

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012015\
 Data File : BF076991.D
 Acq On : 21 Jan 2015 8:48
 Operator : IZ / TP
 Sample : G1111-04
 Misc : S
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 RBDC4-011615

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	1.361	23	24	29	rBV2	7670	14060	1.86%	0.182%
2	1.441	29	31	40	rVB	68384	116296	15.38%	1.508%
3	4.013	254	256	264	rVB	52399	119385	15.78%	1.549%
4	4.962	335	339	349	rBV	357910	707607	93.55%	9.178%
5	7.316	541	545	549	rBV	401570	721015	95.32%	9.352%
6	7.396	549	552	557	rVB	431346	756387	100.00%	9.811%
7	7.910	593	597	602	rVB	113722	186669	24.68%	2.421%
8	8.230	621	625	629	rBV	336227	524598	69.36%	6.805%
9	9.202	707	710	714	rBV	286416	444039	58.71%	5.760%
10	10.814	848	851	855	rBV	162236	254658	33.67%	3.303%
11	12.288	977	980	987	rVB	15533	23638	3.13%	0.307%
12	13.465	1080	1083	1087	rBV	446584	735633	97.26%	9.542%
13	14.540	1174	1177	1180	rVB	25017	37774	4.99%	0.490%
14	14.951	1209	1213	1216	rBV	165844	279607	36.97%	3.627%
15	16.574	1353	1355	1357	rBV	38493	47252	6.25%	0.613%
16	16.631	1357	1360	1363	rVV	430862	531333	70.25%	6.892%
17	17.729	1454	1456	1459	rBV	210887	282775	37.38%	3.668%
18	18.426	1515	1517	1520	rBV	5553	9425	1.25%	0.122%
19	18.723	1539	1543	1547	rBV	12295	17959	2.37%	0.233%
20	19.489	1608	1610	1612	rBV	8527	11019	1.46%	0.143%
21	19.969	1649	1652	1654	rVB	578281	715919	94.65%	9.286%
22	20.506	1696	1699	1700	rBV2	5525	9842	1.30%	0.128%
23	21.077	1746	1749	1751	rBV3	4308	10357	1.37%	0.134%
24	21.226	1758	1762	1765	rBV	218384	358882	47.45%	4.655%
25	21.375	1769	1775	1777	rBV3	13319	29365	3.88%	0.381%
26	21.615	1794	1796	1798	rBV2	8772	14396	1.90%	0.187%
27	21.706	1801	1804	1806	rBV4	6616	16881	2.23%	0.219%
28	22.015	1829	1831	1832	rVB2	8925	12005	1.59%	0.156%
29	22.049	1832	1834	1836	rVB3	6955	9402	1.24%	0.122%
30	22.220	1847	1849	1850	rBV2	6567	8681	1.15%	0.113%
31	22.438	1867	1868	1871	rBV3	13333	21970	2.90%	0.285%
32	22.563	1877	1879	1881	rBV3	11387	17411	2.30%	0.226%
33	22.895	1905	1908	1910	rVB	199934	279153	36.91%	3.621%
34	23.329	1944	1946	1950	rBV5	21226	61623	8.15%	0.799%

Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

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	23.398	1950	1952	1957	rVV6	27041	63217	8.36%	0.820%
36	23.489	1957	1960	1964	rVV4	50483	123994	16.39%	1.608%
37	23.615	1970	1971	1974	rBV3	21264	27701	3.66%	0.359%
38	23.798	1985	1987	1989	rVB	35240	42654	5.64%	0.553%
39	24.244	2024	2026	2028	rVB2	27821	35836	4.74%	0.465%
40	24.941	2085	2087	2091	rBV5	12852	29116	3.85%	0.378%

