

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
 Data File : BG033548.D
 Acq On : 4 Apr 2018 6:59
 Operator : SJ/JU
 Sample : J2177-05
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 032818-DBRI-F-U-M

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-BG031918.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	3.483	27	33	42	rBV	139121	271745	7.48%	1.931%
2	3.571	43	48	57	rVB	90836	145878	4.02%	1.037%
3	5.774	418	423	431	rBV	23558	43316	1.19%	0.308%
4	6.291	505	511	527	rBV	119584	284923	7.84%	2.025%
5	7.984	790	799	819	rBV2	72282	226336	6.23%	1.609%
6	8.377	859	866	890	rBV	280858	657053	18.09%	4.670%
7	8.865	941	949	964	rBV	70688	180804	4.98%	1.285%
8	9.194	996	1005	1020	rBV	435825	893914	24.61%	6.353%
9	10.063	1146	1153	1172	rBV	341150	827791	22.79%	5.883%
10	11.744	1433	1439	1450	rBV	123650	272070	7.49%	1.934%
11	14.106	1834	1841	1860	rBV	1254404	2208260	60.80%	15.694%
12	14.899	1968	1976	1985	rBV	49499	82249	2.26%	0.585%
13	15.481	2069	2075	2085	rBV2	281141	501362	13.80%	3.563%
14	16.955	2319	2326	2344	rBV	753071	1323627	36.44%	9.407%
15	18.213	2533	2540	2554	rBV2	394005	713014	19.63%	5.067%
16	19.006	2671	2675	2682	rBV4	37527	62027	1.71%	0.441%
17	20.733	2963	2969	2979	rBV	2648019	3632209	100.00%	25.813%
18	22.073	3191	3197	3205	rBV4	58570	121989	3.36%	0.867%
19	22.561	3270	3280	3297	rBV2	380353	839056	23.10%	5.963%
20	26.327	3907	3921	3940	rBV	211159	783501	21.57%	5.568%

