

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
 Data File : BG024586.D
 Acq On : 1 Nov 2016 10:50
 Operator : UM/SJ
 Sample : H5447-06
 Misc :
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 RPC-B3

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:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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	3.135	43	50	71	rVB	7893260	16789858	100.00%	24.264%
2	5.332	415	424	432	rBV	537149	880589	5.24%	1.273%
3	5.802	496	504	513	rBV	2309765	3930345	23.41%	5.680%
4	7.406	768	777	789	rVB	2431986	4409065	26.26%	6.372%
5	7.794	835	843	855	rBV	2301713	4113460	24.50%	5.945%
6	8.270	916	924	932	rVB	461939	823000	4.90%	1.189%
7	8.593	969	979	989	rBV	1684721	3070731	18.29%	4.438%
8	9.445	1115	1124	1132	rBV	1461053	2733848	16.28%	3.951%
9	11.096	1397	1405	1414	rBV	599650	1116174	6.65%	1.613%
10	13.511	1804	1816	1823	rBV	3490757	5683423	33.85%	8.214%
11	14.322	1946	1954	1959	rBV	800176	1205054	7.18%	1.742%
12	14.886	2043	2050	2057	rVB	987636	1609139	9.58%	2.326%
13	16.367	2295	2302	2309	rBV	3398758	5206733	31.01%	7.525%
14	17.624	2509	2516	2527	rBV2	1302798	1996505	11.89%	2.885%
15	18.470	2656	2660	2670	rBV4	149285	244773	1.46%	0.354%
16	20.203	2949	2955	2962	rBV	6228121	8804381	52.44%	12.724%
17	21.496	3170	3175	3184	rBV3	236847	400679	2.39%	0.579%
18	21.919	3240	3247	3255	rVB	1504899	2671304	15.91%	3.861%
