

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
 Data File : BG022907.D
 Acq On : 7 Jul 2016 22:42
 Operator : UM/SJ
 Sample : H3834-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1

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-BG070816.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	5.699	479	487	496	rBV	1129904	1931369	17.58%	3.336%
2	6.534	624	629	637	rVB2	94640	152428	1.39%	0.263%
3	7.004	703	709	719	rVB2	172144	322067	2.93%	0.556%
4	7.233	743	748	754	rBV5	74640	145010	1.32%	0.250%
5	7.309	754	761	769	rVB	1020898	1816034	16.53%	3.136%
6	7.497	784	793	805	rBV6	136802	345372	3.14%	0.596%
7	7.685	814	825	833	rBV	1977639	3488961	31.76%	6.026%
8	8.155	896	905	910	rBV3	423056	897944	8.17%	1.551%
9	8.202	910	913	919	rVB2	132158	198169	1.80%	0.342%
10	8.478	953	960	966	rBV	1456406	2500760	22.76%	4.319%
11	8.525	966	968	975	rVB	89022	131627	1.20%	0.227%
12	8.684	990	995	1001	rBV	87775	165992	1.51%	0.287%
13	8.802	1010	1015	1022	rVB	70077	126528	1.15%	0.219%
14	9.325	1097	1104	1111	rBV	1534963	2842714	25.87%	4.909%
15	9.554	1135	1143	1147	rBV8	50856	120207	1.09%	0.208%
16	10.271	1259	1265	1269	rBV2	90905	171254	1.56%	0.296%
17	10.735	1338	1344	1352	rBV6	72623	195497	1.78%	0.338%
18	10.981	1377	1386	1397	rBV	612688	1163779	10.59%	2.010%
19	11.634	1489	1497	1504	rBV4	74484	174637	1.59%	0.302%
20	11.745	1511	1516	1523	rVB3	83974	165397	1.51%	0.286%
21	11.869	1530	1537	1542	rBV2	134948	272470	2.48%	0.471%
22	12.932	1711	1718	1722	rBV8	89129	185012	1.68%	0.320%
23	13.067	1735	1741	1747	rBV9	91083	209238	1.90%	0.361%
24	13.208	1761	1765	1768	rBV2	91985	141627	1.29%	0.245%
25	13.420	1794	1801	1807	rVB	4178203	6651833	60.55%	11.488%
26	13.531	1815	1820	1826	rBV3	109005	180697	1.64%	0.312%
27	13.896	1878	1882	1889	rBV10	76420	177238	1.61%	0.306%
28	14.166	1925	1928	1934	rVB	102166	159049	1.45%	0.275%
29	14.236	1936	1940	1944	rBV	112608	161729	1.47%	0.279%
30	14.313	1948	1953	1957	rVB5	57792	110192	1.00%	0.190%
31	14.436	1970	1974	1978	rVB2	134943	193628	1.76%	0.334%
32	14.795	2024	2035	2044	rBV4	1237988	3115801	28.36%	5.381%
33	15.188	2099	2102	2106	rVB6	80046	117509	1.07%	0.203%
34	16.293	2284	2290	2300	rVB	4541263	7098371	64.61%	12.259%

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

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-BG070816.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	16.563	2332	2336	2342	rVB	258324	375093	3.41%	0.648%
36	17.139	2430	2434	2438	rBV6	83593	154148	1.40%	0.266%
37	17.204	2441	2445	2449	rVB2	319334	444697	4.05%	0.768%
38	17.556	2499	2505	2510	rBV	1517792	2347880	21.37%	4.055%
39	17.967	2572	2575	2580	rVB2	144241	196801	1.79%	0.340%
40	18.114	2596	2600	2603	rBV6	146436	208740	1.90%	0.361%
41	18.185	2609	2612	2614	rBV4	90295	116499	1.06%	0.201%
42	18.432	2649	2654	2663	rBV2	434076	814912	7.42%	1.407%
43	19.360	2808	2812	2817	rVB3	193278	288500	2.63%	0.498%
44	19.689	2865	2868	2878	rVB4	262697	435761	3.97%	0.753%
45	20.153	2941	2947	2954	rBV	8307118	10986490	100.00%	18.974%
46	21.845	3228	3235	3242	rBV2	1671796	2904718	26.44%	5.017%
47	25.194	3796	3805	3818	rVB2	895671	2798140	25.47%	4.833%

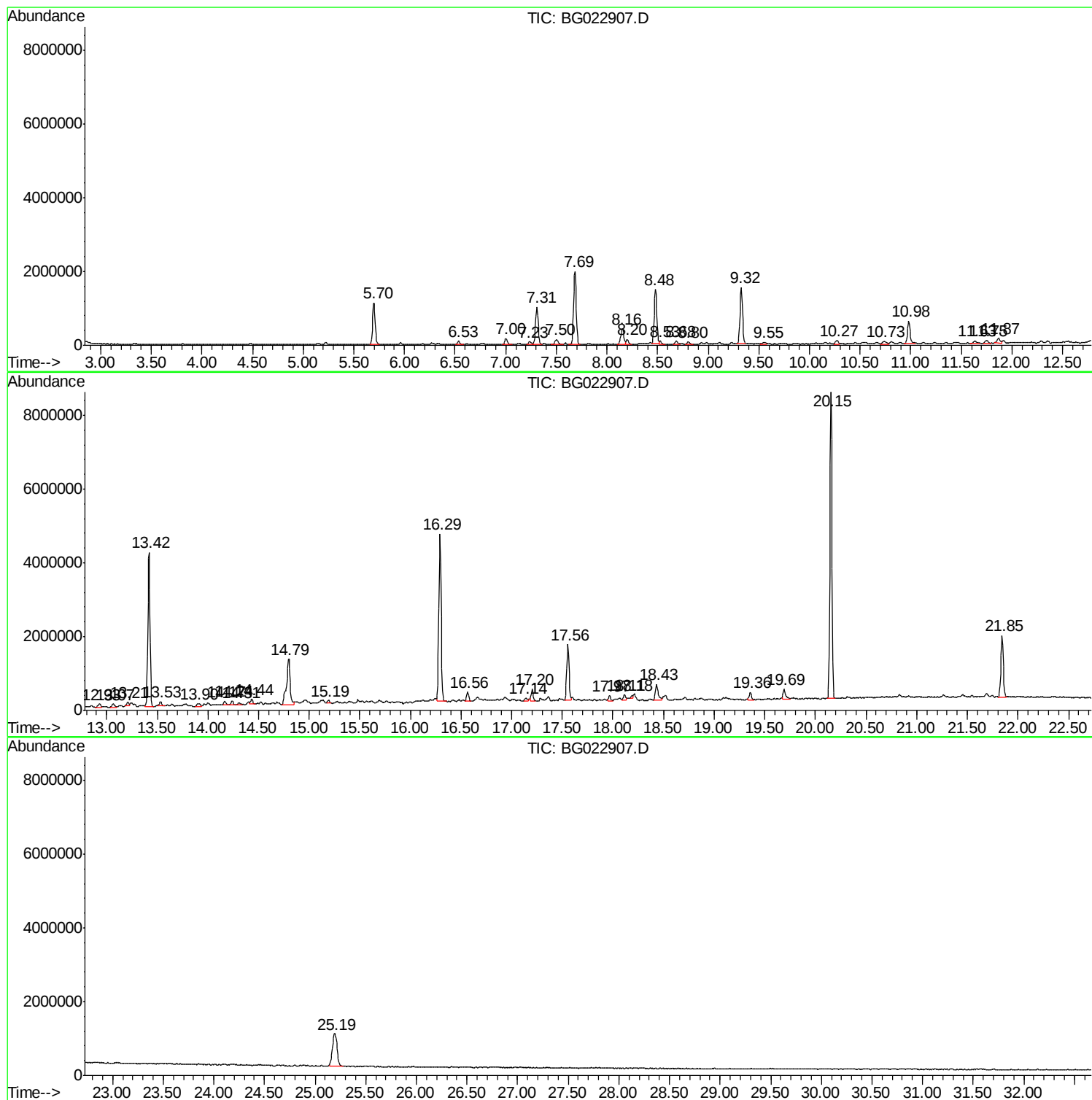
Sum of corrected areas: 57902519

Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.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 G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

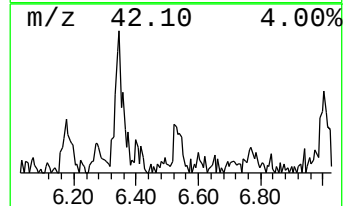
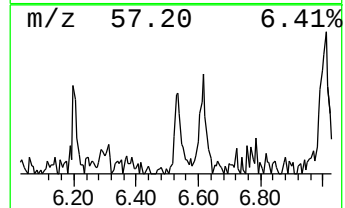
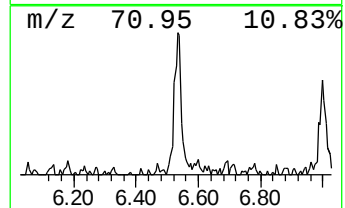
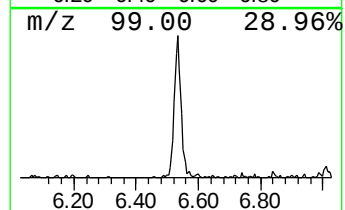
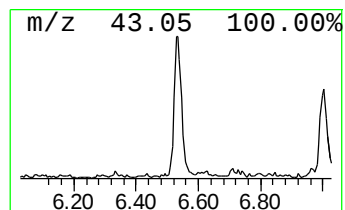
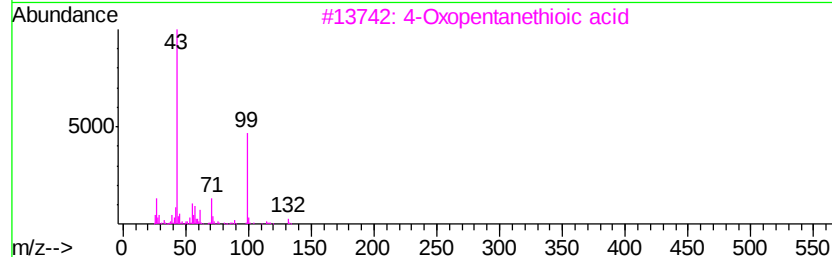
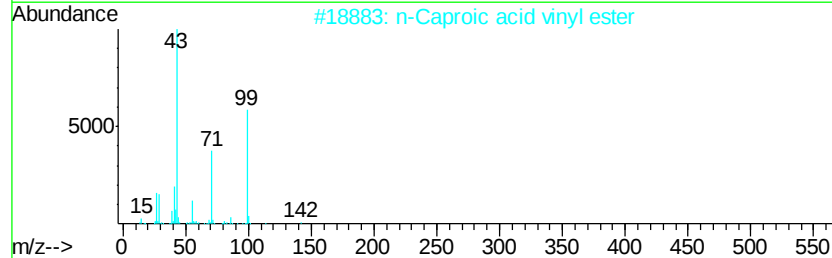
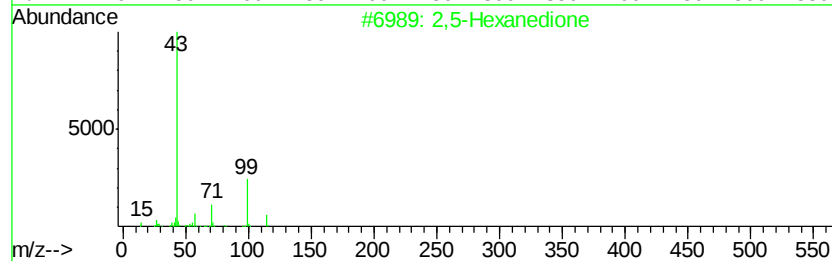
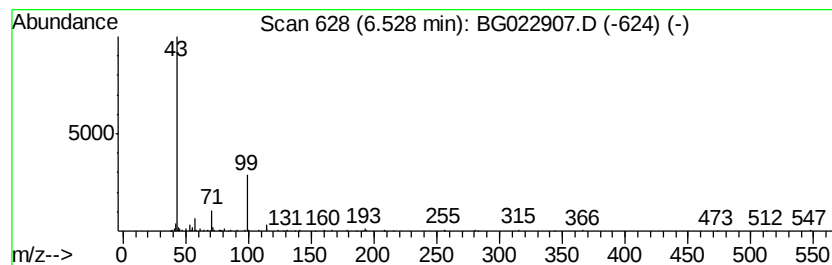
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2,5-Hexanedione Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.53	3.40 ng	152428	1,4-Dichlorobenzene-d4	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2,5-Hexanedione	114	C6H10O2	000110-13-4	59
2			n-Caproic acid vinyl ester	142	C8H14O2	003050-69-9	38
3			4-Oxopentanethioic acid	132	C5H8O2S	1000193-80-6	28
4			3,6-Heptanedione	128	C7H12O2	001703-51-1	28
5			2,3-Octanedione	142	C8H14O2	000585-25-1	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

