

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
 Data File : BF096394.D
 Acq On : 1 Jul 2017 22:24
 Operator : SJ/MA
 Sample : I3982-14
 Misc :
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 163-72-11929-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	492	rVB	434467	540678	17.12%	2.044%
2	5.351	549	555	558	rBV	2780674	2949026	93.36%	11.149%
3	6.328	715	721	723	rBV	31118	37839	1.20%	0.143%
4	6.369	723	728	731	rBV	3085807	3158816	100.00%	11.942%
5	6.504	746	751	754	rBV	3037924	2836632	89.80%	10.724%
6	6.734	786	790	793	rBV	1089731	863820	27.35%	3.266%
7	6.804	799	802	809	rVB	65012	55497	1.76%	0.210%
8	6.893	812	817	820	rVV	2657002	2394707	75.81%	9.053%
9	7.292	880	885	888	rBV	1831187	1653399	52.34%	6.251%
10	7.387	897	901	906	rVB	41514	45325	1.43%	0.171%
11	8.016	1004	1008	1011	rBV	1040128	923981	29.25%	3.493%
12	9.092	1186	1191	1194	rBV	2802419	2524753	79.93%	9.545%
13	9.486	1253	1258	1261	rBV	1195515	1026900	32.51%	3.882%
14	9.710	1293	1296	1299	rVB	45447	39805	1.26%	0.150%
15	9.763	1301	1305	1309	rVV	905529	803335	25.43%	3.037%
16	10.210	1378	1381	1384	rVB	69644	55782	1.77%	0.211%
17	10.551	1434	1439	1442	rBV	1317170	1278535	40.48%	4.833%
18	10.681	1458	1461	1470	rBV	69667	79580	2.52%	0.301%
19	11.128	1534	1537	1540	rBV2	38819	38237	1.21%	0.145%
20	11.245	1553	1557	1559	rBV	834333	728652	23.07%	2.755%
21	11.263	1559	1560	1564	rVB	64068	49713	1.57%	0.188%
22	11.780	1644	1648	1651	rBV2	95739	96902	3.07%	0.366%
23	12.451	1759	1762	1765	rBV	100701	88985	2.82%	0.336%
24	12.674	1795	1800	1803	rBV	124441	122011	3.86%	0.461%
25	12.827	1822	1826	1830	rBV	2213921	2202333	69.72%	8.326%
26	13.727	1976	1979	1988	rVB	165773	171506	5.43%	0.648%
27	13.869	1999	2003	2006	rBV	927099	945801	29.94%	3.576%
