Supplementary Materials

Short-Term Stability of Serum and Liver Extracts for Untargeted Metabolomics and Lipidomics

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Figure S1. Examples of total ion chromatograms for human serum extracts acquired using LC-MS methods: (**a**) RPLC-ESI(+) lipidomics (ACQUITY Premier BEH C18 column); (**b**) RPLC-ESI(–) lipidomics (ACQUITY Premier BEH C18 column); (**c**) HILIC-ESI(+) metabolomics (BEH Amide column); (**d**) HILIC-ESI(–) metabolomics (ACQUITY Premier BEH Amide column); (**e**) RPLC-ESI(–) metabolomics (ACQUITY Premier HSS T3 column).

Figure S2. Examples of total ion chromatograms for mouse liver extracts acquired using LC-MS methods: (**a**) RPLC-ESI(+) lipidomics (ACQUITY Premier BEH C18 column); (**b**) RPLC-ESI(–) lipidomics (ACQUITY Premier BEH C18 column); (**c**) HILIC-ESI(+) metabolomics (BEH Amide column); (**d**) HILIC-ESI(–) metabolomics (ACQUITY Premier BEH Amide column); (**e**) RPLC-ESI(–) metabolomics (ACQUITY Premier HSS T3 column).

Figure S3. Examples of annotated lipids containing odd-chain fatty acids using MS/MS and MS-DIAL software

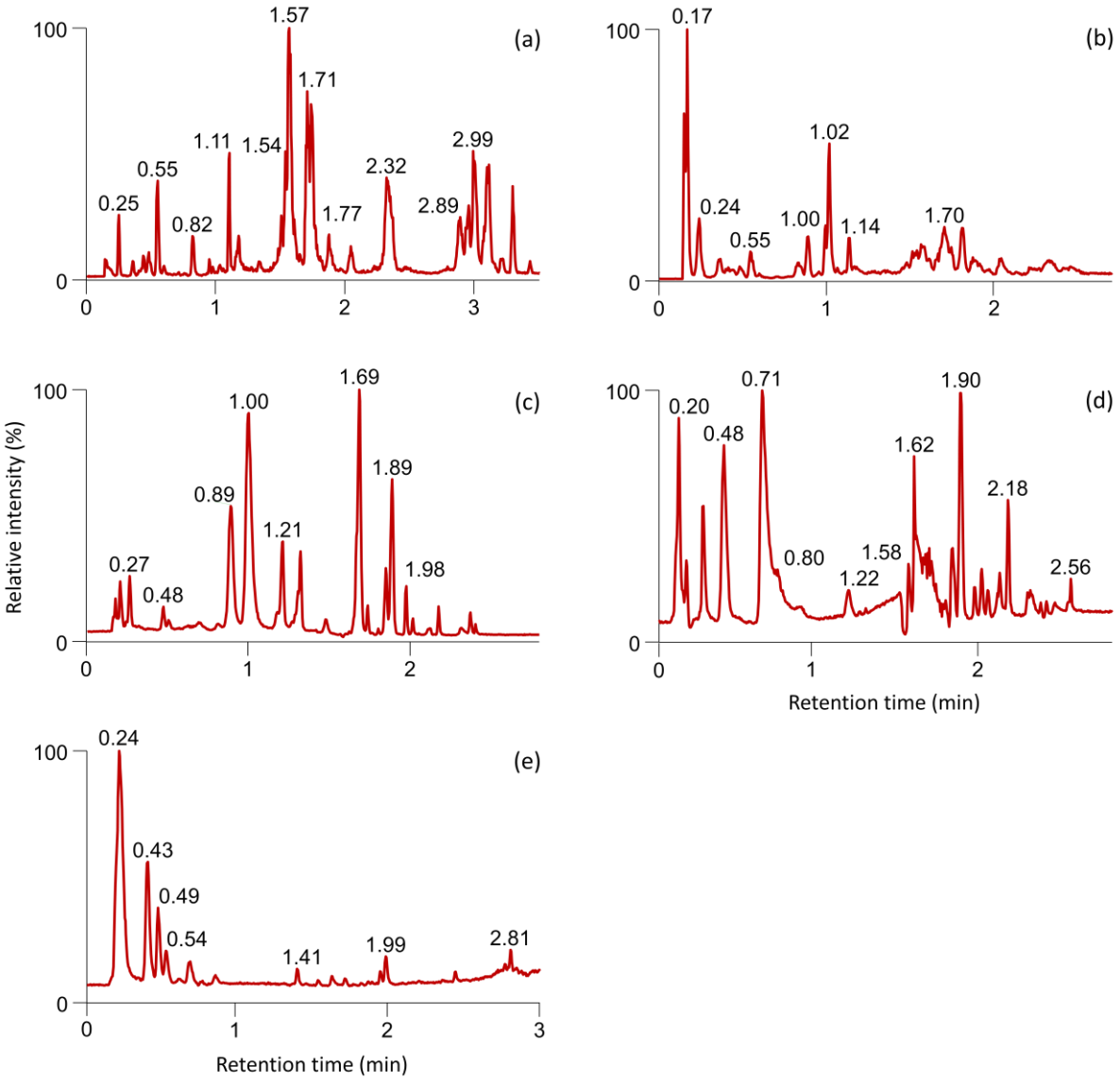
RPLC-ESI(+)

- DG 35:2|DG 17:0_18:2
- LPC 17:0/0:0
- PC 35:2|PC 17:0_18:2
- SM 35:1;O2|SM 18:1;O2/17:0
- TG 51:1|TG 16:0_17:0_18:1

RPLC-ESI(–)

- CL 71:7|CL 17:1_18:2_18:2_18:2
- LPE 17:0
- PE 35:2|PE 17:0_18:2
- PE O-37:5|PE O-17:1_20:4
- PI 39:4|PI 19:0_20:4
- PS 37:4|PS 17:0_20:4

Figure S4. ESI(–)-MS/MS spectrum (zoom of *m*/*z* 200–350) of (**a**) the PC 18:0/20:4 standard (precursor ion *m*/*z* 868.6073, $[M+CH_3COO]^-$, retention time 1.76 min); (**b**) PC 18:0/20:4;O (precursor ion *m*/*z* 884.6021, $[M+CH_3COO]^-$, retention time 1.50 min) formed by oxidation of the PC 18:0/20:4 standard.



