

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF030223\
 Data File : BF132617.D
 Acq On : 02 Mar 2023 20:18
 Operator : CG\JU
 Sample : 01749-13
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CF-15

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-BF022223.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF132617.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.234	445	450	457	rVB	1399783	1728085	44.20%	6.152%
2	5.628	512	517	520	rBV	3779876	3578826	91.54%	12.741%
3	6.622	682	686	690	rBV	3391059	3617424	92.53%	12.878%
4	6.998	747	750	754	rBV	1494579	1190587	30.45%	4.239%
5	7.563	842	846	849	rBV	2773161	2421276	61.93%	8.620%
6	8.287	965	969	972	rBV	1863094	1481374	37.89%	5.274%
7	9.363	1148	1152	1155	rBV	4675425	3909505	100.00%	13.918%
8	10.045	1265	1268	1272	rVB	1755350	1443208	36.92%	5.138%
9	10.757	1386	1389	1393	rVB	108210	87084	2.23%	0.310%
10	10.839	1399	1403	1406	rBV	2293039	1915600	49.00%	6.820%
11	11.545	1519	1523	1526	rBV	1353944	1201220	30.73%	4.276%
12	12.057	1606	1610	1625	rBV	172143	270707	6.92%	0.964%
13	12.763	1727	1730	1734	rBV	82628	82578	2.11%	0.294%
14	12.998	1767	1770	1773	rBV	62601	49717	1.27%	0.177%
15	13.133	1789	1793	1797	rBV	3343319	2942363	75.26%	10.475%
16	14.033	1942	1946	1947	rBV3	96089	114076	2.92%	0.406%
17	14.204	1971	1975	1978	rBV	1262430	1100847	28.16%	3.919%
18	15.063	2118	2121	2126	rVB	120388	128986	3.30%	0.459%
19	15.757	2234	2239	2244	rBV2	640393	825756	21.12%	2.940%

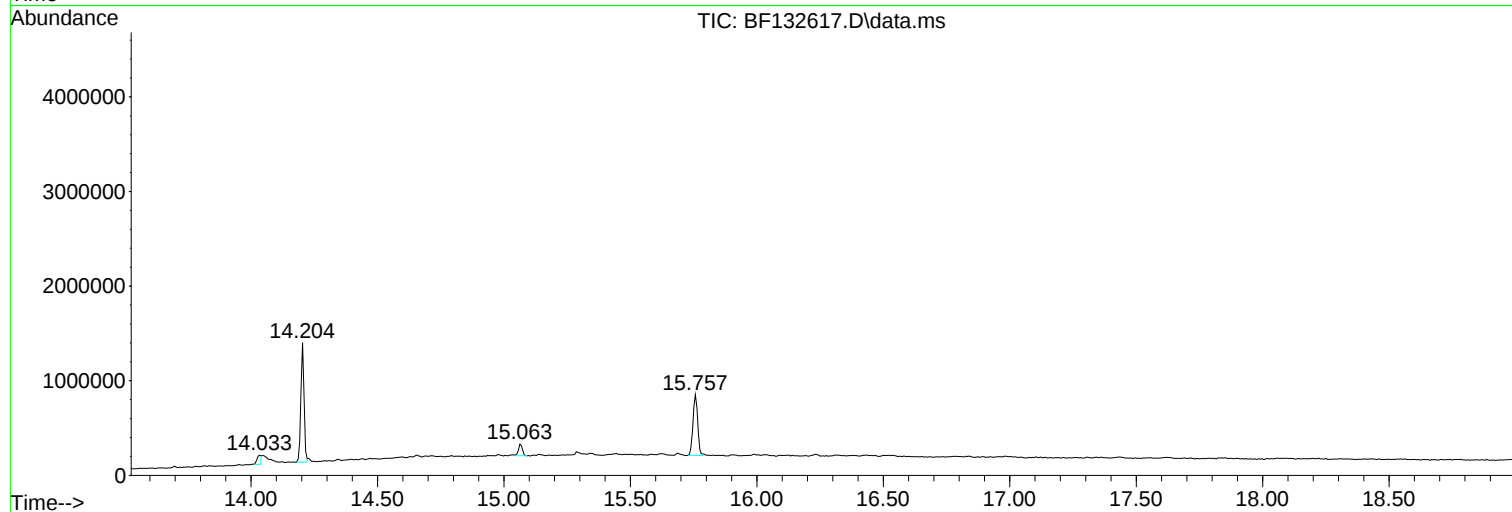
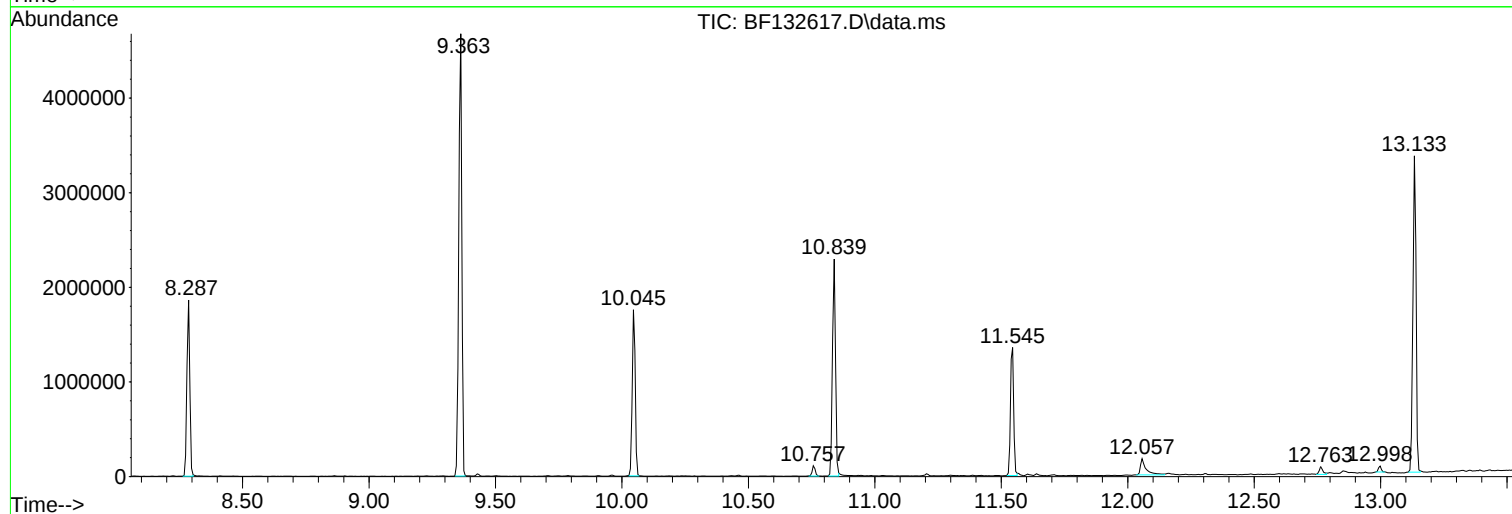
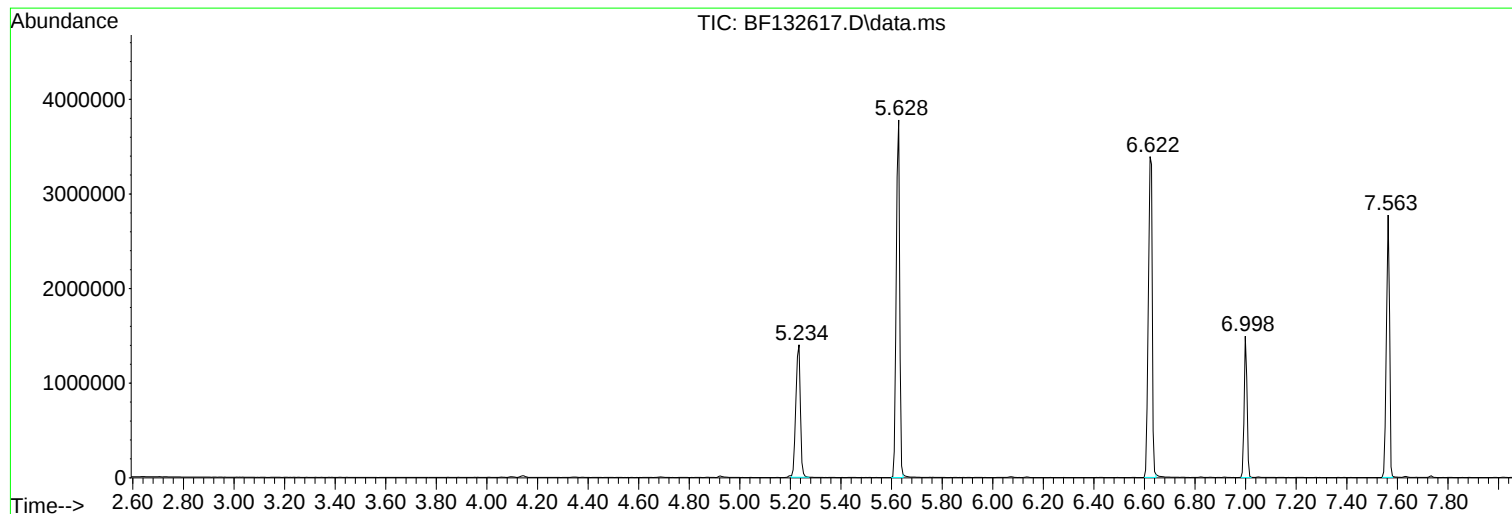
Sum of corrected areas: 28089219

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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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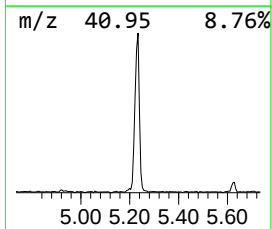
