

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070117\
 Data File : BF096382.D
 Acq On : 1 Jul 2017 16:46
 Operator : SJ/MA
 Sample : I3939-01
 Misc :
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-13-2-4

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	4.916	476	481	488	rVB	309222	347665	14.48%	1.650%
2	5.340	548	553	556	rBV	2251195	2129365	88.66%	10.108%
3	6.369	722	728	732	rVB	2270958	2401828	100.00%	11.402%
4	6.498	746	750	754	rBV	2253681	2230870	92.88%	10.590%
5	6.734	786	790	793	rBV	782256	681592	28.38%	3.236%
6	6.886	812	816	820	rVB	1450826	1242448	51.73%	5.898%
7	7.292	879	885	888	rBV	1487285	1429637	59.52%	6.787%
8	7.386	896	901	906	rVB	44588	50974	2.12%	0.242%
9	7.722	951	958	960	rBV	61317	73356	3.05%	0.348%
10	8.016	1003	1008	1011	rBV	1083772	953976	39.72%	4.529%
11	9.092	1186	1191	1194	rBV	2237152	2014541	83.88%	9.563%
12	9.186	1203	1207	1209	rBV	33196	28282	1.18%	0.134%
13	9.480	1253	1257	1260	rBV	549074	411036	17.11%	1.951%
