

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF020123\
 Data File : BF132270.D
 Acq On : 01 Feb 2023 20:35
 Operator : CG\JU
 Sample : 01356-01
 Misc :
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP-J

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132270.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.301	414	419	428	rVB	890954	1030004	37.54%	4.644%
2	5.690	480	485	488	rBV	2674994	2556301	93.16%	11.526%
3	6.678	648	653	656	rVB	2719841	2508623	91.42%	11.311%
4	7.066	716	719	723	rVB	1188344	964523	35.15%	4.349%
5	7.631	810	815	818	rBV	1860081	1646950	60.02%	7.426%
6	8.354	934	938	941	rBV	1653703	1281744	46.71%	5.779%
7	9.431	1117	1121	1124	rBV	3625689	2743965	100.00%	12.372%
8	10.119	1234	1238	1241	rVB	1768094	1383879	50.43%	6.240%
9	10.831	1356	1359	1362	rVB	77455	58243	2.12%	0.263%
10	10.907	1368	1372	1376	rBV	1871402	1713180	62.43%	7.724%
11	11.025	1387	1392	1396	rVB2	36631	44435	1.62%	0.200%
12	11.619	1489	1493	1496	rBV	1428154	1265419	46.12%	5.706%
13	12.125	1575	1579	1585	rBV	316265	309379	11.27%	1.395%
14	12.383	1620	1623	1625	rBV2	52002	47728	1.74%	0.215%
15	12.836	1697	1700	1705	rVB	59780	60392	2.20%	0.272%
16	12.913	1710	1713	1721	rBV	104808	123100	4.49%	0.555%
17	13.072	1737	1740	1747	rBV2	50758	64583	2.35%	0.291%
18	13.207	1759	1763	1767	rVB	2260869	1959858	71.42%	8.837%
19	14.060	1905	1908	1912	rBV	146873	146029	5.32%	0.658%
20	14.107	1913	1916	1929	rVB5	112980	271933	9.91%	1.226%
21	14.277	1941	1945	1948	rBV	1072404	936801	34.14%	4.224%
22	14.419	1967	1969	1972	rBV2	38592	40197	1.46%	0.181%
