

Data Path : Z:\svoasrv\HPCHEM1\BNA_F\Data\BF040122\
 Data File : BF127625.D
 Acq On : 01 Apr 2022 21:27
 Operator : CG\JU
 Sample : N2207-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 20220341-096-21-02

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-BF032122.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC: BF127625.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.087	473	476	485	rBV	12946	25310	1.05%	0.141%
2	5.463	537	540	568	rBV	2157004	2315021	96.48%	12.939%
3	6.475	708	712	732	rBV	2368952	2323257	96.83%	12.985%
4	6.828	770	772	782	rBV	632951	598550	24.95%	3.345%
5	7.398	866	869	880	rBV	1587163	1526796	63.63%	8.533%
6	8.116	987	991	1008	rBV	862409	803723	33.50%	4.492%
7	9.186	1169	1173	1182	rBV	2625197	2399422	100.00%	13.410%
8	9.251	1182	1184	1190	rVB2	28345	29735	1.24%	0.166%
9	9.469	1218	1221	1227	rBV2	18816	27117	1.13%	0.152%
10	9.869	1286	1289	1301	rBV	1070728	926606	38.62%	5.179%
11	10.663	1421	1424	1439	rBV	1512570	1540032	64.18%	8.607%
12	11.363	1540	1543	1552	rBV	1133669	971449	40.49%	5.429%
13	11.733	1603	1606	1610	rBV	217439	191934	8.00%	1.073%
14	12.445	1719	1727	1730	rBV	259764	254041	10.59%	1.420%
15	12.527	1738	1741	1745	rVB	53557	41034	1.71%	0.229%
16	12.945	1808	1812	1816	rBV	2524613	2269925	94.60%	12.687%
17	13.857	1959	1967	1983	rBV7	25274	130641	5.44%	0.730%
18	14.016	1990	1994	2004	rBV	608802	632316	26.35%	3.534%
19	14.610	2092	2095	2100	rVB2	28632	27934	1.16%	0.156%
20	14.827	2127	2132	2136	rBV	76141	82680	3.45%	0.462%
21	15.086	2172	2176	2181	rVB	34155	41622	1.73%	0.233%
22	15.280	2205	2209	2222	rVB	17362	54507	2.27%	0.305%
23	15.457	2235	2239	2242	rBV	32466	41145	1.71%	0.230%
24	15.498	2242	2246	2257	rVB	348682	489754	20.41%	2.737%
25	15.886	2308	2312	2318	rBV	30875	45595	1.90%	0.255%
26	16.386	2393	2397	2405	rVB4	24474	43053	1.79%	0.241%
27	16.974	2493	2497	2503	rVB4	17189	30269	1.26%	0.169%
