

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
 Data File : BF096393.D
 Acq On : 1 Jul 2017 21:56
 Operator : SJ/MA
 Sample : I3980-10
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-D-COMP

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:\HPCHEM1\BNA_F\METHODS\8270-BF070117.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	4.928	478	483	493	rVB	426829	527212	16.46%	2.022%
2	5.351	549	555	558	rBV	2944741	3203438	100.00%	12.283%
3	6.369	723	728	731	rBV	3064143	3113628	97.20%	11.939%
4	6.504	746	751	754	rBV	3011976	2880590	89.92%	11.045%
5	6.734	786	790	793	rBV	945304	752227	23.48%	2.884%
6	6.892	812	817	820	rBV	2607338	2293030	71.58%	8.792%
7	7.292	880	885	888	rBV	2188226	1965021	61.34%	7.535%
8	8.016	1004	1008	1011	rBV	1212685	1043404	32.57%	4.001%
9	9.092	1186	1191	1194	rBV	3038024	2734628	85.37%	10.485%
10	9.480	1254	1257	1260	rBV	325107	237455	7.41%	0.910%
11	9.710	1293	1296	1300	rVB	41636	34676	1.08%	0.133%
12	9.763	1301	1305	1309	rBV	989059	859756	26.84%	3.297%
13	10.210	1378	1381	1384	rVB	49769	41714	1.30%	0.160%
14	10.545	1434	1438	1442	rBV	1309382	1272148	39.71%	4.878%
15	10.680	1458	1461	1466	rBV	49921	46876	1.46%	0.180%
16	11.245	1553	1557	1560	rVB	733678	666057	20.79%	2.554%
17	11.780	1644	1648	1655	rBV	166133	152152	4.75%	0.583%
18	12.563	1778	1781	1785	rBV3	45930	41095	1.28%	0.158%
19	12.827	1822	1826	1830	rBV	2290451	2203781	68.79%	8.450%
20	13.727	1976	1979	1987	rBV3	150693	208669	6.51%	0.800%
21	13.868	1999	2003	2007	rBV	932813	887901	27.72%	3.405%
