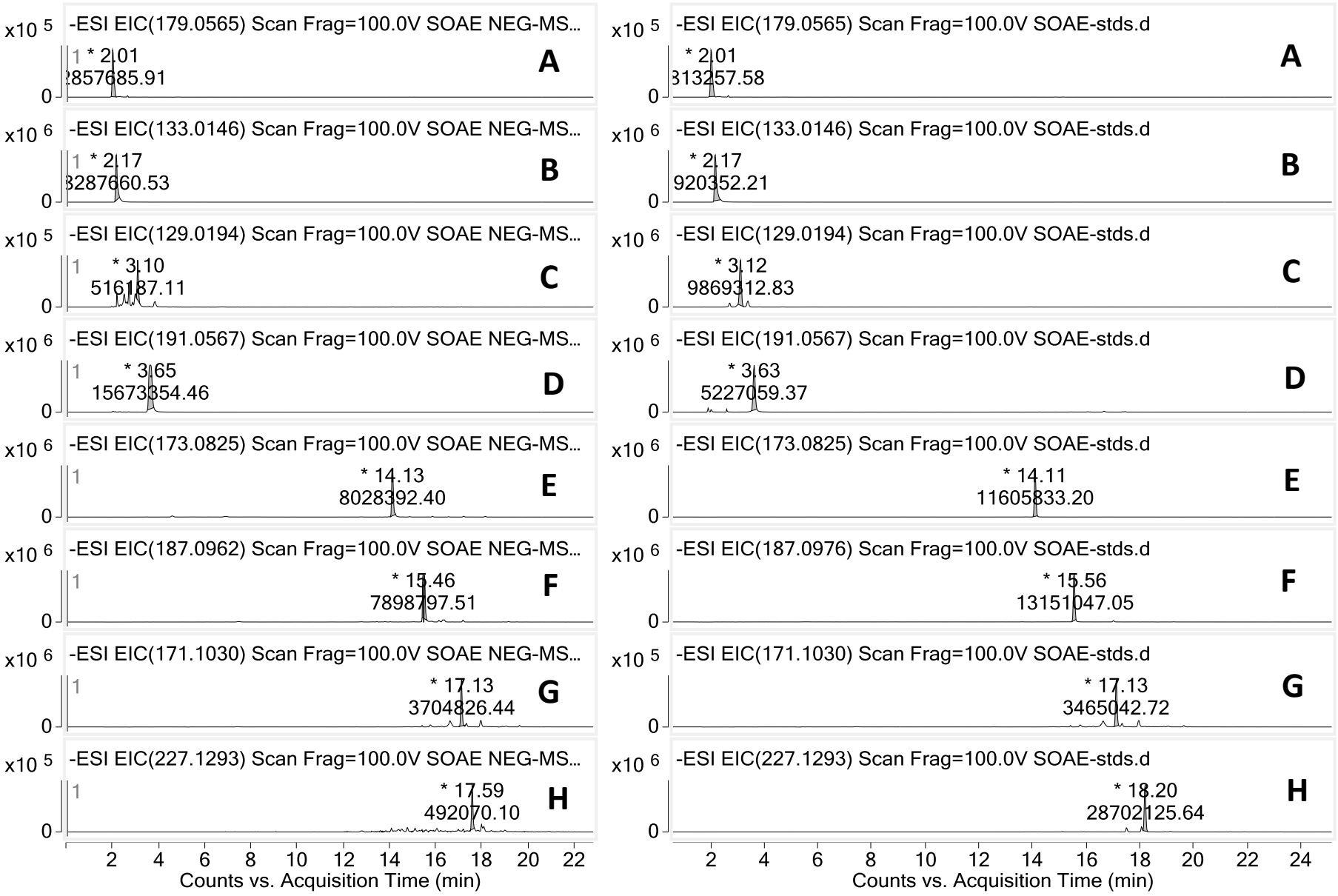


Fig. 1S. LC-ESI-MS-EICs of SOAE molecules in left panel, corresponding reference standards in right panel. A) glucose, B) malic acid, C) glutaconic acid, D) quinic acid, E) suberic acid, F) azelaic acid, G) oxo nonanoic acid and H) traumatic acid.

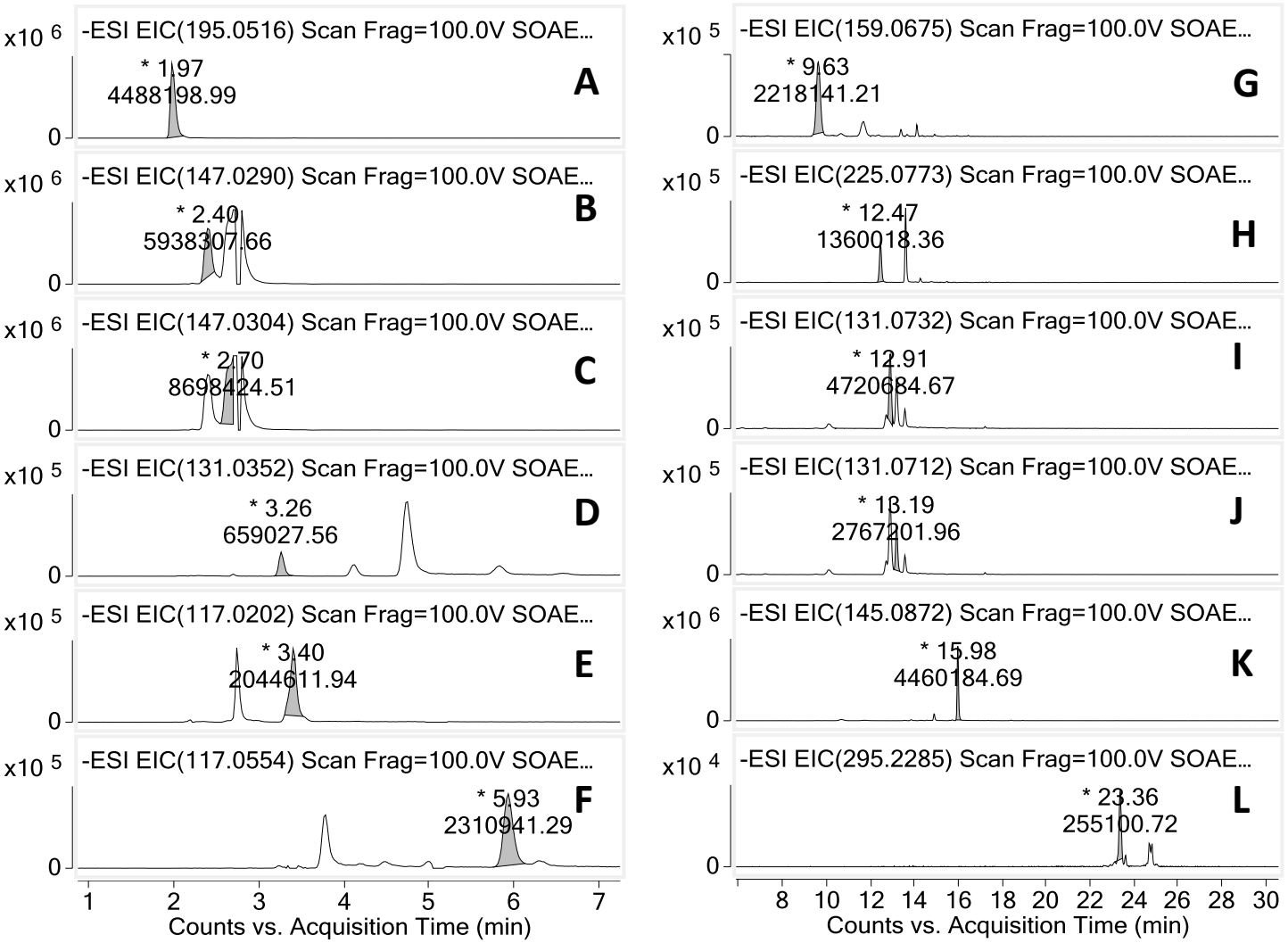


Fig. 2S. LC-ESI-MS-EICs of SOAE molecules, A) gluconic acid, B) hydroxy glutaric acid, C) 2-methylmalic acid, D) 2-hydroxy-4-oxopentanoate, E) erythrono-1,4-lactone, F) L-α-hydroxyisovaleric acid, G) pimelic acid, H) 4-hydroxy-(3',4'-dihydroxyphenyl)-valeric acid, I) hydroxy caproic acid, J) hydroxy caproic acid isomer, K) hydroxy heptanoic acid and L) hydroxy-linoleic acid isomer.

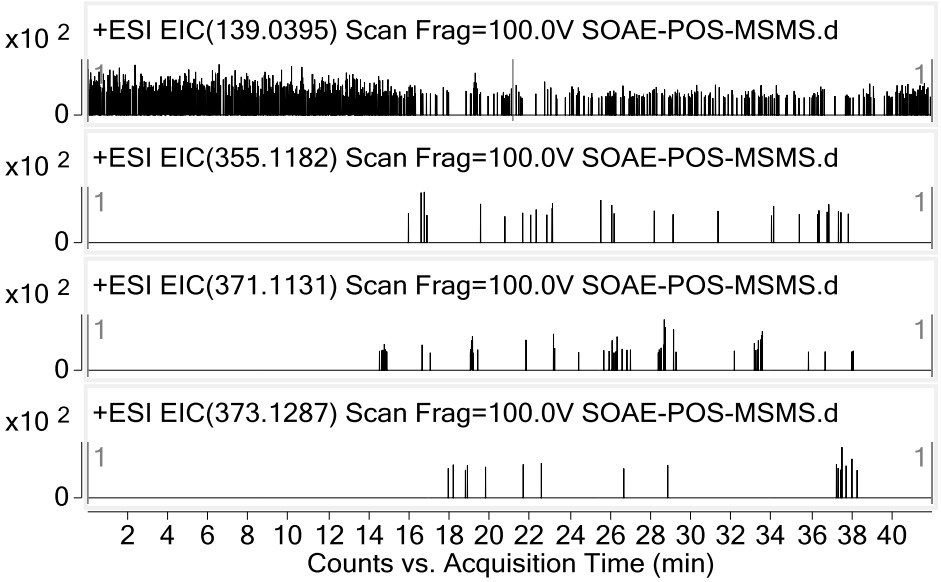


Fig. 3S (A). LC-ESI-MS extracted ion [M+H] chromatograms of A) Sesamol, B) Sesamin, C) Sesamolin and D) sesamolinol .

