Electronic Supplementary Information for

Formation of soluble furanic and carbocyclic oxy-organics during the hydrothermal carbonization of glucose

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Table S1 The elemental contents of hydrochar (HC) and water soluble non-volatile compounds (WSNV)

Sample	Reaction Time	Carbon content (%)	Hydrogen content (%)	Oxygen content (%)
HC	2 h	62.6	3.9	33.5
HC	3 h	63.2	3.6	33.2
HC	4 h	65.2	3.4	31.4
HC	5 h	66.1	3.1	30.8
HC	6 h	67.4	2.9	29.7
HC	8 h	67.7	2.9	29.4
HC	10 h	68.9	2.8	28.3
WSNV	2 h	48.6	6.3	45.1
WSNV	3 h	52.9	5.8	41.3
WSNV	4 h	55.6	5.2	39.2
WSNV	5 h	58.4	4.9	36.7
WSNV	6 h	59.3	4.6	36.1
WSNV	8 h	59.2	4.5	36.3
WSNV	10 h	60.7	4.5	34.8

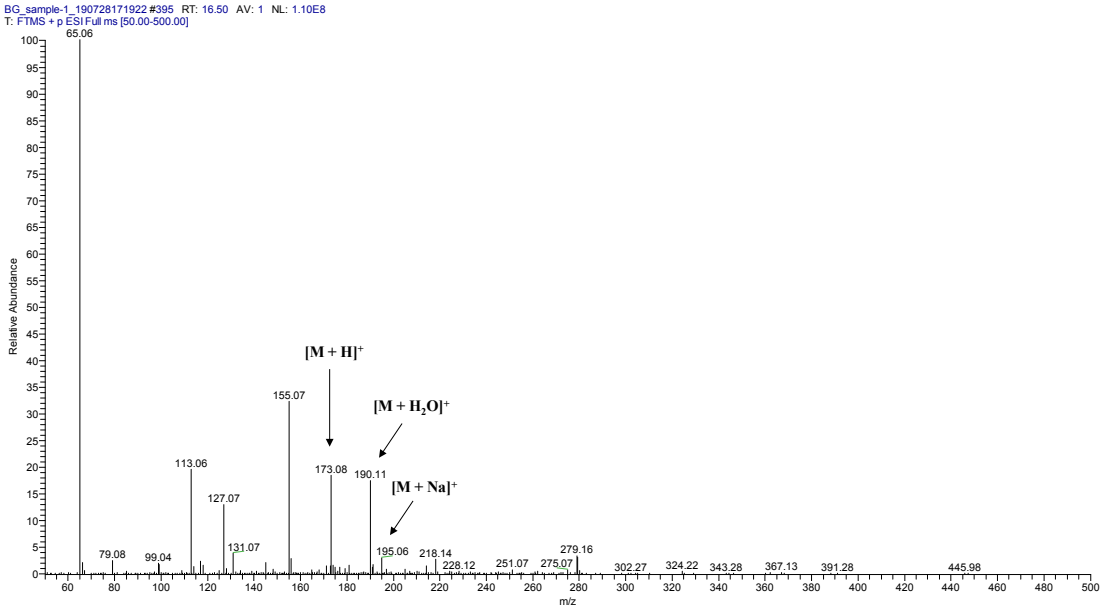

Figure S1 The MS spectrum of compound at 16.50 min under positive ionisation mode

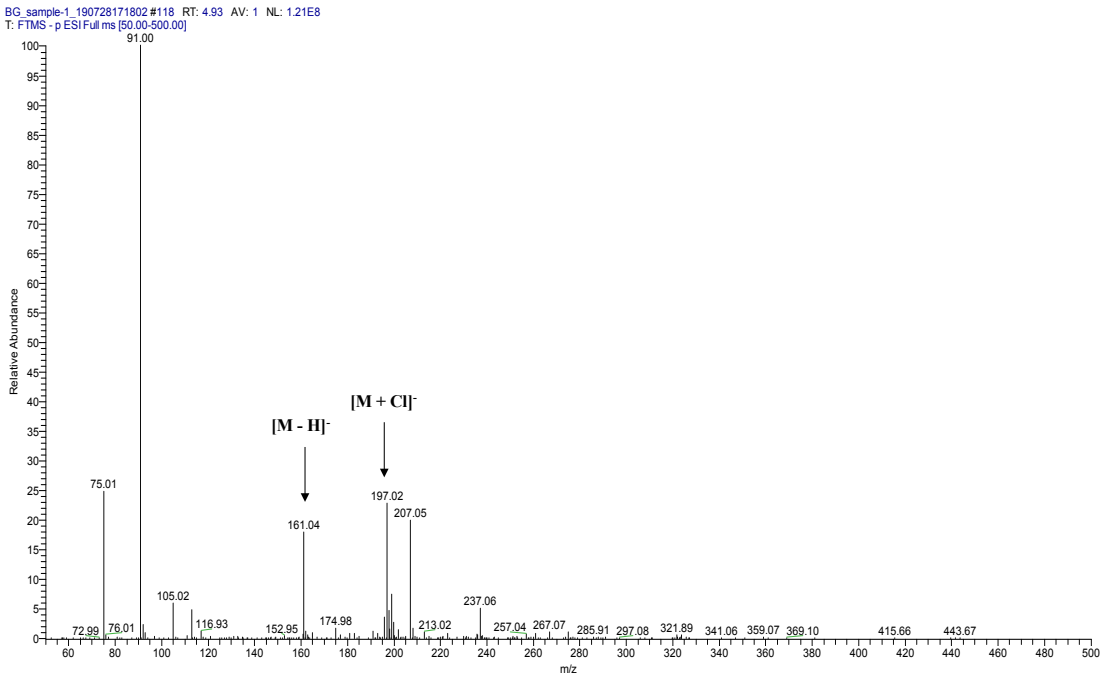

Figure S2 The MS spectrum of compound at 4.89 min under negative ionisation mode

Table S2 The mass loss between the fragment ions and the corresponding functional group

