

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
 Data File : BF076955.D
 Acq On : 20 Jan 2015 8:02
 Operator : IZ / TP
 Sample : G1086-03
 Misc : W
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VESEY-CHURCH-ST-COMPOSITE

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	43	rVB2	22910	56973	4.41%	0.500%
2	4.104	262	264	275	rBV	127509	301870	23.36%	2.647%
3	5.041	342	346	358	rBV	531755	1005543	77.83%	8.818%
4	7.373	547	550	555	rBV	547770	1001549	77.52%	8.783%
5	7.464	555	558	567	rVB	600065	1097931	84.98%	9.628%
6	7.979	599	603	606	rVB	125351	206894	16.01%	1.814%
7	8.299	627	631	634	rBV	518231	808101	62.55%	7.086%
8	9.270	712	716	719	rBV	420268	635678	49.20%	5.574%
9	10.882	854	857	861	rBV	196181	291162	22.54%	2.553%
10	13.534	1085	1089	1092	rBV	804715	1234011	95.51%	10.821%
11	14.597	1179	1182	1185	rBV	71555	104067	8.05%	0.913%
12	15.008	1215	1218	1222	rBV	187178	317428	24.57%	2.784%
13	16.208	1320	1323	1326	rBV	41791	56081	4.34%	0.492%
14	16.631	1357	1360	1362	rBV	35136	46099	3.57%	0.404%
15	16.677	1362	1364	1367	rBV	507068	788749	61.05%	6.917%
16	17.774	1458	1460	1463	rBV	242470	329405	25.50%	2.889%
17	18.757	1544	1546	1551	rBV2	15500	21385	1.66%	0.188%
18	19.454	1603	1607	1609	rBV	29365	34781	2.69%	0.305%
19	19.740	1630	1632	1634	rBV	31884	32479	2.51%	0.285%
20	19.900	1643	1646	1649	rBV	87143	90552	7.01%	0.794%
21	20.003	1653	1655	1658	rVB	1056450	1292029	100.00%	11.330%
22	20.792	1722	1724	1726	rBV	59638	68064	5.27%	0.597%
23	21.272	1761	1766	1768	rBV	346976	578644	44.79%	5.074%
24	21.477	1782	1784	1787	rBV3	16252	21724	1.68%	0.190%
25	21.660	1797	1800	1803	rVB	19602	27785	2.15%	0.244%
26	21.923	1820	1823	1825	rBV3	5165	13511	1.05%	0.118%
27	22.037	1831	1833	1836	rVB	20847	25045	1.94%	0.220%
28	22.415	1864	1866	1867	rBV	16307	23216	1.80%	0.204%
29	22.506	1873	1874	1879	rVB	16716	27533	2.13%	0.241%
30	22.769	1895	1897	1898	rBV	15375	19945	1.54%	0.175%
31	22.849	1901	1904	1907	rVB	17576	28514	2.21%	0.250%
32	22.917	1907	1910	1913	rBV	281715	357803	27.69%	3.138%
33	23.123	1926	1928	1931	rBV4	14811	22568	1.75%	0.198%
34	23.477	1957	1959	1960	rBV	19954	27117	2.10%	0.238%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

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	23.512	1960	1962	1965	rVV4	37542	76149	5.89%	0.668%
36	23.603	1968	1970	1973	rVV3	11285	17661	1.37%	0.155%
37	23.775	1983	1985	1987	rBV2	15804	29218	2.26%	0.256%
38	24.015	2004	2006	2010	rBV4	16809	33692	2.61%	0.295%
39	24.460	2043	2045	2050	rVB5	22234	46239	3.58%	0.405%
40	24.689	2059	2065	2072	rBV3	32883	161768	12.52%	1.419%
41	24.838	2076	2078	2084	rVB7	16328	44909	3.48%	0.394%

