

Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
 Data File : BG021696.D
 Acq On : 15 Apr 2016 21:56
 Operator : UM/SJ
 Sample : H2549-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S8-0574

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_G\METHODS\8270-BG041316.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	3.878	172	177	187	rVB	63802	109164	5.85%	0.514%
2	4.601	295	300	309	rBV3	12360	25054	1.34%	0.118%
3	5.288	410	417	423	rBV3	23919	52029	2.79%	0.245%
4	5.512	448	455	465	rBV	95632	166039	8.90%	0.782%
5	5.770	492	499	507	rVB	277505	463437	24.84%	2.183%
6	6.446	608	614	616	rBV2	15574	27891	1.49%	0.131%
7	6.892	682	690	696	rVB2	18919	36111	1.94%	0.170%
8	7.368	764	771	784	rBV	189271	359428	19.26%	1.693%
9	7.609	798	812	824	rBV5	42275	117625	6.30%	0.554%
10	7.750	828	836	842	rBV	497693	900499	48.26%	4.241%
11	8.214	909	915	926	rBV	129180	229119	12.28%	1.079%
12	8.303	926	930	933	rBV2	19513	31708	1.70%	0.149%
13	8.467	947	958	963	rBV	57464	134158	7.19%	0.632%
14	8.543	963	971	984	rVB	413415	795568	42.64%	3.747%
15	8.684	993	995	1002	rVB4	13274	22686	1.22%	0.107%
16	8.996	1031	1048	1062	rVB4	45320	204916	10.98%	0.965%
17	9.243	1062	1090	1092	rBV3	93776	375657	20.13%	1.769%
18	9.384	1112	1114	1123	rVB	383904	569304	30.51%	2.681%
19	9.507	1129	1135	1146	rVB6	43428	128635	6.89%	0.606%
20	9.601	1146	1151	1154	rBV3	29514	46462	2.49%	0.219%
21	9.642	1154	1158	1166	rVB4	33381	66779	3.58%	0.315%
22	9.777	1174	1181	1187	rBV3	36075	76745	4.11%	0.361%
23	9.871	1187	1197	1202	rBV	94884	187832	10.07%	0.885%
24	9.954	1204	1211	1214	rBV2	75099	141603	7.59%	0.667%
25	10.024	1219	1223	1241	rVB7	47182	142770	7.65%	0.672%
26	10.224	1245	1257	1269	rBV	186994	488774	26.20%	2.302%
27	10.500	1301	1304	1309	rVB2	19343	26704	1.43%	0.126%
28	10.571	1309	1316	1320	rBV6	25065	58529	3.14%	0.276%
29	10.653	1324	1330	1336	rVB2	77545	137753	7.38%	0.649%
30	10.764	1343	1349	1354	rBV5	37533	72194	3.87%	0.340%
31	10.811	1354	1357	1363	rVB4	40403	65602	3.52%	0.309%
32	10.882	1364	1369	1373	rBV3	23395	40204	2.15%	0.189%
33	10.952	1375	1381	1388	rBV5	35927	78809	4.22%	0.371%
34	11.035	1388	1395	1405	rVB	202661	399233	21.40%	1.880%

Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
 Data File : BG021696.D
 Acq On : 15 Apr 2016 21:56
 Operator : UM/SJ
 Sample : H2549-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S8-0574

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_G\METHODS\8270-BG041316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	11.182	1407	1420	1426	rBV8	61779	176915	9.48%	0.833%
36	11.305	1435	1441	1444	rBV5	63533	133953	7.18%	0.631%
37	11.434	1459	1463	1466	rBV5	17482	26829	1.44%	0.126%
38	11.481	1466	1471	1479	rVB5	81118	195414	10.47%	0.920%
39	11.558	1480	1484	1489	rVB7	25195	39003	2.09%	0.184%
40	11.610	1489	1493	1497	rBV3	37274	63323	3.39%	0.298%
41	11.722	1509	1512	1517	rVB4	44511	75627	4.05%	0.356%
42	11.787	1518	1523	1528	rBV7	57355	126555	6.78%	0.596%
43	11.851	1529	1534	1540	rVV6	81666	182273	9.77%	0.858%
44	11.910	1540	1544	1550	rVB4	82967	150504	8.07%	0.709%
45	12.075	1567	1572	1577	rVB5	52997	93564	5.01%	0.441%
46	12.274	1602	1606	1611	rVB	51205	86500	4.64%	0.407%
47	12.321	1611	1614	1616	rBV3	20529	26018	1.39%	0.123%
48	12.357	1616	1620	1625	rVB2	44538	70933	3.80%	0.334%
49	12.421	1628	1631	1633	rBV4	17765	21739	1.17%	0.102%
50	12.692	1669	1677	1680	rBV6	68049	162654	8.72%	0.766%
51	12.727	1680	1683	1689	rVV8	39542	73448	3.94%	0.346%
52	12.838	1699	1702	1706	rVB2	78010	113270	6.07%	0.533%
53	12.885	1706	1710	1718	rVB5	68236	127766	6.85%	0.602%
54	12.968	1718	1724	1729	rBV4	92553	209200	11.21%	0.985%
55	13.062	1736	1740	1742	rBV2	39412	54419	2.92%	0.256%
56	13.450	1800	1806	1812	rVB	1047816	1640261	87.91%	7.725%
57	13.502	1812	1815	1819	rBV4	81674	124814	6.69%	0.588%
58	13.655	1837	1841	1850	rVB8	99296	211726	11.35%	0.997%
59	13.837	1870	1872	1877	rVB4	54341	64762	3.47%	0.305%
60	13.967	1889	1894	1899	rBV3	92262	159688	8.56%	0.752%
61	14.019	1899	1903	1907	rBV4	74625	110337	5.91%	0.520%
62	14.061	1907	1910	1913	rBV5	56734	87629	4.70%	0.413%
63	14.155	1922	1926	1927	rBV2	67686	89224	4.78%	0.420%
64	14.260	1939	1944	1950	rVB2	121809	297430	15.94%	1.401%
65	14.466	1970	1979	1986	rBV3	480912	978576	52.45%	4.609%
66	14.771	2028	2031	2034	rBV	89498	142524	7.64%	0.671%
67	14.824	2035	2040	2050	rVB2	261996	528342	28.32%	2.488%
68	15.253	2109	2113	2117	rVB	131152	201058	10.78%	0.947%
69	15.347	2124	2129	2132	rBV2	148899	296497	15.89%	1.396%
70	15.424	2137	2142	2146	rVV2	230389	398858	21.38%	1.878%
71	15.477	2147	2151	2158	rVB6	165536	305442	16.37%	1.439%

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041516\
 Data File : BG021696.D
 Acq On : 15 Apr 2016 21:56
 Operator : UM/SJ
 Sample : H2549-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S8-0574

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

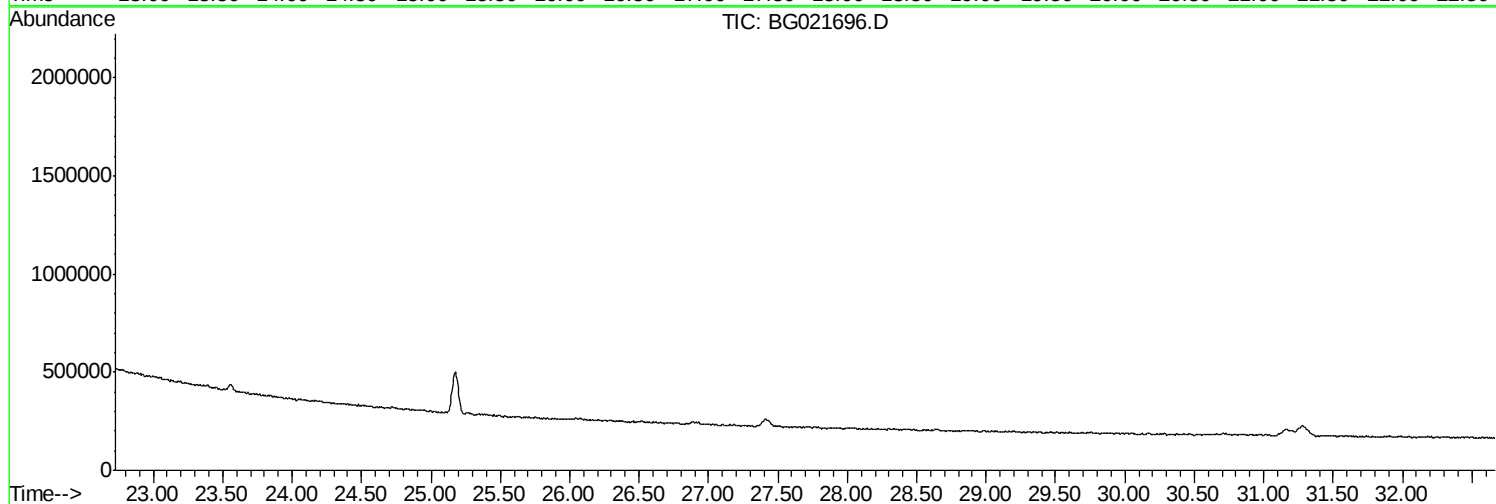
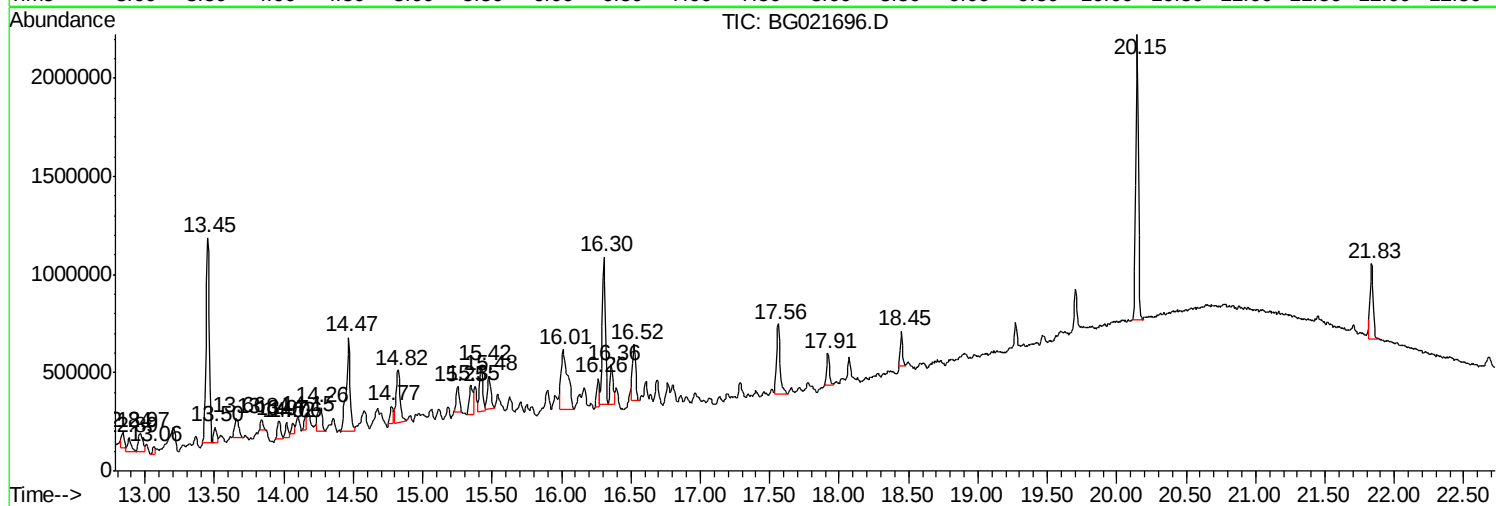
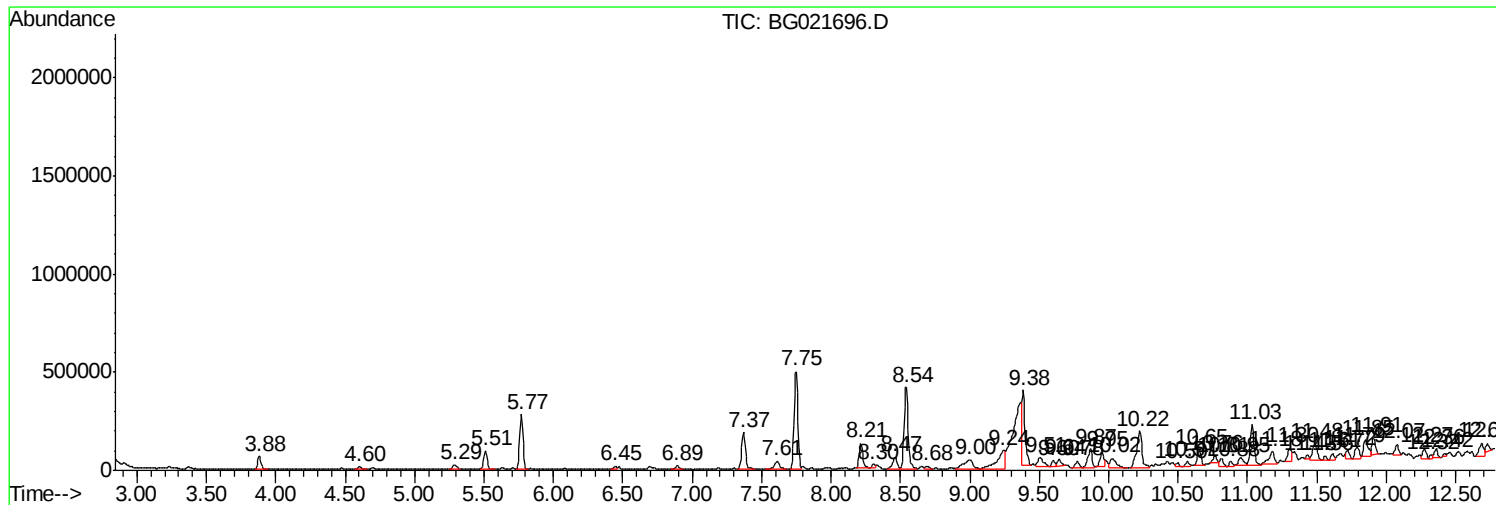
If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041316.M
 Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

