

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
 Data File : BG016364.D
 Acq On : 13 Apr 2015 17:16
 Operator : TP/IZ
 Sample : G1744-09
 Misc :
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TD-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-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	2.767	8	13	23	rBV	115302	249848	11.45%	1.417%
2	2.855	23	28	33	rVV	68576	109580	5.02%	0.622%
3	2.902	33	36	43	rVB2	16658	23451	1.08%	0.133%
4	4.794	352	358	366	rVB	104239	153322	7.03%	0.870%
5	5.264	432	438	449	rBV	836315	1167934	53.54%	6.624%
6	6.862	703	710	722	rBV	816476	1264372	57.97%	7.171%
7	7.209	762	769	778	rBV	800617	1272652	58.35%	7.218%
8	7.673	842	848	856	rVB	265696	424375	19.46%	2.407%
9	7.996	896	903	911	rVB	610227	963670	44.18%	5.466%
10	8.831	1036	1045	1056	rBV	484846	761093	34.89%	4.317%
11	10.464	1315	1323	1330	rBV	381355	634667	29.10%	3.600%
12	12.938	1737	1744	1757	rVB	1157235	1623770	74.44%	9.210%
13	13.778	1881	1887	1897	rBV	48032	67138	3.08%	0.381%
14	14.318	1972	1979	1989	rVB2	559411	815795	37.40%	4.627%
15	15.170	2120	2124	2128	rVB2	18258	22246	1.02%	0.126%
16	15.805	2226	2232	2240	rBV	750048	1030037	47.22%	5.842%
17	16.028	2266	2270	2280	rBV	19901	32990	1.51%	0.187%
18	17.056	2439	2445	2457	rBV2	708391	976304	44.76%	5.537%
19	17.955	2593	2598	2607	rBV2	48575	86300	3.96%	0.489%
20	19.383	2836	2841	2851	rBV	316120	355489	16.30%	2.016%
21	19.500	2858	2861	2866	rVB	66766	72914	3.34%	0.414%
22	19.683	2887	2892	2903	rBV	1746134	2181220	100.00%	12.371%
23	20.376	3007	3010	3014	rVB2	21310	22047	1.01%	0.125%
24	20.429	3014	3019	3025	rBV	238895	258392	11.85%	1.466%
25	20.488	3025	3029	3033	rVV2	41861	51855	2.38%	0.294%
26	20.529	3033	3036	3040	rVB	33582	35486	1.63%	0.201%
27	20.946	3103	3107	3117	rBV2	167465	241144	11.06%	1.368%
28	21.234	3151	3156	3162	rBV	901906	1078534	49.45%	6.117%
29	21.387	3178	3182	3187	rBV	71794	85214	3.91%	0.483%
30	21.815	3251	3255	3260	rBV	64300	85810	3.93%	0.487%
31	22.274	3329	3333	3340	rVB	73171	100350	4.60%	0.569%
32	22.403	3350	3355	3360	rBV	69525	92399	4.24%	0.524%
33	22.779	3415	3419	3430	rVB2	54727	88199	4.04%	0.500%
34	23.343	3511	3515	3524	rVB3	43371	77984	3.58%	0.442%

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-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-BG040615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	23.472	3529	3537	3548	rVB2	537945	1064292	48.79%	6.036%
36	23.989	3623	3625	3634	rVB5	33814	60225	2.76%	0.342%