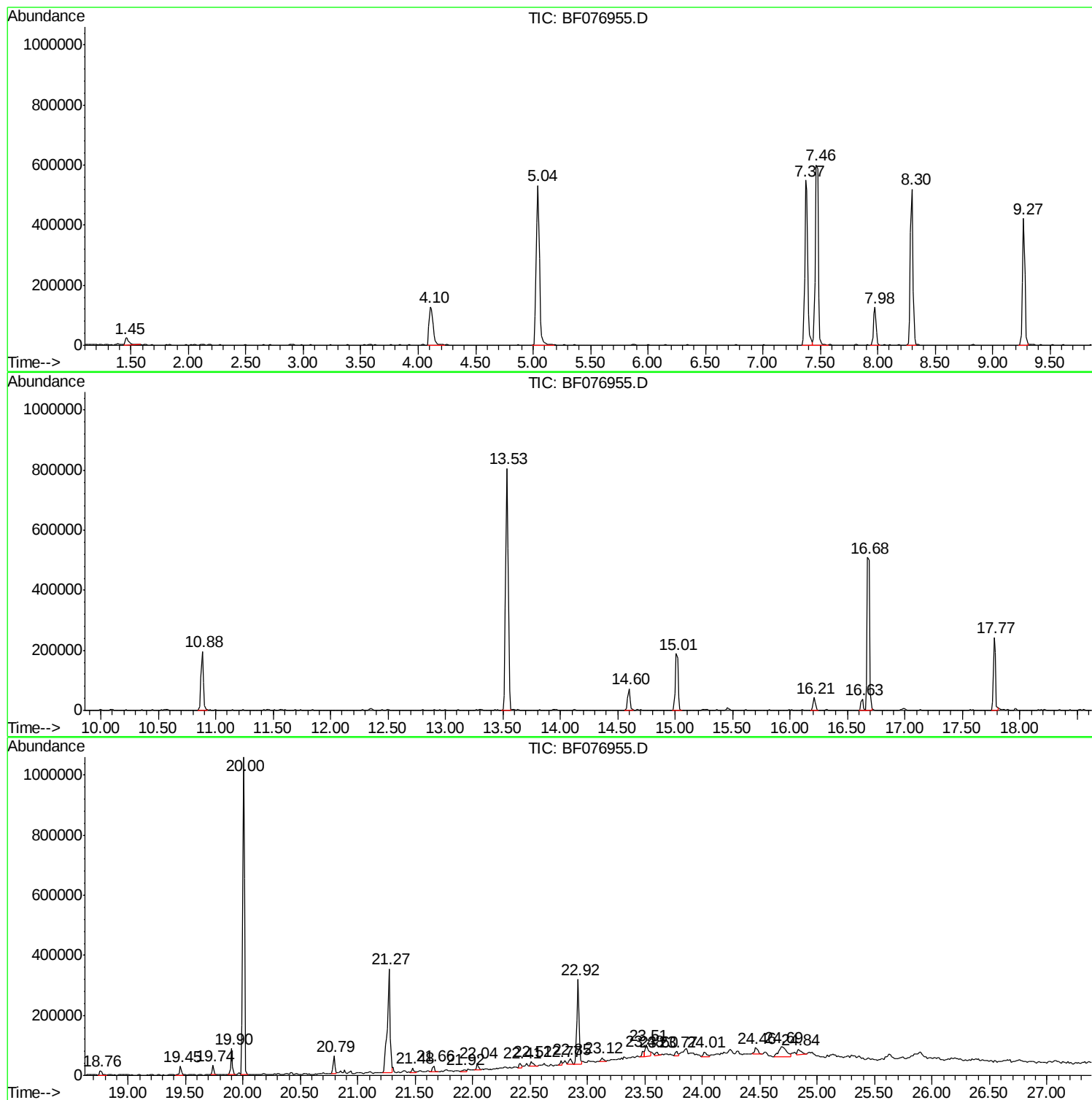
Sum of corrected areas: 11403872

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

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



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

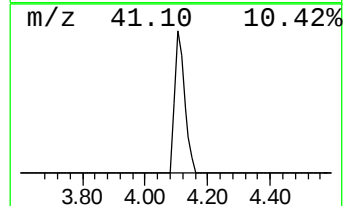
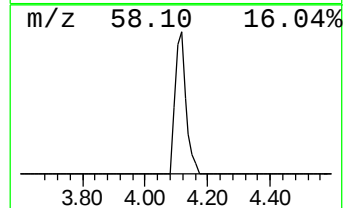
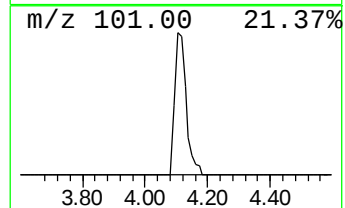
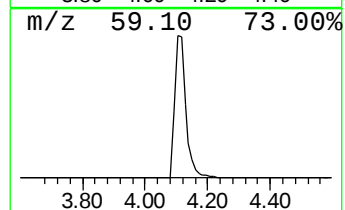
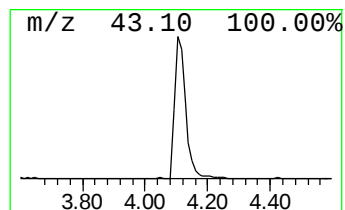
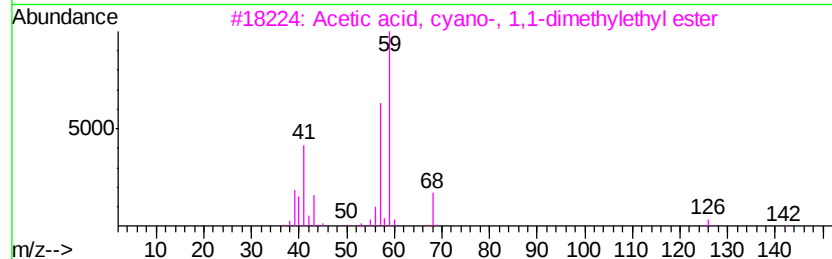
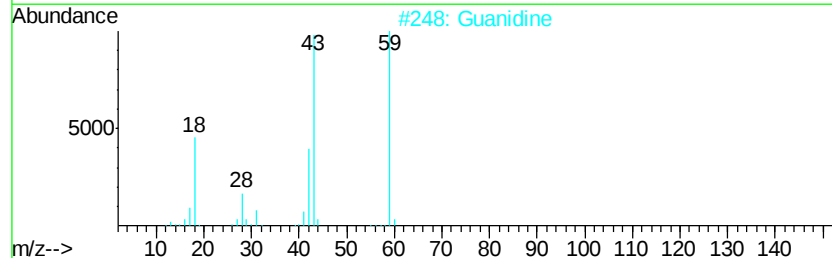
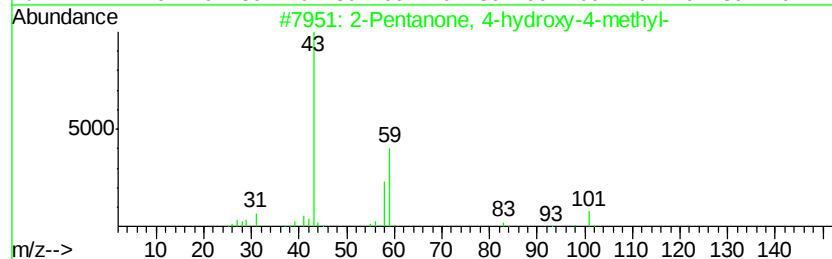
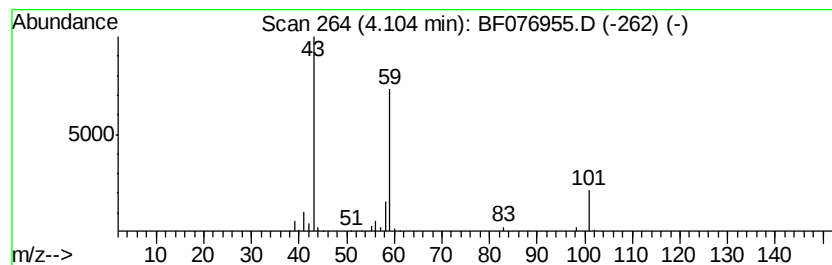
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.10	29.18 ng	301870	1,4-Dichlorobenzene-d4	7.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2		Guanidine	59	CH5N3	000113-00-8	43
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