72	16.011	2237	2242	2255	rVB3	303248	1020668	54.71%	4.807%
73	16.264	2281	2285	2287	rBV	142461	201791	10.82%	0.950%
74	16.305	2287	2292	2297	rVB	748665	1115675	59.80%	5.254%
75	16.358	2297	2301	2305	rBV2	198473	309574	16.59%	1.458%
76	16.522	2325	2329	2335	rVB	286153	456701	24.48%	2.151%
77	17.562	2501	2506	2517	rVB	353868	606129	32.49%	2.855%
78	17.915	2563	2566	2573	rBV2	161354	228519	12.25%	1.076%
79	18.450	2654	2657	2661	rVB	174595	197048	10.56%	0.928%
80	20.148	2941	2946	2953	rVB	1457105	1865749	100.00%	8.787%
81	21.834	3230	3233	3240	rVB	380449	605120	32.43%	2.850%

Sum of corrected areas: 21233070

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



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

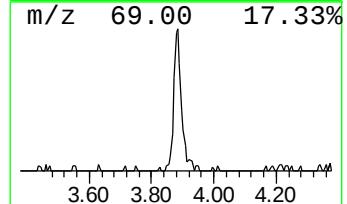
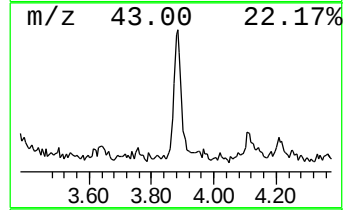
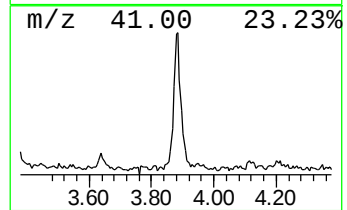
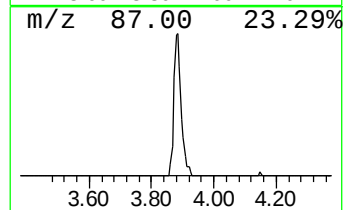
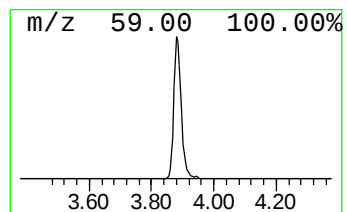
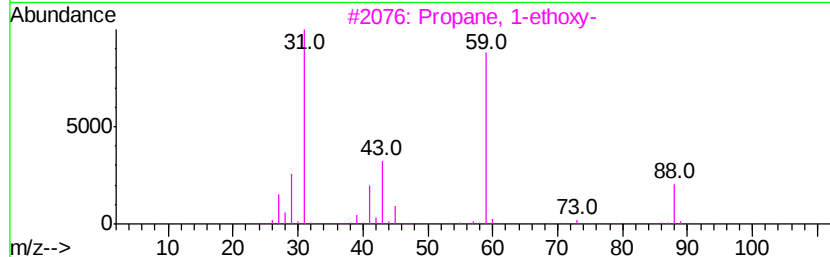
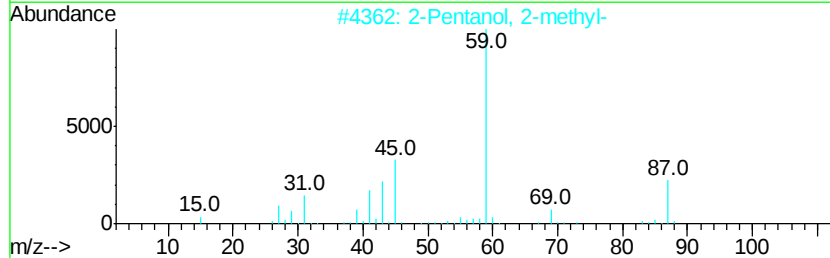
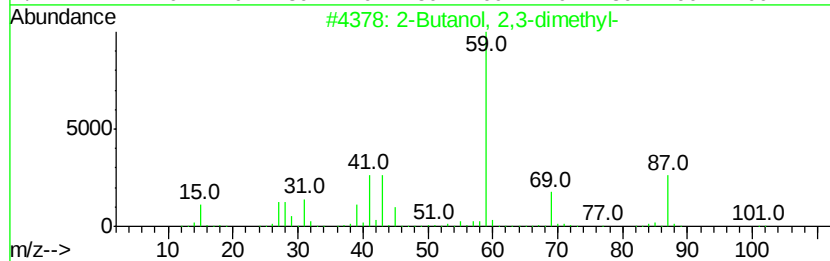
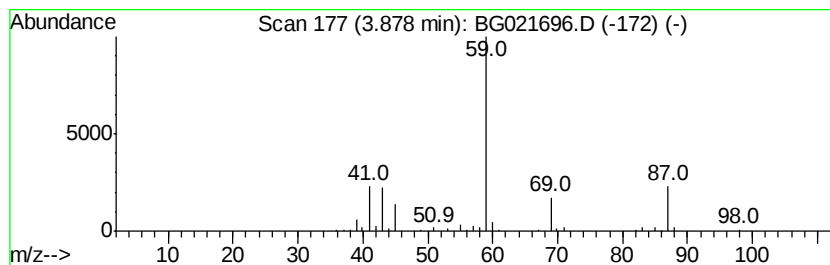
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Butanol, 2,3-dimethyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.88	9.53 ng	109164	1,4-Dichlorobenzene-d4	8.21

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Butanol, 2,3-dimethyl-	102	C6H14O	000594-60-5	83
2			2-Pentanol, 2-methyl-	102	C6H14O	000590-36-3	78
3			Propane, 1-ethoxy-	88	C5H12O	000628-32-0	53
4			Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	50
5			3-Heptanol	116	C7H16O	000589-82-2	40



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
S8-0574

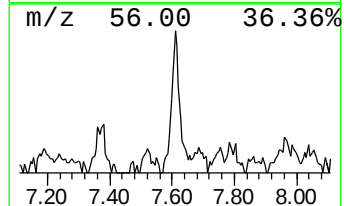
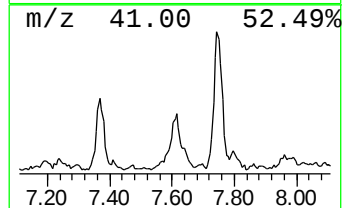
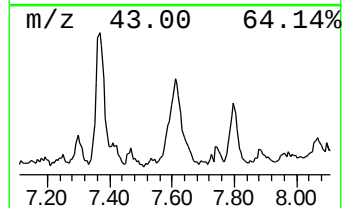
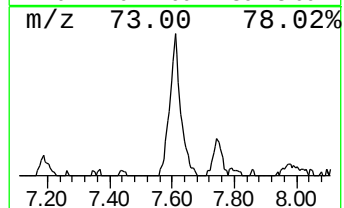
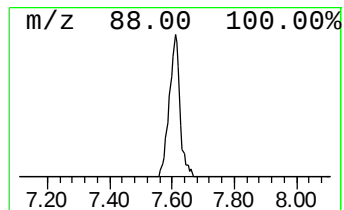
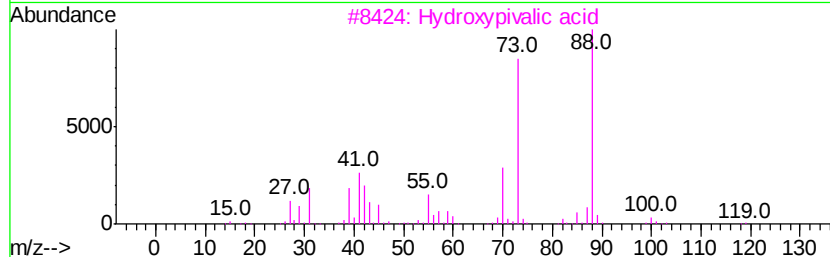
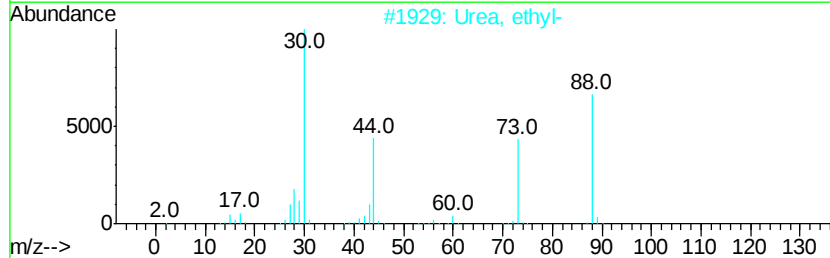
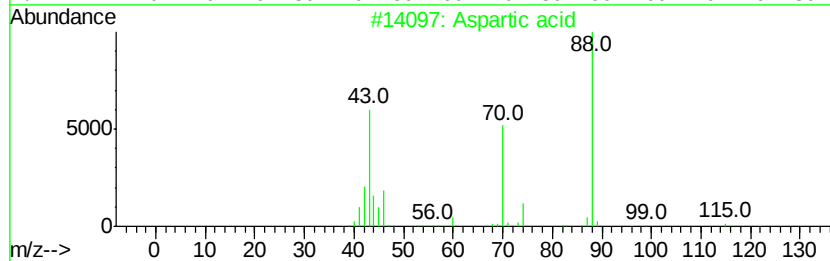
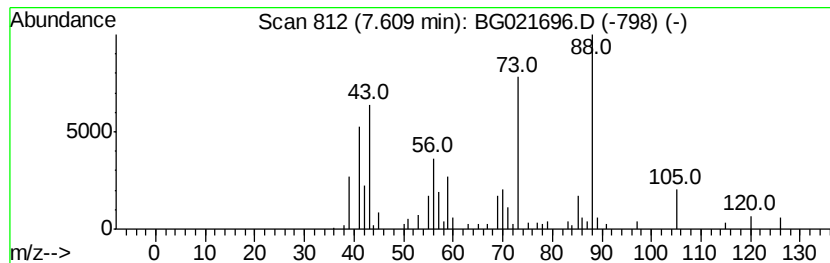
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.61 Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.61	10.27 ng	117625	1,4-Dichlorobenzene-d4	8.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Aspartic acid	133	C4H7N04	000056-84-8	43
2		Urea, ethyl-	88	C3H8N2O	000625-52-5	38
3		Hvdroxyvpivalic acid	118	C5H10O3	004835-90-9	38
4		2-Amino-3-methoxy-2-methyl-propi...	133	C5H11N03	064298-94-8	37
5		Sulfide, allyl methyl	88	C4H8S	010152-76-8	35



