

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070317\
 Data File : BF096447.D
 Acq On : 3 Jul 2017 18:01
 Operator : SJ/MA
 Sample : I3979-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TP3-MH2095-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-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	4.922	475	482	490	rBV	358384	483214	18.21%	2.099%
2	5.340	548	553	557	rBV	2461639	2583378	97.35%	11.221%
3	6.363	722	727	732	rVB	2500228	2653785	100.00%	11.527%
4	6.498	745	750	753	rBV	2614850	2496556	94.08%	10.844%
5	6.722	785	788	792	rBV	792009	729010	27.47%	3.166%
6	6.881	811	815	819	rVB	2103825	1931763	72.79%	8.391%
7	7.287	878	884	887	rBV	1543908	1482019	55.85%	6.437%
8	7.387	895	901	911	rVB3	28811	37616	1.42%	0.163%
9	8.004	1002	1006	1010	rBV	1068230	975831	36.77%	4.239%
10	9.086	1185	1190	1193	rBV	2542171	2483757	93.59%	10.788%
11	9.475	1252	1256	1259	rBV	643836	489978	18.46%	2.128%
12	9.651	1276	1286	1292	rBV4	23916	56395	2.13%	0.245%
13	9.704	1292	1295	1299	rVB	53883	43355	1.63%	0.188%
14	9.757	1299	1304	1308	rBV	951791	816987	30.79%	3.549%
15	10.204	1377	1380	1383	rVB	60727	46548	1.75%	0.202%
16	10.545	1433	1438	1441	rBV	1222290	1138566	42.90%	4.945%
17	10.675	1457	1460	1466	rBV	53728	55015	2.07%	0.239%
18	11.122	1532	1536	1539	rBV2	43547	36292	1.37%	0.158%
19	11.239	1552	1556	1559	rBV	735555	659450	24.85%	2.864%
20	11.475	1593	1596	1599	rBV	108065	87660	3.30%	0.381%
21	11.775	1643	1647	1650	rBV3	59514	55155	2.08%	0.240%
22	11.957	1673	1678	1682	rVB6	19678	34310	1.29%	0.149%
23	12.033	1688	1691	1693	rBV	38237	32764	1.23%	0.142%
24	12.292	1731	1735	1739	rBV	292025	270037	10.18%	1.173%
25	12.351	1742	1745	1747	rVV	62148	59189	2.23%	0.257%
26	12.439	1756	1760	1764	rBV2	26303	36990	1.39%	0.161%
27	12.822	1821	1825	1829	rBV	1697831	1603996	60.44%	6.967%
28	13.039	1858	1862	1865	rBV2	36140	40801	1.54%	0.177%
29	13.280	1900	1903	1905	rBV	51518	50990	1.92%	0.221%
30	13.721	1975	1978	1986	rBV	139435	186164	7.02%	0.809%
