

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016453.D
 Acq On : 16 Apr 2015 10:38
 Operator : TP/IZ
 Sample : G1829-03
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PO-004

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-BG040615.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	2.759	7	12	21	rBV	273823	416748	8.59%	1.475%
2	2.835	21	25	38	rVB	357797	439594	9.06%	1.556%
3	4.780	347	356	364	rVB	75272	107239	2.21%	0.380%
4	5.256	431	437	448	rBV	722323	1016943	20.96%	3.599%
5	6.178	590	594	605	rBV	32441	58449	1.20%	0.207%
6	6.854	703	709	723	rVB	505500	777831	16.03%	2.753%
7	7.200	761	768	778	rBV	1341129	2079844	42.88%	7.361%
8	7.665	841	847	856	rBV	282516	444738	9.17%	1.574%
9	7.982	894	901	912	rVB	1085004	1682834	34.69%	5.956%
10	8.822	1037	1044	1054	rBV	975360	1551051	31.97%	5.489%
11	10.450	1313	1321	1328	rBV	462481	746977	15.40%	2.644%
12	12.659	1690	1697	1707	rBV	43930	72129	1.49%	0.255%
13	12.929	1734	1743	1754	rVB	2775285	4071075	83.92%	14.408%
14	13.763	1880	1885	1894	rVB	39407	55210	1.14%	0.195%
15	14.310	1970	1978	1985	rBV2	731094	1126651	23.23%	3.987%
16	15.544	2181	2188	2196	rBV2	51655	96352	1.99%	0.341%
17	15.667	2201	2209	2214	rBV2	53125	88779	1.83%	0.314%
18	15.802	2225	2232	2244	rBV	2037046	2791665	57.55%	9.880%
19	16.078	2274	2279	2285	rVB	117951	164956	3.40%	0.584%
20	17.048	2438	2444	2449	rBV2	923698	1309736	27.00%	4.635%
21	17.953	2593	2598	2605	rBV	151731	243690	5.02%	0.862%
22	18.047	2606	2614	2619	rVB2	278531	419038	8.64%	1.483%
23	19.110	2787	2795	2799	rBV	55493	105208	2.17%	0.372%
24	19.233	2812	2816	2831	rVB2	59233	101075	2.08%	0.358%
25	19.468	2852	2856	2865	rVB	32973	63662	1.31%	0.225%
26	19.680	2886	2892	2901	rBV	3832623	4850925	100.00%	17.168%
27	20.943	3103	3107	3117	rBV	249839	346808	7.15%	1.227%
28	21.143	3137	3141	3145	rBV	291076	304425	6.28%	1.077%
29	21.231	3150	3156	3160	rBV	982863	1289998	26.59%	4.565%
30	22.388	3349	3353	3359	rBV	137935	199343	4.11%	0.705%
31	23.458	3528	3535	3548	rVB	656782	1233182	25.42%	4.364%

