Supporting Information

Bioactive Diarylheptanoids from *Alpinia coriandriodora*

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Contents

Table S1. M06-2X/def2-TZVP/SMD//B3LYP/def2-SVP/PCM calculated relative thermal energies (ΔE), relative free energies (ΔG), and equilibrium populations (P)[a] of low-energy conformers of compounds **1**, **6**, and **8** in MeOH solution.

conformer	*E* (kcal/mol)	*G* (kcal/mol)	P (%)
(1*S*,3*R*,5*S*)-**1**			
1a	0.0	0.0	33.2
1b	1.203	0.101	28.0
1c	2.222	0.279	20.7
1d	2.998	1.103	5.2
1e	3.104	1.128	4.9
1f	1.261	1.252	4.0
1g	2.682	1.480	2.7
1h [b]	0.972	1.911	1.3
(1*S*,3*R*,5*R*)-**6**			
6a	1.345	0.0	21.9
6b	0.0	0.153	16.9
6c	0.873	0.507	9.3
6d	0.106	0.562	8.5
6e	0.292	0.600	7.9
6f	0.894	0.626	7.6
6g	0.334	0.658	7.2
6h	0.424	0.760	6.1
6i	1.847	1.138	3.2
6j	1.914	1.167	3.1
6k	1.803	1.201	2.9
6l	1.864	1.221	2.8
6m	0.879	1.349	2.2
6n [b]	1.764	2.347	0.4
(1*S*,3*R*,5*R*,7*R*)-**8**			
R-**8a**	0.0	0.0	67.9
R-**8b**	1.568	0.836	16.5
R-**8c**	2.342	1.270	7.9
R-**8d**	0.476	1.764	3.4
R-**8e**	2.229	1.990	2.4
R-**8f**	2.705	2.135	1.8
(1*S*,3*R*,5*R*,7*S*)-**8**			
S-**8a**	0.675	0.0	61.2
S-**8b**	0.0	0.749	17.3
S-**8c**	1.755	1.107	9.4
S-**8d**	0.625	1.492	4.9
S-**8e**	2.819	1.703	3.4
S-**8f**	2.804	1.748	3.2

[a] From G values at 298.15 K. [b] Conformer not applied to ECD/TDDFT calculations

Table S2. The mPW1PW91/6-311+G(d,p)/PCM//B3LYP/def2-SVP calculated ^{13}C NMR data for (1*S*,3*R*,5*R*,7*R*)-**8** and (1*S*,3*R*,5*R*,7*S*)-**8** and their goodness of fit with the measured shifts of **8**.

position	(1*S*,3*R*,5*R*,7*R*)-**8**			(1*S*,3*R*,5*R*,7*S*)-**8**			**8**
	σ^x	δ_u	δ_s	σ^x	δ_u	δ_s	δ_{exp}
C-3"	34.71	152.27	149.36	34.94	152.04	149.11	149.4
C-5"	34.71	152.27	149.36	34.94	152.04	149.11	149.4
C-3'	35.32	151.6	148.76	35.25	151.73	148.81	149.1
C-5'	35.32	151.6	148.76	35.25	151.73	148.81	149.1
C-1'	45.57	141.4	138.71	45.01	141.97	139.23	134.5
C-4'	47.56	139.42	136.76	48.17	138.81	136.13	136.0
C-4"	47.62	139.36	136.70	47.40	139.58	136.89	135.9
C-1"	47.92	139.06	136.41	46.36	140.62	137.91	134.3
C-2"	83.20	106.20	104.17	81.34	105.59	103.55	104.8
C-2'	82.34	104.64	102.64	82.11	104.87	102.85	104.8
C-6'	82.34	104.64	102.64	82.11	104.87	102.85	104.8
C-6"	83.20	106.20	104.17	81.341	105.59	103.55	104.8
C-7	103.66	83.32	81.73	105.58	81.41	79.83	81.8
C-1	106.19	80.79	79.25	106.00	80.98	79.41	79.2
C-5	112.35	74.63	73.21	113.20	73.78	72.35	74.3
C-3	115.77	71.21	69.85	116.08	70.90	69.53	69.0
7-OCH_3	130.19	56.79	55.71	129.80	57.18	56.08	56.7
3'- OCH_3	131.20	55.78	54.72	130.85	56.135	55.05	56.8
3"-OCH_3	131.17	55.81	54.75	130.90	56.08	54.99	56.7
5"-OCH_3	131.17	55.81	54.75	130.90	56.08	54.99	56.7
5'- OCH_3	131.20	55.78	54.72	130.85	56.14	55.05	56.8
C-2	138.13	48.85	47.92	138.08	48.90	47.96	43.7
C-6	138.97	48.01	47.09	137.53	49.45	48.50	46.2
C-4	146.57	40.41	39.649	146.32	40.66	39.88	42.3
Probability	sDP4+ = 98.3% uDP4+ = 52.0% DP4+ = 98.4%			sDP4+ = 1.7% uDP4+ = 48.0% DP4+ = 1.6%			

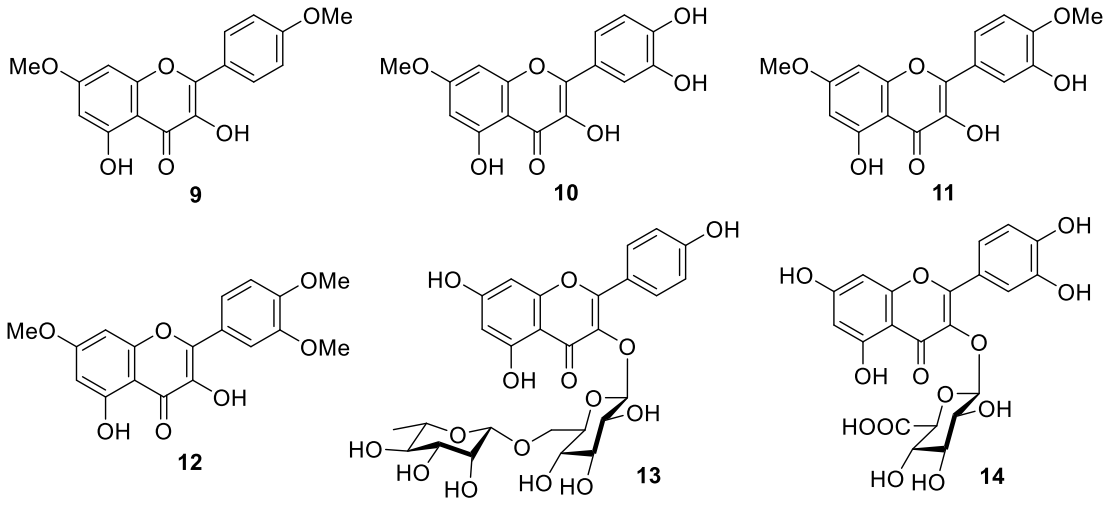


Fig. S1 Structures of compounds **9**–**14**

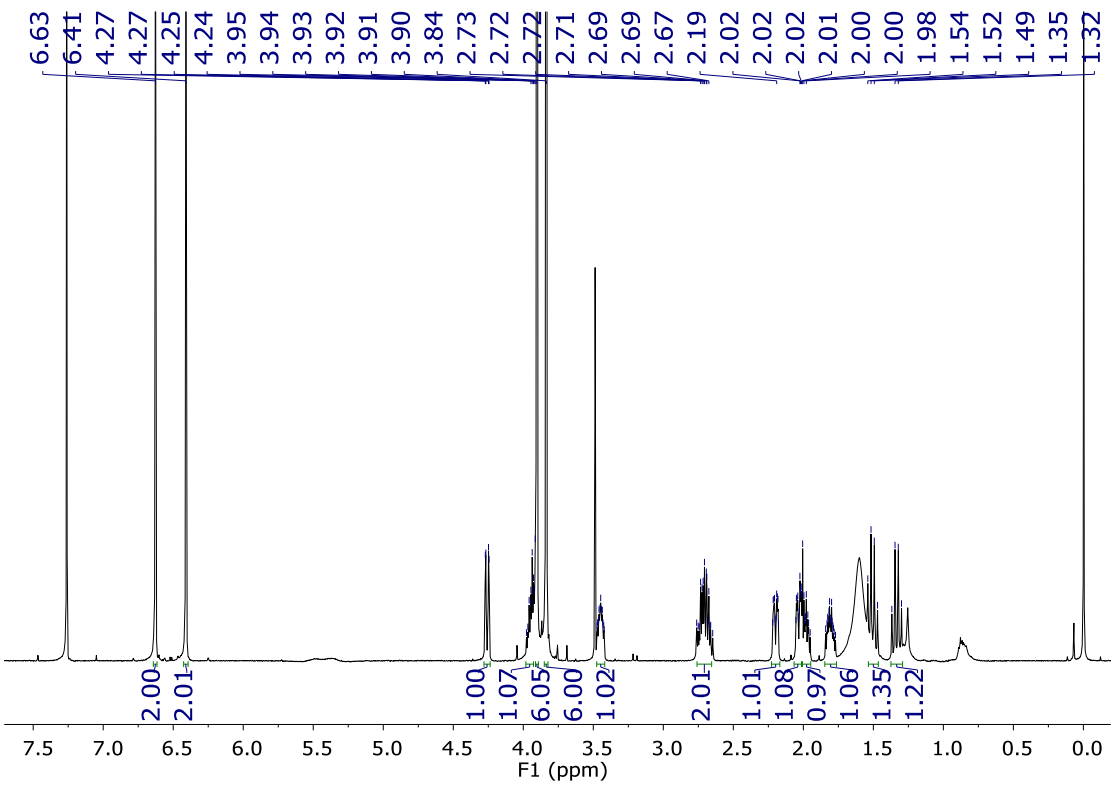


Fig. S2 ^{1}H NMR spectrum of compound **1**.

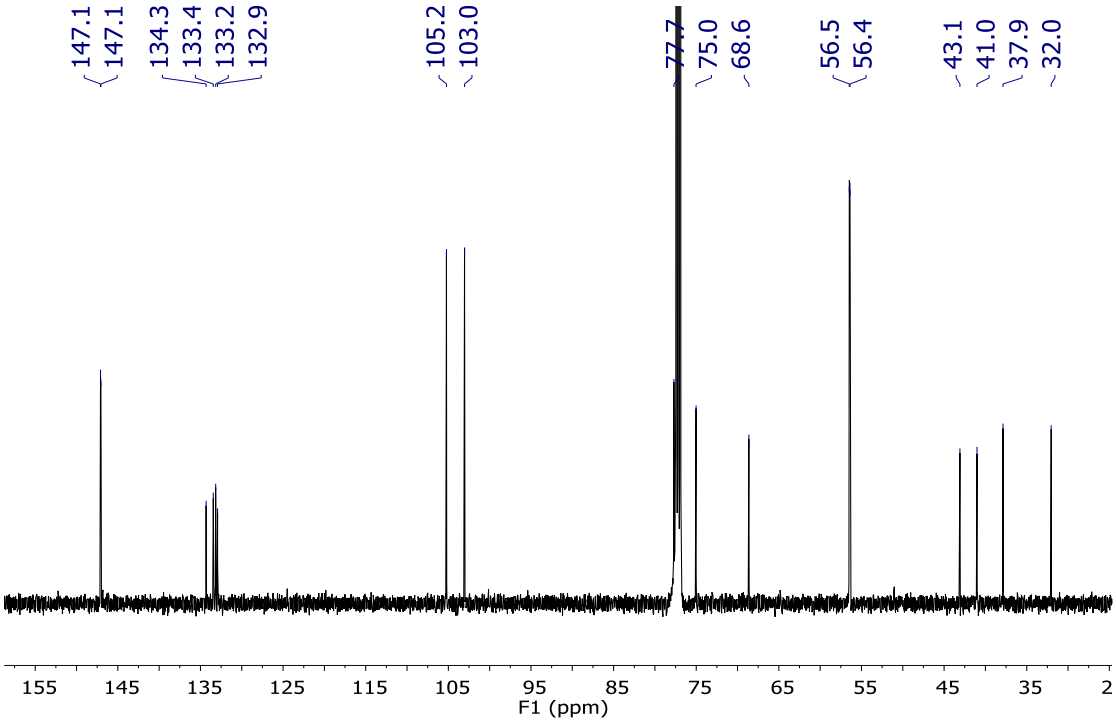


Fig. S3 ^{13}C NMR spectrum of compound **1**.

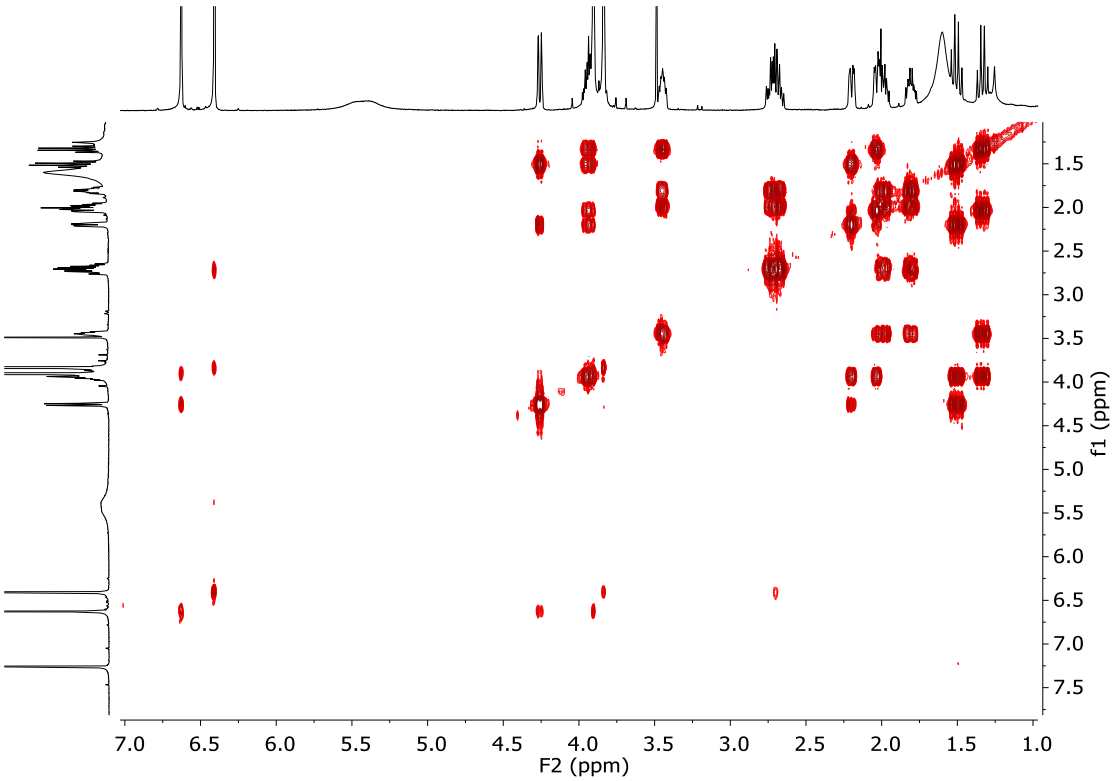


Fig. S4 ^{1}H–^{1}H COSY spectrum of compound **1**.

