

Data Path : Z:\HPCHEM1\BNA_F\Data\BF071417\
 Data File : BF096799.D
 Acq On : 15 Jul 2017 4:06
 Operator : SJ/JU
 Sample : I4187-09
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 CI-SB9-0-2

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	4.798	474	478	490	rVB	156043	210402	10.59%	1.157%
2	5.234	548	552	566	rBV	1852921	1884872	94.88%	10.363%
3	6.275	724	729	732	rBV	2069671	1986484	100.00%	10.922%
4	6.398	745	750	753	rBV	2082144	1902695	95.78%	10.461%
5	6.628	785	789	792	rBV	624519	568148	28.60%	3.124%
6	6.781	811	815	819	rBV	1607978	1411901	71.08%	7.763%
7	7.186	879	884	887	rBV	1236159	1134375	57.10%	6.237%
8	7.904	1002	1006	1010	rBV	922761	854455	43.01%	4.698%
9	8.986	1185	1190	1193	rBV	2122028	1936737	97.50%	10.648%
10	9.374	1253	1256	1260	rBV	298817	273054	13.75%	1.501%
11	9.657	1299	1304	1307	rBV	699862	645021	32.47%	3.546%
12	10.104	1377	1380	1383	rVB	34143	26636	1.34%	0.146%
13	10.439	1433	1437	1443	rBV	1031495	914512	46.04%	5.028%
14	10.574	1456	1460	1466	rVB	36259	45133	2.27%	0.248%