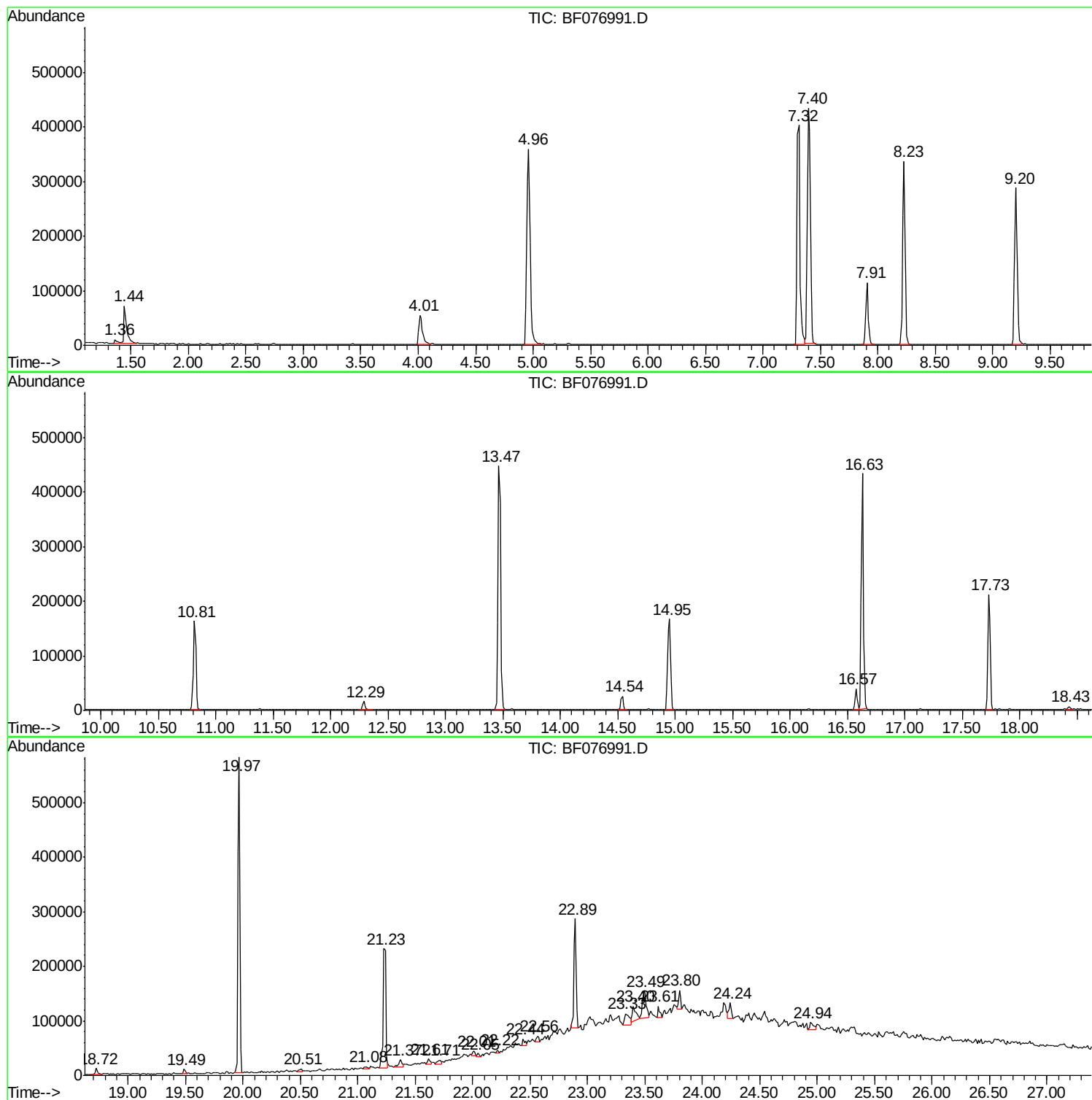
Sum of corrected areas: 7709534

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

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\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

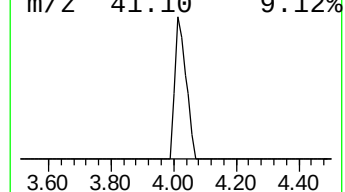
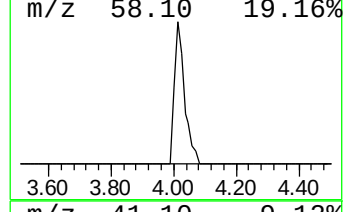
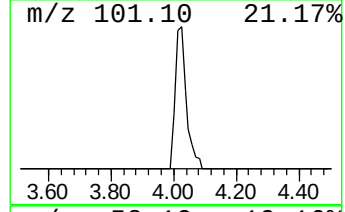
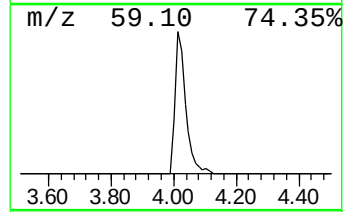
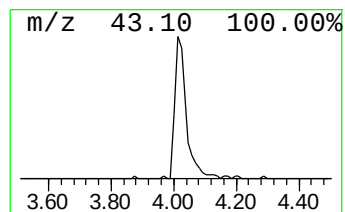
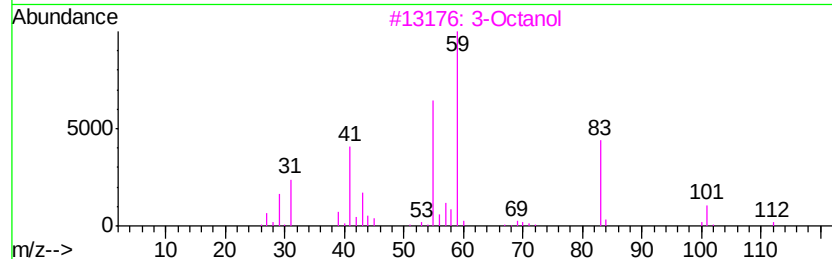
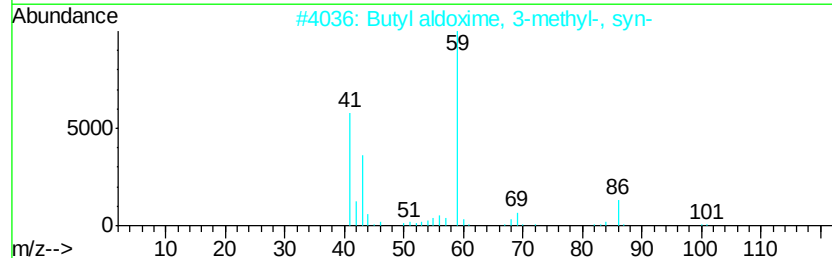
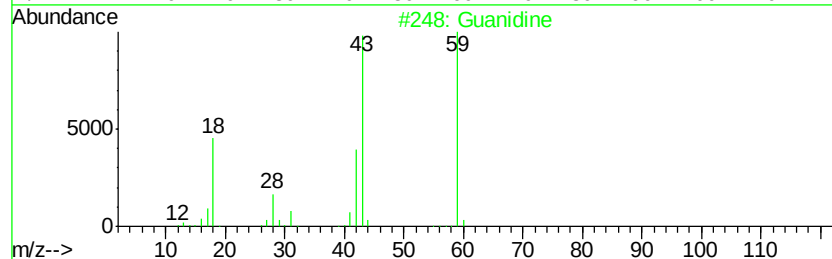
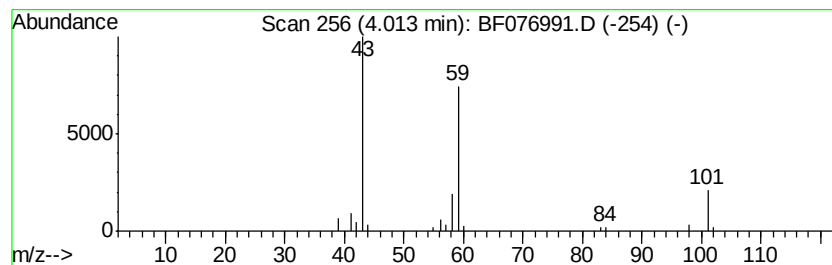
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown4.01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.01	12.79 ng	119385	1,4-Dichlorobenzene-d4	7.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Guanidine	59	CH5N3	000113-00-8	47
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	37
3		3-Octanol	130	C8H18O	000589-98-0	33
4		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	32
5		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

