

Development of a sensitive and quantitative method for the identification of two major furan fatty acids in human plasma

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Supplemental Table S1. Concentrations for furan fatty acid standards in working solutions

Furan fatty acids	Concentration (ng/mL)								
	S1	S2	S3	S4	S5	S6	S7	S8	S9
11D3	0.5	1	5	10	20	40	80	160	320
11D5	2.5	5	25	50	100	200	400	800	1600

Supplemental Table S2. Key parameters for monitoring 11D3 and 11D5

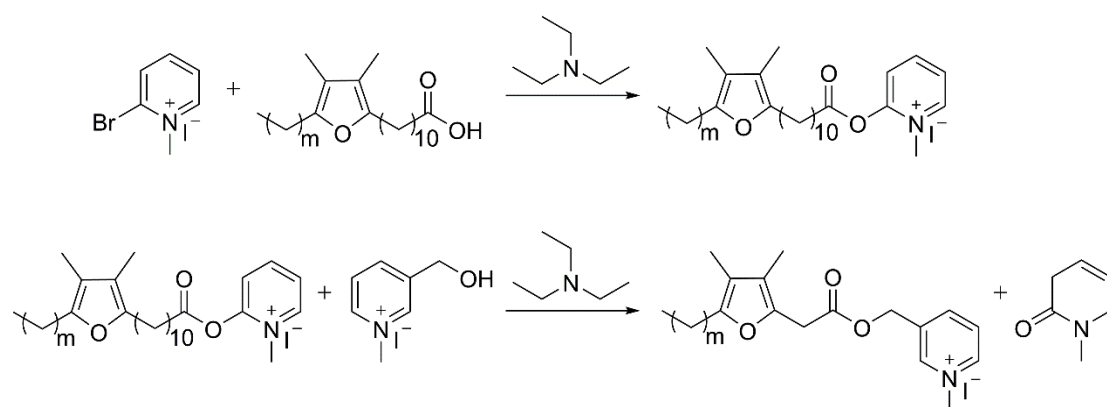
Furan fatty acids	Precursor ion (<i>m/z</i>)	Product ion (<i>m/z</i>)	Dwell time (msec)	Q1 voltage (V)	CE (V)	Q3 voltage (V)
11D3	321	71	19	23	28	25
	321	99	19	14	26	12
	321	141	19	15	33	21
11D5	349	71	19	12	34	16
	349	127	19	24	26	23
	349	141	19	10	38	24

Supplemental Table S3. Key parameters for monitoring 11D3-AMMP and 11D5-AMMP

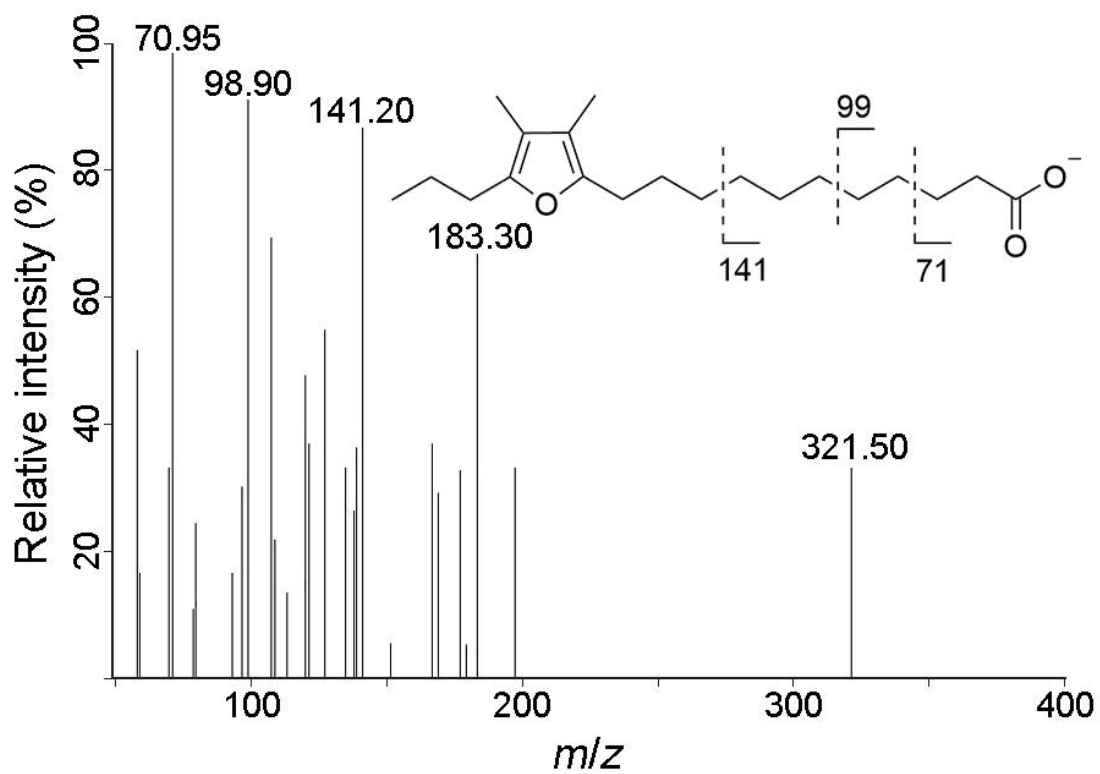
Furan fatty acid derivatives	Precursor ion (<i>m/z</i>)	Product ion (<i>m/z</i>)	Dwell time (msec)	Q1 voltage (V)	CE (V)	Q3 voltage (V)
11D3- AMMP	428	107	13	-12	-52	-18
	428	124	13	-12	-40	-20
	428	178	13	-13	-43	-18
11D5- AMMP	456	107	13	-16	-52	-18
	456	124	13	-10	-45	-22
	456	178	13	-16	-48	-18