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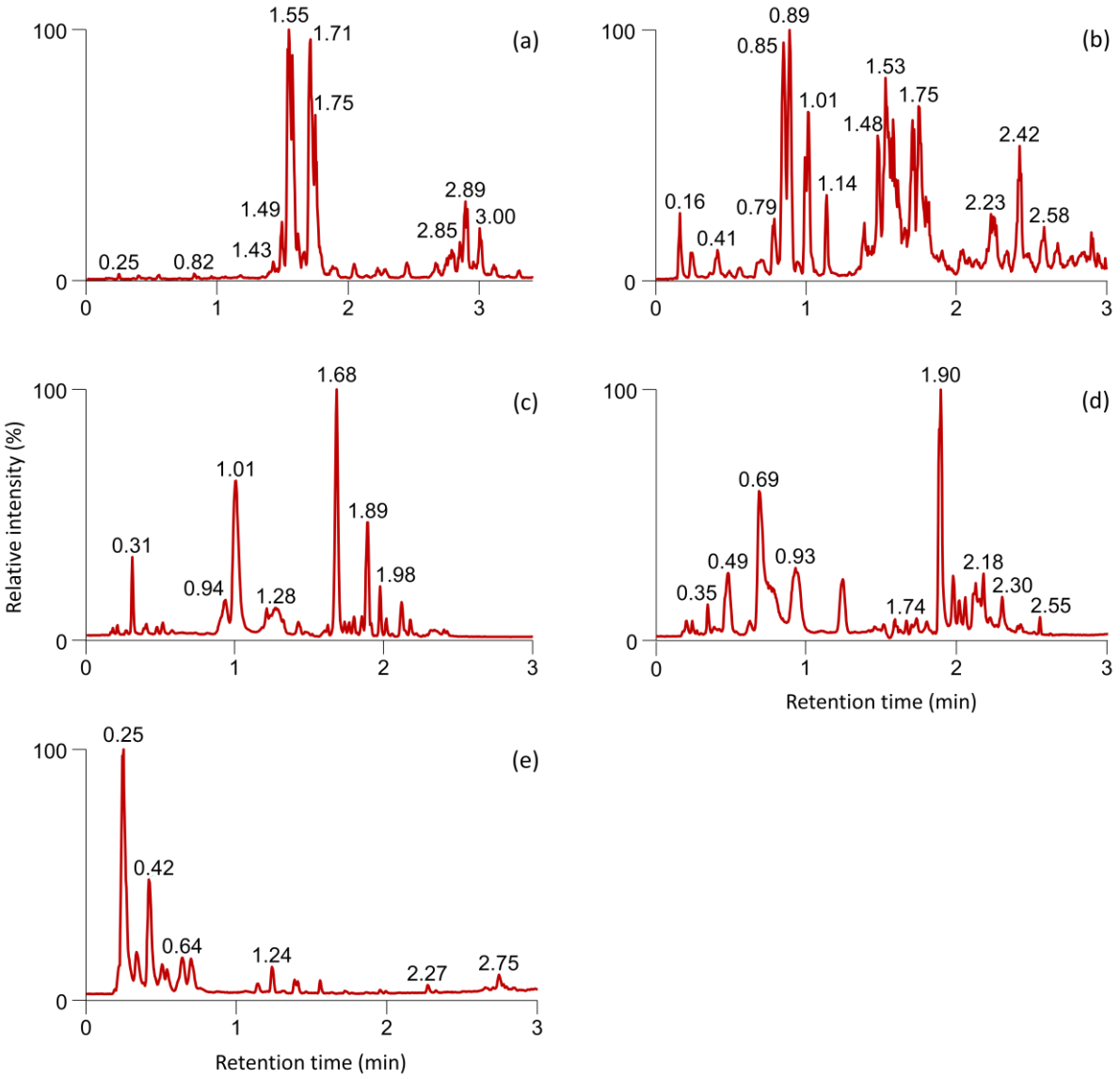
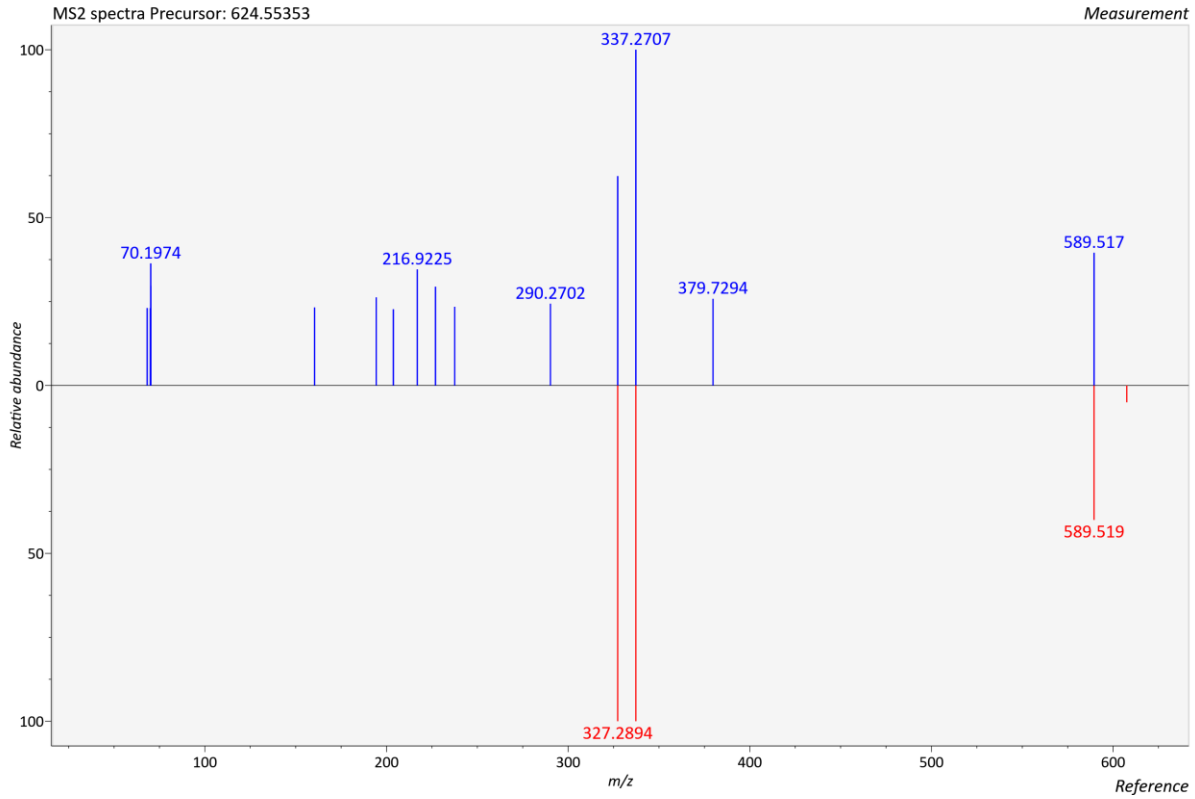


Figure S2. Examples of total ion chromatograms for mouse liver extracts acquired using LC-MS methods: (**a**) RPLC-ESI(+) lipidomics (ACQUITY Premier BEH C18 column); (**b**) RPLC-ESI(–) lipidomics (ACQUITY Premier BEH C18 column); (**c**) HILIC-ESI(+) metabolomics (BEH Amide column); (**d**) HILIC-ESI(–) metabolomics (ACQUITY Premier BEH Amide column); (**e**) RPLC-ESI(–) metabolomics (ACQUITY Premier HSS T3 column).

