

Supplementary Information file 2

LC-MS/MS and high-spatial single-cell MSI reveal selective downregulation of PC(16:0_16:0) and PC(18:0_18:1) due to mPGES-1 knockdown in hormone-resistant prostate cancer cell line

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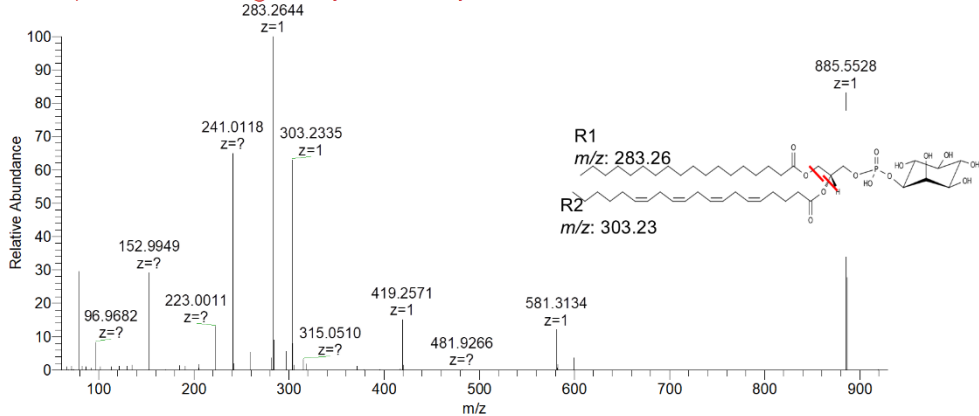
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Lipid molecules obtained in high spatial MALDI-MSI analysis were annotated using LC-MS/MS data analyzed by Qual Browser Software.

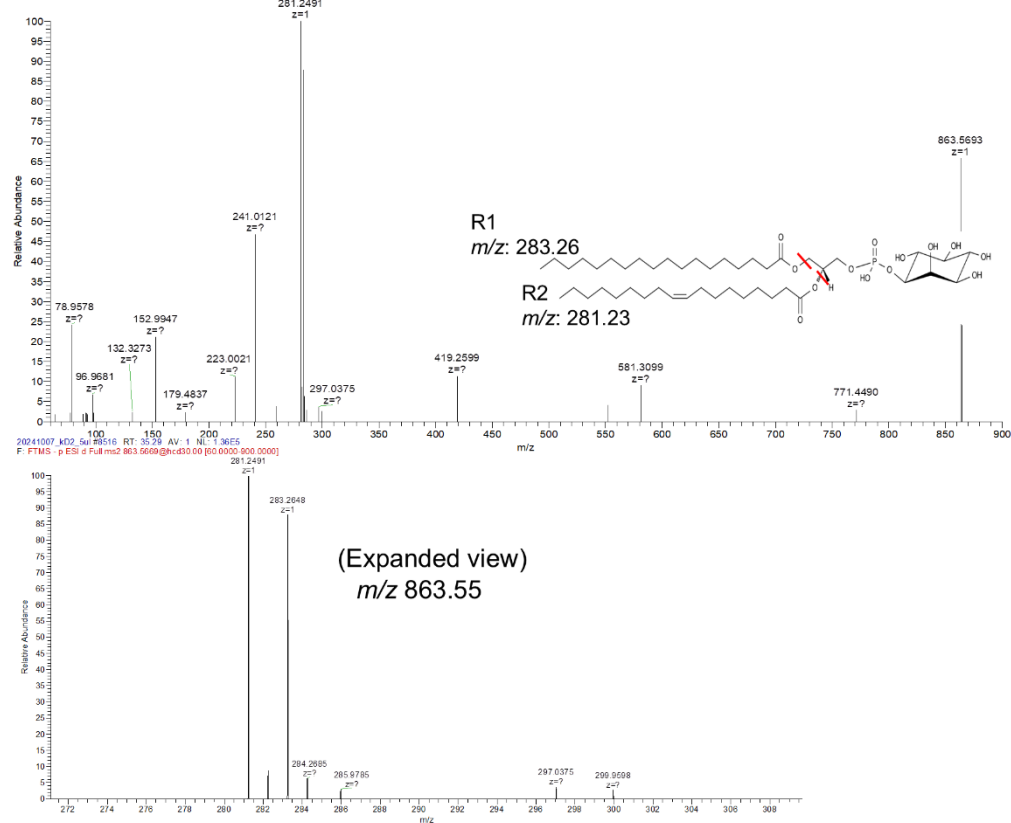
a MS/MS of PI (18:0_20:4 or 38:4) at m/z 885.55

20241007_KD2_5ul#7772-8124 RT: 32.95-33.70 AV: 3 NL: 5.41E5
F: FTMS - p ESI d Full ms2 885.5517@hcd30.00 [61.3333-920.0000]



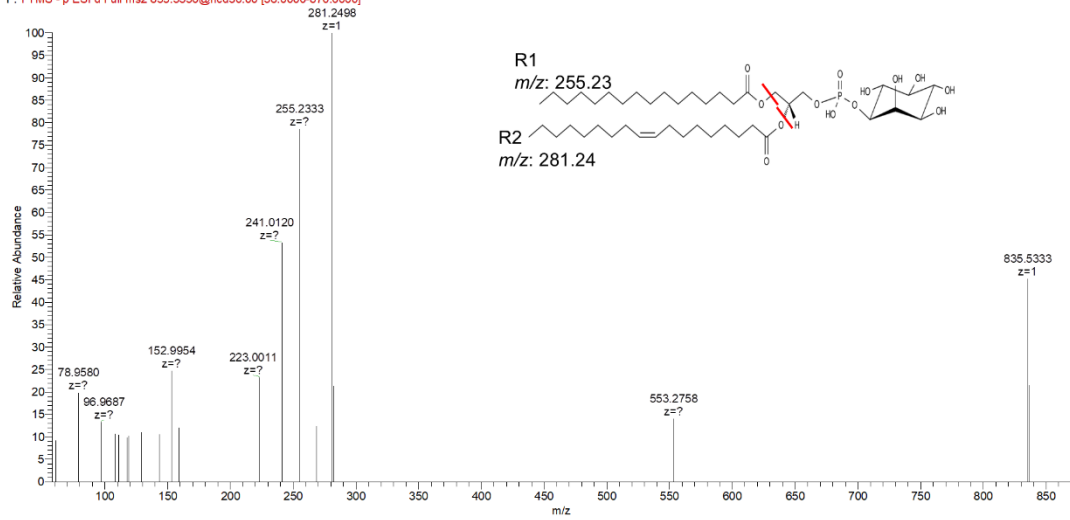
b MS/MS of PI (18:0_18:1 or 36:1) m/z 863.55

