

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
 Data File : BF077649.D
 Acq On : 9 Mar 2015 20:30
 Operator : TP/IZ
 Sample : G1453-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SEP3

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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	1.344	38	40	43	rVB	4202894	5467394	100.00%	23.481%
2	1.470	48	51	64	rVB2	117237	312789	5.72%	1.343%
3	1.641	64	66	69	rVB	56577	71961	1.32%	0.309%
4	1.687	69	70	73	rBV	103467	130222	2.38%	0.559%
5	1.801	79	80	103	rVB	930973	1661893	30.40%	7.137%
6	4.956	354	356	361	rVB	143165	166259	3.04%	0.714%
7	5.482	400	402	405	rBV	1032817	1054064	19.28%	4.527%
8	6.762	511	514	516	rBV	712322	955129	17.47%	4.102%
9	6.899	524	526	529	rBV	997073	1018004	18.62%	4.372%
10	7.196	549	552	553	rBV	234483	306202	5.60%	1.315%
11	7.230	553	555	557	rVB	58513	57532	1.05%	0.247%
12	7.379	564	568	570	rBV	853720	880723	16.11%	3.782%
13	7.539	578	582	588	rVB	80506	117379	2.15%	0.504%
14	7.630	588	590	593	rBV	60603	72320	1.32%	0.311%
15	7.745	598	600	605	rVB2	39043	61325	1.12%	0.263%
16	7.882	610	612	614	rVB	667868	577565	10.56%	2.480%
17	8.762	687	689	692	rBV	295291	411965	7.53%	1.769%
18	10.111	805	807	810	rBV	1171309	1121350	20.51%	4.816%
19	10.934	877	879	882	rBV	412716	476950	8.72%	2.048%
20	11.277	907	909	917	rVB	31203	68428	1.25%	0.294%
21	11.917	962	965	967	rBV	760428	787935	14.41%	3.384%
22	12.111	980	982	986	rBV	37369	56569	1.03%	0.243%
23	12.179	986	988	990	rVV	73894	93375	1.71%	0.401%
24	12.225	990	992	993	rVV2	86383	120069	2.20%	0.516%
25	12.259	993	995	996	rVV2	69152	97664	1.79%	0.419%
26	12.339	999	1002	1005	rVV2	41023	84126	1.54%	0.361%
27	12.397	1005	1007	1009	rVV2	78461	105005	1.92%	0.451%
28	12.442	1009	1011	1013	rVV	96187	109363	2.00%	0.470%
29	12.499	1013	1016	1018	rVB2	44751	70640	1.29%	0.303%
30	12.774	1038	1040	1042	rBV	518818	551730	10.09%	2.370%
31	14.283	1169	1172	1174	rBV	181200	198153	3.62%	0.851%
32	14.363	1176	1179	1181	rVB	87273	107808	1.97%	0.463%
33	14.557	1193	1196	1198	rBV	183724	206005	3.77%	0.885%
34	14.774	1212	1215	1217	rBV	1225794	1396262	25.54%	5.997%

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

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: CENTROID

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
Peak separation: 5

Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	15.528	1279	1281	1284	rVB	61188	81567	1.49%	0.350%
36	15.940	1315	1317	1323	rBV	160422	265231	4.85%	1.139%
37	16.066	1324	1328	1330	rVV	601559	887060	16.22%	3.810%
38	16.123	1330	1333	1335	rVB	312753	493151	9.02%	2.118%
39	16.728	1383	1386	1389	rBV2	75107	119306	2.18%	0.512%
40	17.369	1439	1442	1447	rVB	84093	177085	3.24%	0.761%
41	17.757	1473	1476	1479	rBV	60835	82139	1.50%	0.353%
42	17.826	1479	1482	1486	rVV	443854	673294	12.31%	2.892%
43	18.546	1542	1545	1550	rVB	311867	582979	10.66%	2.504%
44	18.740	1559	1562	1565	rBV	266822	517194	9.46%	2.221%
45	18.923	1576	1578	1582	rVB	28195	60218	1.10%	0.259%
46	19.220	1602	1604	1610	rBV2	20576	66811	1.22%	0.287%
47	19.620	1635	1639	1648	rVB2	67940	212536	3.89%	0.913%
48	19.872	1658	1661	1665	rVB4	42627	91520	1.67%	0.393%

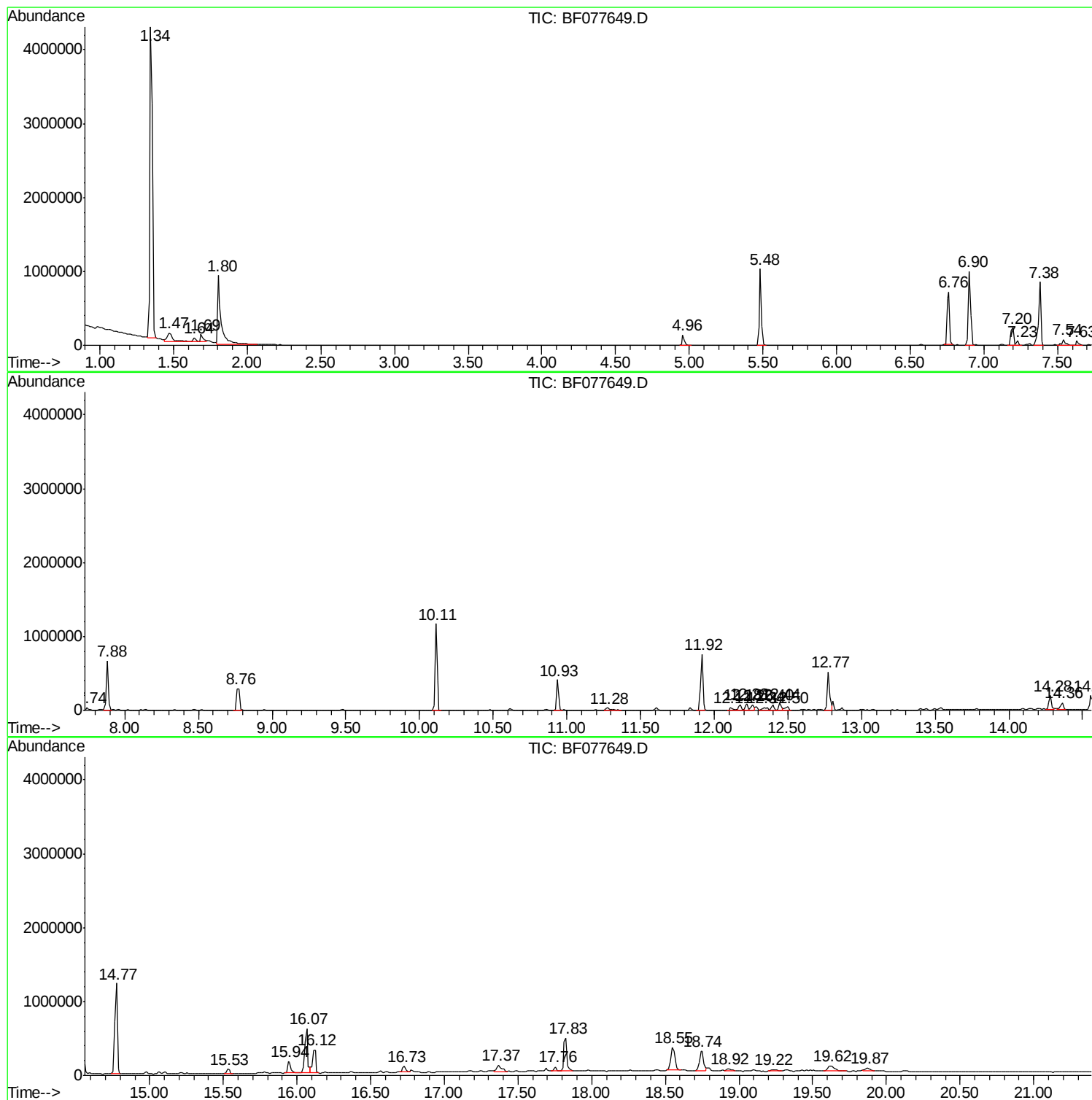
Sum of corrected areas: 23284249

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

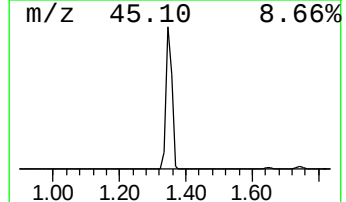
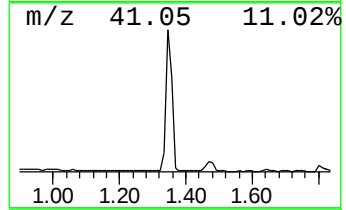
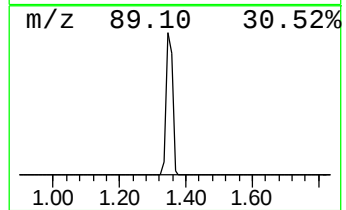
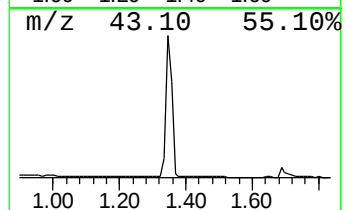
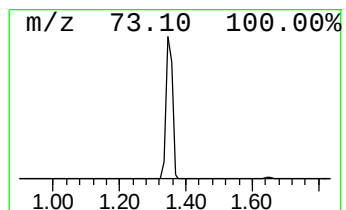
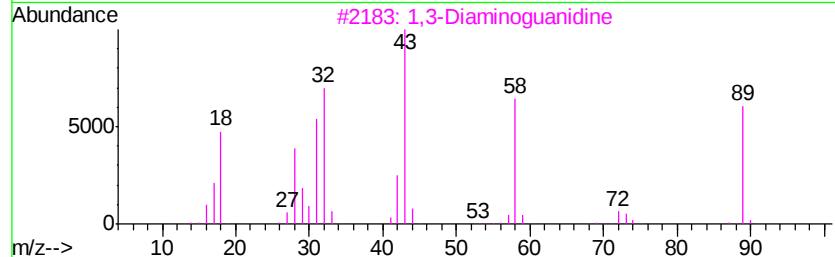
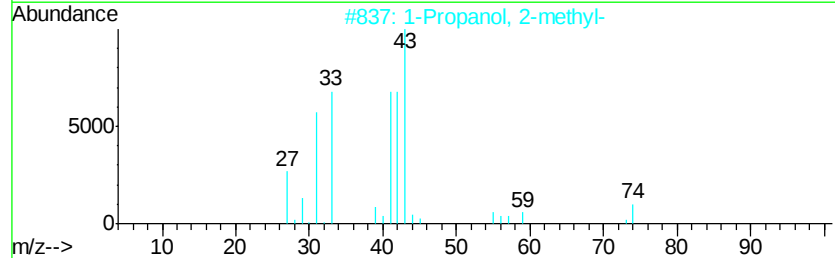
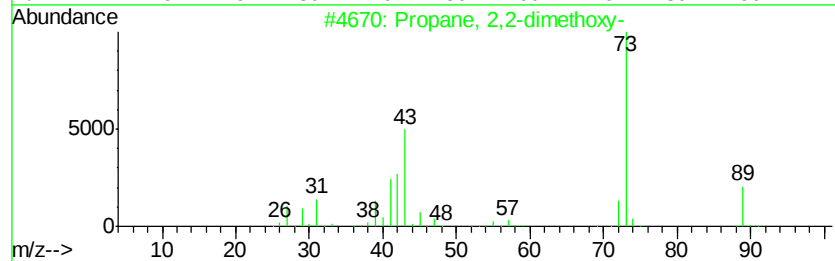
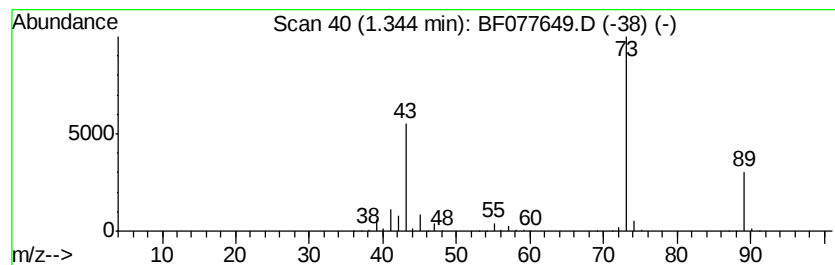
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.34	357.11 ng	5467390	1,4-Dichlorobenzene-d4	7.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2			1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
3			1,3-Diaminoguanidine	89	CH7N5	004364-78-7	9
4			Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
5			Oxirane-2-carboxylic acid, ethyl...	116	C5H8O3	1000192-50-3	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