Figure S3. Examples of annotated lipids containing odd-chain fatty acids using MS/MS and MS-DIAL software

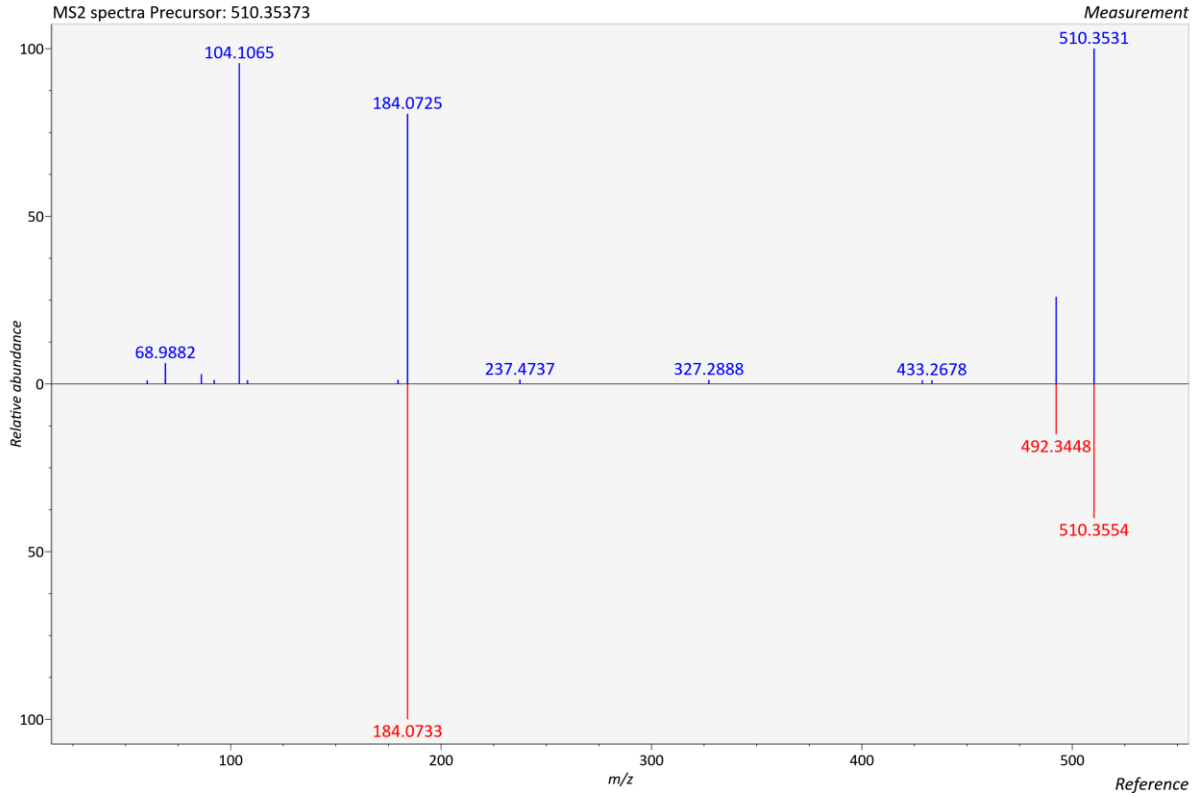
DG 35:2|DG 17:0_18:2

Retention time:	1.99 min
Ion form:	$[M+NH_4]^+$
Precursor ion:	*m/z* 624.55353 (ref. *m/z* 624.55621)



