

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
 Data File : BG016160.D
 Acq On : 27 Mar 2015 3:54
 Operator : TP/IZ
 Sample : G1653-08
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FD4

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-BG032515.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	2.795	13	18	26	rBV	492272	559805	2.24%	0.695%
2	3.271	97	99	101	rVB	427810	303272	1.21%	0.377%
3	4.199	154	257	259	rBV	1124847	17379139	69.42%	21.579%
4	4.710	264	344	346	rBV	1678234	25033552	100.00%	31.083%
5	4.992	388	392	400	rVV	174647	263472	1.05%	0.327%
6	5.110	400	412	424	rVB	160470	388489	1.55%	0.482%
7	5.392	454	460	465	rVV	786537	1197571	4.78%	1.487%
8	5.738	465	519	522	rVB	655352	6788321	27.12%	8.429%
9	6.338	607	621	630	rBV	118241	310515	1.24%	0.386%
10	6.978	699	730	735	rBV	1081161	3026122	12.09%	3.757%
11	7.336	786	791	796	rBV	844038	1504066	6.01%	1.868%
12	7.794	860	869	876	rBV	194283	307529	1.23%	0.382%
13	7.929	876	892	899	rBV2	725029	1480652	5.91%	1.838%
14	8.112	916	923	930	rVB	577004	933031	3.73%	1.158%
15	8.470	970	984	992	rBV	136367	332328	1.33%	0.413%
16	8.552	992	998	1012	rVB	238497	395806	1.58%	0.491%
17	8.946	1056	1065	1074	rBV	443220	745358	2.98%	0.925%
18	9.956	1209	1237	1241	rBV	382589	1721895	6.88%	2.138%
19	10.079	1256	1258	1272	rVB2	692513	692128	2.76%	0.859%
20	10.579	1335	1343	1349	rBV	290069	480208	1.92%	0.596%
21	10.643	1349	1354	1362	rVB	159945	252177	1.01%	0.313%
22	11.155	1432	1441	1452	rBV	138761	308856	1.23%	0.383%
23	11.407	1475	1484	1503	rBV2	144146	305147	1.22%	0.379%
24	12.318	1629	1639	1645	rBV	195484	314903	1.26%	0.391%
25	12.418	1645	1656	1670	rBV	311025	698008	2.79%	0.867%
26	12.723	1699	1708	1717	rBV	217557	423363	1.69%	0.526%
27	13.040	1753	1762	1772	rVB	1191037	1749648	6.99%	2.172%
28	14.415	1983	1996	2004	rBV2	418211	664570	2.65%	0.825%
29	15.901	2242	2249	2255	rBV	997679	1390368	5.55%	1.726%
30	16.559	2354	2361	2369	rBV2	195504	299650	1.20%	0.372%
31	17.152	2458	2462	2468	rVB	587511	804896	3.22%	0.999%
32	17.470	2508	2516	2523	rBV	1864737	2778691	11.10%	3.450%
33	18.045	2609	2614	2622	rBV	309880	486214	1.94%	0.604%
34	18.116	2622	2626	2631	rVB	339830	405429	1.62%	0.503%

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

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-BG032515.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	19.772	2903	2908	2915	rBV	2101978	2614615	10.44%	3.246%
36	21.029	3118	3122	3134	rBV	285892	378736	1.51%	0.470%
37	21.323	3166	3172	3181	rBV	753860	939921	3.75%	1.167%
38	23.608	3553	3561	3571	rBV	452483	888719	3.55%	1.103%
39	26.169	3987	3997	4009	rBV2	361427	991652	3.96%	1.231%

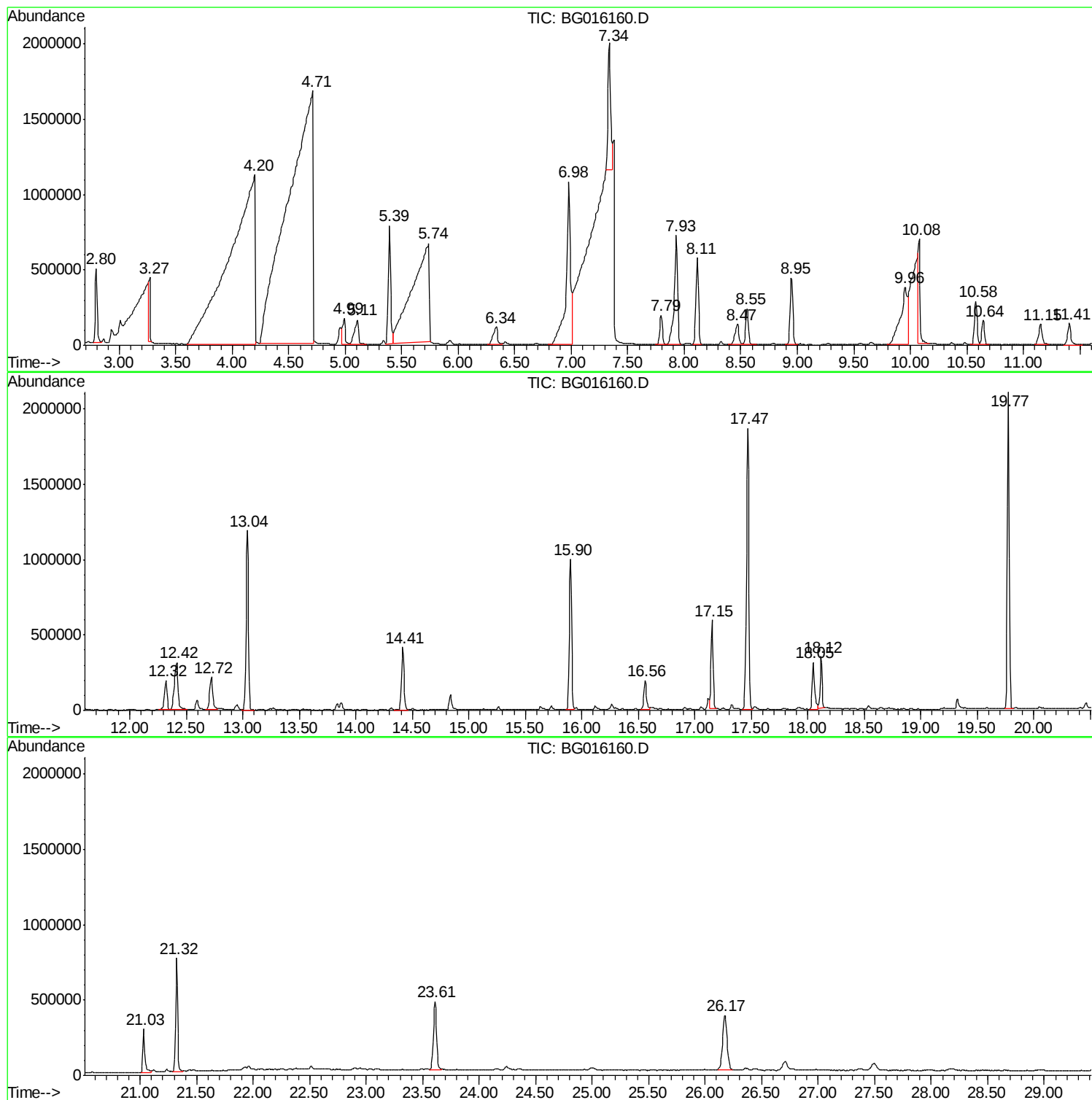
Sum of corrected areas: 80538822

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
FD4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.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\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

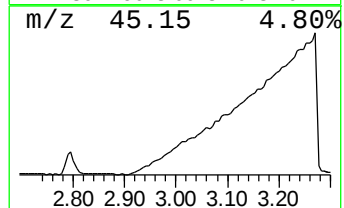
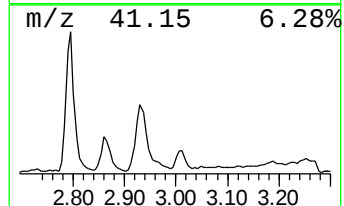
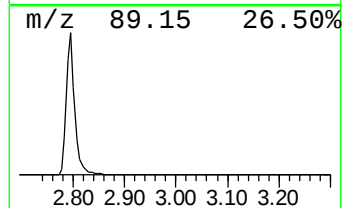
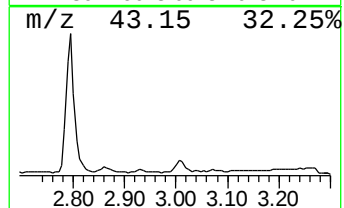
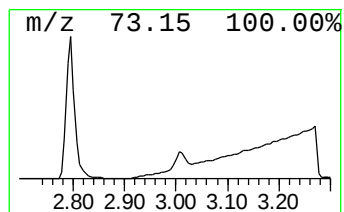
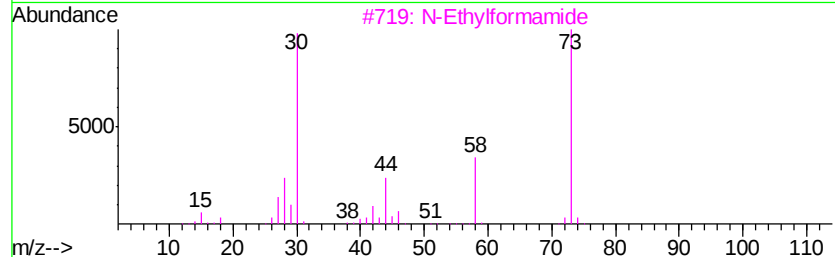
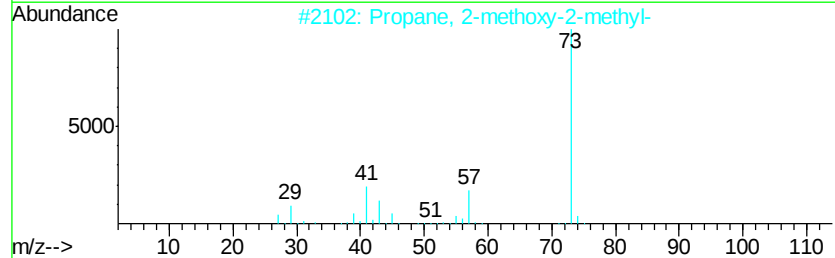
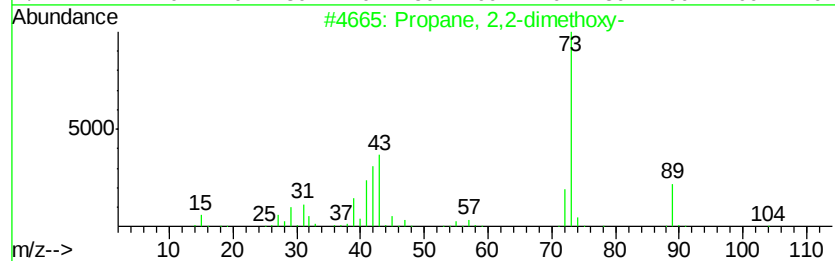
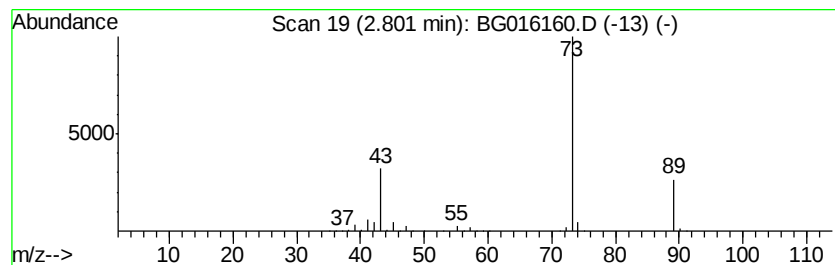
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.80	36.41 ng	559805	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
3		N-Ethylformamide	73	C3H7NO	000627-45-2	7
4		1,3,5-Trioxane	90	C3H6O3	000110-88-3	4
5		1,3-Dioxolane, 2-(6-heptynyl)-	168	C10H16O2	025595-82-8	4