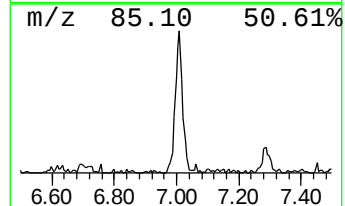
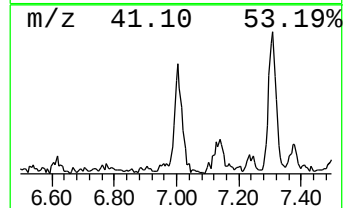
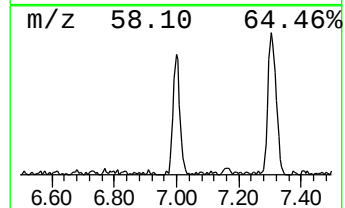
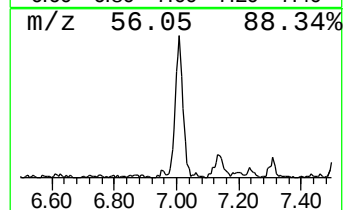
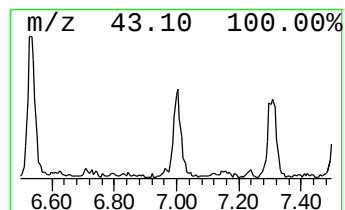
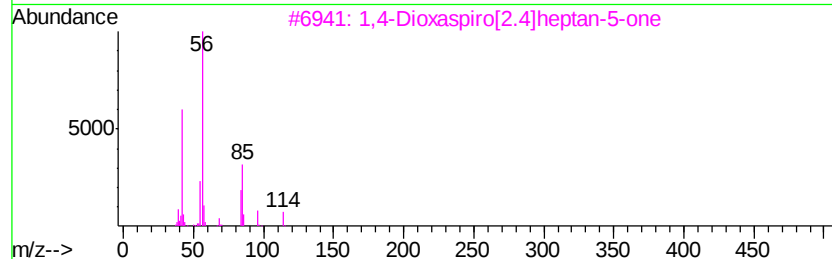
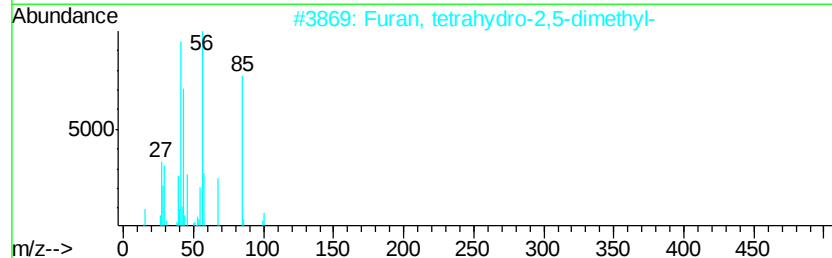
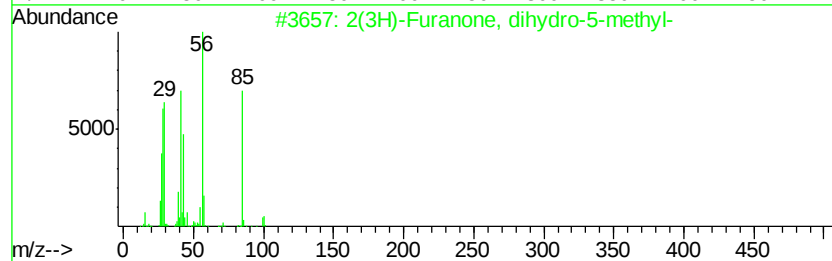
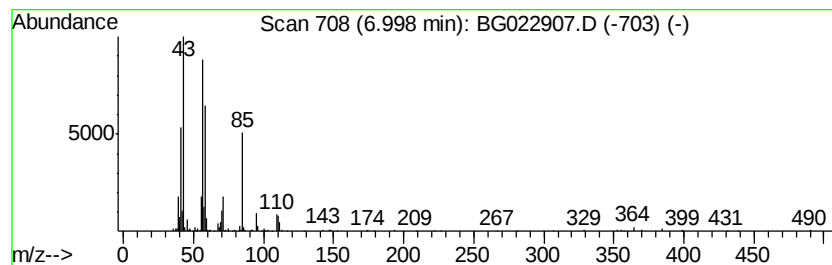
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.00 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.00	7.17 ng	322067	1,4-Dichlorobenzene-d4	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2	(3H)-Furanone, dihydro-5-methyl-	100	C5H8O2	000108-29-2	49	
2		Furan, tetrahydro-2,5-dimethyl-	100	C6H12O	001003-38-9	47	
3	1,4-Dioxaspiro[2.4]heptan-5-one	114	C5H6O3	126091-78-9	47		
4	2H-Pyran, tetrahydro-2-[(2-nitro...	259	C13H25NO4	096039-96-2	47		
5	Furan, tetrahydro-2,5-dimethyl-,...	100	C6H12O	038484-59-2	38		



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

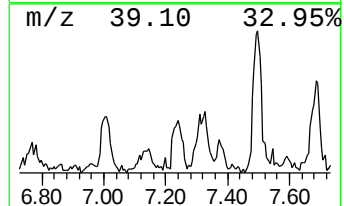
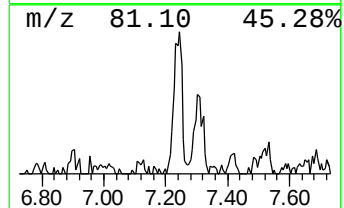
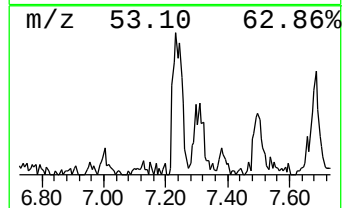
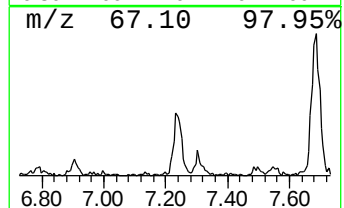
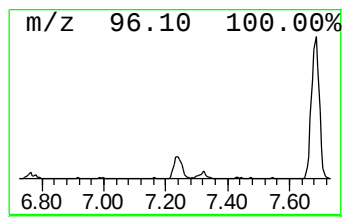
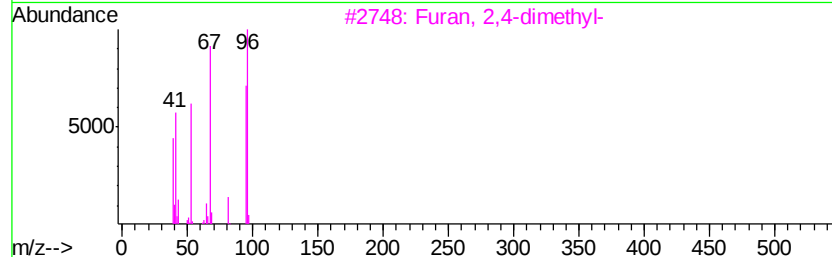
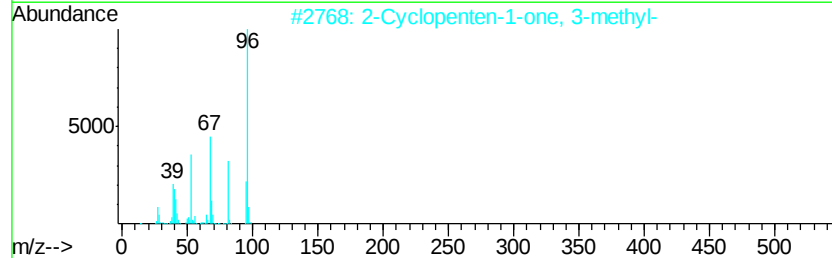
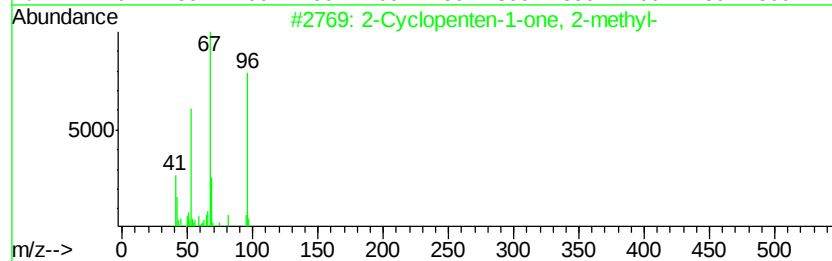
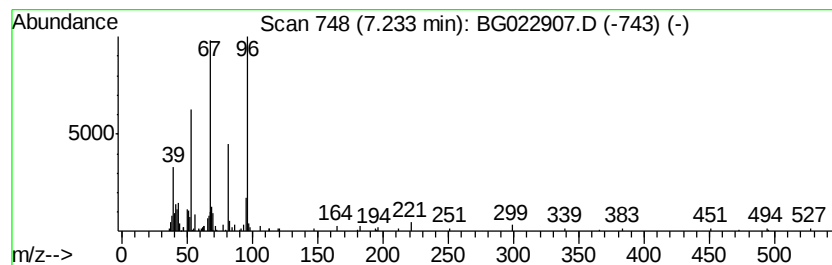
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Cyclopenten-1-one, 2-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.23	3.23 ng	145010	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclopenten-1-one, 2-methyl-	96	C6H8O	001120-73-6	91
2		2-Cyclopenten-1-one, 3-methyl-	96	C6H8O	002758-18-1	90
3		Furan, 2,4-dimethyl-	96	C6H8O	003710-43-8	78
4		Bicyclo[2.1.0]pentane	68	C5H8	000185-94-4	62
5		Cyclopentene	68	C5H8	000142-29-0	62



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

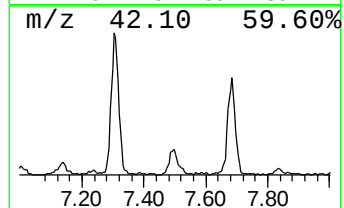
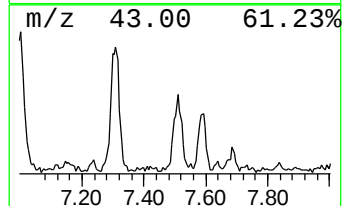
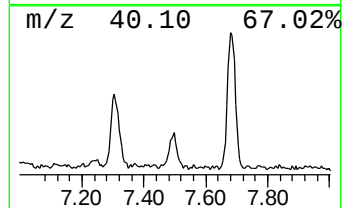
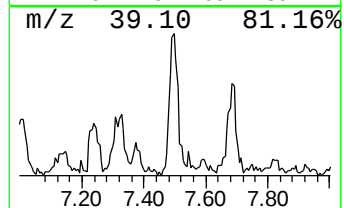
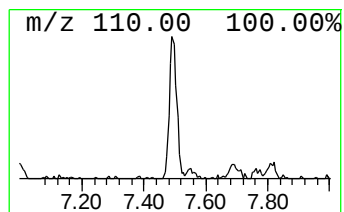
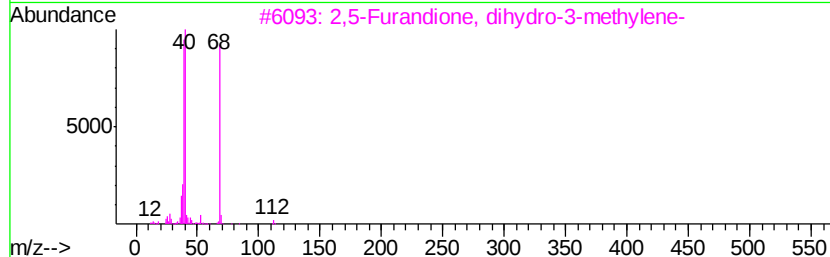
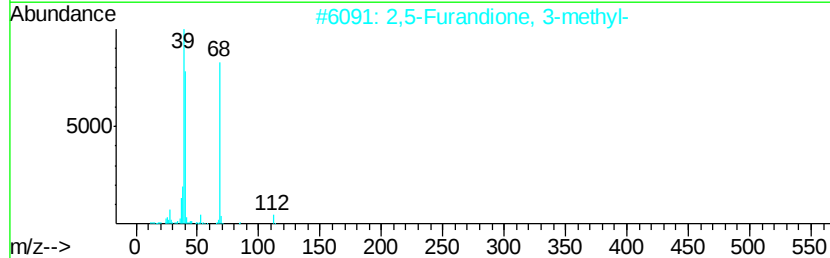
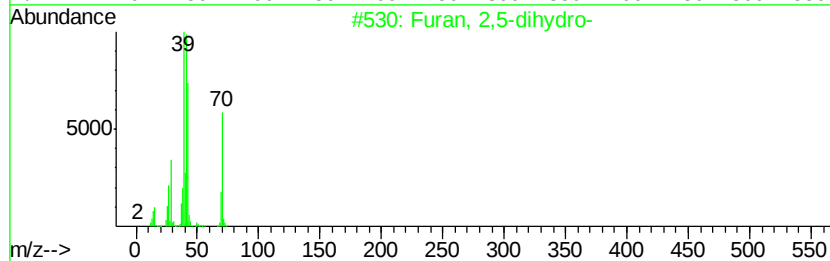
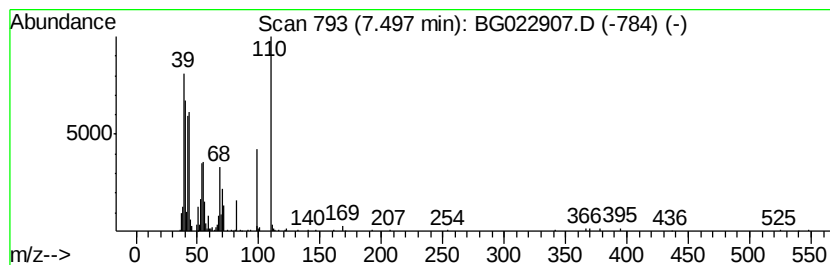
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Furan, 2,5-dihydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.50	7.69 ng	345372	1,4-Dichlorobenzene-d4	8.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan, 2,5-dihydro-	70	C4H6O	001708-29-8	59	
2	2,5-Furandione, 3-methyl-	112	C5H4O3	000616-02-4	50	
3	2,5-Furandione, dihydro-3-methyl...	112	C5H4O3	002170-03-8	50	
4	Bis(3-methylbutyl) fluorene-2,7-...	466	C23H30O6S2	253664-95-8	42	
5	2-Thiophenesulfonyl chloride	182	C4H3ClO2S2	016629-19-9	42	