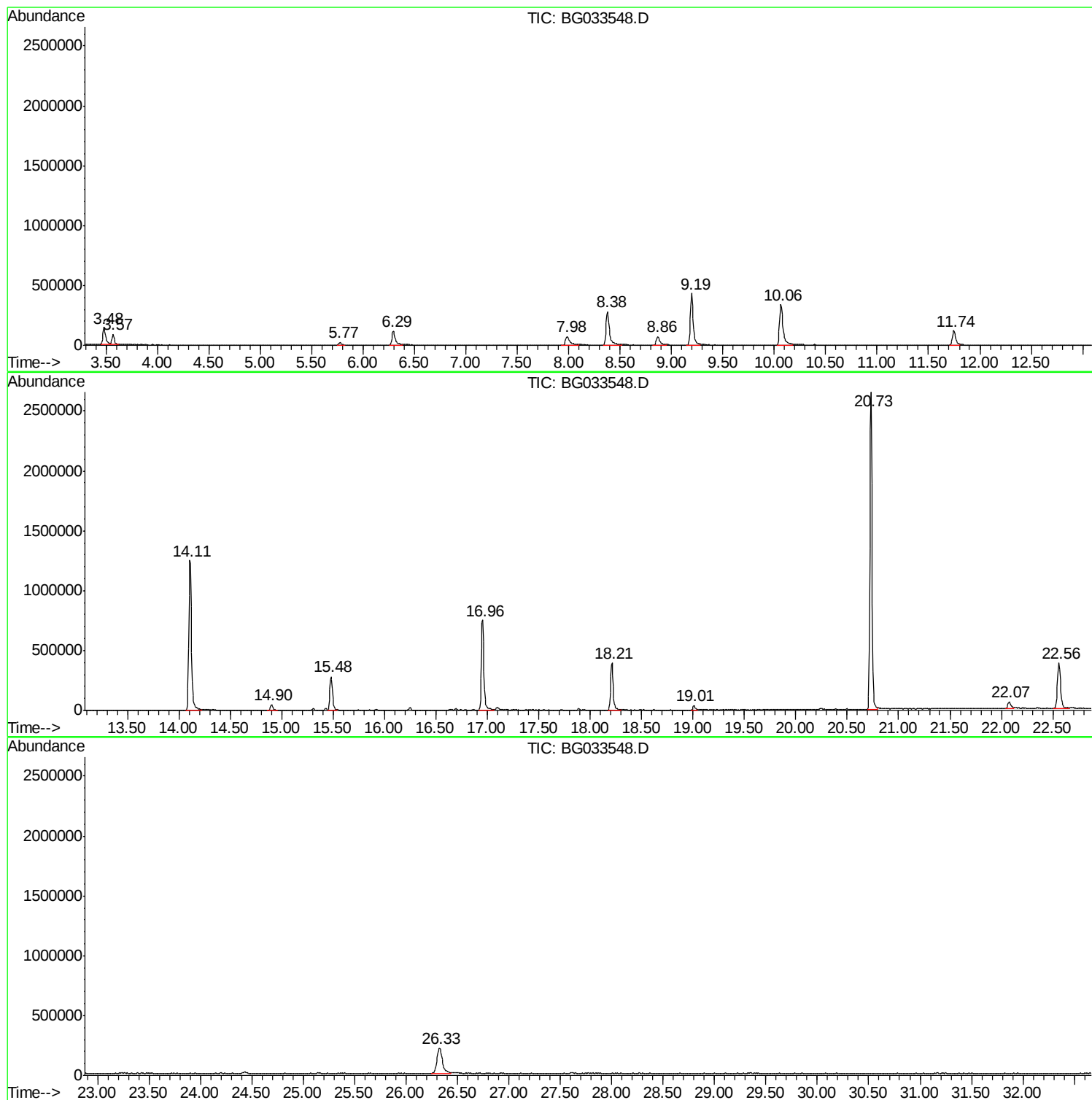
Sum of corrected areas: 14071124

Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
Data File : BG033548.D
Acq On : 4 Apr 2018 6:59
Operator : SJ/JU
Sample : J2177-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
032818-DBRI-F-U-M

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
Data File : BG033548.D
Acq On : 4 Apr 2018 6:59
Operator : SJ/JU
Sample : J2177-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
032818-DBRI-F-U-M

