

Data Path : Z:\HPCHEM1\BNA F\DATA\BF071717\
 Data File : BF096833.D
 Acq On : 17 Jul 2017 21:37
 Operator : SJ/JU
 Sample : I4216-01
 Misc :
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VITALE-FILL-1A

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-BF071317.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	2.893	152	154	159	rBV2	17062	32611	1.46%	0.161%
2	4.787	472	476	483	rBV	158501	213456	9.58%	1.054%
3	5.222	545	550	563	rBV	2183197	2211207	99.20%	10.917%
4	6.263	722	727	737	rBV	1957970	2229127	100.00%	11.005%
5	6.387	743	748	751	rBV	2391210	2142189	96.10%	10.576%
6	6.610	783	786	790	rBV	695985	585460	26.26%	2.890%
7	6.769	809	813	816	rBV	1908119	1645046	73.80%	8.122%
8	7.175	877	882	885	rBV	1406213	1309673	58.75%	6.466%
9	7.298	899	903	908	rVB	36601	37631	1.69%	0.186%
10	7.804	985	989	995	rBV	21667	23056	1.03%	0.114%
11	7.892	1000	1004	1007	rBV	940608	742625	33.31%	3.666%
12	8.969	1182	1187	1190	rBV	2354552	2040061	91.52%	10.072%
13	9.363	1250	1254	1257	rBV	389622	297601	13.35%	1.469%
14	9.639	1297	1301	1304	rBV	770679	652203	29.26%	3.220%
15	10.422	1430	1434	1438	rBV	1047558	914226	41.01%	4.513%
