

SUPPORTING MATERIAL 2: GROUNDWATERS

CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

Data File:

Original Data Path:

Sample Name:

Acquisition Date:

Run Time(min):

Vial:

Injection Volume(µl):

Low Mass(m/z):

High Mass(m/z):

Instrument Method:

Original Processing Method:

Changlung Groundwater

E:\Xcalibur\Data\2024\FEBRUARY-2024

GCMS-FS

03/01/24 02:01:07 AM

49.70

12

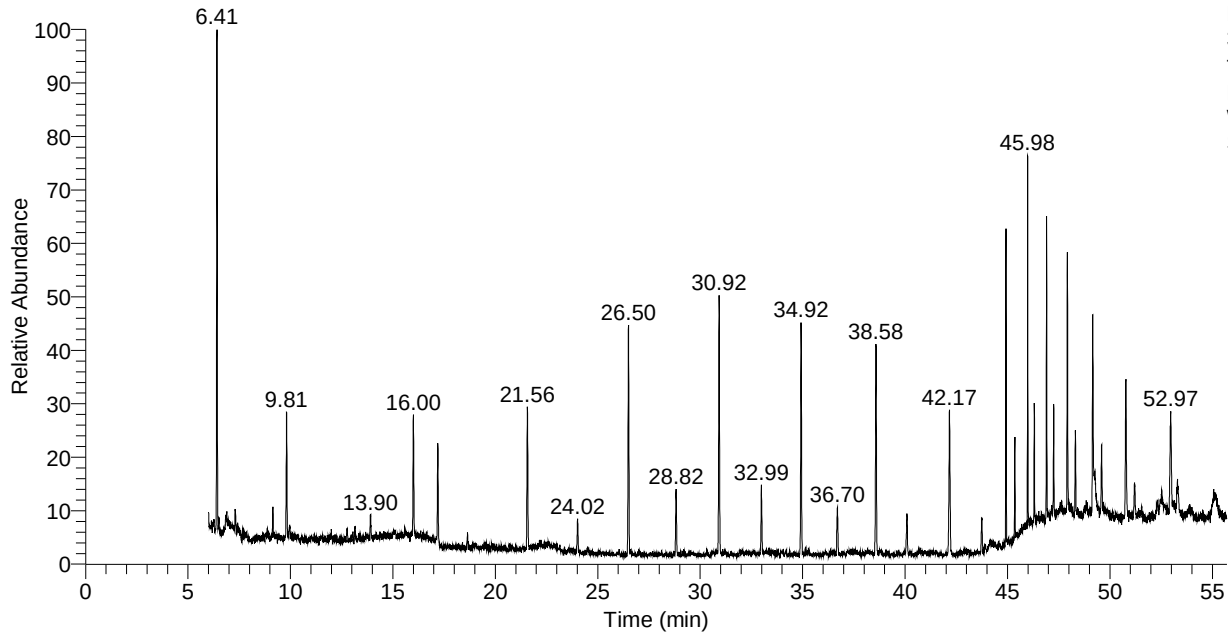
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50

800

E:\Xcalibur\Methods\SAT_EW-DER.meth

RT: 0.00 - 55.70 SM: 7G



NL:
3.19E6
TIC MS
NGA-ZE-
WATER3-
SAMPLE-
INJ1

Qual Peak Table

RT	Peak Area	Peak Height	S/N	Area %
6.41	6278971.77	2522250.44	27.48	8.59
9.14	356965.77	147597.38	3.14	0.49
9.81	1981624.32	666341.43	17.15	2.71
13.90	371176.97	125119.62	3.46	0.51
16.00	2175236.01	674872.99	8.80	2.98
17.19	1574103.69	520871.26	8.69	2.15
18.64	208242.42	73392.33	3.06	0.28
21.56	2459222.01	778882.45	23.80	3.36
24.02	524200.05	168468.56	4.82	0.72
26.50	3900255.28	1250396.14	84.78	5.34
28.82	1163912.89	357343.89	15.51	1.59
30.92	4431781.97	1390698.25	47.39	6.06
32.99	1116136.89	359724.76	10.74	1.53
34.92	3867425.93	1240686.01	43.06	5.29
36.70	934693.16	258426.28	10.91	1.28
38.58	3581834.24	1118967.21	41.49	4.90
40.09	808595.40	218159.39	6.86	1.11
42.17	3088917.84	789646.16	24.45	4.23
43.74	524742.93	171697.79	2.83	0.72
44.93	2871799.01	1421948.89	16.32	3.93

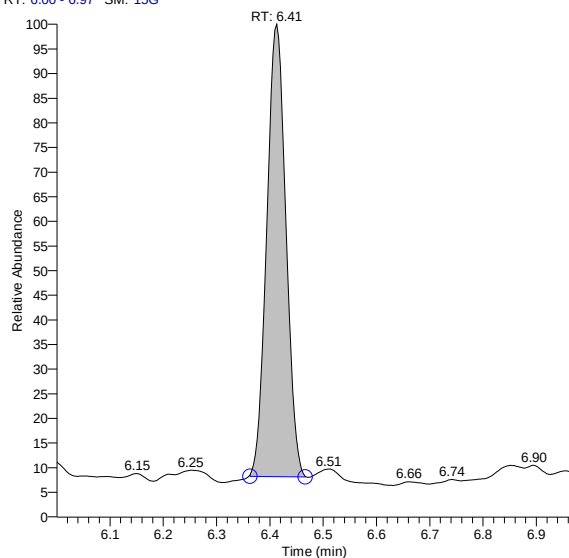
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RT	Peak Area	Peak Height	S/N	Area %
45.36	803061.49	431469.33	5.44	1.10
45.98	3269744.48	1618097.49	20.32	4.47
46.31	1269380.76	561193.72	6.86	1.74
46.91	2943229.77	1397830.84	11.25	4.03
47.25	1313065.02	534515.72	4.47	1.80
47.92	3498245.55	1307667.43	17.78	4.79
48.31	1130508.20	431295.15	4.40	1.55
49.16	5037961.54	1055765.19	17.09	6.89
49.59	1193521.09	365971.22	5.38	1.63
50.78	2655927.08	748119.81	11.94	3.63
52.52	1092368.73	130573.48	2.59	1.49
52.97	3204880.12	596983.47	12.93	4.38
53.30	1392239.52	200565.67	3.74	1.90
55.07	1019651.97	146075.16	2.05	1.39
55.15	706751.97	137492.28	2.76	0.97
55.23	355968.94	97980.26	2.00	0.49

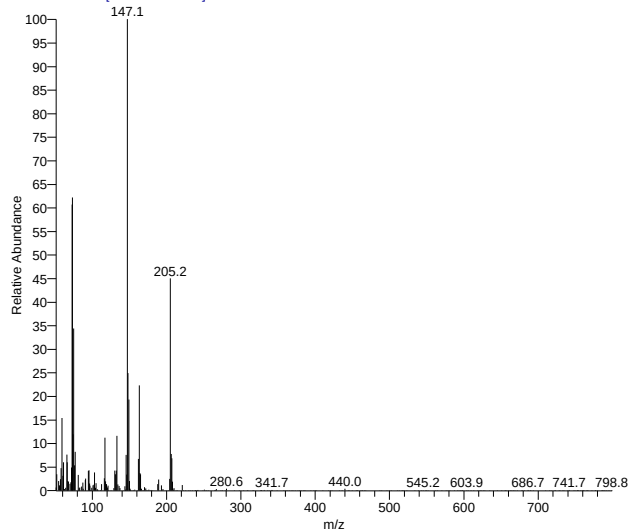
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RT: 6.00 - 6.97 SM: 15G



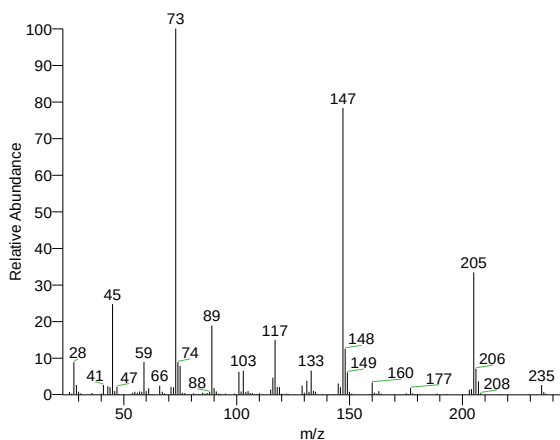
NL:
2.75E6
TIC: MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #124 RT: 6.41 AV: 1 RF: 6.00, 3 NL: 5.42E5
T: + c EI Full ms [50,000-800,000]



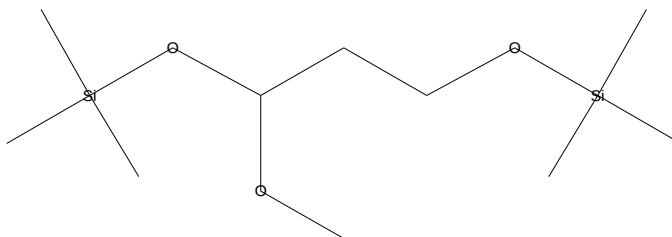
RT	Compound Name	Area	Probability	SI	RSI	Library
6.41	Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis(trimethylglycolic acid, 2TMS derivative	6278971.77	34.57	730	748	mainlib
6.41	L-(+)-Threose, tris(trimethylsilyl) ether, methyloxime (syn	6278971.77	8.28	692	730	mainlib
6.41	L-(+)-Threose, tris(trimethylsilyl) ether, ethyloxime (isomer 1)	6278971.77	4.77	676	688	mainlib
6.41	à-Hydroxyisobutyric acid, 2TMS derivative	6278971.77	3.46	667	694	mainlib
6.41		6278971.77	3.32	666	700	mainlib

Hit Spectrum



Compound Structure

Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis(trimethylglycolic acid, 2TMS derivative
Formula C10H26O3Si2, MW 250, CAS# 62185-57-3, Entry# 42666
Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis(trimethylglycolic acid, 2TMS derivative



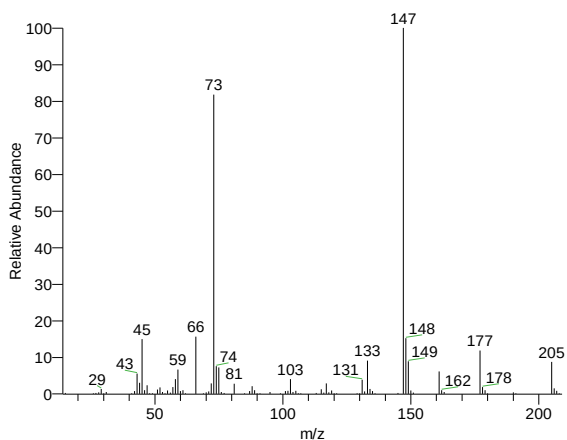
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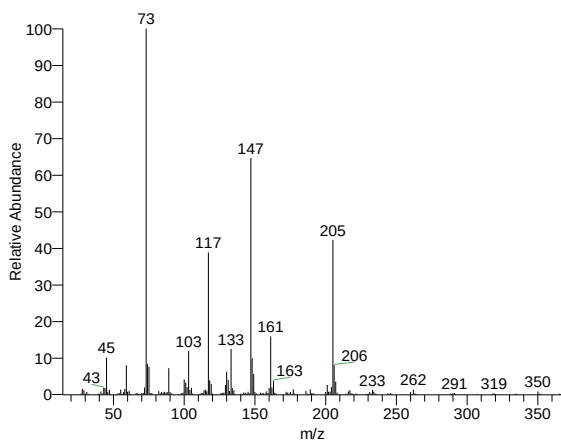
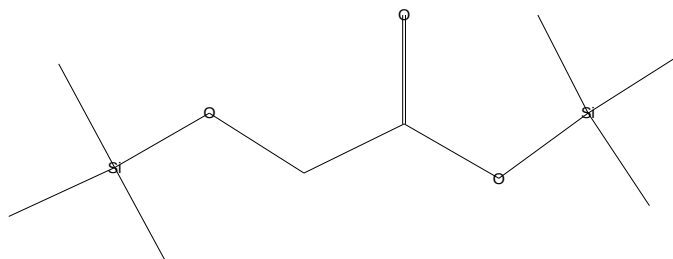
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Hit Spectrum

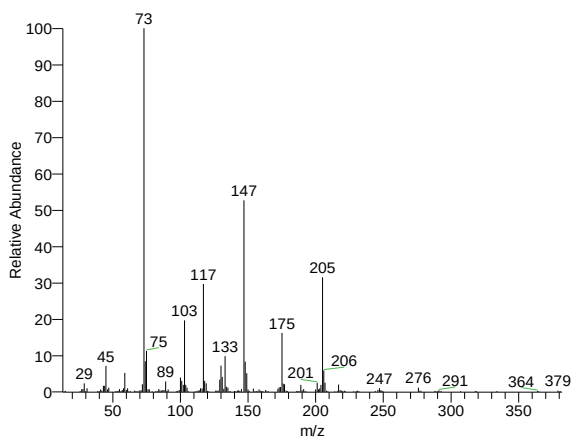
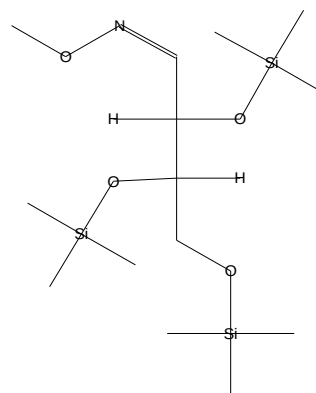
Compound Structure



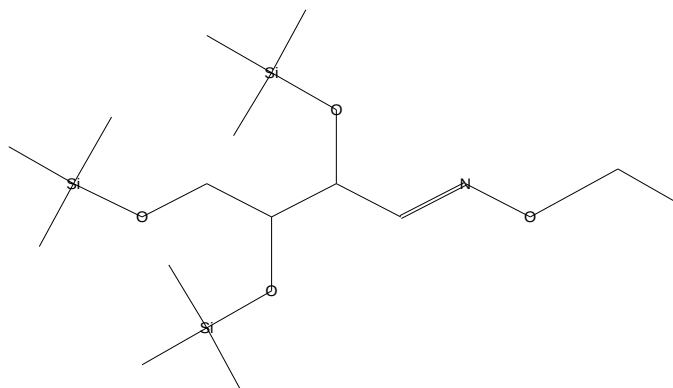
Glycolic acid, 2TMS derivative
Formula C₈H₂₀O₃Si₂, MW 220, CAS# 33581-77-0, Entry# 134871
Acetic acid, [(trimethylsilyl)oxy]-, trimethylsilyl ester



L-(+)-Threonine, tris(trimethylsilyl) ether, methyloxime (syn)
Formula C₁₄H₃₅NO₄Si₃, MW 365, CAS# NA, Entry# 42643
\$:28ALJSKKFUUDIVIZ-PTNGSMBKSA-N



L-(+)-Threonine, tris(trimethylsilyl) ether, ethyloxime (isomer 1)
Formula C₁₅H₃₇NO₄Si₃, MW 379, CAS# NA, Entry# 42660
\$:28XVNGFUHWCI VPNT-FOWTUZBSSA-N



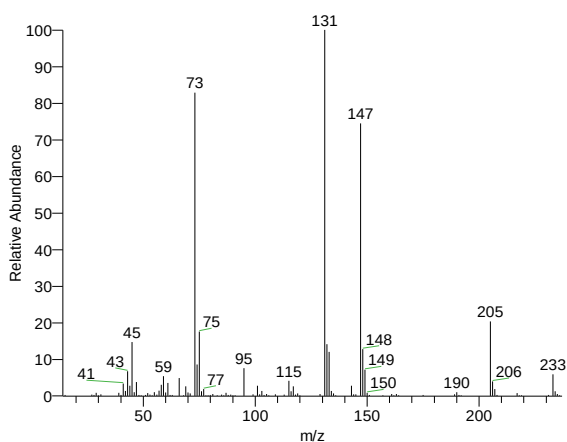
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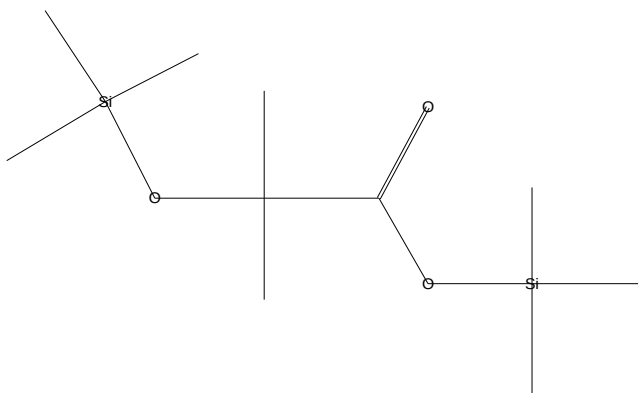
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Hit Spectrum

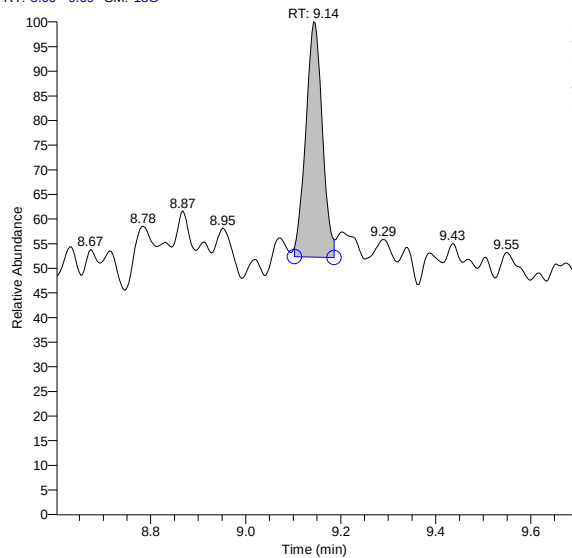
Compound Structure



à-Hydroxyisobutyric acid, 2TMS derivative
Formula C₁₀H₂₄O₃Si₂, MW 248, CAS# 55133-92-1, Entry# 115549
Propanoic acid, 2-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

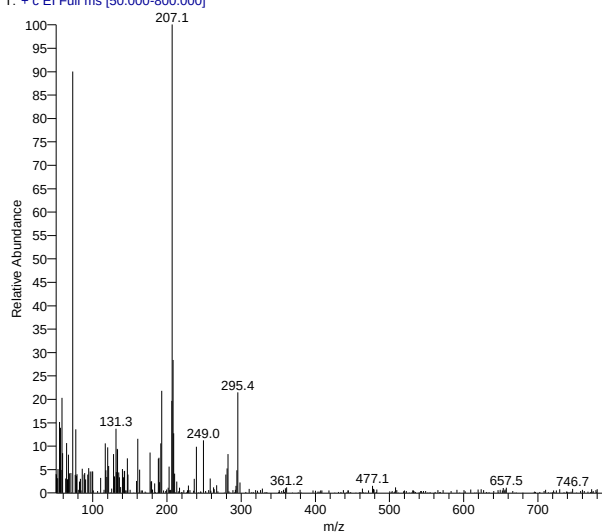


RT: 8.60 - 9.69 SM: 15G



NL: 3.09E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #938 RT: 9.14 AV: 1 RF: 6.00, 3 NL: 4.85E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.14	Methyltris(trimethylsiloxy)silane	356965.77	20.03	504	653	mainlib
9.14	Tetrasiloxane, decamethyl-	356965.77	9.73	485	623	mainlib
9.14	2,4,6-Cycloheptatrien-1-one, 3,5-bis-trimethylsilyl-	356965.77	7.64	479	647	mainlib
9.14	1,2-Bis(trimethylsilyl)benzene	356965.77	6.75	476	658	mainlib
9.14	Tris(tert-butyl dimethylsilyloxy)arsane	356965.77	5.31	470	651	mainlib

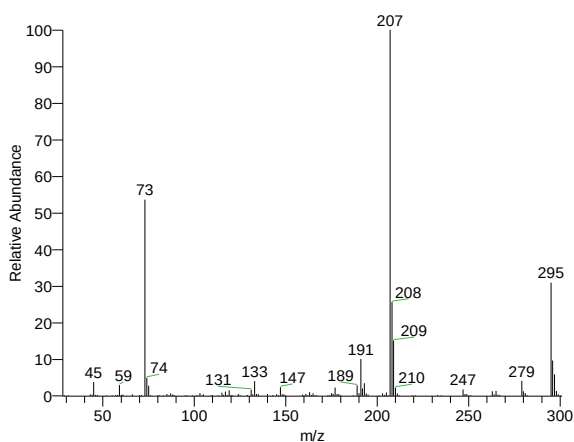
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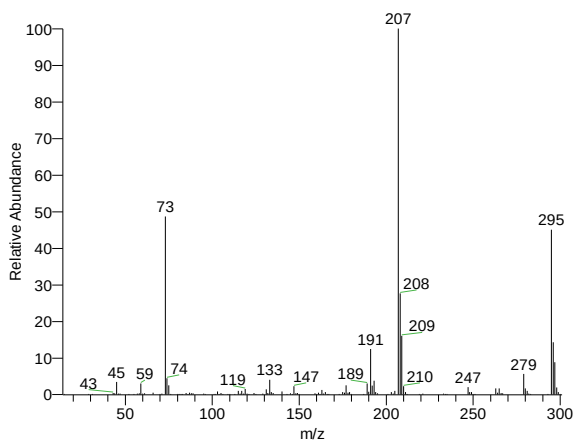
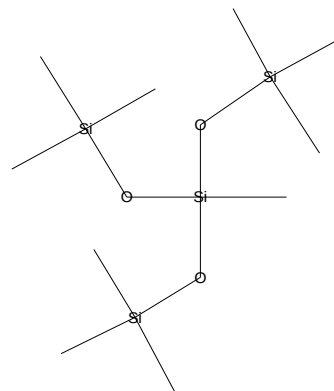
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

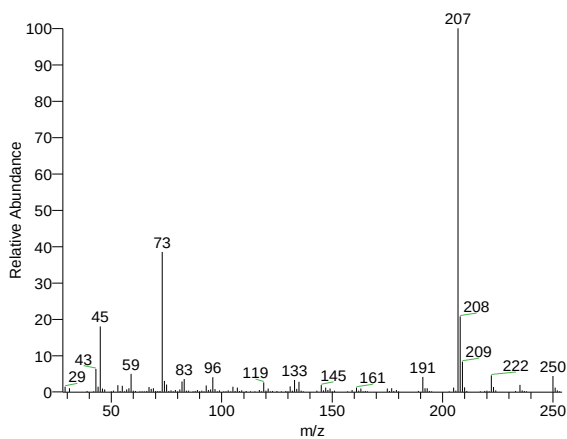
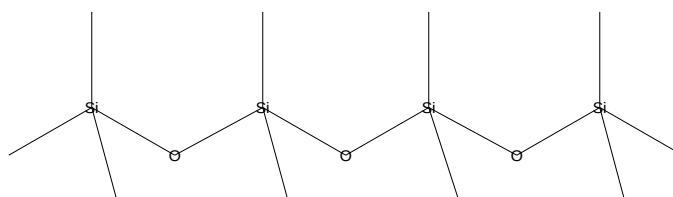
Compound Structure



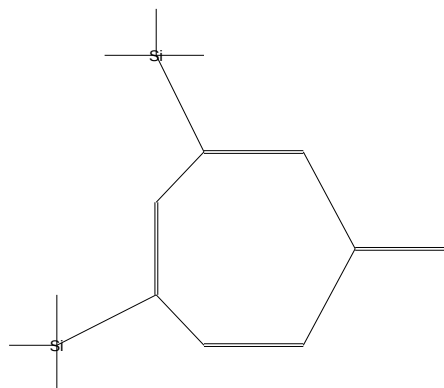
Methyltris(trimethylsiloxy)silane
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



Tetrasiloxane, decamethyl-
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 141-62-8, Entry# 188653
Decamethyltetrasiloxane



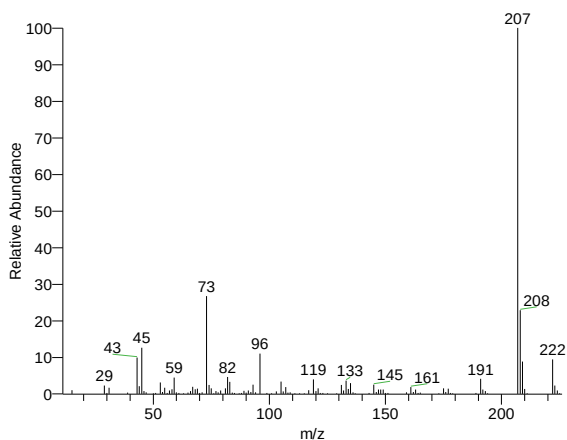
2,4,6-Cycloheptatrien-1-one, 3,5-bis-trimethylsilyl-
Formula C₁₃H₂₂O₂Si₂, MW 250, CAS# NA, Entry# 188644
3,5-Bis(trimethylsilyl)-2,4,6-cycloheptatrien-1-one #



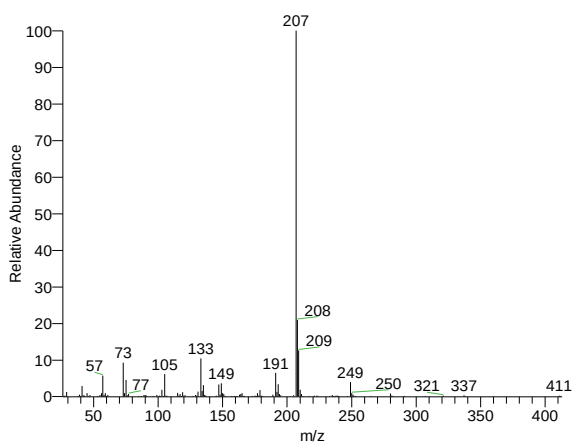
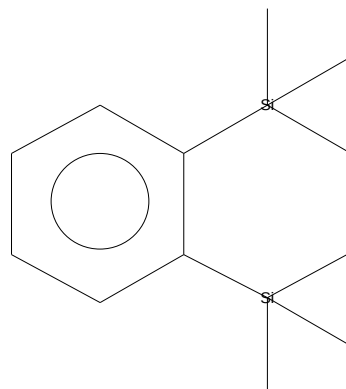
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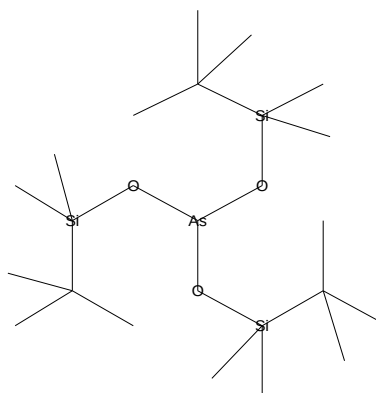
Compound Structure



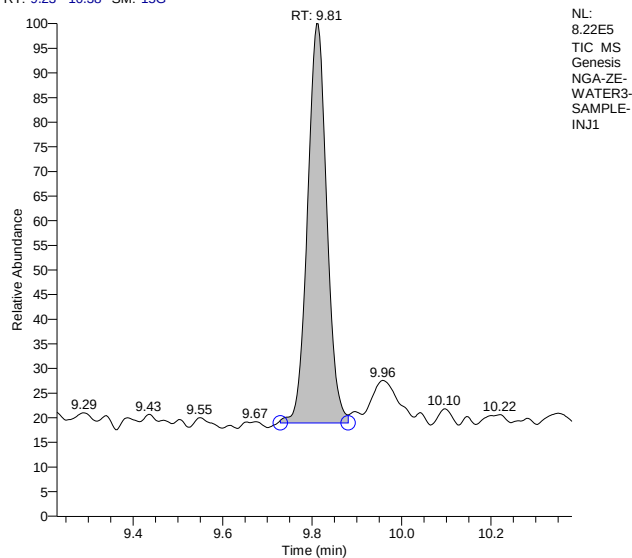
1,2-Bis(trimethylsilyl)benzene
Formula C₁₂H₂₂Si₂, MW 222, CAS# 17151-09-6, Entry# 188650
Trimethyl[2-(trimethylsilyl)phenyl]silane #



Tris(tert-butyl)dimethylsilyloxyarsane
Formula C₁₈H₄₅AsO₃Si₃, MW 468, CAS# NA, Entry# 188959
Arsenous acid, tris(tert-butyl)dimethylsilyl ester

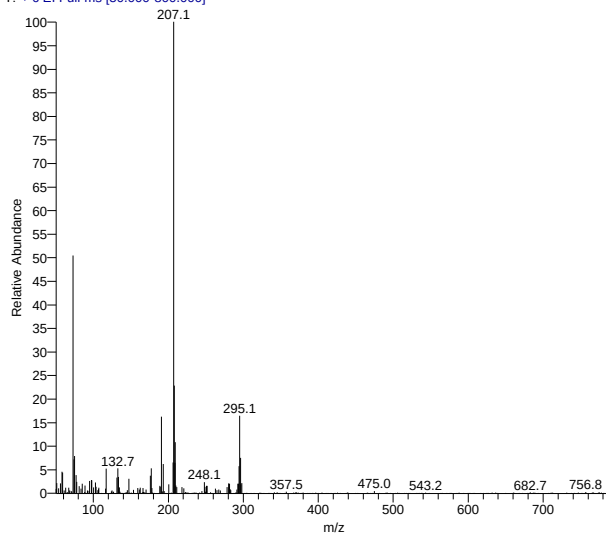


RT: 9.23 - 10.38 SM: 15G



NL:
8.22E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #1137 RT: 9.81 AV: 1 RF: 6.00, 3 NL: 2.51E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	Tetrasiloxane, decamethyl-	1981624.32	43.11	701	763	mainlib
9.81	Methyltris(trimethylsiloxy)silane	1981624.32	43.11	701	766	mainlib

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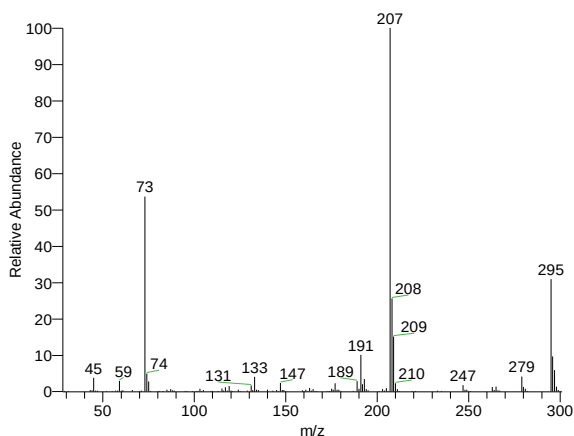
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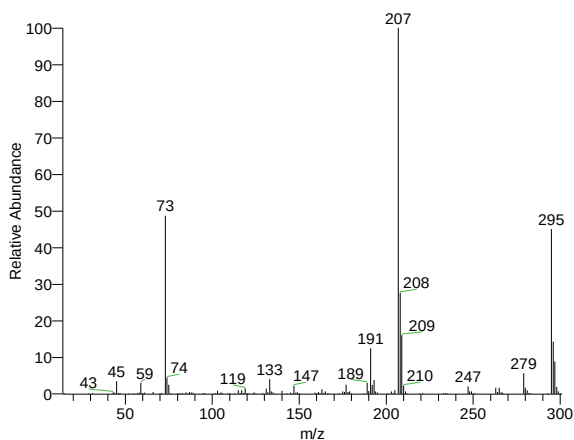
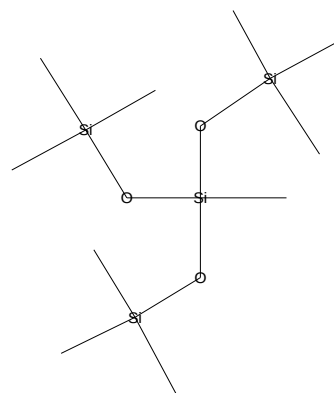
RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane	1981624.32	3.04	598	643	mainlib
9.81	1,1,1,3,5,5,5-Heptamethyltrisiloxane	1981624.32	2.80	596	888	mainlib
9.81	Tris(tert-butyl dimethylsilyl oxy)arsane	1981624.32	2.26	591	732	mainlib

Hit Spectrum

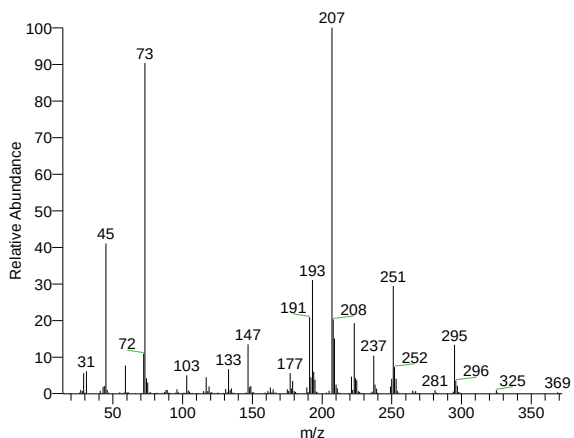
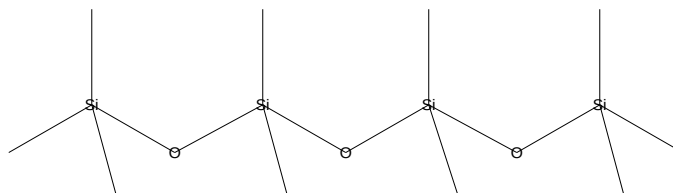
Compound Structure



Methyltris(trimethylsiloxy)silane
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



Tetrasiloxane, decamethyl-
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 141-62-8, Entry# 188653
Decamethyltetrasiloxane



7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane
Formula C₁₄H₃₆O₆Si₃, MW 384, CAS# NA, Entry# 188641
\$:28TUXFBCQKAFVQCP-UHFFFAOYSA-N



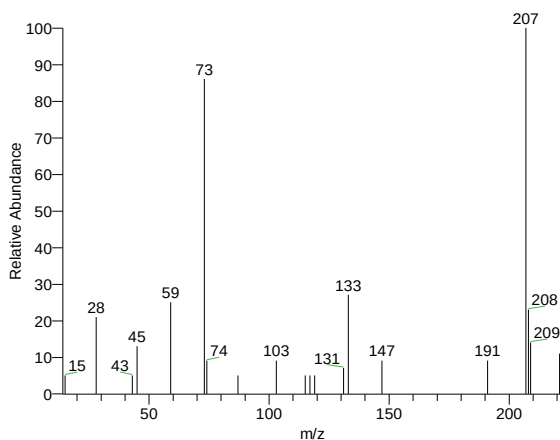
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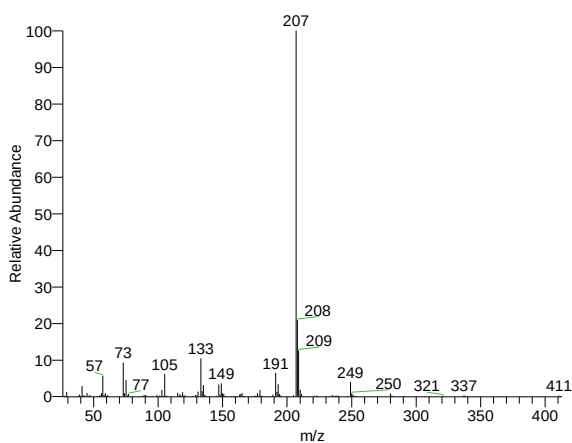
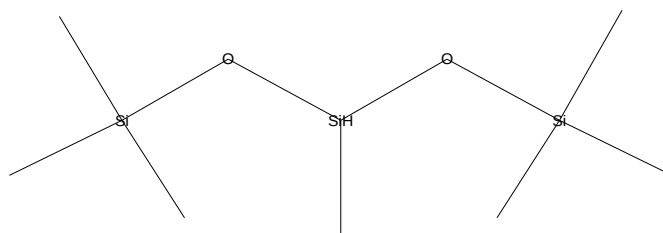
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Hit Spectrum

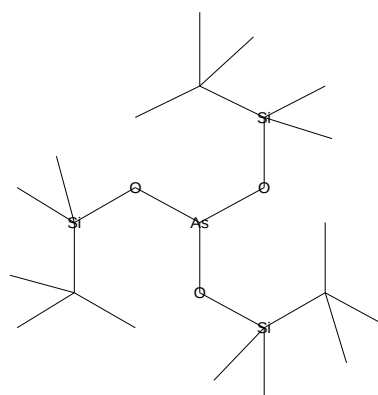
Compound Structure



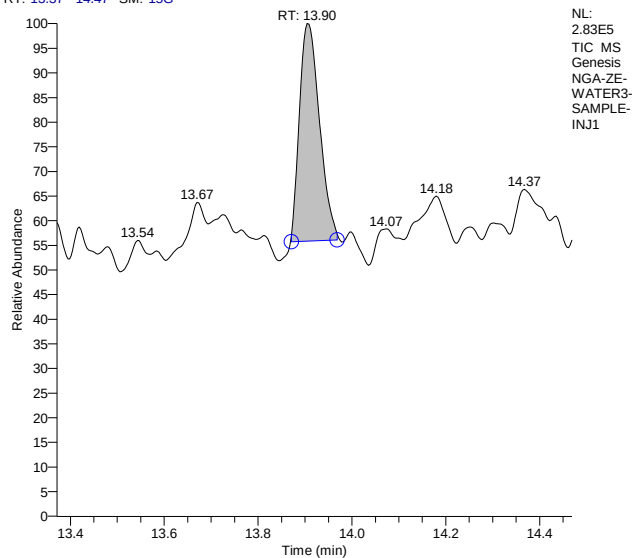
1,1,1,3,5,5,5-Heptamethyltrisiloxane
Formula C₇H₂₂O₂Si₃, MW 222, CAS# 1873-88-7, Entry# 188643
Bis(trimethylsiloxy)methylsilane



Tris(tert-butylidimethylsiloxy)arsane
Formula C₁₈H₄₅AsO₃Si₃, MW 468, CAS# NA, Entry# 188959
Arsenous acid, tris(tert-butylidimethylsilyl) ester

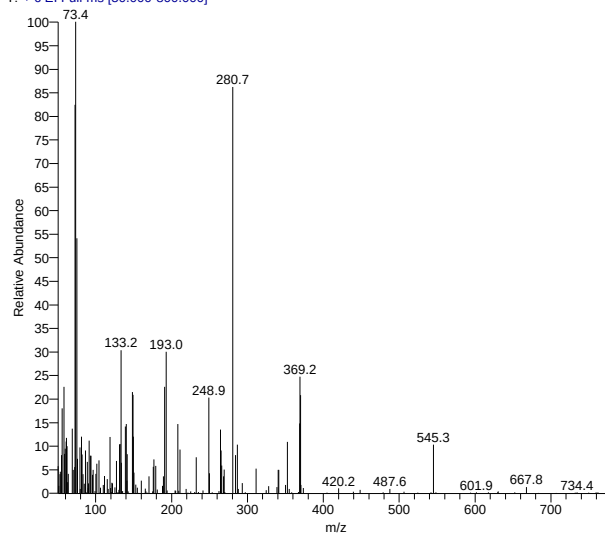


RT: 13.37 - 14.47 SM: 15G



NL:
2.83E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #2358 RT: 13.90 AV: 1 RF: 6.00, 3 NL: 3.24E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
13.90	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	371176.97	28.93	453	703	mainlib

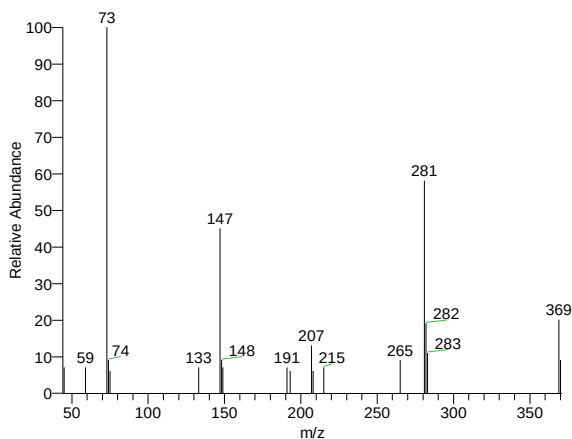
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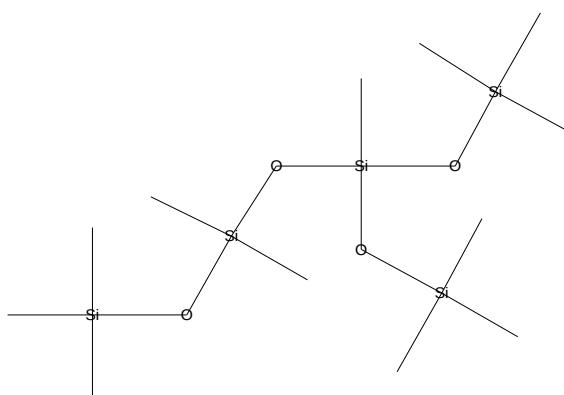
RT	Compound Name	Area	Probability	SI	RSI	Library
13.90	Pentasiloxane,	371176.97	22.74	447	526	mainlib
13.90	dodecamethyl-					
	Trisiloxane,	371176.97	11.72	429	510	mainlib
	1,1,1,5,5,5-hexamethyl-3,					
	3-bis[(trimethylsilyl)oxy]-					
13.90	3-Butoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)tri	371176.97	6.75	413	633	mainlib
	siloxane					
13.90	4-Hydroxybenzaldehyde, 2TMS derivative	371176.97	2.26	389	497	mainlib

Hit Spectrum

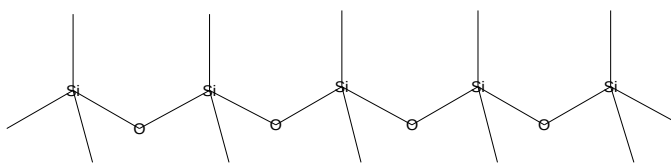
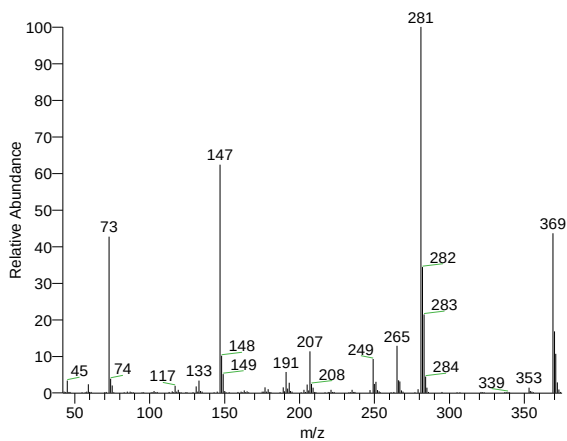


Compound Structure

1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



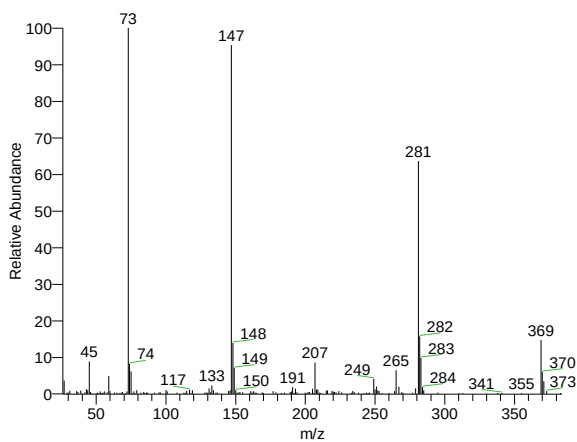
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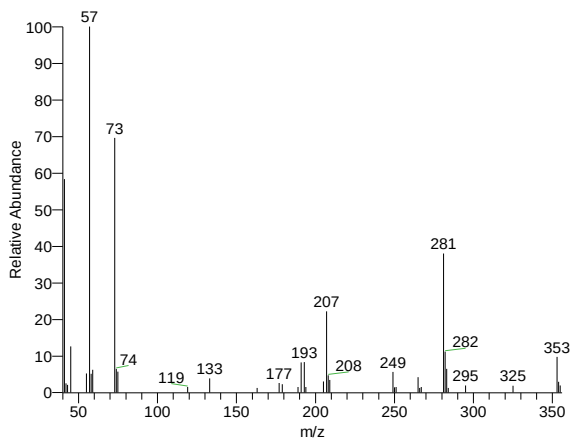
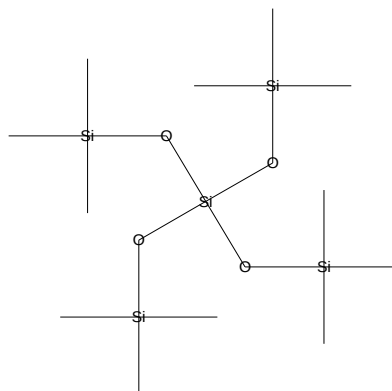
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

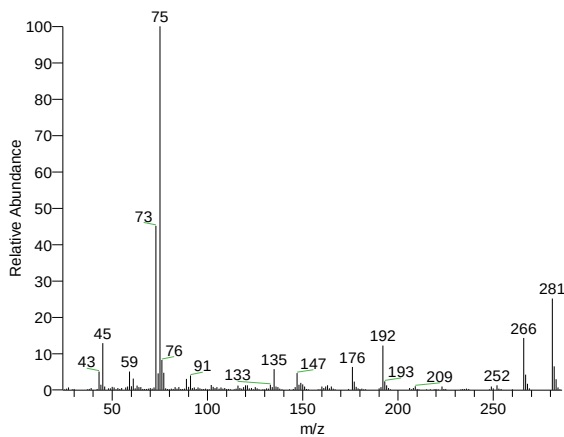
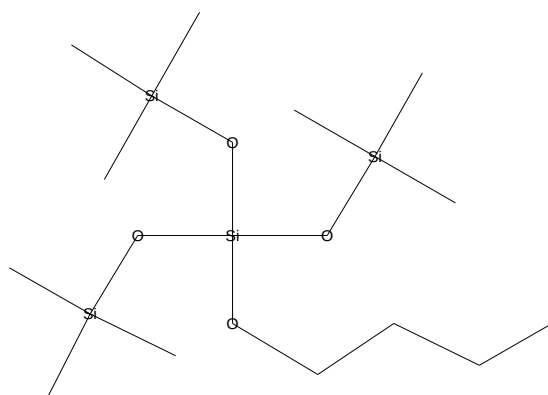
Compound Structure



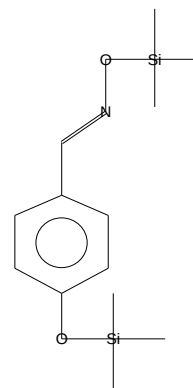
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



3-Butoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)trisiloxane
Formula C₁₃H₃₆O₄Si₄, MW 368, CAS# 87867-97-8, Entry# 25615
Butyl tris(trimethylsilyl) orthosilicate #

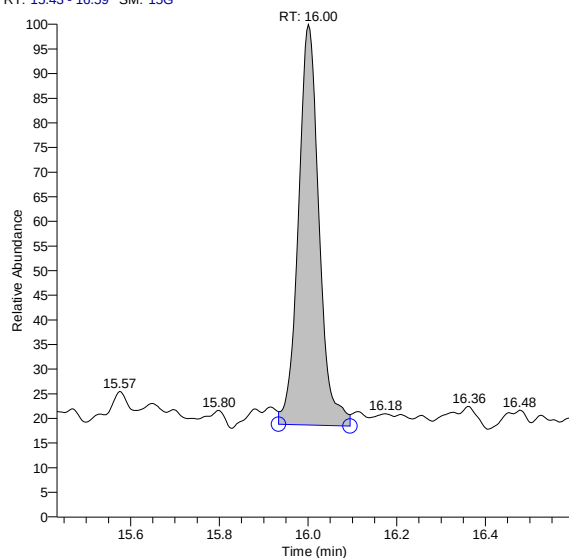


4-Hydroxybenzaldehyde, 2TMS derivative
Formula C₁₃H₂₃NO₂Si₂, MW 281, CAS# 52629-38-6, Entry# 45385
p-Trimethylsiloxybenzaldehyde oxime, trimethylsilyl-



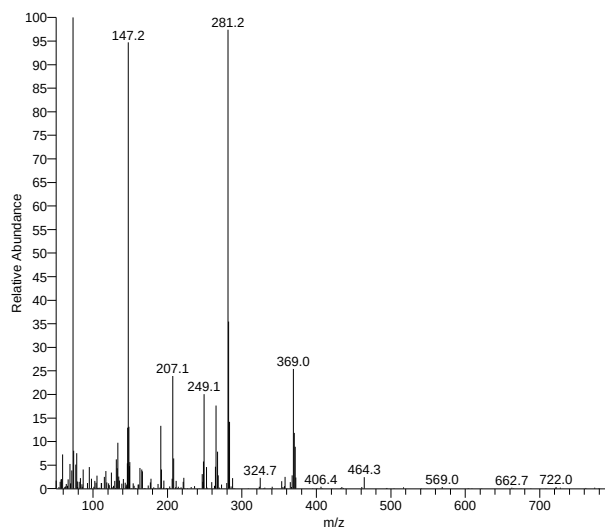
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ANALYTICAL CHEMISTRY DIVISION

RT: 15.43 - 16.59 SM: 15G



NL:
8.30E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

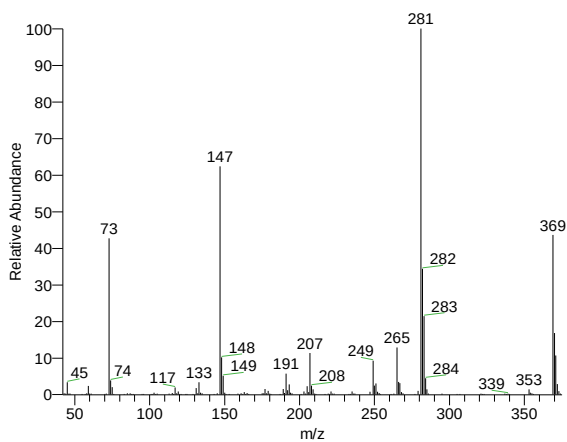
NGA-ZE-WATER3-SAMPLE-INJ1 #2983 RT: 16.00 AV: 1 RF: 6.00, 3 NL: 1.20E5
T: + c EI Full ms [50.000-800.000]



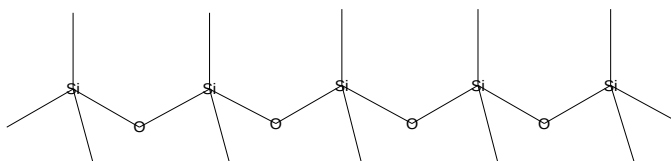
RT	Compound Name	Area	Probability	SI	RSI	Library
16.00	Pentasiloxane, dodecamethyl-	2175236.01	49.35	736	793	mainlib
16.00	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	2175236.01	37.80	729	930	mainlib
16.00	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	2175236.01	10.91	701	770	mainlib
16.00	2,6-Dihydroxyacetophenone, 2TMS derivative	2175236.01	0.52	578	667	mainlib
16.00	Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester	2175236.01	0.38	569	669	mainlib

Hit Spectrum

Compound Structure



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



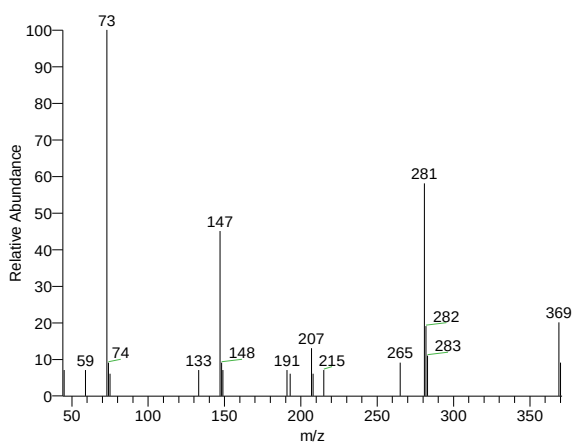
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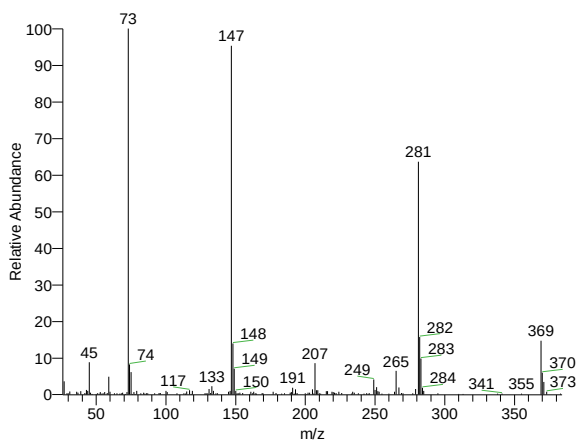
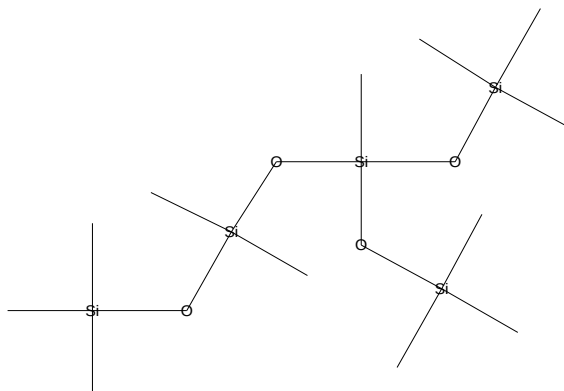
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

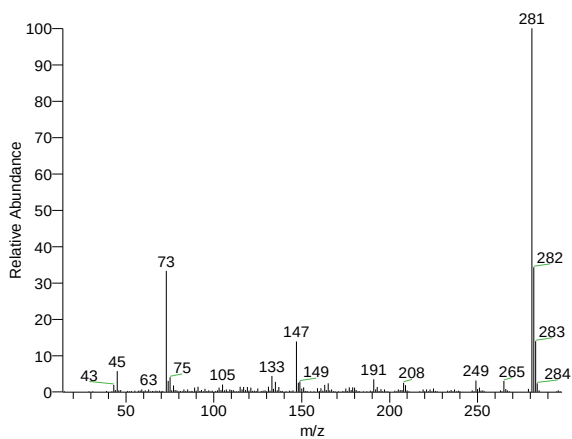
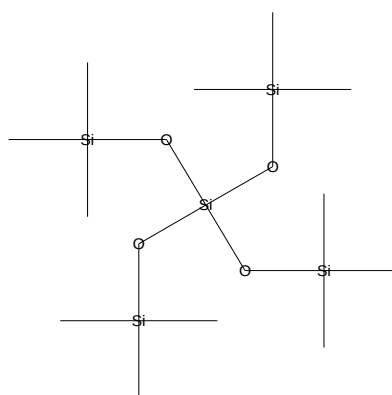
Compound Structure



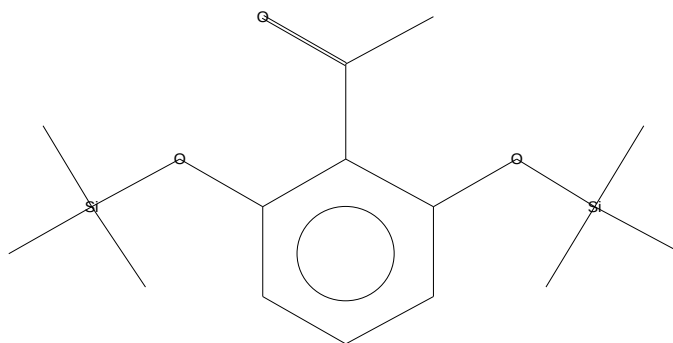
1,1,1,3,5,5,7,7,7-Nonamethyl-3-((trimethylsiloxy)tetrasiloxane)
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-((trimethylsilyl)oxy)tetrasiloxane #



Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis((trimethylsilyl)oxy)-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



2,6-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220073
2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



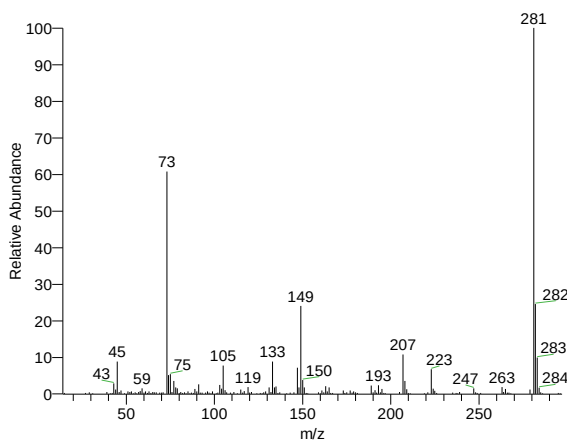
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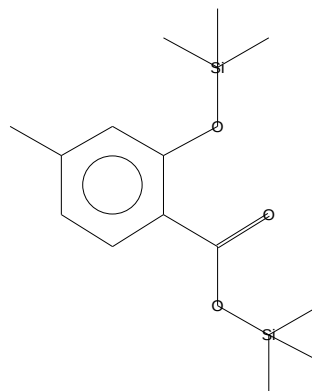
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

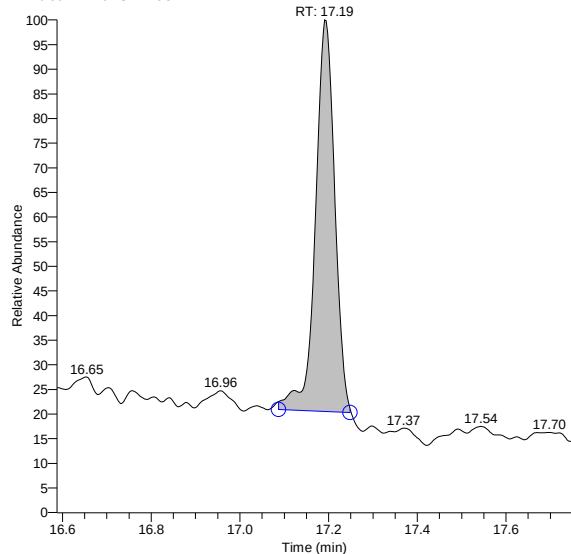
Compound Structure



Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# 35-27-8, Entry# 219921
\$.28WMMUZRDZZSRQEF-UHFFFAOYSA-N

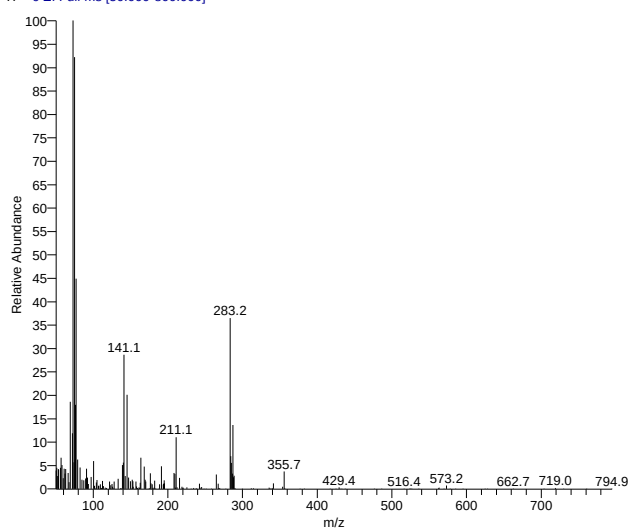


RT: 16.59 - 17.75 SM: 15G



NL:
6.55E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #3338 RT: 17.19 AV: 1 RF: 6.00, 3 NL: 1.27E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
17.19	2,2'-Sulfonyldiethanol, 2TMS derivative	1574103.69	21.80	469	577	mainlib
17.19	N'-(3-Pyridinylmethylene)isonicotinohydrazide, TBDMS derivative	1574103.69	16.69	462	503	mainlib
17.19	n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester	1574103.69	4.73	433	514	mainlib
17.19	N'-(3-Pyridinylmethylene)isonicotinohydrazide, TMS derivative	1574103.69	3.99	429	464	mainlib
17.19	Trimethylsilyl [3-chloro-4-(prop-2-en-1-yloxy)phenyl]acetate	1574103.69	3.84	428	451	mainlib

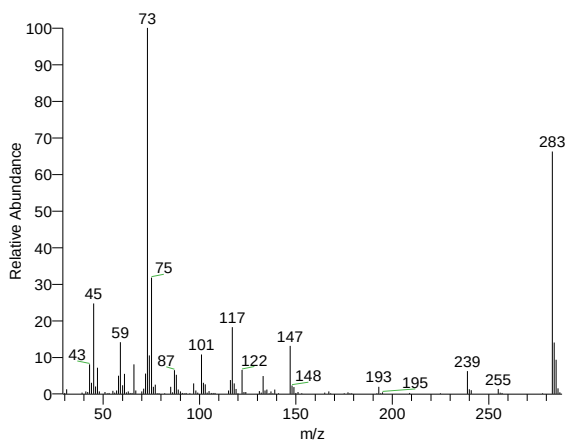
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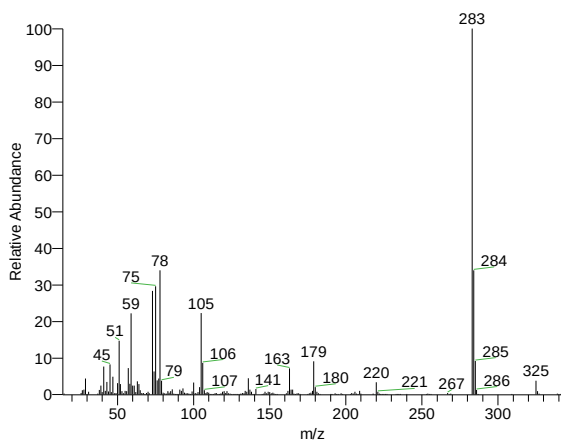
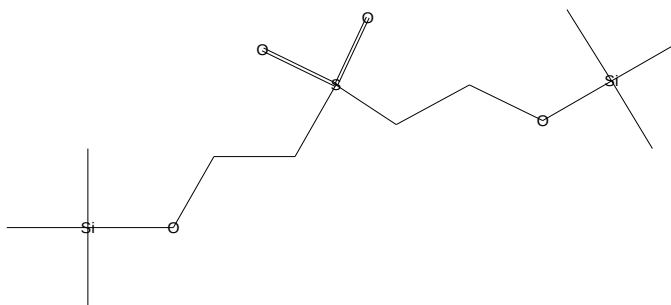
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

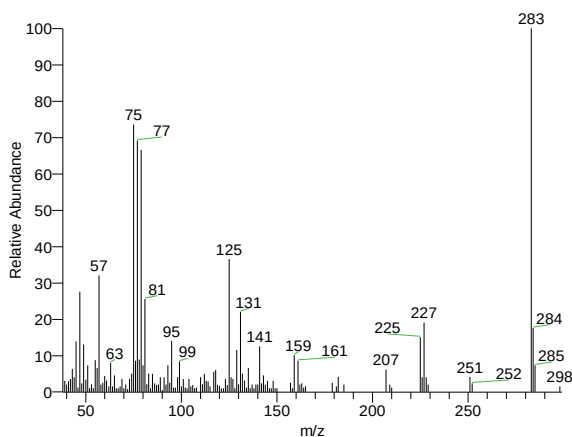
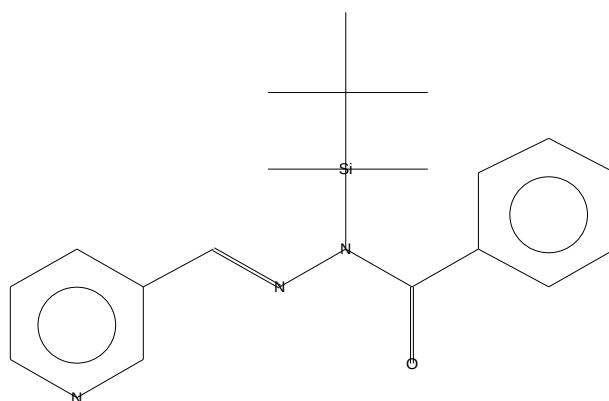
Compound Structure



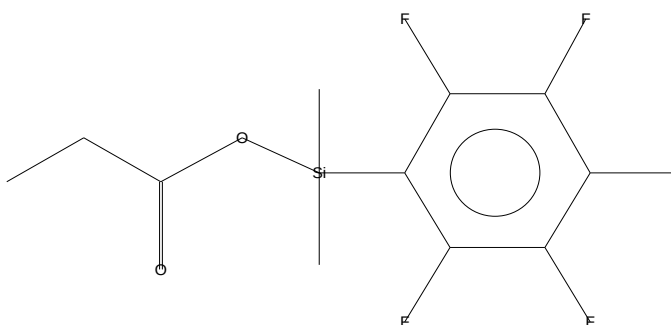
2,2'-Sulfonyldiethanol, 2TMS derivative
Formula C₁₀H₂₆O₄Si₂, MW 298, CAS# 97916-04-6, Entry# 43779
bis [2-Trimethylsiloxy]ethyl sulfone



N'-(3-Pyridinylmethylene)isonicotinohydrazide, TBDMS derivative
Formula C₁₈H₂₄N₄O₂Si, MW 340, CAS# NA, Entry# 220559
N'-(3-Pyridinylmethylene)isonicotinohydrazide tbdms



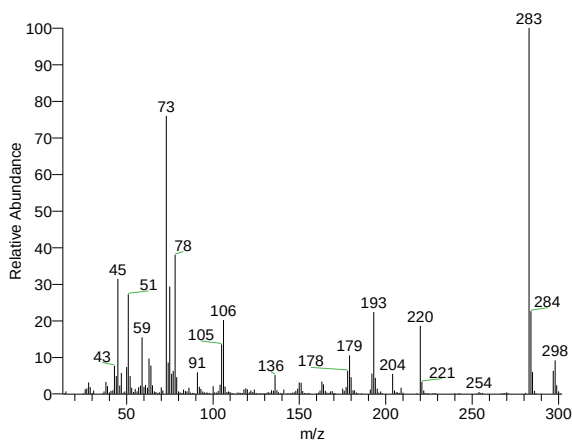
n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester
Formula C₁₁H₁₁F₅O₂Si, MW 298, CAS# NA, Entry# 220549
Dimethyl(2,3,4,5,6-pentafluorophenyl)silyl propionate #



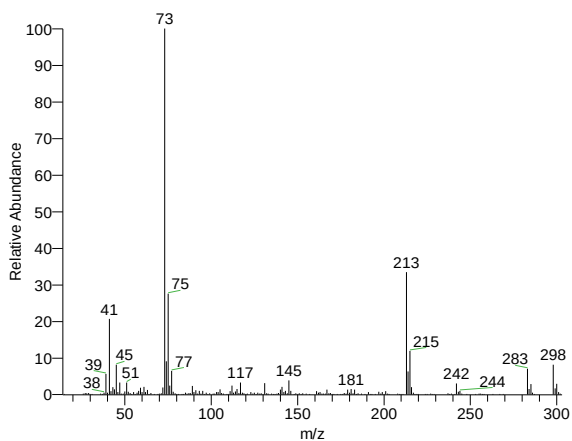
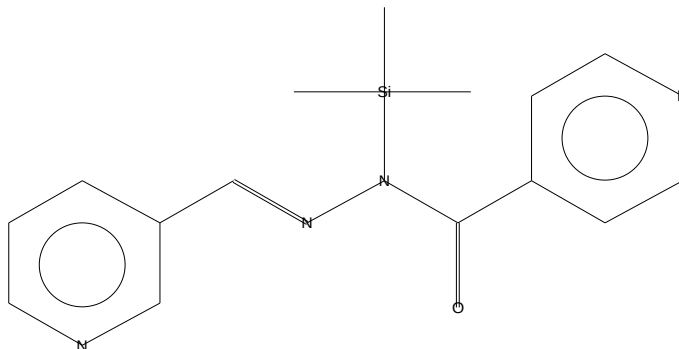
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Hit Spectrum

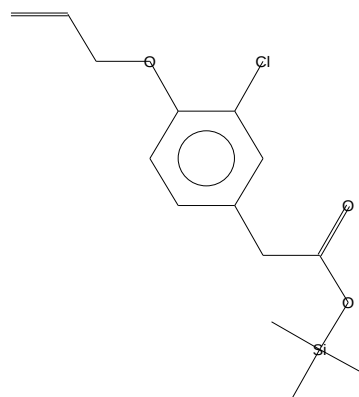
Compound Structure



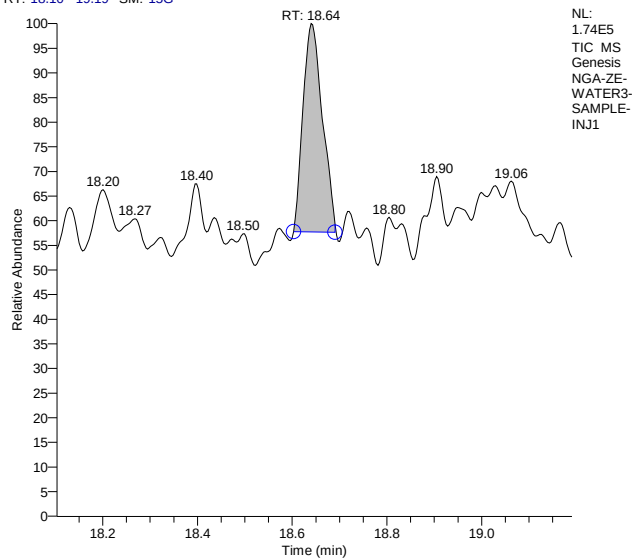
N'-(3-Pyridinylmethylene)isonicotinohydrazide, TMS derivative
Formula C₁₅H₁₈N₄O₃Si, MW 298, CAS# NA, Entry# 220546
N'-(3-Pyridinylmethylene)isonicotinohydrazide tms



Trimethylsilyl [3-chloro-4-(prop-2-en-1-yloxy)phenyl]acetate
Formula C₁₄H₁₉ClO₃Si, MW 298, CAS# NA, Entry# 43332
\$:28ICJPSMUDYUPECL-UHFFFAOYSA-N

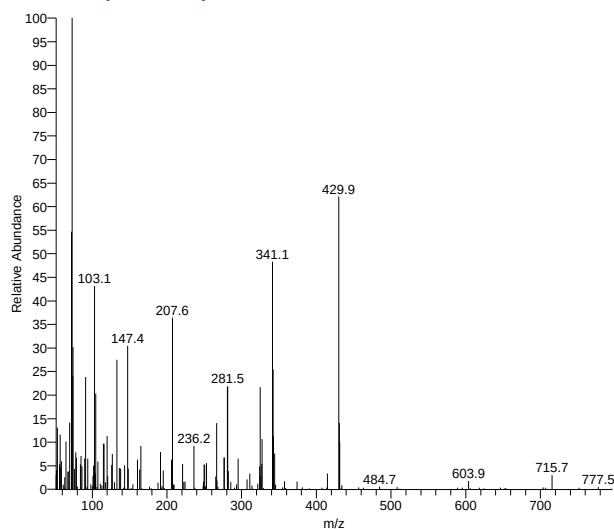


RT: 18.10 - 19.19 SM: 15G



NL:
1.74E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #3770 RT: 18.64 AV: 1 RF: 6.00, 3 NL: 2.32E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
18.64	(S)-(-)-1,1'-Bi-2-naphthol, O,O'-bis(trimethylsilyl)-	208242.42	51.18	471	523	mainlib

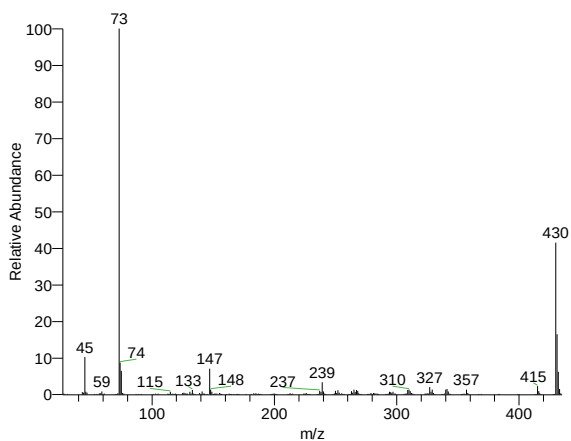
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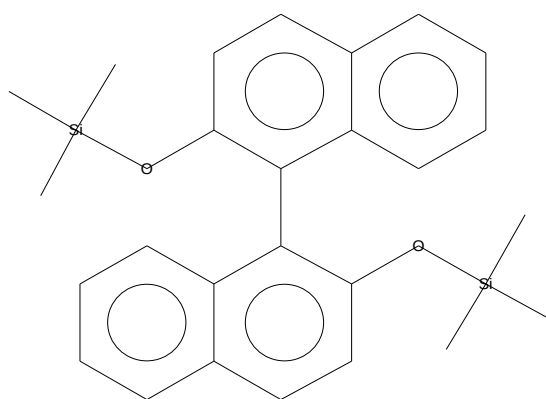
RT	Compound Name	Area	Probability	SI	RSI	Library
18.64	Cyclohexasiloxane,	208242.42	14.78	443	508	mainlib
18.64	dodecamethyl-					
18.64	Octasiloxane,	208242.42	3.71	408	459	mainlib
	1,1,3,3,5,5,7,7,9,9,11,11,1					
	3,13,15,15-hexadecamethy					
	l-					
18.64	Heptasiloxane,	208242.42	3.56	407	460	mainlib
	1,1,3,3,5,5,7,7,9,9,11,11,1					
	3,13-tetradecamethyl-					
18.64	Estra-1,3,5(10)-trien-17-on	208242.42	3.28	405	501	mainlib
	e,					
	3,4-bis[(trimethylsilyl)oxy					
	]-					

Hit Spectrum

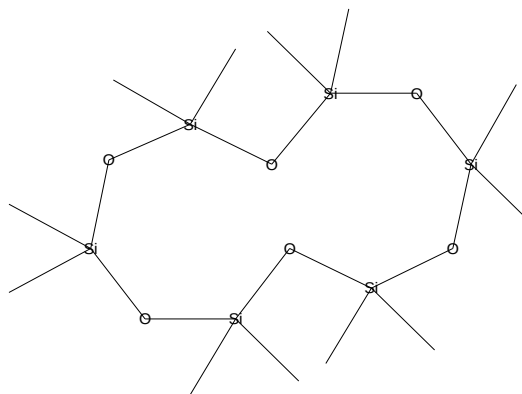
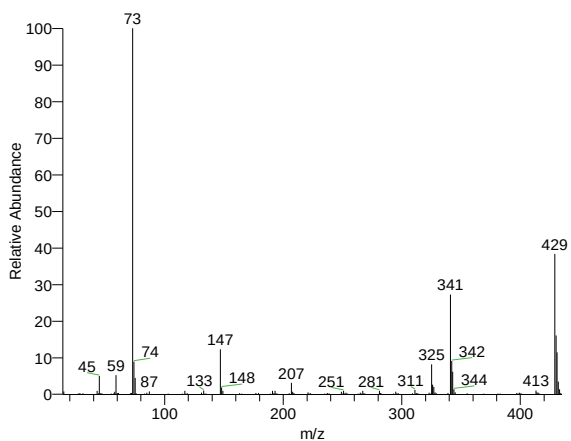


Compound Structure

(S)-(-)-1,1'-Bi-2-naphthol, O,O'-bis(trimethylsilyl)-
Formula C₂₆H₃₀O₂Si₂, MW 430, CAS# NA, Entry# 44305
\$.28HICHTPUMVRXTTH-UHFFFAOYSA-N



Cyclohexasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₆Si₆, MW 444, CAS# 540-97-6, Entry# 44297
Dodecamethylcyclohexasiloxane



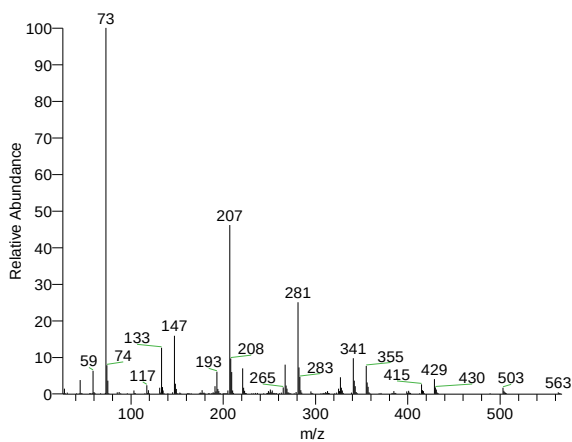
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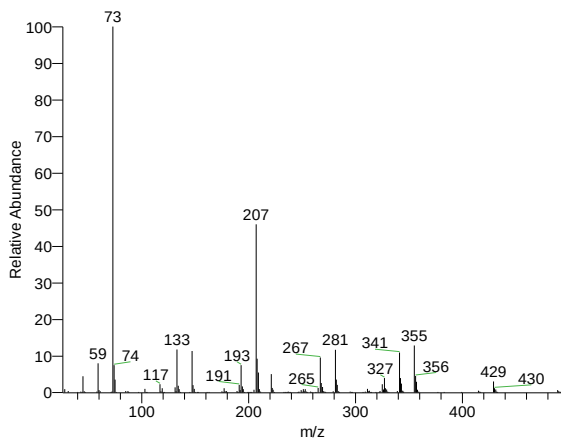
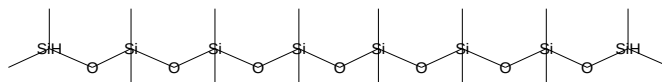
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

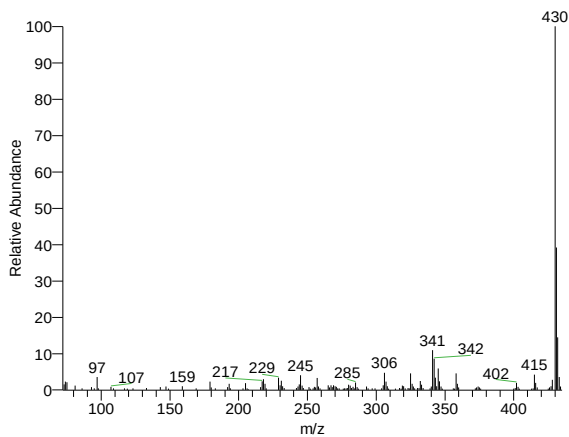
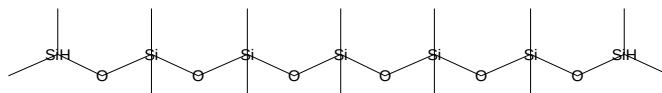
Compound Structure



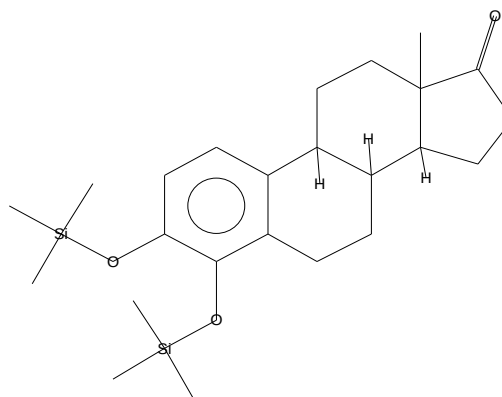
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

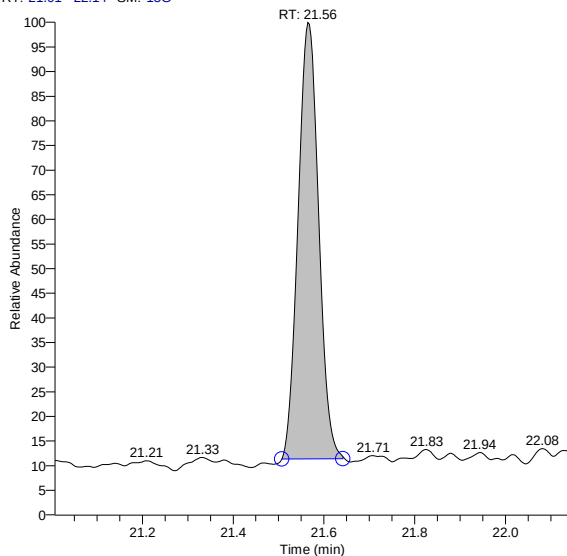


Estra-1,3,5(10)-trien-17-one, 3,4-bis(trimethylsilyl)oxy]-
Formula C₂₄H₃₈O₃Si₂, MW 430, CAS# 51497-39-3, Entry# 239669
3,4-Bis(trimethylsilyl)oxy]estra-1,3,5(10)-trien-17-one #



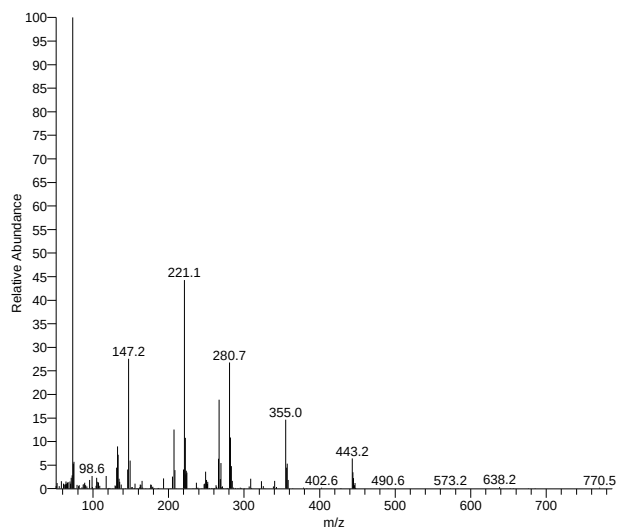
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ANALYTICAL CHEMISTRY DIVISION

RT: 21.01 - 22.14 SM: 15G



NL:
8.79E5
TIC: MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

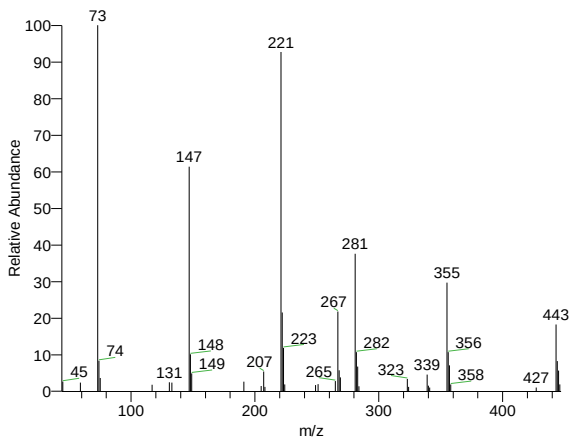
NGA-ZE-WATER3-SAMPLE-INJ1 #4642 RT: 21.56 AV: 1 RF: 6.00, 3 NL: 2.11E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
21.56	Hexasiloxane, tetradecamethyl-	2459222.01	90.61	760	845	mainlib
21.56	1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane	2459222.01	7.74	670	886	mainlib
21.56	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2459222.01	0.52	564	623	mainlib
21.56	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2459222.01	0.26	546	604	mainlib
21.56	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2459222.01	0.13	528	589	mainlib

Hit Spectrum

Compound Structure



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



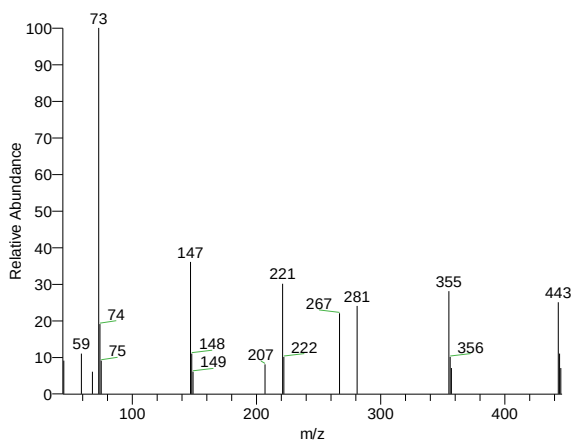
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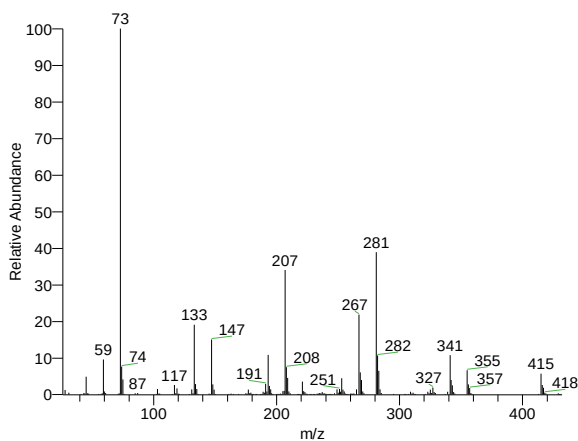
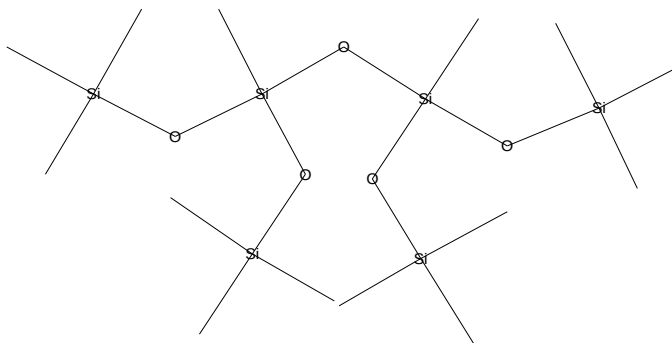
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

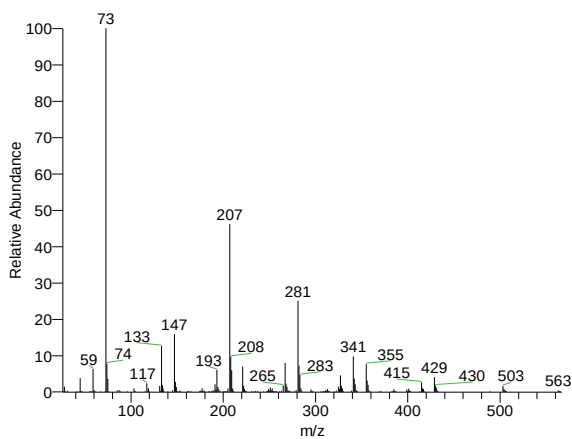
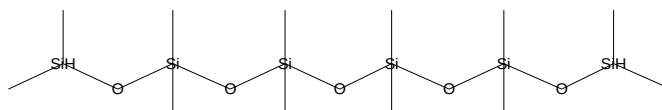
Compound Structure



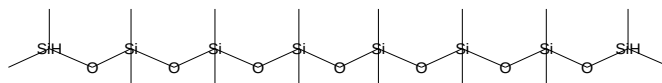
1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 2003-92-1, Entry# 42693
1,1,1,3,5,7,7,7-Octamethyl-3,5-bis[(trimethylsilyl)oxy]tetrasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



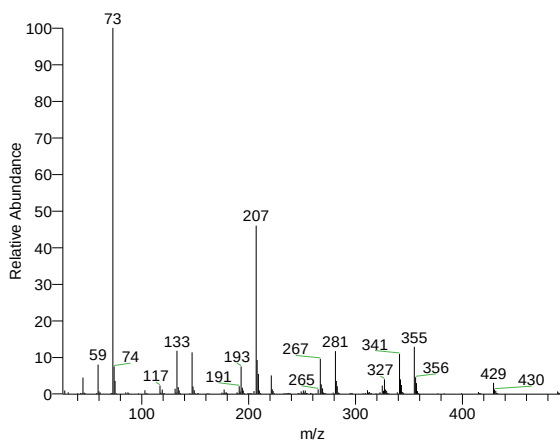
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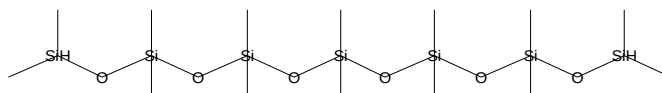
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

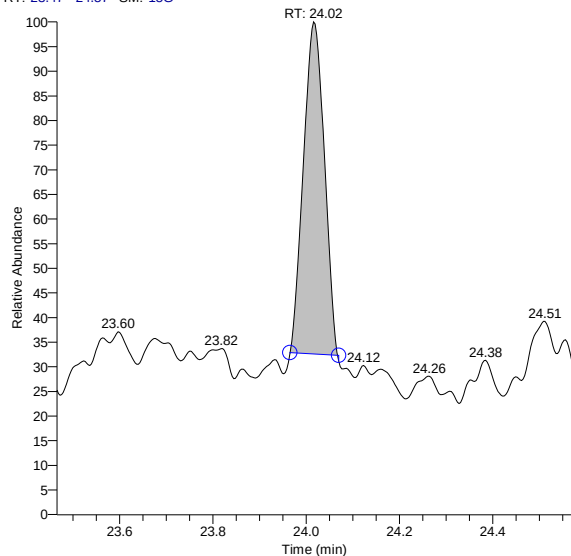
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

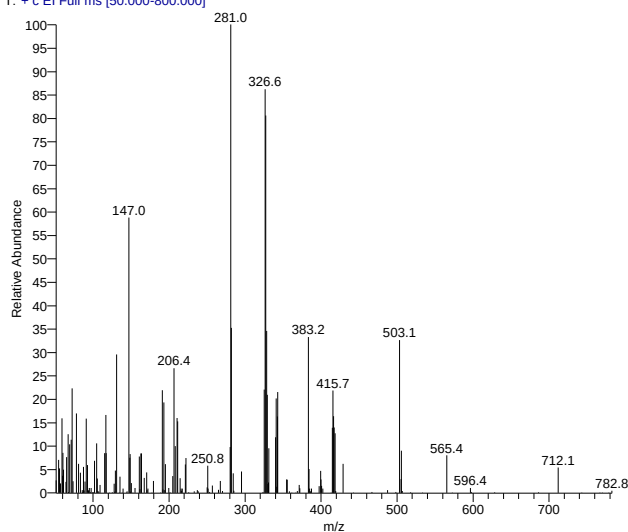


RT: 23.47 - 24.57 SM: 15G



NL:
2.50E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #5373 RT: 24.02 AV: 1 RF: 6.00, 3 NL: 2.74E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
24.02	Cycloheptasiloxane, tetradecamethyl-	524200.05	82.28	540	612	mainlib
24.02	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	524200.05	3.64	414	540	mainlib
24.02	3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	524200.05	2.57	404	531	mainlib
24.02	Cyclodecasiloxane, eicosamethyl-	524200.05	2.17	400	413	mainlib
24.02	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	524200.05	2.17	400	428	mainlib

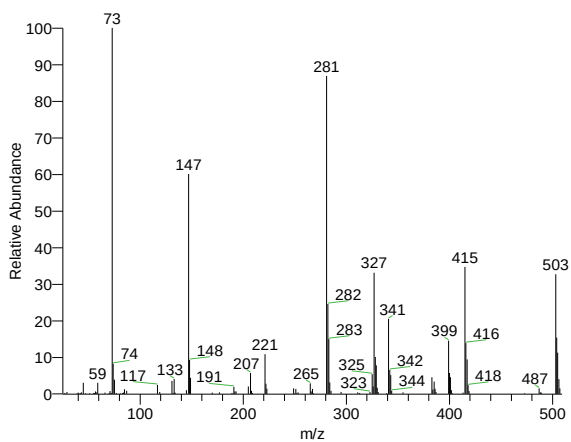
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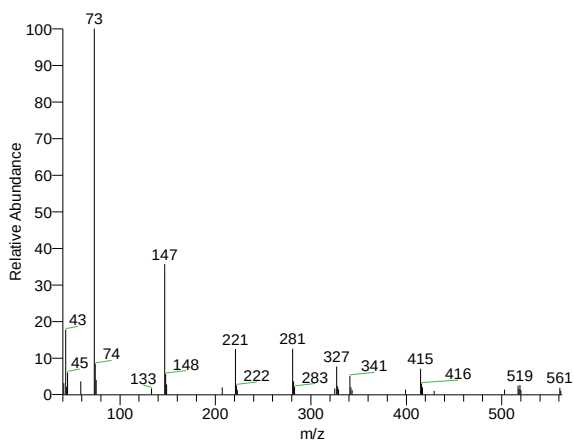
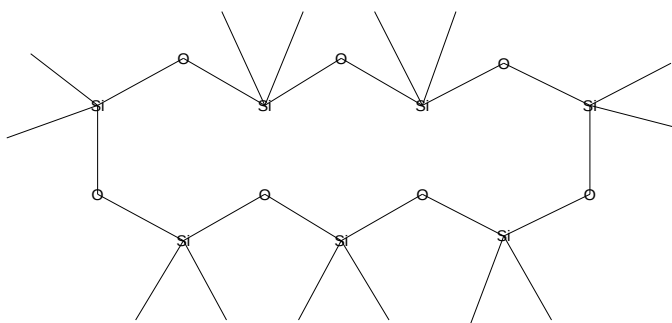
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

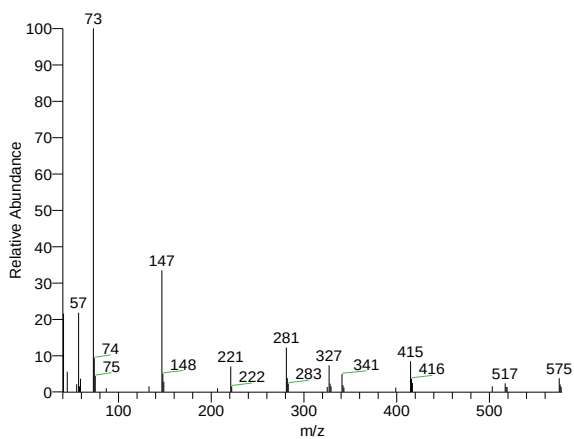
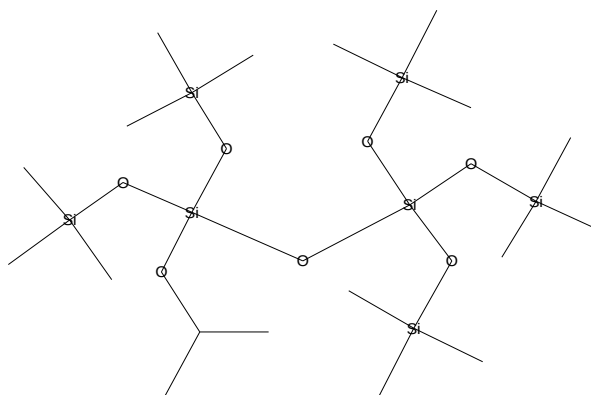
Compound Structure



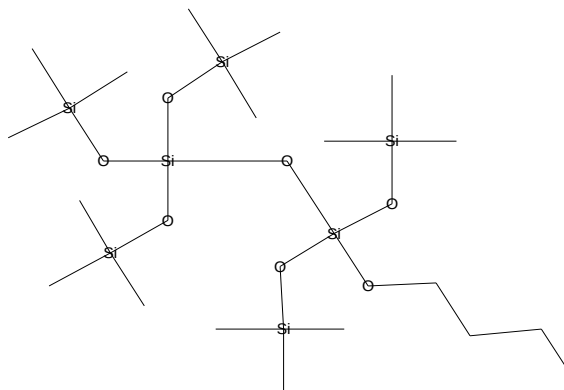
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane
Formula C₁₈H₅₂O₇Si₇, MW 576, CAS# 71579-69-6, Entry# 42479
1-Isopropoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl tris(trimethylsilyl) orthosilicate #



3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane
Formula C₁₉H₅₄O₇Si₇, MW 590, CAS# 72439-84-0, Entry# 42504
1-Butoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl tris(trimethylsilyl) orthosilicate #



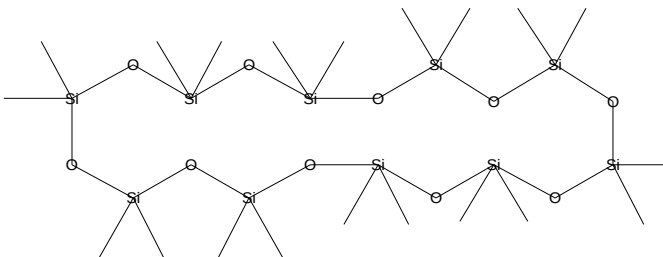
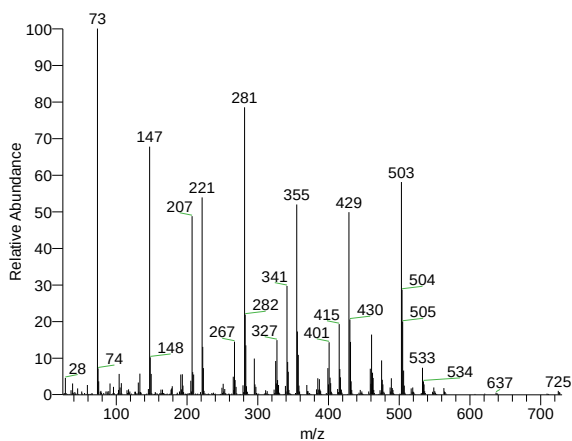
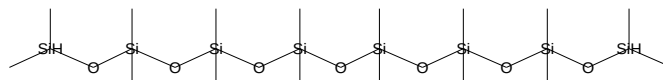
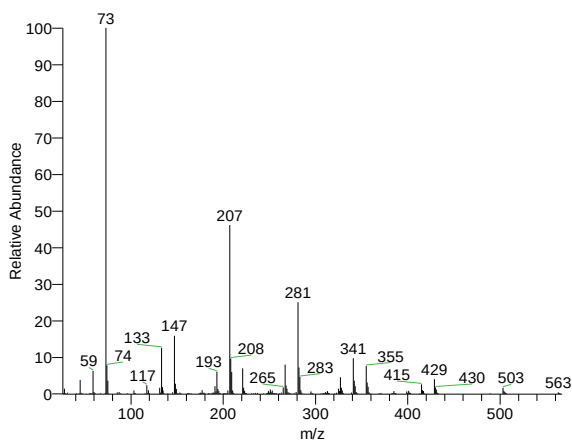
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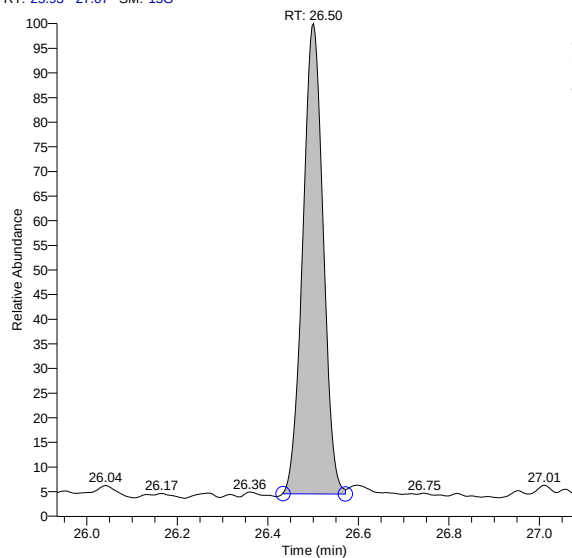
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure

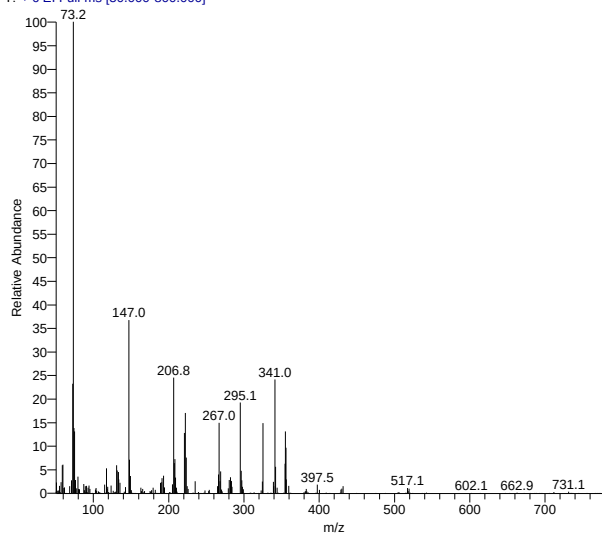


RT: 25.93 - 27.07 SM: 15G



NL:
1.31E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #6114 RT: 26.50 AV: 1 RF: 6.00, 3 NL: 2.34E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
26.50	Heptasiloxane, hexadecamethyl-	3900255.28	75.71	666	753	mainlib

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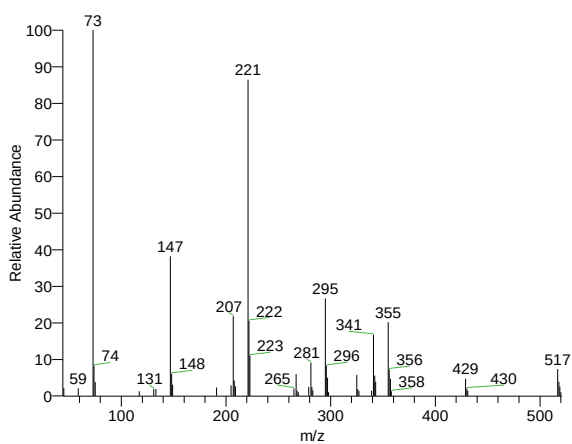
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ANALYTICAL CHEMISTRY DIVISION

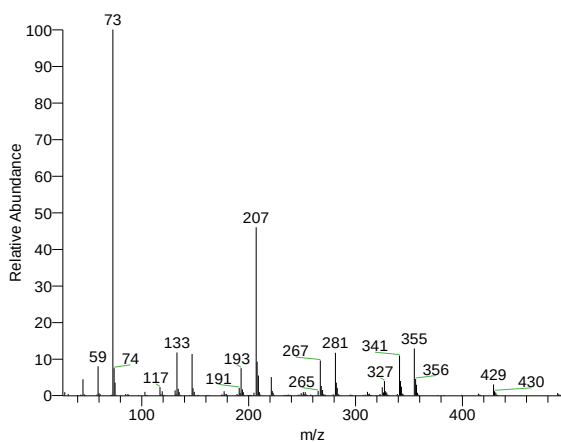
RT	Compound Name	Area	Probability	SI	RSI	Library
26.50	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3900255.28	17.56	626	667	mainlib
26.50	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3900255.28	4.14	587	621	mainlib
26.50	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3900255.28	1.00	550	592	mainlib
26.50	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	3900255.28	0.33	526	551	mainlib

Hit Spectrum

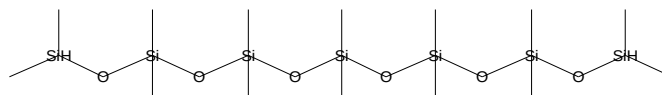
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



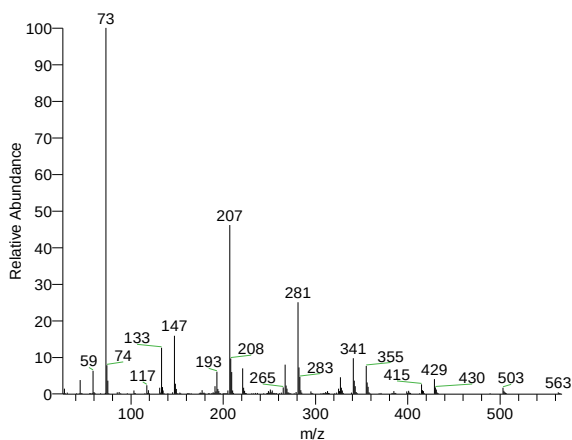
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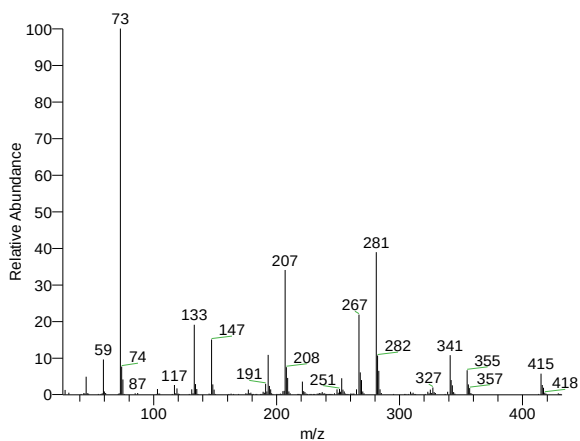
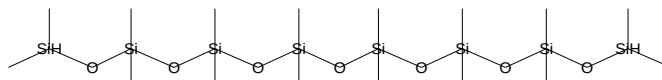
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

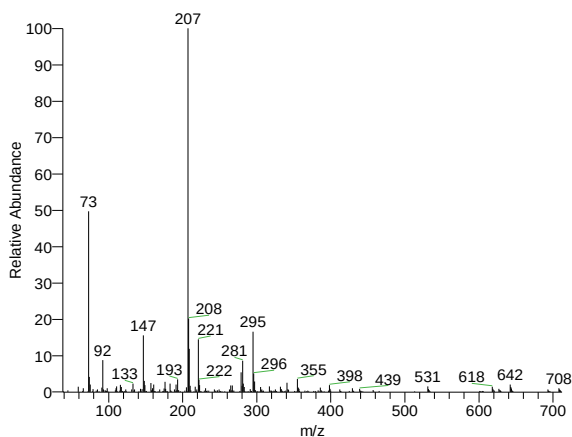
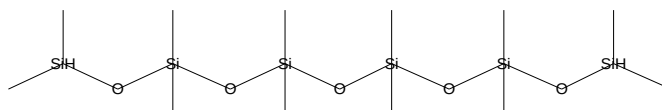
Compound Structure



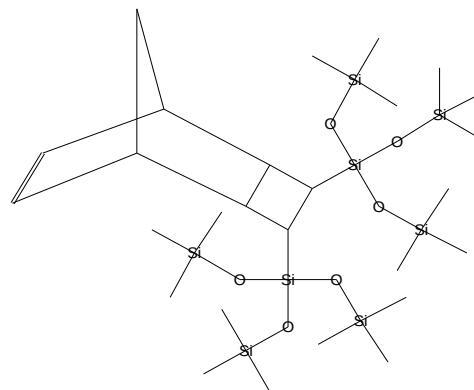
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

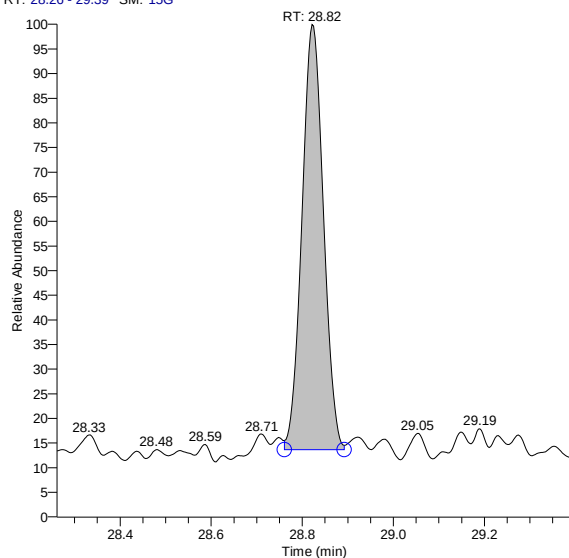


Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:2BJSGSCCAWLAXCNS-UHFFFAOYSA-N



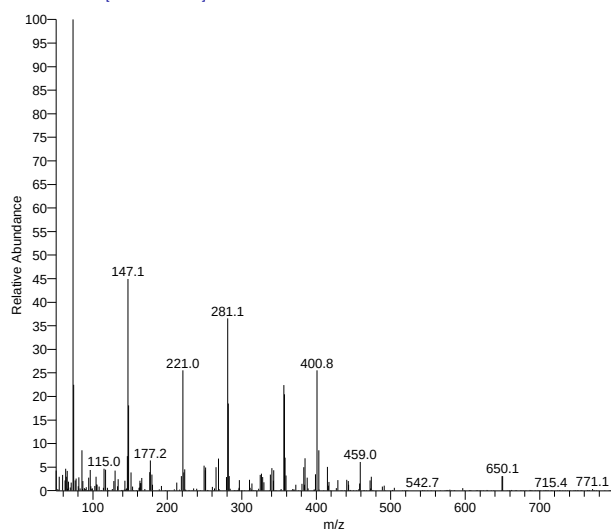
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RT: 28.26 - 29.39 SM: 15G



NL:
4.14E5
TIC: MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

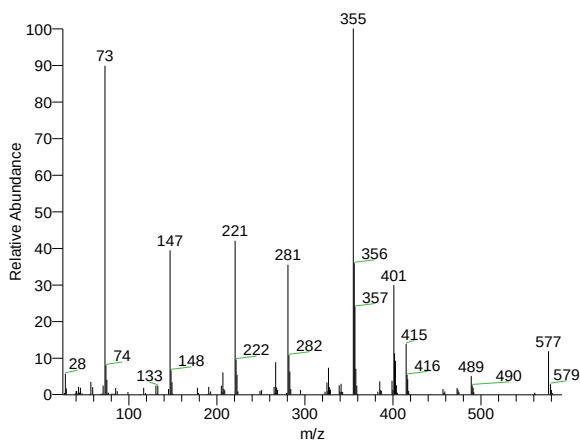
NGA-ZE-WATER3-SAMPLE-INJ1 #6806 RT: 28.82 AV: 1 RF: 6.00, 3 NL: 7.30E4
T: + c EI Full ms [50.000-800.000]



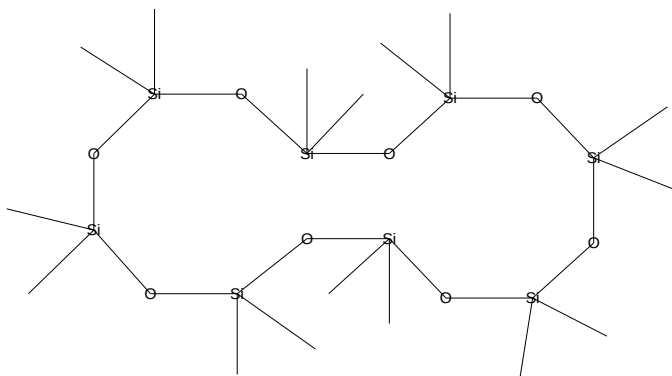
RT	Compound Name	Area	Probability	SI	RSI	Library
28.82	Cyclooctasiloxane, hexadecamethyl-	1163912.89	58.55	486	567	mainlib
28.82	Hexasiloxane, tetradecamethyl-	1163912.89	13.58	446	650	mainlib
28.82	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1163912.89	3.30	409	464	mainlib
28.82	1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane	1163912.89	2.13	396	644	mainlib
28.82	Cyclodecasiloxane, eicosamethyl-	1163912.89	1.97	394	412	mainlib

Hit Spectrum

Compound Structure



Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane



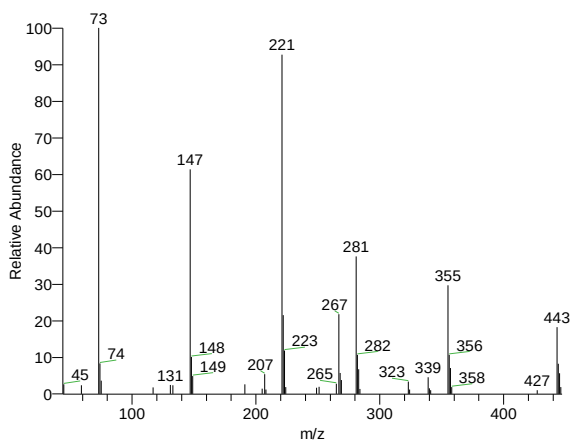
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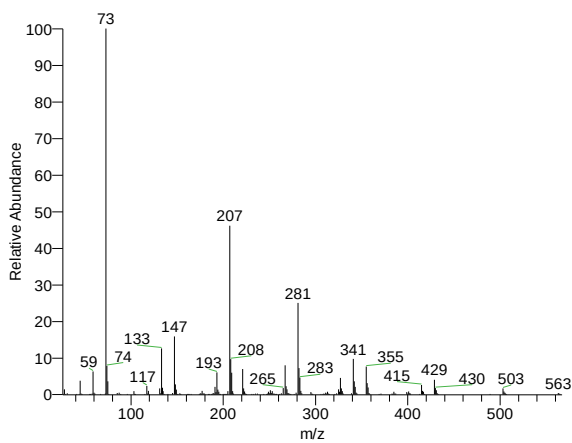
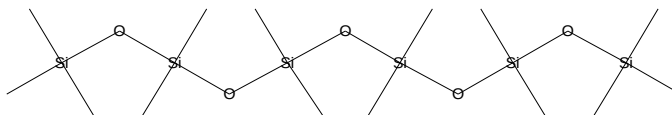
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

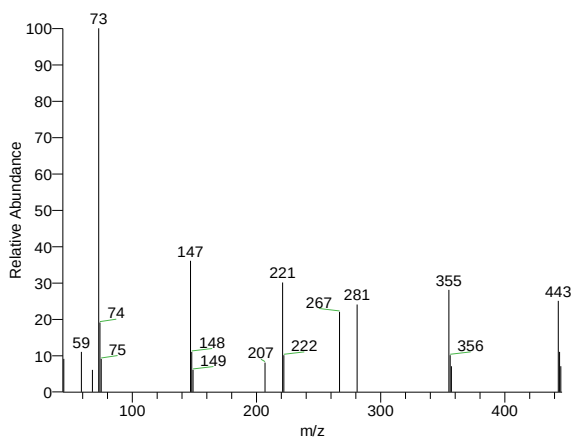
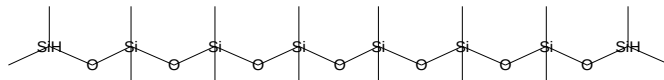
Compound Structure



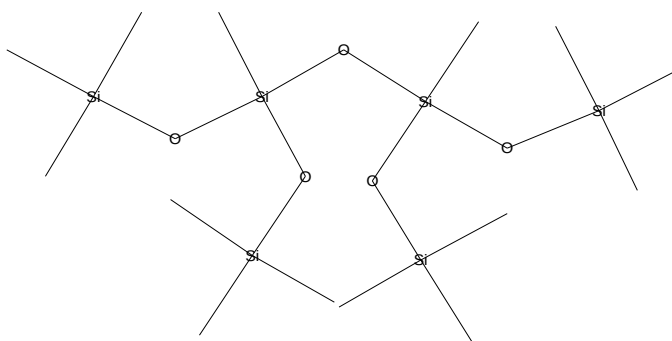
Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



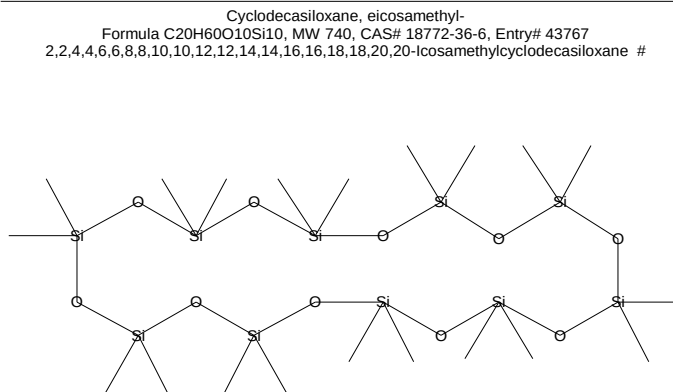
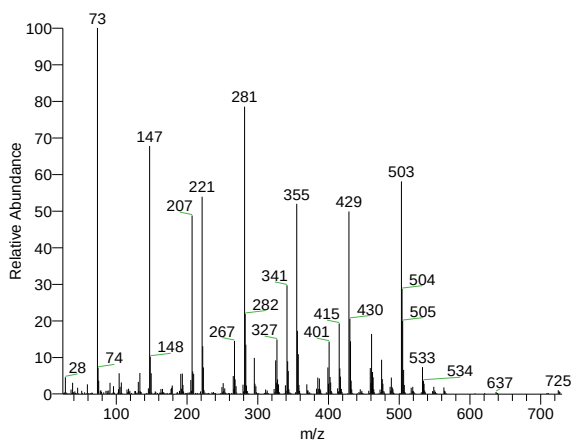
1,1,1,3,5,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 2003-92-1, Entry# 42693
1,1,1,3,5,7,7-Octamethyl-3,5-bis[(trimethylsilyl)oxy]tetrasiloxane #



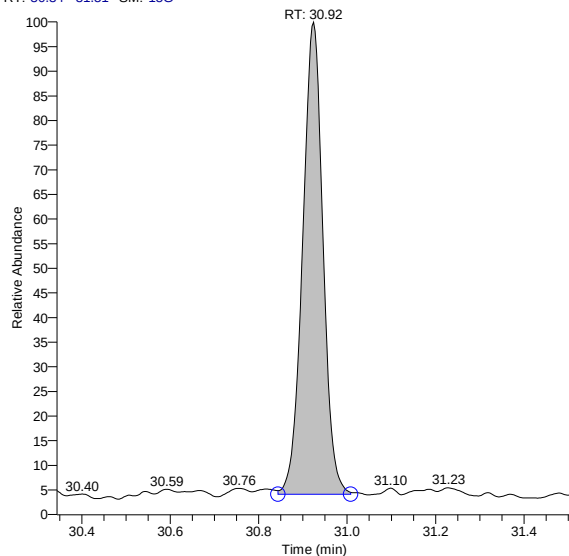
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Hit Spectrum

Compound Structure

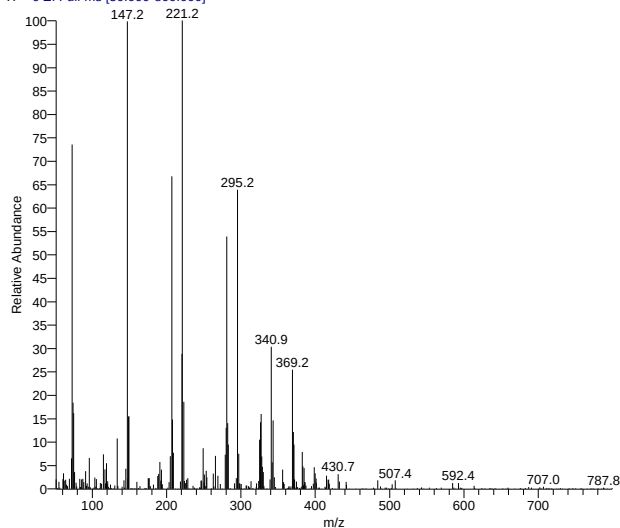


RT: 30.34 - 31.51 SM: 15G



NL:
1.45E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #7433 RT: 30.92 AV: 1 RF: 6.00, 3 NL: 1.32E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
30.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	4431781.97	33.77	545	590	mainlib
30.92	Heptasiloxane, hexadecamethyl-	4431781.97	25.19	537	684	mainlib
30.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	4431781.97	8.44	513	584	mainlib
30.92	Tricyclo[4.2.1.0(2,5)]non-7 -ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	4431781.97	8.11	512	555	mainlib
30.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	4431781.97	6.05	504	584	mainlib

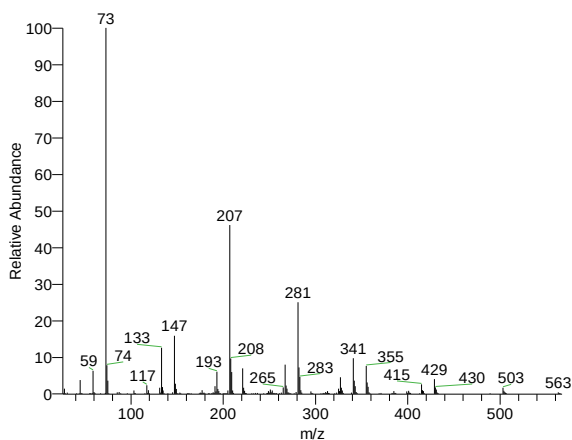
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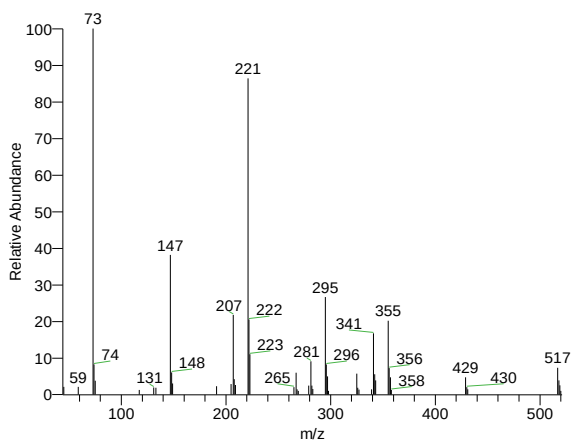
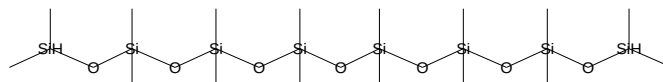
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

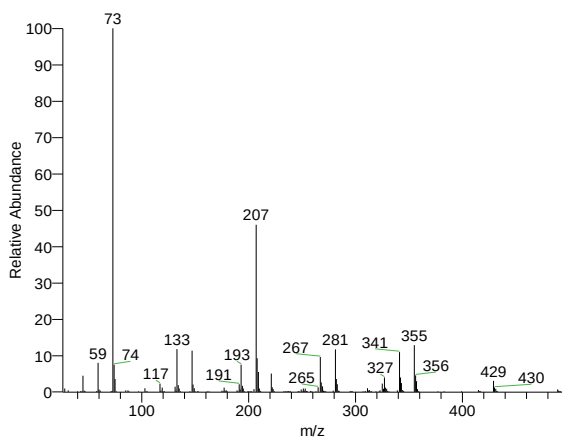
Compound Structure



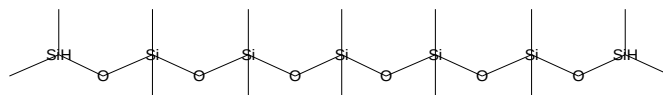
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



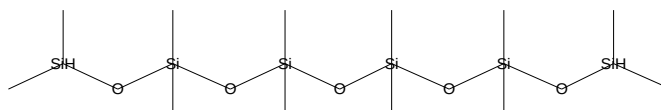
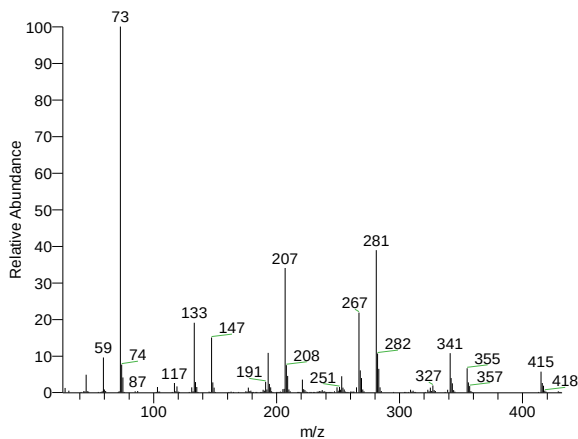
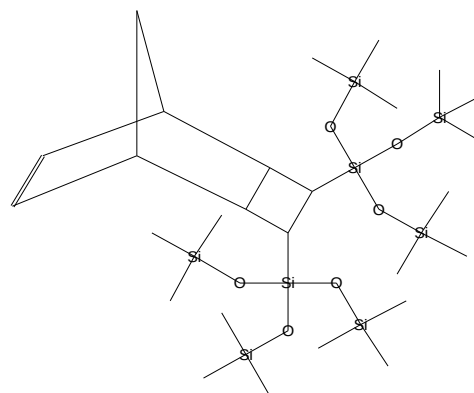
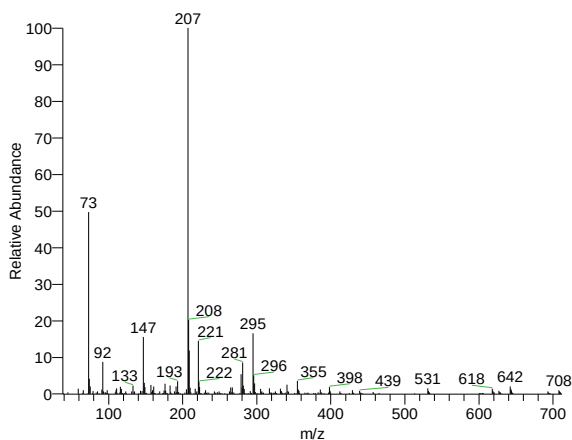
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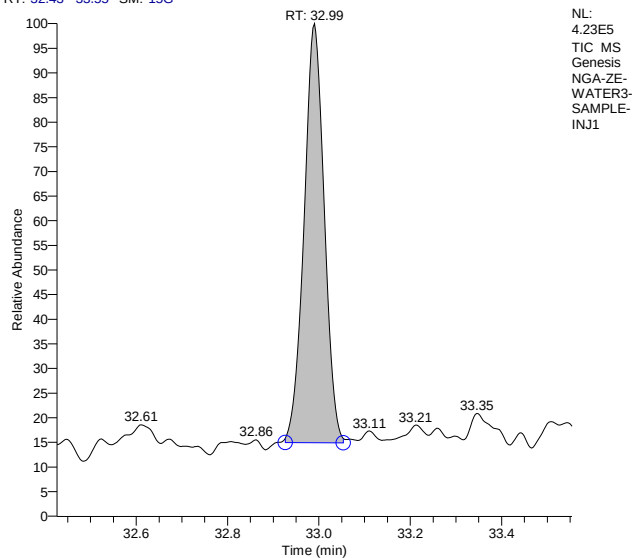
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

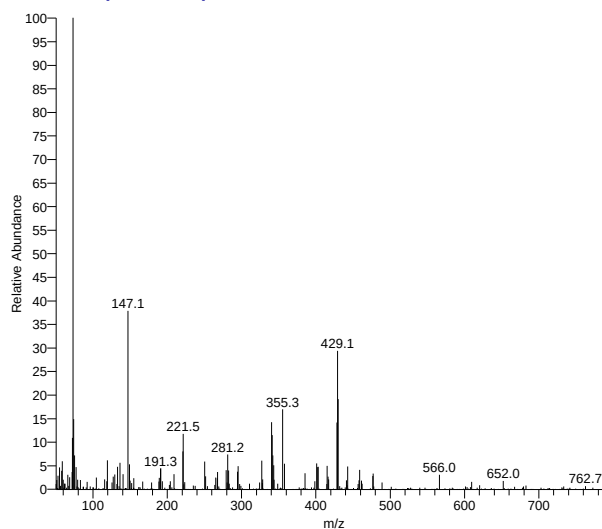
Compound Structure



RT: 32.43 - 33.55 SM: 15G



NGA-ZE-WATER3-SAMPLE-INJ1 #8049 RT: 32.99 AV: 1 RF: 6.00, 3 NL: 8.95E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
32.99	Cyclononasiloxane, octadecamethyl-	1116136.89	56.77	535	640	mainlib

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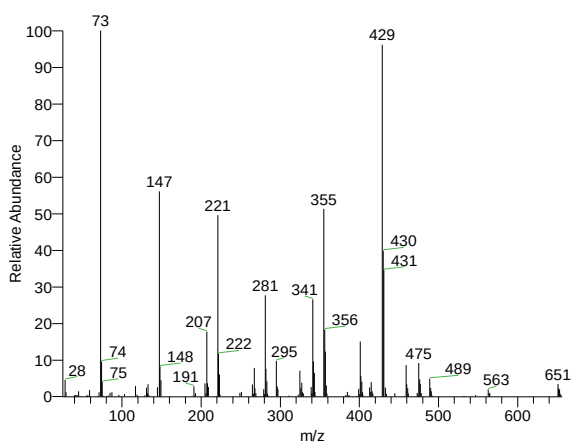
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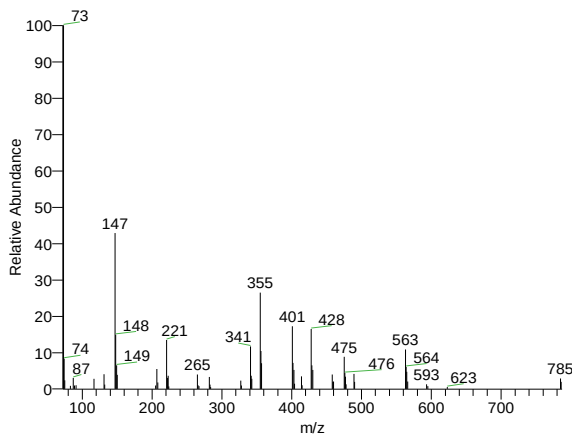
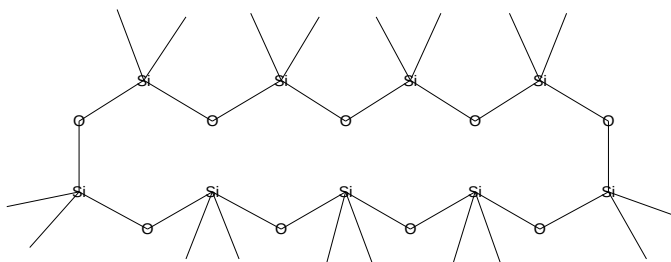
RT	Compound Name	Area	Probability	SI	RSI	Library
32.99	Bis(heptamethylcyclotetrasiloxyl)hexamethyltrisiloxane	1116136.89	9.32	471	623	mainlib
32.99	Cyclodecasiloxane,	1116136.89	6.39	460	514	mainlib
32.99	eicosamethyl-Octasiloxane,	1116136.89	4.51	450	554	mainlib
	1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-					
32.99	Oxazepam, 2TMS derivative	1116136.89	3.99	447	528	mainlib

Hit Spectrum

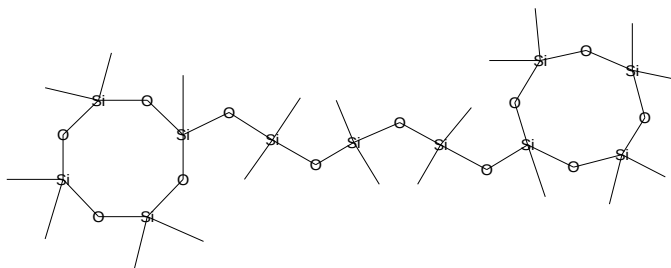
Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C18H54O9Si9, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Bis(heptamethylcyclotetrasiloxyl)hexamethyltrisiloxane
Formula C20H60O12Si11, MW 800, CAS# 71449-67-7, Entry# 42773



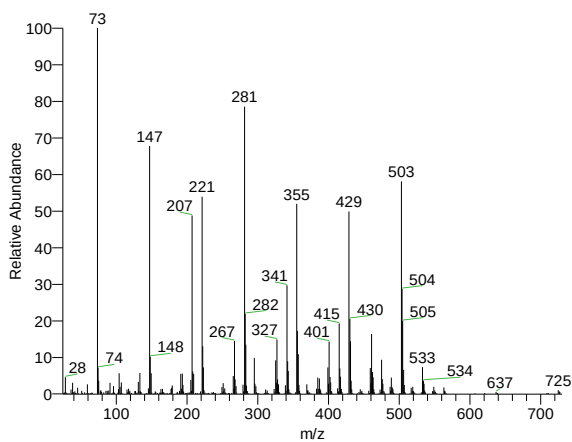
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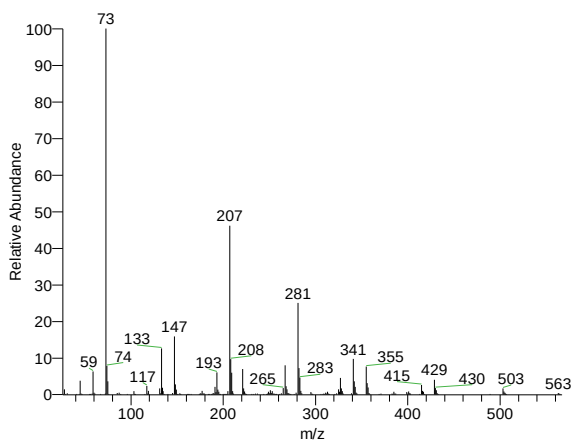
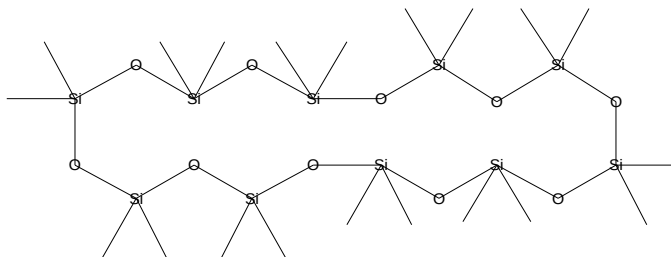
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

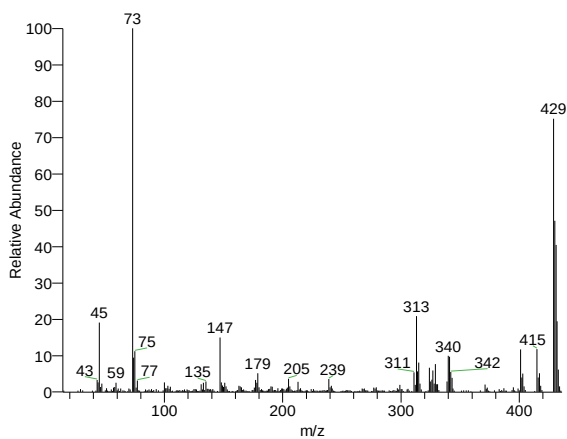
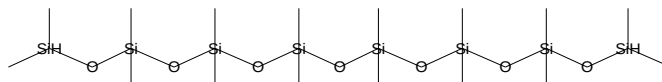
Compound Structure



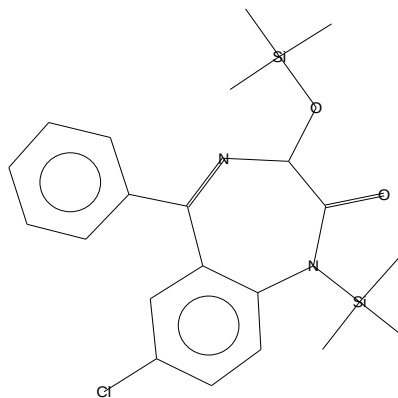
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #

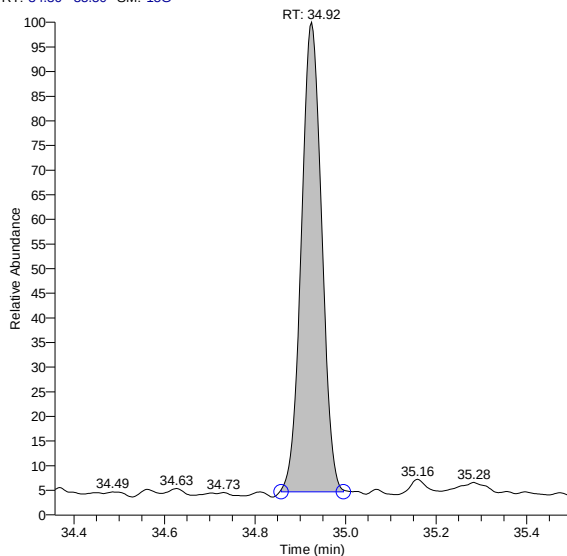


Oxazepam, 2TMS derivative
Formula C₂₁H₂₇ClN₂O₂Si₂, MW 430, CAS# 55319-93-2, Entry# 44302



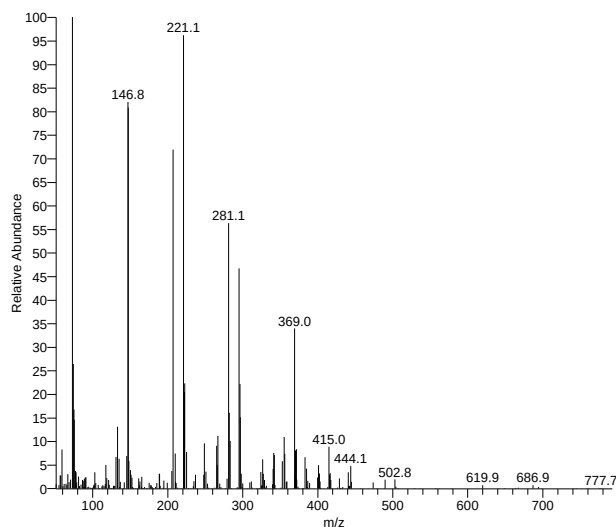
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RT: 34.36 - 35.50 SM: 15G



NL:
1.30E6
TIC: MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

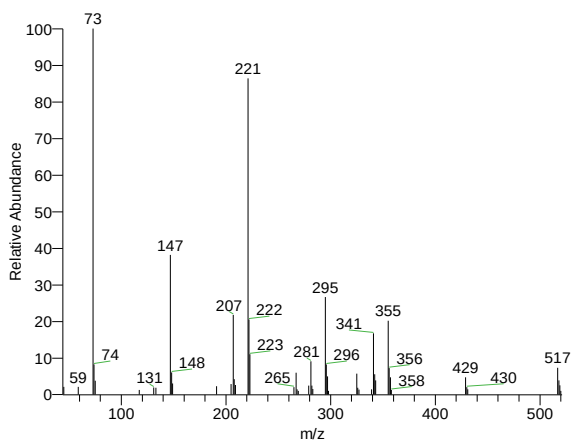
NGA-ZE-WATER3-SAMPLE-INJ1 #8626 RT: 34.92 AV: 1 RF: 6.00, 3 NL: 1.31E5
T: + c EI Full ms [50.000-800.000]



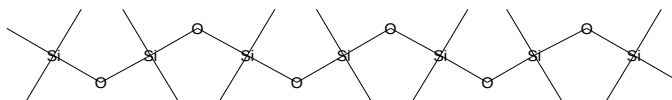
RT	Compound Name	Area	Probability	SI	RSI	Library
34.92	Heptasiloxane, hexadecamethyl-	3867425.93	39.61	564	724	mainlib
34.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3867425.93	29.55	556	593	mainlib
34.92	Pentasiloxane, dodecamethyl-	3867425.93	6.85	516	610	mainlib
34.92	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	3867425.93	6.05	513	633	mainlib
34.92	Cyclodecasiloxane, eicosamethyl-	3867425.93	2.21	490	499	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



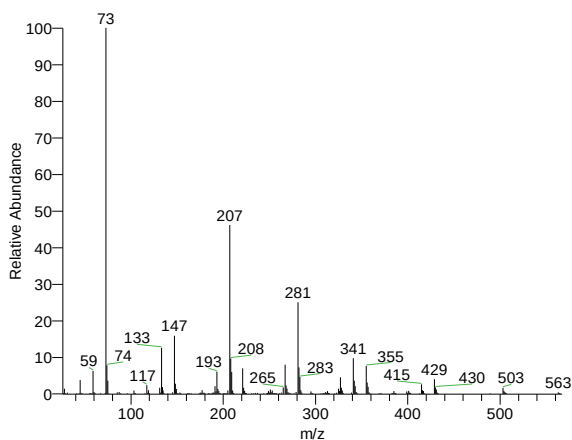
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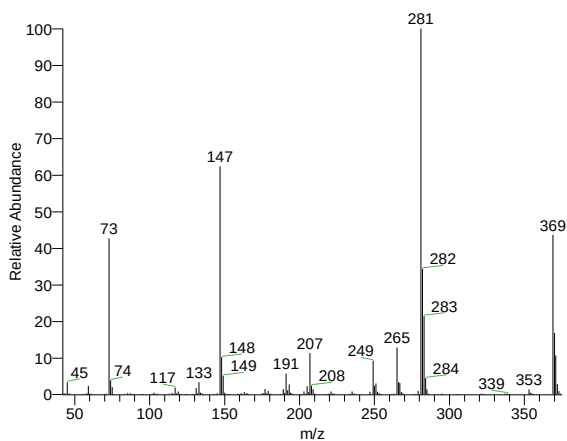
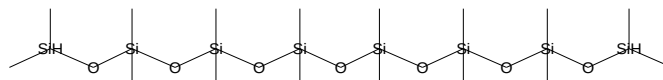
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

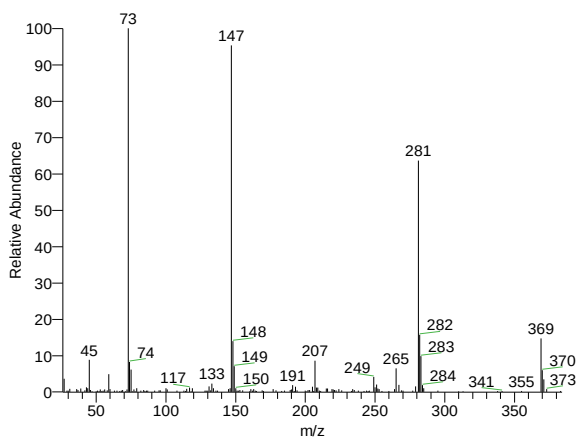
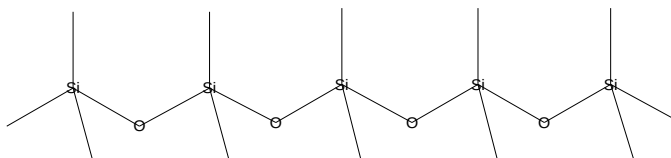
Compound Structure



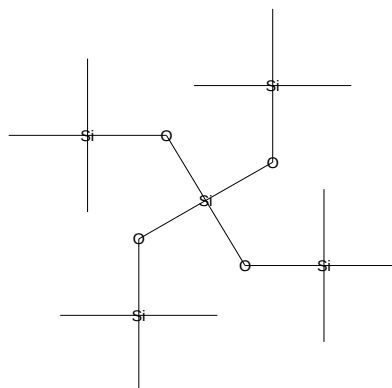
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



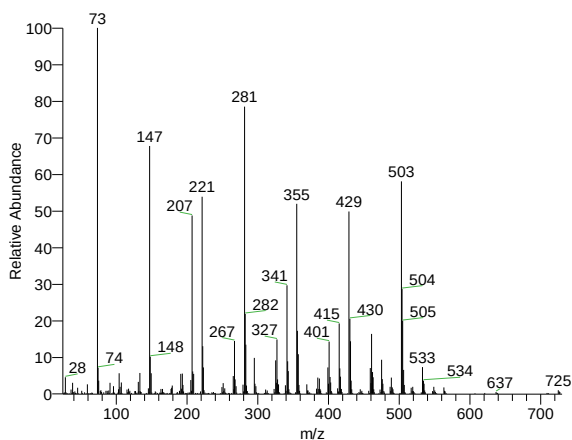
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



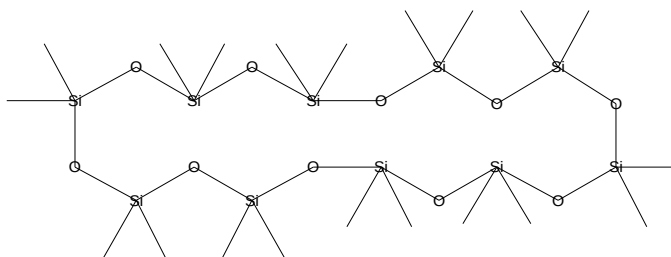
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Hit Spectrum

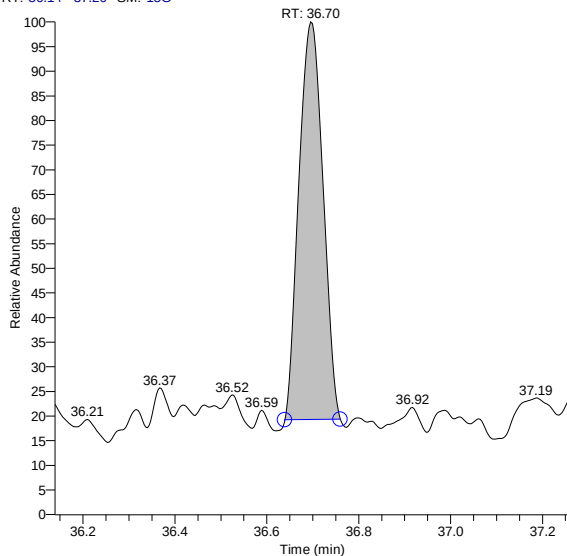
Compound Structure



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #

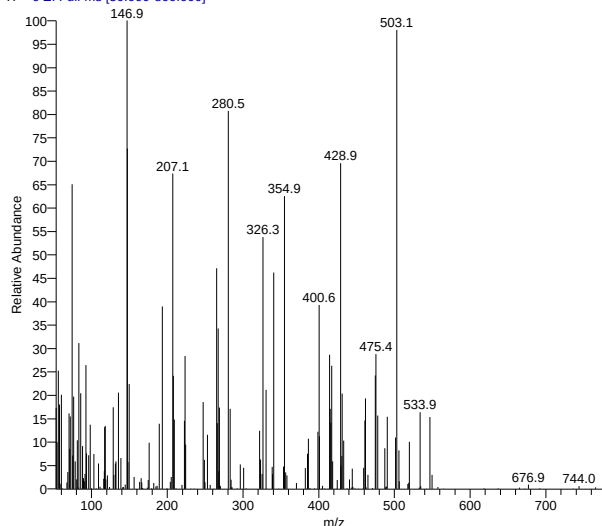


RT: 36.14 - 37.26 SM: 15G



NL:
3.20E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #9154 RT: 36.70 AV: 1 RF: 6.00, 3 NL: 1.52E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
36.70	Cyclodecasiloxane, eicosamethyl-	934693.16	70.57	490	507	mainlib
36.70	Cyclononasiloxane, octadecamethyl-	934693.16	10.48	421	519	mainlib
36.70	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	934693.16	8.45	416	498	mainlib
36.70	Tetracosamethyl-cyclododecasiloxane	934693.16	2.39	387	586	mainlib
36.70	Cycloheptasiloxane, tetradecamethyl-	934693.16	1.83	380	502	mainlib

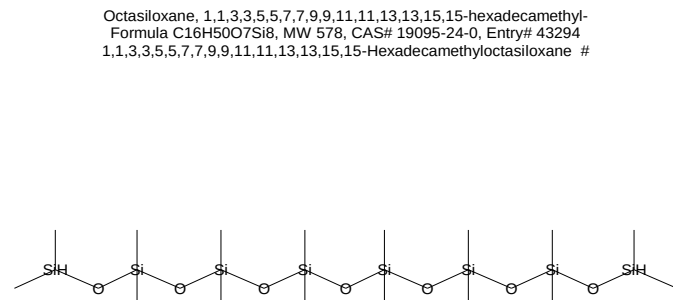
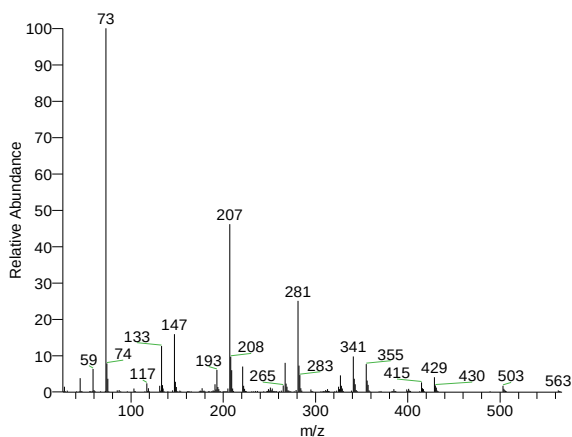
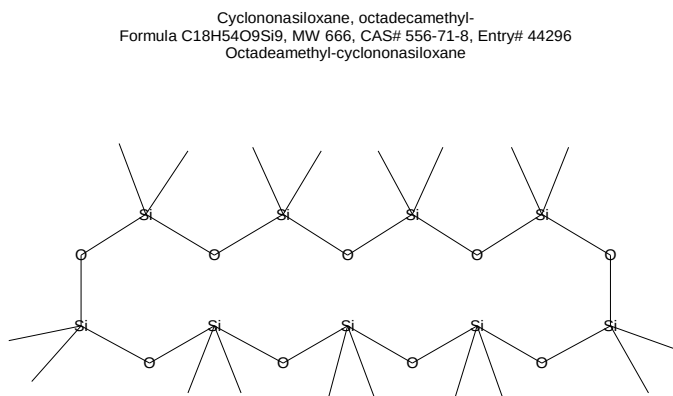
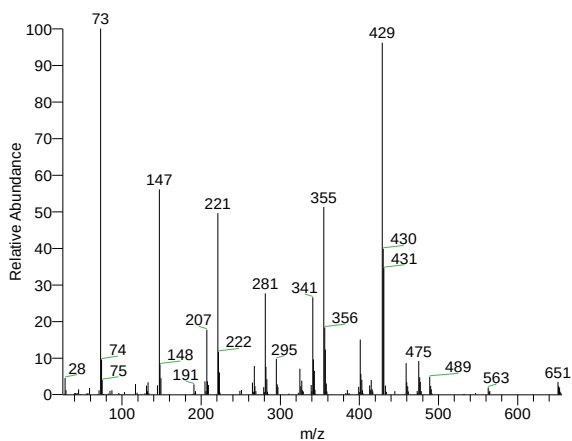
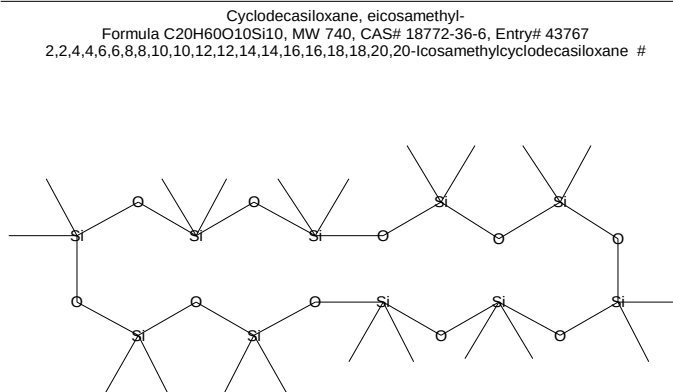
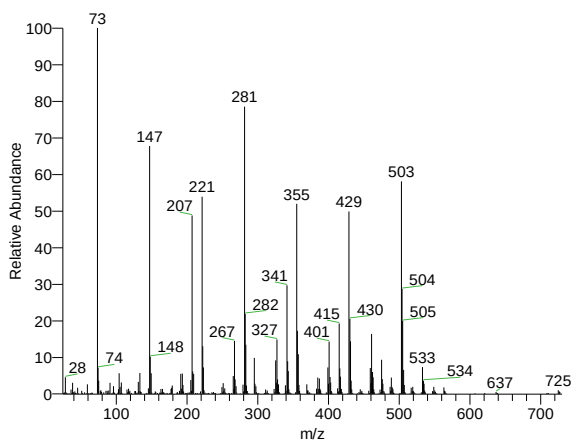
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Hit Spectrum

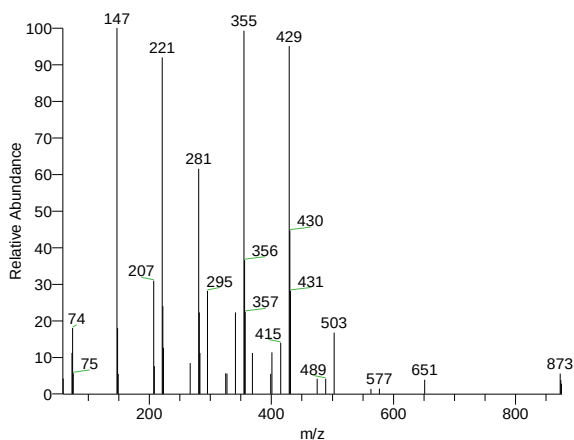
Compound Structure



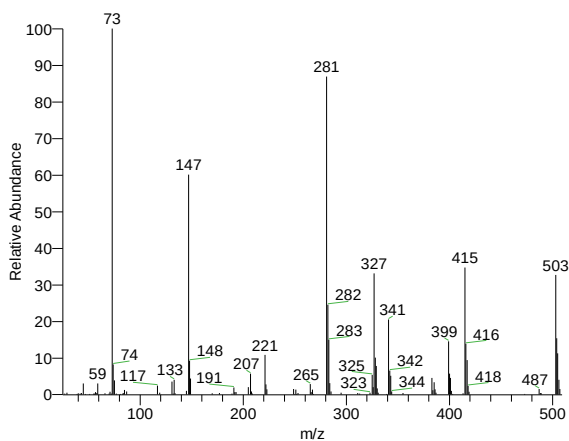
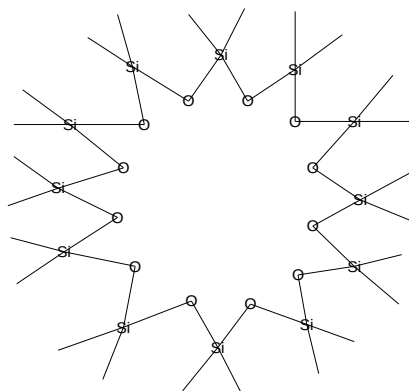
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Hit Spectrum

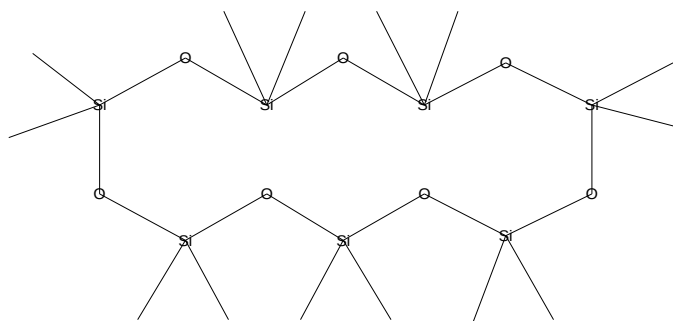
Compound Structure



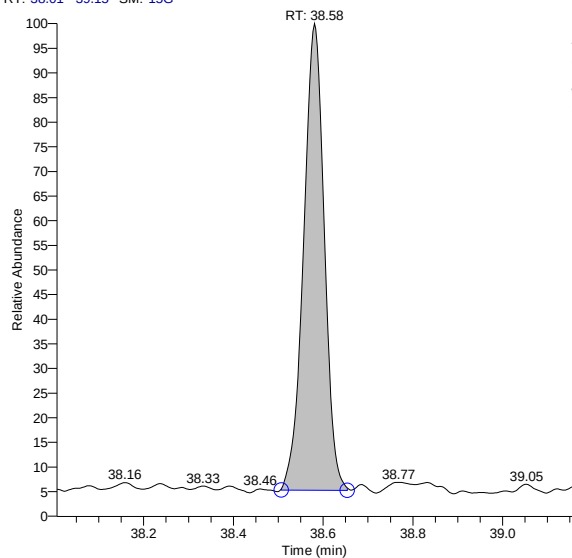
Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #

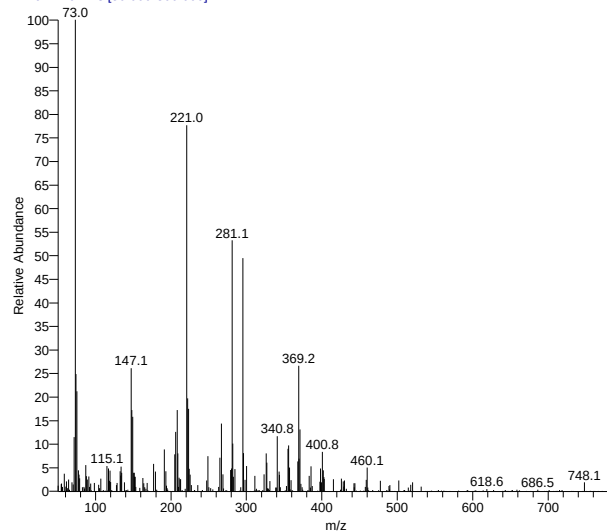


RT: 38.01 - 39.15 SM: 15G



NL:
1.18E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #9716 RT: 38.58 AV: 1 RF: 6.00, 3 NL: 1.22E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
38.58	Heptasiloxane, hexadecamethyl-	3581834.24	25.35	497	719	mainlib

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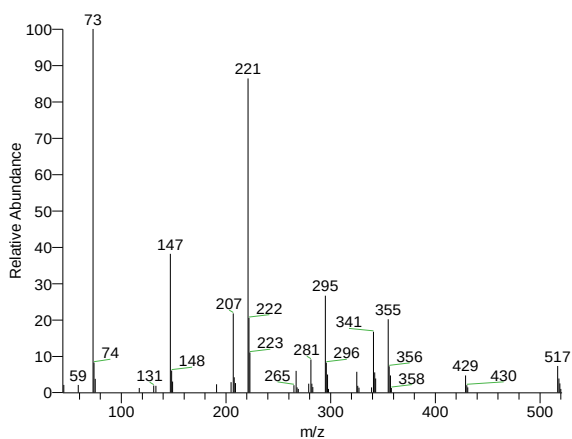
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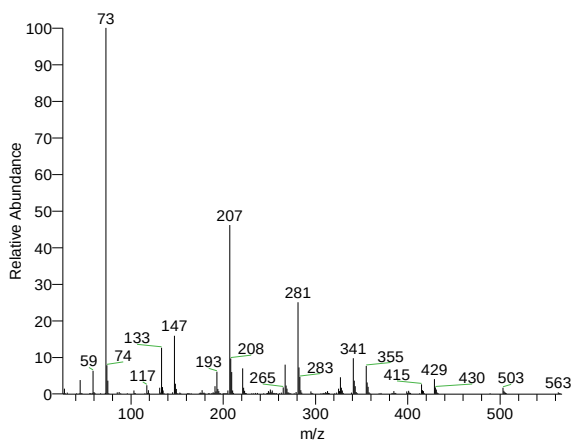
RT	Compound Name	Area	Probability	SI	RSI	Library
38.58	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3581834.24	16.38	484	549	mainlib
38.58	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3581834.24	4.73	456	568	mainlib
38.58	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3581834.24	3.99	452	557	mainlib
38.58	Cyclooctasiloxane, hexadecamethyl-	3581834.24	3.06	445	560	mainlib

Hit Spectrum

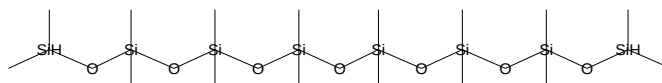
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



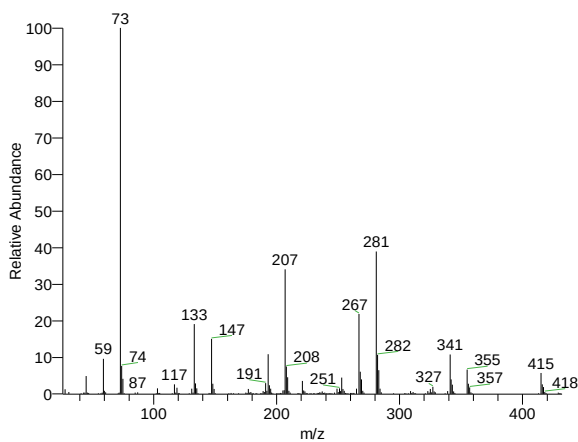
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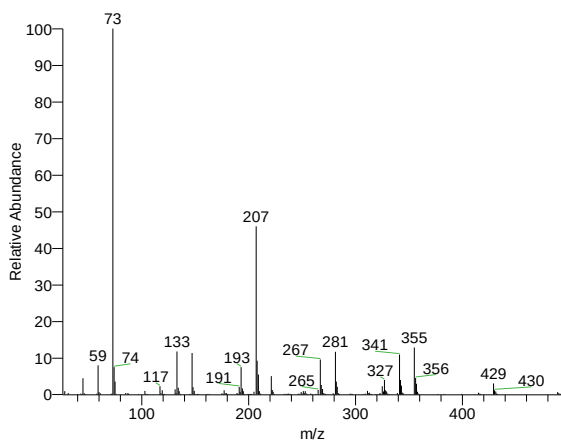
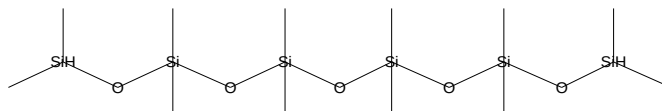
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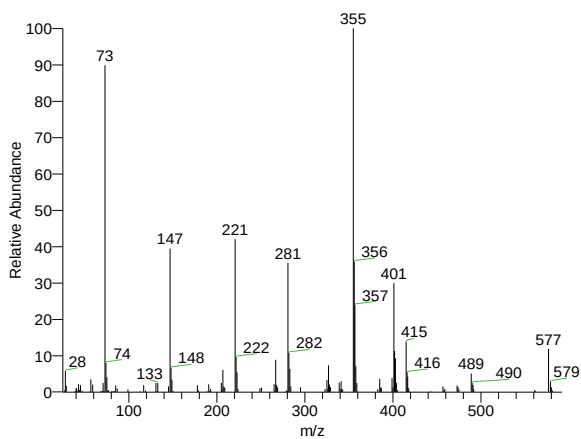
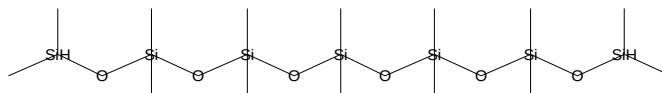
Compound Structure



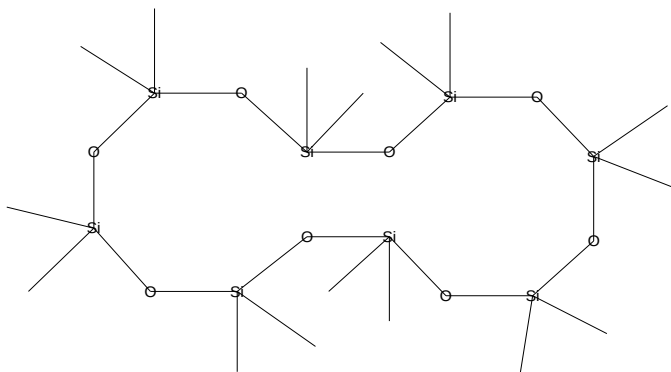
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

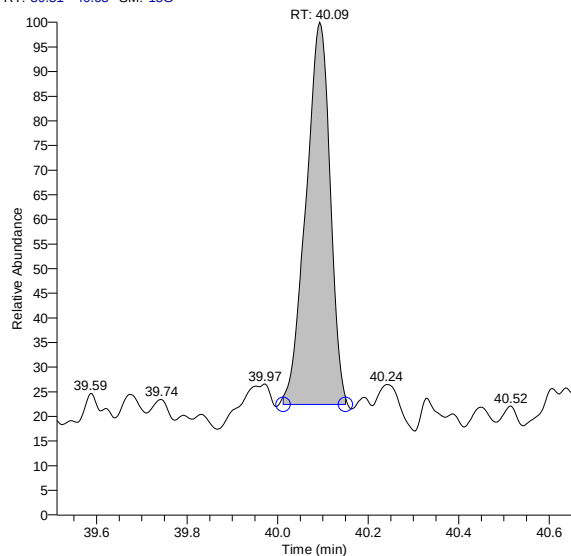


Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane



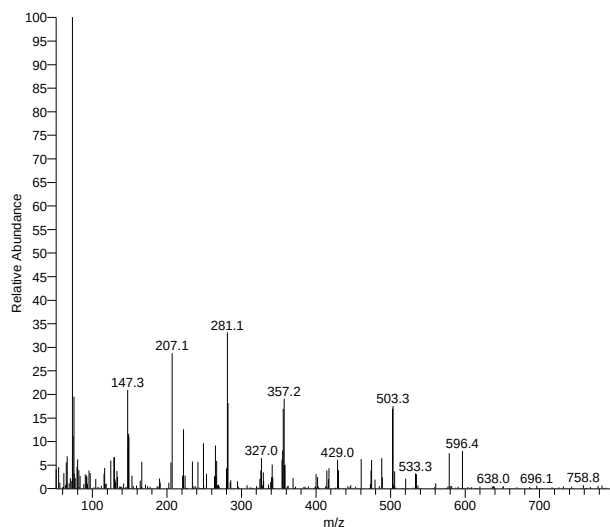
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RT: 39.51 - 40.65 SM: 15G



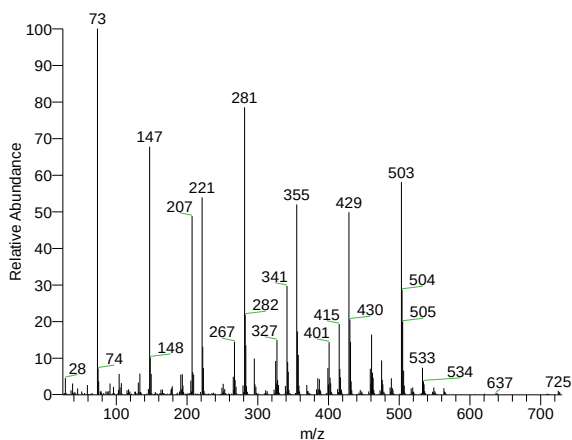
NL:
2.81E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #10167 RT: 40.09 AV: 1 RF: 6.00, 3 NL: 5.68E4
T: + c EI Full ms [50.000-800.000]



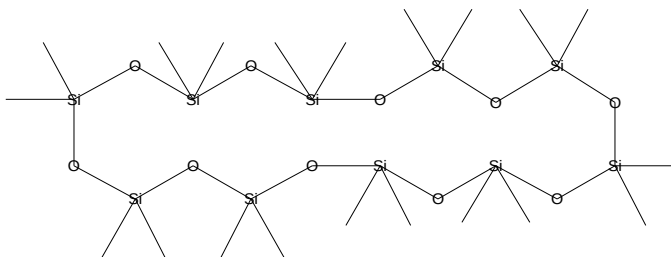
RT	Compound Name	Area	Probability	SI	RSI	Library
40.09	Cyclodecasiloxane, eicosamethyl-	808595.40	60.13	494	553	mainlib
40.09	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	808595.40	13.03	450	576	mainlib
40.09	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	808595.40	3.12	412	595	mainlib
40.09	Cycloheptasiloxane, tetradecamethyl-	808595.40	2.33	404	583	mainlib
40.09	3,4-Dihydroxymandelic acid, ethyl ester, tri-TMS	808595.40	1.45	390	582	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



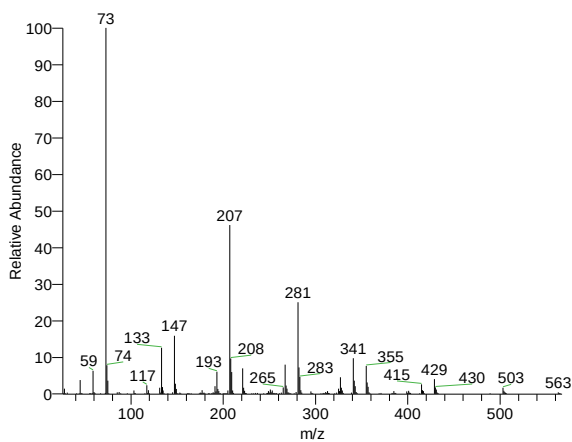
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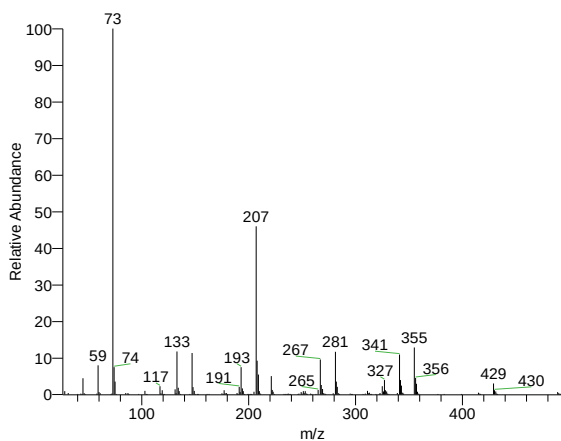
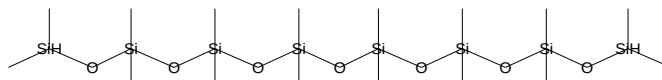
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

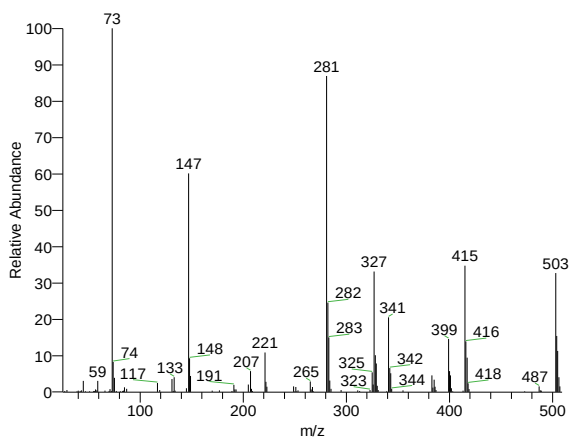
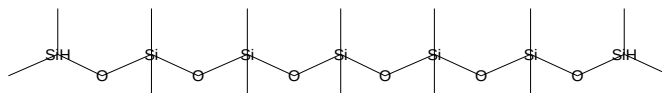
Compound Structure



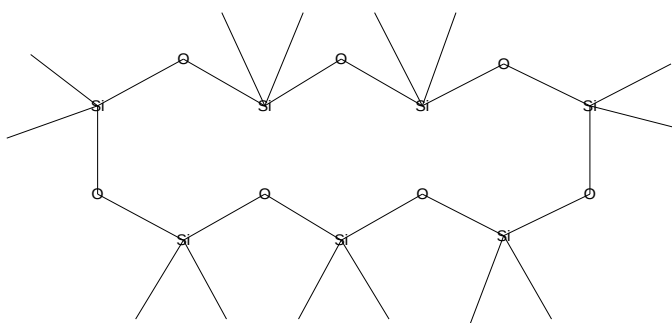
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



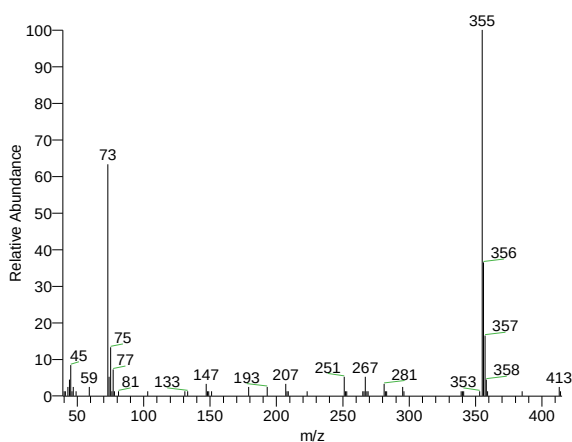
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



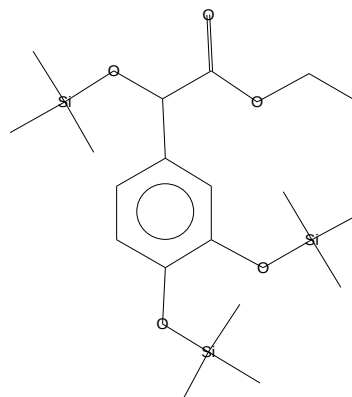
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Hit Spectrum

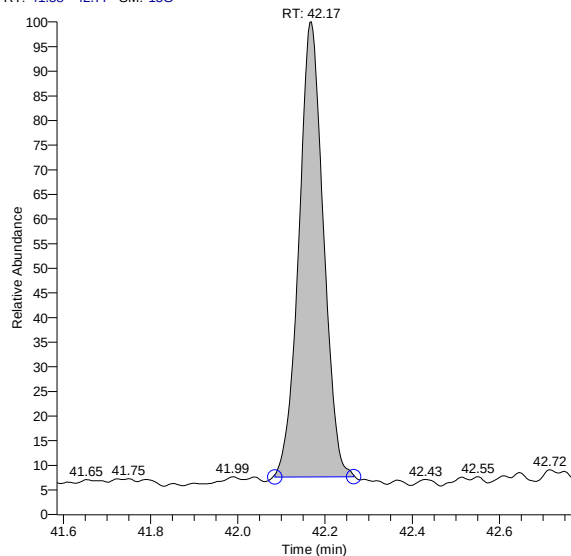
Compound Structure



3,4-Dihydroxymandelic acid, ethyl ester, tri-TMS
Formula C₁₉H₃₆O₅Si₃, MW 428, CAS# NA, Entry# 234280
Ethyl (3,4-bis(trimethylsilyloxy)phenyl)((trimethylsilyloxy)acetate) #

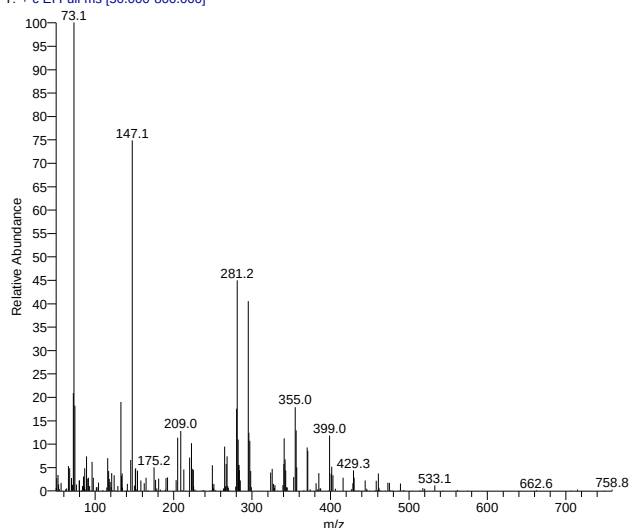


RT: 41.58 - 42.77 SM: 15G



NL: 8.55E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #10786 RT: 42.17 AV: 1 RF: 6.00, 3 NL: 9.22E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
42.17	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3088917.84	19.16	486	549	mainlib
42.17	Pyridoxine, 3TMS derivative	3088917.84	13.14	475	547	mainlib
42.17	Heptasiloxane, hexadecamethyl-	3088917.84	7.17	458	610	mainlib
42.17	Cyclononasiloxane, octadecamethyl-	3088917.84	5.06	448	508	mainlib
42.17	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3088917.84	4.67	446	531	mainlib

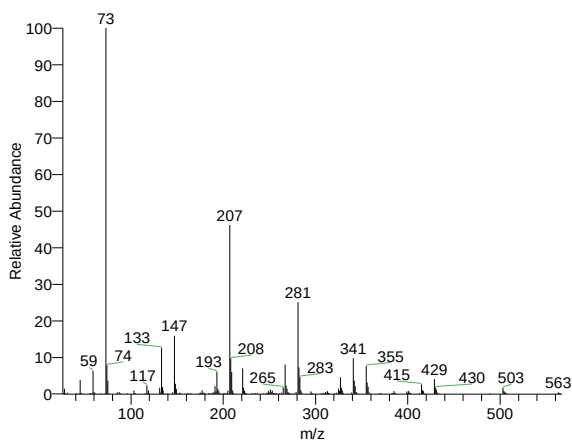
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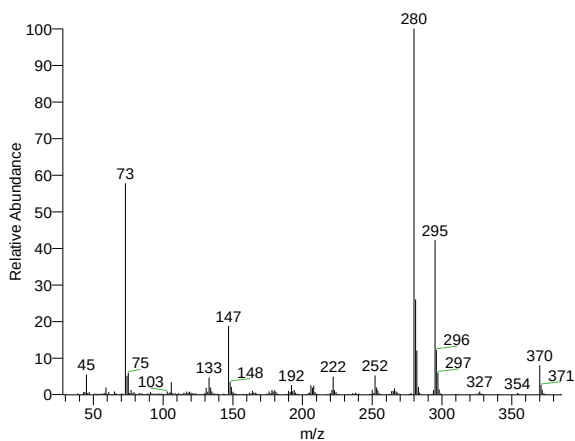
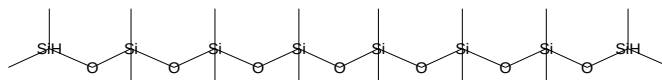
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

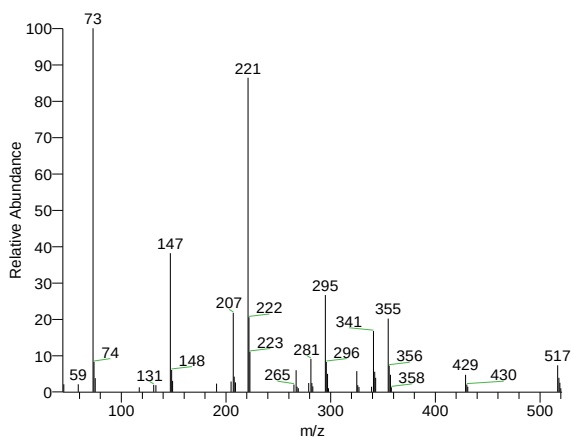
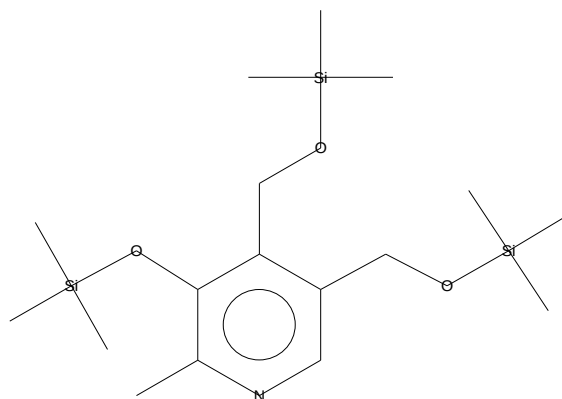
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Pyridoxine, 3TMS derivative
Formula C₁₇H₃₅NO₃Si₃, MW 385, CAS# 14857-17-1, Entry# 219628
Pyridine, 2-methyl-3-(trimethylsilyloxy)-4,5-bis-[(trimethylsilyloxy)methyl]-



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



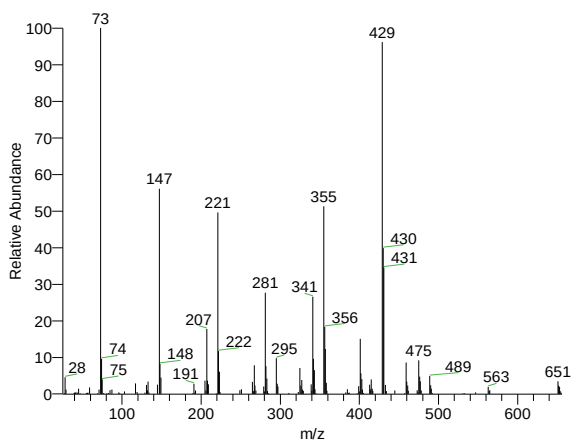
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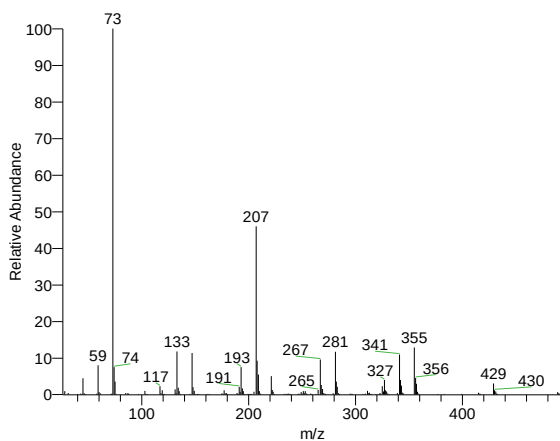
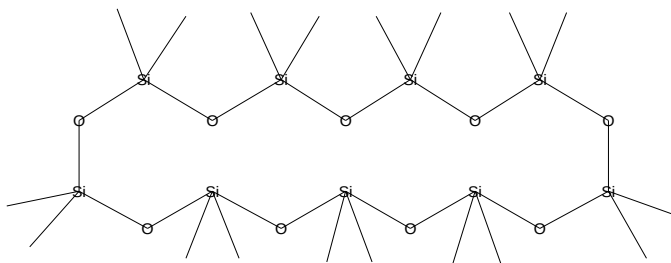
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

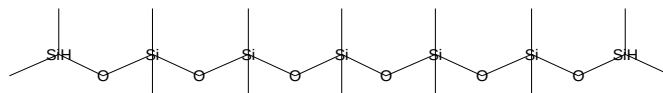
Compound Structure



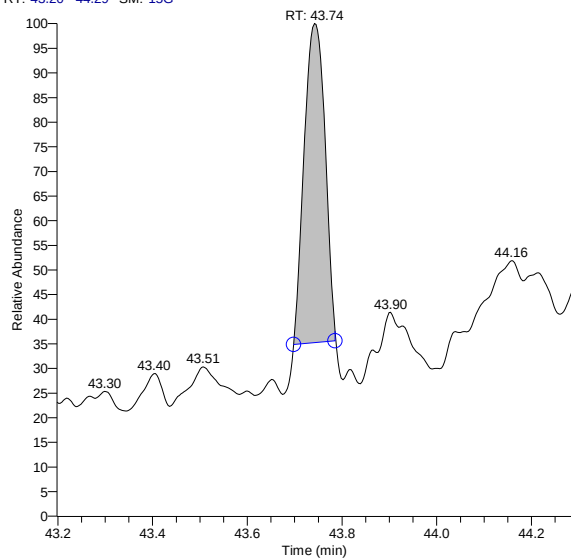
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

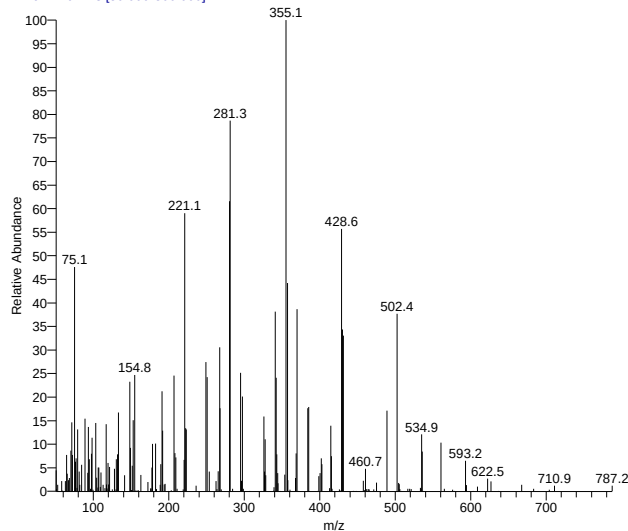


RT: 43.20 - 44.29 SM: 15G



NL:
2.65E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #11255 RT: 43.74 AV: 1 RF: 6.00, 3 NL: 1.57E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
43.74	Cyclononasiloxane, octadecamethyl-	524742.93	36.21	496	602	mainlib

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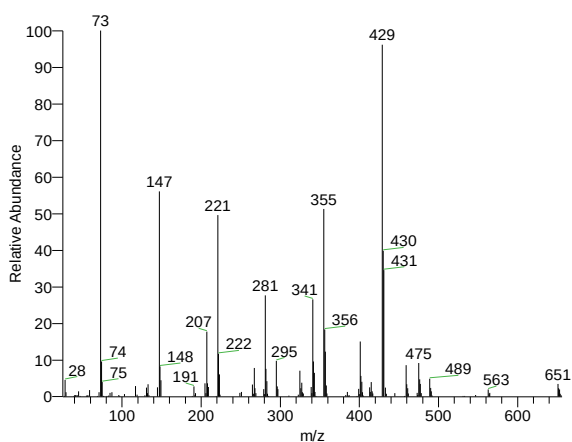
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ANALYTICAL CHEMISTRY DIVISION

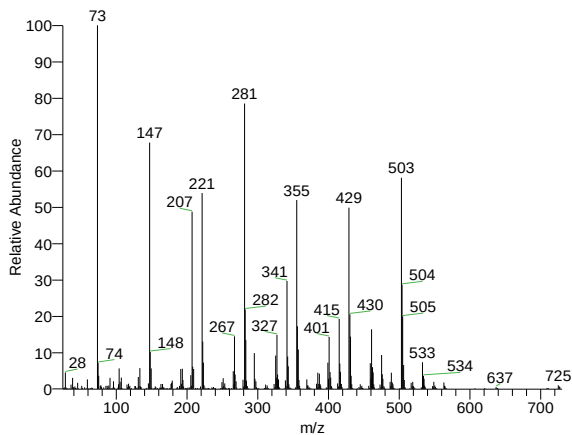
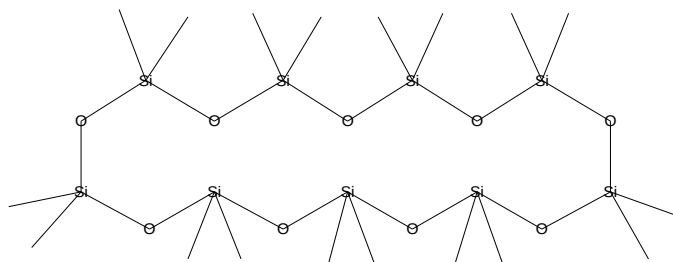
RT	Compound Name	Area	Probability	SI	RSI	Library
43.74	Cyclodecasiloxane,	524742.93	20.85	480	503	mainlib
43.74	eicosamethyl- Octasiloxane,	524742.93	18.42	477	548	mainlib
	1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethy l-					
43.74	Tetracosamethyl-cyclodod ecasiloxane	524742.93	8.94	458	704	mainlib
43.74	Heptasiloxane,	524742.93	6.67	450	536	mainlib
	1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-					

Hit Spectrum

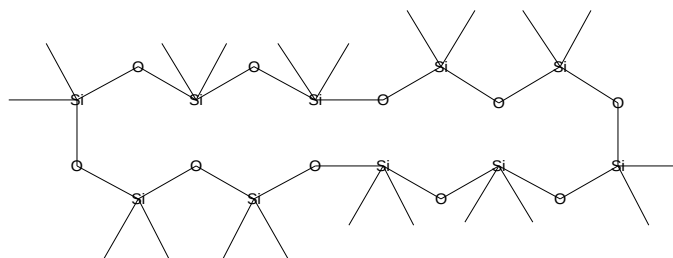
Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



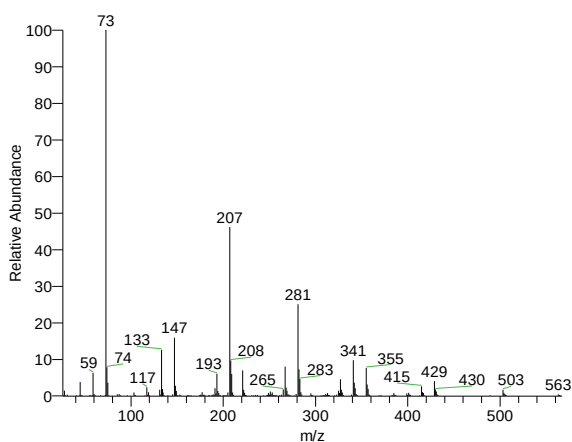
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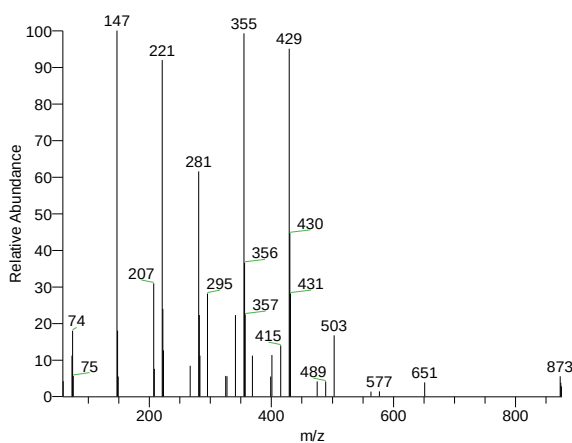
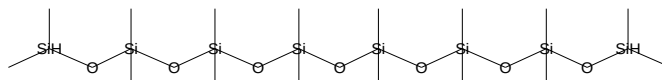
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

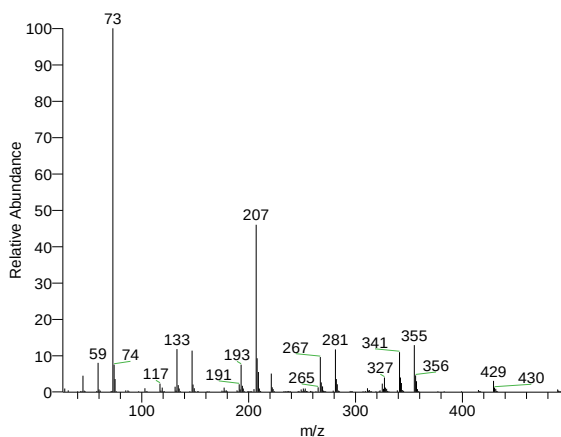
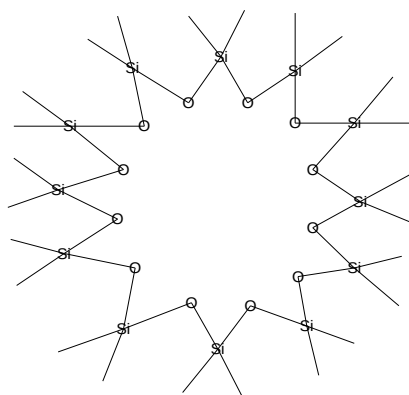
Compound Structure



