

Type of the Paper (Article)

Cyclic hexapeptide from *Bouvardia ternifolia* (Cav.) Schltdl. and neuroprotective effects of root extracts.

Yury Maritza Zapata Lopera ^{1,2}, Gabriela Trejo-Tapia ^{2**}, Manasés González-Cortazar ¹, Maribel Herrera-Ruiz ¹, Alejandro Zamilpa ¹ and Enrique Jiménez-Ferrer ^{1*}

¹ Centro de Investigación Biomédica del Sur, Instituto Mexicano del Seguro Social, Xochitepec 62790, Morelos, México

² Centro de Desarrollo de Productos Bióticos, Instituto Politécnico Nacional, Yautepec 62730, Morelos, México

* Correspondence: enriqueferrer_mx@yahoo.com (E.J.-F.) ** Second corresponding author (G.T.-T.).

Content

Figure S1. GC–MS Analysis of the BtD extract

Figure S2. GC–MS Analysis of the BtH extract

Figure S3. Spectrum UV and HPLC of cyclic hexapeptide

Figure S4. Mass spectrum (MS) of cyclic hexapeptide

Figure S5. ¹H NMR (CD₃OD, 400 MHz) of cyclic hexapeptide

Figure S6. ¹³C NMR (CD₃OD, 400 MHz) of cyclic hexapeptide

Figure S7. The ¹³C NMR (DEPT) spectrum of cyclic hexapeptide

Figure S8. The HMBC spectrum of cyclic hexapeptide

Figure S9. The ¹H-¹H COSY spectrum of cyclic hexapeptide

Figure S1. GC–MS Analysis of the BtD extract

Area Percent Report

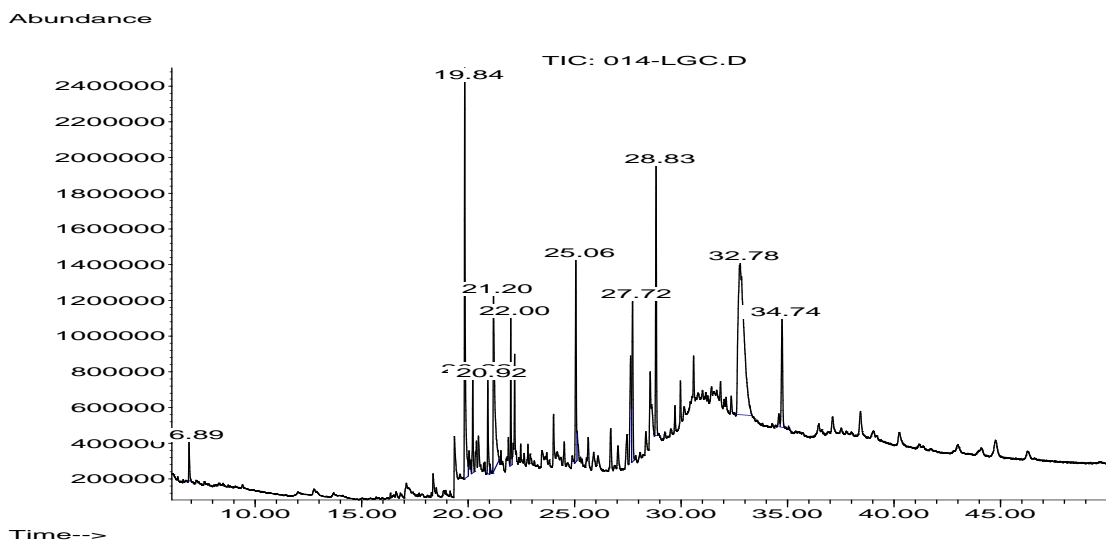
Data File : C:\MSDCHEM\2\DATA\014-LGC.D Vial: 95
 Acq On : 18 Oct 2022 9:59 Operator: M.G.M
 Sample : BTZCDCI3 Splitless 40°C-1min, Inst : Instrumen
 Misc : 10°C/min-250°C-5min,10°C/min-20min Multiplr: 1.00
 Sample Amount: 1.00

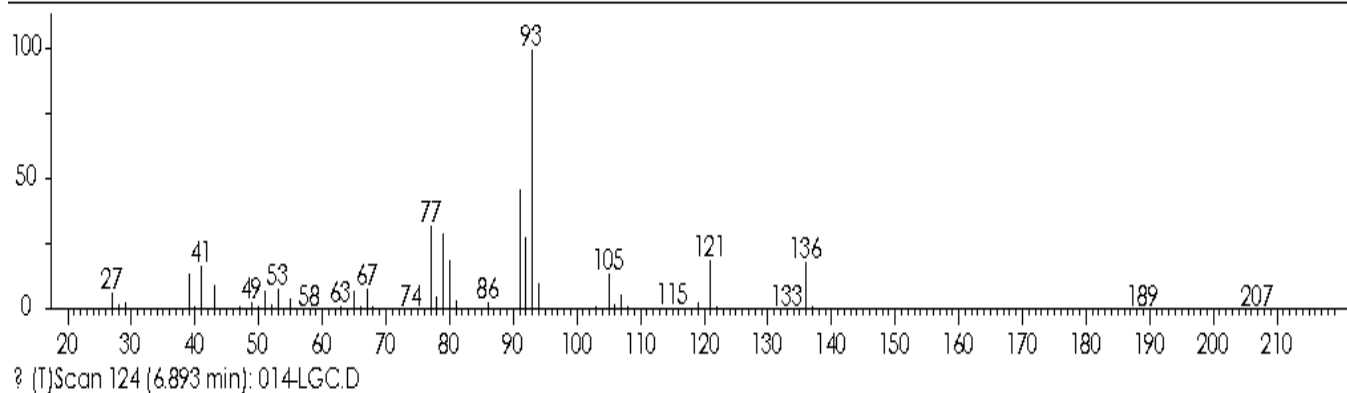
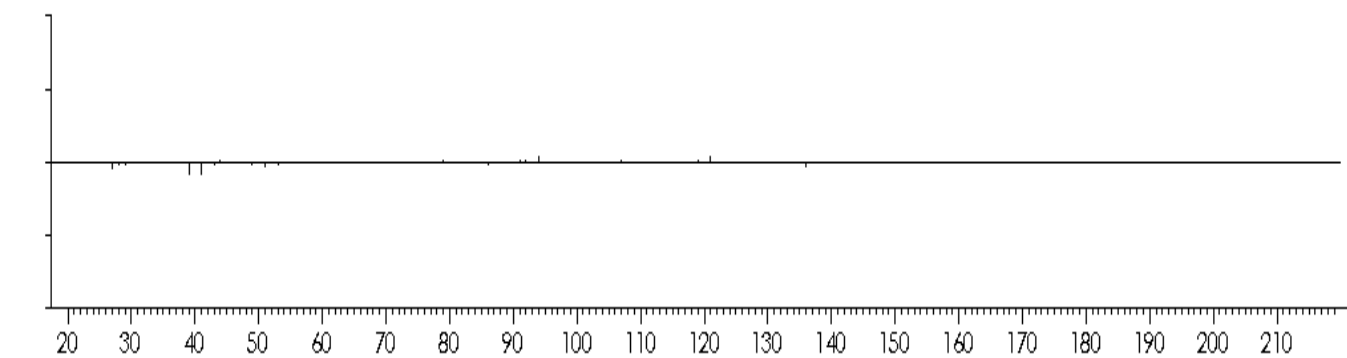
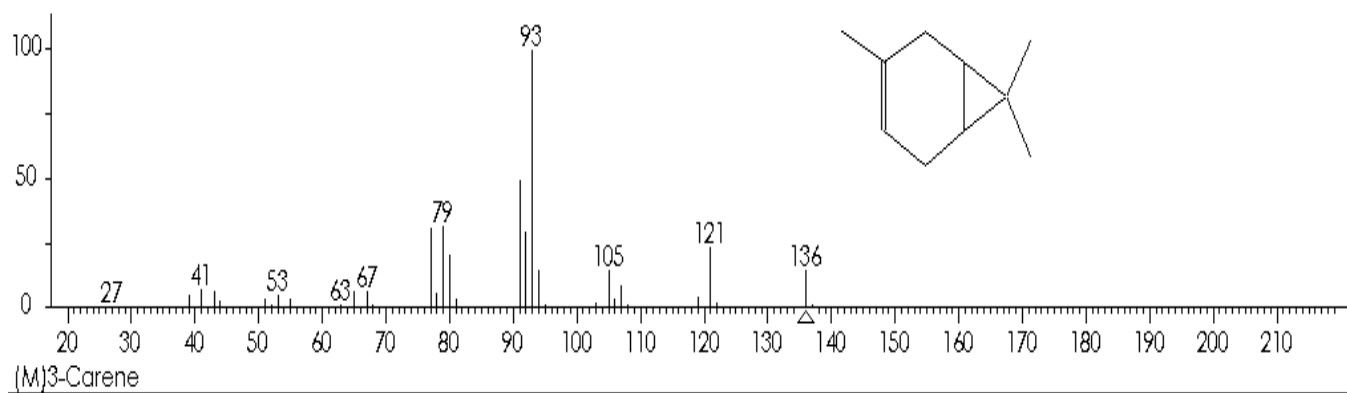
MS Integration Params: autoint1.e

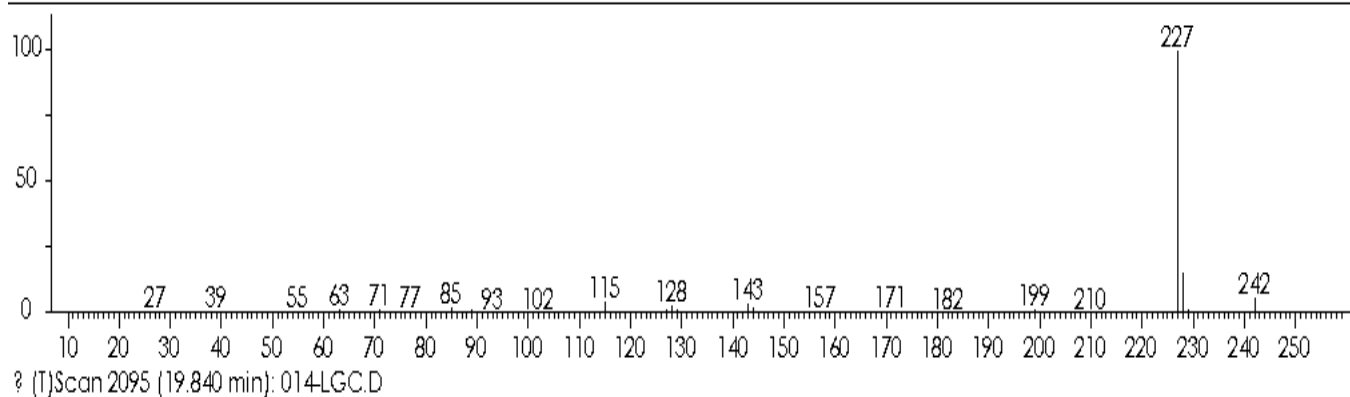
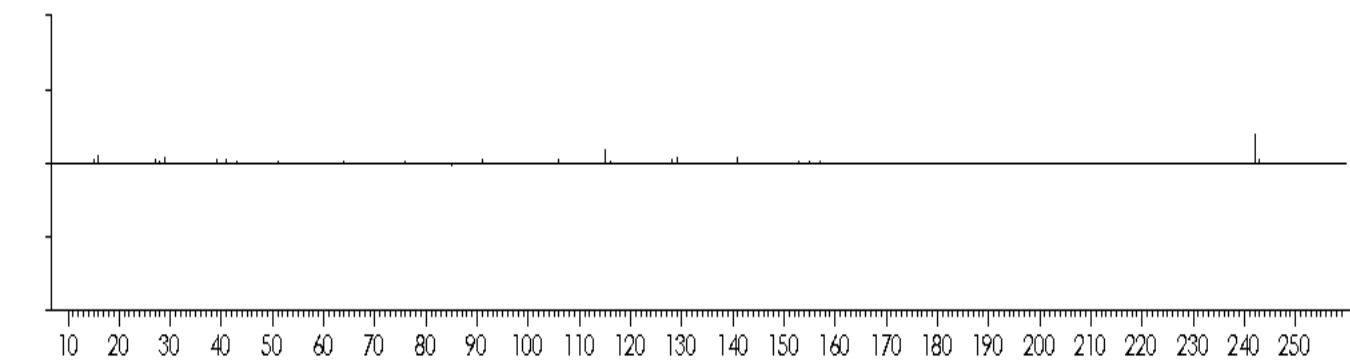
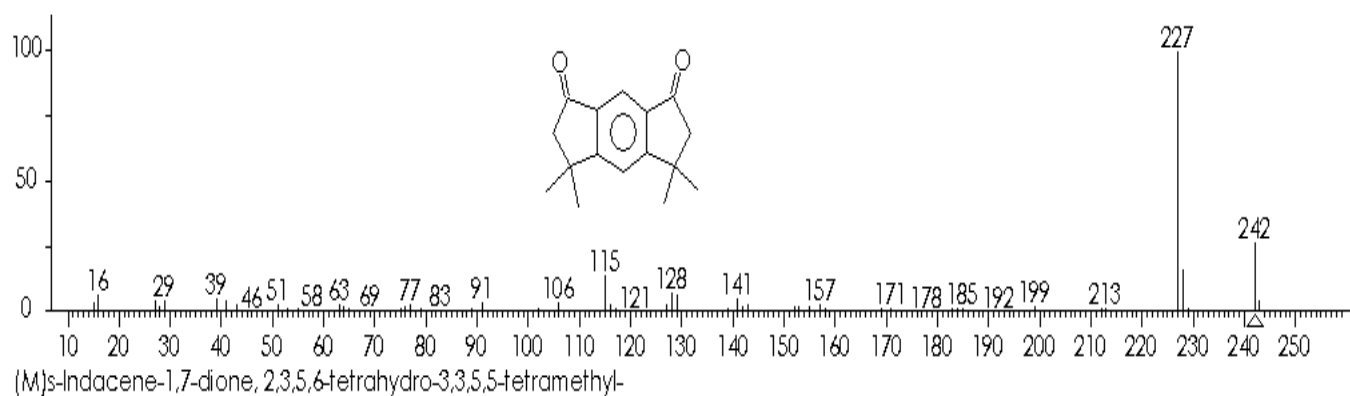
Signal : TIC

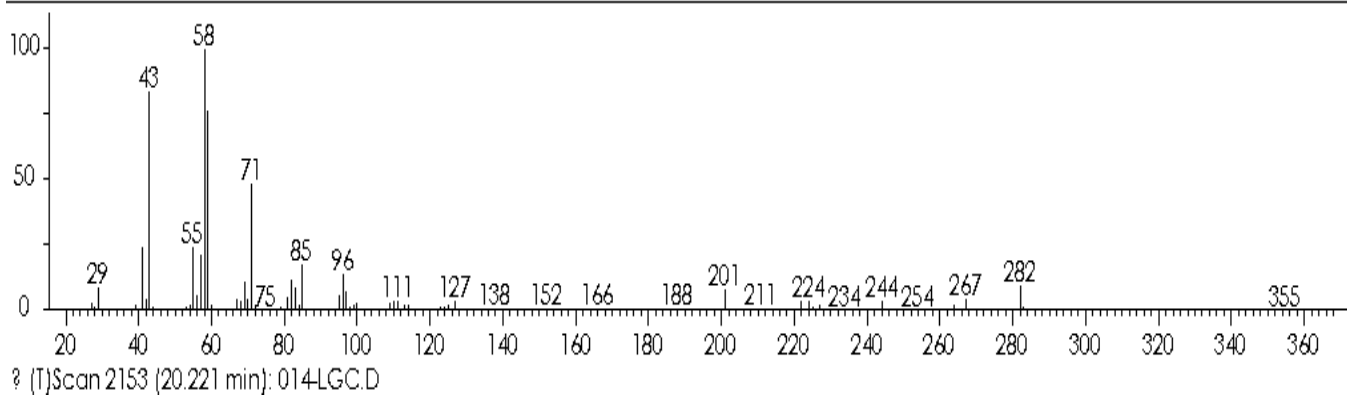
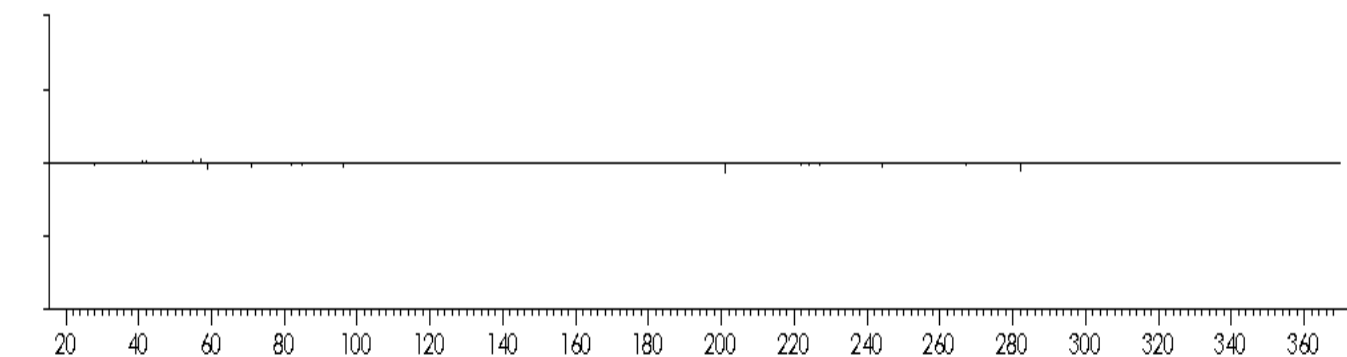
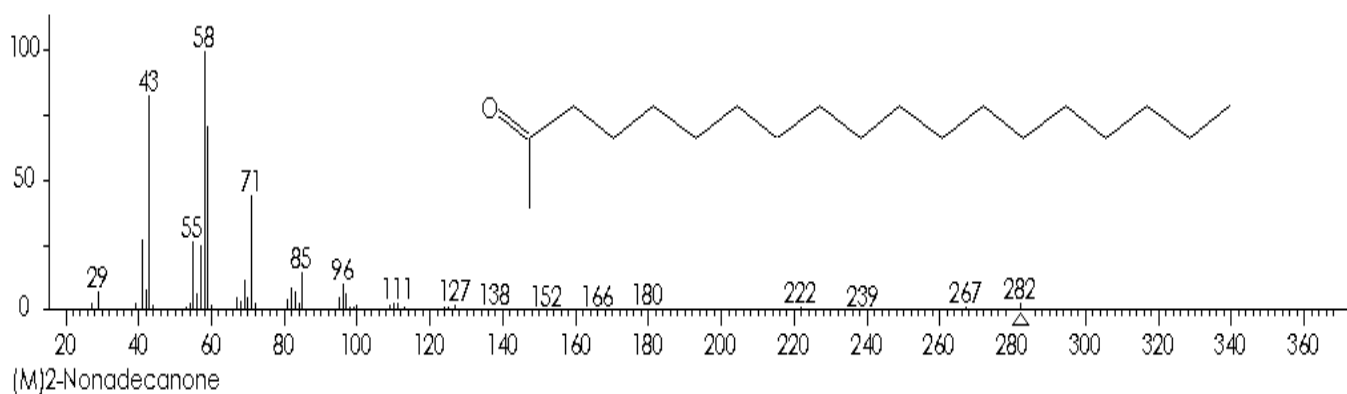
peak #	R.T. min	first scan	max last scan	PK scan	peak TY	peak height	corr. area	corr. % max.	% of total
1	6.893	117	124	137	M	220731	5563550	3.39%	1.208%
2	19.840	2087	2095	2121	BV	2252539	66055036	40.24%	14.343%
3	20.221	2143	2153	2165	VV 2	538038	12801791	7.80%	2.780%
4	20.924	2252	2260	2274	M	528670	13685068	8.34%	2.972%
5	21.193	2295	2301	2342	BB	974166	52105698	31.74%	11.314%
6	22.008	2417	2425	2434	VV	809337	15743630	9.59%	3.419%
7	25.055	2880	2889	2898	M	1138838	32704637	19.92%	7.102%
8	27.722	3288	3295	3310	VB	898734	30700493	18.70%	6.666%
9	28.826	3451	3463	3476	BB	1485641	42057954	25.62%	9.133%
10	32.780	4027	4065	4150	BB 3	848609	164147530	100.00%	35.643%
11	34.744	4350	4364	4384	VB 2	606289	24963514	15.21%	5.421%