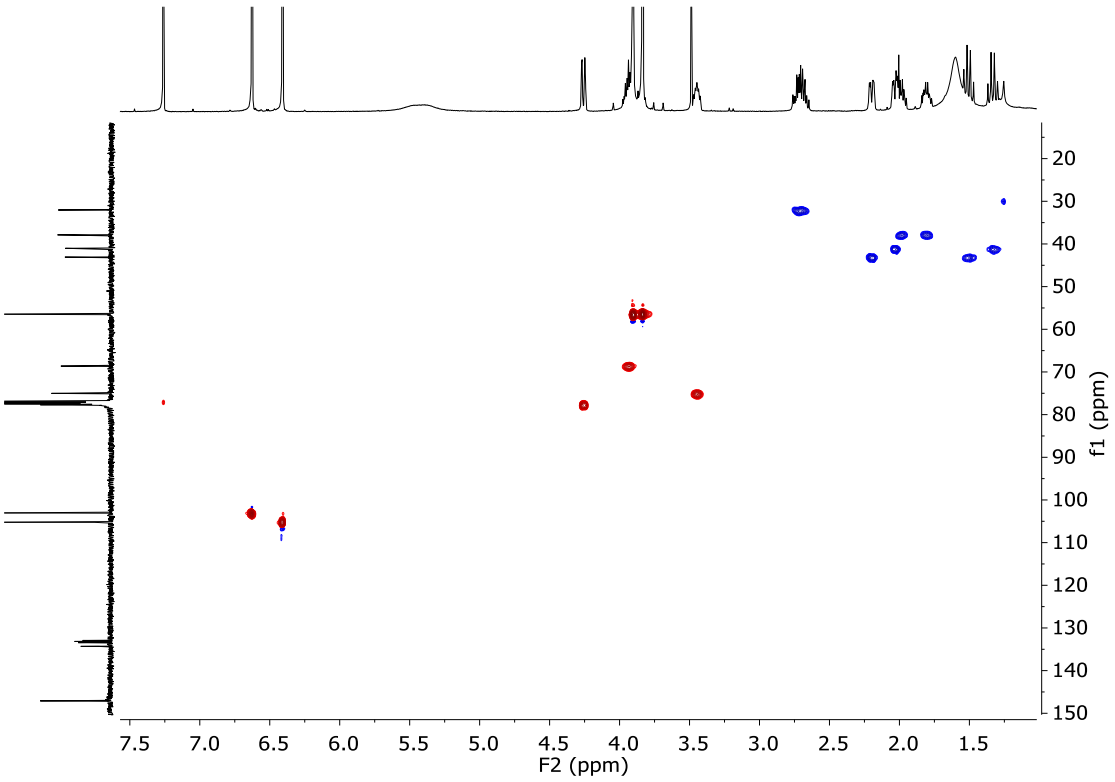


Fig. S5 HSQC spectrum of compound **1**.

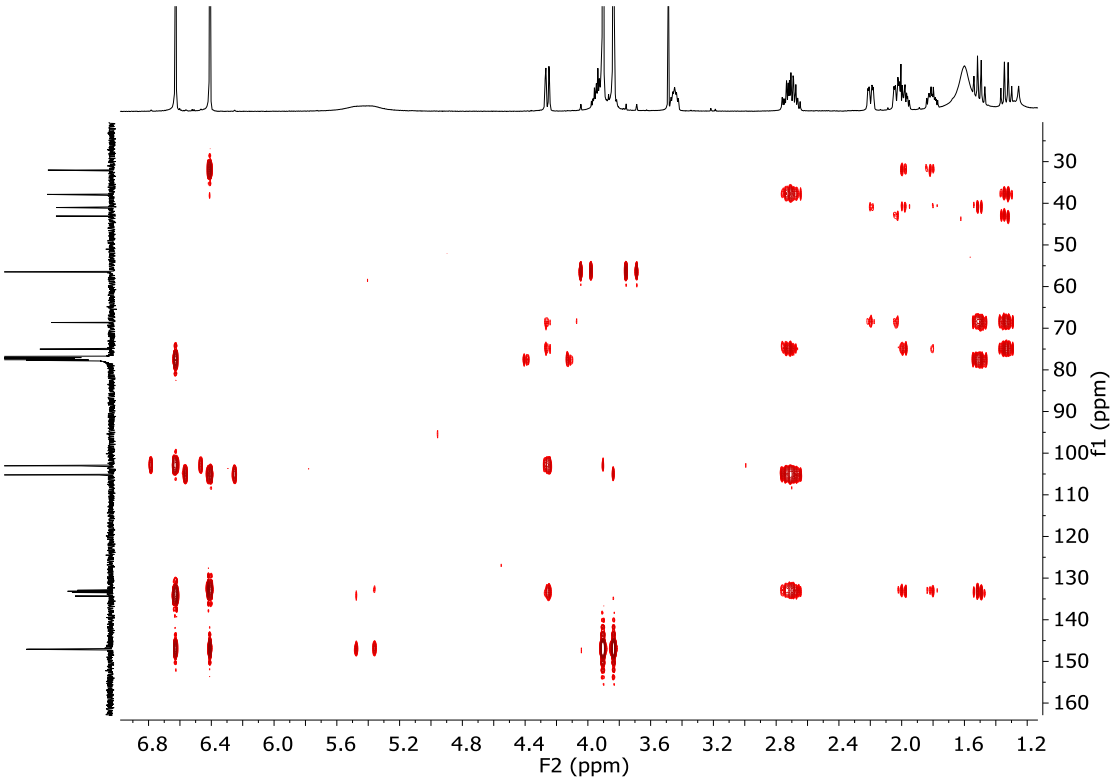


Fig. S6 HMBC spectrum of compound **1**.

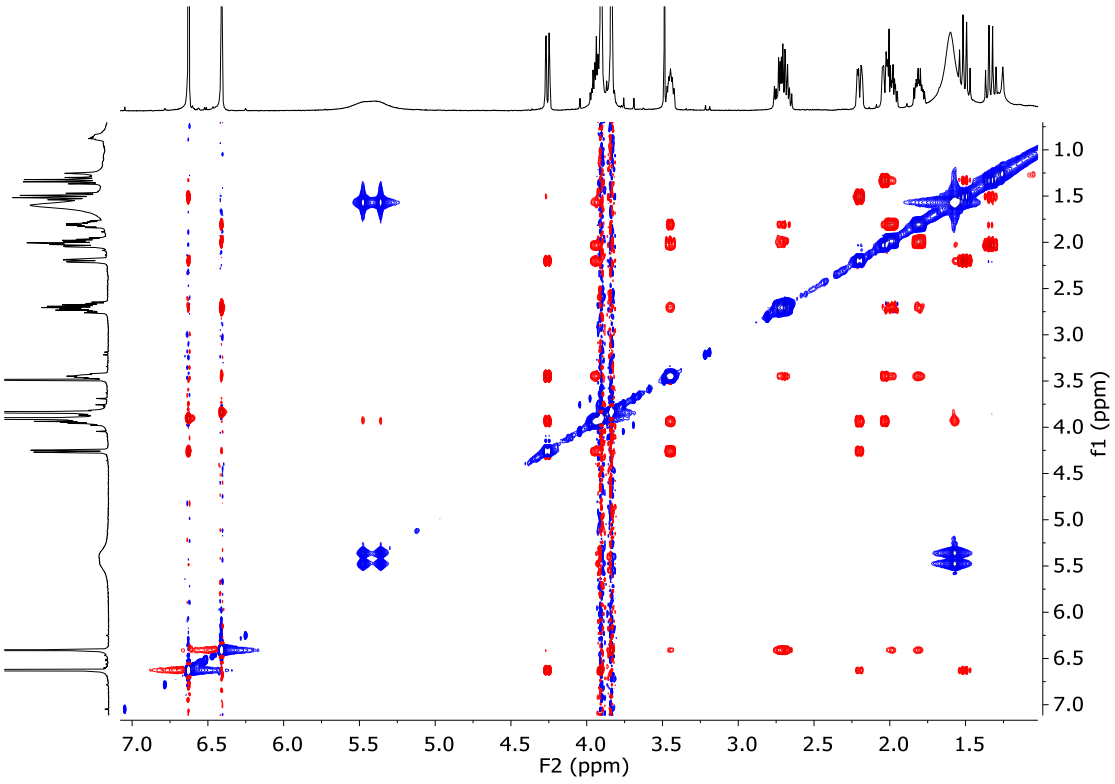
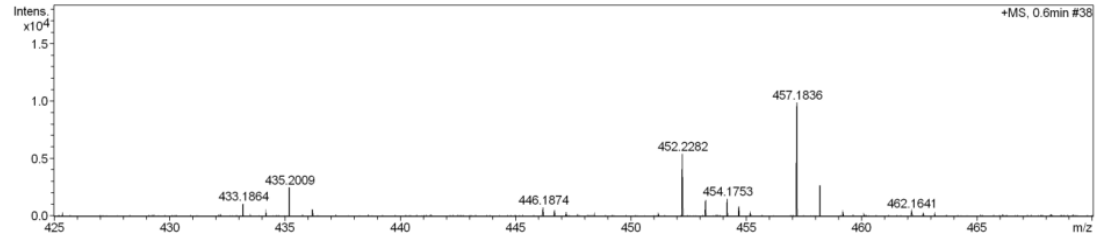


Fig. S7 NOESY spectrum of compound **1**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
435.2009	1	C23H31O8	100.00	435.2013	0.9	0.4	8.4	8.5	even	ok
457.1836	1	C23H30NaO8	100.00	457.1833	0.6	0.3	10.7	8.5	even	ok
869.3954	1	C46H61O16	100.00	869.3954	0.0	0.0	22.2	16.5	even	ok
891.3777	1	C46H60NaO16	100.00	891.3774	-0.4	-0.4	7.1	16.5	even	ok

Fig. S8 HRESI-MS spectrum of compound **1**.

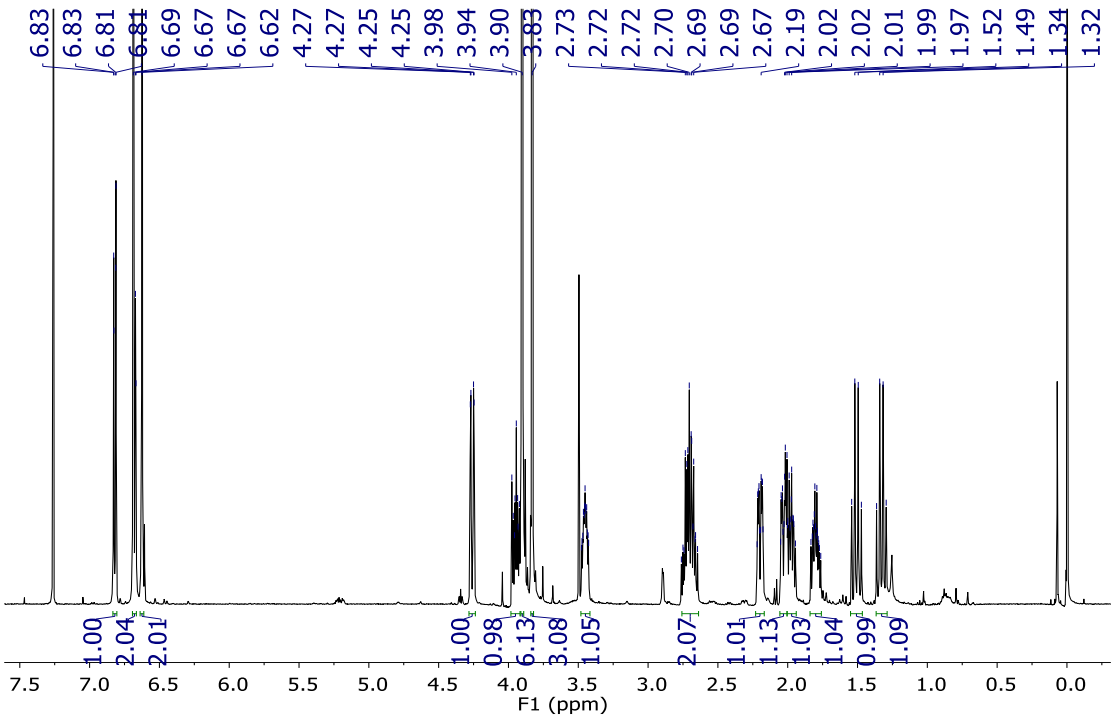


Fig. S9 ^{1}H NMR spectrum of compound **2**.

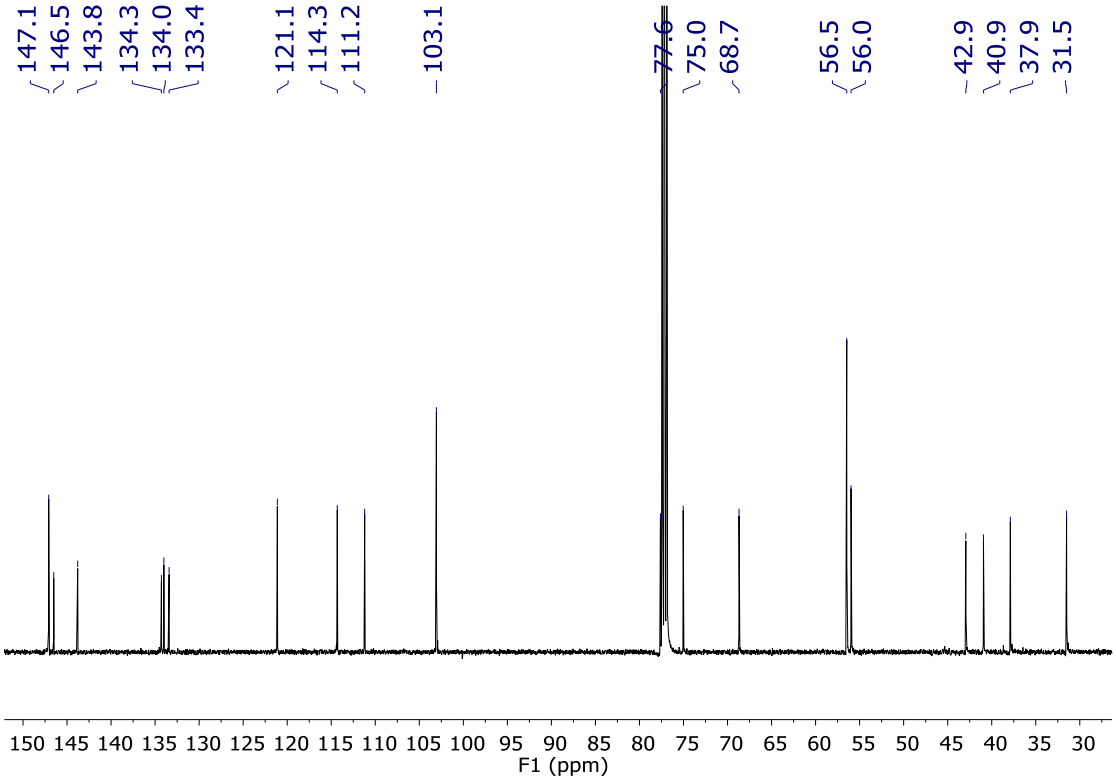
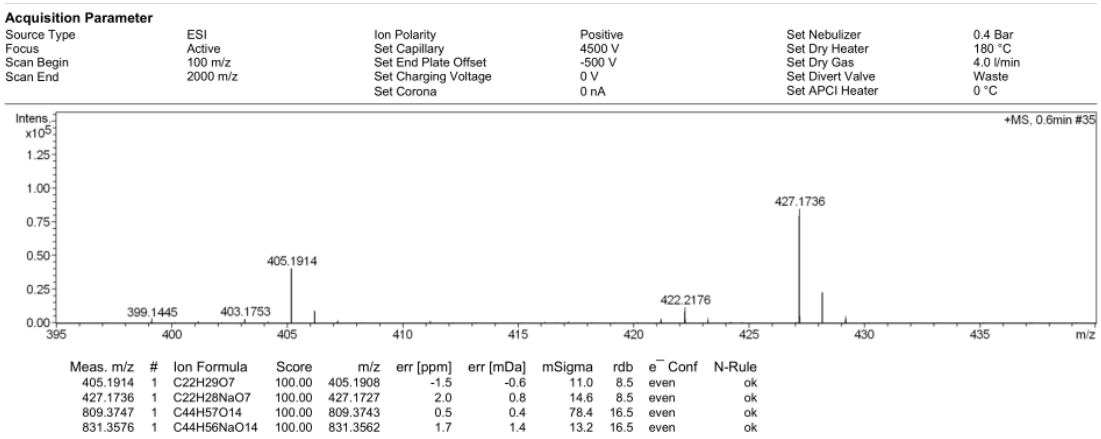


Fig. S10 ^{13}C NMR spectrum of compound **2**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
405.1914	1	C22H29O7	100.00	405.1908	-1.5	-0.6	11.0	8.5	even	ok
427.1736	1	C22H28NaO7	100.00	427.1727	2.0	0.8	14.6	8.5	even	ok
809.3747	1	C44H57O14	100.00	809.3743	0.5	0.4	78.4	16.5	even	ok
831.3576	1	C44H56NaO14	100.00	831.3562	1.7	1.4	13.2	16.5	even	ok

Fig. S11 HRESI-MS spectrum of compound **2**.