Supplemental Figure S1. The derivatization reactions of 11D3 and 11D5 with BMP & CMP

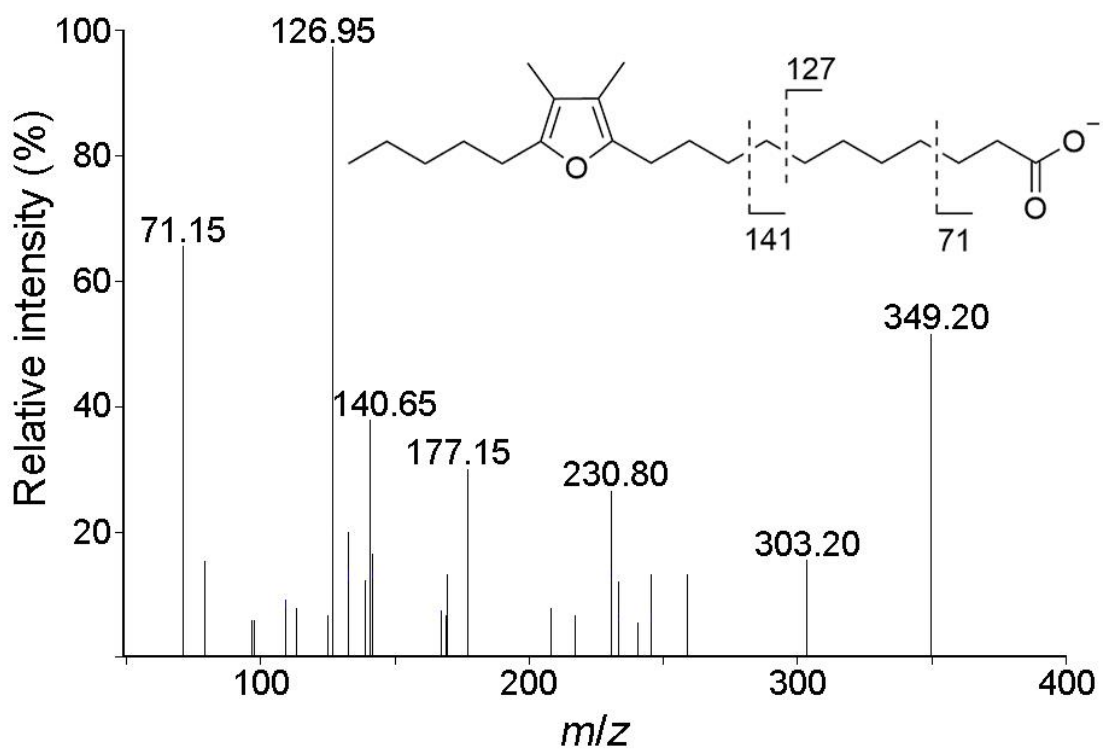
($m=2$ or 4)