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

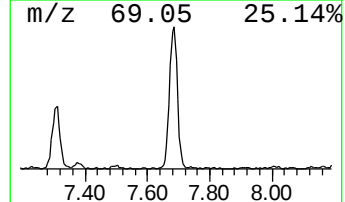
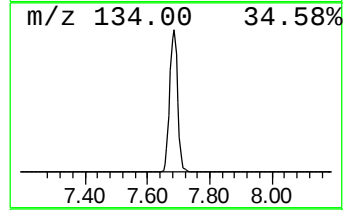
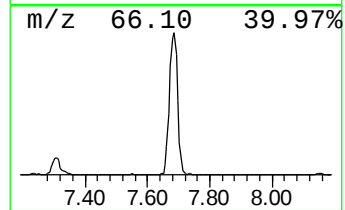
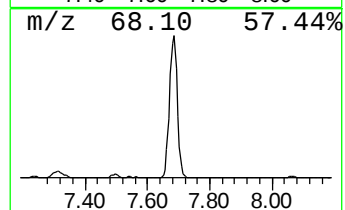
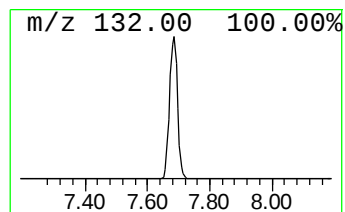
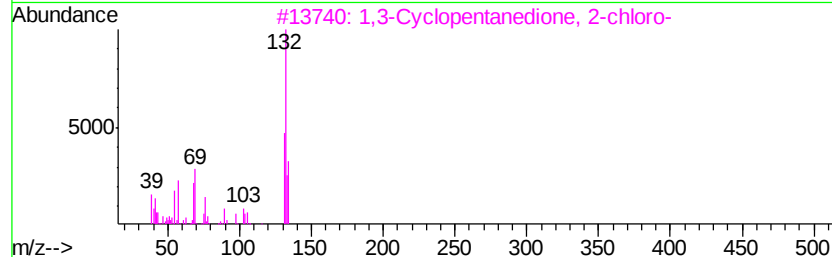
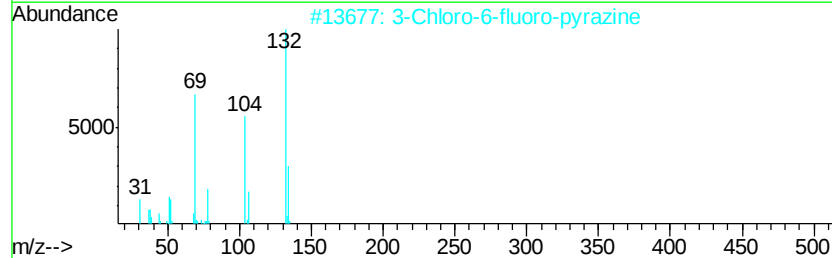
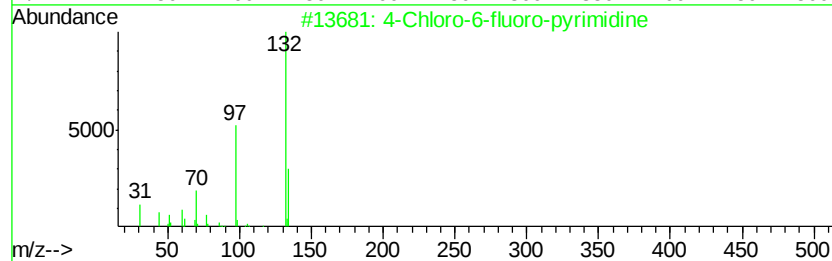
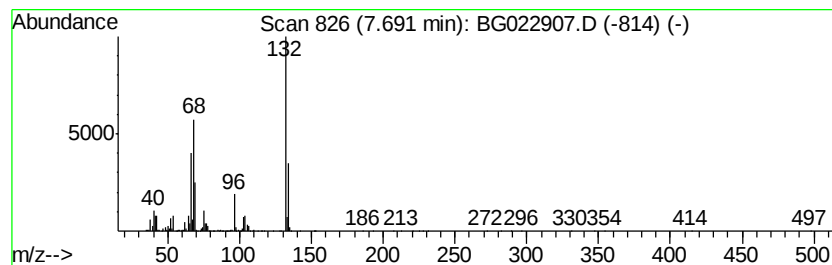
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.69 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.69	77.71 ng	3488960	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12
4		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

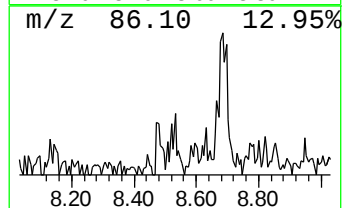
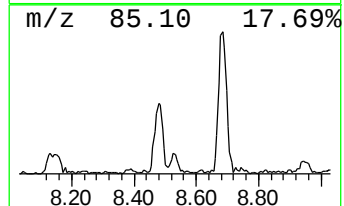
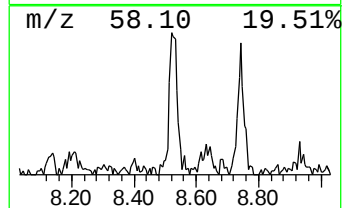
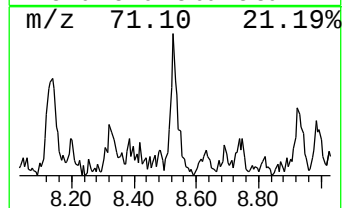
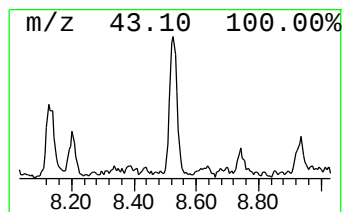
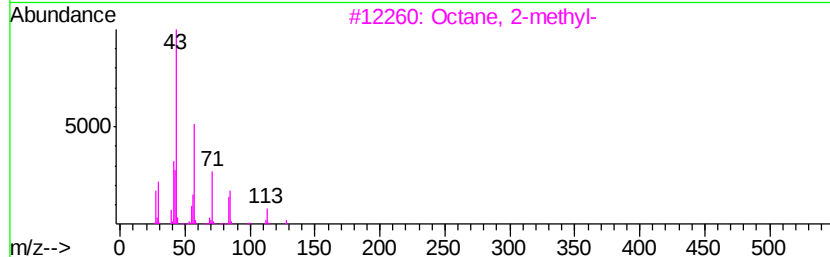
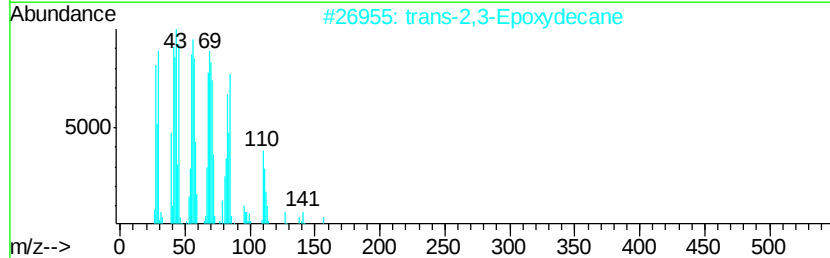
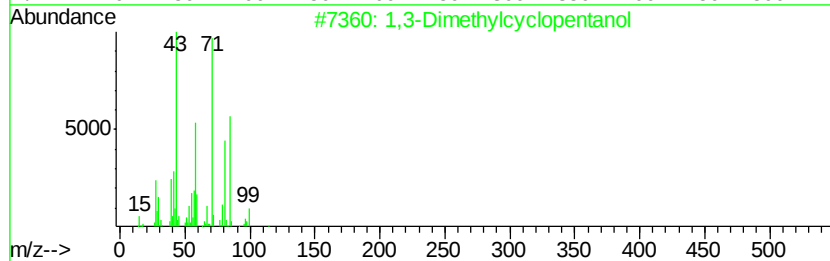
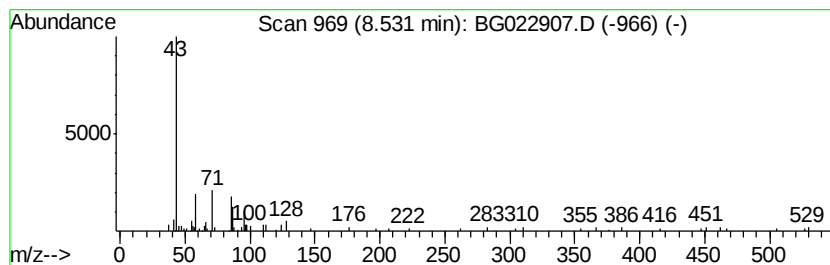
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown8.53 Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.53	2.93 ng	131627	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dimethylcyclopentanol	114	C7H14O	019550-46-0	38
2		trans-2,3-Epoxydecane	156	C10H20O	054125-39-2	38
3		Octane, 2-methyl-	128	C9H20	003221-61-2	38
4		Nonane, 1-iodo-	254	C9H19I	004282-42-2	32
5		Ether, 3-butenyl pentyl	142	C9H18O	034061-78-4	23