22	14.057	2032	2035	2039	rBV	61037	63364	1.98%	0.243%
23	14.362	2084	2087	2091	rVB	58751	51034	1.59%	0.196%
24	14.657	2135	2137	2141	rVB2	37614	36548	1.14%	0.140%
25	14.727	2146	2149	2154	rVB	209879	183865	5.74%	0.705%
26	15.280	2239	2243	2248	rVB	494275	579845	18.10%	2.223%

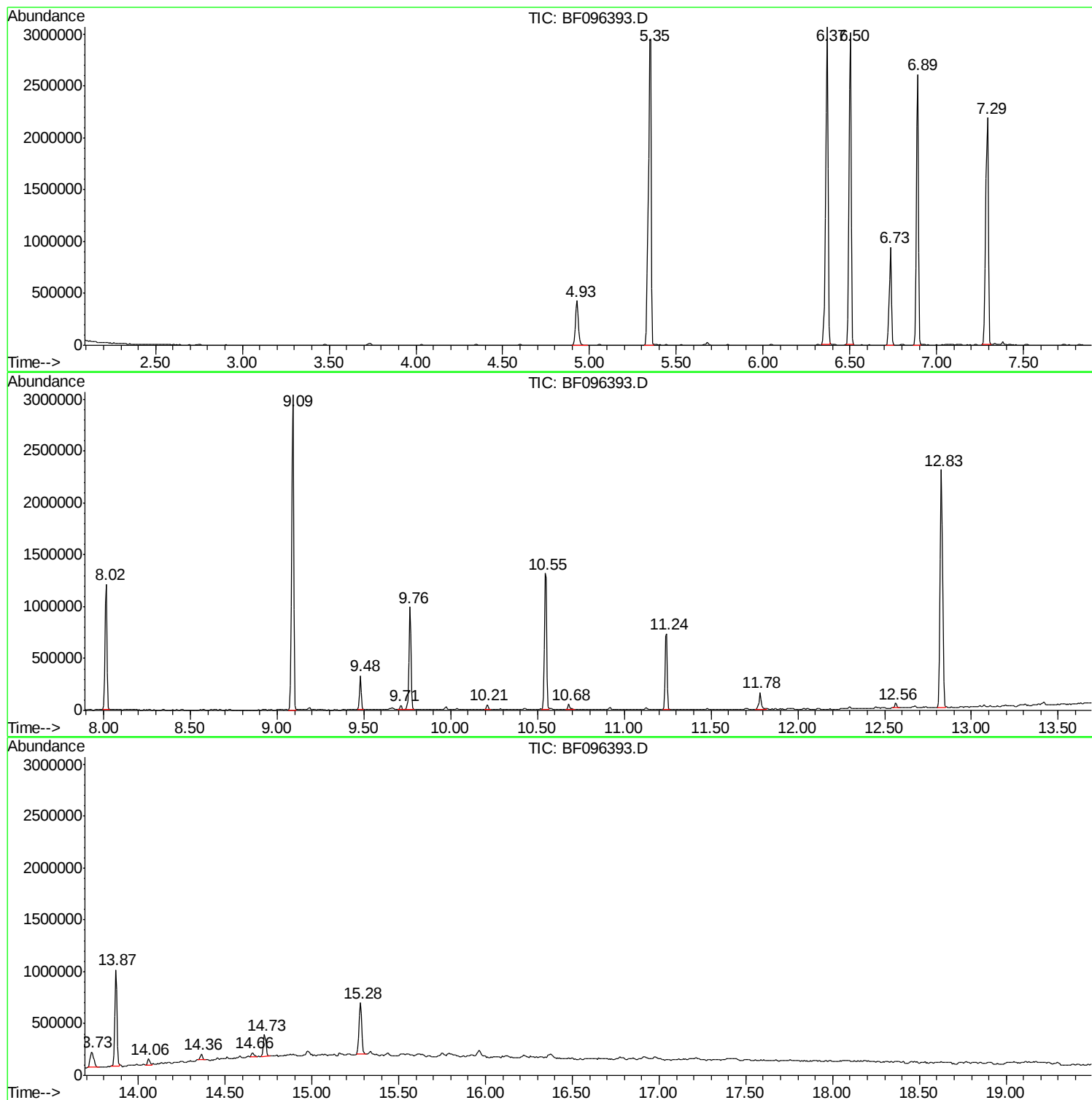
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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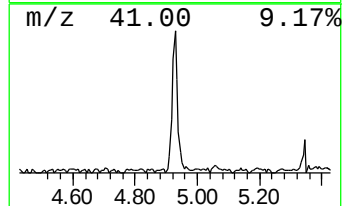
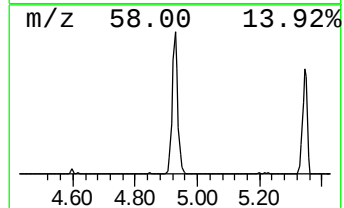
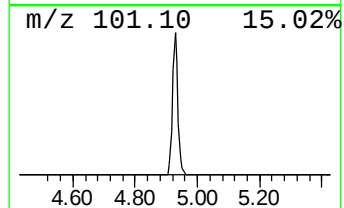
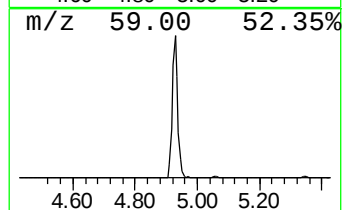
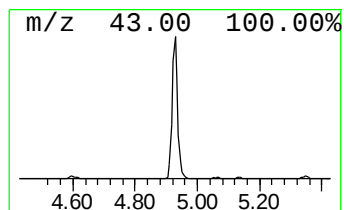
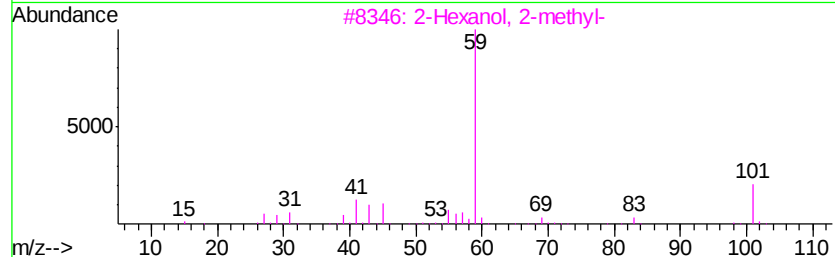
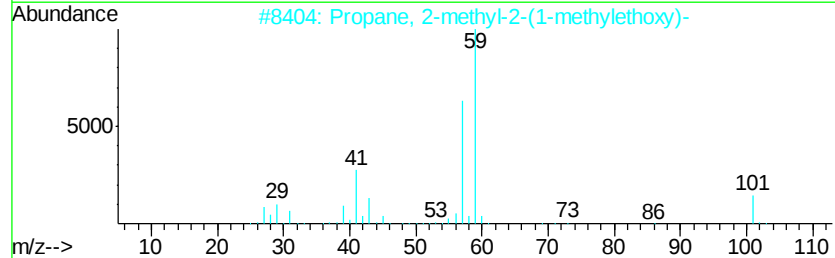
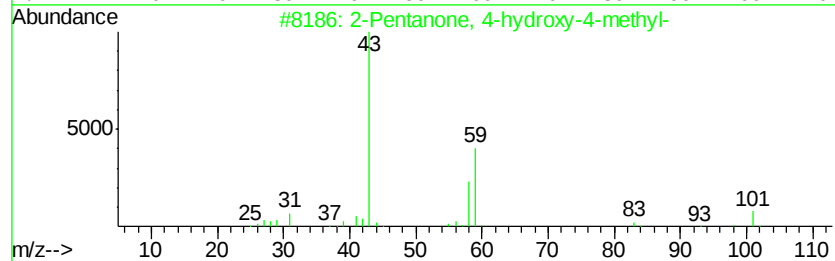