31	13.868	1999	2003	2006	rBV	756199	695719	26.22%	3.022%
32	14.080	2032	2039	2042	rBV9	52156	146660	5.53%	0.637%
33	15.280	2239	2243	2249	rVB	389503	522800	19.70%	2.271%

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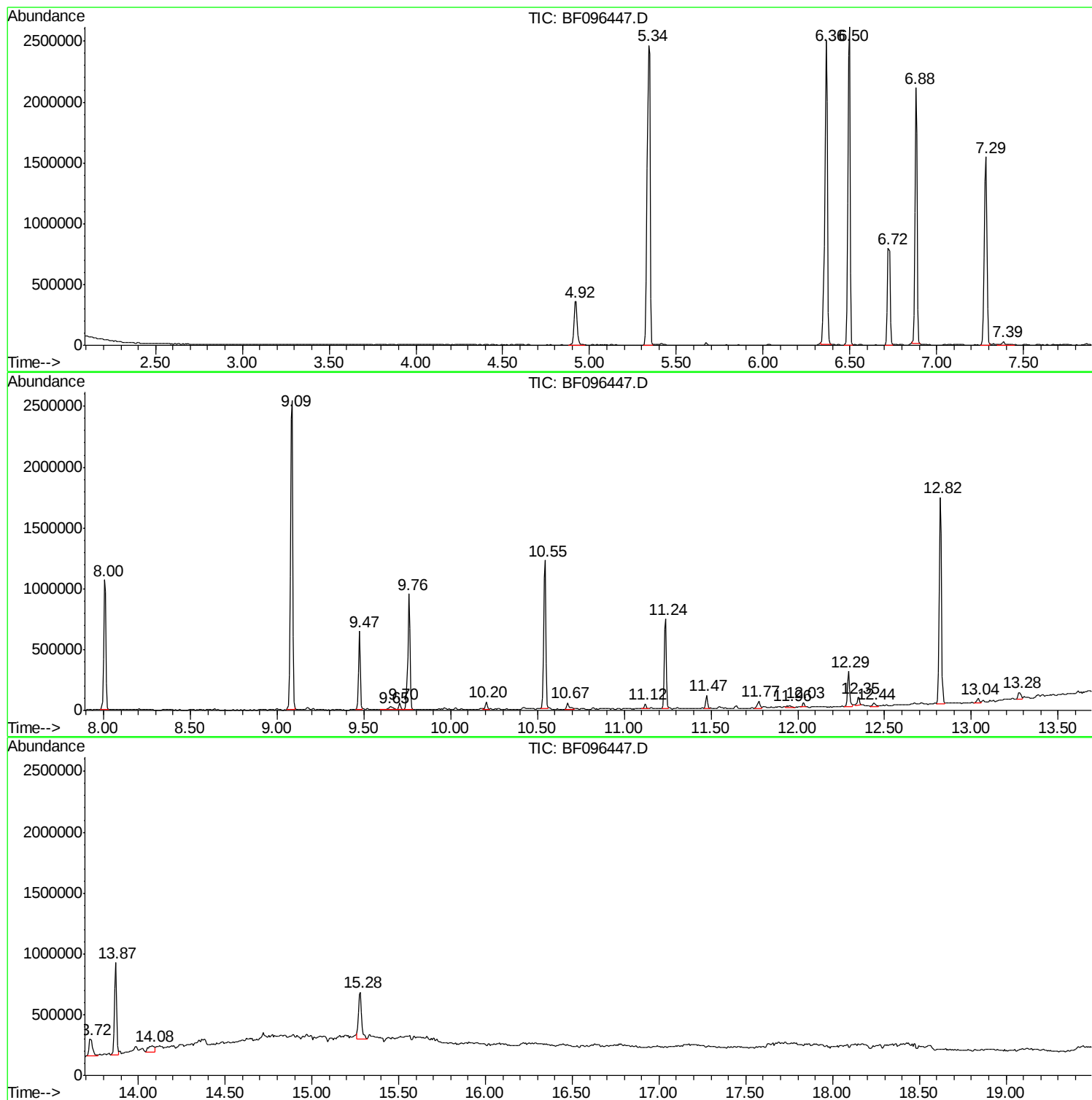
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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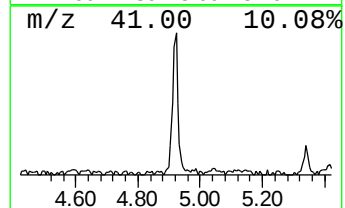
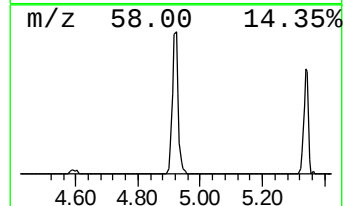
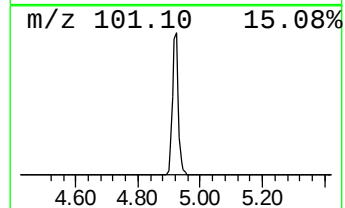
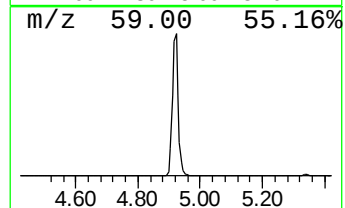
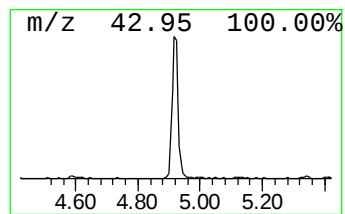
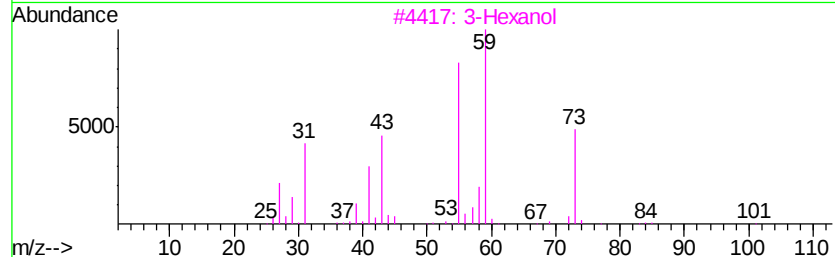
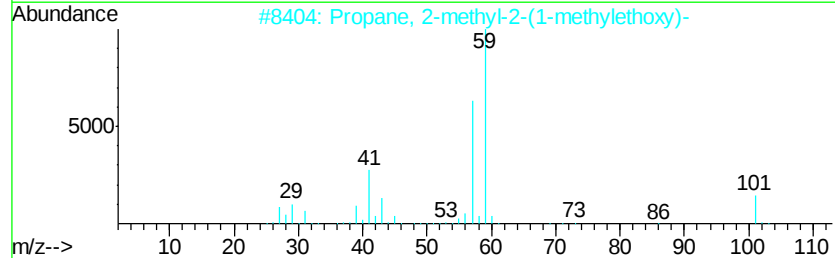
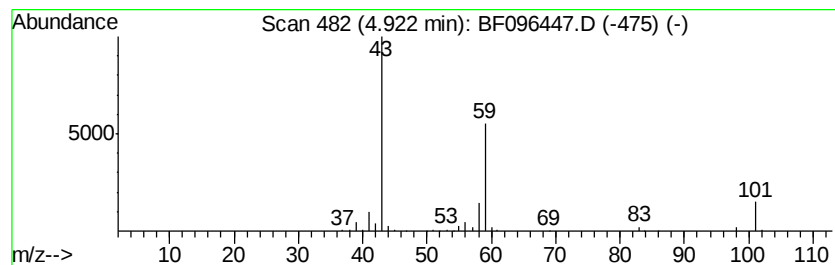
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	13.26 ng	483214	1,4-Dichlorobenzene-d4	6.73

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		3-Hexanol	102	C6H14O	000623-37-0	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	33
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33



