

Data Path : Z:\SVOASRV\HPCHEM1\BNA_F\DATA\BF092718\
Data File : BF109423.D
Acq On : 28 Sep 2018 9:38
Operator : JU/SJ
Sample : J5133-03
Misc :
ALS Vial : 44 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
092618-SIDI-F-D-S

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-BF092218.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	2.693	98	103	110	rVB	28074	44451	1.27%	0.229%
2	4.887	473	476	491	rBV	91655	101524	2.90%	0.523%
3	5.310	545	548	563	rVB	813723	808645	23.09%	4.163%
4	6.340	719	723	734	rBV2	652269	672939	19.22%	3.464%
5	6.475	742	746	749	rBV	1963191	1626241	46.45%	8.372%
6	6.704	782	785	789	rBV	802763	630753	18.01%	3.247%
7	6.863	808	812	815	rBV	2716509	2373367	67.78%	12.218%
8	7.269	876	881	884	rBV	2049349	1944214	55.53%	10.009%
9	7.987	999	1003	1017	rBV	964749	779303	22.26%	4.012%
10	9.063	1182	1186	1189	rBV	3761025	3501419	100.00%	18.026%
11	9.457	1249	1253	1263	rVB	225792	214533	6.13%	1.104%
12	9.734	1296	1300	1309	rBV	934193	837473	23.92%	4.311%
13	10.416	1413	1416	1420	rVB	48659	36214	1.03%	0.186%
14	10.522	1430	1434	1445	rBV	1192935	1157368	33.05%	5.958%
15	11.210	1548	1551	1555	rBV	786454	694699	19.84%	3.576%
16	12.798	1816	1821	1824	rBV	2464137	2351901	67.17%	12.108%
17	13.727	1973	1979	1994	rBV3	39015	128808	3.68%	0.663%
18	13.839	1994	1998	2004	rVB	687481	625960	17.88%	3.222%
19	14.474	2103	2106	2113	rBV2	50730	65602	1.87%	0.338%
20	14.592	2124	2126	2128	rVB	58942	47919	1.37%	0.247%
21	14.686	2138	2142	2147	rBV	170599	156943	4.48%	0.808%
22	15.239	2231	2236	2240	rBV	432259	495217	14.14%	2.549%
23	15.286	2240	2244	2249	rVB	33602	44318	1.27%	0.228%
24	15.680	2307	2311	2317	rBV2	25714	36675	1.05%	0.189%
25	16.368	2422	2428	2437	rBV5	23224	48234	1.38%	0.248%

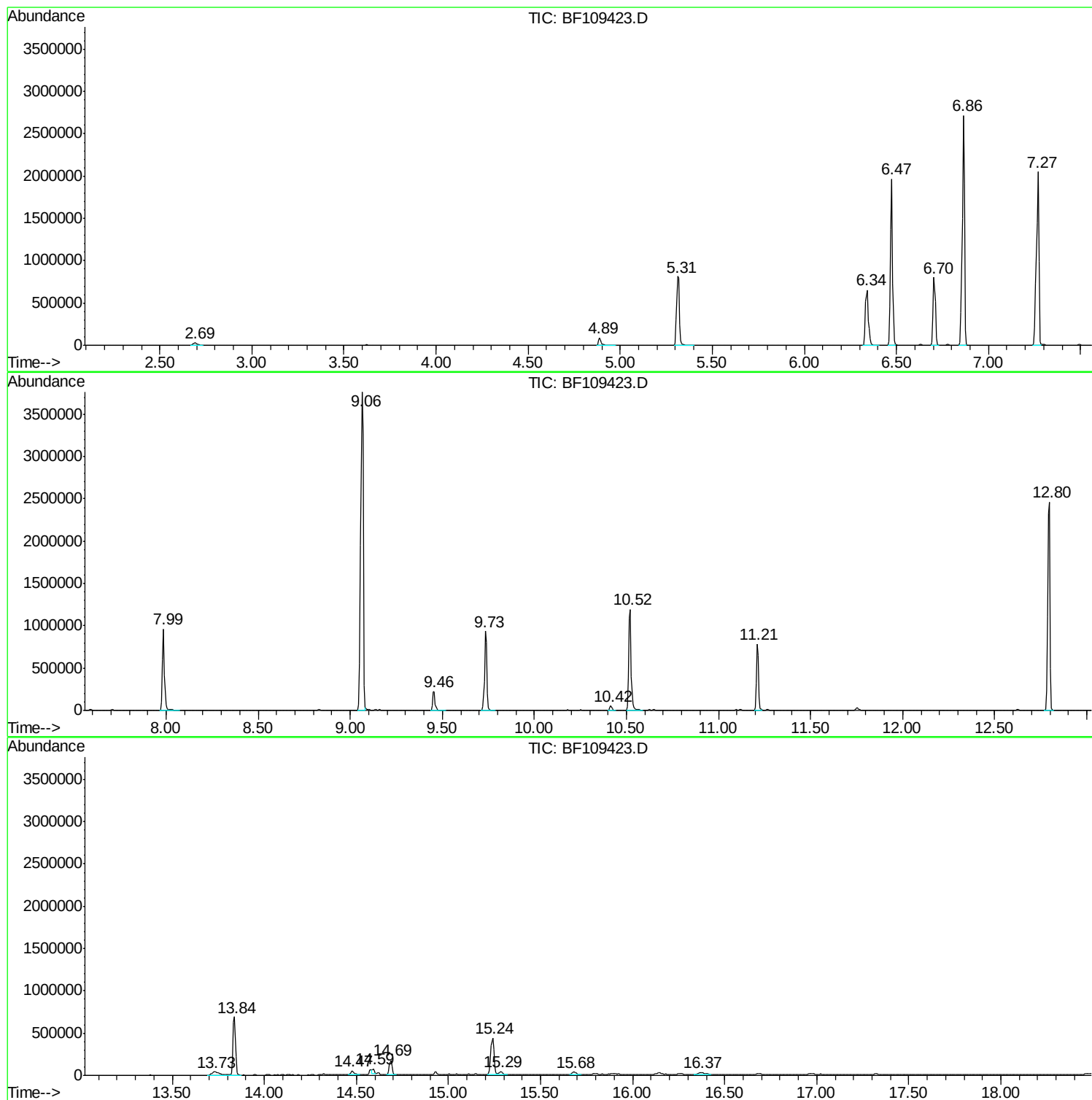