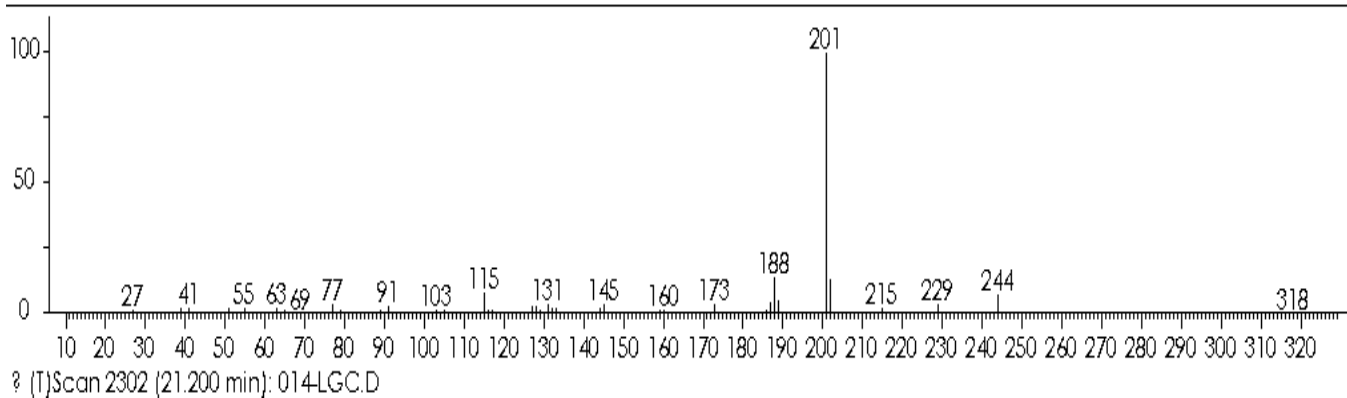
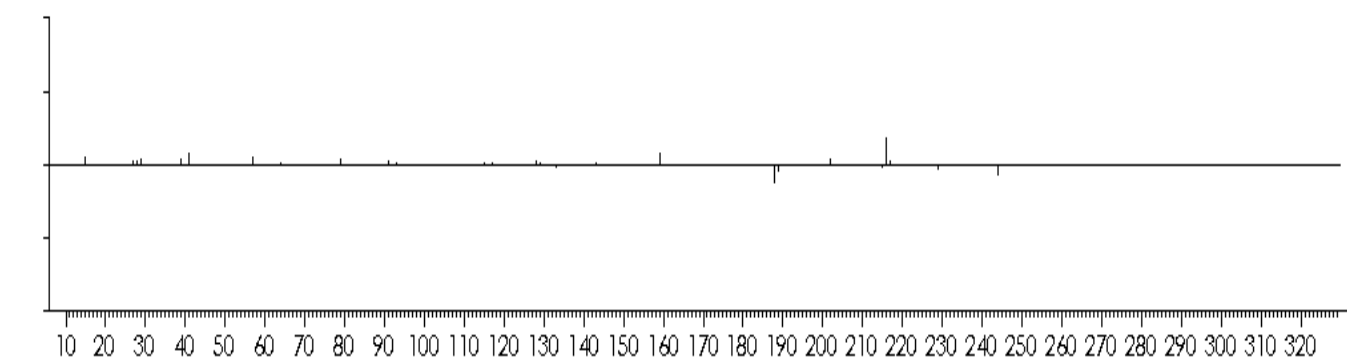
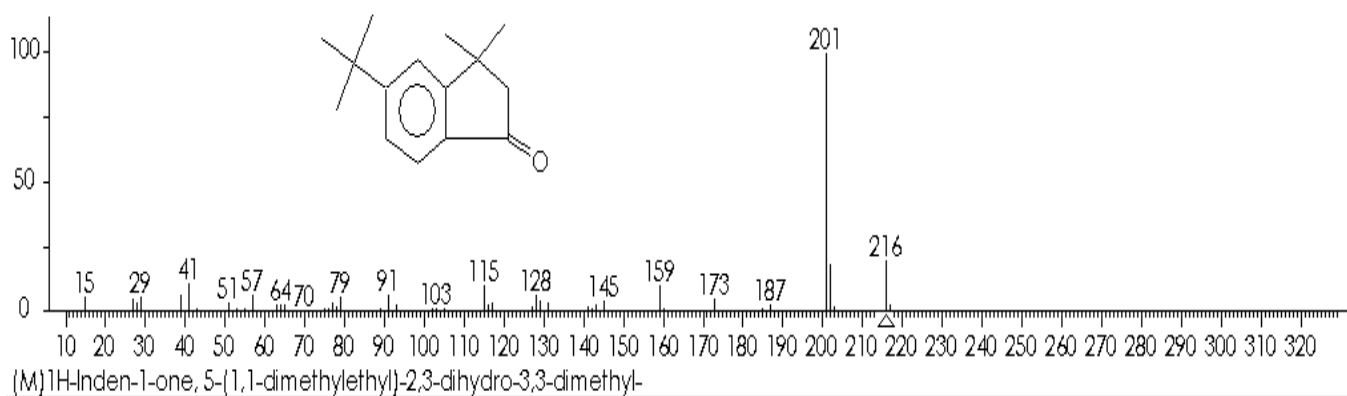
Sum of corrected areas: 460528900

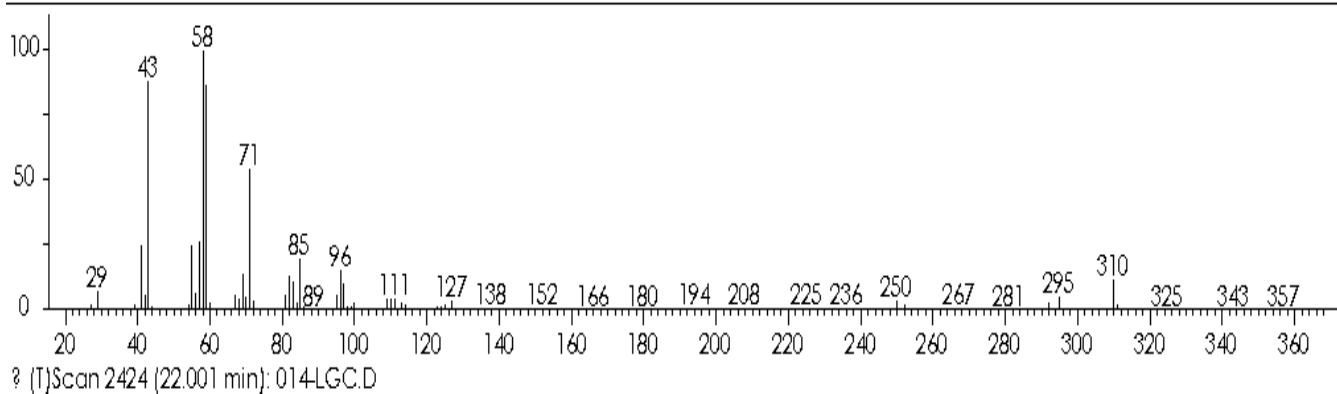
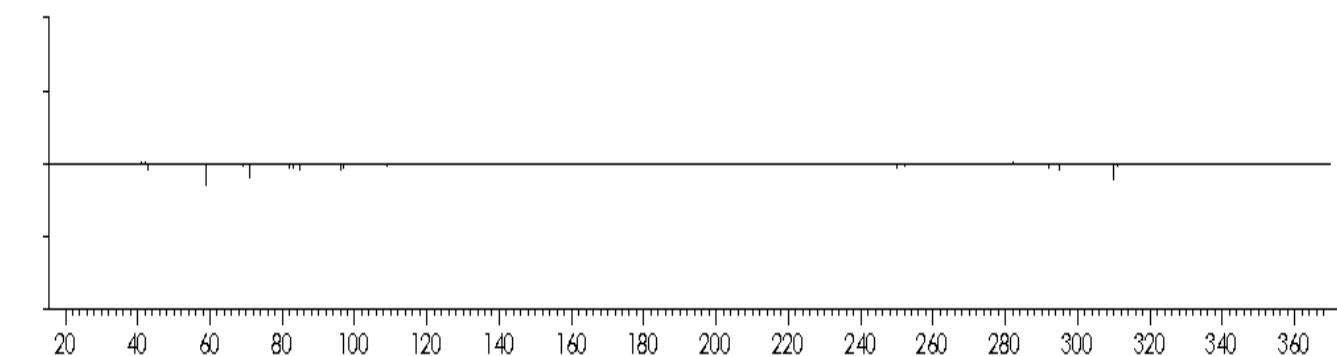
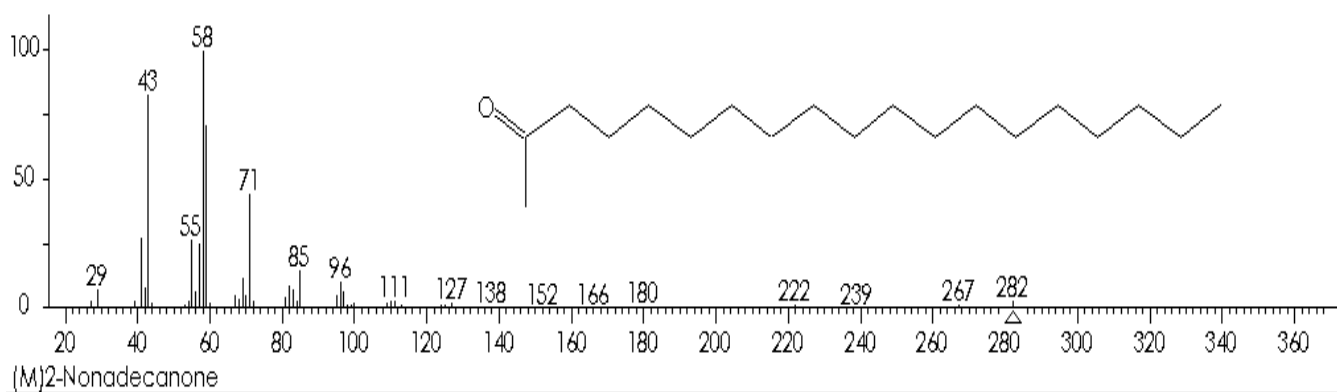


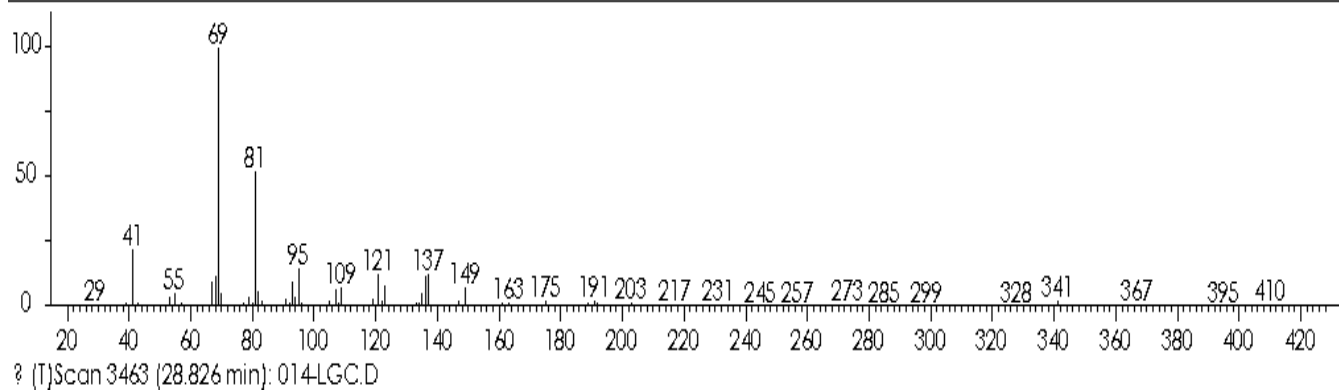
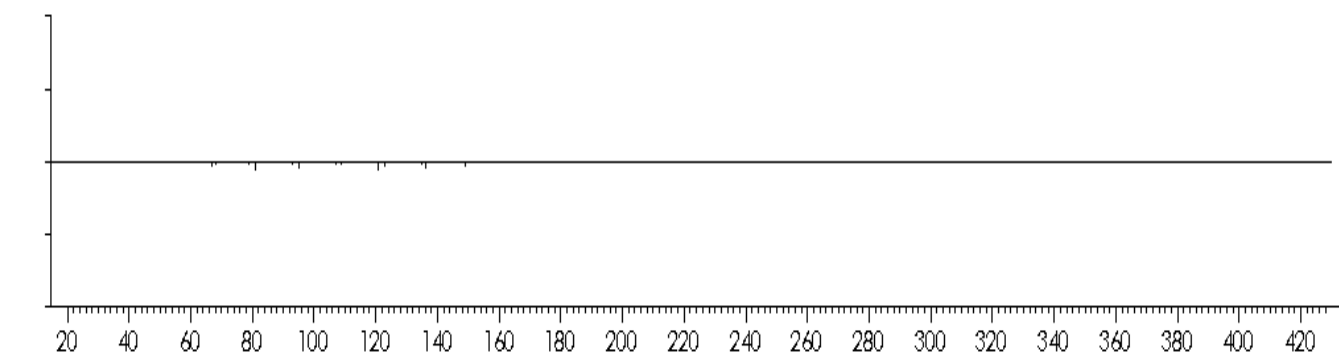
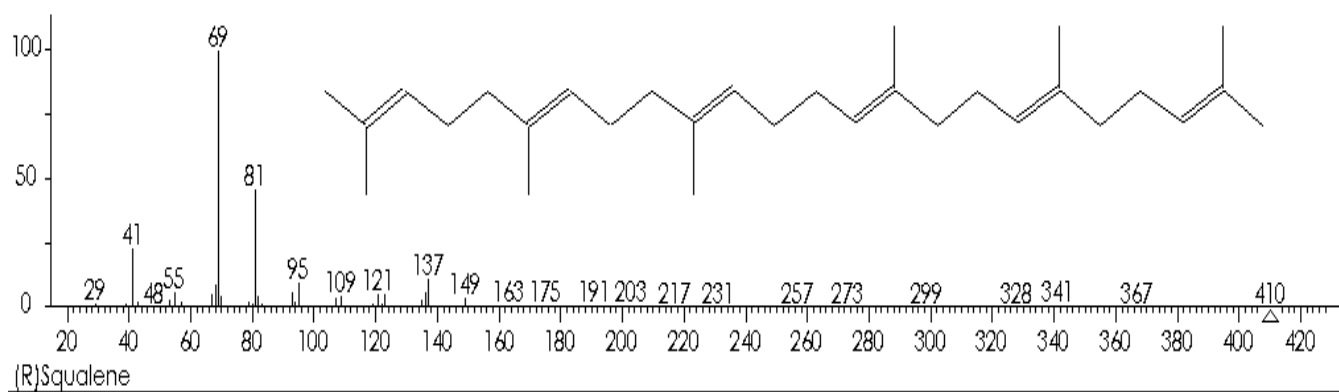