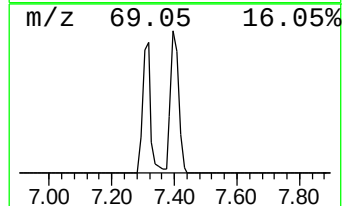
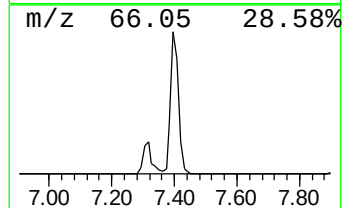
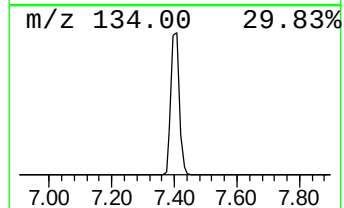
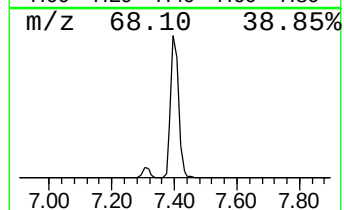
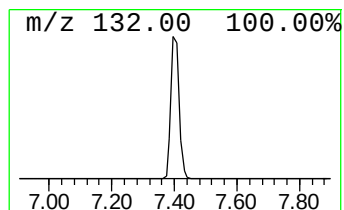
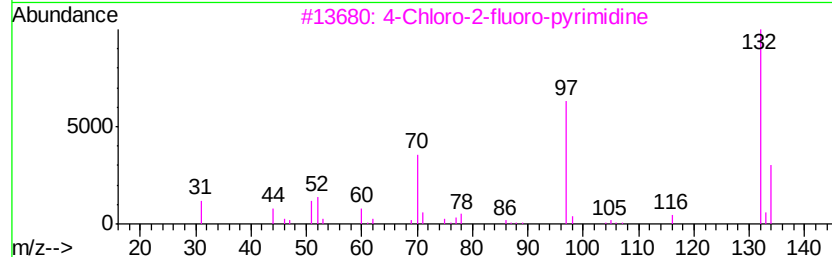
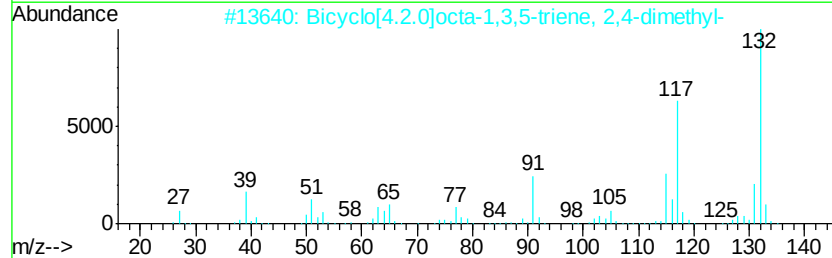
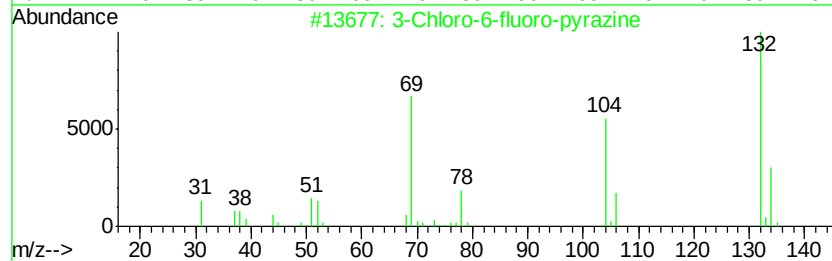
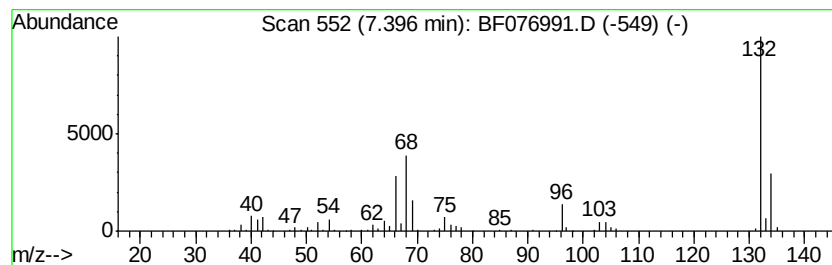
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.40 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.40	81.04 ng	756387	1,4-Dichlorobenzene-d4	7.91