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

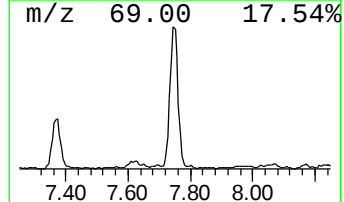
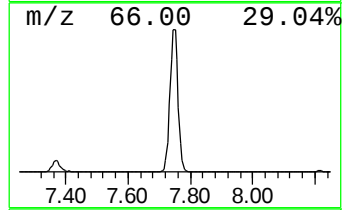
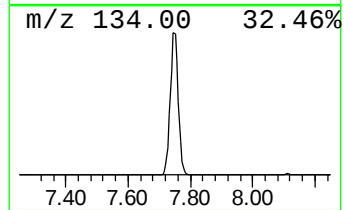
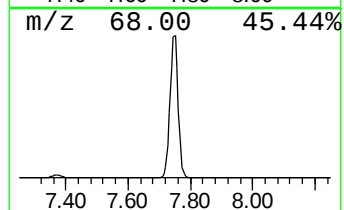
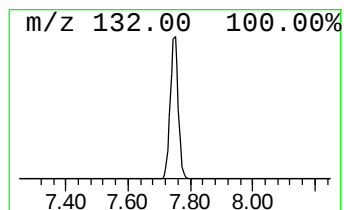
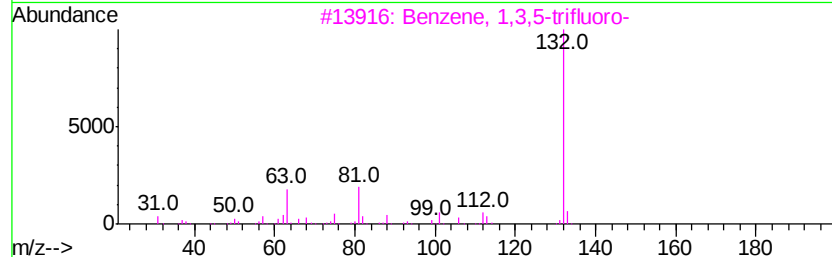
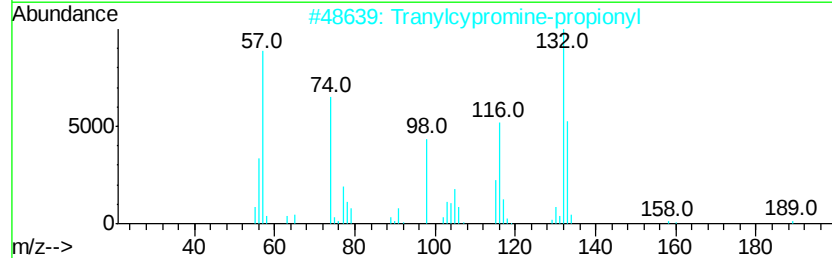
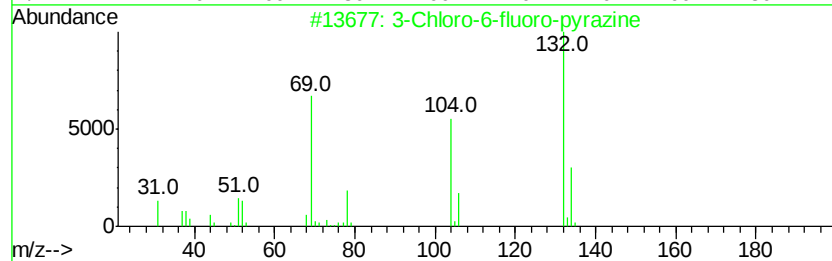
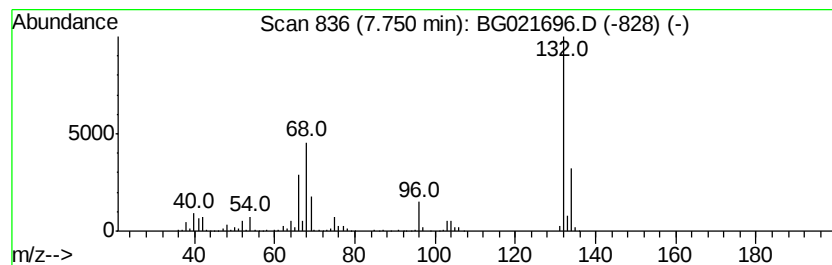
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.75 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.75	78.61 ng	900499	1,4-Dichlorobenzene-d4	8.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

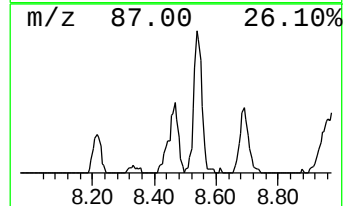
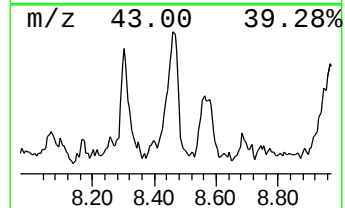
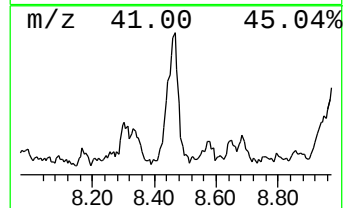
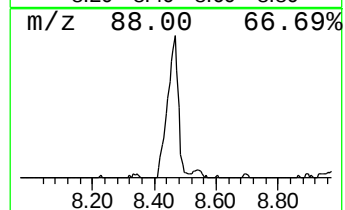
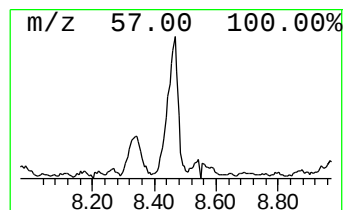
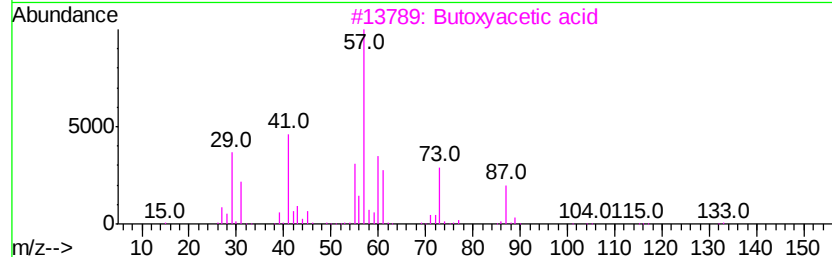
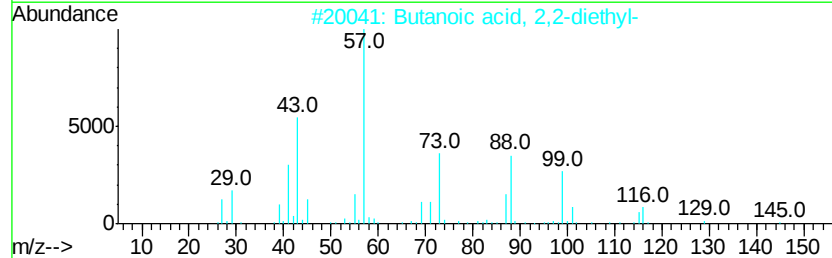
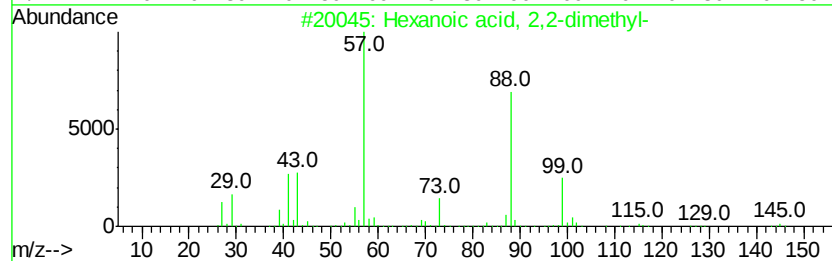
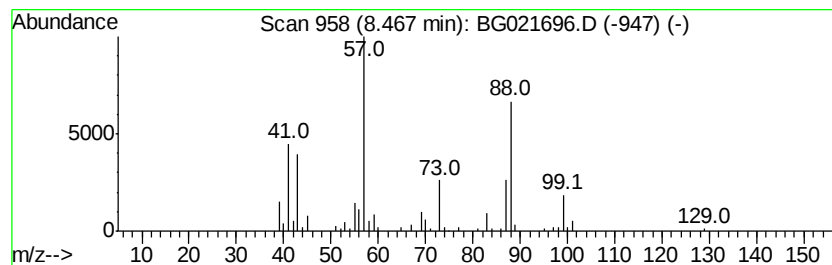
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 2,2-dimethyl- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	11.71 ng	134158	1,4-Dichlorobenzene-d4	8.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2,2-dimethyl-	144	C8H16O2	000813-72-9	50
2		Butanoic acid, 2,2-diethyl-	144	C8H16O2	000813-58-1	37
3		Butoxyacetic acid	132	C6H12O3	002516-93-0	32
4		Methyl propionate	88	C4H8O2	000554-12-1	27
5		Heptane, 3-(chloromethyl)-	148	C8H17Cl	000123-04-6	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

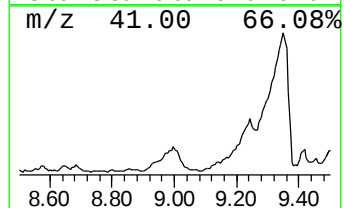
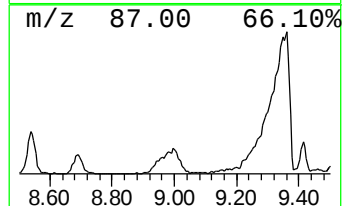
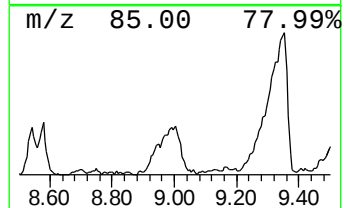
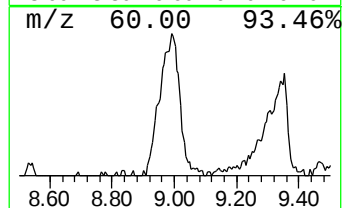
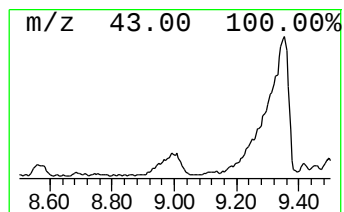
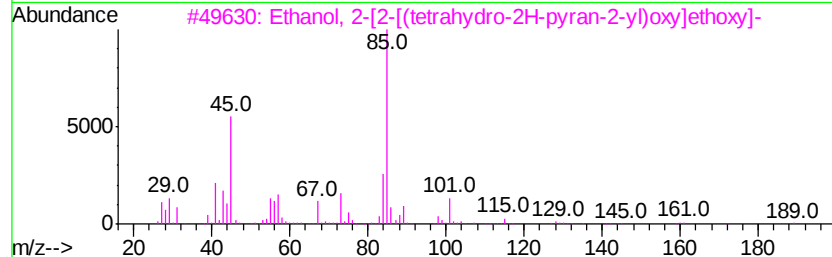
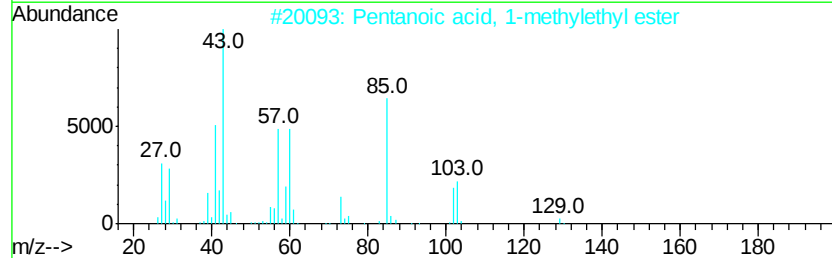
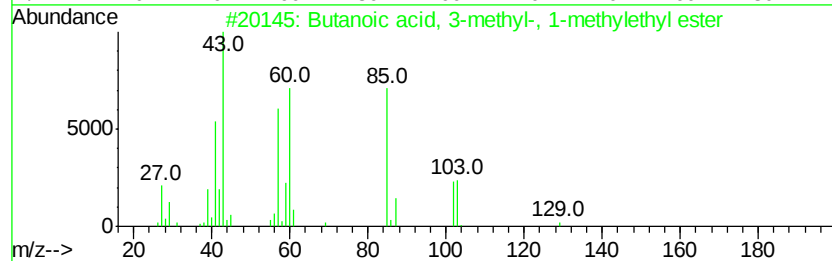
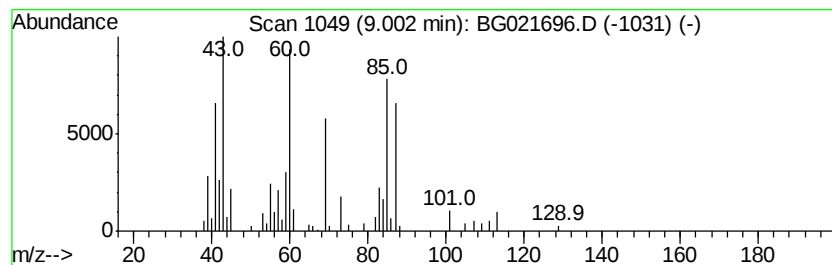
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Butanoic acid, 3-methyl-, 1... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.00	17.89 ng	204916	1,4-Dichlorobenzene-d4	8.21

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 3-methyl-, 1-meth...	144	C8H16O2	032665-23-9	53
2		Pentanoic acid, 1-methylethyl ester	144	C8H16O2	018362-97-5	42
3		Ethanol, 2-[2-[(tetrahydro-2H-py...	190	C9H18O4	002163-11-3	22
4		1-Pentanol, 2,3-dimethyl-	116	C7H16O	010143-23-4	22
5		Ethanol, 2-(2-butoxyethoxy)-, ac...	204	C10H20O4	000124-17-4	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