20241007_KD2_5ul#8503 RT: 35.29 AV: 1 NL: 1.36E5
F: FTMS - p ESI d Full ms2 863.5669@hcd30.00 [60.0000-900.0000]



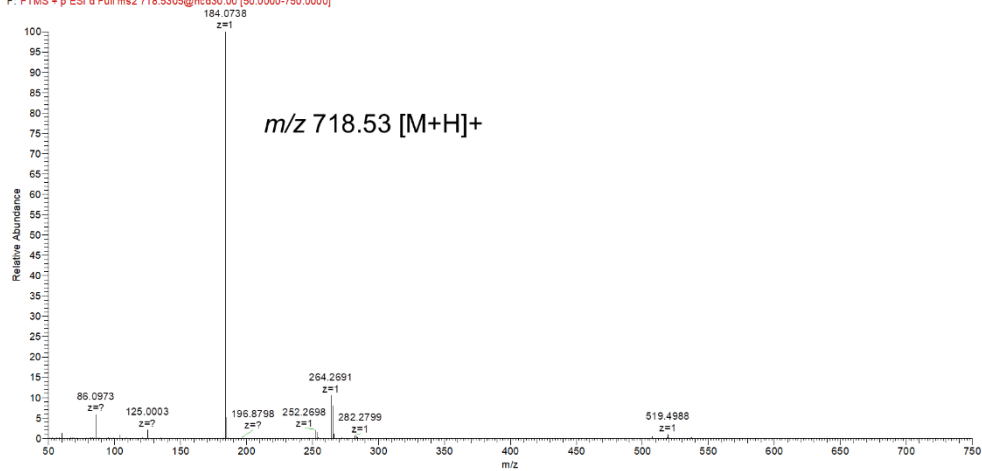
c MS/MS of PI (16:0_18:1 or 34:1) m/z 835.53

20241007_kD2_5ul #7685 RT: 32.41 AV: 1 NL: 2.74E4
F: FTMS -p ESI d Full ms2 835.5350@hcd30.00 [58.0000-870.0000]

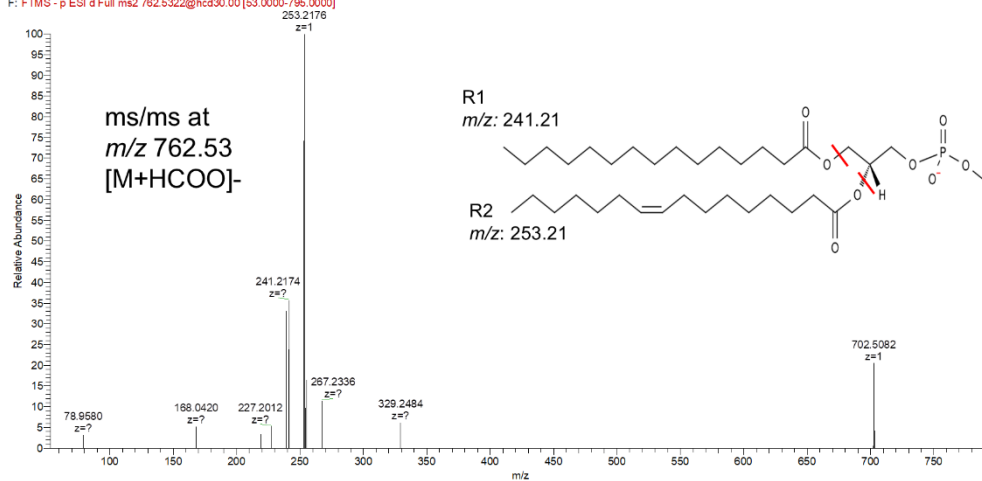


d MS/MS of PC (15:0_16:1 or 31:1) m/z 718.53 $[M+H]^+$

20241007_kD2_5ul#7557 RT: 31.99 AV: 1 NL: 7.87E6
F: FTMS + p ESI d Full ms2 718.5305@hcd30.00 [50.0000-750.0000]

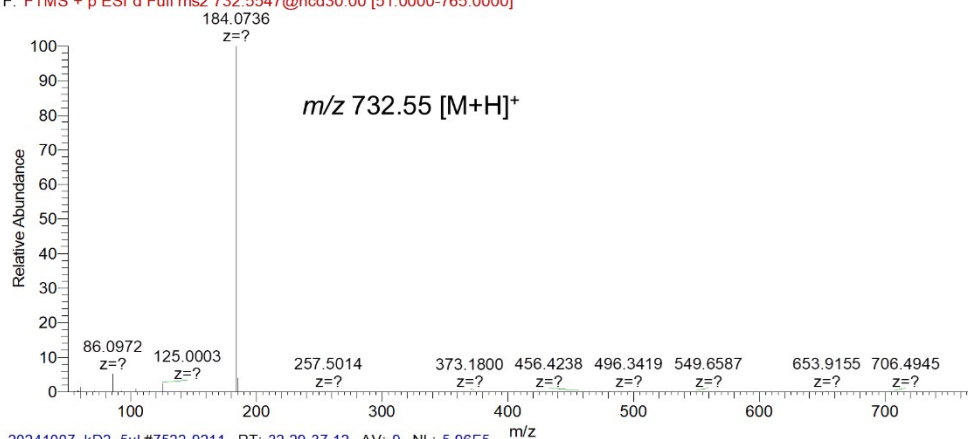


20241007_kD2_5ul#7480 RT: 31.89 AV: 1 NL: 9.01E4
F: FTMS - p ESI d Full ms2 762.5322@hcd30.00 [53.0000-795.0000]