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

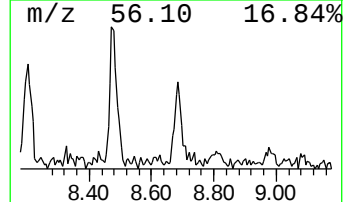
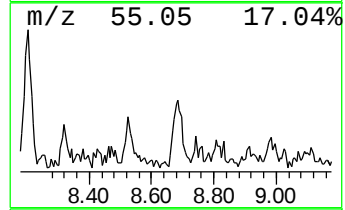
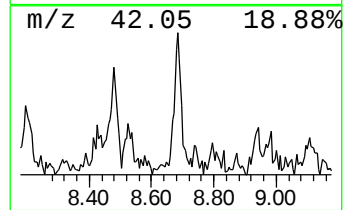
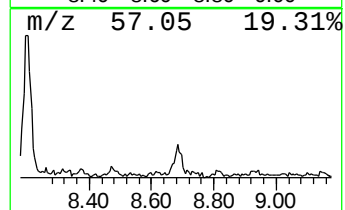
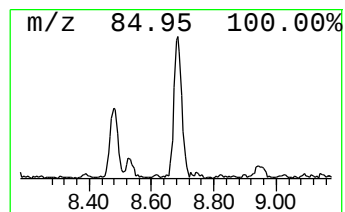
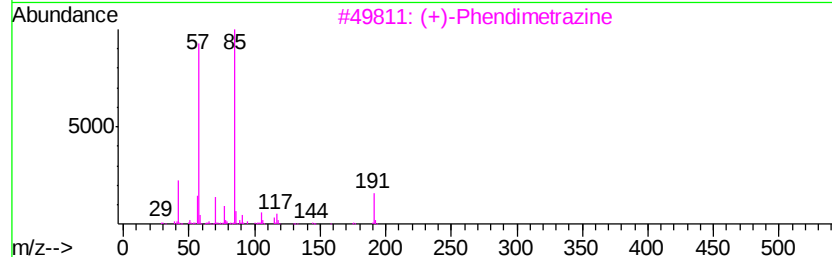
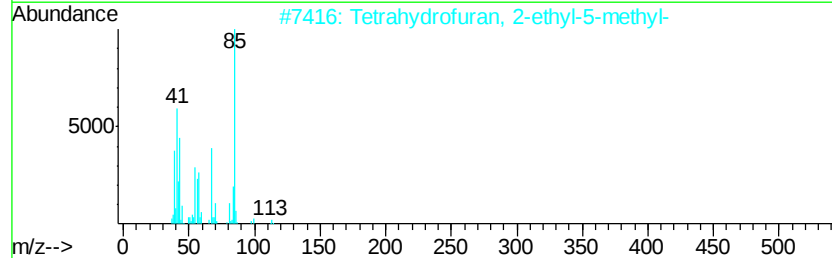
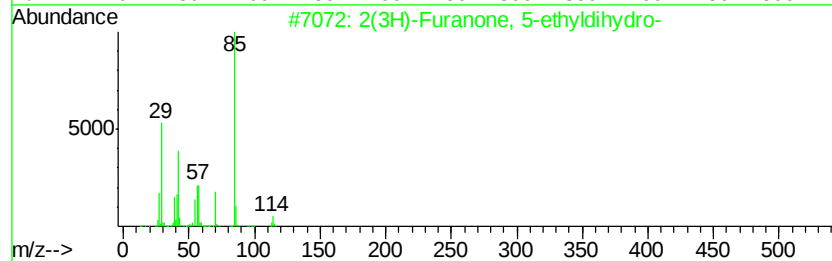
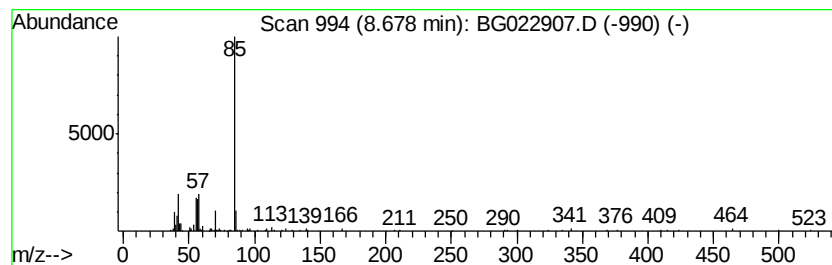
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 2(3H)-Furanone, 5-ethylidihy... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	3.70 ng	165992	1,4-Dichlorobenzene-d4	8.16

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2(3H)-Furanone, 5-ethylidihydro-	114	C6H10O2	000695-06-7	78
2		Tetrahydrofuran, 2-ethyl-5-methyl-	114	C7H14O	000931-39-5	72
3		(+)-Phendimetrazine	191	C12H17NO	000634-03-7	43
4		Pentanal, 5-[1(tetrahydro-2H-pyran-5-ylidene)-1-oxo-5-oxo-1,5-dihydro-2H-pyran-5-ylidene]-	186	C10H18O3	014194-86-6	36
5		5,6-Epoxyhexanol-1	116	C6H12O2	021915-57-1	33



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

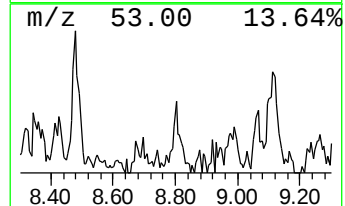
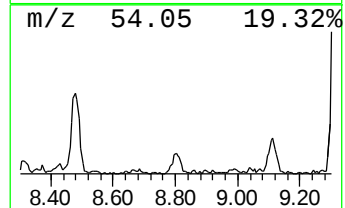
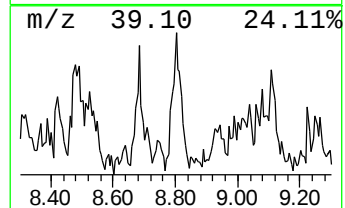
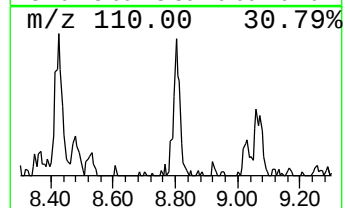
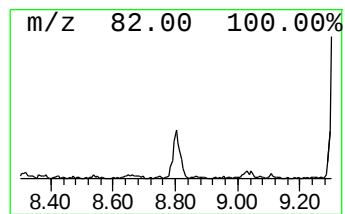
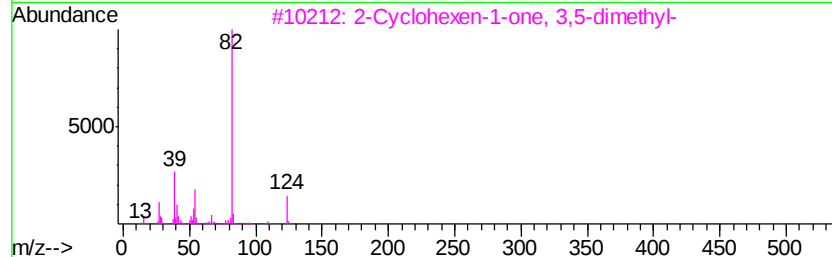
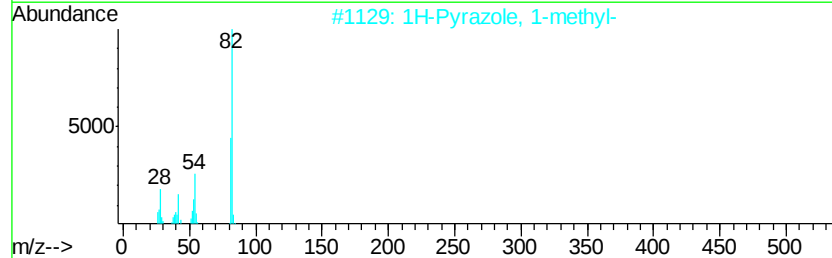
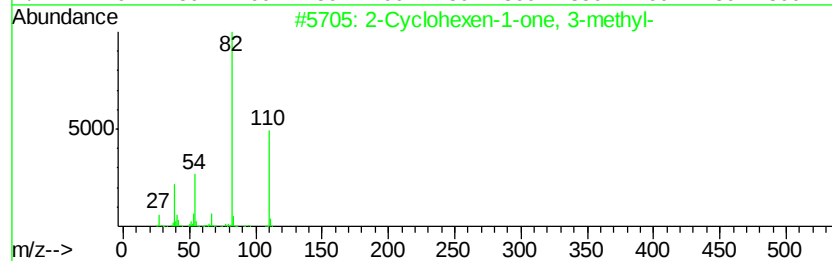
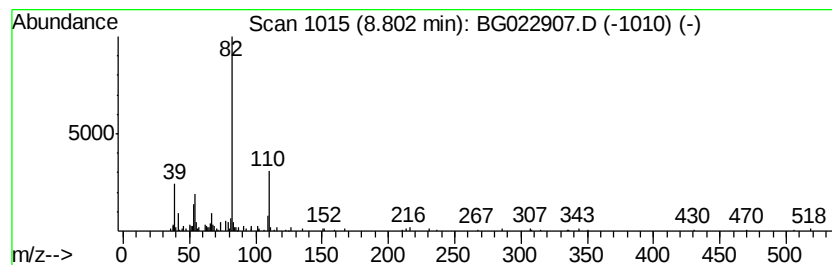
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 2-Cyclohexen-1-one, 3-methyl- Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.80	2.82 ng	126528	1,4-Dichlorobenzene-d4	8.16

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 3-methyl-	110	C7H10O	001193-18-6	72
2		1H-Pyrazole, 1-methyl-	82	C4H6N2	000930-36-9	58
3		2-Cyclohexen-1-one, 3,5-dimethyl-	124	C8H12O	001123-09-7	53
4		Ethylphosphonic acid	110	C2H7O3P	006779-09-5	53
5		Betazole	111	C5H9N3	000105-20-4	47



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

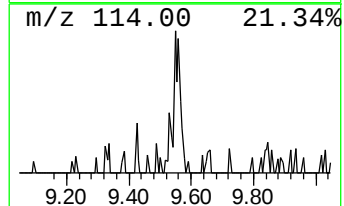
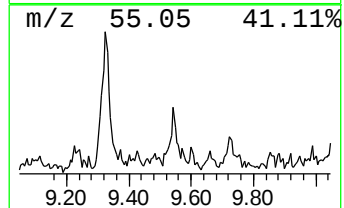
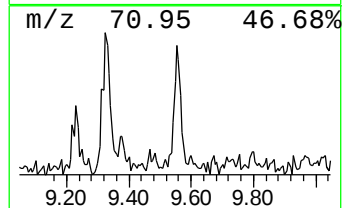
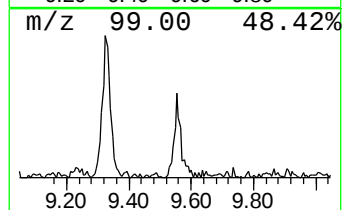
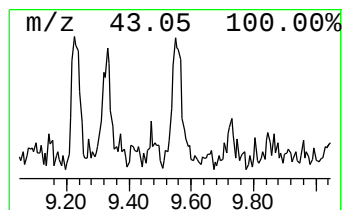
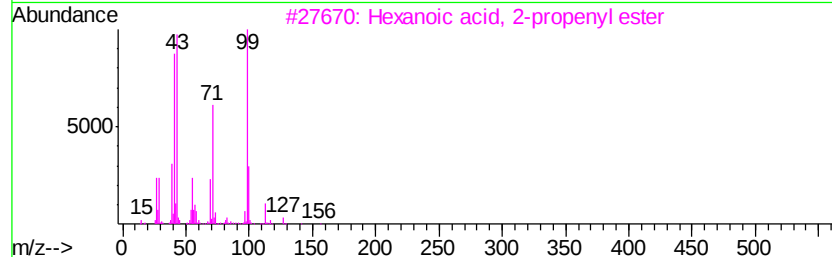
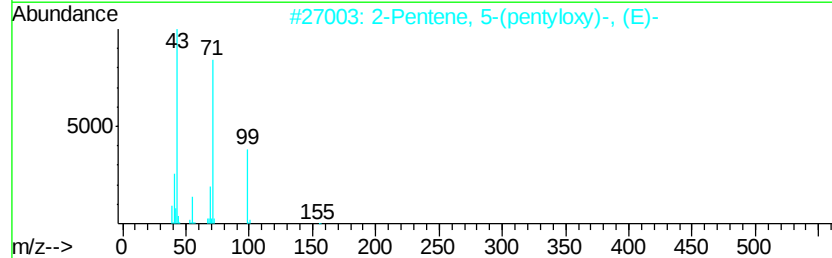
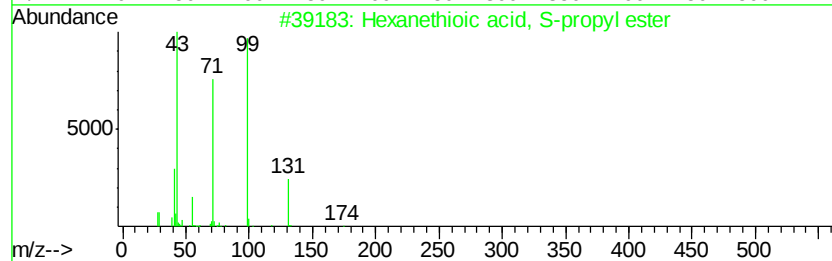
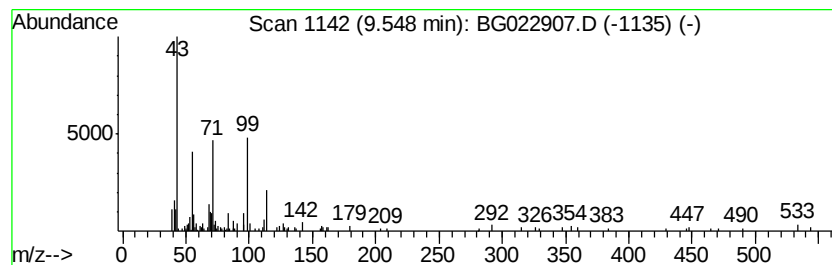
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Hexanethioic acid, S-propyl... Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.55	2.68 ng	120207	1,4-Dichlorobenzene-d4	8.16

