

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
 Data File : BG036818.D
 Acq On : 19 Sep 2018 12:41
 Operator : JU/SJ
 Sample : J4929-13
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SP-PIT-11-BASELINE-WATER

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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	5.156	313	318	328	rVB	33686	50403	1.38%	0.269%
2	5.620	390	397	411	rVB	535107	866632	23.75%	4.631%
3	7.200	659	666	677	rBV	373838	656614	18.00%	3.509%
4	7.576	723	730	742	rBV	809150	1408256	38.59%	7.526%
5	8.047	803	810	817	rBV	190785	323831	8.87%	1.731%
6	8.370	857	865	873	rBV	675681	1146349	31.42%	6.126%
7	9.210	998	1008	1018	rBV	598946	1081536	29.64%	5.780%
8	10.849	1280	1287	1295	rBV	270973	483911	13.26%	2.586%
9	13.293	1696	1703	1710	rBV	1599827	2476587	67.87%	13.235%
10	13.558	1743	1748	1758	rBV	103023	168787	4.63%	0.902%
11	14.116	1838	1843	1849	rBV	85785	121660	3.33%	0.650%
12	14.674	1931	1938	1946	rVB2	432834	706971	19.38%	3.778%
13	16.161	2183	2191	2205	rBV	1267824	2023869	55.47%	10.816%
14	17.412	2398	2404	2411	rBV2	557362	892486	24.46%	4.769%
15	18.076	2512	2517	2523	rBV3	77837	105081	2.88%	0.562%
16	18.299	2550	2555	2563	rBV2	60688	110960	3.04%	0.593%
17	19.568	2767	2771	2777	rBV8	25632	41436	1.14%	0.221%
18	20.021	2842	2848	2854	rBV	2665777	3648863	100.00%	19.499%
19	21.678	3124	3130	3137	rBV2	591790	995998	27.30%	5.323%
20	23.358	3413	3416	3423	rVB2	45649	75716	2.08%	0.405%
21	23.969	3515	3520	3526	rVB2	47445	100101	2.74%	0.535%
22	24.891	3667	3677	3689	rVB2	349958	1070707	29.34%	5.722%
23	26.031	3865	3871	3881	rVB2	57889	155906	4.27%	0.833%