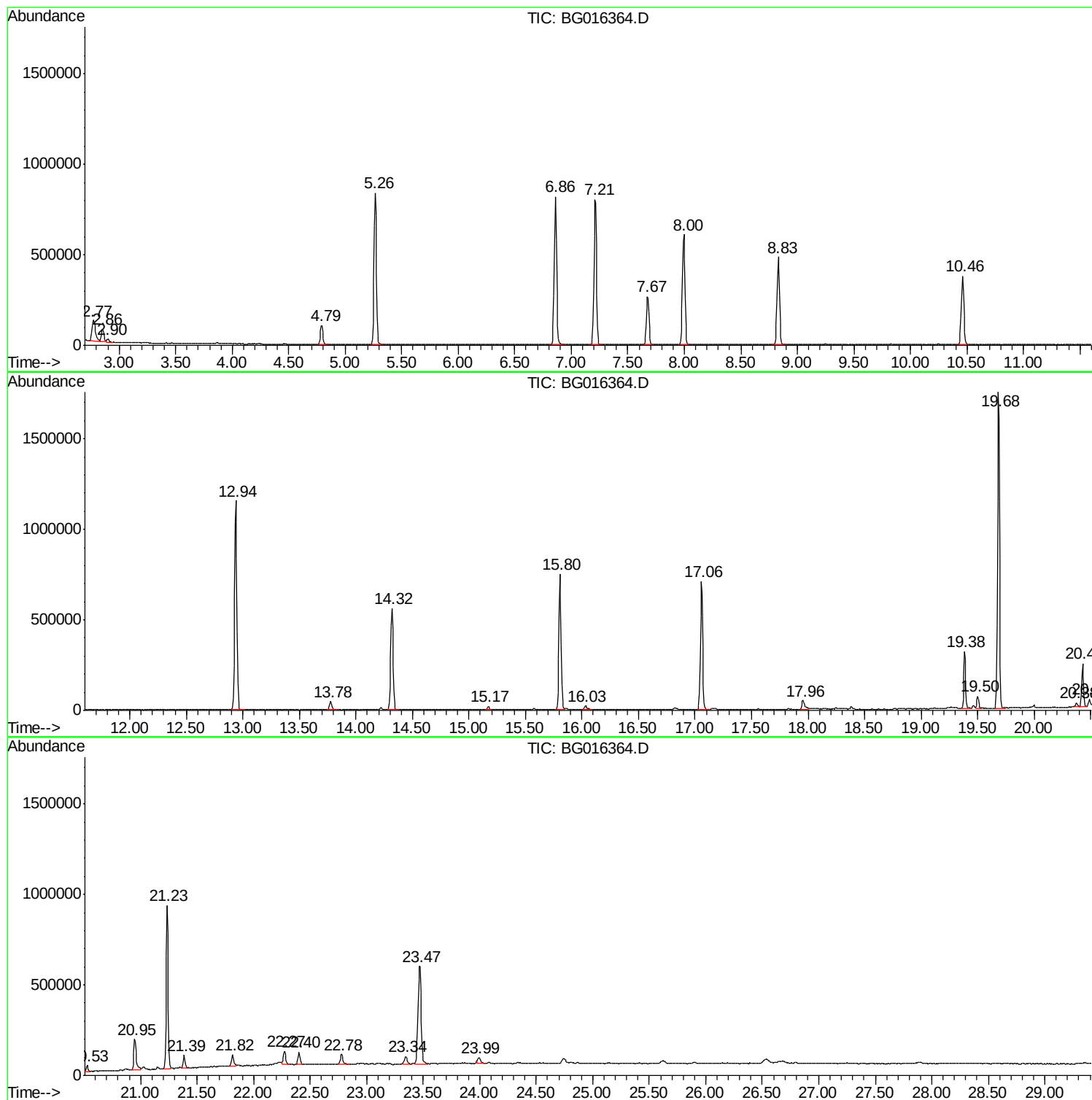
Sum of corrected areas: 17631098

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

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\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

