

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF062218\
 Data File : BF106728.D
 Acq On : 23 Jun 2018 00:07
 Operator : JU/SJ
 Sample : J3622-04
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-A

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-BF061918.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	5.207	484	488	496	rBV	90336	118042	8.17%	0.995%
2	5.601	551	555	559	rBV	1120894	1196925	82.88%	10.088%
3	6.601	720	725	729	rBV	1076540	1244120	86.15%	10.485%
4	6.737	743	748	751	rBV	1231196	1249998	86.55%	10.535%
5	6.960	782	786	789	rBV	363612	296603	20.54%	2.500%
6	7.119	808	813	816	rBV	1063900	1018527	70.53%	8.584%
7	7.525	876	882	885	rBV	829339	834726	57.80%	7.035%
8	8.242	999	1004	1007	rBV	423628	360263	24.95%	3.036%
9	9.319	1181	1187	1190	rBV	1408244	1444199	100.00%	12.172%
10	9.707	1249	1253	1260	rVB	178497	157259	10.89%	1.325%
11	9.907	1283	1287	1291	rBV	18079	15862	1.10%	0.134%
12	10.001	1299	1303	1307	rBV	439849	388300	26.89%	3.273%
13	10.407	1370	1372	1375	rVB	34290	26534	1.84%	0.224%
14	10.795	1433	1438	1441	rBV	924315	856441	59.30%	7.218%
15	10.883	1450	1453	1458	rBV	36999	38476	2.66%	0.324%
16	11.330	1524	1529	1531	rBV	20110	16626	1.15%	0.140%
17	11.489	1552	1556	1560	rBV	403007	358842	24.85%	3.024%
18	13.077	1821	1826	1829	rBV	1402105	1302245	90.17%	10.975%
19	13.954	1971	1975	1986	rBV	117522	125358	8.68%	1.057%
20	14.142	2003	2007	2010	rBV	423308	378617	26.22%	3.191%
21	14.595	2080	2084	2088	rBV5	25408	35345	2.45%	0.298%
22	14.989	2147	2151	2156	rVB	37741	43504	3.01%	0.367%
23	15.671	2262	2267	2274	rVB	256722	326952	22.64%	2.756%
24	18.706	2778	2783	2794	rVB8	11688	31387	2.17%	0.265%

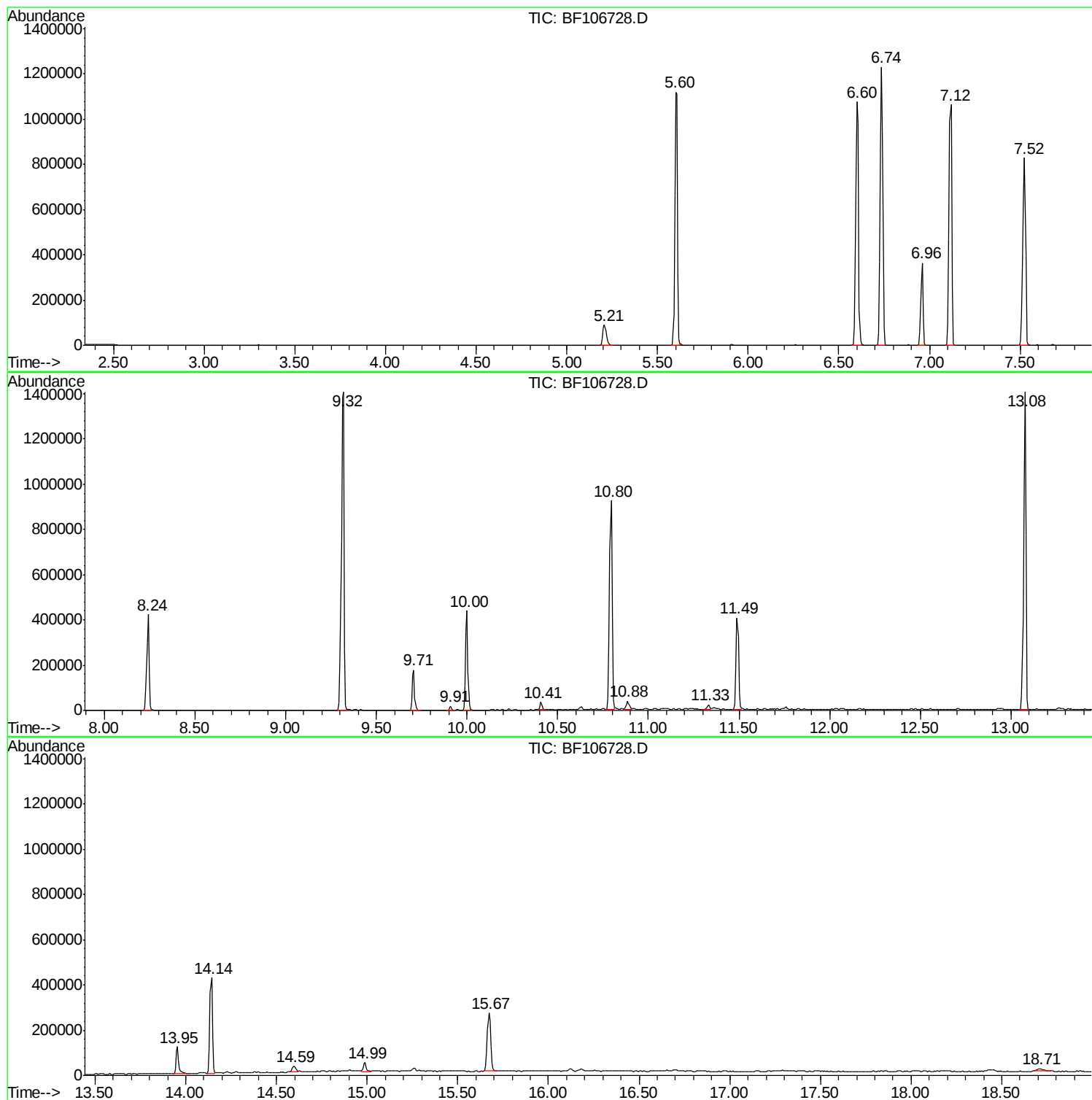
Sum of corrected areas: 11865151