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexanethioic acid, S-propyl ester	174	C9H18OS	002432-78-2	59
2			2-Pentene, 5-(pentyl oxy)-, (E)-	156	C10H20O	056052-85-8	59
3			Hexanoic acid, 2-propenyl ester	156	C9H16O2	000123-68-2	45
4			Hexanethioic acid, S-ethyl ester	160	C8H16OS	002450-12-6	45
5			Hexanoic acid, thio-, S-butyl ester	188	C10H20OS	002432-79-3	45



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

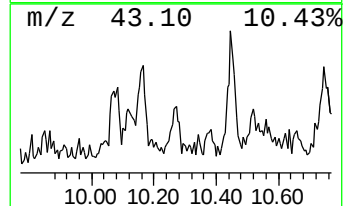
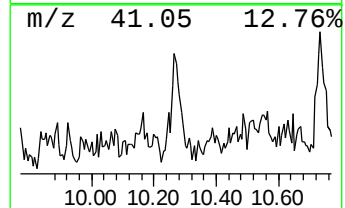
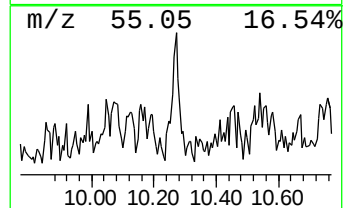
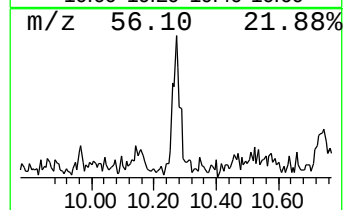
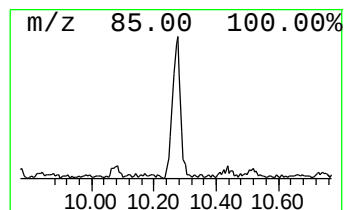
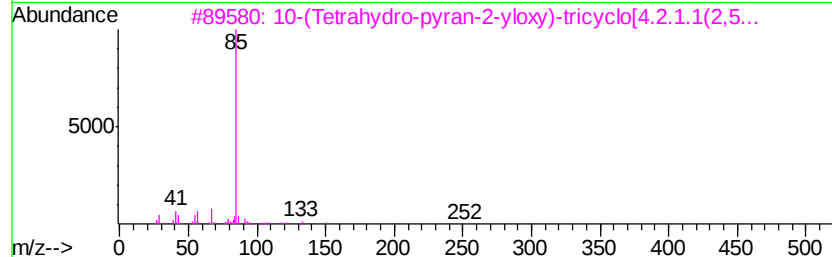
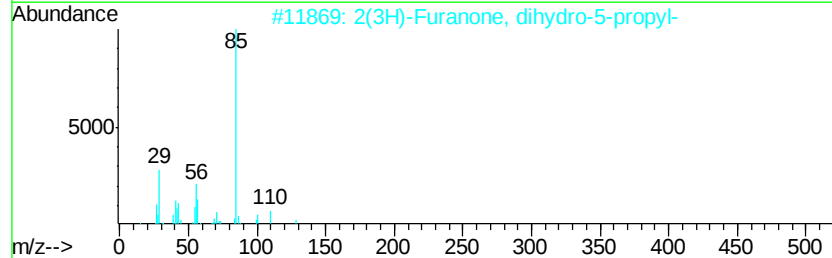
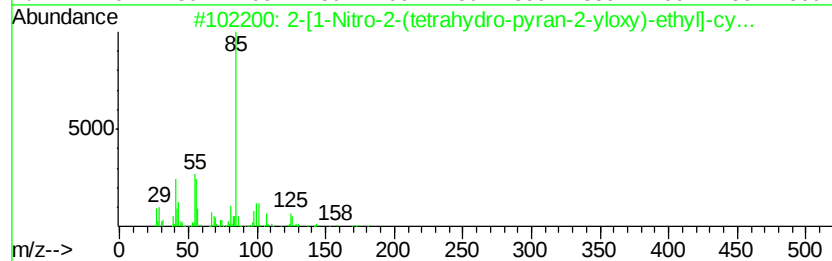
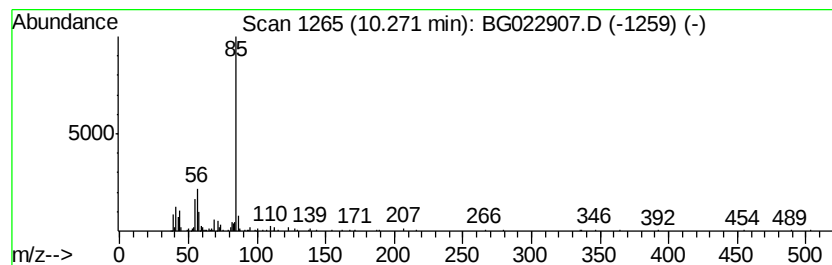
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 2-[1-Nitro-2-(tetrahydro-py... Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.27	2.94 ng	171254	Naphthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-[1-Nitro-2-(tetrahydro-pyran-2-yl)-ethyl]-cyano...	273	C13H23N05	1000190-43-2	64
2		2(3H)-Furanone, dihydro-5-propyl-	128	C7H12O2	000105-21-5	64
3		10-(Tetrahydro-pyran-2-yl)-tricyclo[4.2.1.1(2,5)]hept-2-ene	252	C15H24O3	1000192-28-8	59
4		1-Bromo-7-(tetrahydro-2-pyran-2-yl)-1,2,3,4-tetrahydro-1H-benzodioxole	278	C12H23BrO2	010160-25-5	56
5		3,3,6-Trimethyl-1,5-heptadien-4-ol	154	C10H18O	057590-19-9	52



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

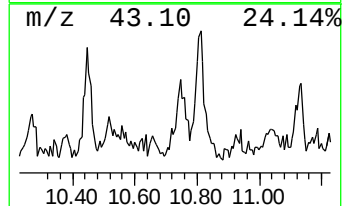
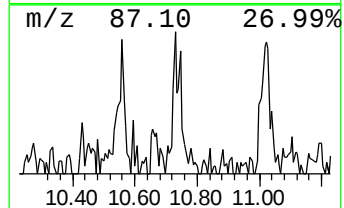
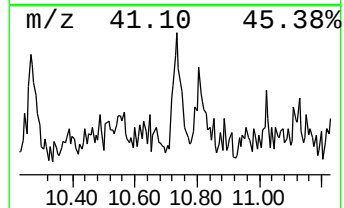
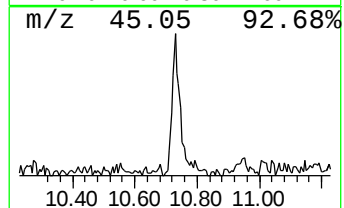
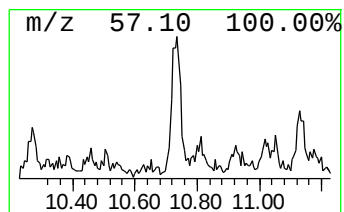
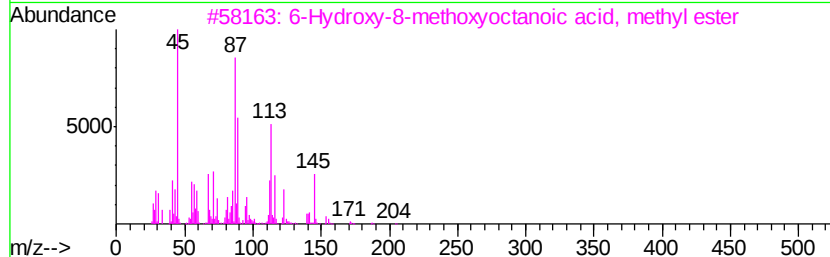
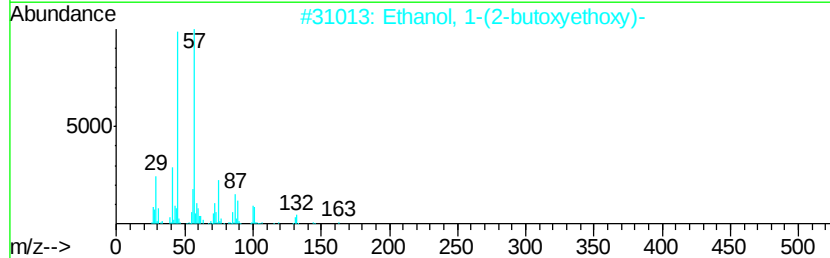
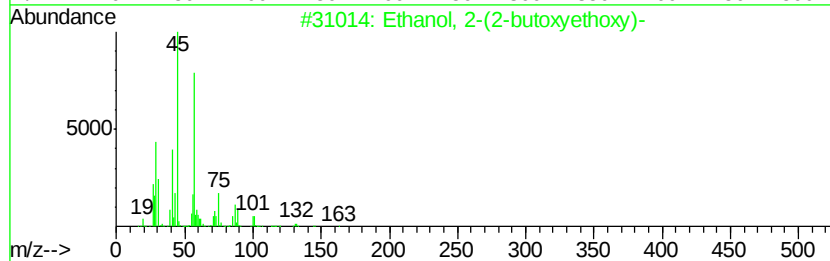
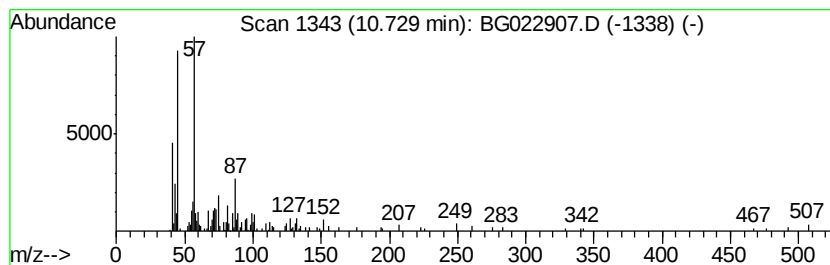
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown10.73 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.73	3.36 ng	195497	Naphthalene-d8	10.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-butoxyethoxy)-	162	C8H18O3	000112-34-5	40
2			Ethanol, 1-(2-butoxyethoxy)-	162	C8H18O3	054446-78-5	37
3			6-Hydroxy-8-methoxyoctanoic acid...	204	C10H20O4	1000197-85-9	32
4			N-Methoxy-2-carbomethoxyvaziridine	131	C5H9NO3	053084-30-3	27
5			Ethylene glycol diglycidyl ether	174	C8H14O4	002224-15-9	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

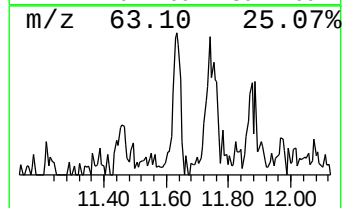
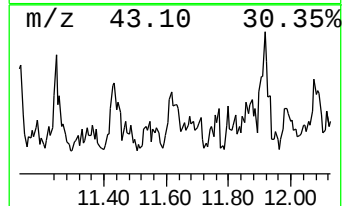
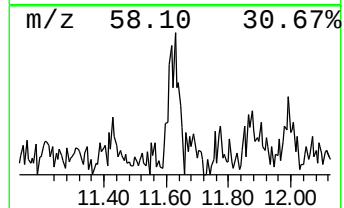
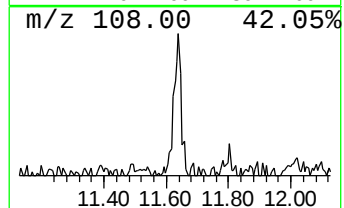
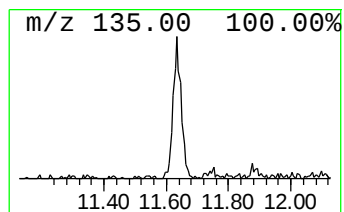
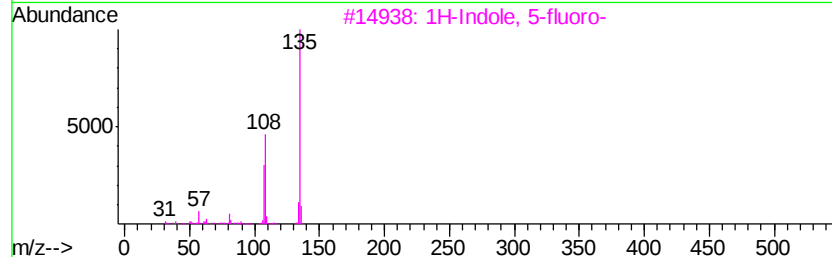
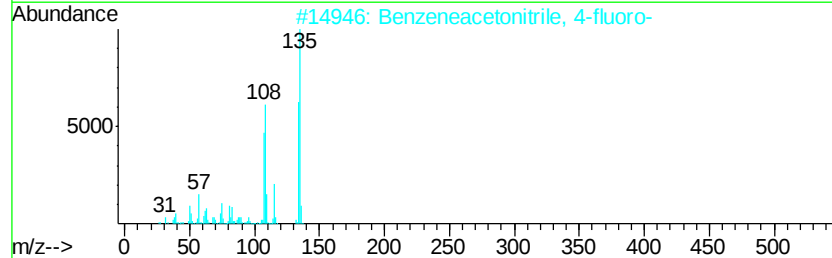
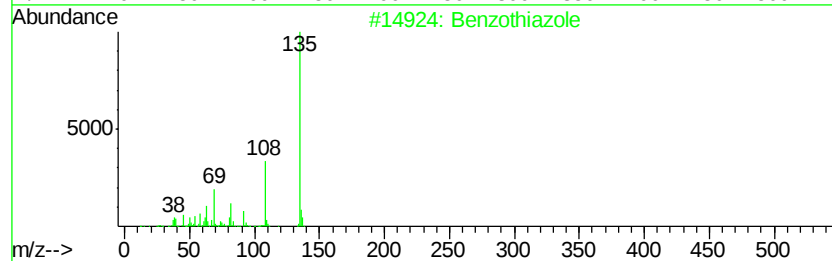
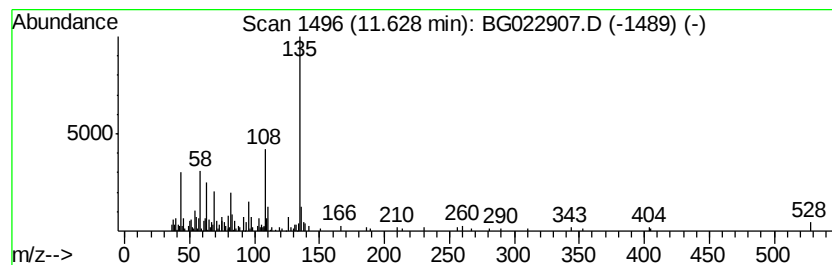
Instrument :
BNA_G
ClientSampleId :
MW-1