28	17.668	2609	2615	2623	rVB7	13187	28831	1.20%	0.161%

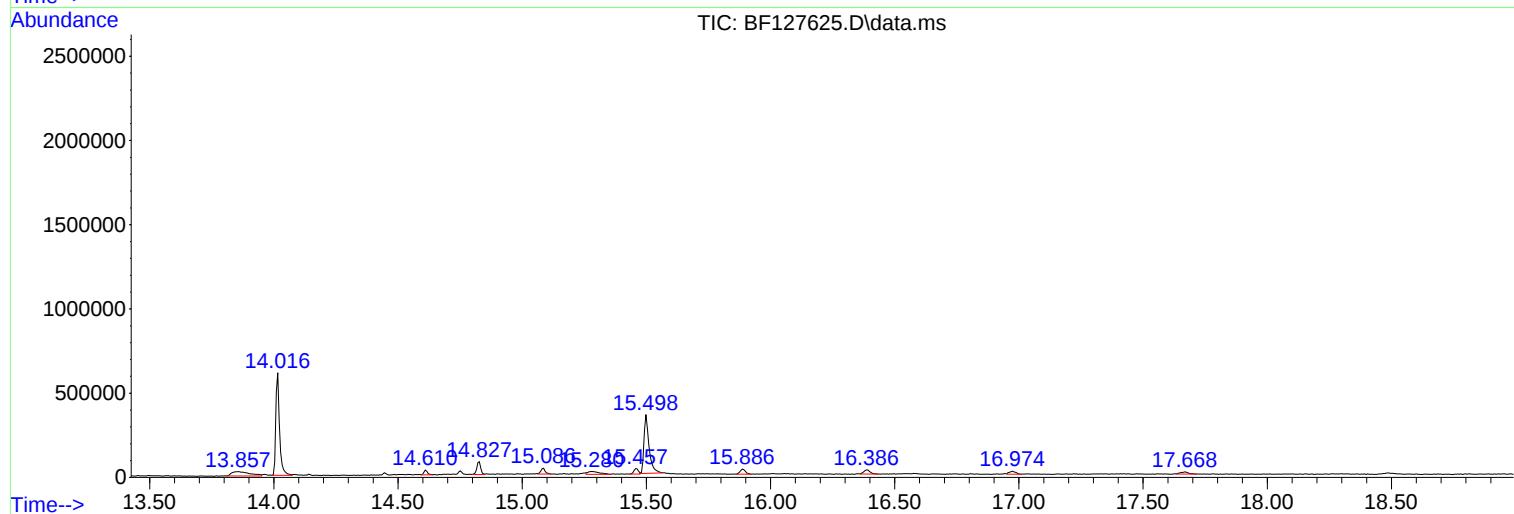
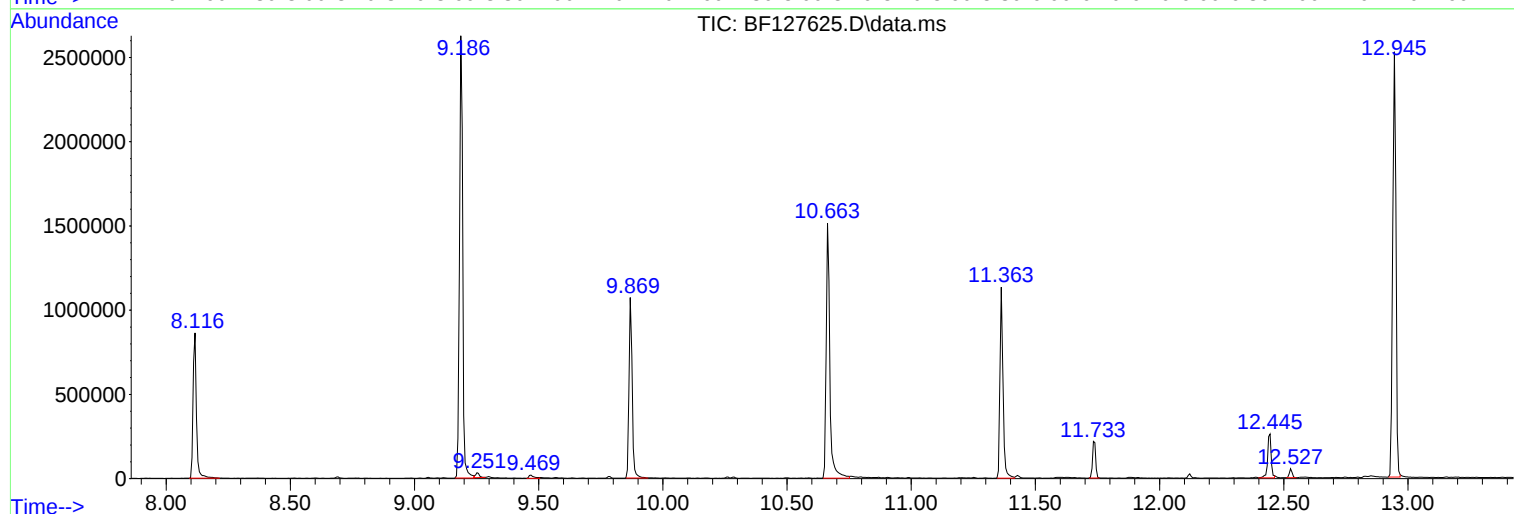
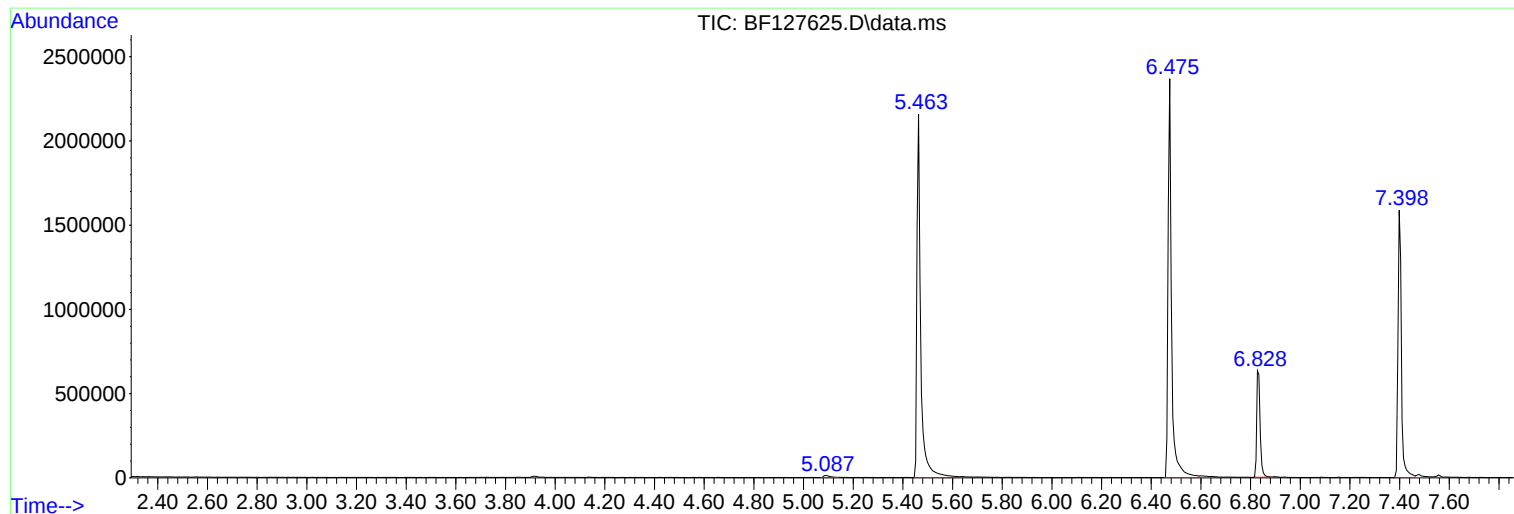
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Misc :
ALS Vial : 20 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
20220341-096-21-02

Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.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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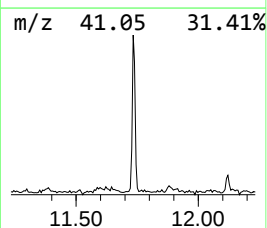
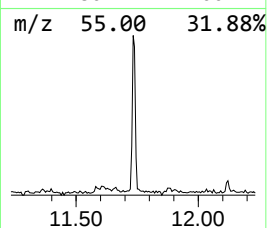
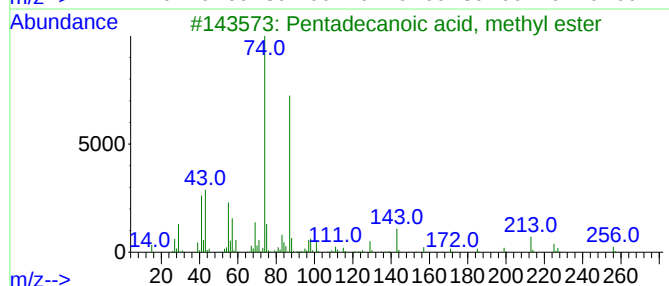
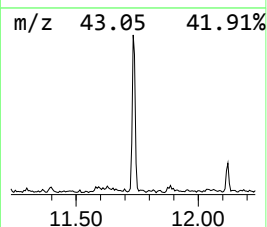
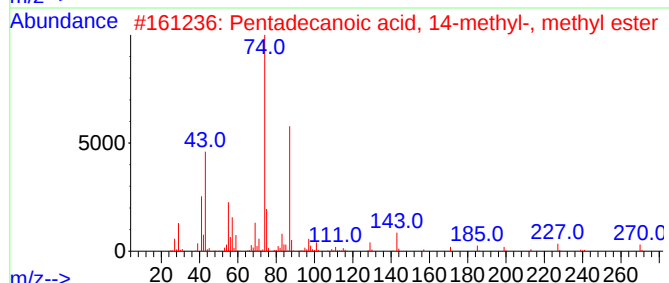
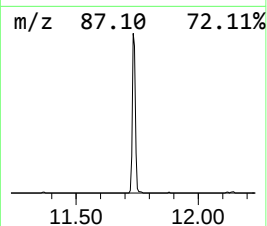
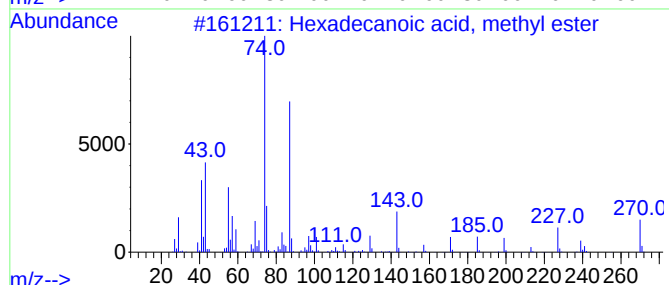
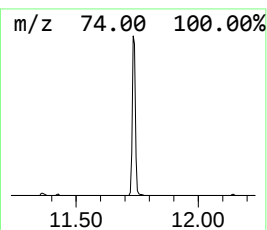
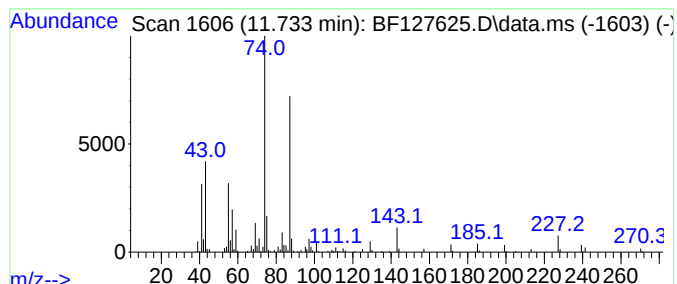
Instrument :
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ClientSampleId :
20220341-096-21-02

