

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
 Data File : BG035672.D
 Acq On : 16 Jul 2018 16:38
 Operator : JU/SJ
 Sample : J3888-02
 Misc :
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 AOC7-BTM-6-6.5

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:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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	5.171	314	320	331	rBV	138130	217108	4.32%	0.831%
2	5.641	393	400	413	rVB	1245020	1932587	38.47%	7.399%
3	7.233	663	671	682	rBV	1298964	2318551	46.16%	8.876%
4	7.597	725	733	742	rBV	1213652	2087731	41.56%	7.993%
5	8.055	803	811	818	rBV	195971	337498	6.72%	1.292%
6	8.378	859	866	876	rBV	825853	1437069	28.61%	5.502%
7	9.219	1001	1009	1022	rBV	721809	1315377	26.19%	5.036%
8	10.863	1281	1289	1300	rVB	272669	493558	9.83%	1.890%
9	13.301	1695	1704	1715	rBV	2122643	3335019	66.39%	12.768%
10	14.124	1838	1844	1854	rBV	250260	369472	7.36%	1.415%
11	14.676	1932	1938	1948	rVB2	483740	790913	15.74%	3.028%
12	16.168	2182	2192	2209	rBV	1649306	2612043	52.00%	10.000%
13	17.419	2398	2405	2412	rBV	672013	1039022	20.68%	3.978%
14	18.300	2550	2555	2562	rBV2	125005	175790	3.50%	0.673%
15	19.146	2695	2699	2704	rBV2	42535	55366	1.10%	0.212%
16	20.027	2842	2849	2854	rBV	3795846	5023321	100.00%	19.231%
17	21.320	3065	3069	3078	rBV	103797	196965	3.92%	0.754%
18	21.684	3124	3131	3142	rVB	690148	1155229	23.00%	4.423%
19	22.536	3270	3276	3279	rBV6	36933	66071	1.32%	0.253%
20	23.975	3514	3521	3527	rVB5	22938	51165	1.02%	0.196%
21	24.909	3669	3680	3692	rBV2	396220	1110431	22.11%	4.251%