14	9.710	1293	1296	1301	rVB	73482	60856	2.53%	0.289%
15	9.763	1301	1305	1309	rBV	1046953	942954	39.26%	4.476%
16	9.969	1338	1340	1343	rVB	35804	29929	1.25%	0.142%
17	10.210	1378	1381	1384	rVB	101642	73060	3.04%	0.347%
18	10.433	1414	1419	1421	rBV	24418	34651	1.44%	0.164%
19	10.551	1434	1439	1442	rBV	1492097	1408042	58.62%	6.684%
20	10.680	1458	1461	1471	rVB	91333	102388	4.26%	0.486%
21	11.127	1534	1537	1540	rBV2	52350	44528	1.85%	0.211%
22	11.245	1553	1557	1559	rBV	809455	733641	30.55%	3.483%
23	11.263	1559	1560	1564	rVB	39276	28849	1.20%	0.137%
24	11.780	1644	1648	1652	rBV2	126120	127079	5.29%	0.603%
25	12.445	1759	1761	1765	rVB	82582	80027	3.33%	0.380%
26	12.563	1778	1781	1786	rBV3	50785	50860	2.12%	0.241%
27	12.674	1795	1800	1805	rVB	83739	104782	4.36%	0.497%
28	12.827	1822	1826	1829	rBV	1733946	1552818	64.65%	7.371%
29	13.727	1974	1979	1984	rBV2	138622	161406	6.72%	0.766%
30	13.868	1998	2003	2006	rBV	644699	641136	26.69%	3.044%