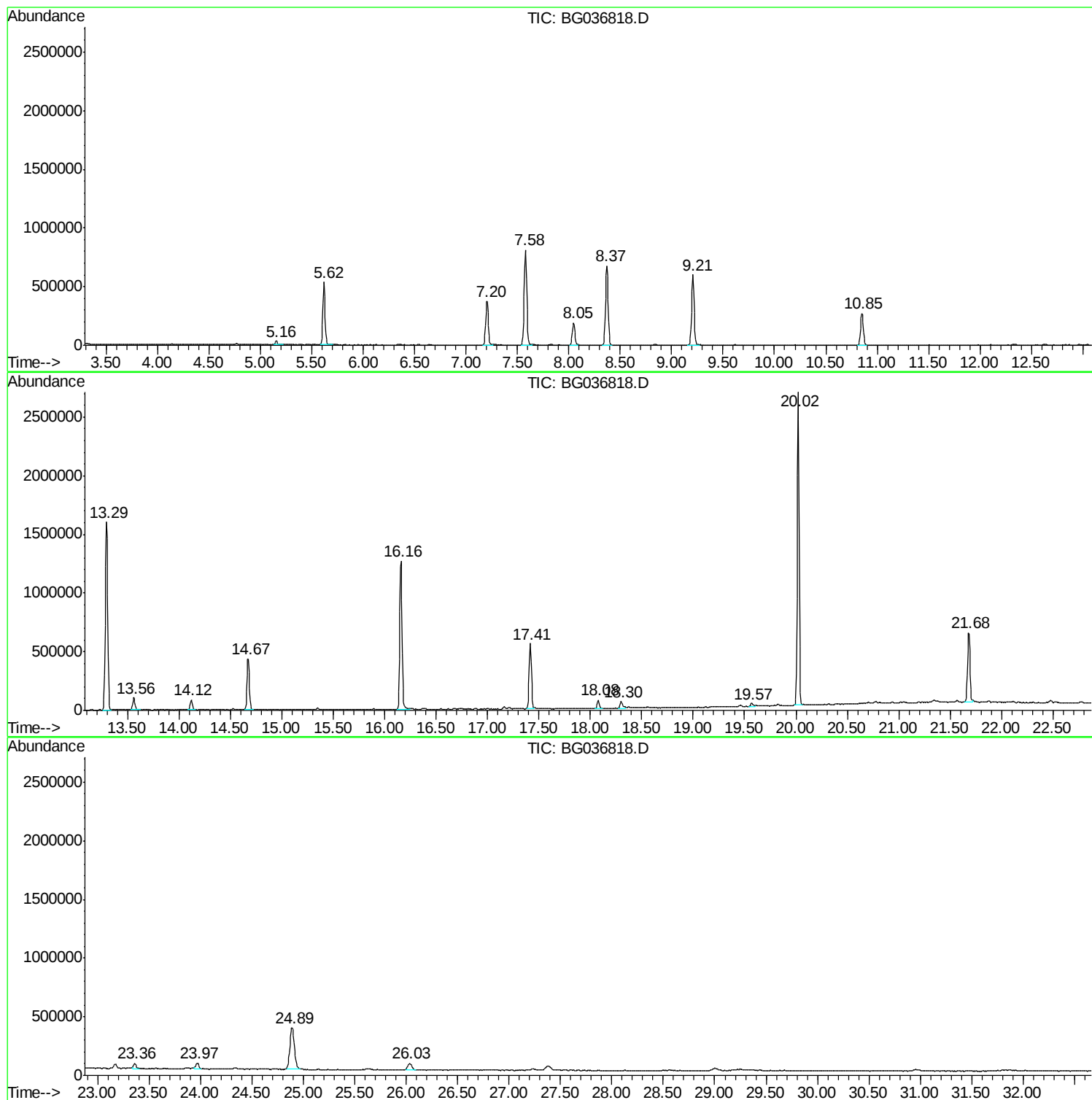
Sum of corrected areas: 18712660

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.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\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

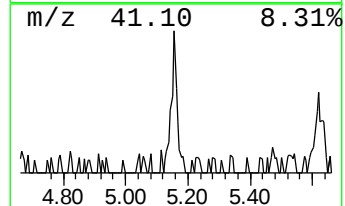
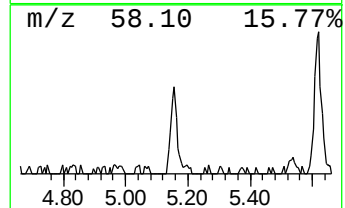
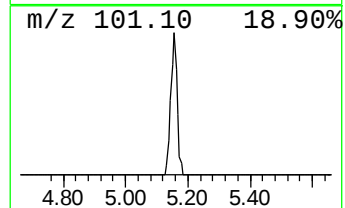
