

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
 Data File : BG019962.D
 Acq On : 6 Dec 2015 11:54
 Operator : UM/NP
 Sample : G4650-13
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

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

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

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.980	20	24	41	rVB	463012	667422	5.64%	2.753%
2	3.139	45	51	76	rVB	7084900	11824227	100.00%	48.771%
3	5.178	393	398	407	rBV	94778	147132	1.24%	0.607%
4	5.654	471	479	489	rVB	459250	748766	6.33%	3.088%
5	7.258	744	752	761	rBV	499517	860960	7.28%	3.551%
6	7.640	809	817	827	rVB	497817	831567	7.03%	3.430%
7	8.110	890	897	904	rBV	126848	211618	1.79%	0.873%
8	8.439	945	953	961	rVB	346662	597998	5.06%	2.467%
9	9.279	1088	1096	1105	rBV	311234	551084	4.66%	2.273%
10	10.930	1370	1377	1385	rBV	173571	308315	2.61%	1.272%
11	13.368	1783	1792	1799	rBV	904639	1389486	11.75%	5.731%
12	14.185	1925	1931	1940	rBV	194704	279656	2.37%	1.153%
13	14.743	2020	2026	2034	rVB2	293778	482874	4.08%	1.992%
14	16.224	2270	2278	2285	rBV	708204	1042083	8.81%	4.298%
15	17.481	2486	2492	2499	rBV2	405582	618925	5.23%	2.553%
16	20.084	2927	2935	2941	rBV	1507593	1949152	16.48%	8.040%
17	21.388	3152	3157	3167	rVB2	92751	144525	1.22%	0.596%
18	21.753	3213	3219	3228	rVB	495178	802108	6.78%	3.308%
19	25.031	3766	3777	3792	rBV	266925	786526	6.65%	3.244%