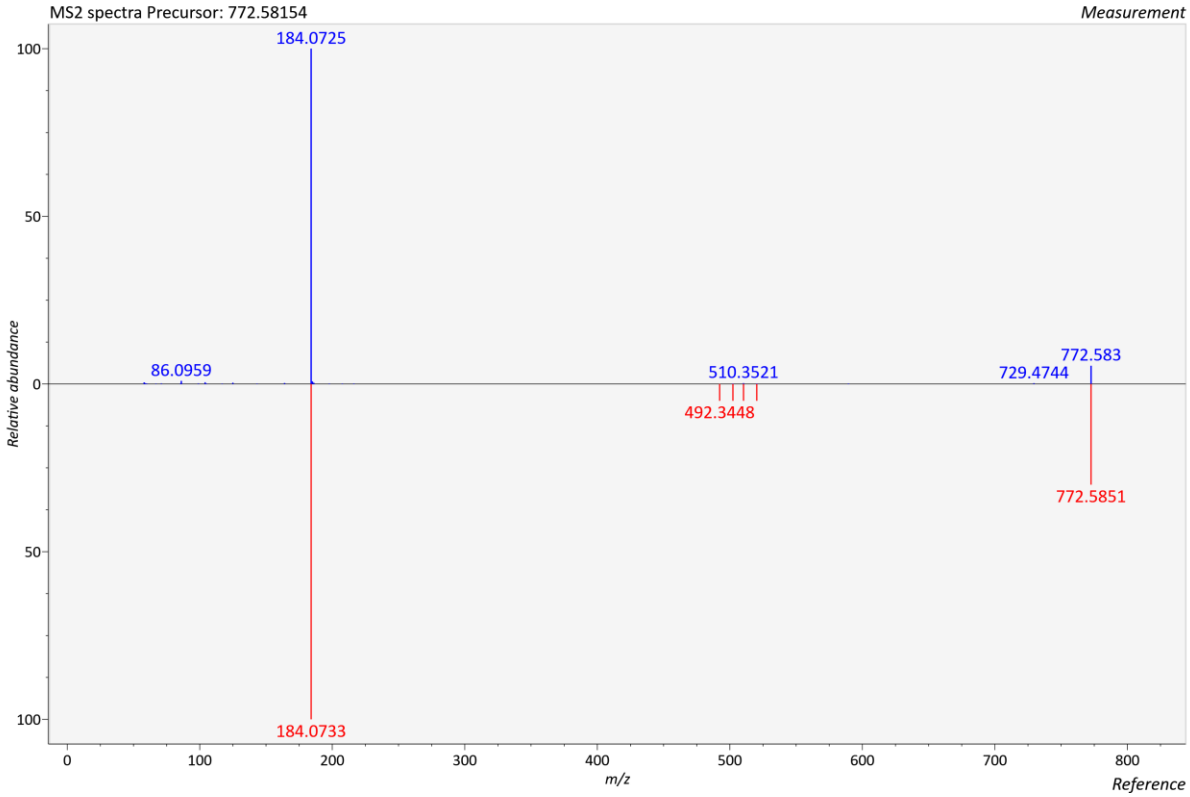
LPC 17:0/0:0

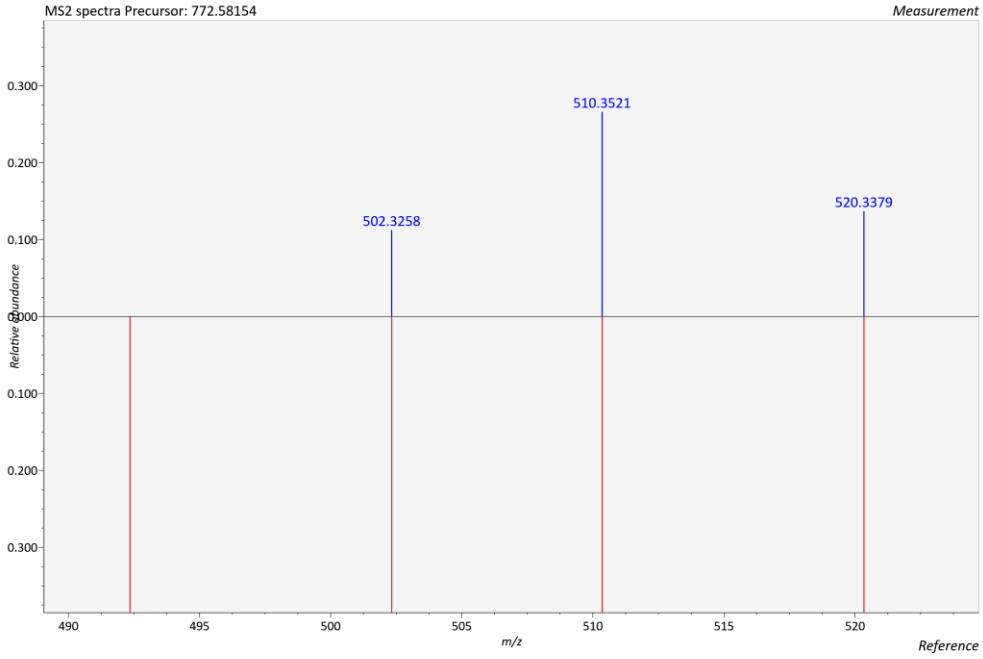
Retention time:	0.69 min
Ion form:	$[M+H]^+$
Precursor ion:	*m/z* 510.35373 (ref. *m/z* 510.35541)



PC 35:2|PC 17:0_18:2

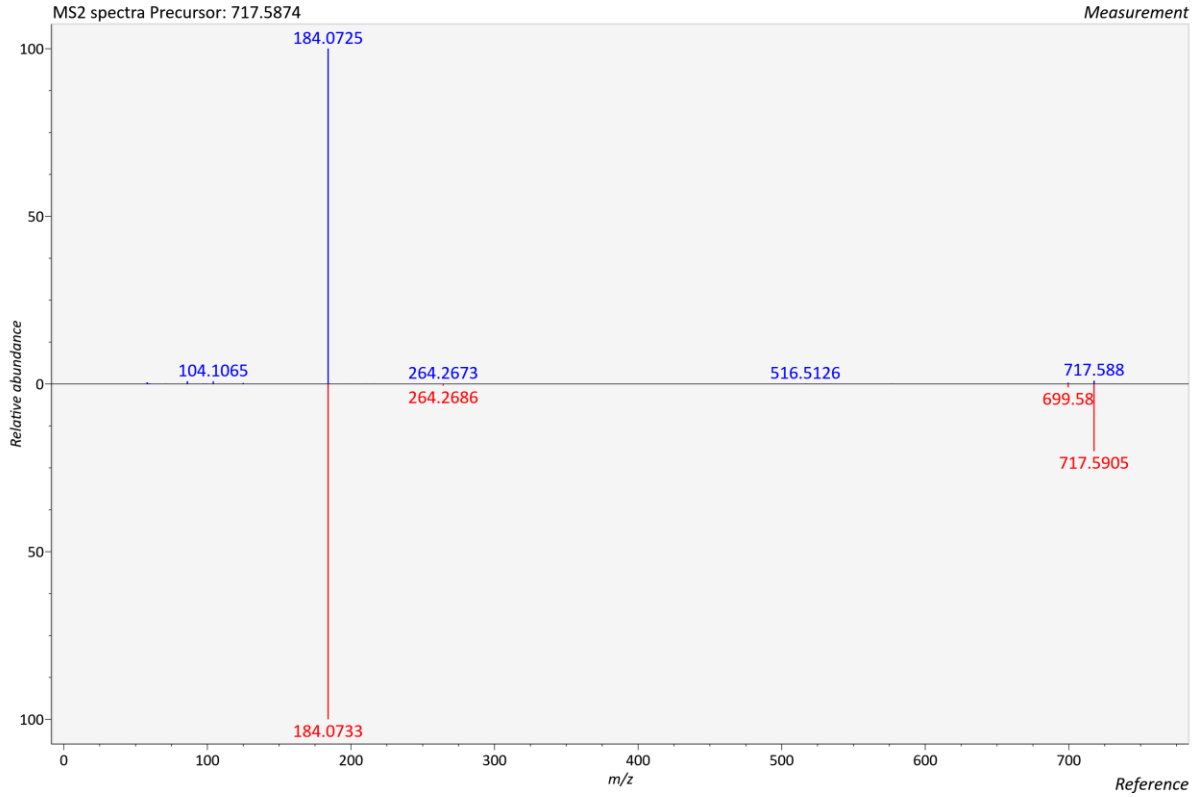
Retention time:	1.66 min
Ion form:	$[M+H]^+$
Precursor ion:	*m/z* 772.58154 (ref. *m/z* 772.58508)