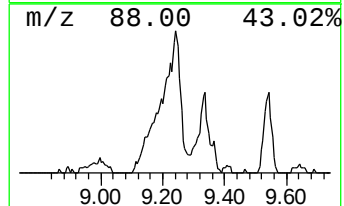
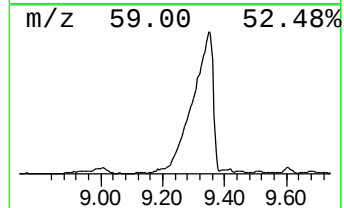
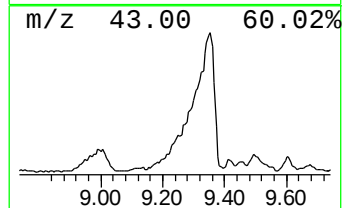
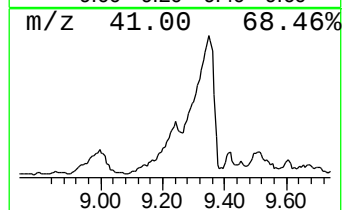
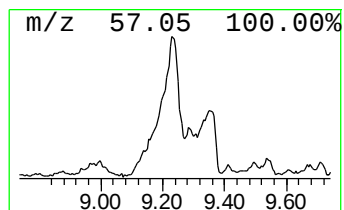
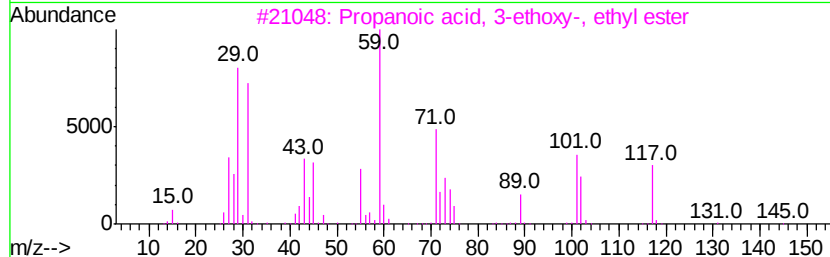
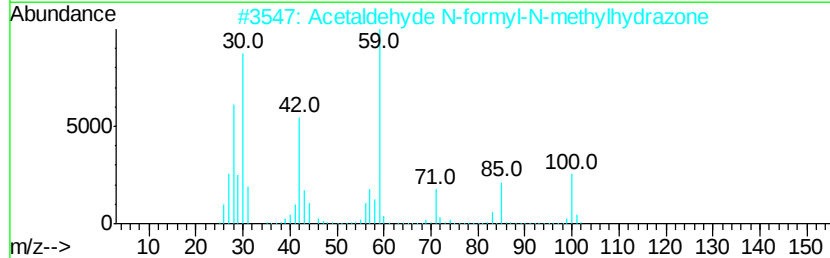
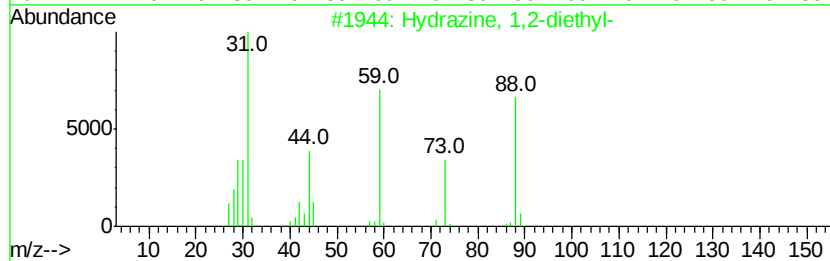
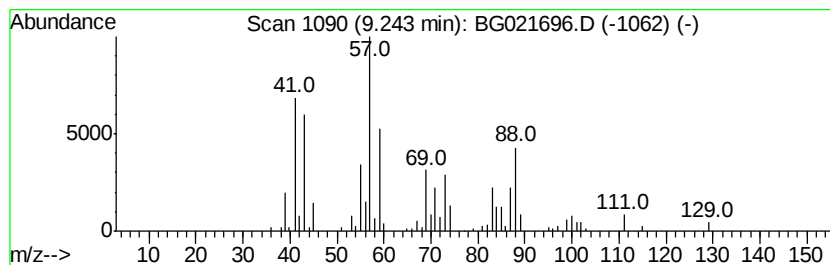
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown9.24 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.24	32.79 ng	375657	1,4-Dichlorobenzene-d4	8.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hydrazine, 1,2-diethyl-	88	C4H12N2	001615-80-1	43
2		Acetaldehyde N-formyl-N-methylhy...	100	C4H8N2O	016568-02-8	22
3		Propanoic acid, 3-ethoxy-, ethyl...	146	C7H14O3	000763-69-9	22
4		Butanoic acid, 4-ethoxy-, methyl...	146	C7H14O3	029006-04-0	16
5		3-Octanol	130	C8H18O	000589-98-0	14



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

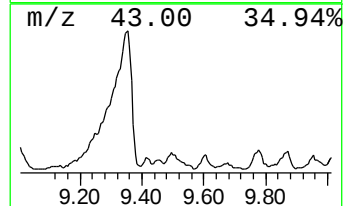
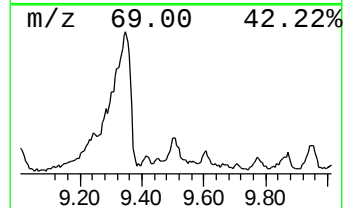
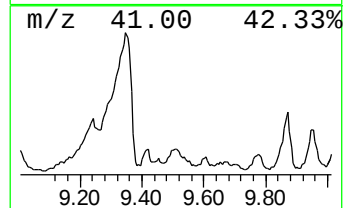
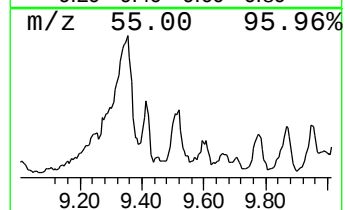
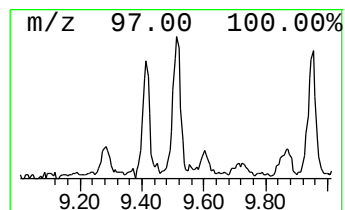
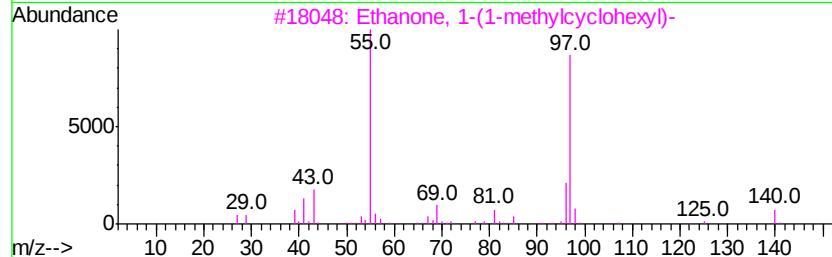
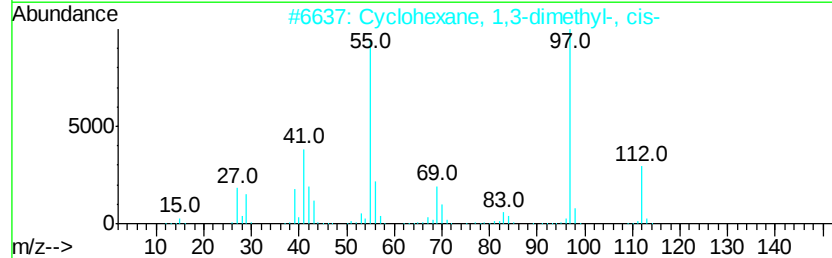
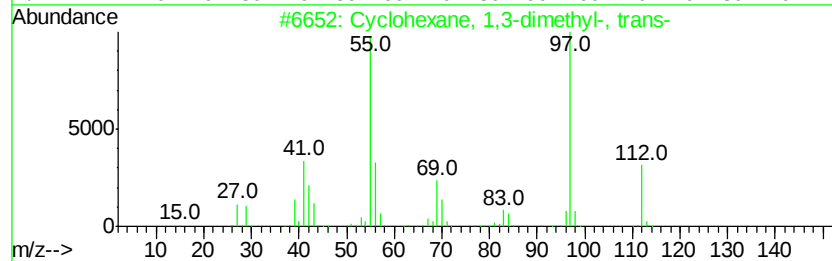
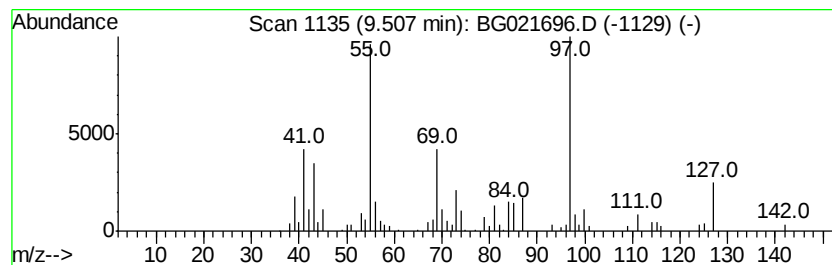
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown9.51 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.51	11.23 ng	128635	1,4-Dichlorobenzene-d4	8.21

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,3-dimethyl-, trans-	112	C8H16	002207-03-6	43
2		Cyclohexane, 1,3-dimethyl-, cis-	112	C8H16	000638-04-0	43
3		Ethanone, 1-(1-methylcyclohexyl)-	140	C9H16O	002890-62-2	43
4		Cyclohexane, 1-ethyl-2-methyl-, ...	126	C9H18	004923-78-8	43
5		Cyclohexane, 1-methyl-4-(1-methy...	140	C10H20	006069-98-3	38



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

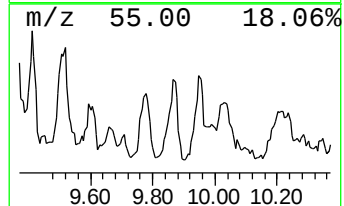
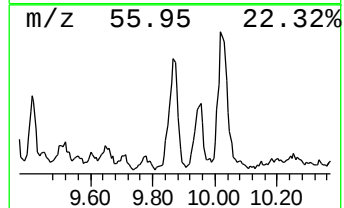
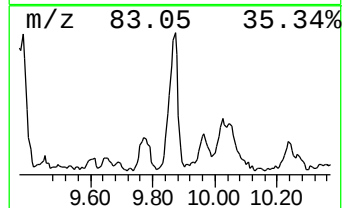
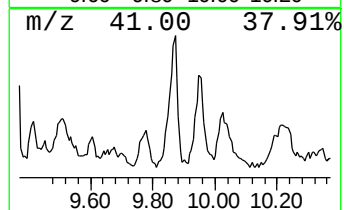
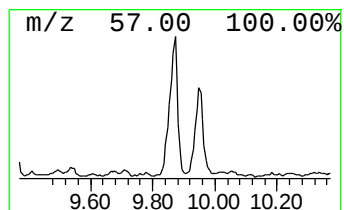
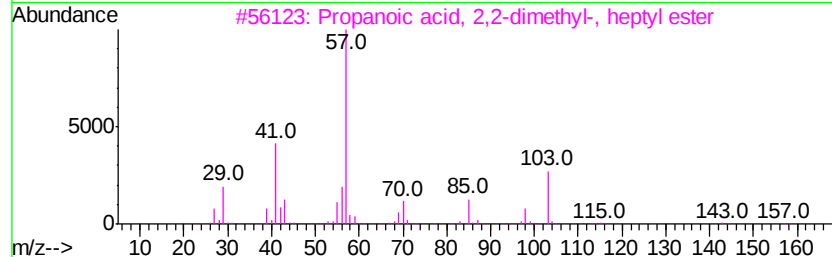
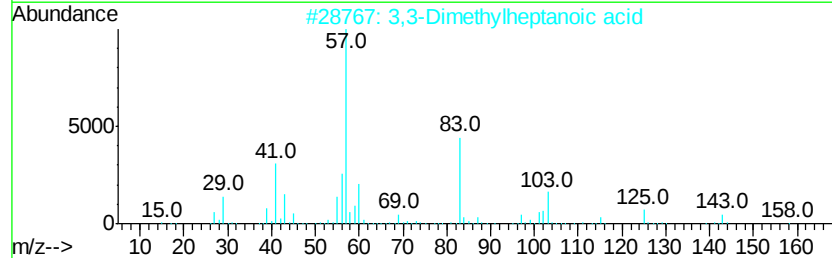
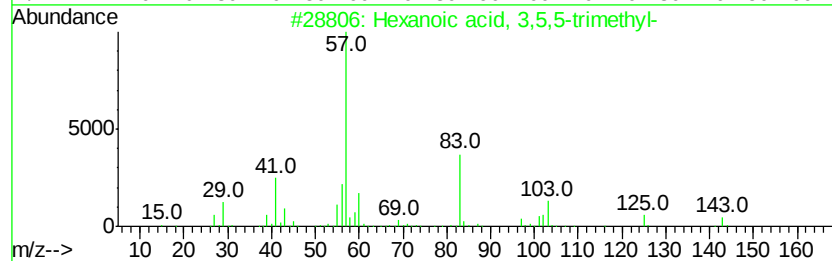
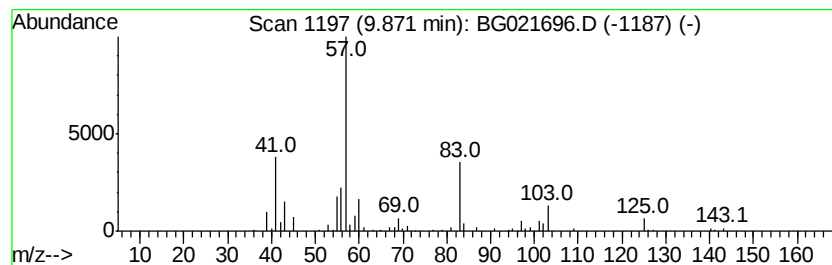
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexanoic acid, 3,5,5-trimet... Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.87	9.41 ng	187832	Naphthalene-d8	11.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanoic acid, 3,5,5-trimethyl-	158	C9H18O2	003302-10-1	90
2			3,3-Dimethylheptanoic acid	158	C9H18O2	067061-30-7	83
3			Propanoic acid, 2,2-dimethyl-, h...	200	C12H24O2	017660-61-6	38
4			Propanoic acid, 2,2-dimethyl-, h...	186	C11H22O2	005434-57-1	35
5			Hexanal, 3,5,5-trimethyl-	142	C9H18O	005435-64-3	23



