

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF090723\
 Data File : BF135135.D
 Acq On : 07 Sep 2023 15:35
 Operator : CG\JU
 Sample : 04283-05
 Misc :
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-5

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-BF083023.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF135135.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.169	10	14	22	rVB	25121	34296	1.34%	0.204%
2	5.016	493	498	505	rVB	32960	44417	1.74%	0.264%
3	5.410	560	565	568	rBV	2314818	2226985	87.32%	13.250%
4	6.410	730	735	738	rBV	2106454	2209157	86.62%	13.144%
5	6.604	765	768	774	rBV	28135	29824	1.17%	0.177%
6	6.769	793	796	800	rBV	667345	564854	22.15%	3.361%
7	7.334	887	892	895	rBV	1555868	1414046	55.44%	8.413%
8	8.051	1009	1014	1017	rBV	854852	763527	29.94%	4.543%
9	9.128	1192	1197	1201	rBV	2702047	2550435	100.00%	15.174%
10	9.245	1214	1217	1221	rVB	29742	27930	1.10%	0.166%
11	9.810	1308	1313	1316	rBV	940504	849136	33.29%	5.052%
12	10.598	1443	1447	1451	rBV	1653428	1599355	62.71%	9.516%
13	11.298	1563	1566	1570	rBV	963697	820032	32.15%	4.879%
14	11.839	1652	1658	1669	rBV	230608	259501	10.17%	1.544%
15	12.627	1788	1792	1806	rBV	78170	104105	4.08%	0.619%
16	12.898	1834	1838	1841	rBV	2490525	2171273	85.13%	12.919%
17	13.816	1988	1994	2003	rBV2	44386	84689	3.32%	0.504%
18	13.957	2014	2018	2026	rVB	544762	485229	19.03%	2.887%
19	14.816	2161	2164	2168	rBV	69425	68612	2.69%	0.408%
20	15.427	2262	2268	2274	rBV	391969	499985	19.60%	2.975%

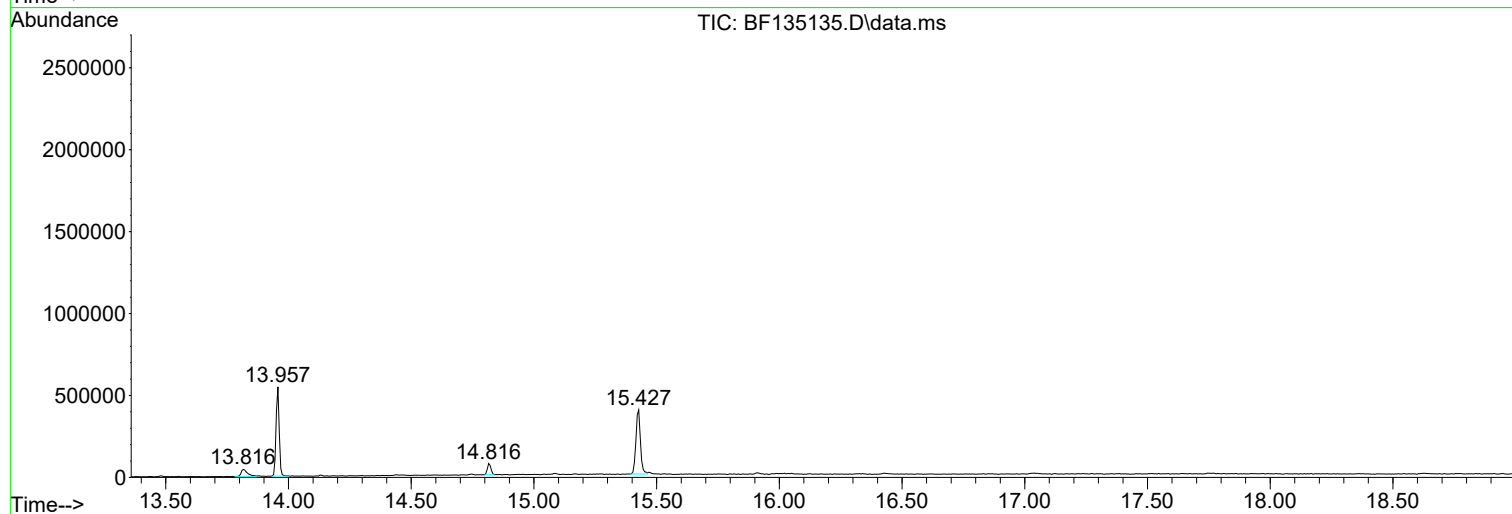
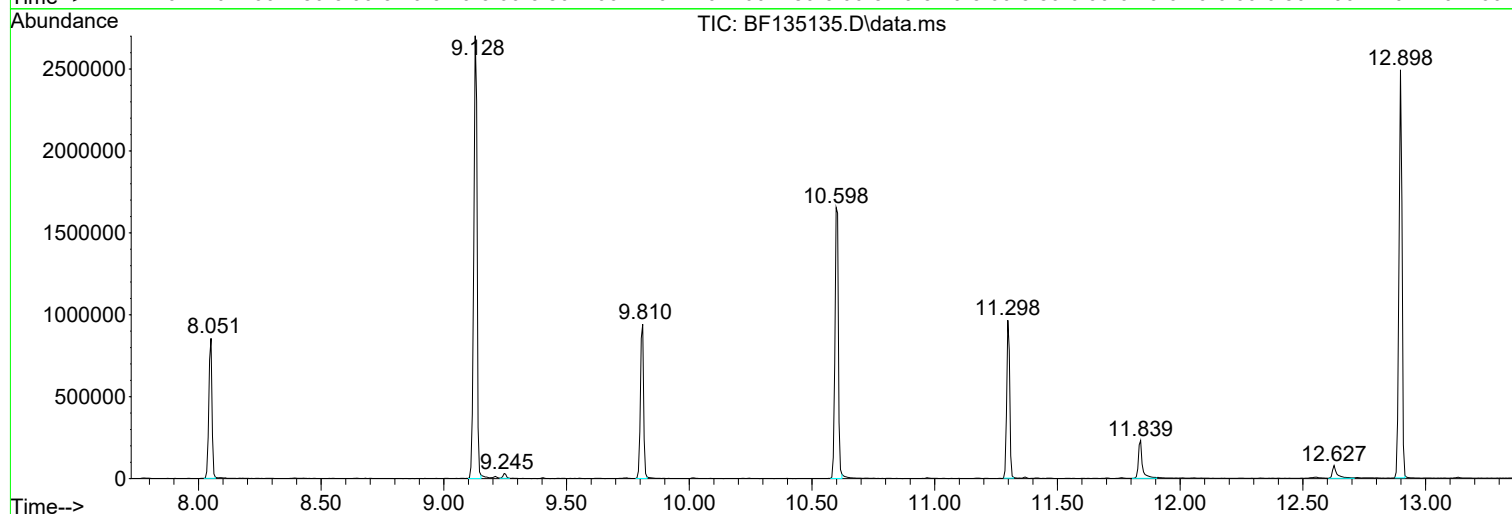
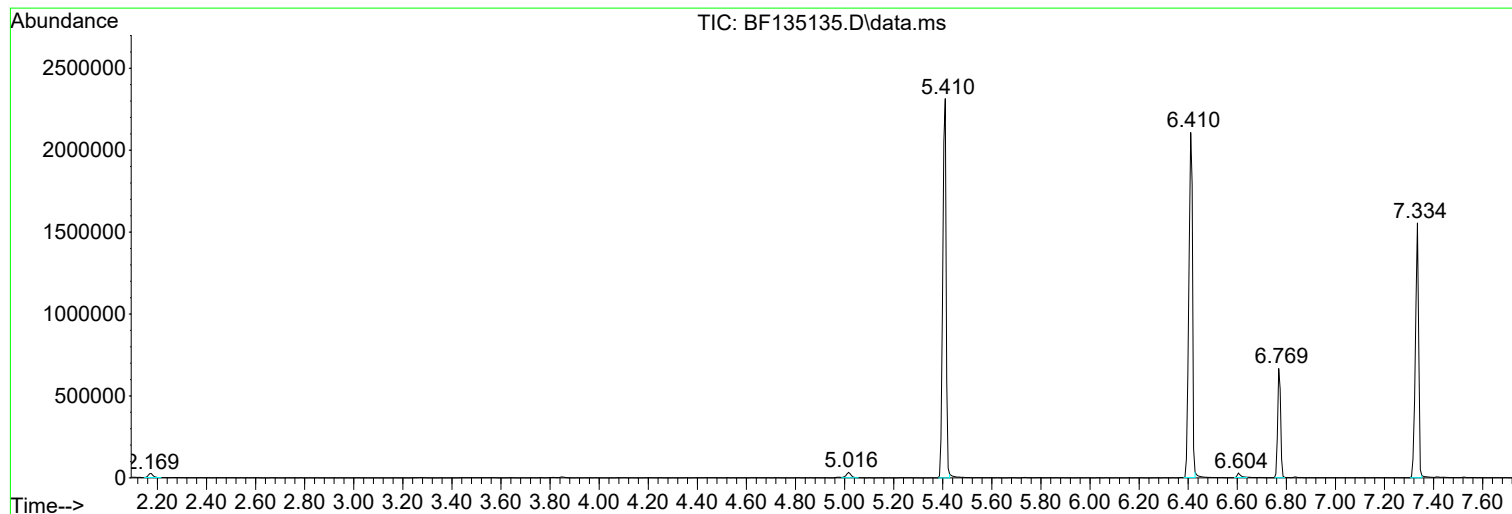
Sum of corrected areas: 16807388

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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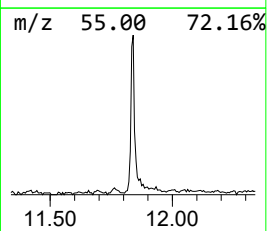