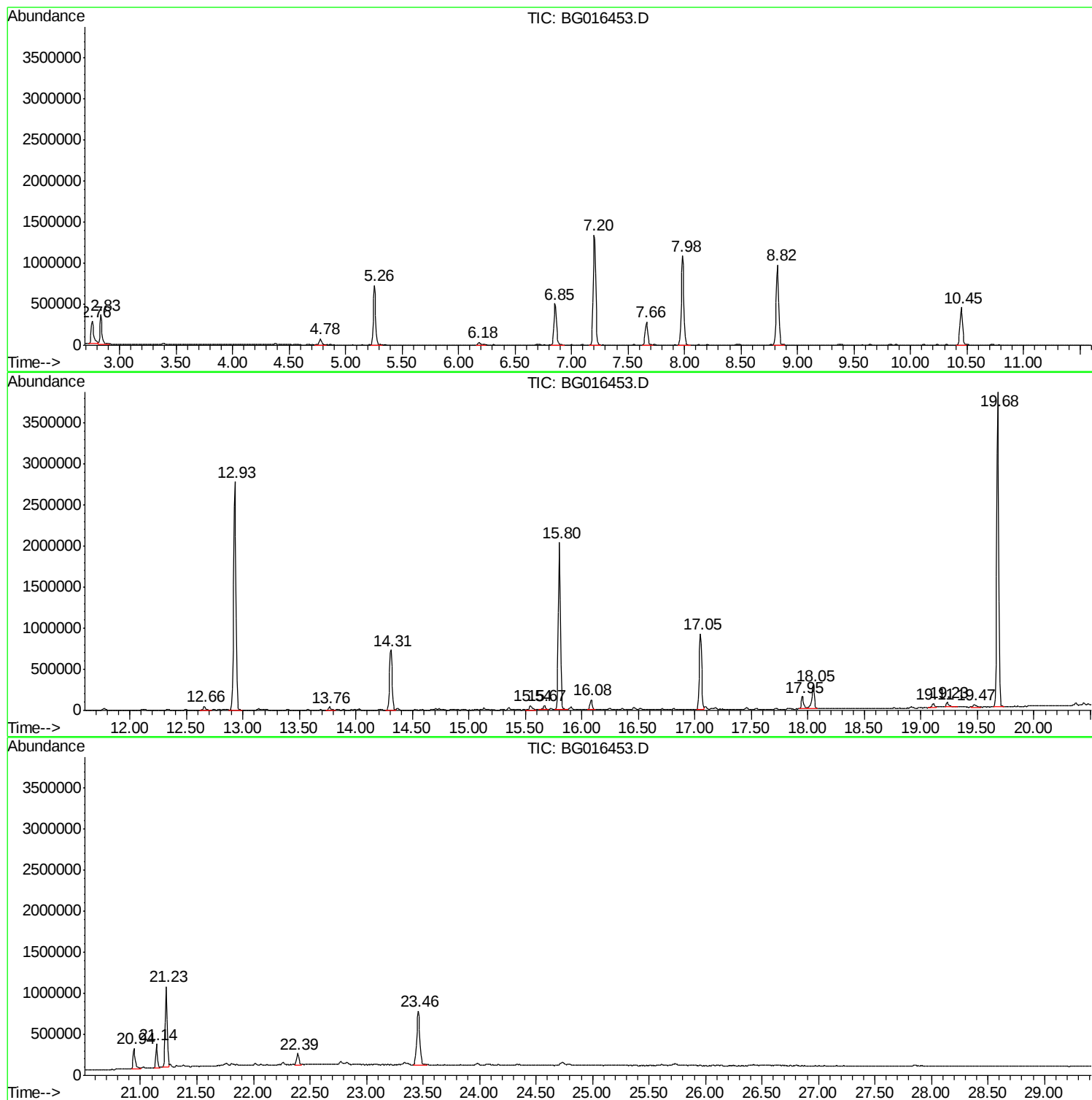
Sum of corrected areas: 28256155

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

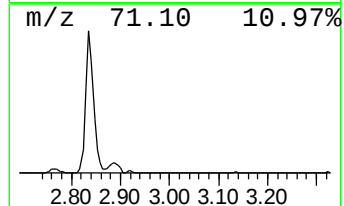
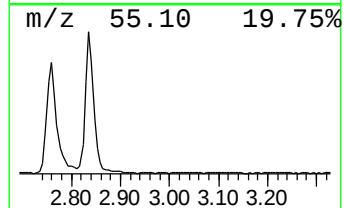
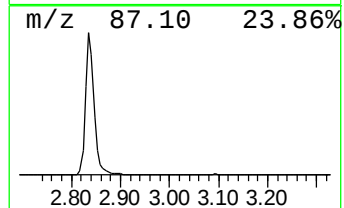
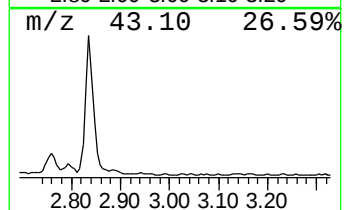
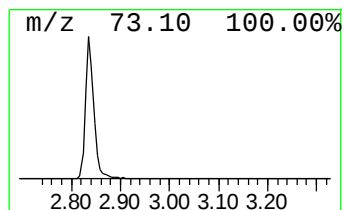
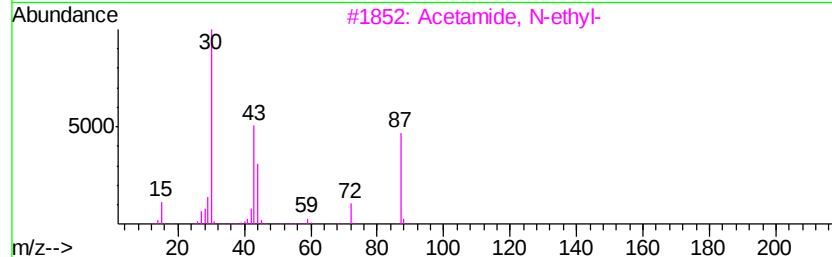
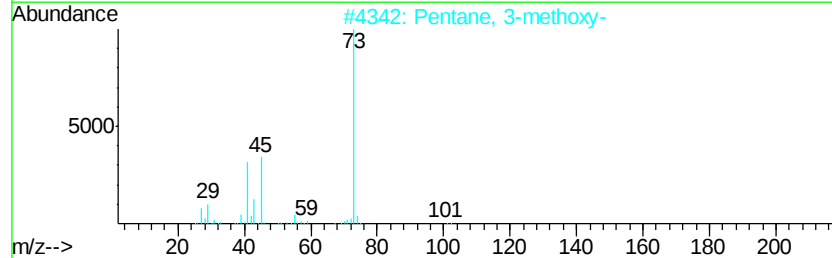
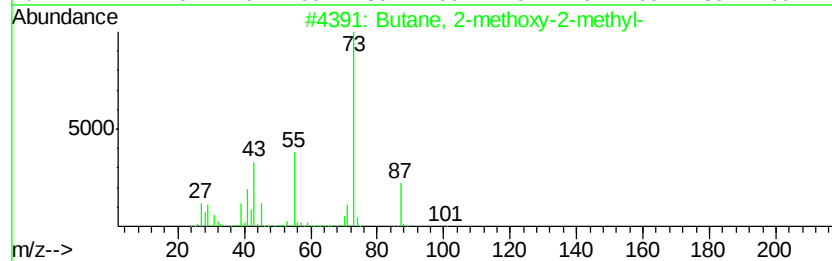
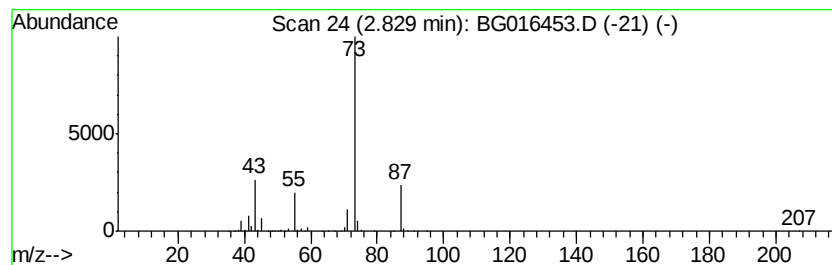
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.83	19.77 ng	439594	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	74
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetic acid, 3-[1,3]dioxolan-2-y...	174	C8H14O4	1000186-02-3	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

