

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
 Data File : BF076956.D
 Acq On : 20 Jan 2015 8:36
 Operator : IZ / TP
 Sample : G1101-02
 Misc : W
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PO-004

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-BF011415.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	1.452	31	32	39	rBV	29849	61415	5.19%	0.672%
2	4.104	262	264	272	rBV	18520	42898	3.62%	0.469%
3	5.041	342	346	360	rVB	181090	354577	29.94%	3.879%
4	7.373	547	550	555	rBV	103672	198665	16.78%	2.173%
5	7.465	555	558	565	rVB	414006	759685	64.15%	8.311%
6	7.979	599	603	611	rBV	112067	181631	15.34%	1.987%
7	8.299	627	631	634	rBV	480801	746646	63.05%	8.168%
8	9.270	712	716	718	rBV	397604	595375	50.28%	6.513%
9	9.316	718	720	725	rVB	45031	72799	6.15%	0.796%
10	10.882	854	857	861	rBV	178015	255581	21.58%	2.796%
11	13.534	1085	1089	1092	rBV	783405	1179740	99.62%	12.906%
12	15.008	1215	1218	1222	rVB	165987	282171	23.83%	3.087%
13	16.551	1350	1353	1357	rBV	45992	55326	4.67%	0.605%
14	16.631	1357	1360	1361	rBV	11383	15795	1.33%	0.173%
15	16.677	1361	1364	1367	rBV	496204	716615	60.51%	7.839%
16	16.825	1375	1377	1381	rBV3	9790	12802	1.08%	0.140%
17	16.905	1381	1384	1387	rBV	143904	187135	15.80%	2.047%
18	17.134	1401	1404	1407	rBV	40427	60674	5.12%	0.664%
19	17.774	1457	1460	1463	rBV	236395	306113	25.85%	3.349%
20	18.757	1543	1546	1549	rBV	83413	112375	9.49%	1.229%
21	19.386	1598	1601	1604	rVB	62490	63239	5.34%	0.692%
22	19.466	1605	1608	1611	rVB	74192	106474	8.99%	1.165%
23	19.900	1643	1646	1649	rBV	63595	68552	5.79%	0.750%
24	20.003	1653	1655	1658	rVV	1021126	1184224	100.00%	12.955%
25	20.792	1720	1724	1726	rBV	45312	50219	4.24%	0.549%
26	20.849	1726	1729	1731	rVV	13984	19182	1.62%	0.210%
27	20.929	1734	1736	1739	rVB	7100	12582	1.06%	0.138%
28	21.146	1753	1755	1757	rBV	21768	29086	2.46%	0.318%
29	21.180	1757	1758	1760	rVB	51745	50259	4.24%	0.550%
30	21.272	1761	1766	1769	rBV	322722	397880	33.60%	4.353%
31	21.477	1781	1784	1786	rBV	110338	156834	13.24%	1.716%
32	21.660	1798	1800	1804	rVB2	19593	24377	2.06%	0.267%
33	22.037	1830	1833	1838	rBV	19301	33473	2.83%	0.366%
34	22.255	1849	1852	1855	rBV5	3845	11852	1.00%	0.130%

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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-BF011415.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.403	1863	1865	1868	rVB2	16953	22204	1.87%	0.243%
36	22.472	1868	1871	1873	rBV	14771	25241	2.13%	0.276%
37	22.769	1894	1897	1900	rBV2	11420	23523	1.99%	0.257%
38	22.906	1906	1909	1912	rBV	257001	307995	26.01%	3.369%
39	23.112	1925	1927	1931	rBV5	12159	20490	1.73%	0.224%
40	23.192	1931	1934	1936	rVV	125075	188317	15.90%	2.060%
41	23.466	1955	1958	1959	rBV2	15610	21821	1.84%	0.239%
42	23.500	1959	1961	1963	rVB3	8837	13402	1.13%	0.147%
43	24.186	2017	2021	2022	rBV4	7194	15123	1.28%	0.165%
44	24.449	2042	2044	2048	rVB5	15045	25939	2.19%	0.284%
45	24.803	2074	2075	2078	rBV3	8516	18161	1.53%	0.199%
46	25.089	2096	2100	2104	rBV2	19843	52664	4.45%	0.576%

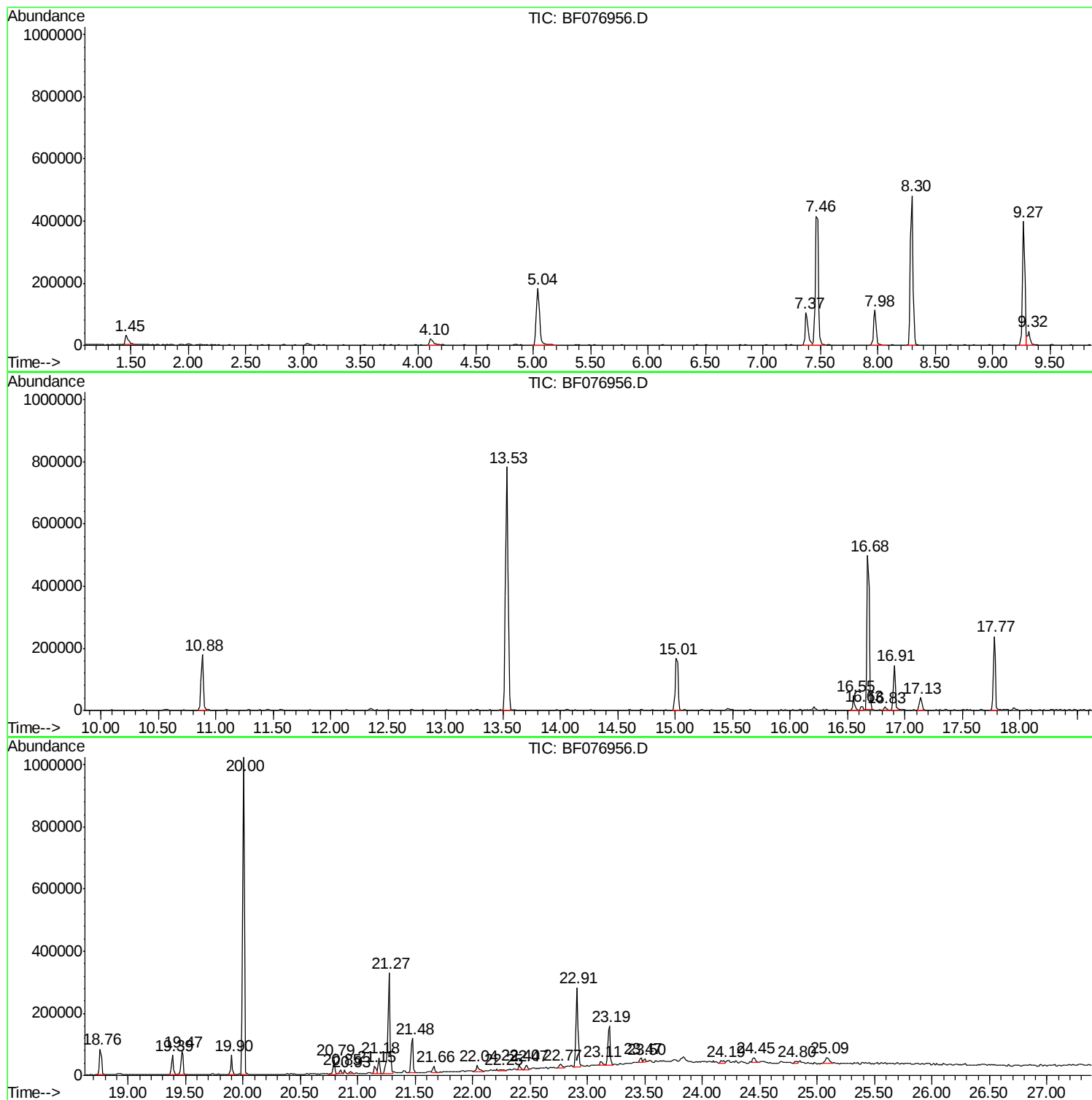
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



