

Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
 Data File : BG031762.D
 Acq On : 26 Dec 2017 15:22
 Operator : SJ/JU
 Sample : I7040-03
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 LIP-22

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-BG122117.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	3.434	19	25	35	rBV	76367	158848	3.85%	0.904%
2	3.528	37	41	47	rVB2	29897	44566	1.08%	0.254%
3	6.225	493	500	509	rBV	290180	490172	11.89%	2.790%
4	7.905	774	786	801	rVB	182970	345536	8.38%	1.967%
5	8.317	847	856	865	rBV	575969	1053970	25.58%	5.999%
6	8.804	932	939	950	rBV	130927	239251	5.81%	1.362%
7	9.145	989	997	1009	rVB	544363	1024762	24.87%	5.833%
8	10.009	1135	1144	1157	rBV	383793	725431	17.60%	4.129%
9	10.861	1279	1289	1297	rBV4	20565	56372	1.37%	0.321%
10	11.689	1421	1430	1442	rBV	194314	379205	9.20%	2.158%
11	14.069	1827	1835	1845	rBV	1531534	2476417	60.09%	14.096%
12	15.438	2060	2068	2079	rVB2	351001	625002	15.17%	3.558%
13	16.019	2162	2167	2173	rBV8	33780	75778	1.84%	0.431%
14	16.907	2311	2318	2327	rVB	1268855	2116617	51.36%	12.048%
15	18.170	2527	2533	2539	rVB2	500318	779815	18.92%	4.439%
16	18.992	2668	2673	2683	rBV	140754	233682	5.67%	1.330%
17	20.226	2879	2883	2893	rBV	237263	367963	8.93%	2.094%
18	20.702	2958	2964	2973	rVB	3092540	4120890	100.00%	23.456%
19	21.607	3113	3118	3125	rBV	79391	129054	3.13%	0.735%
20	22.512	3265	3272	3284	rVB2	529721	1045744	25.38%	5.952%
21	26.266	3899	3911	3925	rBV2	332683	1079463	26.19%	6.144%