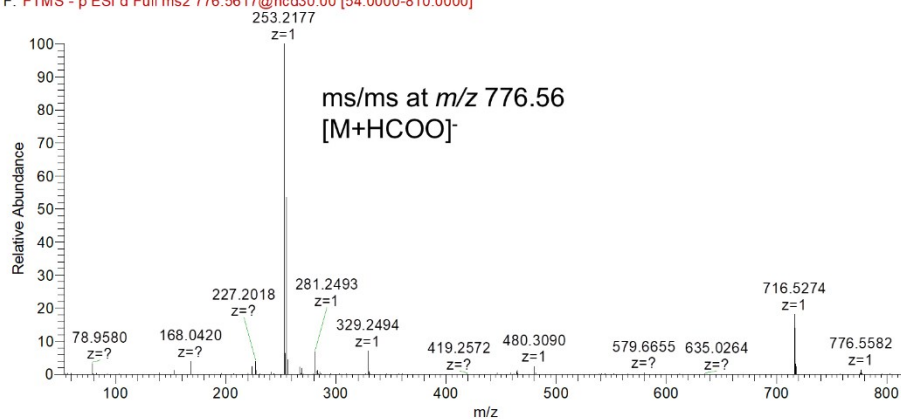


e MS/MS of PC (16:0_16:1 or 32:1) m/z 732.55 $[M+H]^+$

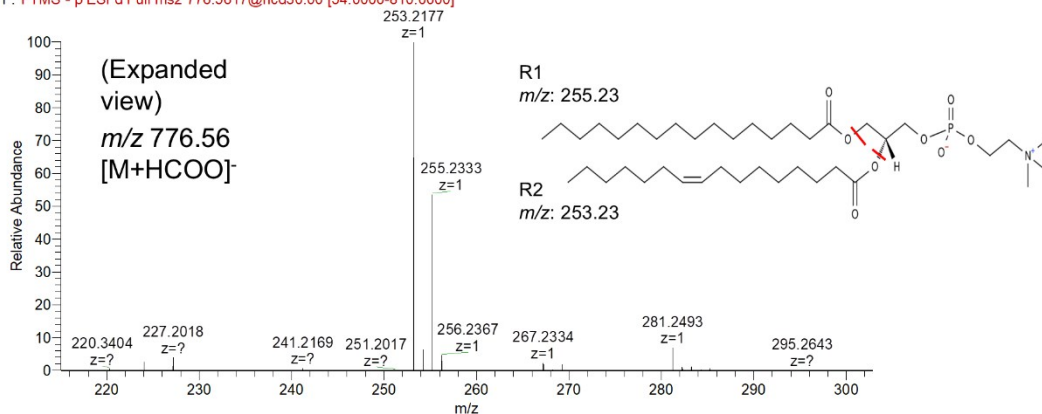
20241007_kD2_5ul #7324-8003 RT: 32.43-33.37 AV: 4 NL: 3.37E8
F: FTMS + p ESI d Full ms2 732.5547@hcd30.00 [51.0000-765.0000]



20241007_kD2_5ul #7522-9211 RT: 32.29-37.12 AV: 9 NL: 5.96E5
F: FTMS - p ESI d Full ms2 776.5617@hcd30.00 [54.0000-810.0000]

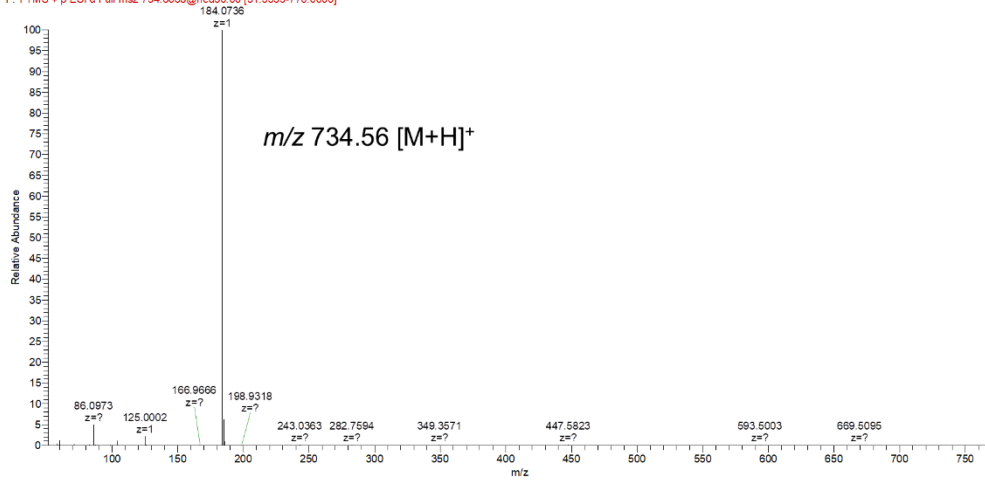


20241007_kD2_5ul #7522-9211 RT: 32.29-37.12 AV: 9 NL: 5.96E5
F: FTMS - p ESI d Full ms2 776.5617@hcd30.00 [54.0000-810.0000]

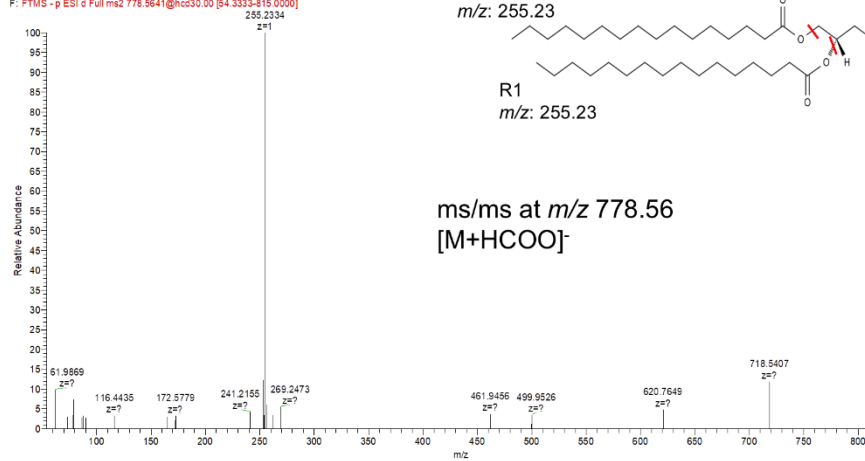


f MS/MS of PC (16:0_16:0 or 32:0) m/z 734.56 $[M+H]^+$

20240924_KD_cell_x10_5ui #7809 RT: 34.25 AV: 1 NL: 7.23E8
F: FTMS -p ESI d Full ms2 734.6069@hcd30.00 [51.3333-770.0000]



20240924_KD_cell_x10_5ui #7809 RT: 34.27 AV: 1 NL: 9.34E4
F: FTMS -p ESI d Full ms2 778.5641@hcd30.00 [54.3333-815.0000]