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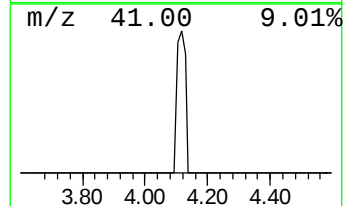
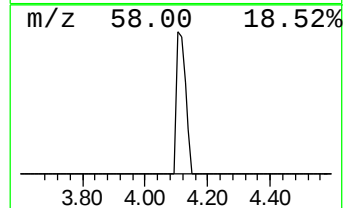
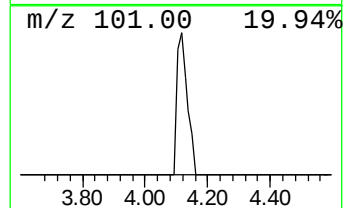
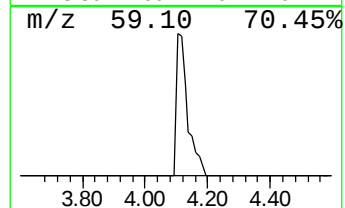
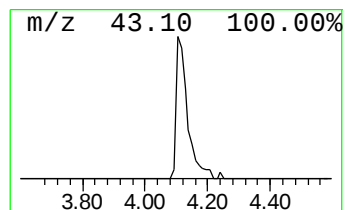
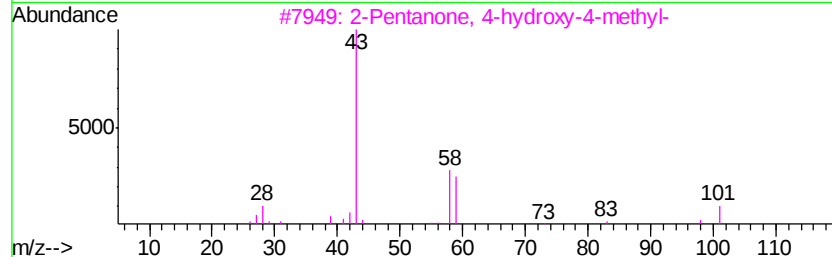
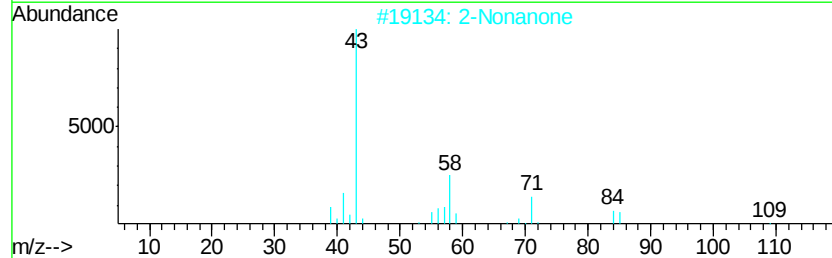
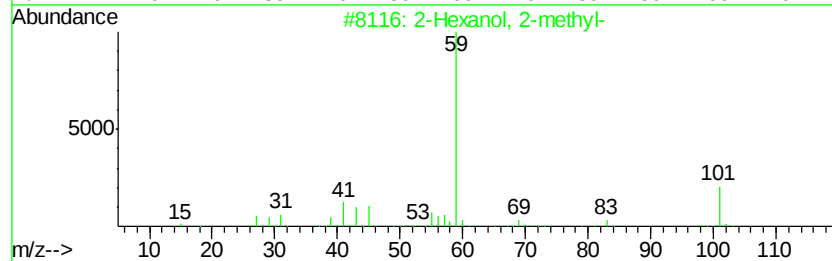
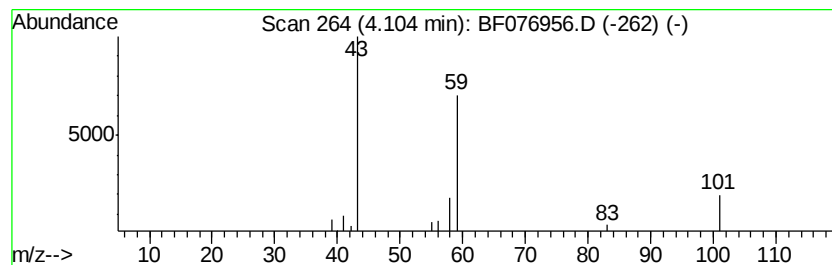
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown4.10 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	4.72 ng	42898	1,4-Dichlorobenzene-d4	7.98

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	36
2	2-Nonanone	142	C9H18O	000821-55-6	9
3	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	9
4	Guanidine	59	CH5N3	000113-00-8	5
5	Acetone	58	C3H6O	000067-64-1	5