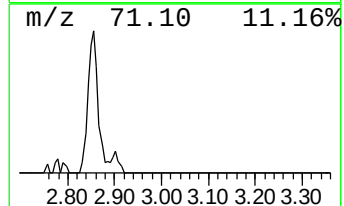
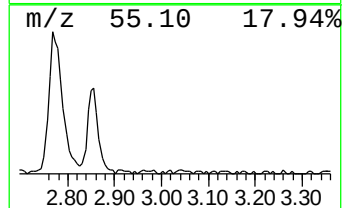
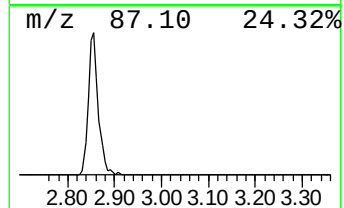
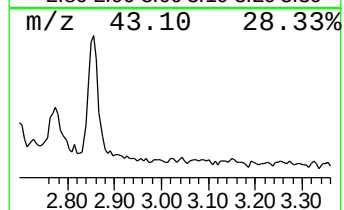
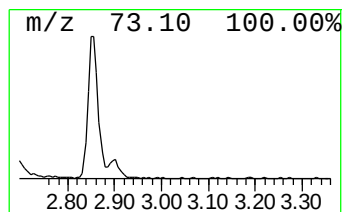
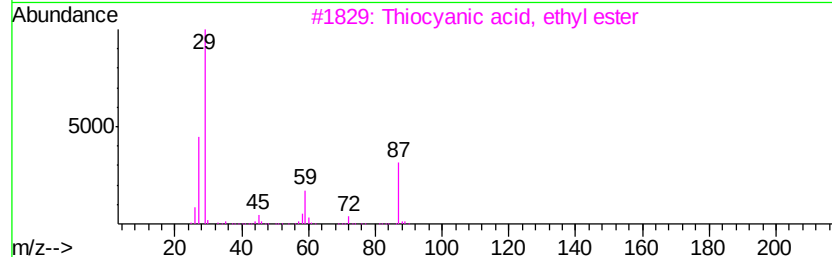
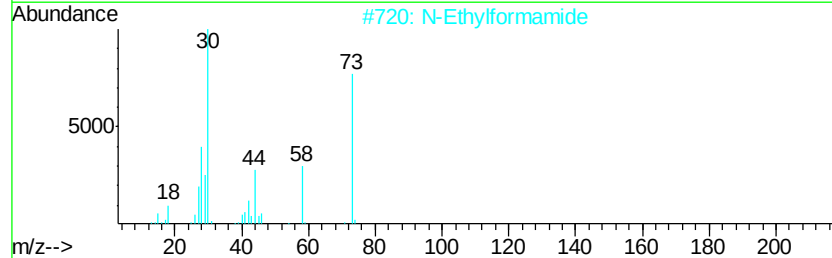
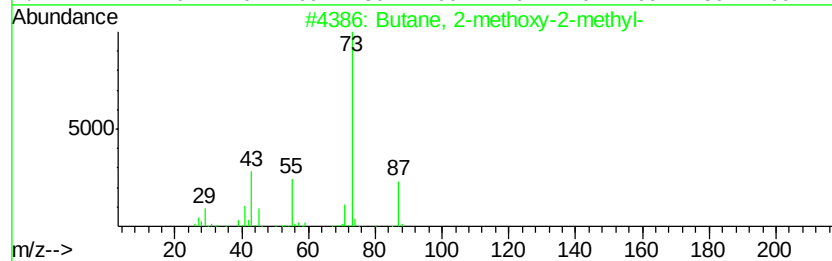
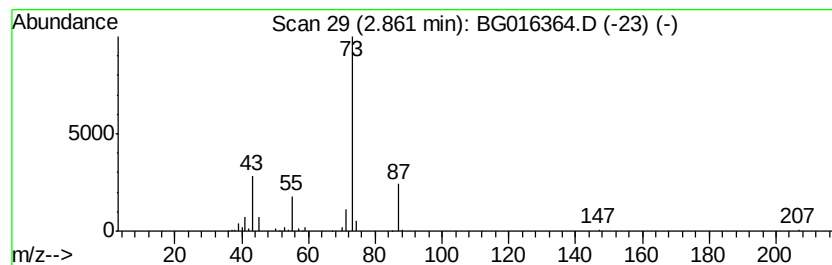
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.86	5.16 ng	109580	1,4-Dichlorobenzene-d4	7.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	56
2			N-Ethylformamide	73	C3H7NO	000627-45-2	9
3			Thiocyanic acid, ethyl ester	87	C3H5NS	000542-90-5	9
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	7
5			Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	5



