

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
 Data File : BG019967.D
 Acq On : 6 Dec 2015 15:06
 Operator : UM/NP
 Sample : G4650-19
 Misc :
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 COFF(0-2)-5

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-BG120215.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	2.991	21	26	38	rBV	69521	105566	6.64%	1.006%
2	5.188	395	400	411	rVB	75819	113735	7.15%	1.083%
3	5.658	473	480	489	rBV	369821	577738	36.34%	5.504%
4	7.257	745	752	762	rBV	405000	698200	43.92%	6.651%
5	7.638	809	817	825	rBV	381035	647419	40.72%	6.167%
6	8.114	890	898	904	rBV	118695	193227	12.15%	1.841%
7	8.438	946	953	962	rBV	243970	419435	26.38%	3.996%
8	9.278	1089	1096	1106	rBV	245412	428892	26.98%	4.086%
9	10.929	1370	1377	1385	rBV	169119	293443	18.46%	2.795%
10	13.367	1783	1792	1801	rBV	701180	1049101	65.99%	9.994%
11	14.184	1925	1931	1940	rBV	136501	201019	12.64%	1.915%
12	14.624	2001	2006	2011	rBV	22248	26687	1.68%	0.254%
13	14.742	2015	2026	2036	rBV2	291726	457427	28.77%	4.357%
14	15.576	2163	2168	2172	rVB	33082	42729	2.69%	0.407%
15	15.976	2228	2236	2241	rBV5	9708	19388	1.22%	0.185%
16	16.223	2271	2278	2288	rBV	574223	854019	53.72%	8.135%
17	16.434	2309	2314	2317	rBV	32838	43530	2.74%	0.415%
18	16.869	2385	2388	2397	rVB6	6690	16092	1.01%	0.153%
19	17.227	2442	2449	2453	rBV2	17093	24372	1.53%	0.232%
20	17.486	2486	2493	2500	rBV	373766	578859	36.41%	5.514%
21	18.355	2636	2641	2648	rBV2	54683	77312	4.86%	0.736%
22	18.878	2723	2730	2735	rBV2	12137	21941	1.38%	0.209%
23	19.131	2768	2773	2777	rBV3	10885	17263	1.09%	0.164%
24	19.213	2783	2787	2794	rBV	24547	36712	2.31%	0.350%
25	19.507	2828	2837	2839	rBV9	7001	16831	1.06%	0.160%
26	19.624	2853	2857	2863	rBV5	23370	38534	2.42%	0.367%