23	15.160	2092	2095	2100	rVB	129213	137587	5.01%	0.620%
24	15.866	2210	2215	2225	rVB	642014	883805	32.21%	3.985%

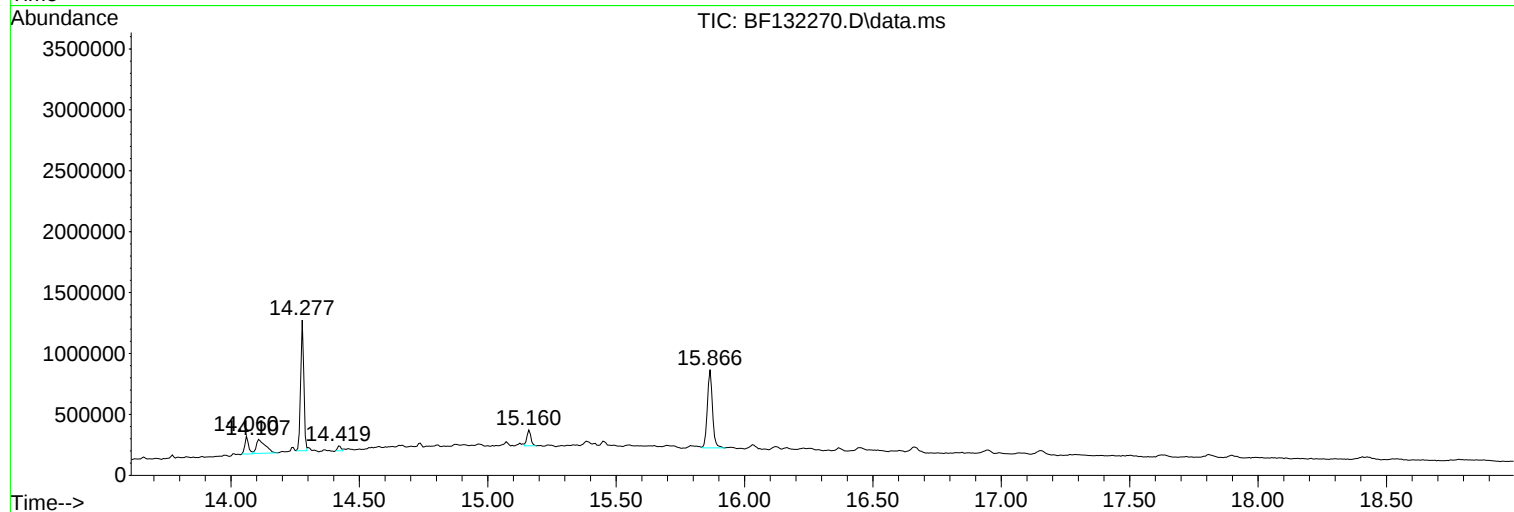
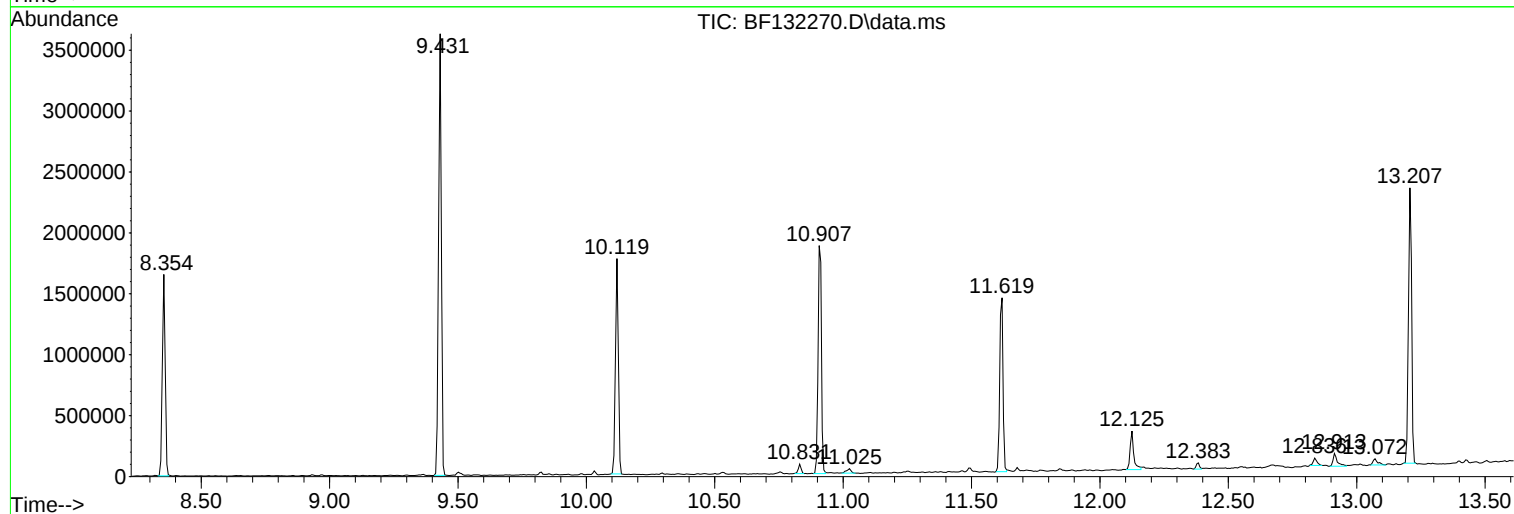
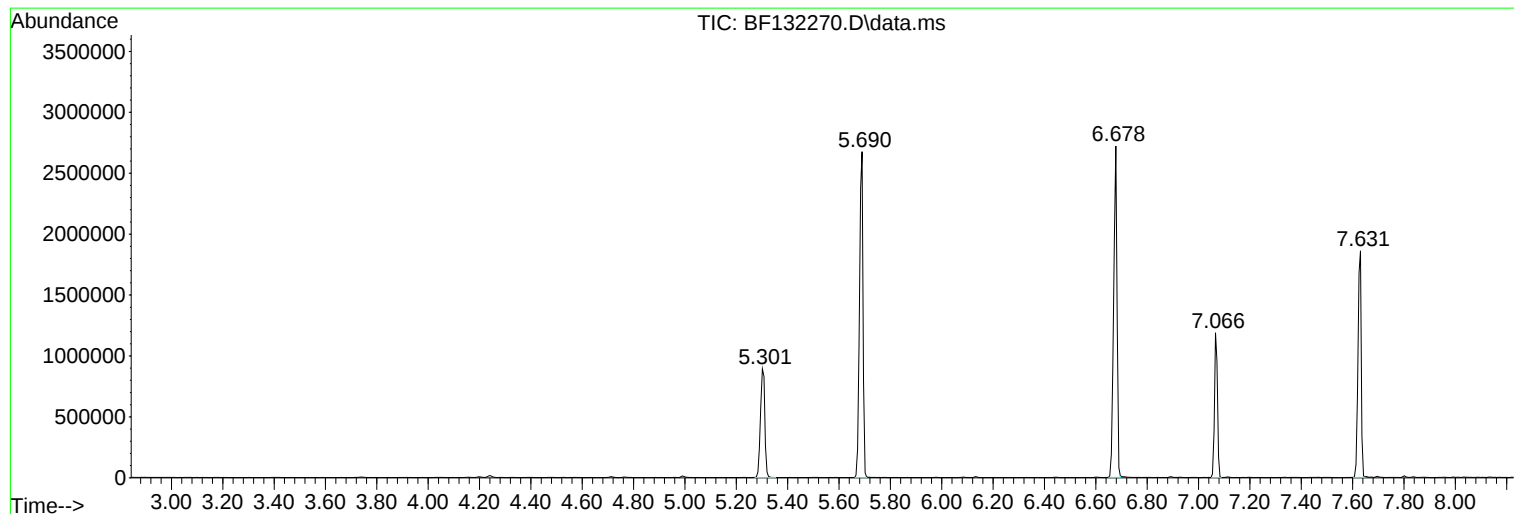
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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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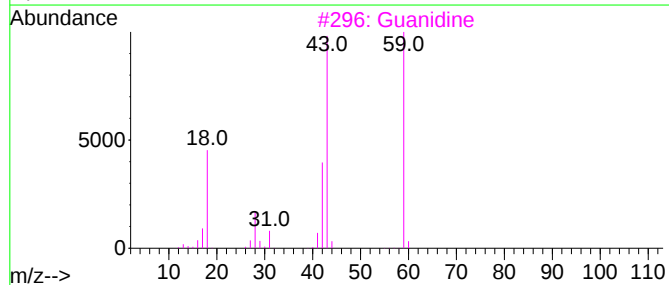
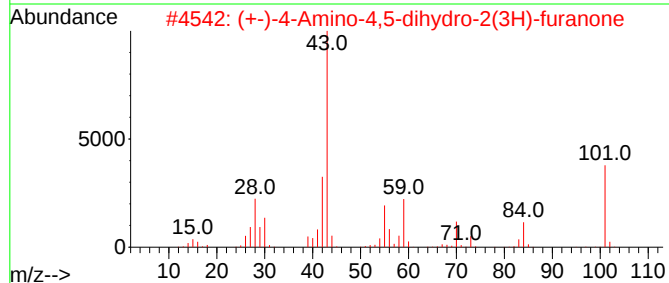
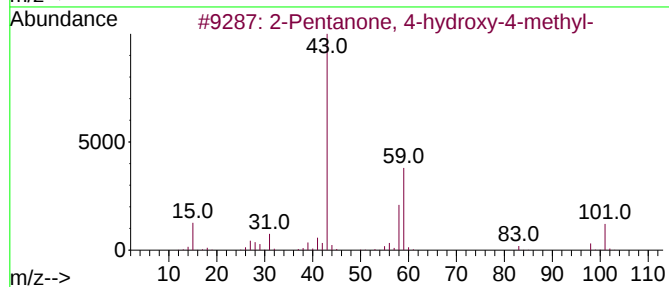
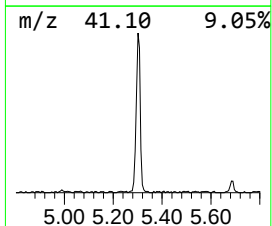
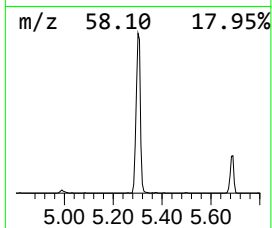
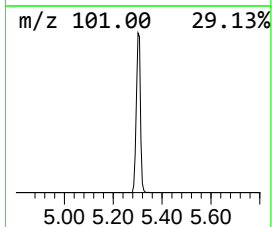
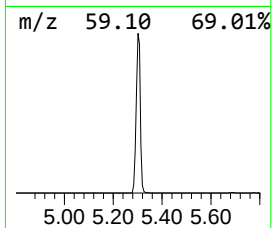
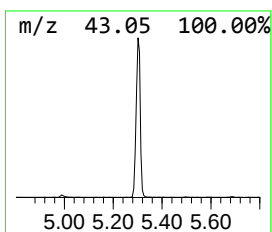
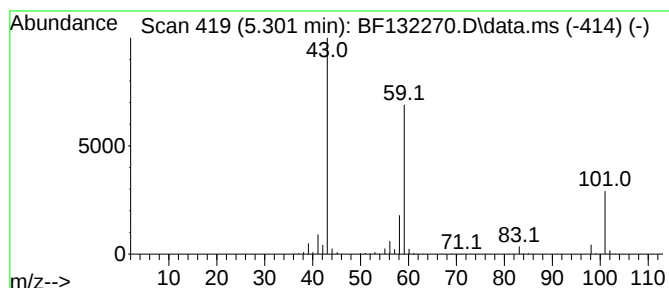