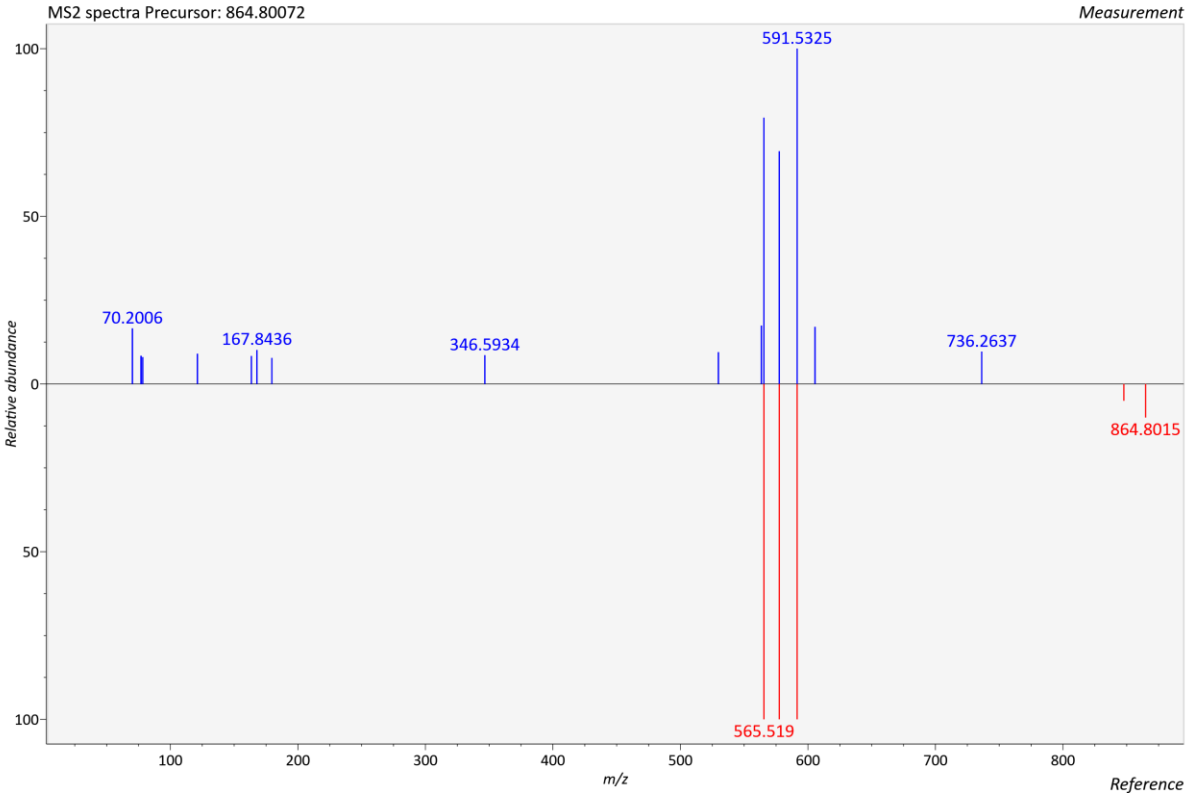
SM 35:1;O2|SM 18:1;O2/17:0

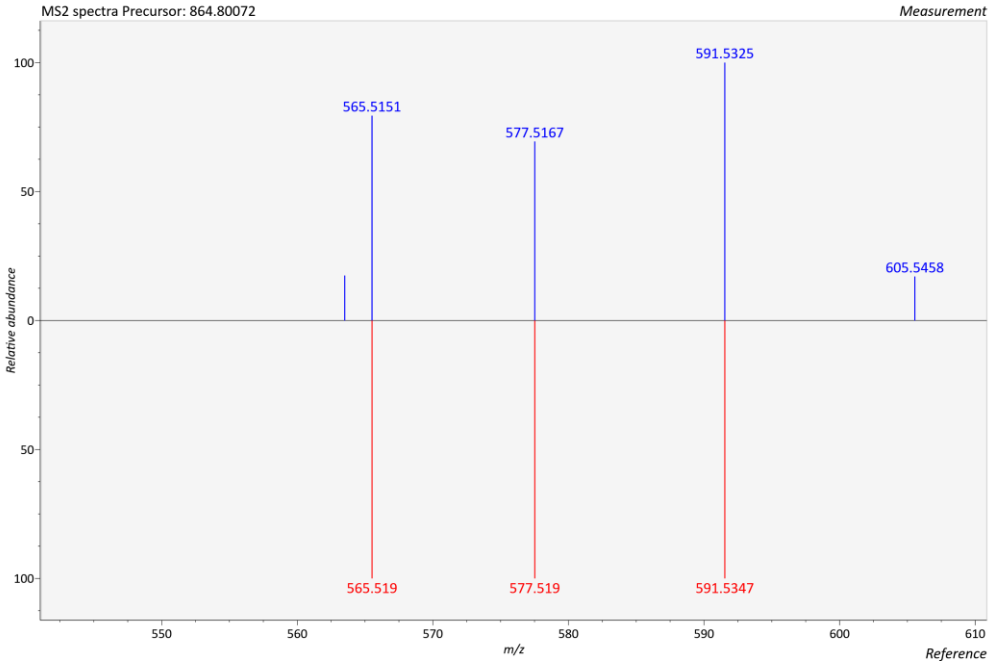
Retention time:	1.60 min
Ion form:	$[M+H]^+$
Precursor ion:	*m/z* 717.58740 (ref. *m/z* 717.59052)



