

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF090617\
 Data File : BF098291.D
 Acq On : 6 Sep 2017 23:54
 Operator : SJ/JU
 Sample : I5075-04
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 72-12020

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	4.875	471	474	487	rVB	111651	143612	7.46%	0.861%
2	5.304	542	547	550	rBV	1875403	1813330	94.21%	10.866%
3	6.340	719	723	726	rBV	1953043	1924725	100.00%	11.534%
4	6.469	740	745	748	rBV	2004932	1830887	95.12%	10.971%
5	6.698	780	784	791	rBV	791953	699294	36.33%	4.190%
6	6.851	806	810	813	rBV	1456788	1196182	62.15%	7.168%
7	7.263	875	880	883	rBV	1263653	1091843	56.73%	6.543%
8	7.298	883	886	889	rVB2	18049	20392	1.06%	0.122%
9	7.981	996	1002	1005	rBV	1044506	896587	46.58%	5.373%
10	8.692	1120	1123	1126	rBV	54756	38376	1.99%	0.230%
11	9.057	1181	1185	1188	rBV	1729186	1473029	76.53%	8.827%
12	9.139	1195	1199	1201	rBV2	26654	29391	1.53%	0.176%
13	9.175	1203	1205	1209	rVB	25218	24190	1.26%	0.145%
14	9.451	1248	1252	1256	rBV	308247	264074	13.72%	1.582%