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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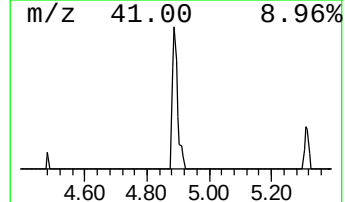
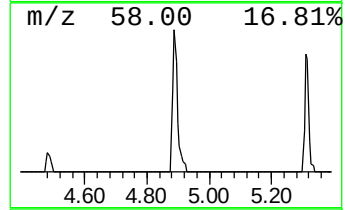
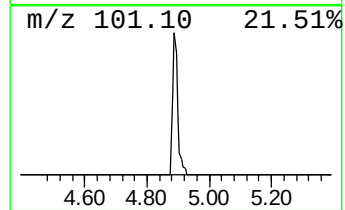
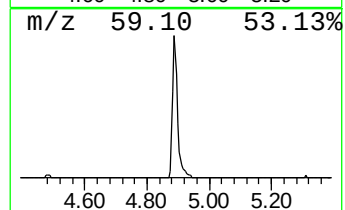
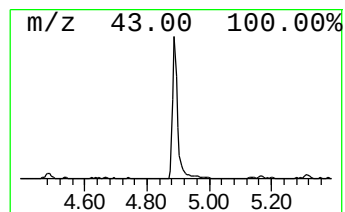
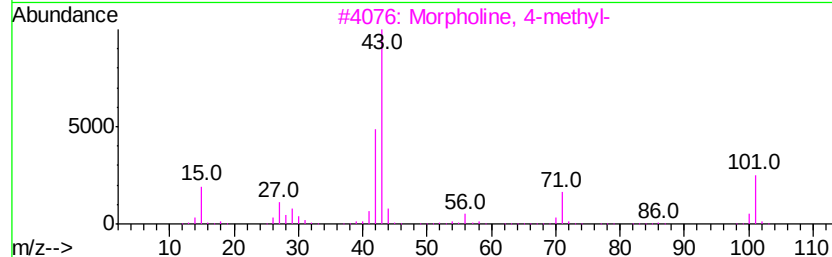
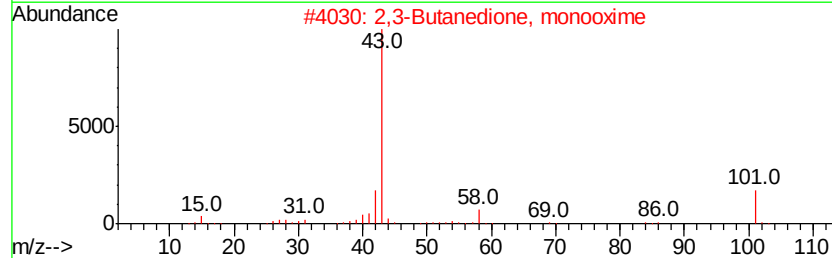
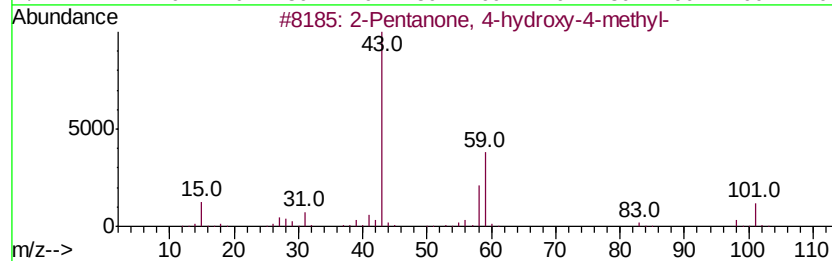
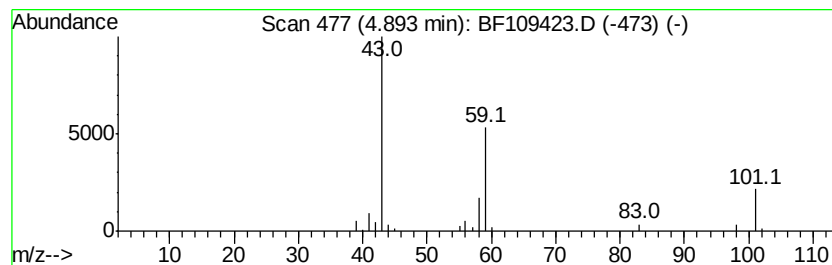
Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF092218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.89	3.22 ng	101524	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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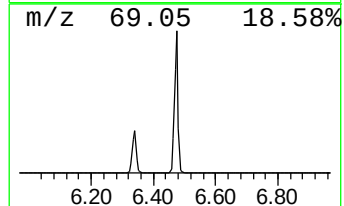
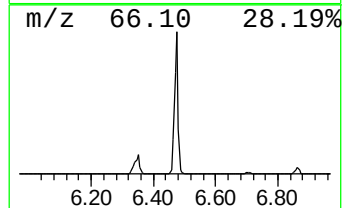
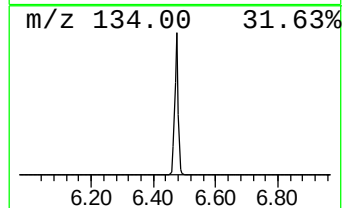
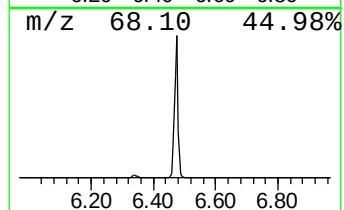
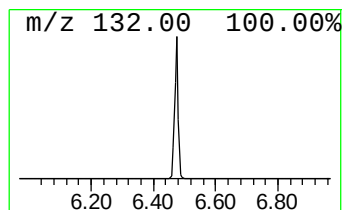