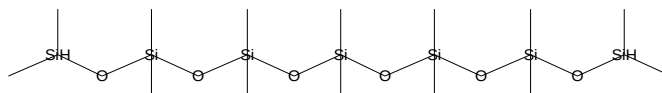
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752

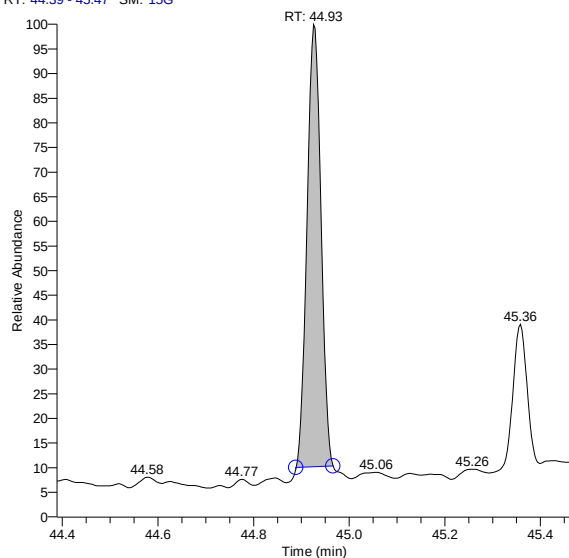


Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



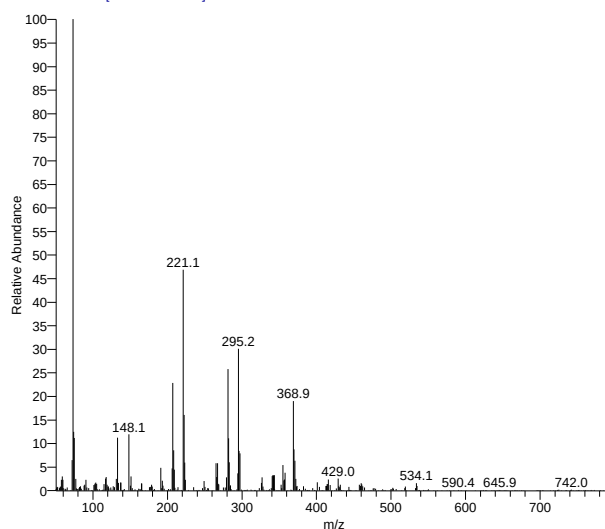
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RT: 44.39 - 45.47 SM: 15G



NL:
1.58E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

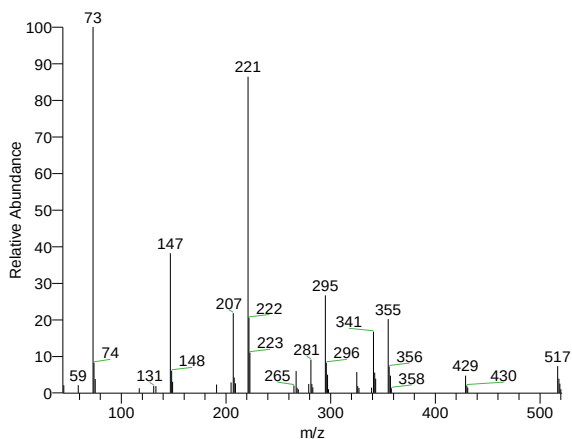
NGA-ZE-WATER3-SAMPLE-INJ1 #11608 RT: 44.93 AV: 1 RF: 6.00, 3 NL: 3.80E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
44.93	Heptasiloxane, hexadecamethyl-	2871799.01	61.66	595	763	mainlib
44.93	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2871799.01	17.80	567	631	mainlib
44.93	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2871799.01	5.33	541	645	mainlib
44.93	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2871799.01	3.23	526	642	mainlib
44.93	Cyclodecasiloxane, eicosamethyl-	2871799.01	1.76	509	522	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



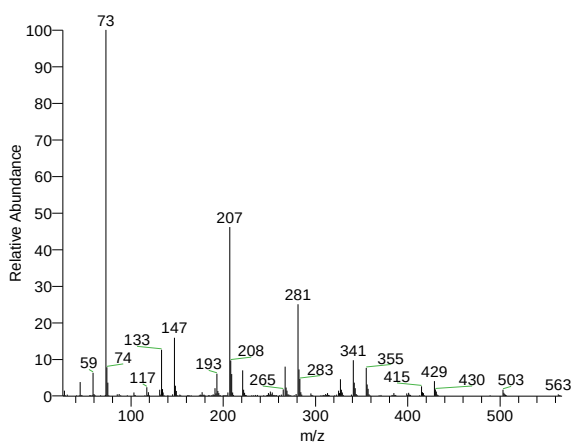
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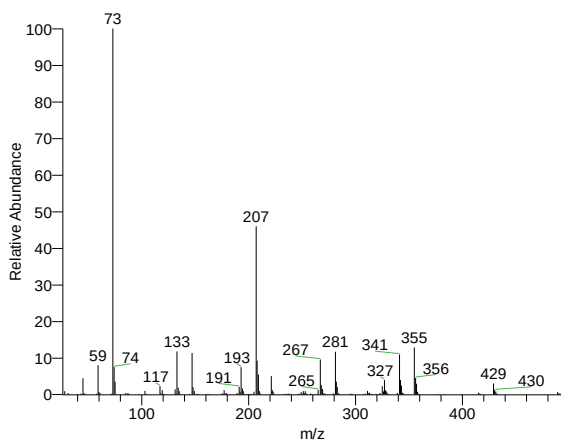
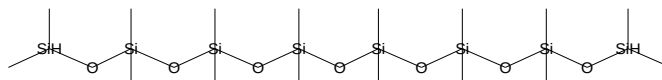
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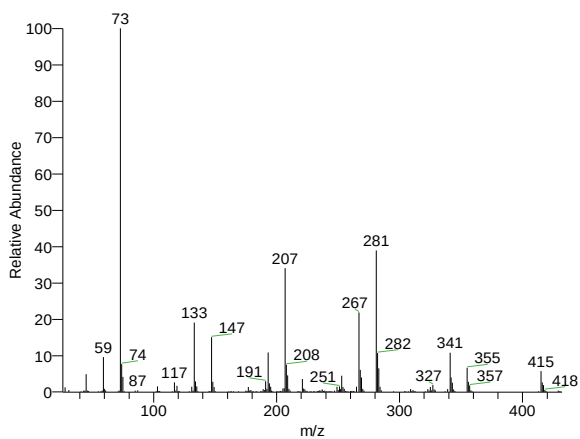
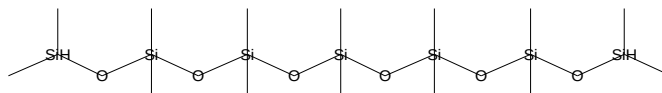
Compound Structure



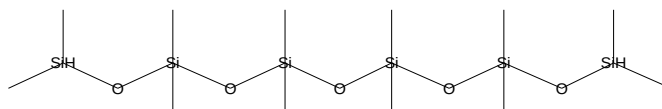
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



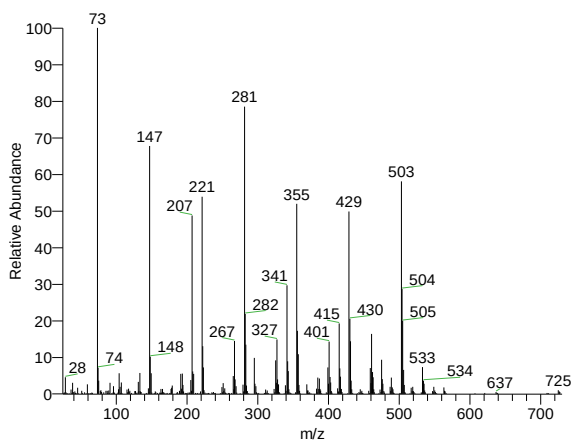
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



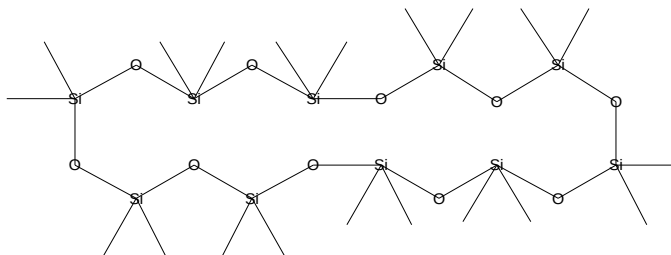
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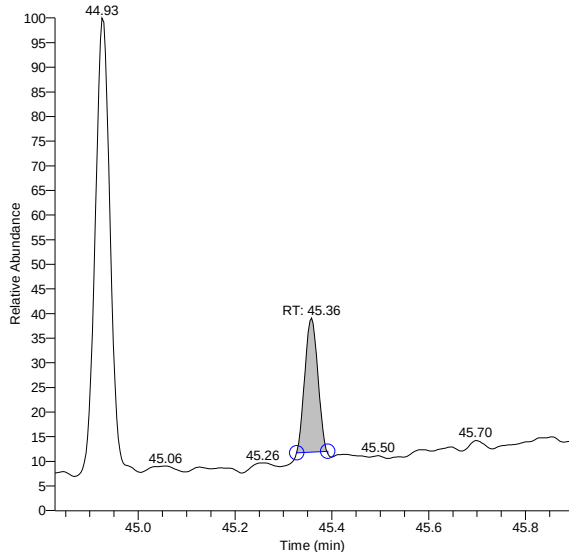
Compound Structure



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-icosamethylcyclodecasiloxane #

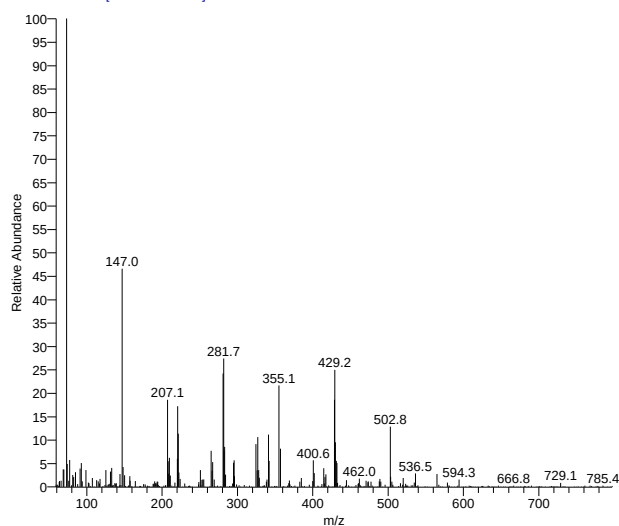


RT: 44.83 - 45.89 SM: 15G



NL:
1.58E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #11737 RT: 45.36 AV: 1 RF: 6.00, 3 NL: 1.37E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
45.36	Cyclodecasiloxane, eicosamethyl-	803061.49	40.16	626	667	mainlib
45.36	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	803061.49	29.96	618	691	mainlib
45.36	Cyclononasiloxane, octadecamethyl-	803061.49	19.35	605	711	mainlib
45.36	Tetracosamethyl-cyclododecasiloxane	803061.49	3.97	556	755	mainlib
45.36	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	803061.49	3.51	553	659	mainlib

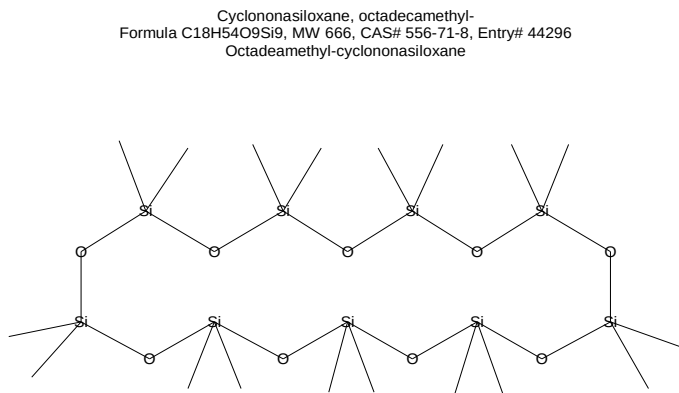
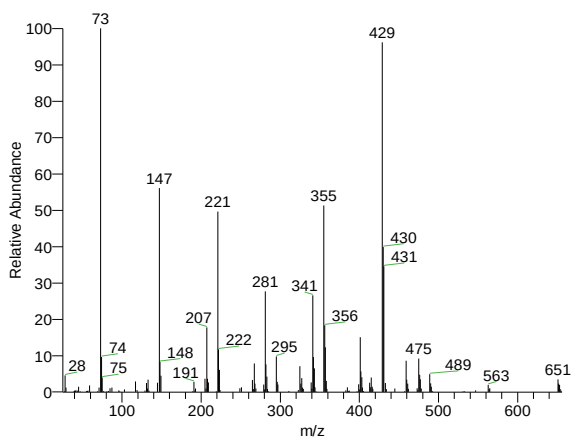
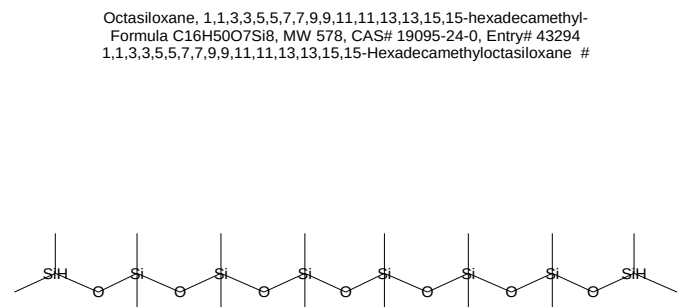
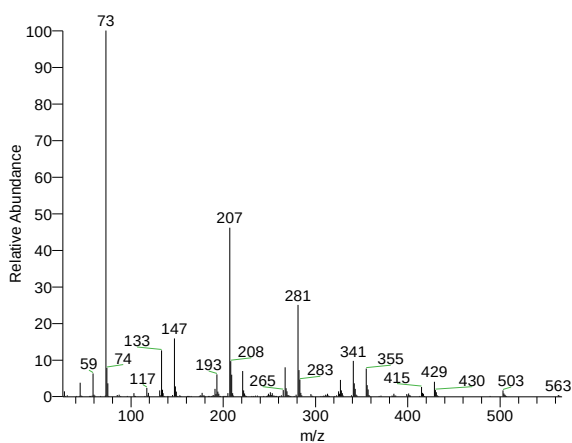
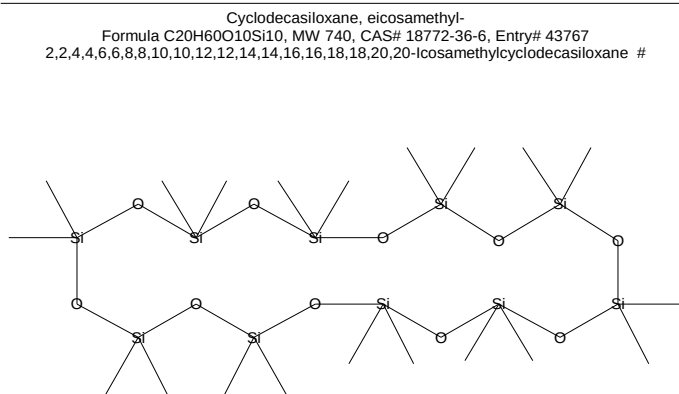
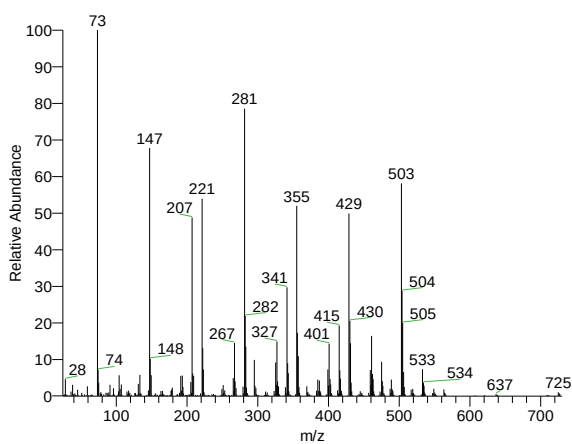
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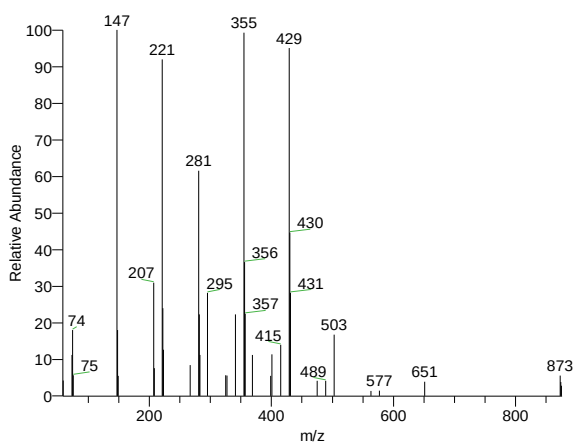
Compound Structure



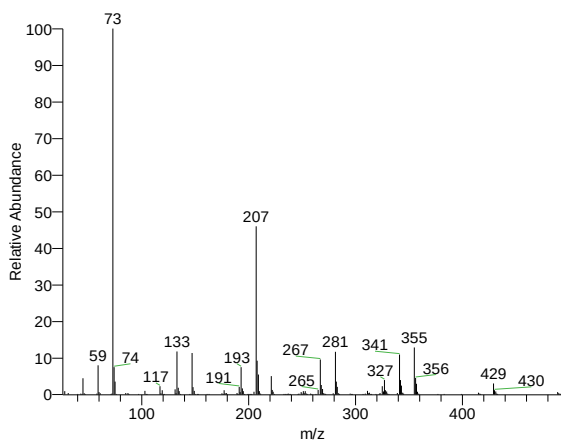
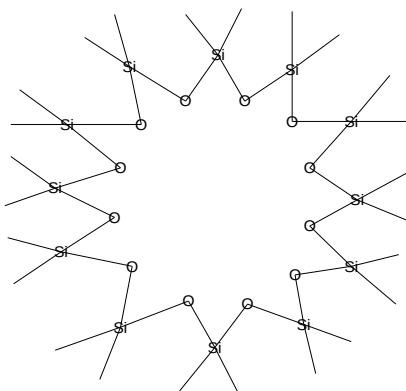
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Hit Spectrum

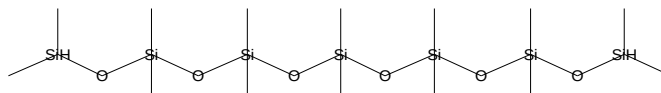
Compound Structure



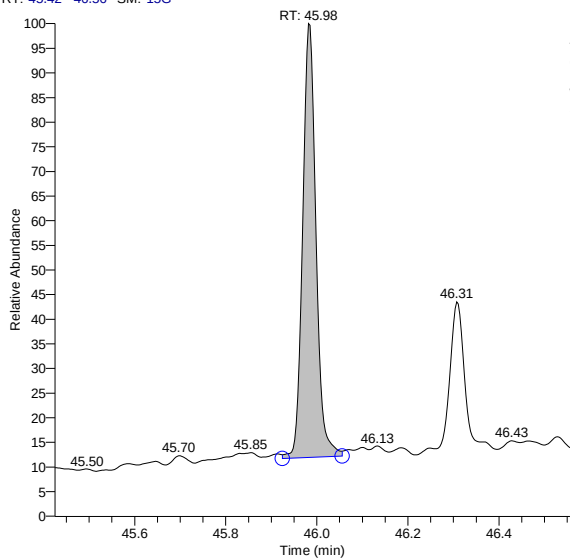
Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

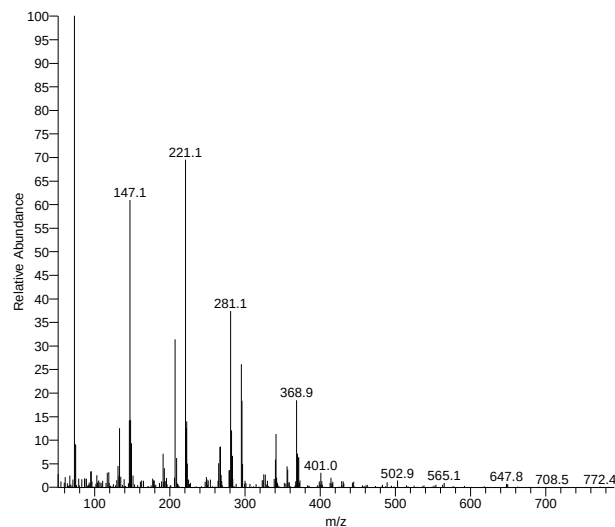


RT: 45.42 - 46.56 SM: 15G



NL:
1.84E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #11923 RT: 45.98 AV: 1 RF: 6.00, 3 NL: 3.93E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Heptasiloxane, hexadecamethyl-	3269744.48	41.68	613	774	mainlib

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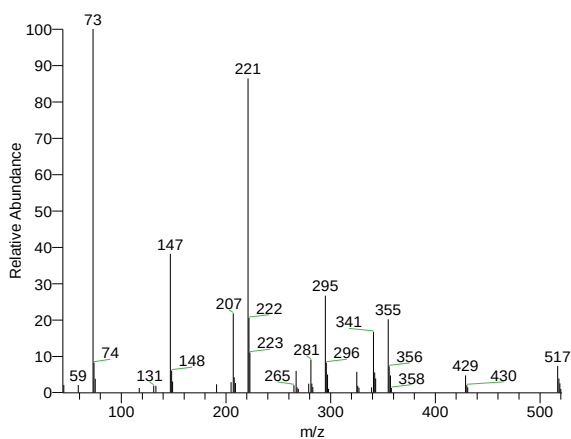
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ANALYTICAL CHEMISTRY DIVISION

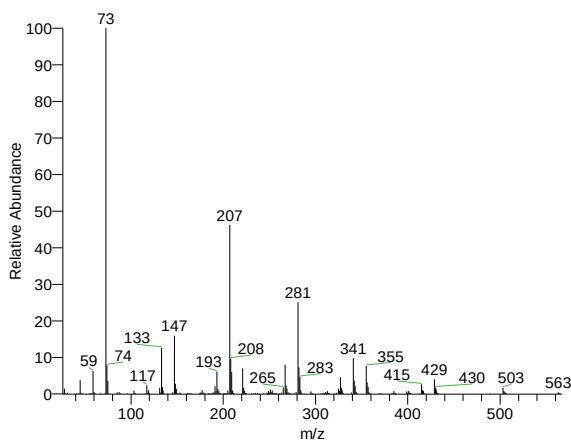
RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3269744.48	27.76	601	655	mainlib
45.98	Pentasiloxane, dodecamethyl-	3269744.48	6.22	559	659	mainlib
45.98	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3269744.48	5.50	556	666	mainlib
45.98	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3269744.48	4.43	551	640	mainlib

Hit Spectrum

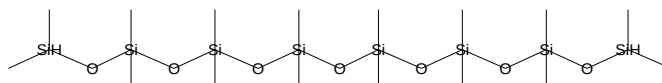
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



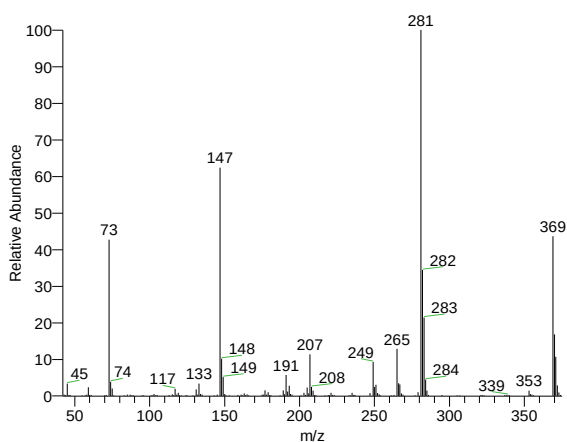
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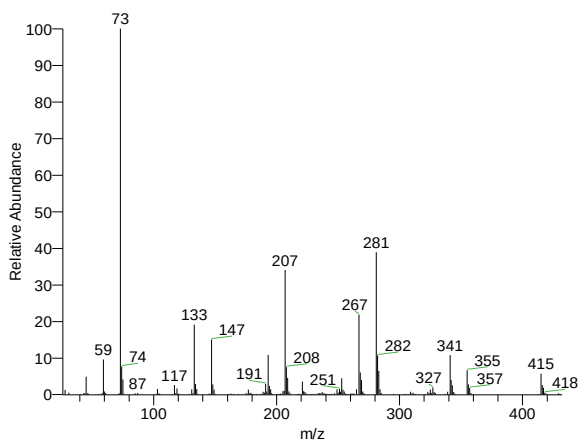
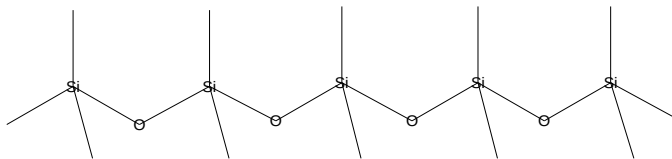
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

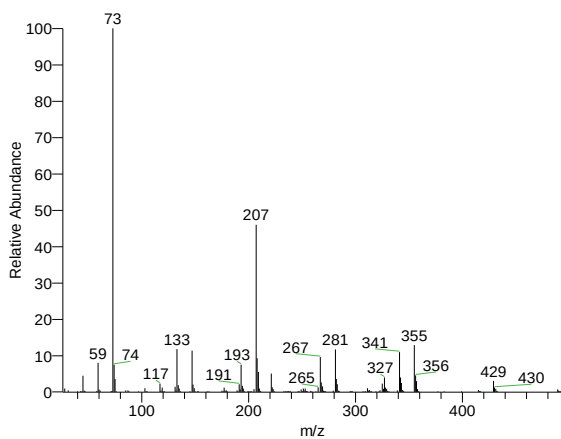
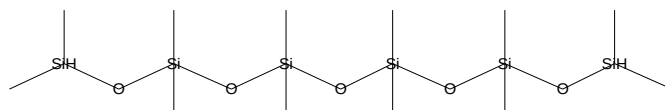
Compound Structure



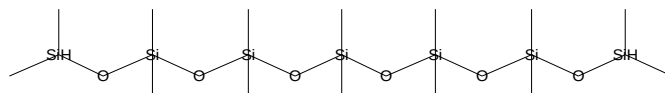
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



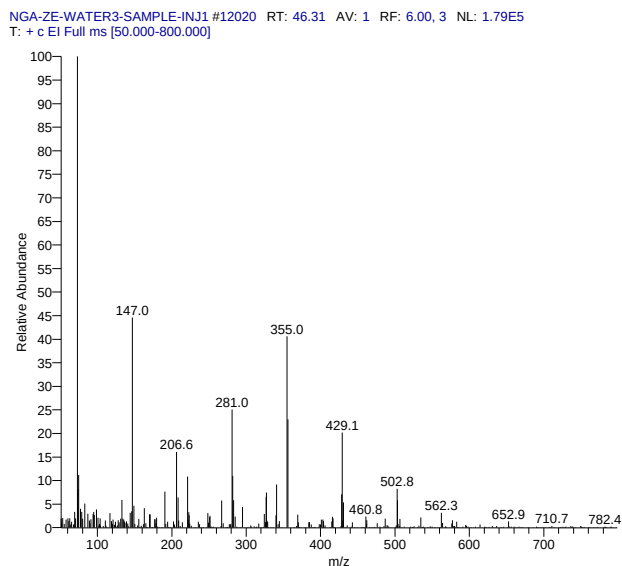
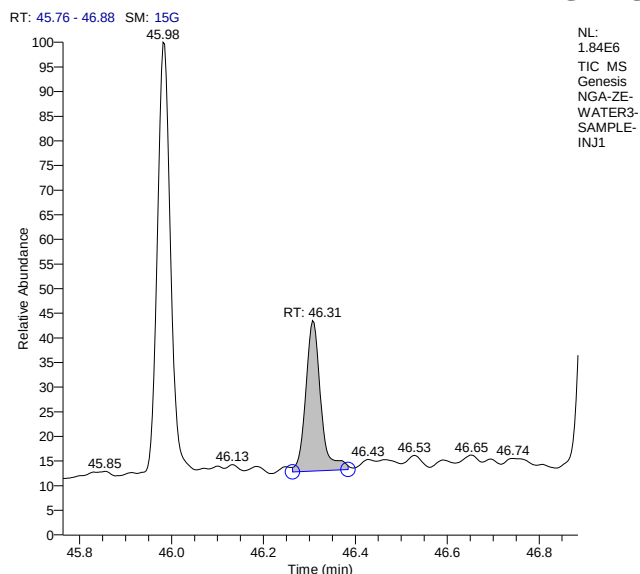
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

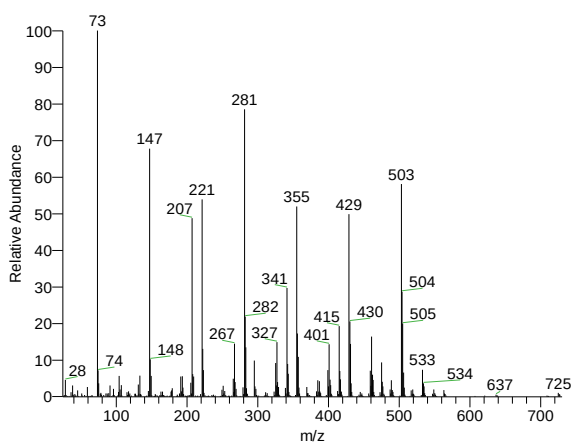


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ANALYTICAL CHEMISTRY DIVISION



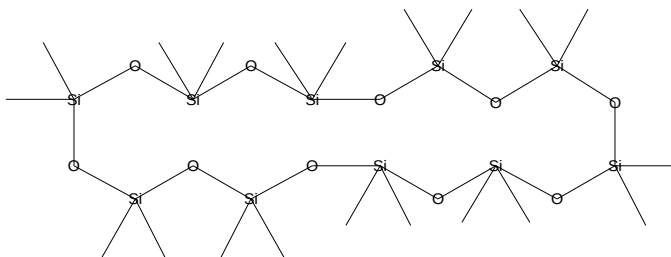
RT	Compound Name	Area	Probability	SI	RSI	Library
46.31	Cyclodecasiloxane, eicosamethyl-	1269380.76	42.10	564	620	mainlib
46.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1269380.76	30.57	555	655	mainlib
46.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1269380.76	7.67	520	661	mainlib
46.31	Tetracosamethyl-cyclododecasiloxane	1269380.76	6.78	517	708	mainlib
46.31	Cyclooctasiloxane, hexadecamethyl-	1269380.76	4.10	502	670	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



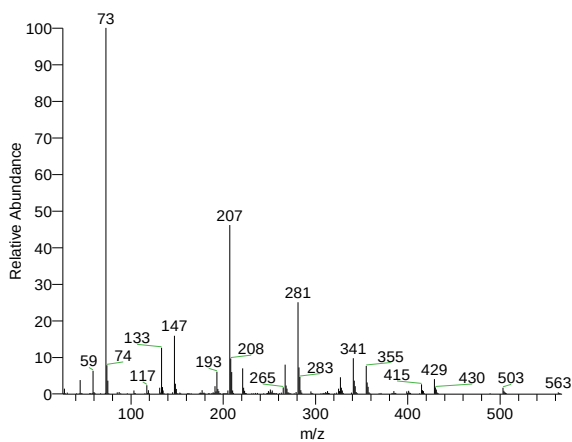
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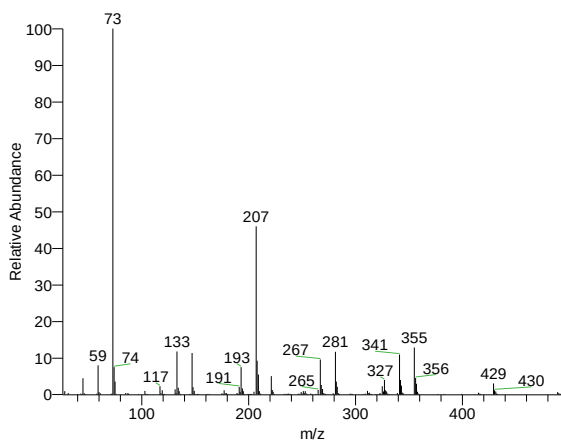
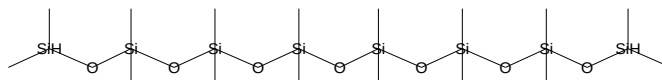
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

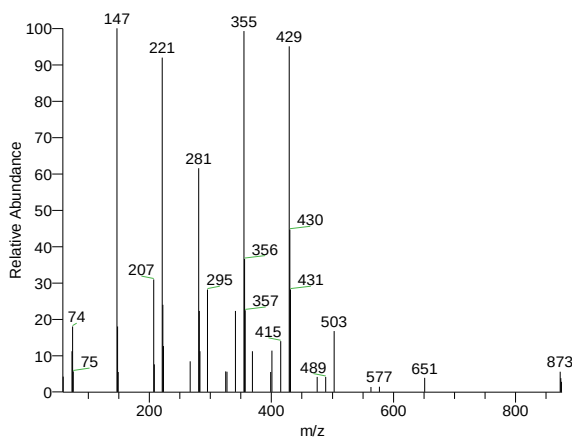
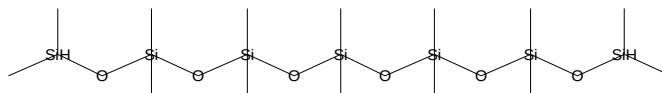
Compound Structure



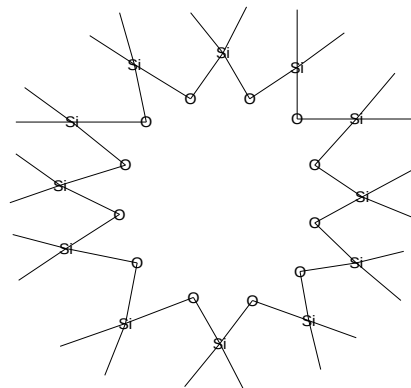
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



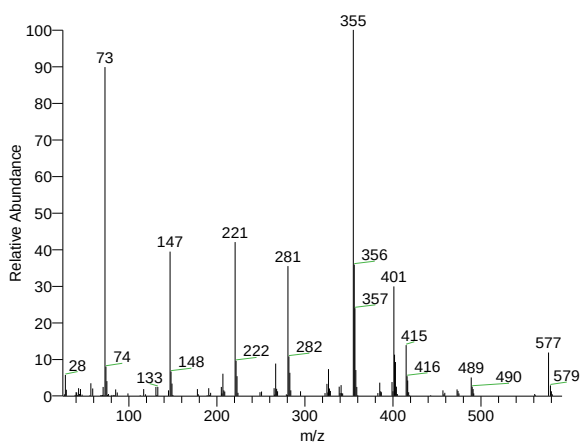
Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



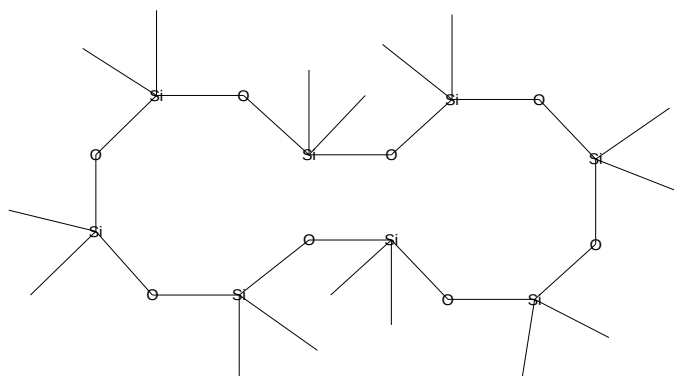
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Hit Spectrum

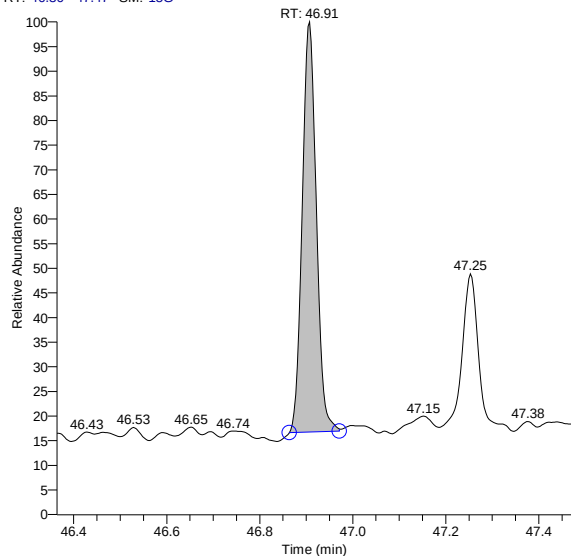
Compound Structure



Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane

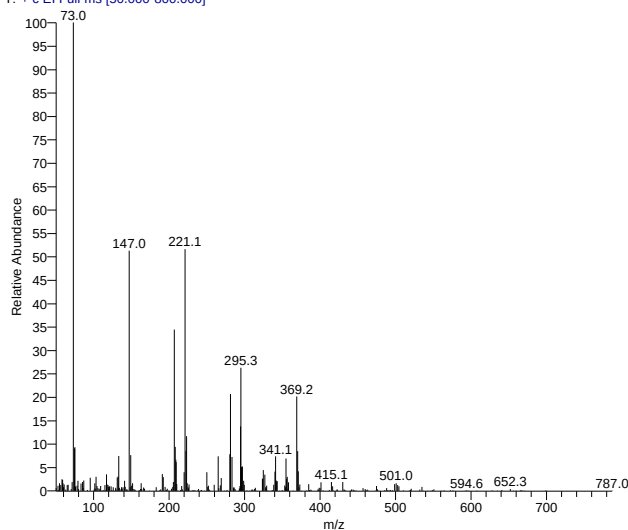


RT: 46.36 - 47.47 SM: 15G



NL:
1.68E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #12199 RT: 46.91 AV: 1 RF: 6.00, 3 NL: 3.52E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
46.91	Heptasiloxane, hexadecamethyl-	2943229.77	57.13	568	741	mainlib
46.91	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2943229.77	22.58	546	602	mainlib
46.91	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2943229.77	6.52	518	612	mainlib
46.91	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	2943229.77	1.95	492	543	mainlib
46.91	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2943229.77	1.53	486	575	mainlib

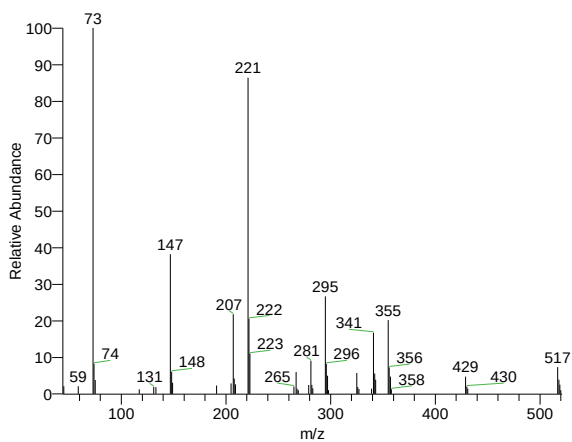
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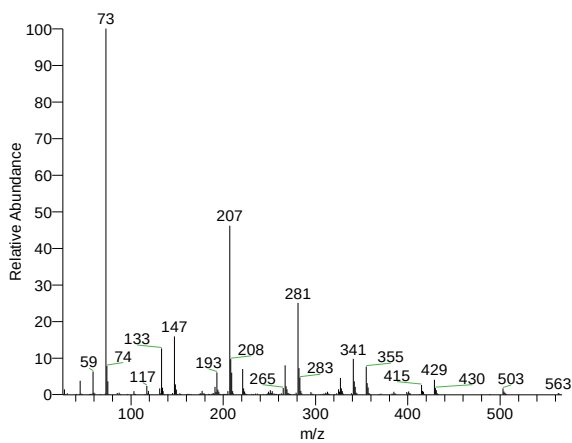
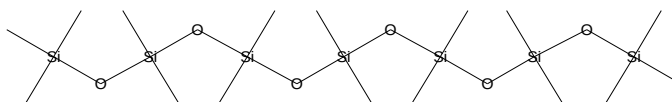
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

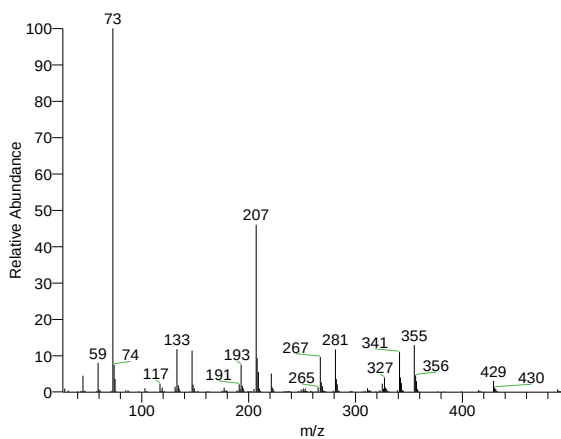
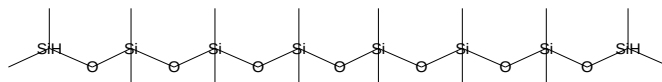
Compound Structure



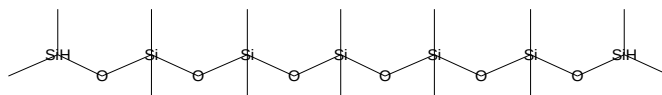
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



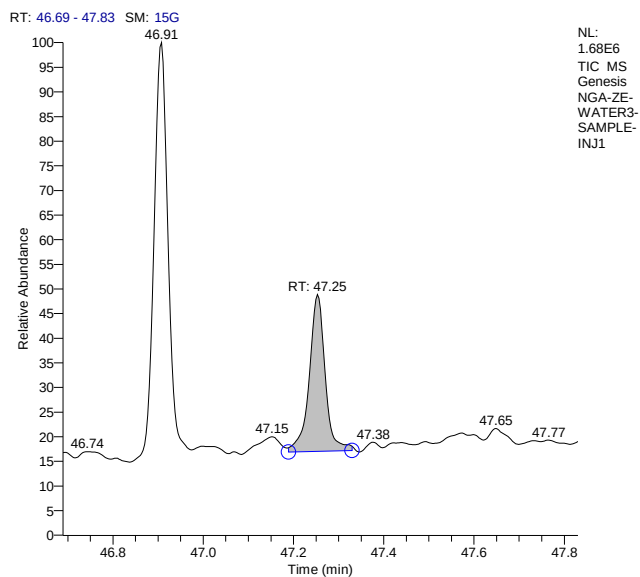
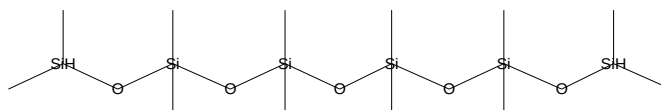
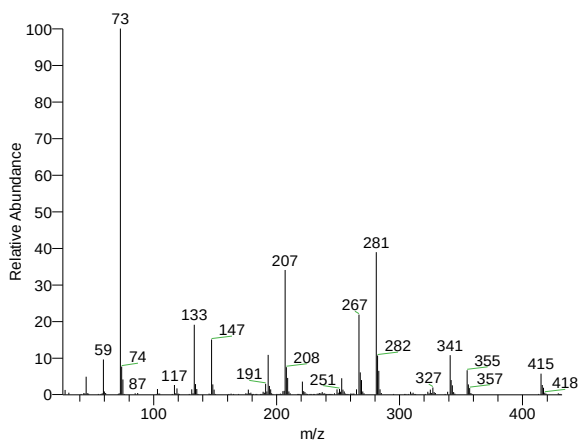
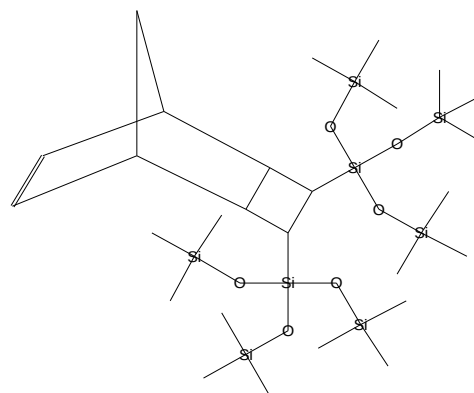
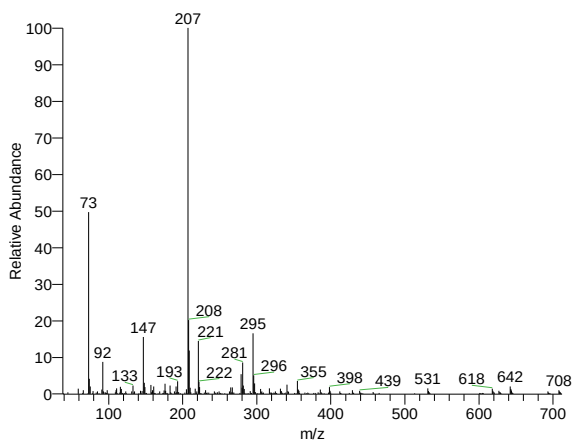
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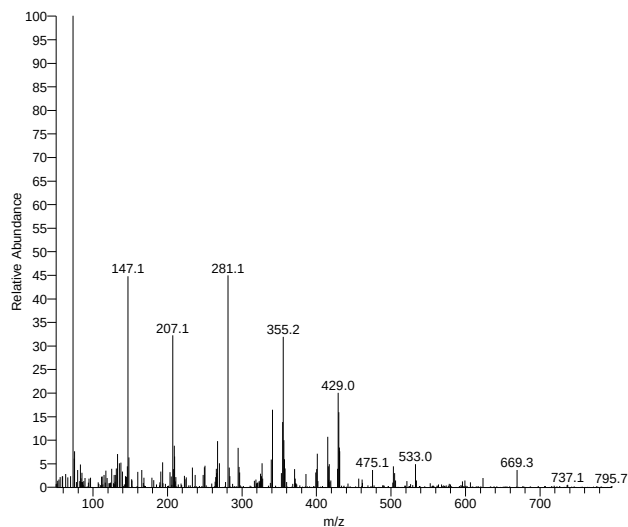
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure



NGA-ZE-WATER3-SAMPLE-INJ1 #12302 RT: 47.25 AV: 1 RF: 6.00, 3 NL: 1.34E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
47.25	Cyclodecasiloxane, eicosamethyl-	1313065.02	43.84	564	625	mainlib

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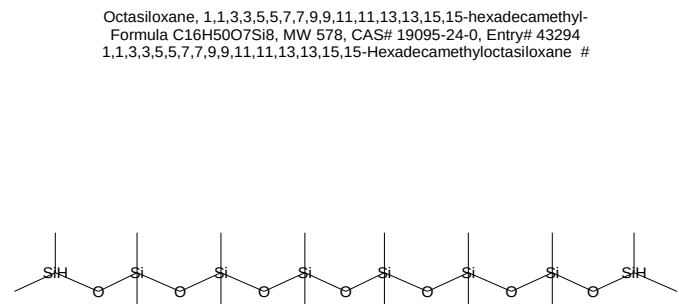
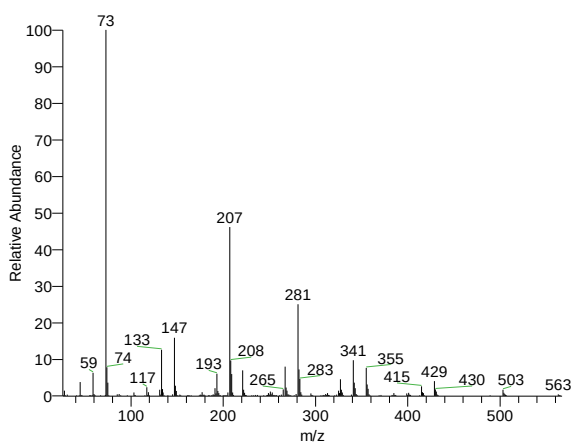
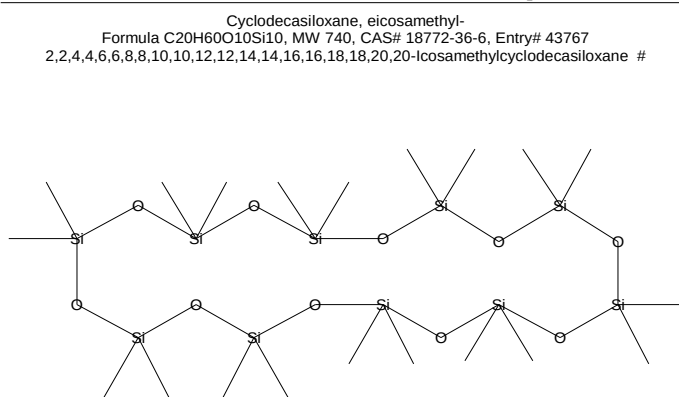
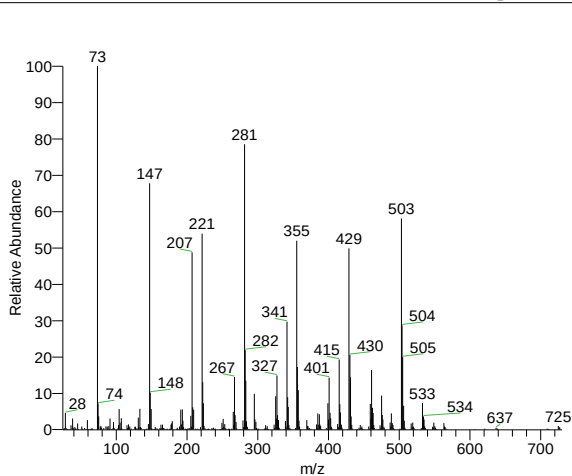
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
47.25	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1313065.02	31.83	555	657	mainlib
47.25	Cyclononasiloxane, octadecamethyl-	1313065.02	7.99	520	652	mainlib
47.25	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1313065.02	6.12	513	651	mainlib
47.25	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1313065.02	3.52	497	612	mainlib

Hit Spectrum

Compound Structure



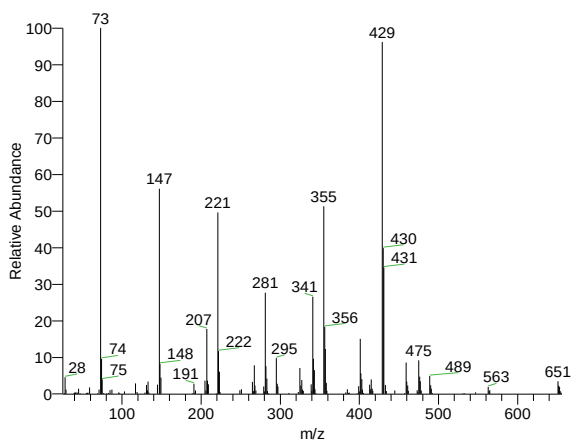
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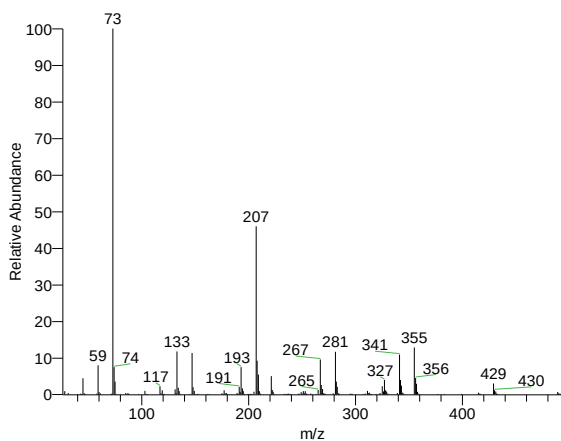
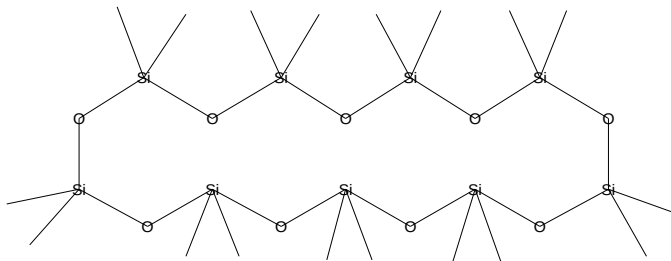
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

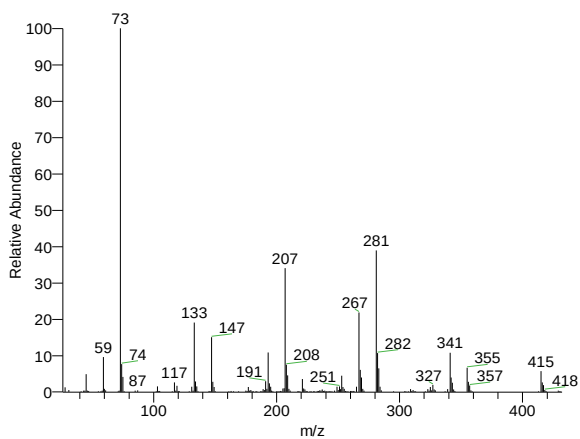
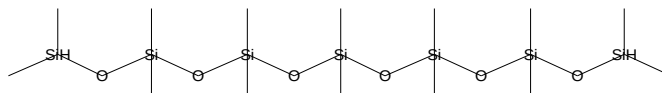
Compound Structure



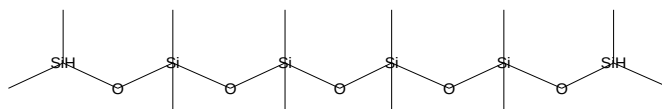
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

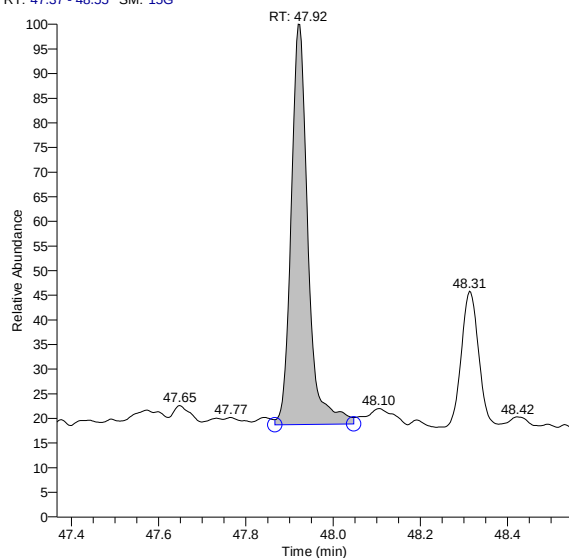


Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



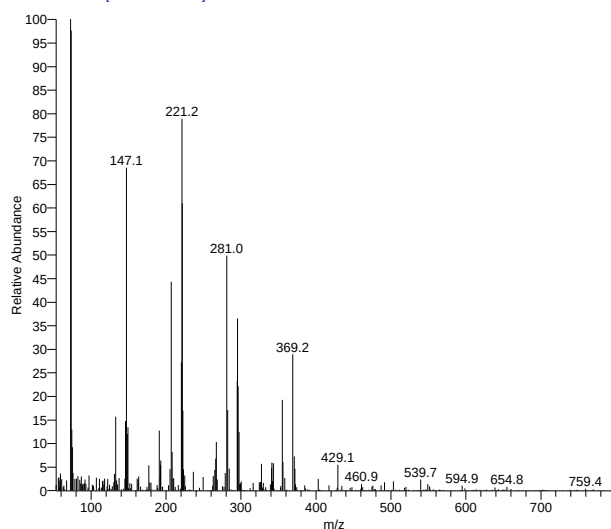
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RT: 47.37 - 48.55 SM: 15G



NL:
1.61E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

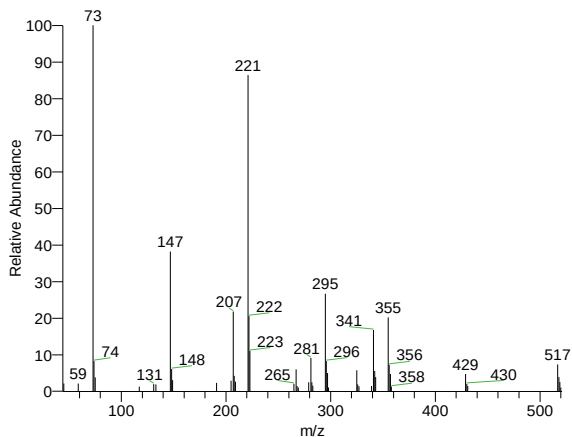
NGA-ZE-WATER3-SAMPLE-INJ1 #12501 RT: 47.92 AV: 1 RF: 6.00, 3 NL: 2.01E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
47.92	Heptasiloxane, hexadecamethyl-	3498245.55	78.41	631	781	mainlib
47.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3498245.55	6.04	533	591	mainlib
47.92	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	3498245.55	4.26	523	580	mainlib
47.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3498245.55	3.44	518	603	mainlib
47.92	Hexasiloxane, tetradecamethyl-	3498245.55	0.93	487	713	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



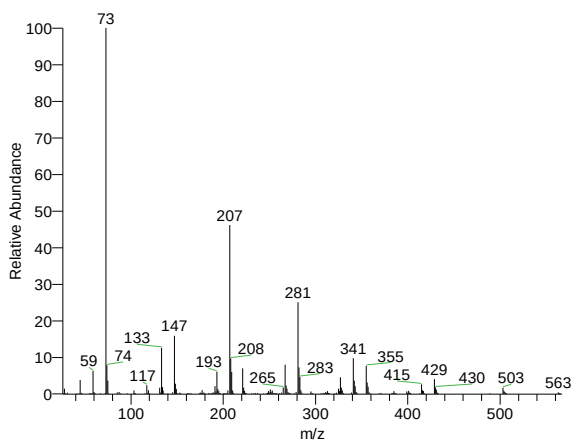
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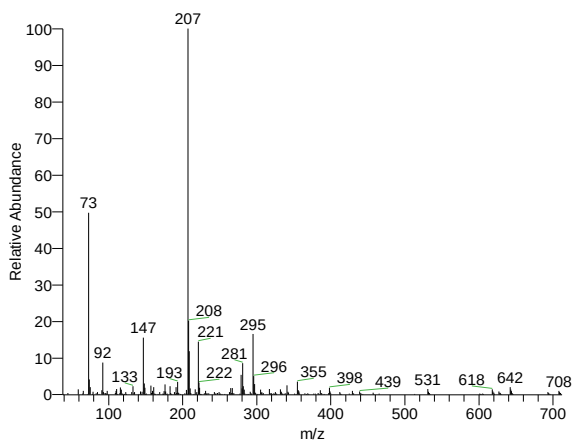
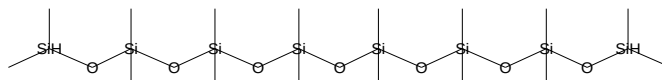
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

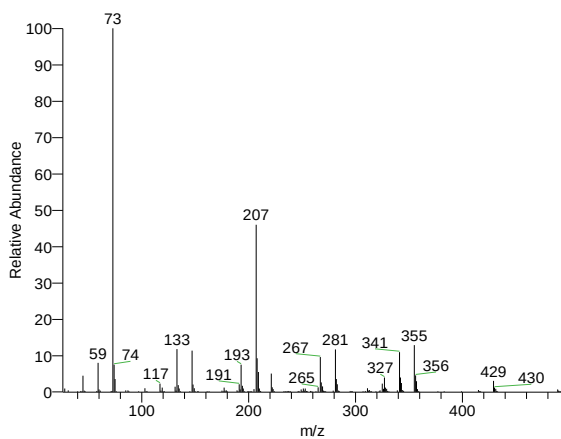
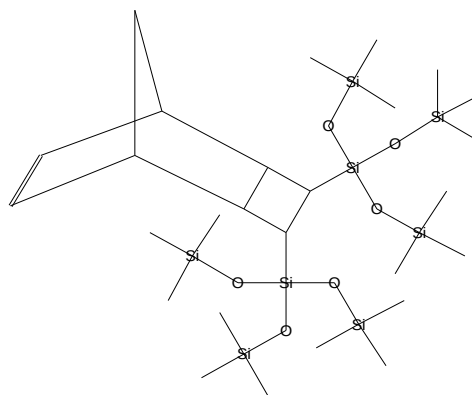
Compound Structure



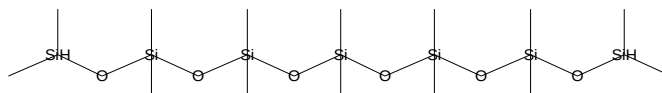
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:28JSGSCAWLXCNS-UHFFFAOYSA-N



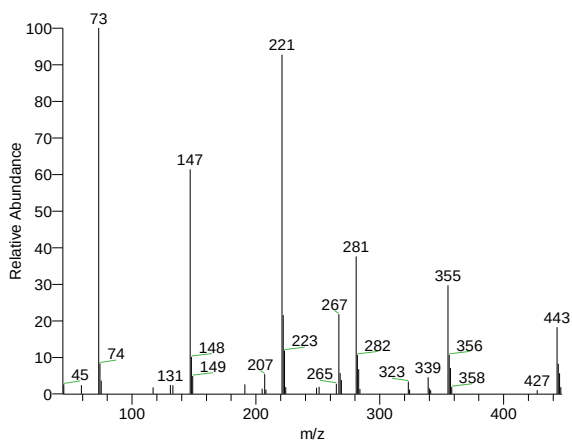
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



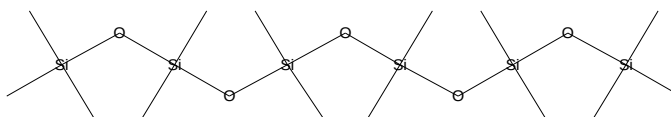
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

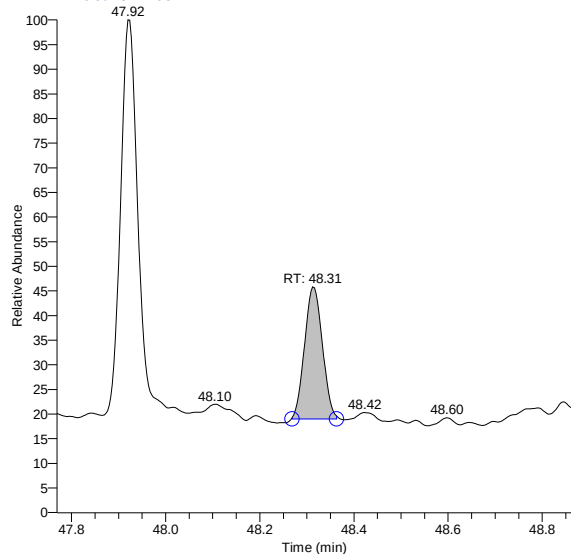
Compound Structure



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane

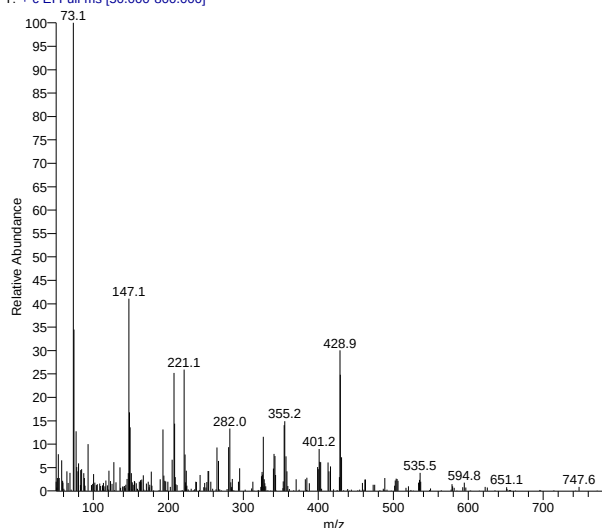


RT: 47.77 - 48.86 SM: 15G



NL:
1.61E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #12618 RT: 48.31 AV: 1 RF: 6.00, 3 NL: 1.04E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
48.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	1130508.20	25.03	503	597	mainlib
48.31	Cyclononasiloxane, octadecamethyl-	1130508.20	22.12	500	627	mainlib
48.31	Cyclodecasiloxane, eicosamethyl-	1130508.20	16.94	493	523	mainlib
48.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	1130508.20	10.60	479	610	mainlib
48.31	Cyclohexasiloxane, dodecamethyl-	1130508.20	2.02	423	550	mainlib

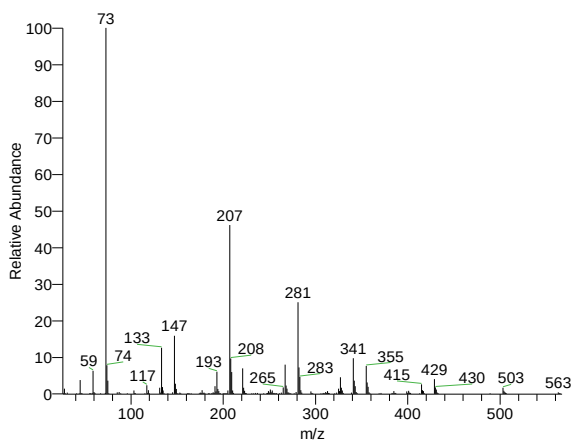
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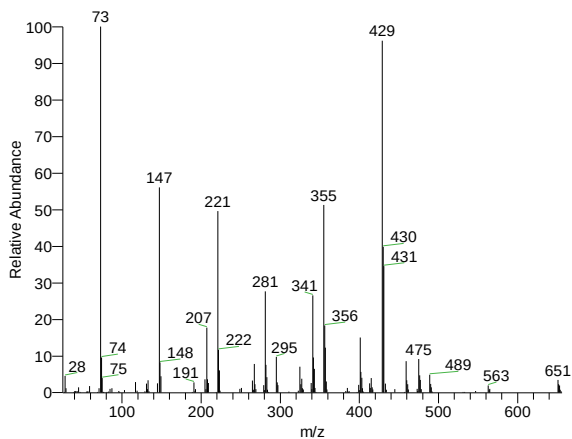
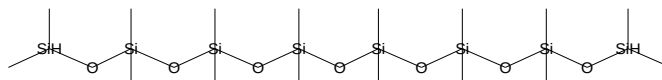
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

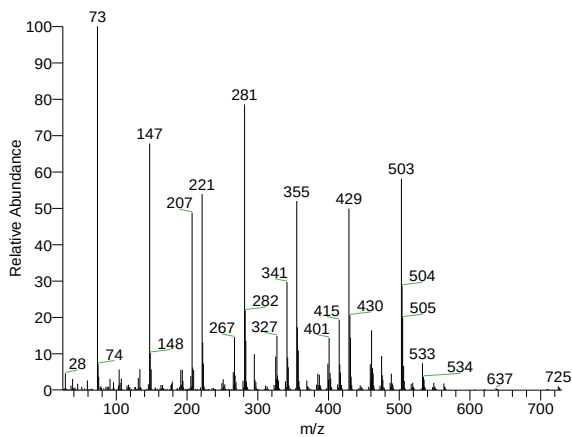
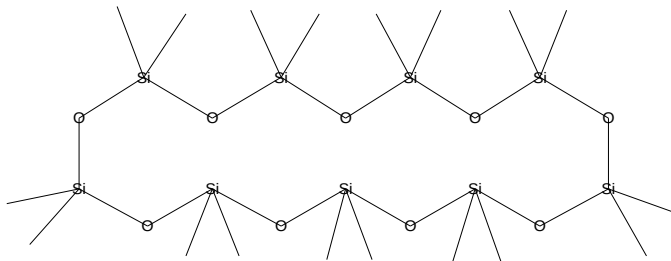
Compound Structure



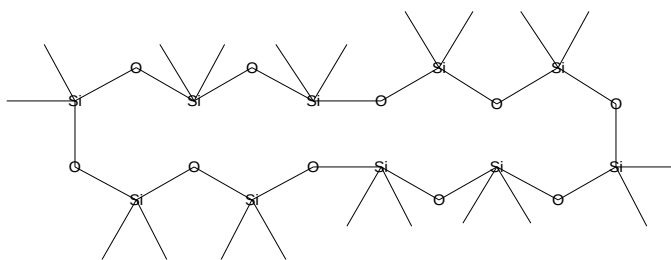
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



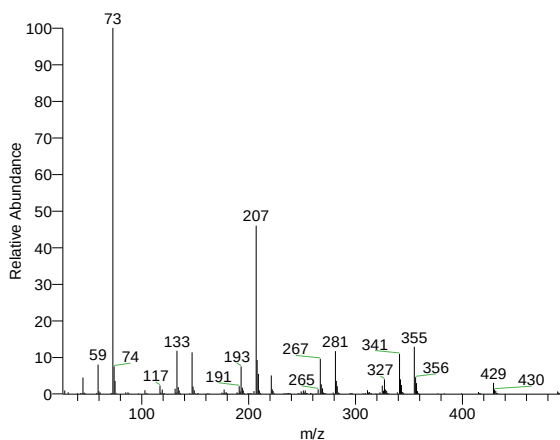
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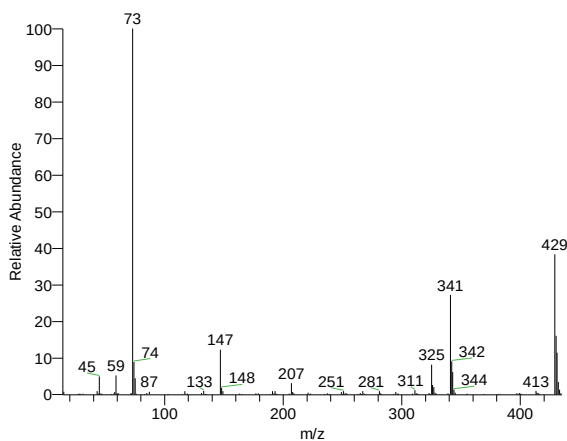
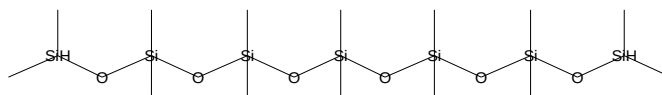
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

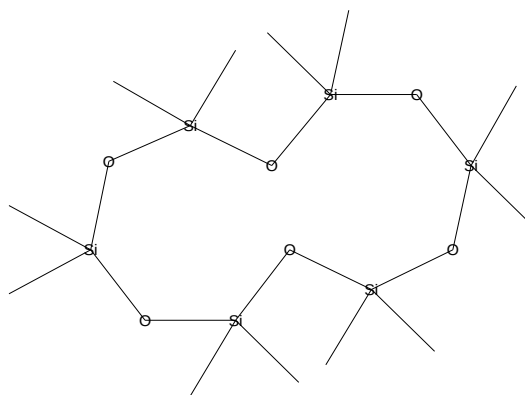
Compound Structure



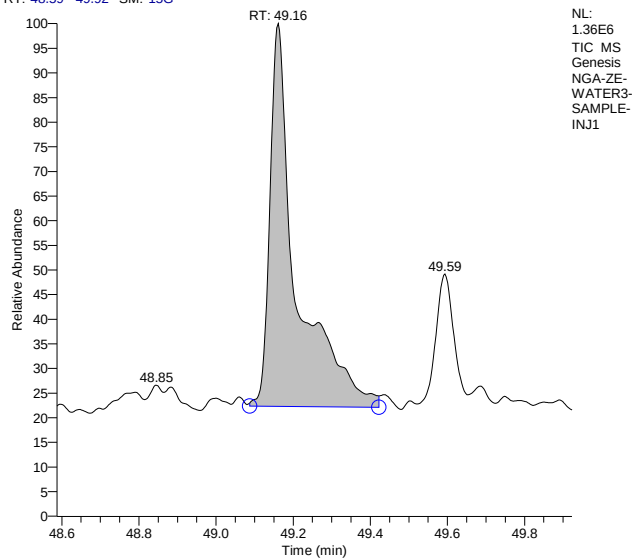
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclohexasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₆Si₆, MW 444, CAS# 540-97-6, Entry# 44297
Dodecamethylcyclohexasiloxane

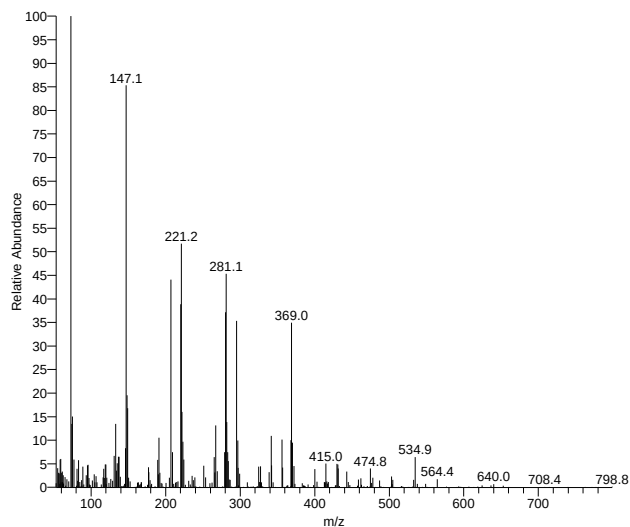


RT: 48.59 - 49.92 SM: 15G



NL:
1.36E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #12871 RT: 49.16 AV: 1 RF: 6.00, 3 NL: 1.56E5
T: + c EI Full ms [50.000-800.000]



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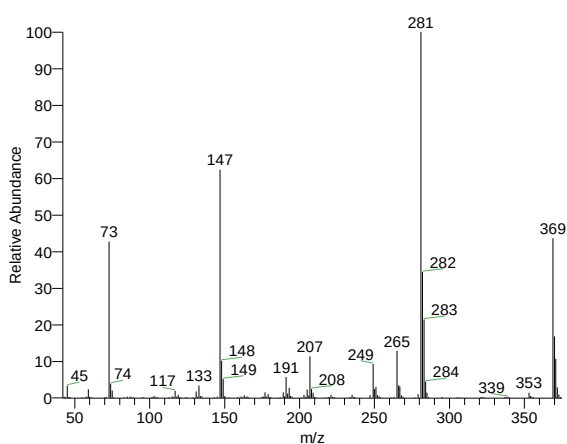
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

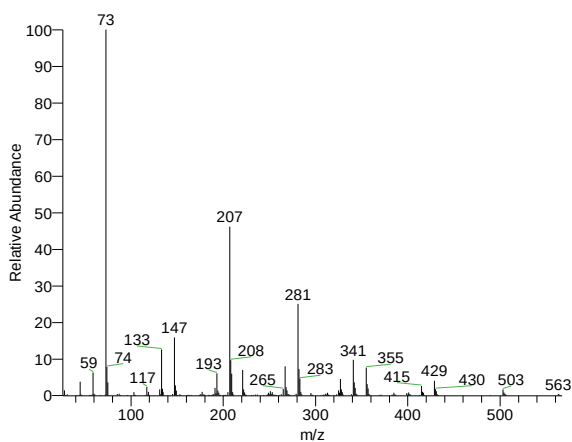
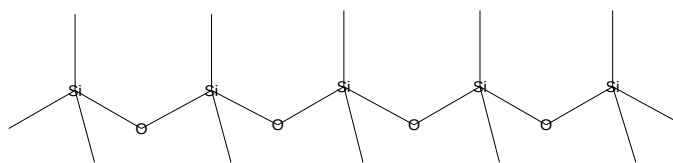
RT	Compound Name	Area	Probability	SI	RSI	Library
49.16	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	5037961.54	17.62	524	601	mainlib
49.16	Pentasiloxane, dodecamethyl-	5037961.54	17.62	524	629	mainlib
49.16	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	5037961.54	12.79	515	668	mainlib
49.16	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	5037961.54	9.54	507	626	mainlib
49.16	Cyclodecasiloxane, eicosamethyl-	5037961.54	8.80	505	536	mainlib

Hit Spectrum

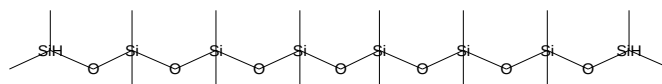
Compound Structure



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



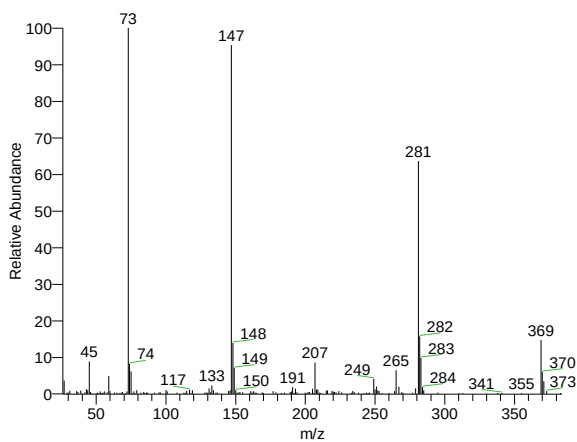
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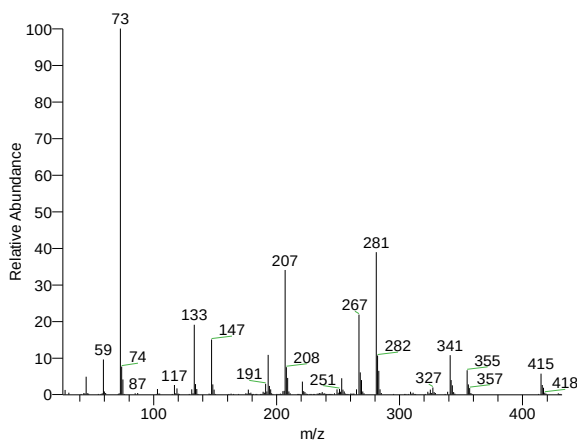
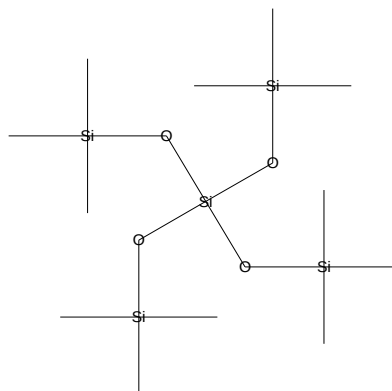
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

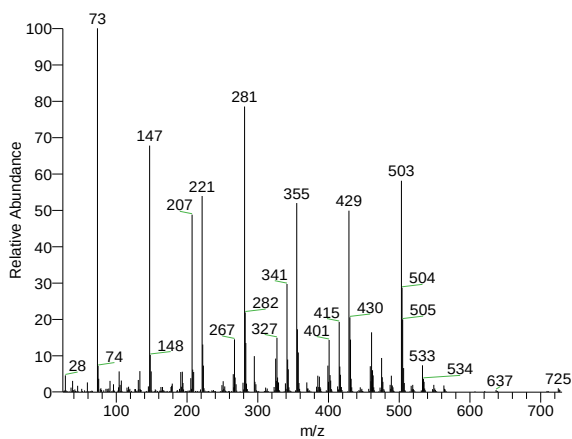
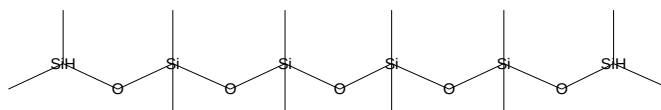
Compound Structure



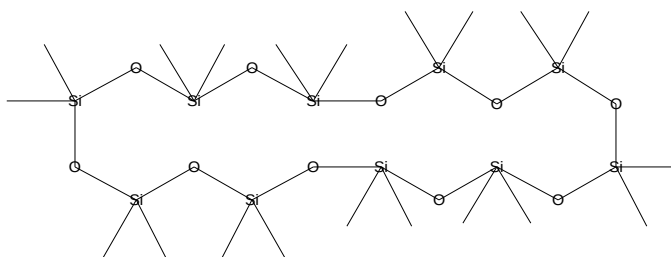
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

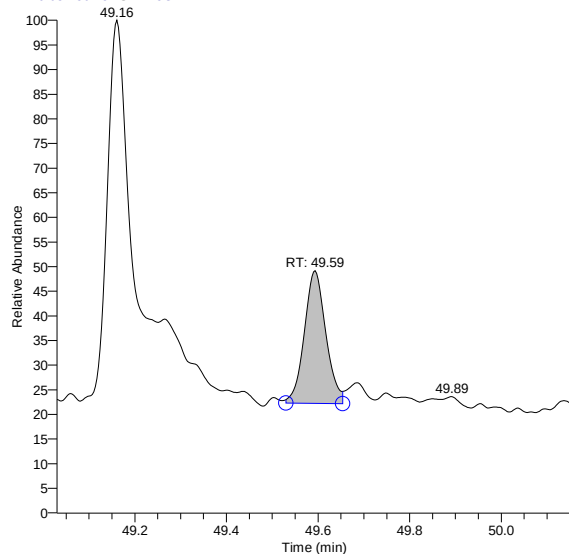


Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



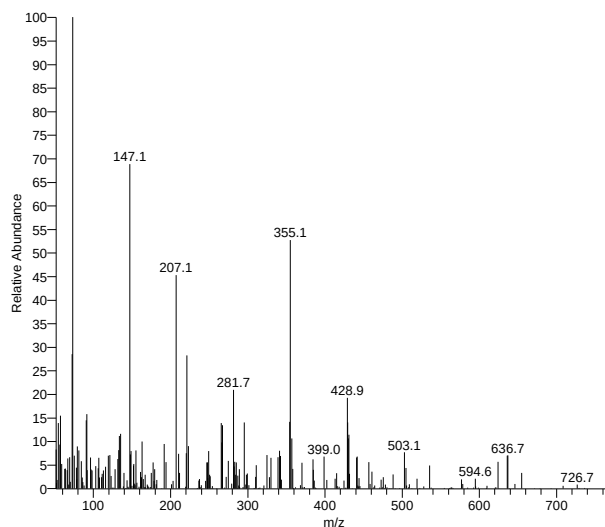
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RT: 49.03 - 50.15 SM: 15G



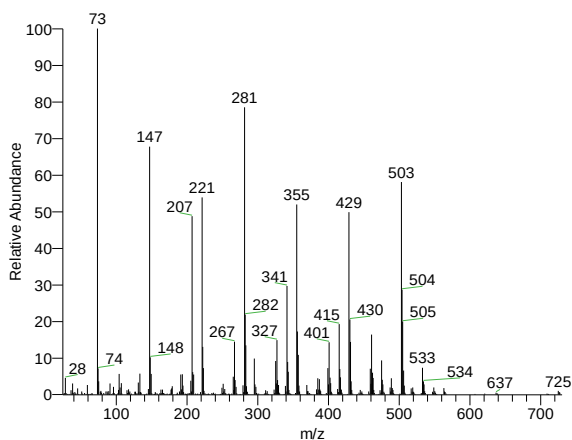
NL:
1.36E6
TIC: MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #13000 RT: 49.59 AV: 1 RF: 6.00, 3 NL: 6.85E4
T: + c EI Full ms [50.000-800.000]



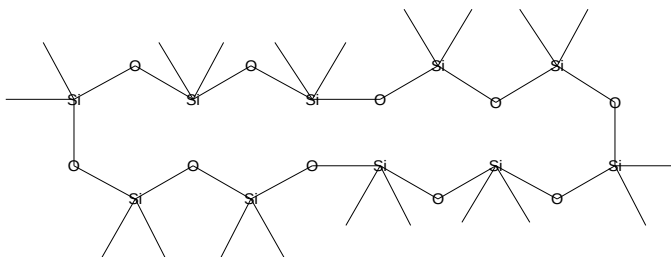
RT	Compound Name	Area	Probability	SI	RSI	Library
49.59	Cyclodecasiloxane, eicosamethyl-	1193521.09	36.09	453	500	mainlib
49.59	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1193521.09	21.87	438	556	mainlib
49.59	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1193521.09	7.33	414	553	mainlib
49.59	Cyclononasiloxane, octadecamethyl-	1193521.09	4.73	401	571	mainlib
49.59	Tetracosamethyl-cyclododecasiloxane	1193521.09	2.29	382	683	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



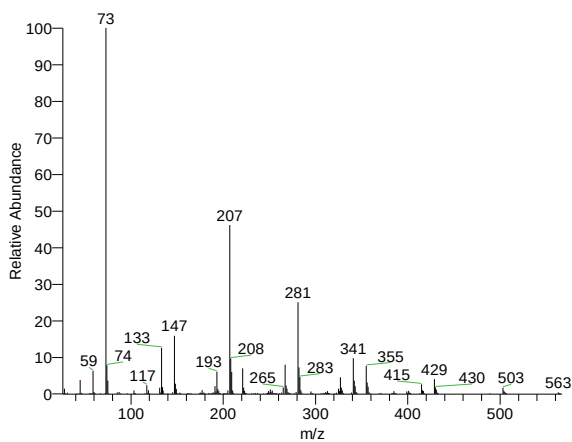
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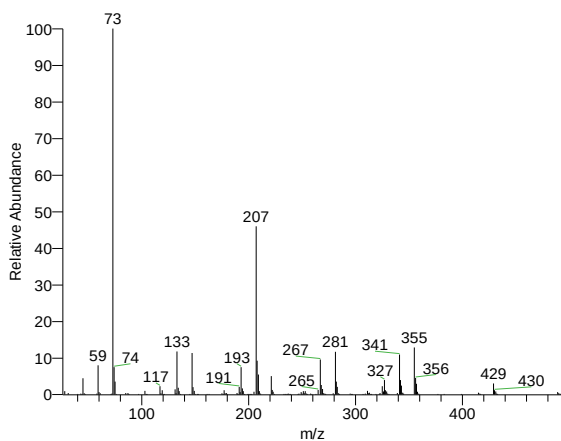
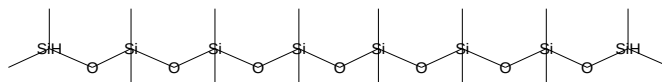
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

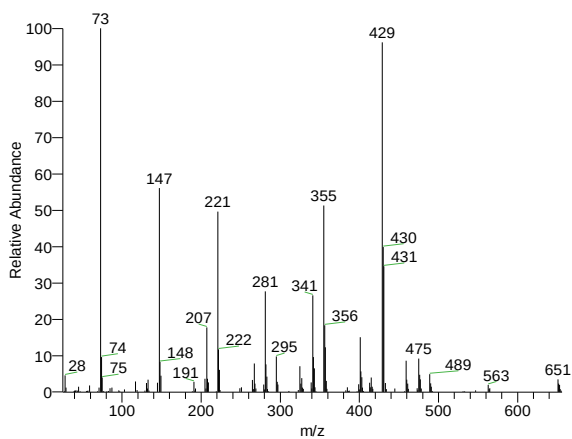
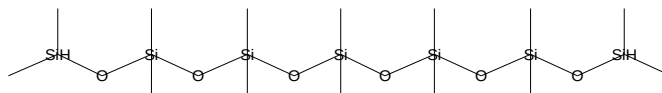
Compound Structure



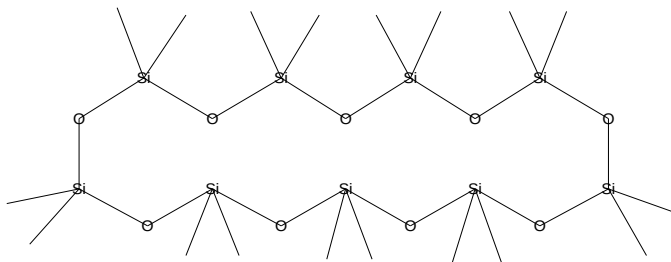
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



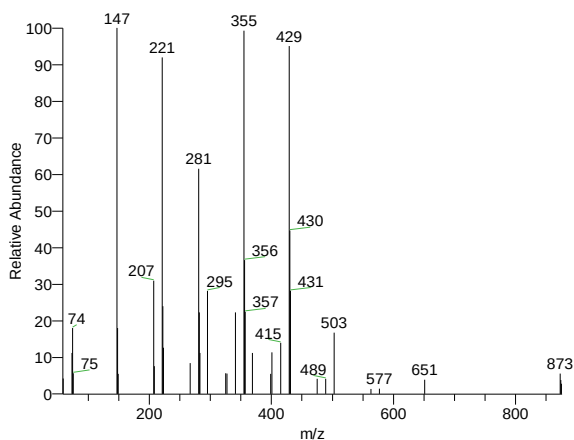
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



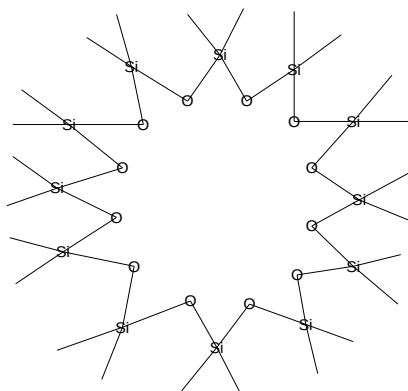
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Hit Spectrum

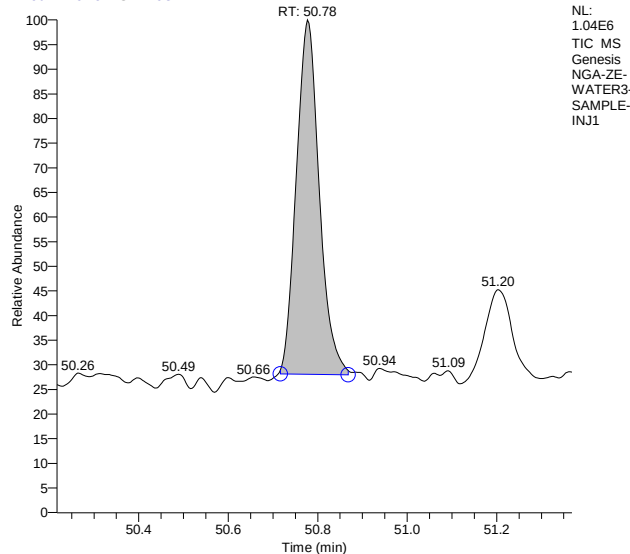
Compound Structure



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752

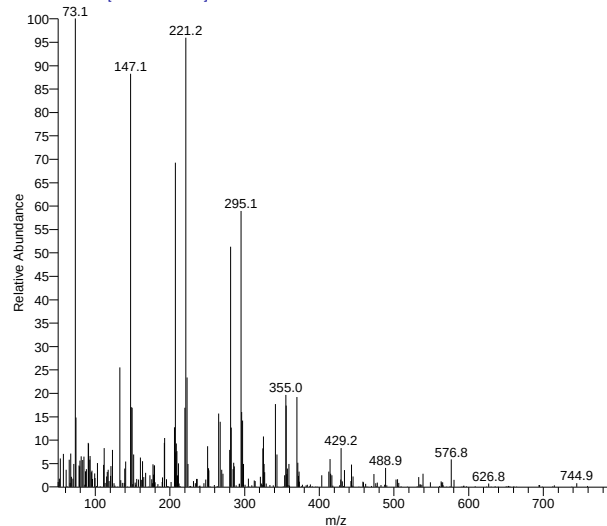


RT: 50.22 - 51.37 SM: 15G



NL:
1.04E6
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #13353 RT: 50.78 AV: 1 RF: 6.00, 3 NL: 8.70E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
50.78	Heptasiloxane, hexadecamethyl-	2655927.08	66.63	561	756	mainlib
50.78	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2655927.08	14.69	518	614	mainlib
50.78	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2655927.08	4.32	491	605	mainlib
50.78	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	2655927.08	3.31	484	550	mainlib
50.78	Cyclododecasiloxane, eicosamethyl-	2655927.08	1.30	462	498	mainlib

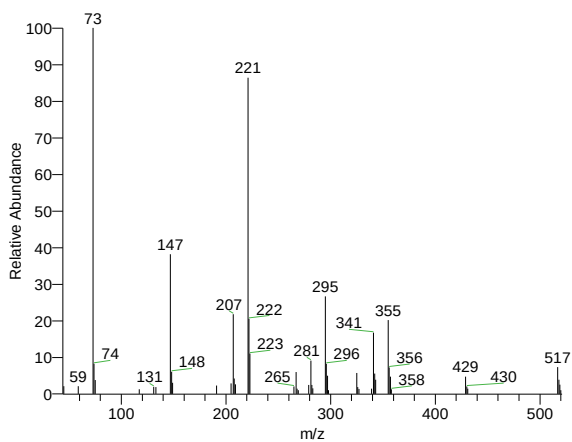
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH

GC-MS/MS QUAL REPORT

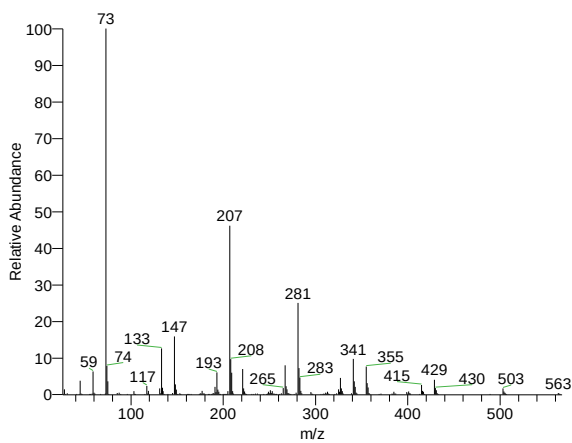
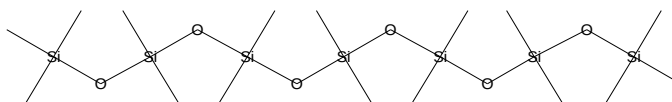
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

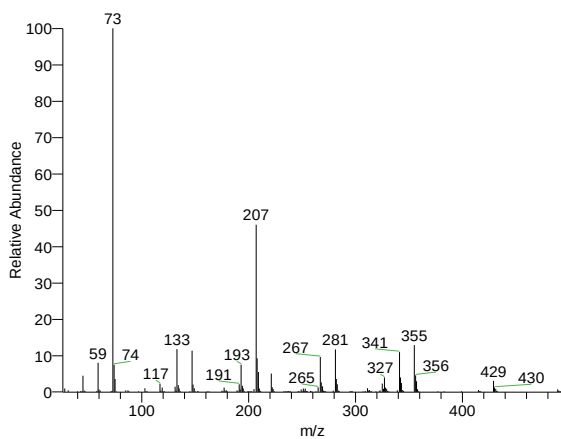
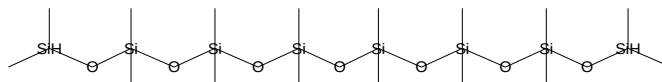
Compound Structure



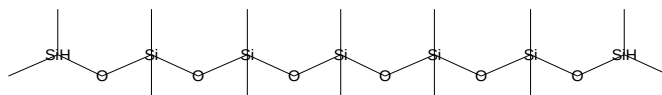
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



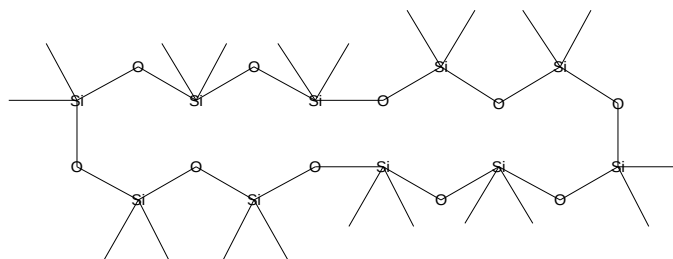
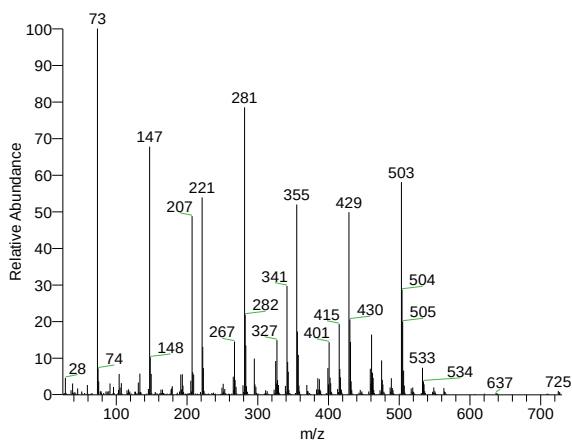
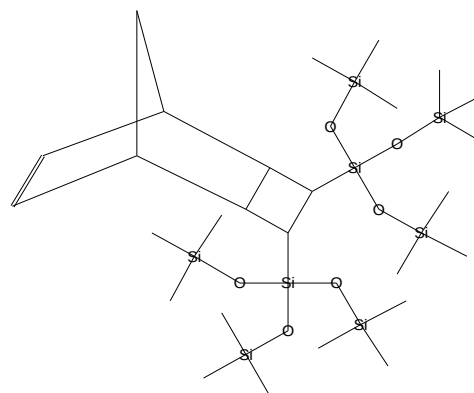
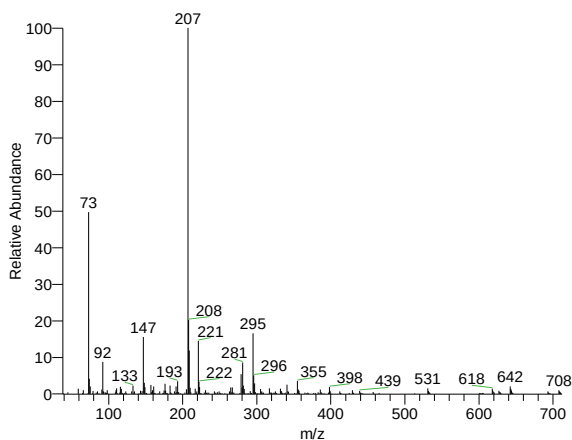
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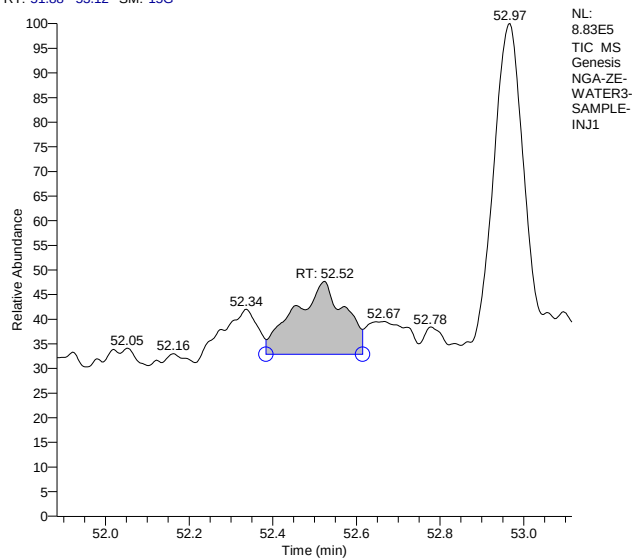
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Hit Spectrum

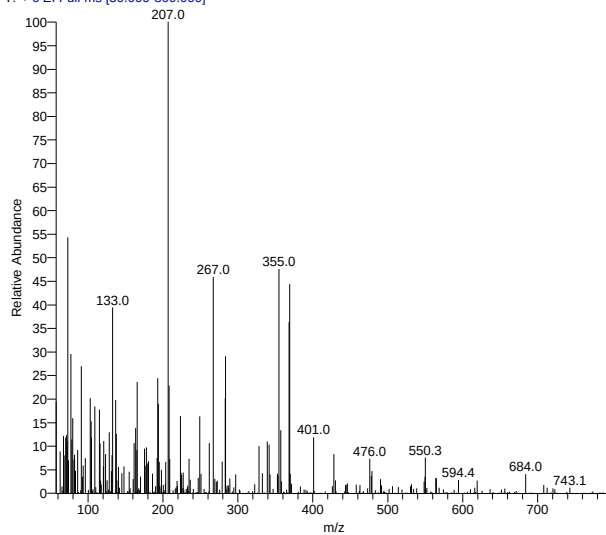
Compound Structure



RT: 51.88 - 53.12 SM: 15G



NGA-ZE-WATER3-SAMPLE-INJ1 #13874 RT: 52.52 AV: 1 RF: 6.00, 3 NL: 3.08E4
T: + c EI Full ms [50.000-800.000]



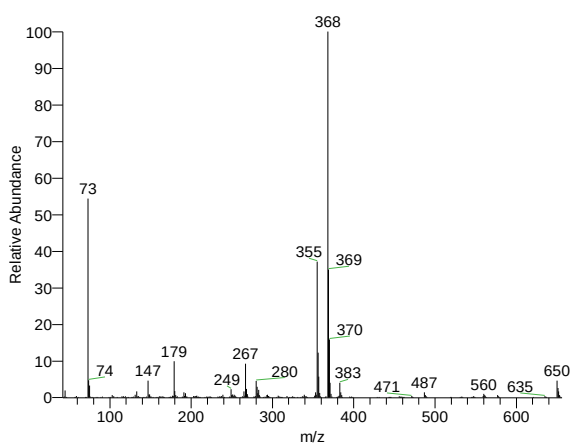
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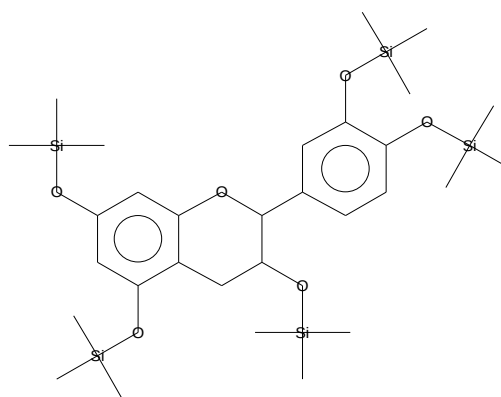
RT	Compound Name	Area	Probability	SI	RSI	Library
52.52	[(2-{3,4-Bis[(trimethylsilyl)oxy]phenyl}-3,5-bis[(trimethylsilyl)oxy]-3,4-dihydro-2H-chromen-7-yl)oxy](trimethyl)silane	1092368.73	4.71	374	449	mainlib
52.52	(E)-1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenylprop-2-en-1-one	1092368.73	3.41	365	556	mainlib
52.52	4,8-Ditert-butyl-N,N-diethyl-2,10-dimethyl-12H-dibenzoc[1,3,2]dioxaphosphocin-6-amine	1092368.73	2.68	359	457	mainlib
52.52	Tibolone, trimethylsilyl ether	1092368.73	2.58	358	422	mainlib
52.52	Lysergol, TBDMS derivative	1092368.73	2.18	354	447	mainlib

Hit Spectrum

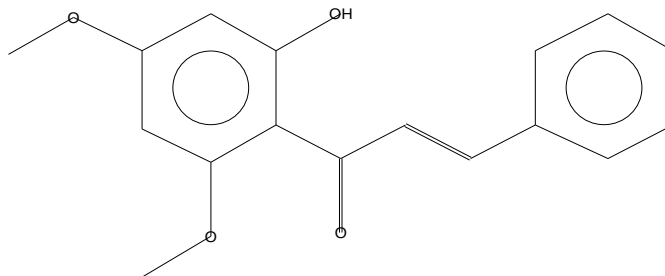
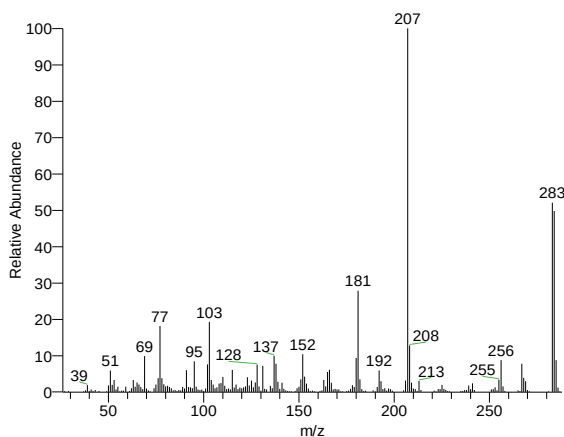


Compound Structure

Formula C30H54O6Si5, MW 650, CAS# NA, Entry# 235642
\$:28QKMSLFRFGOTVEJ-UHFFFAOYSA-N



(E)-1-(2-Hydroxy-4,6-dimethoxyphenyl)-3-phenylprop-2-en-1-one
Formula C17H16O4, MW 284, CAS# 1775-97-9, Entry# 189081
2-Propen-1-one, 1-(2-hydroxy-4,6-dimethoxyphenyl)-3-phenyl-, (E)-



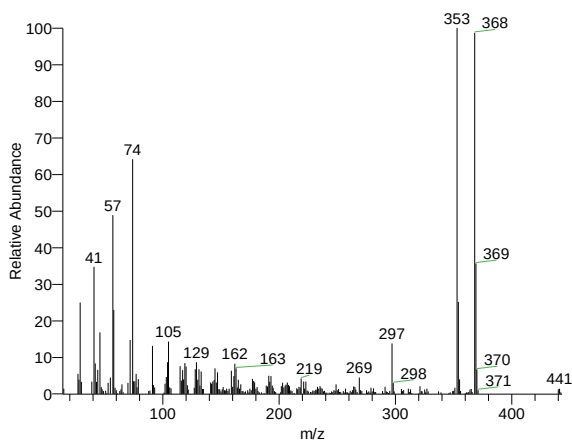
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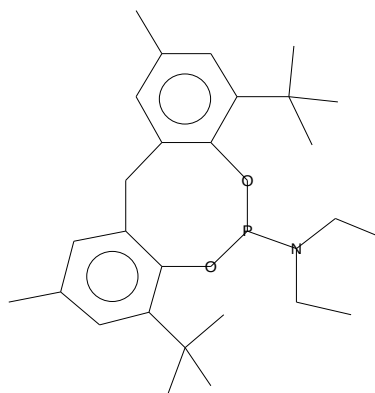
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

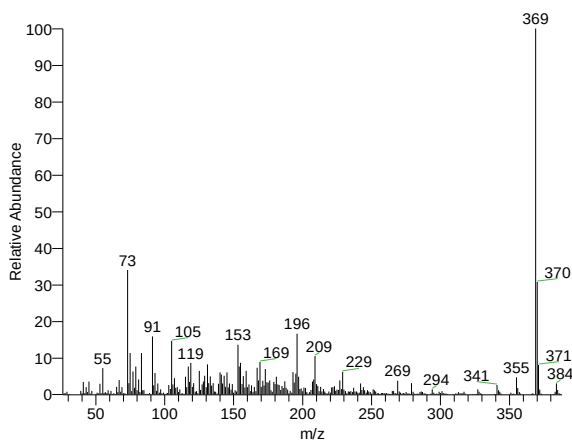
Compound Structure



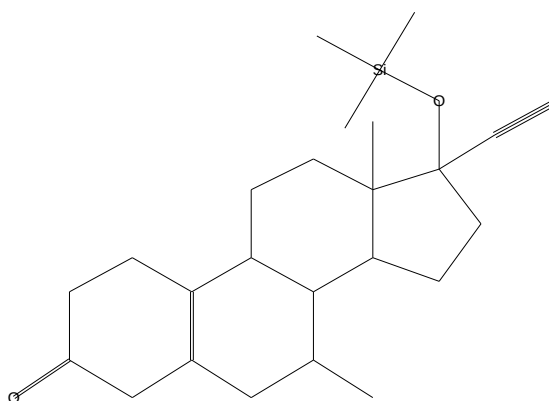
4,8-Ditert-butyl-N,N-diethyl-2,10-dimethyl-12H-dibenzo[d,g][1,3,2]dioxaphosphocin-6-amine
Formula C₂₇H₄₀NO₂P, MW 441, CAS# NA, Entry# 234127
\$:28NRGOJRVWTVSCJH-UHFFFAOYSA-N



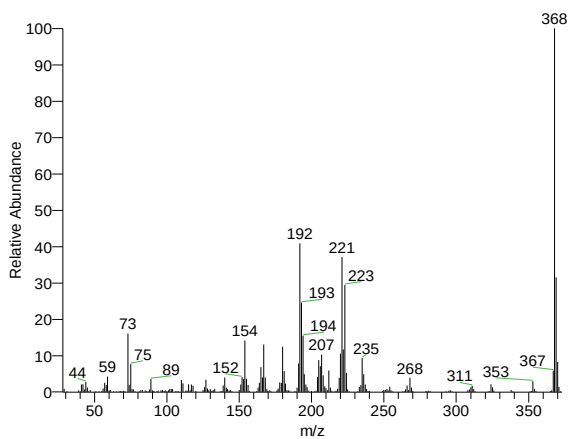
SI 358, RSI 422, mainlib, Entry# 235766, CAS# NA, Tibolone, trimethylsilyl ether



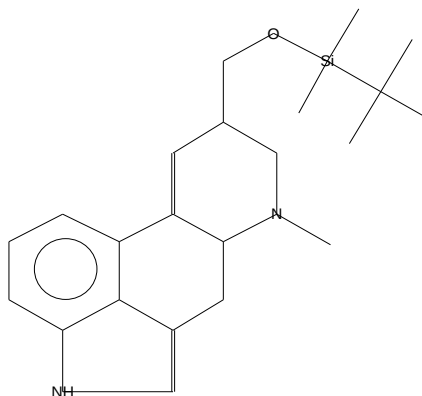
Tibolone, trimethylsilyl ether
Formula C₂₄H₃₆O₂Si, MW 384, CAS# NA, Entry# 235766
\$:28YHYCUPXRLXXQKC-UHFFFAOYSA-N



SI 354, RSI 447, mainlib, Entry# 235676, CAS# NA, Lysergol, TBDMS derivative

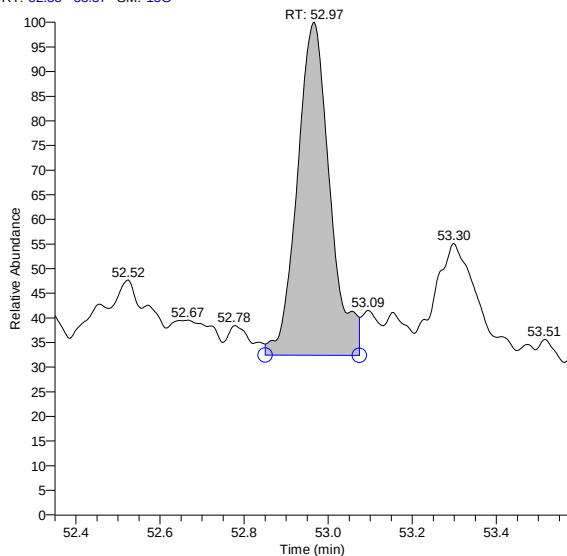


Lysergol, TBDMS derivative
Formula C₂₂H₃₂N₂O₂Si, MW 368, CAS# NA, Entry# 235676
Lysergol-TBDMS Derivative



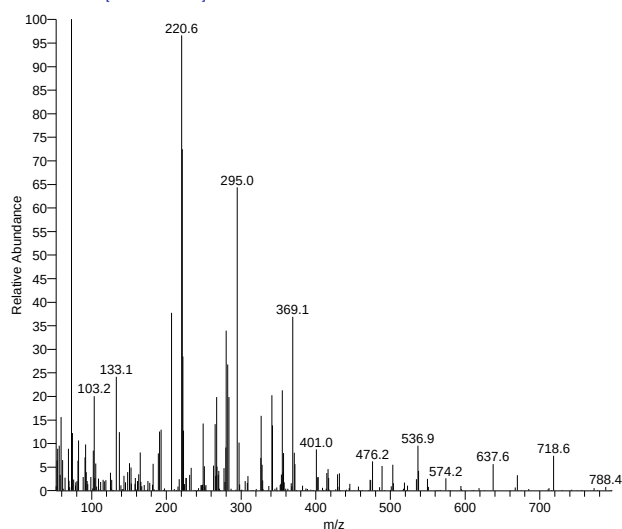
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RT: 52.35 - 53.57 SM: 15G



NL:
8.83E5
TIC MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

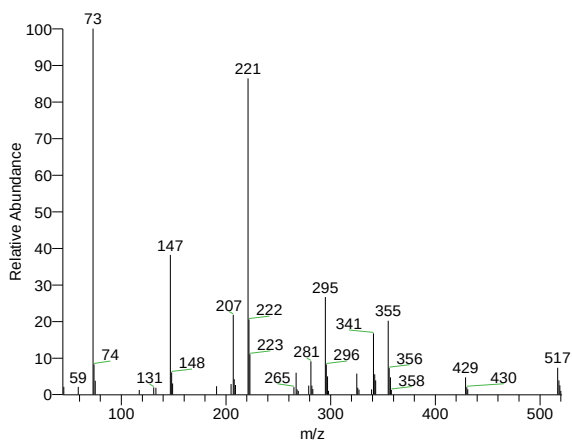
NGA-ZE-WATER3-SAMPLE-INJ1 #14006 RT: 52.97 AV: 1 RF: 6.00, 3 NL: 7.03E4
T: + c EI Full ms [50.000-800.000]



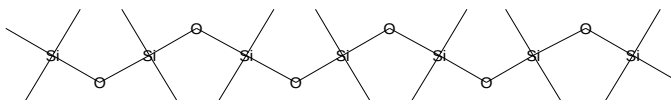
RT	Compound Name	Area	Probability	SI	RSI	Library
52.97	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	3204880.12	23.90	455	534	mainlib
52.97	Heptasiloxane, hexadecamethyl-	3204880.12	23.90	455	691	mainlib
52.97	Cyclodecasiloxane, eicosamethyl-	3204880.12	10.16	434	461	mainlib
52.97	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	3204880.12	8.58	430	550	mainlib
52.97	Cyclononasiloxane, octadecamethyl-	3204880.12	5.54	417	506	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



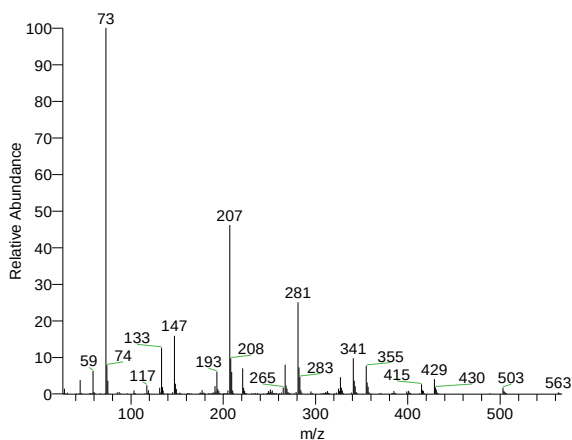
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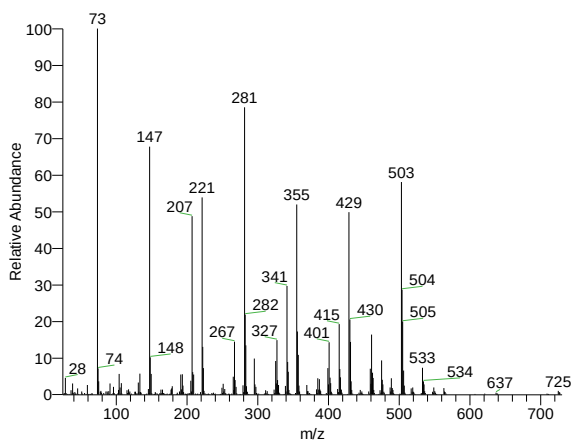
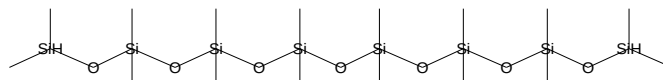
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

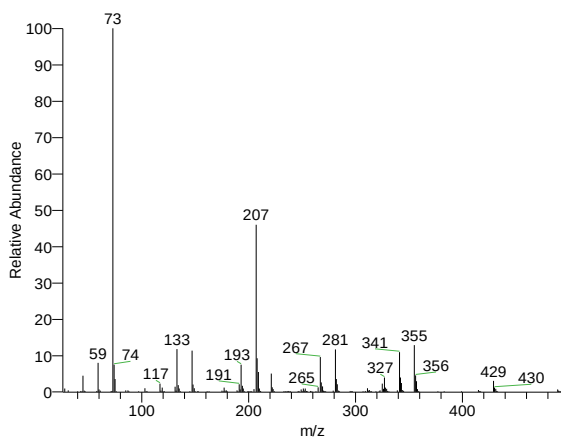
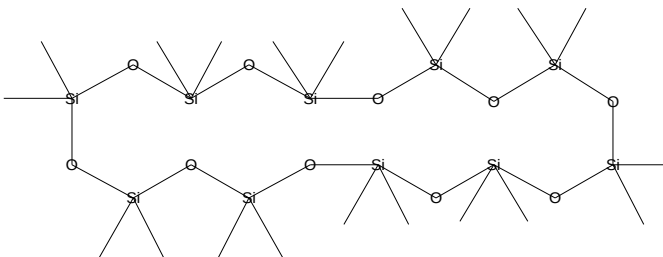
Compound Structure



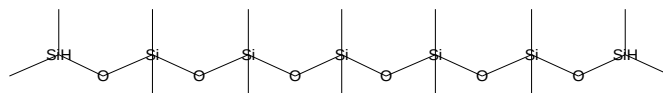
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



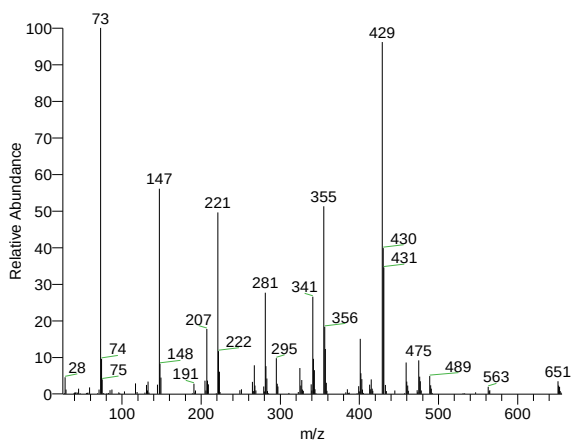
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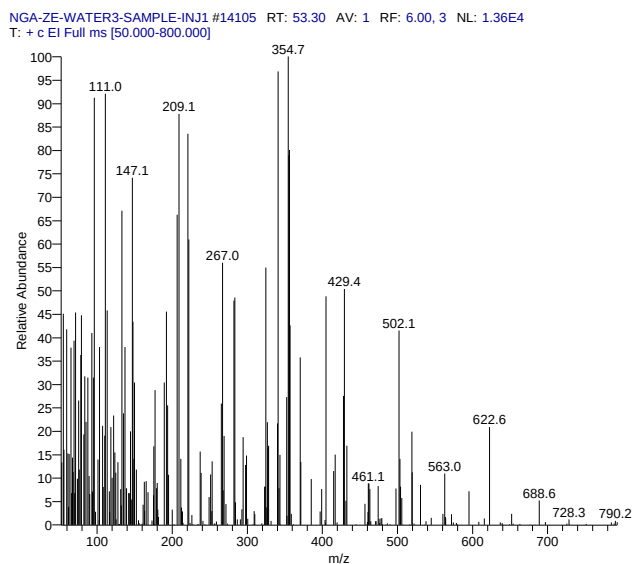
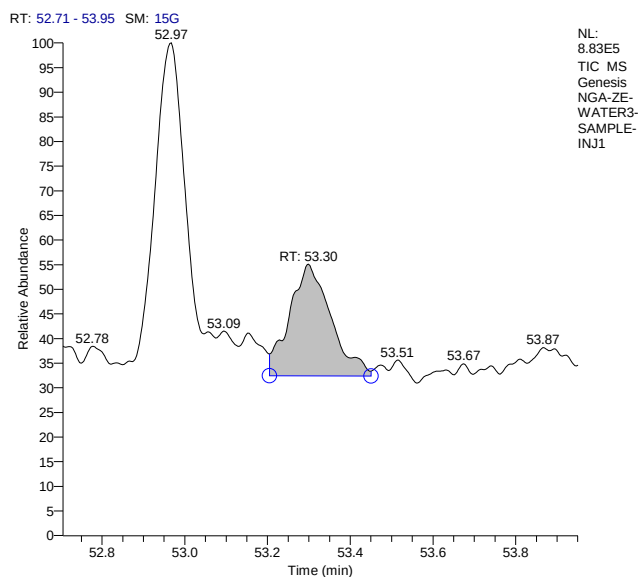
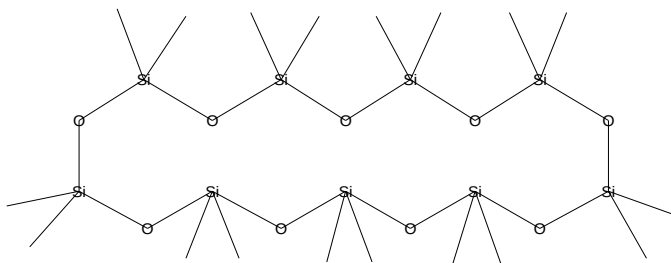
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



RT	Compound Name	Area	Probability	SI	RSI	Library
53.30	Cyclodecasiloxane, eicosamethyl-	1392239.52	25.33	436	483	mainlib
53.30	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1392239.52	20.41	431	555	mainlib
53.30	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1392239.52	12.37	416	564	mainlib
53.30	1,3,5,7,9-Pentaethylbicyclo[5.3.1]pentasiloxane	1392239.52	3.77	391	728	mainlib
53.30	Heptasiloxane, hexadecamethyl-	1392239.52	2.96	385	572	mainlib

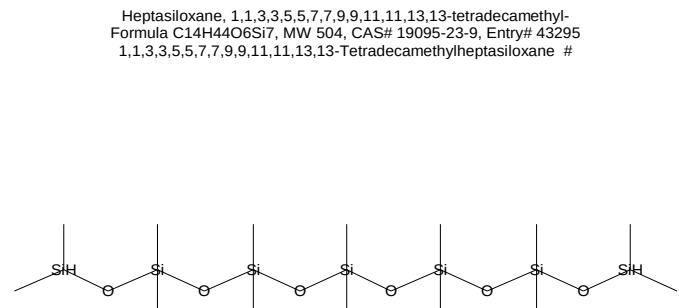
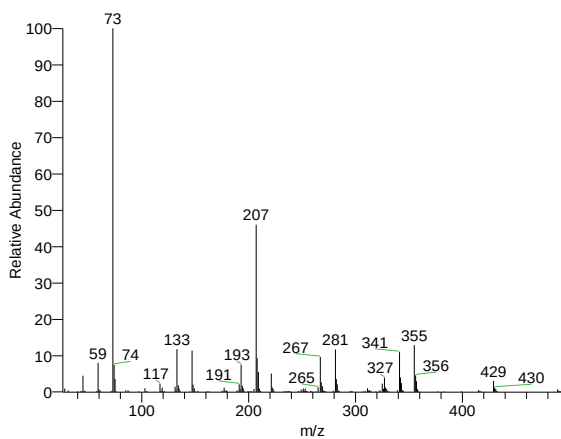
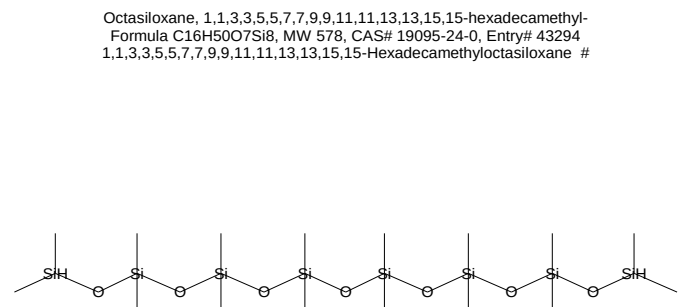
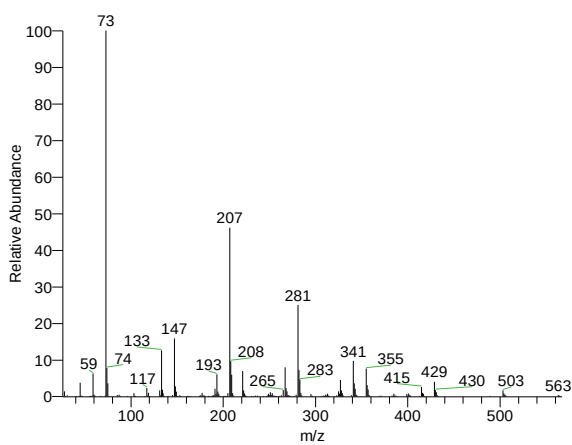
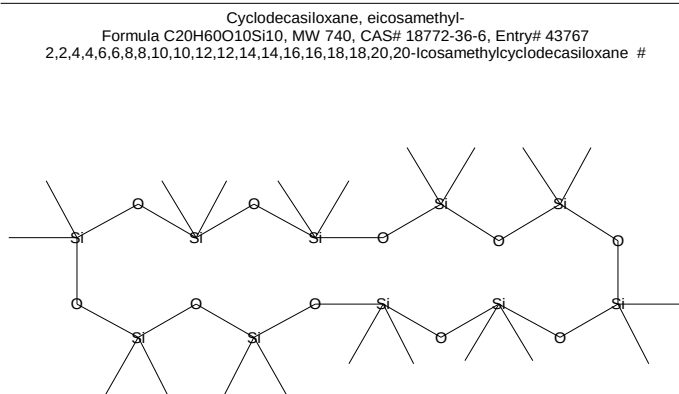
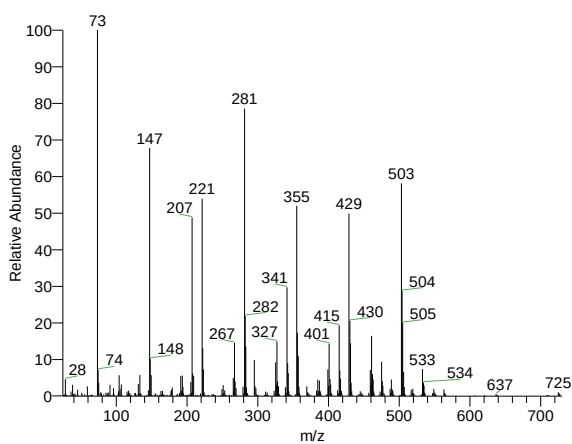
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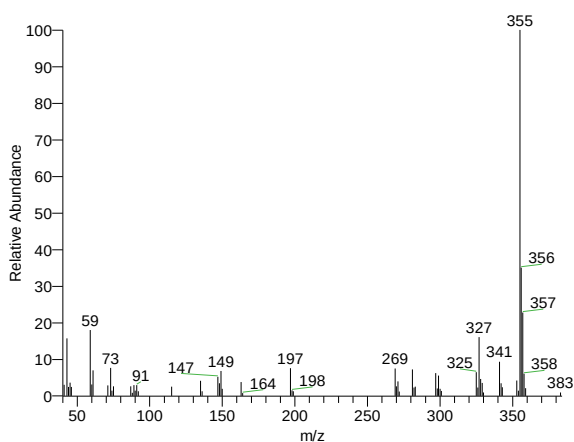
Compound Structure



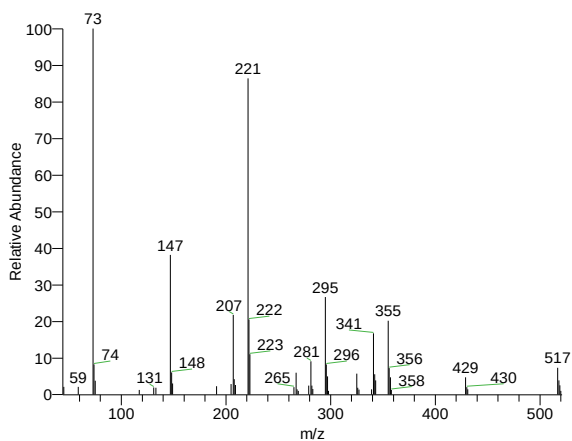
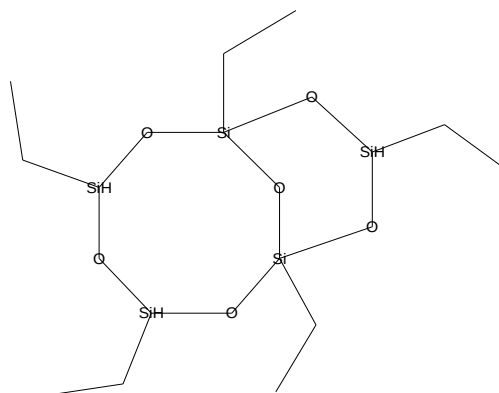
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Compound Structure



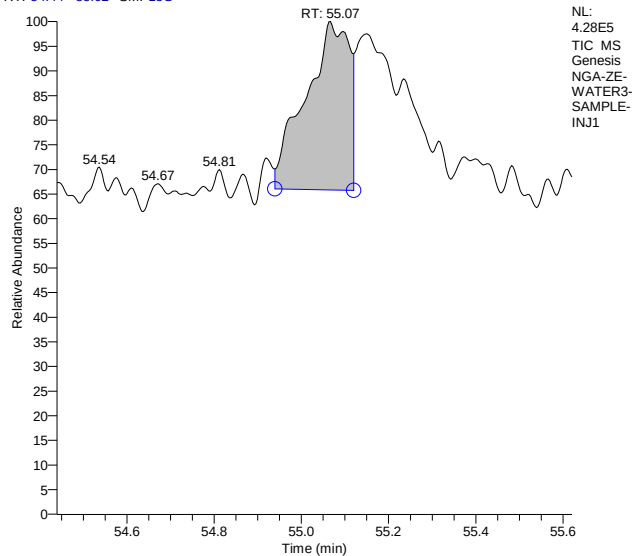
1,3,5,7,9-Pentaethylbicyclo[5.3.1]pentasiloxane
Formula C₁₀H₂₈O₆Si₅, MW 384, CAS# 73420-26-5, Entry# 234399
\$:28IBTWGHXUBZSUFI-UHFFFAOYSA-N



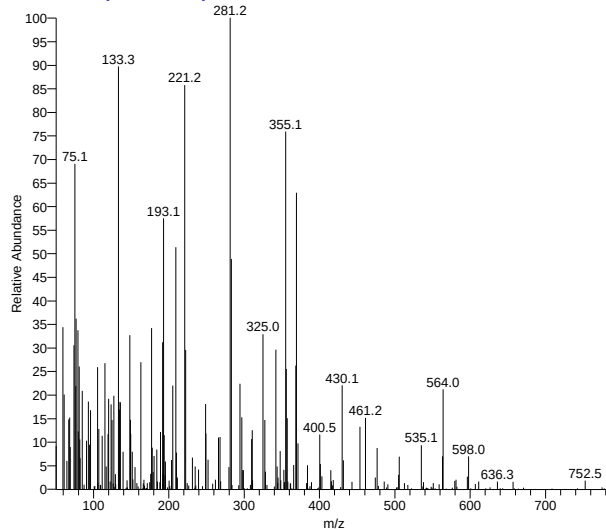
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



RT: 54.44 - 55.62 SM: 15G



NGA-ZE-WATER3-SAMPLE-INJ1 #14632 RT: 55.07 AV: 1 RF: 6.00, 3 NL: 1.91E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
55.07	2,4-Dihydroxybenzoic acid, 3TMS derivative	1019651.97	8.83	384	449	mainlib

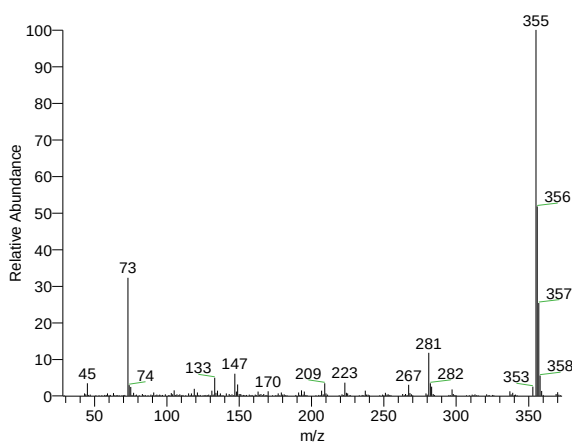
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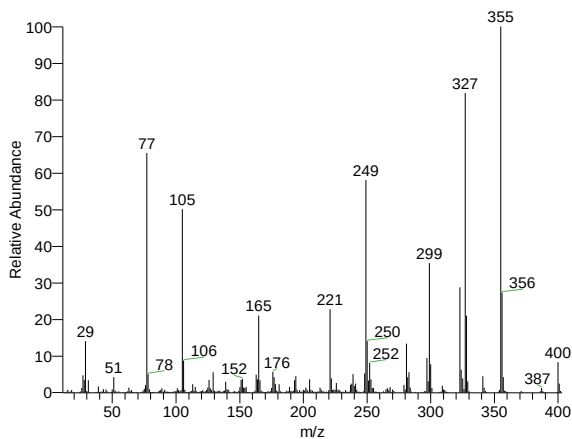
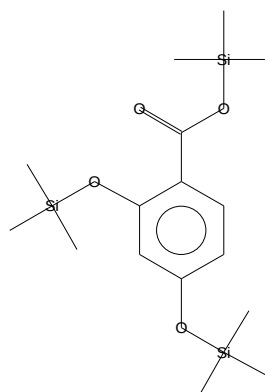
RT	Compound Name	Area	Probability	SI	RSI	Library
55.07	2H-1-Benzopyran-3-carboxylic acid, 2-ethoxy-2,4-diphenyl-, ethyl ester	1019651.97	6.41	375	442	mainlib
55.07	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1019651.97	6.16	374	425	mainlib
55.07	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1019651.97	5.44	371	465	mainlib
55.07	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1019651.97	4.60	367	469	mainlib

Hit Spectrum

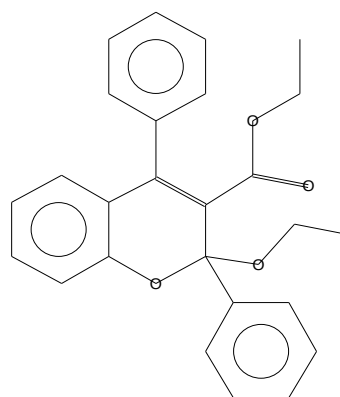


Compound Structure

2,4-Dihydroxybenzoic acid, 3TMS derivative
 Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 10586-16-0, Entry# 234374
 Benzoic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester



2H-1-Benzopyran-3-carboxylic acid, 2-ethoxy-2,4-diphenyl-, ethyl ester
 Formula C₂₆H₂₄O₄, MW 400, CAS# 19723-39-8, Entry# 234351
 Ethyl 2-ethoxy-2,4-diphenyl-2H-chromene-3-carboxylate #



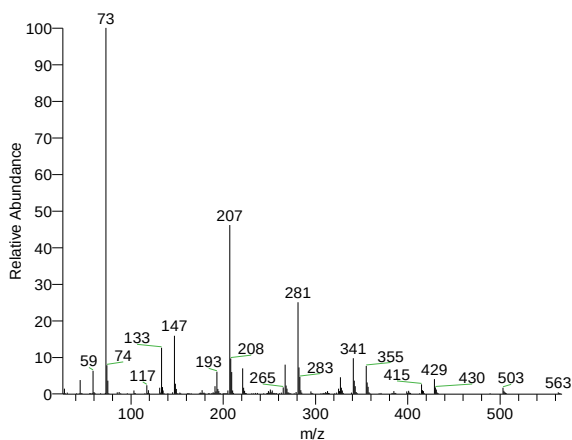
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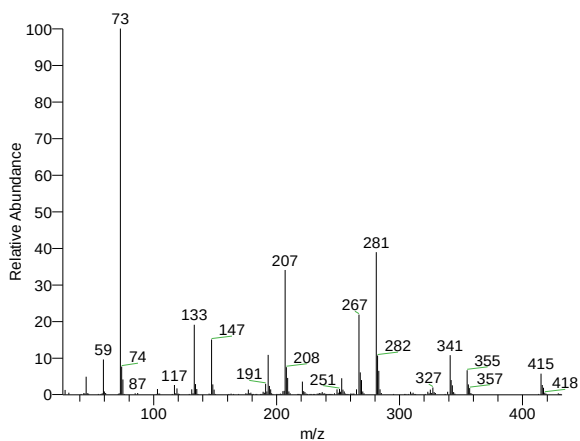
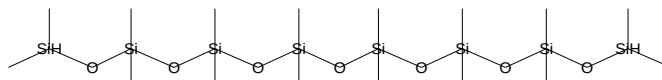
ANALYTICAL CHEMISTRY DIVISION

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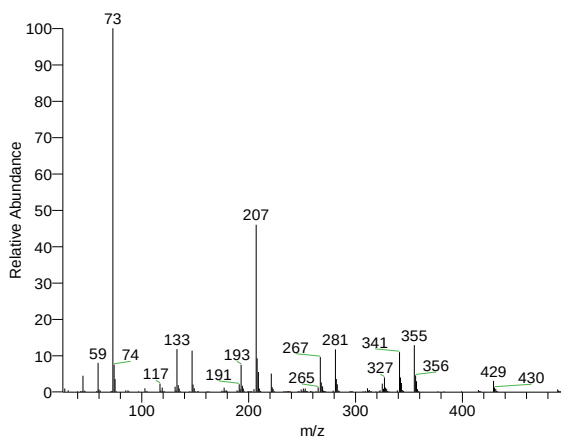
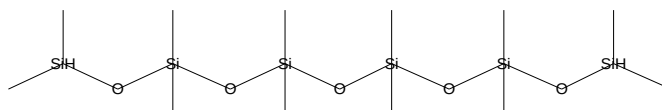
Compound Structure



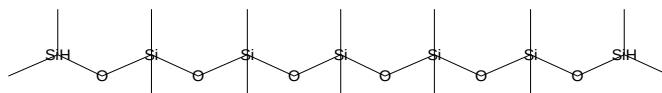
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

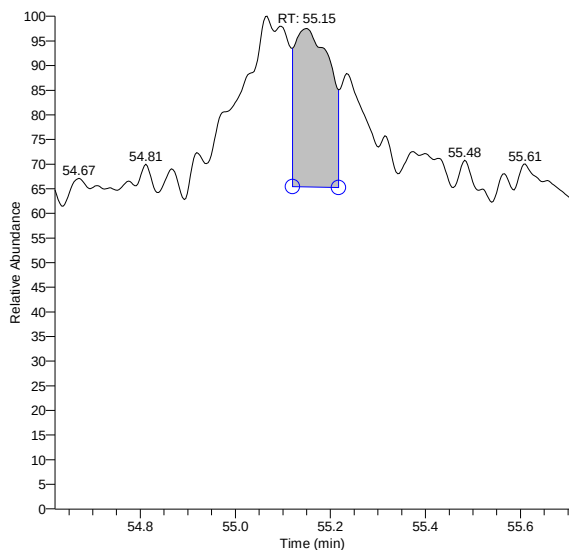


Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



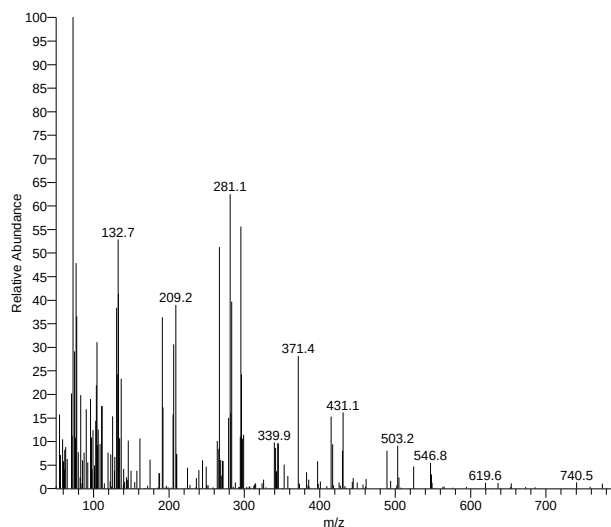
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ANALYTICAL CHEMISTRY DIVISION

RT: 54.62 - 55.70 SM: 15G



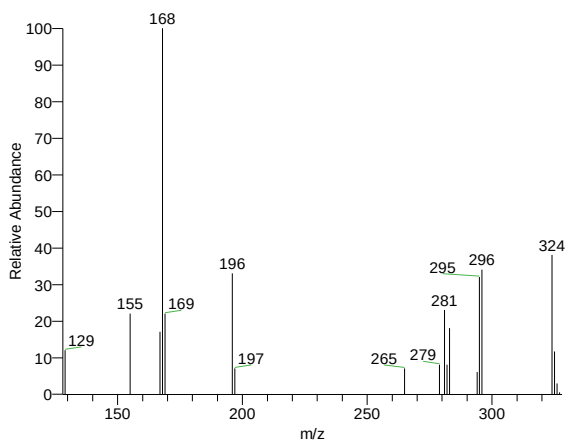
NL:
4.28E5
TIC: MS
Genesis
NGA-ZE-
WATER3-
SAMPLE-
INJ1

NGA-ZE-WATER3-SAMPLE-INJ1 #14657 RT: 55.15 AV: 1 RF: 6.00, 3 NL: 2.44E4
T: + c EI Full ms [50.000-800.000]



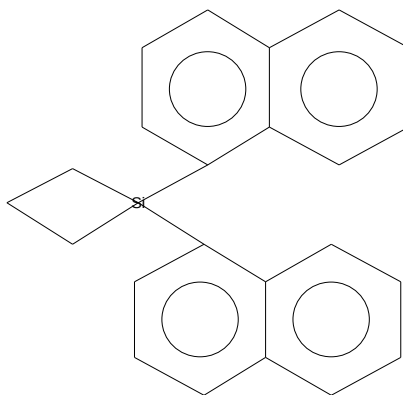
RT	Compound Name	Area	Probability	SI	RSI	Library
55.15	2,4-Dihydroxypropio-phenone, 2TMS derivative	706751.97	8.93	371	541	mainlib
55.15	1,1-Di(1-naphthyl)-1-silacyclobutane	706751.97	8.93	371	567	mainlib
55.15	1-Phenylpropene-3,3-diol diacetate	706751.97	2.99	347	728	mainlib
55.15	2,4-Dihydroxyacetophenone, 2TMS derivative	706751.97	2.41	342	442	mainlib
55.15	2-Hydroxy-4-methylanthraquinone, O-trimethylsilyl	706751.97	2.22	340	644	mainlib

Hit Spectrum



Compound Structure

1,1-Di(1-naphthyl)-1-silacyclobutane
Formula C23H20Si, MW 324, CAS# 54600-10-1, Entry# 157554
1,1-Di(1-naphthyl)siletane #



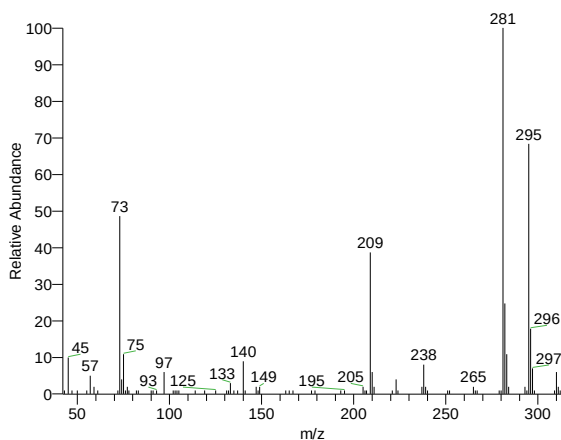
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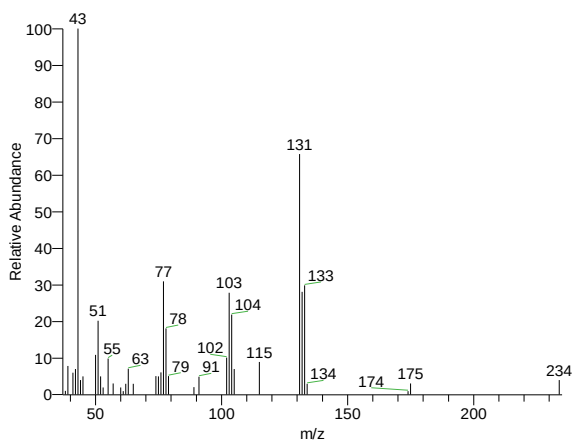
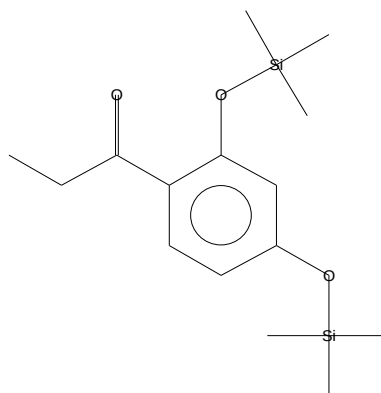
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

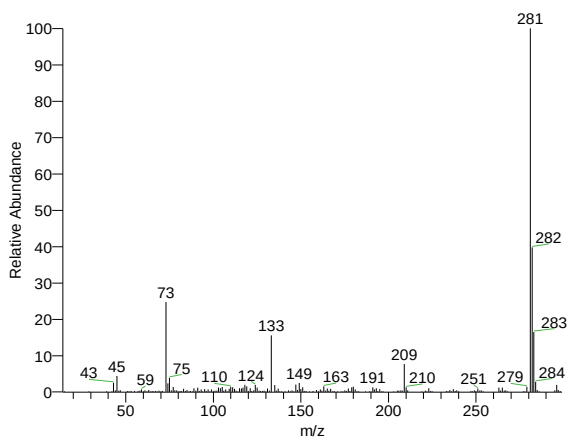
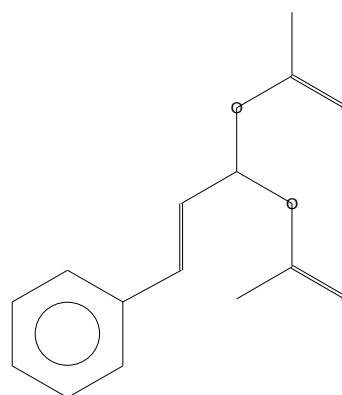
Compound Structure



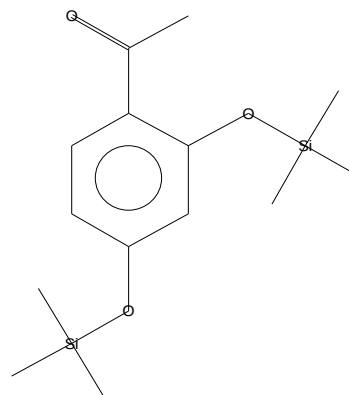
2,4-Dihydroxypropiophenone, 2TMS derivative
Formula C₁₅H₂₆O₃Si₂, MW 310, CAS# 55724-93-1, Entry# 220126
1-Propanone, 1-[2,4-bis[(trimethylsilyl)oxy]phenyl]-



1-Phenylpropene-3,3-diol diacetate
Formula C₁₃H₁₄O₄, MW 234, CAS# NA, Entry# 11997
(2E)-1-(Acetyloxy)-3-phenyl-2-propenyl acetate #



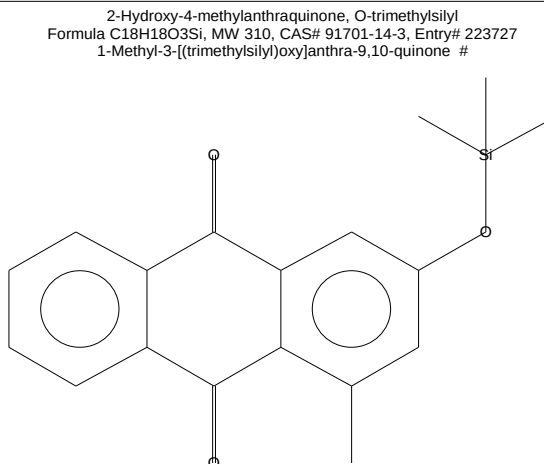
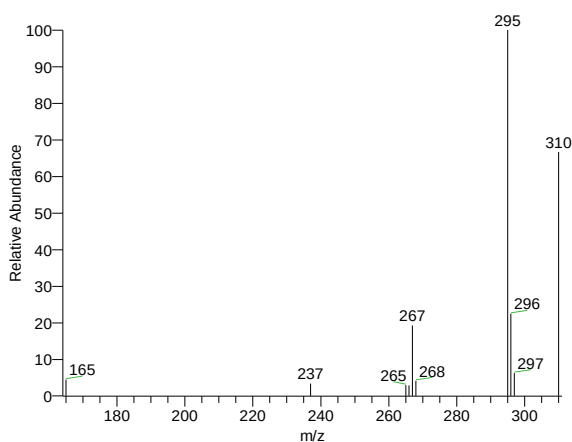
2,4-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220074
2',4'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



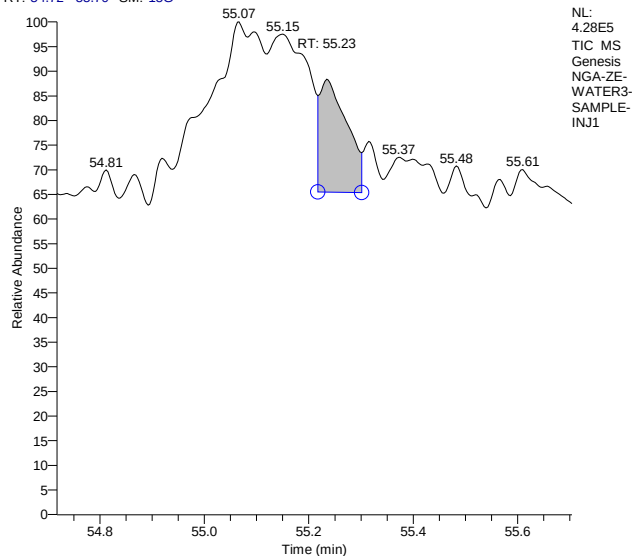
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Hit Spectrum

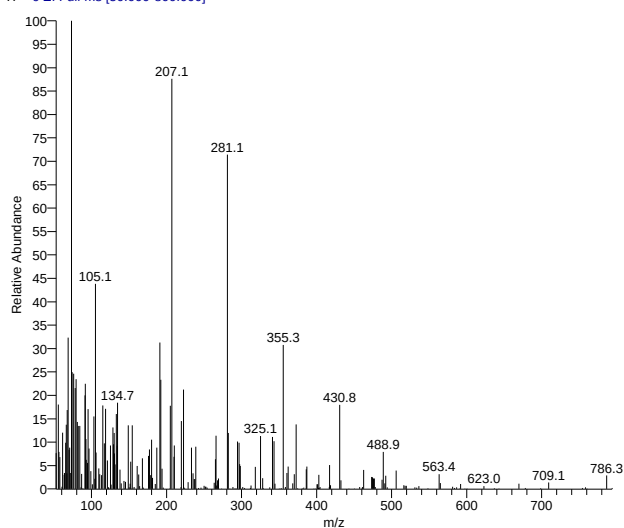
Compound Structure



RT: 54.72 - 55.70 SM: 15G



NGA-ZE-WATER3-SAMPLE-INJ1 #14682 RT: 55.23 AV: 1 RF: 6.00, 3 NL: 2.89E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
55.23	4-Dehydroxy-N-(4,5-methylenedioxy-2-nitrobenzylidene)tyramine	355968.94	8.19	396	515	mainlib
55.23	Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester	355968.94	5.95	387	513	mainlib
55.23	2,5-Dihydroxyacetophenone, 2TMS derivative	355968.94	5.25	384	478	mainlib
55.23	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	355968.94	5.25	384	486	mainlib
55.23	Trimethylsilyl 3-methyl-4-[(trimethylsilyl)oxy]benzoate	355968.94	4.02	377	489	mainlib

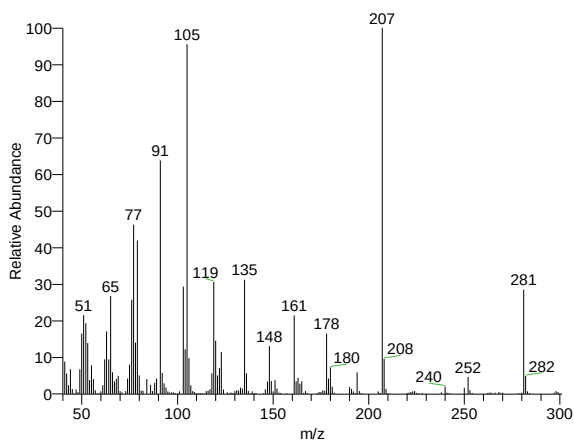
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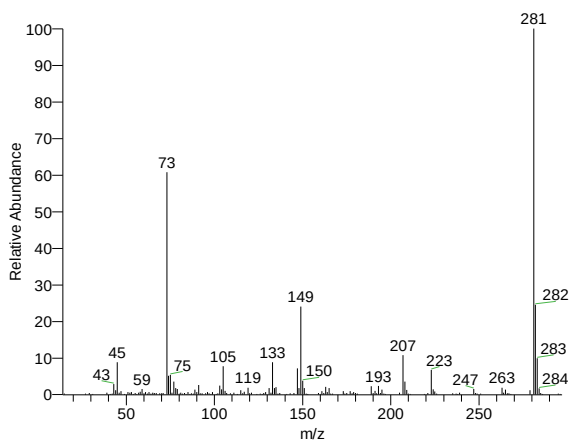
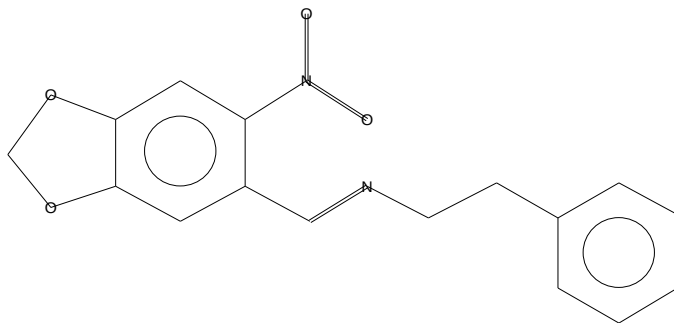
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

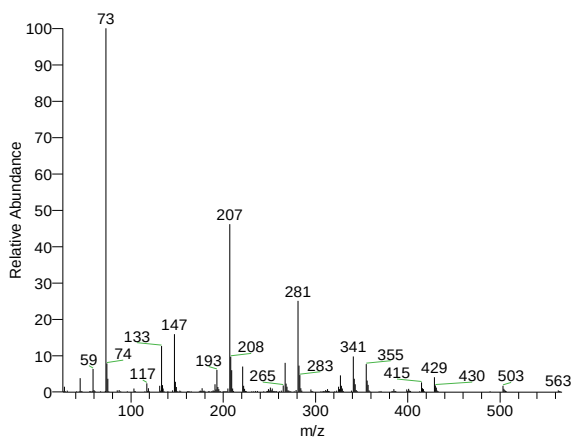
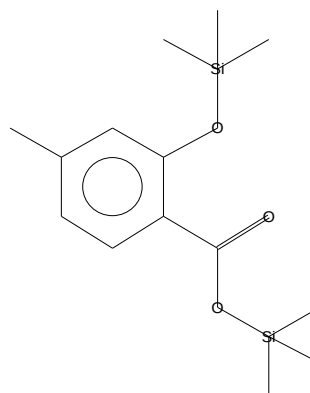
Compound Structure



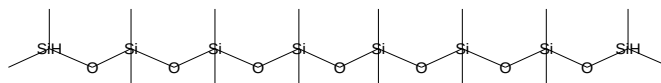
4-Dehydroxy-N-(4,5-methylenedioxy-2-nitrobenzylidene)tyramine
Formula C₁₆H₁₄N₂O₄, MW 298, CAS# NA, Entry# 188699
N-[(E)-(6-Nitro-1,3-benzodioxol-5-yl)methylidene]-2-phenylethanamine #



Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# 35-27-8, Entry# 219921
\$.28WMMUZRDZZSRQEF-UHFFFAOYSA-N



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



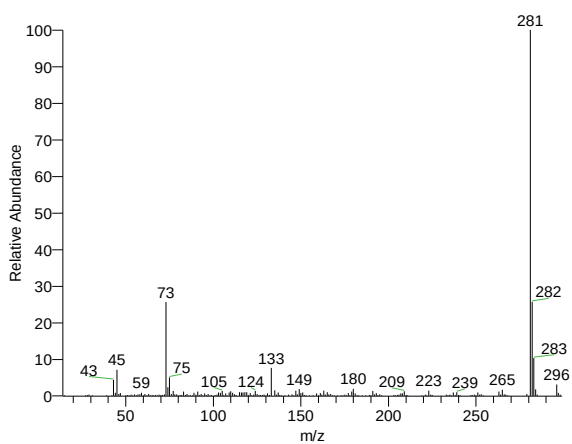
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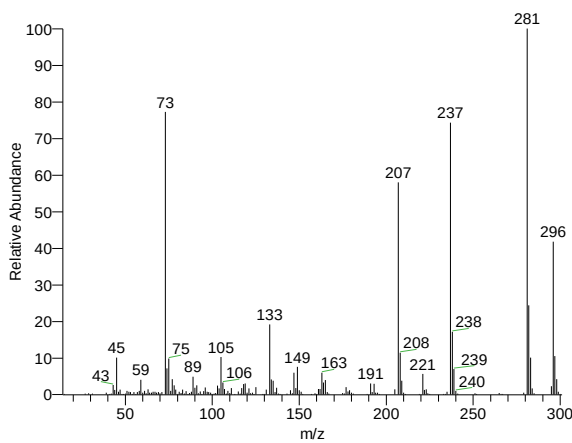
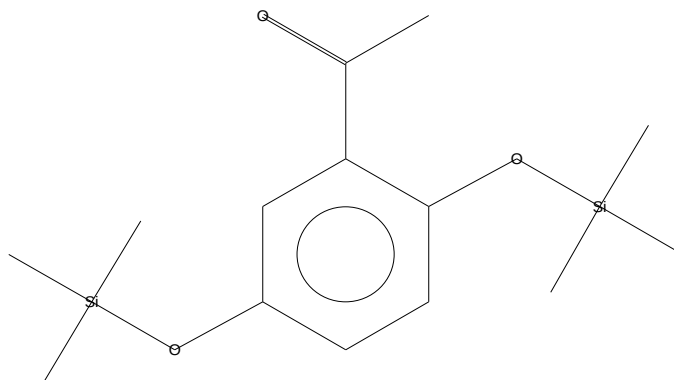
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

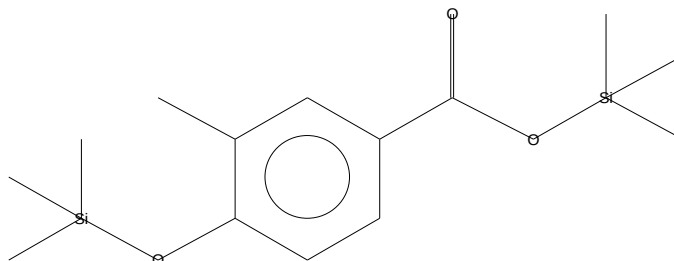
Compound Structure



2,5-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220075
2,5-Dihydroxyacetophenone, bis(trimethylsilyl) ether



Trimethylsilyl 3-methyl-4-[(trimethylsilyl)oxy]benzoate
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 219915
4-(Trimethylsilyl)oxy-3-methylbenzoic acid, trimethylsilyl ester



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Data File:

Panamik Groundwater

Original Data Path:

E:\Xcalibur\Data\2024\FEBRUARY-2024

Sample Name:

GCMS-FS

Acquisition Date:

03/01/24 12:59:18 AM

Run Time(min):

49.67

Vial:

11

Injection Volume(µl):

1.00

Low Mass(m/z):

50

High Mass(m/z):

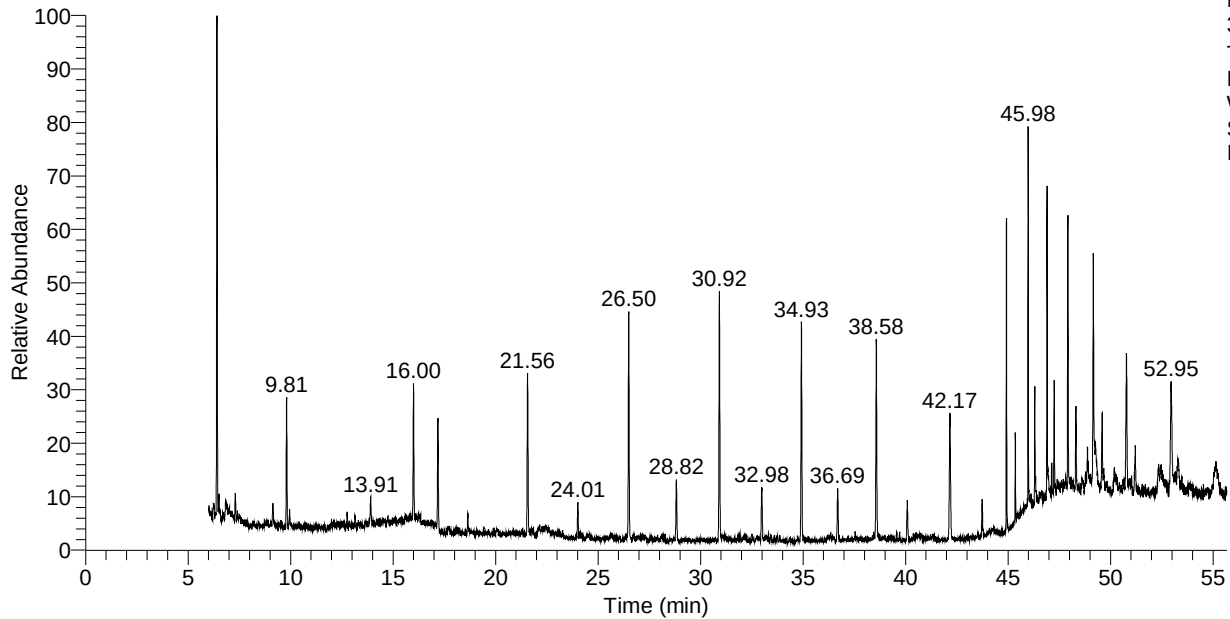
800

Instrument Method:

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Original Processing Method:

RT: 0.00 - 55.67 SM: 7G



NL:
3.29E6
TIC MS
NGA-ZE-
WATER2-
SAMPLE-
INJ1

Qual Peak Table

RT	Peak Area	Peak Height	S/N	Area %
6.41	6781505.20	2679717.99	37.62	8.85
6.84	443440.92	96348.03	2.10	0.58
9.14	439629.75	125139.68	3.34	0.57
9.81	1996102.51	707553.19	21.28	2.61
9.95	270872.06	89030.23	2.76	0.35
13.91	480076.81	145014.90	4.13	0.63
16.00	2416677.42	751100.49	10.67	3.16
17.19	1724179.98	586598.68	9.55	2.25
21.56	2912737.18	913162.00	31.81	3.80
24.02	496923.20	181235.41	3.28	0.65
26.50	3973410.43	1254651.52	32.89	5.19
28.82	1139809.28	339111.59	12.85	1.49
30.92	4424459.96	1390178.10	56.09	5.78
32.99	1064970.54	304579.99	7.57	1.39
34.92	3950484.56	1239026.69	80.72	5.16
36.69	1015218.62	296505.82	15.58	1.33
38.58	3769728.92	1102127.76	40.91	4.92
40.09	741941.14	218066.71	5.61	0.97
42.17	3051906.76	725180.55	16.48	3.98
43.74	616909.62	203912.52	4.39	0.81

Analysed by Satyanarayana

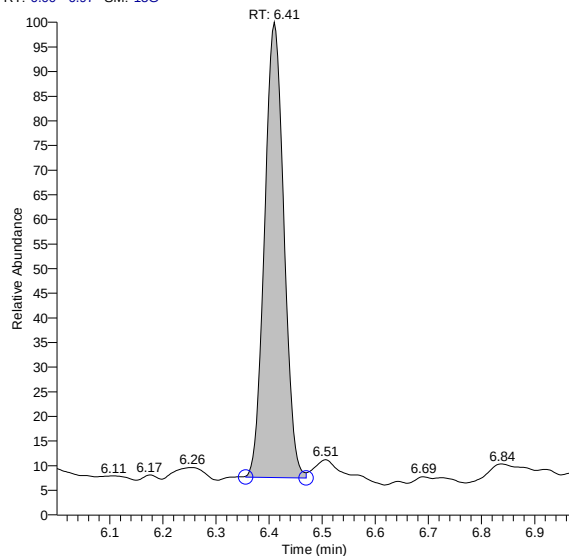
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ANALYTICAL CHEMISTRY DIVISION

RT	Peak Area	Peak Height	S/N	Area %
44.93	2794722.57	1409178.08	10.23	3.65
45.35	695241.95	381974.54	3.23	0.91
45.98	3455900.31	1697267.82	17.88	4.51
46.31	1450527.55	540764.23	5.83	1.89
46.91	3610289.13	1496336.46	10.14	4.71
47.25	1305395.02	557530.55	4.72	1.70
47.92	3390519.81	1386272.83	12.15	4.43
48.31	1115720.14	430630.73	3.22	1.46
48.88	1126402.36	217270.99	2.63	1.47
49.16	4522682.90	1273211.96	15.44	5.91
49.59	1229843.07	394275.85	4.20	1.61
50.78	2991809.71	777491.72	11.18	3.91
52.96	3690110.79	636119.42	13.12	4.82
53.12	322066.21	102303.55	2.03	0.42
53.19	284823.50	102835.59	2.04	0.37
53.29	1294565.22	191311.76	4.31	1.69
55.15	1597438.26	172466.73	2.83	2.09

Analysed by Satyanarayana

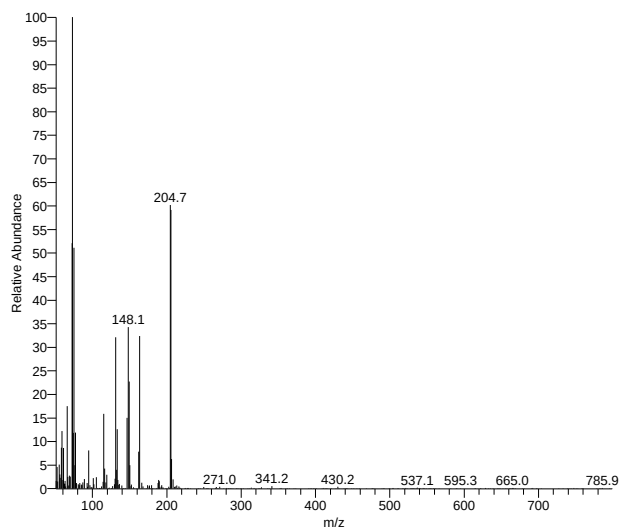
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RT: 6.00 - 6.97 SM: 15G



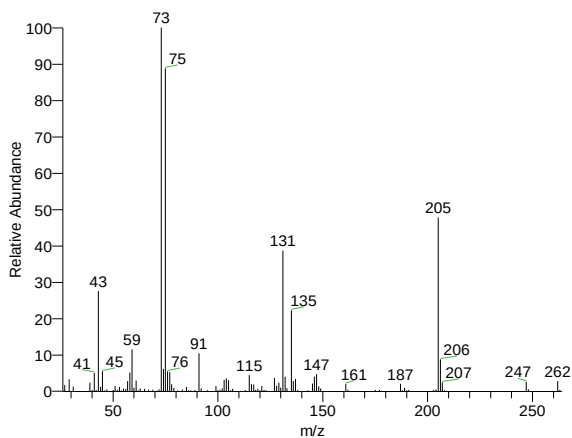
NL:
2.90E6
TIC: MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #123 RT: 6.41 AV: 1 RF: 6.00, 3 NL: 4.22E5
T: + c EI Full ms [50.000-800.000]



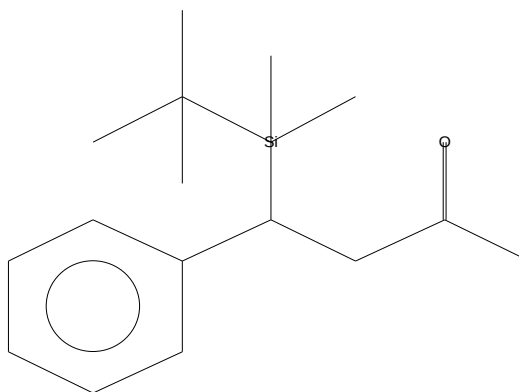
RT	Compound Name	Area	Probability	SI	RSI	Library
6.41	3-Butanone, 1-(t-butyl dimethylsilyl)-1-phenyl-	6781505.20	13.60	563	614	mainlib
6.41	à-Hydroxyisobutyric acid, 2TMS derivative	6781505.20	10.96	558	595	mainlib
6.41	4-Phenyl-3-buten-2-ol, (E)-, TMS derivative	6781505.20	8.62	552	560	mainlib
6.41	3-Phenyl-1-buten-1-ol, TMS derivative	6781505.20	6.60	545	588	mainlib
6.41	1-Phenyl-1-hepten-3-ol, (E)-, TMS derivative	6781505.20	4.92	537	596	mainlib

Hit Spectrum



Compound Structure

3-Butanone, 1-(t-butyl dimethylsilyl)-1-phenyl-
Formula C₁₆H₂₆OSi, MW 262, CAS# 118356-59-5, Entry# 41510
4-[tert-Butyl(dimethyl)silyl]-4-phenyl-2-butanone #



Analysed by Satyanarayana

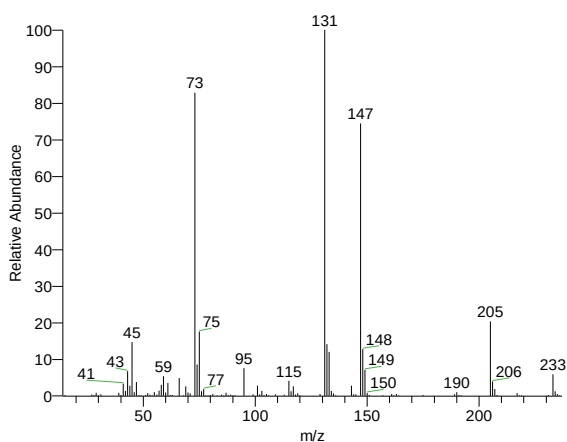
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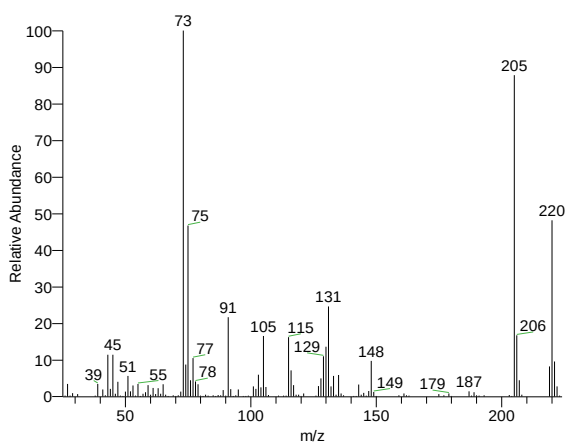
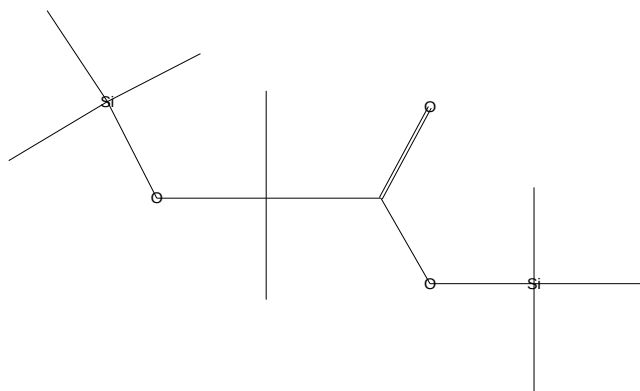
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

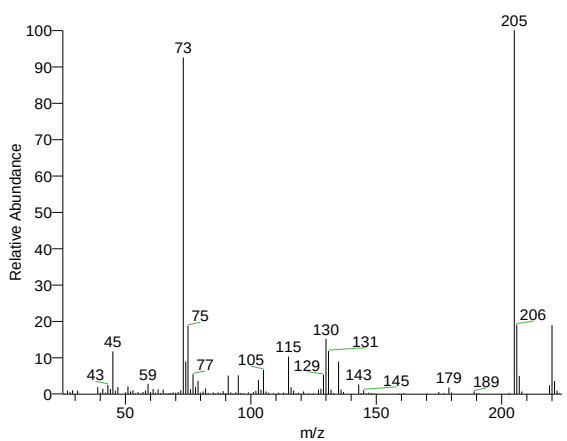
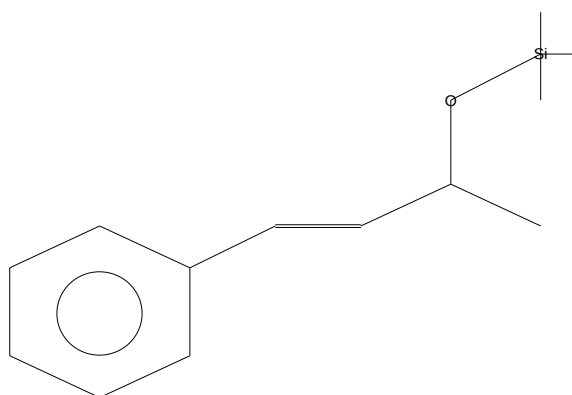
Compound Structure



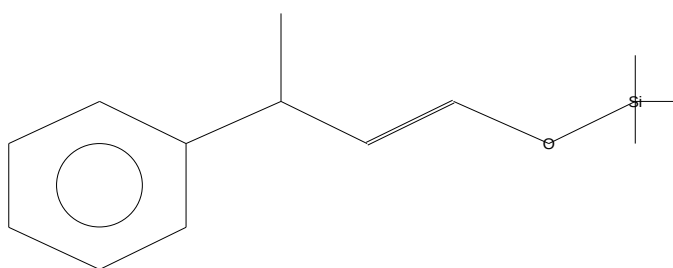
2-Hydroxyisobutyric acid, 2TMS derivative
Formula C₁₀H₂₄O₃Si₂, MW 248, CAS# 55133-92-1, Entry# 115549
Propanoic acid, 2-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester



4-Phenyl-3-buten-2-ol, (E)-, TMS derivative
Formula C₁₃H₂₀O₂Si, MW 220, CAS# 76987-16-1, Entry# 43284
1-Butene, 1-phenyl-3-(trimethylsilyloxy)-, (E)



3-Phenyl-1-buten-1-ol, TMS derivative
Formula C₁₃H₂₀O₂Si, MW 220, CAS# 55543-95-8, Entry# 187248
1-Butene, 3-phenyl-1-(trimethylsilyloxy)-, (Z- or E-)

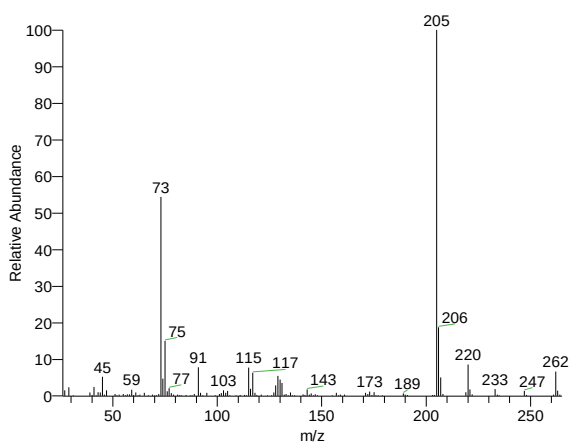


Analysed by Satyanarayana

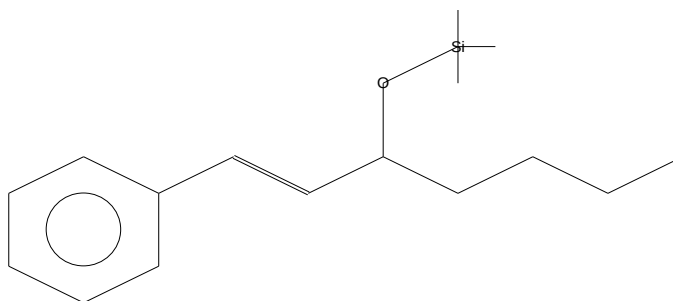
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Hit Spectrum

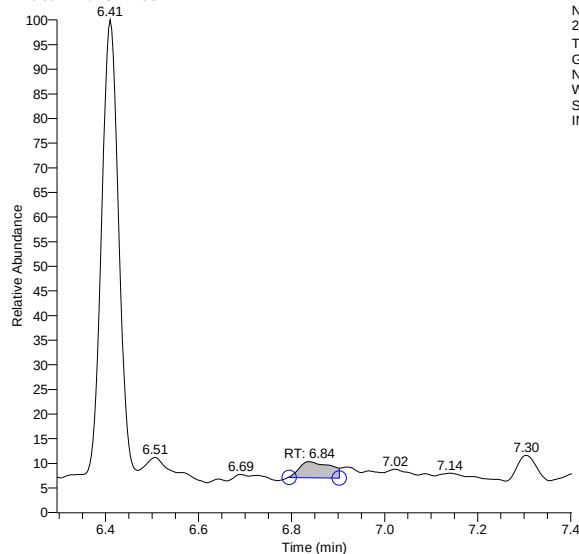
Compound Structure



1-Phenyl-1-hepten-3-ol, (E)-, TMS derivative
Formula C₁₆H₂₆OSi, MW 262, CAS# NA, Entry# 187246
1-Heptene, 1-phenyl-3-(trimethylsilyloxy)-

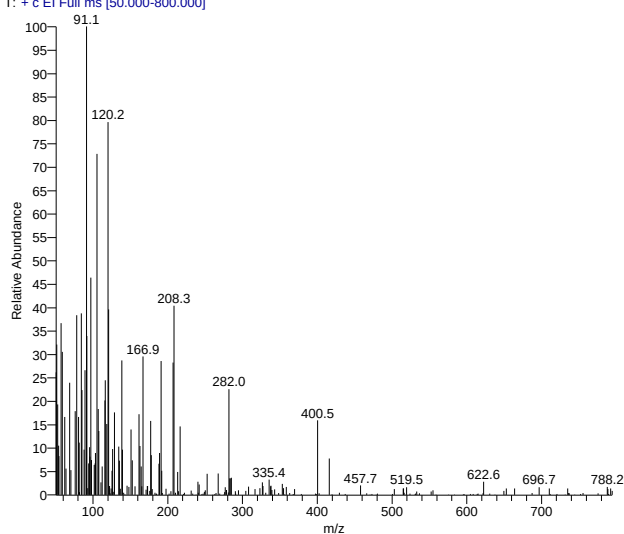


RT: 6.30 - 7.40 SM: 15G



NL:
2.90E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #251 RT: 6.84 AV: 1 RF: 6.00, 3 NL: 1.93E4
T: + c EI Full ms [50.000-800.000]



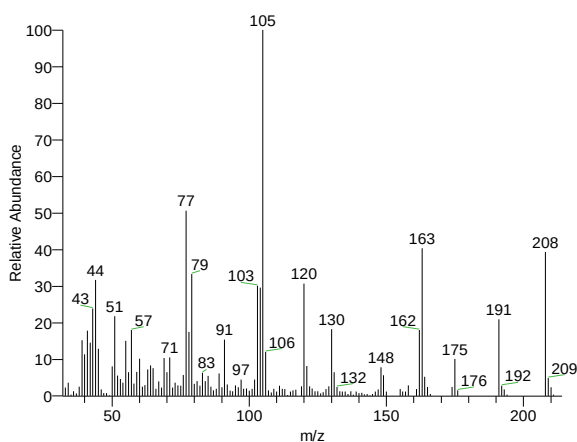
RT	Compound Name	Area	Probability	SI	RSI	Library
6.84	2-(1-Phenyl-ethylamino)-2-thioxo-acetamide	443440.92	4.94	375	511	mainlib
6.84	4-Dehydroxy-N-(4,5-methylenedioxy-2-nitrobenzylidene)tyramine	443440.92	4.36	372	445	mainlib
6.84	Aminoacetamide, N-methyl-N-[4-(1-pyrrolidinyl)-2-butyryl]-	443440.92	4.19	371	458	mainlib
6.84	3,5-Dimethoxycinnamic acid	443440.92	4.19	371	466	mainlib
6.84	4-Hydroxy-3-nitrocoumarin	443440.92	2.79	359	500	mainlib

Analysed by Satyanarayana

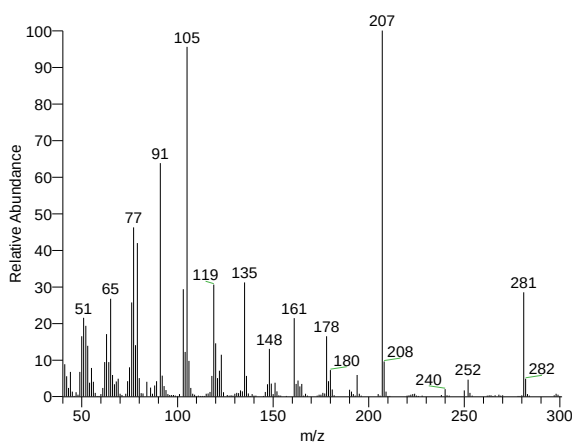
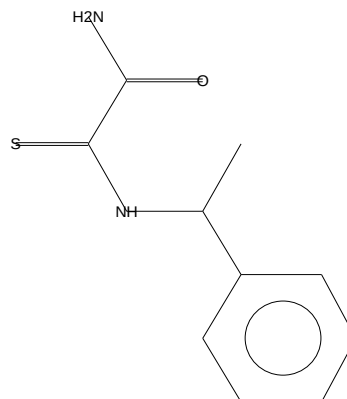
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Hit Spectrum

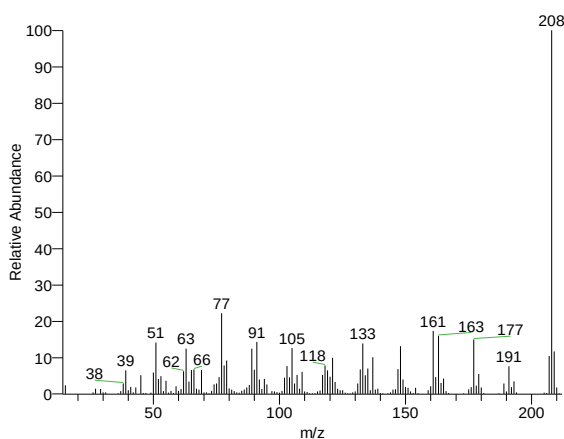
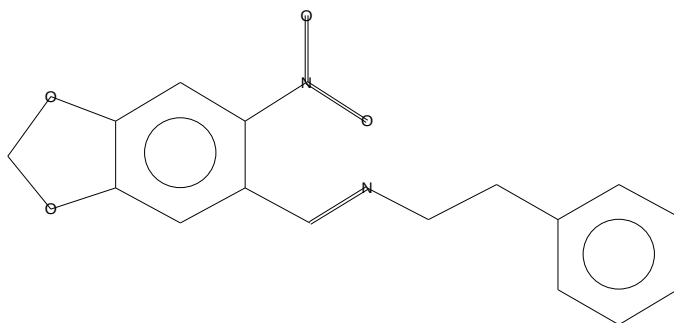
Compound Structure



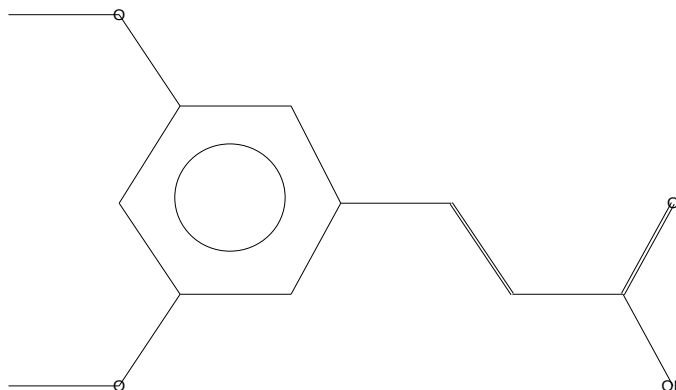
2-(1-Phenyl-ethylamino)-2-thioxo-acetamide
Formula C₁₀H₁₂N₂O₂S, MW 208, CAS# NA, Entry# 79466
S:28JUUJUPNDOLRJDSH-UHFFFAOYSA-N



4-Dehydroxy-N-(4,5-methylenedioxy-2-nitrobenzylidene)tyramine
Formula C₁₆H₁₄N₂O₄, MW 298, CAS# NA, Entry# 188699
N-[(E)-(6-Nitro-1,3-benzodioxol-5-yl)methylidene]-2-phenylethanamine #



3,5-Dimethoxycinnamic acid
Formula C₁₁H₁₂O₄, MW 208, CAS# 16909-11-8, Entry# 189175
2-Propenoic acid, 3-(3,5-dimethoxyphenyl)-

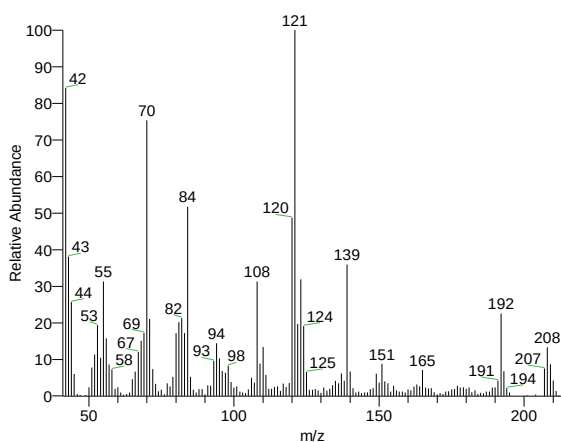


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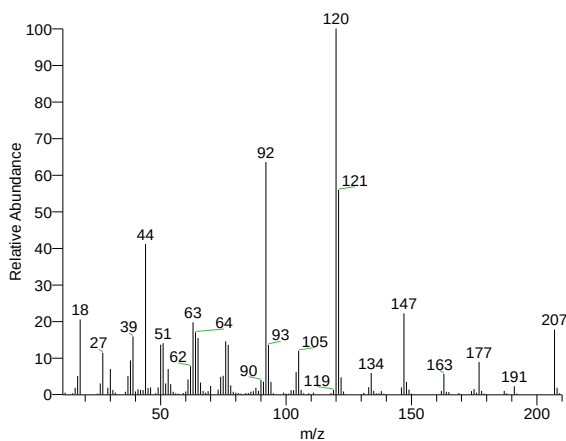
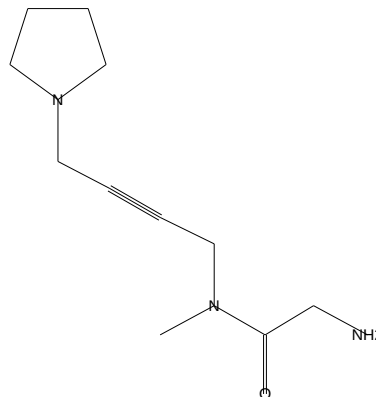
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Hit Spectrum

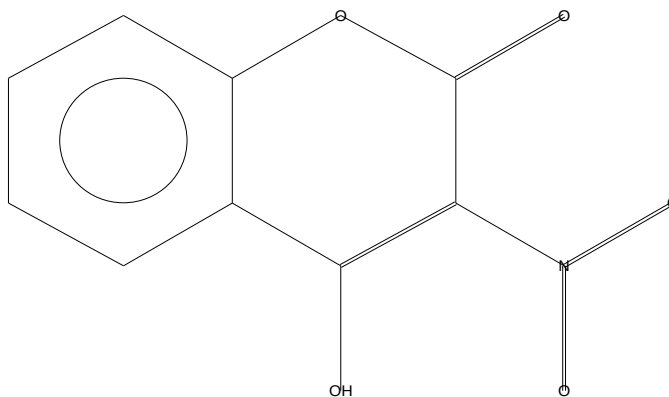
Compound Structure



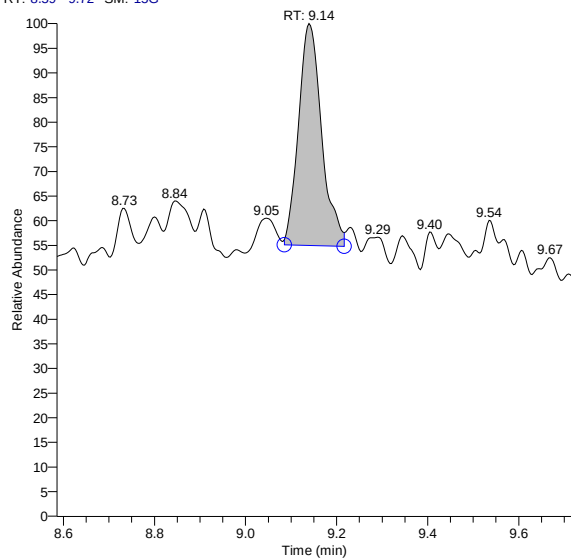
Aminoacetamide, N-methyl-N-[4-(1-pyrrolidinyl)-2-butynyl]-
Formula C₁₁H₁₉N₃O, MW 209, CAS# 124045-52-9, Entry# 102245
2-Amino-N-methyl-N-[4-(1-pyrrolidinyl)-2-butynyl]acetamide #