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

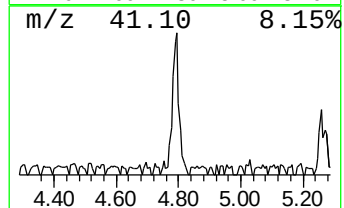
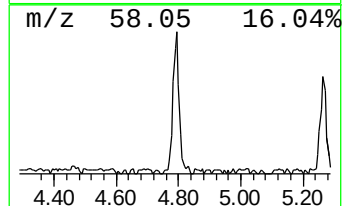
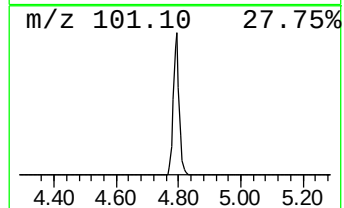
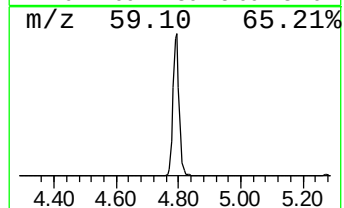
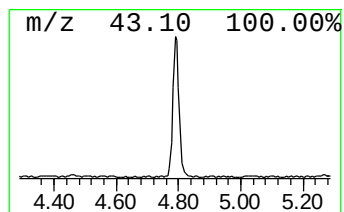
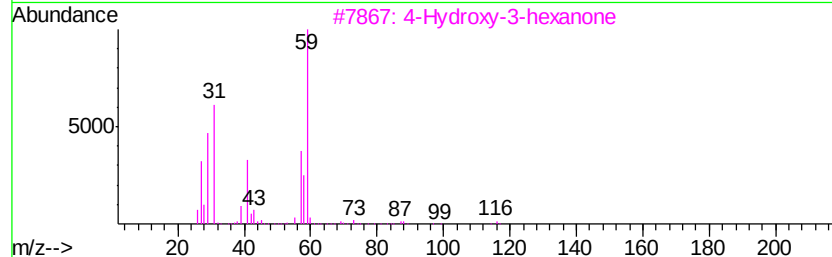
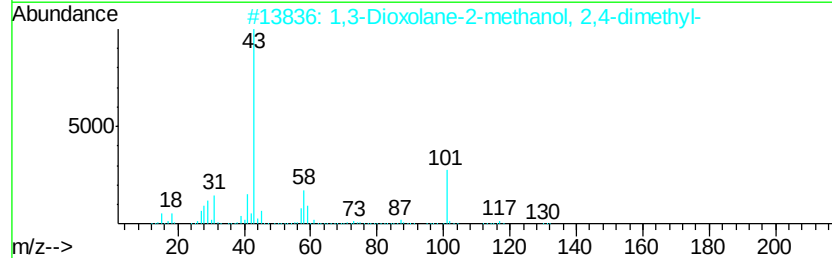
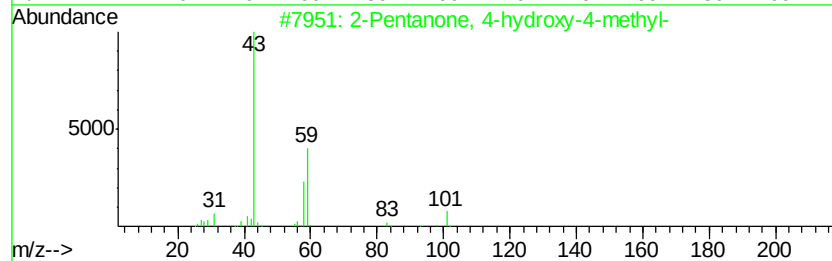
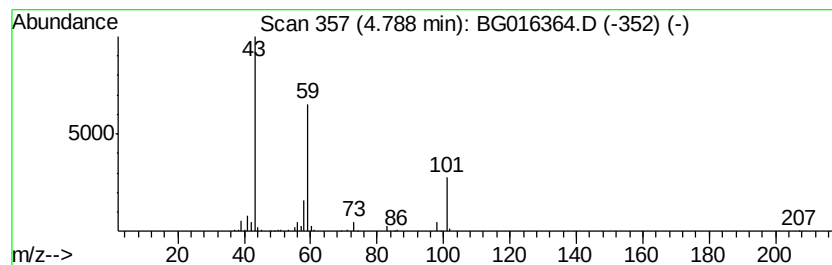
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.79	7.23 ng	153322	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	47
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	25
3		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	23
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	17
5		1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	17