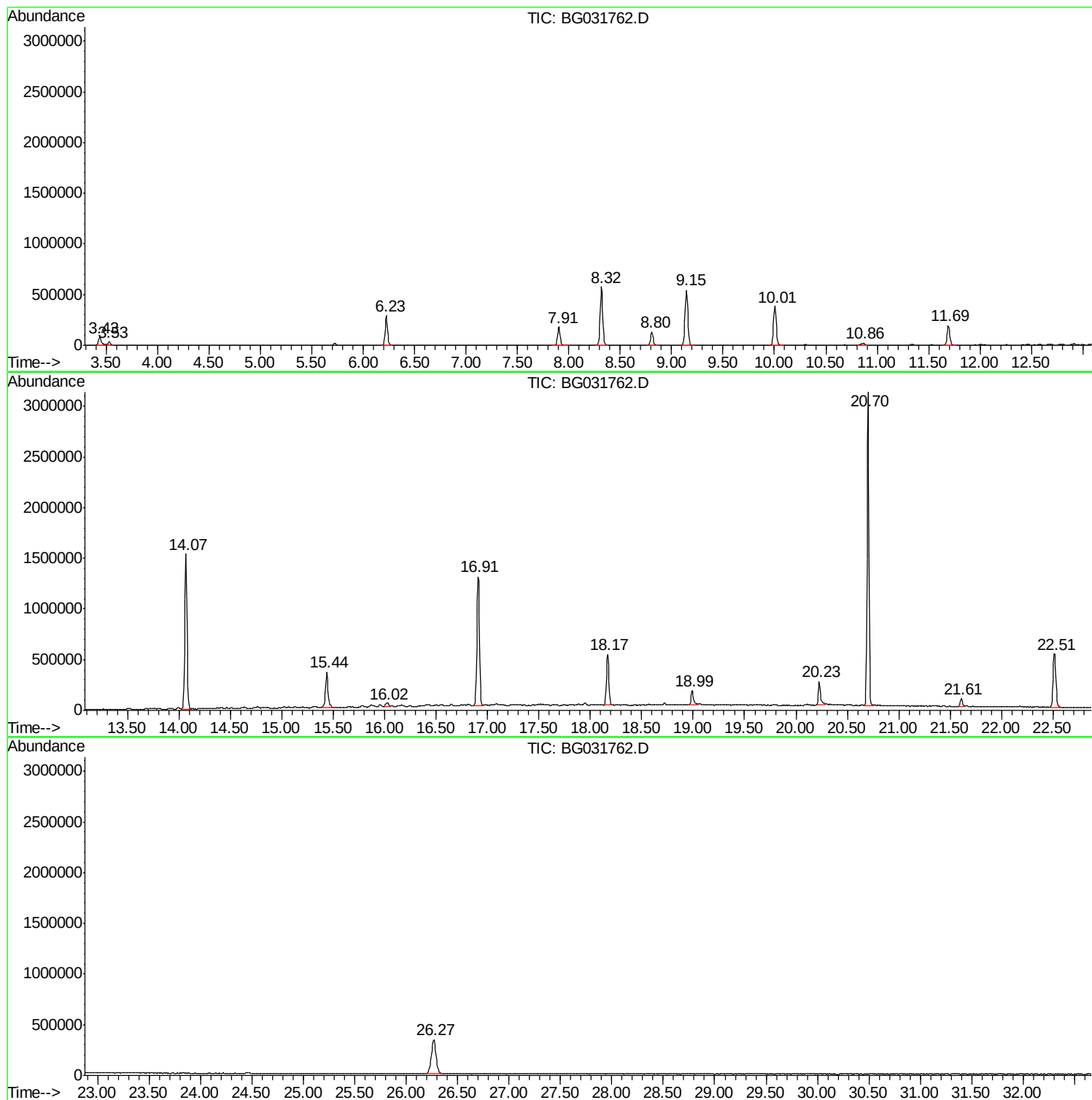
Sum of corrected areas: 17568538

Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampled :
LIP-22

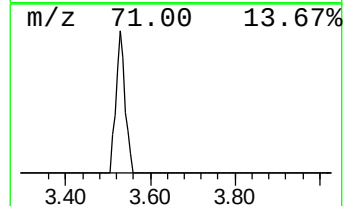
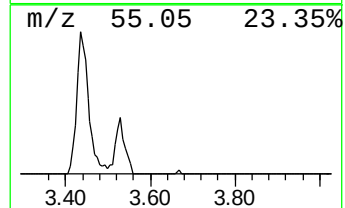
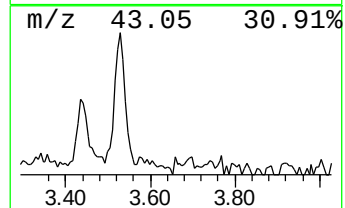
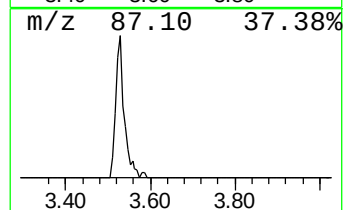