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

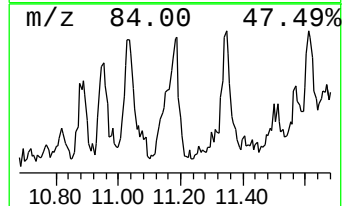
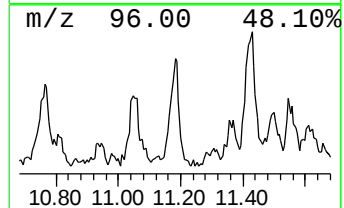
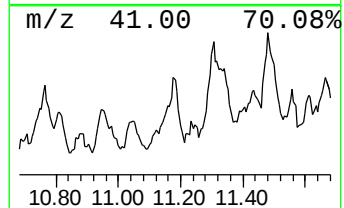
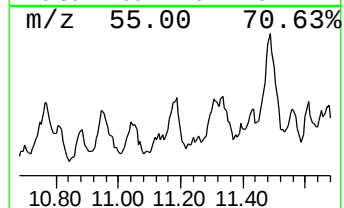
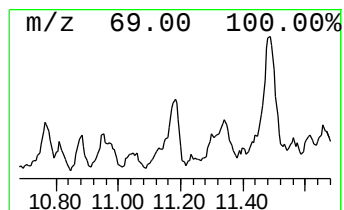
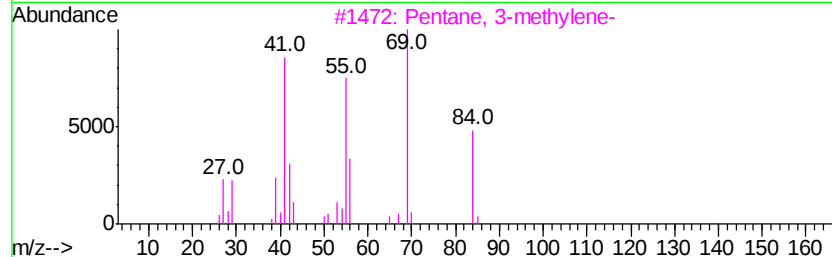
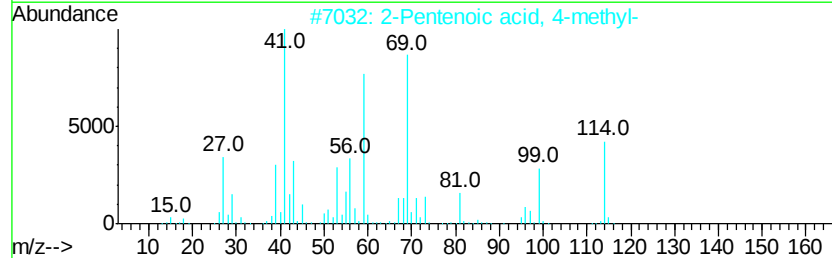
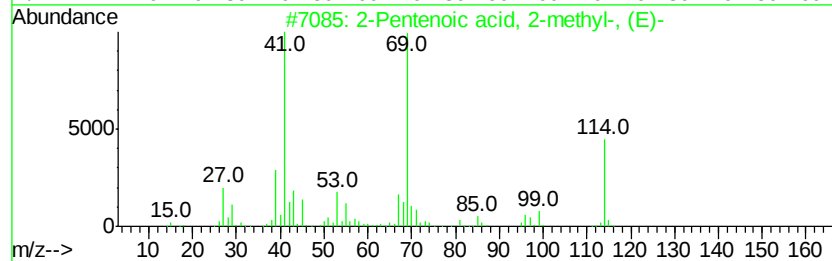
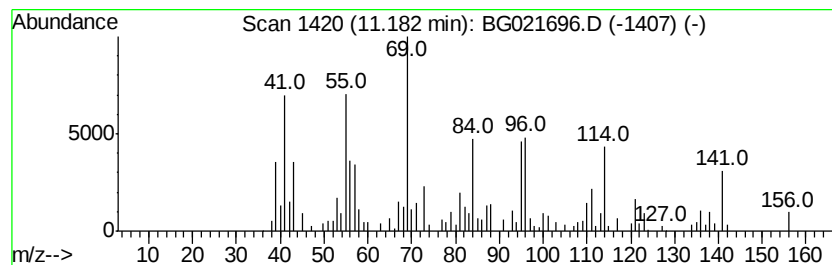
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown11.18 Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.18	8.86 ng	176915	Naphthalene-d8	11.03

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentenoic acid, 2-methyl-, (E)-		114	C6H10O2		016957-70-3	42
2	2-Pentenoic acid, 4-methyl-		114	C6H10O2		010321-71-8	38
3	Pentane, 3-methylene-		84	C6H12		000760-21-4	38
4	Furan, 2,3-dihydro-3-methyl-		84	C5H8O		001708-27-6	38
5	2-Pentene, 3-methyl-, (E)-		84	C6H12		000616-12-6	30



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

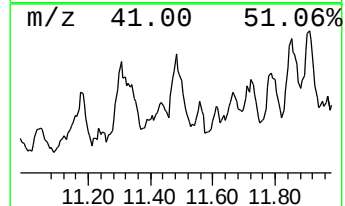
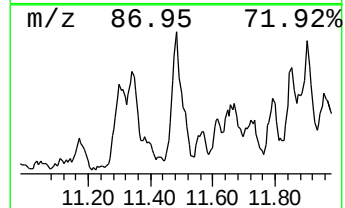
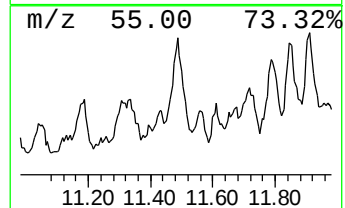
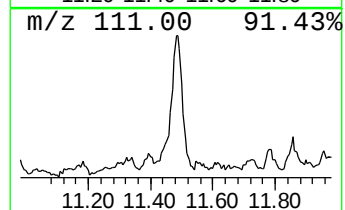
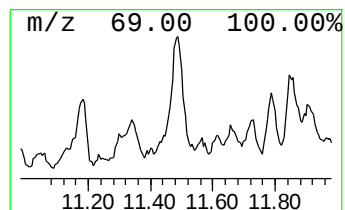
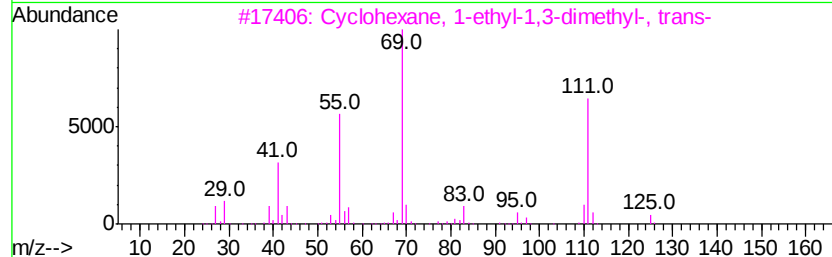
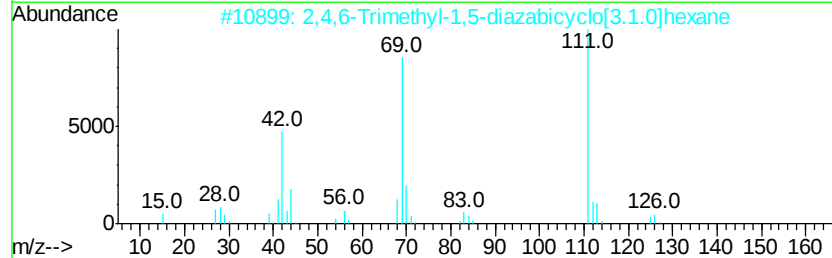
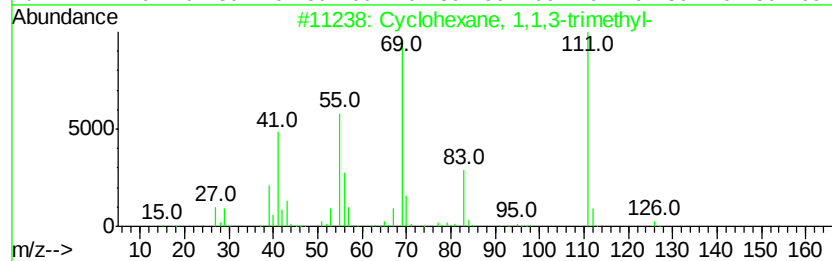
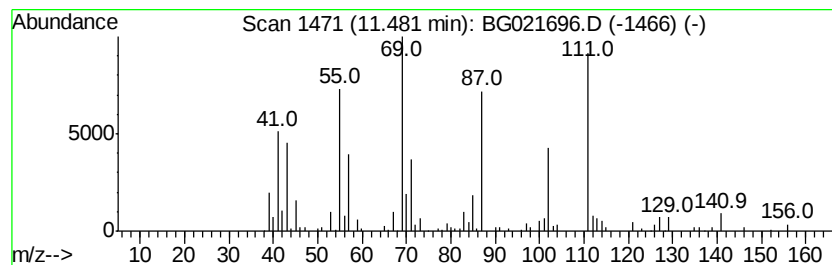
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Cyclohexane, 1,1,3-trimethyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.48	9.79 ng	195414	Napthalene-d8	11.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexane, 1,1,3-trimethyl-	126	C9H18	003073-66-3	53
2		2,4,6-Trimethyl-1,5-diazabicyclo...	126	C7H14N2	1000283-21-2	47
3		Cyclohexane, 1-ethyl-1,3-dimethyl...	140	C10H20	062238-29-3	47
4		Cyclohexane, 1-ethyl-1,4-dimethyl...	140	C10H20	062238-32-8	47
5		Cyclohexane, 1-ethyl-1,3-dimethyl...	140	C10H20	062238-31-7	43