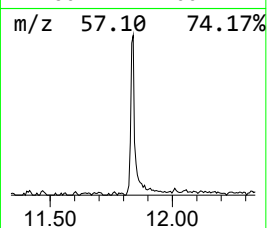
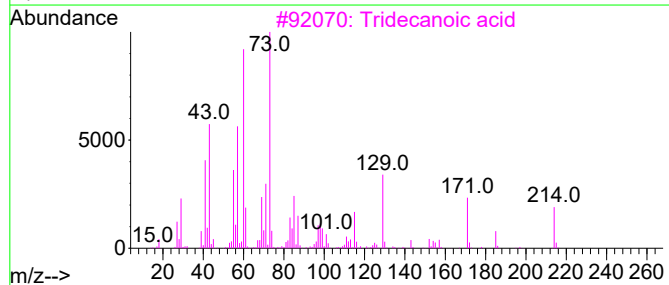
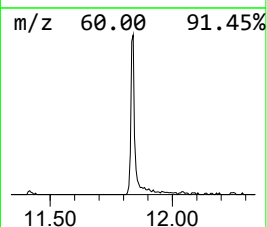
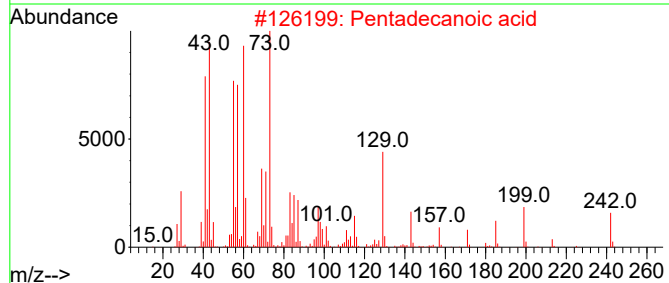
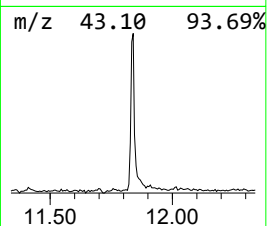
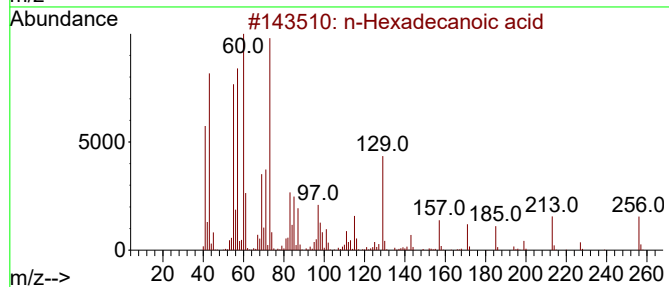
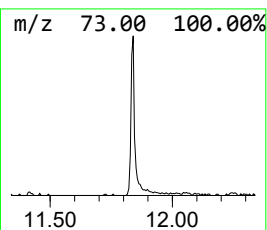
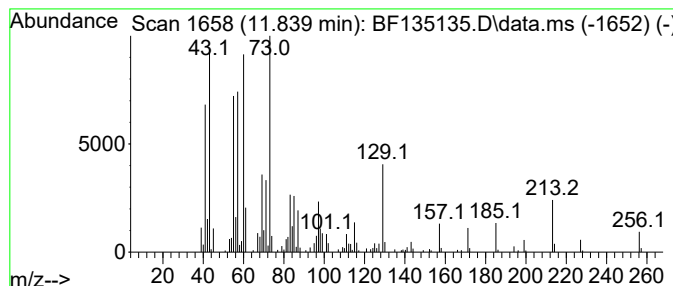
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 n-Hexadecanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.839	6.33 ng	259501	Phenanthrene-d10	11.298

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3			Tridecanoic acid	214	C13H26O2	000638-53-9	74
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	74
5			Dodecanoic acid	200	C12H24O2	000143-07-7	72



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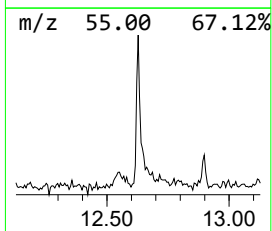
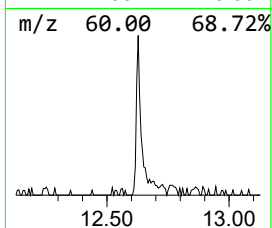
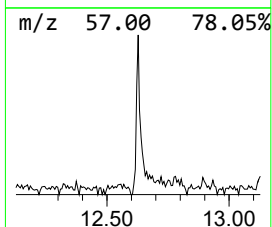