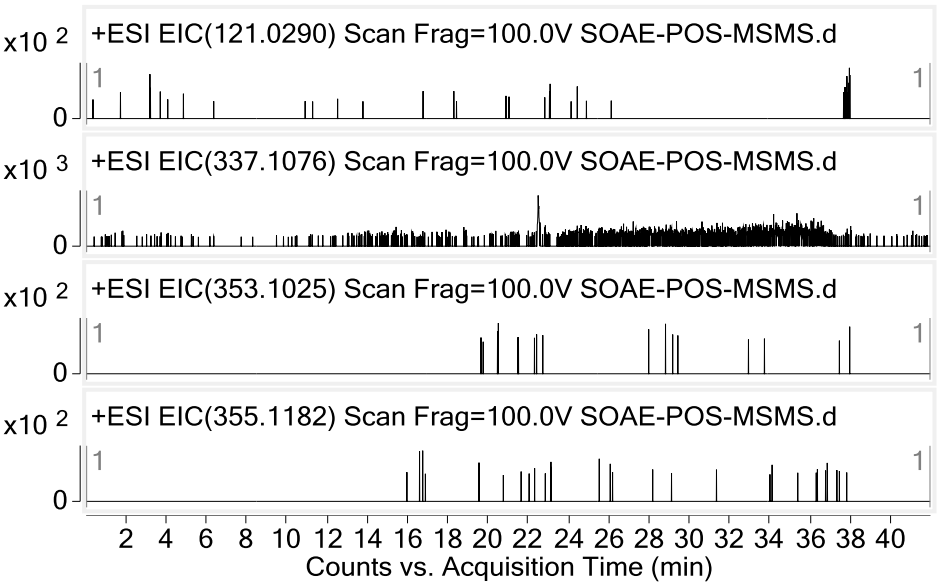


Fig. 3S (B). LC-ESI-MS extracted ion [M+H-H2O] chromatograms of A) Sesamol, B) Sesamin, C) Sesamolin and D) sesamolinol .

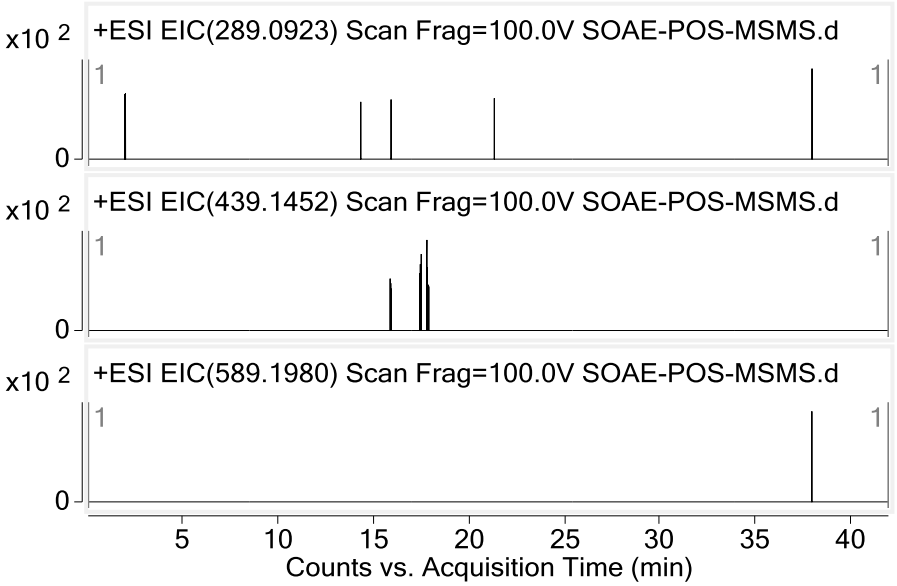


Fig. 3S (C). LC-ESI-MS extracted ion [M+H] chromatograms of sesamol A) mono glucosides B) di-glucosides C) tri-glucosides

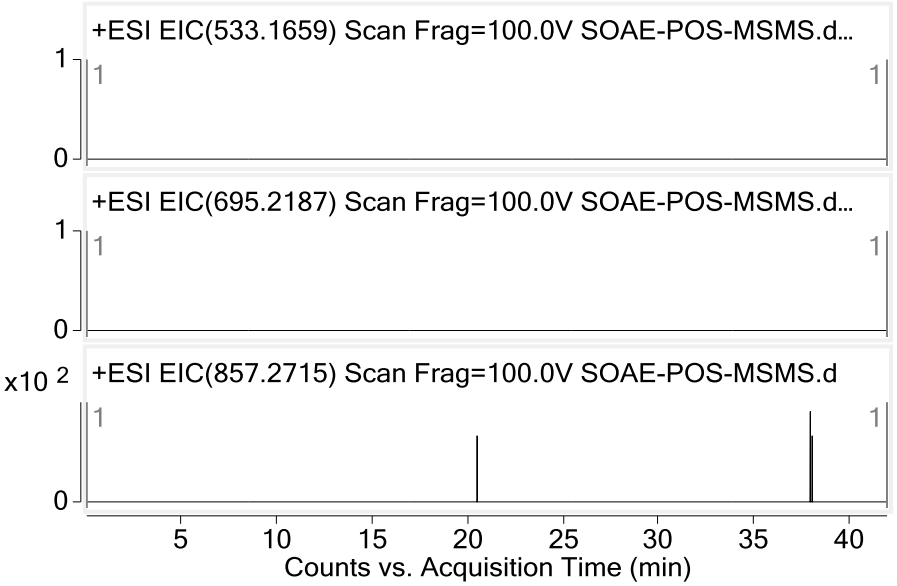


Fig. 3S (D). LC-ESI-MS extracted ion [M+H] chromatograms of sesaminol A) mono glucosides B) di-glucosides C) tri-glucosides

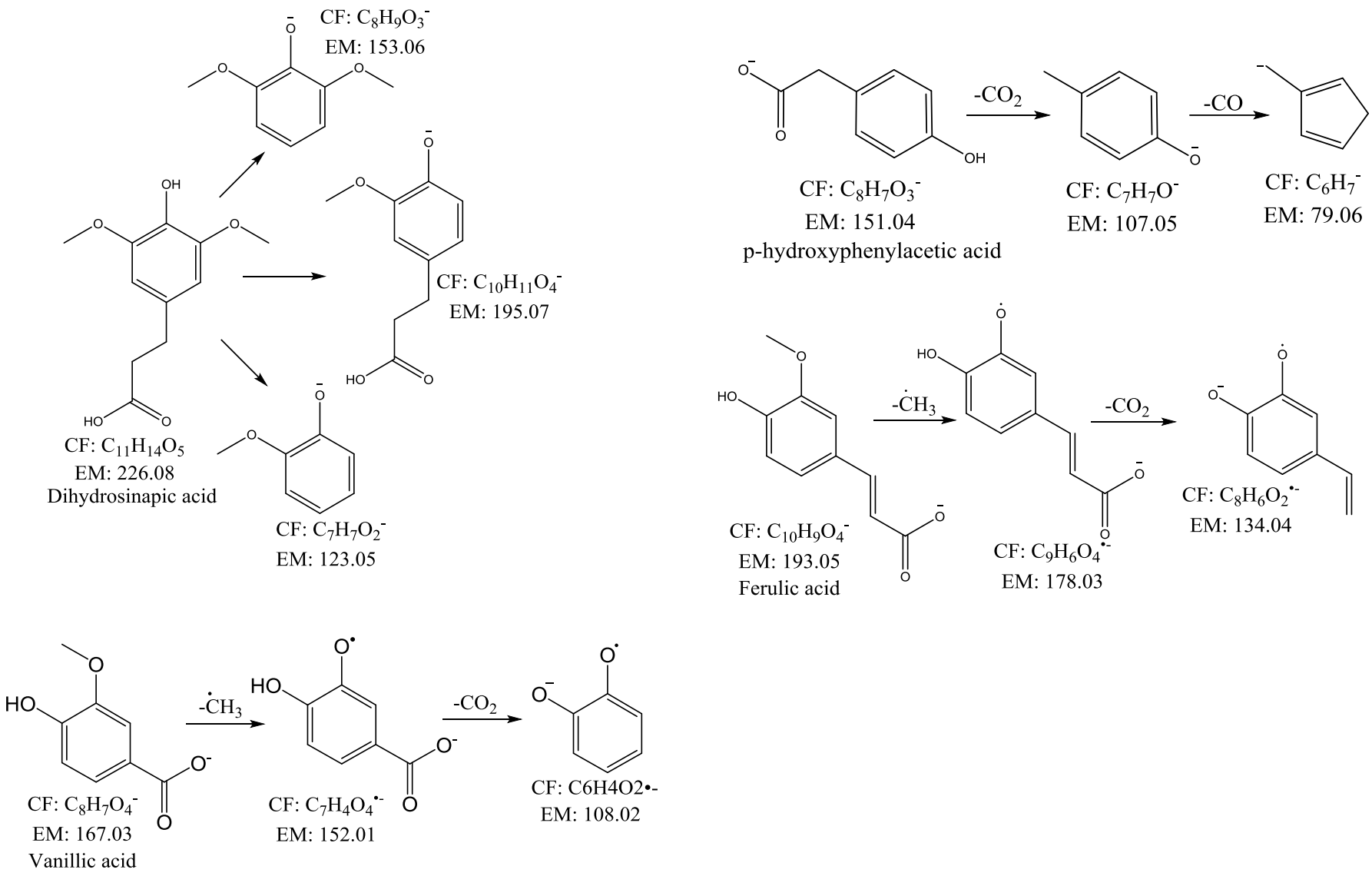


Fig. 4S. Fragmentation pattern of methoxyphenol derivatives and phenol derivatives.