27	19.771	2876	2882	2888	rBV2	59830	90602	5.70%	0.863%
28	19.889	2898	2902	2905	rVB2	24150	26201	1.65%	0.250%
29	20.083	2929	2935	2941	rBV	1242442	1589763	100.00%	15.144%
30	20.764	3047	3051	3056	rVB2	17691	23913	1.50%	0.228%
31	20.811	3056	3059	3067	rBV4	53440	66208	4.16%	0.631%
32	21.029	3093	3096	3100	rVB2	15368	18918	1.19%	0.180%
33	21.387	3152	3157	3164	rVB4	46128	75649	4.76%	0.721%
34	21.751	3213	3219	3227	rVB	460476	758450	47.71%	7.225%

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

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-BG120215.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	21.945	3249	3252	3256	rVB2	17810	23745	1.49%	0.226%
36	22.568	3355	3358	3363	rVB4	13782	18575	1.17%	0.177%
37	23.279	3474	3479	3486	rVB6	13100	23037	1.45%	0.219%
38	23.479	3506	3513	3518	rBV3	32663	68363	4.30%	0.651%
39	25.036	3767	3778	3793	rVB2	243641	714604	44.95%	6.807%

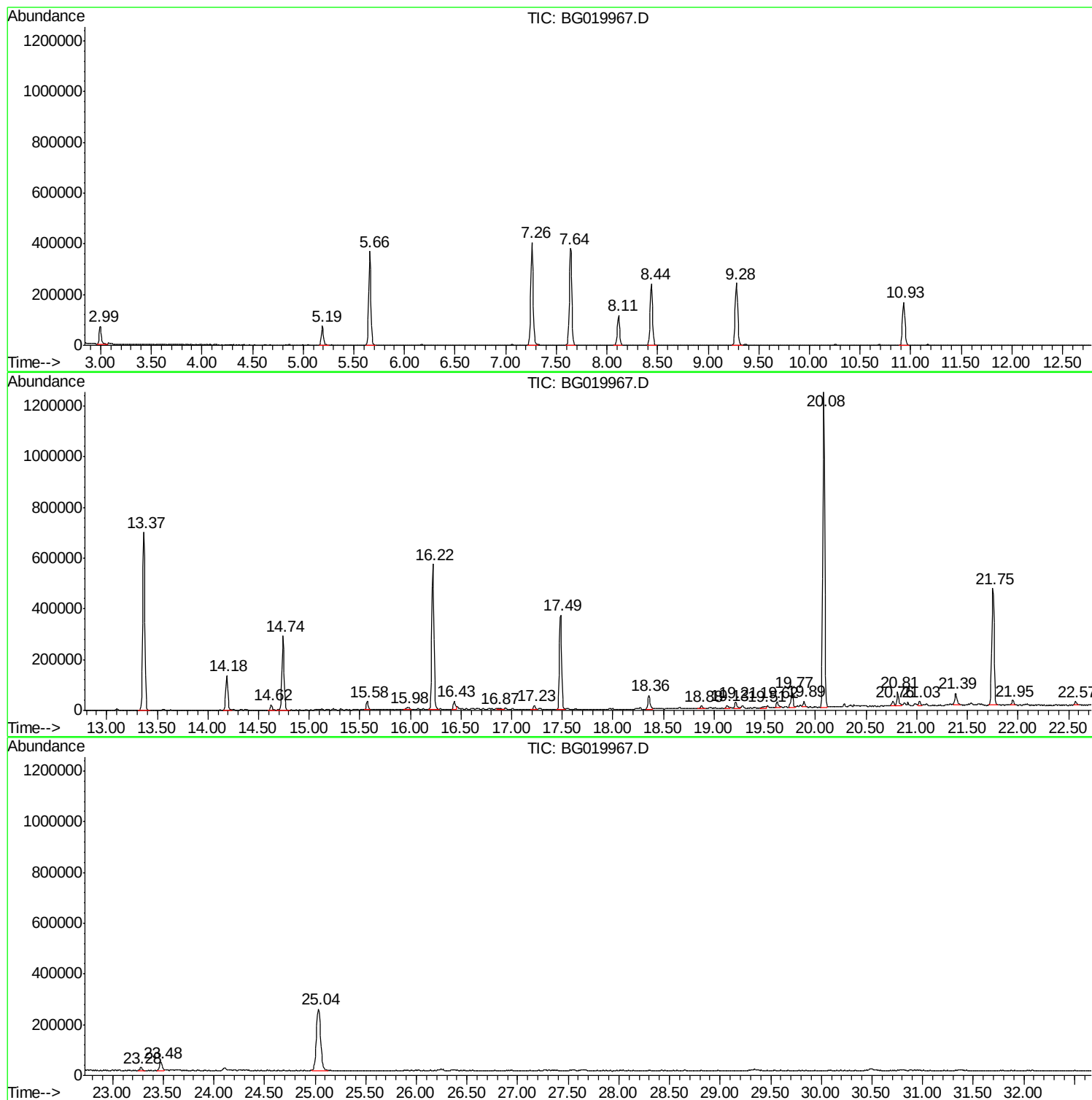
Sum of corrected areas: 10497499

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.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\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

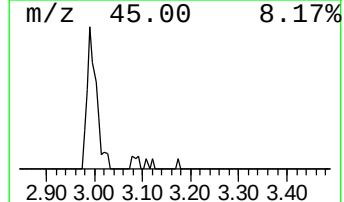
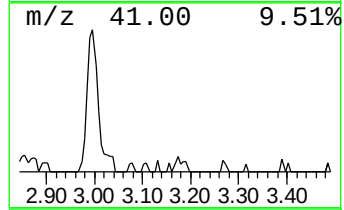
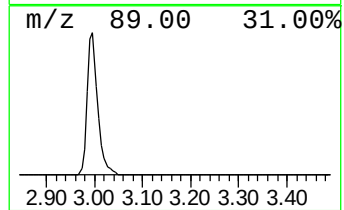
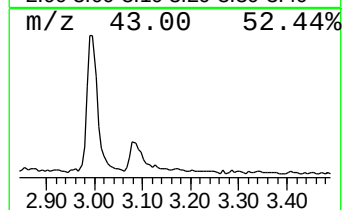
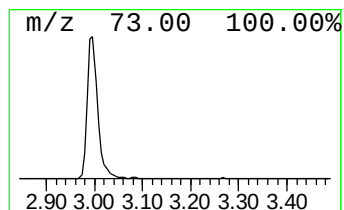
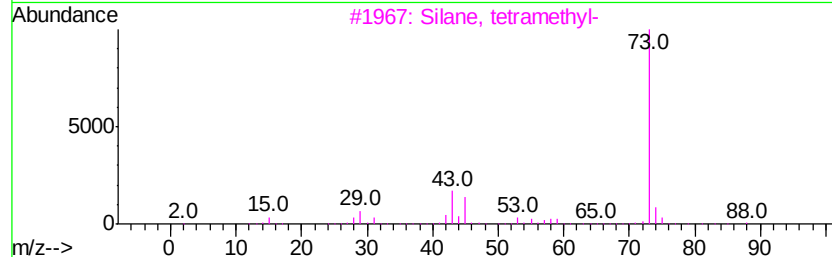
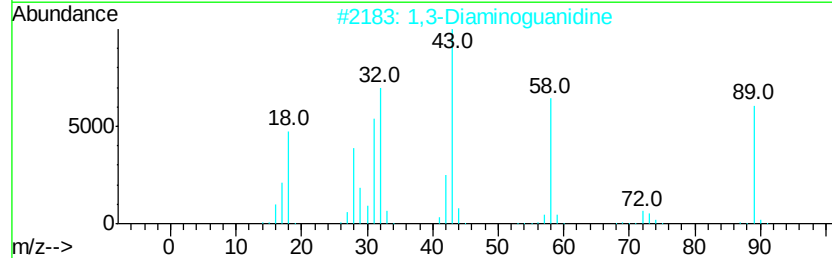
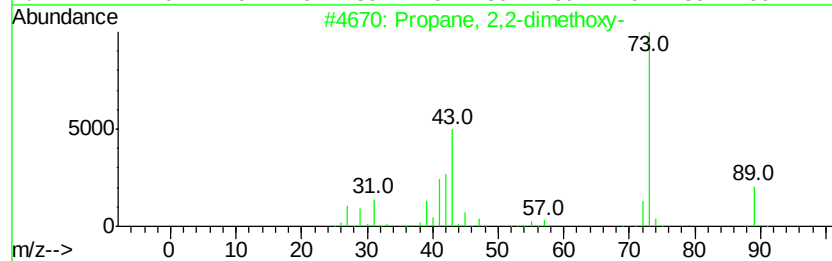
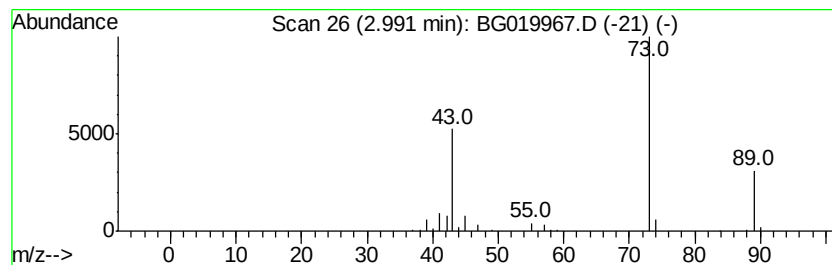
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.99 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	10.93 ng	105566	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
5		1,3-Dioxolane, 2-(3-bromo-5,5,5-...	352	C10H16BrCl3O2	1000115-31-4	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