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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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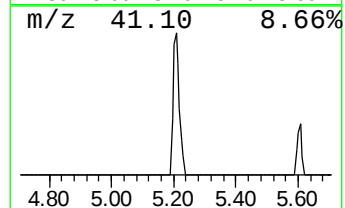
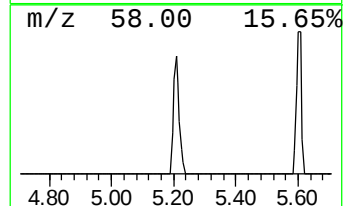
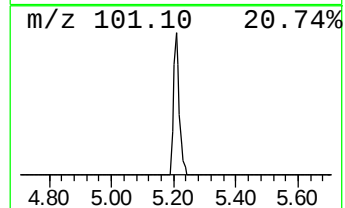
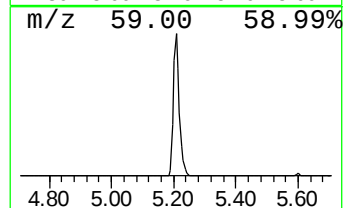
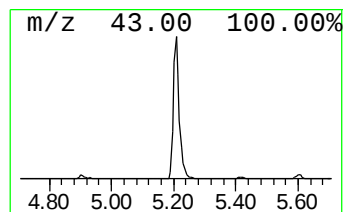
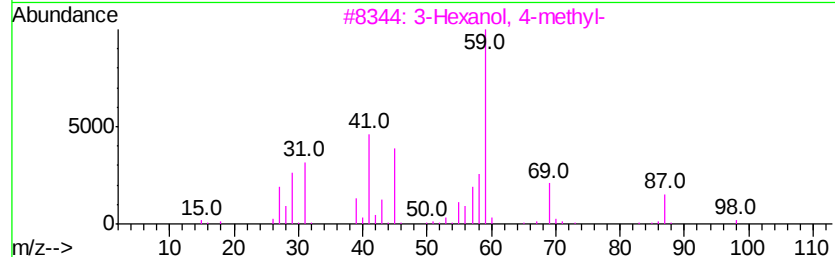
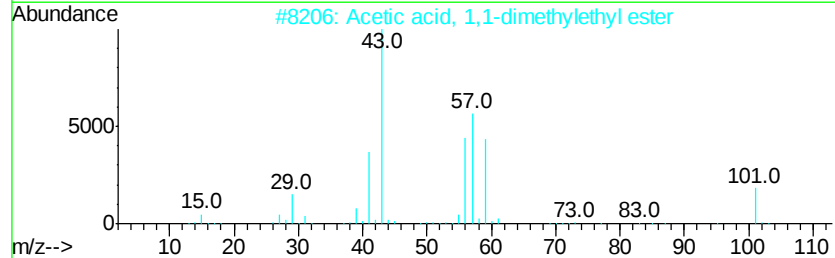
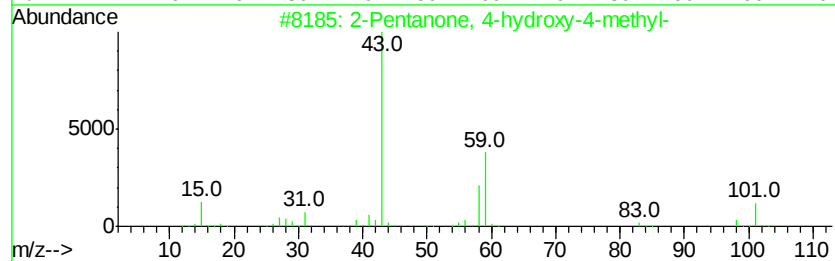
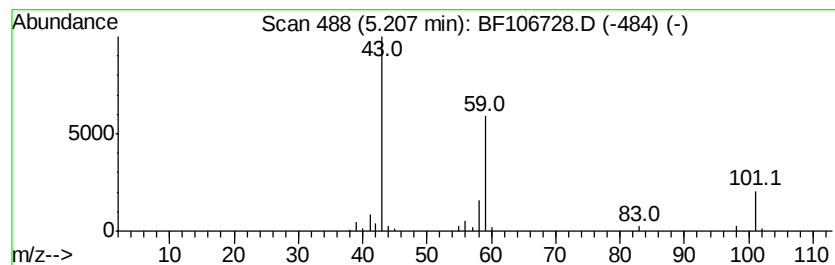
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.21	7.96 ng	118042	1,4-Dichlorobenzene-d4	6.96

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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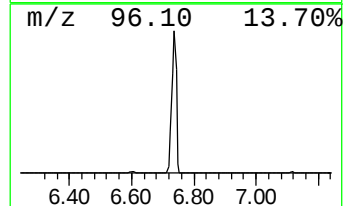
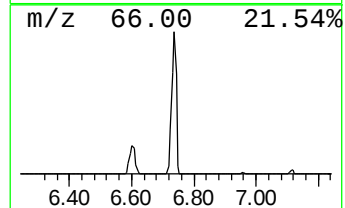
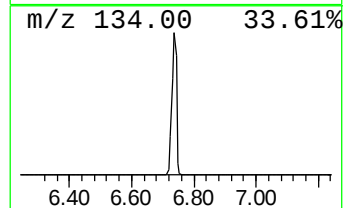