16	10.557	1454	1457	1464	rBV	40121	44411	1.99%	0.219%
17	11.004	1530	1533	1536	rBV2	41200	32312	1.45%	0.160%
18	11.116	1548	1552	1554	rBV	537634	507370	22.76%	2.505%
19	11.133	1554	1555	1558	rVB	154780	106427	4.77%	0.525%
20	11.186	1558	1564	1568	rBV	61413	48929	2.19%	0.242%
21	11.427	1602	1605	1611	rVB	28039	25364	1.14%	0.125%
22	11.639	1639	1641	1643	rBV	31508	29424	1.32%	0.145%
23	11.686	1647	1649	1652	rVB	27257	23555	1.06%	0.116%
24	11.722	1652	1655	1658	rBV	44087	48163	2.16%	0.238%
25	11.910	1682	1687	1689	rBV	23874	29258	1.31%	0.144%
26	12.163	1727	1730	1733	rBV2	20827	30108	1.35%	0.149%
27	12.316	1753	1756	1760	rBV	254512	233927	10.49%	1.155%
28	12.545	1789	1795	1797	rBV2	214108	254323	11.41%	1.256%
29	12.580	1797	1801	1806	rVB	105773	169465	7.60%	0.837%
30	12.698	1817	1821	1824	rVB	1618350	1536989	68.95%	7.588%
31	12.874	1849	1851	1855	rVB	66474	48076	2.16%	0.237%
32	12.939	1860	1862	1866	rVB3	50905	40288	1.81%	0.199%
33	12.974	1866	1868	1870	rBV2	32257	33251	1.49%	0.164%
34	13.069	1882	1884	1887	rVB3	30570	24965	1.12%	0.123%

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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