Experimental mass loss	Lost group	Theoretical mass of lost group [a]	Corresponding functional group
14.02	CH_2	14.0157	methylene
18.01	H_2O	18.0106	hydroxy
26.02	C_2H_2	26.0157	acetylene
27.99	CO	27.9949	carbonyl
28.03	C_2H_4	28.0313	ethylene
30.01	CH_2O	30.0106	aldehyde
43.99	CO_2	43.9898	carboxyl
82.04	C_5H_6O	82.0417	methyl furan
94.04	C_6H_6O	94.0417	phenol
96.02	$C_5H_4O_2$	96.0210	furfural
98.03	$C_5H_6O_2$	98.0326	furfuryl alcohol

[a] the theoretical mass of lost group was calculated by the following equation:

Mass of lost group =12 × (mol of C) + 1.0078 × (mole of H) + 15.9949 × (mole of O)

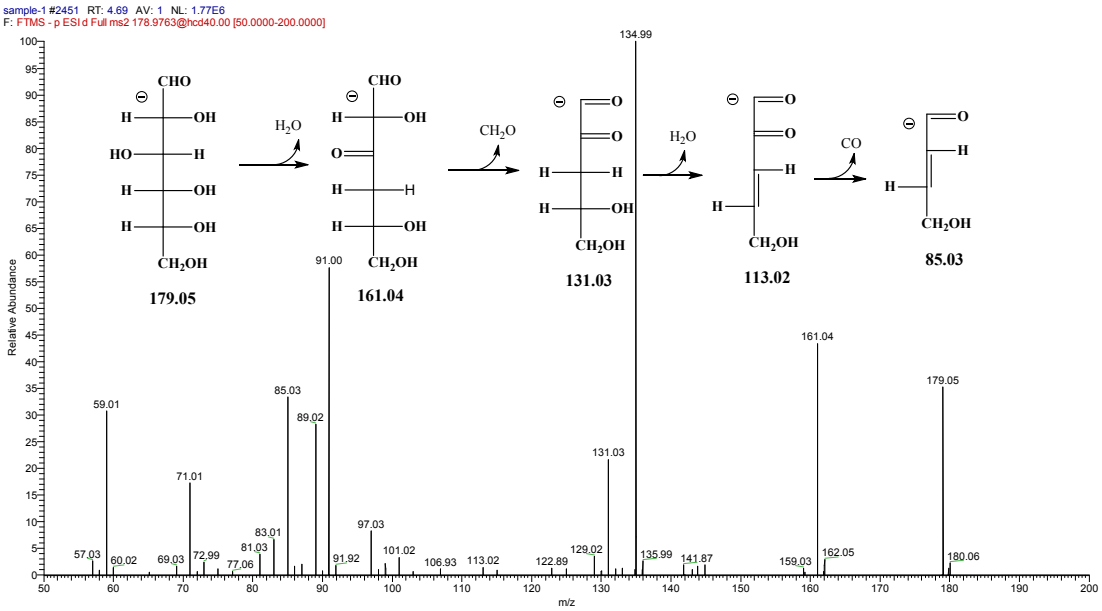

Figure S3 The MS^2 spectrum of de-protonated $C_6H_{12}O_6$ (4.26 min) and its possible fragmentation process

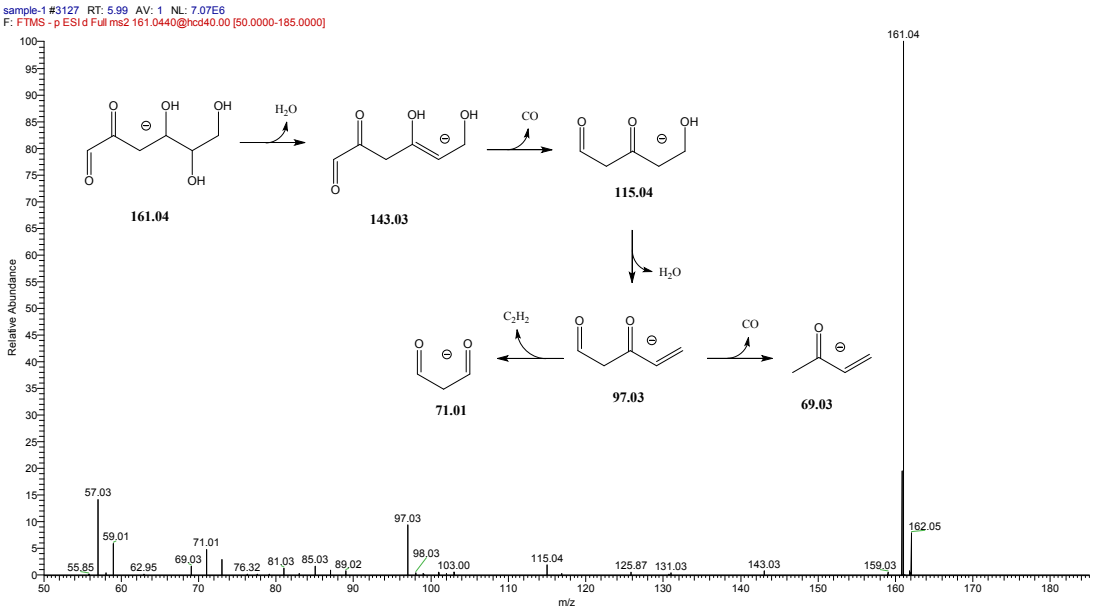

Figure S4 The MS^2 spectrum of de-protonated $C_6H_{10}O_5$ (4.89 min) and its possible fragmentation process