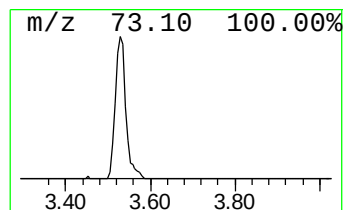
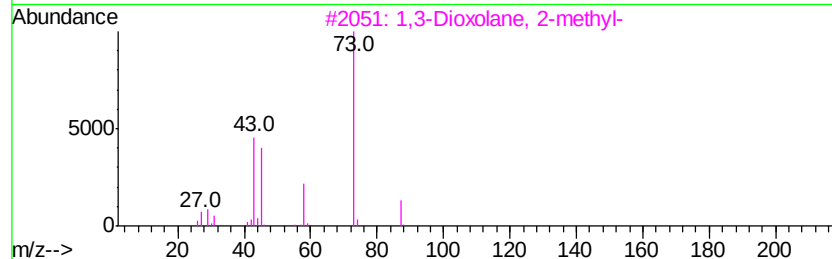
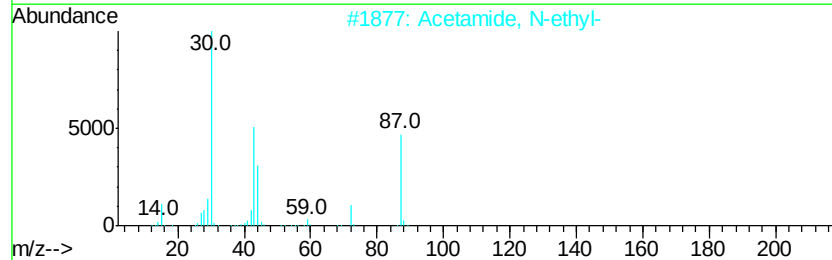
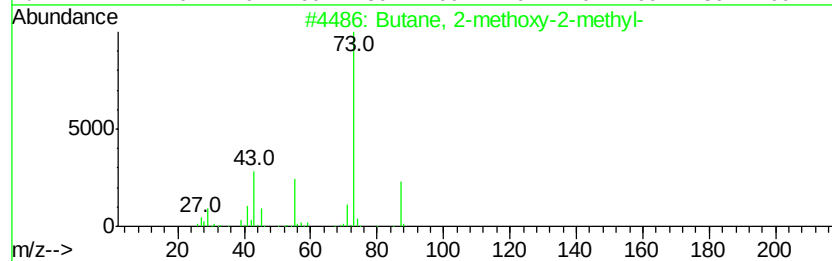
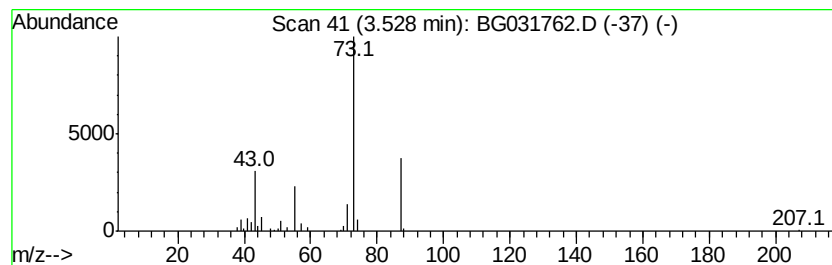
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.53	3.73 ng	44566	1,4-Dichlorobenzene-d4	8.81

