

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF021623\
 Data File : BF132438.D
 Acq On : 16 Feb 2023 17:36
 Operator : CG\JU
 Sample : 01553-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TWP-06

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-BF021623.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132438.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.196	227	231	237	rVB	358795	427029	5.81%	1.140%
2	5.260	408	412	423	rVB	799561	783333	10.66%	2.091%
3	5.648	474	478	481	rBV	2374633	2024215	27.55%	5.404%
4	6.637	642	646	654	rBV	1487278	1265983	17.23%	3.380%
5	7.025	709	712	716	rBV	1295504	1133632	15.43%	3.026%
6	7.595	803	809	812	rBV	4233660	4355396	59.28%	11.628%
7	8.313	927	931	935	rBV	1850337	1477018	20.10%	3.943%
8	9.395	1110	1115	1118	rBV	7329751	6920269	94.19%	18.475%
9	10.078	1227	1231	1234	rBV	2107837	1693287	23.05%	4.521%
10	10.483	1297	1300	1304	rVB	515143	403280	5.49%	1.077%
11	10.789	1347	1352	1357	rVB	151412	133711	1.82%	0.357%
12	10.872	1361	1366	1369	rBV	3526182	3214258	43.75%	8.581%
13	11.572	1481	1485	1489	rBV	2151156	1830428	24.91%	4.887%
14	12.083	1568	1572	1589	rBV	471246	555691	7.56%	1.484%
15	12.871	1703	1706	1716	rBV	140668	201762	2.75%	0.539%
16	13.171	1751	1757	1760	rBV	7287949	7346968	100.00%	19.614%
17	14.130	1910	1920	1927	rBV9	32839	136217	1.85%	0.364%
18	14.230	1933	1937	1941	rBV	1787588	1582130	21.53%	4.224%
19	14.318	1949	1952	1957	rVB	121223	111582	1.52%	0.298%
20	15.101	2080	2085	2093	rVB	269154	310614	4.23%	0.829%
21	15.795	2197	2203	2219	rBV	1182509	1550413	21.10%	4.139%