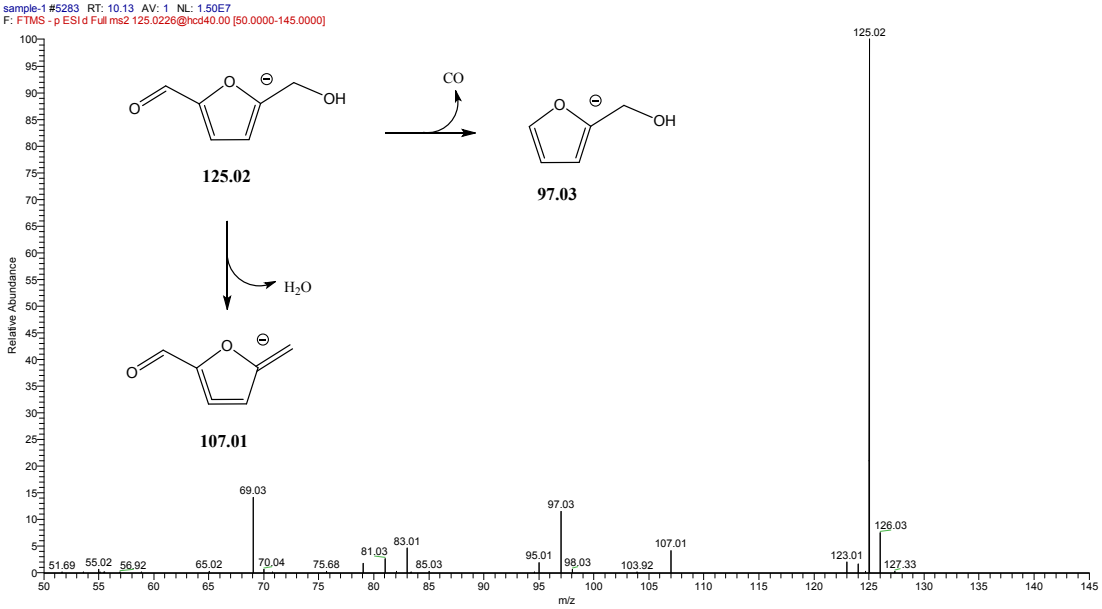

Figure S5 The MS^2 spectrum of de-protonated $C_6H_6O_3$ (10.17 min) and its possible fragmentation process

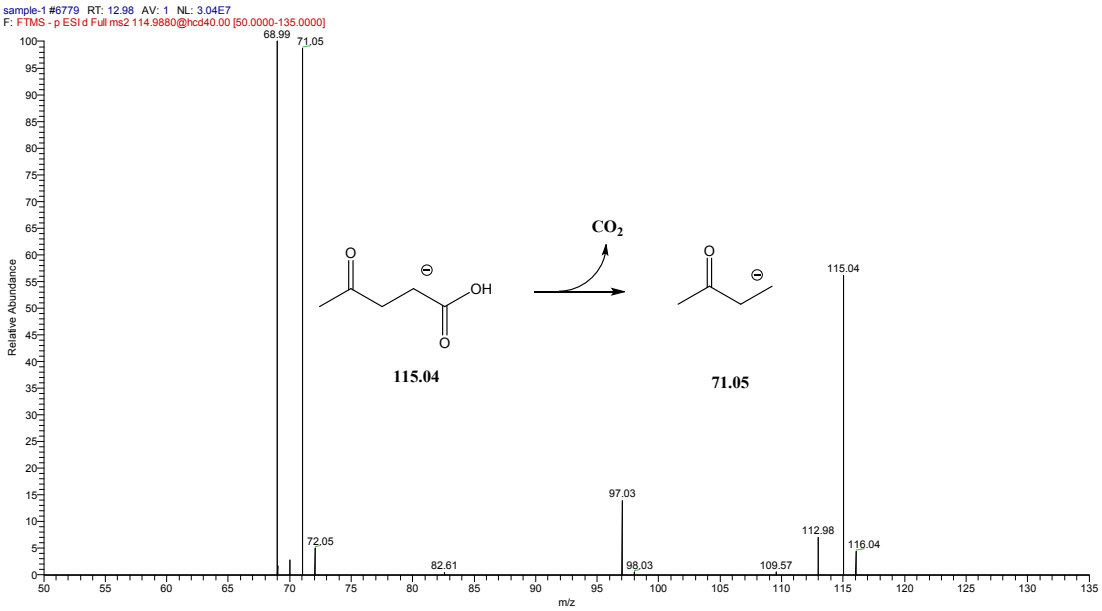

Figure S6 The MS^2 spectrum of de-protonated $C_5H_8O_3$ (12.91 min) and its possible fragmentation process

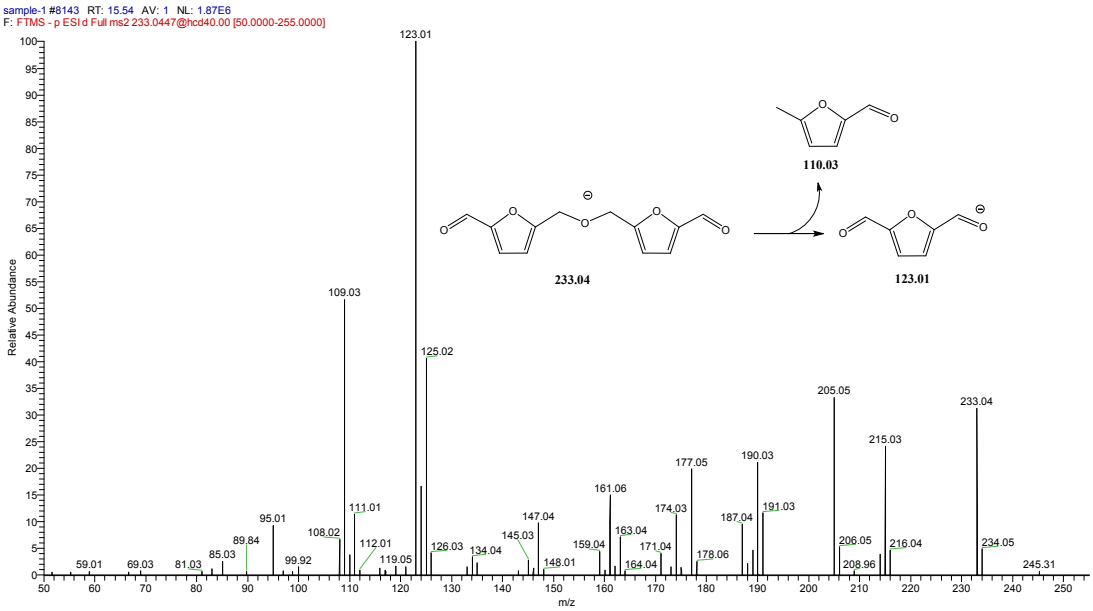

Figure S7 The MS^2 spectrum of de-protonated $C_{12}H_{10}O_5$ (15.45 min) and its possible fragmentation process