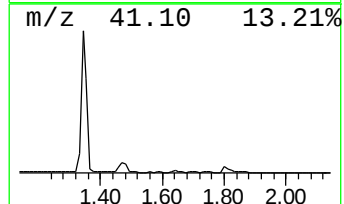
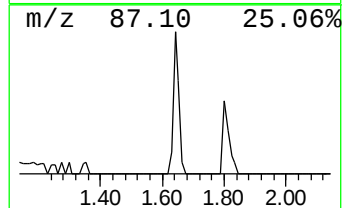
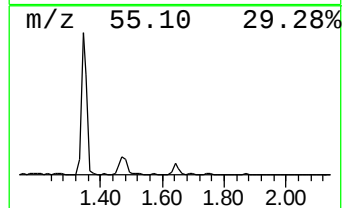
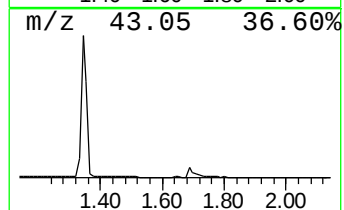
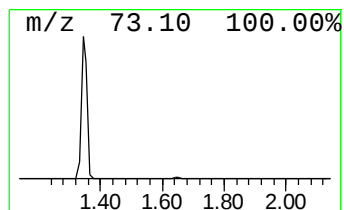
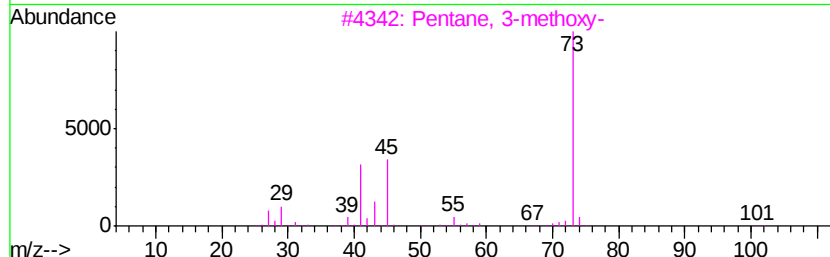
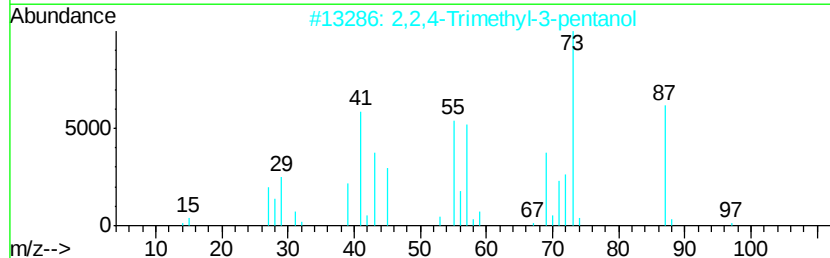
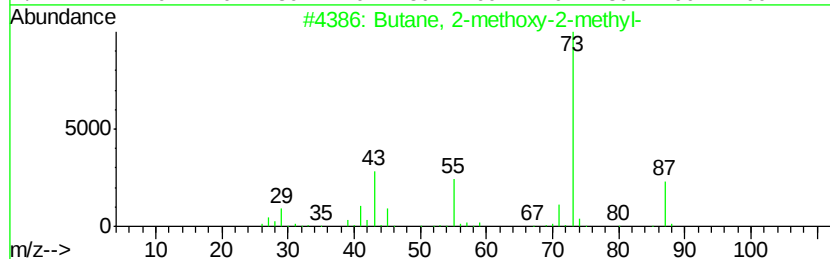
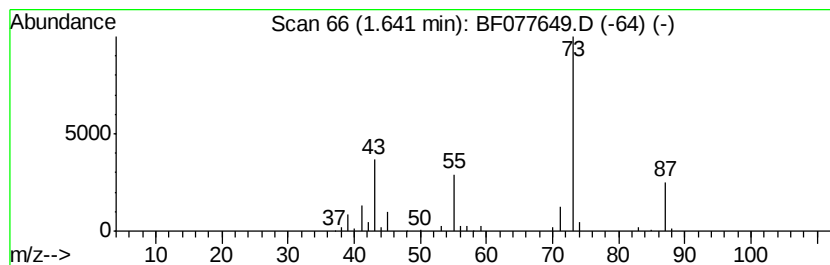
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.64	4.70 ng	71961	1,4-Dichlorobenzene-d4	7.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

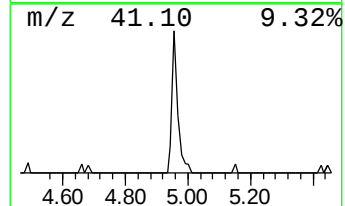
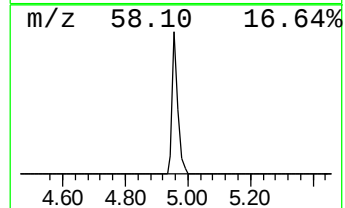
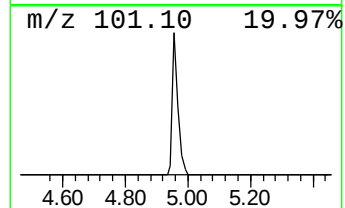
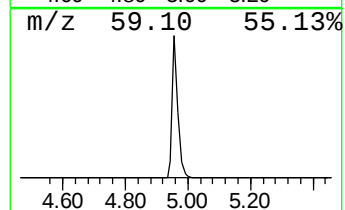
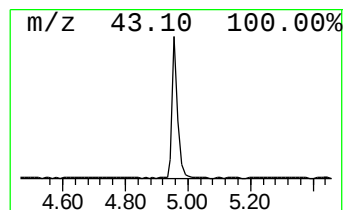
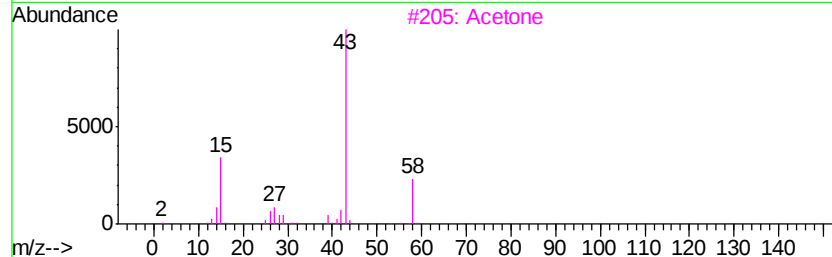
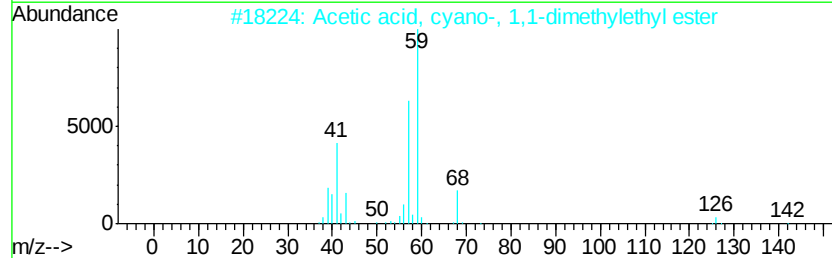
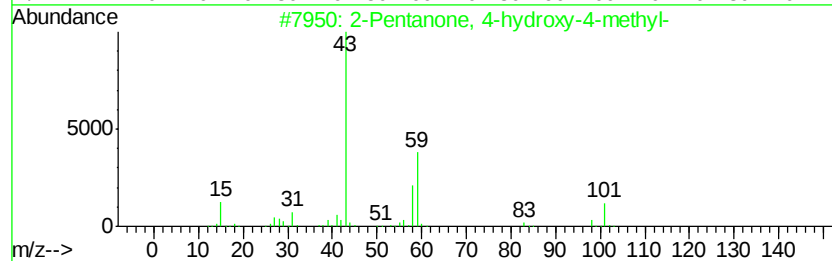
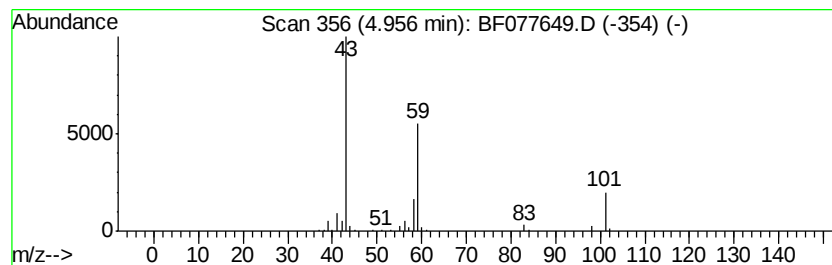
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.96	10.86 ng	166259	1,4-Dichlorobenzene-d4	7.19