15	9.669	1287	1289	1293	rBV3	22418	20788	1.08%	0.125%
16	9.733	1293	1300	1303	rVV	903626	811259	42.15%	4.861%
17	9.763	1303	1305	1309	rVB	61757	52860	2.75%	0.317%
18	9.933	1331	1334	1340	rVB	39640	41092	2.13%	0.246%
19	10.139	1366	1369	1371	rBV4	21012	25191	1.31%	0.151%
20	10.169	1371	1374	1376	rVB	31165	26068	1.35%	0.156%
21	10.275	1389	1392	1400	rBV	42181	42722	2.22%	0.256%
22	10.522	1430	1434	1438	rBV	778145	733094	38.09%	4.393%
23	10.639	1451	1454	1459	rBV	55579	66108	3.43%	0.396%
24	11.086	1523	1530	1532	rBV2	41124	39917	2.07%	0.239%
25	11.116	1532	1535	1539	rVB2	29514	30499	1.58%	0.183%
26	11.216	1548	1552	1554	rBV	779638	682135	35.44%	4.088%
27	11.233	1554	1555	1559	rVV	89499	73132	3.80%	0.438%
28	11.286	1561	1564	1567	rVB	26715	29448	1.53%	0.176%
29	12.421	1754	1757	1761	rBV	99164	85376	4.44%	0.512%
30	12.651	1791	1796	1798	rBV	101241	101661	5.28%	0.609%
31	12.798	1817	1821	1824	rBV	1117373	983325	51.09%	5.892%
32	13.492	1936	1939	1944	rBV6	27811	42332	2.20%	0.254%