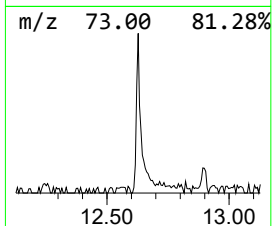
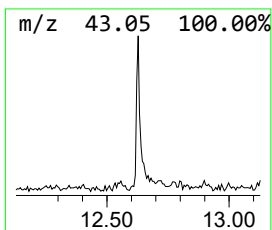
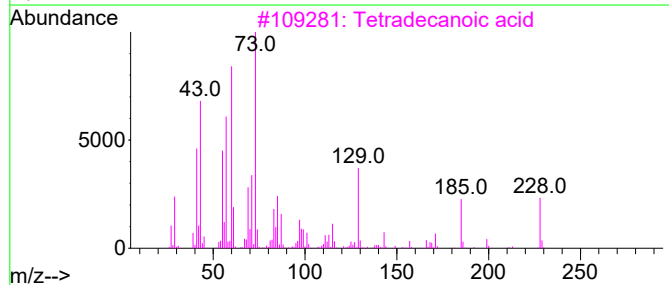
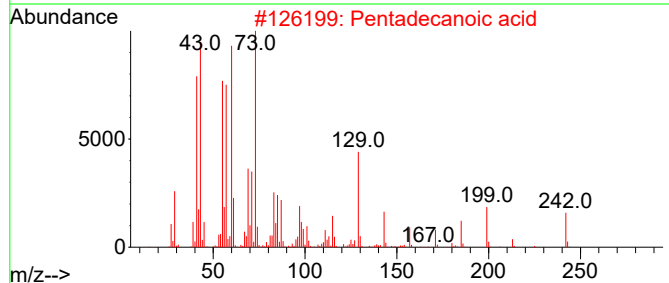
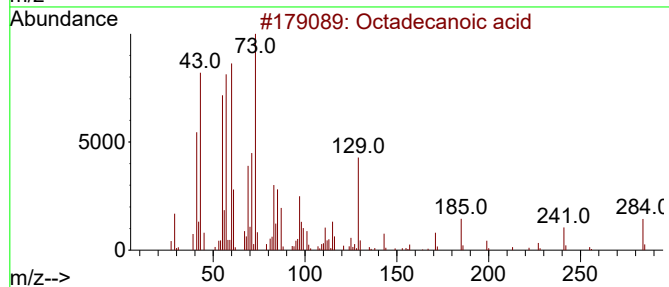
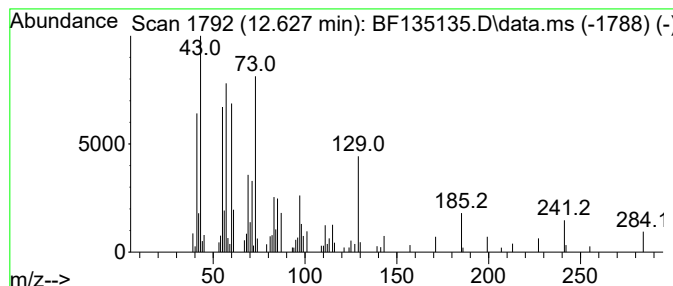
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF083023.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Octadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.628	4.29 ng	104105	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	98
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	58
4			Ethanone, 1-(4,5-dihydro-2-thiaz...	129	C5H7NOS	029926-41-8	30
5			Oxalic acid, cyclobutyl hexadecy...	368	C22H40O4	1000309-70-6	15



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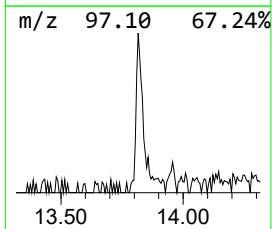
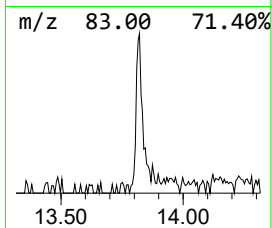
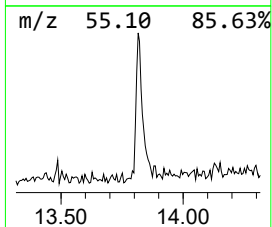