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	64	
2	Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	10	
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9	
4	1-Propene-1-thiol	74	C3H6S	000925-89-3	9	
5	Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9	



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LIP-22

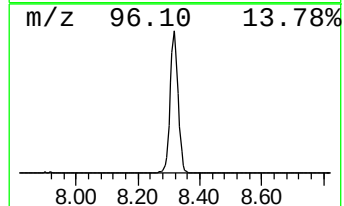
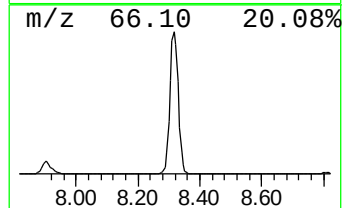
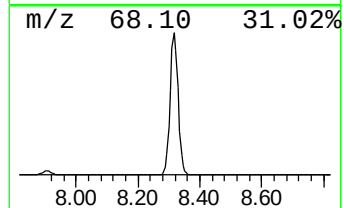
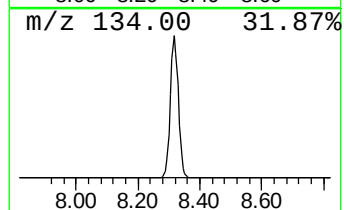
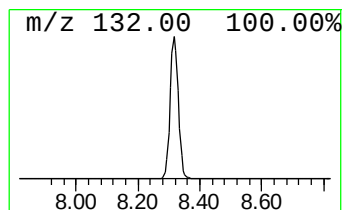
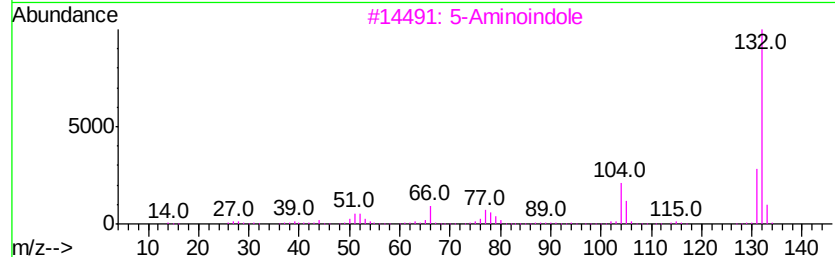
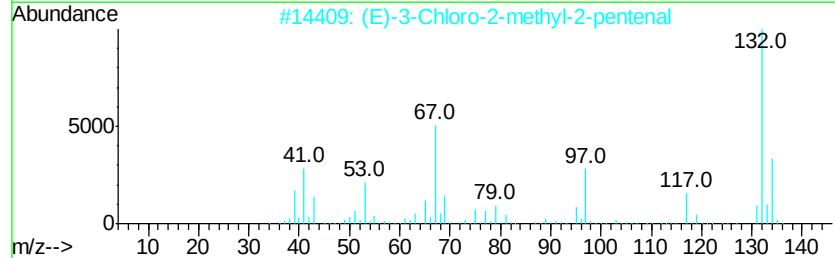
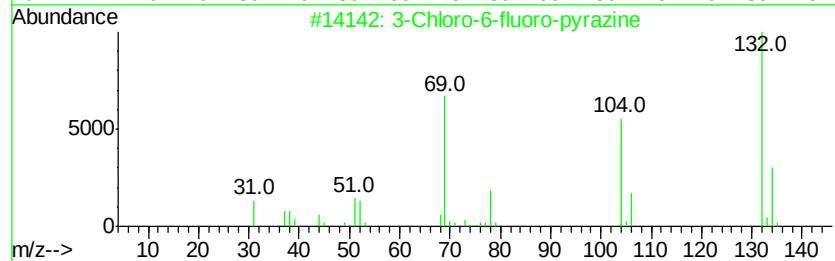
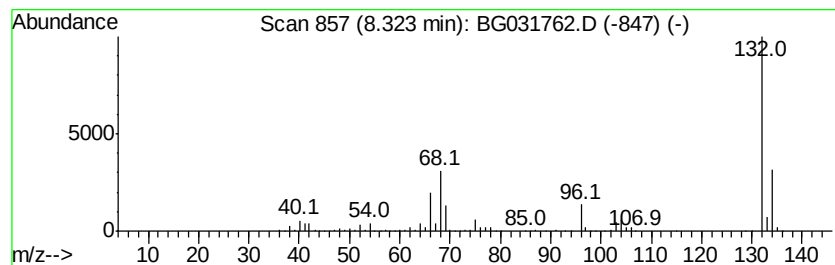
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown8.32 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.32	88.11 ng	1053970	1,4-Dichlorobenzene-d4	8.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	35
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