28	13.892	2006	2007	2012	rVB	63904	52038	1.65%	0.197%
29	14.880	2172	2175	2185	rVB2	49377	110728	3.51%	0.419%
30	15.280	2239	2243	2251	rBV	480507	576266	18.24%	2.179%

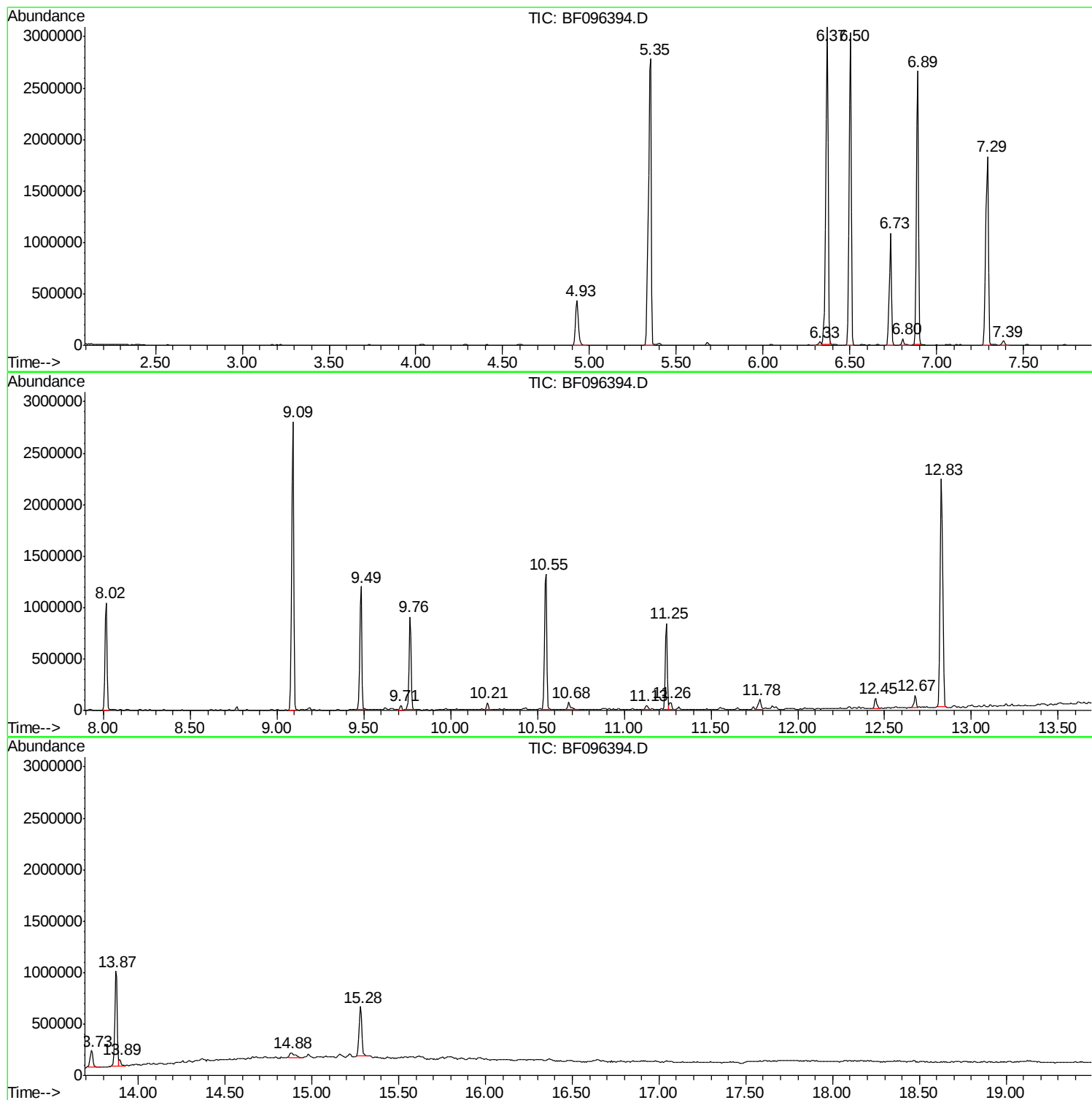
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ALS Vial : 17 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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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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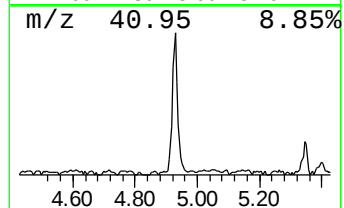
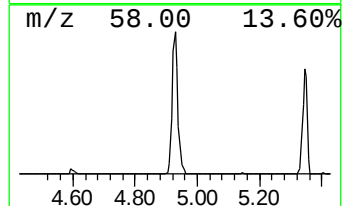
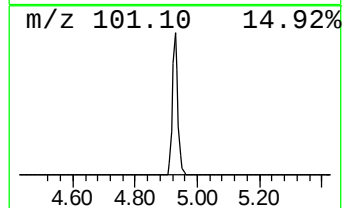
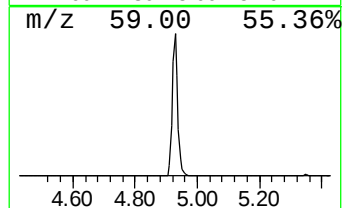
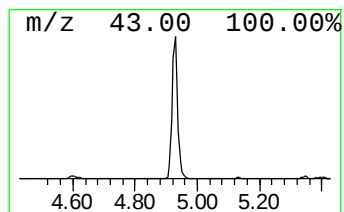
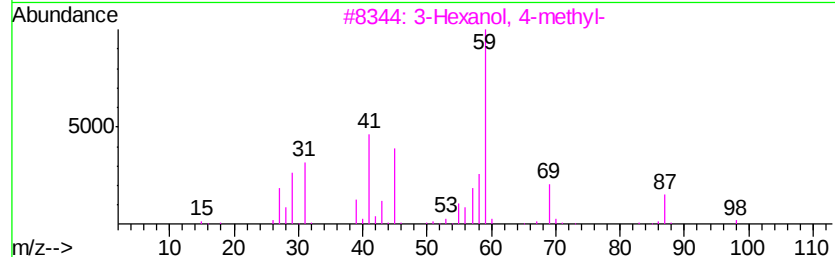
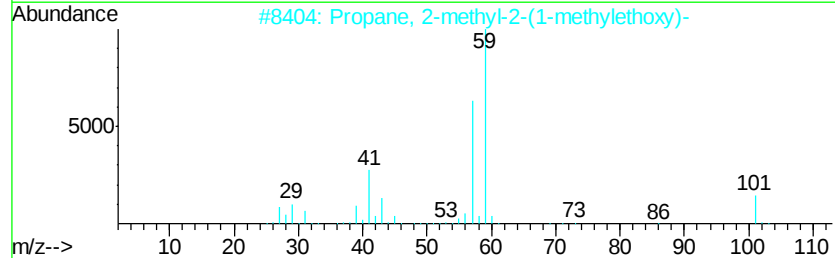
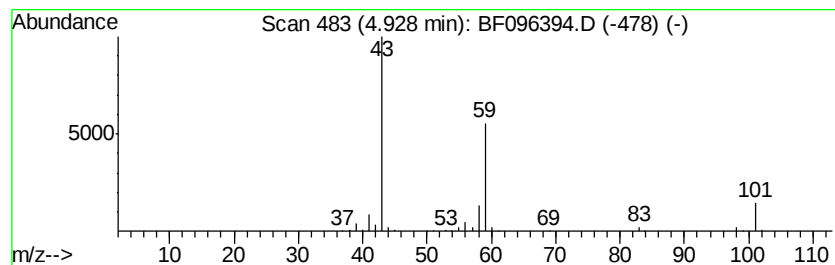
