

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
 Data File : BF096391.D
 Acq On : 1 Jul 2017 21:00
 Operator : SJ/MA
 Sample : I3980-04
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-B-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	491	rVB	384074	472025	16.23%	1.899%
2	5.345	549	554	558	rBV	2698235	2909185	100.00%	11.703%
3	6.369	723	728	731	rBV	2725886	2853584	98.09%	11.479%
4	6.504	746	751	754	rBV	2962684	2785648	95.75%	11.206%
5	6.734	786	790	793	rBV	891353	727365	25.00%	2.926%
6	6.892	812	817	820	rBV	2367335	2139342	73.54%	8.606%
7	7.292	880	885	888	rBV	1904481	1728078	59.40%	6.952%
8	8.016	1004	1008	1011	rBV	1061986	927617	31.89%	3.732%
9	9.092	1186	1191	1194	rBV	2975035	2680938	92.15%	10.785%
10	9.480	1252	1257	1260	rBV	440194	346990	11.93%	1.396%
11	9.710	1293	1296	1299	rVB	53661	44494	1.53%	0.179%
12	9.763	1301	1305	1309	rBV	906412	815848	28.04%	3.282%
13	10.210	1378	1381	1384	rVB	75200	57566	1.98%	0.232%
14	10.545	1434	1438	1442	rBV	1251098	1228530	42.23%	4.942%
15	10.680	1458	1461	1466	rBV	67831	68140	2.34%	0.274%
16	11.245	1553	1557	1560	rBV	738704	670702	23.05%	2.698%
17	11.780	1644	1648	1657	rBV	184317	180259	6.20%	0.725%
18	12.563	1778	1781	1787	rBV3	44581	50401	1.73%	0.203%
19	12.674	1793	1800	1806	rBV2	20438	32242	1.11%	0.130%
20	12.827	1822	1826	1829	rBV	2387529	2200303	75.63%	8.851%
21	13.727	1976	1979	1986	rBV	323815	311616	10.71%	1.254%
22	13.868	1999	2003	2007	rBV	936952	895420	30.78%	3.602%
23	13.986	2020	2023	2026	rBV5	31064	33853	1.16%	0.136%
24	14.362	2084	2087	2090	rBV2	32759	36566	1.26%	0.147%