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleID :
RBDC4-011615

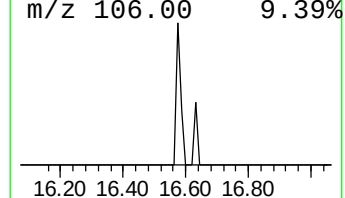
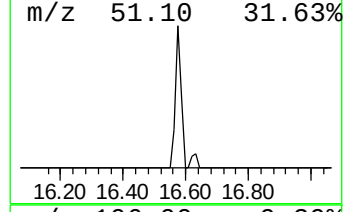
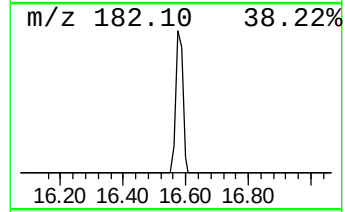
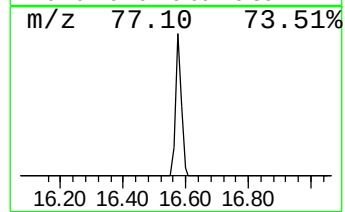
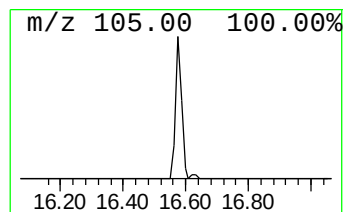
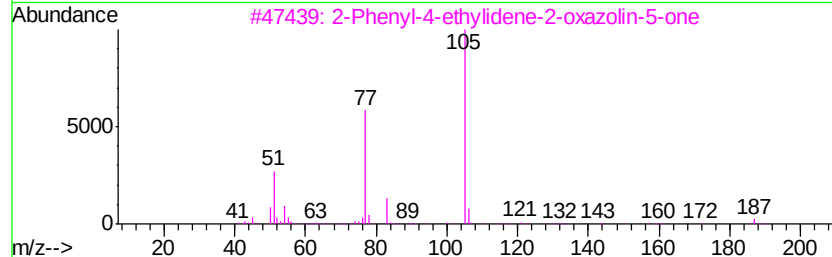
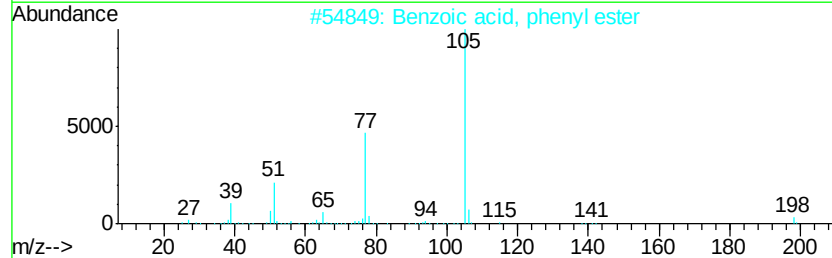
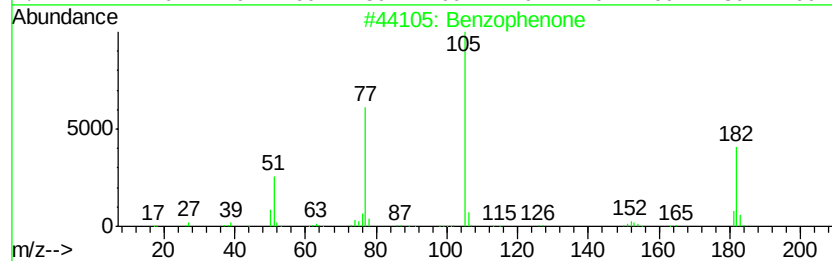
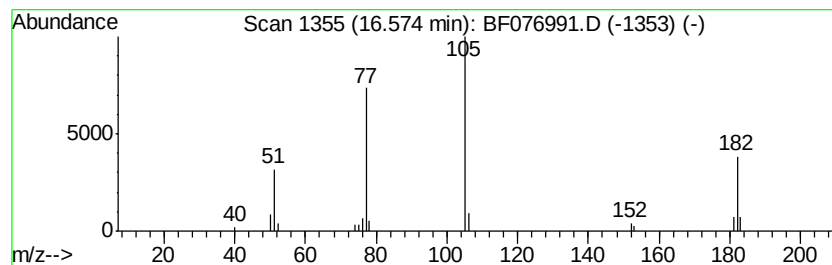
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
16.57	3.34 ng	47252	Phenanthrene-d10	17.73