R1

m/z : 255.23

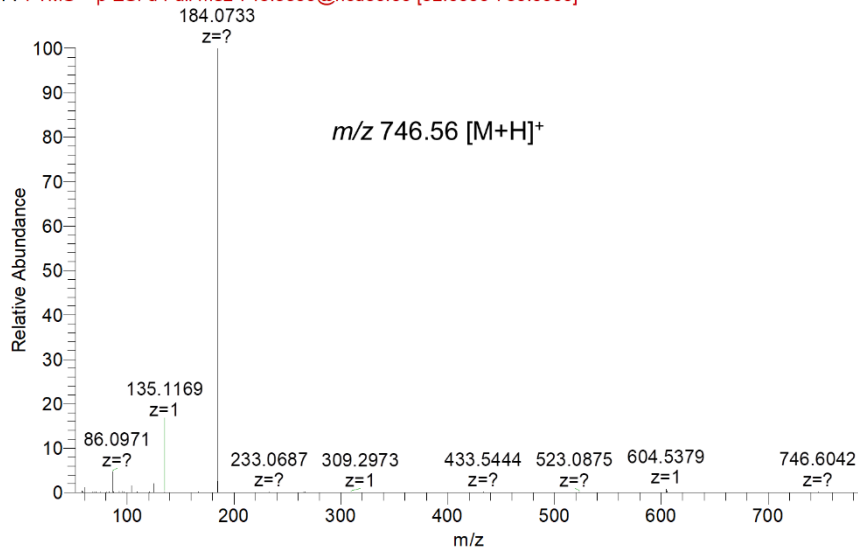
R1

m/z : 255.23

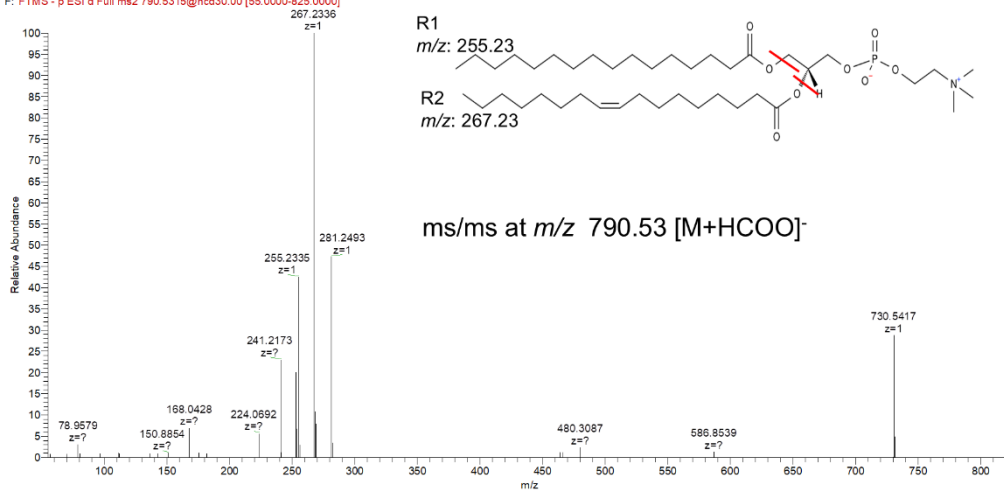
ms/ms at m/z 778.56
 $[M+HCOO]^-$

g MS/MS of PC (16:0_17:1 or 33:1) m/z 746.57 $[M+H]^+$

20250515_NC1_x5_2ul #7486-7765 RT: 35.87-36.84 AV: 3 NL: 4.61E7
F: FTMS + p ESI d Full ms2 746.5590@hcd30.00 [52.0000-780.0000]

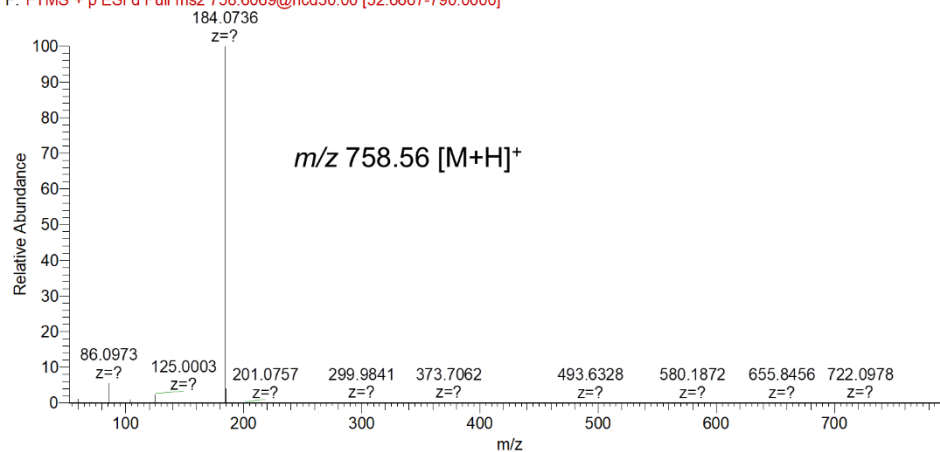


20240924_KD_cell_x10_5ul #7680 RT: 33.79 AV: 1 NL: 8.98E5
F: FTMS + p ESI d Full ms2 790.5315@hcd30.00 [55.0000-825.0000]