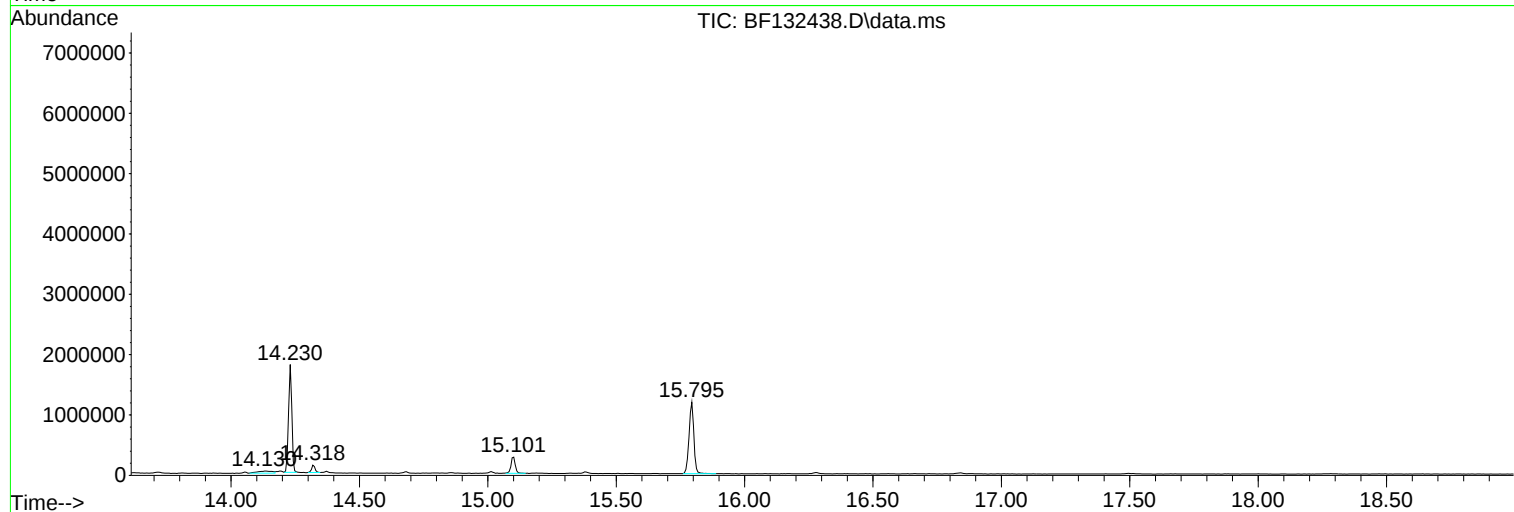
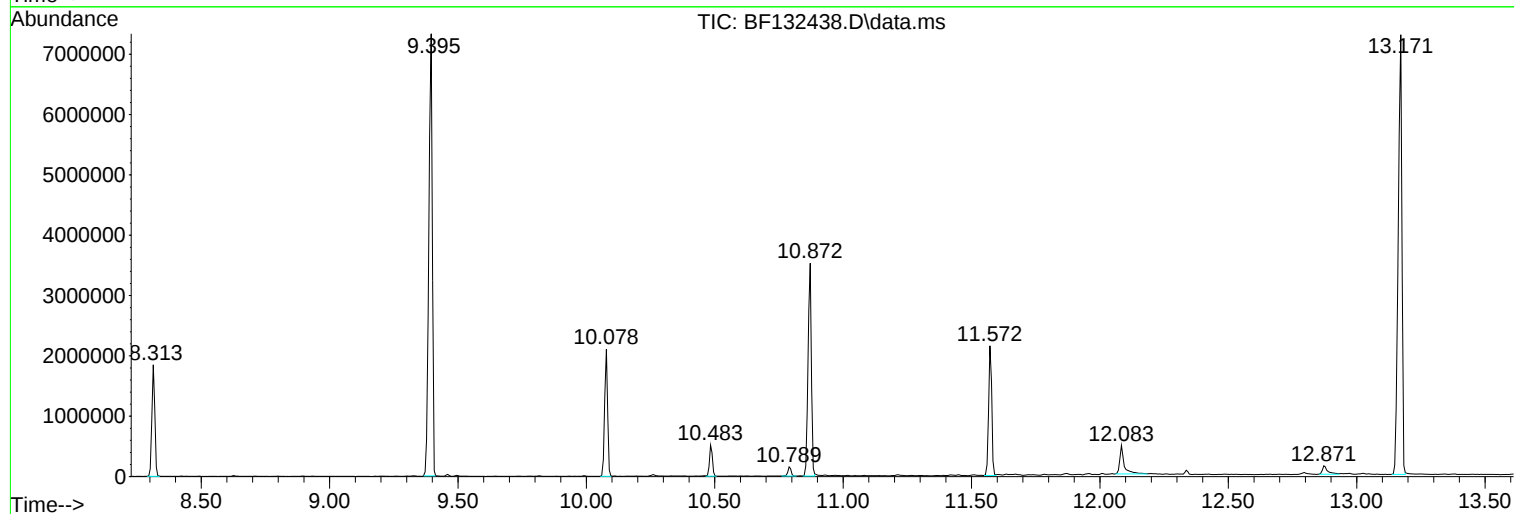
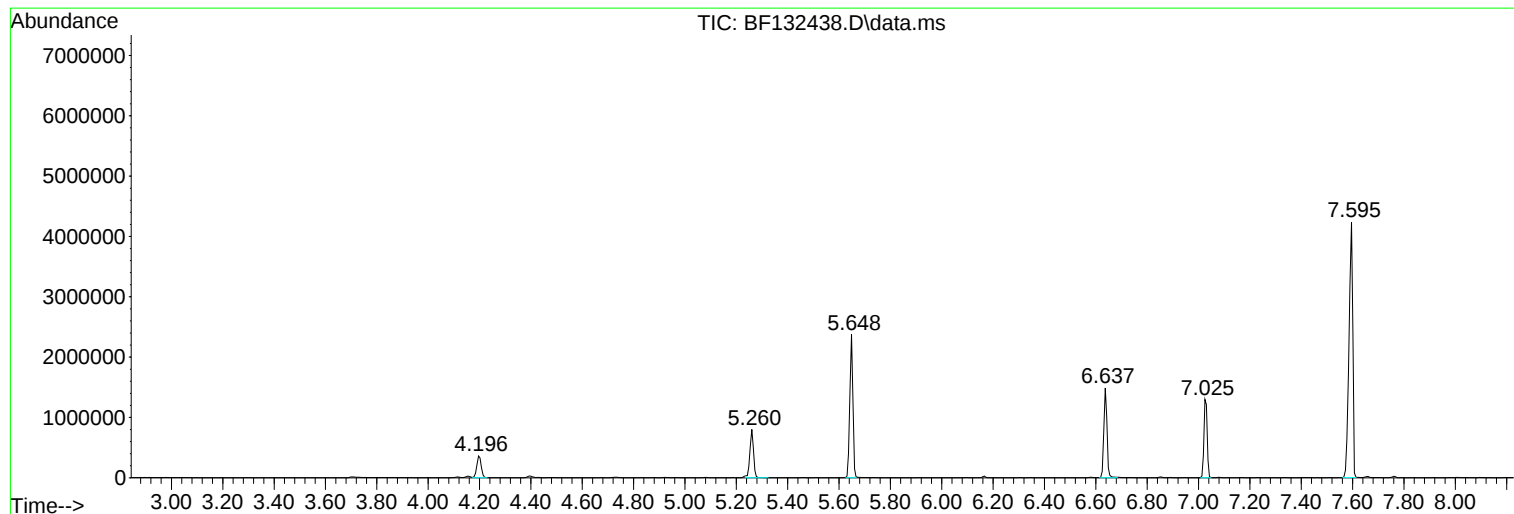
Sum of corrected areas: 37457216

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Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.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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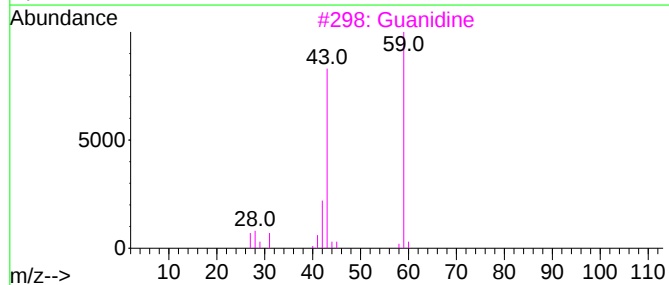
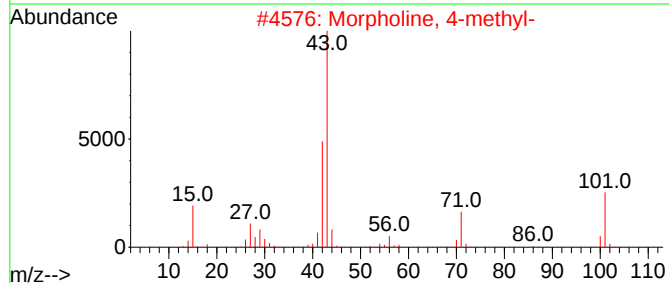
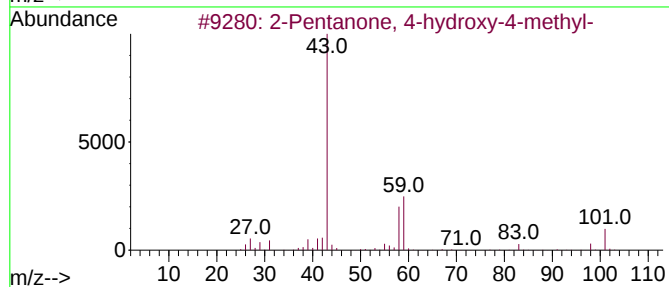
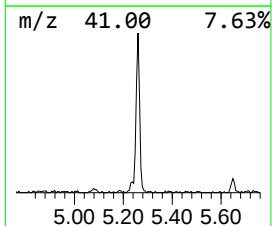
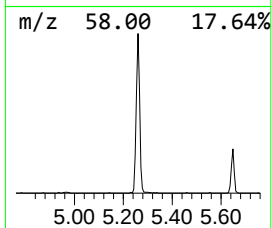
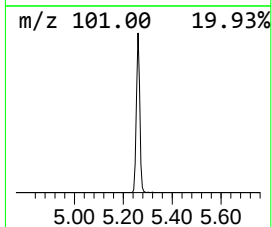
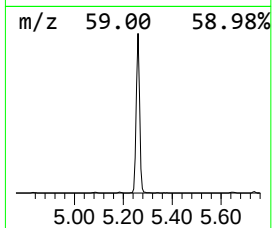
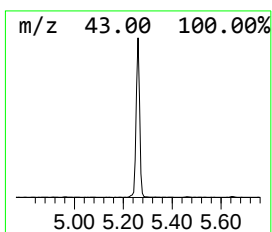
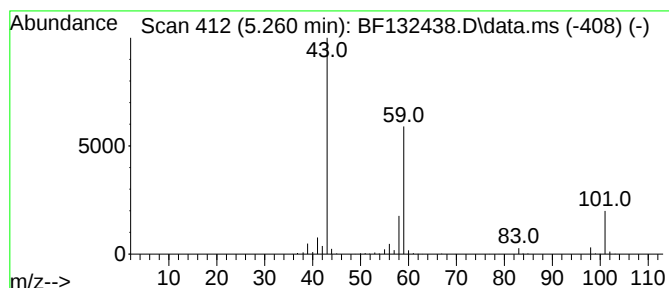