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF013123.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.301	21.36 ng	1030000	1,4-Dichlorobenzene-d4	7.066

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	47
3			Guanidine	59	CH5N3	000113-00-8	43
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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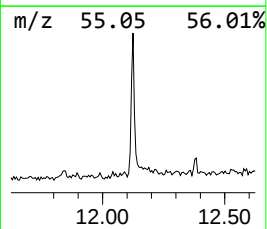
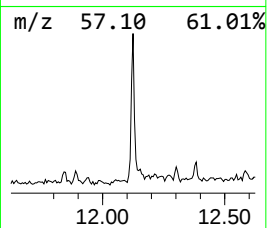
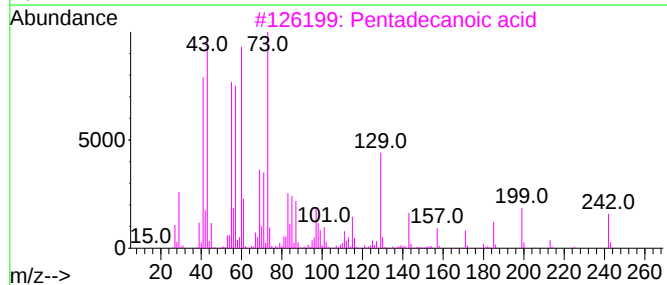
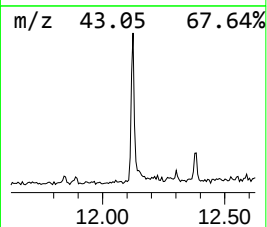
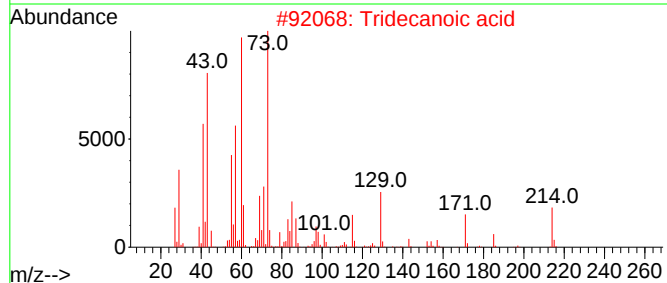
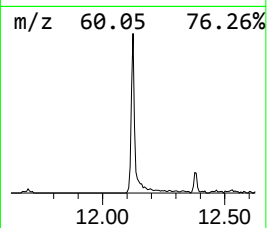
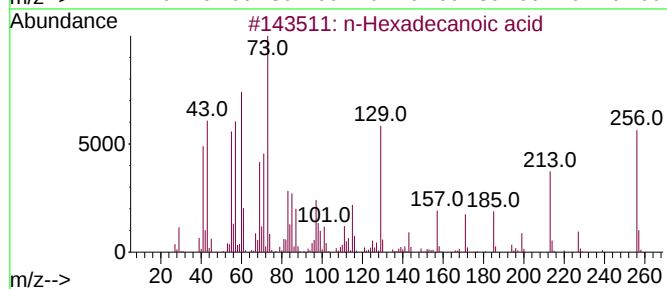
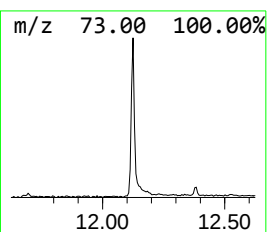
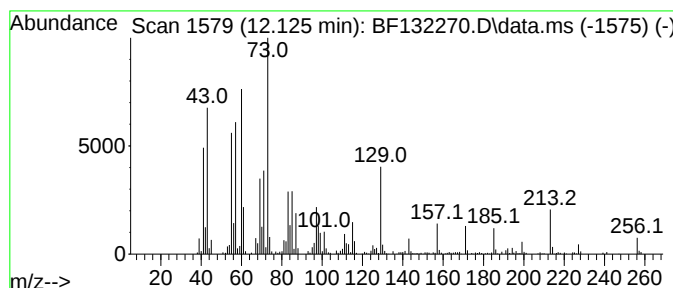
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.125	4.89 ng	309379	Phenanthrene-d10	11.619