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
3		Acetone	58	C3H6O	000067-64-1	10
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

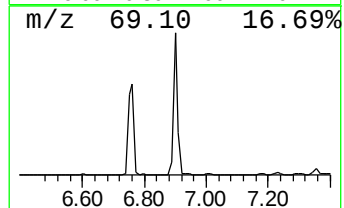
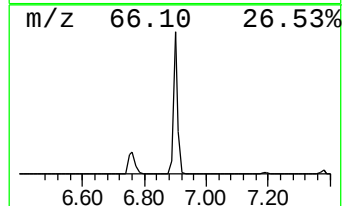
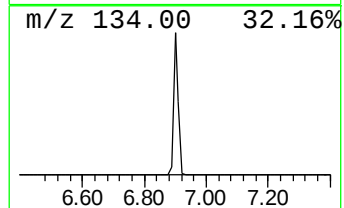
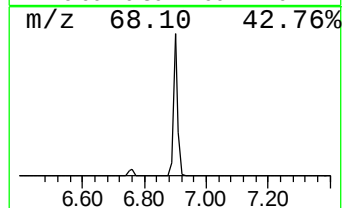
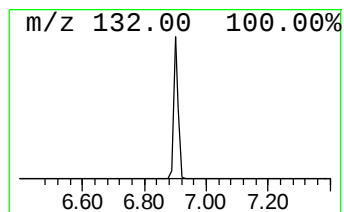
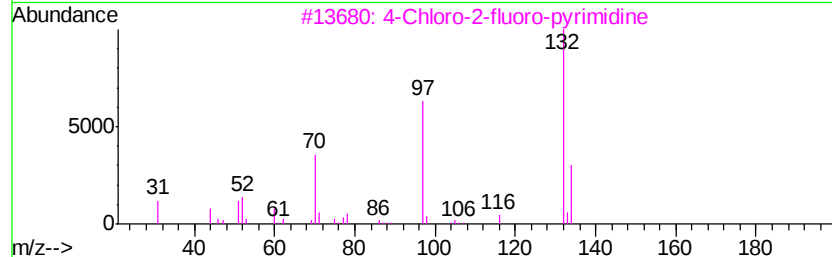
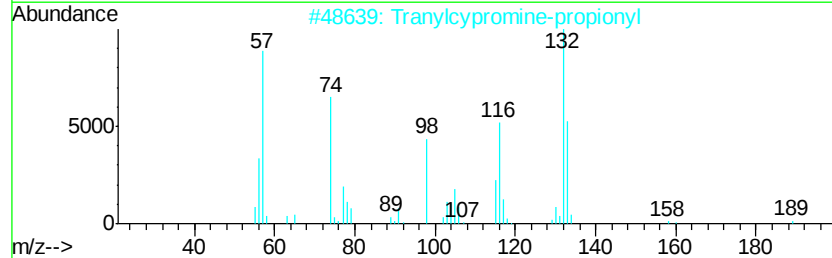
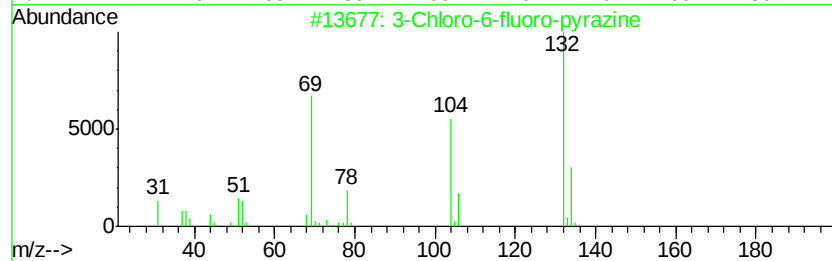
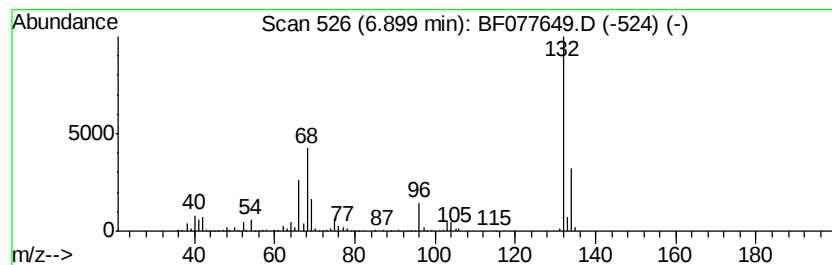
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.90 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.90	66.49 ng	1018000	1,4-Dichlorobenzene-d4	7.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

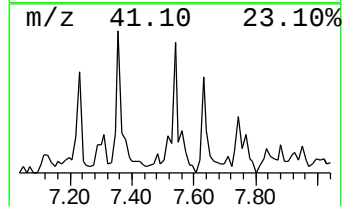
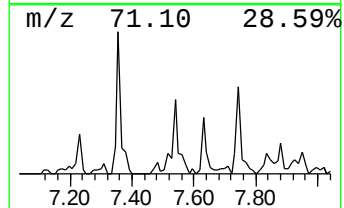
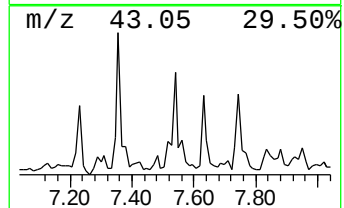
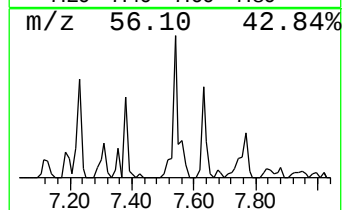
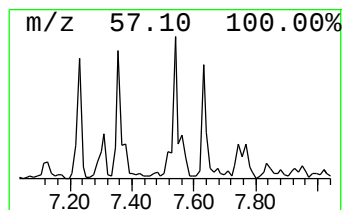
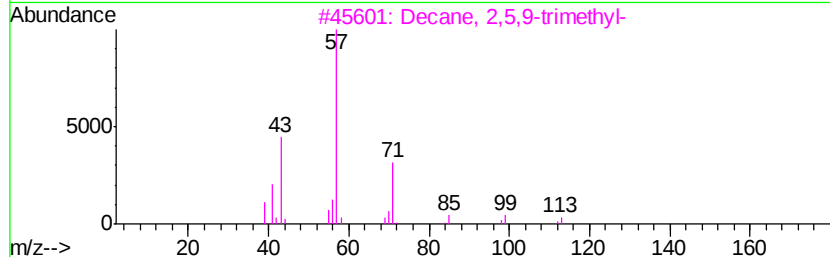
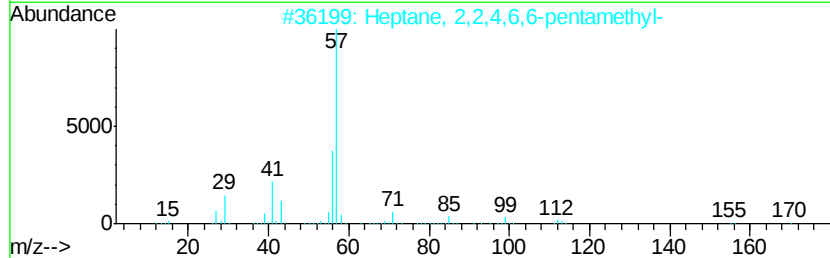
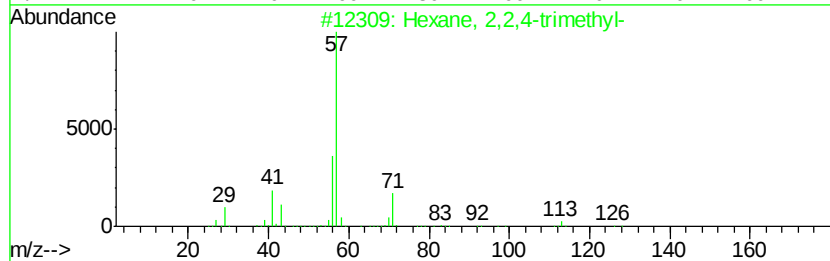
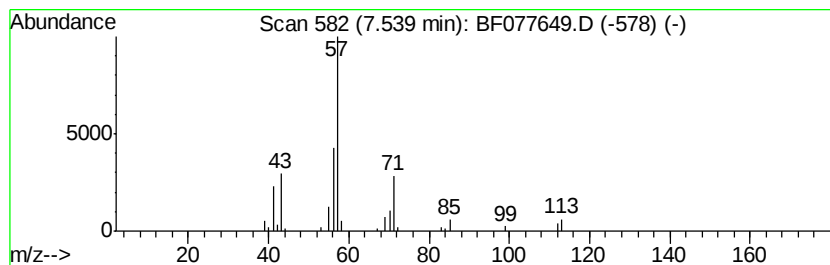
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Hexane, 2,2,4-trimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.54	7.67 ng	117379	1,4-Dichlorobenzene-d4	7.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	56
2			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
3			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	50
4			Undecane, 2,5-dimethyl-	184	C13H28	017301-22-3	50
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	45