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

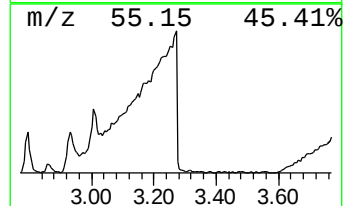
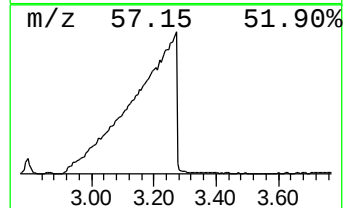
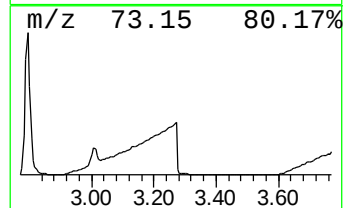
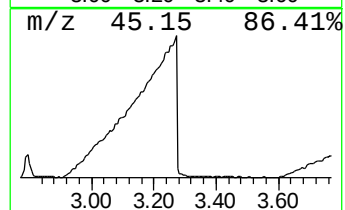
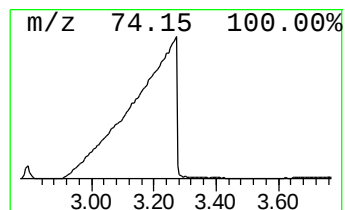
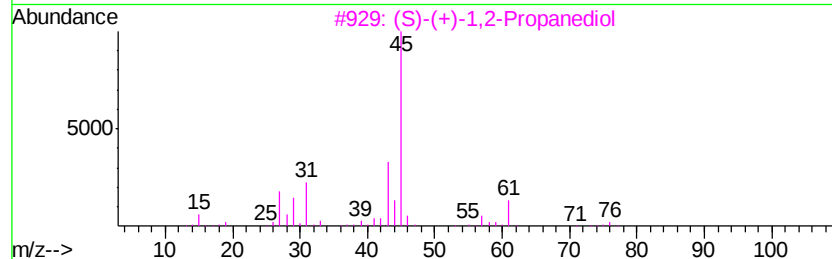
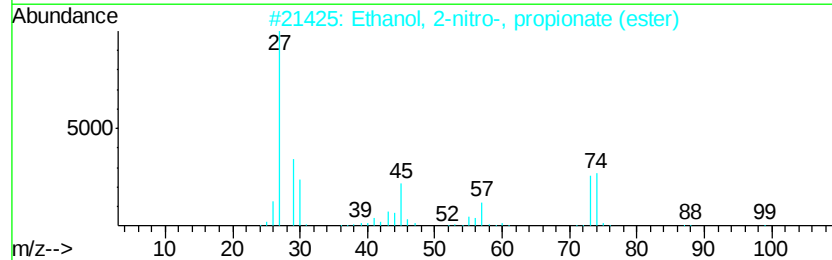
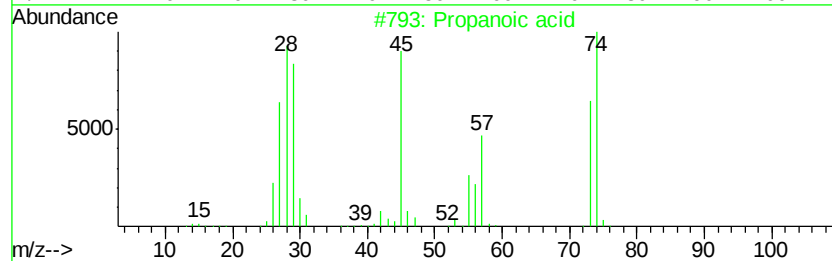
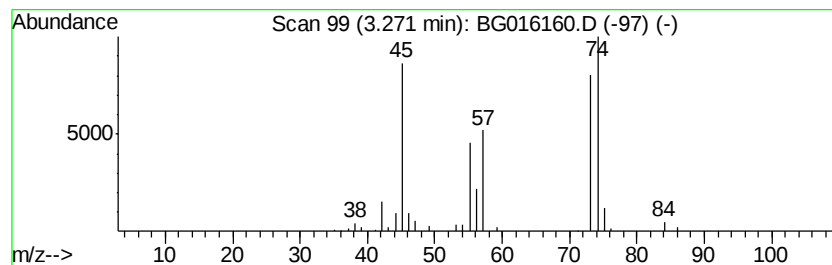
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propanoic acid Concentration Rank 15

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.27	19.72 ng	303272	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid		74	C3H6O2	000079-09-4	87
2	Ethanol, 2-nitro-, propionate (e...		147	C5H9NO4	005390-28-3	42
3	(S)-(+)-1,2-Propanediol		76	C3H8O2	004254-15-3	9
4	Acetic acid, hydroxy-		76	C2H4O3	000079-14-1	9
5	Diethanolamine		105	C4H11NO2	000111-42-2	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

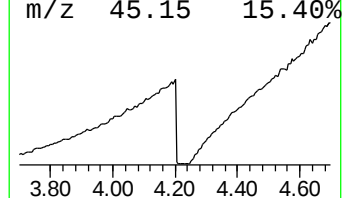
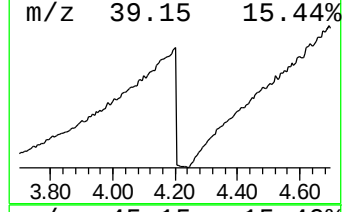
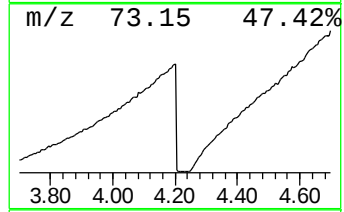
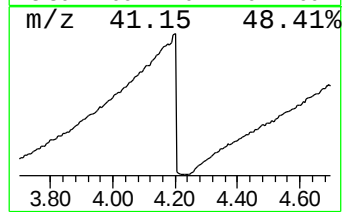
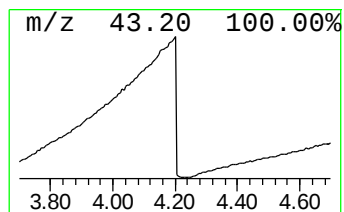
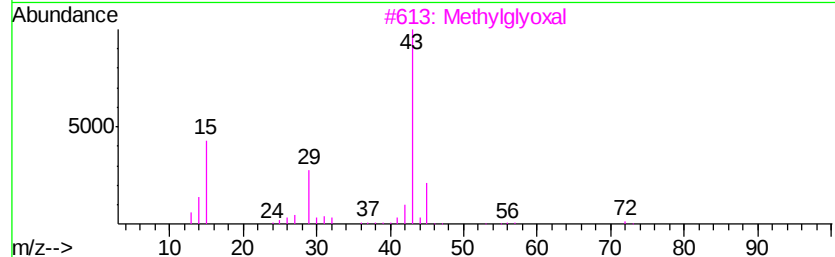
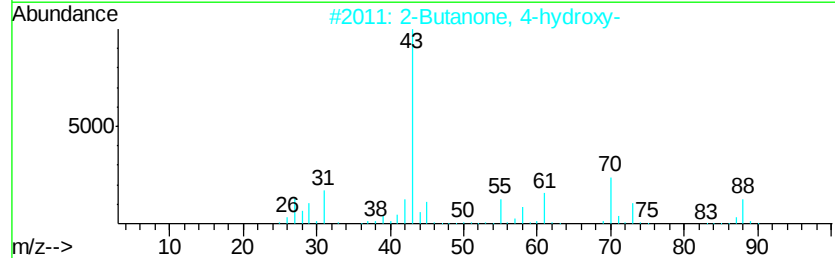
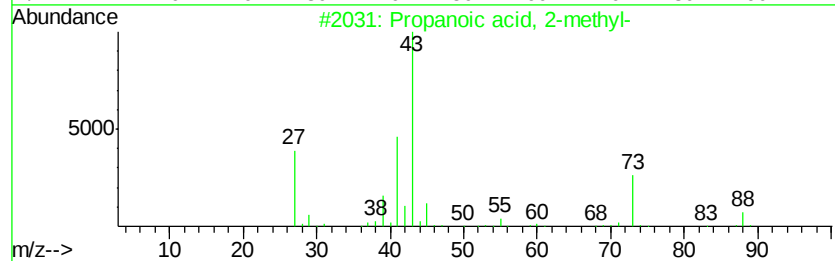
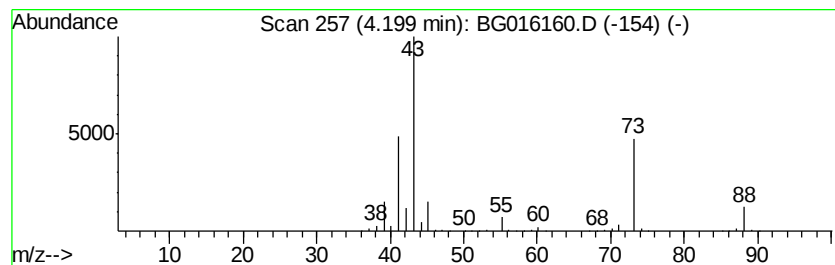
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 Propanoic acid, 2-methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.20	1130.24 ng	17379100	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanoic acid, 2-methyl-	88	C4H8O2	000079-31-2	91
2		2-Butanone, 4-hydroxy-	88	C4H8O2	000590-90-9	50
3		Methylglyoxal	72	C3H4O2	000078-98-8	9
4		Propanoyl chloride, 2-methyl-	106	C4H7ClO	000079-30-1	9
5		2-Oxo-n-valeric acid	116	C5H8O3	001821-02-9	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