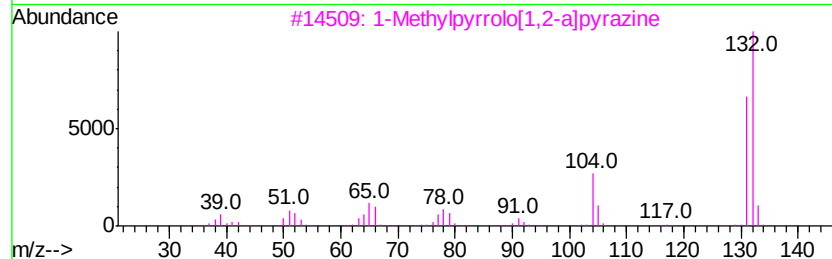
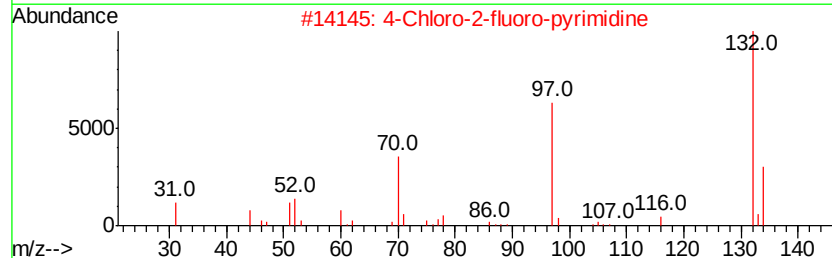
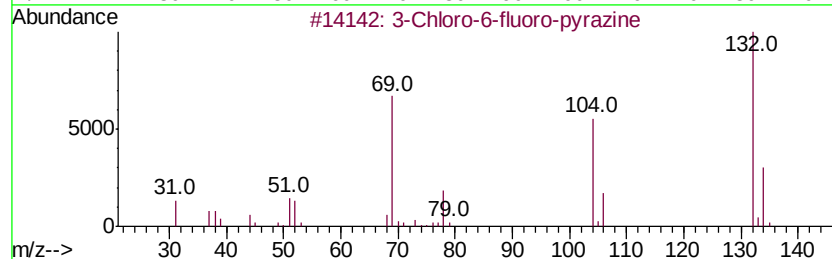
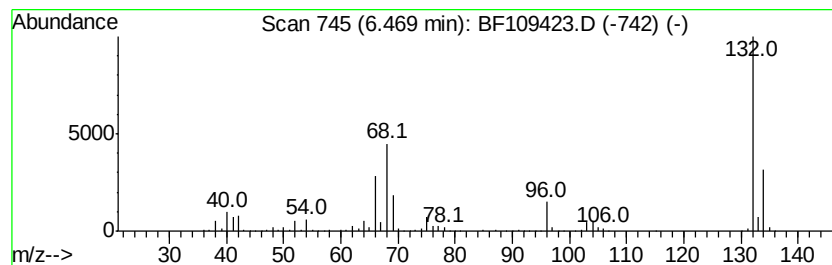
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.47 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	51.57 ng	1626240	1,4-Dichlorobenzene-d4	6.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
3		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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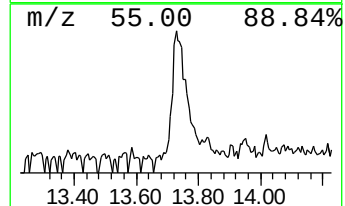
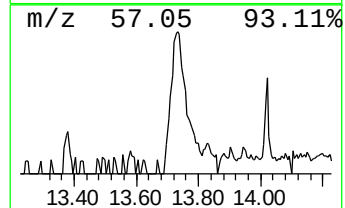
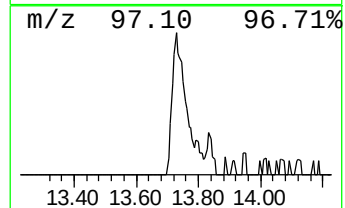
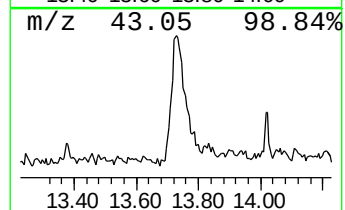
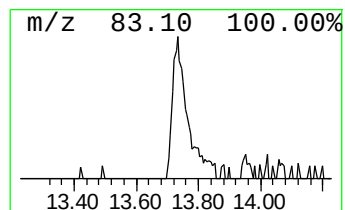
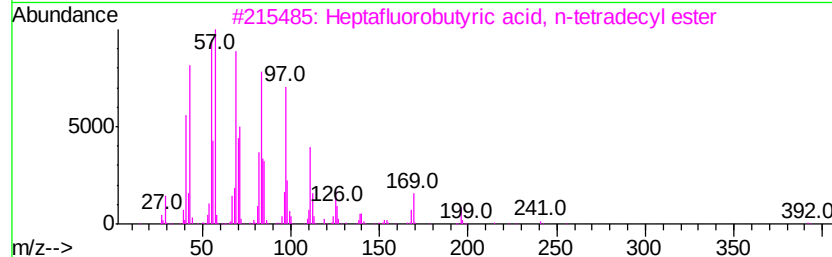
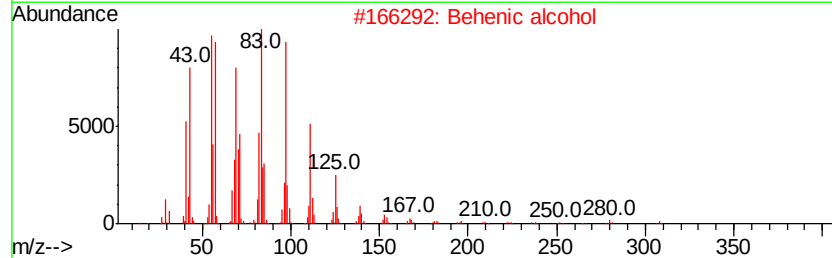
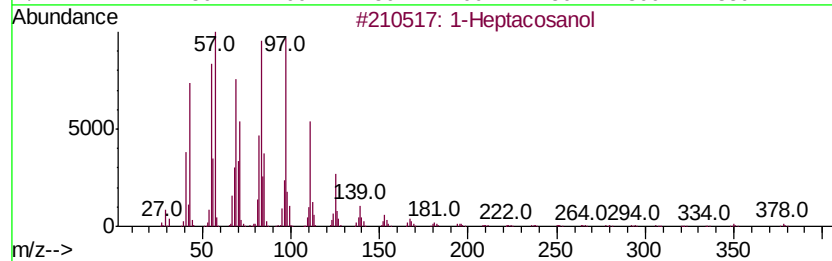
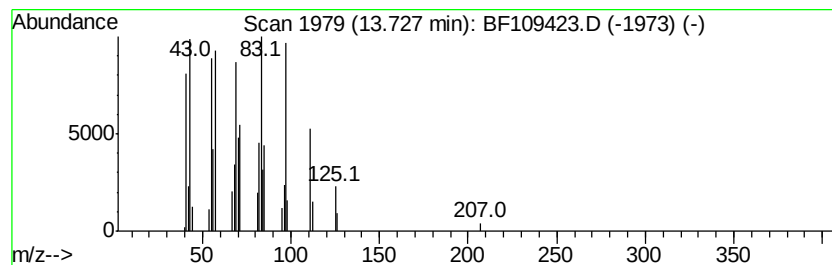
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ClientSampleId :