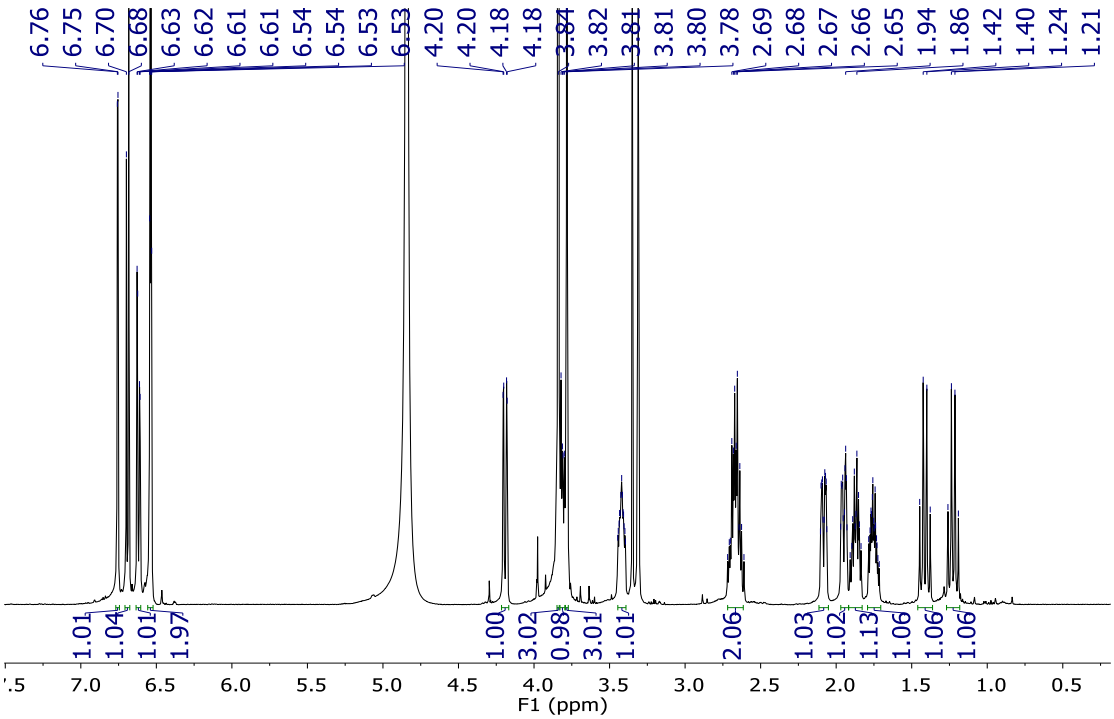


Fig. S12 ^{1}H NMR spectrum of compound **3**.

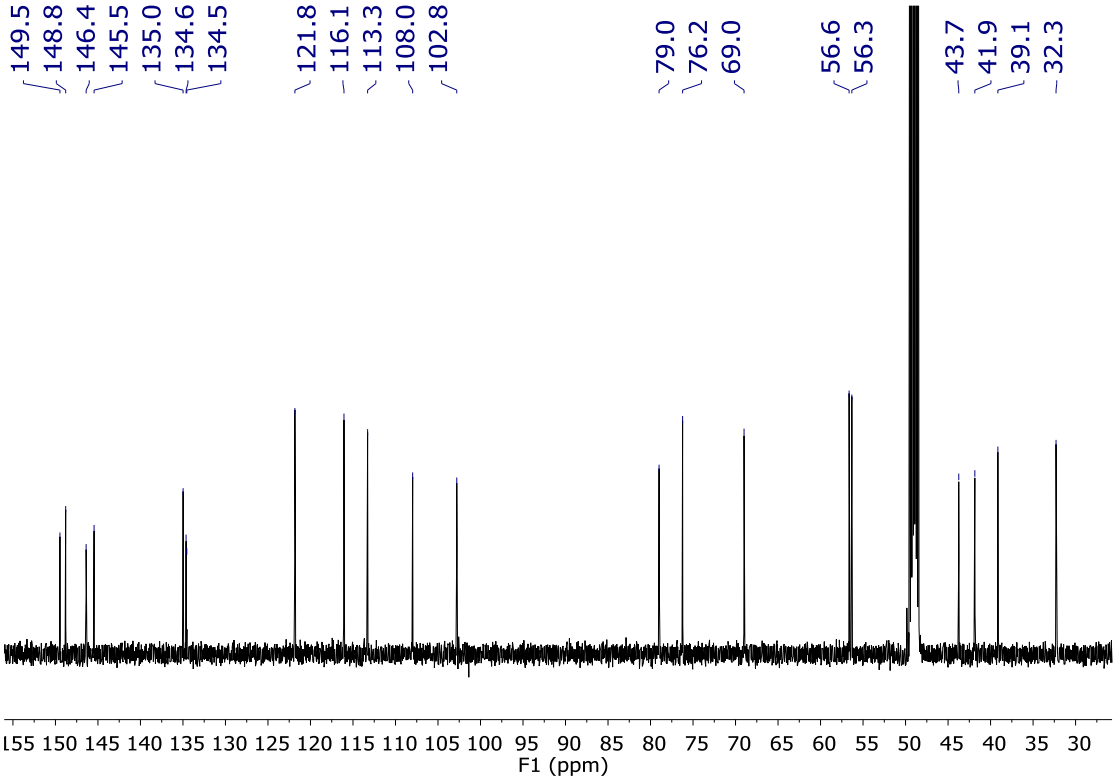
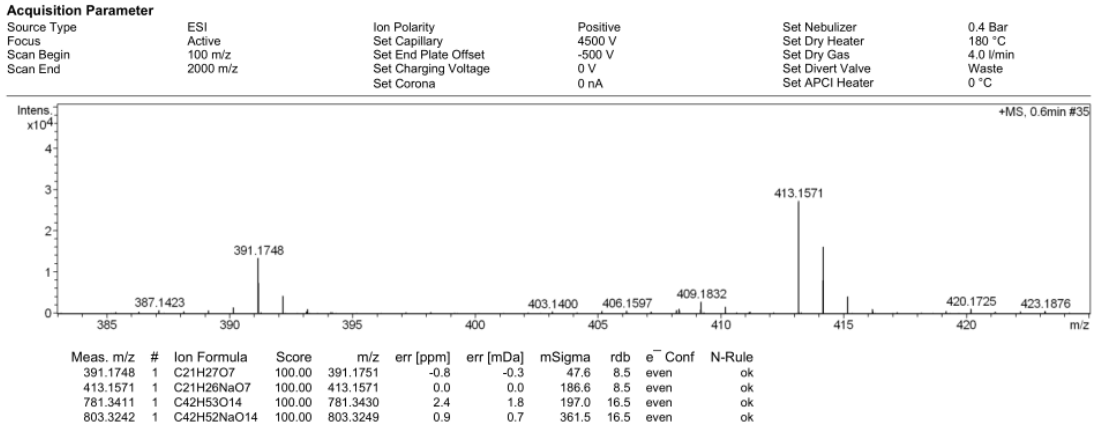


Fig. S13 ^{13}C NMR spectrum of compound **3**.



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
391.1748	1	C21H27O7	100.00	391.1751	-0.8	-0.3	47.6	8.5	even	ok
413.1571	1	C21H26NaO7	100.00	413.1571	0.0	0.0	186.6	8.5	even	ok
781.3411	1	C42H53O14	100.00	781.3430	2.4	1.8	197.0	16.5	even	ok
803.3242	1	C42H52NaO14	100.00	803.3249	0.9	0.7	361.5	16.5	even	ok

Fig. S14 HRESI-MS spectrum of compound **3**.

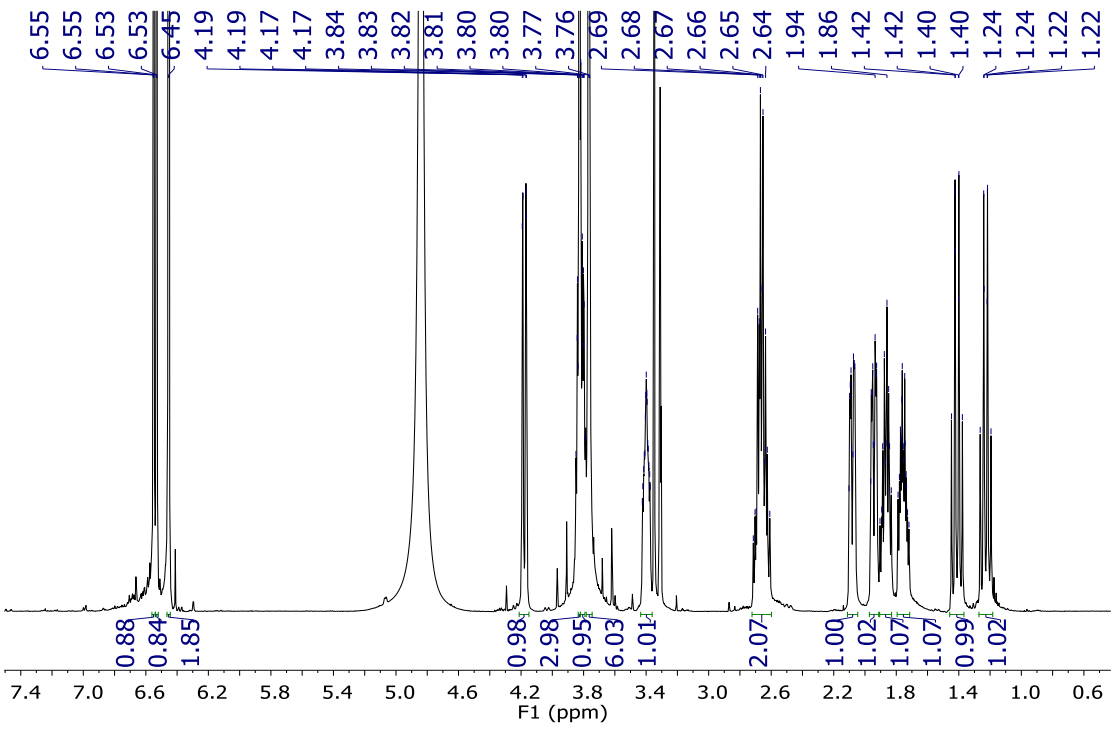


Fig. S15 ^{1}H NMR spectrum of compound **4**.

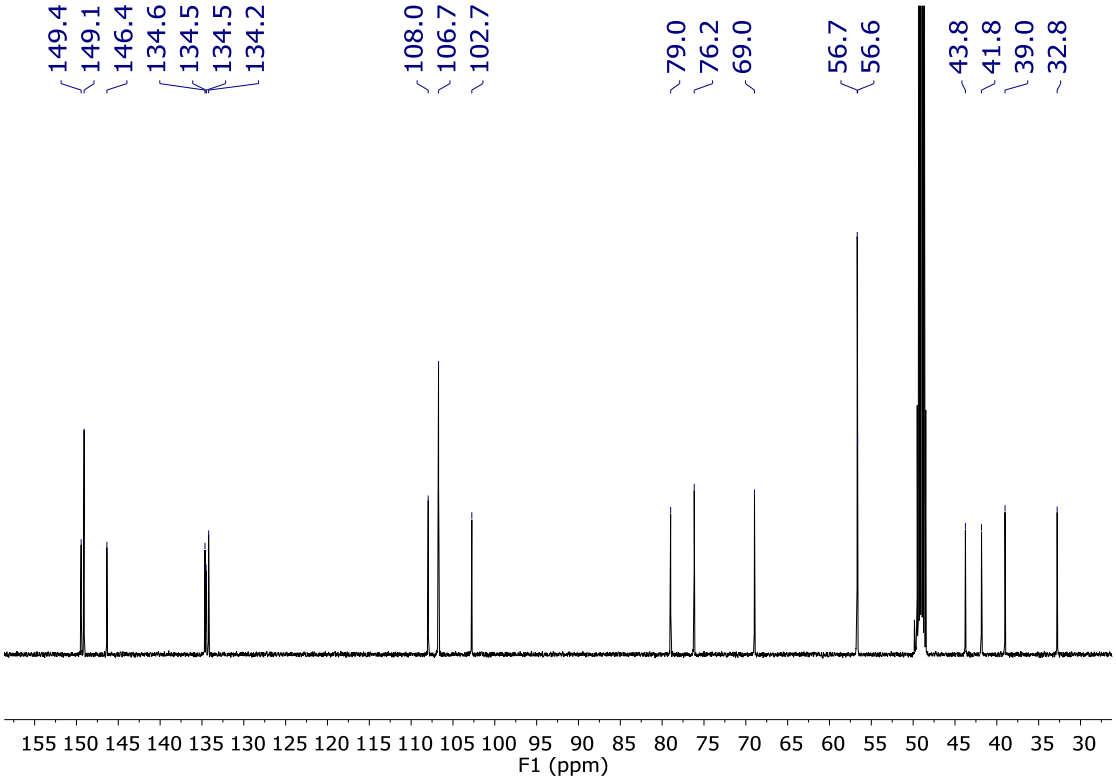


Fig. S16 ^{13}C NMR spectrum of compound **4**.

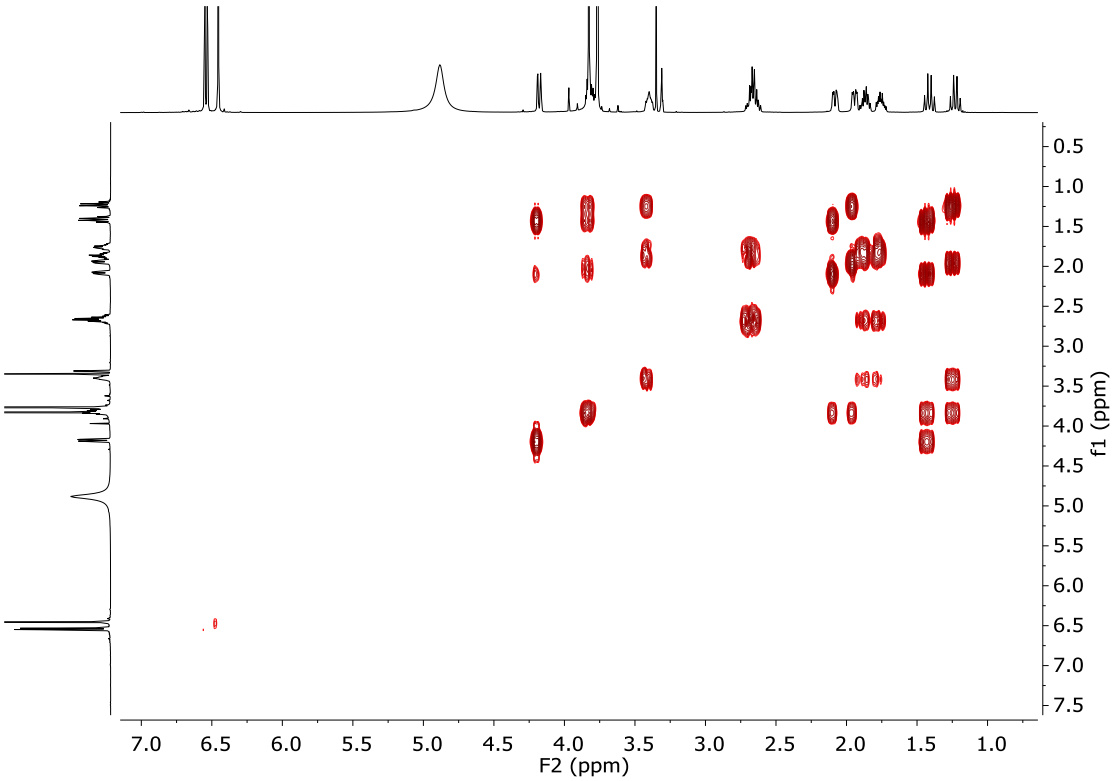


Fig. S17 ^{1}H–^{1}H COSY spectrum of compound **4**.