4-Hydroxy-3-nitrocoumarin
Formula C₉H₅NO₅, MW 207, CAS# 20261-31-8, Entry# 101423
2H-1-Benzopyran-2-one, 4-hydroxy-3-nitro-

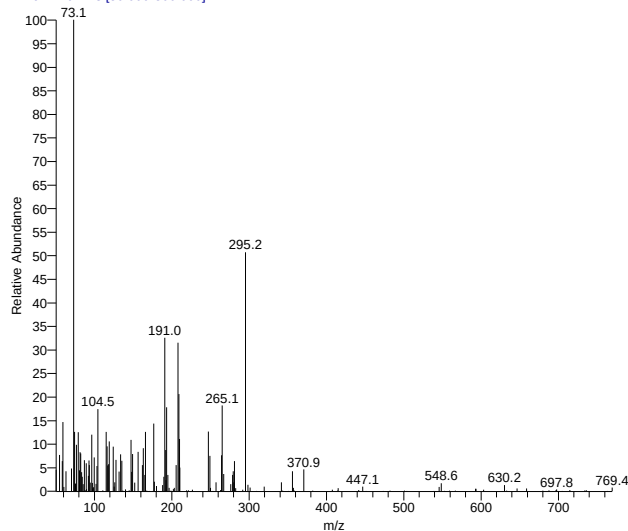


RT: 8.59 - 9.72 SM: 15G



NL:
2.78E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #937 RT: 9.14 AV: 1 RF: 6.00, 3 NL: 3.86E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.14	Tetrasiloxane, decamethyl-	439629.75	18.57	438	488	mainlib
9.14	Methyltris(trimethylsiloxy)silane	439629.75	14.59	432	483	mainlib

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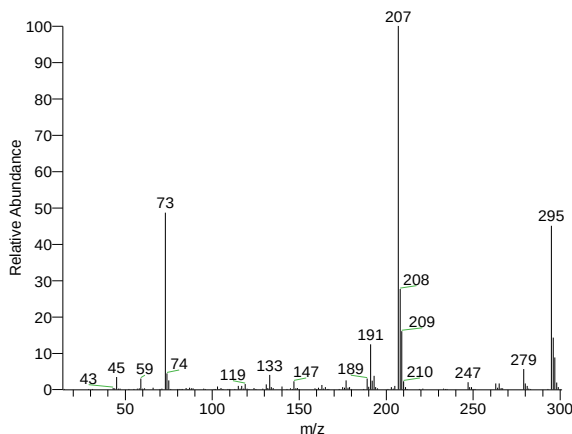
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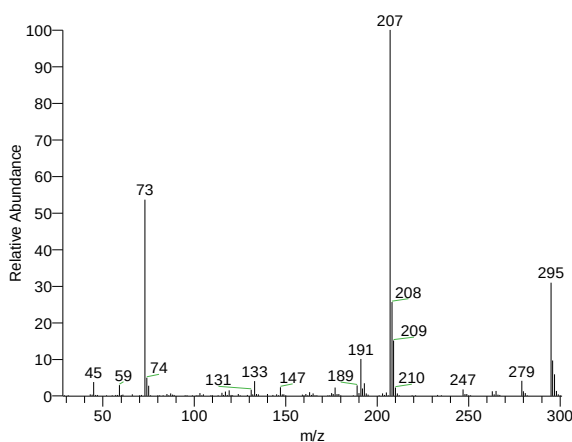
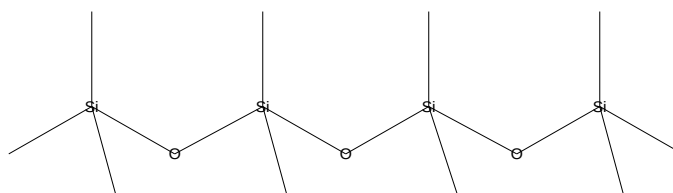
RT	Compound Name	Area	Probability	SI	RSI	Library
9.14	Benzaldehyde,	439629.75	3.90	400	535	mainlib
9.14	2-nitro-4-trimethylsilyl-	439629.75	3.74	399	531	mainlib
9.14	1,2-Benzenedimethanethio	439629.75	3.60	398	466	mainlib
	l, TMS derivative					
	3,5-Hexadien-1-yne,					
	1,3,6-tris(trimethylsilyl)-,					
	(E,E)-					

Hit Spectrum

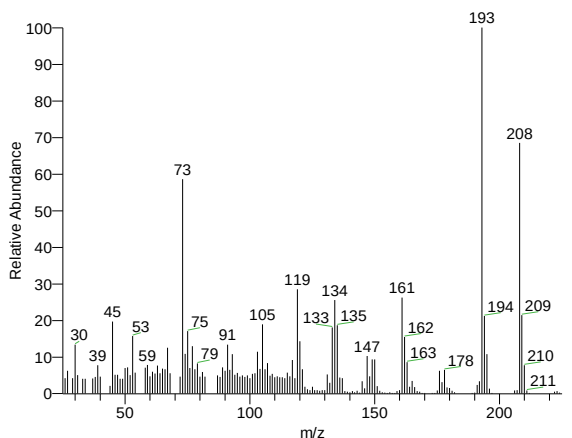
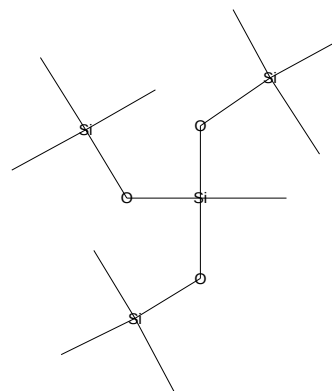
Compound Structure



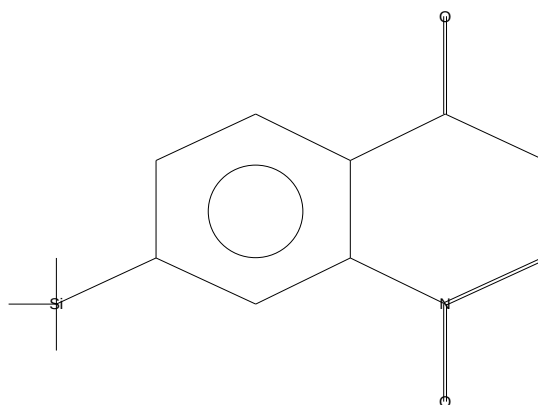
Tetrasiloxane, decamethyl-
Formula C10H30O3Si4, MW 310, CAS# 141-62-8, Entry# 188653
Decamethyltetrasiloxane



Methyltris(trimethylsiloxy)silane
Formula C10H30O3Si4, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



Benzaldehyde, 2-nitro-4-trimethylsilyl-
Formula C10H13NO3Si, MW 223, CAS# 30127-94-7, Entry# 179899
2-Nitro-4-(trimethylsilyl)benzaldehyde #

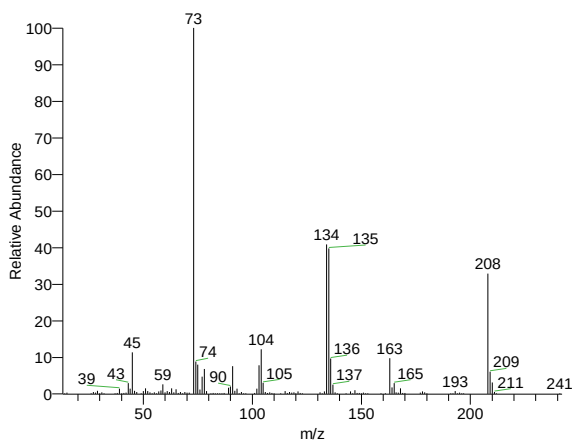


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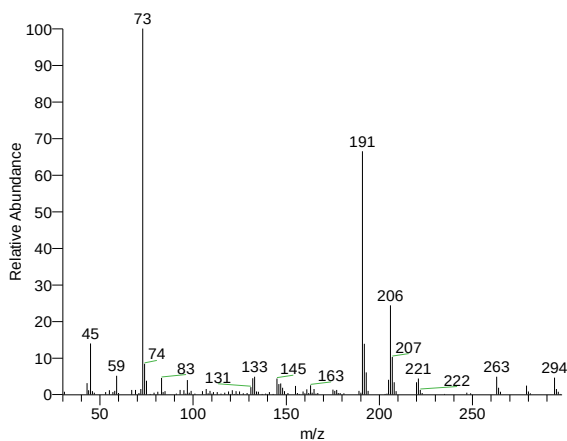
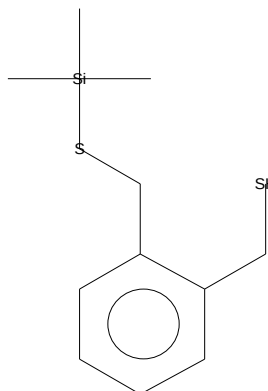
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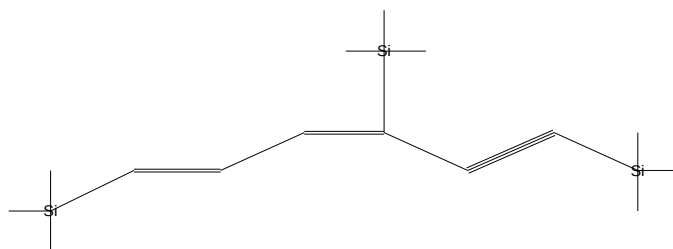
Compound Structure



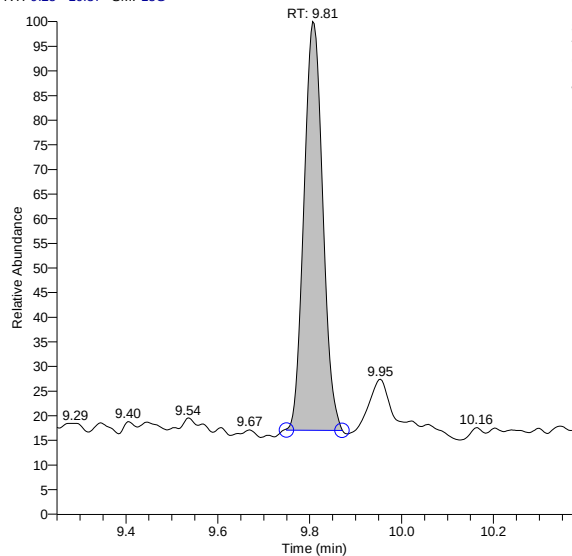
1,2-Benzenedimethanethiol, TMS derivative
Formula C₁₁H₁₈S₂Si, MW 242, CAS# NA, Entry# 42385
1,2-Benzenedimethanethiol, S-trimethylsilyl-



3,5-Hexadien-1-yne, 1,3,6-tris(trimethylsilyl)-, (E,E)-
Formula C₁₅H₃₀Si₃, MW 294, CAS# NA, Entry# 43125
[(1E,3E)-4,6-Bis(trimethylsilyl)-1,3-hexadien-5-ynyl](trimethyl)silane #

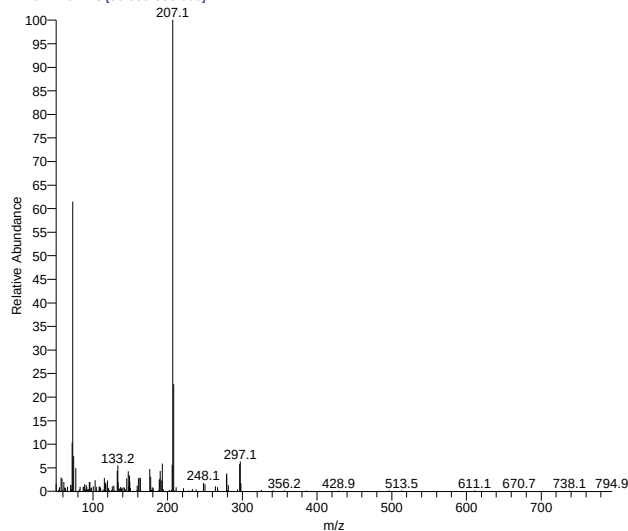


RT: 9.25 - 10.37 SM: 15G



NL:
8.53E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #1136 RT: 9.81 AV: 1 RF: 6.00, 3 NL: 2.57E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	Methyltris(trimethylsiloxy)silane	1996102.51	16.86	617	638	mainlib
9.81	Tetrasiloxane, decamethyl-	1996102.51	10.55	603	630	mainlib

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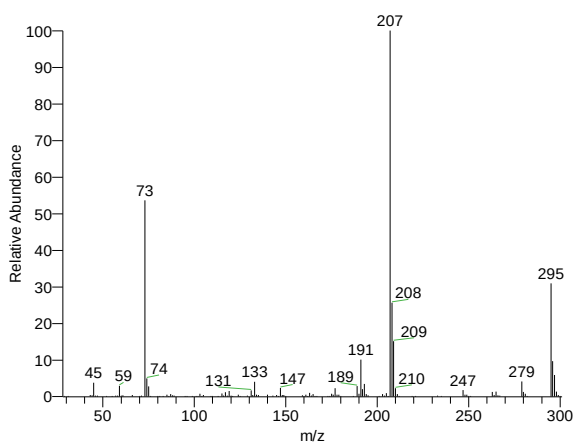
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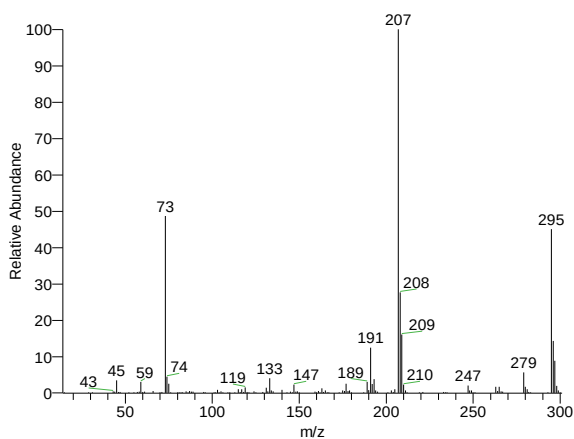
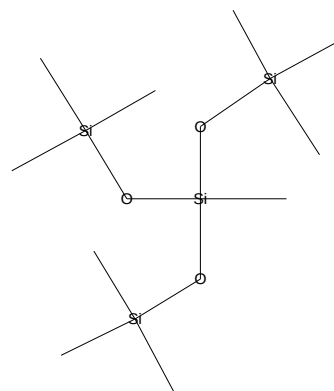
RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	Arsenous acid, tris(trimethylsilyl) ester	1996102.51	9.33	600	709	mainlib
9.81	Thymol, TBDMS derivative	1996102.51	7.88	596	695	mainlib
9.81	4-tert-Amylphenol, TMS derivative	1996102.51	7.27	594	665	mainlib

Hit Spectrum

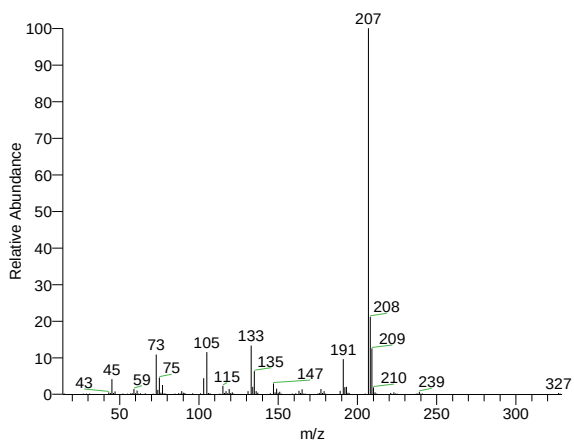
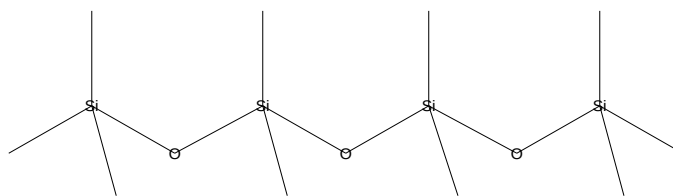
Compound Structure



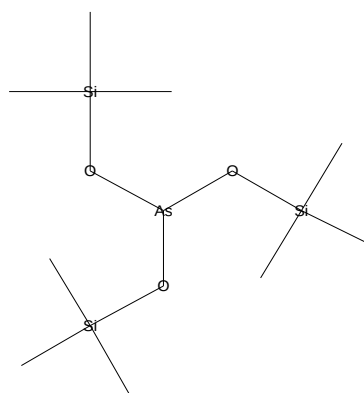
Methyltris(trimethylsiloxy)silane
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



Tetrasiloxane, decamethyl-
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 141-62-8, Entry# 188653
Decamethyltetrasiloxane



Arsenous acid, tris(trimethylsilyl) ester
Formula C₉H₂₇AsO₃Si₃, MW 342, CAS# 55429-29-3, Entry# 188948
\$:28CWZNQWMMDOIFQC-UHFFFAOYSA-N



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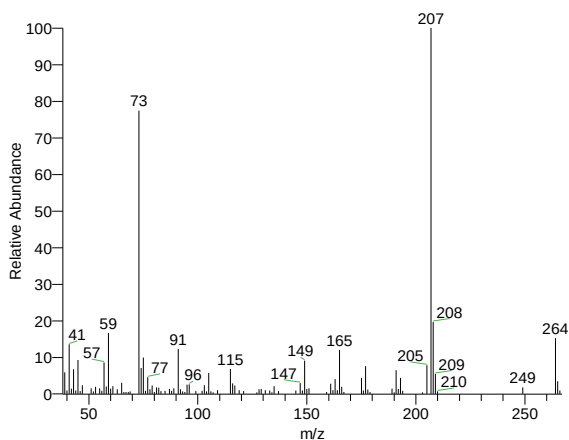
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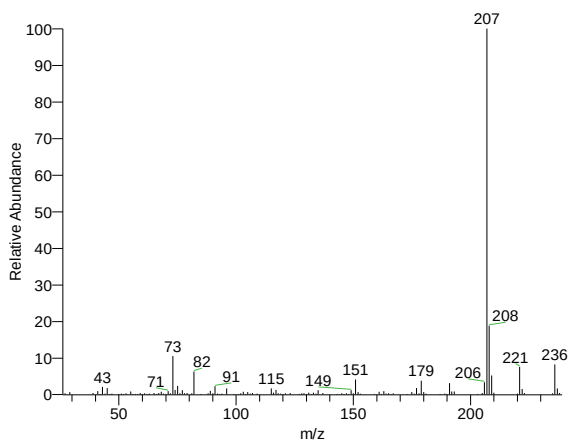
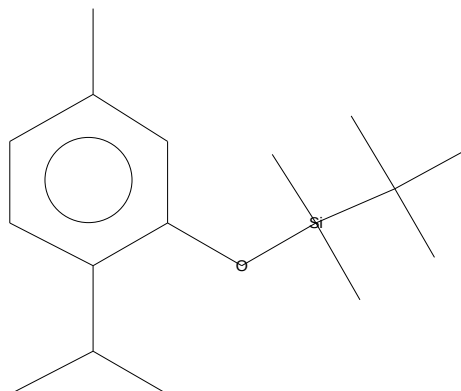
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

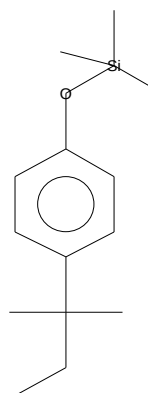
Compound Structure



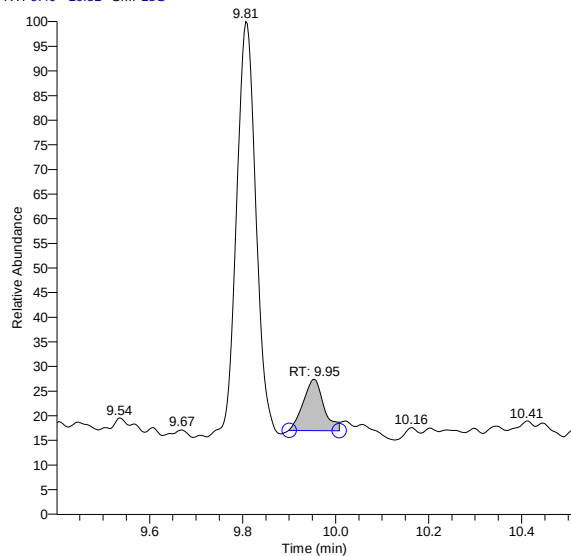
Thymol, TBDMS derivative
Formula C₁₆H₂₈O₂Si, MW 264, CAS# 330455-64-6, Entry# 188649
Benzene, 2-[(tert-butyltrimethylsilyl)oxy]-1-isopropyl-4-methyl-



4-tert-Amylphenol, TMS derivative
Formula C₁₄H₂₄O₂Si, MW 236, CAS# NA, Entry# 188939
4-(1,1-Dimethylpropyl)phenol, trimethylsilyl ether

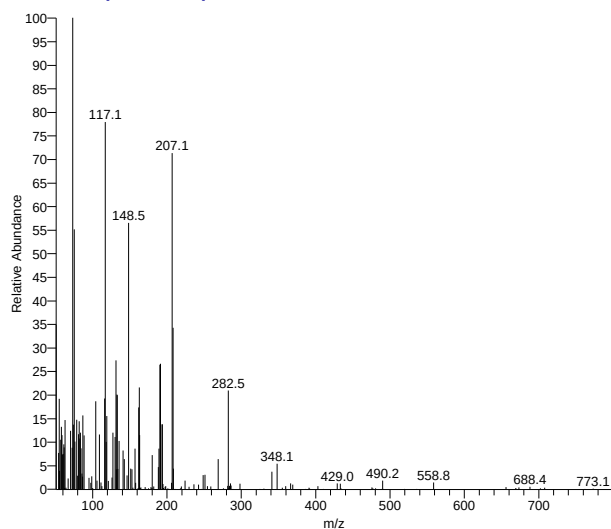


RT: 9.40 - 10.51 SM: 15G



NL:
8.53E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #1180 RT: 9.95 AV: 1 RF: 6.00, 3 NL: 2.31E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.95	2-Methylbenzamide oxime, O-tert.-butyldimethylsilyl-	270872.06	7.52	454	519	mainlib

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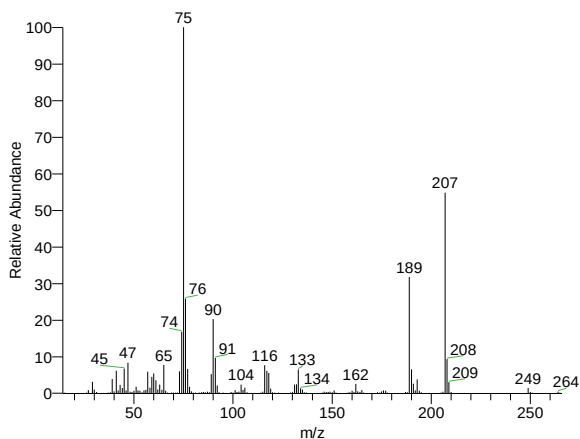
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

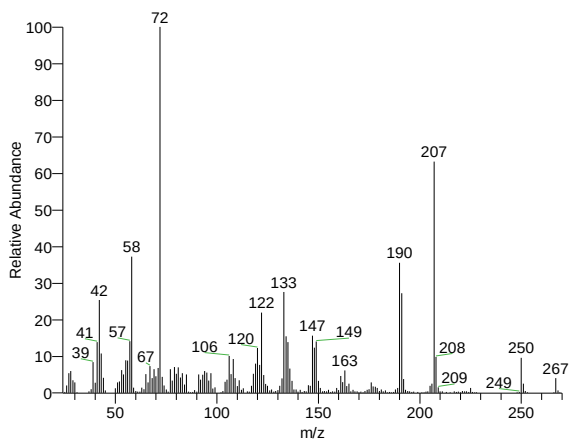
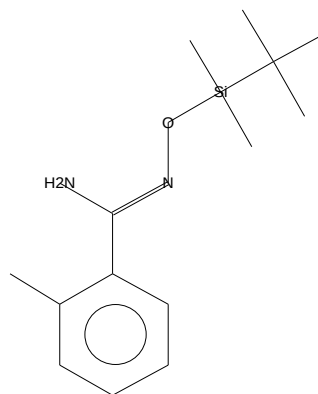
RT	Compound Name	Area	Probability	SI	RSI	Library
9.95	1-(2-Acetoxyethyl)-3,6-diazahomoadamantan-9-one oxime	270872.06	6.35	450	482	mainlib
9.95	2-Acetoxyacetate, TMS derivative	270872.06	5.12	445	686	mainlib
9.95	4-Trimethylsilylmethylbenzamide	270872.06	3.30	432	474	mainlib
9.95	3,7,11,15,18-Pentaoxa-2,19-disilaicosane, 2,2,19,19-tetramethyl-	270872.06	2.79	428	482	mainlib

Hit Spectrum

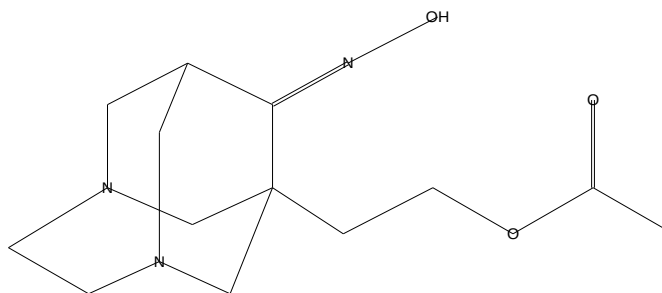
Compound Structure



2-Methylbenzamide oxime, O-tert.-butyldimethylsilyl-
Formula C₁₄H₂₄N₂O₂Si, MW 264, CAS# NA, Entry# 46002
\$:28DXZOOUSILHIGHJ-UHFFFAOYSA-N



1-(2-Acetoxyethyl)-3,6-diazahomoadamantan-9-one oxime
Formula C₁₃H₂₁N₃O₃, MW 267, CAS# NA, Entry# 40369
\$:28AJPFDLSTNHSVQG-OWBHPGMISA-N



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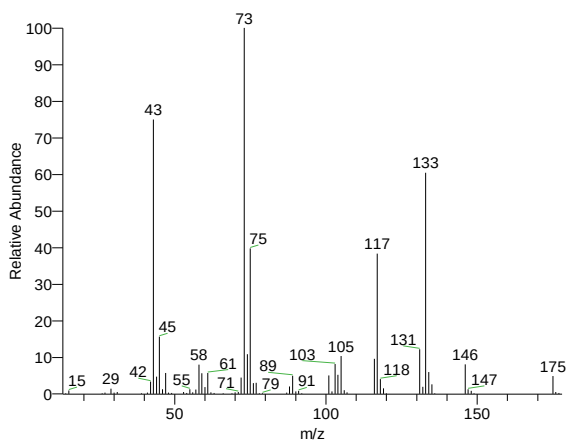
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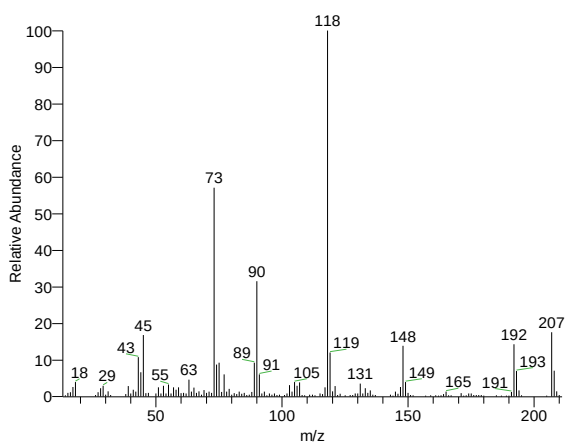
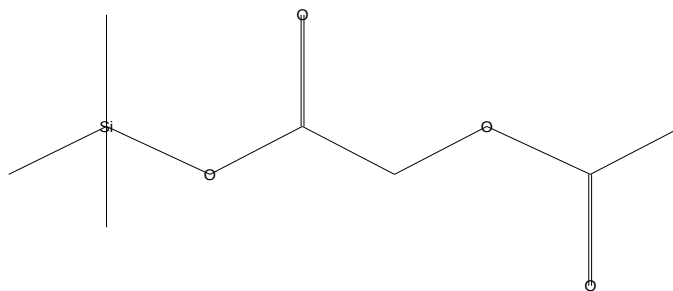
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

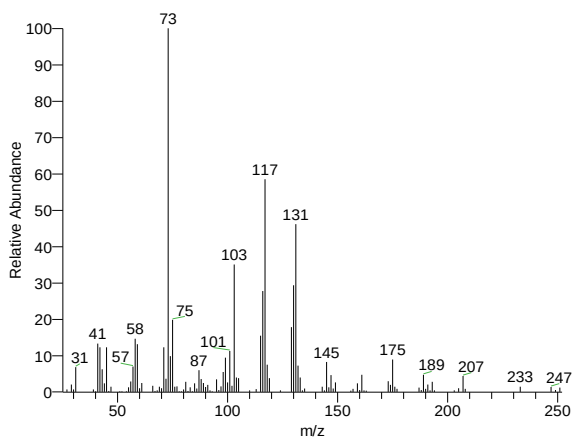
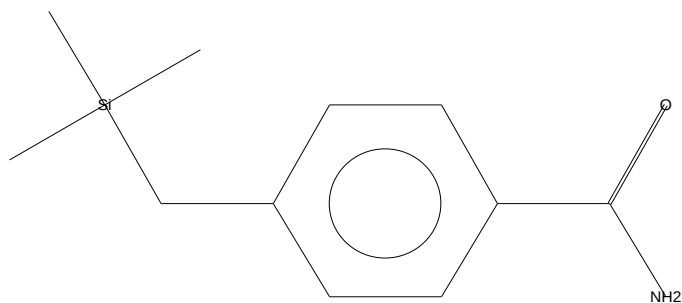
Compound Structure



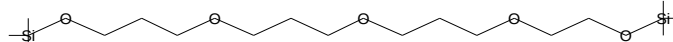
2-Acetoxyacetate, TMS derivative
Formula C₇H₁₄O₄Si, MW 190, CAS# NA, Entry# 40668
Trimethylsilyl 2-acetoxyacetate



4-Trimethylsilylmethylbenzamide
Formula C₁₁H₁₇NOSi, MW 207, CAS# 17095-22-6, Entry# 97868
\$.28APSUDKBZJORVFP-UHFFFAOYSA-N



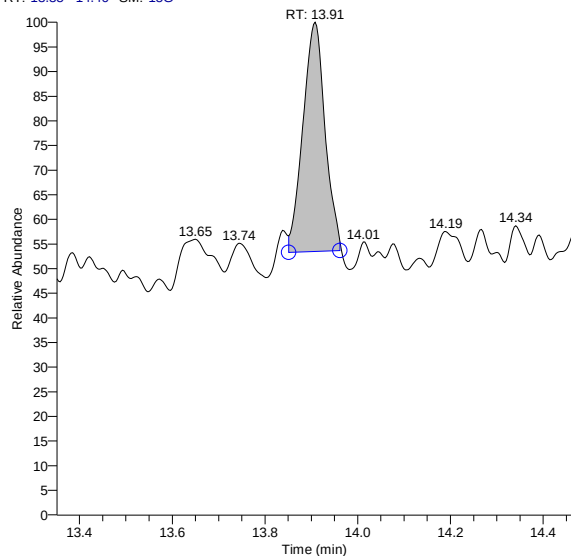
3,7,11,15,18-Pentaoxa-2,19-disilaicosane, 2,2,19,19-tetramethyl-
Formula C₁₇H₄₀O₅Si₂, MW 380, CAS# NA, Entry# 42186
2,2,19,19-Tetramethyl-3,6,10,14,18-pentaoxa-2,19-disilaicosane #



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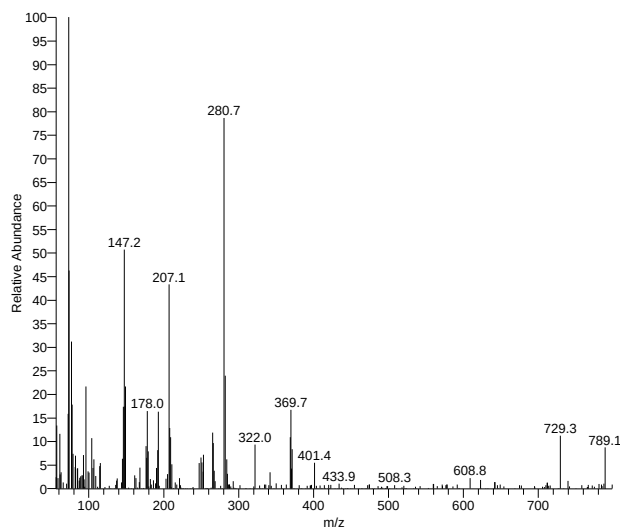
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RT: 13.35-14.46 SM: 15G



NL:
3.12E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

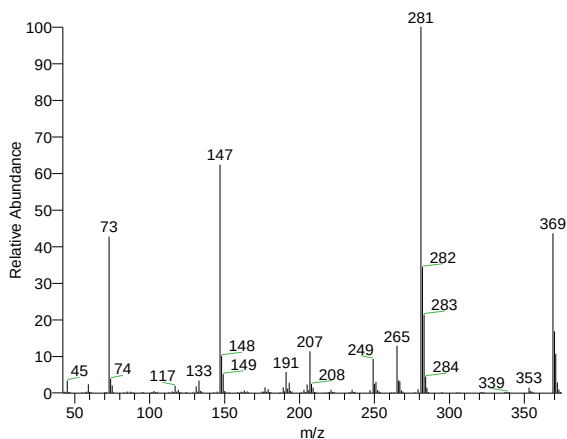
NGA-ZE-WATER2-SAMPLE-INJ1 #2359 RT: 13.91 AV: 1 RF: 6.00, 3 NL: 3.78E4
T: + c EI Full ms [50.000-800.000]



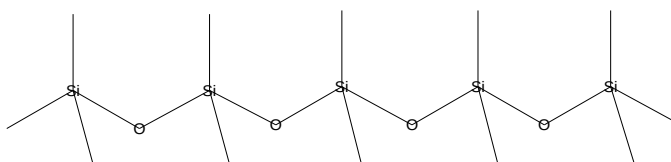
RT	Compound Name	Area	Probability	SI	RSI	Library
13.91	Pentasiloxane, dodecamethyl-	480076.81	30.57	486	629	mainlib
13.91	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3, 3-bis[(trimethylsilyl)oxy]-	480076.81	27.01	483	655	mainlib
13.91	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	480076.81	13.11	464	815	mainlib
13.91	benzoic acid, 4-[[[(trimethylsilyl)oxy]methyl]-, trimethylsilyl ester	480076.81	3.64	434	631	mainlib
13.91	Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester	480076.81	3.36	432	609	mainlib

Hit Spectrum

Compound Structure



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



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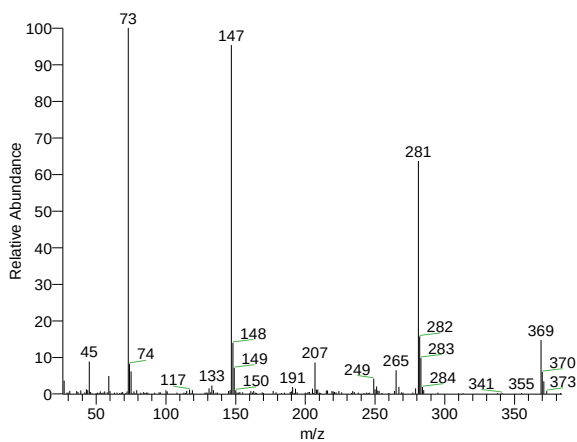
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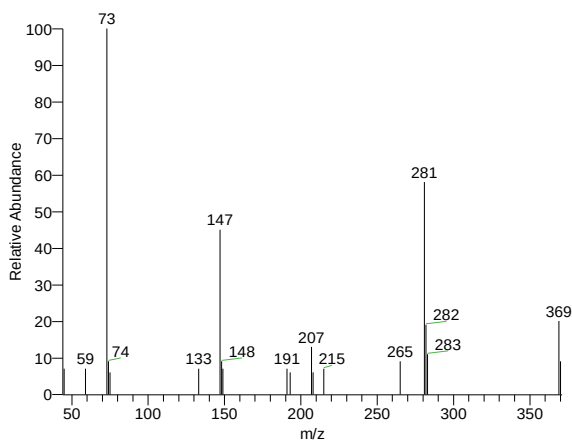
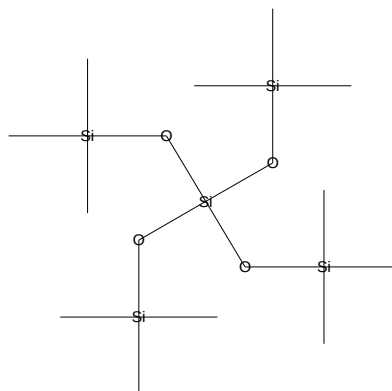
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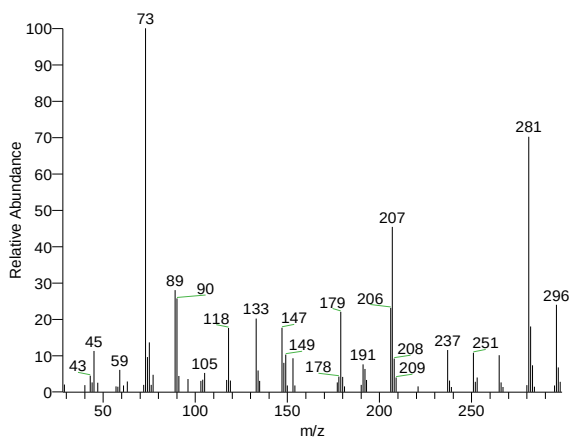
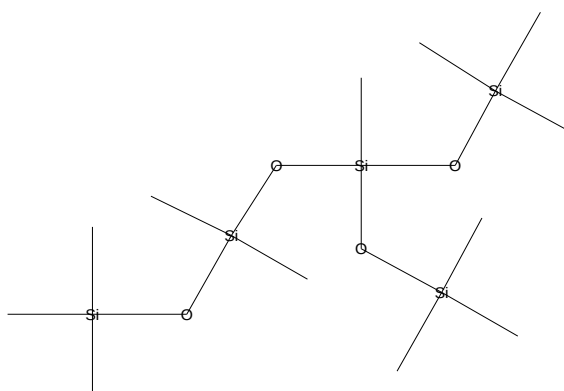
Compound Structure



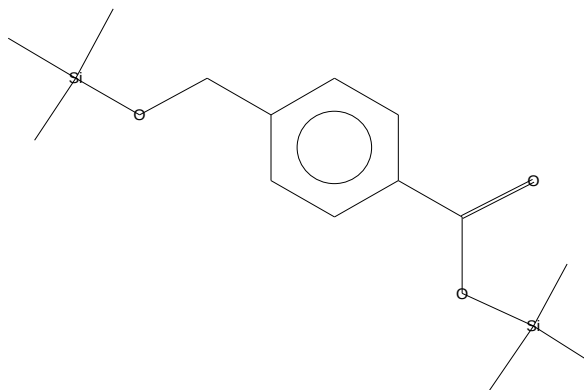
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



benzoic acid, 4-[[[(trimethylsilyl)oxy]methyl]-, trimethylsilyl ester
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 43770
trimethylsilyl 4-[[[(trimethylsilyl)oxy]methyl]benzoate

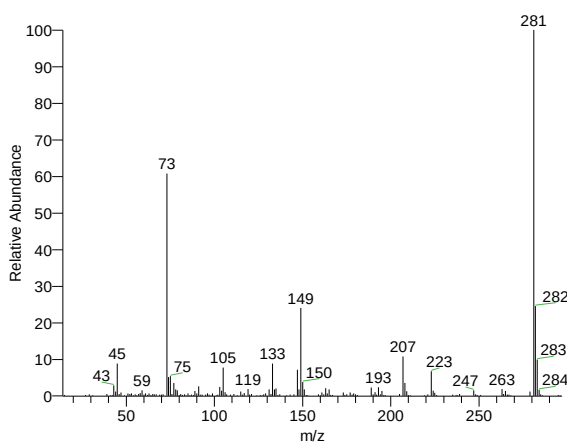


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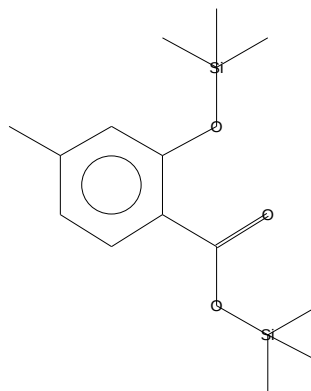
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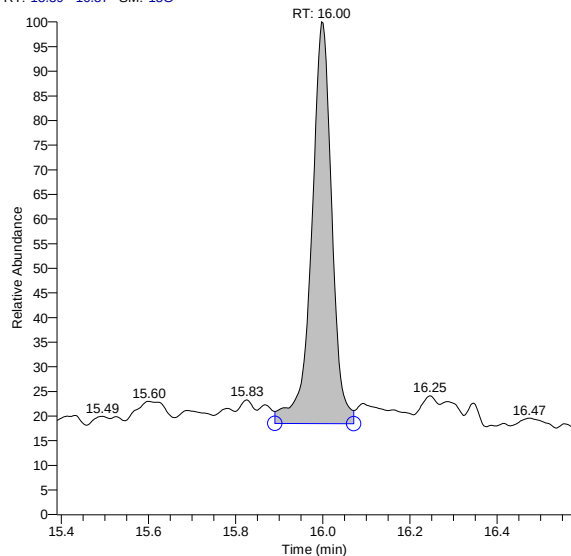
Compound Structure



Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# 35-27-8, Entry# 219921
\$.28WMMUZRDZZSRQEF-UHFFFAOYSA-N

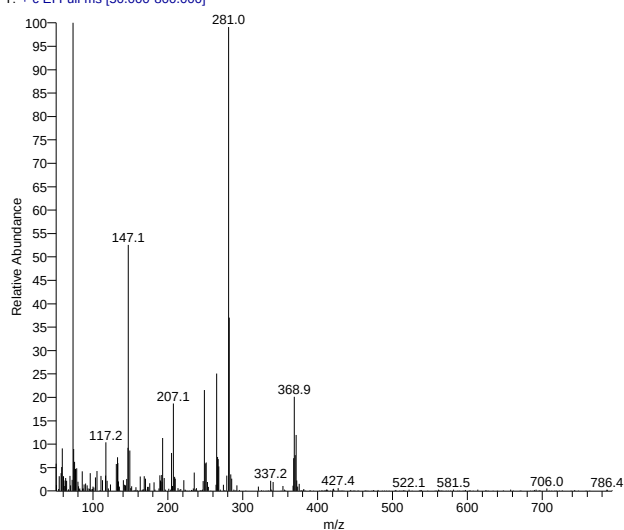


RT: 15.39 - 16.57 SM: 15G



NL:
9.22E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #2982 RT: 16.00 AV: 1 RF: 6.00, 3 NL: 1.40E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
16.00	Pentasiloxane, dodecamethyl-	2416677.42	79.37	721	782	mainlib
16.00	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3, 3-bis[(trimethylsilyl)oxy]-	2416677.42	14.08	661	739	mainlib
16.00	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	2416677.42	2.36	598	871	mainlib
16.00	trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-	2416677.42	1.90	593	787	mainlib
16.00	2,6-Dihydroxyacetophenone, 2TMS derivative	2416677.42	0.55	566	656	mainlib

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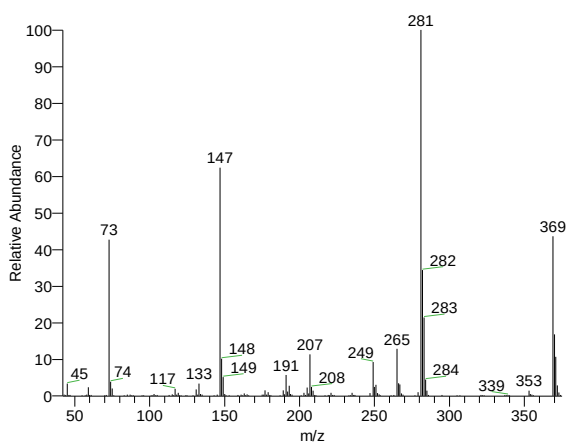
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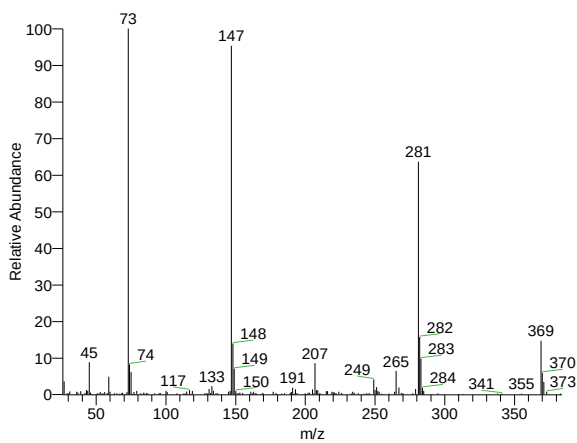
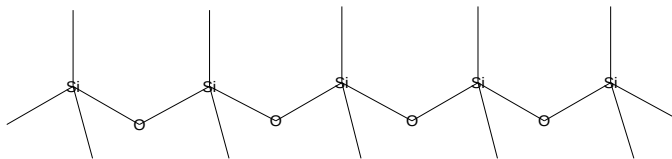
ANALYTICAL CHEMISTRY DIVISION

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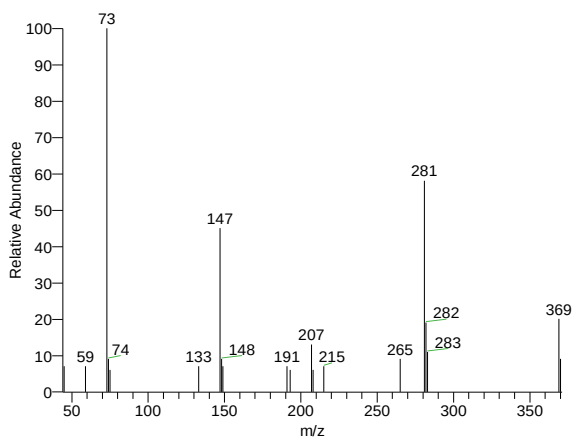
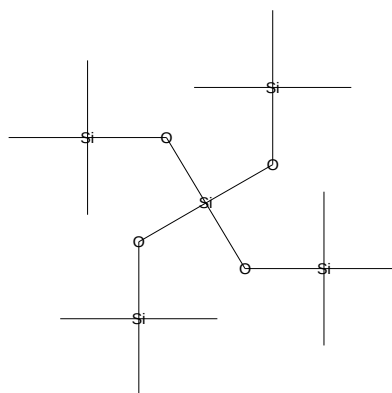
Compound Structure



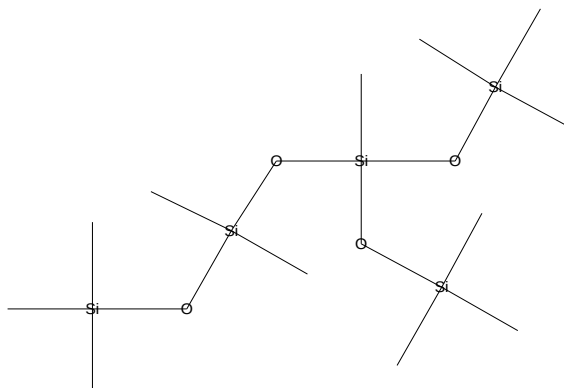
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

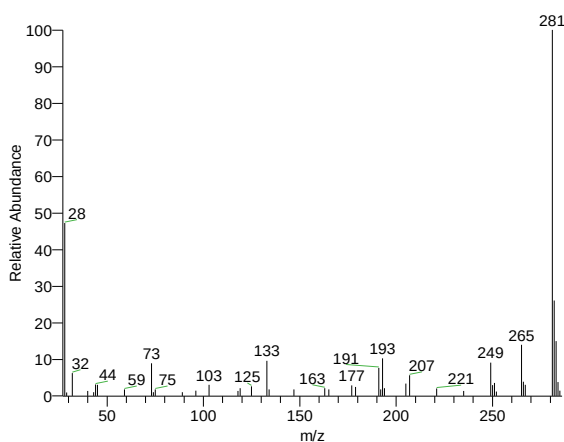


Analysed by Satyanarayana

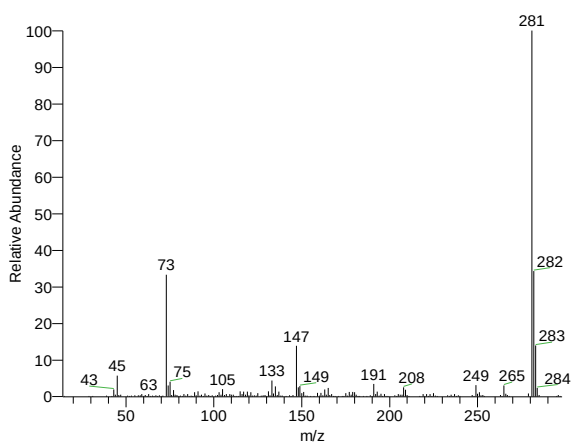
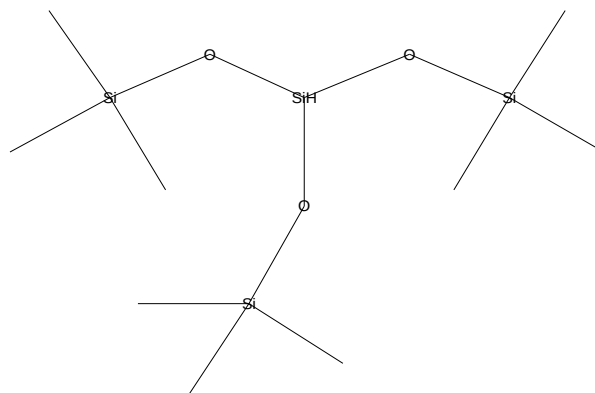
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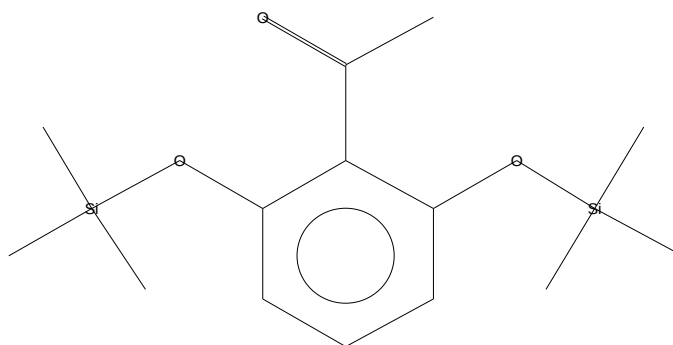
Compound Structure



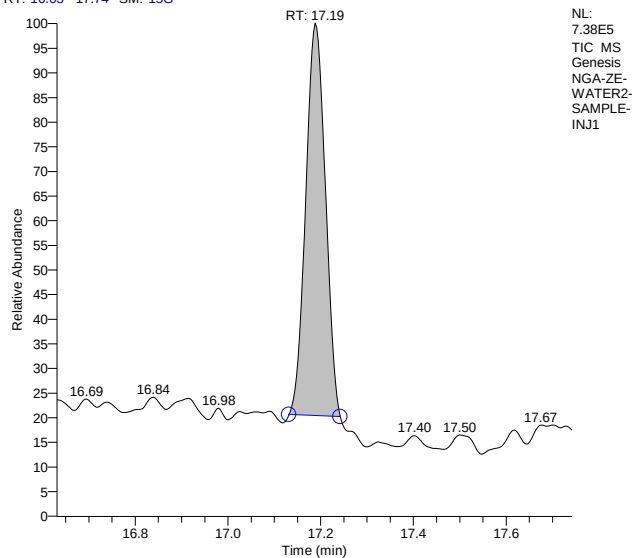
trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-
Formula C₉H₂₈O₃Si₄, MW 296, CAS# NA, Entry# 219896
1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]trisiloxane



2,6-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220073
2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

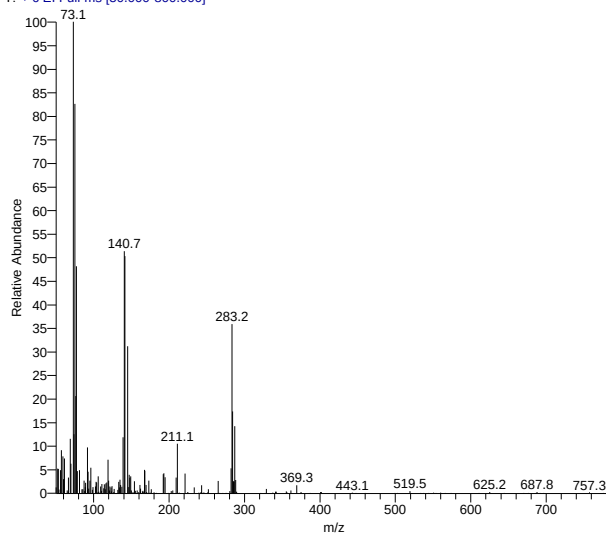


RT: 16.63 - 17.74 SM: 15G



NL:
7.38E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #3337 RT: 17.19 AV: 1 RF: 6.00, 3 NL: 1.23E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
17.19	N'-(3-Pyridinylmethylene) isonicotinohydrazide, TBDMS derivative	1724179.98	8.32	454	480	mainlib

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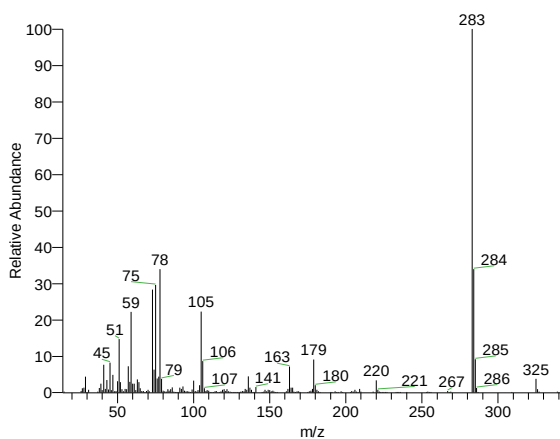
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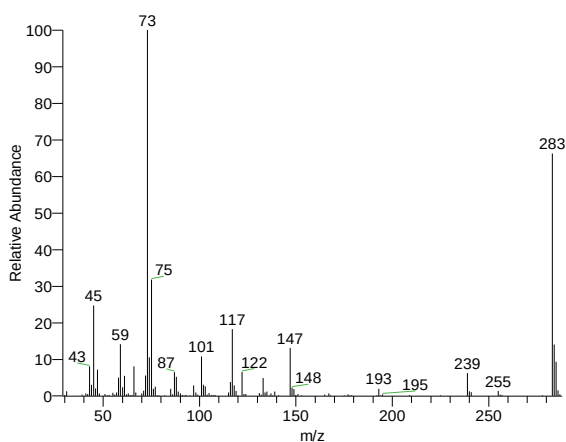
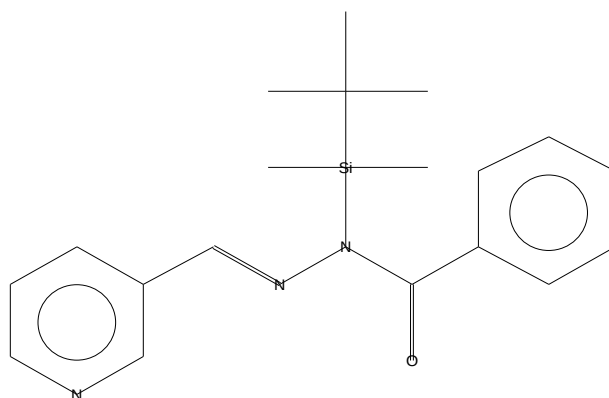
RT	Compound Name	Area	Probability	SI	RSI	Library
17.19	2,2'-Sulfonyldiethanol, 2TMS derivative	1724179.98	6.37	447	513	mainlib
17.19	t-Butyl-(2-[3-(2,2-dimethyl-6-methylene-cyclohexyl)-propyl]-[1,3]dithian-2-yl)-dimethyl-silane	1724179.98	5.01	441	463	mainlib
17.19	N'-(3-Pyridinylmethylene)isonicotinohydrazide, TMS derivative	1724179.98	3.94	435	459	mainlib
17.19	n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester	1724179.98	2.94	427	487	mainlib

Hit Spectrum

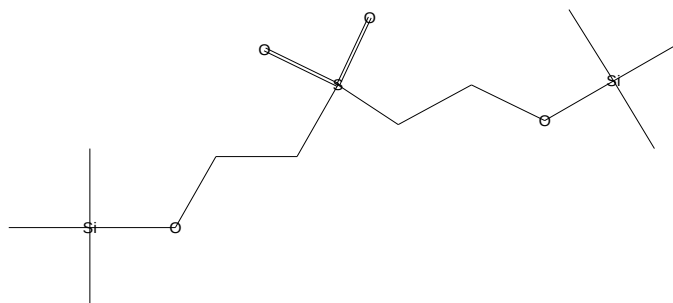
Compound Structure



N'-(3-Pyridinylmethylene)isonicotinohydrazide, TBDMS derivative
Formula C₁₈H₂₄N₄O₃Si, MW 340, CAS# NA, Entry# 220559
N'-(3-Pyridinylmethylene)isonicotinohydrazide tbdms



2,2'-Sulfonyldiethanol, 2TMS derivative
Formula C₁₀H₂₆O₄Si₂, MW 298, CAS# 97916-04-6, Entry# 43779
bis [2-Trimethylsiloxy]ethyl sulfone

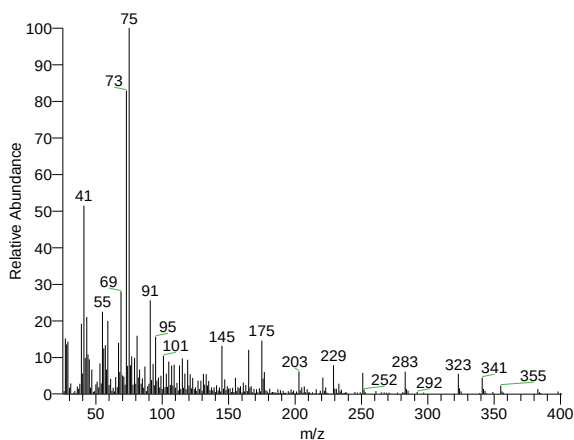


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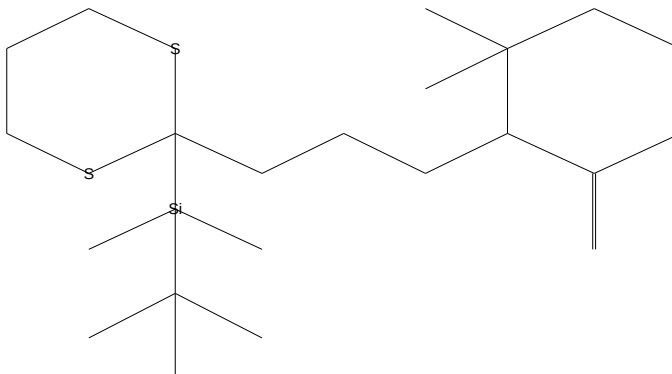
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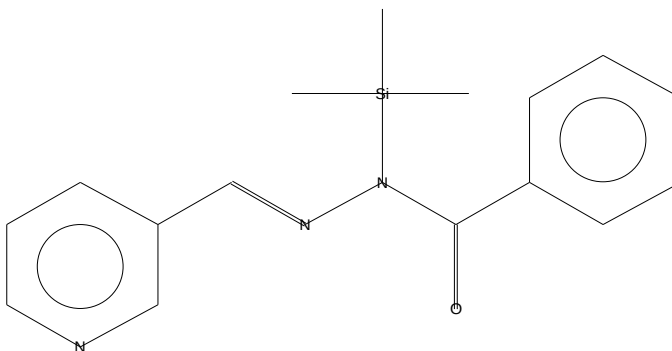
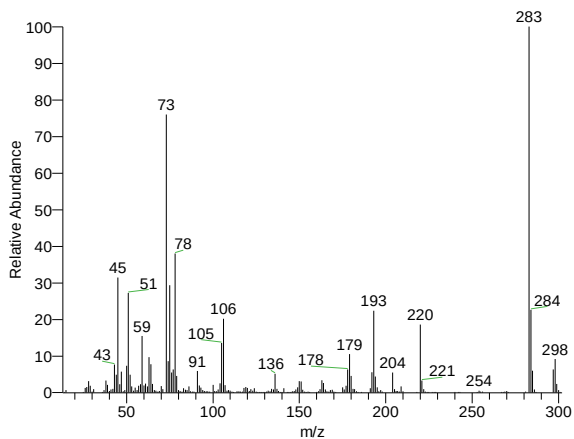
Compound Structure



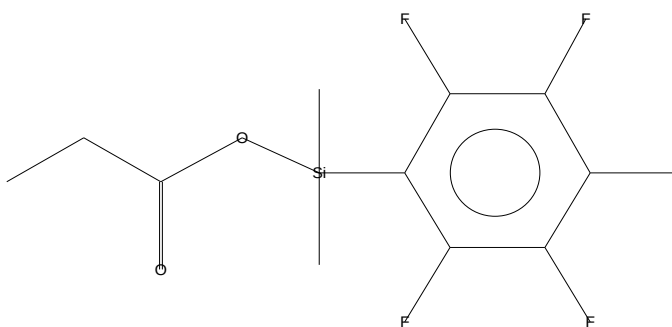
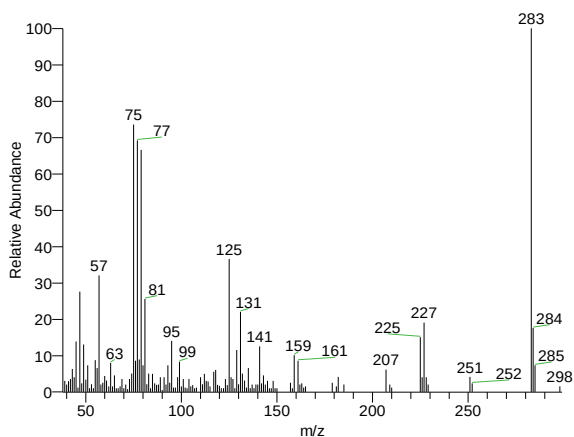
t-Butyl(2-[3-(2,2-dimethyl-6-methylene-cyclohexyl)-propyl]-[1,3]dithian-2-yl)-dimethyl-silane
Formula C₂₂H₄₂S₂Si, MW 398, CAS# 95472-42-7, Entry# 45252
tert-Butyl(2-[3-(2,2-dimethyl-6-methylenecyclohexyl)propyl]-1,3-dithian-2-yl)dimethylsilane #



N'-(3-Pyridinylmethylene)isonicotinohydrazide, TMS derivative
Formula C₁₅H₁₈N₄O₂Si, MW 298, CAS# NA, Entry# 220546
N'-(3-Pyridinylmethylene)isonicotinohydrazide tms



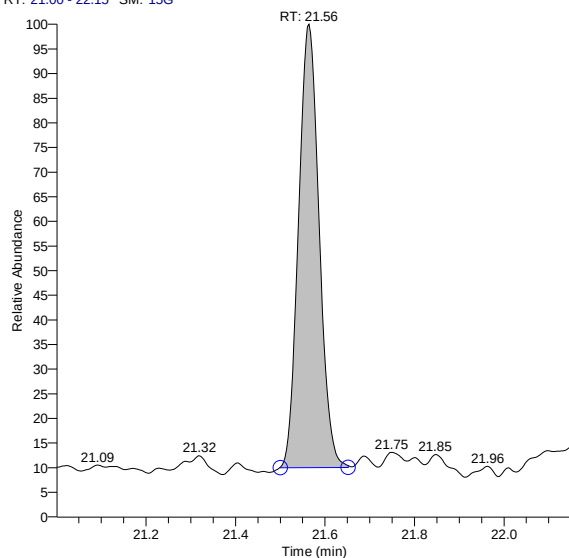
n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester
Formula C₁₁H₁₁F₅O₂Si, MW 298, CAS# NA, Entry# 220549
Dimethyl(2,3,4,5,6-pentafluorophenyl)silyl propionate #



Analysed by Satyanarayana

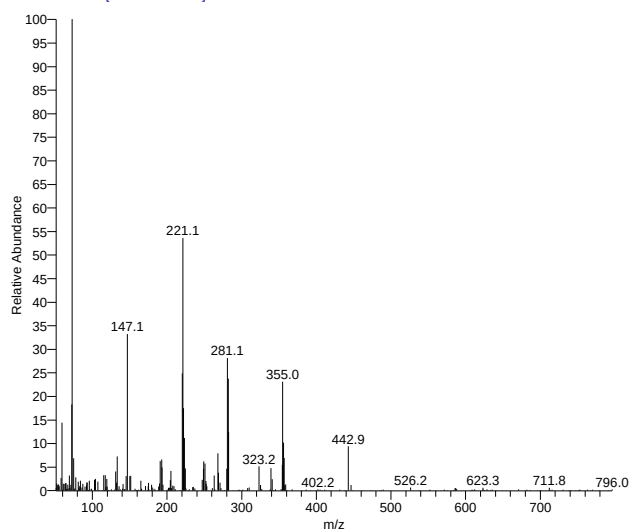
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RT: 21.00 - 22.15 SM: 15G



NL:
1.01E6
TIC: MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

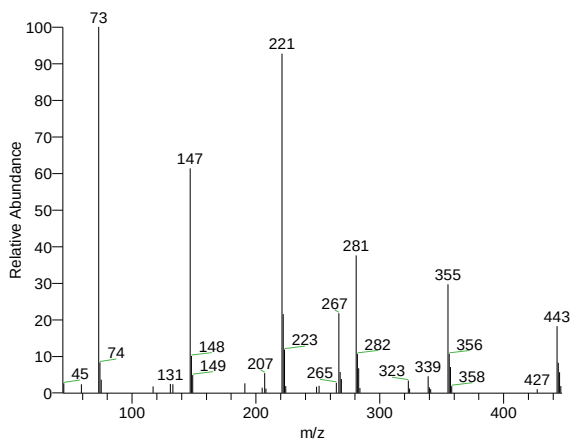
NGA-ZE-WATER2-SAMPLE-INJ1 #4642 RT: 21.56 AV: 1 RF: 6.00, 3 NL: 1.53E5
T: + c EI Full ms [50.000-800.000]



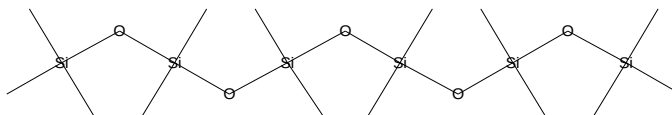
RT	Compound Name	Area	Probability	SI	RSI	Library
21.56	Hexasiloxane, tetradecamethyl-	2912737.18	82.87	638	787	mainlib
21.56	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2912737.18	2.48	493	552	mainlib
21.56	2,5-Dihydroxybenzoic acid, 3TMS derivative	2912737.18	1.80	484	514	mainlib
21.56	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2912737.18	1.38	477	534	mainlib
21.56	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2912737.18	1.32	476	531	mainlib

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Compound Structure



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



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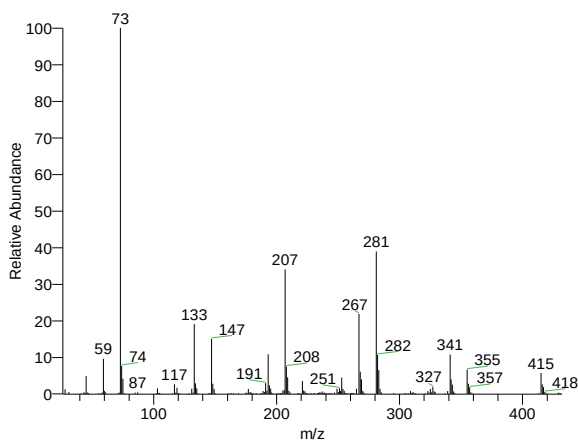
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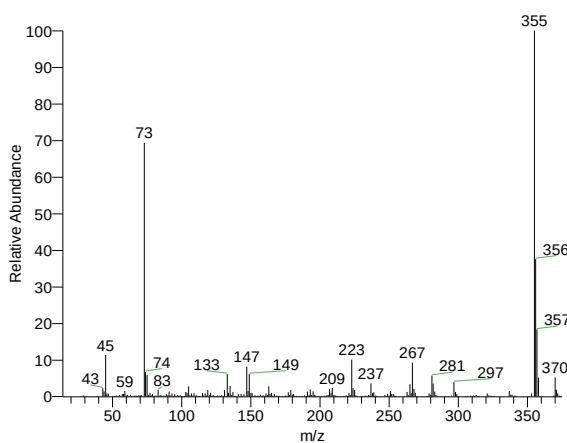
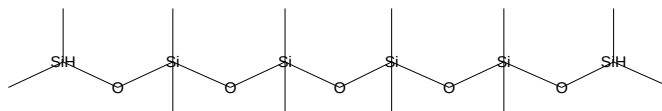
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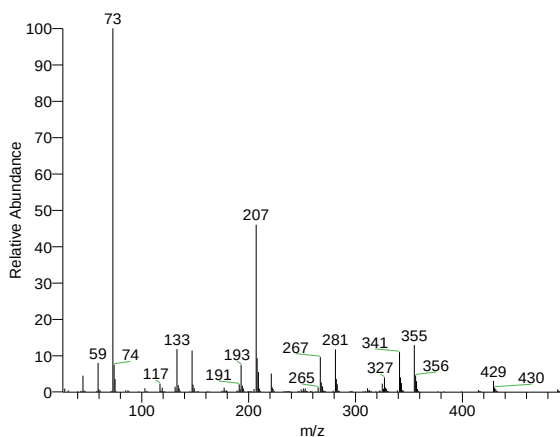
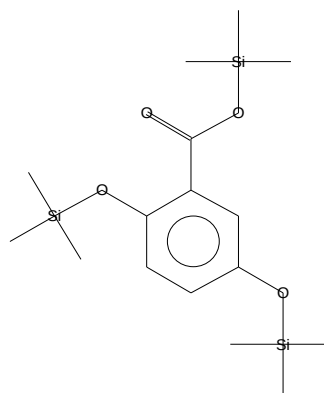
Compound Structure



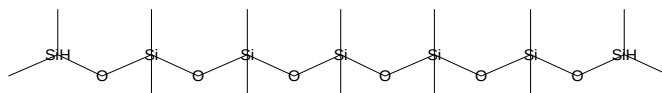
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



2,5-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-20-0, Entry# 234286
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

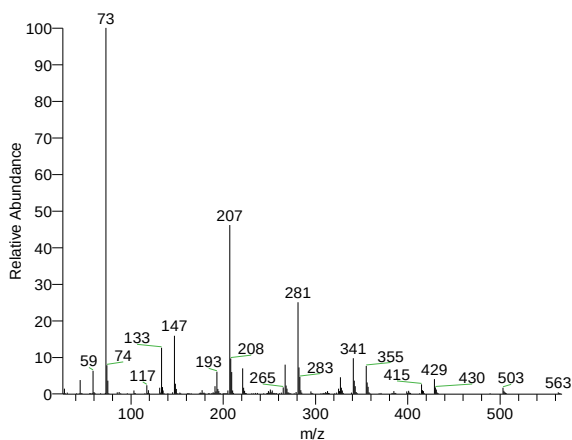


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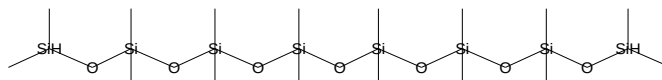
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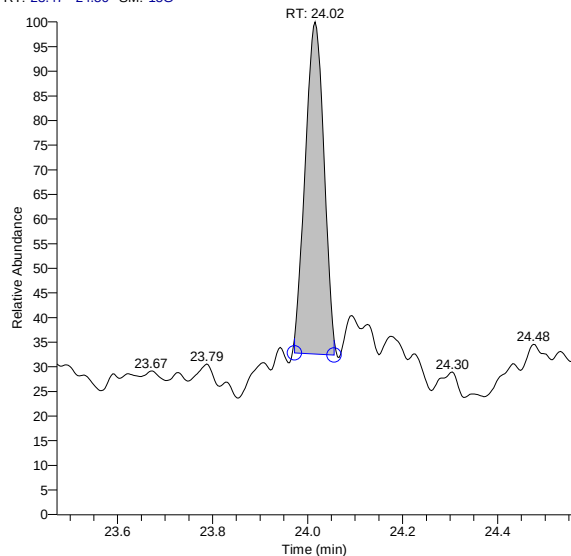
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #

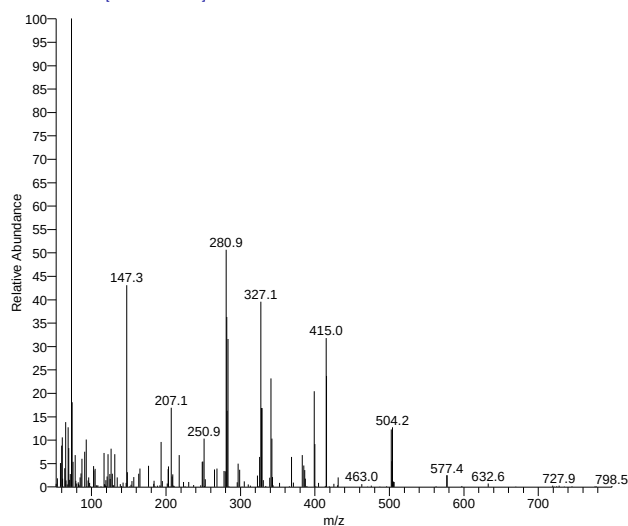


RT: 23.47 - 24.56 SM: 15G



NL:
2.69E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #5373 RT: 24.02 AV: 1 RF: 6.00, 3 NL: 3.88E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
24.02	Cycloheptasiloxane, tetradecamethyl-	496923.20	89.92	650	739	mainlib
24.02	3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	496923.20	3.98	524	660	mainlib
24.02	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	496923.20	3.21	519	652	mainlib
24.02	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	496923.20	1.17	496	527	mainlib
24.02	Tetrasiloxane, 3,5-diethoxy-1,1,1,7,7,7-hexamethyl-3,5-bis(trimethylsiloxy)-	496923.20	0.46	474	751	mainlib

Analysed by Satyanarayana

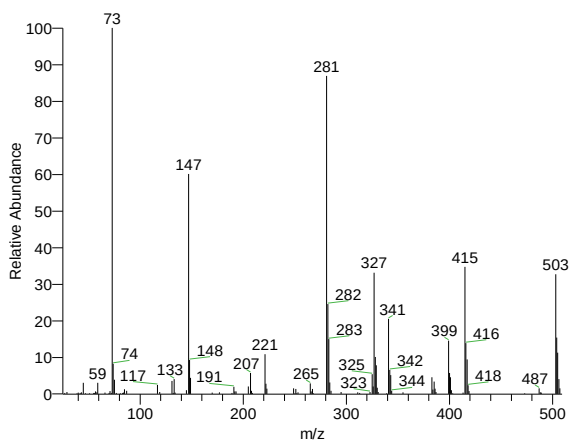
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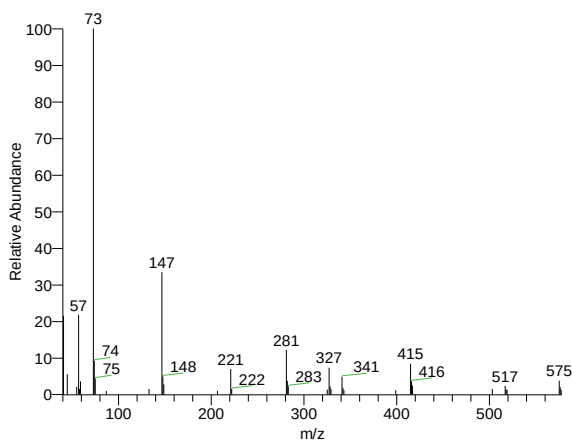
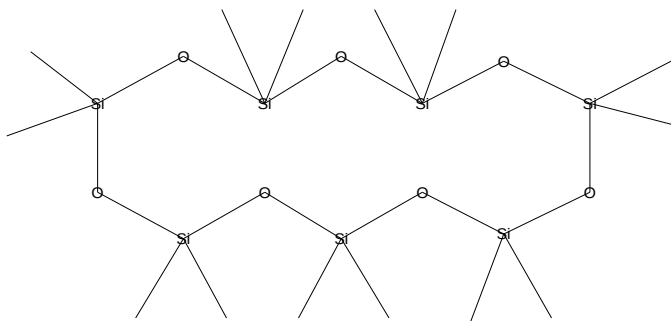
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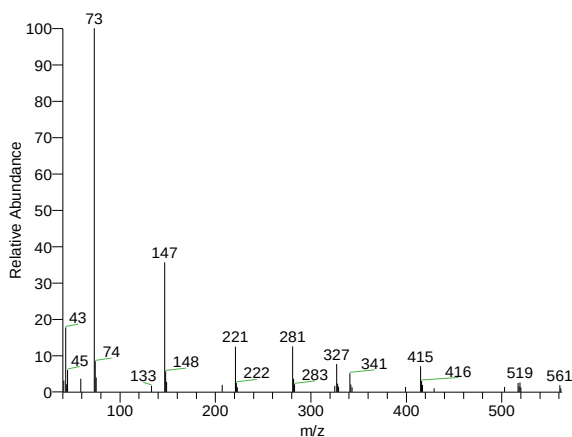
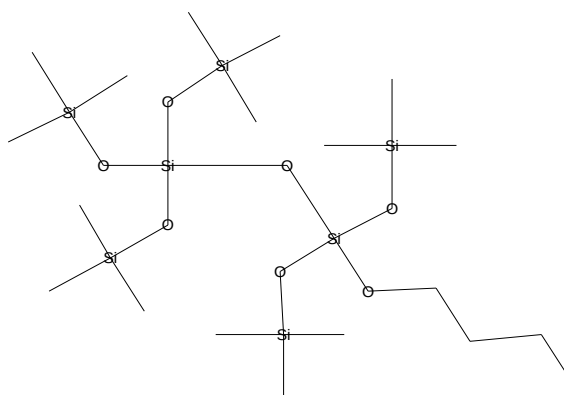
Compound Structure



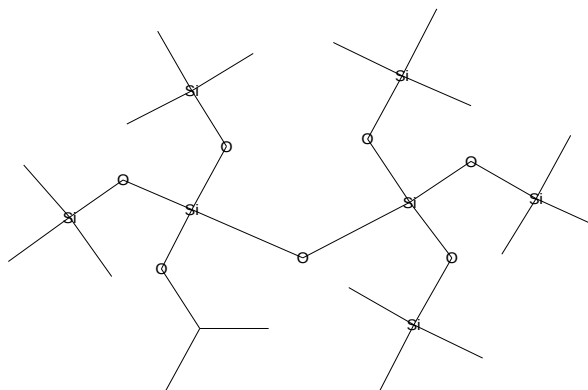
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane
Formula C₁₉H₅₄O₇Si₇, MW 590, CAS# 72439-84-0, Entry# 42504
1-Butoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl tris(trimethylsilyl) orthosilicate #



3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane
Formula C₁₈H₅₂O₇Si₇, MW 576, CAS# 71579-69-6, Entry# 42479
1-Isopropoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl tris(trimethylsilyl) orthosilicate #

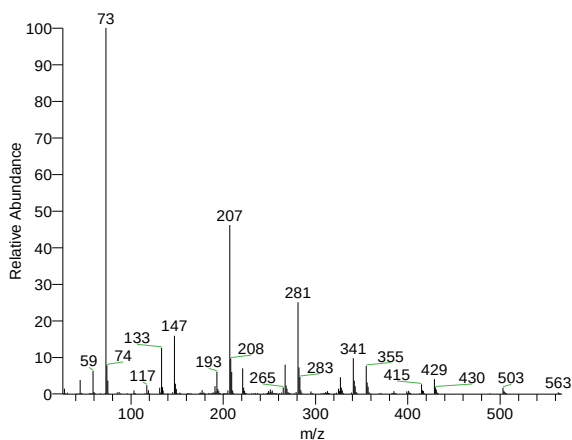


Analysed by Satyanarayana

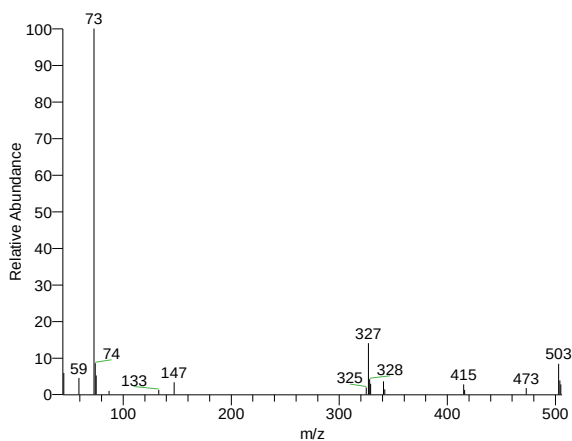
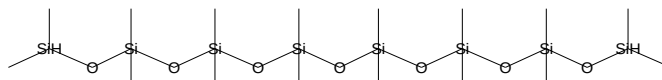
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Hit Spectrum

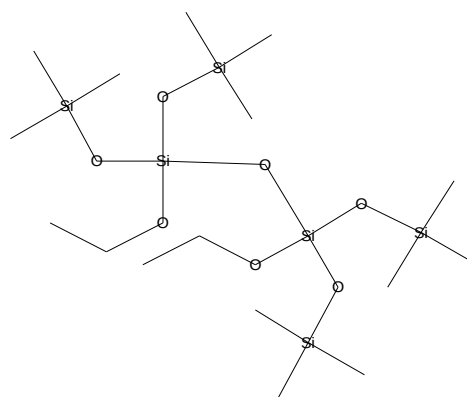
Compound Structure



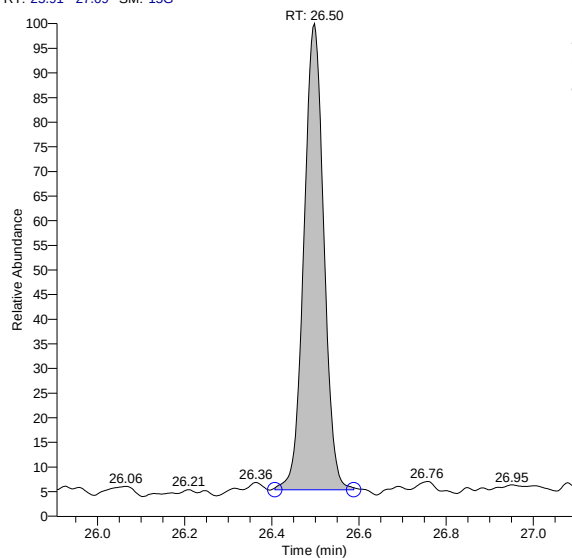
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Tetrasiloxane, 3,5-diethoxy-1,1,1,7,7,7-hexamethyl-3,5-bis(trimethylsiloxy)-
Formula C₁₆H₄₆O₇Si₆, MW 518, CAS# 72439-78-2, Entry# 44057
1-Ethoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl ethyl bis(trimethylsilyl) orthosilicate #

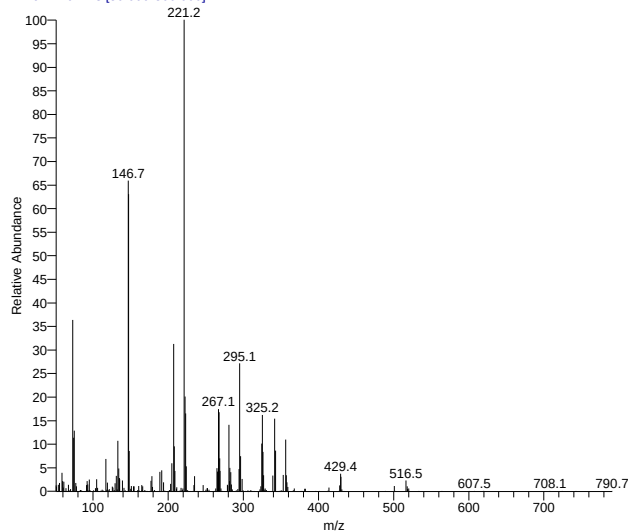


RT: 25.91 - 27.09 SM: 15G



NL:
1.33E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #6113 RT: 26.50 AV: 1 RF: 6.00, 3 NL: 1.91E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
26.50	Heptasiloxane, hexadecamethyl-	3973410.43	89.36	682	744	mainlib

Analysed by Satyanarayana

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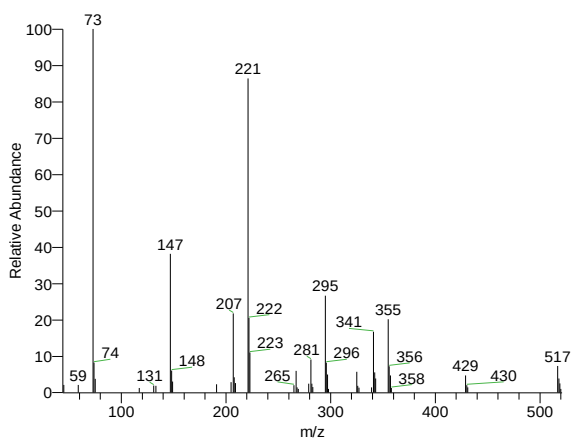
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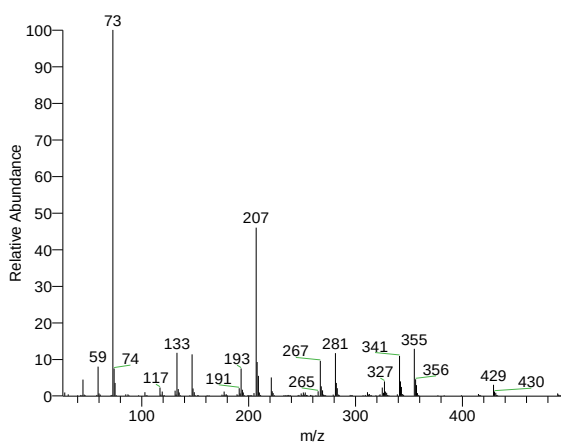
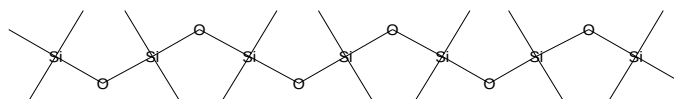
RT	Compound Name	Area	Probability	SI	RSI	Library
26.50	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3973410.43	2.82	539	564	mainlib
26.50	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3973410.43	2.38	535	561	mainlib
26.50	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3973410.43	1.23	517	546	mainlib
26.50	Hexasiloxane, tetradecamethyl-	3973410.43	1.23	517	677	mainlib

Hit Spectrum

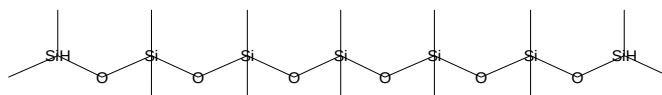
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

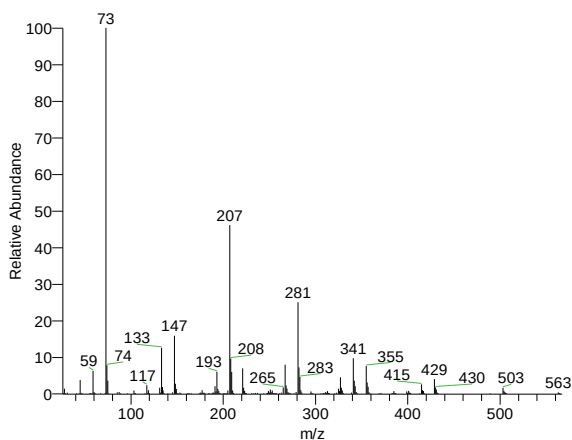


Analysed by Satyanarayana

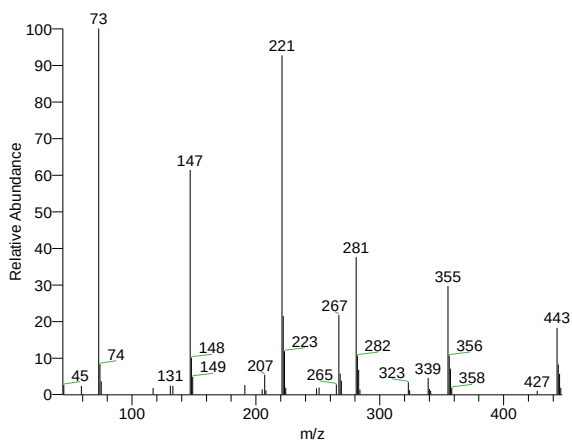
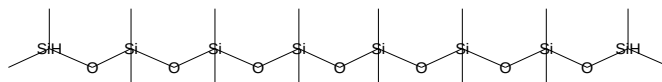
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Hit Spectrum

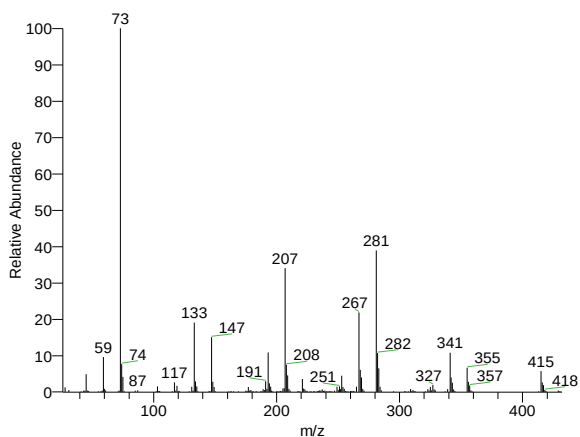
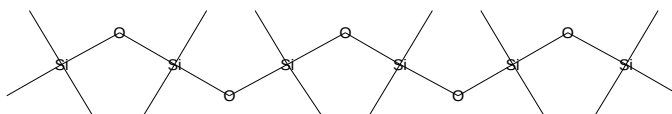
Compound Structure



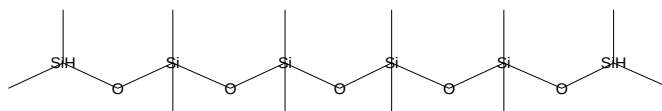
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



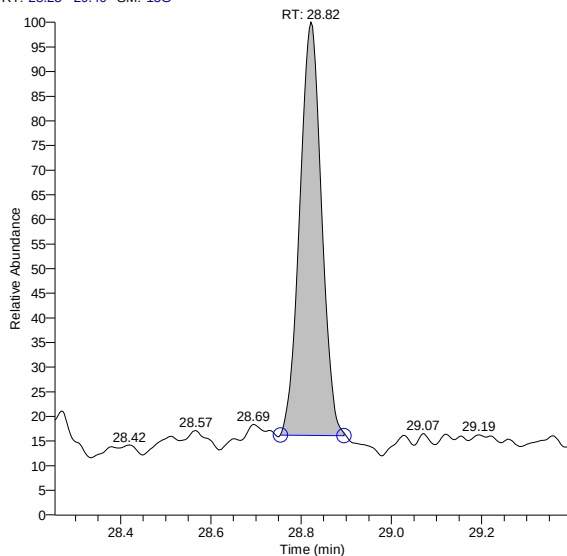
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Analysed by Satyanarayana

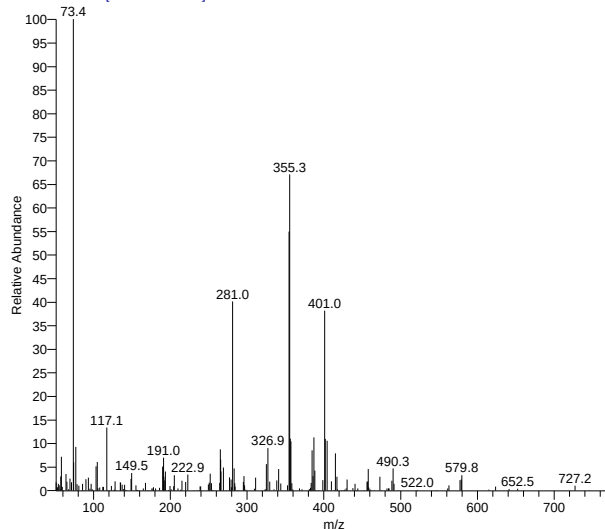
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RT: 28.25 - 29.40 SM: 15G



NL:
4.04E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

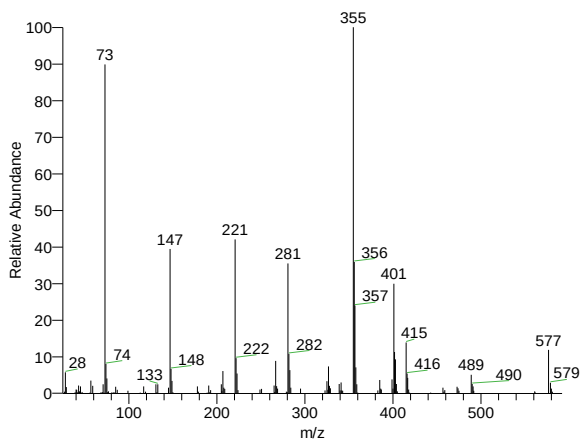
NGA-ZE-WATER2-SAMPLE-INJ1 #6806 RT: 28.82 AV: 1 RF: 6.00, 3 NL: 7.37E4
T: + c EI Full ms [50.000-800.000]



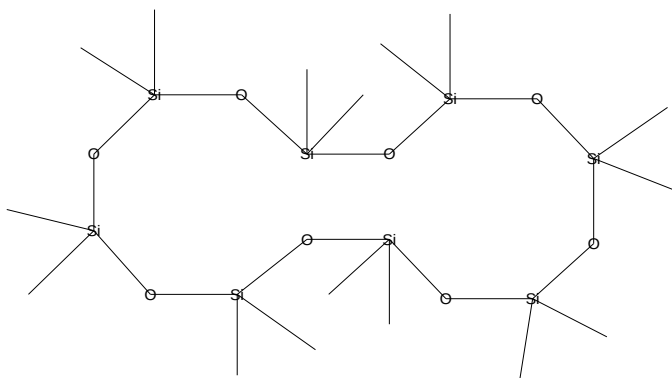
RT	Compound Name	Area	Probability	SI	RSI	Library
28.82	Cyclooctasiloxane, hexadecamethyl-	1139809.28	56.89	580	653	mainlib
28.82	3,4-Dihydroxyphenylglycol, 4TMS derivative	1139809.28	8.10	509	676	mainlib
28.82	(-)-Epinephrine, 3TMS derivative	1139809.28	5.07	495	645	mainlib
28.82	N-(Trifluoroacetyl)-O,O', O"-tris(trimethylsilyl)norepinephrine	1139809.28	3.27	482	754	mainlib
28.82	N-(Trifluoroacetyl)-O,O', O"-tris(trimethylsilyl)epinephrine	1139809.28	2.76	478	736	mainlib

Hit Spectrum

Compound Structure



Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane



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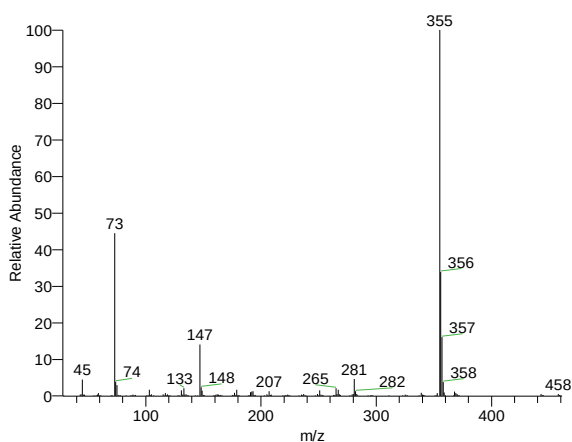
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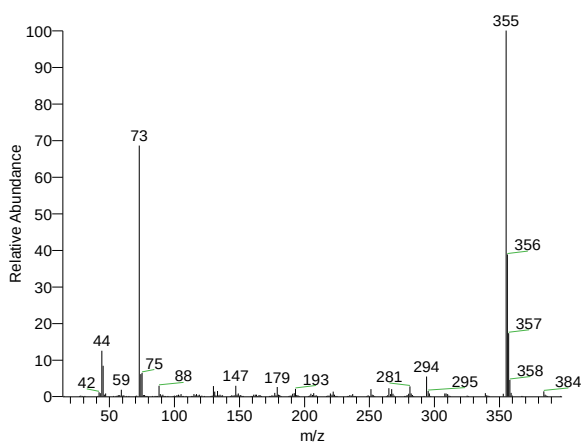
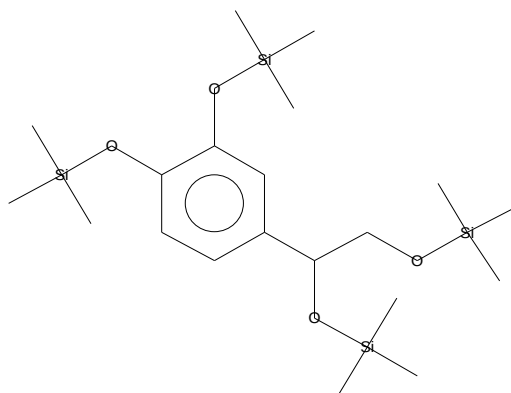
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

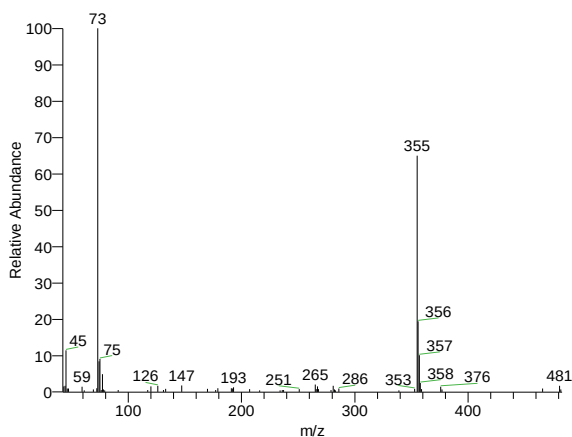
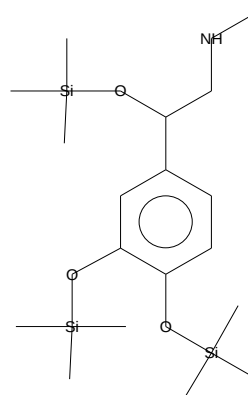
Compound Structure



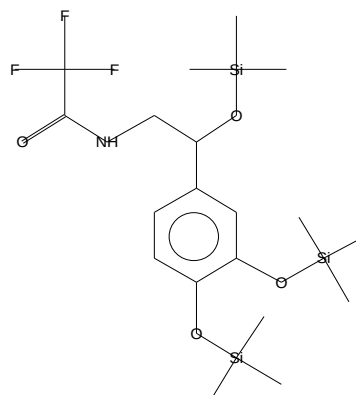
3,4-Dihydroxyphenylglycol, 4TMS derivative
Formula C₂₀H₄₂O₄Si₄, MW 458, CAS# 56114-62-6, Entry# 234287
Silane, [[4-[1,2-bis(trimethylsilyl)oxy]ethyl]-1,2-phenylene]bis(oxy)]bis(trimethyl-



(-)-Epinephrine, 3TMS derivative
Formula C₁₈H₃₇NO₃Si₃, MW 399, CAS# NA, Entry# 234281
(-)-Epinephrine, tris(trimethylsilyl) ether



N-(Trifluoroacetyl)-O,O'-tris(trimethylsilyl)norepinephrine
Formula C₁₉H₃₄F₃NO₄Si₃, MW 481, CAS# NA, Entry# 44143
N-(2-(3,4-Bis(trimethylsilyl)oxy)phenyl)-2-[(trimethylsilyl)oxy]ethyl)-2,2,2-trifluoroacetamide #

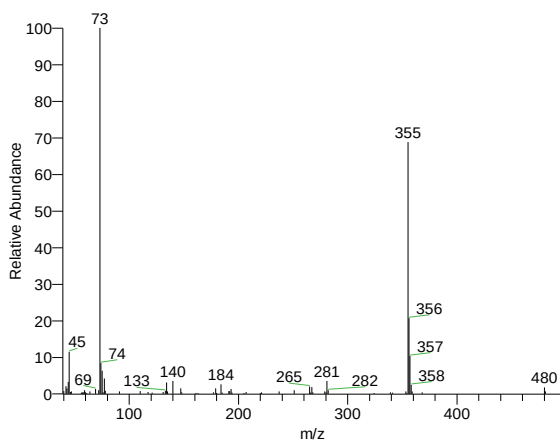


Analysed by Satyanarayana

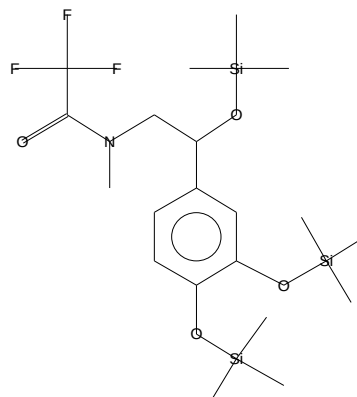
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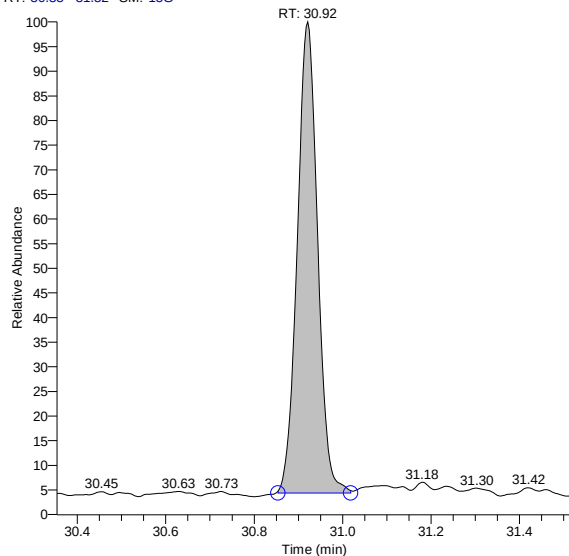
Compound Structure



N-(Trifluoroacetyl)-O,O',O''-tris(trimethylsilyl)epinephrine
Formula C₂₀H₃₆F₃NO₄Si₃, MW 495, CAS# 54135-51-2, Entry# 44146

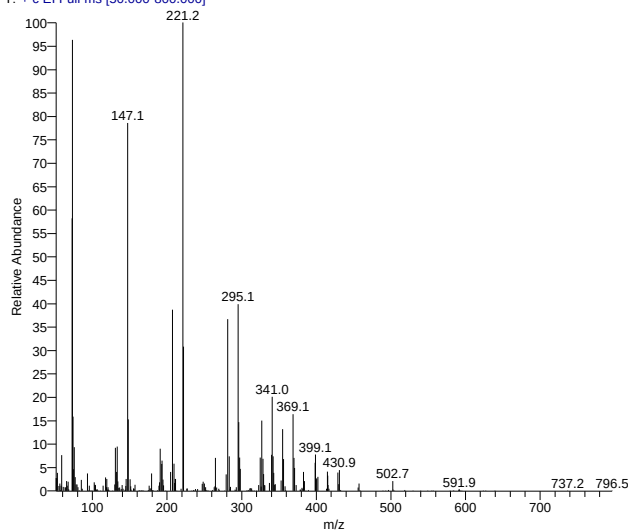


RT: 30.35 - 31.52 SM: 15G



NL:
1.45E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #7432 RT: 30.92 AV: 1 RF: 6.00, 3 NL: 1.75E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
30.92	Heptasiloxane, hexadecamethyl-	4424459.96	50.13	614	769	mainlib
30.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	4424459.96	35.39	604	635	mainlib
30.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	4424459.96	7.53	559	615	mainlib
30.92	Cyclodecasiloxane, eicosamethyl-	4424459.96	2.01	527	534	mainlib
30.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	4424459.96	0.60	501	583	mainlib

Analysed by Satyanarayana

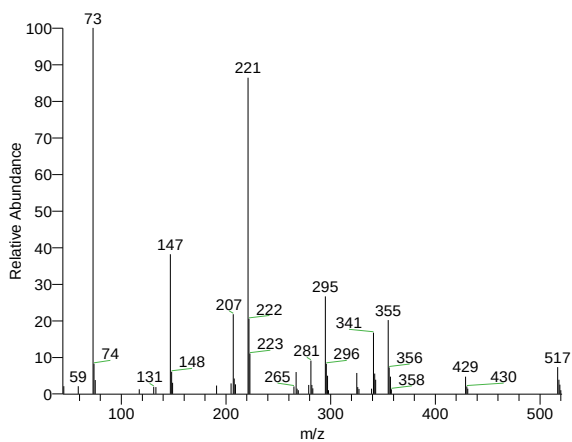
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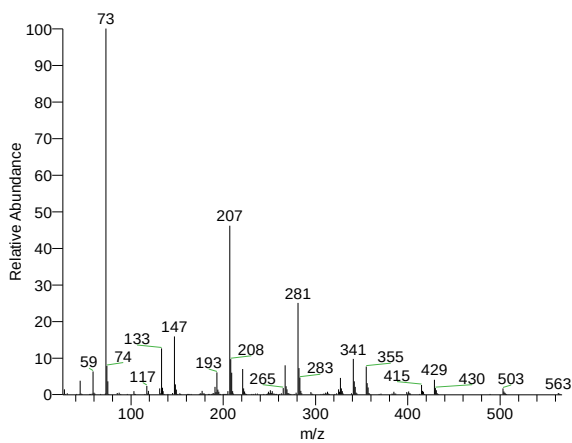
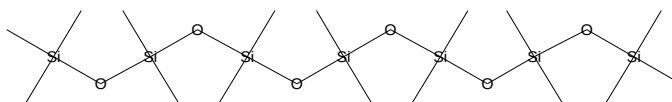
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

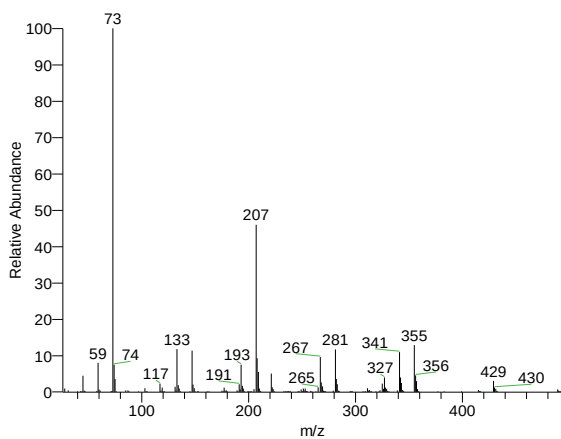
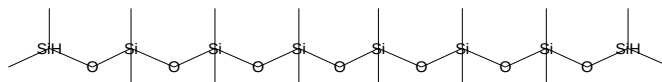
Compound Structure



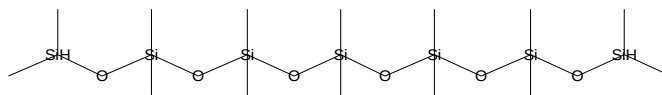
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

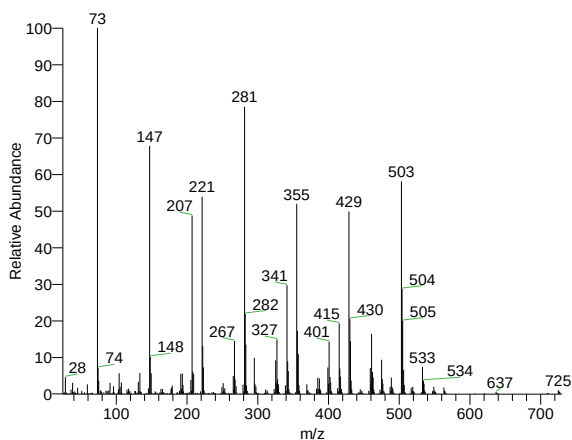


Analysed by Satyanarayana

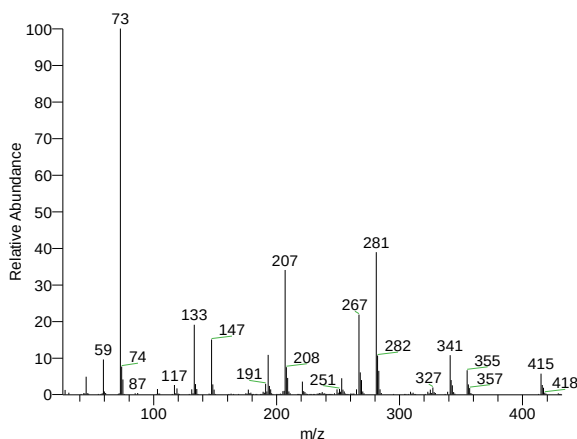
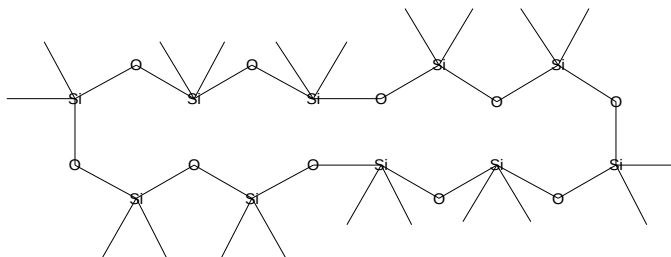
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Hit Spectrum

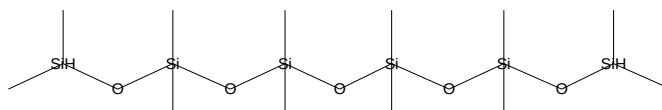
Compound Structure



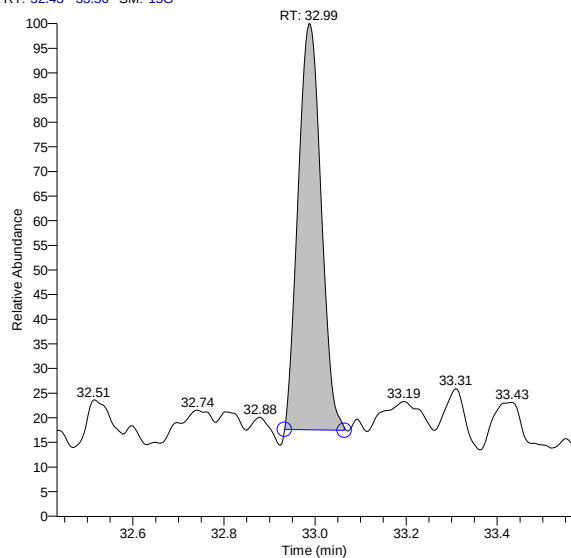
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

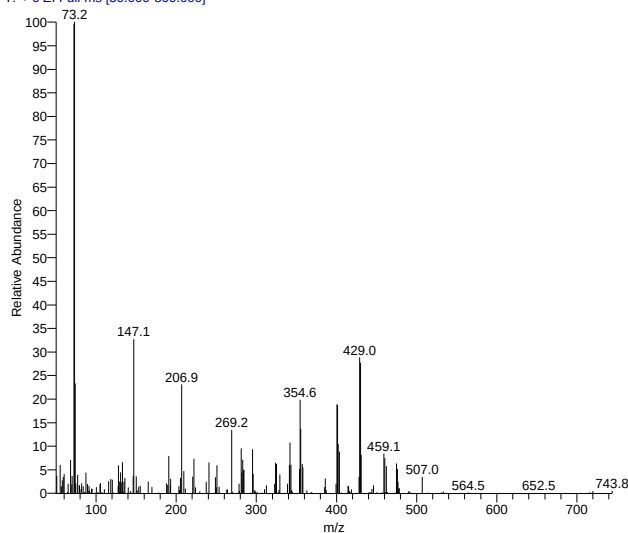


RT: 32.43 - 33.56 SM: 15G



NL:
3.69E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #8048 RT: 32.99 AV: 1 RF: 6.00, 3 NL: 6.70E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
32.99	Cyclononasiloxane, octadecamethyl-	1064970.54	67.41	571	632	mainlib

Analysed by Satyanarayana

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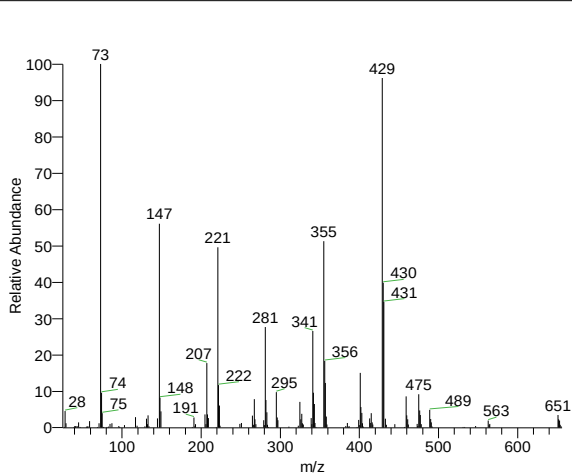
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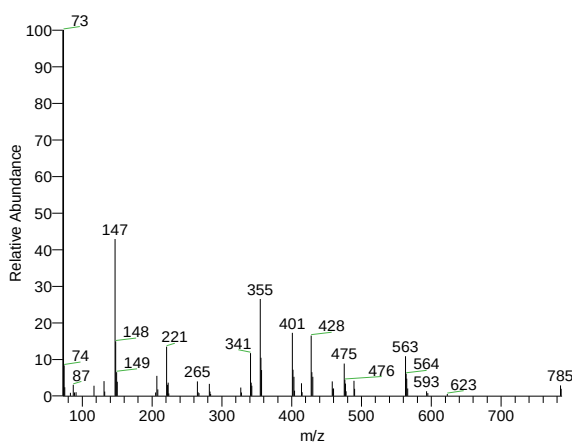
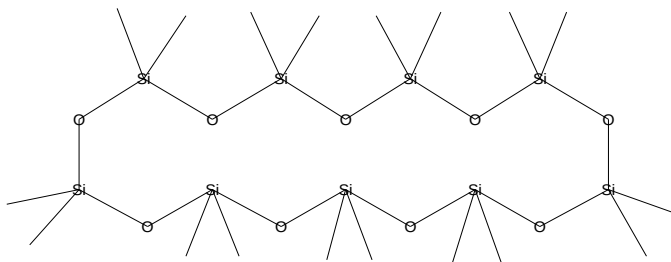
RT	Compound Name	Area	Probability	SI	RSI	Library
32.99	Bis(heptamethylcyclotetrasiloxyl)hexamethyltrisiloxane	1064970.54	8.76	496	618	mainlib
32.99	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1064970.54	6.71	489	554	mainlib
32.99	Cyclodecasiloxane, eicosamethyl-	1064970.54	4.33	476	492	mainlib
32.99	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1064970.54	2.80	463	596	mainlib

Hit Spectrum

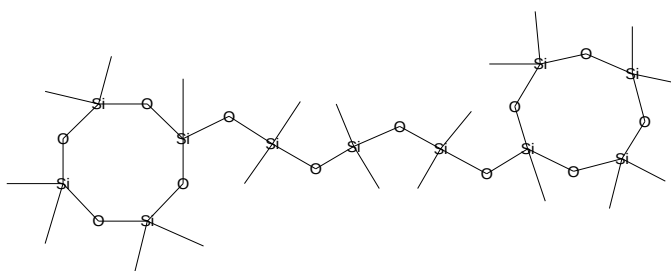
Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Bis(heptamethylcyclotetrasiloxyl)hexamethyltrisiloxane
Formula C₂₀H₆₀O₁₂Si₁₁, MW 800, CAS# 71449-67-7, Entry# 42773



Analysed by Satyanarayana

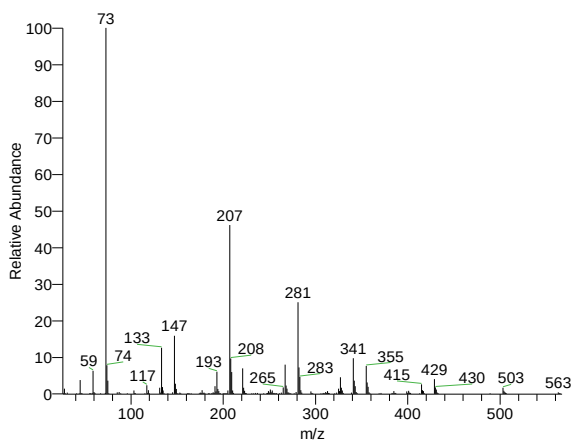
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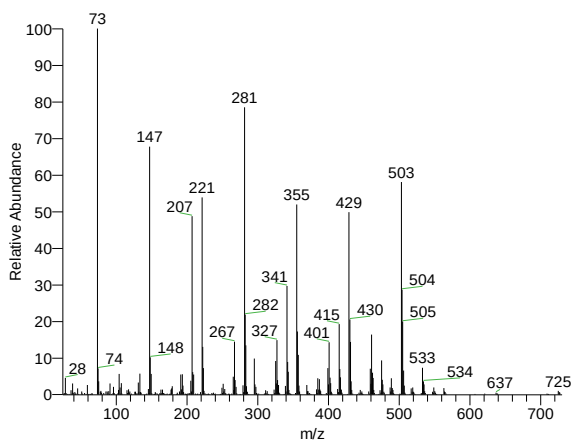
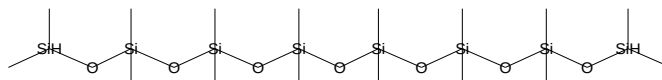
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

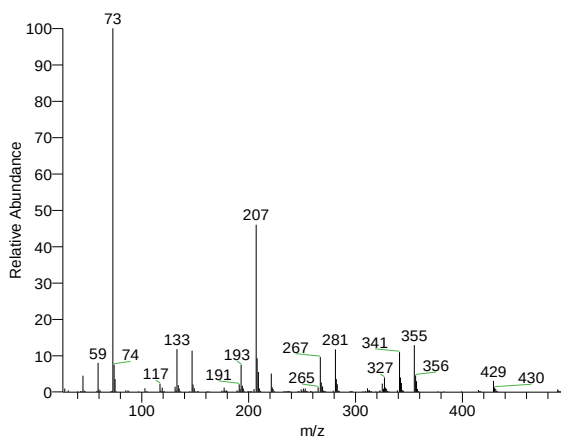
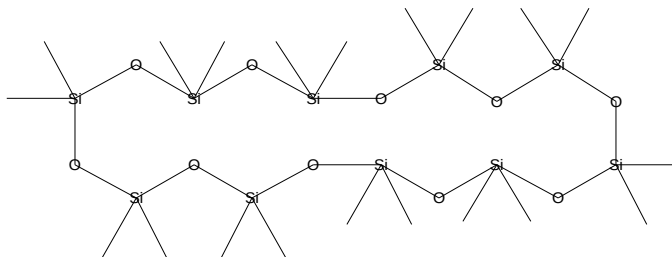
Compound Structure



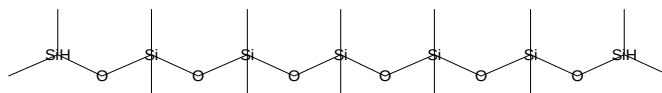
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



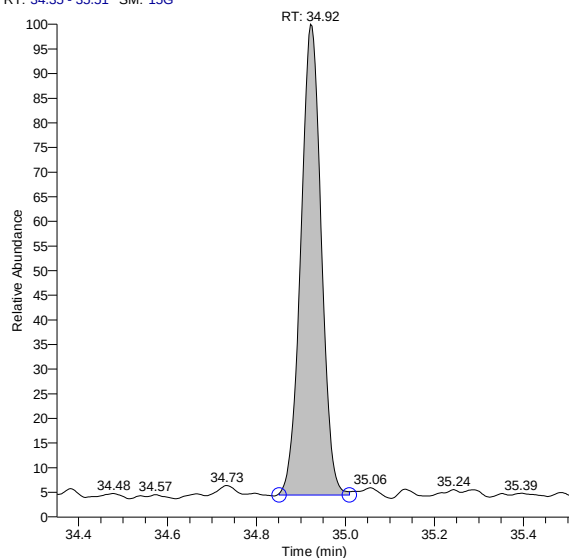
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



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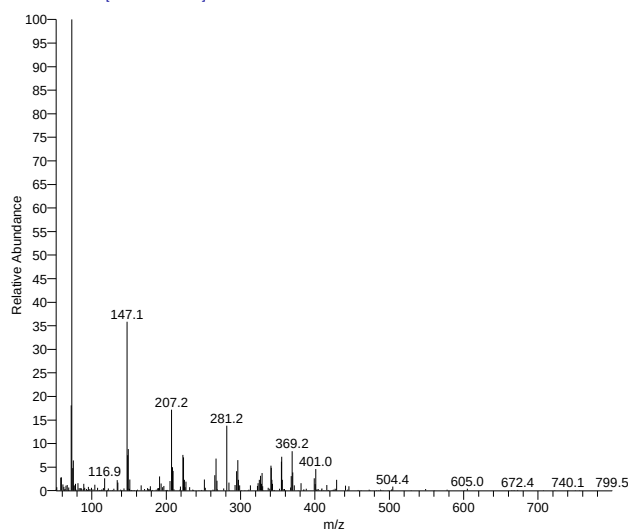
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RT: 34.35 - 35.51 SM: 15G



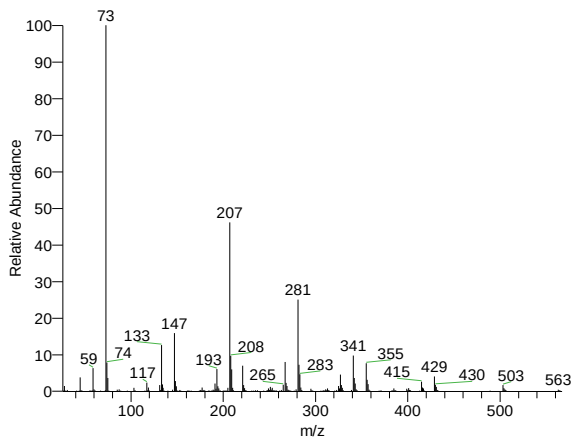
NL:
1.30E6
TIC: MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #8625 RT: 34.92 AV: 1 RF: 6.00, 3 NL: 3.14E5
T: + c EI Full ms [50.000-800.000]



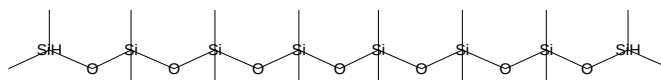
RT	Compound Name	Area	Probability	SI	RSI	Library
34.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3950484.56	45.20	588	635	mainlib
34.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3950484.56	31.91	578	673	mainlib
34.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3950484.56	5.87	520	620	mainlib
34.92	Heptasiloxane, hexadecamethyl-	3950484.56	5.41	518	661	mainlib
34.92	1,1,1,3,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	3950484.56	1.33	482	793	mainlib

Hit Spectrum



Compound Structure

Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



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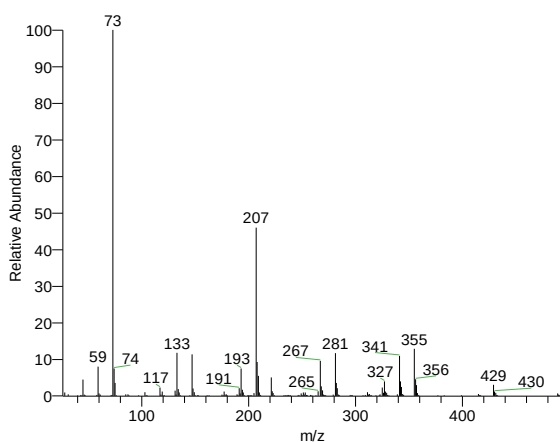
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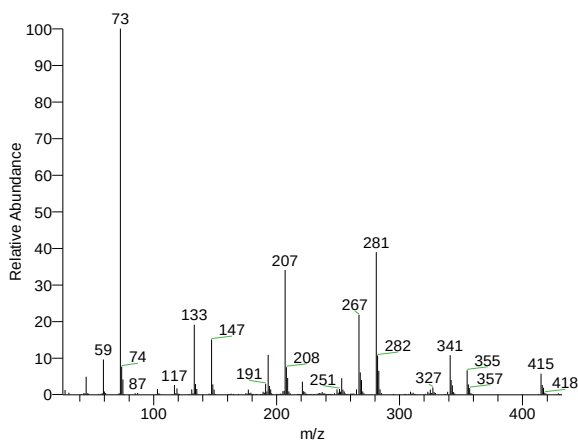
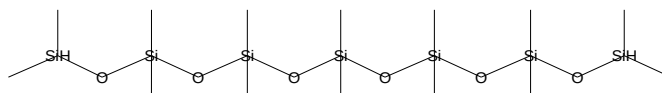
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Hit Spectrum

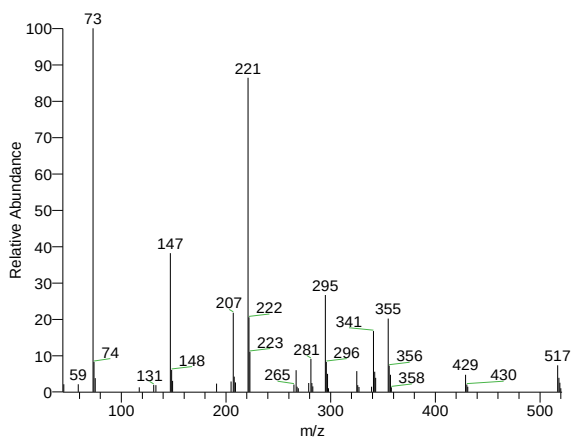
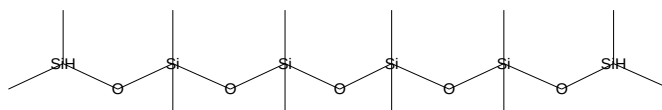
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane

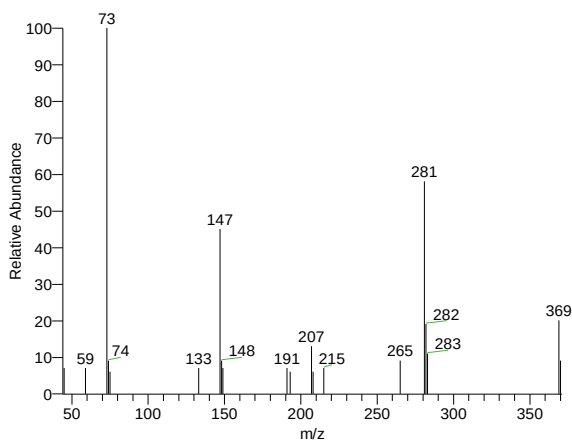


Analysed by Satyanarayana

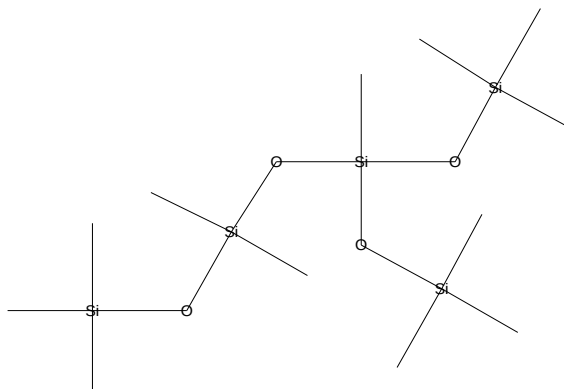
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Hit Spectrum

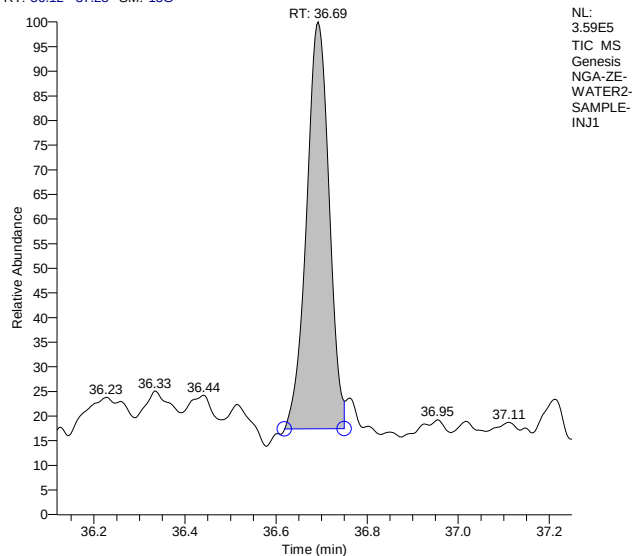
Compound Structure



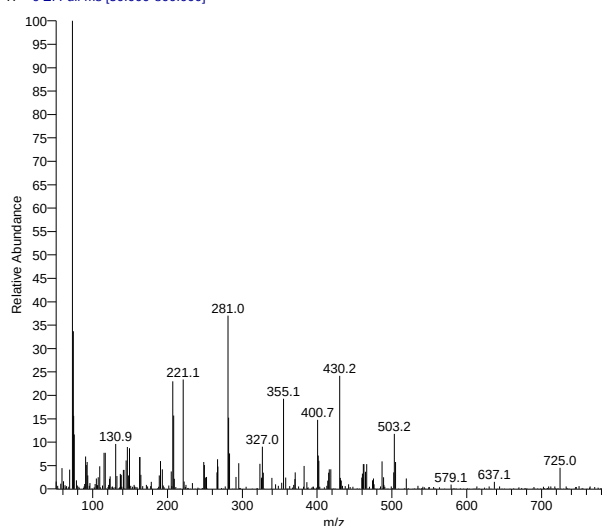
1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



RT: 36.12 - 37.25 SM: 15G



NGA-ZE-WATER2-SAMPLE-INJ1 #9153 RT: 36.69 AV: 1 RF: 6.00, 3 NL: 5.71E4
T: + c EI Full ms [50.000-800.000]



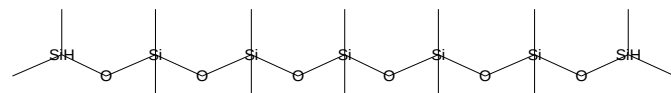
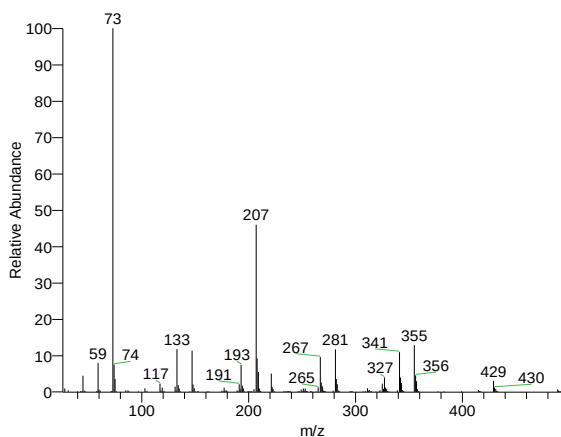
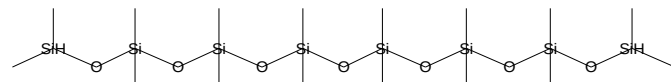
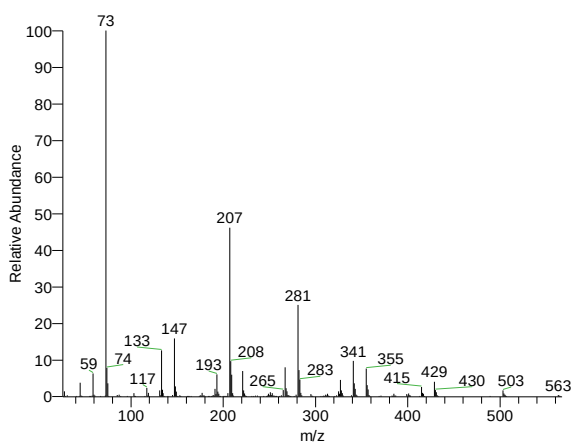
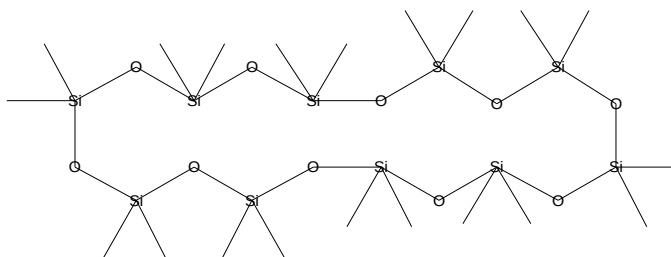
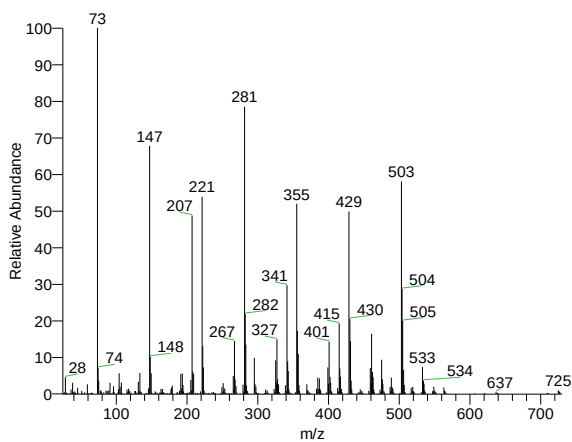
RT	Compound Name	Area	Probability	SI	RSI	Library
36.69	Cyclodecasiloxane, eicosamethyl-	1015218.62	67.51	492	527	mainlib
36.69	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1015218.62	12.20	433	531	mainlib
36.69	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1015218.62	2.28	376	528	mainlib
36.69	Cyclononasiloxane, octadecamethyl-	1015218.62	2.10	374	475	mainlib
36.69	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1015218.62	1.78	370	516	mainlib

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Hit Spectrum

Compound Structure



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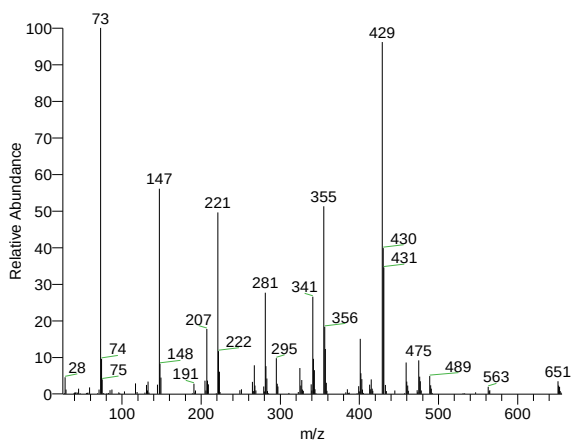
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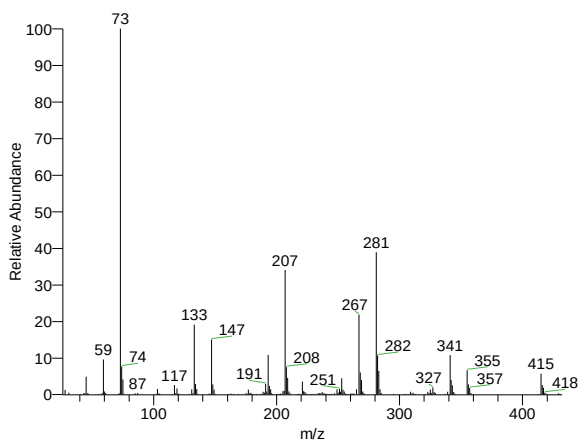
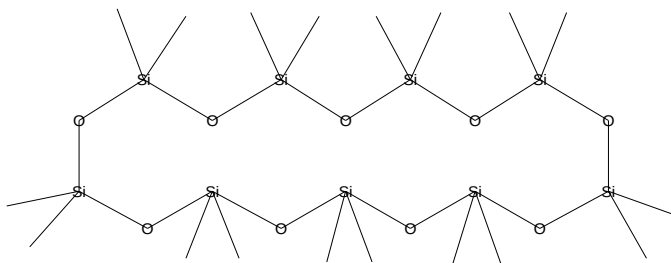
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

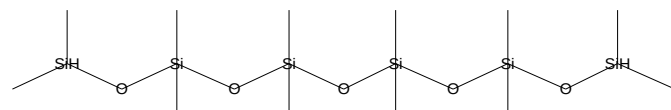
Compound Structure



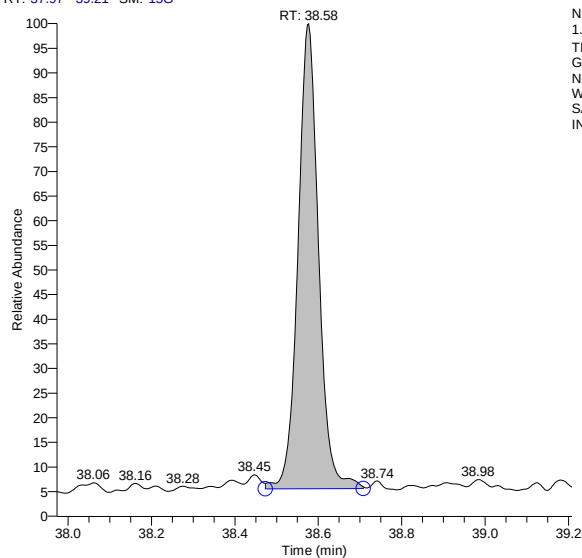
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

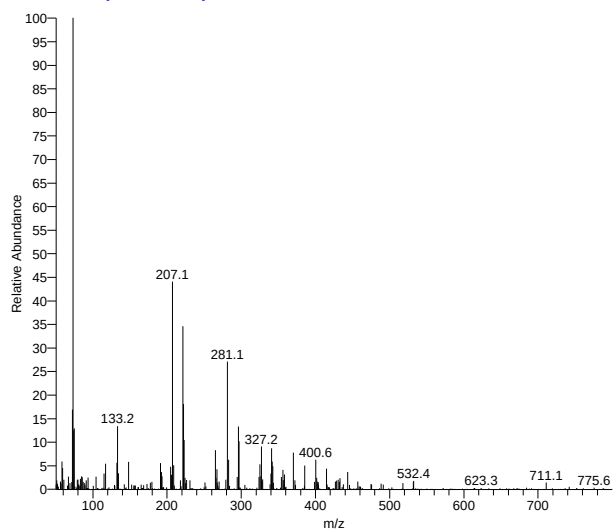


RT: 37.97 - 39.21 SM: 15G



NL:
1.17E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #9715 RT: 38.58 AV: 1 RF: 6.00, 3 NL: 1.83E5
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

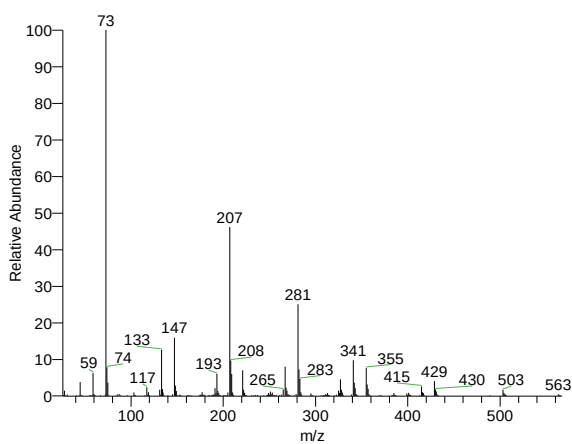
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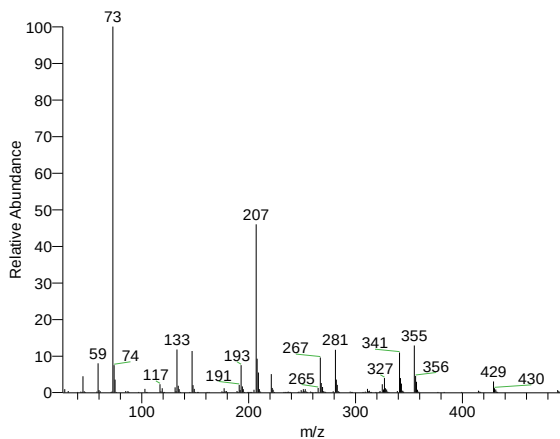
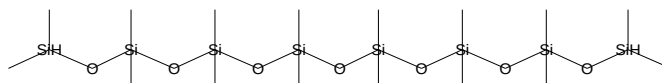
RT	Compound Name	Area	Probability	SI	RSI	Library
38.58	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3769728.92	56.09	545	633	mainlib
38.58	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3769728.92	25.54	525	636	mainlib
38.58	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3769728.92	7.51	498	626	mainlib
38.58	Cyclononasiloxane, octadecamethyl-	3769728.92	1.68	456	516	mainlib
38.58	Cyclodecasiloxane, eicosamethyl-	3769728.92	1.62	455	475	mainlib

Hit Spectrum

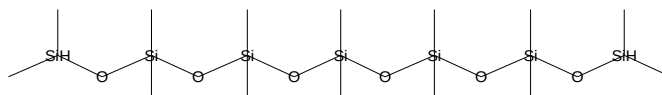
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

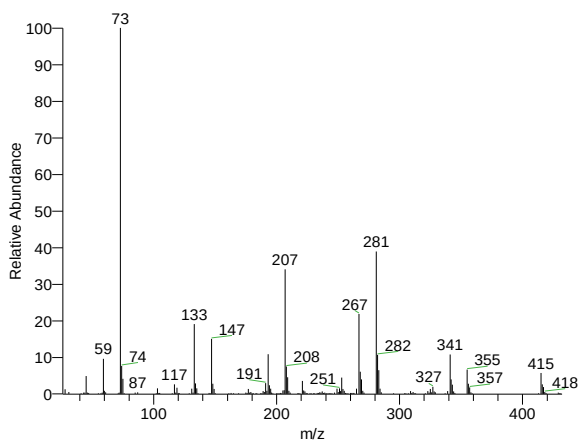


Analysed by Satyanarayana

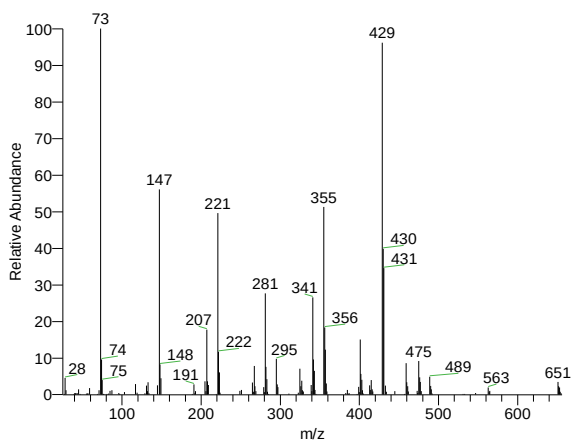
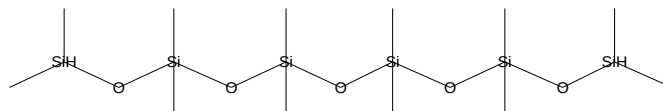
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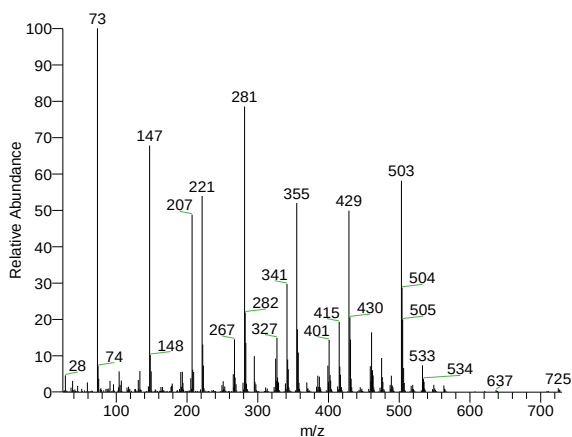
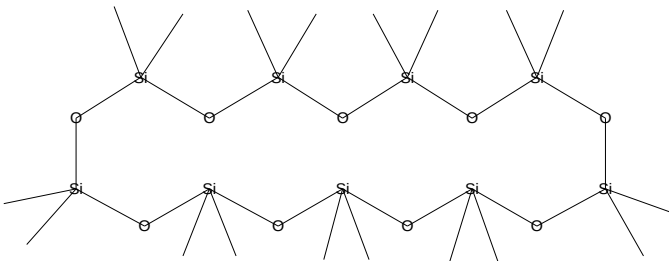
Compound Structure



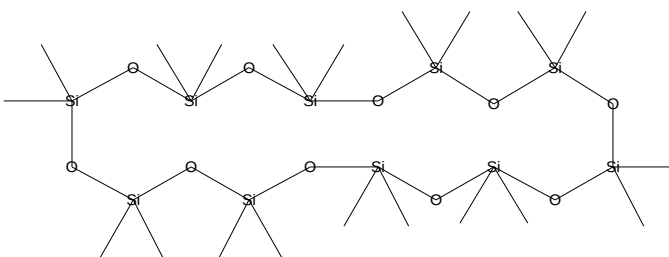
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



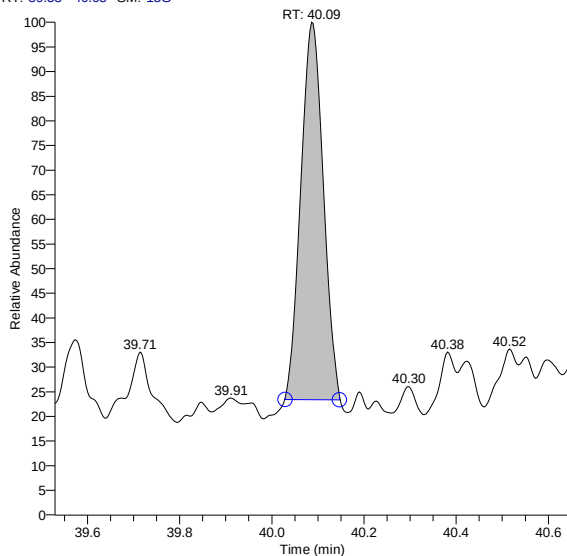
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



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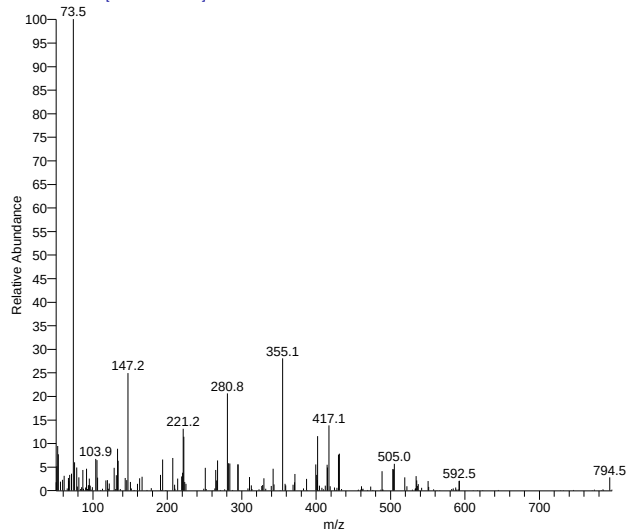
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RT: 39.53 - 40.65 SM: 15G



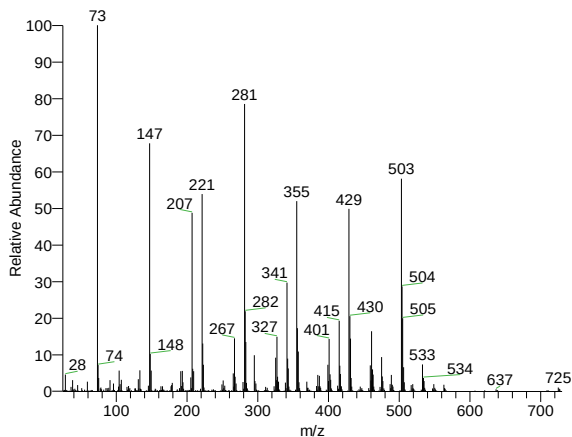
NL:
2.85E5
TIC: MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #10165 RT: 40.09 AV: 1 RF: 6.00, 3 NL: 6.34E4
T: + c EI Full ms [50.000-800.000]



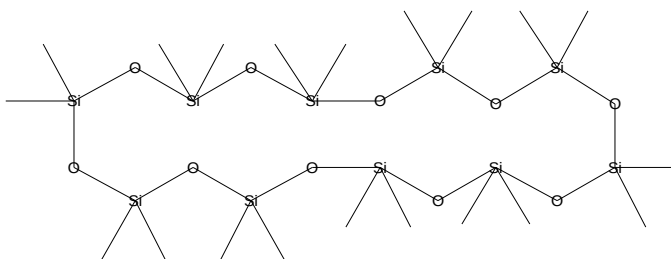
RT	Compound Name	Area	Probability	SI	RSI	Library
40.09	Cyclodecasiloxane, eicosamethyl-	741941.14	72.92	503	538	mainlib
40.09	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	741941.14	13.90	447	523	mainlib
40.09	Cycloheptasiloxane, tetradecamethyl-	741941.14	2.90	400	514	mainlib
40.09	Cyclooctasiloxane, hexadecamethyl-	741941.14	2.17	392	543	mainlib
40.09	Cyclononasiloxane, octadecamethyl-	741941.14	0.92	371	466	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #

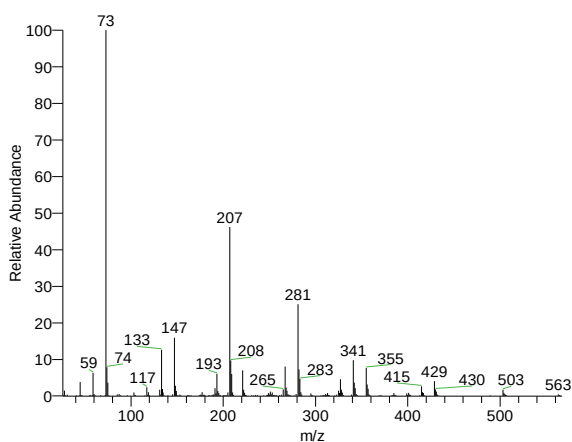


Analysed by Satyanarayana

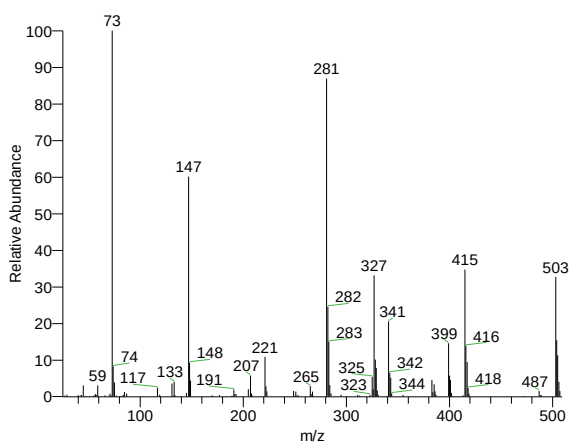
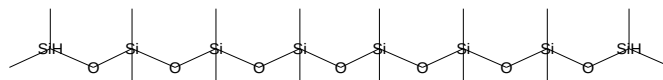
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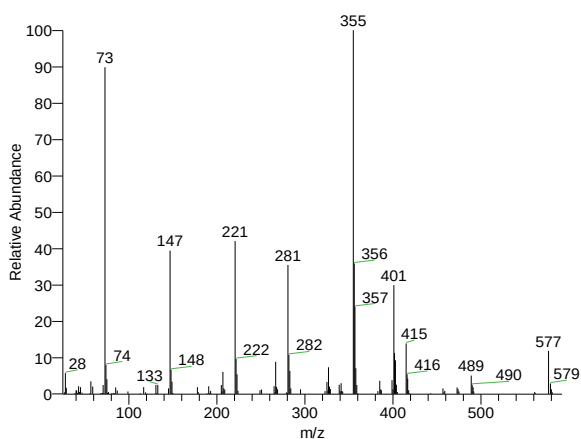
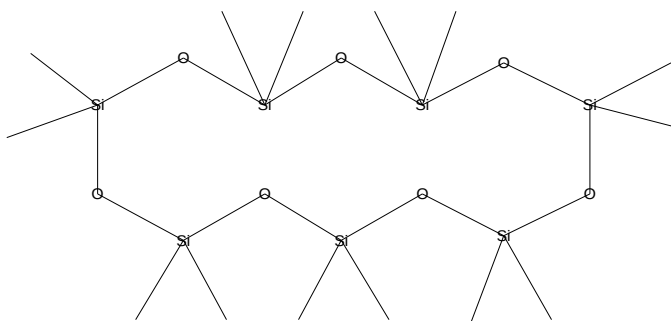
Compound Structure



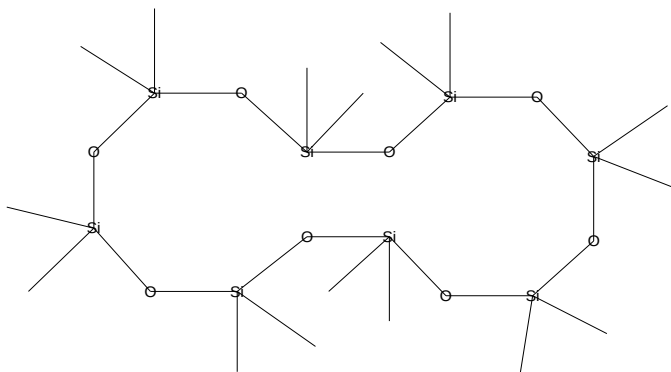
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane

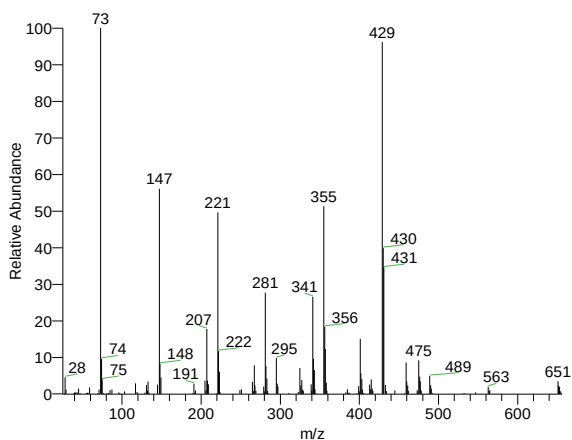


Analysed by Satyanarayana

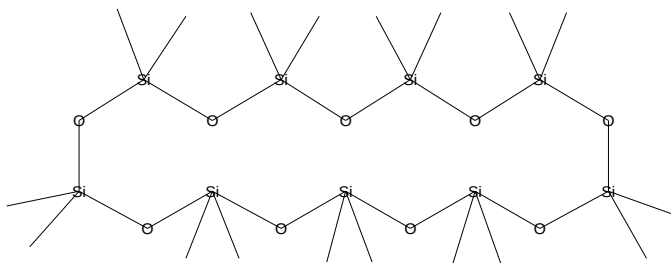
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Hit Spectrum

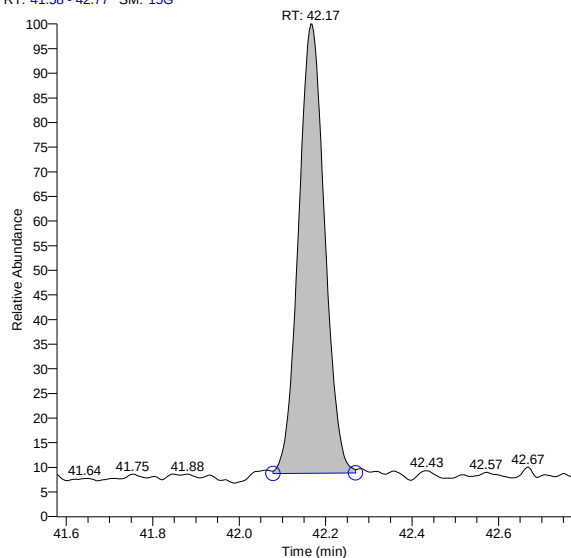
Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane

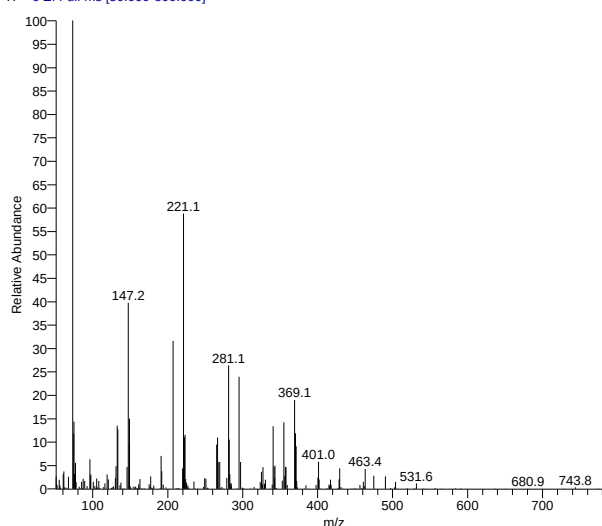


RT: 41.58 - 42.77 SM: 15G



NL:
7.95E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #10785 RT: 42.17 AV: 1 RF: 6.00, 3 NL: 1.24E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
42.17	Heptasiloxane, hexadecamethyl-	3051906.76	48.27	593	751	mainlib
42.17	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3051906.76	21.98	573	623	mainlib
42.17	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3051906.76	8.69	551	647	mainlib
42.17	Cyclodecasiloxane, eicosamethyl-	3051906.76	5.78	539	546	mainlib
42.17	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3051906.76	4.31	531	631	mainlib

Analysed by Satyanarayana

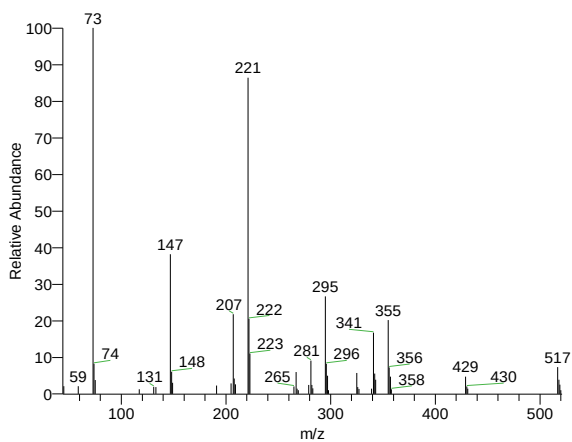
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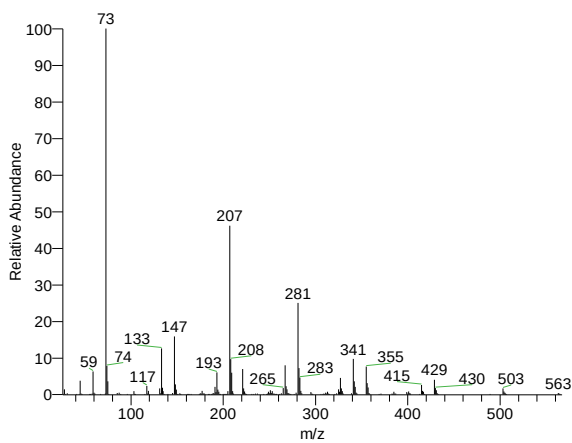
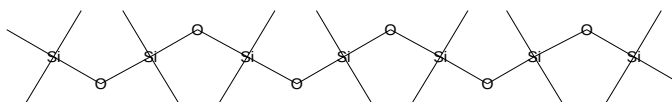
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

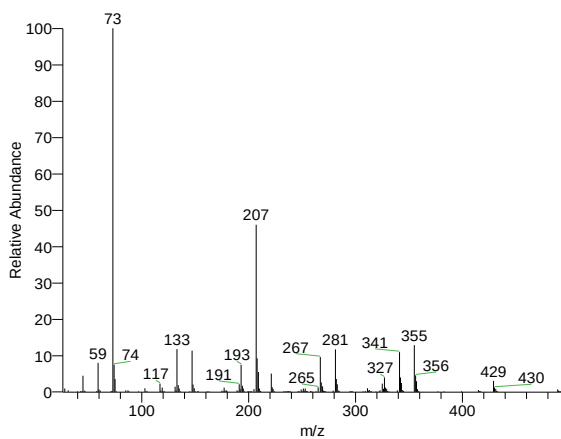
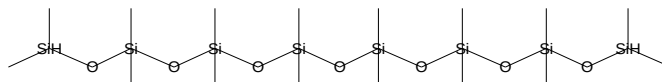
Compound Structure



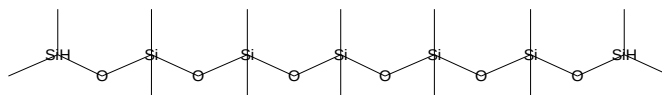
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

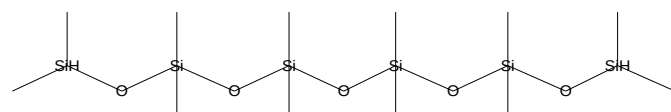
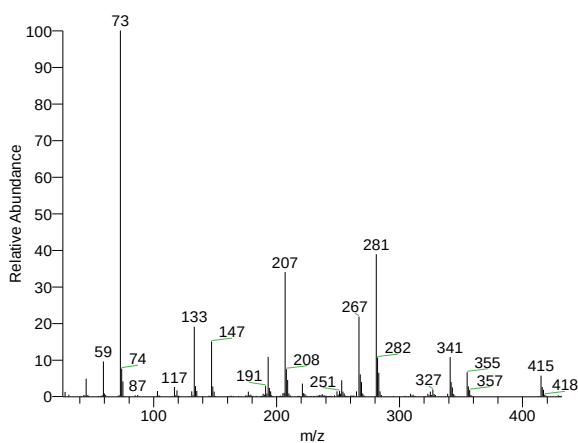
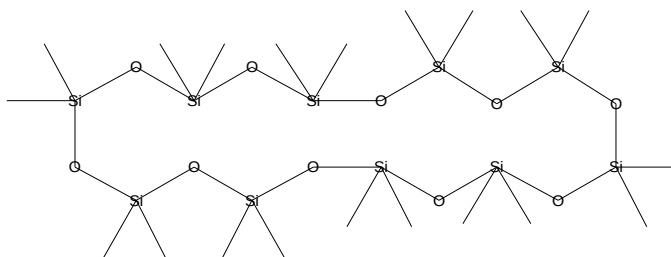
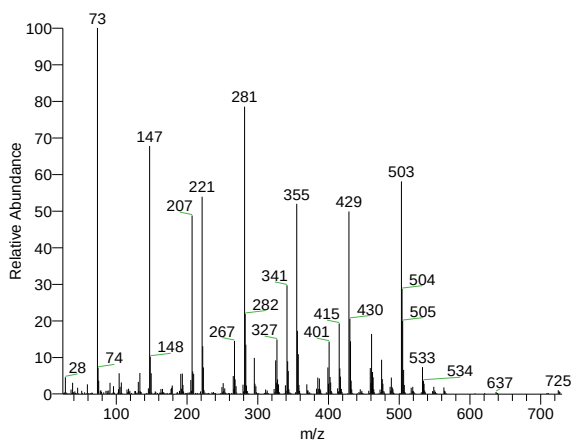


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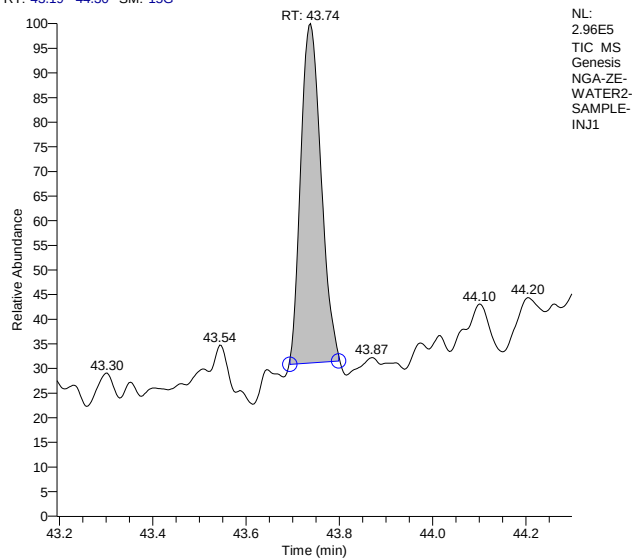
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

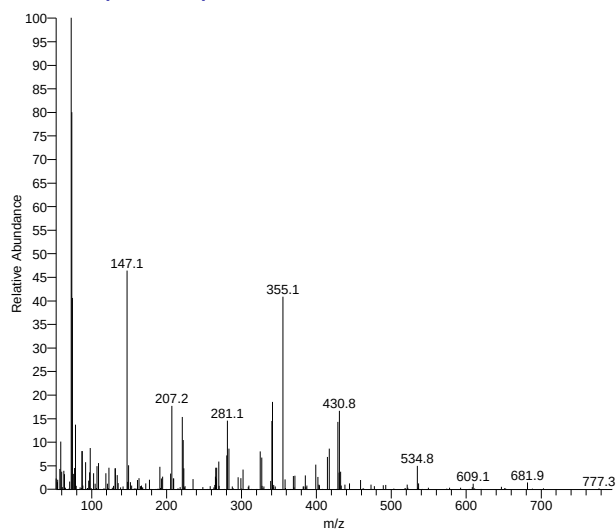
Compound Structure



RT: 43.19 - 44.30 SM: 15G



NGA-ZE-WATER2-SAMPLE-INJ1 #11254 RT: 43.74 AV: 1 RF: 6.00, 3 NL: 5.31E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

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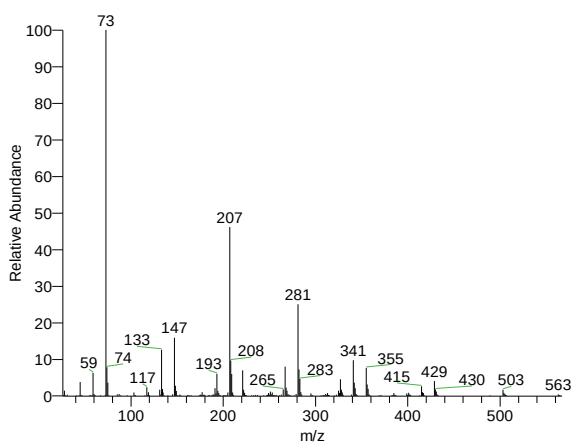
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ANALYTICAL CHEMISTRY DIVISION

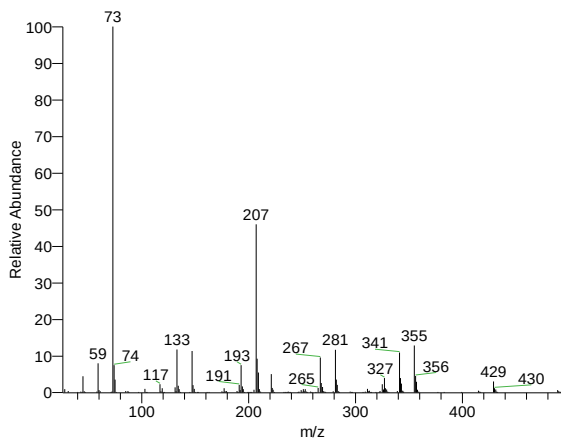
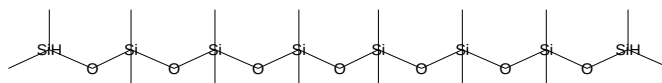
RT	Compound Name	Area	Probability	SI	RSI	Library
43.74	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	616909.62	41.45	552	614	mainlib
43.74	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	616909.62	22.62	535	608	mainlib
43.74	Cyclononasiloxane, octadecamethyl-	616909.62	16.42	526	606	mainlib
43.74	Cyclodecasiloxane, eicosamethyl-	616909.62	9.45	510	531	mainlib
43.74	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	616909.62	2.01	465	547	mainlib

Hit Spectrum

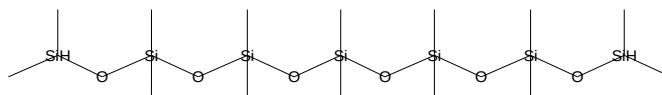
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

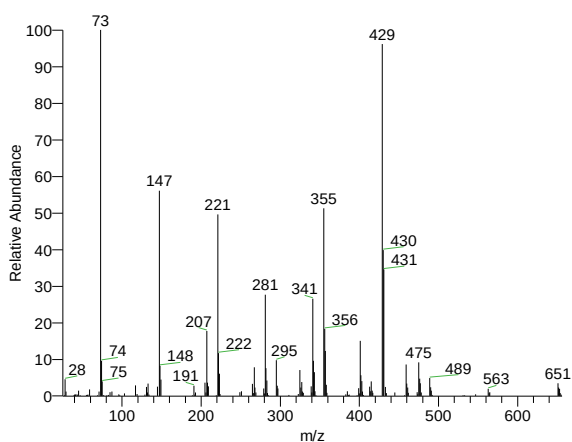
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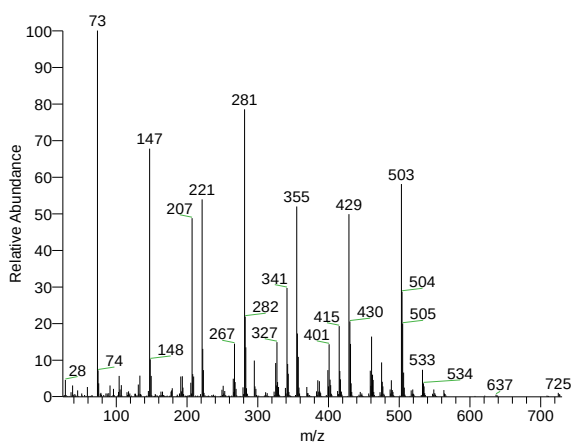
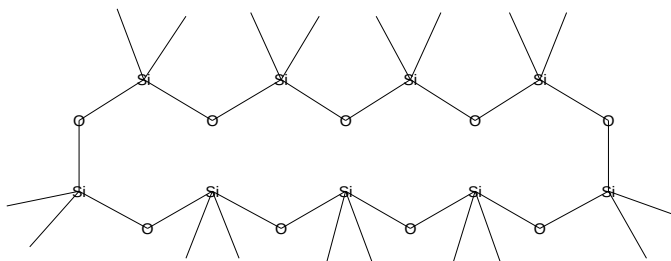
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

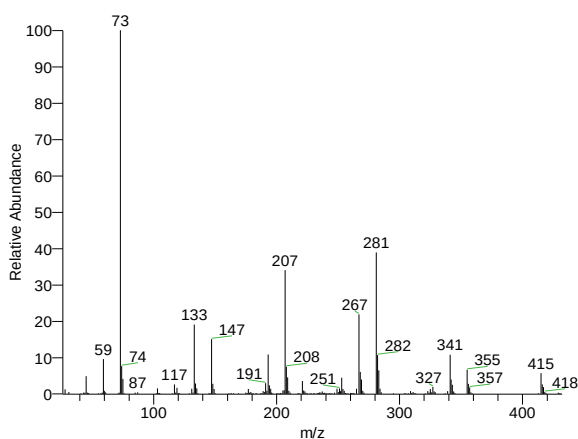
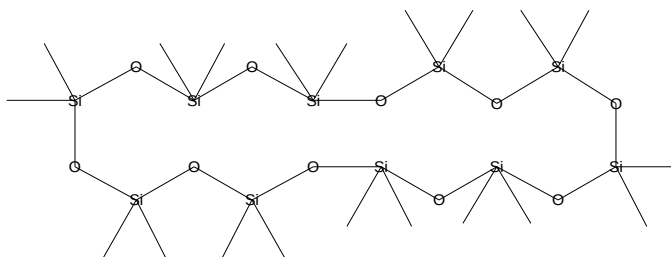
Compound Structure



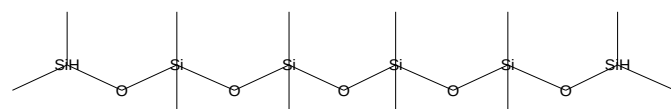
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



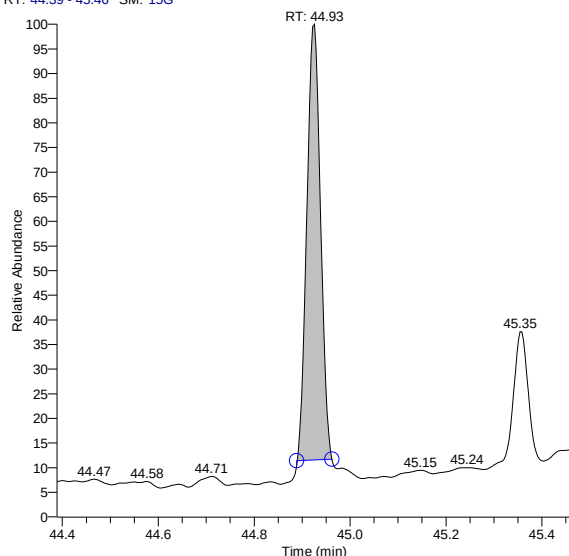
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



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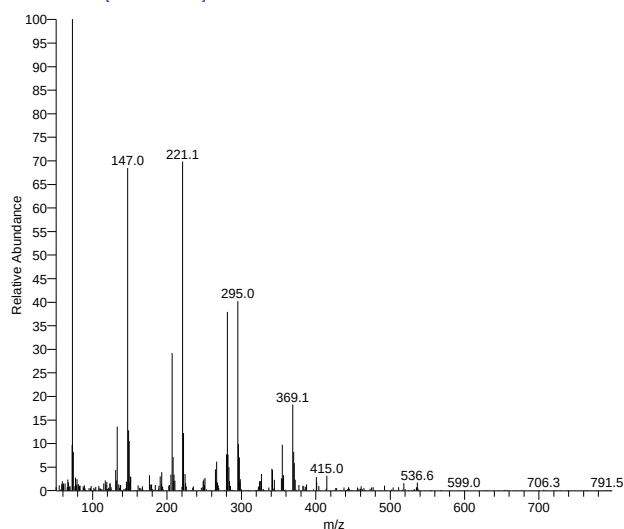
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ANALYTICAL CHEMISTRY DIVISION

RT: 44.39 - 45.46 SM: 15G



NL:
1.59E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

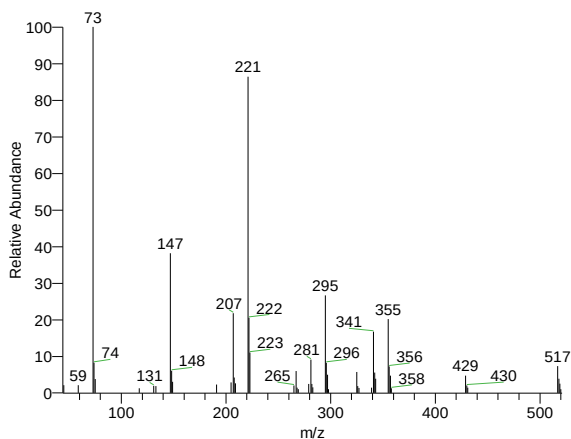
NGA-ZE-WATER2-SAMPLE-INJ1 #11608 RT: 44.93 AV: 1 RF: 6.00, 3 NL: 3.18E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
44.93	Heptasiloxane, hexadecamethyl-	2794722.57	42.57	597	766	mainlib
44.93	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3, 3-bis[(trimethylsilyl)oxy]-	2794722.57	10.36	560	662	mainlib
44.93	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	2794722.57	9.95	559	615	mainlib
44.93	Pentasiloxane, dodecamethyl-	2794722.57	7.62	552	641	mainlib
44.93	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	2794722.57	5.99	546	635	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Analysed by Satyanarayana

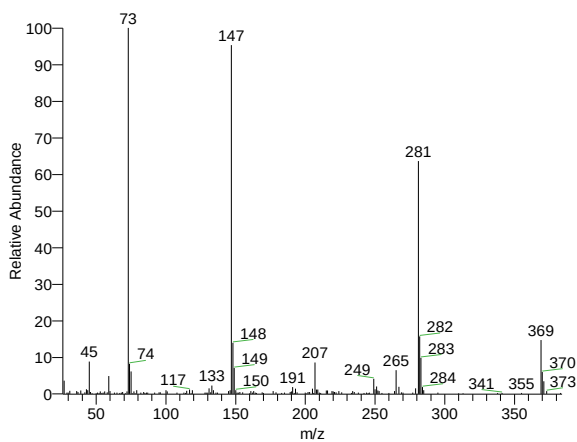
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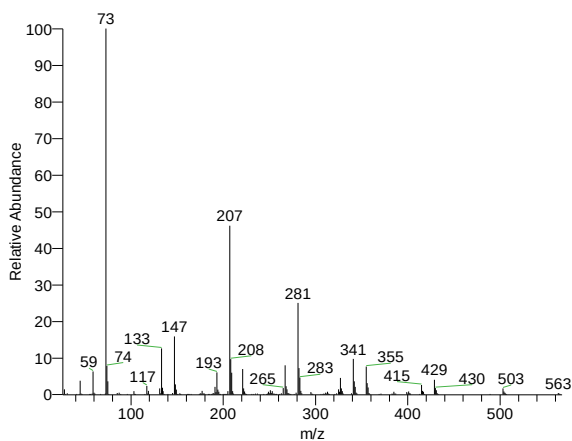
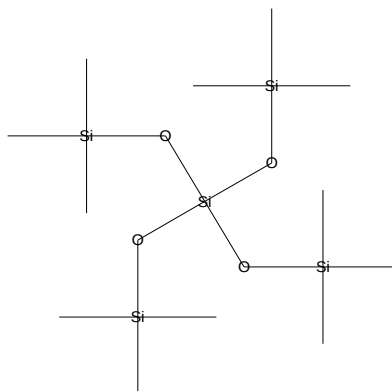
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

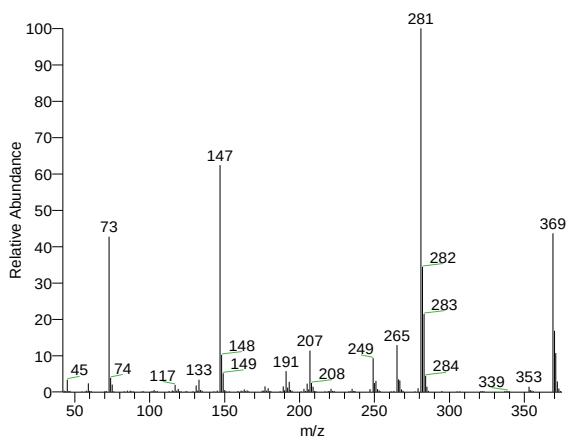
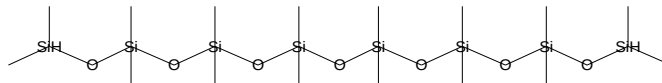
Compound Structure



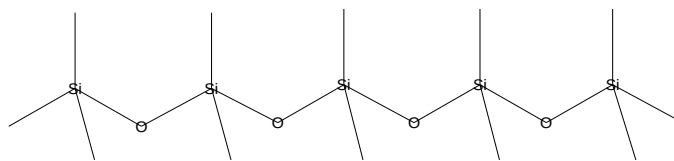
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane

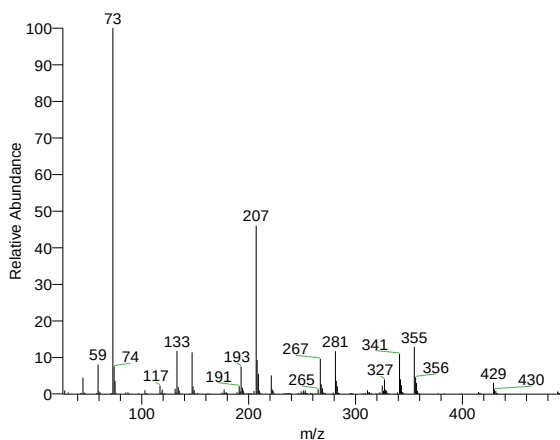


Analysed by Satyanarayana

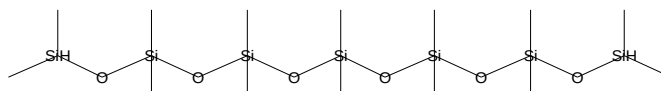
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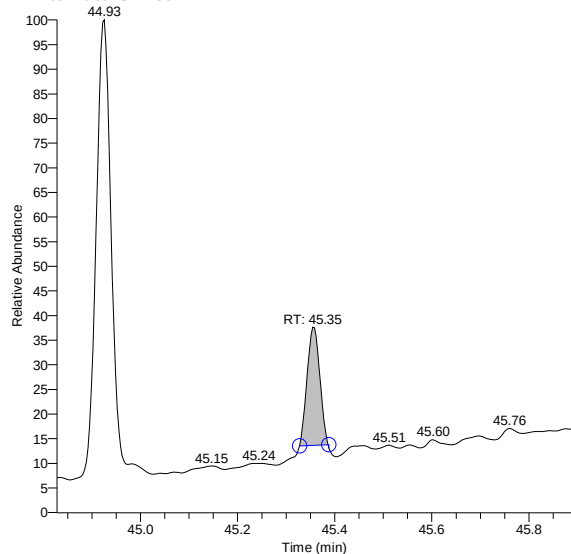
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

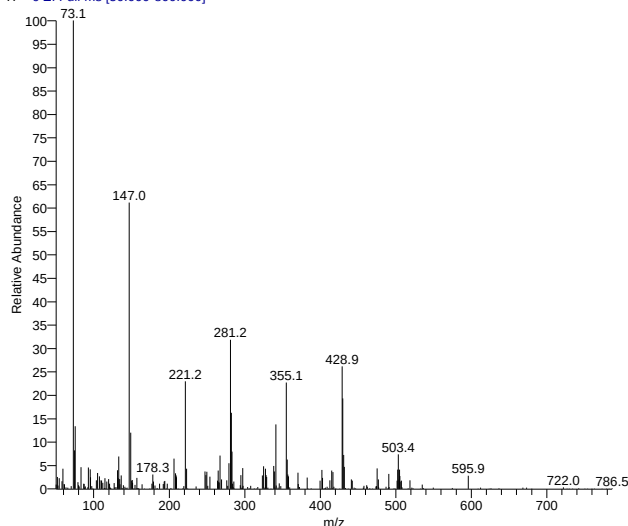


RT: 44.83 - 45.89 SM: 15G



NL:
1.59E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #11736 RT: 45.35 AV: 1 RF: 6.00, 3 NL: 1.25E5
T: + c EI Full ms [50.000-800.000]



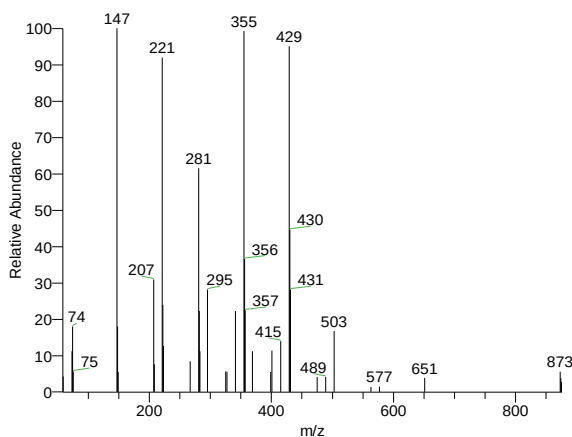
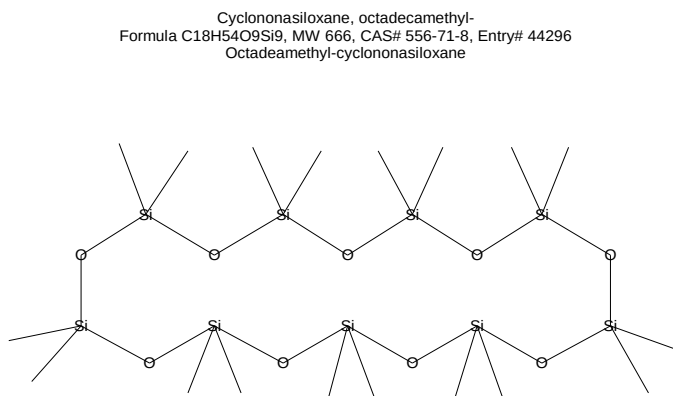
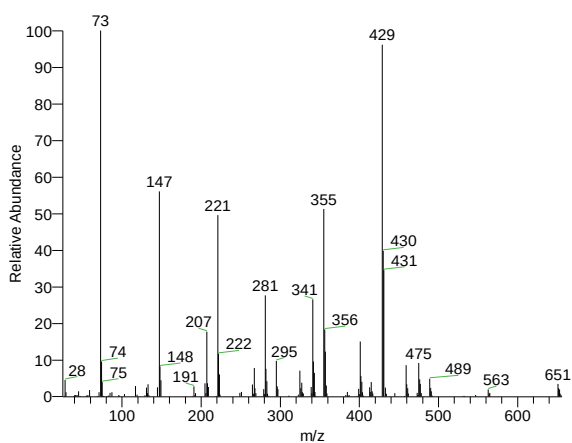
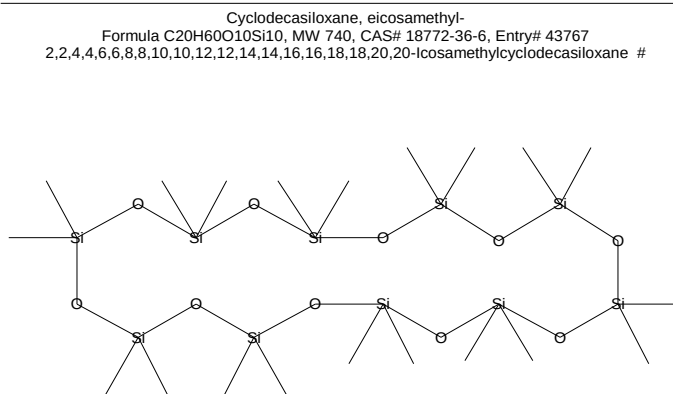
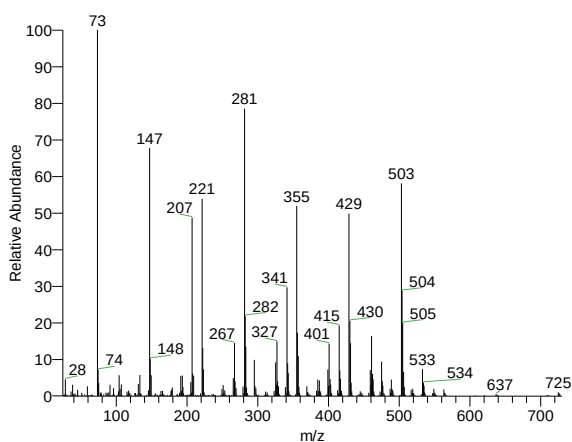
RT	Compound Name	Area	Probability	SI	RSI	Library
45.35	Cyclodecasiloxane, eicosamethyl-	695241.95	66.20	610	639	mainlib
45.35	Cyclononasiloxane, octadecamethyl-	695241.95	11.31	548	666	mainlib
45.35	Tetracosamethyl-cyclododecasiloxane	695241.95	9.55	544	768	mainlib
45.35	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	695241.95	7.51	538	601	mainlib
45.35	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	695241.95	1.13	470	570	mainlib

Analysed by Satyanarayana

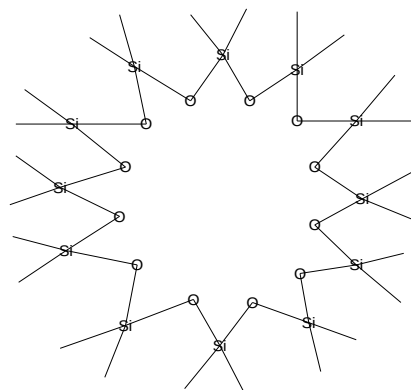
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Hit Spectrum