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Hexadecanoic acid, methyl e... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.733	3.95 ng	191934	Phenanthrene-d10		11.363	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Hexadecanoic acid, methyl ester		270	C17H34O2	000112-39-0	96
2	Pentadecanoic acid, 14-methyl-, ...		270	C17H34O2	005129-60-2	91
3	Pentadecanoic acid, methyl ester		256	C16H32O2	007132-64-1	90
4	Undecanoic acid, 10-methyl-, met...		214	C13H26O2	005129-56-6	90
5	Methyl 11-methyl-dodecanoate		228	C14H28O2	1000336-45-1	90



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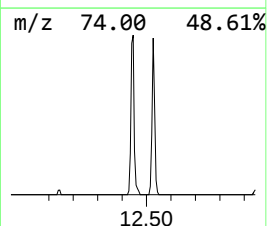
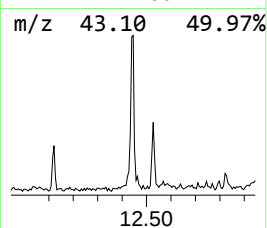
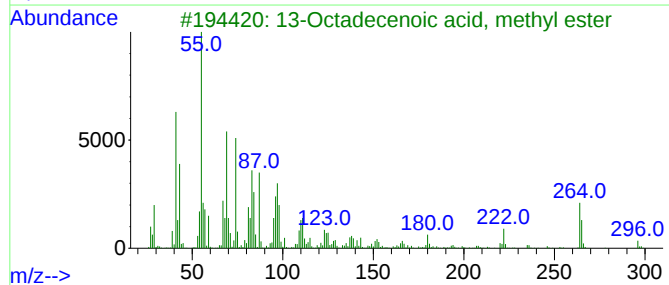
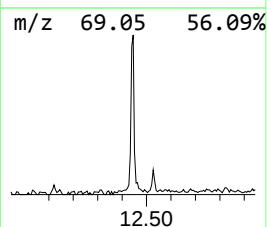
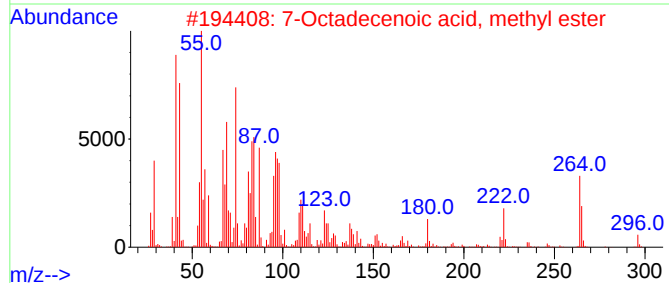
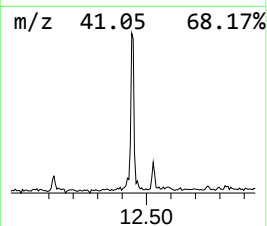
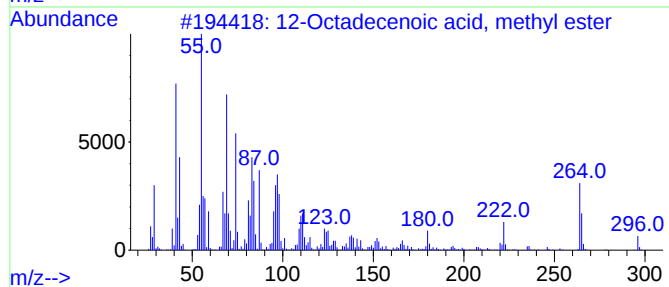
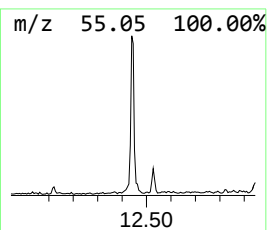
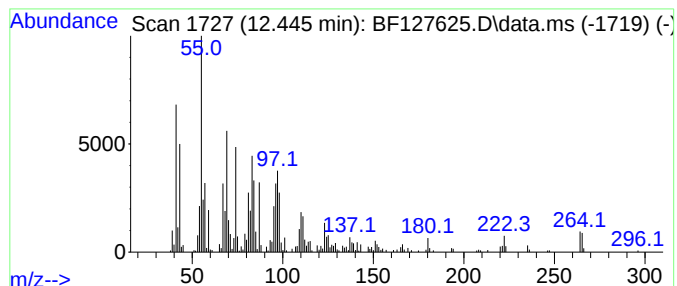