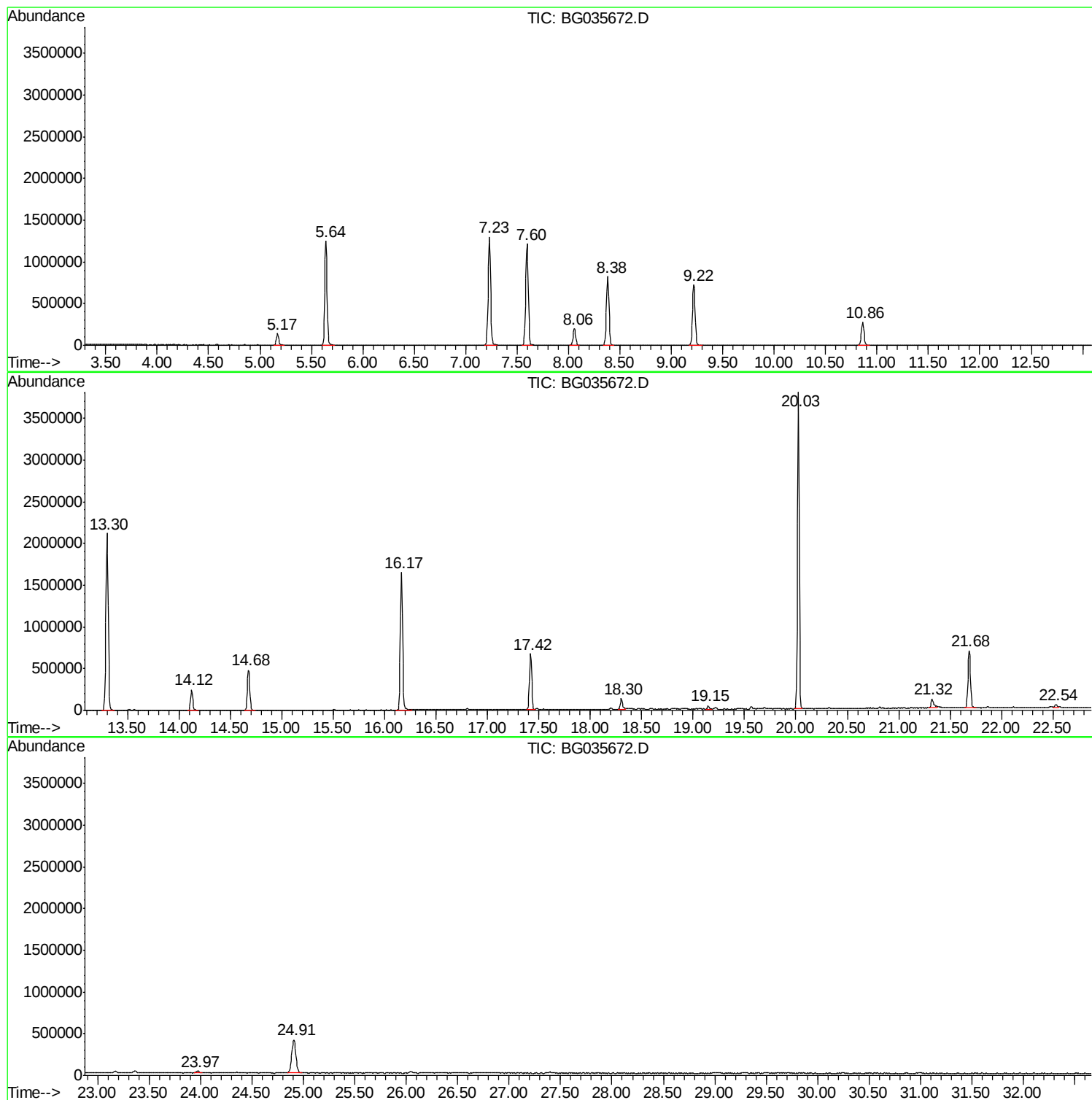
Sum of corrected areas: 26120286

Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035672.D
Acq On : 16 Jul 2018 16:38
Operator : JU/SJ
Sample : J3888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AOC7-BTM-6-6.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071218.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\BG071618\
Data File : BG035672.D
Acq On : 16 Jul 2018 16:38
Operator : JU/SJ
Sample : J3888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AOC7-BTM-6-6.5

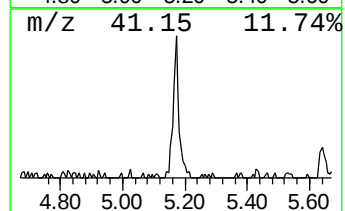
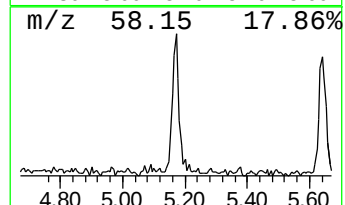
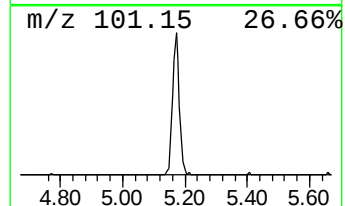
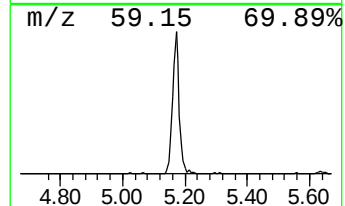