25	15.280	2239	2243	2247	rVB	588749	661529	22.74%	2.661%

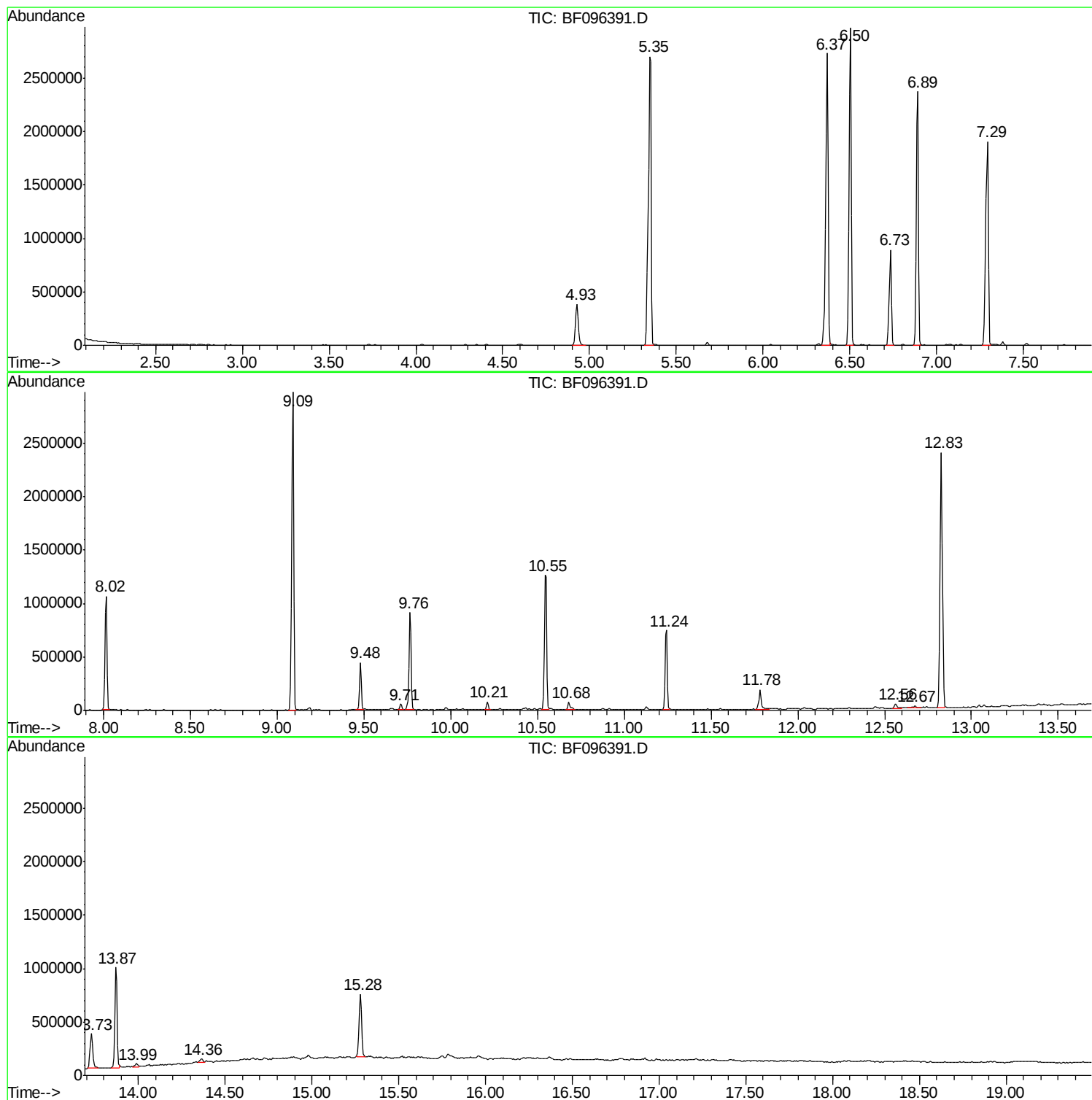
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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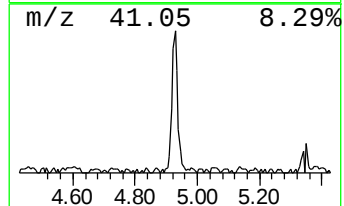
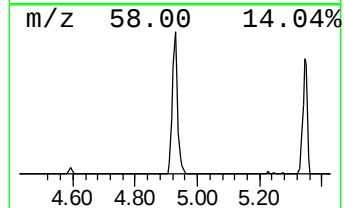
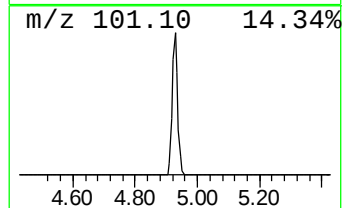
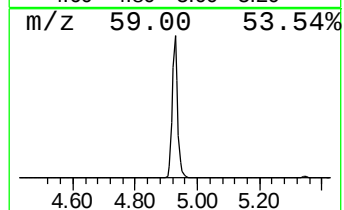
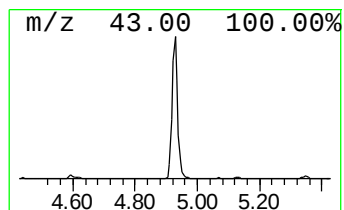
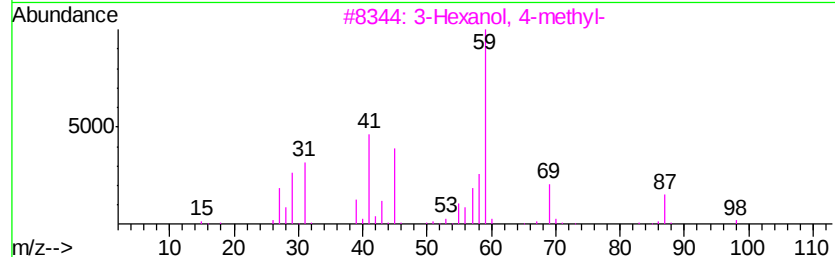
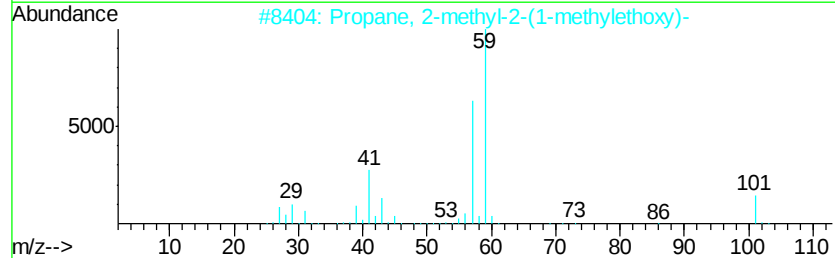
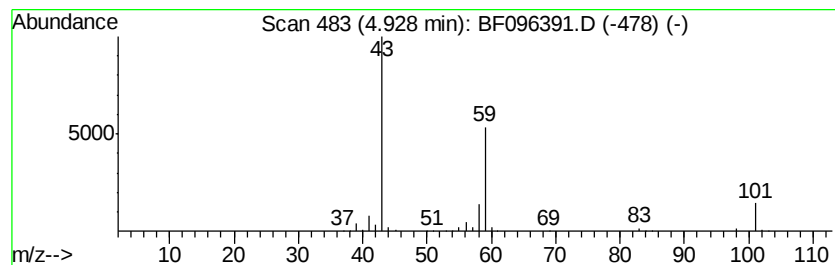
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.93	12.98 ng	472025	1,4-Dichlorobenzene-d4	6.73

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, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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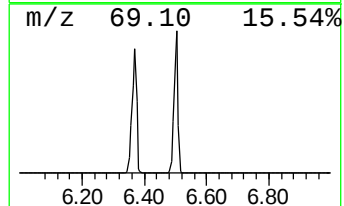