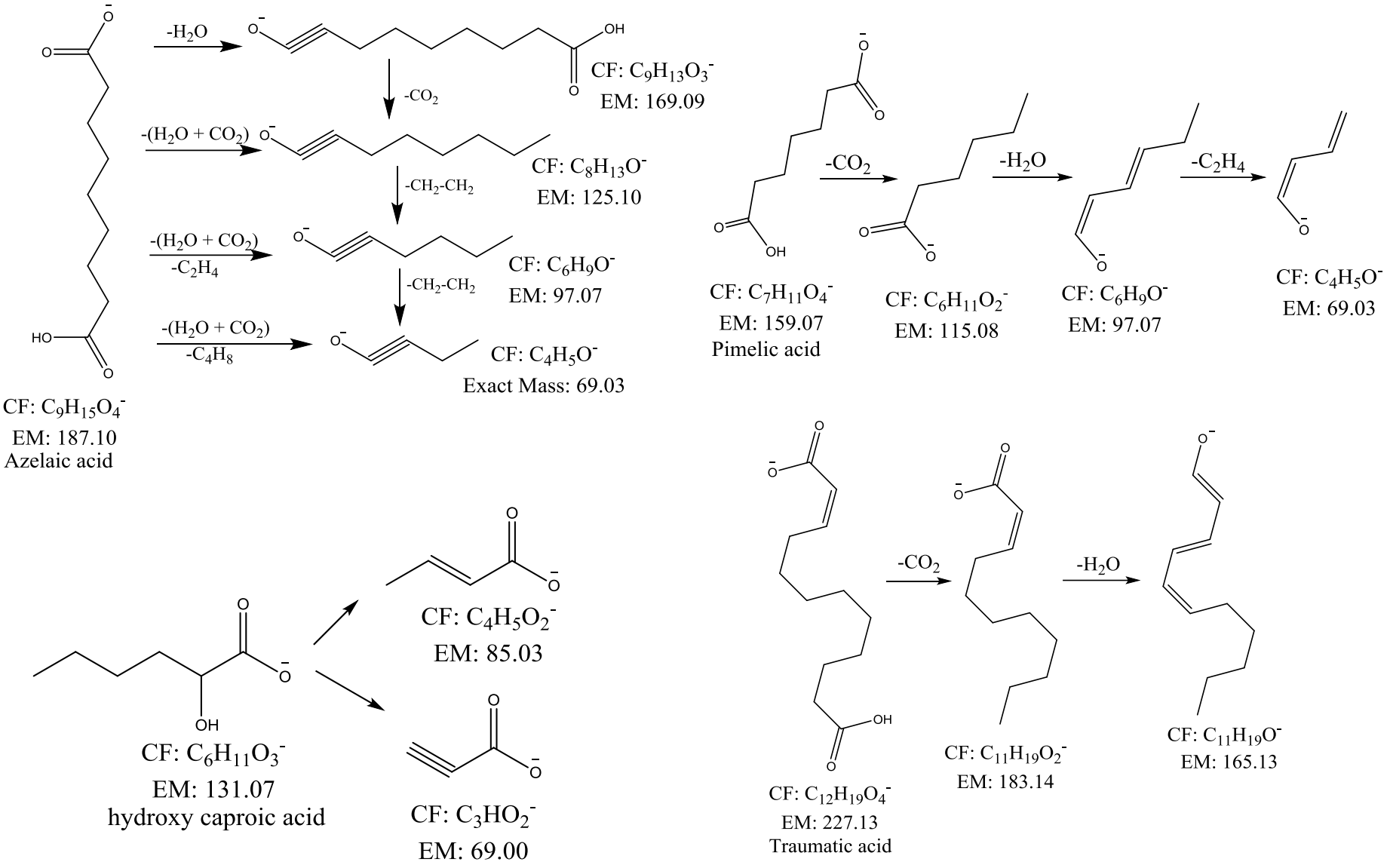


Fig. 5S. Fragmentation pattern of di-carboxylic acids and hydroxy carboxylic acids

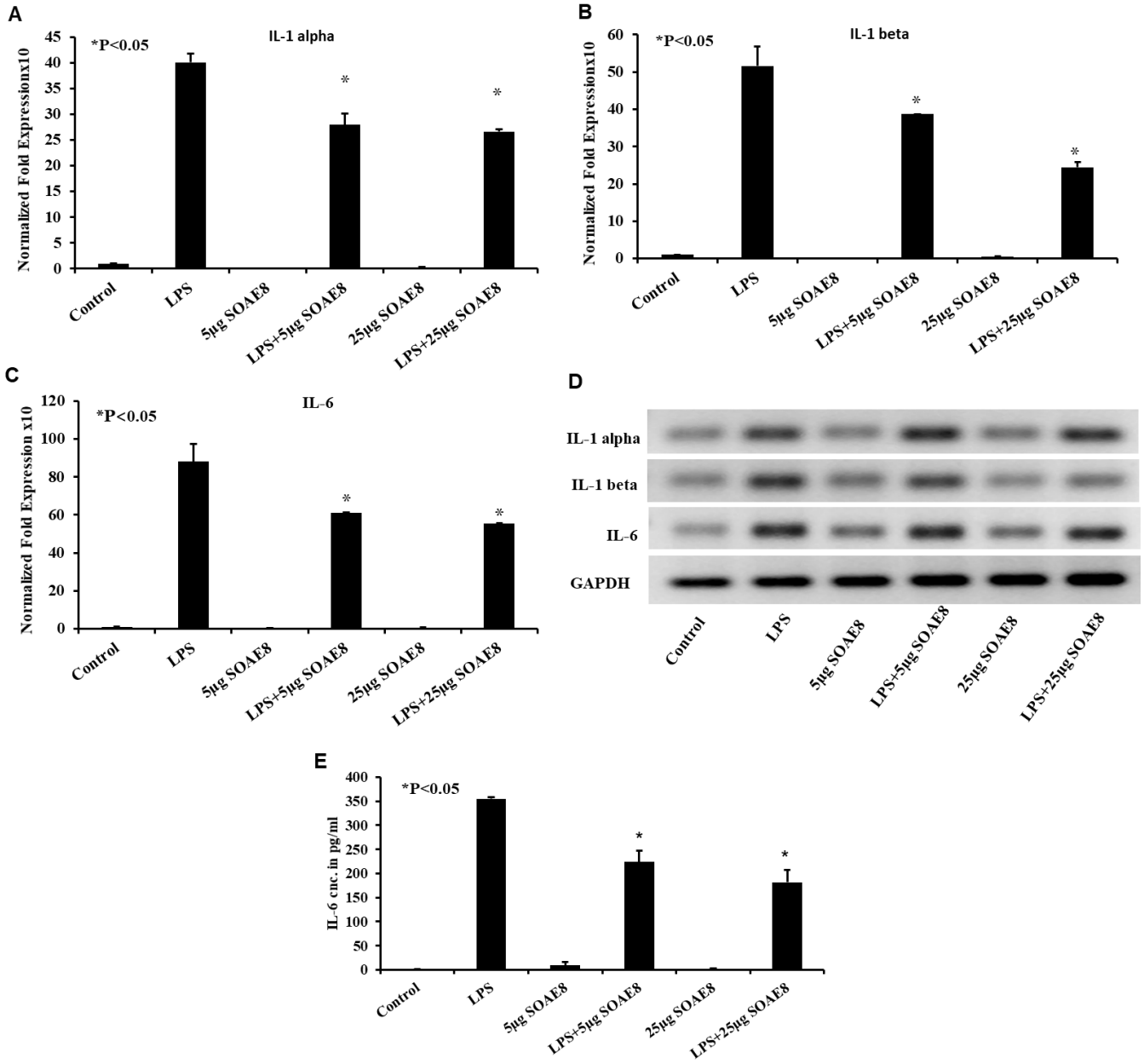


Fig. 6S: SOAE-8 attenuates LPS-induced inflammatory cytokines in RAW 264.7 macrophages: RAW macrophages were pre-treated with SOAE -8 (5 and 25µg/ml) followed by addition of 10ng/ml LPS. Cells were incubated for 24 hours following which RNA was isolated and real time PCR analysis was performed for IL-1α (A), IL- 1β (B), IL-6 (C) gene expression, PCR products (D). (n>3; * P<0.05) and (E) ELISA for IL-6.

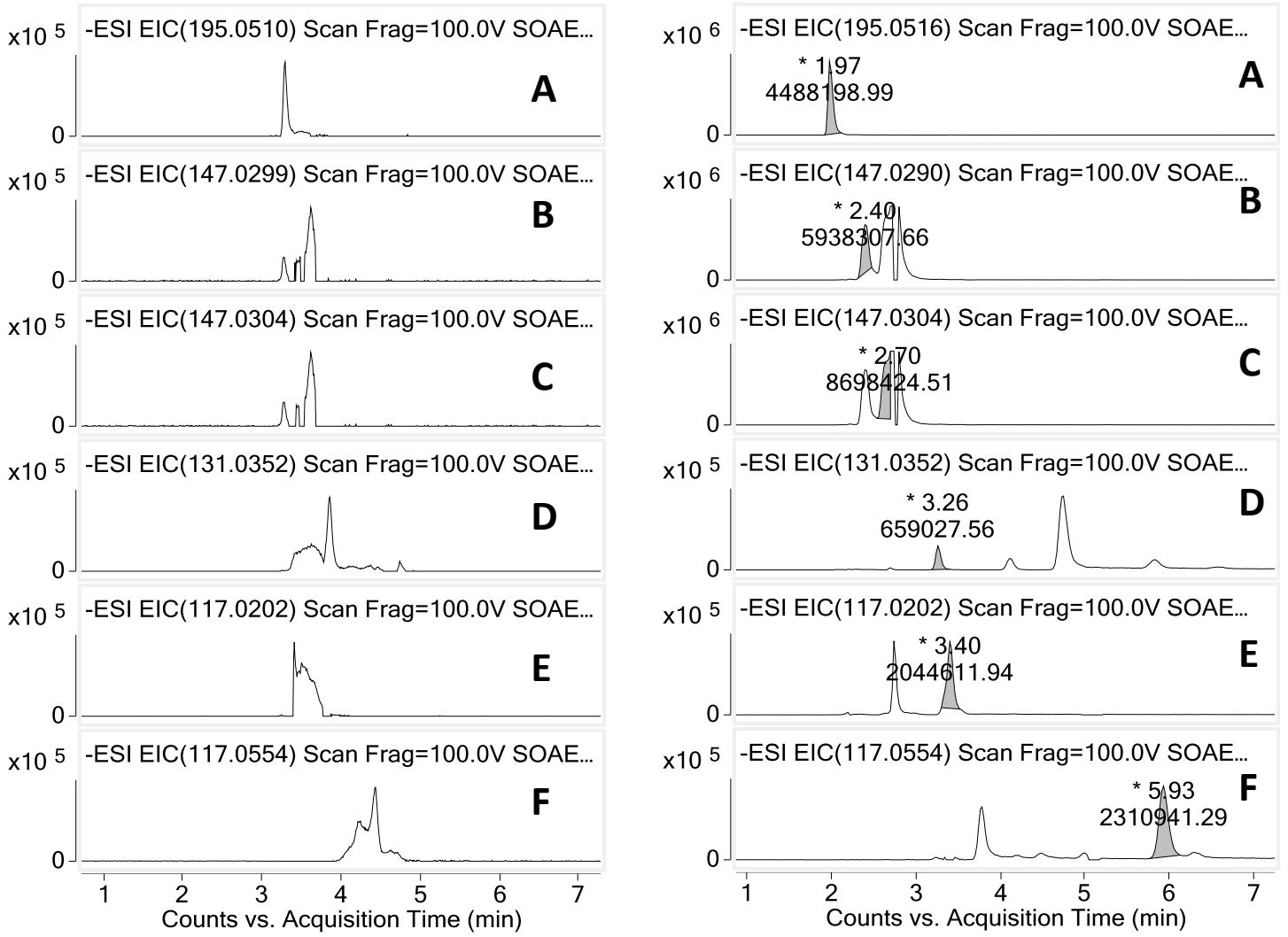


Fig 7S. LC-ESI-MS-EICs of SOAE identified molecules of A) gluconic acid, B) hydroxy glutaric acid, C) 2-methylmalic acid, D) 2-hydroxy-4-oxopentanoate, E) erythrono-1,4-lactone and F) L-α-hydroxyisovaleric acid analyzed on different columns, Hilic (left panel) and Zorbax C18 (right panel)