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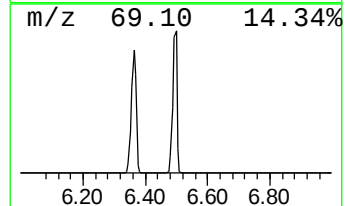
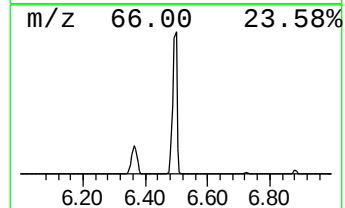
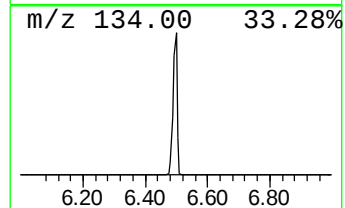
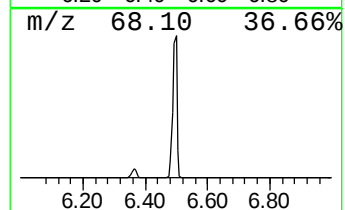
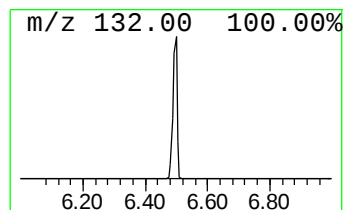
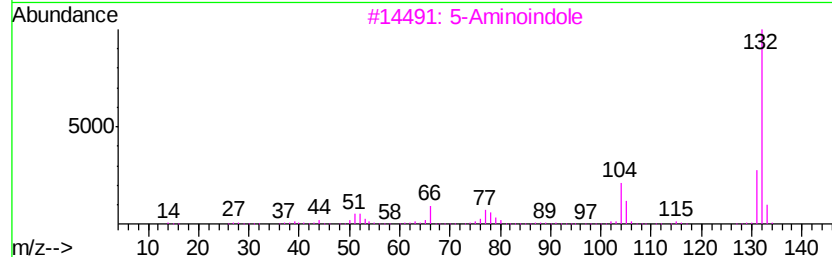
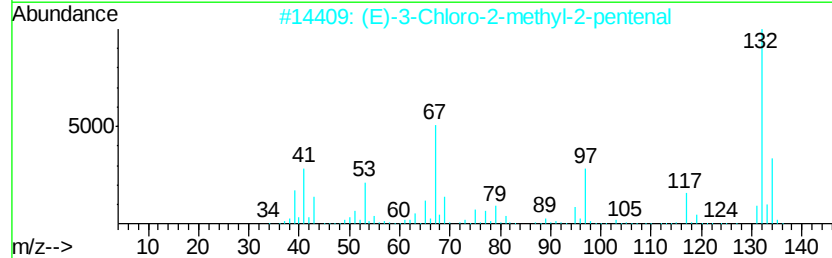
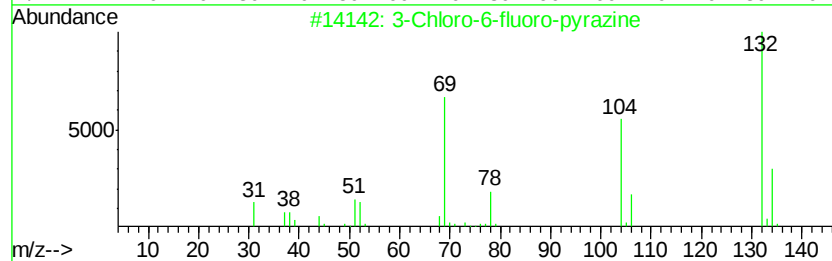
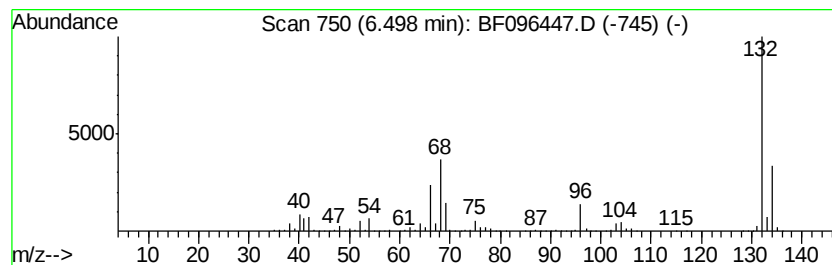
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.50 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.50	68.49 ng	2496560	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	35
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	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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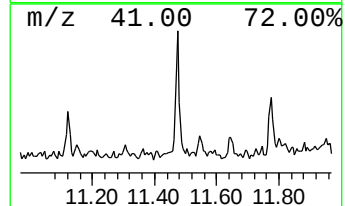
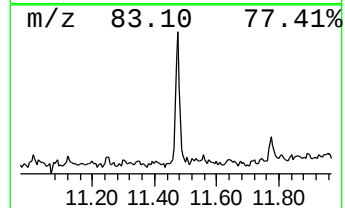
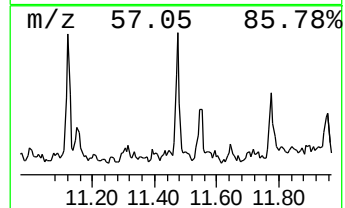
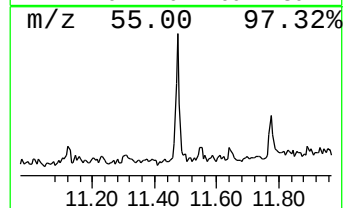
