

Data Path : Z:\HPCHEM1\BNA F\DATA\BF070517\
 Data File : BF096495.D
 Acq On : 5 Jul 2017 20:23
 Operator : SJ/MA
 Sample : I4049-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RO-72-12000

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	3.063	165	166	175	rBV3	23971	49322	2.03%	0.243%
2	4.904	474	479	485	rBV	257379	346549	14.25%	1.707%
3	5.328	546	551	554	rBV	2543917	2431217	100.00%	11.975%
4	6.351	720	725	729	rBV	2434883	2393900	98.47%	11.791%
5	6.481	743	747	750	rBV	2591177	2337761	96.16%	11.515%
6	6.710	783	786	790	rBV	911808	728558	29.97%	3.589%
7	6.869	809	813	816	rBV	1977024	1656872	68.15%	8.161%
8	7.269	876	881	884	rBV	1550303	1481735	60.95%	7.298%
9	7.369	894	898	906	rVB	31076	36322	1.49%	0.179%
10	7.992	1000	1004	1008	rBV	1164017	943080	38.79%	4.645%
11	9.069	1183	1187	1191	rBV	2119017	2032663	83.61%	10.012%
12	9.198	1206	1209	1216	rVB	30878	30225	1.24%	0.149%
13	9.463	1251	1254	1257	rBV	432079	334285	13.75%	1.647%