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

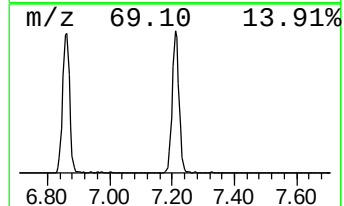
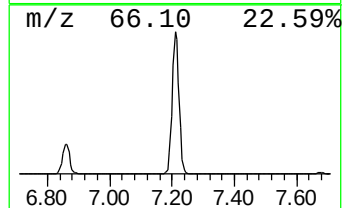
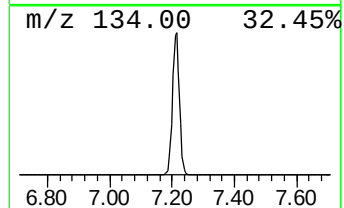
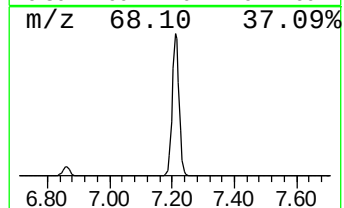
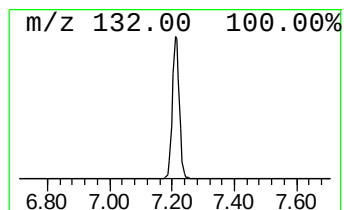
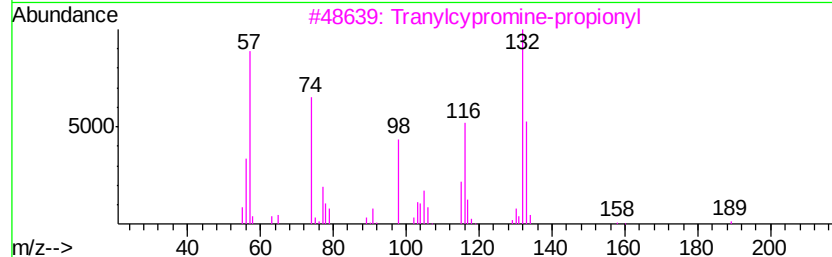
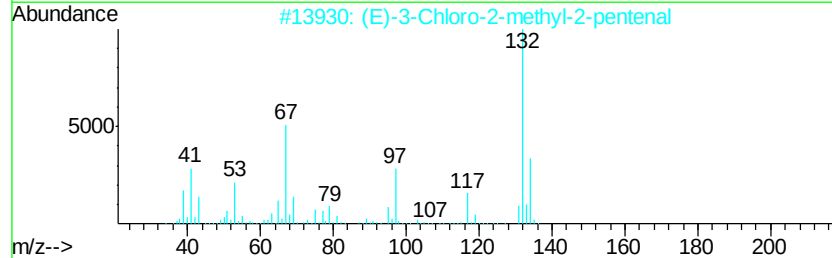
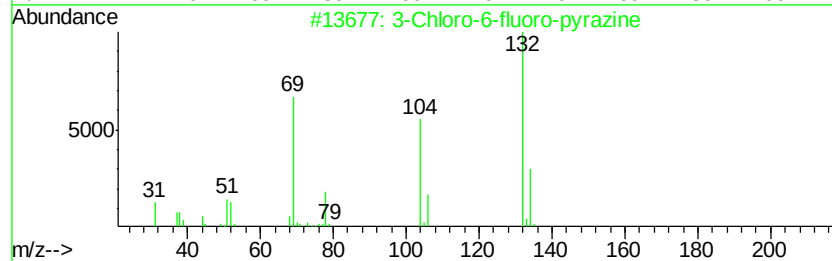
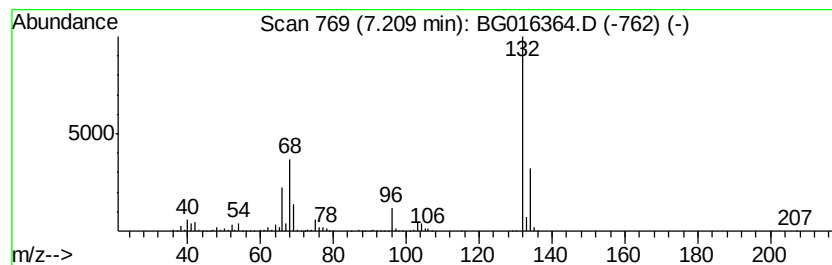
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.21 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.21	59.98 ng	1272650	1,4-Dichlorobenzene-d4	7.67