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

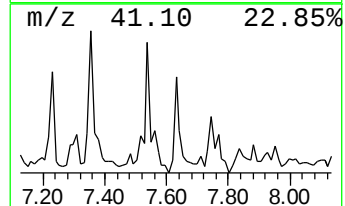
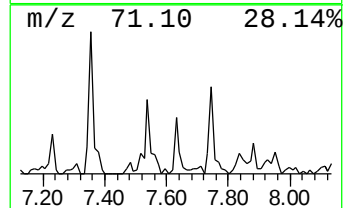
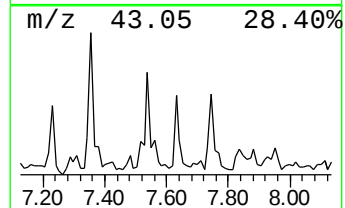
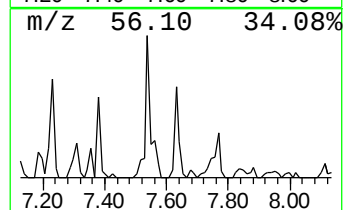
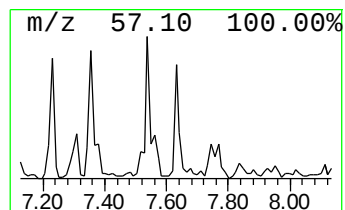
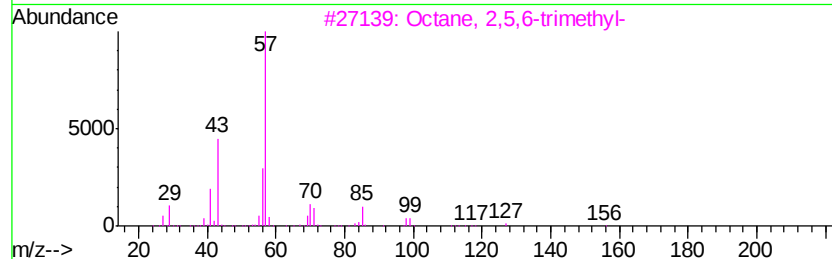
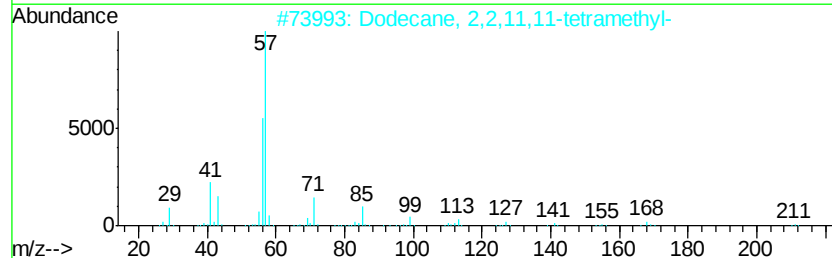
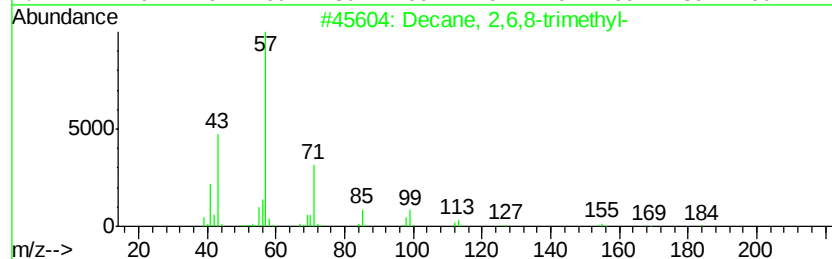
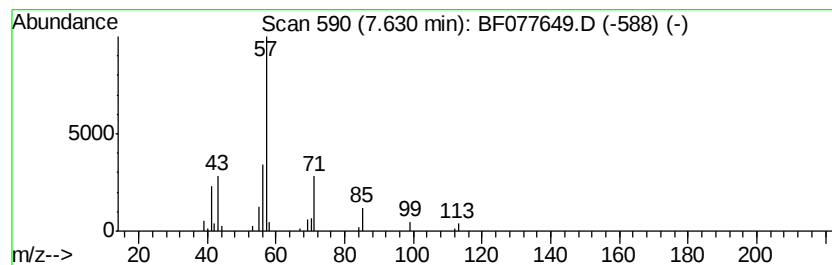
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Decane, 2,6,8-trimethyl- Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.63	4.72 ng	72320	1,4-Dichlorobenzene-d4	7.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,6,8-trimethyl-	184	C13H28	062108-26-3	64
2			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	59
3			Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	59
4			Decane, 2,5,9-trimethyl-	184	C13H28	062108-22-9	59
5			Undecane, 2,6-dimethyl-	184	C13H28	017301-23-4	53



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

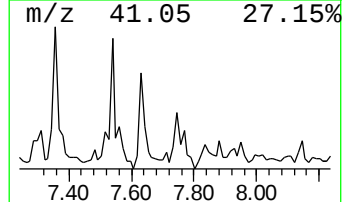
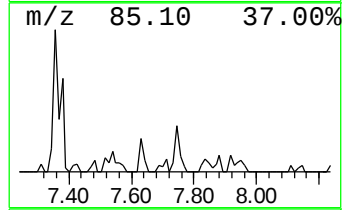
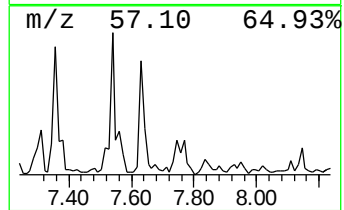
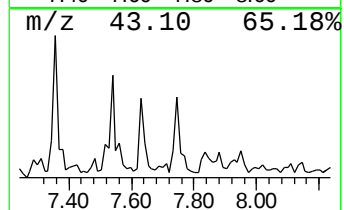
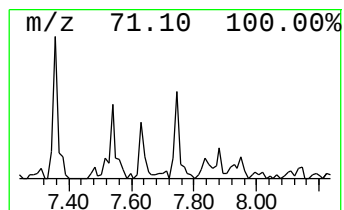
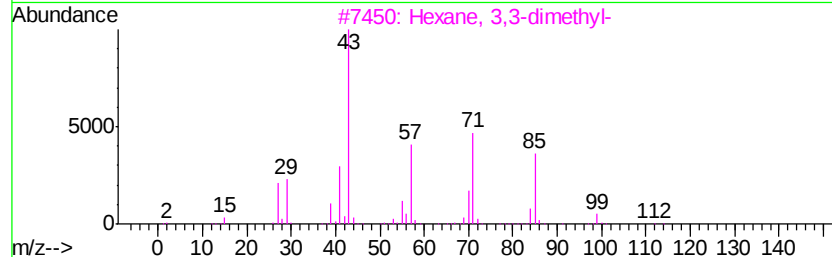
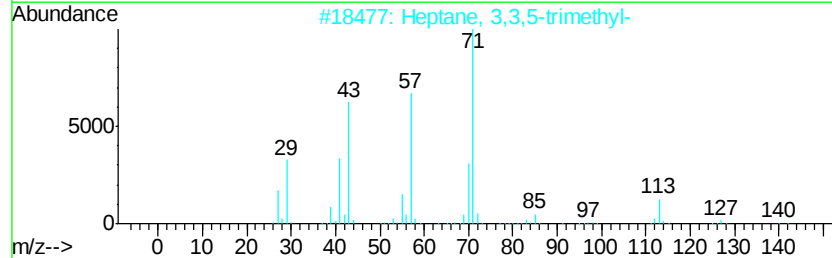
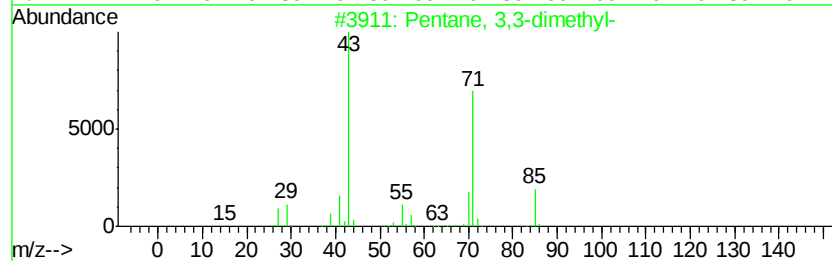
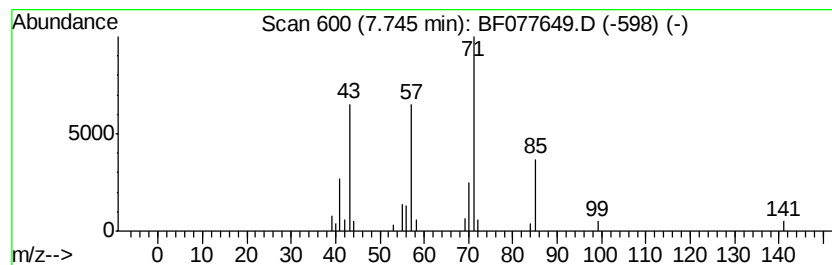
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Pentane, 3,3-dimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.74	4.01 ng	61325	1,4-Dichlorobenzene-d4	7.19

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3,3-dimethyl-	100	C7H16	000562-49-2	64
2			Heptane, 3,3,5-trimethyl-	142	C10H22	007154-80-5	59
3			Hexane, 3,3-dimethyl-	114	C8H18	000563-16-6	59
4			Octane, 3,3-dimethyl-	142	C10H22	004110-44-5	59
5			Heptane, 2,5,5-trimethyl-	142	C10H22	001189-99-7	59



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

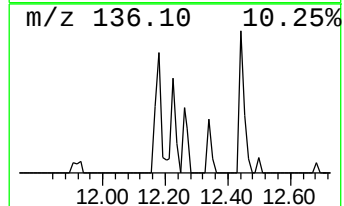
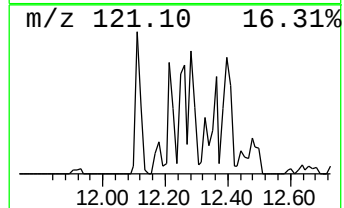
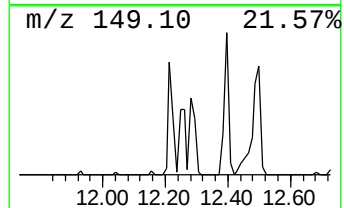
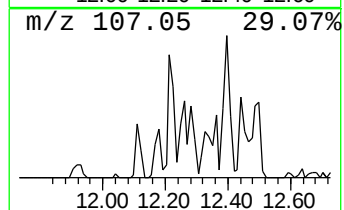
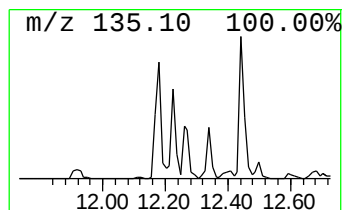
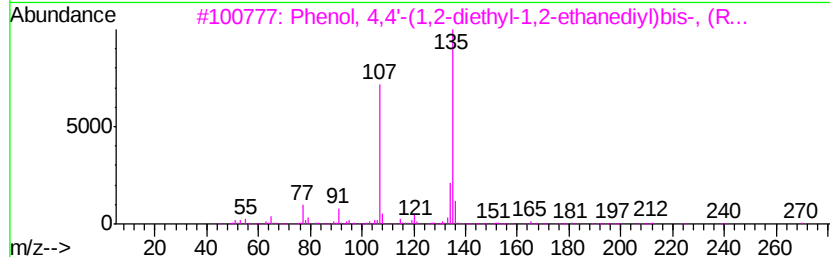
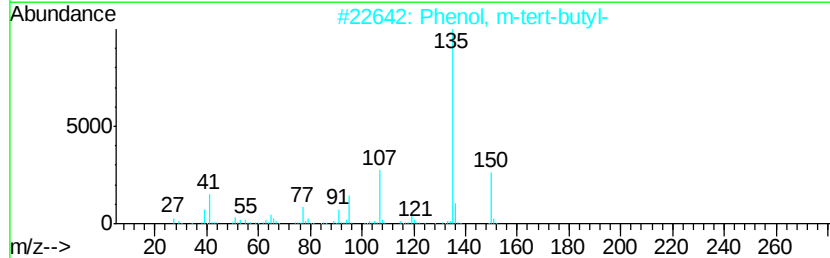
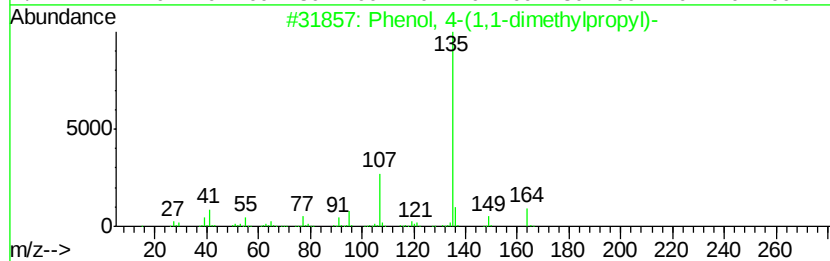
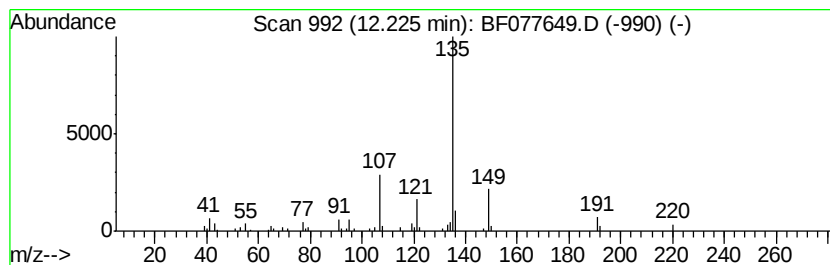
Instrument :
BNA_F
ClientSampleId :
SEP3