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Peak Number 4 1-Heptacosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	4.12 ng	128808	Chrysene-d12	13.84
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		1-Heptacosanol	396 C27H56O	002004-39-9 95
2		Behenic alcohol	326 C22H46O	000661-19-8 91
3		Heptafluorobutyric acid, n-tetra...	410 C18H29F7O2	007365-36-8 91
4		n-Tetracosanol-1	354 C24H50O	000506-51-4 91
5		Pentafluoropropionic acid, tetra...	360 C17H29F5O2	006222-06-6 90



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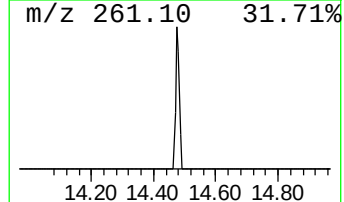
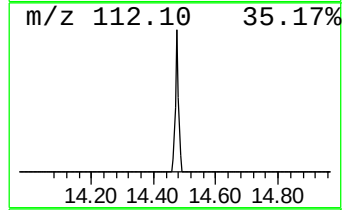
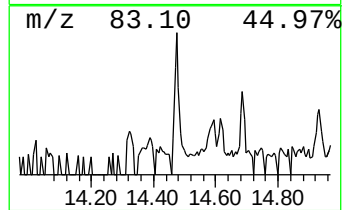
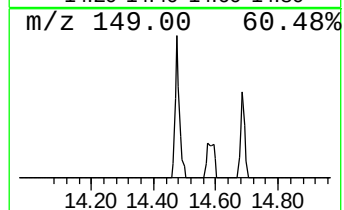
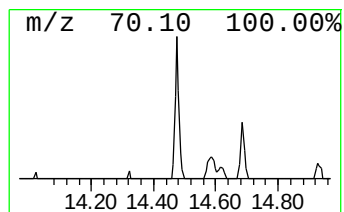
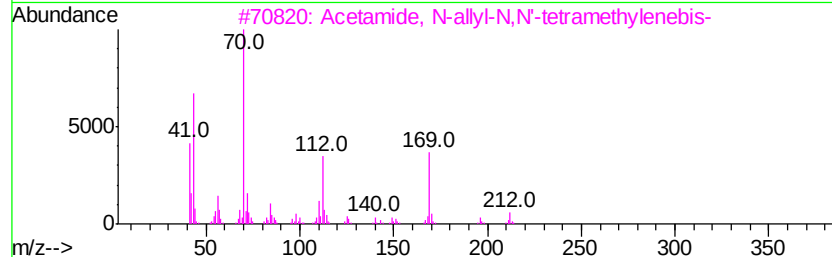
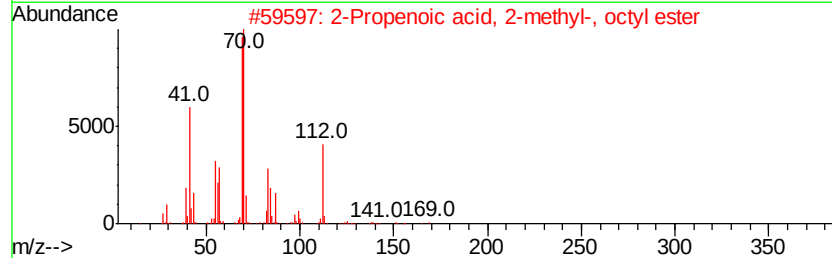
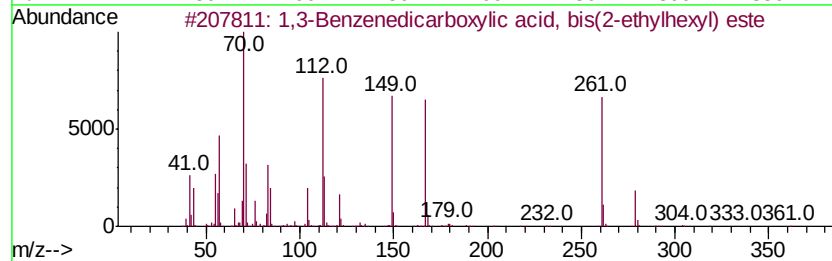
