

Data Path : Z:\SVOASRV\HPCHEM1\BNA F\DATA\BF062818\
 Data File : BF106945.D
 Acq On : 29 Jun 2018 2:17
 Operator : JU/SJ
 Sample : J3593-01
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S39-9005

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	4.095	294	299	307	rBB	89685	108372	6.80%	0.849%
2	5.195	480	486	489	rBV	622935	679585	42.64%	5.325%
3	5.595	550	554	565	rBV	848563	741657	46.53%	5.812%
4	6.595	719	724	735	rBV	1343055	1447489	90.82%	11.343%
5	6.731	743	747	750	rBV	1387011	1189046	74.60%	9.318%
6	6.954	781	785	788	rBV	422471	330508	20.74%	2.590%
7	7.113	807	812	815	rBV	1383042	1325197	83.15%	10.385%
8	7.519	876	881	884	rBV	1058191	996524	62.52%	7.809%
9	8.236	999	1003	1023	rBB	400758	369865	23.21%	2.898%
10	9.307	1181	1185	1188	rBV	1792535	1562584	98.04%	12.245%
11	9.701	1248	1252	1258	rBV	172182	151681	9.52%	1.189%
12	9.995	1298	1302	1312	rVB	354149	331744	20.81%	2.600%
13	10.401	1368	1371	1374	rVB	31086	23407	1.47%	0.183%
14	10.783	1433	1436	1444	rBV	281843	271809	17.05%	2.130%
15	10.877	1444	1452	1457	rVV2	25112	33344	2.09%	0.261%
16	11.483	1552	1555	1563	rVB	331843	330043	20.71%	2.586%
17	12.936	1794	1802	1807	rBV5	19220	47230	2.96%	0.370%
18	13.071	1820	1825	1828	rBV	1729339	1593803	100.00%	12.489%
19	13.401	1878	1881	1886	rBV3	18627	25648	1.61%	0.201%
20	13.589	1910	1913	1915	rBV	22067	20541	1.29%	0.161%
21	13.948	1971	1974	1977	rBV	89800	82245	5.16%	0.644%
22	14.054	1990	1992	1996	rBV3	22937	31691	1.99%	0.248%
23	14.089	1996	1998	2002	rVB	42044	38551	2.42%	0.302%
24	14.136	2002	2006	2009	rBV	541862	496510	31.15%	3.891%
25	14.977	2146	2149	2152	rBV	66392	69202	4.34%	0.542%
26	15.671	2262	2267	2275	rVB	326275	462868	29.04%	3.627%

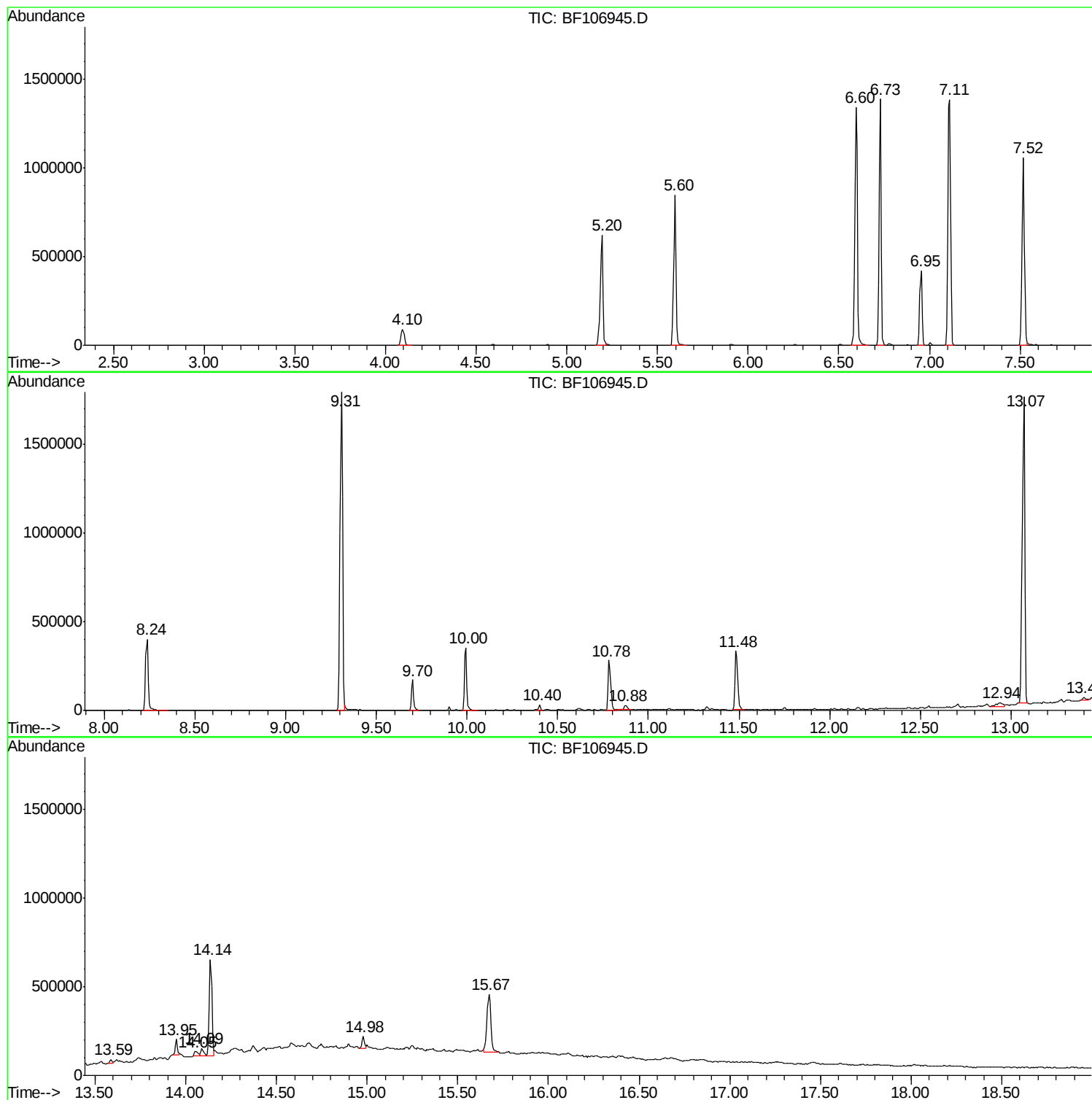
