

Data Path : U:\HPCHEM1\BNA F\DATA\BF082117\
 Data File : BF097926.D
 Acq On : 22 Aug 2017 00:58
 Operator : SJ/JU
 Sample : I4889-01
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SASP2P-TP-106-L(0-5)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-BF081517.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	4.934	481	484	493	rVB	186821	224210	10.49%	1.116%
2	5.351	551	555	559	rBV	2015266	1981244	92.68%	9.863%
3	6.381	725	730	733	rBV	2152837	2137795	100.00%	10.642%
4	6.516	749	753	756	rBV	2211205	1993776	93.26%	9.925%
5	6.751	789	793	796	rBV	792946	673122	31.49%	3.351%
6	6.904	815	819	822	rBV	1776845	1490549	69.72%	7.420%
7	7.310	883	888	891	rBV	1368944	1180531	55.22%	5.877%
8	8.034	1006	1011	1014	rBV	976505	821602	38.43%	4.090%
9	9.110	1189	1194	1197	rBV	2145028	1973664	92.32%	9.825%
10	9.498	1258	1260	1264	rVB	138928	110240	5.16%	0.549%
11	9.781	1304	1308	1312	rBV2	802046	729220	34.11%	3.630%
12	10.569	1438	1442	1445	rBV	1098703	936876	43.82%	4.664%
13	10.692	1460	1463	1469	rVB	39666	37392	1.75%	0.186%
14	11.263	1556	1560	1563	rBV	770023	669103	31.30%	3.331%
15	11.286	1563	1564	1567	rVV	133750	77259	3.61%	0.385%
