Complementary analytical platforms of H NMR spectroscopy and LCMS analysis in the metabolite profiling of *Isochrysis galbana*

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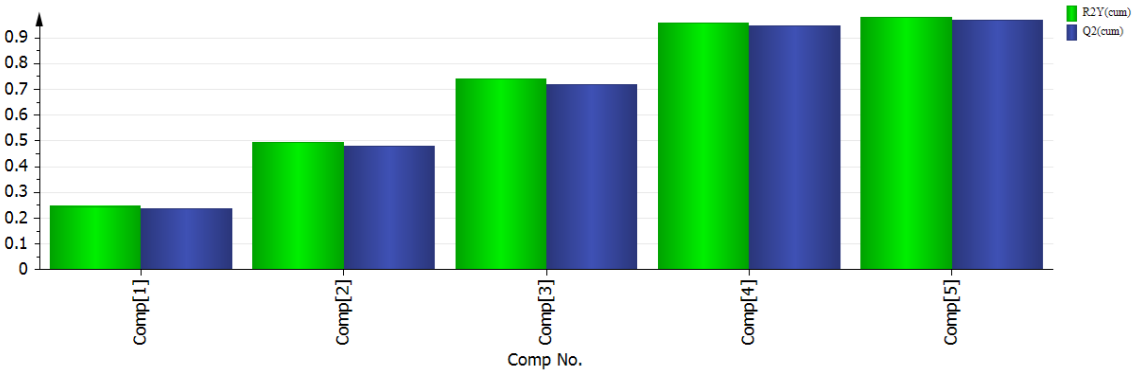
a)



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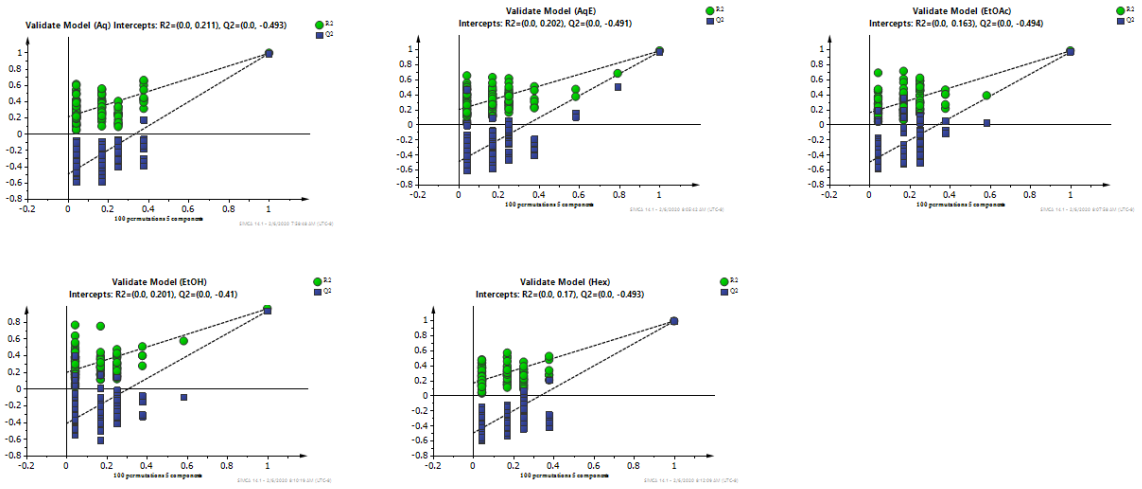
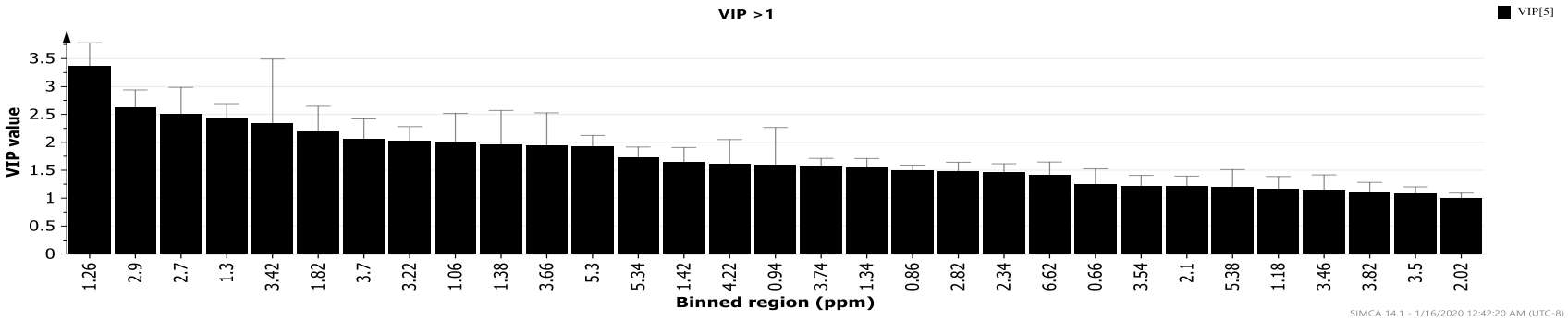


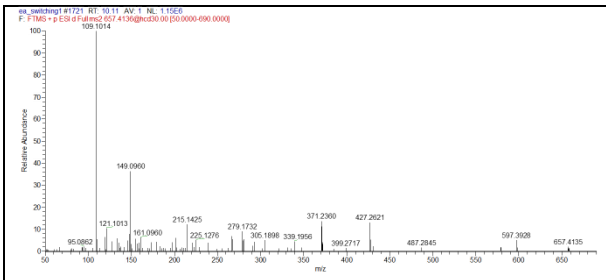
Figure S1 (a) R2 and Q2 values from summary of fit model and (b) the R2- and Q2- intercepts derived from 100 permutation tests for each of the solvent extracts