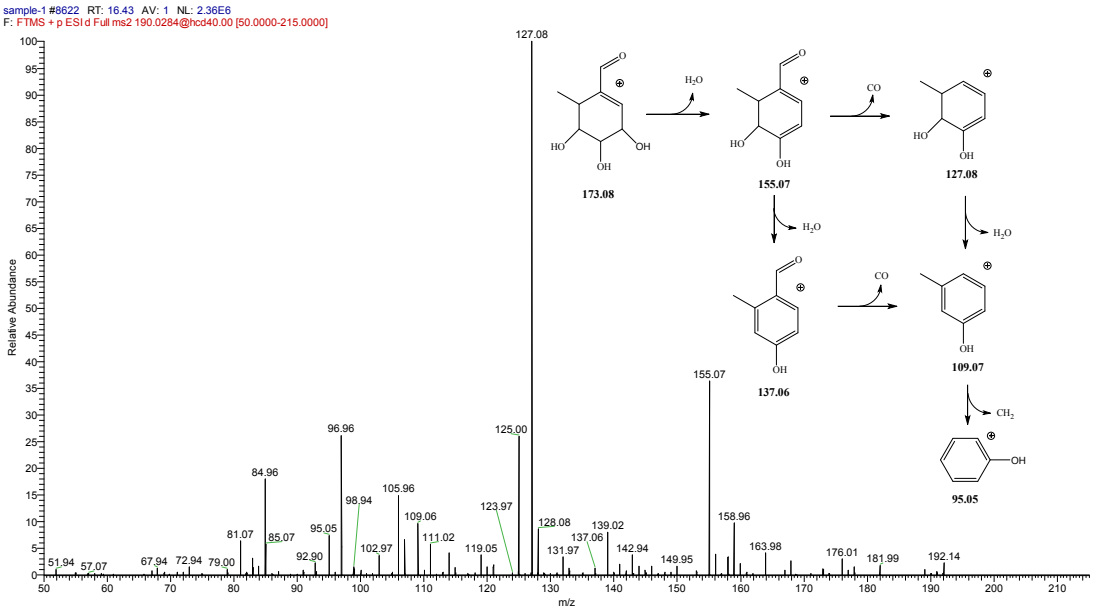

Figure S8 The MS^2 spectrum of protonated $C_8H_{12}O_4$ (16.50 min) and its possible fragmentation process

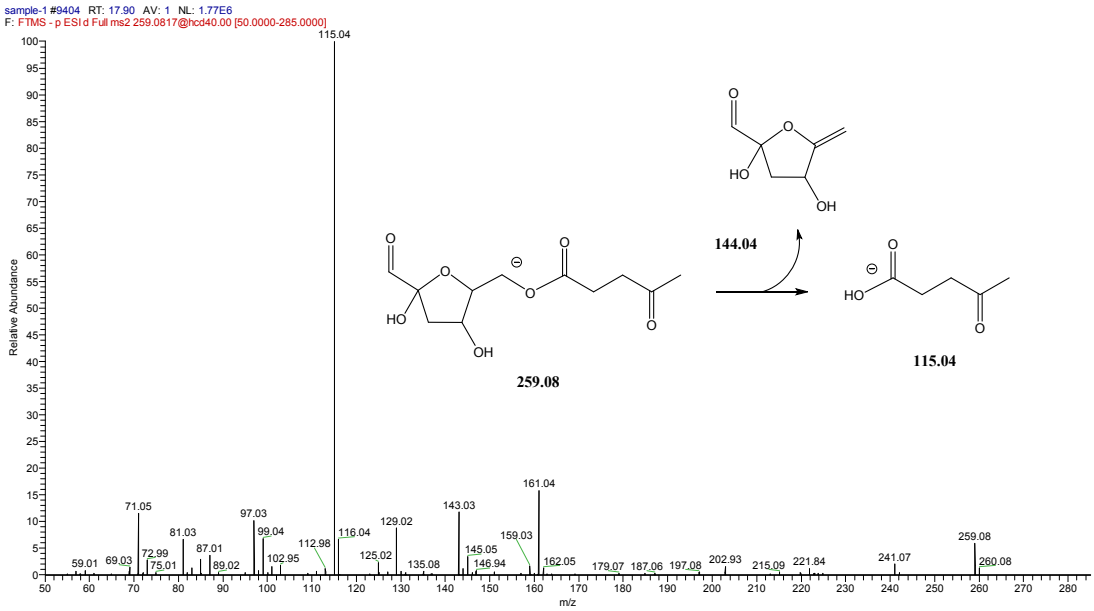

Figure S9 The MS^2 spectrum of de-protonated $C_{11}H_{16}O_7$ (17.97 min) and its possible fragmentation process