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Quant Method : Z:\SVOASRV\HPCHEM1\BNA F\METHODS\8270-BF061918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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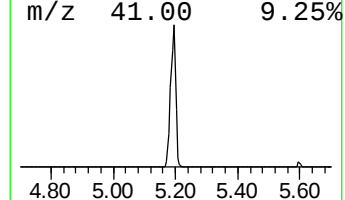
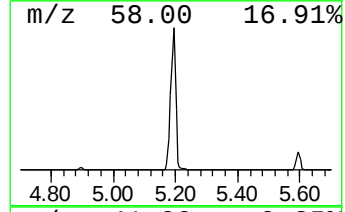
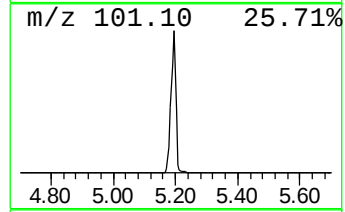
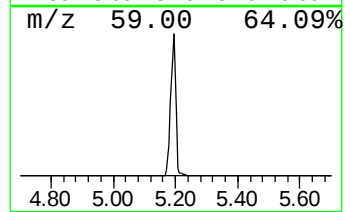
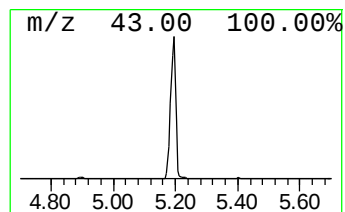
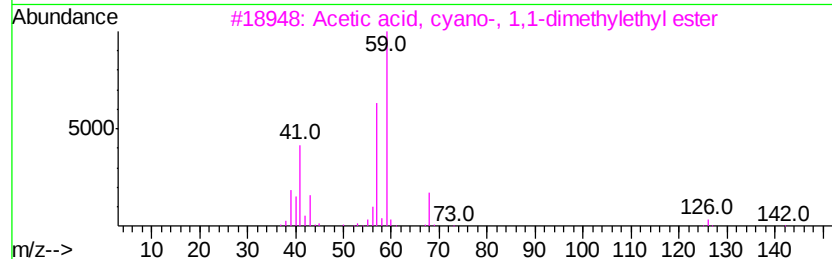
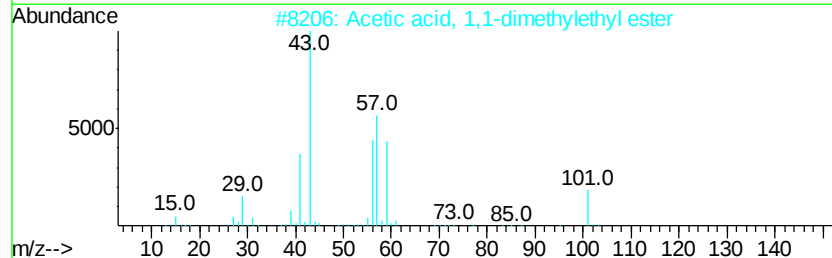
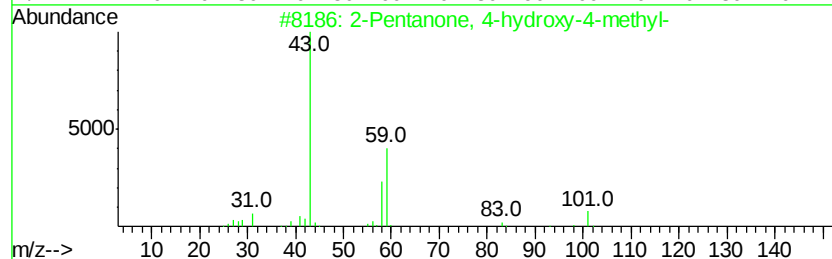
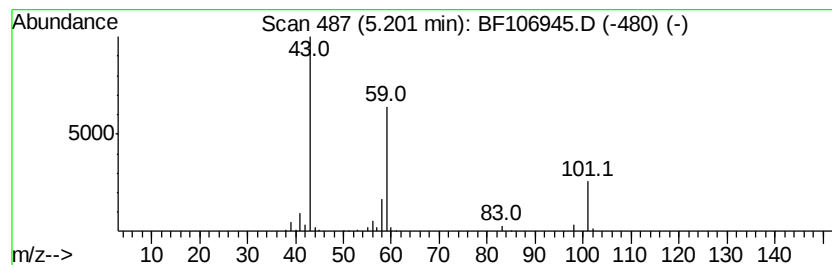
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.20	41.12 ng	679585	1,4-Dichlorobenzene-d4	6.95

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, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
4			Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5			5-Hexen-2-one	98	C6H10O	000109-49-9	9