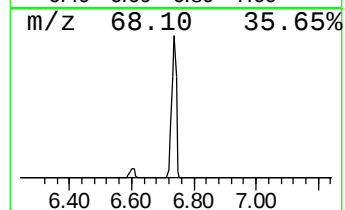
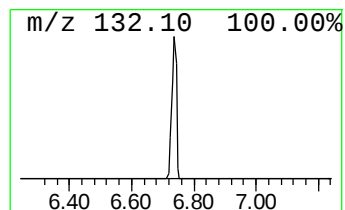
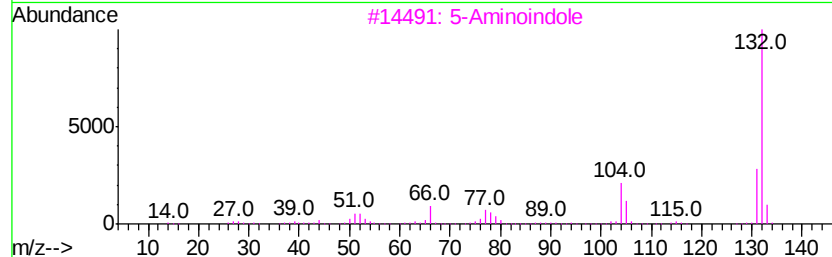
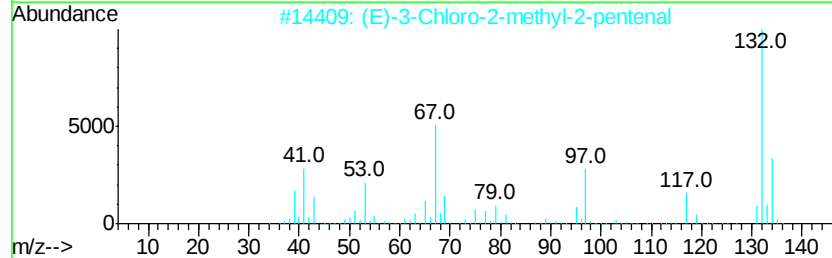
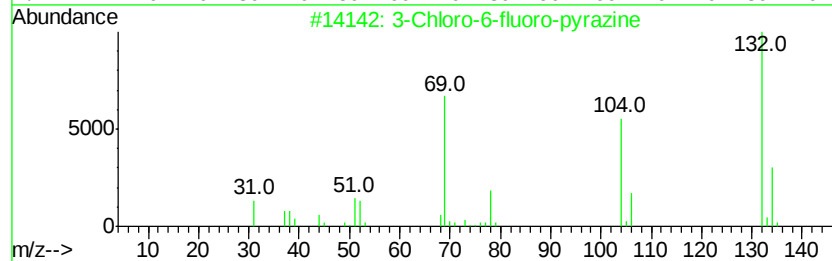
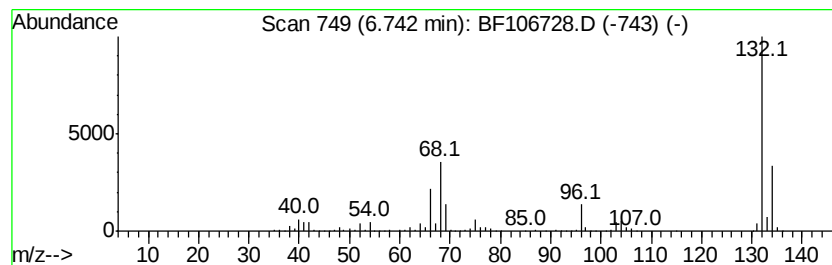
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Peak Number 2 unknown6.74 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.74	84.29 ng	1250000	1,4-Dichlorobenzene-d4	6.96

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	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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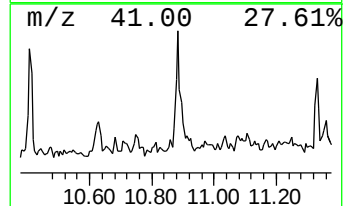
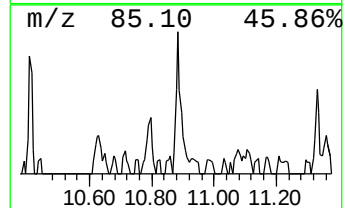
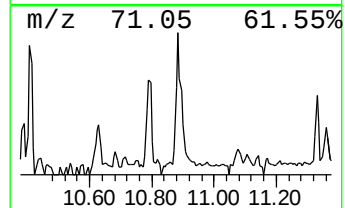
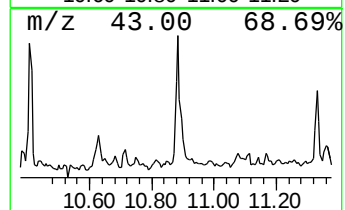
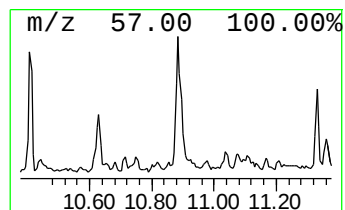
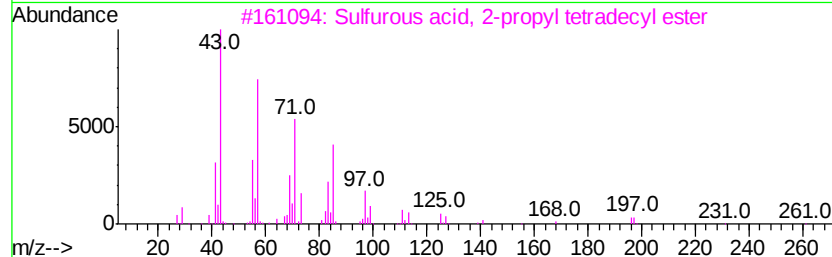
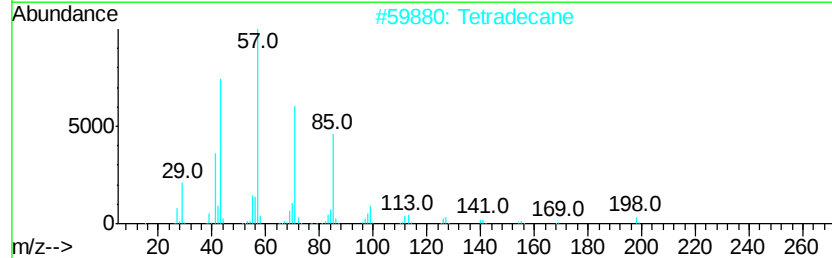
