

Data Path : Z:\HPCHEM1\BNA F\DATA\BF072517\
 Data File : BF097044.D
 Acq On : 25 Jul 2017 22:16
 Operator : SJ/JU
 Sample : I4290-03
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 S-3

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:\HPCHEM1\BNA_F\METHODS\8270-BF072517.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	4.669	470	473	488	rBV	242315	460223	10.71%	1.383%
2	5.110	543	548	561	rBV	3253095	4099820	95.38%	12.319%
3	6.169	722	728	741	rBV	3178770	4298412	100.00%	12.916%
4	6.275	741	746	749	rBV	3505580	3854116	89.66%	11.581%
5	6.498	780	784	791	rBV	952688	845747	19.68%	2.541%
6	6.657	806	811	814	rBV	2754390	2830206	65.84%	8.504%
7	7.069	875	881	884	rBV	2350163	2644474	61.52%	7.946%
8	7.781	997	1002	1006	rBV	1294422	1170333	27.23%	3.517%
9	8.863	1180	1186	1189	rBV	3421345	3788539	88.14%	11.384%
10	9.257	1249	1253	1256	rBV	373406	287964	6.70%	0.865%
11	9.528	1294	1299	1302	rBV	1235075	1198780	27.89%	3.602%
12	9.981	1373	1376	1379	rVB	87094	68743	1.60%	0.207%
13	10.198	1408	1413	1416	rBV2	30403	44391	1.03%	0.133%
14	10.316	1428	1433	1436	rBV	1962103	2090462	48.63%	6.281%
15	10.451	1449	1456	1463	rBV	105918	129881	3.02%	0.390%
16	10.898	1524	1532	1534	rBV2	43094	44712	1.04%	0.134%
17	10.998	1545	1549	1552	rBV	1213701	1050503	24.44%	3.156%
18	11.551	1640	1643	1652	rBV2	132593	140685	3.27%	0.423%
19	12.586	1813	1819	1822	rBV	2458972	2654154	61.75%	7.975%
20	13.492	1969	1973	1983	rBV	174884	201307	4.68%	0.605%
21	13.616	1990	1994	2003	rBV	752712	776508	18.06%	2.333%
22	14.968	2219	2224	2230	rBV	521419	600936	13.98%	1.806%

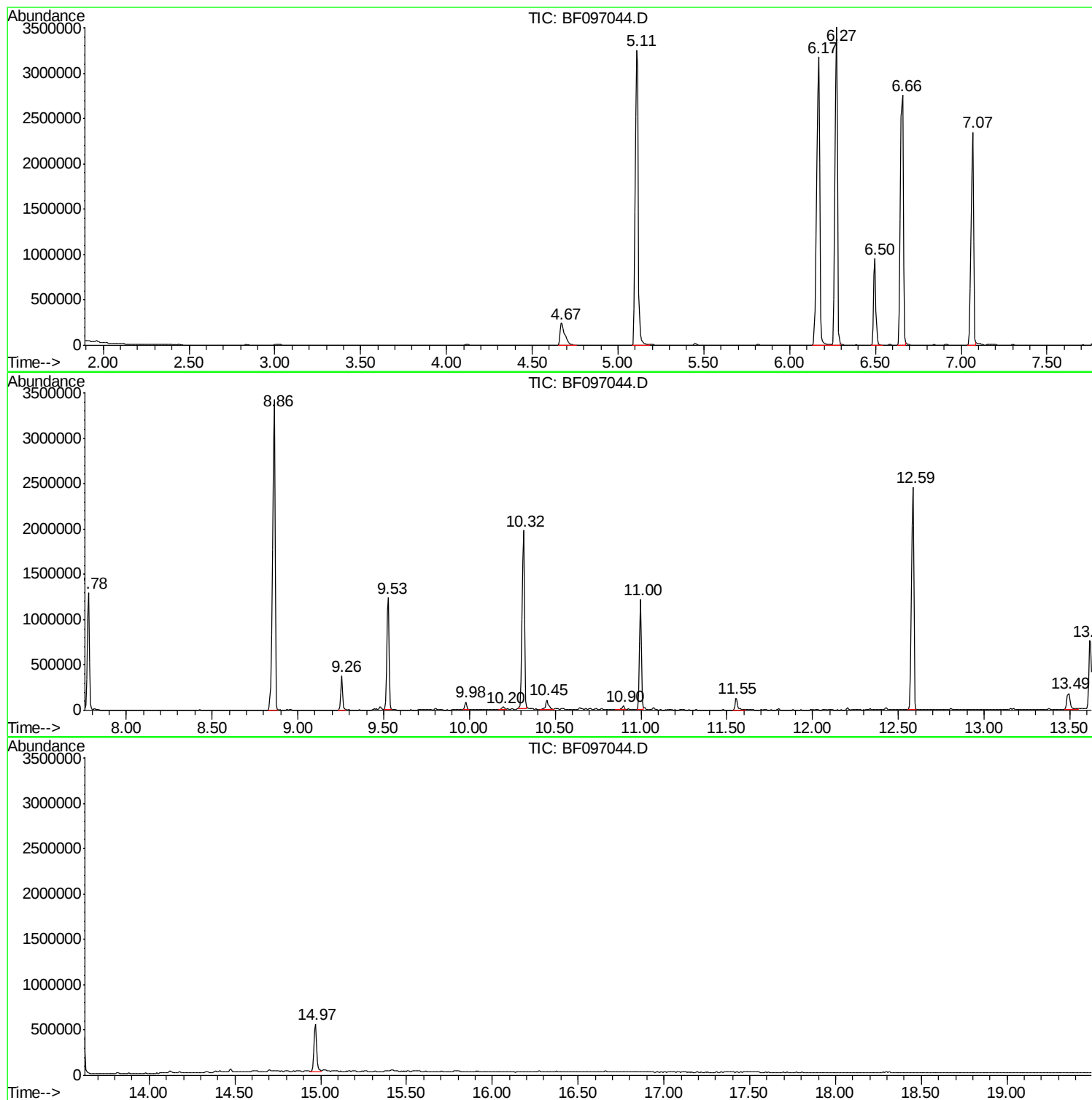
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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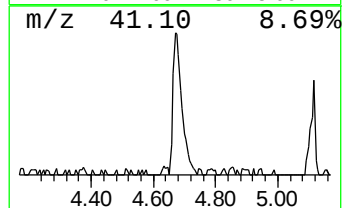