19	23.435	3499	3505	3514	rVB4	149747	297836	1.77%	0.430%
20	23.640	3534	3540	3548	rVB3	221384	489308	2.91%	0.707%
21	25.344	3819	3830	3843	rVB2	908572	2719045	16.19%	3.930%

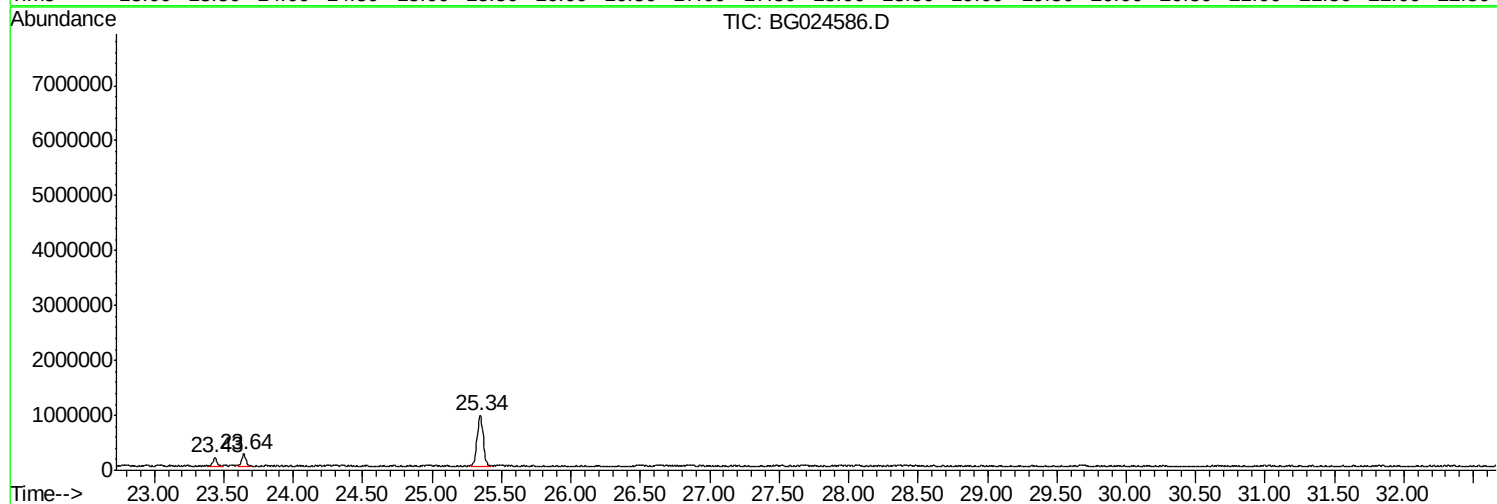
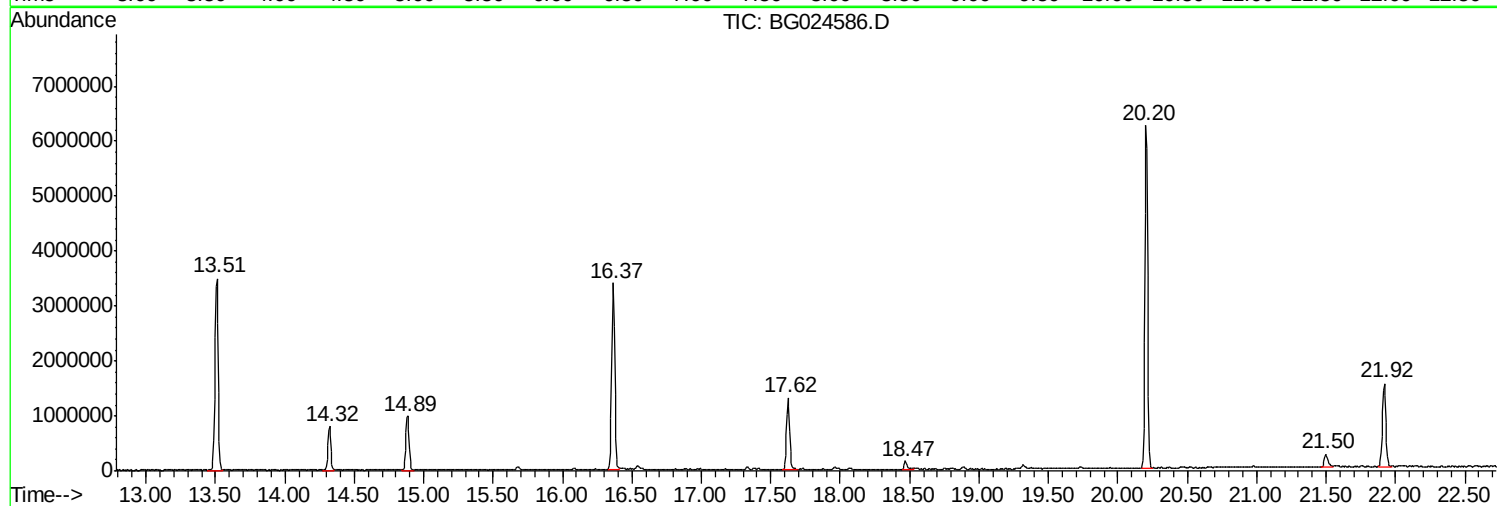
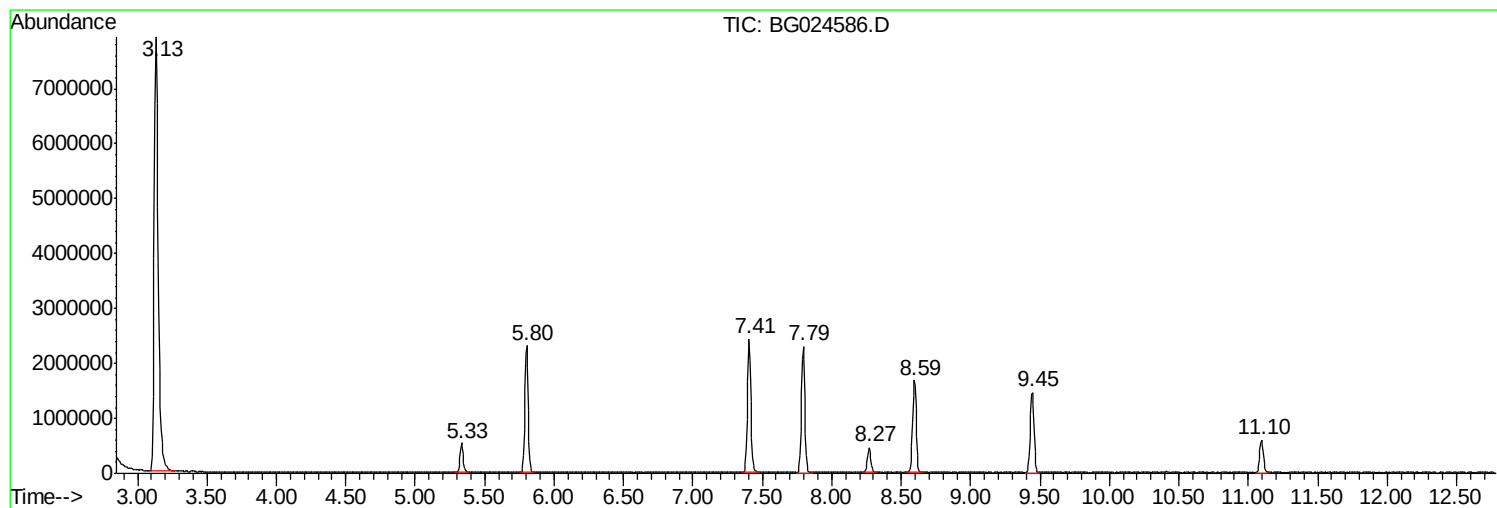
Sum of corrected areas: 69195250

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

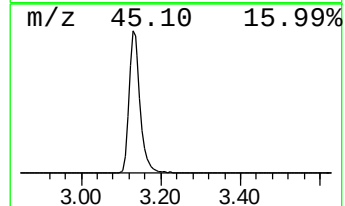
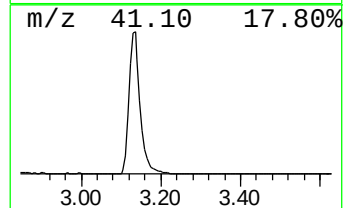
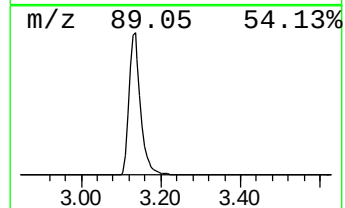
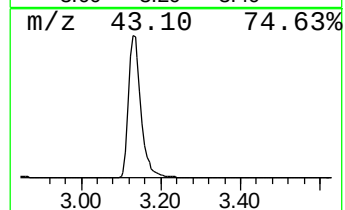
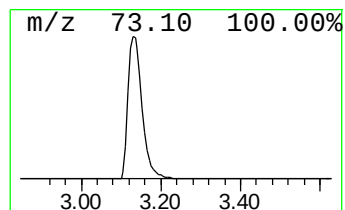
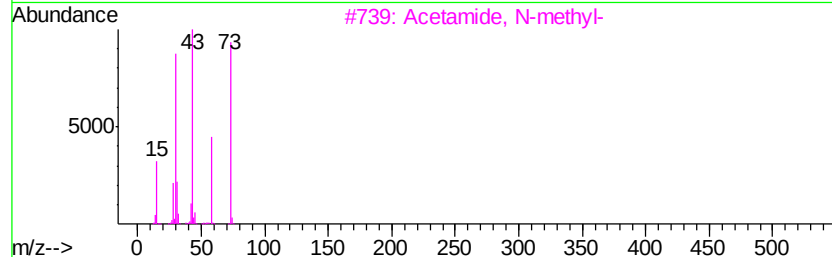
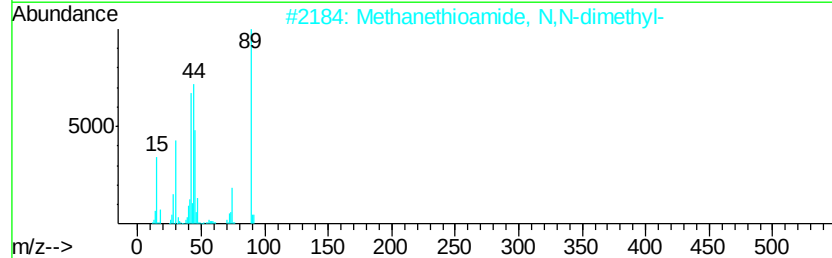