Supplemental Figure S2. MS/MS spectra of (a) 11D3 and (b) 11D5 in the negative mode

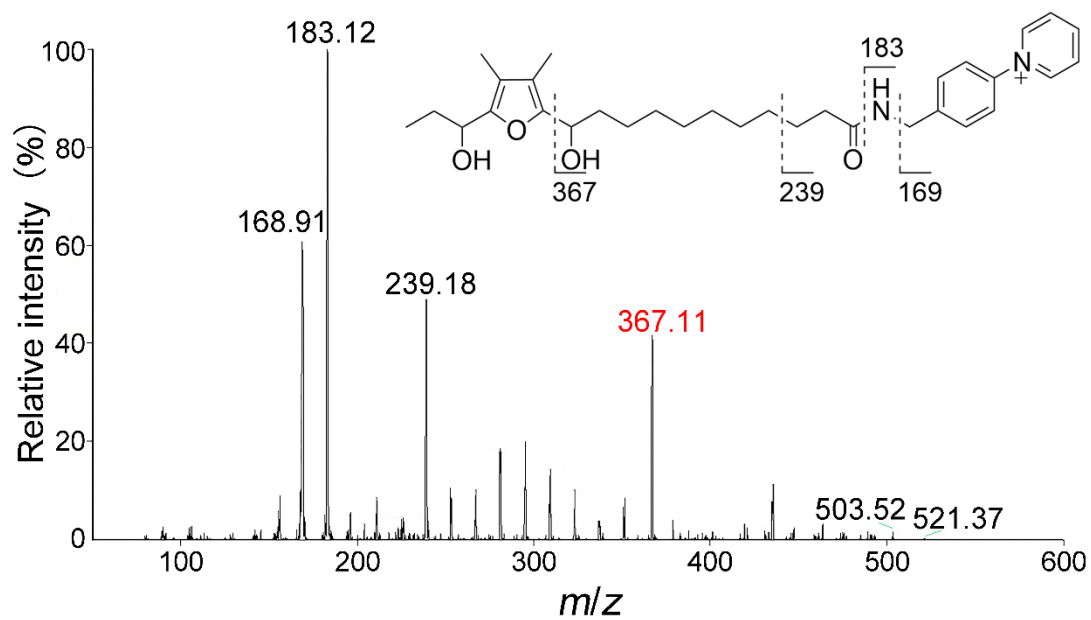


(a)

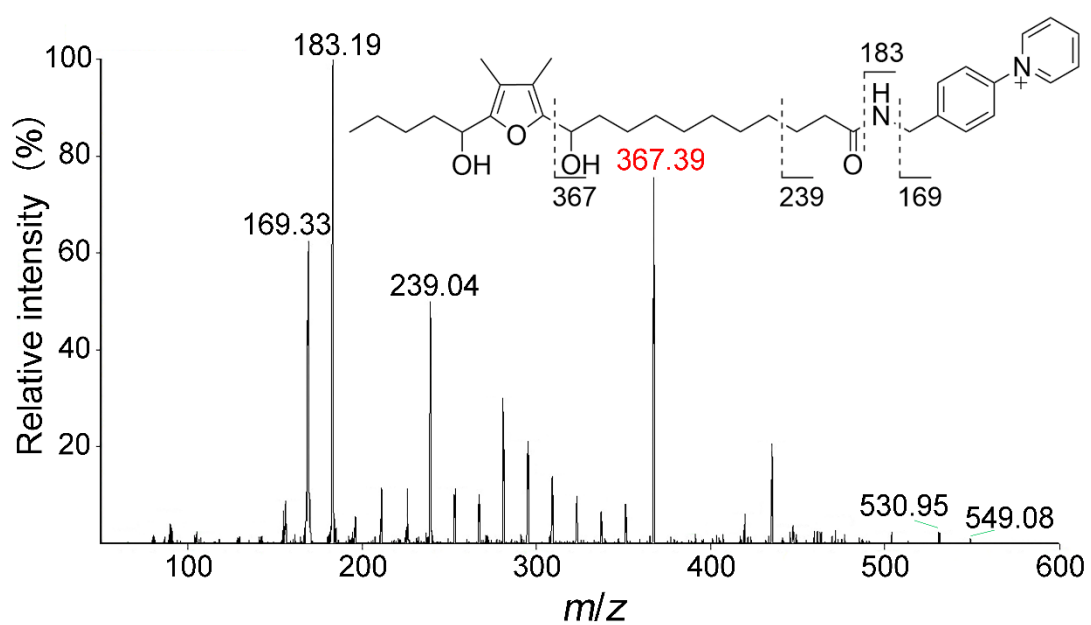


(b)

Supplemental Figure S3. MS/MS spectra of oxidized furan fatty acids-AMPP. (a) $[11D3\text{-AMPP} + 32]^+$; (b) $[11D5\text{-AMPP} + 32]^+$.