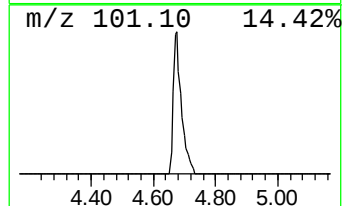
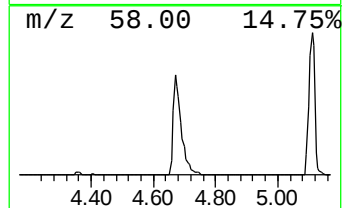
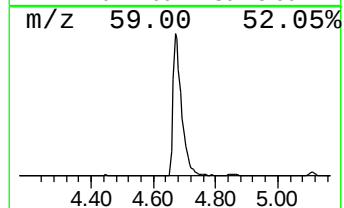
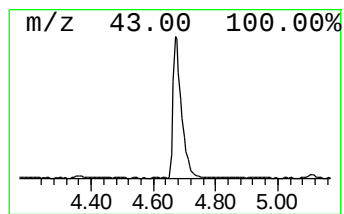
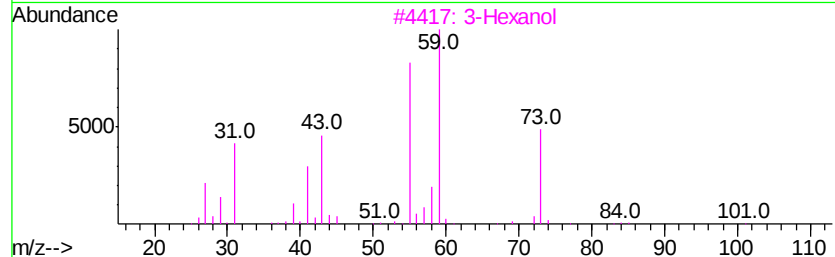
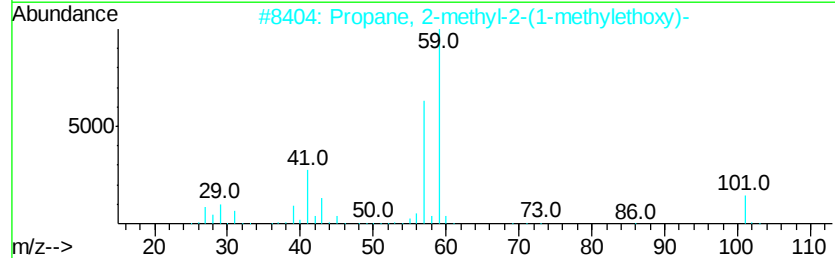
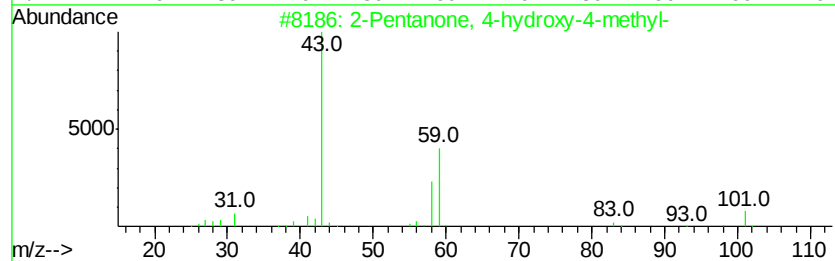
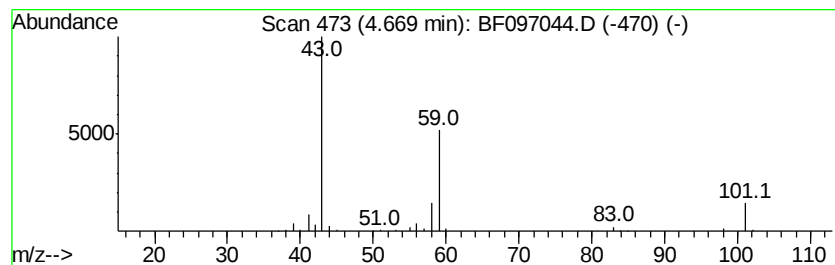
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF072517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.67	10.88 ng	460223	1,4-Dichlorobenzene-d4	6.50

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28



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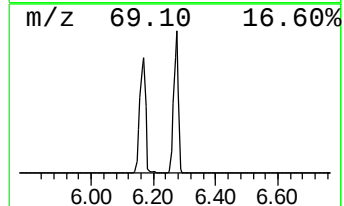
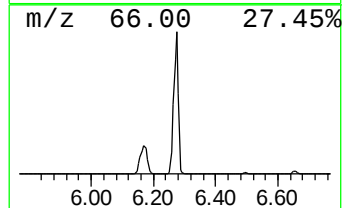
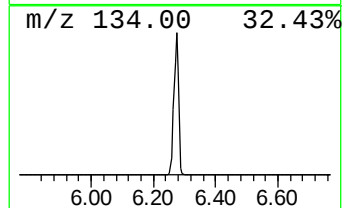
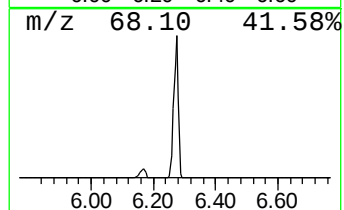
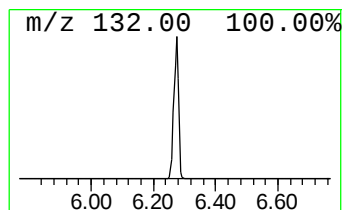
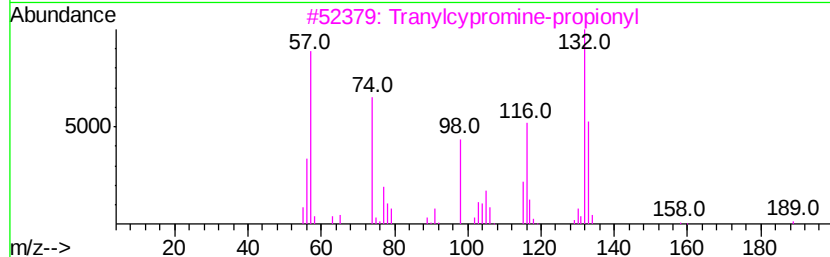