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	12.52 ng	540678	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	56
2			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5			1,2-Butanediol	90	C4H10O2	000584-03-2	25



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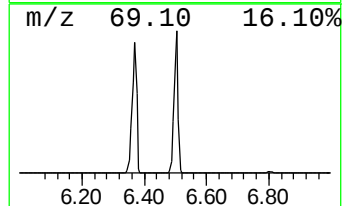
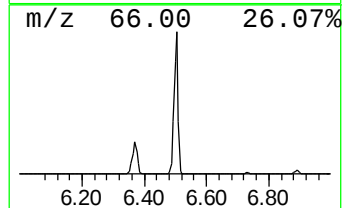
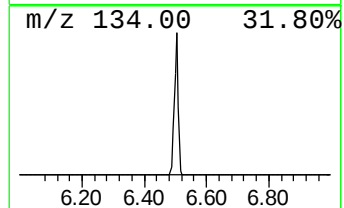
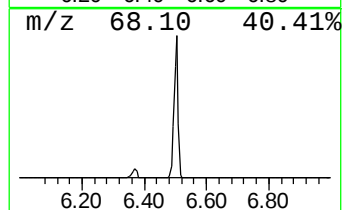
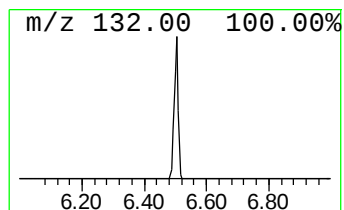
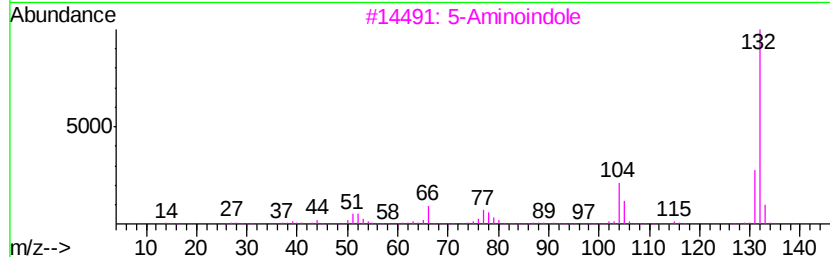
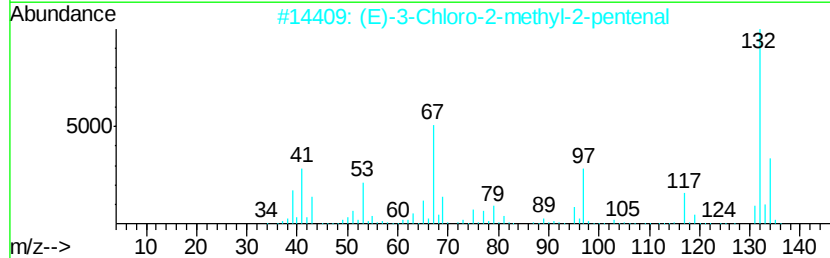
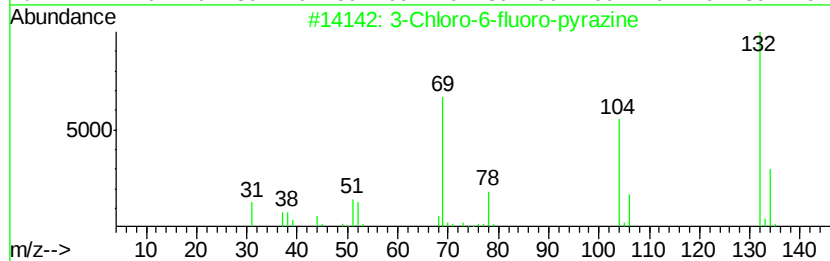
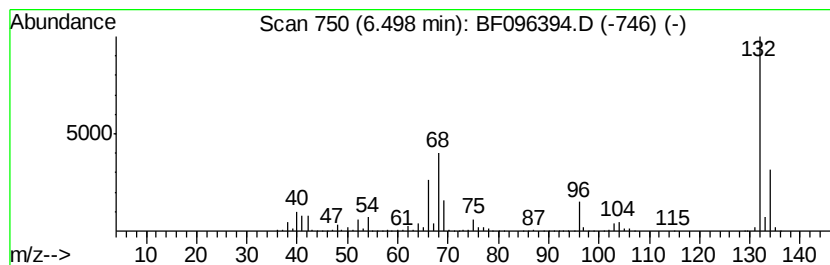
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	65.68 ng	2836630	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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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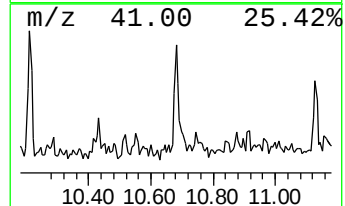