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

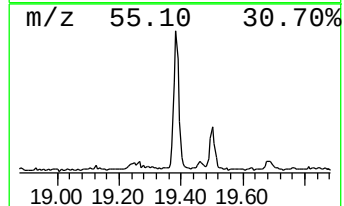
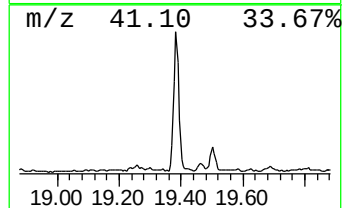
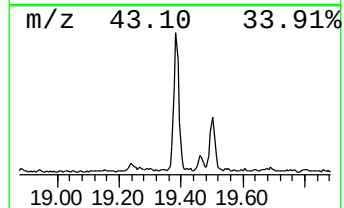
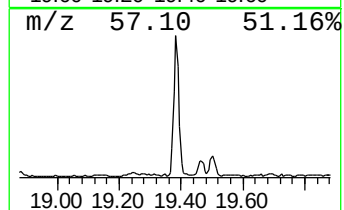
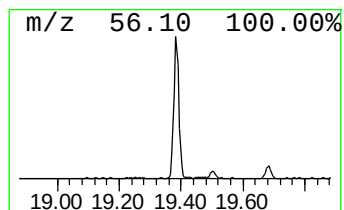
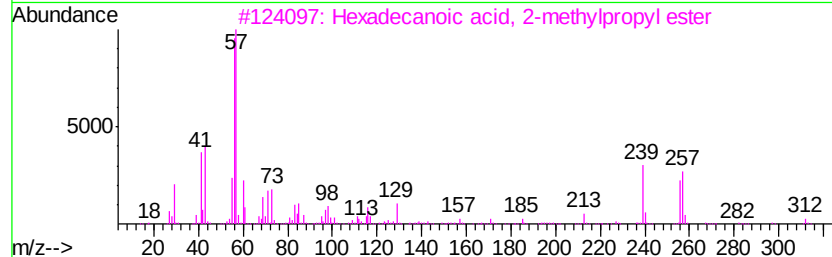
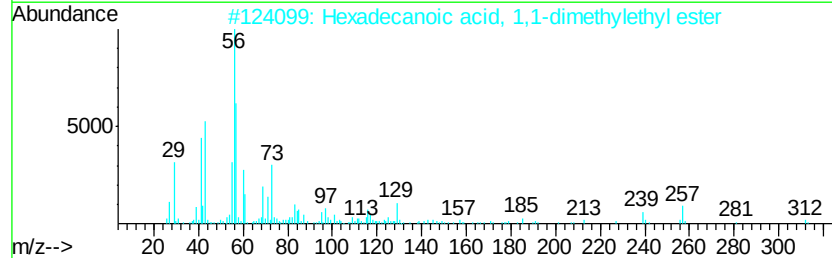
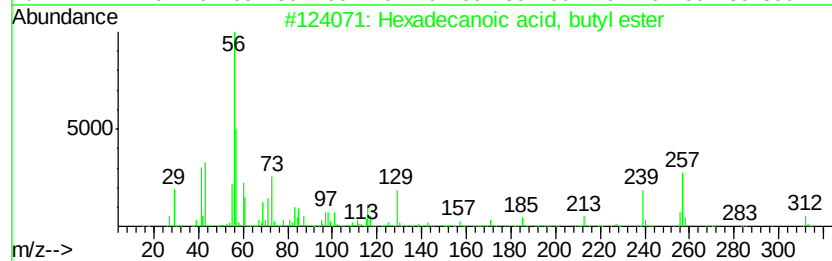
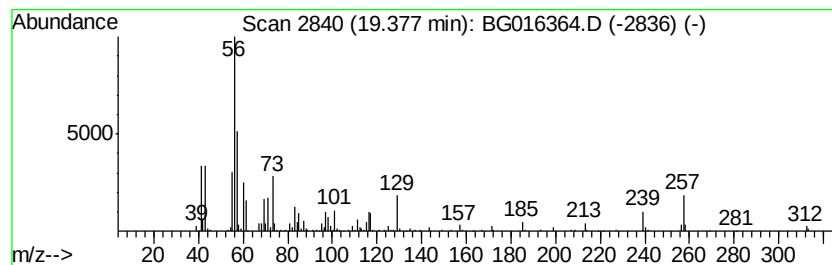
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.38	6.59 ng	355489	Chrysene-d12	21.23

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	99
2			Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	86
3			Hexadecanoic acid, 2-methylpropy...	312	C20H40O2	000110-34-9	81
4			Nipecotic acid	129	C6H11NO2	000498-95-3	50
5			2,4-Dipropyl-5-ethyl-1,3-dioxane	200	C12H24O2	006413-83-8	32



