

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF081919\
 Data File : BF116404.D
 Acq On : 19 Aug 2019 22:50
 Operator : HP/JU
 Sample : K4290-04
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 B-4

Integration Parameters: rteint.p

Integrator: RTE

Smoothing : ON

Sampling : 1

Start Thrs: 0.2

Stop Thrs : 0

Filtering: 5

Min Area: 3 % of largest Peak

Max Peaks: 100

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-BF073019.M

Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	5.434	566	569	599	rBV	1209153	1637526	56.89%	6.565%
2	6.445	738	741	760	rBV	1540969	1892115	65.73%	7.586%
3	6.581	760	764	772	rVB	1934736	1975487	68.63%	7.920%
4	6.804	799	802	812	rBV	690739	642458	22.32%	2.576%
5	6.957	825	828	846	rBV	2044804	1836184	63.79%	7.362%
6	7.369	894	898	927	rBV	1432482	1467829	50.99%	5.885%
7	8.081	1016	1019	1036	rVB	848631	825810	28.69%	3.311%
8	9.151	1198	1201	1212	rBV	2912374	2723528	94.61%	10.920%
9	9.551	1265	1269	1277	rBV	508752	446155	15.50%	1.789%
10	9.834	1313	1317	1321	rBV	1248767	1003261	34.85%	4.022%
11	10.628	1448	1452	1466	rBV	1113160	1237255	42.98%	4.961%
12	11.322	1566	1570	1573	rBV	1201252	1113847	38.69%	4.466%
13	11.345	1573	1574	1579	rVB	210778	166263	5.78%	0.667%
14	11.845	1653	1659	1668	rBV3	242297	413826	14.38%	1.659%
15	11.939	1672	1675	1678	rVV	43568	38581	1.34%	0.155%
16	12.539	1773	1777	1782	rBV	356704	372518	12.94%	1.494%
17	12.622	1788	1791	1795	rBV3	53391	81253	2.82%	0.326%
18	12.692	1800	1803	1805	rVV3	32221	41468	1.44%	0.166%
19	12.763	1810	1815	1823	rVB	332792	555073	19.28%	2.225%
20	12.898	1834	1838	1841	rBV	3192749	2878634	100.00%	11.541%
21	13.098	1870	1872	1874	rBV	36441	32205	1.12%	0.129%
22	13.204	1887	1890	1893	rBV3	28716	35275	1.23%	0.141%
23	13.363	1914	1917	1921	rBV2	61724	61767	2.15%	0.248%
24	13.786	1984	1989	1996	rBV3	279977	430125	14.94%	1.725%
25	13.963	2015	2019	2022	rBV2	1050661	1082148	37.59%	4.339%
26	13.992	2022	2024	2032	rVB	165275	198579	6.90%	0.796%
27	14.404	2092	2094	2096	rVB2	44176	34386	1.19%	0.138%
28	14.704	2143	2145	2149	rVB	77267	71169	2.47%	0.285%
29	14.774	2154	2157	2164	rVB	175002	193881	6.74%	0.777%
30	15.010	2193	2197	2198	rBV	114875	144569	5.02%	0.580%
31	15.304	2244	2247	2251	rBV	66391	74072	2.57%	0.297%
32	15.368	2255	2258	2260	rVV	95682	120189	4.18%	0.482%
33	15.416	2263	2266	2279	rVB	579315	852978	29.63%	3.420%
34	15.804	2330	2332	2338	rVB	61453	81468	2.83%	0.327%

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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 >
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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.904	2516	2519	2526	rvB3	40746	72294	2.51%	0.290%
36	17.345	2590	2594	2605	rvB	43955	107464	3.73%	0.431%