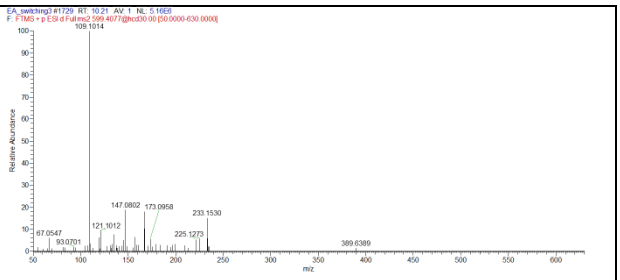
Binned region (ppm)	VIP value	Tentative metabolite
1.26	3.37	Fatty acid derivatatties
2.9	2.61	DMSP
2.7	2.49	DMSP
1.3	2.43	Fatty acid derivatatties
3.42	2.33	DMSP
1.82	2.18	D-1,4/2,5-cyclohexanetetrol
3.7	2.05	Amino acid derivatatties
3.22	2.02	Choline
1.06	2.01	valine/violaxanthin
1.38	1.96	Threonine/DPA/Fucoxanthin
3.66	1.93	Sucrose
5.3	1.92	Fatty acid derivatatties
5.34	1.73	Fatty acid derivatatties
1.42	1.64	Arachidic acid
4.22	1.61	Sucrose
0.94	1.59	Leucine/α-linoleic acid

Binned region (ppm)	VIP value	Tentative metabolite
3.74	1.57	D-1,4/2,5-cyclohexanetetrol
1.34	1.54	Palmitic acid
0.86	1.48	Palmitic acid
2.82	1.48	α-linoleic acid
2.34	1.45	Fatty acid derivatatties
2.94	1.45	DMSP
6.62	1.41	Astaxanthin
0.66	1.25	Cholesterol
3.54	1.21	Glucose
2.1	1.20	Carotenoid derivatives
5.38	1.19	Sucrose/DHA/DPA
1.18	1.16	Carotenoid derivatives
3.46	1.15	DMSP
3.82	1.10	Glucose
3.5	1.08	Amino acid derivatatives
2.02	1.00	Oleic acid

Figure S2 VIP plot with values more than 1.0 and error bars not crossing baseline



1. m/z 597.3928



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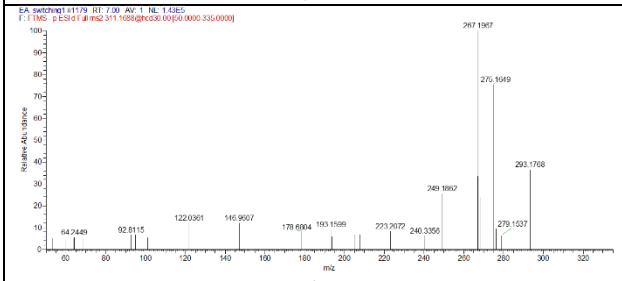

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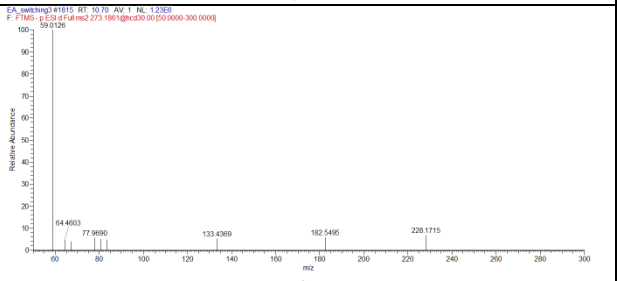

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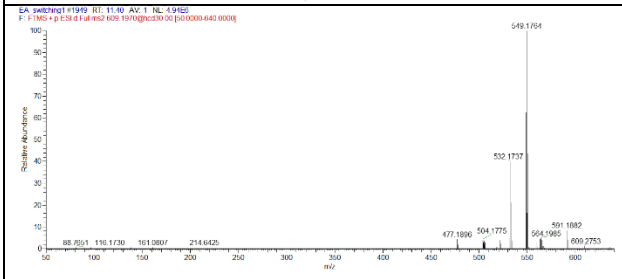

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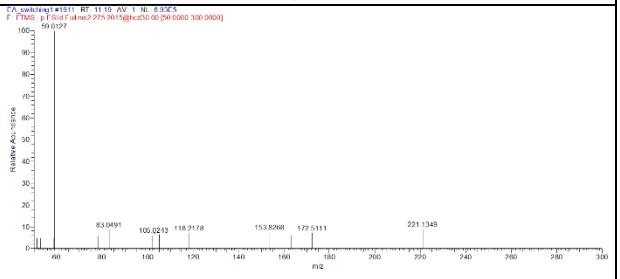

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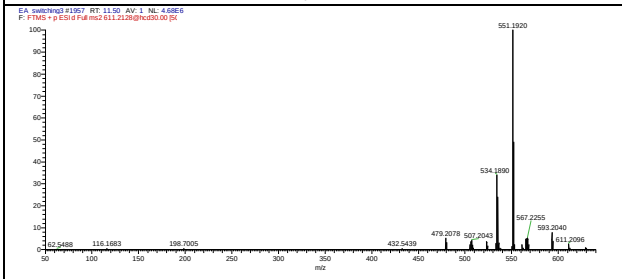

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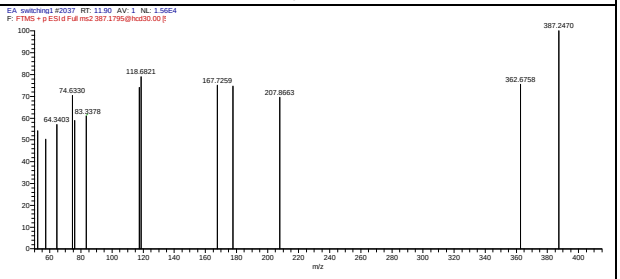