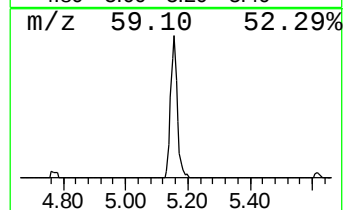
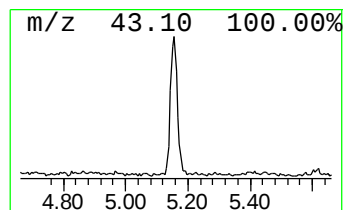
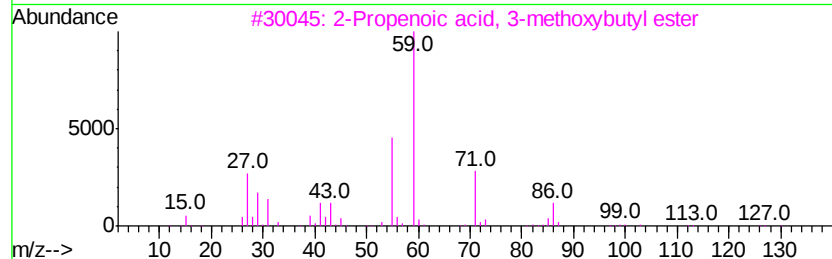
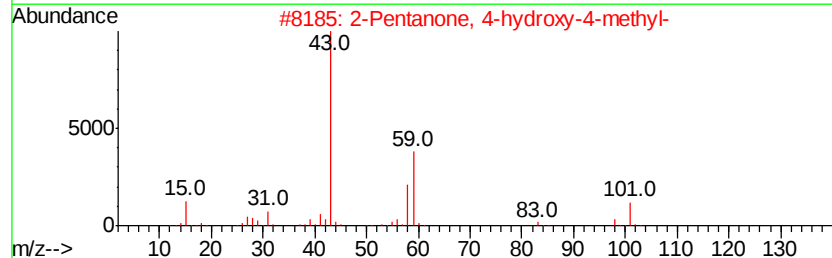
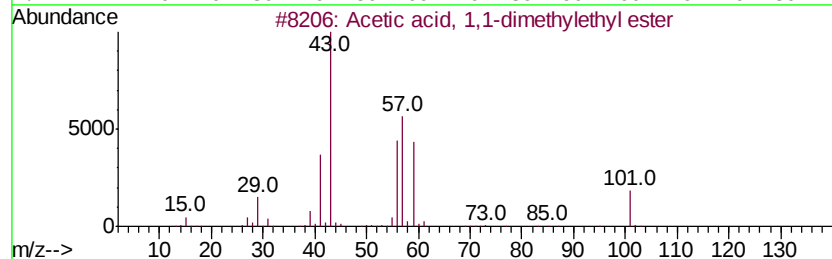
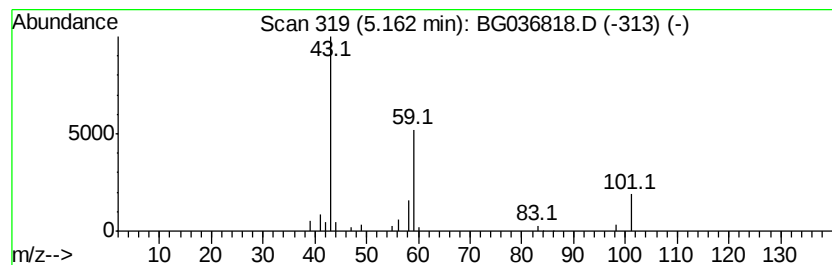
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.16	3.11 ng	50403	1,4-Dichlorobenzene-d4	8.05