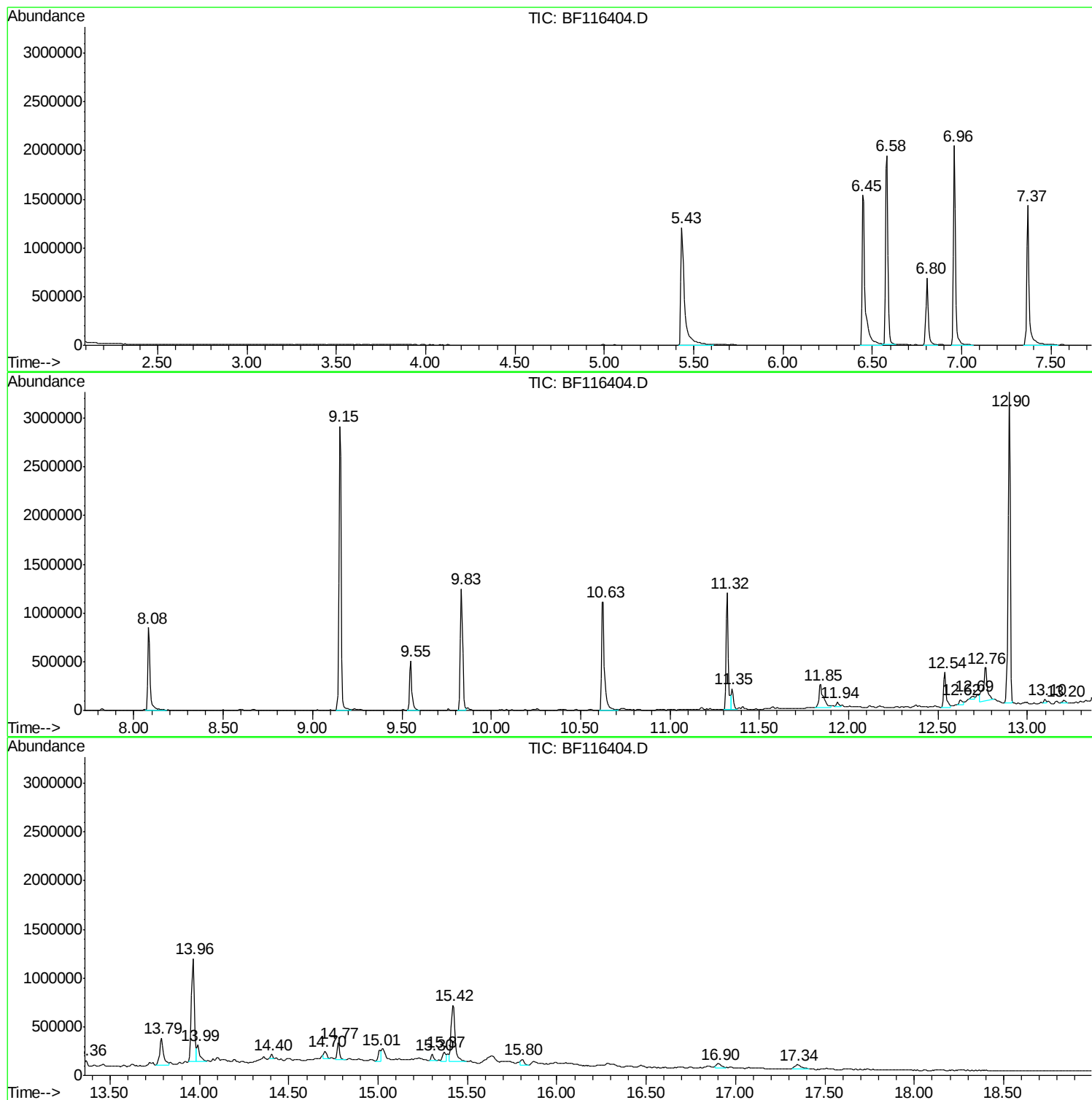
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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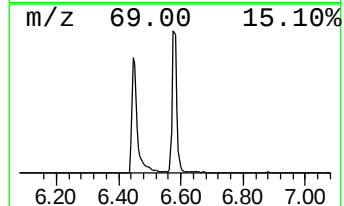
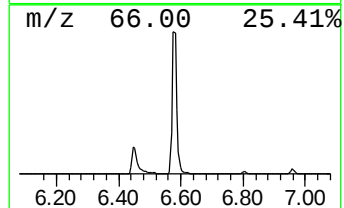
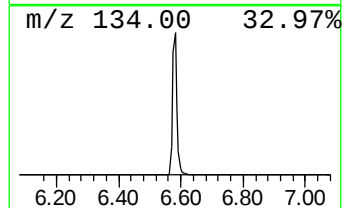
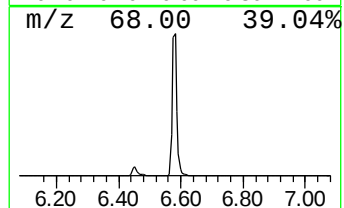
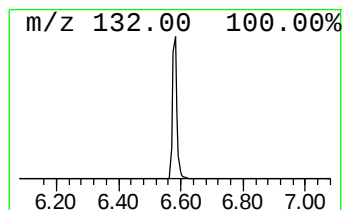
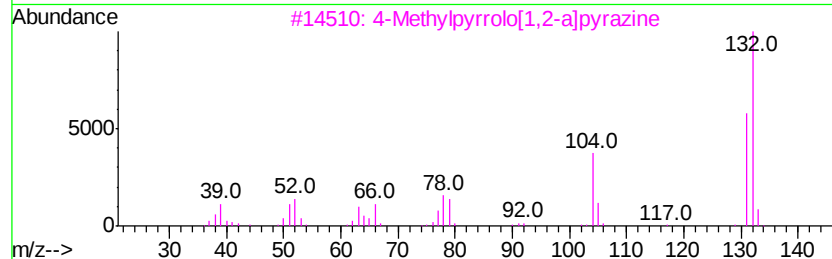
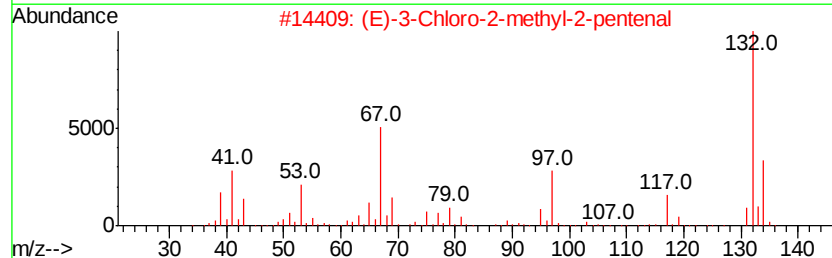
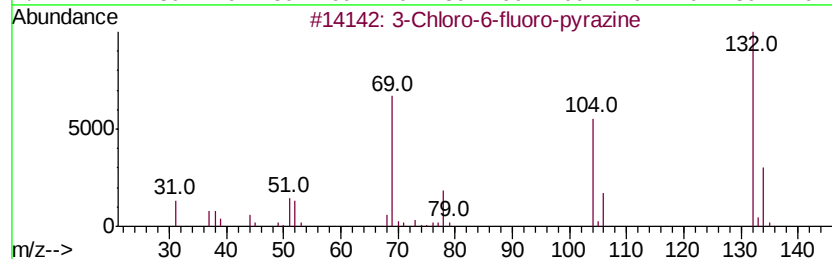