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

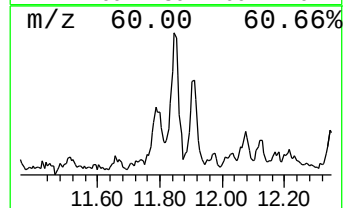
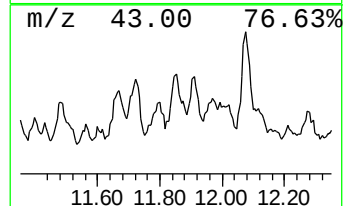
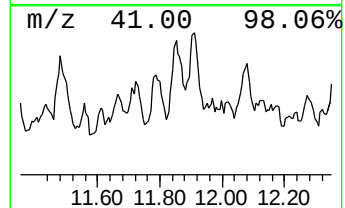
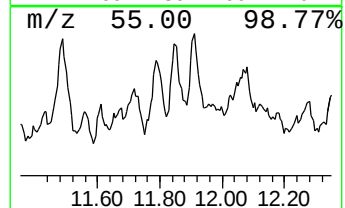
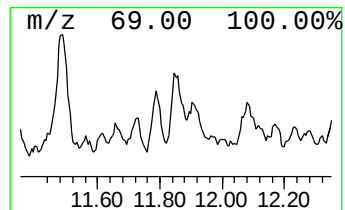
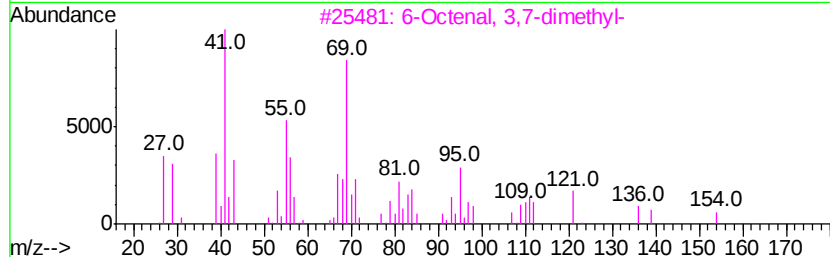
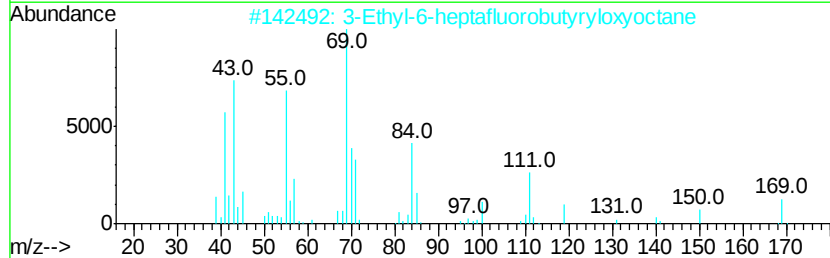
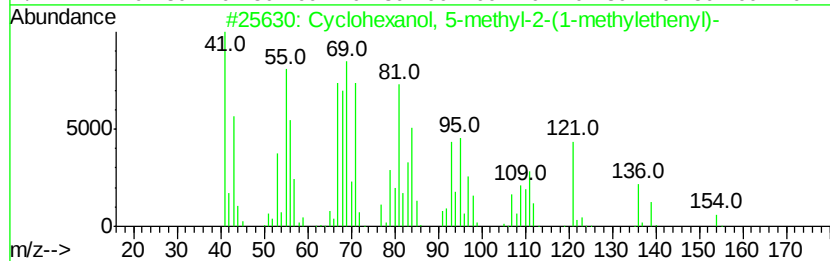
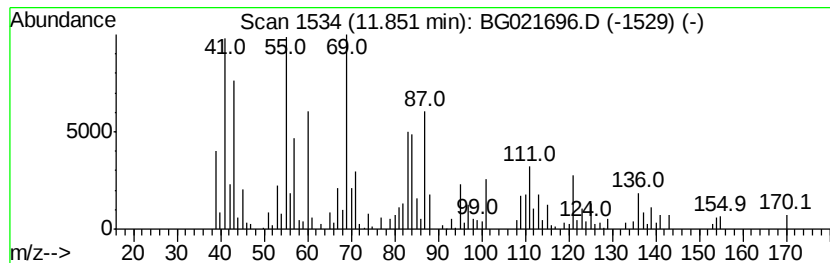
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 unknown11.85 Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.85	9.13 ng	182273	Napthalene-d8	11.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 5-methyl-2-(1-meth...	154	C10H18O	007786-67-6	38
2		3-Ethyl-6-heptafluorobutyryloxy...	354	C14H21F7O2	1000215-97-4	35
3		6-Octenal, 3,7-dimethyl-	154	C10H18O	000106-23-0	30
4		2-Nonen-4-one	140	C9H16O	032064-72-5	27
5		Cyclohexane, (1,2-dimethylbutyl)-	168	C12H24	061142-37-8	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

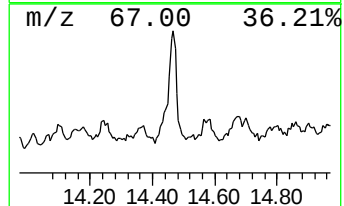
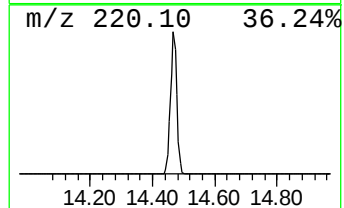
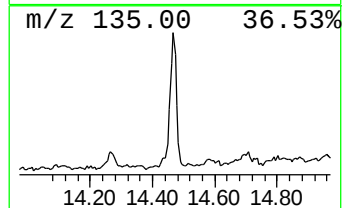
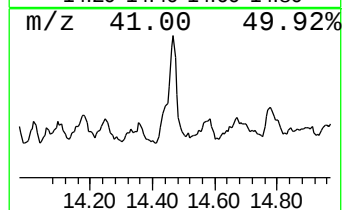
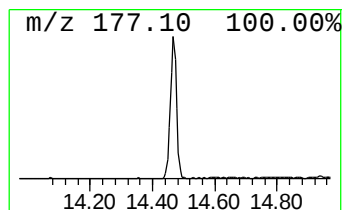
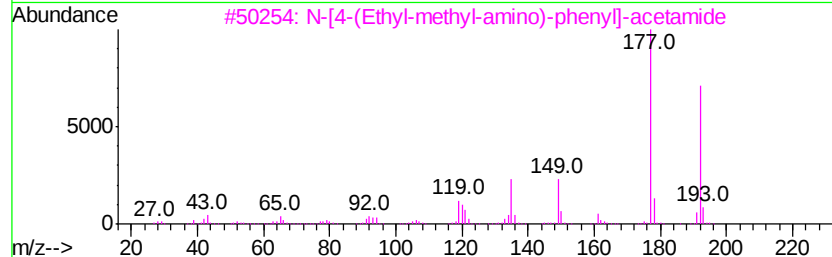
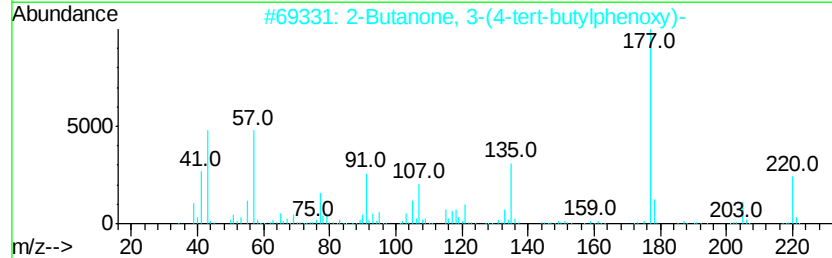
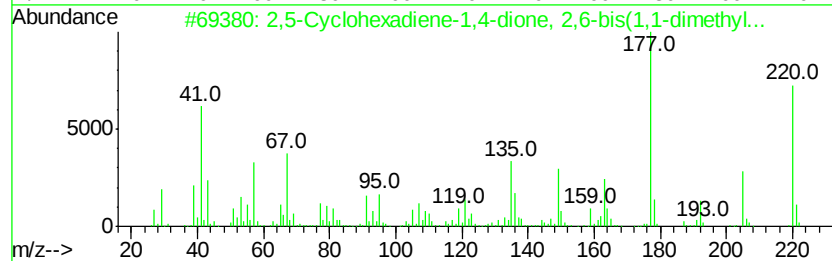
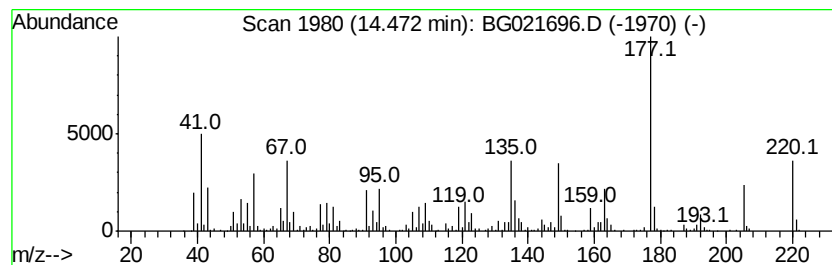
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,5-Cyclohexadiene-1,4-dion... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.47	37.04 ng	978576	Acenaphthene-d10	14.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5-Cyclohexadiene-1,4-dione, 2,...	220	C14H20O2	000719-22-2	99
2		2-Butanone, 3-(4-tert-butylpheno...	220	C14H20O2	160875-28-5	64
3		N-[4-(Ethyl-methyl-amino)-phenyl]...	192	C11H16N2O	099981-45-0	49
4		3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	000079-77-6	49
5		4(1H)-Pteridinone, 2-amino-7-met...	177	C7H7N5O	013040-58-9	46



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

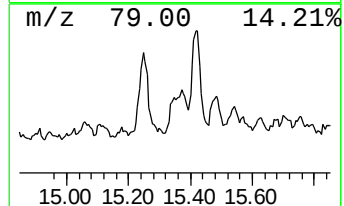
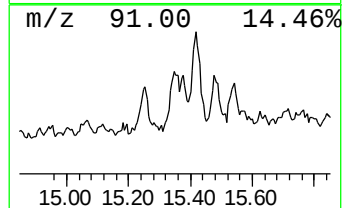
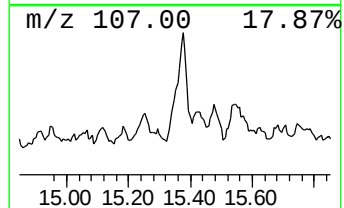
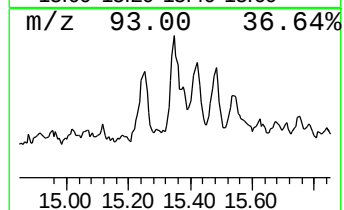
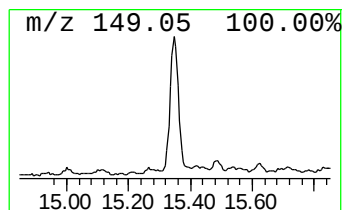
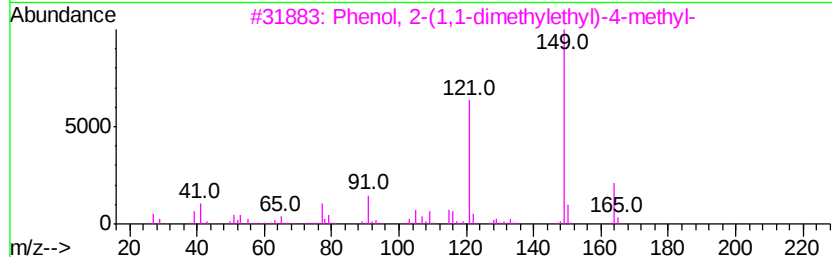
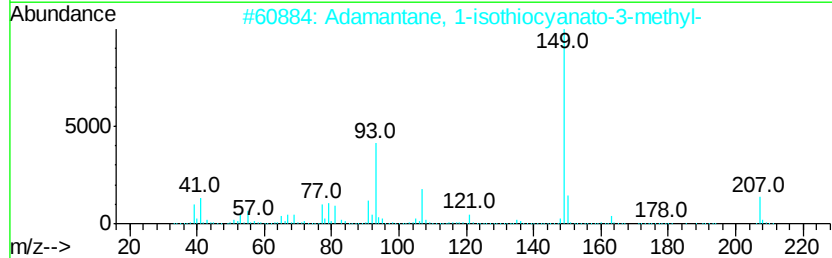
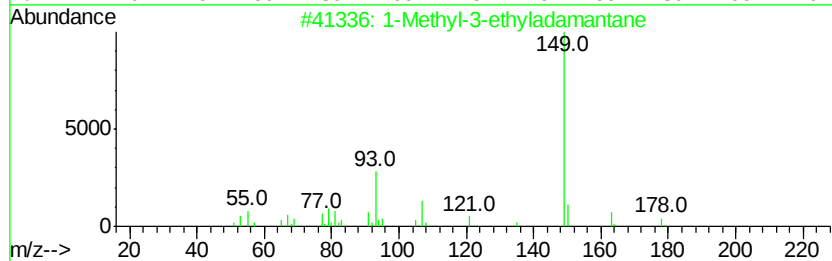
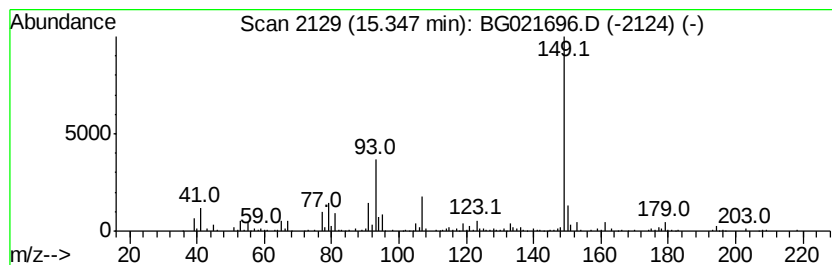
Instrument :
BNA_G
ClientSampled :
S8-0574

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 1-Methyl-3-ethyladamantane Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.		
15.35	11.22 ng	296497	Acenaphthene-d10	14.82		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	74
2		Adamantane, 1-isothiocyanato-3-m...	207	C12H17NS	136860-48-5	64
3		Phenol, 2-(1,1-dimethylethyl)-4-...	164	C11H16O	002409-55-4	50
4		Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	50
5		Cis-1,4-dimethyladamantane	164	C12H20	024145-89-9	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