14	9.692	1291	1293	1296	rVB	38795	29780	1.22%	0.147%
15	9.745	1296	1302	1306	rBV	1015526	886897	36.48%	4.369%
16	10.192	1375	1378	1381	rVB	53435	37736	1.55%	0.186%
17	10.416	1411	1416	1421	rBV3	51664	74452	3.06%	0.367%
18	10.527	1431	1435	1439	rBV	957508	934721	38.45%	4.604%
19	10.663	1455	1458	1467	rBV	74356	101748	4.19%	0.501%
20	11.110	1531	1534	1537	rBV2	58203	52197	2.15%	0.257%
21	11.145	1537	1540	1543	rVB2	31611	33985	1.40%	0.167%
22	11.227	1550	1554	1557	rBV	710573	627077	25.79%	3.089%
23	12.433	1756	1759	1763	rBV	64186	50413	2.07%	0.248%
24	12.657	1793	1797	1800	rBV	42241	45912	1.89%	0.226%
25	12.810	1819	1823	1827	rVB	1269720	1106094	45.50%	5.448%
26	13.715	1973	1977	1985	rBV	141648	156645	6.44%	0.772%
27	13.857	1996	2001	2004	rBV	742333	671830	27.63%	3.309%
28	14.351	2081	2085	2091	rBV5	19971	33469	1.38%	0.165%
29	14.715	2143	2147	2151	rBV2	28133	32825	1.35%	0.162%
30	14.862	2169	2172	2175	rBV	28955	34972	1.44%	0.172%