33	13.698	1971	1974	1980	rBV2	93668	127379	6.62%	0.763%
34	13.851	1995	2000	2002	rBV	706301	726011	37.72%	4.350%

LSC Area Percent Report

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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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Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.257	2235	2239	2248	rVB	385899	501700	26.07%	3.006%
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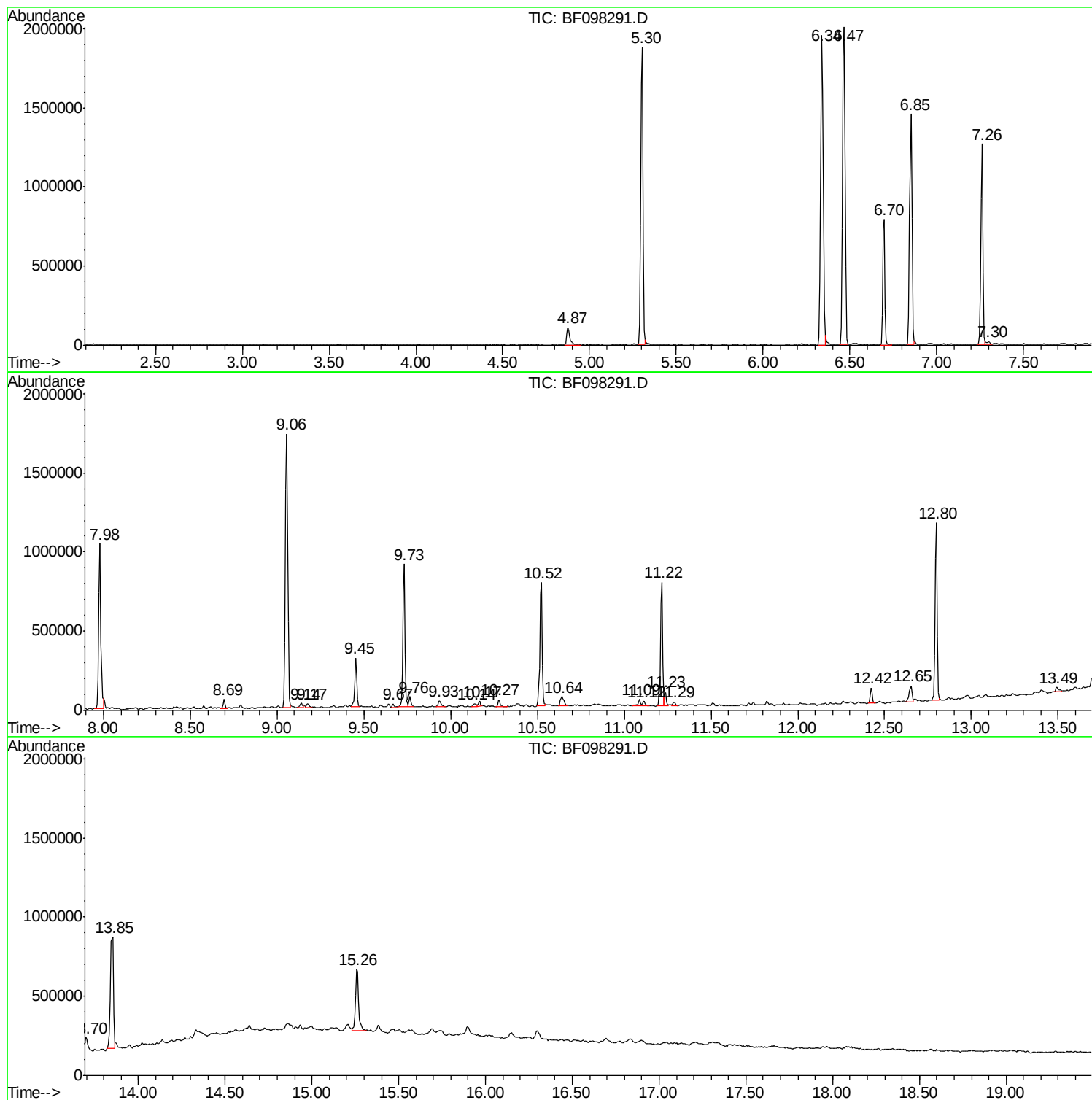
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF081517.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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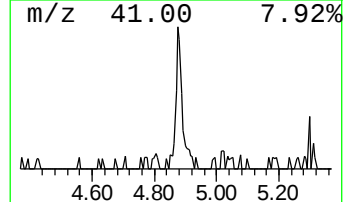
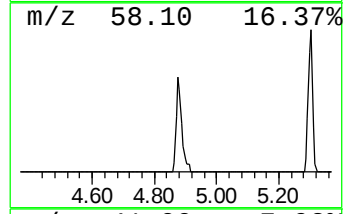
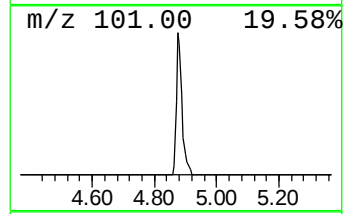
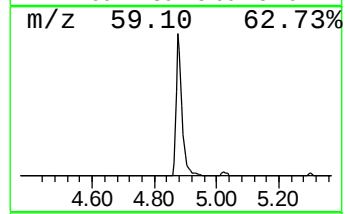
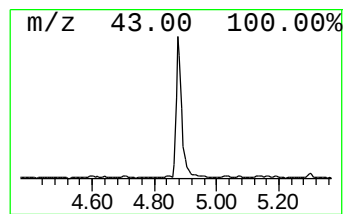
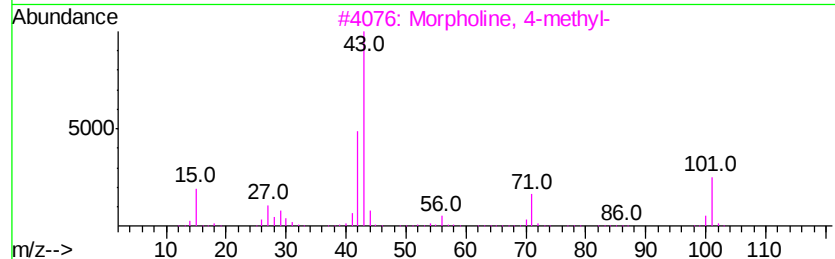
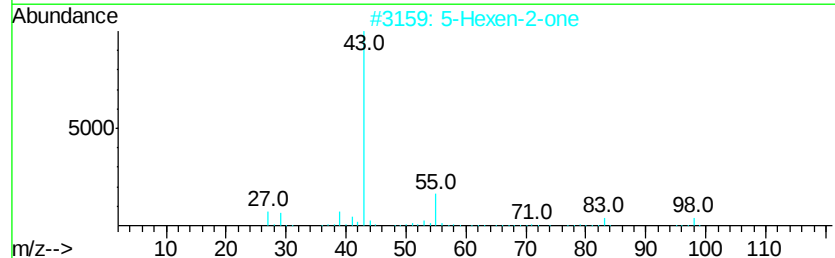
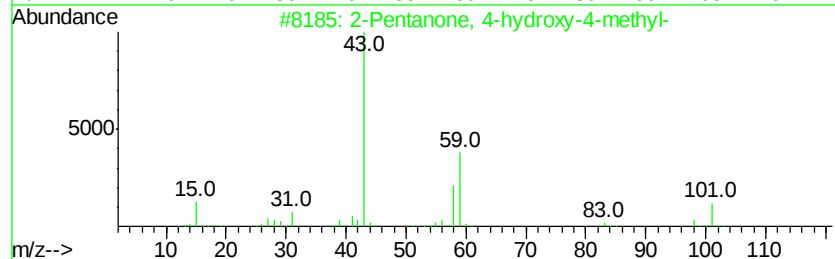
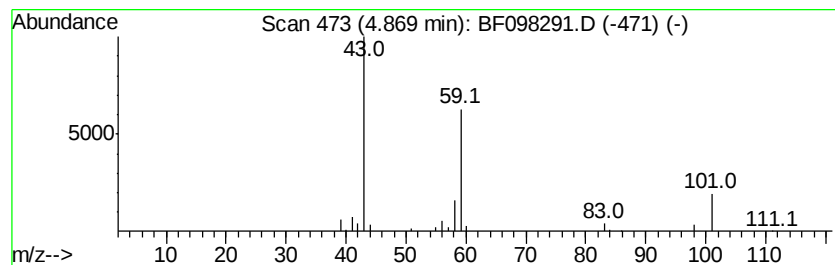