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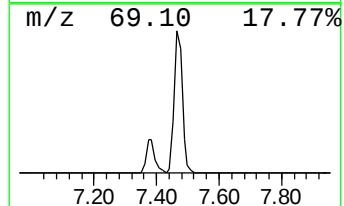
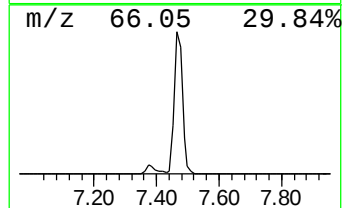
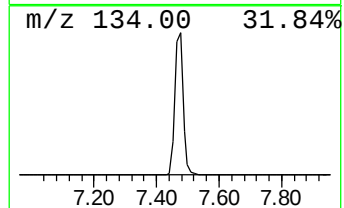
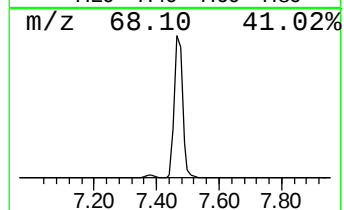
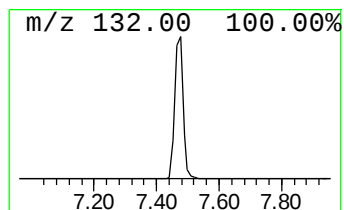
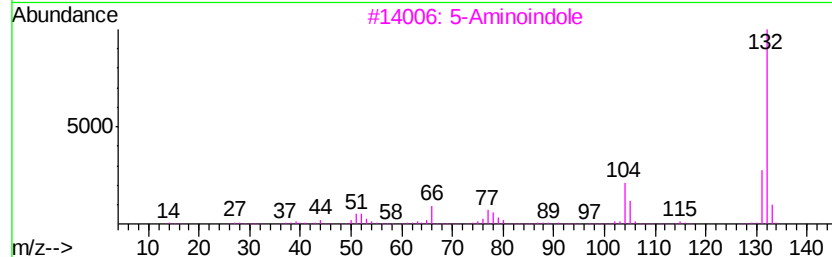
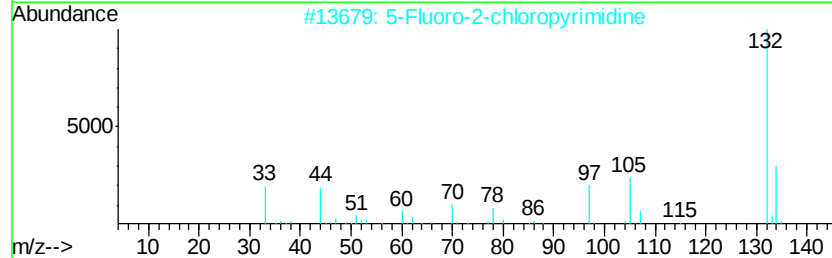
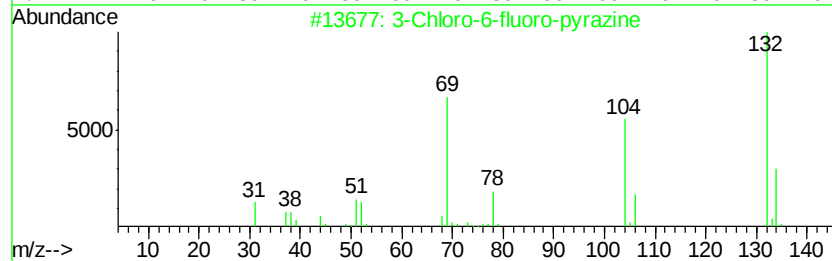
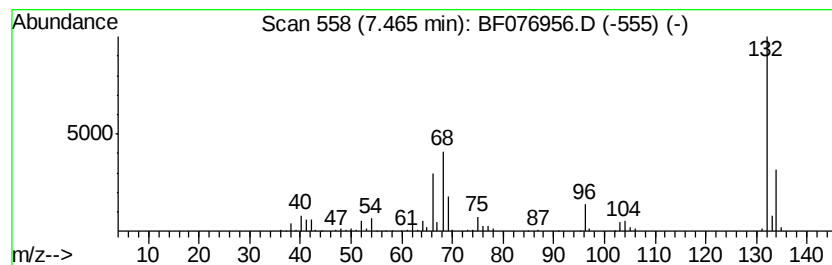
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Peak Number 3 unknown7.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	83.65 ng	759685	1,4-Dichlorobenzene-d4	7.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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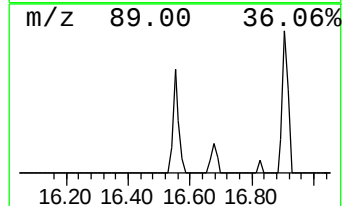
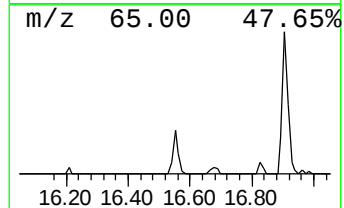
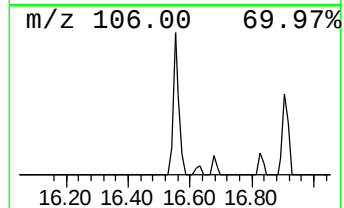
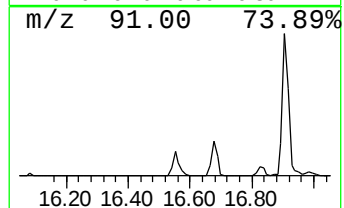
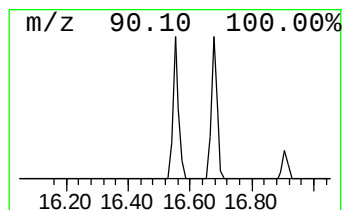
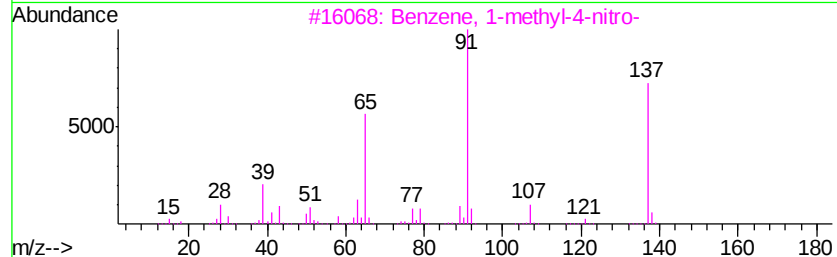
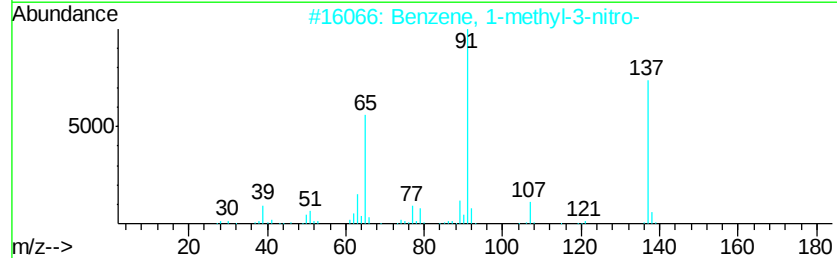
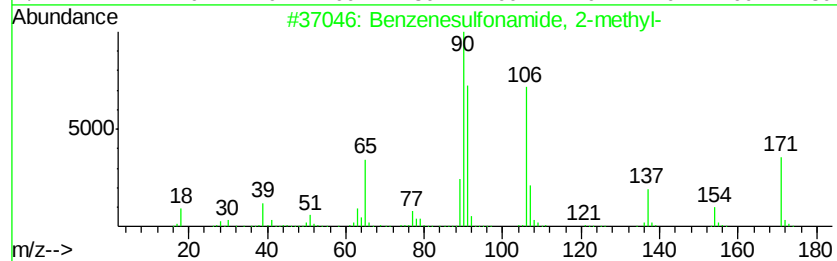
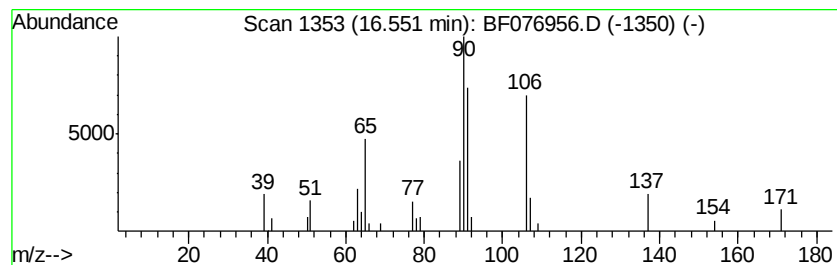
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Benzenesulfonamide, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.55	3.61 ng	55326	Phenanthrene-d10	17.77

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzenesulfonamide, 2-methyl-	171	C7H9NO2S	000088-19-7	91
2		Benzene, 1-methyl-3-nitro-	137	C7H7NO2	000099-08-1	22
3		Benzene, 1-methyl-4-nitro-	137	C7H7NO2	000099-99-0	22
4		2,4-Octadiyne	106	C8H10	002809-71-4	22
5		Cycloheptatrienylium, iodide	218	C7H7I	001316-80-9	14



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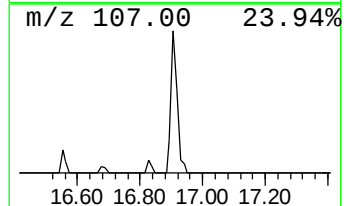
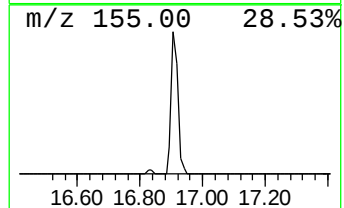
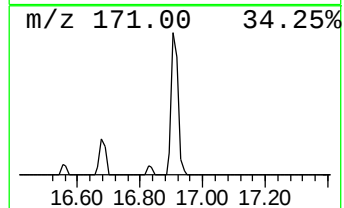
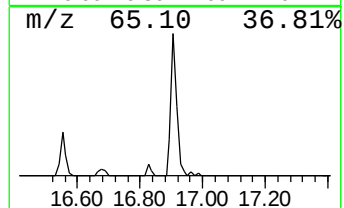
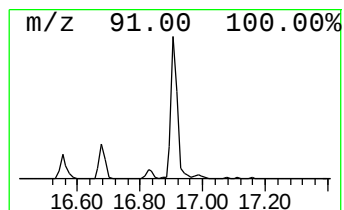
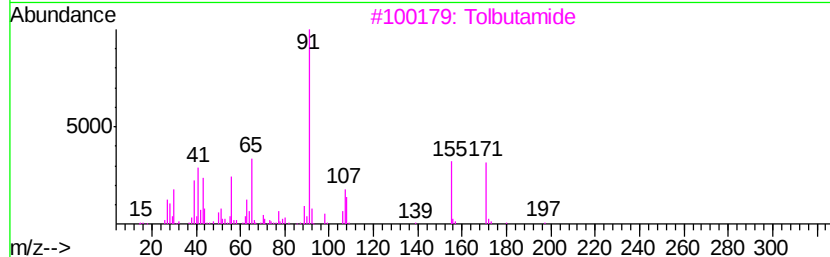
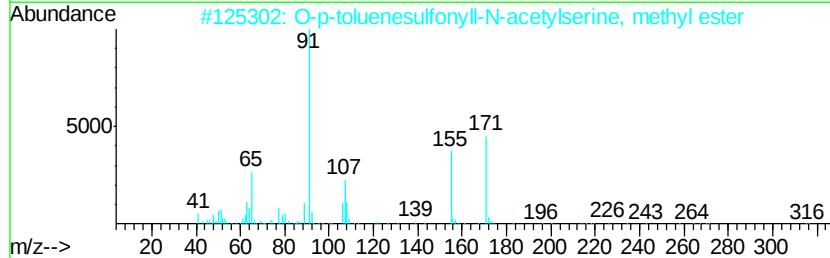
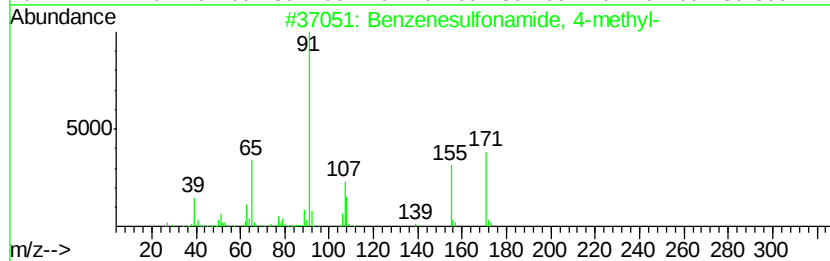
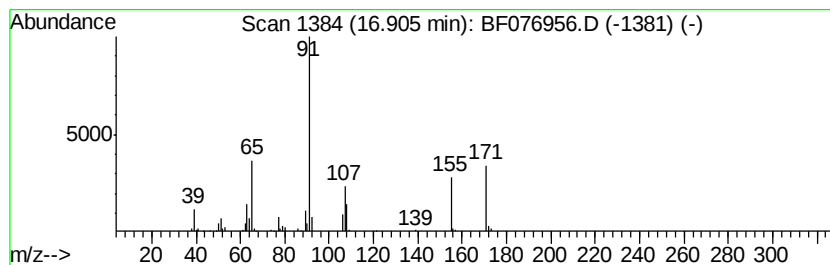
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Benzenesulfonamide, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.91	12.23 ng	187135	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenesulfonamide, 4-methyl-	171	C7H9NO2S	000070-55-3	96
2		O-p-toluenesulfonyl-N-acetylser...	315	C13H17NO6S	1000126-44-8	90
3		Tolbutamide	270	C12H18N2O3S	000064-77-7	87
4		Thiosulfuric acid, S-[2-[3-(4-me...	381	C12H19N3O5S3	1000255-60-3	86
5		N-p-toluenesulfonyl-L-threonine,...	363	C18H21NO5S	1000130-34-4	83