TG 51:1|TG 16:0_17:0_18:1

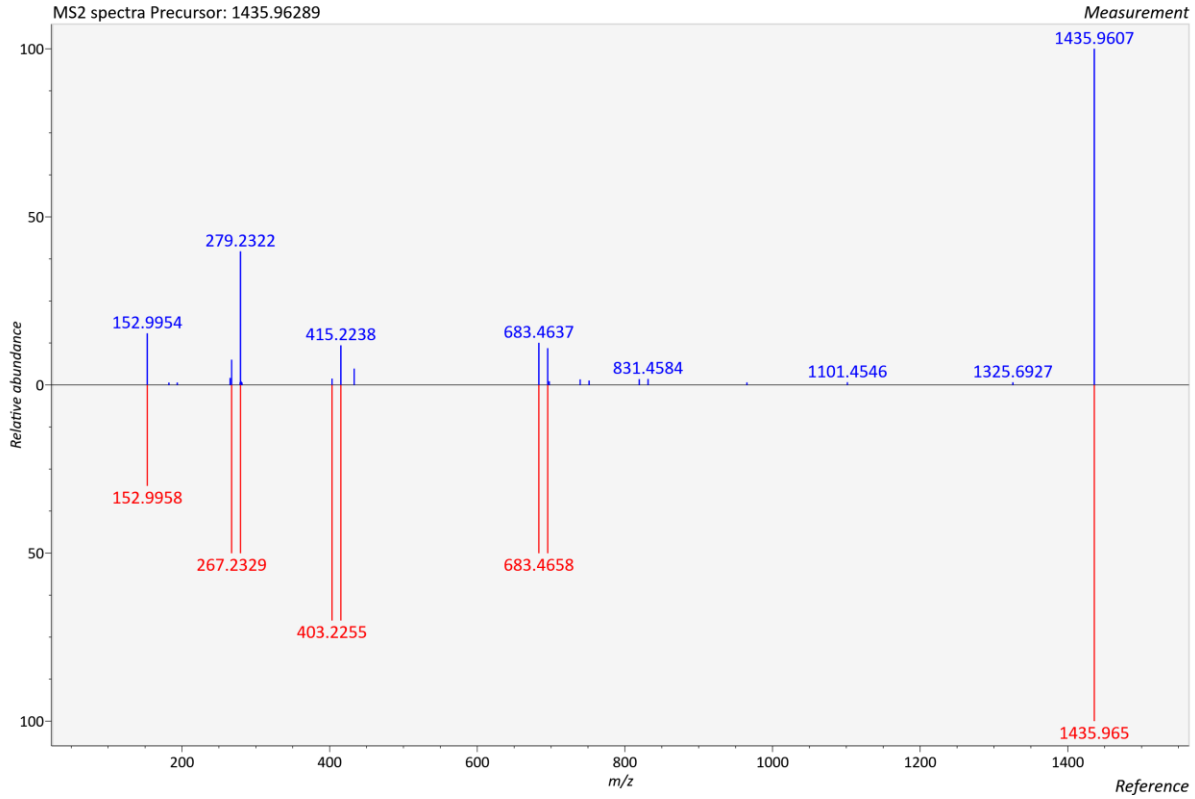
Retention time:	3.16 min
Ion form:	$[M+NH_4]^+$
Precursor ion:	*m/z* 864.80072 (ref. *m/z* 864.80151)





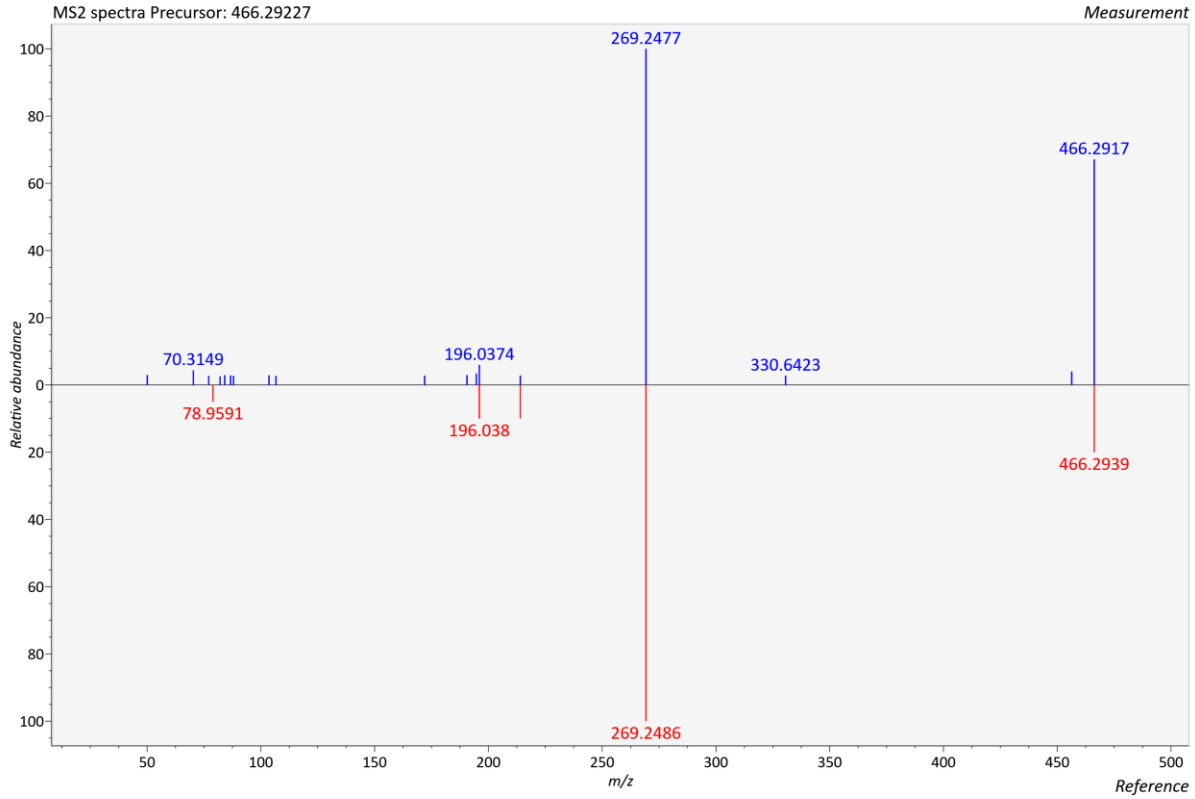
CL 71:7|CL 17:1_18:2_18:2_18:2

Retention time:	2.62 min
Ion form:	$[M–H]^-$
Precursor ion:	*m/z* 1435.96289 (ref. *m/z* 1435.96484)