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF021623.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.260	13.82 ng	783333	1,4-Dichlorobenzene-d4	7.025

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
3			Guanidine	59	CH5N3	000113-00-8	9
4			Acetone	58	C3H6O	000067-64-1	9
5			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	9



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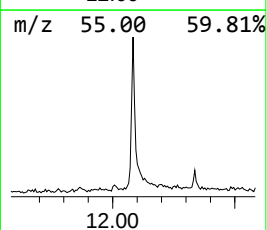
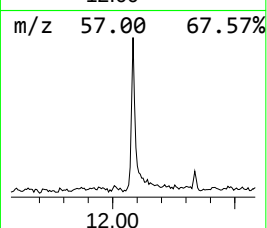
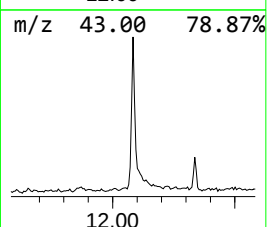
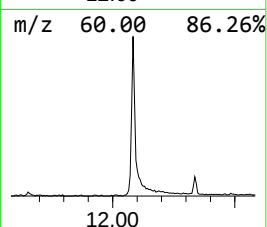
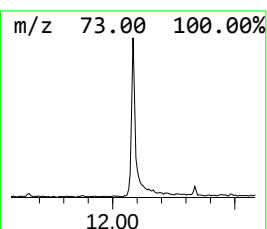
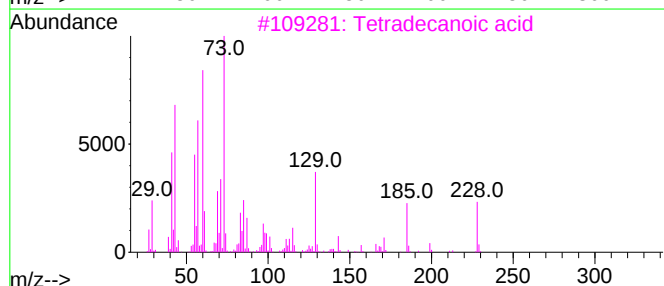
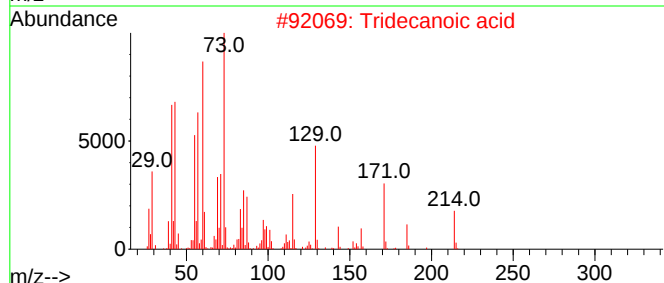
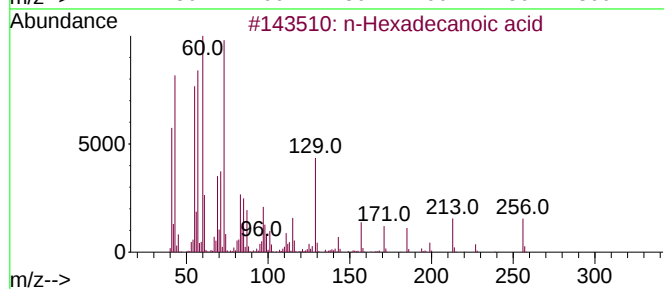
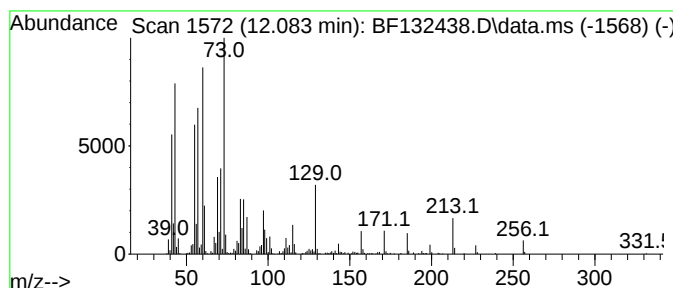