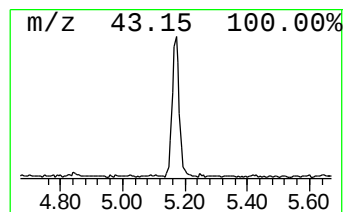
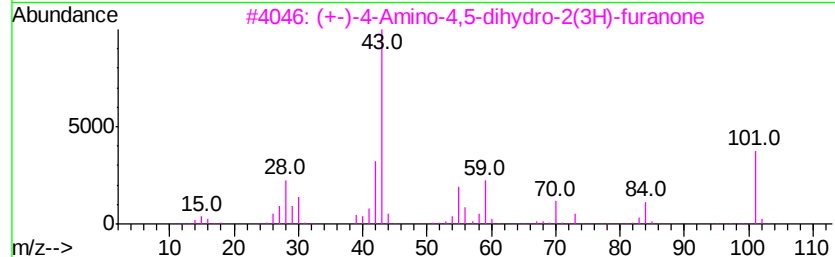
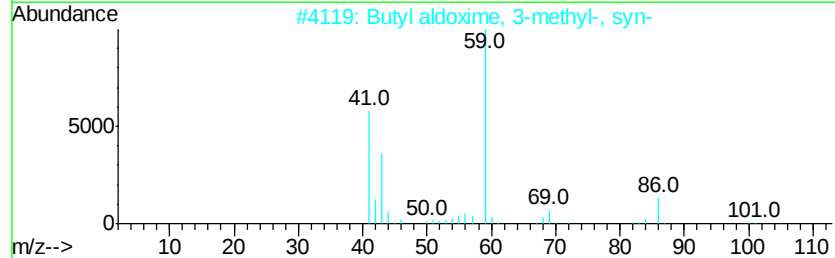
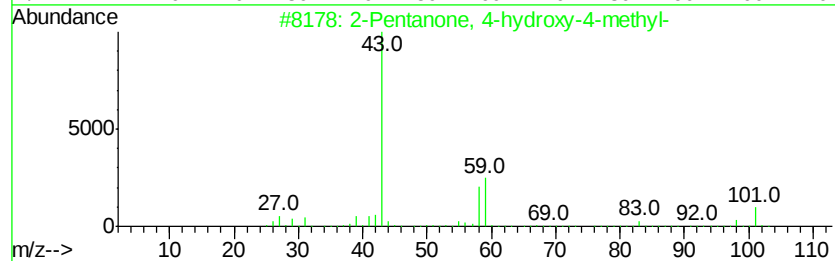
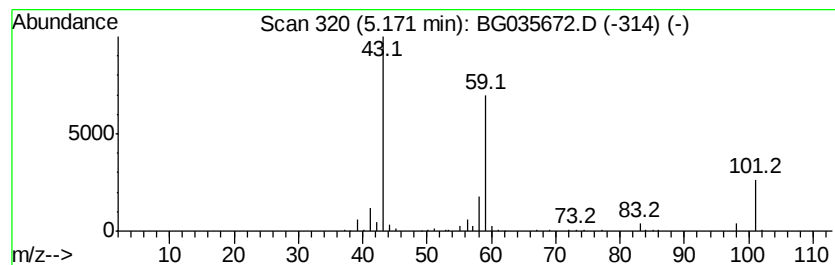
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.17	12.87 ng	217108	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	45
2		Butyl aldoxime, 3-methyl-, syn-	101	C5H11NO	005780-40-5	35
3		(+)-4-Amino-4,5-dihydro-2(3H)-furanone	101	C4H7NO2	016504-58-8	25
4		3-Hexanol	102	C6H14O	000623-37-0	25
5		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035672.D
Acq On : 16 Jul 2018 16:38
Operator : JU/SJ
Sample : J3888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AOC7-BTM-6-6.5