Compound Structure



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



Analysed by Satyanarayana

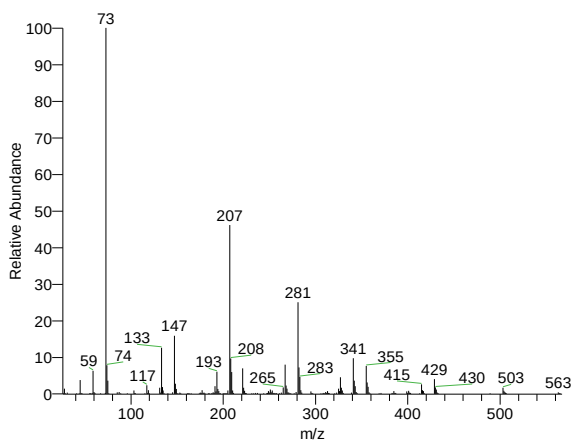
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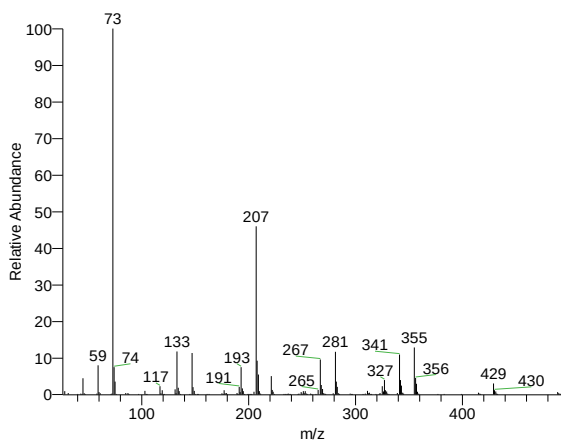
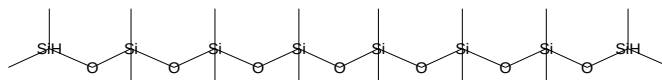
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

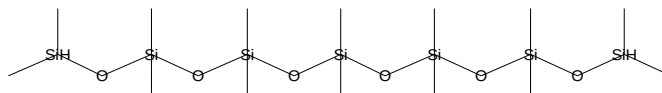
Compound Structure



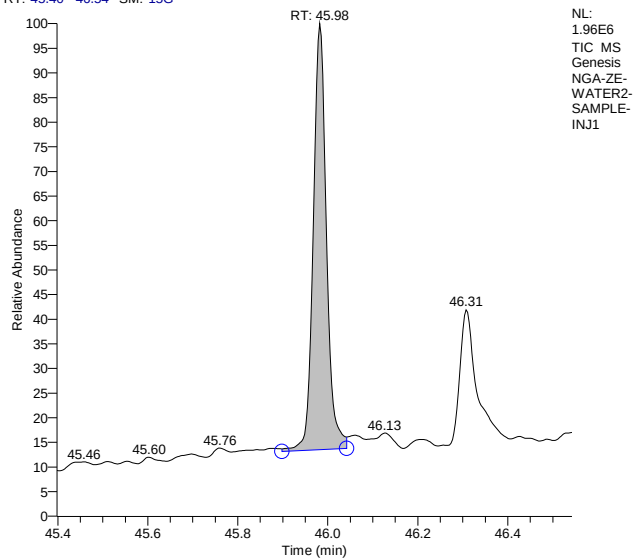
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

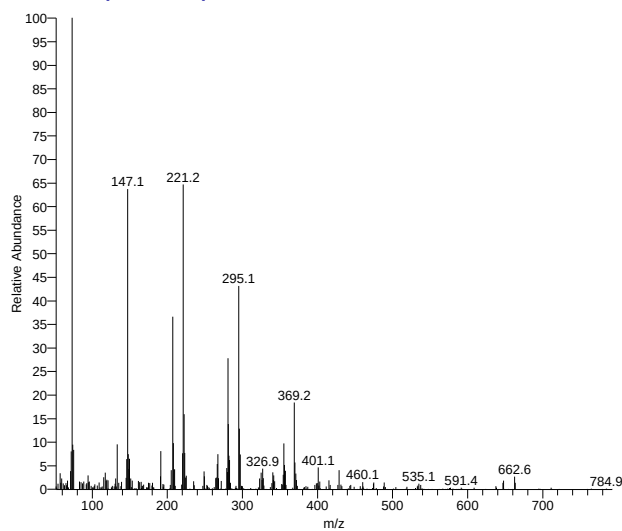


RT: 45.40 - 46.54 SM: 15G



NL:
1.96E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #11923 RT: 45.98 AV: 1 RF: 6.00, 3 NL: 3.88E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Heptasiloxane, hexadecamethyl-	3455900.31	68.96	649	827	mainlib

Analysed by Satyanarayana

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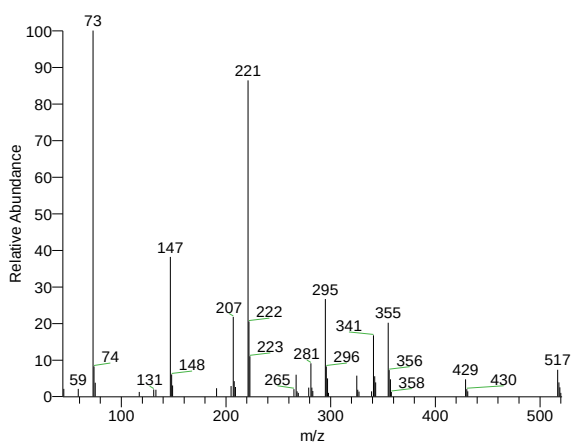
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

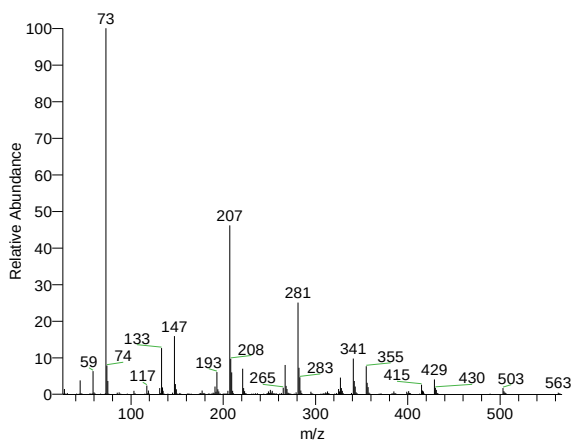
RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3455900.31	15.73	608	676	mainlib
45.98	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3455900.31	3.47	565	666	mainlib
45.98	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	3455900.31	2.10	550	617	mainlib
45.98	Hexasiloxane, tetradecamethyl-	3455900.31	2.02	549	802	mainlib

Hit Spectrum

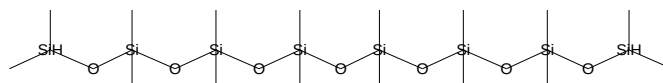
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

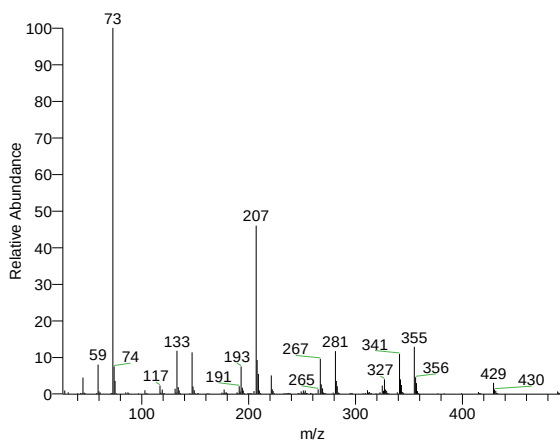
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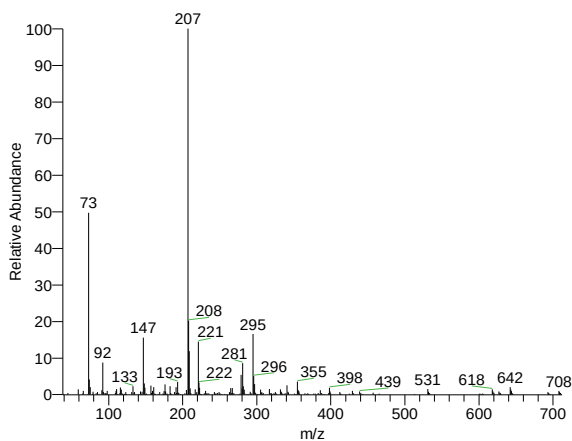
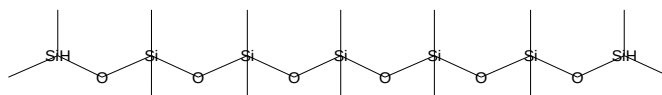
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

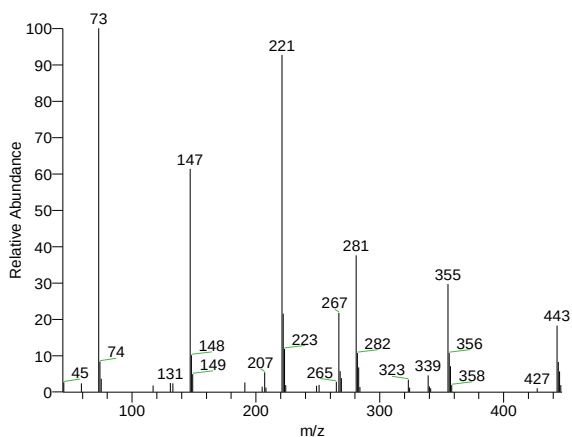
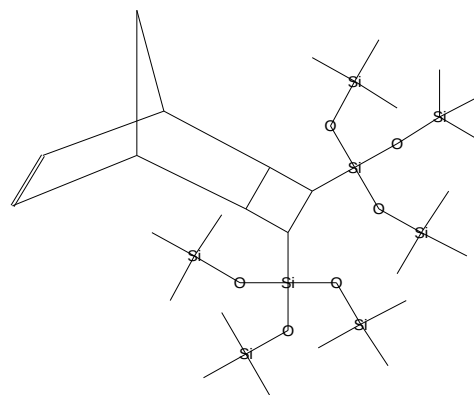
Compound Structure



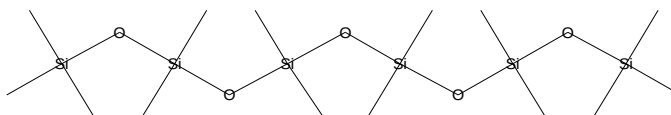
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Tricyclo[4.2.1.0(2.5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:2BJSGCCAWLXCNS-UHFFFAOYSA-N

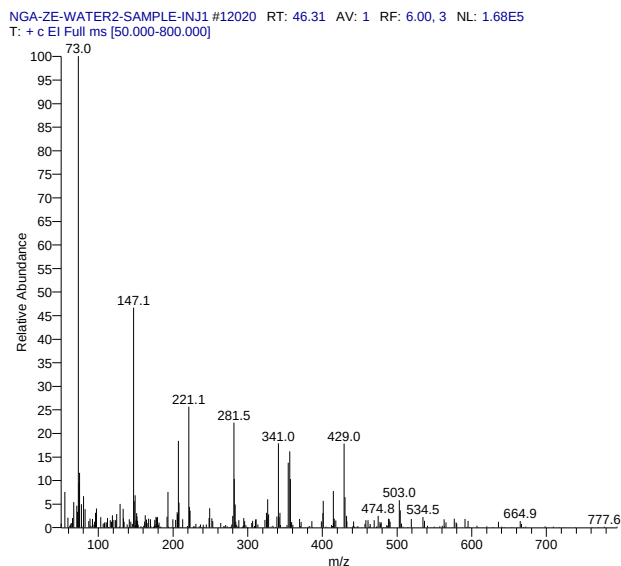
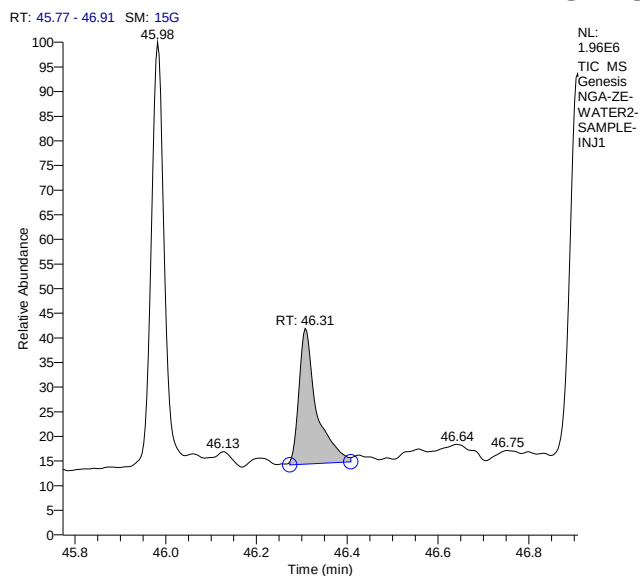


Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



Analysed by Satyanarayana

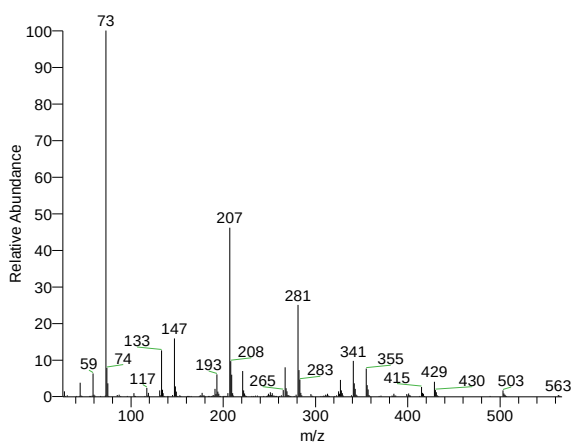
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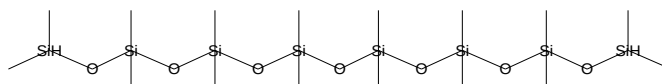
RT	Compound Name	Area	Probability	SI	RSI	Library
46.31	Cyclodecasiloxane, eicosamethyl-	1450527.55	34.54	525	567	mainlib
46.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1450527.55	34.54	525	613	mainlib
46.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1450527.55	9.23	493	617	mainlib
46.31	Cyclononasiloxane, octadecamethyl-	1450527.55	5.59	478	593	mainlib
46.31	Heptasiloxane, hexadecamethyl-	1450527.55	2.54	458	646	mainlib

Hit Spectrum

Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



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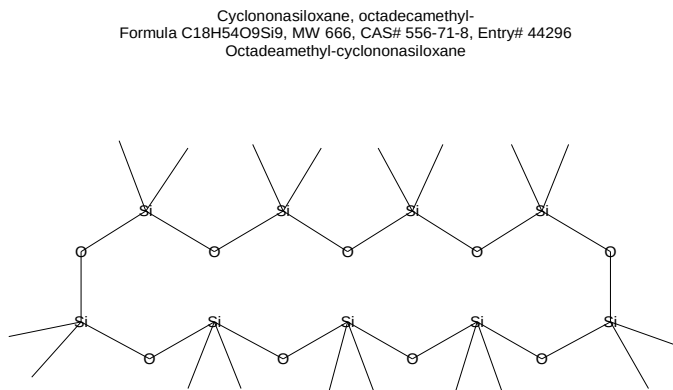
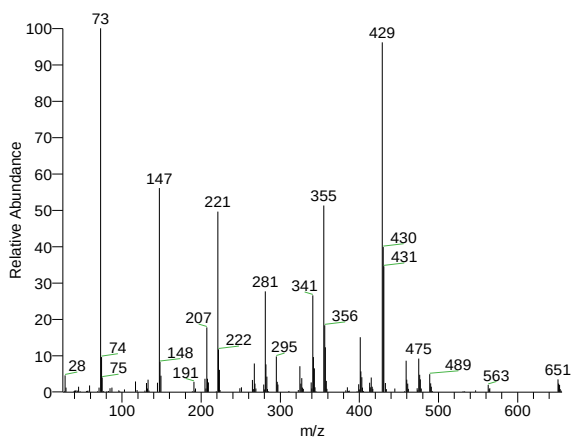
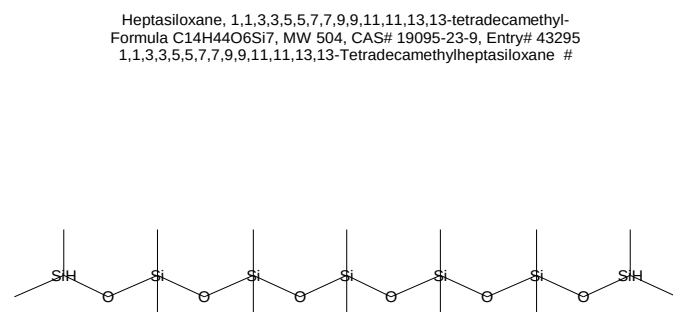
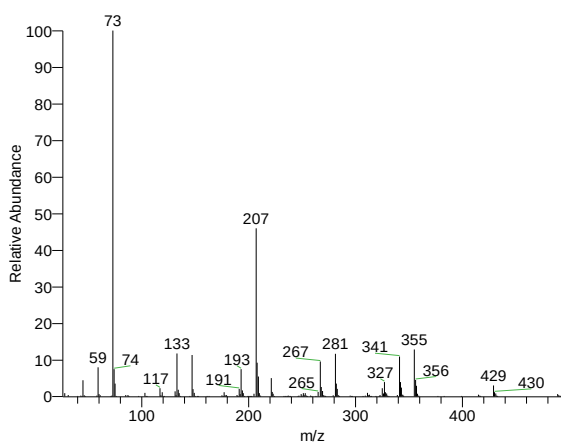
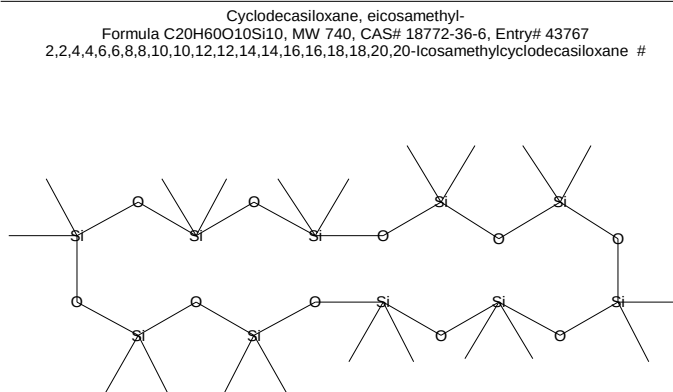
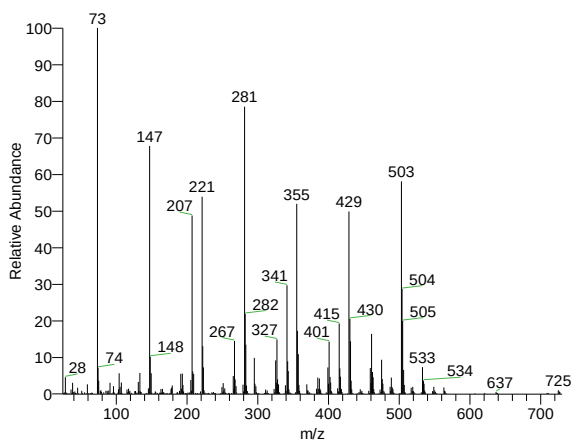
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Hit Spectrum

Compound Structure

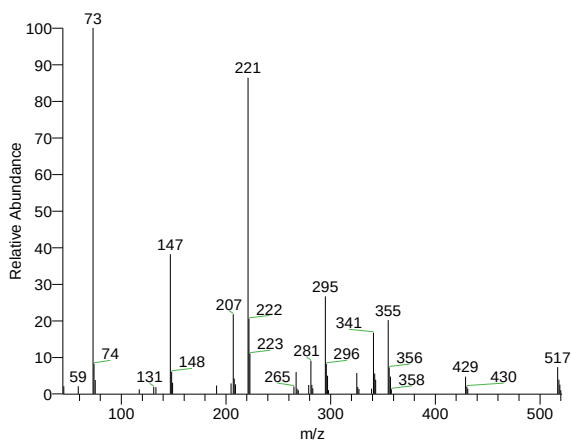


Analysed by Satyanarayana

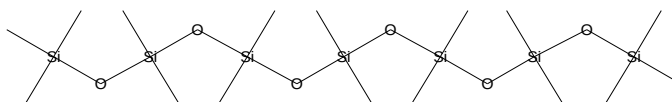
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Hit Spectrum

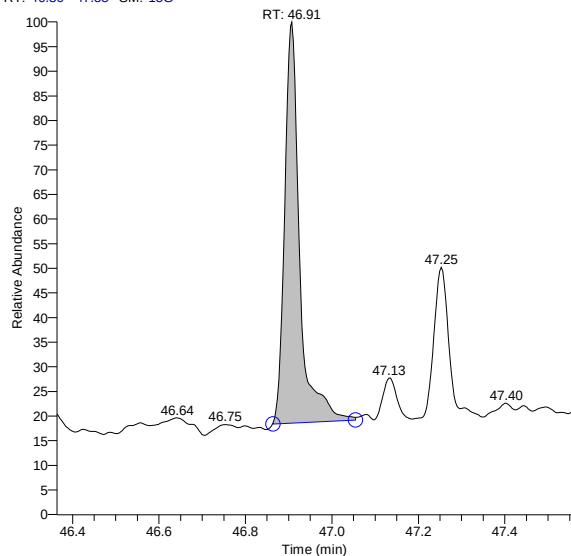
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane

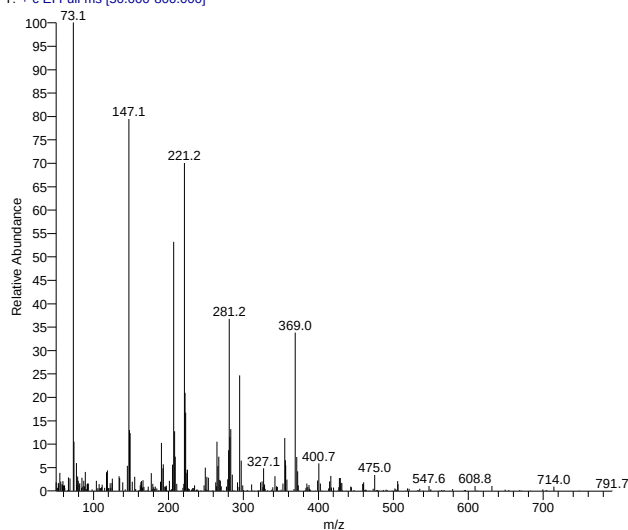


RT: 46.36 - 47.55 SM: 15G



NL:
1.84E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #12199 RT: 46.91 AV: 1 RF: 6.00, 3 NL: 2.68E5
T: + c EI Full ms [50.000-800.000]



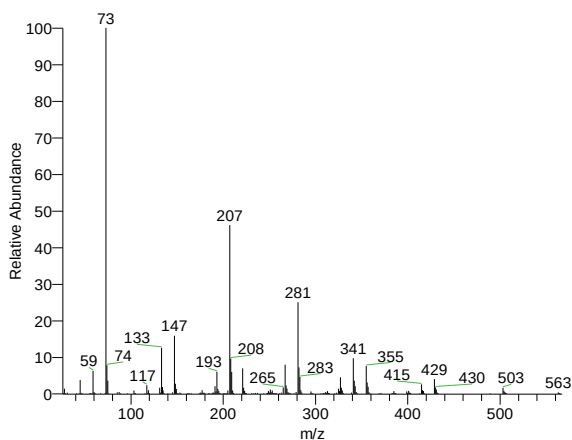
RT	Compound Name	Area	Probability	SI	RSI	Library
46.91	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3610289.13	45.56	600	660	mainlib
46.91	Heptasiloxane, hexadecamethyl-	3610289.13	18.01	578	770	mainlib
46.91	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3610289.13	8.74	559	671	mainlib
46.91	Hexasiloxane, tetradecamethyl-	3610289.13	7.04	554	793	mainlib
46.91	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3610289.13	5.95	550	661	mainlib

Analysed by Satyanarayana

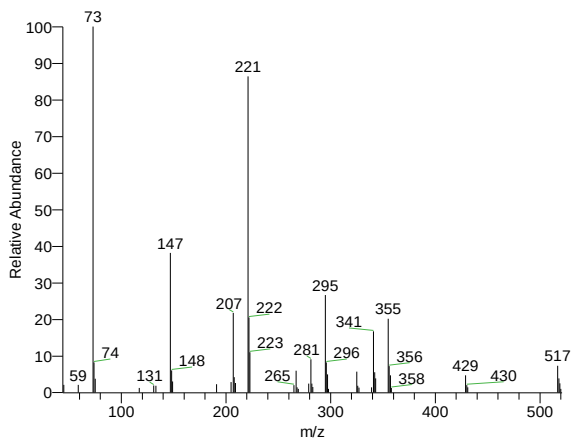
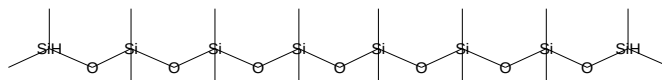
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Hit Spectrum

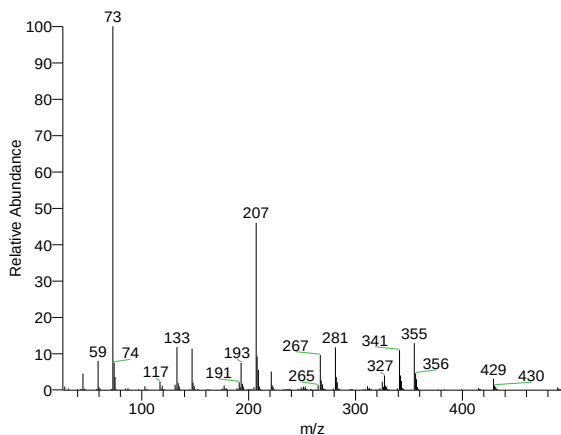
Compound Structure



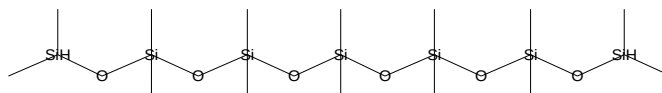
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

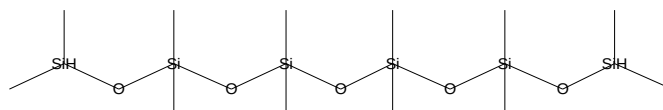
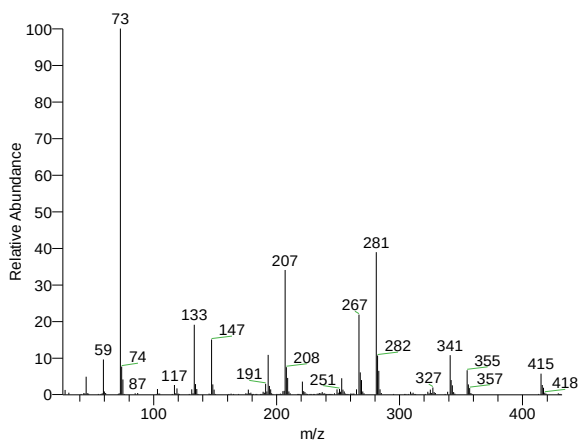
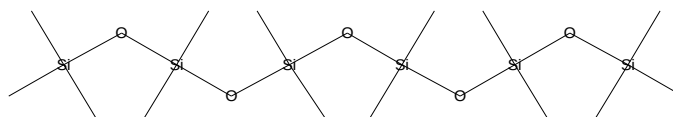
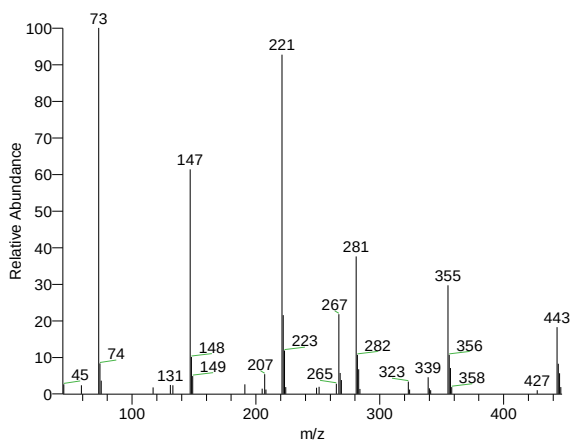
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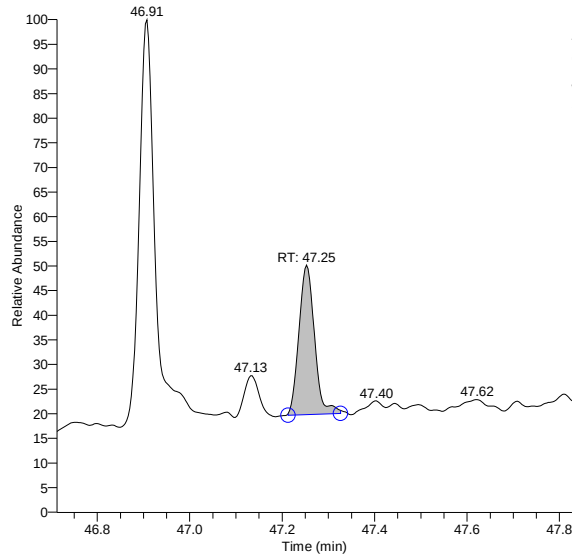
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

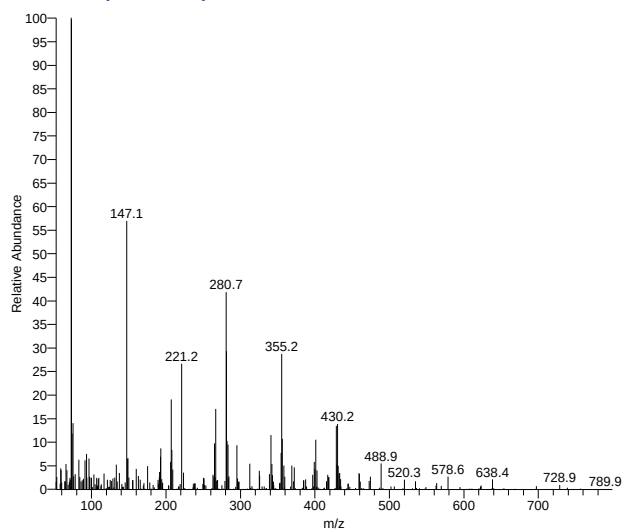
Compound Structure



RT: 46.71 - 47.83 SM: 15G



NGA-ZE-WATER2-SAMPLE-INJ1 #12302 RT: 47.25 AV: 1 RF: 6.00, 3 NL: 1.39E5
T: + c EI Full ms [50.000-800.000]



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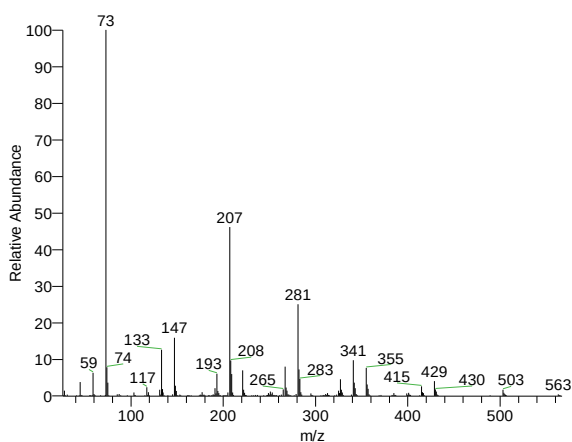
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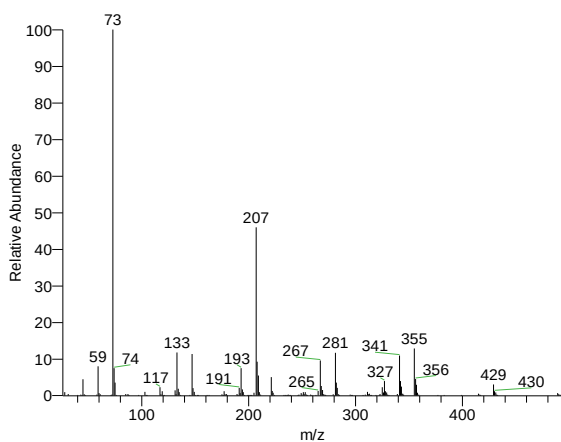
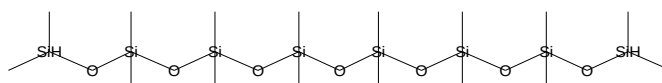
RT	Compound Name	Area	Probability	SI	RSI	Library
47.25	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1305395.02	51.01	621	706	mainlib
47.25	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1305395.02	17.09	597	711	mainlib
47.25	Cyclononasiloxane, octadecamethyl-	1305395.02	16.43	596	686	mainlib
47.25	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1305395.02	5.50	572	689	mainlib
47.25	Cyclodecasiloxane, eicosamethyl-	1305395.02	5.07	570	593	mainlib

Hit Spectrum

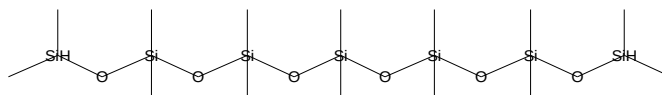
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

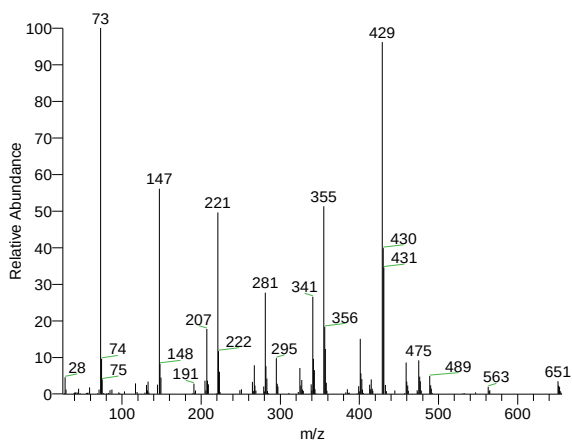


Analysed by Satyanarayana

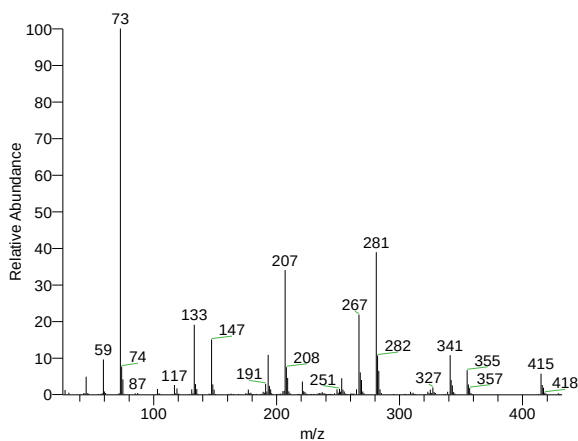
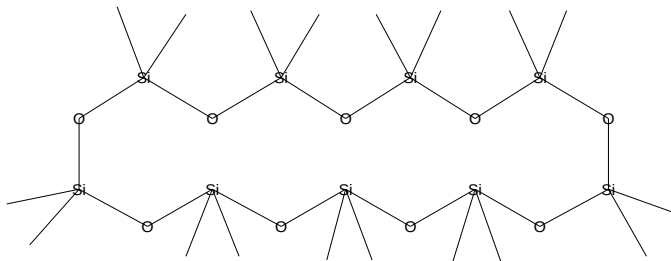
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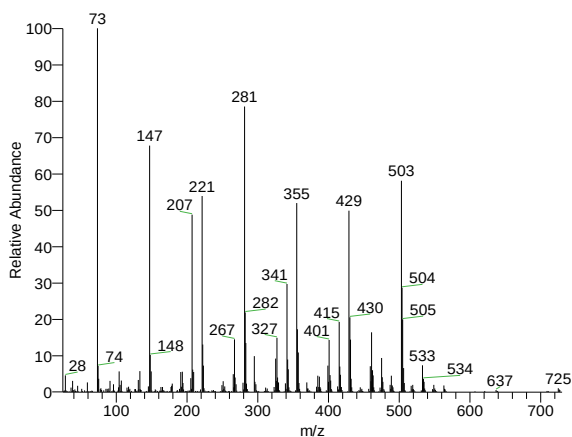
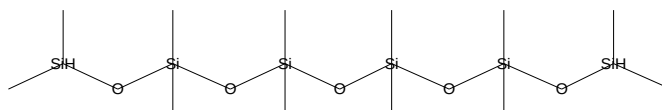
Compound Structure



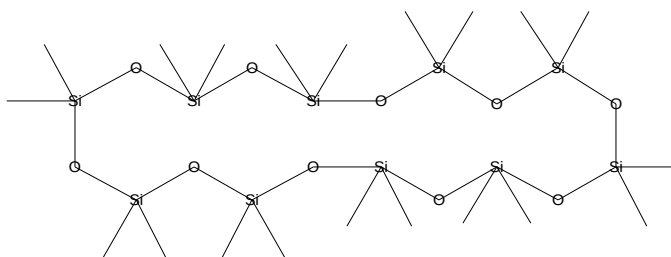
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



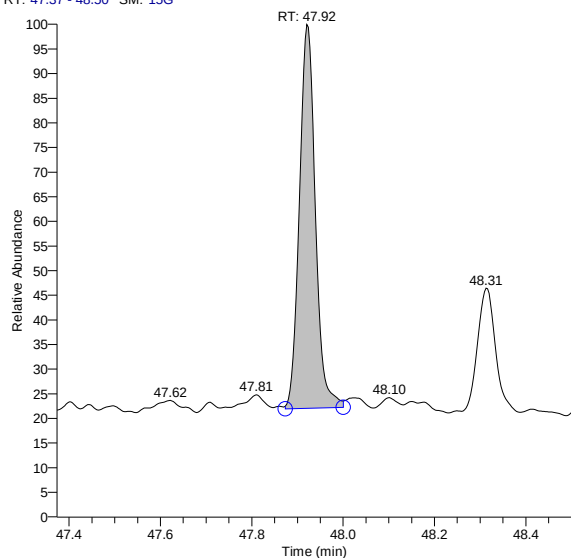
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Analysed by Satyanarayana

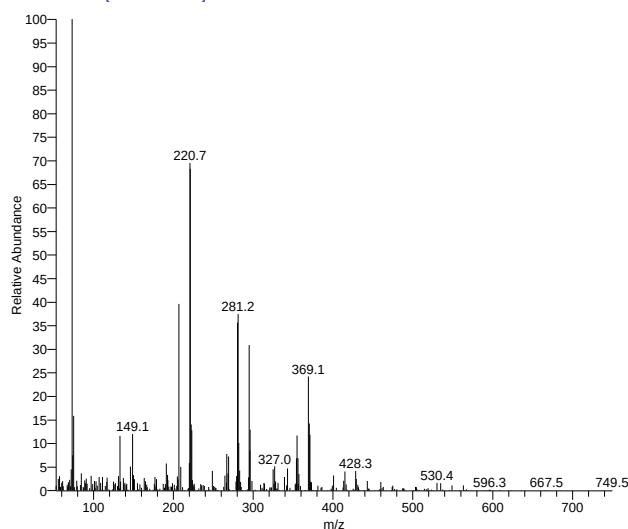
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RT: 47.37 - 48.50 SM: 15G



NL:
1.78E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

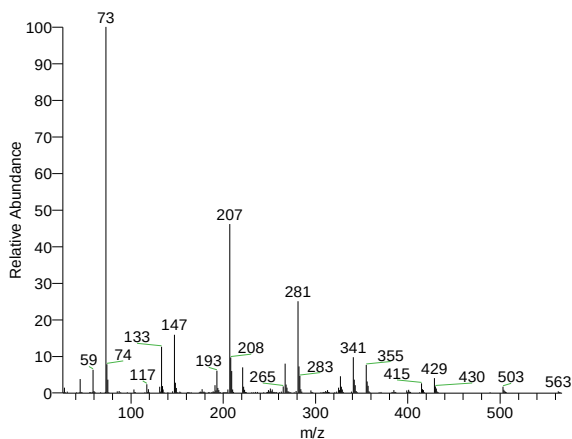
NGA-ZE-WATER2-SAMPLE-INJ1 #12501 RT: 47.92 AV: 1 RF: 6.00, 3 NL: 2.77E5
T: + c EI Full ms [50.000-800.000]



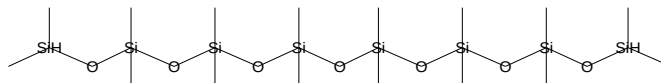
RT	Compound Name	Area	Probability	SI	RSI	Library
47.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	3390519.81	25.24	527	589	mainlib
47.92	Heptasiloxane, hexadecamethyl-	3390519.81	15.30	512	694	mainlib
47.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	3390519.81	9.88	499	590	mainlib
47.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	3390519.81	7.57	492	600	mainlib
47.92	Hexasiloxane, tetradecamethyl-	3390519.81	6.98	490	725	mainlib

Hit Spectrum

Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

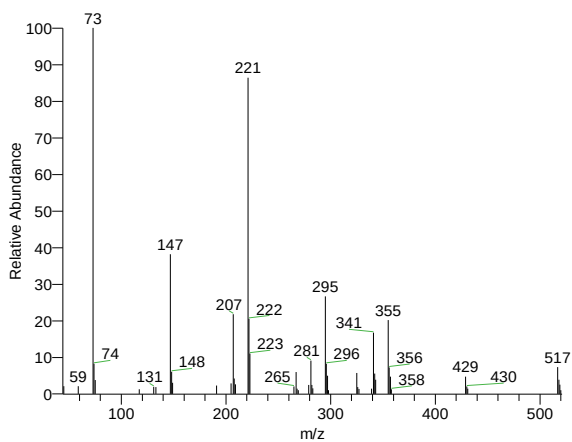
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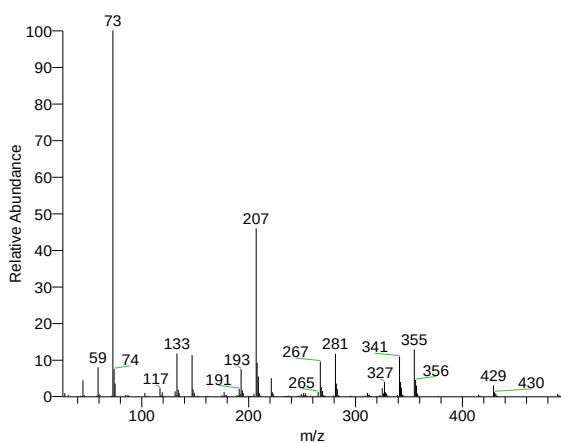
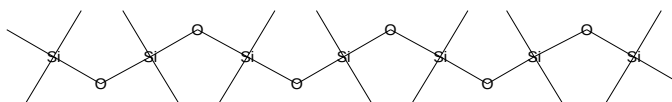
ANALYTICAL CHEMISTRY DIVISION

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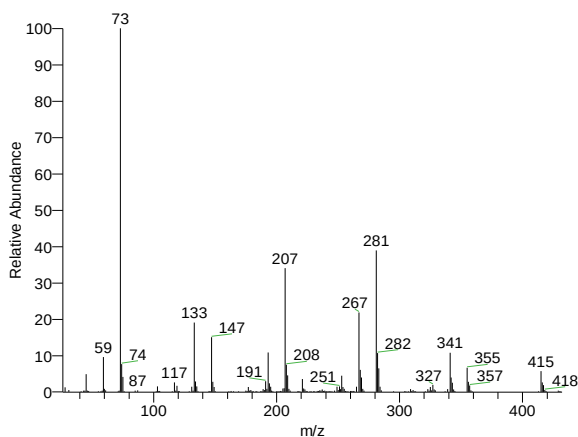
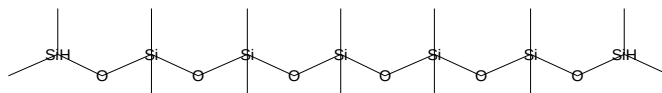
Compound Structure



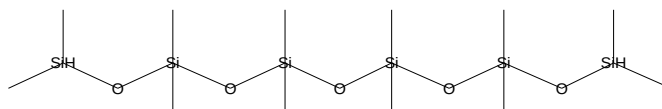
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C12H38O5Si6, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

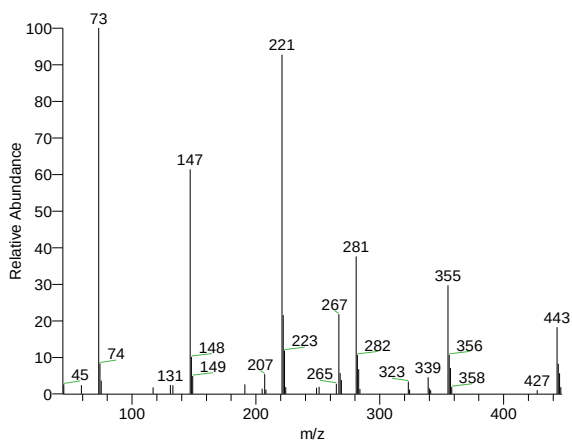


Analysed by Satyanarayana

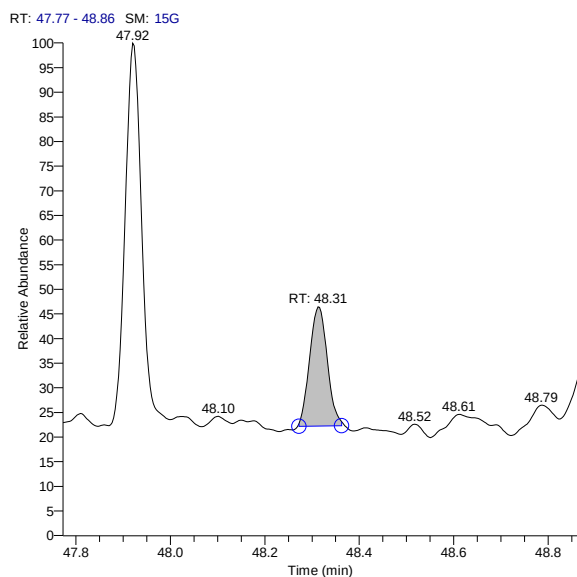
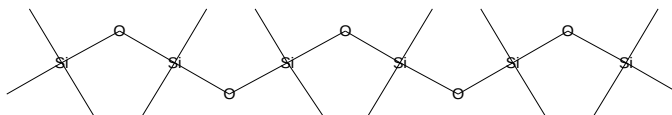
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

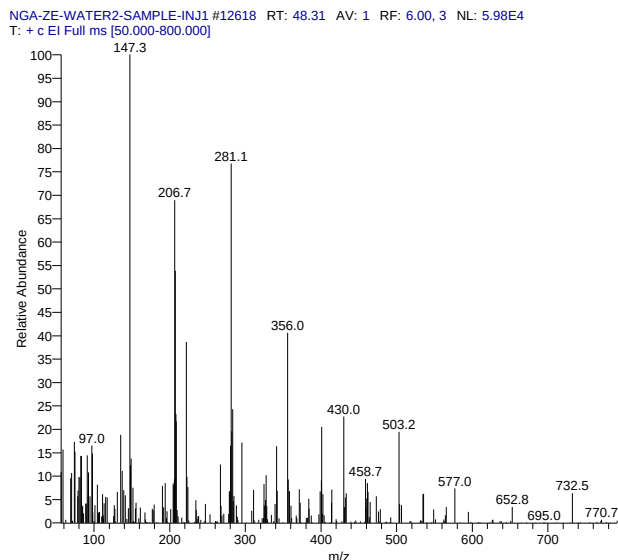
Compound Structure



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



NL: 1.78E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1



RT	Compound Name	Area	Probability	SI	RSI	Library
48.31	Cyclodecasiloxane, eicosamethyl-	1115720.14	39.59	481	520	mainlib
48.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1115720.14	20.41	463	566	mainlib
48.31	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1115720.14	4.89	425	566	mainlib
48.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1115720.14	3.84	419	559	mainlib
48.31	Cyclononasiloxane, octadecamethyl-	1115720.14	2.48	406	486	mainlib

Analysed by Satyanarayana

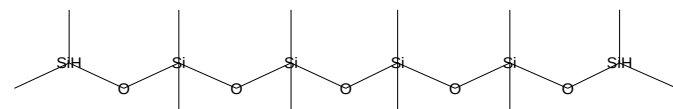
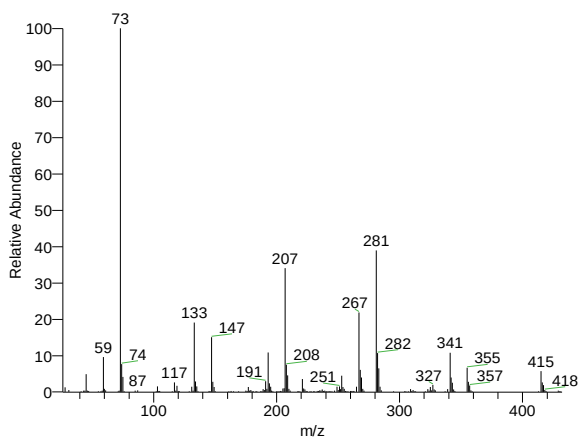
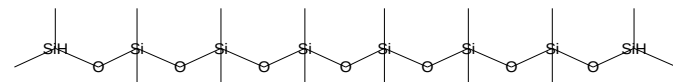
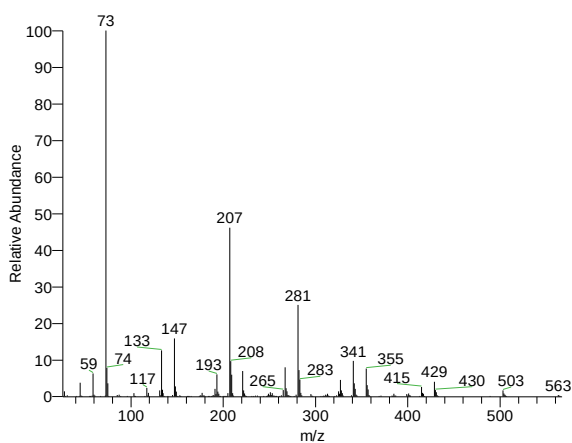
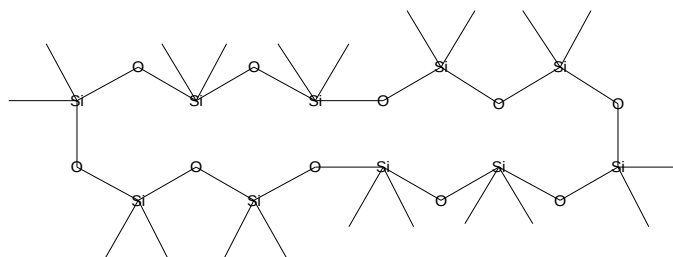
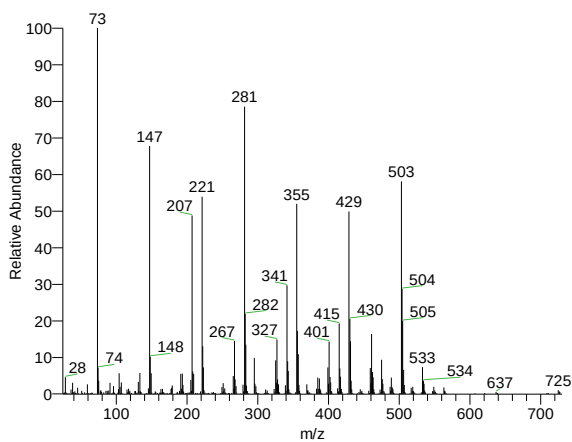
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure



Analysed by Satyanarayana

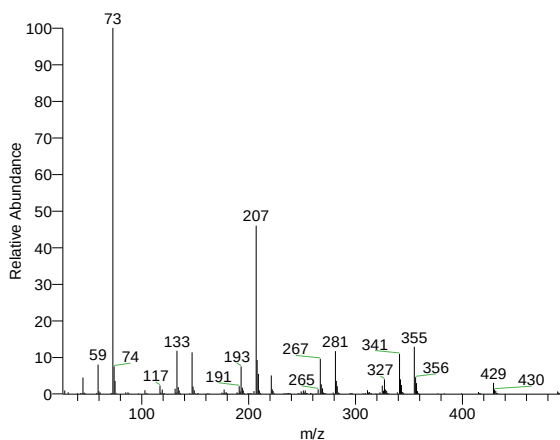
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GC-MS/MS QUAL REPORT

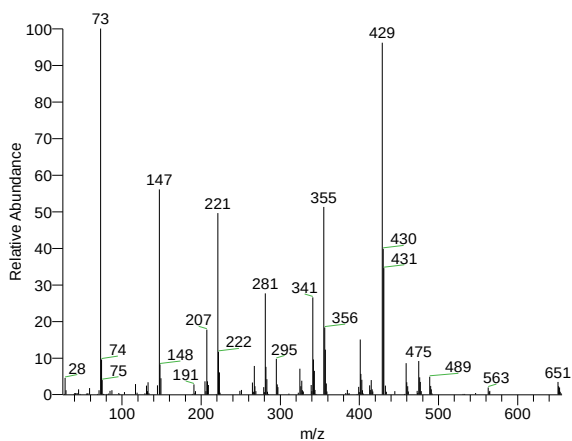
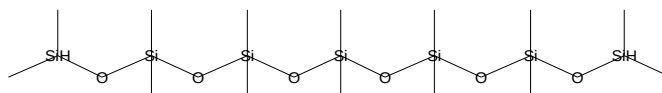
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

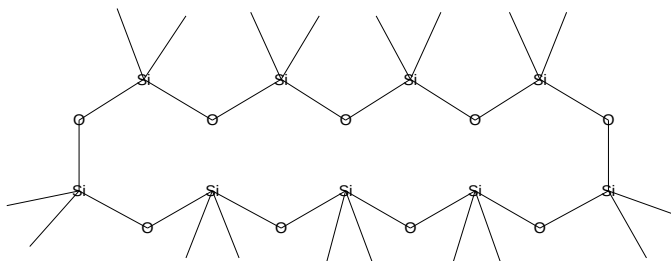
Compound Structure



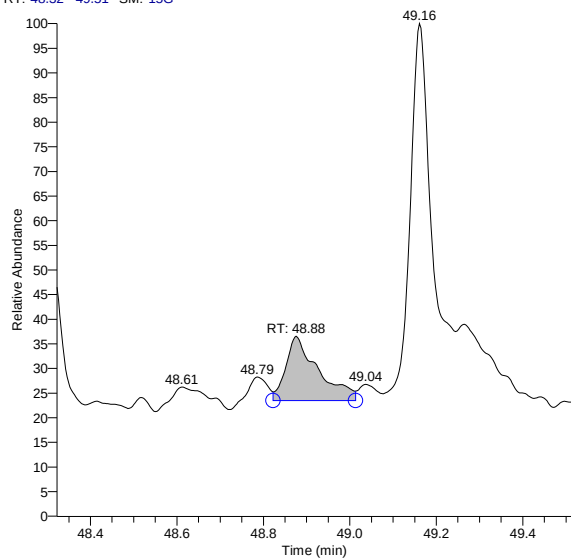
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane

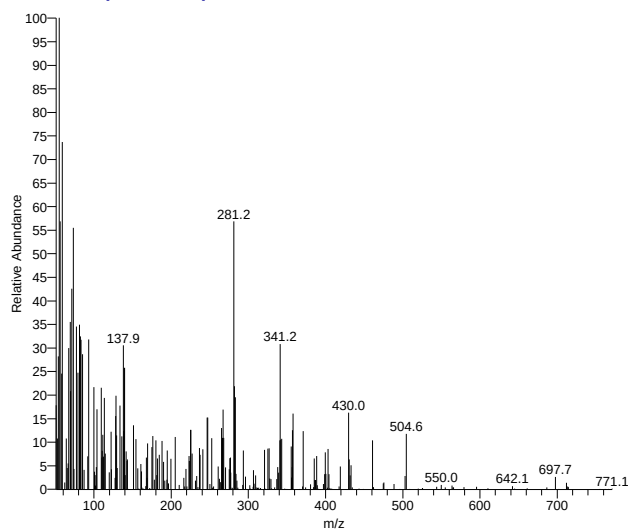


RT: 48.32 - 49.51 SM: 15G



NL:
1.67E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #12786 RT: 48.88 AV: 1 RF: 6.00, 3 NL: 2.92E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

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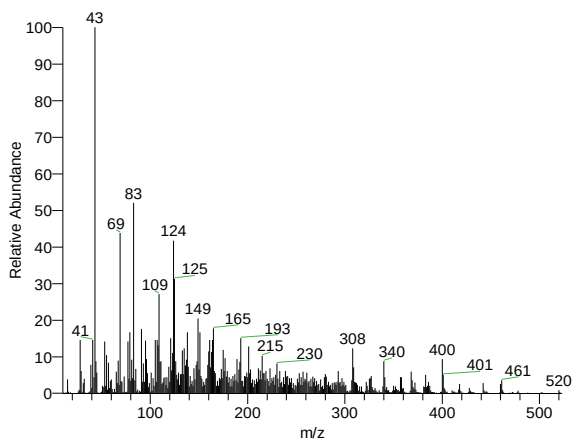
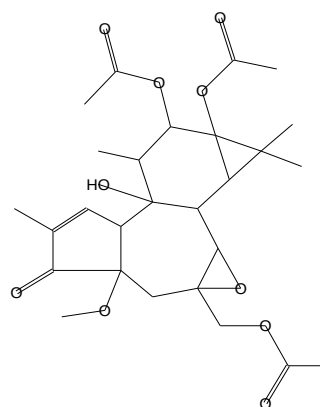
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
48.88	4H-Cyclopropa[5',6']benz[1',2':7,8]azuleno[5,6]oxiren-4-one, 8,8a-bis(acetyloxy)-2a-[(a cetyloxy)methyl]-1,1a,1b, 1c,2a,3,3a,6a,6b,7,8,8a-do decahydro-6b-hydroxy-3a- methoxy-1,1,5,7-tetrameth yl-, [1aR-(1aà,1bà,1cà,2aà,3aà ,6aà,6bà,7à,8à,8aà)]-	1126402.36	8.85	395	405	mainlib
48.88	Propanoic acid, 2-(3-acetoxy-4,4,14-trimeth ylandro-8-en-17-yl)-	1126402.36	7.13	390	406	mainlib
48.88	1,3,5,7,9-Pentaethyl-1,9-di butoxypentasiloxane	1126402.36	5.75	385	569	mainlib
48.88	Cholestan-3-one, cyclic 1,2-ethanediyl aetal, (5à)-	1126402.36	4.86	381	440	mainlib
48.88	7aH-Cyclopenta[a]cyclopro pa[f]cycloundecene-2,4,7, 7a,10,11-hexol, 1,1a,2,3,4,4a,5,6,7,10,11,1 1a-dodecahydro-1,1,3,6,9- pentamethyl-, 2,4,7,10,11-pentaacetate	1126402.36	4.10	377	398	mainlib

Hit Spectrum

Compound Structure

Formula C₂₇H₃₆O₁₀, MW 520, CAS# 64838-69-3, Entry# 9653

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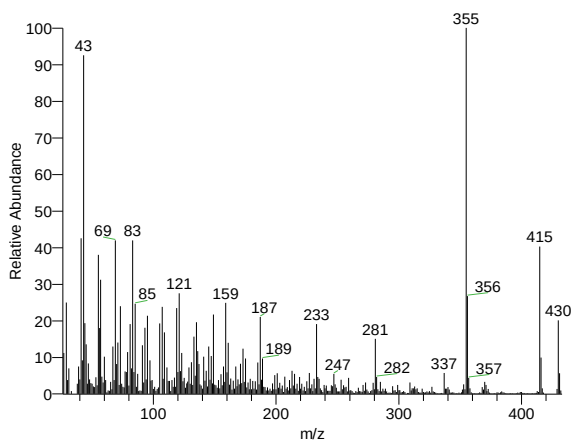
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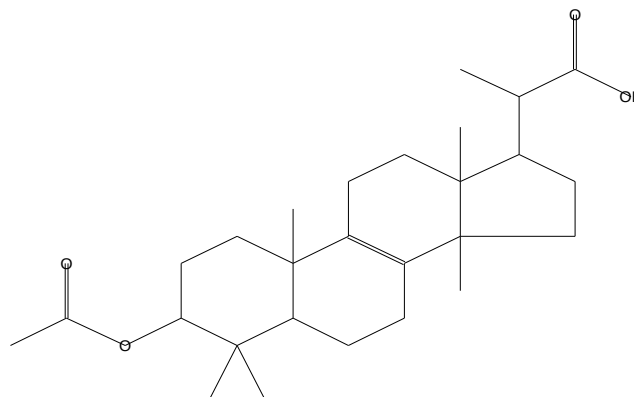
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

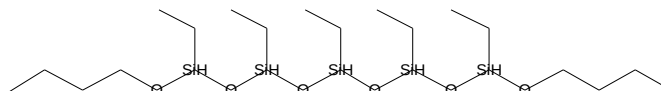
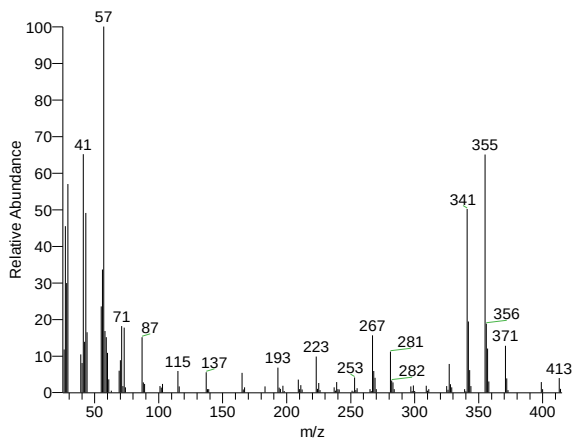
Compound Structure



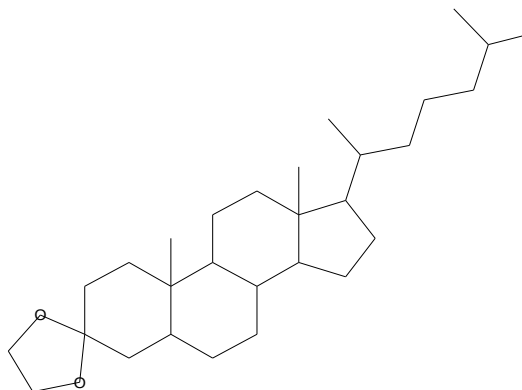
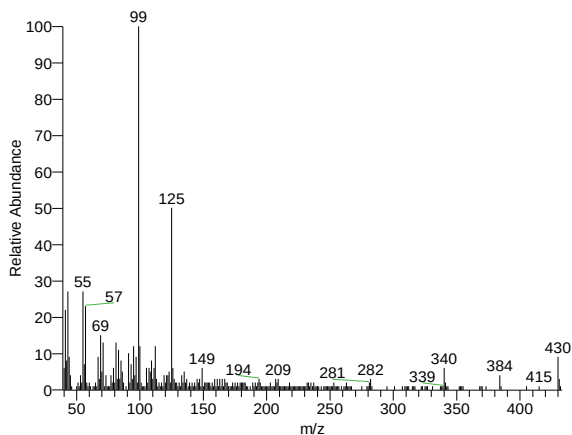
Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandrosta-8-en-17-yl)-
Formula C₂₇H₄₂O₄, MW 430, CAS# NA, Entry# 234266



1,3,5,7,9-Pentaethyl-1,9-dibutoxypentasiloxane
Formula C₁₈H₄₈O₆Si₅, MW 500, CAS# 73420-35-6, Entry# 23889
1,9-Dibutoxy-1,3,5,7,9-pentaethylpentasiloxane #



Cholestan-3-one, cyclic 1,2-ethanediyl aetal, (5 α)-
Formula C₂₉H₅₀O₂, MW 430, CAS# 25328-53-4, Entry# 72469
5 α -Cholestan-3-one, cyclic ethylene acetal

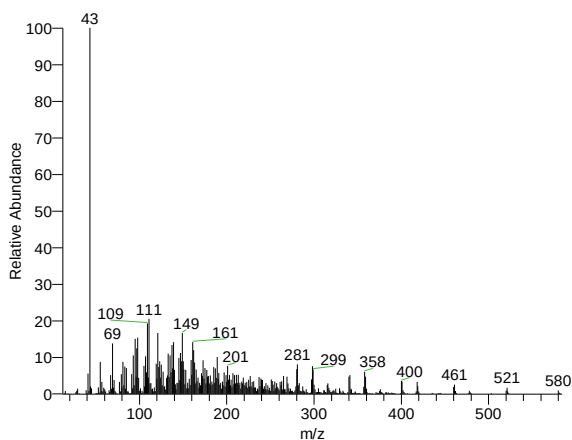


Analysed by Satyanarayana

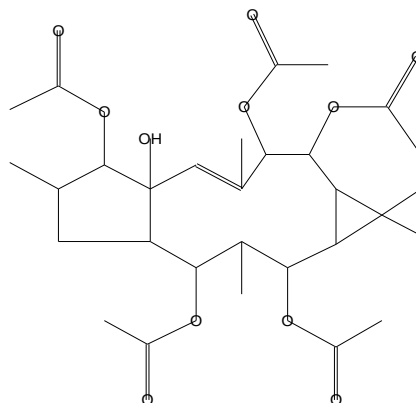
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

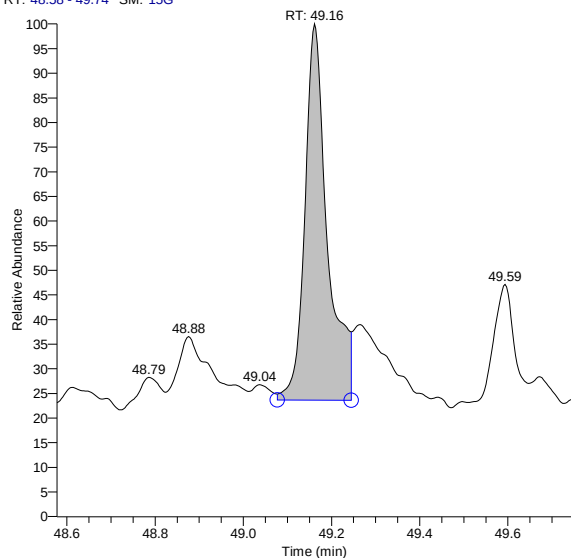
Compound Structure



Formula C₃₀H₄₄O₁₁, MW 580, CAS# 51906-08-2, Entry# 11163

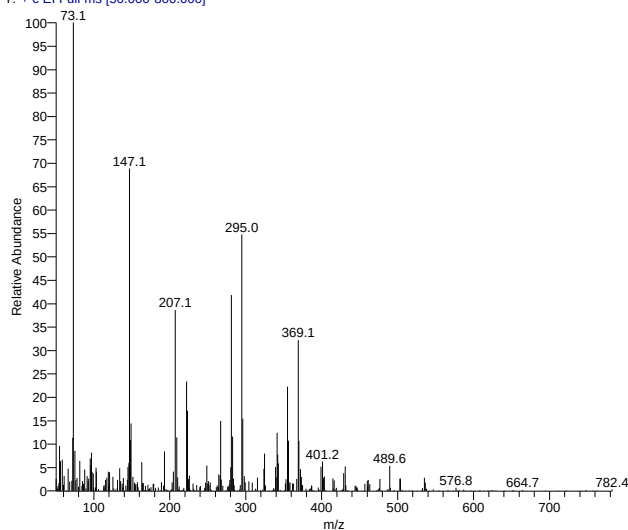


RT: 48.58 - 49.74 SM: 15G



NL:
1.67E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #12871 RT: 49.16 AV: 1 RF: 6.00, 3 NL: 1.77E5
T: + c EI Full ms [50.000-800.000]



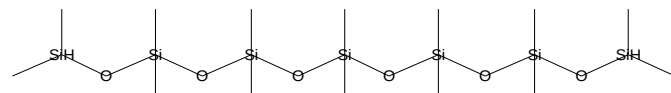
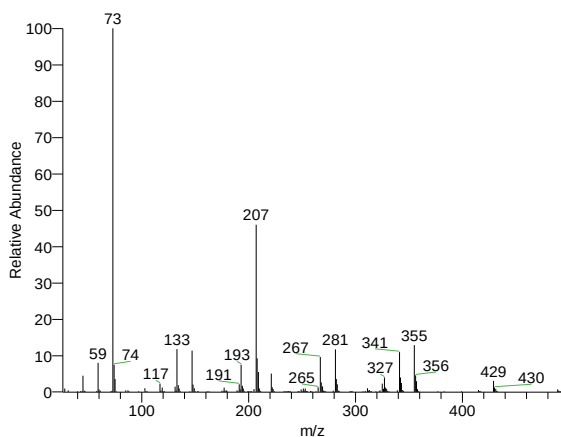
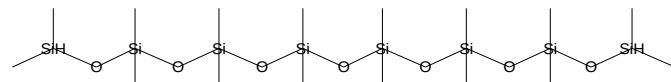
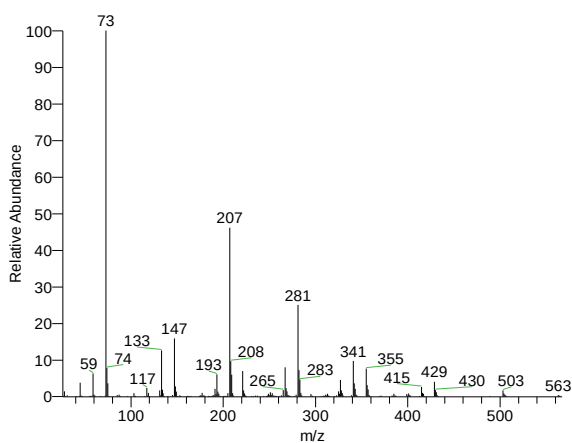
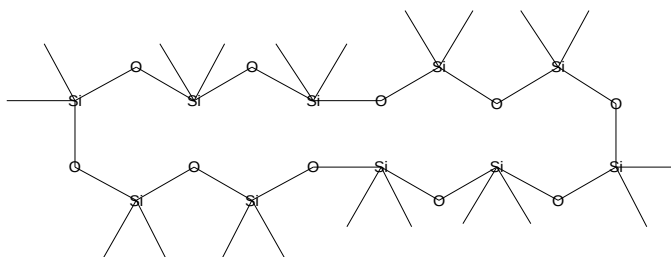
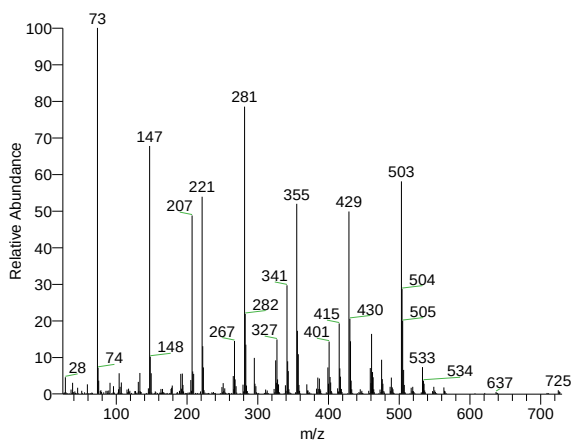
RT	Compound Name	Area	Probability	SI	RSI	Library
49.16	Cyclodecasiloxane, eicosamethyl-	4522682.90	22.49	515	540	mainlib
49.16	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	4522682.90	20.74	513	605	mainlib
49.16	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	4522682.90	8.82	492	622	mainlib
49.16	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	4522682.90	6.40	483	648	mainlib
49.16	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	4522682.90	4.39	472	610	mainlib

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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure



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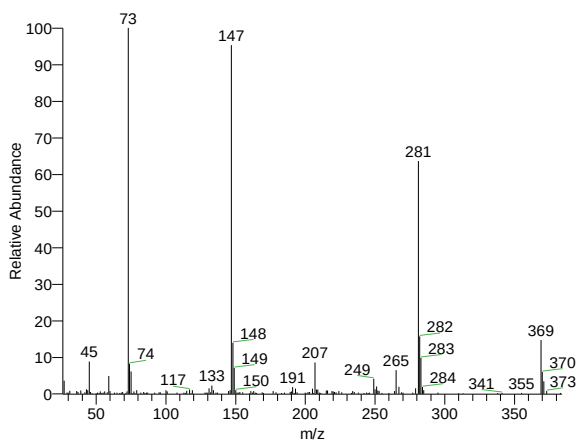
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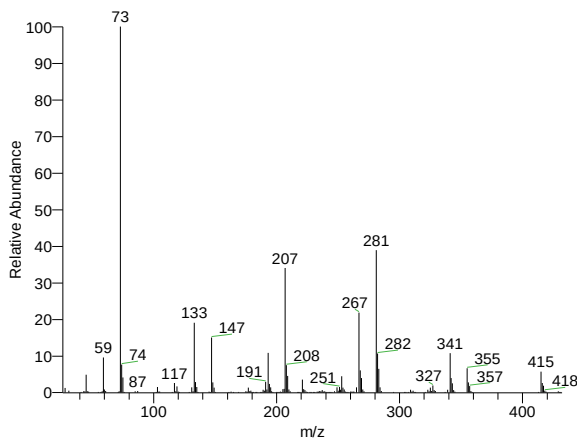
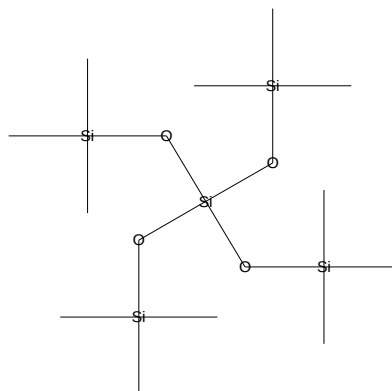
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

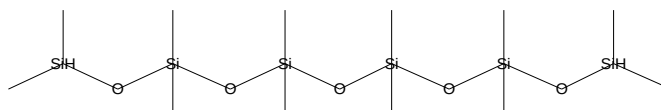
Compound Structure



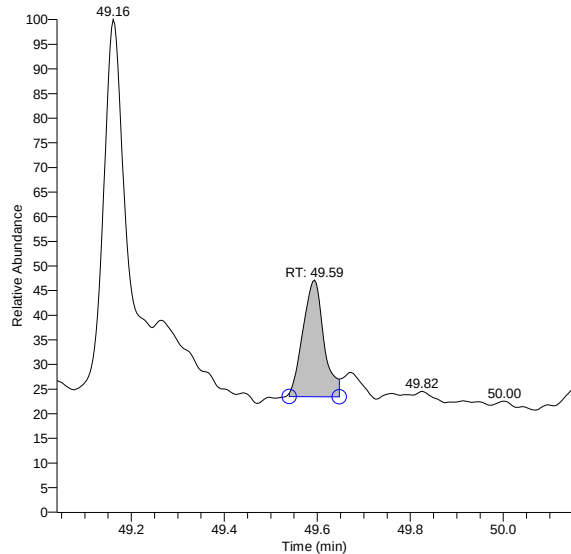
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

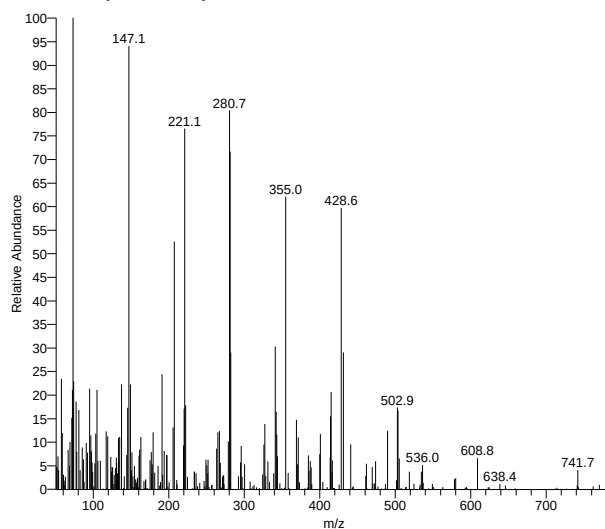


RT: 49.04 - 50.15 SM: 15G



NL:
1.67E6
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #13000 RT: 49.59 AV: 1 RF: 6.00, 3 NL: 4.92E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
49.59	Cyclodecasiloxane, eicosamethyl-	1229843.07	43.12	535	588	mainlib

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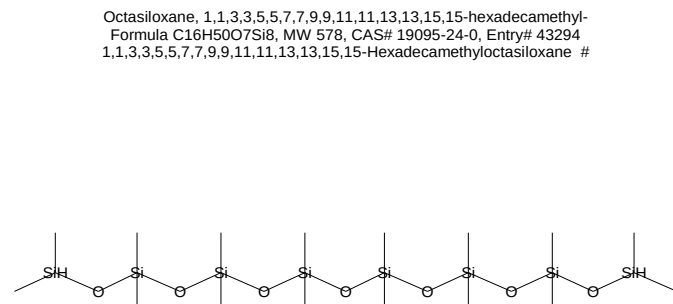
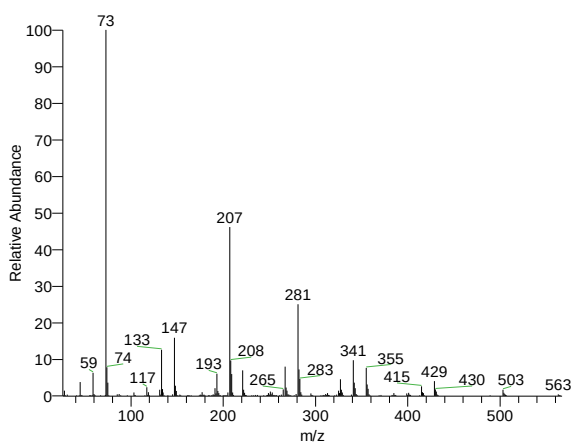
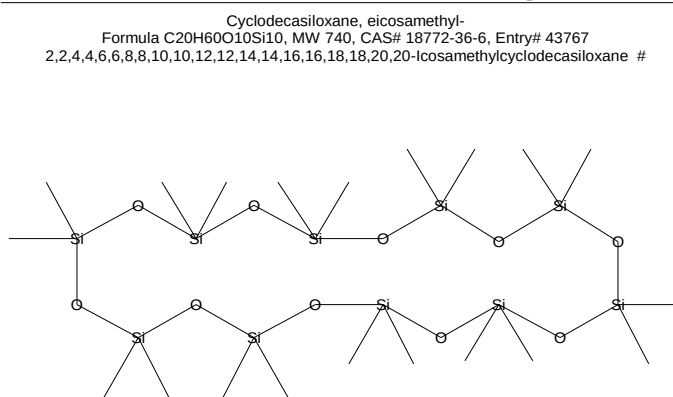
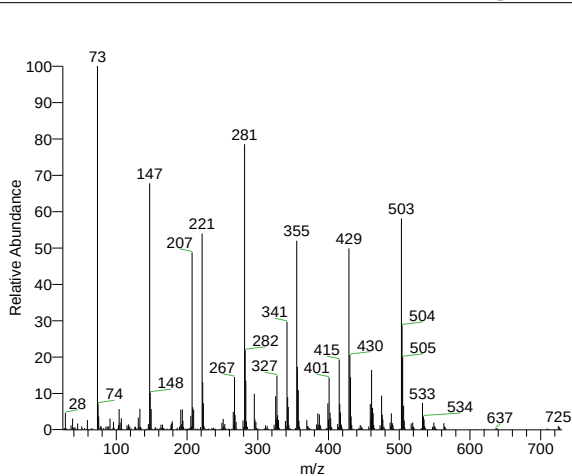
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RT	Compound Name	Area	Probability	SI	RSI	Library
49.59	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1229843.07	26.99	521	626	mainlib
49.59	Cyclononasiloxane, octadecamethyl-	1229843.07	5.05	464	593	mainlib
49.59	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1229843.07	4.07	459	587	mainlib
49.59	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1229843.07	2.55	445	580	mainlib

Hit Spectrum

Compound Structure



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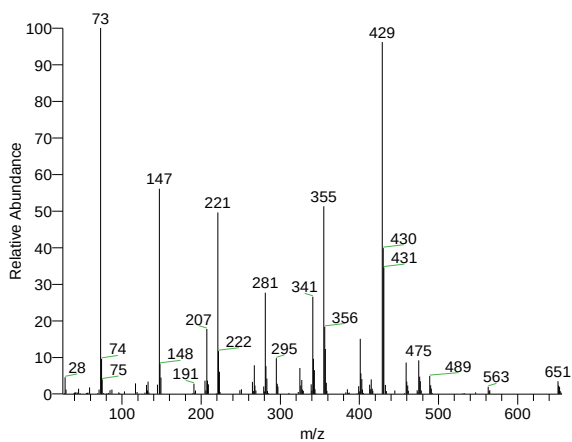
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GC-MS/MS QUAL REPORT

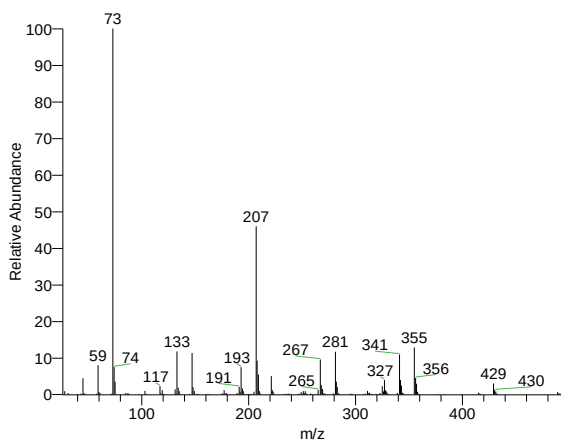
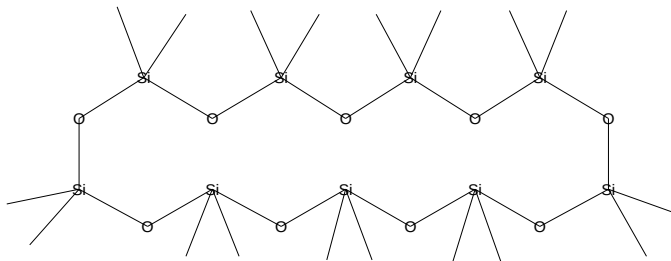
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

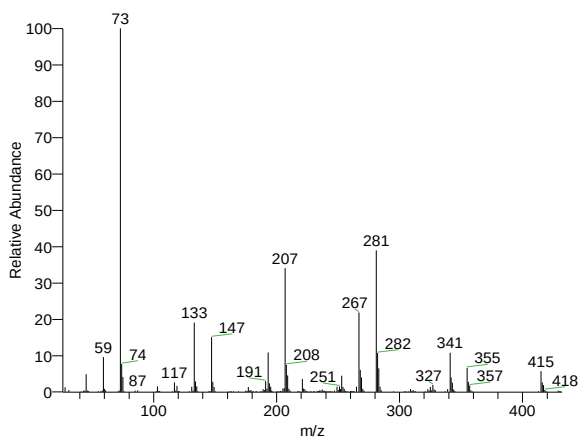
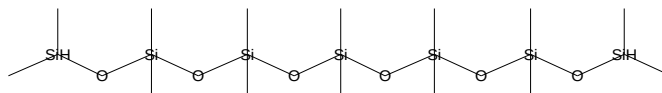
Compound Structure



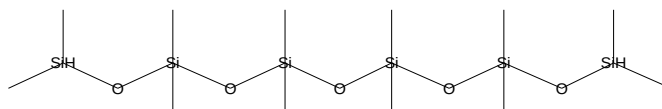
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



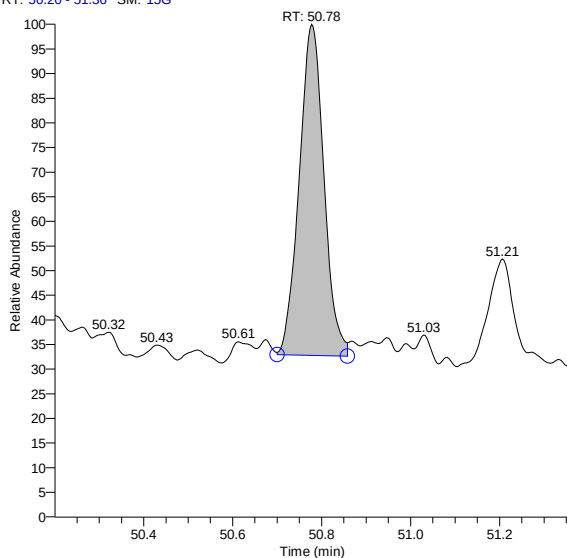
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Analysed by Satyanarayana

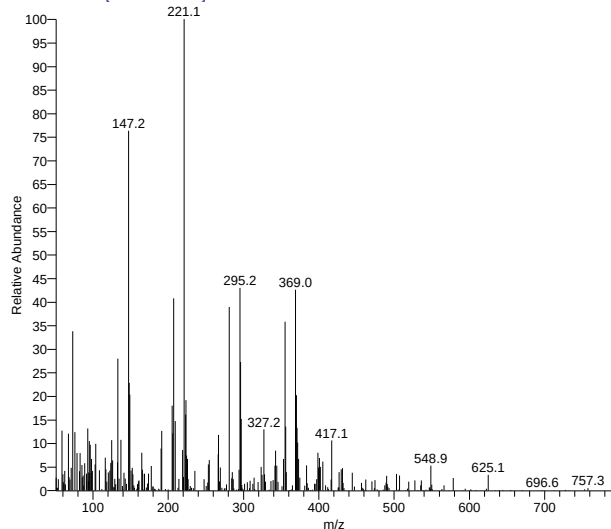
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RT: 50.20 - 51.36 SM: 15G



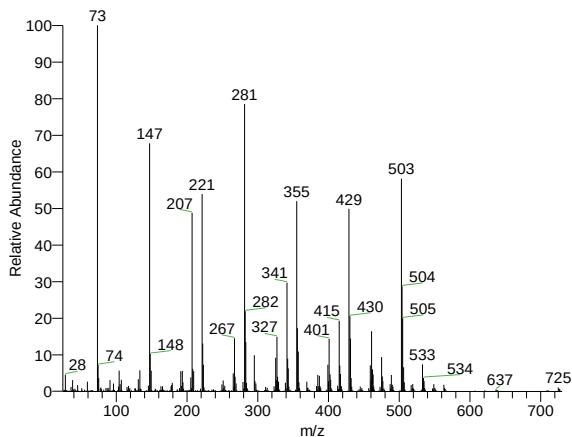
NL:
1.16E6
TIC: MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #13353 RT: 50.78 AV: 1 RF: 6.00, 3 NL: 8.06E4
T: + c EI Full ms [50.000-800.000]



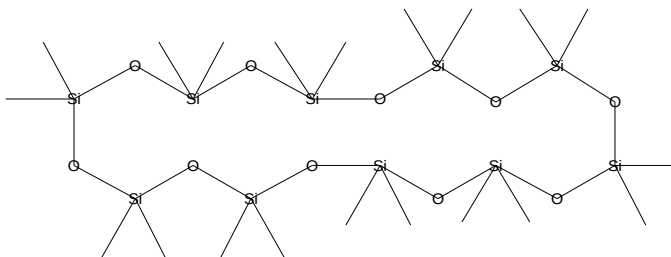
RT	Compound Name	Area	Probability	SI	RSI	Library
50.78	Cyclodecasiloxane, eicosamethyl-	2991809.71	13.30	445	474	mainlib
50.78	Heptasiloxane, hexadecamethyl-	2991809.71	7.66	429	691	mainlib
50.78	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2991809.71	7.36	428	514	mainlib
50.78	1,3,5,7,9,11,13-Heptaethyl cycloheptasiloxane	2991809.71	5.20	418	610	mainlib
50.78	1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isobutyl ester	2991809.71	3.87	410	555	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



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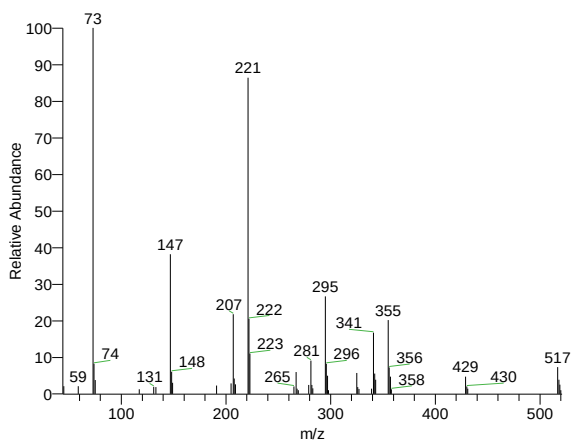
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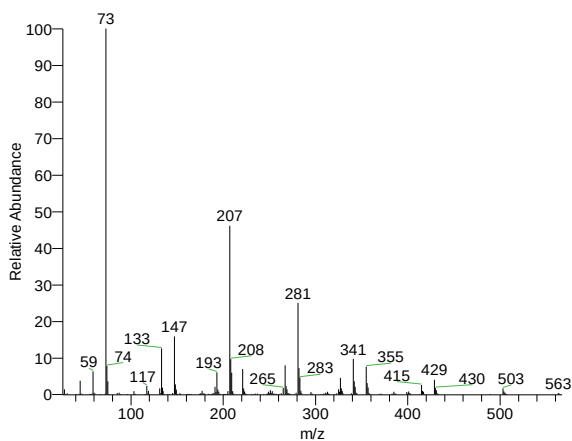
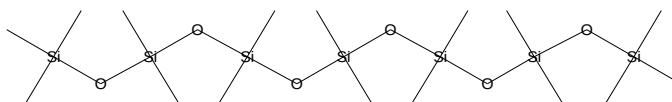
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

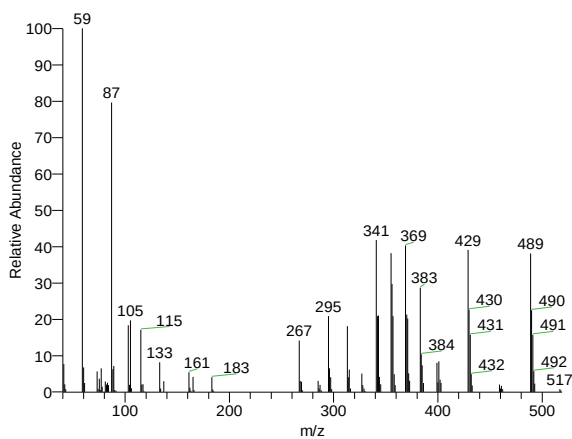
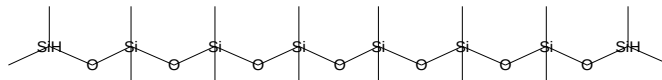
Compound Structure



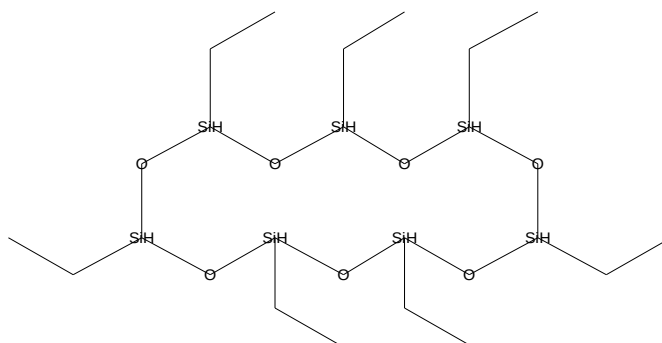
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



1,3,5,7,9,11,13-Heptaethylcycloheptasiloxane
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 17909-36-3, Entry# 30265
2,4,6,8,10,12,14-Heptaethylcycloheptasiloxane #

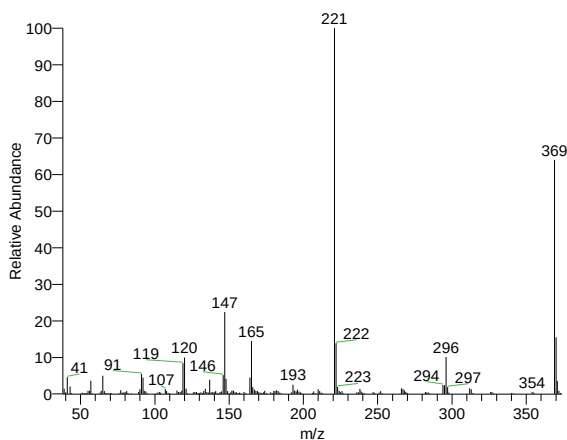


Analysed by Satyanarayana

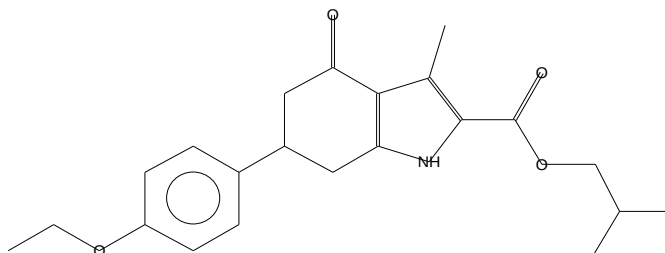
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Hit Spectrum

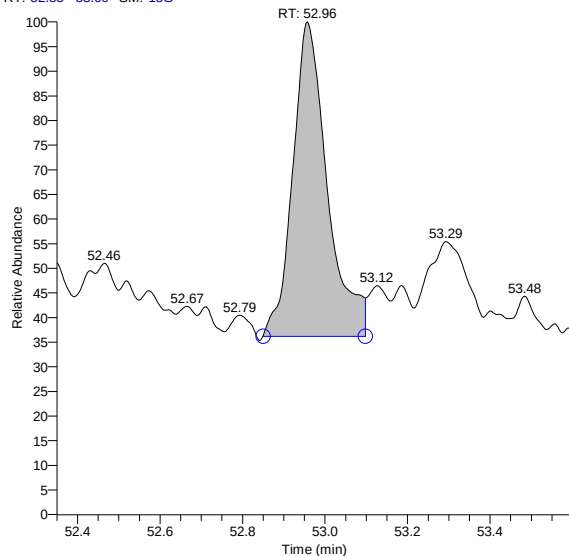
Compound Structure



1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isobutyl ester
Formula C₂₂H₂₇NO₄, MW 369, CAS# NA, Entry# 196839
\$:28XORXIIIMNPHEBIN-UHFFFAOYSA-N

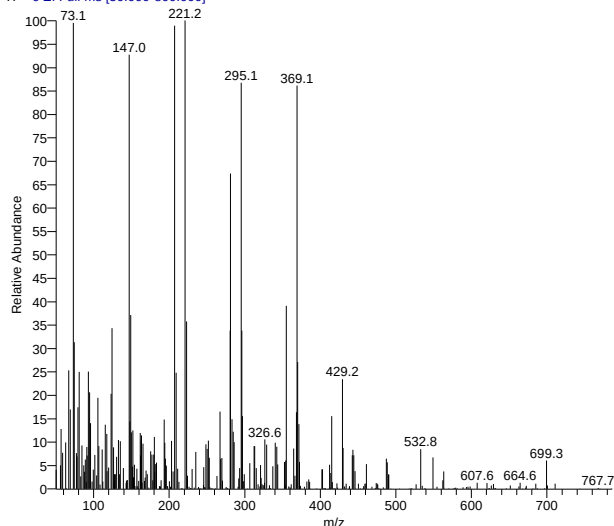


RT: 52.35 - 53.60 SM: 15G



NL:
9.97E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #14003 RT: 52.96 AV: 1 RF: 6.00, 3 NL: 4.58E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
52.96	Pentasiloxane, dodecamethyl-	3690110.79	7.98	426	544	mainlib
52.96	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3690110.79	6.43	421	523	mainlib
52.96	Acetic acid, 2-(2,3-dihydro-1,3-dioxo-1H-inden-2-yl)-2-(3,4-dimethoxyphenyl)-, ethyl ester	3690110.79	4.93	414	520	mainlib
52.96	Cyclodecasiloxane, eicosamethyl-	3690110.79	4.16	410	451	mainlib
52.96	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3690110.79	4.16	410	542	mainlib

Analysed by Satyanarayana

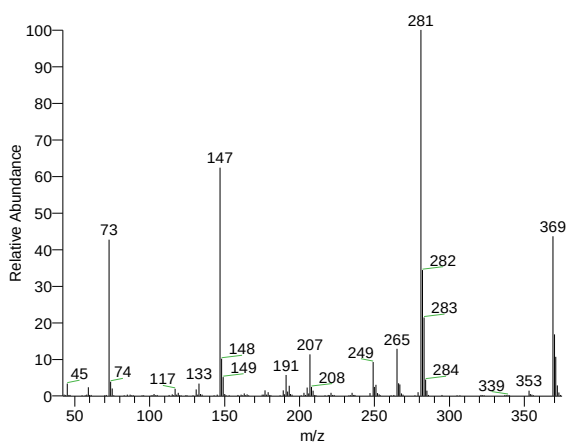
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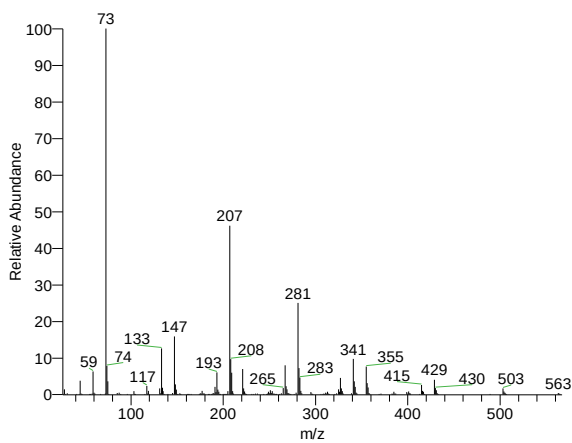
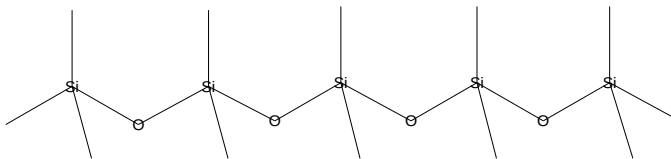
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

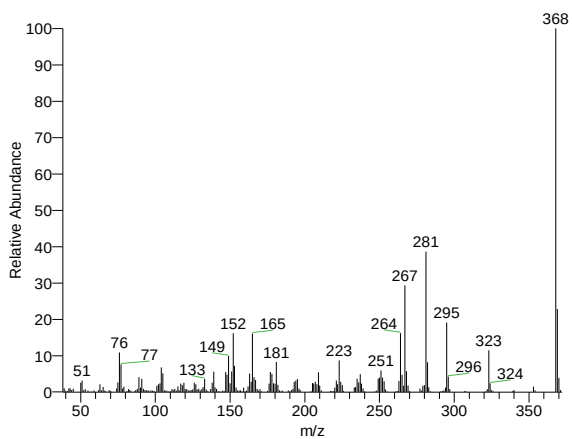
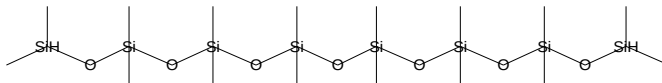
Compound Structure



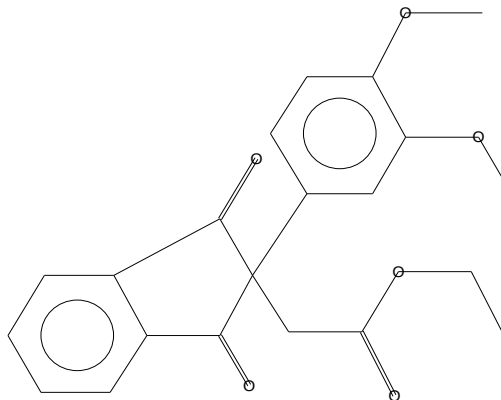
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Acetic acid, 2-(2,3-dihydro-1,3-dioxo-1H-inden-2-yl)-2-(3,4-dimethoxyphenyl)-, ethyl ester
Formula C₂₁H₂₀O₆, MW 368, CAS# 7185-23-1, Entry# 235699
Ethyl [2-(3,4-dimethoxyphenyl)-1,3-dioxo-2,3-dihydro-1H-inden-2-yl]acetate #

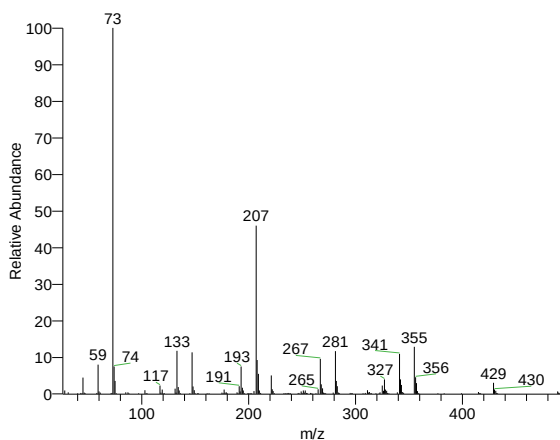


Analysed by Satyanarayana

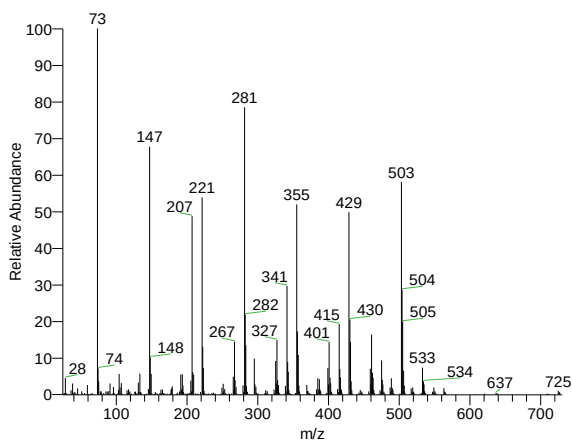
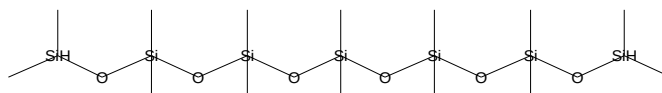
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Hit Spectrum

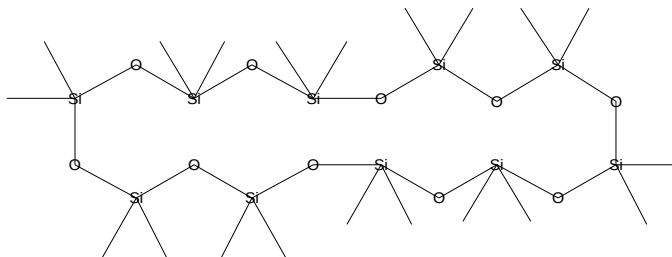
Compound Structure



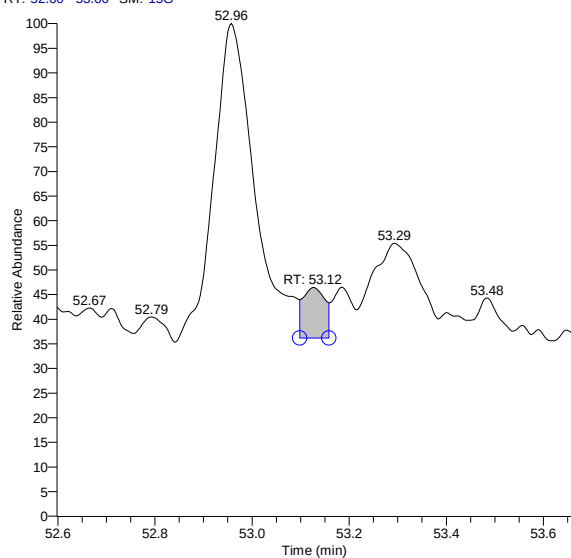
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #

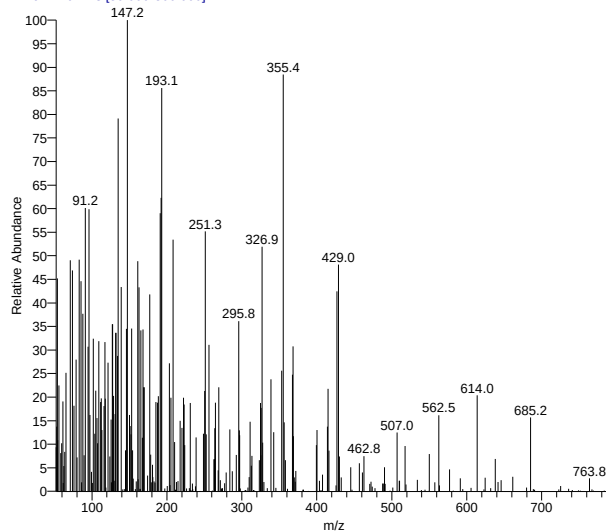


RT: 52.60 - 53.66 SM: 15G



NL:
9.97E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #14053 RT: 53.12 AV: 1 RF: 6.00, 3 NL: 1.34E4
T: + c EI Full ms [50.000-800.000]



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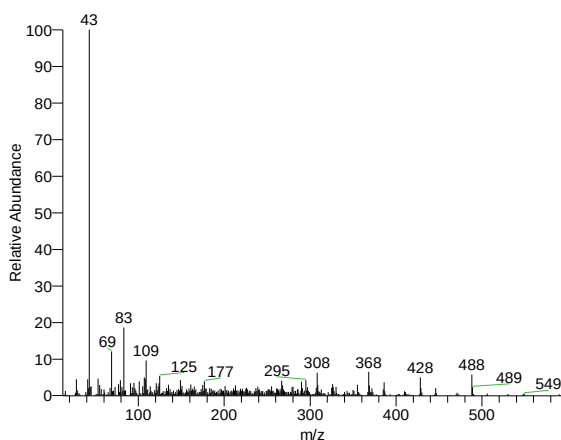
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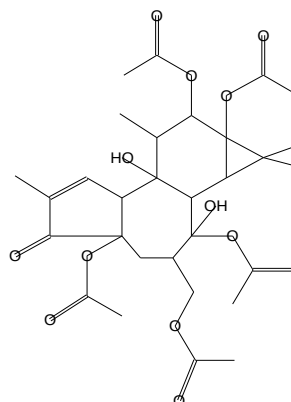
RT	Compound Name	Area	Probability	SI	RSI	Library
53.12	5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-one, 2,4a,9,9a-tetrakis(acetyloxy)-3,[(acetyloxy)methyl]-1,1a,1b,2,3,4,4a,7a,7b,8,9,9a-dodecahydro-2,7b-dihydroxy-1,1,6,8-tetramethyl-, [1aR-(1aà,1bá,2à,3á,4aá,7aà,7bà,8à,9á,9aà)]-	322066.21	7.47	389	417	mainlib
53.12	5H-Cyclopropa[3,4]benz[1,2-e]azulen-5-one, 2,9,9a-tris(acetyloxy)-3-[(acetyloxy)methyl]-1,1a,1b,2,4a,7a,7b,8,9,9a-decahydro-4a,7b-dihydroxy-1,1,6,8-tetramethyl-, [1aR-(1aà,1bá,2á,4aá,7aà,7bà,8à,9á,9aà)]-	322066.21	4.67	375	404	mainlib
53.12	3,9á:14,15-Diepoxypregn-16-en-20-one, 3,11á,18-triacetoxy-	322066.21	4.49	374	432	mainlib
53.12	4-(cis-2,3,4,trans-6-Tetramethyl-3-cyclohexenyl)butan-2-one	322066.21	4.49	374	449	mainlib
53.12	2,4-dinitrophenylhydrazone Formyl colchicine	322066.21	4.14	372	413	mainlib

Hit Spectrum

Compound Structure



Formula C₃₀H₄₀O₁₃, MW 608, CAS# 77573-25-2, Entry# 9659

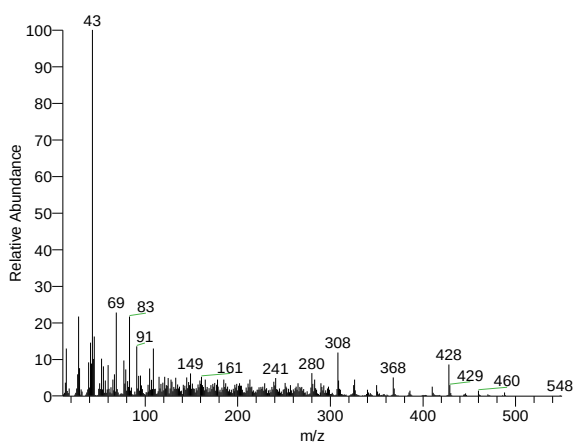


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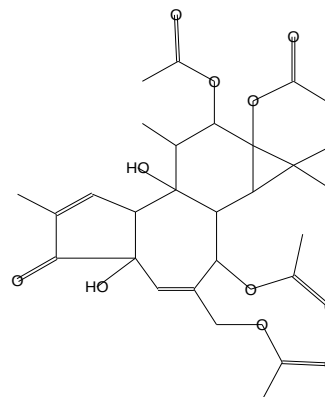
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Hit Spectrum

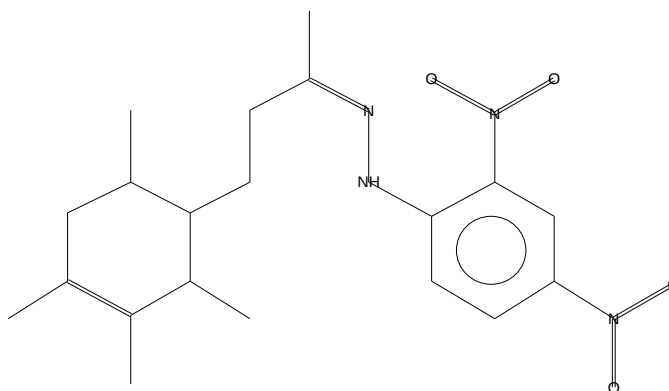
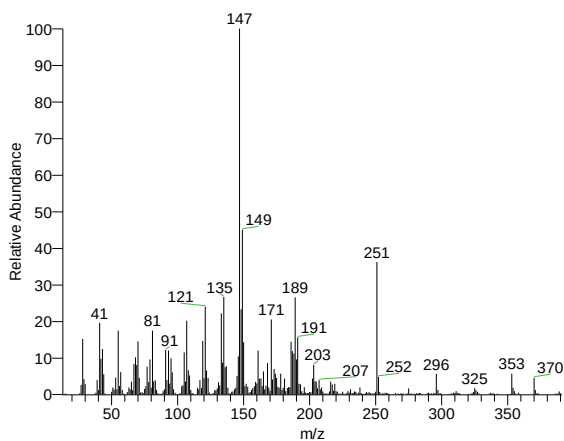
Compound Structure



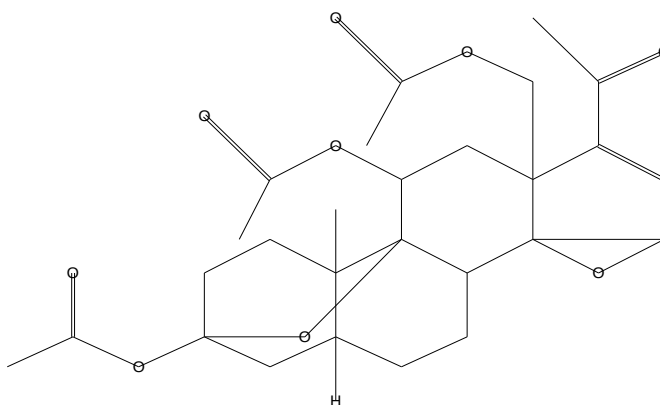
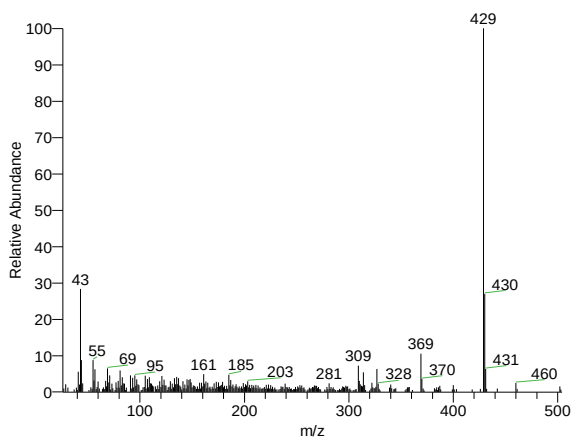
Formula C₂₈H₃₆O₁₁, MW 548, CAS# 77573-17-2, Entry# 8447



4-(cis-2,3,4,trans-6-Tetramethyl-3-cyclohexenyl)butan-2-one, 2,4-dinitrophenylhydrazone
Formula C₂₀H₂₈N₄O₄, MW 388, CAS# NA, Entry# 135471
(2Z)-4-(2,3,4,6-Tetramethyl-3-cyclohexen-1-yl)-2-butanone, (2,4-dinitrophenyl)hydrazone #



3,9á,14,15-Diepoxypregn-16-en-20-one, 3,11á,18-triacetoxy-
Formula C₂₇H₃₄O₉, MW 502, CAS# NA, Entry# 239582
\$:28GBYXRTQLWMZHST-UHFFFAOYSA-N



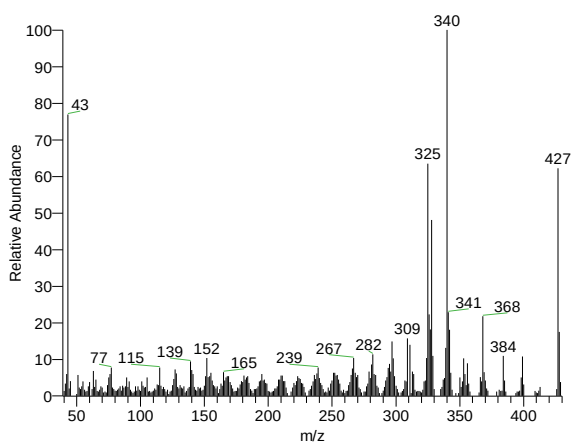
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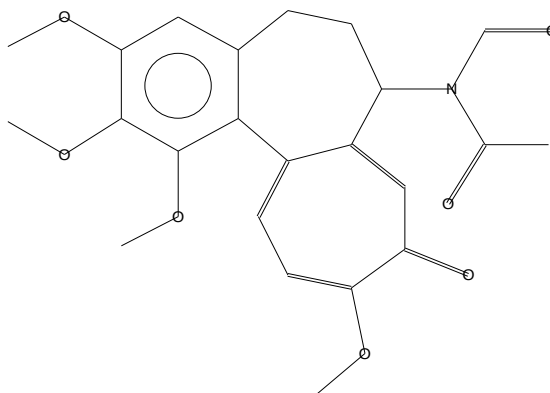
Hit Spectrum

Compound Structure

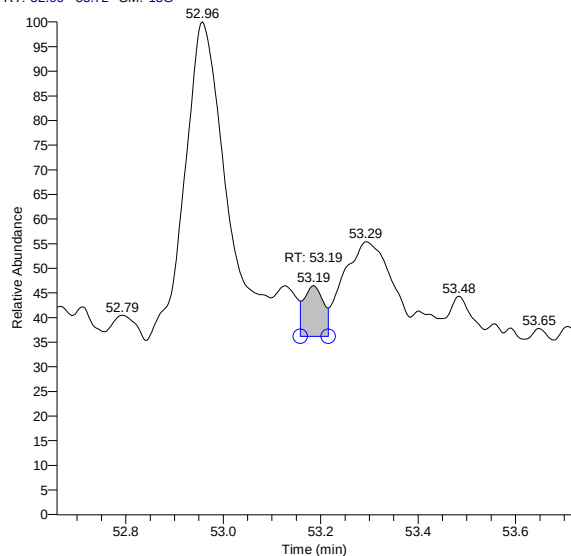
SI 372, RSI 413, mainlib, Entry# 232349, CAS# NA, Formyl colchicine



Formyl colchicine
Formula C₂₃H₂₅NO₇, MW 427, CAS# NA, Entry# 232349
N-Formyl-N-(1,2,3,10-tetramethoxy-9-oxo-5,6,7,9-tetrahydrobenzo[a]heptalen-7-yl)acetamide #

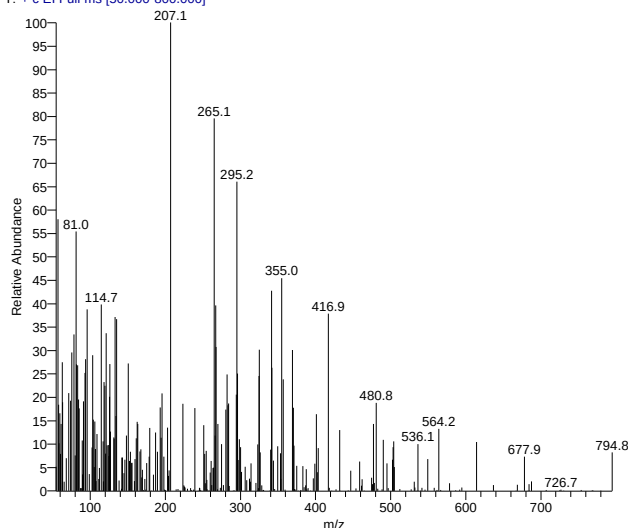


RT: 52.66 - 53.72 SM: 15G



NL:
9.97E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #14071 RT: 53.19 AV: 1 RF: 6.00, 3 NL: 2.22E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
53.19	2-Demethylthiocolchicine formate	284823.50	6.83	393	481	mainlib
53.19	Bufa-20,22-dienolide, 3,14-dihydroxy-, (3à,5á)-	284823.50	4.95	384	476	mainlib
53.19	Pregnan-20-one, 3,11,21-tris[(trimethylsilyl)oxy]-, O-(phenylmethyl)oxime, (3à,5á,11á)-	284823.50	4.18	380	455	mainlib
53.19	Acetic acid, 3-acetoxy-6-(2-cyanovinyl)-3a,6-dimethyl-2,3,4a,4,5,5a,6,9,9a,9b-decahydro-1H-cyclopenta[a]naphthalen-7-ylmethyl ester	284823.50	3.86	378	496	mainlib
53.19	Ethyl iso-allocholate	284823.50	3.26	374	422	mainlib

Analysed by Satyanarayana

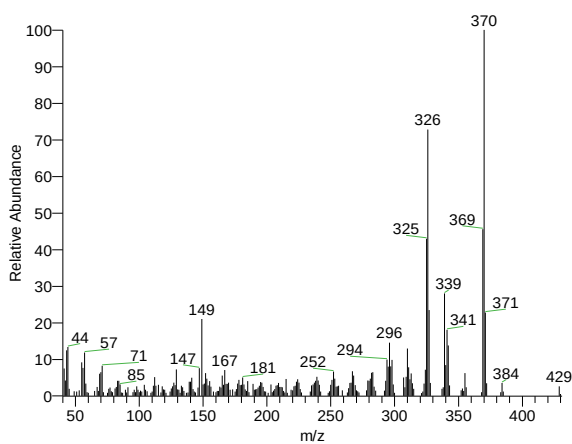
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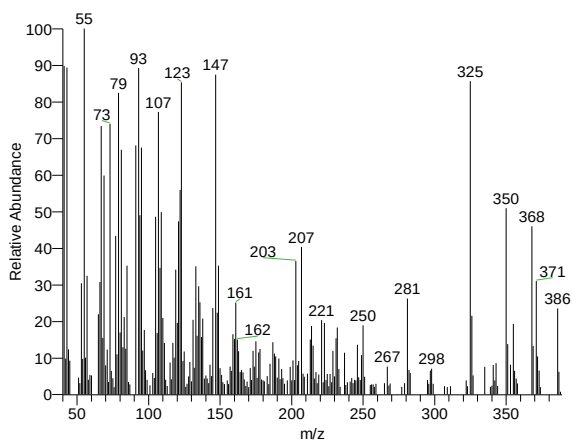
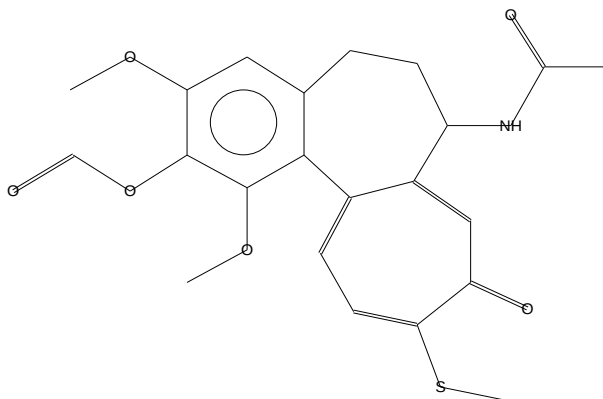
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

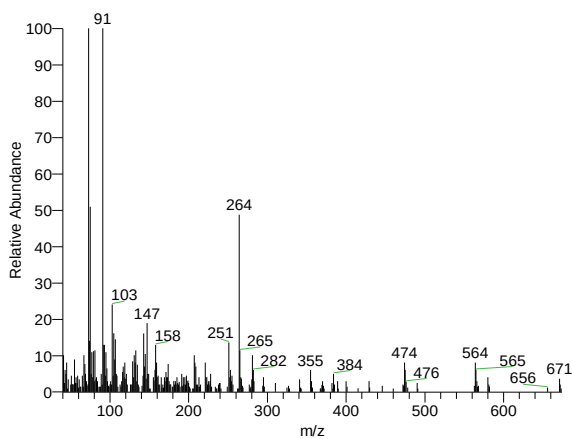
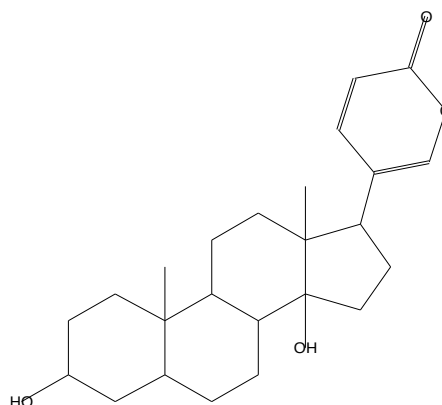
Compound Structure



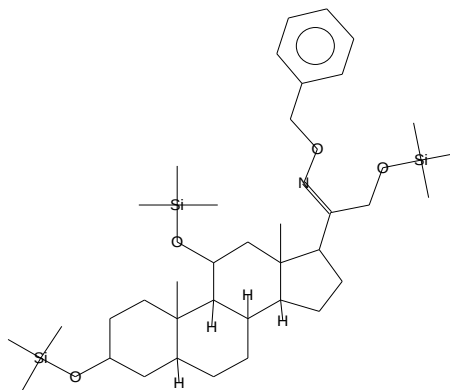
2-Demethylthiocolchicine formate
Formula C₂₂H₂₃NO₆S, MW 429, CAS# NA, Entry# 235943



Bufo-20,22-dienolide, 3,14-dihydroxy-, (3a,5a)-
Formula C₂₄H₃₄O₄, MW 386, CAS# 465-21-4, Entry# 19060
5a-Bufo-20,22-dienolide, 3a,14-dihydroxy-



Pregnan-20-one, 3,11,21-tris(trimethylsilyl)oxy]-, O-(phenylmethyl)oxime, (3a,5a,11a)-
Formula C₃₇H₆₅NO₄Si₃, MW 671, CAS# 57326-18-8, Entry# 41727
3,11,21-Tris(trimethylsilyl)oxy]pregnan-20-one o-benzoyloxime #

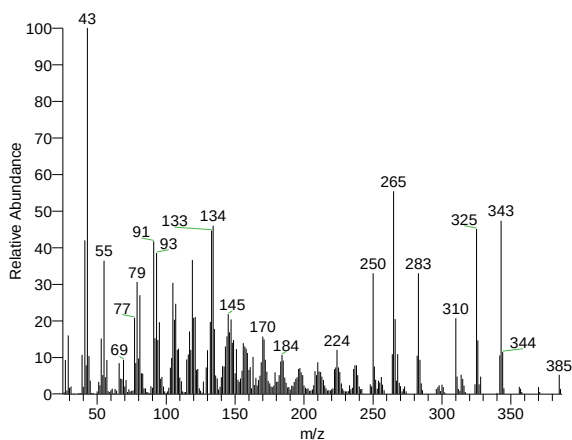


Analysed by Satyanarayana

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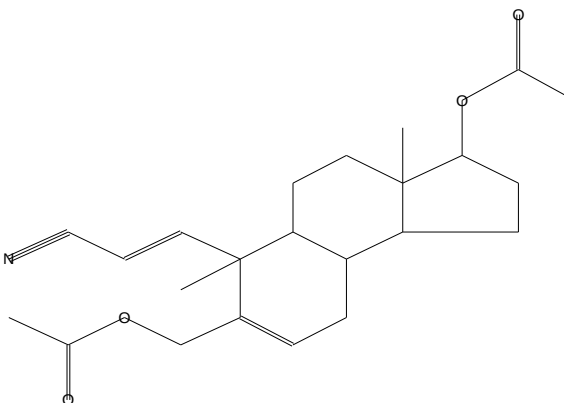
Hit Spectrum

Compound Structure

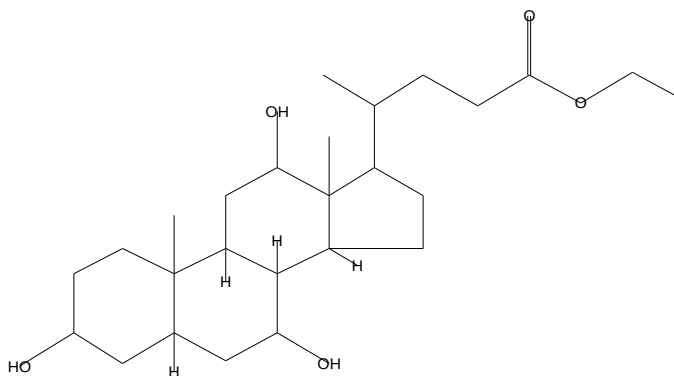
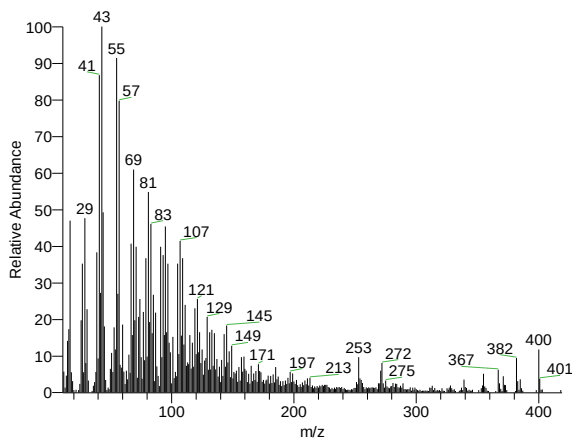


SI 374, RSI 422, mainlib, Entry# 7020, CAS# NA, Ethyl iso-allochololate

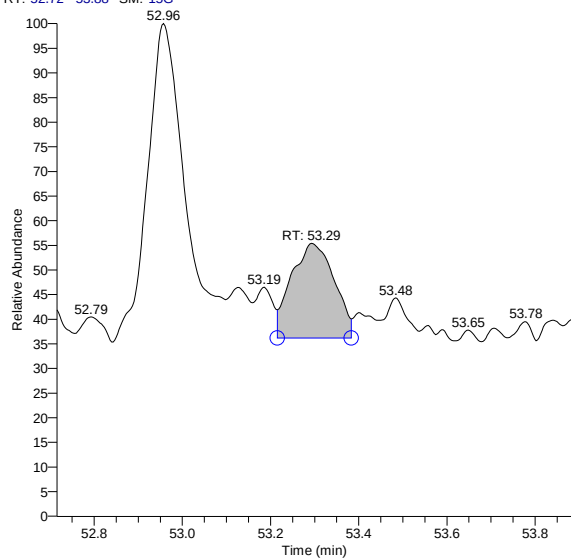
Formula C23H31NO4, MW 385, CAS# NA, Entry# 14223



Ethyl iso-allochololate
Formula C26H44O5, MW 436, CAS# NA, Entry# 7020
Ethyl 3,7,12-trihydroxycholan-24-oate #

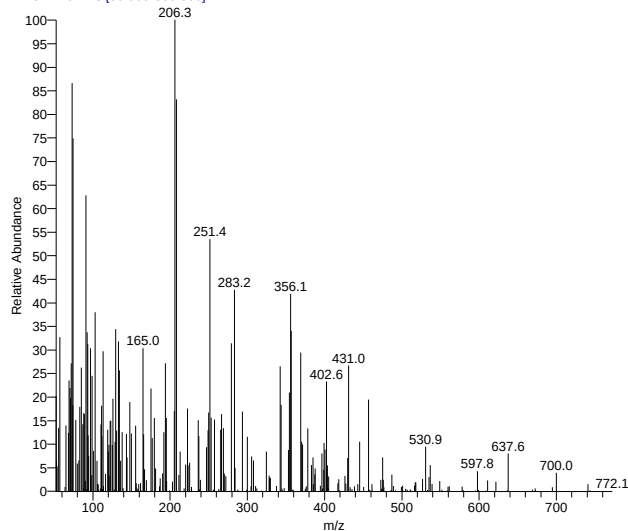


RT: 52.72 - 53.88 SM: 15G



NL:
9.97E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #14103 RT: 53.29 AV: 1 RF: 6.00, 3 NL: 1.99E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
53.29	Corticosterone, bis(O-ethyloxime)	1294565.22	6.19	347	379	mainlib

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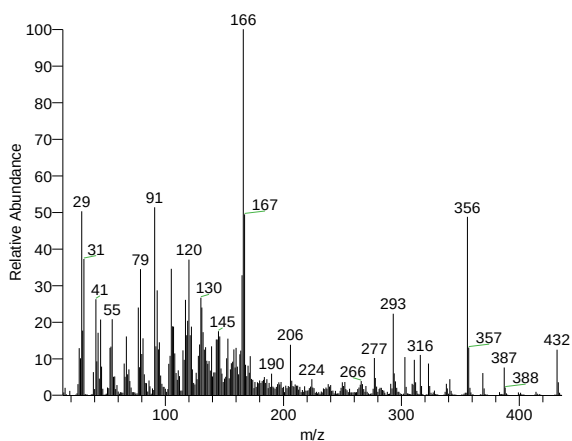
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ANALYTICAL CHEMISTRY DIVISION

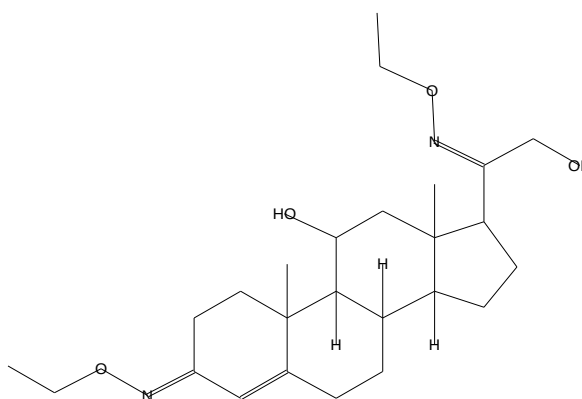
RT	Compound Name	Area	Probability	SI	RSI	Library
53.29	3-(4-Chlorophenyl)-1-[4-(3-fluorophenyl)-4-oxobutyl]piperidin-3-yl decanoate	1294565.22	4.25	336	440	mainlib
53.29	Glycodeoxycholic acid	1294565.22	3.34	330	355	mainlib
53.29	.psi.,.psi.-Carotene, 3,3',4,4'-tetrahydro-1,1',2,2'-tetrahydro-1,1'-dimethoxy-2,2'-dioxo-	1294565.22	3.34	330	352	mainlib
53.29	2-Phosphonobutanoic acid, tris(trimethylsilyl); ester	1294565.22	3.34	330	419	mainlib

Hit Spectrum

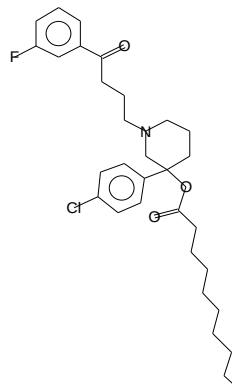
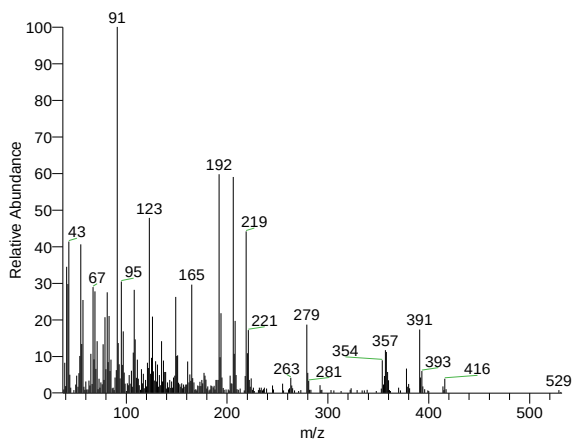
Compound Structure



Corticosterone, bis(O-ethylxime)
Formula C₂₅H₄₀N₂O₄, MW 432, CAS# NA, Entry# 155101
\$:28FDDJMLCQVAFATE-WZGXAYAEVSA-N



3-(4-Chlorophenyl)-1-[4-(3-fluorophenyl)-4-oxobutyl]piperidin-3-yl decanoate
Formula C₃₁H₄₁ClFNO₃, MW 529, CAS# NA, Entry# 63375
\$:28ZAGSBITYFUOAHT-UHFFFAOYSA-N



Analysed by Satyanarayana

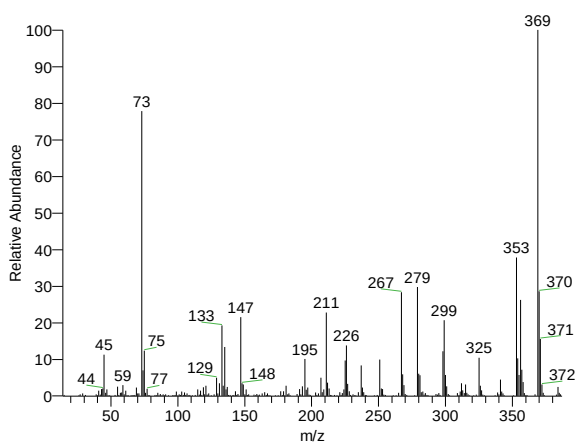
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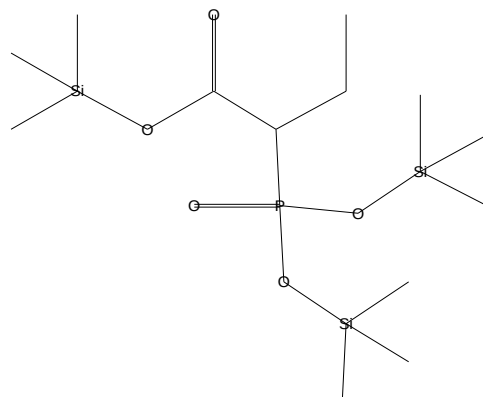
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Hit Spectrum

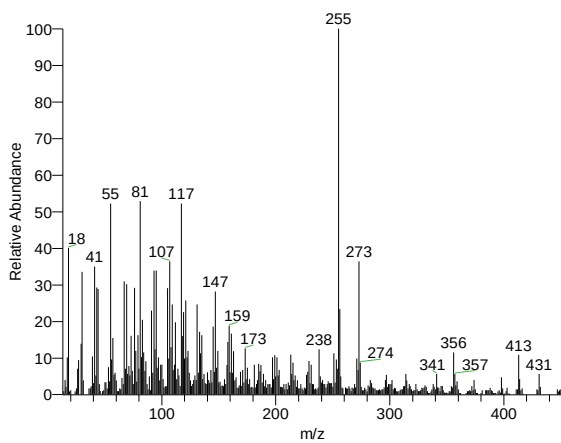
Compound Structure



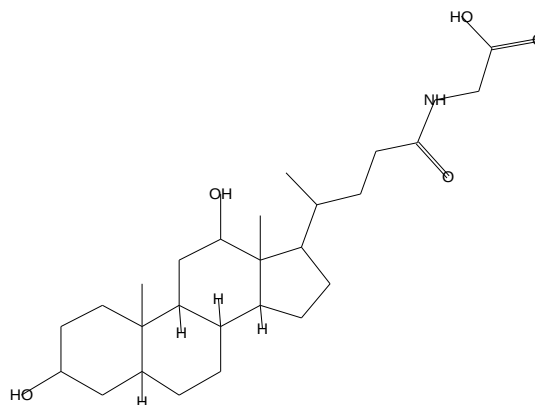
2-Phosphonobutanoic acid, trimethylsilyl; ester
Formula C₁₃H₃₃O₅PSi₃, MW 384, CAS# 959220-68-9, Entry# 235765
Trimethylsilyl 2-(bis[(trimethylsilyl)oxy]phosphoryl)butanoate #



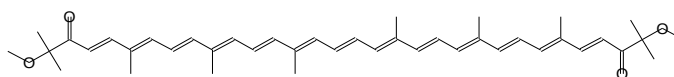
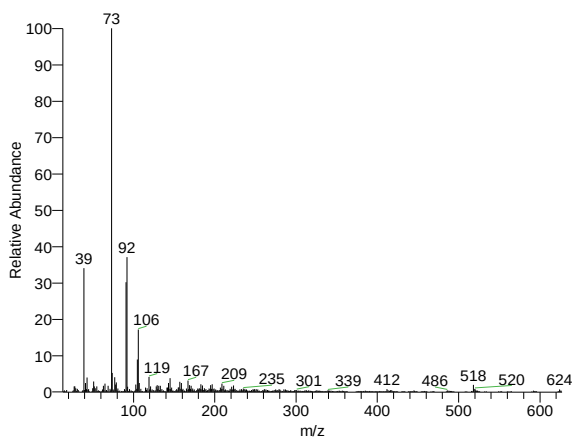
SI 330, RSI 355, mainlib, Entry# 211333, CAS# 360-65-6, Glycodeoxycholic acid



Glycodeoxycholic acid
Formula C₂₆H₄₃NO₅, MW 449, CAS# 360-65-6, Entry# 211333
Glycine, N-[(3α,5α,12α)-3,12-dihydroxy-24-oxocholan-24-yl]-



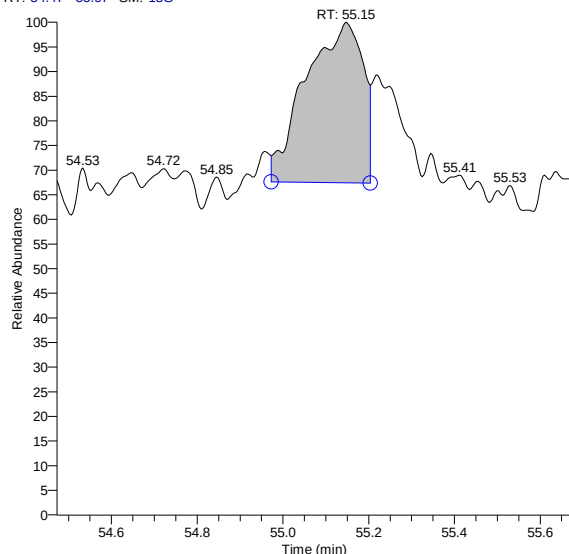
.psi.,.psi.-Carotene, 3,3',4,4'-tetrahydro-1,1',2,2'-tetrahydro-1,1'-dimethoxy-2,2'-dioxo-
Formula C₄₂H₅₆O₄, MW 624, CAS# 1185-31-5, Entry# 41763
Lycopene, 3,3',4,4'-tetrahydro-1,1',2,2'-tetrahydro-1,1'-dimethoxy-2,2'-dioxo-, all-trans-



Analysed by Satyanarayana

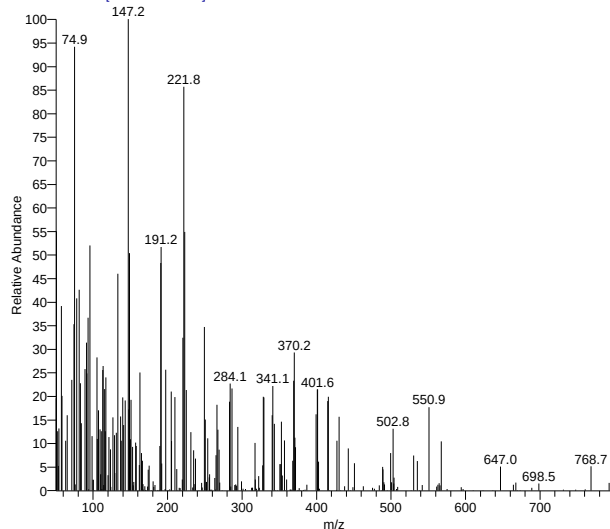
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ANALYTICAL CHEMISTRY DIVISION

RT: 54.47 - 55.67 SM: 15G



NL:
5.30E5
TIC MS
Genesis
NGA-ZE-
WATER2-
SAMPLE-
INJ1

NGA-ZE-WATER2-SAMPLE-INJ1 #14656 RT: 55.15 AV: 1 RF: 6.00, 3 NL: 1.90E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
55.15	Acetamide, N-[5-(diethylamino)-2-[(2, 4-dinitrophenyl)azo]-4-me thoxyphenyl]-	1597438.26	7.55	369	397	mainlib
55.15	5à-Cholan-24-oic acid, 3,7-dioxo-, methyl ester	1597438.26	6.67	366	441	mainlib
55.15	5,5'-Dimethoxy-3,3',7,7'-tet ramethyl-2,2'-binaphthale ne-1,1',4,4'-tetrone	1597438.26	4.04	351	443	mainlib
55.15	17-(1,5-Dimethylhexyl)-2, 3-dihydroxy-10,13-dimeth yl-1,2,3,7,8,9,10,11,12,13, 14,15,16,17-tetradecahydr ocyclopenta[a]phenanthren -6-one	1597438.26	3.88	350	389	mainlib
55.15	2,4a-Oxymethano-1,2,3,4,4 a,4b,5,6,7,8,8a,9-dodec ah ydrophenanthren-9-one, 8-cyanomethyl-2-methoxy- 7-methoxycarbonyl-1,1,7-t rimethyl-	1597438.26	3.88	350	396	mainlib

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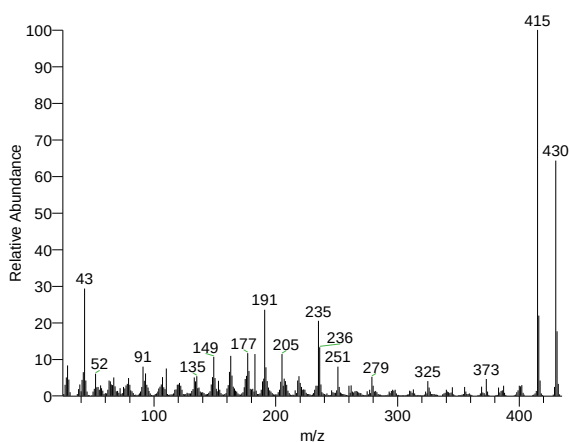
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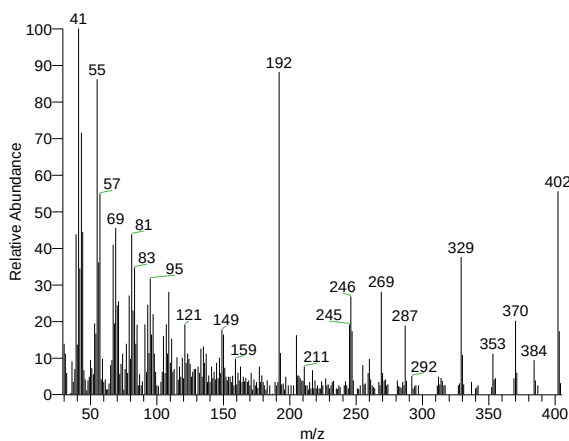
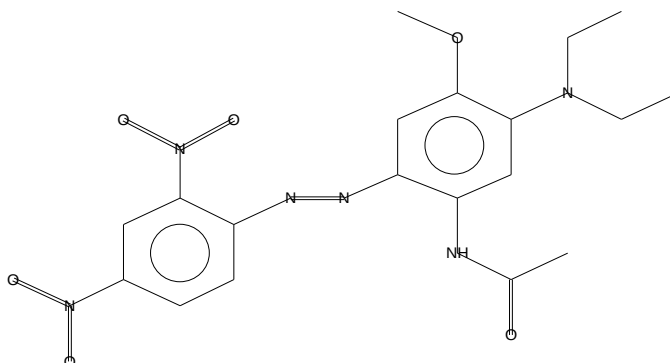
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

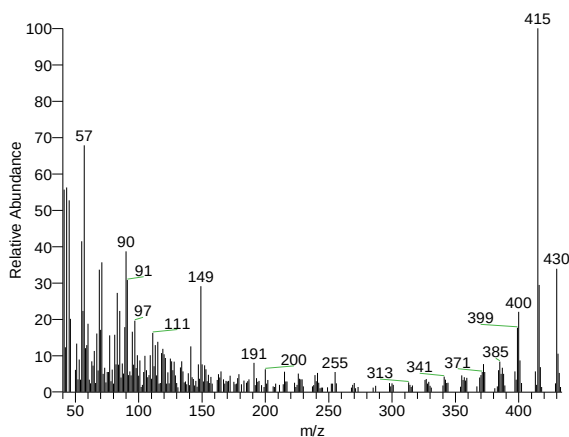
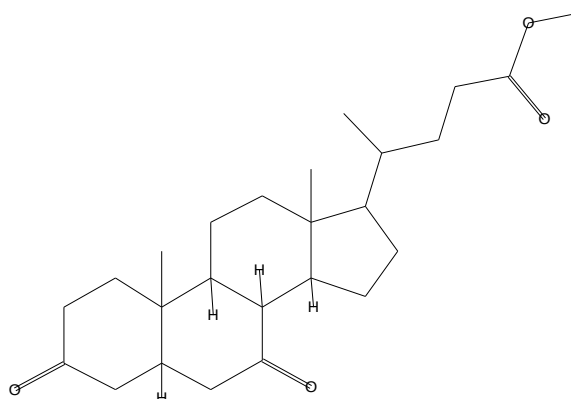
Compound Structure



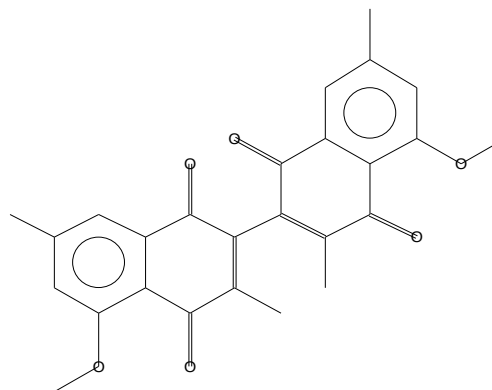
Acetamide, N-[5-(diethylamino)-2-[(2,4-dinitrophenyl)azo]-4-methoxyphenyl]-
Formula C₁₉H₂₂N₆O₆, MW 430, CAS# 80988-29-0, Entry# 239068
N-(5-(Diethylamino)-2-[(E)-(2,4-dinitrophenyl)diazenyl]-4-methoxyphenyl)acetamide #



5α-Cholan-24-oic acid, 3,7-dioxo-, methyl ester
Formula C₂₅H₃₈O₄, MW 402, CAS# 16656-68-1, Entry# 4209
Methyl-3,7-diketo-5α-cholanoate



5,5'-Dimethoxy-3,3',7,7'-tetramethyl-2,2'-binaphthalene-1,1',4,4'-tetrone
Formula C₂₆H₂₂O₆, MW 430, CAS# 85485-13-8, Entry# 239043
\$:28ATPIQUNDZDKBDS-UHFFFAOYSA-N

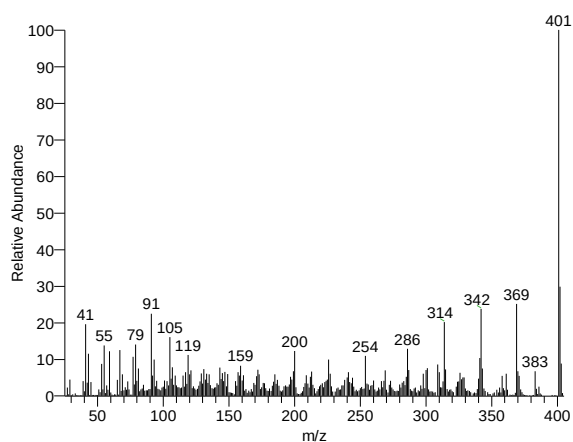


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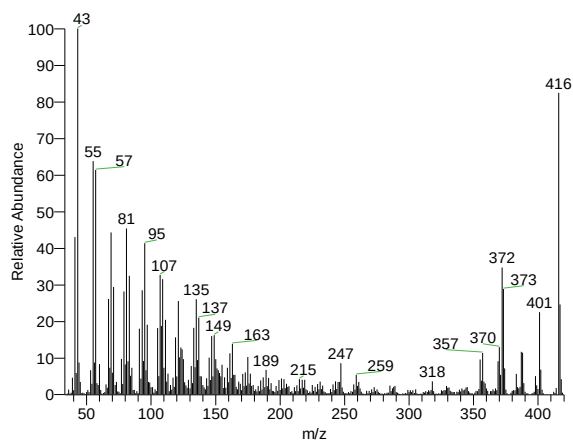
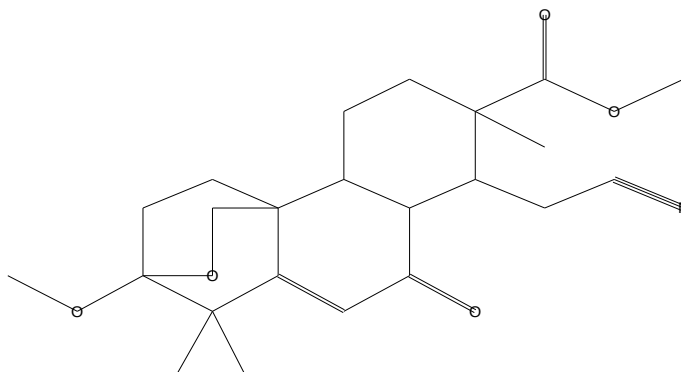
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Hit Spectrum

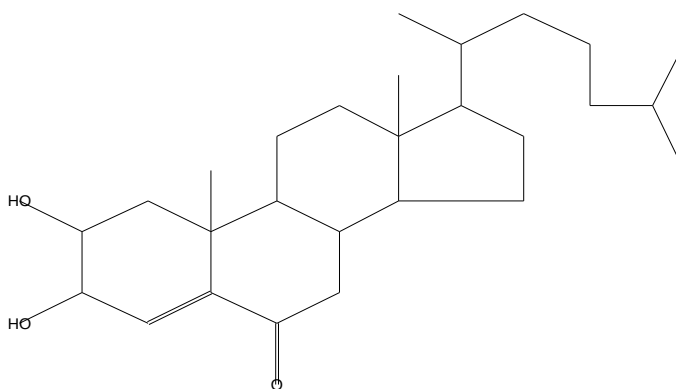
Compound Structure



Formula C₂₃H₃₁NO₅, MW 401, CAS# NA, Entry# 238339
\$:28SSQKXQDLZRHEKL-UHFFFAOYSA-N



Formula C₂₇H₄₄O₃, MW 416, CAS# NA, Entry# 14996
2,3-Dihydroxycholest-4-en-6-one #



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ANALYTICAL CHEMISTRY DIVISION

Data File:

Chumathang Groundwater

Original Data Path:

E:\Xcalibur\Data\2024\FEBRUARY-2024

Sample Name:

GCMS-FS

Acquisition Date:

02/29/24 11:57:31 PM

Run Time(min):

49.67

Vial:

10

Injection Volume(µl):

1.00

Low Mass(m/z):

50

High Mass(m/z):

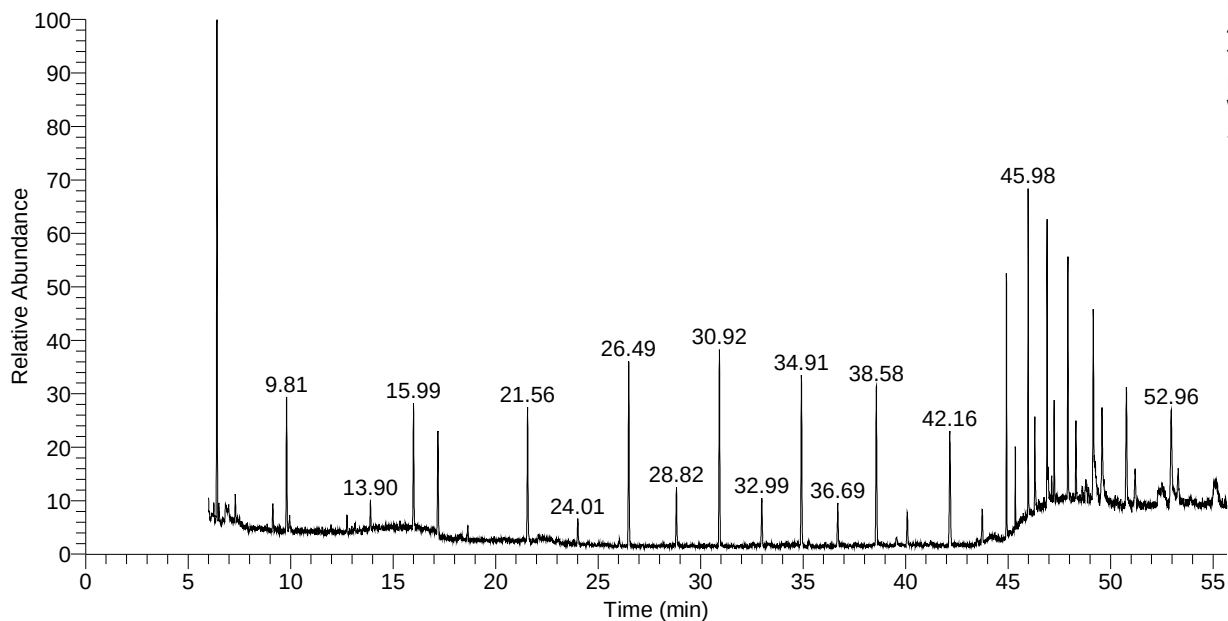
800

Instrument Method:

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Original Processing Method:

RT: 0.00 - 55.67 SM: 7G



NL:
4.18E6
TIC MS
NGA-ZE-
WATER1-
SAMPLE-
INJ1

Qual Peak Table

RT	Peak Area	Peak Height	S/N	Area %
6.41	8097919.72	3288473.74	48.00	8.90
7.30	555916.01	197705.13	3.13	0.61
9.14	473953.90	181077.78	6.15	0.52
9.81	2586571.69	931566.39	31.03	2.84
9.95	355472.67	102364.44	3.27	0.39
12.75	255824.69	101190.97	2.40	0.28
13.90	554642.94	195039.87	5.43	0.61
16.00	2804800.02	899212.20	10.47	3.08
17.19	2184589.29	729839.15	11.49	2.40
18.65	301893.55	98719.54	4.13	0.33
21.56	2917961.89	927990.34	24.18	3.21
24.01	547683.56	180230.88	5.07	0.60
26.04	146411.70	44682.53	2.11	0.16
26.49	4097079.02	1315126.83	60.12	4.50
28.82	1335996.65	411881.66	21.49	1.47
30.92	4361413.12	1384094.74	71.37	4.79
32.99	1157583.09	340962.56	10.21	1.27
34.92	4003161.48	1235497.74	36.03	4.40
36.69	1004098.94	296614.95	12.32	1.10
38.57	3870136.40	1140307.25	56.63	4.25

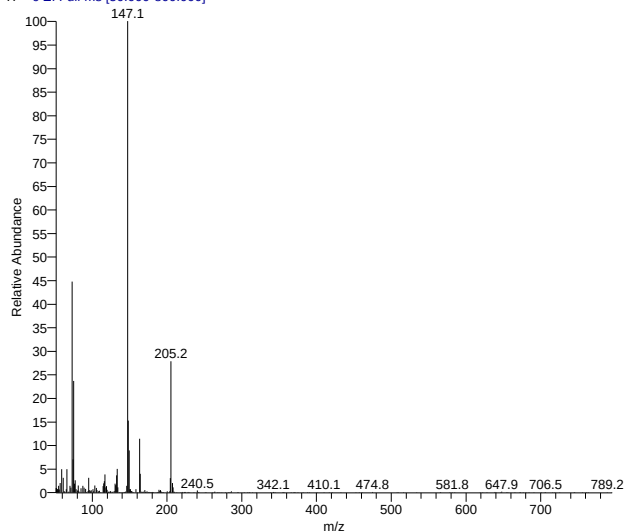
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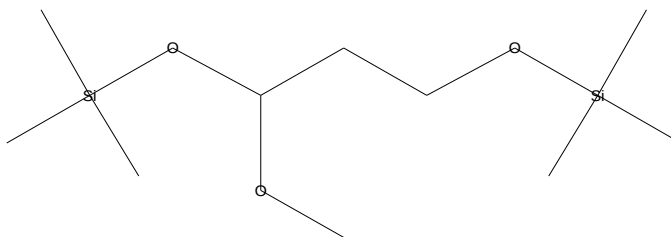
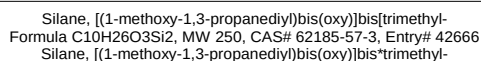
RT	Peak Area	Peak Height	S/N	Area %
39.56	301292.45	58155.03	2.57	0.33
40.08	871749.55	242137.23	9.77	0.96
42.16	3379575.26	831714.23	38.78	3.71
43.74	751977.63	235910.19	3.62	0.83
44.92	3061238.52	1541053.81	11.97	3.36
45.35	777460.27	442037.68	3.43	0.85
45.98	3742547.54	1869488.54	16.57	4.11
46.31	1838058.61	599410.78	5.24	2.02
46.90	4525139.34	1745228.27	11.81	4.97
47.25	1520082.97	646999.63	4.94	1.67
47.92	3825974.67	1569974.17	12.94	4.21
48.31	1301092.46	509850.95	4.08	1.43
48.80	529378.67	138019.25	2.09	0.58
49.16	6257999.77	1349386.58	22.38	6.88
49.58	3426430.09	668073.06	11.18	3.77
50.77	3201182.88	847580.15	15.16	3.52
51.20	1017803.23	250825.26	4.85	1.12
52.51	876479.40	155020.78	2.86	0.96
52.96	4282862.87	701064.12	14.40	4.71
53.30	1524693.34	255537.01	5.19	1.68
55.14	2357776.36	179477.20	2.86	2.59

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Compound Structure



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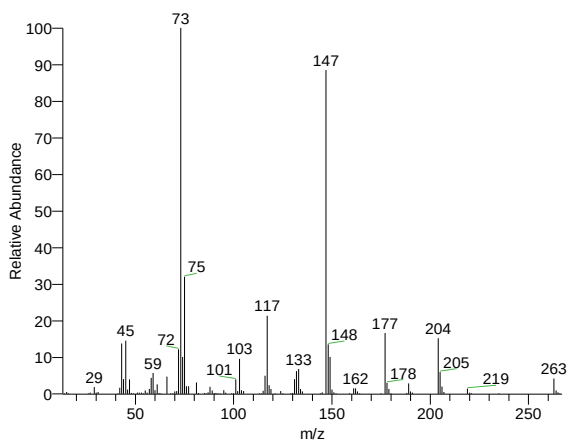
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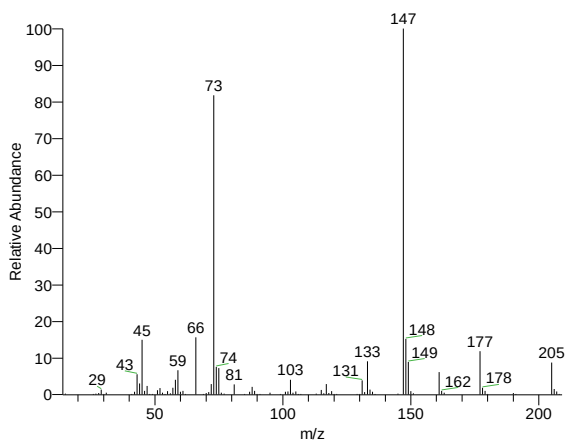
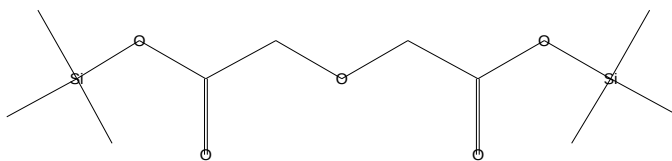
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Hit Spectrum

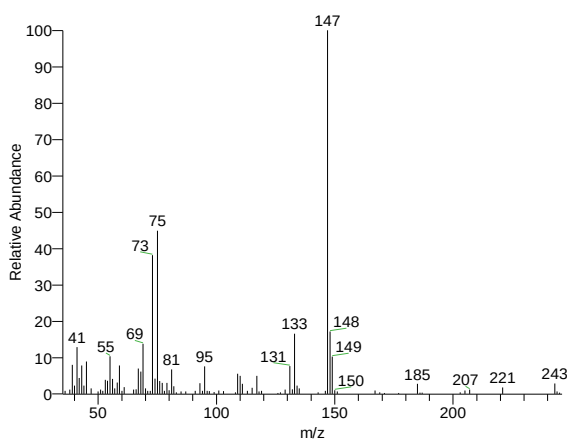
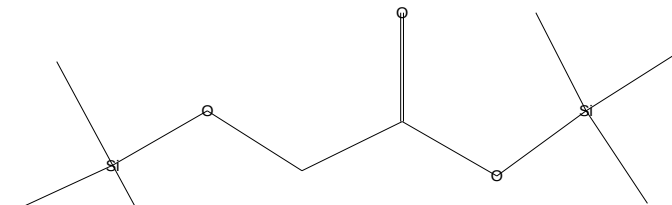
Compound Structure



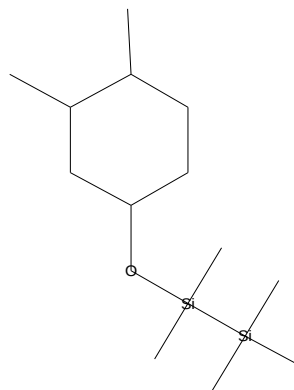
Diglycolic acid, 2TMS derivative
Formula C₁₀H₂₂O₅Si₂, MW 278, CAS# 55557-25-0, Entry# 42542
Acetic acid, 2,2'-oxybis-, bis(trimethylsilyl) ester



Glycolic acid, 2TMS derivative
Formula C₈H₂₀O₃Si₂, MW 220, CAS# 33581-77-0, Entry# 134871
Acetic acid, [(trimethylsilyl)oxy]-, trimethylsilyl ester



3,4-Dimethyl-1-pentamethyldisilyloxycyclohexane
Formula C₁₃H₃₀O₂Si₂, MW 258, CAS# NA, Entry# 135026
1-[(3,4-Dimethylcyclohexyl)oxy]-1,1,2,2,2-pentamethyldisilane #

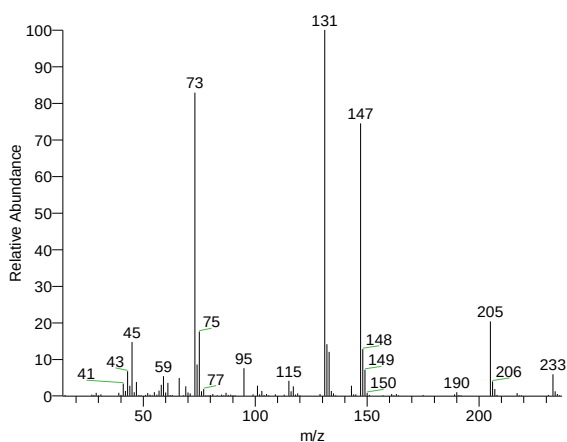


Analysed by Satyanarayana

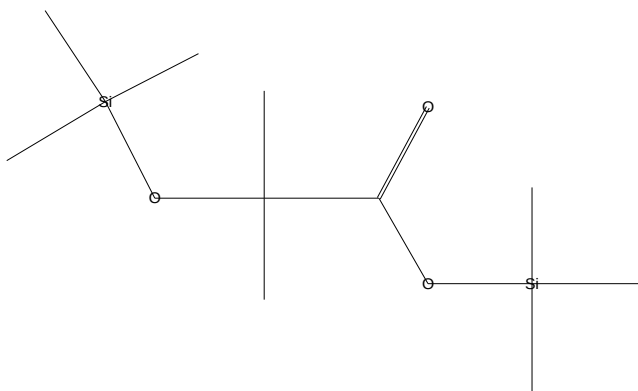
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Hit Spectrum

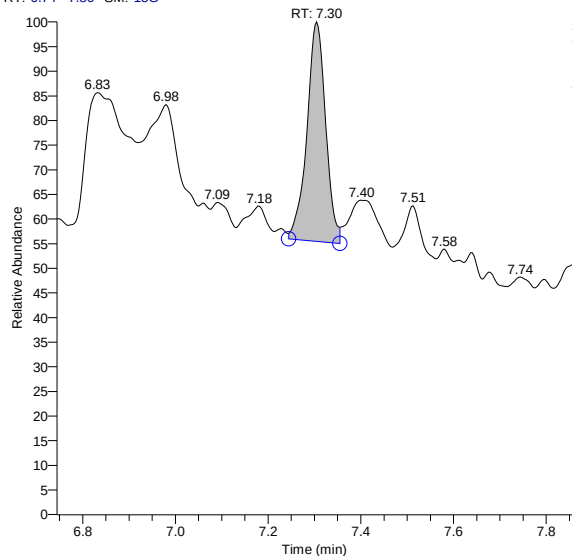
Compound Structure



à-Hydroxyisobutyric acid, 2TMS derivative
Formula C₁₀H₂₄O₃Si₂, MW 248, CAS# 55133-92-1, Entry# 115549
Propanoic acid, 2-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester

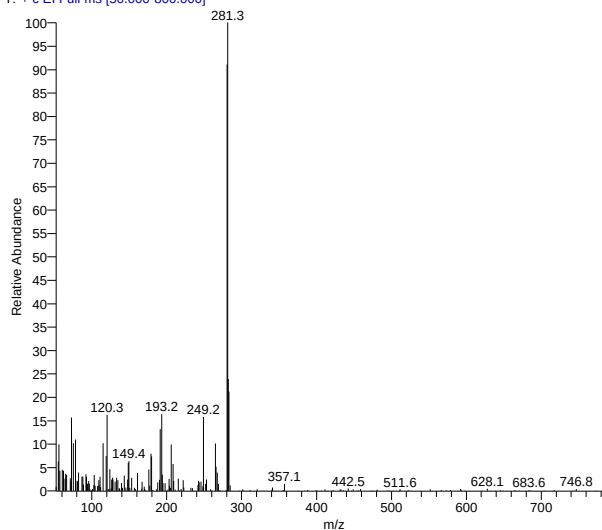


RT: 6.74 - 7.86 SM: 15G



NL:
4.44E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #390 RT: 7.30 AV: 1 RF: 6.00, 3 NL: 9.36E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
7.30	Cyclotetrasiloxane, octamethyl-	555916.01	24.76	672	770	mainlib
7.30	2,6-Dihydroxyacetophenone, 2TMS derivative	555916.01	19.46	666	696	mainlib
7.30	trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-	555916.01	15.29	660	840	mainlib
7.30	2,5-Dihydroxyacetophenone, 2TMS derivative	555916.01	12.02	654	680	mainlib
7.30	1-[2,4-Bis(trimethylsiloxy)phenyl]-2-[(4-trimethylsiloxy)phenyl]propan-1-one	555916.01	8.48	644	699	mainlib

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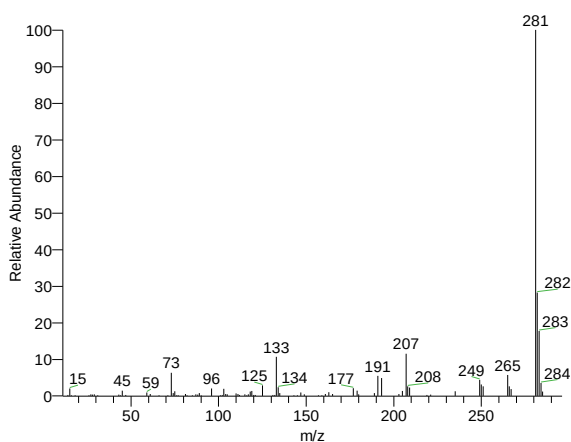
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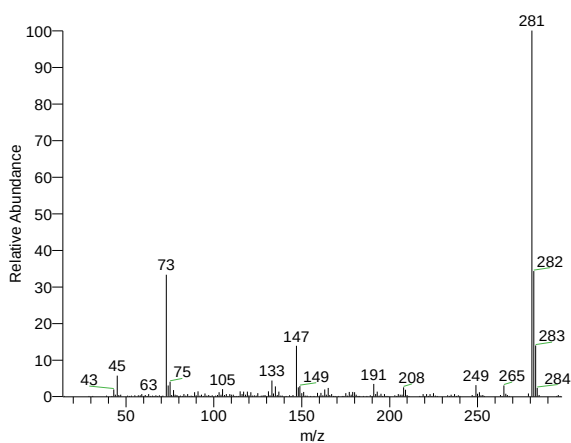
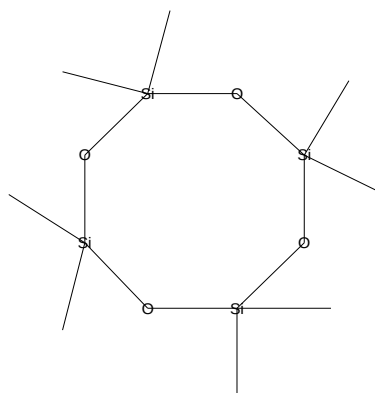
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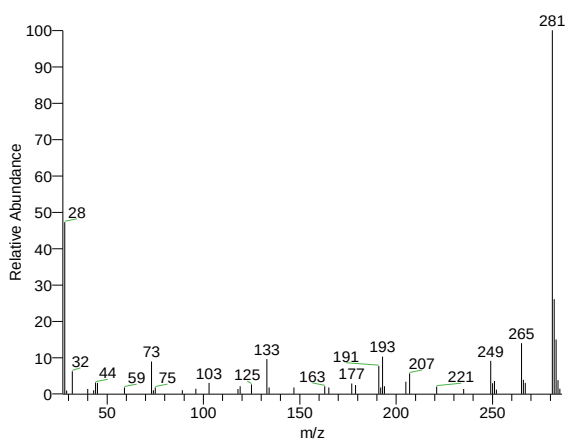
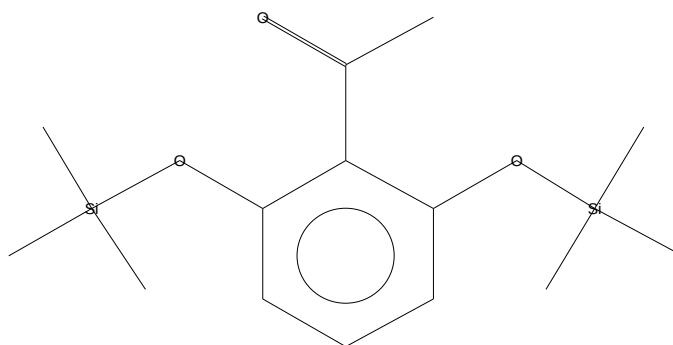
Compound Structure



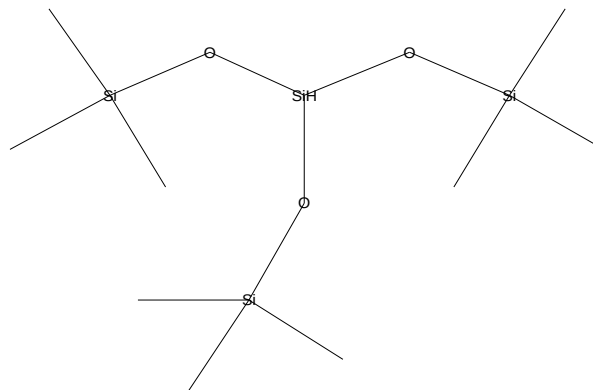
Cyclotetrasiloxane, octamethyl-
Formula C₈H₂₄O₄Si₄, MW 296, CAS# 556-67-2, Entry# 220100
Oktamethylcyklotetrasiloxan



2,6-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220073
2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-
Formula C₉H₂₈O₃Si₄, MW 296, CAS# NA, Entry# 219896
1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]trisiloxane

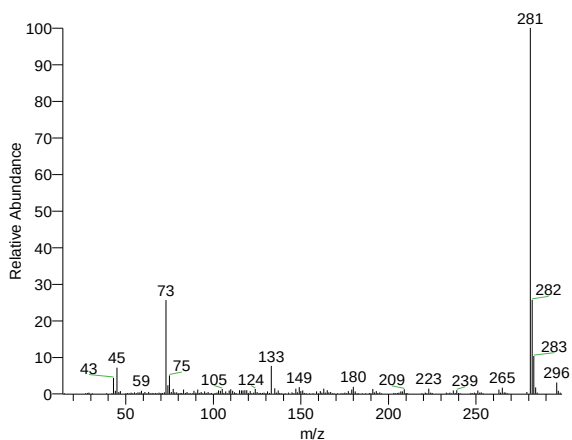


Analysed by Satyanarayana

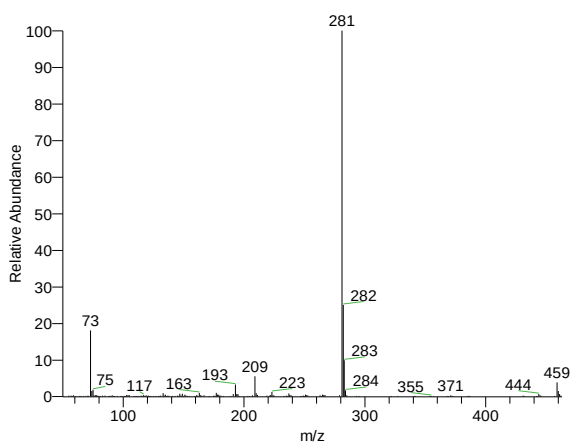
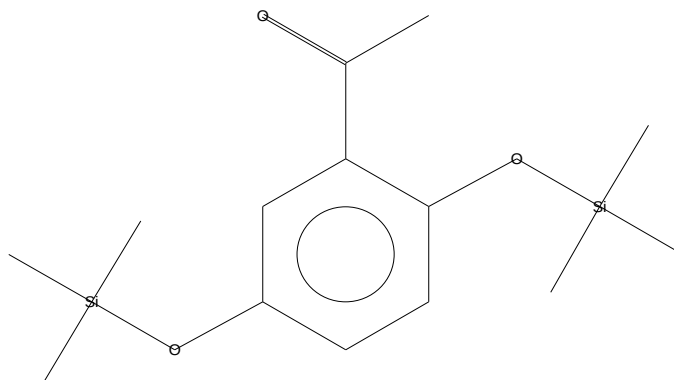
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Hit Spectrum

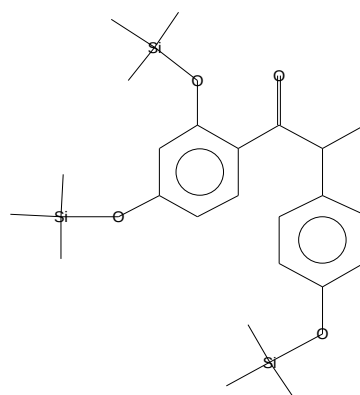
Compound Structure



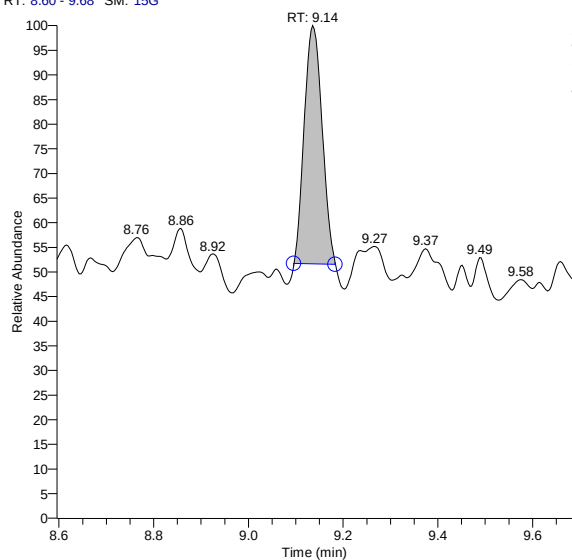
2,5-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220075
2,5-Dihydroxyacetophenone, bis(trimethylsilyl) ether



1-[2,4-Bis(trimethylsiloxy)phenyl]-2-[(4-trimethylsiloxy)phenyl]propan-1-one
Formula C₂₄H₃₈O₄Si₃, MW 474, CAS# 102907-88-0, Entry# 220076
1-[2,4-Bis(trimethylsilyloxy)phenyl]-2-[(4-trimethylsilyloxy)phenyl]propan-1-one

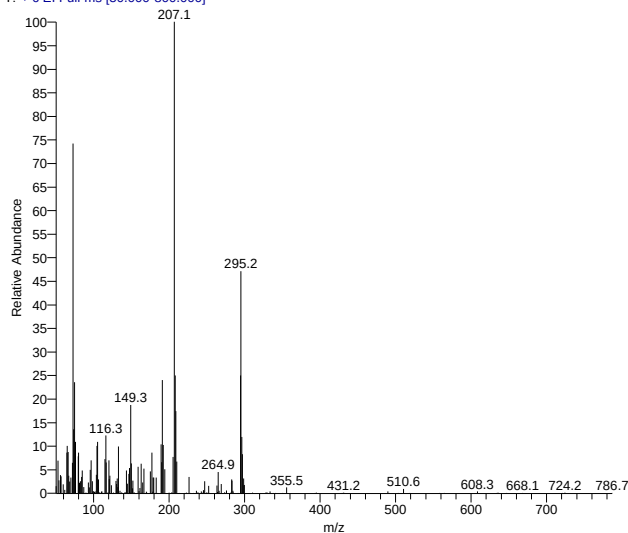


RT: 8.60 - 9.68 SM: 15G



NL:
3.75E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #936 RT: 9.14 AV: 1 RF: 6.00, 3 NL: 6.23E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.14	Methyltris(trimethylsiloxy)silane	473953.90	51.03	654	702	mainlib
9.14	Tetrasiloxane, decamethyl-	473953.90	38.07	646	685	mainlib

Analysed by Satyanarayana

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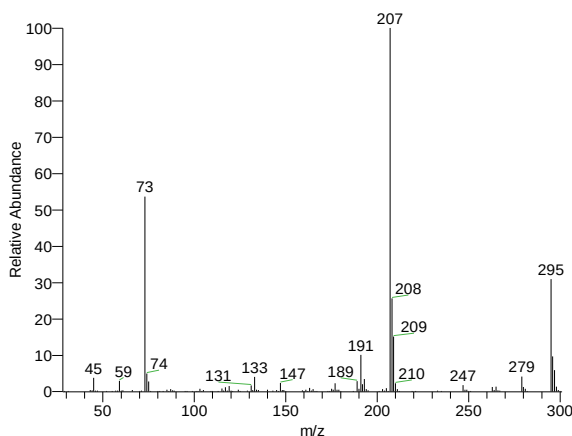
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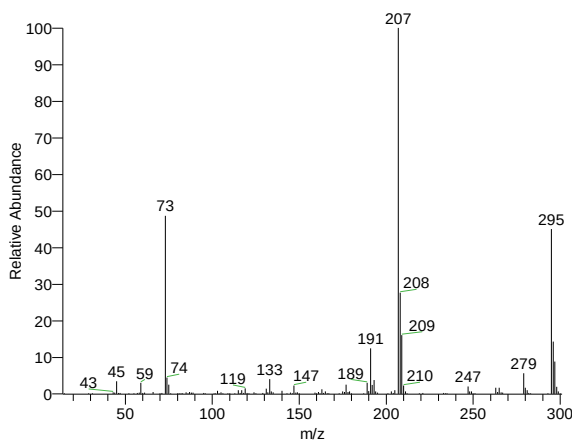
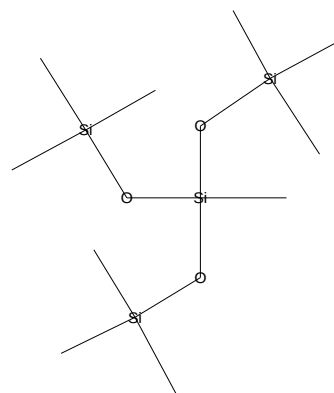
RT	Compound Name	Area	Probability	SI	RSI	Library
9.14	Thymol, TBDMS derivative	473953.90	1.38	509	667	mainlib
9.14	2-tert-Octylhydroquinone, 2TMS derivative	473953.90	1.03	501	519	mainlib
9.14	7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane	473953.90	0.99	500	527	mainlib

Hit Spectrum

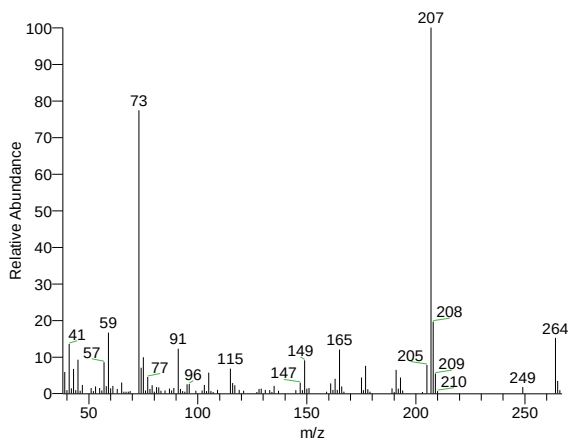
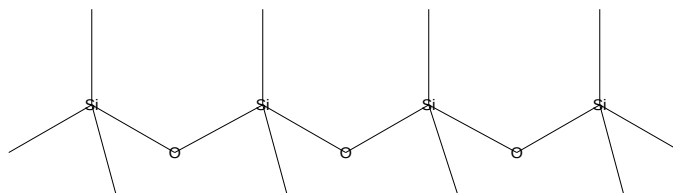
Compound Structure



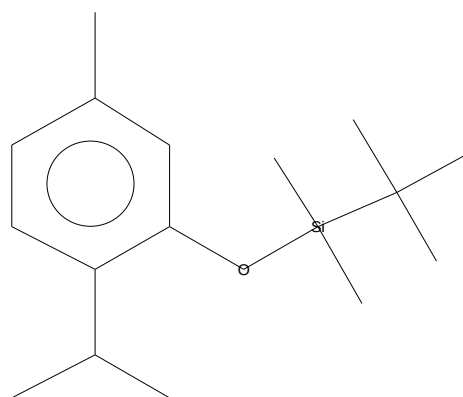
Methyltris(trimethylsiloxy)silane
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



Tetrasiloxane, decamethyl-
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 141-62-8, Entry# 188653
Decamethyltetrasiloxane



Thymol, TBDMS derivative
Formula C₁₆H₂₈O₂Si, MW 264, CAS# 330455-64-6, Entry# 188649
Benzene, 2-[(tert-butyl)dimethylsilyl]oxy]-1-isopropyl-4-methyl-

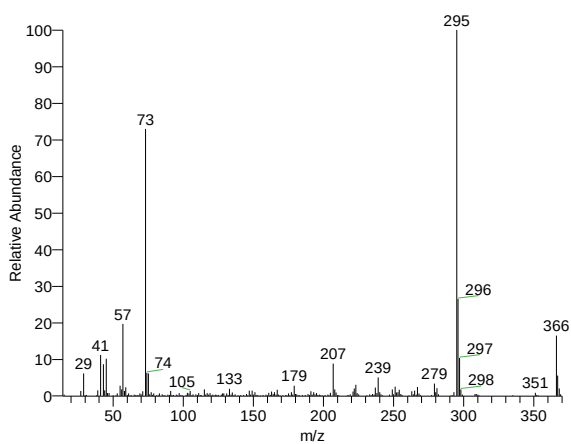


Analysed by Satyanarayana

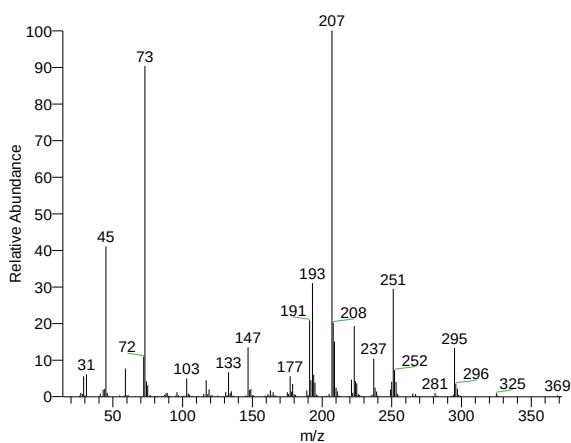
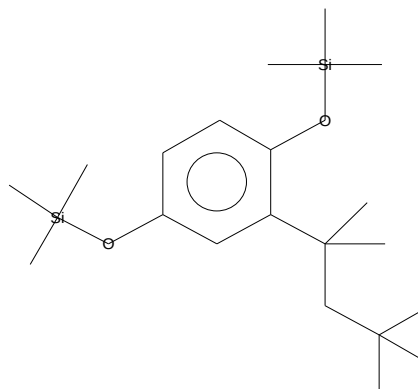
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
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Hit Spectrum

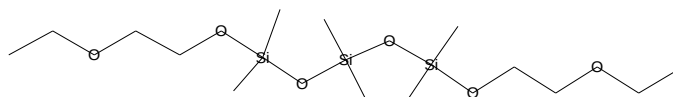
Compound Structure



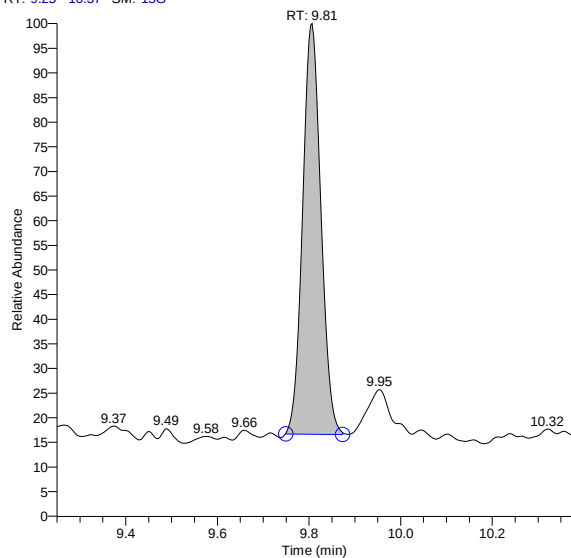
2-tert-Octylhydroquinone, 2TMS derivative
Formula C₂₀H₃₈O₂Si₂, MW 366, CAS# NA, Entry# 223590
2-(1,1,3,3-Tetramethylbutyl)-1,4-benzenediol ditms



7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane
Formula C₁₄H₃₆O₆Si₃, MW 384, CAS# NA, Entry# 188641
\$.28TUXFBCQKAFVQCP-UHFFFAOYSA-N

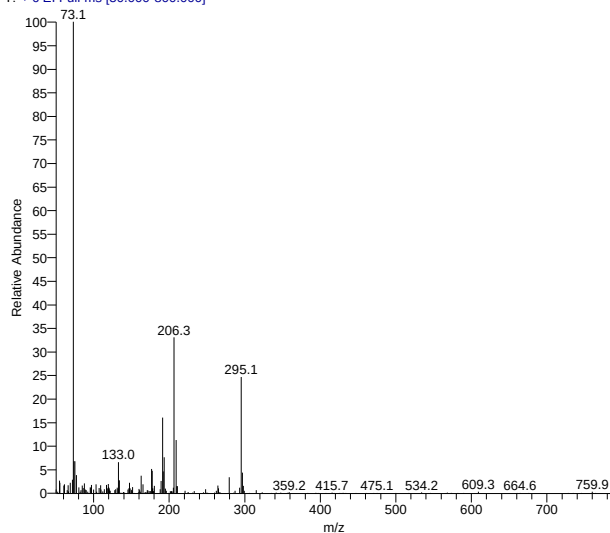


RT: 9.25 - 10.37 SM: 15G



NL:
1.12E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #1136 RT: 9.81 AV: 1 RF: 6.00, 3 NL: 2.98E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	3,5-Hexadien-1-yne, 1,3,6-tris(trimethylsilyl)-, (E,E)-	2586571.69	31.53	520	562	mainlib

Analysed by Satyanarayana

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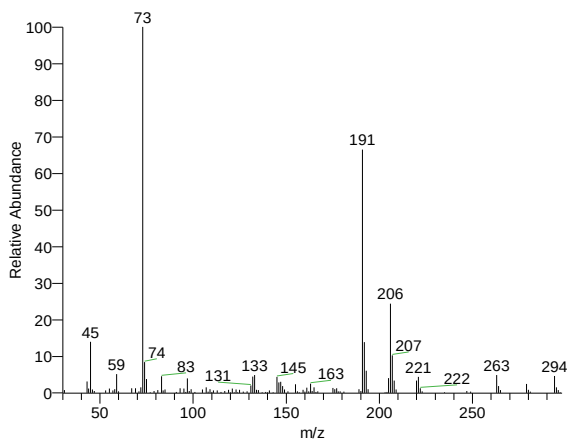
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ANALYTICAL CHEMISTRY DIVISION