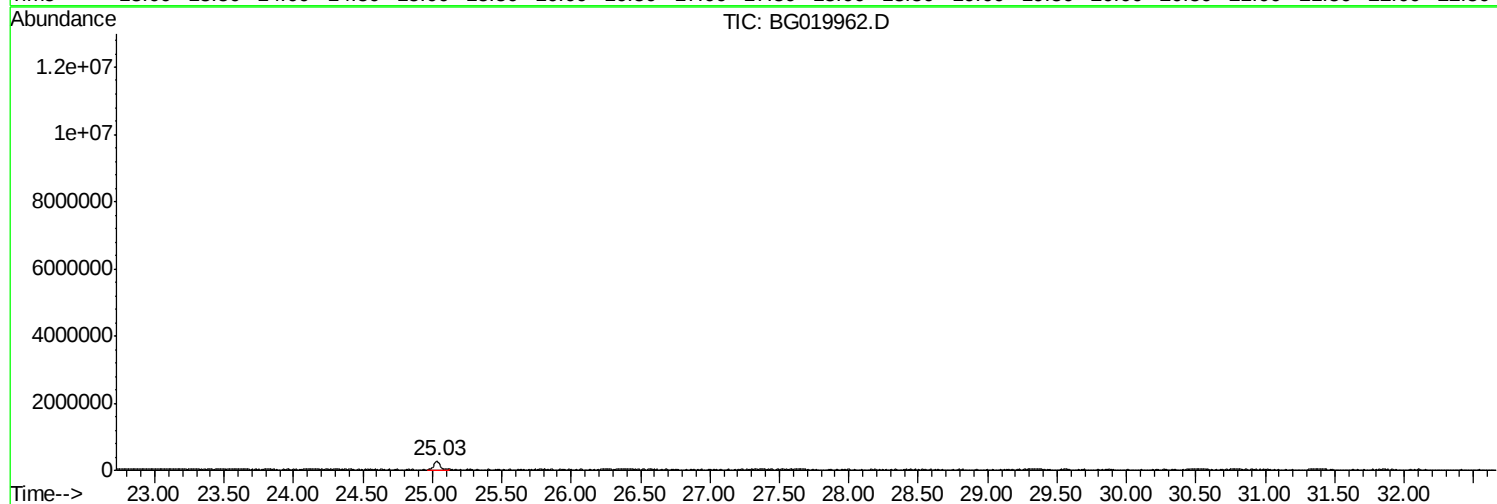
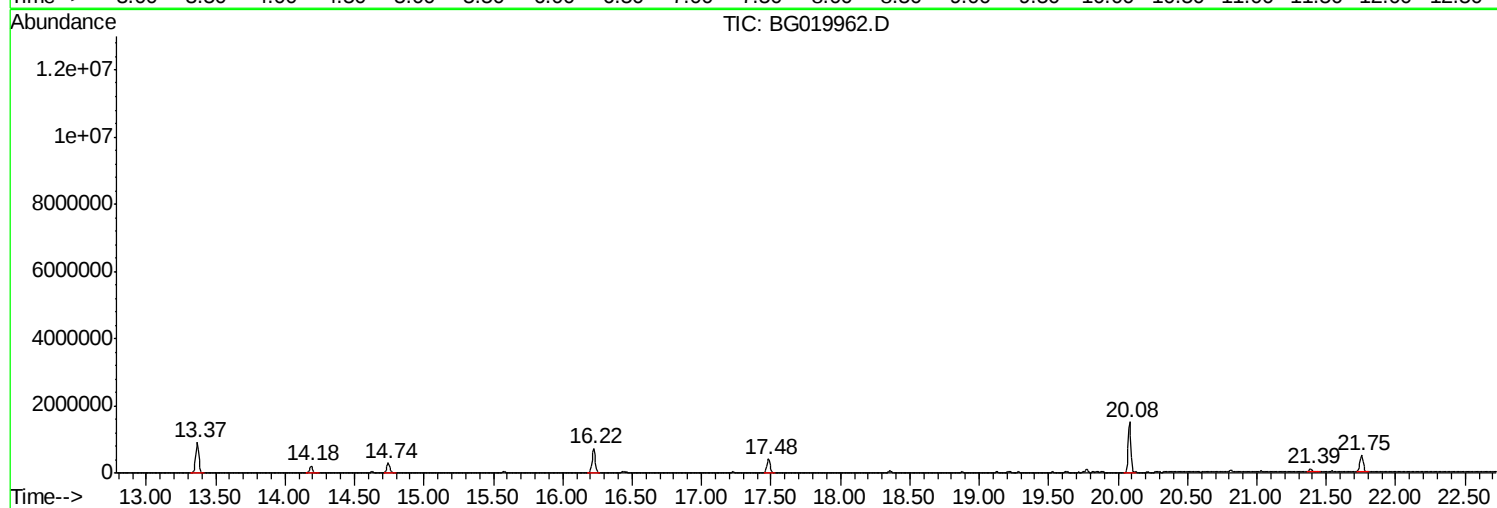