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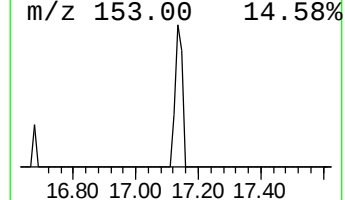
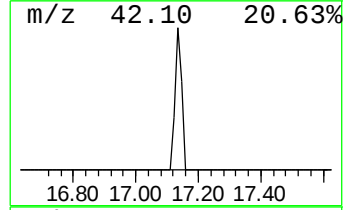
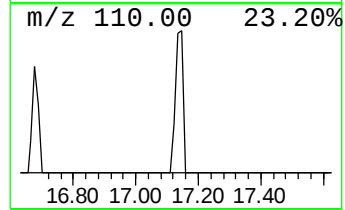
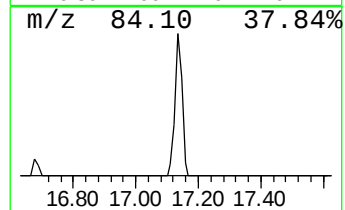
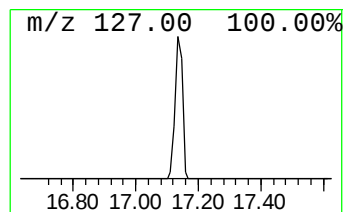
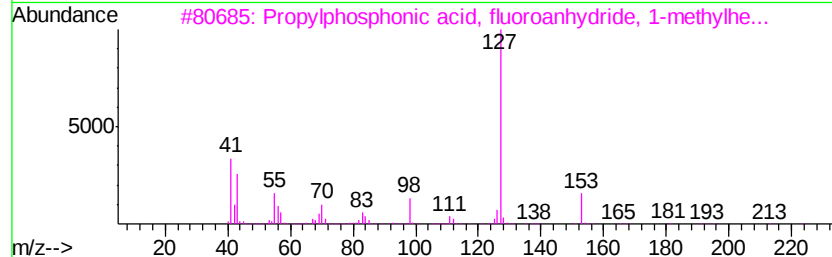
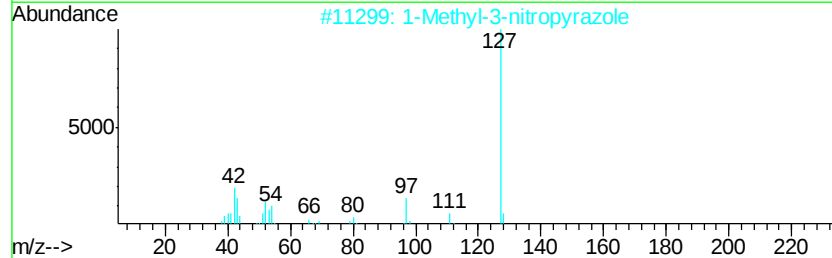
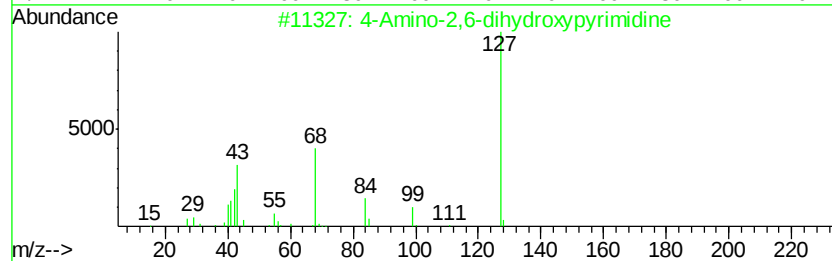
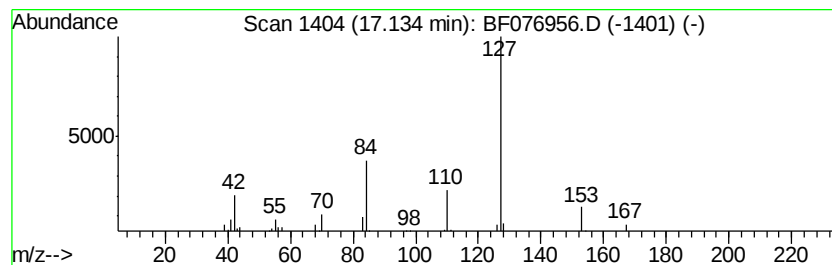
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 unknown17.13 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.13	3.96 ng	60674	Phenanthrene-d10	17.77

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	47
2	1-Methyl-3-nitropyrazole	127	C4H5N3O2	054210-32-1	46
3	Propylphosphonic acid, fluoroanh...	238	C11H24F02P	1000273-50-7	42
4	6-Azathymine	127	C4H5N3O2	000932-53-6	40
5	2,5-Pyrrolidinedione, 1-ethyl-	127	C6H9N02	002314-78-5	38



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076956.D
Acq On : 20 Jan 2015 8:36
Operator : IZ / TP
Sample : G1101-02
Misc : W
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
PO-004