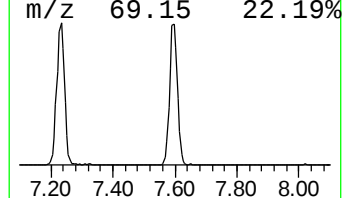
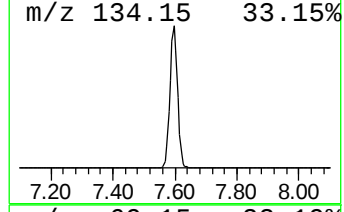
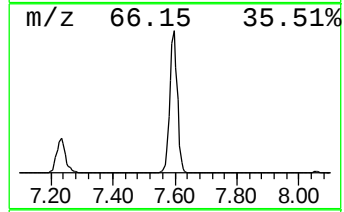
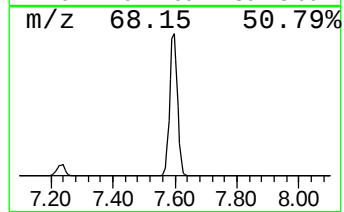
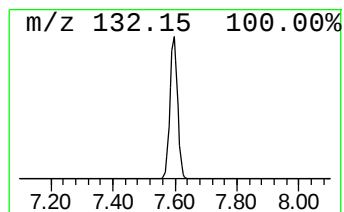
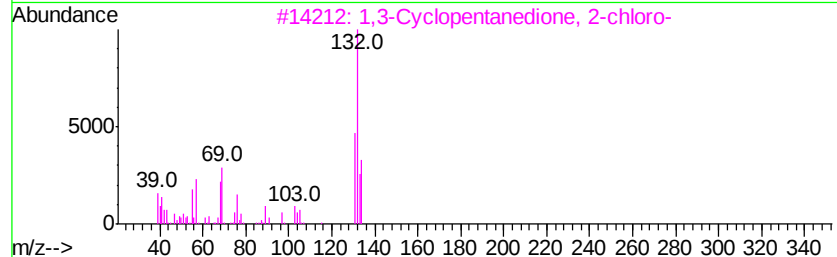
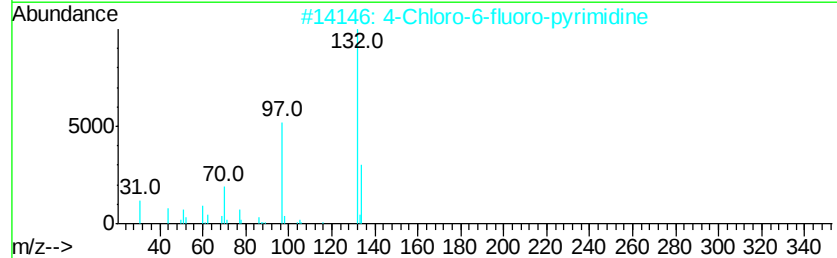
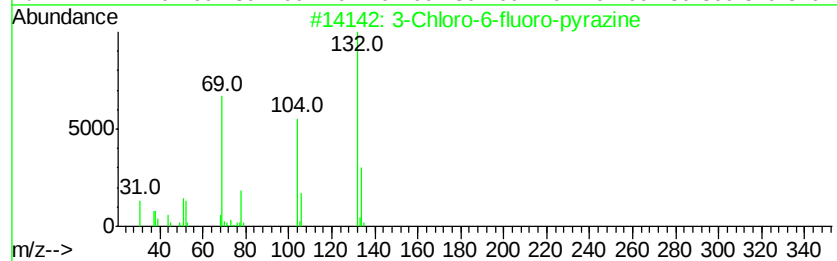
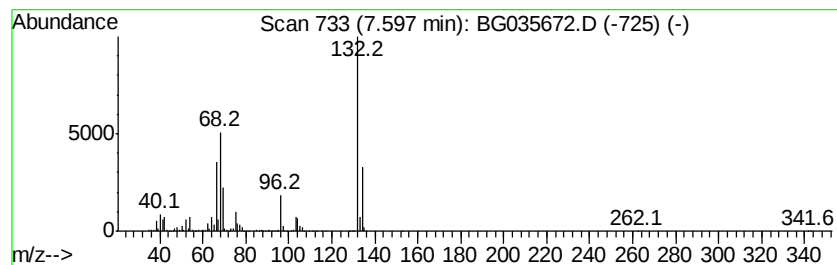
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown7.60 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.60	123.72 ng	2087730	1,4-Dichlorobenzene-d4	8.06