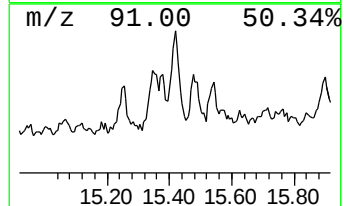
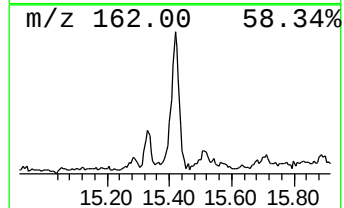
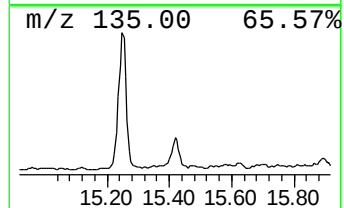
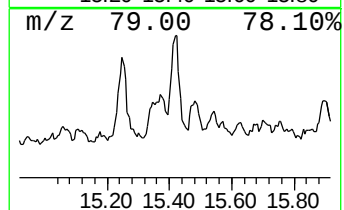
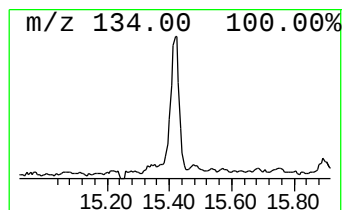
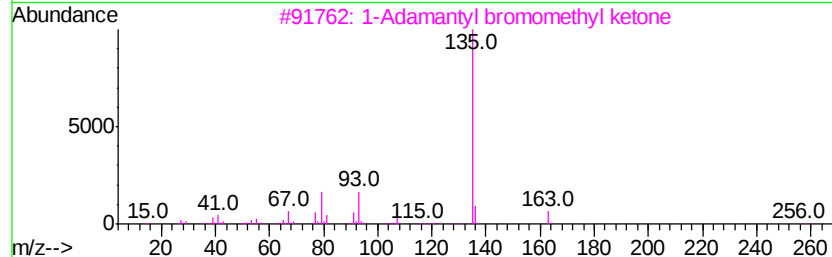
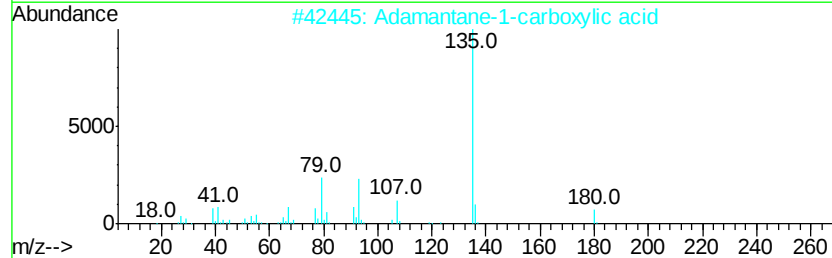
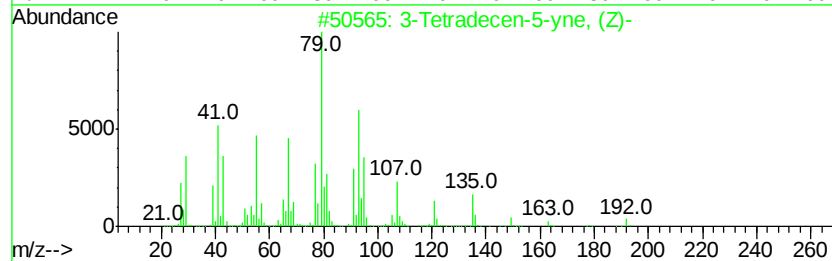
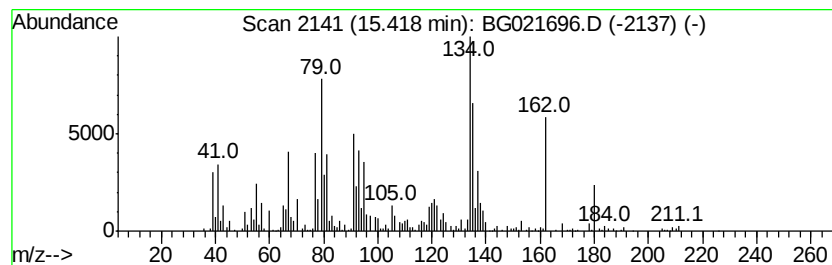
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 unknown15.42 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.42	15.10 ng	398858	Acenaphthene-d10	14.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Tetradecen-5-yne, (Z)-	192	C14H24	074663-68-6	38
2		Adamantane-1-carboxylic acid	180	C11H16O2	000828-51-3	38
3		1-Adamantyl bromomethyl ketone	256	C12H17BrO	005122-82-7	27
4		4-Tridecen-6-yne, (Z)-	178	C13H22	074744-42-6	25
5		2-Methyl-1-nonene-3-yne	136	C10H16	070058-00-3	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

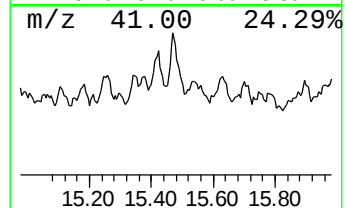
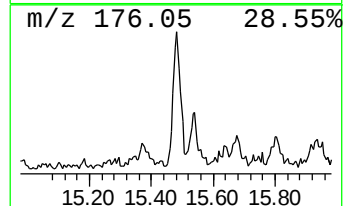
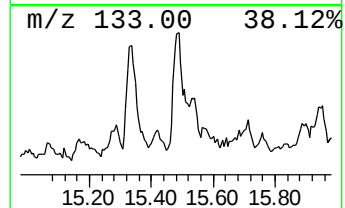
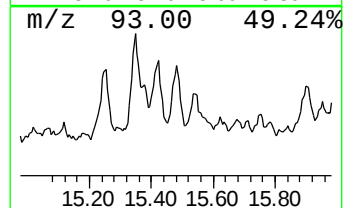
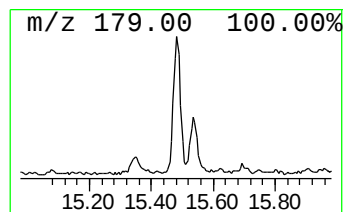
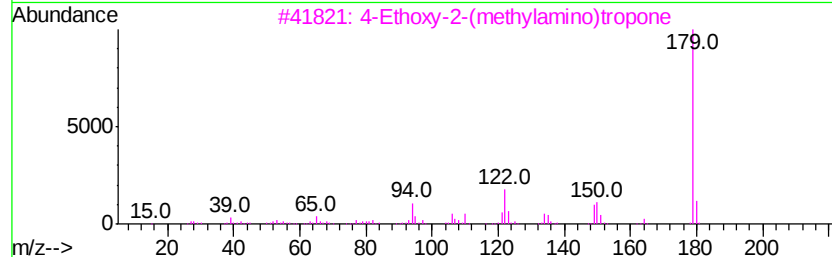
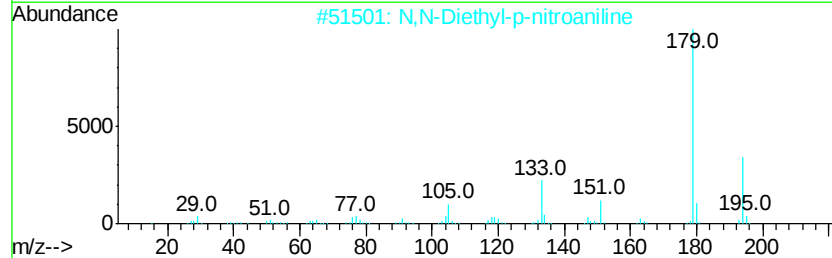
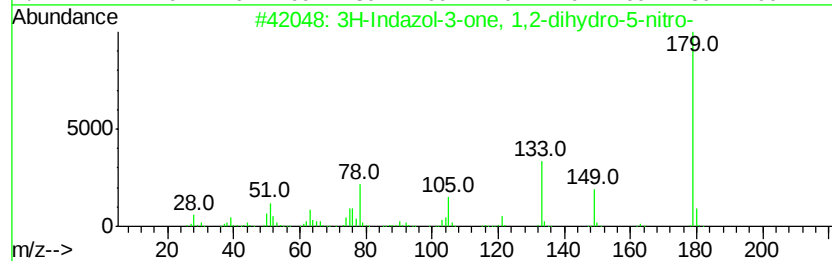
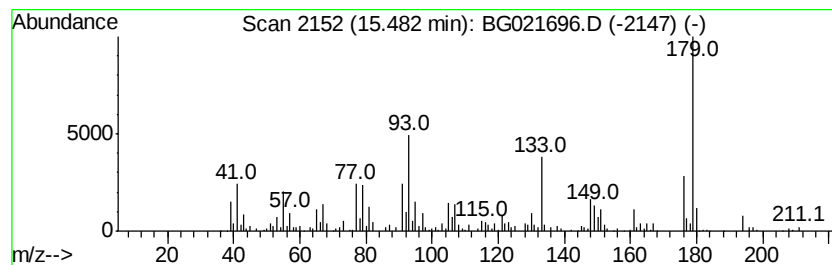
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown15.48 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.48	11.56 ng	305442	Acenaphthene-d10	14.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3H-Indazol-3-one, 1,2-dihydro-5-...	179	C7H5N3O3	061346-19-8	43
2		N,N-Diethyl-p-nitroaniline	194	C10H14N2O2	002216-15-1	38
3		4-Ethoxy-2-(methylamino)troponone	179	C10H13NO2	1000241-45-1	38
4		Benzoic acid, 2-acetyl-3-methoxy-	194	C10H10O4	120714-42-3	27
5		(p-Butyrylphenoxy)acetic acid	222	C12H14O4	001141-96-4	27



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

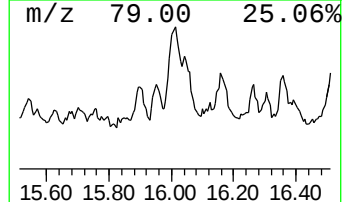
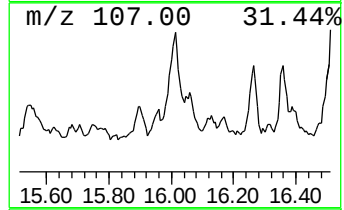
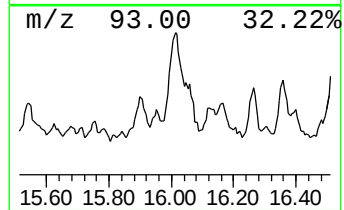
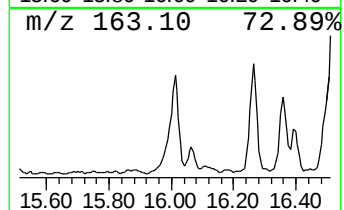
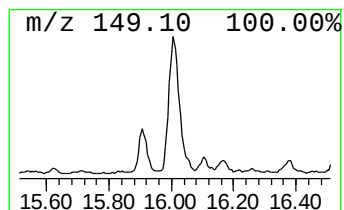
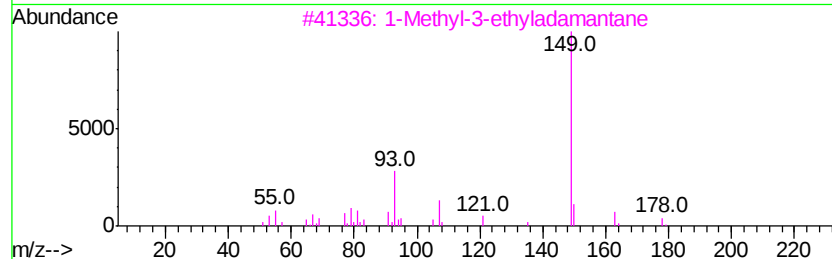
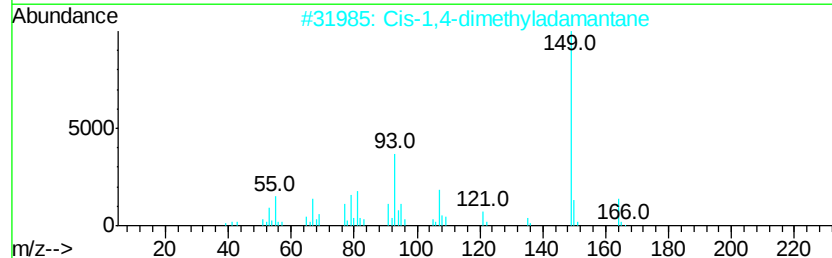
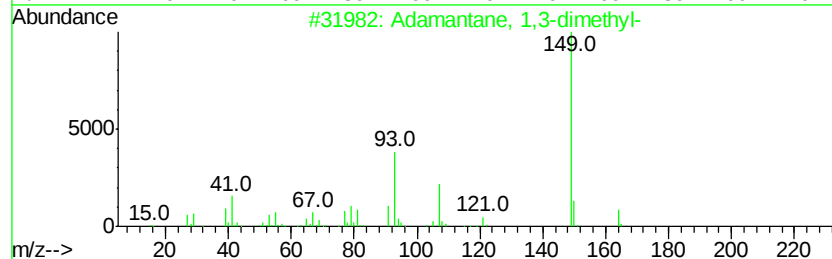
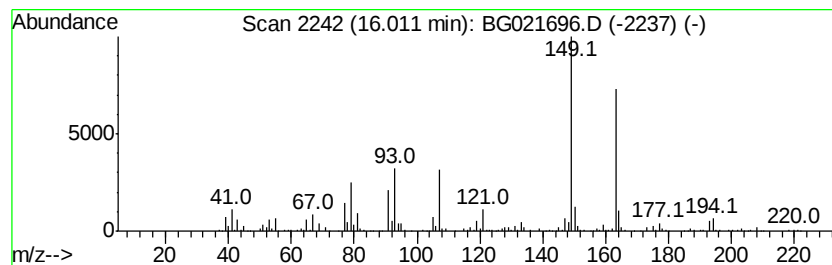
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 Adamantane, 1,3-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.01	38.64 ng	1020670	Acenaphthene-d10	14.82