15	11.021	1532	1536	1539	rBV2	27319	23245	1.17%	0.128%
16	11.133	1551	1555	1557	rBV	609030	515145	25.93%	2.832%
17	11.151	1557	1558	1562	rVB	55055	42081	2.12%	0.231%
18	11.739	1655	1658	1661	rBV	29610	29263	1.47%	0.161%
19	12.180	1730	1733	1736	rBV	19672	20741	1.04%	0.114%
20	12.339	1756	1760	1764	rBV	178439	153192	7.71%	0.842%
21	12.563	1793	1798	1801	rBV	204632	211068	10.63%	1.160%
22	12.715	1820	1824	1828	rVB	1367436	1263478	63.60%	6.947%
23	12.786	1832	1836	1839	rBV3	18785	24082	1.21%	0.132%
24	12.880	1847	1852	1853	rBV5	15588	23311	1.17%	0.128%
25	12.892	1853	1854	1858	rVB	26866	21724	1.09%	0.119%
26	12.998	1868	1872	1876	rBV	27887	27068	1.36%	0.149%
27	13.121	1890	1893	1897	rBV	22622	23877	1.20%	0.131%
28	13.510	1955	1959	1961	rBV2	26027	32761	1.65%	0.180%
29	13.627	1974	1979	1985	rVB3	78464	113095	5.69%	0.622%
30	13.757	1996	2001	2004	rBV2	679672	784368	39.49%	4.313%
31	13.786	2004	2006	2008	rVB	100294	82609	4.16%	0.454%
32	14.145	2065	2067	2071	rVB	30279	24015	1.21%	0.132%