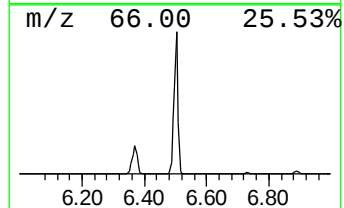
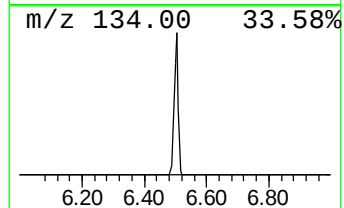
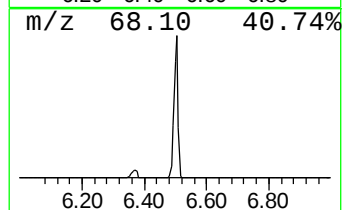
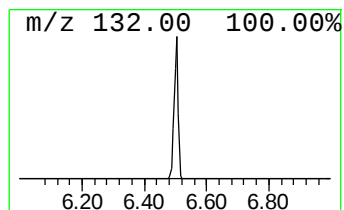
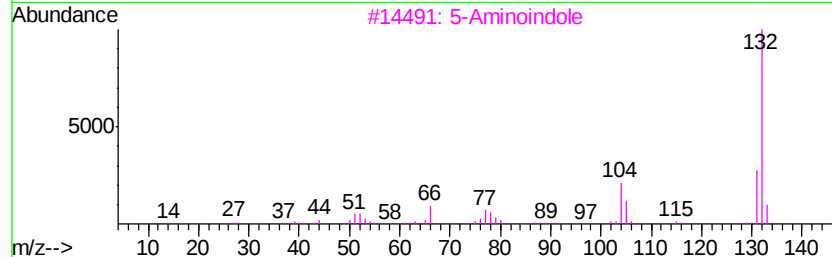
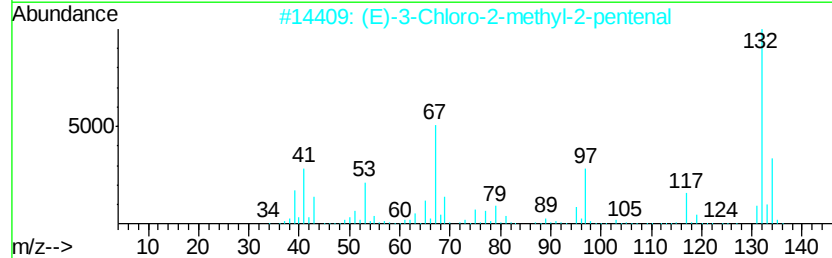
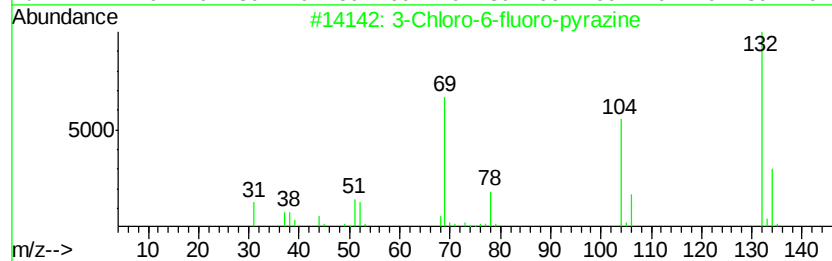
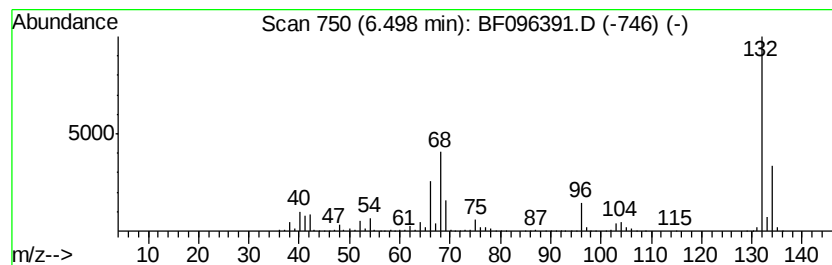
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	76.60 ng	2785650	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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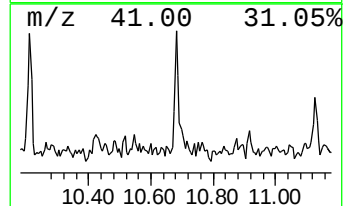
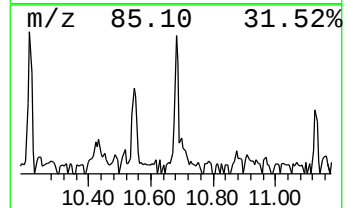
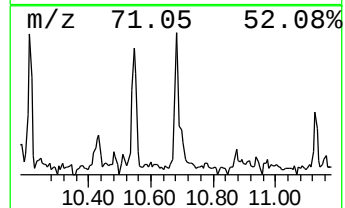
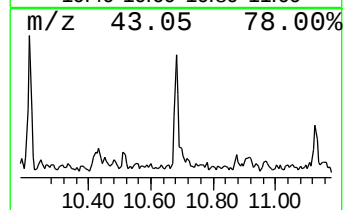
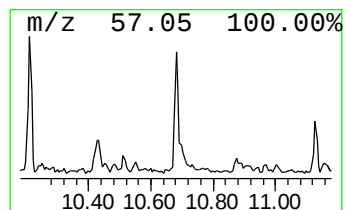