31	15.262	2236	2240	2247	rBV	444810	552743	22.74%	2.723%
32	15.774	2323	2327	2334	rBV7	18698	36067	1.48%	0.178%

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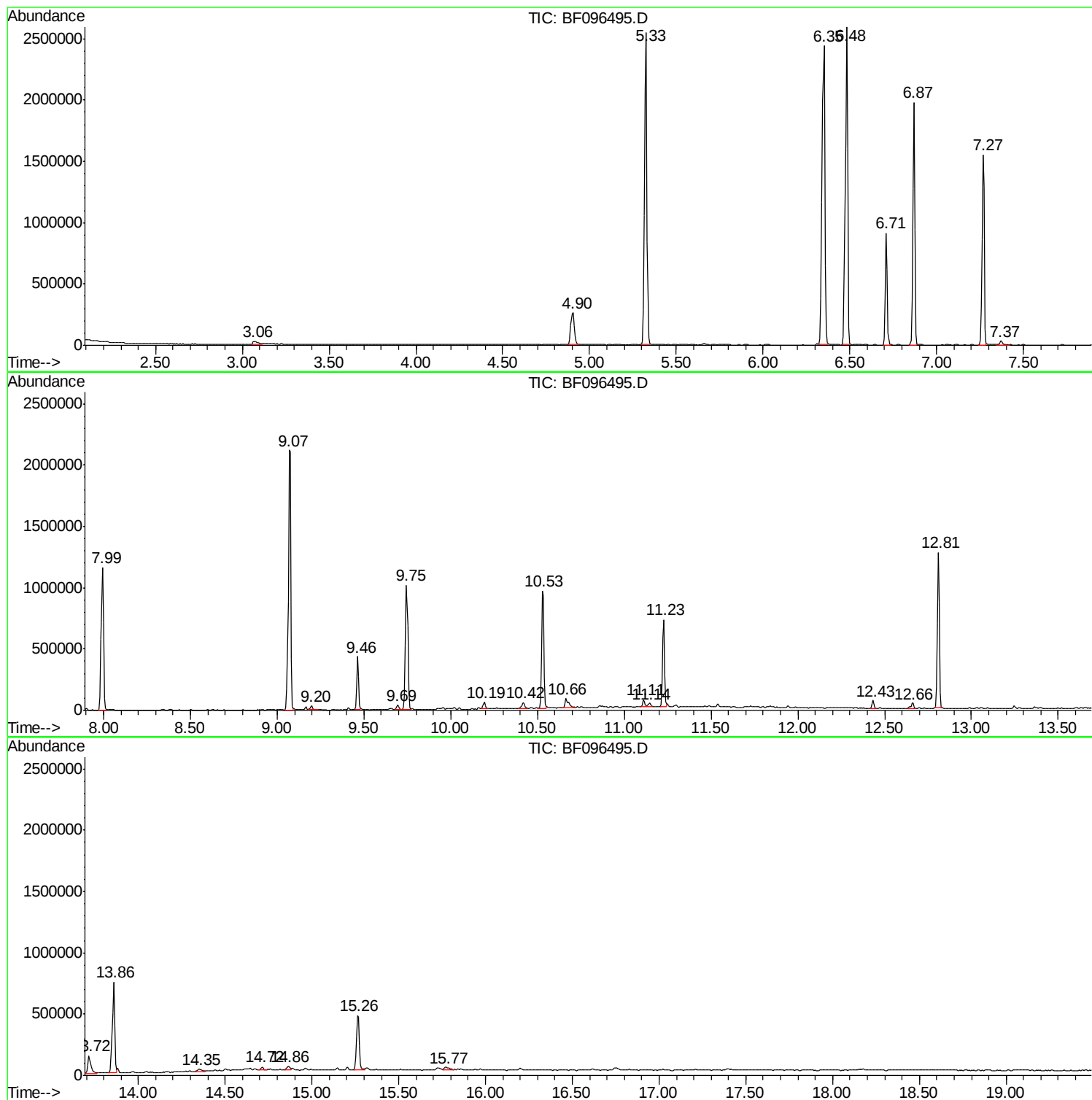
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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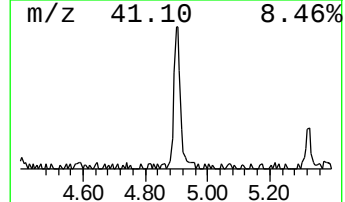
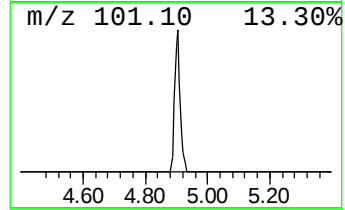
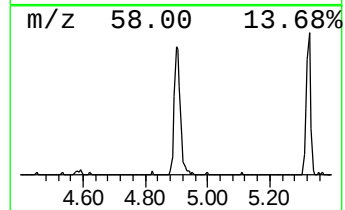
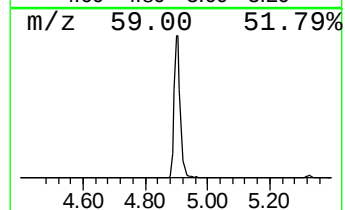
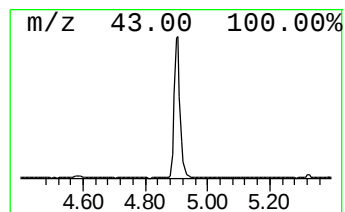
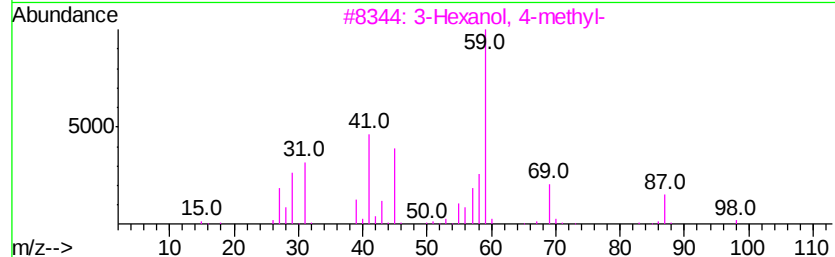
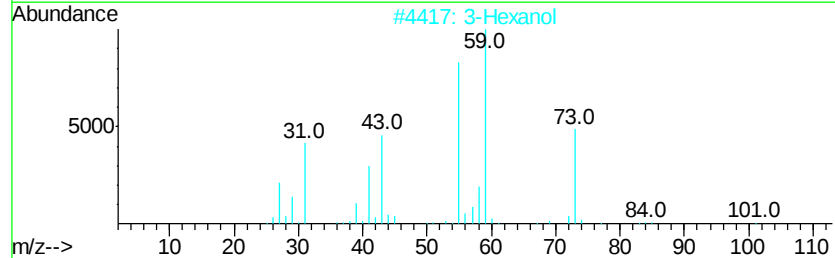
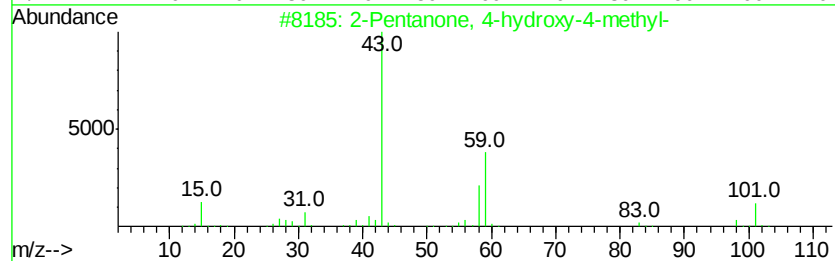
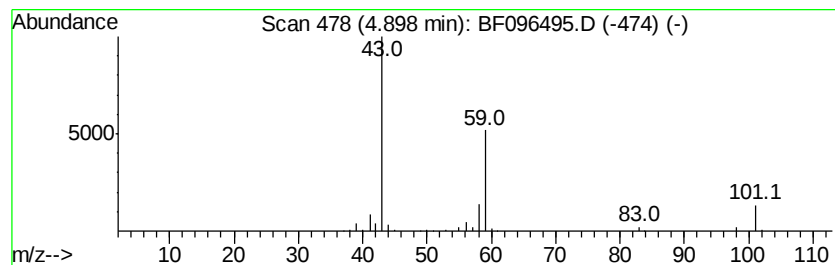
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.	
4.90	9.51 ng	346549	1,4-Dichlorobenzene-d4	6.71	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2	3-Hexanol	102	C6H14O	000623-37-0	33