16	11.339	1570	1573	1576	rVB	31906	29175	1.36%	0.145%
17	11.763	1640	1645	1648	rBV	23149	23525	1.10%	0.117%
18	11.792	1648	1650	1653	rVB	36002	27845	1.30%	0.139%
19	11.839	1653	1658	1660	rBV2	19382	21639	1.01%	0.108%
20	11.874	1660	1664	1667	rBV	49225	52509	2.46%	0.261%
21	12.316	1735	1739	1742	rBV2	38173	42891	2.01%	0.214%
22	12.398	1750	1753	1758	rVB4	26695	31287	1.46%	0.156%
23	12.474	1762	1766	1769	rBV	429085	374346	17.51%	1.864%
24	12.698	1799	1804	1807	rBV	405876	434848	20.34%	2.165%
25	12.751	1810	1813	1818	rVB2	22465	28135	1.32%	0.140%
26	12.851	1826	1830	1833	rBV	1697088	1527060	71.43%	7.602%
27	12.921	1837	1842	1845	rBV3	35244	57165	2.67%	0.285%
28	13.004	1853	1856	1858	rBV3	25456	32255	1.51%	0.161%
29	13.027	1858	1860	1863	rVB	53893	45234	2.12%	0.225%
30	13.092	1869	1871	1874	rBV2	27926	25937	1.21%	0.129%
31	13.133	1874	1878	1881	rBV2	48965	52153	2.44%	0.260%
32	13.221	1891	1893	1896	rVB	28176	21791	1.02%	0.108%
33	13.257	1896	1899	1901	rBV	30844	28262	1.32%	0.141%
34	13.533	1943	1946	1952	rVB	28347	35868	1.68%	0.179%

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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