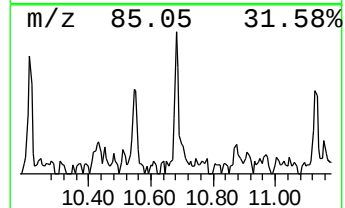
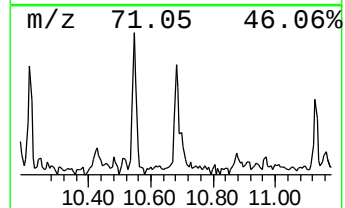
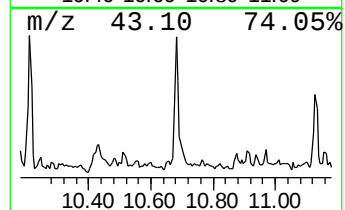
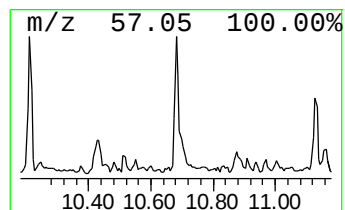
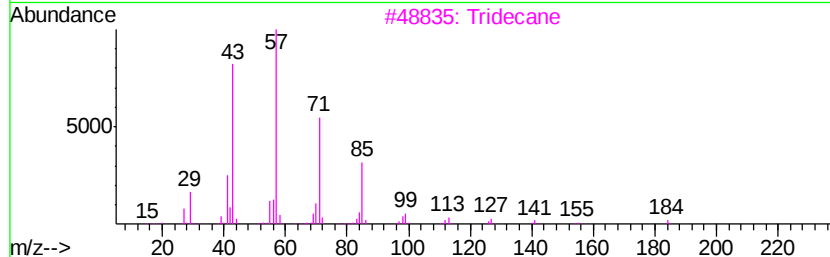
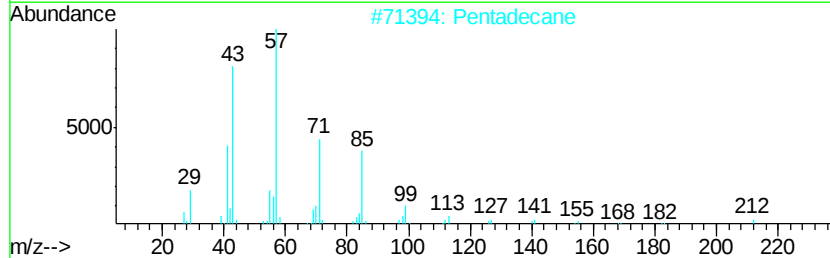
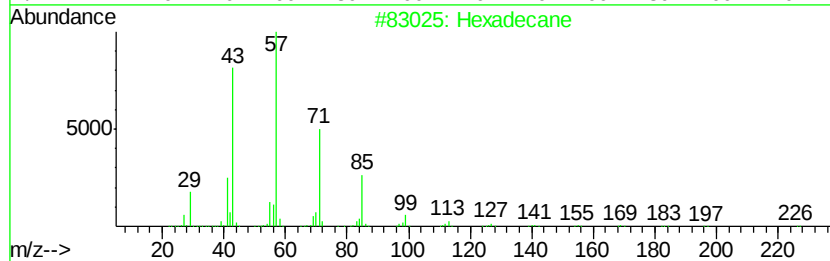
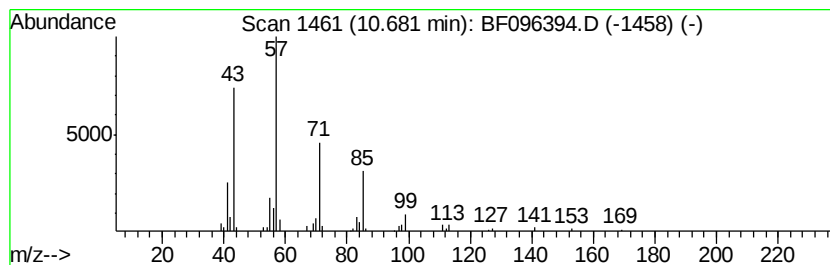
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.18 ng	79580	Phenanthrene-d10	11.25

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane		226	C16H34	000544-76-3	91
2	Pentadecane		212	C15H32	000629-62-9	90
3	Tridecane		184	C13H28	000629-50-5	86
4	Heneicosane		296	C21H44	000629-94-7	83
5	Tetradecane		198	C14H30	000629-59-4	72



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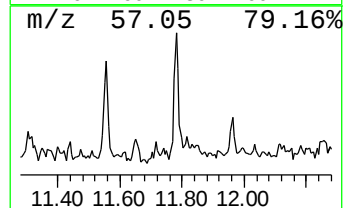
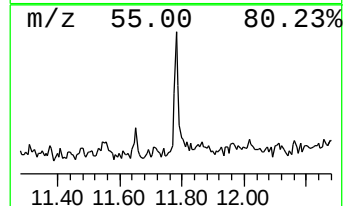