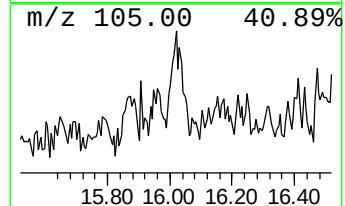
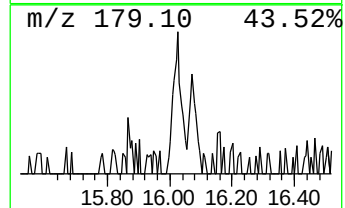
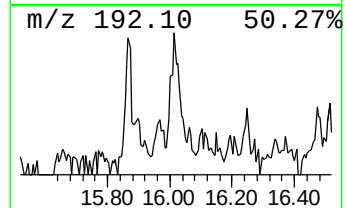
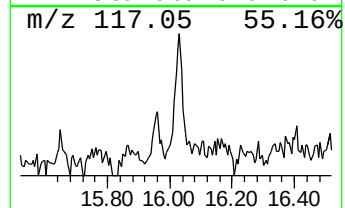
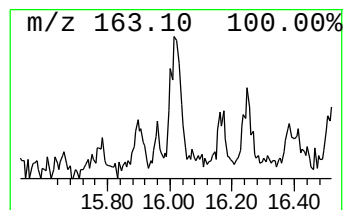
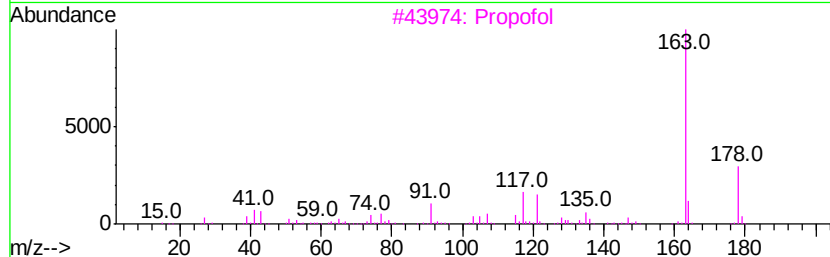
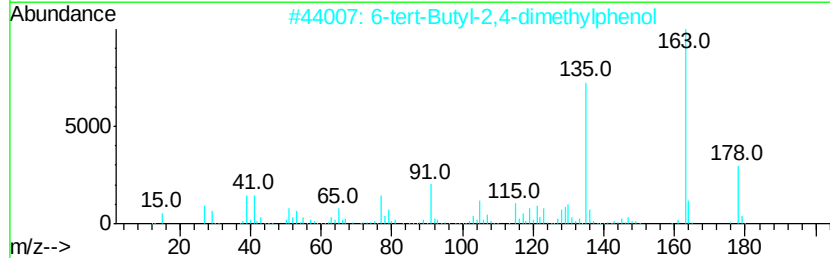
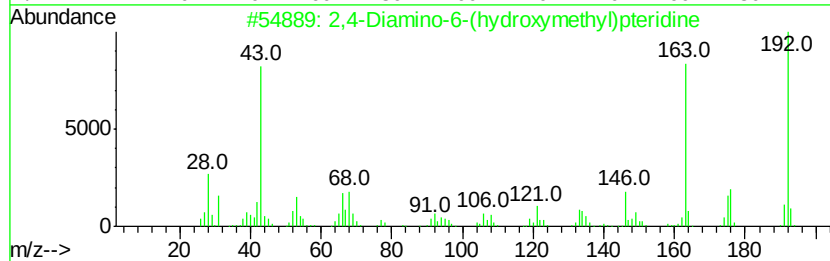
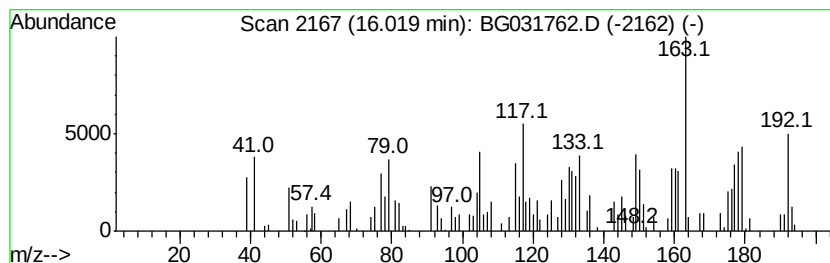
Instrument :
BNA_G
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown16.02 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.02	2.42 ng	75778	Acenaphthene-d10	15.44
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2,4-Diamino-6-(hydroxymethyl)pte...	192 C7H8N6O	000945-24-4	27
2	6-tert-Butyl-2,4-dimethylphenol	178 C12H18O	001879-09-0	22
3	Propofol	178 C12H18O	002078-54-8	22
4	Benzoic acid, 4-(1-methylethyl)-...	178 C11H14O2	020185-55-1	18
5	2-Allyl-1,4-dimethoxy-3-methyl-b...	192 C12H16O2	1000187-53-7	15