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27		
2	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27		
3	1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25		
4	1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22		
5	5-Aminoindole	132	C8H8N2	005192-03-0	22		



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035672.D
Acq On : 16 Jul 2018 16:38
Operator : JU/SJ
Sample : J3888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AOC7-BTM-6-6.5

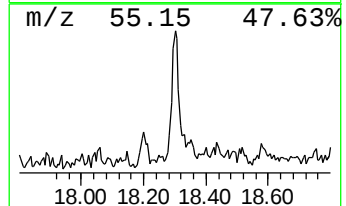
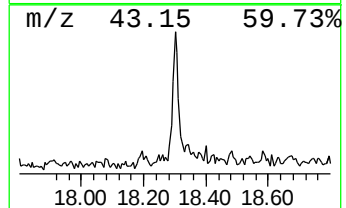
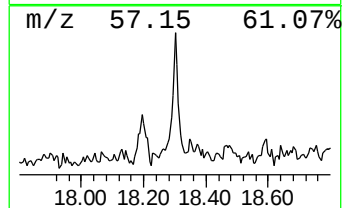
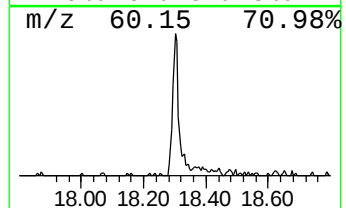
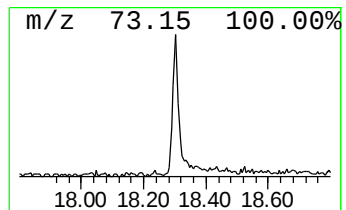
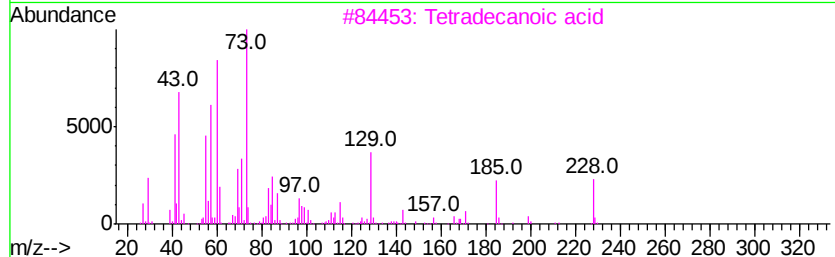
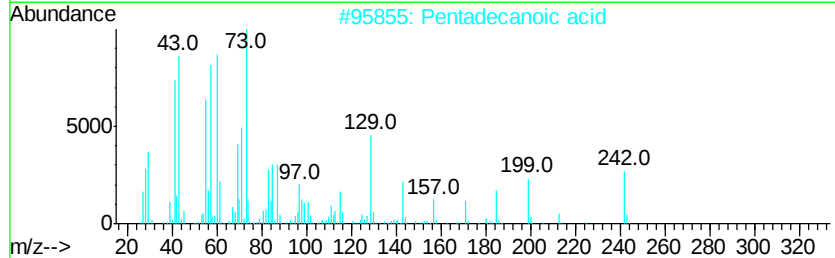
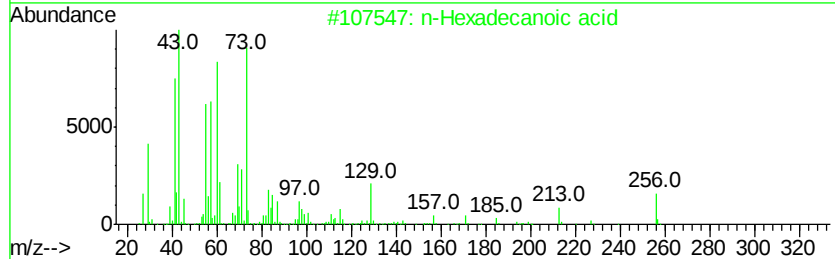
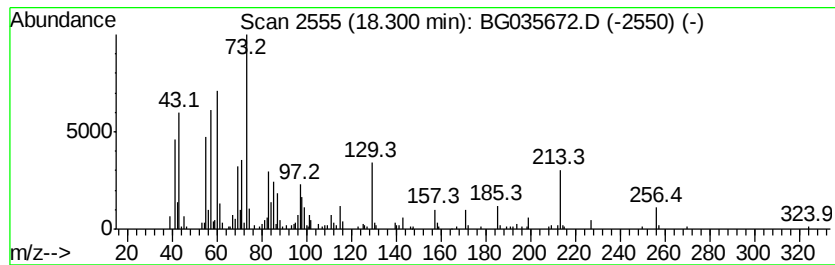
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.30	3.38 ng	175790	Phenanthrene-d10	17.42

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	58
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	53
4		Heptadecanoic acid	270	C17H34O2	000506-12-7	53
5		n-Decanoic acid	172	C10H20O2	000334-48-5	38



Data Path : Z:\SVOASRV\HPCHEM1\BNA G\DATA\BG071618\
Data File : BG035672.D
Acq On : 16 Jul 2018 16:38
Operator : JU/SJ
Sample : J3888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AOC7-BTM-6-6.5