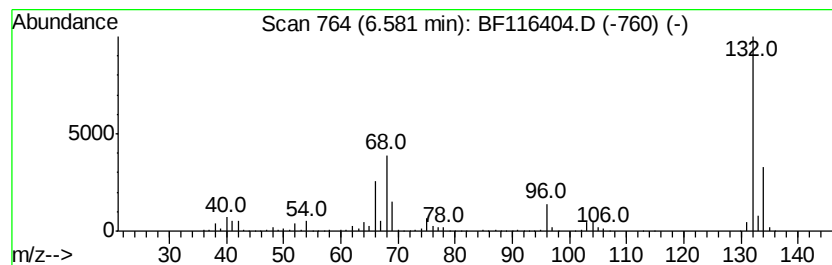
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF073019.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	61.50 ng	1975490	1,4-Dichlorobenzene-d4	6.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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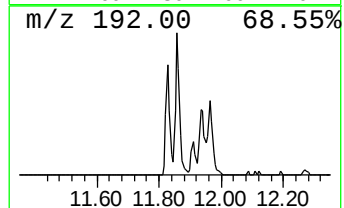
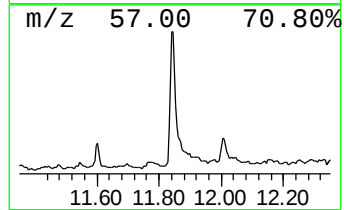
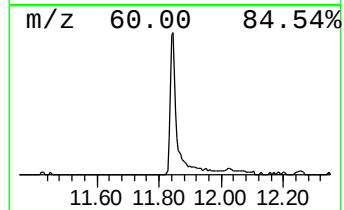
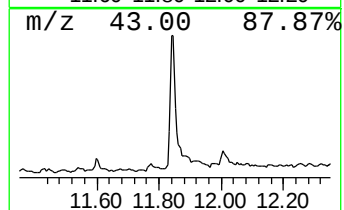