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phenol, 4-(1,1-dimethylprop... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.	
12.23	4.35 ng	120069	Phenanthrene-d10	12.78	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4-(1,1-dimethylpropyl)-	164	C11H16O	000080-46-6	59
2	Phenol, m-tert-butyl-	150	C10H14O	000585-34-2	58
3	Phenol, 4,4'-(1,2-diethyl-1,2-eth...	270	C18H22O2	000084-16-2	53
4	4-(3,4-Methylenedioxyphenyl)-2-b...	192	C11H12O3	055418-52-5	53
5	Phenol, 4-(1,1,3,3-tetramethylbu...	206	C14H22O	000140-66-9	50



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

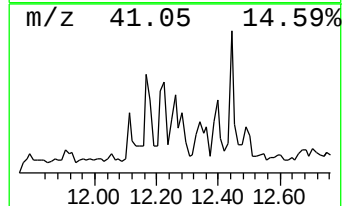
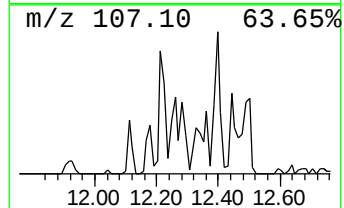
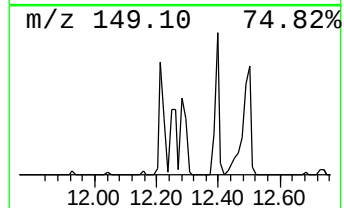
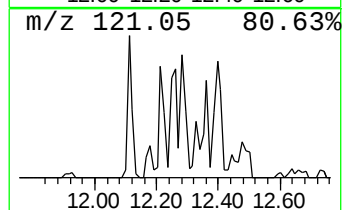
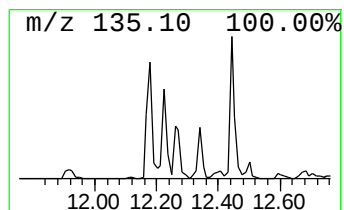
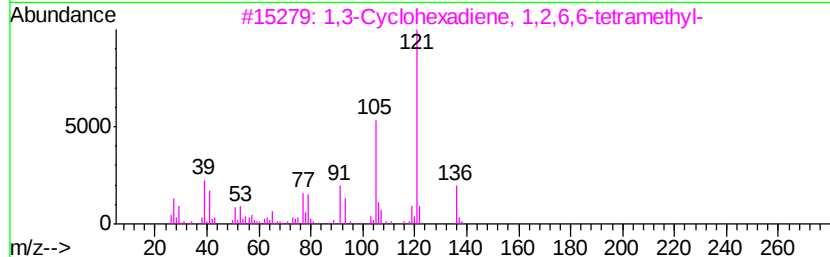
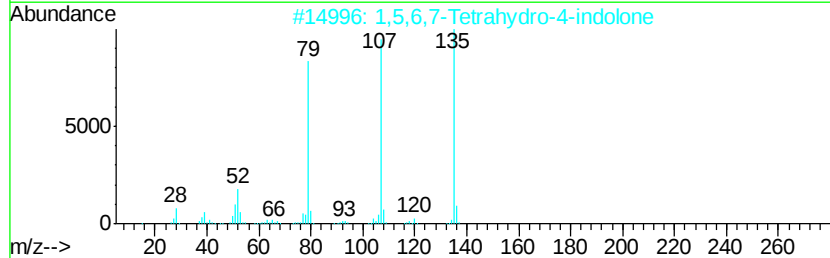
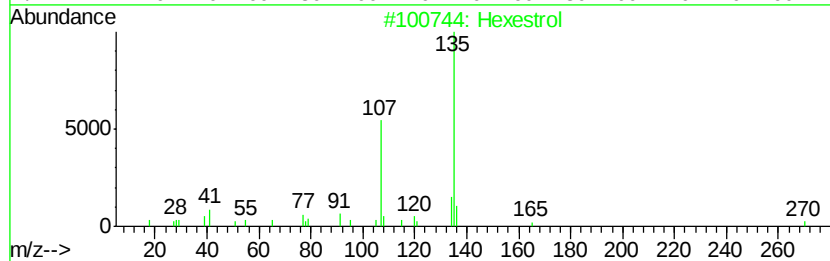
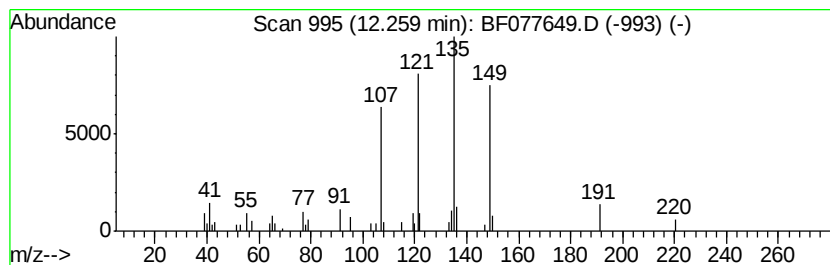
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown12.26 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.26	3.54 ng	97664	Phenanthrene-d10	12.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexestrol	270	C18H22O2	005635-50-7	27
2		1,5,6,7-Tetrahydro-4-indolone	135	C8H9NO	013754-86-4	27
3		1,3-Cyclohexadiene, 1,2,6,6-tetr...	136	C10H16	000514-96-5	18
4		ortho-Methoxyacetophenone	150	C9H10O2	000579-74-8	18
5		trans-8-Ethyl-bicyclo[4.3.0]non-...	150	C11H18	1000145-84-8	18



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

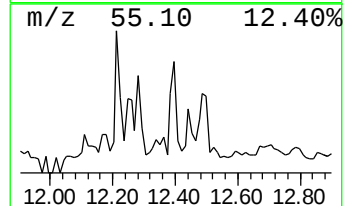
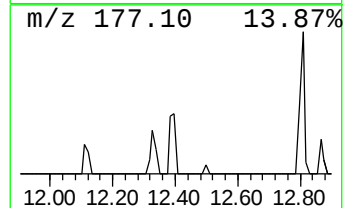
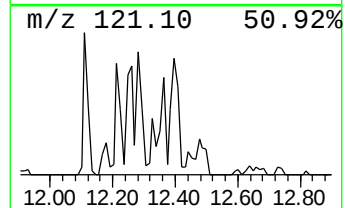
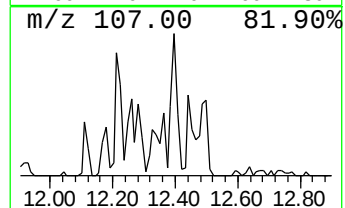
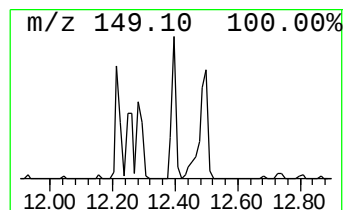
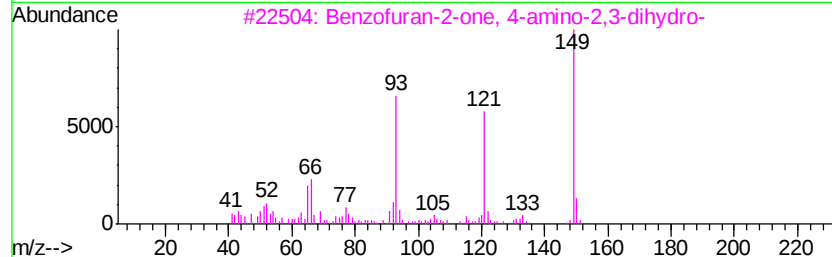
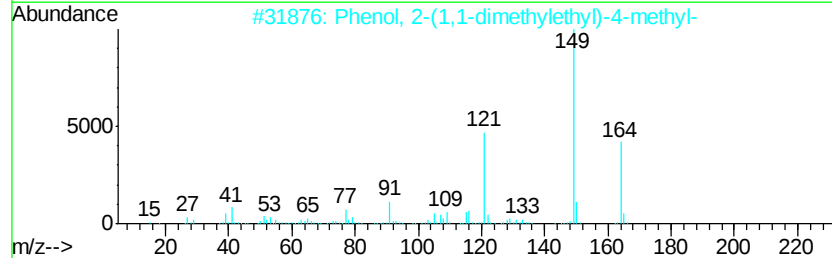
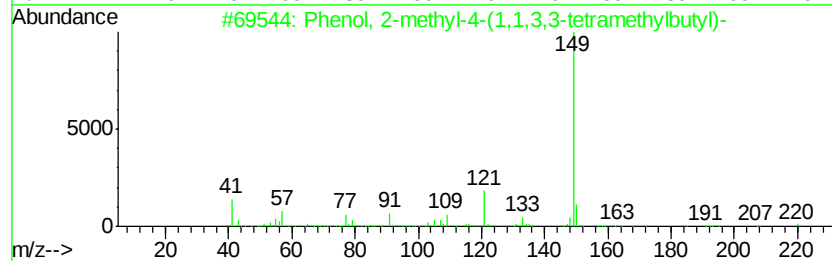
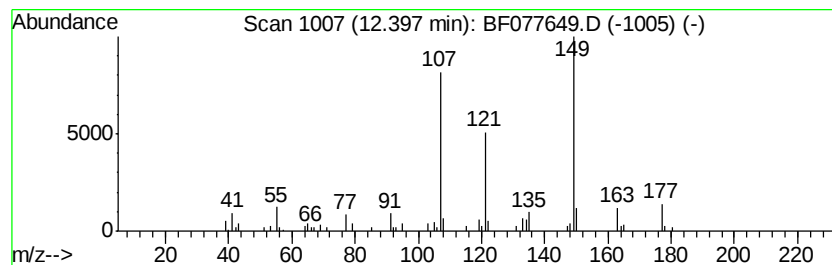
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 unknown12.40 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.40	3.81 ng	105005	Phenanthrene-d10	12.78