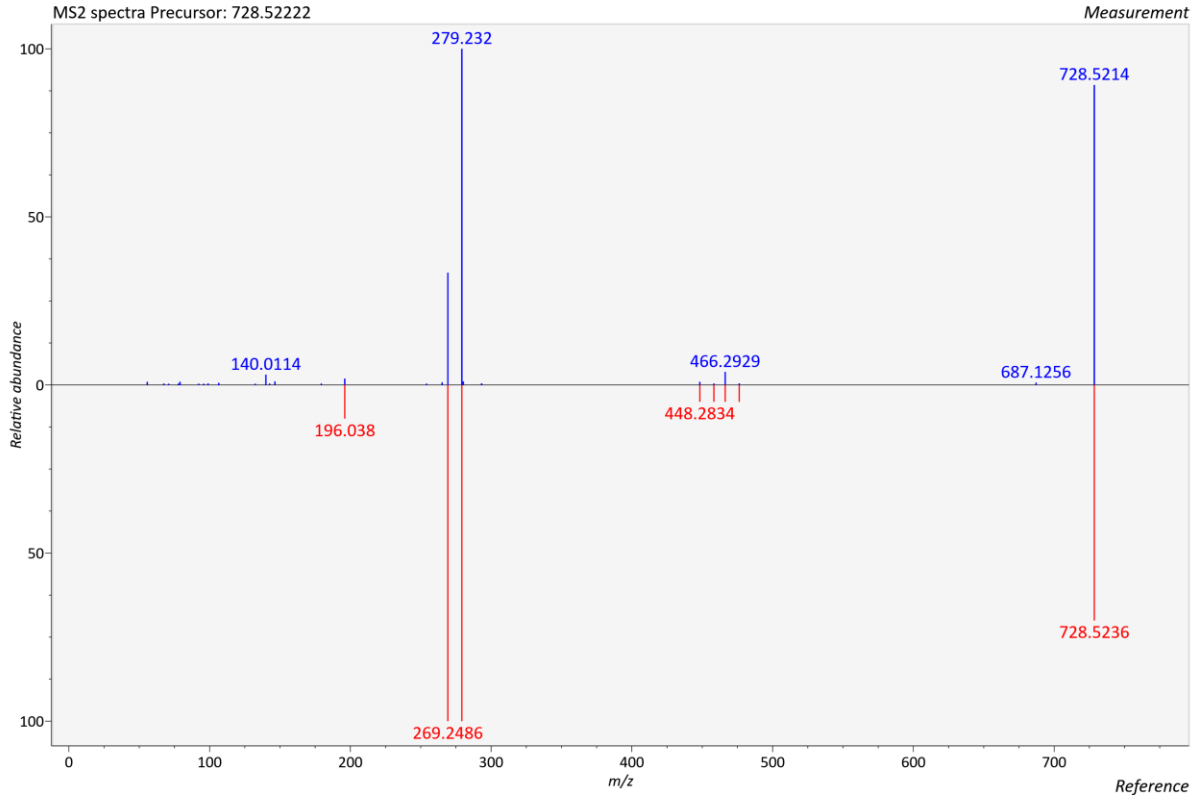
LPE 17:0

Retention time:	0.70 min
Ion form:	$[M–H]^-$
Precursor ion:	*m/z* 466.29227 (ref. *m/z* 466.29391)



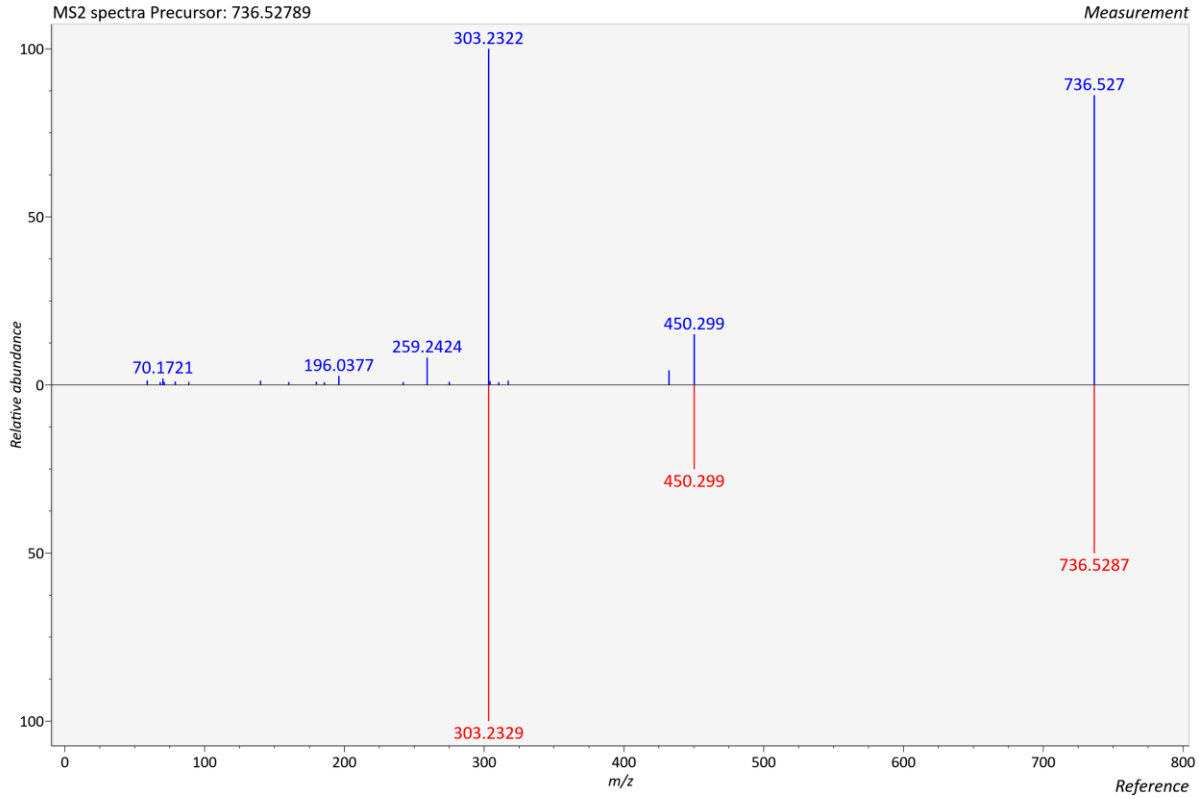
PE 35:2 | PE 17:0_18:2

Retention time:	1.71 min
Ion form:	$[M–H]^-$
Precursor ion:	*m/z* 728.52222 (ref. *m/z* 728.52362)