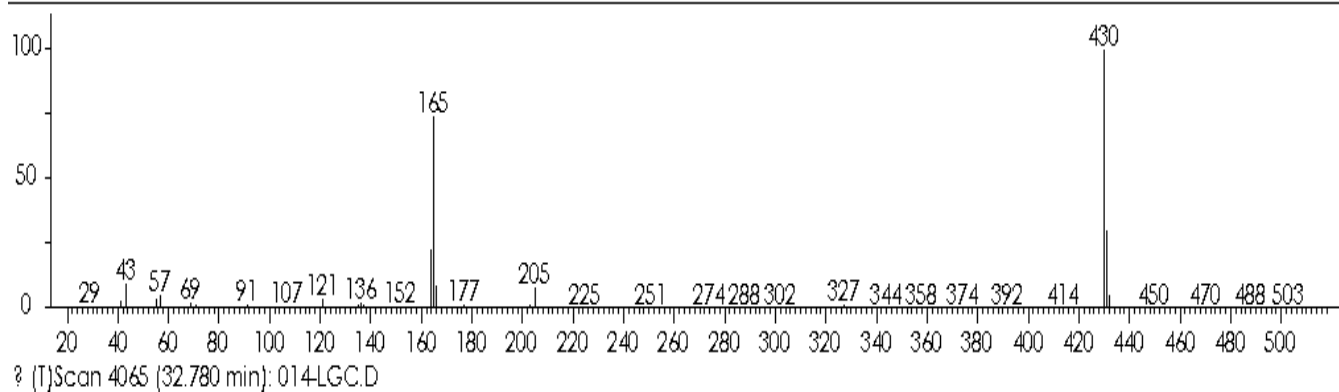
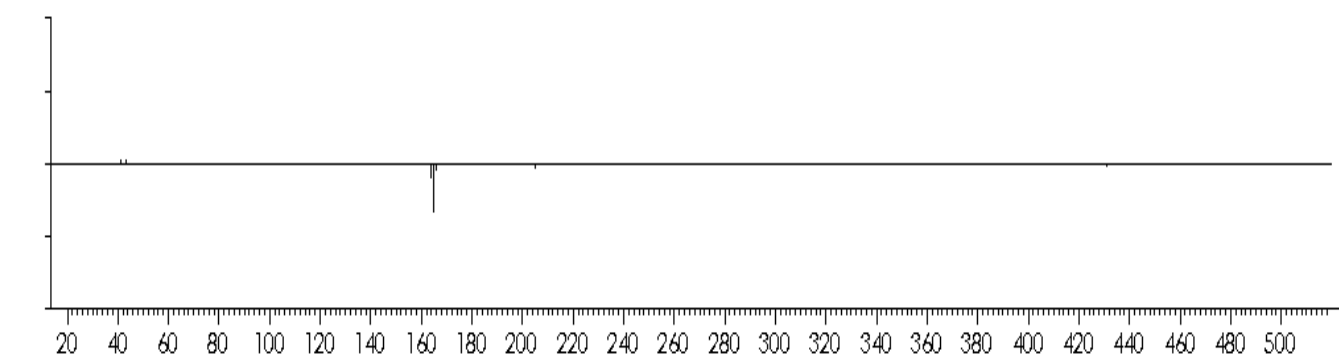
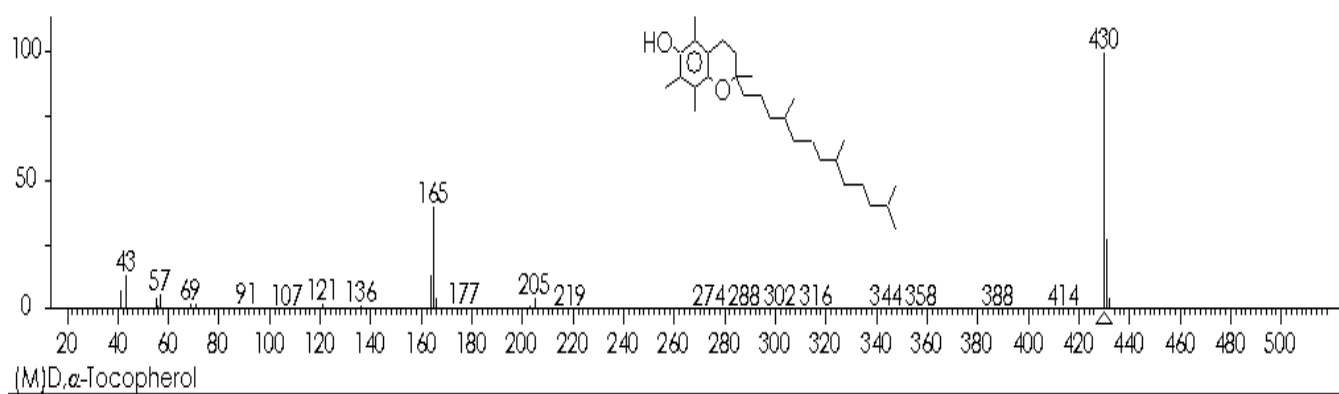












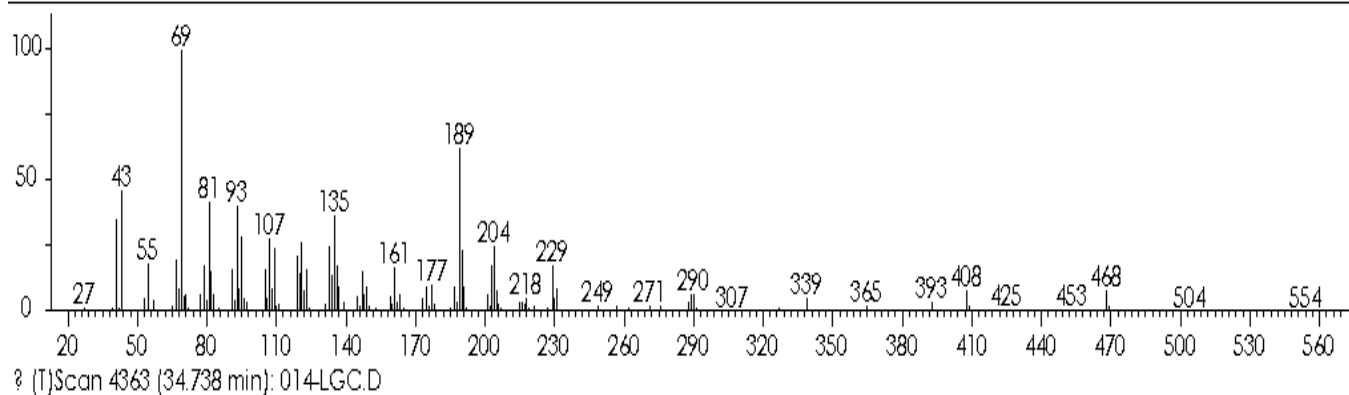
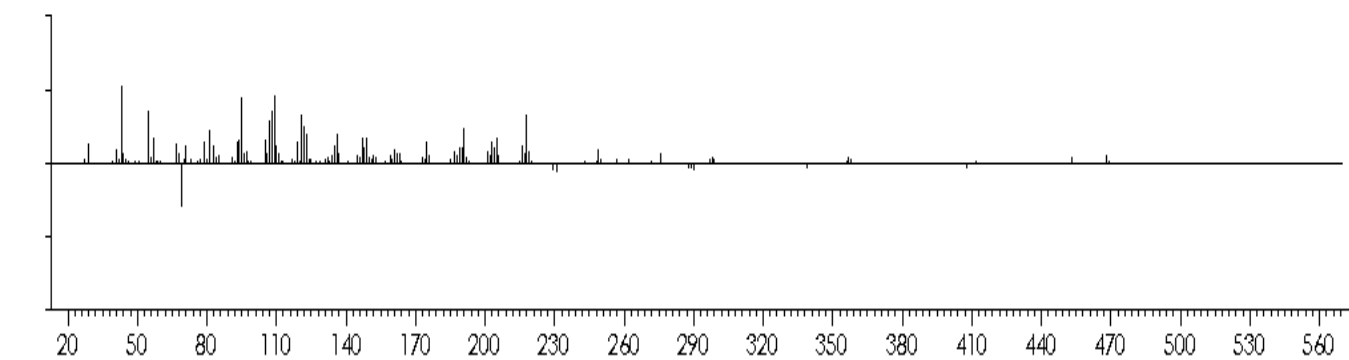
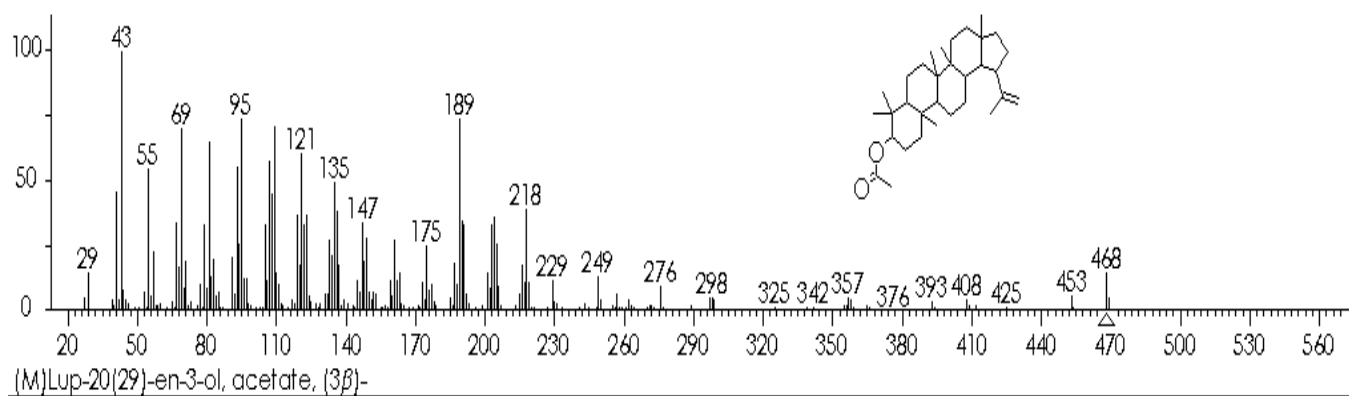


Figure S2. GC-MS Analysis of the BtH extract

Area Percent Report

Data File : C:\MSDCHEM\2\DATA\015-LGC.D Vial: 96
 Acq On : 18 Oct 2022 11:15 Operator: M.G.M
 Sample : BtzHex Splitless 40°C-1min, Inst : Instrumen
 Misc : 10°C/min-250°C-5min,10°C/min-20min Multiplr: 1.00
 Sample Amount: 1.00

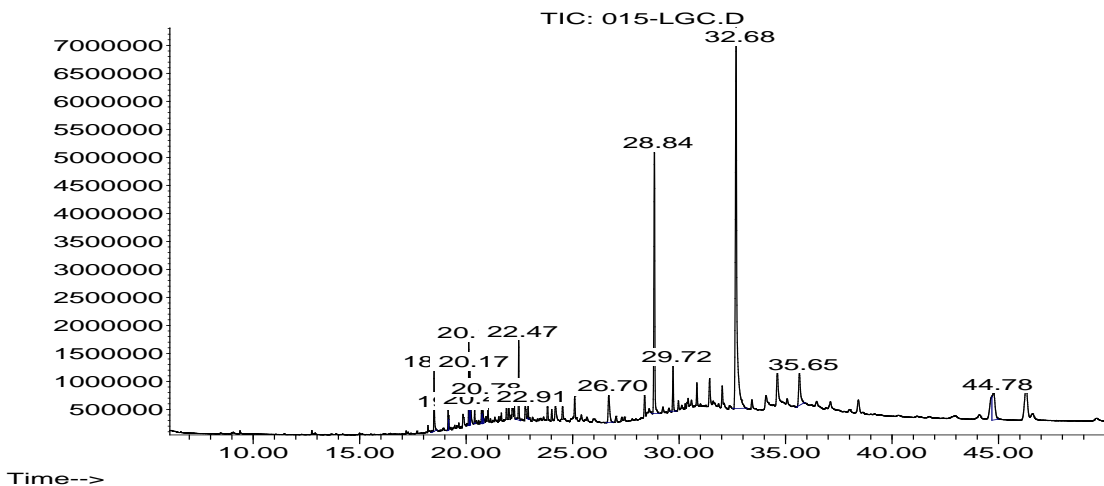
MS Integration Params: autoint1.e

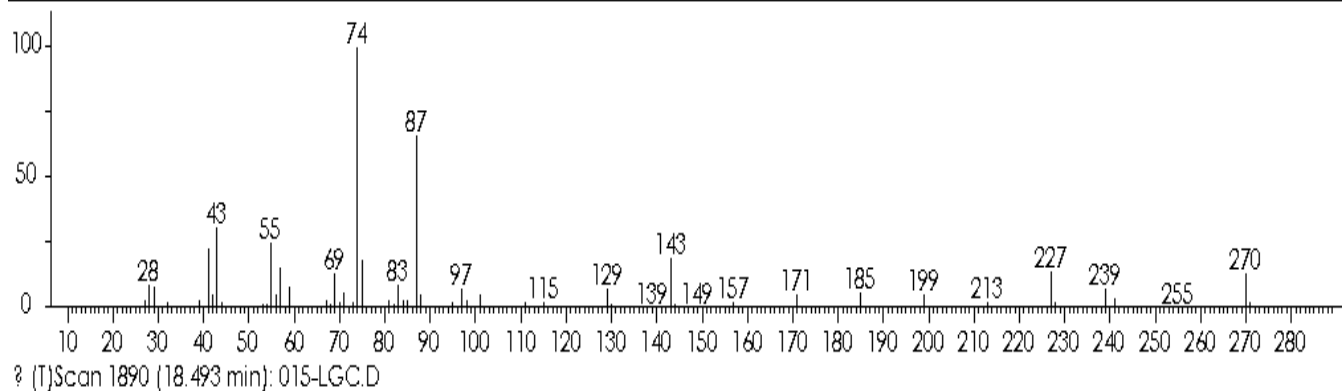
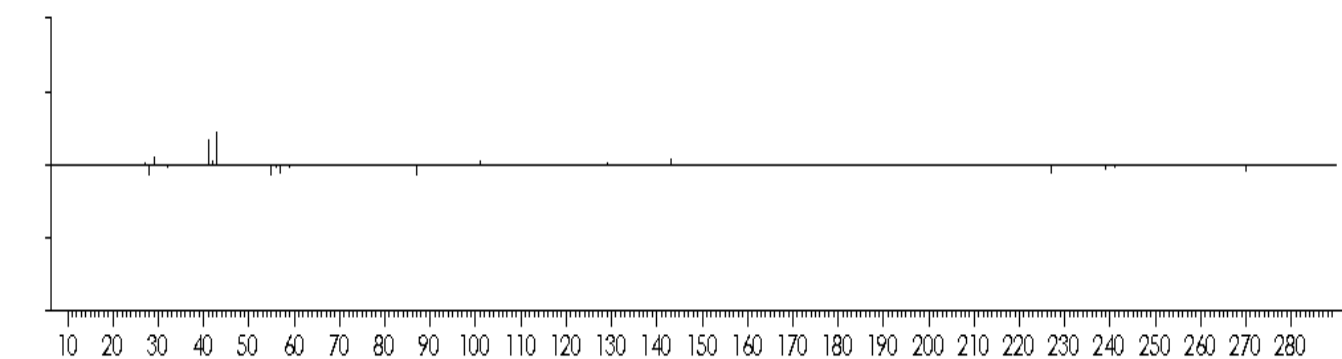
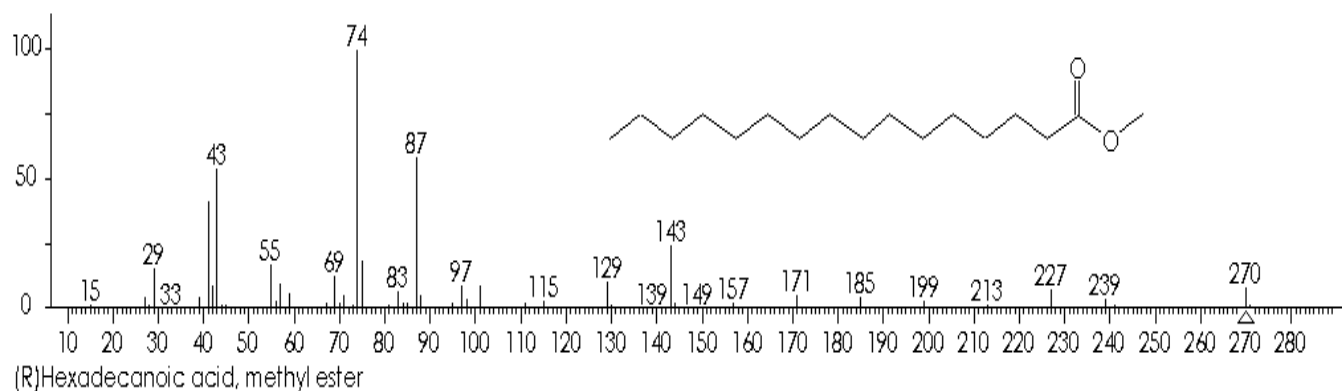
Signal : TIC