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5	Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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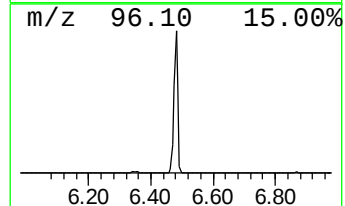
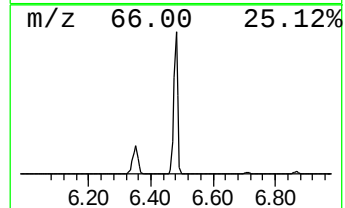
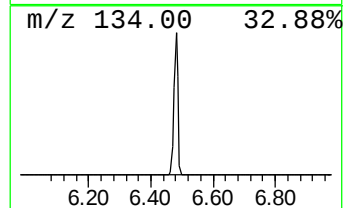
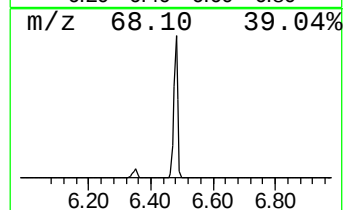
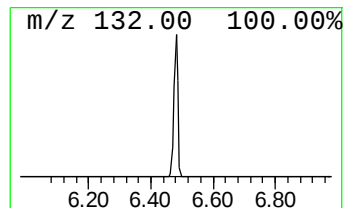
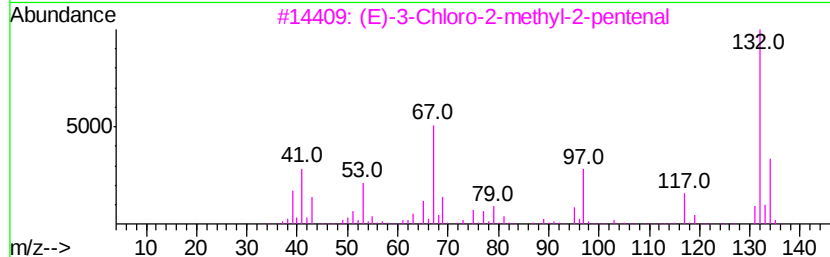
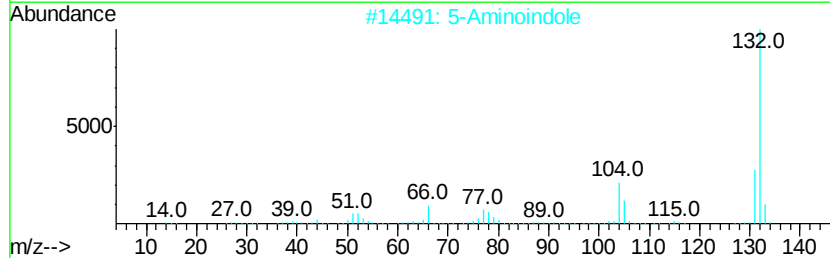
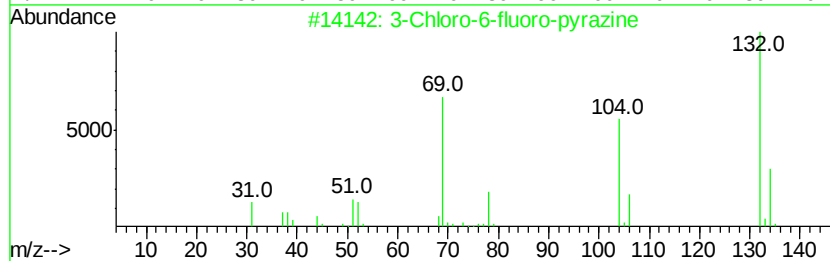
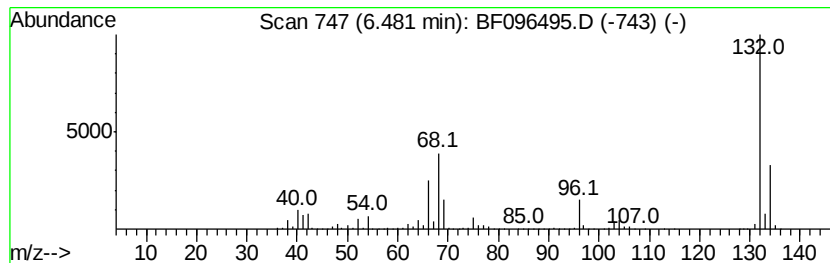
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Peak Number 2 unknown6.48 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.48	64.18 ng	2337760	1,4-Dichlorobenzene-d4	6.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Aminoindole	132	C8H8N2	005192-03-0	12
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Amphetaminil	250	C17H18N2	017590-01-1	10



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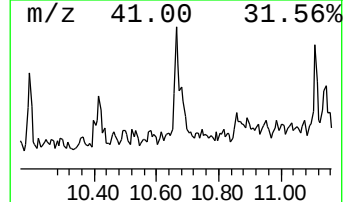