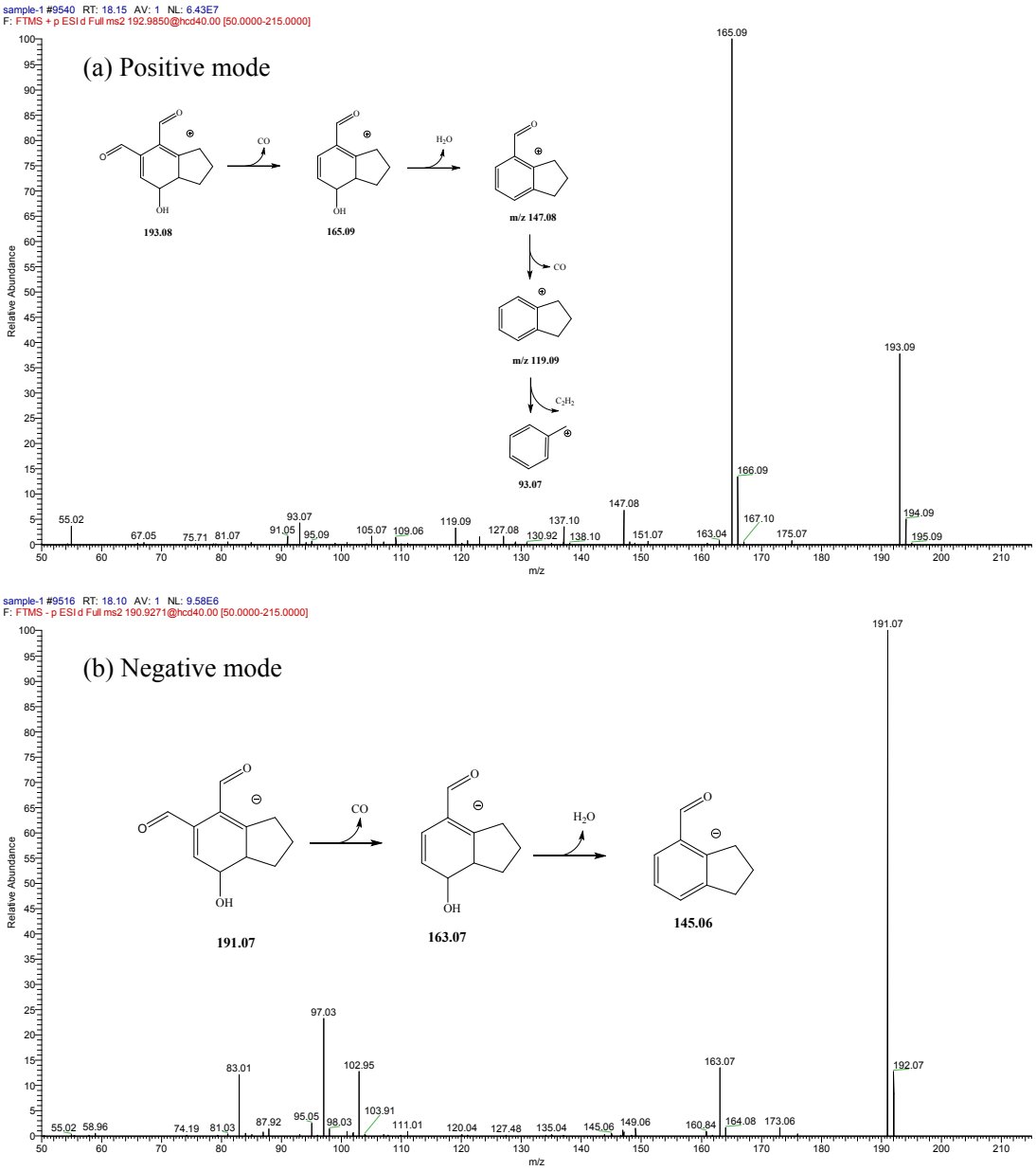

Figure S10 The MS² spectrum of (a) protonated and (b) de-protonated $C_{11}H_{12}O_3$ (18.11 min) and its possible fragmentation process

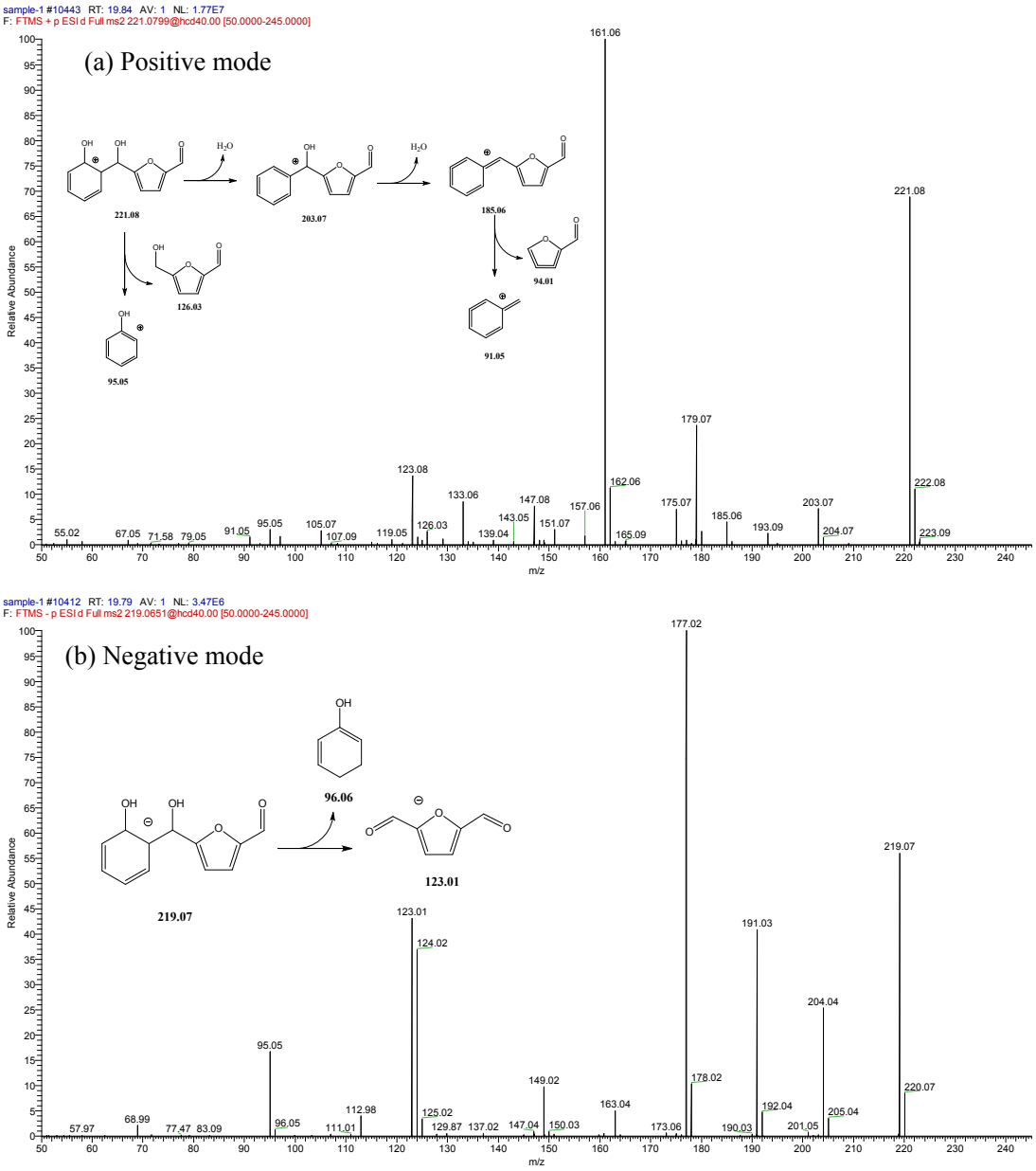

Figure S11 The MS² spectra of (a) protonated and (b) de-protonated $C_{12}H_{12}O_4$ (19.81 min) and its possible fragmentation process