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	50
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	45
3		2-Propenoic acid, 3-methoxybutyl...	158	C8H14O3	002768-07-2	12
4		1,2-Butanediol	90	C4H10O2	000584-03-2	9
5		Propane, 2-ethoxy-2-methyl-	102	C6H14O	000637-92-3	9



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

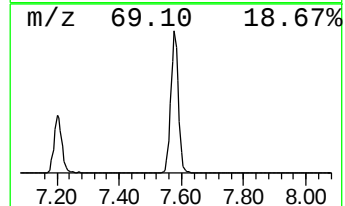
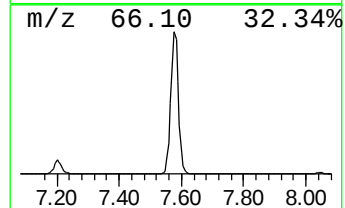
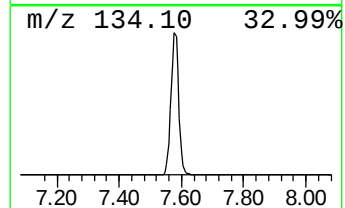
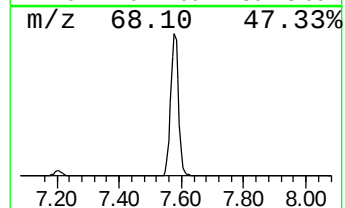
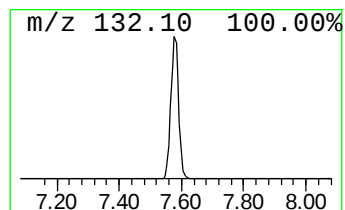
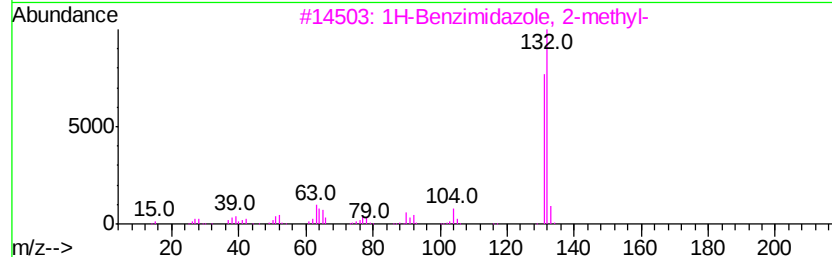
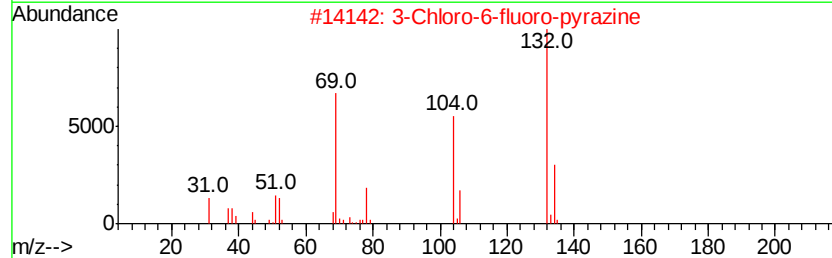
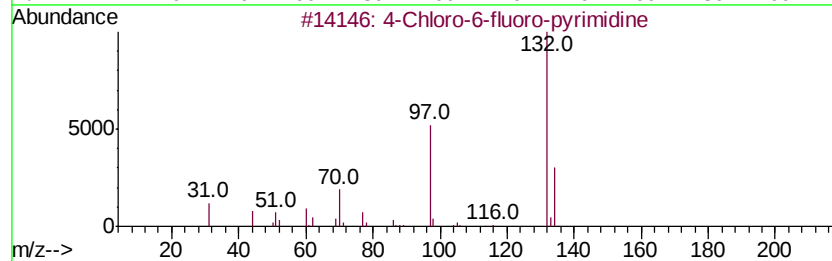
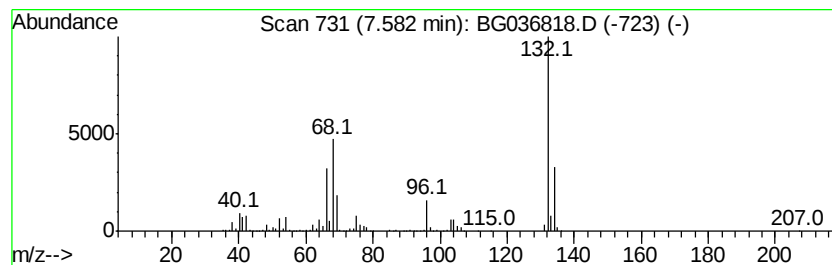
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	86.97 ng	1408260	1,4-Dichlorobenzene-d4	8.05