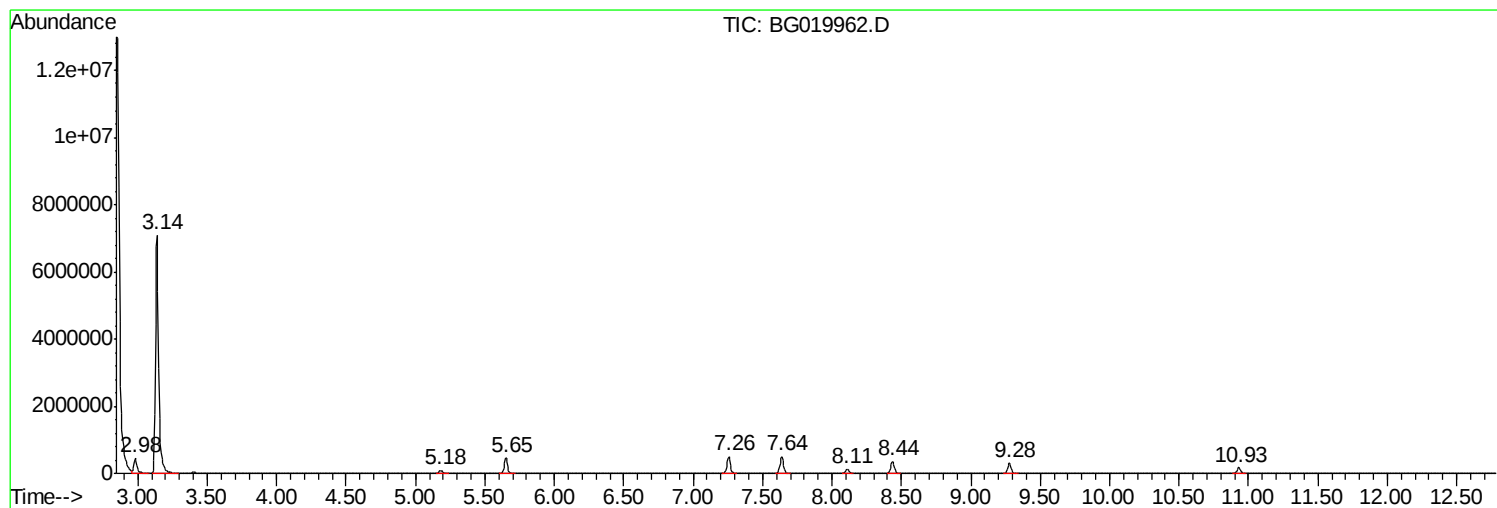
Sum of corrected areas: 24244424

Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019962.D
Acq On : 6 Dec 2015 11:54
Operator : UM/NP
Sample : G4650-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

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 : BG019962.D
Acq On : 6 Dec 2015 11:54
Operator : UM/NP
Sample : G4650-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

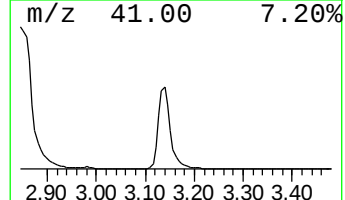
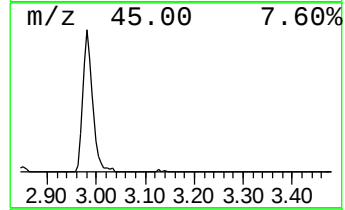
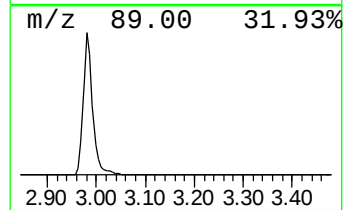
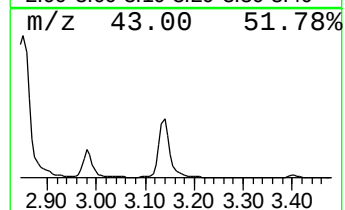
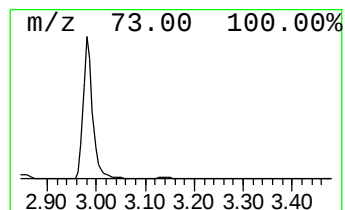
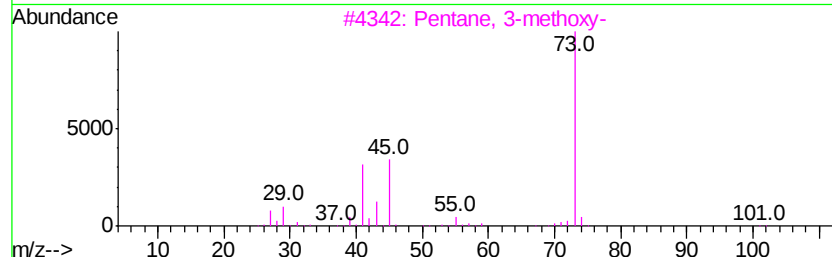
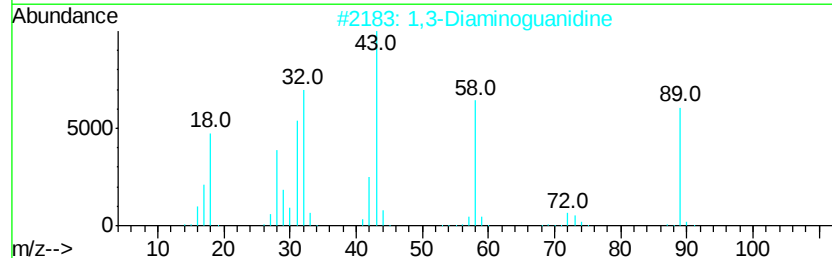
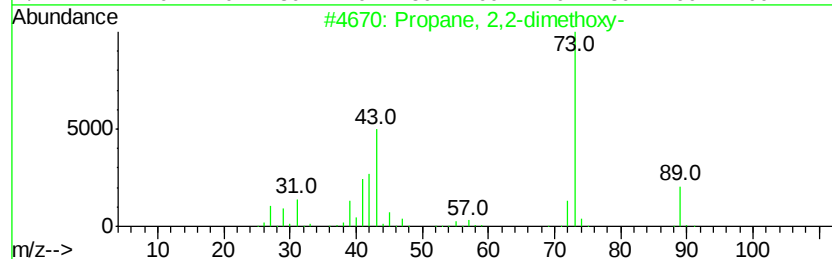
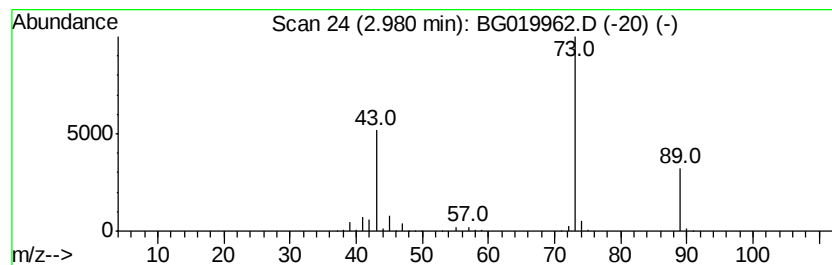
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.98	63.08 ng	667422	1,4-Dichlorobenzene-d4	8.11