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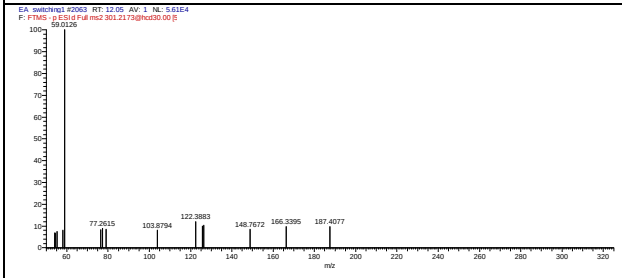

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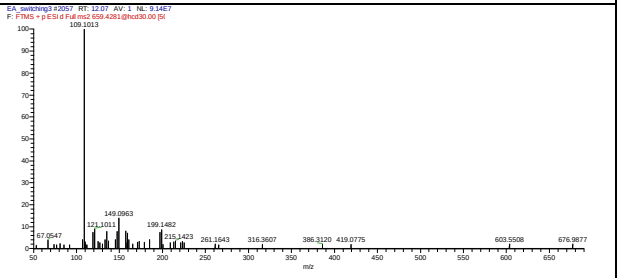

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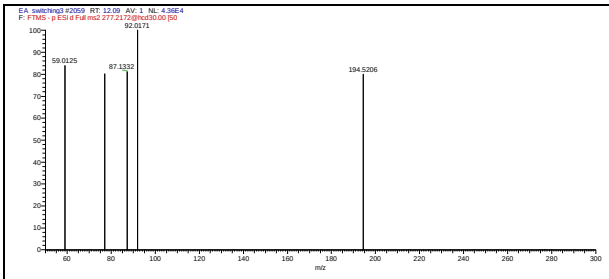
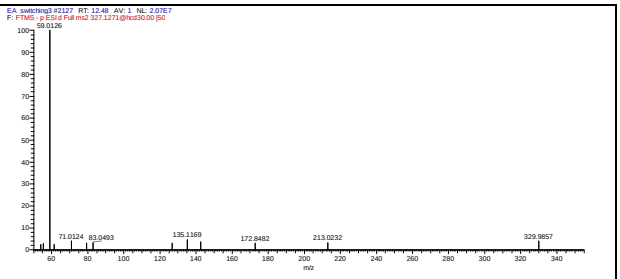


11. m/z 277.2172



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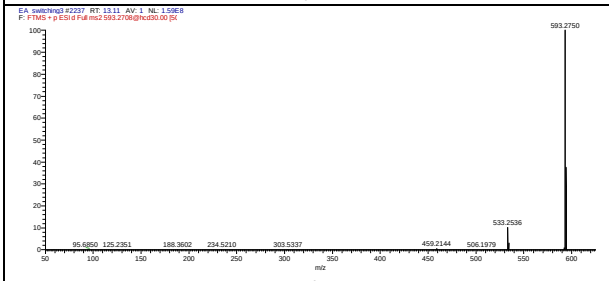

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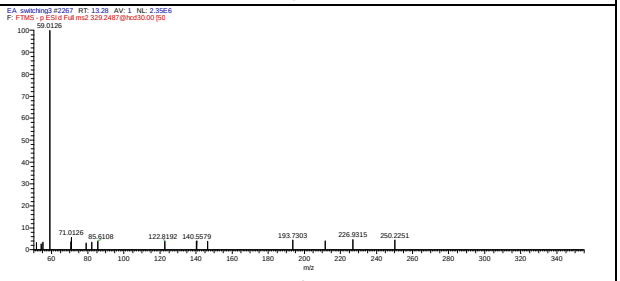

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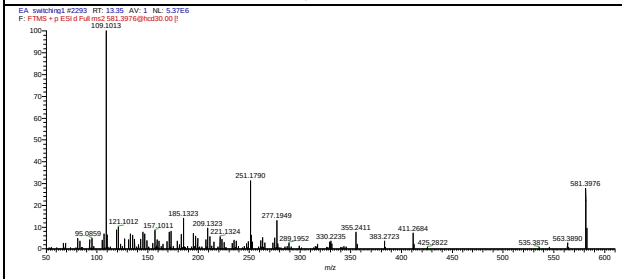
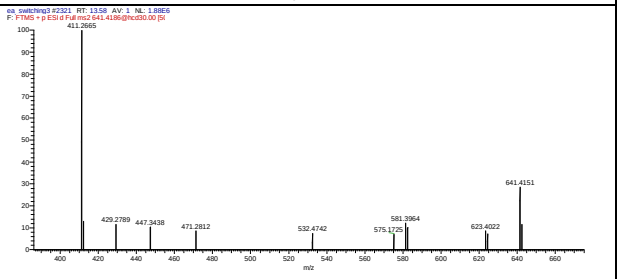
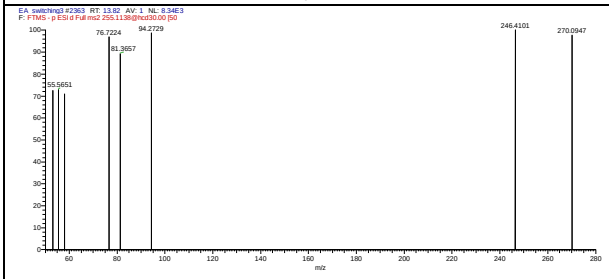


15. m/z 581.3976



16. m/z 581.3964



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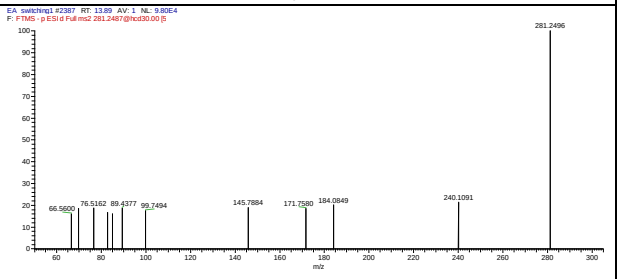