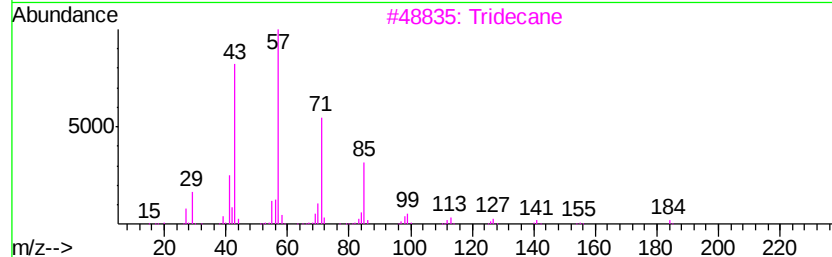
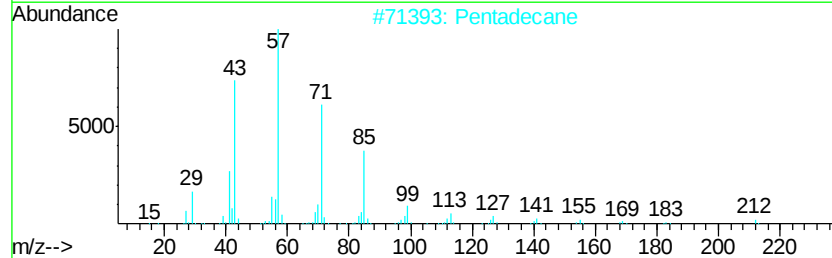
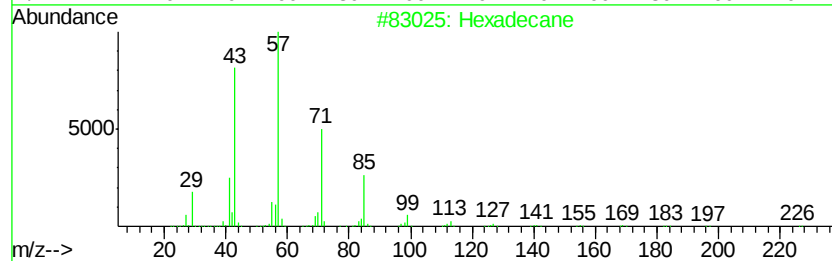
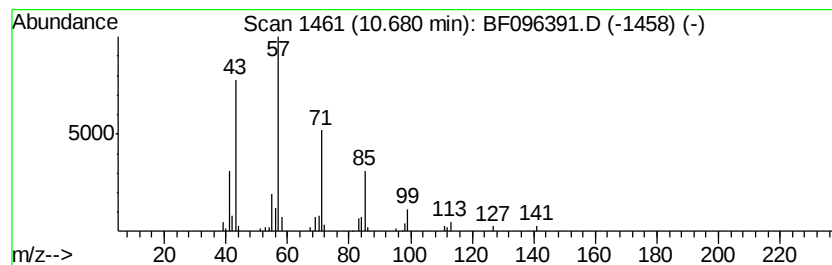
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Peak Number 4 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.03 ng	68140	Phenanthrene-d10	11.24

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	83
4	Eicosane		282	C20H42	000112-95-8	78
5	Tetradecane		198	C14H30	000629-59-4	64



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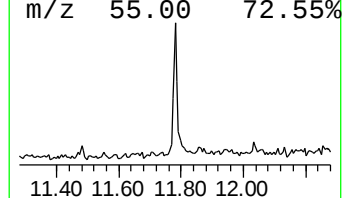
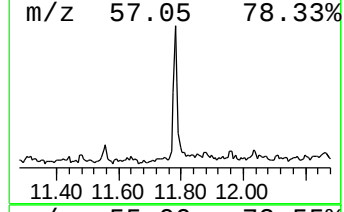
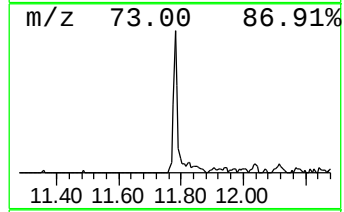
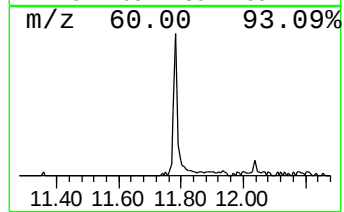
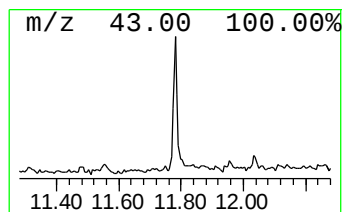
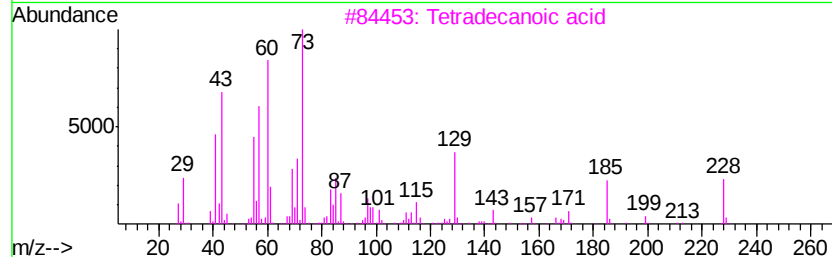