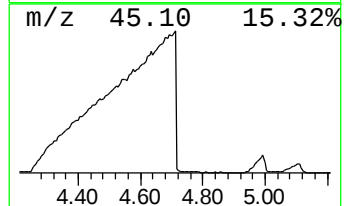
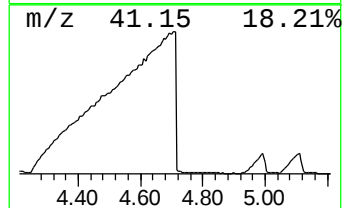
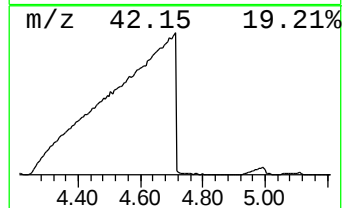
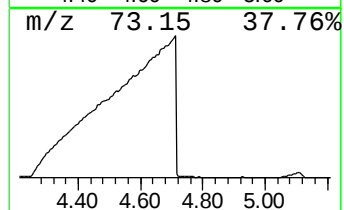
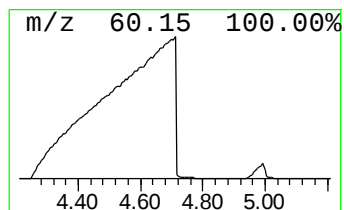
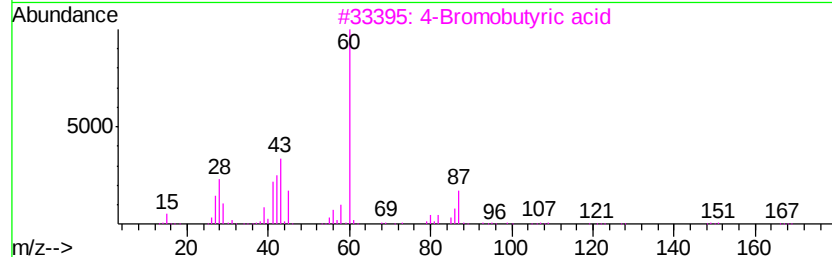
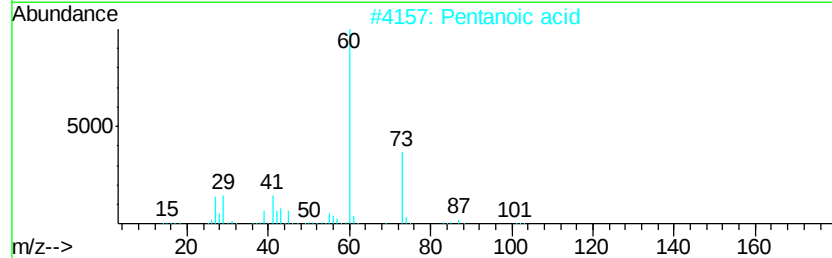
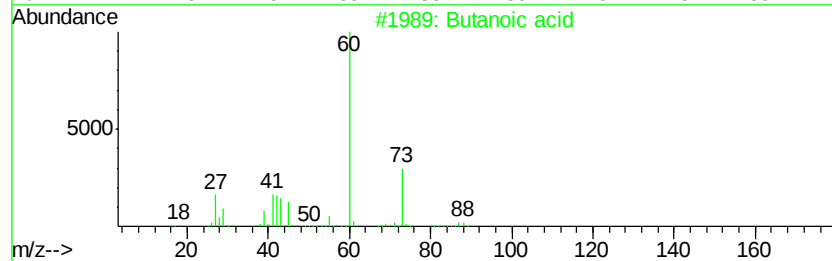
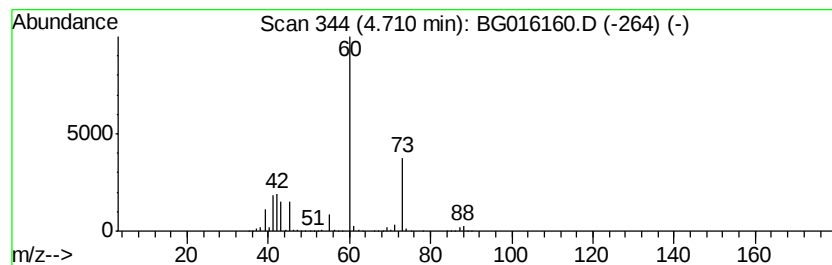
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Butanoic acid Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.71	1628.04 ng	25033600	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanoic acid	88	C4H8O2	000107-92-6	91
2		Pentanoic acid	102	C5H10O2	000109-52-4	50
3		4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	9
4		Hexanoic acid	116	C6H12O2	000142-62-1	9
5		Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

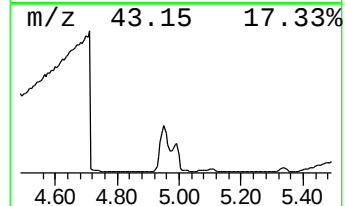
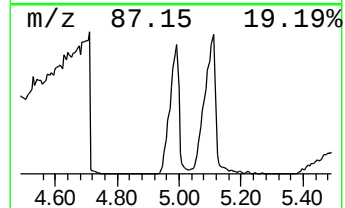
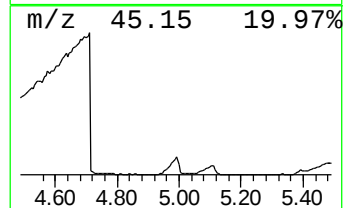
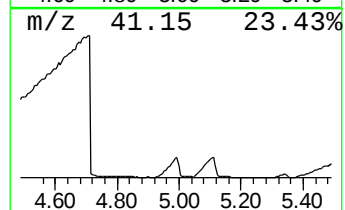
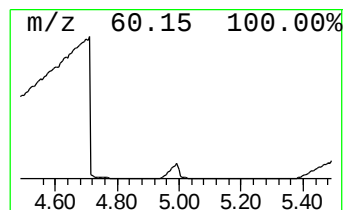
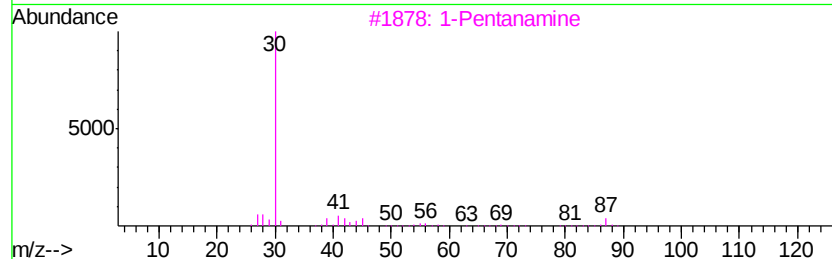
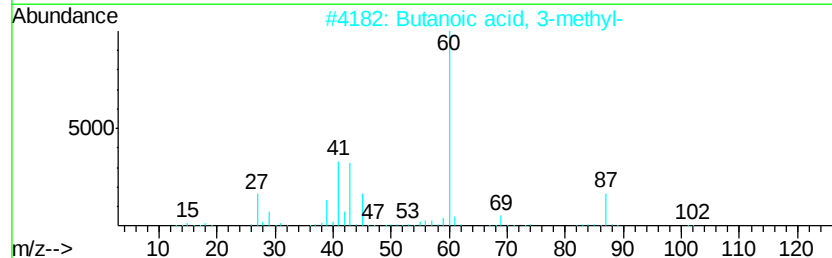
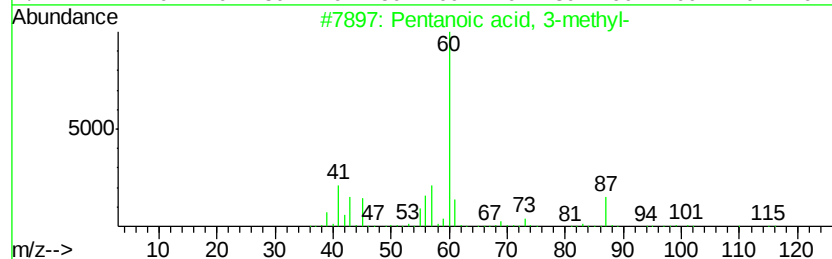
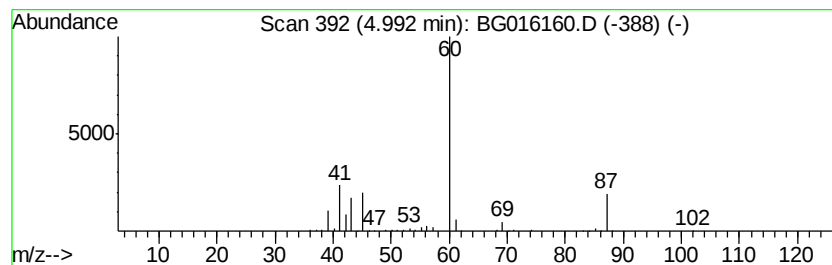
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentanoic acid, 3-methyl- Concentration Rank 16

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	17.13 ng	263472	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	64
2		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	64
3		1-Pentanamine	87	C5H13N	000110-58-7	7
4		Ethyne, chloro-	60	C2HCl	000593-63-5	7
5		Hydrazine, 1,1-dimethyl-	60	C2H8N2	000057-14-7	5



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

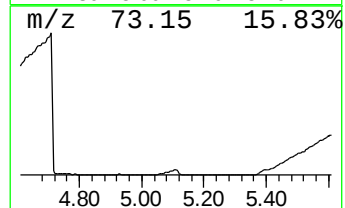
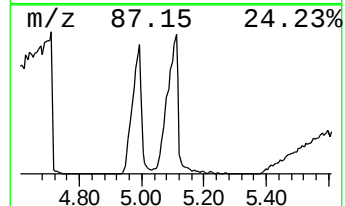
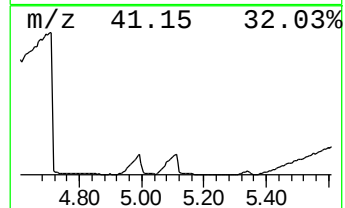
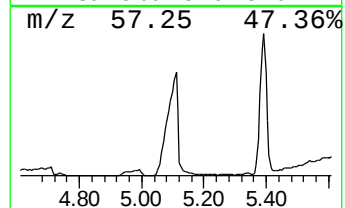
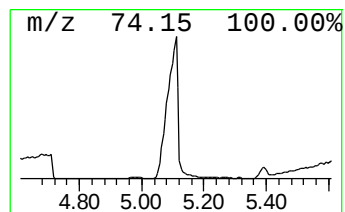
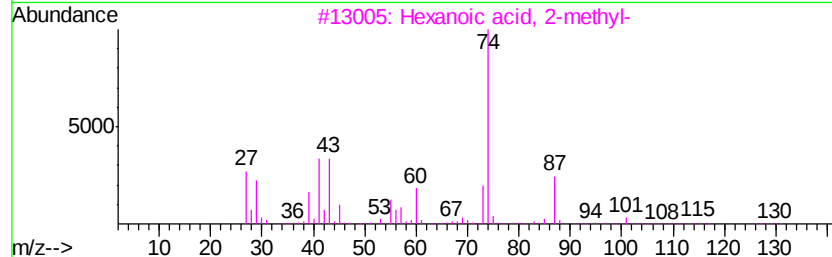
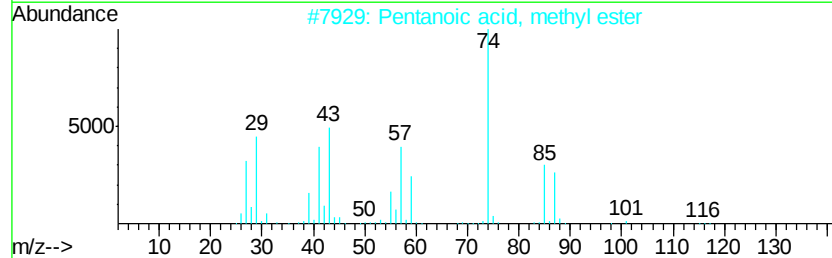
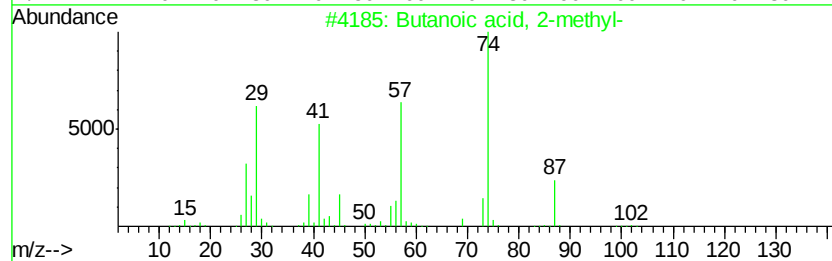
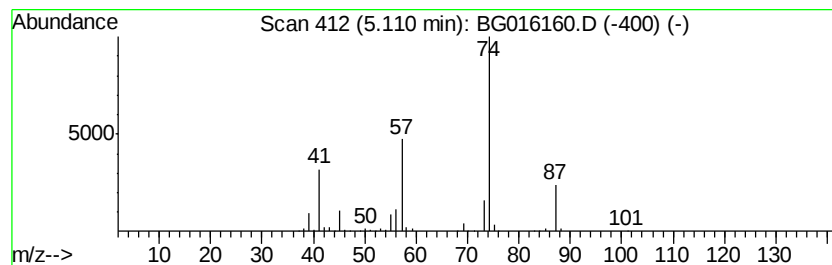
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Butanoic acid, 2-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	25.27 ng	388489	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	83
2		Pentanoic acid, methyl ester	116	C6H12O2	000624-24-8	50
3		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	43
4		Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	39
5		2-Methylheptanoic acid	144	C8H16O2	001188-02-9	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