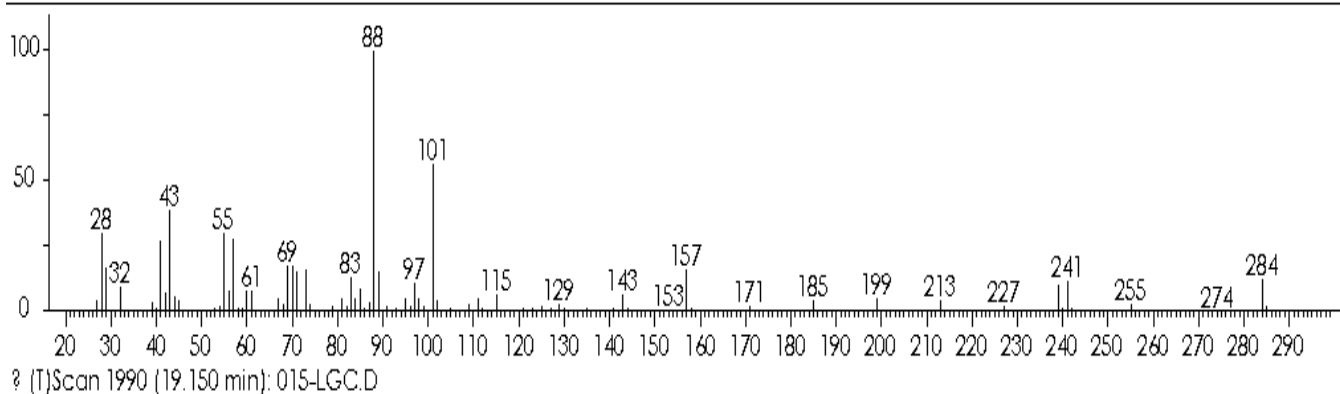
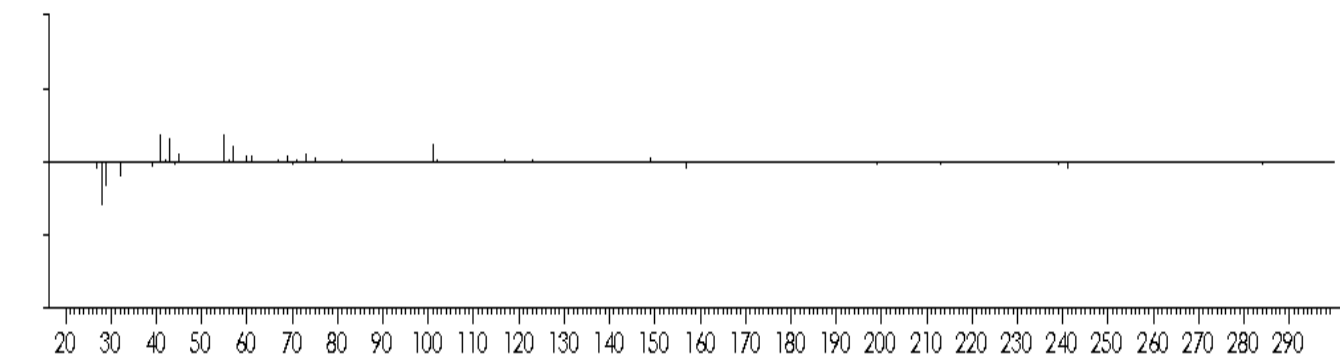
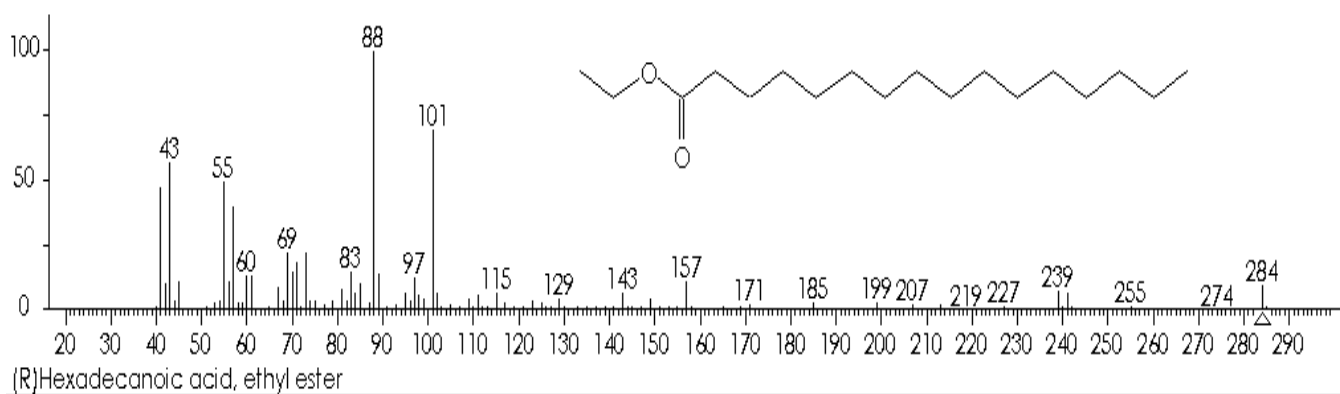
peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	18.493	1870	1890	1910	BB	1054859	23320727	7.17%	3.216%
2	19.150	1986	1990	1994	M	371667	5936264	1.83%	0.819%
3	20.122	2133	2138	2142	M	1521626	25098555	7.72%	3.462%
4	20.175	2143	2146	2150	M3	988264	18038391	5.55%	2.488%
5	20.398	2176	2180	2185	M	284165	4668471	1.44%	0.644%
6	20.727	2224	2230	2234	M	513857	8499903	2.61%	1.172%
7	20.773	2235	2237	2245	M2	478580	10314151	3.17%	1.422%
8	22.474	2473	2496	2508	BB	1397806	27913041	8.58%	3.850%
9	22.907	2558	2562	2568	M2	244262	4606328	1.42%	0.635%
10	26.704	3120	3140	3164	BB 3	500167	24591938	7.56%	3.392%
11	28.845	3446	3466	3496	BB	4676899	145442645	44.72%	20.059%
12	29.719	3580	3599	3616	BB	811542	20855076	6.41%	2.876%
13	32.681	4025	4050	4122	BB	6757043	325236826	100.00%	44.855%
14	35.657	4479	4503	4536	BB 4	575766	35057274	10.78%	4.835%
15	44.774	5878	5891	5920	M4	480756	45497576	13.99%	6.275%

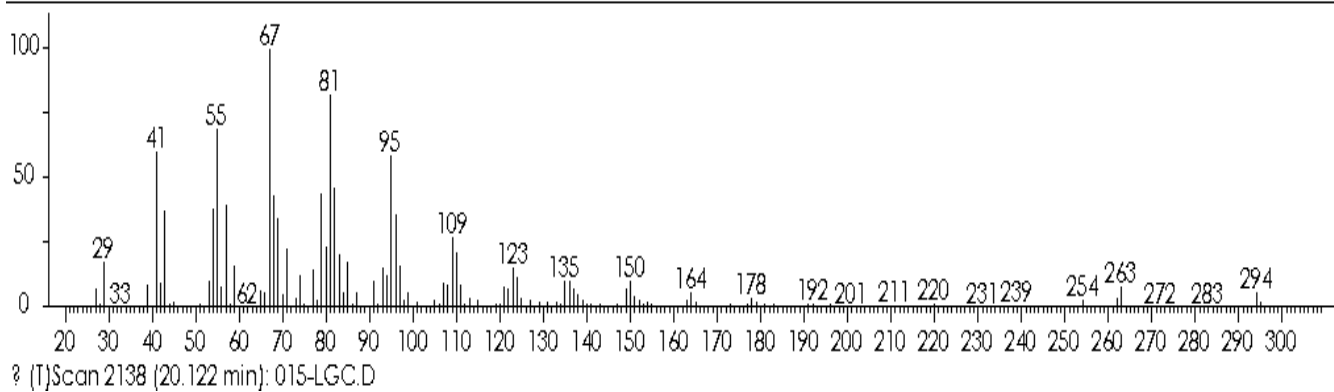
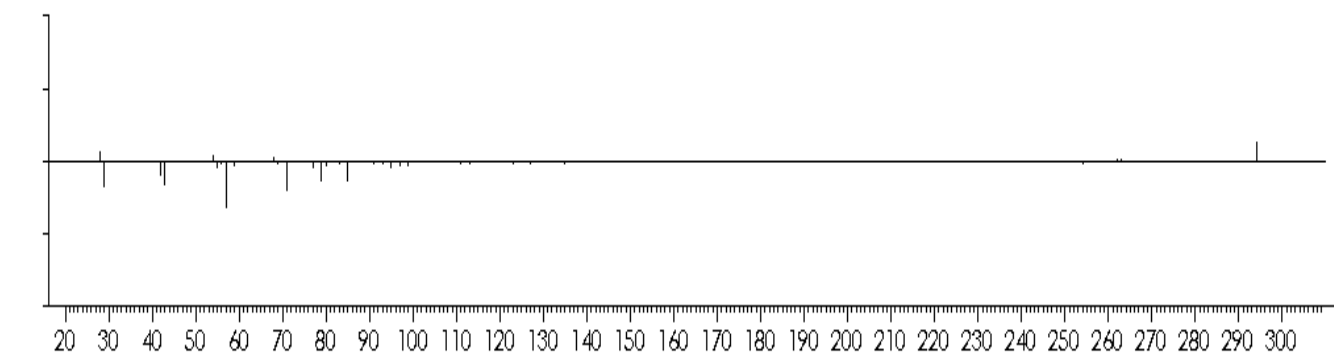
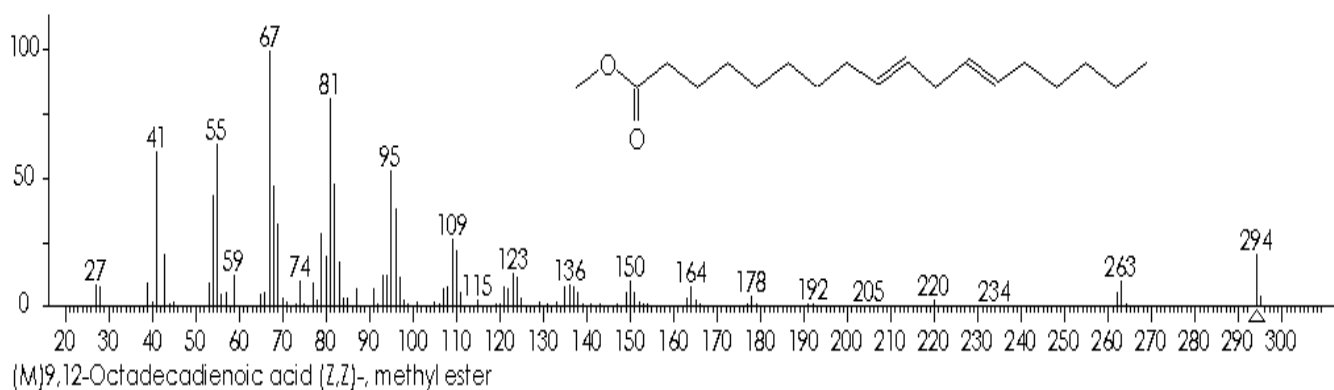
Sum of corrected areas: 725077165

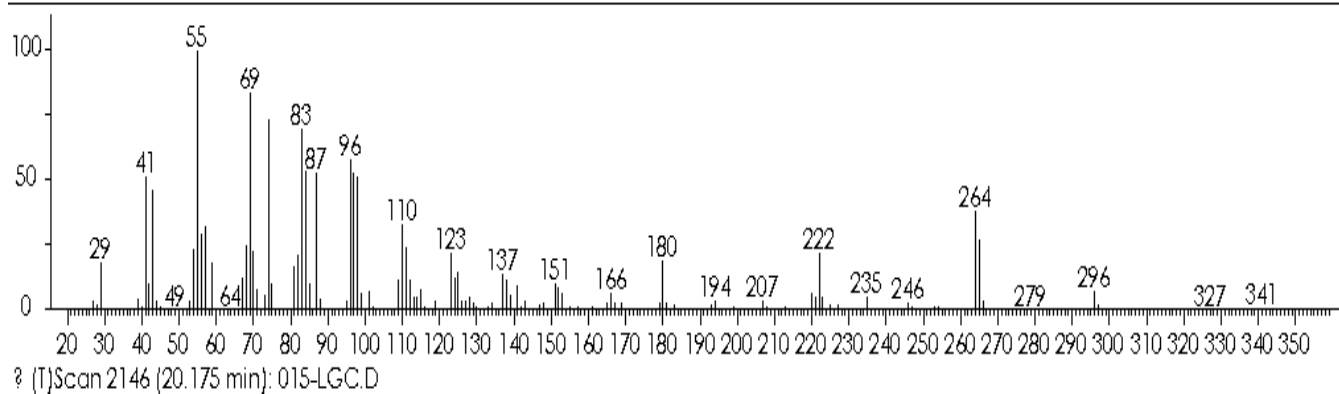
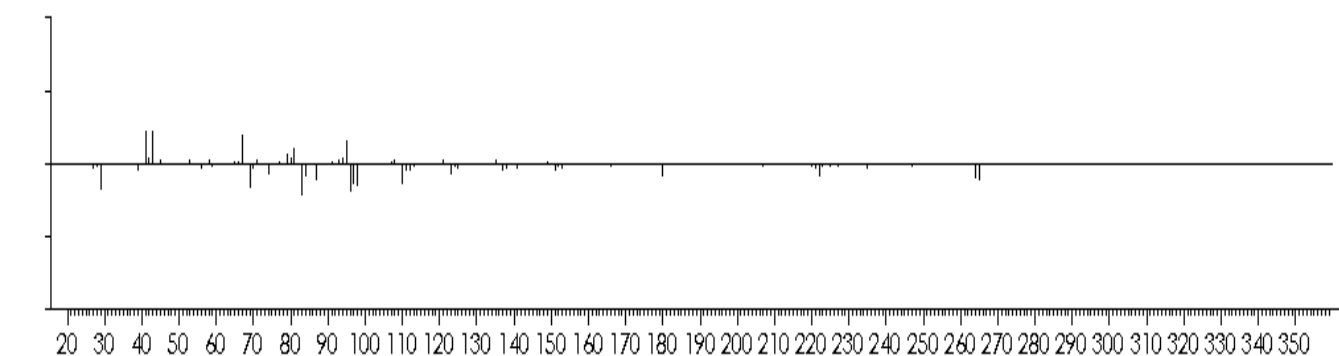
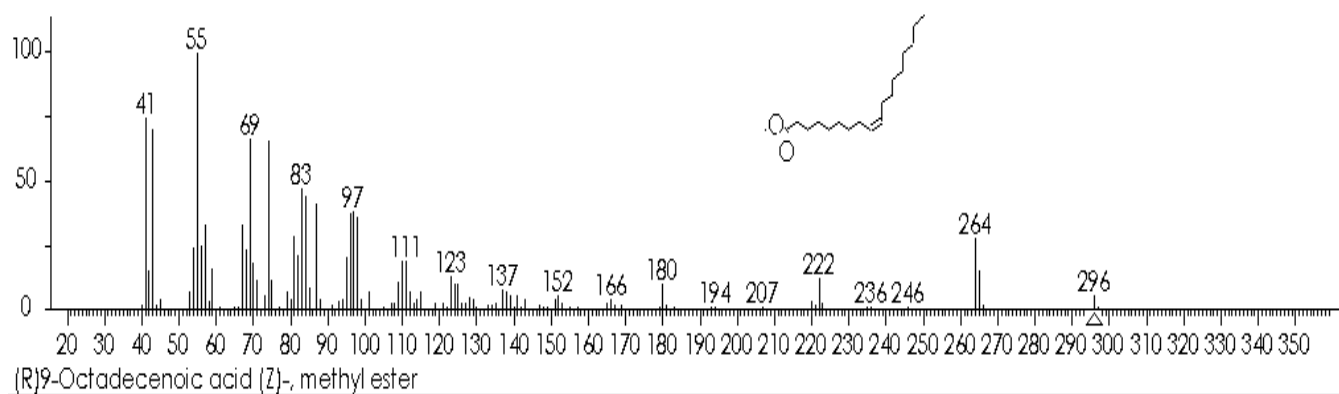
Abundance

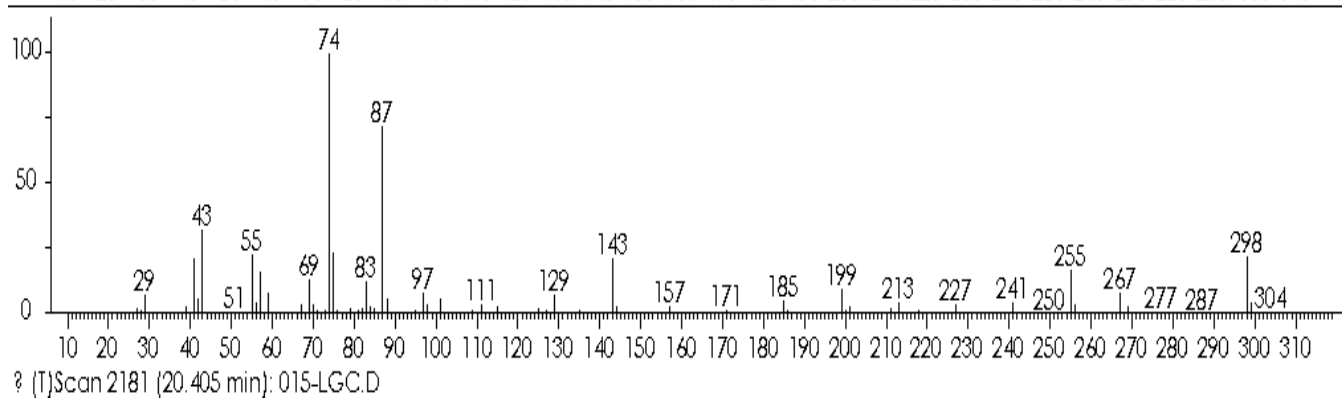
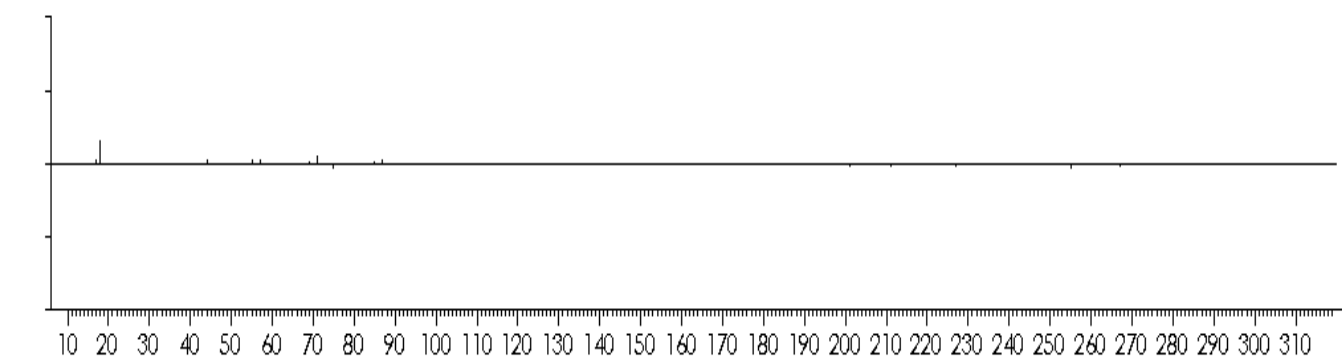
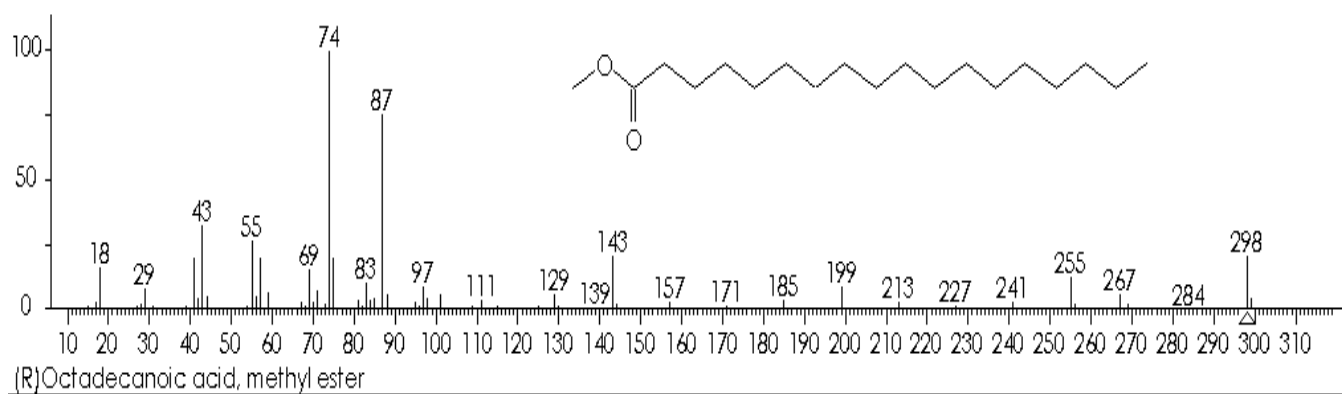