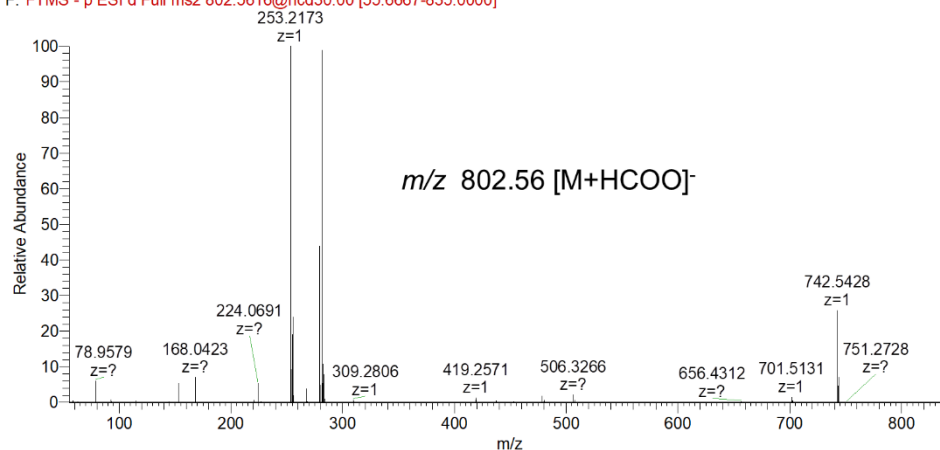


h MS/MS of PC (16:1_18:1 or 34:2) m/z 758.56 $[M+H]^+$

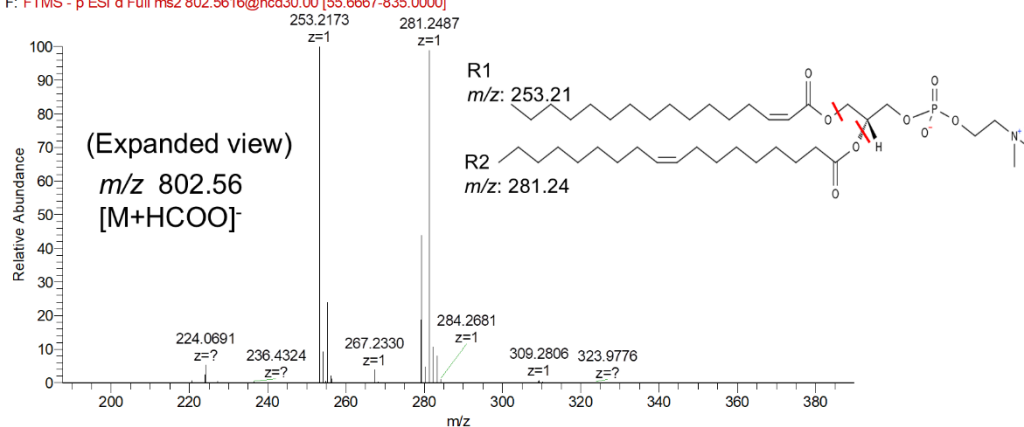
20241007 WT2 5ul #7767-8739 RT: 33.02-35.43 AV: 6 NL: 7.91E7
F: FTMS + p ESI d Full ms2 758.6069@hcd30.00 [52.6667-790.0000]



20241007 WT2 5ul #7767-8739 RT: 32.66-35.41 AV: 7 NL: 4.48E5
F: FTMS - p ESI d Full ms2 802.5616@hcd30.00 [55.6667-835.0000]

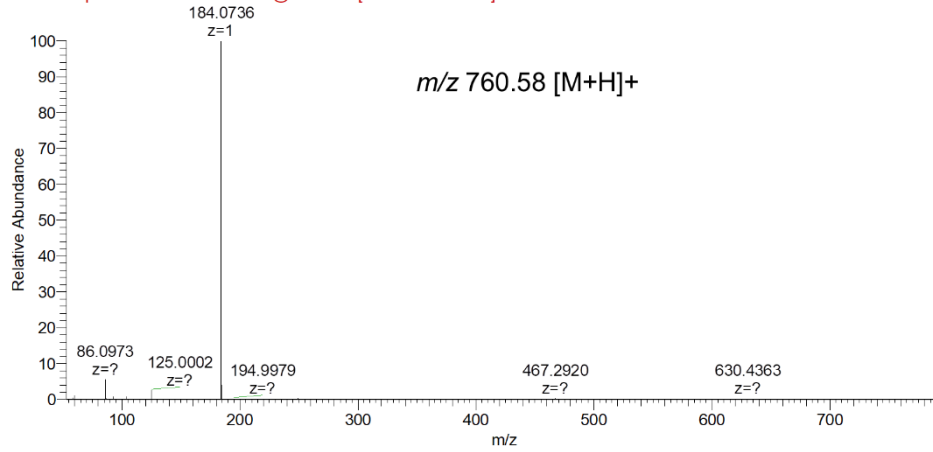


20241007_WT2_5ul #7767-8739 RT: 32.66-35.41 AV: 7 NL: 4.48E5
F: FTMS - p ESI d Full ms2 802.5616@hcd30.00 [55.6667-835.0000]