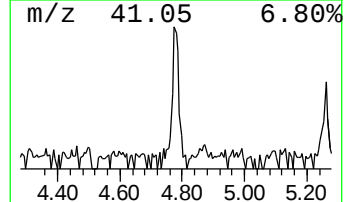
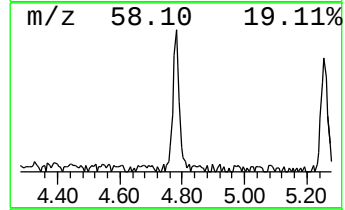
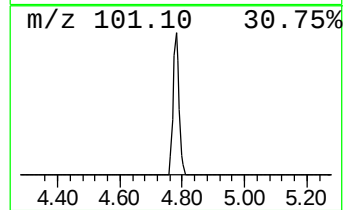
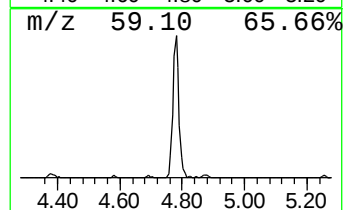
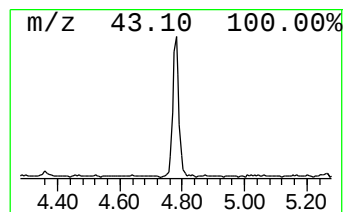
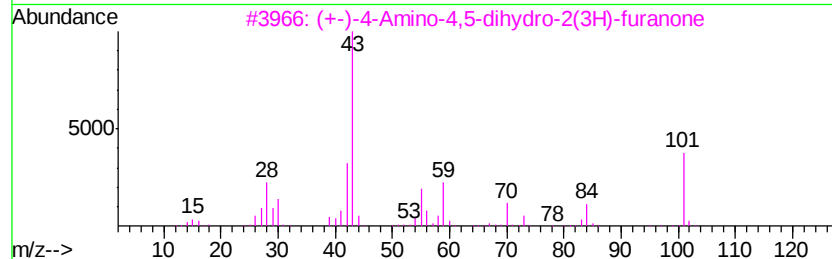
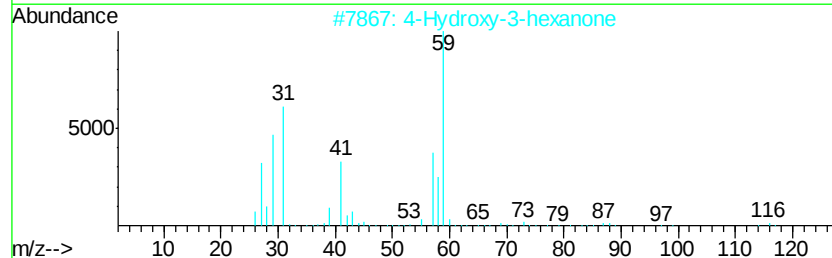
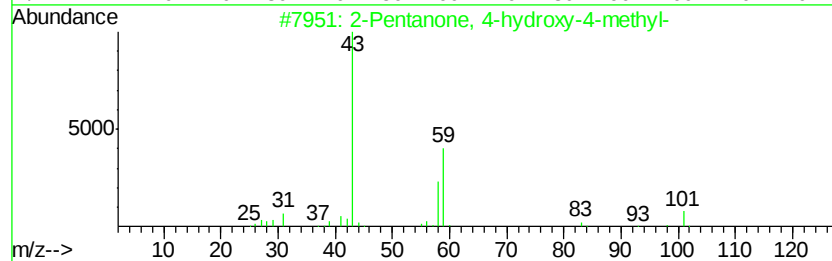
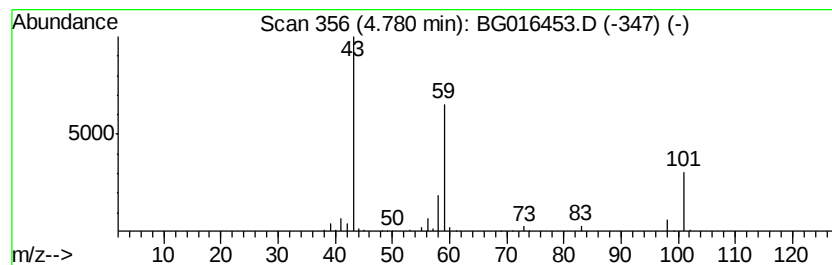
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	4.82 ng	107239	1,4-Dichlorobenzene-d4	7.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
3		(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	23
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23
5		Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	16



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

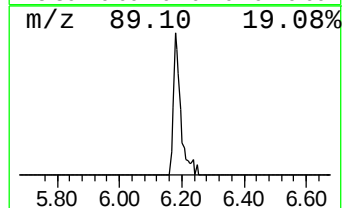
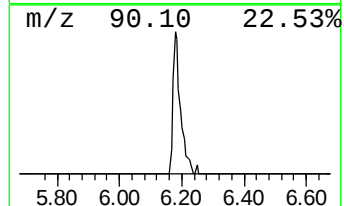
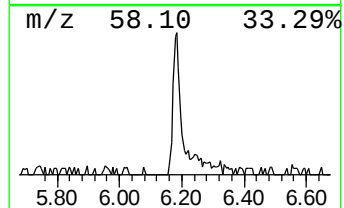
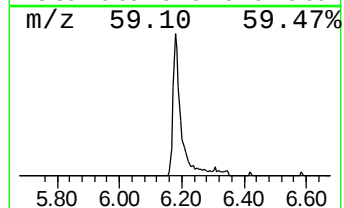
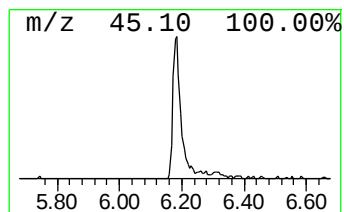
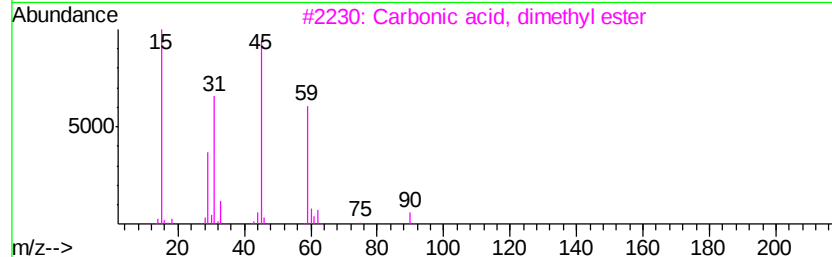
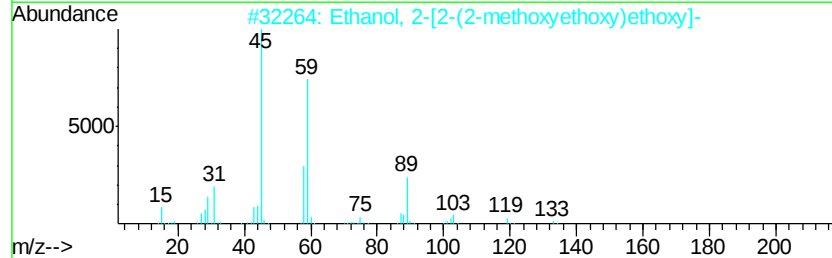
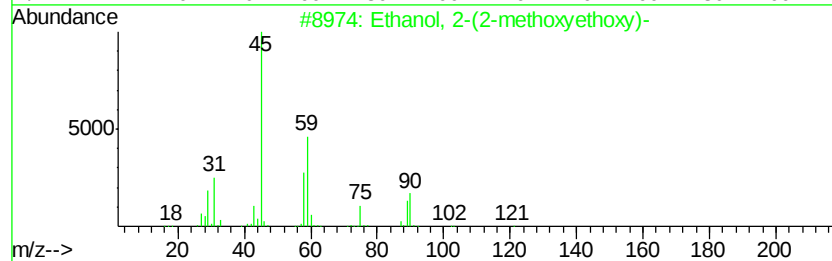
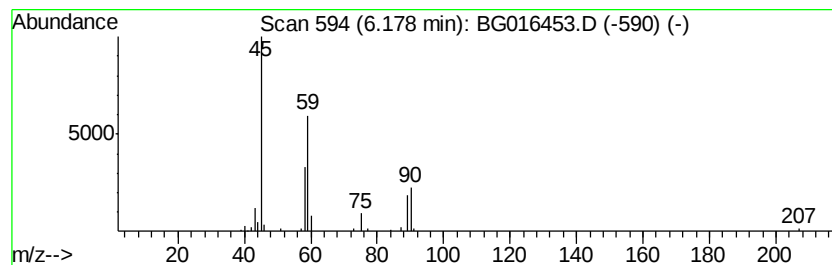
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 Ethanol, 2-(2-methoxyethoxy)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.18	2.63 ng	58449	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanol, 2-(2-methoxyethoxy)-	120	C5H12O3	000111-77-3	78
2		Ethanol, 2-[2-(2-methoxyethoxy)e...	164	C7H16O4	000112-35-6	39
3		Carbonic acid, dimethyl ester	90	C3H6O3	000616-38-6	33
4		Butanoic acid, 4-methoxy-, methy...	132	C6H12O3	029006-01-7	33
5		Ethene, (2-methoxyethoxy)-	102	C5H10O2	001663-35-0	28