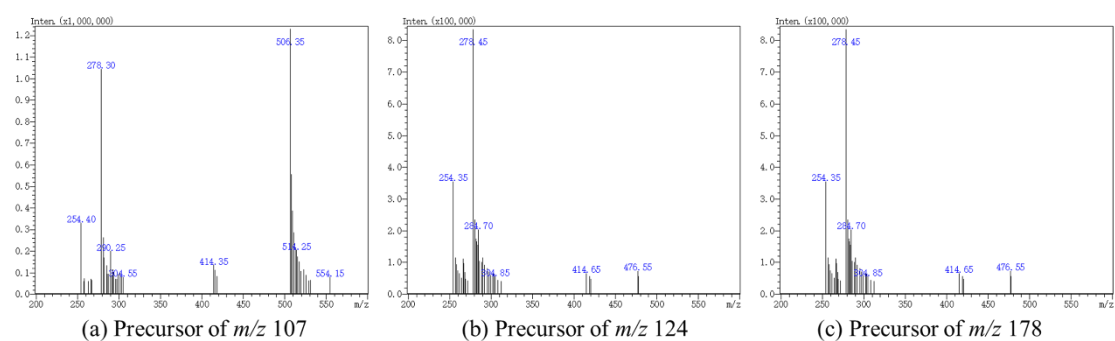


(a)

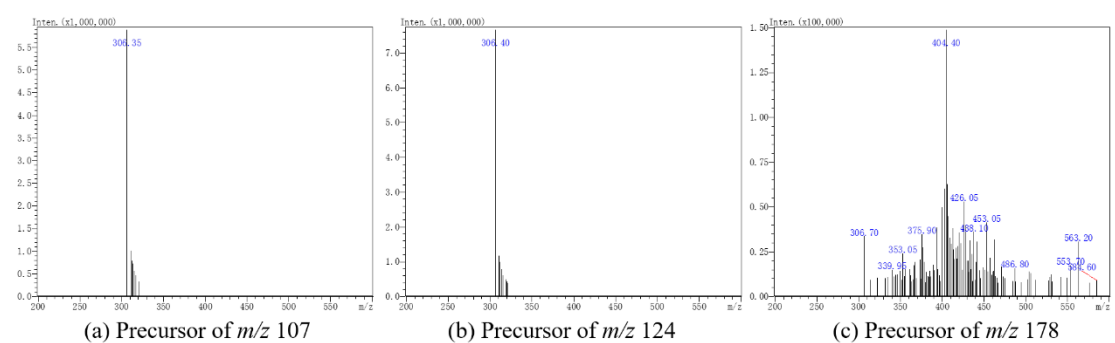


(b)

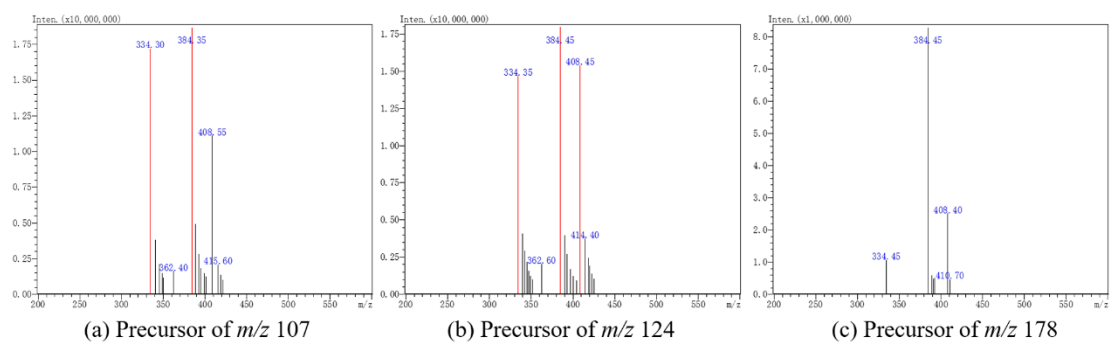
Supplemental Figure S4 Precursor ions at retention time of 4.05 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