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

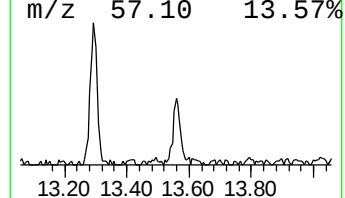
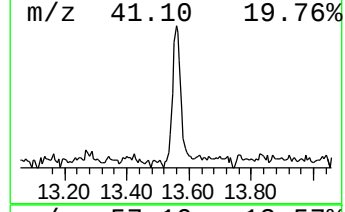
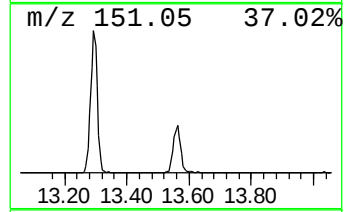
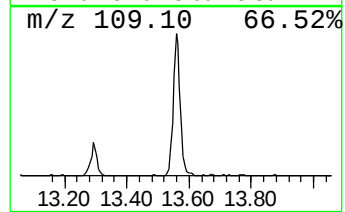
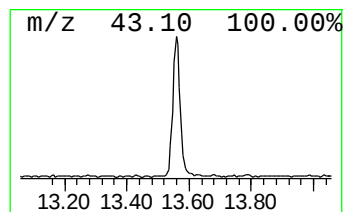
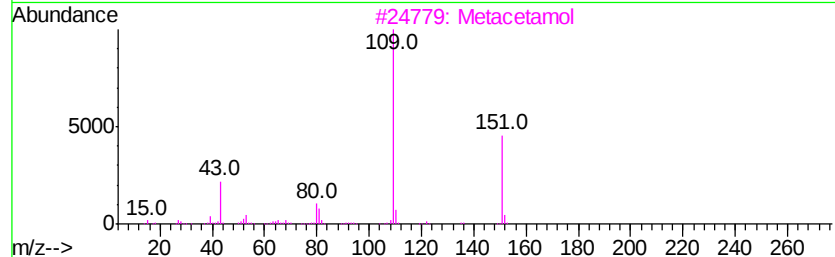
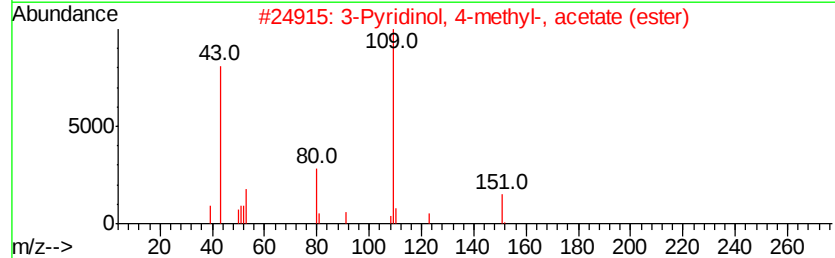
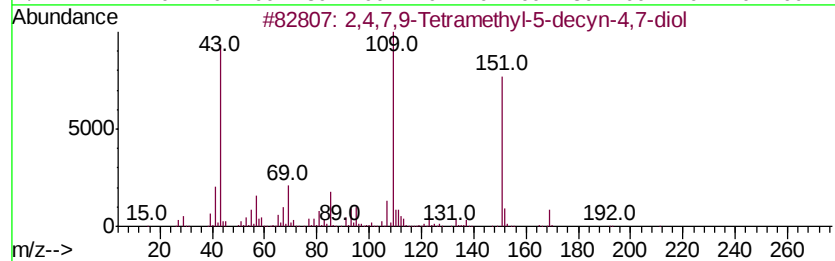
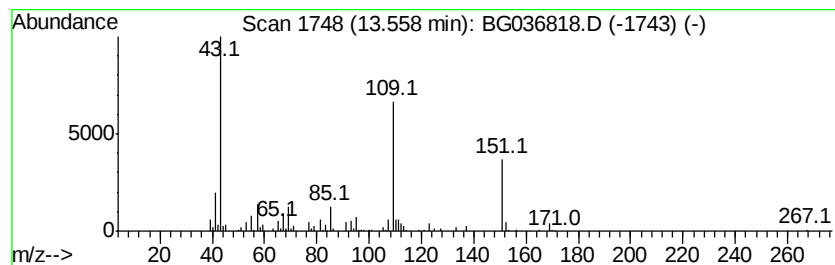
Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 2,4,7,9-Tetramethyl-5-decyn... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
13.56	4.77 ng	168787	Acenaphthene-d10		14.67	
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4,7,9-Tetramethyl-5-decyn-4,7-...	226	C14H26O2		000126-86-3	90
2	3-Pyridinol, 4-methyl-, acetate ...	151	C8H9NO2		001006-96-8	58
3	Metacetamol	151	C8H9NO2		000621-42-1	52
4	Acetaminophen	151	C8H9NO2		000103-90-2	52
5	Tiocarlide	400	C23H32N2O2S		000910-86-1	50