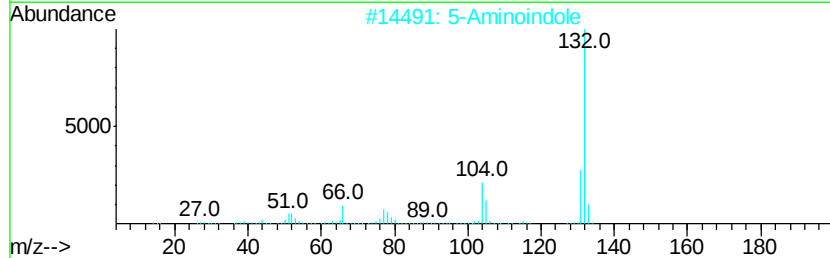
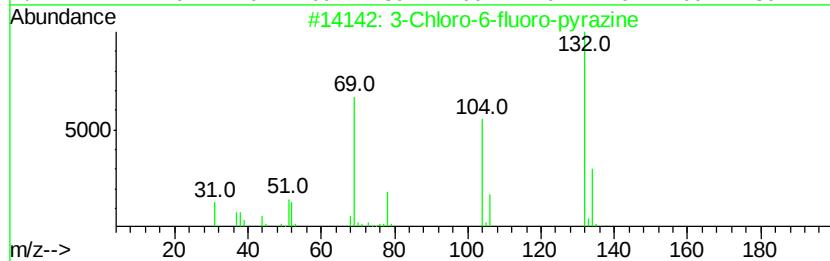
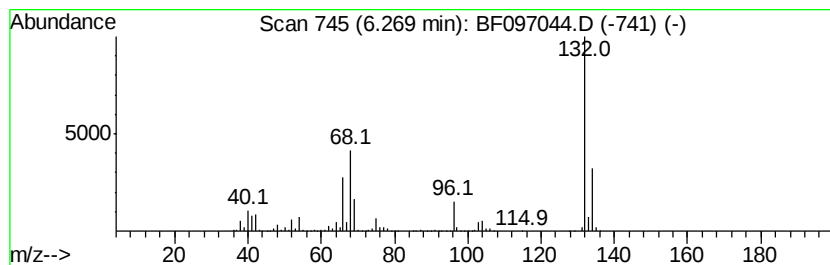
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Peak Number 2 unknown6.27 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.27	91.14 ng	3854120	1,4-Dichlorobenzene-d4	6.50

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3		Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2	5		Aminoindole	132	C8H8N2	005192-03-0	12
3			Tranvlcvpromine-propionyl	189	C12H15NO	1000123-86-3	10
4			(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5			1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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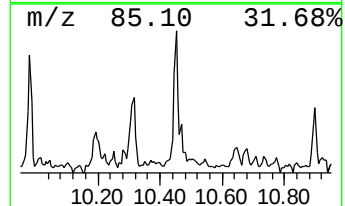
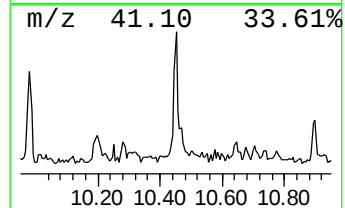
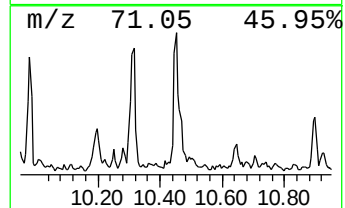
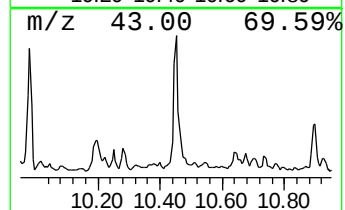
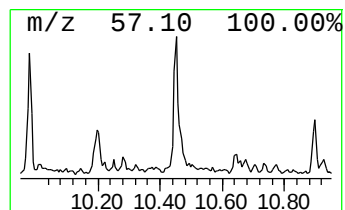