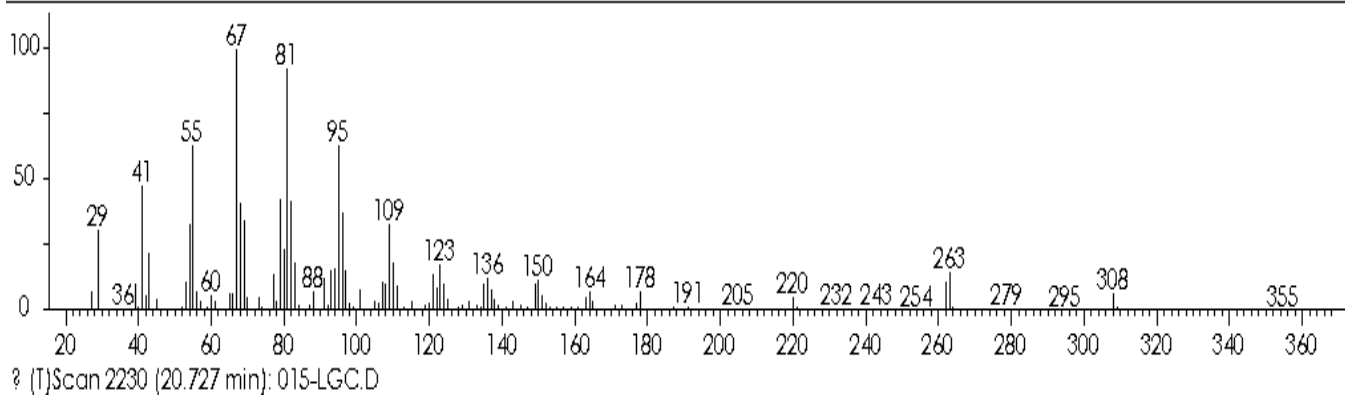
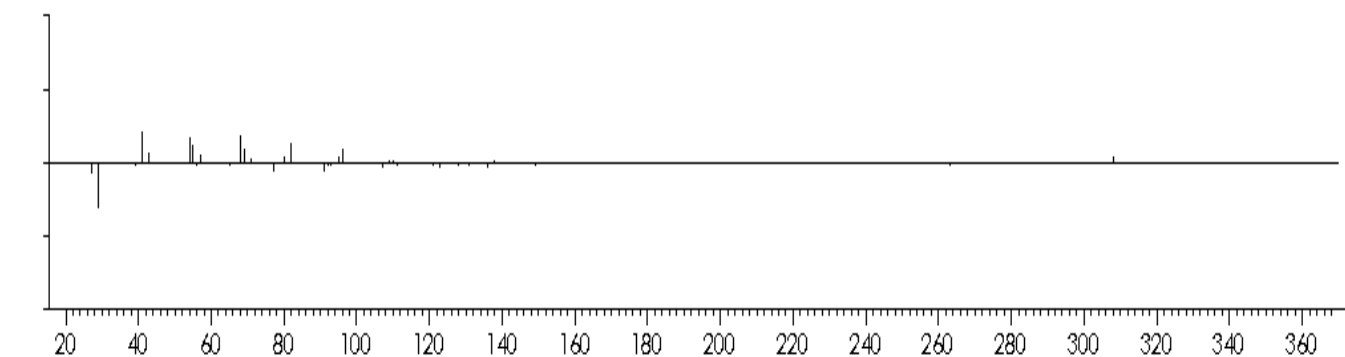
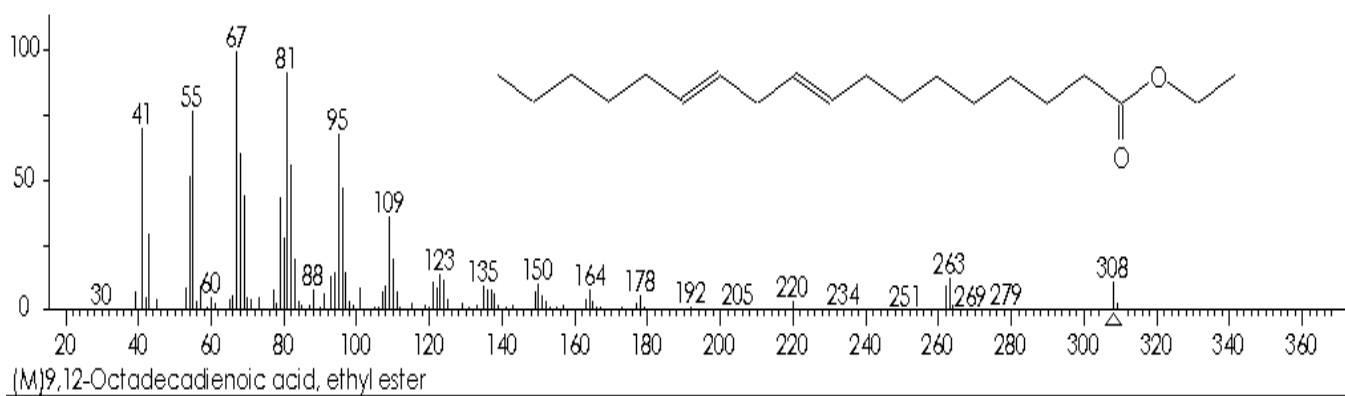


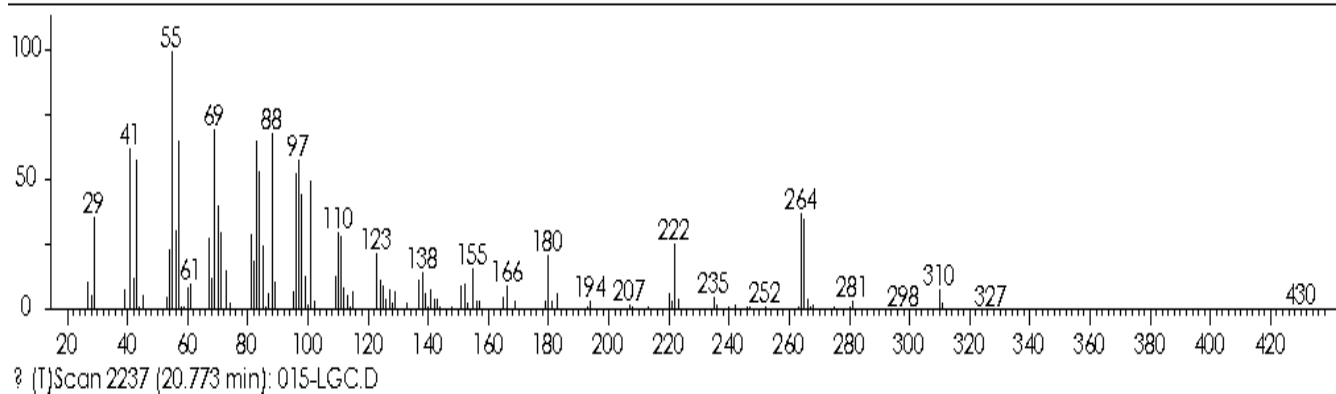
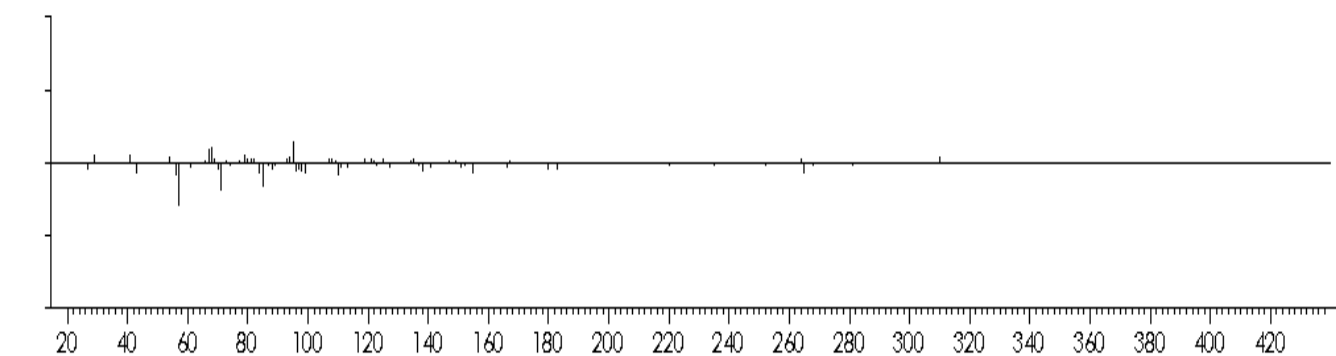
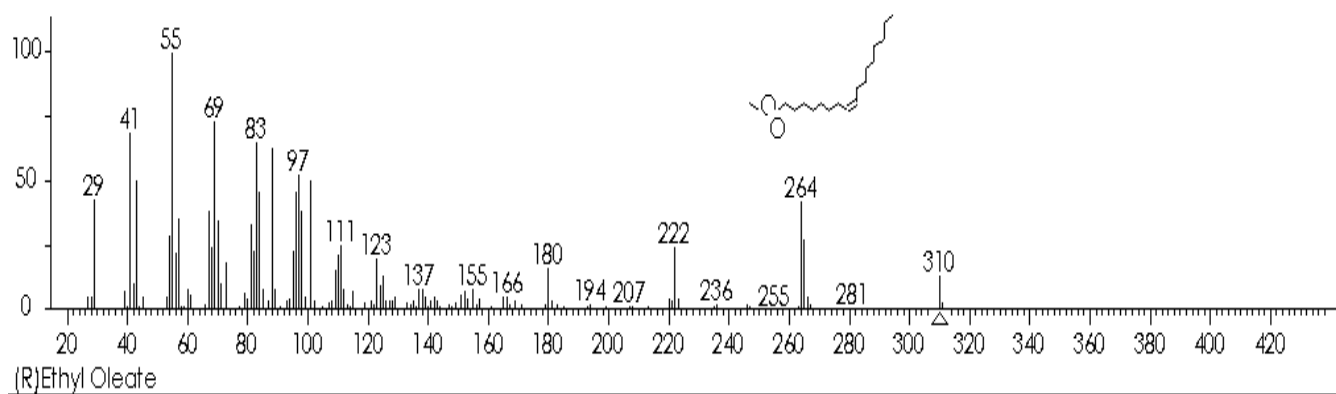


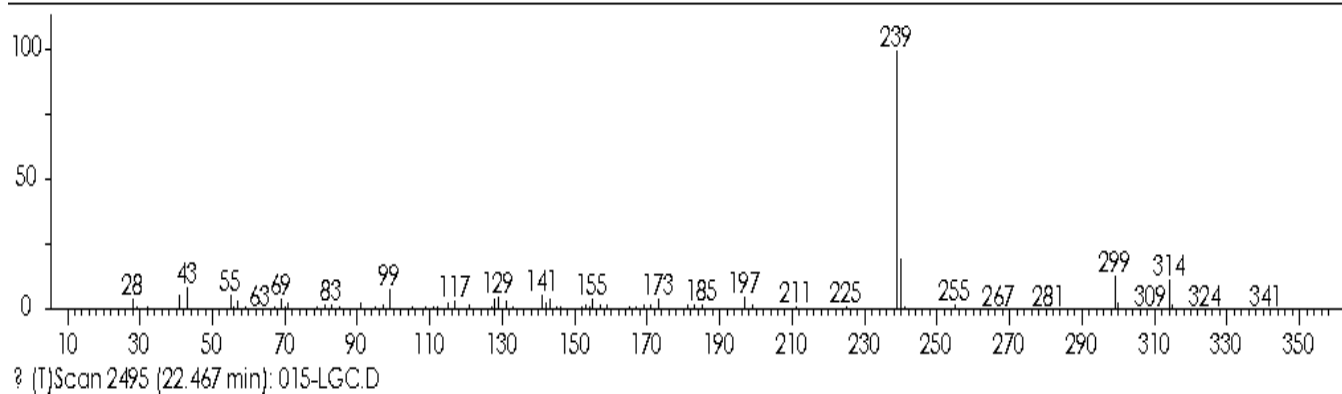
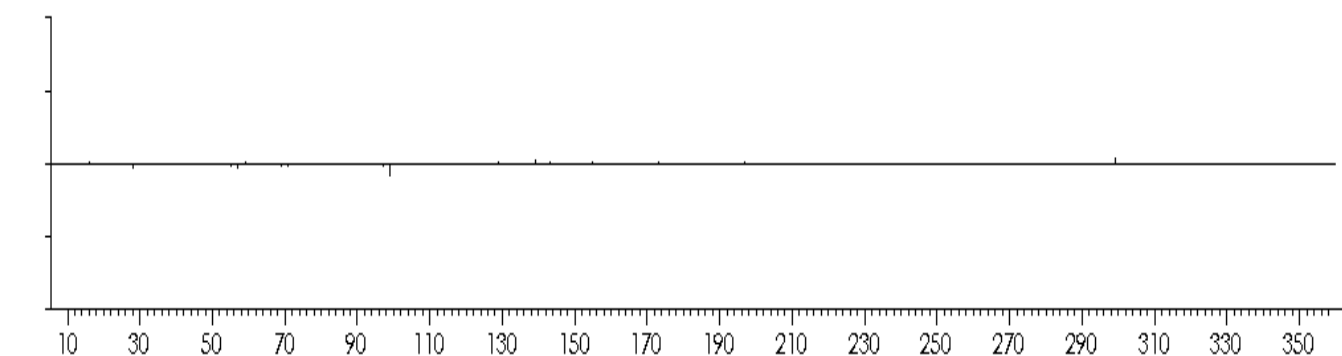
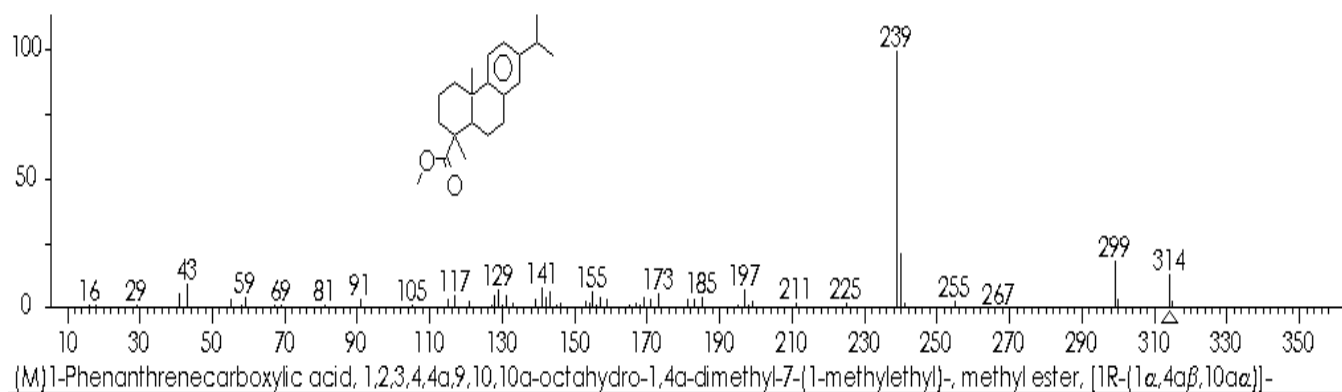