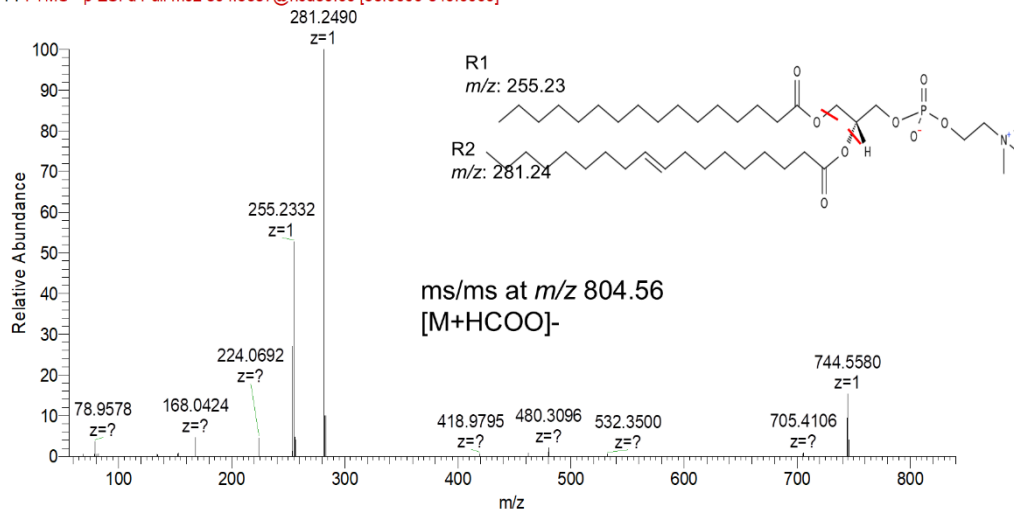


i MS/MS of PC (16:0_18:1 or 34:1) at m/z 760.58 $[M+H]^+$

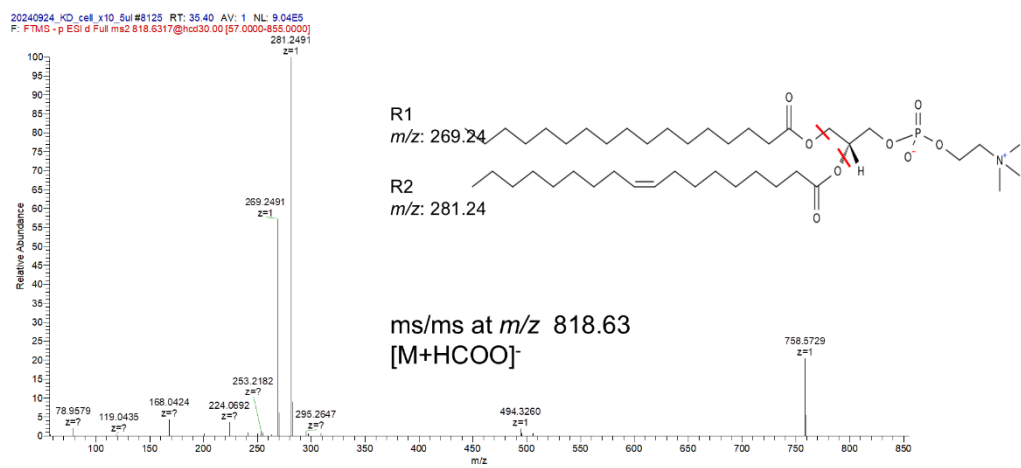
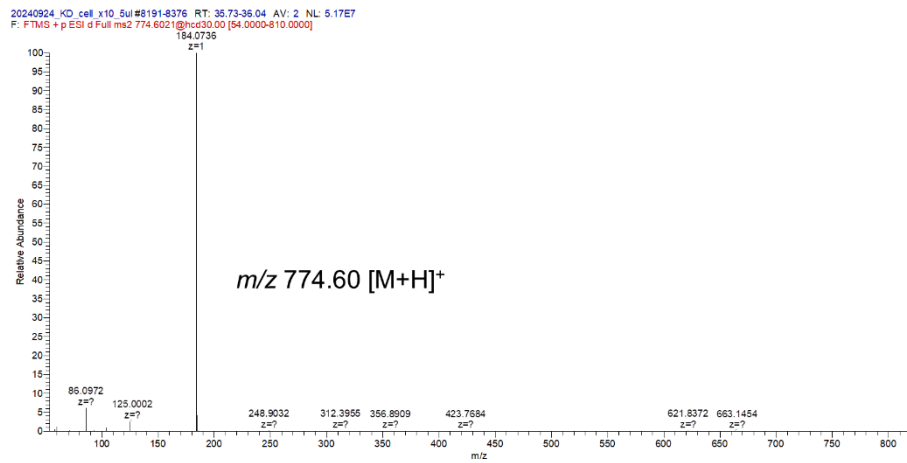
20241007_kD2_5ul #8575 RT: 35.30 AV: 1 NL: 1.60E8
F: FTMS + p ESI d Full ms2 760.5854@hcd30.00 [53.0000-795.0000]



20241007_kD2_5ul #8569 RT: 35.28 AV: 1 NL: 1.12E6
F: FTMS - p ESI d Full ms2 804.5687@hcd30.00 [56.0000-840.0000]

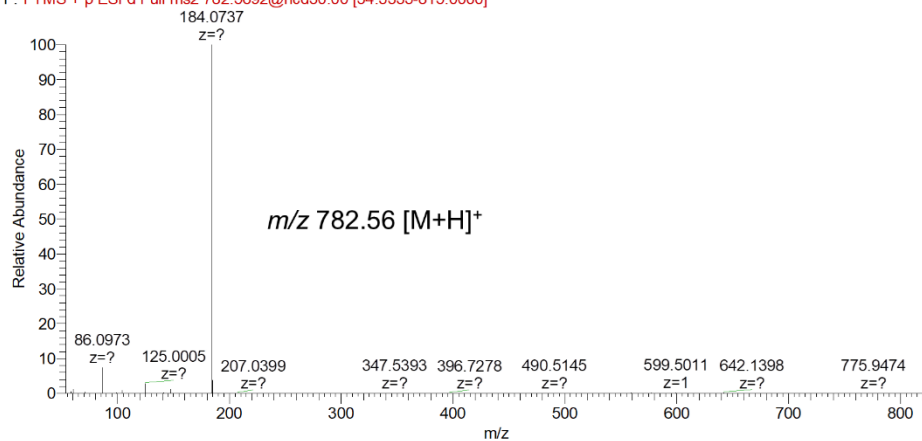


j MS/MS of PC (17:0_18:1 or 35:1) at m/z 774.60 $[M+H]^+$

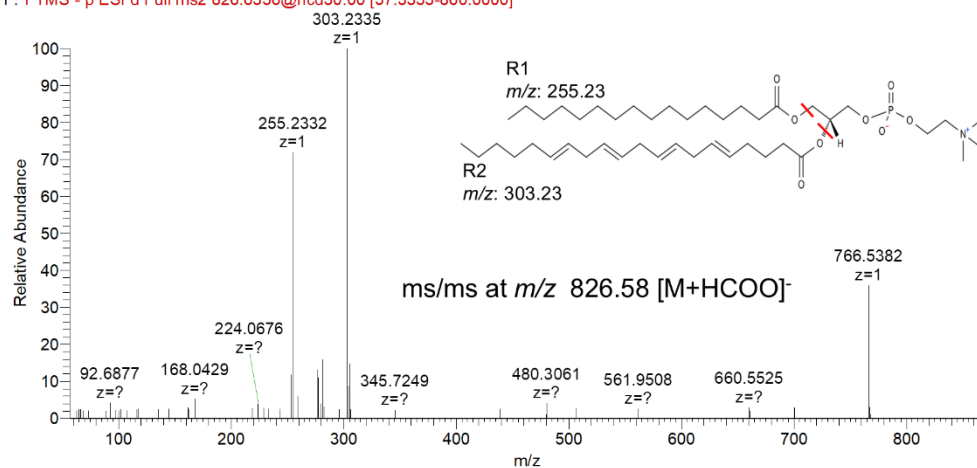


k MS/MS of PC (16:0_20:4 or 36:4) m/z 782.56 $[M+H]^+$

20241007_VT2_5ul #7767-8739 RT: 32.75-35.19 AV: 5 NL: 1.25E7
F: FTMS + p ESI d Full ms2 782.5692@hcd30.00 [54.3333-815.0000]