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35	13.639	1961	1964	1968	rBV3	35622	63073	2.95%	0.314%
36	13.751	1979	1983	1988	rVB2	102398	117569	5.50%	0.585%
37	13.898	2000	2008	2010	rBV2	726186	925836	43.31%	4.609%
38	13.921	2010	2012	2014	rVB	172338	128858	6.03%	0.641%
39	13.998	2023	2025	2028	rVB	39462	35199	1.65%	0.175%
40	14.280	2071	2073	2076	rVB	38733	34533	1.62%	0.172%
41	14.316	2077	2079	2082	rVB2	34962	25143	1.18%	0.125%
42	14.910	2177	2180	2183	rBV	144881	195231	9.13%	0.972%
43	15.198	2226	2229	2234	rVB	80177	94719	4.43%	0.472%
44	15.257	2235	2239	2244	rVB	121523	144357	6.75%	0.719%
45	15.315	2245	2249	2253	rBV	348184	395298	18.49%	1.968%

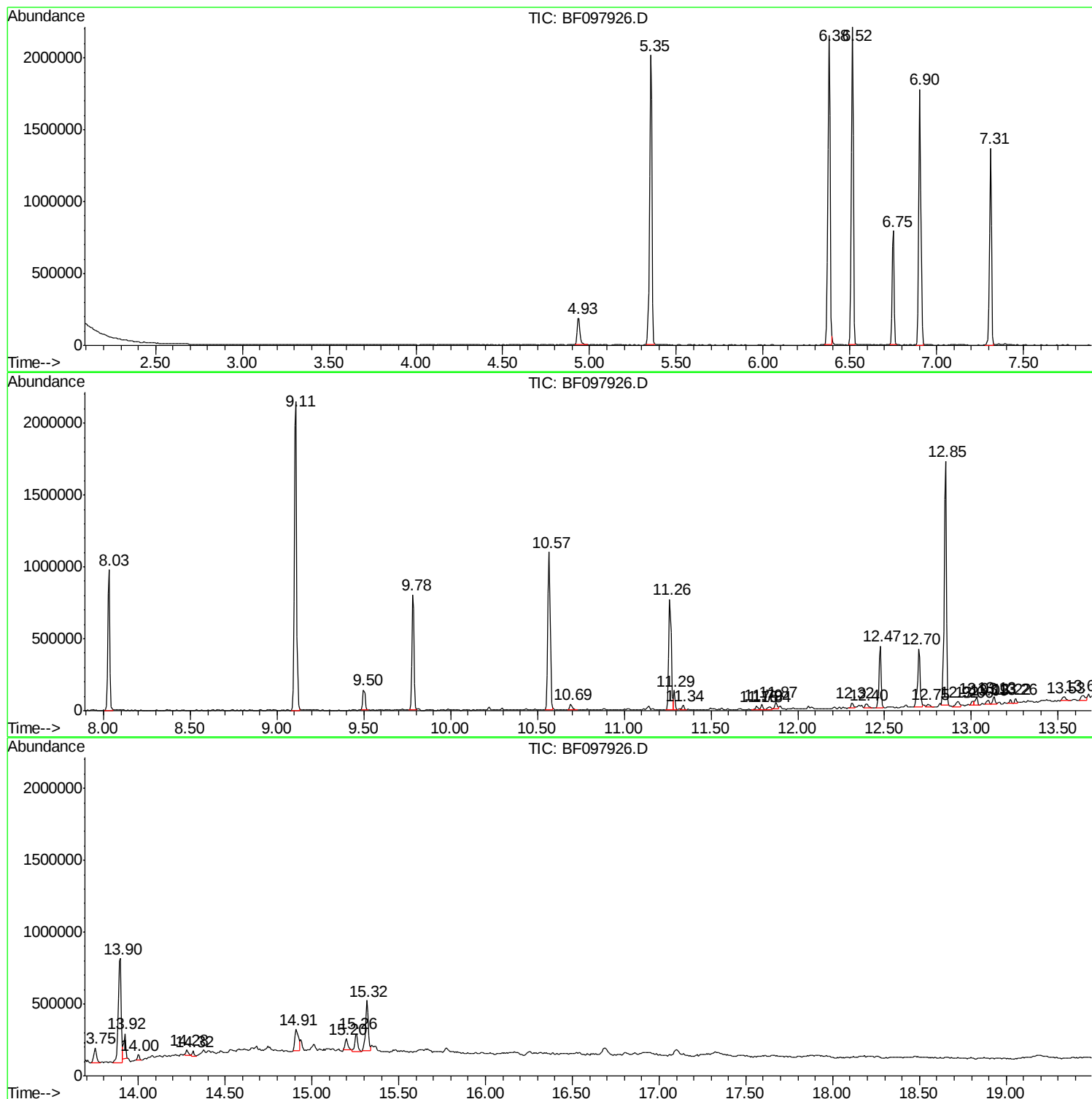
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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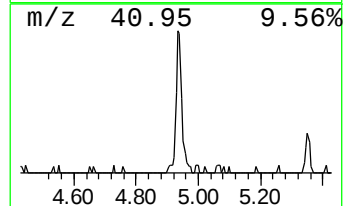
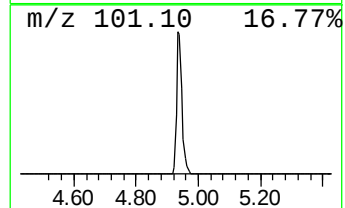
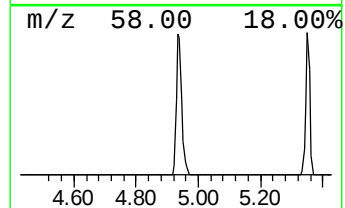
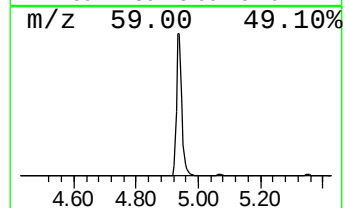
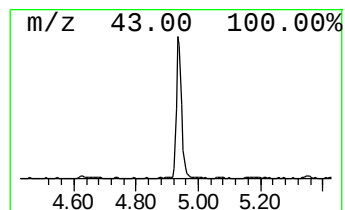
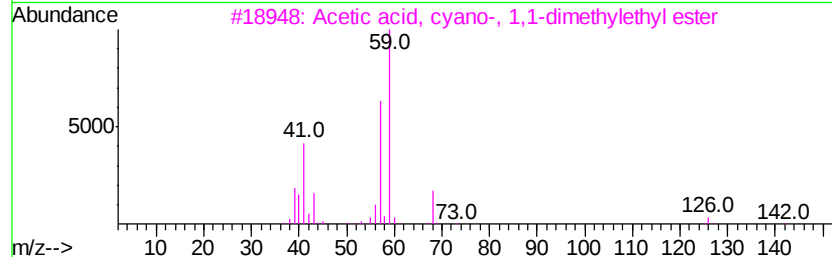
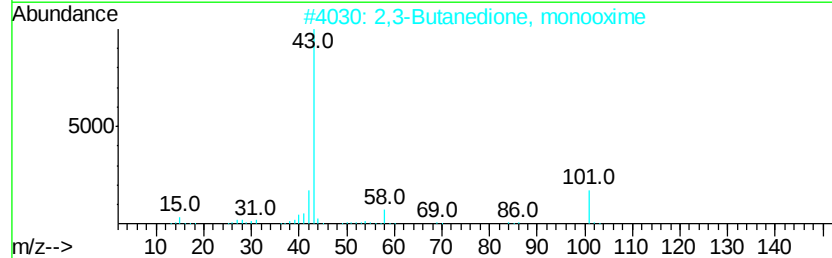
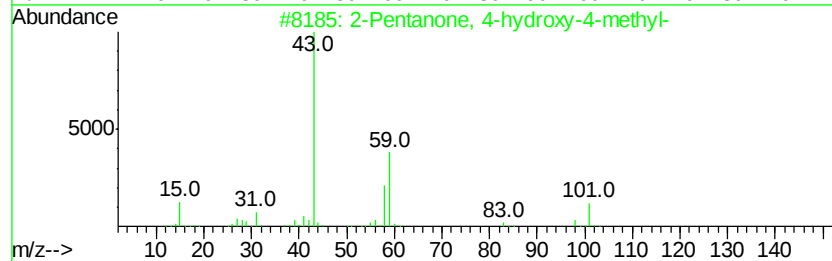