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.083	6.07 ng	555691	Phenanthrene-d10	11.572

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	95
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	94
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	86
5			Octadecanoic acid	284	C18H36O2	000057-11-4	70



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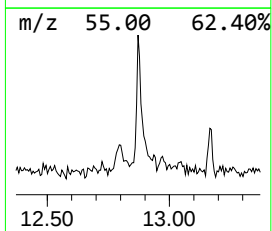
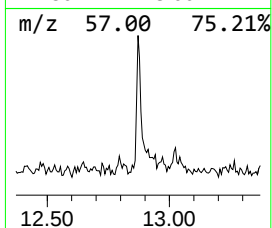
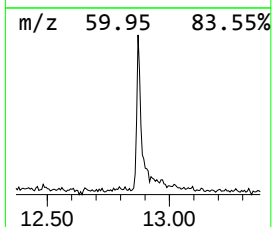
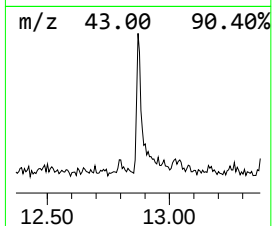
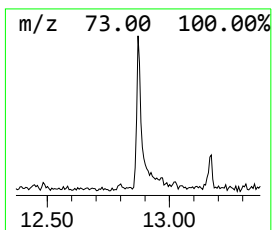
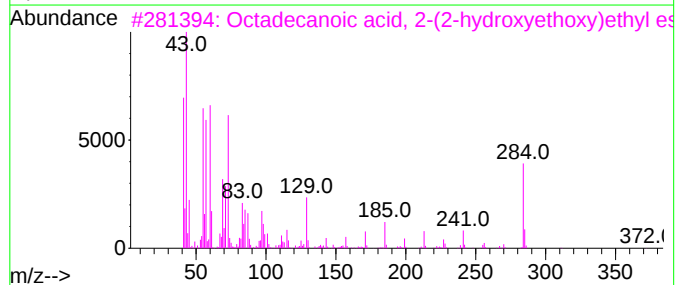
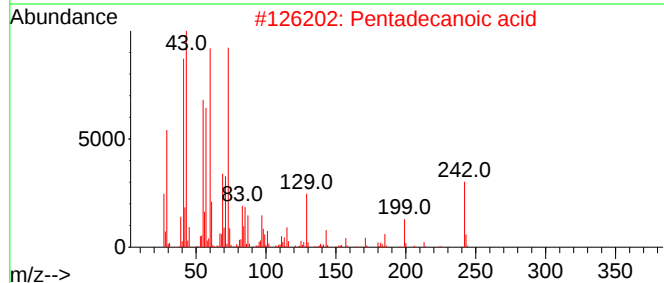
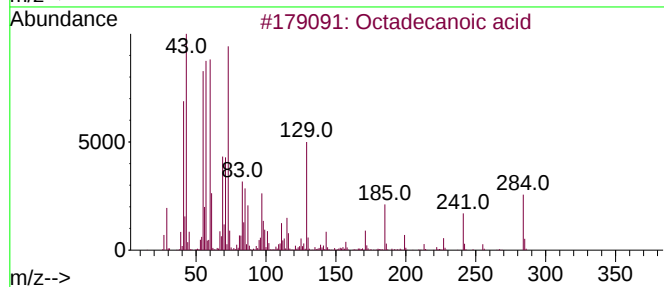
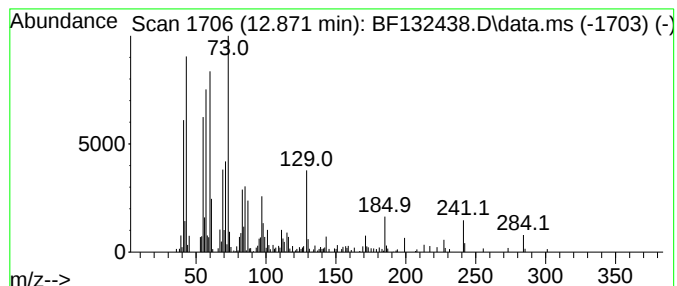