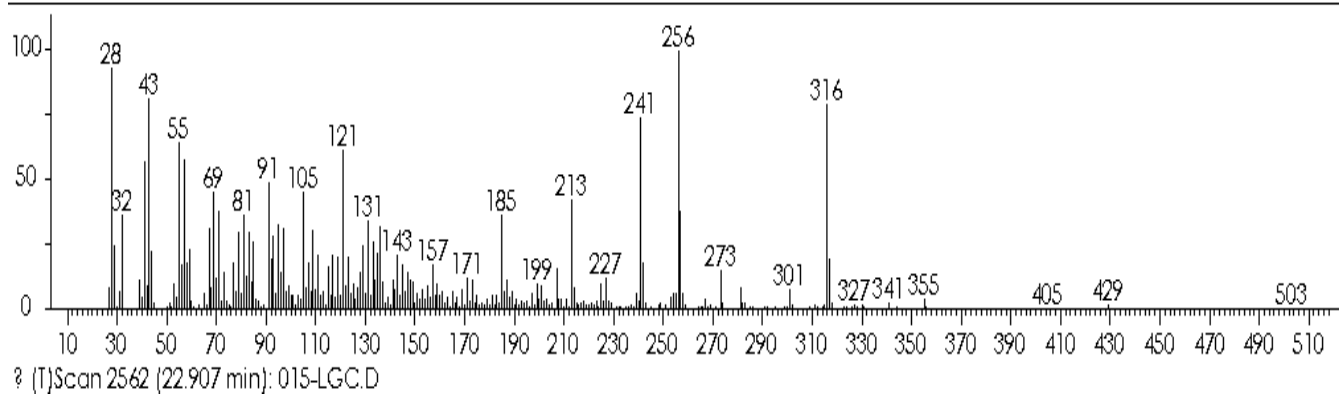
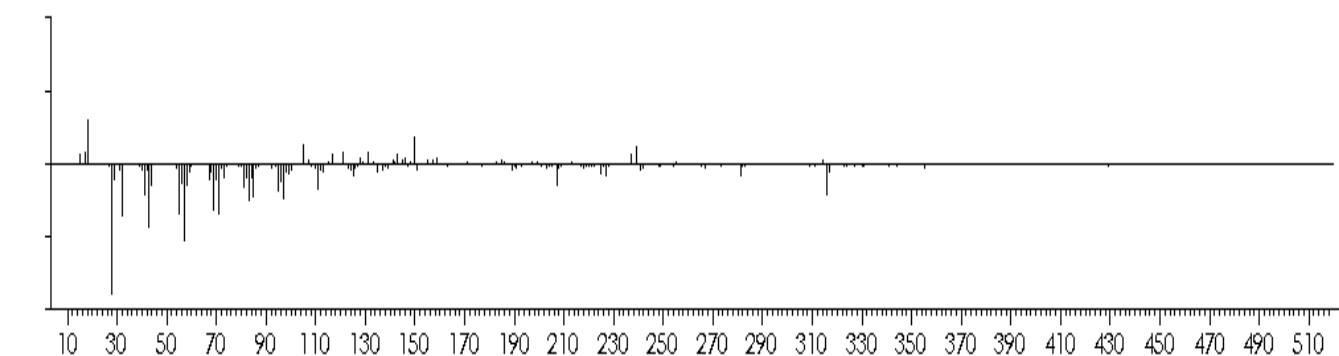
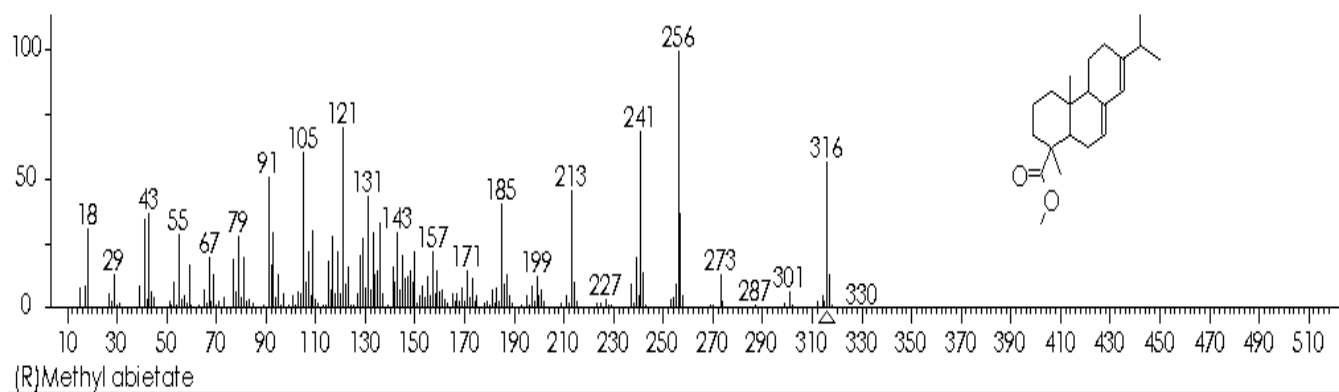


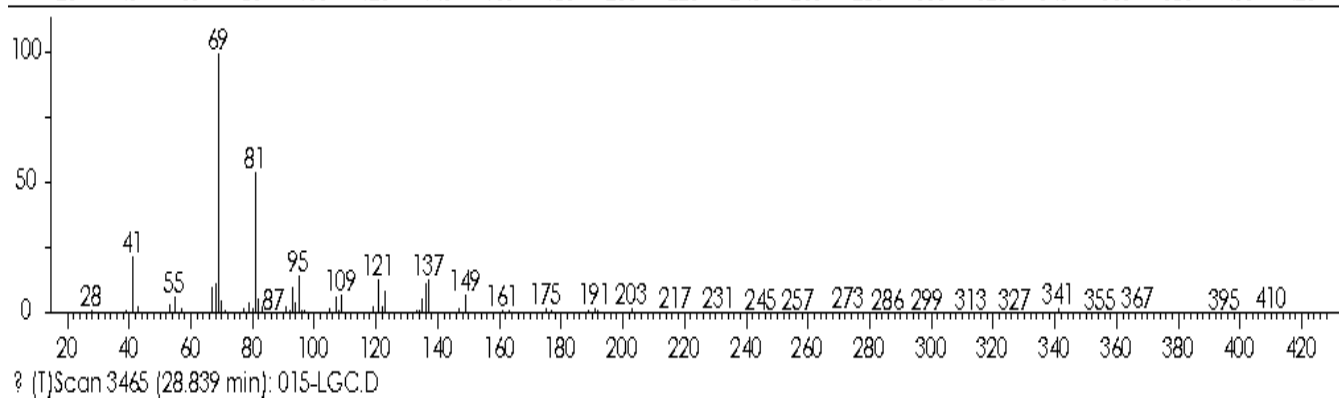
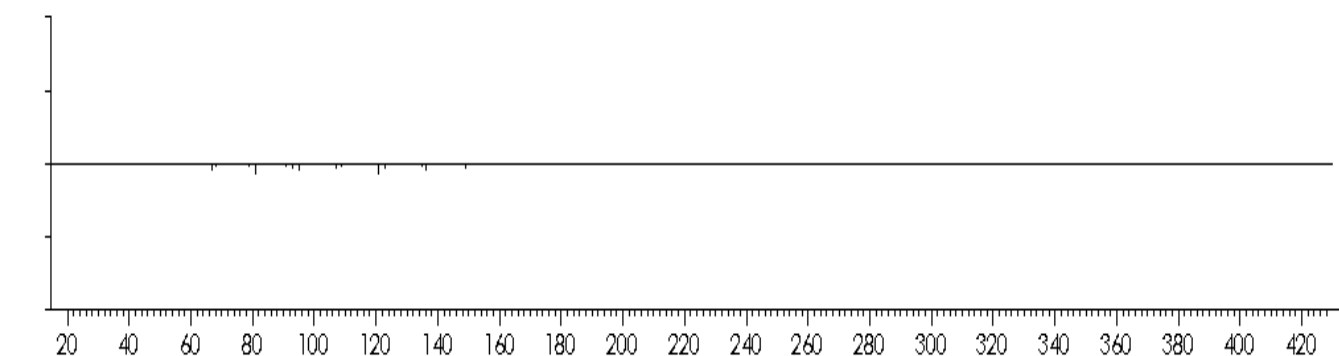
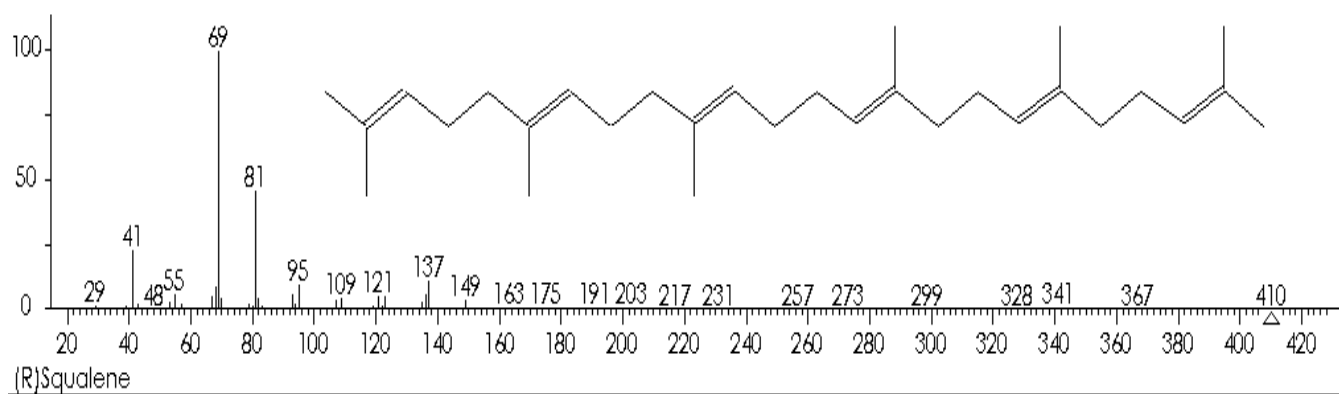


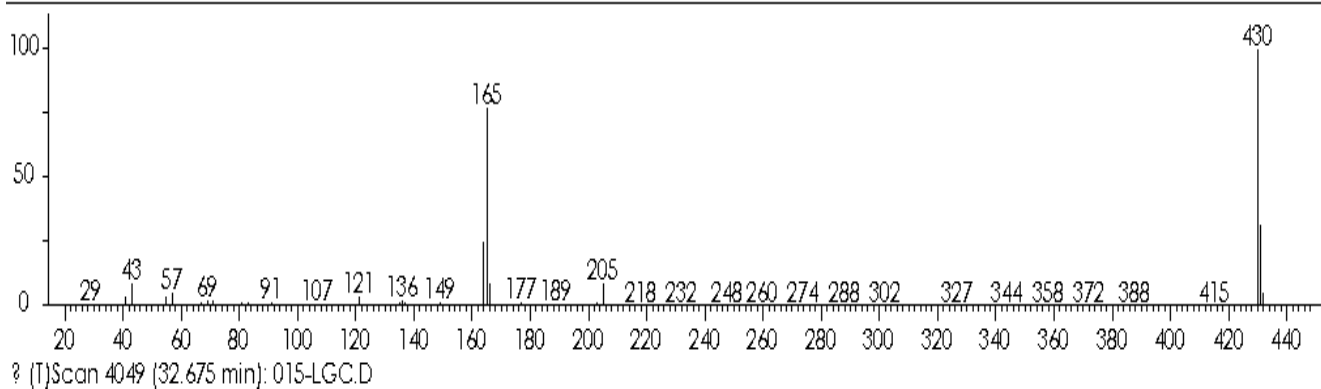
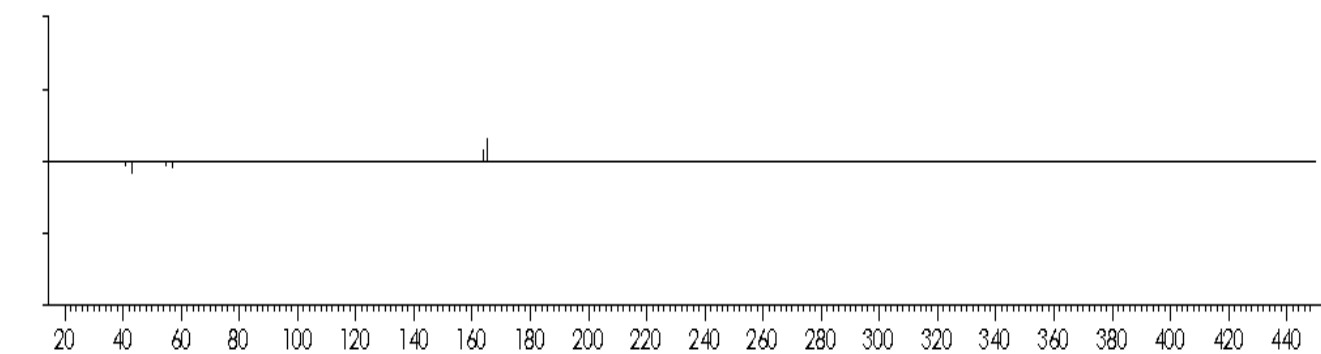
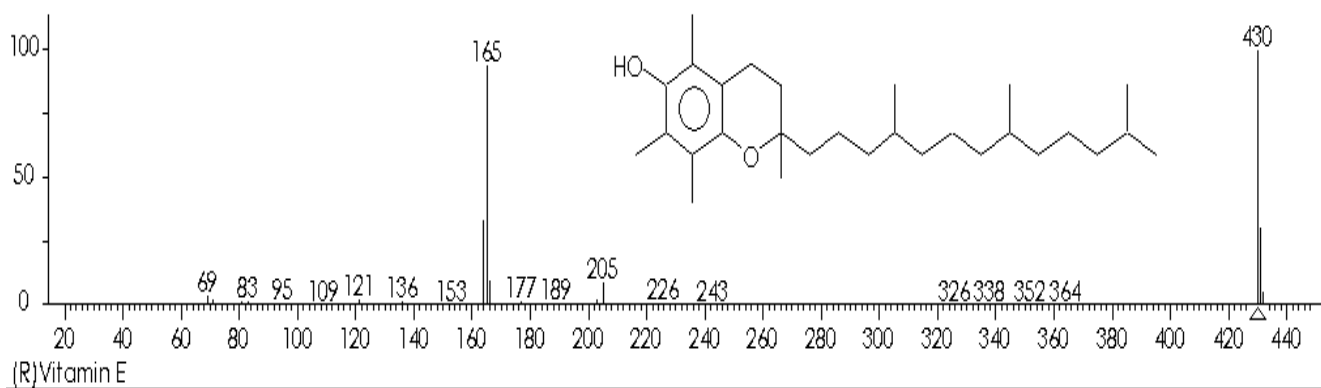


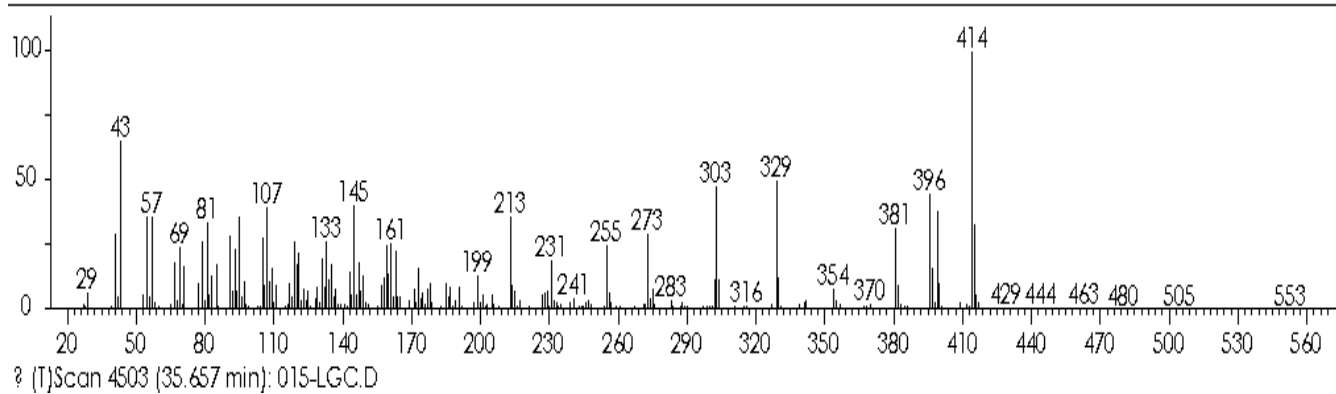
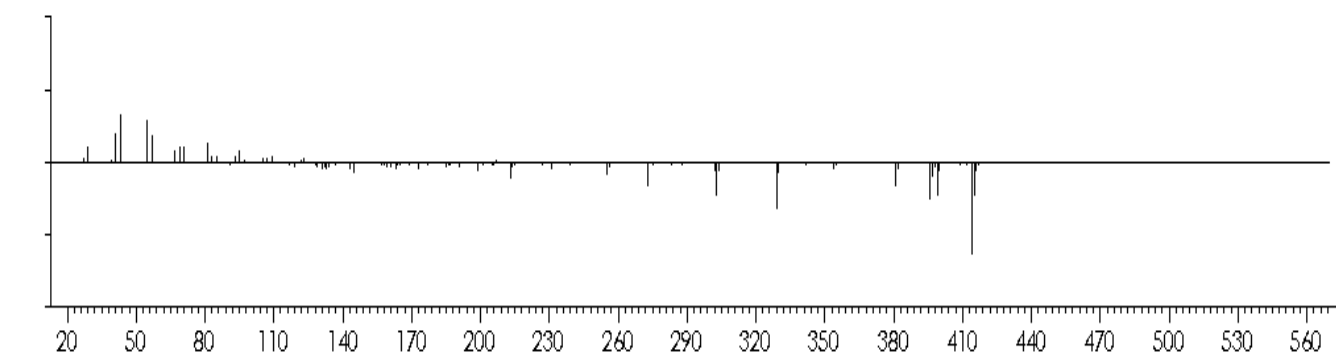
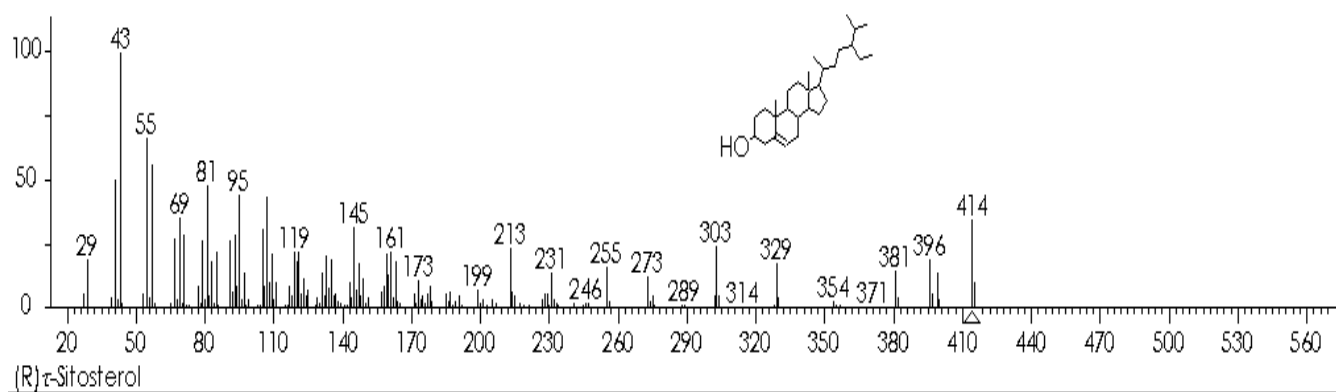