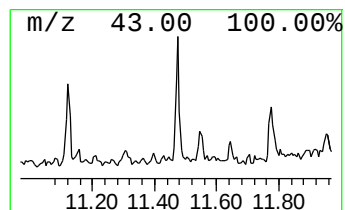
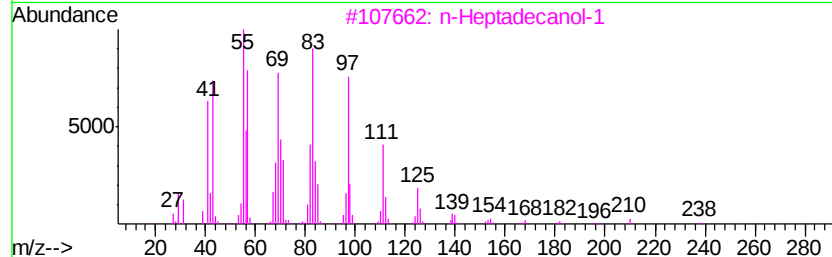
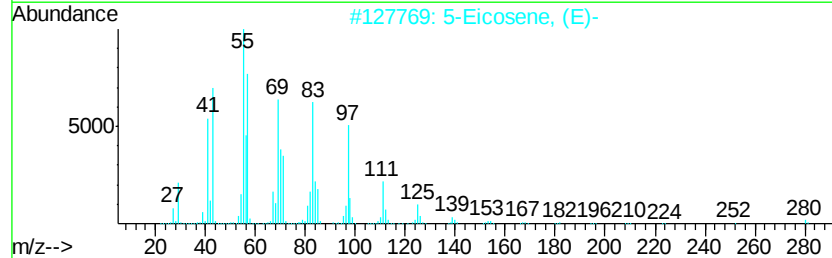
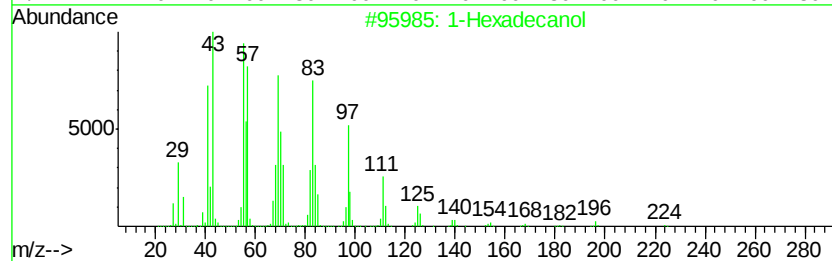
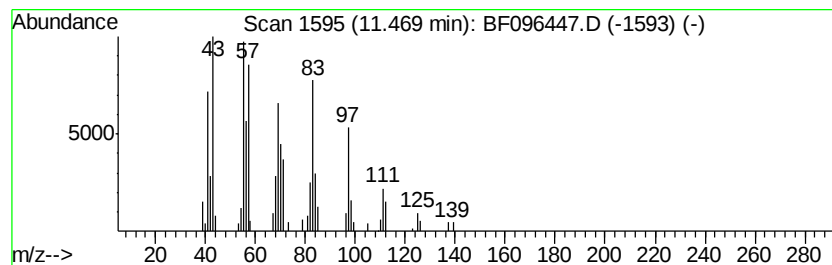
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 1-Hexadecanol Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.47	2.66 ng	87660	Phenanthrene-d10		11.24
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexadecanol	242	C16H34O	036653-82-4	91
2	5-Eicosene, (E)-	280	C20H40	074685-30-6	91
3	n-Heptadecanol-1	256	C17H36O	001454-85-9	91
4	5-Octadecene, (E)-	252	C18H36	007206-21-5	91
5	Isobutyl tetradecyl carbonate	314	C19H38O3	959275-58-2	90



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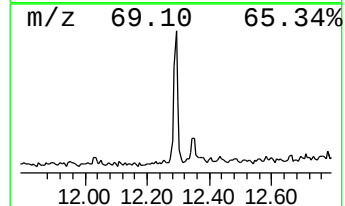
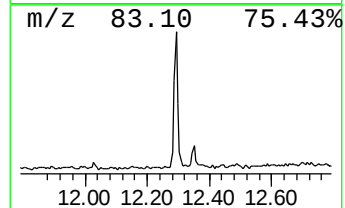
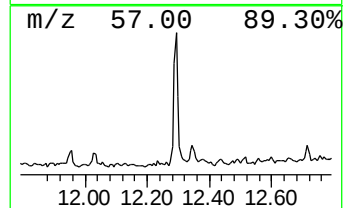
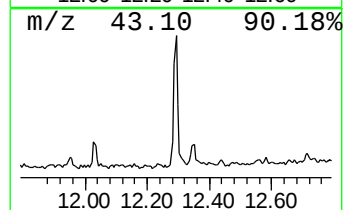
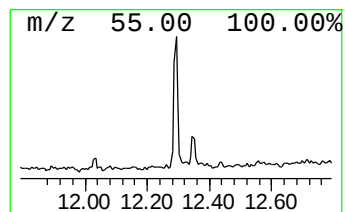
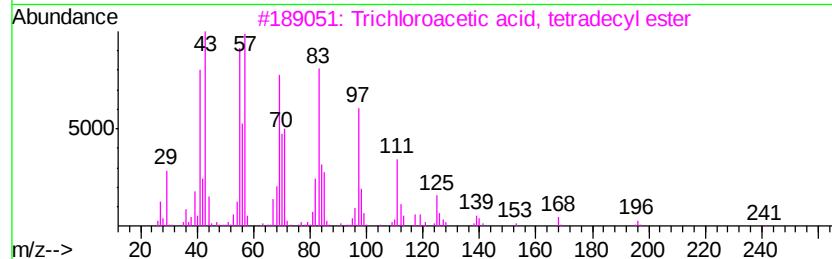
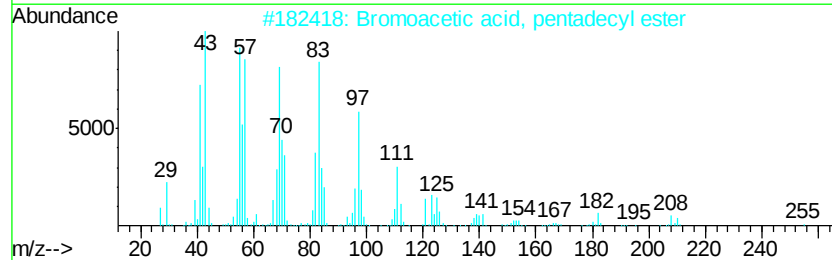