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	50
2			1,3-Diaminoquinidine	89	CH7N5	004364-78-7	9
3			Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
4			2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9
5			N-Ethylformamide	73	C3H7NO	000627-45-2	7



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019962.D
Acq On : 6 Dec 2015 11:54
Operator : UM/NP
Sample : G4650-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

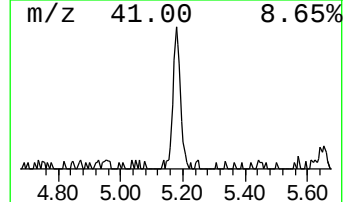
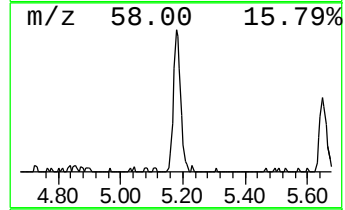
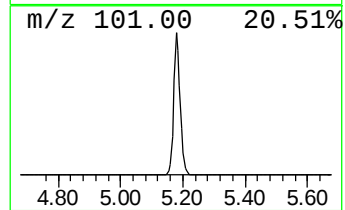
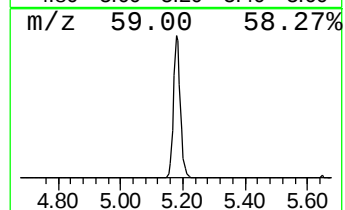
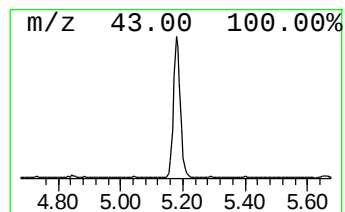
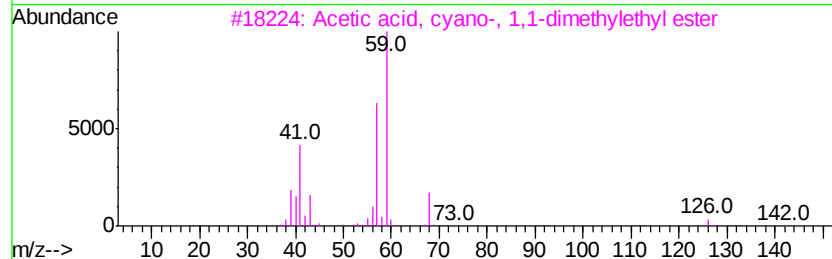
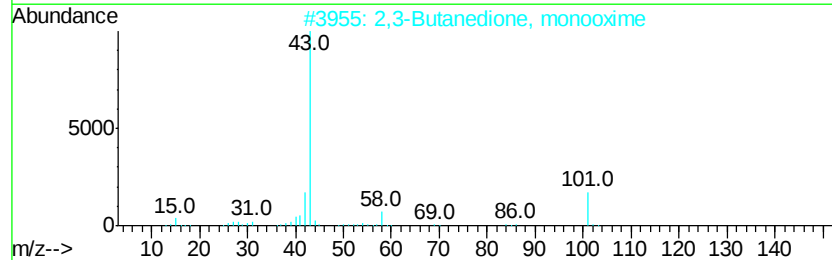
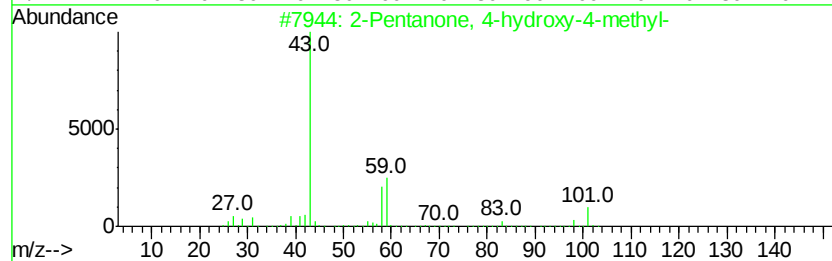
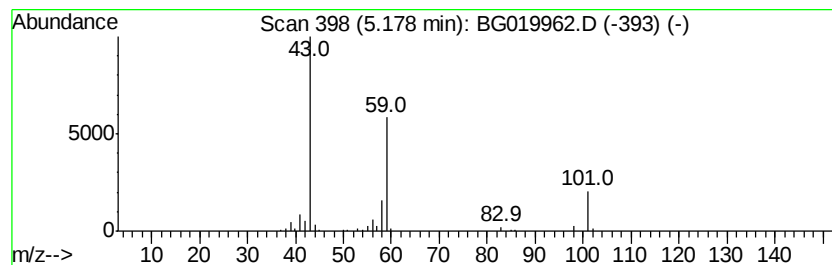
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.18	13.91 ng	147132	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	56
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	25
3		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		3-Octanol	130	C8H18O	000589-98-0	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019962.D
Acq On : 6 Dec 2015 11:54
Operator : UM/NP
Sample : G4650-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