31	14.627	2130	2132	2135	rBV3	32828	30405	1.27%	0.144%
32	14.874	2171	2174	2183	rVB2	64862	136796	5.70%	0.649%
33	15.162	2220	2223	2226	rVB	41392	49454	2.06%	0.235%
34	15.215	2229	2232	2238	rVB	53198	63600	2.65%	0.302%

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Instrument :
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ClientSampleId :
SB-13-2-4

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-BF070117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.280	2238	2243	2247	rBV	504936	612581	25.50%	2.908%
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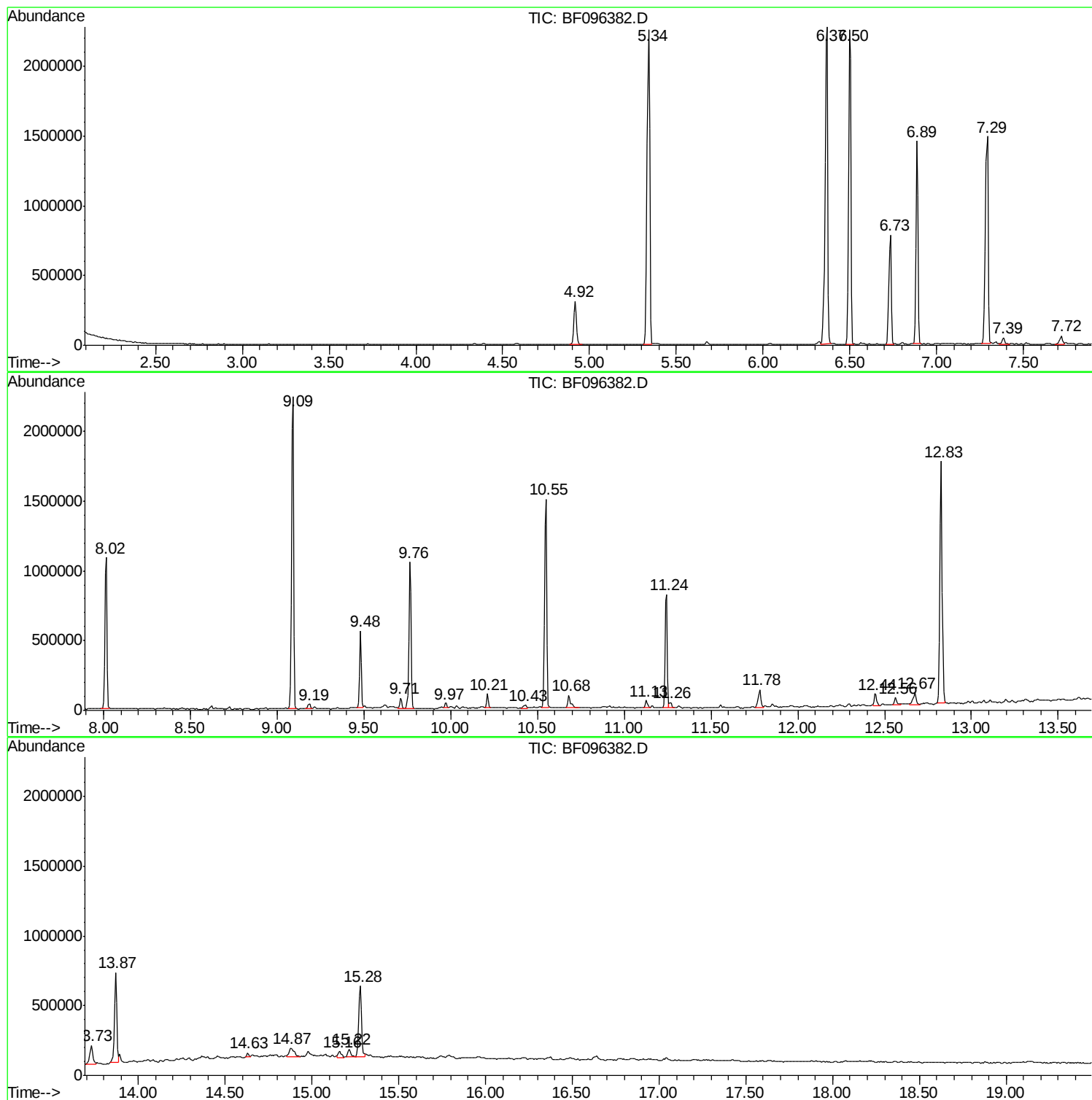
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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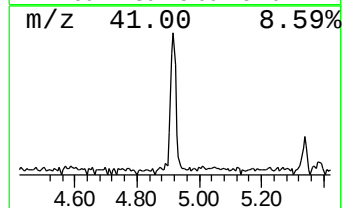
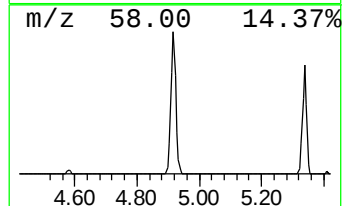
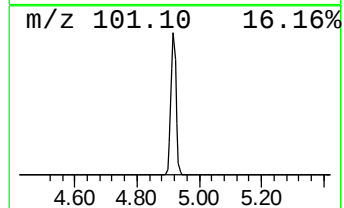
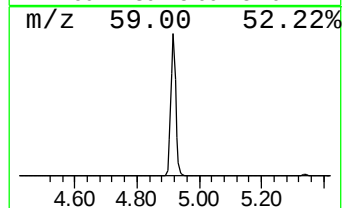
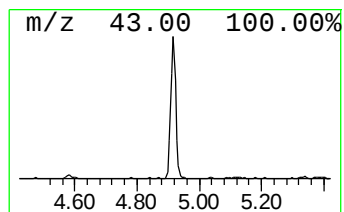