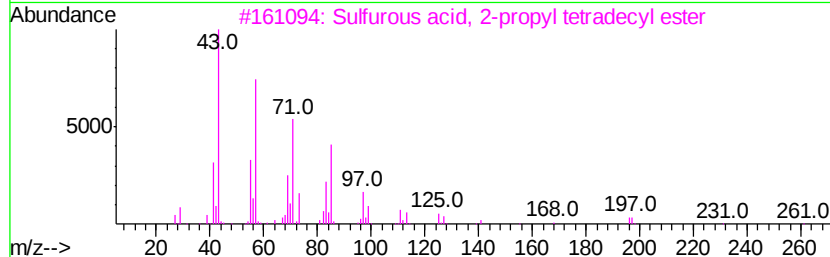
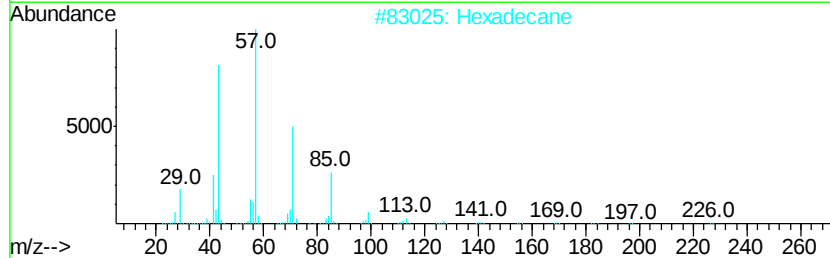
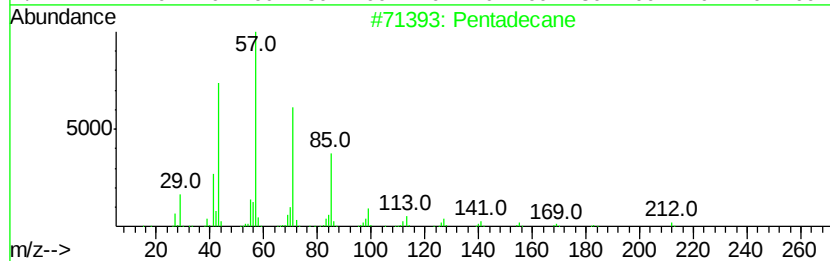
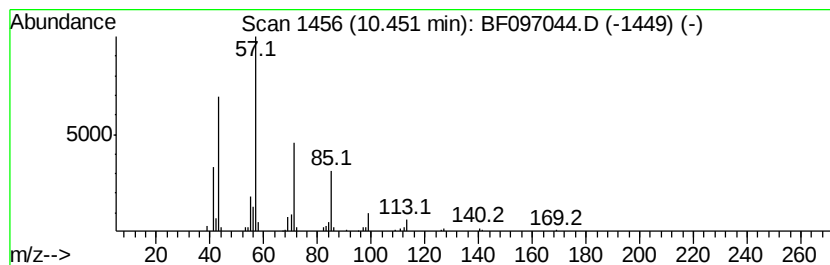
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Peak Number 4 Pentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
10.45	2.47 ng	129881	Phenanthrene-d10		11.00	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecane	212	C15H32	000629-62-9	90
2		Hexadecane	226	C16H34	000544-76-3	87
3		Sulfurous acid, 2-propyl tetradec...	320	C17H36O3S	1000309-12-5	86
4		Tetradecane	198	C14H30	000629-59-4	80
5		Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	80



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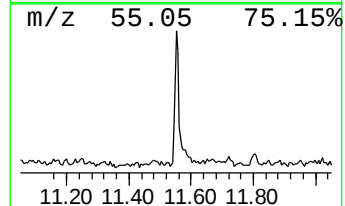
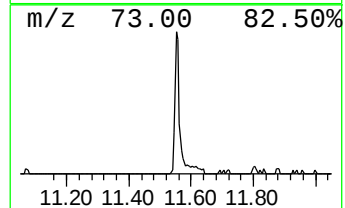
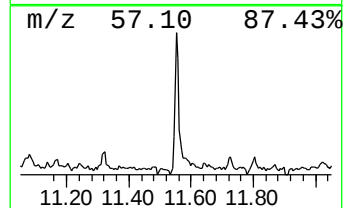
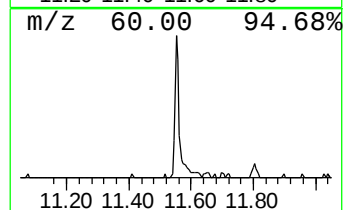