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

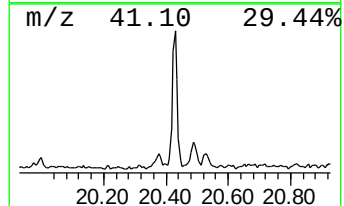
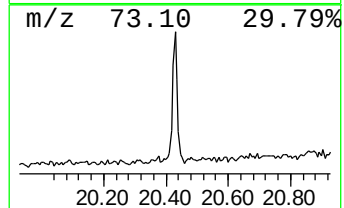
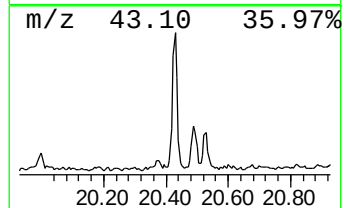
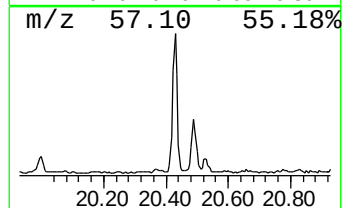
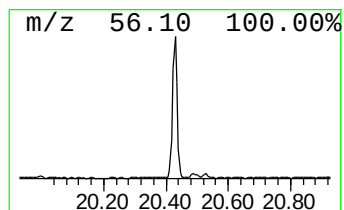
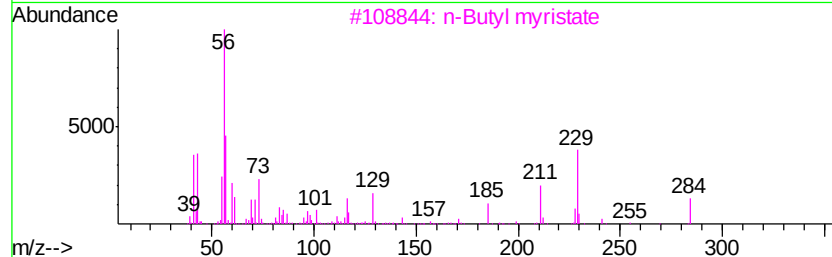
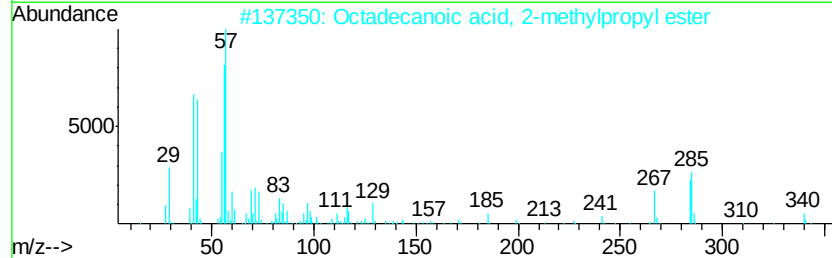
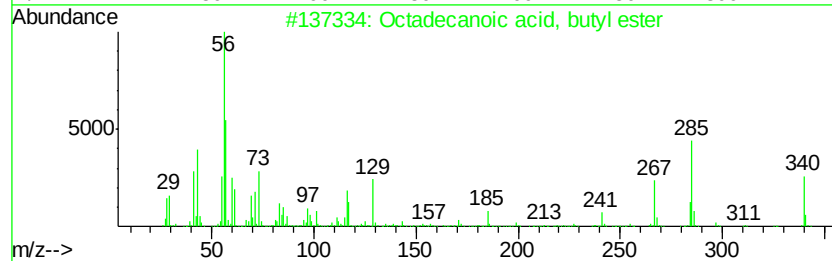
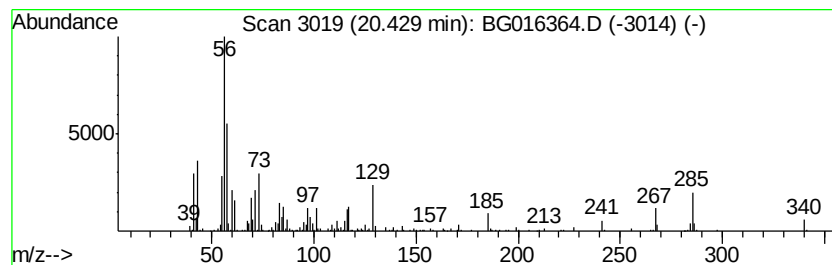
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid, butyl ester Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.43	4.79 ng	258392	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid, butyl ester	340	C22H44O2	000123-95-5	97
2		Octadecanoic acid, 2-methylpropy...	340	C22H44O2	000646-13-9	70
3		n-Butyl myristate	284	C18H36O2	000110-36-1	58
4		Nipecotic acid	129	C6H11NO2	000498-95-3	47
5		1-Hexene, 4-methyl-	98	C7H14	003769-23-1	30