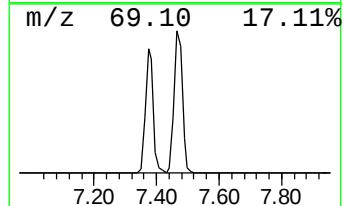
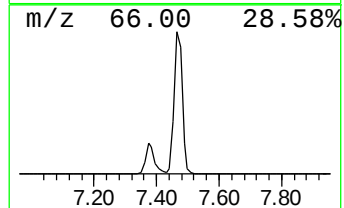
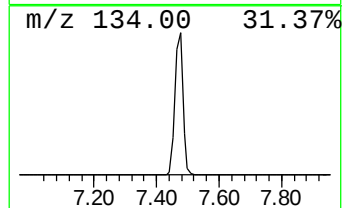
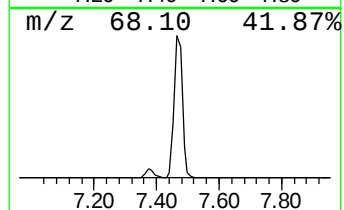
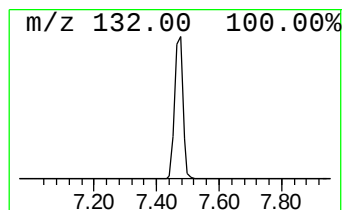
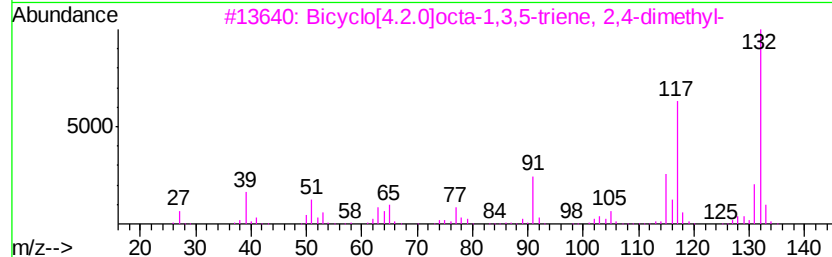
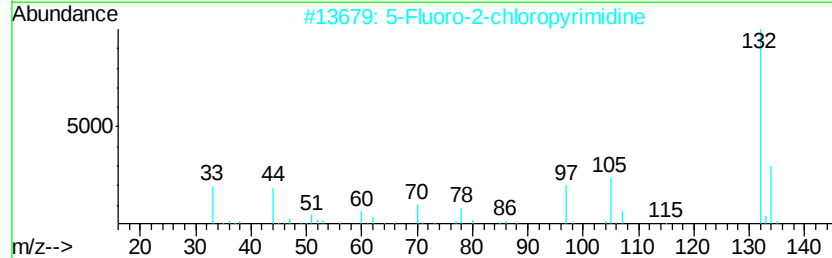
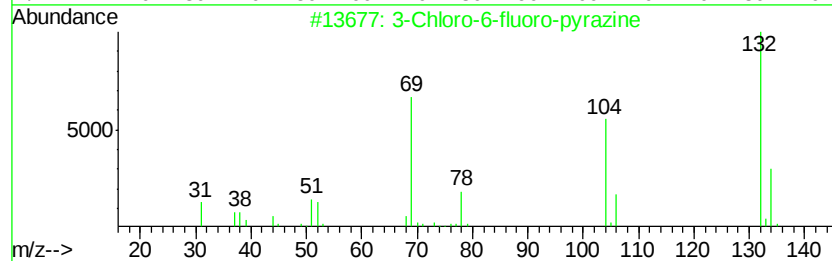
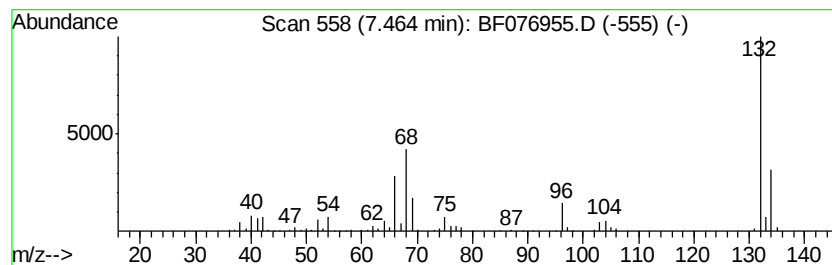
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.46	106.14 ng	1097930	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	35
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		Benzene, 1-ethenyl-3,5-dimethyl-	132	C10H12	005379-20-4	9
5		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

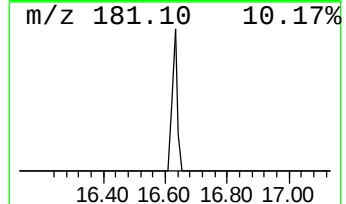
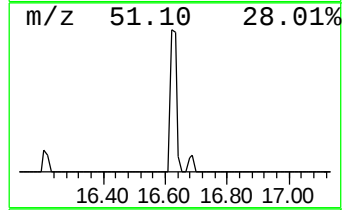
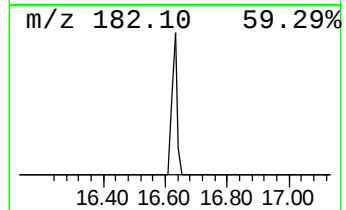
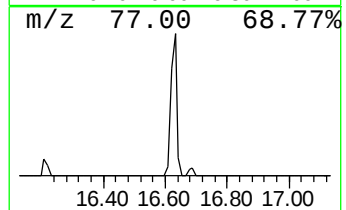
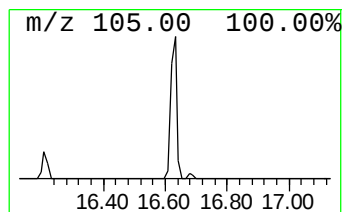
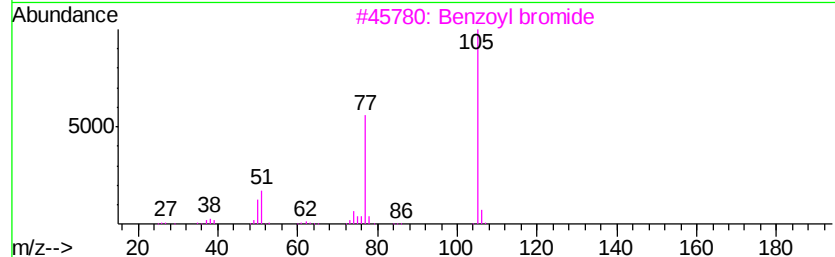
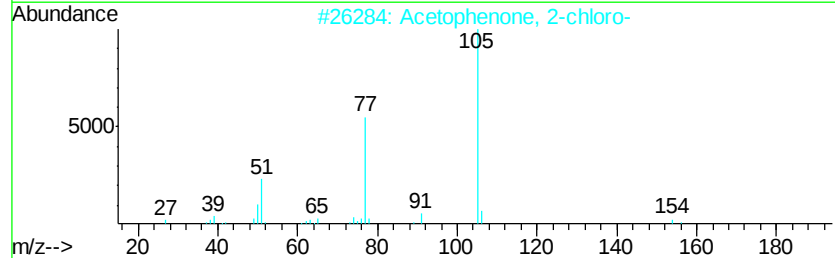
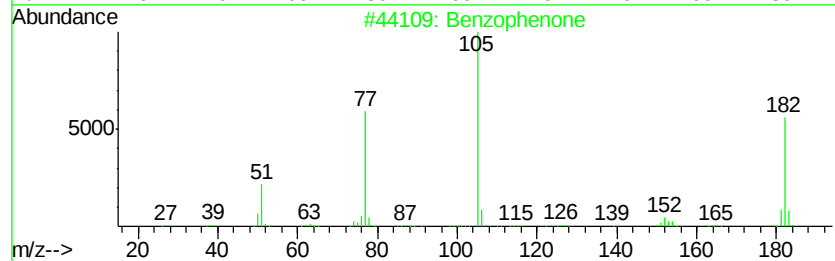
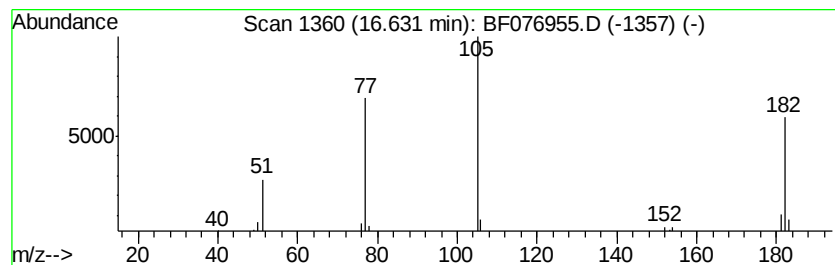
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Benzophenone Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.63	2.80 ng	46099	Phenanthrene-d10	17.77