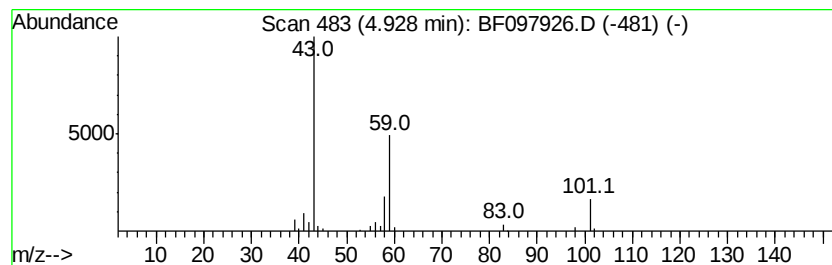
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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	6.66 ng	224210	1,4-Dichlorobenzene-d4	6.75

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53	
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25	
3	Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23	
4	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9	
5	Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9	



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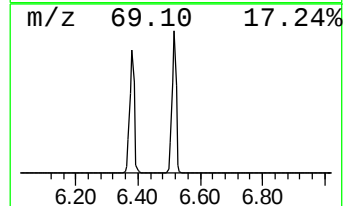
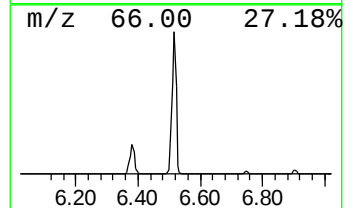
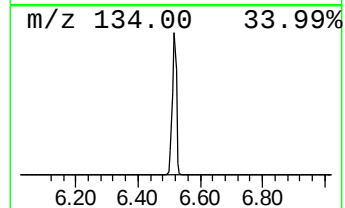
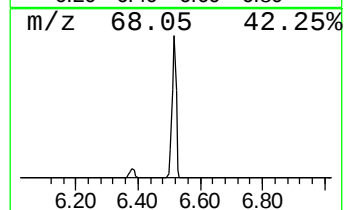
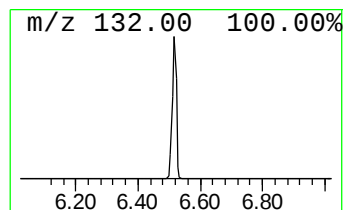
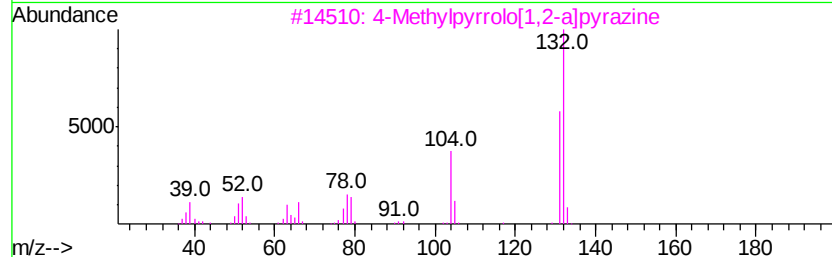
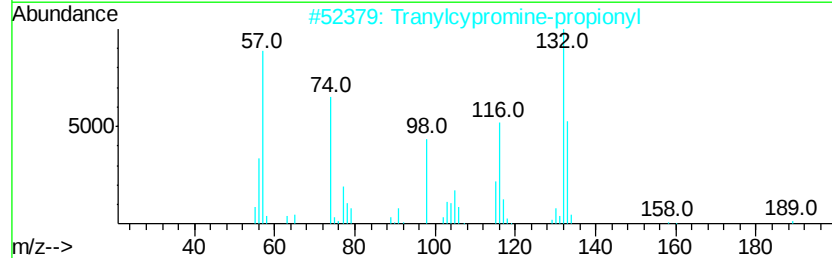
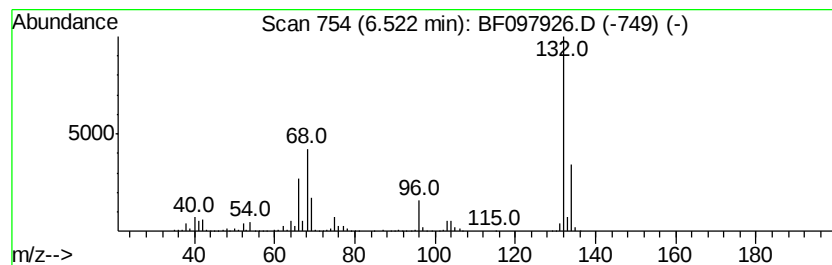
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Peak Number 2 unknown6.52 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.52	59.24 ng	1993780	1,4-Dichlorobenzene-d4	6.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
4		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9