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Adamantane, 1,3-dimethyl-	164	C12H20	000702-79-4	52
2		Cis-1,4-dimethyladamantane	164	C12H20	024145-89-9	50
3		1-Methyl-3-ethyladamantane	178	C13H22	001687-34-9	47
4		2-(3-Methylbuta-1,3-dienyl)cyclo...	164	C11H16O	1000191-75-5	47
5		Pyridinium, 1-(acetylamino)-2,6-...	164	C9H12N2O	031020-35-6	46



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

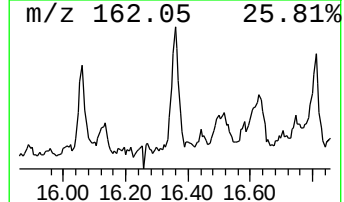
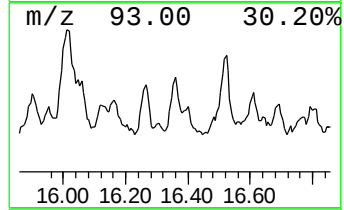
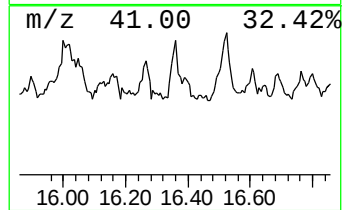
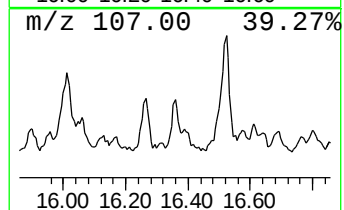
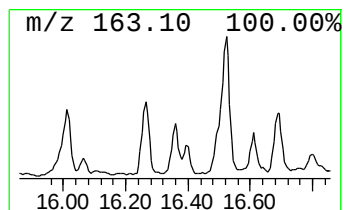
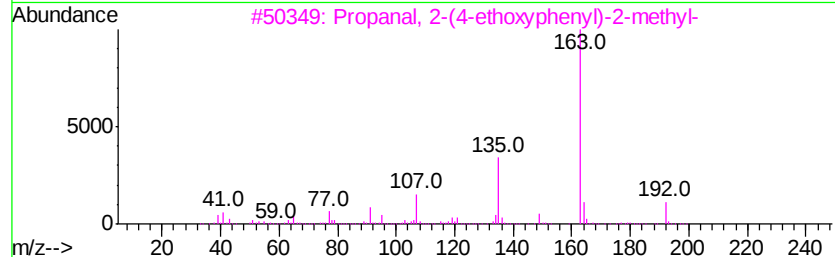
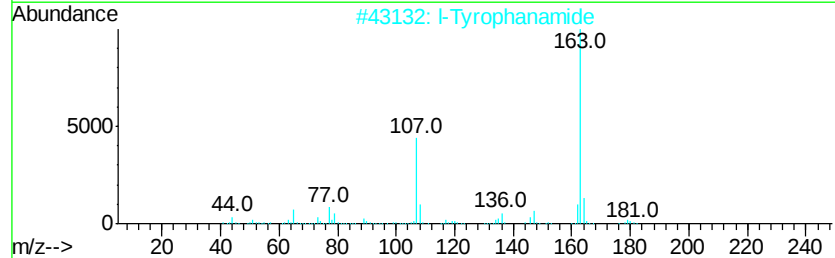
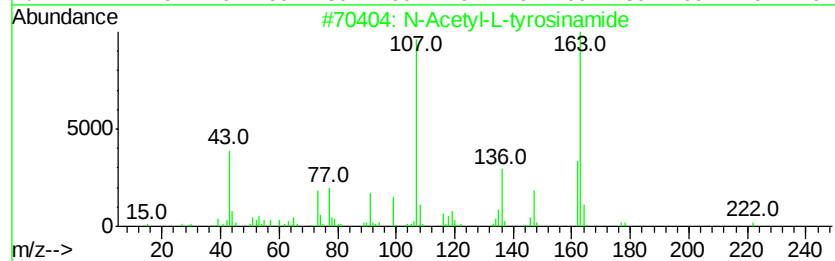
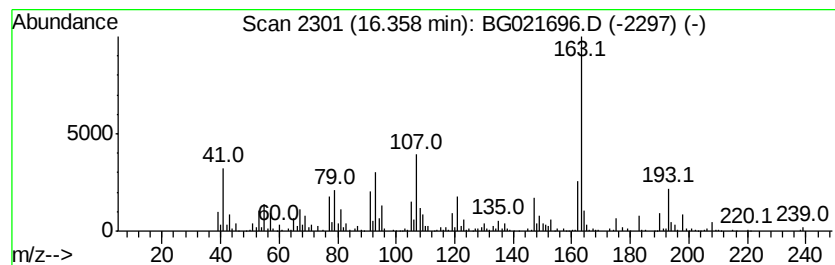
Instrument :
BNA_G
ClientSampleId :
S8-0574

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 N-Acetyl-L-tyrosinamide Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.		
16.36	10.21 ng	309574	Phenanthrene-d10	17.56		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		N-Acetyl-L-tyrosinamide	222	C11H14N2O3	001948-71-6	59
2		l-Tyrosinamide	180	C9H12N2O2	1000131-25-3	53
3		Propanal, 2-(4-ethoxyphenyl)-2-methyl-	192	C12H16O2	093622-71-0	50
4		1,3-Dimethyladamantan-5-carboxyl-	236	C15H24O2	063263-09-2	50
5		6-Amino-2,4-dimethyl-5,7-diazabenzofluorene	163	C8H9N3O	022727-43-1	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG041516\
Data File : BG021696.D
Acq On : 15 Apr 2016 21:56
Operator : UM/SJ
Sample : H2549-02
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S8-0574

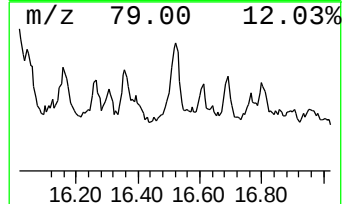
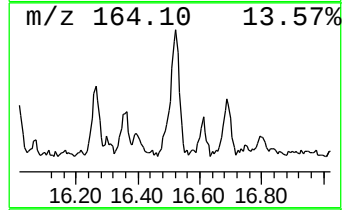
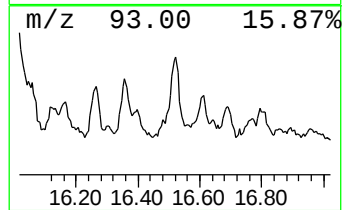
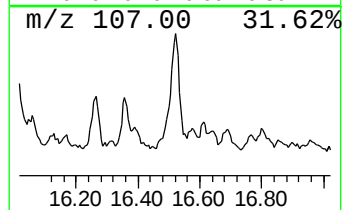
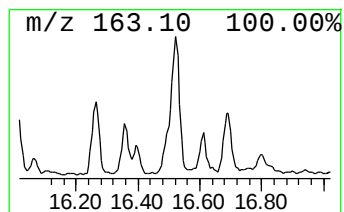
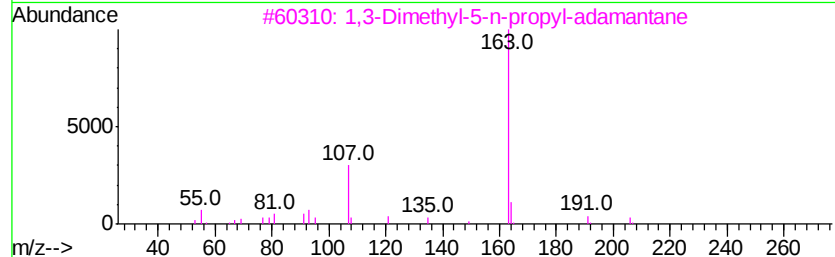
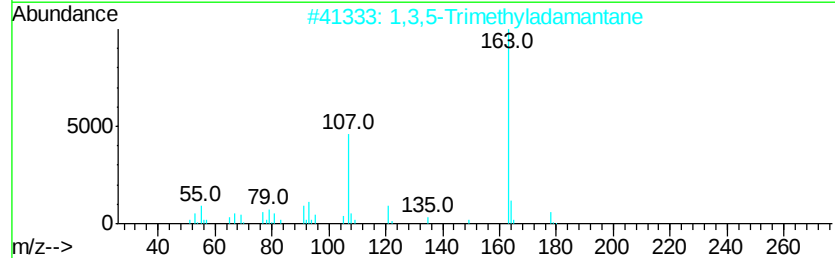
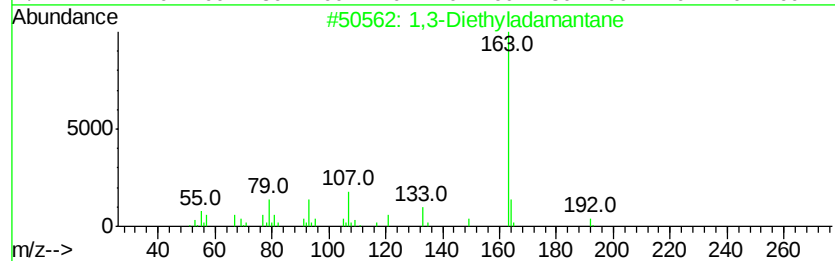
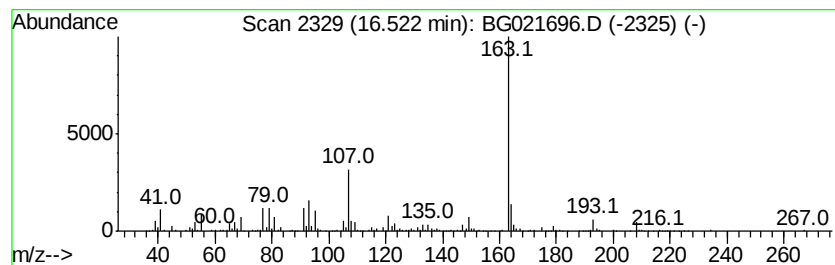
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG041316.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 1,3-Diethyladamantane Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.52	15.07 ng	456701	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Diethyladamantane	192	C14H24	025074-51-5	87
2		1,3,5-Trimethyladamantane	178	C13H22	000707-35-7	64
3		1,3-Dimethyl-5-n-propyl-adamantane	206	C15H26	019385-87-6	64
4		1,3-Dimethyladamantan-5-carboxyl...	236	C15H24O2	063263-09-2	64
5		1,3-Dimethyl-5-n-hexyladamantane	248	C18H32	052873-50-4	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041516\
 Data File : BG021696.D
 Acq On : 15 Apr 2016 21:56
 Operator : UM/SJ
 Sample : H2549-02
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S8-0574

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG041316.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-Butanol, 2,3-di...	3.88	9.5	ng	109164	1	8.21	229119	20.0
unknown7.61	7.61	10.3	ng	117625	1	8.21	229119	20.0
unknown7.75	7.75	78.6	ng	900499	1	8.21	229119	20.0
Hexanoic acid, 2,...	8.47	11.7	ng	134158	1	8.21	229119	20.0
Butanoic acid, 3-...	9.00	17.9	ng	204916	1	8.21	229119	20.0
unknown9.24	9.24	32.8	ng	375657	1	8.21	229119	20.0
unknown9.51	9.51	11.2	ng	128635	1	8.21	229119	20.0
Hexanoic acid, 3,...	9.87	9.4	ng	187832	2	11.03	399233	20.0
unknown11.18	11.18	8.9	ng	176915	2	11.03	399233	20.0
Cyclohexane, 1,1,...	11.48	9.8	ng	195414	2	11.03	399233	20.0
unknown11.85	11.85	9.1	ng	182273	2	11.03	399233	20.0
2,5-Cyclohexadien...	14.47	37.0	ng	978576	3	14.82	528342	20.0
1-Methyl-3-ethyla...	15.35	11.2	ng	296497	3	14.82	528342	20.0
unknown15.42	15.42	15.1	ng	398858	3	14.82	528342	20.0
unknown15.48	15.48	11.6	ng	305442	3	14.82	528342	20.0
Adamantane, 1,3-d...	16.01	38.6	ng	1020670	3	14.82	528342	20.0
N-Acetyl-L-tyrosi...	16.36	10.2	ng	309574	4	17.56	606129	20.0
1,3-Diethyladaman...	16.52	15.1	ng	456701	4	17.56	606129	20.0