33	14.257	2084	2086	2090	rVB2	48924	53614	2.70%	0.295%
34	14.551	2134	2136	2139	rVB3	24029	21302	1.07%	0.117%

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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
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35	14.674	2155	2157	2162	rVB4	37172	34539	1.74%	0.190%
36	14.756	2167	2171	2174	rBV	102635	148737	7.49%	0.818%
37	14.851	2185	2187	2189	rBV	53307	52347	2.64%	0.288%
38	15.027	2214	2217	2221	rVB	64866	73016	3.68%	0.401%
39	15.086	2224	2227	2232	rVB	72644	78624	3.96%	0.432%
40	15.139	2232	2236	2243	rBV	374984	463603	23.34%	2.549%
41	15.580	2308	2311	2315	rBV2	41526	52747	2.66%	0.290%

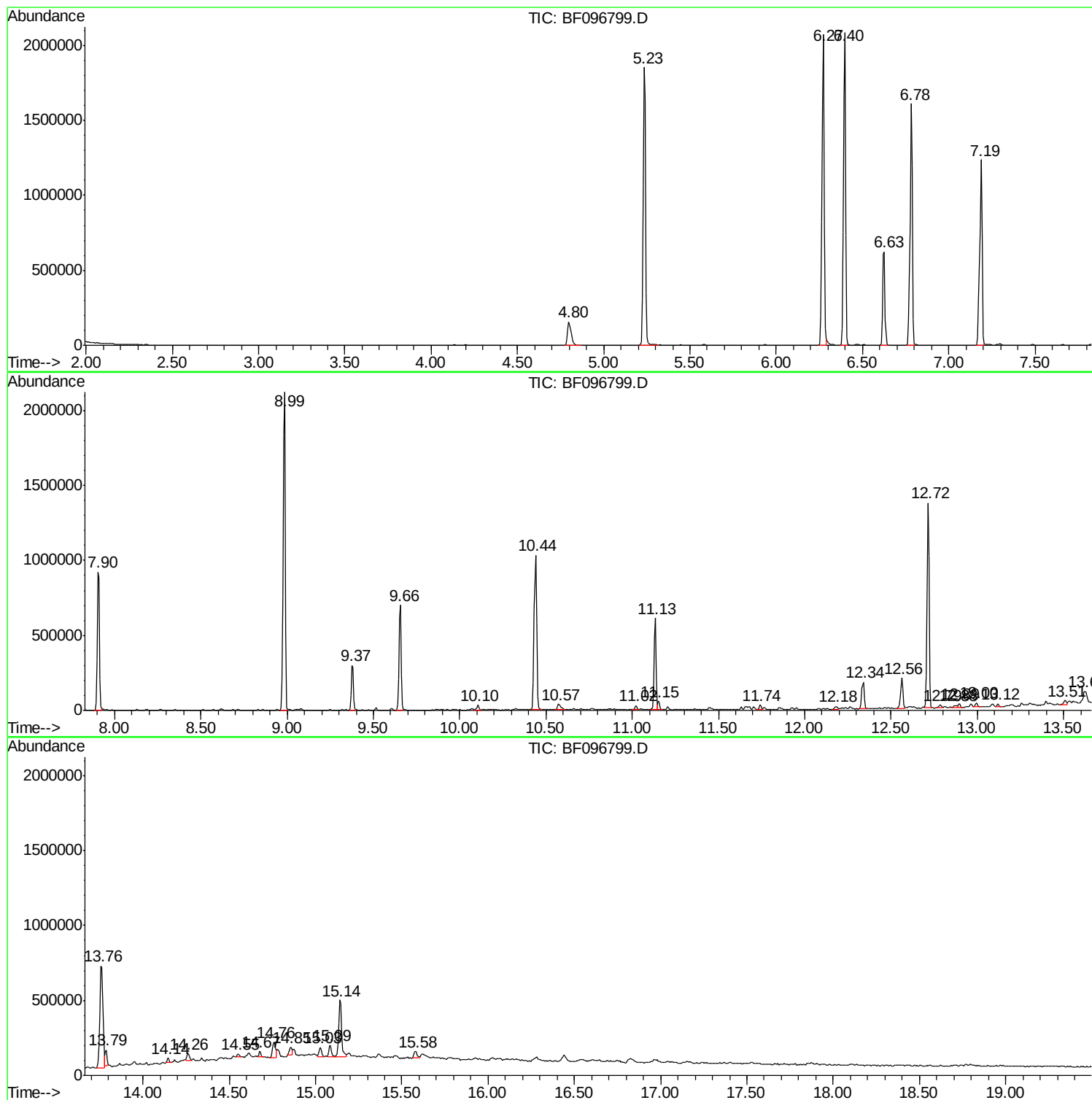
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF071317.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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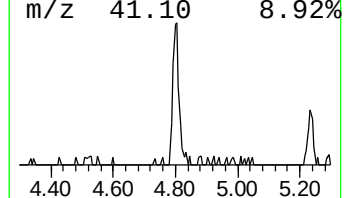
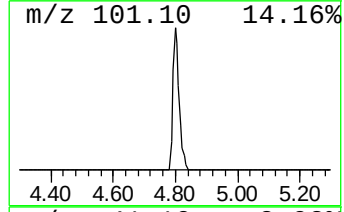
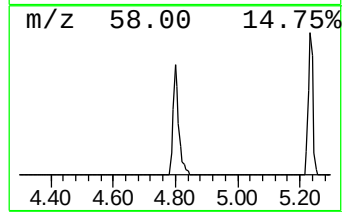
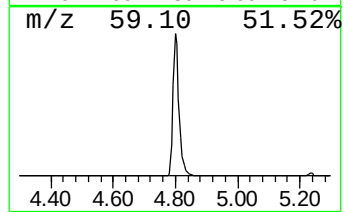
