

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
 Data File : BG038649.D
 Acq On : 16 Dec 2018 20:45
 Operator : JU/SJ
 Sample : J6424-05
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SODUP02_121318

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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	3.734	107	110	115	rBV	15350	23328	1.46%	0.262%
2	5.145	345	350	357	rVB	21117	34710	2.17%	0.390%
3	5.609	422	429	441	rBV	408926	688433	42.97%	7.729%
4	7.213	695	702	713	rBV	427298	811043	50.63%	9.105%
5	7.589	758	766	777	rVB	400816	717156	44.77%	8.051%
6	8.059	839	846	858	rVB	84082	150407	9.39%	1.689%
7	8.382	894	901	910	rVB	308150	553145	34.53%	6.210%
8	9.240	1039	1047	1057	rBV	252367	489075	30.53%	5.491%
9	10.879	1319	1326	1339	rBV	107116	201188	12.56%	2.259%
10	13.317	1734	1741	1749	rBV	695648	1101022	68.73%	12.361%
11	14.140	1875	1881	1892	rVB	83024	126589	7.90%	1.421%
12	14.698	1969	1976	1984	rVB2	172348	281076	17.55%	3.156%
13	16.185	2223	2229	2247	rBV	526186	838436	52.34%	9.413%
14	17.442	2437	2443	2454	rBV2	223817	352911	22.03%	3.962%
15	18.306	2585	2590	2600	rBV5	19840	35719	2.23%	0.401%
16	20.045	2880	2886	2895	rBV	1243820	1602007	100.00%	17.985%
17	21.320	3098	3103	3117	rBV2	47929	95272	5.95%	1.070%
18	21.725	3165	3172	3184	rVB	231243	396034	24.72%	4.446%
19	23.170	3414	3418	3426	rVB4	8536	16485	1.03%	0.185%
20	25.021	3724	3733	3743	rVB	125787	372886	23.28%	4.186%
21	26.091	3904	3915	3922	rBV5	6879	20380	1.27%	0.229%