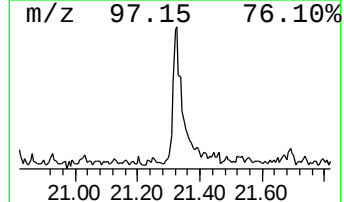
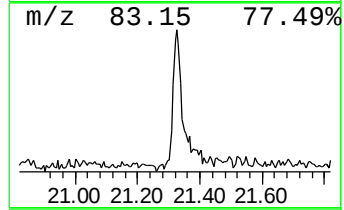
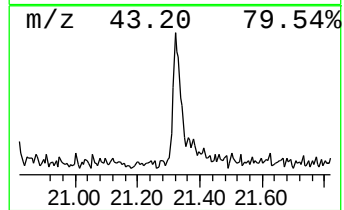
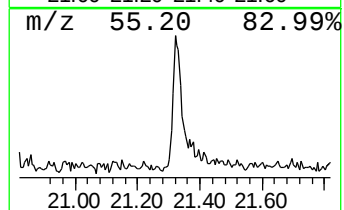
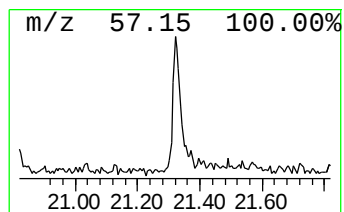
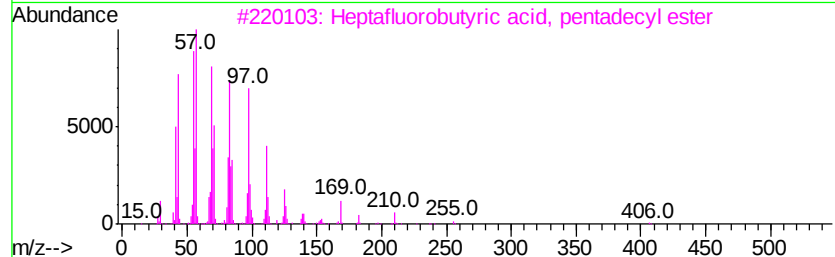
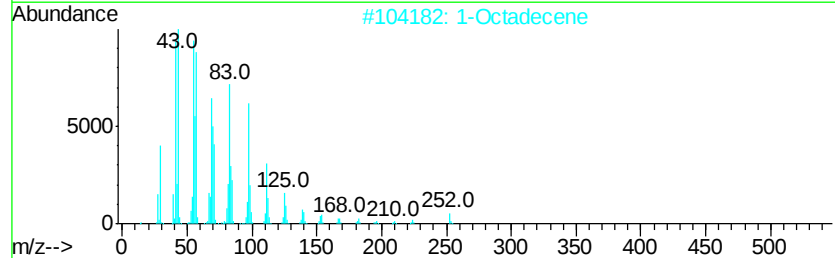
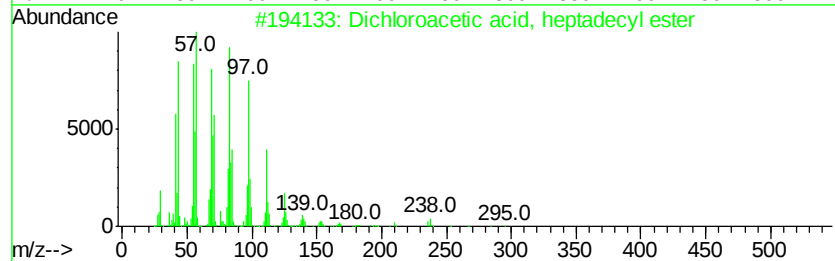
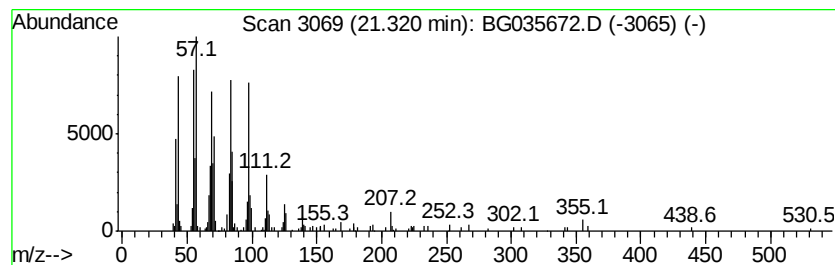
Quant Method : Z:\SVOASRV\HPCHEM1\BNA G\METHODS\8270-BG071218.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Dichloroacetic acid, heptad... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.32	3.41 ng	196965	Chrysene-d12	21.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	95
2		1-Octadecene	252	C18H36	000112-88-9	95
3		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	94
4		Heptadecyl heptafluorobutyrate	452	C21H35F7O2	959085-66-6	91
5		Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	87



Data Path : Z:\SVOASRV\HPCHEM1\BNA_G\DATA\BG071618\
Data File : BG035672.D
Acq On : 16 Jul 2018 16:38
Operator : JU/SJ
Sample : J3888-02
Misc :
ALS Vial : 12 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
AOC7-BTM-6-6.5

Quant Method : Z:\SVOASRV\HPCHEM1\BNA_G\METHODS\8270-BG071218.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...	5.17	12.9	ng	217108	1	8.06	337498	20.0
unknown7.60	7.60	123.7	ng	2087730	1	8.06	337498	20.0
n-Hexadecanoic acid	18.30	3.4	ng	175790	4	17.42	1039020	20.0
Dichloroacetic ac...	21.32	3.4	ng	196965	5	21.68	1155230	20.0