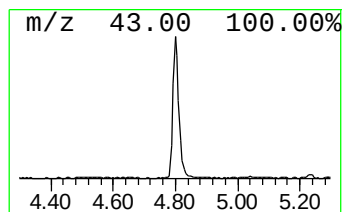
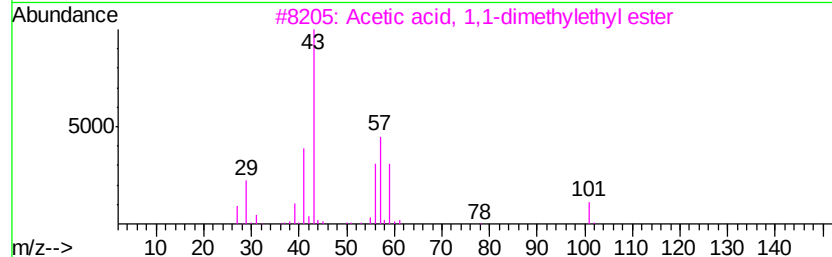
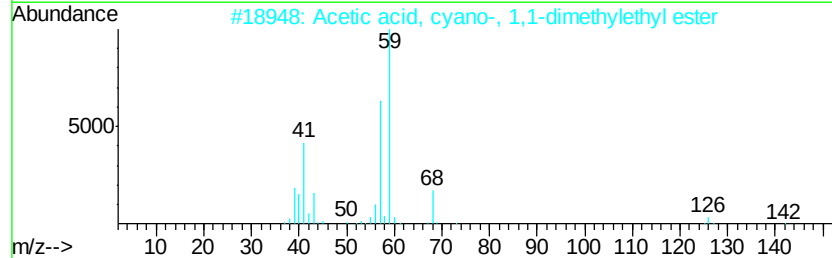
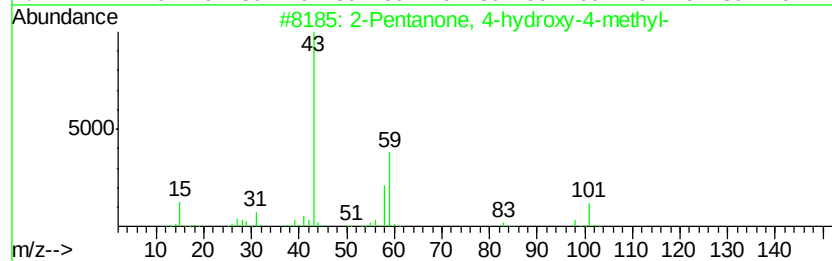
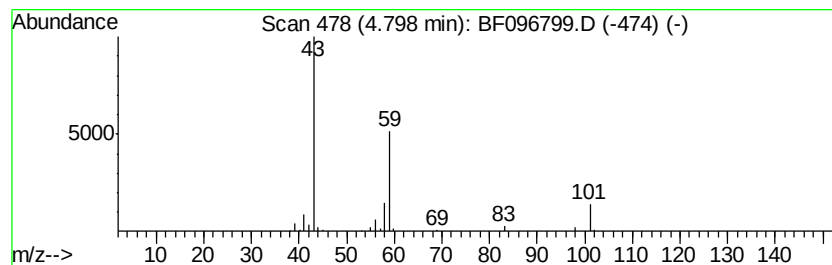
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
4.80	7.41 ng	210402	1,4-Dichlorobenzene-d4	6.63

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	17
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	9



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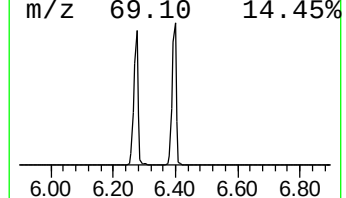
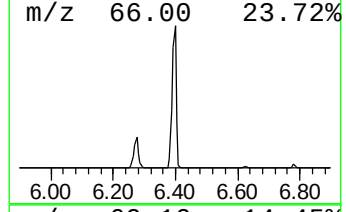
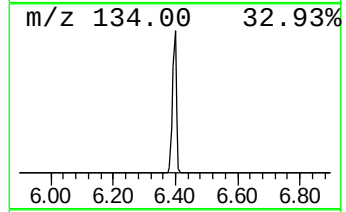
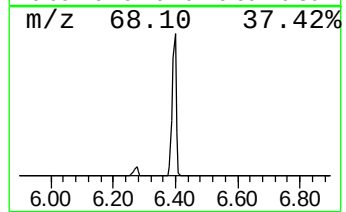
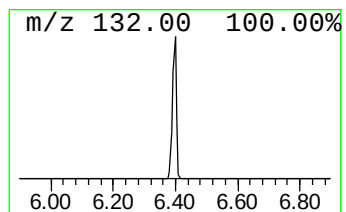
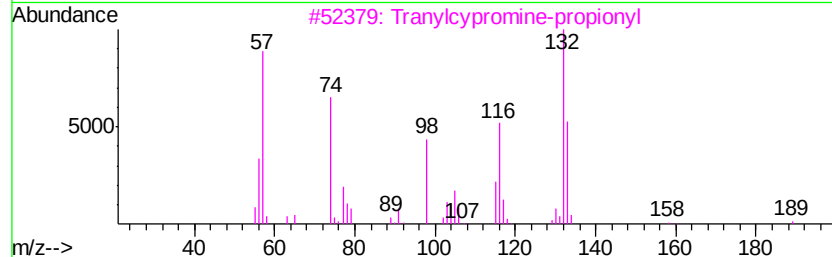
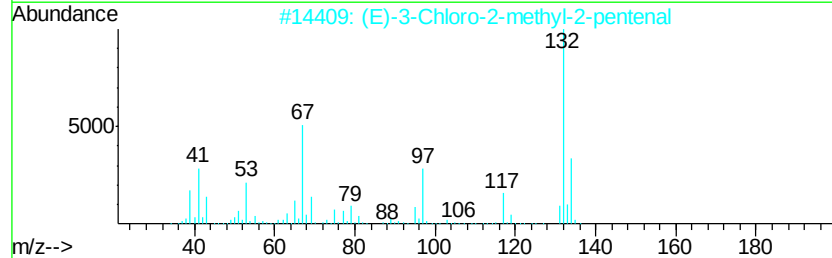
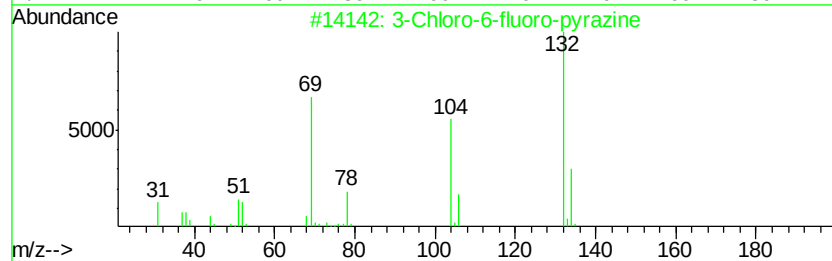
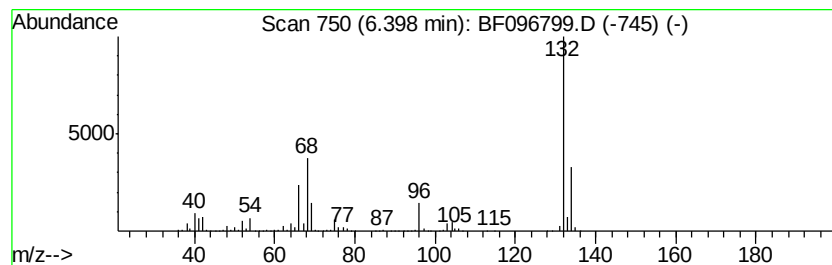
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Peak Number 2 unknown6.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.40	66.98 ng	1902700	1,4-Dichlorobenzene-d4	6.63