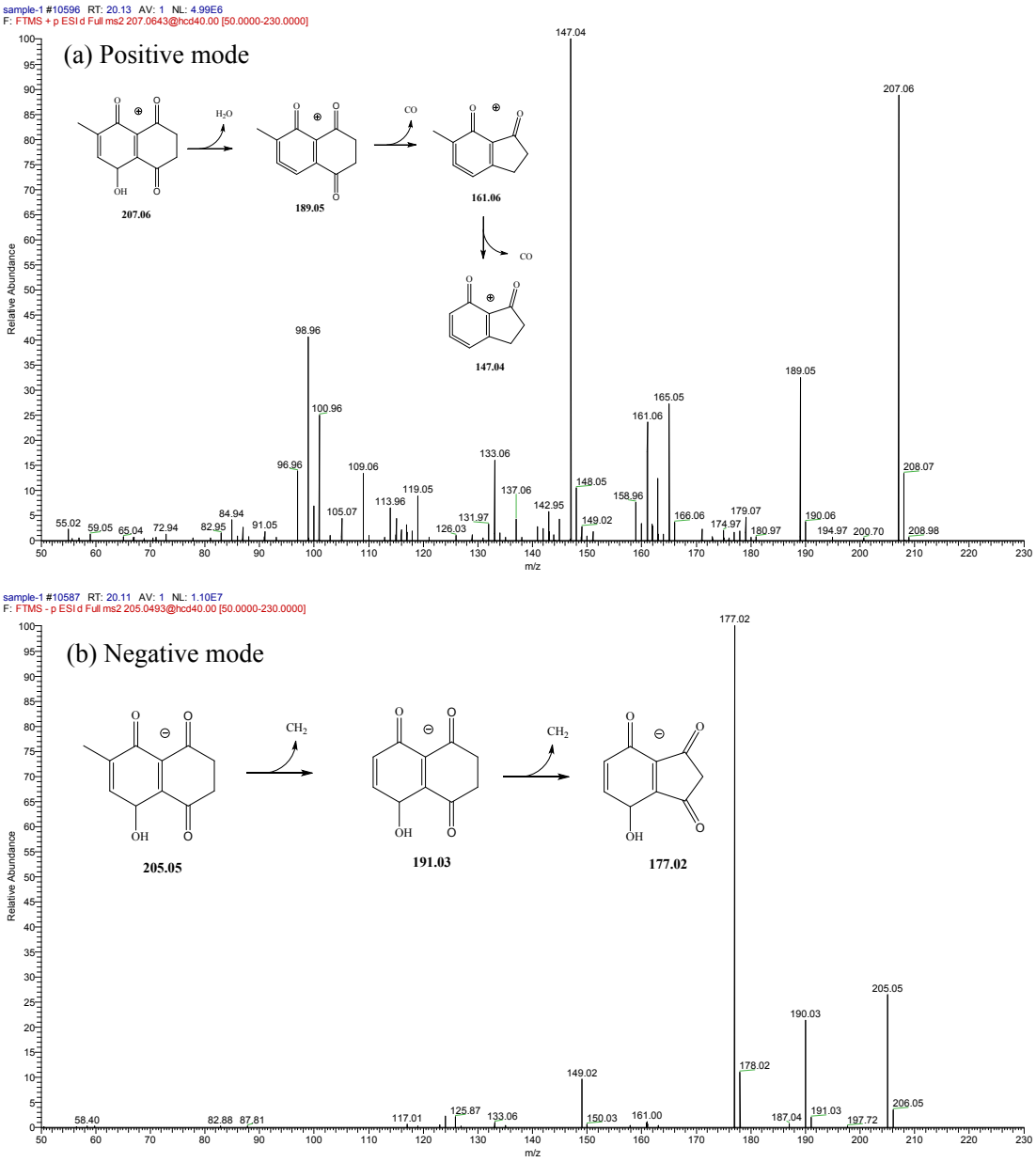

Figure S12 The MS^2 spectrum of (a) protonated and (b) de-protonated $C_{11}H_{10}O_4$ (20.07 min) and its possible fragmentation process

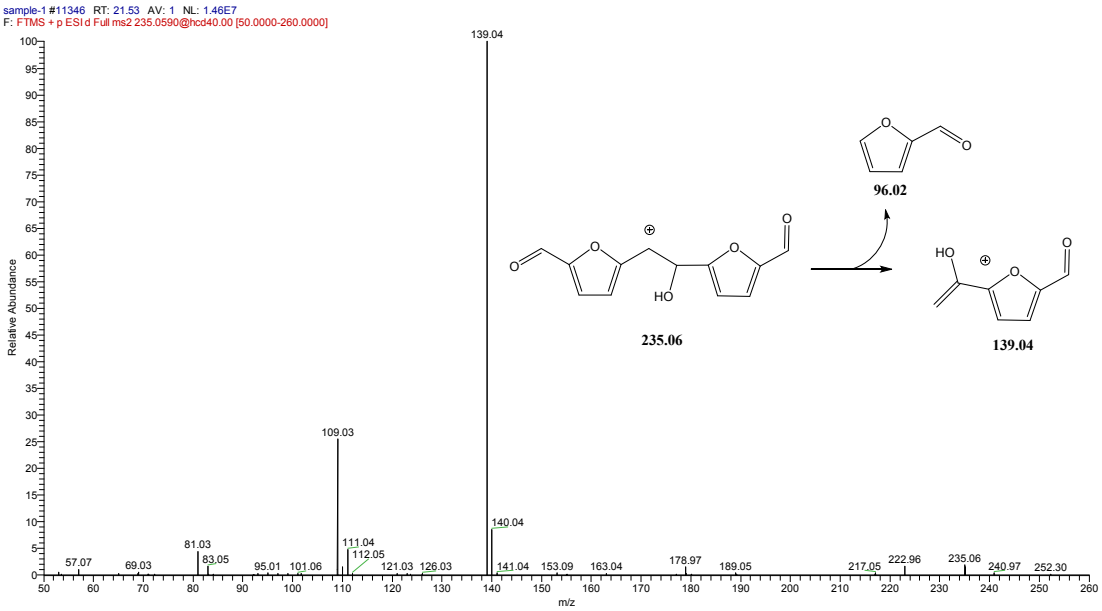

Figure S13 The MS^2 spectrum of protonated $C_{12}H_{10}O_5$ (21.45 min) and its possible fragmentation process