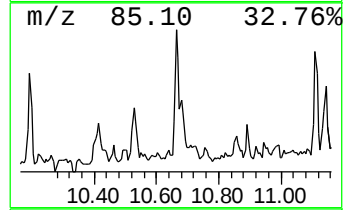
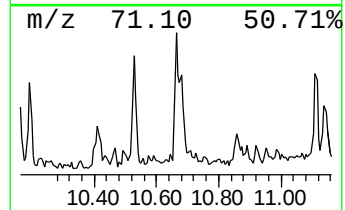
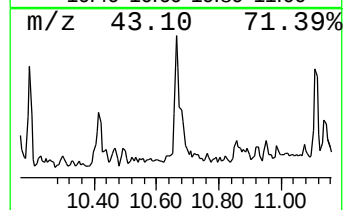
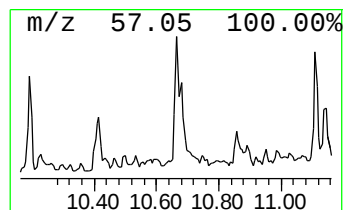
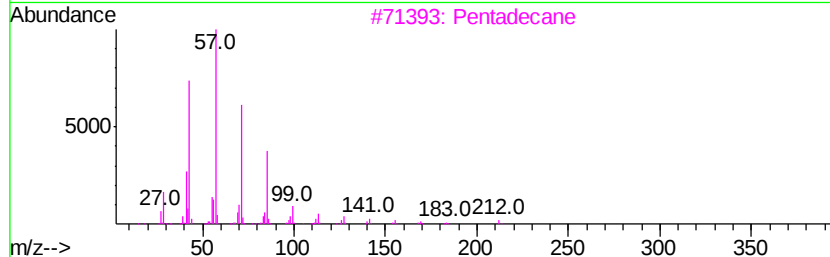
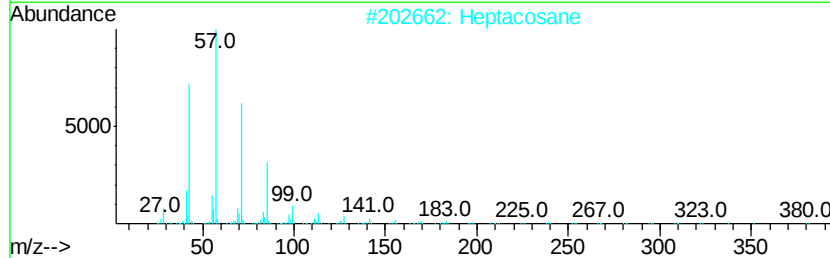
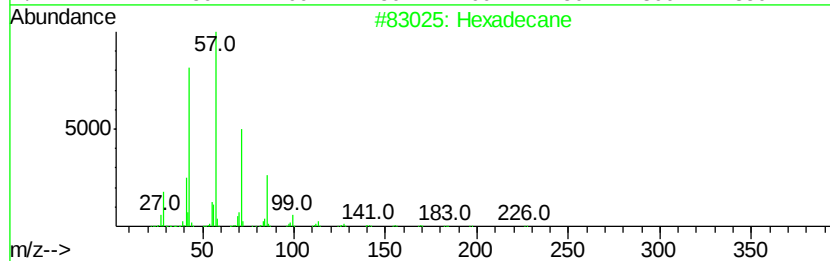
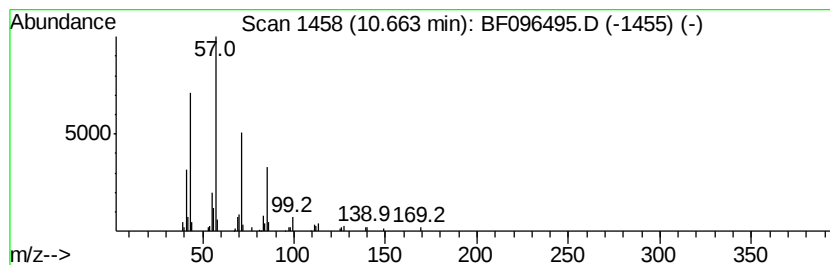
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Peak Number 4 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.66	3.25 ng	101748	Phenanthrene-d10	11.23	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Hexadecane	226	C16H34	000544-76-3	87
2	Heptacosane	380	C27H56	000593-49-7	78
3	Pentadecane	212	C15H32	000629-62-9	78
4	Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	72
5	Tetradecane	198	C14H30	000629-59-4	72



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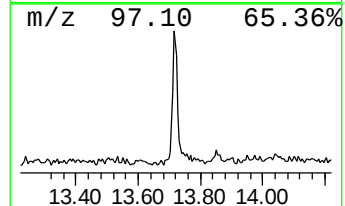
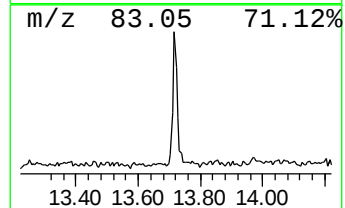