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

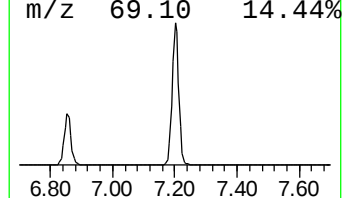
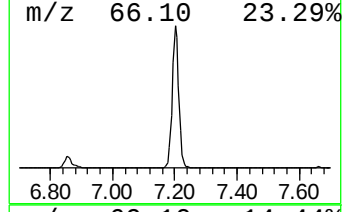
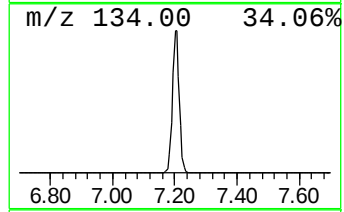
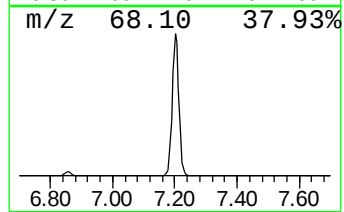
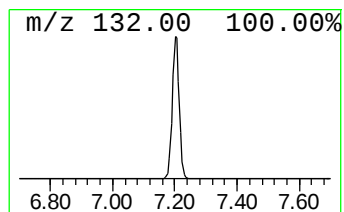
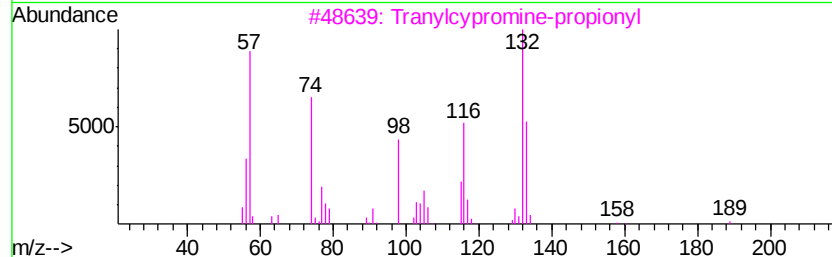
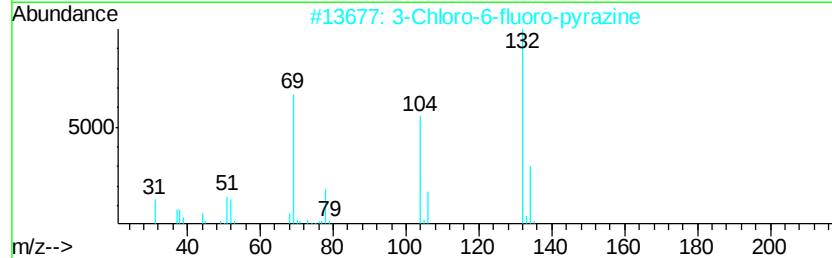
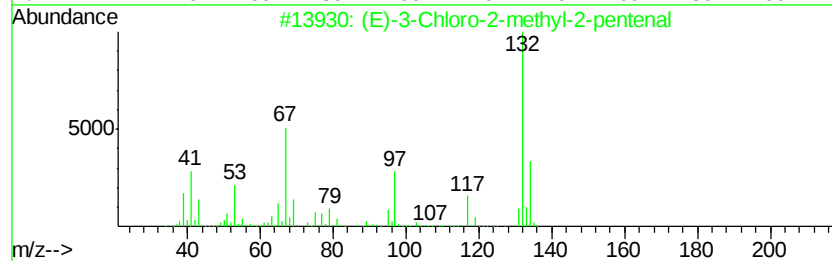
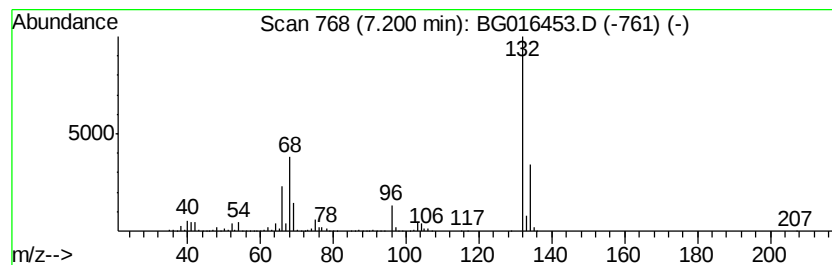
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	93.53 ng	2079840	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