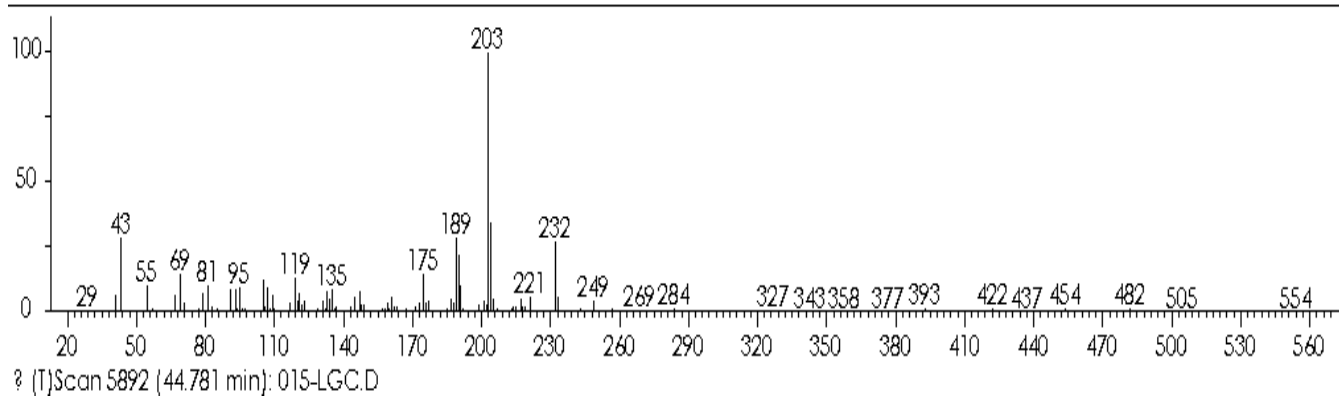
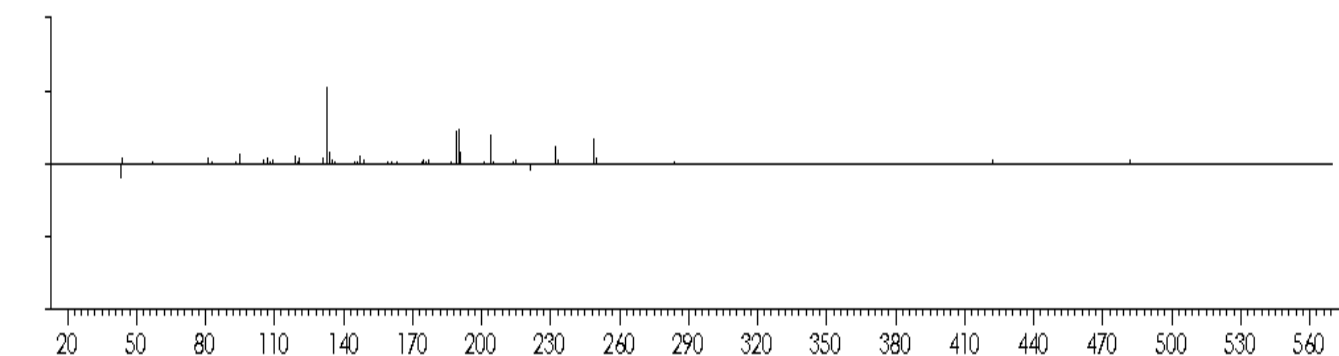
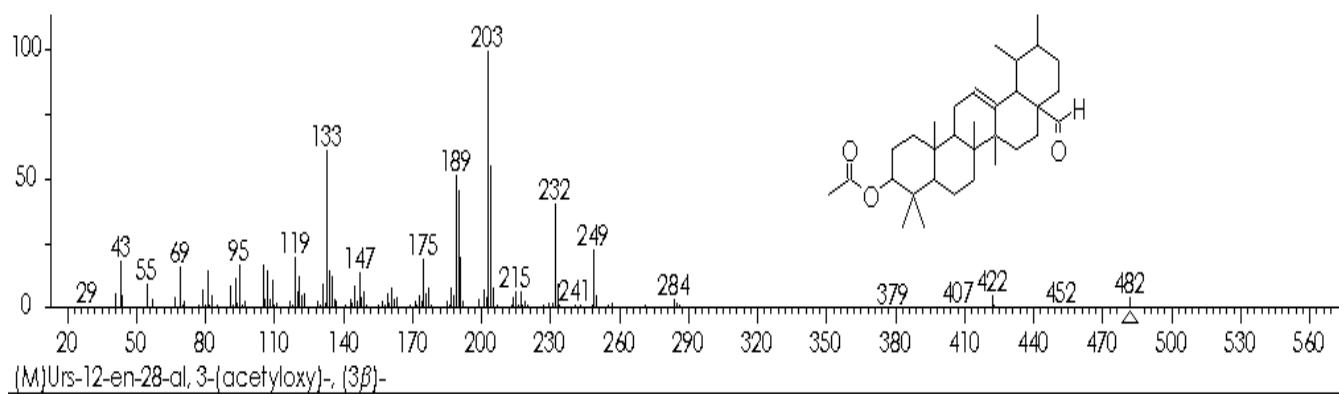












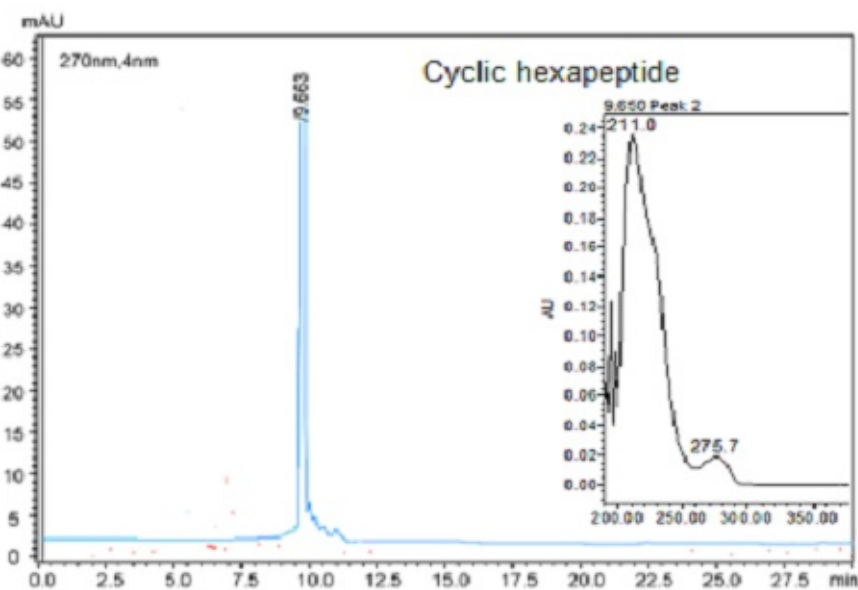
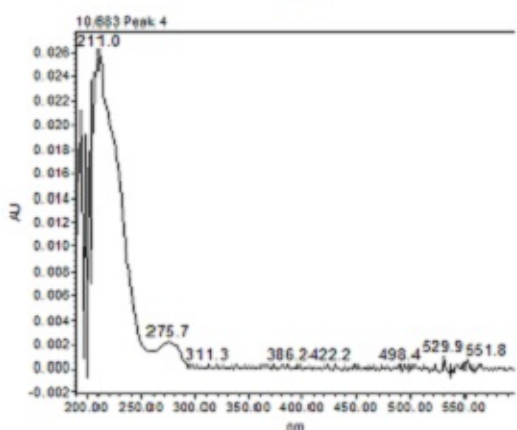
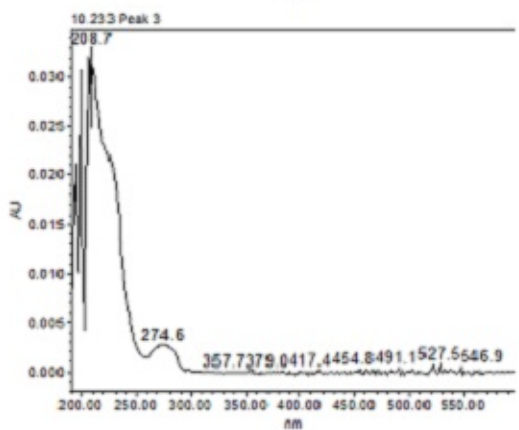
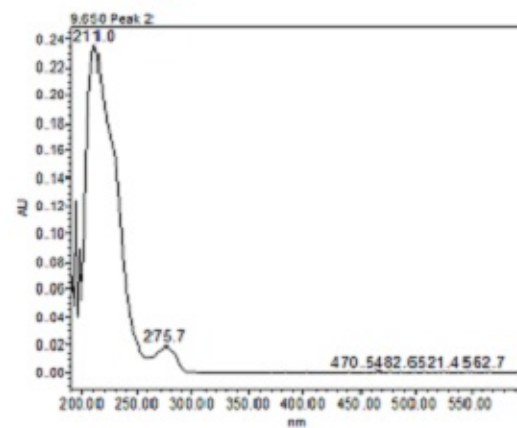
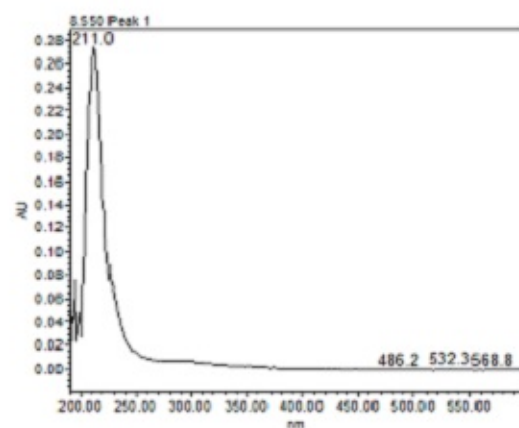
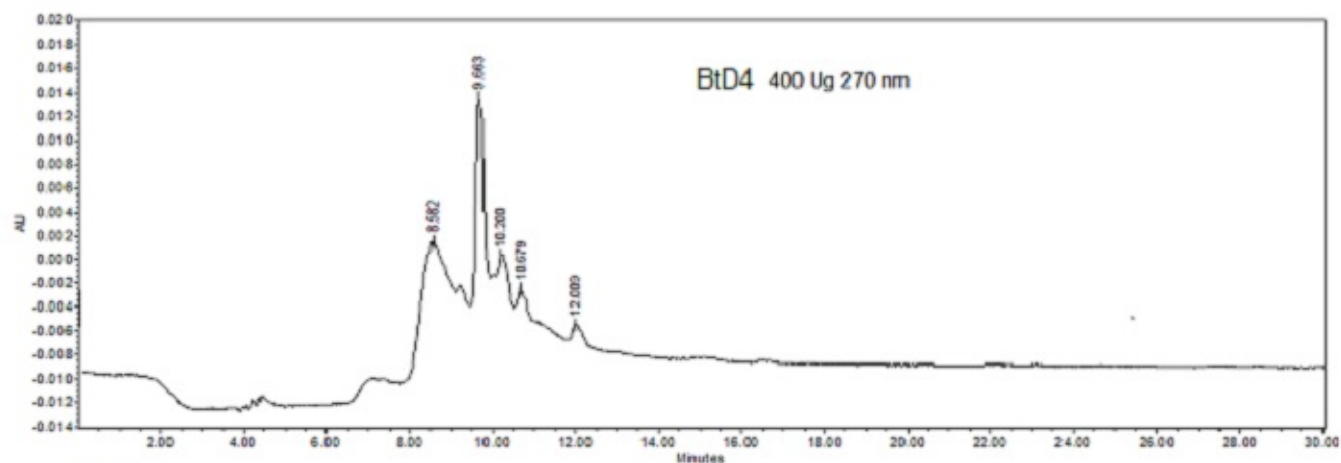
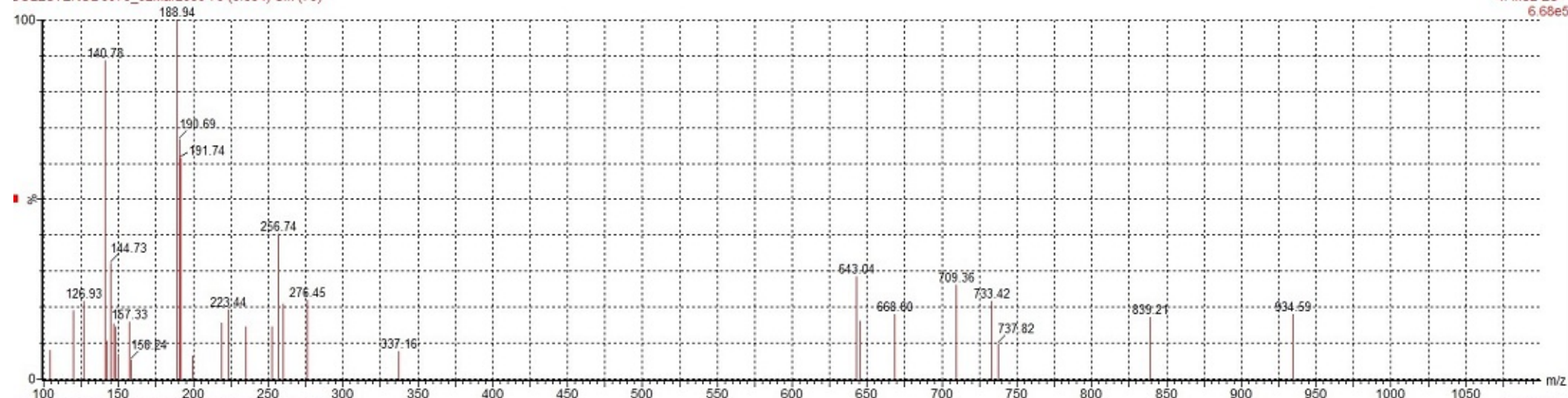


Figure S3. Spectrum UV and HPLC of cyclic hexapeptide

DOLESTEROL 3073_02Mar2350 73 (3.684) Cm (73)

4: MS2 ES+
6.68e5

DOLESTEROL 3073_02Mar2350 69 (3.480) Cm (68.79)