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	13.098	1887	1889	1891	rBV3	29143	24573	1.10%	0.121%
36	13.145	1895	1897	1899	rBV3	22100	23351	1.05%	0.115%
37	13.169	1899	1901	1907	rVB6	24788	40186	1.80%	0.198%
38	13.280	1918	1920	1924	rBV4	29349	38033	1.71%	0.188%
39	13.486	1953	1955	1958	rBV2	45949	54630	2.45%	0.270%
40	13.604	1970	1975	1983	rBV4	129121	225487	10.12%	1.113%
41	13.739	1993	1998	2000	rBV2	653702	718122	32.22%	3.545%
42	13.763	2000	2002	2005	rVB	105060	92515	4.15%	0.457%
43	14.027	2045	2047	2050	rBV3	33775	51303	2.30%	0.253%
44	14.121	2060	2063	2065	rVB2	54489	46263	2.08%	0.228%
45	14.733	2164	2167	2169	rBV	77741	90952	4.08%	0.449%
46	15.057	2219	2222	2225	rVB2	53575	59331	2.66%	0.293%
47	15.110	2227	2231	2235	rBV	370376	447894	20.09%	2.211%

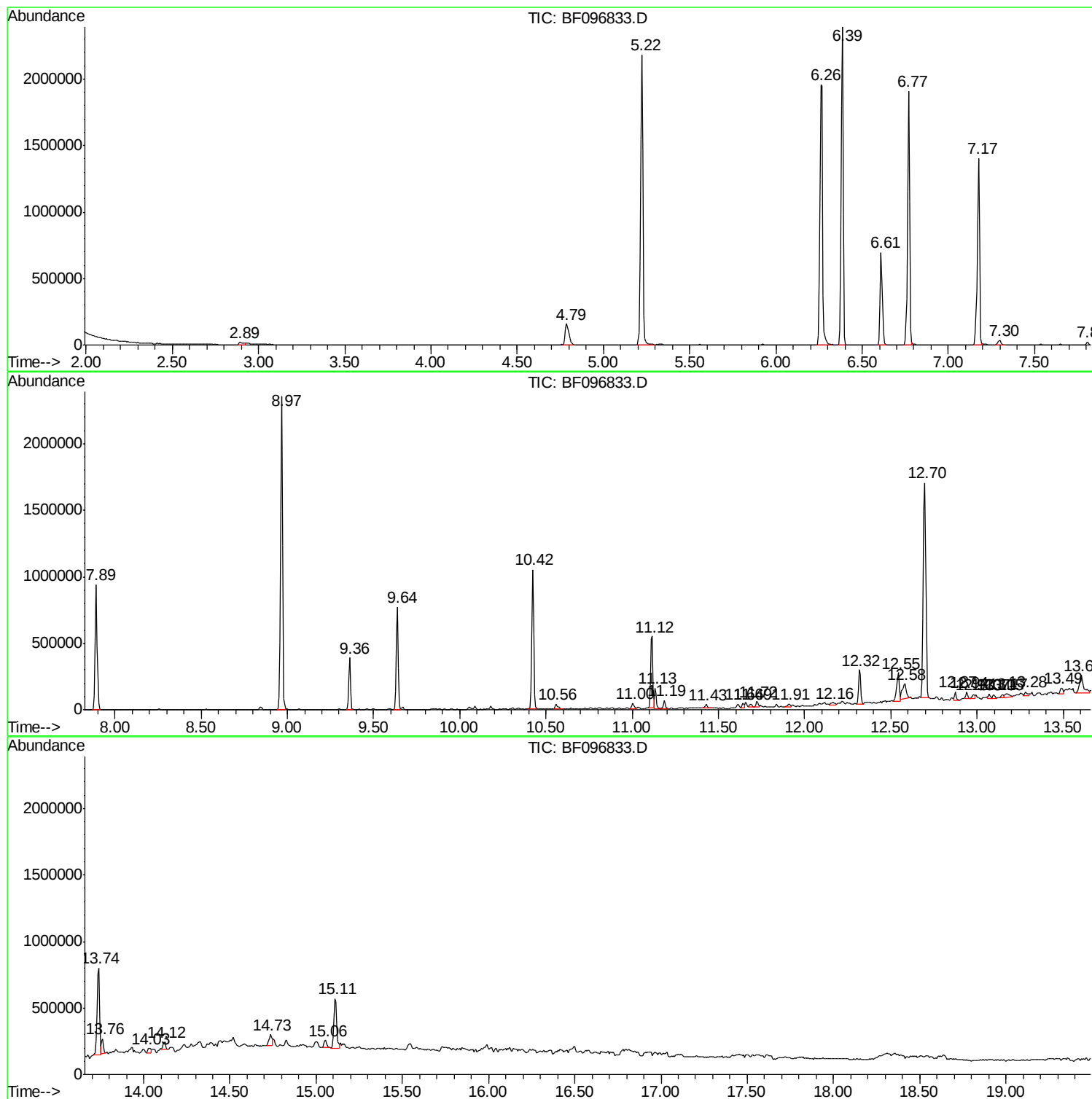
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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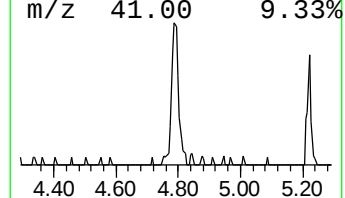
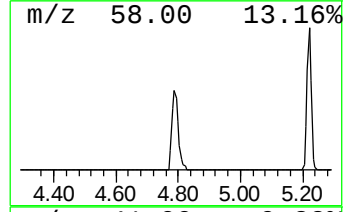
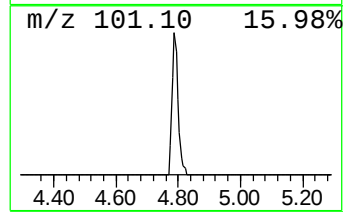
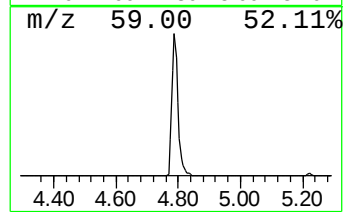
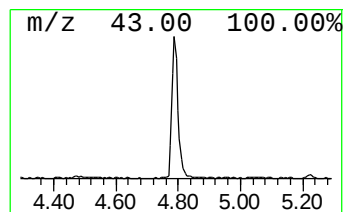