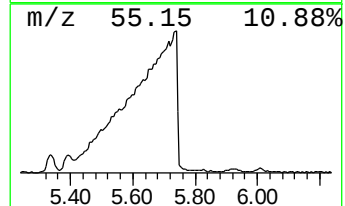
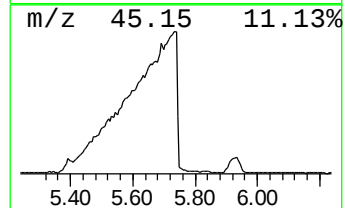
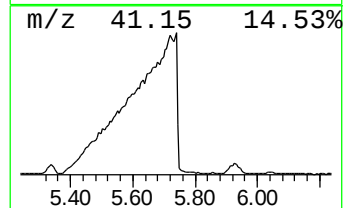
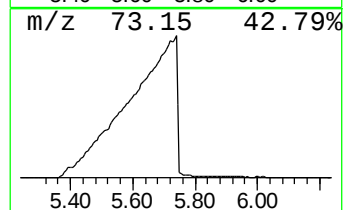
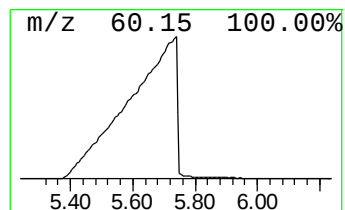
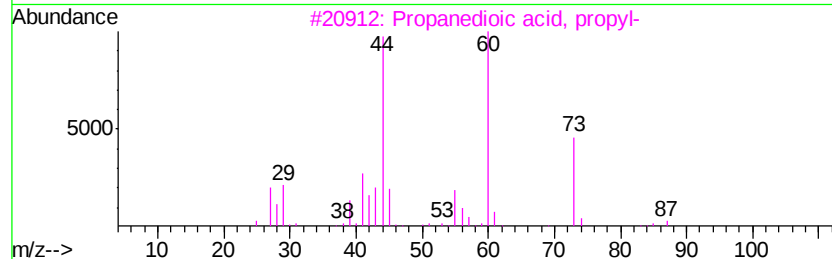
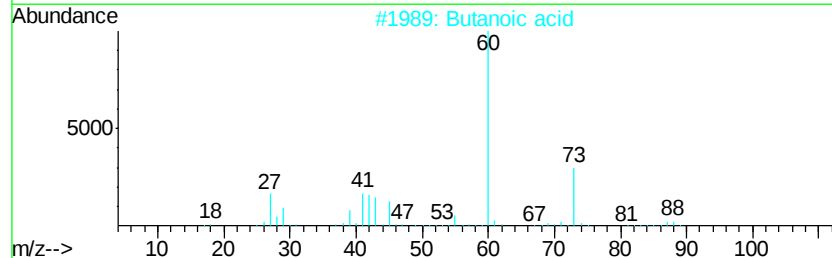
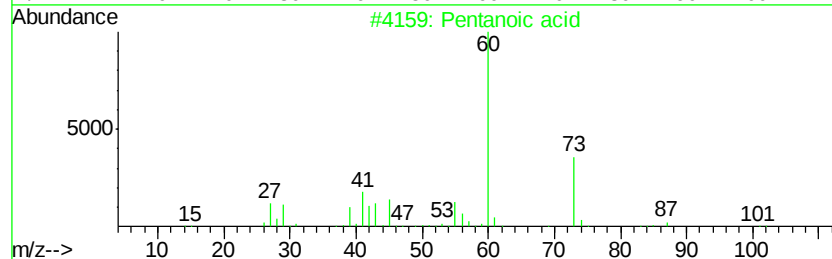
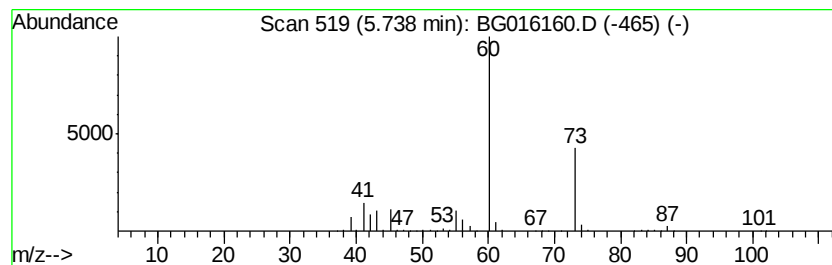
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Pentanoic acid Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.74	441.48 ng	6788320	1,4-Dichlorobenzene-d4	7.79

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanoic acid	102	C5H10O2	000109-52-4	83	
2	Butanoic acid	88	C4H8O2	000107-92-6	83	
3	Propanedioic acid, propyl-	146	C6H10O4	000616-62-6	42	
4	Hexanoic acid	116	C6H12O2	000142-62-1	40	
5	Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	38	



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

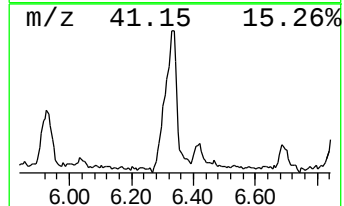
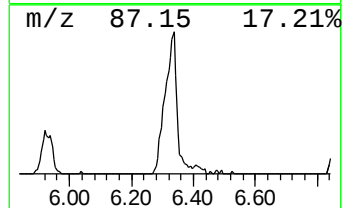
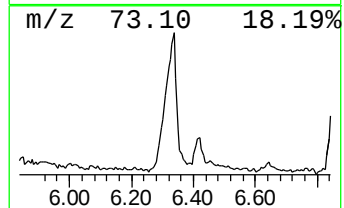
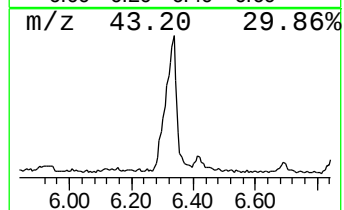
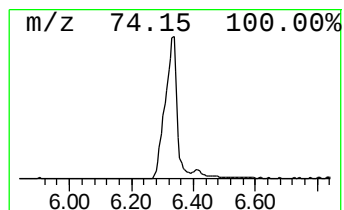
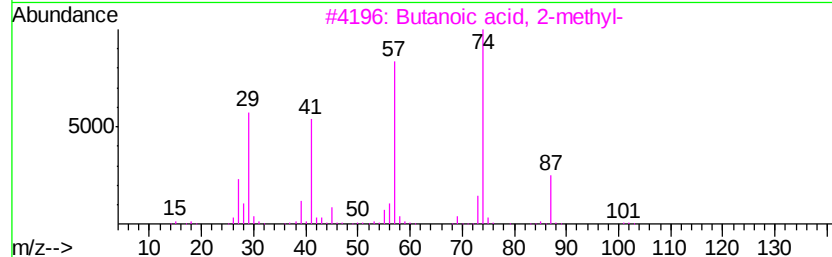
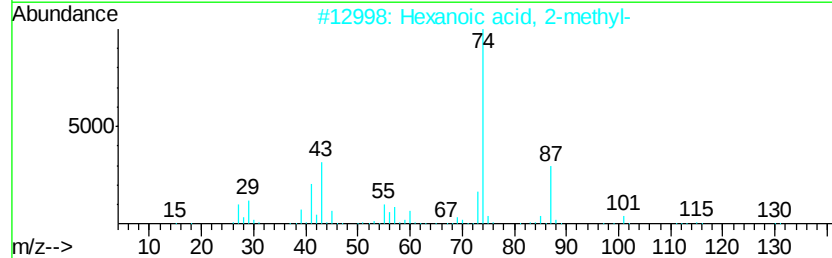
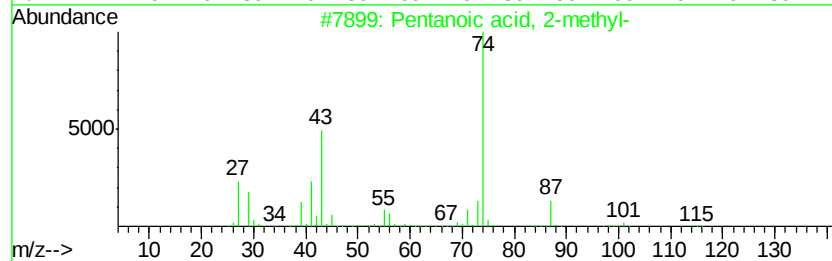
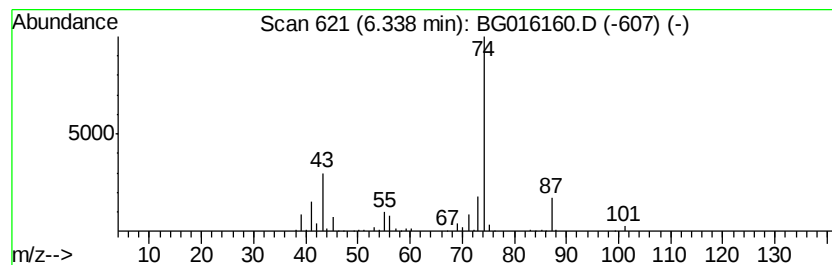
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Pentanoic acid, 2-methyl- Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.34	20.19 ng	310515	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, 2-methyl-	116	C6H12O2	000097-61-0	83
2		Hexanoic acid, 2-methyl-	130	C7H14O2	004536-23-6	72
3		Butanoic acid, 2-methyl-	102	C5H10O2	000116-53-0	64
4		2-Methylheptanoic acid	144	C8H16O2	001188-02-9	40
5		N-Nitrosodimethylamine	74	C2H6N2O	000062-75-9	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

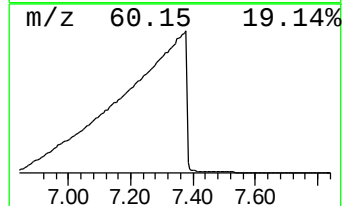
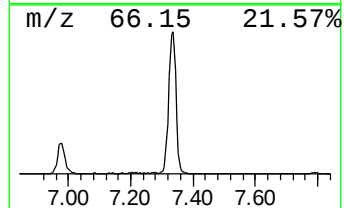
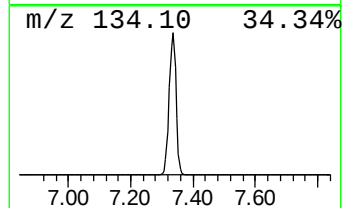
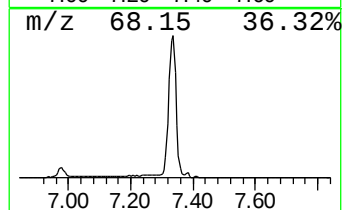
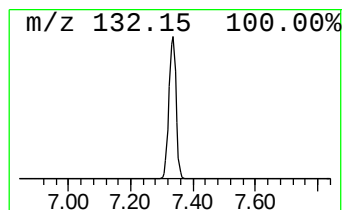
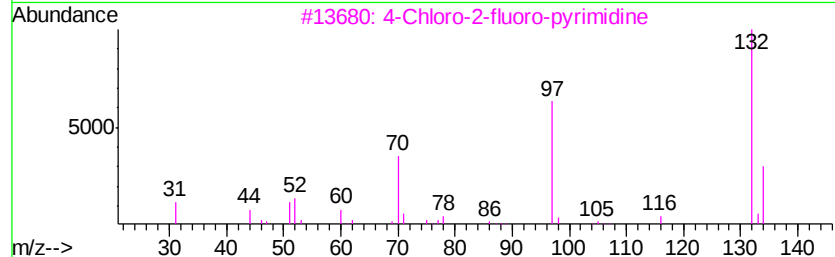
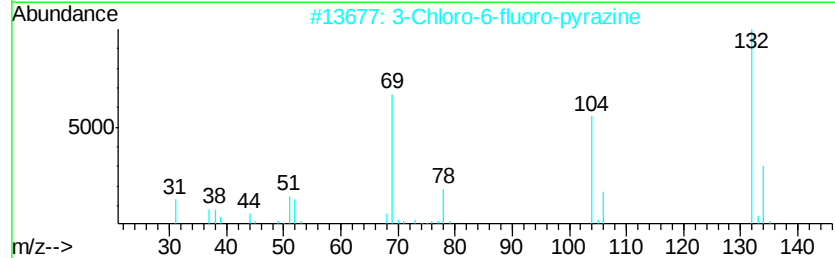
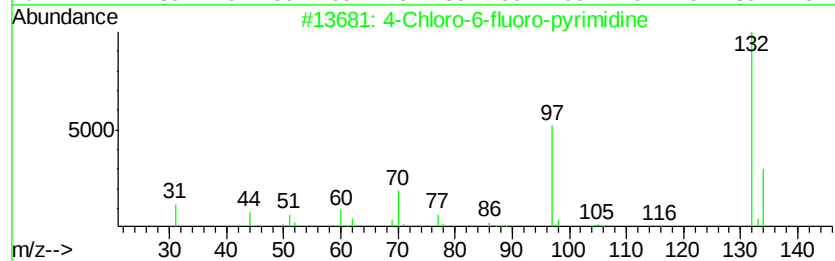
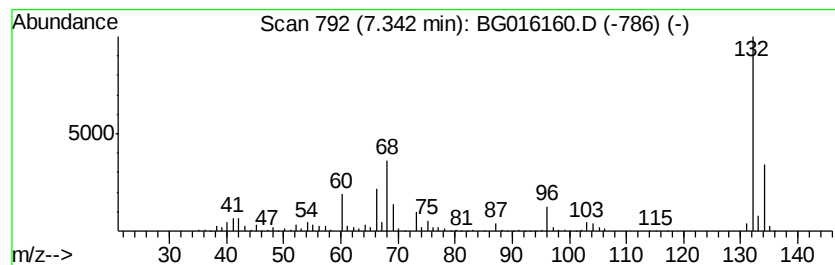
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown7.34 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.34	97.82 ng	1504070	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	25
3		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	25
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	17
5		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