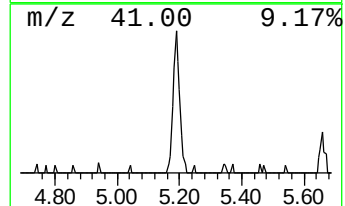
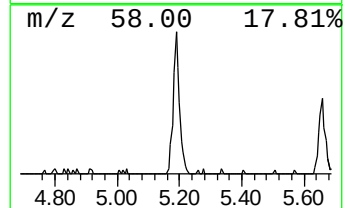
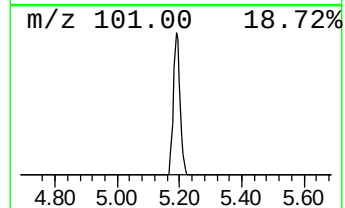
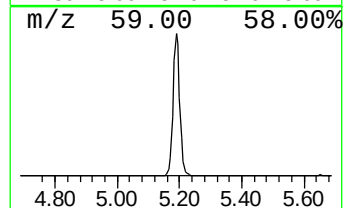
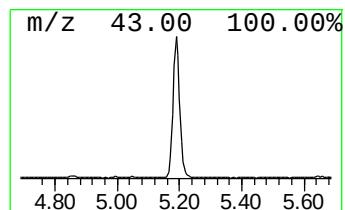
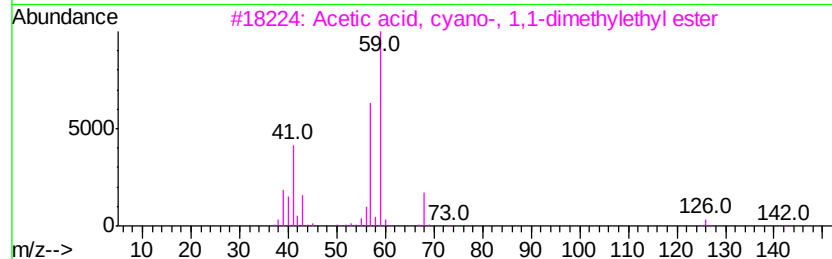
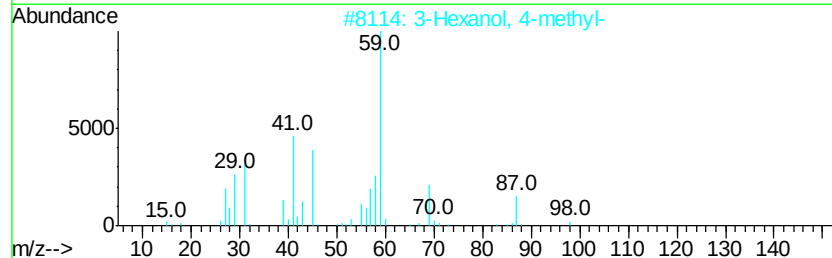
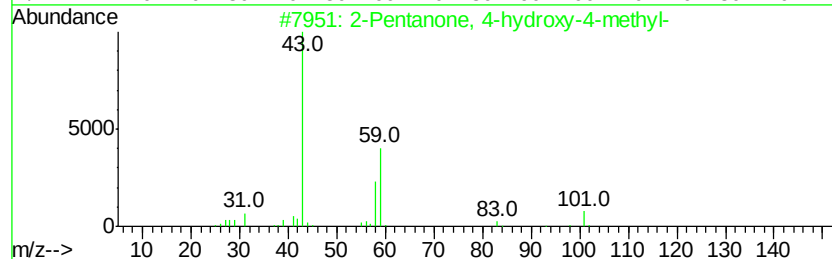
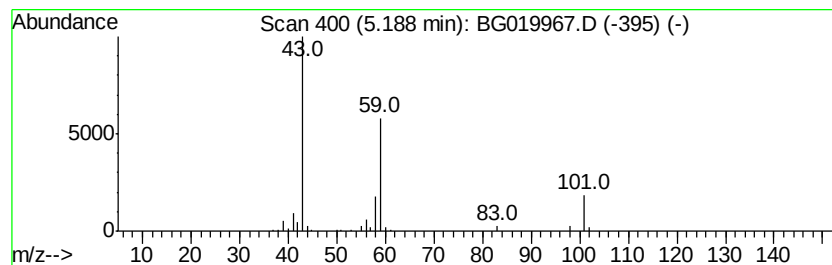
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	11.77 ng	113735	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
2		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	25
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		Acetone	58	C3H6O	000067-64-1	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

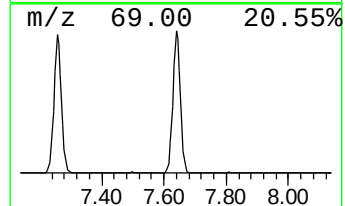
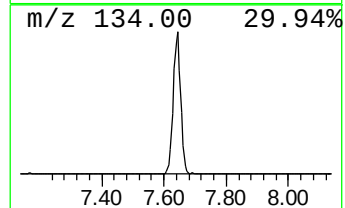
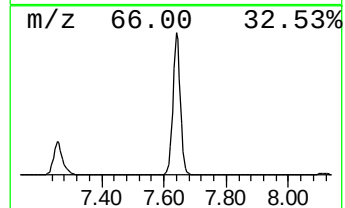