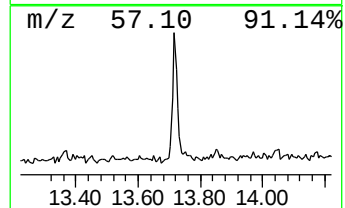
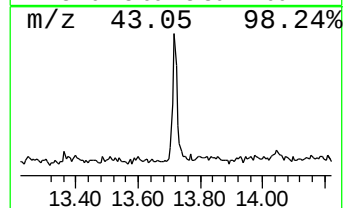
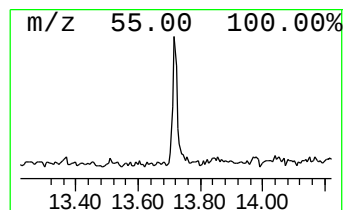
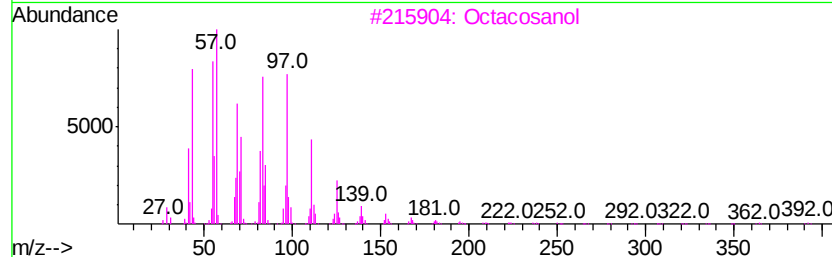
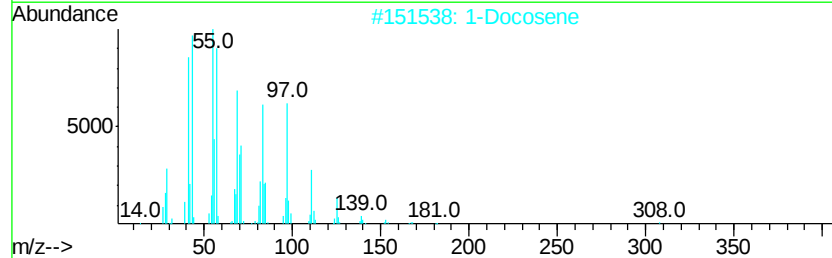
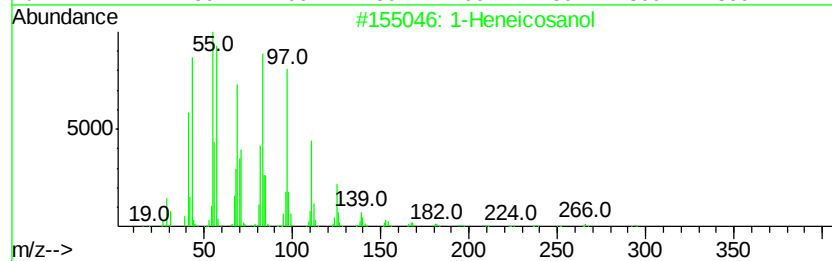
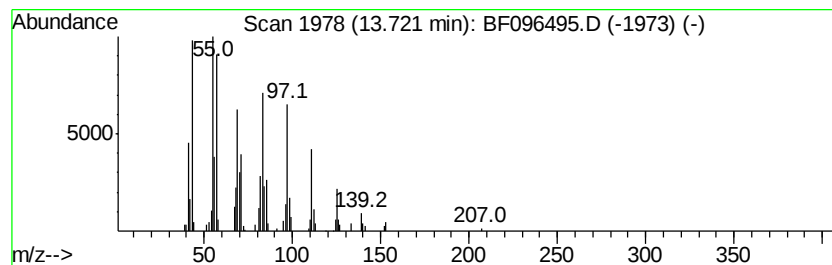
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 1-Heneicosanol Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	4.66 ng	156645	Chrysene-d12	13.86

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol		312	C21H44O	015594-90-8	95
2	1-Docosene		308	C22H44	001599-67-3	94
3	Octacosanol		410	C28H58O	000557-61-9	94
4	Behenic alcohol		326	C22H46O	000661-19-8	93
5	n-Heptadecanol-1		256	C17H36O	001454-85-9	91



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.90	9.5	ng	346549	1	6.71	728558	20.0
unknown6.48	6.48	64.2	ng	2337760	1	6.71	728558	20.0
Hexadecane	10.66	3.3	ng	101748	4	11.23	627077	20.0
1-Heneicosanol	13.72	4.7	ng	156645	5	13.86	671830	20.0