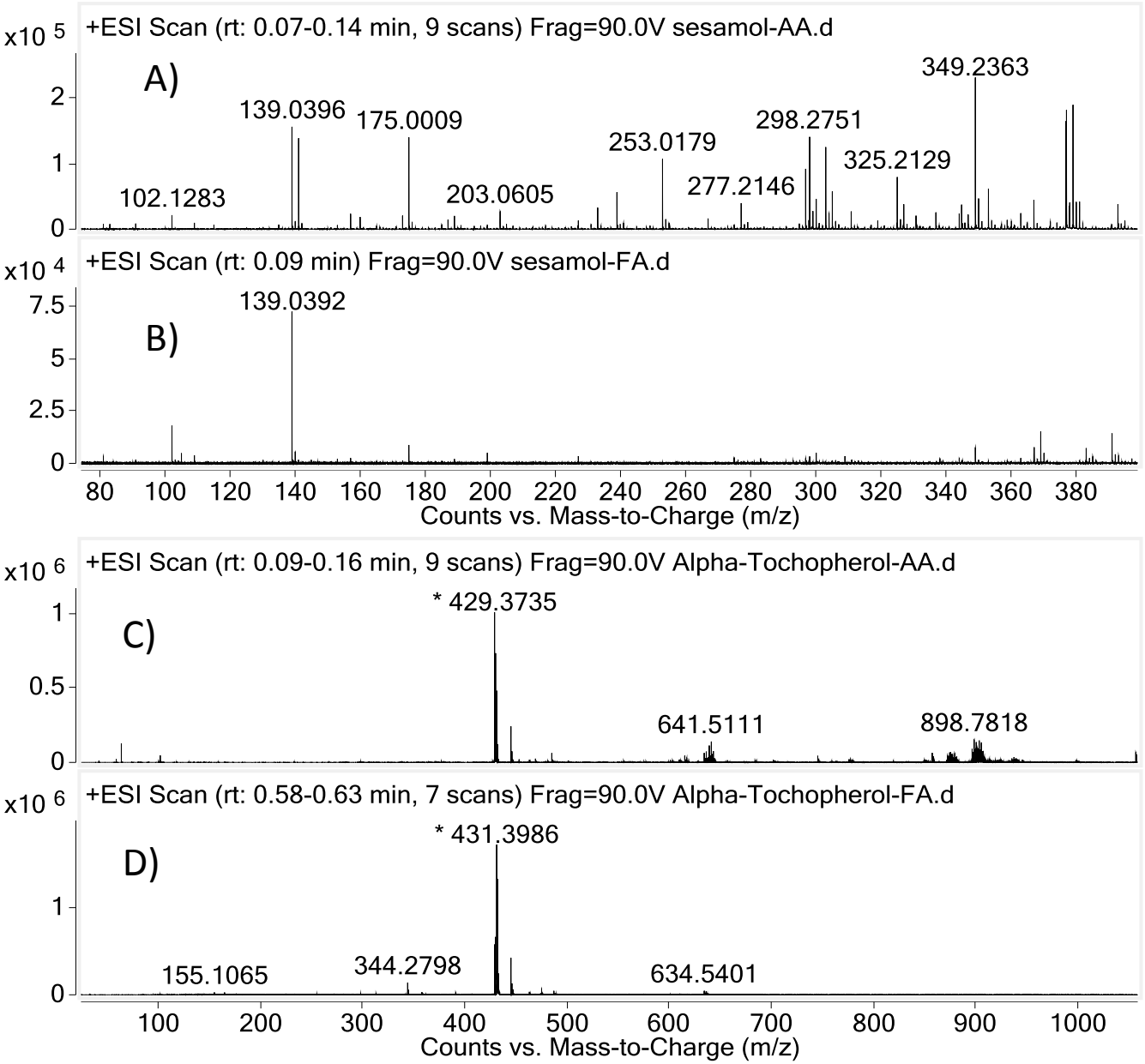
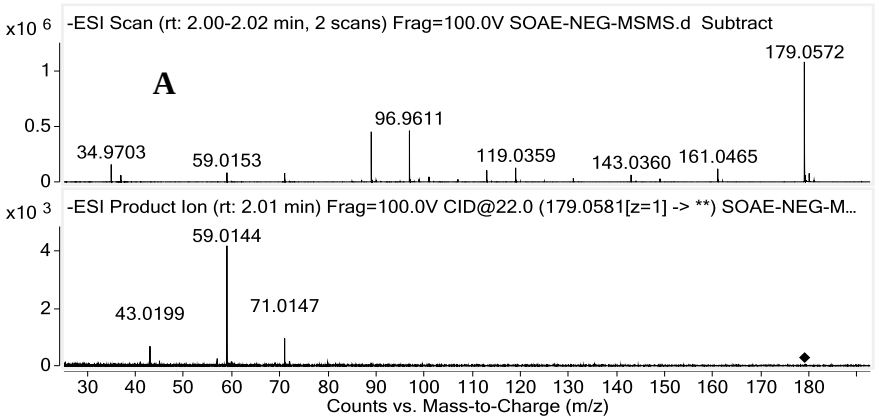
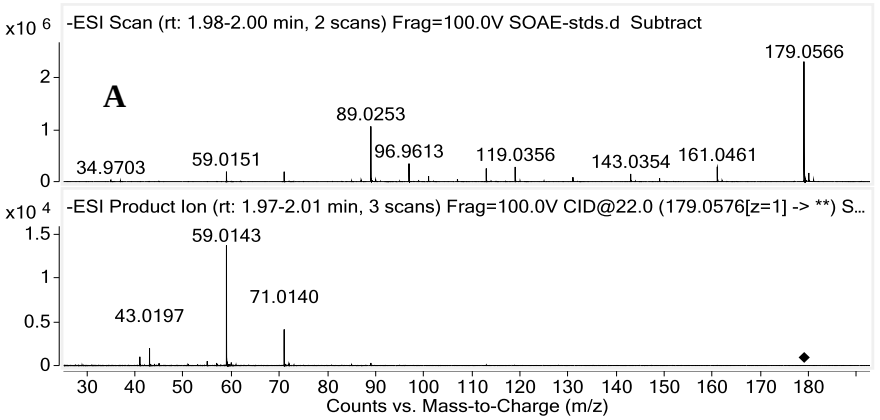
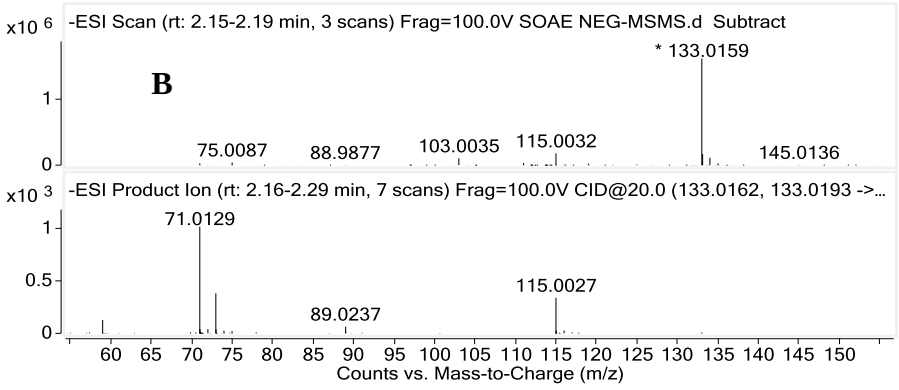
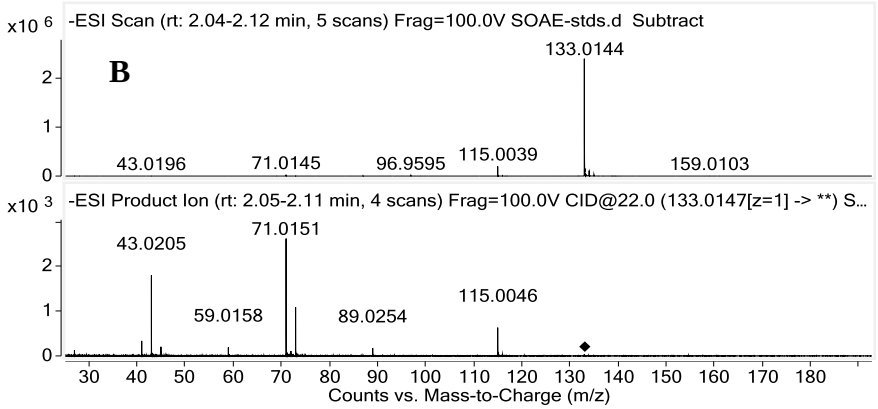


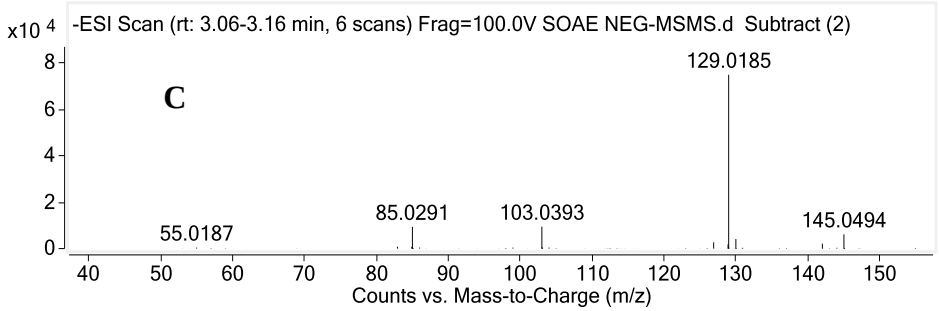
Fig. 8S. ESI-HRMS spectra of sesamol analyzed in A) ammonium acetate and B) formic acid buffers, α-tocopherol analyzed in C) ammonium acetate and D) formic acid.











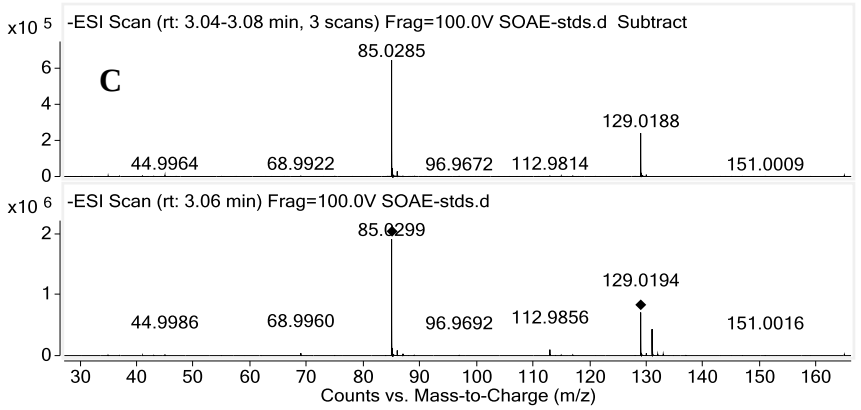


Fig. 9S (A). ESI-HRMS and MS/MS spectra of SOAE (left panel) and standards (right panel) of A) glucose, B) malic acid and C) glutaconic acid.