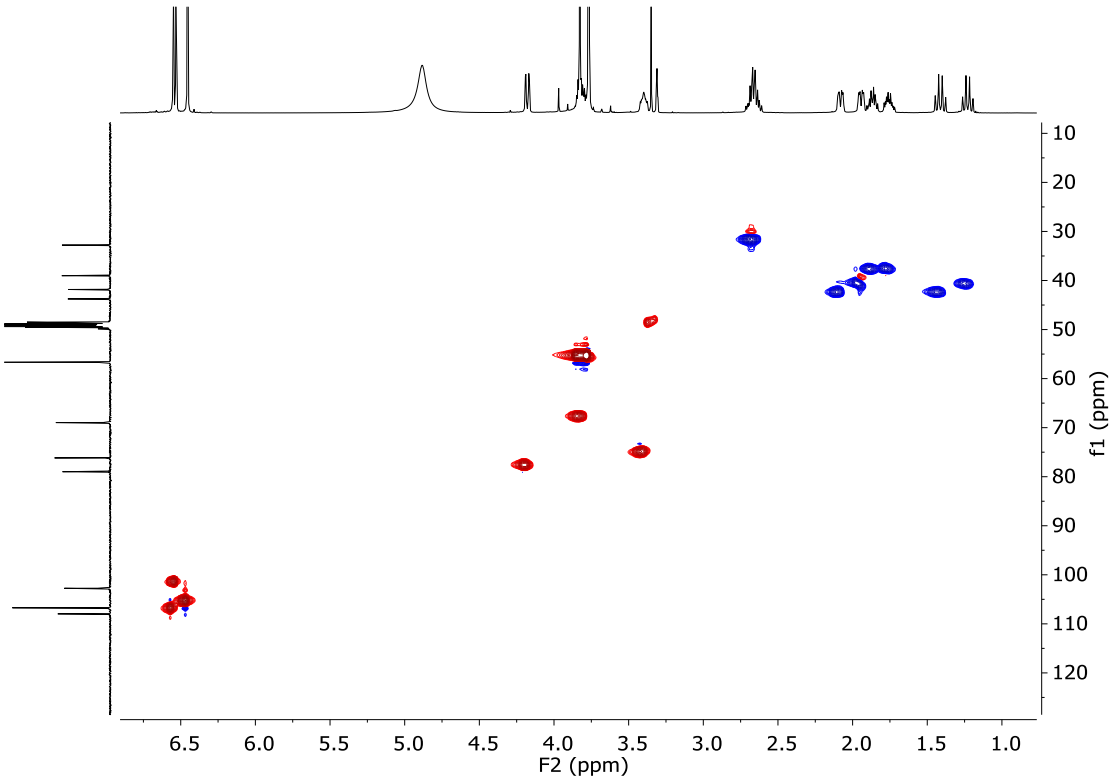


Fig. S18 HSQC spectrum of compound **4**.

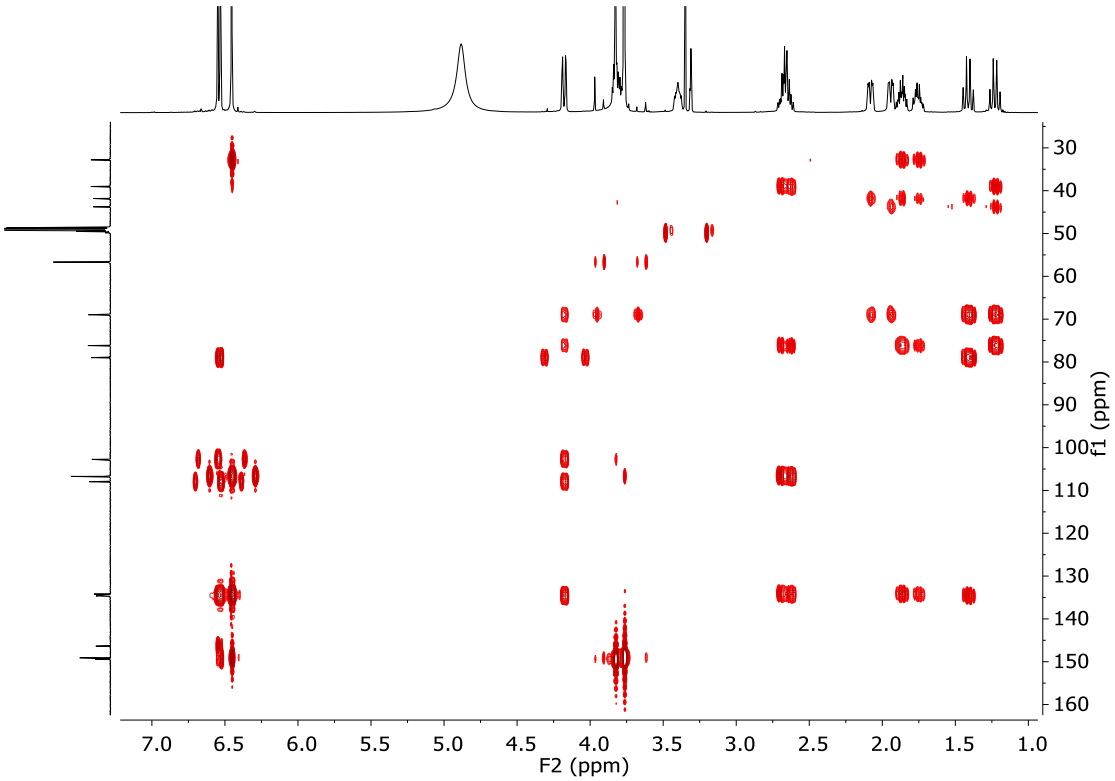


Fig. S19 HMBC spectrum of compound **4**.

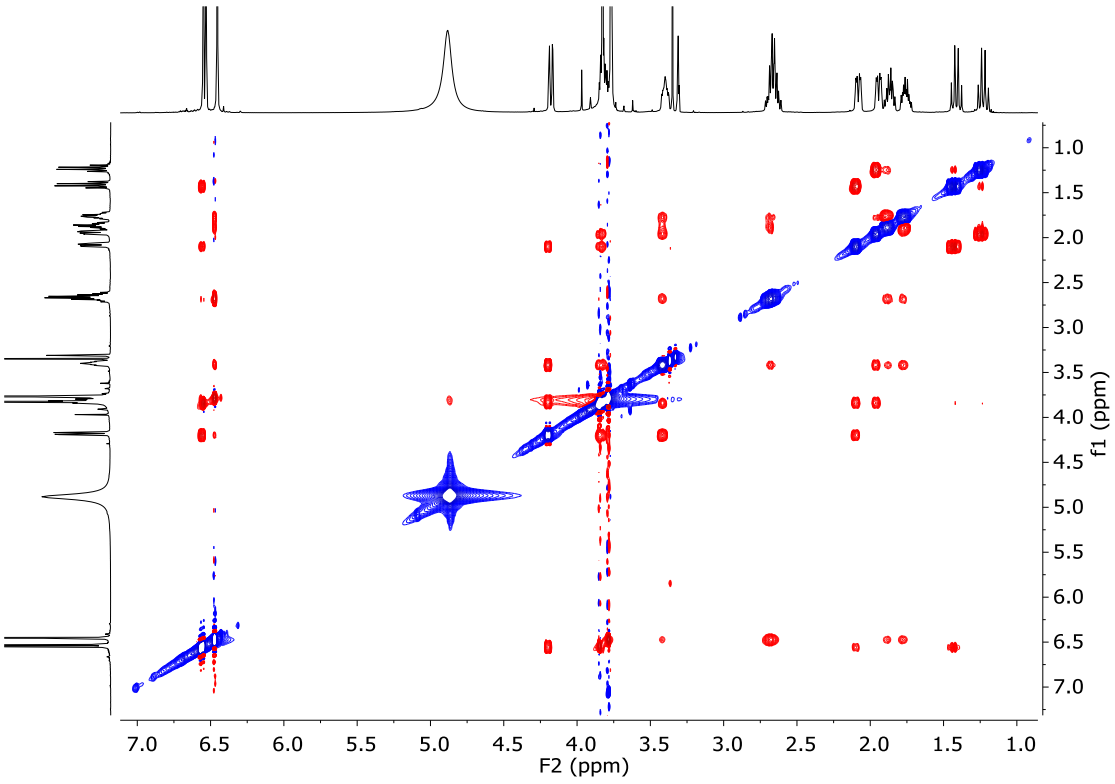
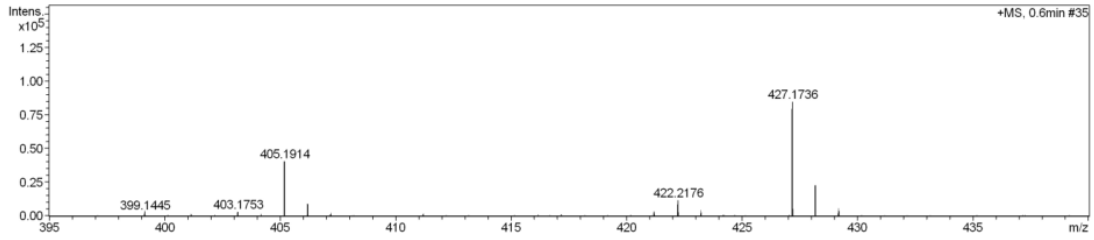


Fig. S20 NOESY spectrum of compound **4**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e¯ Conf	N-Rule
405.1914	1	C22H29O7	100.00	405.1908	-1.5	-0.6	11.0	8.5	even	ok
427.1736	1	C22H28NaO7	100.00	427.1727	2.0	0.8	14.6	8.5	even	ok
809.3747	1	C44H57O14	100.00	809.3743	0.5	0.4	78.4	16.5	even	ok
831.3576	1	C44H56NaO14	100.00	831.3562	1.7	1.4	13.2	16.5	even	ok

Fig. S21 HRESI-MS spectrum of compound **4**.

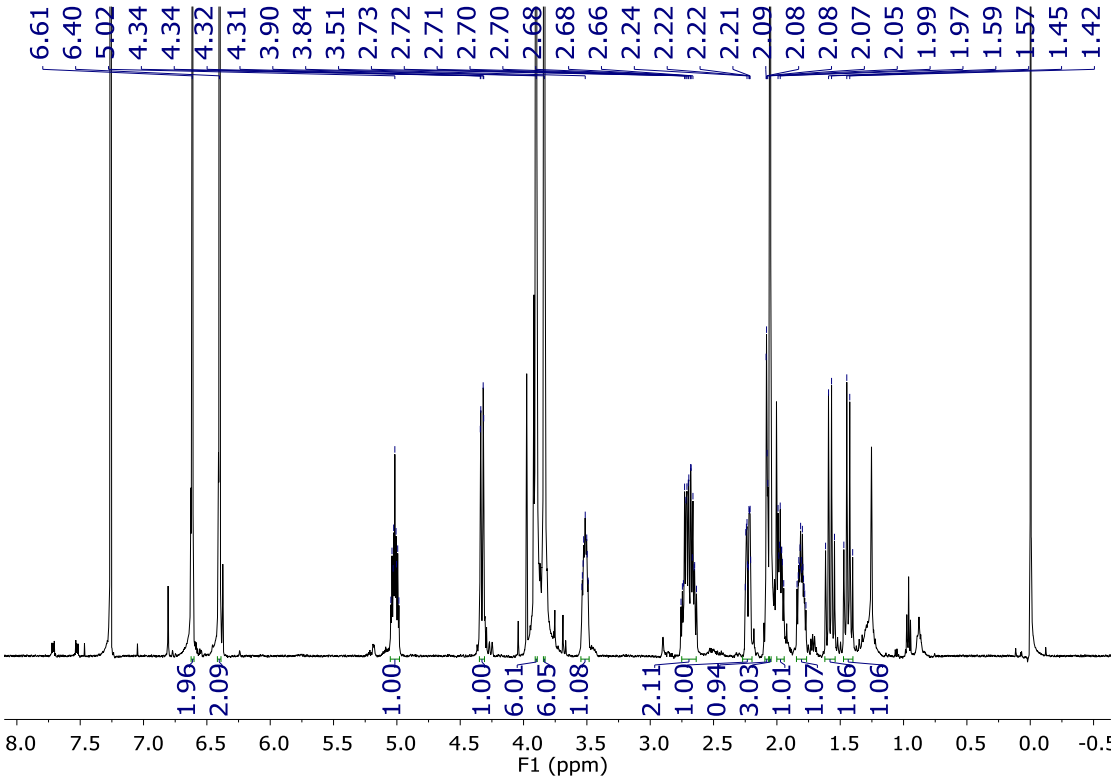


Fig. S22 ^{1}H NMR spectrum of compound **5**.

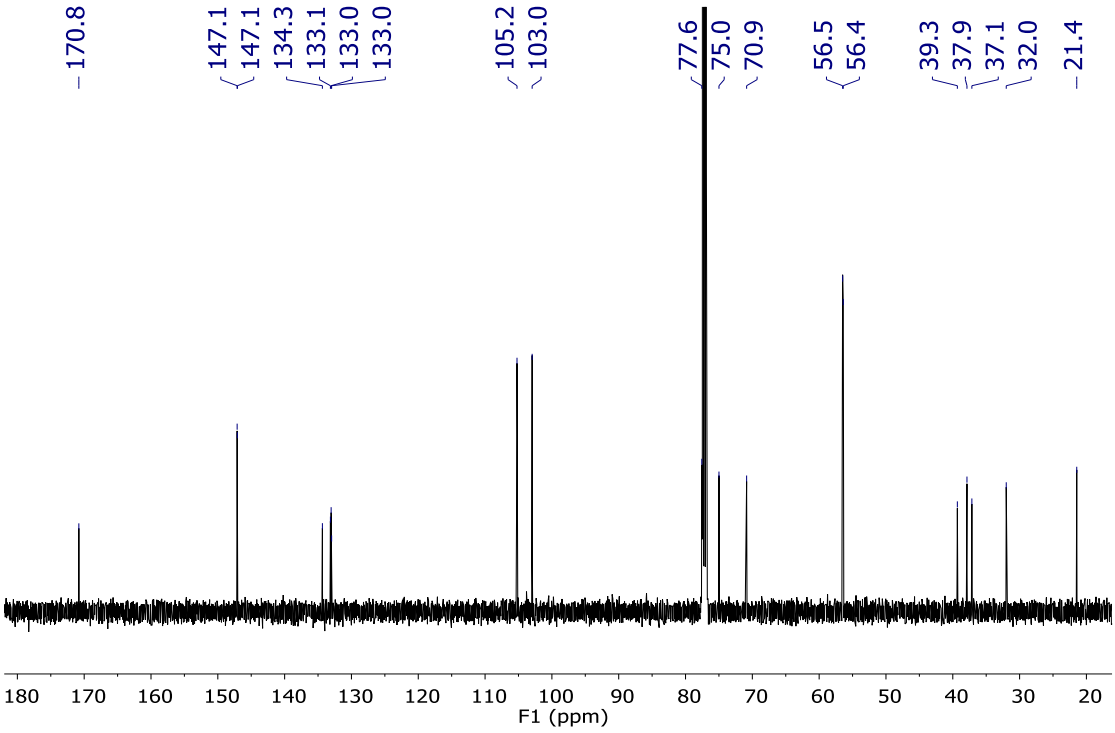


Fig. S23 ^{13}C NMR spectrum of compound **5**.

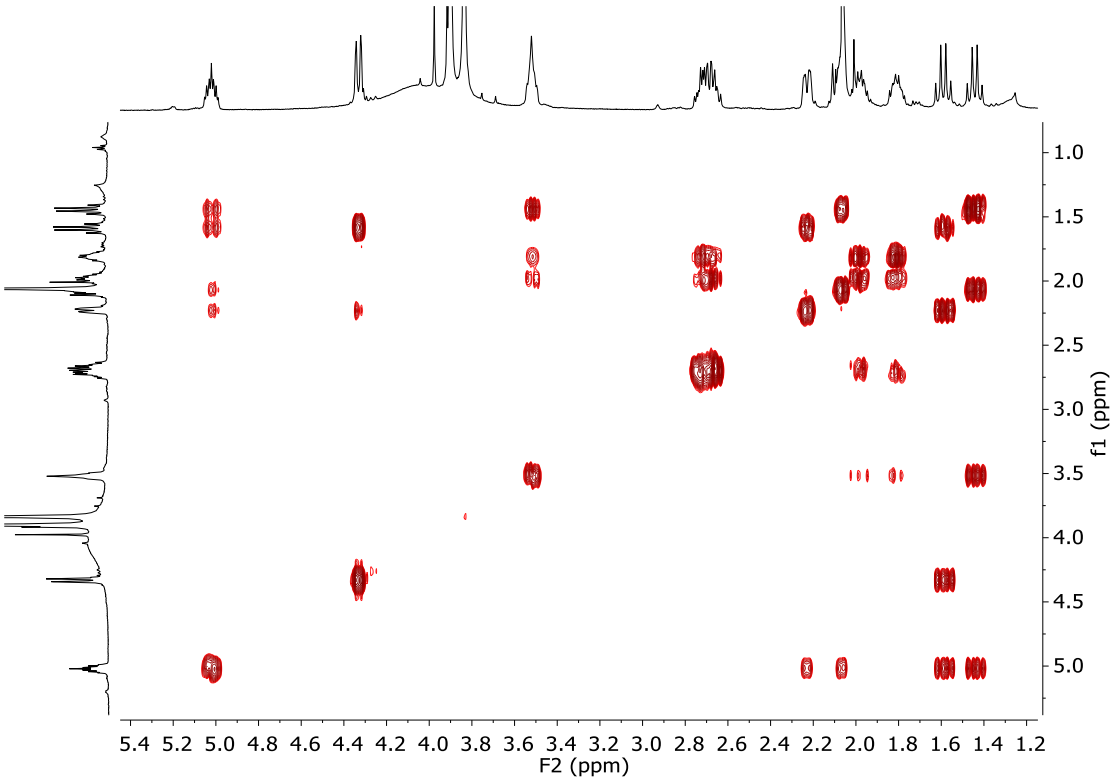


Fig. S24 ^{1}H–^{1}H COSY spectrum of compound **5**.