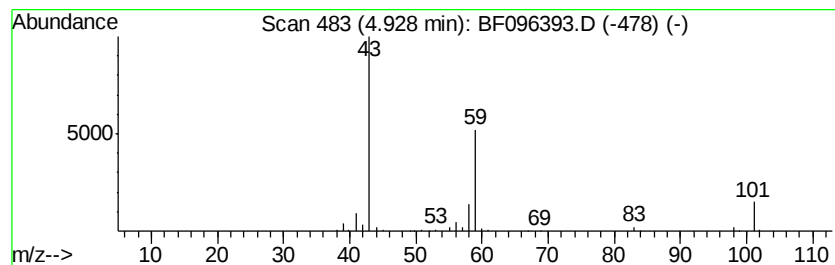
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.93	14.02 ng	527212	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
4			1,2-Butanediol	90	C4H10O2	000584-03-2	9
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9



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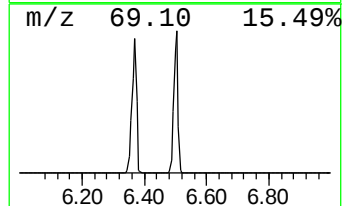
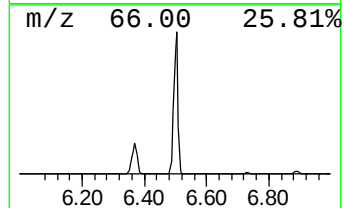
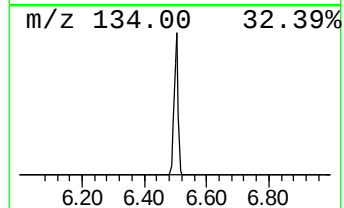
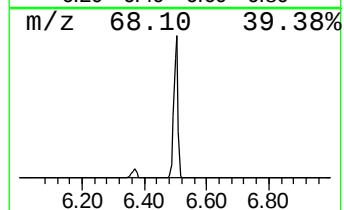
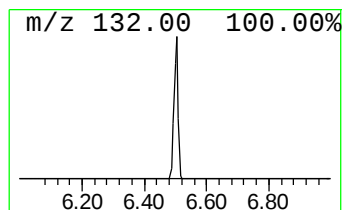
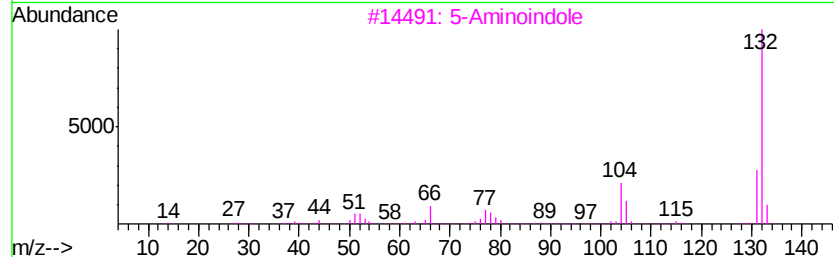
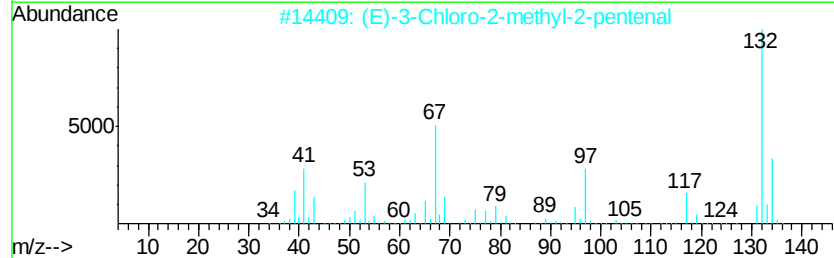
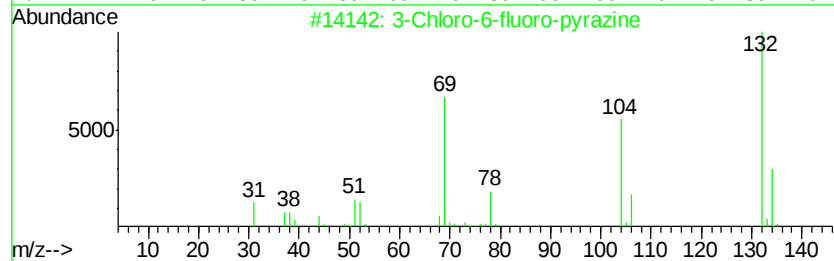
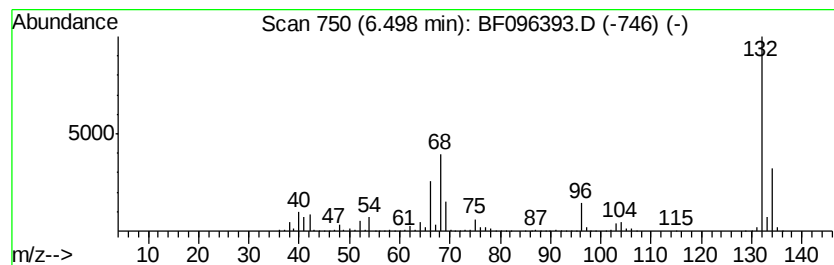
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	76.59 ng	2880590	1,4-Dichlorobenzene-d4	6.73