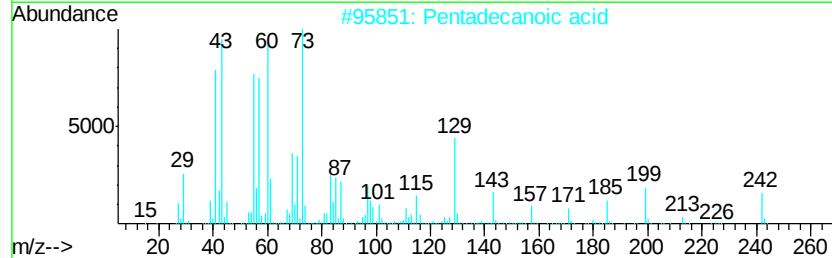
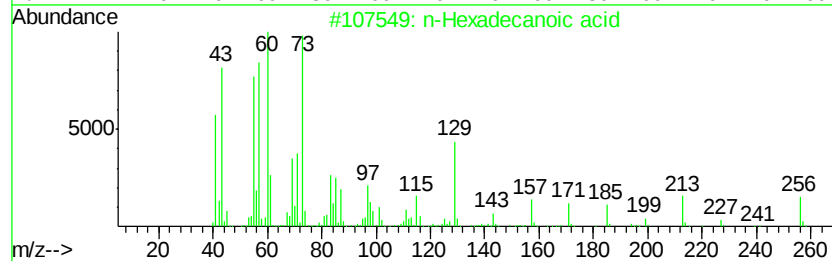
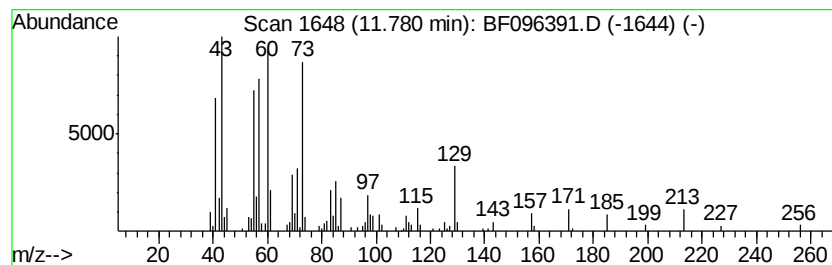
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	5.38 ng	180259	Phenanthrene-d10	11.24

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	87
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	80
4	Dodecanoic acid	200	C12H24O2	000143-07-7	78
5	Undecanoic acid	186	C11H22O2	000112-37-8	72



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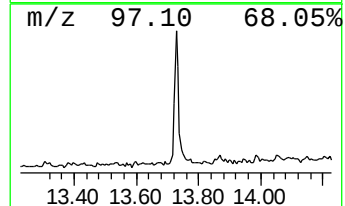
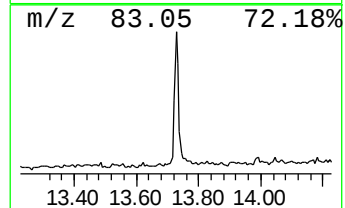
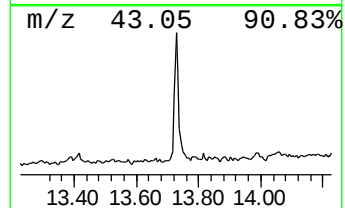
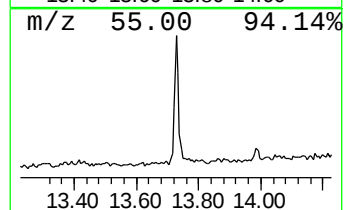
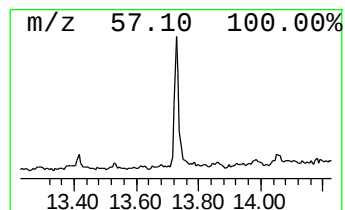
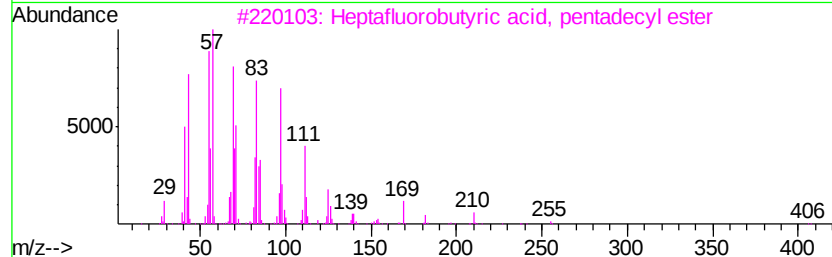
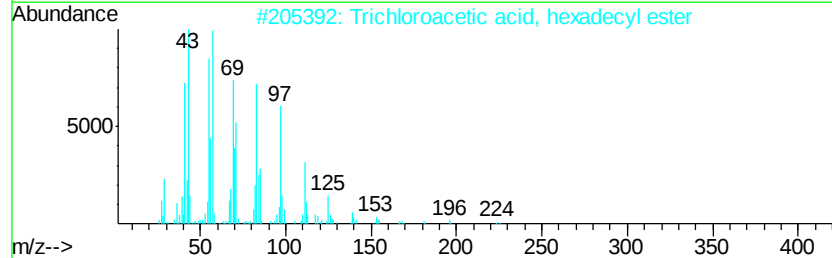