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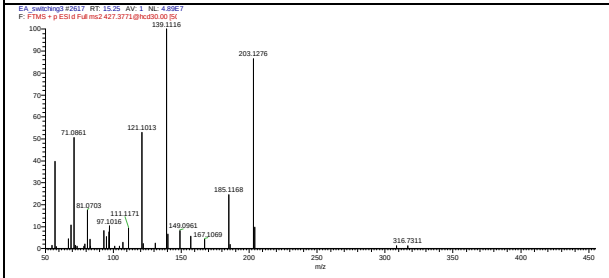

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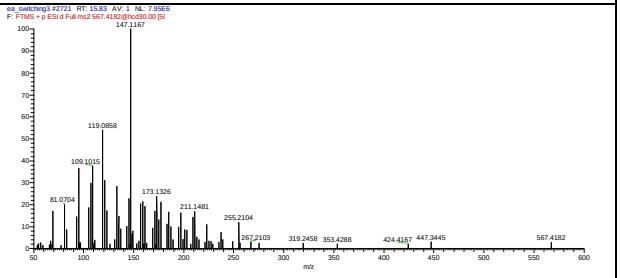

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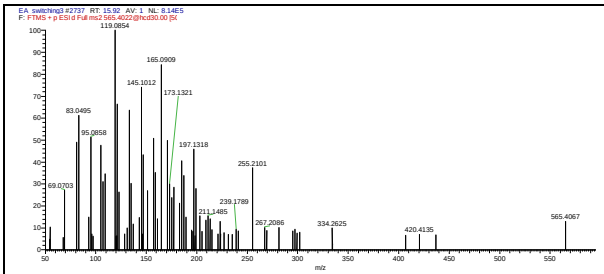

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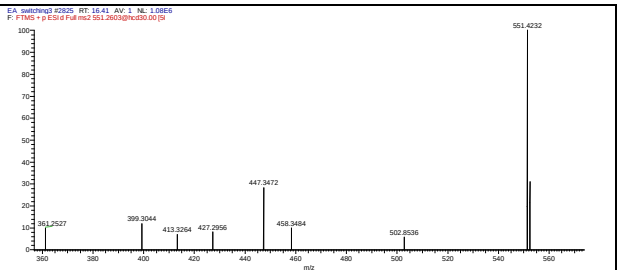

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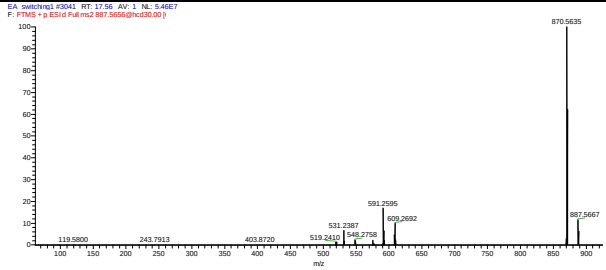

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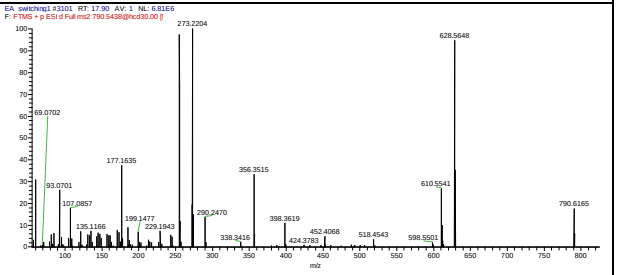

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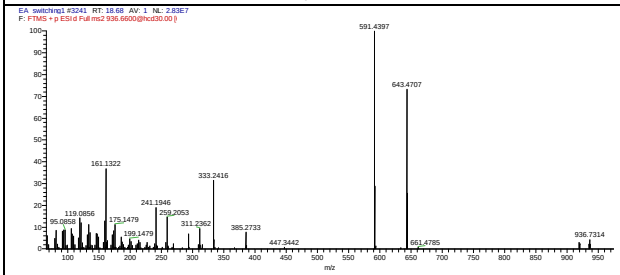
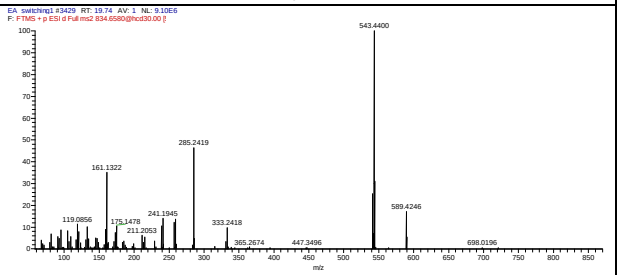
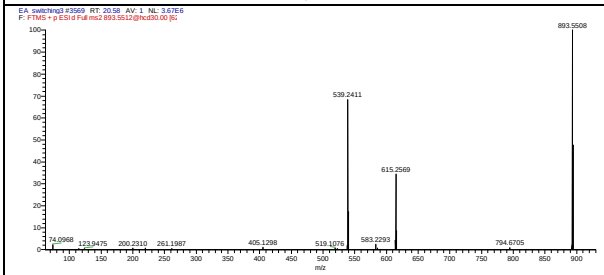