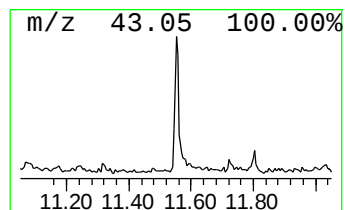
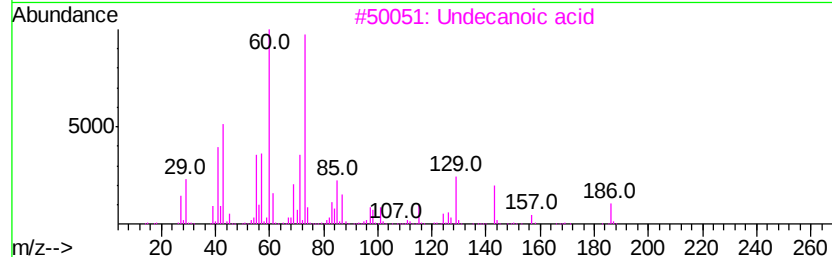
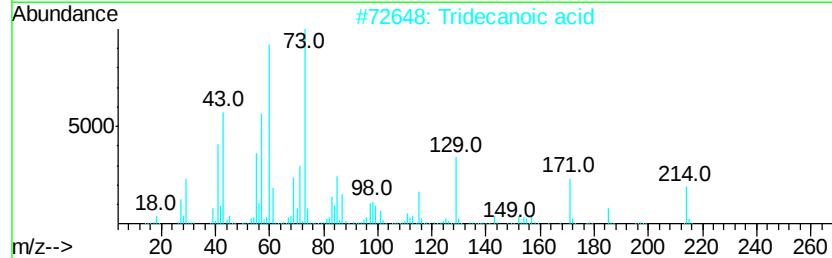
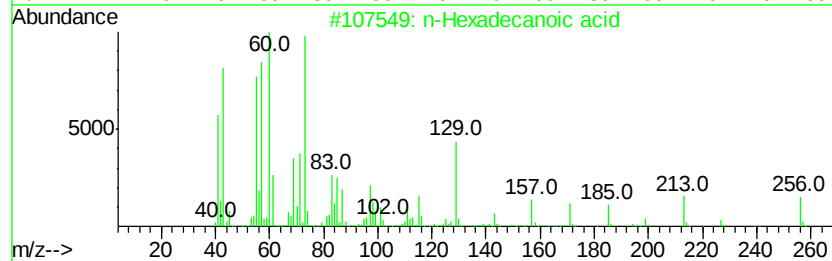
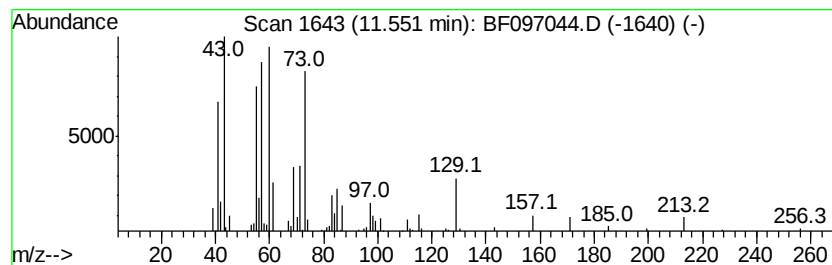
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.55	2.68 ng	140685	Phenanthrene-d10	11.00

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Tridecanoic acid	214	C13H26O2	000638-53-9	80
3	Undecanoic acid	186	C11H22O2	000112-37-8	64
4	Dodecanoic acid	200	C12H24O2	000143-07-7	64
5	Pentadecanoic acid	242	C15H30O2	001002-84-2	58



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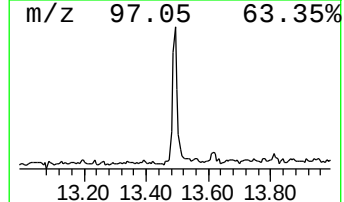
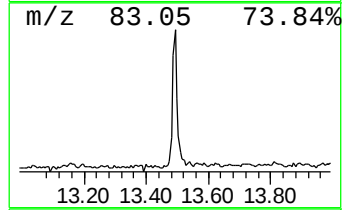
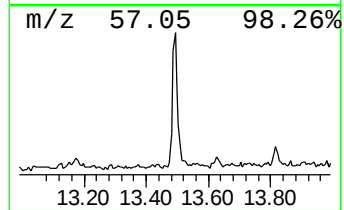
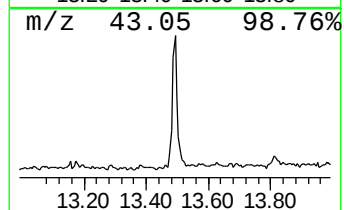
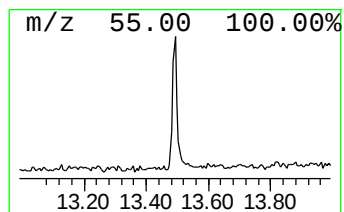
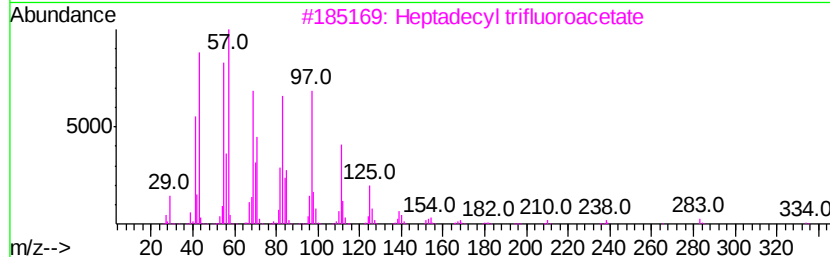
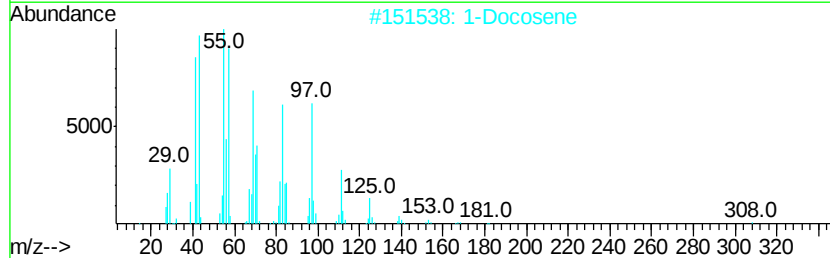