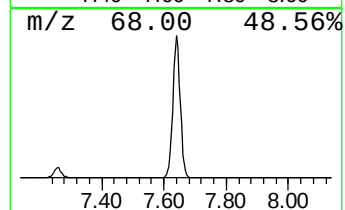
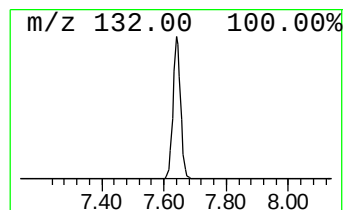
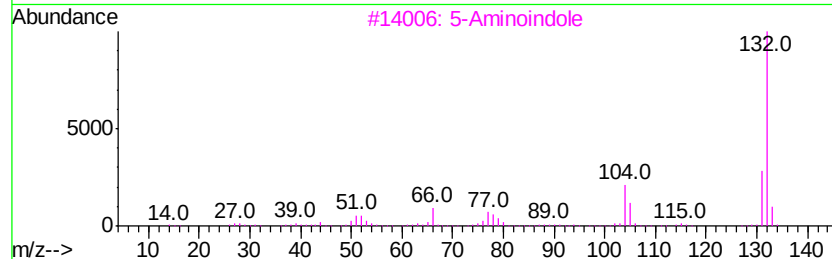
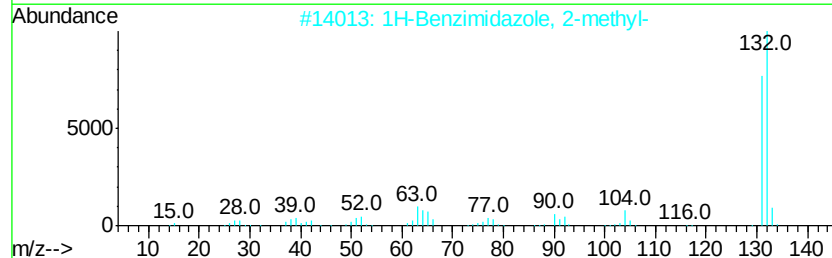
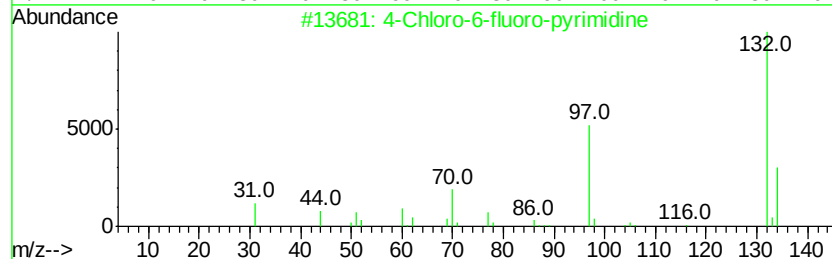
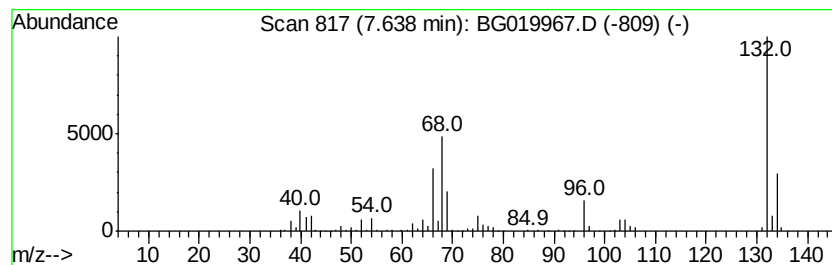
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.64 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	67.01 ng	647419	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		5-Aminoindole	132	C8H8N2	005192-03-0	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

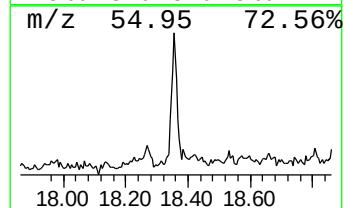
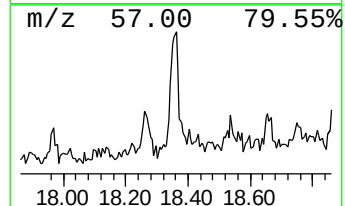
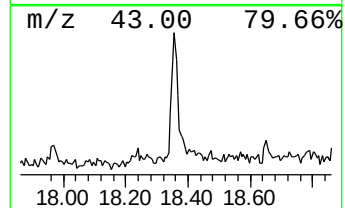
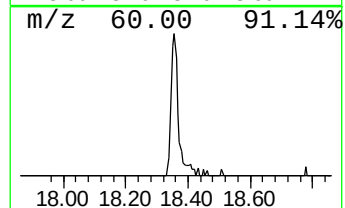
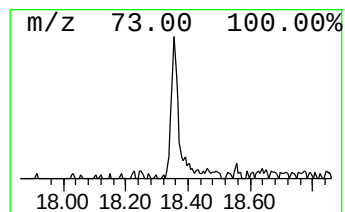
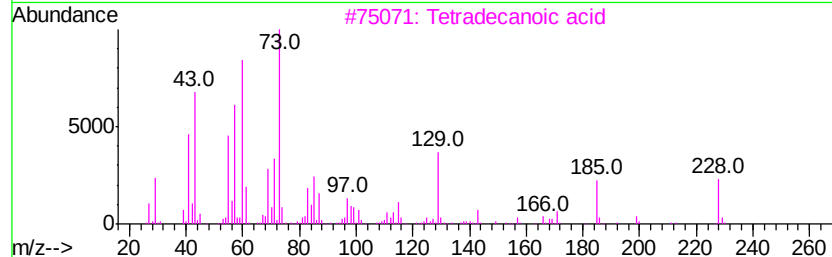
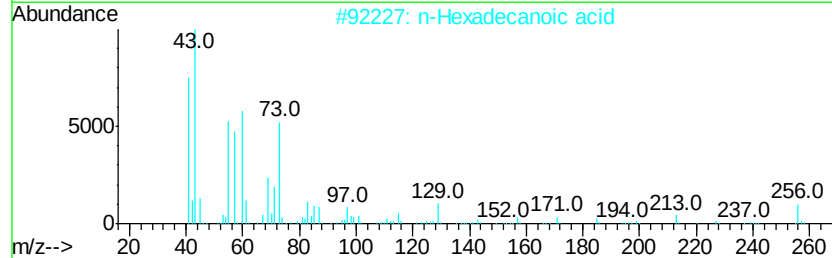
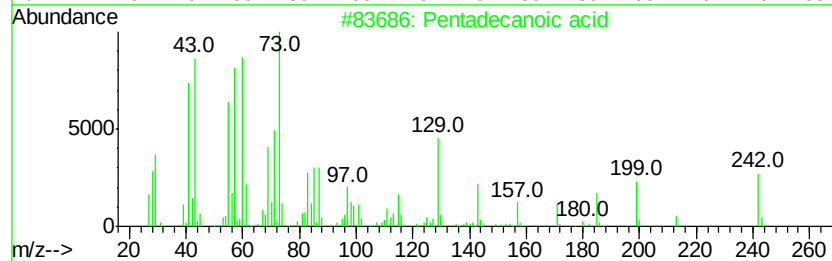
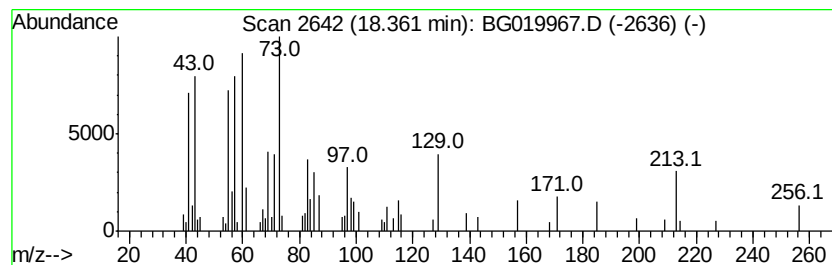