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Phenol, 2-methyl-4-(1,1,3,3-tetr...	220	C15H24O	002219-84-3	38
2			Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	35
3			Benzofuran-2-one, 4-amino-2,3-di...	149	C8H7NO2	075990-99-7	35
4			Phenol, 2-(1,1-dimethylethyl)-5-...	164	C11H16O	000088-60-8	35
5			Phenol, 2-(1,1-dimethylethyl)-3-...	164	C11H16O	013037-79-1	35



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

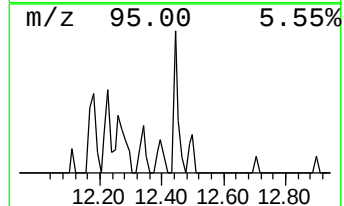
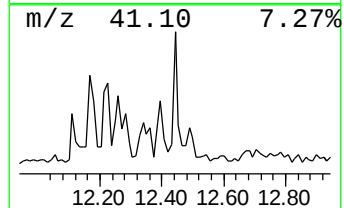
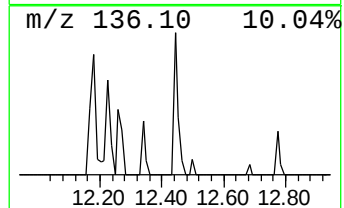
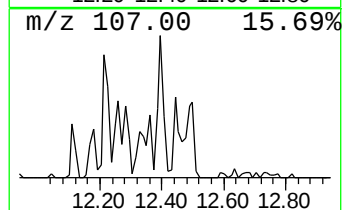
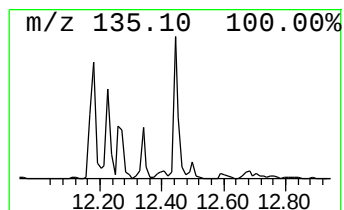
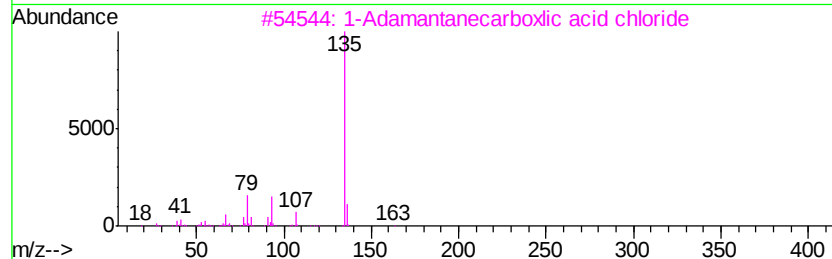
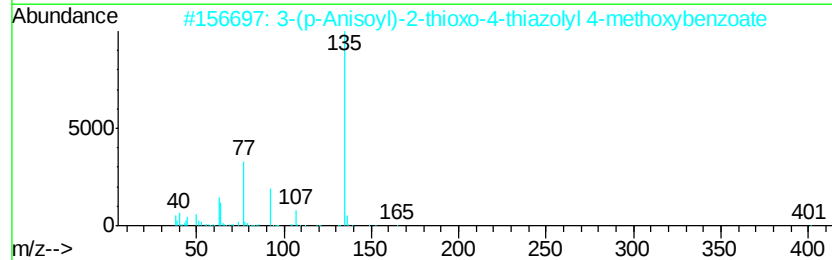
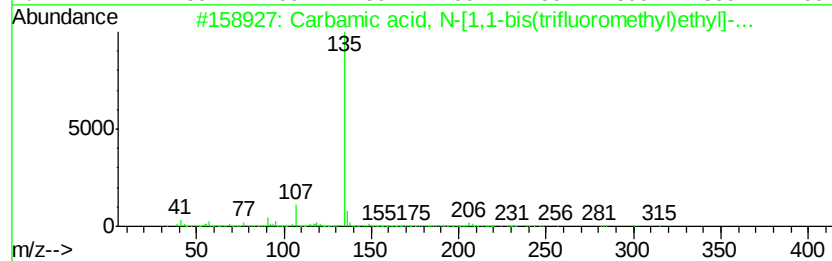
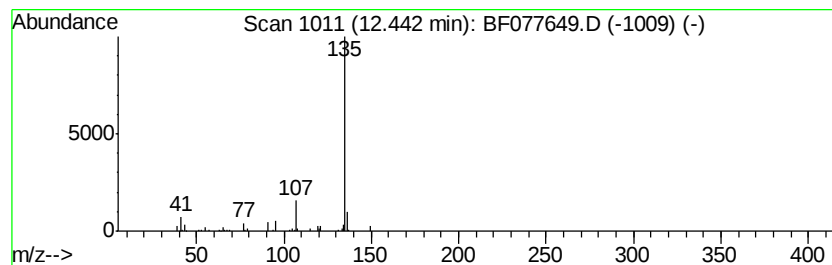
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Carbamic acid, N-[1,1-bis(t... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.44	3.96 ng	109363	Phenanthrene-d10	12.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Carbamic acid, N-[1,1-bis(triflu...	413	C19H25F6N02	296242-69-8	72
2		3-(p-Anisoyl)-2-thioxo-4-thiazol...	401	C19H15N05S2	299970-55-1	50
3		1-Adamantanecarboxylic acid chloride	198	C11H15Cl0	002094-72-6	45
4		Hexestrol	270	C18H22O2	005635-50-7	45
5		Adenosine 3',5'-cyclic monosp...	329	C10H12N5O6P	000060-92-4	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

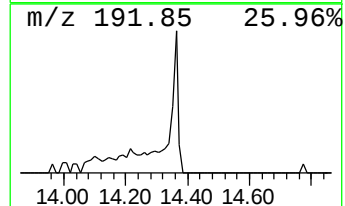
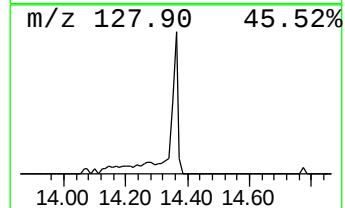
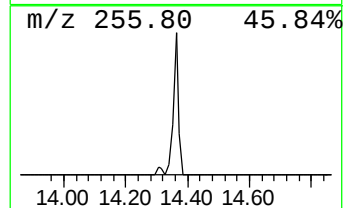
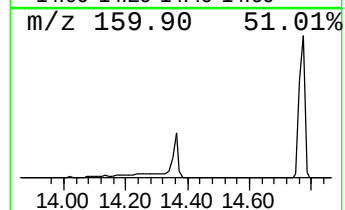
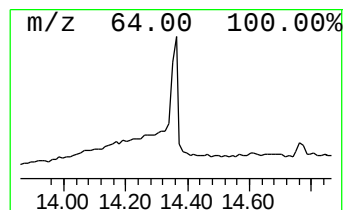
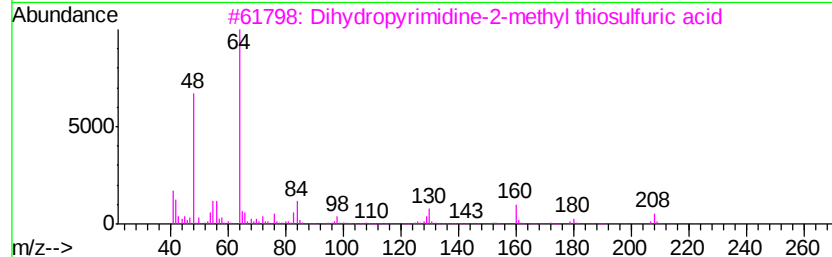
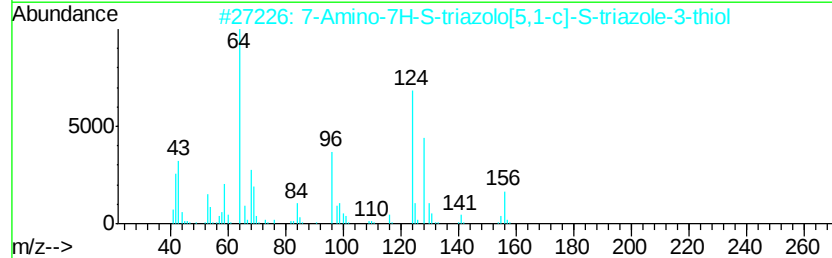
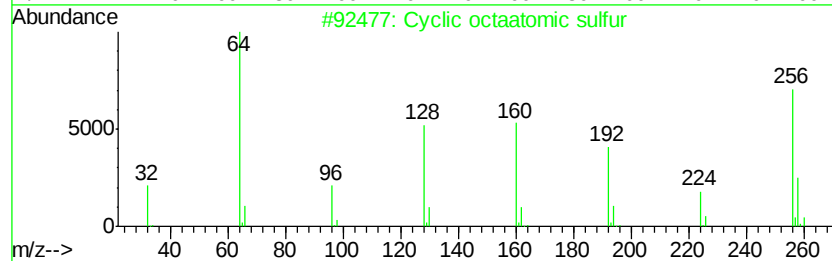
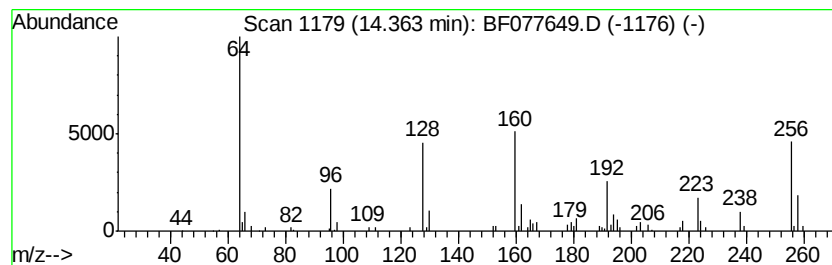
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Cyclic octaatomic sulfur Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.36	3.91 ng	107808	Phenanthrene-d10	12.78

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclic octaatomic sulfur	256	S8	010544-50-0	94
2		7-Amino-7H-S-triazolo[5,1-c]-S-t...	156	C3H4N6S	013728-28-4	36
3		Dihydroprymidine-2-methyl thiosul...	208	C5H8N2O3S2	1000256-28-8	28
4		2-Nitroso-1-naphthol-4-sulfonic ...	253	C10H7NO5S	003682-32-4	28
5		2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1000256-39-2	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