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

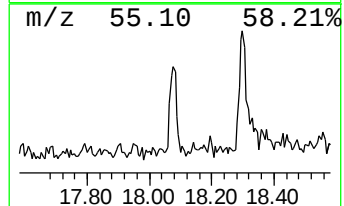
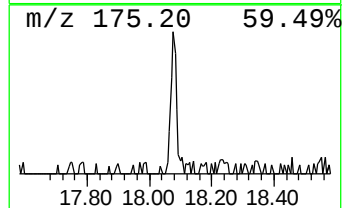
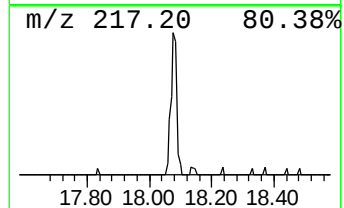
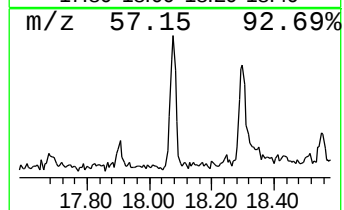
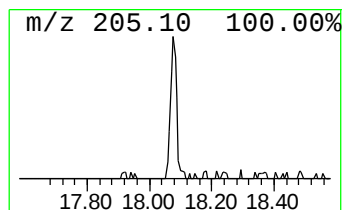
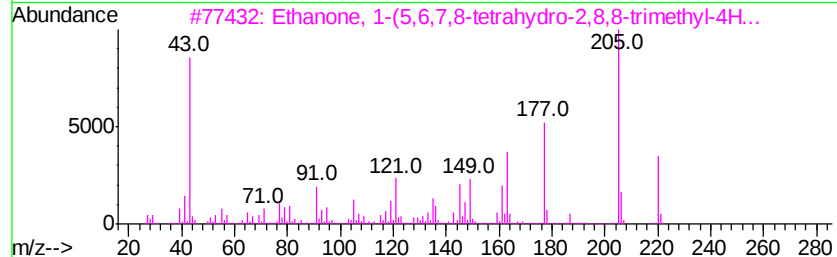
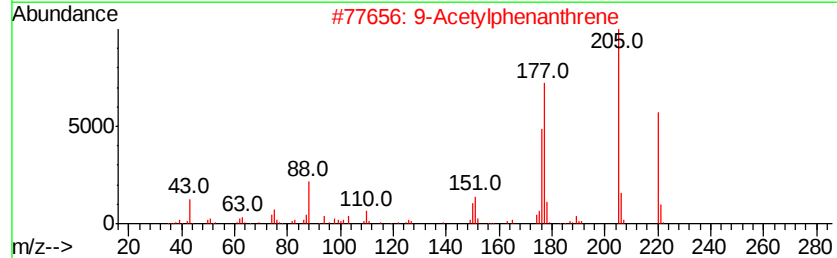
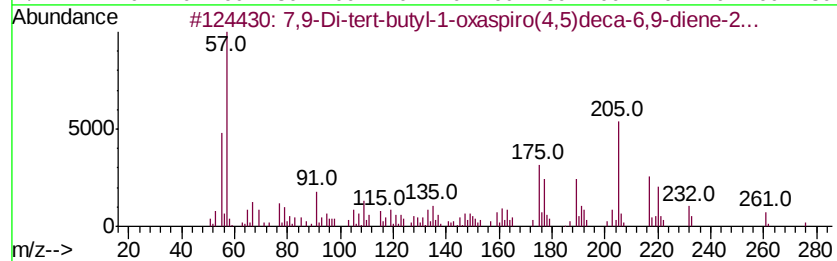
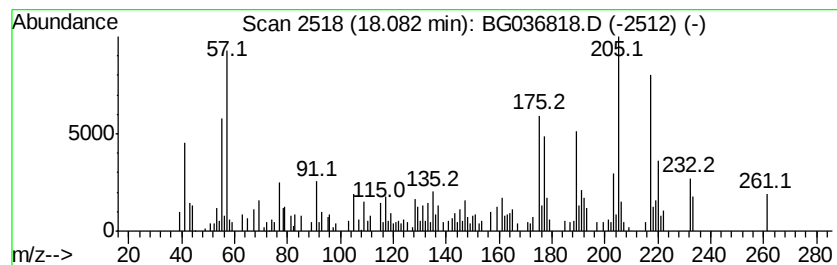
Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 7,9-Di-tert-butyl-1-oxaspiro... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.08	2.35 ng	105081	Phenanthrene-d10	17.41	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	7,9-Di-tert-butyl-1-oxaspiro(4,5...	276	C17H24O3	082304-66-3	91
2	9-Acetylphenanthrene	220	C16H12O	002039-77-2	51
3	Ethanone, 1-(5,6,7,8-tetrahydro-...	220	C14H20O2	071596-88-8	38
4	2H-2a,7-Methanoazuleno[5,6-b]oxi...	220	C15H24O	029597-36-2	38
5	1,3-Pentadiene, 1,1-diphenyl-, (Z)-	220	C17H16	015295-31-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