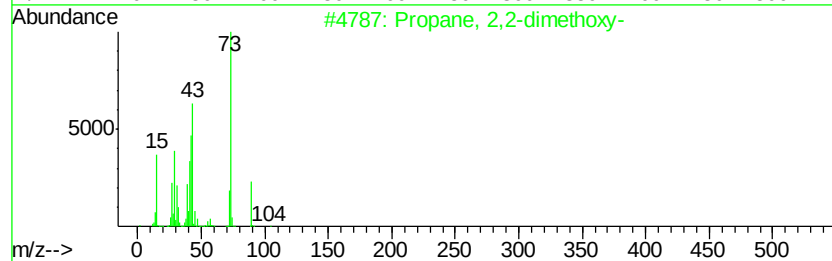
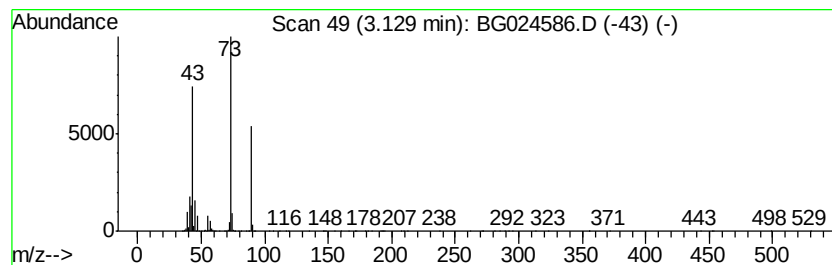
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.13 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.13	408.02 ng	16789900	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	33
2		Methanethioamide, N,N-dimethyl-	89	C3H7NS	000758-16-7	32
3		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	25
4		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	10
5		Thiazole, tetrahydro-	89	C3H7NS	000504-78-9	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

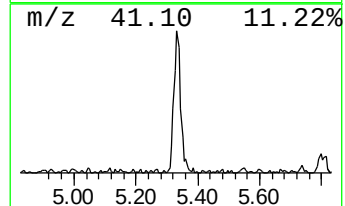
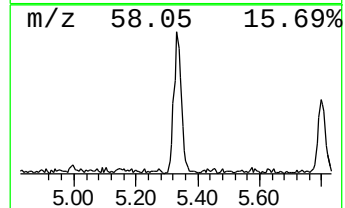
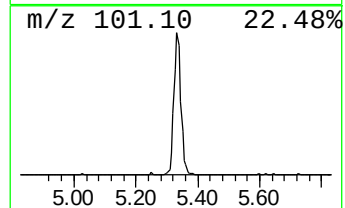