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 Benzothiazole Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.63	3.00 ng	174637	Napthalene-d8	10.98	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzothiazole	135	C7H5NS	000095-16-9	78
2	Benzeneacetonitrile, 4-fluoro-	135	C8H6FN	000459-22-3	78
3	1H-Indole, 5-fluoro-	135	C8H6FN	000399-52-0	53
4	1H-Pyrazolo[3,4-d]pyrimidin-4-amine	135	C5H5N5	002380-63-4	52
5	Adenine	135	C5H5N5	000073-24-5	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

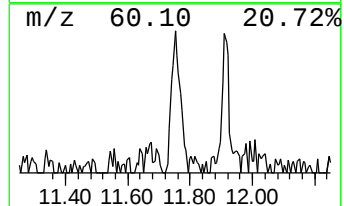
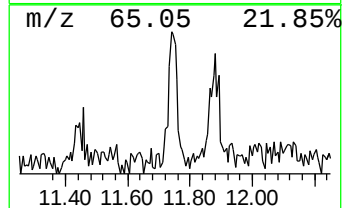
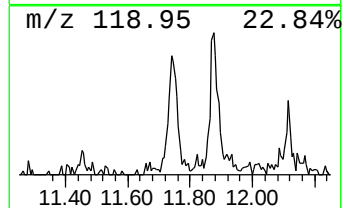
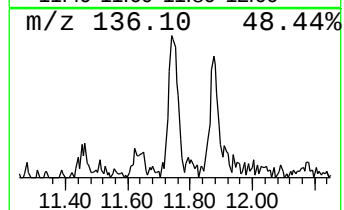
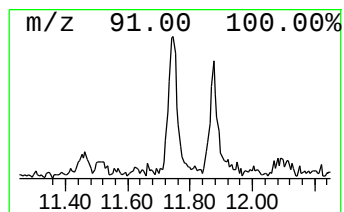
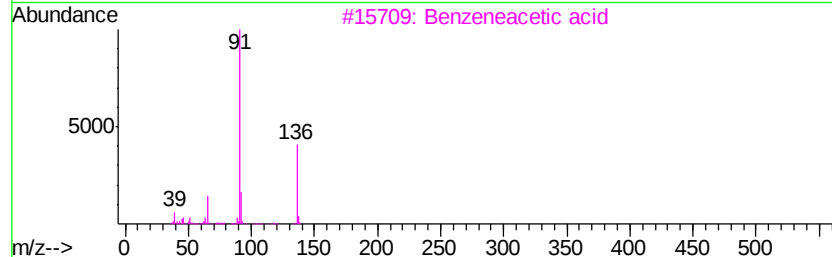
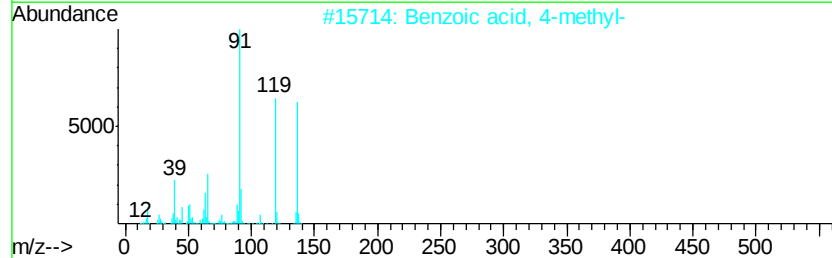
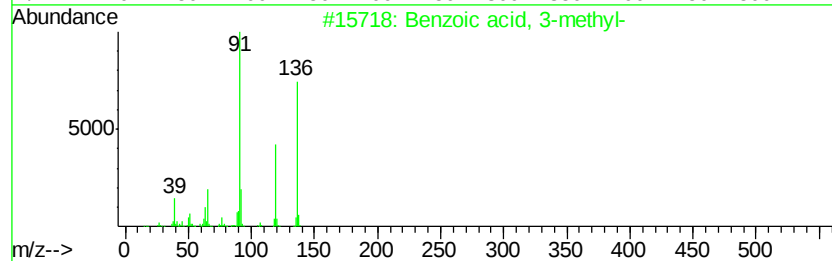
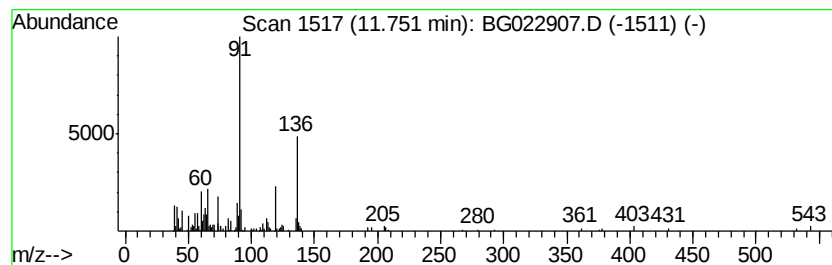
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzoic acid, 3-methyl- Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.75	2.84 ng	165397	Naphthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzoic acid, 3-methyl-	136	C8H8O2	000099-04-7	76
2		Benzoic acid, 4-methyl-	136	C8H8O2	000099-94-5	53
3		Benzeneacetic acid	136	C8H8O2	000103-82-2	52
4		p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	47
5		Bicyclo[4.2.0]octa-1,3,5-trien-7-ol	120	C8H8O	035447-99-5	43



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

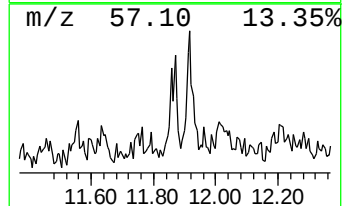
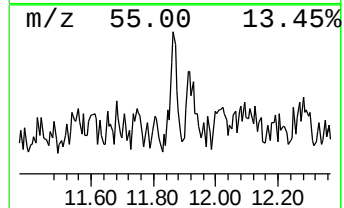
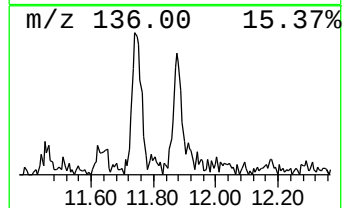
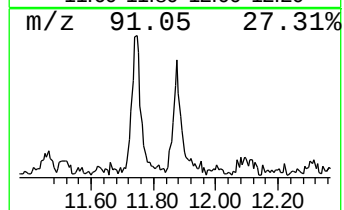
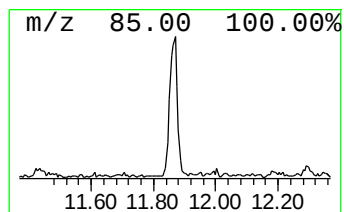
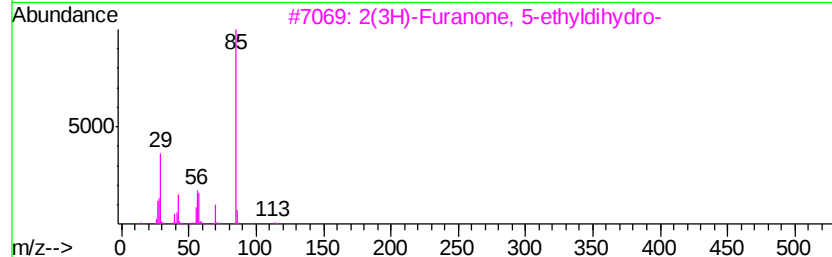
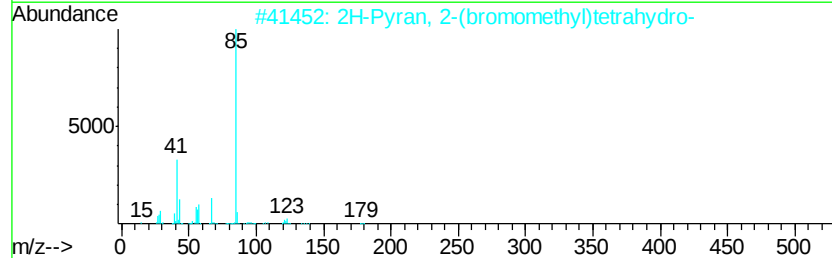
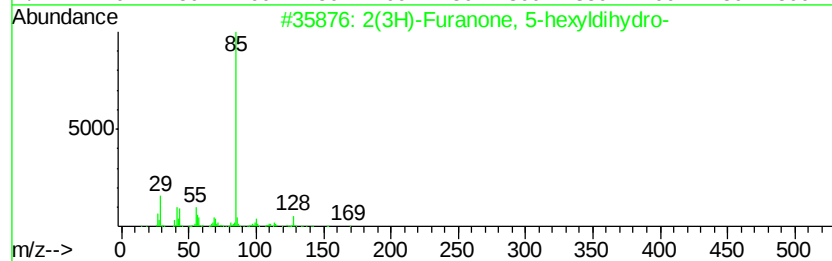
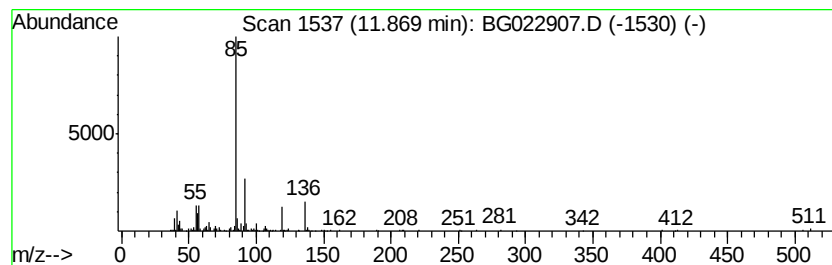
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 2(3H)-Furanone, 5-hexyldihy... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.87	4.68 ng	272470	Napthalene-d8	10.98

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2(3H)-Furanone, 5-hexvldihydro-	170	C10H18O2	000706-14-9	53
2			2H-Pyran, 2-(bromomethyl)tetrahy...	178	C6H11BrO	034723-82-5	50
3			2(3H)-Furanone, 5-ethvldihydro-	114	C6H10O2	000695-06-7	50
4			2(3H)-Furanone, dihydro-5-pentyl-	156	C9H16O2	000104-61-0	50
5			2(3H)-Furanone, 5-butyldihydro-	142	C8H14O2	000104-50-7	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