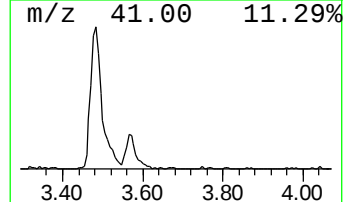
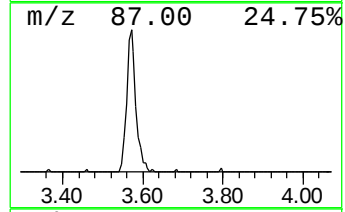
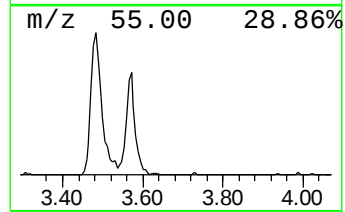
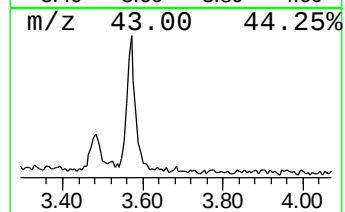
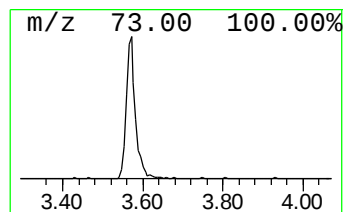
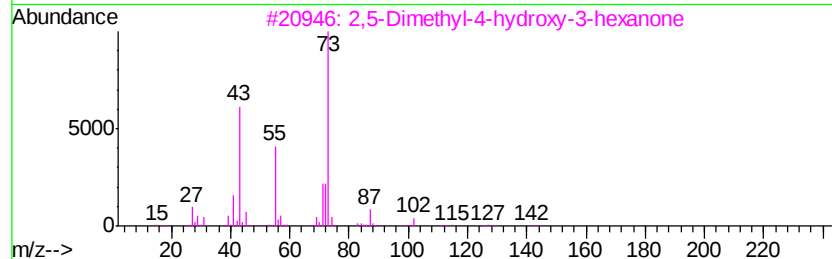
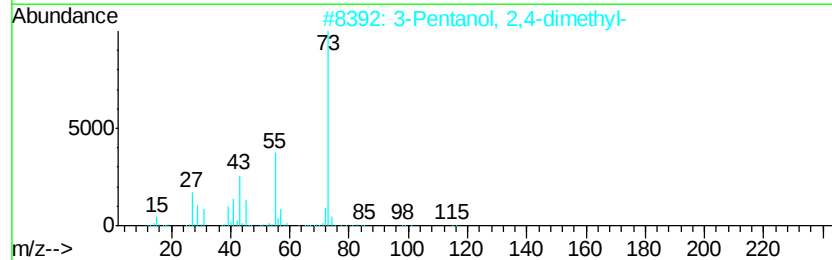
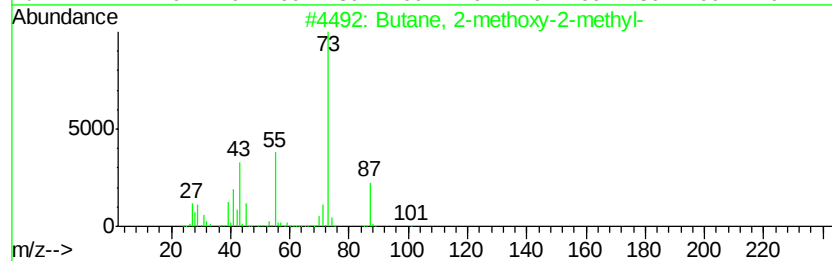
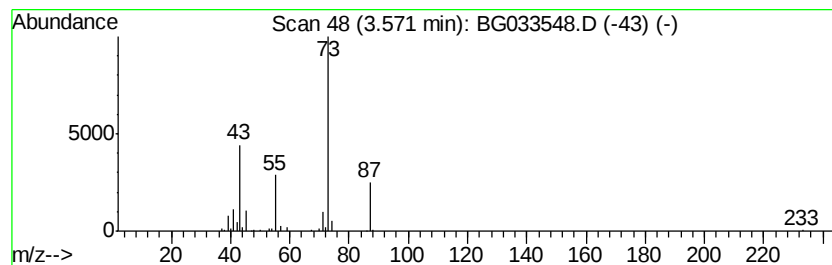
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.57	16.14 ng	145878	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	37
3		2,5-Dimethyl-4-hydroxy-3-hexanone	144	C8H16O2	000815-77-0	25
4		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
Data File : BG033548.D
Acq On : 4 Apr 2018 6:59
Operator : SJ/JU
Sample : J2177-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
032818-DBRI-F-U-M