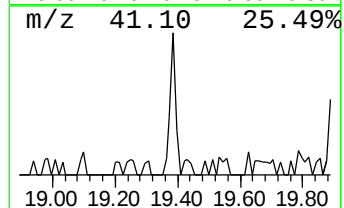
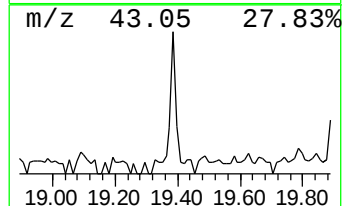
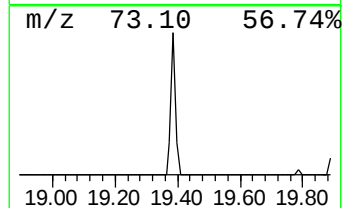
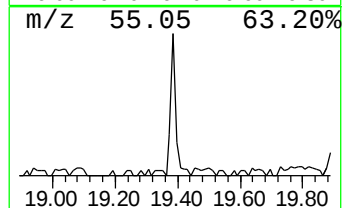
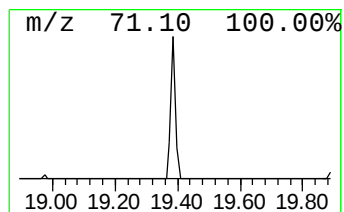
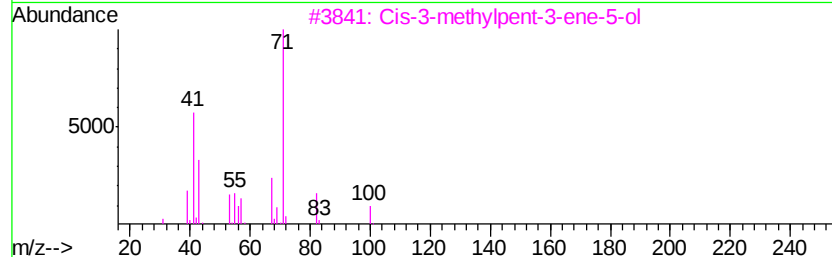
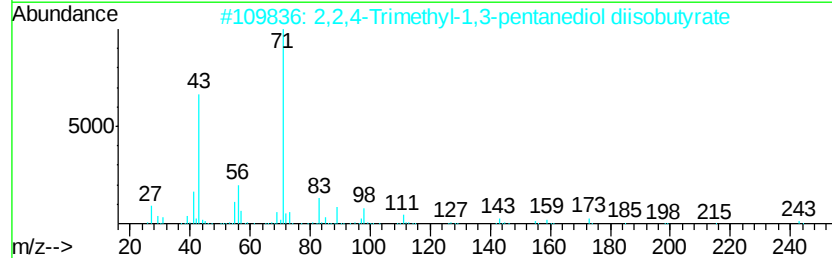
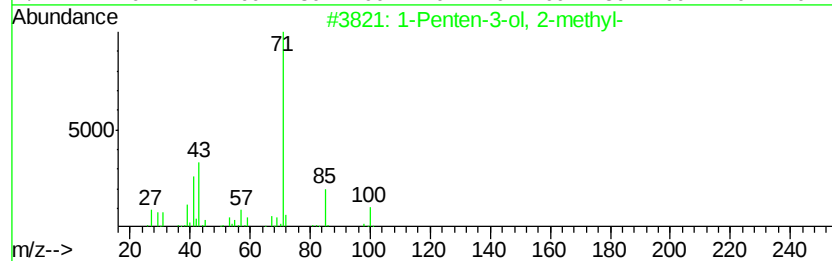
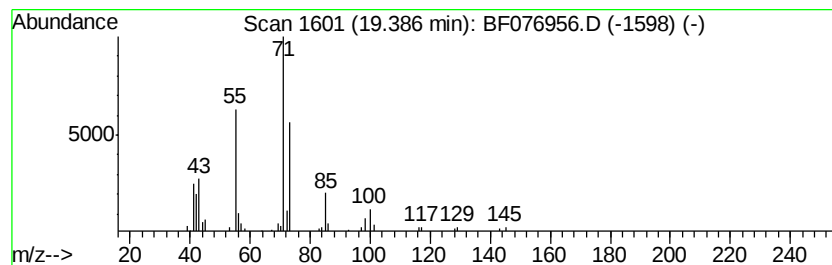
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 1-Penten-3-ol, 2-methyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.39	4.13 ng	63239	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Penten-3-ol, 2-methyl-	100	C6H12O	002088-07-5	59
2		2,2,4-Trimethyl-1,3-pentanediol ...	286	C16H30O4	006846-50-0	43
3		Cis-3-methylpent-3-ene-5-ol	100	C6H12O	030804-75-2	37
4		Acetaldehyde, propylhydrazine	100	C5H12N2	007422-88-0	36
5		(+)-3-Methyl-1-penten-3-ol	100	C6H12O	086361-10-6	36



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
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Sample : G1101-02
Misc : W
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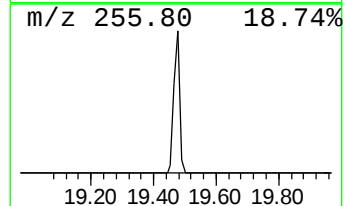
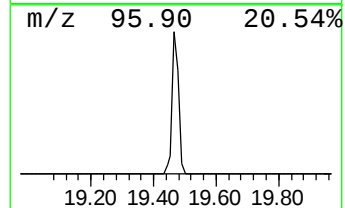
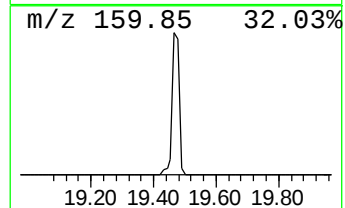
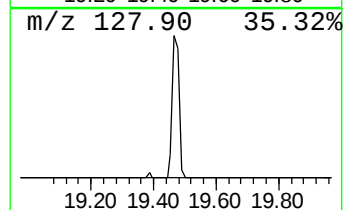
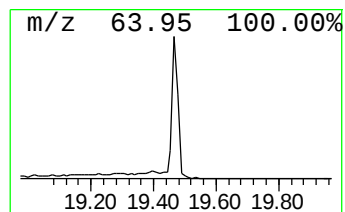
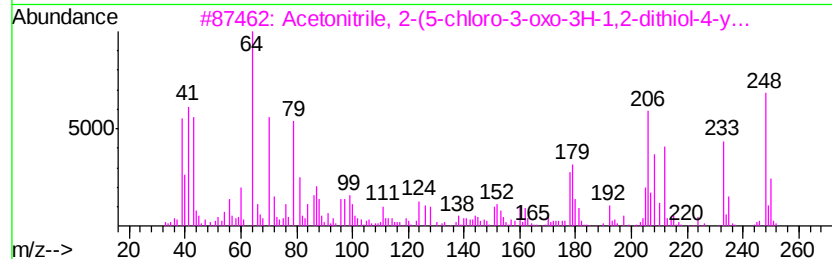
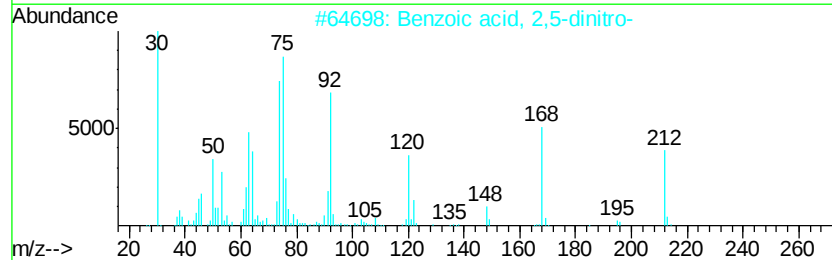
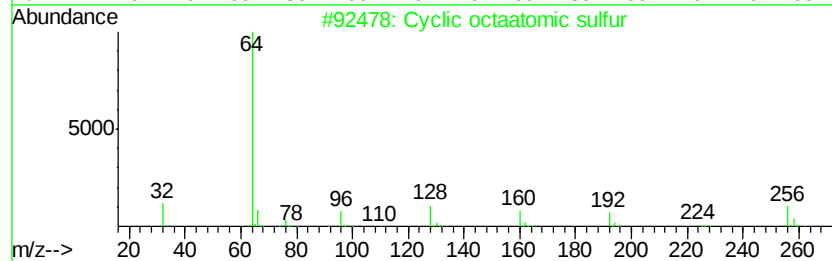
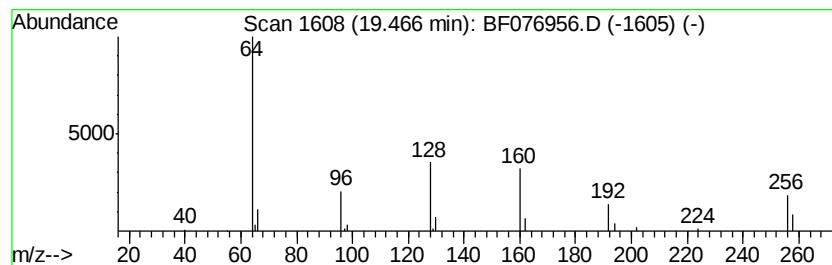
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 10 Cyclic octaatomic sulfur Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.47	6.96 ng	106474	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclic octaatomic sulfur	256	S8	010544-50-0	90
2		Benzoic acid, 2,5-dinitro-	212	C7H4N2O6	000610-28-6	59
3		Acetonitrile, 2-(5-chloro-3-oxo-...	248	C8H9ClN2OS2	1000269-94-4	9
4		2,3-Diazabicyclo[3.2.0]hept-2-en...	176	C7H7F3N2	1000258-92-2	9
5		7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	9