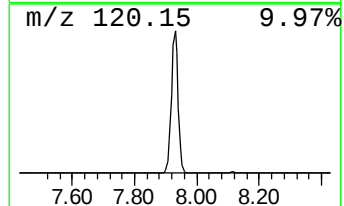
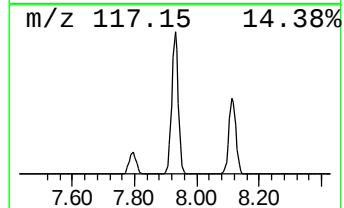
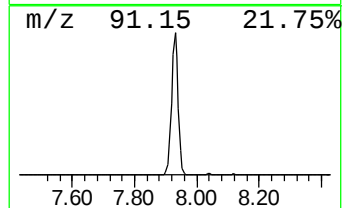
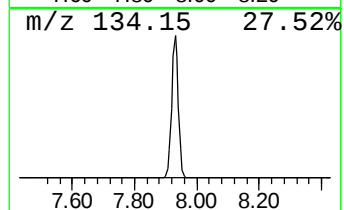
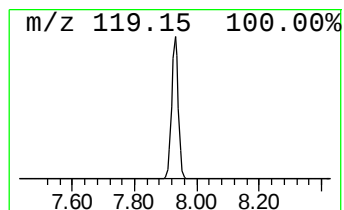
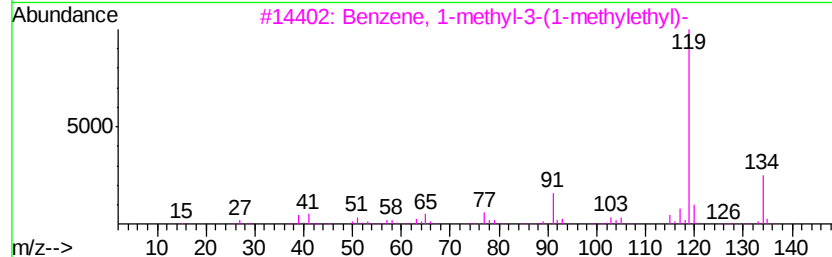
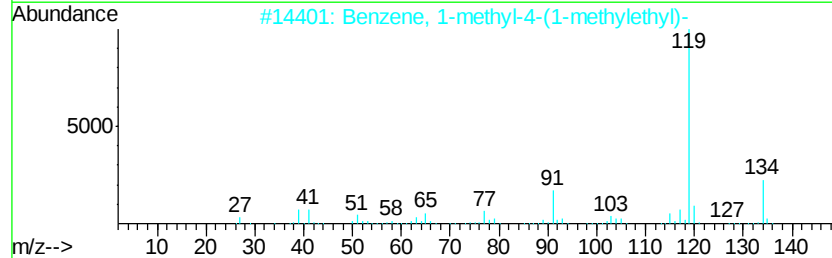
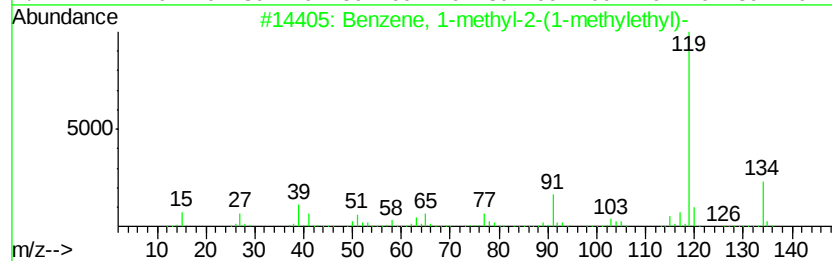
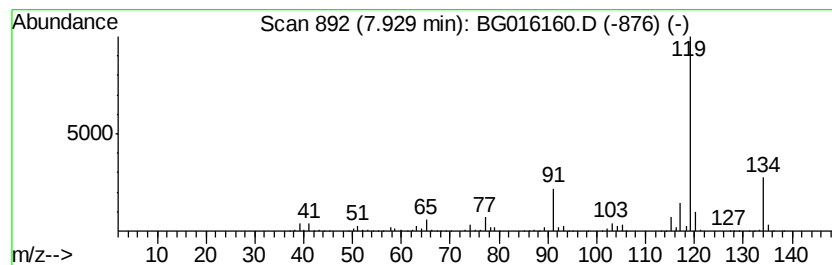
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Benzene, 1-methyl-2-(1-meth... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.93	96.29 ng	1480650	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	97
2		Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	97
3		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	95
4		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	91
5		Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	91



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

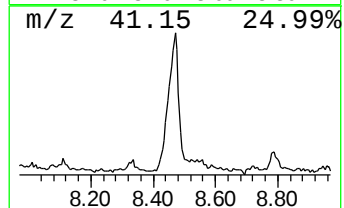
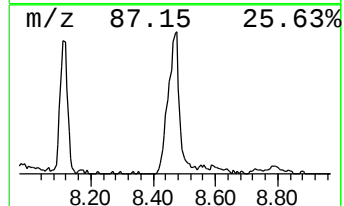
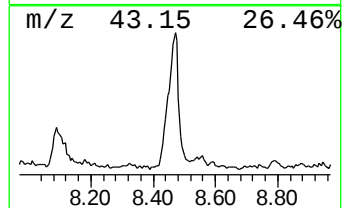
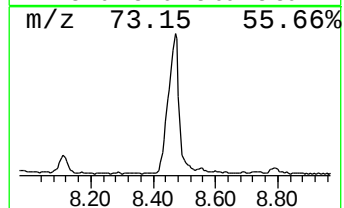
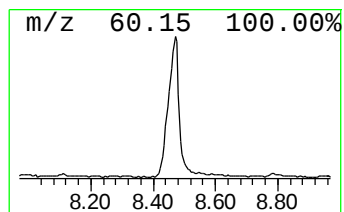
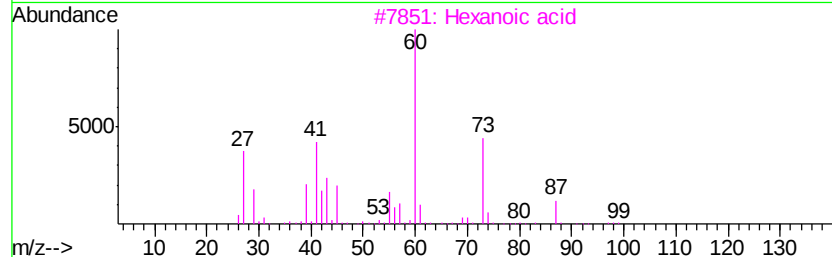
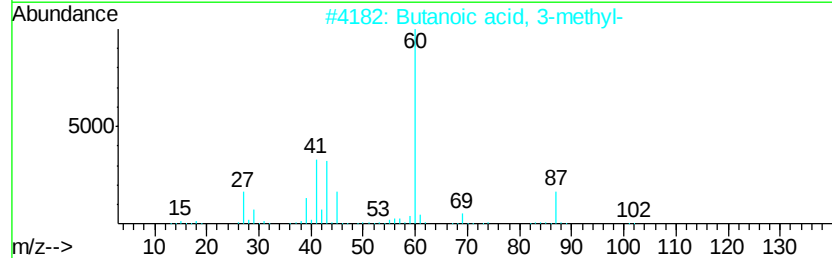
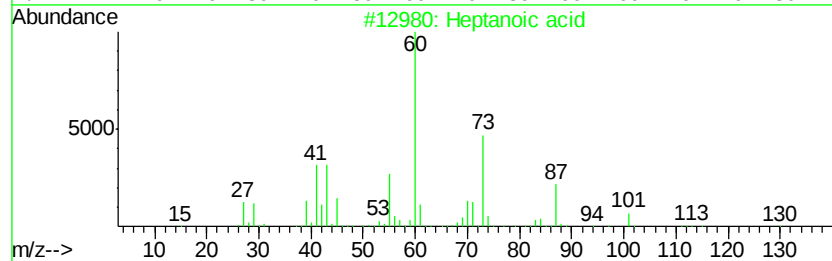
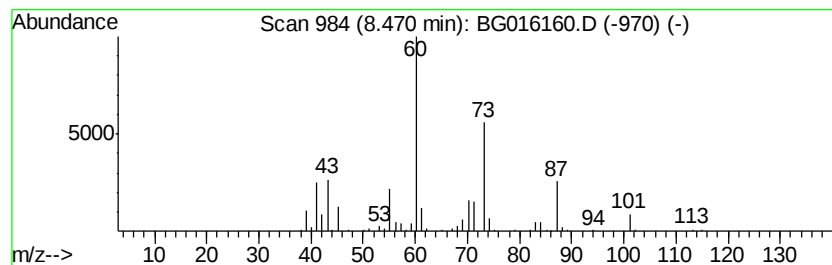
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Heptanoic acid Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.47	21.61 ng	332328	1,4-Dichlorobenzene-d4	7.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptanoic acid	130	C7H14O2	000111-14-8	90
2			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	59
3			Hexanoic acid	116	C6H12O2	000142-62-1	56
4			Octanoic Acid	144	C8H16O2	000124-07-2	53
5			Pentanoic acid	102	C5H10O2	000109-52-4	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