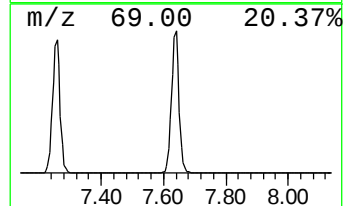
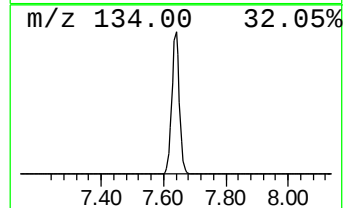
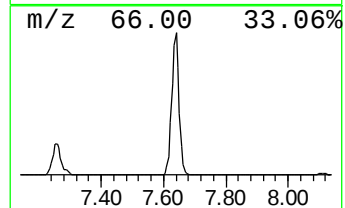
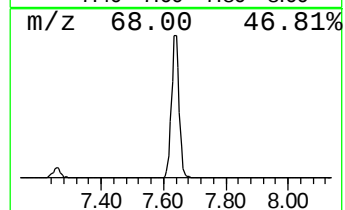
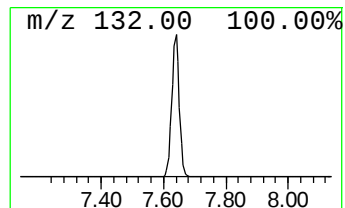
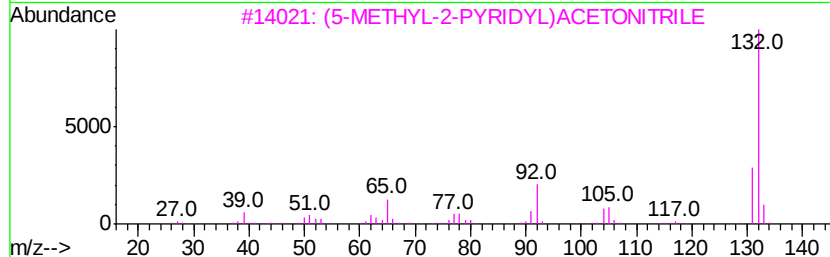
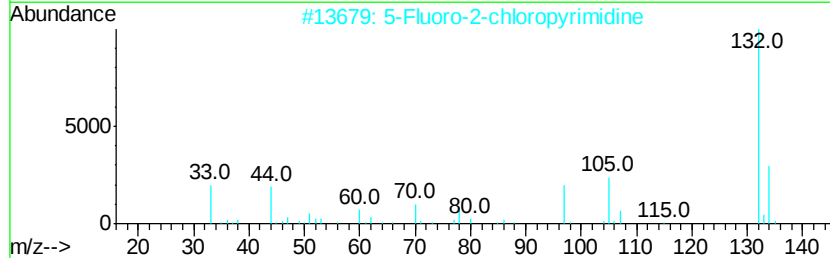
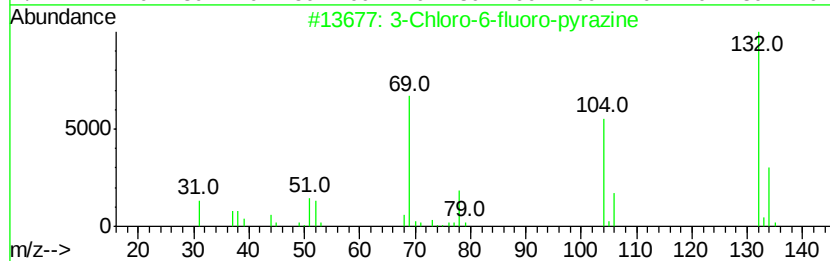
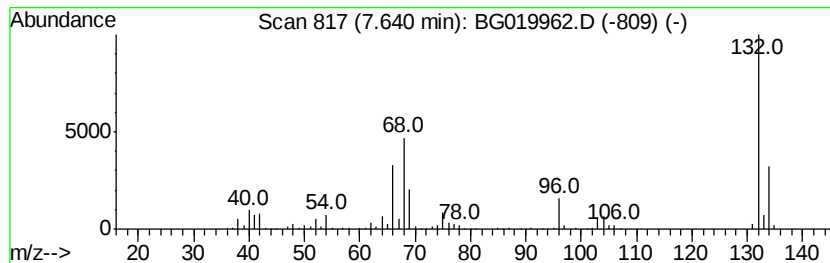
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG120215.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.64 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.64	78.59 ng	831567	1,4-Dichlorobenzene-d4	8.11