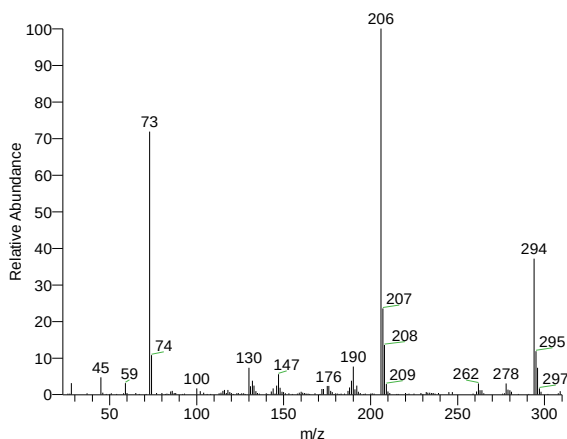
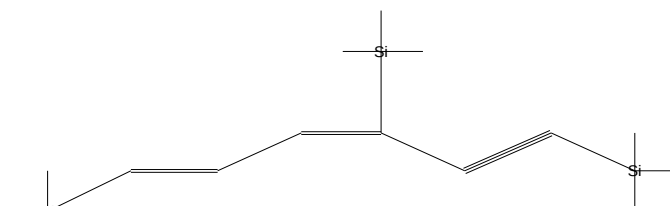
RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	4,6-Dioxa-5-aza-2,3,7,8-tetrasilanonane,	2586571.69	7.91	485	515	mainlib
9.81	2,2,3,3,7,7,8,8-octamethyl-1-Trimethylsilyl-4-(1-methyl-1-silacyclobutyl)benzene	2586571.69	6.22	479	591	mainlib
9.81	Paracetamol, 2TMS derivative	2586571.69	4.26	468	504	mainlib
9.81	Isophthalic acid, 2TMS derivative	2586571.69	3.77	465	480	mainlib

Hit Spectrum

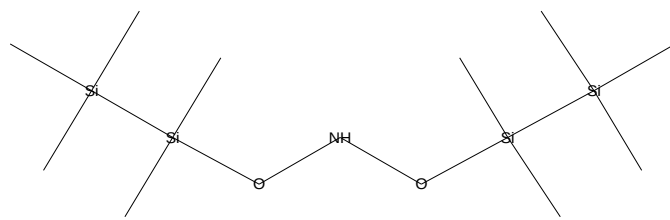
Compound Structure



3,5-Hexadien-1-yne, 1,3,6-tris(trimethylsilyl)-, (E,E)-
Formula C₁₅H₃₀Si₃, MW 294, CAS# NA, Entry# 43125
[(1E,3E)-4,6-Bis(trimethylsilyl)-1,3-hexadien-5-ynyl](trimethyl)silane #



4,6-Dioxa-5-aza-2,3,7,8-tetrasilanonane, 2,2,3,3,7,7,8,8-octamethyl-
Formula C₁₀H₃₁NO₂Si₄, MW 309, CAS# 74793-29-6, Entry# 188072
o-[(1,1,2,2-Pentamethyldisilanyl)-N-[(1,1,2,2,2-pentamethyldisilanyl)oxy]hydroxylamine #



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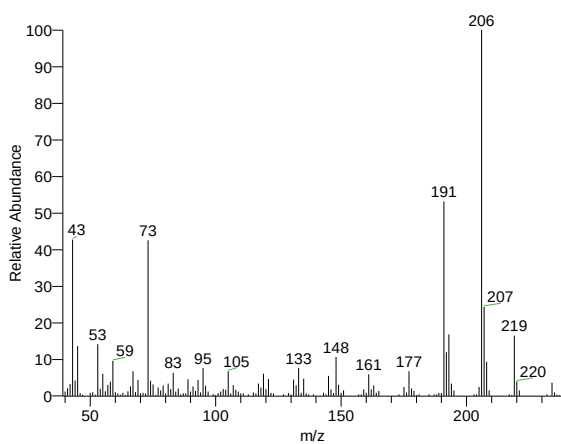
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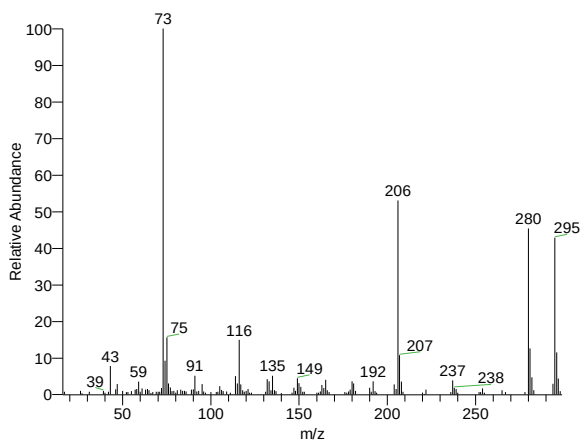
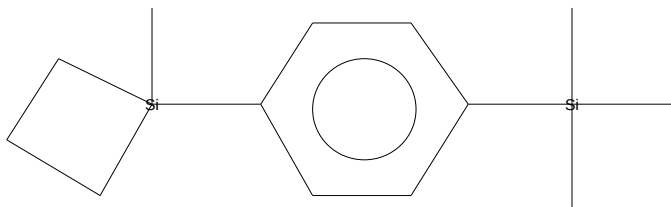
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

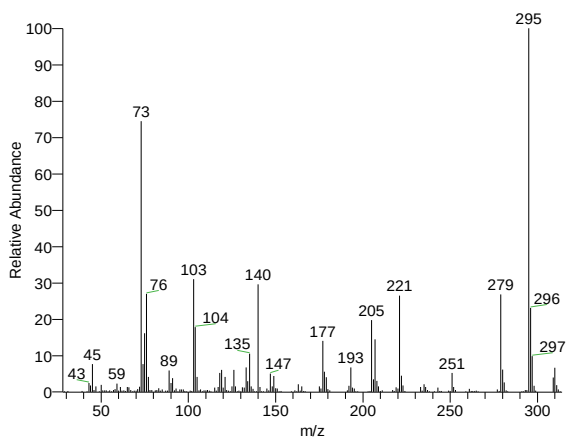
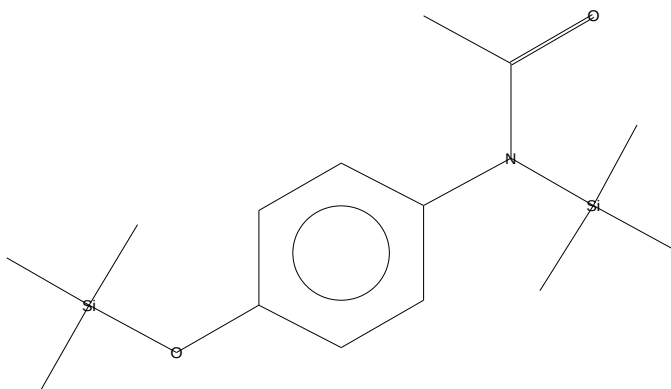
Compound Structure



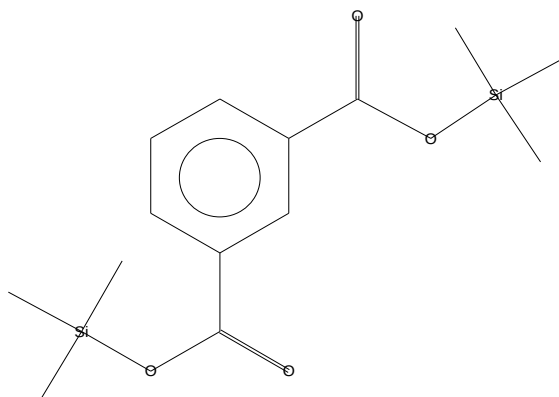
1-Trimethylsilyl-4-(1-methyl-1-silacyclobutyl)benzene
Formula C₁₃H₂₂Si₂, MW 234, CAS# 141682-10-2, Entry# 188323
1-Methyl-1-[4-(trimethylsilyl)phenyl]siletane #



Paracetamol, 2TMS derivative
Formula C₁₄H₂₅NO₂Si₂, MW 295, CAS# 55530-61-5, Entry# 43287
Acetamide, N-(trimethylsilyl)-N-[4-[(trimethylsilyl)oxy]phenyl]-



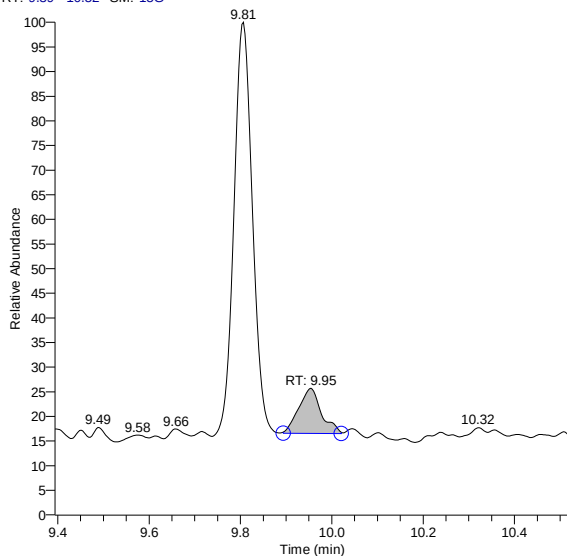
Isophthalic acid, 2TMS derivative
Formula C₁₄H₂₂O₄Si₂, MW 310, CAS# 106450-31-1, Entry# 223588
1,3-Benzenedicarboxylic acid, bis(trimethylsilyl) ester



Analysed by Satyanarayana

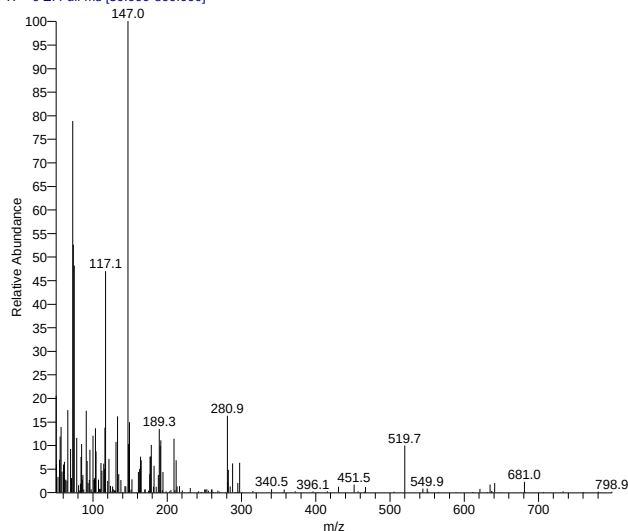
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RT: 9.39 - 10.52 SM: 15G



NL:
1.12E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

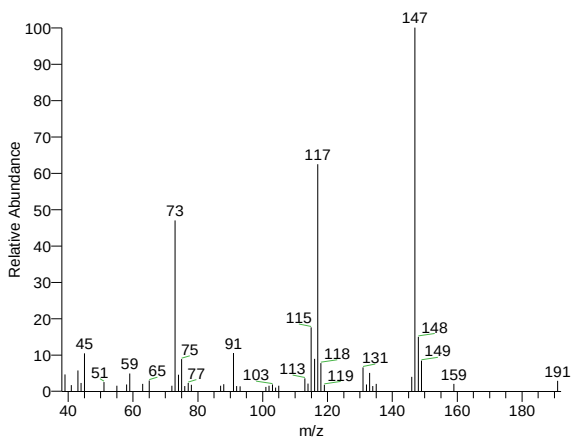
NGA-ZE-WATER1-SAMPLE-INJ1 #1180 RT: 9.95 AV: 1 RF: 6.00, 3 NL: 3.89E4
T: + c EI Full ms [50.000-800.000]



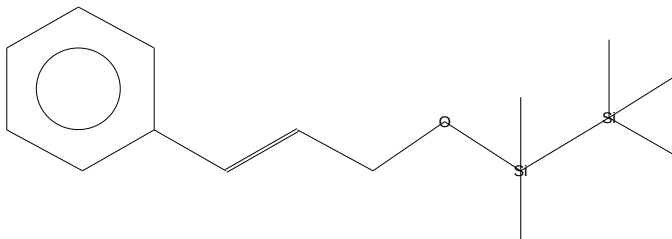
RT	Compound Name	Area	Probability	SI	RSI	Library
9.95	1-Pentamethyldisilyloxy-3-phenylprop-2-ene	355472.67	8.25	457	730	mainlib
9.95	1-Pentamethyldisilyloxybutane	355472.67	5.99	448	692	mainlib
9.95	Propanal, 2,3-bis[(trimethylsilyl)oxy]-, O-methyloxime, (S)-	355472.67	5.99	448	697	mainlib
9.95	2-Pentamethyldisilanyloxybutane	355472.67	5.75	447	699	mainlib
9.95	Dimethyl(trimethylsilyl)ethoxysilane	355472.67	5.53	446	694	mainlib

Hit Spectrum

Compound Structure



1-Pentamethyldisilyloxy-3-phenylprop-2-ene
Formula C₁₄H₂₄OSi₂, MW 264, CAS# NA, Entry# 135197
1,1,2,2,2-Pentamethyldisilanyl (2E)-3-phenyl-2-propenyl ether #



Analysed by Satyanarayana

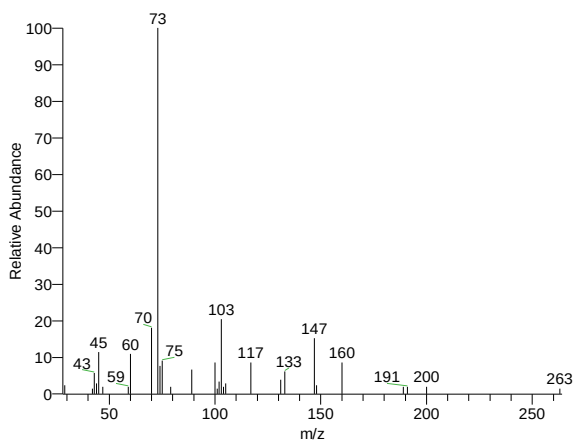
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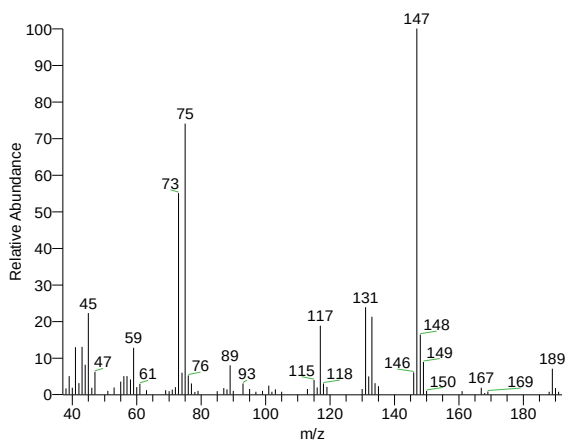
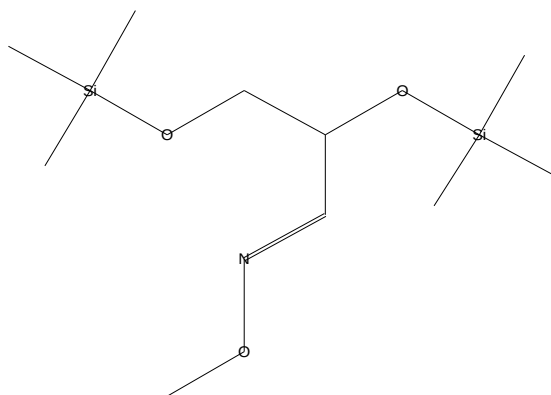
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

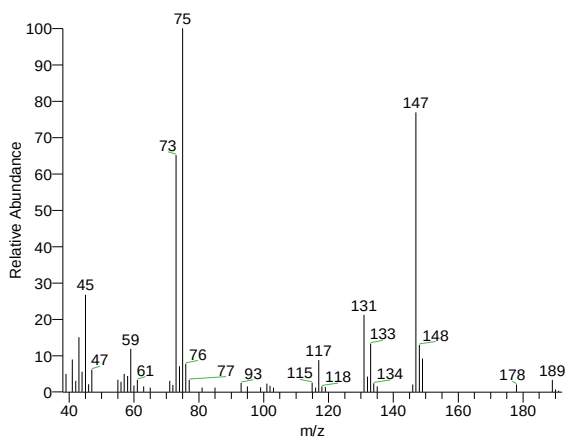
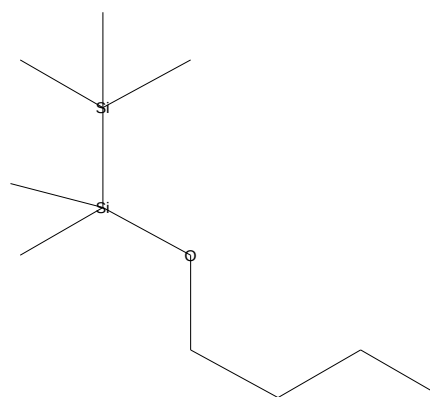
Compound Structure



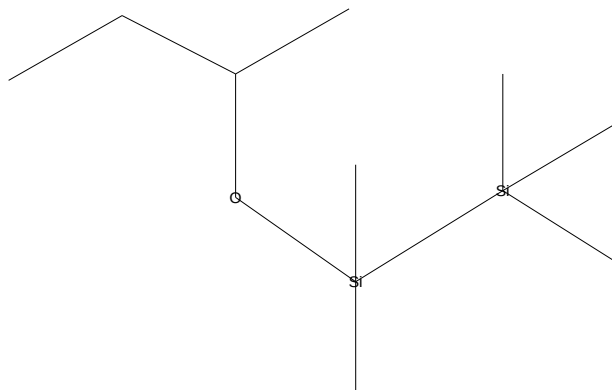
Propanal, 2,3-bis[(trimethylsilyl)oxy]-, O-methyloxime, (S)-
Formula C₁₀H₂₅NO₃Si₂, MW 263, CAS# 56196-02-2, Entry# 41873
(1E)-2,3-Bis[(trimethylsilyl)oxy]propanal o-methyloxime #



1-Pentamethyldisilyloxybutane
Formula C₉H₂₄O₂Si₂, MW 204, CAS# 81500-46-1, Entry# 135031
\$:28FVMARYSDBQQJIZ-UHFFFAOYSA-N



2-Pentamethyldisilanyloxybutane
Formula C₉H₂₄O₂Si₂, MW 204, CAS# NA, Entry# 45784
1-Sec-butoxy-1,1,2,2,2-pentamethyldisilane #

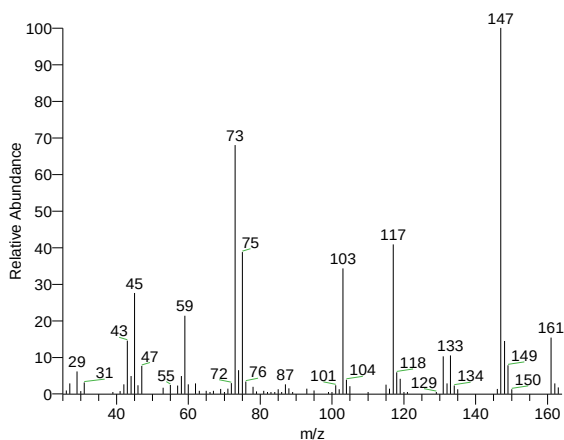


Analysed by Satyanarayana

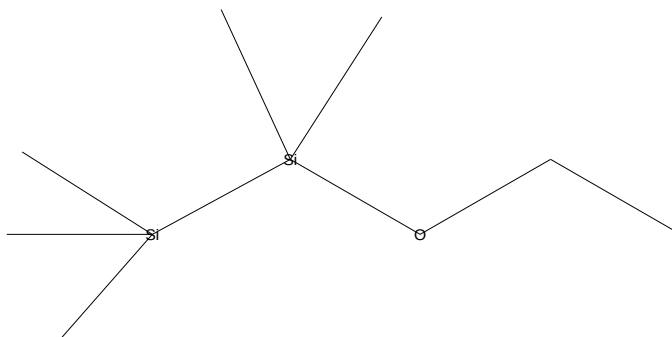
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Hit Spectrum

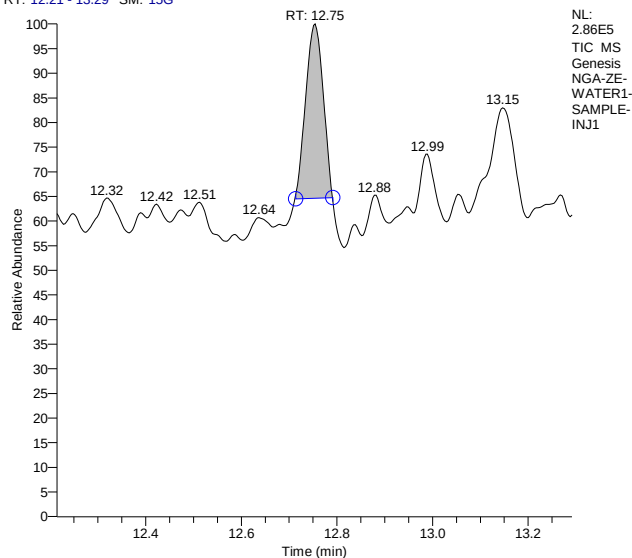
Compound Structure



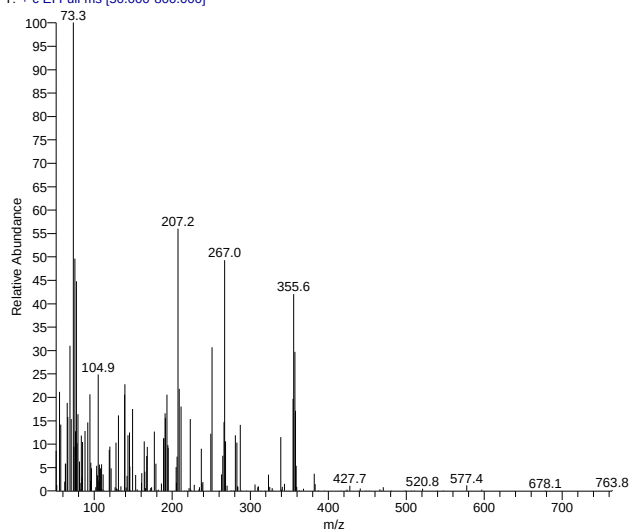
Dimethyl(trimethylsilyl)ethoxysilane
Formula C₇H₂₀OSi₂, MW 176, CAS# 18297-47-7, Entry# 134908
1-Ethoxy-1,1,2,2,2-pentamethyldisilane #



RT: 12.21 - 13.29 SM: 15G



NGA-ZE-WATER1-SAMPLE-INJ1 #2015 RT: 12.75 AV: 1 RF: 6.00, 3 NL: 2.75E4
T: + c EI Full ms [50.000-800.000]



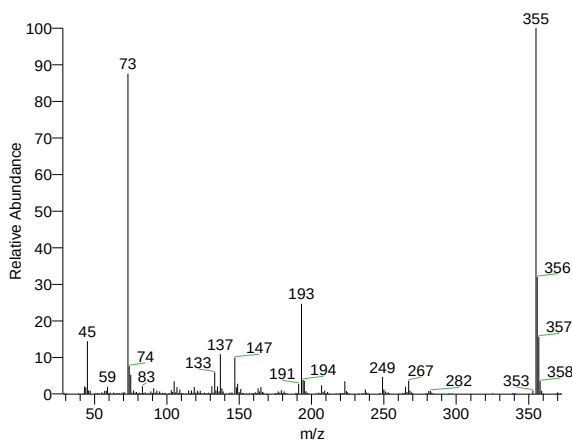
RT	Compound Name	Area	Probability	SI	RSI	Library
12.75	2,3-Dihydroxybenzoic acid, 3TMS derivative	255824.69	21.53	502	521	mainlib
12.75	2,5-Dihydroxybenzoic acid, 3TMS derivative	255824.69	15.63	493	507	mainlib
12.75	2,6-Dihydroxybenzoic acid, 3TMS derivative	255824.69	15.63	493	525	mainlib
12.75	2,4-Dihydroxybenzoic acid, 3TMS derivative	255824.69	9.47	478	494	mainlib
12.75	1,1,3,3,5,5,7,7,9,9-Decamethyl-9-(2-methylpropoxy)pentasiloxan-1-ol	255824.69	7.25	471	520	mainlib

Analysed by Satyanarayana

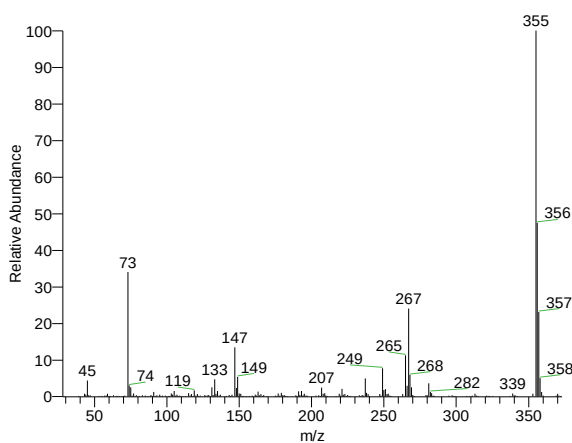
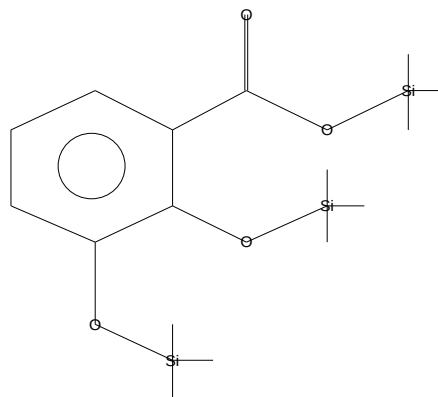
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Hit Spectrum

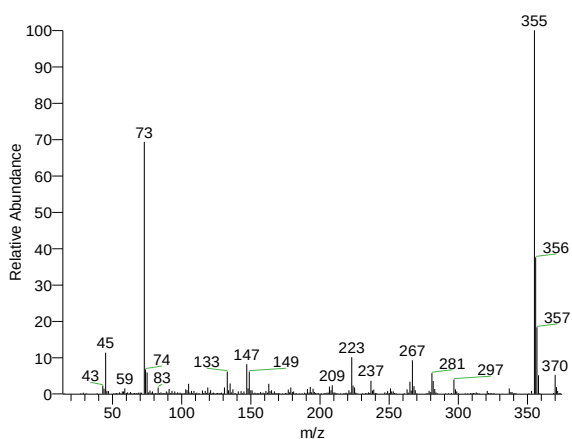
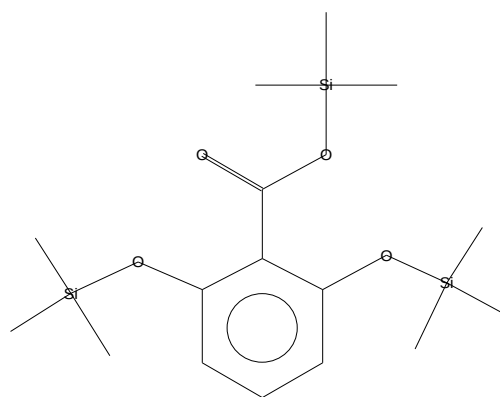
Compound Structure



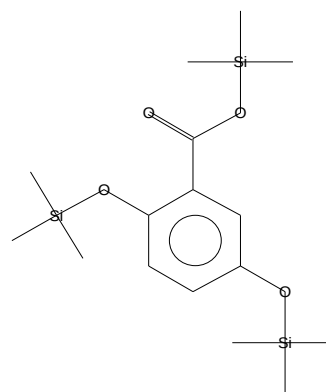
2,3-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-19-7, Entry# 234285
Benzoic acid, 2,3-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester



2,6-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3782-85-2, Entry# 234377
Benzoic acid, 2,6-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester



2,5-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-20-0, Entry# 234286
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester

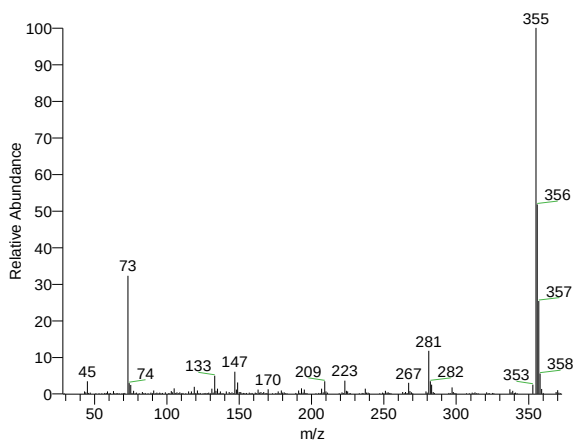


Analysed by Satyanarayana

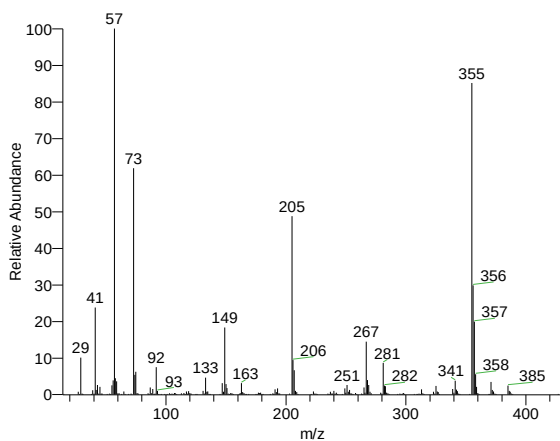
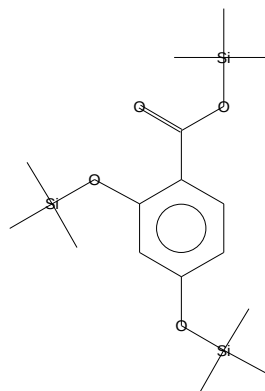
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

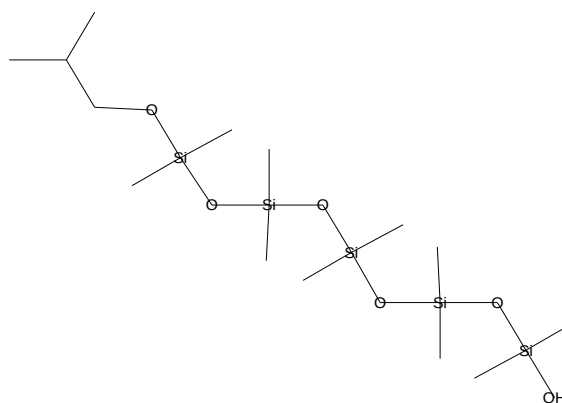
Compound Structure



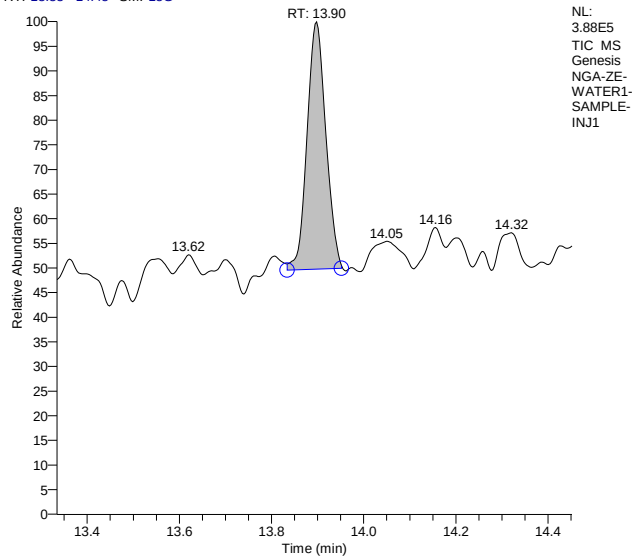
2,4-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 10586-16-0, Entry# 234374
Benzoic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester



1,1,3,3,5,5,7,7,9,9-Decamethyl-9-(2-methylpropoxy)pentasiloxan-1-ol
Formula C₁₄H₄₀O₆Si₅, MW 444, CAS# NA, Entry# 27596
\$:28RUVMAVDYFDDASU-UHFFFAOYSA-N

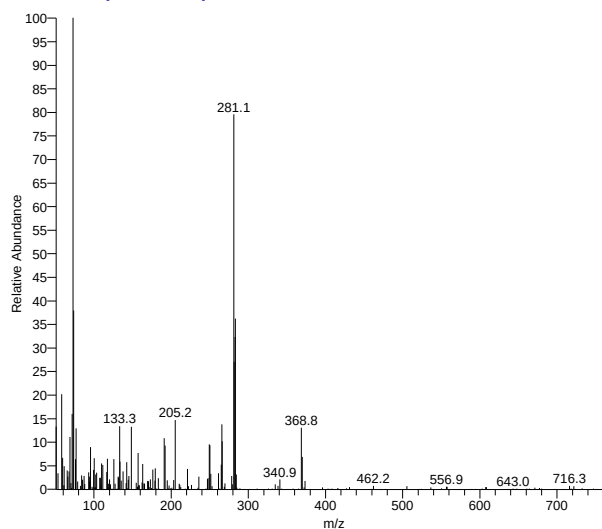


RT: 13.33 - 14.45 SM: 15G



NL:
3.88E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #2356 RT: 13.90 AV: 1 RF: 6.00, 3 NL: 5.91E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
13.90	2,6-Dihydroxyacetophenone, 2TMS derivative	554642.94	16.89	544	603	mainlib

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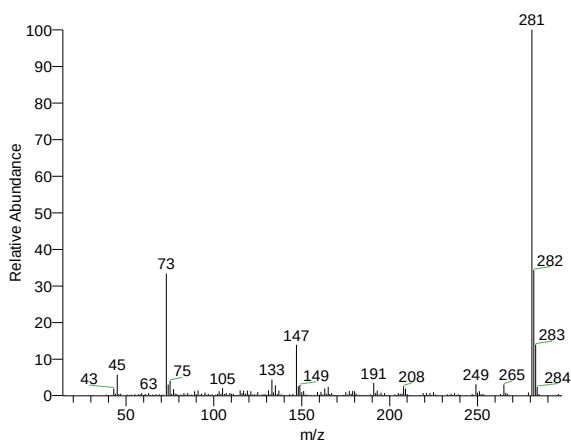
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

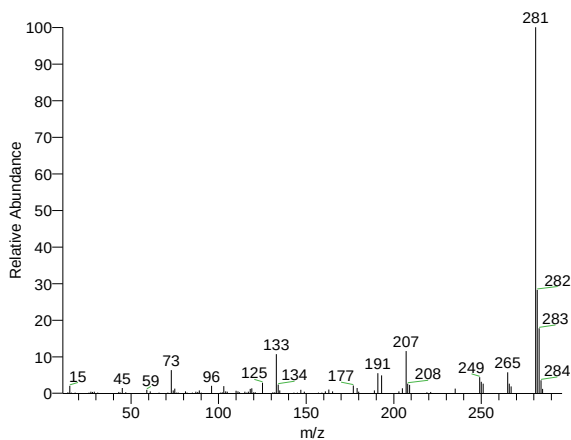
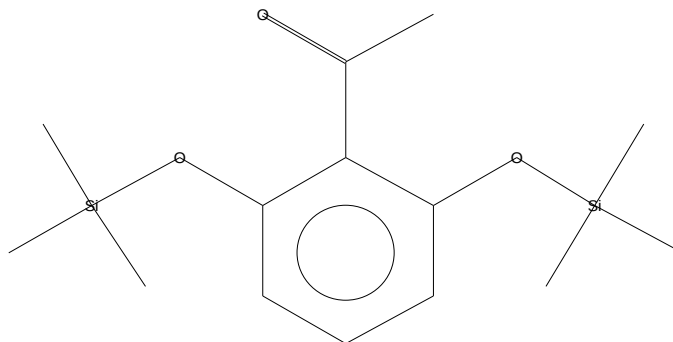
RT	Compound Name	Area	Probability	SI	RSI	Library
13.90	Cyclotetrasiloxane, octamethyl-	554642.94	15.58	542	666	mainlib
13.90	Pentasiloxane, dodecamethyl-	554642.94	14.37	540	605	mainlib
13.90	2,4-Dihydroxyacetophenone, 2TMS derivative	554642.94	9.28	527	579	mainlib
13.90	2,5-Dihydroxyacetophenone, 2TMS derivative	554642.94	5.99	514	567	mainlib

Hit Spectrum

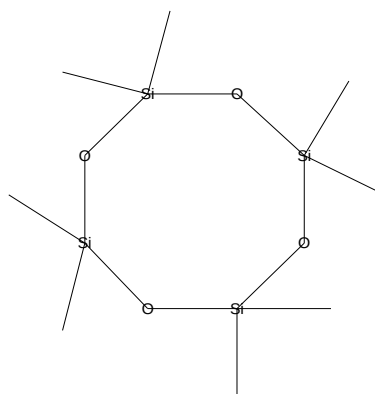
Compound Structure



2,6-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220073
2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



Cyclotetrasiloxane, octamethyl-
Formula C₈H₂₄O₄Si₄, MW 296, CAS# 556-67-2, Entry# 220100
Oktamethylcyclotetrasiloxan



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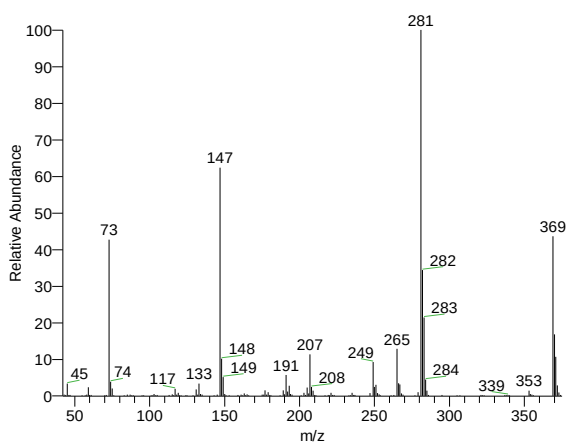
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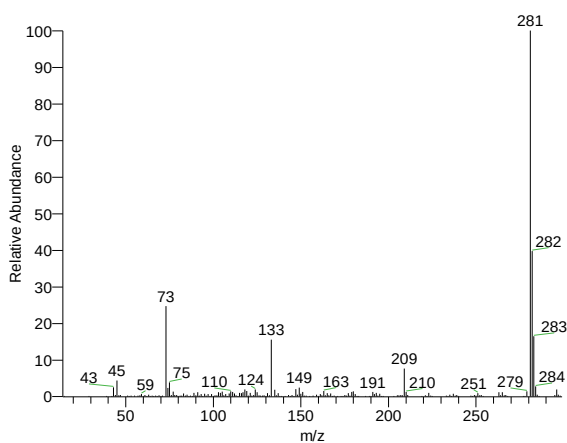
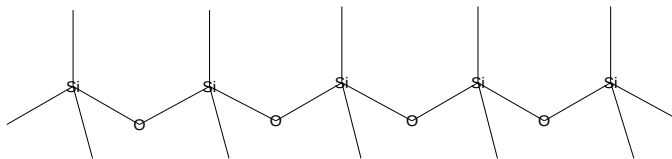
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

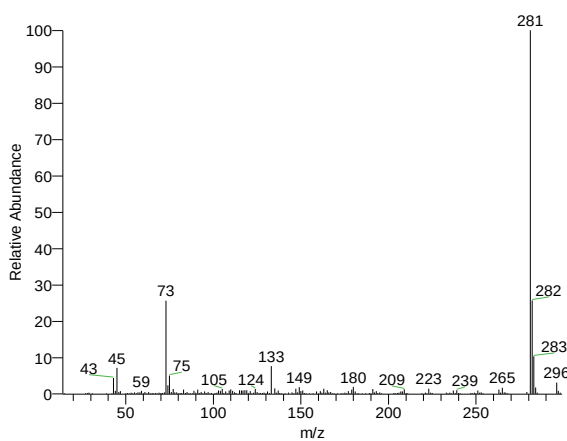
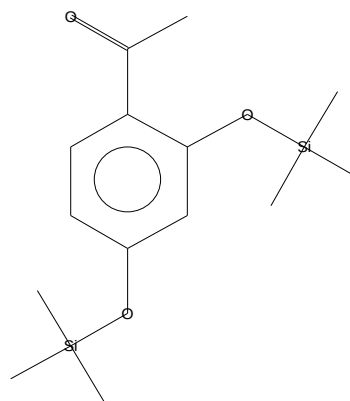
Compound Structure



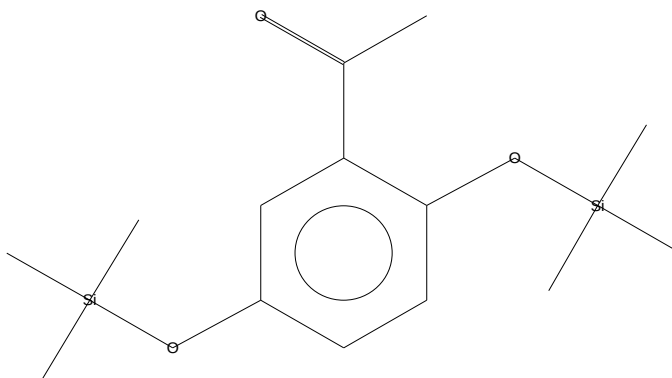
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



2,4-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220074
2',4'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



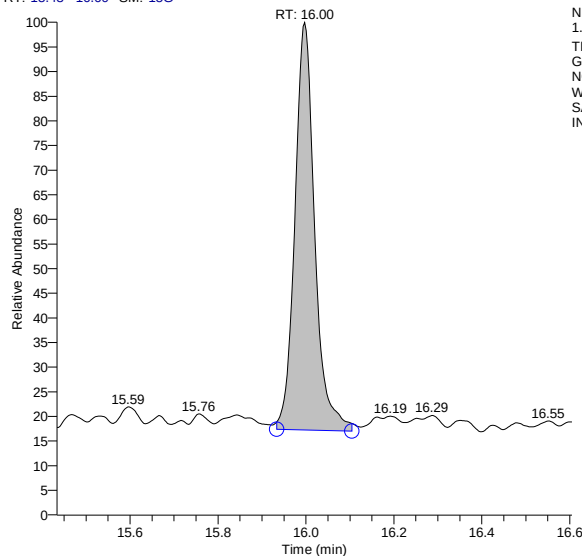
2,5-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220075
2,5-Dihydroxyacetophenone, bis(trimethylsilyl) ether



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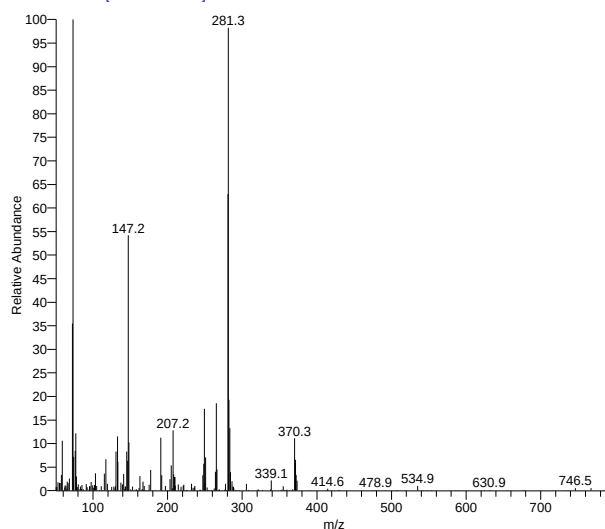
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RT: 15.43 - 16.60 SM: 15G



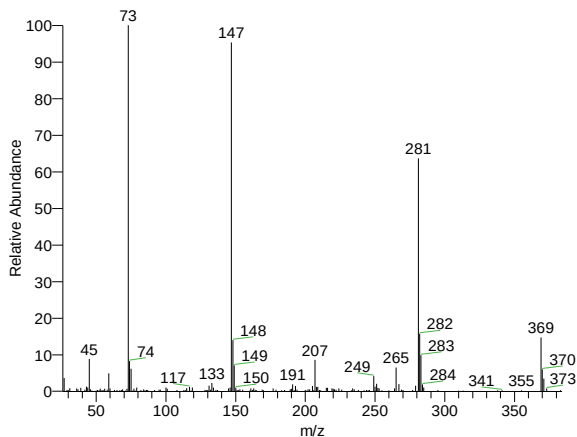
NL:
1.09E6
TIC: MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #2982 RT: 16.00 AV: 1 RF: 6.00, 3 NL: 1.87E5
T: + c EI Full ms [50.000-800.000]



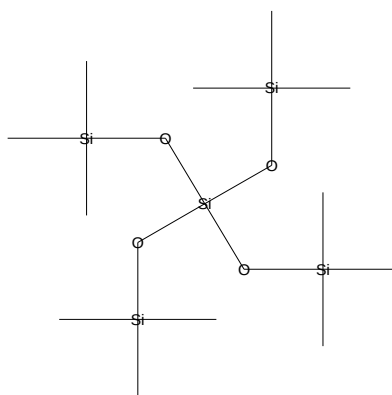
RT	Compound Name	Area	Probability	SI	RSI	Library
16.00	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	2804800.02	49.85	688	739	mainlib
16.00	Pentasiloxane, dodecamethyl-	2804800.02	13.86	658	709	mainlib
16.00	2,6-Dihydroxyacetophenone, 2TMS derivative	2804800.02	7.14	640	705	mainlib
16.00	Cyclotetrasiloxane, octamethyl-	2804800.02	5.33	632	756	mainlib
16.00	trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-	2804800.02	4.71	629	793	mainlib

Hit Spectrum



Compound Structure

Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Analysed by Satyanarayana

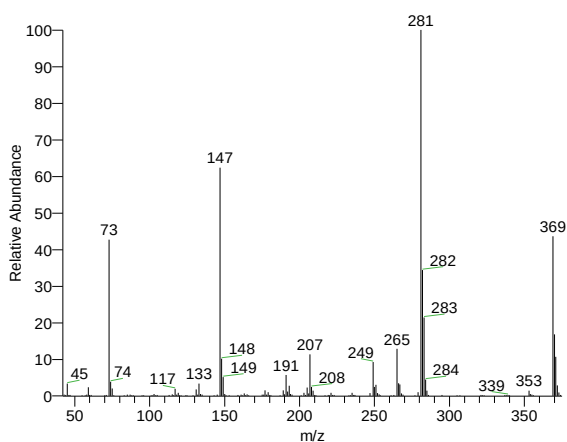
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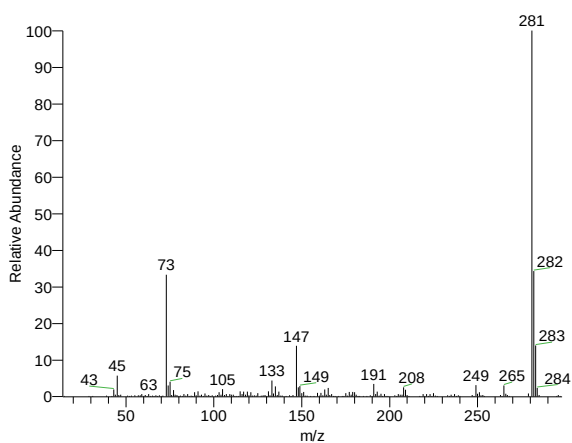
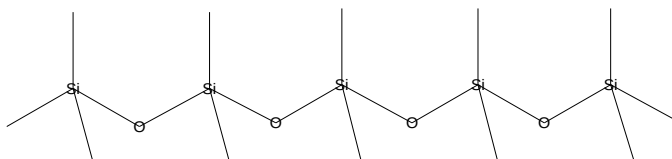
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

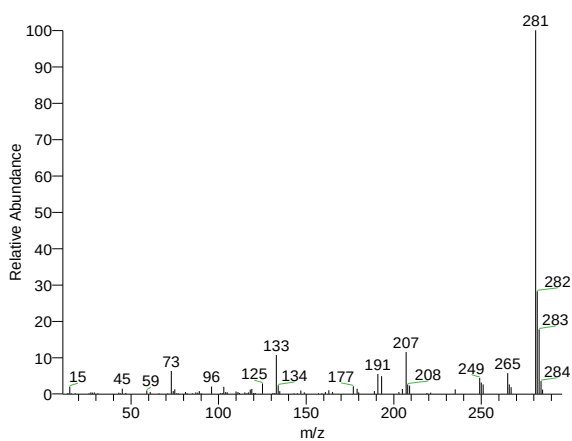
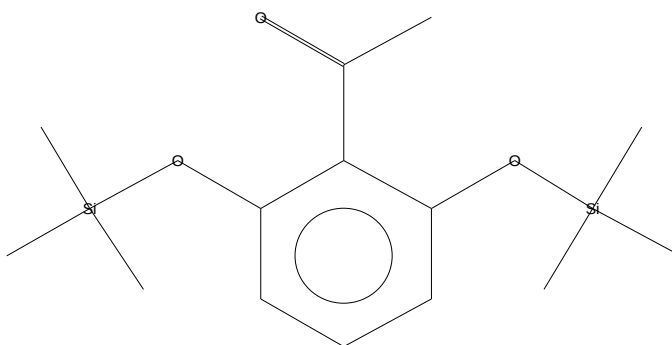
Compound Structure



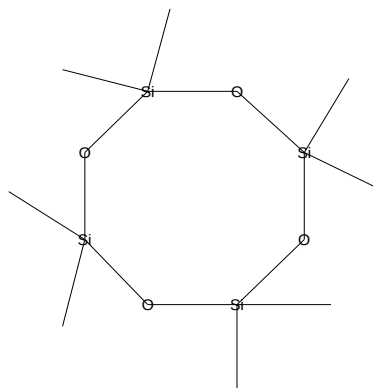
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



2,6-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220073
2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether



Cyclotetrasiloxane, octamethyl-
Formula C₈H₂₄O₄Si₄, MW 296, CAS# 556-67-2, Entry# 220100
Oktamethylcyclotetrasiloxan

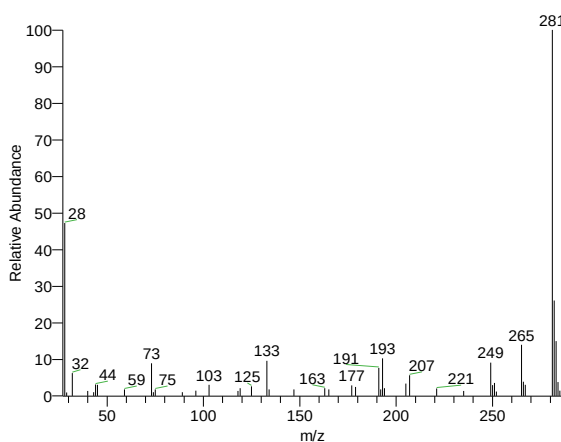


Analysed by Satyanarayana

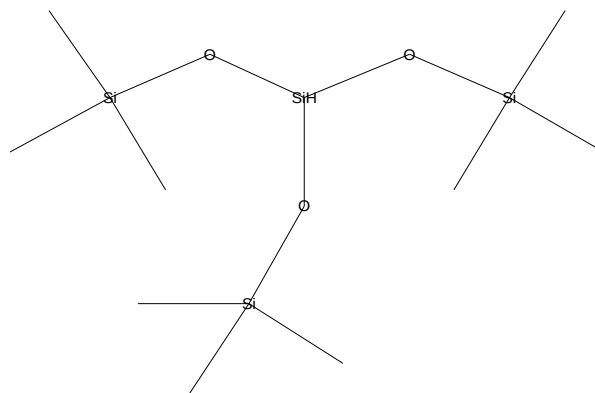
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Hit Spectrum

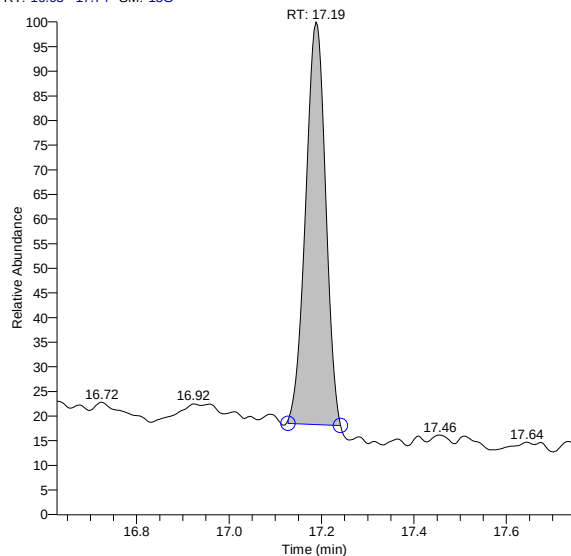
Compound Structure



trisiloxane, 1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]-
Formula C₉H₂₈O₃Si₄, MW 296, CAS# NA, Entry# 219896
1,1,1,5,5,5-hexamethyl-3-[(trimethylsilyl)oxy]trisiloxane

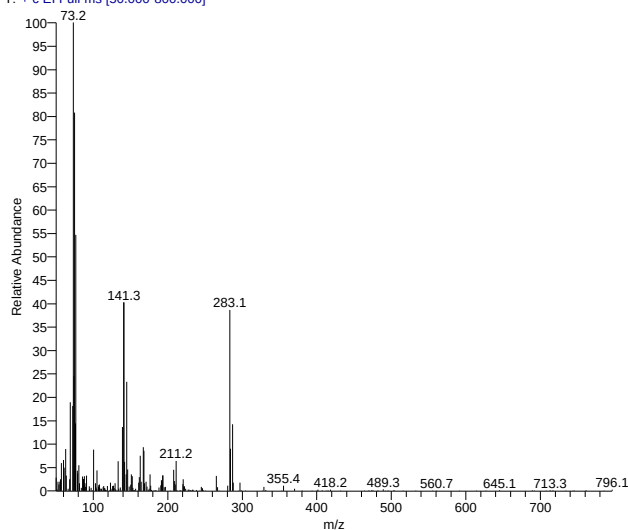


RT: 16.63 - 17.74 SM: 15G



NL: 8.93E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #3337 RT: 17.19 AV: 1 RF: 6.00, 3 NL: 1.53E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
17.19	N'-(3-Pyridinylmethylene)isonicotinohydrazide, TMS derivative	2184589.29	11.15	461	485	mainlib
17.19	N'-(3-Pyridinylmethylene)isonicotinohydrazide, TBDMS derivative	2184589.29	8.09	452	479	mainlib
17.19	n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester	2184589.29	7.15	449	518	mainlib
17.19	Quinoxaline, 6-nitro-2-phenyl-, 1,4-dioxide	2184589.29	5.76	444	500	mainlib
17.19	5,8,11-Eicosatriynoic acid, TMS derivative	2184589.29	4.18	435	438	mainlib

Analysed by Satyanarayana

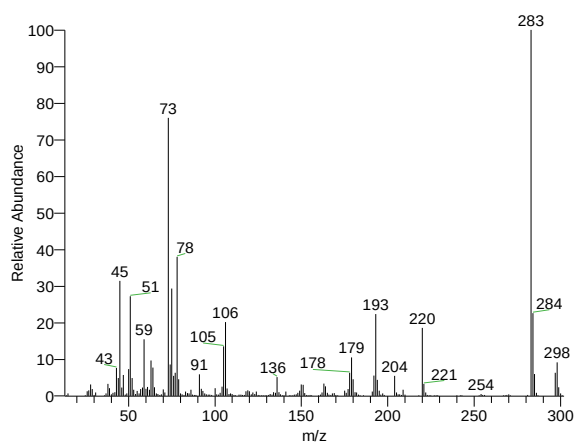
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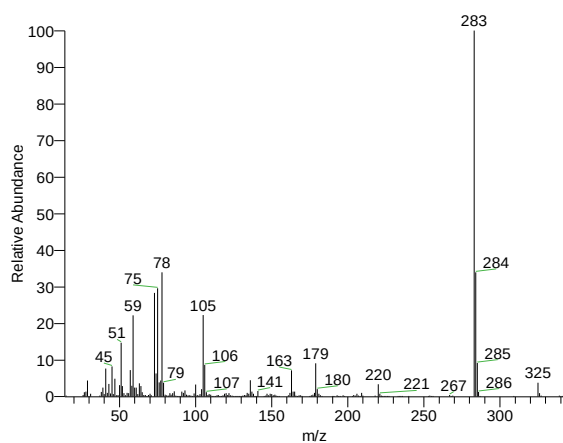
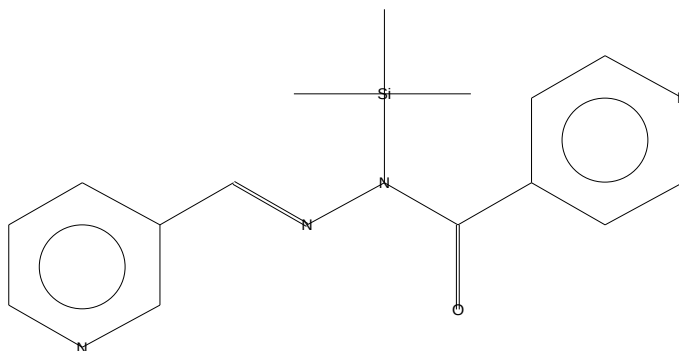
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

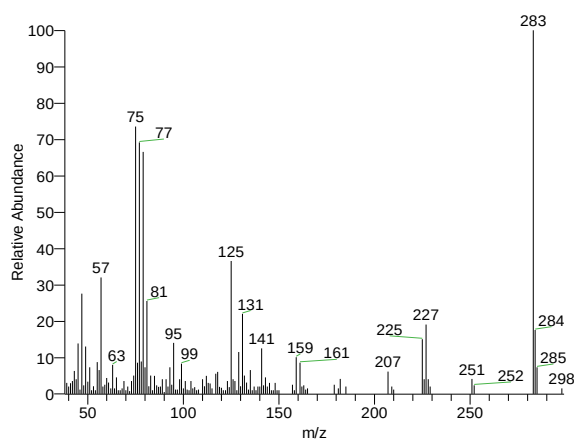
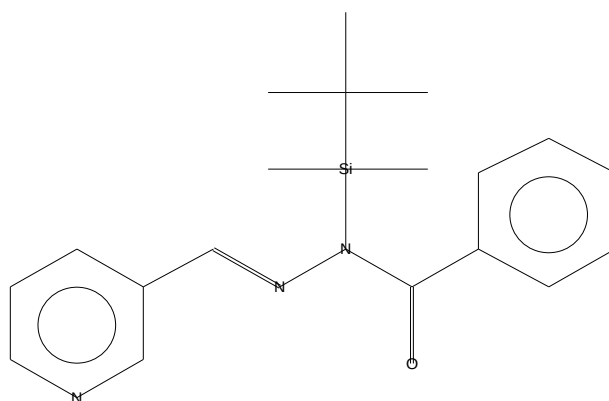
Compound Structure



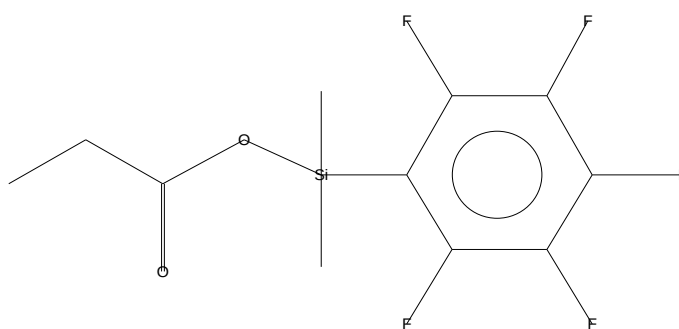
N'-(3-Pyridinylmethylene)isonicotinohydrazide, TMS derivative
Formula C₁₅H₁₈N₄OSi, MW 298, CAS# NA, Entry# 220546
N'-(3-Pyridinylmethylene)isonicotinohydrazide tms



N'-(3-Pyridinylmethylene)isonicotinohydrazide, TBDMS derivative
Formula C₁₈H₂₄N₄OSi, MW 340, CAS# NA, Entry# 220559
N'-(3-Pyridinylmethylene)isonicotinohydrazide tbdms



n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester
Formula C₁₁H₁₁F₅O₂Si, MW 298, CAS# NA, Entry# 220549
Dimethyl(2,3,4,5,6-pentafluorophenyl)silyl propionate #

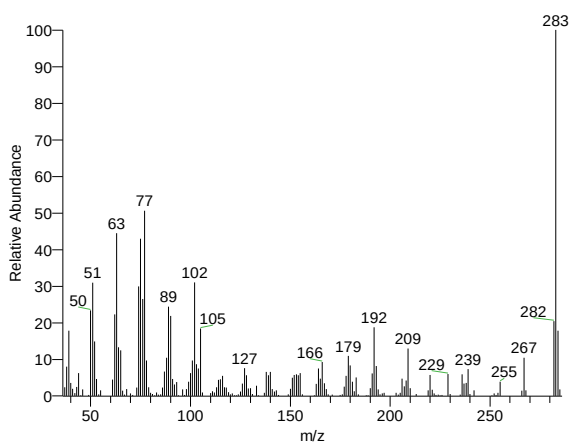


Analysed by Satyanarayana

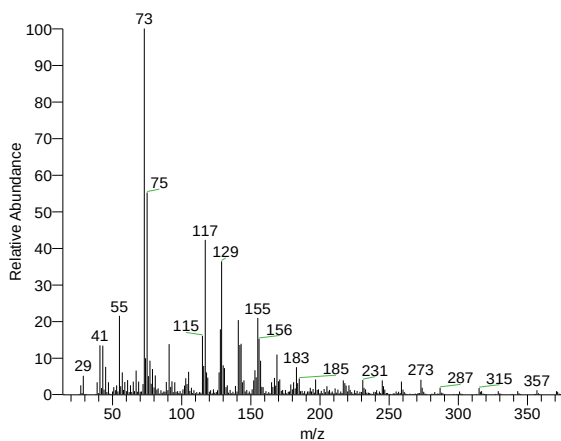
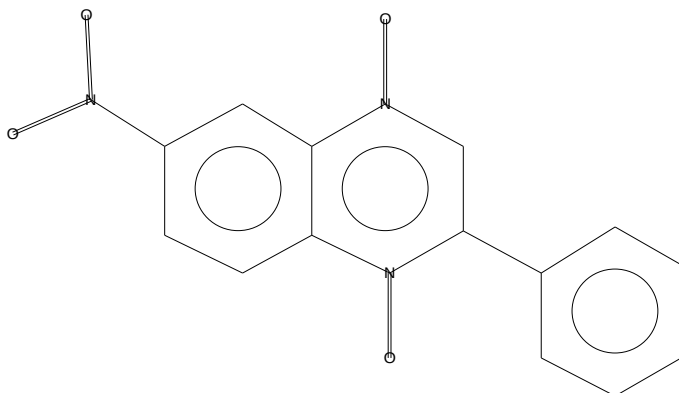
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Hit Spectrum

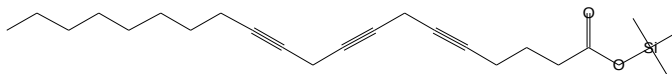
Compound Structure



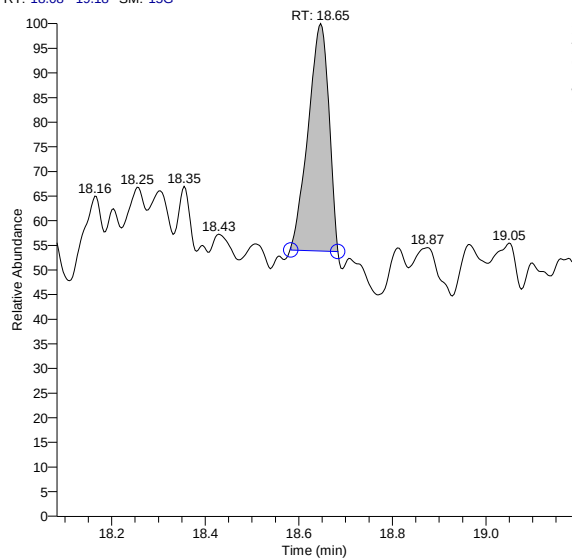
Quinoxaline, 6-nitro-2-phenyl-, 1,4-dioxide
Formula C₁₄H₉N₃O₄, MW 283, CAS# 351065-06-0, Entry# 220553
6-Nitro-2-phenylquinoxaline 1,4-dioxide #



5,8,11-Eicosatriynoic acid, TMS derivative
Formula C₂₃H₃₆O₂Si, MW 372, CAS# NA, Entry# 41372
5,8,11-Eicosatriynoic acid, trimethylsilyl ester

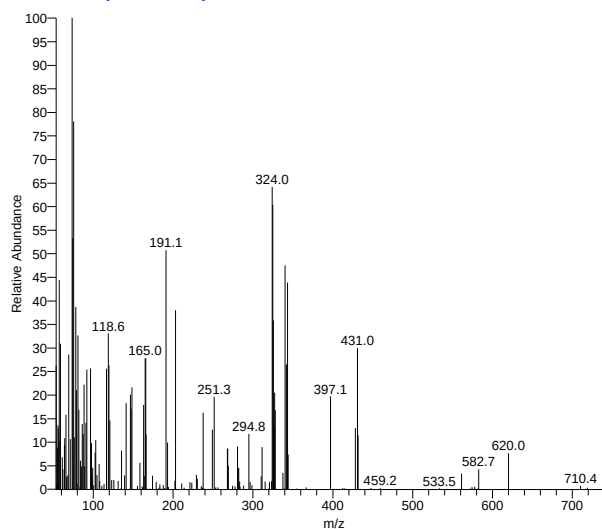


RT: 18.08 - 19.18 SM: 15G



NL:
2.14E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #3772 RT: 18.65 AV: 1 RF: 6.00, 3 NL: 1.31E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
18.65	5-Chloro-1-trimethylsilyl-indole-2-carboxylic acid, trimethylsilyl ester	301893.55	12.86	408	448	mainlib

Analysed by Satyanarayana

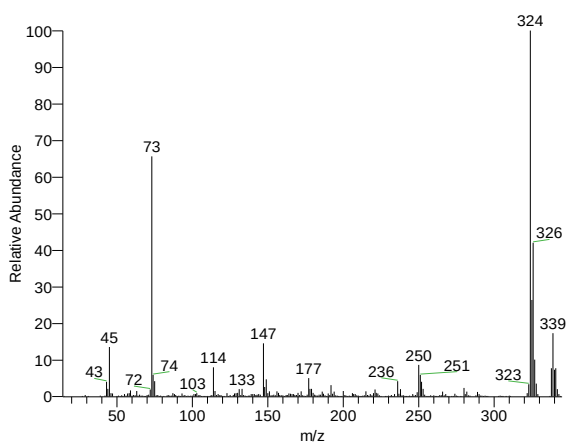
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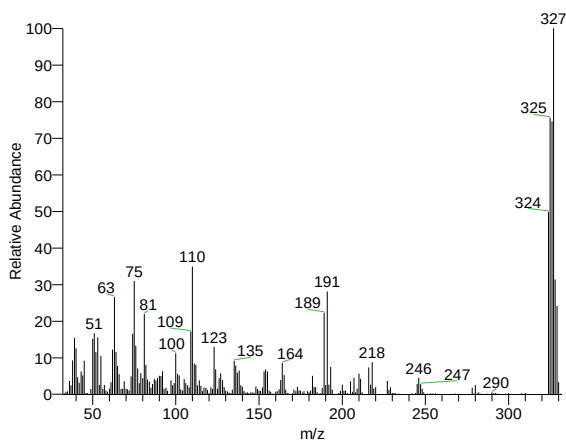
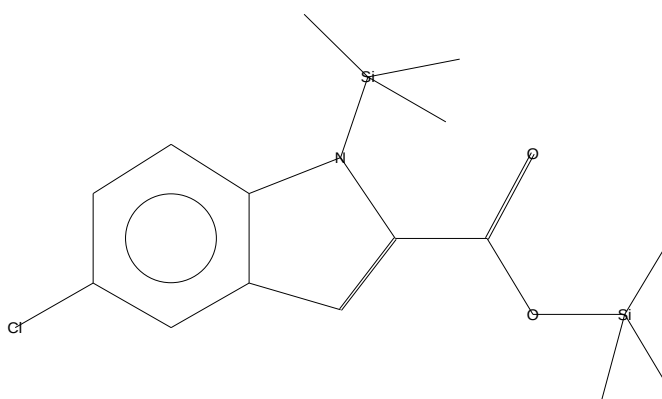
RT	Compound Name	Area	Probability	SI	RSI	Library
18.65	Benzene-1,2-diol, 4-(4-bromo-3-chlorophenyl iminomethyl)-	301893.55	5.85	388	499	mainlib
18.65	Octadecanoic acid, 1,3-propanediyl ester	301893.55	5.63	387	456	mainlib
18.65	1H-Indole-2,3-dione, 5-chloro-1-(trimethylsilyl)-	301893.55	4.08	378	506	mainlib
18.65	3-[O-(trimethylsilyl)oxime] 1,2,4-Triazol-5(1H)-thione	301893.55	2.80	367	495	mainlib
	4-(4-acetylphenyl)-3-(4-methoxyphenyl)-					

Hit Spectrum

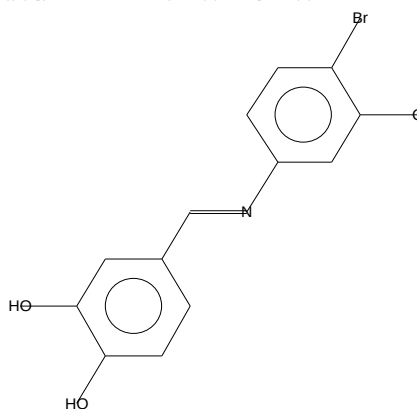


Compound Structure

5-Chloro-1-(trimethylsilyl)-indole-2-carboxylic acid, trimethylsilyl ester
 Formula C₁₅H₂₂ClNO₂Si₂, MW 339, CAS# NA, Entry# 229704
 5-Chloro-1H-indole-2-carboxylic acid, N,O-diTMS



Benzene-1,2-diol, 4-(4-bromo-3-chlorophenyl iminomethyl)-
 Formula C₁₃H₉BrClNO₂, MW 325, CAS# 304456-09-5, Entry# 230369
 4-((E)-[(4-Bromo-3-chlorophenyl)imino]methyl)-1,2-benzenediol #



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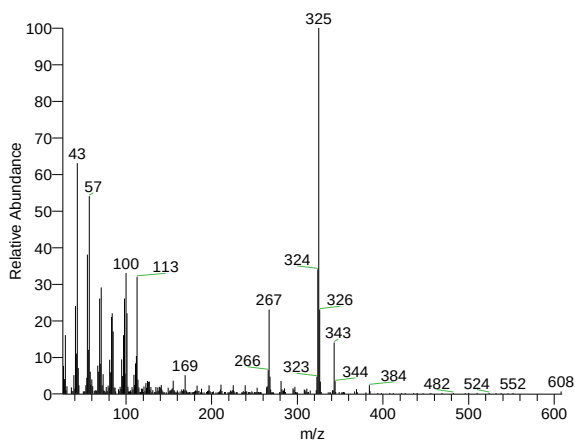
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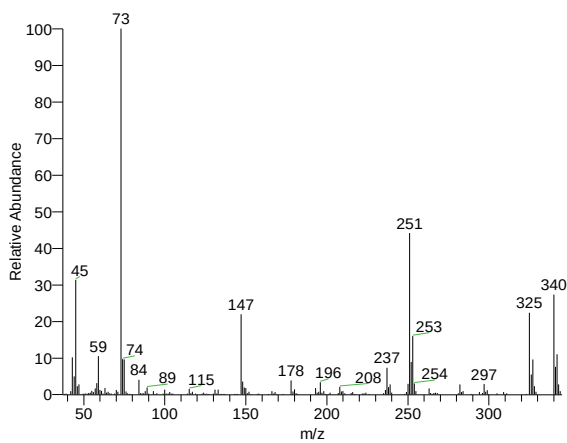
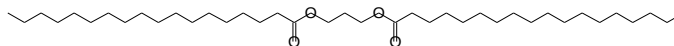
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Hit Spectrum

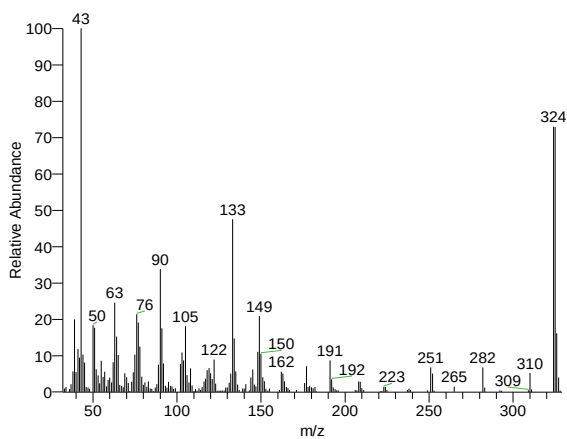
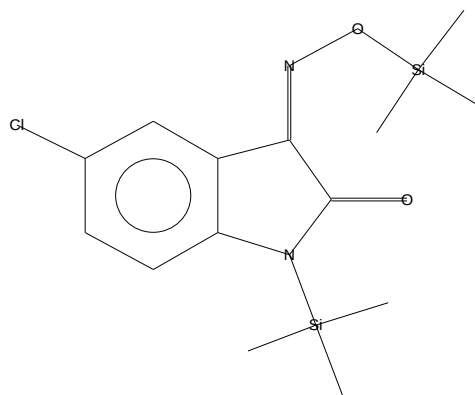
Compound Structure



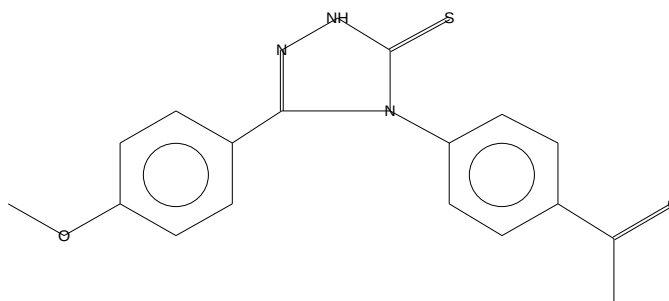
Octadecanoic acid, 1,3-propanediyl ester
Formula C₃₉H₇₆O₄, MW 608, CAS# 17367-44-1, Entry# 229887
Stearic acid, trimethylene ester



1H-Indole-2,3-dione, 5-chloro-1-(trimethylsilyl)-, 3-[O-(trimethylsilyl)oxime]
Formula C₁₄H₂₁ClN₂O₂Si₂, MW 340, CAS# NA, Entry# 43600
(3Z)-5-Chloro-1-(trimethylsilyl)-1H-indole-2,3-dione 3-[O-(trimethylsilyl)oxime] #



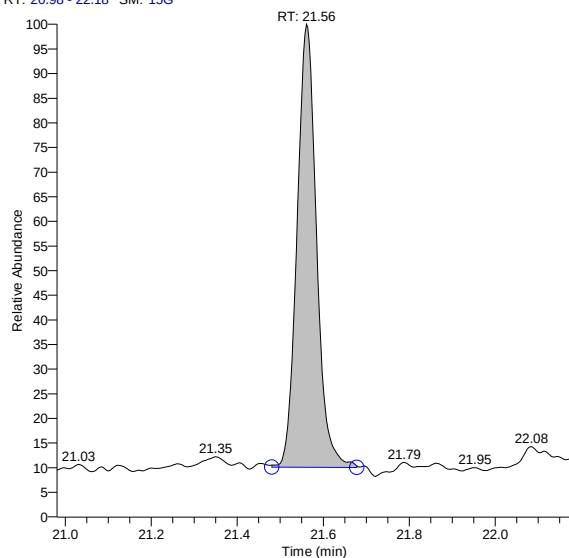
1,2,4-Triazol-5(1H)-thione, 4-(4-acetylphenyl)-3-(4-methoxyphenyl)-
Formula C₁₇H₁₅N₃O₂S, MW 325, CAS# NA, Entry# 14665
1-(4-[3-(4-Methoxyphenyl)-5-thioxo-1,5-dihydro-4H-1,2,4-triazol-4-yl]phenyl)ethanone #



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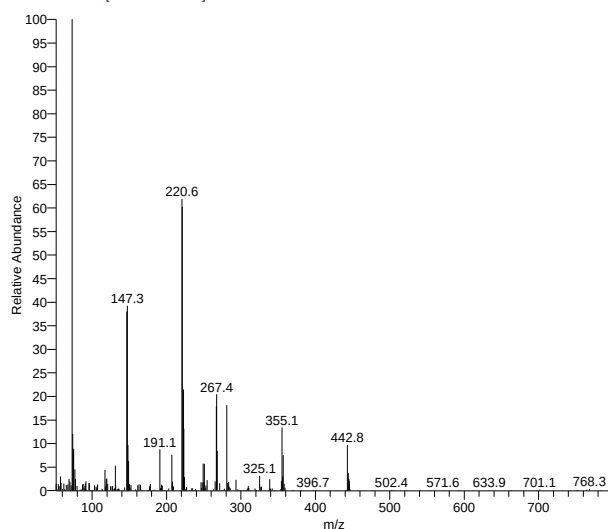
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RT: 20.98 - 22.18 SM: 15G



NL:
1.03E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

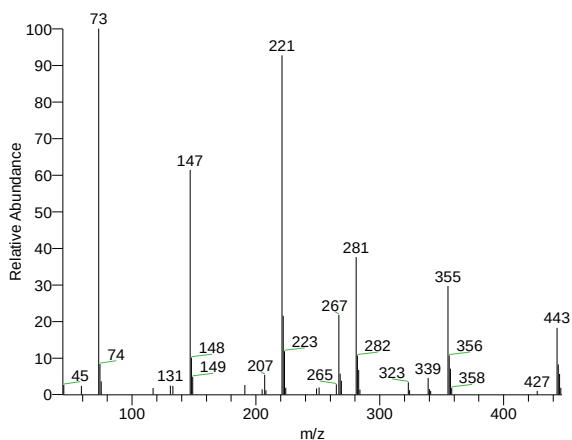
NGA-ZE-WATER1-SAMPLE-INJ1 #4641 RT: 21.56 AV: 1 RF: 6.00, 3 NL: 2.35E5
T: + c EI Full ms [50.000-800.000]



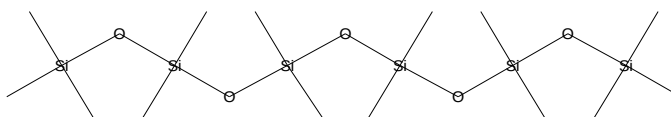
RT	Compound Name	Area	Probability	SI	RSI	Library
21.56	Hexasiloxane, tetradecamethyl-	2917961.89	92.42	741	811	mainlib
21.56	1,1,1,3,5,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane	2917961.89	5.40	625	786	mainlib
21.56	Heptasiloxane, hexadecamethyl-	2917961.89	0.37	521	604	mainlib
21.56	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2917961.89	0.27	512	550	mainlib
21.56	3,6-Dioxa-2,4,5,7-tetrasiloxane, 2,2,4,4,5,5,7,7-octamethyl-	2917961.89	0.19	502	675	mainlib

Hit Spectrum

Compound Structure



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



Analysed by Satyanarayana

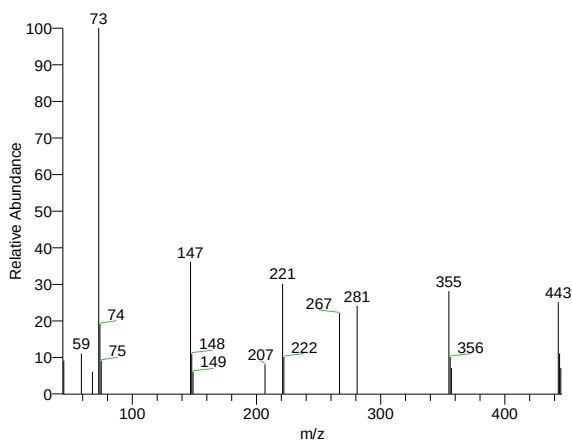
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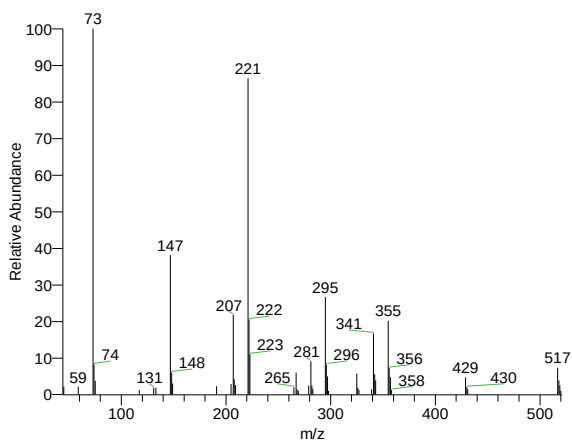
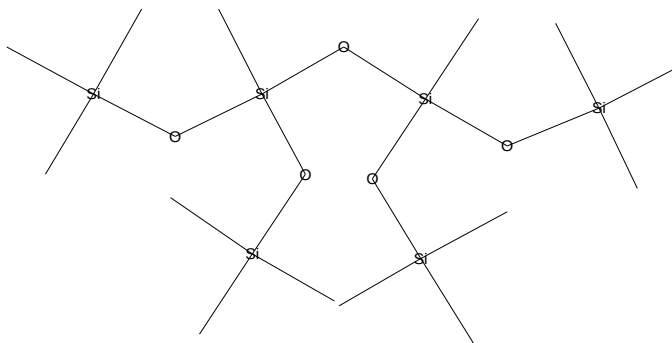
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

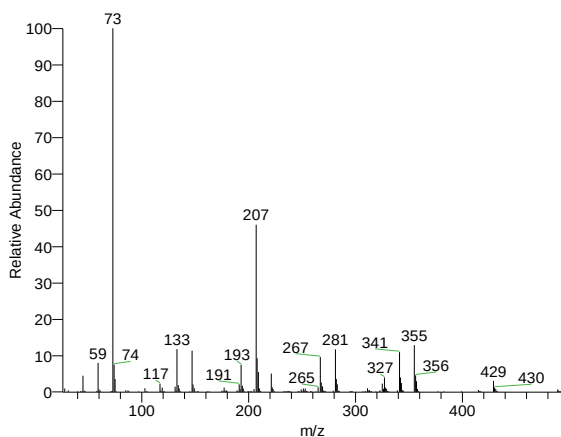
Compound Structure



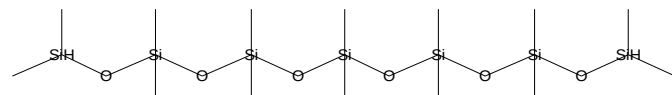
1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 2003-92-1, Entry# 42693
1,1,1,3,5,7,7,7-Octamethyl-3,5-bis(trimethylsilyl)oxy)tetrasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

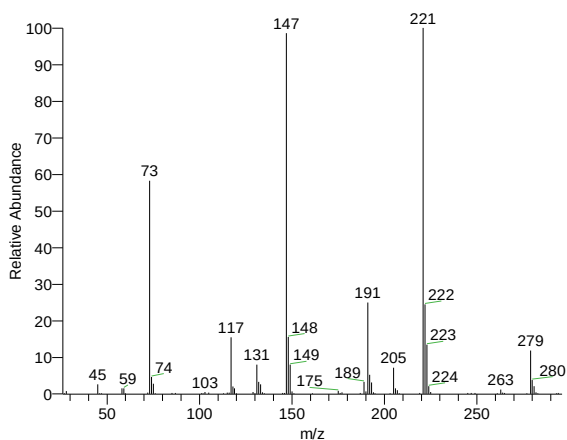


Analysed by Satyanarayana

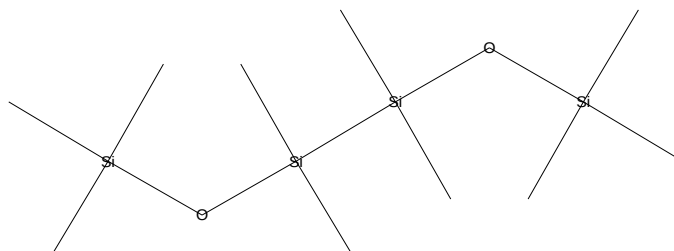
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Hit Spectrum

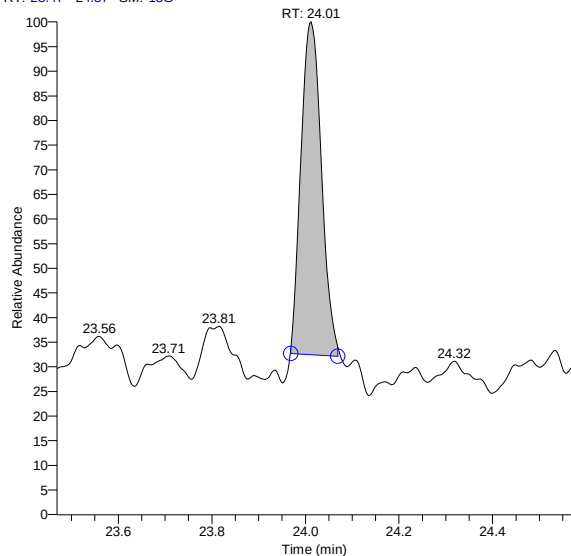
Compound Structure



3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-
Formula C₁₀H₃₀O₂Si₄, MW 294, CAS# 4342-25-0, Entry# 196522
2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxa-2,4,5,7-tetrasilaoctane #

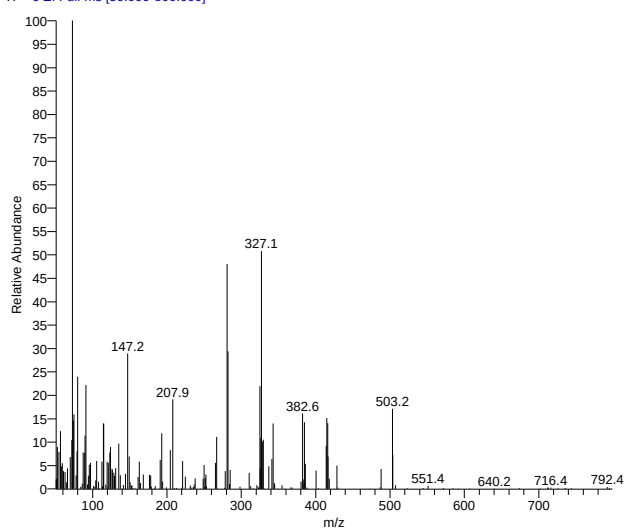


RT: 23.47 - 24.57 SM: 15G



NL:
2.67E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #5372 RT: 24.01 AV: 1 RF: 6.00, 3 NL: 3.59E4
T: + c EI Full ms [50.000-800.000]



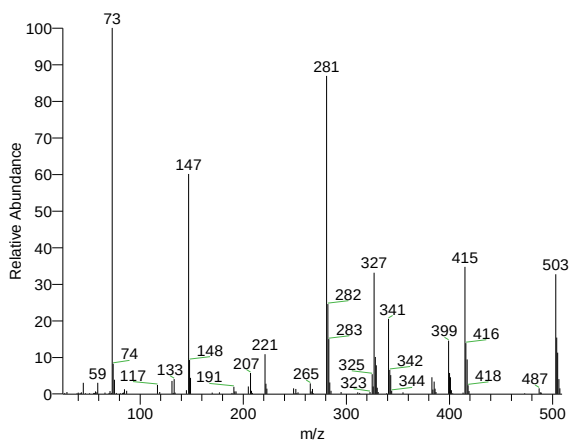
RT	Compound Name	Area	Probability	SI	RSI	Library
24.01	Cycloheptasiloxane, tetradecamethyl-	547683.56	73.37	530	619	mainlib
24.01	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	547683.56	8.07	450	491	mainlib
24.01	Ethyl gallate, 3TMS derivative	547683.56	2.70	426	492	mainlib
24.01	Cyclodecasiloxane, eicosamethyl-	547683.56	1.96	417	432	mainlib
24.01	3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	547683.56	1.96	417	631	mainlib

Analysed by Satyanarayana

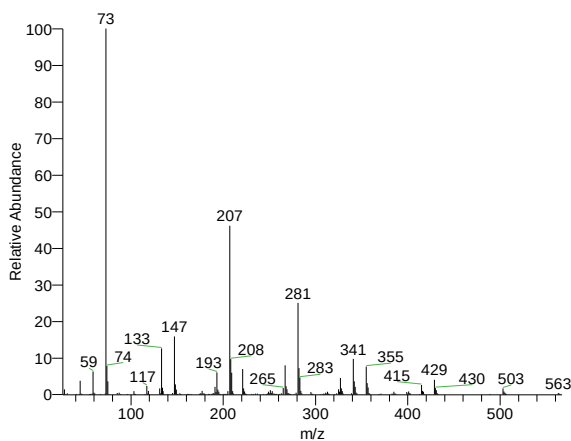
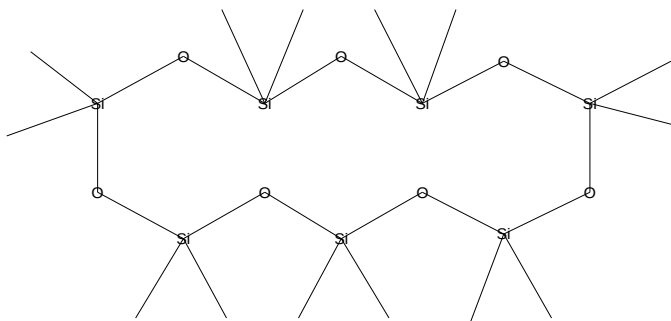
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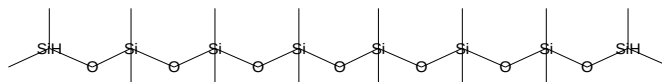
Compound Structure



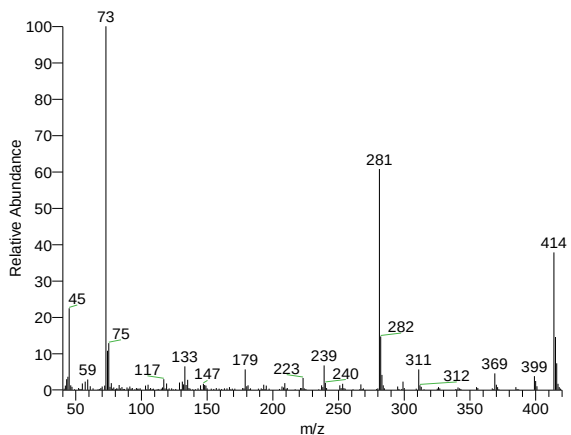
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



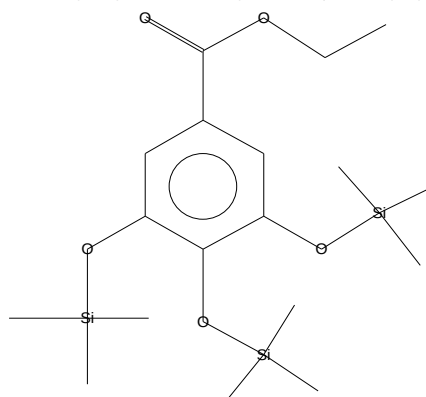
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



SI 426, RSI 492, mainlib, Entry# 43774, CAS# NA, Ethyl gallate, 3TMS derivative



Ethyl gallate, 3TMS derivative
Formula C₁₈H₃₄O₅Si₃, MW 414, CAS# NA, Entry# 43774
3,4,5-Trihydroxybenzoic acid ethyl ester, tris(O-trimethylsilyl)-

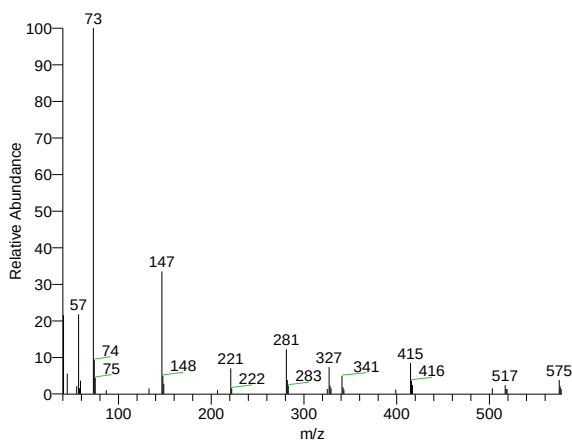


Analysed by Satyanarayana

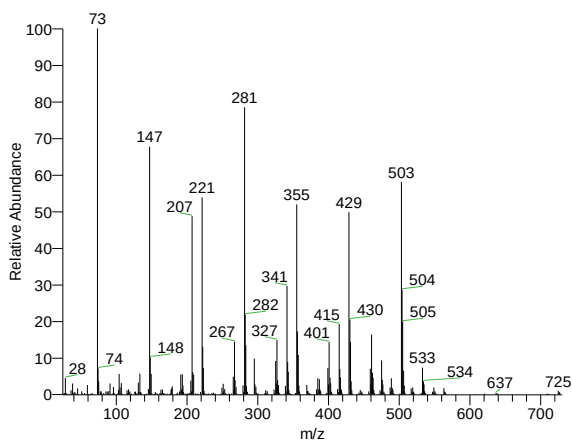
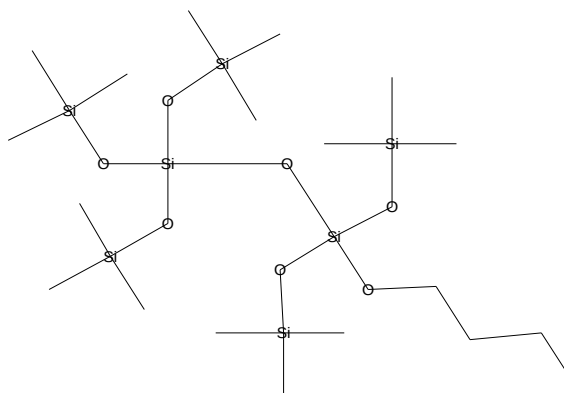
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Hit Spectrum

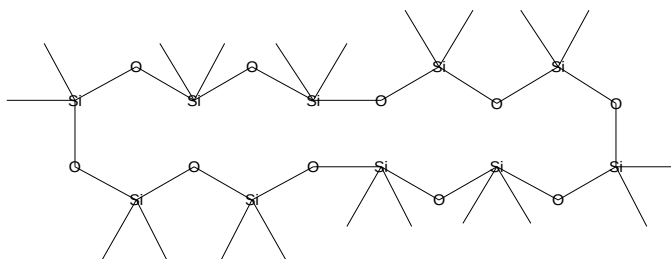
Compound Structure



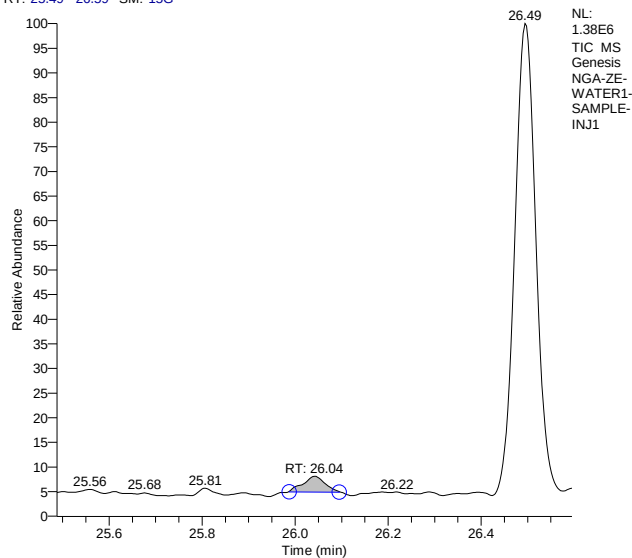
3-Butoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane
Formula C₁₉H₅₄O₇Si₇, MW 590, CAS# 72439-84-0, Entry# 42504
1-Butoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl tris(trimethylsilyl) orthosilicate #



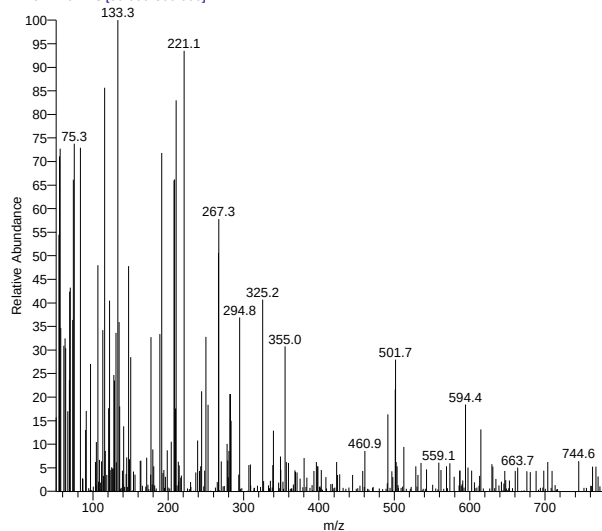
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



RT: 25.49 - 26.59 SM: 15G



NGA-ZE-WATER1-SAMPLE-INJ1 #5977 RT: 26.04 AV: 1 RF: 6.00, 3 NL: 5.15E3
T: + c EI Full ms [50,000-800,000]



RT	Compound Name	Area	Probability	SI	RSI	Library
26.04	Benzene, (2-bromo-1-cyclobuten-1-yl)-	146411.70	7.60	320	752	mainlib

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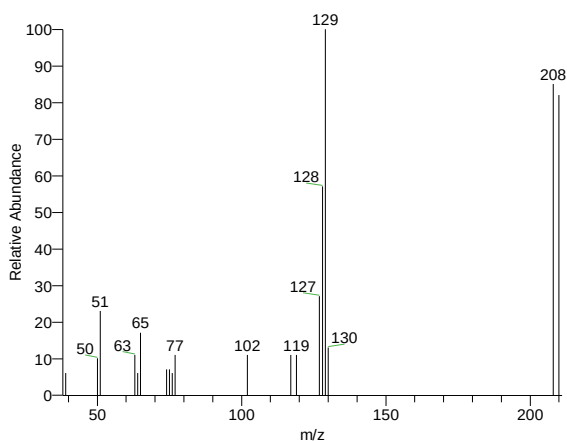
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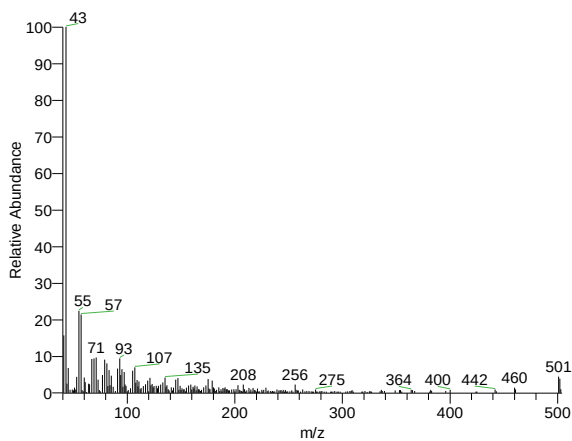
ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
26.04	Serverogenin acetate	146411.70	5.98	314	419	mainlib
26.04	{Sulfanediylbis[(4,6-dichlorobenzene-2,1-diyl)oxy]}bis(trimethylsilane)	146411.70	5.05	310	348	mainlib
26.04	7,8-Epoxy lanostan-11-ol, 3-acetoxy-	146411.70	4.07	305	353	mainlib
26.04	17 α -Acetoxy-1',1'-dicarboethoxy-1 α ,2 α -dihydro-17 α -methyl-3'H-cycloprop[1,2]-5 α -androst-1-en-3-one	146411.70	3.44	301	348	mainlib

Hit Spectrum

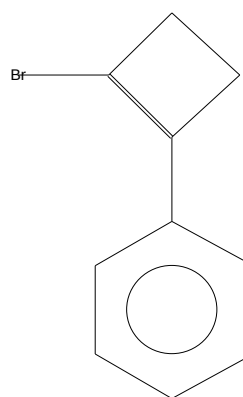


SI 314, RSI 419, mainlib, Entry# 7203, CAS# NA, Serverogenin acetate

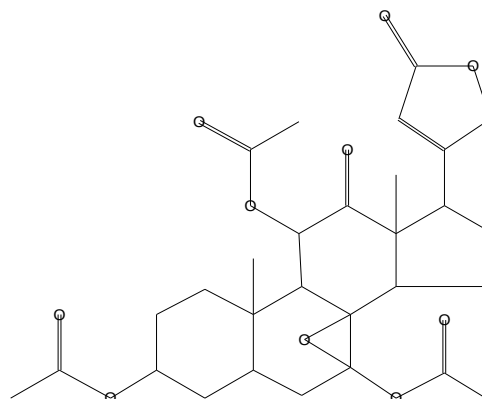


Compound Structure

Benzene, (2-bromo-1-cyclobuten-1-yl)-
Formula C₁₀H₉Br, MW 208, CAS# 41893-67-8, Entry# 114189
(2-Bromo-1-cyclobuten-1-yl)benzene #



Serverogenin acetate
Formula C₂₉H₃₆O₁₀, MW 544, CAS# NA, Entry# 7203



Analysed by Satyanarayana

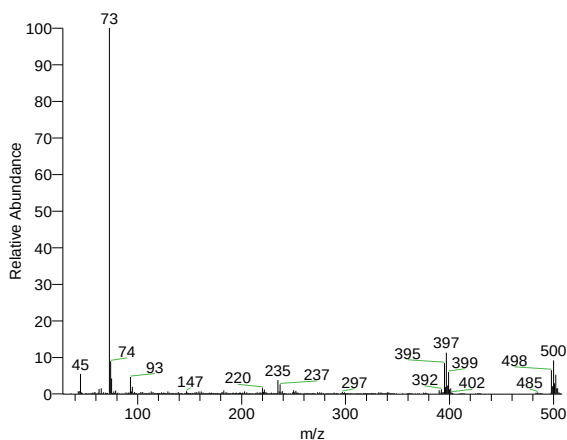
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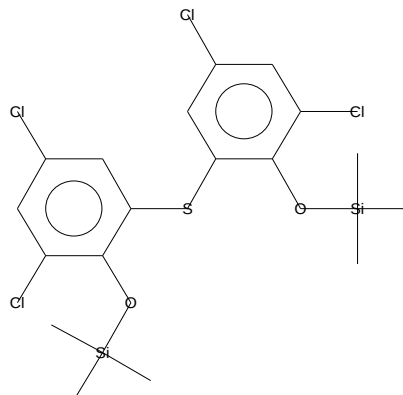
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

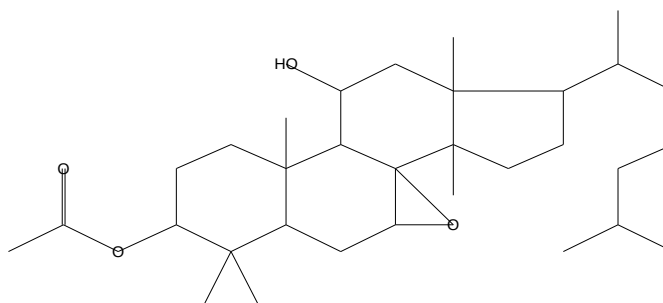
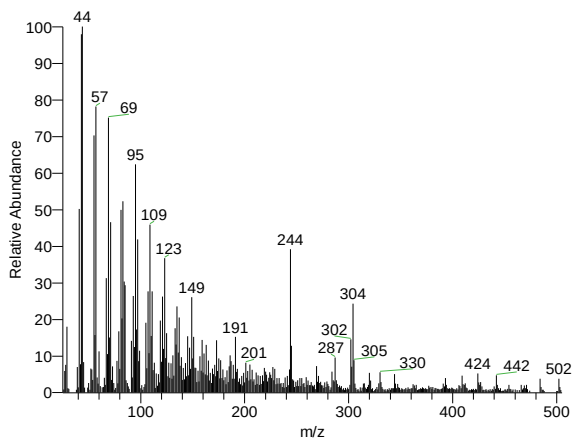
Compound Structure



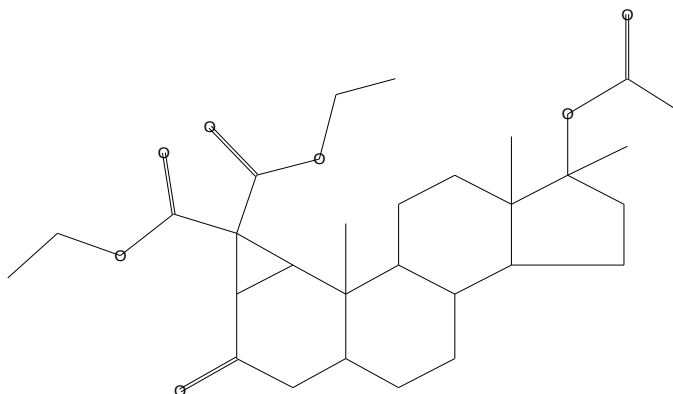
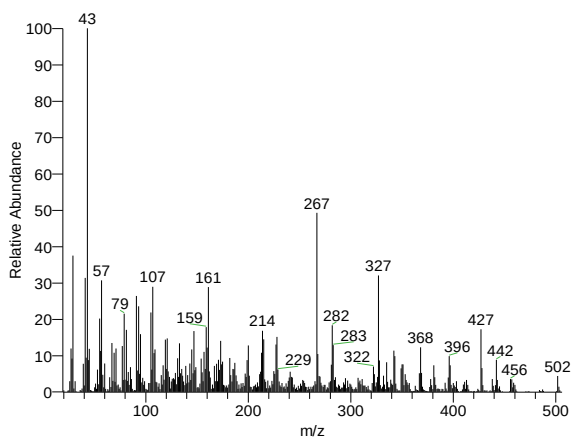
{Sulfanediylbis[(4,6-dichlorobenzene-2,1-diyl)oxy]]bis(trimethylsilane)
Formula C₁₈H₂₂Cl₄O₂Si₂, MW 498, CAS# NA, Entry# 44234
\$:28RBRYOHZYNTTMX-UHFFFAOYSA-N



7,8-Epoxylostan-11-ol, 3-acetoxy-
Formula C₃₂H₅₄O₄, MW 502, CAS# NA, Entry# 15359



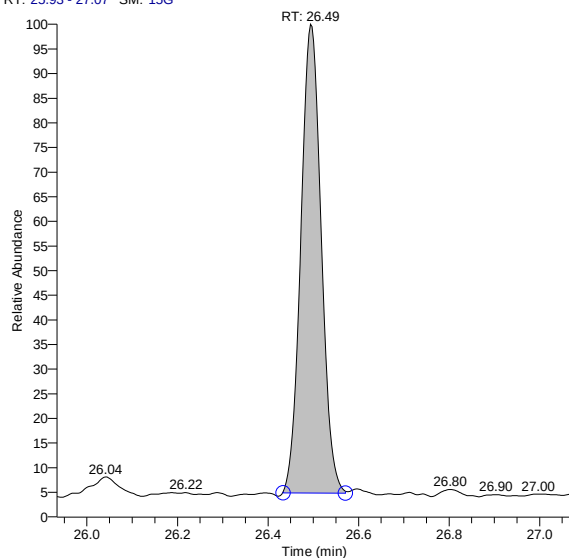
Formula C₂₉H₄₂O₇, MW 502, CAS# 80097-22-9, Entry# 14237



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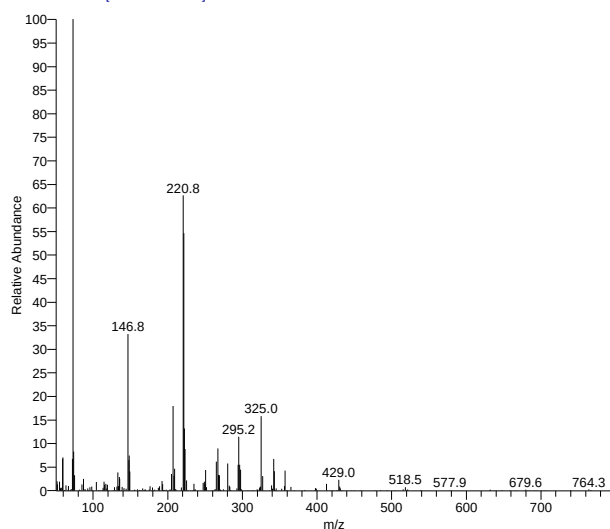
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RT: 25.93 - 27.07 SM: 15G



NL:
1.38E6
TIC: MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

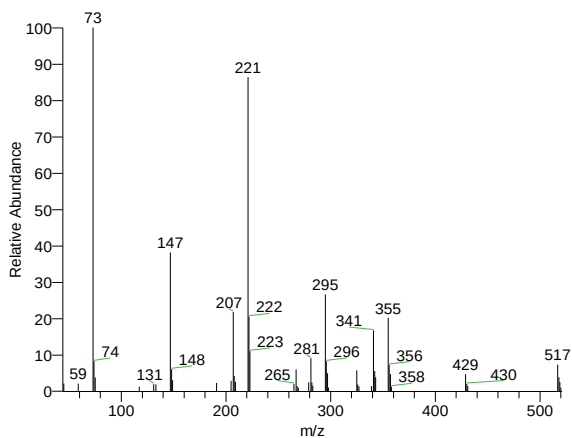
NGA-ZE-WATER1-SAMPLE-INJ1 #6112 RT: 26.49 AV: 1 RF: 6.00, 3 NL: 3.18E5
T: + c EI Full ms [50.000-800.000]



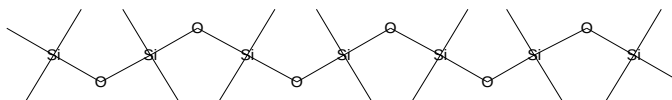
RT	Compound Name	Area	Probability	SI	RSI	Library
26.49	Heptasiloxane, hexadecamethyl-	4097079.02	81.36	652	725	mainlib
26.49	Trisiloxane, octamethyl-	4097079.02	3.60	526	760	mainlib
26.49	3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-	4097079.02	1.85	508	652	mainlib
26.49	Hexasiloxane, tetradecamethyl-	4097079.02	1.57	504	633	mainlib
26.49	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	4097079.02	1.32	500	528	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



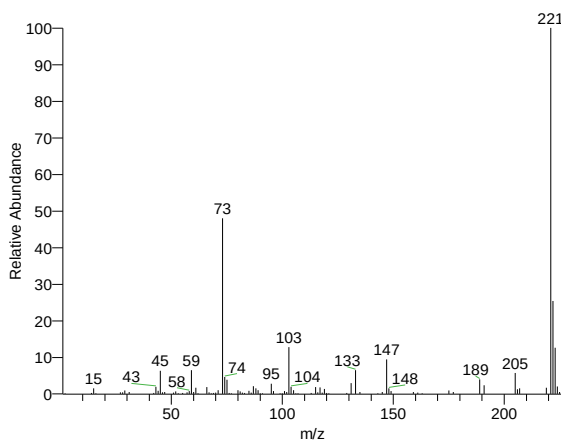
Analysed by Satyanarayana

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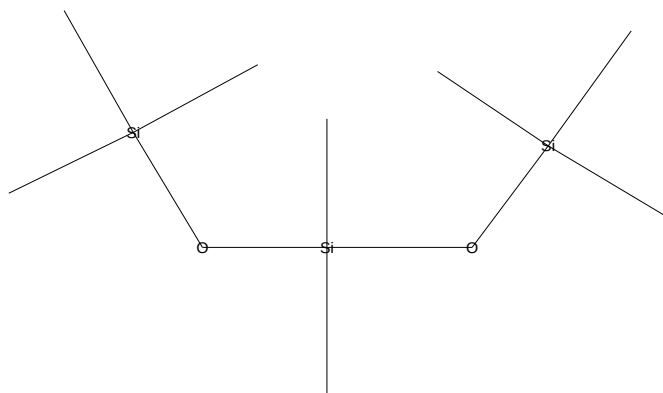
Hit Spectrum

Compound Structure

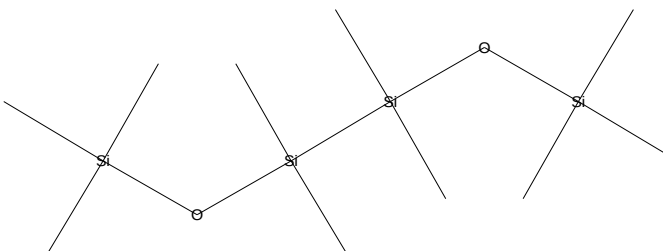
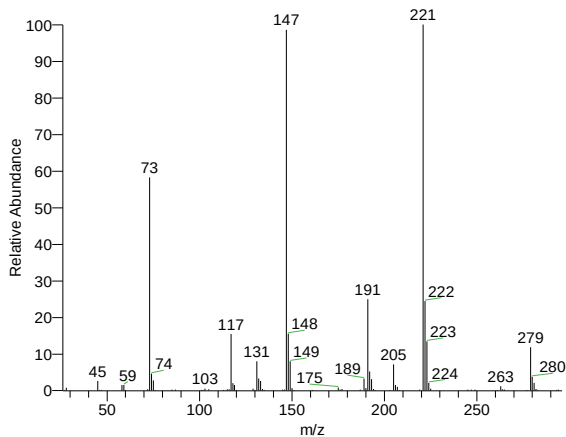
SI 526, RSI 760, mainlib, Entry# 196438, CAS# 107-51-7, Trisiloxane, octamethyl-



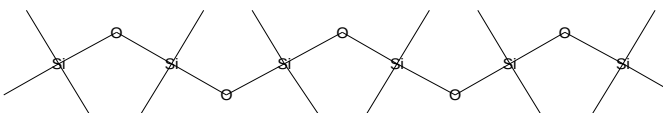
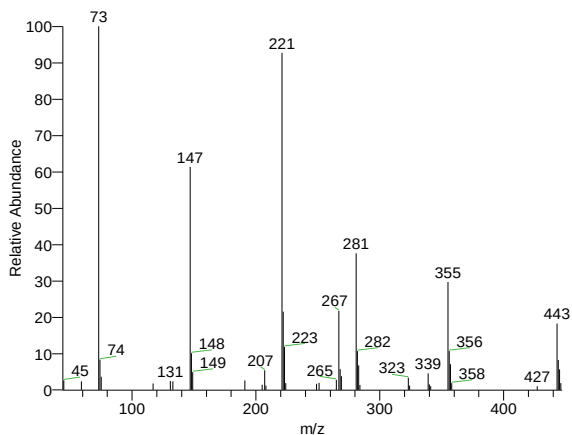
Trisiloxane, octamethyl-
Formula C₈H₂₄O₂Si₃, MW 236, CAS# 107-51-7, Entry# 196438
Octamethyltrisiloxane



3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-
Formula C₁₀H₃₀O₂Si₄, MW 294, CAS# 4342-25-0, Entry# 196522
2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxa-2,4,5,7-tetrasilaoctane #



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane

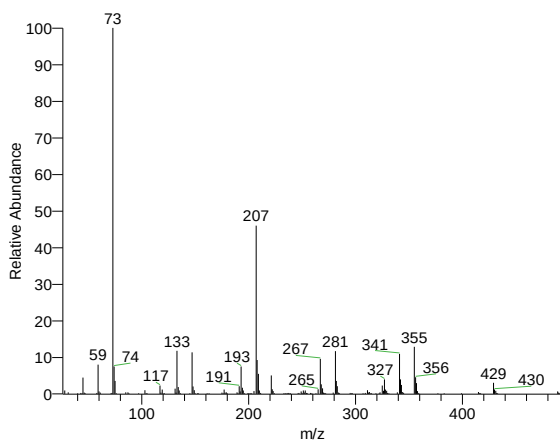


Analysed by Satyanarayana

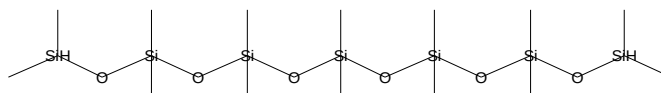
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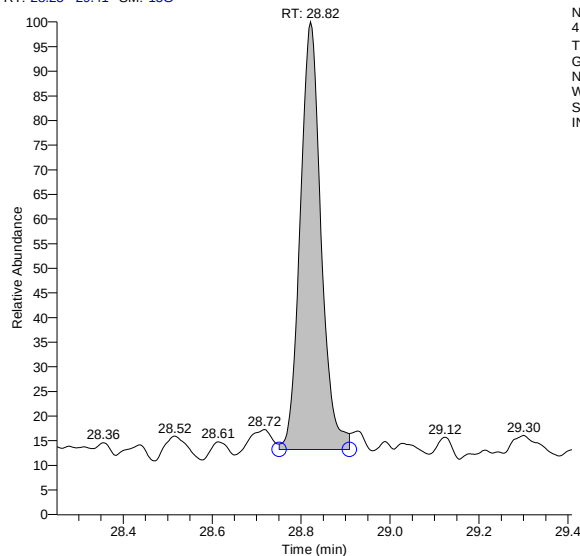
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

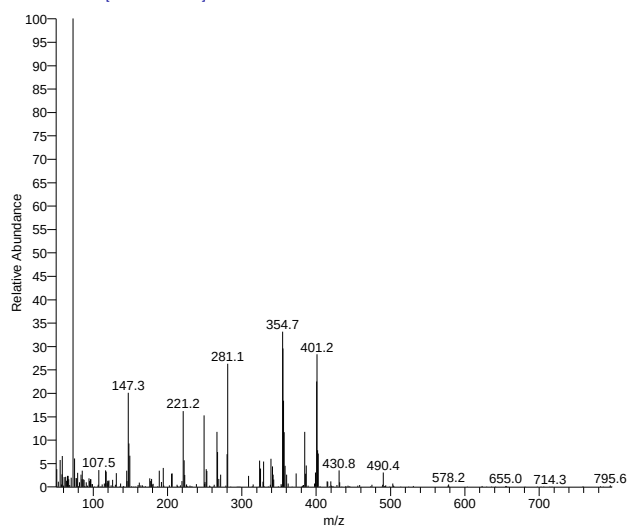


RT: 28.25 - 29.41 SM: 15G



NL:
4.74E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #6806 RT: 28.82 AV: 1 RF: 6.00, 3 NL: 1.12E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
28.82	Cyclooctasiloxane, hexadecamethyl-	1335996.65	64.85	609	673	mainlib
28.82	3,4-Dihydroxyphenylglycol, 4TMS derivative	1335996.65	3.11	486	653	mainlib
28.82	3,4-Dihydroxymandelic acid, ethyl ester, tri-TMS	1335996.65	3.11	486	756	mainlib
28.82	(-)-Epinephrine, 3TMS derivative	1335996.65	2.62	482	608	mainlib
28.82	2,5-Dihydroxybenzoic acid, 3TMS derivative	1335996.65	2.22	478	610	mainlib

Analysed by Satyanarayana

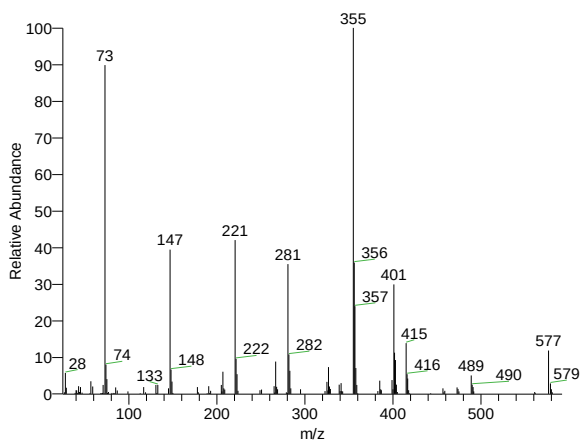
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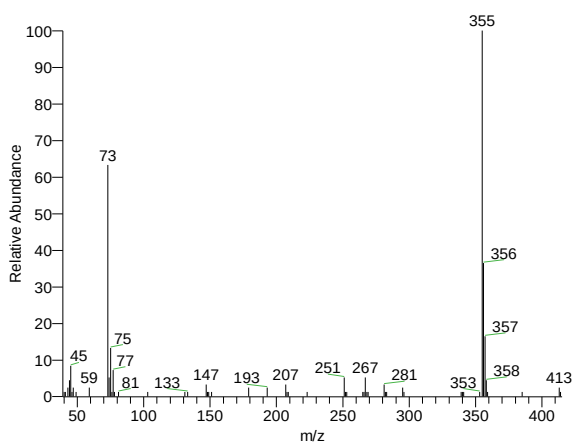
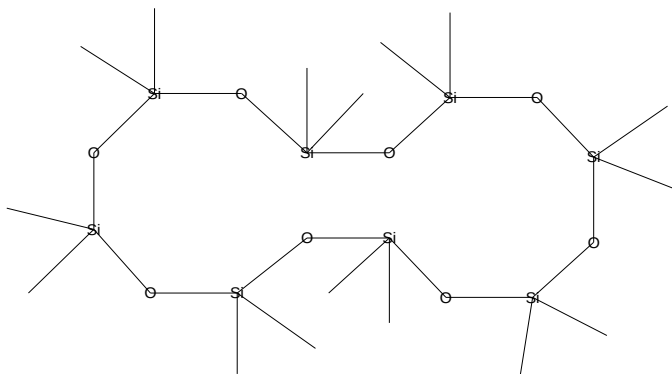
ANALYTICAL CHEMISTRY DIVISION

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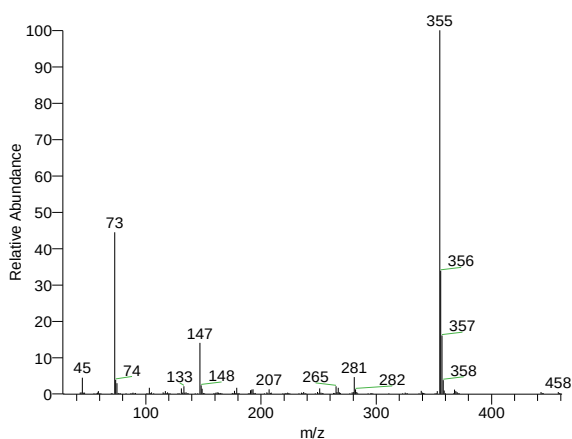
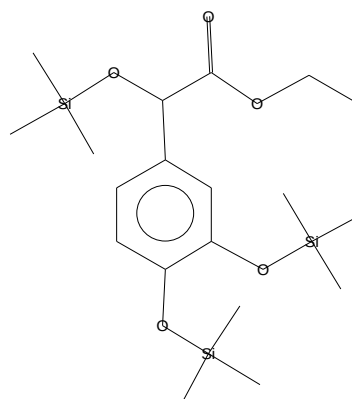
Compound Structure



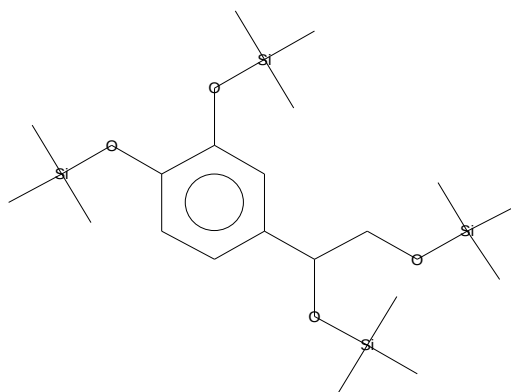
Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane



3,4-Dihydroxymandelic acid, ethyl ester, tri-TMS
Formula C₁₉H₃₆O₅Si₃, MW 428, CAS# NA, Entry# 234280
Ethyl (3,4-bis[(trimethylsilyl)oxy]phenyl)[(trimethylsilyl)oxy]acetate #



3,4-Dihydroxyphenylglycol, 4TMS derivative
Formula C₂₀H₄₂O₄Si₄, MW 458, CAS# 56114-62-6, Entry# 234287
Silane, [[4-[1,2-bis[(trimethylsilyl)oxy]ethyl]-1,2-phenylene]bis(oxy)]bis[trimethyl-

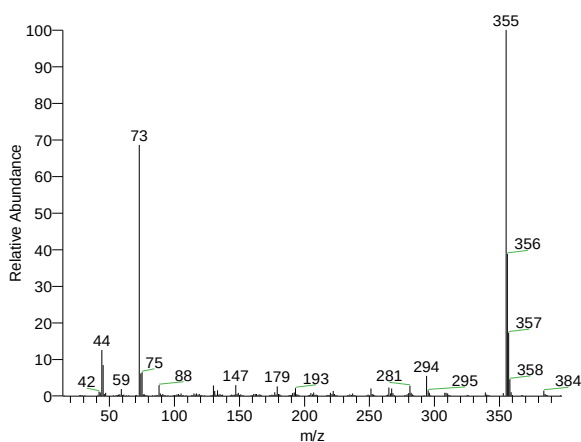


Analysed by Satyanarayana

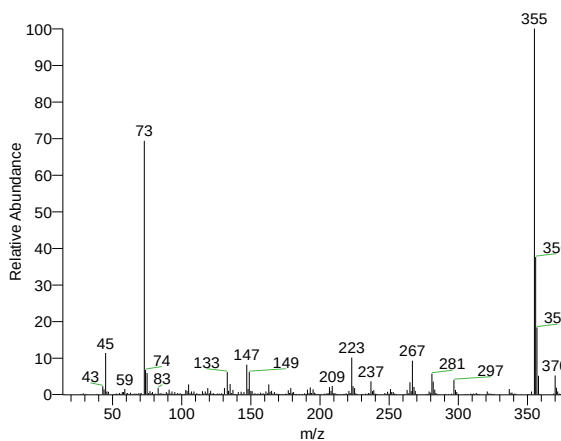
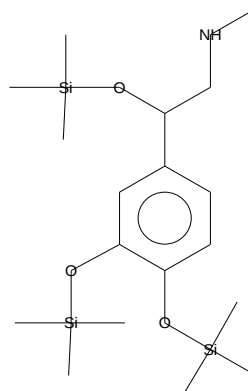
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

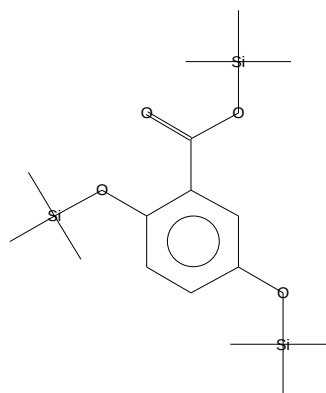
Compound Structure



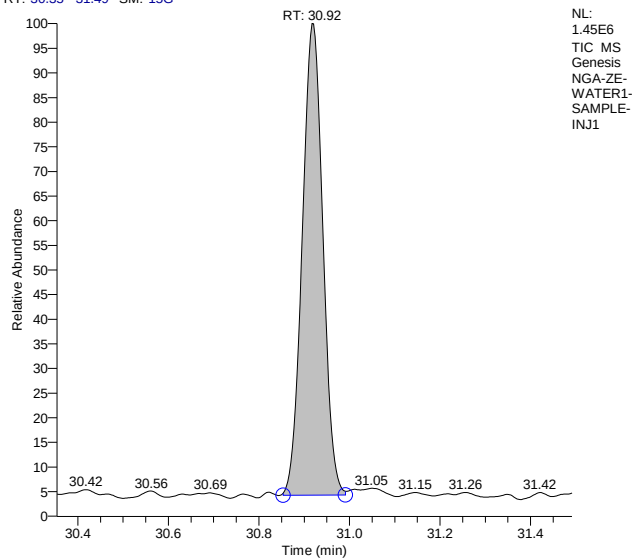
(-)-Epinephrine, 3TMS derivative
Formula C₁₈H₃₇NO₃Si₃, MW 399, CAS# NA, Entry# 234281
(-)-Epinephrine, tris(trimethylsilyl) ether



2,5-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-20-0, Entry# 234286
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester

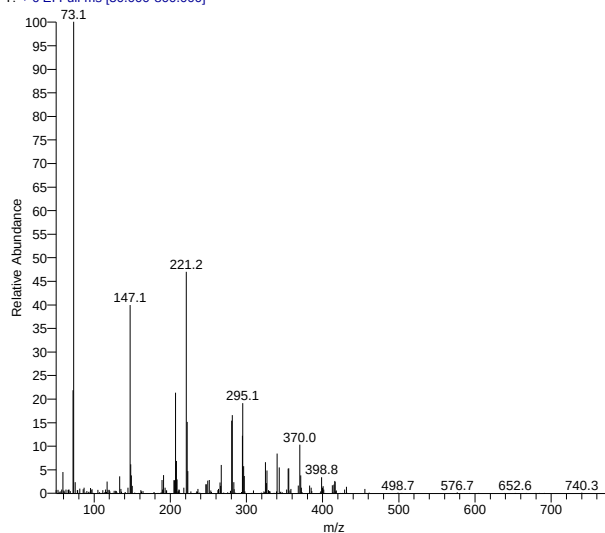


RT: 30.35 - 31.49 SM: 15G



NL:
1.45E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #7431 RT: 30.92 AV: 1 RF: 6.00, 3 NL: 3.47E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
30.92	Heptasiloxane, hexadecamethyl-	4361413.12	56.59	577	728	mainlib

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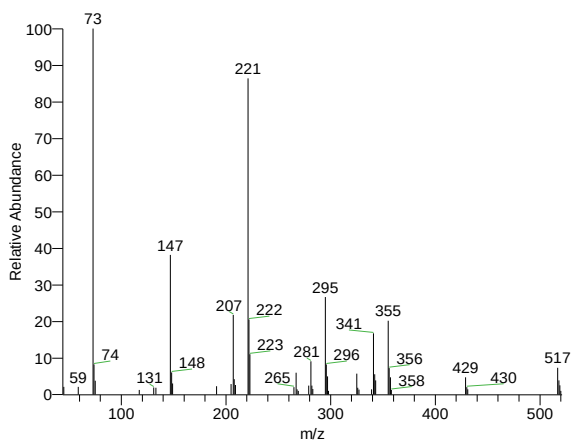
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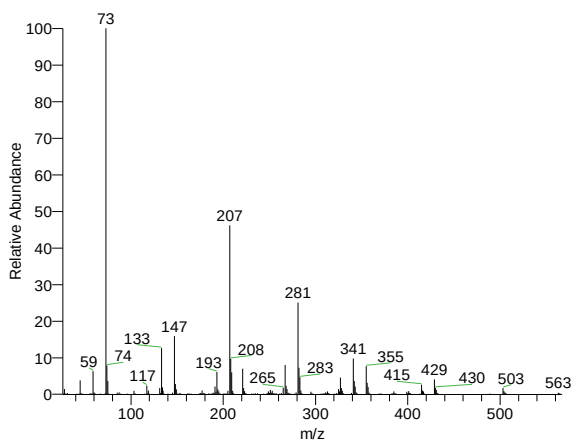
RT	Compound Name	Area	Probability	SI	RSI	Library
30.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	4361413.12	9.29	513	555	mainlib
30.92	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	4361413.12	6.37	502	541	mainlib
30.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	4361413.12	3.67	486	538	mainlib
30.92	4-Hydroxybenzyl alcohol, 2TBDMS derivative	4361413.12	3.67	486	660	mainlib

Hit Spectrum

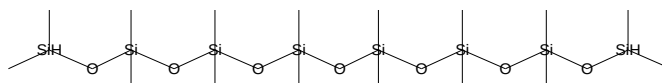
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

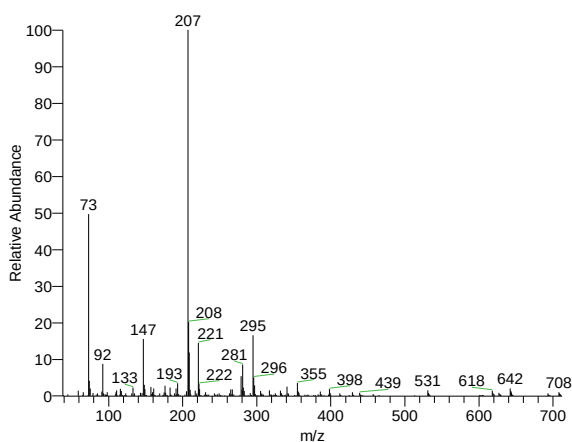
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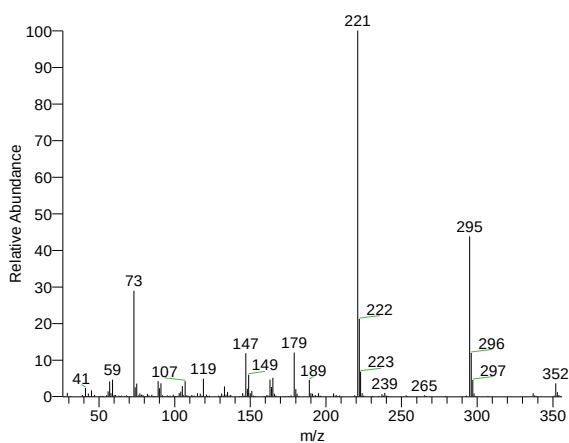
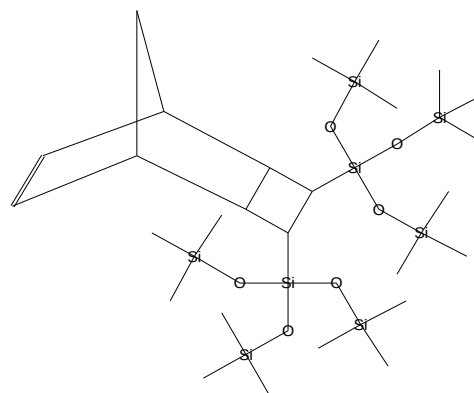
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

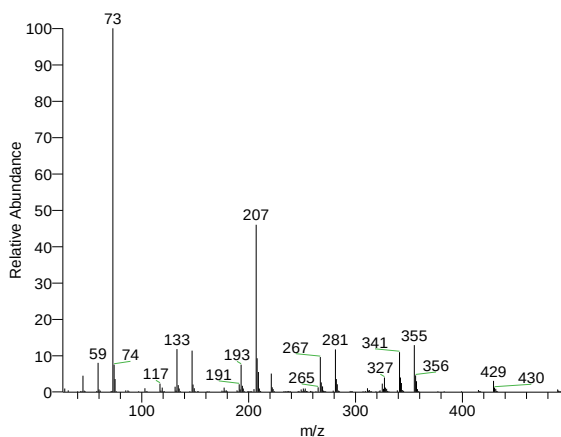
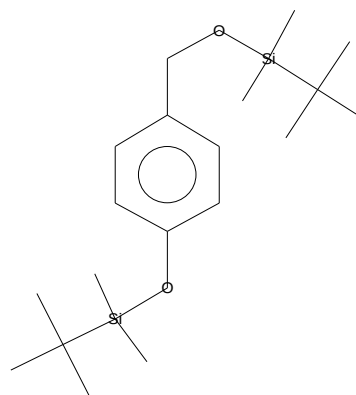
Compound Structure



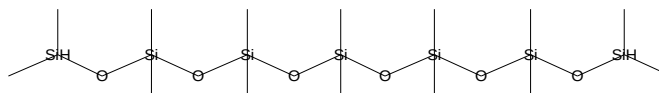
Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:2BJSGSCCAWLAXCNS-UHFFFAOYSA-N



4-Hydroxybenzyl alcohol, 2TBDMS derivative
Formula C₁₉H₃₆O₂Si₂, MW 352, CAS# NA, Entry# 196813
4-Hydroxybenzyl alcohol, bis(tert-butylidimethylsilyl) ether



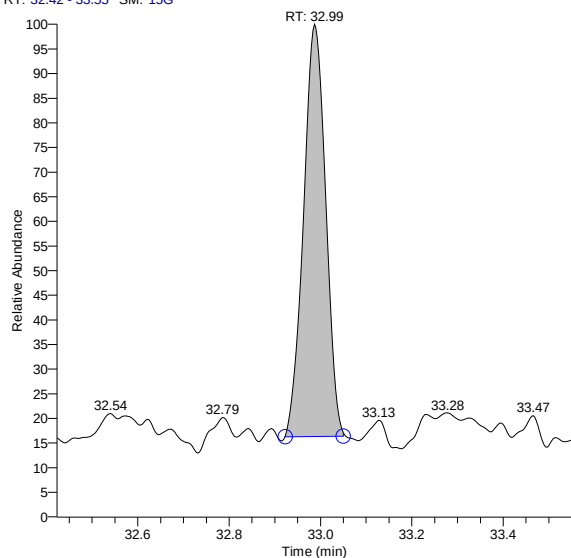
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

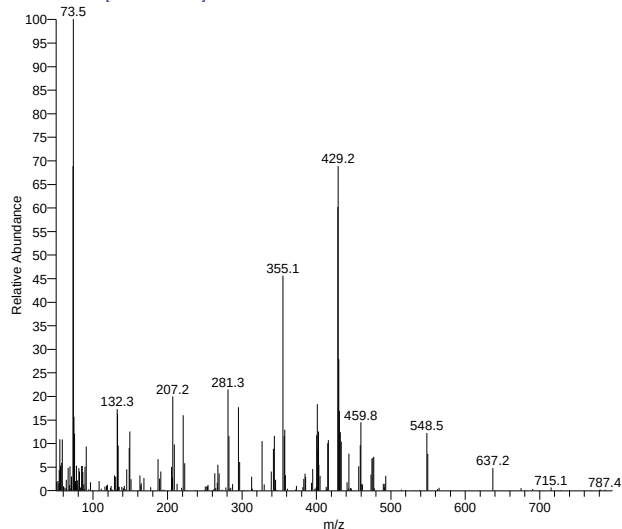
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RT: 32.42 - 33.55 SM: 15G



NL:
4.08E5
TIC: MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

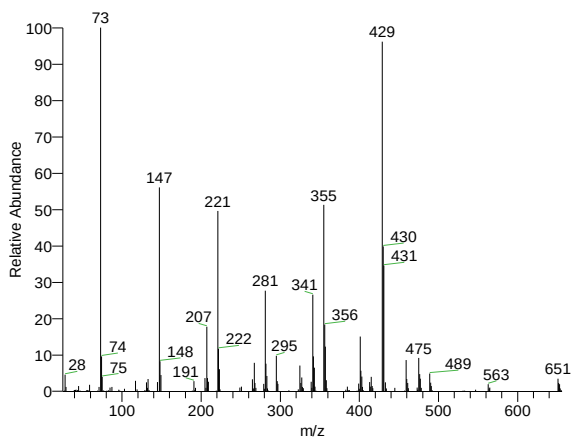
NGA-ZE-WATER1-SAMPLE-INJ1 #8048 RT: 32.99 AV: 1 RF: 6.00, 3 NL: 4.55E4
T: + c EI Full ms [50.000-800.000]



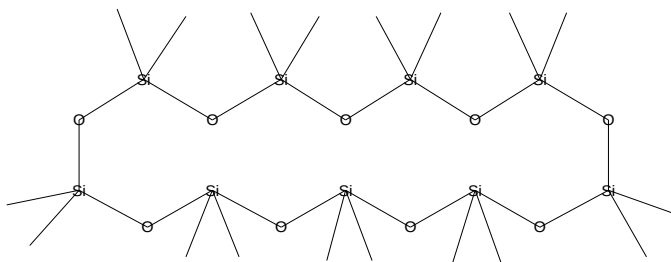
RT	Compound Name	Area	Probability	SI	RSI	Library
32.99	Cyclononasiloxane, octadecamethyl-	1157583.09	79.32	570	637	mainlib
32.99	Oxazepam, 2TMS derivative	1157583.09	9.36	492	559	mainlib
32.99	Cyclodecasiloxane, eicosamethyl-	1157583.09	3.13	468	477	mainlib
32.99	Lorazepam, 2TMS derivative	1157583.09	0.83	436	501	mainlib
32.99	2-(2,6-Bis(tert-butyldimethylsilyl)-3,4-2H-3-pyridyl)isoindoline-1,3-dione	1157583.09	0.77	434	526	mainlib

Hit Spectrum

Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Analysed by Satyanarayana

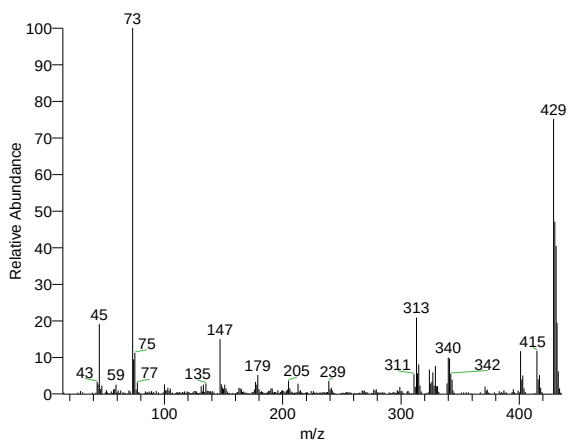
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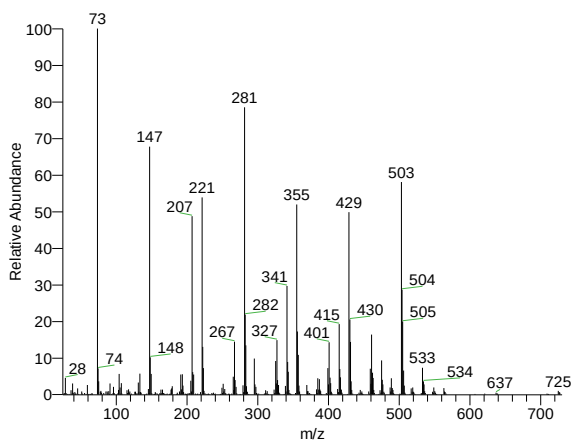
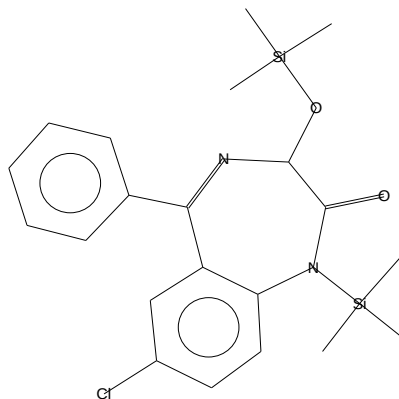
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

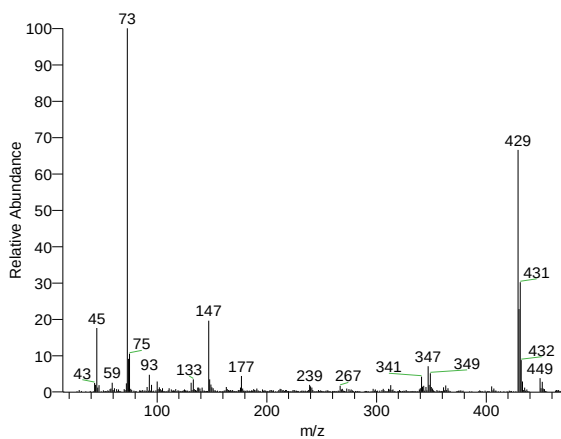
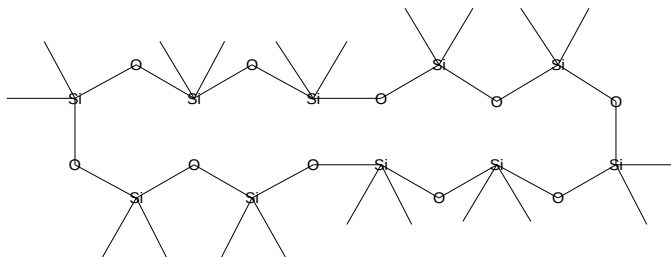
Compound Structure



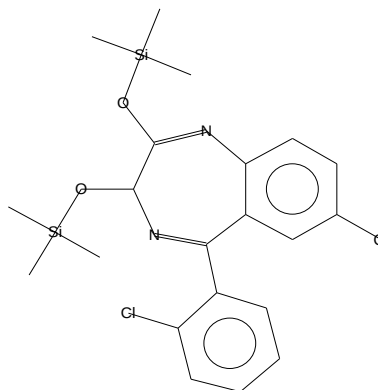
Oxazepam, 2TMS derivative
Formula C₂₁H₂₇ClN₂O₂Si₂, MW 430, CAS# 55319-93-2, Entry# 44302



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Lorazepam, 2TMS derivative
Formula C₂₁H₂₆Cl₂N₂O₂Si₂, MW 464, CAS# 959089-69-1, Entry# 44303
7-Chloro-5-(2-chlorophenyl)-2,3-bis[(trimethylsilyl)oxy]-3H-1,4-benzodiazepine

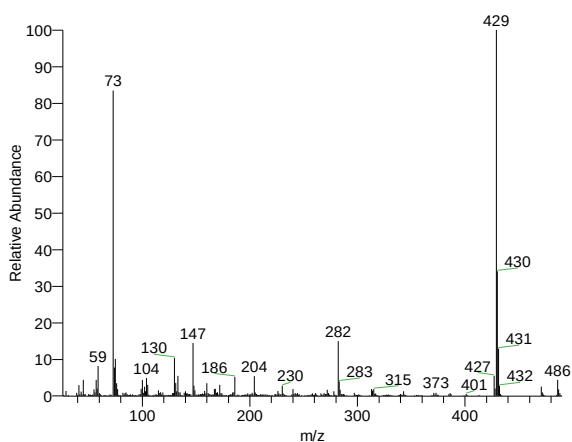


Analysed by Satyanarayana

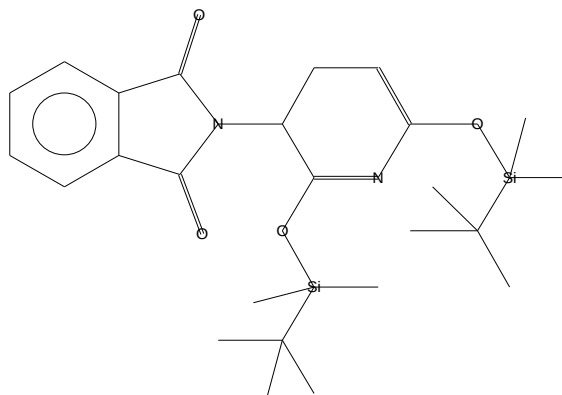
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

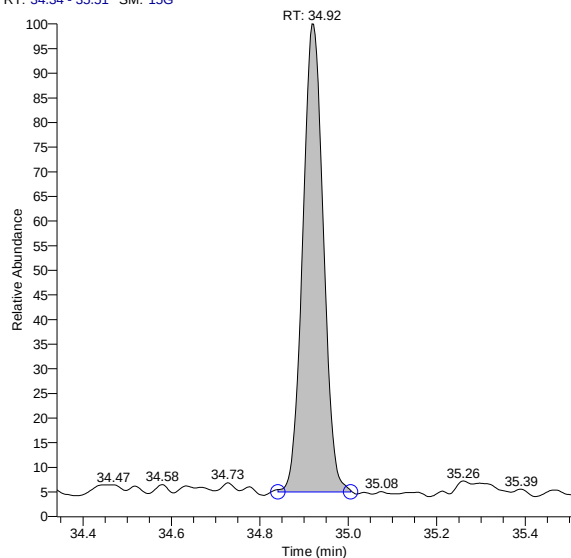
Compound Structure



2-(2,6-Bis(tert-butyl(dimethyl)silyl)-3,4-2H-3-pyridyl)isoindoline-1,3-dione
Formula C₂₅H₃₈N₂O₄Si₂, MW 486, CAS# NA, Entry# 239586
Calmore BDMS

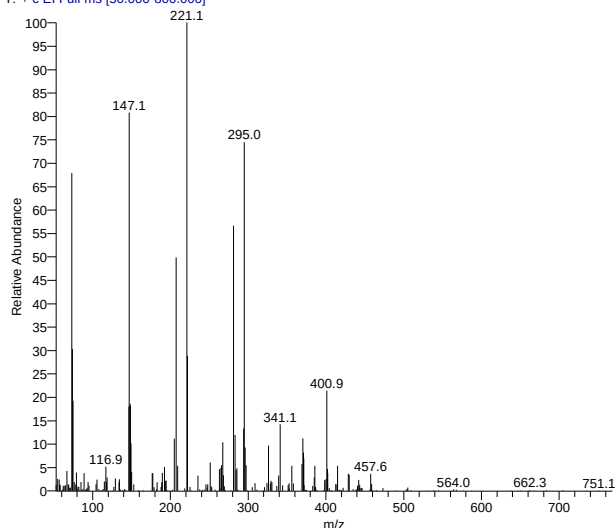


RT: 34.34 - 35.51 SM: 15G



NL:
1.30E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #8624 RT: 34.92 AV: 1 RF: 6.00, 3 NL: 1.18E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
34.92	Heptasiloxane, hexadecamethyl-	4003161.48	52.75	516	676	mainlib
34.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	4003161.48	11.23	471	516	mainlib
34.92	Hexasiloxane, tetradecamethyl-	4003161.48	7.48	459	679	mainlib
34.92	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	4003161.48	2.28	434	532	mainlib
34.92	1,3-Dithiane, 2-butyl-2-[2-(1,3-dithian-2-yl)phenyl]-	4003161.48	2.28	434	667	mainlib

Analysed by Satyanarayana

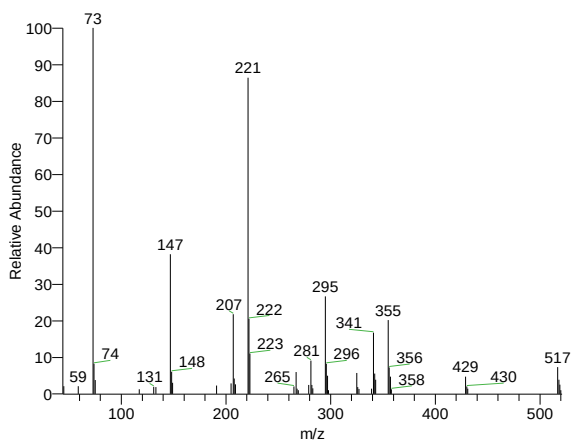
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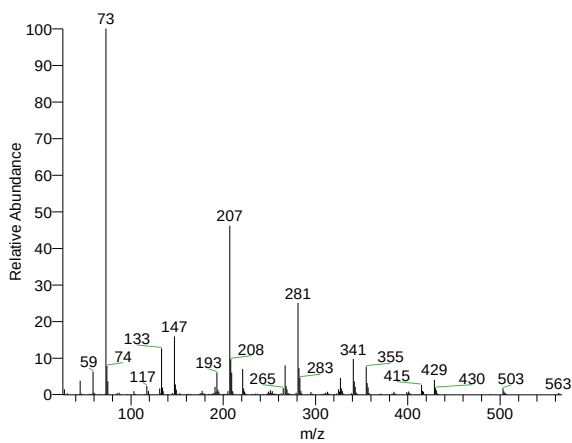
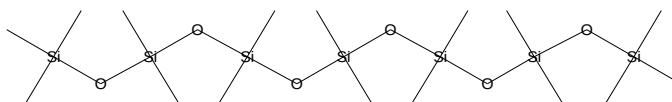
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

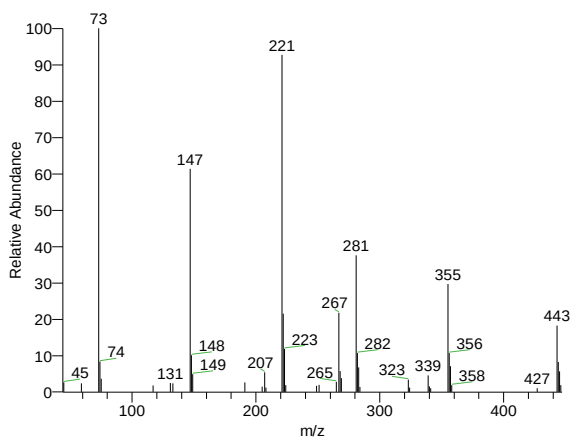
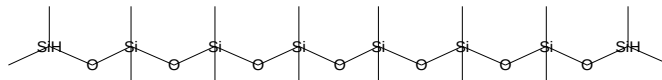
Compound Structure



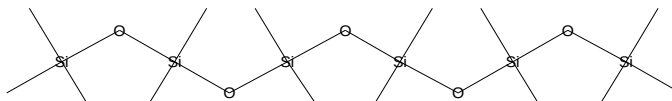
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



Analysed by Satyanarayana

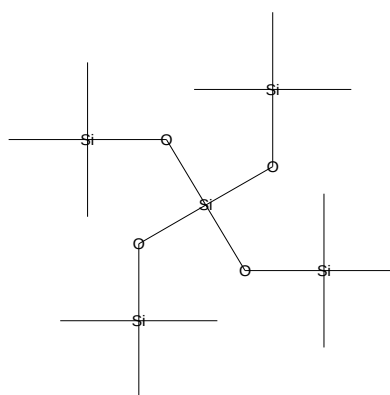
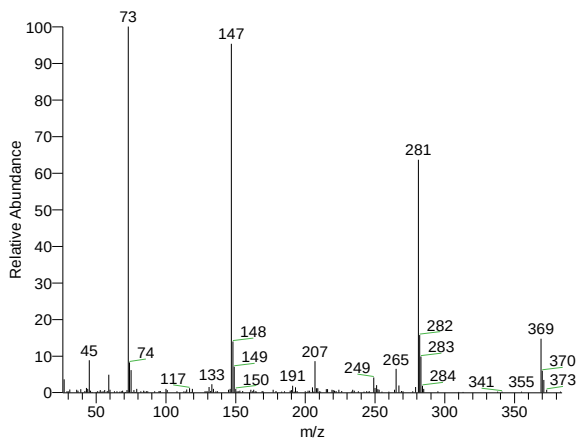
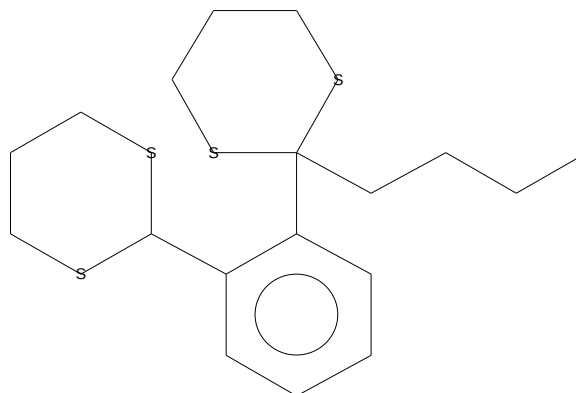
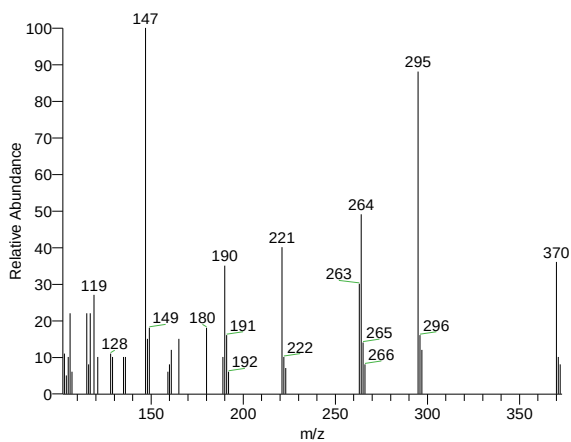
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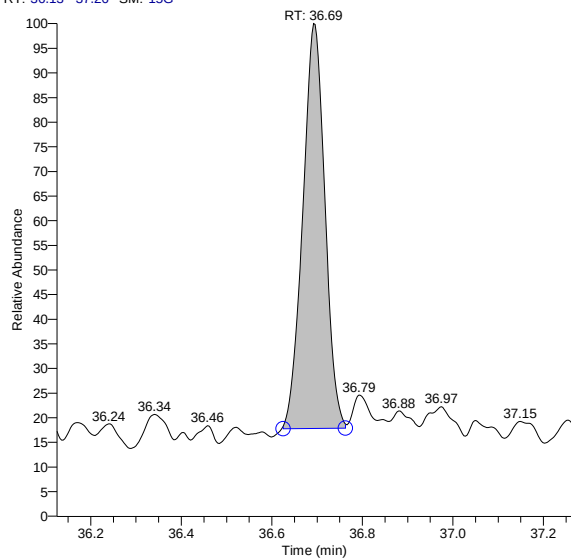
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure

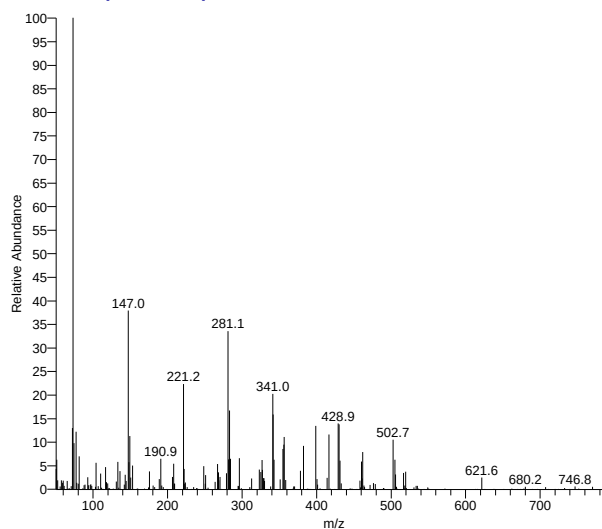


RT: 36.13 - 37.26 SM: 15G



NL:
3.61E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #9153 RT: 36.69 AV: 1 RF: 6.00, 3 NL: 7.34E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
36.69	Cyclodecasiloxane, eicosamethyl-	1004098.94	53.45	573	611	mainlib

Analysed by Satyanarayana

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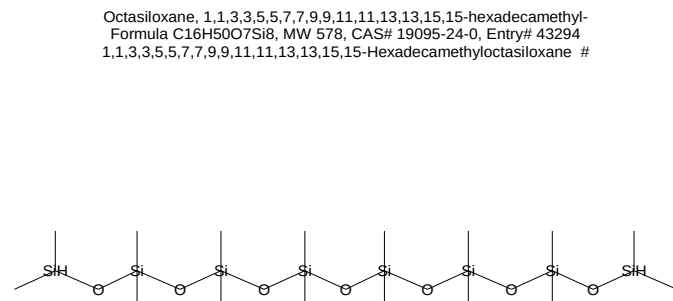
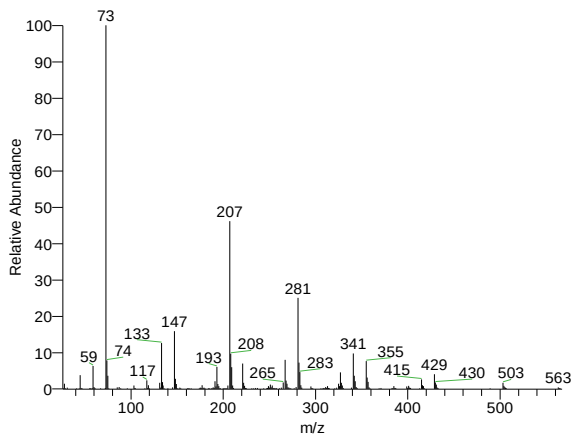
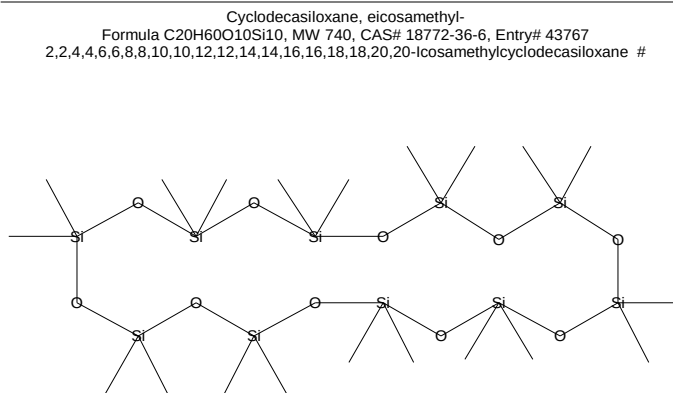
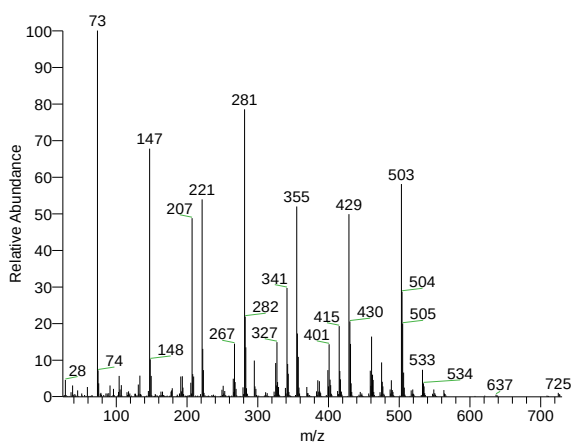
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
36.69	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1004098.94	27.56	555	637	mainlib
36.69	Cyclononasiloxane, octadecamethyl-	1004098.94	5.81	509	605	mainlib
36.69	Heptasiloxane, hexadecamethyl-	1004098.94	3.52	494	665	mainlib
36.69	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1004098.94	3.25	492	599	mainlib

Hit Spectrum

Compound Structure

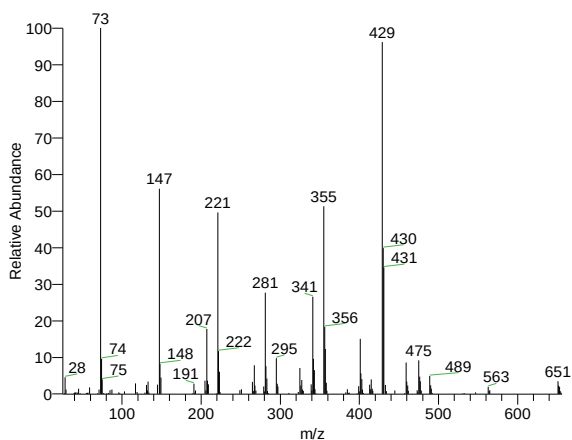


Analysed by Satyanarayana

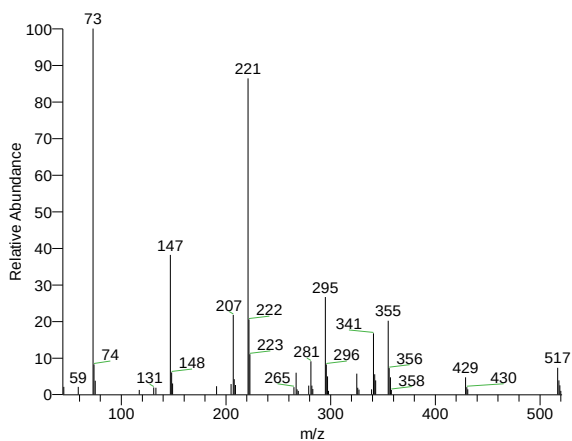
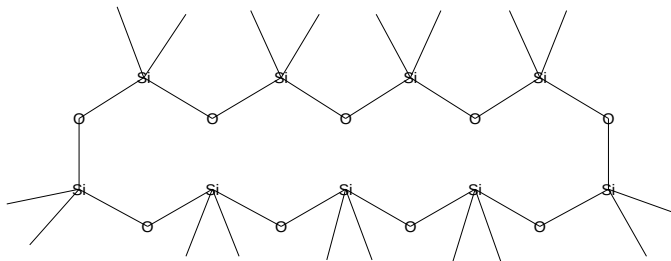
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GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

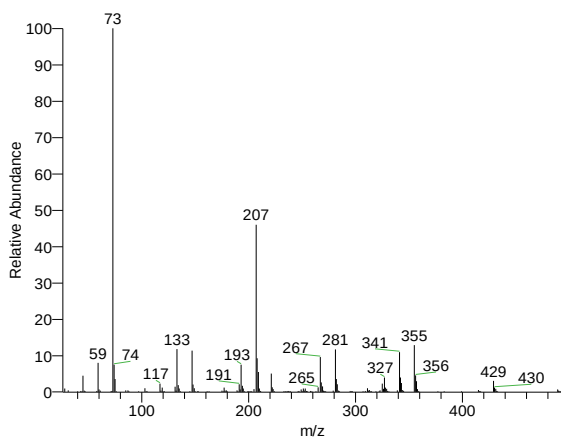
Compound Structure



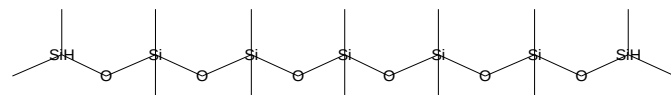
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



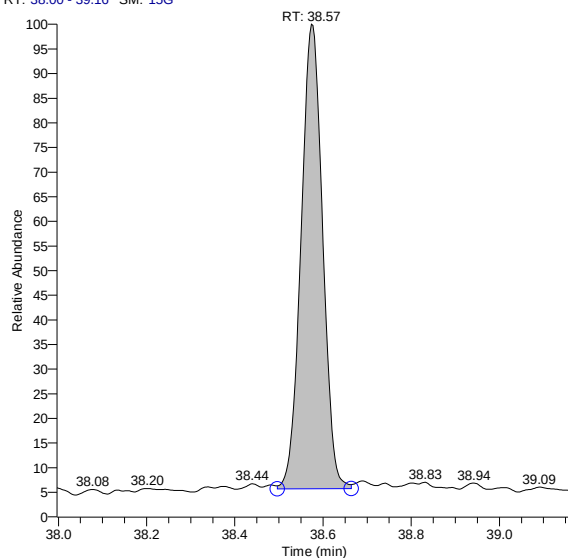
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

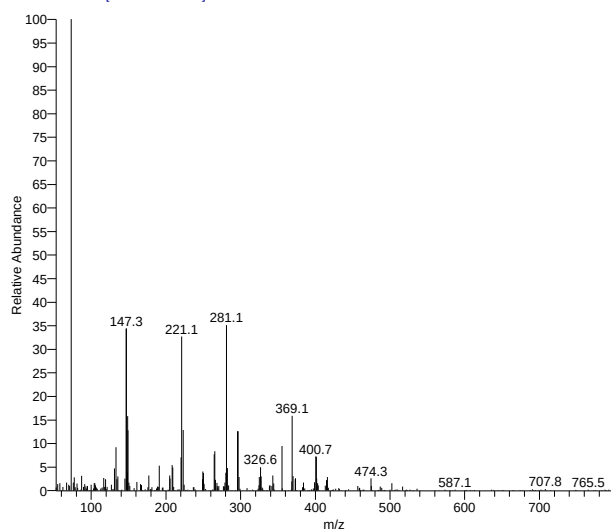
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GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

RT: 38.00 - 39.16 SM: 15G



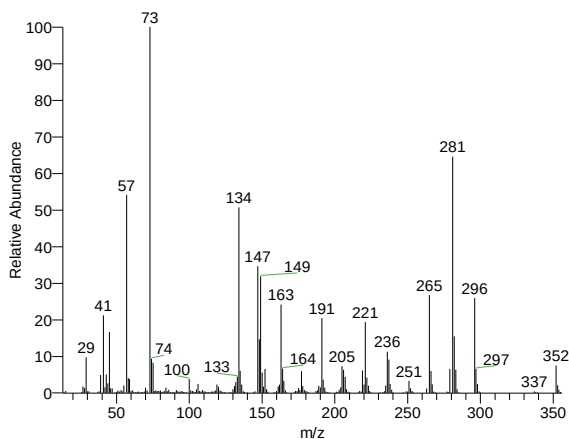
NL:
1.21E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #9714 RT: 38.57 AV: 1 RF: 6.00, 3 NL: 2.16E5
T: + c EI Full ms [50.000-800.000]



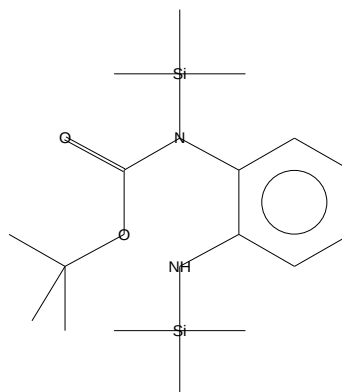
RT	Compound Name	Area	Probability	SI	RSI	Library
38.57	tert-Butyl (2-aminophenyl)carbamate, 2TMS derivative	3870136.40	15.05	462	575	mainlib
38.57	Pentasiloxane, dodecamethyl-	3870136.40	14.47	461	582	mainlib
38.57	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3870136.40	8.33	445	489	mainlib
38.57	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	3870136.40	7.68	443	620	mainlib
38.57	Cyclooctasiloxane, hexadecamethyl-	3870136.40	7.09	441	553	mainlib

Hit Spectrum



Compound Structure

tert-Butyl (2-aminophenyl)carbamate, 2TMS derivative
Formula C₁₇H₃₂N₂O₂Si₂, MW 352, CAS# NA, Entry# 43765
tert-Butyl 2-aminophenylcarbamate ditms



Analysed by Satyanarayana

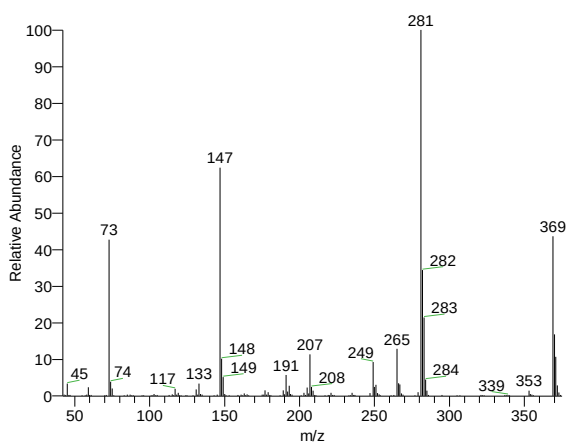
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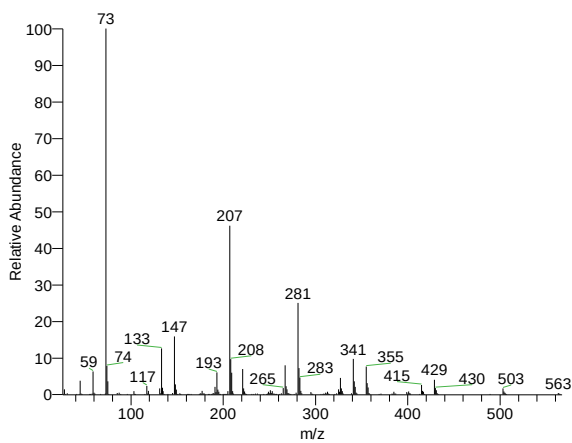
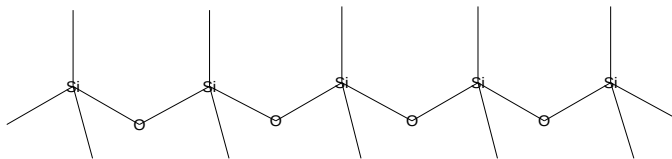
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

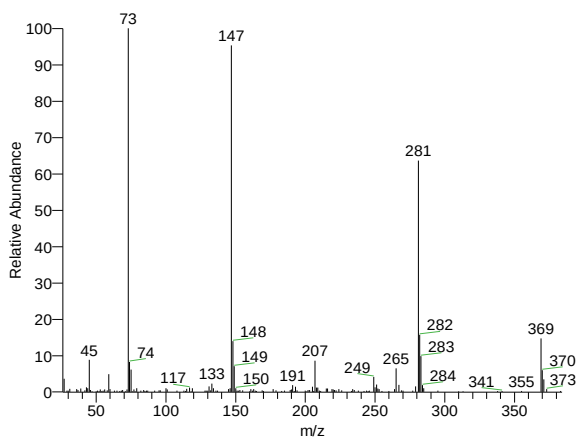
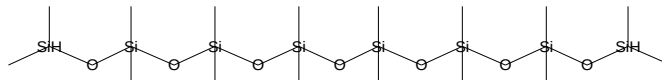
Compound Structure



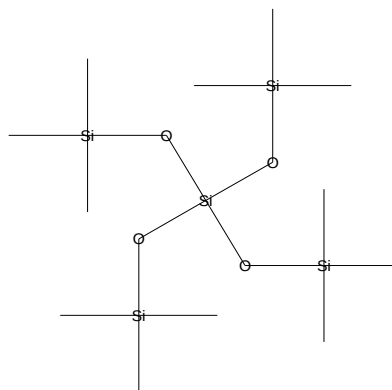
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane

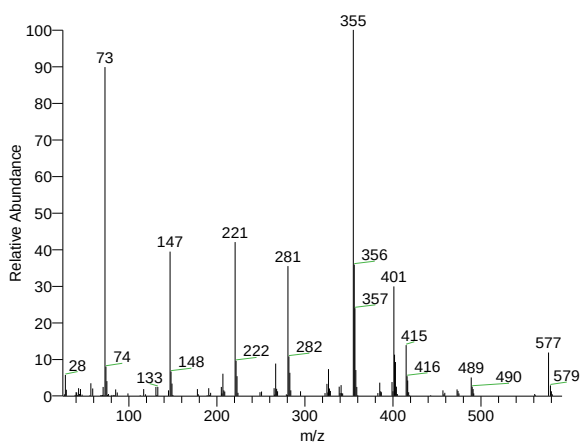


Analysed by Satyanarayana

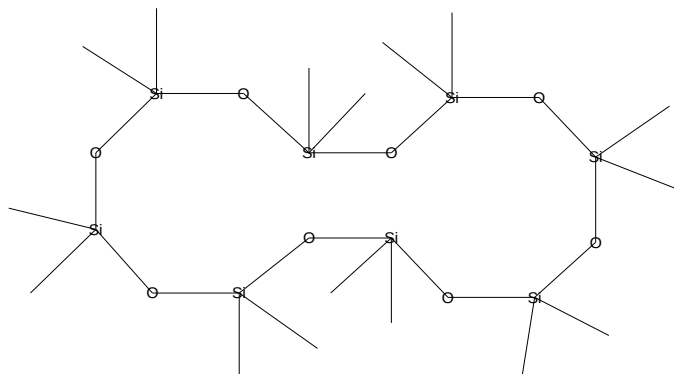
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Hit Spectrum

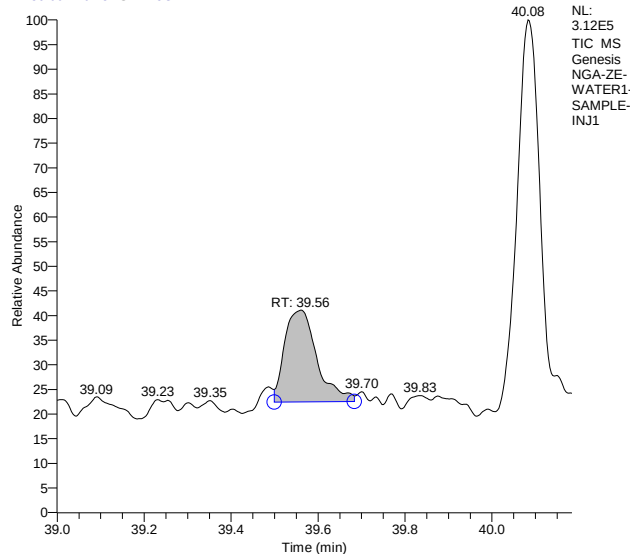
Compound Structure



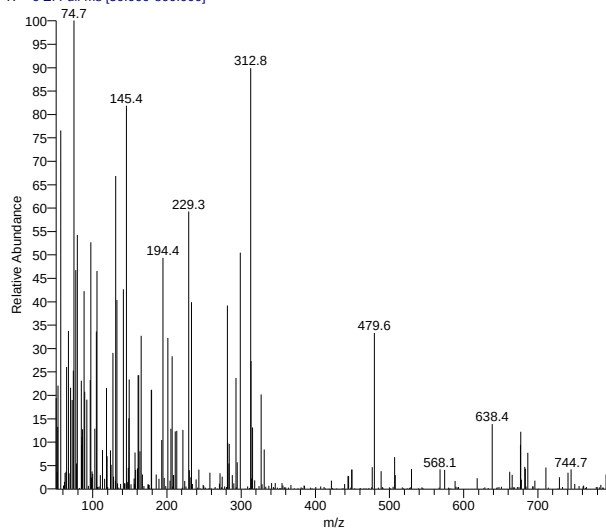
Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane



RT: 39.00 - 40.18 SM: 15G



NGA-ZE-WATER1-SAMPLE-INJ1 #10008 RT: 39.56 AV: 1 RF: 6.00, 3 NL: 8.30E3
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
39.56	2,4,6-Decatrienoic acid, 1a,2,5,5a,6,9,10,10a-octahydro-5,5a-dihydroxy-4-(hydroxymethyl)-1,1,7,9-tetramethyl-11-oxo-1H-2,8a-methanocyclopenta[a]cyclopropana[cyclo]decen-6-yl ester, [1aR-(1a,2a,5a,5a,6a,8a,9a,10a)]-	301292.45	4.33	296	334	mainlib
39.56	Morphinan, 7,8-didehydro-4,5-epoxy-3,6-dimethoxy-17-methyl-, (5a,6a)-	301292.45	3.05	286	373	mainlib
39.56	2-Methoxy-4-nitrophenyl 3-trifluoromethylphenyl ether	301292.45	2.34	279	368	mainlib

Analysed by Satyanarayana

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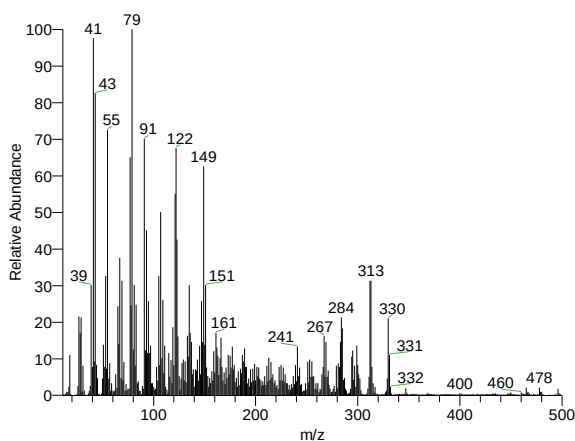
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

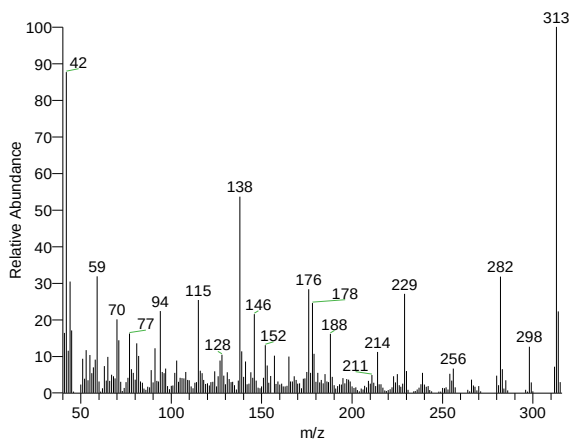
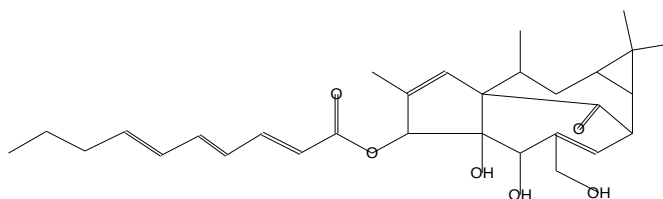
RT	Compound Name	Area	Probability	SI	RSI	Library
39.56	Hexadecanoic acid, 1-[[[(2-aminoethoxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl ester	301292.45	2.07	276	311	mainlib
39.56	2,7:3,6-Dimethanonaphth[2,3-b]oxirene, 3,4,6,9,9-pentachloro-1a,2,2a,3,6,6a,7,7a-octahydro-, (1aà,2á,2aá,3á,6á,6aá,7á,7aà)-	301292.45	2.07	276	336	mainlib

Hit Spectrum

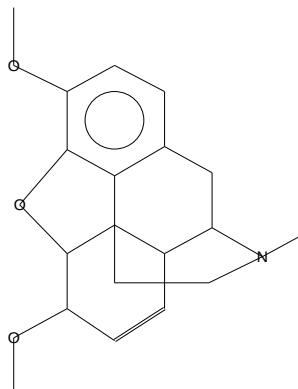
Compound Structure



Formula C30H40O6, MW 496, CAS# 52557-28-5, Entry# 48499
\$:28XIQPHOZUEKAYJG-GTEMLCSVSA-N



Morphinan, 7,8-didehydro-4,5-epoxy-3,6-dimethoxy-17-methyl-, (5à,6à)-
Formula C19H23NO3, MW 313, CAS# 2859-16-7, Entry# 227615
Morphinan, 7,8-didehydro-4,5à-epoxy-3,6à-dimethoxy-17-methyl-

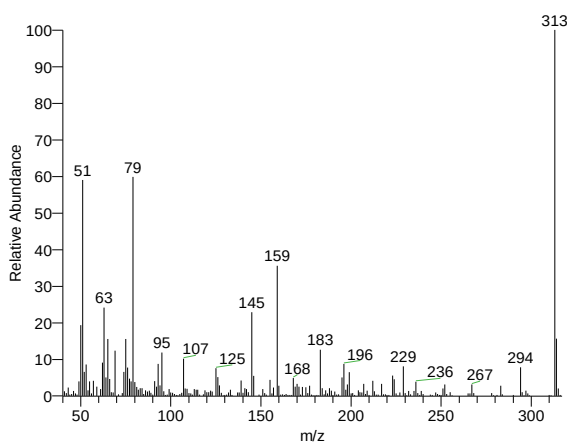


Analysed by Satyanarayana

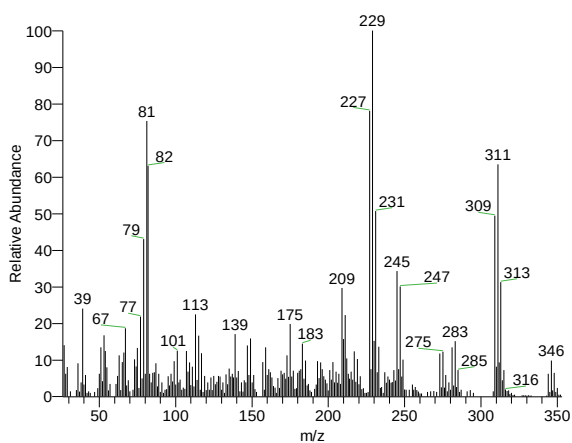
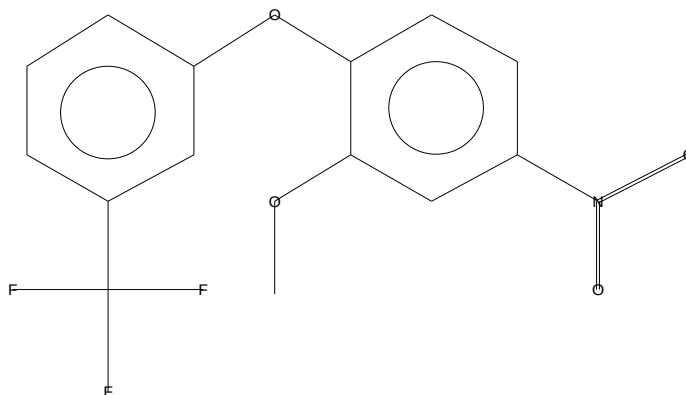
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Hit Spectrum

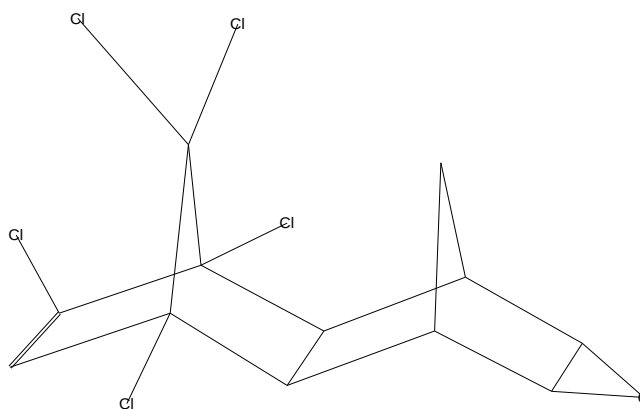
Compound Structure



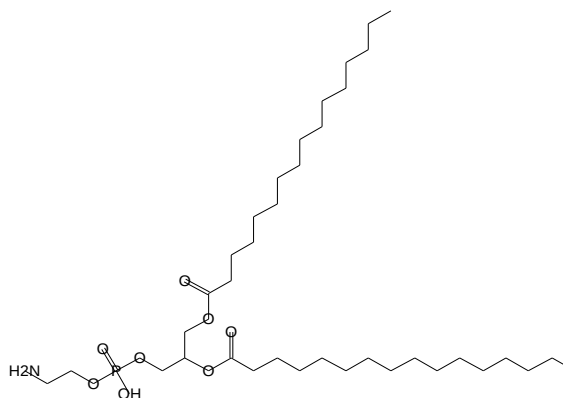
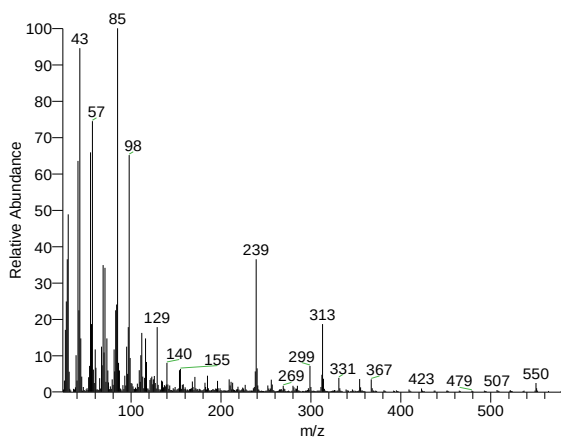
2-Methoxy-4-nitrophenyl 3-trifluoromethylphenyl ether
Formula C₁₄H₁₀F₃NO₄, MW 313, CAS# NA, Entry# 227664
2-Methoxy-4-nitro-1-[3-(trifluoromethyl)phenoxy]benzene #



Formula C₁₂H₉Cl₅O, MW 344, CAS# 33487-96-6, Entry# 200505
\$:28MKVOLIOOHSQALO-UHFFFAOYSA-N



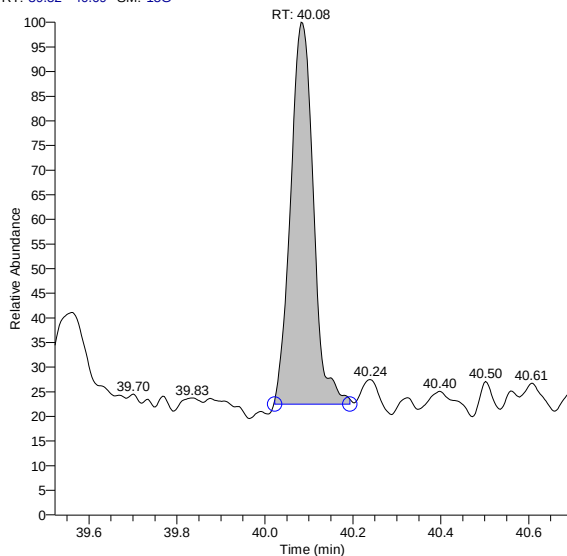
Hexadecanoic acid, 1-[[[(2-aminoethoxy)hydroxyphosphinyl]oxy]methyl]-1,2-ethanediyl ester
Formula C₃₇H₇₄NO₈P, MW 691, CAS# 3026-45-7, Entry# 54704
Palmitin, 1,2-di-, 2-aminoethyl hydrogen phosphate



Analysed by Satyanarayana

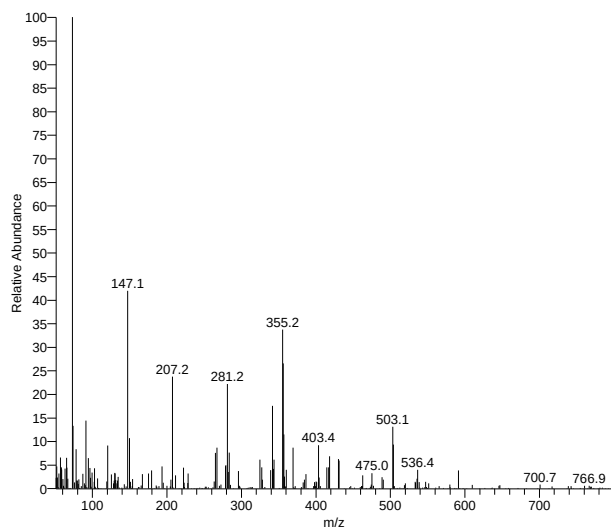
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RT: 39.52 - 40.69 SM: 15G