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LIP-22

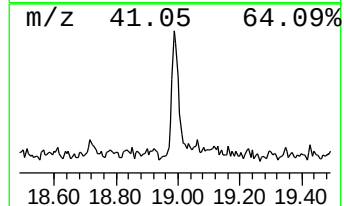
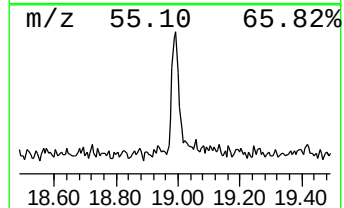
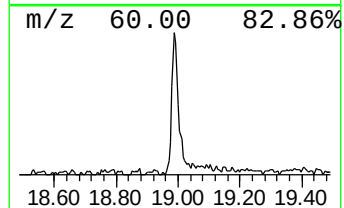
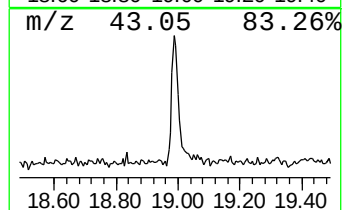
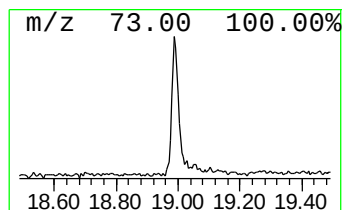
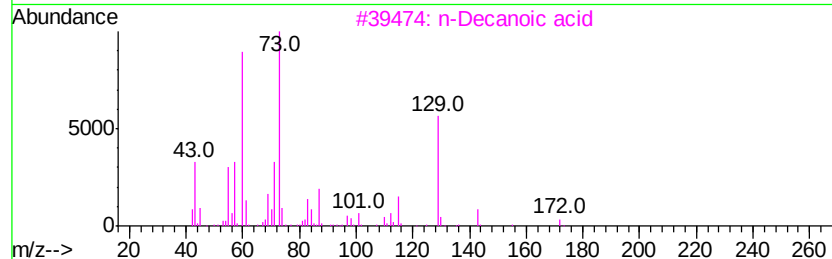
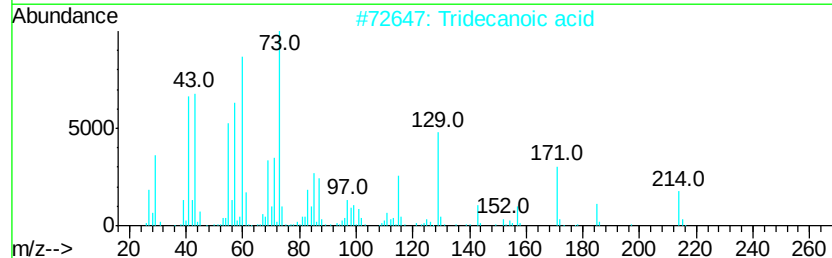
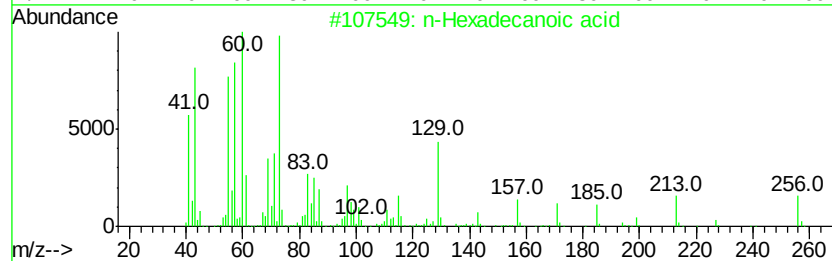
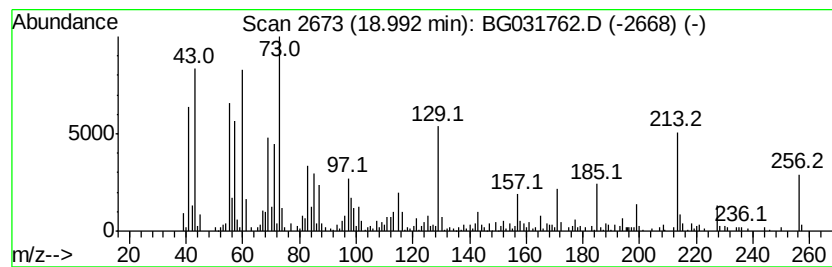
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 n-Hexadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.99	5.99 ng	233682	Phenanthrene-d10	18.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tridecanoic acid	214	C13H26O2	000638-53-9	93
3		n-Decanoic acid	172	C10H20O2	000334-48-5	87
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
5		Undecanoic acid	186	C11H22O2	000112-37-8	55