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3		(5-METHYL-2-PYRIDYL)ACETONITRILE	132	C8H8N2	1000241-93-9	10
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		Benzene, 1,2,4-trifluoro-	132	C6H3F3	000367-23-7	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG120615\
Data File : BG019962.D
Acq On : 6 Dec 2015 11:54
Operator : UM/NP
Sample : G4650-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

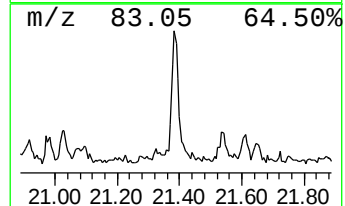
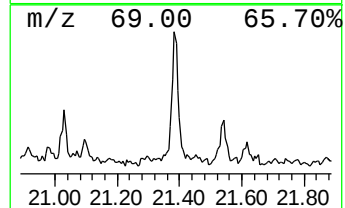
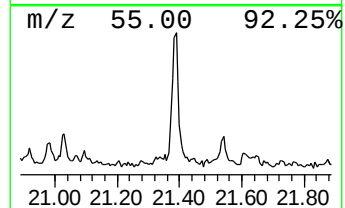
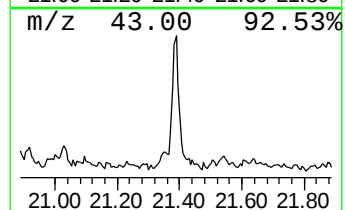
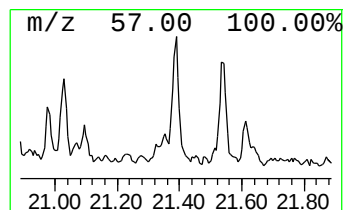
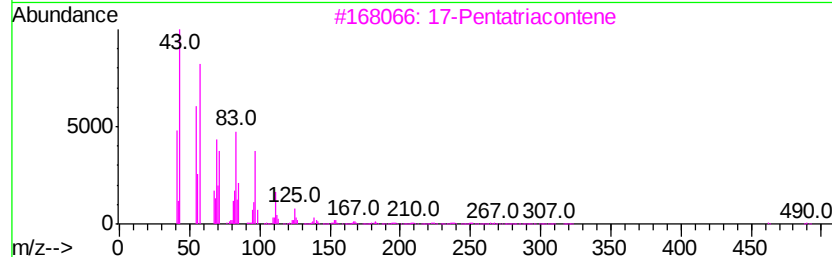
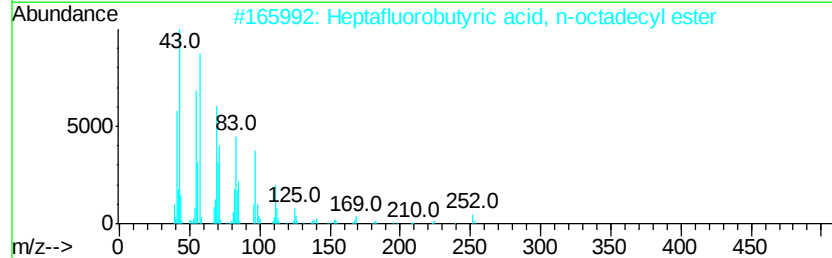
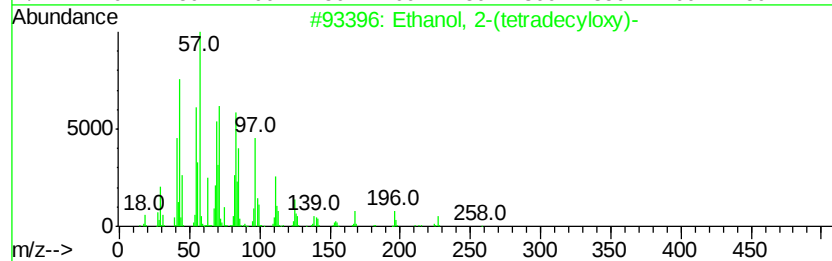
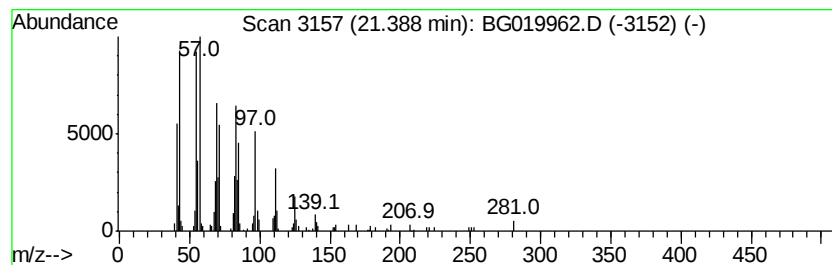
Instrument :
BNA_G
ClientSampleId :
COFF(0-2)-2

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 Ethanol, 2-(tetradecyloxy)- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD		R.T.	
21.39	3.60 ng	144525	Chrysene-d12		21.75	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Ethanol, 2-(tetradecyloxy)-	258	C16H34O2	002136-70-1	87
2		Heptafluorobutyric acid, n-octadecyl ester	466	C22H37F7O2	000400-57-7	83
3		17-Pentatriacontene	491	C35H70	006971-40-0	80
4		Pentafluoropropionic acid, heptafluorooctyl ester	402	C20H35F5O2	1000283-04-2	80
5		Cyclopentane, (4-octyldodecyl)-	350	C25H50	005638-09-5	72



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG120615\
Data File : BG019962.D
Acq On : 6 Dec 2015 11:54
Operator : UM/NP
Sample : G4650-13
Misc :
ALS Vial : 4 Sample Multiplier: 1

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

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
Propane, 2,2-dime...	2.98	63.1	ng	667422	1	8.11	211618	20.0
2-Pentanone, 4-hy...	5.18	13.9	ng	147132	1	8.11	211618	20.0
unknown7.64	7.64	78.6	ng	831567	1	8.11	211618	20.0
Ethanol, 2-(tetra...	21.39	3.6	ng	144525	5	21.75	802108	20.0