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	94
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
3		Benzoyl bromide	184	C7H5BrO	000618-32-6	43
4		Benzoyl chloride	140	C7H5ClO	000098-88-4	43
5		Ethanone, 2-bromo-1-phenyl-	198	C8H7BrO	000070-11-1	43



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

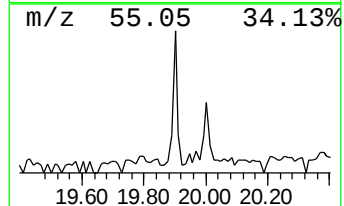
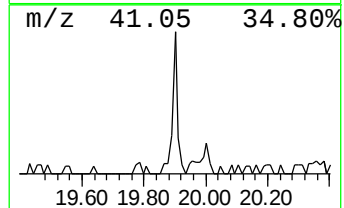
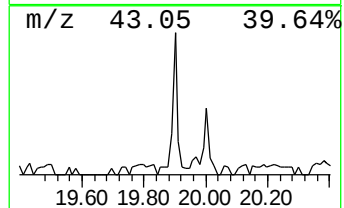
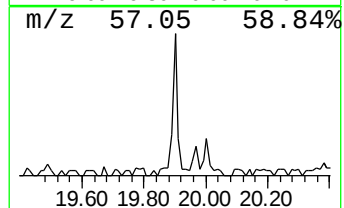
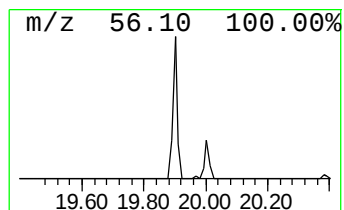
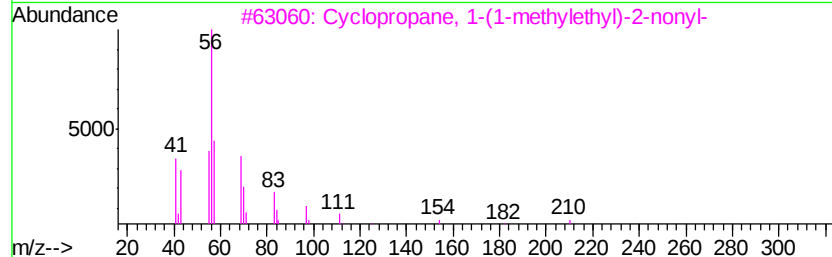
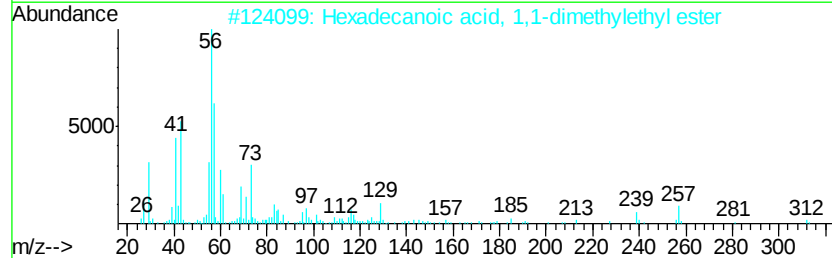
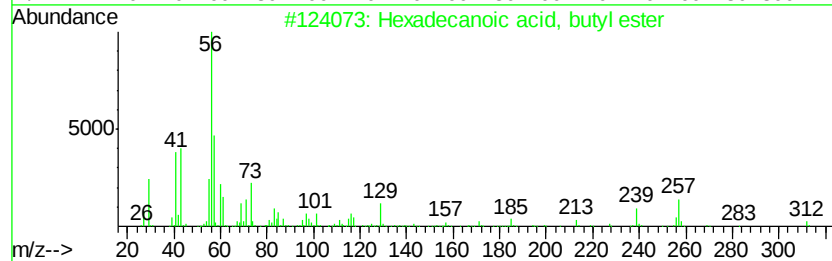
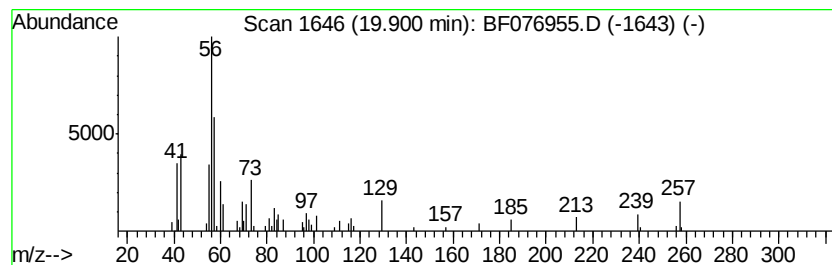
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.90	3.13 ng	90552	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	91
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	91
3		Cyclopropane, 1-(1-methylethyl)-...	210	C15H30	041977-39-3	38
4		Cyclopentanecarboxylic acid, 2-a...	129	C6H11NO2	037910-65-9	37
5		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	37