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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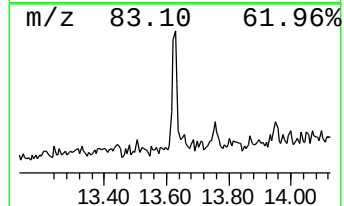
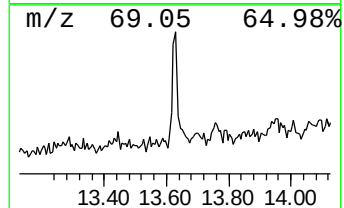
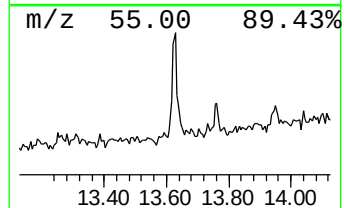
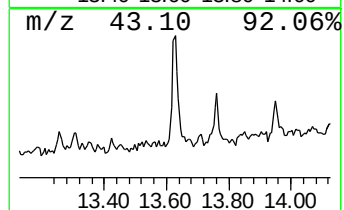
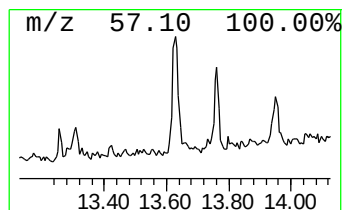
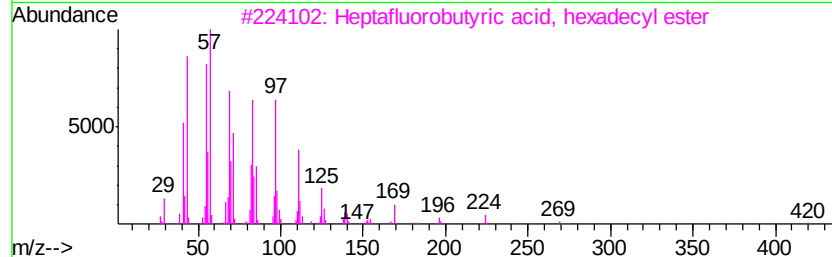
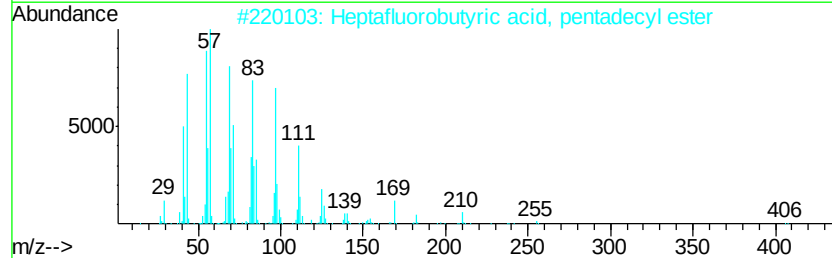
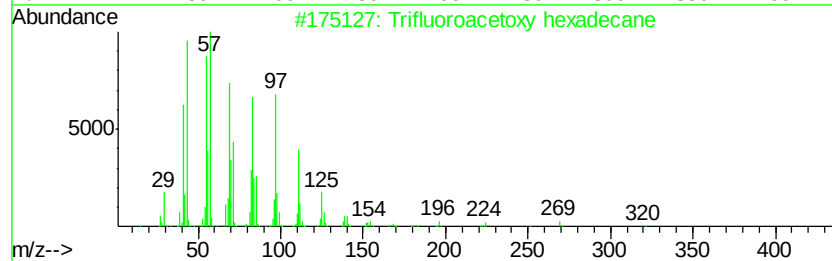
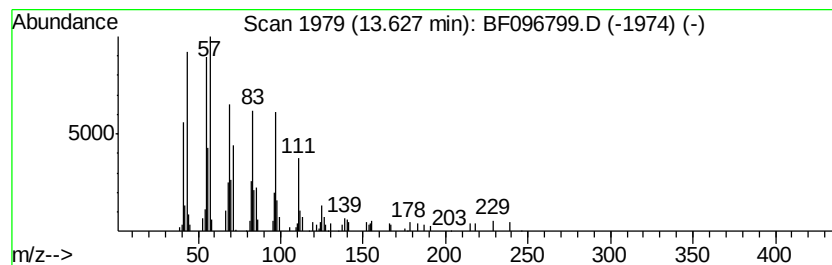
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Trifluoroacetoxy hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.63	2.88 ng	113095	Chrysene-d12	13.76	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	95
2	Heptafluorobutyric acid, pentadec...	424	C19H31F7O2	959261-23-5	93
3	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
4	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91



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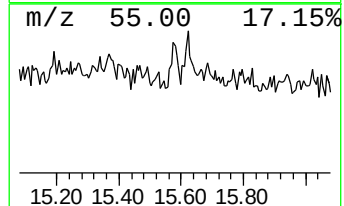