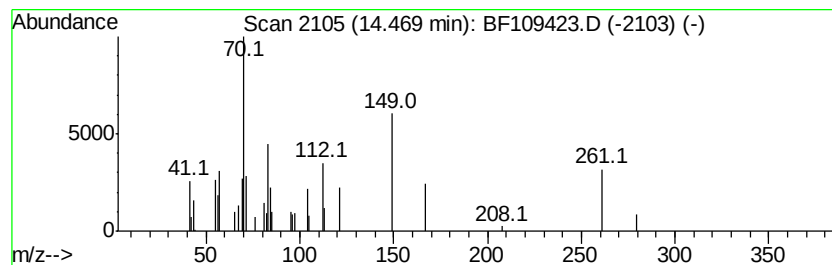
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 Peak Number 5 unknown14.47 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	2.10 ng	65602	Chrysene-d12	13.84

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Benzenedicarboxylic acid, bi...	390	C24H38O4	000137-89-3	38
2		2-Propenoic acid, 2-methyl-, oct...	198	C12H22O2	002157-01-9	32
3		Acetamide, N-allyl-N,N'-tetramet...	212	C11H20N2O2	020944-07-4	32
4		Carbonic acid, 2-chloroethyl 2-e...	236	C11H21ClO3	1000357-88-2	27
5		Bromoacetic acid, 2-ethylhexyl e...	250	C10H19BrO2	068144-73-0	27



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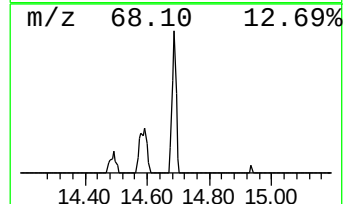
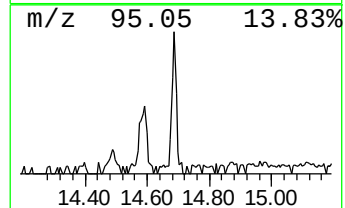
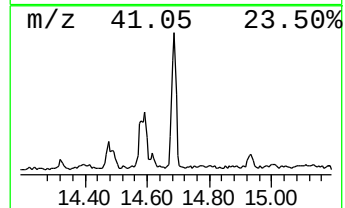
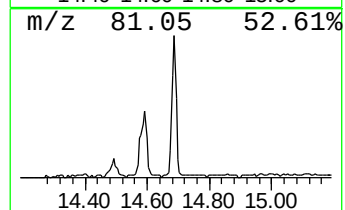
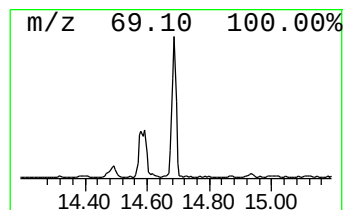
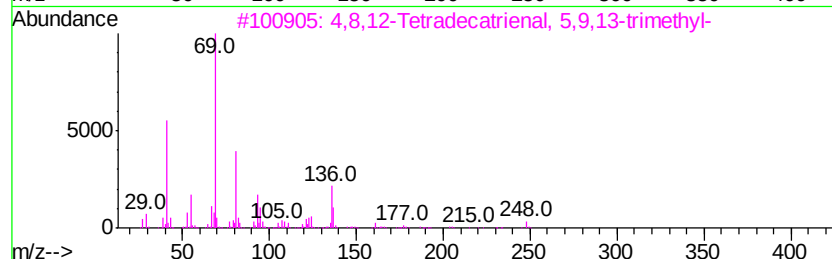