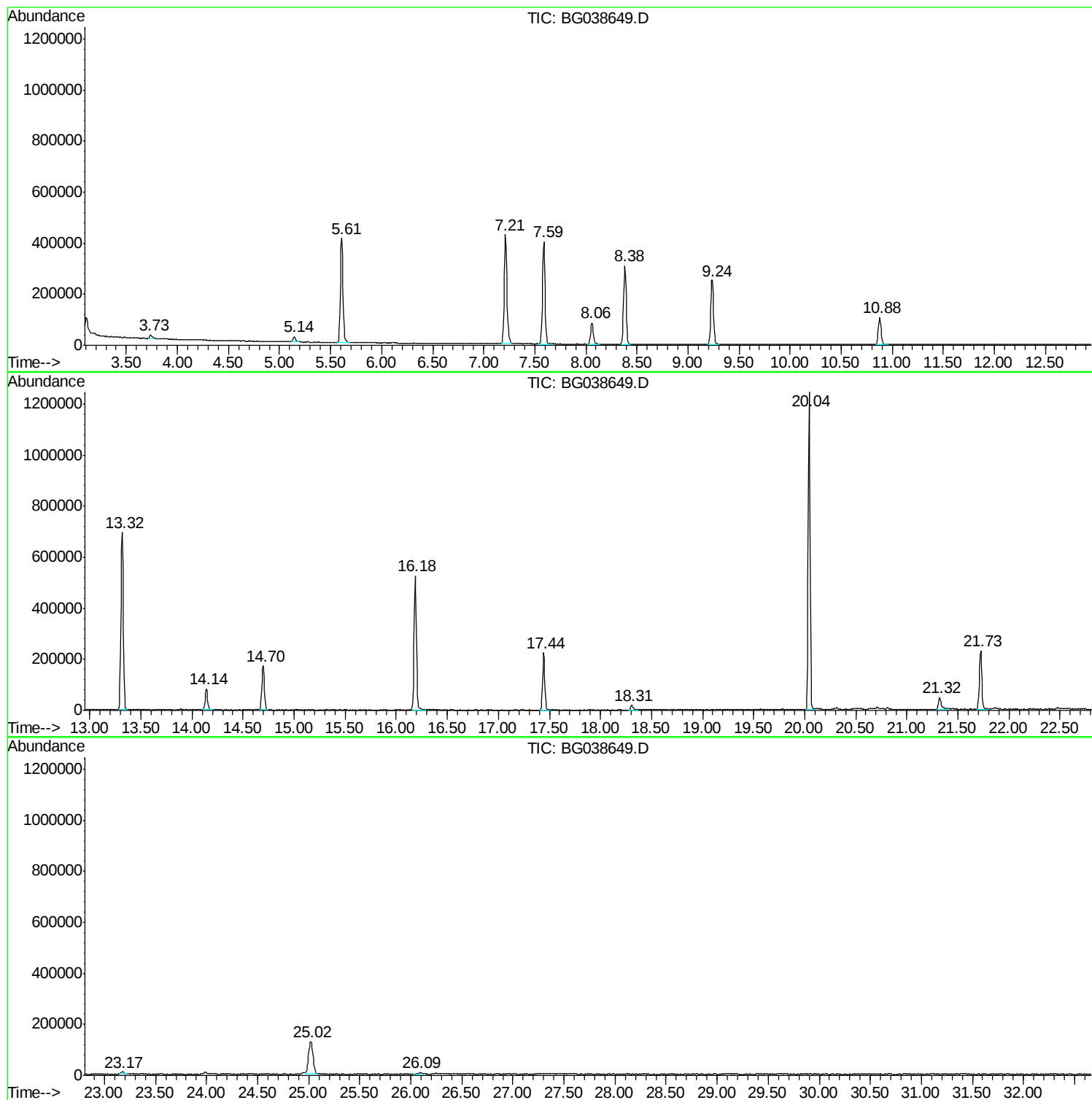
Sum of corrected areas: 8907302

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

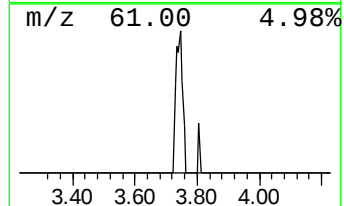
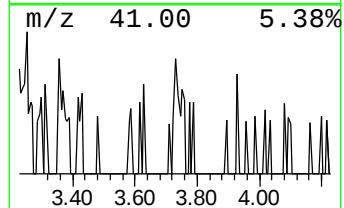
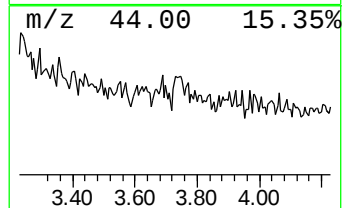
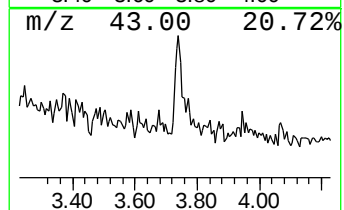
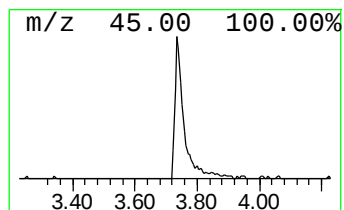
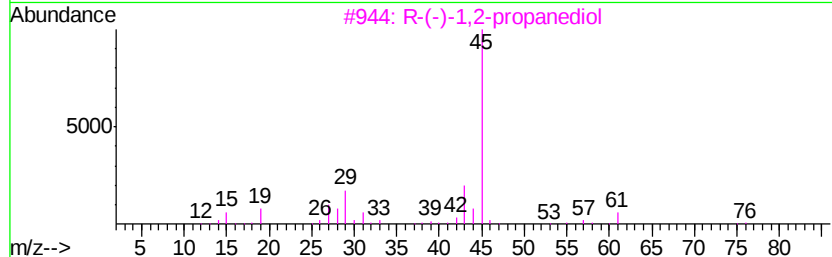
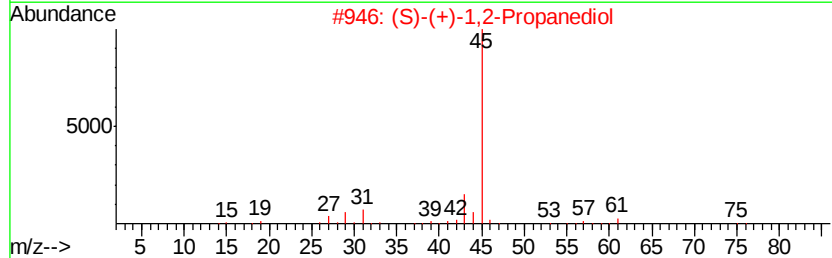
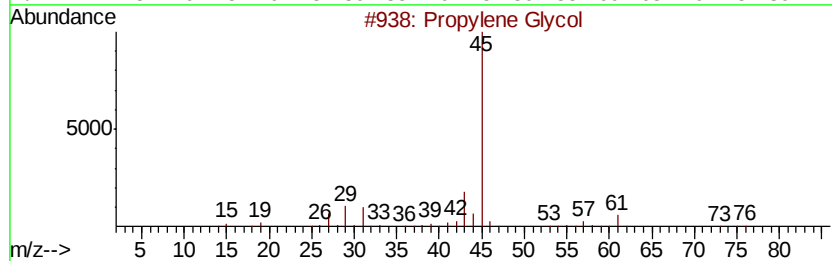
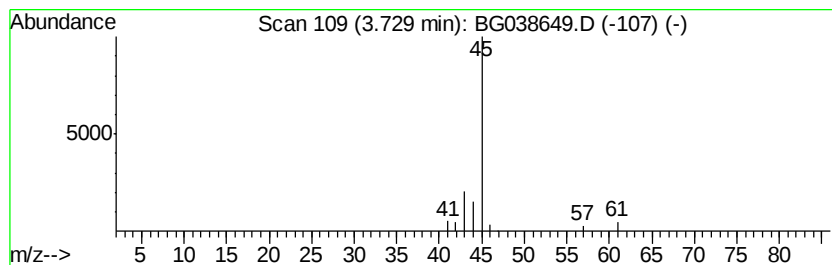
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propylene Glycol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.73	3.10 ng	23328	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propylene Glycol	76	C3H8O2	000057-55-6	64
2		(S)-(+)-1,2-Propanediol	76	C3H8O2	004254-15-3	64
3		R-(-)-1,2-propanediol	76	C3H8O2	004254-14-2	43
4		Methyltartronic acid	134	C4H6O5	000595-98-2	9
5		2-Butanol, (R)-	74	C4H10O	014898-79-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