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	95
2		Benzoic acid, phenyl ester	198	C13H10O2	000093-99-2	53
3		2-Phenyl-4-ethylidene-2-oxazolin...	187	C11H9N02	037791-41-6	53
4		Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	53
5		Benzeneacetic acid, .alpha.-oxo-...	164	C9H8O3	015206-55-0	53



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

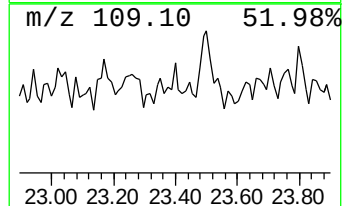
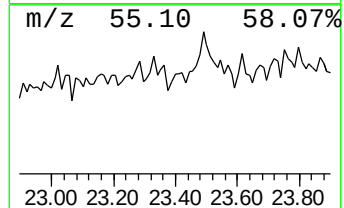
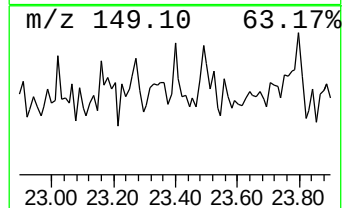
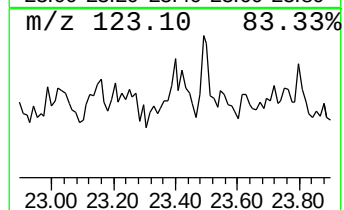
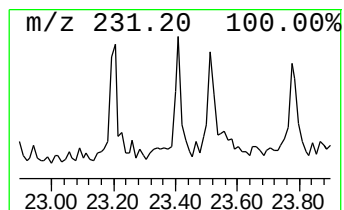
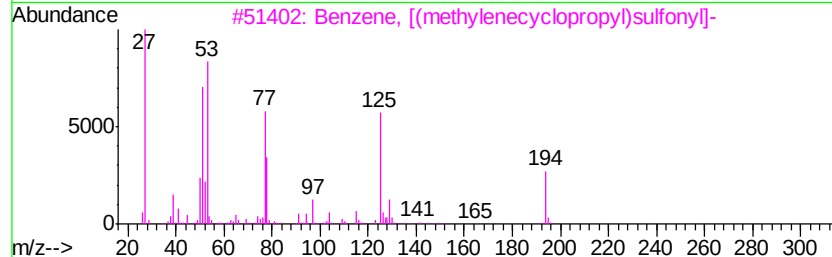
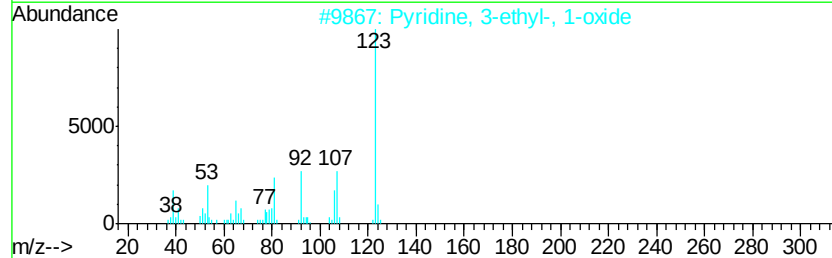
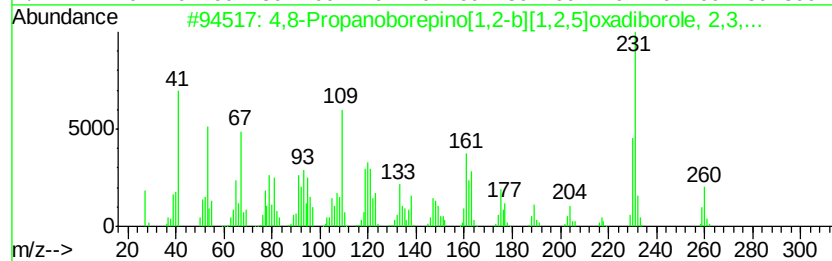
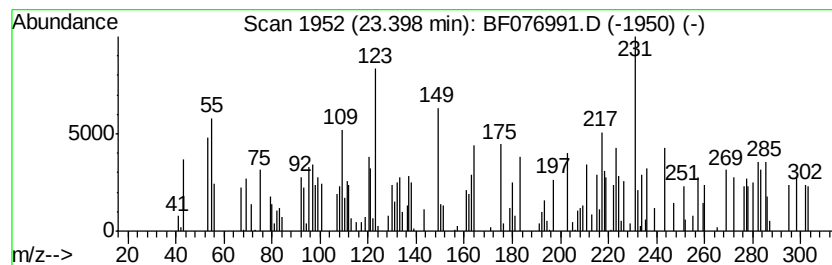
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown23.40 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.40	4.53 ng	63217	Perylene-d12	22.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	4,8-Propanoborepino[1,2-b][1,2,5...	260	C16H30B2O	139688-22-5	43		
2	Pyridine, 3-ethyl-, 1-oxide	123	C7H9NO	014906-62-8	38		
3	Benzene, [(methylenecyclopropyl)...	194	C10H10O2S	078656-83-4	22		
4	Spirohexan-4-one, 5,5-dichloro-6...	192	C8H10Cl2O	110079-12-4	12		
5	Bicyclo[4.1.0]heptane-7-carboxam...	222	C11H14N2OS	329912-72-3	10		