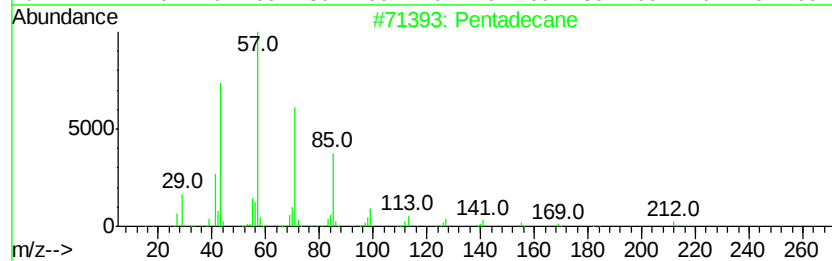
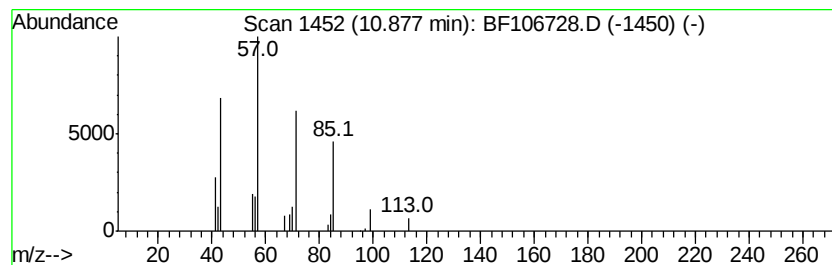
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Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.14 ng	38476	Phenanthrene-d10	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentadecane		212	C15H32	000629-62-9	86
2	Tetradecane		198	C14H30	000629-59-4	86
3	Sulfurous acid, 2-propyl tetradecyl ester		320	C17H36O3S	1000309-12-5	78
4	Hexadecane		226	C16H34	000544-76-3	78
5	Nonadecane		268	C19H40	000629-92-5	72



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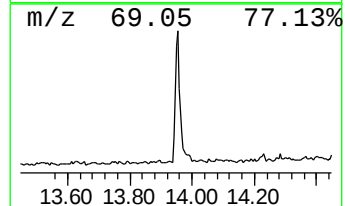
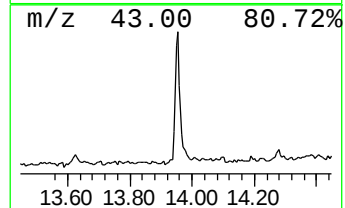
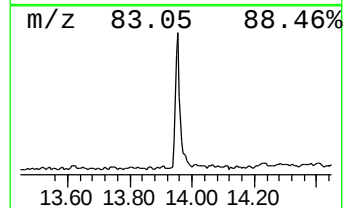
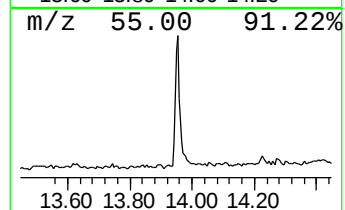
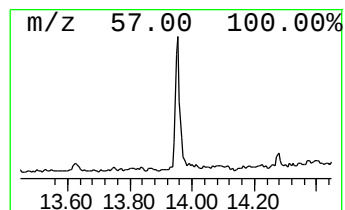
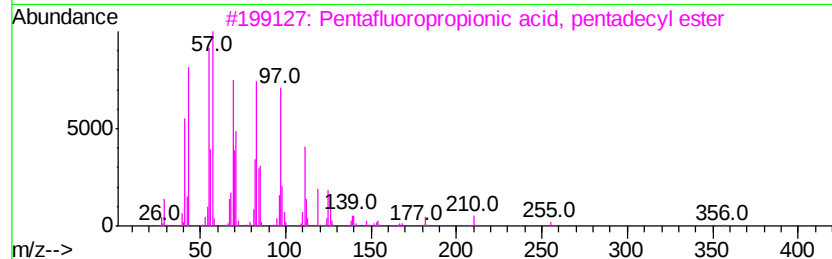
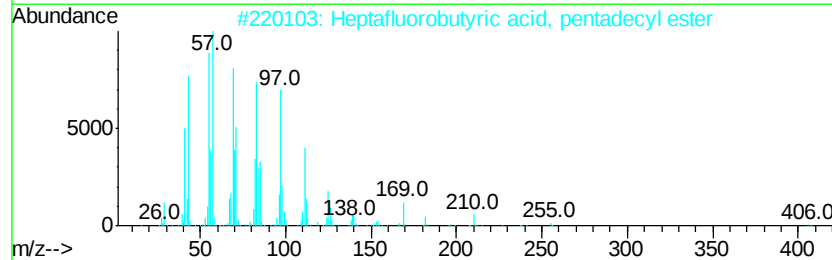
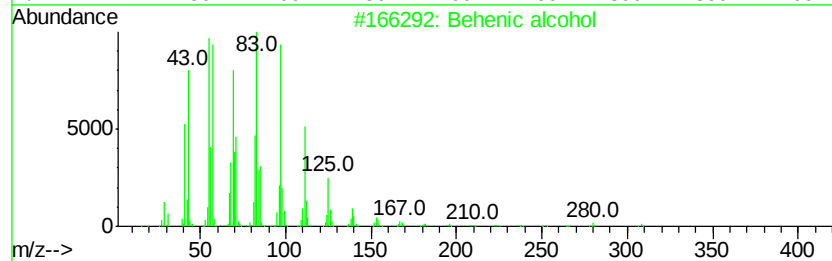