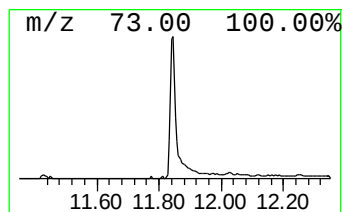
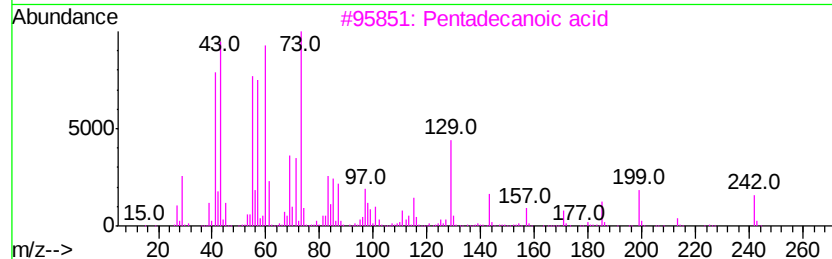
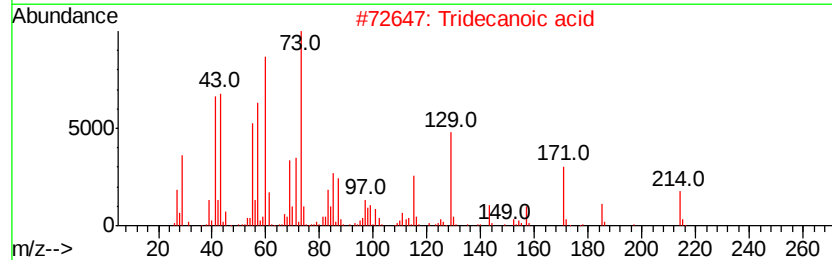
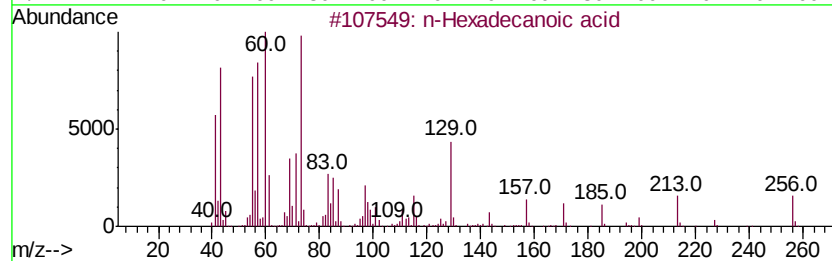
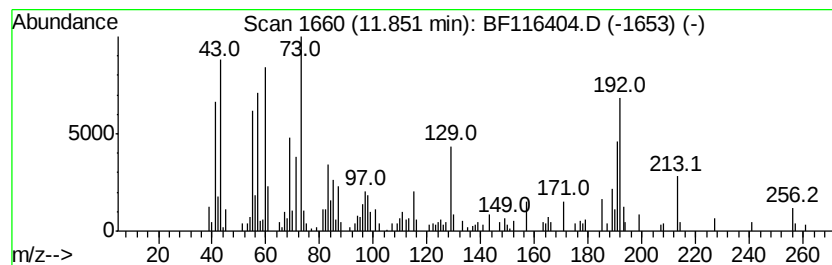
Instrument :
BNA_F
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
11.85	7.43 ng	413826	Phenanthrene-d10		11.32	
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	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	87
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	58