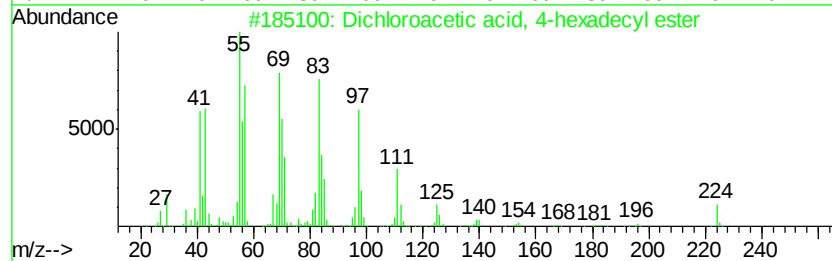
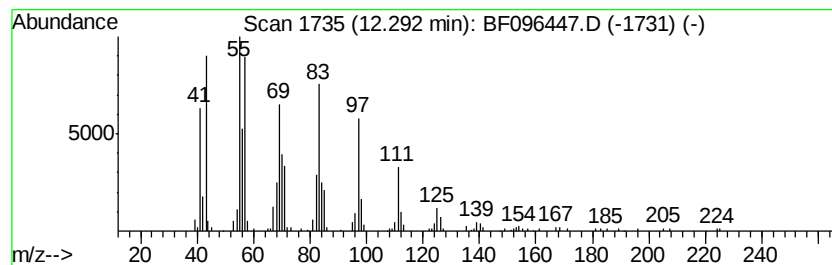
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Dichloroacetic acid, 4-hexa... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.29	8.19 ng	270037	Phenanthrene-d10	11.24

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Dichloroacetic acid, 4-hexadecyl...	352	C18H34Cl2O2	1000282-98-1	95
2		Bromoacetic acid, pentadecyl ester	348	C17H33BrO2	131143-01-6	94
3		Trichloroacetic acid, tetradecyl...	358	C16H29Cl3O2	074339-52-9	91
4		1-Nonadecene	266	C19H38	018435-45-5	91
5		1-Heptadecene	238	C17H34	006765-39-5	91



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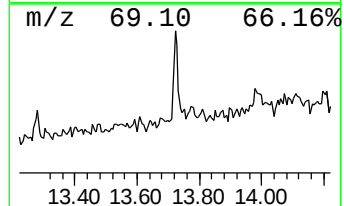
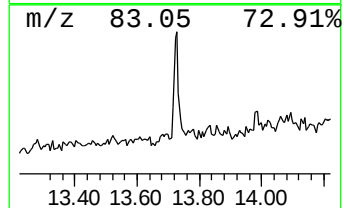
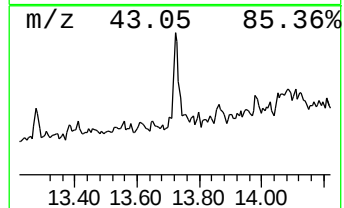
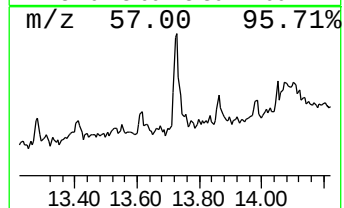
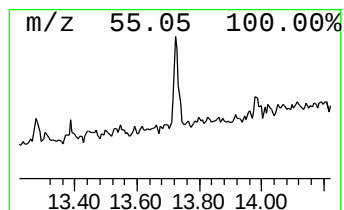
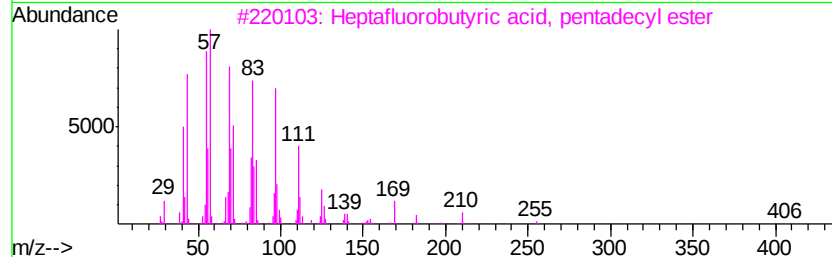
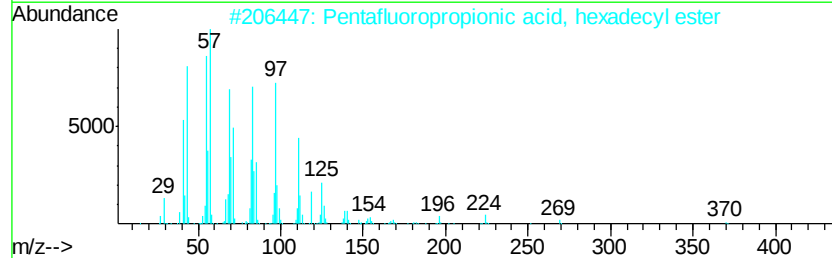
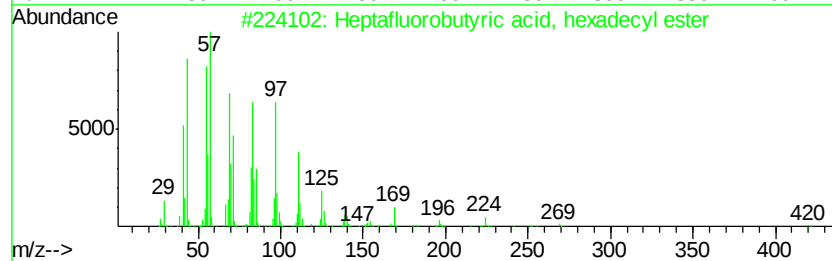