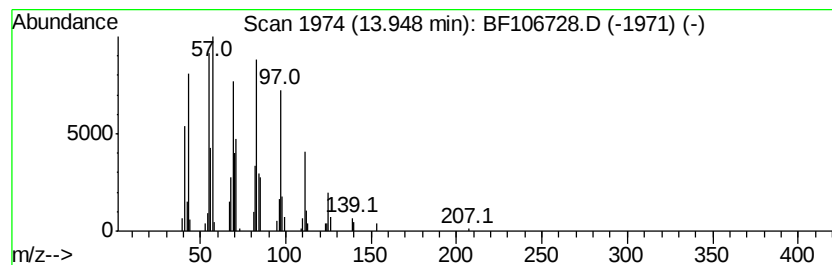
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Peak Number 5 Behenic alcohol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	6.62 ng	125358	Chrysene-d12	14.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Behenic alcohol	326 C22H46O	000661-19-8 95
2		Heptafluorobutyric acid, pentade...	424 C19H31F7O2	959261-23-5 94
3		Pentafluoropropionic acid, penta...	374 C18H31F5O2	959092-08-1 94
4		Trifluoroacetoxy hexadecane	338 C18H33F3O2	006222-03-3 94
5		Trifluoroacetic acid, pentadecyl...	324 C17H31F3O2	959010-23-2 94



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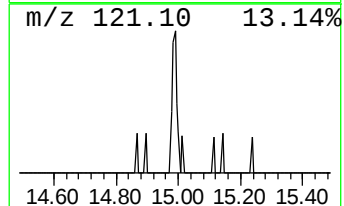
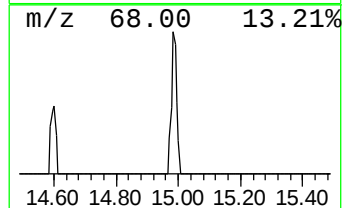
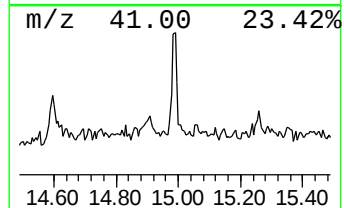
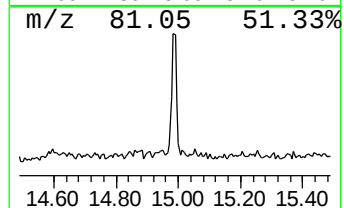
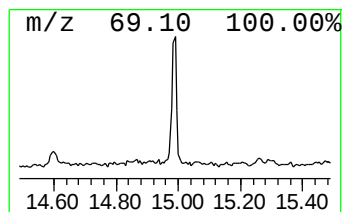