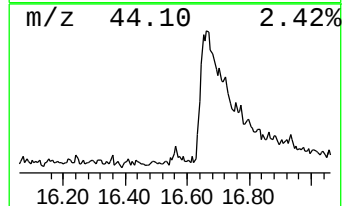
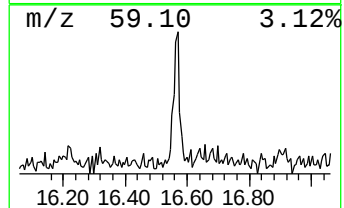
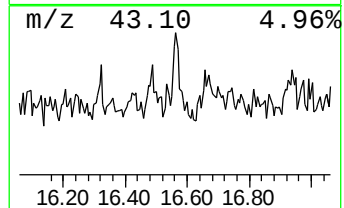
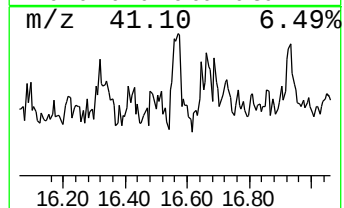
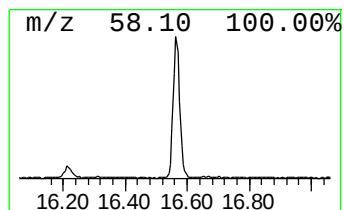
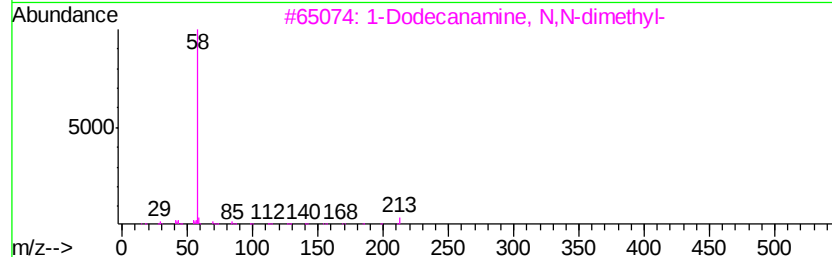
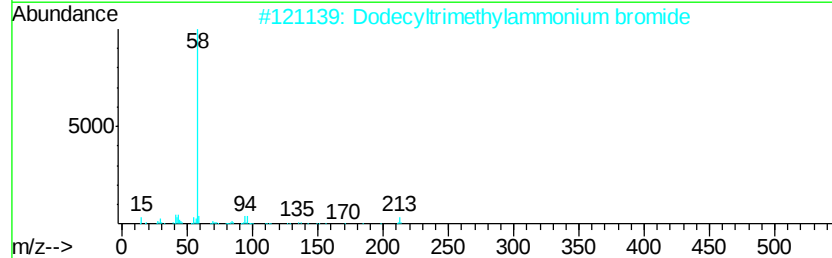
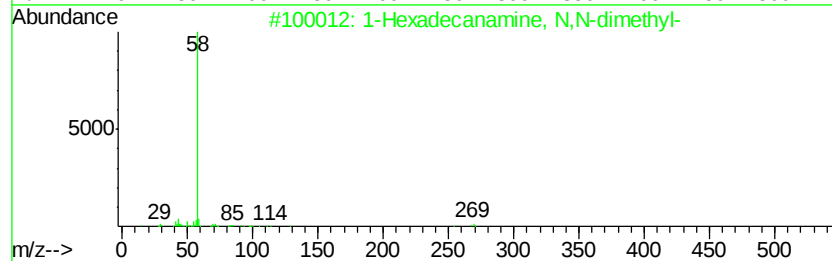
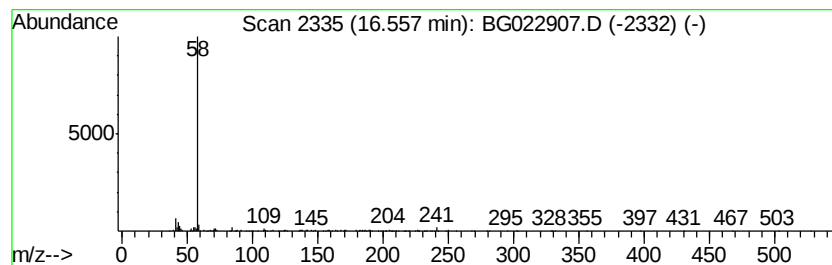
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 1-Hexadecanamine, N,N-dimet... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.56	3.20 ng	375093	Phenanthrene-d10	17.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexadecanamine, N,N-dimethyl-	269	C18H39N	000112-69-6	64
2			Dodecyltrimethylammonium bromide	307	C15H34BrN	001119-94-4	64
3			1-Dodecanamine, N,N-dimethyl-	213	C14H31N	000112-18-5	56
4			3(N,N-Dimethylmyristylammonio)pr...	363	C19H41N03S	014933-09-6	56
5			2-Butanol, 1-(dimethylamino)-	117	C6H15NO	003760-96-1	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

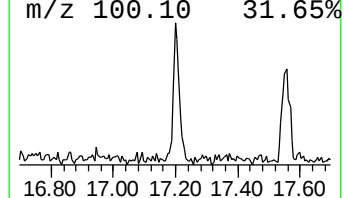
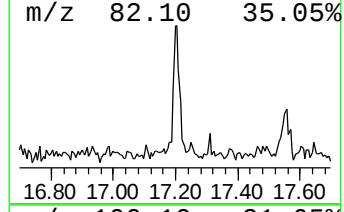
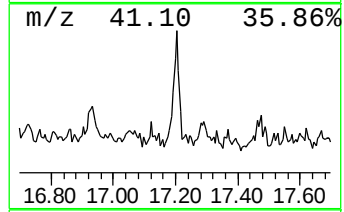
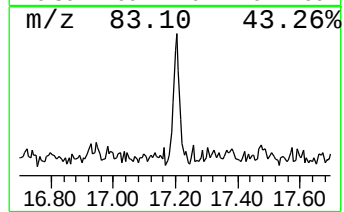
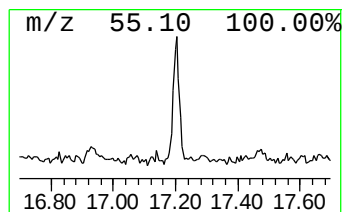
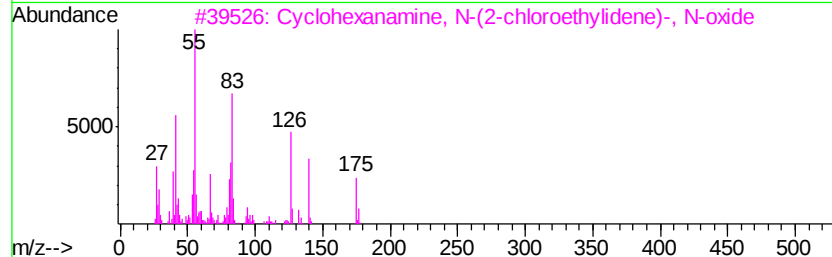
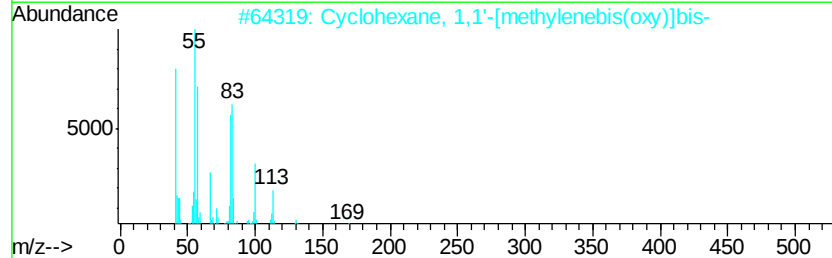
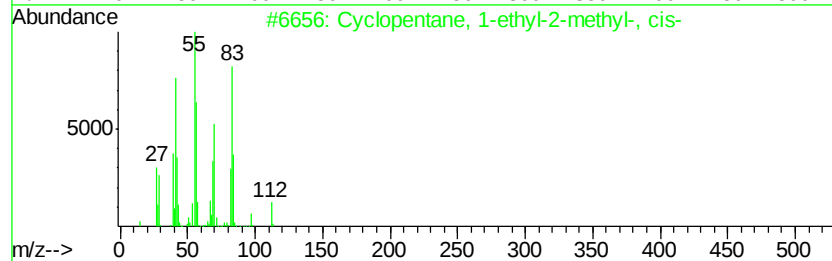
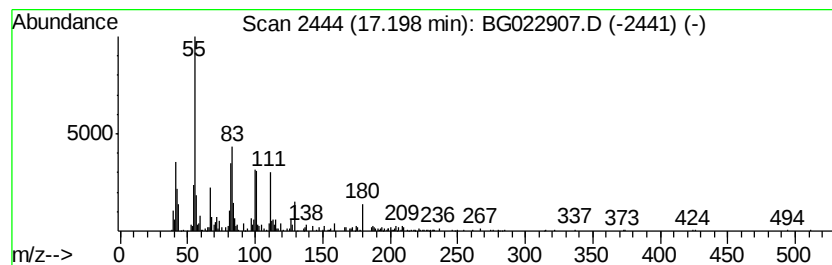
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 unknown17.20 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.20	3.79 ng	444697	Phenanthrene-d10	17.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 1-ethyl-2-methyl-,...	112	C8H16	000930-89-2	25
2			Cyclohexane, 1,1'-[methylenebis(...	212	C13H24O2	001453-21-0	25
3			Cyclohexanamine, N-(2-chloroethy...	175	C8H14ClNO	037898-41-2	22
4			Pyridine, 2,3,4,5-tetrahydro-	83	C5H9N	000505-18-0	22
5			1,4-Cyclooctanedione	140	C8H12O2	055794-45-1	16



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

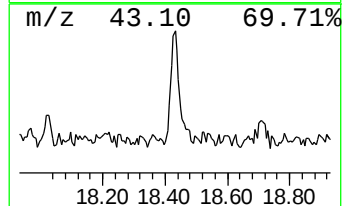
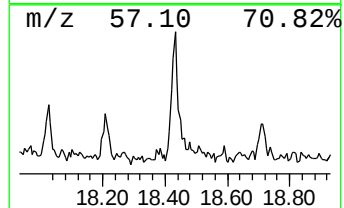
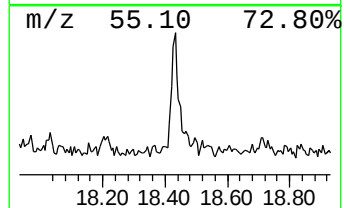
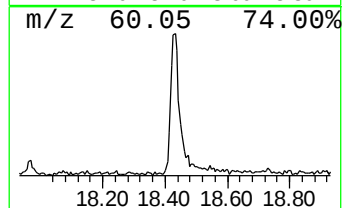
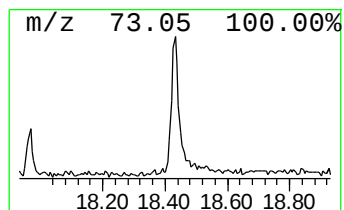
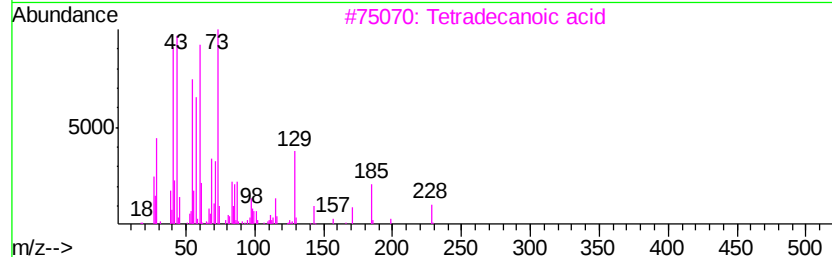
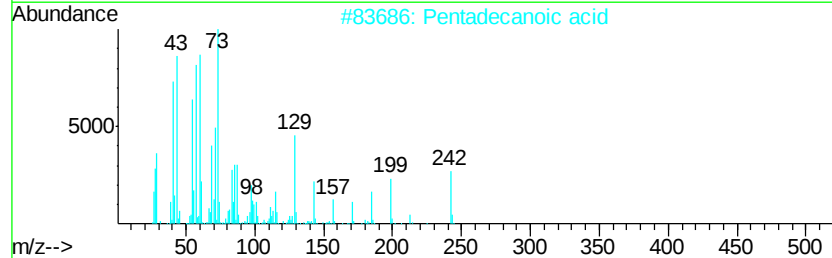
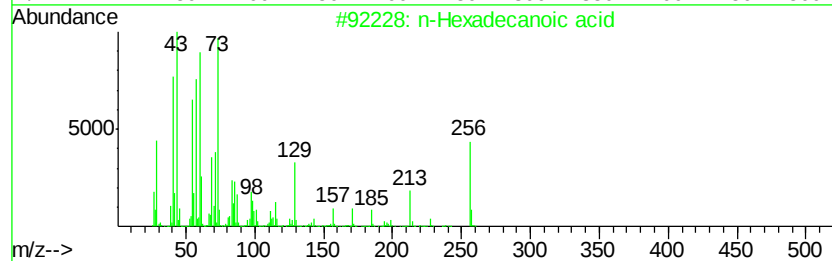
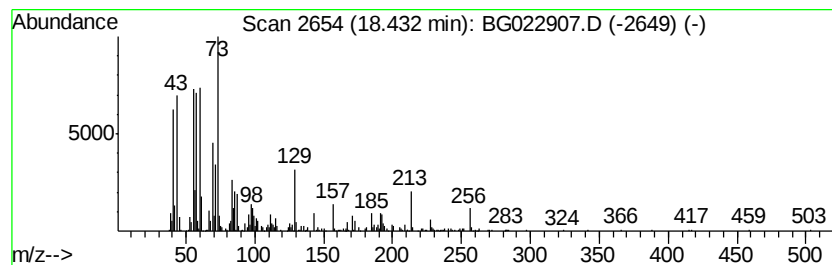
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.43	6.94 ng	814912	Phenanthrene-d10	17.56