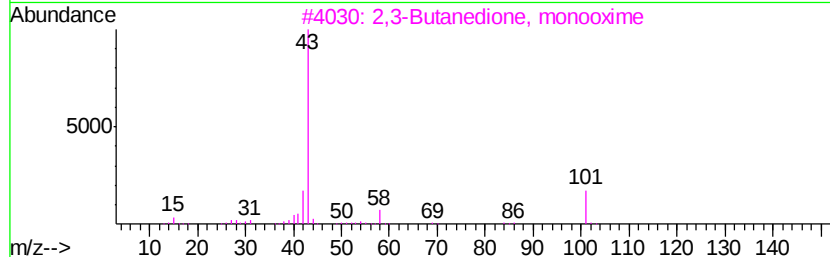
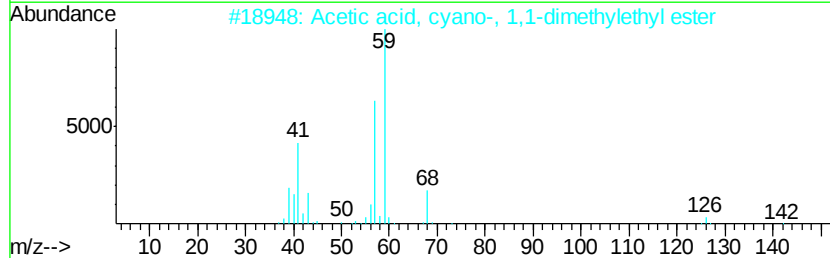
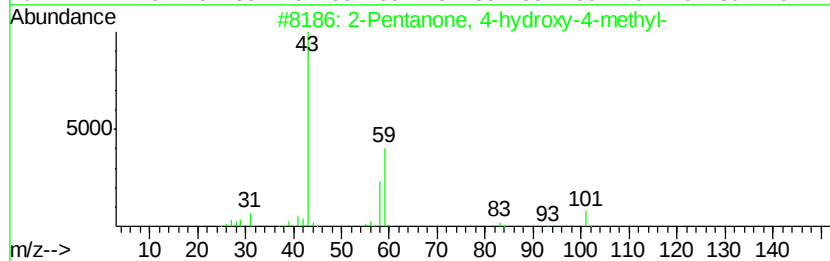
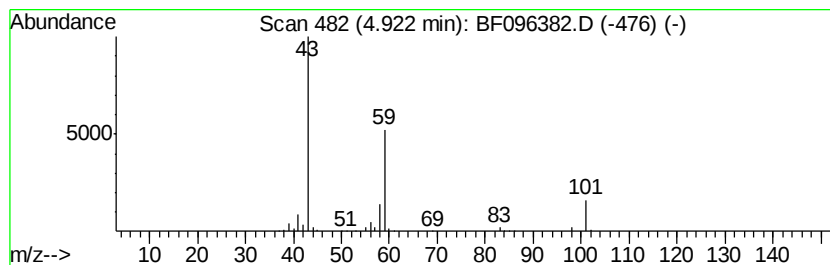
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	10.20 ng	347665	1,4-Dichlorobenzene-d4	6.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5			1,2-Butanediol	90	C4H10O2	000584-03-2	9



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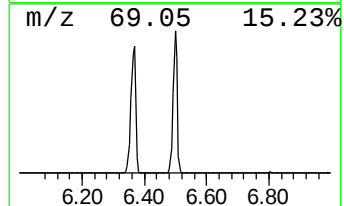
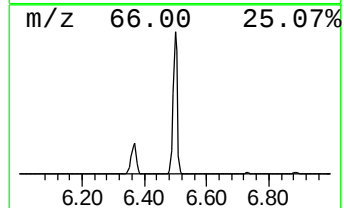
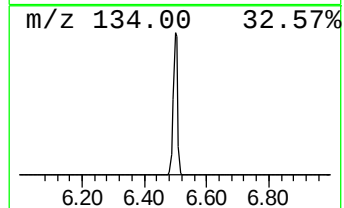
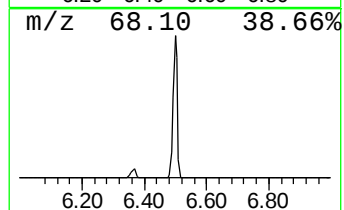
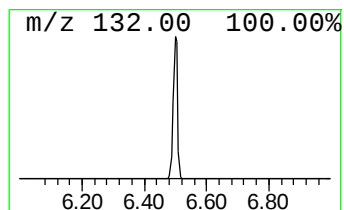
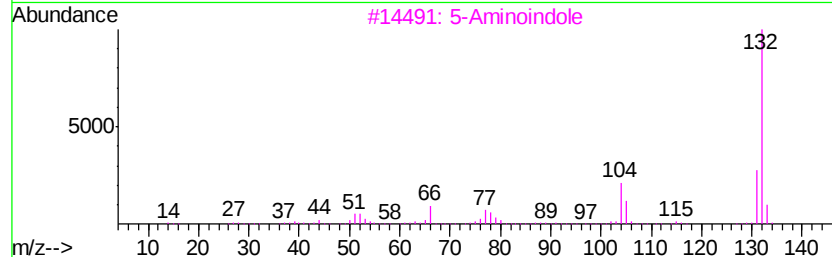
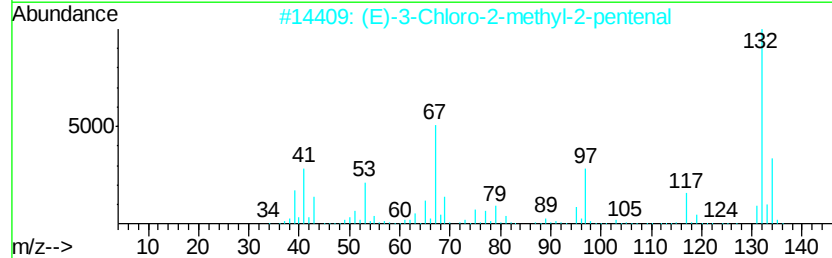
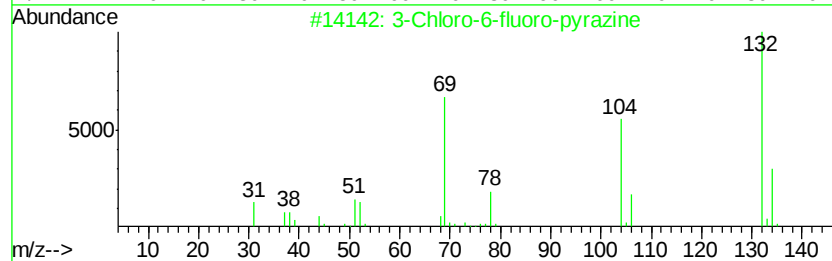
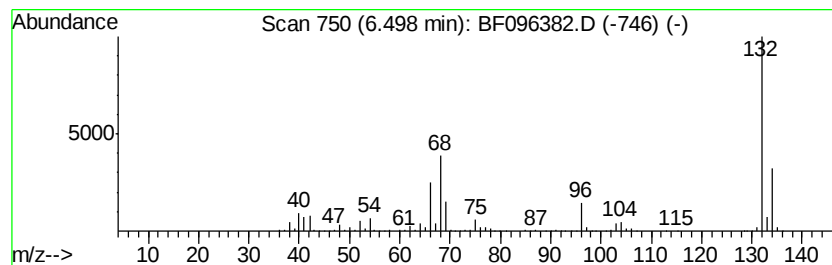
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	65.46 ng	2230870	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	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9