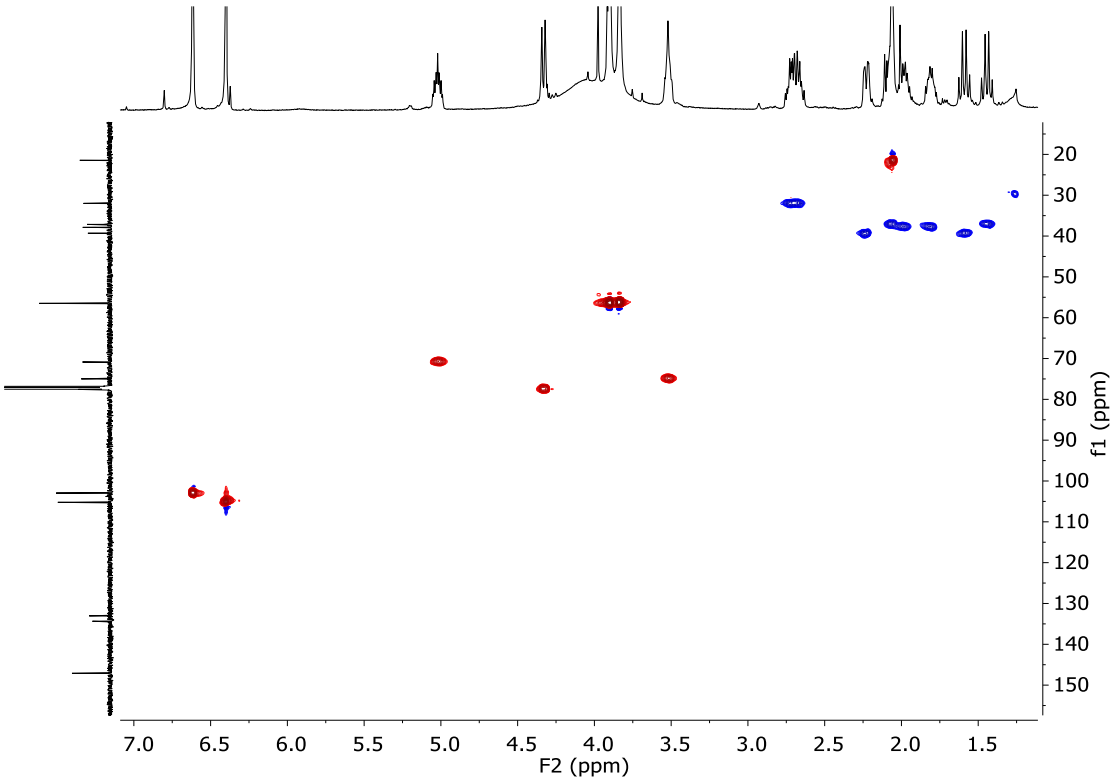


Fig. S25 HSQC spectrum of compound **5**.

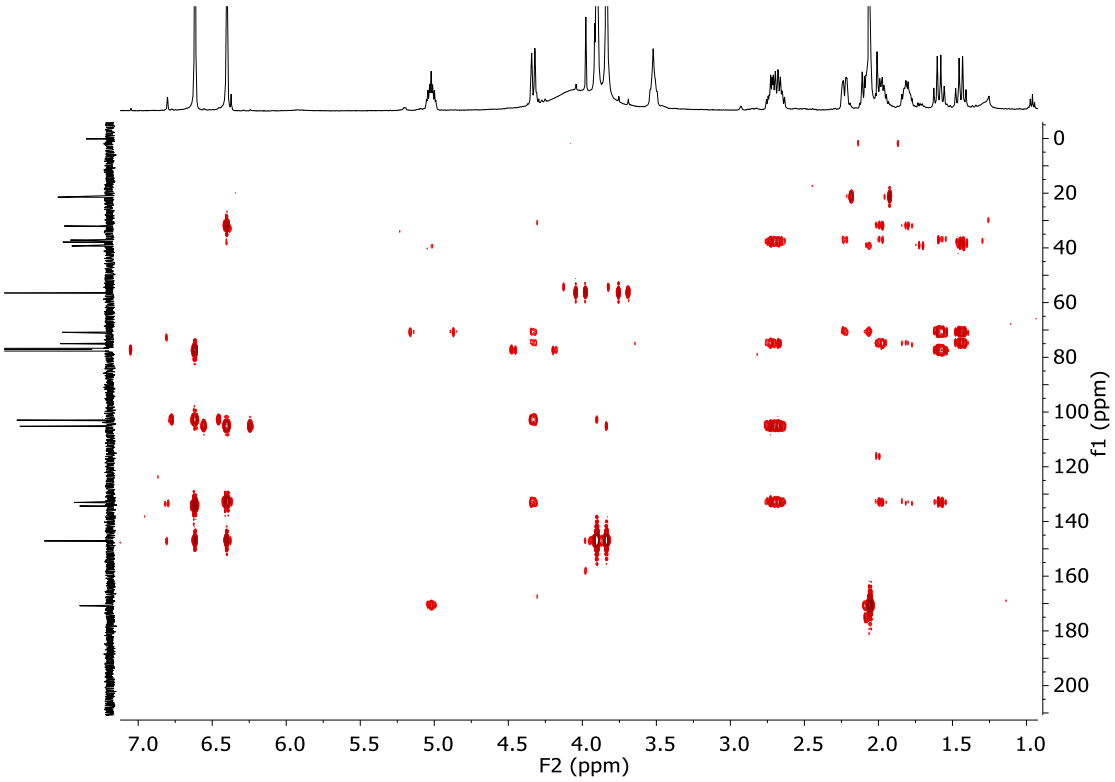


Fig. S26 HMBC spectrum of compound **5**.

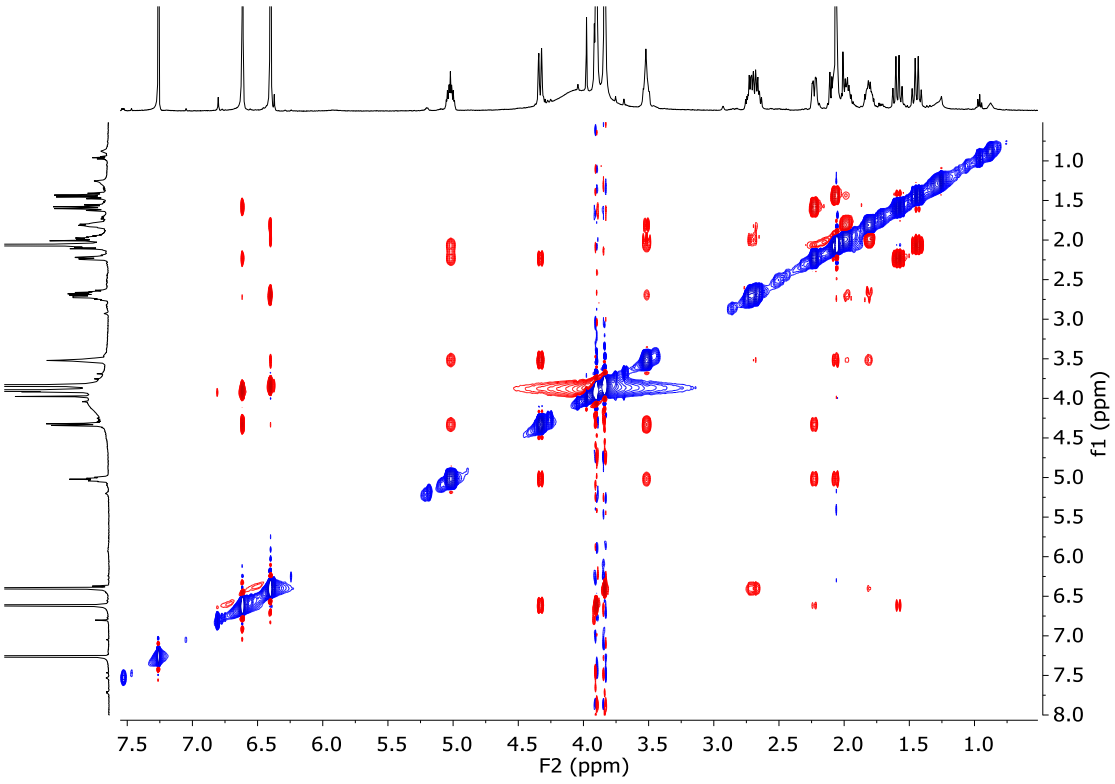


Fig. S27 NOESY spectrum of compound **5**.

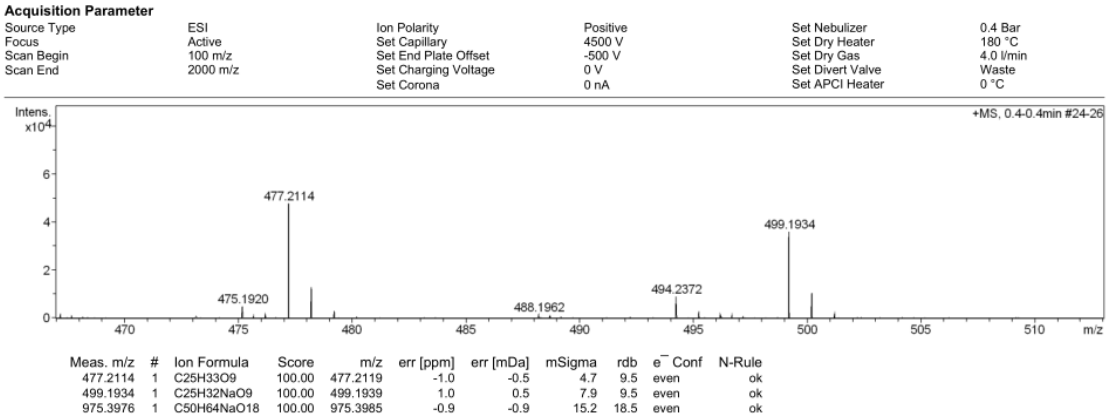


Fig. S28 HRESI-MS spectrum of compound **5**.

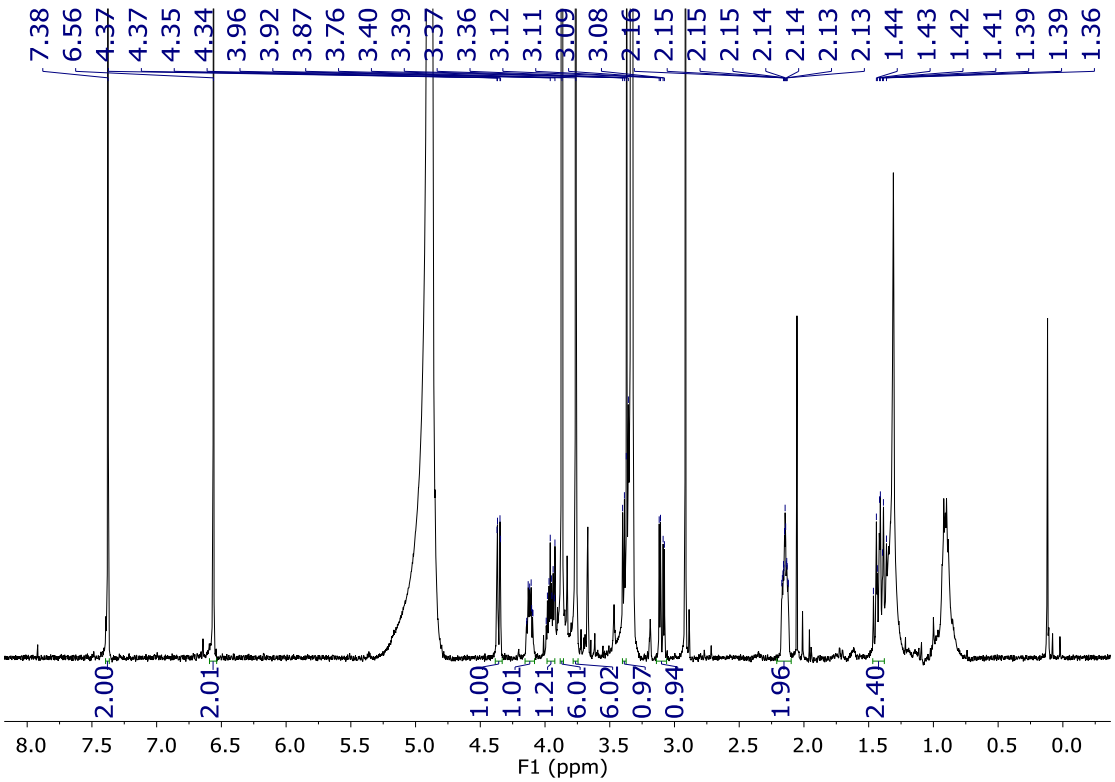


Fig. S29 ^{1}H NMR spectrum of compound **6**.

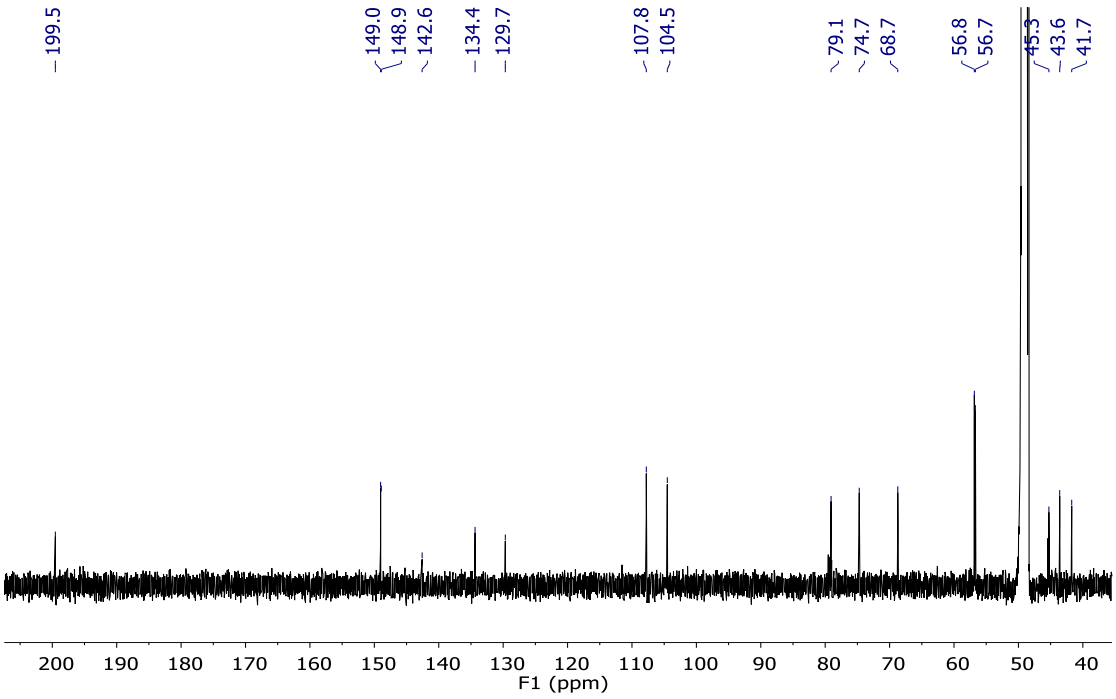


Fig. S30 ^{13}C NMR spectrum of compound **6**.