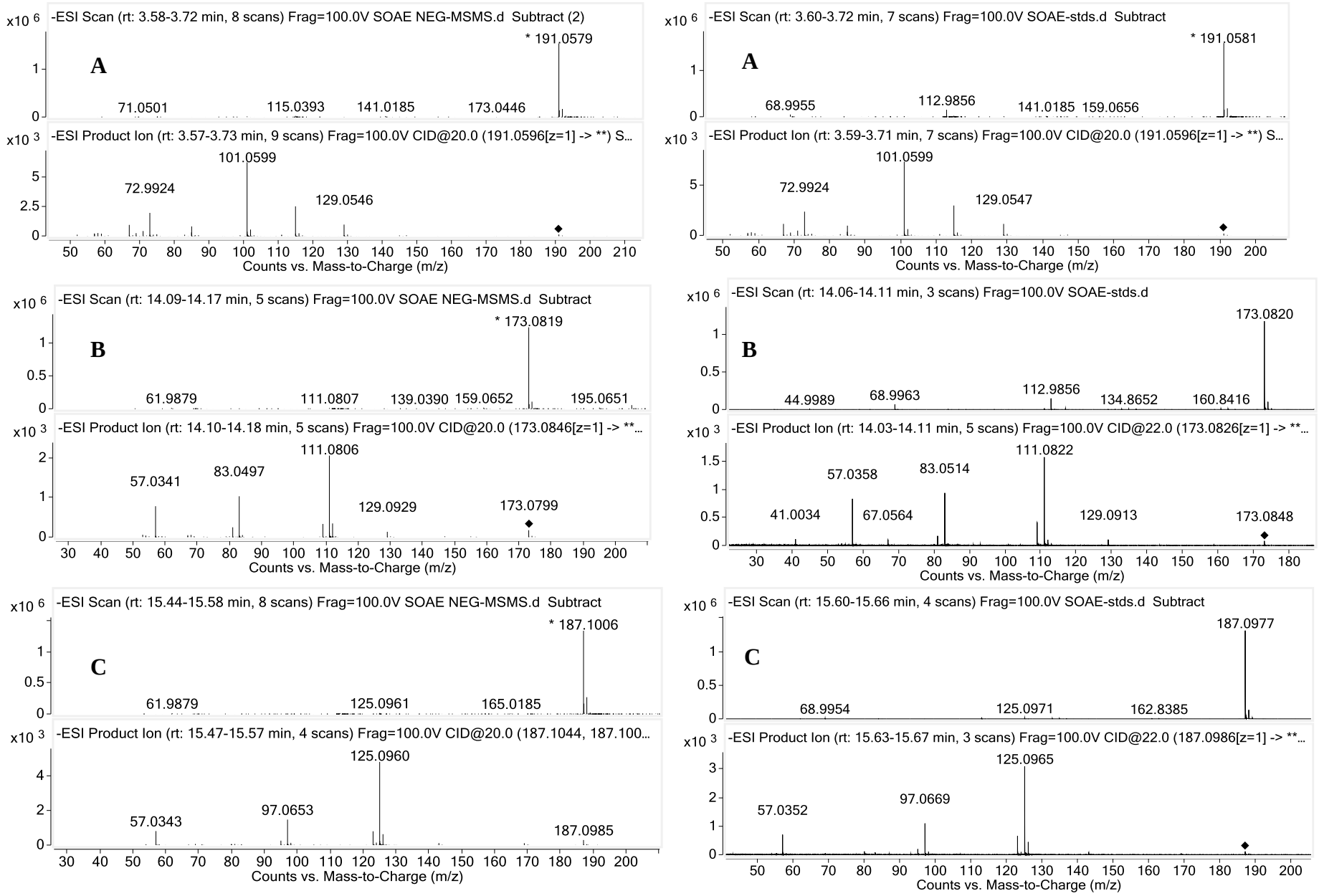
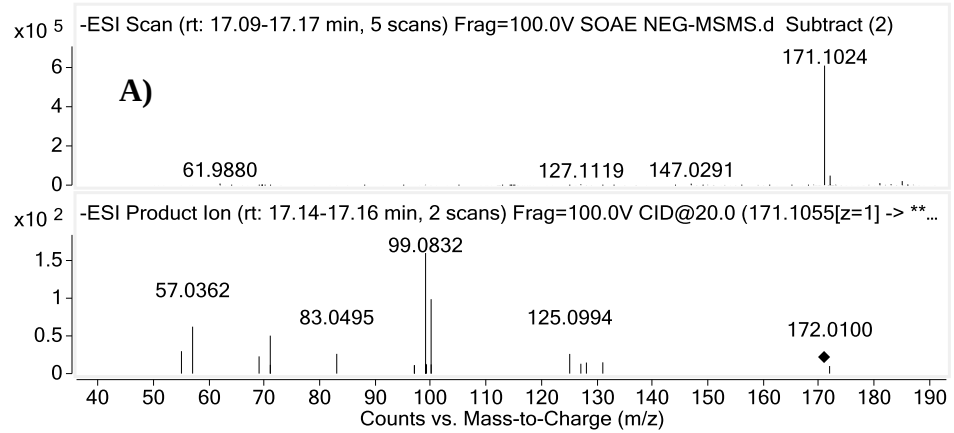
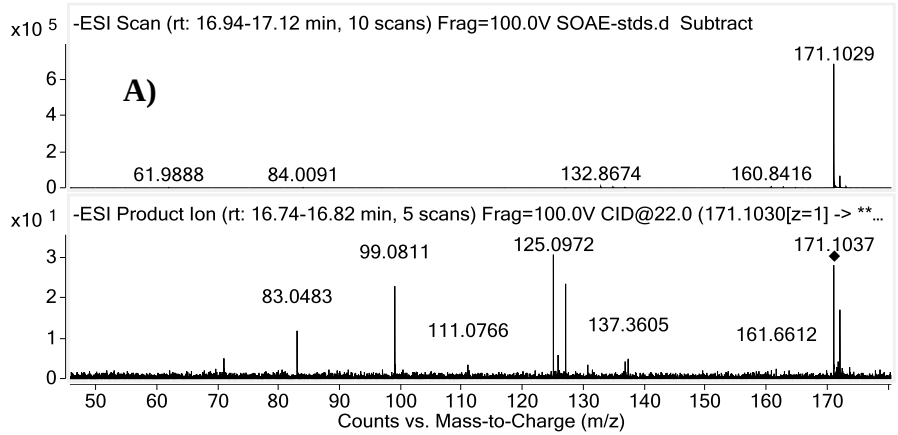
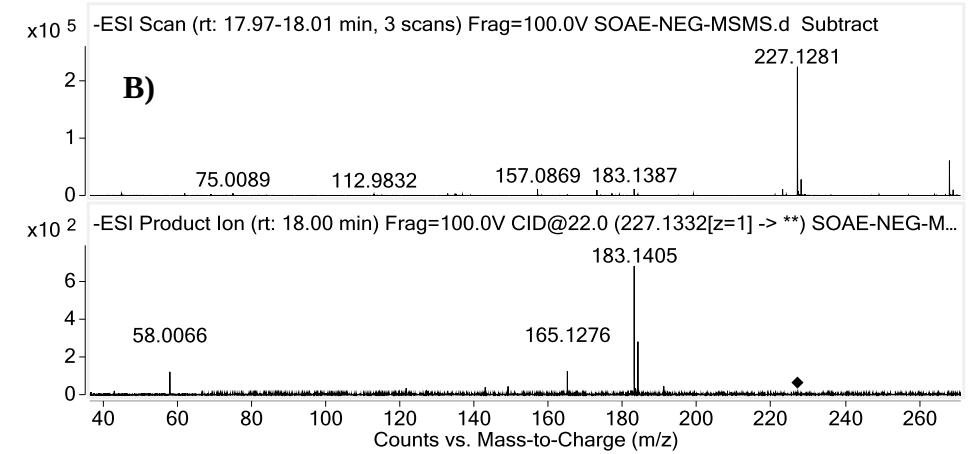


Fig. 9S(B). ESI-HRMS and MS/MS spectra of SOAE (left panel) and standards (right panel) of A) quinic acid, B) suberic acid and C) azelaic acid.







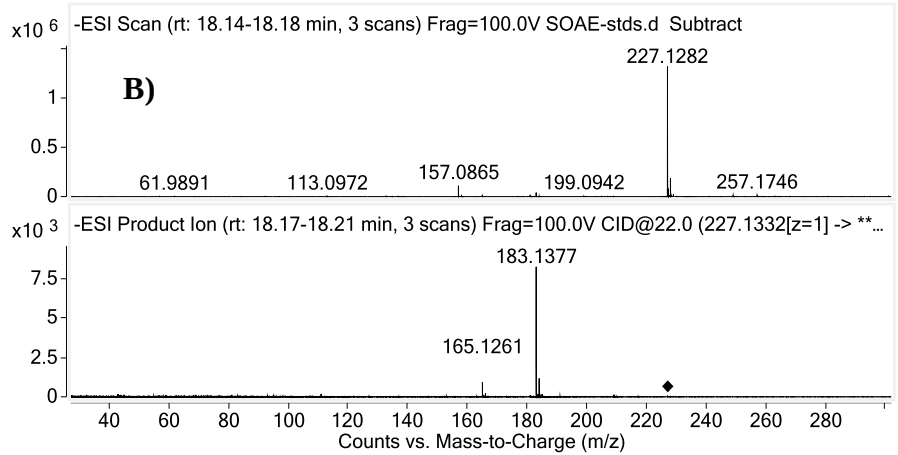


Fig. 9S(C). ESI-HRMS and MS/MS spectra of SOAE (left panel) and standards (right panel) of A) oxo nonanoic acid and B) traumatic acid.