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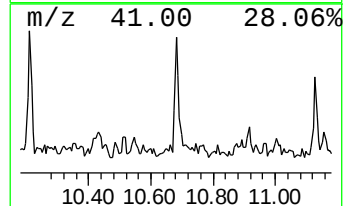
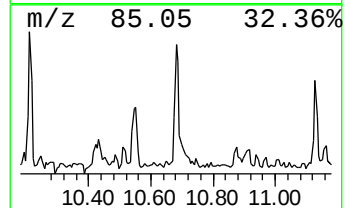
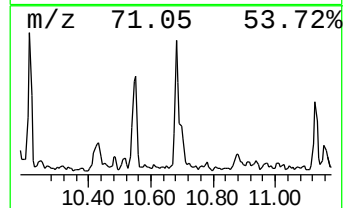
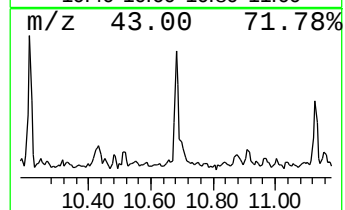
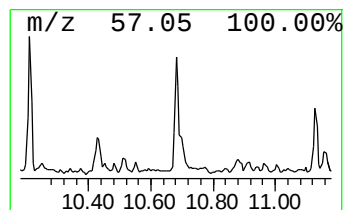
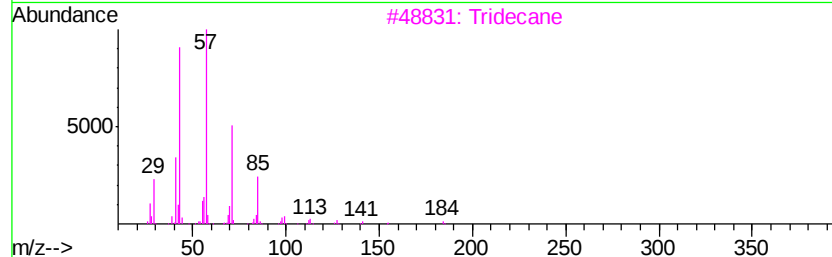
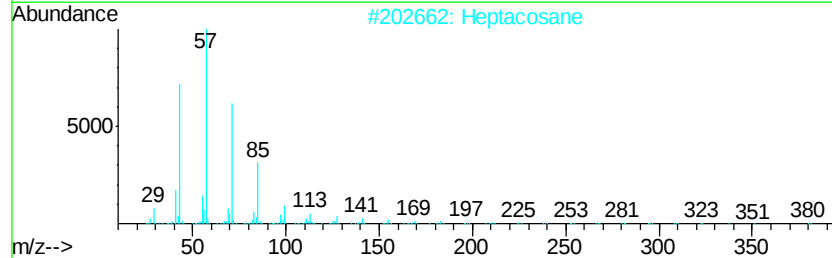
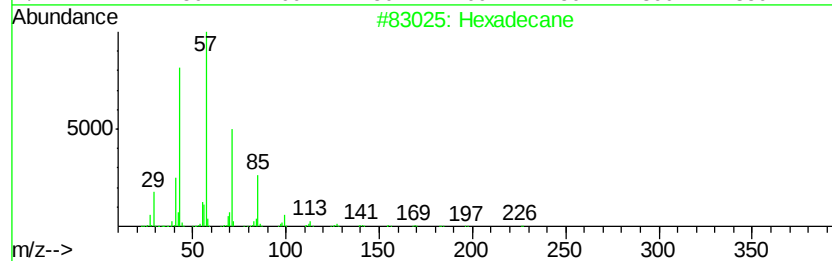
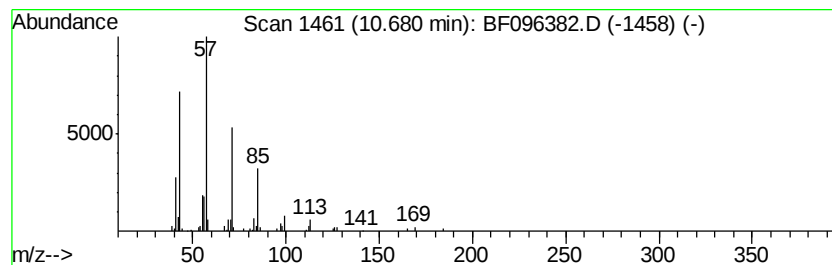
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Hexadecane Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.68	2.79 ng	102388	Phenanthrene-d10	11.24

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	80
2		Heptacosane	380	C27H56	000593-49-7	80
3		Tridecane	184	C13H28	000629-50-5	80
4		Pentadecane	212	C15H32	000629-62-9	72
5		Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	64



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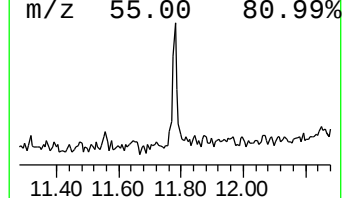