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		1-Aminoindan	133	C9H11N	034698-41-4	9



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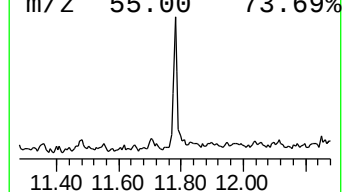
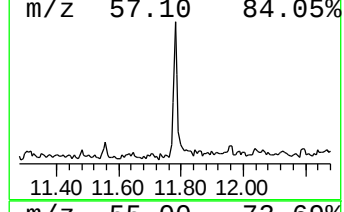
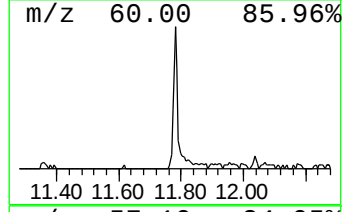
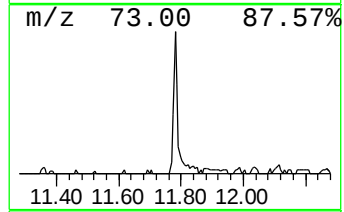
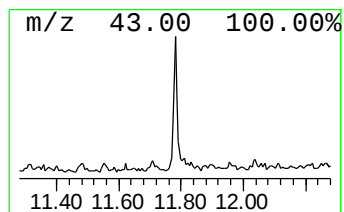
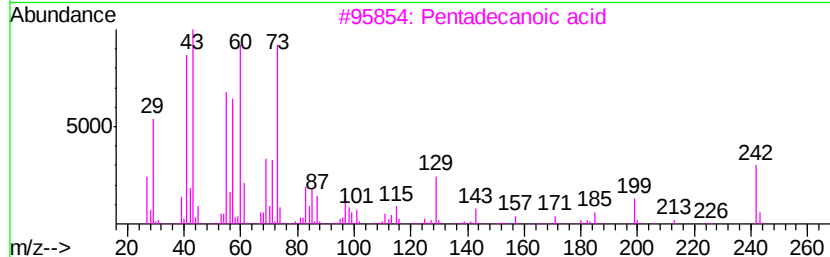
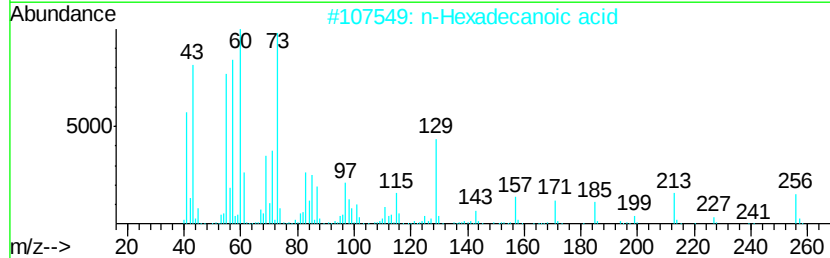
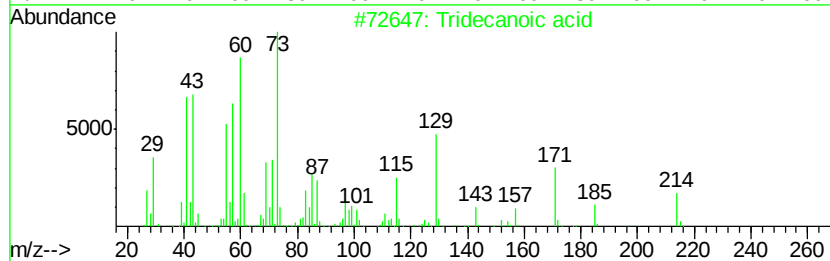
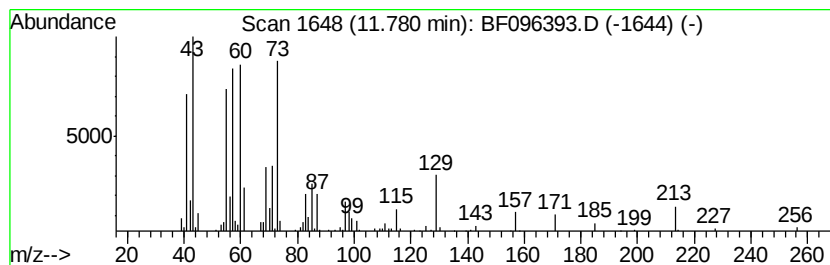
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Peak Number 4 Tridecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.78	4.57 ng	152152	Phenanthrene-d10	11.24	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Tridecanoic acid	214	C13H26O2	000638-53-9	96