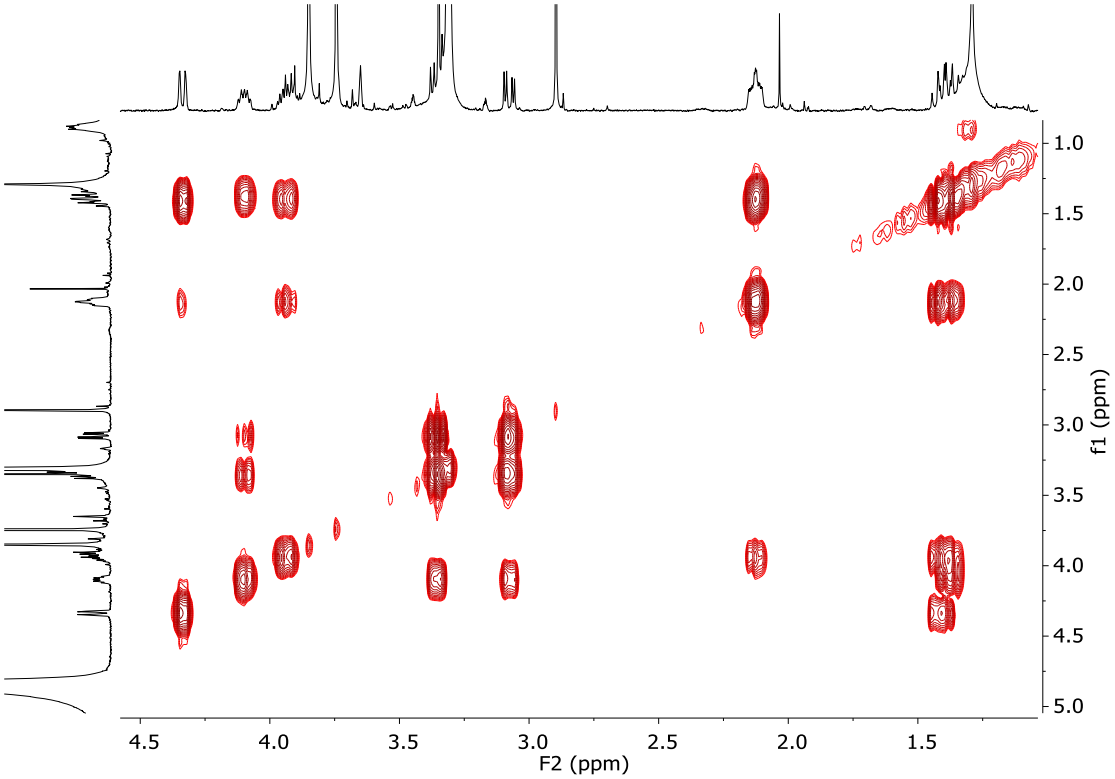


Fig. S31 ^{1}H–^{1}H COSY spectrum of compound **6**.

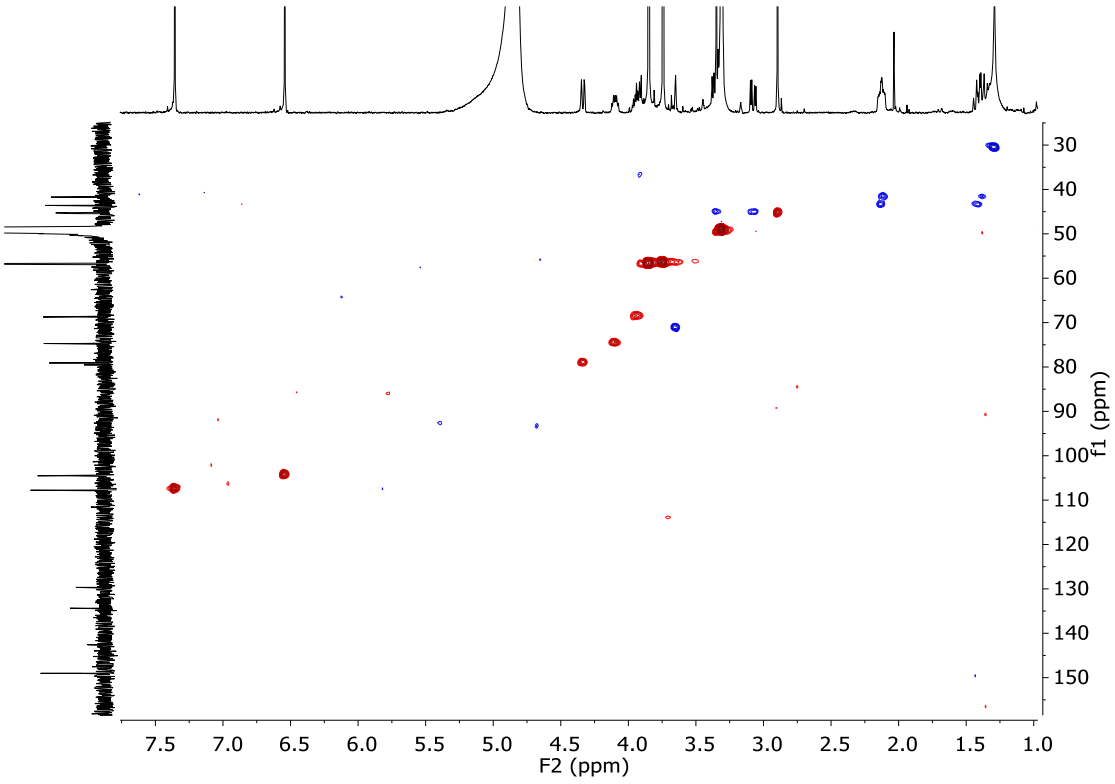


Fig. S32 HSQC spectrum of compound **6**.

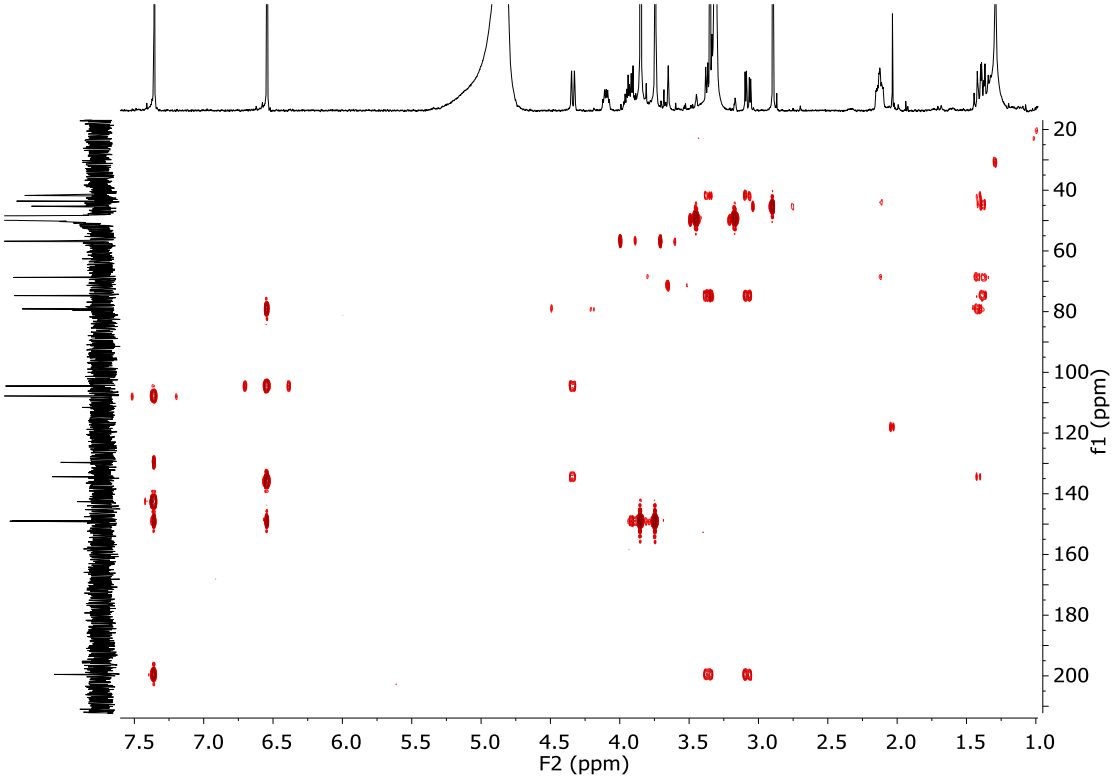


Fig. S33 HMBC spectrum of compound **6**.

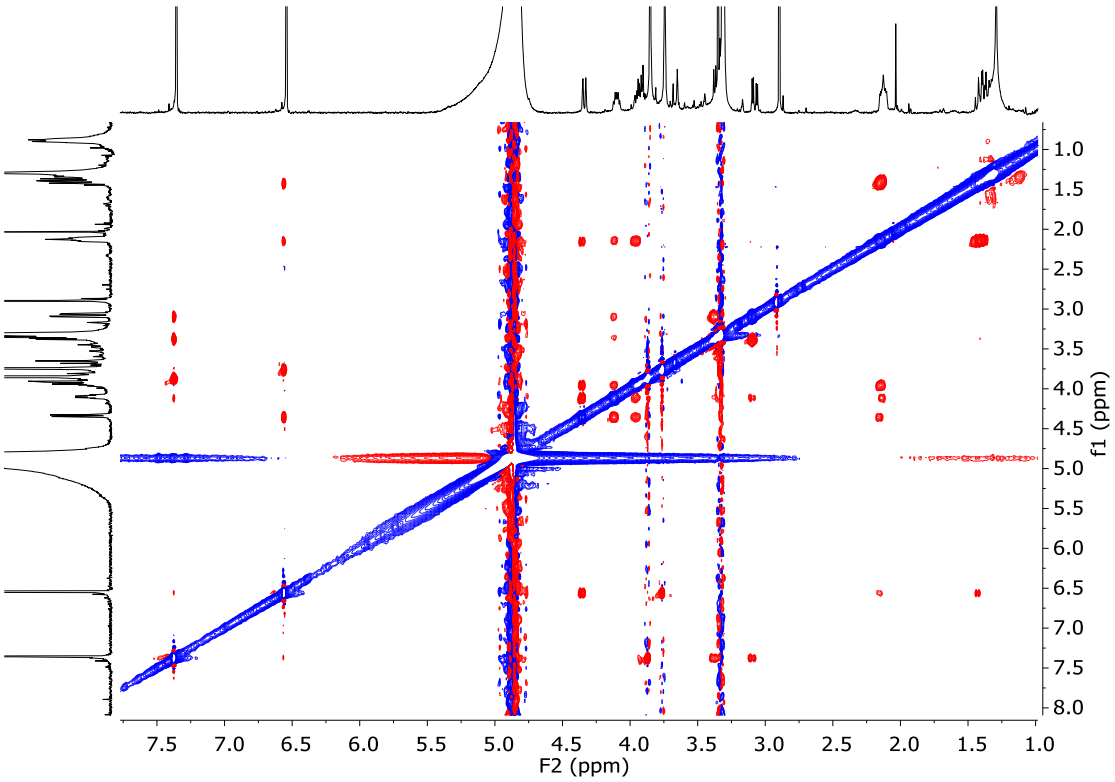
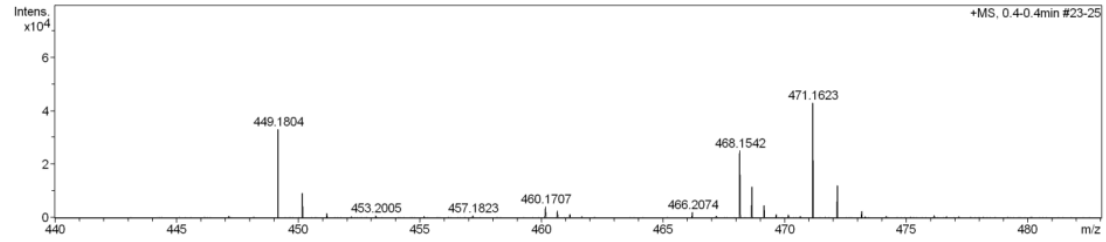


Fig. S34 NOESY spectrum of compound **6**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
449.1804	1	C23H29O9	100.00	449.1806	0.4	0.2	12.3	9.5	even	ok
471.1623	1	C23H28NaO9	100.00	471.1626	0.5	0.2	14.5	9.5	even	ok
897.3545	1	C46H57O18	100.00	897.3539	0.6	0.6	80.6	18.5	even	ok
919.3356	1	C46H56NaO18	100.00	919.3359	0.4	0.3	33.5	18.5	even	ok

Fig. S35 HRESI-MS spectrum of compound **6**.

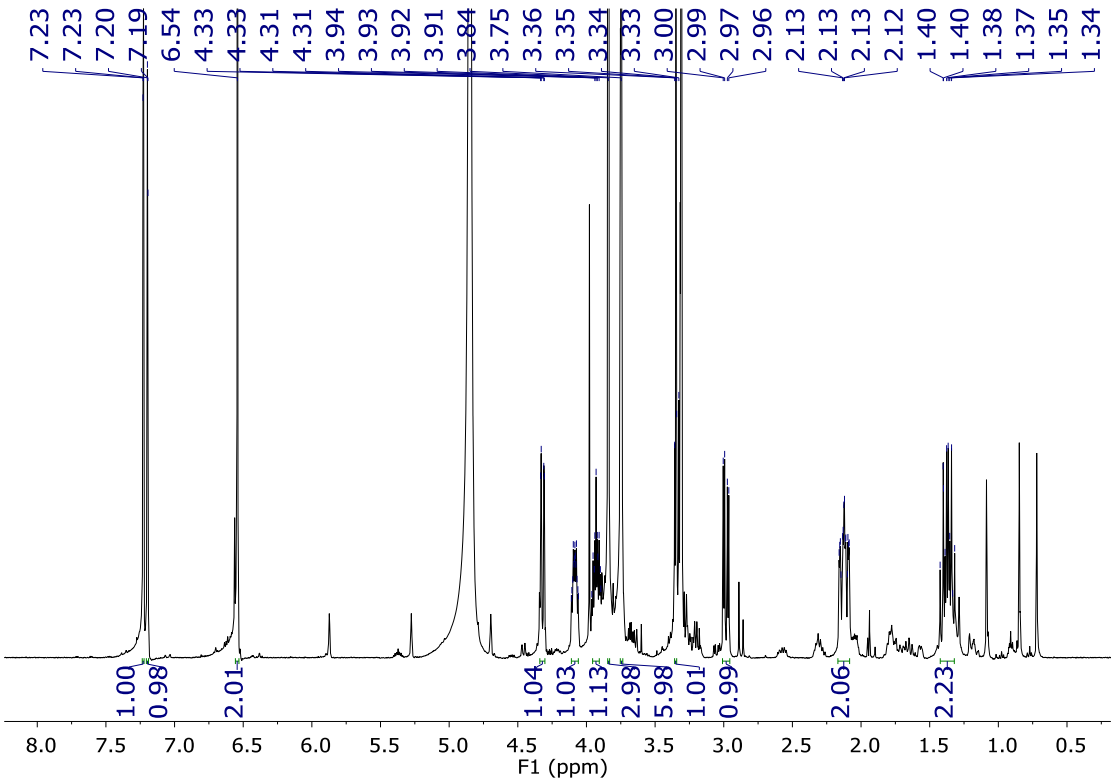


Fig. S36 ^{1}H NMR spectrum of compound **7**.