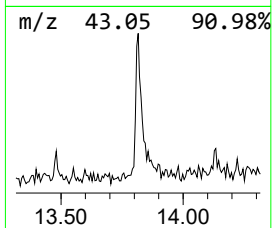
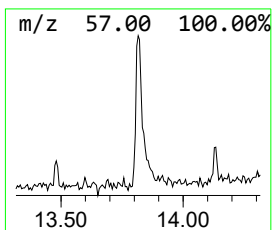
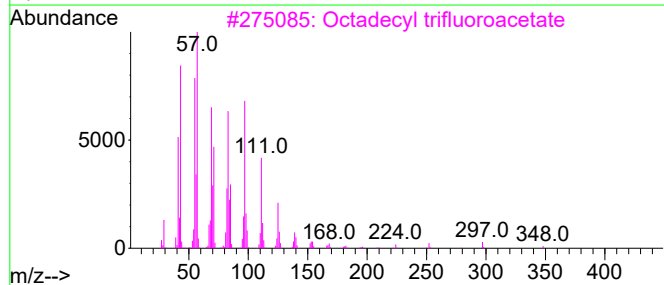
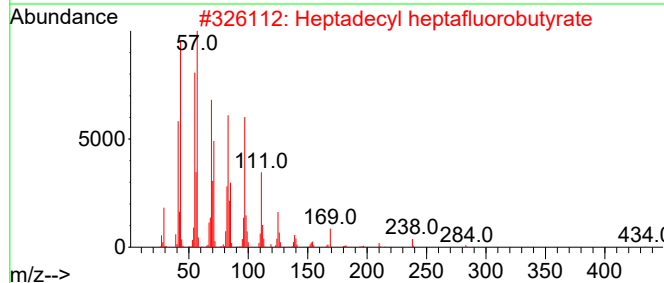
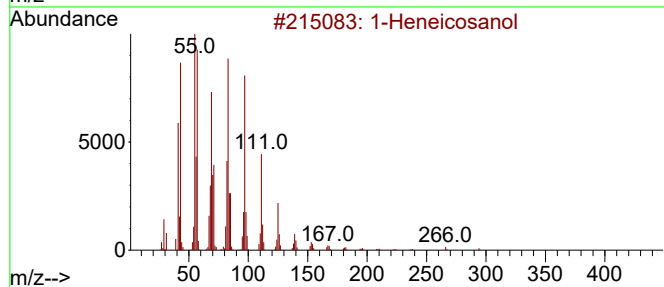
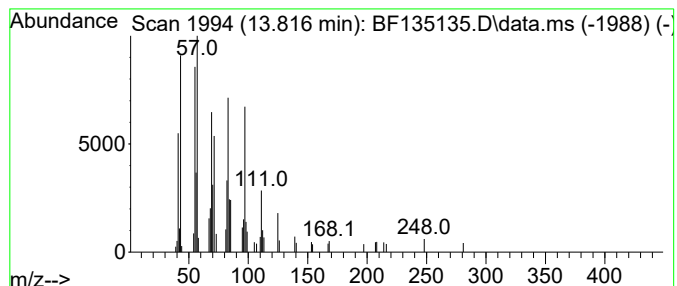
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Peak Number 3 1-Heneicosanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.816	3.49 ng	84689	Chrysene-d12	13.957

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Heneicosanol	312	C21H44O	015594-90-8	93
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	93
3			Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	90
4			Heptadecyl trifluoroacetate	352	C19H35F3O2	1010351-87-0	90
5			Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	90



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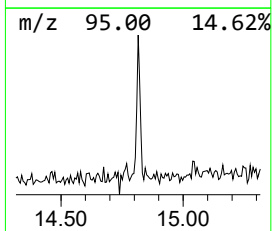
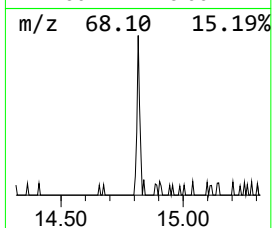