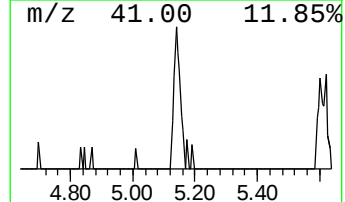
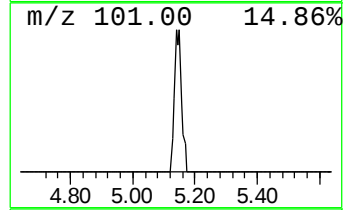
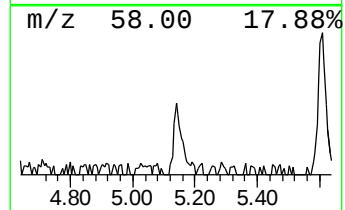
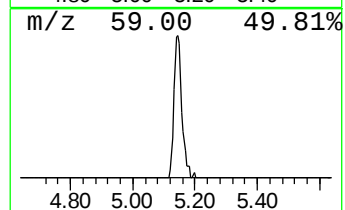
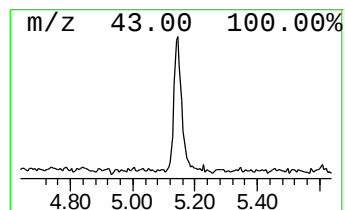
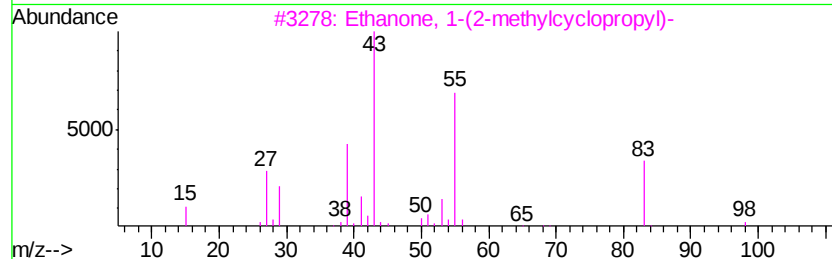
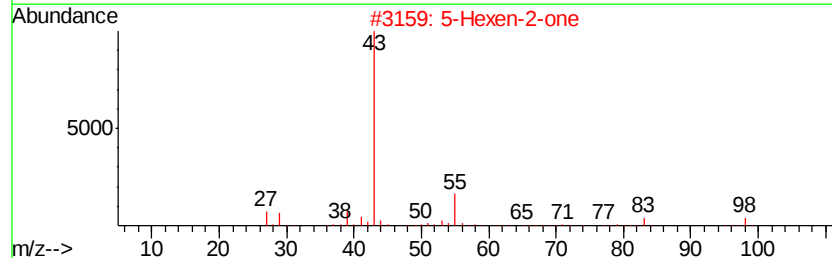
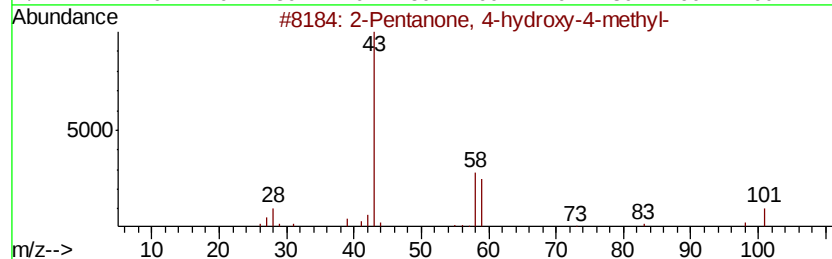
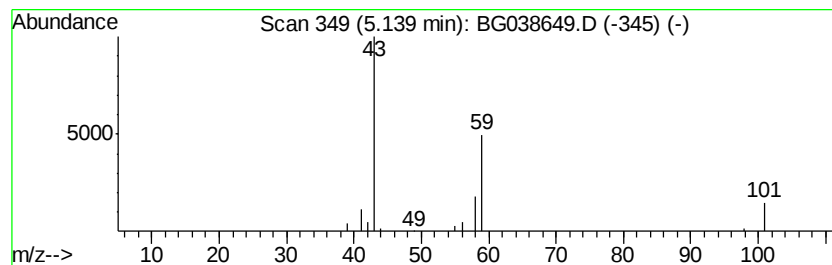
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	4.62 ng	34710	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		5-Hexen-2-one	98	C6H10O	000109-49-9	9
3		Ethanone, 1-(2-methylcyclopropyl)-	98	C6H10O	000930-56-3	9
4		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	9
5		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