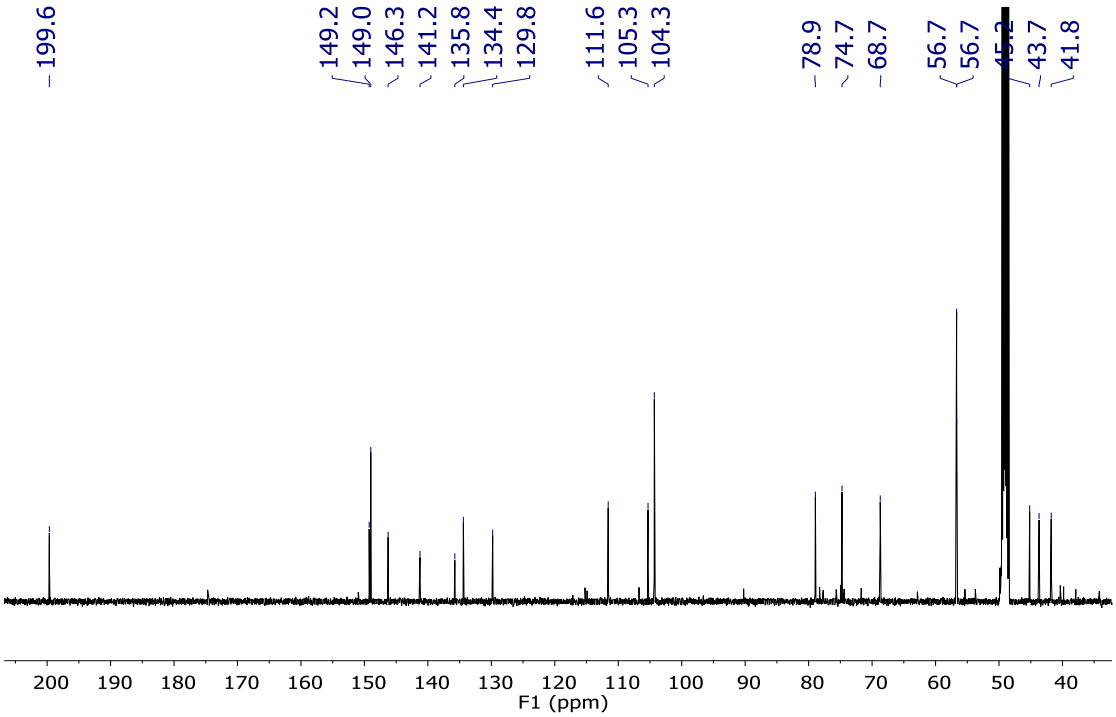


Fig. S37 ^{13}C NMR spectrum of compound **7**.

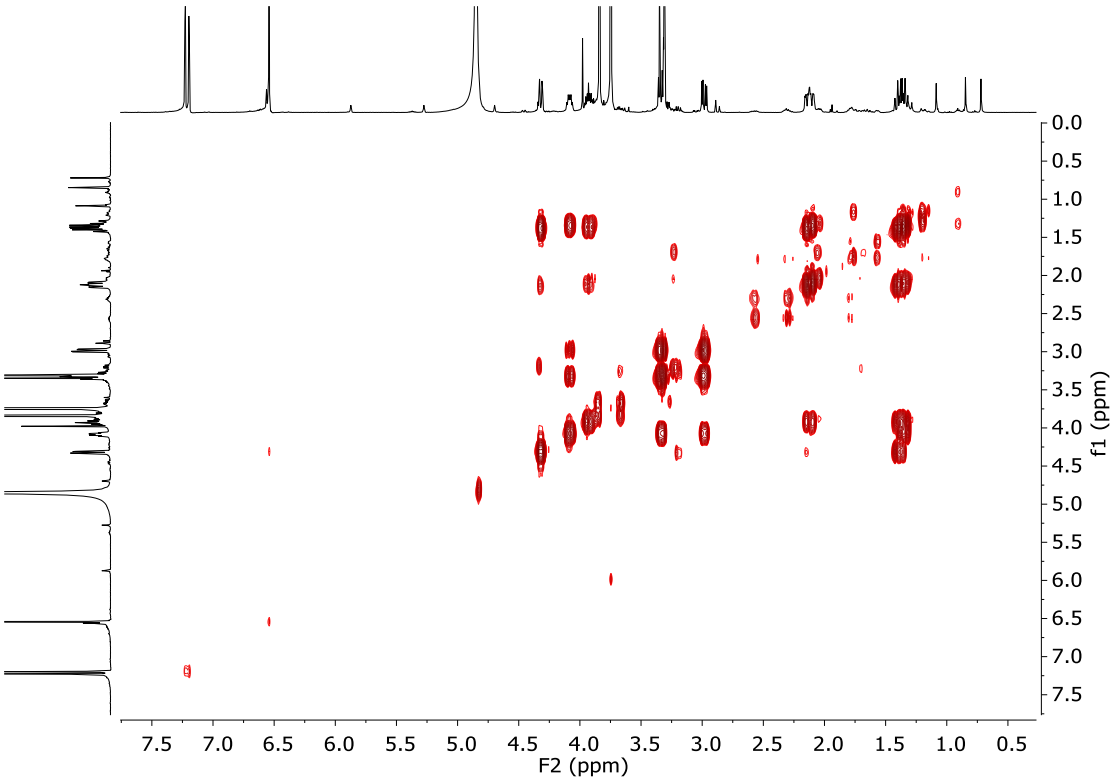


Fig. S38 ^{1}H–^{1}H COSY spectrum of compound **7**.

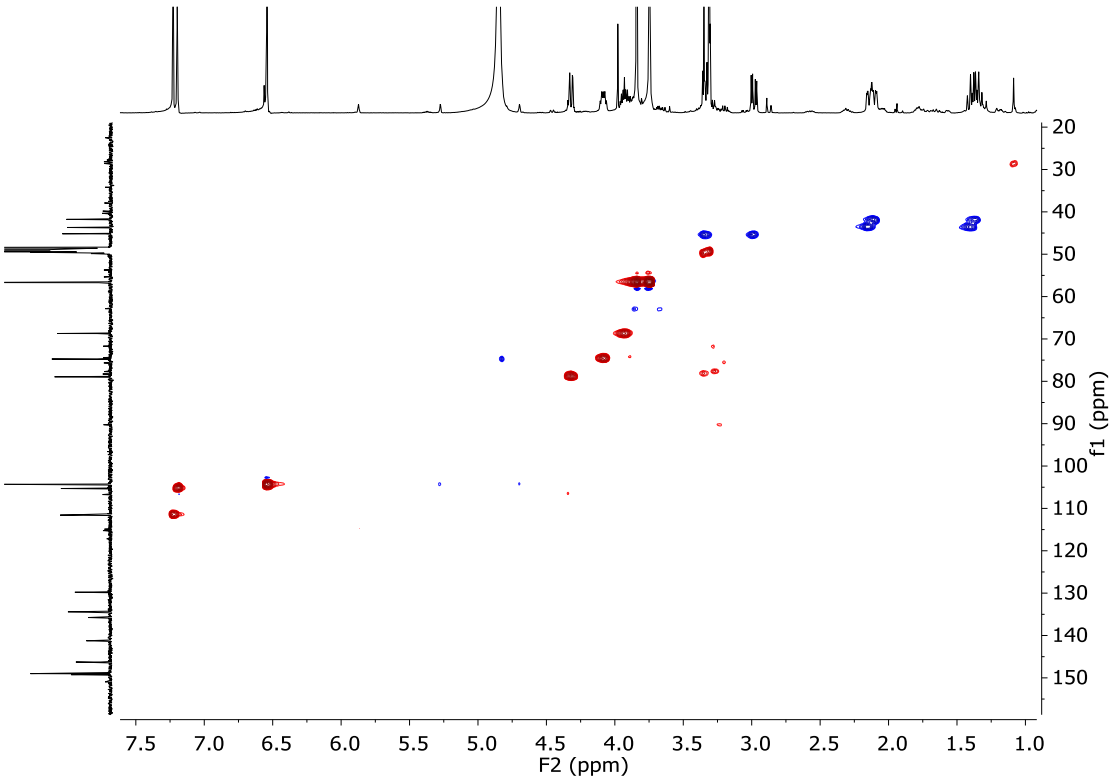


Fig. S39 HSQC spectrum of compound **7**.

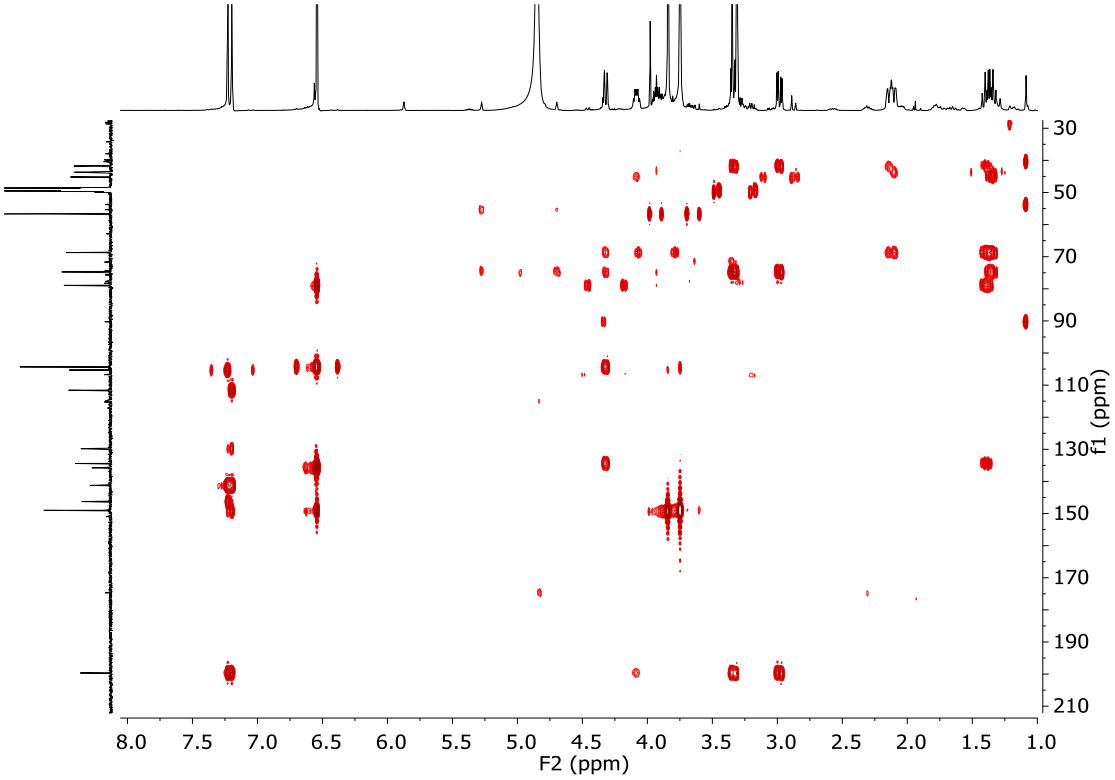


Fig. S40 HMBC spectrum of compound **7**.

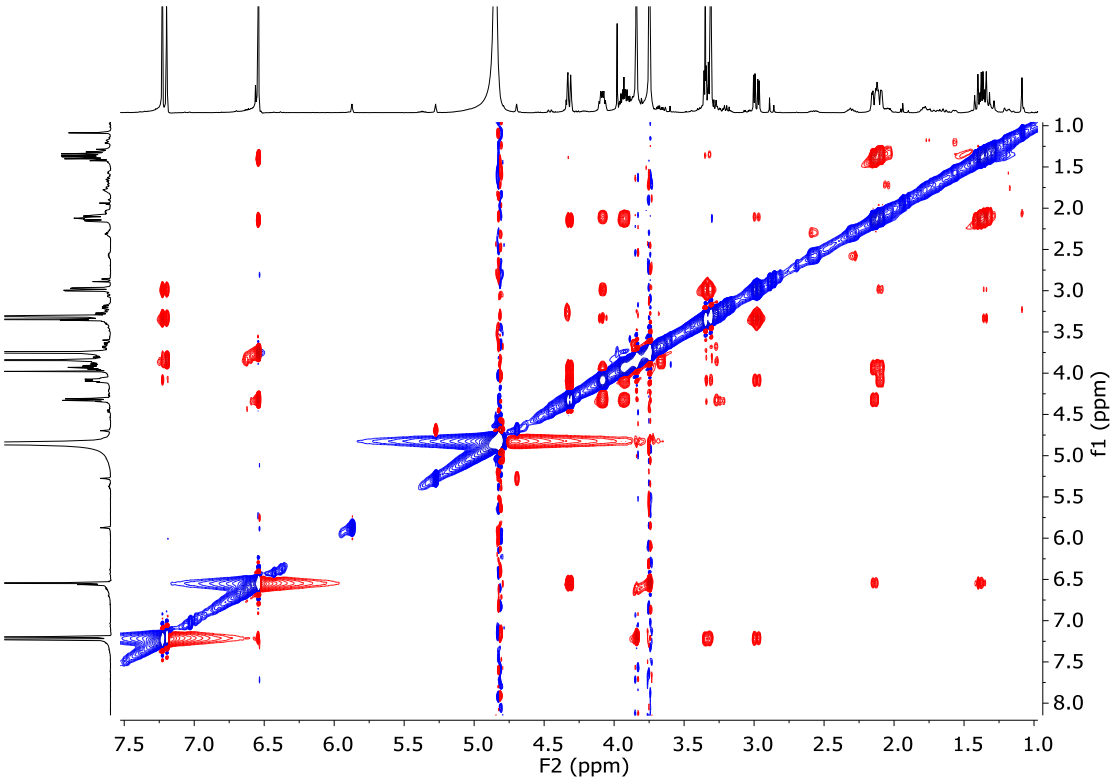
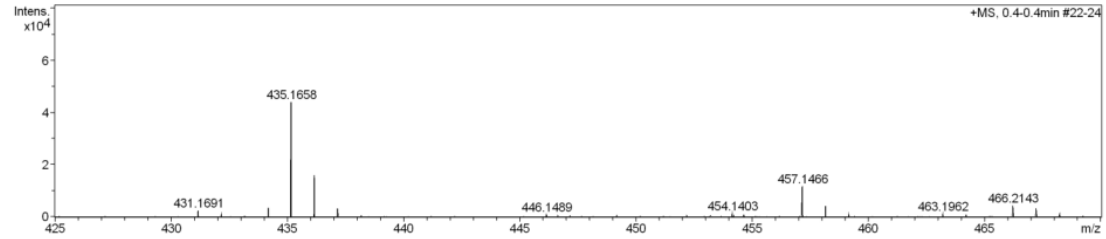


Fig. S41 NOESY spectrum of compound **7**.

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.4 Bar
Focus	Active	Set Capillary	4500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	0 °C



Meas. m/z	#	Ion Formula	Score	m/z	err [ppm]	err [mDa]	mSigma	rdb	e⁻ Conf	N-Rule
435.1658	1	C22H27O9	100.00	435.1650	-1.9	-0.8	63.0	9.5	even	ok
457.1466	1	C22H26NaO9	100.00	457.1469	0.6	0.3	60.1	9.5	even	ok
869.3237	1	C44H53O18	100.00	869.3226	-1.2	-1.1	104.8	18.5	even	ok
891.3044	1	C44H52NaO18	100.00	891.3046	0.2	0.2	95.7	18.5	even	ok

Fig. S42 HRESI-MS spectrum of compound **7**.

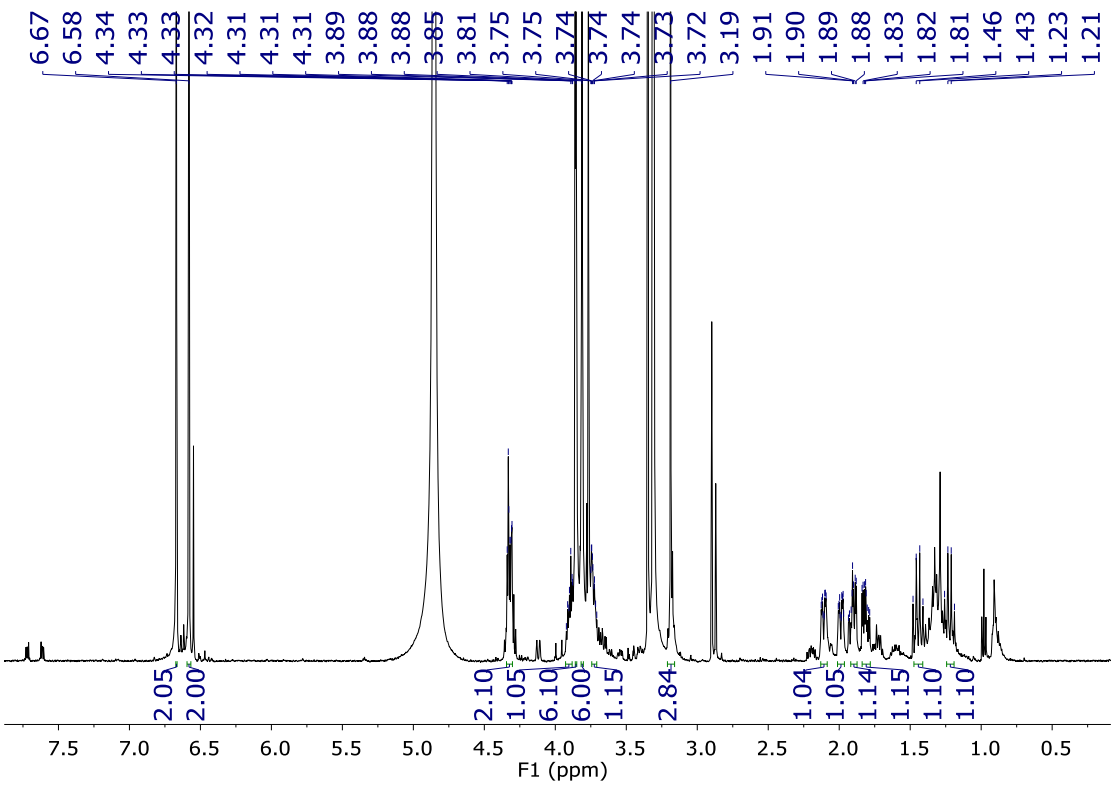


Fig. S43 ^{1}H NMR spectrum of compound **8**.