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexadecanoic acid	256	C16H32O2	000057-10-3	97
2			Pentadecanoic acid	242	C15H30O2	001002-84-2	93
3			Tetradecanoic acid	228	C14H28O2	000544-63-8	68
4			Tridecanoic acid	214	C13H26O2	000638-53-9	64
5			Dodecanoic acid	200	C12H24O2	000143-07-7	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

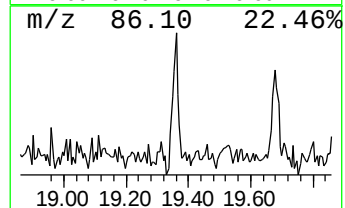
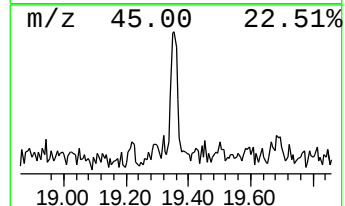
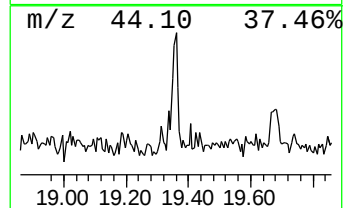
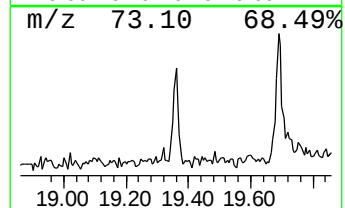
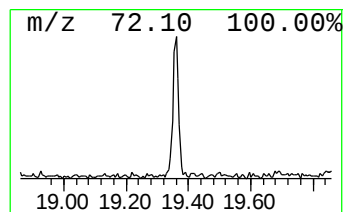
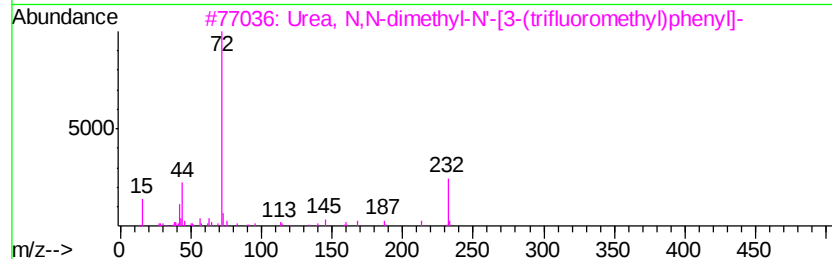
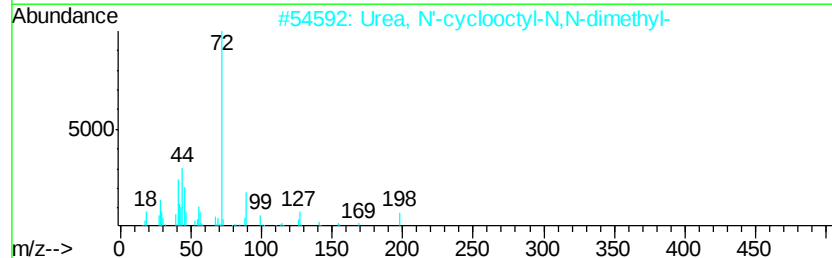
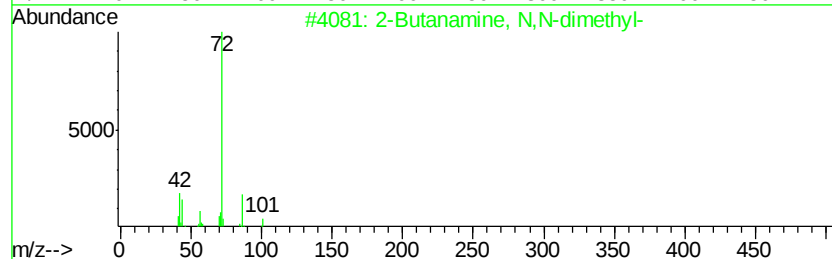
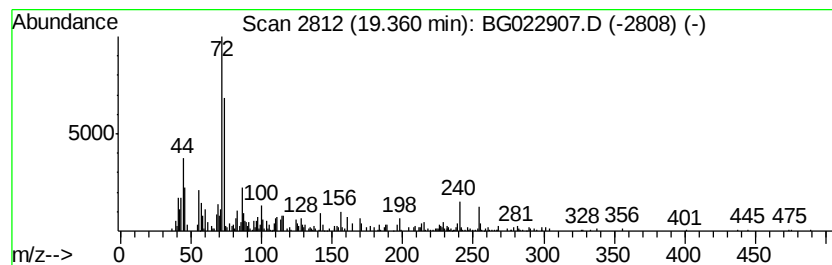
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 2-Butanamine, N,N-dimethyl- Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.36	2.46 ng	288500	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butanamine, N,N-dimethyl-	101	C6H15N	000921-04-0	50
2		Urea, N'-cyclooctyl-N,N-dimethyl-	198	C11H22N2O	002163-69-1	46
3		Urea, N,N-dimethyl-N'-[3-(triflu...	232	C10H11F3N2O	002164-17-2	43
4		1-Butanamine, N-ethyl-N-methyl-	115	C7H17N	066225-40-9	43
5		N,N'-Diisopropylethylenediamine	144	C8H20N2	004013-94-9	43



Data Path : Z:\HPCHEM1\BNA G\DATA\BG070816\
Data File : BG022907.D
Acq On : 7 Jul 2016 22:42
Operator : UM/SJ
Sample : H3834-01
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-1

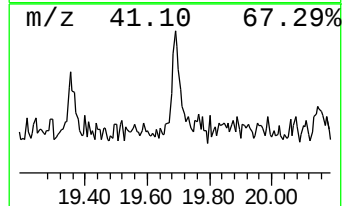
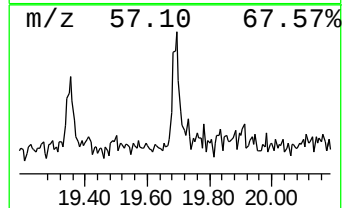
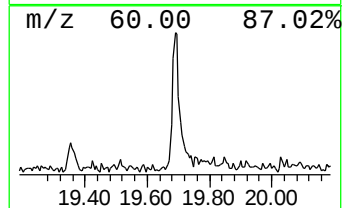
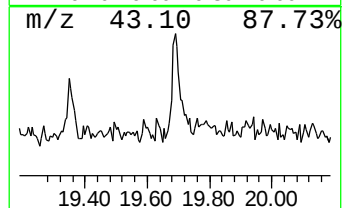
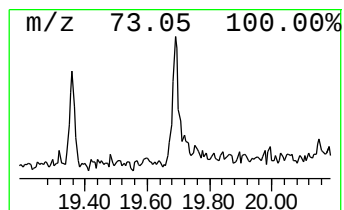
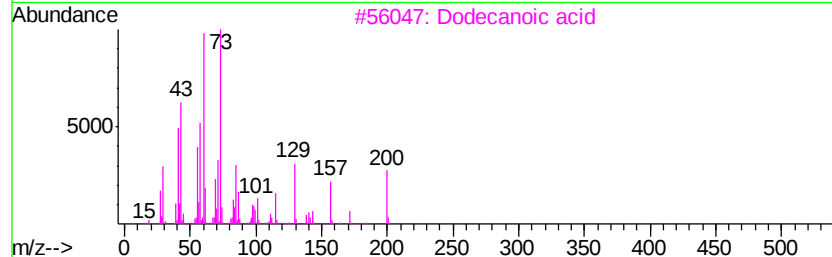
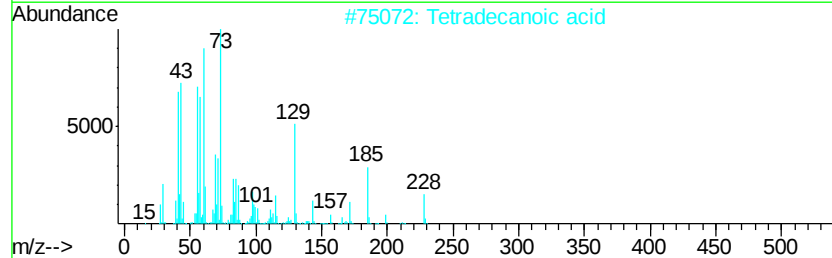
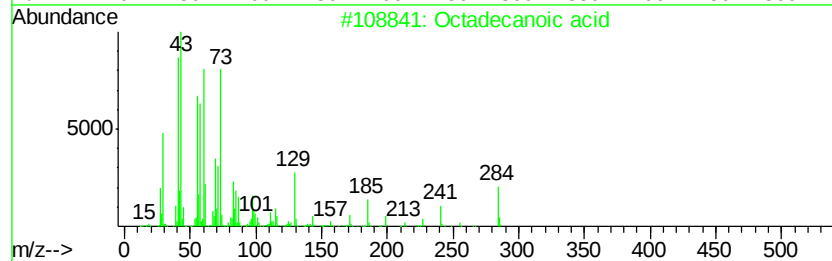
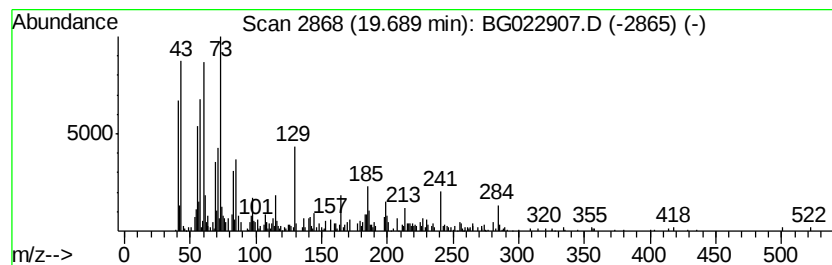
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 Octadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.71 ng	435761	Phenanthrene-d10	17.56

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	83
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	64
3	Dodecanoic acid	200	C12H24O2	000143-07-7	53
4	Tridecanoic acid	214	C13H26O2	000638-53-9	53
5	Undecanoic acid	186	C11H22O2	000112-37-8	46



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG070816\
 Data File : BG022907.D
 Acq On : 7 Jul 2016 22:42
 Operator : UM/SJ
 Sample : H3834-01
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-1

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
2,5-Hexanedione	6.53	3.4	ng	152428	1	8.16	897944	20.0
unknown7.00	7.00	7.2	ng	322067	1	8.16	897944	20.0
2-Cyclopenten-1-o...	7.23	3.2	ng	145010	1	8.16	897944	20.0
Furan, 2,5-dihydro-	7.50	7.7	ng	345372	1	8.16	897944	20.0
unknown7.69	7.69	77.7	ng	3488960	1	8.16	897944	20.0
unknown8.53	8.53	2.9	ng	131627	1	8.16	897944	20.0
2(3H)-Furanone, 5...	8.68	3.7	ng	165992	1	8.16	897944	20.0
2-Cyclohexen-1-on...	8.80	2.8	ng	126528	1	8.16	897944	20.0
Hexanethioic acid...	9.55	2.7	ng	120207	1	8.16	897944	20.0
2-[1-Nitro-2-(tet...	10.27	2.9	ng	171254	2	10.98	1163780	20.0
unknown10.73	10.73	3.4	ng	195497	2	10.98	1163780	20.0
Benzothiazole	11.63	3.0	ng	174637	2	10.98	1163780	20.0
Benzoic acid, 3-m...	11.75	2.8	ng	165397	2	10.98	1163780	20.0
2(3H)-Furanone, 5...	11.87	4.7	ng	272470	2	10.98	1163780	20.0
1-Hexadecanamine, ...	16.56	3.2	ng	375093	4	17.56	2347880	20.0
unknown17.20	17.20	3.8	ng	444697	4	17.56	2347880	20.0
n-Hexadecanoic acid	18.43	6.9	ng	814912	4	17.56	2347880	20.0
2-Butanamine, N,N...	19.36	2.5	ng	288500	4	17.56	2347880	20.0
Octadecanoic acid	19.69	3.7	ng	435761	4	17.56	2347880	20.0