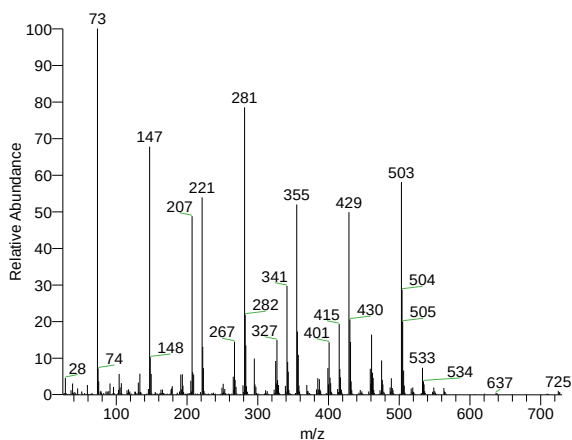
NL:
3.12E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #10164 RT: 40.08 AV: 1 RF: 6.00, 3 NL: 5.29E4
T: + c EI Full ms [50.000-800.000]



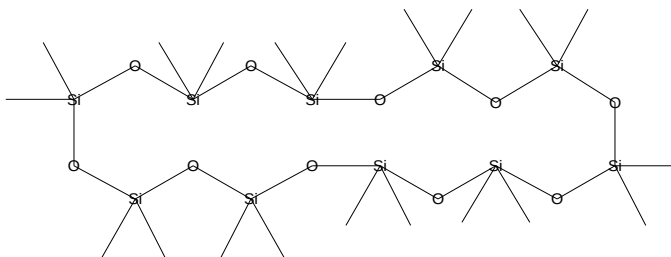
RT	Compound Name	Area	Probability	SI	RSI	Library
40.08	Cyclodecasiloxane, eicosamethyl-	871749.55	58.19	509	540	mainlib
40.08	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	871749.55	14.92	475	556	mainlib
40.08	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	871749.55	3.74	440	592	mainlib
40.08	Cyclooctasiloxane, hexadecamethyl-	871749.55	2.41	427	586	mainlib
40.08	2,4-Dihydroxybenzoic acid, 3TMS derivative	871749.55	1.51	413	554	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Analysed by Satyanarayana

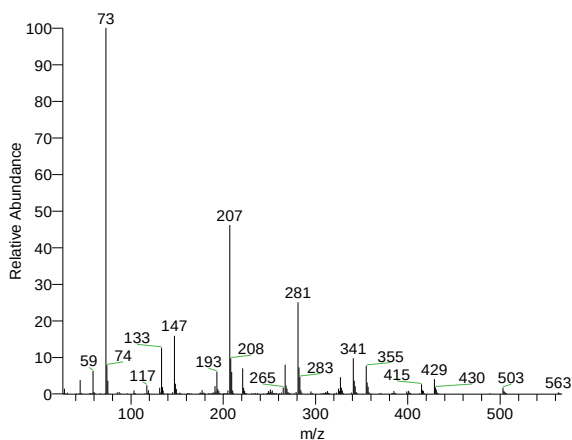
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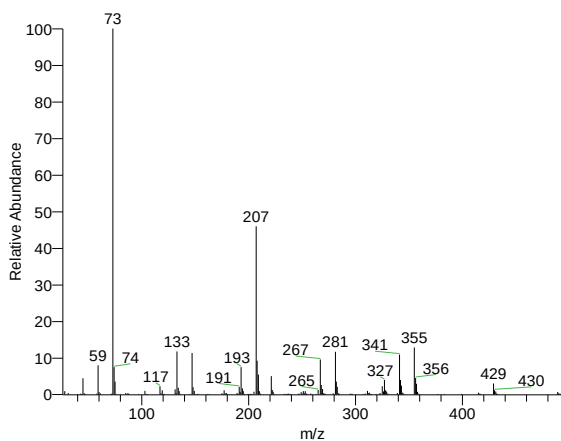
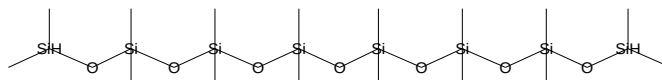
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

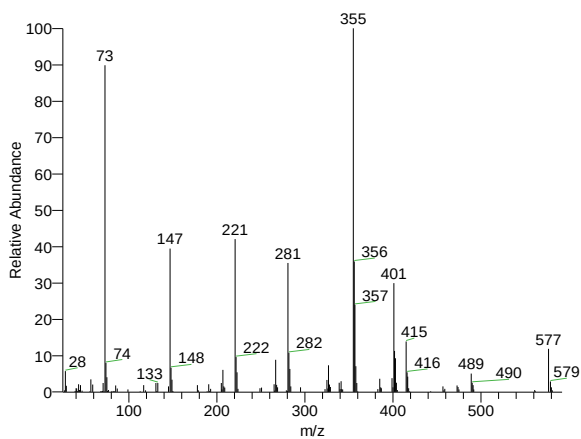
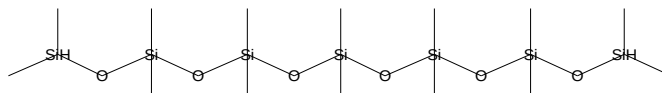
Compound Structure



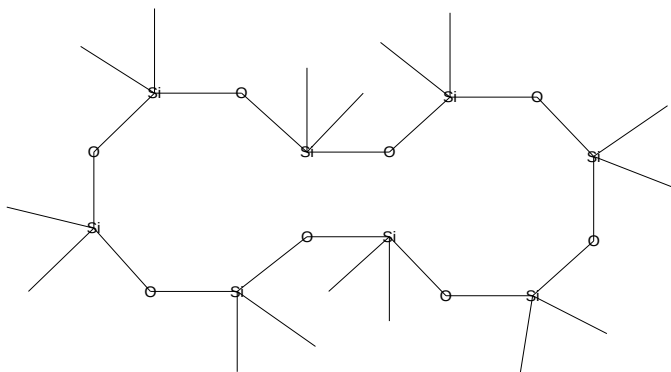
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclooctasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₈Si₈, MW 592, CAS# 556-68-3, Entry# 234277
Hexadecamethyl-cyclooctasiloxane

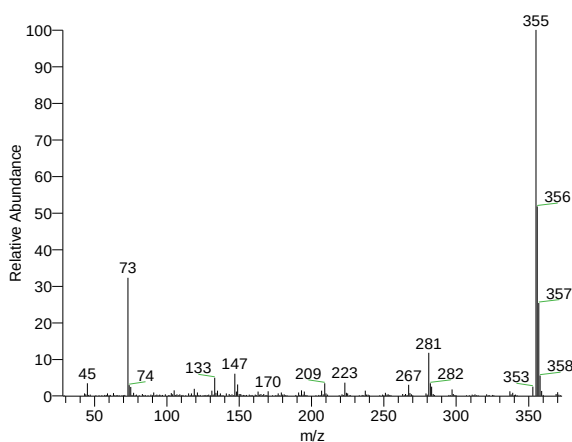


Analysed by Satyanarayana

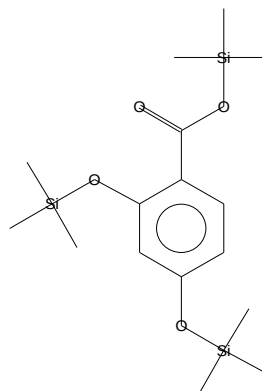
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
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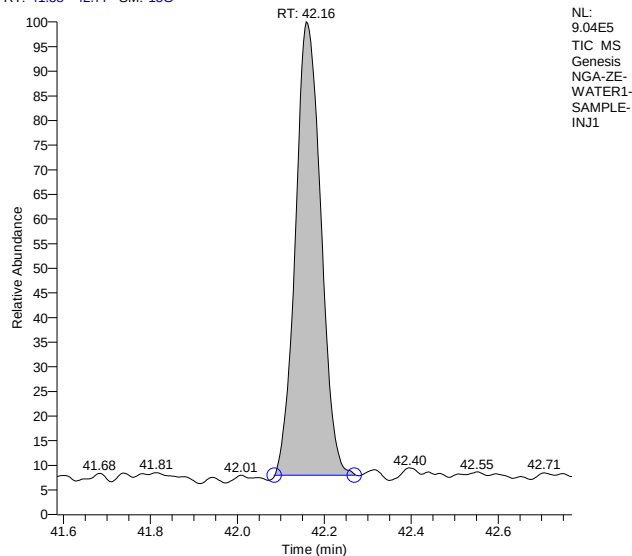
Compound Structure



2,4-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 10586-16-0, Entry# 234374
Benzoic acid, 2,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

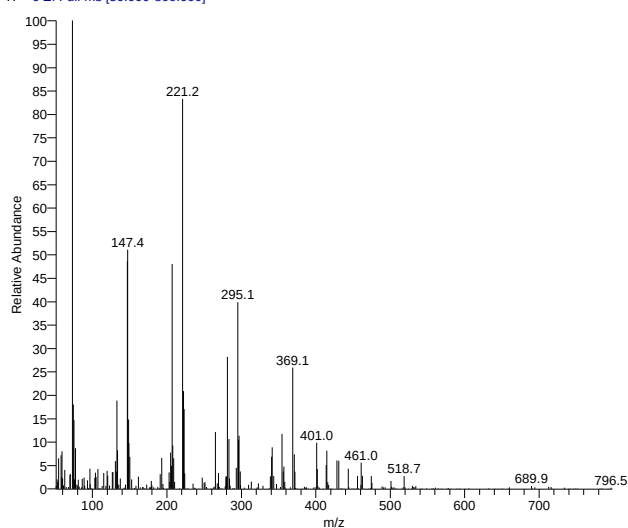


RT: 41.58 - 42.77 SM: 15G



NL:
9.04E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #10783 RT: 42.16 AV: 1 RF: 6.00, 3 NL: 9.99E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
42.16	Heptasiloxane, hexadecamethyl-	3379575.26	64.38	592	778	mainlib
42.16	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3379575.26	11.21	531	589	mainlib
42.16	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3379575.26	3.36	505	598	mainlib
42.16	Hexasiloxane, tetradecamethyl-	3379575.26	3.36	505	729	mainlib
42.16	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3379575.26	2.70	500	601	mainlib

Analysed by Satyanarayana

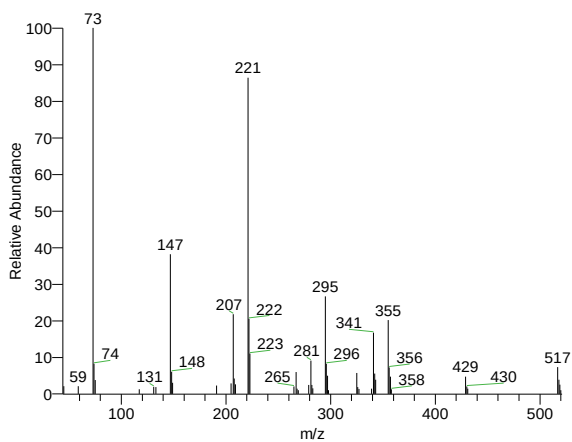
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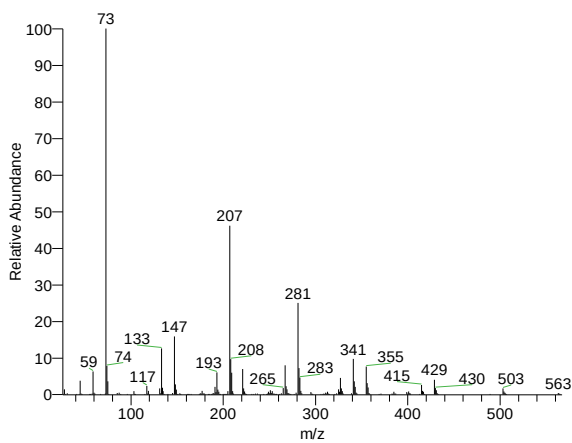
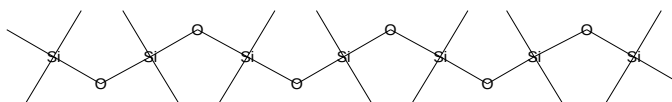
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

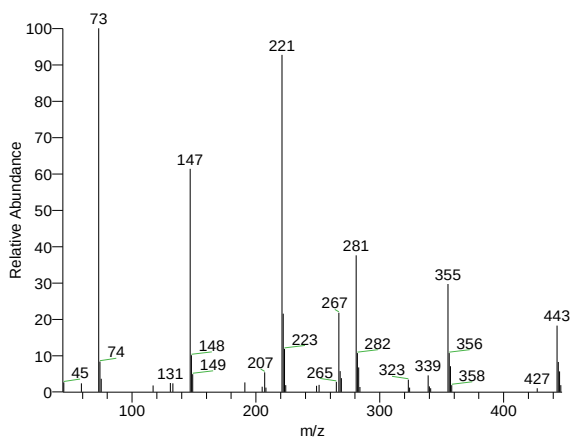
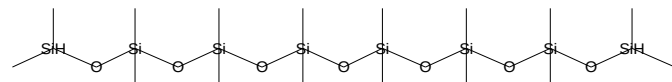
Compound Structure



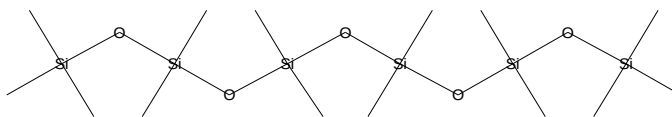
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



Analysed by Satyanarayana

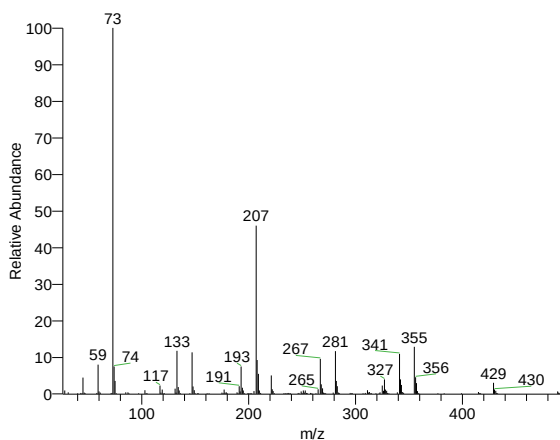
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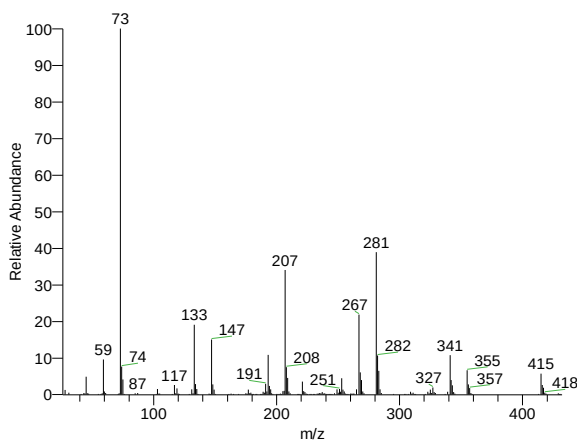
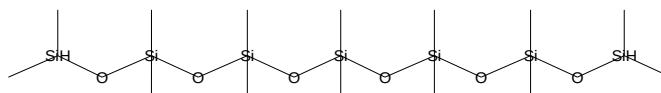
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

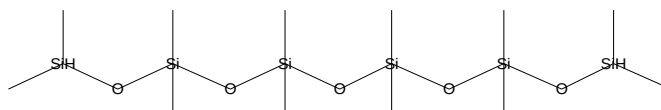
Compound Structure



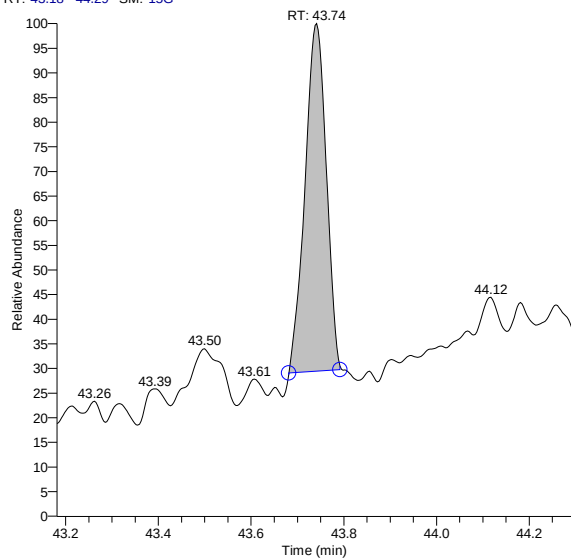
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

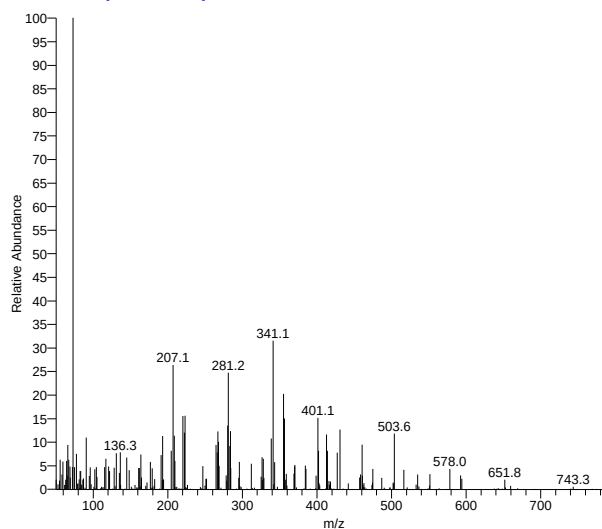


RT: 43.18 - 44.29 SM: 15G



NL:
3.34E5
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #11255 RT: 43.74 AV: 1 RF: 6.00, 3 NL: 4.75E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
43.74	Cyclodecasiloxane, eicosamethyl-	751977.63	45.23	430	461	mainlib

Analysed by Satyanarayana

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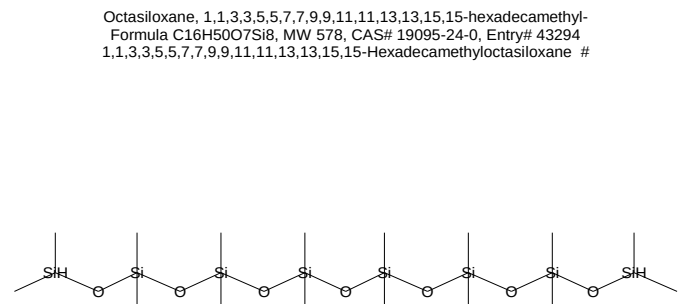
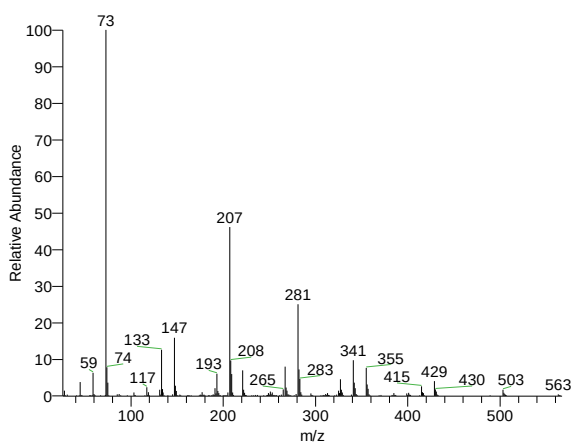
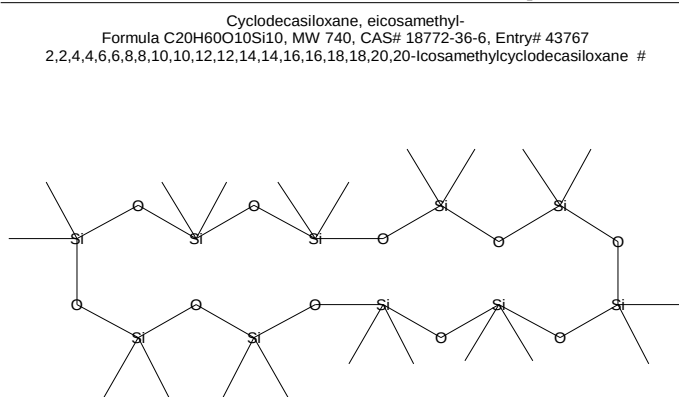
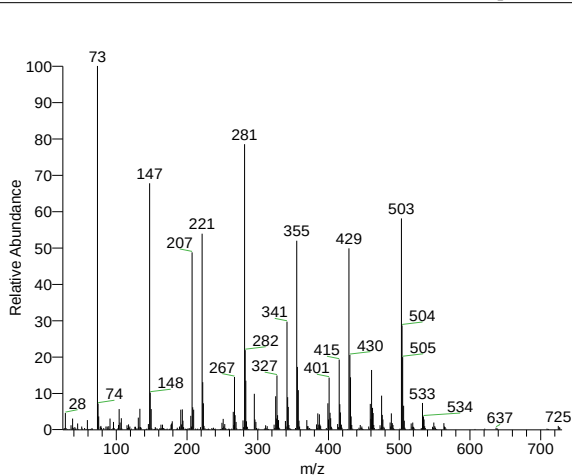
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
43.74	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	751977.63	12.57	400	506	mainlib
43.74	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	751977.63	3.76	374	525	mainlib
43.74	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	751977.63	3.62	373	550	mainlib
43.74	Cyclononasiloxane, octadecamethyl-	751977.63	2.41	361	443	mainlib

Hit Spectrum

Compound Structure



Analysed by Satyanarayana

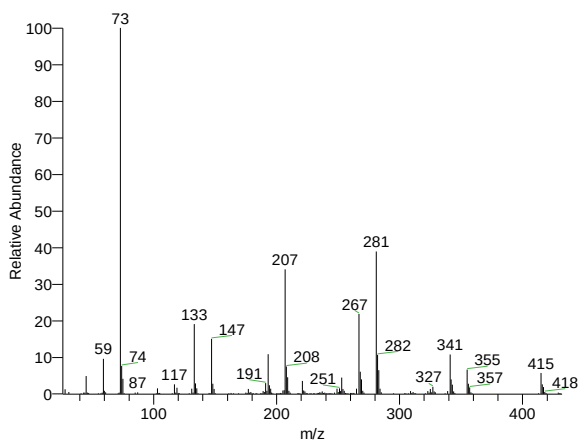
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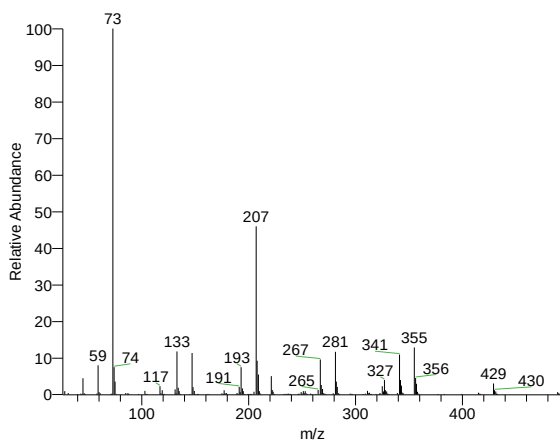
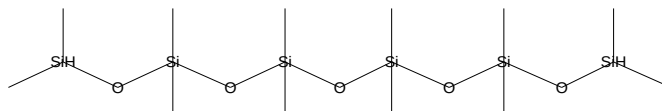
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

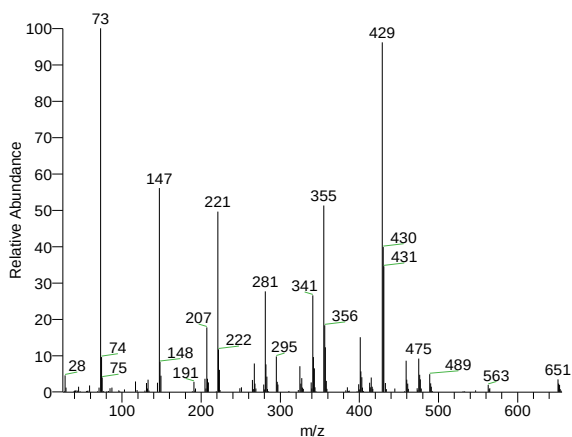
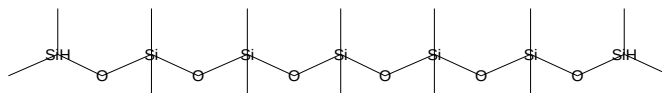
Compound Structure



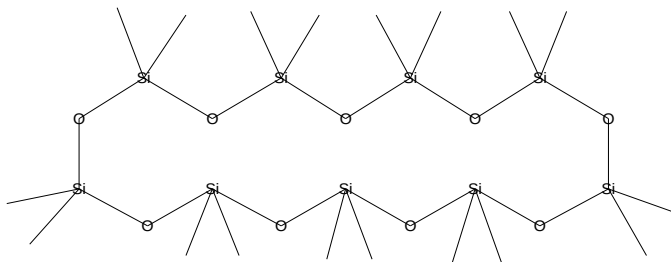
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



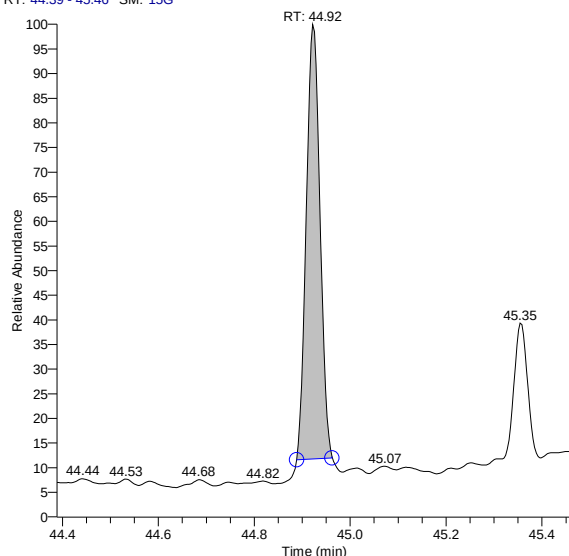
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Analysed by Satyanarayana

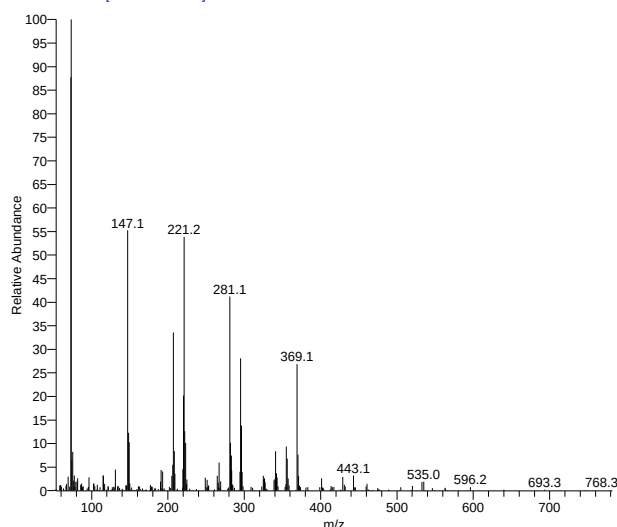
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ANALYTICAL CHEMISTRY DIVISION

RT: 44.39 - 45.46 SM: 15G



NL:
1.75E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

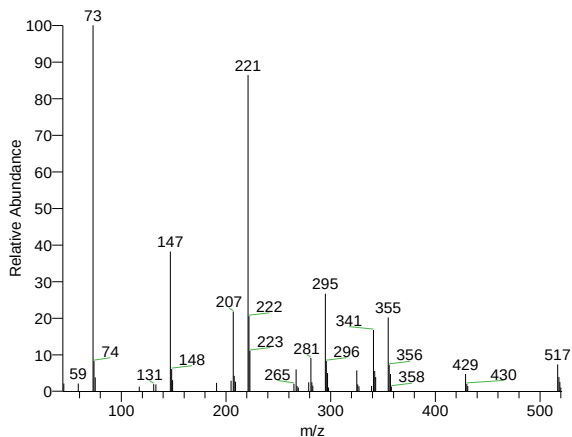
NGA-ZE-WATER1-SAMPLE-INJ1 #11607 RT: 44.92 AV: 1 RF: 6.00, 3 NL: 3.53E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
44.92	Heptasiloxane, hexadecamethyl-	3061238.52	39.67	631	806	mainlib
44.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3061238.52	31.18	625	693	mainlib
44.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3061238.52	7.23	585	692	mainlib
44.92	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	3061238.52	5.39	577	682	mainlib
44.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3061238.52	3.91	568	683	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Analysed by Satyanarayana

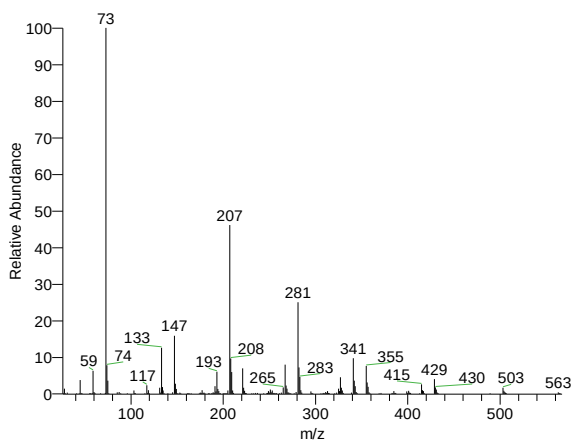
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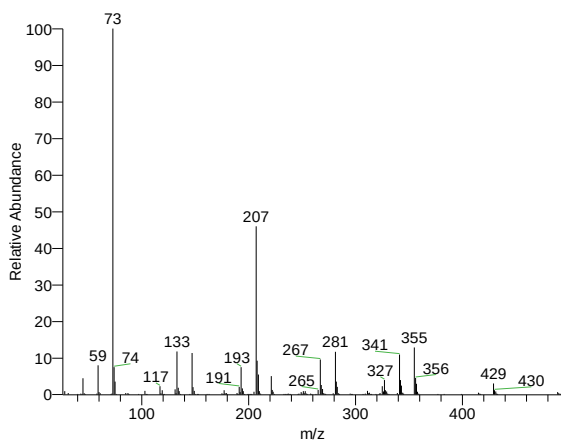
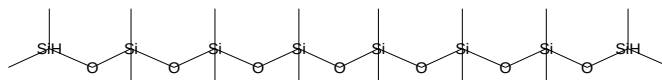
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

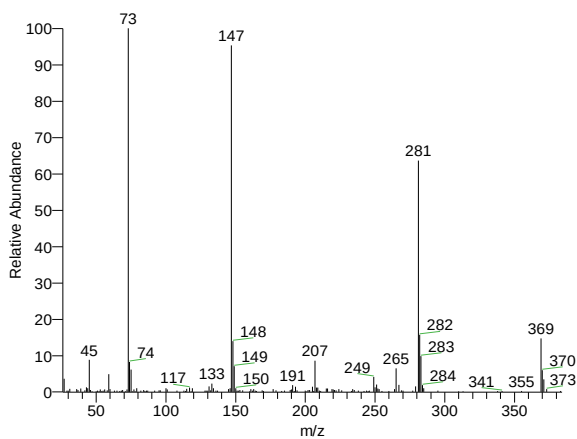
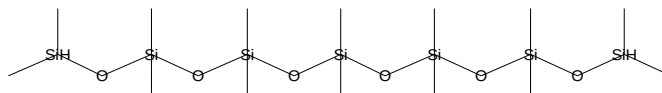
Compound Structure



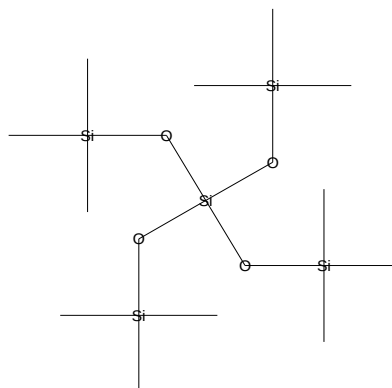
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane

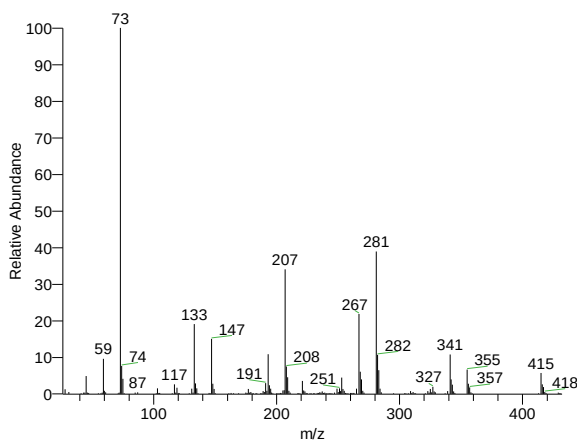


Analysed by Satyanarayana

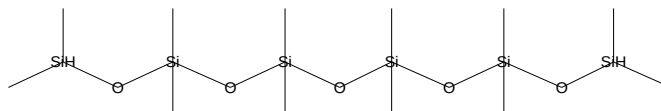
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

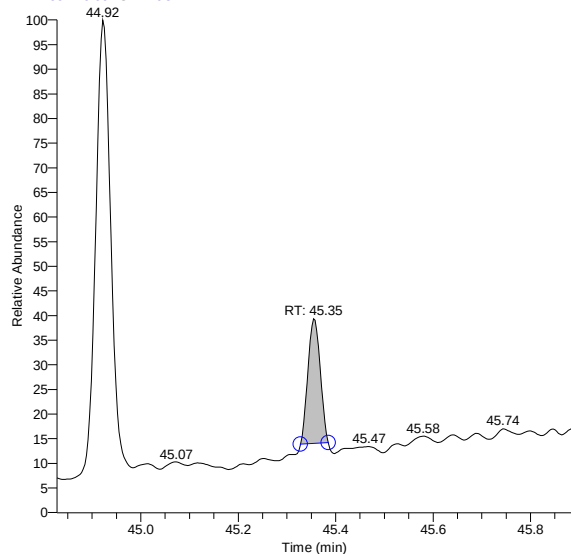
Compound Structure



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

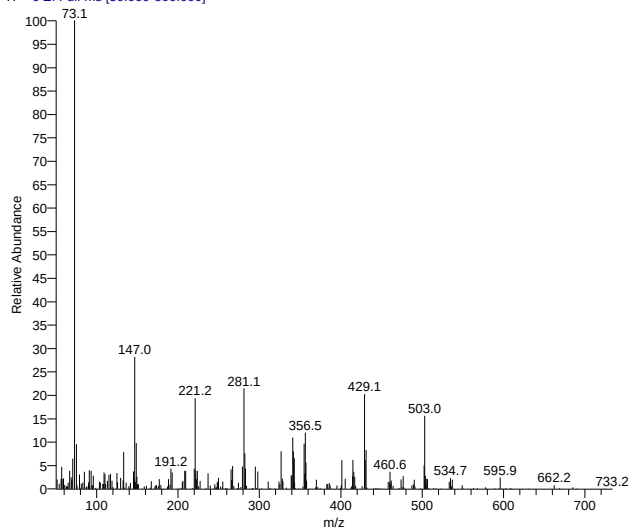


RT: 44.83 - 45.88 SM: 15G



NL:
1.75E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #11736 RT: 45.35 AV: 1 RF: 6.00, 3 NL: 1.53E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
45.35	Cyclodecasiloxane, eicosamethyl-	777460.27	78.61	639	668	mainlib
45.35	Cyclononasiloxane, octadecamethyl-	777460.27	8.33	558	678	mainlib
45.35	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	777460.27	7.68	556	653	mainlib
45.35	Cycloheptasiloxane, tetradecamethyl-	777460.27	1.66	512	720	mainlib
45.35	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	777460.27	0.60	489	749	mainlib

Analysed by Satyanarayana

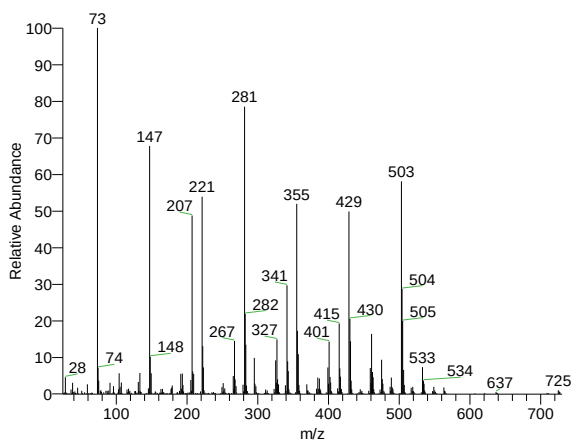
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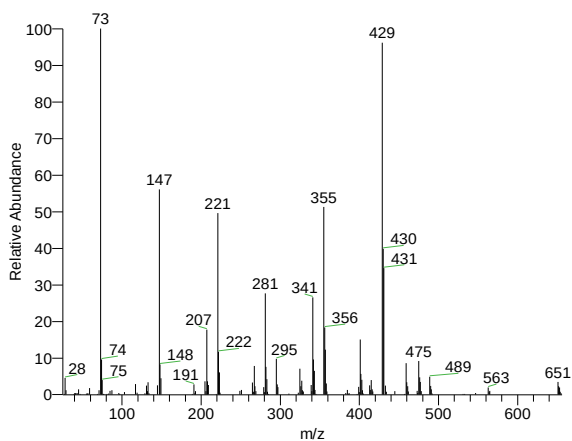
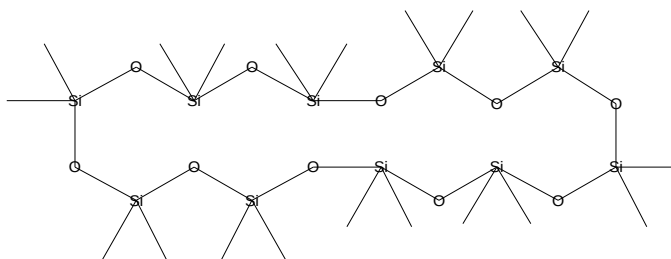
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

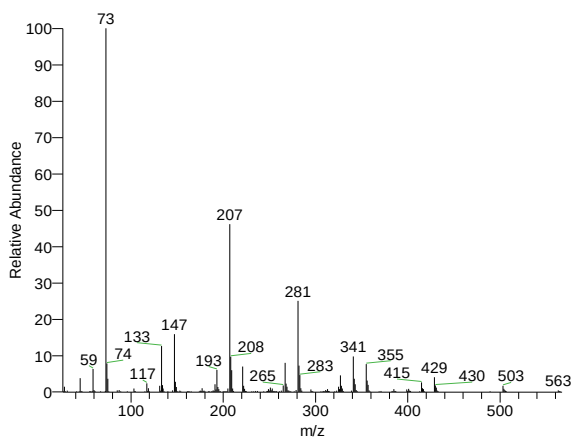
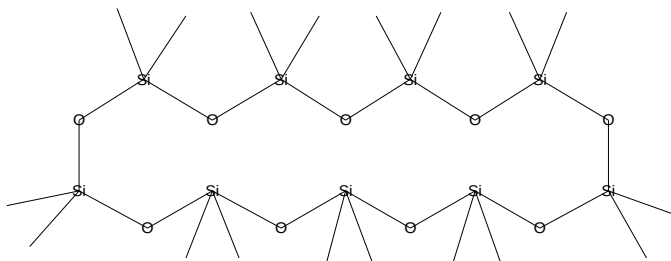
Compound Structure



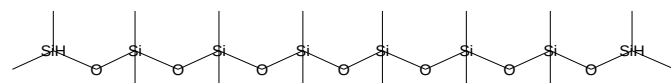
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

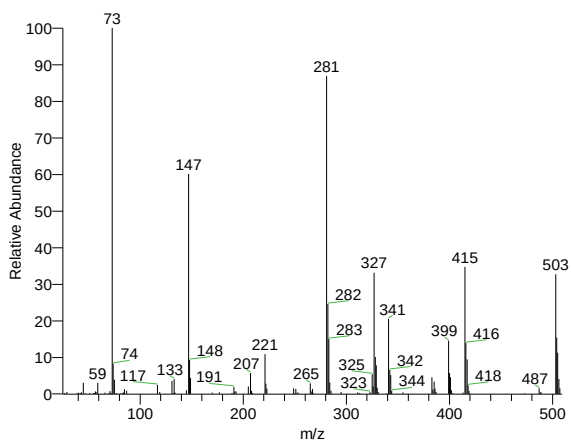
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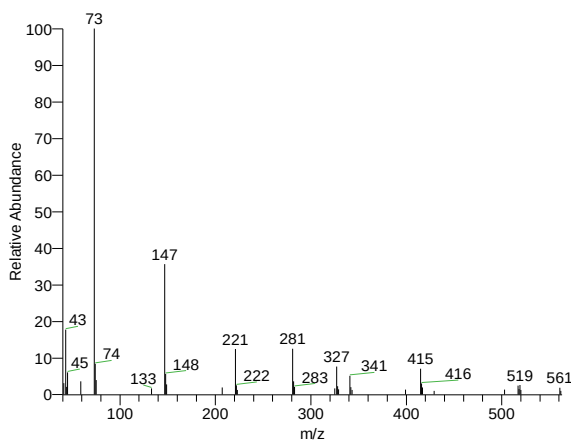
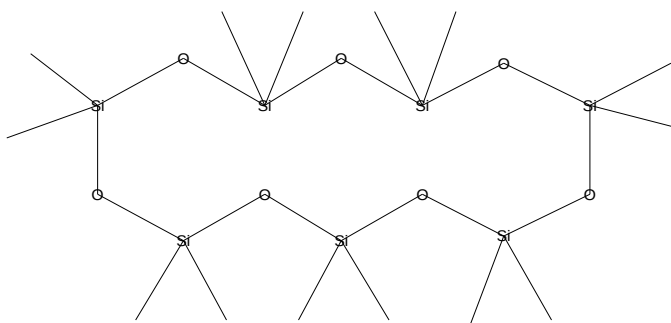
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

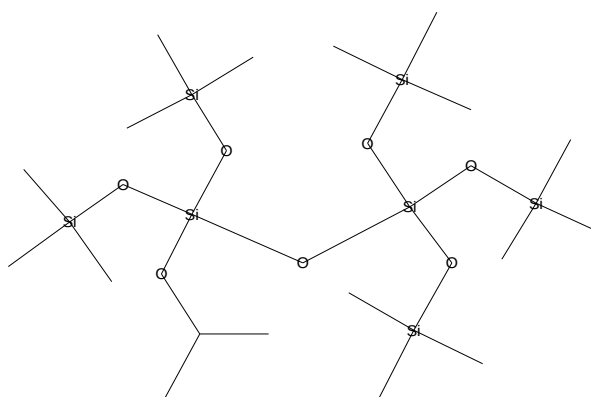
Compound Structure



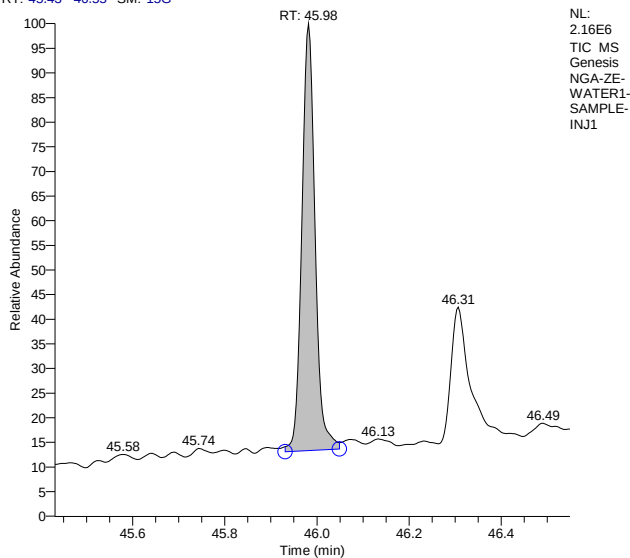
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane
Formula C₁₈H₅₂O₇Si₇, MW 576, CAS# 71579-69-6, Entry# 42479
1-Isopropoxy-3,3,3-trimethyl-1-[(trimethylsilyl)oxy]disiloxanyl tris(trimethylsilyl) orthosilicate #

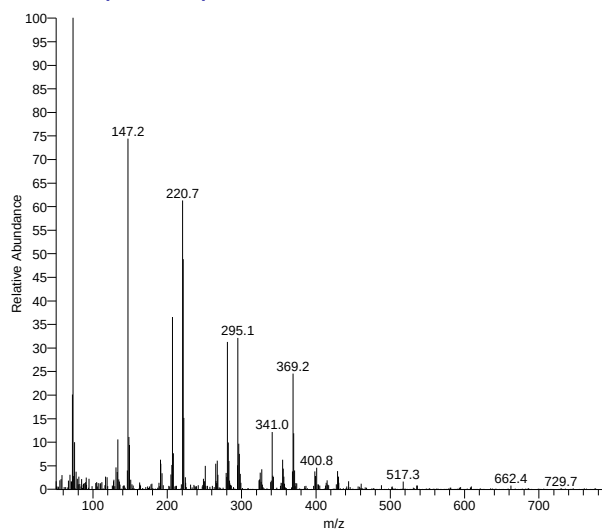


RT: 45.43 - 46.55 SM: 15G



NL:
2.16E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #11923 RT: 45.98 AV: 1 RF: 6.00, 3 NL: 3.98E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Heptasiloxane, hexadecamethyl-	3742547.54	67.57	640	833	mainlib

Analysed by Satyanarayana

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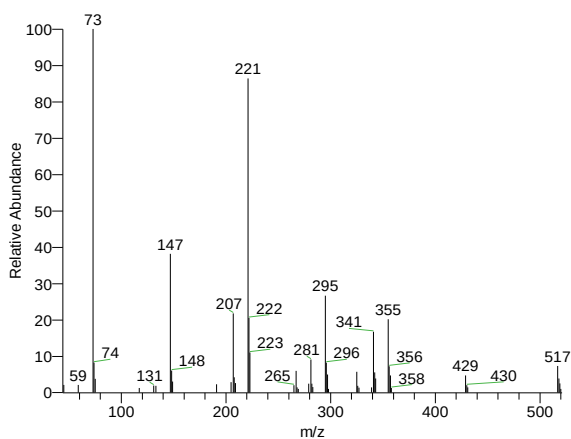
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

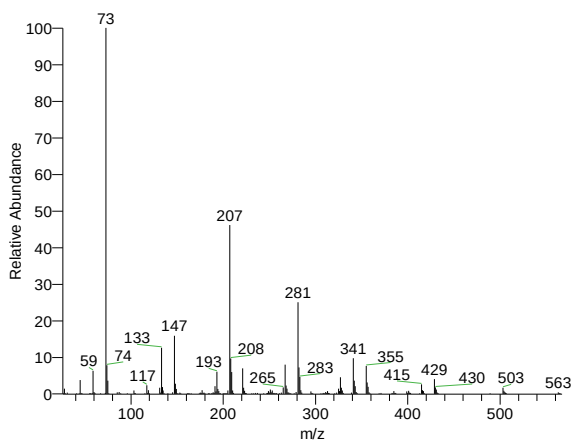
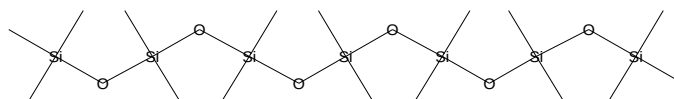
RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3742547.54	19.51	612	685	mainlib
45.98	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3742547.54	5.00	578	684	mainlib
45.98	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3742547.54	2.27	558	666	mainlib
45.98	Cyclododecasiloxane, eicosamethyl-	3742547.54	0.90	536	558	mainlib

Hit Spectrum

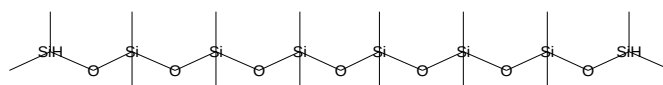
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

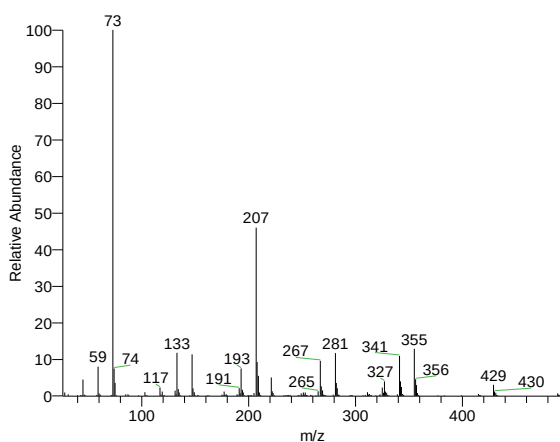
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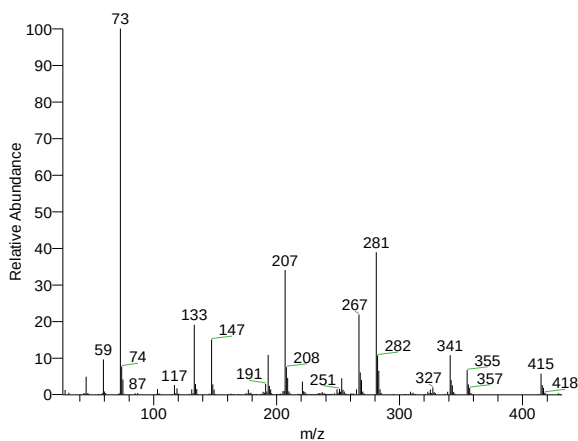
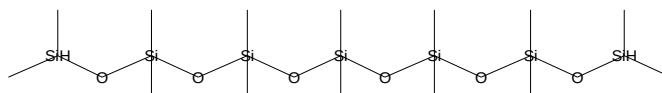
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

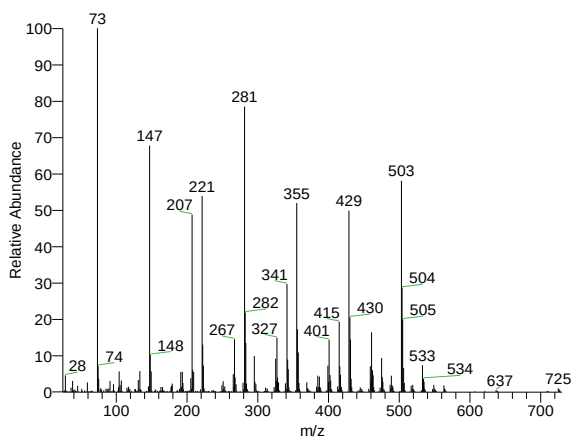
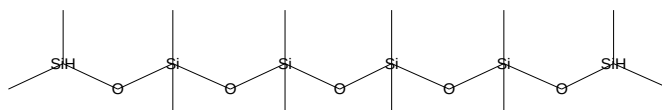
Compound Structure



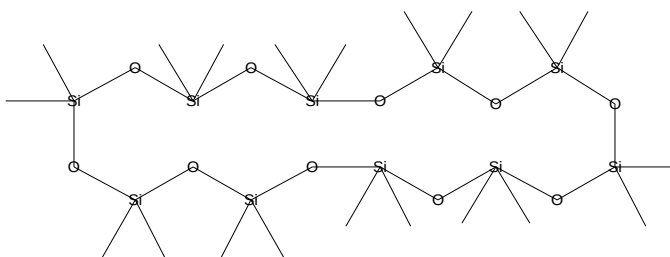
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



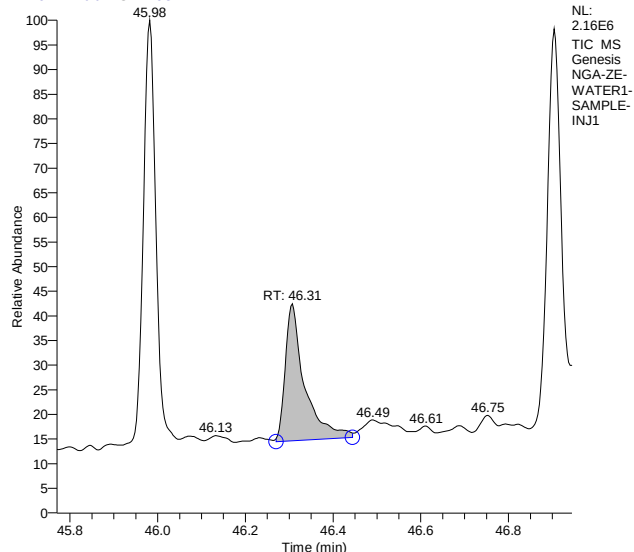
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



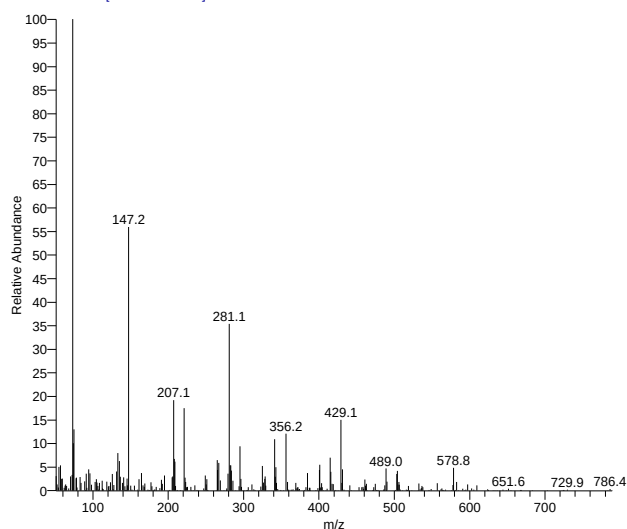
Analysed by Satyanarayana

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GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

RT: 45.77 - 46.94 SM: 15G

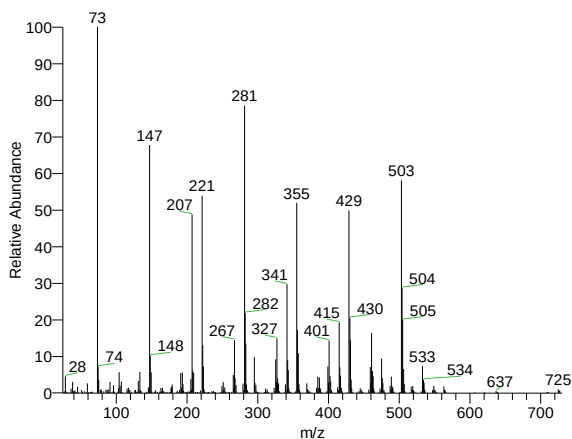


NGA-ZE-WATER1-SAMPLE-INJ1 #12020 RT: 46.31 AV: 1 RF: 6.00, 3 NL: 1.70E5
T: + c EI Full ms [50.000-800.000]



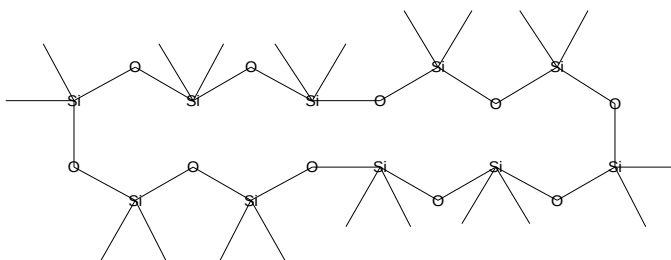
RT	Compound Name	Area	Probability	SI	RSI	Library
46.31	Cyclodecasiloxane, eicosamethyl-	1838058.61	51.32	609	658	mainlib
46.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1838058.61	32.12	595	695	mainlib
46.31	Cyclononasiloxane, octadecamethyl-	1838058.61	5.38	532	638	mainlib
46.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1838058.61	4.34	527	655	mainlib
46.31	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	1838058.61	3.49	522	655	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Analysed by Satyanarayana

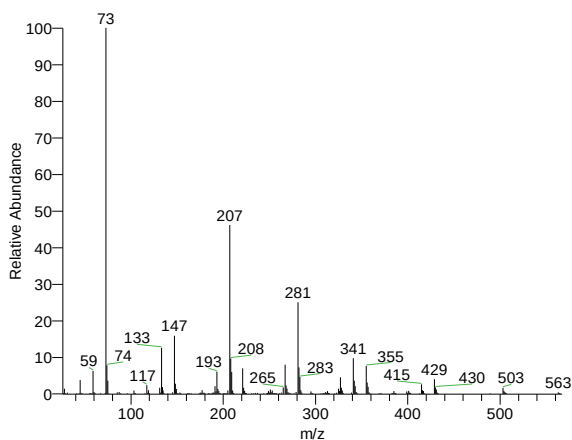
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH

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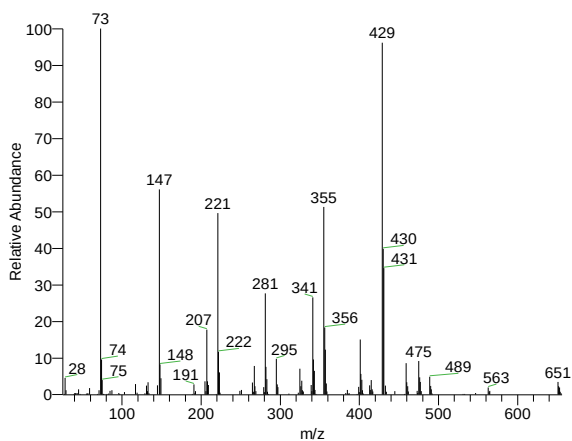
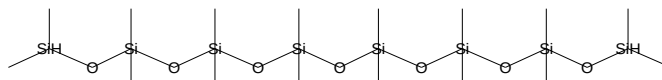
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

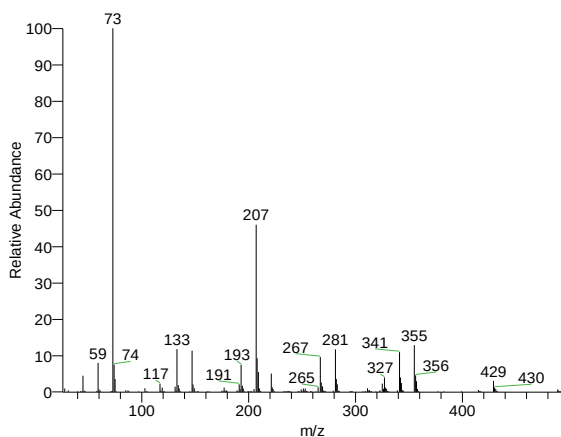
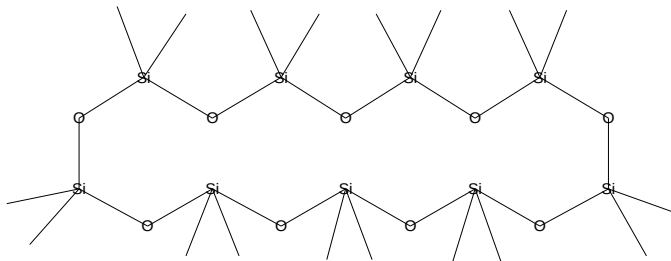
Compound Structure



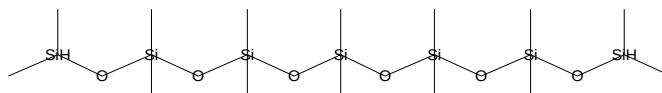
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

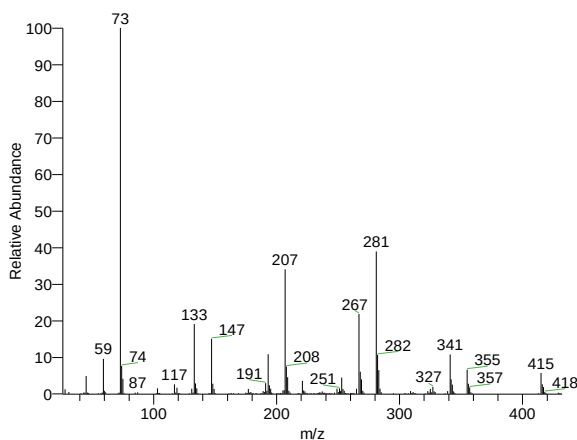


Analysed by Satyanarayana

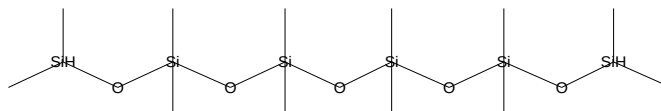
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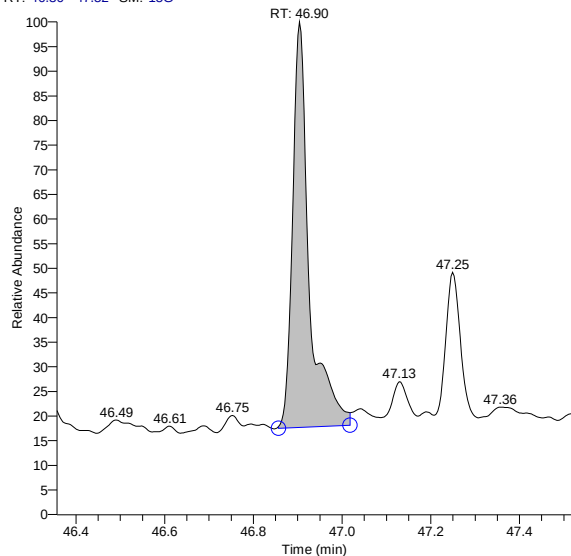
Compound Structure



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

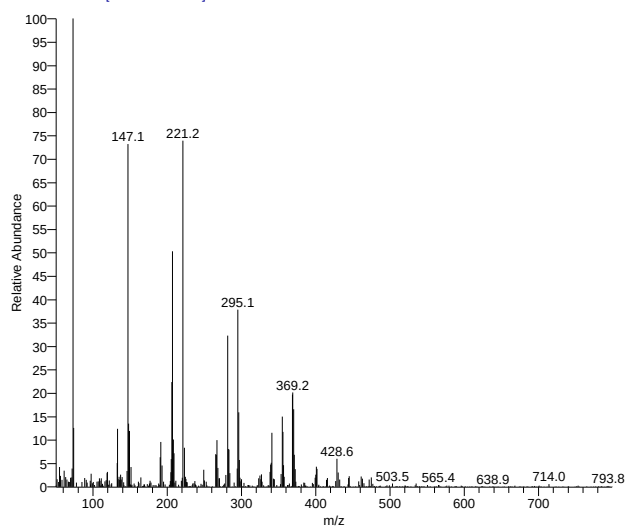


RT: 46.36 - 47.52 SM: 15G



NL:
2.12E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #12198 RT: 46.90 AV: 1 RF: 6.00, 3 NL: 3.09E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
46.90	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	4525139.34	28.86	565	648	mainlib
46.90	Heptasiloxane, hexadecamethyl-	4525139.34	28.86	565	782	mainlib
46.90	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	4525139.34	7.24	530	669	mainlib
46.90	Pentasiloxane, dodecamethyl-	4525139.34	3.95	513	611	mainlib
46.90	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	4525139.34	2.79	503	635	mainlib

Analysed by Satyanarayana

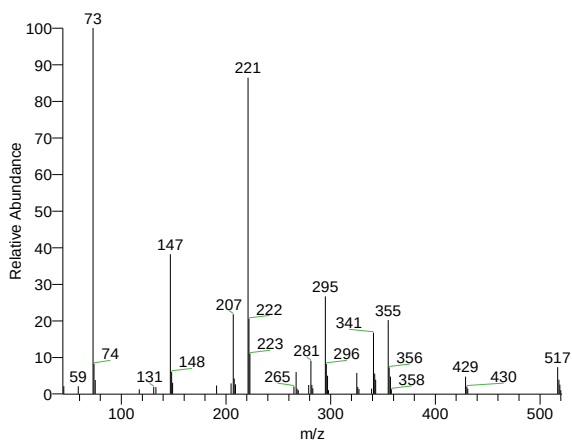
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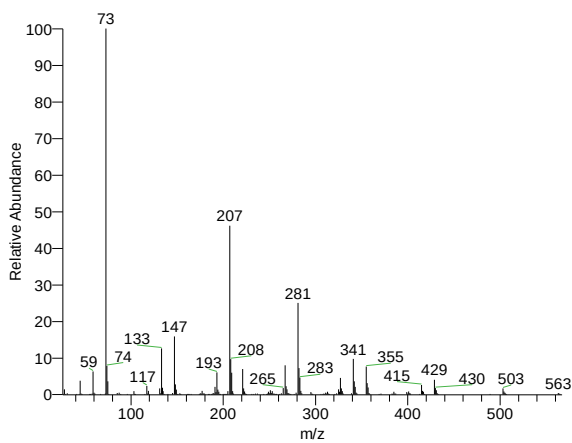
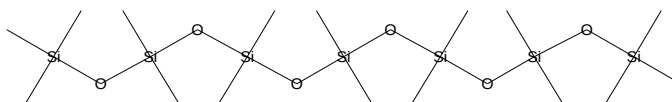
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

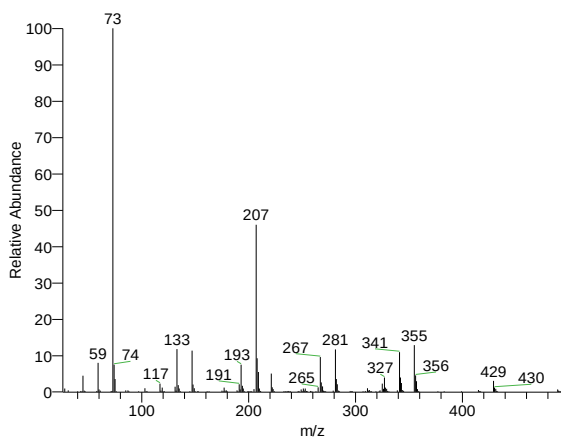
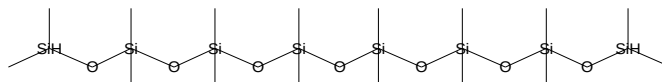
Compound Structure



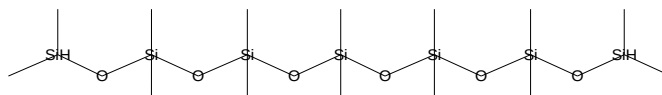
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

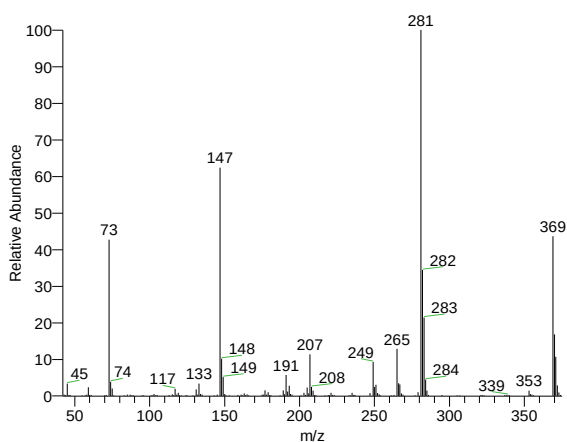
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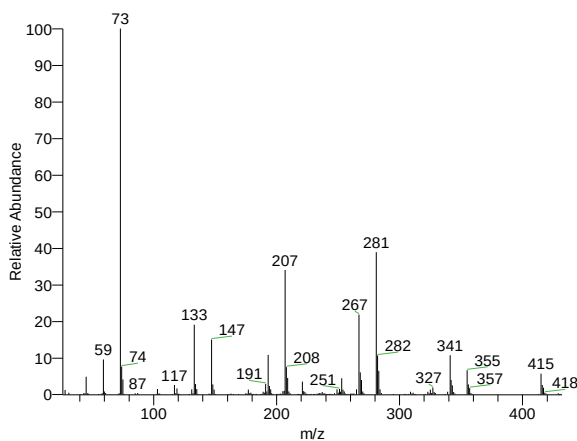
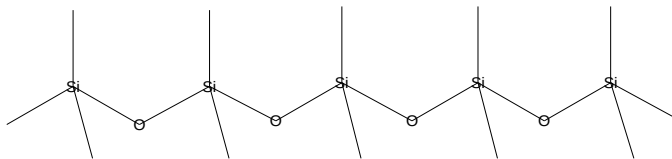
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

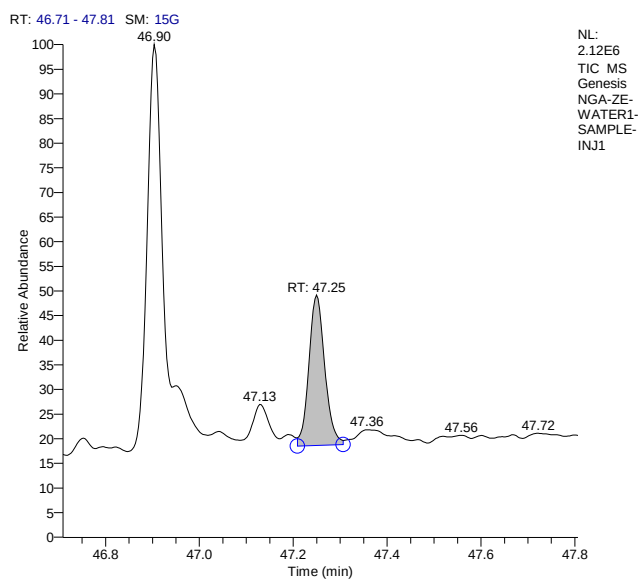
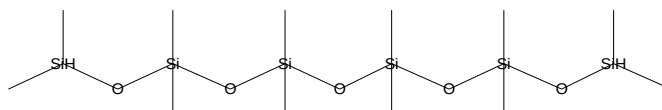
Compound Structure



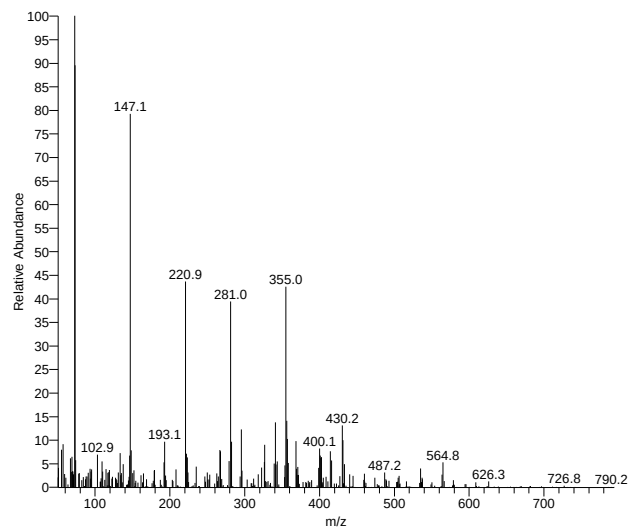
Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



NGA-ZE-WATER1-SAMPLE-INJ1 #12301 RT: 47.25 AV: 1 RF: 6.00, 3 NL: 1.36E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
47.25	Cyclodecasiloxane, eicosamethyl-	1520082.97	27.90	536	574	mainlib

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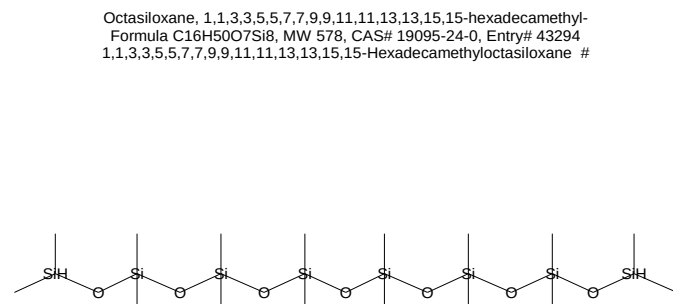
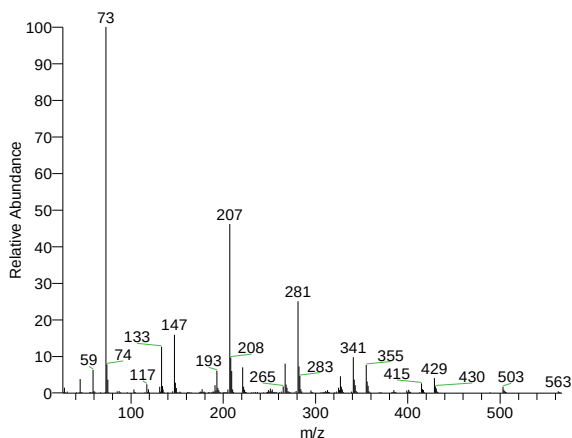
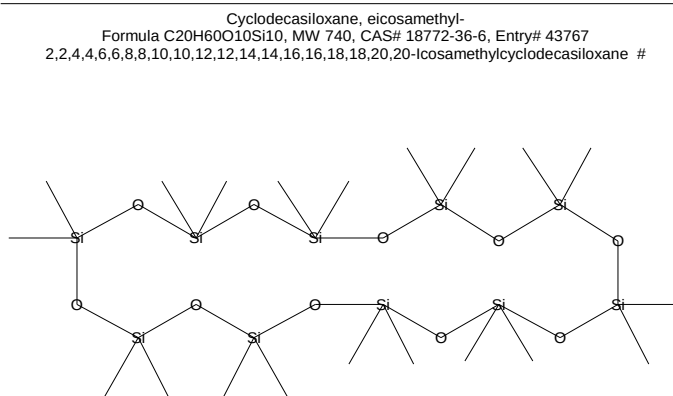
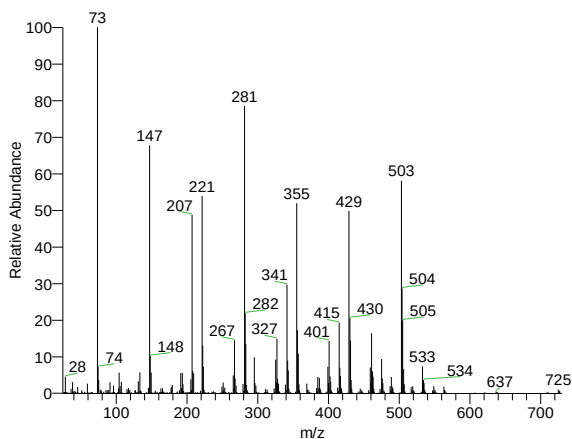
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ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
47.25	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1520082.97	17.46	522	606	mainlib
47.25	Heptasiloxane, hexadecamethyl-	1520082.97	14.07	517	721	mainlib
47.25	Cyclooctasiloxane, hexadecamethyl-	1520082.97	9.37	505	680	mainlib
47.25	Cyclononasiloxane, octadecamethyl-	1520082.97	4.55	486	596	mainlib

Hit Spectrum

Compound Structure



Analysed by Satyanarayana

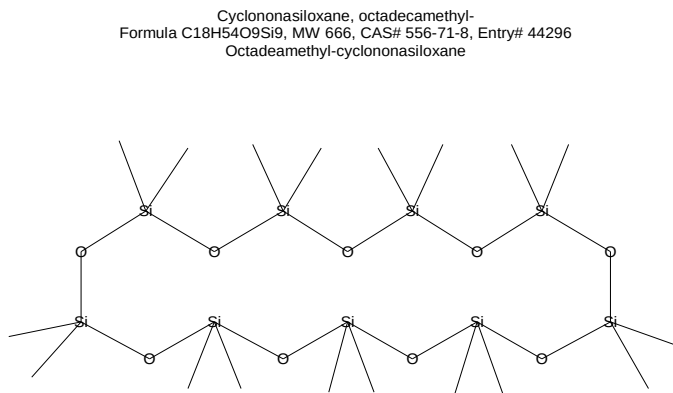
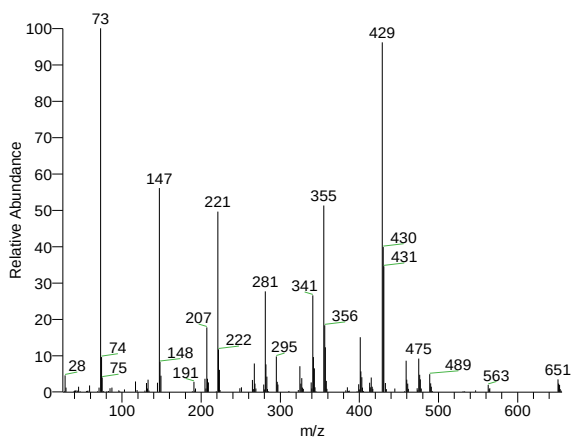
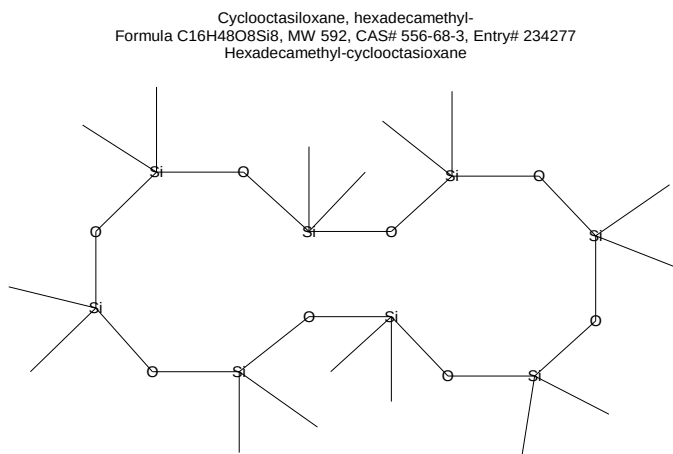
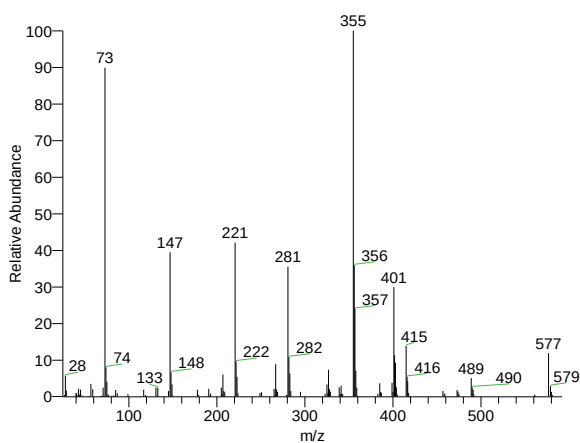
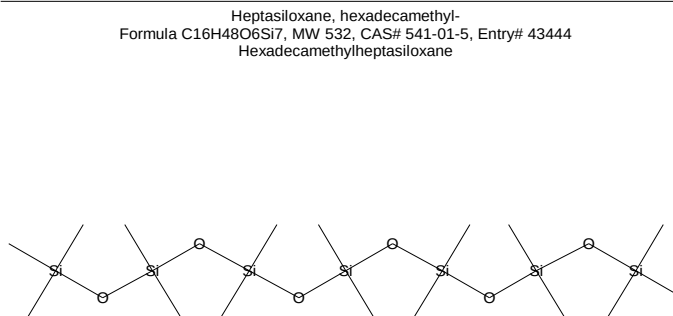
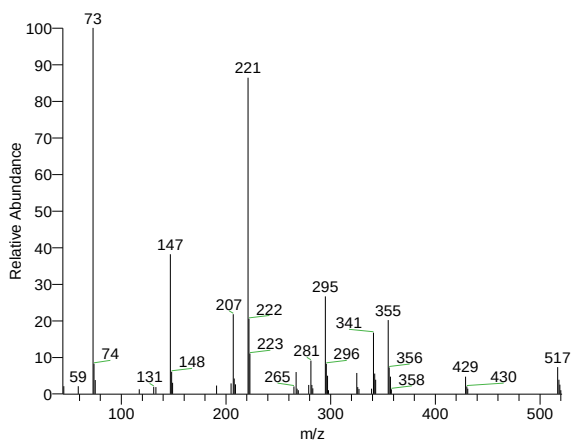
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Hit Spectrum

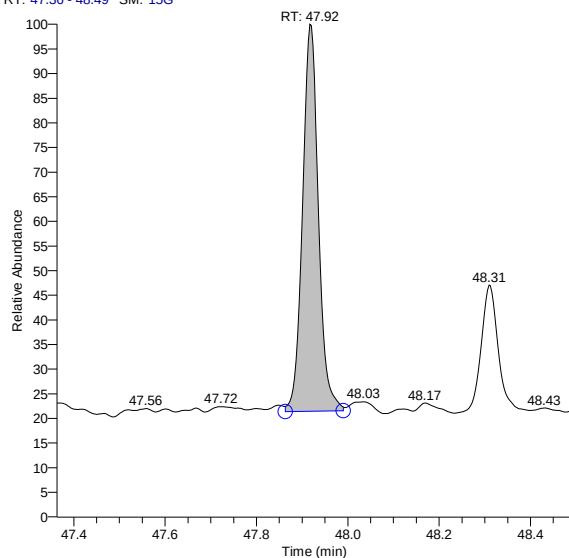
Compound Structure



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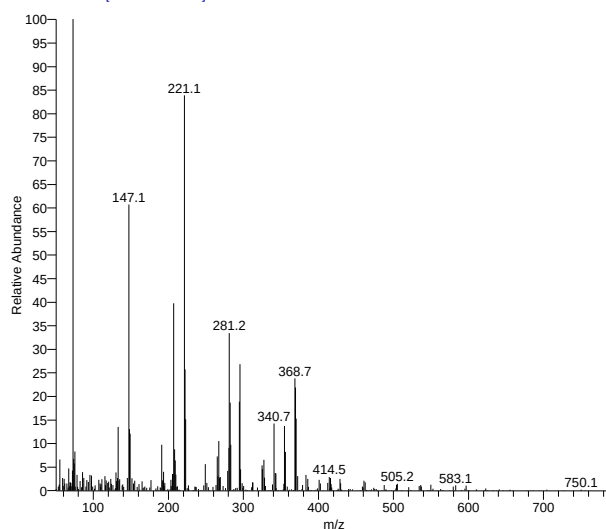
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RT: 47.36 - 48.49 SM: 15G



NL:
2.00E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

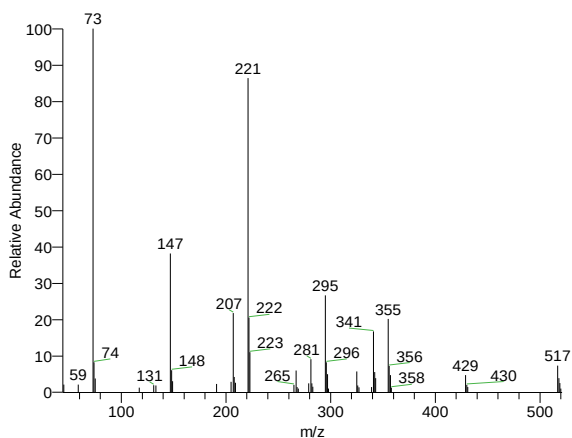
NGA-ZE-WATER1-SAMPLE-INJ1 #12500 RT: 47.92 AV: 1 RF: 6.00, 3 NL: 2.73E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
47.92	Heptasiloxane, hexadecamethyl-	3825974.67	32.83	604	797	mainlib
47.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3825974.67	27.74	600	665	mainlib
47.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3825974.67	11.80	579	692	mainlib
47.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3825974.67	11.80	579	692	mainlib
47.92	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	3825974.67	3.28	549	594	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



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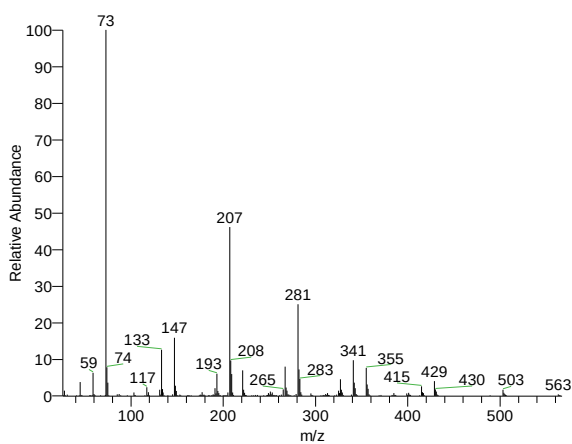
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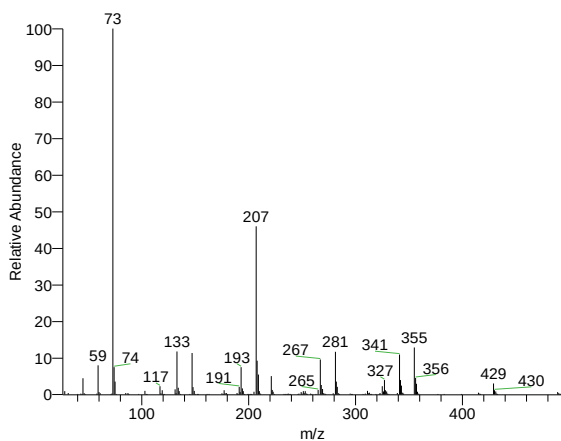
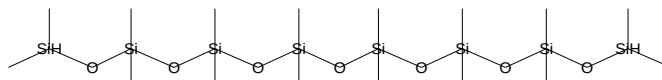
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

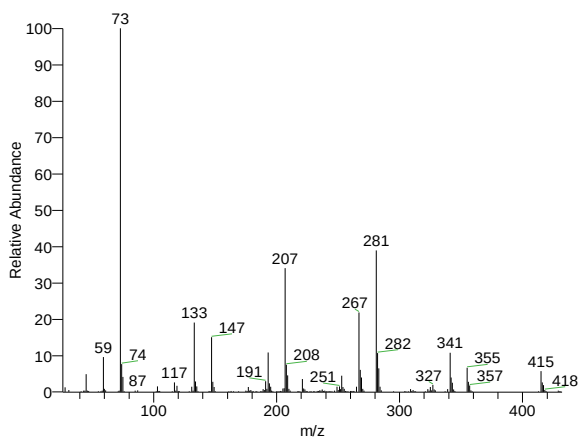
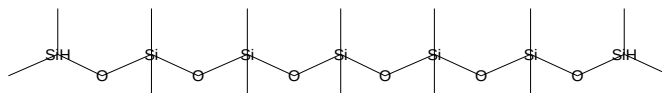
Compound Structure



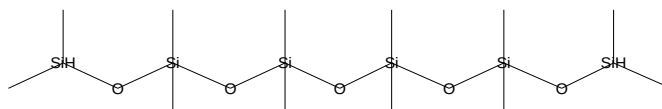
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

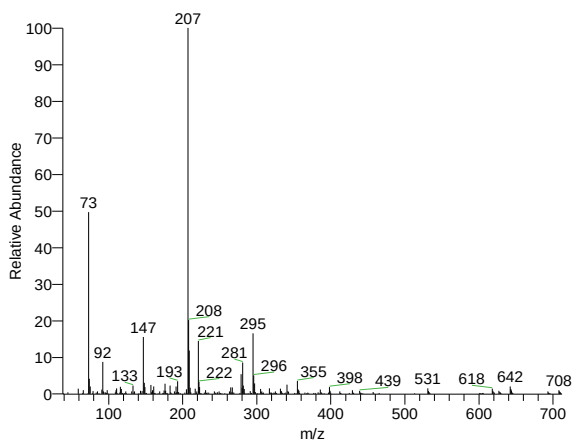


Analysed by Satyanarayana

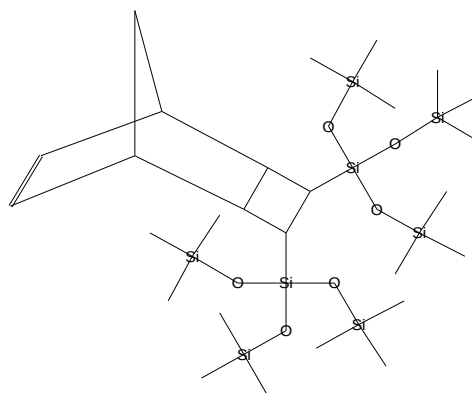
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Hit Spectrum

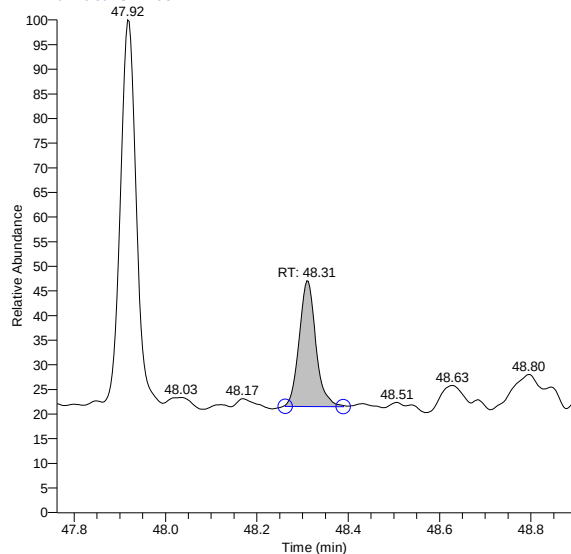
Compound Structure



Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:2BJSGSCCAWLXCNS-UHFFFAOYSA-N

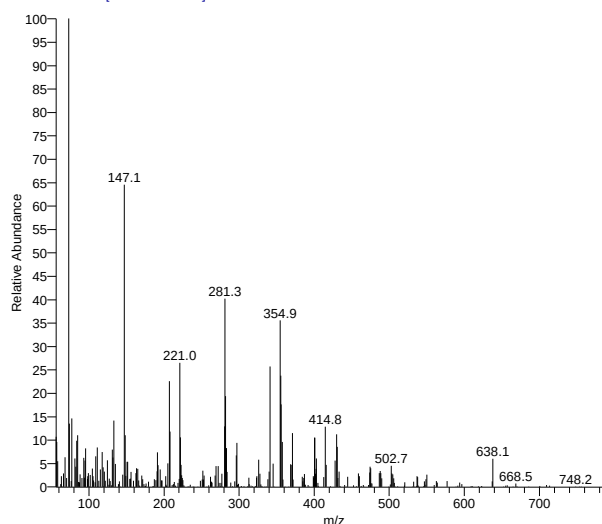


RT: 47.76 - 48.89 SM: 15G



NL:
2.00E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #12617 RT: 48.31 AV: 1 RF: 6.00, 3 NL: 1.05E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
48.31	Cyclodecasiloxane, eicosamethyl-	1301092.46	39.53	556	591	mainlib
48.31	Cyclooctasiloxane, hexadecamethyl-	1301092.46	19.19	537	704	mainlib
48.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1301092.46	16.96	534	619	mainlib
48.31	Tetracosamethyl-cyclododecasiloxane	1301092.46	5.68	510	744	mainlib
48.31	Cyclononasiloxane, octadecamethyl-	1301092.46	3.44	495	596	mainlib

Analysed by Satyanarayana

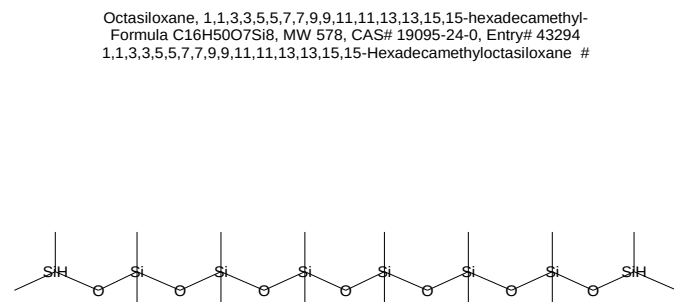
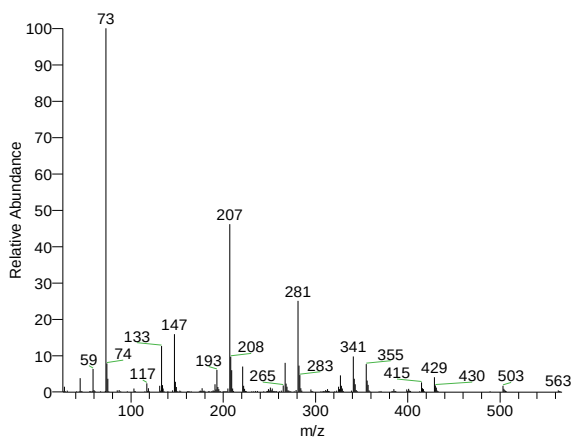
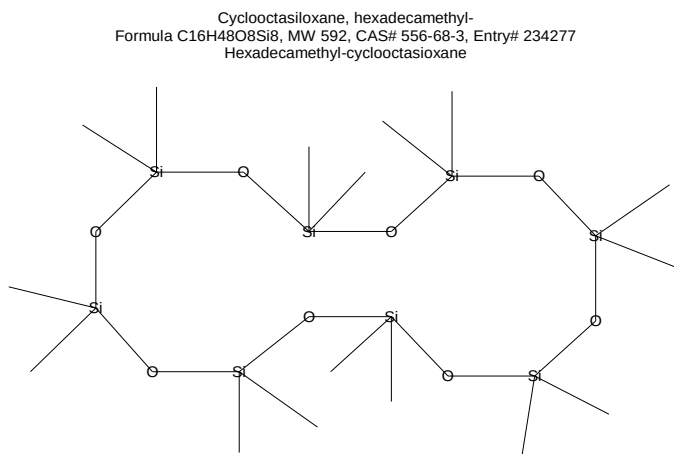
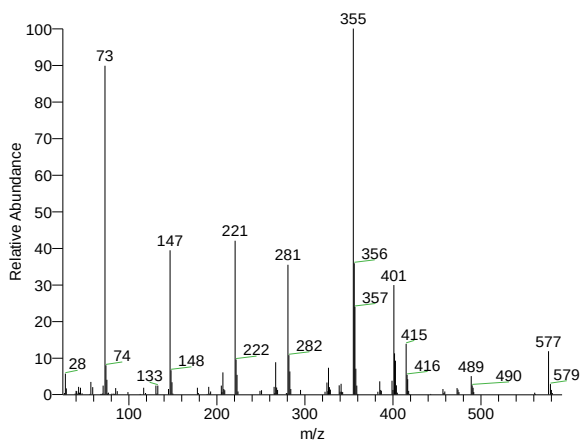
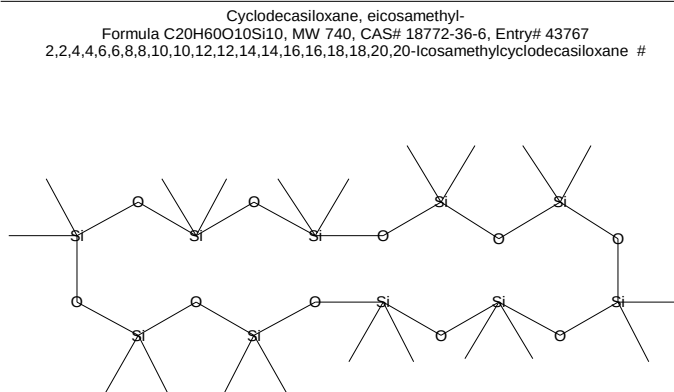
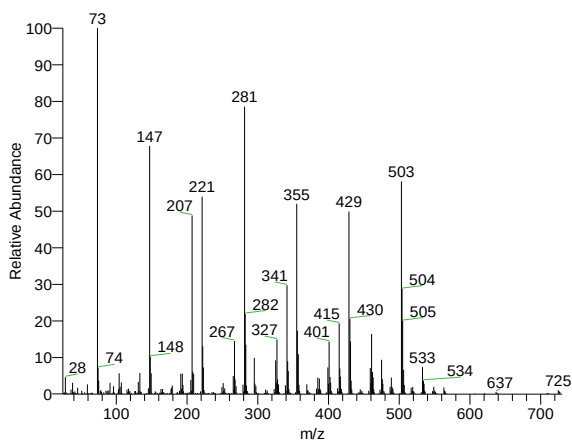
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Hit Spectrum

Compound Structure



Analysed by Satyanarayana

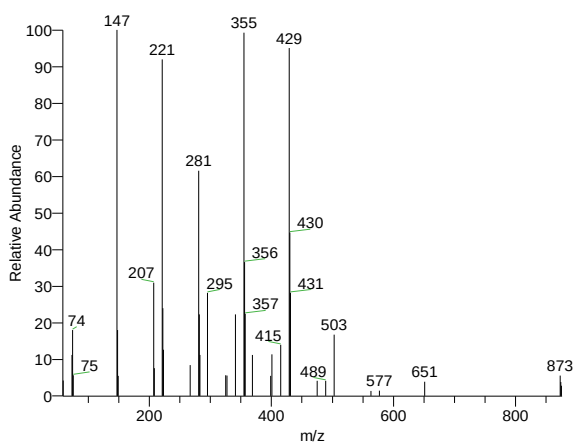
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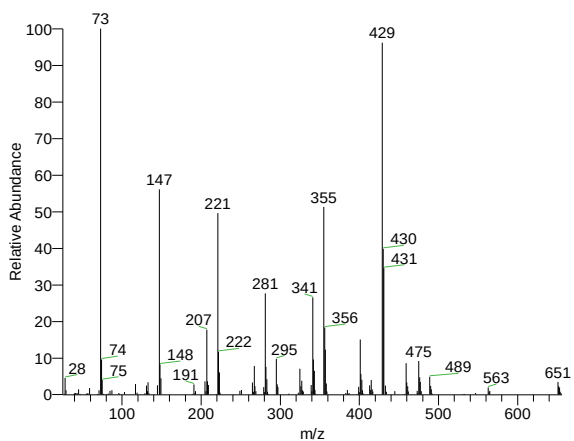
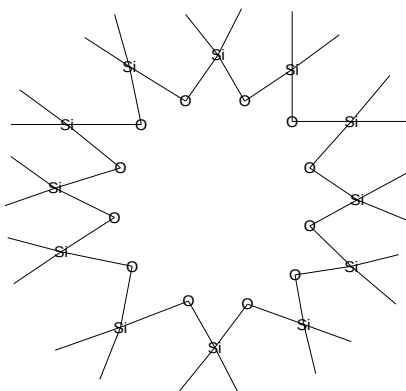
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

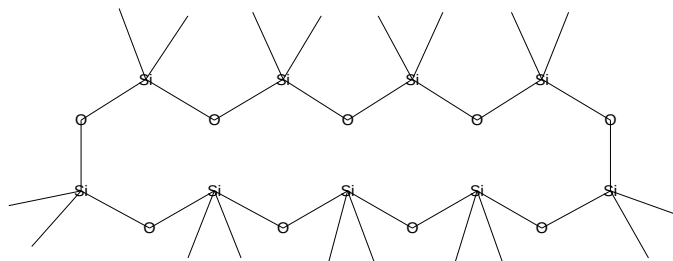
Compound Structure



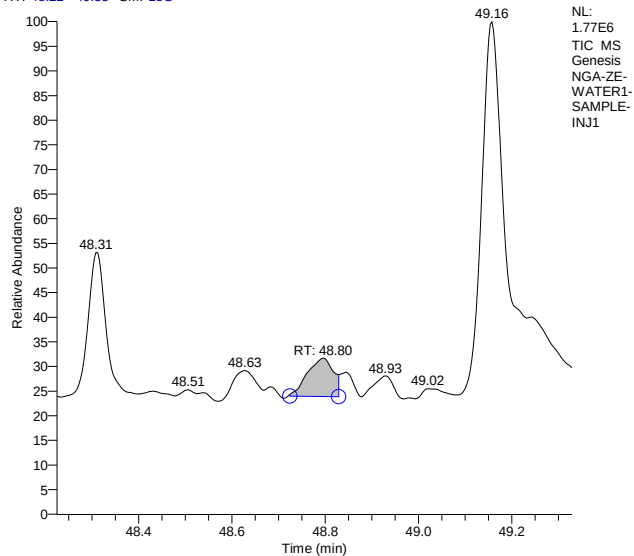
Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



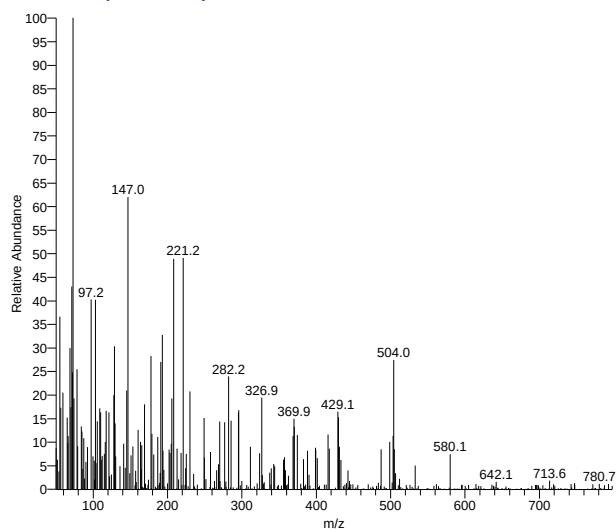
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



RT: 48.22 - 49.33 SM: 15G



NGA-ZE-WATER1-SAMPLE-INJ1 #12762 RT: 48.80 AV: 1 RF: 6.00, 3 NL: 3.09E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

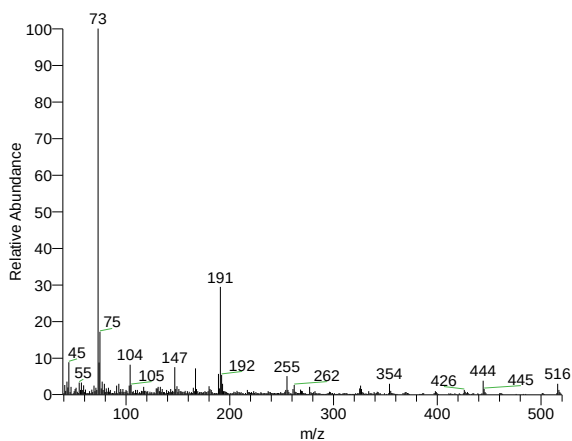
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ANALYTICAL CHEMISTRY DIVISION

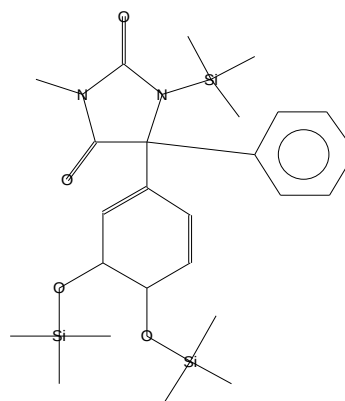
RT	Compound Name	Area	Probability	SI	RSI	Library
48.80	2,4-Imidazolidinedione, 5-[3,4-bis[(trimethylsilyl)oxy]phenyl]-3-methyl-5-phenyl-1-(trimethylsilyl)-	529378.67	5.80	367	418	mainlib
48.80	androsta--2,4,16-triene-3,6,17-triol, tri-TMS	529378.67	5.35	365	397	mainlib
48.80	(+)-Prostaglandin F2α, 4TMS derivative	529378.67	4.20	359	396	mainlib
48.80	3,9α:14,15-Diepoxypregn-16-en-20-one, 3,11α,18-triacetoxy-	529378.67	3.71	356	418	mainlib
48.80	Dihydromorphine, 2TMS derivative	529378.67	3.14	352	419	mainlib

Hit Spectrum

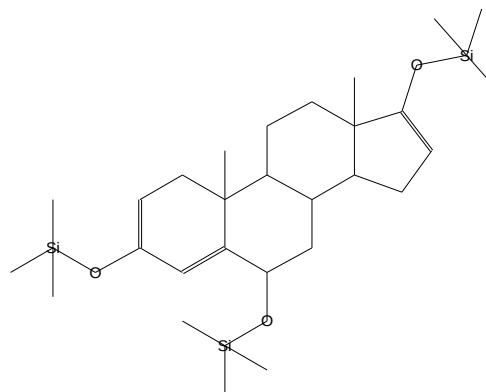
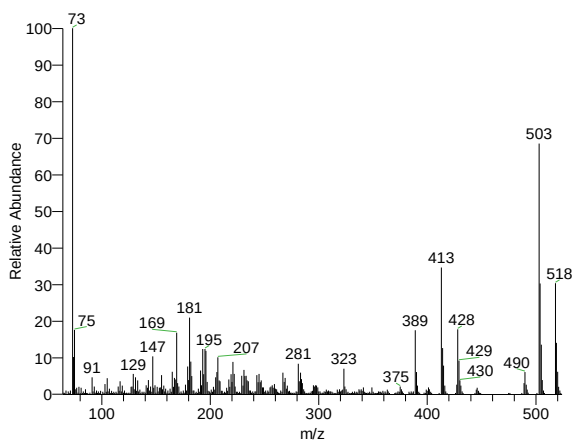


Compound Structure

2,4-Imidazolidinedione, 5-[3,4-bis[(trimethylsilyl)oxy]phenyl]-3-methyl-5-phenyl-1-(trimethylsilyl)-
Formula C₂₅H₄₀N₂O₄Si₃, MW 516, CAS# 55517-85-6, Entry# 43118



androsta--2,4,16-triene-3,6,17-triol, tri-TMS
Formula C₂₈H₅₀O₃Si₃, MW 518, CAS# NA, Entry# 44428
\$.28CQOMSMVEBAFHDM-UHFFFAOYSA-N



Analysed by Satyanarayana

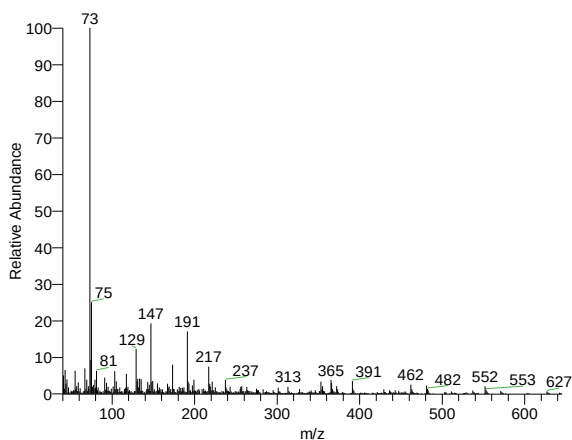
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GC-MS/MS QUAL REPORT

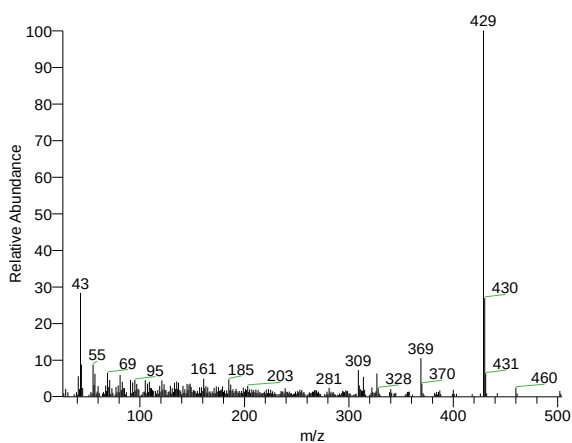
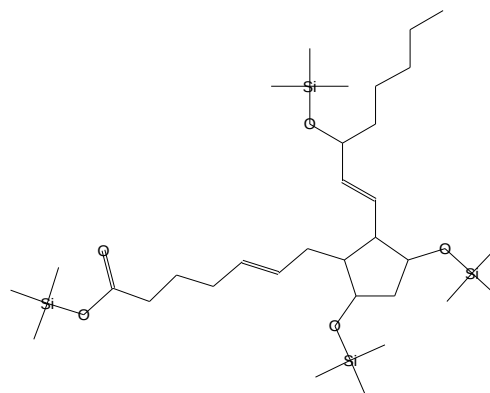
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

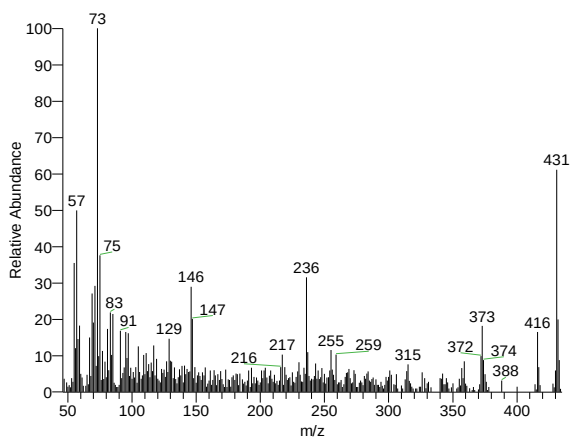
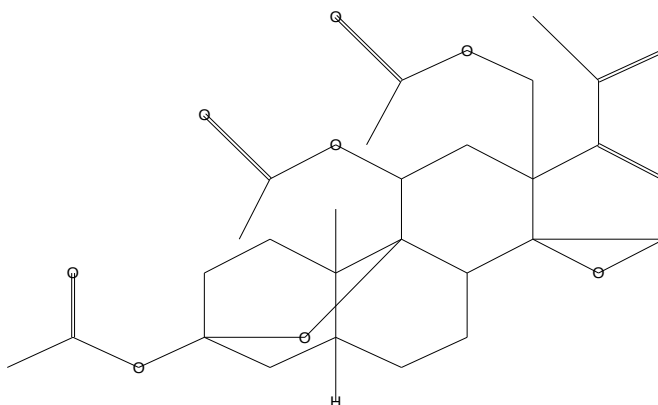
Compound Structure



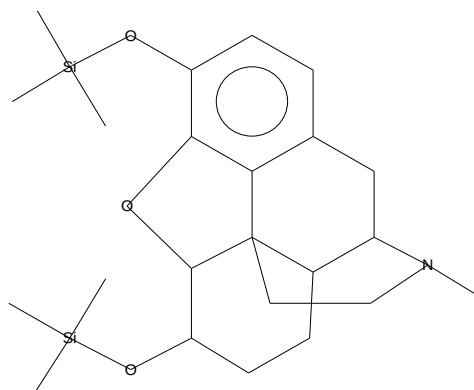
(+)-Prostaglandin F2 α , 4TMS derivative
Formula C32H66O5Si4, MW 642, CAS# 50669-95-9, Entry# 41447



3,9 α ,14,15-Diepoxypregn-16-en-20-one, 3,11 α ,18-triacetoxy-
Formula C27H34O9, MW 502, CAS# NA, Entry# 239582
\$:28GBYXRTQLWMZHST-UHFFFAOYSA-N



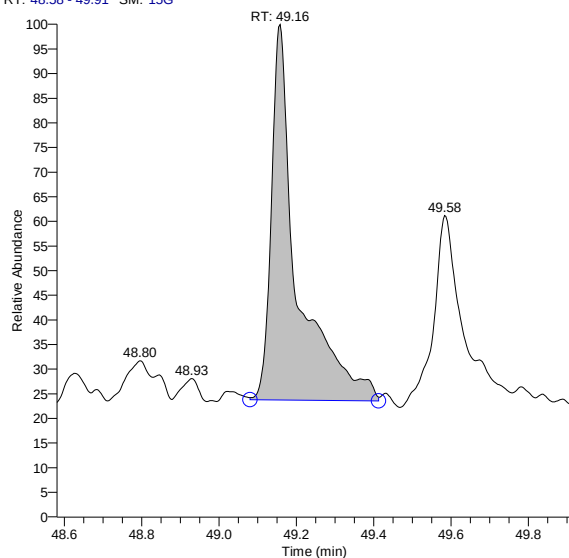
Dihydromorphine, 2TMS derivative
Formula C23H37NO3Si2, MW 431, CAS# NA, Entry# 44307
Dihydromorphine , di(trimethylsilyl) ether



Analysed by Satyanarayana

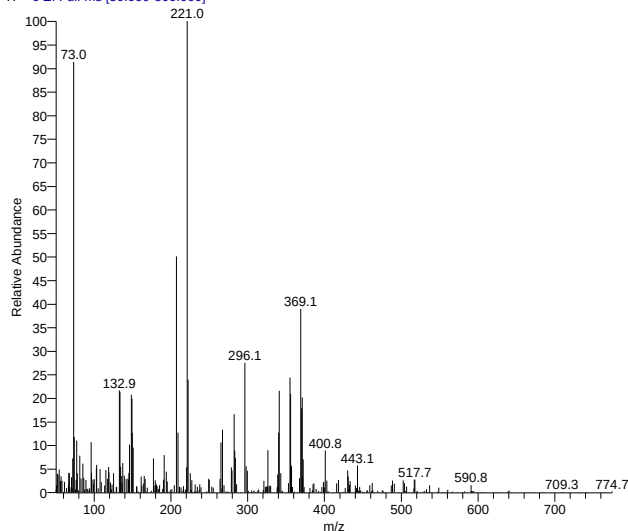
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GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

RT: 48.58 - 49.91 SM: 15G



NL:
1.77E6
TIC: MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

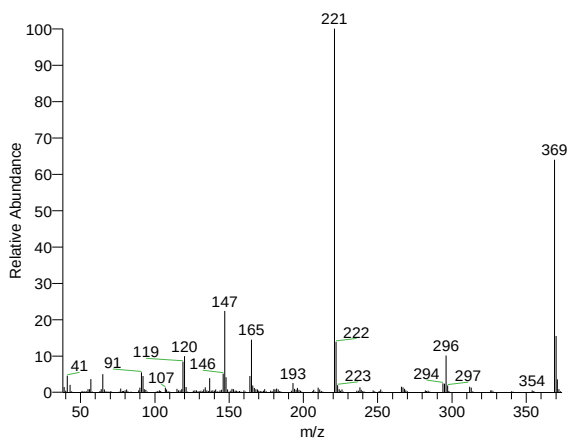
NGA-ZE-WATER1-SAMPLE-INJ1 #12870 RT: 49.16 AV: 1 RF: 6.00, 3 NL: 1.50E5
T: + c EI Full ms [50,000-800,000]



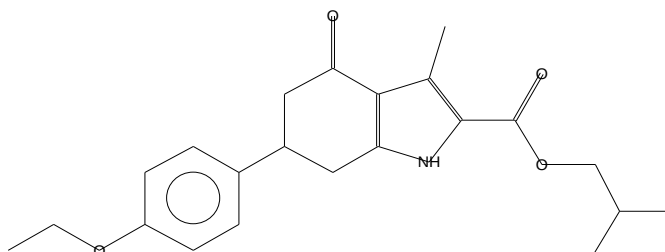
RT	Compound Name	Area	Probability	SI	RSI	Library
49.16	1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isobutyl ester	6257999.77	8.29	434	562	mainlib
49.16	Cyclodecasiloxane, eicosamethyl-	6257999.77	7.32	431	455	mainlib
49.16	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	6257999.77	6.75	429	505	mainlib
49.16	Heptasiloxane, hexadecamethyl-	6257999.77	5.17	422	662	mainlib
49.16	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	6257999.77	4.37	418	554	mainlib

Hit Spectrum

Compound Structure



1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isobutyl ester
Formula C22H27NO4, MW 369, CAS# NA, Entry# 196839
\$.28XORXIIMNPHEBIN-UHFFFAOYSA-N



Analysed by Satyanarayana

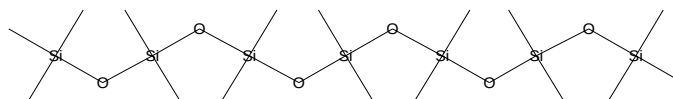
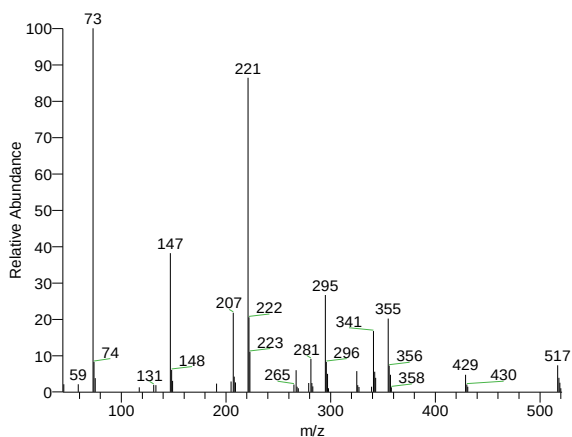
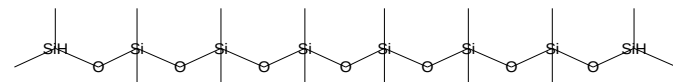
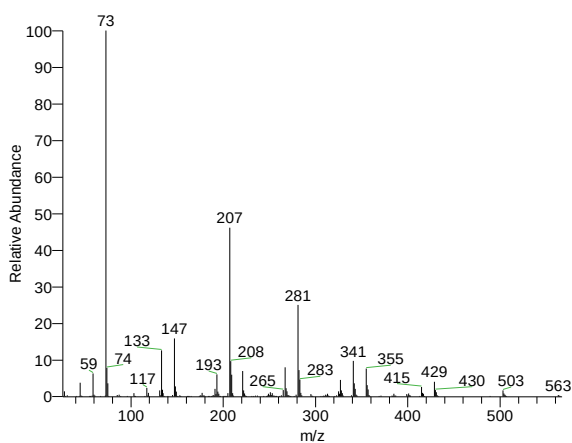
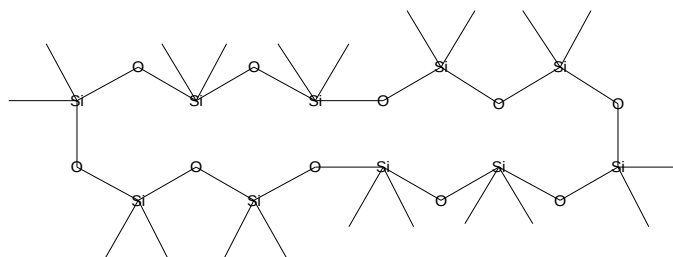
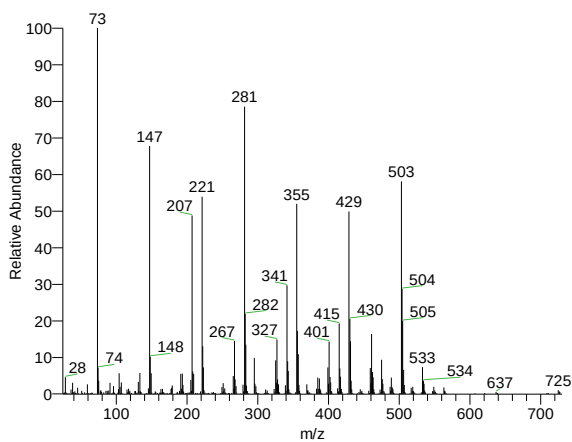
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Hit Spectrum

Compound Structure

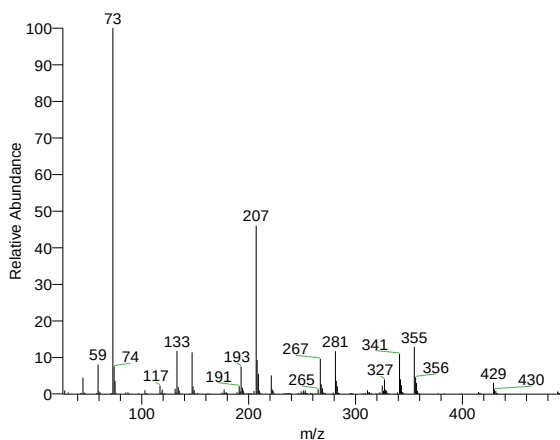


Analysed by Satyanarayana

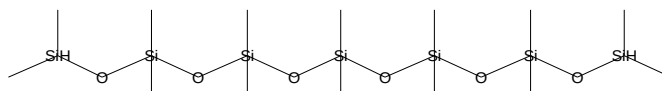
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

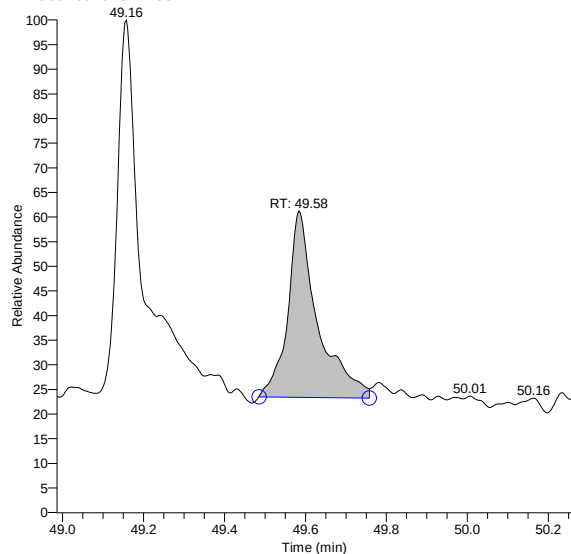
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

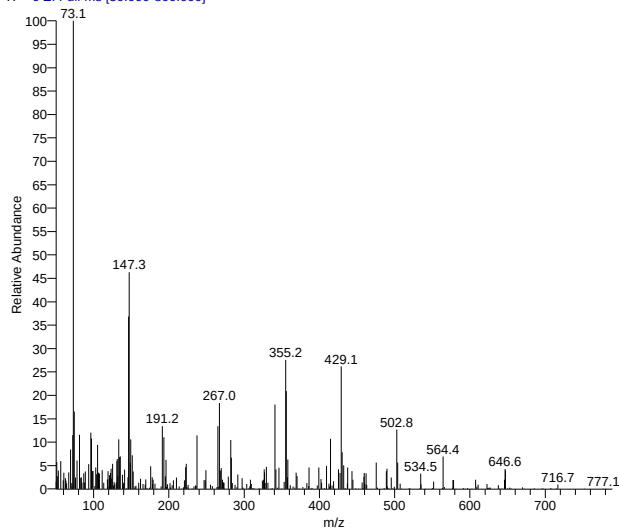


RT: 48.99 - 50.26 SM: 15G



NL:
1.77E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #12997 RT: 49.58 AV: 1 RF: 6.00, 3 NL: 1.11E5
T: + c EI Full ms [50.000-800.000]



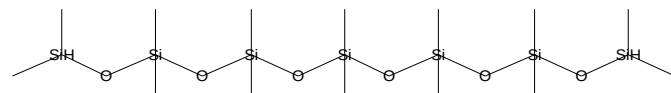
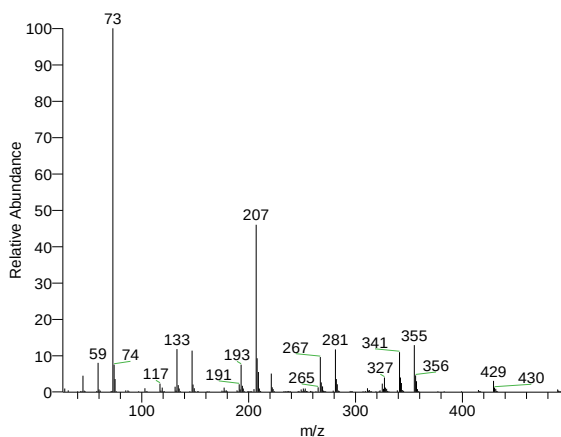
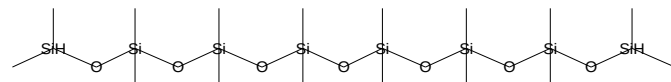
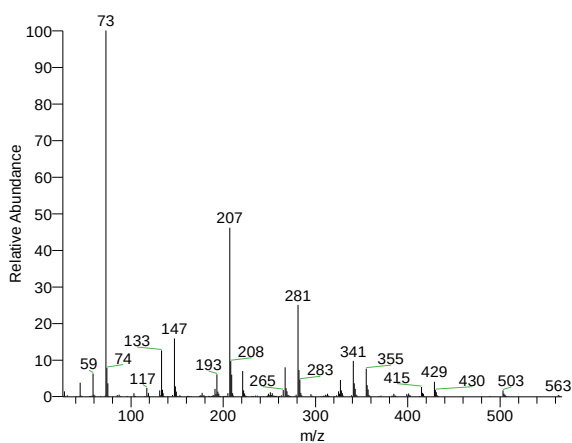
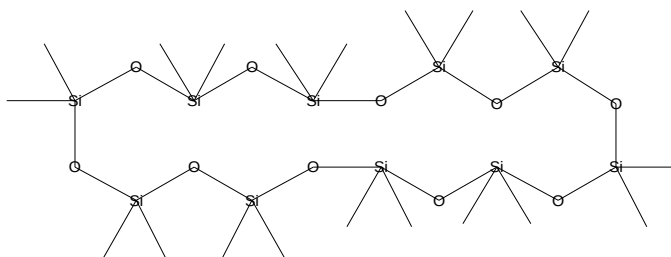
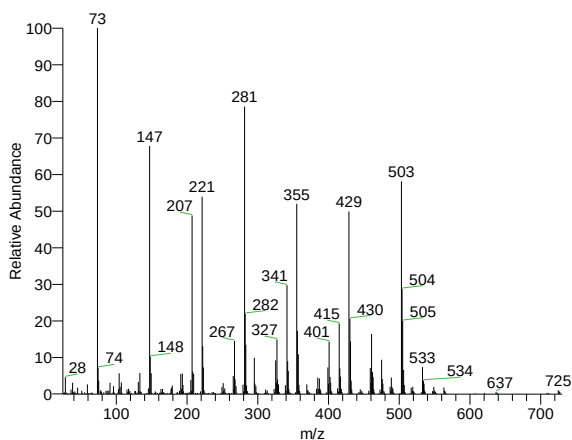
RT	Compound Name	Area	Probability	SI	RSI	Library
49.58	Cyclodecasiloxane, eicosamethyl-	3426430.09	41.12	461	522	mainlib
49.58	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3426430.09	11.20	430	521	mainlib
49.58	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3426430.09	6.45	414	541	mainlib
49.58	Cyclononasiloxane, octadecamethyl-	3426430.09	5.07	408	546	mainlib
49.58	2,5-Dihydroxybenzoic acid, 3TMS derivative	3426430.09	3.68	399	545	mainlib

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Hit Spectrum

Compound Structure



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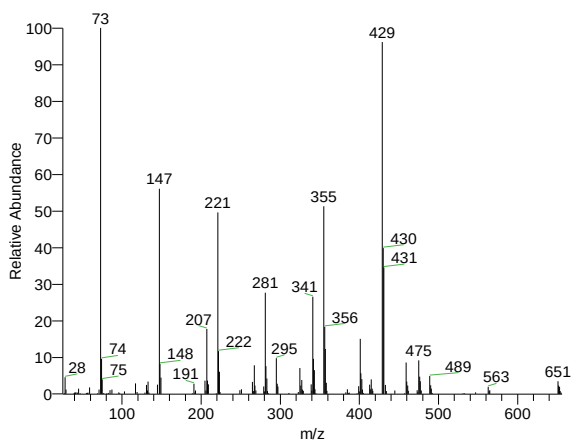
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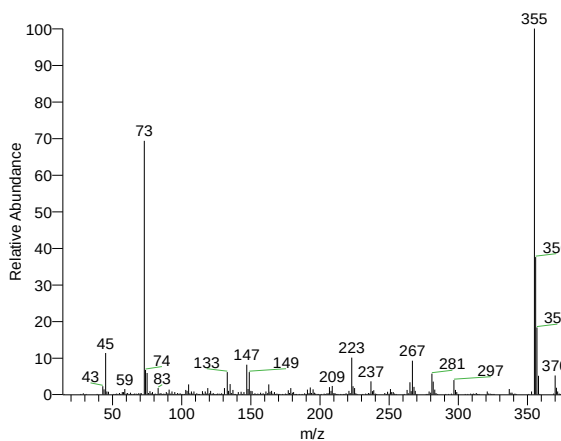
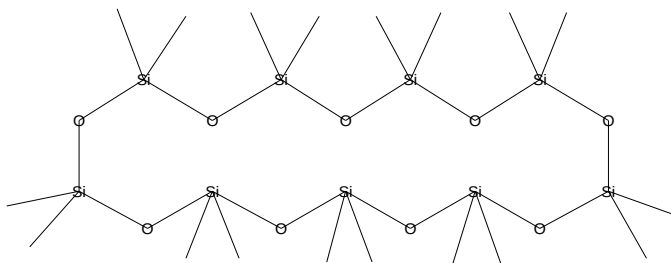
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

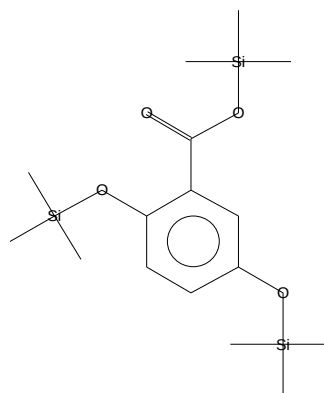
Compound Structure



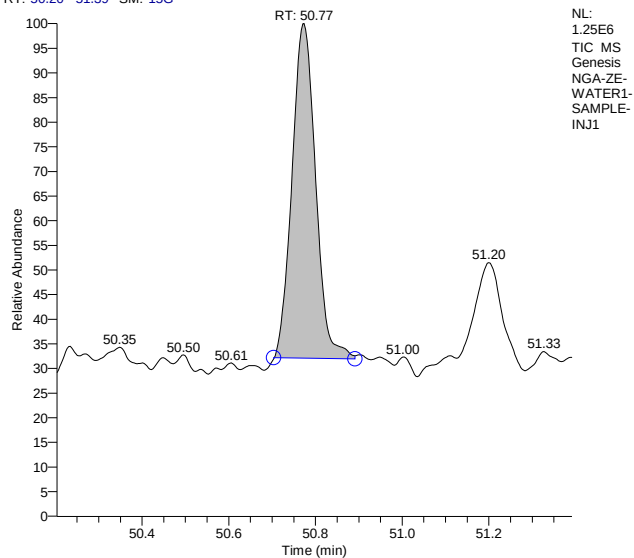
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



2,5-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-20-0, Entry# 234286
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester

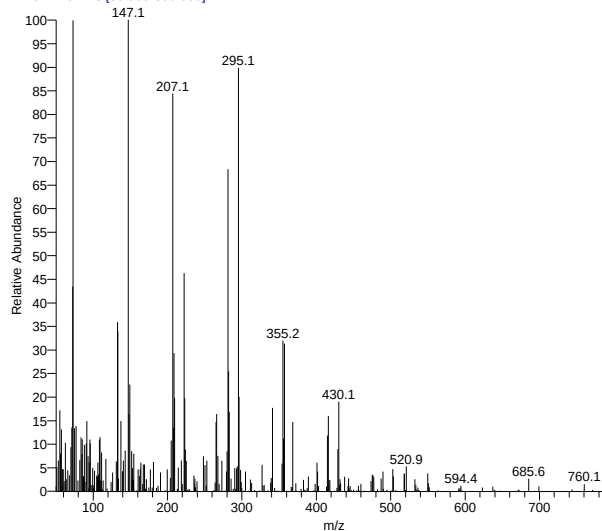


RT: 50.20 - 51.39 SM: 15G



NL:
1.25E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #13352 RT: 50.77 AV: 1 RF: 6.00, 3 NL: 7.10E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

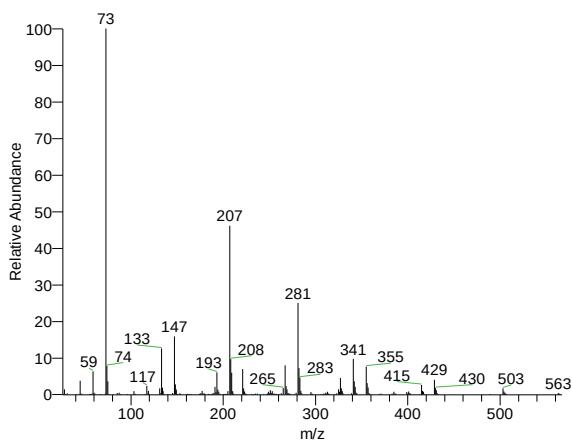
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ANALYTICAL CHEMISTRY DIVISION

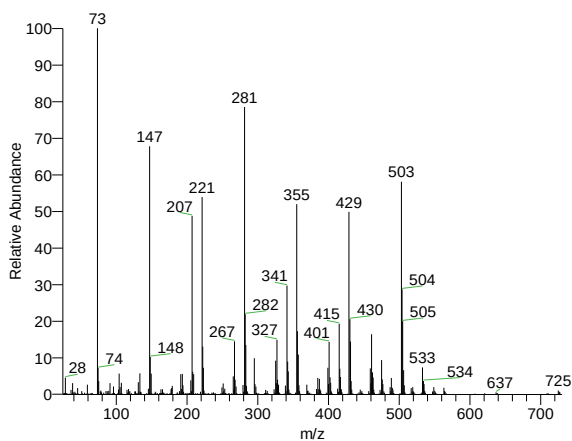
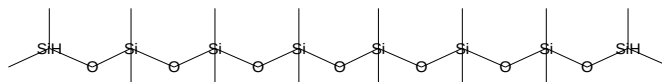
RT	Compound Name	Area	Probability	SI	RSI	Library
50.77	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3201182.88	48.25	514	627	mainlib
50.77	Cyclodecasiloxane, eicosamethyl-	3201182.88	12.63	481	520	mainlib
50.77	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3201182.88	8.16	468	587	mainlib
50.77	Cyclononasiloxane, octadecamethyl-	3201182.88	3.22	446	539	mainlib
50.77	Heptasiloxane, hexadecamethyl-	3201182.88	2.97	444	611	mainlib

Hit Spectrum

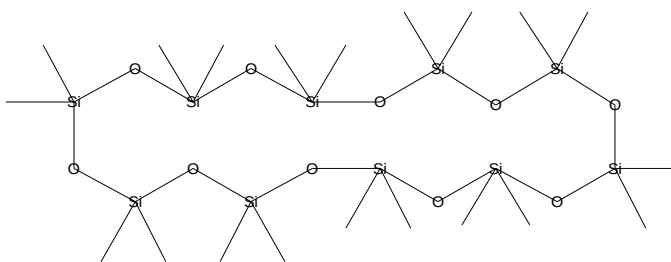


Compound Structure

Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Analysed by Satyanarayana

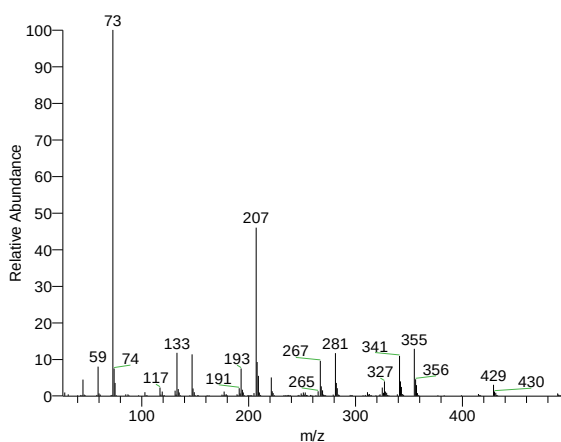
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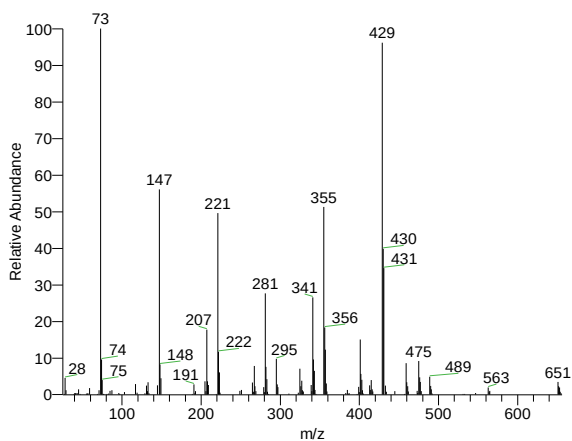
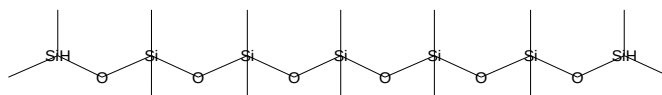
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

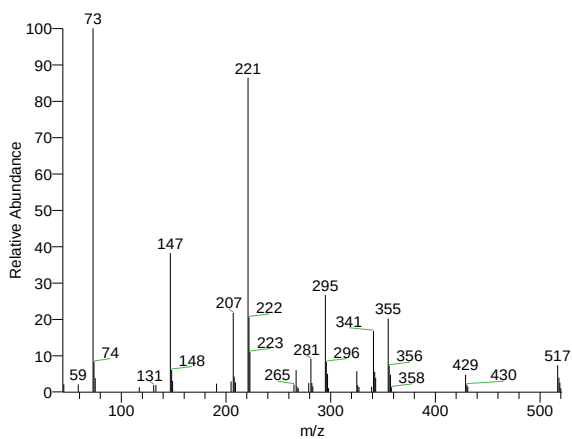
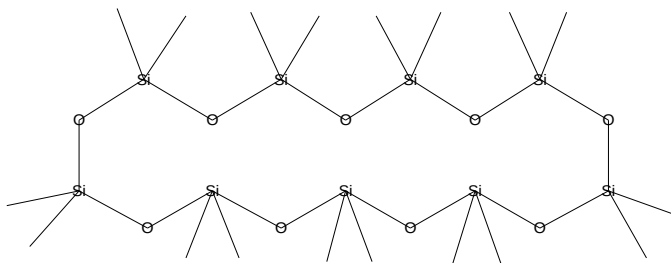
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



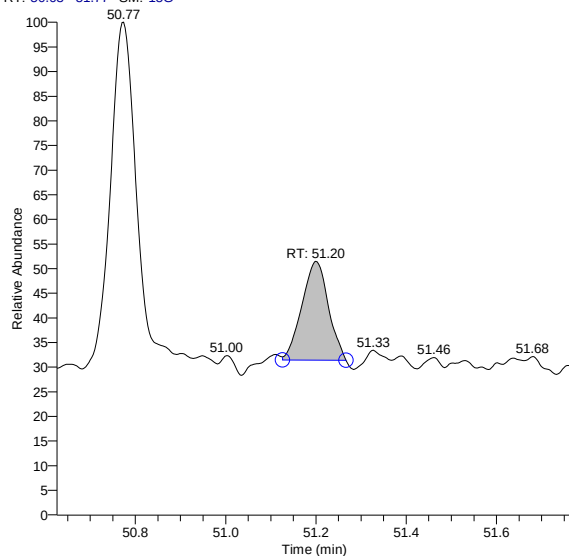
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Analysed by Satyanarayana

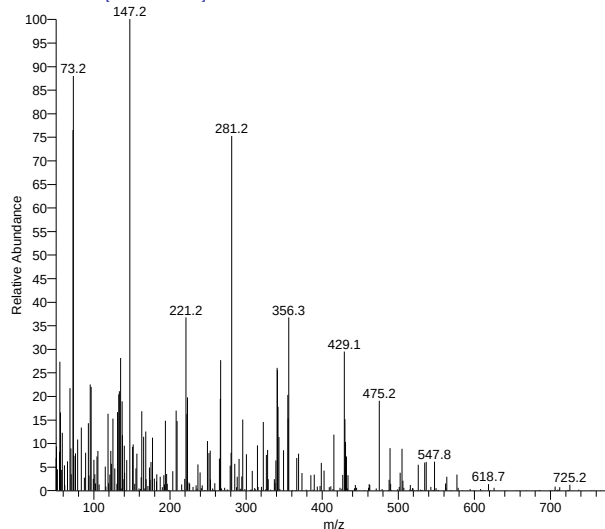
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

RT: 50.63 - 51.77 SM: 15G



NL:
1.25E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

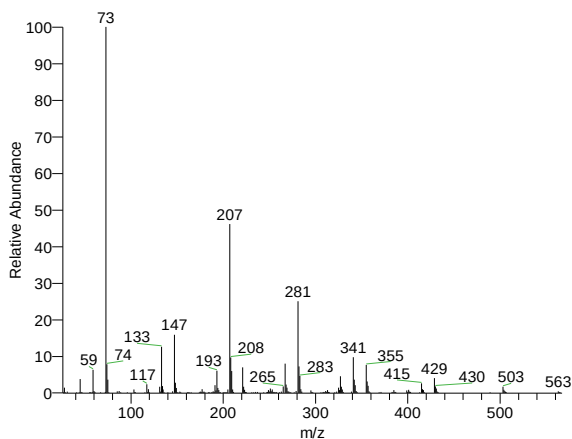
NGA-ZE-WATER1-SAMPLE-INJ1 #13479 RT: 51.20 AV: 1 RF: 6.00, 3 NL: 4.07E4
T: + c EI Full ms [50.000-800.000]



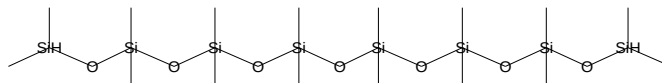
RT	Compound Name	Area	Probability	SI	RSI	Library
51.20	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1017803.23	23.38	454	562	mainlib
51.20	Cyclodecasiloxane, eicosamethyl-	1017803.23	14.17	439	487	mainlib
51.20	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1017803.23	11.97	435	564	mainlib
51.20	Cyclononasiloxane, octadecamethyl-	1017803.23	6.53	418	553	mainlib
51.20	1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane	1017803.23	5.52	414	775	mainlib

Hit Spectrum

Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

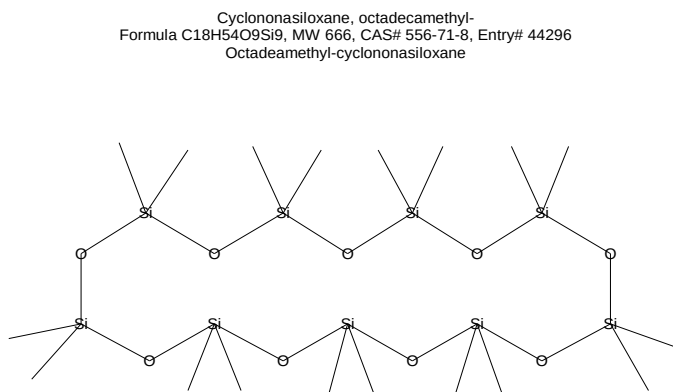
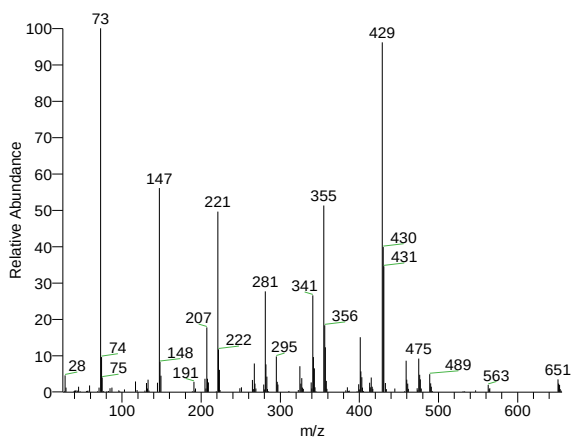
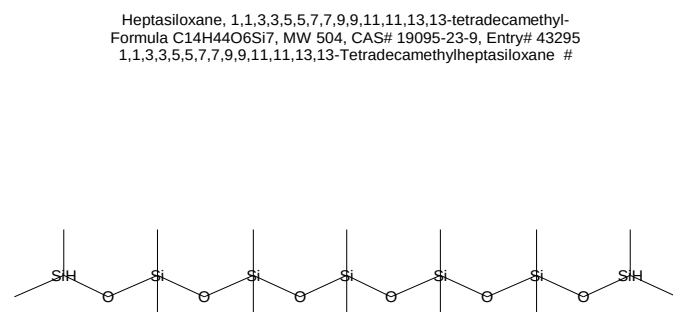
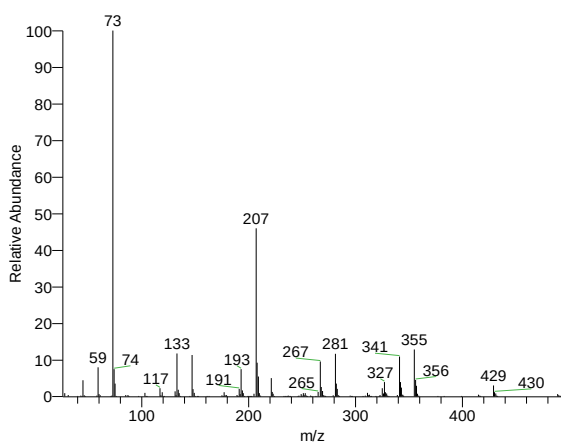
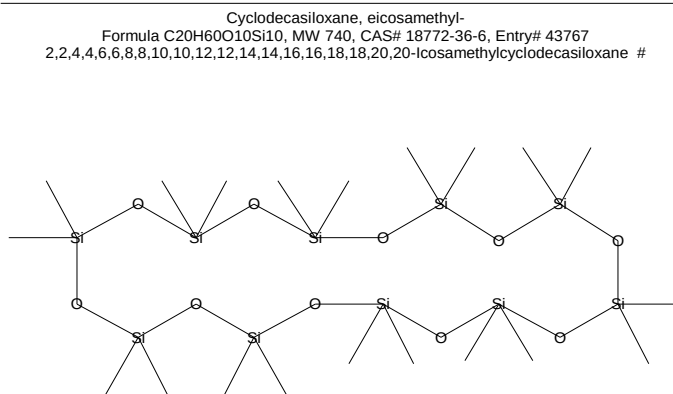
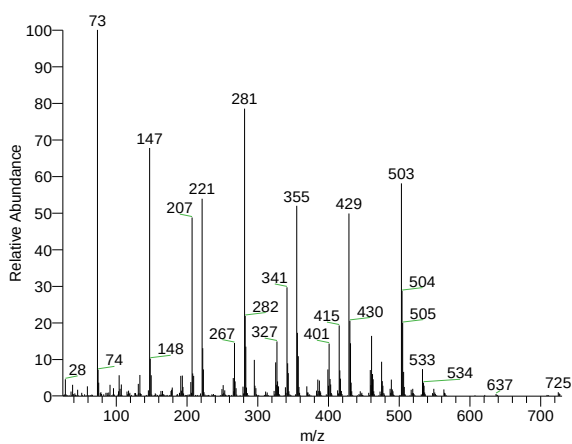
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Hit Spectrum

Compound Structure

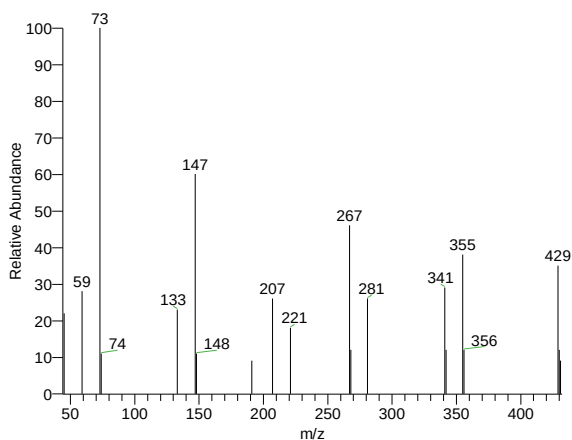


Analysed by Satyanarayana

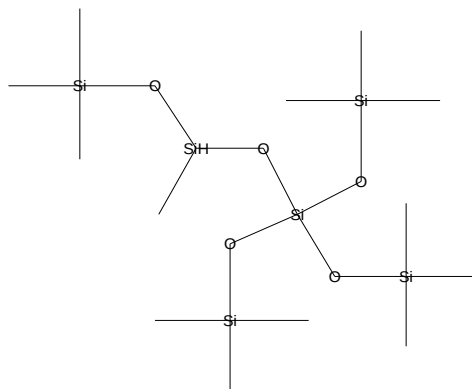
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Hit Spectrum

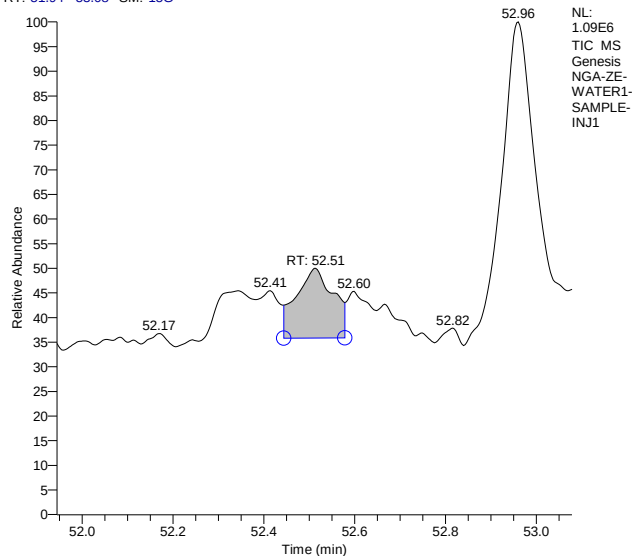
Compound Structure



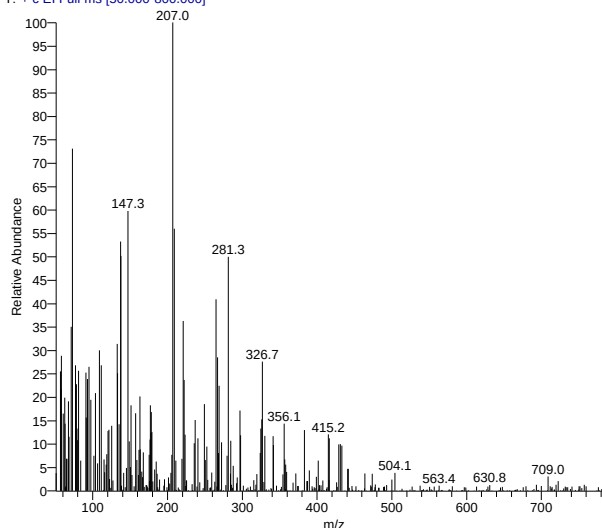
1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane
Formula C₁₃H₄₀O₅Si₆, MW 444, CAS# 38147-00-1, Entry# 42719
1,3,3,3-Tetramethyldisiloxanyl tris(trimethylsilyl) orthosilicate #



RT: 51.94 - 53.08 SM: 15G



NGA-ZE-WATER1-SAMPLE-INJ1 #13871 RT: 52.51 AV: 1 RF: 6.00, 3 NL: 2.75E4
T: + c EI Full ms [50.000-800.000]

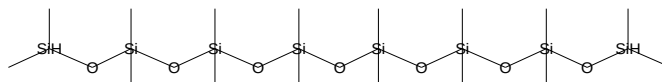
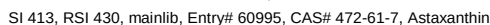


RT	Compound Name	Area	Probability	SI	RSI	Library
52.51	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	876479.40	13.87	426	550	mainlib
52.51	Astaxanthin	876479.40	8.96	413	430	mainlib
52.51	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	876479.40	8.26	411	536	mainlib
52.51	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	876479.40	7.94	410	548	mainlib
52.51	Spiro[adamantane-2,2'-[1,3]dithiolane]-1,5-dicarboxy lic acid, 6-oxo-	876479.40	3.38	389	463	mainlib

Analysed by Satyanarayana

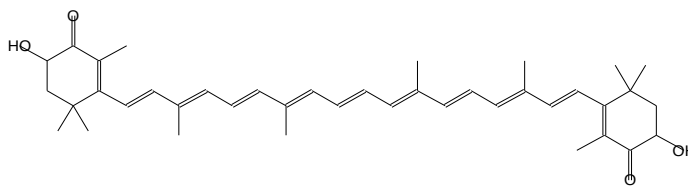
Hit Spectrum

Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #

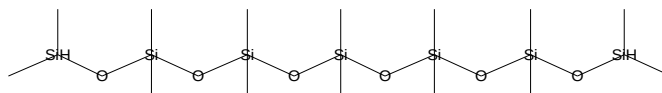


Astaxanthin

Formula C40H52O4, MW 596, CAS# 472-61-7, Entry# 60995
 á,á-Carotene-4,4'-dione, 3,3'-dihydroxy-, (3S,3'S)-



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₀O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

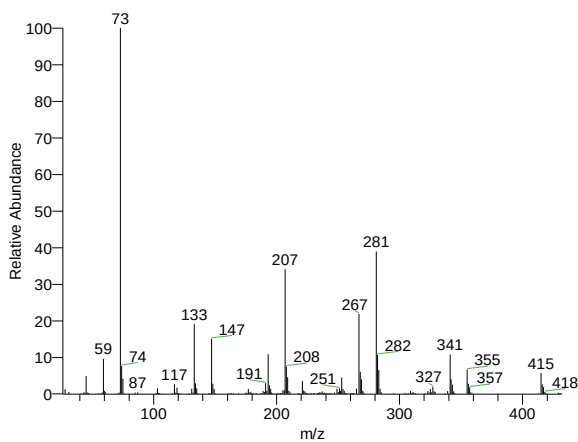
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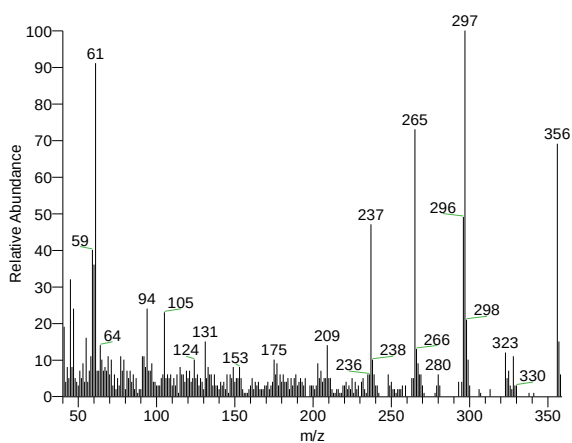
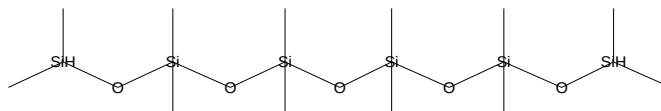
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Hit Spectrum

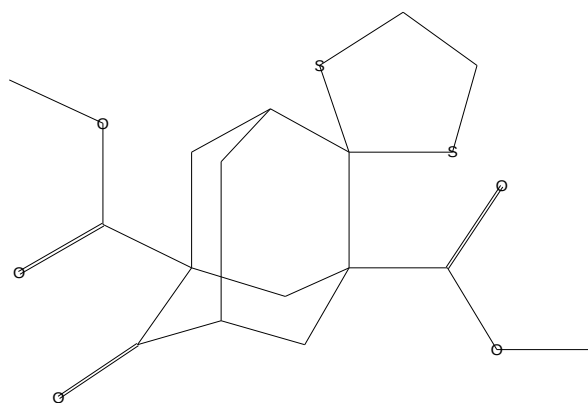
Compound Structure



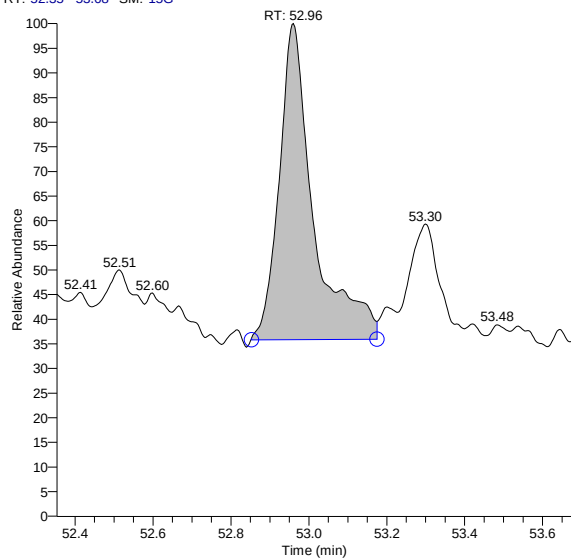
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Spiro[adamantane-2,2'-[1,3]dithiolane]-1,5-dicarboxylic acid, 6-oxo-
Formula C₁₆H₂₀O₅S₂, MW 356, CAS# 19930-84-8, Entry# 224096
\$:28GJWLQHCSAVLWOT-UHFFFAOYSA-N

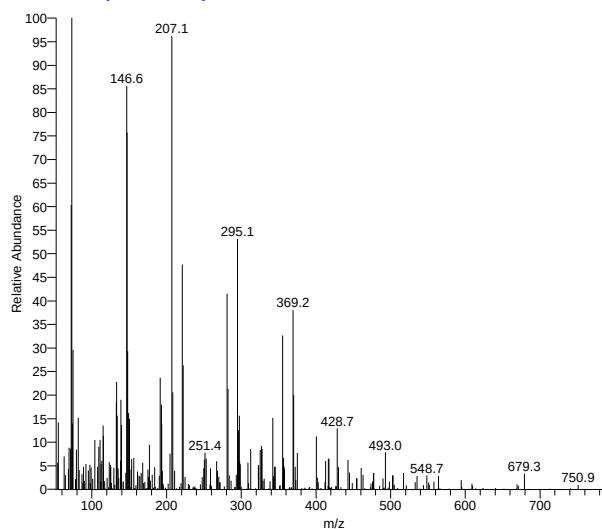


RT: 52.35 - 53.68 SM: 15G



NL:
1.09E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

NGA-ZE-WATER1-SAMPLE-INJ1 #14004 RT: 52.96 AV: 1 RF: 6.00, 3 NL: 6.55E4
T: + c EI Full ms [50.000-800.000]



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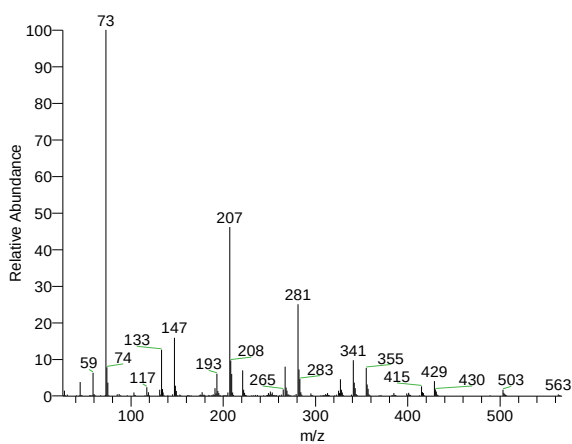
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ANALYTICAL CHEMISTRY DIVISION

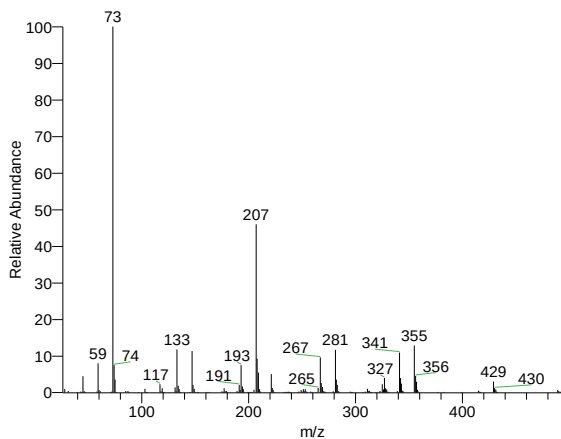
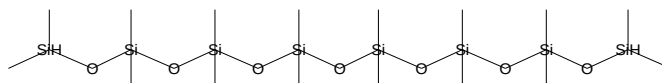
RT	Compound Name	Area	Probability	SI	RSI	Library
52.96	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	4282862.87	35.94	494	594	mainlib
52.96	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	4282862.87	10.96	469	599	mainlib
52.96	Heptasiloxane, hexadecamethyl-	4282862.87	9.68	466	696	mainlib
52.96	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	4282862.87	7.61	460	795	mainlib
52.96	Cyclodecasiloxane, eicosamethyl-	4282862.87	5.07	448	482	mainlib

Hit Spectrum

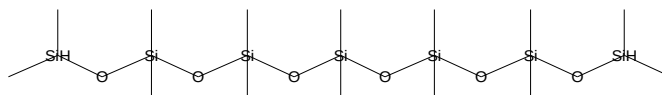
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



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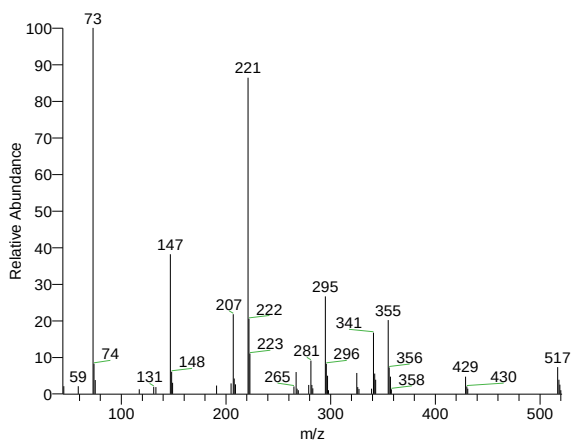
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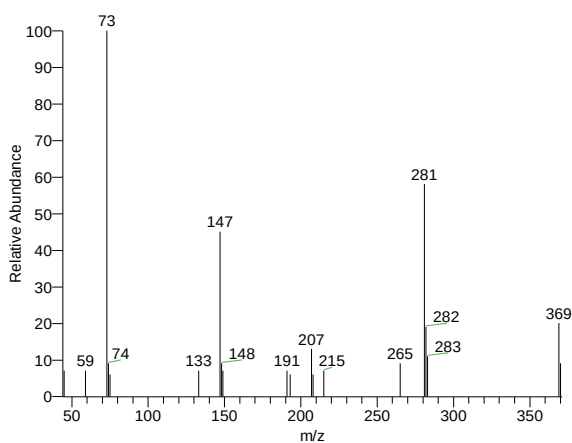
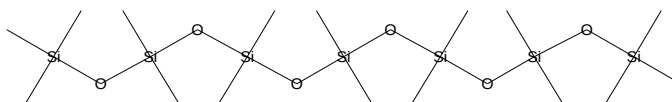
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Hit Spectrum

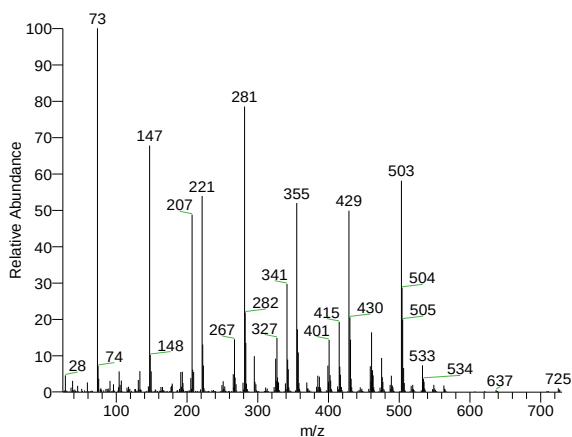
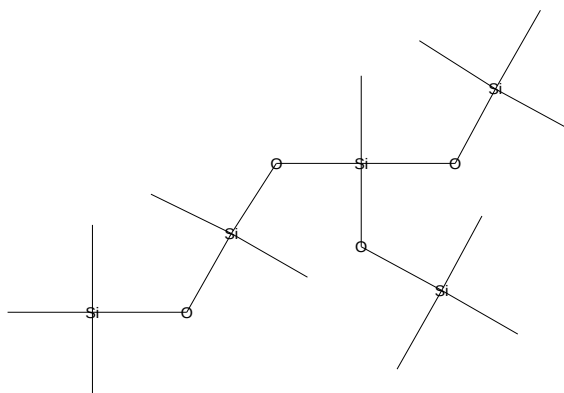
Compound Structure



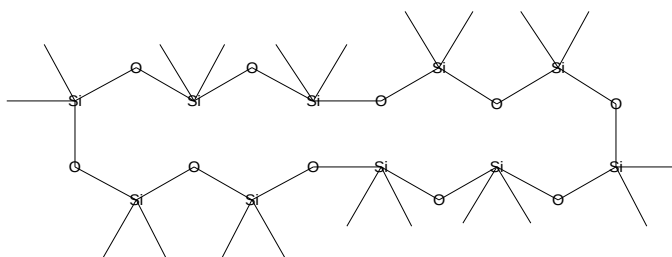
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

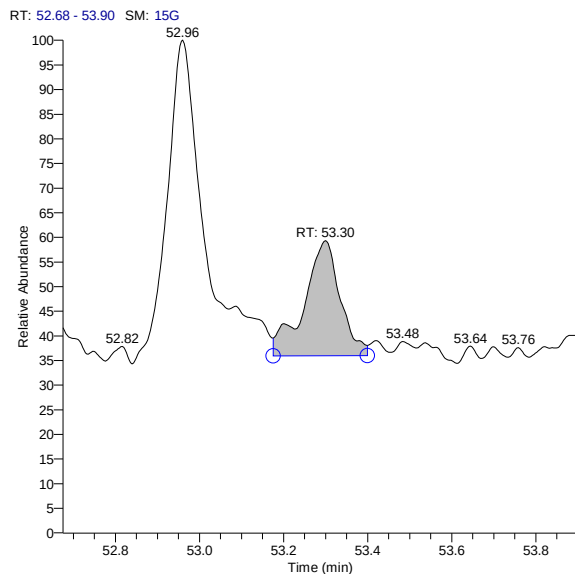


Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



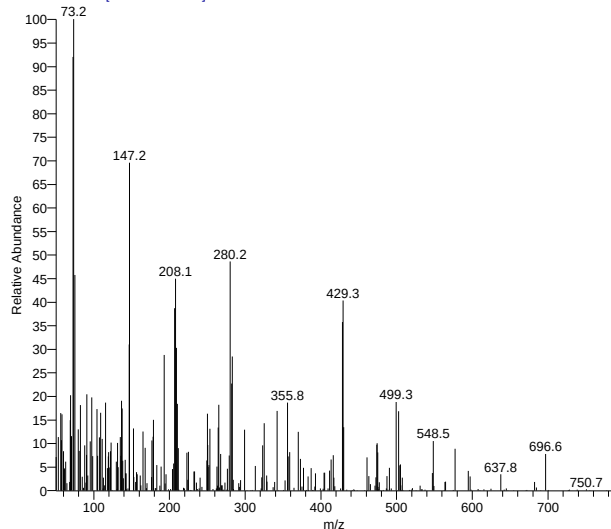
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NL:
1.09E6
TIC MS
Genesis
NGA-ZE-
WATER1-
SAMPLE-
INJ1

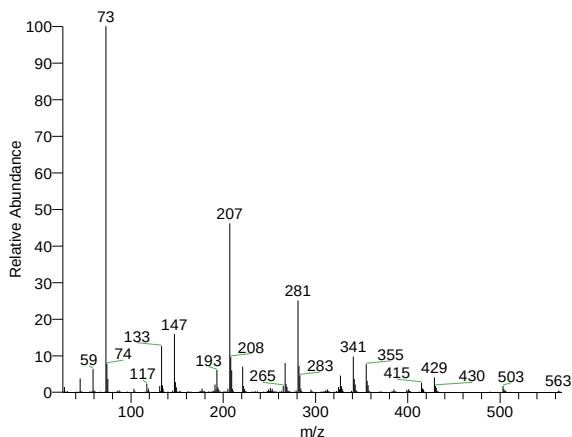
NGA-ZE-WATER1-SAMPLE-INJ1 #14105 RT: 53.30 AV: 1 RF: 6.00, 3 NL: 3.46E4
T: + c EI Full ms [50.000-800.000]



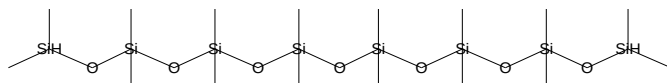
RT	Compound Name	Area	Probability	SI	RSI	Library
53.30	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1524693.34	9.43	392	513	mainlib
53.30	3,9á:14,15-Diepoxy pregn-16-en-20-one, 3,11á,18-triacetoxy-	1524693.34	7.41	386	459	mainlib
53.30	Cyclodecasiloxane, eicosamethyl-	1524693.34	6.84	384	436	mainlib
53.30	Norcodeine, N-trimethylsilyl-, trimethylsilyl ether	1524693.34	5.10	376	429	mainlib
53.30	Pregnan-20-one, 3,11,21-tris[(trimethylsilyl)oxy]-, O-(phenylmethyl)oxime, (3á,5á,11á)-	1524693.34	3.70	367	449	mainlib

Hit Spectrum

Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



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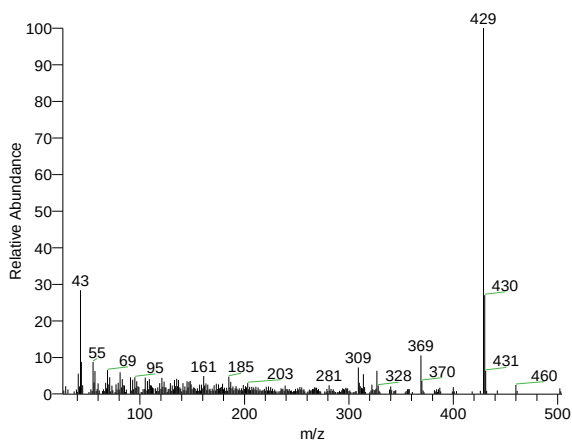
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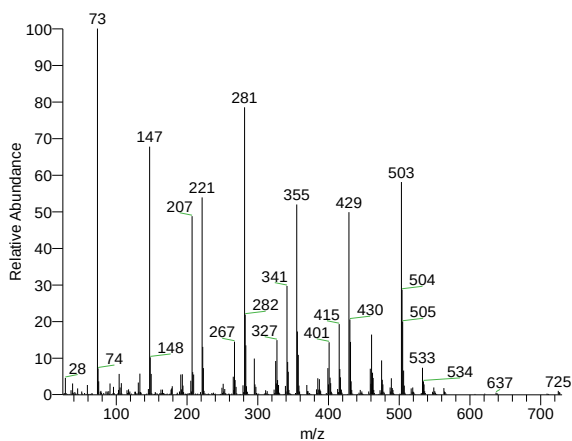
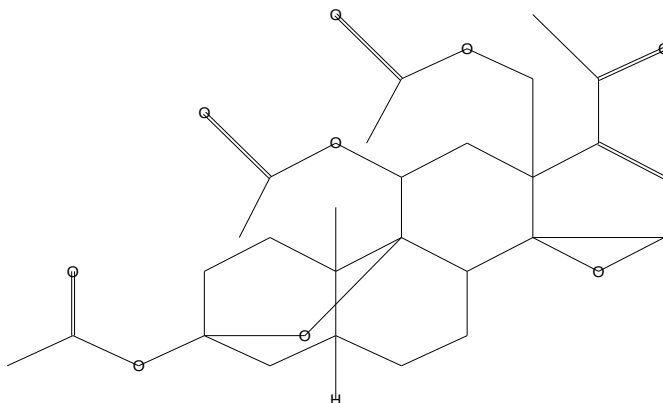
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

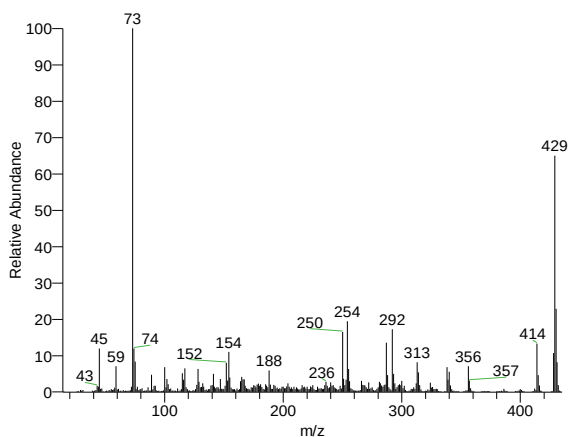
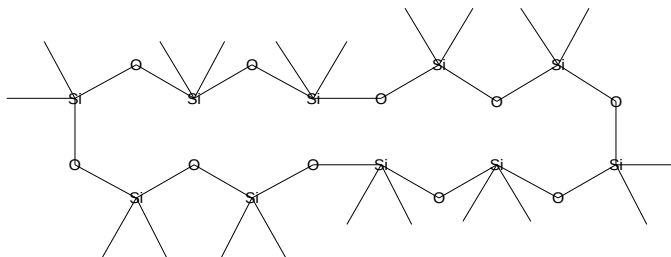
Compound Structure



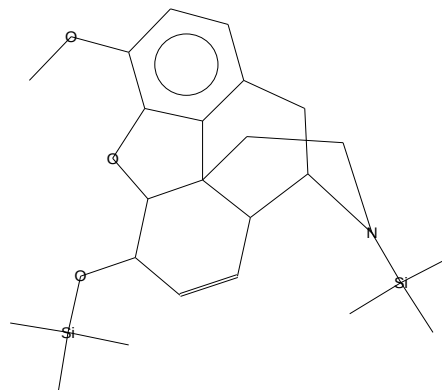
3,9a:14,15-Diepoxypregn-16-en-20-one, 3,11a,18-triacetoxy-
Formula C₂₇H₃₄O₉, MW 502, CAS# NA, Entry# 239582
\$:28GBYXRTQLWMZHST-UHFFFAOYSA-N



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Norcodeine, N-trimethylsilyl-, trimethylsilyl ether
Formula C₂₃H₃₅NO₃Si₂, MW 429, CAS# NA, Entry# 44301
\$:28VDNJLECFBKILGS-UHFFFAOYSA-N

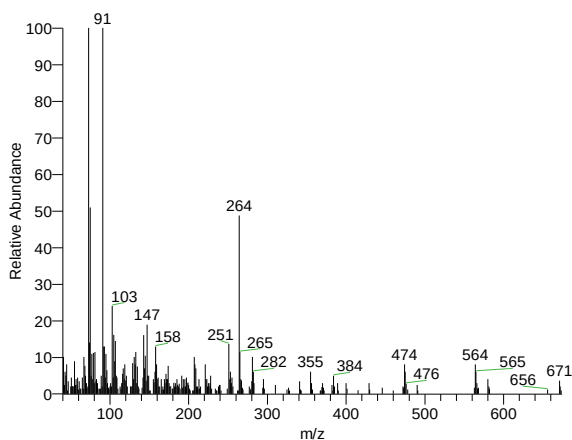


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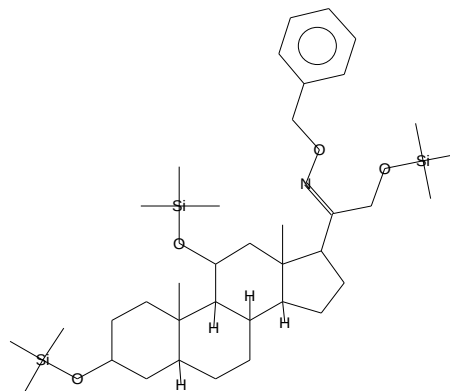
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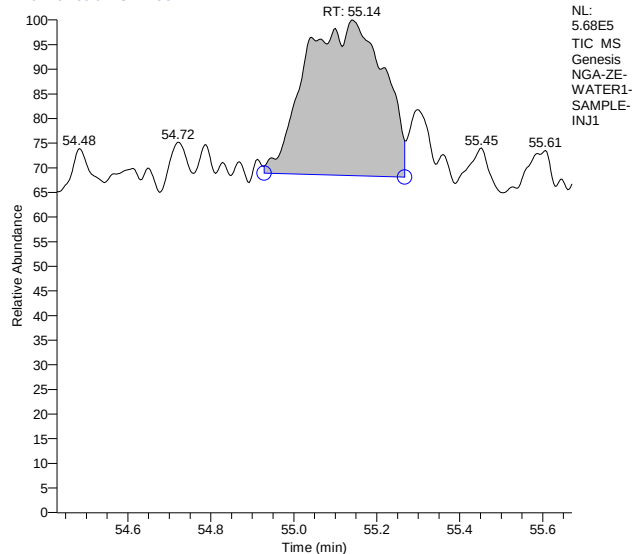
Compound Structure



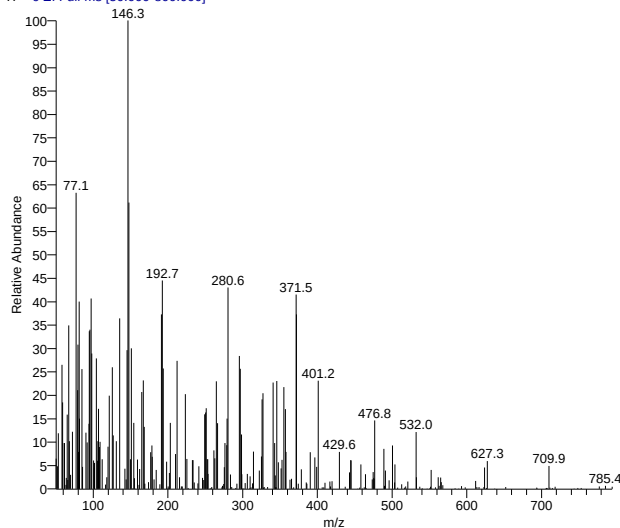
Pregnan-20-one, 3,11,21-tris[(trimethylsilyl)oxy]-, O-(phenylmethyl)oxime, (3 α ,5 α ,11 α)-
Formula C₃₇H₆₅NO₄Si₃, MW 671, CAS# 57326-18-8, Entry# 41727
3,11,21-Tris[(trimethylsilyl)oxy]pregnan-20-one o-benzyloxime #



RT: 54.43 - 55.67 SM: 15G



NGA-ZE-WATER1-SAMPLE-INJ1 #14654 RT: 55.14 AV: 1 RF: 6.00, 3 NL: 2.13E4
T: + c EI Full ms [50.000-800.000]



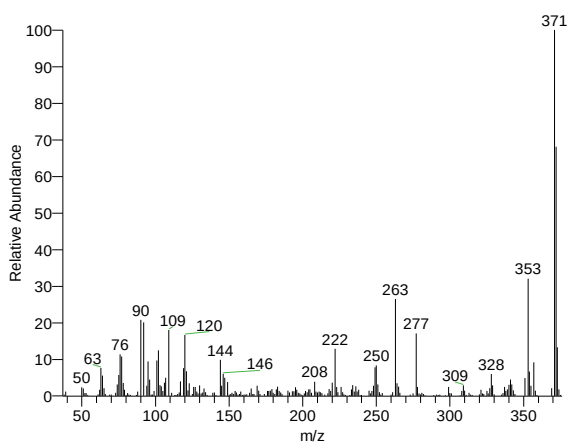
RT	Compound Name	Area	Probability	SI	RSI	Library
55.14	Quinazolin-4(3H)-one, 2-[2-(2-fluorophenyl)eth enyl]-3-(3-methoxyphenyl)-	2357776.36	5.27	341	430	mainlib
55.14	17 α -Hydroxyprogesterone, bis(O-ethyloxime)	2357776.36	5.06	340	383	mainlib
55.14	Medroxyprogesterone, bis(O-methyloxime)	2357776.36	4.28	336	391	mainlib
55.14	3-Desoxo-3,16-dihydroxy-1 2-desoxyphorbol	2357776.36	3.94	334	364	mainlib
55.14	3,13,16,20-tetraacetate Bufo-20,22-dienolide, 3,14-dihydroxy-, (3 α ,5 α)-	2357776.36	3.64	332	425	mainlib

Analysed by Satyanarayana

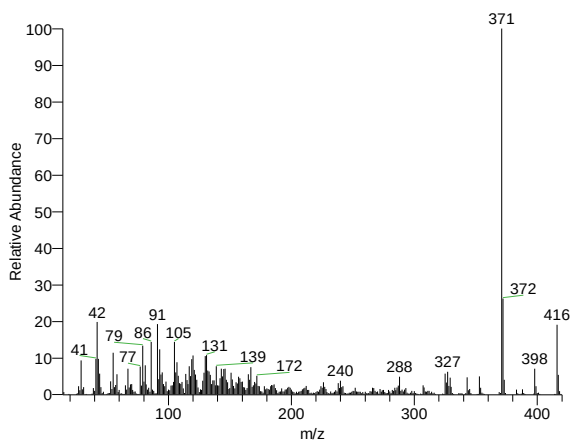
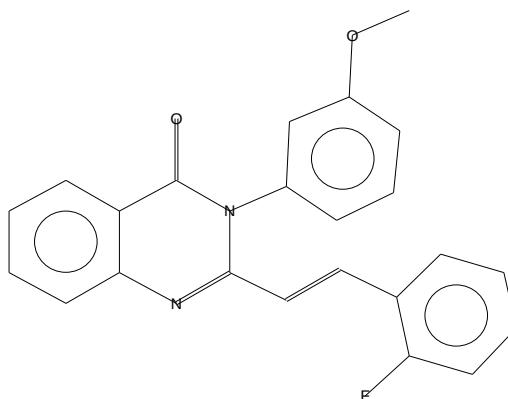
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Hit Spectrum

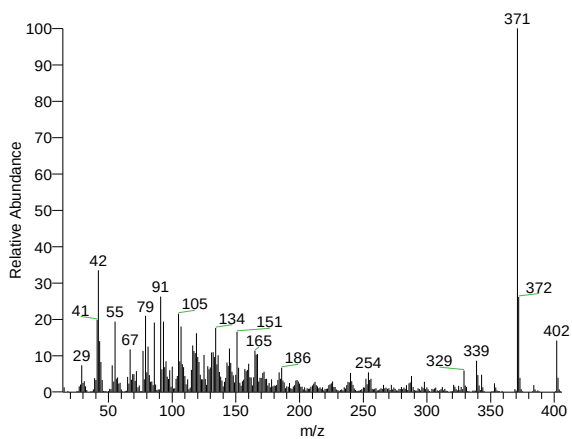
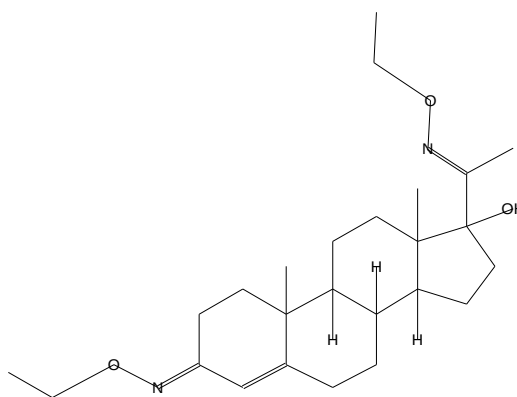
Compound Structure



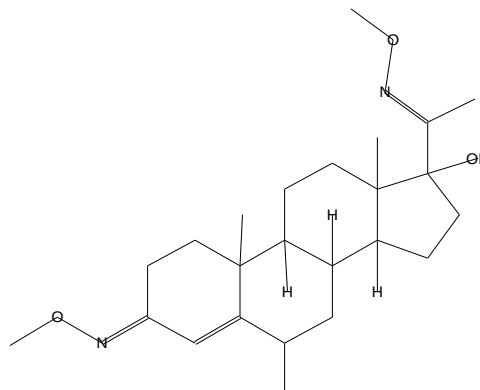
Quinazolin-4(3H)-one, 2-[2-(2-fluorophenyl)ethenyl]-3-(3-methoxyphenyl)-
Formula C₂₃H₁₇FN₂O₂, MW 372, CAS# 304880-63-5, Entry# 236089
2-[(E)-2-(2-Fluorophenyl)ethenyl]-3-(3-methoxyphenyl)-4(3H)-quinazolinone #



17α-Hydroxyprogesterone, bis(O-ethyloxime)
Formula C₂₅H₄₀N₂O₃, MW 416, CAS# NA, Entry# 236061
\$:28MMQREWWMXUHPU-QRFHMDMSA-N



Medroxyprogesterone, bis(O-methyloxime)
Formula C₂₄H₃₈N₂O₃, MW 402, CAS# NA, Entry# 235991
\$:28BSOUGPXCMBNBNR-ZZZAPRPPSA-N

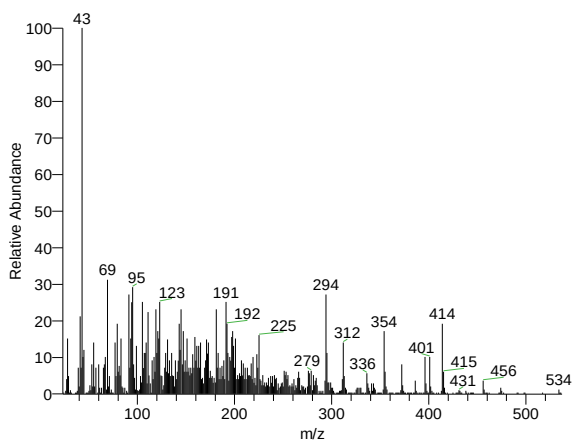


Analysed by Satyanarayana

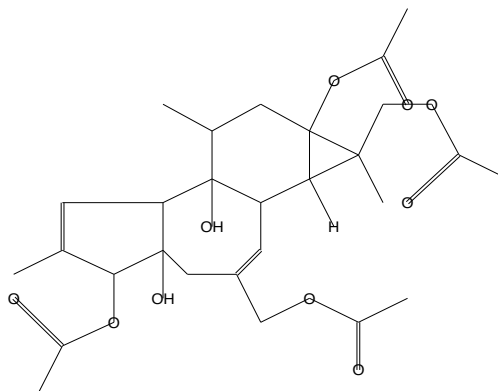
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

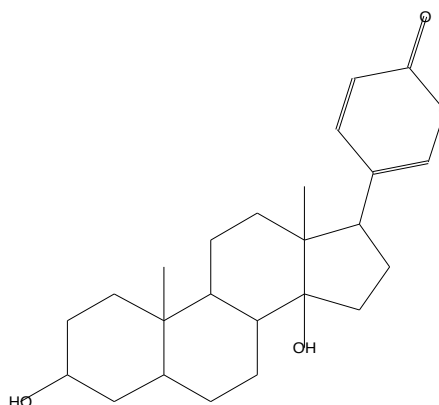
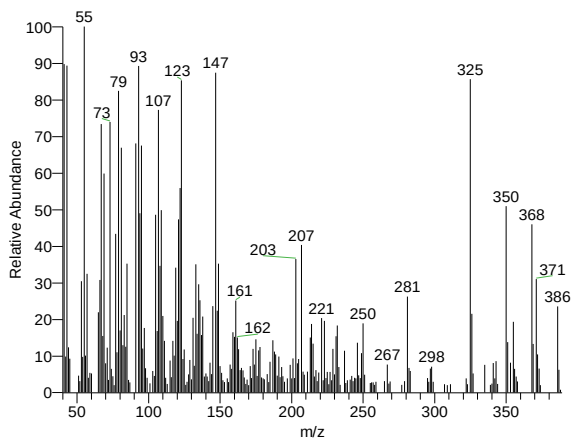
Compound Structure



3-Desoxo-3,16-dihydroxy-12-desoxyphorbol 3,13,16,20-tetraacetate
Formula C₂₈H₃₈O₁₀, MW 534, CAS# NA, Entry# 8568



Bufo-20,22-dienolide, 3,14-dihydroxy-, (3 α ,5 α)-
Formula C₂₄H₃₄O₄, MW 386, CAS# 465-21-4, Entry# 19060
5 α -Bufo-20,22-dienolide, 3 α ,14-dihydroxy-



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Data File:

Puga Groundwater

Original Data Path:

E:\Xcalibur\Data\2024\FEBRUARY-2024

Sample Name:

GCMS-FS

Acquisition Date:

03/01/24 03:02:52 AM

Run Time(min):

49.69

Vial:

13

Injection Volume(µl):

1.00

Low Mass(m/z):

50

High Mass(m/z):

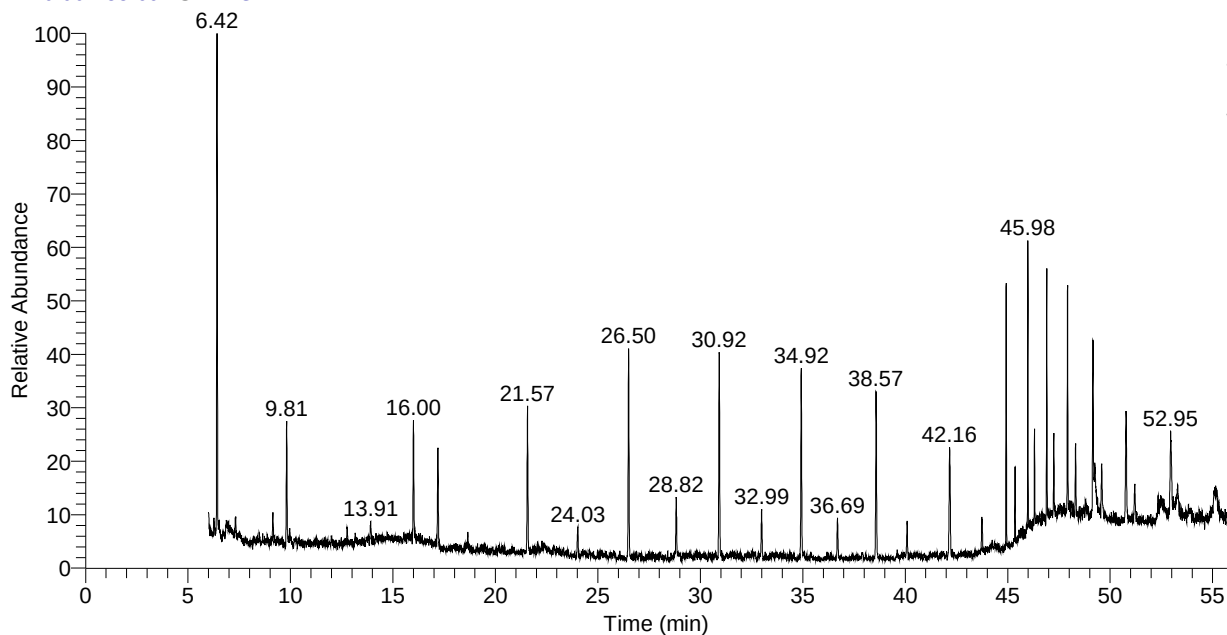
800

Instrument Method:

E:\Xcalibur\Methods\SAT_EW-DER.meth

Original Processing Method:

RT: 0.00 - 55.69 SM: 7G



NL:
2.91E6
TIC MS
NGA-ZE-
WATER4-
SAMPLE-
INJ1

Qual Peak Table

RT	Peak Area	Peak Height	S/N	Area %
6.41	5745925.60	2280904.40	33.50	9.69
9.14	353715.77	128807.57	2.68	0.60
9.81	1644439.75	579991.72	17.25	2.77
12.76	187585.90	71726.33	2.15	0.32
13.91	291230.57	93553.60	3.39	0.49
16.00	1857987.08	591485.33	10.46	3.13
17.19	1410989.82	469640.36	9.46	2.38
21.57	2180797.26	693509.50	17.35	3.68
24.02	385712.78	131551.69	3.08	0.65
26.50	3137474.30	1021915.57	26.69	5.29
28.82	972691.68	291431.86	8.04	1.64
30.92	3195655.80	1004167.11	33.60	5.39
32.99	732484.29	229003.85	6.00	1.24
34.93	2972016.78	933708.96	26.62	5.01
36.69	654999.85	199426.87	11.55	1.11
38.58	2682573.28	821546.56	37.26	4.53
40.09	560368.05	177730.82	6.77	0.95
42.17	2198754.08	552274.82	15.08	3.71
43.74	584799.78	167265.38	4.67	0.99
44.93	2028933.71	1049839.15	10.69	3.42

Analysed by Satyanarayana

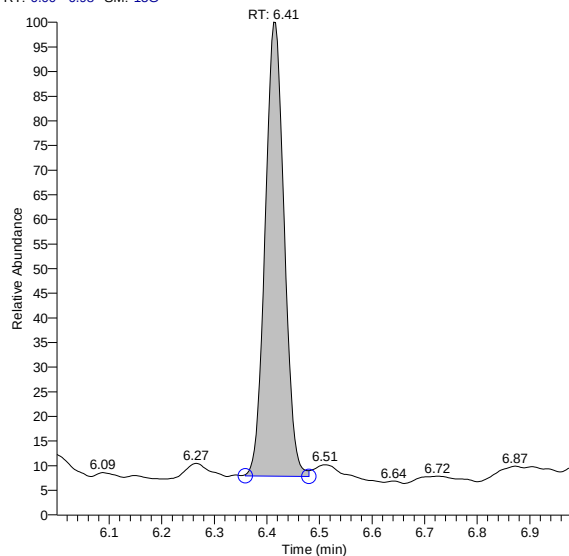
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RT	Peak Area	Peak Height	S/N	Area %
45.36	462492.73	270132.55	3.04	0.78
45.98	2312742.61	1163126.27	14.52	3.90
46.31	880288.86	404997.22	5.00	1.49
46.90	2417905.33	1065233.70	9.00	4.08
47.25	1002071.72	380111.63	3.15	1.69
47.92	2661753.57	1034408.36	9.64	4.49
48.31	881399.29	338141.59	3.16	1.49
49.16	2902502.77	869590.81	17.21	4.90
49.25	1474146.32	261127.08	5.33	2.49
49.59	1019817.26	262764.41	5.35	1.72
50.77	2099841.88	546167.12	14.71	3.54
51.20	667883.05	177641.98	5.60	1.13
52.33	362988.58	99444.71	2.40	0.61
52.50	913068.46	109296.47	2.53	1.54
52.95	2580592.09	445737.65	9.67	4.35
53.29	1178436.49	162929.40	3.27	1.99
55.10	822936.34	149538.97	2.54	1.39
55.15	852662.63	139735.52	2.38	1.44

Analysed by Satyanarayana

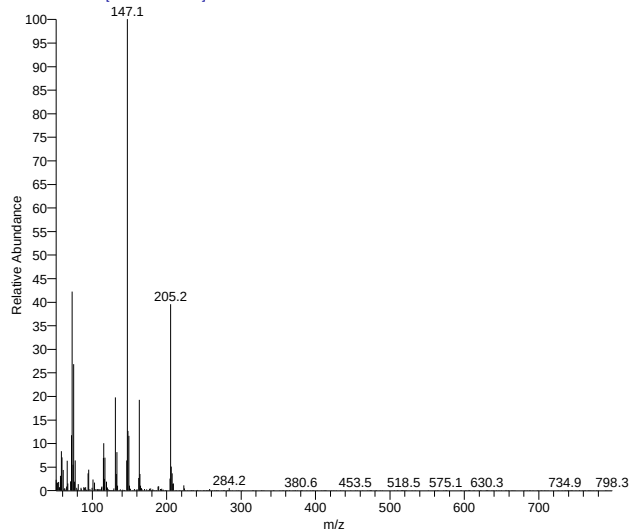
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RT: 6.00 - 6.98 SM: 15G



NL:
2.48E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

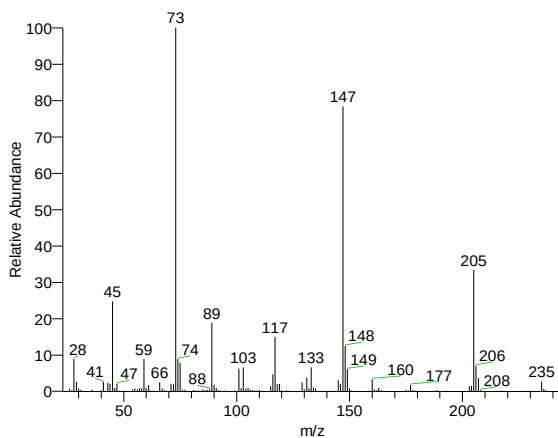
NGA-ZE-WATER4-SAMPLE-INJ1 #124 RT: 6.41 AV: 1 RF: 6.00, 3 NL: 7.38E5
T: + c EI Full ms [50.000-800.000]



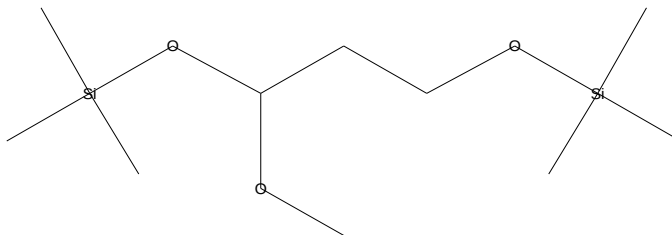
RT	Compound Name	Area	Probability	SI	RSI	Library
6.41	Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis(trimethyl-à-Hydroxyisobutyric acid, 2TMS derivative	5745925.60	31.80	723	740	mainlib
6.41	Glycolic acid, 2TMS derivative	5745925.60	29.33	721	758	mainlib
6.41	1,3-Propanediol, 2TMS derivative	5745925.60	7.83	689	724	mainlib
6.41	3-Trimethylsiloxyvaleric acid, trimethylsilyl ester	5745925.60	2.62	665	695	mainlib
6.41		5745925.60	1.90	656	692	mainlib

Hit Spectrum

Compound Structure



Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis(trimethyl-
Formula C10H26O3Si2, MW 250, CAS# 62185-57-3, Entry# 42666
Silane, [(1-methoxy-1,3-propanediyl)bis(oxy)]bis(trimethyl-



Analysed by Satyanarayana

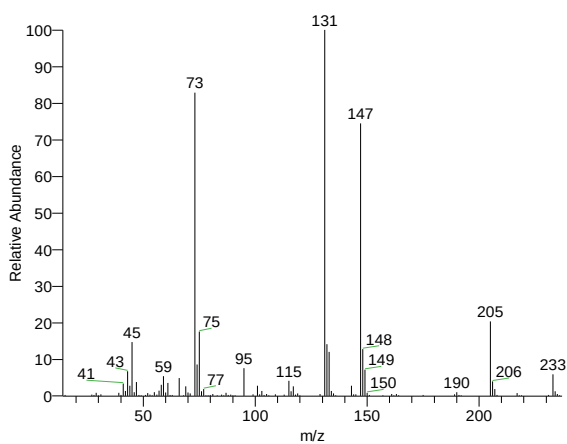
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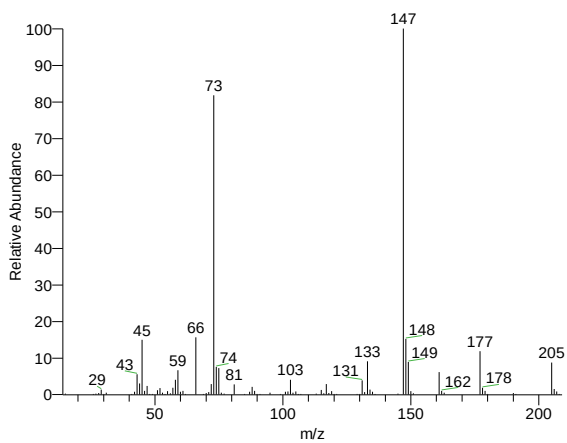
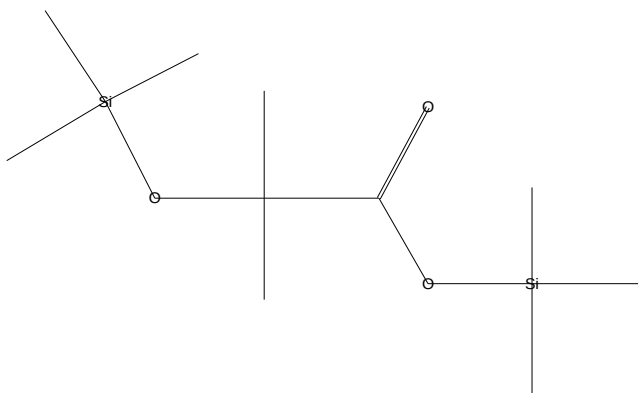
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

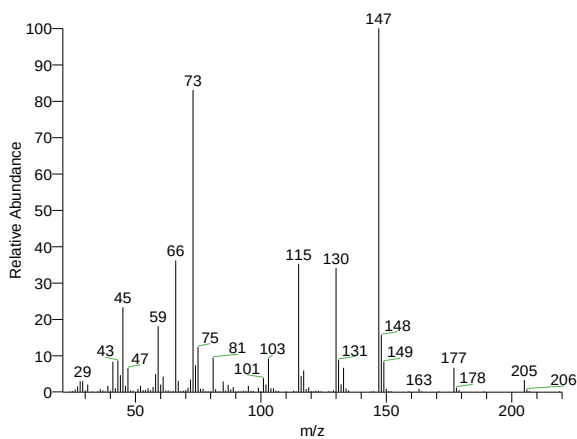
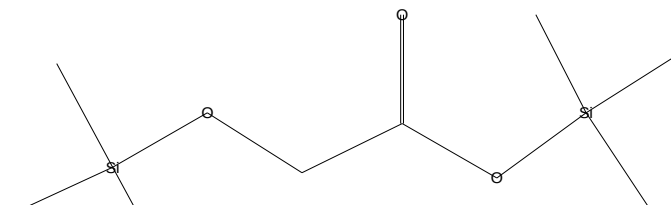
Compound Structure



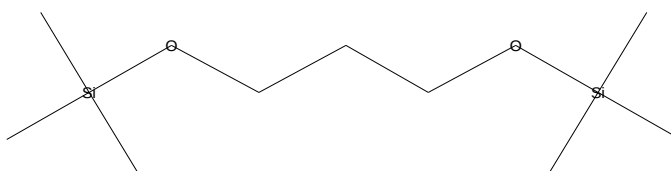
2-Hydroxyisobutyric acid, 2TMS derivative
Formula C₁₀H₂₄O₃Si₂, MW 248, CAS# 55133-92-1, Entry# 115549
Propanoic acid, 2-methyl-2-[(trimethylsilyl)oxy]-, trimethylsilyl ester



Glycolic acid, 2TMS derivative
Formula C₈H₂₀O₃Si₂, MW 220, CAS# 33581-77-0, Entry# 134871
Acetic acid, [(trimethylsilyl)oxy]-, trimethylsilyl ester



1,3-Propanediol, 2TMS derivative
Formula C₉H₂₄O₂Si₂, MW 220, CAS# 17887-80-8, Entry# 134870
3,7-Dioxa-2,8-disilanonane, 2,2,8,8-tetramethyl-

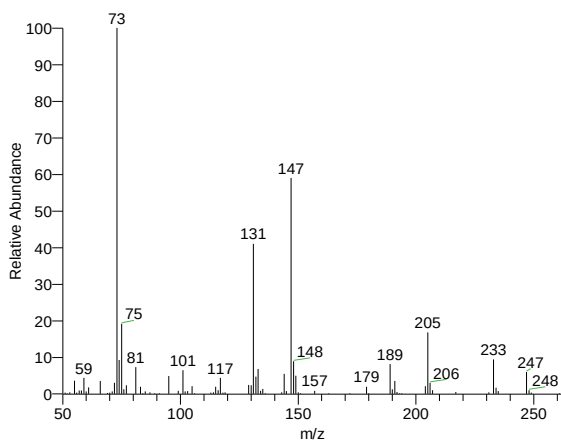


Analysed by Satyanarayana

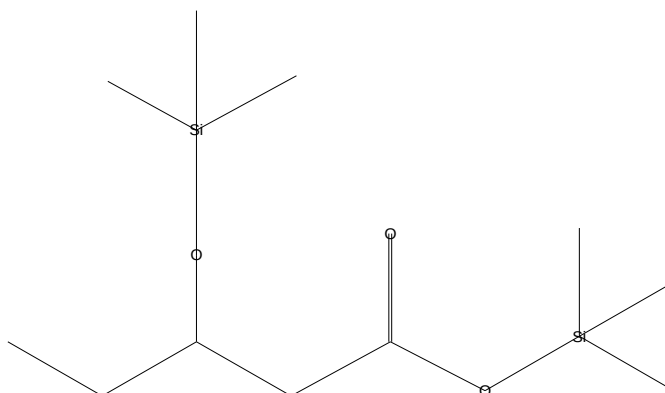
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Hit Spectrum

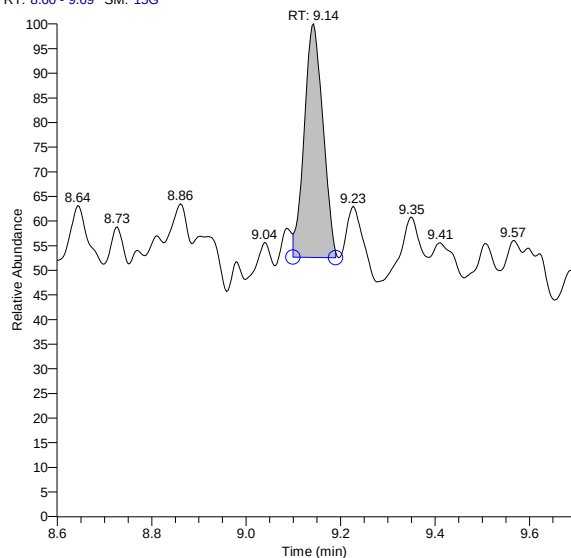
Compound Structure



3-Trimethylsiloxyvaleric acid, trimethylsilyl ester
Formula C₁₁H₂₆O₃Si₂, MW 262, CAS# 79628-62-9, Entry# 42595
3-Trimethylsilyloxyvaleric acid, trimethylsilyl ester

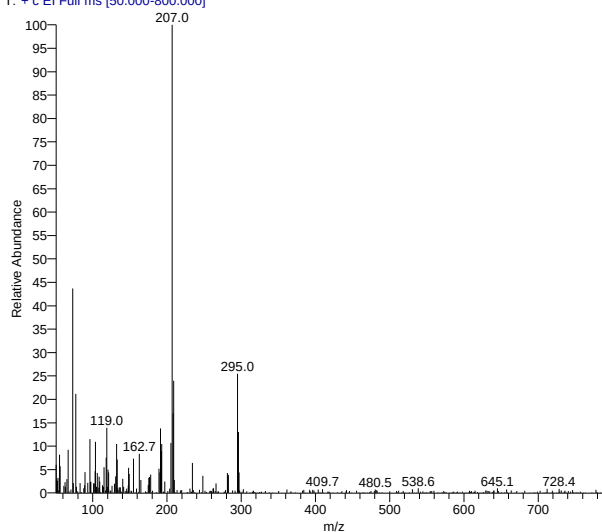


RT: 8.60 - 9.69 SM: 15G



NL:
2.72E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #938 RT: 9.14 AV: 1 RF: 6.00, 3 NL: 6.07E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.14	Tetrasiloxane, decamethyl-	353715.77	29.31	540	660	mainlib
9.14	Methyltris(trimethylsiloxy) silane	353715.77	29.31	540	680	mainlib
9.14	Cyclotrisiloxane, hexamethyl-	353715.77	4.08	468	725	mainlib
9.14	1,2-Benzisothiazol-3-amine , TBDMS derivative	353715.77	2.88	458	629	mainlib
9.14	Arsenous acid, tris(trimethylsilyl) ester	353715.77	2.32	453	684	mainlib

Analysed by Satyanarayana

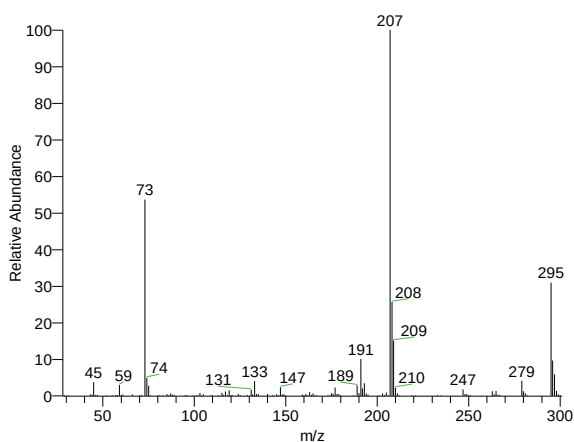
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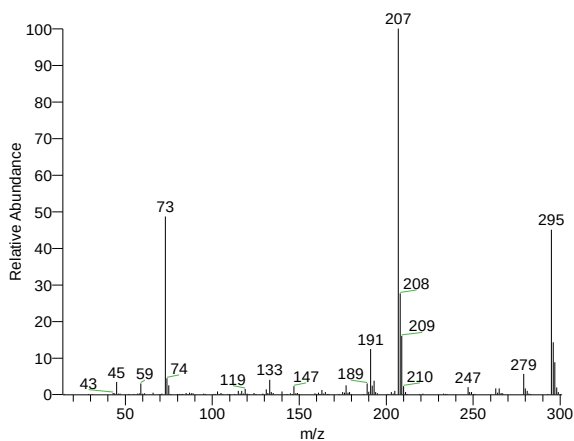
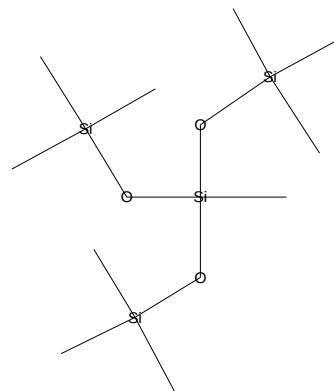
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

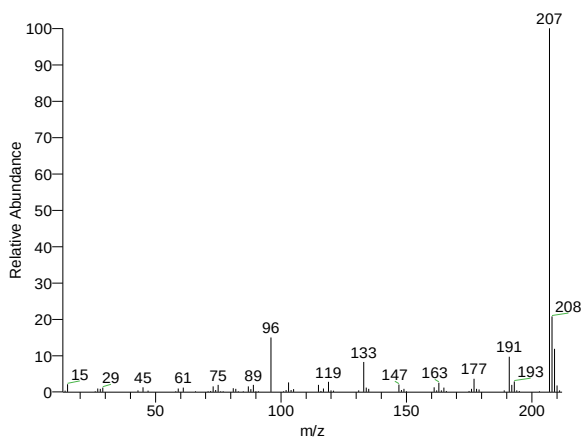
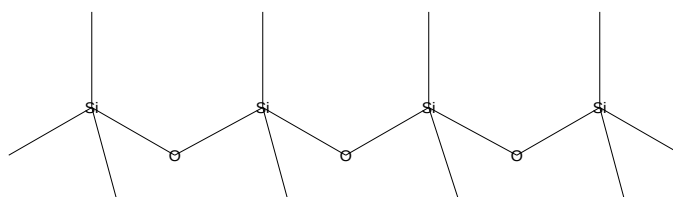
Compound Structure



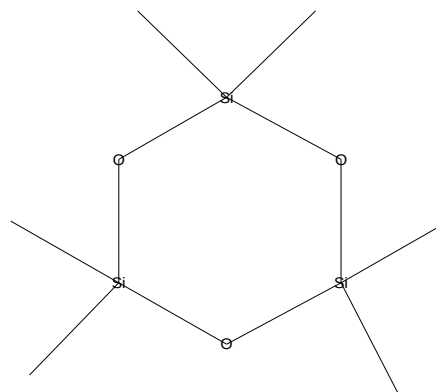
Methyltris(trimethylsiloxy)silane
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



Tetrasiloxane, decamethyl-
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 141-62-8, Entry# 188653
Decamethyltetrasiloxane



Cyclotrisiloxane, hexamethyl-
Formula C₆H₁₈O₃Si₃, MW 222, CAS# 541-05-9, Entry# 188945
Dimethylsiloxane cyclic trimer



Analysed by Satyanarayana

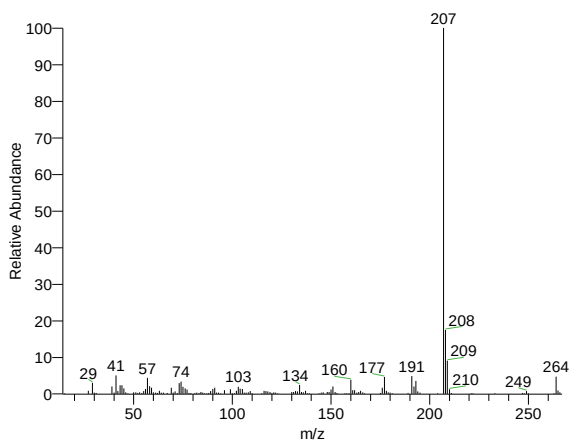
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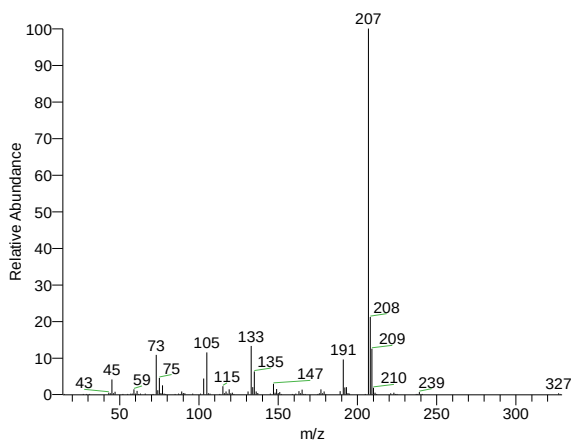
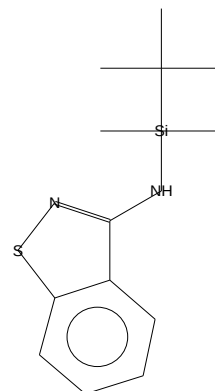
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

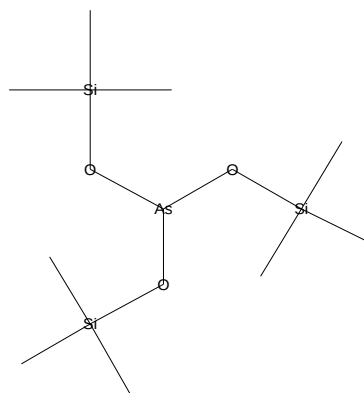
Compound Structure



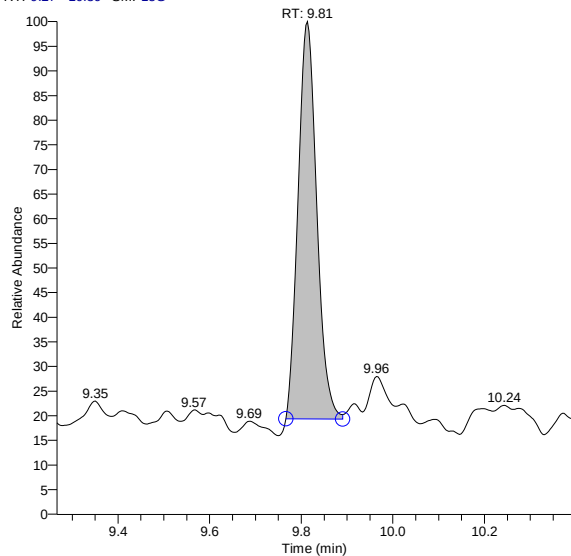
1,2-Benzisothiazol-3-amine, TBDMS derivative
Formula C₁₃H₂₀N₂SSi, MW 264, CAS# NA, Entry# 188958
1,2-Benzisothiazol-3-amine tbdms



Arsenous acid, tris(trimethylsilyl) ester
Formula C₉H₂₇AsO₃Si₃, MW 342, CAS# 55429-29-3, Entry# 188948
\$.28CWZNQWMMDOIFQC-UHFFFAOYSA-N

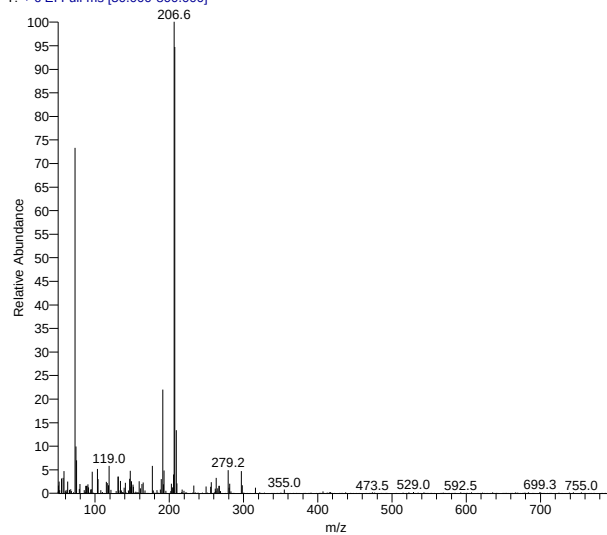


RT: 9.27 - 10.39 SM: 15G



NL:
7.19E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #1138 RT: 9.81 AV: 1 RF: 6.00, 3 NL: 1.96E5
T: + c EI Full ms [50,000-800,000]



RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	4-tert-Octylphenol, TMS derivative	1644439.75	20.82	642	793	mainlib

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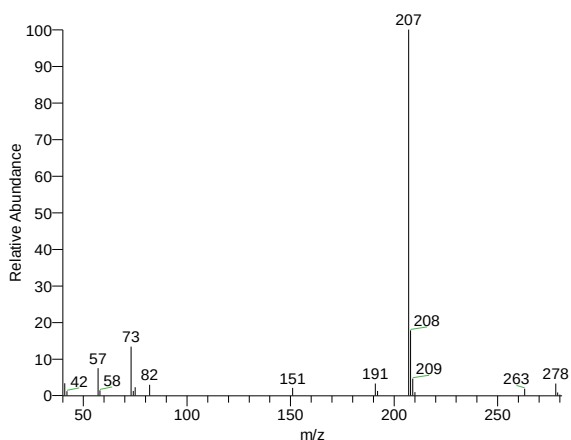
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

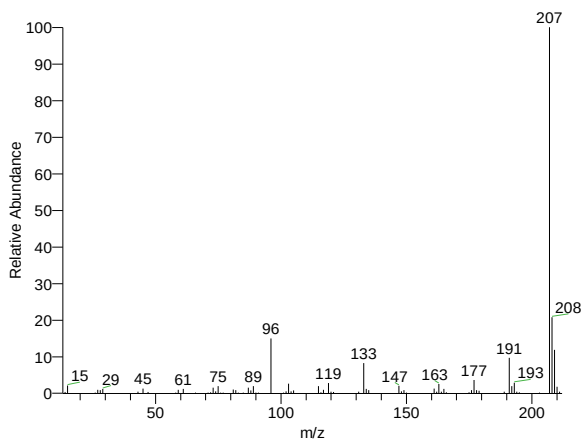
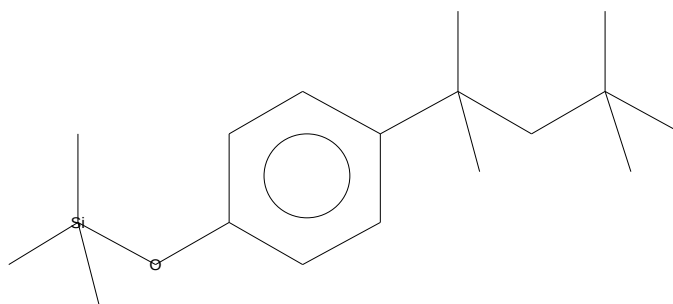
RT	Compound Name	Area	Probability	SI	RSI	Library
9.81	Cyclotrisiloxane, hexamethyl-	1644439.75	12.62	627	723	mainlib
9.81	Arsenous acid, tris(trimethylsilyl) ester	1644439.75	11.64	625	702	mainlib
9.81	Methyltris(trimethylsiloxy)silane	1644439.75	7.05	610	636	mainlib
9.81	2,4,6-Cycloheptatrien-1-one, 3,5-bis-trimethylsilyl-	1644439.75	5.95	606	665	mainlib

Hit Spectrum

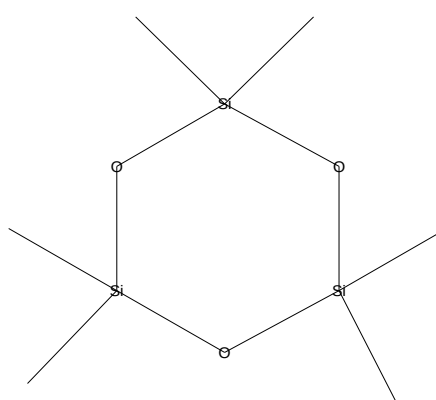
Compound Structure



4-tert-Octylphenol, TMS derivative
Formula C₁₇H₃₀O₂Si, MW 278, CAS# 78721-87-6, Entry# 188940
Trimethyl[4-(1,1,3,3,-tetramethylbutyl)phenoxy]silane



Cyclotrisiloxane, hexamethyl-
Formula C₆H₁₈O₃Si₃, MW 222, CAS# 541-05-9, Entry# 188945
Dimethylsiloxane cyclic trimer



Analysed by Satyanarayana

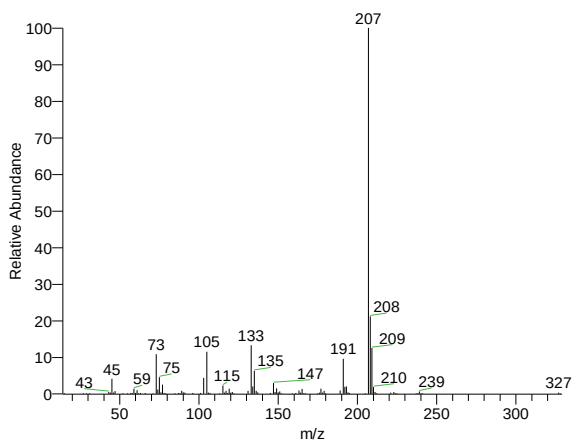
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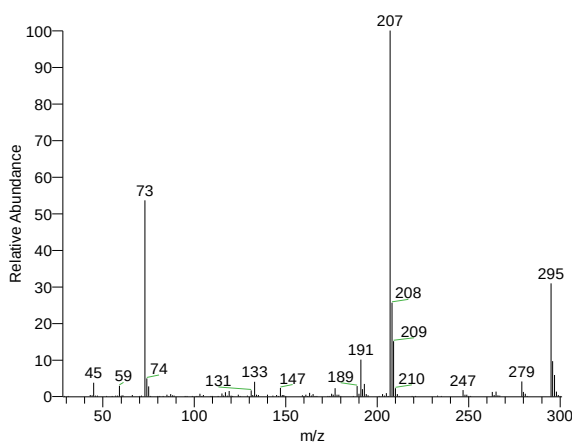
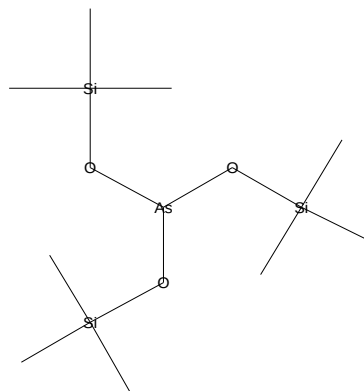
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

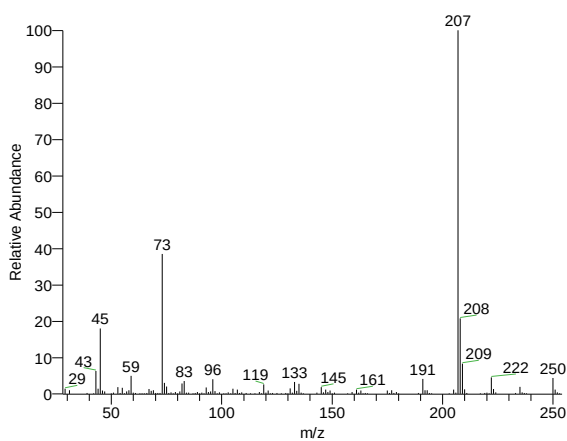
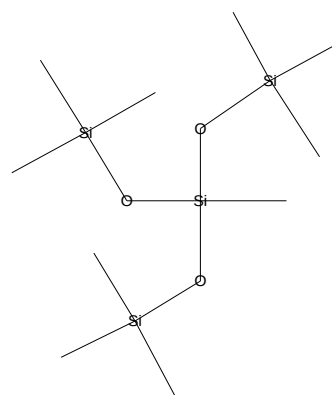
Compound Structure



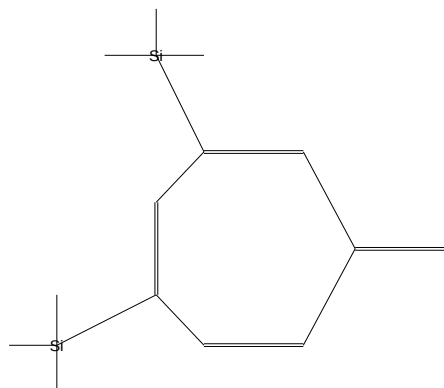
Arsenous acid, tris(trimethylsilyl) ester
Formula C₉H₂₇AsO₃Si₃, MW 342, CAS# 55429-29-3, Entry# 188948
\$:28CWZNQWMMDOIFQC-UHFFFAOYSA-N



Methyltris(trimethylsiloxy)silane
Formula C₁₀H₃₀O₃Si₄, MW 310, CAS# 17928-28-8, Entry# 188654
Trisiloxane, 1,1,1,3,5,5,5-heptamethyl-3-[(trimethylsilyl)oxy]-



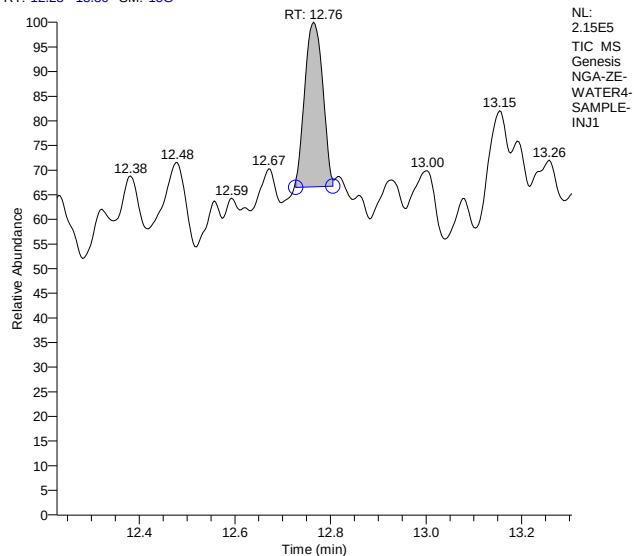
2,4,6-Cycloheptatrien-1-one, 3,5-bis(trimethylsilyl)-
Formula C₁₃H₂₂O₂Si₂, MW 250, CAS# NA, Entry# 188644
3,5-Bis(trimethylsilyl)-2,4,6-cycloheptatrien-1-one #



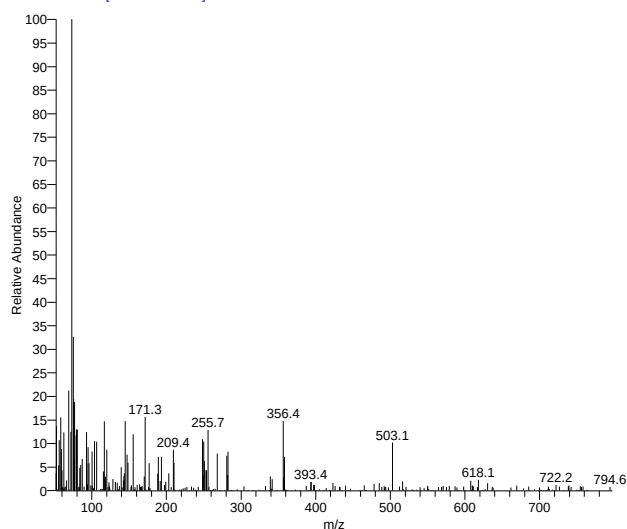
Analysed by Satyanarayana

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ANALYTICAL CHEMISTRY DIVISION

RT: 12.23 - 13.30 SM: 15G



NGA-ZE-WATER4-SAMPLE-INJ1 #2018 RT: 12.76 AV: 1 RF: 6.00, 3 NL: 3.06E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
12.76	4-(5-Chloro-2-methoxyphenyl)-5-cyclopropyl-1,2,4-triazole-3-thiol	187585.90	5.56	340	479	mainlib
12.76	t-Butyl-(2-[3-(2,2-dimethyl-6-methylene-cyclohexyl)-propyl]-[1,3]dithian-2-yl)-dimethyl-silane	187585.90	4.91	337	451	mainlib
12.76	Prost-13-en-1-oic acid, 9-(methoxyimino)-11,15-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester, (8.xi.,12.xi.)-	187585.90	3.66	329	382	mainlib
12.76	Thiazolo[3,2-a]benzimidazole-3(2H)-one, 2-(3-bromobenzylidene)-	187585.90	2.95	324	424	mainlib
12.76	Acetic acid, (2,4,5-trichlorophenoxy)-, 2-(2-methylpropoxy)ethyl ester	187585.90	2.32	318	400	mainlib

Analysed by Satyanarayana

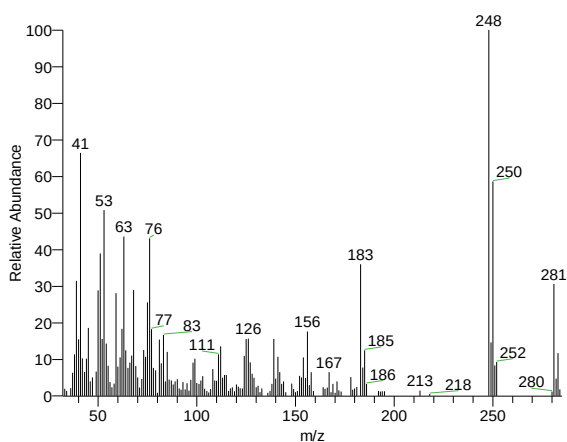
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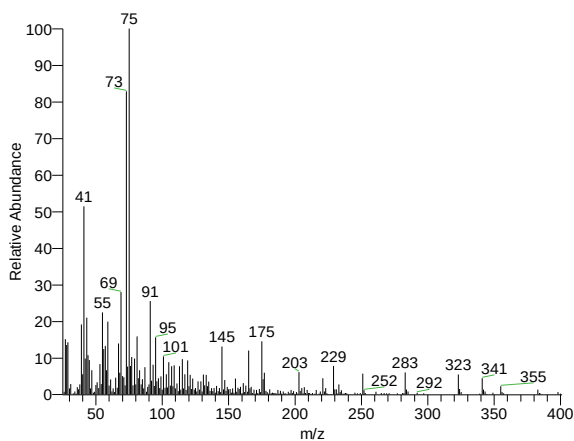
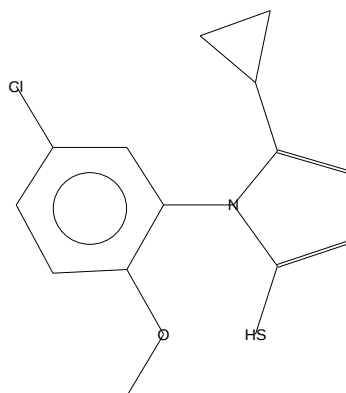
ANALYTICAL CHEMISTRY DIVISION

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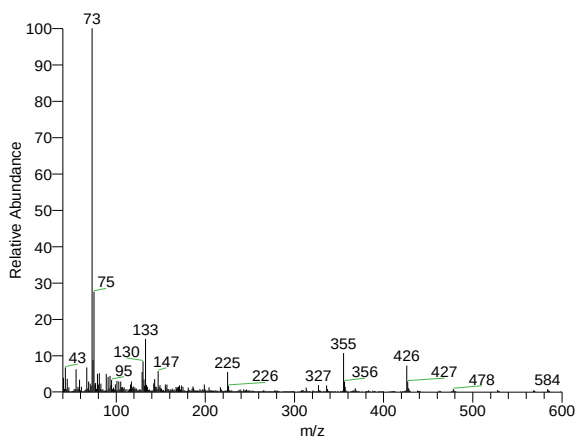
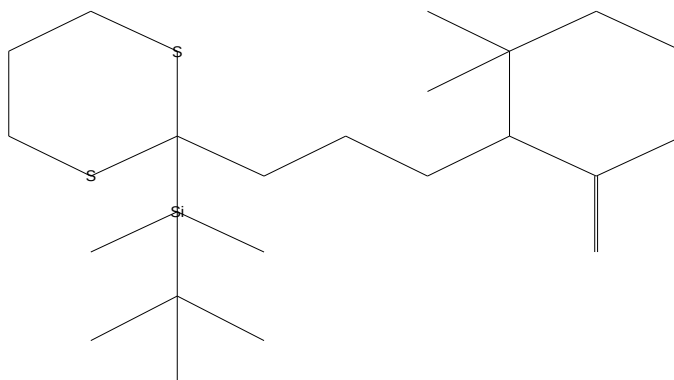
Compound Structure



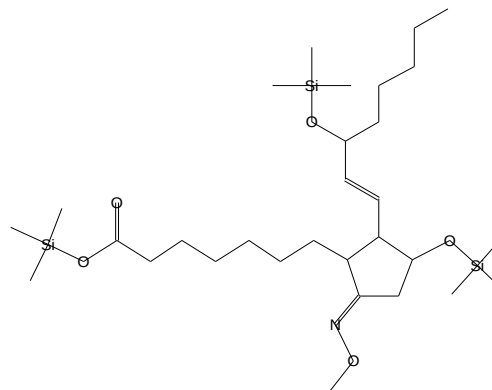
4-(5-Chloro-2-methoxyphenyl)-5-cyclopropyl-1,2,4-triazole-3-thiol
Formula C₁₂H₁₂ClN₃OS, MW 281, CAS# NA, Entry# 208744
\$28GOBZELKVUTXIJY-UHFFFAOYSA-N



t-Butyl-(2-[3-(2,2-dimethyl-6-methylene-cyclohexyl)-propyl]-[1,3]dithian-2-yl)-dimethyl-silane
Formula C₂₂H₄₂S₂Si, MW 398, CAS# 95472-42-7, Entry# 45252
tert-Butyl(2-[3-(2,2-dimethyl-6-methylenecyclohexyl)propyl]-1,3-dithian-2-yl)dimethylsilane #



Formula C₃₀H₆₁NO₅Si₃, MW 599, CAS# 72150-30-2, Entry# 41413
Trimethylsilyl 9-(methoxyimino)-11,15-bis(trimethylsilyloxy)prost-13-en-1-oate

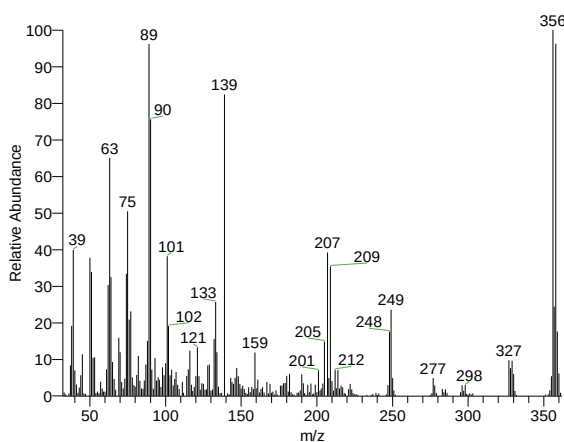


Analysed by Satyanarayana

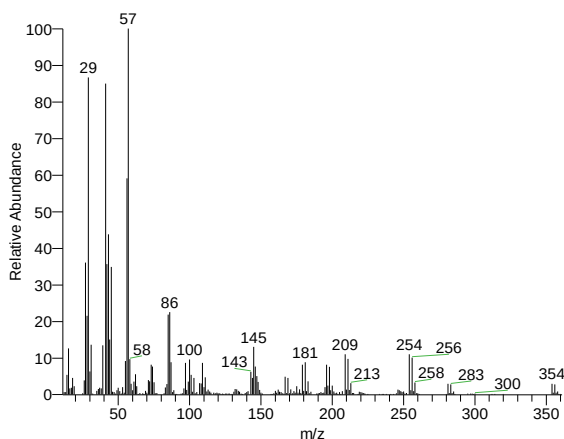
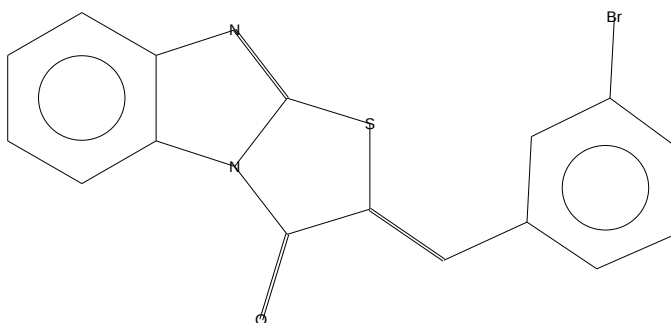
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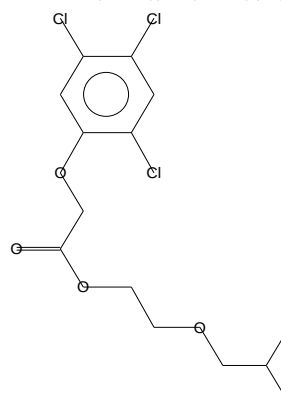
Compound Structure



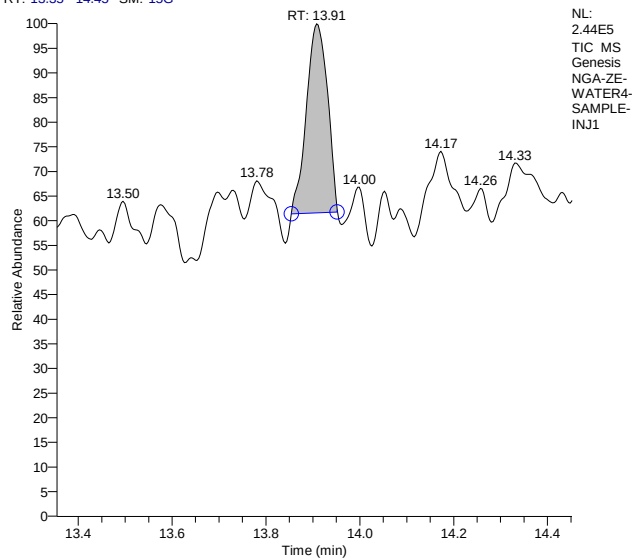
Thiazolo[3,2-a]benzimidazol-3(2H)-one, 2-(3-bromobenzylidene)-
Formula C₁₆H₉BrN₂OS, MW 356, CAS# 299953-38-1, Entry# 234523
(2Z)-2-(3-Bromobenzylidene)[1,3]thiazolo[3,2-a]benzimidazol-3(2H)-one #



Acetic acid, (2,4,5-trichlorophenoxy)-, 2-(2-methylpropoxy)ethyl ester
Formula C₁₄H₁₇Cl₃O₄, MW 354, CAS# 62059-40-9, Entry# 23100
Acetic acid,(2,4,5-trichlorophenoxy)-, 2-(2-methylpropoxy)ethyl ester

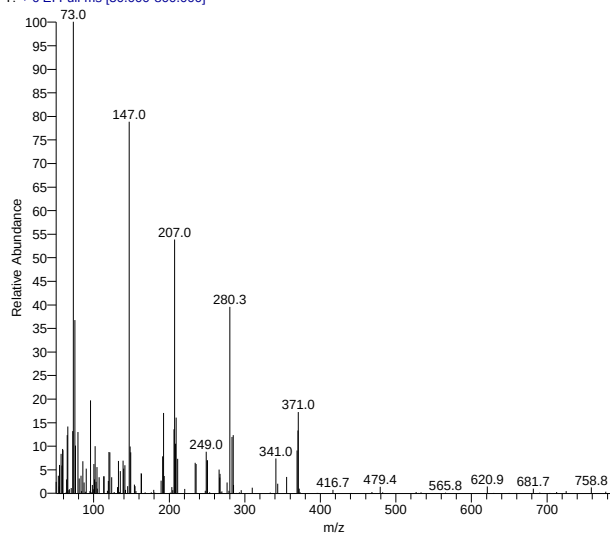


RT: 13.35 - 14.45 SM: 15G



NL:
2.44E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #2359 RT: 13.91 AV: 1 RF: 6.00, 3 NL: 3.20E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
13.91	Bis(carboxymethyl) trithiocarbonate, 2TMS derivative	291230.57	13.31	414	536	mainlib

Analysed by Satyanarayana

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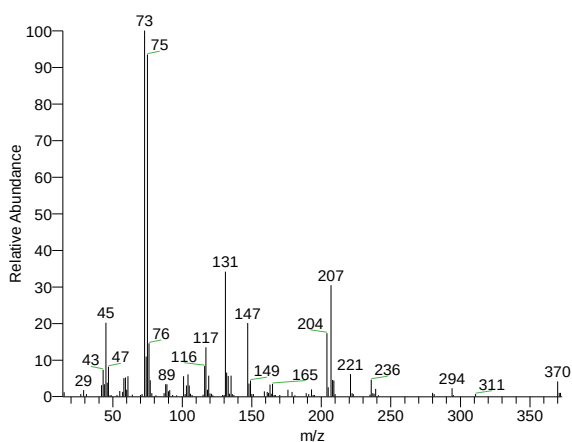
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ANALYTICAL CHEMISTRY DIVISION

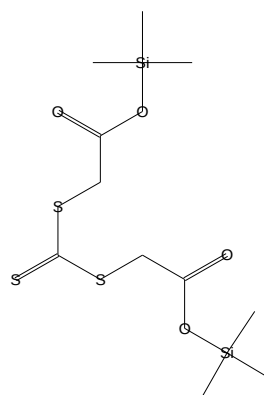
RT	Compound Name	Area	Probability	SI	RSI	Library
13.91	7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane	291230.57	5.26	392	480	mainlib
13.91	(Dimethyl)[4-(2-phenyl-1,9b-dihydro-5-oxa-3,3a-diazacyclopenta[a]naphthalen-4-yl)phenyl]-amine	291230.57	5.06	391	450	mainlib
13.91	3,4-Dimethoxyphenyllactic acid, di-TMS	291230.57	4.07	386	496	mainlib
13.91	Mercaptoethanol, 2TMS derivative	291230.57	4.07	386	681	mainlib

Hit Spectrum

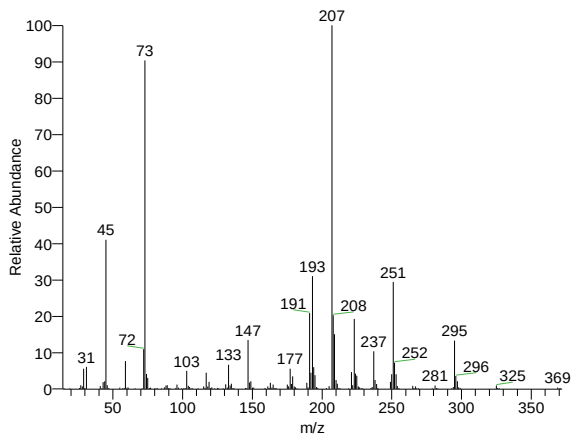
Compound Structure



Bis(carboxymethyl) trithiocarbonate, 2TMS derivative
Formula C₁₁H₂₂O₄S₃Si₂, MW 370, CAS# NA, Entry# 41408
(((Carboxymethyl)thio)carbothioyl)thio)acetic acid dtms



7,7,9,9,11,11-Hexamethyl-3,6,8,10,12,15-hexaoxa-7,9,11-trisilaheptadecane
Formula C₁₄H₃₆O₆Si₃, MW 384, CAS# NA, Entry# 188641
\$:28TUXFBCQKAFVQCP-UHFFFAOYSA-N

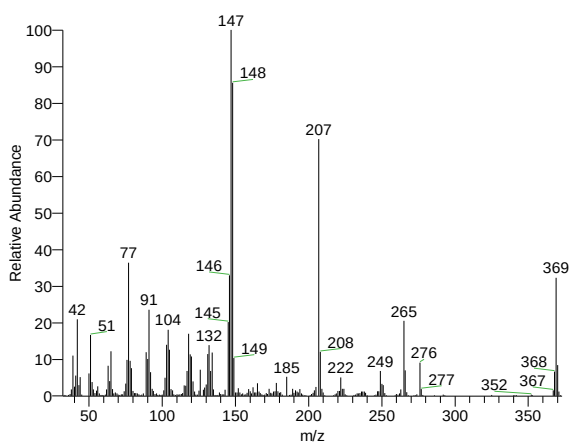


Analysed by Satyanarayana

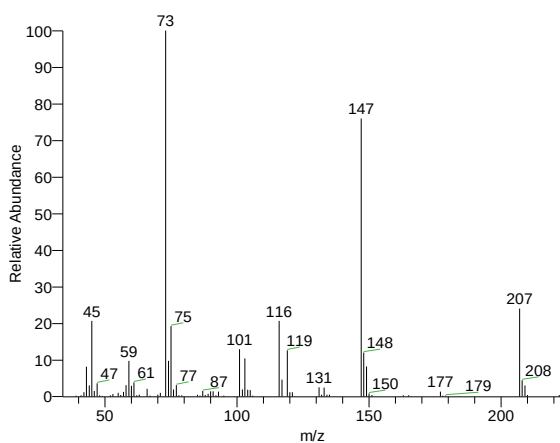
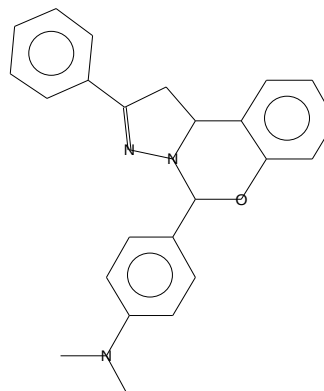
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Hit Spectrum

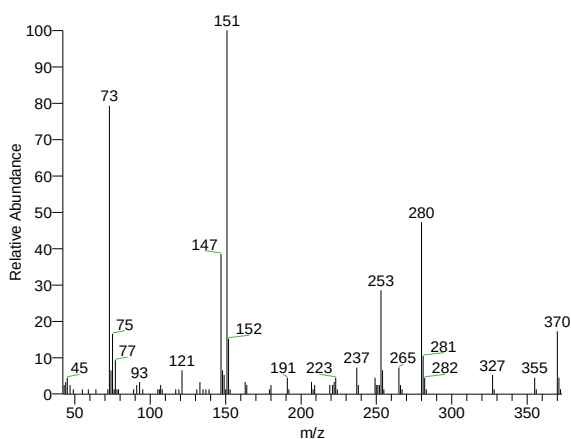
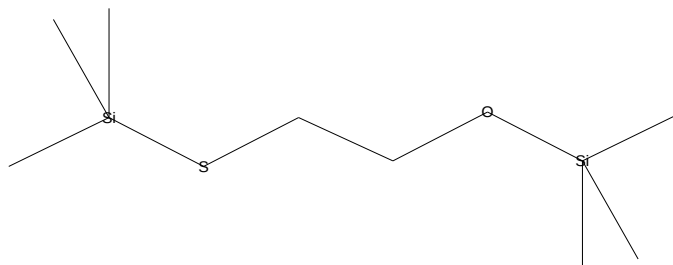
Compound Structure



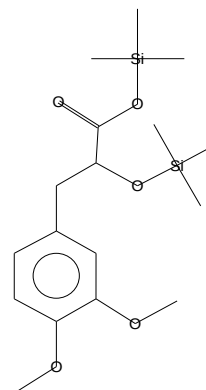
(Dimethyl)[4-(2-phenyl-1,9b-dihydro-5-oxa-3,3a-diazacyclopenta[a]naphthalen-4-yl)phenyl]-amine
Formula C₂₄H₂₃N₃O, MW 369, CAS# NA, Entry# 135451
N,N-Dimethyl-4-(2-phenyl-1,10b-dihydropyrazolo[1,5-c][1,3]benzoxazin-5-yl)aniline #



Mercaptoethanol, 2TMS derivative
Formula C₈H₂₂OSSi₂, MW 222, CAS# 78921-31-0, Entry# 42672
3-Oxa-6-thia-2,7-disilaoctane, 2,2,7,7-tetramethyl-



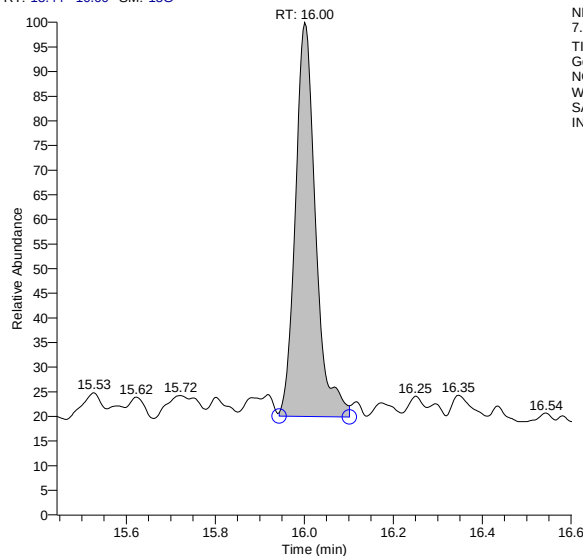
3,4-Dimethoxyphenyllactic acid, di-TMS
Formula C₁₇H₃₀O₅Si₂, MW 370, CAS# NA, Entry# 141121
Trimethylsilyl 3-(3,4-dimethoxyphenyl)-2-[(trimethylsilyl)oxy]propanoate #



Analysed by Satyanarayana

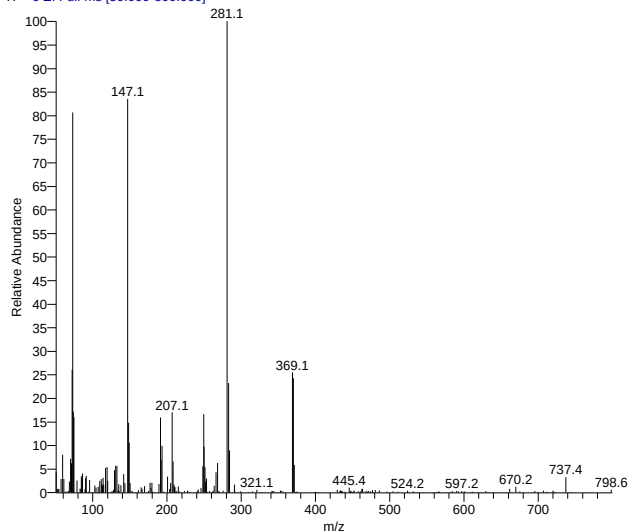
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RT: 15.44 - 16.60 SM: 15G



NL:
7.39E5
TIC: MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

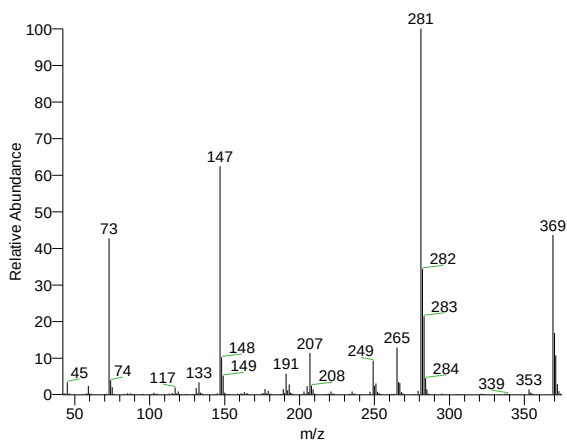
NGA-ZE-WATER4-SAMPLE-INJ1 #2983 RT: 16.00 AV: 1 RF: 6.00, 3 NL: 1.03E5
T: + c EI Full ms [50.000-800.000]



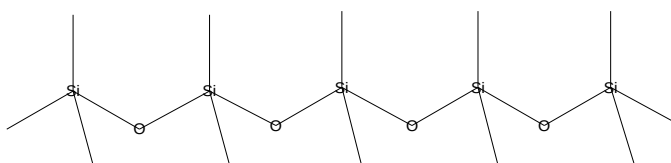
RT	Compound Name	Area	Probability	SI	RSI	Library
16.00	Pentasiloxane, dodecamethyl-	1857987.08	41.53	630	705	mainlib
16.00	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3, 3-bis[(trimethylsilyl)oxy]-	1857987.08	36.69	627	710	mainlib
16.00	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	1857987.08	16.71	607	830	mainlib
16.00	2,6-Dihydroxyacetophenone, 2TMS derivative	1857987.08	1.10	500	604	mainlib
16.00	Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester	1857987.08	0.98	497	616	mainlib

Hit Spectrum

Compound Structure



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



Analysed by Satyanarayana

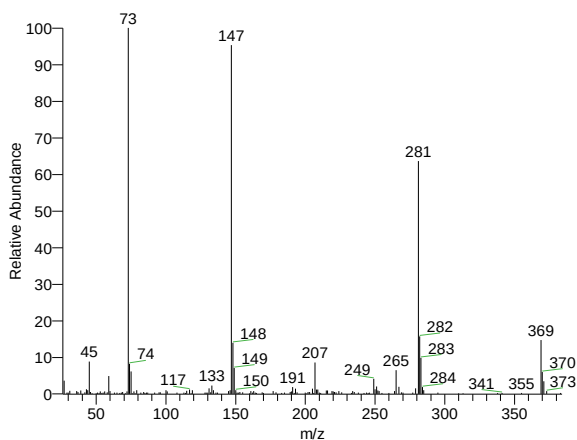
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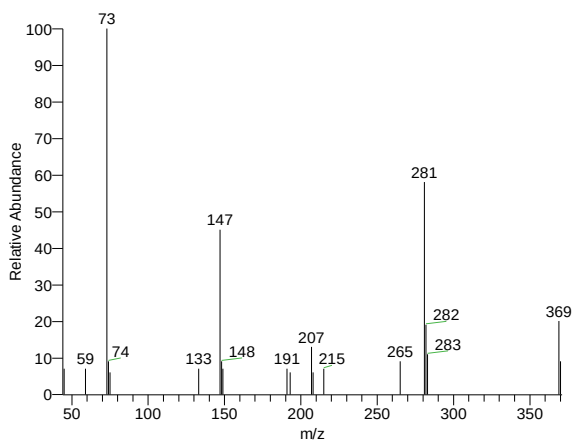
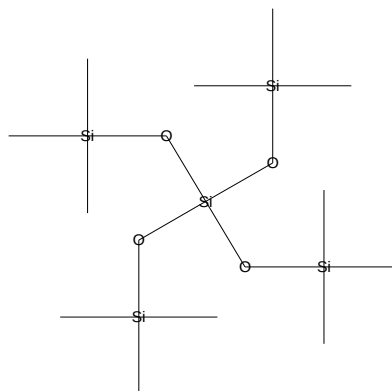
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

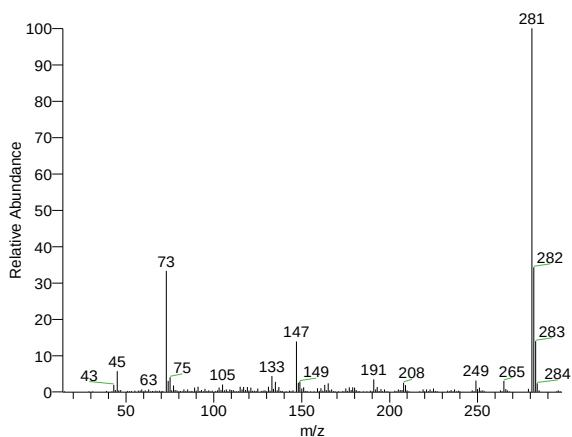
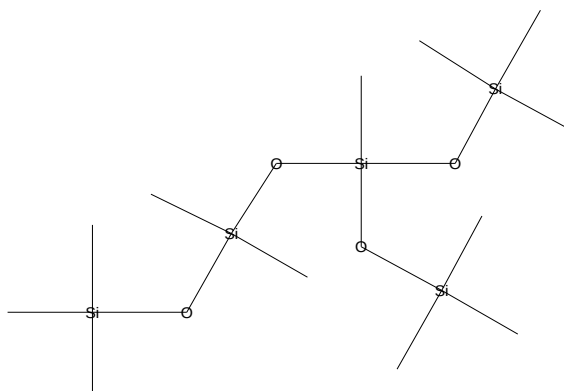
Compound Structure



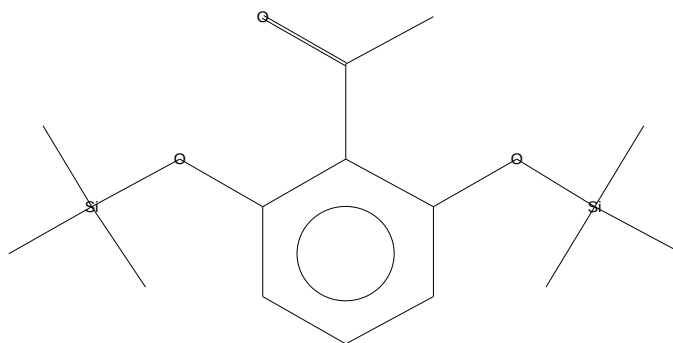
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



1,1,1,3,5,5,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #



2,6-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220073
2',6'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

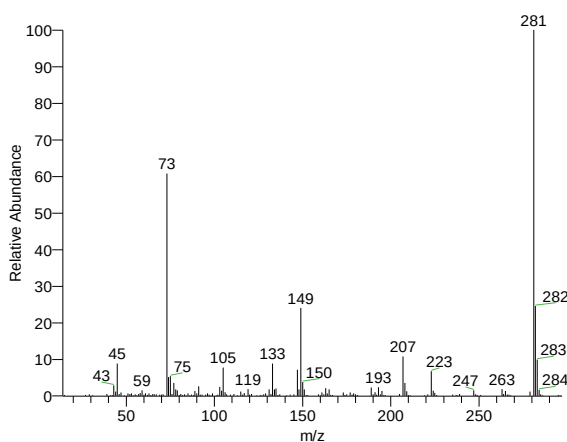


Analysed by Satyanarayana

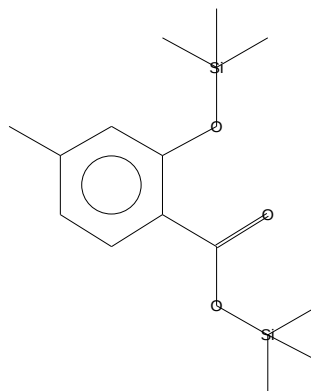
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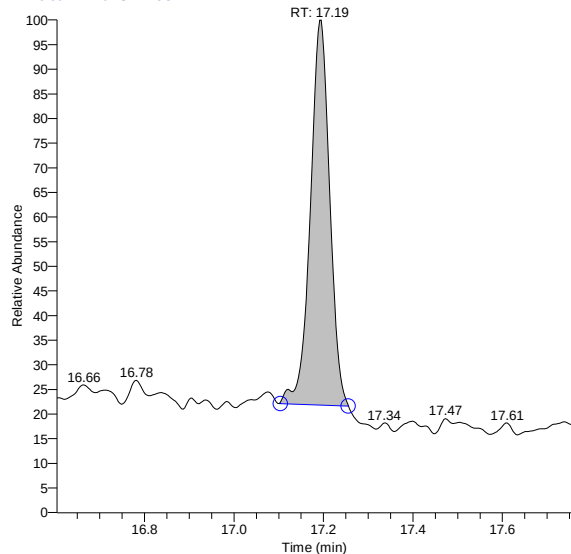
Compound Structure



Benzoic acid, 4-methyl-2-trimethylsilyloxy-, trimethylsilyl ester
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# 35-27-8, Entry# 219921
\$.28WMMUZRDZZSRQEF-UHFFFAOYSA-N

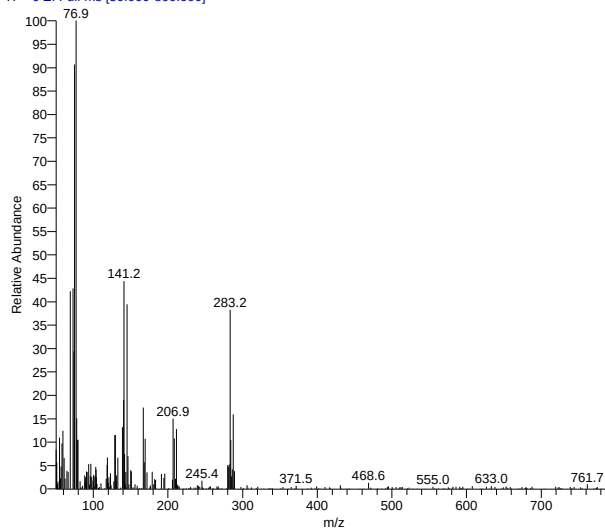


RT: 16.60 - 17.76 SM: 15G



NL:
6.01E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #3338 RT: 17.19 AV: 1 RF: 6.00, 3 NL: 7.59E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
17.19	n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester	1410989.82	9.89	444	542	mainlib
17.19	Bicyclo[4.3.0]nonan-2-one, (Z)-cis-8-(1-phenyl-1-trimethylsilylmethylene)-Hydrosulfide, [5-(4-methoxyphenyl)-4-(3-pyridinyl)-4H-1,2,4-triazol-3-yl]-	1410989.82	4.50	424	487	mainlib
17.19	1-Dimethyl(pentafluorophenyl)silyloxybutane	1410989.82	3.98	421	460	mainlib
17.19	Toluene, 2-(4-dimethylaminobenzylidenamino)-4-nitro-	1410989.82	3.51	418	501	mainlib
17.19		1410989.82	3.10	415	481	mainlib

Analysed by Satyanarayana

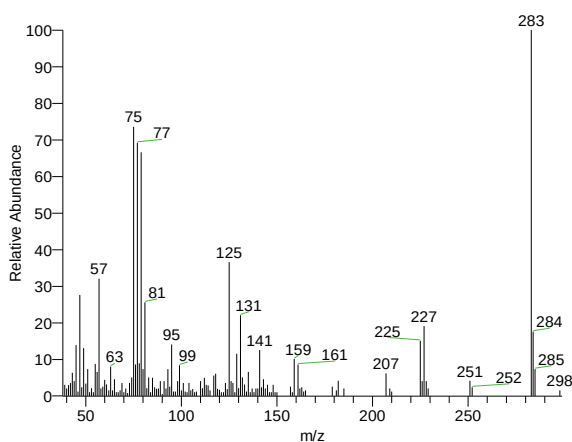
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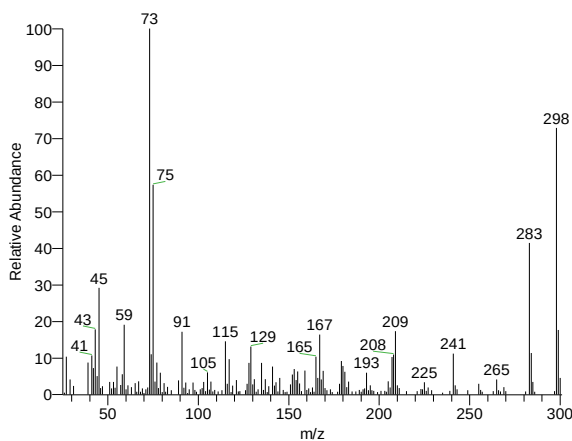
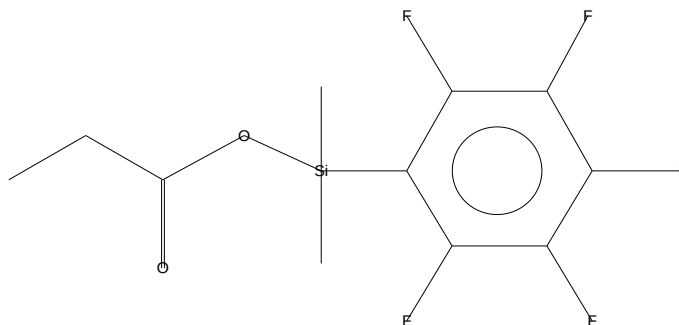
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

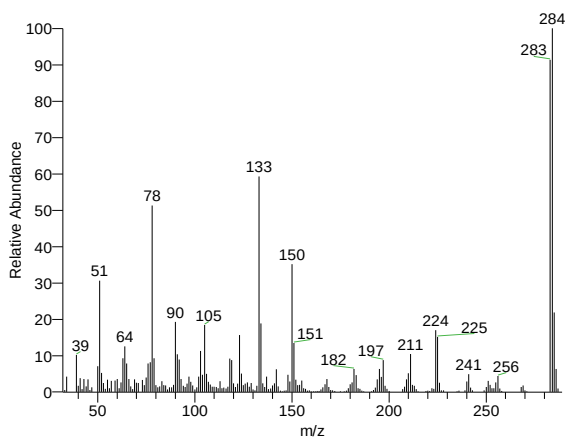
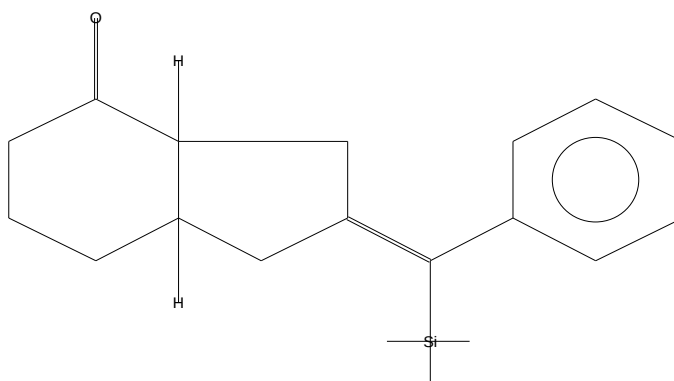
Compound Structure



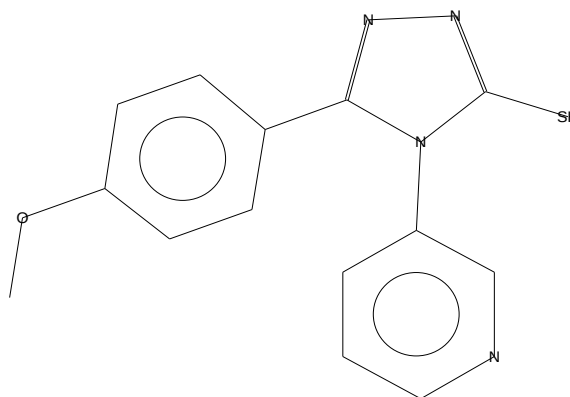
n-Propanoic acid, dimethyl(pentafluorophenyl)silyl ester
Formula C₁₁H₁₁F₅O₂Si, MW 298, CAS# NA, Entry# 220549
Dimethyl(2,3,4,5,6-pentafluorophenyl)silyl propionate #



Bicyclo[4.3.0]nonan-2-one, (Z)-cis-8-(1-phenyl-1-trimethylsilylmethylene)-
Formula C₁₉H₂₆O₂Si, MW 298, CAS# NA, Entry# 43840
(2E)-2-[Phenyl(trimethylsilyl)methylene]octahydro-4H-inden-4-one #



Hydrosulfide, [5-(4-methoxyphenyl)-4-(3-pyridinyl)-4H-1,2,4-triazol-3-yl]-
Formula C₁₄H₁₂N₄O₂S, MW 284, CAS# NA, Entry# 221040
\$.28NPWRXOGFWLAFKG-UHFFFAOYSA-N



Analysed by Satyanarayana

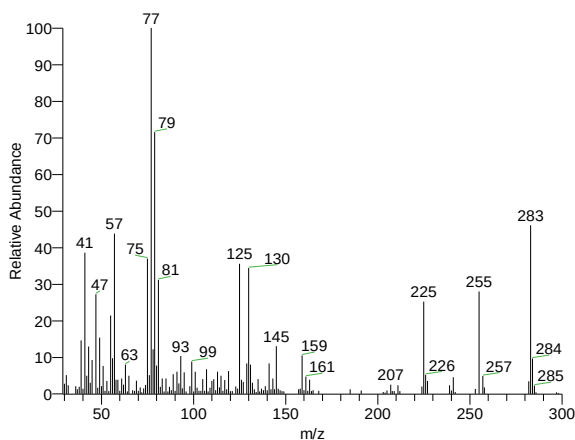
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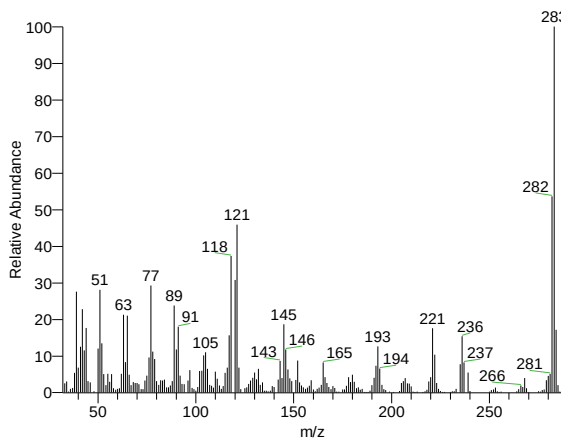
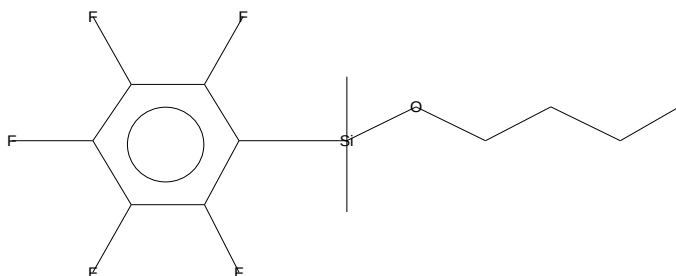
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

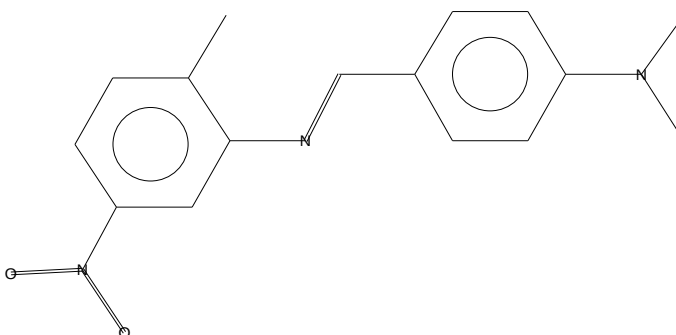
Compound Structure



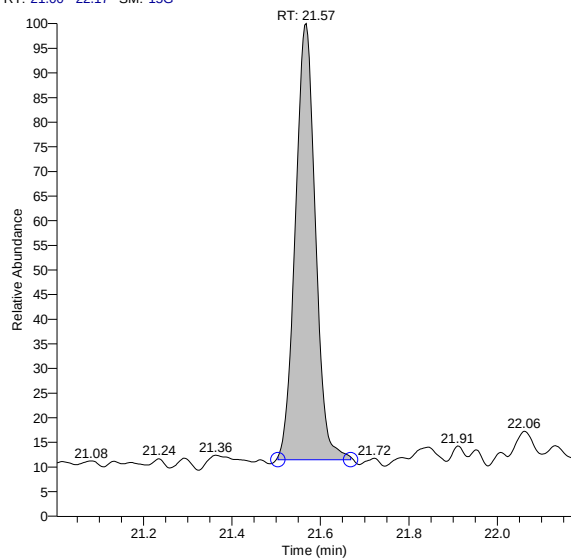
1-Dimethyl(pentafluorophenyl)silyloxybutane
Formula C₁₂H₁₅F₅OSi, MW 298, CAS# 62394-61-0, Entry# 46823
Butoxy(dimethyl)(2,3,4,5,6-pentafluorophenyl)silane #



Toluene, 2-(4-dimethylaminobenzylidenamino)-4-nitro-
Formula C₁₆H₁₇N₃O₂, MW 283, CAS# 199791-21-4, Entry# 220701
N-((E)-[4-(Dimethylamino)phenyl]methylidene)-2-methyl-5-nitroaniline #

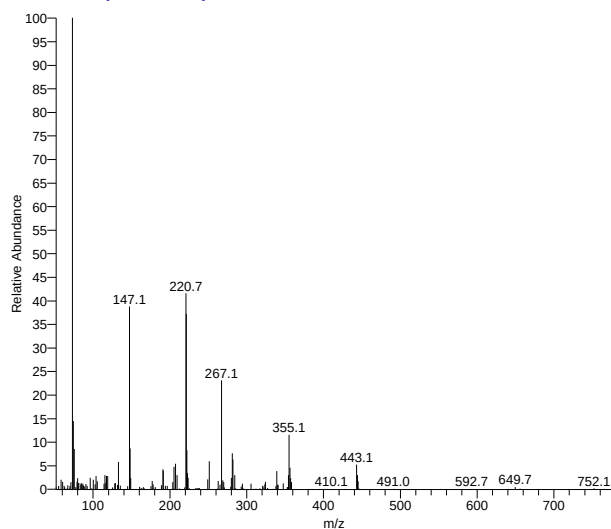


RT: 21.00 - 22.17 SM: 15G



NL:
7.84E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #4643 RT: 21.57 AV: 1 RF: 6.00, 3 NL: 2.17E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
21.57	Hexasiloxane, tetradecamethyl-	2180797.26	85.80	739	823	mainlib

Analysed by Satyanarayana

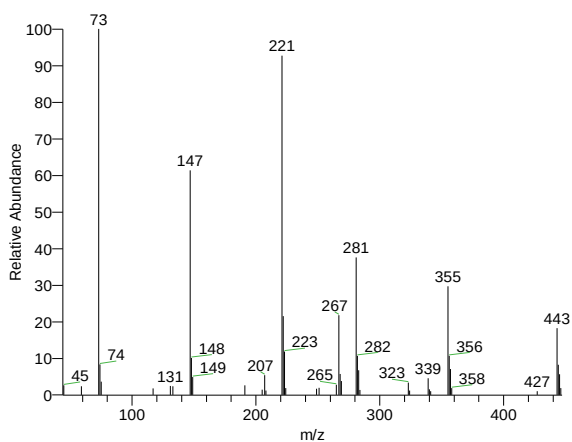
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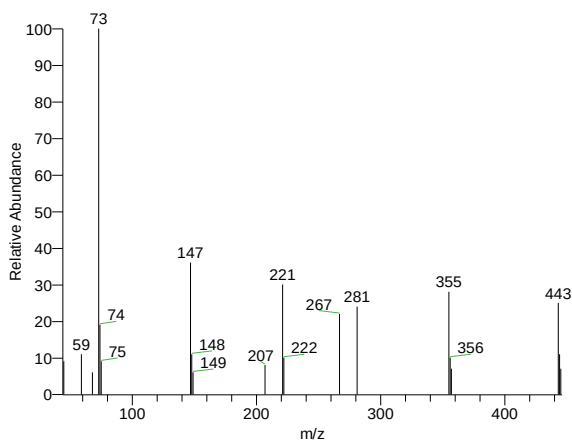
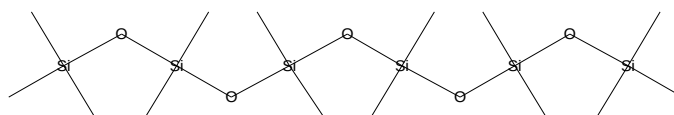
ANALYTICAL CHEMISTRY DIVISION

RT	Compound Name	Area	Probability	SI	RSI	Library
21.57	1,1,1,3,5,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane	2180797.26	12.21	668	843	mainlib
21.57	Heptasiloxane, hexadecamethyl-	2180797.26	0.48	536	641	mainlib
21.57	3,6-Dioxa-2,4,5,7-tetrasilaoctane,	2180797.26	0.36	528	750	mainlib
21.57	2,2,4,4,5,5,7,7-octamethyl-Trisiloxane, octamethyl-	2180797.26	0.19	511	750	mainlib

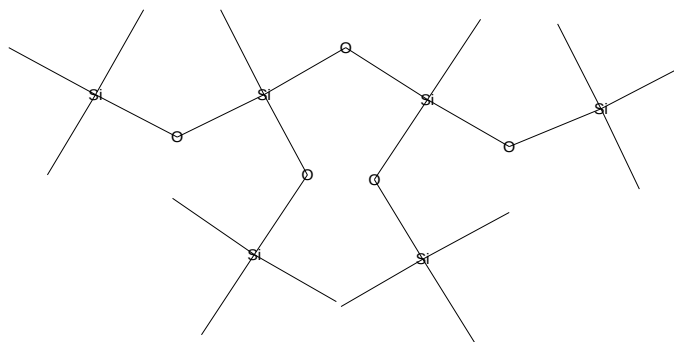
Hit Spectrum



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



1,1,1,3,5,7,7-Octamethyl-3,5-bis(trimethylsiloxy)tetrasiloxane
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 2003-92-1, Entry# 42693
1,1,1,3,5,7,7-Octamethyl-3,5-bis[(trimethylsilyl)oxy]tetrasiloxane #



Analysed by Satyanarayana

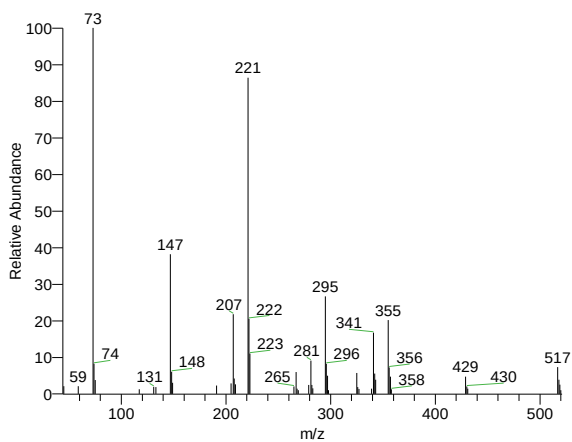
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GC-MS/MS QUAL REPORT

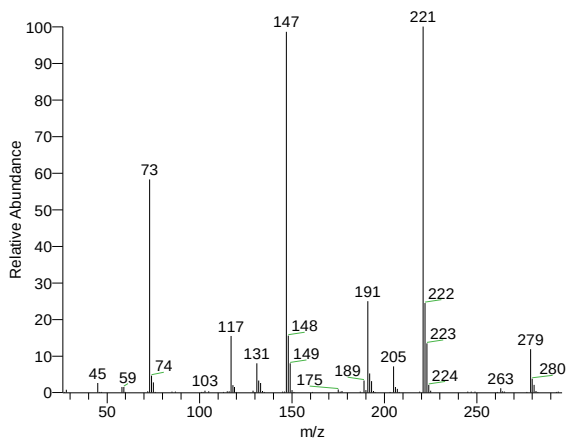
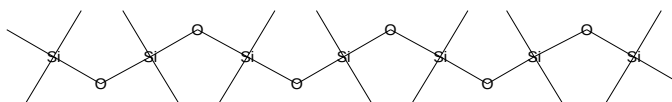
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

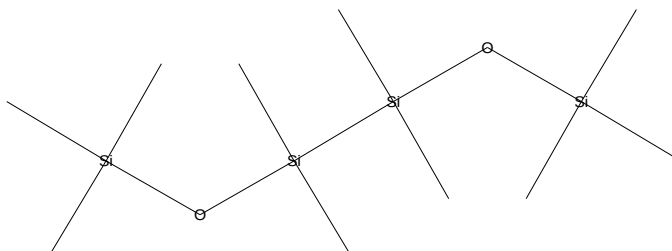
Compound Structure



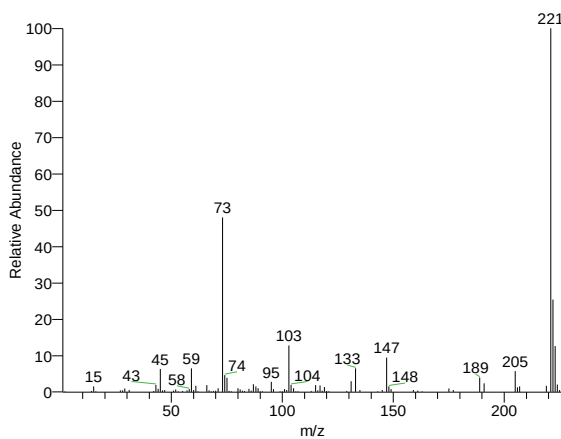
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



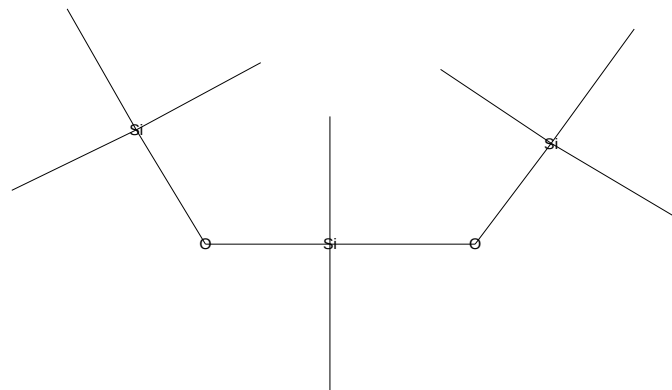
3,6-Dioxa-2,4,5,7-tetrasilaoctane, 2,2,4,4,5,5,7,7-octamethyl-
Formula C₁₀H₃₀O₂Si₄, MW 294, CAS# 4342-25-0, Entry# 196522
2,2,4,4,5,5,7,7-Octamethyl-3,6-dioxa-2,4,5,7-tetrasilaoctane #



SI 511, RSI 750, mainlib, Entry# 196438, CAS# 107-51-7, Trisiloxane, octamethyl-



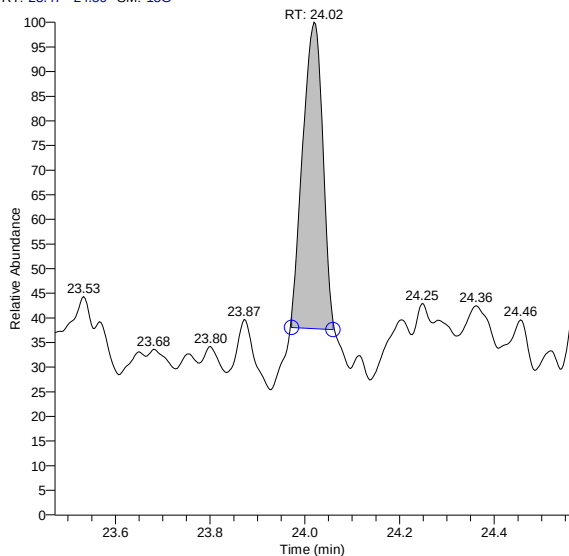
Trisiloxane, octamethyl-
Formula C₈H₂₄O₂Si₃, MW 236, CAS# 107-51-7, Entry# 196438
Octamethyltrisiloxane



Analysed by Satyanarayana

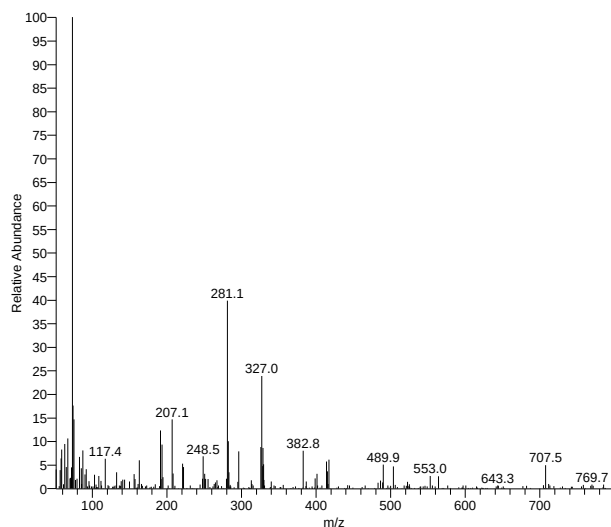
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

RT: 23.47 - 24.56 SM: 15G



NL:
2.12E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

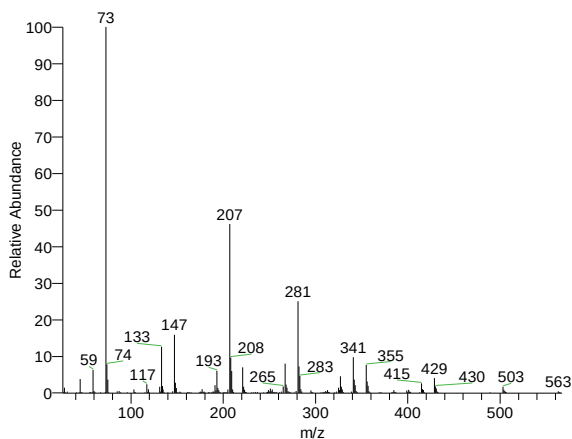
NGA-ZE-WATER4-SAMPLE-INJ1 #5374 RT: 24.02 AV: 1 RF: 6.00, 3 NL: 4.84E4
T: + c EI Full ms [50.000-800.000]



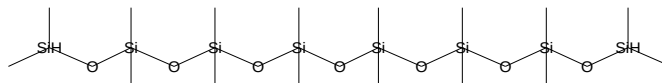
RT	Compound Name	Area	Probability	SI	RSI	Library
24.02	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	385712.78	15.44	427	526	mainlib
24.02	3-Ethoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)tri siloxane	385712.78	12.13	421	701	mainlib
24.02	3,4,5-Trihydroxybenzoic acid ethyl ester (3TMS)	385712.78	9.29	414	529	mainlib
24.02	3-Butoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)tri siloxane	385712.78	7.30	408	752	mainlib
24.02	Cycloheptasiloxane, tetradecamethyl-	385712.78	6.74	406	532	mainlib

Hit Spectrum

Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

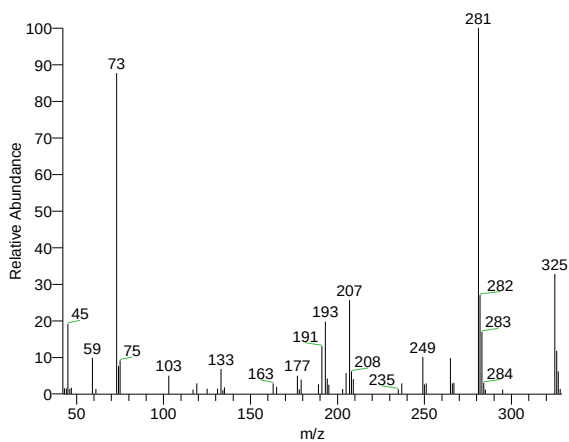
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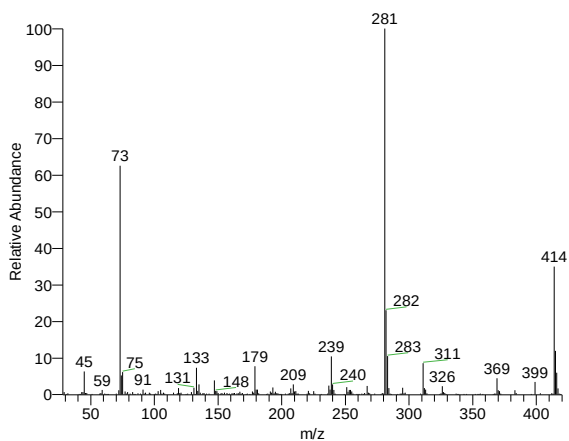
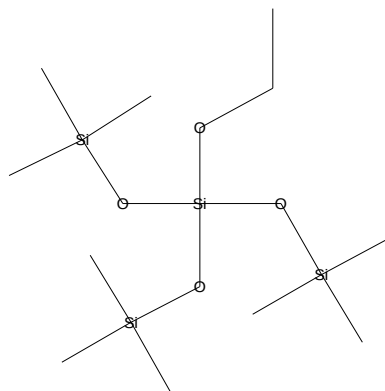
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

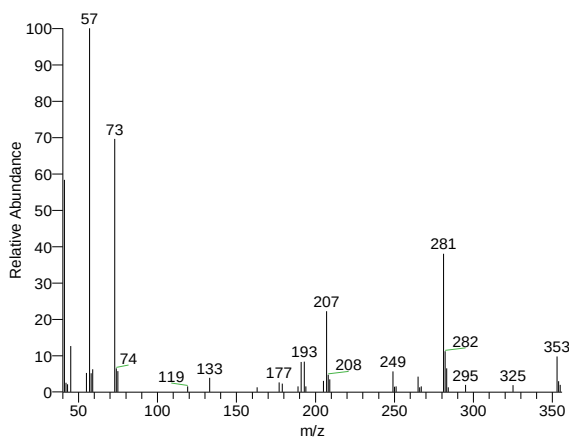
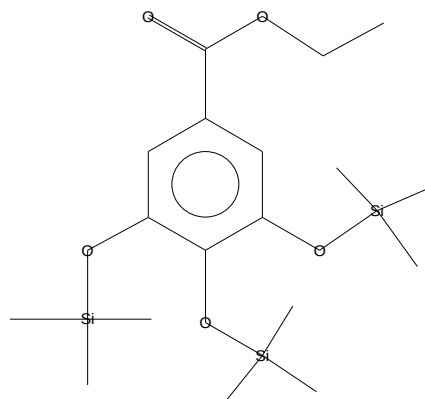
Compound Structure



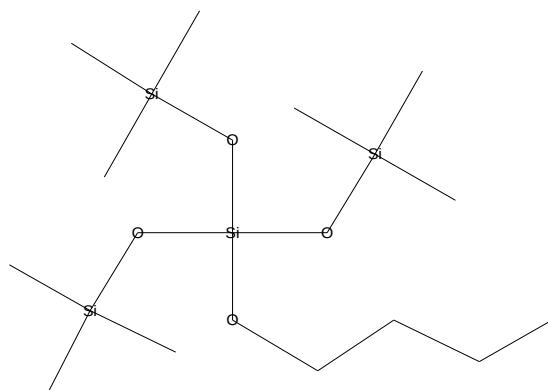
3-Ethoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)trisiloxane
Formula C₁₁H₃₂O₄Si₄, MW 340, CAS# 18030-67-6, Entry# 219923
3-Ethoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsilyloxy)trisiloxane



3,4,5-Trihydroxybenzoic acid ethyl ester (3TMS)
Formula C₁₈H₃₄O₅Si₃, MW 414, CAS# NA, Entry# 219924
Ethyl 3,4,5-tris((trimethylsilyl)oxy)benzoate



3-Butoxy-1,1,1,5,5,5-hexamethyl-3-(trimethylsiloxy)trisiloxane
Formula C₁₃H₃₆O₄Si₄, MW 368, CAS# 87867-97-8, Entry# 25615
Butyl tris(trimethylsilyl) orthosilicate #



Analysed by Satyanarayana

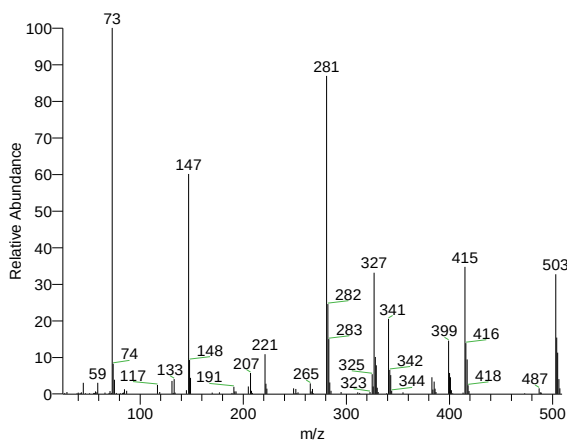
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH

GC-MS/MS QUAL REPORT

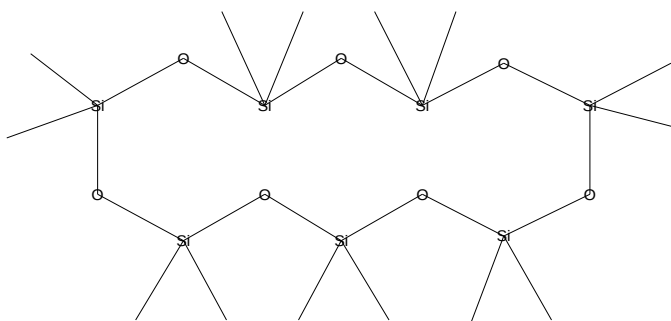
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

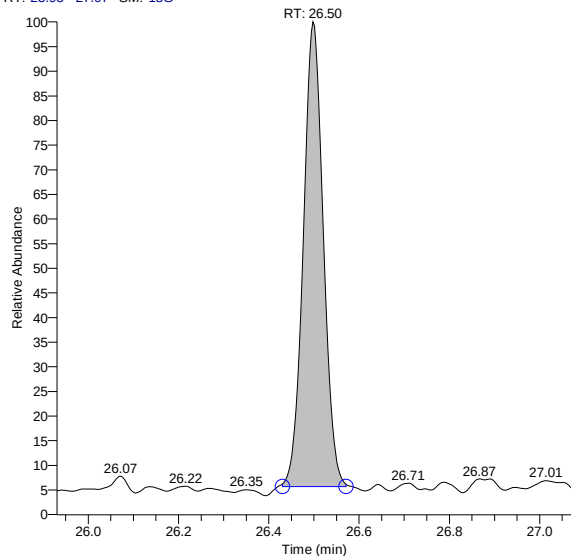
Compound Structure



Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #

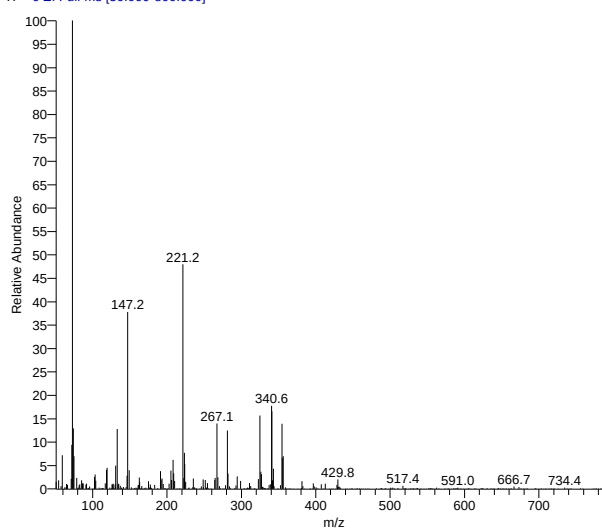


RT: 25.93 - 27.07 SM: 15G



NL:
1.08E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #6113 RT: 26.50 AV: 1 RF: 6.00, 3 NL: 2.13E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
26.50	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3137474.30	58.17	600	645	mainlib
26.50	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3137474.30	17.74	575	611	mainlib
26.50	Heptasiloxane, hexadecamethyl-	3137474.30	9.68	558	661	mainlib
26.50	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3137474.30	6.83	548	585	mainlib
26.50	Hexasiloxane, tetradecamethyl-	3137474.30	1.66	511	656	mainlib

Analysed by Satyanarayana

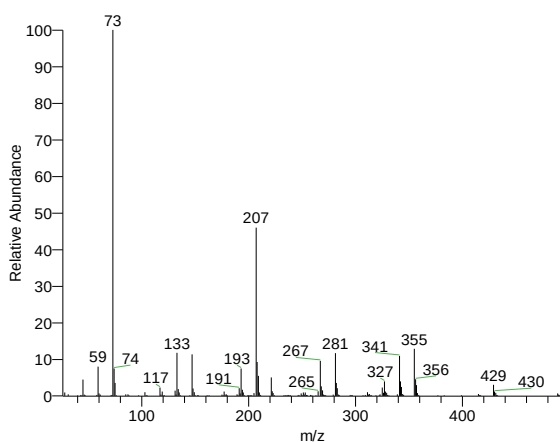
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH

GC-MS/MS QUAL REPORT

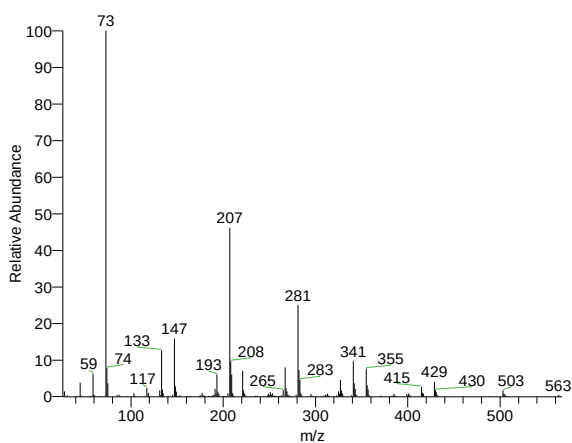
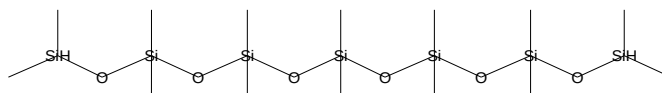
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

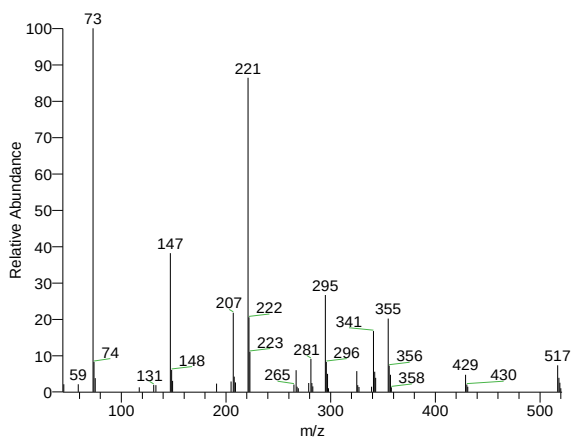
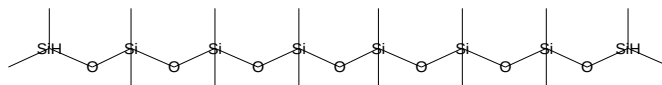
Compound Structure



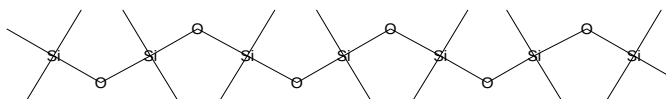
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Analysed by Satyanarayana

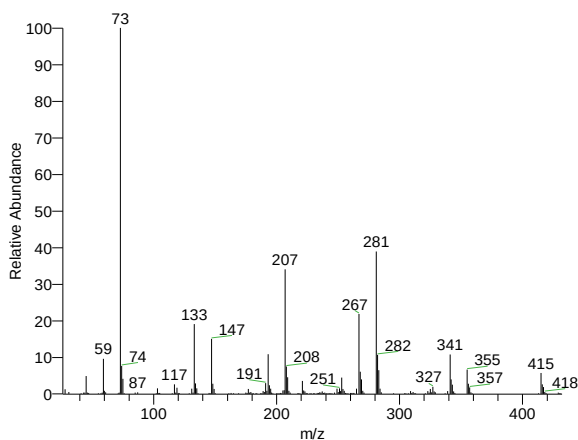
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH

GC-MS/MS QUAL REPORT

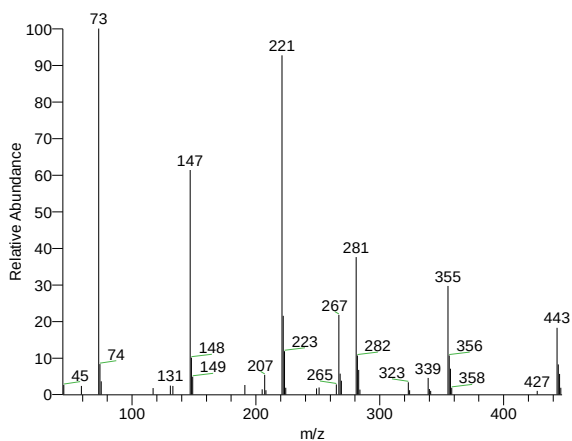
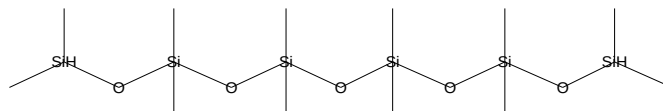
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

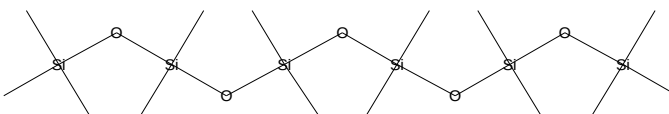
Compound Structure



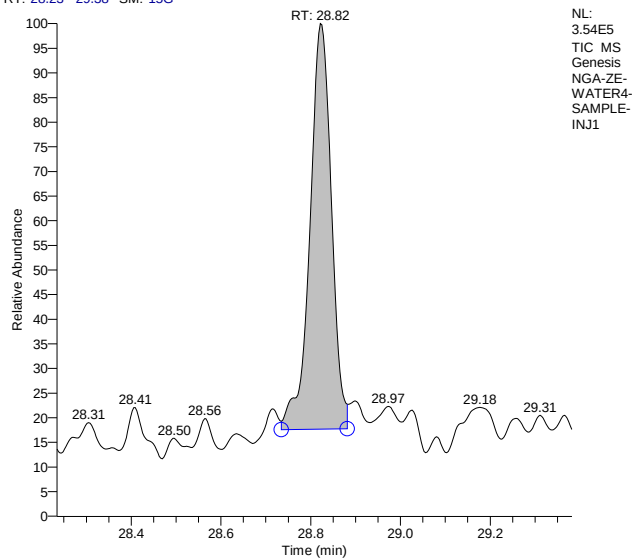
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane

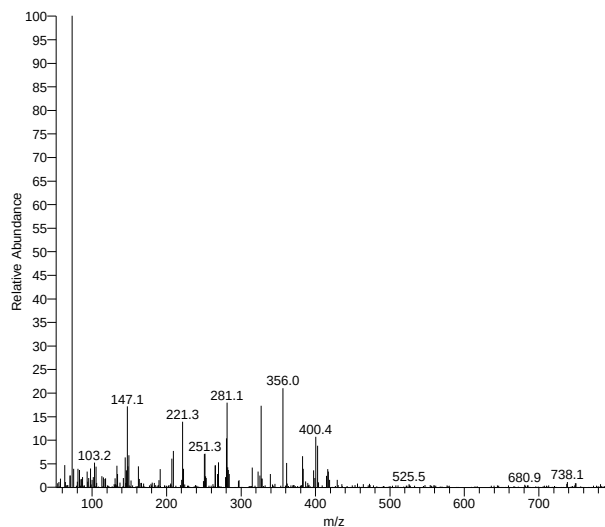


RT: 28.23 - 29.38 SM: 15G



NL:
3.54E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #6806 RT: 28.82 AV: 1 RF: 6.00, 3 NL: 8.38E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

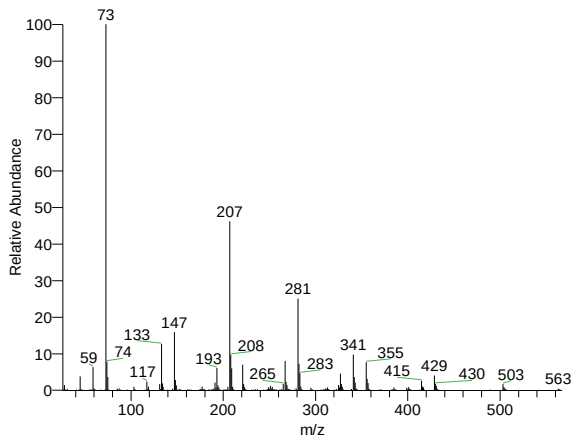
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

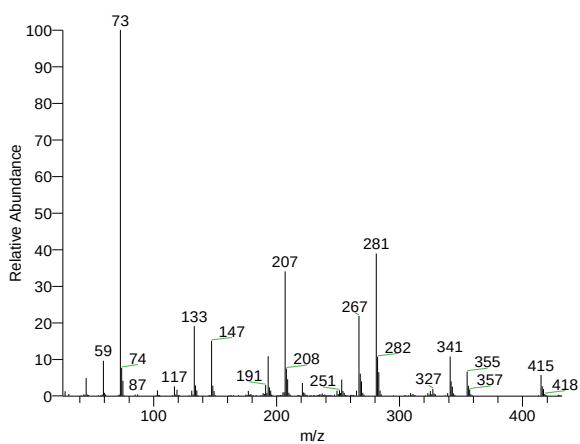
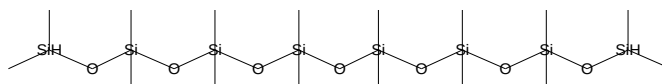
RT	Compound Name	Area	Probability	SI	RSI	Library
28.82	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	972691.68	16.09	420	510	mainlib
28.82	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	972691.68	12.97	415	551	mainlib
28.82	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	972691.68	3.81	388	602	mainlib
28.82	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	972691.68	3.22	384	491	mainlib
28.82	Cycloheptasiloxane, tetradecamethyl-	972691.68	2.84	381	519	mainlib

Hit Spectrum

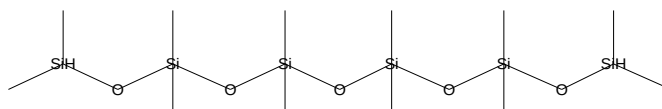
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Analysed by Satyanarayana

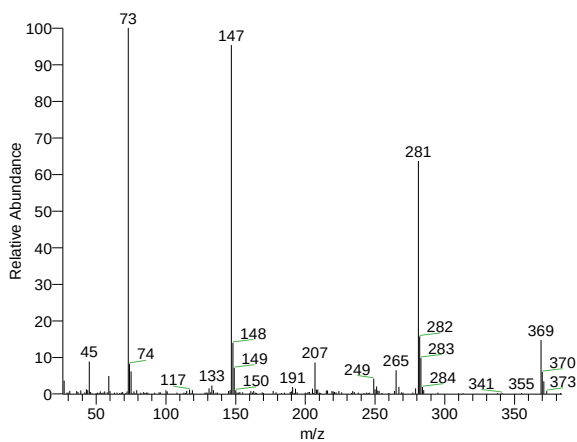
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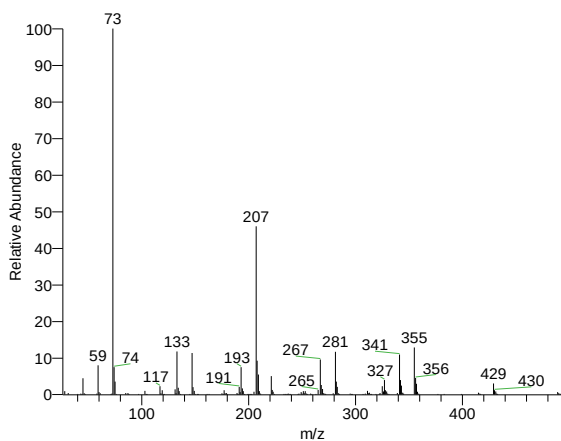
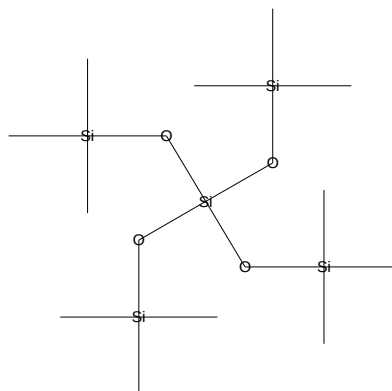
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

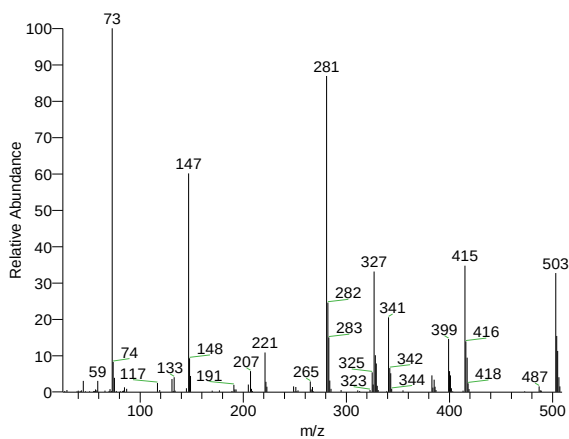
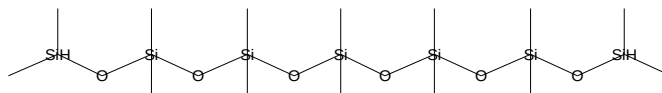
Compound Structure



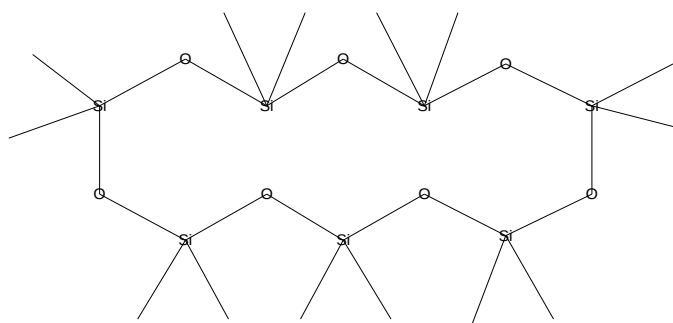
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



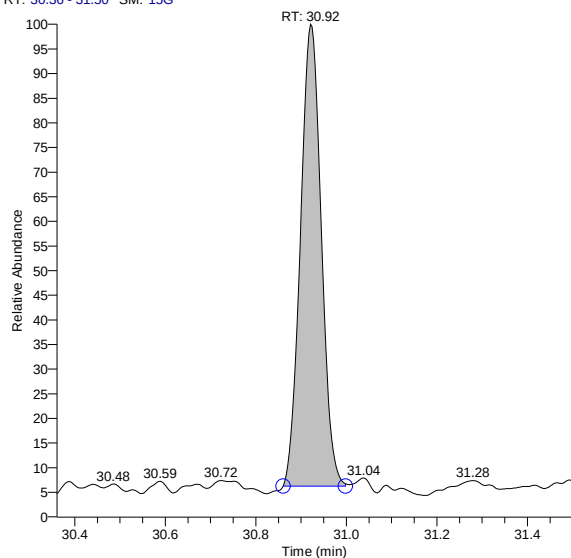
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



Analysed by Satyanarayana

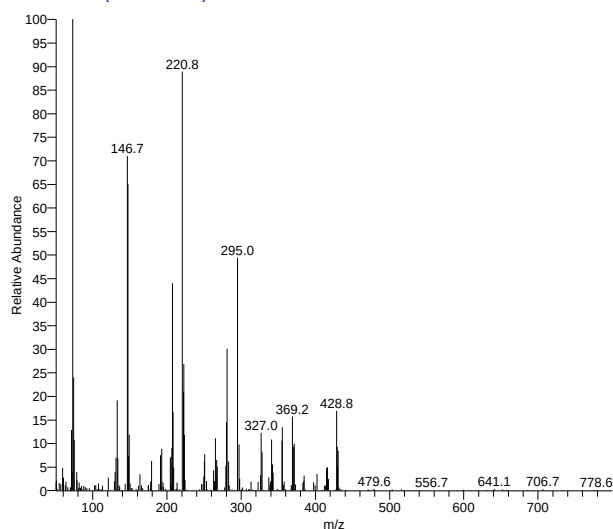
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GC-MS/MS QUAL REPORT
ANALYTICAL CHEMISTRY DIVISION

RT: 30.36 - 31.50 SM: 15G



NL:
1.07E6
TIC: MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

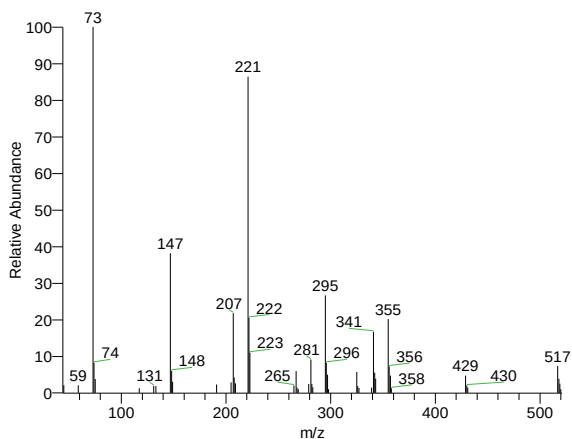
NGA-ZE-WATER4-SAMPLE-INJ1 #7432 RT: 30.92 AV: 1 RF: 6.00, 3 NL: 1.19E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
30.92	Heptasiloxane, hexadecamethyl-	3195655.80	35.62	584	728	mainlib
30.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	3195655.80	32.86	582	624	mainlib
30.92	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	3195655.80	18.92	566	627	mainlib
30.92	Cyclononasiloxane, octadecamethyl-	3195655.80	4.95	533	586	mainlib
30.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	3195655.80	1.51	508	563	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Analysed by Satyanarayana

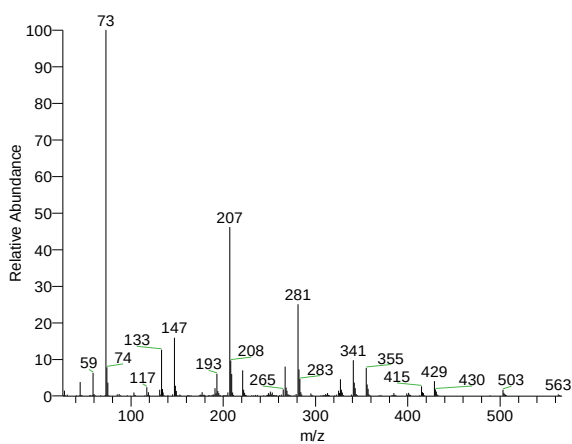
CSIR-INDIAN INSTITUTE OF TOXICOLOGY RESEARCH

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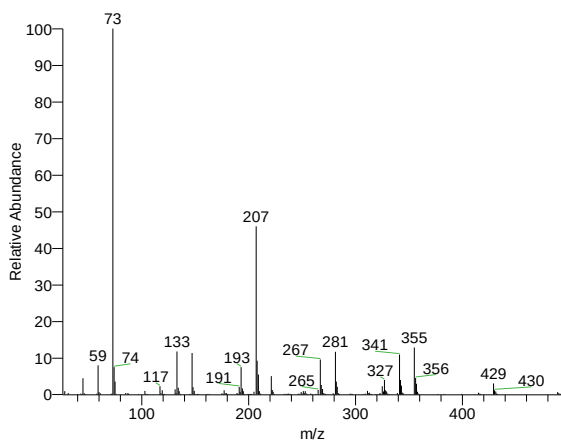
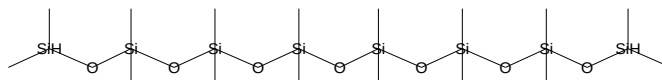
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

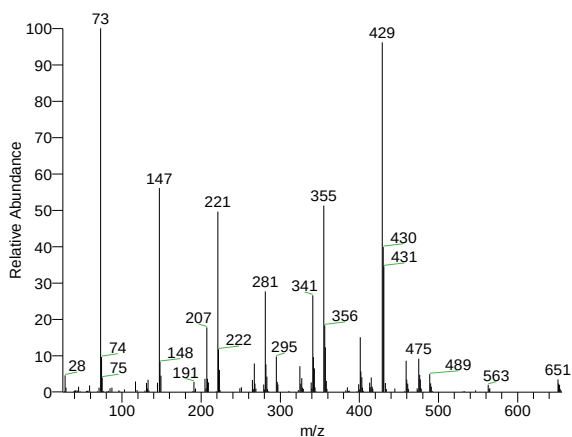
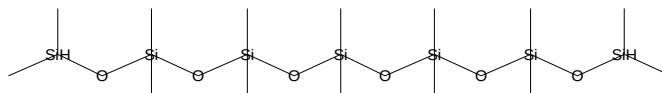
Compound Structure



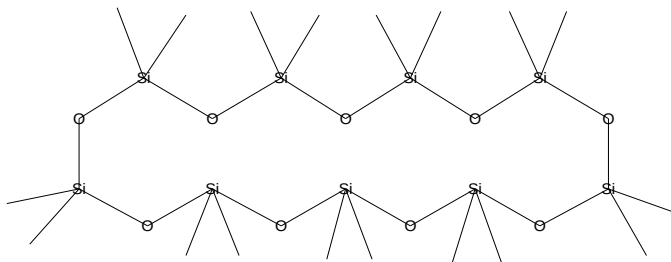
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane

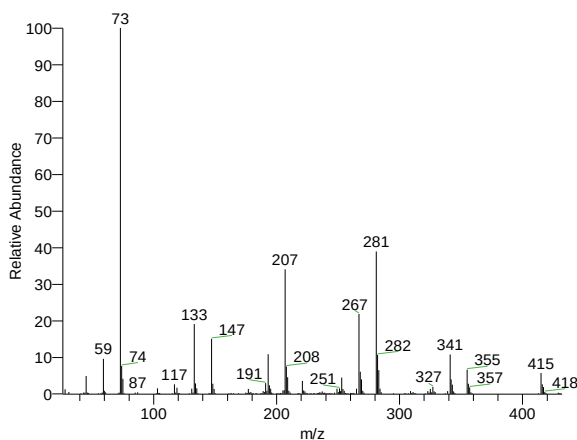


Analysed by Satyanarayana

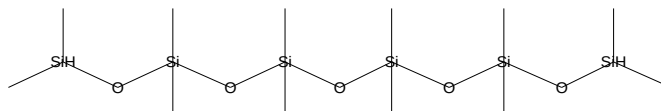
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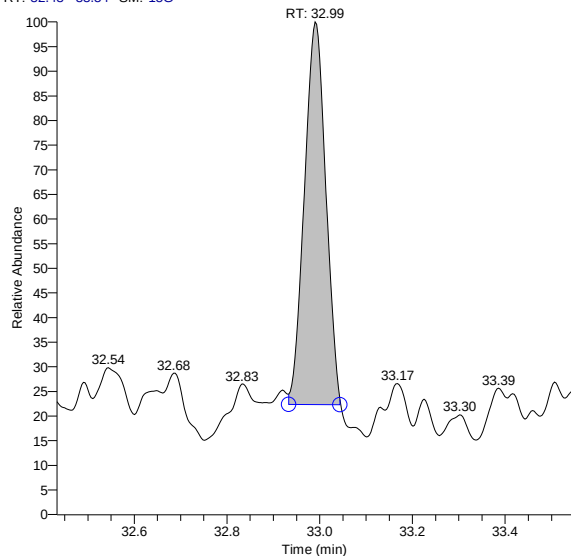
Compound Structure



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

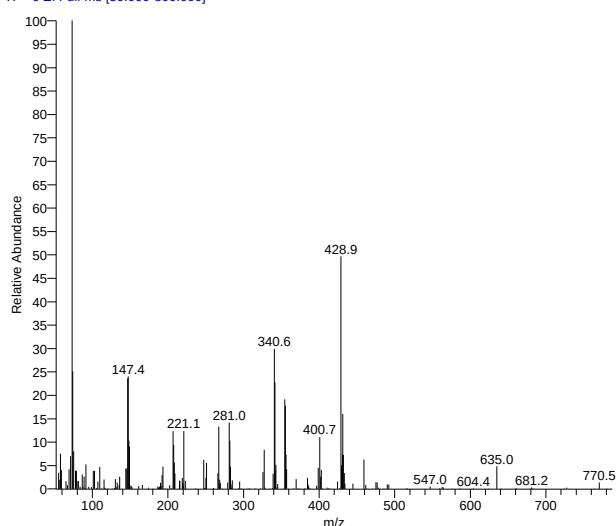


RT: 32.43 - 33.54 SM: 15G



NL:
2.95E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #8049 RT: 32.99 AV: 1 RF: 6.00, 3 NL: 6.57E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
32.99	Cyclononasiloxane, octadecamethyl-	732484.29	69.70	637	693	mainlib
32.99	Tetracosamethyl-cyclododecasiloxane	732484.29	6.27	552	686	mainlib
32.99	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	732484.29	6.02	551	596	mainlib
32.99	1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane	732484.29	4.37	542	790	mainlib
32.99	Cyclohexasiloxane, dodecamethyl-	732484.29	4.20	541	620	mainlib

Analysed by Satyanarayana

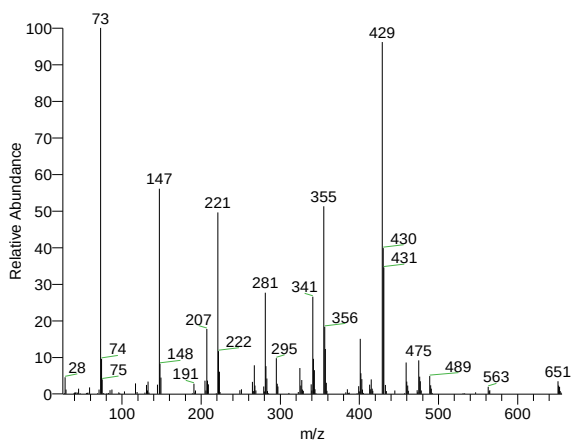
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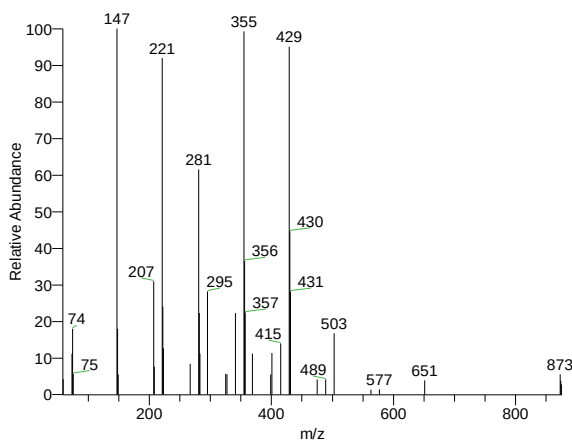
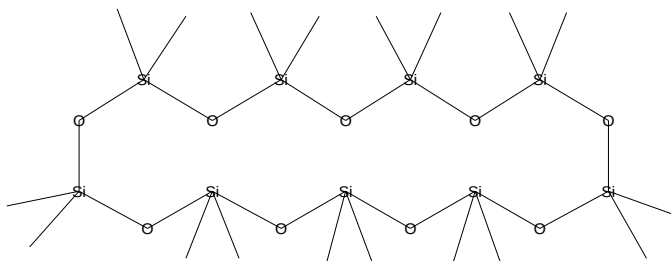
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

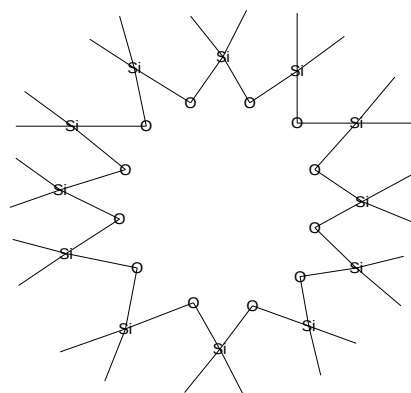
Compound Structure



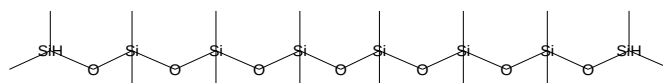
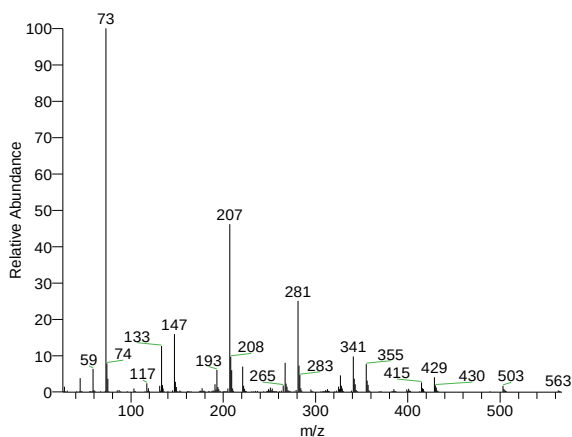
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

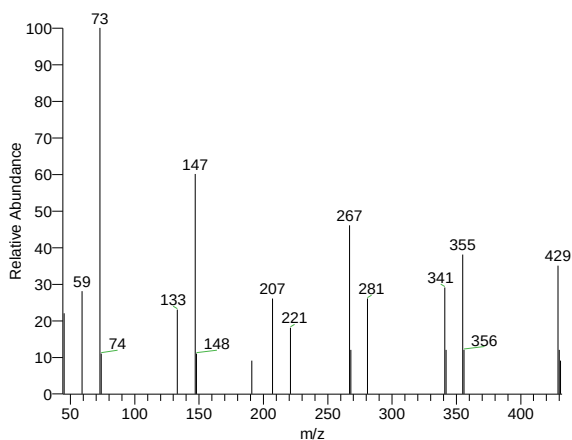
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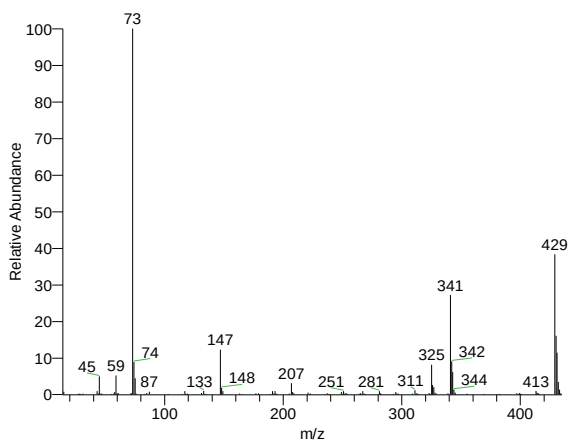
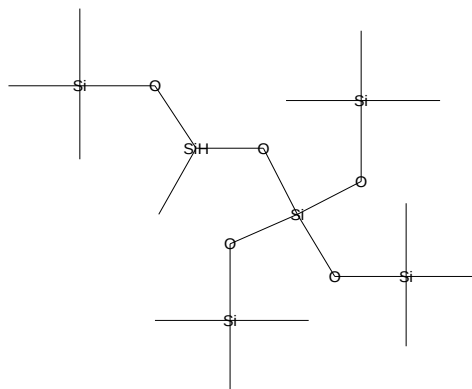
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

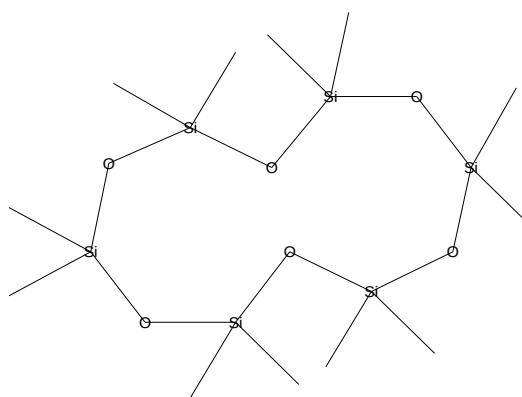
Compound Structure



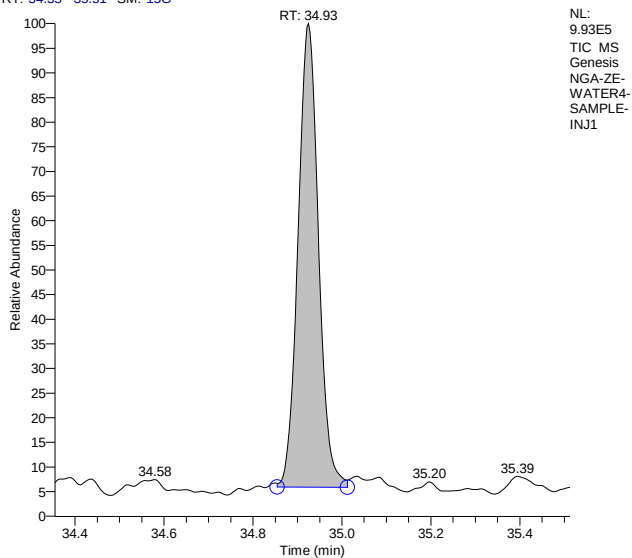
1,1,1,5,7,7,7-Heptamethyl-3,3-bis(trimethylsiloxy)tetrasiloxane
Formula C₁₃H₄₀O₅Si₆, MW 444, CAS# 38147-00-1, Entry# 42719
1,3,3,3-Tetramethyldisiloxanyl tris(trimethylsilyl) orthosilicate #



Cyclohexasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₆Si₆, MW 444, CAS# 540-97-6, Entry# 44297
Dodecamethylcyclohexasiloxane

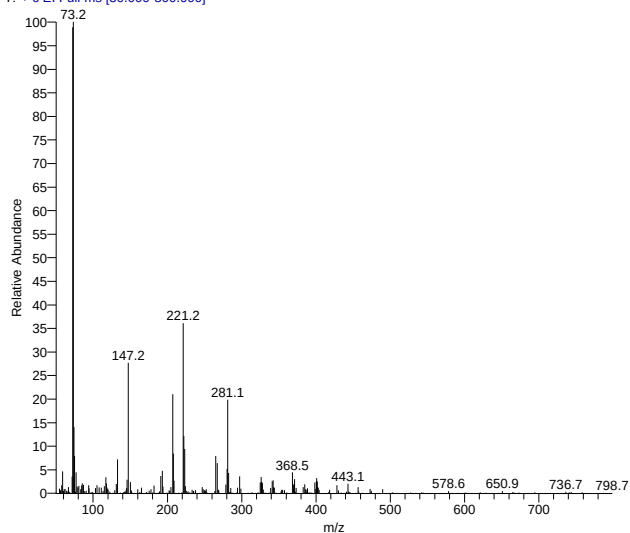


RT: 34.35 - 35.51 SM: 15G



NL:
9.93E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #8626 RT: 34.93 AV: 1 RF: 6.00, 3 NL: 2.37E5
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

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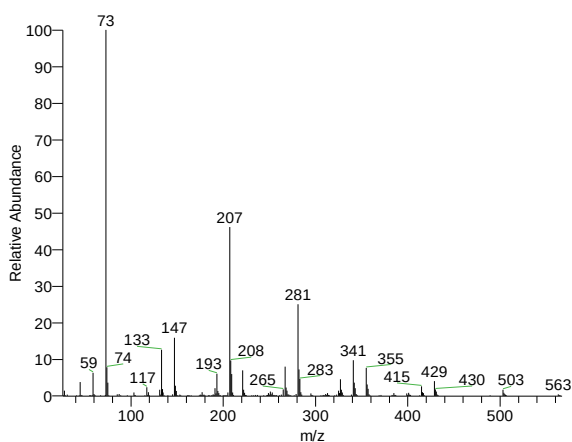
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

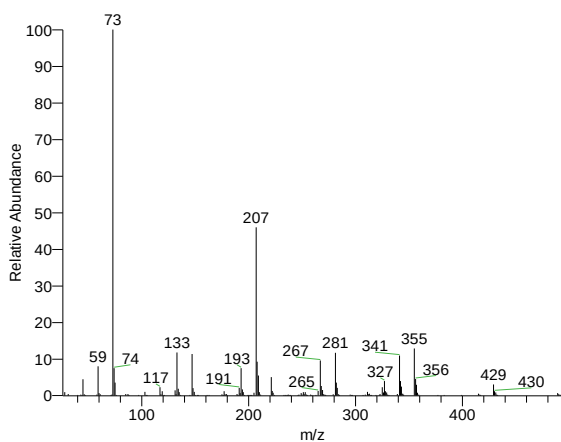
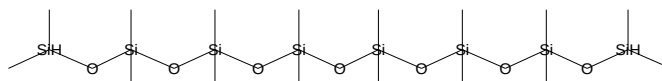
RT	Compound Name	Area	Probability	SI	RSI	Library
34.93	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2972016.78	60.46	575	627	mainlib
34.93	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2972016.78	17.13	546	634	mainlib
34.93	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2972016.78	7.80	526	616	mainlib
34.93	Heptasiloxane, hexadecamethyl-	2972016.78	3.08	504	624	mainlib
34.93	Hexasiloxane, tetradecamethyl-	2972016.78	2.96	503	666	mainlib

Hit Spectrum

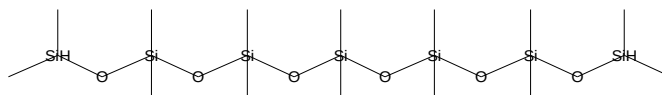
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

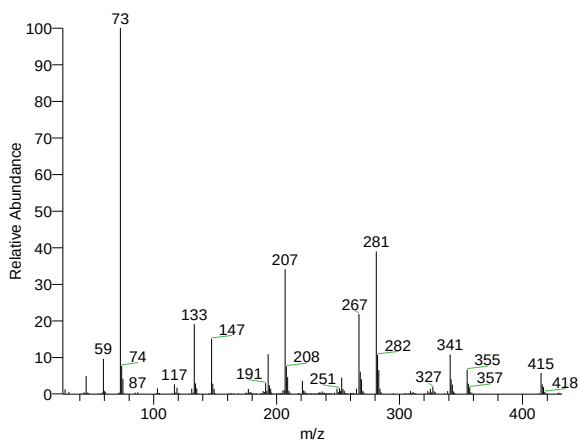


Analysed by Satyanarayana

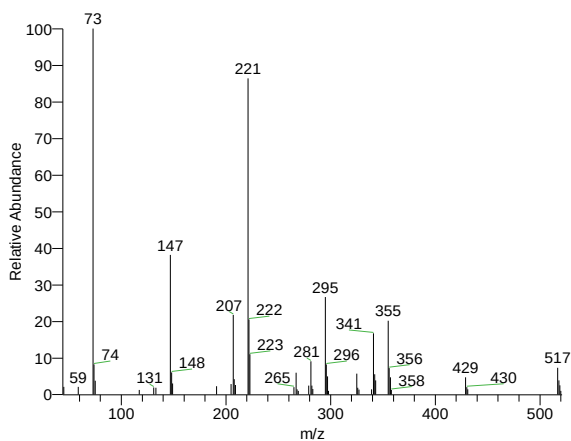
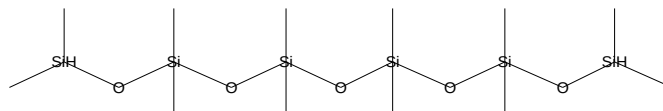
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Hit Spectrum

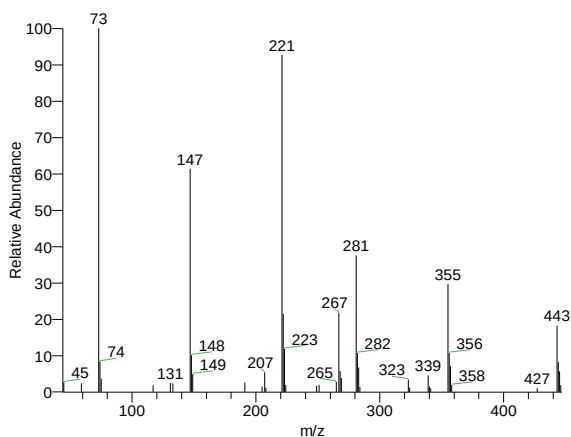
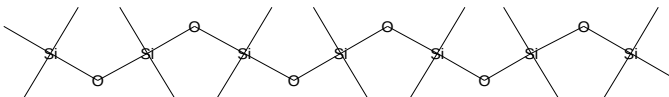
Compound Structure



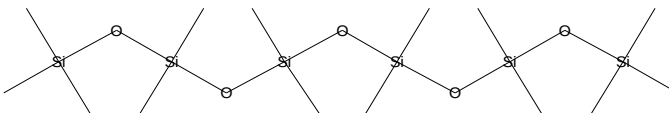
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



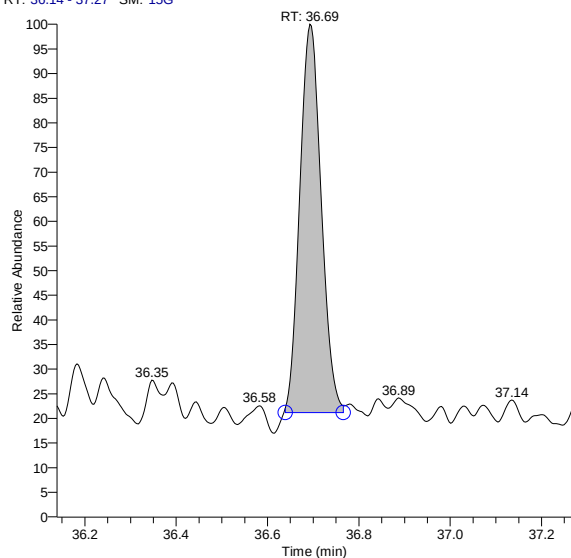
Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane



Analysed by Satyanarayana

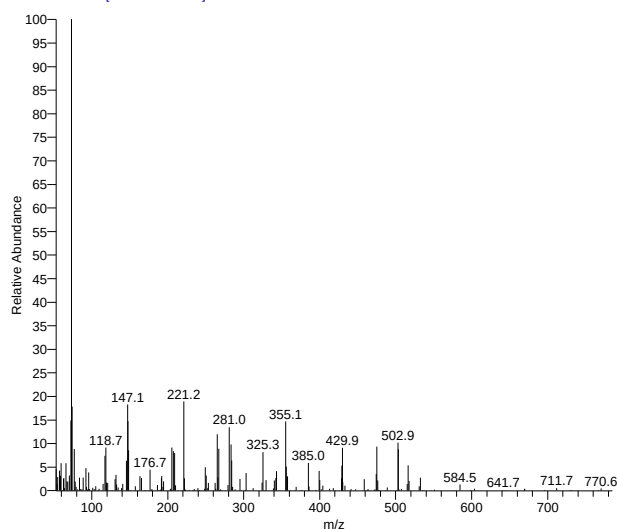
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RT: 36.14 - 37.27 SM: 15G



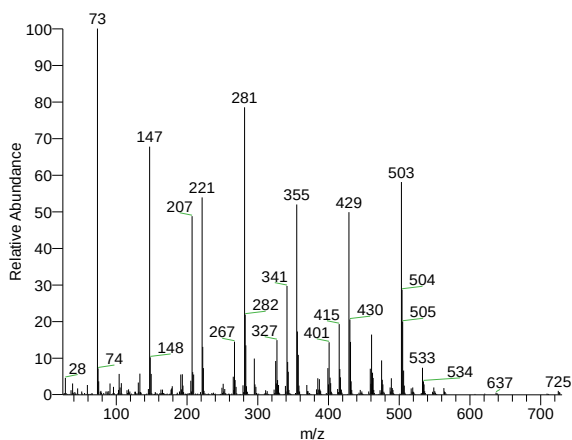
NL:
2.53E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #9153 RT: 36.69 AV: 1 RF: 6.00, 3 NL: 6.48E4
T: + c EI Full ms [50.000-800.000]



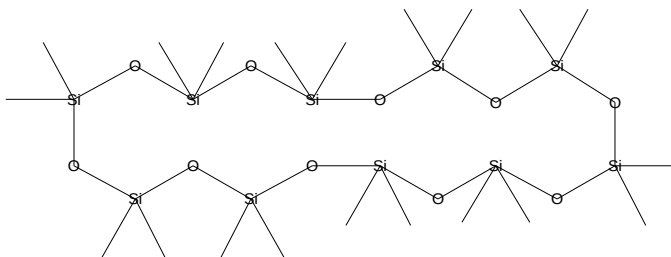
RT	Compound Name	Area	Probability	SI	RSI	Library
36.69	Cyclodecasiloxane, eicosamethyl-	654999.85	68.32	520	553	mainlib
36.69	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	654999.85	20.84	495	576	mainlib
36.69	Cyclononasiloxane, octadecamethyl-	654999.85	5.15	459	547	mainlib
36.69	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	654999.85	1.51	432	565	mainlib
36.69	Heptasiloxane, hexadecamethyl-	654999.85	1.13	424	628	mainlib

Hit Spectrum



Compound Structure

Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Analysed by Satyanarayana

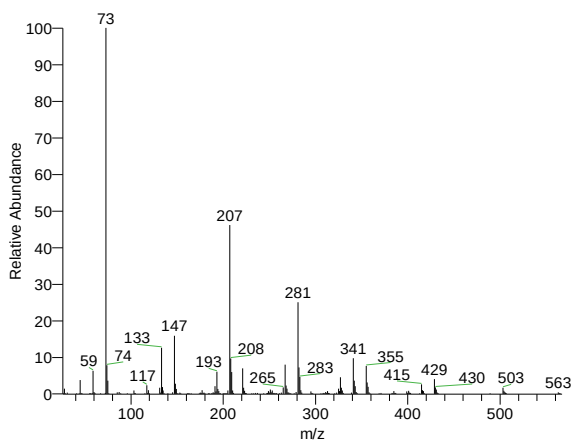
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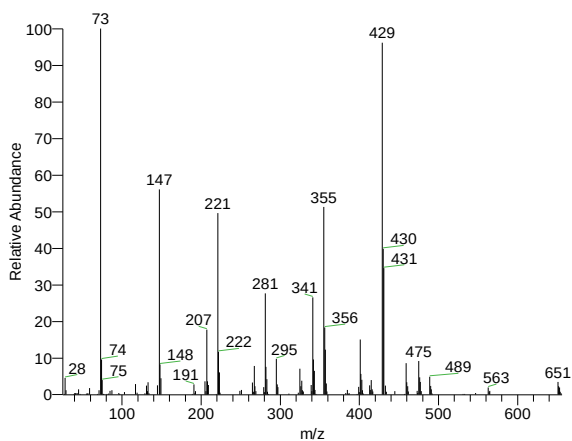
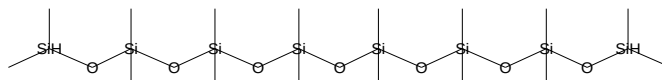
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

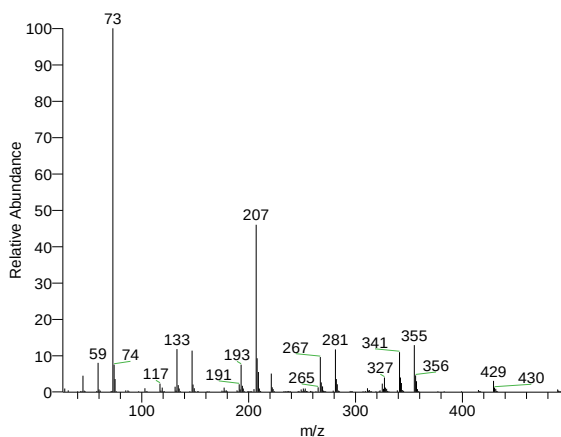
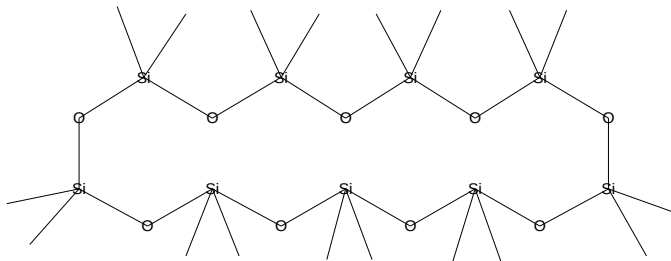
Compound Structure



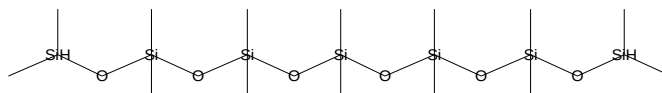
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

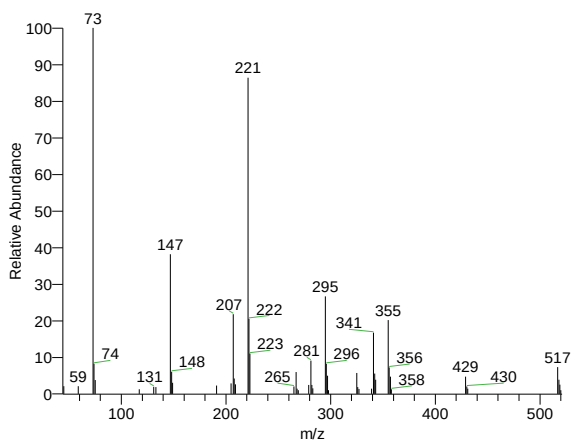


Analysed by Satyanarayana

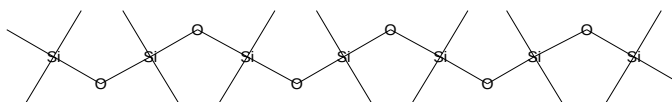
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Hit Spectrum

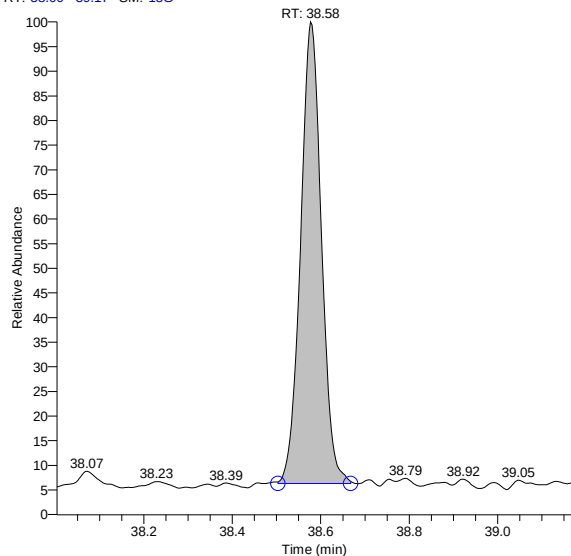
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane

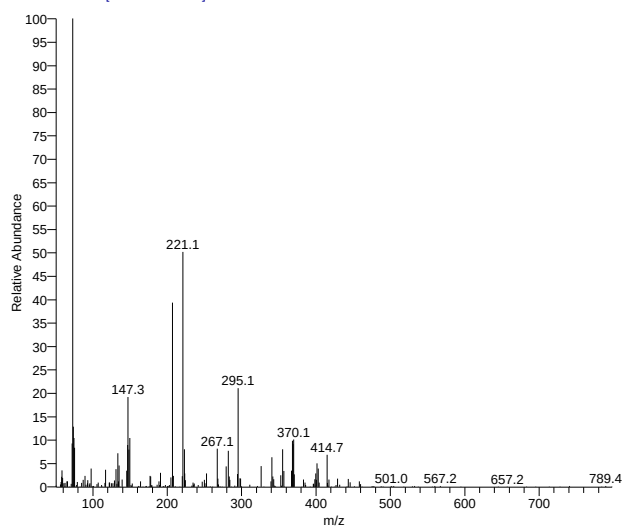


RT: 38.00 - 39.17 SM: 15G



NL:
8.77E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #9715 RT: 38.58 AV: 1 RF: 6.00, 3 NL: 1.72E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
38.58	Heptasiloxane, hexadecamethyl-	2682573.28	45.09	501	690	mainlib
38.58	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2682573.28	20.53	481	540	mainlib
38.58	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2682573.28	7.50	458	555	mainlib
38.58	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2682573.28	5.14	447	539	mainlib
38.58	Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-	2682573.28	2.49	428	481	mainlib

Analysed by Satyanarayana

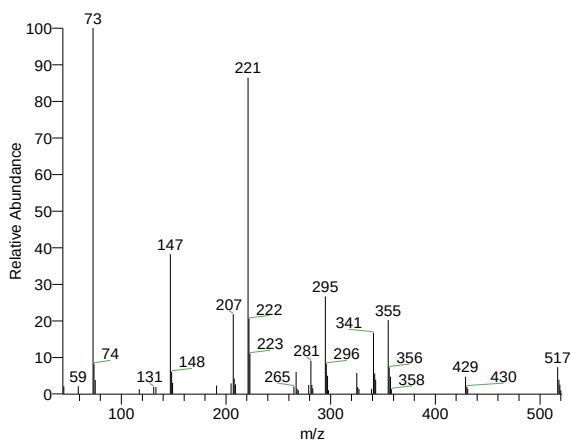
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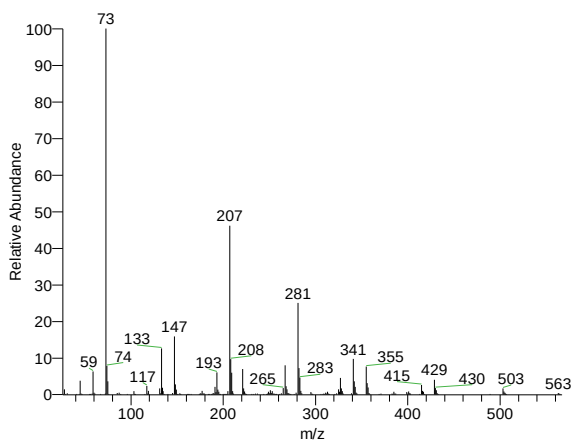
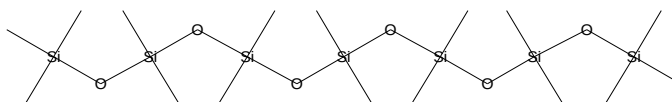
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

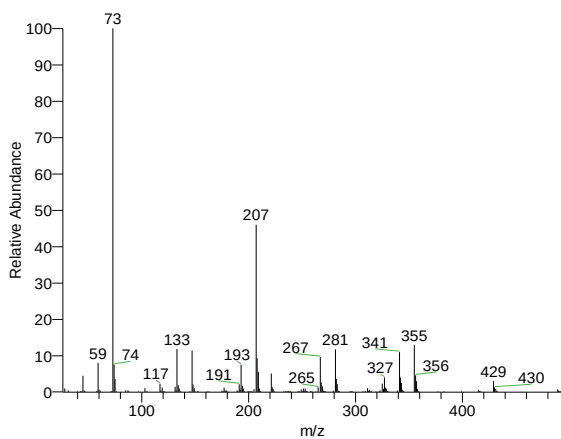
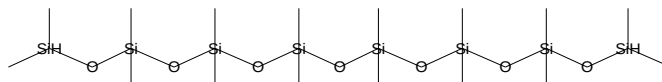
Compound Structure



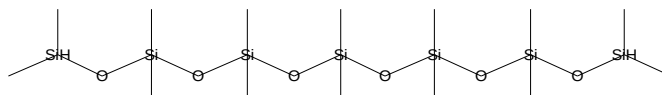
Heptasiloxane, hexadecamethyl-
Formula C16H48O6Si7, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C14H44O6Si7, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

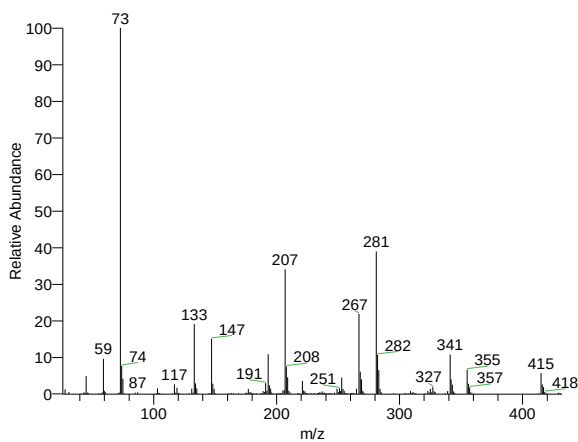
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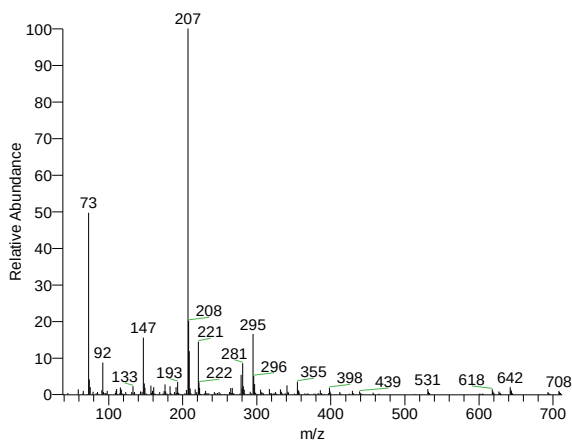
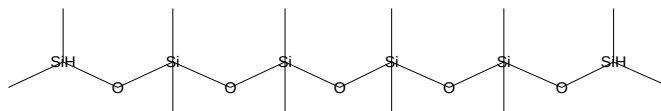
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

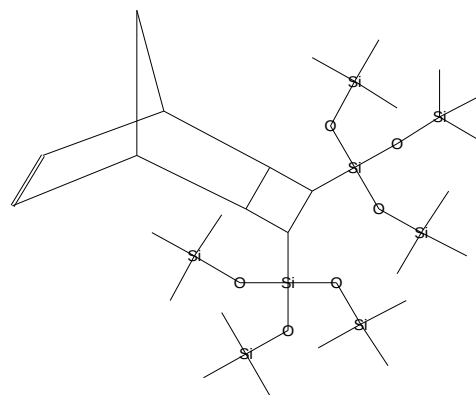
Compound Structure



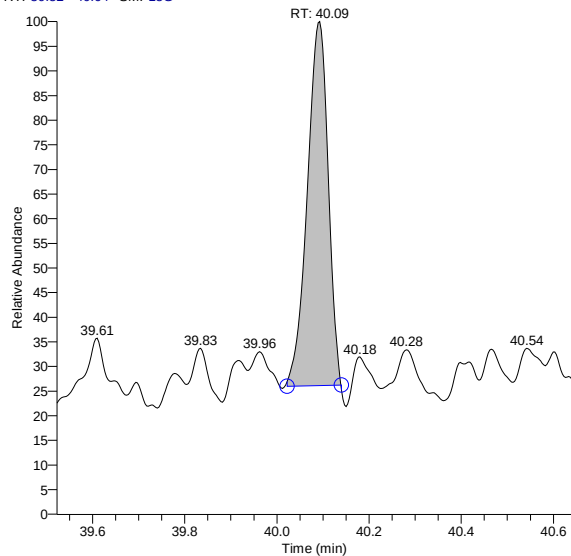
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Tricyclo[4.2.1.0(2,5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:28JSGSCCAWLXCNS-UHFFFAOYSA-N

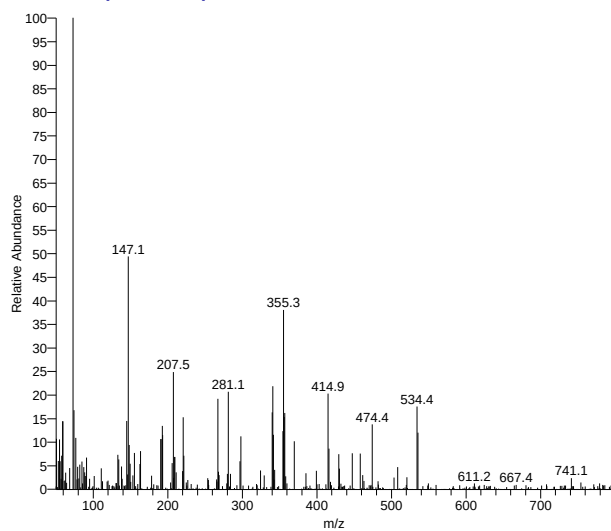


RT: 39.52 - 40.64 SM: 15G



NL:
2.41E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #10167 RT: 40.09 AV: 1 RF: 6.00, 3 NL: 3.59E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

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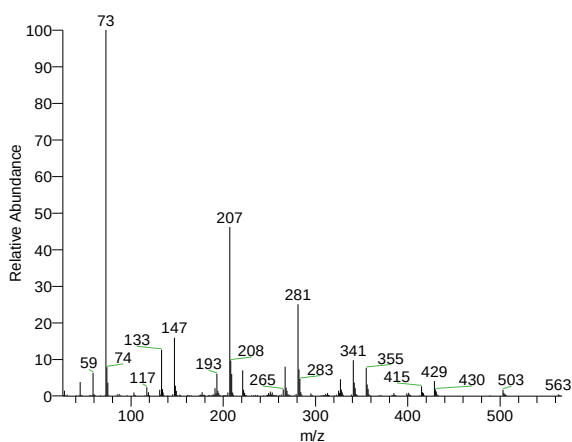
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

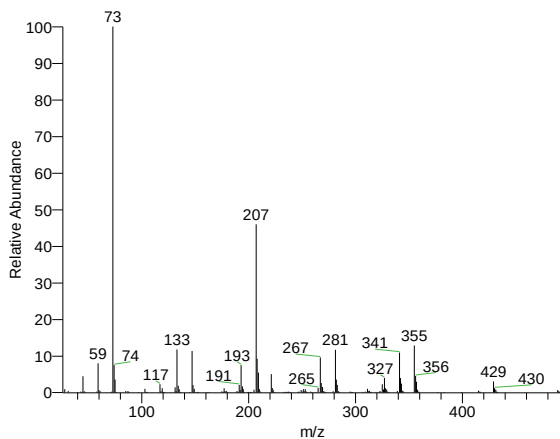
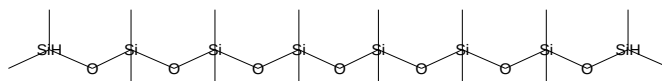
RT	Compound Name	Area	Probability	SI	RSI	Library
40.09	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	560368.05	18.55	451	626	mainlib
40.09	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	560368.05	14.21	444	641	mainlib
40.09	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	560368.05	6.90	425	610	mainlib
40.09	2,5-Dihydroxybenzoic acid, 3TMS derivative	560368.05	4.45	412	547	mainlib
40.09	Cyclodecasiloxane, eicosamethyl-	560368.05	4.11	410	458	mainlib

Hit Spectrum

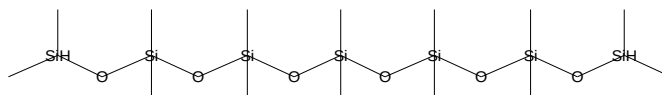
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

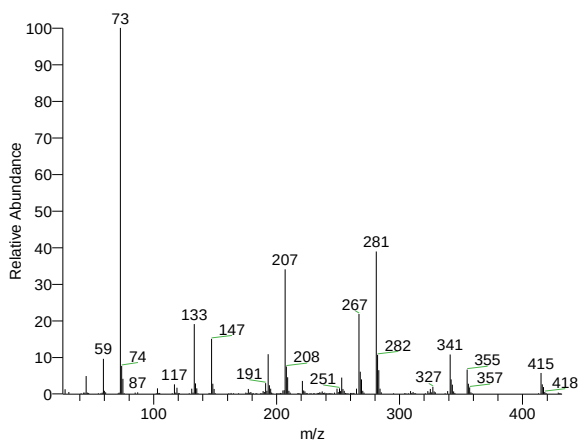
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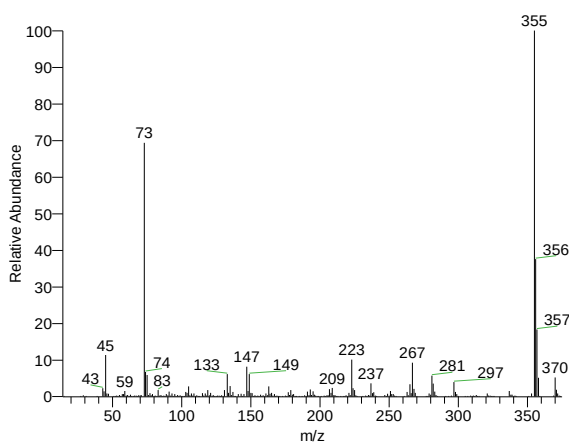
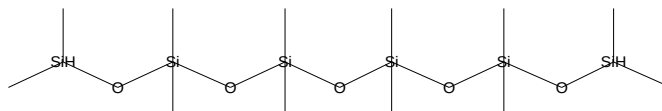
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

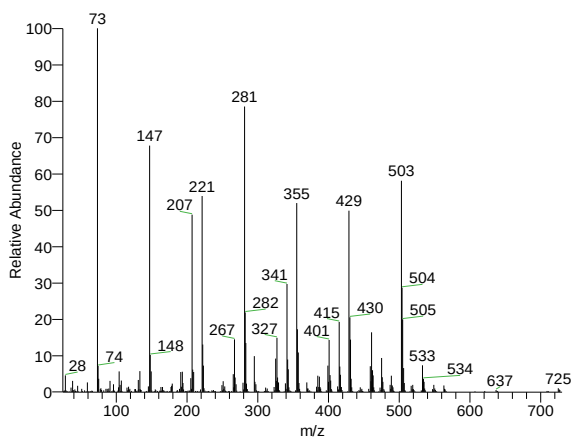
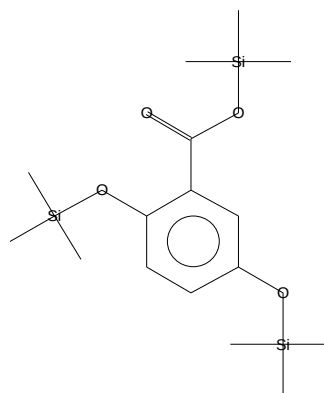
Compound Structure



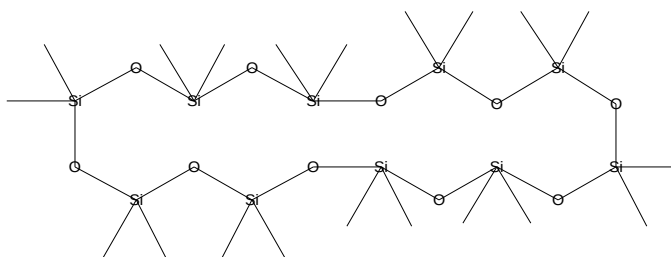
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



2,5-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-20-0, Entry# 234286
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester



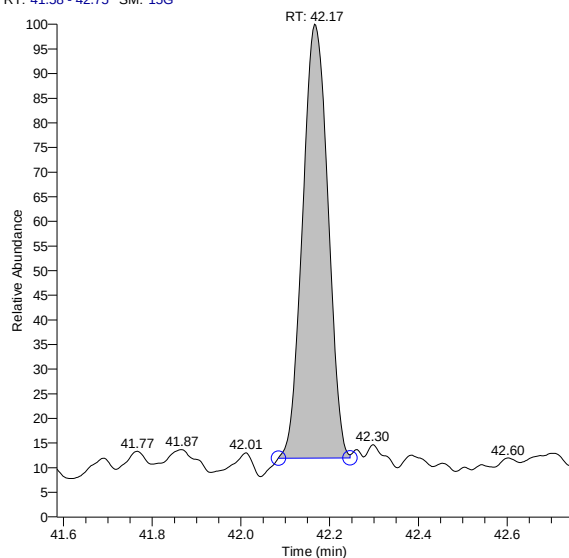
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



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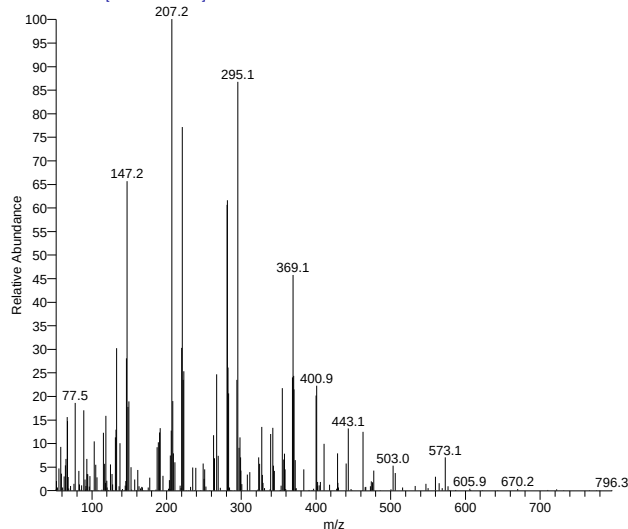
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RT: 41.58 - 42.75 SM: 15G



NL:
6.27E5
TIC: MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

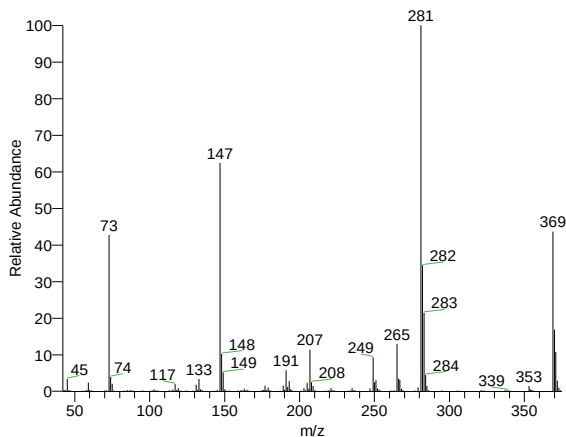
NGA-ZE-WATER4-SAMPLE-INJ1 #10785 RT: 42.17 AV: 1 RF: 6.00, 3 NL: 3.56E4
T: + c EI Full ms [50,000-800,000]



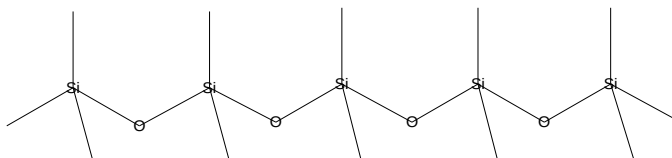
RT	Compound Name	Area	Probability	SI	RSI	Library
42.17	Pentasiloxane, dodecamethyl-	2198754.08	26.46	470	592	mainlib
42.17	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2198754.08	12.05	450	525	mainlib
42.17	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	2198754.08	8.99	442	566	mainlib
42.17	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2198754.08	6.34	432	554	mainlib
42.17	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	2198754.08	5.85	430	770	mainlib

Hit Spectrum

Compound Structure



Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane

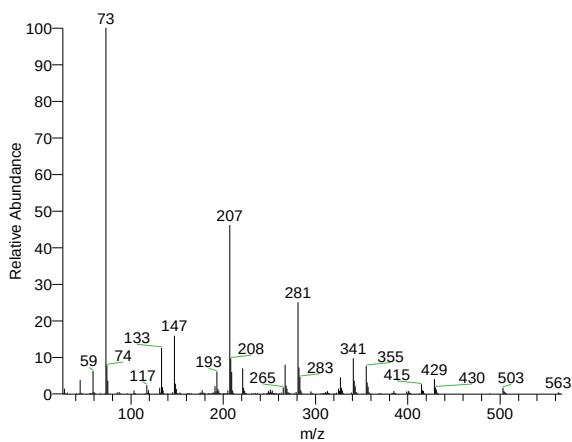


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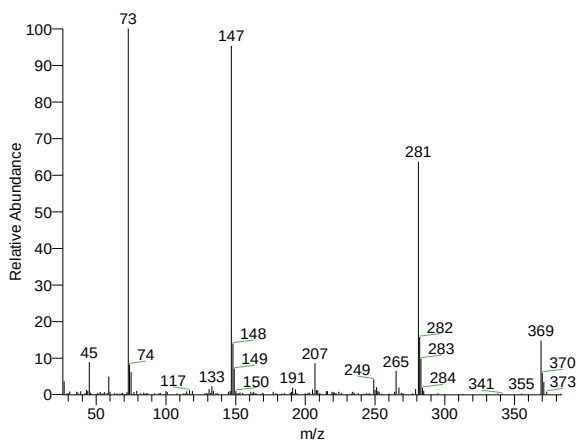
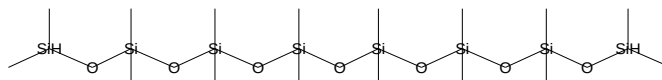
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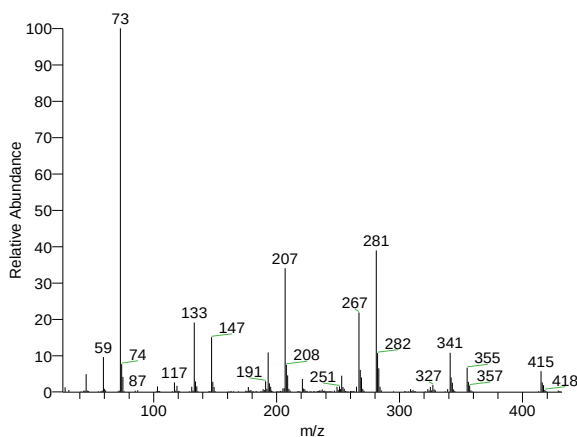
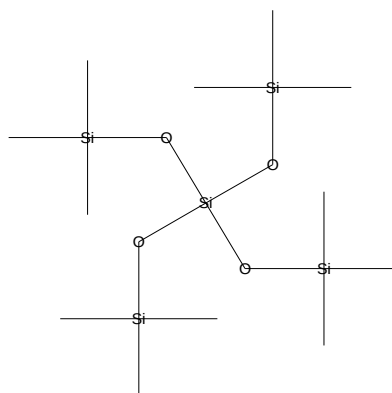
Compound Structure



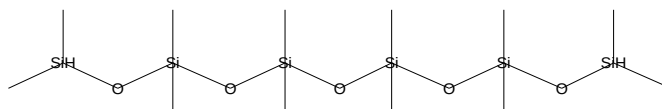
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #

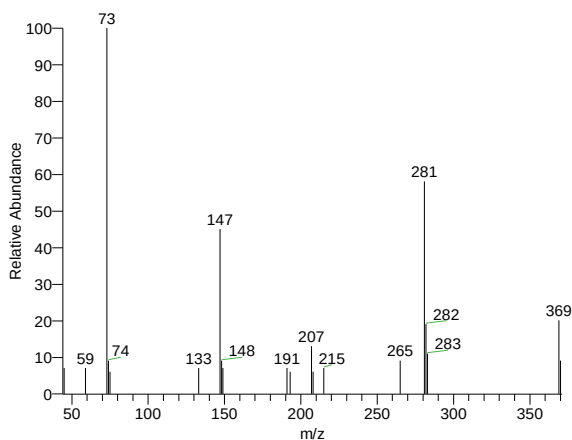


Analysed by Satyanarayana

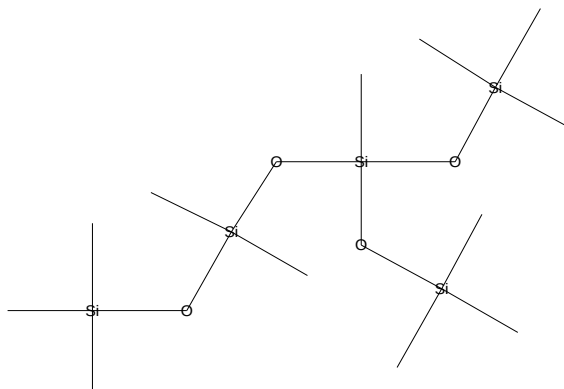
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Hit Spectrum

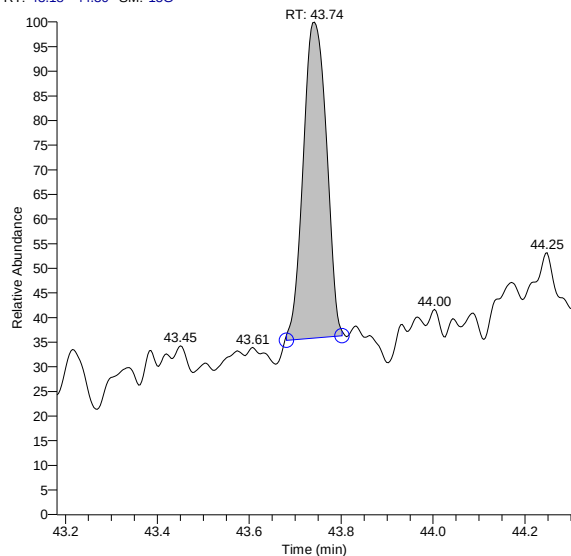
Compound Structure



1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-[(trimethylsilyl)oxy]tetrasiloxane #

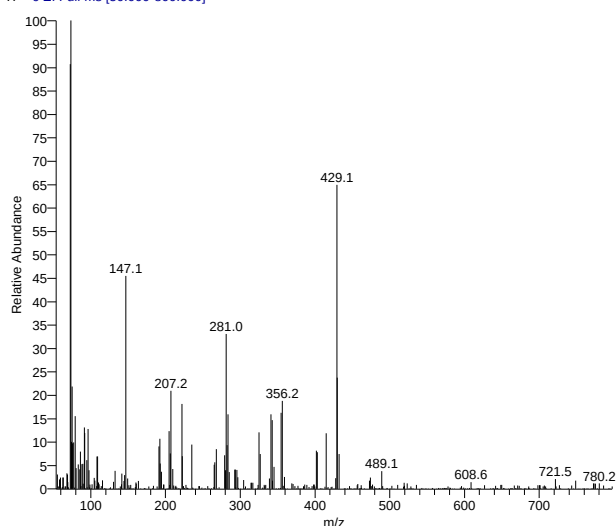


RT: 43.18 - 44.30 SM: 15G



NL: 2.61E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #11255 RT: 43.74 AV: 1 RF: 6.00, 3 NL: 3.69E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
43.74	Cyclononasiloxane, octadecamethyl-	584799.78	24.07	452	548	mainlib
43.74	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	584799.78	14.58	437	524	mainlib
43.74	Cyclohexasiloxane, dodecamethyl-	584799.78	9.71	425	588	mainlib
43.74	Cyclodecasiloxane, eicosamethyl-	584799.78	6.47	413	459	mainlib
43.74	2-(2,6-Bis(tert-butyl-dimethylsilyl)-3,4-dihydro-3-pyridyl)isoindoline-1,3-dione	584799.78	4.95	406	508	mainlib

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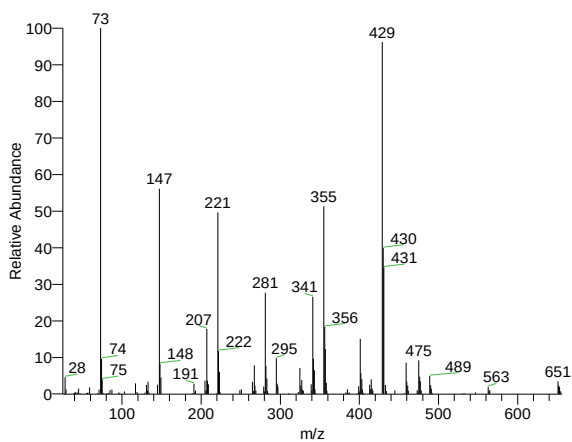
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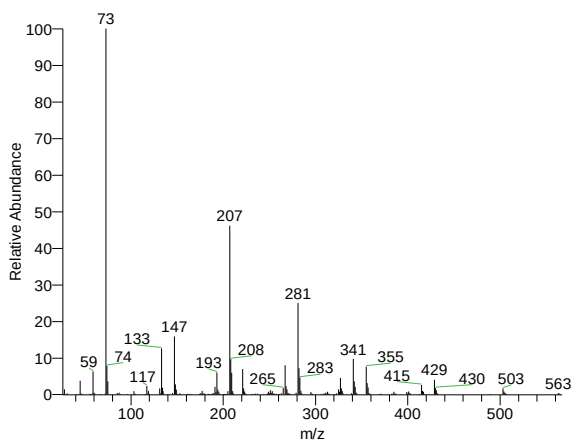
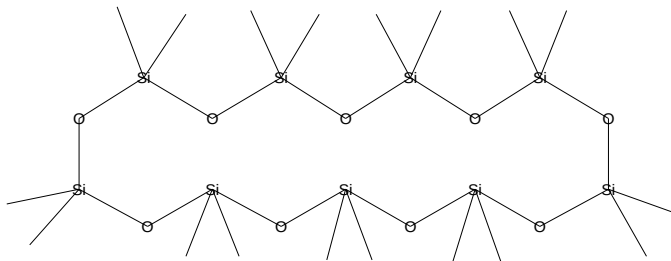
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

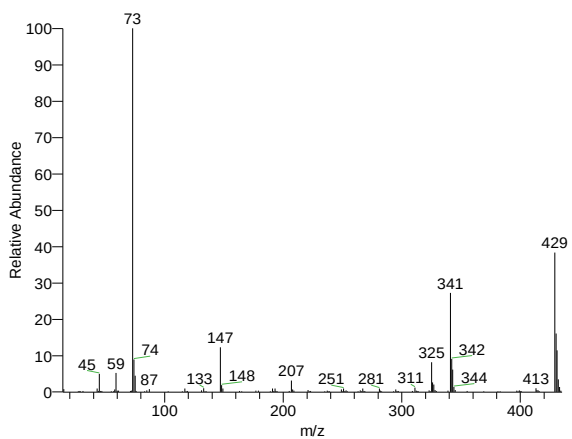
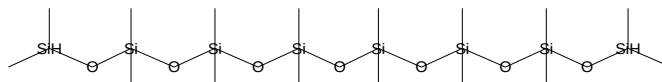
Compound Structure



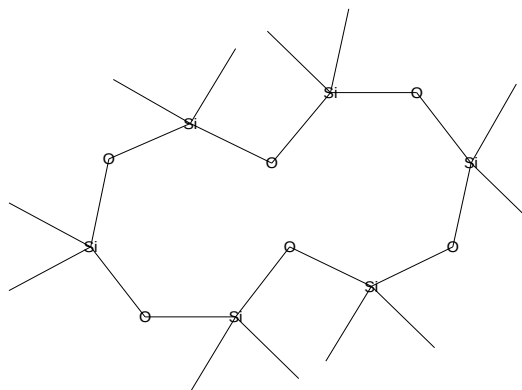
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclohexasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₆Si₆, MW 444, CAS# 540-97-6, Entry# 44297
Dodecamethylcyclohexasiloxane

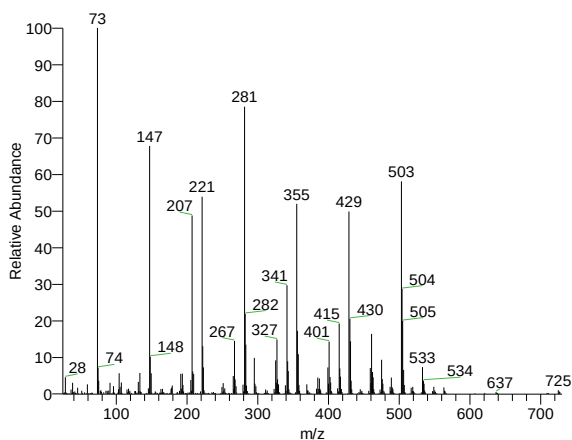


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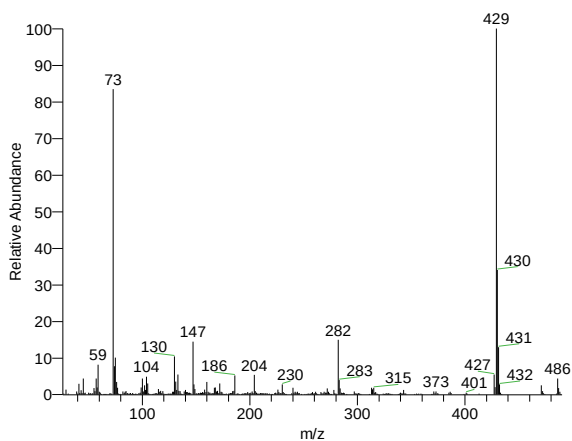
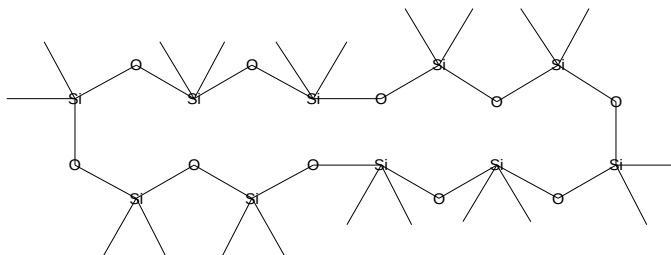
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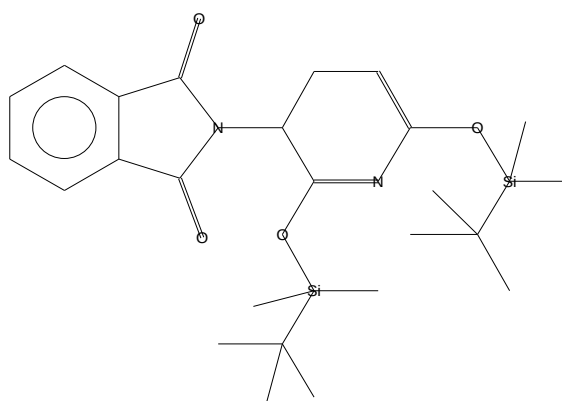
Compound Structure