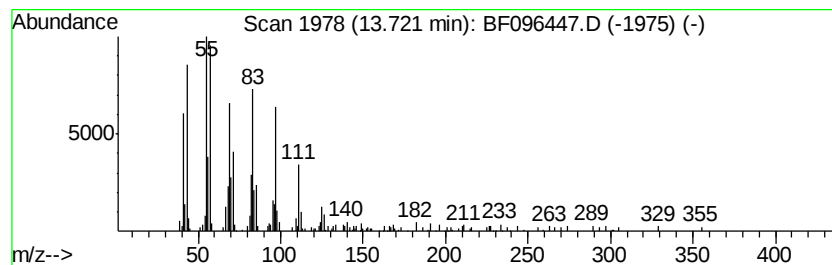
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Heptafluorobutyric acid, he... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.72	5.35 ng	186164	Chrysene-d12	13.87

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	91
2		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	91
4		Octacosanol	410	C28H58O	000557-61-9	91
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	91



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TP3-MH2095-COMP

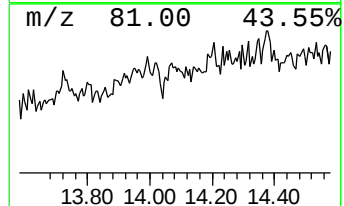
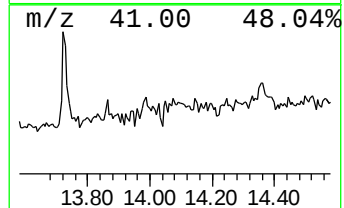
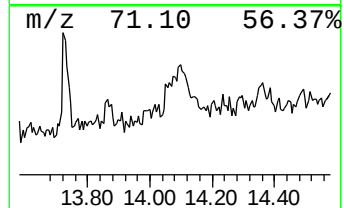
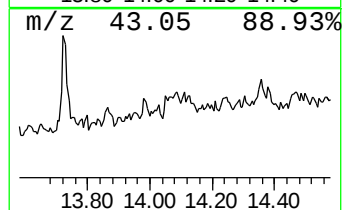
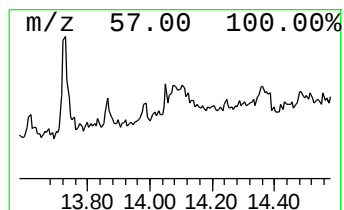
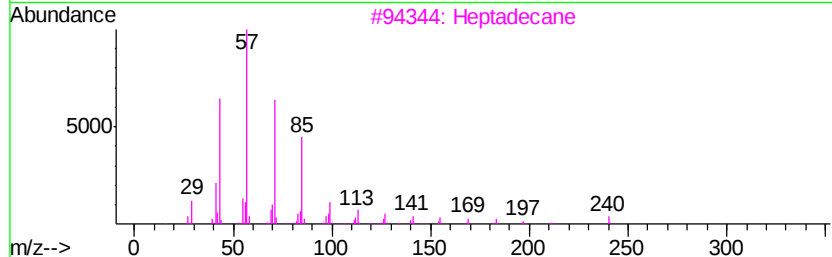
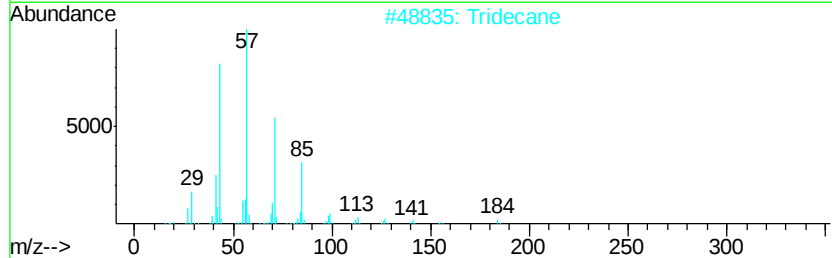
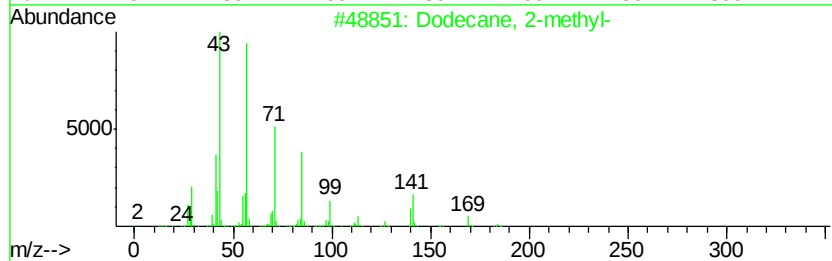
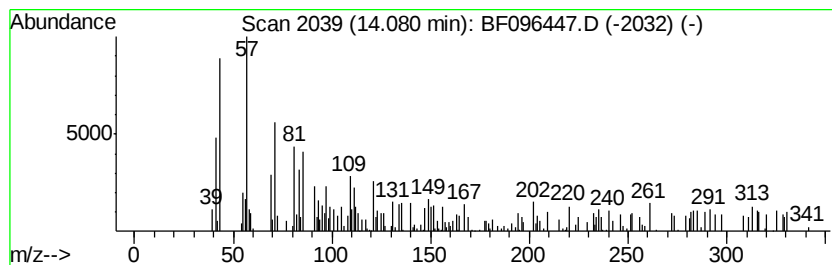
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF070117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown14.08 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.08	4.22 ng	146660	Chrysene-d12	13.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dodecane, 2-methyl-	184	C13H28	001560-97-0	47
2		Tridecane	184	C13H28	000629-50-5	35
3		Heptadecane	240	C17H36	000629-78-7	35
4		Eicosane	282	C20H42	000112-95-8	22
5		Sulfurous acid, pentadecyl 2-pro...	334	C18H38O3S	1000309-12-6	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF070317\
Data File : BF096447.D
Acq On : 3 Jul 2017 18:01
Operator : SJ/MA
Sample : I3979-01
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TP3-MH2095-COMP

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	13.3	ng	483214	1	6.73	729010	20.0
unknown6.50	6.50	68.5	ng	2496560	1	6.73	729010	20.0
1-Hexadecanol	11.47	2.7	ng	87660	4	11.24	659450	20.0
Dichloroacetic ac...	12.29	8.2	ng	270037	4	11.24	659450	20.0
Heptafluorobutyri...	13.72	5.3	ng	186164	5	13.87	695719	20.0
unknown14.08	14.08	4.2	ng	146660	5	13.87	695719	20.0