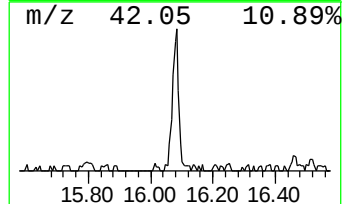
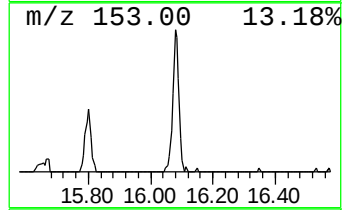
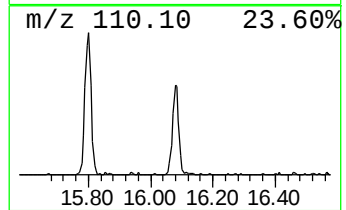
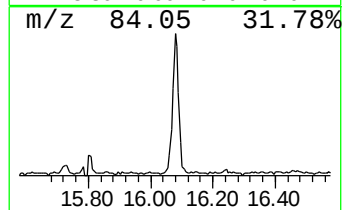
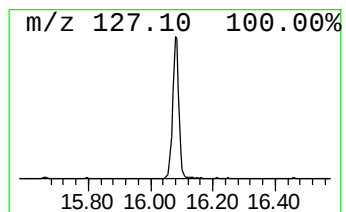
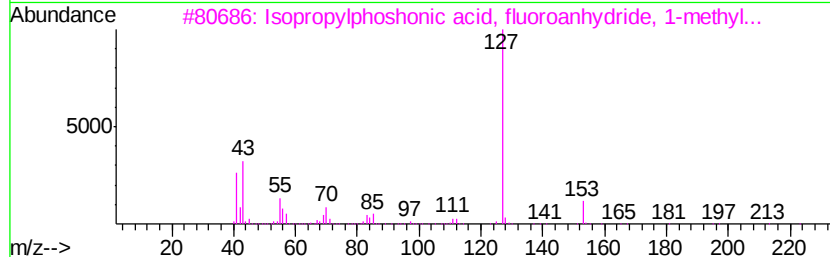
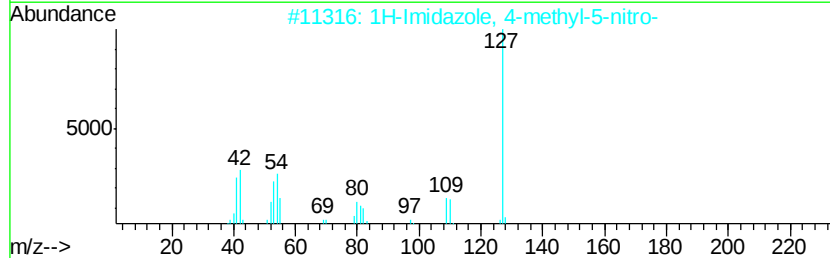
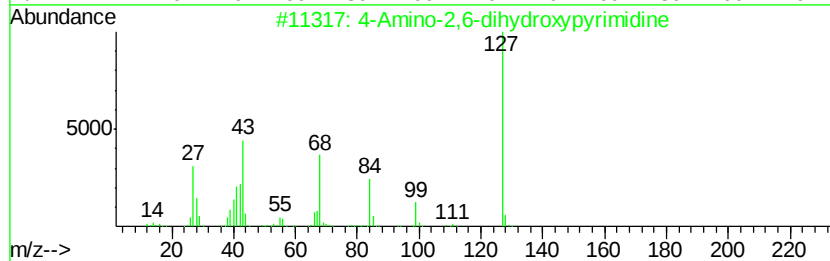
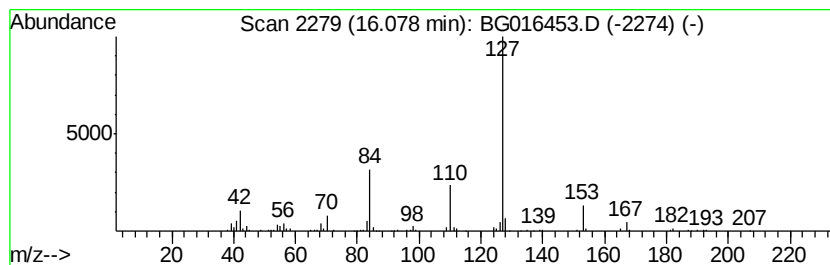
Instrument :
BNA_G
ClientSampleId :
PO-004

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 4-Amino-2,6-dihydroxypyrimi... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.	
16.08	2.52 ng	164956	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Amino-2,6-dihydroxypyrimidine	127	C4H5N3O2	000873-83-6	50
2	1H-Imidazole, 4-methyl-5-nitro-	127	C4H5N3O2	014003-66-8	50
3	Isopropylphosphonic acid, fluoroa...	238	C11H24F02P	1000273-54-8	50
4	1H-Imidazole, 1-methyl-5-nitro-	127	C4H5N3O2	003034-42-2	47
5	1-(4-Fluoro-benzenesulfonyl)-pip...	286	C12H15FN2O3S	1000295-13-0	45