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

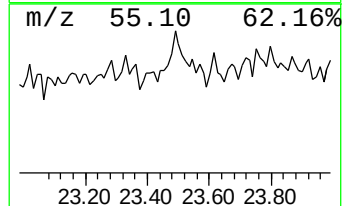
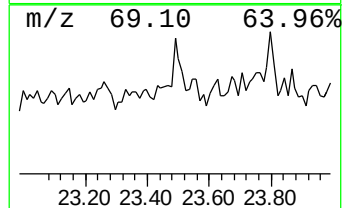
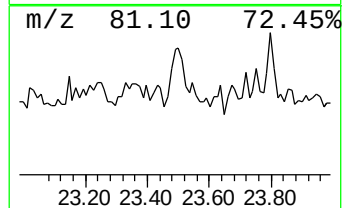
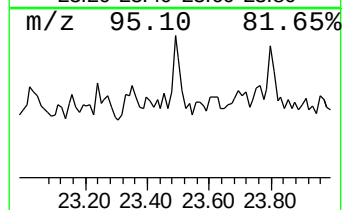
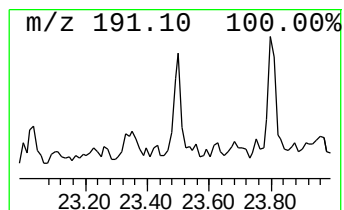
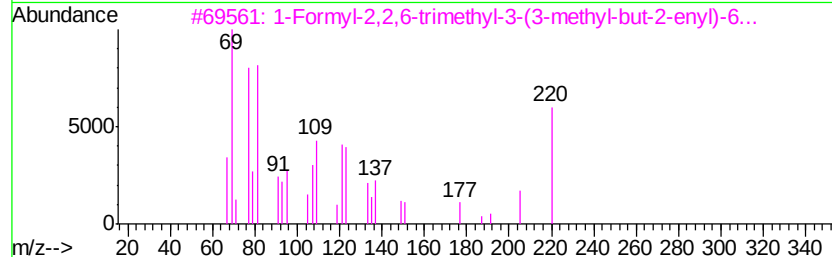
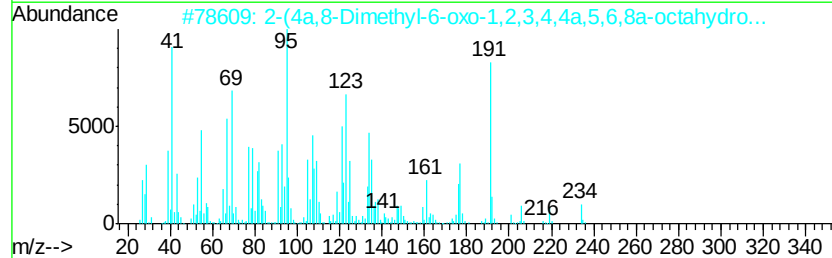
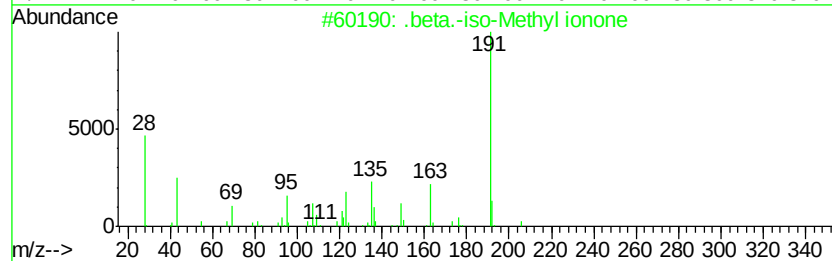
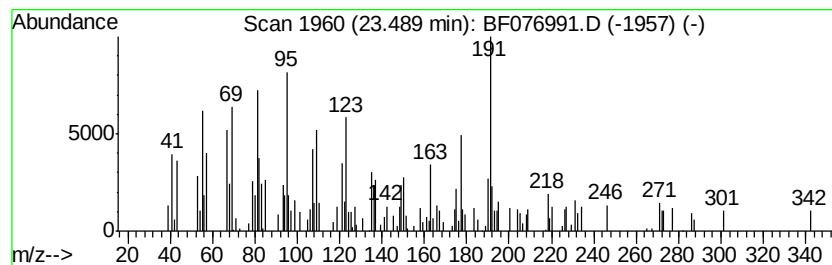
Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

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 .beta.-iso-Methyl ionone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
23.49	8.88 ng	123994	Perylene-d12	22.89	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	.beta.-iso-Methyl ionone	206	C14H22O	1000285-40-2	86
2	2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4...	234	C15H22O2	1000190-21-8	58
3	1-Formyl-2,2,6-trimethyl-3-(3-me...	220	C15H24O	108287-18-9	42
4	5-Bromo-4-oxo-4,5,6,7-tetrahydro...	216	C6H5BrN2O2	300574-36-1	35
5	Cyclohexene, 1,5,5-trimethyl-6-a...	180	C12H20O	211563-96-1	27