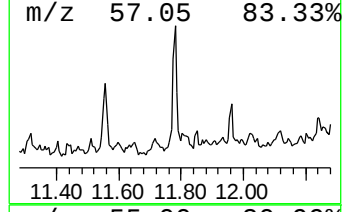
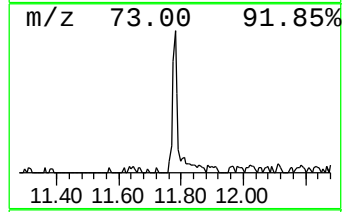
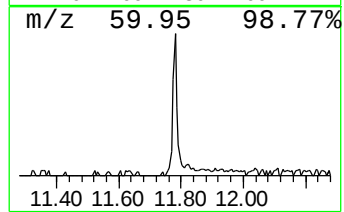
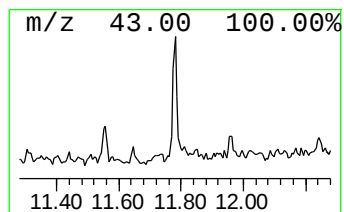
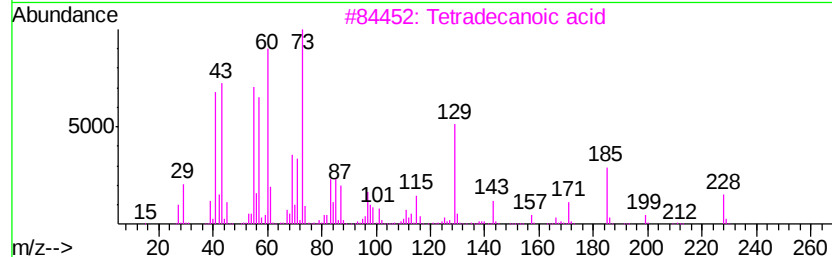
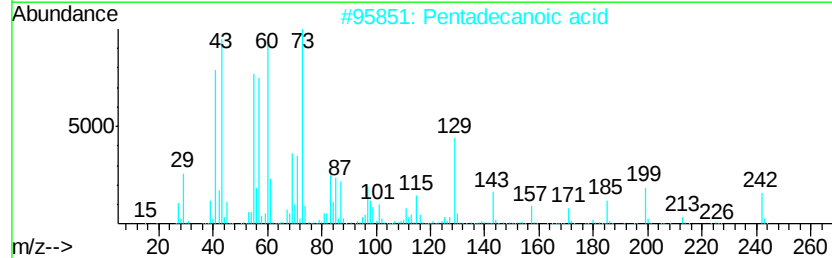
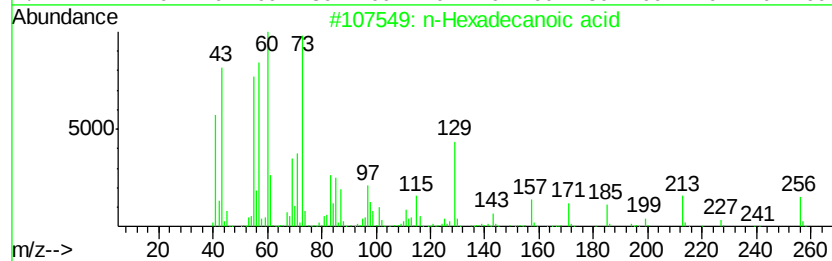
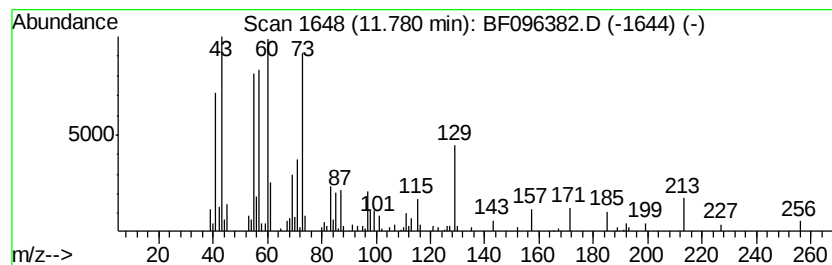
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.78	3.46 ng	127079	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	90
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		Tridecanoic acid	214	C13H26O2	000638-53-9	64
5		Dodecanoic acid	200	C12H24O2	000143-07-7	53



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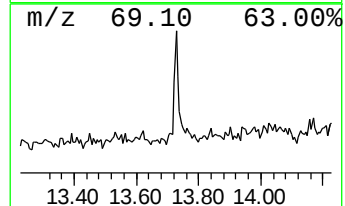
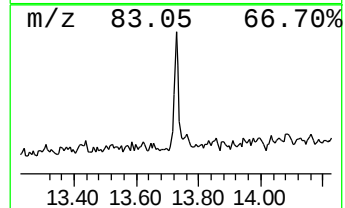
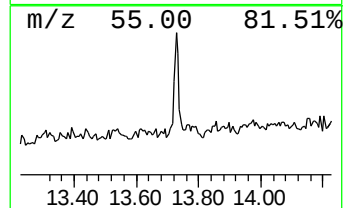
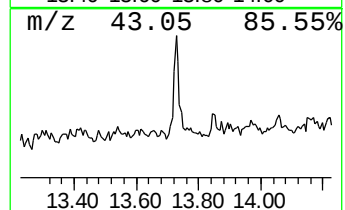
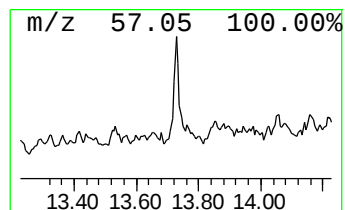
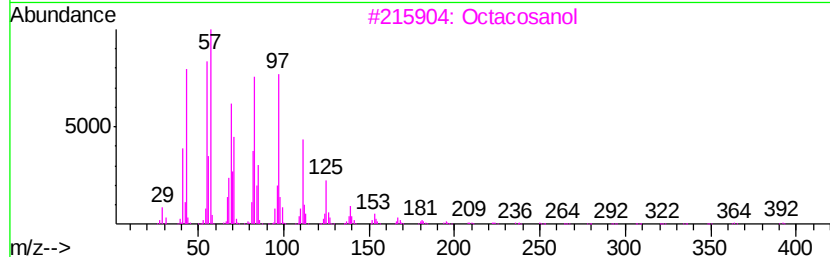
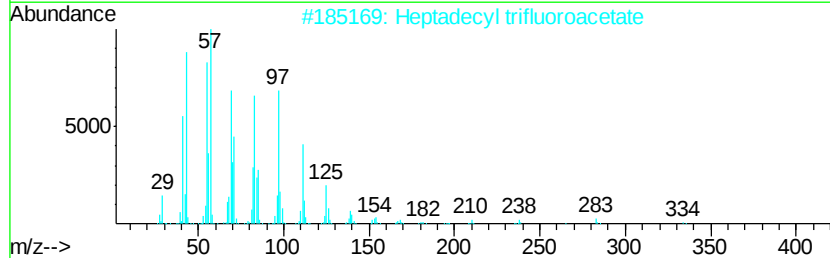
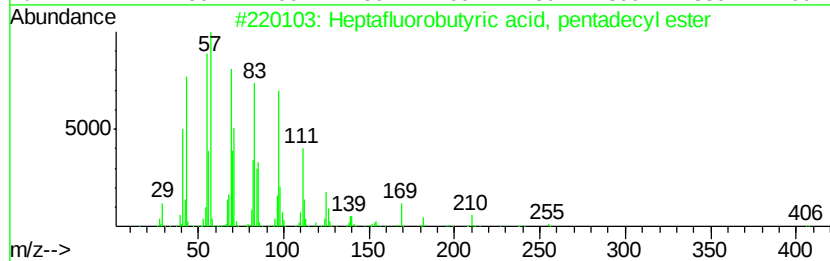