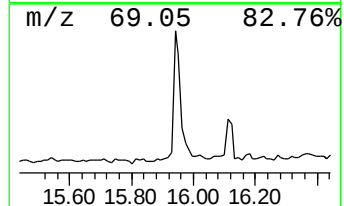
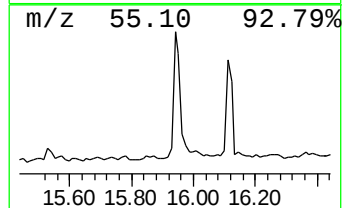
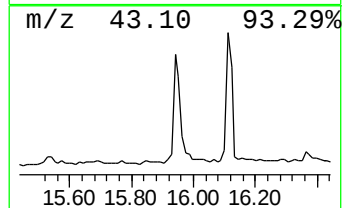
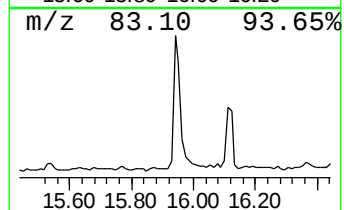
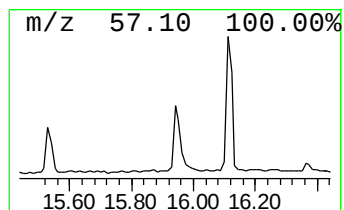
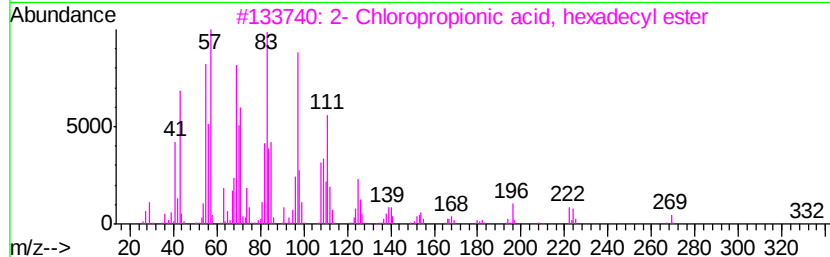
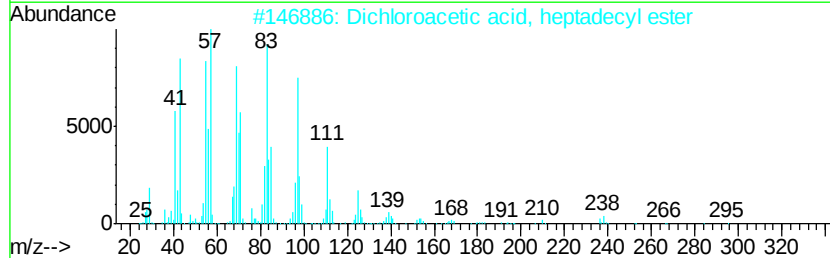
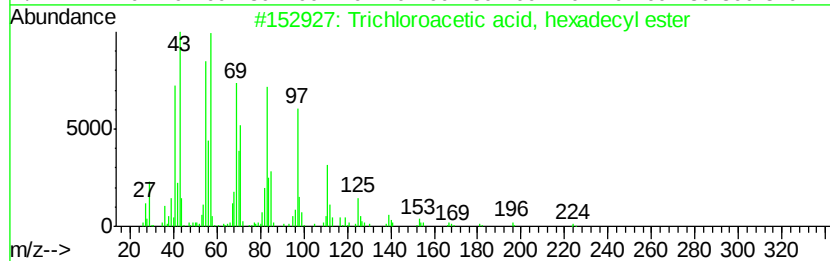
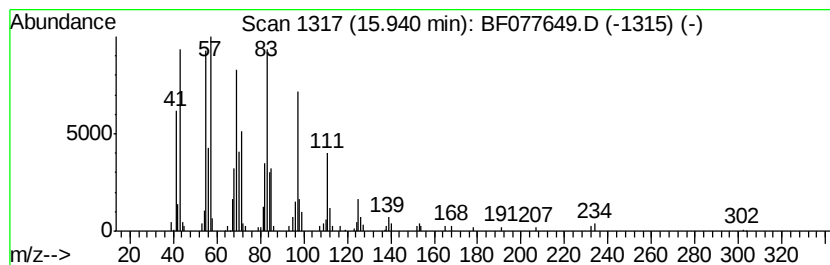
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Trichloroacetic acid, hexad... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.94	5.98 ng	265231	Chrysene-d12	16.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2			Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	94
3			2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
4			3-Eicosene, (E)-	280	C20H40	074685-33-9	91
5			1-Heneicosyl formate	340	C22H44O2	077899-03-7	91



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

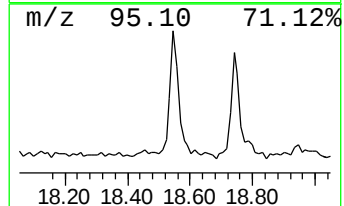
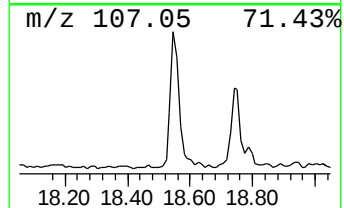
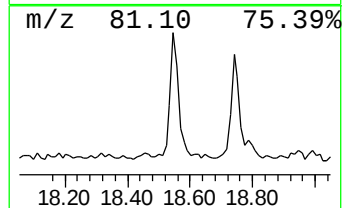
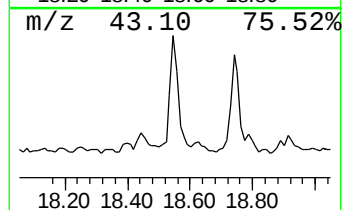
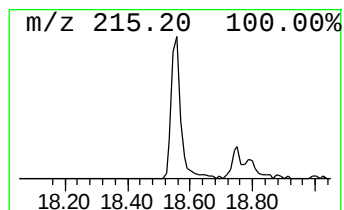
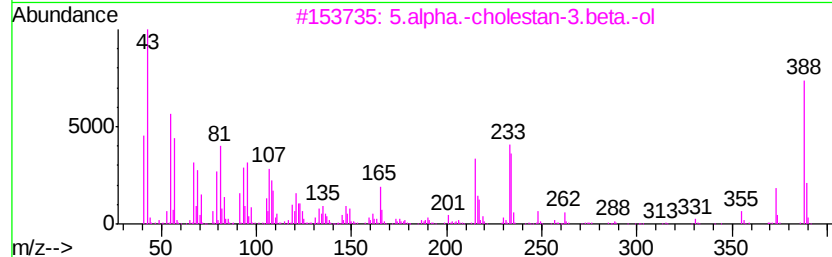
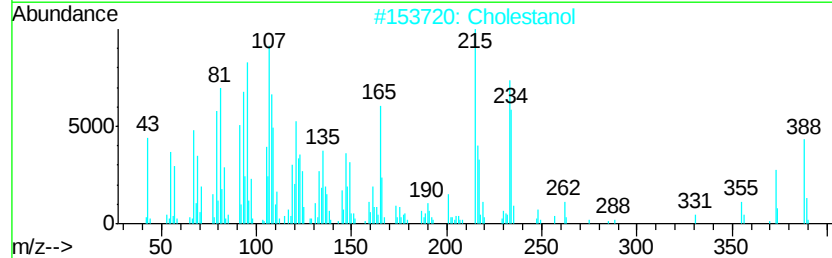
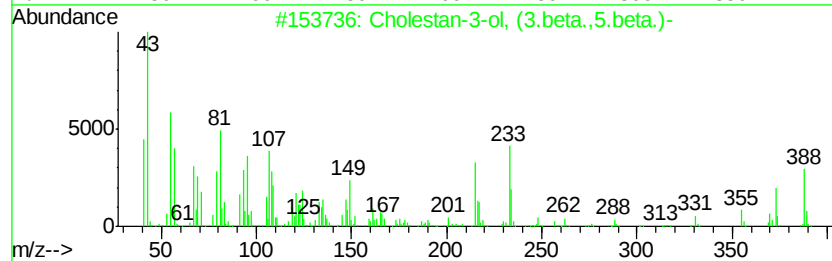
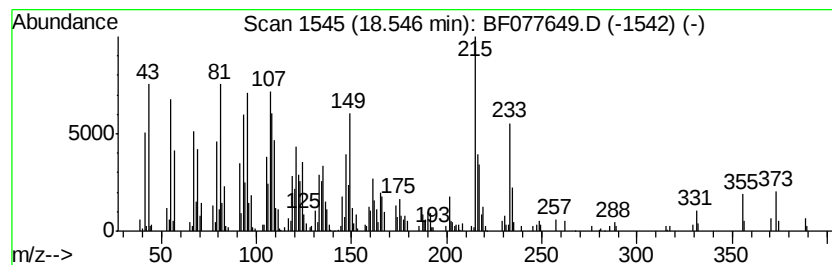
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Cholestan-3-ol, (3.beta.,5.... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.55	17.32 ng	582979	Perylene-d12	17.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholestan-3-ol, (3.beta.,5.beta.)-	388	C27H48O	000360-68-9	93
2		Cholestanol	388	C27H48O	000080-97-7	87
3		5.alpha.-cholestan-3.beta.-ol	388	C27H48O	1000213-40-9	70
4		Cholestan-3-ol	388	C27H48O	027409-41-2	53
5		Cholestan-3.beta.-ol	388	C27H48O	017608-41-2	52