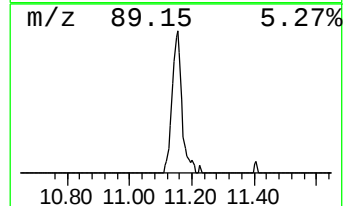
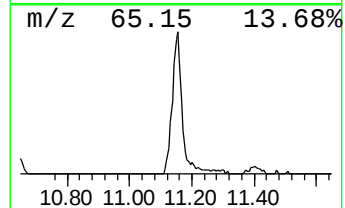
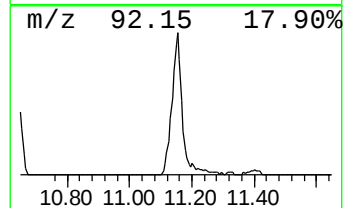
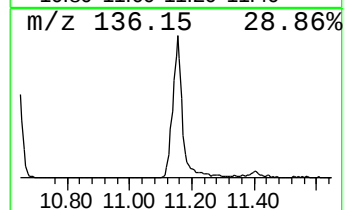
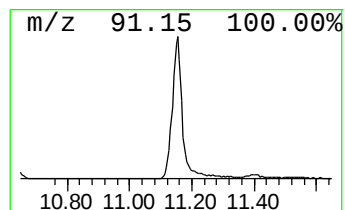
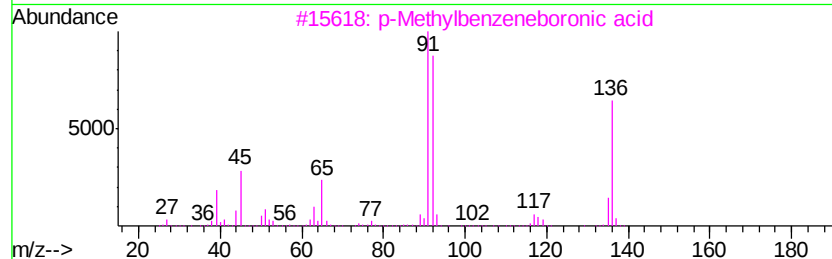
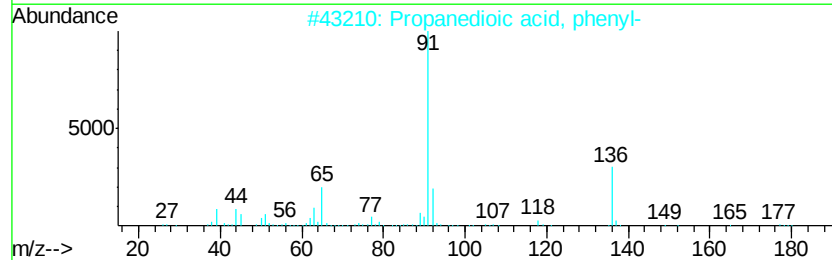
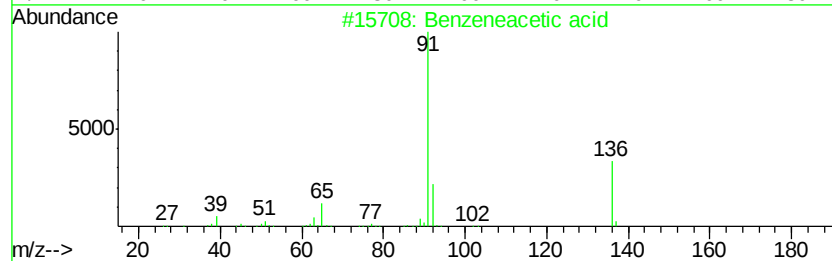
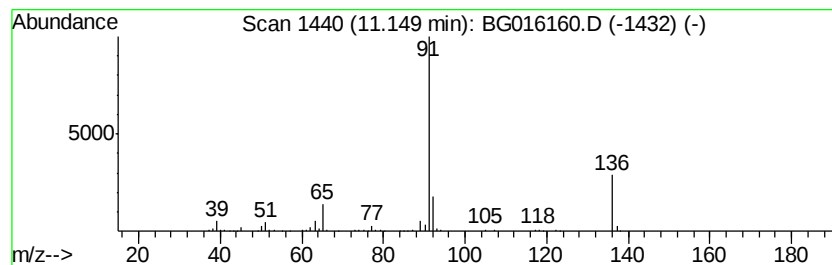
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Benzeneacetic acid Concentration Rank 18

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.15	12.86 ng	308856	Naphthalene-d8	10.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzeneacetic acid	136	C8H8O2	000103-82-2	90
2		Propanedioic acid, phenyl-	180	C9H8O4	002613-89-0	72
3		p-Methylbenzeneboronic acid	136	C7H9BO2	005720-05-8	64
4		Benzene, (iodomethyl)-	218	C7H7I	000620-05-3	53
5		2-Benzyloxy-4-bromobutane-1,3-diol	274	C11H15BrO3	1000191-12-1	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

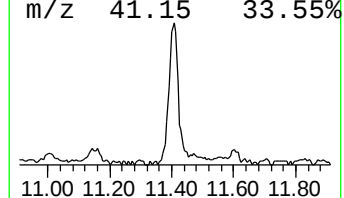
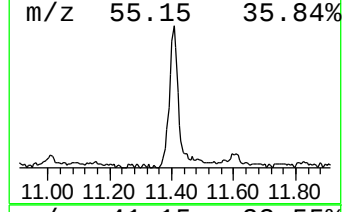
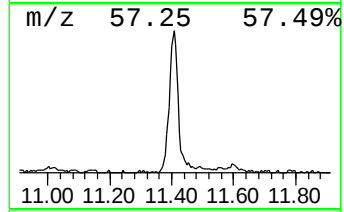
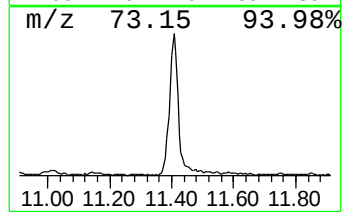
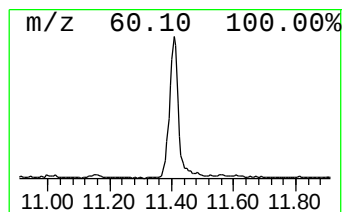
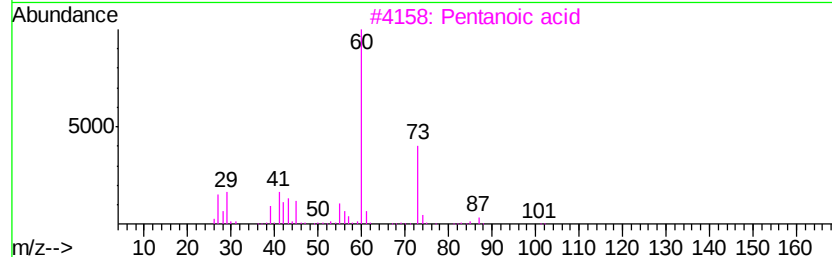
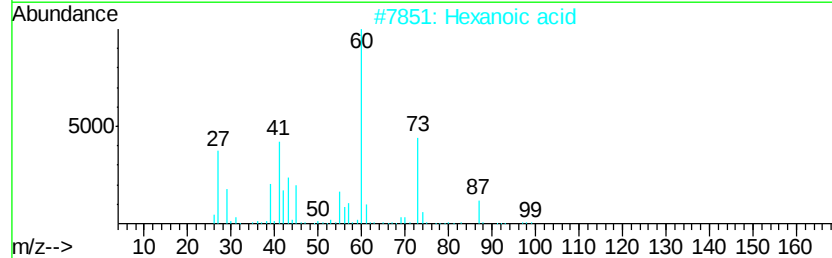
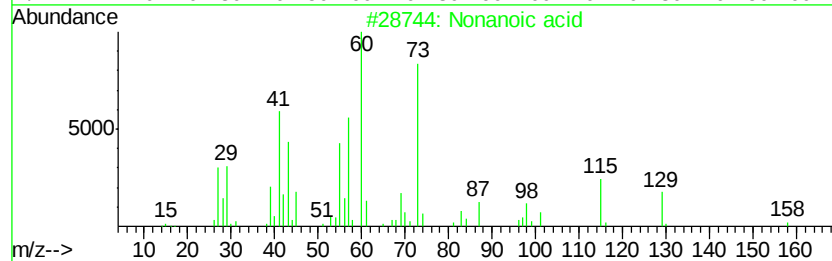
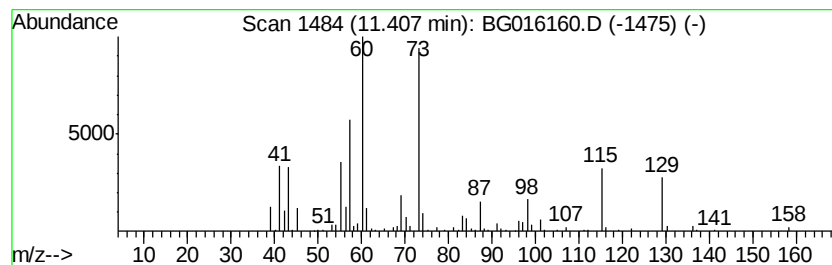
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 15 Nonanoic acid Concentration Rank 20

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.41	12.71 ng	305147	Napthalene-d8	10.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonanoic acid	158	C9H18O2	000112-05-0	90
2		Hexanoic acid	116	C6H12O2	000142-62-1	47
3		Pentanoic acid	102	C5H10O2	000109-52-4	46
4		Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	43
5		Pentanoic acid, 3-methyl-	116	C6H12O2	000105-43-1	43



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

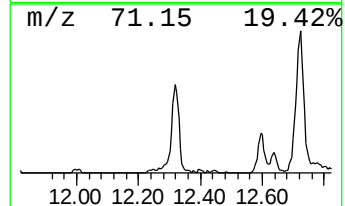
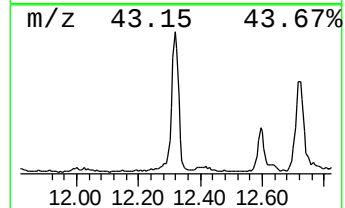
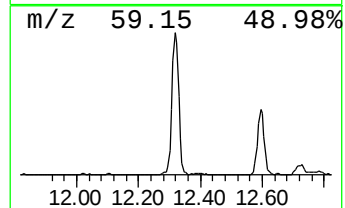
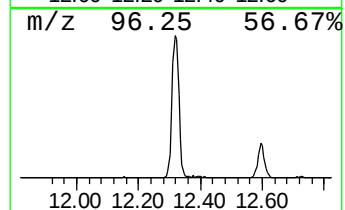
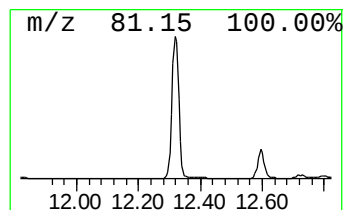
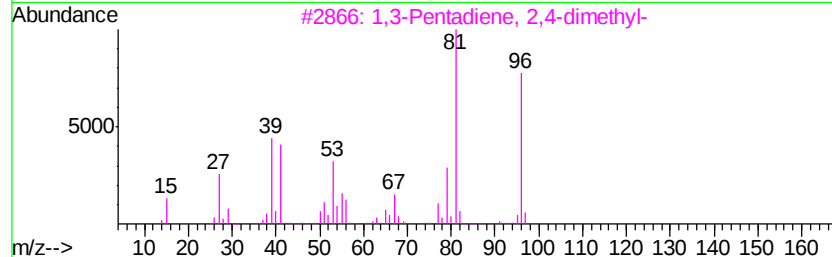
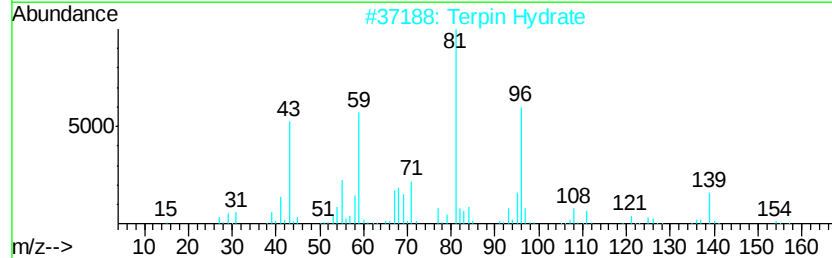
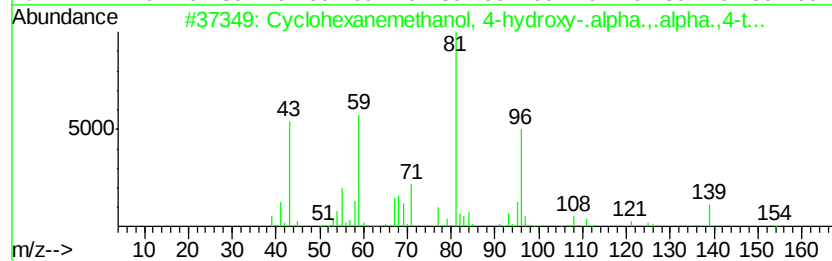
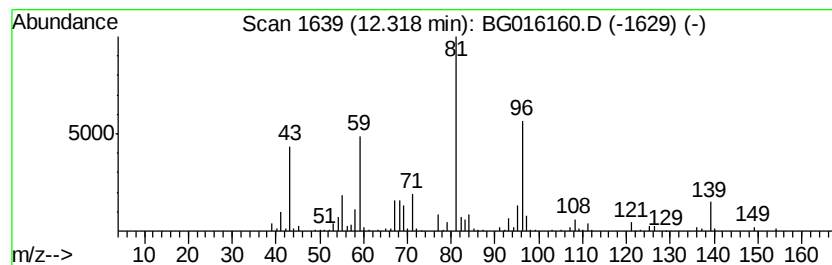
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 16 Cyclohexanemethanol, 4-hydr... Concentration Rank 17