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

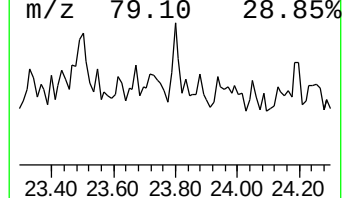
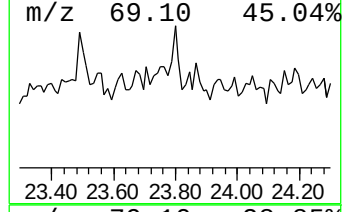
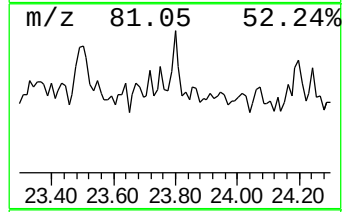
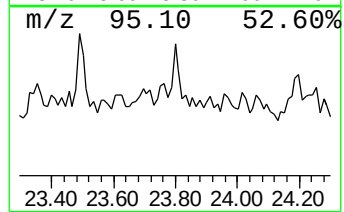
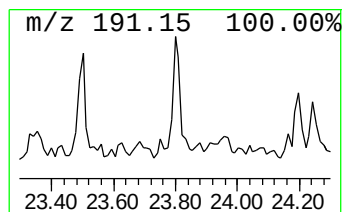
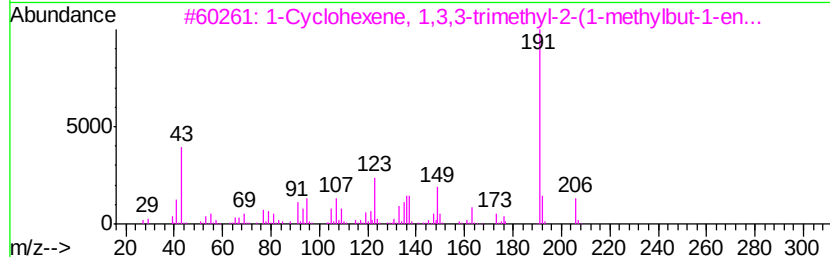
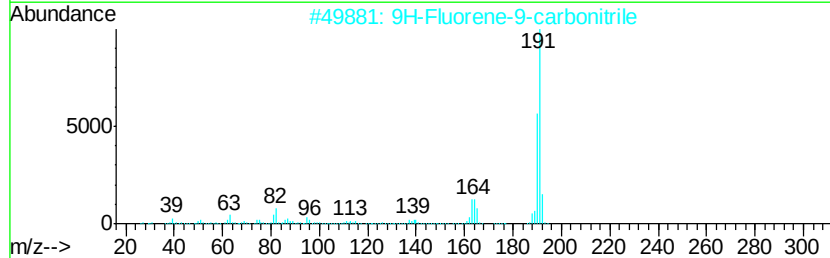
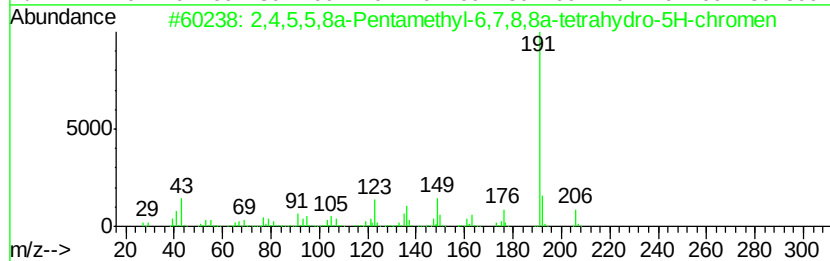
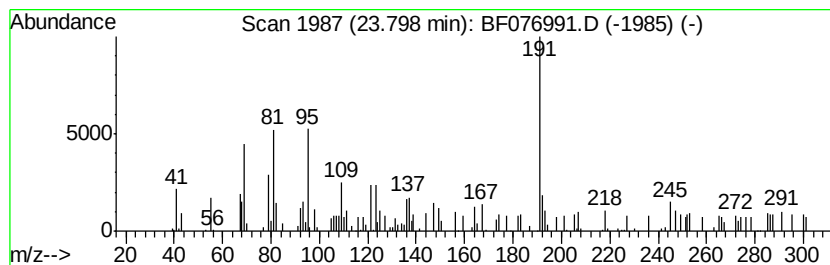
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown23.80 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.80	3.06 ng	42654	Perylene-d12	22.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4,5,5,8a-Pentamethyl-6,7,8,8a-...	206	C14H22O	1000195-40-9	38
2		9H-Fluorene-9-carbonitrile	191	C14H9N	001529-40-4	38
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	38
4		2-Chloro-4,6-dimethylquinoline	191	C11H10ClN	003913-18-6	35
5		Pyrido[3,4-d]pyridazin-1(2H)-one...	191	C8H9N5O	1000263-69-7	30



Data Path : Z:\HPCHEM1\BNA F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