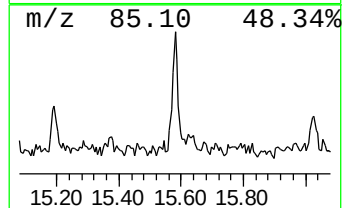
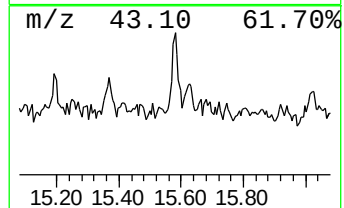
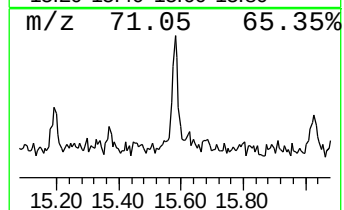
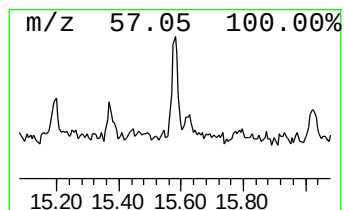
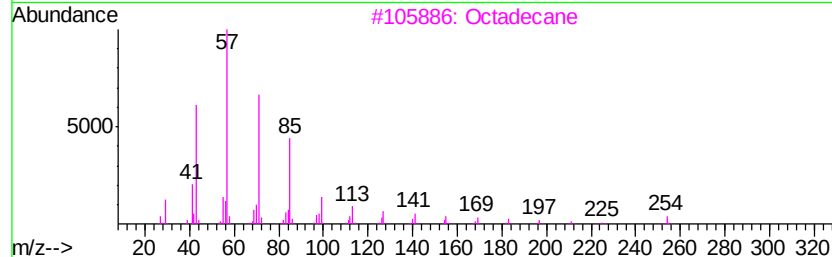
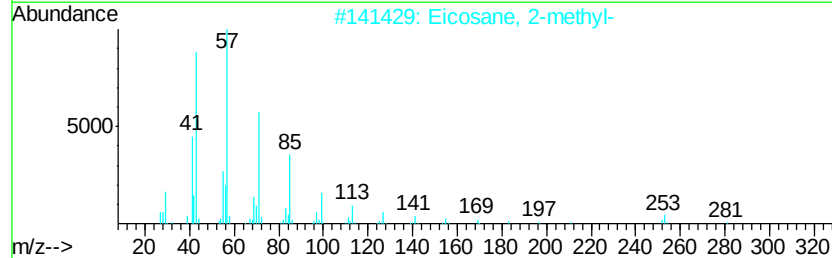
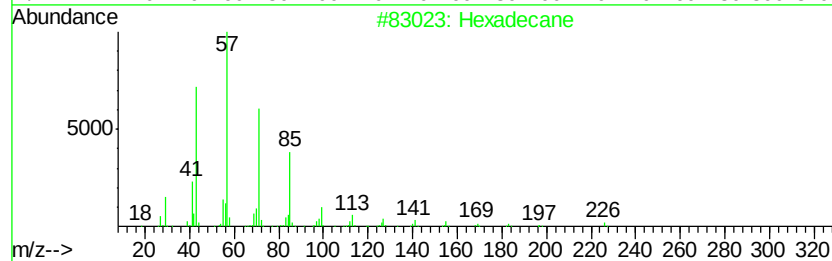
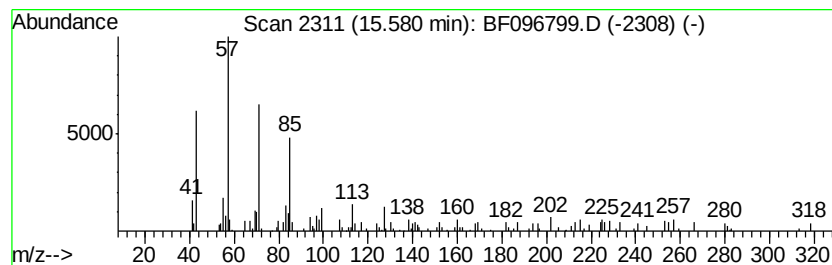
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Hexadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.58	2.28 ng	52747	Perylene-d12	15.14
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Hexadecane	226 C16H34	000544-76-3	64
2	Eicosane, 2-methyl-	296 C21H44	001560-84-5	58
3	Octadecane	254 C18H38	000593-45-3	58
4	Octacosane	394 C28H58	000630-02-4	58
5	Hexadecane, 2,6,10,14-tetramethyl-	282 C20H42	000638-36-8	55



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.80	7.4	ng	210402	1	6.63	568148	20.0
unknown6.40	6.40	67.0	ng	1902700	1	6.63	568148	20.0
Trifluoroacetoxy ...	13.63	2.9	ng	113095	5	13.76	784368	20.0
Hexadecane	15.58	2.3	ng	52747	6	15.14	463603	20.0