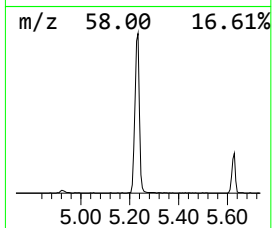
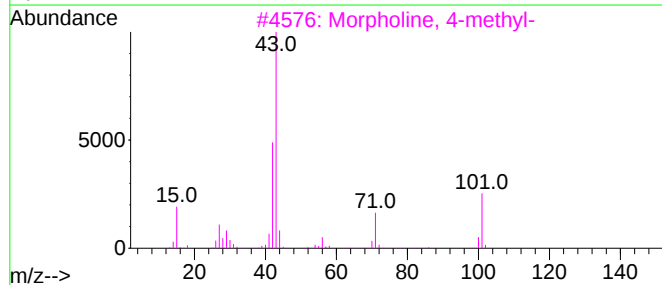
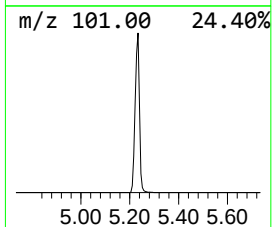
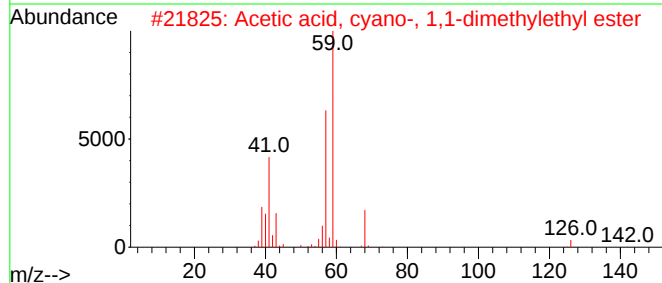
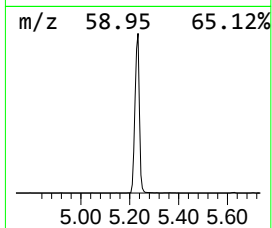
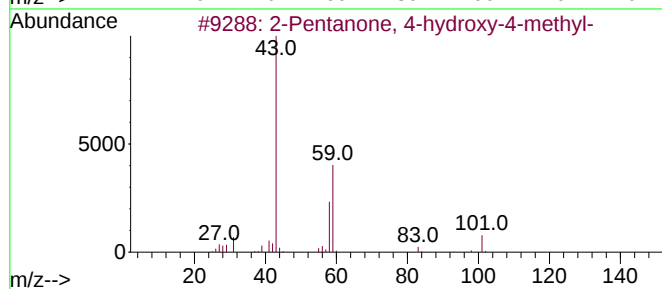
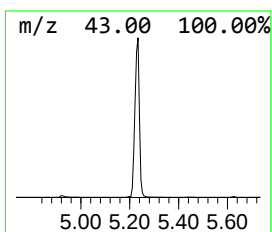
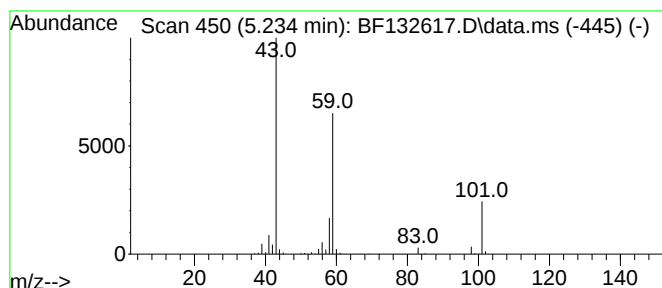
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF022223.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.234	29.03 ng	1728090	1,4-Dichlorobenzene-d4	6.998

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



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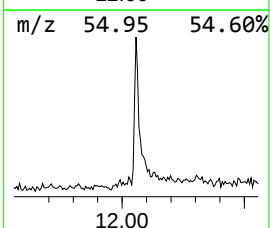
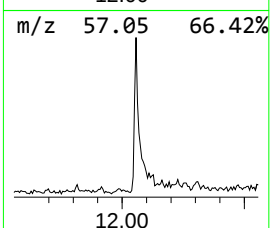
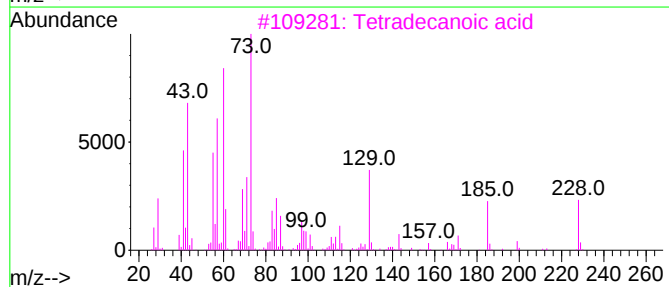
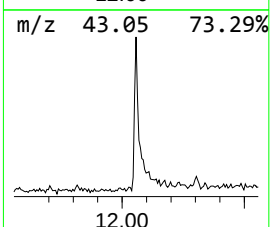
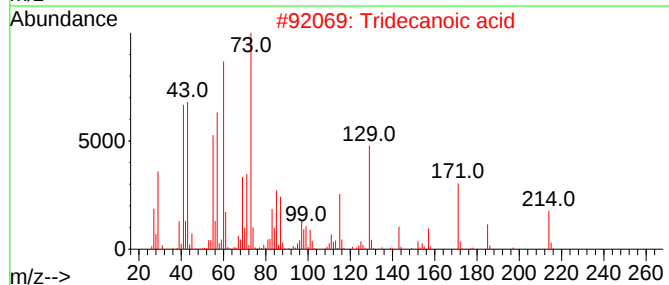