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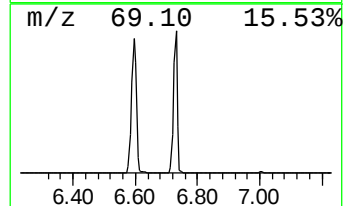
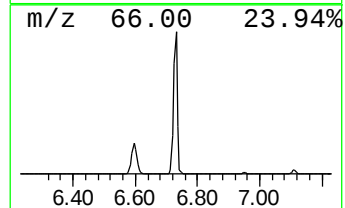
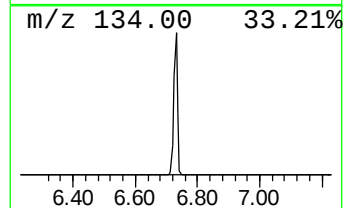
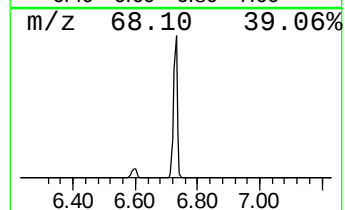
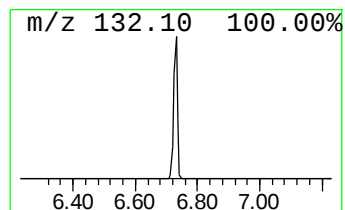
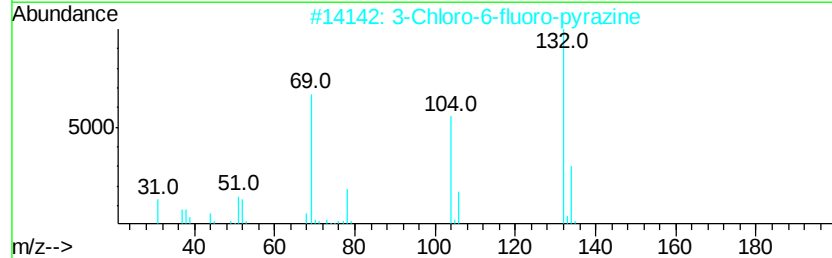
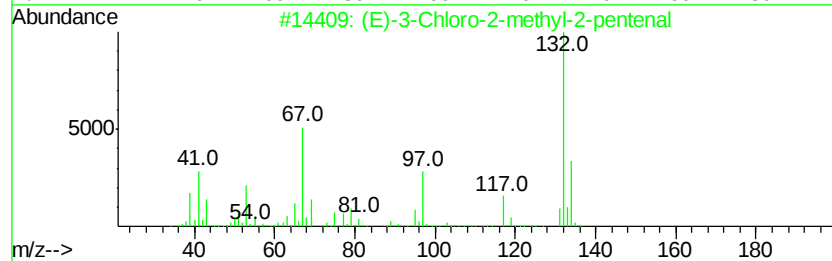
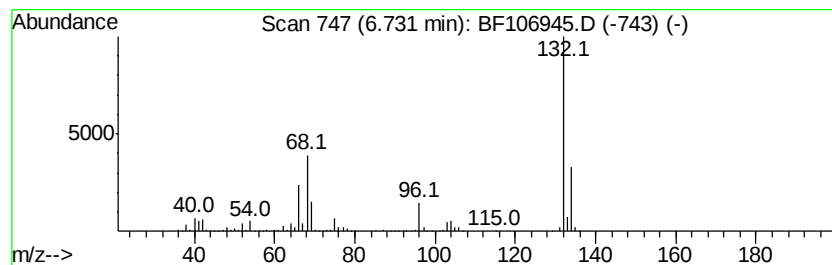
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 3 unknown6.73 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.73	71.95 ng	1189050	1,4-Dichlorobenzene-d4	6.95

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
3		Tranvlcypropine-propionyl	189	C12H15NO	1000123-86-3	10
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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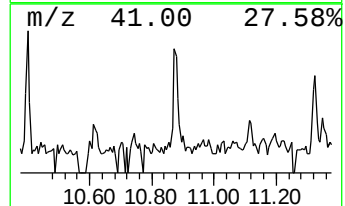
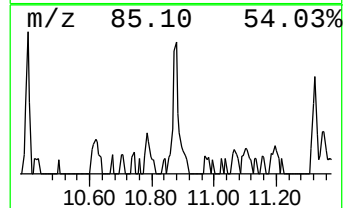
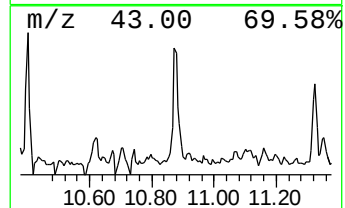