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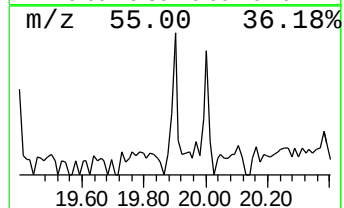
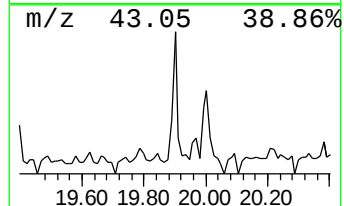
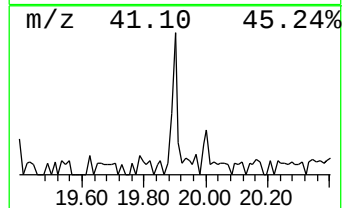
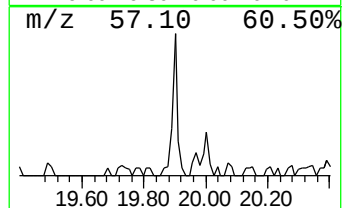
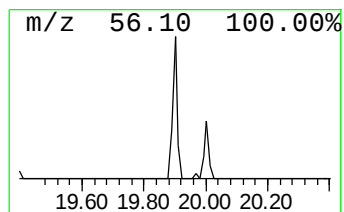
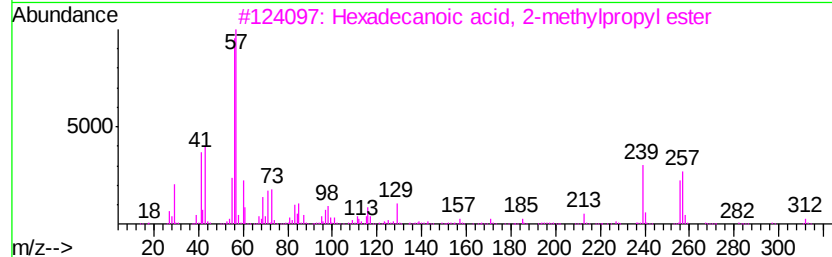
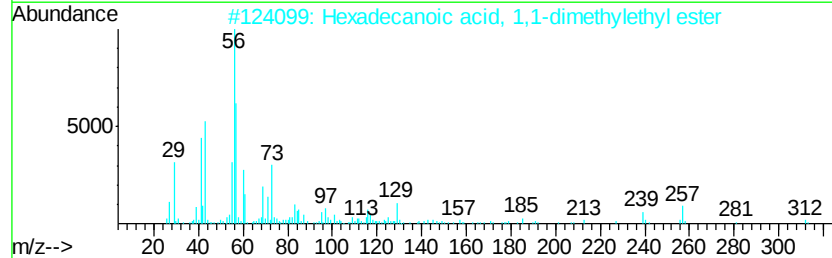
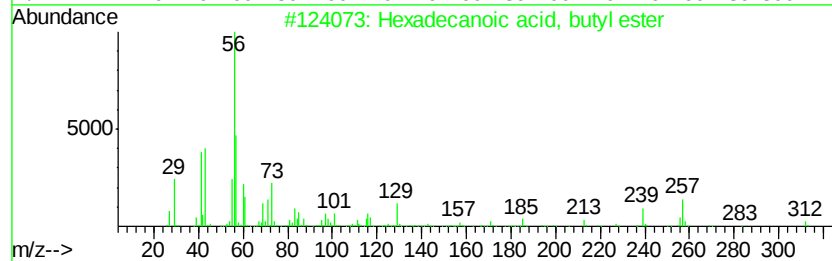
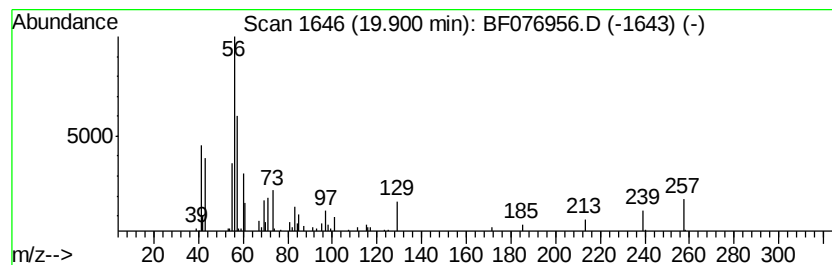
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 11 Hexadecanoic acid, butyl ester Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	3.45 ng	68552	Chrysene-d12	21.27

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	80
3			Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
4			Pentadecane, 8-methylene-	224	C16H32	055668-09-2	37
5			1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
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ALS Vial : 33 Sample Multiplier: 1

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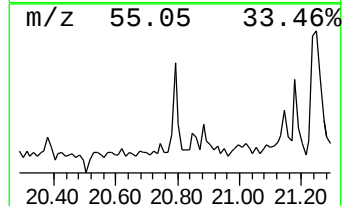
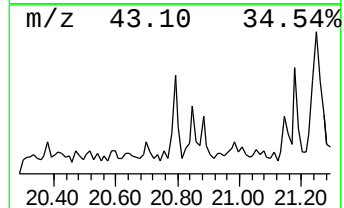
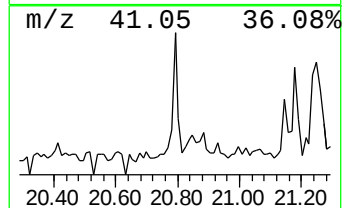
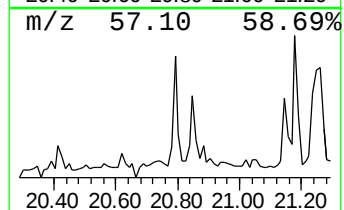
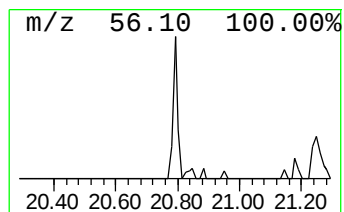
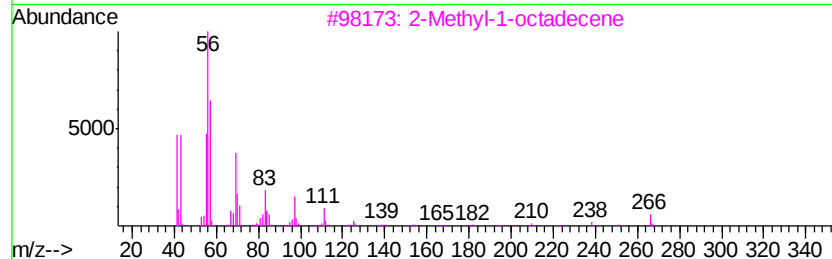
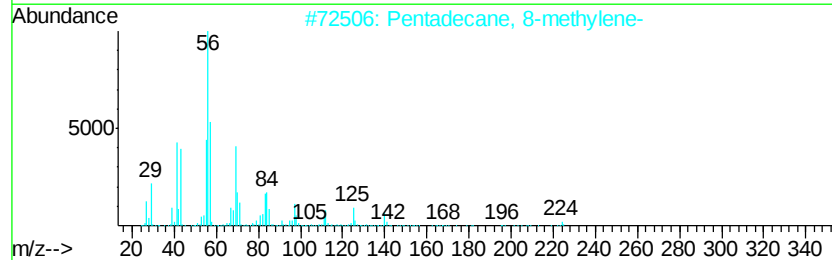
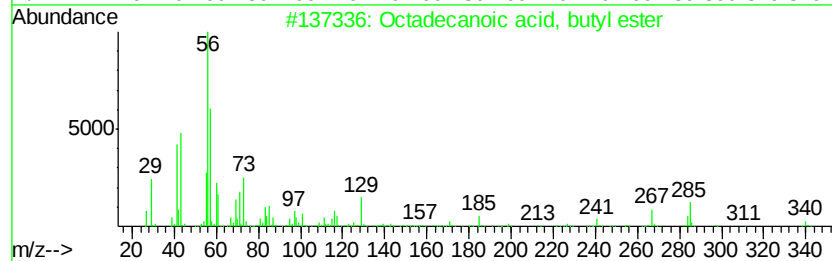
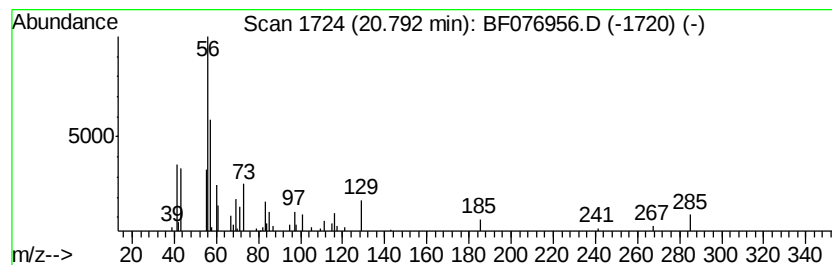
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 12 Octadecanoic acid, butyl ester Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	2.52 ng	50219	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	91
2		Pentadecane, 8-methylene-	224	C16H32	055668-09-2	38
3		2-Methyl-1-octadecene	266	C19H38	061868-20-0	38
4		2-Methylhexadec-1-ene	238	C17H34	061868-19-7	32
5		2-Methyl-1-tetradecene	210	C15H30	052254-38-3	32