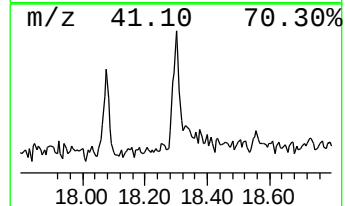
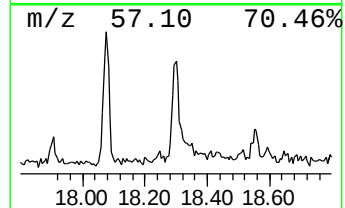
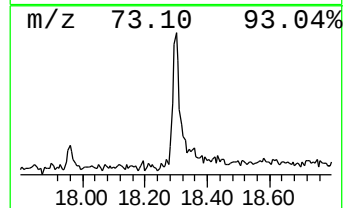
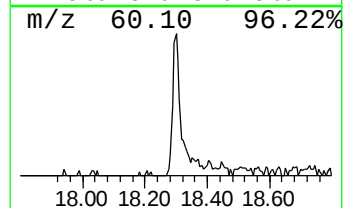
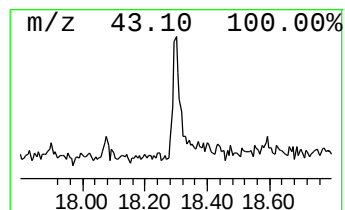
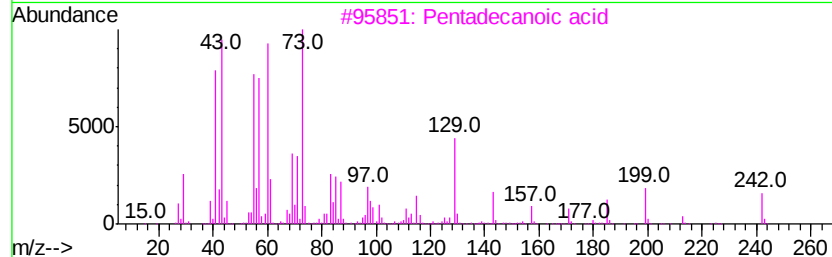
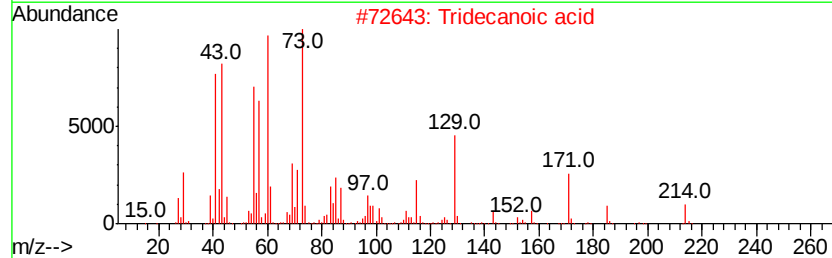
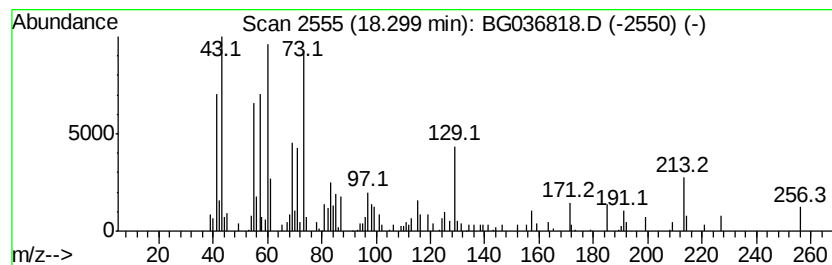
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	2.49 ng	110960	Phenanthrene-d10	17.41