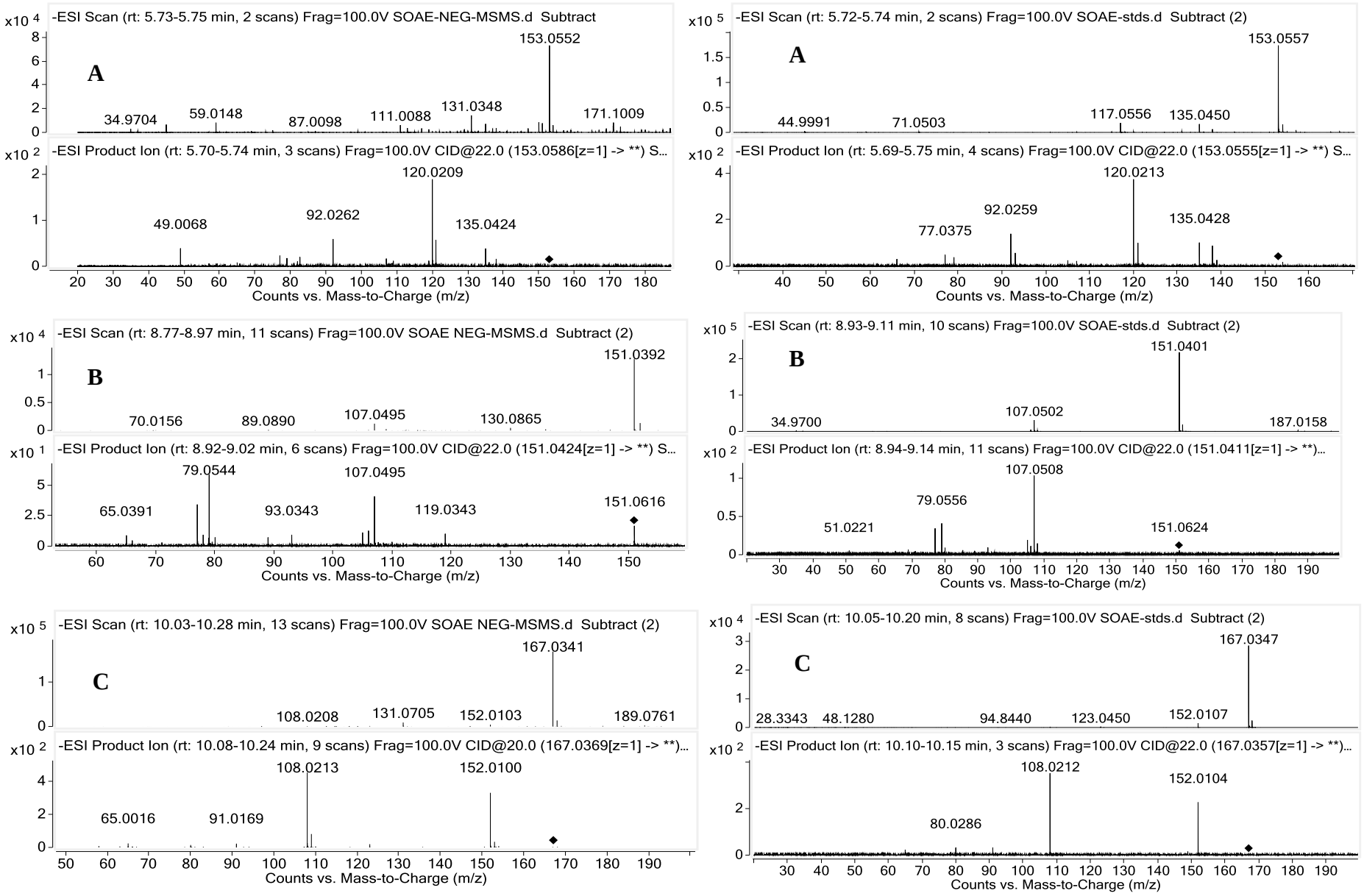


Fig. 9S(D): ESI-HRMS and MS/MS spectra of SOAE molecules (left panel) and standards (right panel) of A)vanillyl alcohol, B) p-hydroxyphenylacetic acid and C) vanillic acid

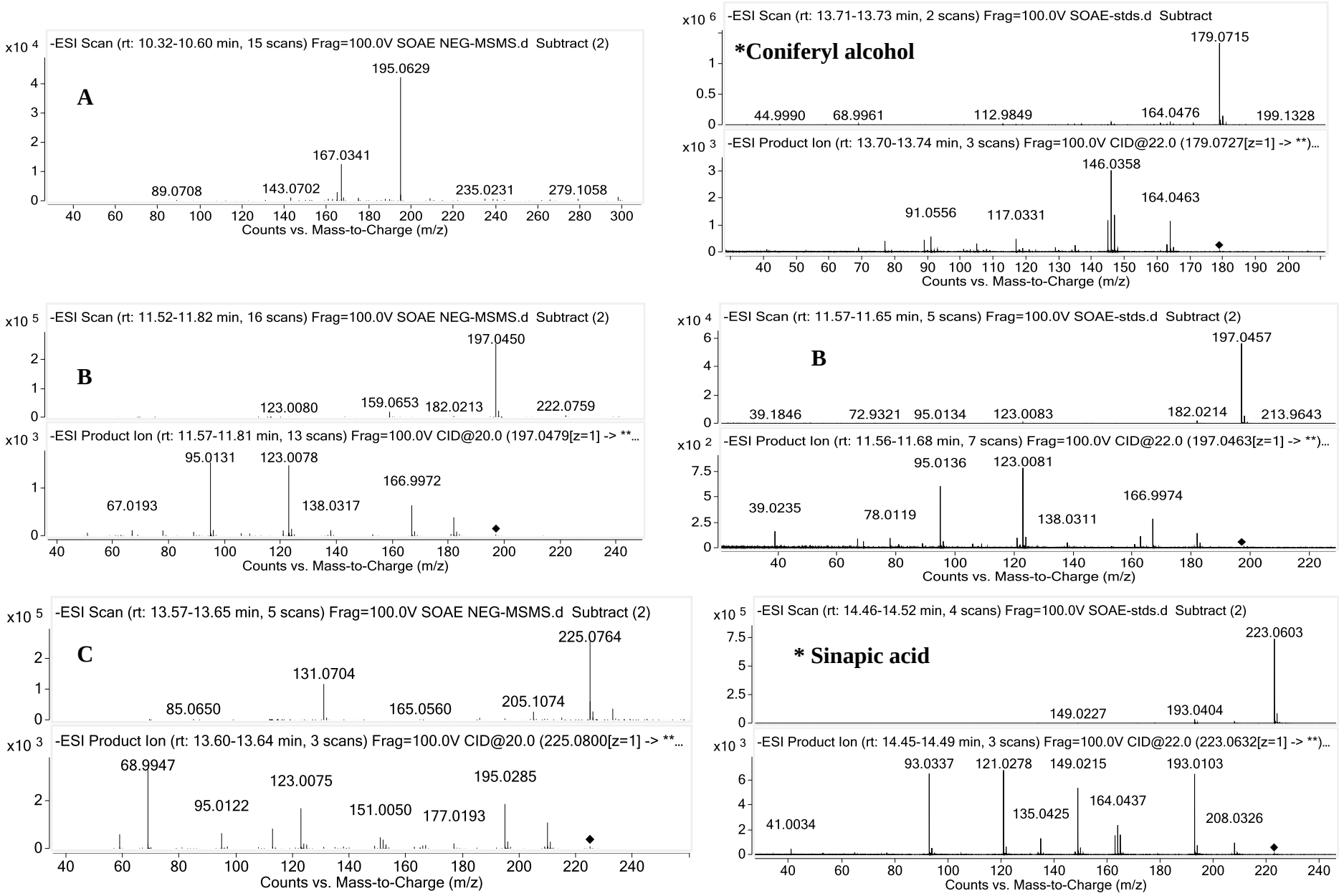


Fig. 9S(E): ESI-HRMS and MS/MS spectra of SOAE molecules (left panel) and standards* (right panel) of A) 5-hydroxy coniferyl alcohol, B) syringic acid and C) dihydrosinapic acid

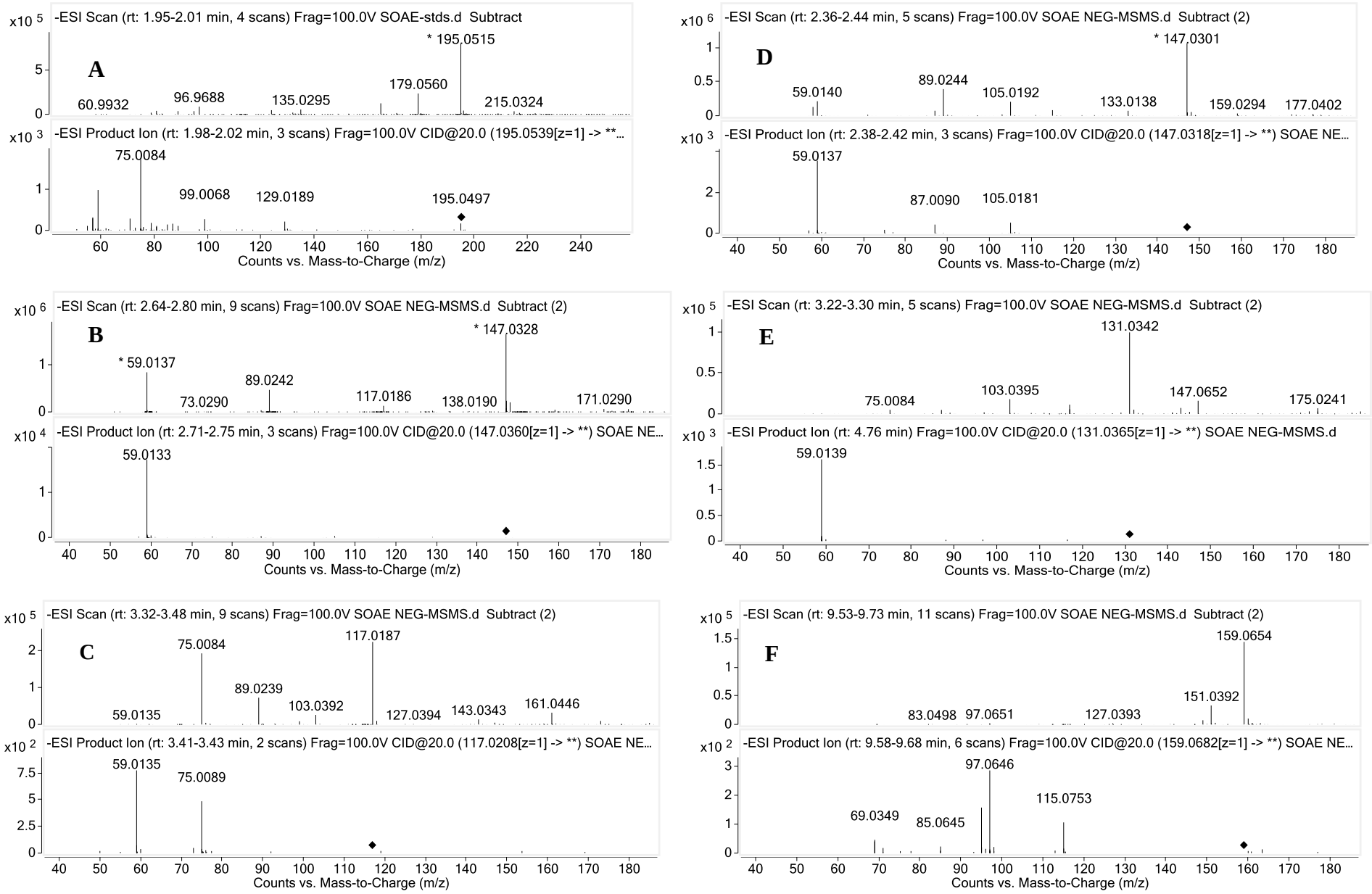


Fig. 9S(F) : ESI-HRMS and MS/MS spectra of SOAE molecules of A) gluconic acid, B) 2-methylmalic acid, C) erythrono-1,4-lactone, D) hydroxy glutaric acid, E) 2-hydroxy-4-oxopentanoate and F) pimelic acid.