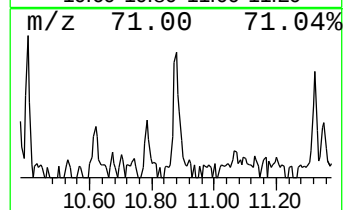
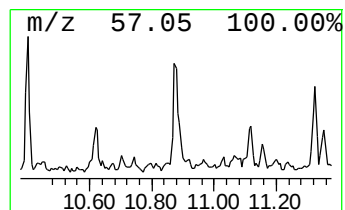
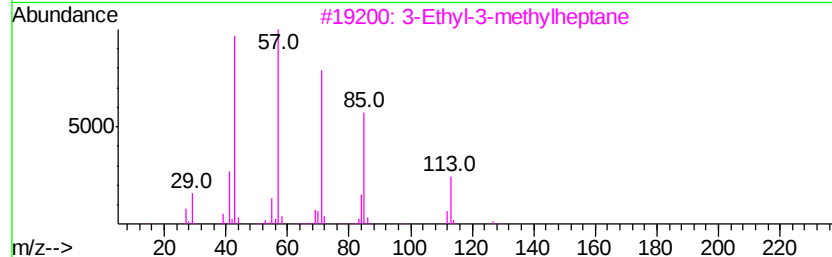
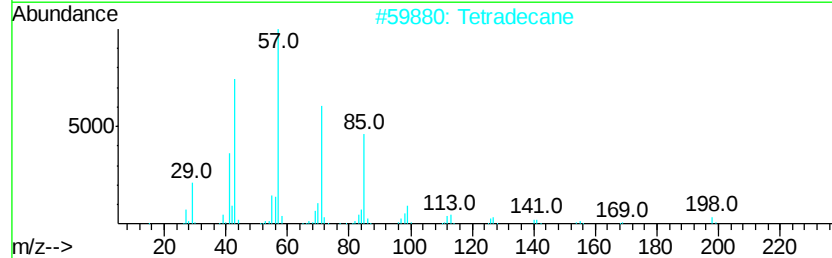
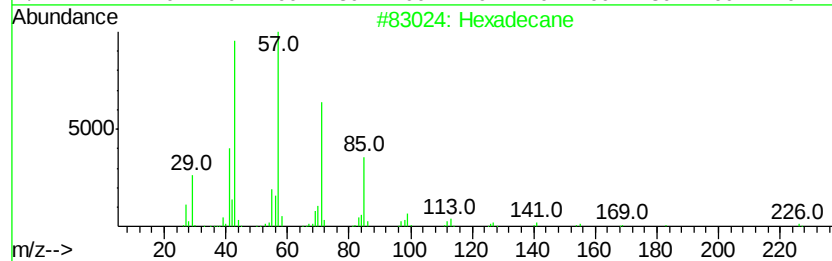
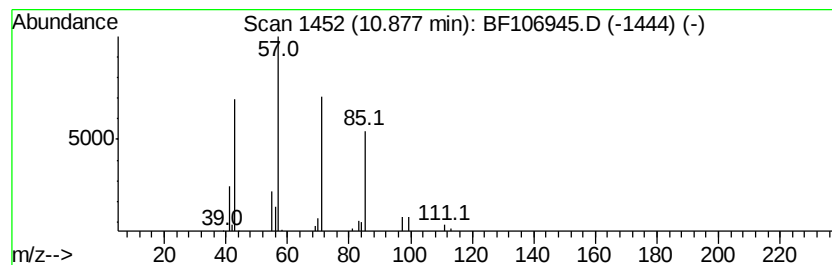
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Peak Number 5 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.88	2.02 ng	33344	Phenanthrene-d10	11.48

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	72
2	Tetradecane		198	C14H30	000629-59-4	72
3	3-Ethyl-3-methylheptane		142	C10H22	017302-01-1	59
4	Sulfurous acid, 2-ethylhexyl hex...		278	C14H30O3S	1000309-20-2	59
5	Sulfurous acid, hexyl pentyl ester		236	C11H24O3S	1000309-14-1	53



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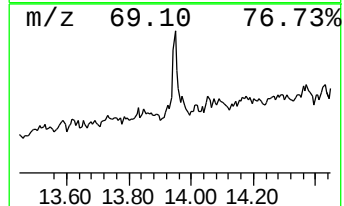
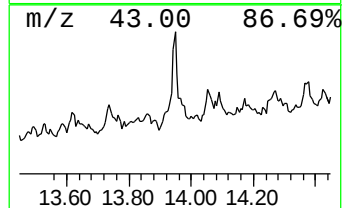
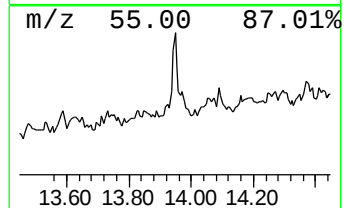