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

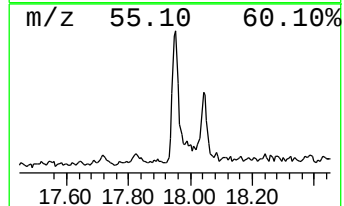
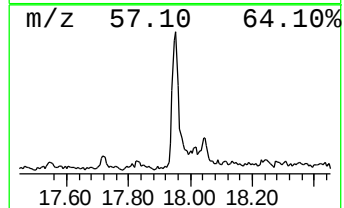
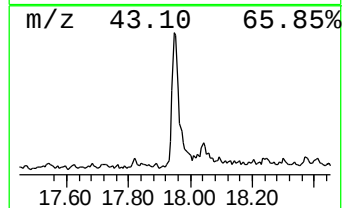
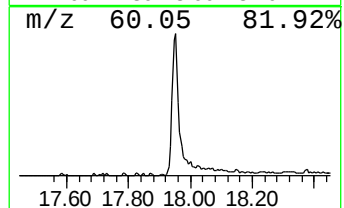
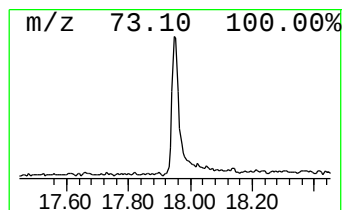
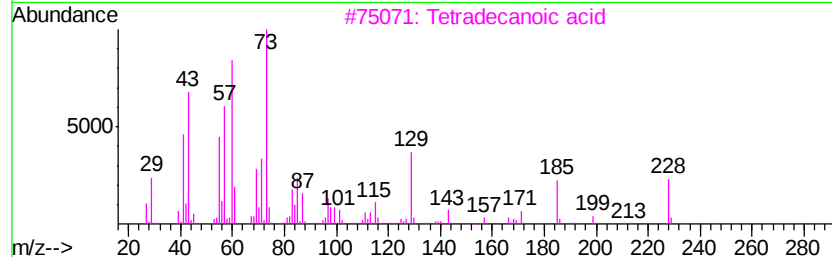
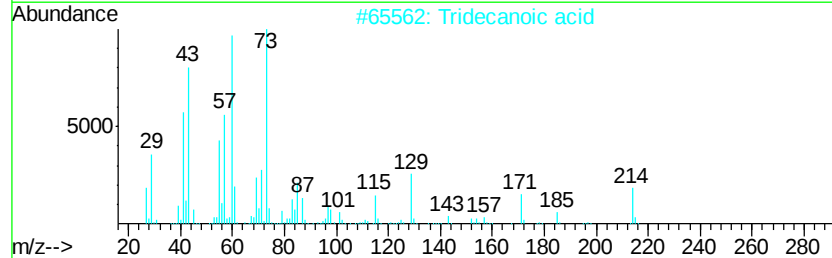
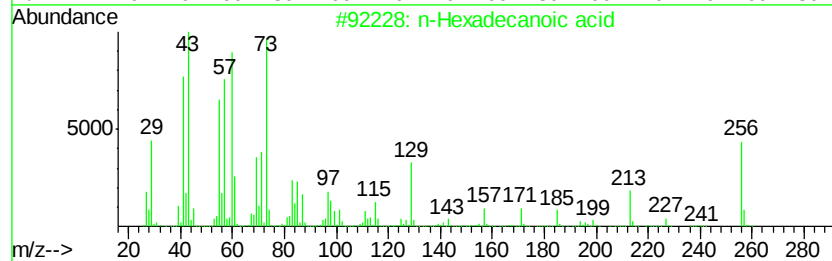
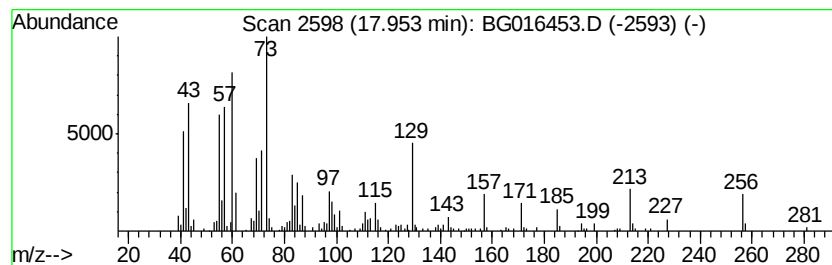
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	3.72 ng	243690	Phenanthrene-d10	17.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	86
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Undecanoic acid	186	C11H22O2	000112-37-8	62



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

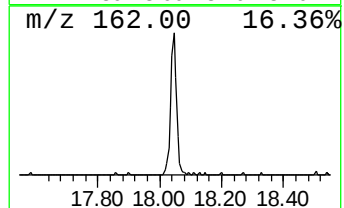
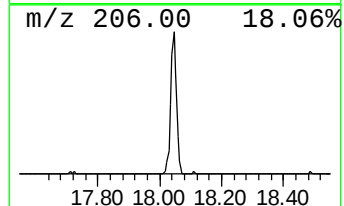
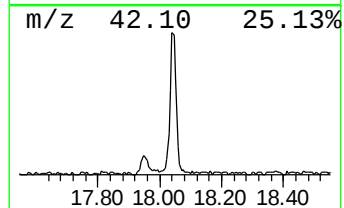
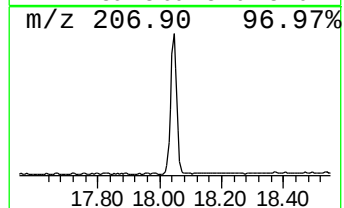
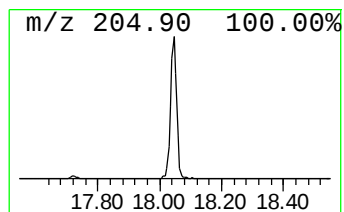
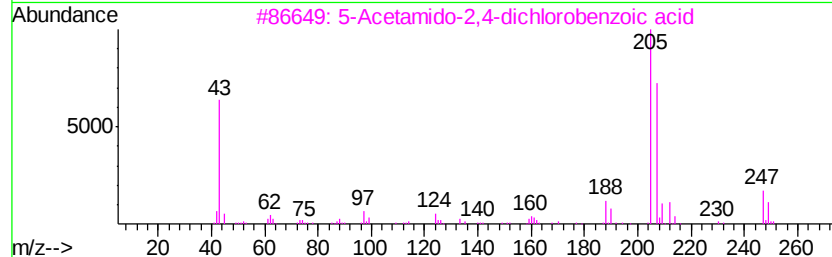
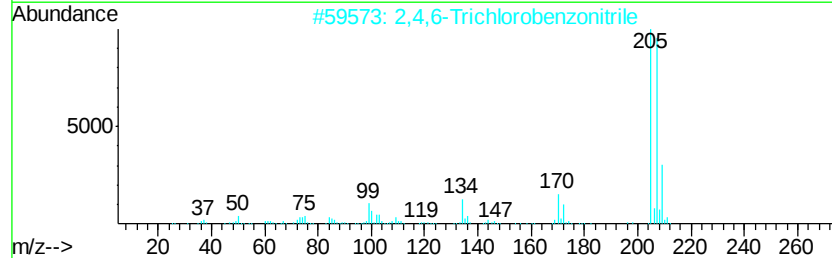
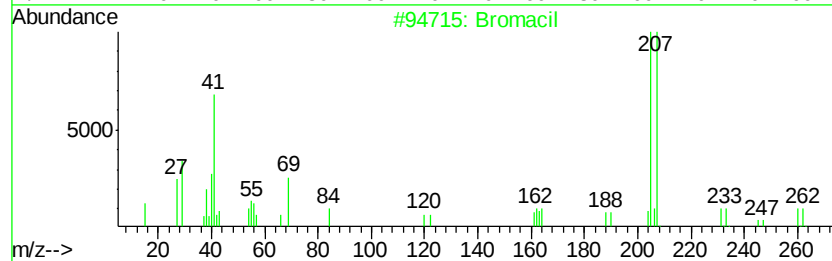
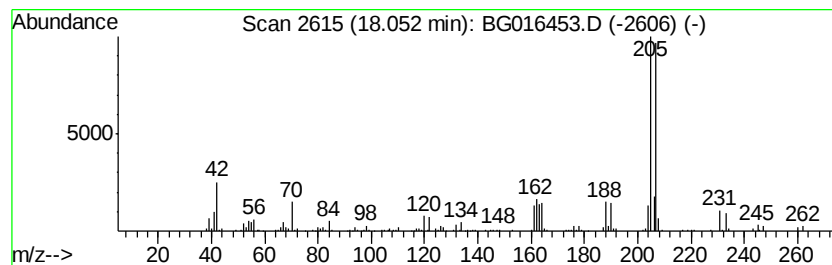
Instrument :
BNA_G
ClientSampleId :
PO-004