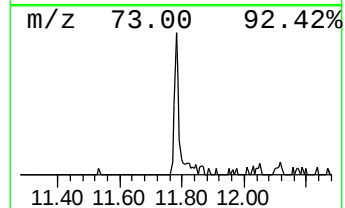
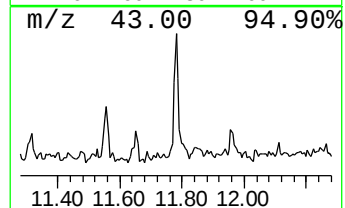
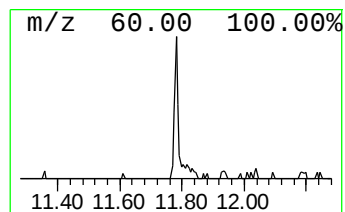
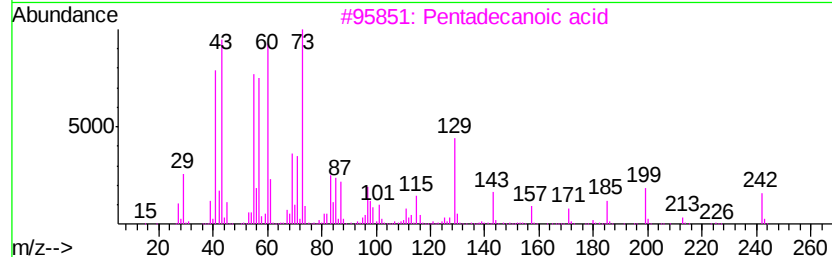
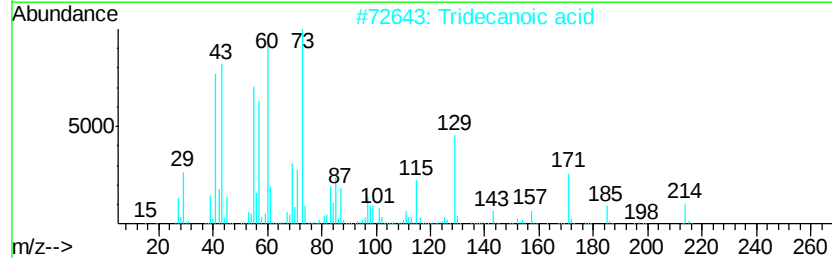
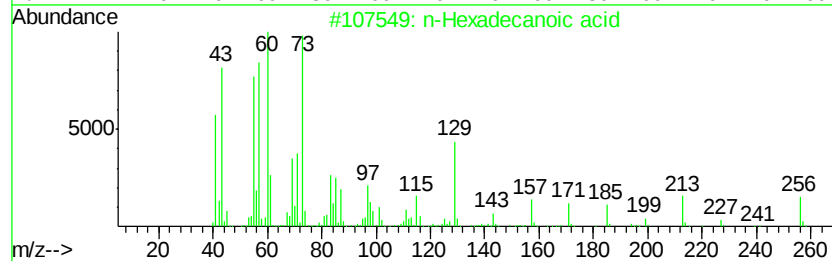
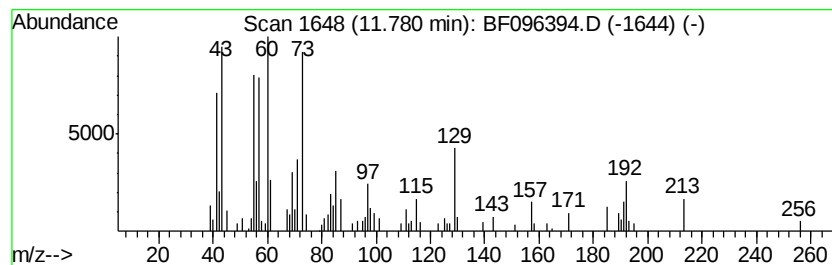
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	2.66 ng	96902	Phenanthrene-d10	11.25

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	76
2		Tridecanoic acid	214	C13H26O2	000638-53-9	58
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	47



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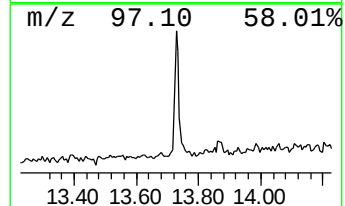
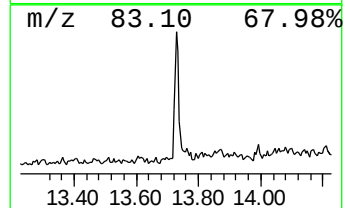
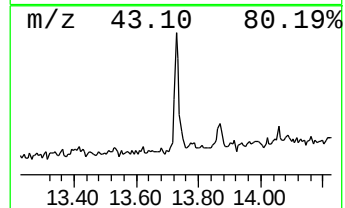
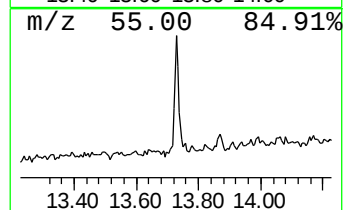
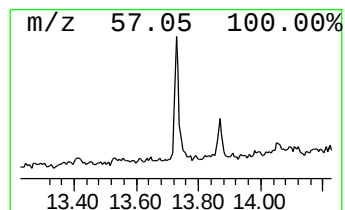
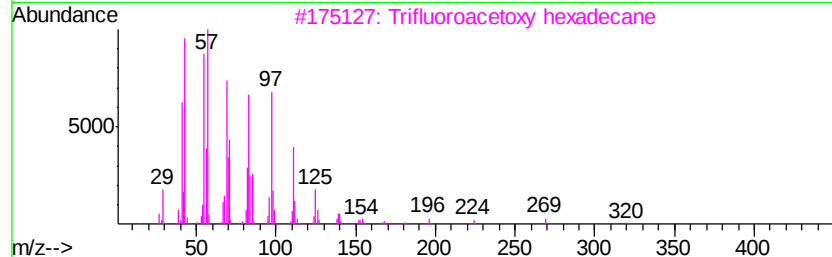