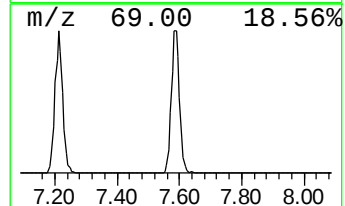
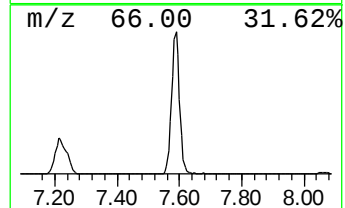
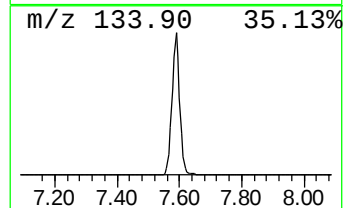
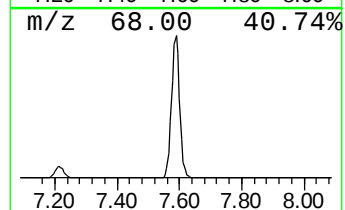
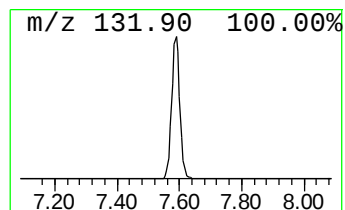
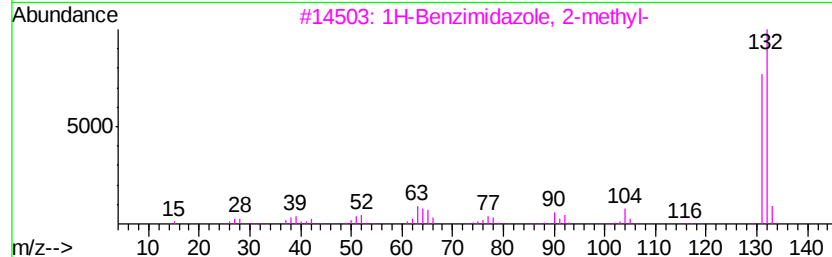
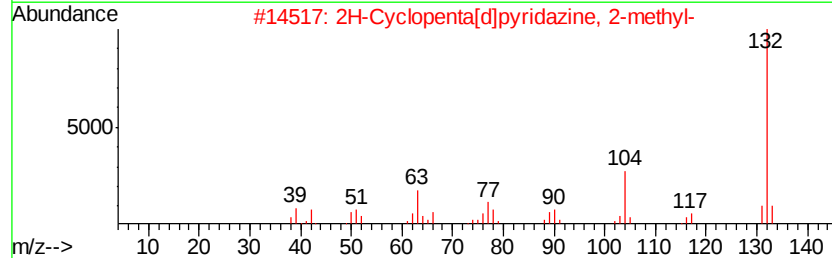
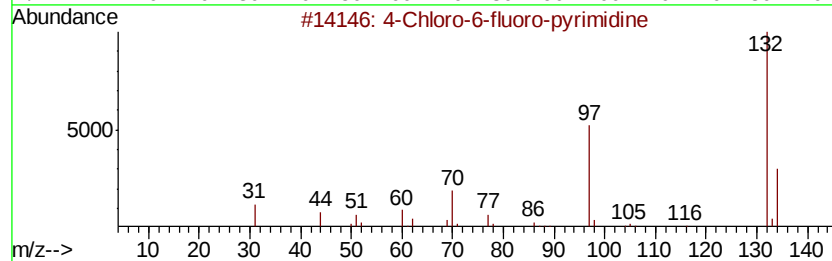
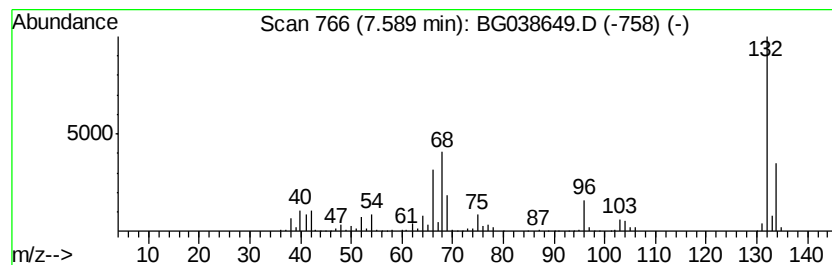
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.59 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.59	95.36 ng	717156	1,4-Dichlorobenzene-d4	8.06