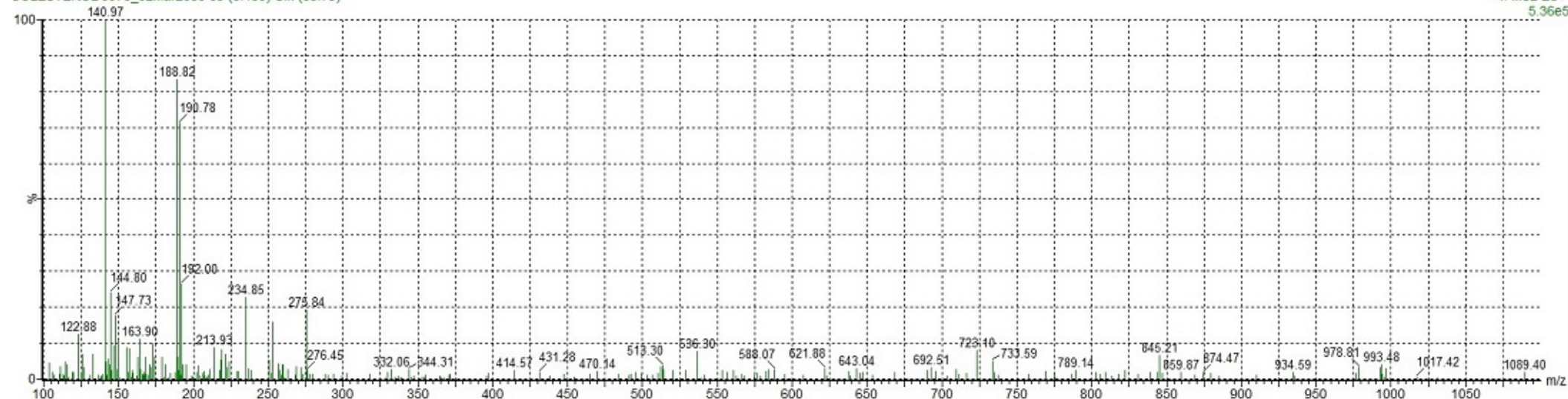
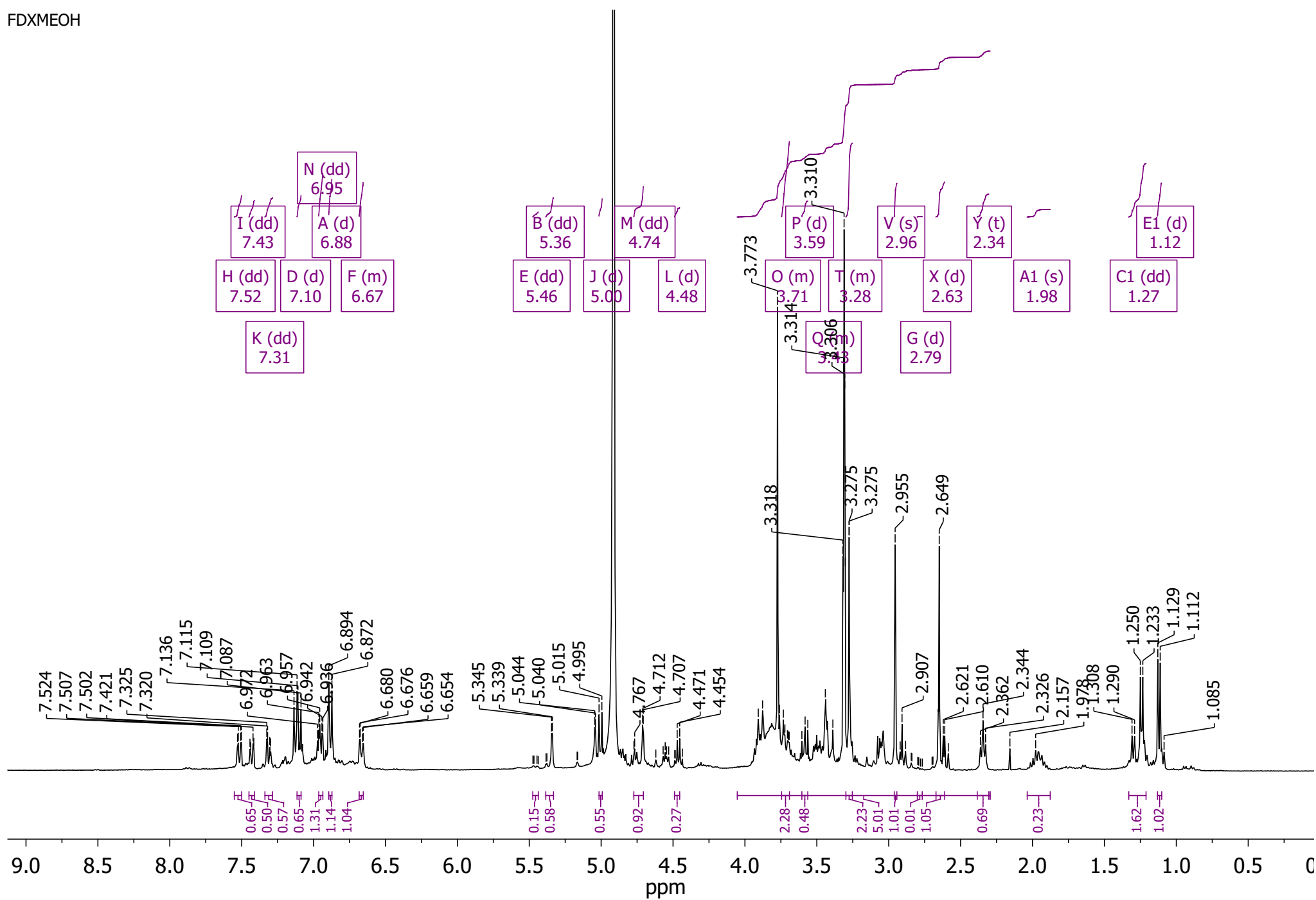
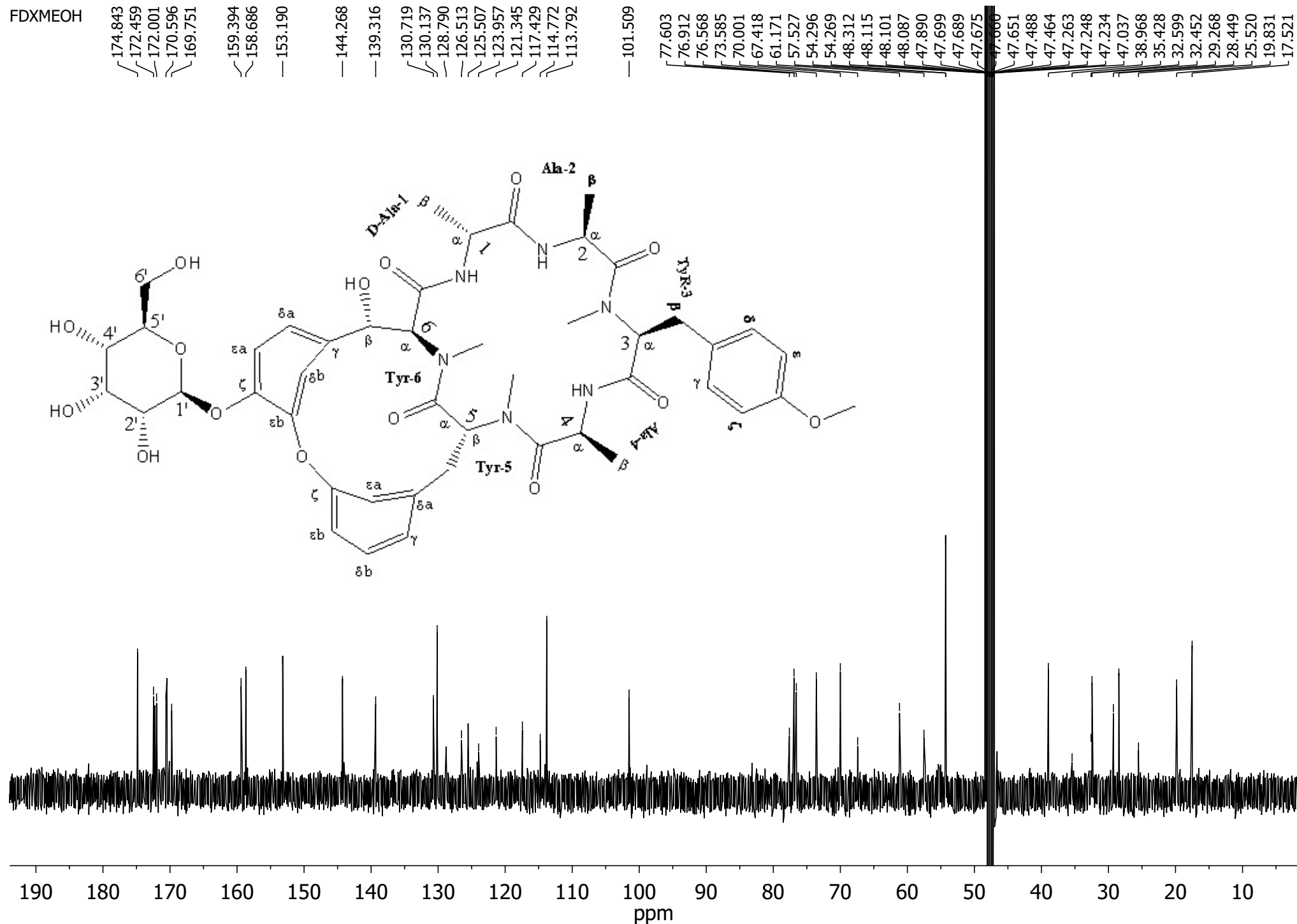
4: MS2 ES+
5.36e5 $m/z = 934.59 [M+H]^+$

Figure S4. Mass spectrum (MS) cyclic hexapeptide

Figure S5. ^1H NMR (CD_3OD , 500 MHz) Rubiayunnanesis H



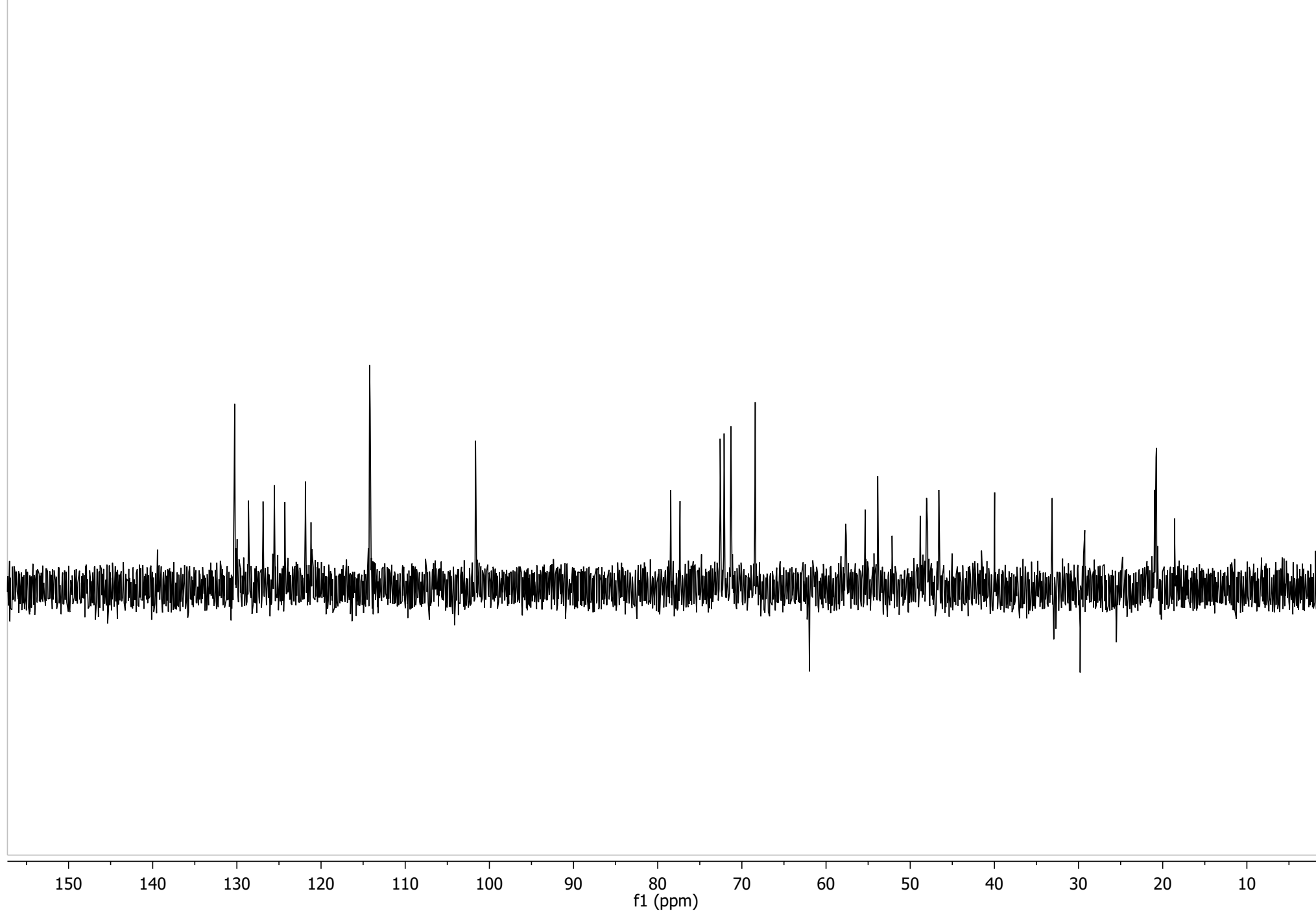


Figure S7. ^{13}C NMR (DEPT) Rubiayunnanesis H

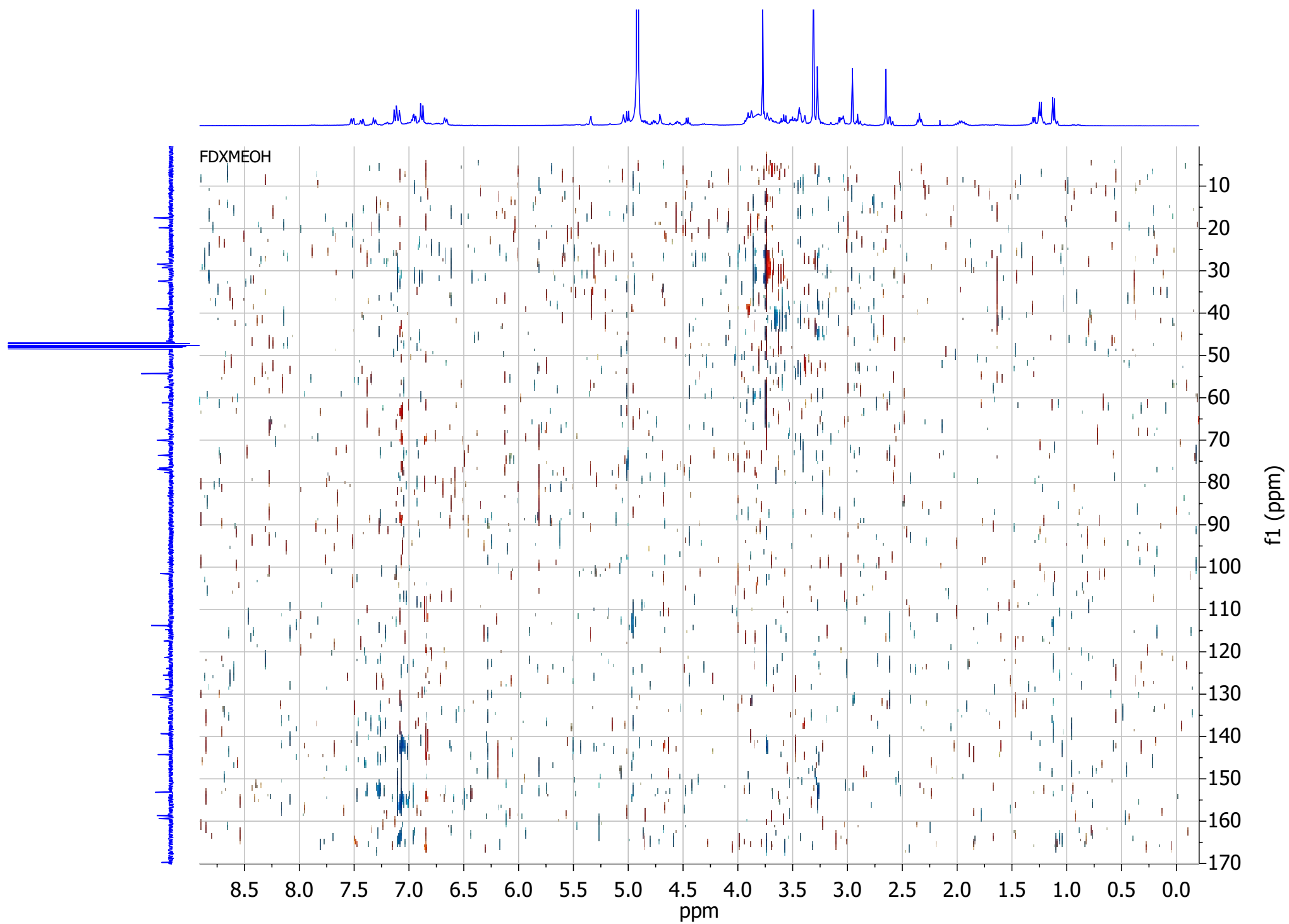


Figure S8. Spectrum HSQC Rubiayunnanesis H

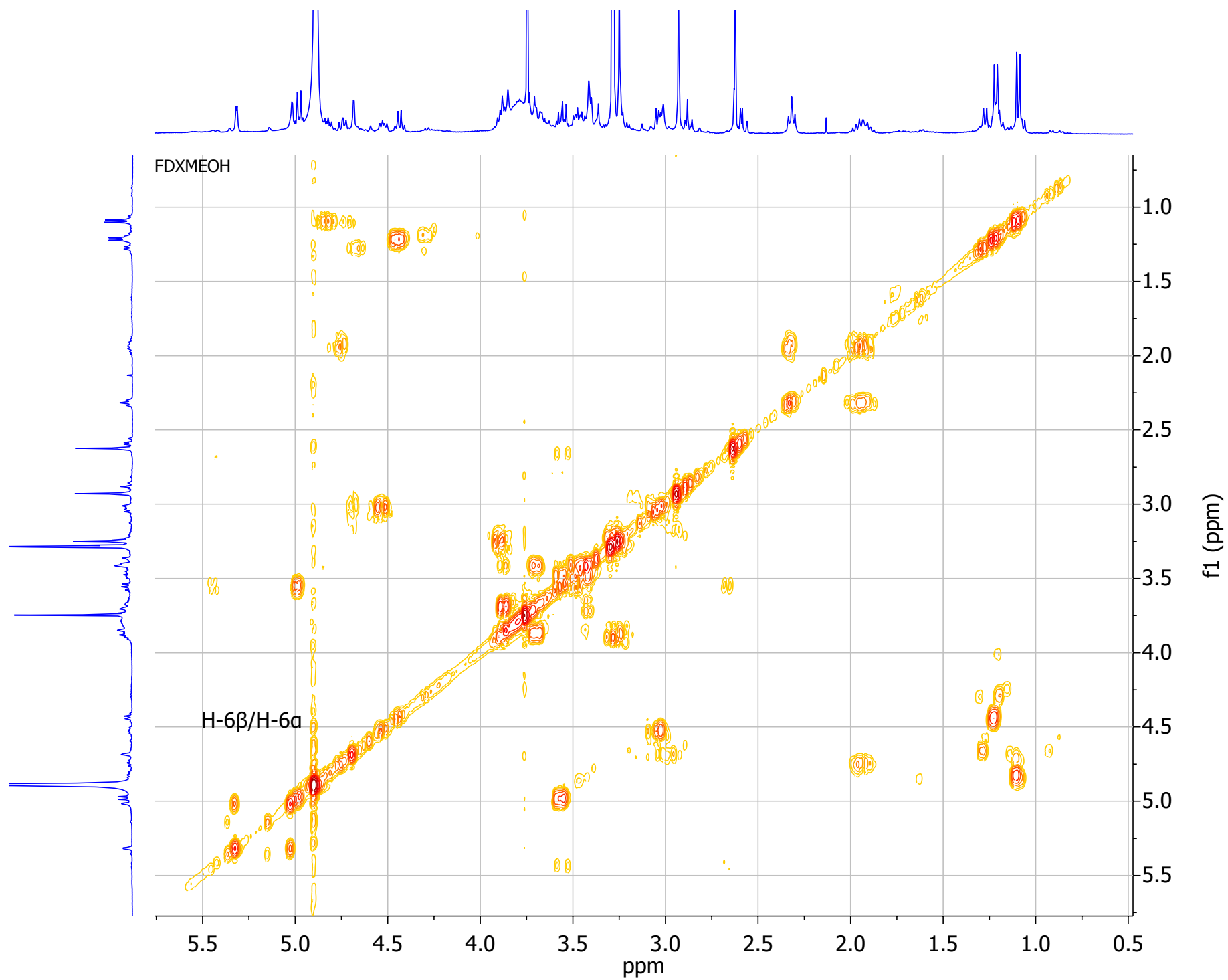


Figure S9. ^1H - ^1H COSY Rubiayunnanesis H