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LIP-22

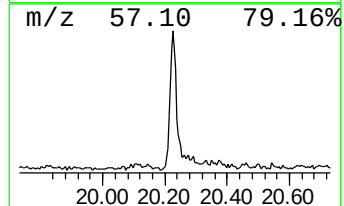
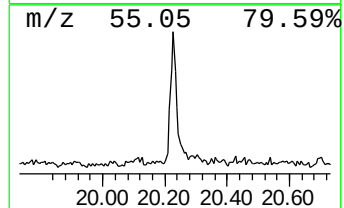
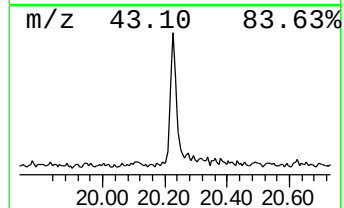
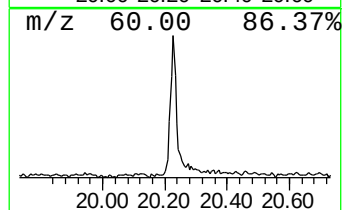
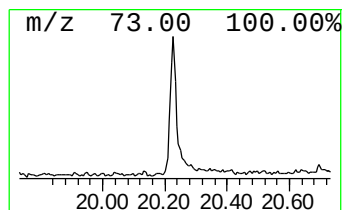
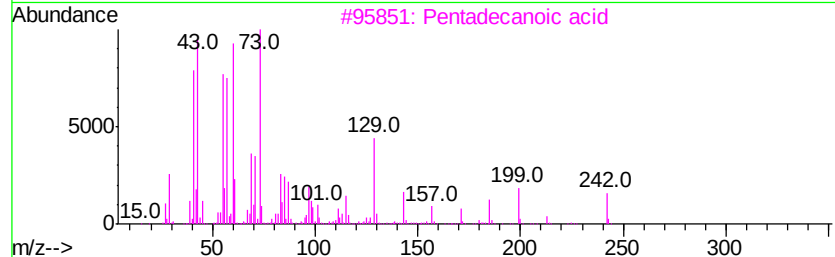
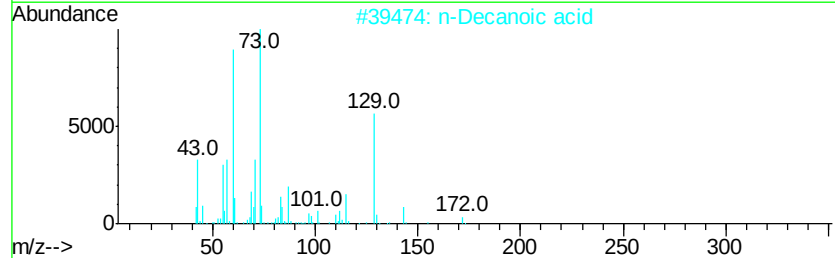
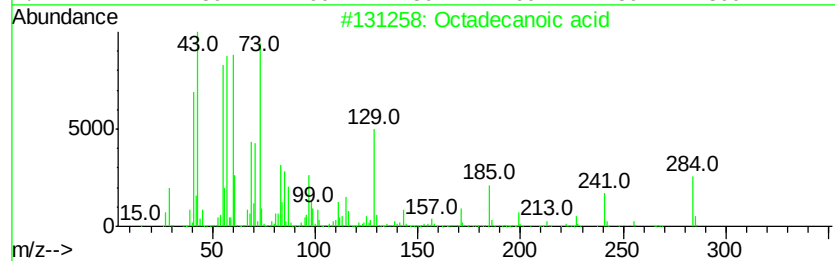
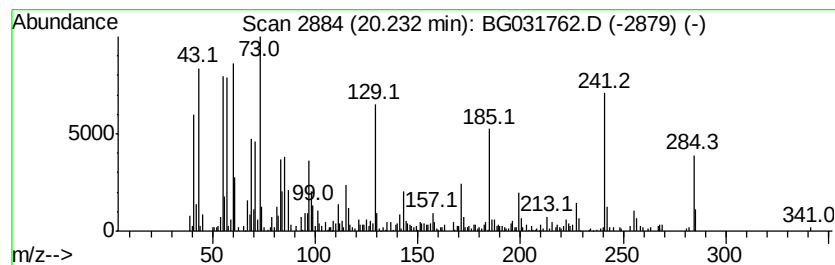
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Octadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.23	9.44 ng	367963	Phenanthrene-d10	18.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		n-Decanoic acid	172	C10H20O2	000334-48-5	89
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	68
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : U:\HPCHEM1\BNA G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LIP-22