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

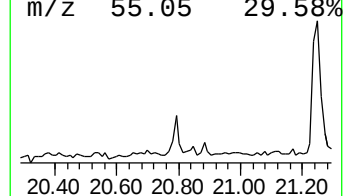
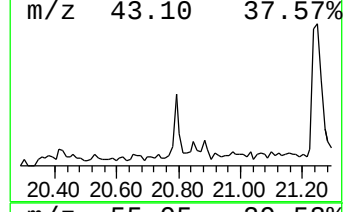
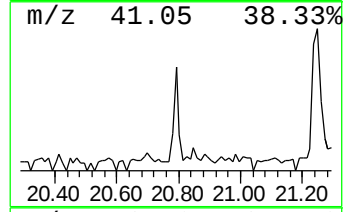
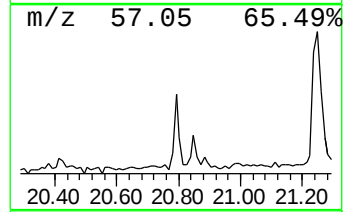
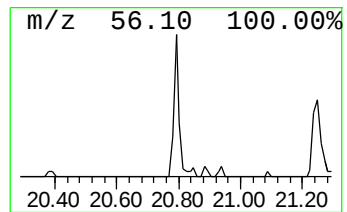
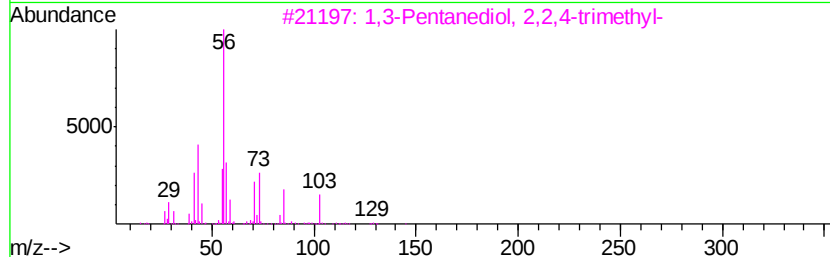
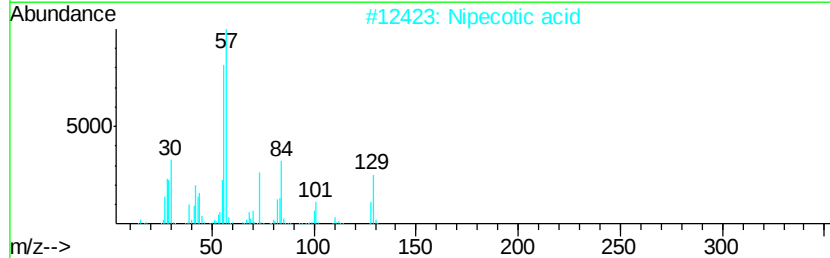
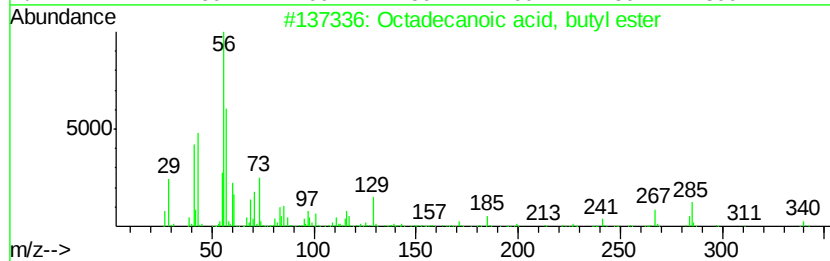
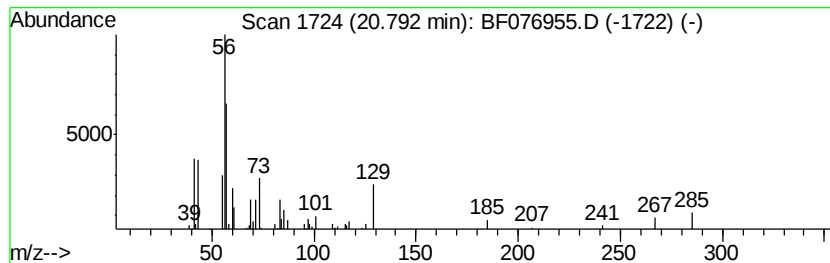
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid, butyl ester Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.79	2.35 ng	68064	Chrysene-d12	21.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	90
2		Nipecotic acid	129	C6H11NO2	000498-95-3	50
3		1,3-Pentanediol, 2,2,4-trimethyl-	146	C8H18O2	000144-19-4	37
4		Decane, 2,2,3-trimethyl-	184	C13H28	062338-09-4	35
5		Urea, N,N'-di-2-propenyl-	140	C7H12N2O	001801-72-5	35