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Bromacil Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.05	6.40 ng	419038	Phenanthrene-d10	17.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Bromacil	260	C9H13BrN2O2	000314-40-9	94
2	2,4,6-Trichlorobenzonitrile	205	C7H2Cl3N	006575-05-9	58
3	5-Acetamido-2,4-dichlorobenzoic ...	247	C9H7Cl2NO3	050602-49-8	45
4	Benzoic acid, 3-amino-2,5-dichloro-	205	C7H5Cl2NO2	000133-90-4	45
5	Phenol, 2,4-bis(1,1-dimethylprop...	234	C16H26O	000120-95-6	27



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

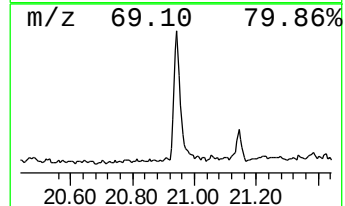
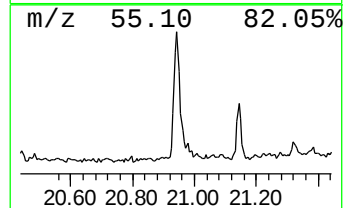
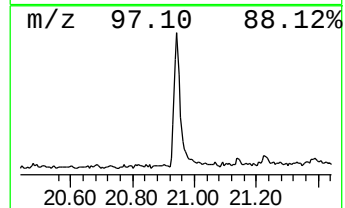
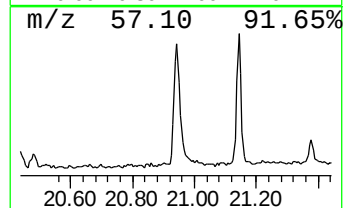
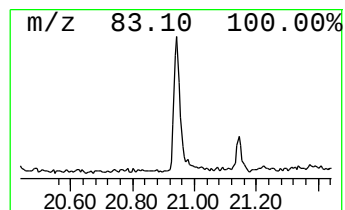
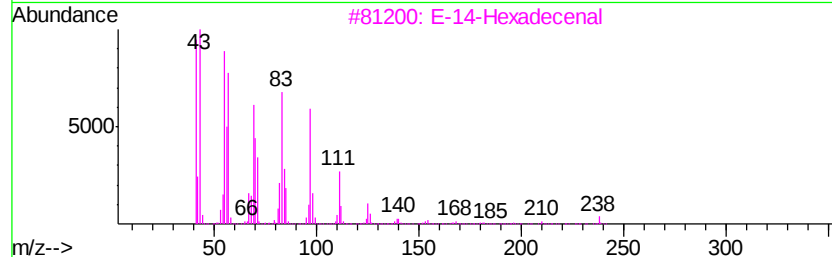
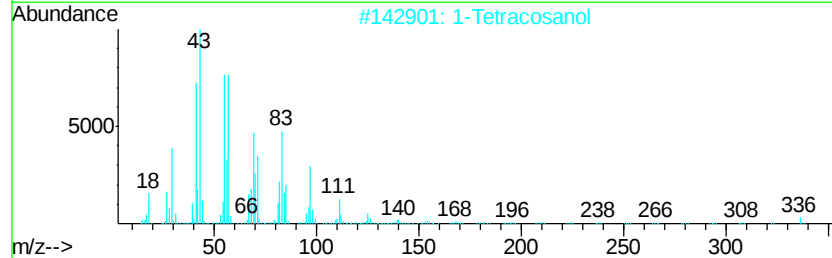
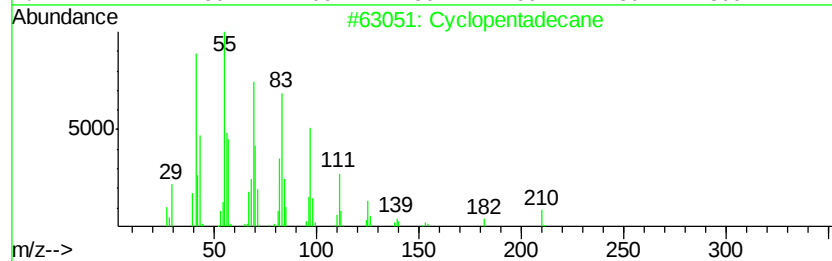
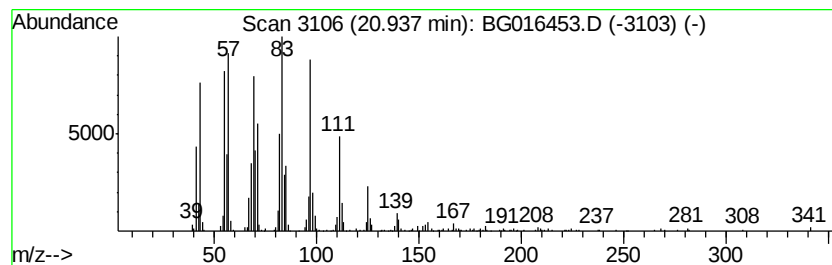
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Cyclopentadecane Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	5.38 ng	346808	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclopentadecane	210	C15H30	000295-48-7	93
2		1-Tetracosanol	354	C24H50O	000506-51-4	91
3		E-14-Hexadecenal	238	C16H30O	330207-53-9	91
4		Trifluoroacetic acid, n-octadecyl...	366	C20H37F3O2	079392-43-1	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