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.32	13.12 ng	314903	Naphthalene-d8	10.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanemethanol, 4-hydroxy-....	172	C10H20O2	000080-53-5	91
2		Terpin Hydrate	172	C10H20O2	002451-01-6	58
3		1,3-Pentadiene, 2,4-dimethyl-	96	C7H12	001000-86-8	47
4		6-Methyl-bicyclo[4.2.0]octan-7-ol	140	C9H16O	1000193-87-3	47
5		4-Methylcyclohexanol acetate	156	C9H16O2	022597-23-5	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

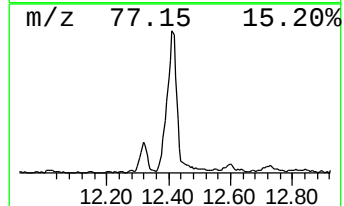
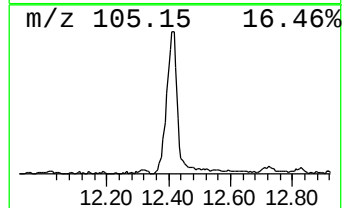
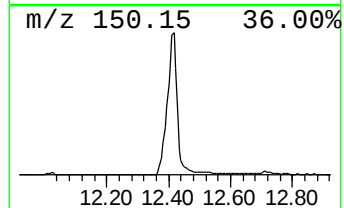
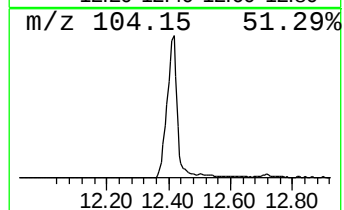
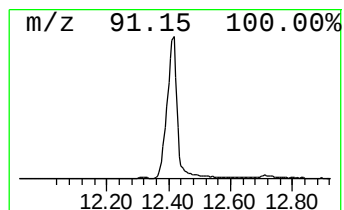
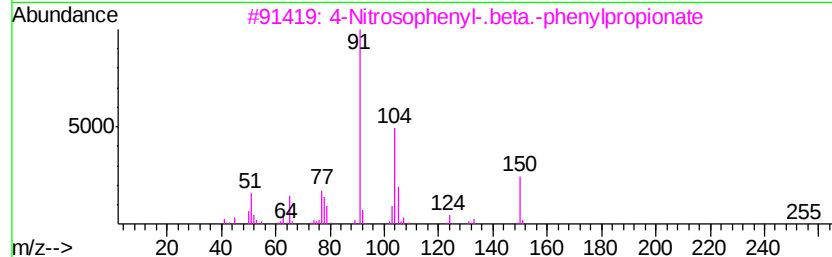
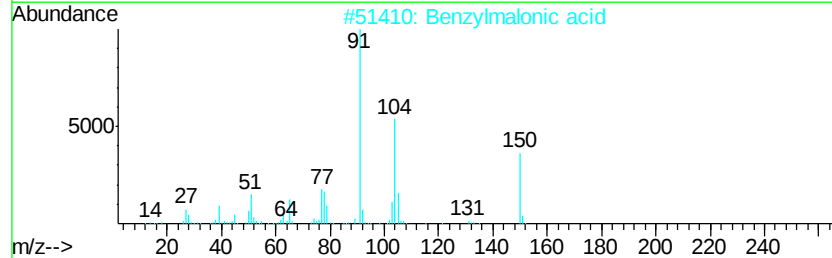
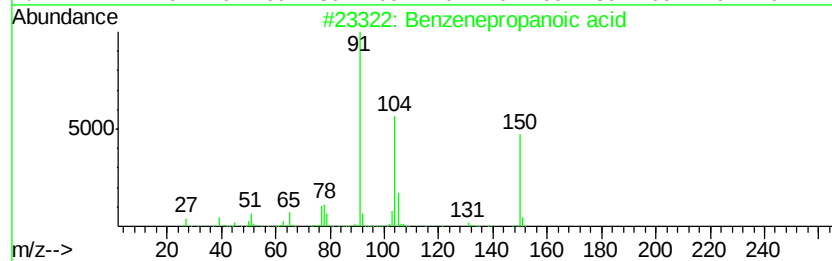
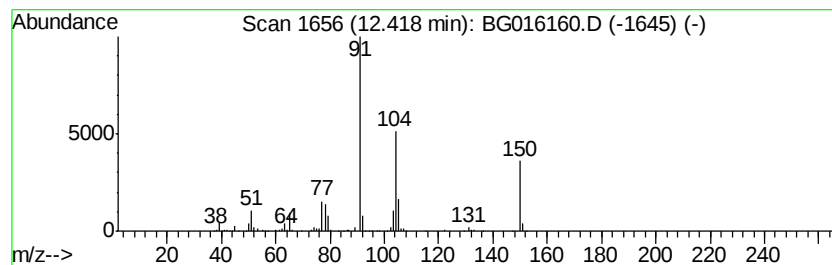
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 17 Benzenepropanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.42	29.07 ng	698008	Napthalene-d8	10.58

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzenepropanoic acid	150	C9H10O2	000501-52-0	95
2		Benzylmalonic acid	194	C10H10O4	000616-75-1	91
3		4-Nitrosophenyl-.beta.-phenylpro...	255	C15H13NO3	1000129-40-0	78
4		3-Phenyl-propionic acid, isoprop...	192	C12H16O2	022767-95-9	78
5		2-Butenoic acid, 3-methyl-, 2-ph...	204	C13H16O2	042078-65-9	53



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

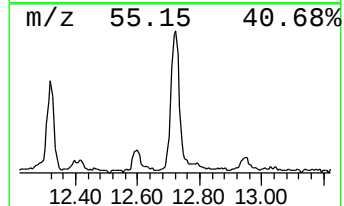
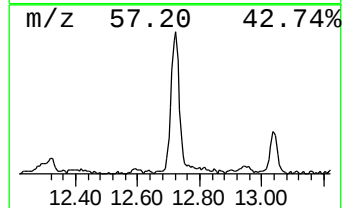
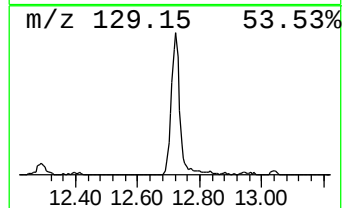
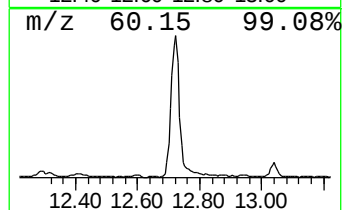
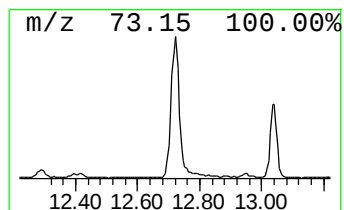
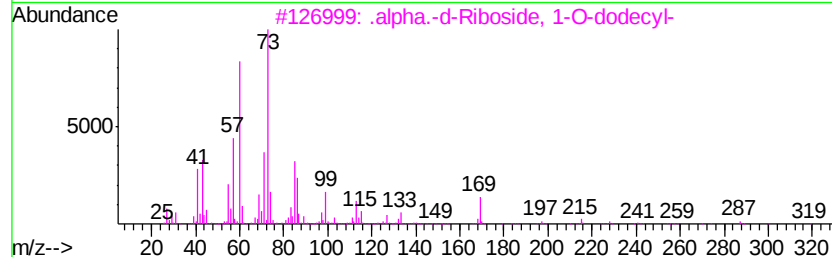
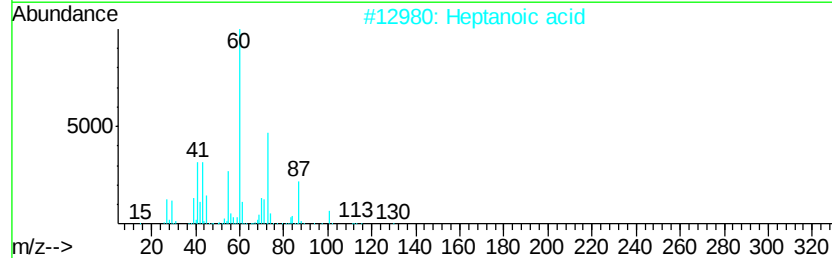
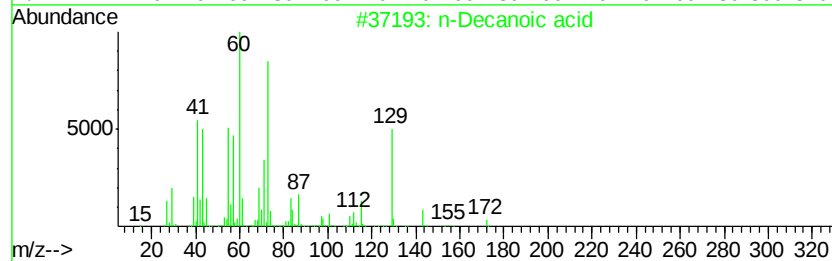
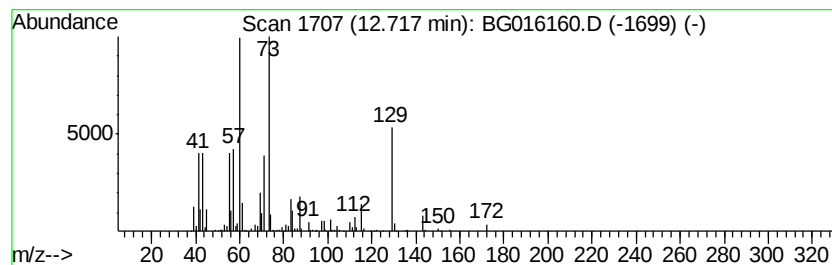
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 18 n-Decanoic acid Concentration Rank 19

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	12.74 ng	423363	Acenaphthene-d10	14.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Decanoic acid	172	C10H20O2	000334-48-5	98
2		Heptanoic acid	130	C7H14O2	000111-14-8	43
3		.alpha.-d-Riboside, 1-O-dodecyl-	318	C17H34O5	1000154-76-8	42
4		.alpha.-L-Galactopyranoside, met...	178	C7H14O5	014687-15-1	38
5		Nonanoic acid	158	C9H18O2	000112-05-0	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