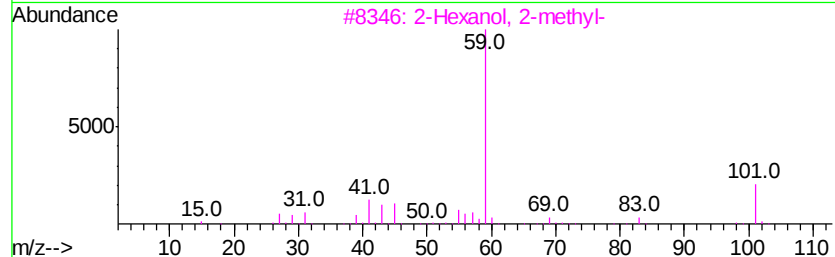
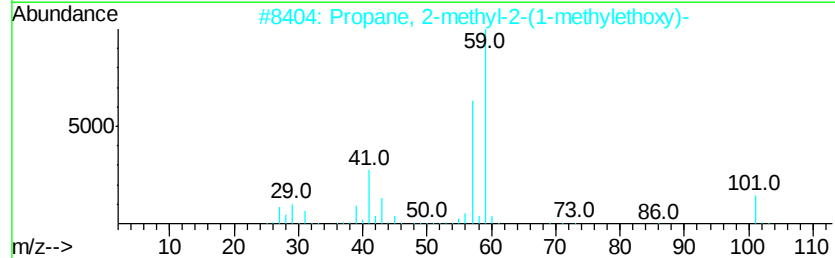
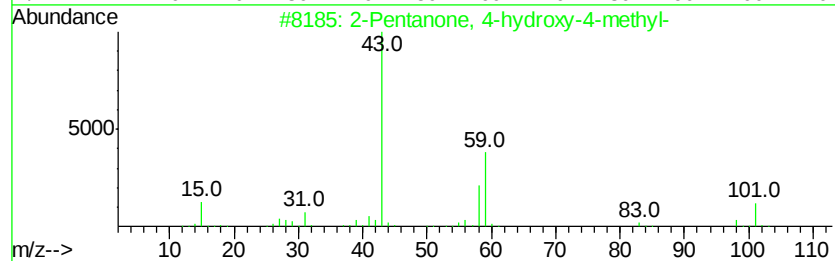
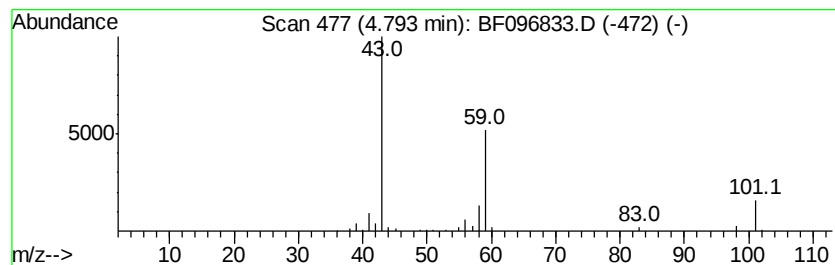
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.79	7.29 ng	213456	1,4-Dichlorobenzene-d4	6.61

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		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
4		3-Hexanol	102	C6H14O	000623-37-0	33
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27



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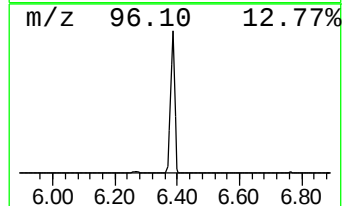
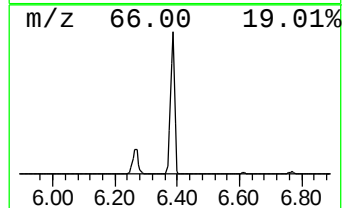
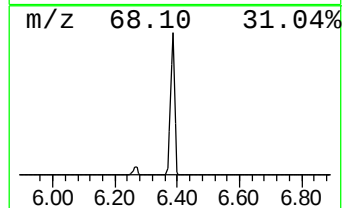
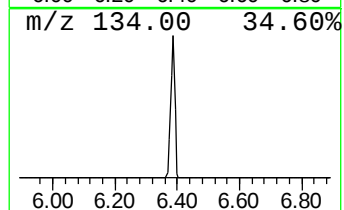
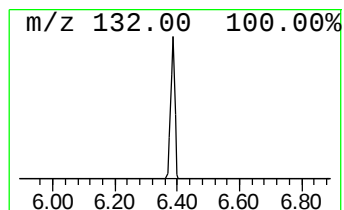
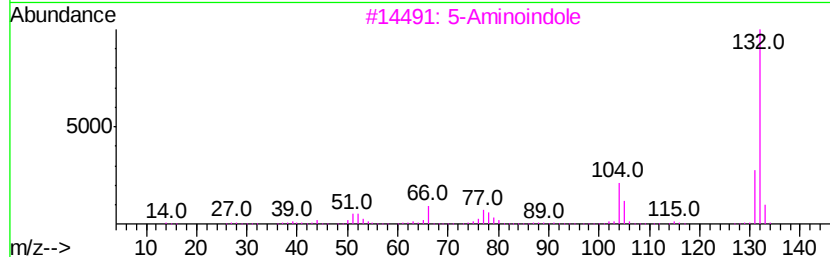
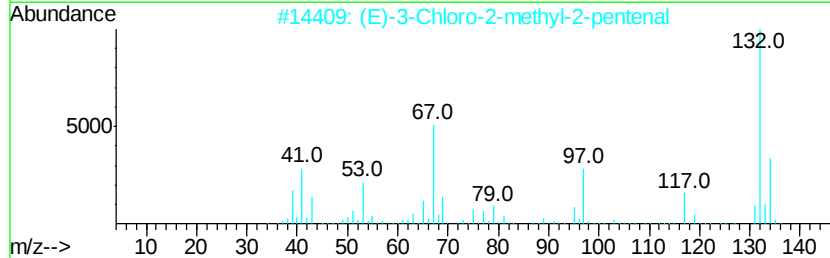
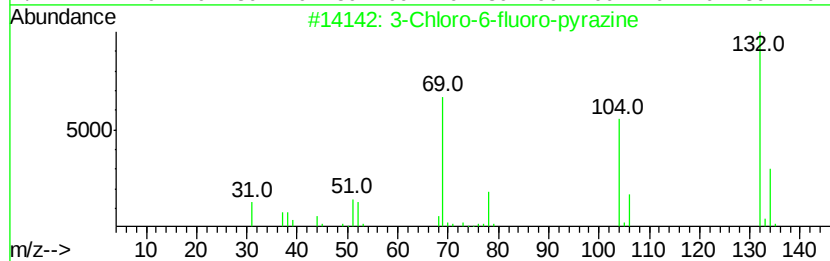
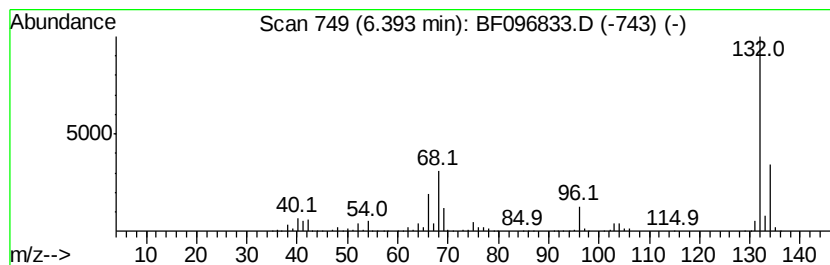
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Peak Number 2 unknown6.39 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.39	73.18 ng	2142190	1,4-Dichlorobenzene-d4	6.61