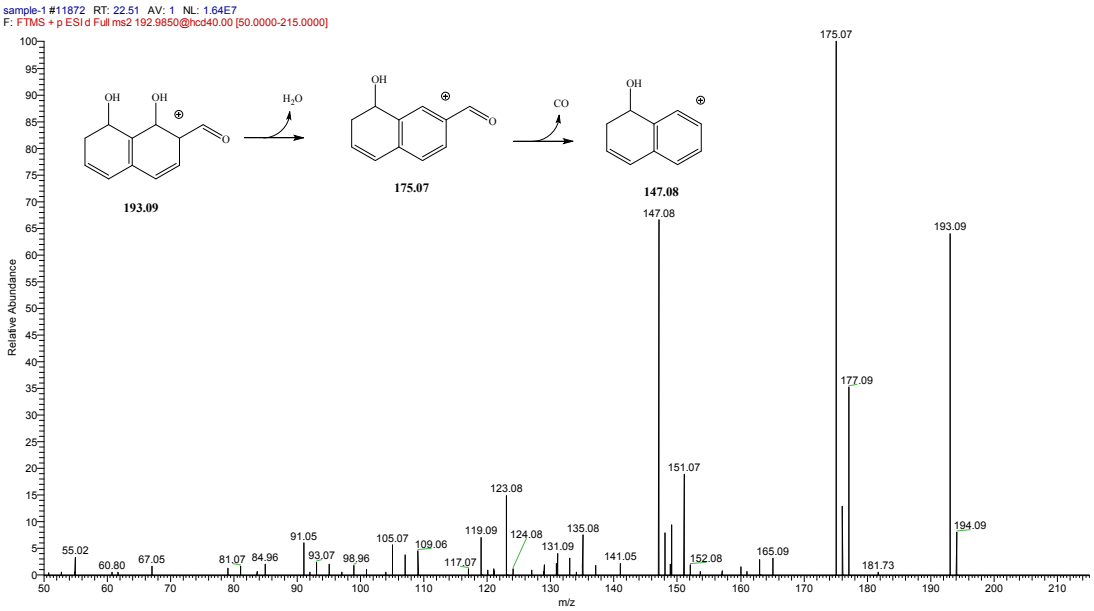

Figure S14 The MS^2 spectrum of protonated $C_{11}H_{12}O_3$ (22.43 min) and its possible fragmentation process

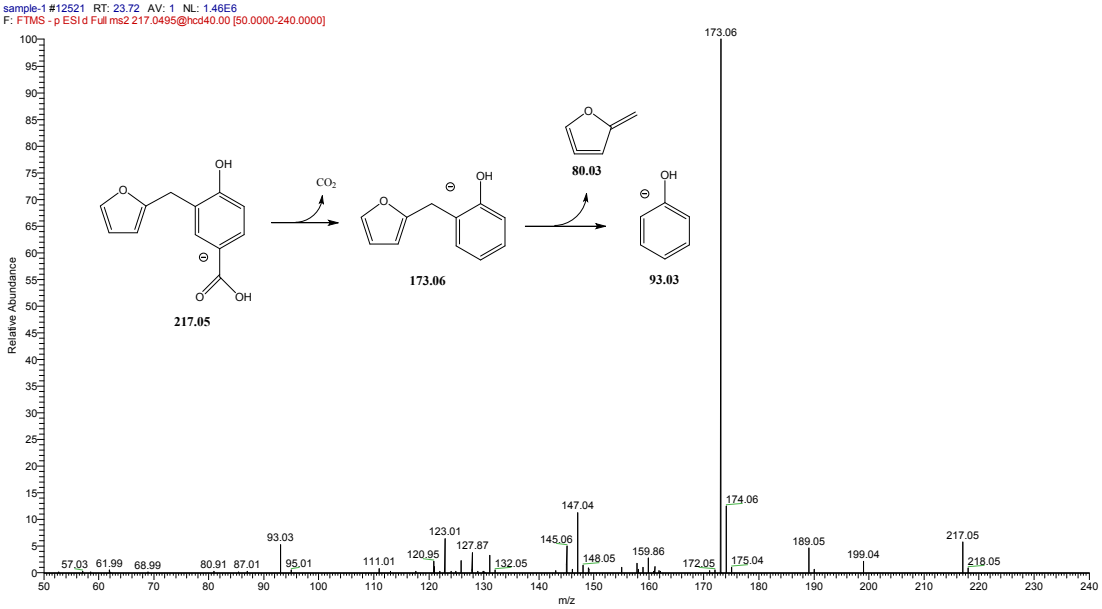

Figure S15 The MS^2 spectrum of de-protonated $C_{12}H_{10}O_4$ (23.64 min) and its possible fragmentation process