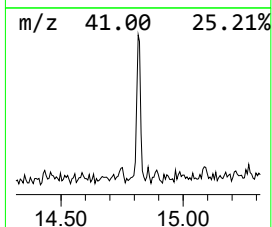
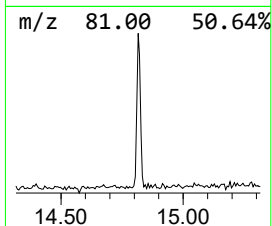
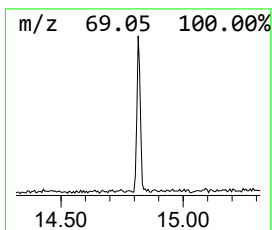
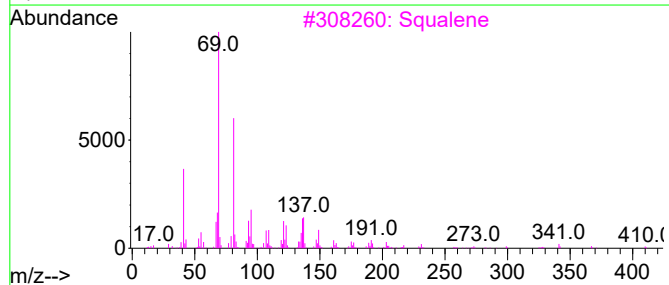
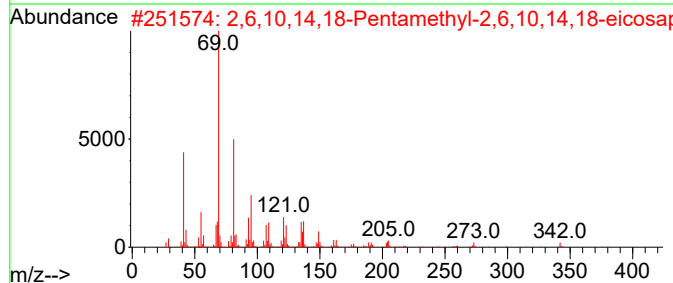
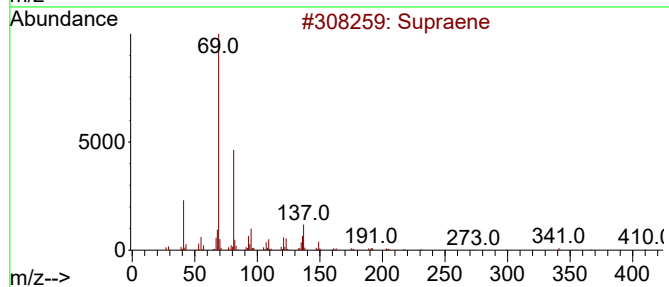
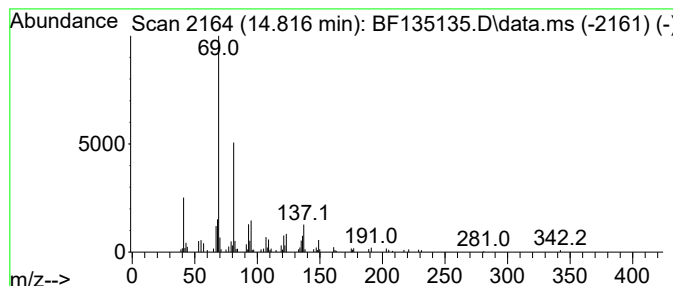
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.816	2.74 ng	68612	Perylene-d12	15.427

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			2,6,10,14,18-Pentamethyl-2,6,10,...	342	C25H42	075581-03-2	91
3			Squalene	410	C30H50	000111-02-4	91
4			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	83
5			Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexadecanoic ...	11.839	6.3	ng	259501	4	11.298	820032	20.0
Octadecanoic acid	12.628	4.3	ng	104105	5	13.957	485229	20.0
1-Heneicosanol	13.816	3.5	ng	84689	5	13.957	485229	20.0
Supraene	14.816	2.7	ng	68612	6	15.427	499985	20.0