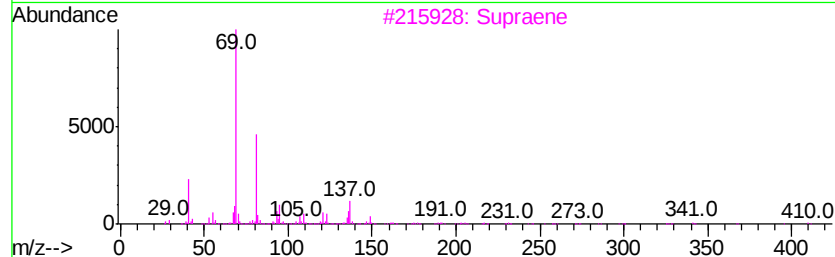
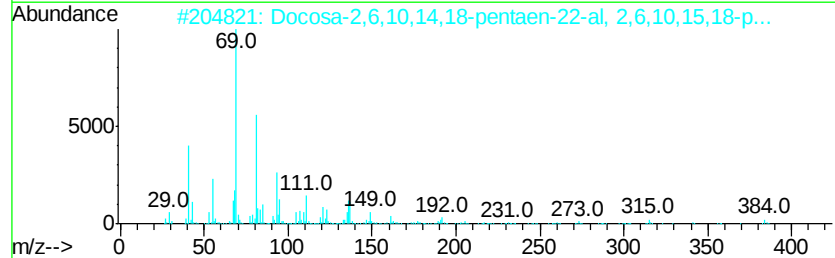
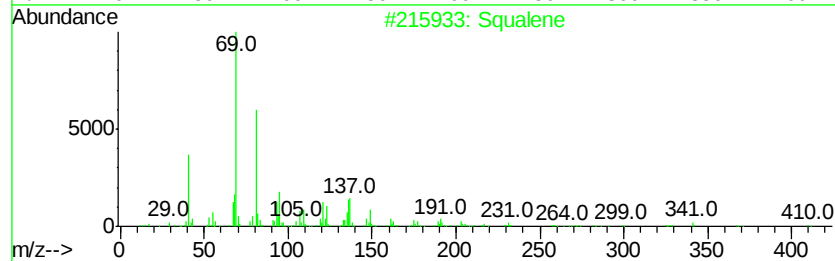
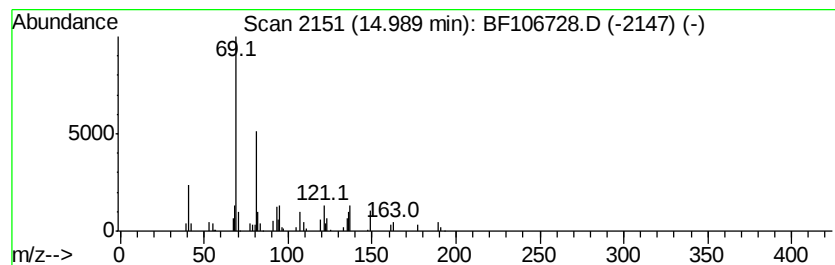
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Peak Number 6 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.99	2.66 ng	43504	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	86
2		Docosa-2,6,10,14,18-pentaen-22-a...	384	C27H44O	1000163-04-7	80
3		Supraene	410	C30H50	007683-64-9	64
4		2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	64
5		Hexadeca-2,6,10,14-tetraen-1-ol,...	290	C20H34O	007614-21-3	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.21	8.0	ng	118042	1	6.96	296603	20.0
unknown6.74	6.74	84.3	ng	1250000	1	6.96	296603	20.0
Pentadecane	10.88	2.1	ng	38476	4	11.49	358842	20.0
Behenic alcohol	13.95	6.6	ng	125358	5	14.14	378617	20.0
Squalene	14.99	2.7	ng	43504	6	15.67	326952	20.0