2	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tetradecanoic acid	228	C14H28O2	000544-63-8	59
5	n-Decanoic acid	172	C10H20O2	000334-48-5	47



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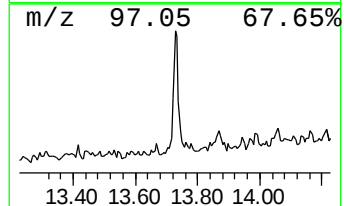
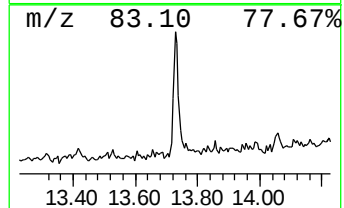
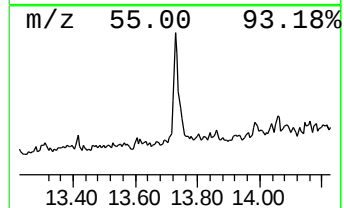
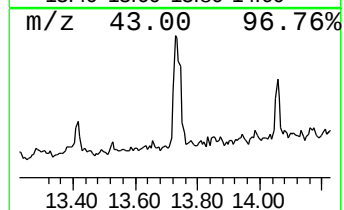
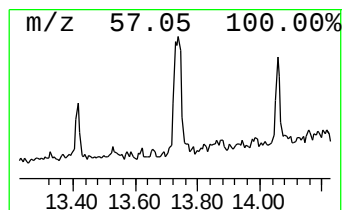
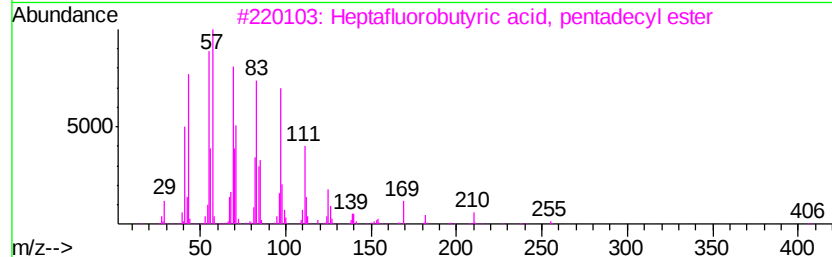
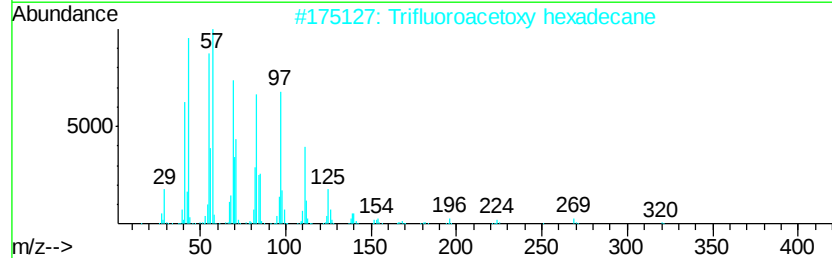
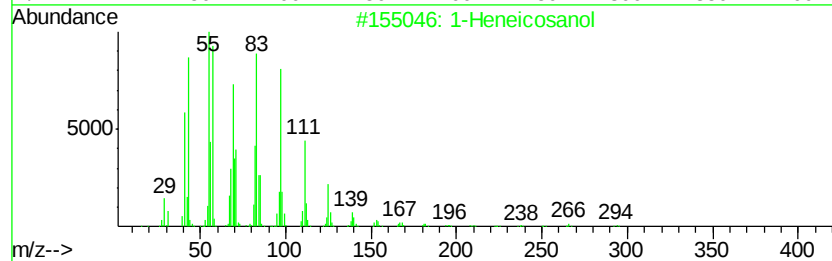
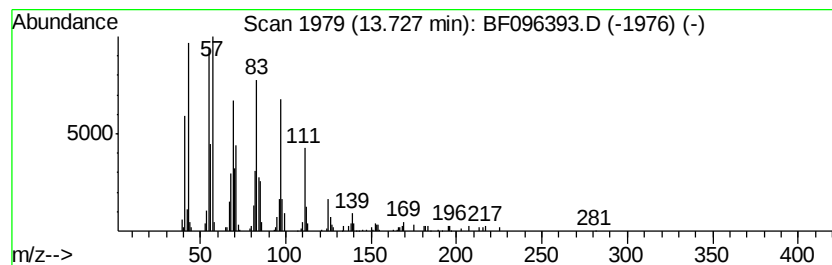
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Peak Number 5 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.		