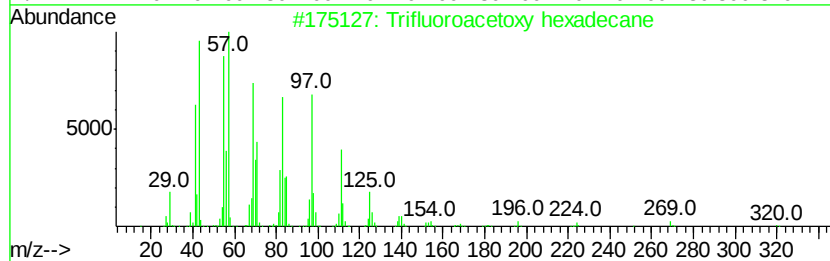
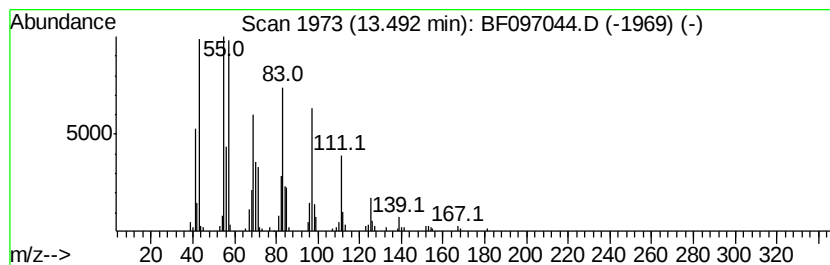
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Peak Number 6 Trifluoroacetoxy hexadecane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.49	5.18 ng	201307	Chrysene-d12	13.62	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxv hexadecane	338	C18H33F3O2	006222-03-3	94
2	1-Docosene	308	C22H44	001599-67-3	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4	1-Heneicosanol	312	C21H44O	015594-90-8	91
5	1-Octadecanol	270	C18H38O	000112-92-5	91



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.67	10.9	ng	460223	1	6.50	845747	20.0
unknown6.27	6.27	91.1	ng	3854120	1	6.50	845747	20.0
Pentadecane	10.45	2.5	ng	129881	4	11.00	1050500	20.0
n-Hexadecanoic acid	11.55	2.7	ng	140685	4	11.00	1050500	20.0
Trifluoroacetoxy ...	13.49	5.2	ng	201307	5	13.62	776508	20.0