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

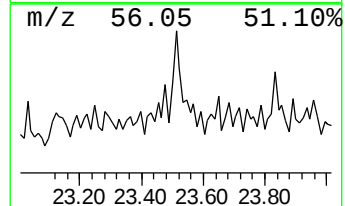
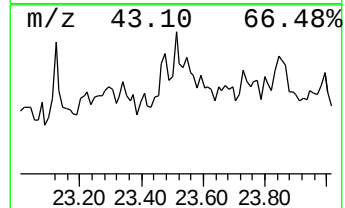
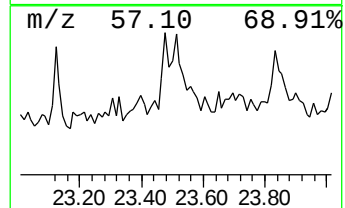
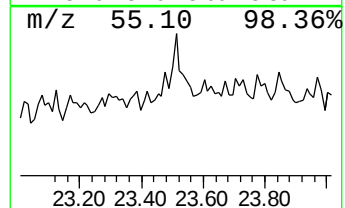
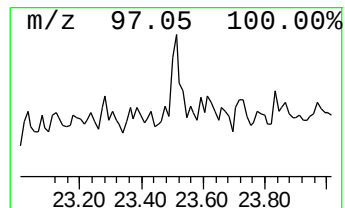
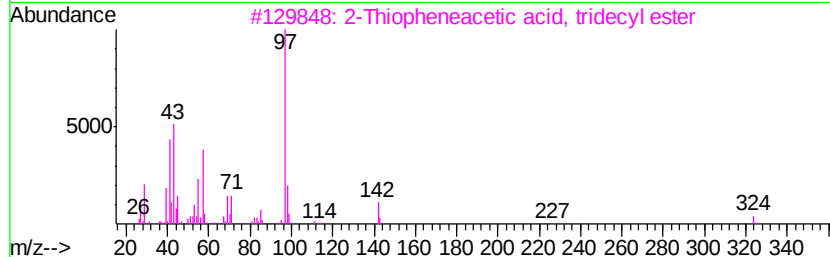
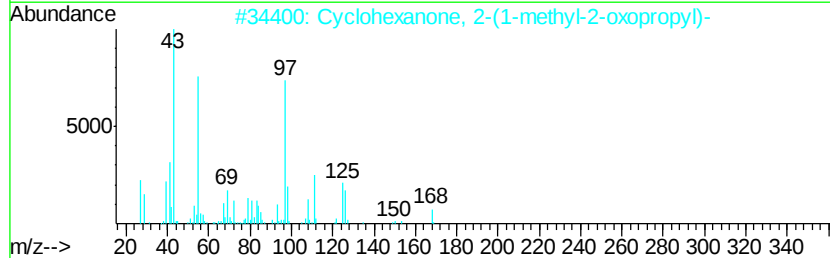
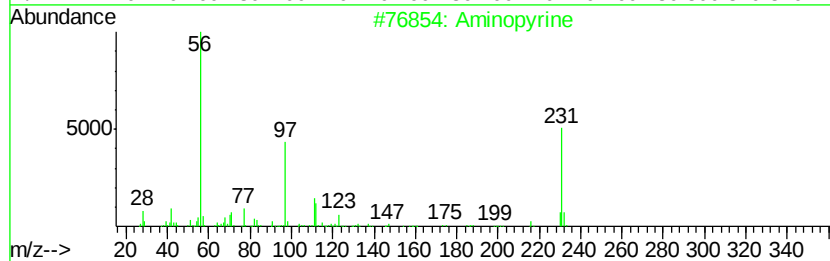
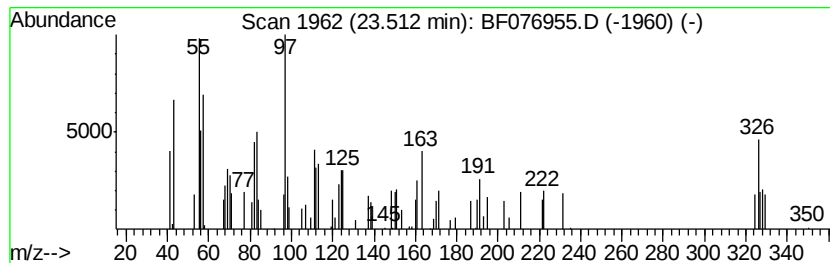
Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

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 9 unknown23.51 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.51	4.26 ng	76149	Perylene-d12	22.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Aminopvrine	231	C13H17N3O	000058-15-1	30
2	Cyclohexanone, 2-(1-methyl-2-oxo...	168	C10H16O2	067722-25-2	27
3	2-Thiopheneacetic acid, tridecyl...	324	C19H32O2S	1000278-91-8	14
4	Cyclohexane, 1,2-dimethyl-, trans-	112	C8H16	006876-23-9	11
5	Cyclohexane, 1,2-dimethyl-	112	C8H16	000583-57-3	11



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

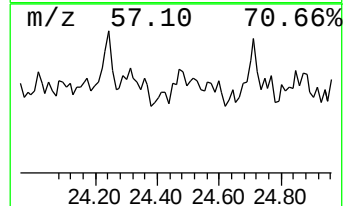
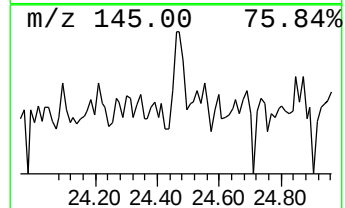
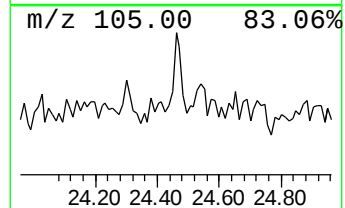
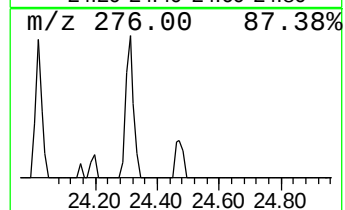
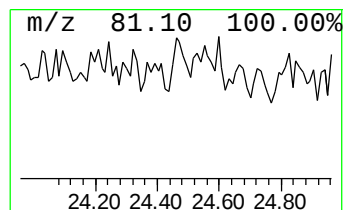
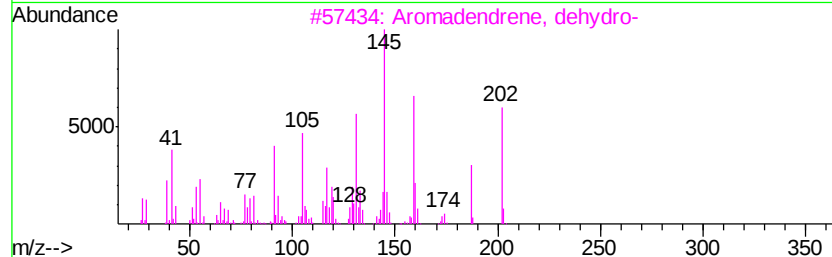
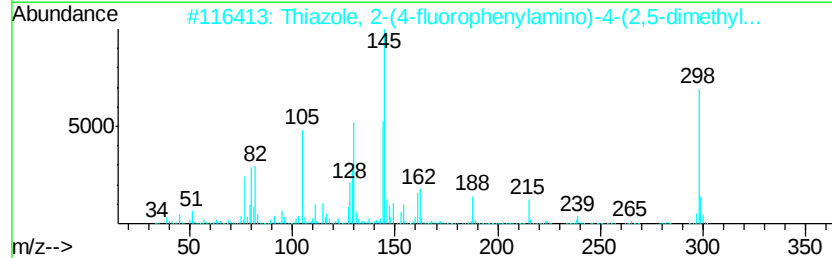
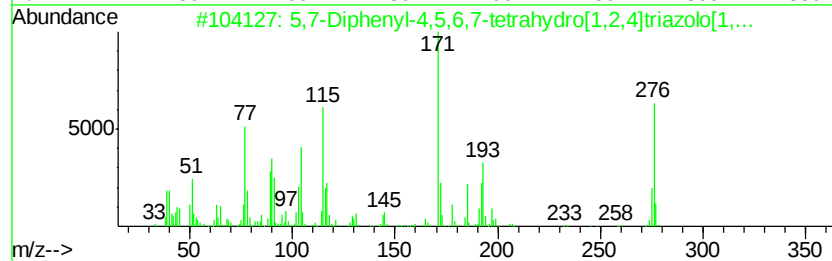
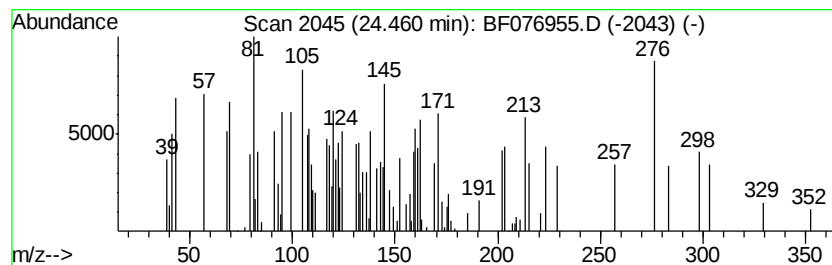
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown24.46 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.46	2.58 ng	46239	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5,7-Diphenyl-4,5,6,7-tetrahydro[...]	276	C17H16N4	133533-71-8	25
2		Thiazole, 2-(4-fluorophenylamino...	298	C17H15FN2S	339197-00-1	11
3		Aromadendrene, dehydro-	202	C15H22	1000156-12-5	10
4		Norflurazon	303	C12H9ClF3N3O	027314-13-2	9
5		.alpha.-1-Naphthylisobutyric aci...	276	C16H17FO3	1000129-24-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