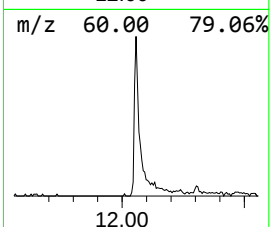
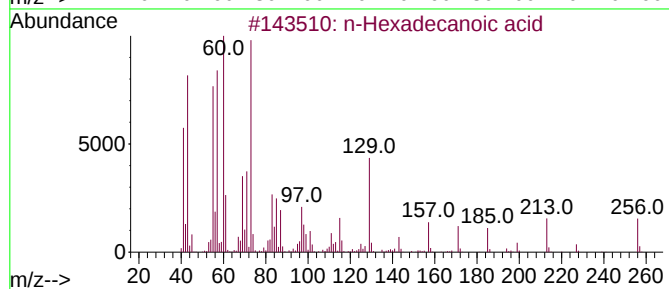
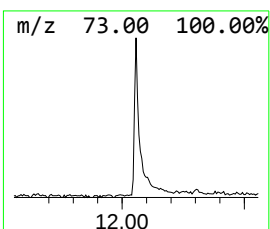
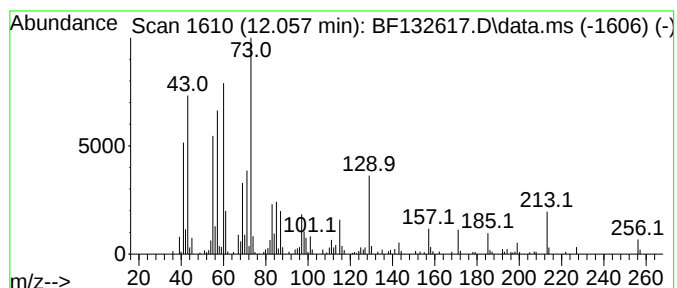
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Peak Number 2 n-Hexadecanoic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	4.51 ng	270707	Phenanthrene-d10	11.545

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	83
4			Pentadecanoic acid	242	C15H30O2	001002-84-2	81
5			Nonanoic acid	158	C9H18O2	000112-05-0	38



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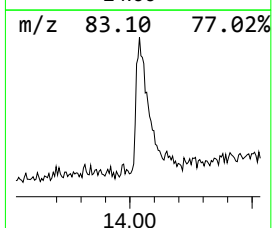
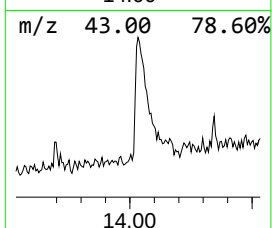
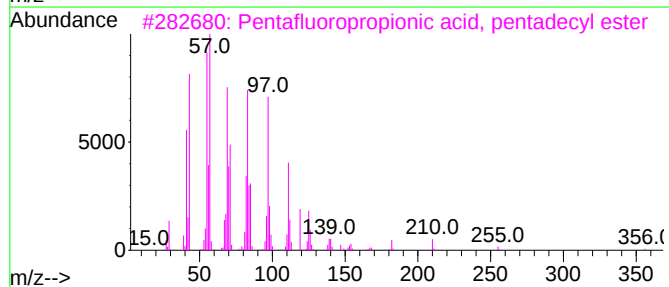
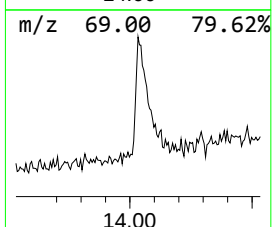
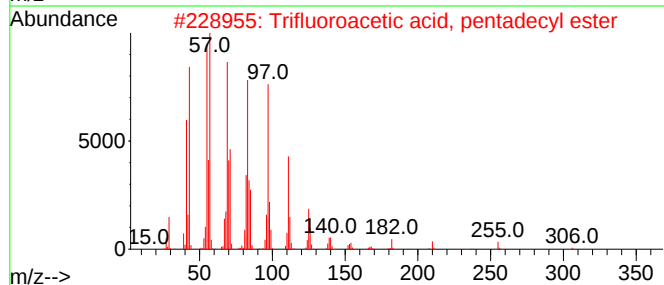
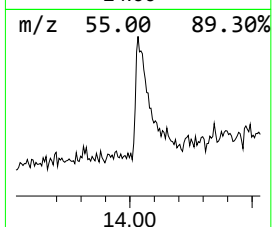
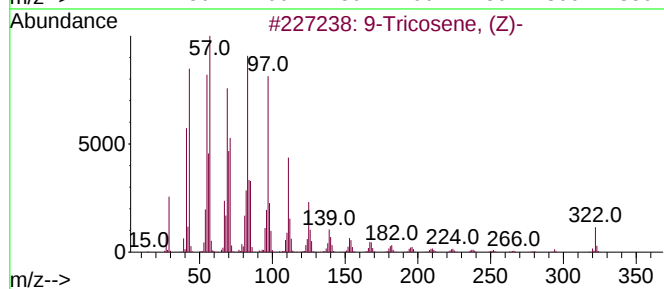