25. m/z 936.7314



26. m/z 834.6580



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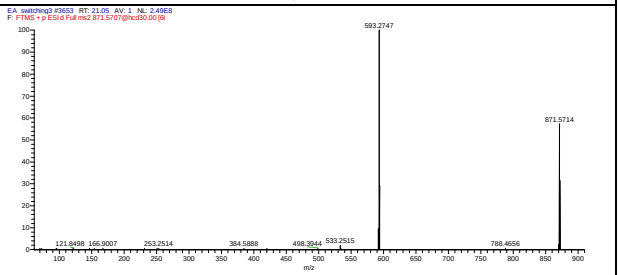
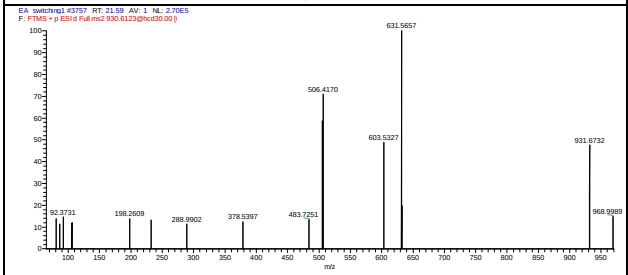


28. m/z 871.5711



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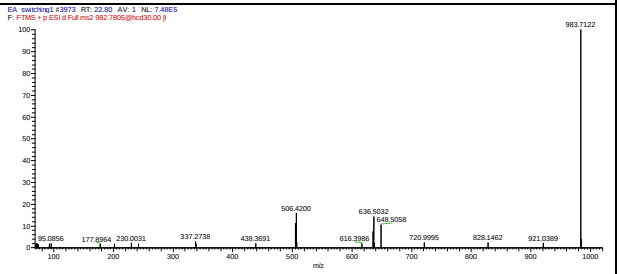

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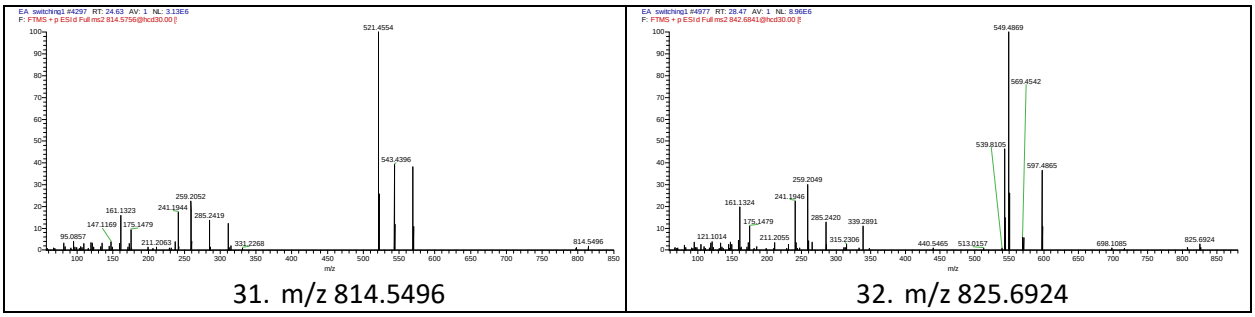
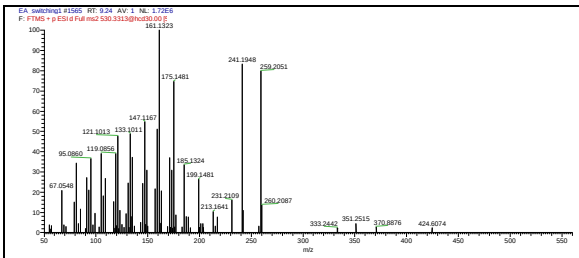


Figure S3 MS/MS spectrums of molecular ion detected by LCMS/MS in positive and negative mode



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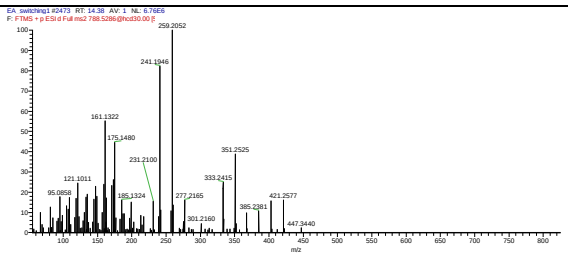

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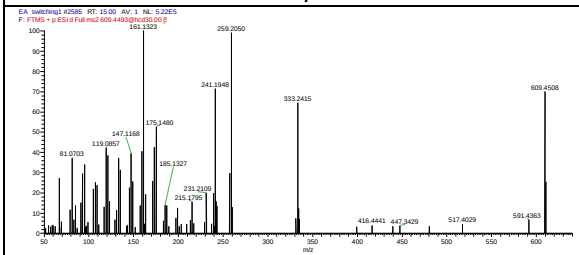

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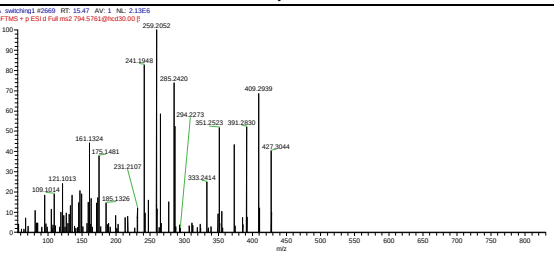
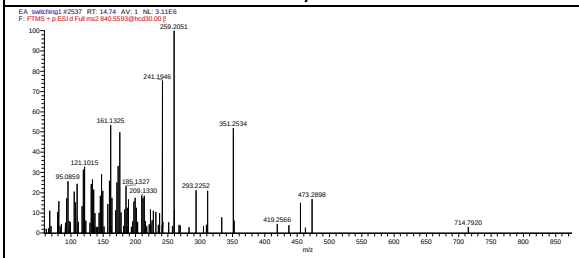