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Misc : W
ALS Vial : 33 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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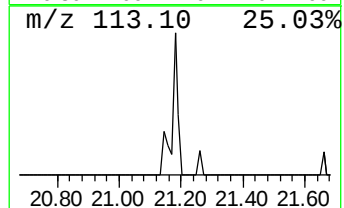
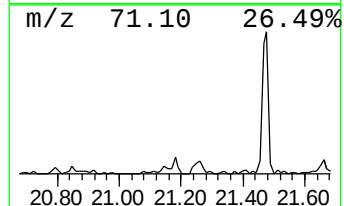
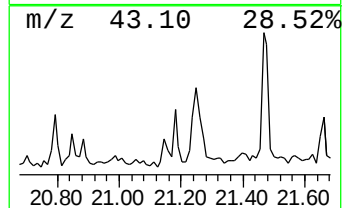
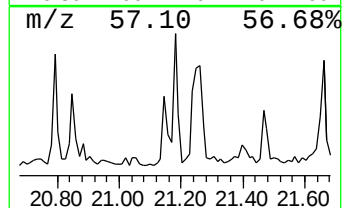
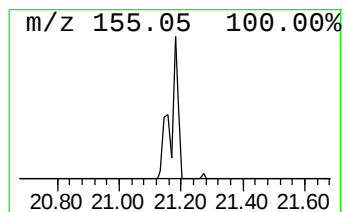
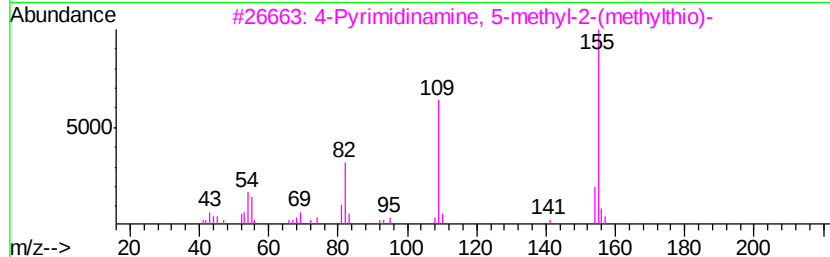
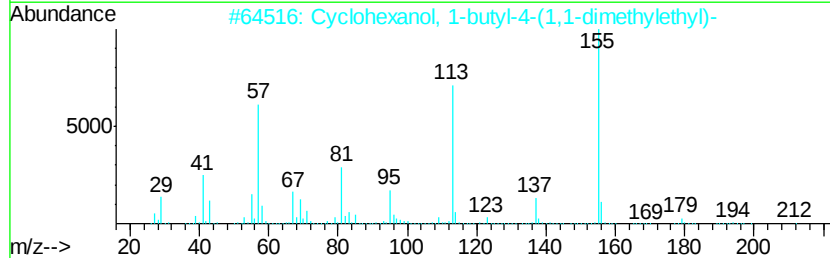
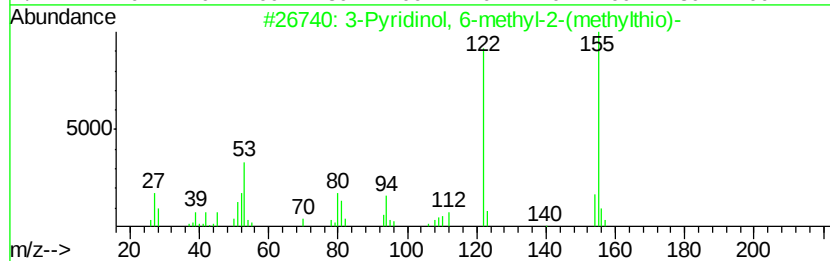
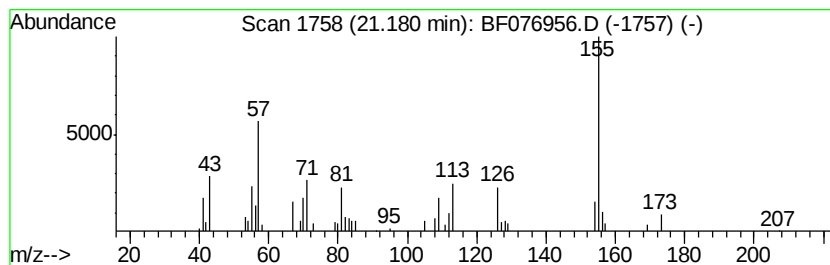
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 13 unknown21.18 Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.18	2.53 ng	50259	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Pyridinol, 6-methyl-2-(methylt...	155	C7H9NOS	023003-25-0	43
2		Cyclohexanol, 1-butyl-4-(1,1-dim...	212	C14H28O	053188-79-7	43
3		4-Pyrimidinamine, 5-methyl-2-(me...	155	C6H9N3S	054308-64-4	38
4		Benzaldehyde, 4-chloro-, oxime, ...	155	C7H6ClNO	003717-23-5	38
5		Hexadecanoic acid, 9,10,16-trihy...	304	C16H32O5	006949-98-0	38



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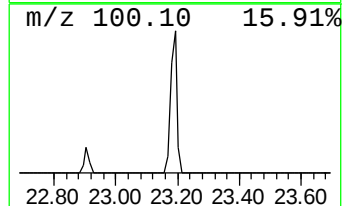
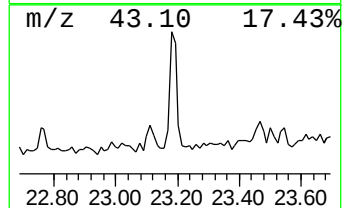
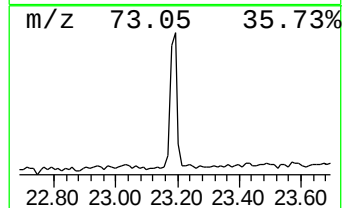
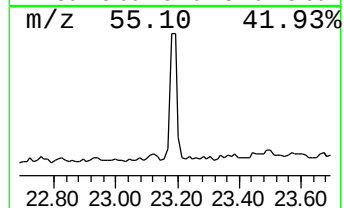
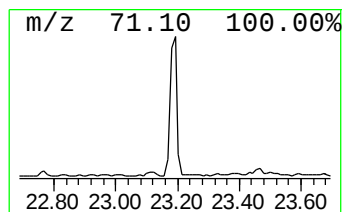
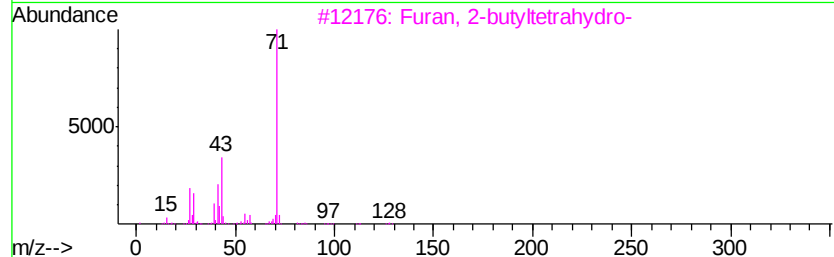
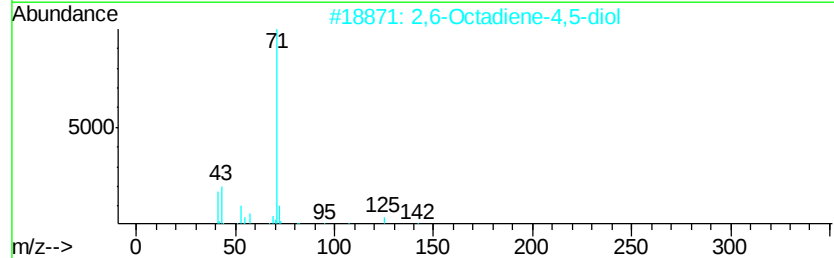
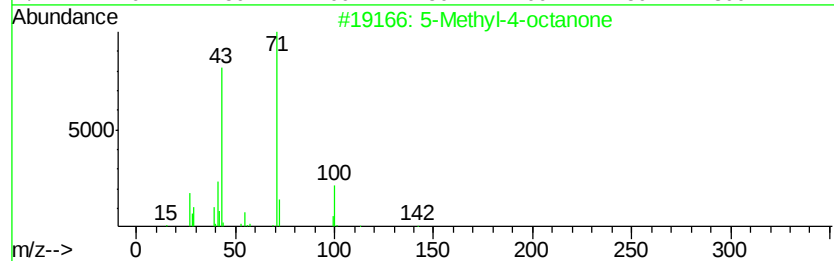
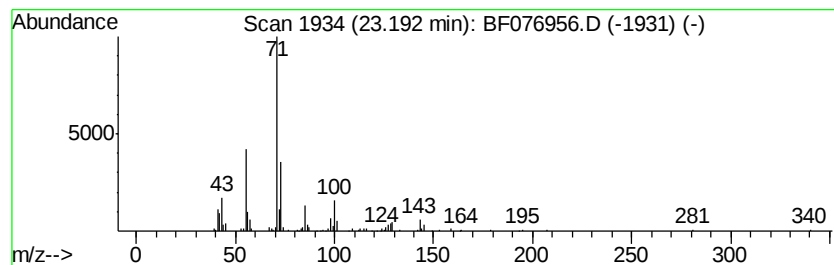
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 15 unknown23.19 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.19	12.23 ng	188317	Perylene-d12	22.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Methyl-4-octanone	142	C9H18O	006175-51-5	40
2		2,6-Octadiene-4,5-diol	142	C8H14O2	004486-59-3	38
3		Furan, 2-butyltetrahydro-	128	C8H16O	001004-29-1	37
4		2,2-Dimethylperhydro-1,3-oxazine	115	C6H13NO	073155-29-0	36
5		Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	33