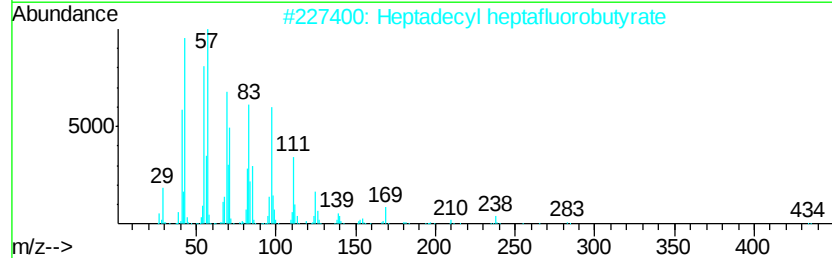
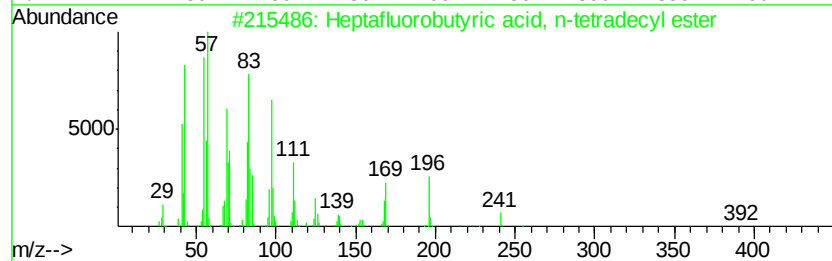
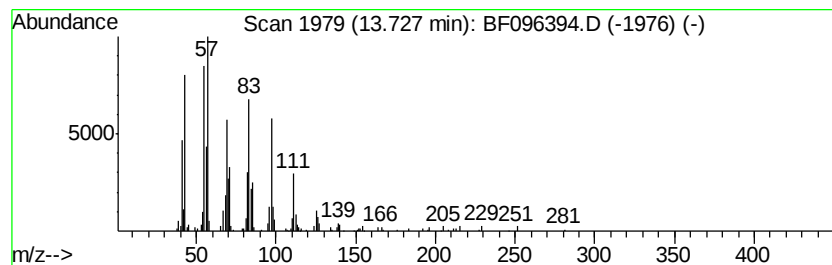
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Peak Number 7 Heptafluorobutyric acid, n-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	3.63 ng	171506	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptafluorobutyric acid, n-tetra...	410	C18H29F7O2	007365-36-8	91
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91
4			Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	91
5			1,2-Octadecanediol	286	C18H38O2	020294-76-2	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	12.5	ng	540678	1	6.73	863820	20.0
unknown6.50	6.50	65.7	ng	2836630	1	6.73	863820	20.0
Hexadecane	10.68	2.2	ng	79580	4	11.25	728652	20.0
n-Hexadecanoic acid	11.78	2.7	ng	96902	4	11.25	728652	20.0
Heptafluorobutyri...	13.73	3.6	ng	171506	5	13.87	945801	20.0