4. m/z 794.5761



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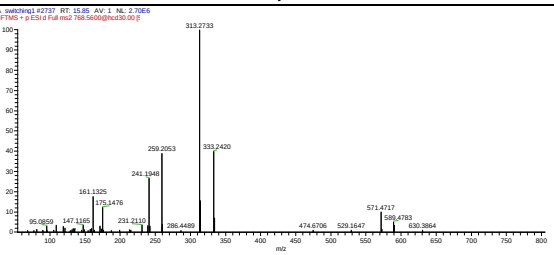

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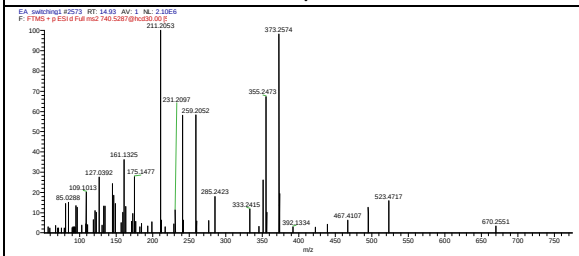

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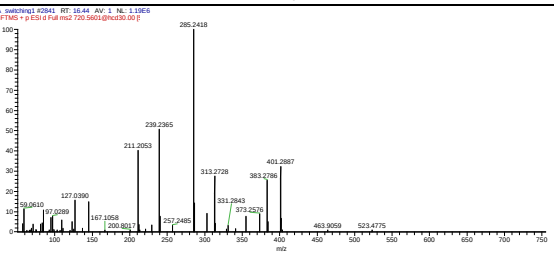

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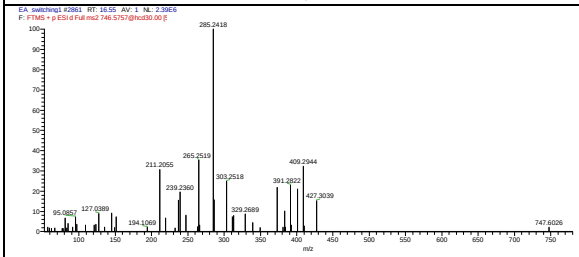

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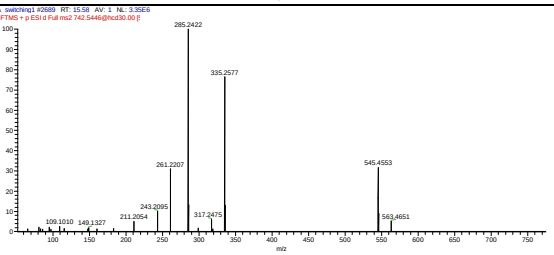


10. m/z 742.5446

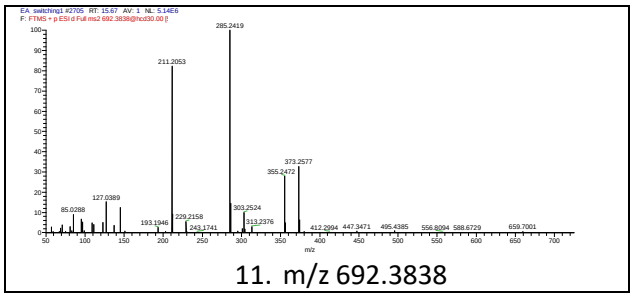


Figure S4 MS/MS spectrums of metabolites from cluster of glycerophospholipids identified in EtOAc extract of *I. galbana*. in positive mode