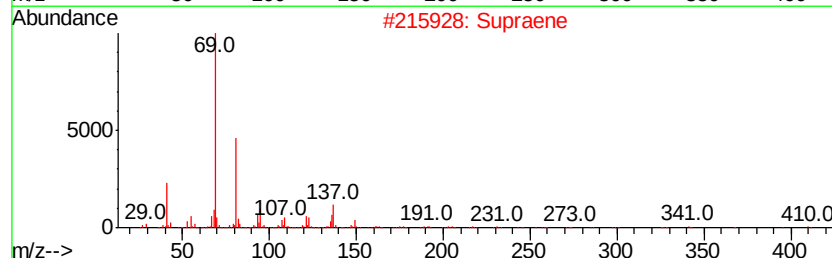
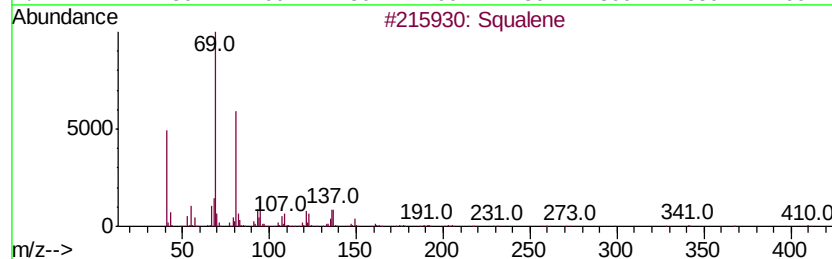
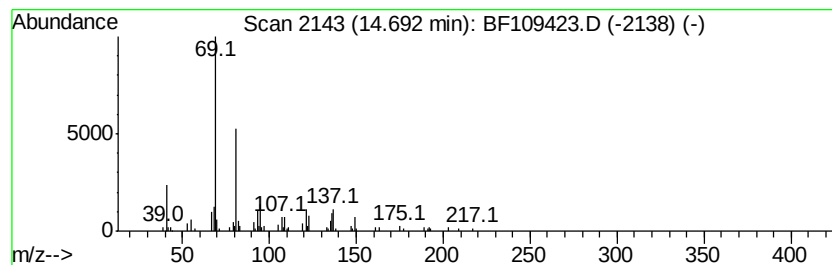
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Peak Number 6 Squalene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.69	6.34 ng	156943	Perylene-d12	15.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	91
2		Supraene	410	C30H50	007683-64-9	91
3		4,8,12-Tetradecatrienal, 5,9,13-...	248	C17H28O	066408-55-7	78
4		4-Methyl-1,5-Heptadiene	110	C8H14	000998-94-7	50
5		2,3,5-Trimethyl-2,3,5-hexanetric...	203	C12H17N3	003974-79-6	50



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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.89	3.2	ng	101524	1	6.70	630753	20.0
unknown6.47	6.47	51.6	ng	1626240	1	6.70	630753	20.0
1-Heptacosanol	13.73	4.1	ng	128808	5	13.84	625960	20.0
unknown14.47	14.47	2.1	ng	65602	5	13.84	625960	20.0
Squalene	14.69	6.3	ng	156943	6	15.24	495217	20.0