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 12-Octadecenoic acid, methyl... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.445	5.23 ng	254041	Phenanthrene-d10	11.363

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			12-Octadecenoic acid, methyl ester	296	C19H36O2	056554-46-2	99
2			7-Octadecenoic acid, methyl ester	296	C19H36O2	057396-98-2	99
3			13-Octadecenoic acid, methyl ester	296	C19H36O2	056554-47-3	98
4			14-Octadecenoic acid, methyl ester	296	C19H36O2	056554-48-4	97
5			9-Octadecenoic acid (Z)-, methyl...	296	C19H36O2	000112-62-9	97



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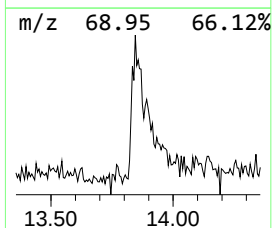
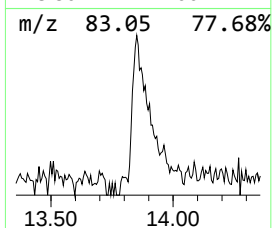
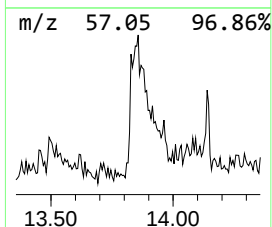
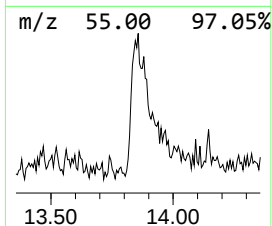
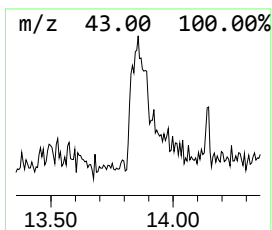
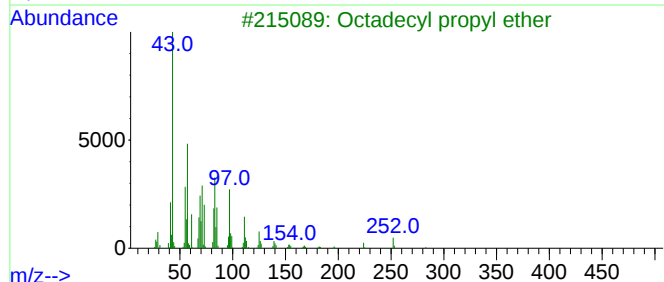
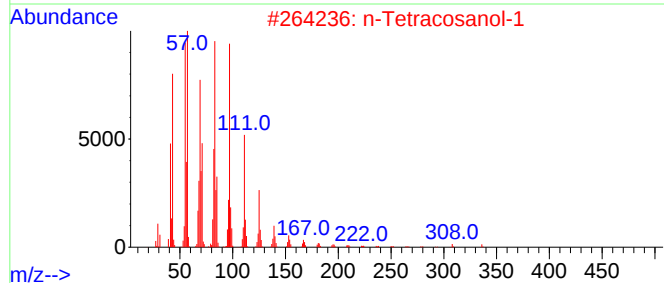