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Peak Number 4 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.871	2.20 ng	201762	Phenanthrene-d10	11.572

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octadecanoic acid	284	C18H36O2	000057-11-4	99
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	94
3			Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	90
4			Tetradecanoic acid	228	C14H28O2	000544-63-8	76
5			n-Decanoic acid	172	C10H20O2	000334-48-5	53



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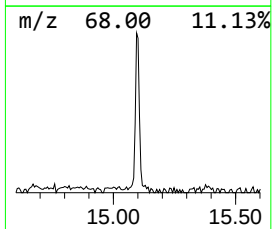
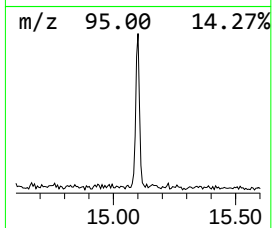
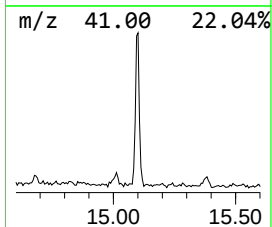
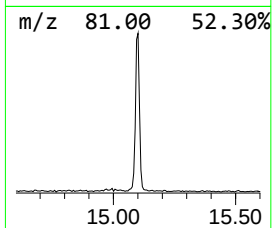
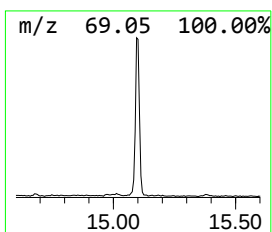
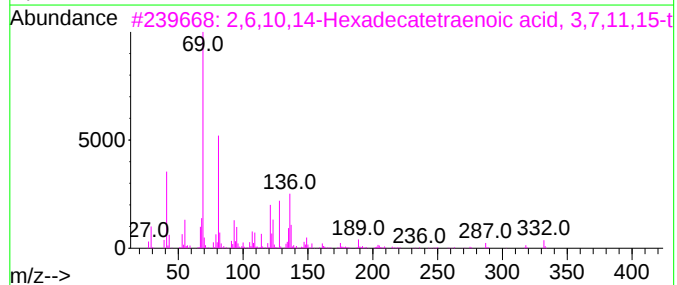
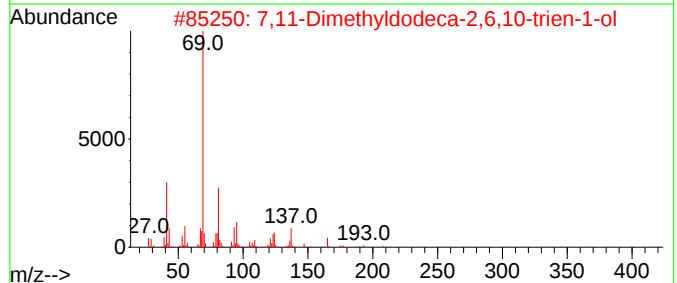