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Tridecanoic acid	214	C13H26O2	000638-53-9	90
3			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	80
5			n-Decanoic acid	172	C10H20O2	000334-48-5	62



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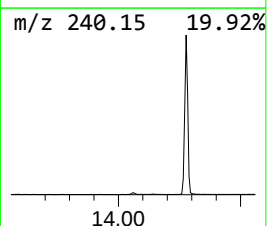
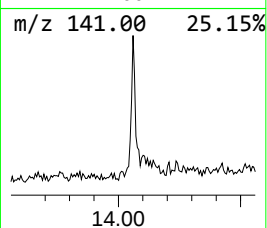
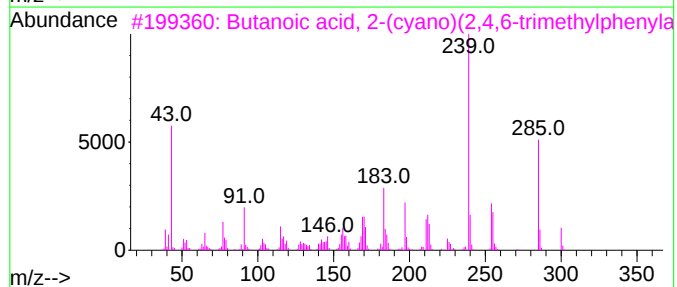
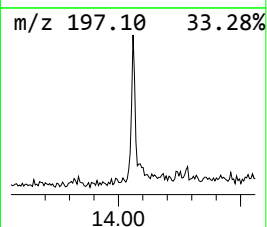
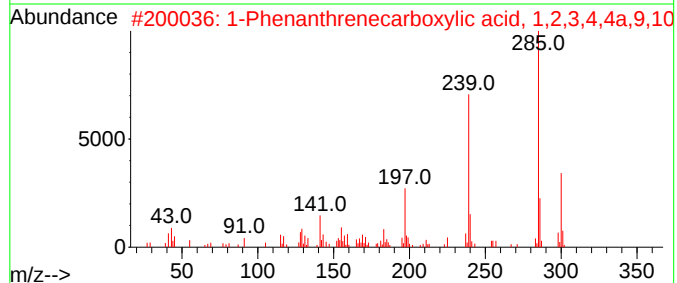
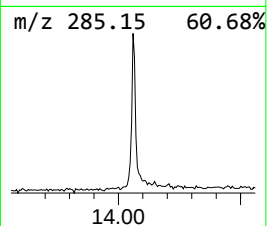
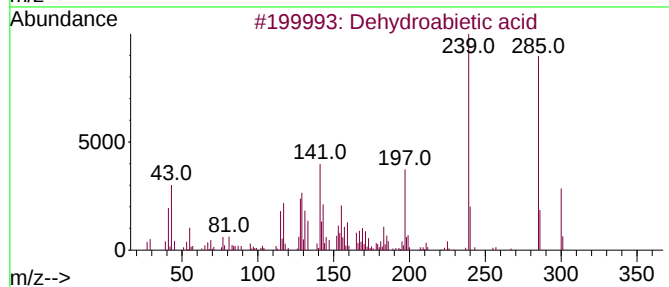
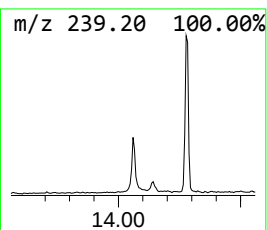
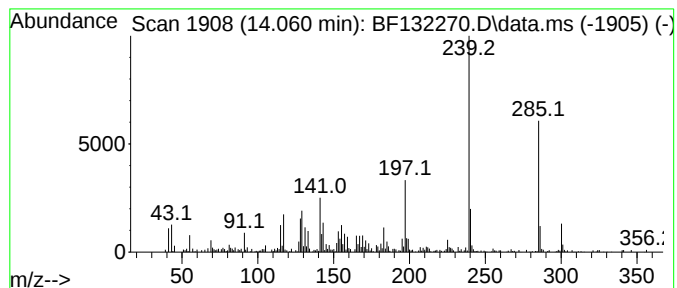
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Peak Number 3 Dehydroabiatic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.060	3.12 ng	146029	Chrysene-d12	14.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dehydroabiatic acid	300	C20H28O2	001740-19-8	96