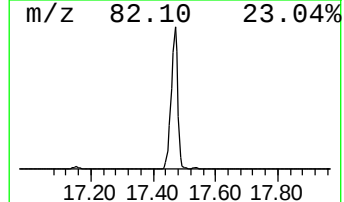
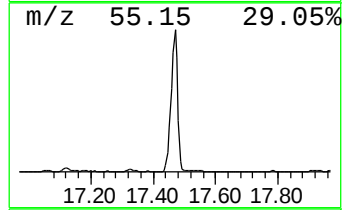
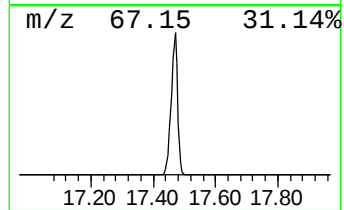
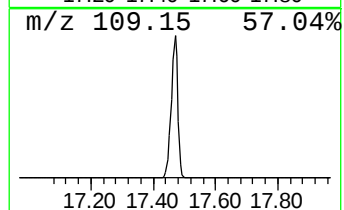
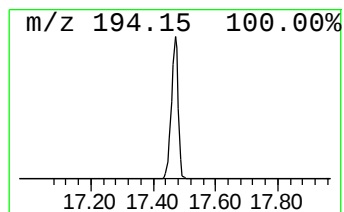
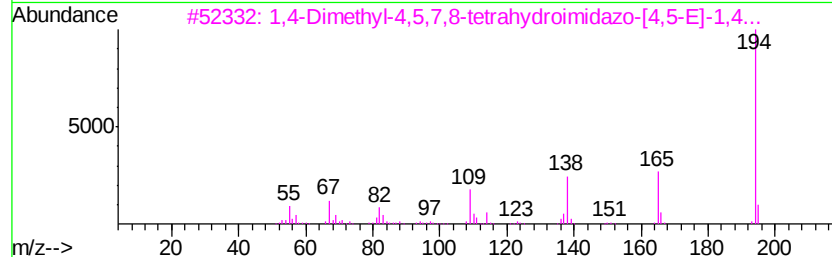
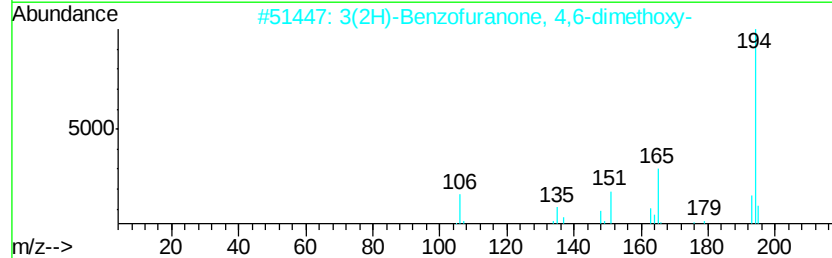
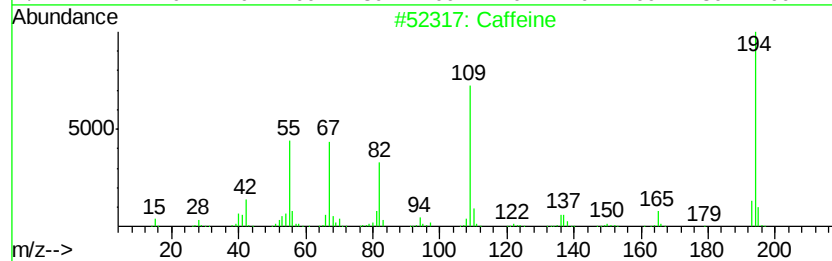
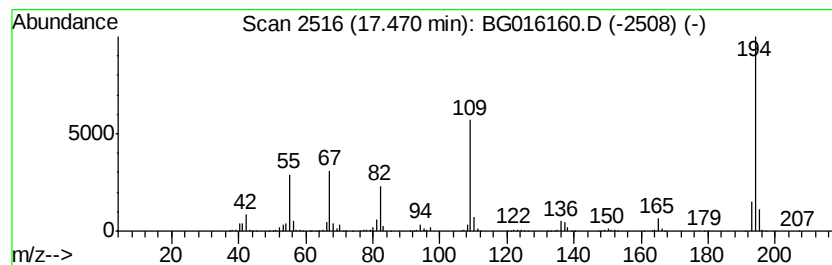
Instrument :
BNA_G
ClientSampleId :
FD4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 19 Caffeine Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD		R.T.
17.47	69.04 ng	2778690	Phenanthrene-d10		17.15
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Caffeine	194	C8H10N4O2	000058-08-2	97
2	3(2H)-Benzofuranone, 4,6-dimethoxy-	194	C10H10O4	004225-35-8	50
3	1,4-Dimethyl-4,5,7,8-tetrahydroi...	194	C8H10N4O2	130063-15-9	47
4	Anthrone	194	C14H10O	000090-44-8	43
5	.alpha.-Methylstilbene	194	C15H14	000779-51-1	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016160.D
Acq On : 27 Mar 2015 3:54
Operator : TP/IZ
Sample : G1653-08
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
FD4

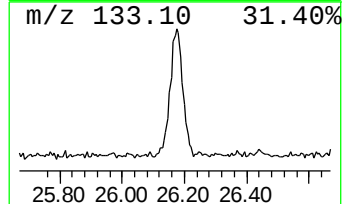
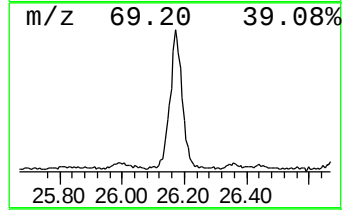
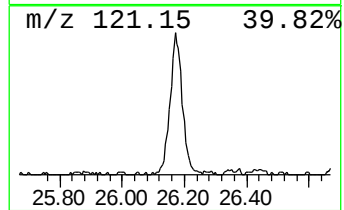
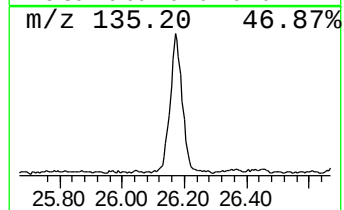
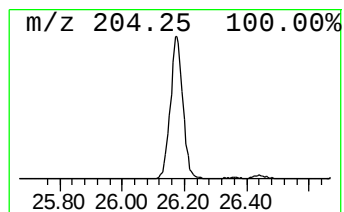
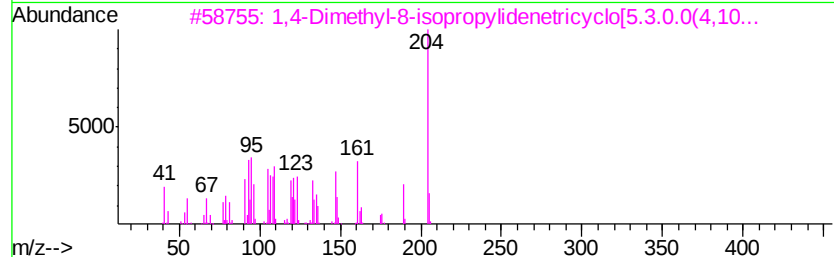
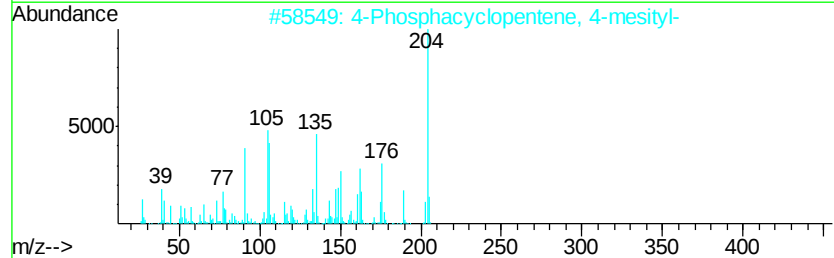
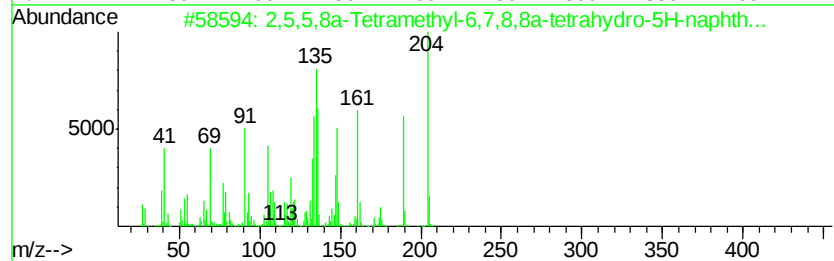
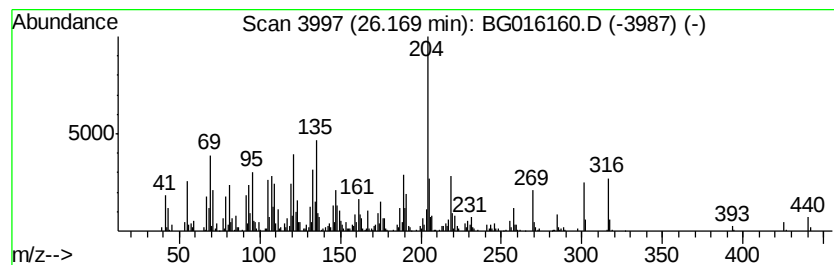
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 20 2,5,5,8a-Tetramethyl-6,7,8,... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.17	22.32 ng	991652	Perylene-d12	23.61

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2,5,5,8a-Tetramethyl-6,7,8,8a-te...	204	C14H20O	124957-09-1	50
2		4-Phosphacyclopentene, 4-mesityl-	204	C13H17P	214605-01-3	43
3		1,4-Dimethyl-8-isopropylidenetri...	204	C15H24	1000140-07-7	42
4		Naphthalene, 1,2,3,5,6,7,8,8a-oc...	204	C15H24	004630-07-3	37
5		1H-Cycloprop[e]azulene, 1a,2,3,4...	204	C15H24	000489-40-7	25



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
 Data File : BG016160.D
 Acq On : 27 Mar 2015 3:54
 Operator : TP/IZ
 Sample : G1653-08
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 FD4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2,2-dime...	2.80	36.4	ng	559805	1	7.79	307529	20.0
Propanoic acid	3.27	19.7	ng	303272	1	7.79	307529	20.0
Propanoic acid, 2...	4.20	1130.2	ng	17379100	1	7.79	307529	20.0
Butanoic acid	4.71	1628.0	ng	25033600	1	7.79	307529	20.0
Pentanoic acid, 3...	4.99	17.1	ng	263472	1	7.79	307529	20.0
Butanoic acid, 2-...	5.11	25.3	ng	388489	1	7.79	307529	20.0
Pentanoic acid	5.74	441.5	ng	6788320	1	7.79	307529	20.0
Pentanoic acid, 2...	6.34	20.2	ng	310515	1	7.79	307529	20.0
unknown7.34	7.34	97.8	ng	1504070	1	7.79	307529	20.0
Benzene, 1-methyl...	7.93	96.3	ng	1480650	1	7.79	307529	20.0
Heptanoic acid	8.47	21.6	ng	332328	1	7.79	307529	20.0
Benzeneacetic acid	11.15	12.9	ng	308856	2	10.58	480208	20.0
Nonanoic acid	11.41	12.7	ng	305147	2	10.58	480208	20.0
Cyclohexanemethan...	12.32	13.1	ng	314903	2	10.58	480208	20.0
Benzenepropanoic ...	12.42	29.1	ng	698008	2	10.58	480208	20.0
n-Decanoic acid	12.72	12.7	ng	423363	3	14.41	664570	20.0
Caffeine	17.47	69.0	ng	2778690	4	17.15	804896	20.0
2,5,5,8a-Tetramet...	26.17	22.3	ng	991652	6	23.61	888719	20.0