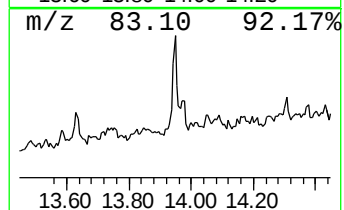
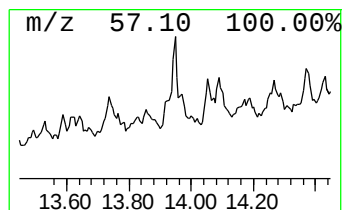
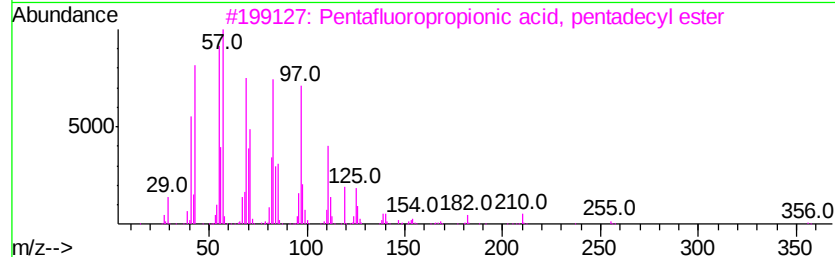
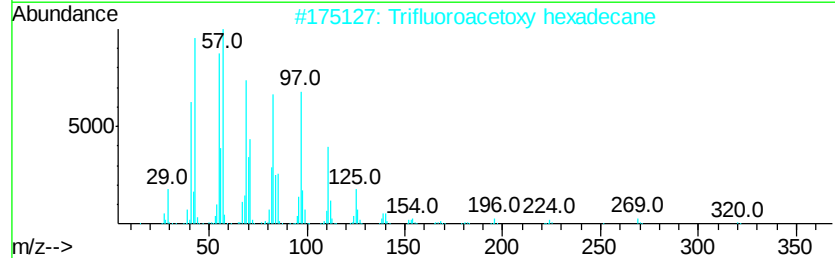
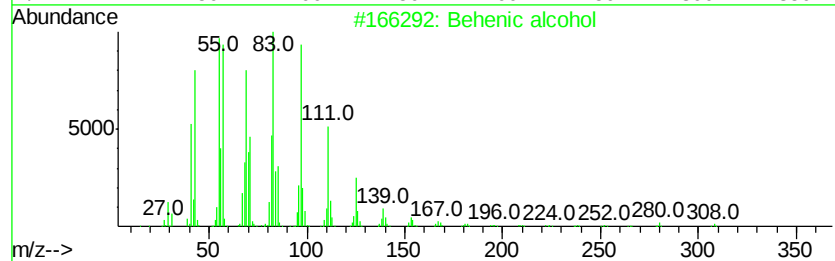
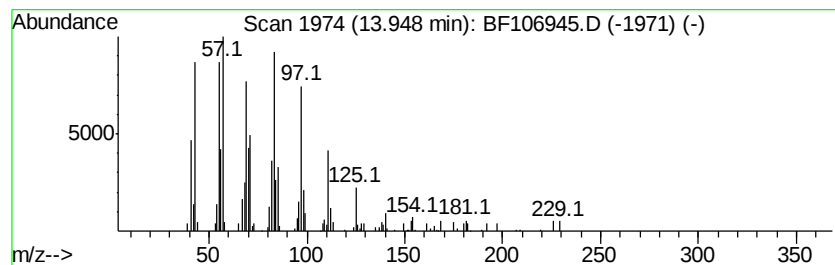
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Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.95	3.31 ng	82245	Chrysene-d12	14.14

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	94
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94
3		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
4		3-Chloropropionic acid, heptadec...	346	C20H39ClO2	1000283-05-1	91
5		1-Heneicosanol	312	C21H44O	015594-90-8	91



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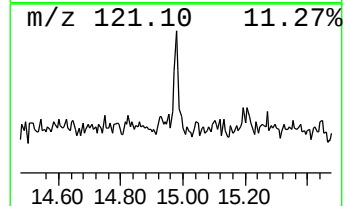
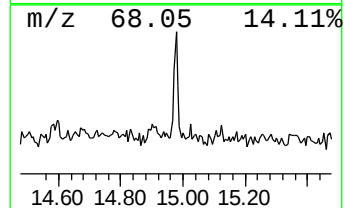
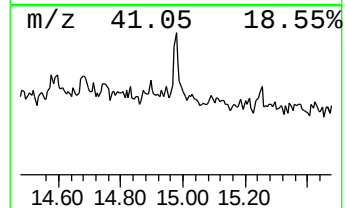
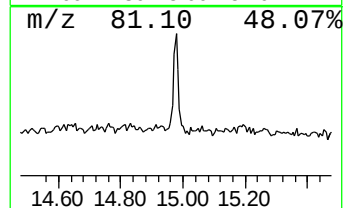