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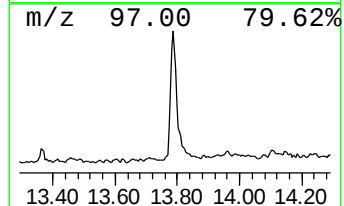
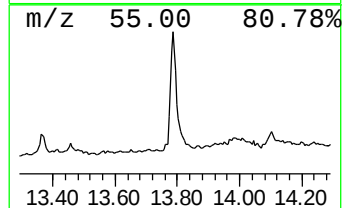
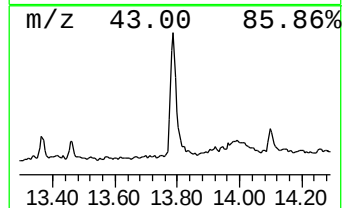
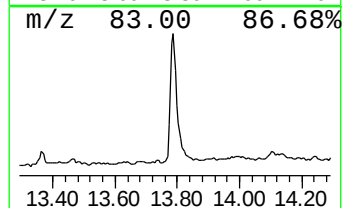
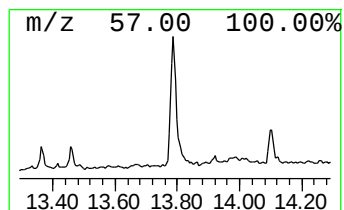
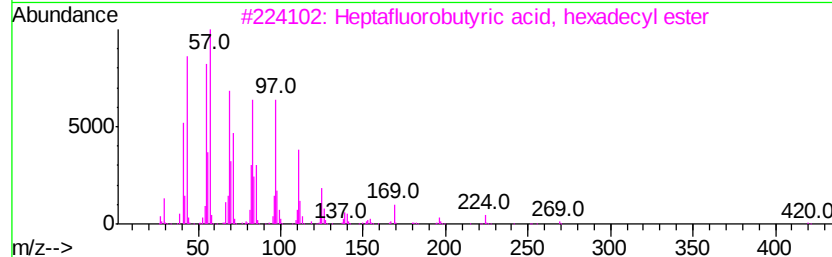
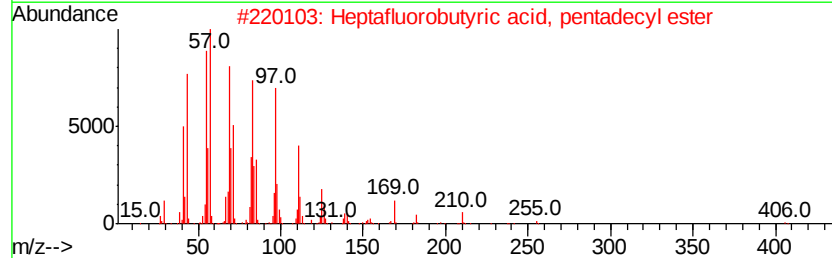
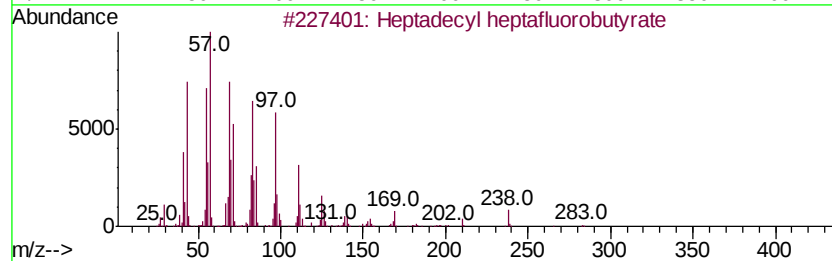
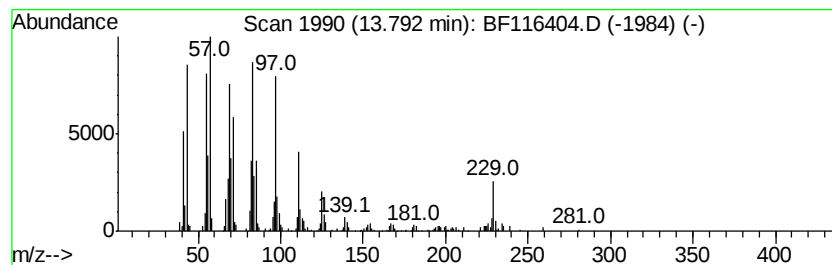
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heptadecyl heptafluorobutyrate Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.79	7.95 ng	430125	Chrysene-d12	13.96