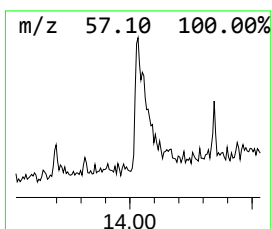
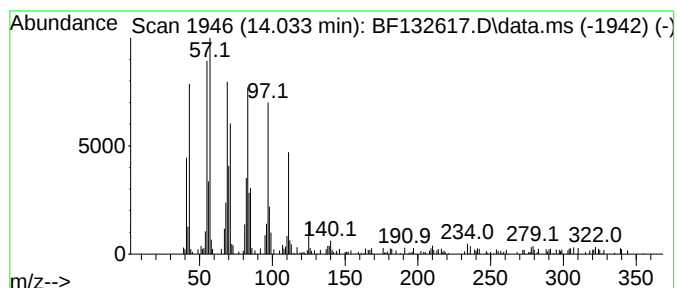
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Peak Number 3 9-Tricosene, (Z)- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
14.033	2.07 ng	114076	Chrysene-d12	14.204	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	9-Tricosene, (Z)-	322	C23H46	027519-02-4	93
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
3	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	91
4	Pentadecafluorooctanoic acid, pe...	624	C23H31F15O2	1000406-04-5	90
5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	90



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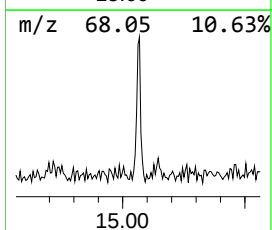
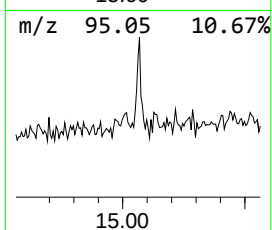
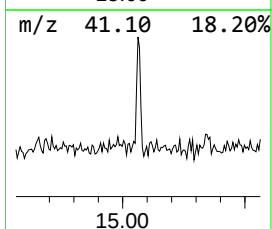
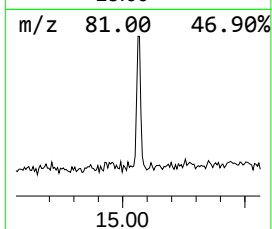
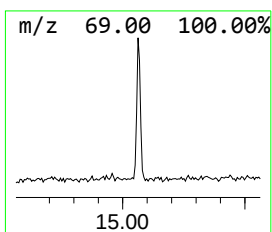
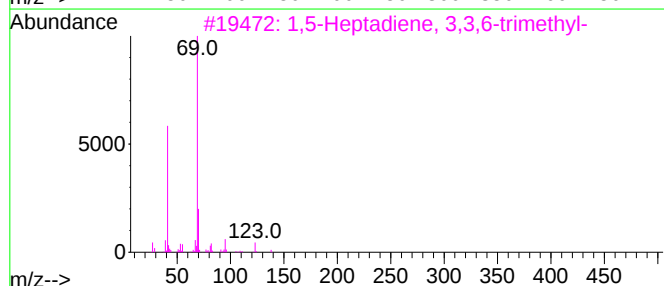