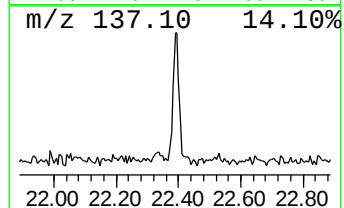
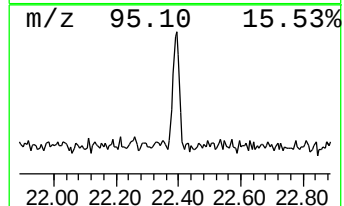
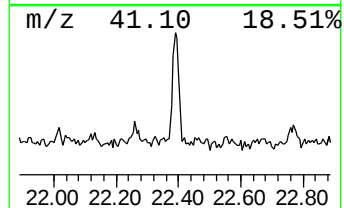
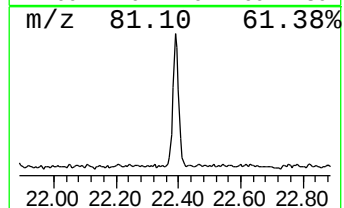
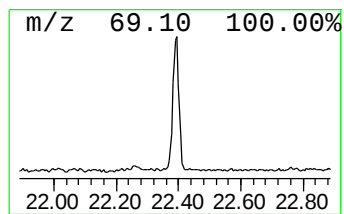
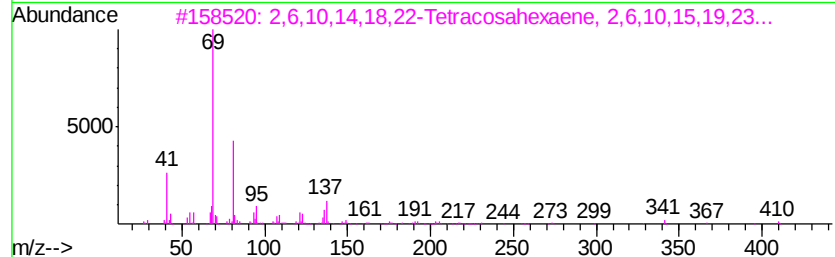
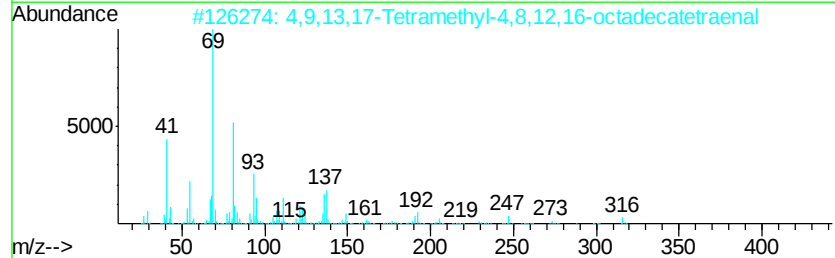
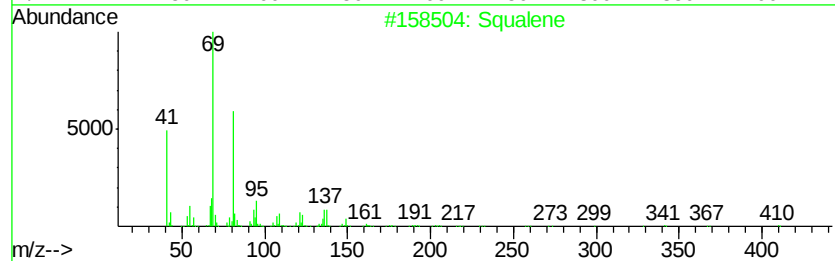
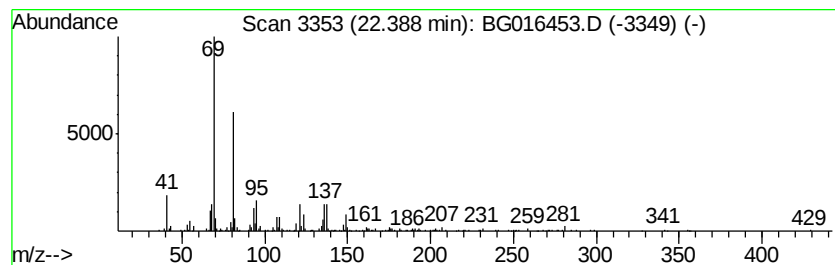
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Squalene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.39	3.23 ng	199343	Perylene-d12	23.46

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	007683-64-9	91
2		4,9,13,17-Tetramethyl-4,8,12,16-...	316	C22H36O	056882-09-8	83
3		2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	78
4		3,7,11-Tridecatricienoic acid, 4,8...	264	C17H28O2	036237-70-4	72
5		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
Data File : BG016453.D
Acq On : 16 Apr 2015 10:38
Operator : TP/IZ
Sample : G1829-03
Misc :
ALS Vial : 18 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PO-004

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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
Butane, 2-methoxy...	2.83	19.8	ng	439594	1	7.66	444738	20.0
2-Pentanone, 4-hy...	4.78	4.8	ng	107239	1	7.66	444738	20.0
Ethanol, 2-(2-met...	6.18	2.6	ng	58449	1	7.66	444738	20.0
unknown7.20	7.20	93.5	ng	2079840	1	7.66	444738	20.0
4-Amino-2,6-dihyd...	16.08	2.5	ng	164956	4	17.05	1309740	20.0
n-Hexadecanoic acid	17.95	3.7	ng	243690	4	17.05	1309740	20.0
Bromacil	18.05	6.4	ng	419038	4	17.05	1309740	20.0
Cyclopentadecane	20.94	5.4	ng	346808	5	21.23	1290000	20.0
Squalene	22.39	3.2	ng	199343	6	23.46	1233180	20.0