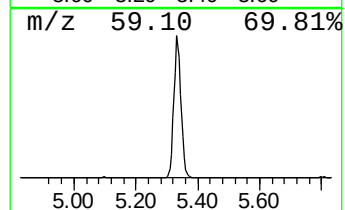
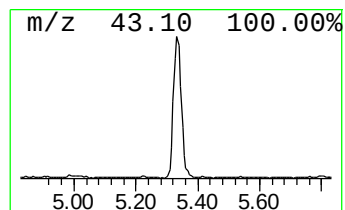
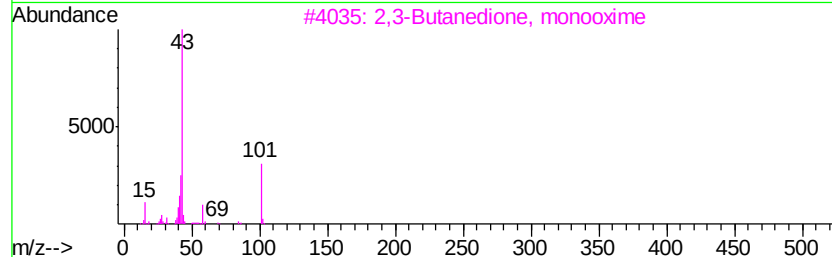
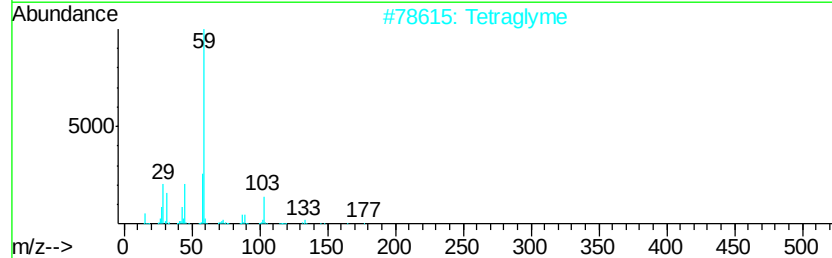
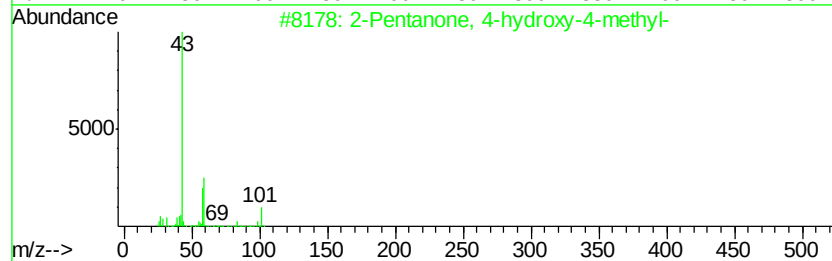
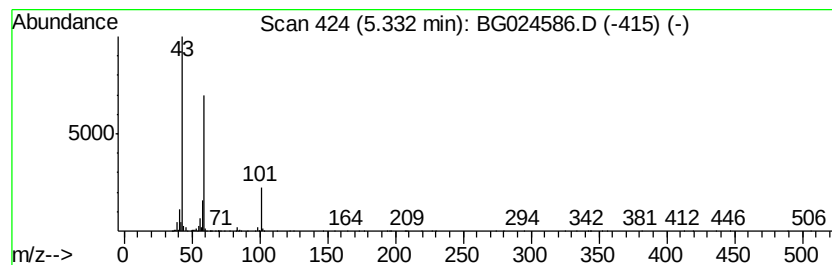
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
5.33	21.40 ng	880589	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38
2		Tetraglyme	222	C10H22O5	000143-24-8	25
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	23
4		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

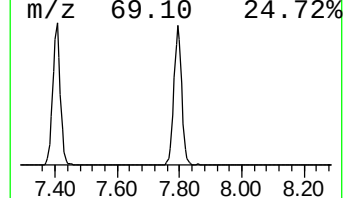
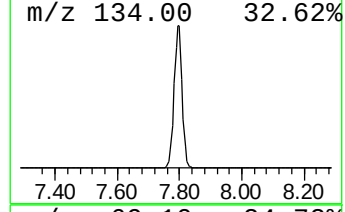
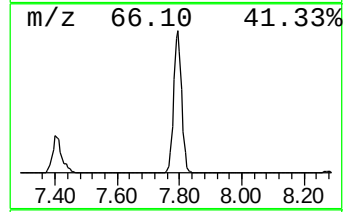