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

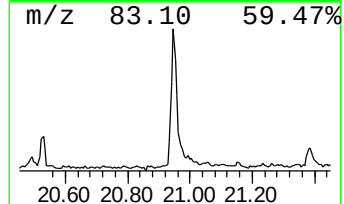
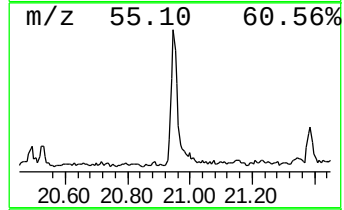
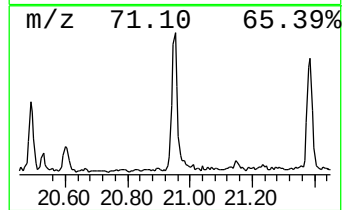
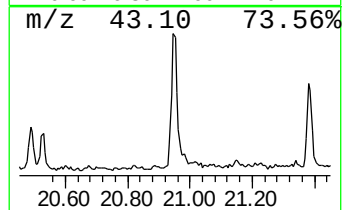
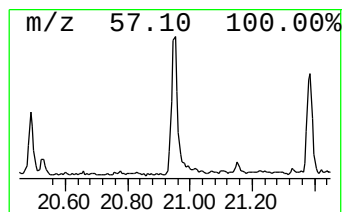
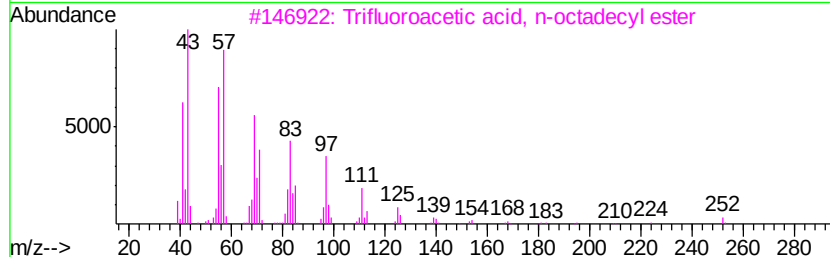
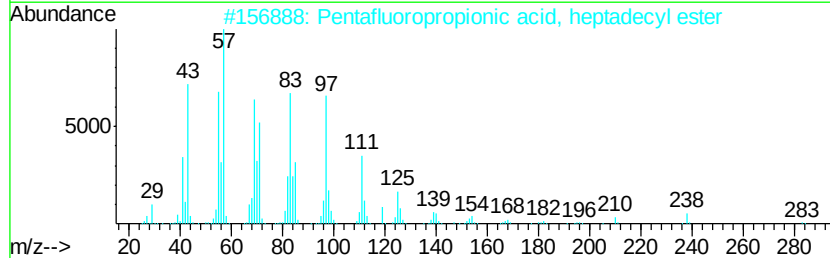
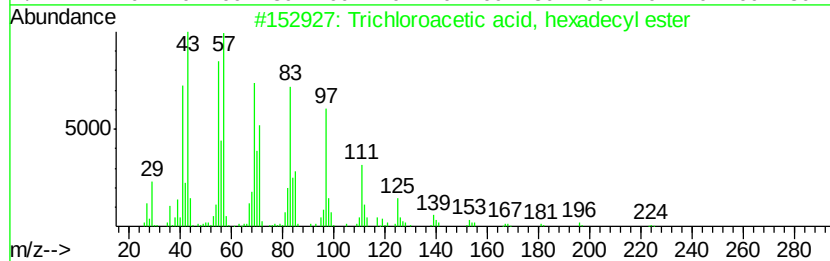
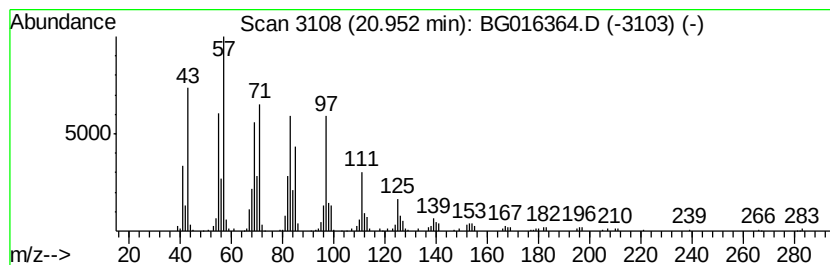
Instrument :
BNA_G
ClientSampleId :
TD-5

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 Trichloroacetic acid, hexadecyl... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.		
20.95	4.47 ng	241144	Chrysene-d12	21.23		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	90
2		Pentafluoropropionic acid, hepta...	402	C20H35F5O2	1000283-04-2	90
3		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	90
4		Cycloeicosane	280	C20H40	000296-56-0	87
5		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041315\
Data File : BG016364.D
Acq On : 13 Apr 2015 17:16
Operator : TP/IZ
Sample : G1744-09
Misc :
ALS Vial : 7 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
TD-5

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...	2.86	5.2	ng	109580	1	7.67	424375	20.0
2-Pentanone, 4-hy...	4.79	7.2	ng	153322	1	7.67	424375	20.0
unknown7.21	7.21	60.0	ng	1272650	1	7.67	424375	20.0
Hexadecanoic acid...	19.38	6.6	ng	355489	5	21.23	1078530	20.0
Octadecanoic acid...	20.43	4.8	ng	258392	5	21.23	1078530	20.0
Trichloroacetic a...	20.95	4.5	ng	241144	5	21.23	1078530	20.0