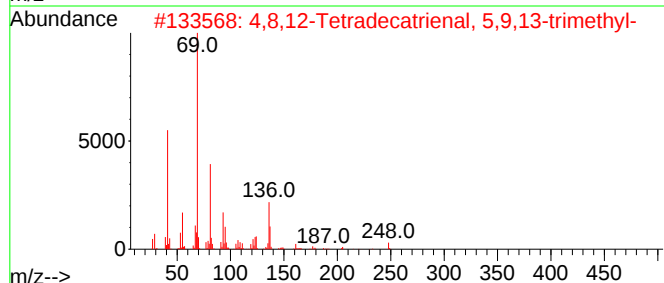
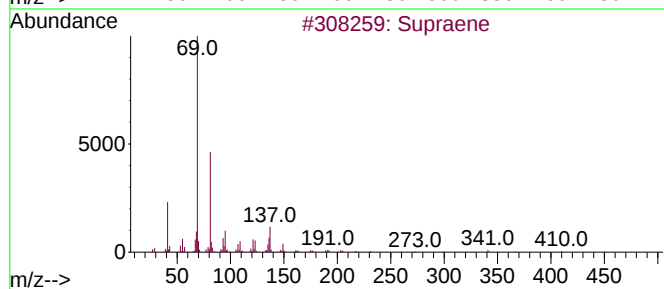
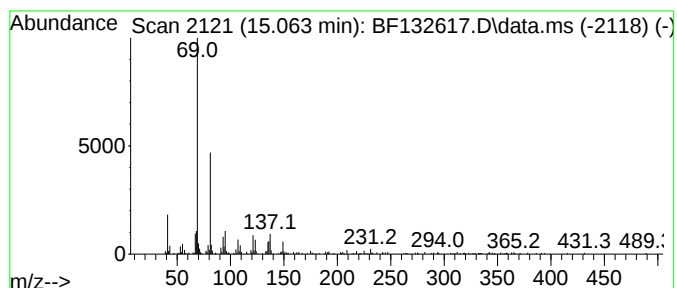
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Peak Number 4 Supraene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.063	3.12 ng	128986	Perylene-d12	15.757

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	72
2			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64
3			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	64
4			2,6-Octadiene, 2,6-dimethyl-	138	C10H18	002792-39-4	59
5			5-Bromo-1-pentanol	166	C5H11BrO	034626-51-2	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-...	5.234	29.0	ng	1728090	1	6.998	1190590	20.0
n-Hexadecanoic ...	12.057	4.5	ng	270707	4	11.545	1201220	20.0
9-Tricosene, (Z)-	14.033	2.1	ng	114076	5	14.204	1100850	20.0
Supraene	15.063	3.1	ng	128986	6	15.757	825756	20.0