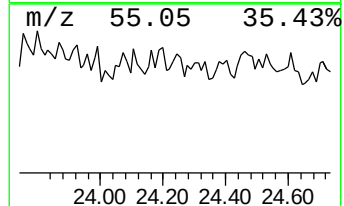
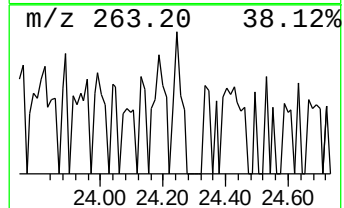
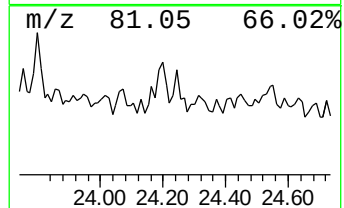
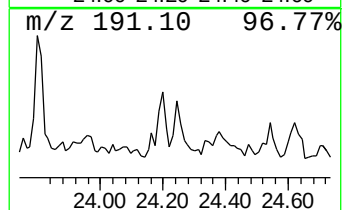
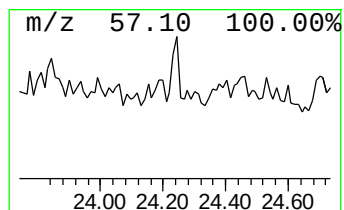
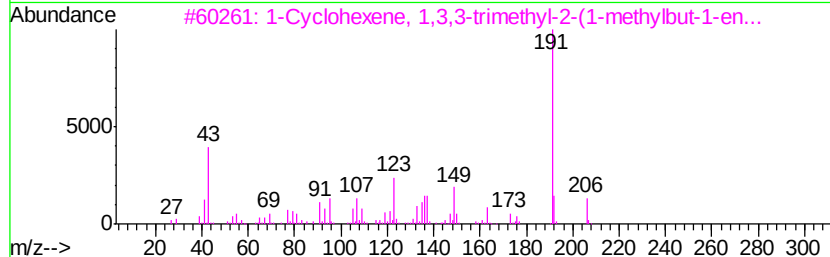
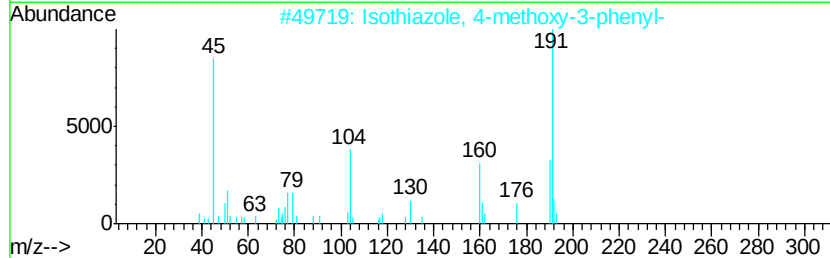
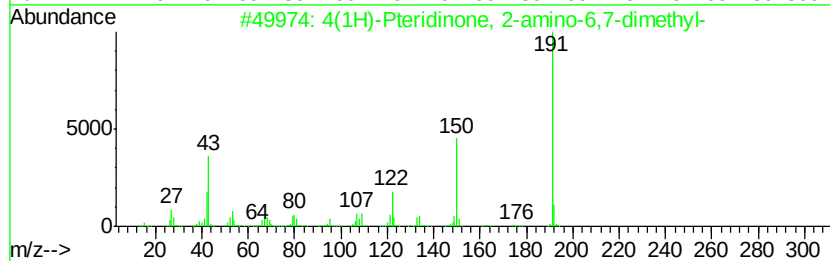
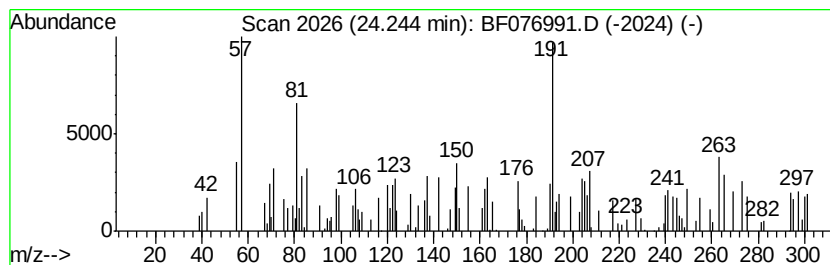
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF011415.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 unknown24.24 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
24.24	2.57 ng	35836	Perylene-d12	22.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4(1H)-Pteridinone, 2-amino-6,7-d...	191	C8H9N5O	000611-55-2	35
2		Isothiazole, 4-methoxy-3-phenyl-	191	C10H9NOS	019574-25-5	18
3		1-Cyclohexene, 1,3,3-trimethyl-2...	206	C14H22O	1000197-08-4	14
4		5-(p-Aminophenyl)-2-thiazolamine	191	C9H9N3S	090349-87-4	14
5		Oxirane, [[4-(1,1-dimethylethyl)...]	206	C13H18O2	003101-60-8	14



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF012015\
Data File : BF076991.D
Acq On : 21 Jan 2015 8:48
Operator : IZ / TP
Sample : G1111-04
Misc : S
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
RBDC4-011615

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
unknown4.01	4.01	12.8	ng	119385	1	7.91	186669	20.0
unknown7.40	7.40	81.0	ng	756387	1	7.91	186669	20.0
Benzophenone	16.57	3.3	ng	47252	4	17.73	282775	20.0
unknown23.40	23.40	4.5	ng	63217	6	22.89	279153	20.0
.beta.-iso-Methyl...	23.49	8.9	ng	123994	6	22.89	279153	20.0
unknown23.80	23.80	3.1	ng	42654	6	22.89	279153	20.0
unknown24.24	24.24	2.6	ng	35836	6	22.89	279153	20.0