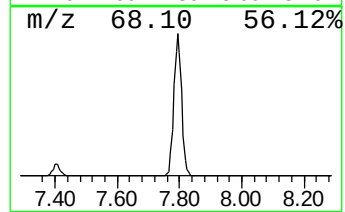
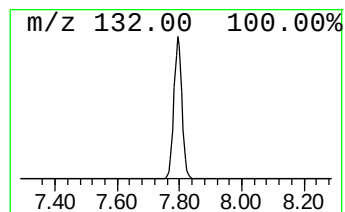
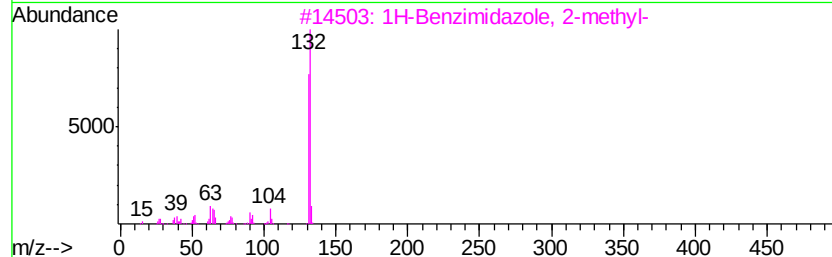
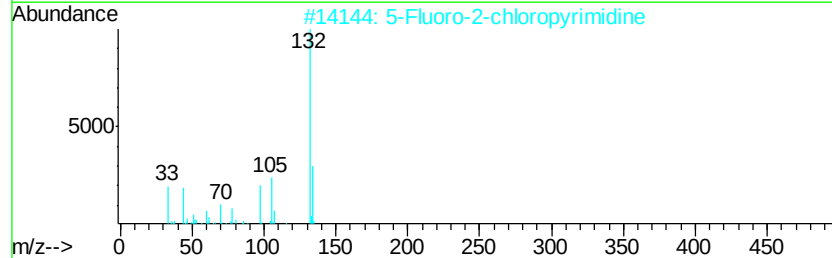
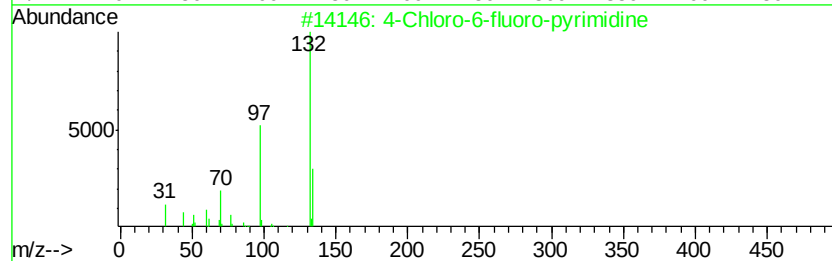
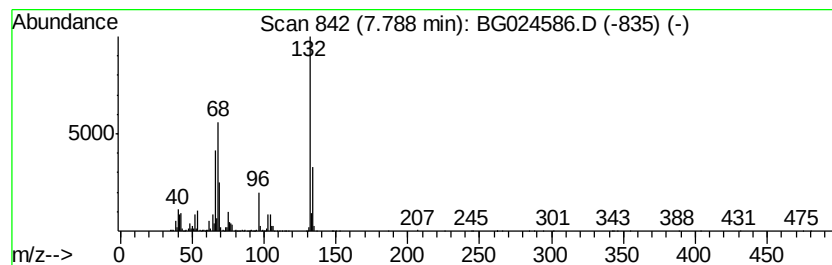
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.79 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	99.96 ng	4113460	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	17
5		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

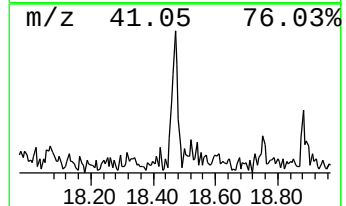
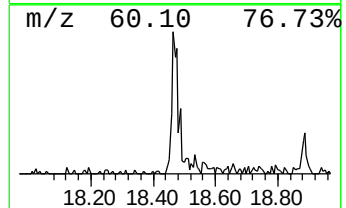
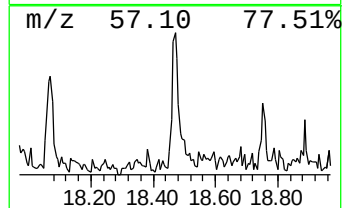
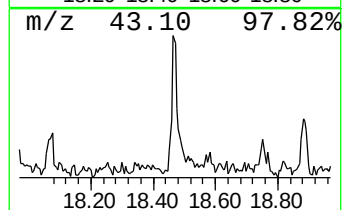
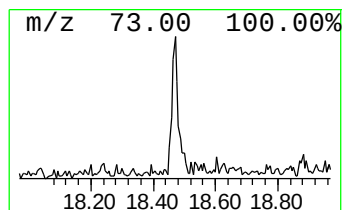