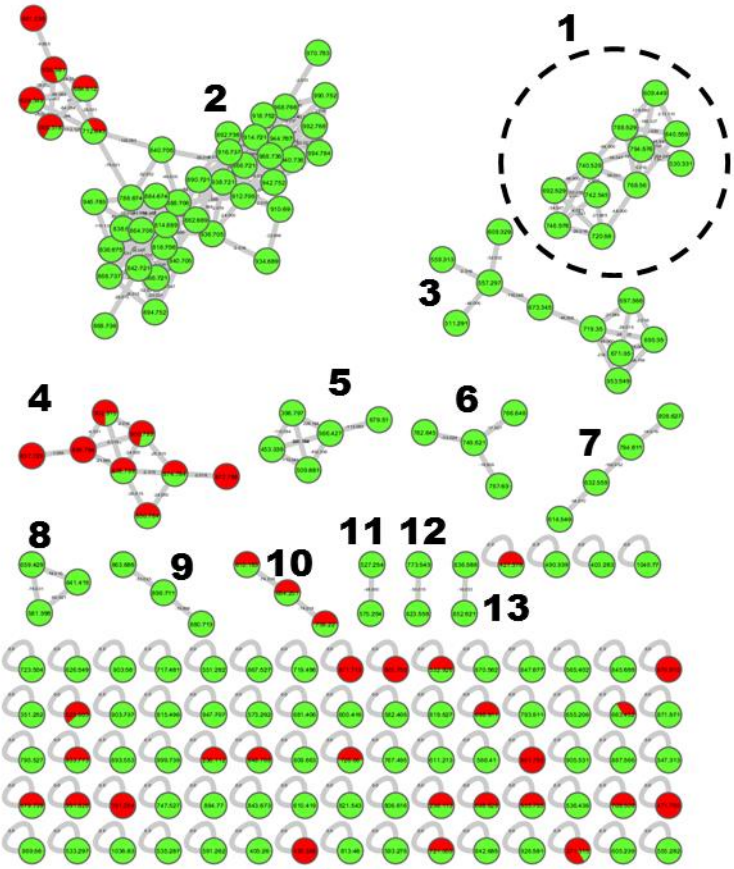
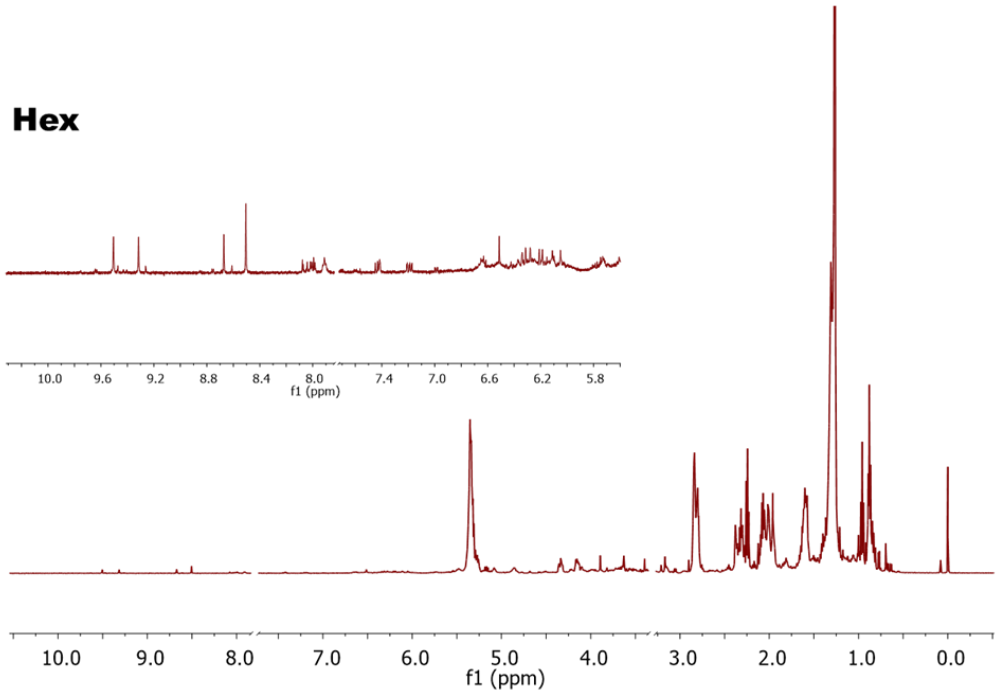
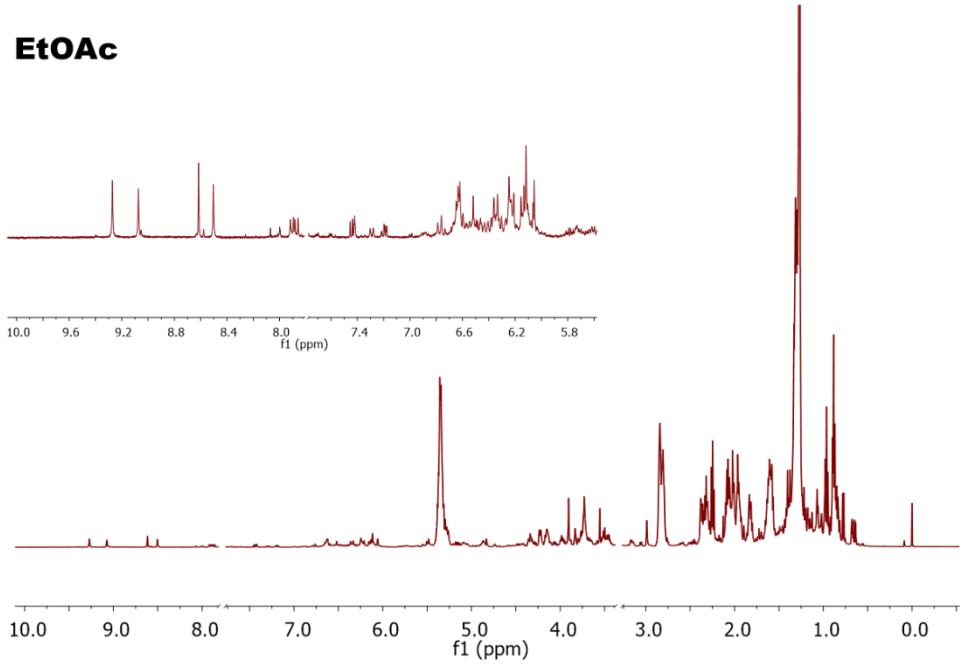


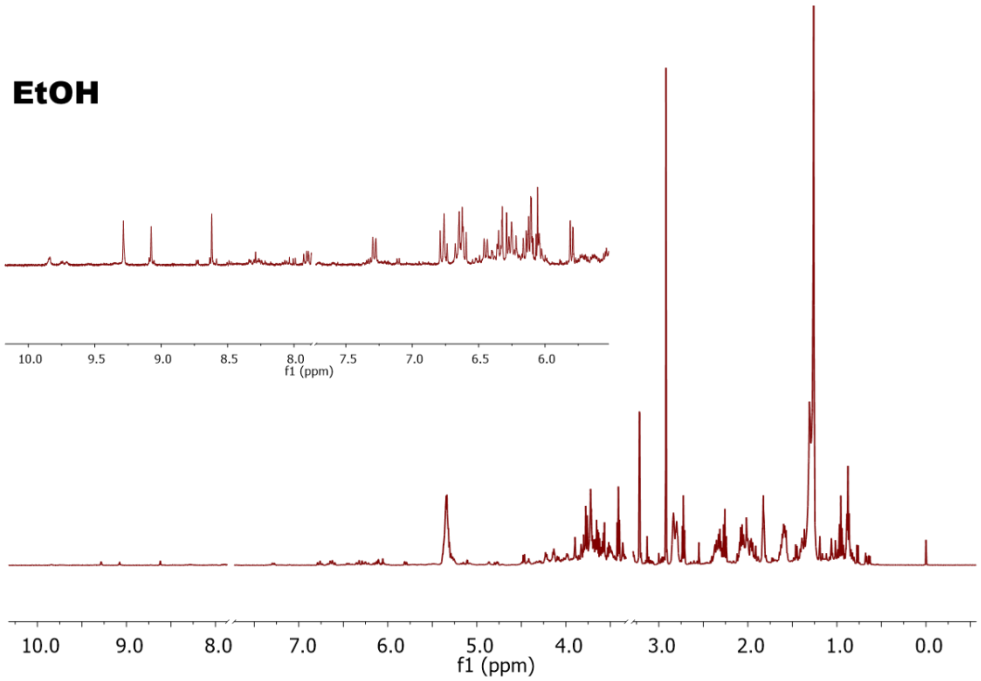
Figure S5 Full molecular network of EtOAc extract of *I. galbana* showing 13 clusters including cluster of glycerophospholipids (cluster no. 1) with 11 new identified putative structures. Green node is EtOAc extract and red node is blank sample.