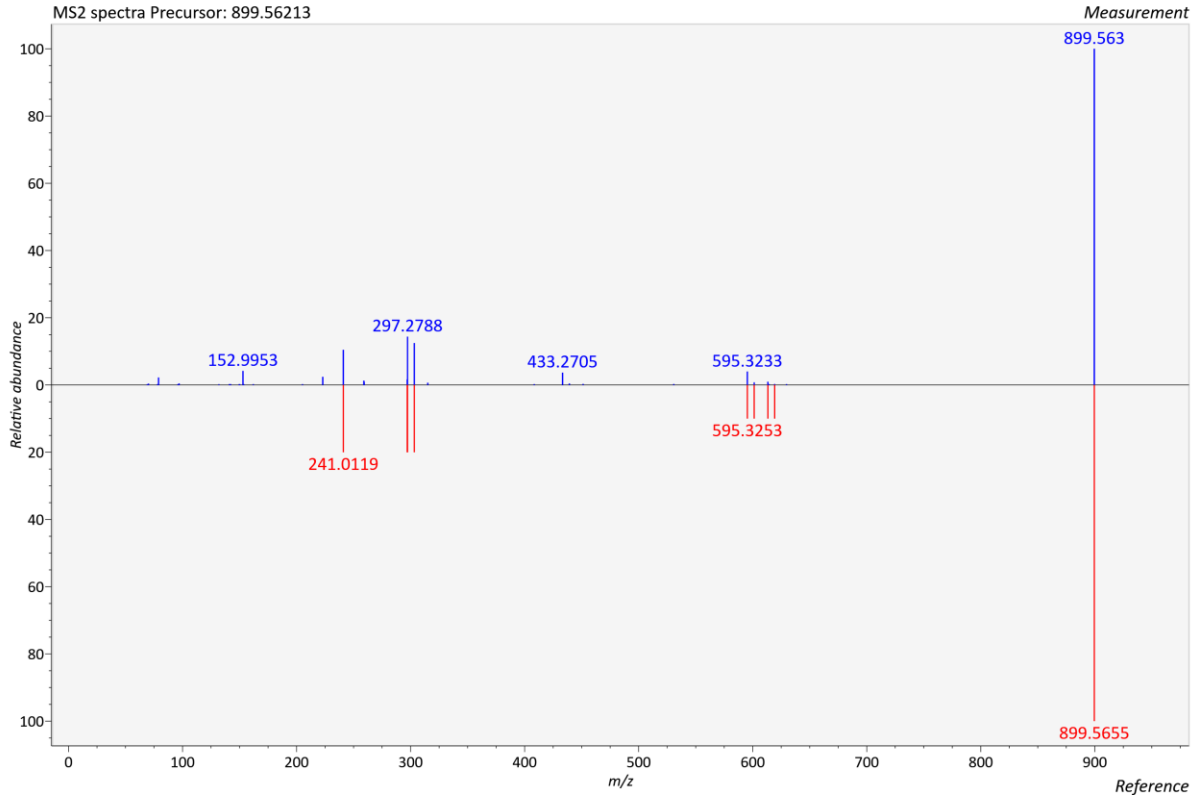
PE O-37:5|PE O-17:1_20:4

Retention time:	1.72 min
Ion form:	$[M–H]^-$
Precursor ion:	*m/z* 736.52789 (ref. *m/z* 736.52869)



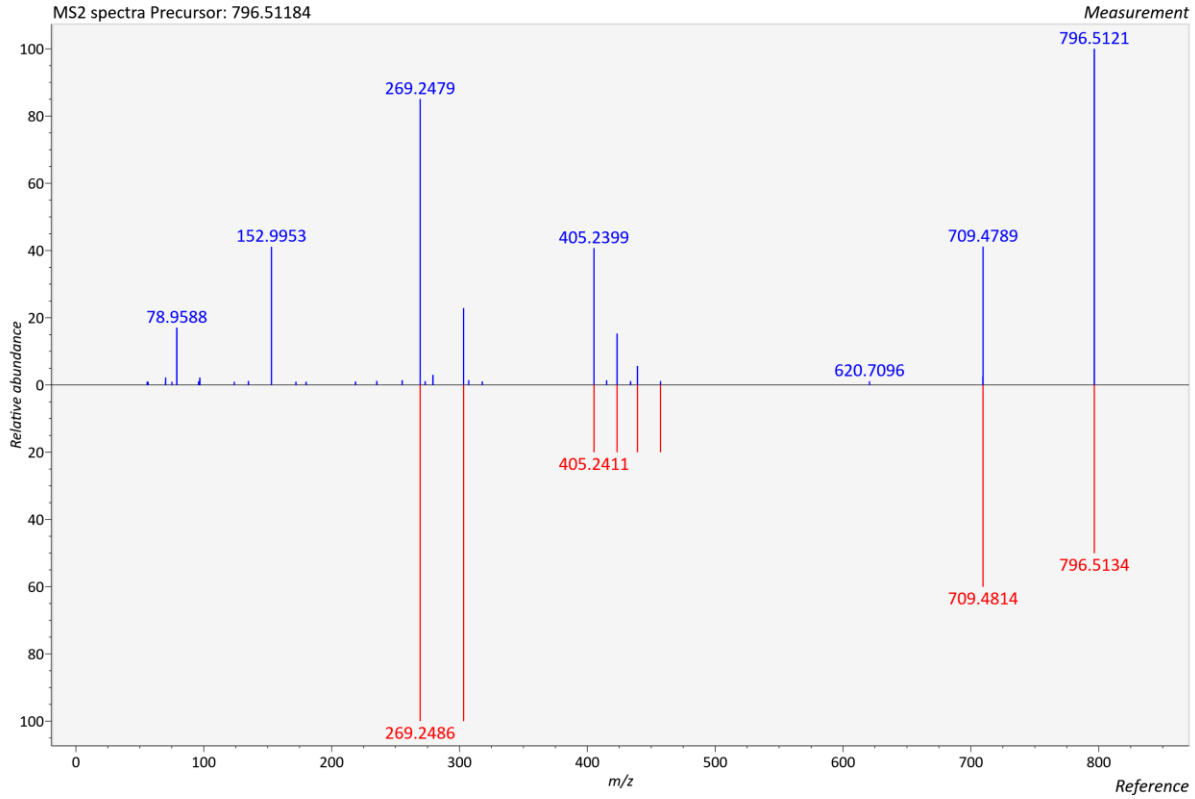
PI 39:4|PI 19:0_20:4

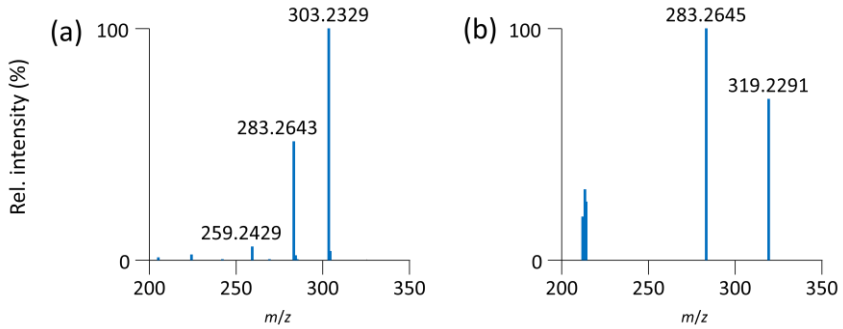
Retention time:	1.61 min
Ion form:	$[M–H]^-$
Precursor ion:	*m/z* 899.56213 (ref. *m/z* 899.56549)



PS 37:4|PS 17:0_20:4

Retention time:	1.48 min
Ion form:	$[M–H]^-$
Precursor ion:	*m/z* 796.51184 (ref. *m/z* 796.51343)





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