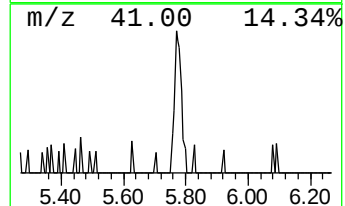
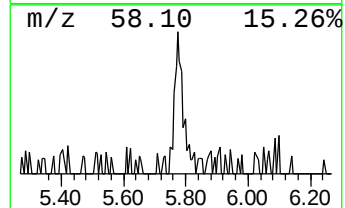
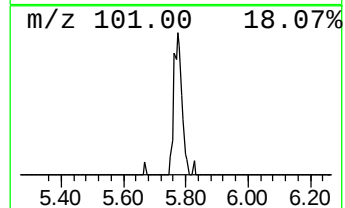
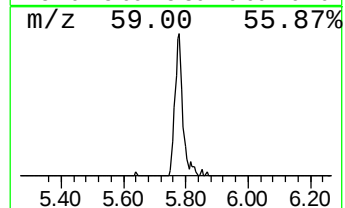
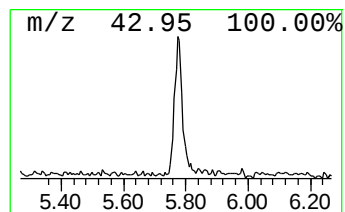
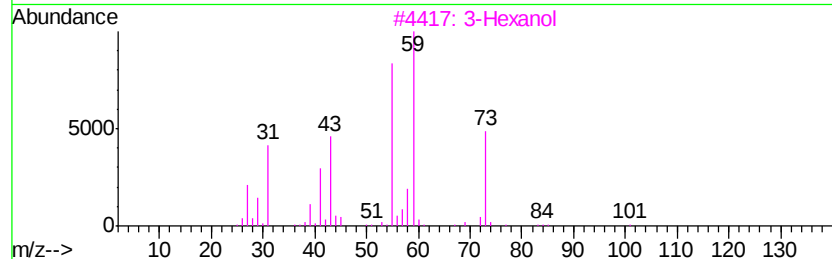
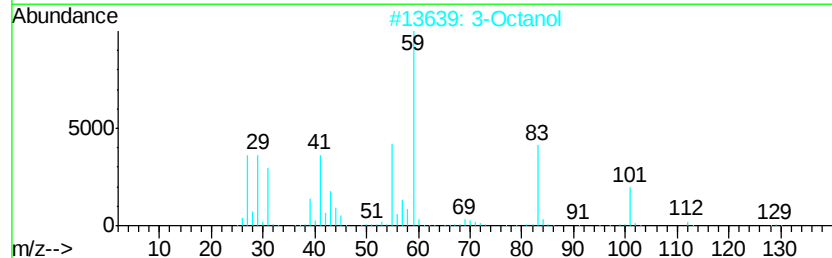
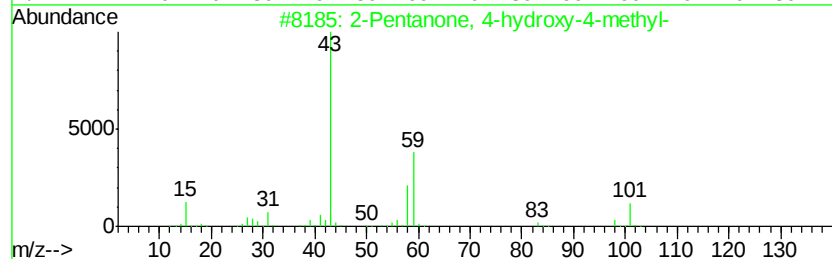
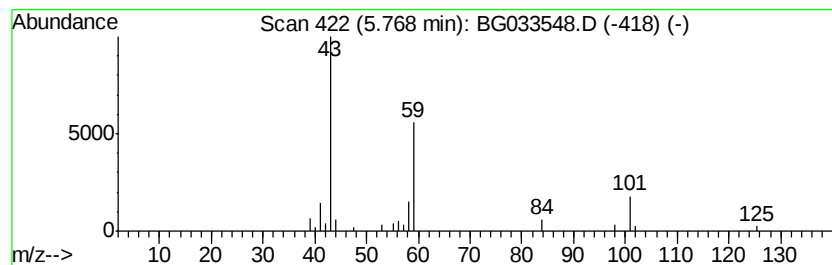
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.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.
5.77	4.79 ng	43316	1,4-Dichlorobenzene-d4	8.86

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			3-Octanol	130	C8H18O	000589-98-0	40
3			3-Hexanol	102	C6H14O	000623-37-0	33
4			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5			Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	23



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
Data File : BG033548.D
Acq On : 4 Apr 2018 6:59
Operator : SJ/JU
Sample : J2177-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
032818-DBRI-F-U-M