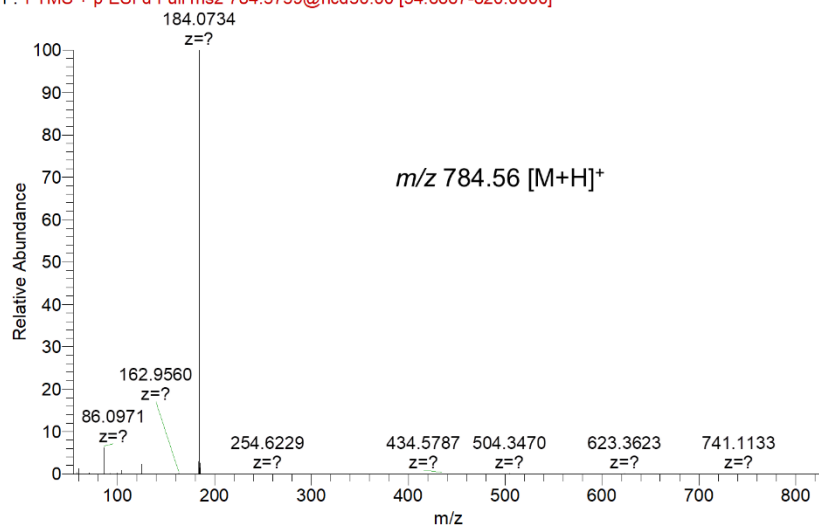
20241007_VT2_5ul #7767-8739 RT: 32.65-33.24 AV: 3 NL: 4.11E4
F: FTMS - p ESI d Full ms2 826.6356@hcd30.00 [57.3333-860.0000]



I MS/MS of PC (16:0_20:3 or 36:3) m/z 784.56 $[M+H]^+$

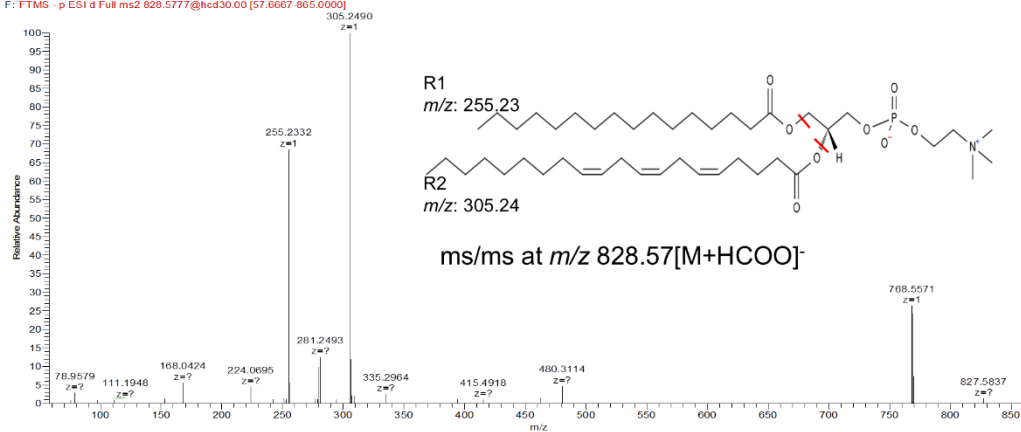
20250515_NC1_x5_2ul #6546-7476 RT: 32.11-34.62 AV: 6 NL: 7.85E6

F: FTMS + p ESI d Full ms2 784.5759@hcd30.00 [54.6667-820.0000]



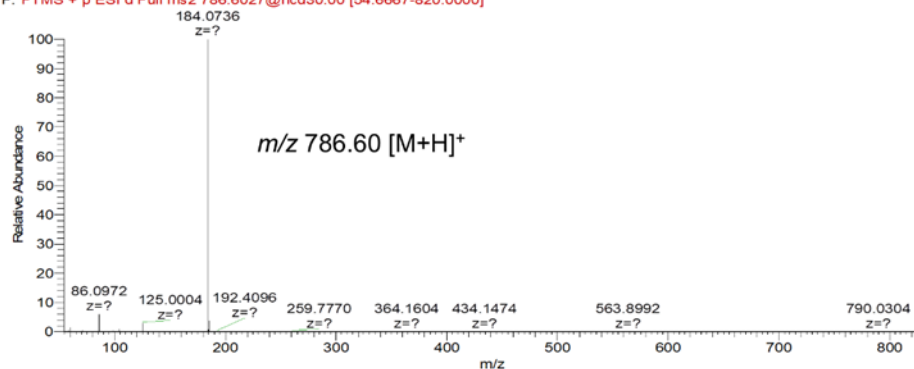
20241007_KD3_5ul #8271 RT: 34.52 AV: 1 NL: 3.29E5

F: FTMS - p ESI d Full ms2 828.5777@hcd30.00 [57.6667-865.0000]