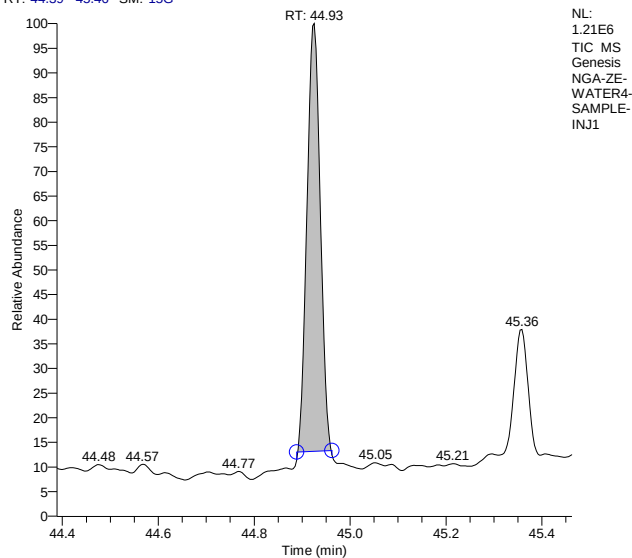
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



2-(2,6-Bis(tert-butylidimethylsilyl)-3,4-2H-3-pyridyl)isoindoline-1,3-dione
Formula C₂₅H₃₈N₂O₄Si₂, MW 486, CAS# NA, Entry# 239586
Calmore BDMS

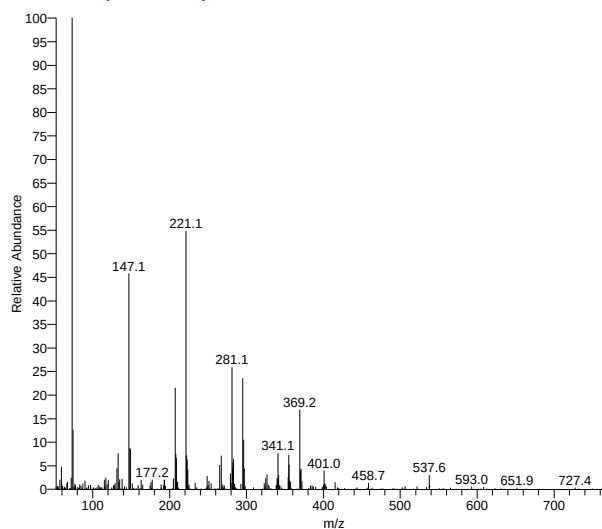


RT: 44.39 - 45.46 SM: 15G



NL:
1.21E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #11608 RT: 44.93 AV: 1 RF: 6.00, 3 NL: 2.94E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
44.93	Heptasiloxane, hexadecamethyl-	2028933.71	45.06	632	796	mainlib

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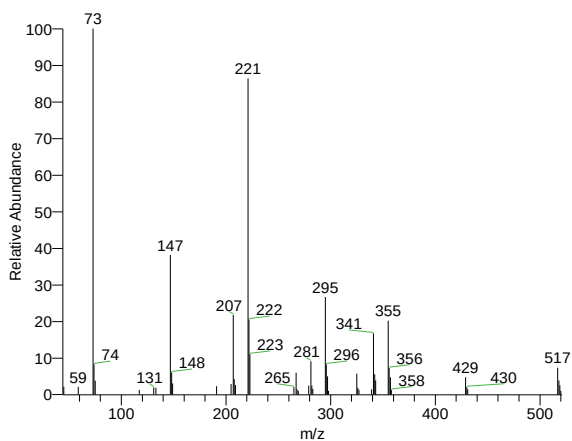
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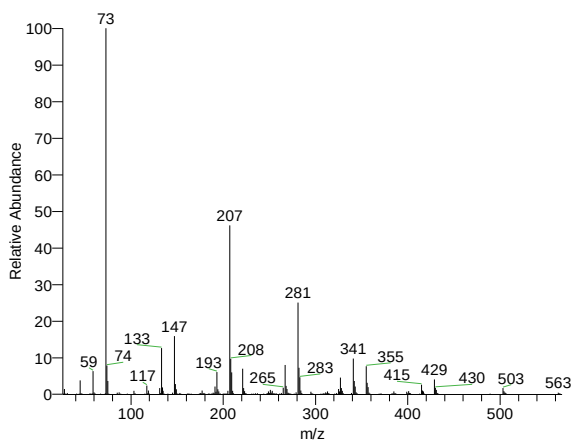
RT	Compound Name	Area	Probability	SI	RSI	Library
44.93	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2028933.71	30.01	620	668	mainlib
44.93	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2028933.71	8.01	588	682	mainlib
44.93	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2028933.71	6.77	584	695	mainlib
44.93	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	2028933.71	1.77	551	659	mainlib

Hit Spectrum

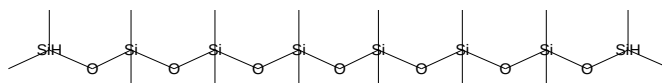
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



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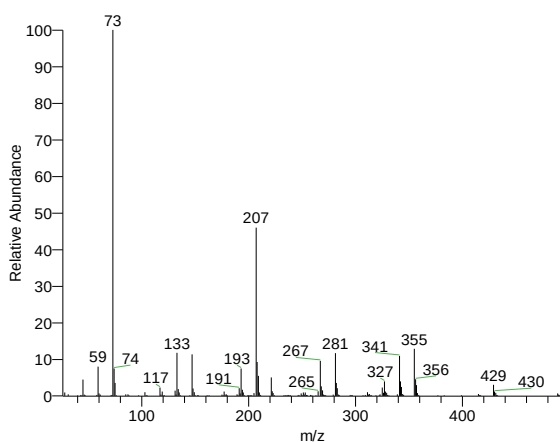
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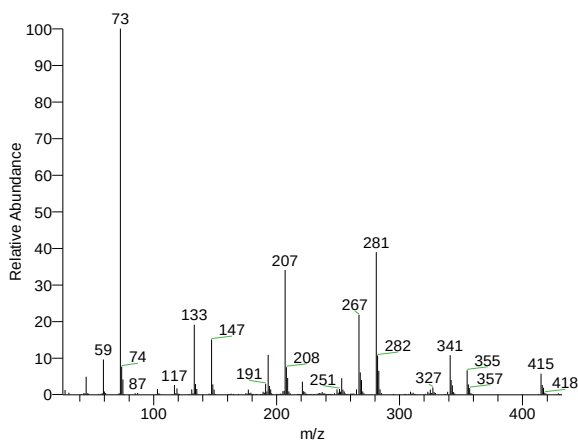
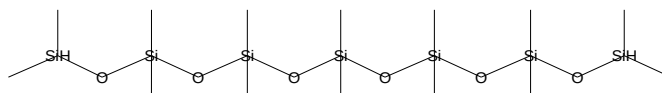
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

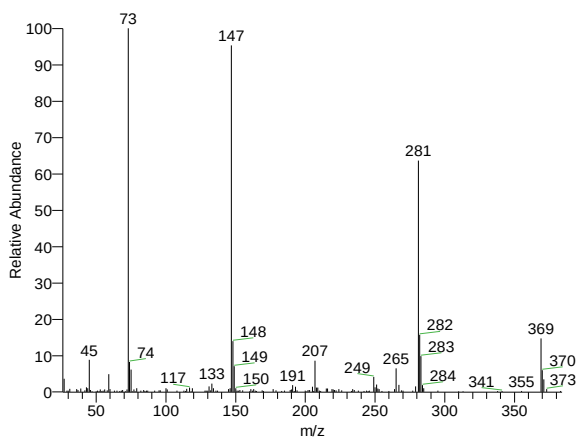
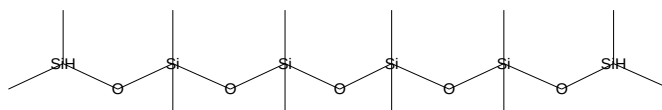
Compound Structure



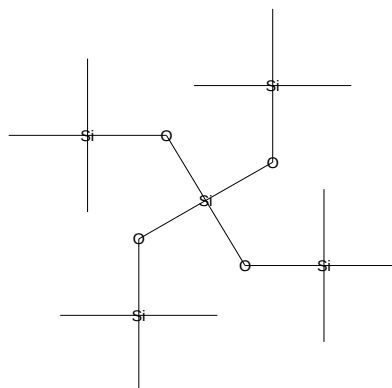
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



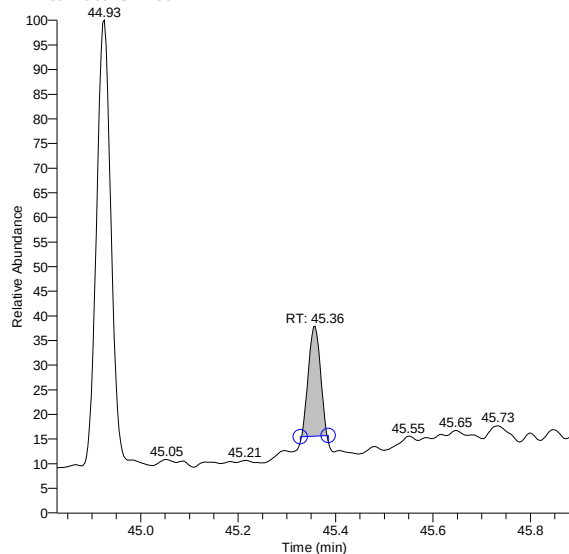
Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsiloxy)silane



Analysed by Satyanarayana

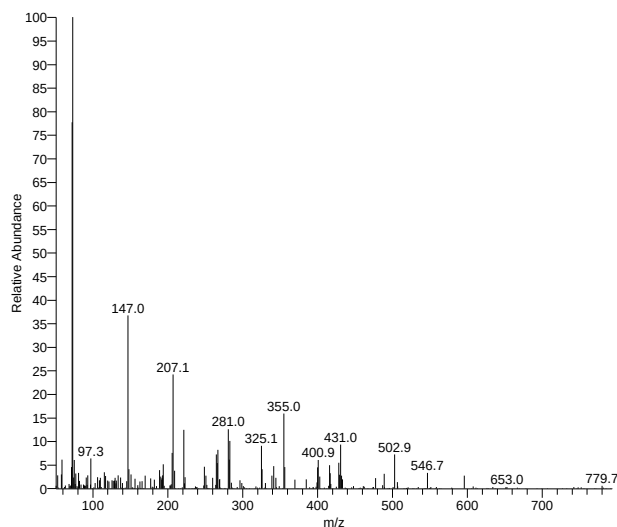
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RT: 44.83 - 45.88 SM: 15G



NL:
1.21E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

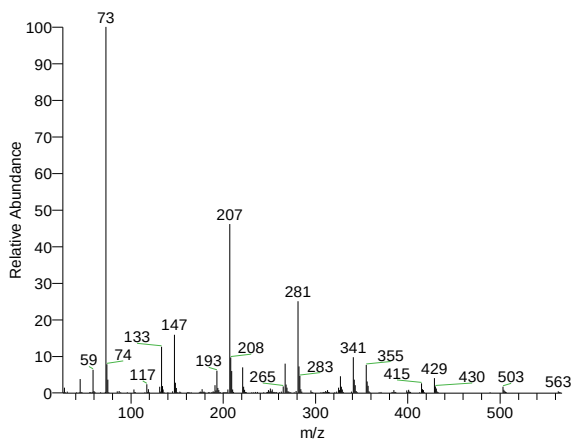
NGA-ZE-WATER4-SAMPLE-INJ1 #11737 RT: 45.36 AV: 1 RF: 6.00, 3 NL: 1.14E5
T: + c EI Full ms [50.000-800.000]



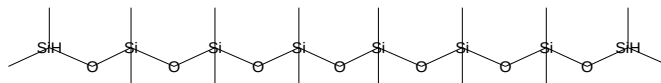
RT	Compound Name	Area	Probability	SI	RSI	Library
45.36	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	462492.73	45.82	513	594	mainlib
45.36	Cyclodecasiloxane, eicosamethyl-	462492.73	26.39	497	551	mainlib
45.36	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	462492.73	11.22	476	595	mainlib
45.36	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	462492.73	6.12	459	580	mainlib
45.36	Cyclononasiloxane, octadecamethyl-	462492.73	1.57	425	520	mainlib

Hit Spectrum

Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C16H50O7Si8, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #

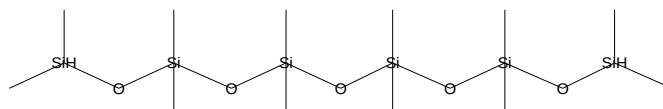
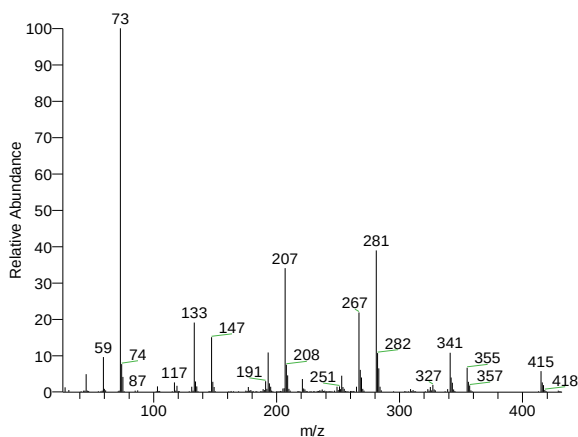
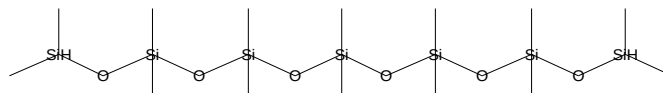
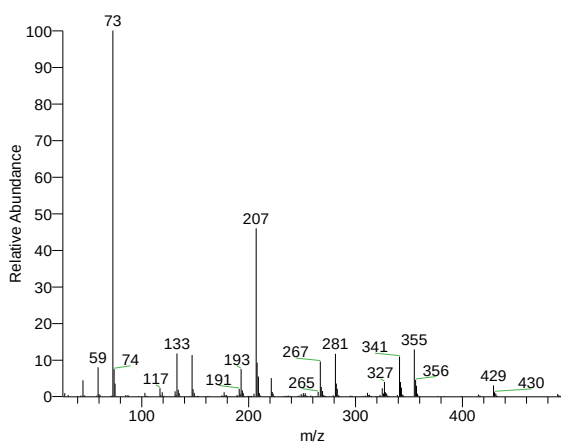
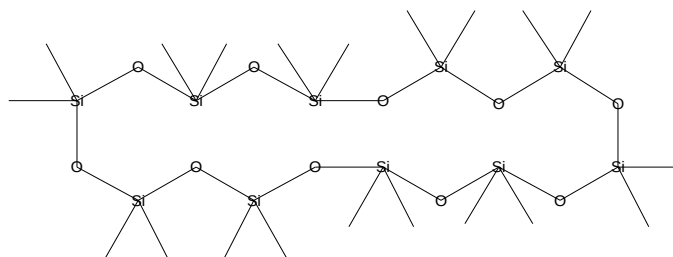
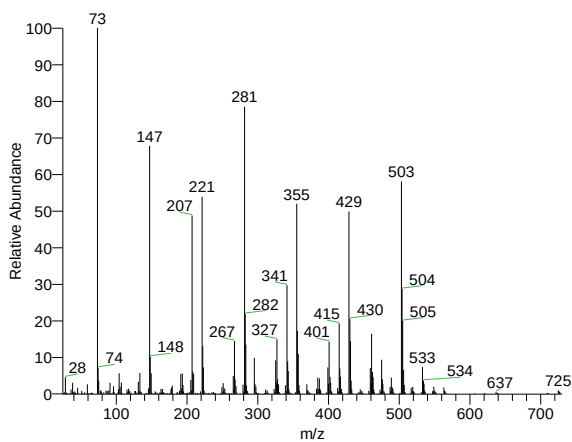


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Hit Spectrum

Compound Structure

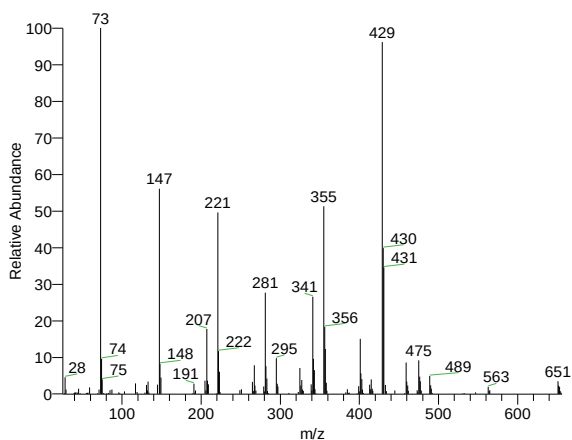


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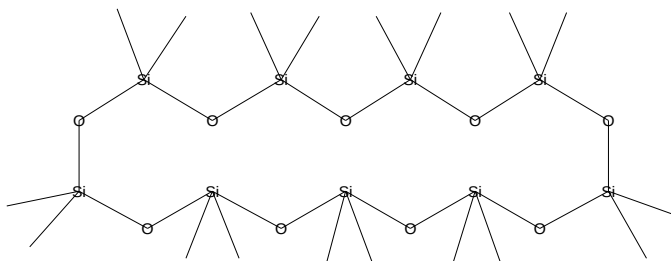
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Hit Spectrum

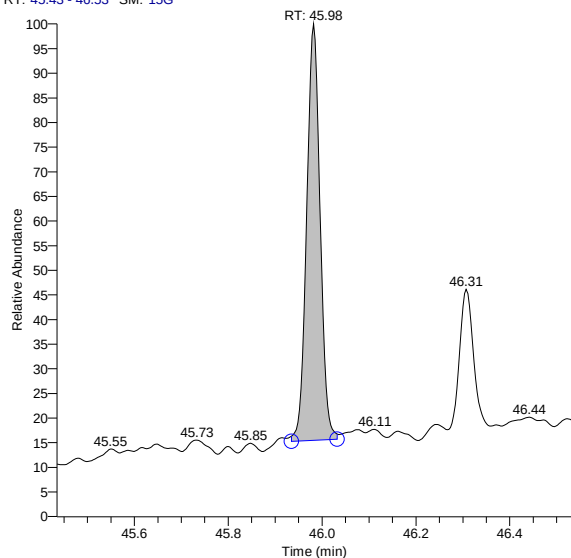
Compound Structure



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane

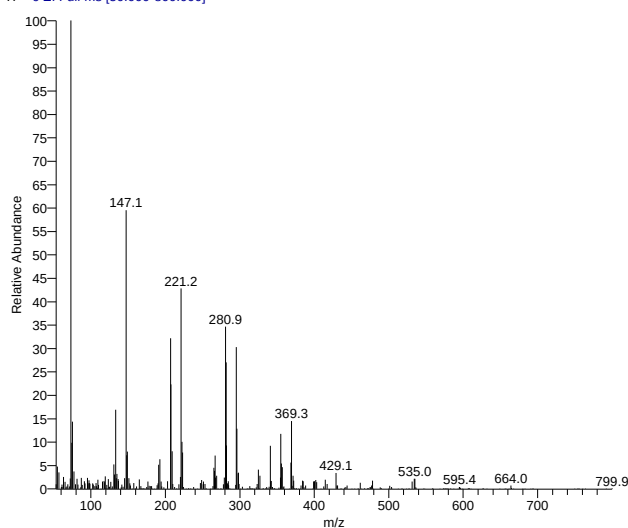


RT: 45.43 - 46.53 SM: 15G



NL: 1.38E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #11923 RT: 45.98 AV: 1 RF: 6.00, 3 NL: 2.89E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
45.98	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	2312742.61	56.75	624	680	mainlib
45.98	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	2312742.61	16.39	596	689	mainlib
45.98	Heptasiloxane, hexadecamethyl-	2312742.61	13.21	591	731	mainlib
45.98	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	2312742.61	3.74	562	675	mainlib
45.98	Tricyclo[4.2.1.0(2,5)]non-7 -ene, 3,4-di(tris(trimethylsilyloxy silyl)-	2312742.61	2.49	550	592	mainlib

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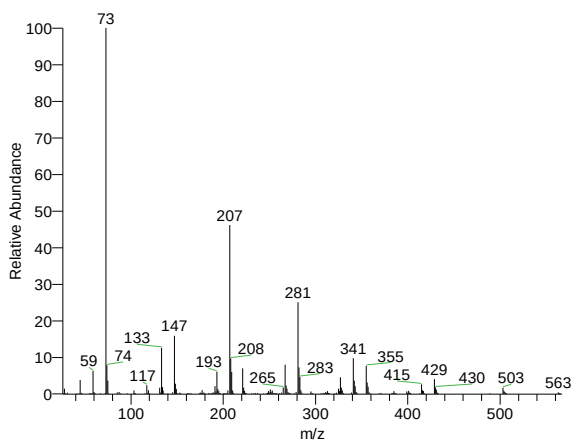
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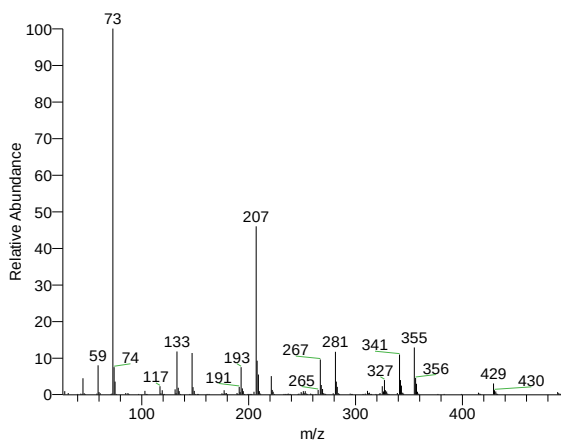
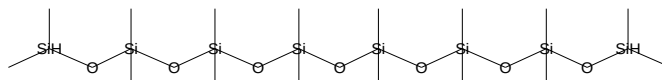
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

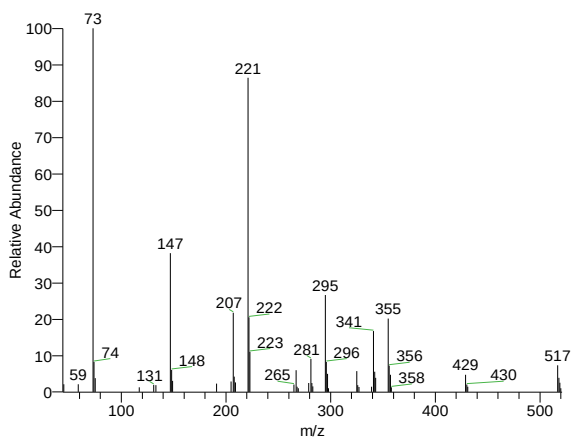
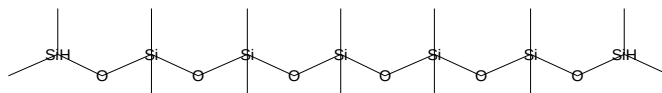
Compound Structure



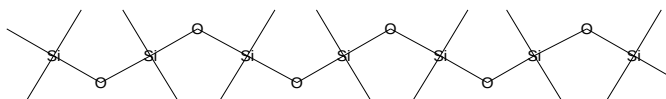
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



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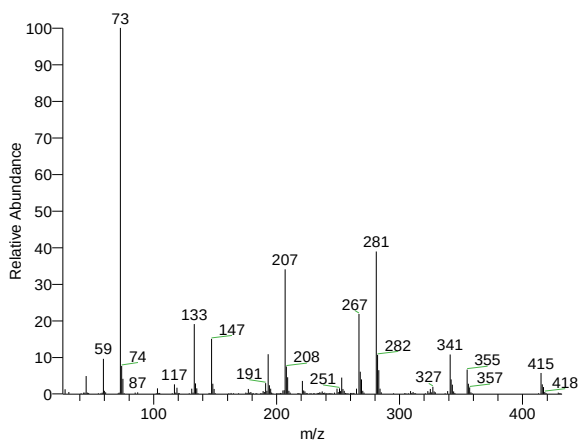
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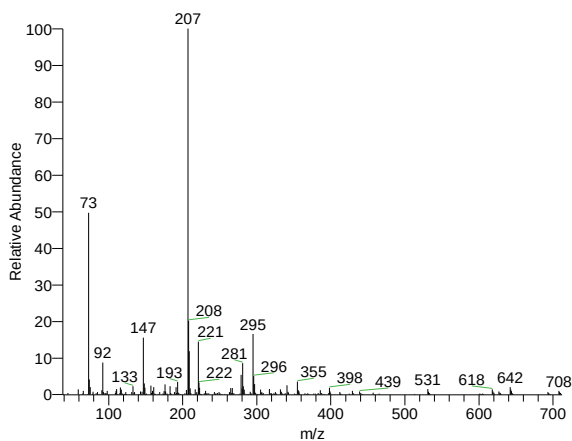
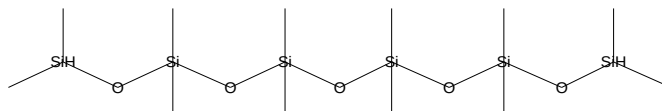
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

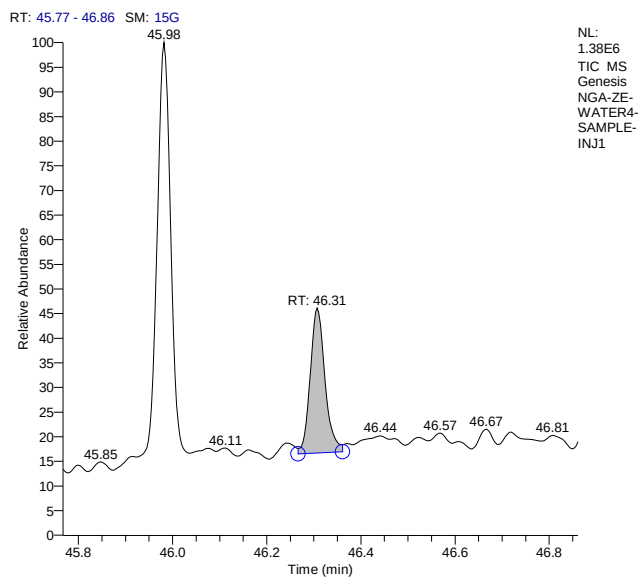
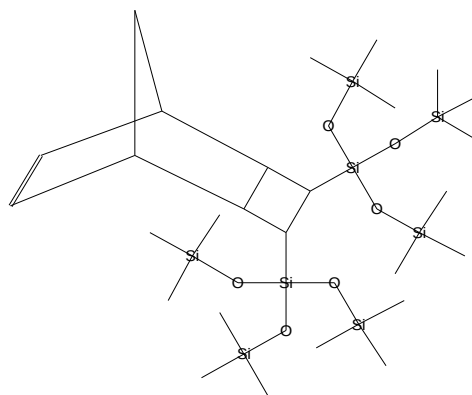
Compound Structure



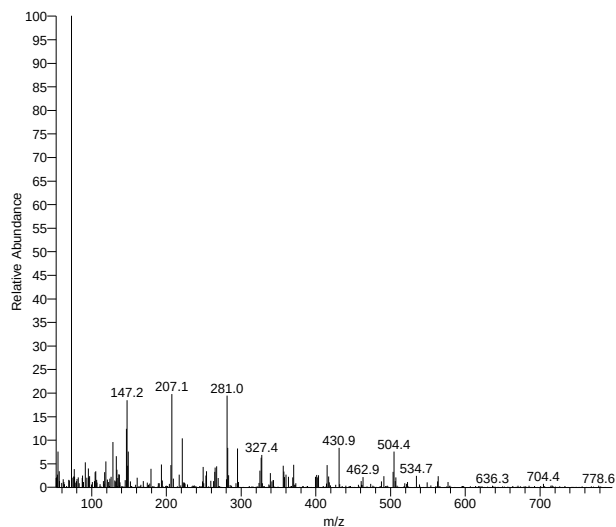
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Tricyclo[4.2.1.0(2.5)]non-7-ene, 3,4-di(tris(trimethylsilyloxy)silyl)-
Formula C₂₇H₆₄O₆Si₈, MW 708, CAS# NA, Entry# 188647
\$:2BJSGSCCAWLXCNS-UHFFFAOYSA-N



NGA-ZE-WATER4-SAMPLE-INJ1 #12020 RT: 46.31 AV: 1 RF: 6.00, 3 NL: 1.48E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
46.31	Cyclodecasiloxane, eicosamethyl-	880288.86	38.47	494	536	mainlib

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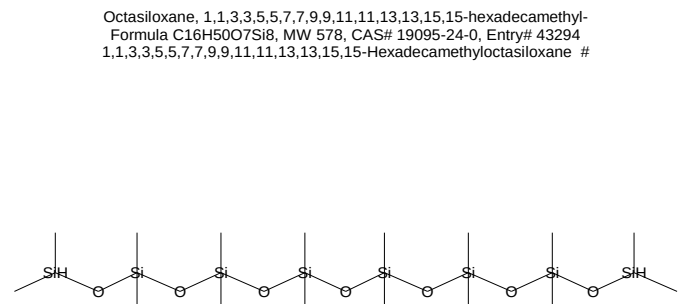
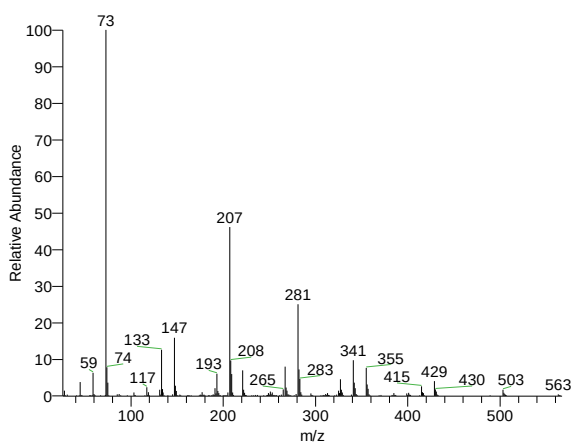
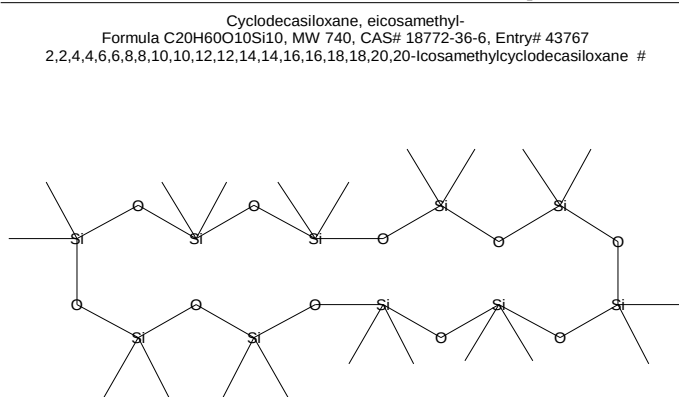
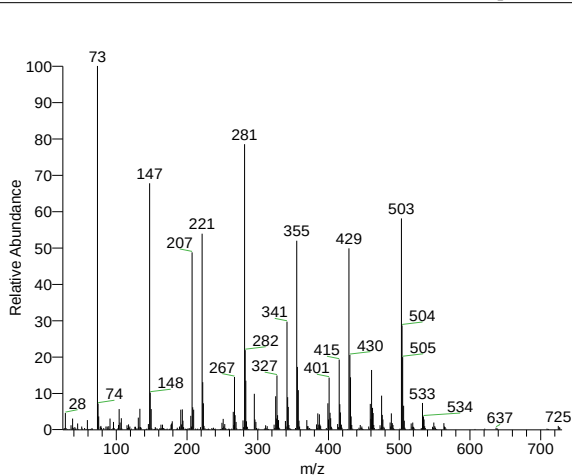
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RT	Compound Name	Area	Probability	SI	RSI	Library
46.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	880288.86	33.99	491	605	mainlib
46.31	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	880288.86	10.18	465	620	mainlib
46.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	880288.86	3.71	442	584	mainlib
46.31	Cycloheptasiloxane, tetradecamethyl-	880288.86	0.97	409	597	mainlib

Hit Spectrum

Compound Structure



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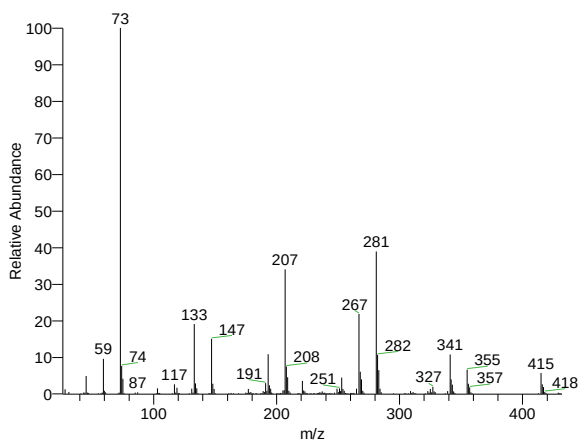
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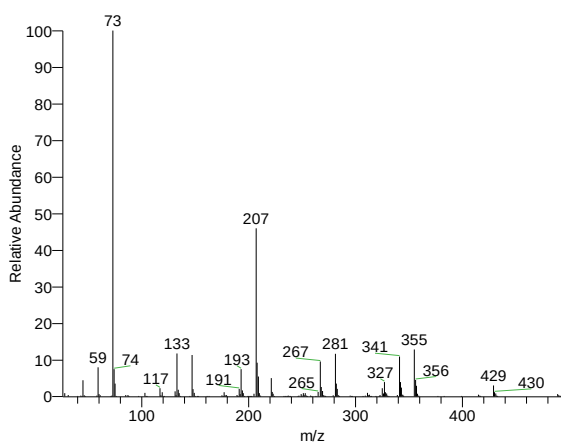
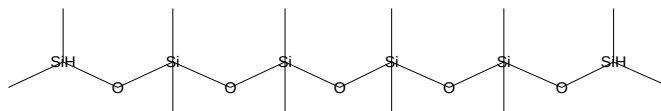
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

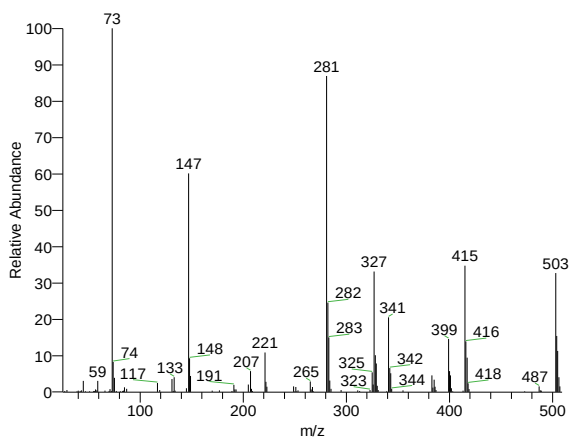
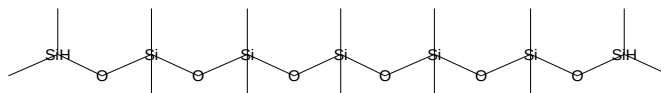
Compound Structure



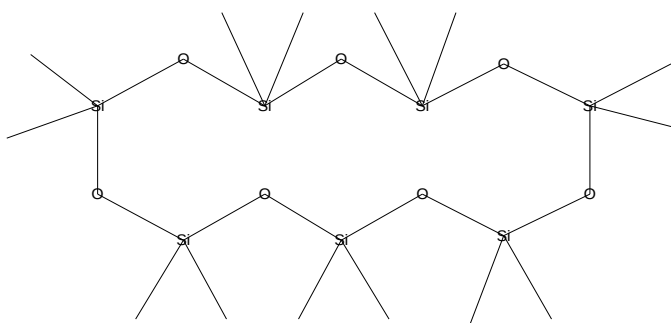
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



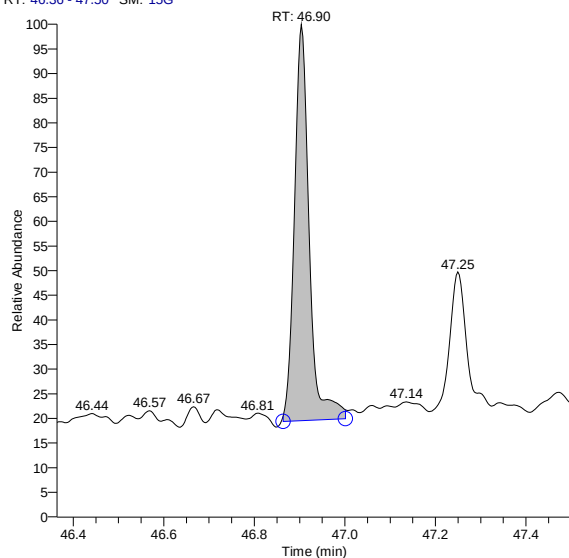
Cycloheptasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₇Si₇, MW 518, CAS# 107-50-6, Entry# 43769
2,2,4,4,6,6,8,8,10,10,12,12,14,14-Tetradecamethylcycloheptasiloxane #



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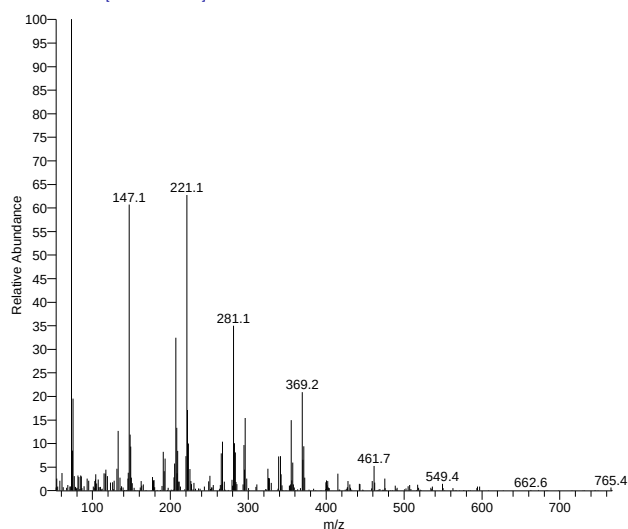
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RT: 46.36 - 47.50 SM: 15G



NL:
1.32E6
TIC: MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

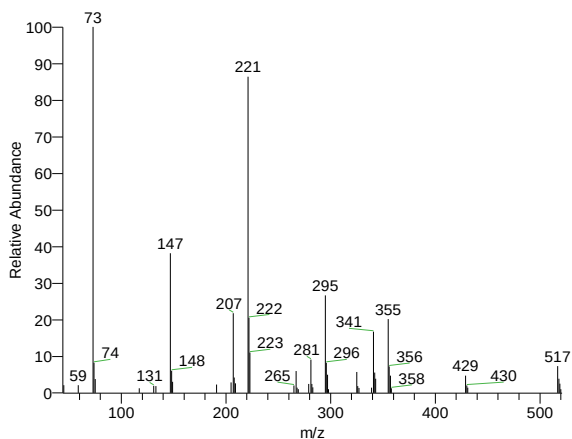
NGA-ZE-WATER4-SAMPLE-INJ1 #12198 RT: 46.90 AV: 1 RF: 6.00, 3 NL: 2.23E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
46.90	Heptasiloxane, hexadecamethyl-	2417905.33	28.62	585	771	mainlib
46.90	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2417905.33	20.21	575	653	mainlib
46.90	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	2417905.33	10.42	557	689	mainlib
46.90	Hexasiloxane, tetradecamethyl-	2417905.33	9.61	555	792	mainlib
46.90	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2417905.33	6.01	541	679	mainlib

Hit Spectrum

Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Analysed by Satyanarayana

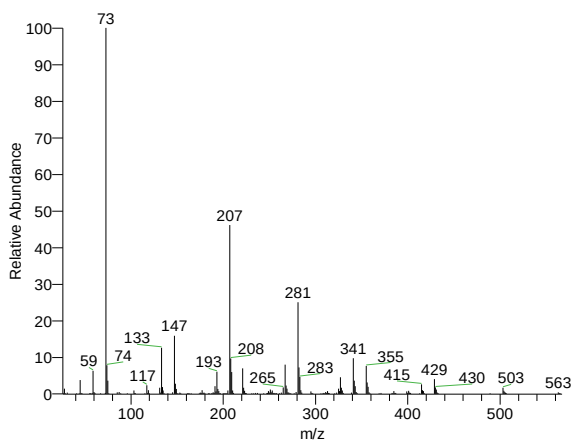
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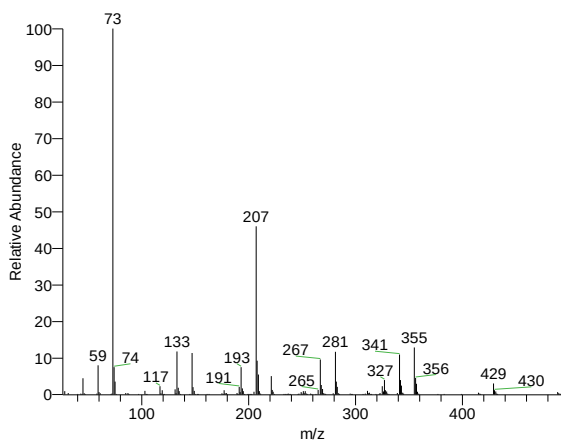
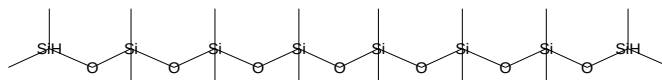
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

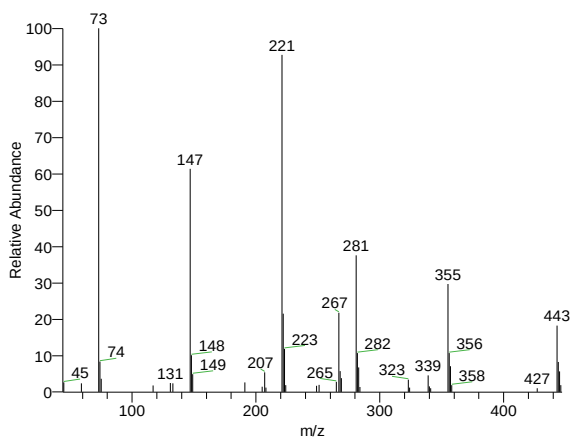
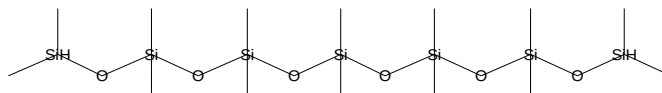
Compound Structure



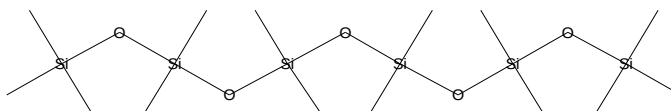
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, tetradecamethyl-
Formula C₁₄H₄₂O₅Si₆, MW 458, CAS# 107-52-8, Entry# 43443
Tetradecamethylhexasiloxane

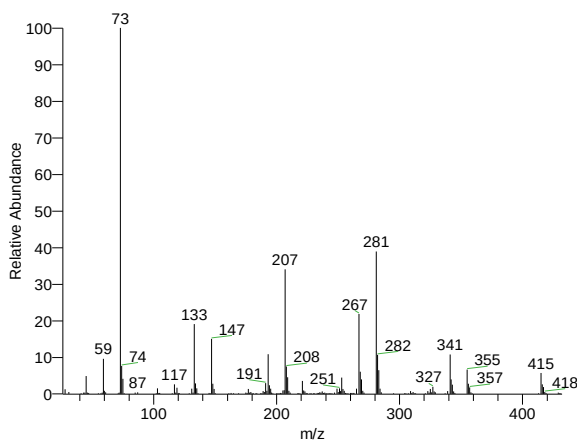


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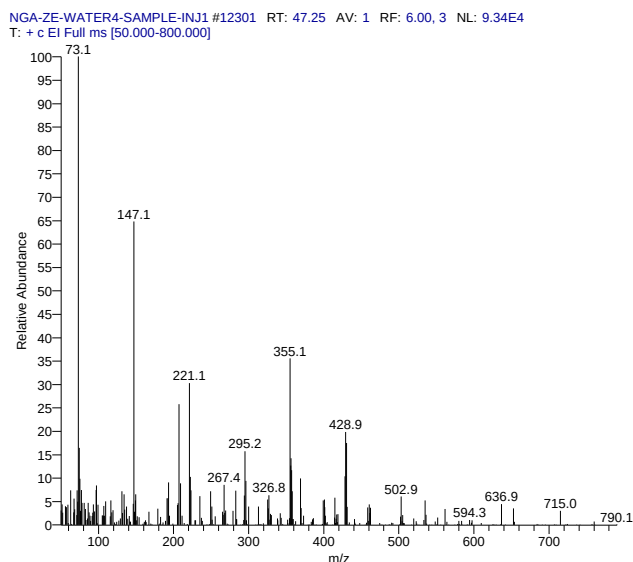
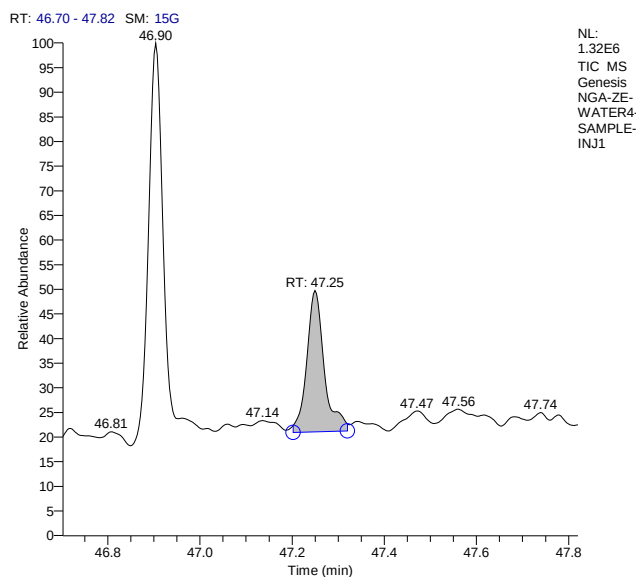
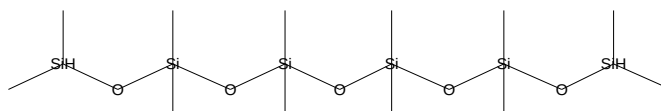
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Hit Spectrum

Compound Structure



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



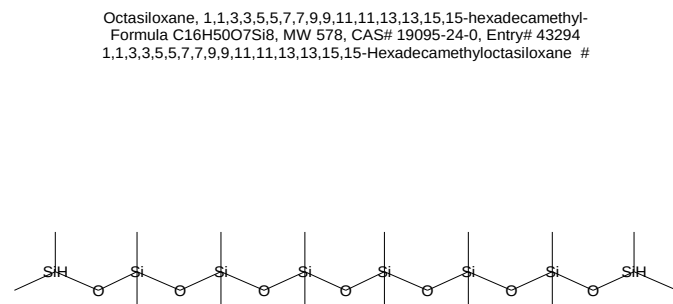
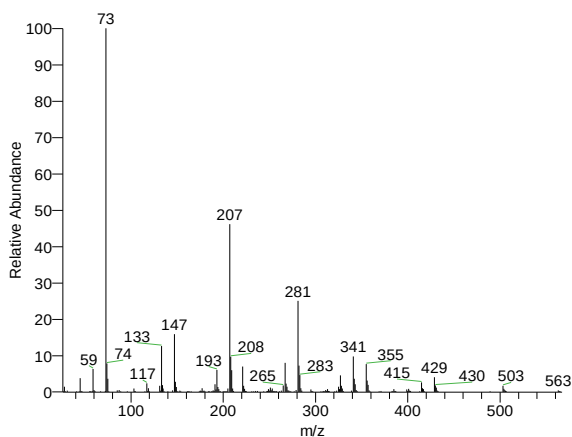
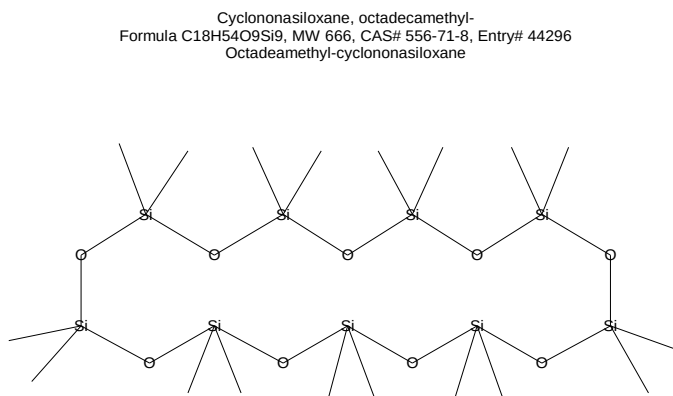
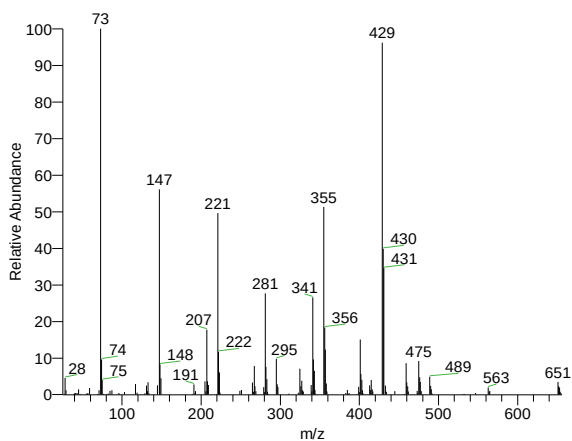
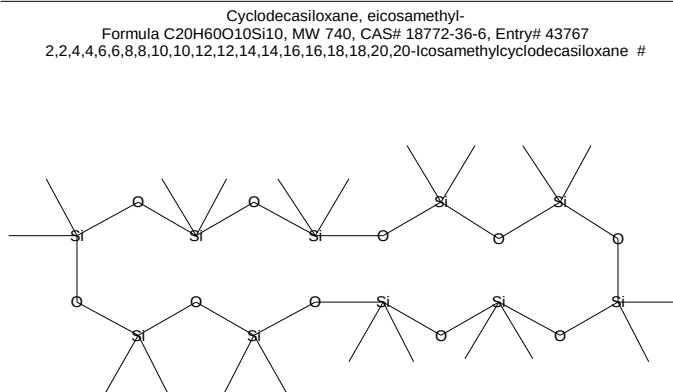
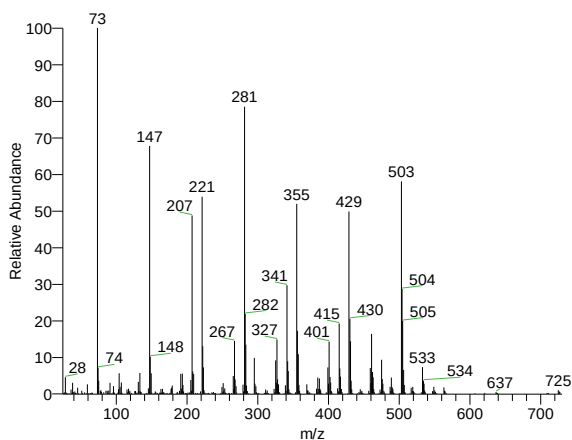
RT	Compound Name	Area	Probability	SI	RSI	Library
47.25	Cyclodecasiloxane, eicosamethyl-	1002071.72	34.34	535	584	mainlib
47.25	Cyclononasiloxane, octadecamethyl-	1002071.72	26.30	528	651	mainlib
47.25	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1002071.72	5.70	484	585	mainlib
47.25	Heptasiloxane, hexadecamethyl-	1002071.72	4.81	480	702	mainlib
47.25	Tetracosamethyl-cyclododecasiloxane	1002071.72	4.44	478	733	mainlib

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Hit Spectrum

Compound Structure



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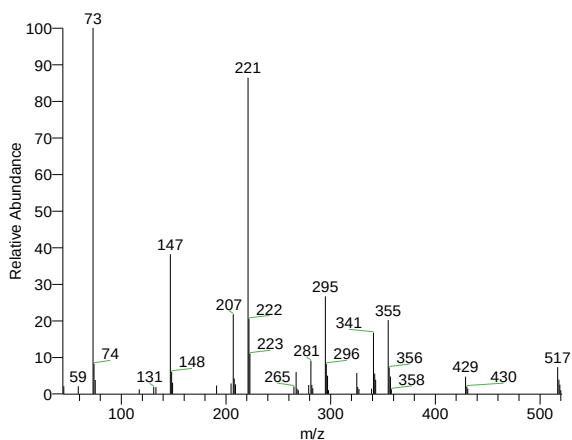
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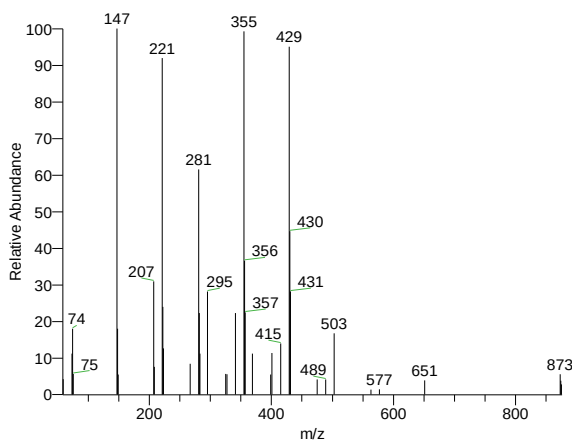
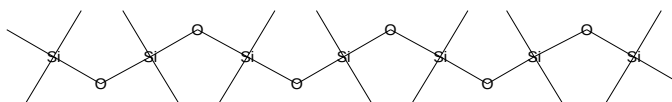
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

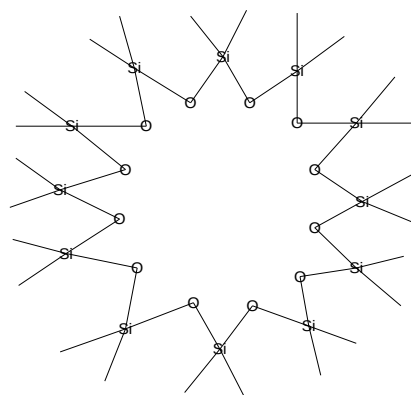
Compound Structure



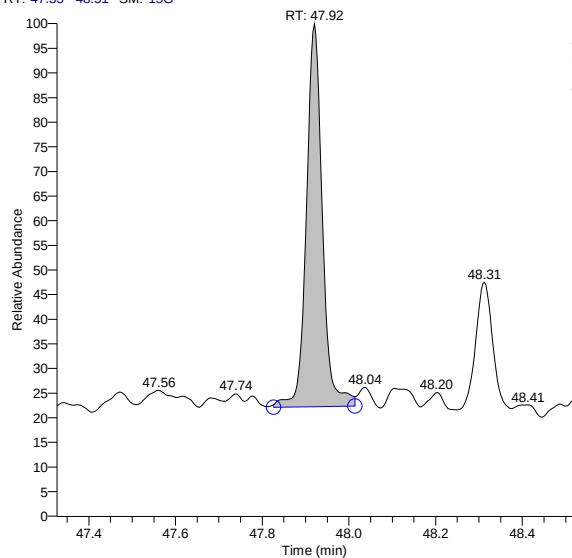
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752

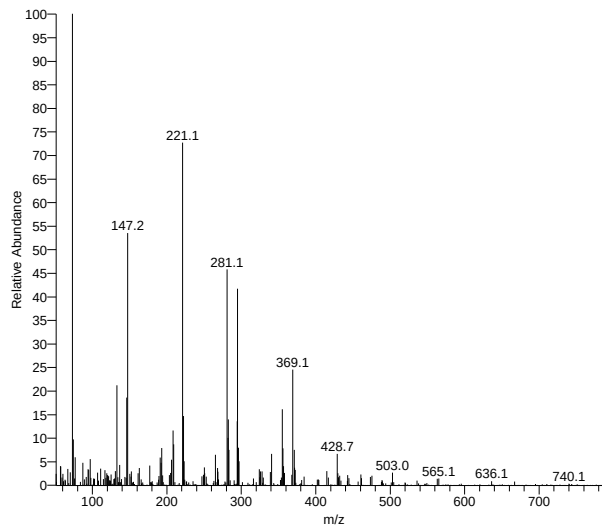


RT: 47.33 - 48.51 SM: 15G



NL:
1.33E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #12501 RT: 47.92 AV: 1 RF: 6.00, 3 NL: 1.88E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
47.92	Heptasiloxane, hexadecamethyl-	2661753.57	36.61	527	710	mainlib

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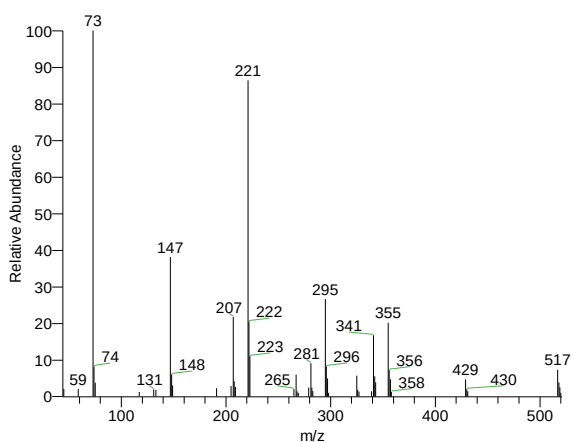
GC-MS/MS QUAL REPORT

ANALYTICAL CHEMISTRY DIVISION

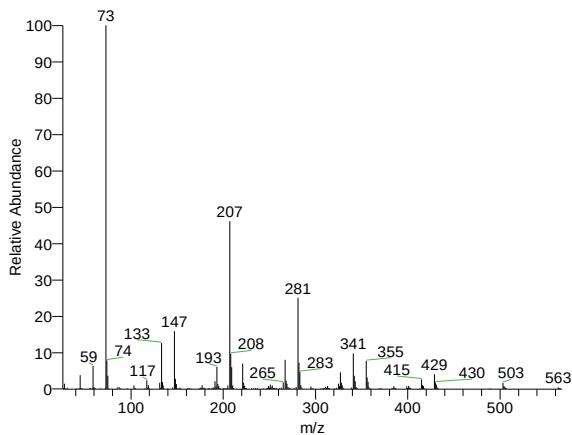
RT	Compound Name	Area	Probability	SI	RSI	Library
47.92	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2661753.57	15.57	506	568	mainlib
47.92	Cyclodecasiloxane, eicosamethyl-	2661753.57	8.96	490	511	mainlib
47.92	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	2661753.57	4.62	472	555	mainlib
47.92	Tetracosamethyl-cyclododecasiloxane	2661753.57	4.44	471	658	mainlib

Hit Spectrum

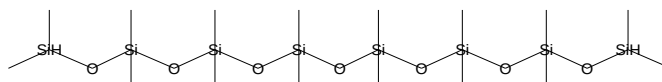
Compound Structure



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyl-octasiloxane #

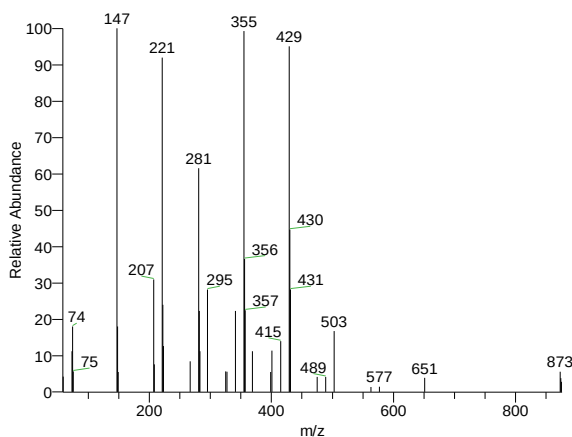
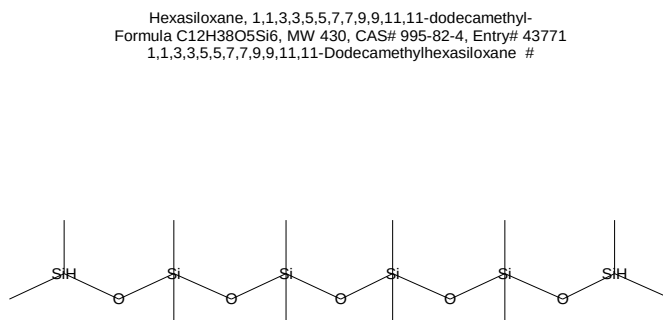
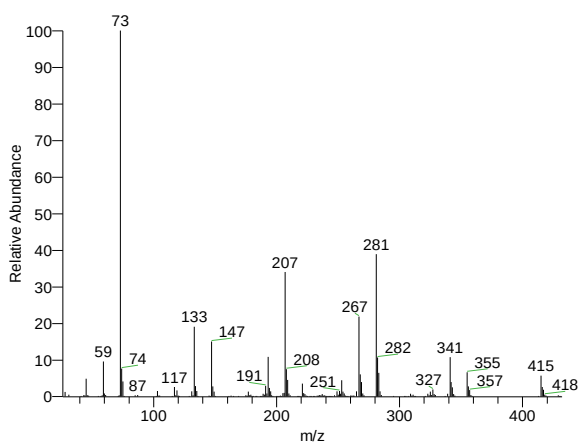
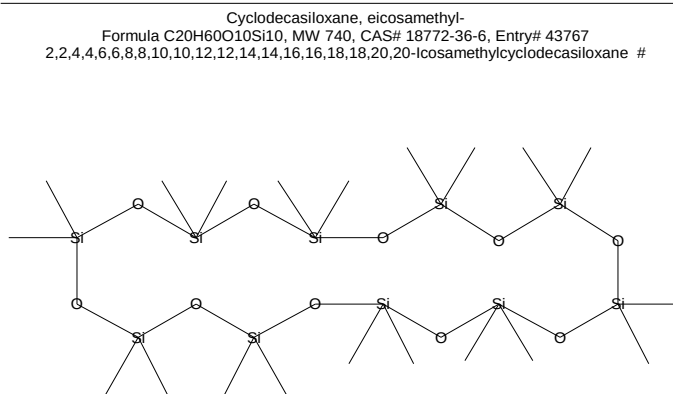
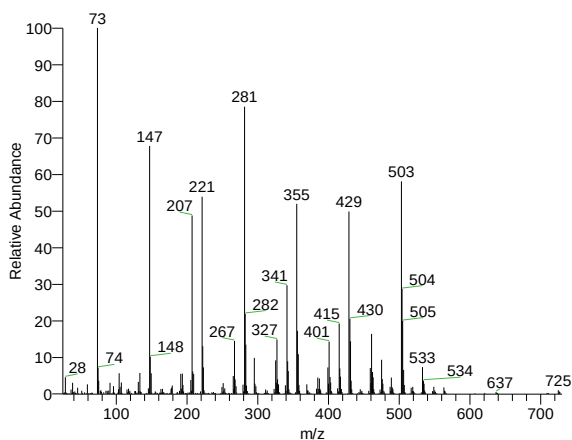


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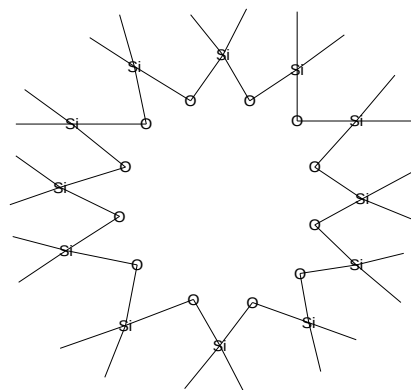
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ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

Compound Structure

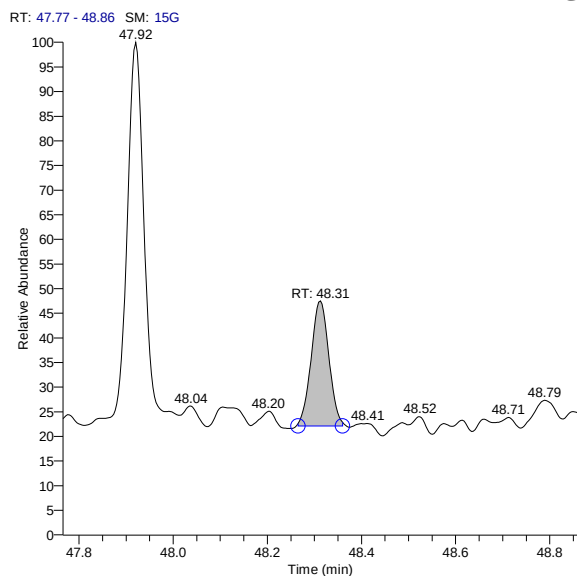


Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752



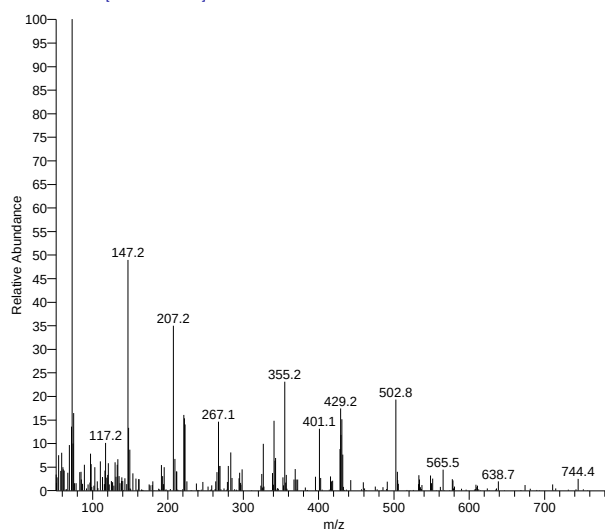
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NL:
1.33E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

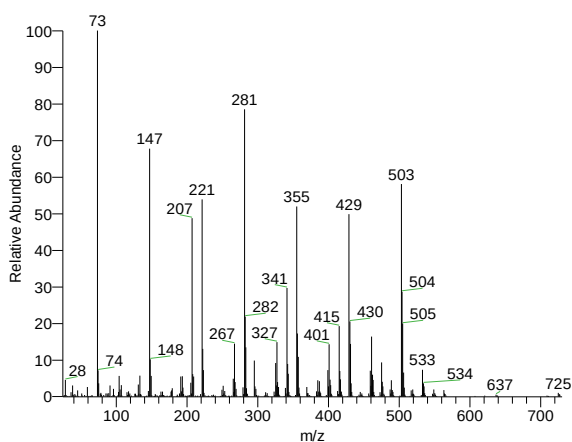
NGA-ZE-WATER4-SAMPLE-INJ1 #12618 RT: 48.31 AV: 1 RF: 6.00, 3 NL: 8.84E4
T: + c EI Full ms [50.000-800.000]



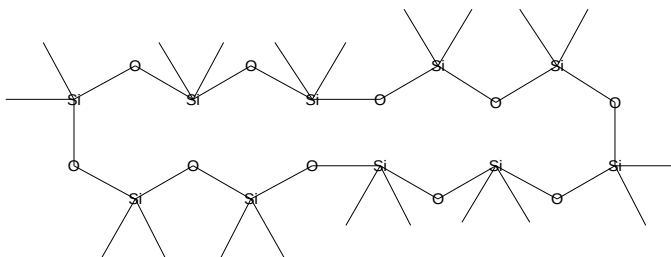
RT	Compound Name	Area	Probability	SI	RSI	Library
48.31	Cyclodecasiloxane, eicosamethyl-	881399.29	68.63	553	610	mainlib
48.31	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	881399.29	15.40	511	605	mainlib
48.31	Cyclononasiloxane, octadecamethyl-	881399.29	4.36	482	642	mainlib
48.31	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	881399.29	2.51	466	621	mainlib
48.31	Heptasiloxane, hexadecamethyl-	881399.29	2.51	466	678	mainlib

Hit Spectrum

Compound Structure



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



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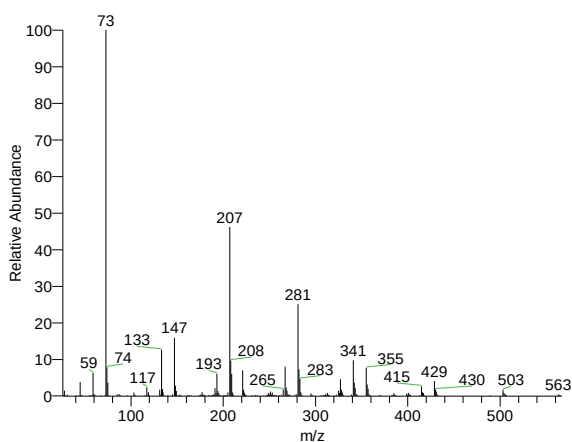
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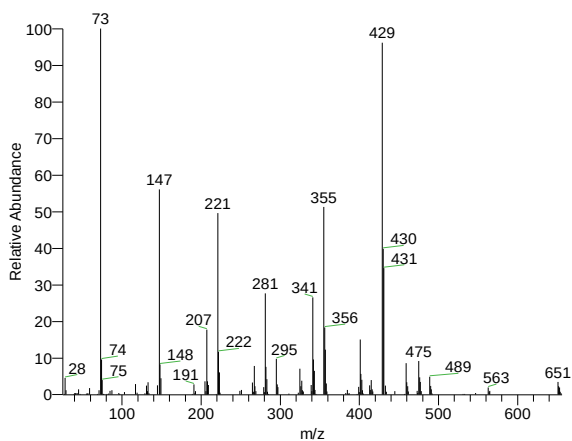
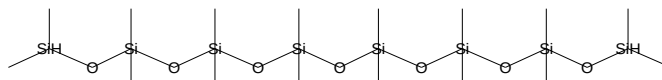
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

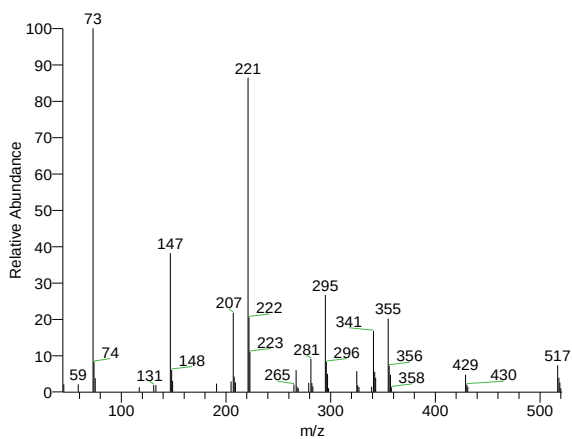
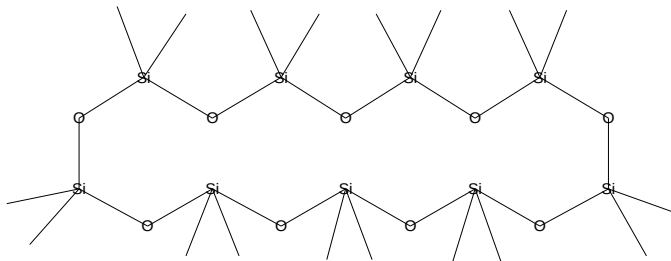
Compound Structure



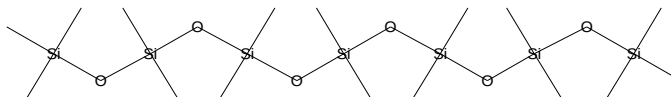
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane

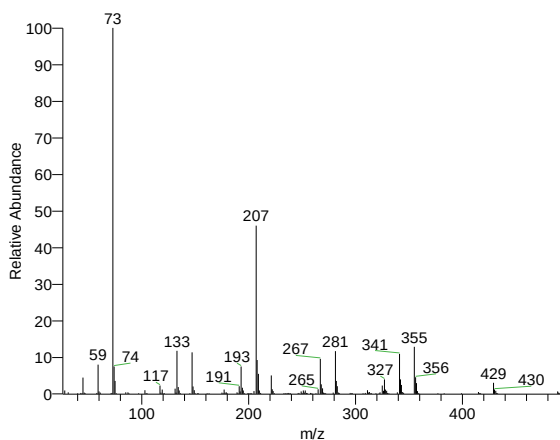


Analysed by Satyanarayana

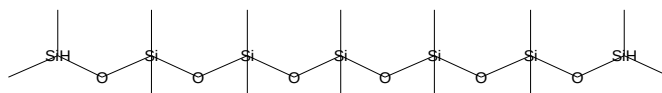
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Hit Spectrum

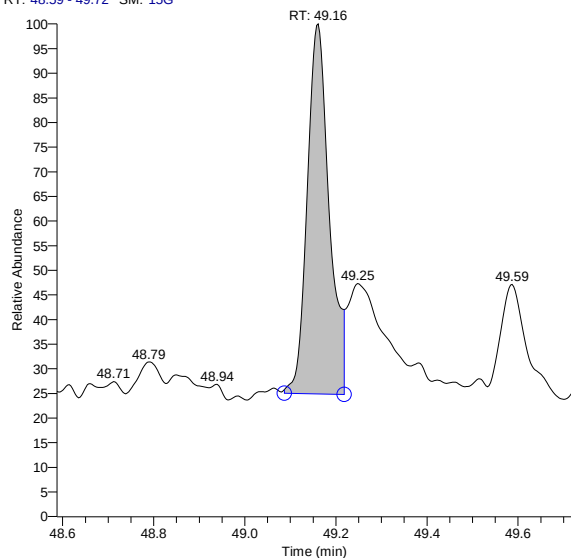
Compound Structure



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #

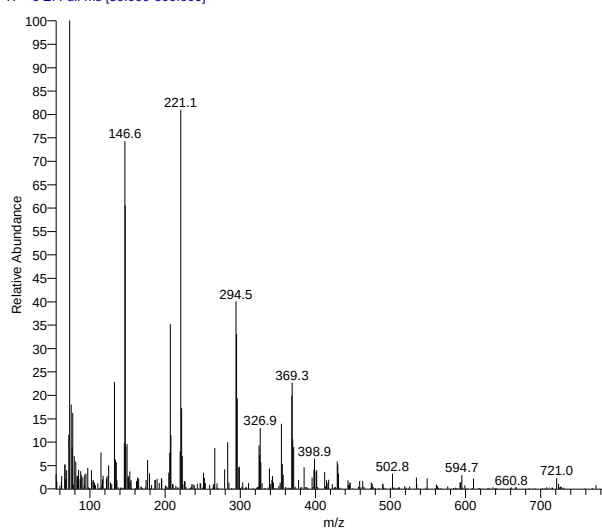


RT: 48.59 - 49.72 SM: 15G



NL: 1.16E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #12871 RT: 49.16 AV: 1 RF: 6.00, 3 NL: 1.30E5
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
49.16	Heptasiloxane, hexadecamethyl-	2902502.77	23.19	482	729	mainlib
49.16	1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isobutyl ester	2902502.77	9.16	460	593	mainlib
49.16	Cyclodecasiloxane, eicosamethyl-	2902502.77	6.47	450	496	mainlib
49.16	Cyclononasiloxane, octadecamethyl-	2902502.77	4.18	437	570	mainlib
49.16	Tetracosamethyl-cyclododecasiloxane	2902502.77	3.53	433	628	mainlib

Analysed by Satyanarayana

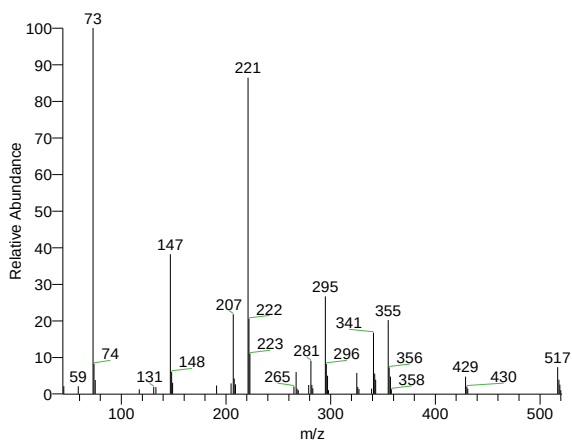
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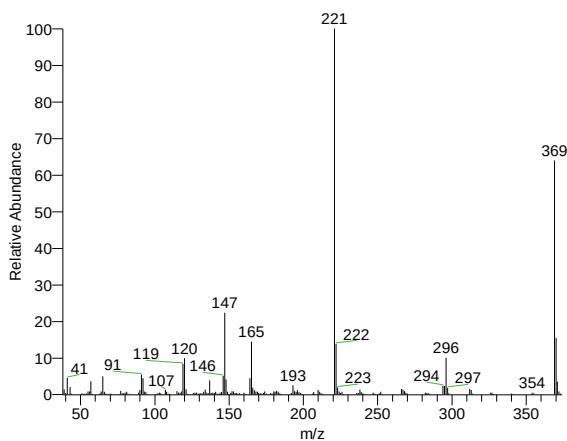
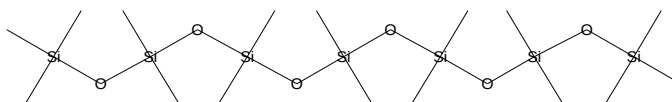
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

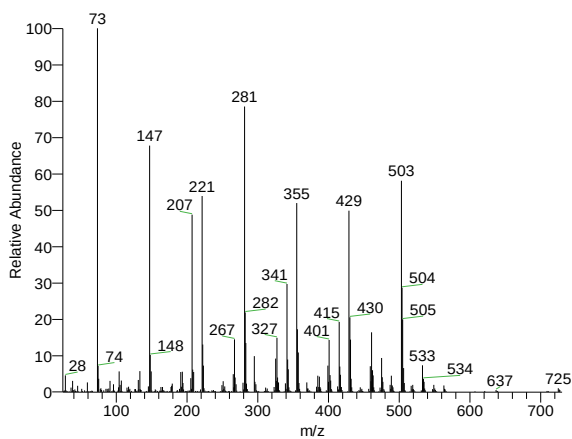
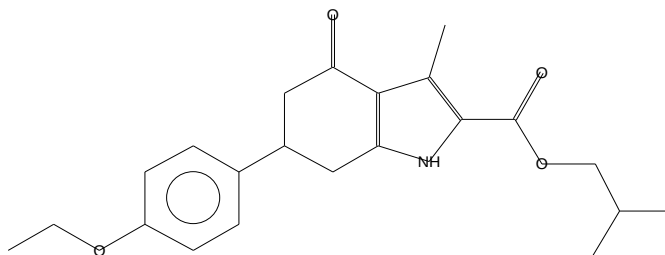
Compound Structure



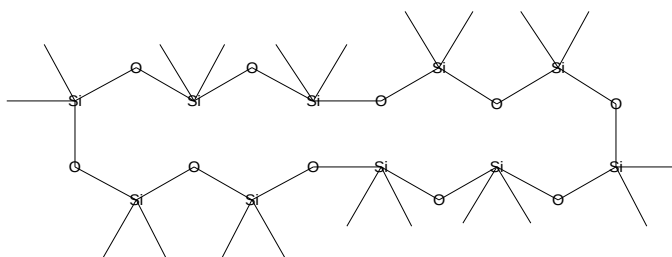
Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



1H-Indole-2-carboxylic acid, 6-(4-ethoxyphenyl)-3-methyl-4-oxo-4,5,6,7-tetrahydro-, isobutyl ester
Formula C₂₂H₂₇NO₄, MW 369, CAS# NA, Entry# 196839
\$.28XORXIIMNPHEBIN-UHFFFAOYSA-N



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



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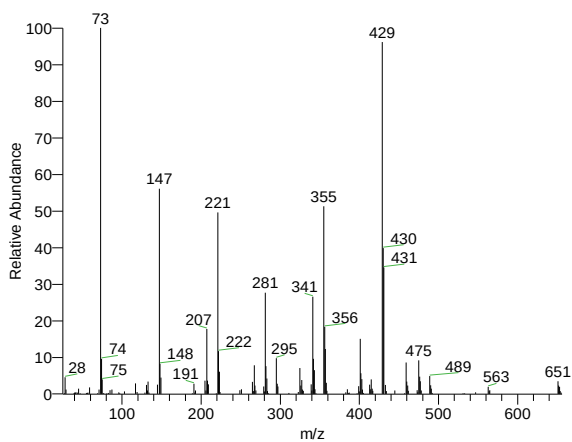
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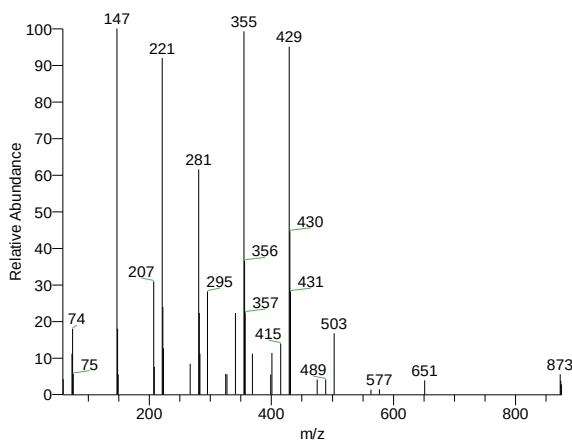
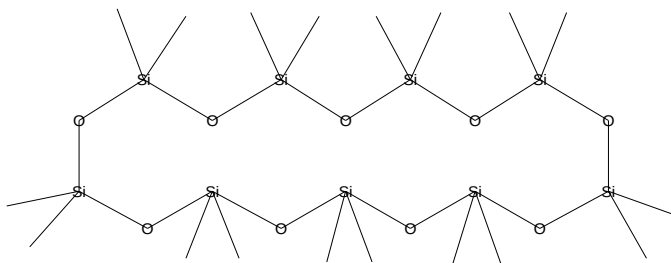
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

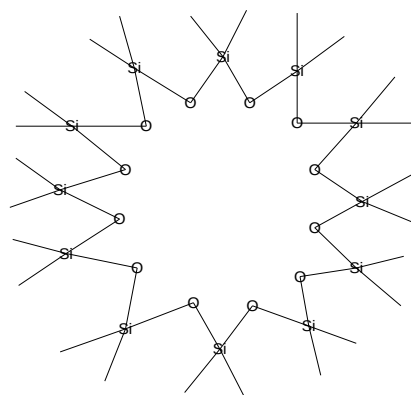
Compound Structure



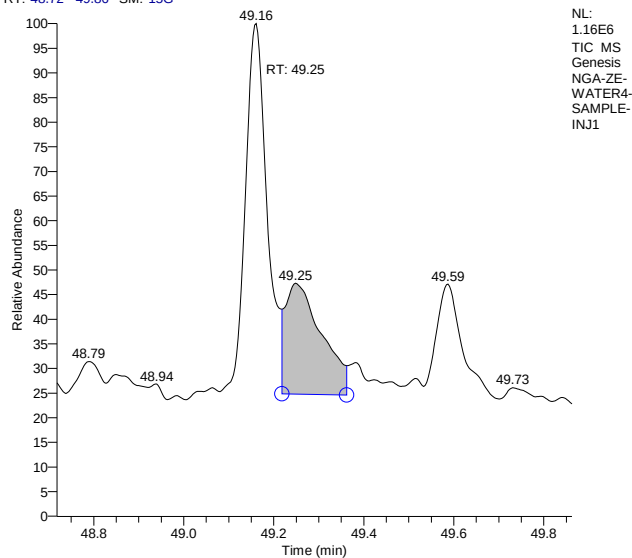
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752

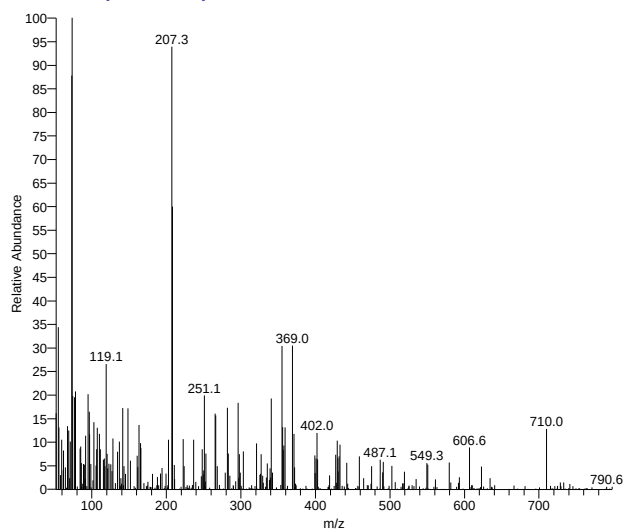


RT: 48.72 - 49.86 SM: 15G



NL:
1.16E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #12897 RT: 49.25 AV: 1 RF: 6.00, 3 NL: 3.79E4
T: + c EI Full ms [50.000-800.000]



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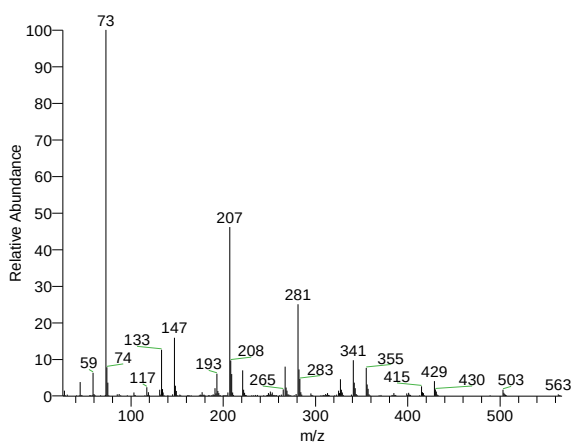
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ANALYTICAL CHEMISTRY DIVISION

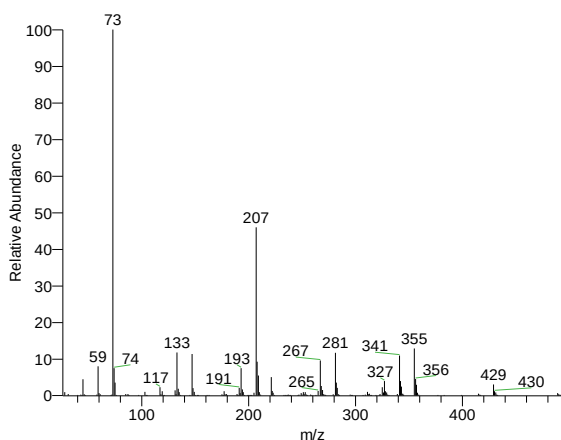
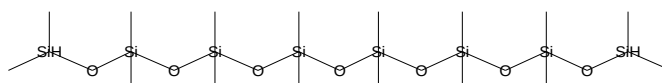
RT	Compound Name	Area	Probability	SI	RSI	Library
49.25	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1474146.32	13.64	407	524	mainlib
49.25	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1474146.32	9.35	396	576	mainlib
49.25	Cyclodecasiloxane, eicosamethyl-	1474146.32	5.85	382	425	mainlib
49.25	2,5-Dihydroxybenzoic acid, 3TMS derivative	1474146.32	3.66	368	457	mainlib
49.25	3,9á:14,15-Diepoxypregn- 16-en-20-one, 3,11á,18-triacetoxy-	1474146.32	2.73	360	425	mainlib

Hit Spectrum

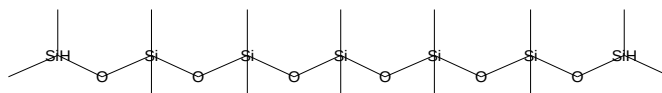
Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Analysed by Satyanarayana

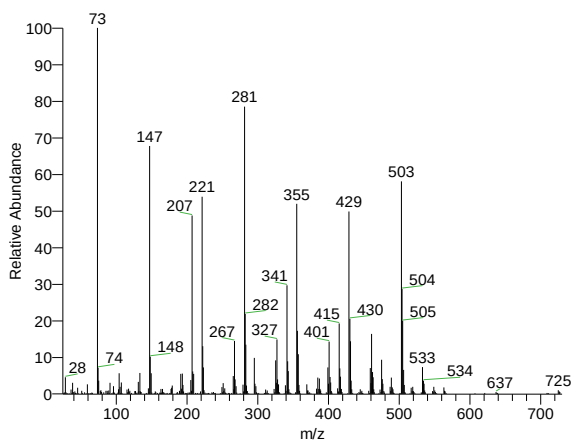
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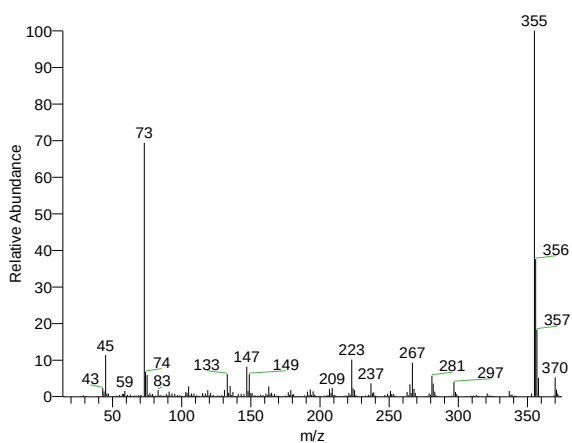
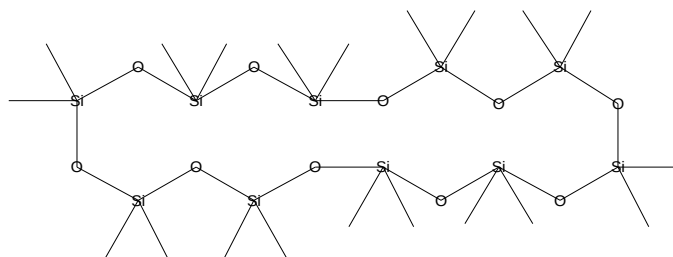
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Hit Spectrum

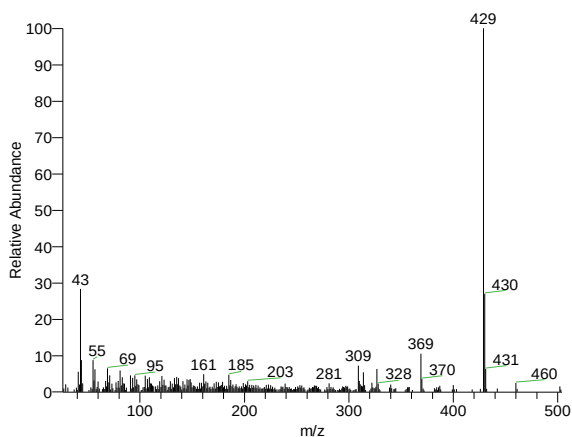
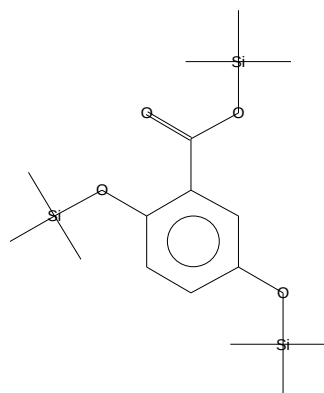
Compound Structure



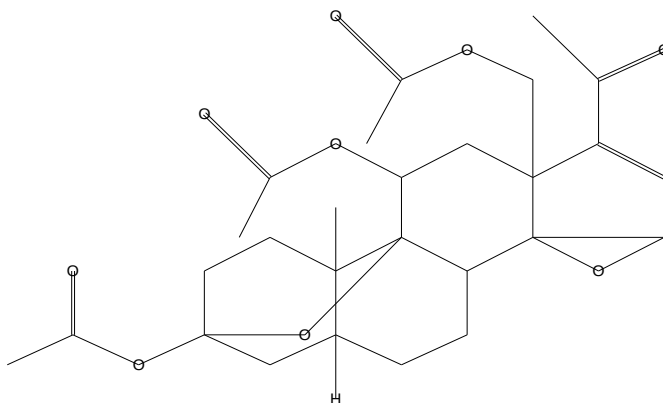
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



2,5-Dihydroxybenzoic acid, 3TMS derivative
Formula C₁₆H₃₀O₄Si₃, MW 370, CAS# 3618-20-0, Entry# 234286
Benzoic acid, 2,5-bis(trimethylsiloxy)-, trimethylsilyl ester



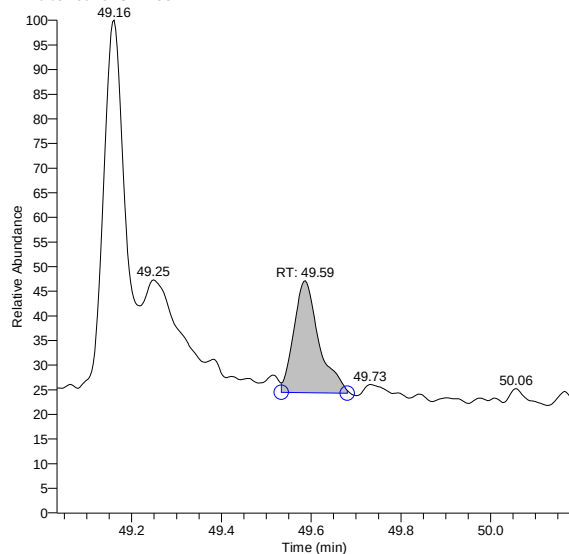
3,9a:14,15-Diepoxypregn-16-en-20-one, 3,11a,18-triacetoxy-
Formula C₂₇H₃₄O₉, MW 502, CAS# NA, Entry# 239582
\$:28GBYXRTQLWMZHST-UHFFFAOYSA-N



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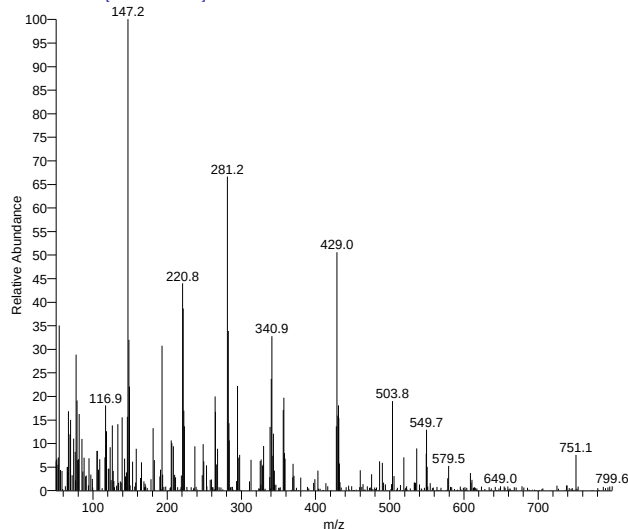
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RT: 49.03 - 50.18 SM: 15G



NL:
1.16E6
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

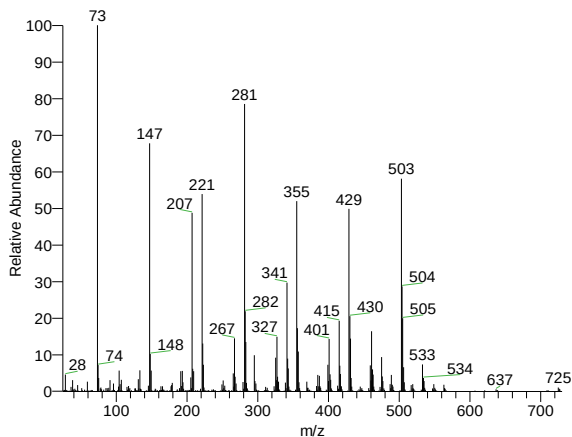
NGA-ZE-WATER4-SAMPLE-INJ1 #12998 RT: 49.59 AV: 1 RF: 6.00, 3 NL: 3.83E4
T: + c EI Full ms [50.000-800.000]



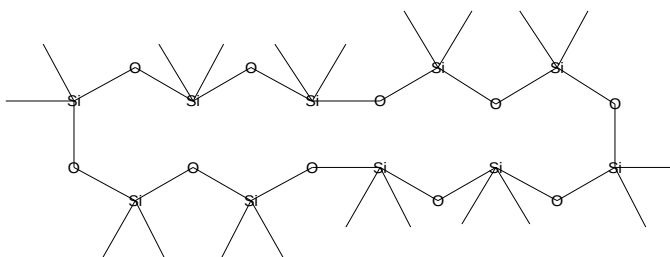
RT	Compound Name	Area	Probability	SI	RSI	Library
49.59	Cyclodecasiloxane, eicosamethyl-	1019817.26	26.22	454	510	mainlib
49.59	Cyclononasiloxane, octadecamethyl-	1019817.26	20.08	447	590	mainlib
49.59	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1019817.26	6.73	423	530	mainlib
49.59	Heptasiloxane, hexadecamethyl-	1019817.26	6.73	423	621	mainlib
49.59	Cyclohexasiloxane, dodecamethyl-	1019817.26	3.26	404	551	mainlib

Hit Spectrum

Compound Structure



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



Analysed by Satyanarayana

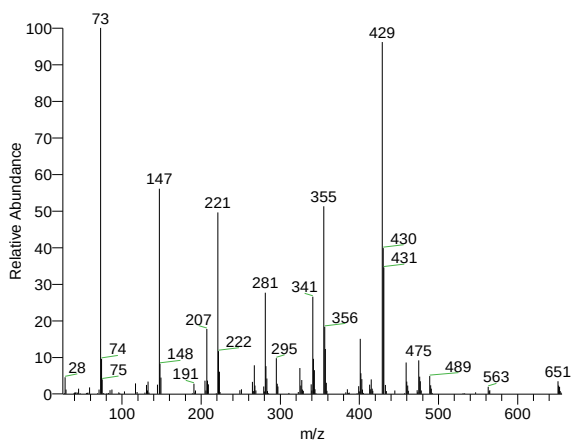
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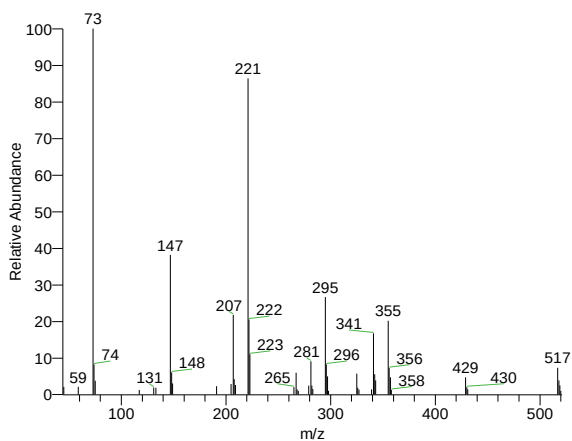
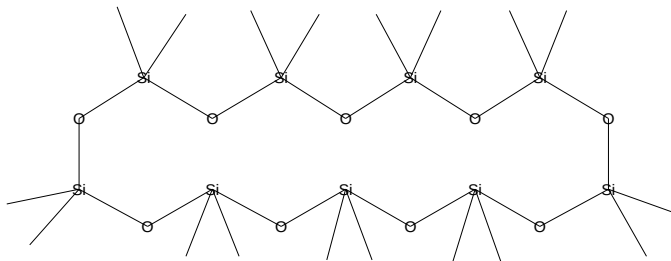
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

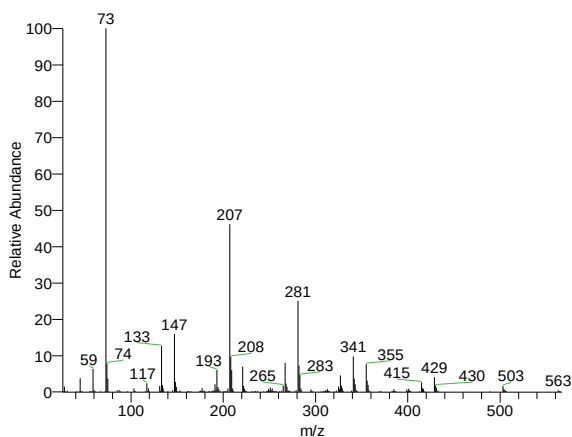
Compound Structure



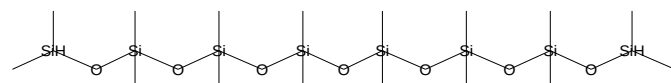
Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #

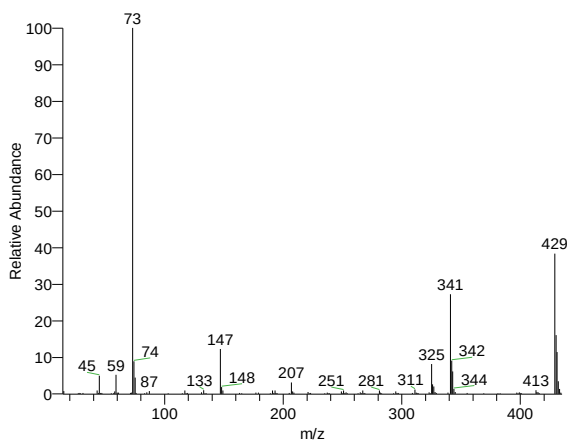


Analysed by Satyanarayana

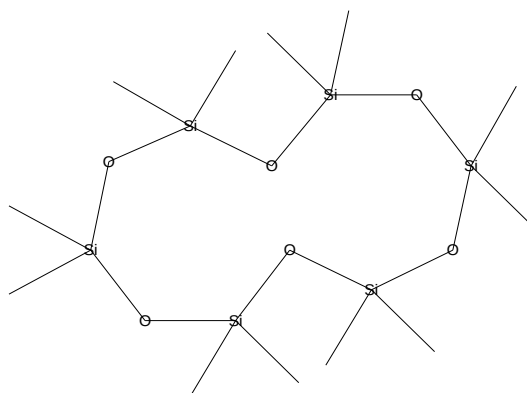
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Hit Spectrum

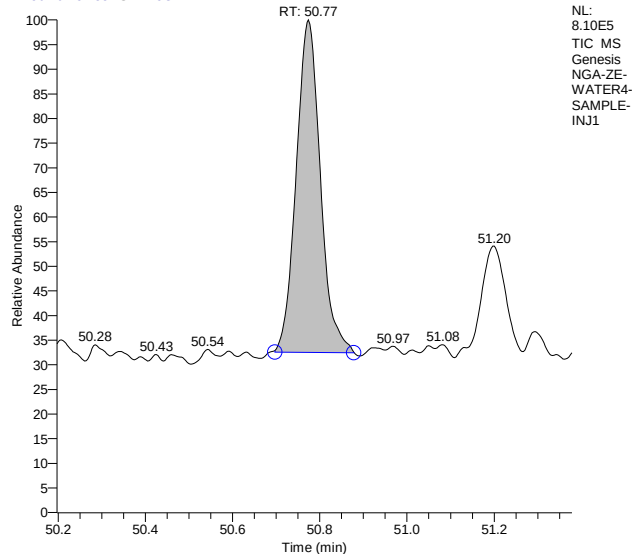
Compound Structure



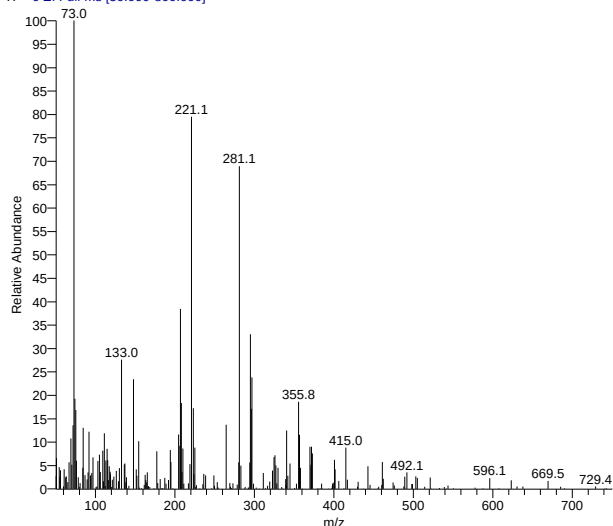
Cyclohexasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₆Si₆, MW 444, CAS# 540-97-6, Entry# 44297
Dodecamethylcyclohexasiloxane



RT: 50.20 - 51.38 SM: 15G



NGA-ZE-WATER4-SAMPLE-INJ1 #13352 RT: 50.77 AV: 1 RF: 6.00, 3 NL: 6.79E4
T: + c EI Full ms [50.000-800.000]



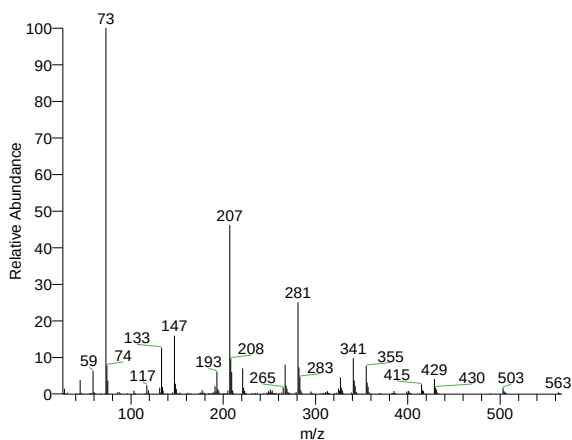
RT	Compound Name	Area	Probability	SI	RSI	Library
50.77	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13,15,15-hexadecamethyl-	2099841.88	25.46	462	546	mainlib
50.77	Cyclodecasiloxane, eicosamethyl-	2099841.88	10.06	440	471	mainlib
50.77	Heptasiloxane, hexadecamethyl-	2099841.88	10.06	440	624	mainlib
50.77	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,1 3,13-tetradecamethyl-	2099841.88	9.67	439	531	mainlib
50.77	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-d odecamethyl-	2099841.88	3.24	415	522	mainlib

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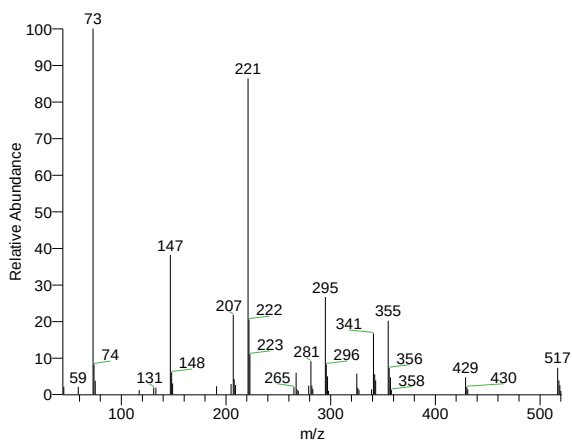
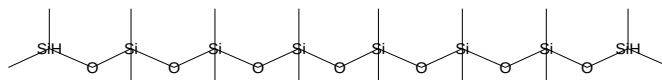
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Hit Spectrum

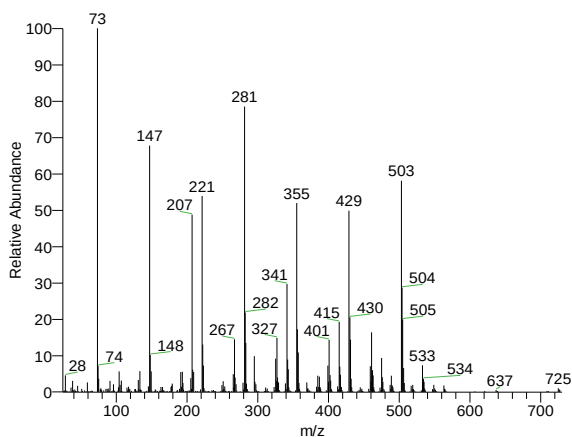
Compound Structure



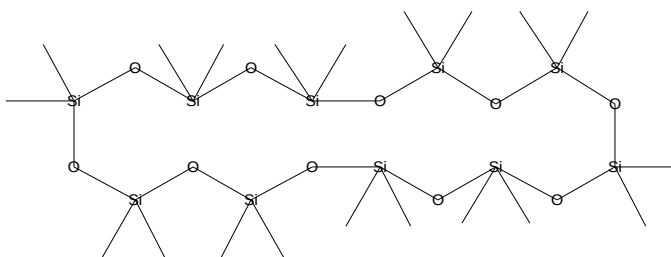
Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Heptasiloxane, hexadecamethyl-
Formula C₁₆H₄₈O₆Si₇, MW 532, CAS# 541-01-5, Entry# 43444
Hexadecamethylheptasiloxane



Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #

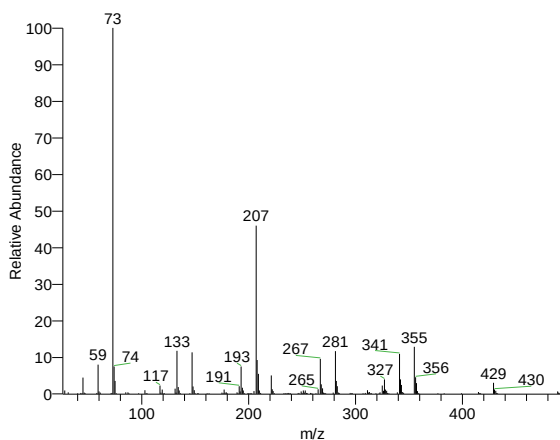


Analysed by Satyanarayana

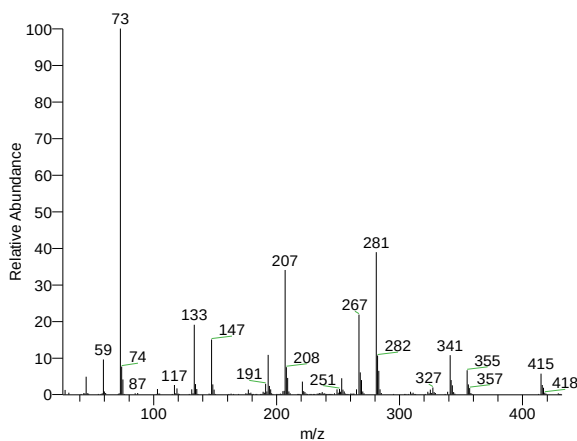
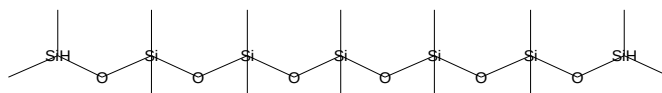
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Hit Spectrum

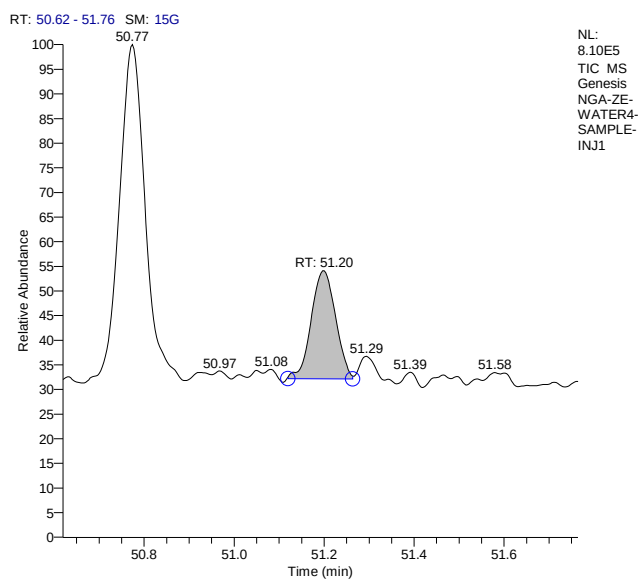
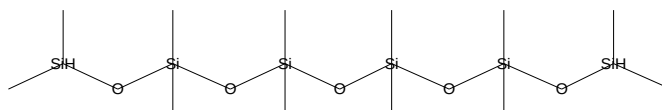
Compound Structure



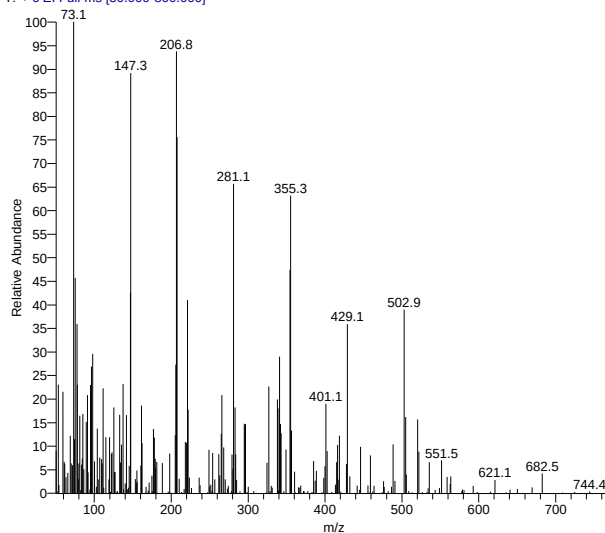
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



NGA-ZE-WATER4-SAMPLE-INJ1 #13479 RT: 51.20 AV: 1 RF: 6.00, 3 NL: 2.64E4
T: + c EI Full ms [50.000-800.000]



RT	Compound Name	Area	Probability	SI	RSI	Library
51.20	Cyclodecasiloxane, eicosamethyl-	667883.05	63.48	498	547	mainlib

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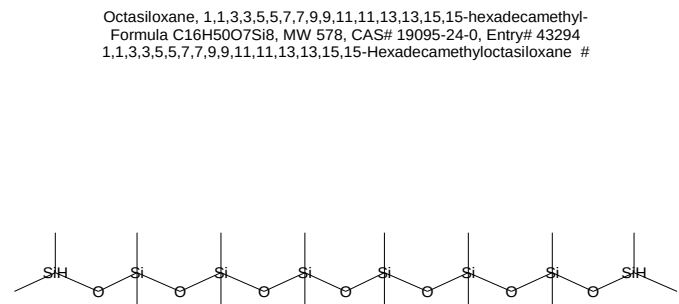
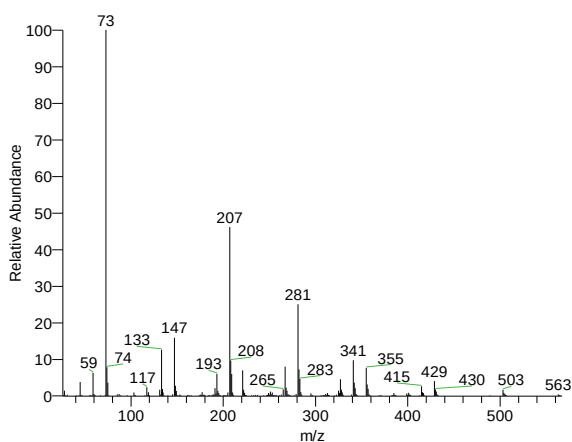
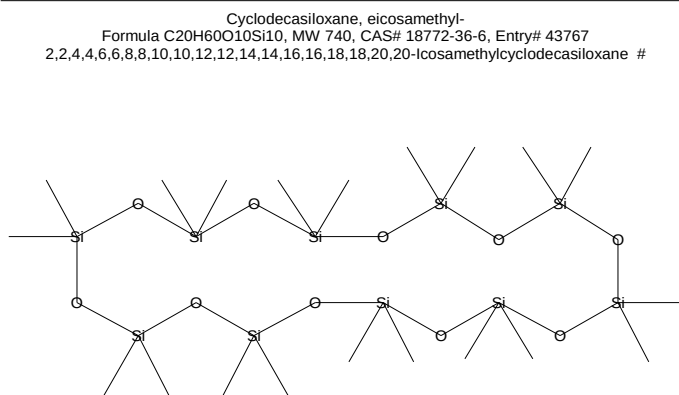
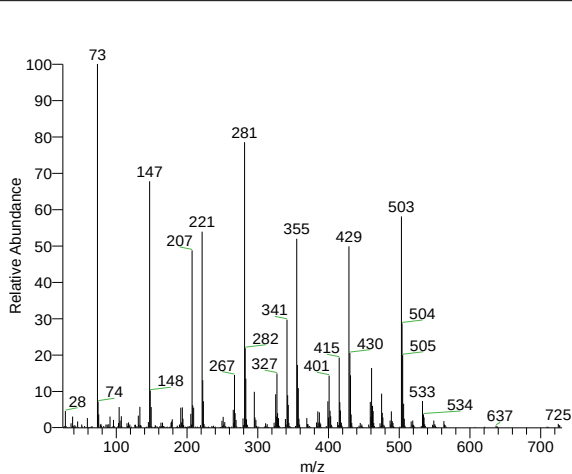
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RT	Compound Name	Area	Probability	SI	RSI	Library
51.20	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	667883.05	15.93	463	588	mainlib
51.20	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	667883.05	3.45	419	589	mainlib
51.20	Cyclononasiloxane, octadecamethyl-	667883.05	1.78	401	538	mainlib
51.20	Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-	667883.05	1.18	389	536	mainlib

Hit Spectrum

Compound Structure



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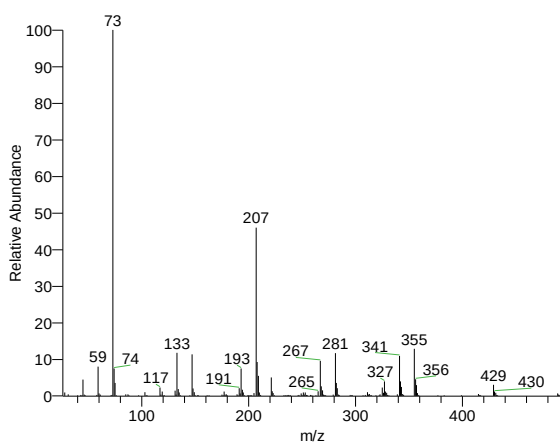
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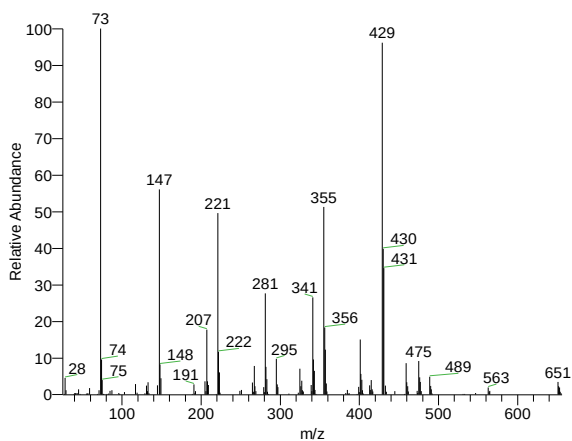
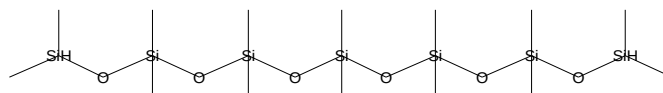
ANALYTICAL CHEMISTRY DIVISION

Hit Spectrum

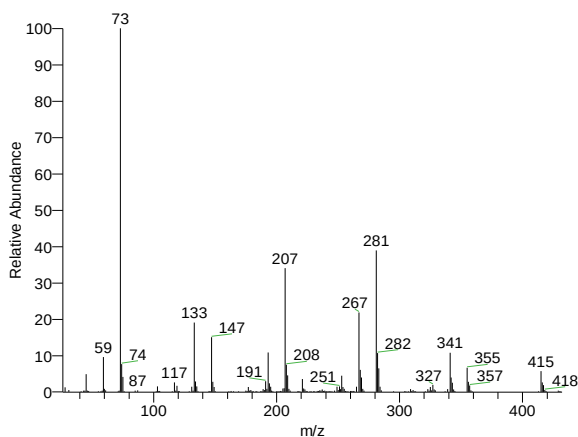
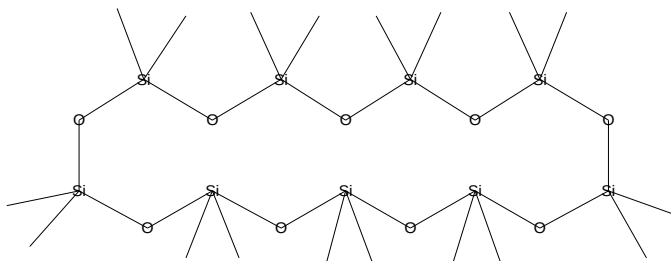
Compound Structure



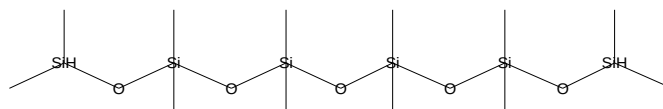
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Cyclononasiloxane, octadecamethyl-
Formula C₁₈H₅₄O₉Si₉, MW 666, CAS# 556-71-8, Entry# 44296
Octadecamethyl-cyclononasiloxane



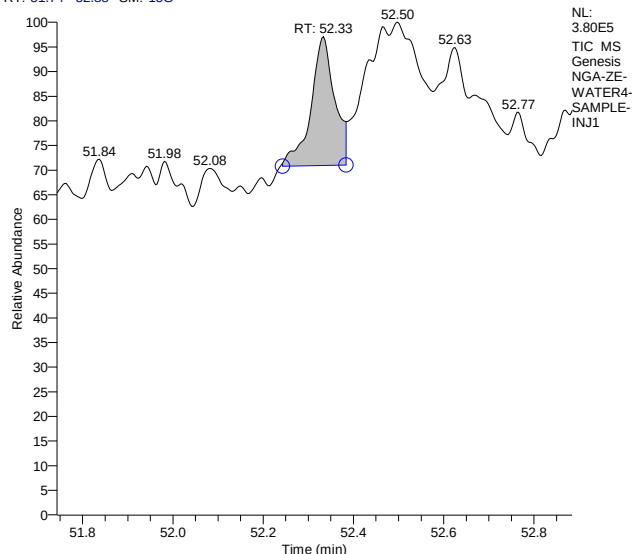
Hexasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11-dodecamethyl-
Formula C₁₂H₃₈O₅Si₆, MW 430, CAS# 995-82-4, Entry# 43771
1,1,3,3,5,5,7,7,9,9,11,11-Dodecamethylhexasiloxane #



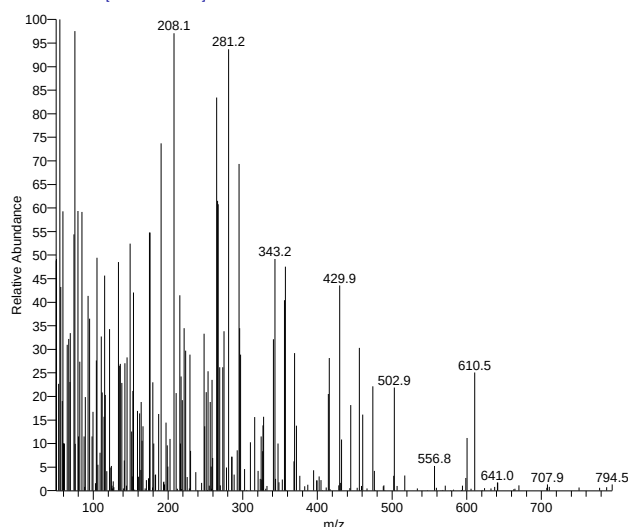
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RT: 51.74 - 52.88 SM: 15G



NGA-ZE-WATER4-SAMPLE-INJ1 #13817 RT: 52.33 AV: 1 RF: 6.00, 3 NL: 9.71E3
T: + c EI Full ms [50.000-800.000]



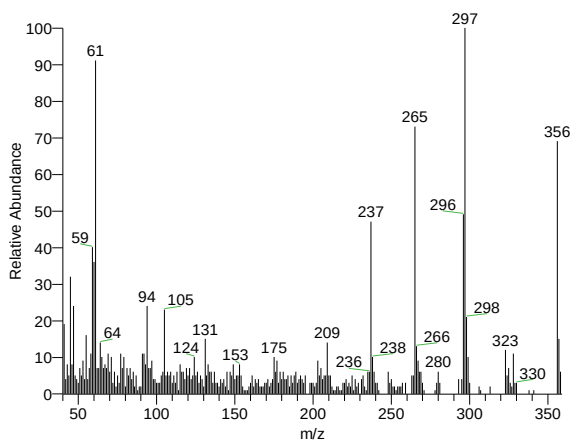
RT	Compound Name	Area	Probability	SI	RSI	Library
52.33	Spiro[adamantane-2,2'-[1,3]dithiolane]-1,5-dicarboxylic acid, 6-oxo-	362988.58	9.61	349	440	mainlib
52.33	Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandro-8-en-17-yl)-	362988.58	7.74	344	371	mainlib
52.33	1H-Cyclopropa[3,4]benz[1,2-e]azulene-5,7b,9,9a-tetrol, 3-[(acetyloxy)methyl]-1a,1b,4,4a,5,7a,8,9-octahydro-1,1,6,8-tetramethyl-, 9,9a-diacetate, [1aR-(1aà,1bà,4aà,5á,7aà,7bà,8à,9á,9aà)]-	362988.58	6.24	339	358	mainlib
52.33	Methyl glycocholate, 3TMS derivative	362988.58	4.53	330	364	mainlib
52.33	Acetic acid, 17-acetoxy-4,4,10,13-tetramethyl-7-oxo-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[a]phenanthren-3-yl (ester)	362988.58	4.00	327	373	mainlib

Analysed by Satyanarayana

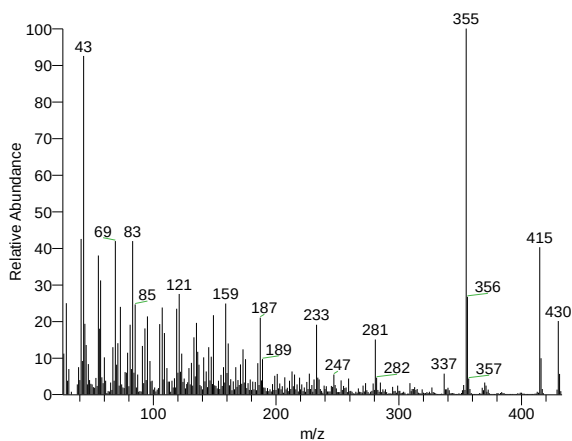
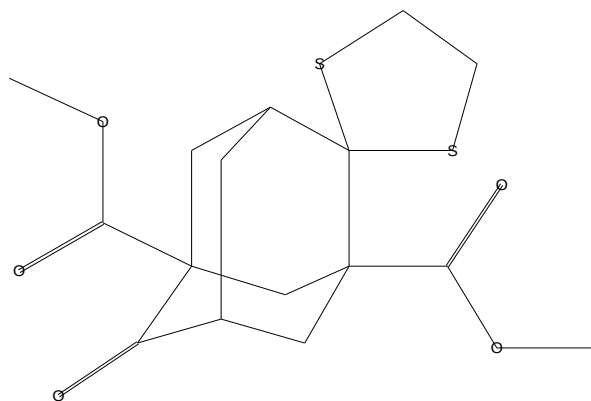
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Hit Spectrum

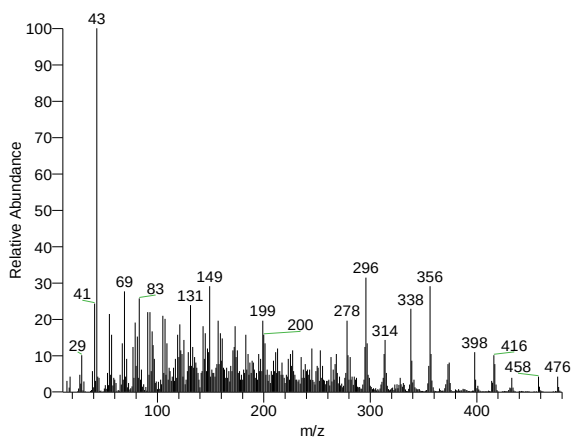
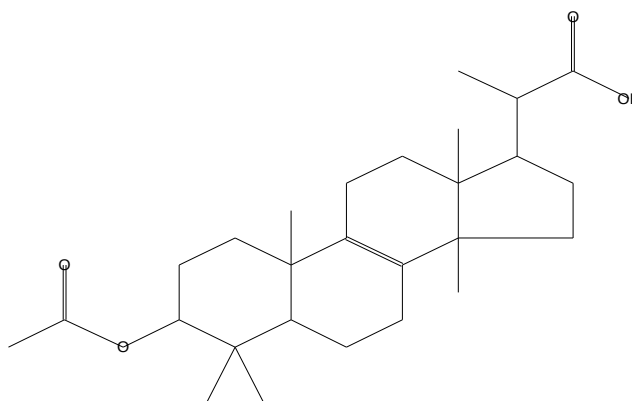
Compound Structure



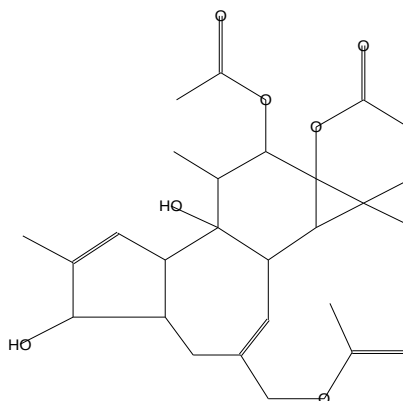
Spiro[adamantane-2,2'-[1,3]dithiolane]-1,5-dicarboxylic acid, 6-oxo-
Formula C₁₆H₂₀O₅S₂, MW 356, CAS# 19930-84-8, Entry# 224096
\$:28GJWLQHCSAVLWOT-UHFFFAOYSA-N



Propanoic acid, 2-(3-acetoxy-4,4,14-trimethylandrosta-8-en-17-yl)-
Formula C₂₇H₄₂O₄, MW 430, CAS# NA, Entry# 234266



Formula C₂₆H₃₆O₈, MW 476, CAS# 77550-15-3, Entry# 14490

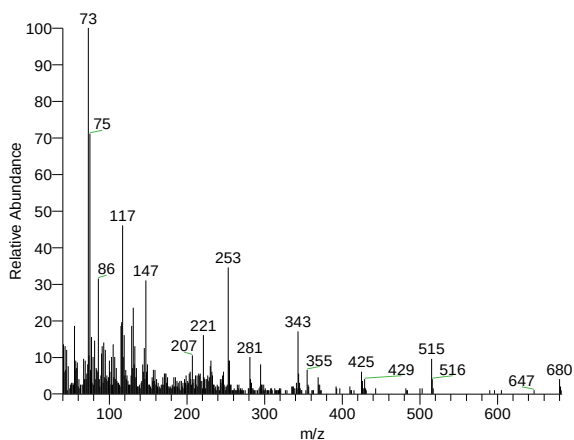


Analysed by Satyanarayana

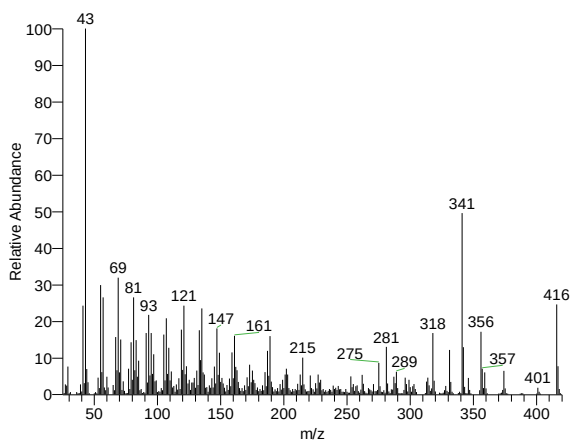
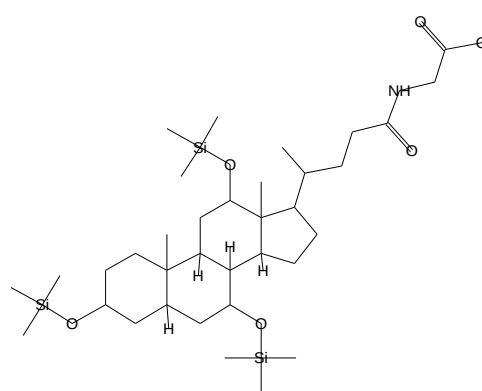
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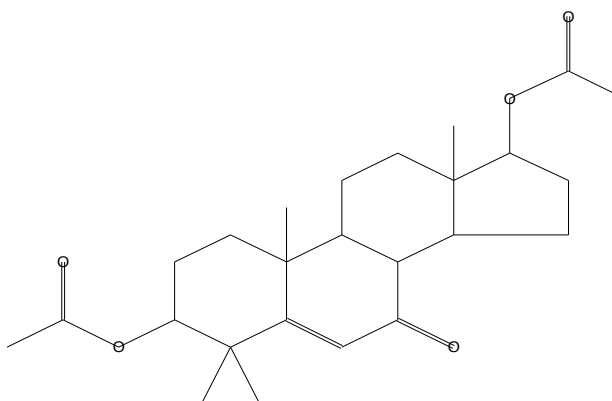
Compound Structure



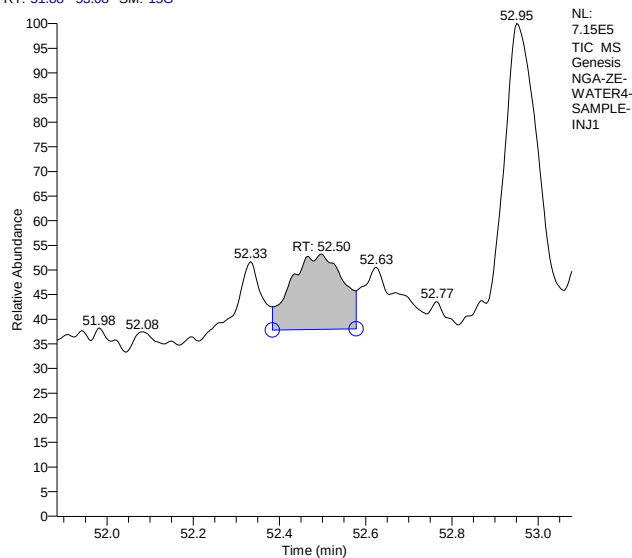
Methyl glycocholate, 3TMS derivative
Formula C₃₆H₆₉NO₆Si₃, MW 695, CAS# 57326-16-6, Entry# 41378
Glycine, N-[(3à,5à,7à,12à)-24-oxo-3,7,12-tris[(trimethylsilyl)oxy]cholan-24-yl]-, methyl ester



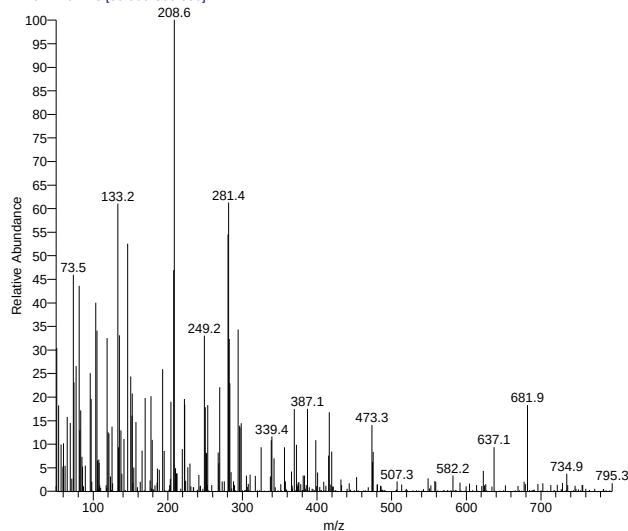
Formula C₂₅H₃₆O₅, MW 416, CAS# NA, Entry# 14772
17-(Acetyloxy)-4,4-dimethyl-7-oxoandrost-5-en-3-yl acetate #



RT: 51.88 - 53.08 SM: 15G



NGA-ZE-WATER4-SAMPLE-INJ1 #13866 RT: 52.50 AV: 1 RF: 6.00, 3 NL: 1.77E4
T: + c EI Full ms [50.000-800.000]



Analysed by Satyanarayana

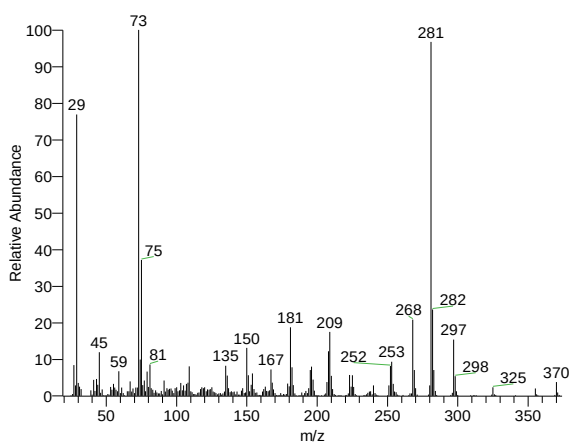
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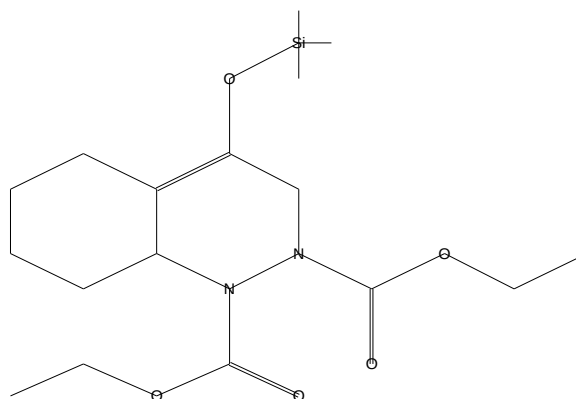
RT	Compound Name	Area	Probability	SI	RSI	Library
52.50	1,2-Cinnolinedicarboxylic acid, 1,2,3,5,6,7,8,8a-octahydro-4-trimethylsilyloxy-, diethyl ester	913068.46	8.73	365	495	mainlib
52.50	2,4-Dihydroxyacetophenone, 2TMS derivative	913068.46	6.51	357	494	mainlib
52.50	3-Hydroxy-4-methoxyphenylpropionic acid, ethyl ester, TMS	913068.46	5.25	352	494	mainlib
52.50	Cyclotetrasiloxane, octamethyl-	913068.46	5.05	351	599	mainlib
52.50	2,5-Dihydroxyacetophenone, 2TMS derivative	913068.46	4.46	348	473	mainlib

Hit Spectrum

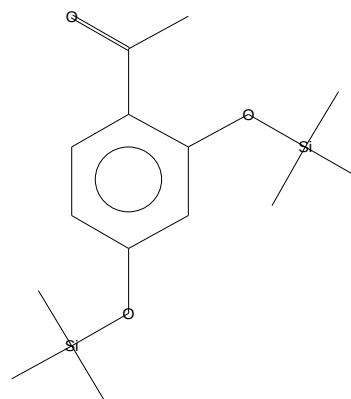
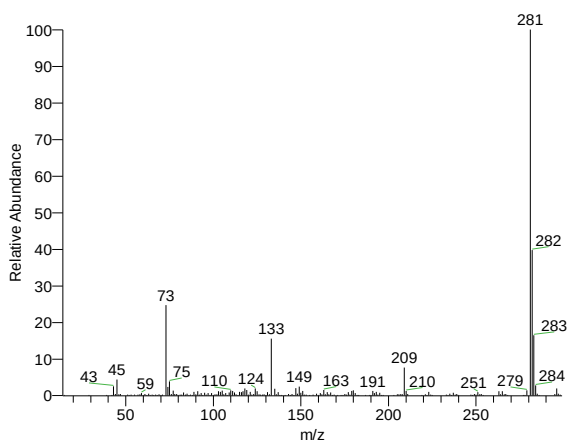


Compound Structure

1,2-Cinnolinedicarboxylic acid, 1,2,3,5,6,7,8,8a-octahydro-4-trimethylsilyloxy-, diethyl ester
Formula C₁₇H₃₀N₂O₅Si, MW 370, CAS# 215712-69-9, Entry# 43762
Diethyl 4-[(trimethylsilyl)oxy]-3,5,6,7,8,8a-hexahydro-1,2-cinnolinedicarboxylate #



2,4-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220074
2',4'-Dihydroxyacetophenone, bis(trimethylsilyl) ether

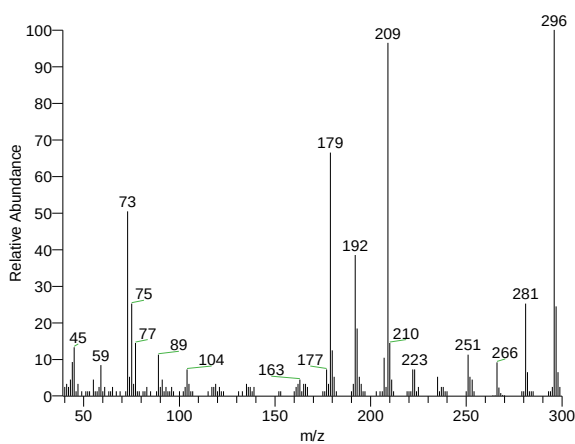


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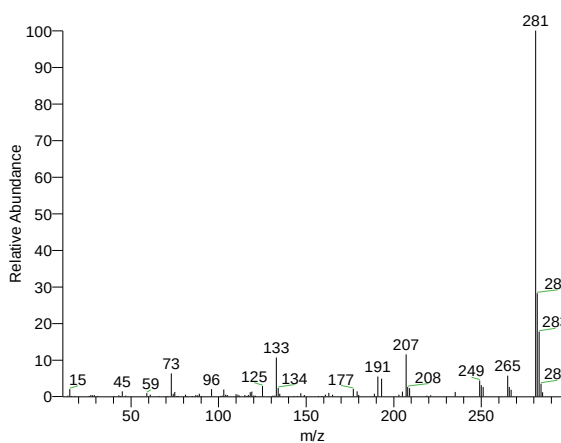
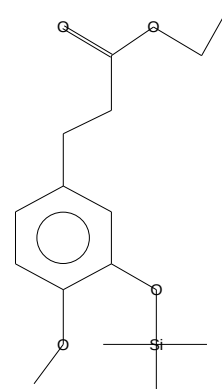
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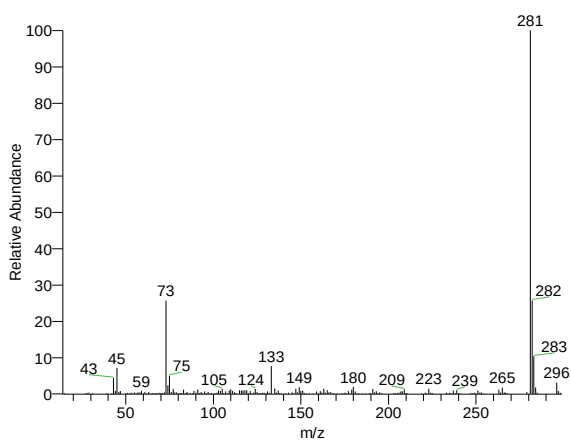
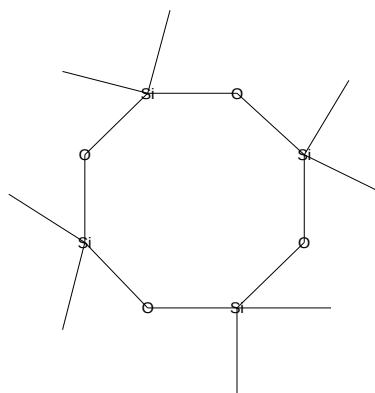
Compound Structure



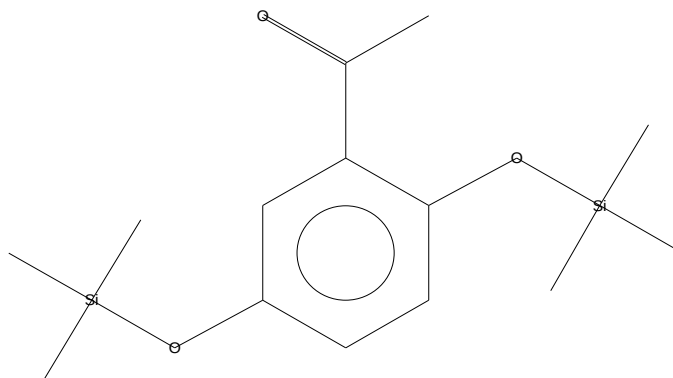
3-Hydroxy-4-methoxyphenylpropionic acid, ethyl ester, TMS
Formula C₁₅H₂₄O₄Si, MW 296, CAS# NA, Entry# 223905
Ethyl 3-(4-methoxy-3-[(trimethylsilyl)oxy]phenyl)propanoate #



Cyclotetrasiloxane, octamethyl-
Formula C₈H₂₄O₄Si₄, MW 296, CAS# 556-67-2, Entry# 220100
Oktamethylcyclotetrasiloxan



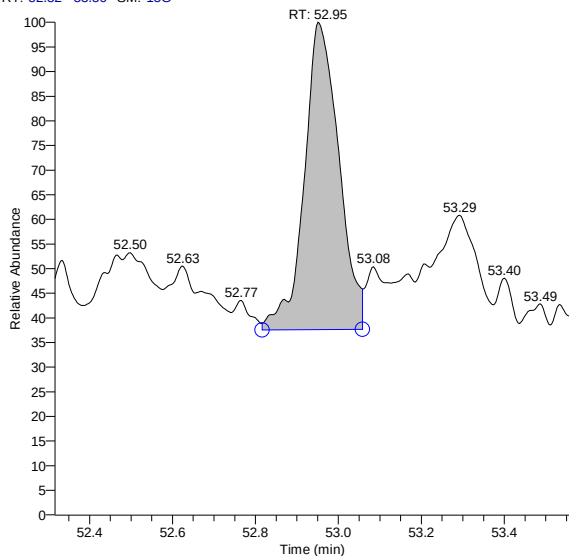
2,5-Dihydroxyacetophenone, 2TMS derivative
Formula C₁₄H₂₄O₃Si₂, MW 296, CAS# NA, Entry# 220075
2,5-Dihydroxyacetophenone, bis(trimethylsilyl) ether



Analysed by Satyanarayana

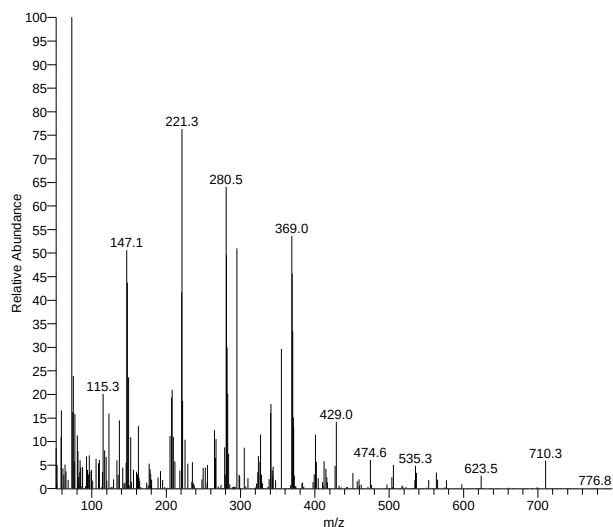
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RT: 52.32 - 53.56 SM: 15G



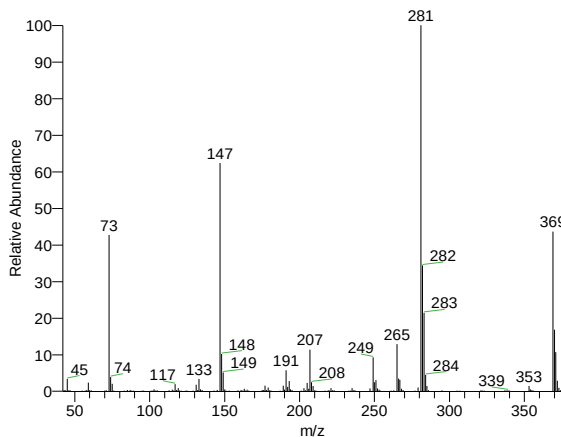
NL:
7.15E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #14001 RT: 52.95 AV: 1 RF: 6.00, 3 NL: 5.43E4
T: + c EI Full ms [50.000-800.000]



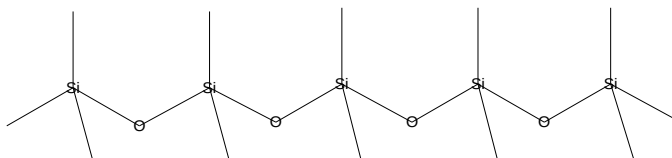
RT	Compound Name	Area	Probability	SI	RSI	Library
52.95	Pentasiloxane, dodecamethyl-	2580592.09	15.68	476	601	mainlib
52.95	1,1,1,3,5,5,7,7,7-Nonamethyl-3-(trimethylsiloxy)tetrasiloxane	2580592.09	10.13	463	800	mainlib
52.95	Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis[(trimethylsilyl)oxy]-	2580592.09	6.95	452	583	mainlib
52.95	3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsiloxy)tetrasiloxane	2580592.09	6.95	452	727	mainlib
52.95	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	2580592.09	4.63	440	545	mainlib

Hit Spectrum



Compound Structure

Pentasiloxane, dodecamethyl-
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 141-63-9, Entry# 219964
Dodecamethylpentasiloxane



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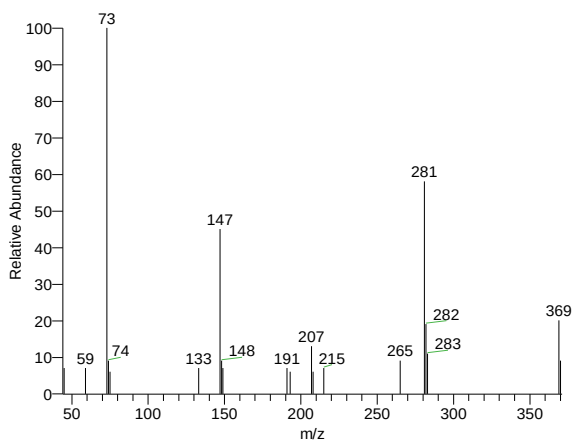
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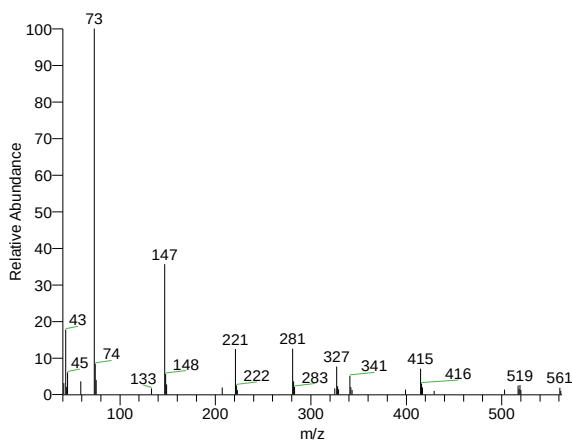
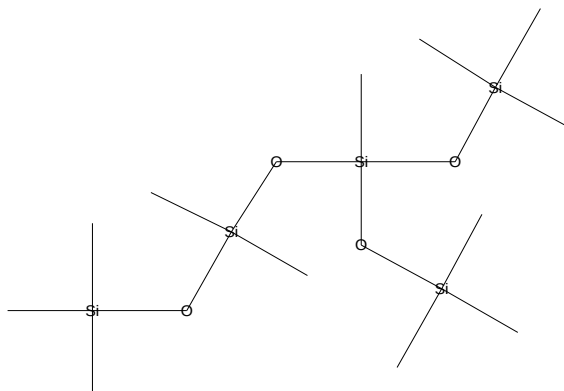
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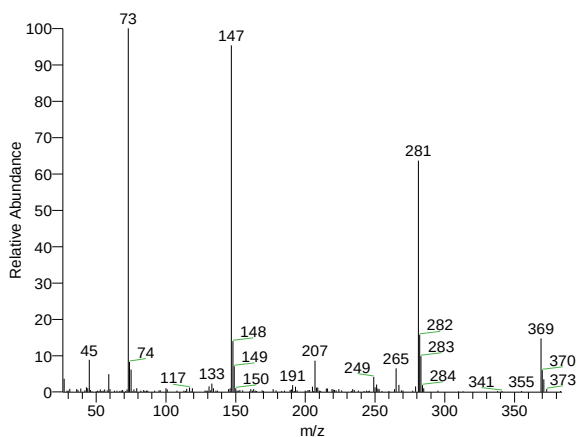
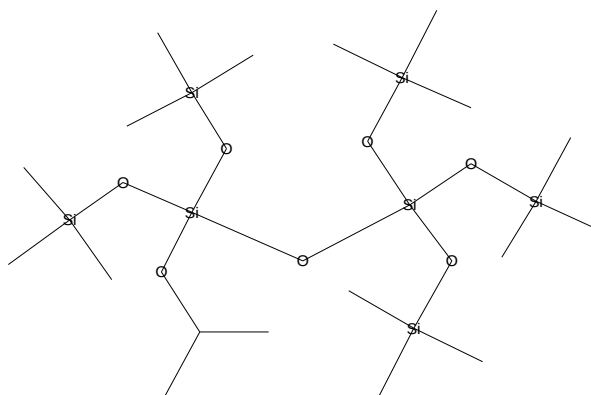
Compound Structure



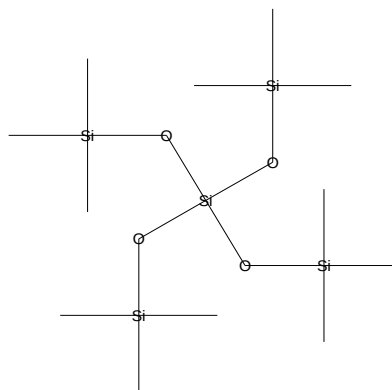
1,1,1,3,5,5,7,7-Nonamethyl-3-((trimethylsilyloxy)tetrasiloxane)
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 38146-99-5, Entry# 43768
1,1,1,3,3,5,7,7,7-Nonamethyl-5-((trimethylsilyloxy)oxy)tetrasiloxane #



3-Isopropoxy-1,1,1,7,7,7-hexamethyl-3,5,5-tris(trimethylsilyloxy)tetrasiloxane
Formula C₁₈H₅₂O₇Si₇, MW 576, CAS# 71579-69-6, Entry# 42479
1-Isopropoxy-3,3,3-trimethyl-1-((trimethylsilyloxy)disiloxanyl tris(trimethylsilyloxy) orthosilicate #



Trisiloxane, 1,1,1,5,5,5-hexamethyl-3,3-bis(trimethylsilyloxy)silane
Formula C₁₂H₃₆O₄Si₅, MW 384, CAS# 3555-47-3, Entry# 42730
Tetrakis(trimethylsilyloxy)silane

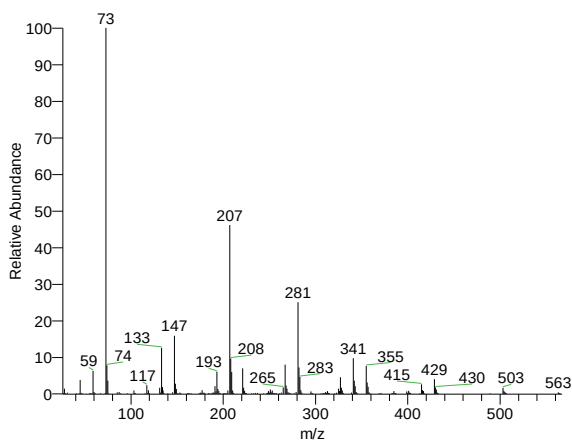


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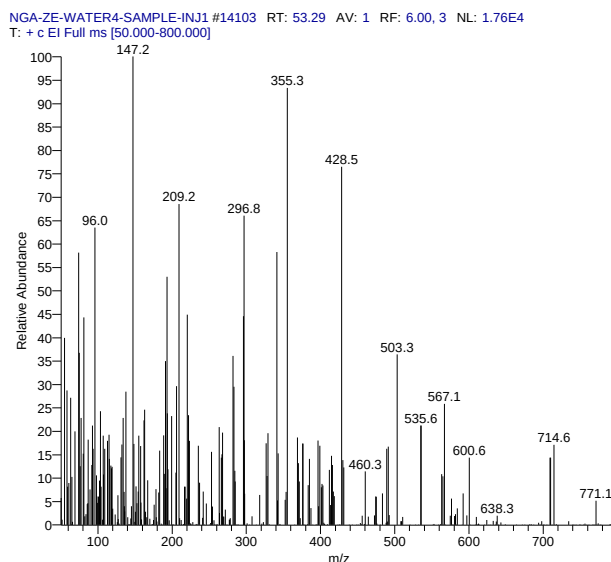
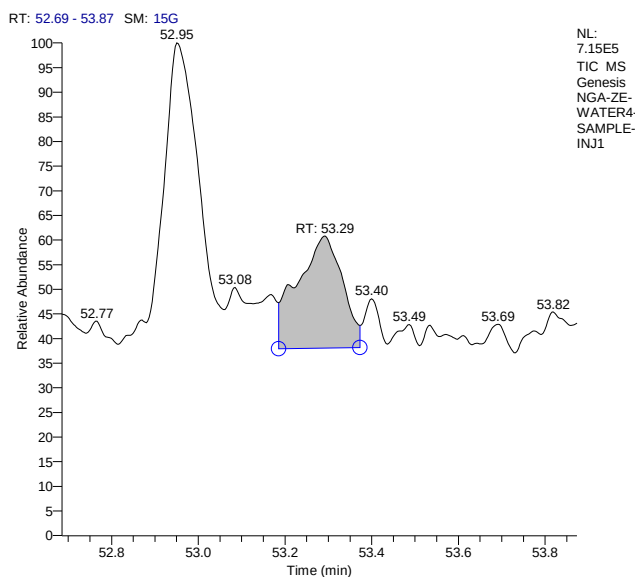
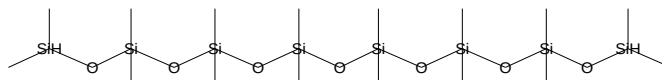
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Compound Structure



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



RT	Compound Name	Area	Probability	SI	RSI	Library
53.29	Cyclodecasiloxane, eicosamethyl-	1178436.49	32.98	404	455	mainlib
53.29	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	1178436.49	13.03	382	473	mainlib
53.29	Cyclononasiloxane, octadecamethyl-	1178436.49	10.24	376	500	mainlib
53.29	Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-	1178436.49	2.53	340	446	mainlib
53.29	Tetracosamethyl-cyclododecasiloxane	1178436.49	2.43	339	676	mainlib

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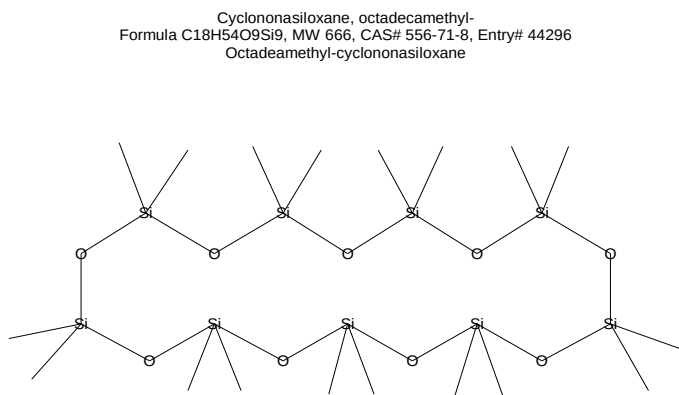
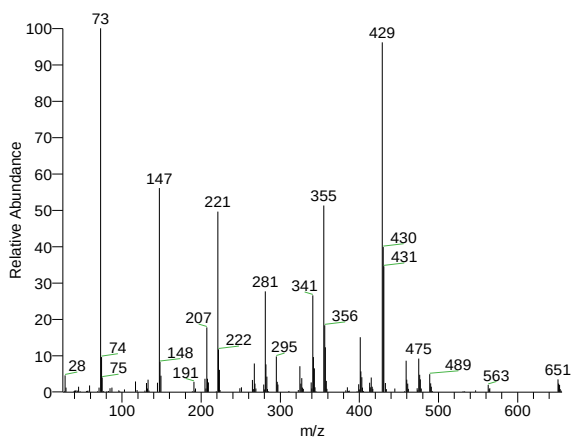
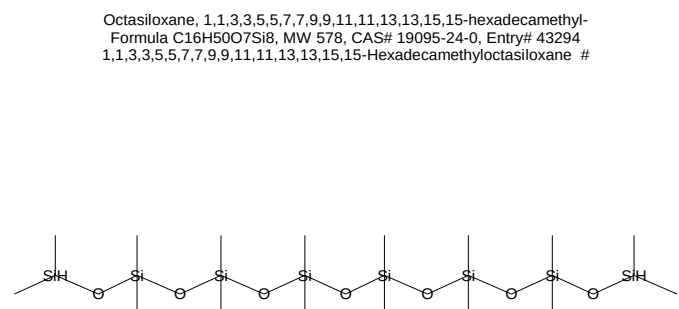
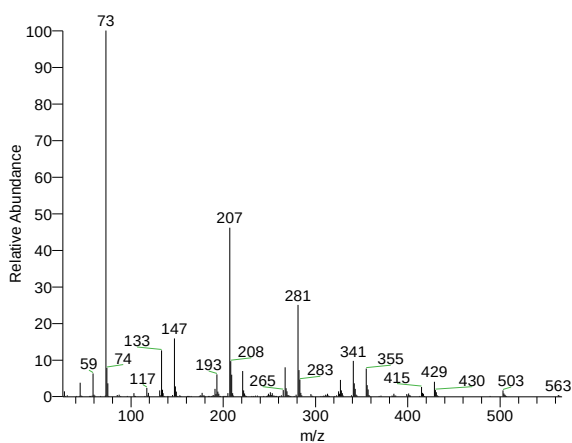
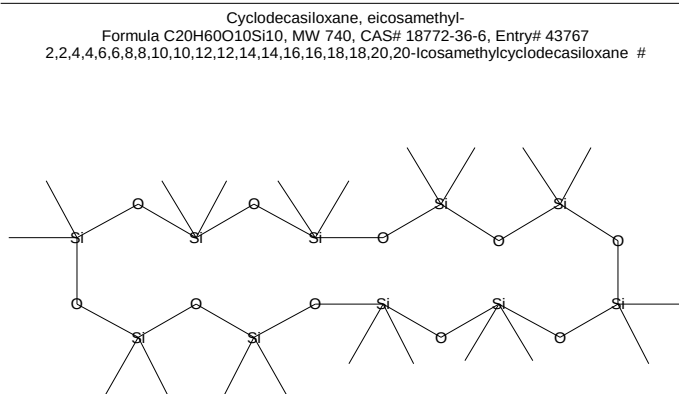
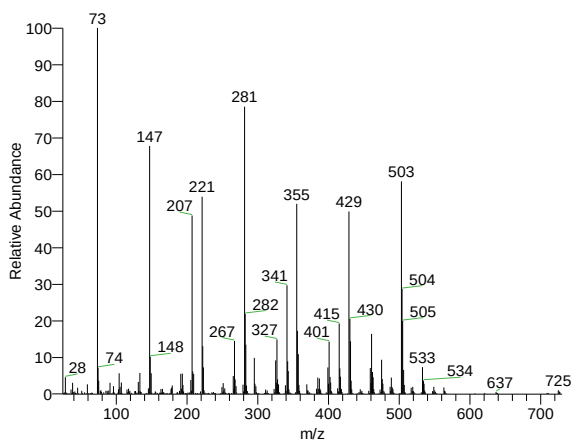
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Compound Structure

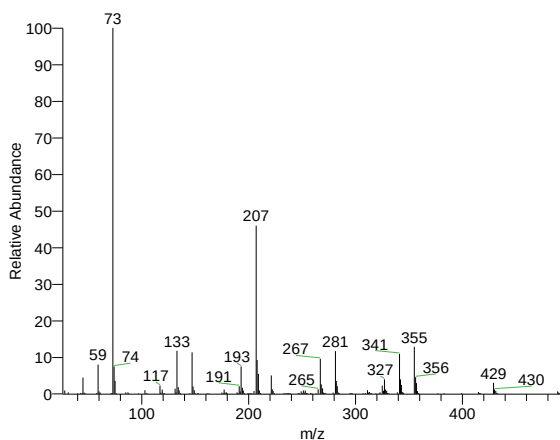


Analysed by Satyanarayana

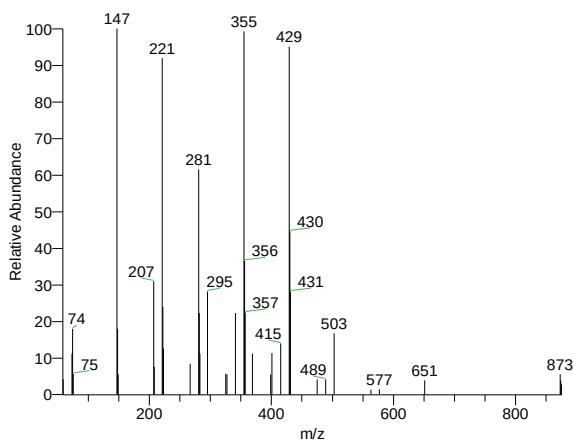
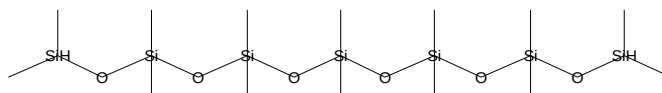
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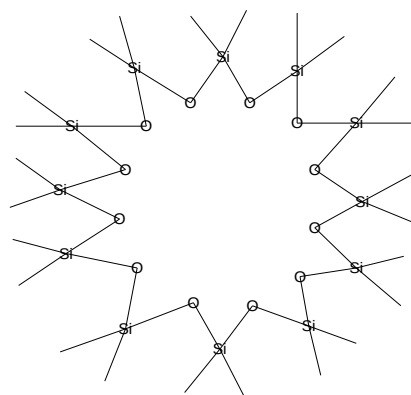
Compound Structure



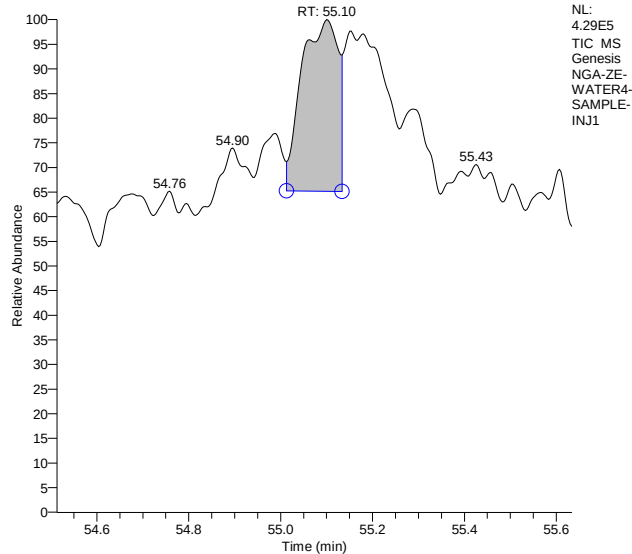
Heptasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13-tetradecamethyl-
Formula C₁₄H₄₄O₆Si₇, MW 504, CAS# 19095-23-9, Entry# 43295
1,1,3,3,5,5,7,7,9,9,11,11,13,13-Tetradecamethylheptasiloxane #



Tetracosamethyl-cyclododecasiloxane
Formula C₂₄H₇₂O₁₂Si₁₂, MW 888, CAS# 18919-94-3, Entry# 135752

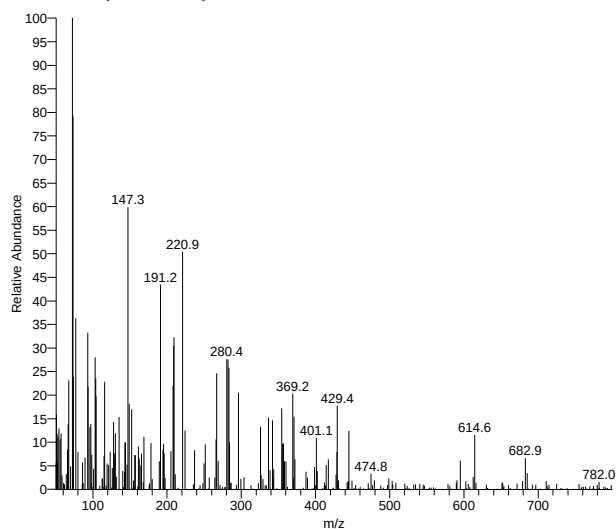


RT: 54.51 - 55.63 SM: 15G



NL:
4.29E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #14642 RT: 55.10 AV: 1 RF: 6.00, 3 NL: 2.85E4
T: + c EI Full ms [50.000-800.000]



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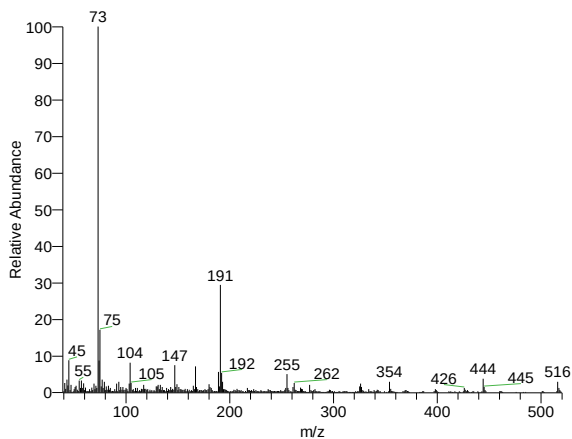
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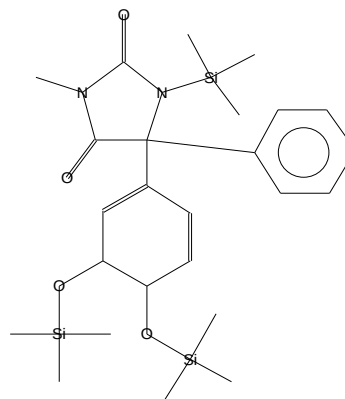
RT	Compound Name	Area	Probability	SI	RSI	Library
55.10	2,4-Imidazolidinedione, 5-[3,4-bis(trimethylsilyloxy)phenyl]-3-methyl-5-phenyl-1-(trimethylsilyl)-	822936.34	11.28	366	406	mainlib
55.10	Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-	822936.34	8.86	360	474	mainlib
55.10	Cyclodecasiloxane, eicosamethyl-	822936.34	3.50	338	390	mainlib
55.10	(22S)-21-Acetoxy-6 α ,11 α -dihydroxy-16 α ,17 α -propylmethylenedioxypregna-1,4-diene-3,20-dione	822936.34	2.96	334	361	mainlib
55.10	(+)-Prostaglandin F 2α , 4TMS derivative	822936.34	2.84	333	372	mainlib

Hit Spectrum

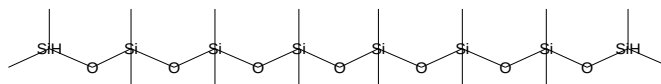
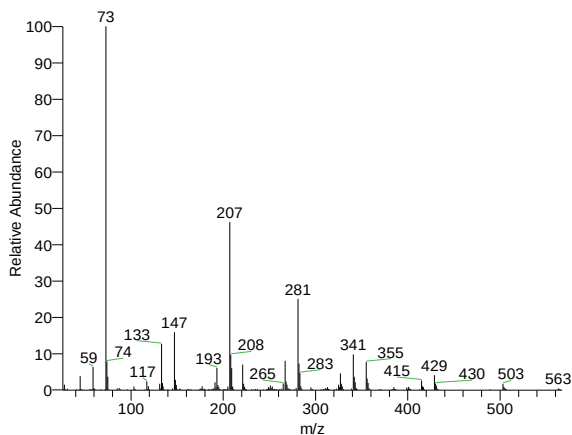
Compound Structure



2,4-Imidazolidinedione, 5-[3,4-bis(trimethylsilyloxy)phenyl]-3-methyl-5-phenyl-1-(trimethylsilyl)-
Formula C₂₅H₄₀N₂O₄Si₃, MW 516, CAS# 55517-85-6, Entry# 43118



Octasiloxane, 1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-hexadecamethyl-
Formula C₁₆H₅₀O₇Si₈, MW 578, CAS# 19095-24-0, Entry# 43294
1,1,3,3,5,5,7,7,9,9,11,11,13,13,15,15-Hexadecamethyloctasiloxane #



Analysed by Satyanarayana

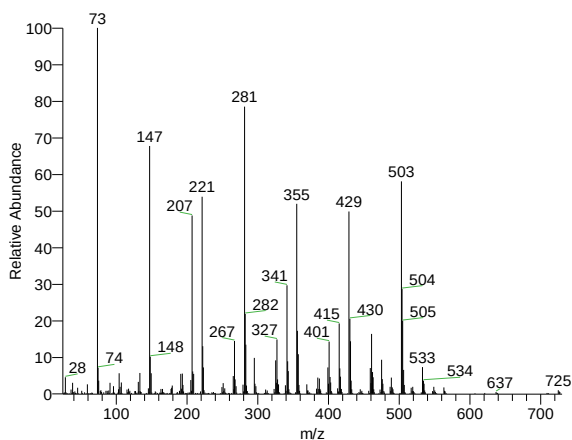
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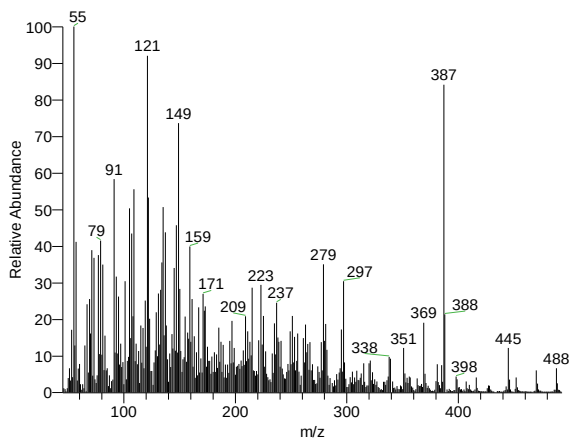
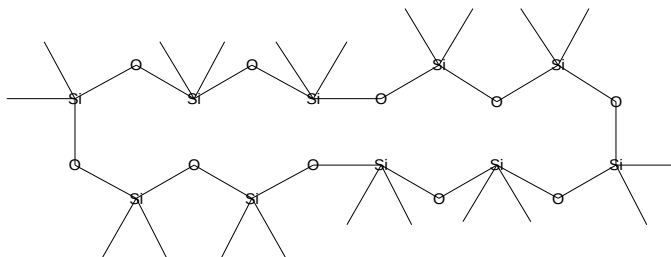
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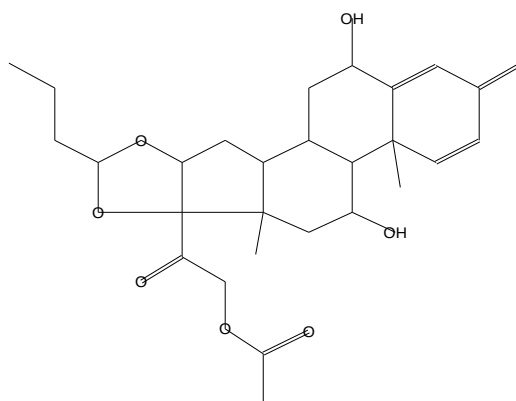
Compound Structure



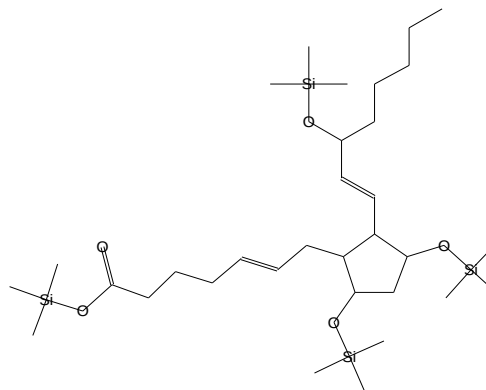
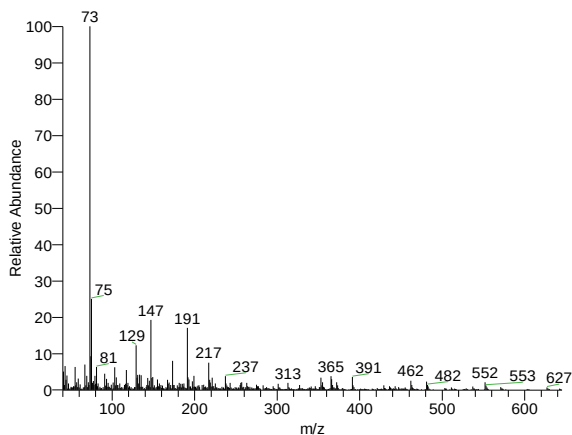
Cyclodecasiloxane, eicosamethyl-
Formula C₂₀H₆₀O₁₀Si₁₀, MW 740, CAS# 18772-36-6, Entry# 43767
2,2,4,4,6,6,8,8,10,10,12,12,14,14,16,16,18,18,20,20-Icosamethylcyclodecasiloxane #



(22S)-21-Acetoxy-6α,11α-dihydroxy-16α,17α-propylmethylenedioxyregna-1,4-diene-3,20-dione
Formula C₂₇H₃₆O₈, MW 488, CAS# 93789-66-3, Entry# 21437



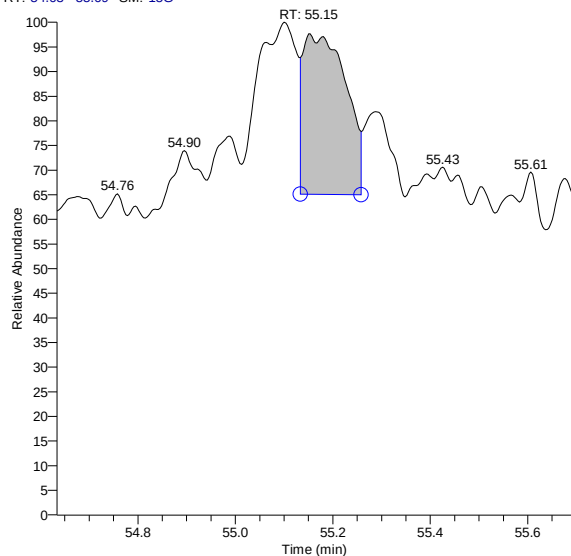
(+)-Prostaglandin F_{2α}, 4TMS derivative
Formula C₃₂H₆₆O₅Si₄, MW 642, CAS# 50669-95-9, Entry# 41447



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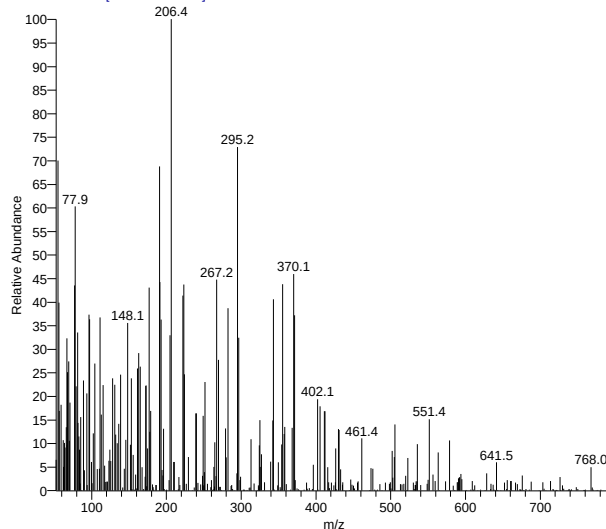
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RT: 54.63 - 55.69 SM: 15G



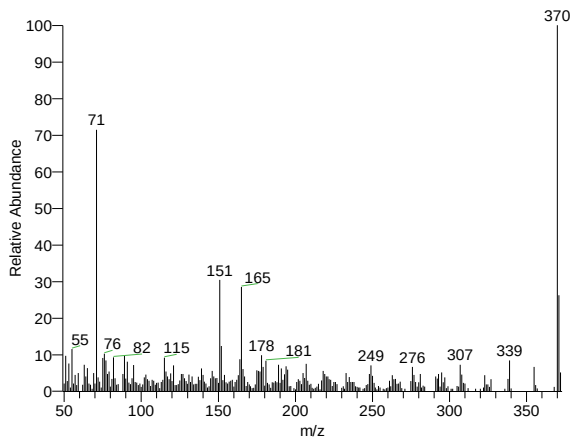
NL:
4.29E5
TIC MS
Genesis
NGA-ZE-
WATER4-
SAMPLE-
INJ1

NGA-ZE-WATER4-SAMPLE-INJ1 #14657 RT: 55.15 AV: 1 RF: 6.00, 3 NL: 1.61E4
T: + c EI Full ms [50.000-800.000]



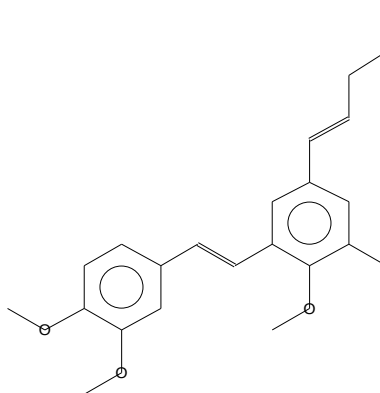
RT	Compound Name	Area	Probability	SI	RSI	Library
55.15	2,3,3',4'-tetramethoxy-5-(3-methoxyprop-1-enyl)stilbene	852662.63	7.83	340	440	mainlib
55.15	12,13-Di-O-acetyl-20-desoxytigla-(1,6(20),7)-trien-3-one	852662.63	5.05	327	393	mainlib
55.15	Milbemycin B, 6,28-anhydro-15-chloro-25-isopropyl-13-dehydro-5-O-demethyl-4-methyl-	852662.63	4.86	326	353	mainlib
55.15	2,4-Diamino-5,6-dihydro-6,8-diphenyl-8H-thiapyrano [4',3'-4,5]thieno[2,3-d]pyrimidine-7-oxide	852662.63	3.82	320	444	mainlib
55.15	Phorbol 12,13,20-triacetate	852662.63	3.08	315	380	mainlib

Hit Spectrum



Compound Structure

2,3,3',4'-tetramethoxy-5-(3-methoxyprop-1-enyl)stilbene
Formula C22H26O5, MW 370, CAS# 850894-64-3, Entry# 235882
\$:28CHTMUFUUYLTCJG-LQPGMRMSA-N

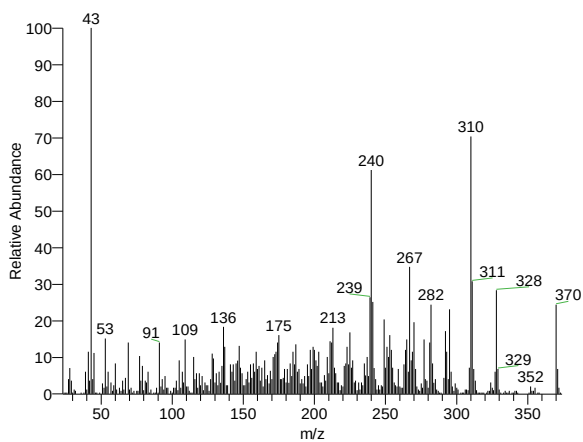


Analysed by Satyanarayana

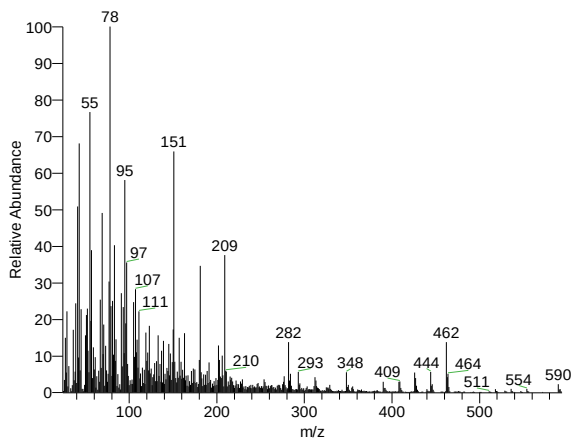
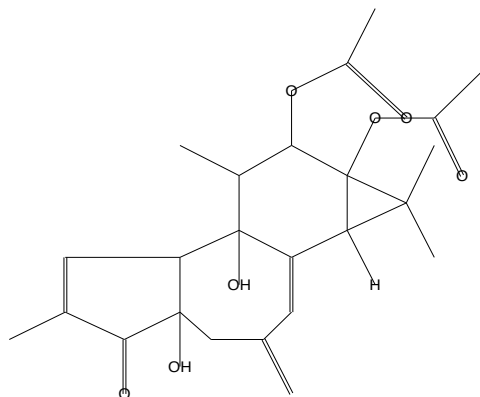
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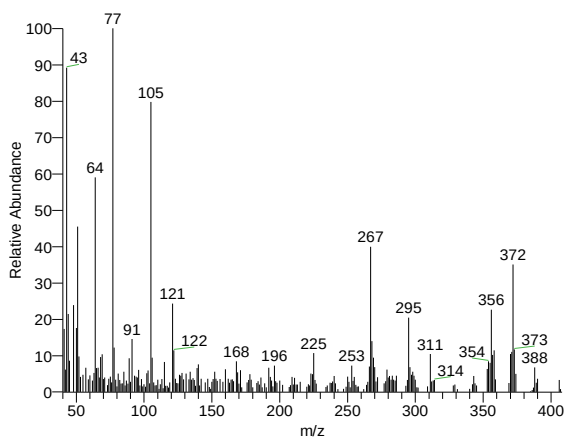
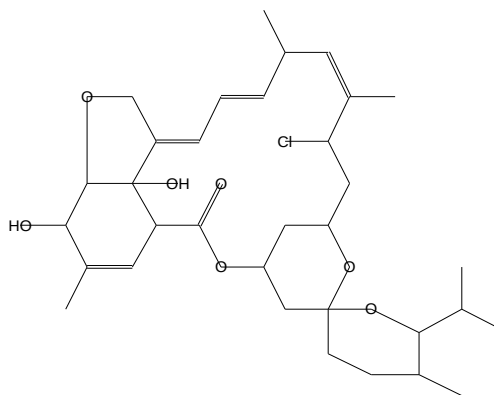
Compound Structure



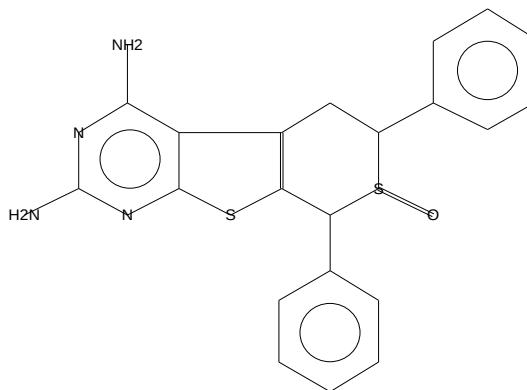
12,13-Di-O-acetyl-20-desoxytigla-(1,6(20),7)-trien-3-one
Formula C₂₄H₃₀O₇, MW 430, CAS# NA, Entry# 14574



Milbemycin B, 6,28-anhydro-15-chloro-25-isopropyl-13-dehydro-5-O-demethyl-4-methyl-
Formula C₃₃H₄₇ClO₇, MW 590, CAS# NA, Entry# 48120
\$.28NCJXUYSQIFYACX-CSMIWHQNSA-N



2,4-Diamino-5,6-dihydro-6,8-diphenyl-8H-thiapyrano[4',3':4,5]thieno[2,3-d]pyrimidine-7-oxide
Formula C₂₁H₁₈N₄O₂S, MW 406, CAS# NA, Entry# 46492
6,8-Diphenyl-5,8-dihydro-6H-thiapyrano[4',3':4,5]thieno[2,3-d]pyrimidine-2,4-diamine 7-oxide #



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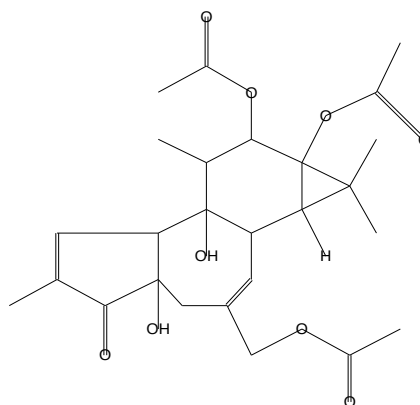
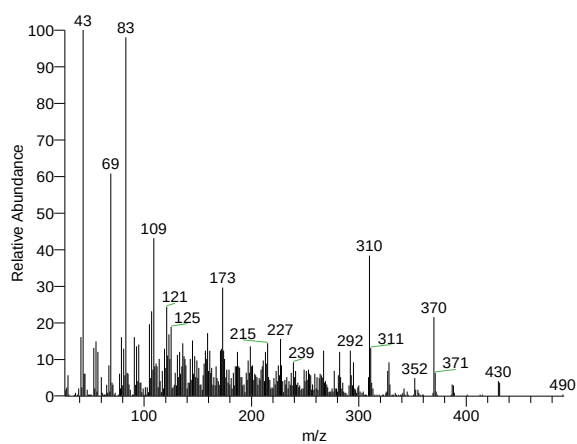
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Hit Spectrum

Compound Structure

SI 315, RSI 380, mainlib, Entry# 9650, CAS# NA, Phorbol 12,13,20-triacetate

Phorbol 12,13,20-triacetate
Formula C₂₆H₃₄O₉, MW 490, CAS# NA, Entry# 9650



Analysed by Satyanarayana