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		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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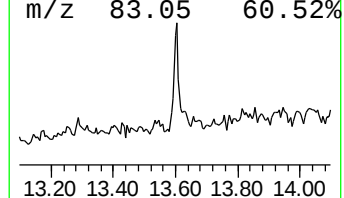
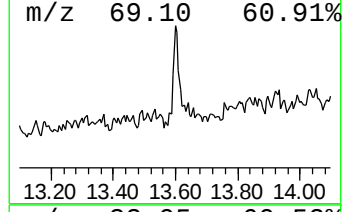
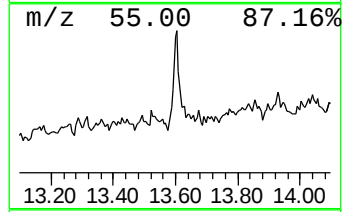
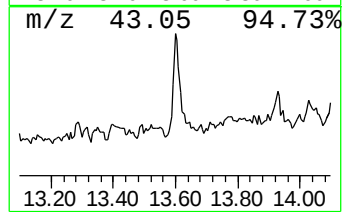
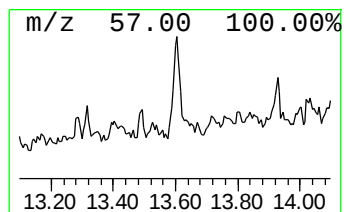
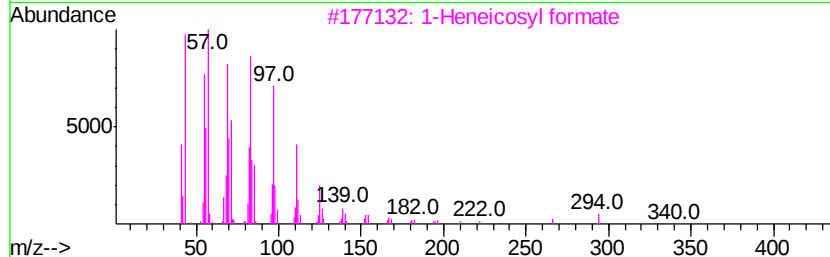
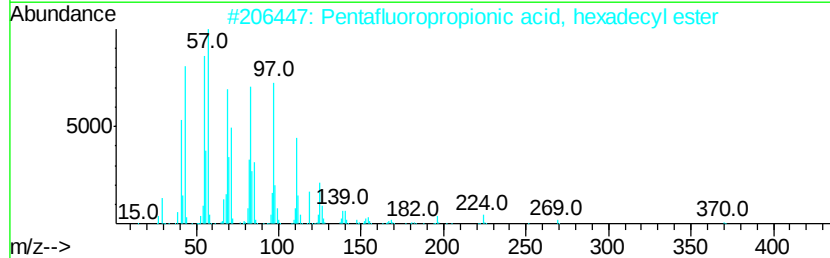
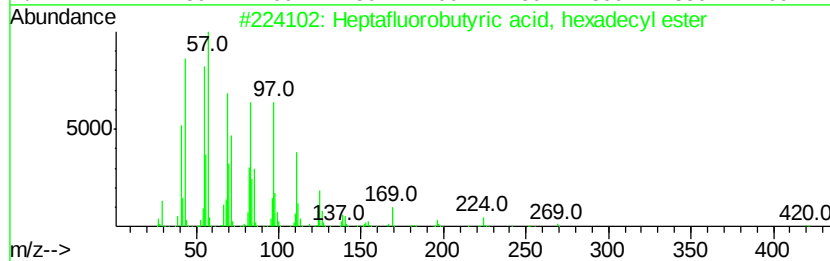
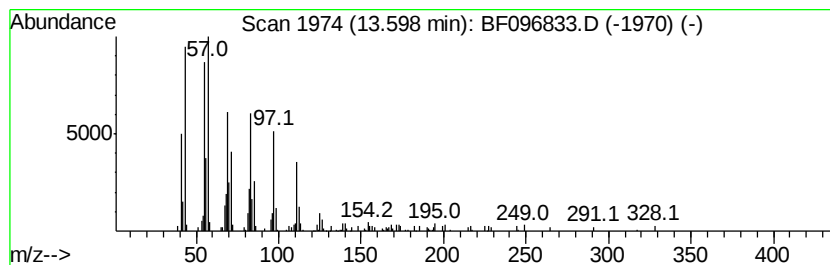
Instrument :
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 4 Heptafluorobutyric acid, he... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.60	6.28 ng	225487	Chrysene-d12		13.74	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutvric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3		1-Heneicosvl formate	340	C22H44O2	077899-03-7	91
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	91
5		5-Eicosene, (E)-	280	C20H40	074685-30-6	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.79	7.3	ng	213456	1	6.61	585460	20.0
unknown6.39	6.39	73.2	ng	2142190	1	6.61	585460	20.0
Heptafluorobutyri...	13.60	6.3	ng	225487	5	13.74	718122	20.0