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ALS Vial : 33 Sample Multiplier: 1

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PO-004

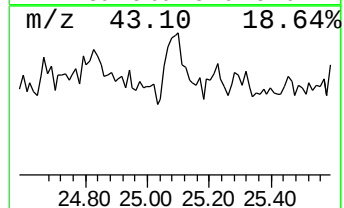
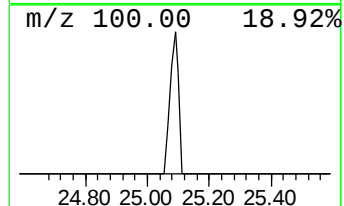
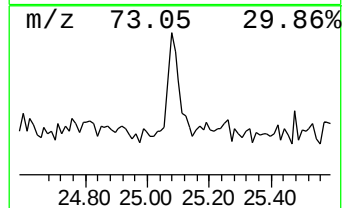
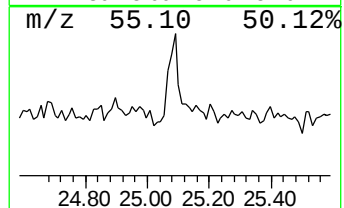
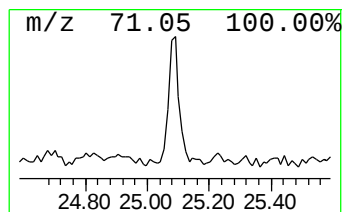
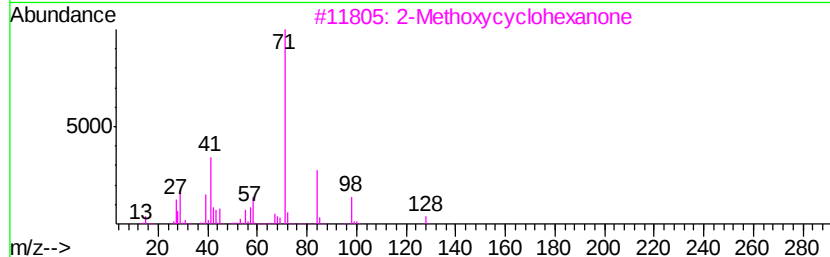
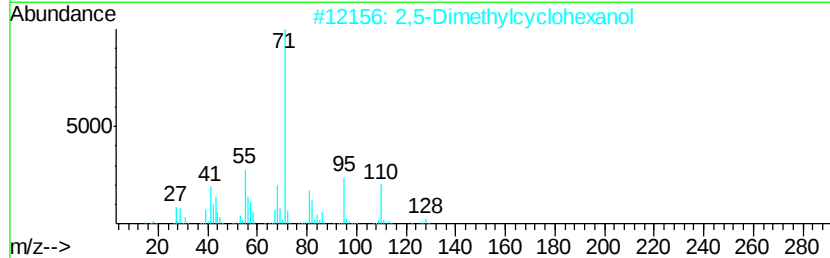
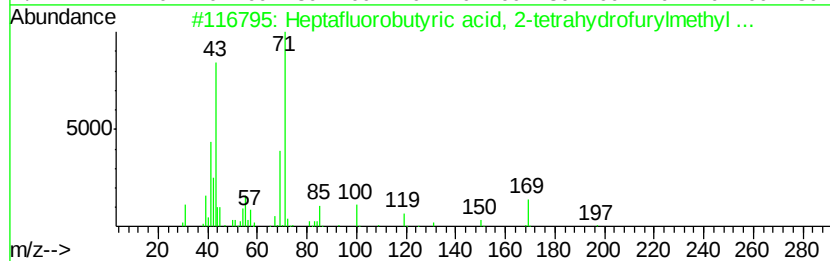
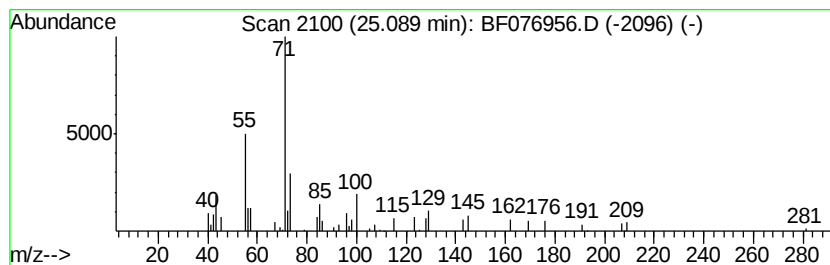
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 16 Heptafluorobutyric acid, 2-... Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
25.09	3.42 ng	52664	Perylene-d12	22.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, 2-tetra...	298	C9H9F7O3	1000216-78-5	50
2		2,5-Dimethylcyclohexanol	128	C8H16O	003809-32-3	43
3		2-Methoxycyclohexanone	128	C7H12O2	007429-44-9	43
4		2,2-Dimethylperhydro-1,3-oxazine	115	C6H13NO	073155-29-0	40
5		Butane, 2,2'-[methylenebis(oxy)]...	188	C11H24O2	054699-28-4	36



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
 Data File : BF076956.D
 Acq On : 20 Jan 2015 8:36
 Operator : IZ / TP
 Sample : G1101-02
 Misc : W
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 PO-004

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown4.10	4.10	4.7	ng	42898	1	7.98	181631	20.0
unknown7.46	7.46	83.7	ng	759685	1	7.98	181631	20.0
Benzenesulfonamid...	16.55	3.6	ng	55326	4	17.77	306113	20.0
Benzenesulfonamid...	16.91	12.2	ng	187135	4	17.77	306113	20.0
unknown17.13	17.13	4.0	ng	60674	4	17.77	306113	20.0
1-Penten-3-ol, 2-...	19.39	4.1	ng	63239	4	17.77	306113	20.0
Cyclic octaatomic...	19.47	7.0	ng	106474	4	17.77	306113	20.0
Hexadecanoic acid...	19.90	3.5	ng	68552	5	21.27	397880	20.0
Octadecanoic acid...	20.79	2.5	ng	50219	5	21.27	397880	20.0
unknown21.18	21.18	2.5	ng	50259	5	21.27	397880	20.0
unknown23.19	23.19	12.2	ng	188317	6	22.91	307995	20.0
Heptafluorobutyri...	25.09	3.4	ng	52664	6	22.91	307995	20.0