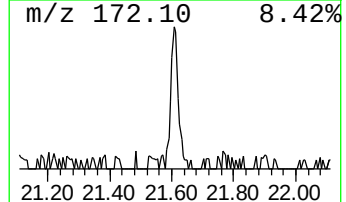
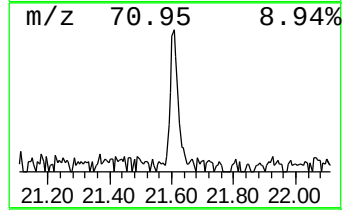
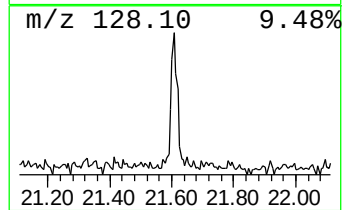
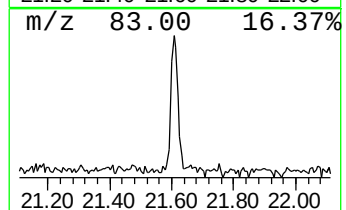
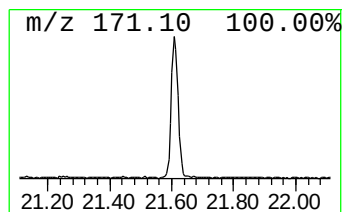
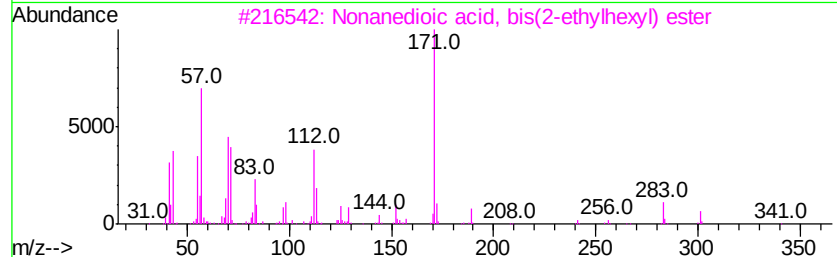
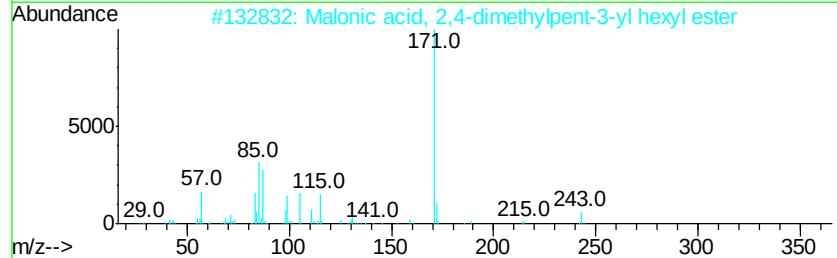
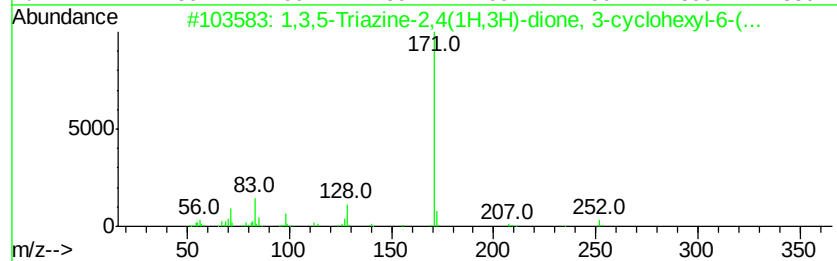
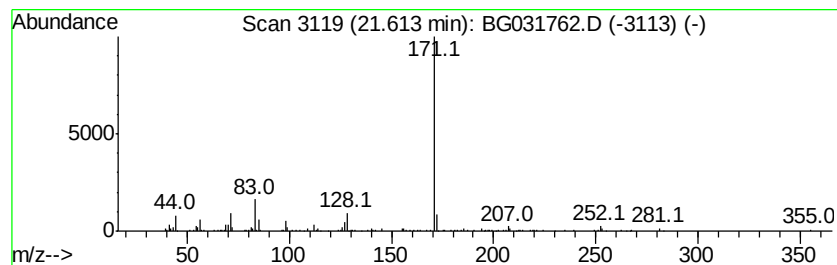
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG122117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.61	2.47 ng	129054	Chrysene-d12	22.52

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	96
2		Malonic acid, 2,4-dimethylpent-3...	286	C16H30O4	1000349-01-3	50
3		Nonanedioic acid, bis(2-ethylhex...	412	C25H48O4	000103-24-2	39
4		1,3,5-Triazaspiro[4.4]nonane-2-...	171	C7H13N3S	1000277-58-6	38
5		Benzoic acid, 2,6-difluoro-4-met...	202	C9H8F2O3	084937-82-6	38



Data Path : U:\HPCHEM1\BNA_G\DATA\BG122617\
Data File : BG031762.D
Acq On : 26 Dec 2017 15:22
Operator : SJ/JU
Sample : I7040-03
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
LIP-22

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG122117.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...	3.53	3.7	ng	44566	1	8.81	239251	20.0
unknown8.32	8.32	88.1	ng	1053970	1	8.81	239251	20.0
unknown16.02	16.02	2.4	ng	75778	3	15.44	625002	20.0
n-Hexadecanoic acid	18.99	6.0	ng	233682	4	18.17	779815	20.0
Octadecanoic acid	20.23	9.4	ng	367963	4	18.17	779815	20.0
1,3,5-Triazine-2,...	21.61	2.5	ng	129054	5	22.52	1045740	20.0