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.87	4.11 ng	143612	1,4-Dichlorobenzene-d4	6.70

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	9



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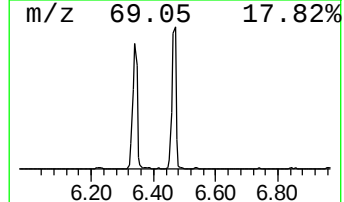
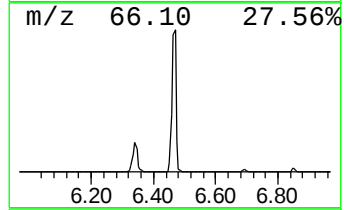
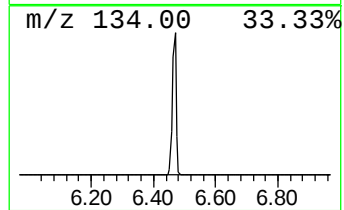
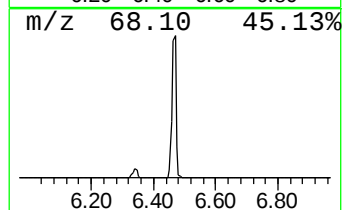
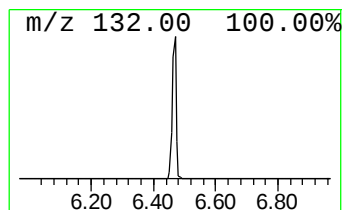
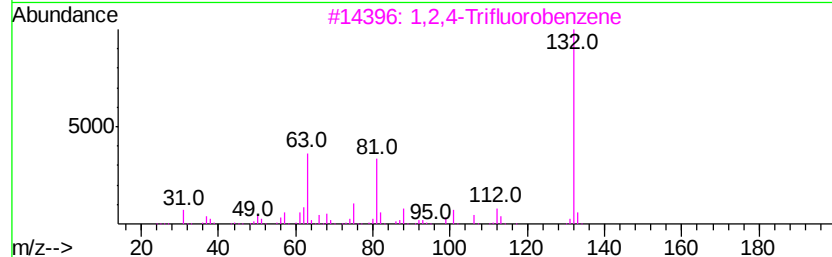
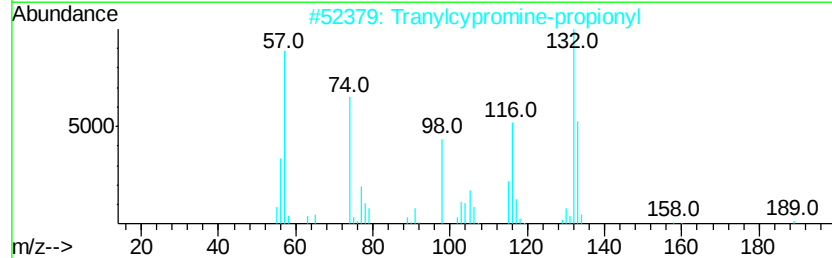
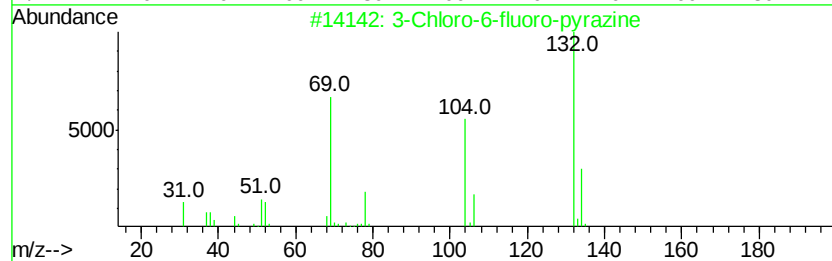
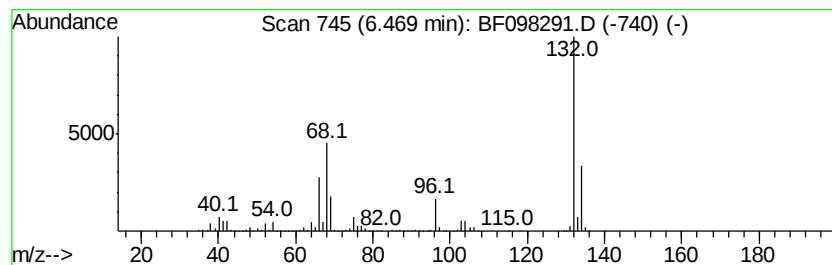
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Peak Number 2 unknown6.47 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.47	52.36 ng	1830890	1,4-Dichlorobenzene-d4	6.70

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		1,2,4-Trifluorobenzene	132	C6H3F3	000367-23-7	9
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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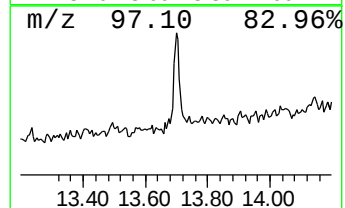