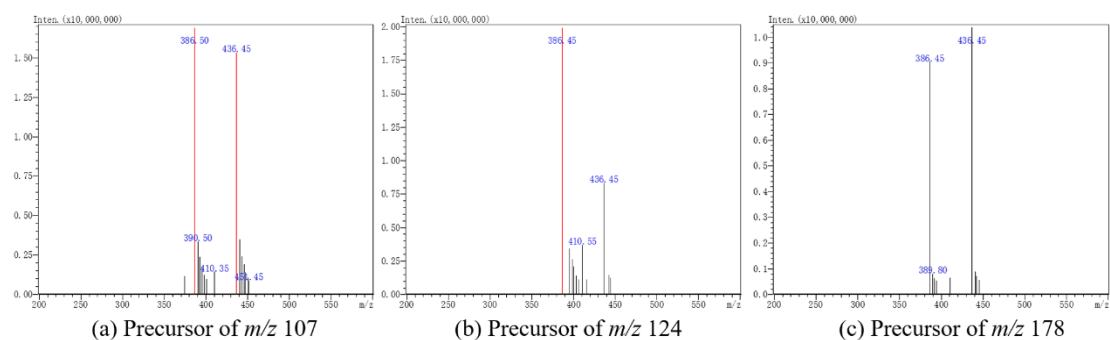
Supplemental Figure S5 Precursor ions at retention time of 4.56 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



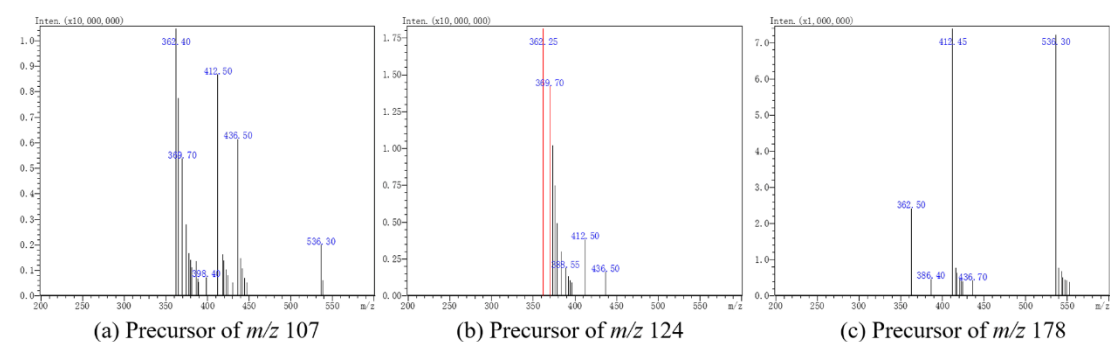
Supplemental Figure S6 Precursor ions at retention time of 5.04 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



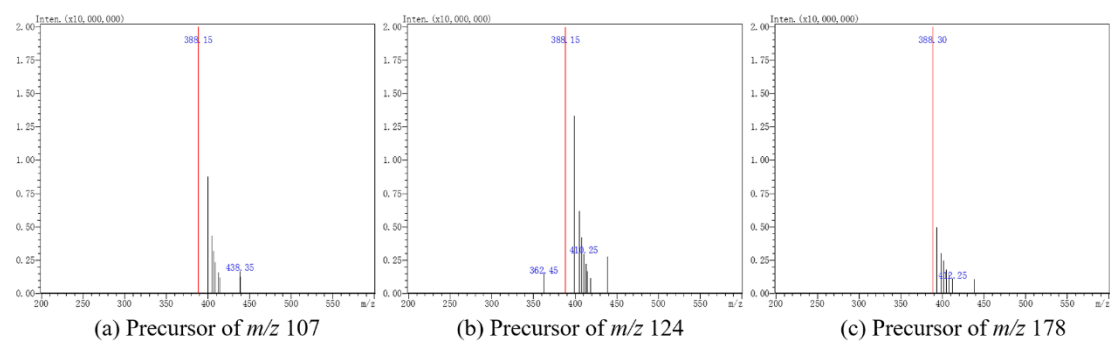
Supplemental Figure S7 Precursor ions at retention time of 5.38 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