2			1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	93
3			Butanoic acid, 2-(cyano)(2,4,6-t...	300	C17H20N2O3	1000267-71-7	81
4			Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3NO3	000391-02-6	52
5			Methyl dehydroabietate	314	C21H30O2	001235-74-1	47



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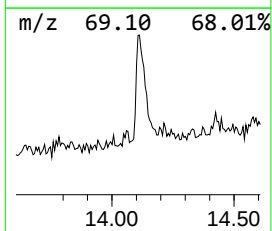
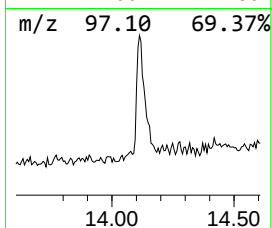
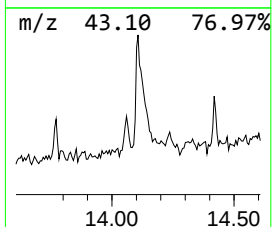
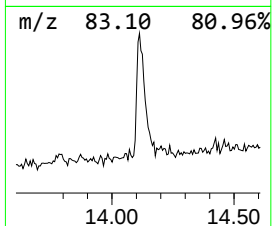
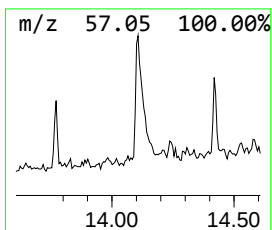
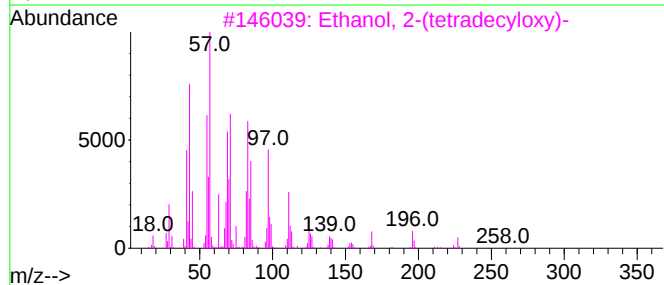
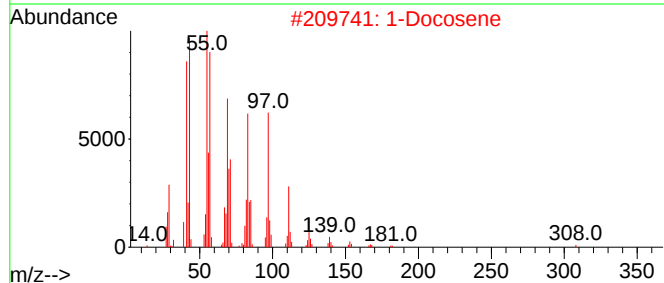
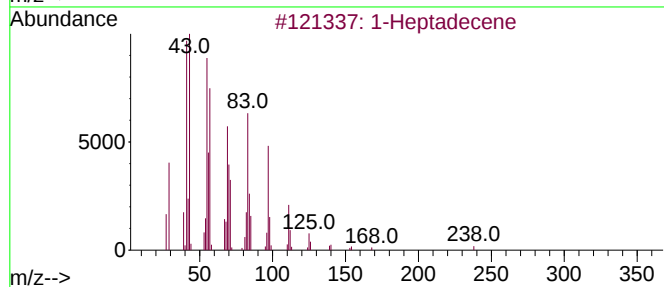
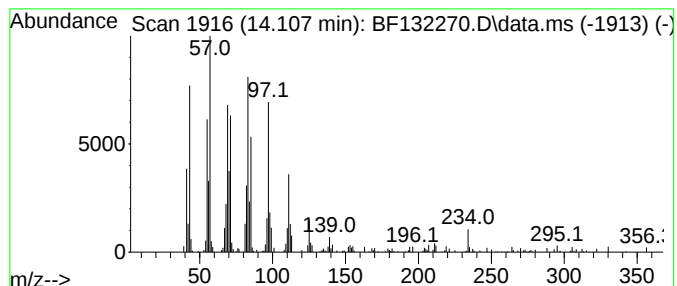