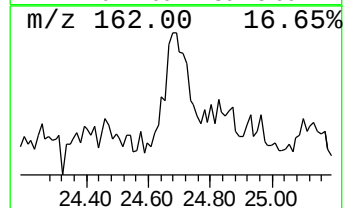
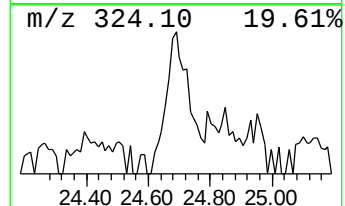
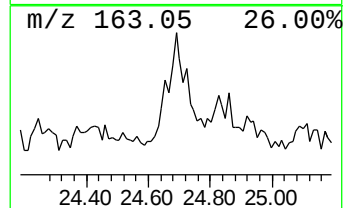
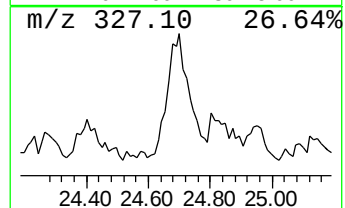
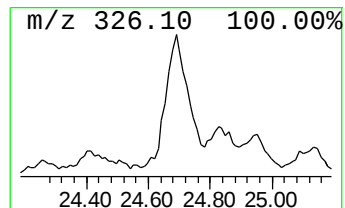
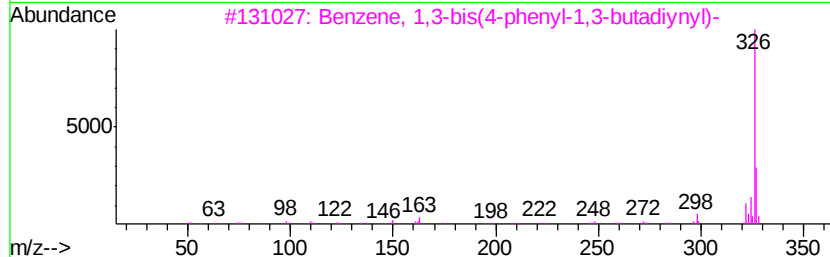
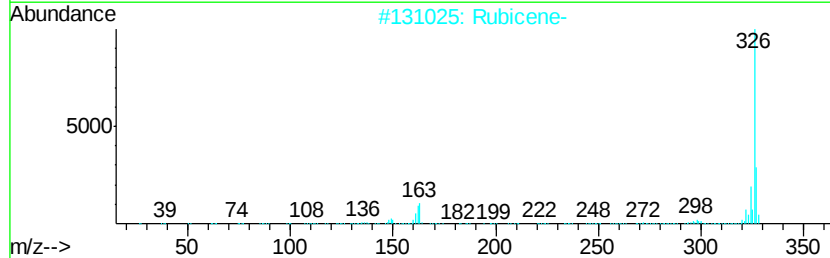
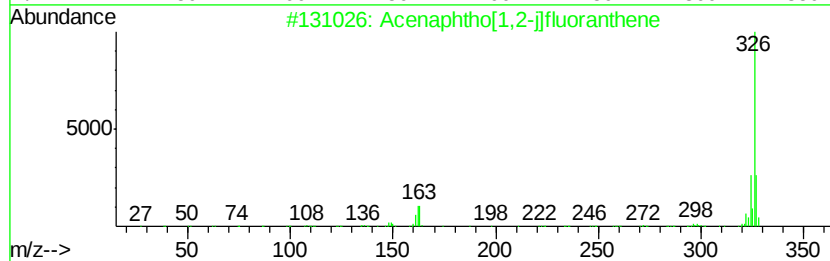
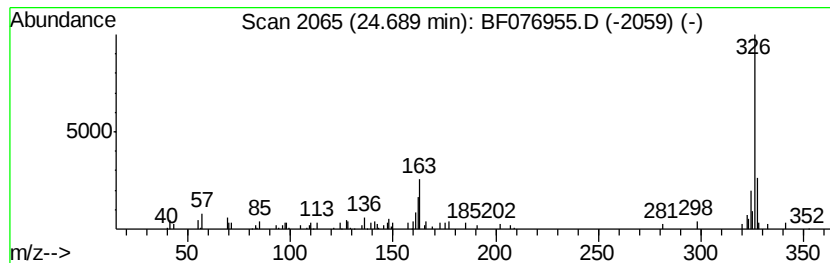
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Acenaphtho[1,2-j]fluoranthene Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.69	9.04 ng	161768	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Acenaphtho[1,2-il]fluoranthene	326	C26H14	000193-21-5	76
2		Rubicene-	326	C26H14	000197-61-5	76
3		Benzene, 1,3-bis(4-phenyl-1,3-butadienyl)-	326	C26H14	037902-13-9	52
4		Bis(pentamethylcyclopentadienyl)iron	326	C20H30Fe	012126-50-0	50
5		2-(4-Biphenyl)imidazo[2,1-b]benzimidazole	326	C21H14N2S	038956-29-5	50