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2		Heptafluorobutyric acid, pentadec...	424	C19H31F7O2	959261-23-5	94
3		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	94
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	93



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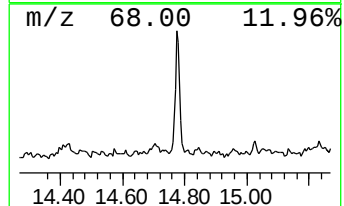
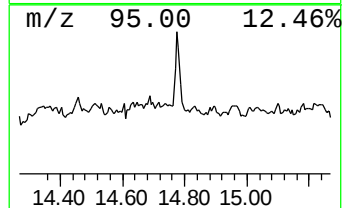
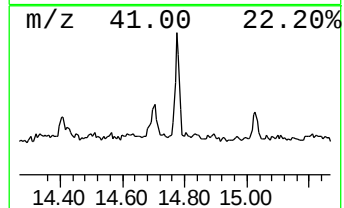
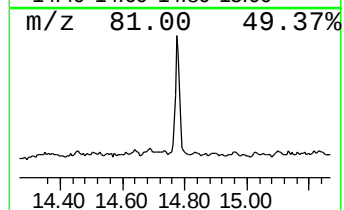
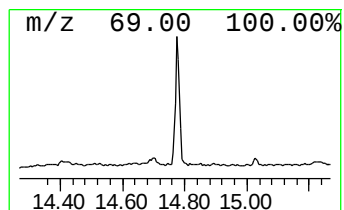
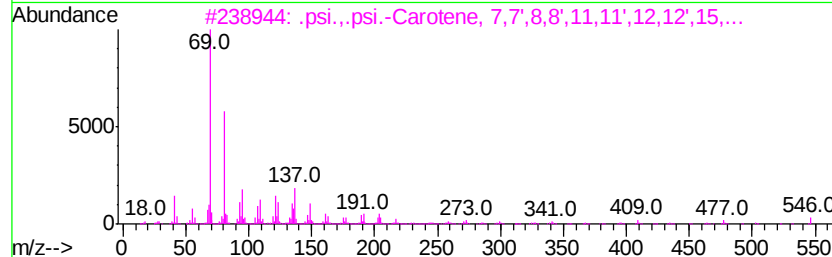
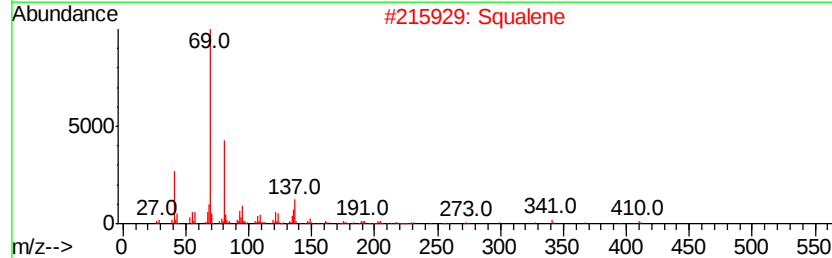
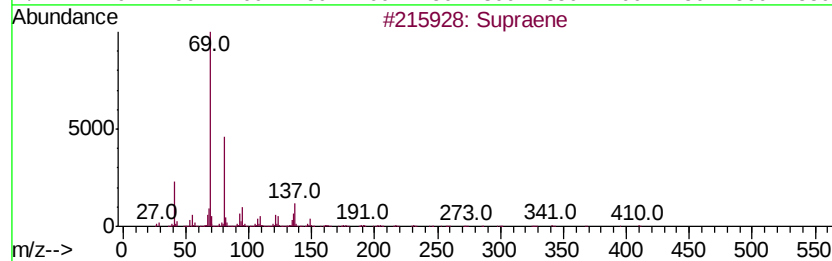
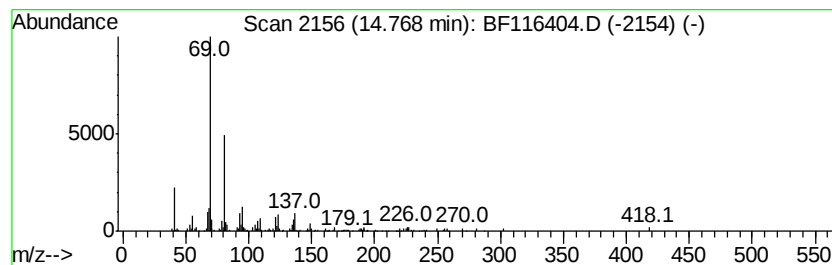
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Peak Number 5 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.77	4.55 ng	193881	Perylene-d12	15.42

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Supraene	410	C30H50	007683-64-9	91
2		Squalene	410	C30H50	000111-02-4	90
3		.psi.,.psi.-Carotene, 7,7',8,8',...	547	C40H66	000502-62-5	83
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	72
5		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	64



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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown6.58	6.58	61.5	ng	1975490	1	6.80	642458	20.0
n-Hexadecanoic acid	11.85	7.4	ng	413826	4	11.32	1113850	20.0
Heptadecyl heptaf...	13.79	8.0	ng	430125	5	13.96	1082150	20.0
Squalene	14.77	4.5	ng	193881	6	15.42	852978	20.0