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

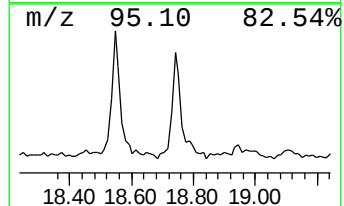
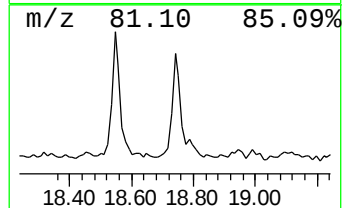
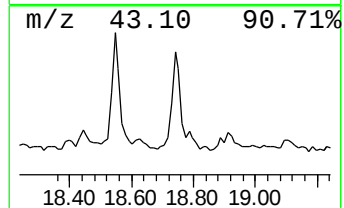
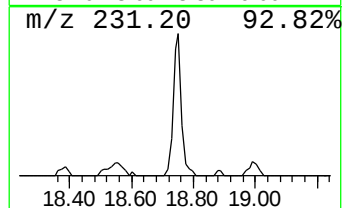
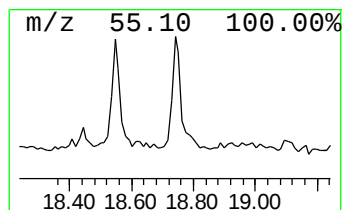
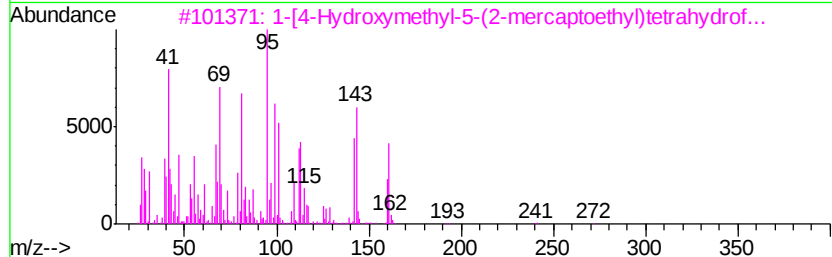
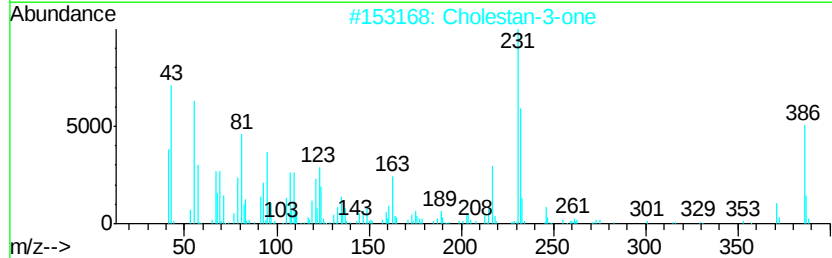
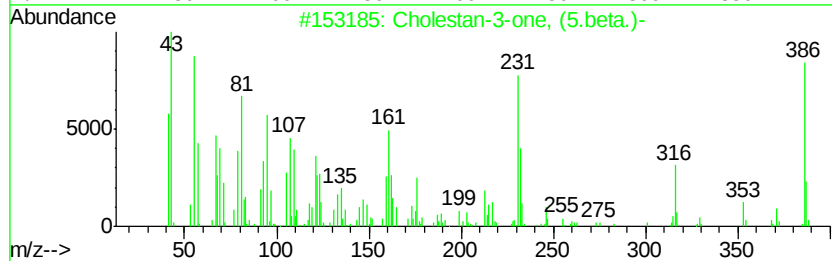
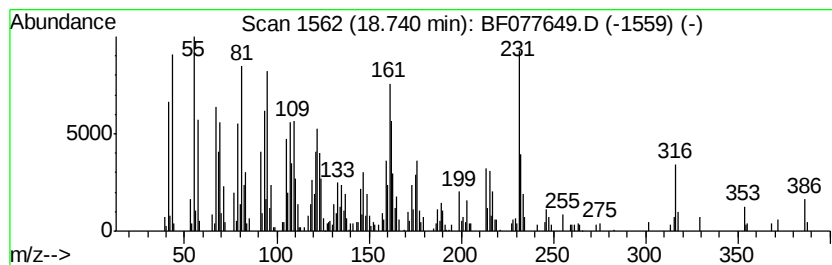
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Cholestan-3-one, (5.beta.)- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.74	15.36 ng	517194	Perylene-d12	17.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cholestan-3-one, (5.beta.)-	386	C27H46O	000601-53-6	97
2		Cholestan-3-one	386	C27H46O	015600-08-5	97
3		1-[4-Hydroxymethyl-5-(2-mercapto...	272	C11H16N2O4S	128453-39-4	72
4		Cholestan-3-one, (5.alpha.)-	386	C27H46O	000566-88-1	52
5		Cholestan-2-one	386	C27H46O	1000210-43-4	42



Data Path : Z:\HPCHEM1\BNA F\DATA\BF030915\
Data File : BF077649.D
Acq On : 9 Mar 2015 20:30
Operator : TP/IZ
Sample : G1453-02
Misc :
ALS Vial : 13 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SEP3

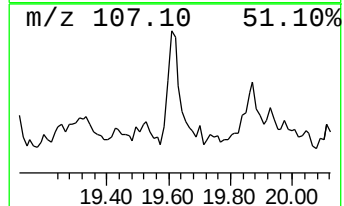
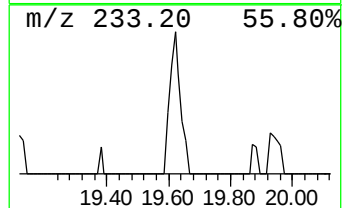
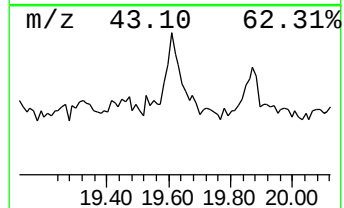
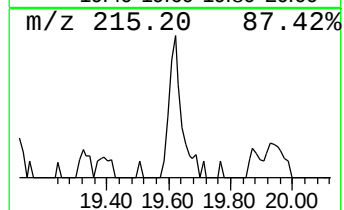
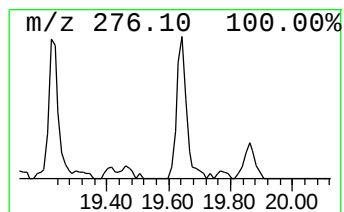
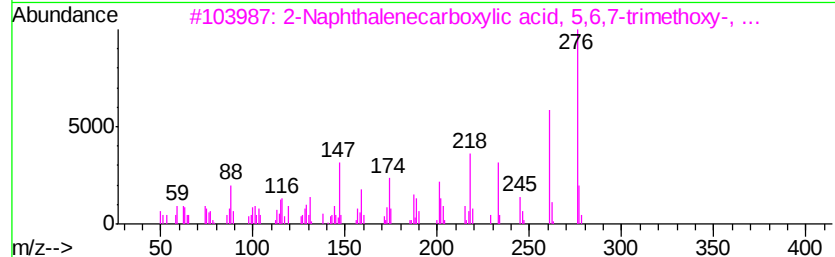
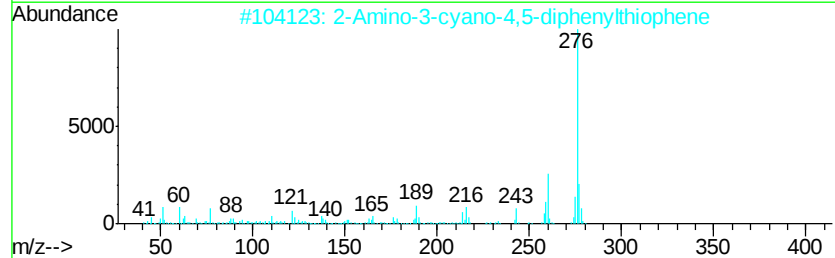
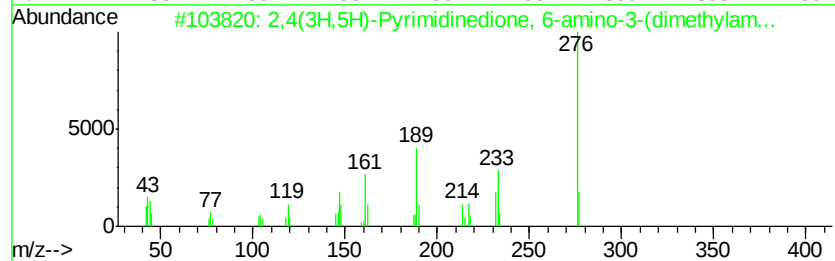
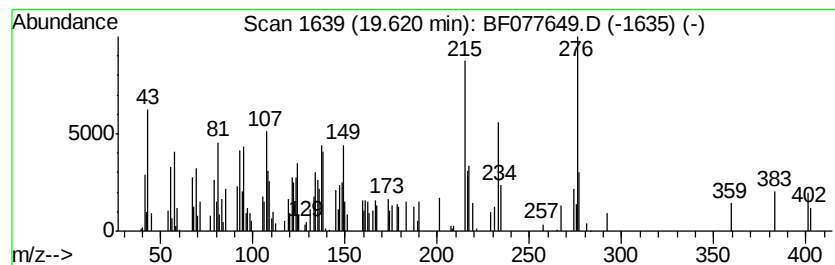
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF021915.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 unknown19.62 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.62	6.31 ng	212536	Perylene-d12	17.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,4(3H,5H)-Pvrimidinedione, 6-am...	276	C13H16N4O3	039265-99-1	30
2		2-Amino-3-cyano-4,5-diphenylthio...	276	C17H12N2S	042160-34-9	22
3		2-Naphthalenecarboxylic acid, 5....	276	C15H16O5	023673-53-2	22
4		Androstan-17-ol, (5.alpha.,17.be...	276	C19H32O	001225-43-0	18
5		6H-Pyrido[4,3-b]carbazole, 9-met...	276	C18H16N2O	010371-86-5	18



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF030915\
 Data File : BF077649.D
 Acq On : 9 Mar 2015 20:30
 Operator : TP/IZ
 Sample : G1453-02
 Misc :
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SEP3

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF021915.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
Propane, 2,2-dime...	1.34	357.1	ng	5467390	1	7.19	306202	20.0
Butane, 2-methoxy...	1.64	4.7	ng	71961	1	7.19	306202	20.0
2-Pentanone, 4-hy...	4.96	10.9	ng	166259	1	7.19	306202	20.0
unknown6.90	6.90	66.5	ng	1018000	1	7.19	306202	20.0
Hexane, 2,2,4-tri...	7.54	7.7	ng	117379	1	7.19	306202	20.0
Decane, 2,6,8-tri...	7.63	4.7	ng	72320	1	7.19	306202	20.0
Pentane, 3,3-dime...	7.74	4.0	ng	61325	1	7.19	306202	20.0
Phenol, 4-(1,1-di...	12.23	4.3	ng	120069	4	12.78	551730	20.0
unknown12.26	12.26	3.5	ng	97664	4	12.78	551730	20.0
unknown12.40	12.40	3.8	ng	105005	4	12.78	551730	20.0
Carbamic acid, N-...	12.44	4.0	ng	109363	4	12.78	551730	20.0
Cyclic octaatomic...	14.36	3.9	ng	107808	4	12.78	551730	20.0
Trichloroacetic a...	15.94	6.0	ng	265231	5	16.06	887060	20.0
Cholestan-3-ol, (...)	18.55	17.3	ng	582979	6	17.82	673294	20.0
Cholestan-3-one, ...	18.74	15.4	ng	517194	6	17.82	673294	20.0
unknown19.62	19.62	6.3	ng	212536	6	17.82	673294	20.0