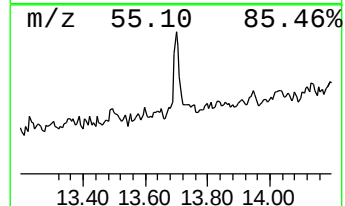
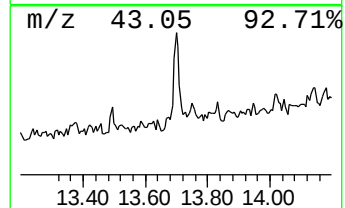
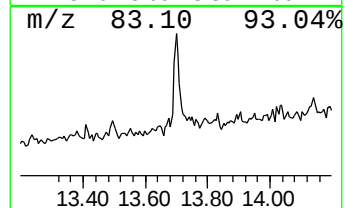
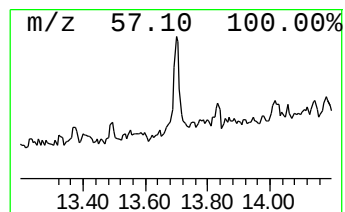
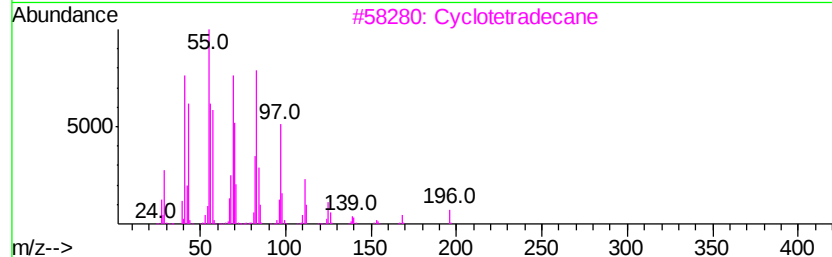
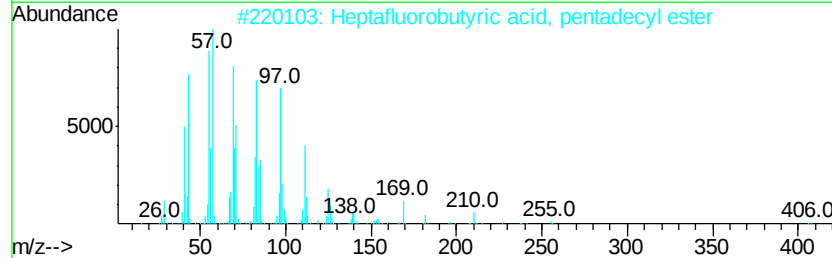
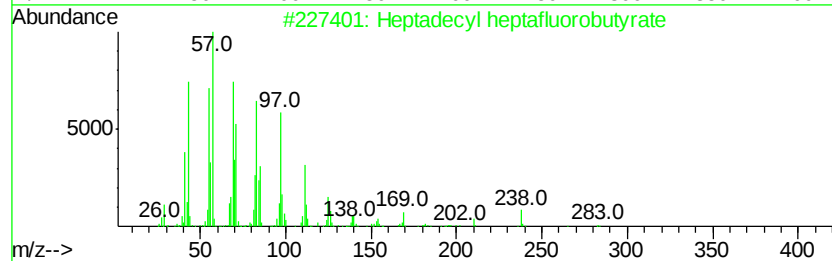
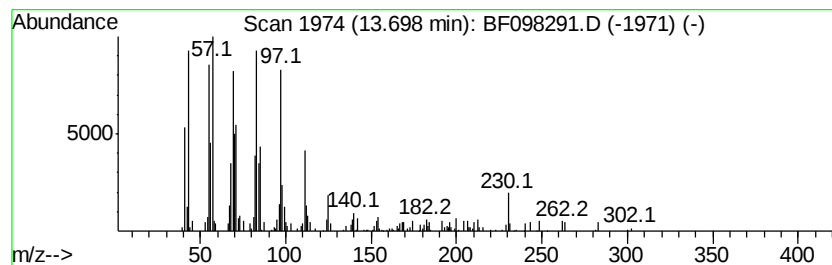
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 5 Heptadecyl heptafluorobutyrate Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.70	3.51 ng	127379	Chrysene-d12	13.85	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	94
2	Heptafluorobutyric acid, pentadecyl ester	424	C19H31F7O2	959261-23-5	94
3	Cyclotetradecane	196	C14H28	000295-17-0	93
4	Trifluoroacetic acid, pentadecyl ester	324	C17H31F3O2	959010-23-2	93
5	Pentafluoropropionic acid, pentadecyl ester	374	C18H31F5O2	959092-08-1	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.87	4.1	ng	143612	1	6.70	699294	20.0
unknown6.47	6.47	52.4	ng	1830890	1	6.70	699294	20.0
Heptadecyl heptaf...	13.70	3.5	ng	127379	5	13.85	726011	20.0