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	22
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

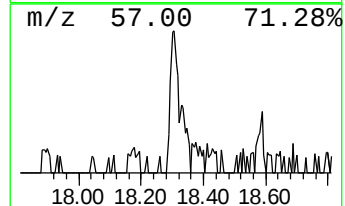
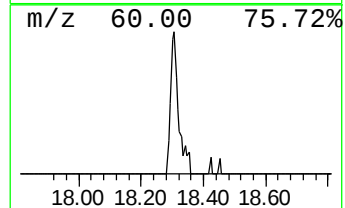
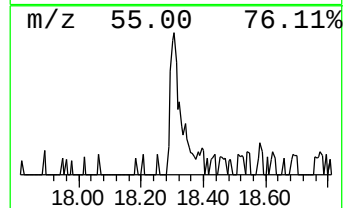
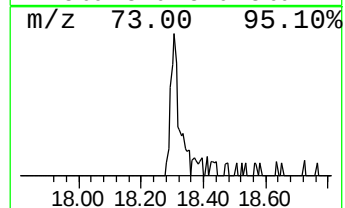
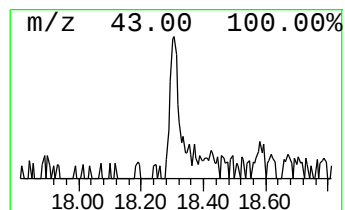
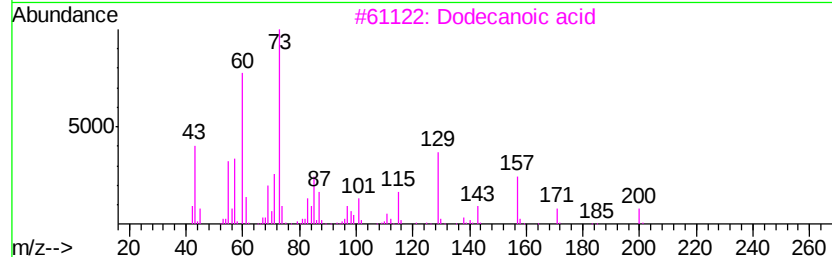
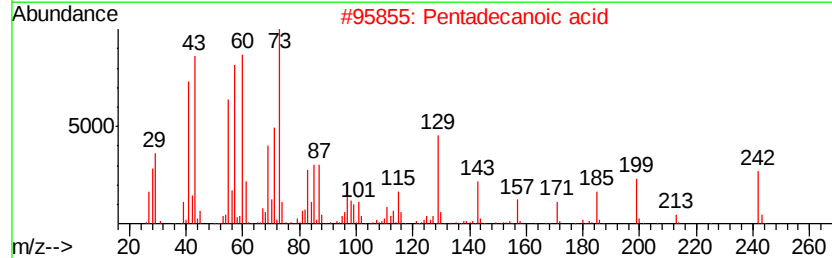
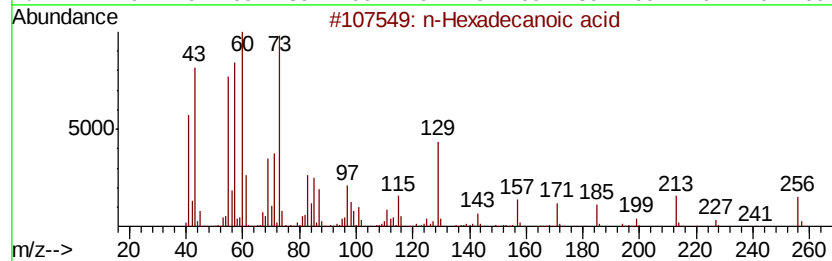
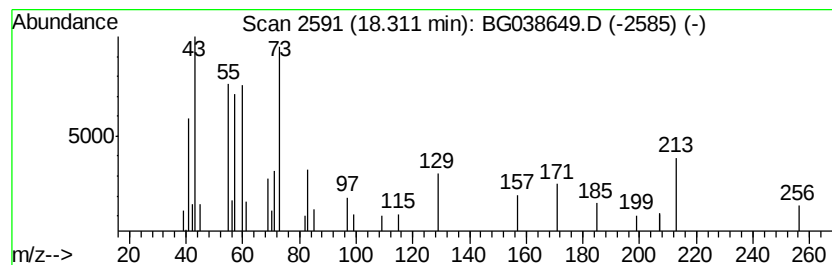
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.31	2.02 ng	35719	Phenanthrene-d10	17.44

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	91
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	59
3		Dodecanoic acid	200	C12H24O2	000143-07-7	59
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	47