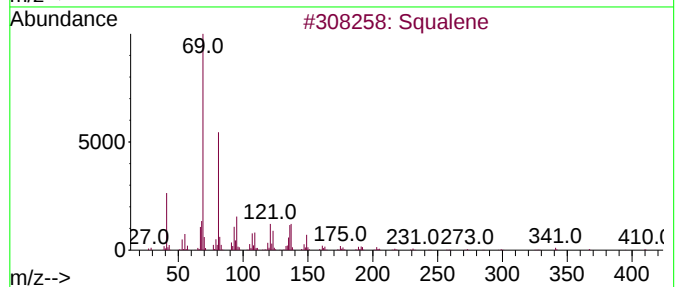
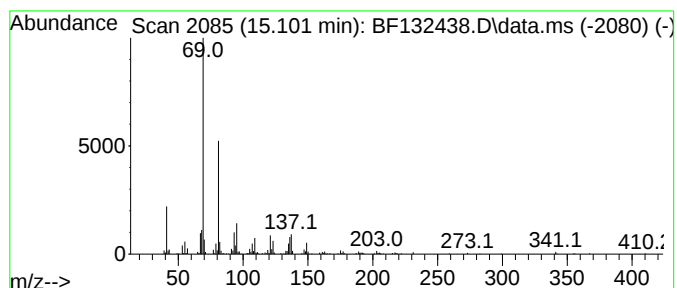
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Peak Number 5 Squalene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.101	4.01 ng	310614	Perylene-d12	15.795

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Squalene	410	C30H50	000111-02-4	97
2			7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
3			2,6,10,14-Hexadecatetraenoic aci...	332	C22H36O2	024035-35-6	72
4			Methanone, dicyclopentyl-	110	C7H10O	001121-37-5	50
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.260	13.8	ng	783333	1	7.025	1133630	20.0
n-Hexadecanoic ...	12.083	6.1	ng	555691	4	11.572	1830430	20.0
Octadecanoic acid	12.871	2.2	ng	201762	4	11.572	1830430	20.0
Squalene	15.101	4.0	ng	310614	6	15.795	1550410	20.0