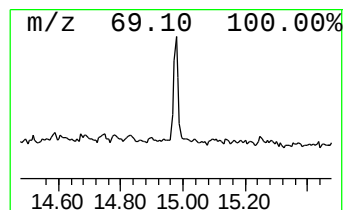
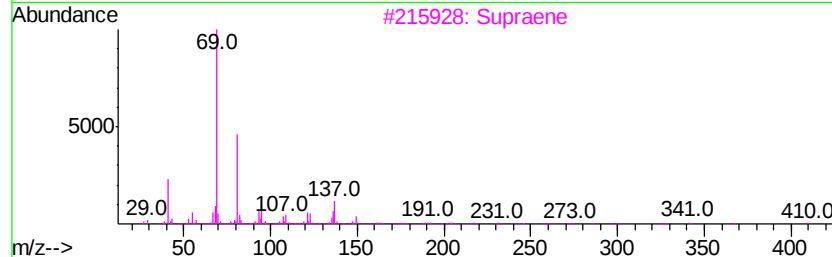
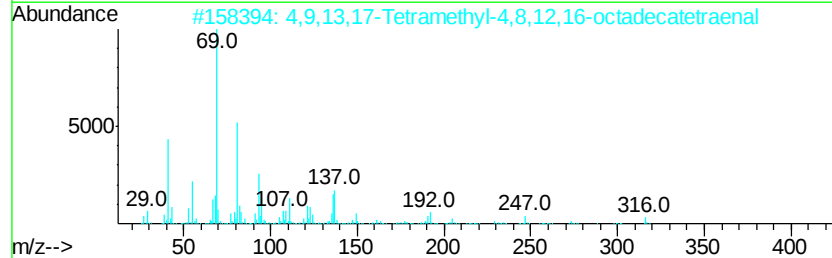
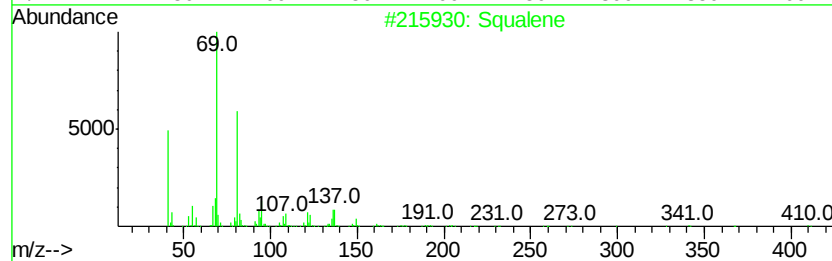
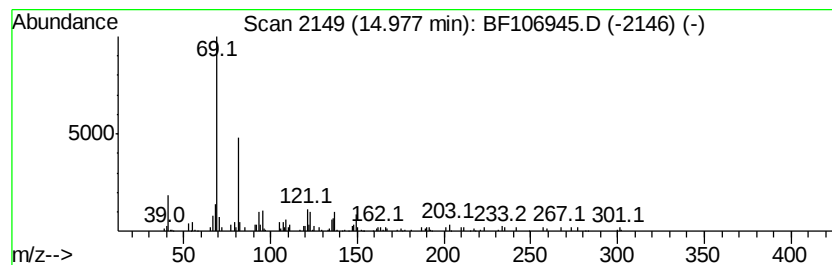
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 7 Squalene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.98	2.99 ng	69202	Perylene-d12	15.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	87
2		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	72
3		Supraene	410	C30H50	007683-64-9	72
4		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
5		2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.20	41.1	ng	679585	1	6.95	330508	20.0
unknown6.73	6.73	72.0	ng	1189050	1	6.95	330508	20.0
Hexadecane	10.88	2.0	ng	33344	4	11.48	330043	20.0
Behenic alcohol	13.95	3.3	ng	82245	5	14.14	496510	20.0
Squalene	14.98	3.0	ng	69202	6	15.67	462868	20.0