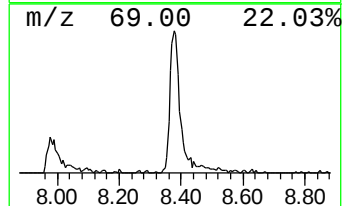
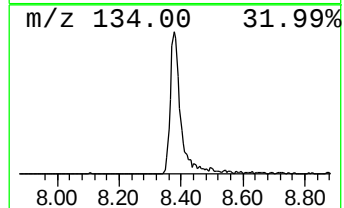
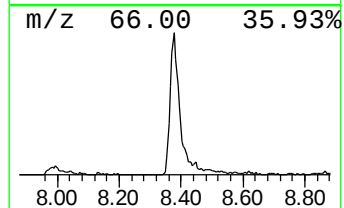
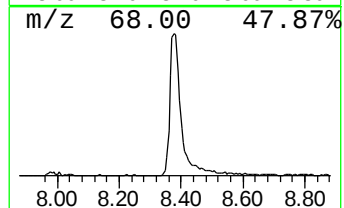
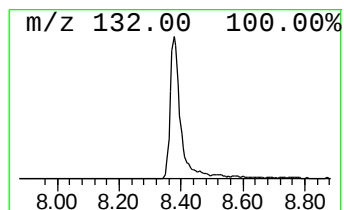
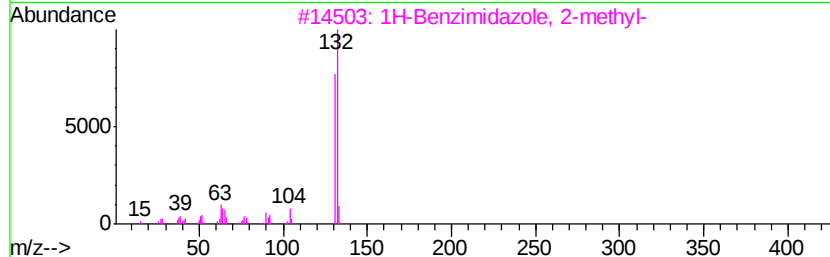
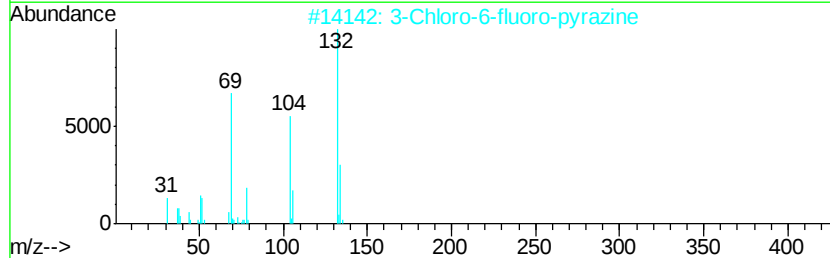
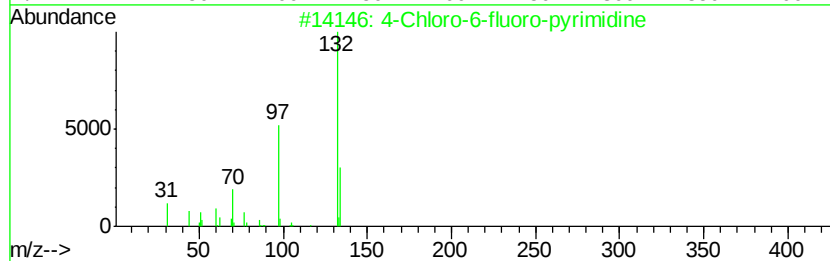
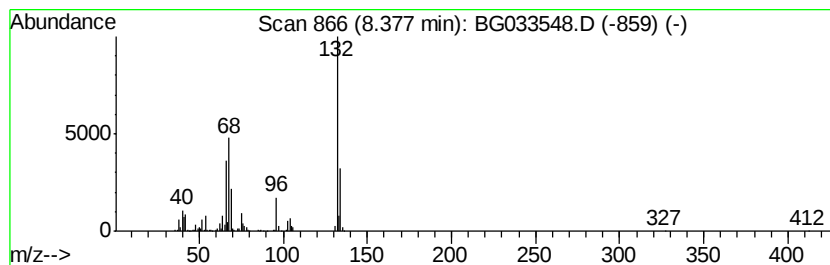
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown8.38 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.38	72.68 ng	657053	1,4-Dichlorobenzene-d4	8.86

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG040318\
Data File : BG033548.D
Acq On : 4 Apr 2018 6:59
Operator : SJ/JU
Sample : J2177-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
032818-DBRI-F-U-M