13.73	4.70 ng	208669	Chrysene-d12	13.87		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Heneicosanol	312	C21H44O	015594-90-8	95
2		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5		Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	94



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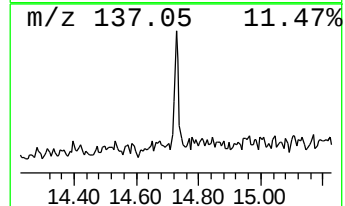
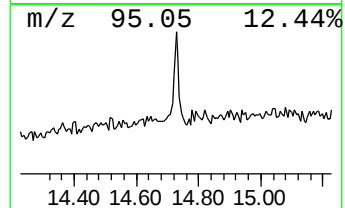
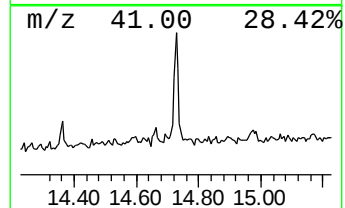
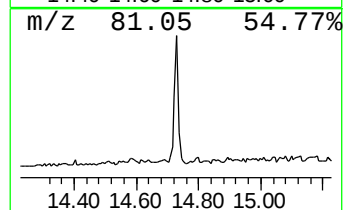
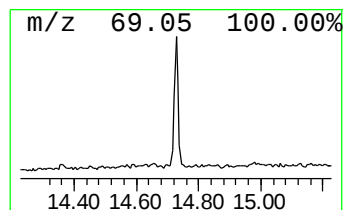
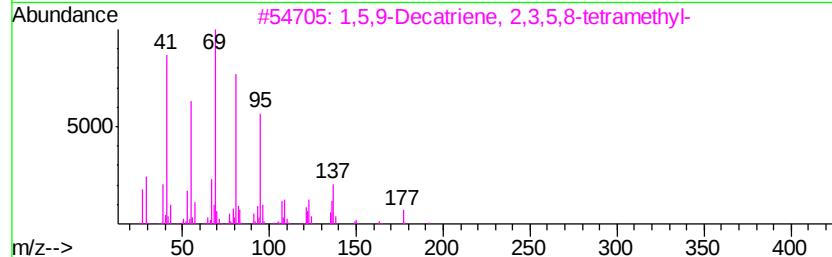
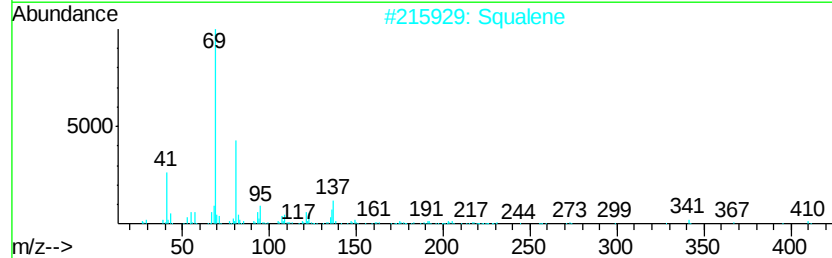
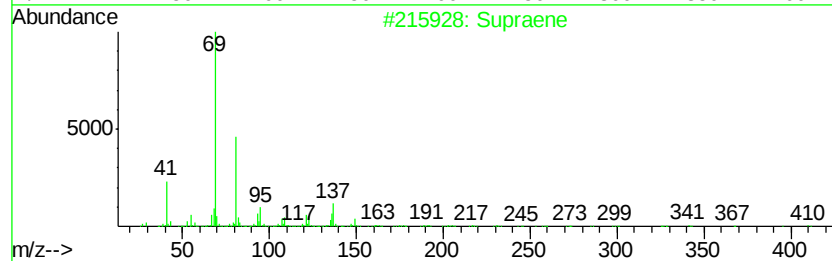
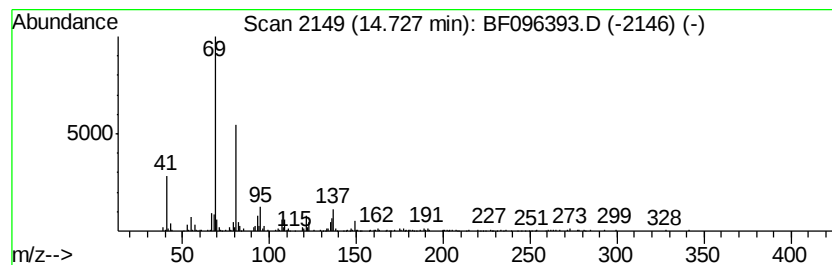
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Supraene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.73	6.34 ng	183865	Perylene-d12	15.28

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Supraene		410	C30H50	007683-64-9	91
2	Squalene		410	C30H50	000111-02-4	90
3	1,5,9-Decatriene, 2,3,5,8-tetram...		192	C14H24	230646-72-7	64
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...		264	C17H28O2	004128-17-0	64
5	2,6-Octadiene, 2,6-dimethyl-		138	C10H18	002792-39-4	58



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	14.0	ng	527212	1	6.73	752227	20.0
unknown6.50	6.50	76.6	ng	2880590	1	6.73	752227	20.0
Tridecanoic acid	11.78	4.6	ng	152152	4	11.24	666057	20.0
1-Heneicosanol	13.73	4.7	ng	208669	5	13.87	887901	20.0
Supraene	14.73	6.3	ng	183865	6	15.28	579845	20.0