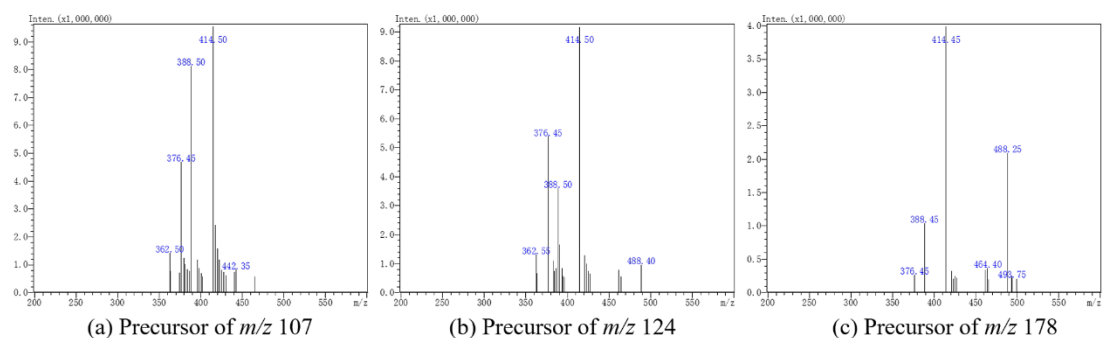
Supplemental Figure S8 Precursor ions at retention time of 5.46 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



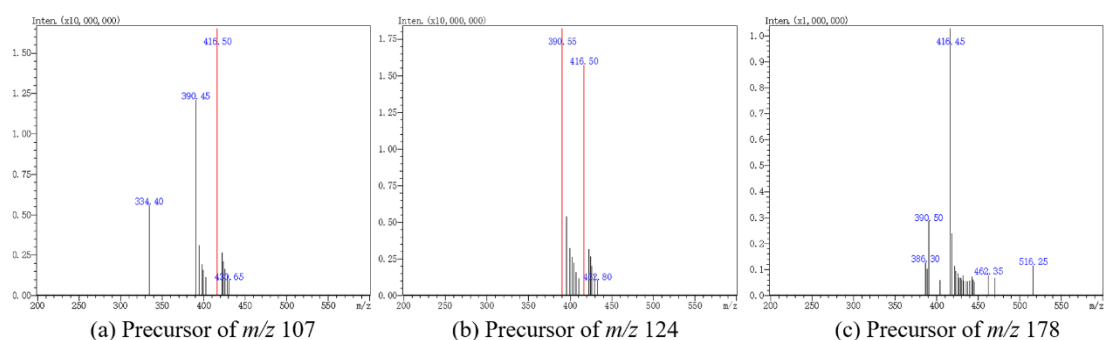
Supplemental Figure S9 Precursor ions at retention time of 5.64 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



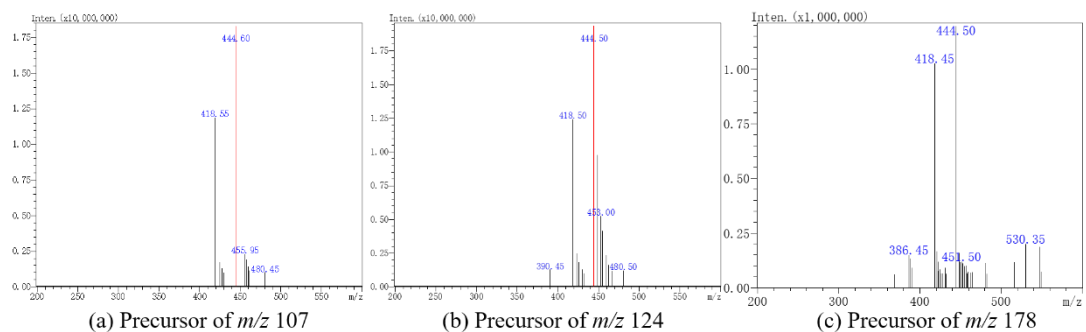
Supplemental Figure S10 Precursor ions at retention time of 5.77 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



Supplemental Figure S11 Precursor ions at retention time of 6.01 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



Supplemental Figure S12 Precursor ions at retention time of 6.48 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.



Supplemental Figure S13 Precursor ions at retention time of 6.89 min. (a) precursor of m/z 107, (b) precursor of m/z 124, (c) precursor of m/z 178.