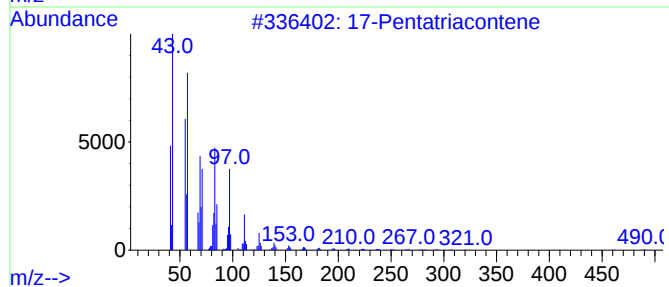
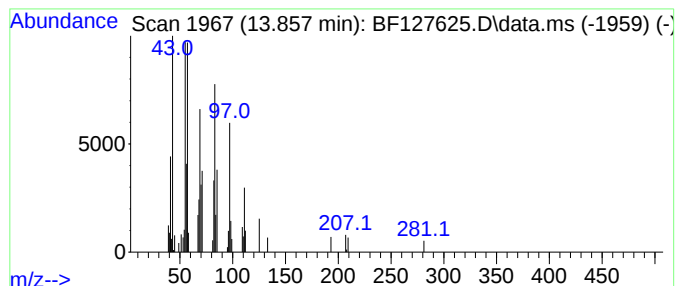
Quant Method : Z:\svoasrv\HPCHEM1\BNA_F\Methods\8270-BF032122.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 17-Pentatriacontene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.857	4.13 ng	130641	Chrysene-d12	14.015

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			17-Pentatriacontene	491	C35H70	006971-40-0	91
2			n-Tetracosanol-1	354	C24H50O	000506-51-4	83
3			Octadecyl propyl ether	312	C21H44O	1000406-28-0	83
4			Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	81
5			1-Octadecanol	270	C18H38O	000112-92-5	81



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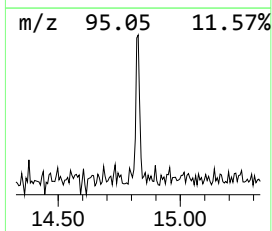
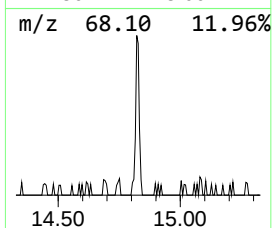
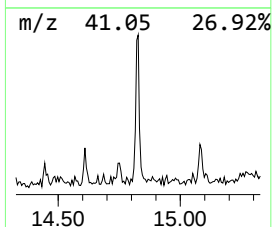
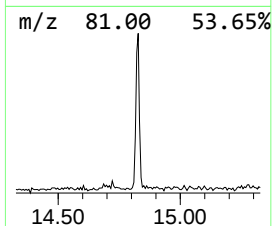
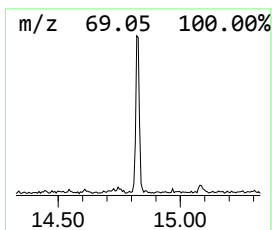
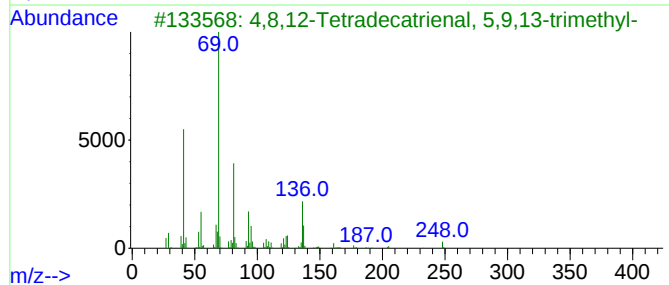
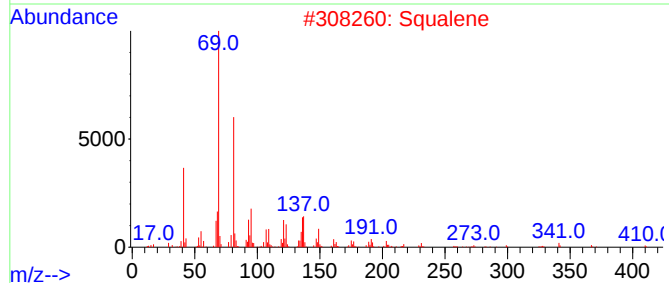