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Peak Number 4 1-Heptadecene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.107	5.81 ng	271933	Chrysene-d12	14.277

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heptadecene	238	C17H34	006765-39-5	95
2			1-Docosene	308	C22H44	001599-67-3	90
3			Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	90
4			1-Tricosene	322	C23H46	018835-32-0	89
5			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	87



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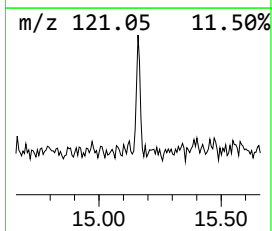
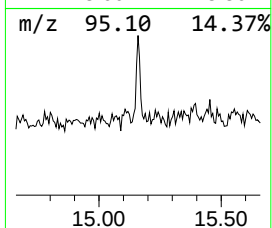
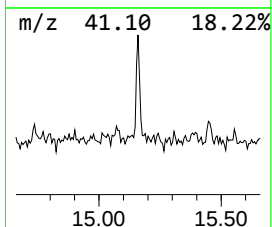
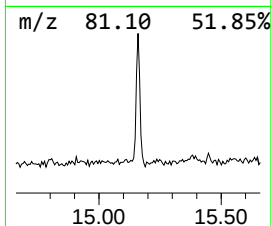
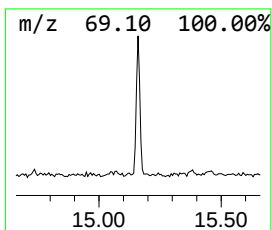
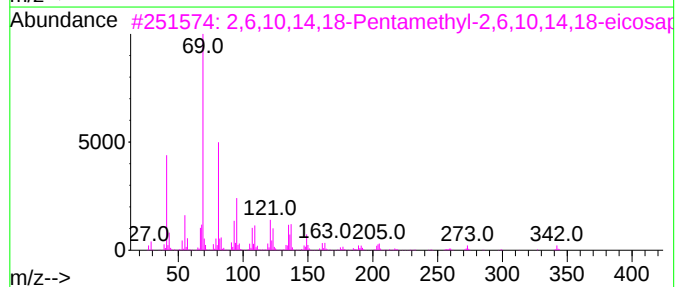