Hex
10.0 9.6 9.2 8.8 8.4 8.0 7.4 7.0 6.6 6.2 5.8
f1 (ppm)
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

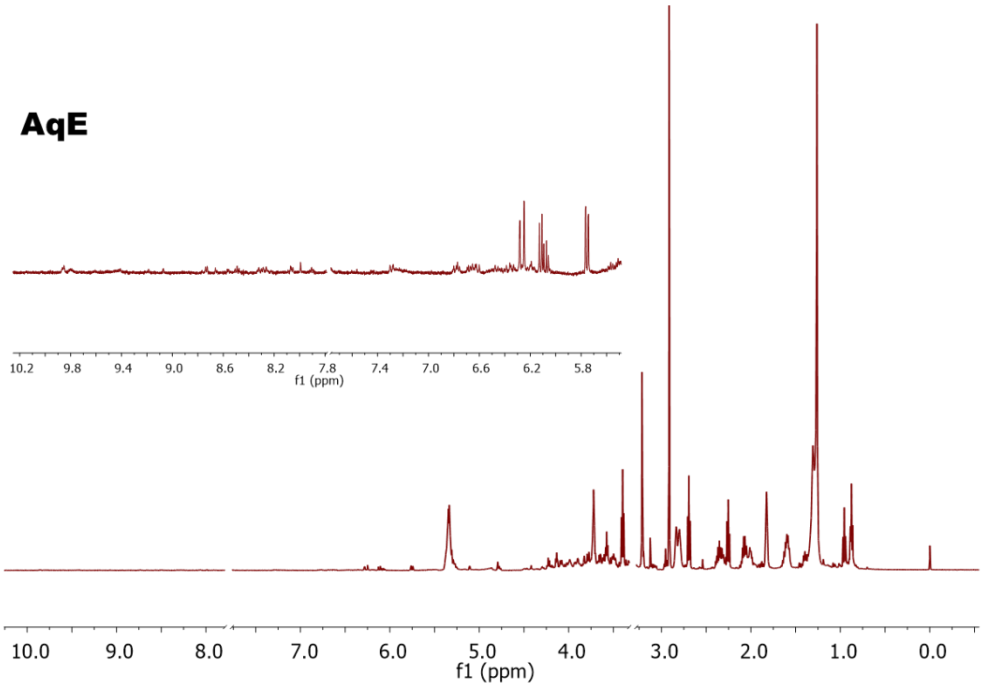
(a)


EtOAc
10.0 9.6 9.2 8.8 8.4 8.0 7.4 7.0 6.6 6.2 5.8
f1 (ppm)
10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0
f1 (ppm)

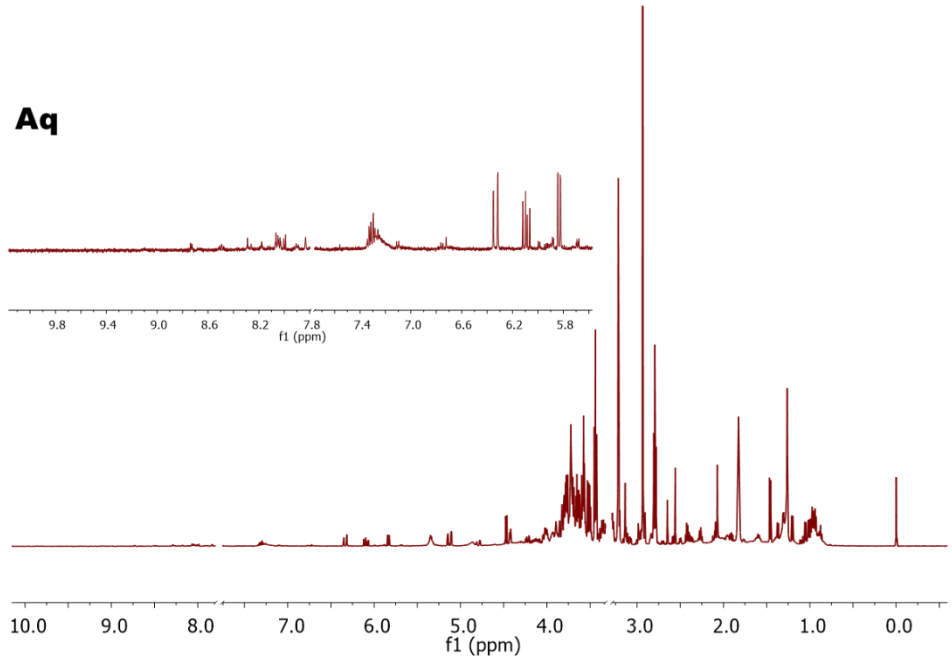
(b)


EtOH
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

(c)


AqE
10.2
9.8
9.4
9.0
8.6
8.2
7.8
7.4
7.0
6.6
6.2
5.8
f1 (ppm)
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)

(d)



(e)

Figure S6 Representatives 1D 500 MHz ^{1}H NMR individual spectrum of (a) hexane (Hex), (b) ethyl acetate (EtOAc), (c) absolute ethanol (EtOH), (d) 50% ethanol (AqE) and (e) aqueous (Aq) extracts of *I. galbana*.