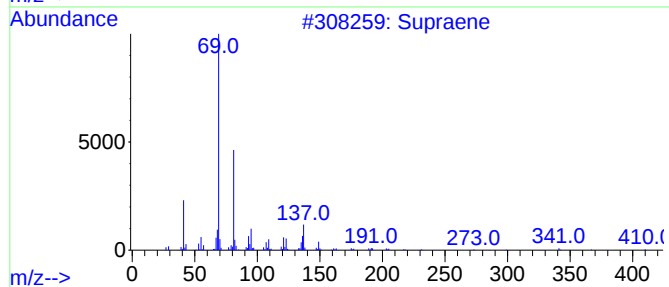
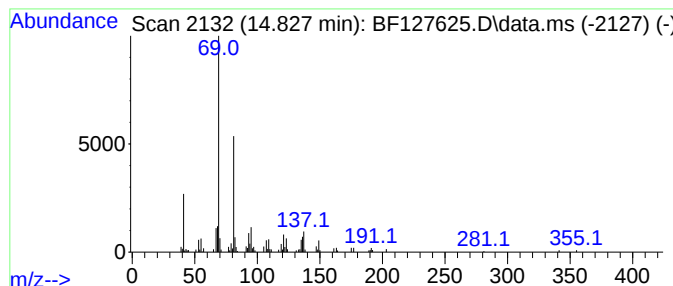
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TIC Library : C:\Database\NIST20.L
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Peak Number 4 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.827	3.38 ng	82680	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Supraene	410	C30H50	007683-64-9	91
2			Squalene	410	C30H50	000111-02-4	91
3			4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	72
4			2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64
5			1,5-Heptadiene, 3,3,6-trimethyl-	138	C10H18	035387-63-4	58



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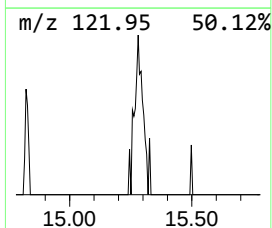
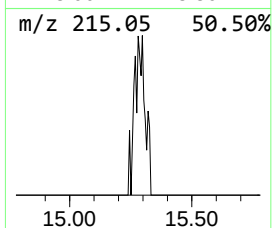
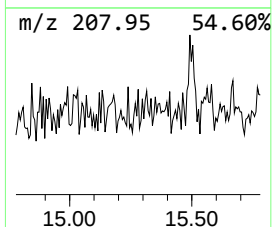
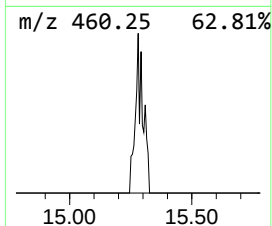
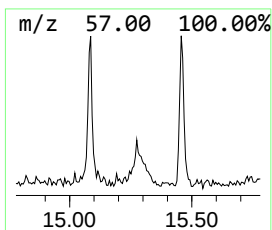
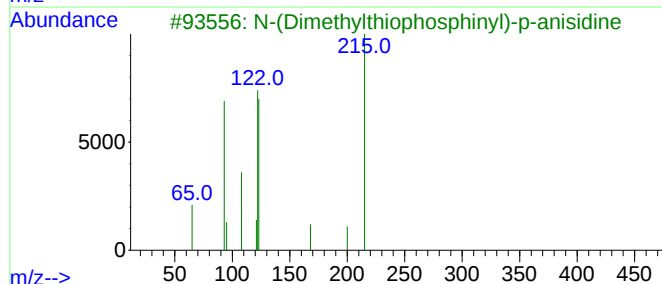
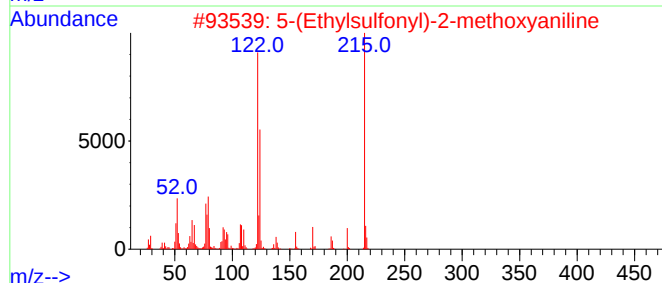