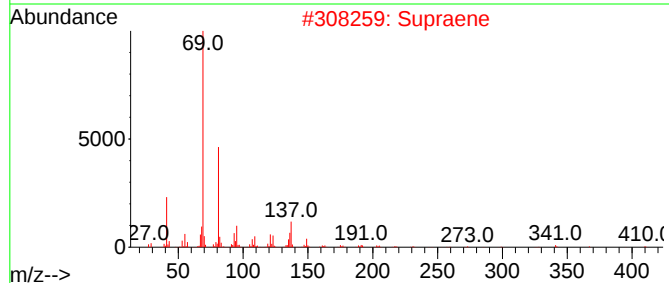
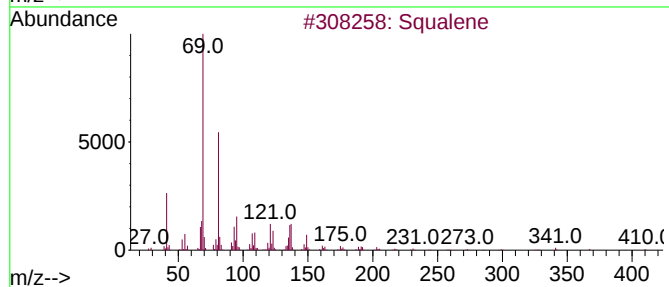
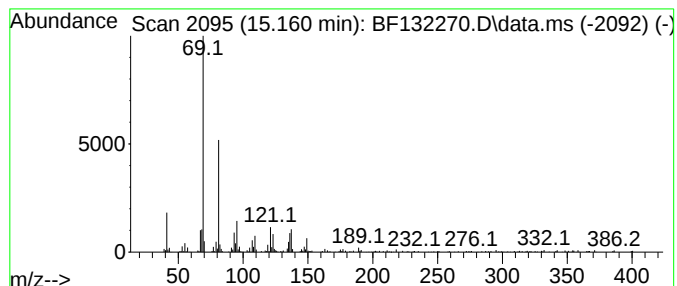
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.160	3.11 ng	137587	Perylene-d12	15.866

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	91
2			Supraene	410	C30H50	007683-64-9	90
3			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	87
4			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	87
5			trans-Farnesol	222	C15H26O	000106-28-5	78



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.301	21.4	ng	1030000	1	7.066	964523	20.0
n-Hexadecanoic ...	12.125	4.9	ng	309379	4	11.619	1265420	20.0
Dehydroabietic ...	14.060	3.1	ng	146029	5	14.277	936801	20.0
1-Heptadecene	14.107	5.8	ng	271933	5	14.277	936801	20.0
Squalene	15.160	3.1	ng	137587	6	15.866	883805	20.0