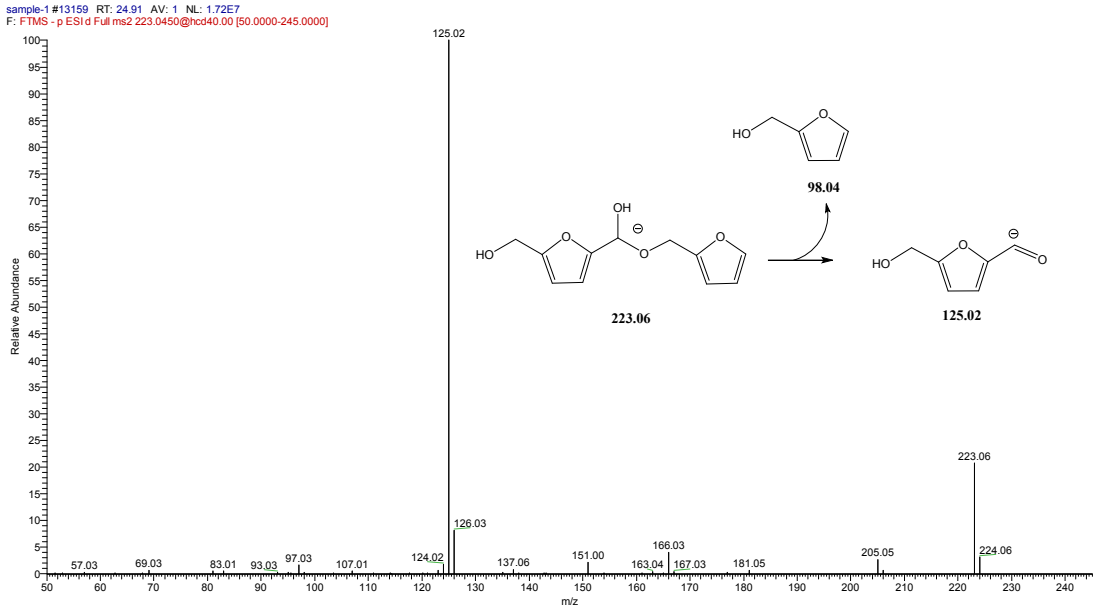

Figure S16 The MS^2 spectrum of de-protonated $C_{11}H_{12}O_5$ (24.82 min) and its possible fragmentation process

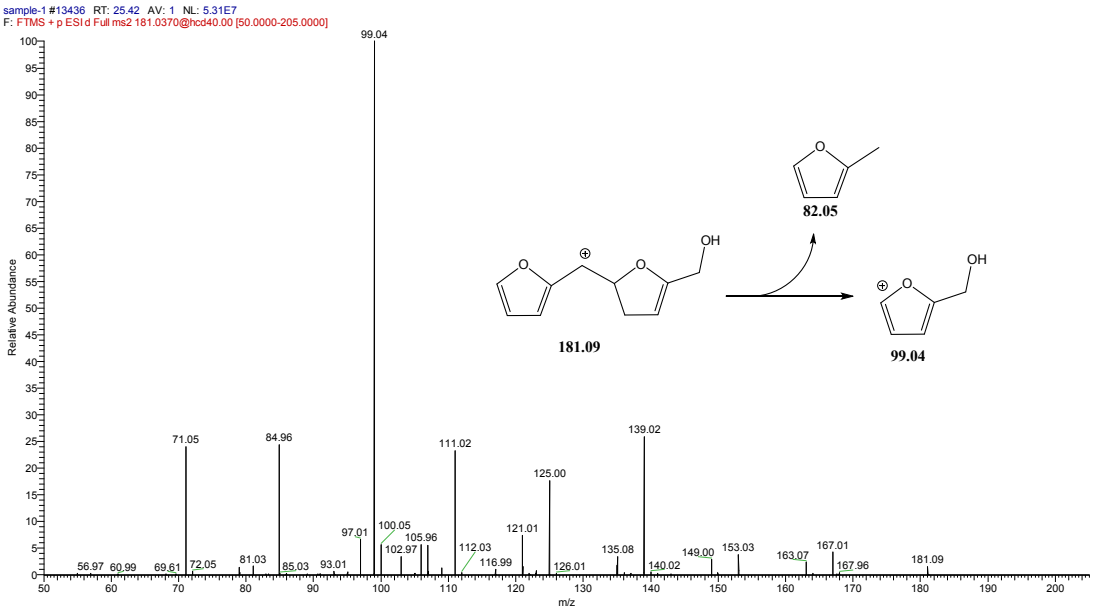

Figure S17 The MS^2 spectrum of protonated $C_{10}H_{12}O_3$ (25.42 min) and its possible fragmentation process

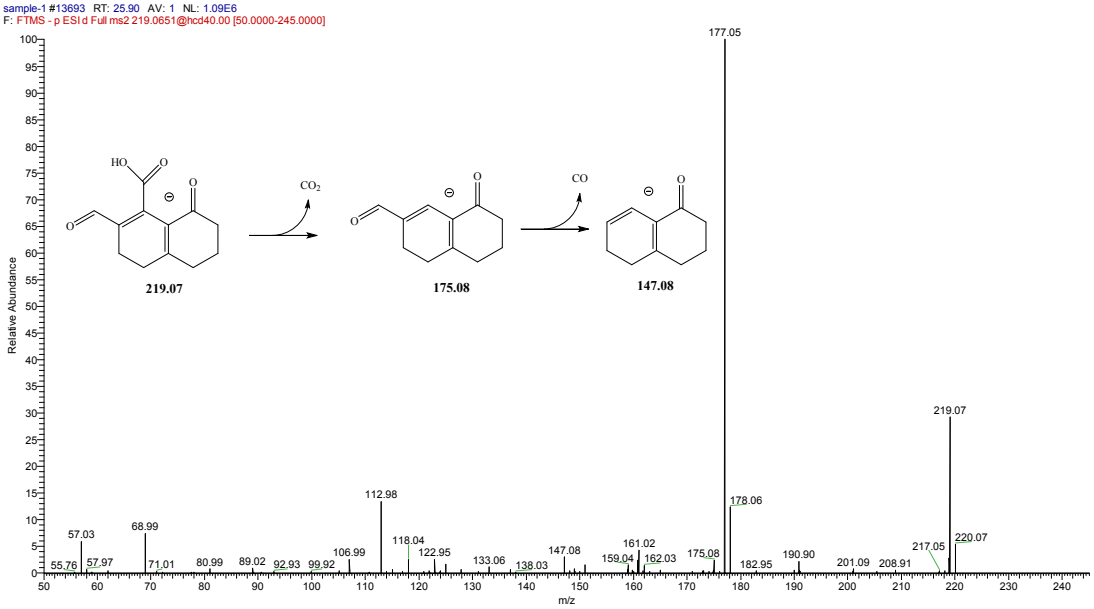

Figure S18 The MS^2 spectrum of de-protonated $C_{12}H_{12}O_4$ (25.56 min) and its possible fragmentation process