5		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9



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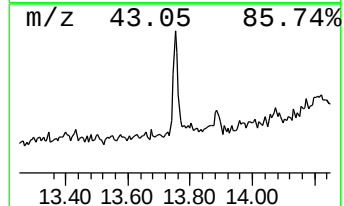
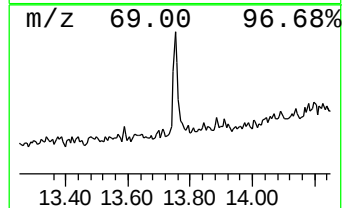
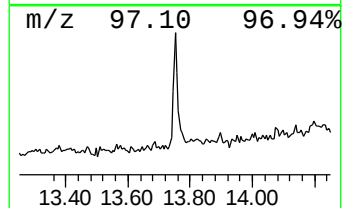
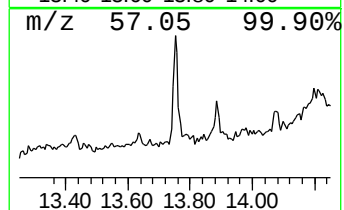
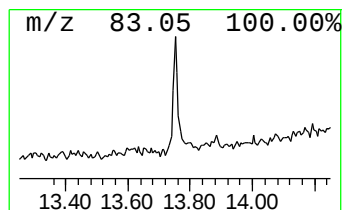
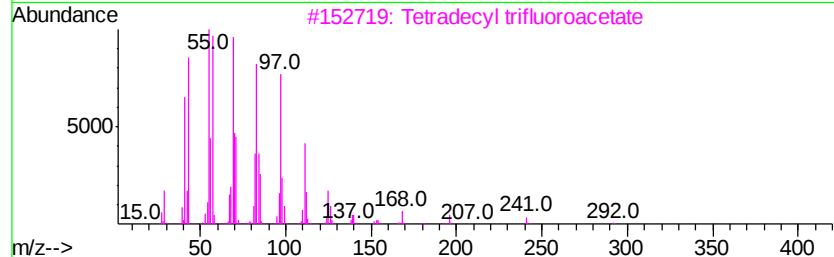
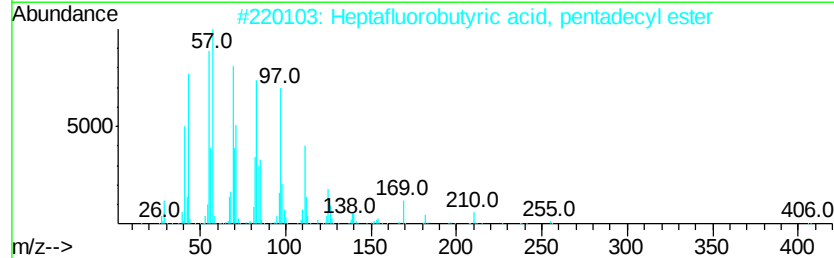
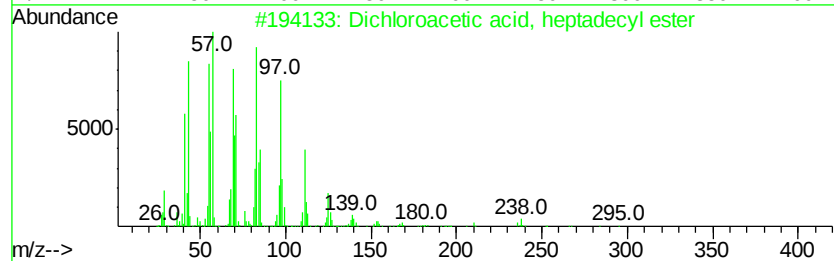
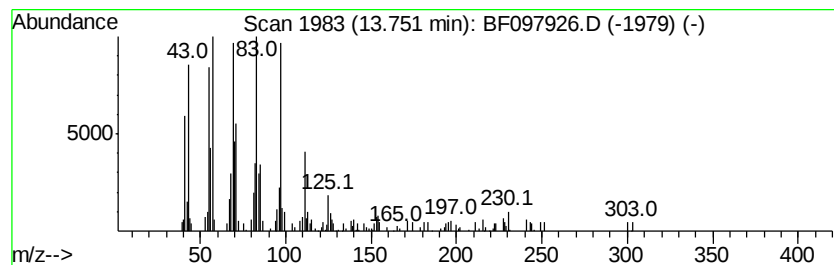
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Dichloroacetic acid, heptad... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.75	2.54 ng	117569	Chrysene-d12	13.90	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	91
2	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
3	Tetradecyl trifluoroacetate	310	C16H29F3O2	006222-02-2	87
4	11-Tricosene	322	C23H46	052078-56-5	87
5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	83



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.93	6.7	ng	224210	1	6.75	673122	20.0
unknown6.52	6.52	59.2	ng	1993780	1	6.75	673122	20.0
Dichloroacetic ac...	13.75	2.5	ng	117569	5	13.90	925836	20.0