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Pentadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.36	2.67 ng	77312	Phenanthrene-d10	17.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	70
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	59
5		.alpha.-D-Glucopyranose, 4-O-.be...	342	C12H22O11	014641-93-1	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

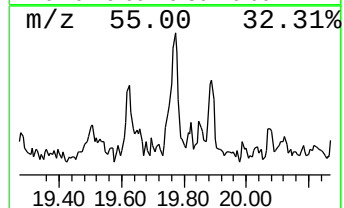
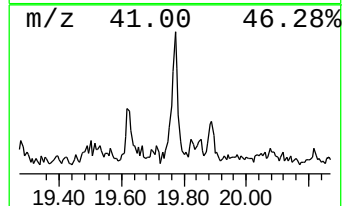
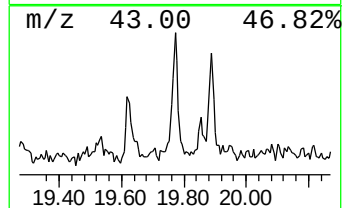
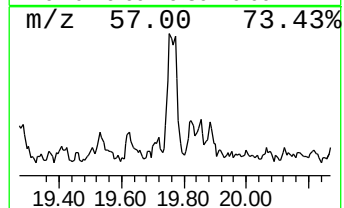
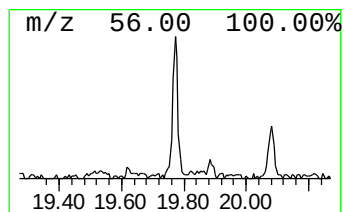
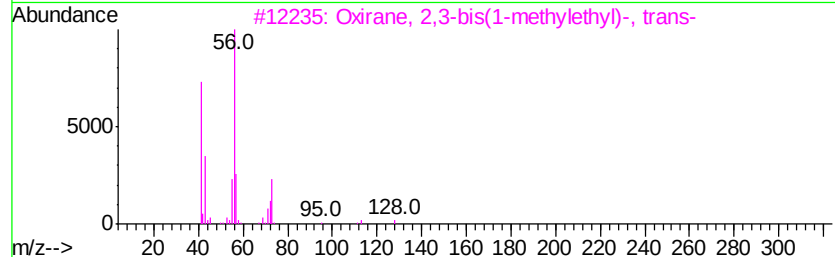
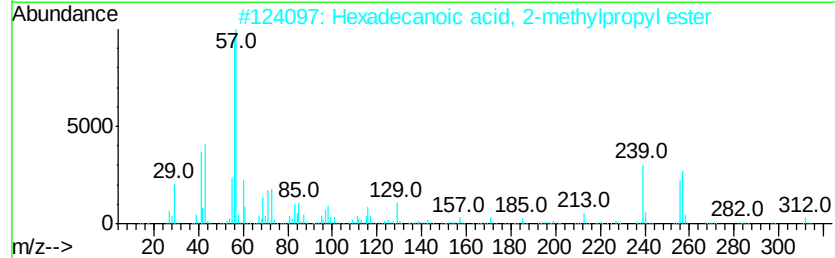
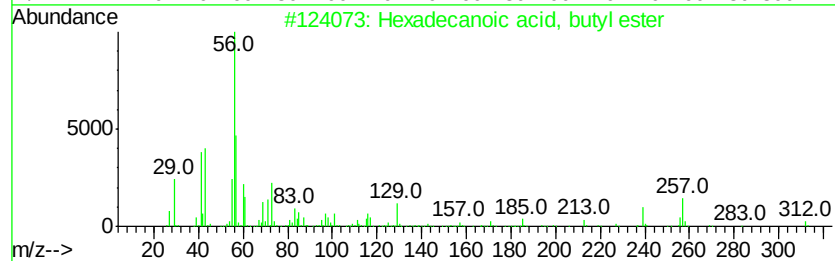
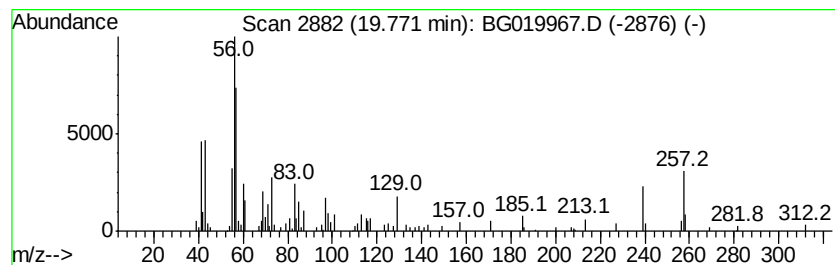
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.77	2.39 ng	90602	Chrysene-d12	21.75

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	95
2		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	90
3		Oxirane, 2,3-bis(1-methylethyl)-...	128	C8H16O	054644-32-5	38
4		1-Pentene, 2,4-dimethyl-	98	C7H14	002213-32-3	35
5		Cyclobutanone, 3,3-dimethyl-	98	C6H10O	001192-33-2	35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120615\
Data File : BG019967.D
Acq On : 6 Dec 2015 15:06
Operator : UM/NP
Sample : G4650-19
Misc :
ALS Vial : 9 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-5

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG120215.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
unknown2.99	2.99	10.9	ng	105566	1	8.11	193227	20.0
2-Pentanone, 4-hy...	5.19	11.8	ng	113735	1	8.11	193227	20.0
unknown7.64	7.64	67.0	ng	647419	1	8.11	193227	20.0
Pentadecanoic acid	18.36	2.7	ng	77312	4	17.49	578859	20.0
Hexadecanoic acid...	19.77	2.4	ng	90602	5	21.75	758450	20.0