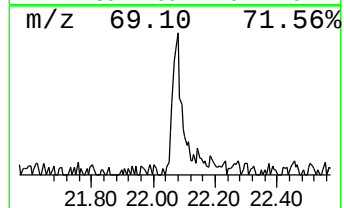
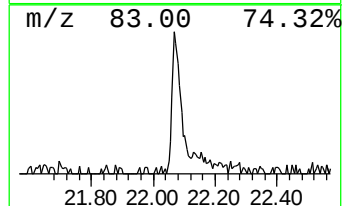
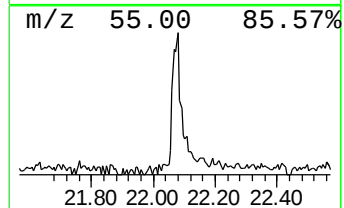
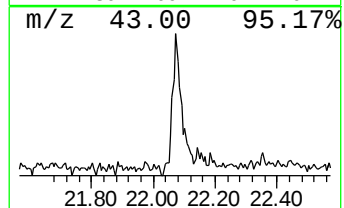
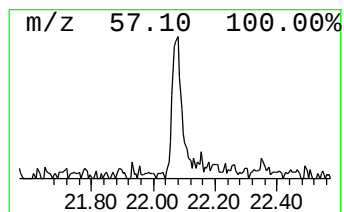
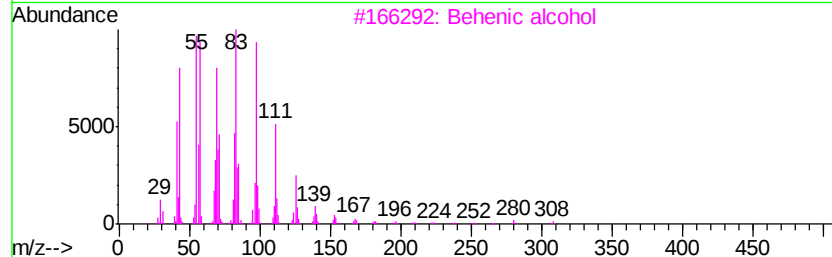
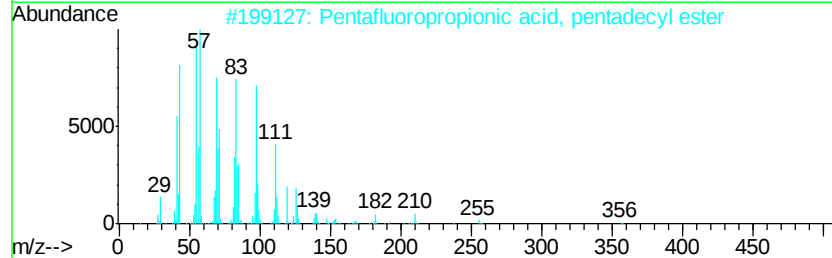
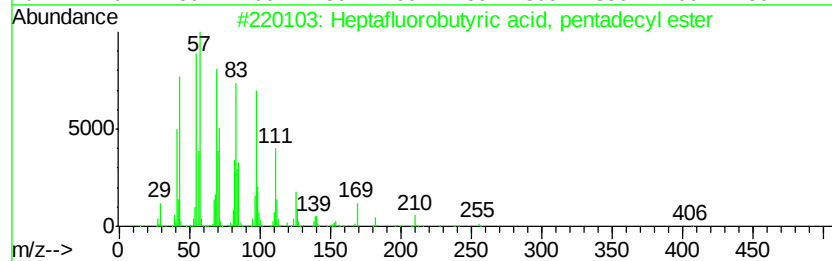
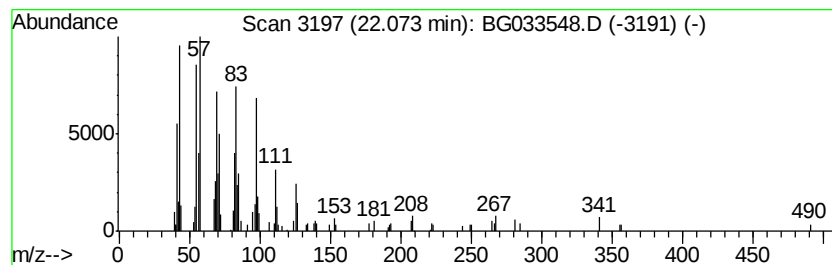
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 Heptafluorobutyric acid, pe... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.07	2.91 ng	121989	Chrysene-d12	22.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	93
2		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	93
3		Behenic alcohol	326	C22H46O	000661-19-8	91
4		Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91
5		1-Tricosene	322	C23H46	018835-32-0	90



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG040318\
Data File : BG033548.D
Acq On : 4 Apr 2018 6:59
Operator : SJ/JU
Sample : J2177-05
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
032818-DBRI-F-U-M

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG031918.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\Database\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	3.57	16.1	ng	145878	1	8.86	180804	20.0
2-Pentanone, 4-hy...	5.77	4.8	ng	43316	1	8.86	180804	20.0
unknown8.38	8.38	72.7	ng	657053	1	8.86	180804	20.0
Heptafluorobutyri...	22.07	2.9	ng	121989	5	22.56	839056	20.0