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	70



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

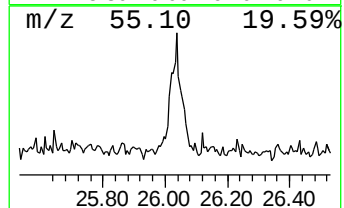
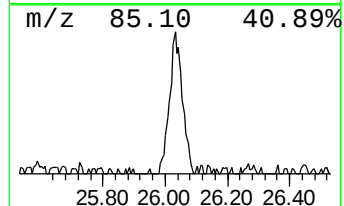
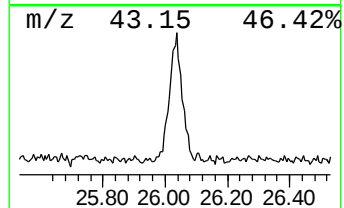
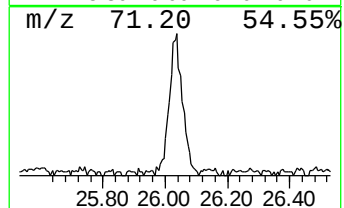
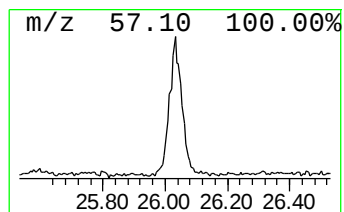
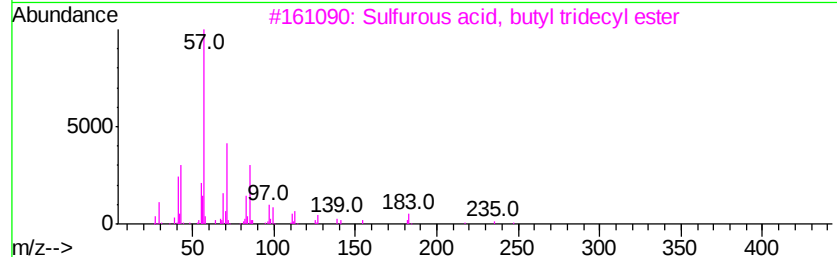
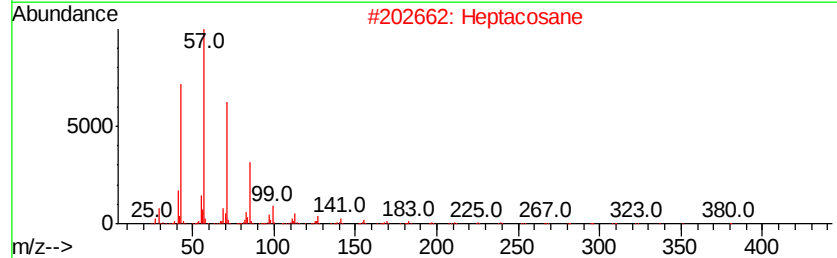
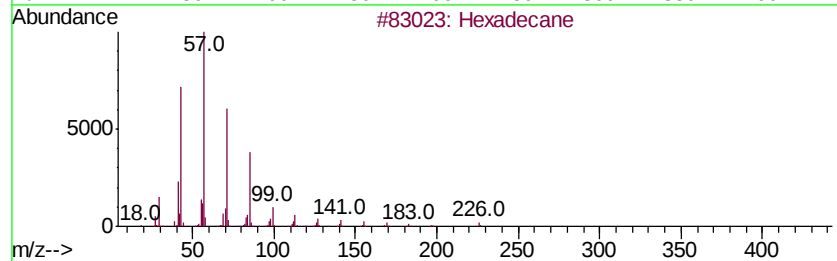
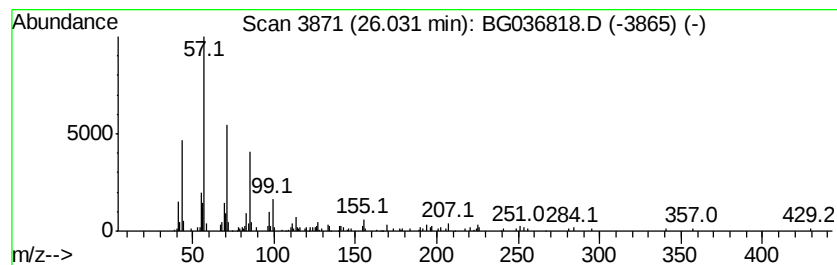
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG082318.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecane Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
26.03	2.91 ng	155906	Perylene-d12	24.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecane	226	C16H34	000544-76-3	81
2		Heptacosane	380	C27H56	000593-49-7	80
3		Sulfurous acid, butyl tridecyl e...	320	C17H36O3S	1000309-18-0	80
4		2-Thiopheneacetic acid, 4-tetrad...	338	C20H34O2S	1000280-67-0	72
5		Eicosane	282	C20H42	000112-95-8	72



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG091818\
Data File : BG036818.D
Acq On : 19 Sep 2018 12:41
Operator : JU/SJ
Sample : J4929-13
Misc :
ALS Vial : 32 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SP-PIT-11-BASELINE-WATER

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG082318.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
2-Pentanone, 4-hy...	5.16	3.1	ng	50403	1	8.05	323831	20.0
unknown7.58	7.58	87.0	ng	1408260	1	8.05	323831	20.0
2,4,7,9-Tetrameth...	13.56	4.8	ng	168787	3	14.67	706971	20.0
7,9-Di-tert-butyl...	18.08	2.4	ng	105081	4	17.41	892486	20.0
n-Hexadecanoic acid	18.30	2.5	ng	110960	4	17.41	892486	20.0
Hexadecane	26.03	2.9	ng	155906	6	24.89	1070710	20.0