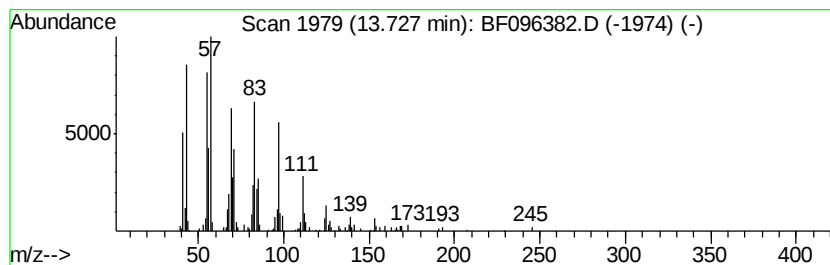
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Heptafluorobutyric acid, pe... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.73	5.04 ng	161406	Chrysene-d12	13.87	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
2	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
3	Octacosanol	410	C28H58O	000557-61-9	87
4	Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	83
5	Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	83



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ALS Vial : 5 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-13-2-4

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	4.92	10.2	ng	347665	1	6.73	681592	20.0
unknown6.50	6.50	65.5	ng	2230870	1	6.73	681592	20.0
Hexadecane	10.68	2.8	ng	102388	4	11.24	733641	20.0
n-Hexadecanoic acid	11.78	3.5	ng	127079	4	11.24	733641	20.0
Heptafluorobutyri...	13.73	5.0	ng	161406	5	13.87	641136	20.0