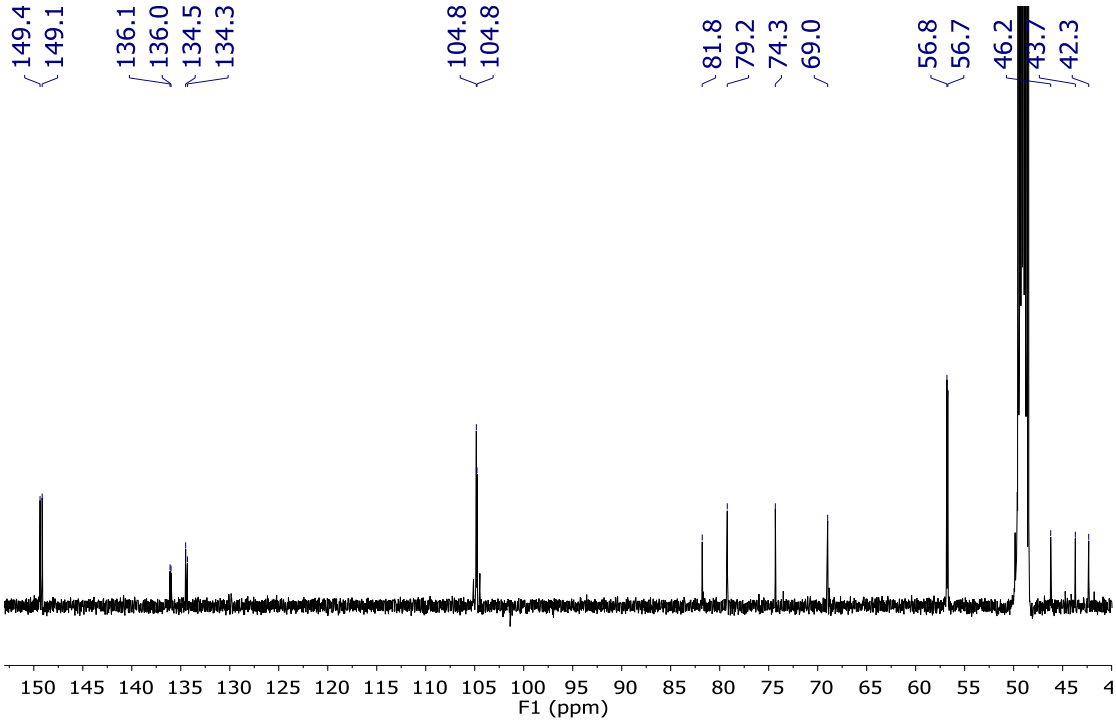


Fig. S44 ^{13}C NMR spectrum of compound **8**.

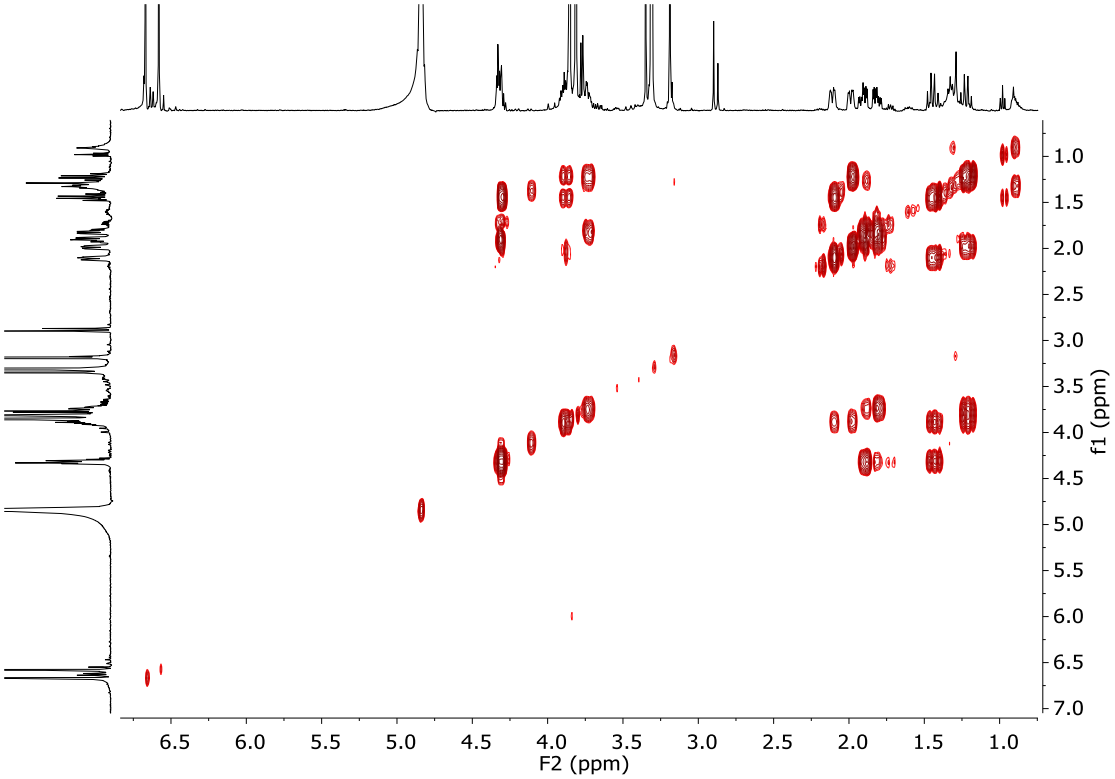


Fig. S45 ^{1}H–^{1}H COSY spectrum of compound **8**.

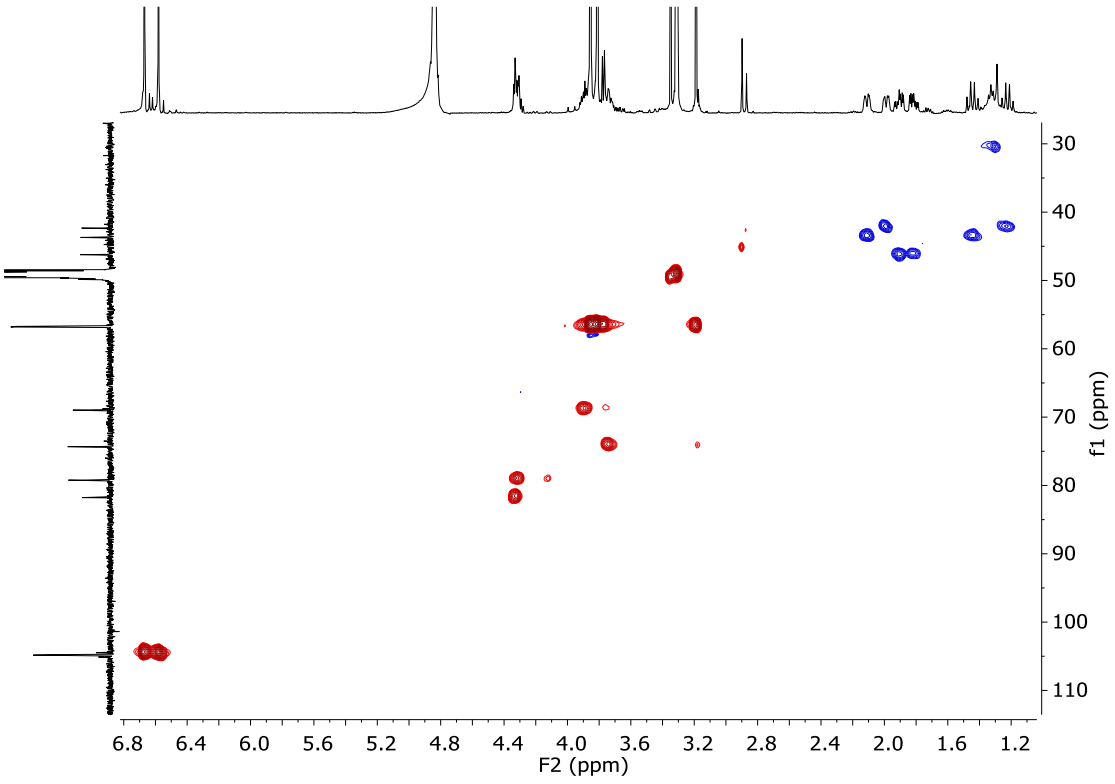


Fig. S46 HSQC spectrum of compound **8**.

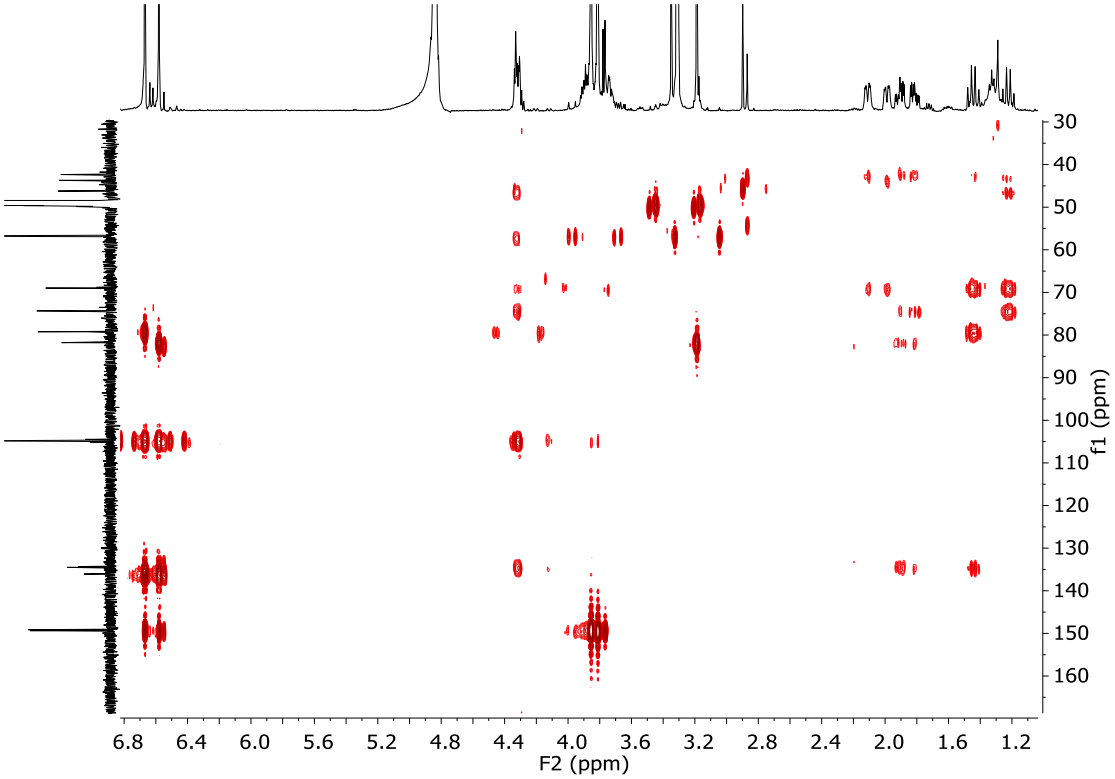


Fig. S47 HMBC spectrum of compound **8**.

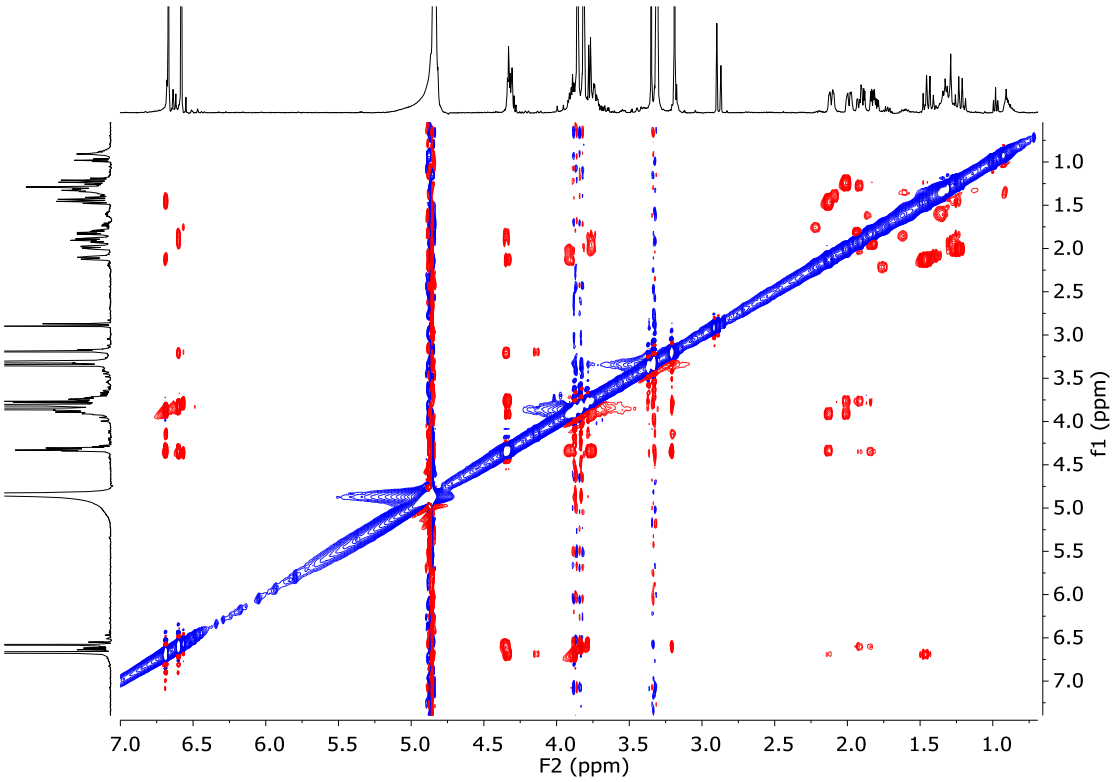


Fig. S48 NOESY spectrum of compound **8**.

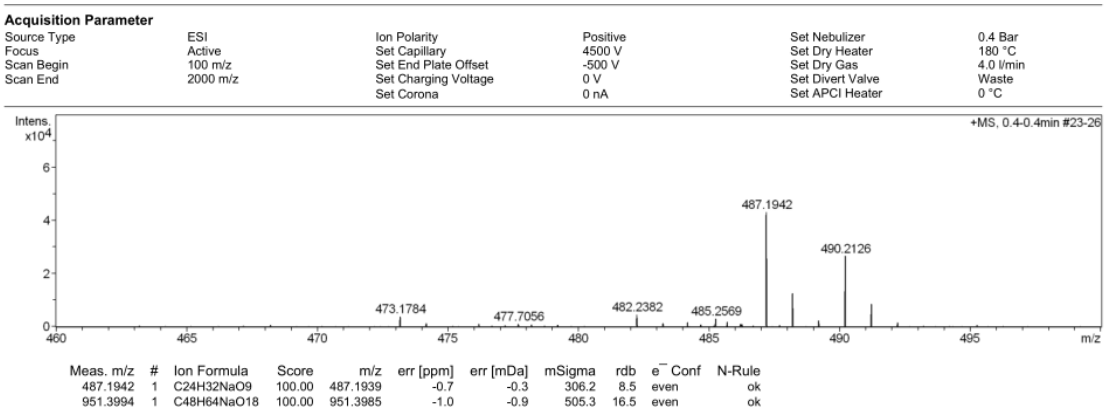


Fig. S49 HRESI-MS spectrum of compound **8**.