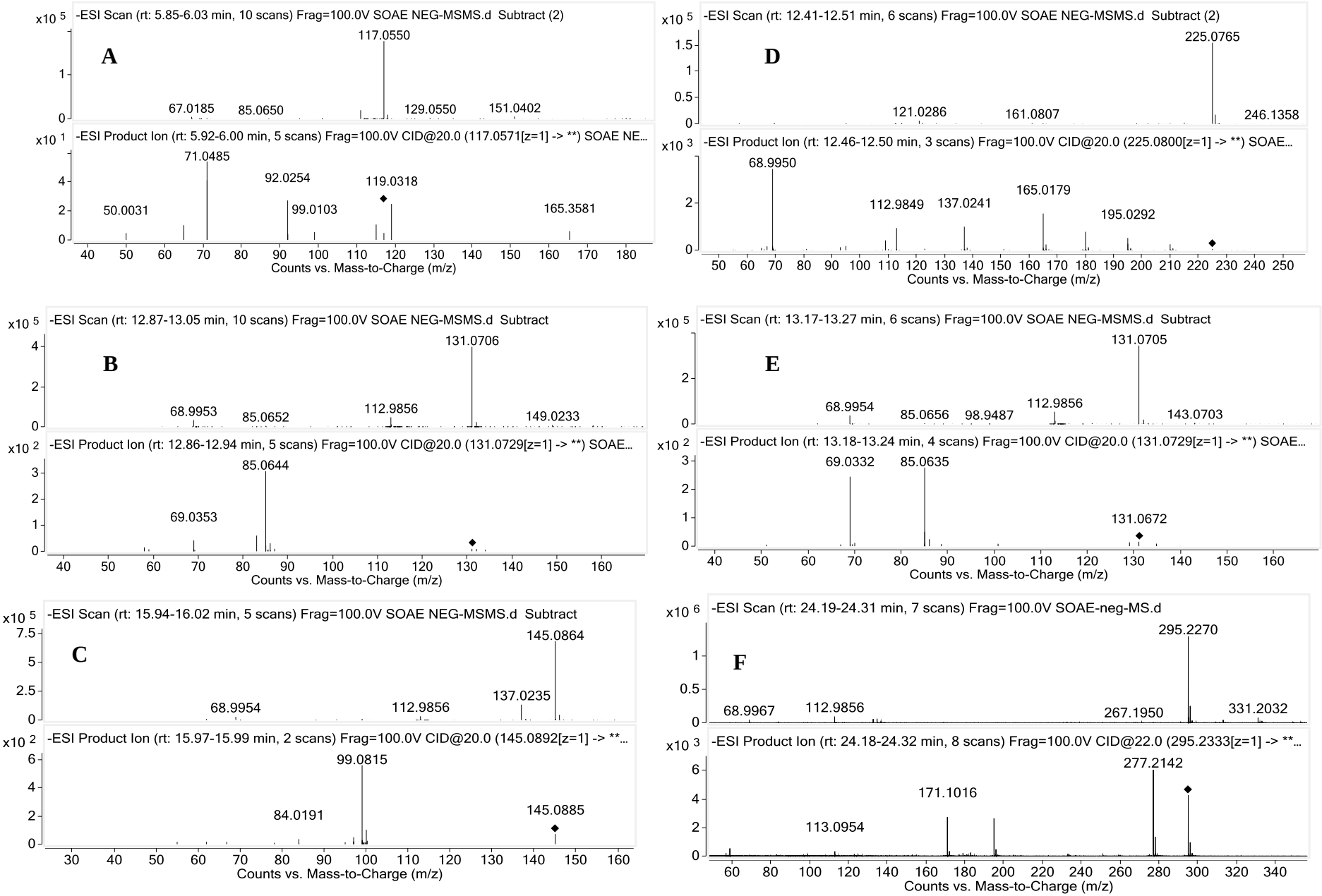


Fig. 9S(G).: ESI-HRMS and MS/MS spectra of SOAE molecules of A) L-α-hydroxyisovaleric acid, B) hydroxy caproic acid, C) hydroxy heptanoic acid, , D) 4-hydroxy-(3',4'-dihydroxyphenyl)-valeric acid, E) hydroxy caproic acid isomer and F) hydroxy linoleic acid isomer.

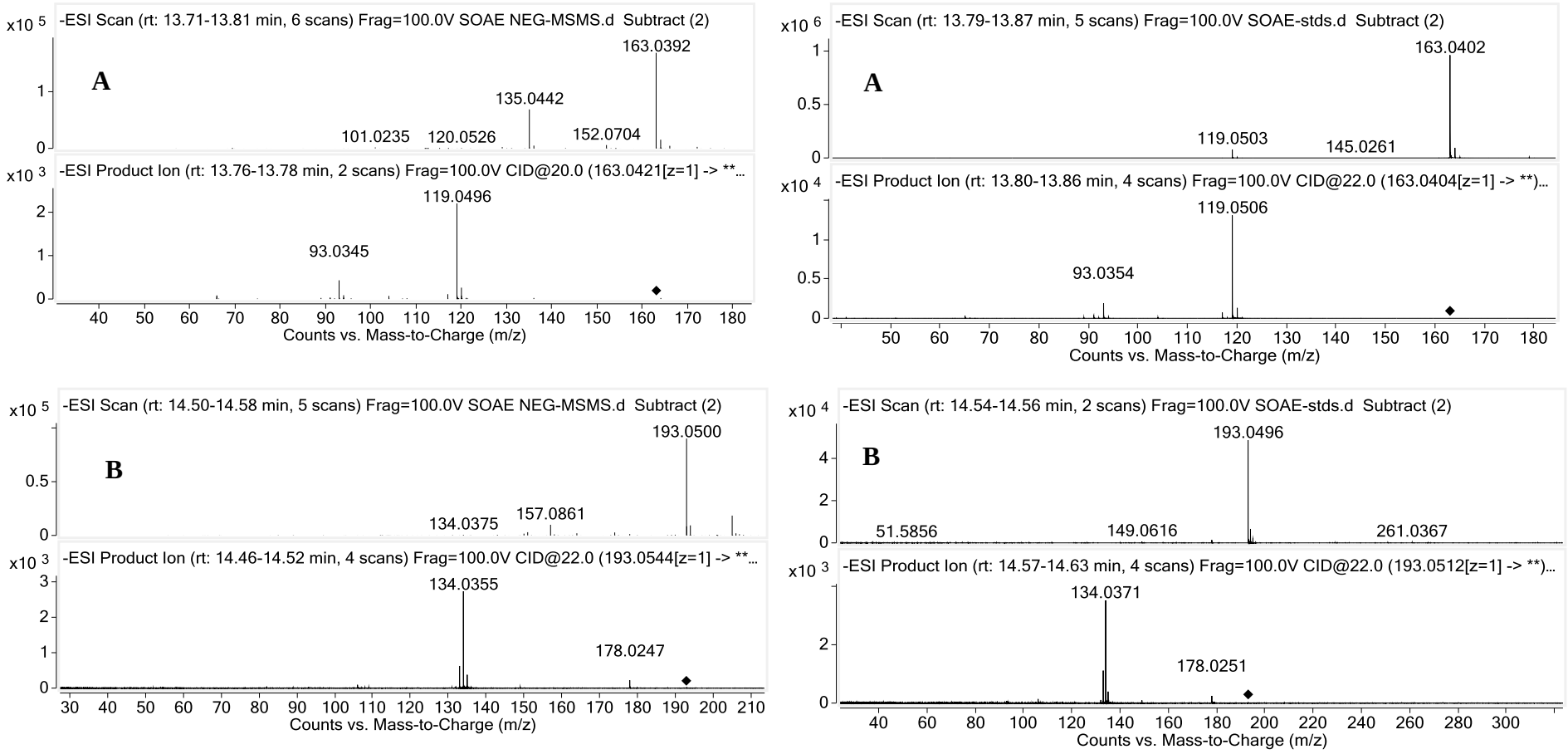


Fig. 9S(H): ESI-HRMS and MS/MS spectra of SOAE molecules (left panel) and standards (right panel) of A) p-coumaric acid and B) ferulic acid.

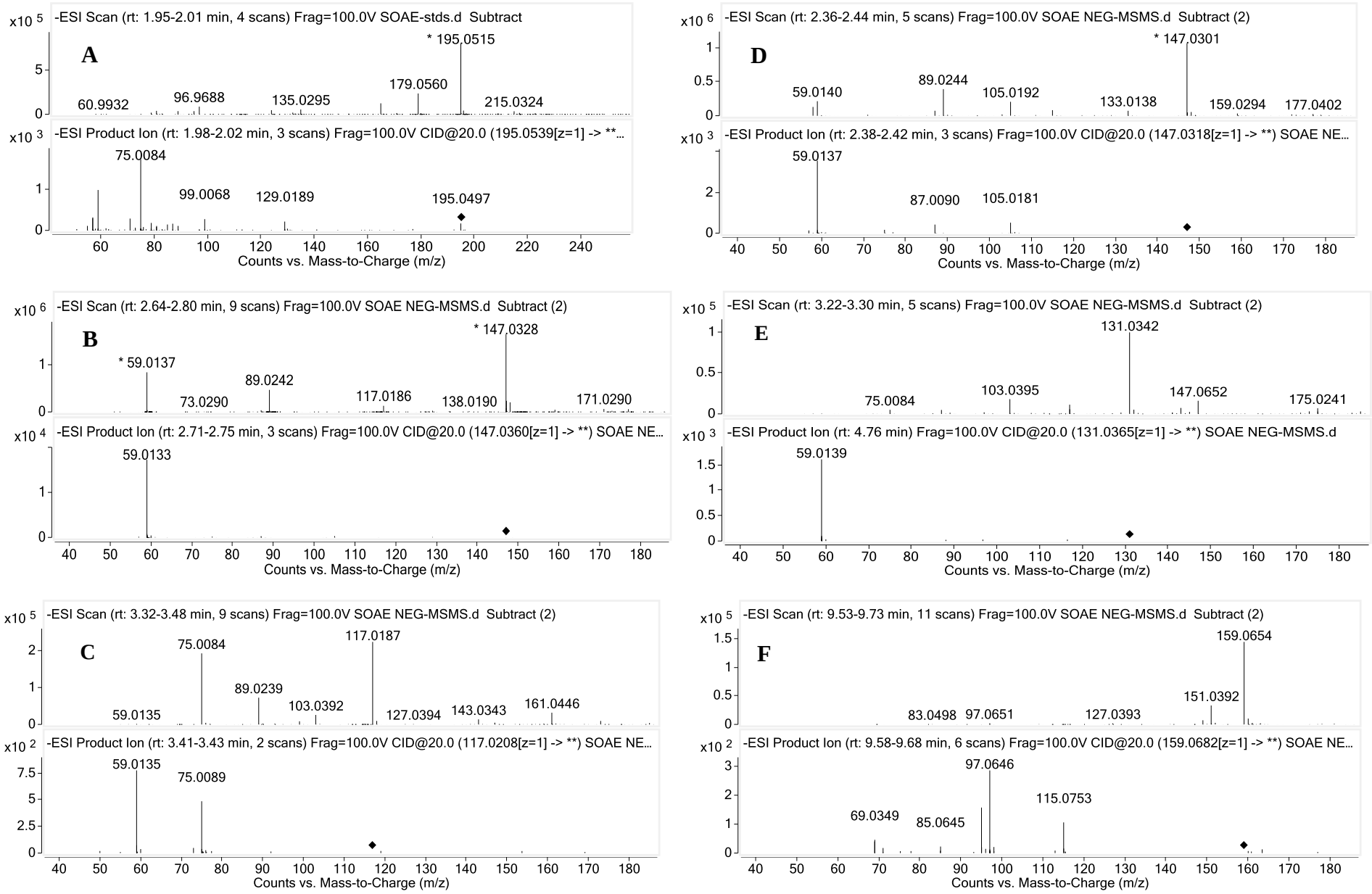


Fig. 9S(I): ESI-HRMS and MS/MS spectra of SOAE molecules of A) gluconic acid, B) 2-methylmalic acid, C) erythrono-1,4-lactone, D) hydroxy glutaric acid, E) 2-hydroxy-4-oxopentanoate and F) pimelic acid.