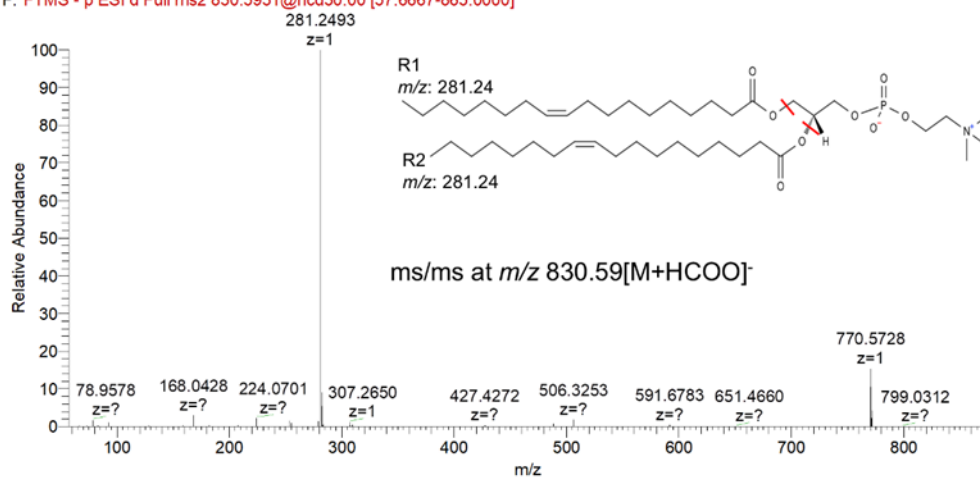


m MS/MS of PC (18:1_18:1 or 36:2) m/z 786.60 $[M+H]^+$

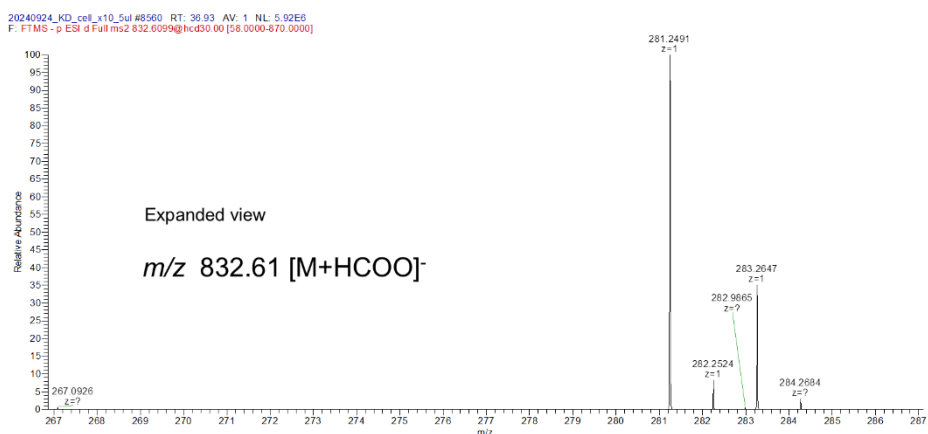
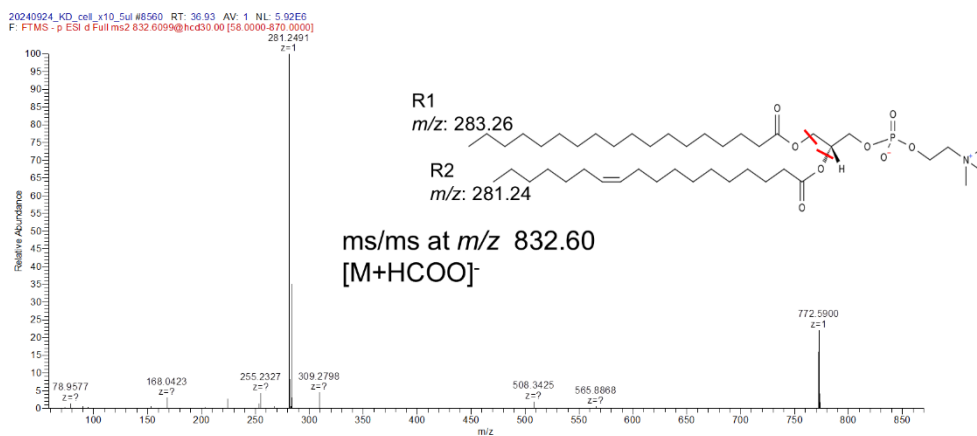
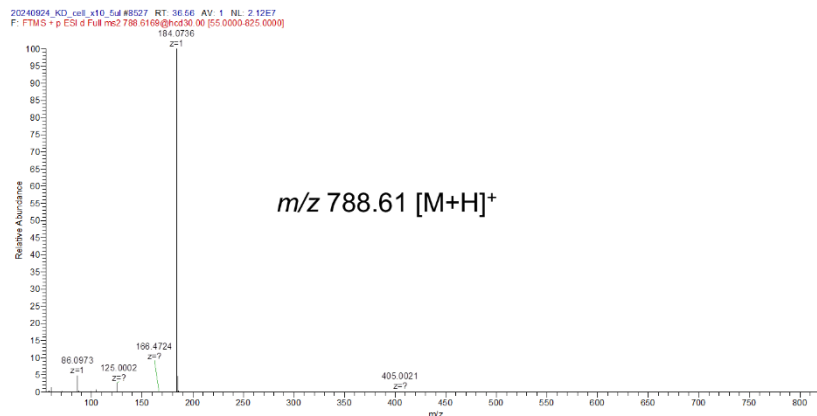
20241007_KD2_5ul #8357-8899 RT: 35.07-36.31 AV: 5 NL: 4.20E8
F: FTMS + p ESI d Full ms2 786.6027@hcd30.00 [54.6667-820.0000]



20241007_KD2_5ul #8521-9521 RT: 35.13-38.41 AV: 6 NL: 4.02E6
F: FTMS - p ESI d Full ms2 830.5931@hcd30.00 [57.6667-865.0000]

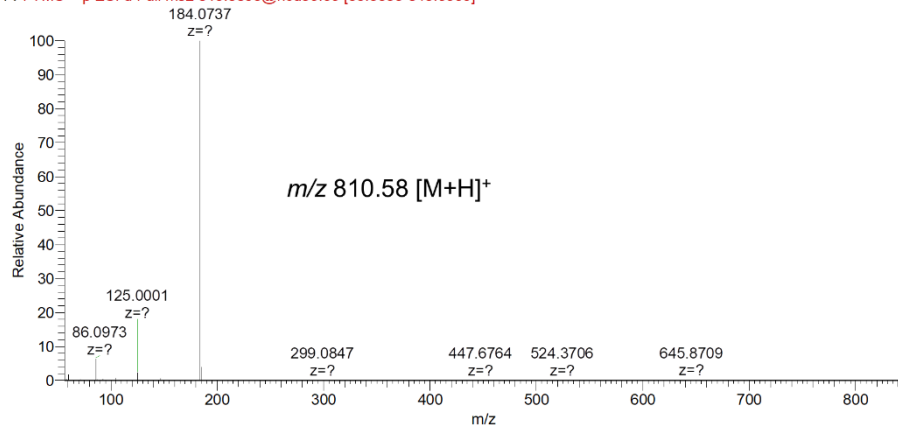


n MS/MS of PC PC(18:0_18:1 or 36:1) m/z 788.61 $[M+H]^+$



o MS/MS of PC PC(18:0_20:4 or 38:4) m/z 810.60 $[M+H]^+$

20241007_WT2_5ul #8649 RT: 35.42 AV: 1 NL: 1.72E7
F: FTMS + p ESI d Full ms2 810.5895@hcd30.00 [56.3333-845.0000]



20241007_WT2_5ul #8683 RT: 35.53 AV: 1 NL: 3.09E4
F: FTMS - p ESI d Full ms2 854.6747@hcd30.00 [59.3333-890.0000]