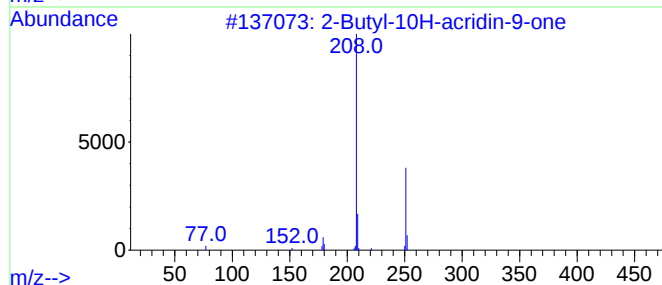
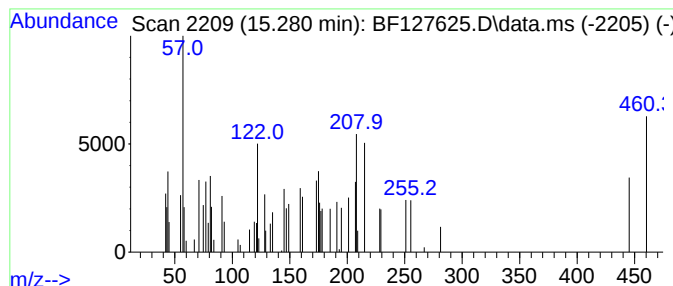
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 unknown15.280 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.280	2.23 ng	54507	Perylene-d12	15.498

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butyl-10H-acridin-9-one	251	C17H17NO	055751-69-4	11		
2	5-(Ethylsulfonyl)-2-methoxyaniline	215	C9H13NO3S	005339-62-8	9		
3	N-(Dimethylthiophosphinyl)-p-ani...	215	C9H14NOPS	100074-00-6	9		
4	5-Iodohistidine	281	C6H8IN3O2	1000131-15-8	9		
5	p-Methylbenzylidene p-butylaniline	251	C18H21N	038549-81-4	9		



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Hexadecanoic ac...	11.733	4.0	ng	191934	4	11.363	971449	20.0
12-Octadecenoic...	12.445	5.2	ng	254041	4	11.363	971449	20.0
17-Pentatriacon...	13.857	4.1	ng	130641	5	14.015	632316	20.0
Supraene	14.827	3.4	ng	82680	6	15.498	489754	20.0
unknown15.280	15.280	2.2	ng	54507	6	15.498	489754	20.0