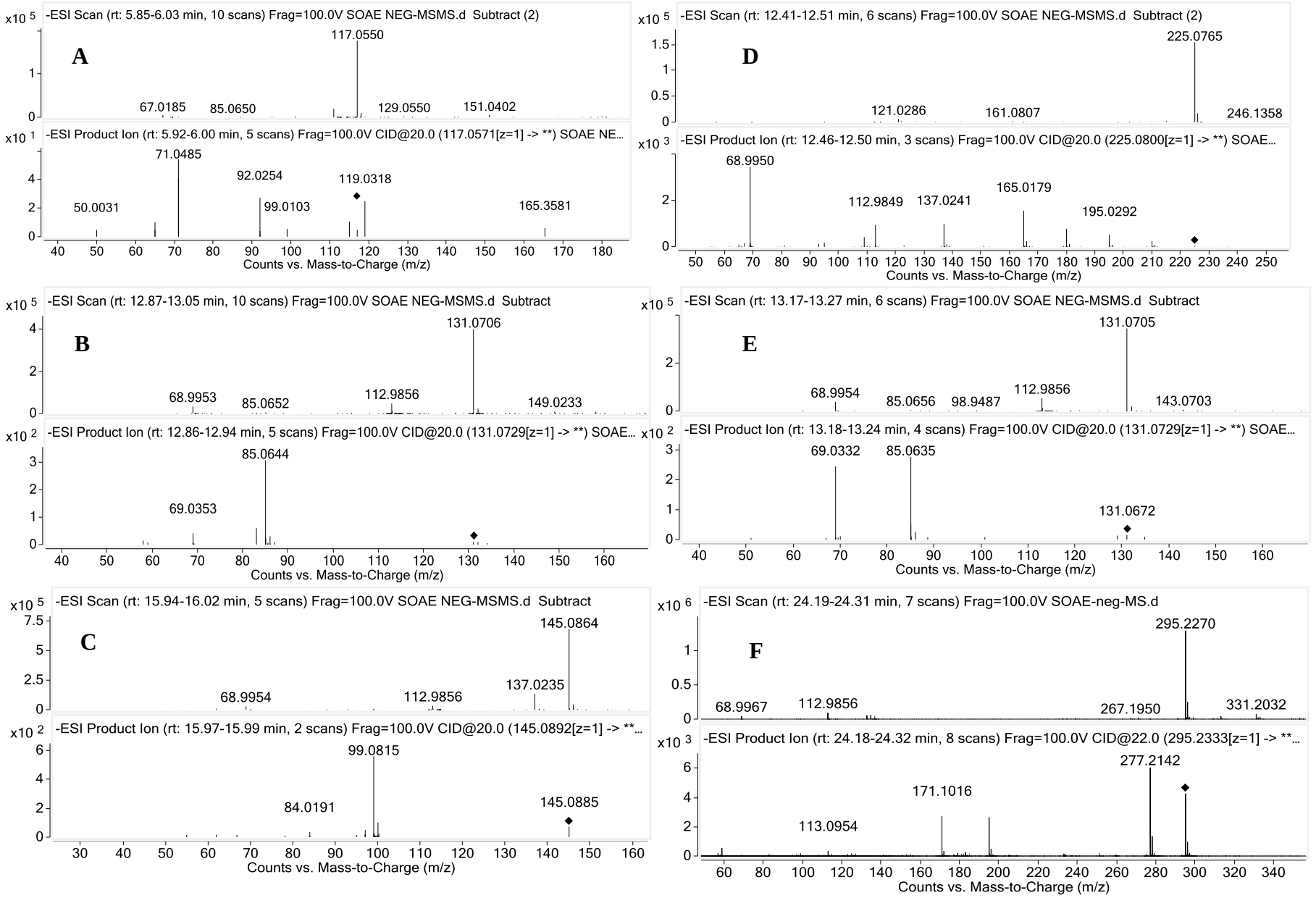
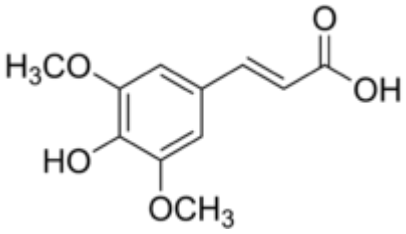
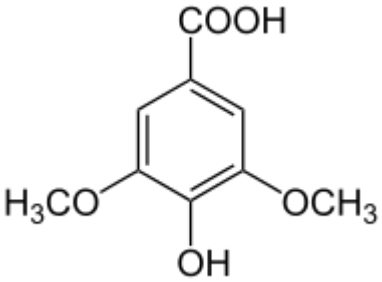


Fig. 9S(J): ESI-HRMS and MS/MS spectra of SOAE molecules of A) L-α-hydroxyisovaleric acid, B) hydroxy caproic acid, C) hydroxy heptanoic acid, D) 4-hydroxy-(3',4'-dihydroxyphenyl)-valeric acid, E) hydroxy caproic acid isomer and F) hydroxy linoleic acid isomer.



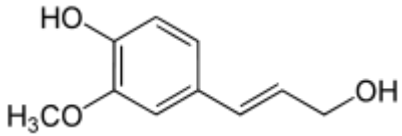
Sinapic acid

[M-H] = 223.06118



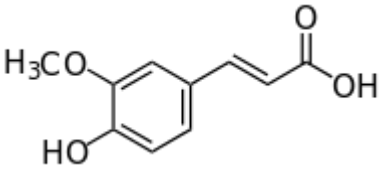
syrengic acid

[M-H] = 197.04553



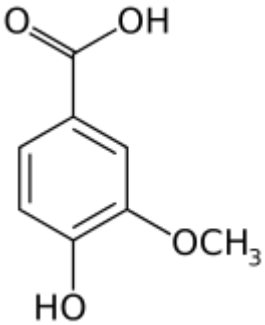
Coniferyl alcohol

[M-H] = 179.07136



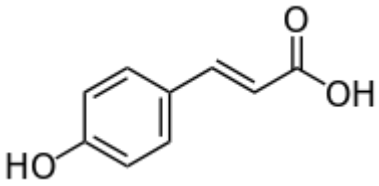
Ferulic acids

[M-H] = 193.05062



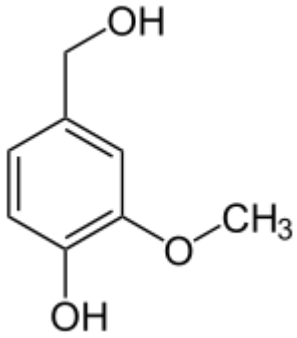
vanillic acid

[M-H] = 167.03497



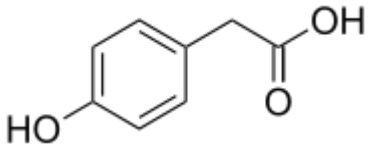
p-coumaric acid

[M-H] = 163.04006



vanillyl alcohol

[M-H] = 153.05571



p-hydroxy phenylacetic acid

[M-H] = 151.04006

Fig. 10S. Structures of SOAE-8 molecules.

Table 1S. The average relative percentage of each individual molecule identified in SOAE samples.

S. No.	Compound	Relative (%)
1	Gluconic acid	3.31
2	Glucose	3.80
3	Malic acid	1.10
4	Hydroxy glutaric acid	7.90
5	2-methylmalic acid	4.74
6	Glutaconic acid	0.69
7	2-hydroxy-4-oxopentanoate	0.88
8	Erythrono-1,4-lactone	2.72
9	Quinic acid	10.21
10	Vanillyl alcohol	1.10
11	L-α-hydroxyisovaleric acid	3.08
12	p-hydroxyphenylacetic acid	1.16
13	Pimelic acid	2.95
14	Vanillic acid	3.99
15	5-hydroxyconiferyl alcohol	1.45
16	Syringic acid	3.31
17	4-hydroxy-(3',4'-dihydroxyphenyl)-valeric acid	1.81
18	Hydroxy caproic acid	6.28
19	Hydroxy caproic acid isomer	3.68
20	Dihydrosinapic acid	2.30
21	p-coumaric acid	2.19
22	Suberic acid	5.36
23	Ferulic acid	0.94
24	Azelaic acid	15.84
25	Hydroxy heptanoic acid	5.94
26	Oxo nonannoic acid	2.27
27	Traumatic acid	0.65
28	Hydroxy-linoleic acid isomer	0.34

Table 2S. List of oligonucleotide primers used for RT-PCR.

Species	Target	Forward Primer	Reverse Primer
Mouse	GAPDH	5'-ACCCAGAAGACTGTGGATGG-3'	5'-CACATTGGGGGTAGGAACAC-3'
	IL-1α	5'-GCAACGGGAAGATTCTGAAG-3'	5'-TGACAAACTTCTGCCTGACG-3'
	IL-1β	5'-AACCTGCTGGTGTGTGACTTC-3'	5'-CAGCACGAGGCTTTTTTGT-3'
	IL-6	5'-AGTTGCCTTCTTGGGACTGA-3'	5'-TCCACGATTTCCCAGAGAAC-3'
	TNF-α	5'-CACACTCAGATCATCTTCTCAAAA-3'	5'-GCAATGACTCTAAAGTAGACCT
Human	GAPDH	5'-GGAACATGTAAACCATGTAGTTGAG-3'	5'-AGTCAACGGATTTGGTCGTA-3'
	IL1β	5'-CTTCGAGGCACAAGGCACAA-3'	5'-CCCTTGCTGTAGTGGTGGTC-3'
	IL6	5'-GCCCACCAAAGTGGCAAAG-3'	5'-CACAAGGCTGGTTTGGCAGA-3'
	TNF-α	5'- ATGAGCACTGAAAGCATGATCC -3'	5'-GAGGCTGATTAGAGAGAGGTC-3'