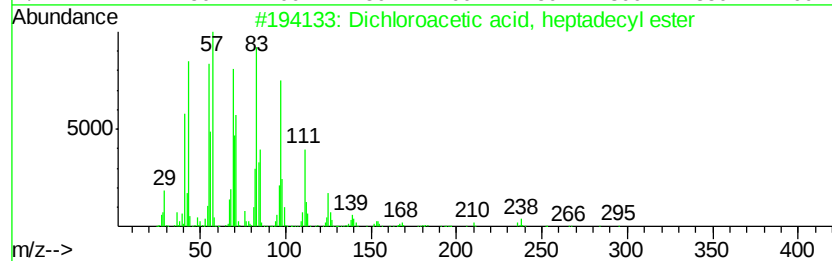
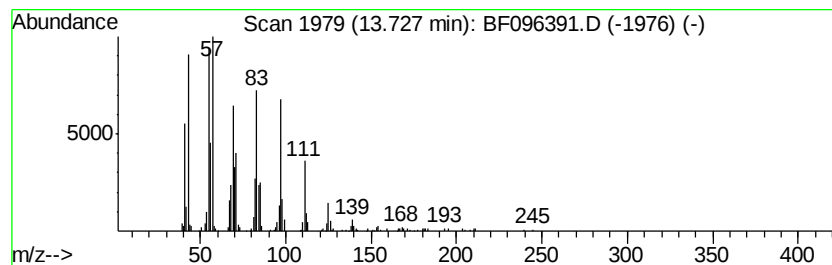
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 Peak Number 6 Dichloroacetic acid, heptadecyl... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.73	6.96 ng	311616	Chrysene-d12	13.87

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
3			Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4			1-Docosene	308	C22H44	001599-67-3	94
5			Cyclopentadecane	210	C15H30	000295-48-7	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	13.0	ng	472025	1	6.73	727365	20.0
unknown6.50	6.50	76.6	ng	2785650	1	6.73	727365	20.0
Hexadecane	10.68	2.0	ng	68140	4	11.24	670702	20.0
n-Hexadecanoic acid	11.78	5.4	ng	180259	4	11.24	670702	20.0
Dichloroacetic ac...	13.73	7.0	ng	311616	5	13.87	895420	20.0