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
Data File : BF076955.D
Acq On : 20 Jan 2015 8:02
Operator : IZ / TP
Sample : G1086-03
Misc : W
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
VESEY-CHURCH-ST-COMPOSITE

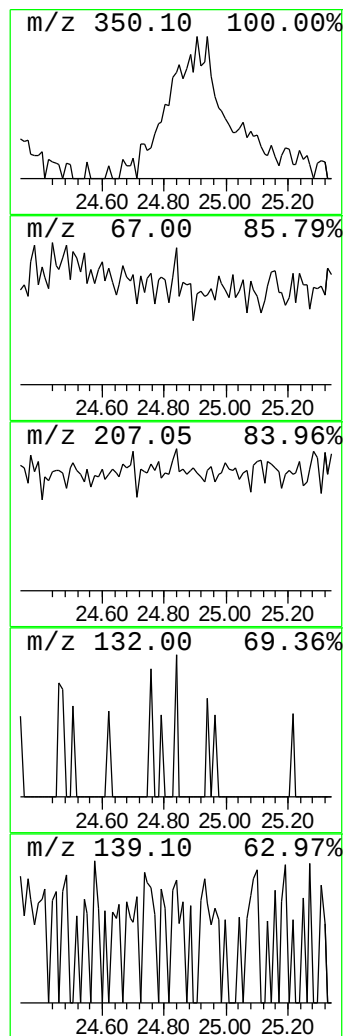
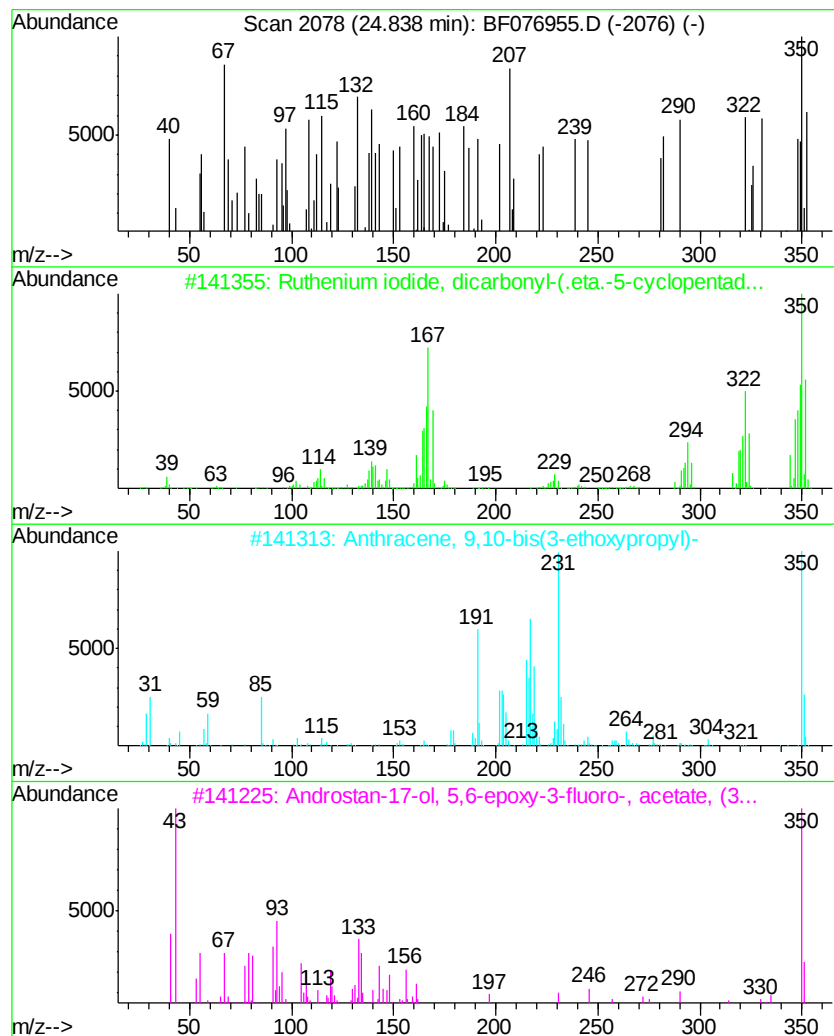
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Ruthenium iodide, dicarbonyl... Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.84	2.51 ng	44909	Perylene-d12	22.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ruthenium iodide, dicarbonyl-(.e...	350	C7H5IO2Ru	031781-83-6	55
2		Anthracene, 9,10-bis(3-ethoxypro...	350	C24H30O2	102954-64-3	11
3		Androstan-17-ol, 5,6-epoxy-3-flu...	350	C21H31FO3	028344-39-0	9
4		Benzo[a]coronene	350	C28H14	000190-70-5	9
5		4-[2-[5-(4-fluoro-phenyl)-furan-...	350	C17H10F4N2O2	1000297-02-5	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF011915\
 Data File : BF076955.D
 Acq On : 20 Jan 2015 8:02
 Operator : IZ / TP
 Sample : G1086-03
 Misc : W
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 VESEY-CHURCH-ST-COMPOSITE

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
2-Pentanone, 4-hy...	4.10	29.2	ng	301870	1	7.98	206894	20.0
unknown7.46	7.46	106.1	ng	1097930	1	7.98	206894	20.0
Benzophenone	16.63	2.8	ng	46099	4	17.77	329405	20.0
Hexadecanoic acid...	19.90	3.1	ng	90552	5	21.27	578644	20.0
Octadecanoic acid...	20.79	2.4	ng	68064	5	21.27	578644	20.0
unknown23.51	23.51	4.3	ng	76149	6	22.92	357803	20.0
unknown24.46	24.46	2.6	ng	46239	6	22.92	357803	20.0
Acenaphtho[1,2-j]...	24.69	9.0	ng	161768	6	22.92	357803	20.0
Ruthenium iodide,...	24.84	2.5	ng	44909	6	22.92	357803	20.0