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

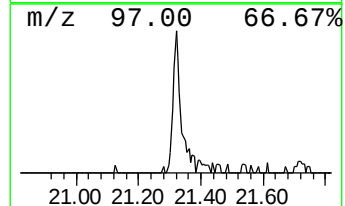
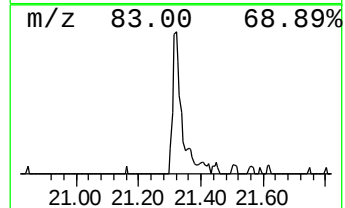
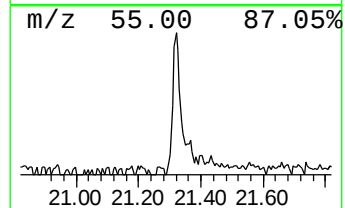
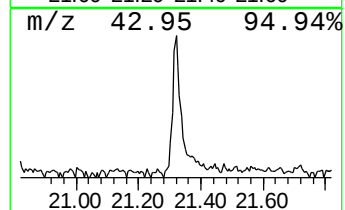
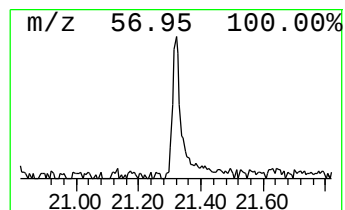
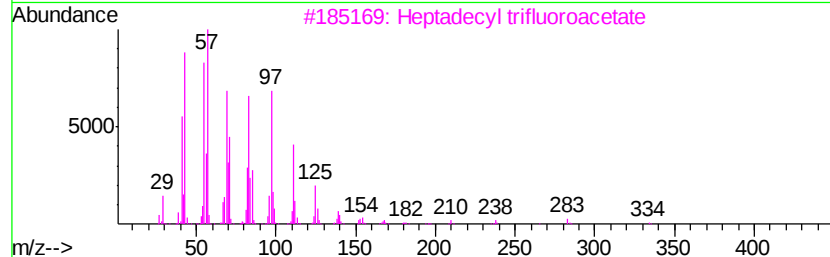
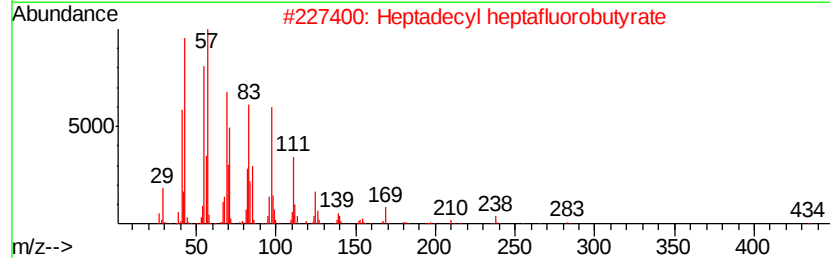
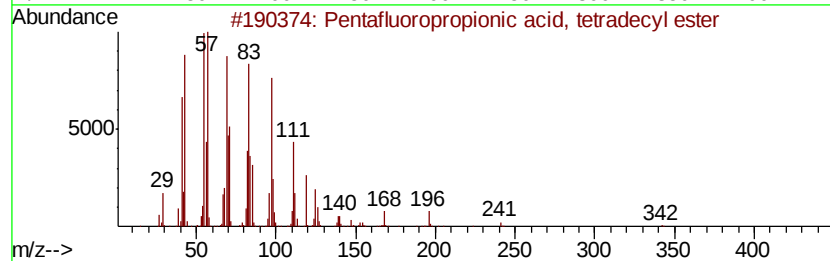
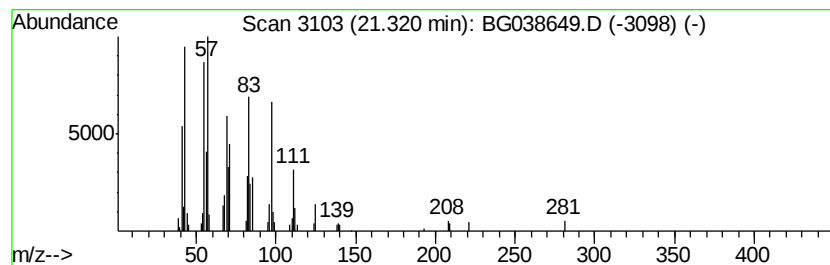
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG121218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	4.81 ng	95272	Chrysene-d12	21.73

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	94
2			Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
3			Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
4			Pentafluoropropionic acid, hepta...	402	C20H35F5O2	959218-78-1	91
5			Pentafluoropropionic acid, hexad...	388	C19H33F5O2	006222-07-7	91



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG121618\
Data File : BG038649.D
Acq On : 16 Dec 2018 20:45
Operator : JU/SJ
Sample : J6424-05
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SODUP02_121318

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG121218.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
Propylene Glycol	3.73	3.1	ng	23328	1	8.06	150407	20.0
2-Pentanone, 4-hy...	5.14	4.6	ng	34710	1	8.06	150407	20.0
unknown7.59	7.59	95.4	ng	717156	1	8.06	150407	20.0
n-Hexadecanoic acid	18.31	2.0	ng	35719	4	17.44	352911	20.0
Pentafluoropropio...	21.32	4.8	ng	95272	5	21.73	396034	20.0