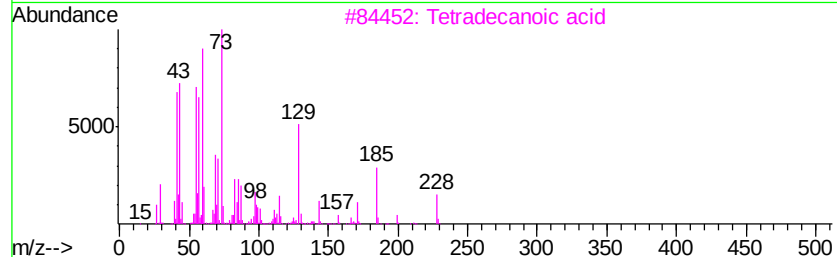
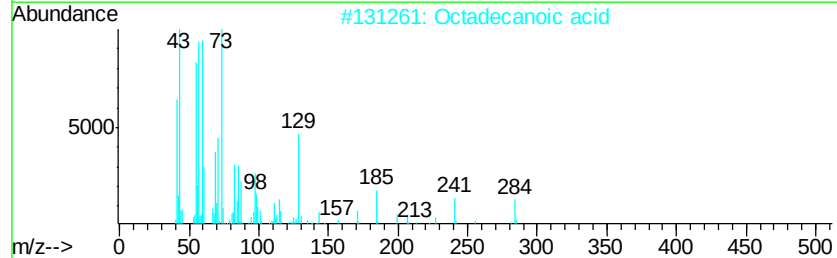
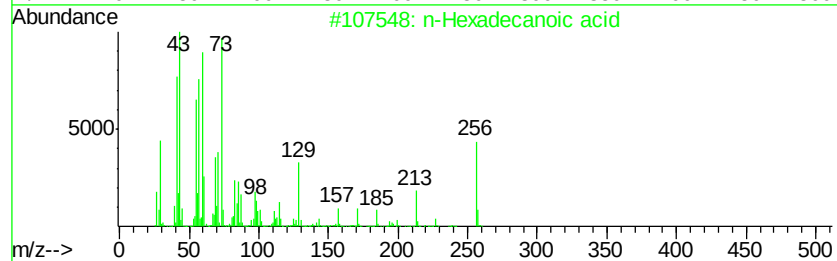
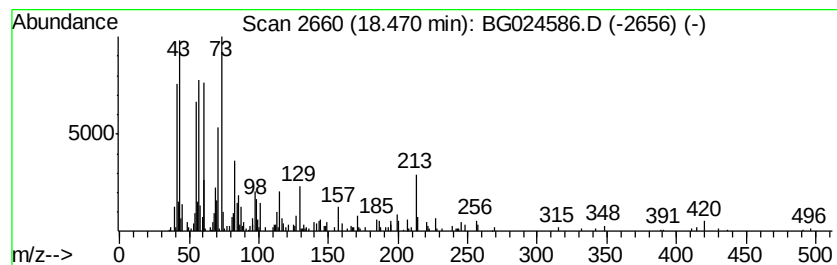
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.45 ng	244773	Phenanthrene-d10	17.62

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	64
2	Octadecanoic acid	284	C18H36O2	000057-11-4	62
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	50
4	Pentadecanoic acid	242	C15H30O2	001002-84-2	50
5	Trehalose	342	C12H22O11	000099-20-7	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

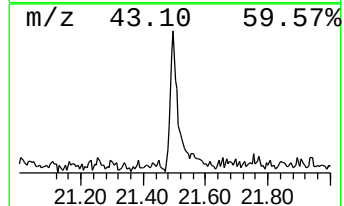
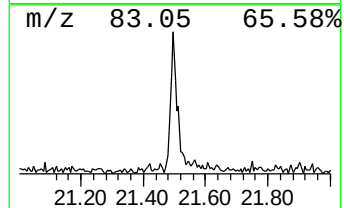
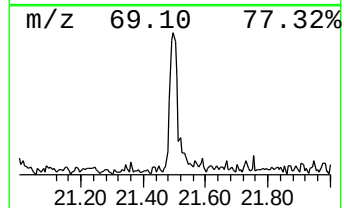
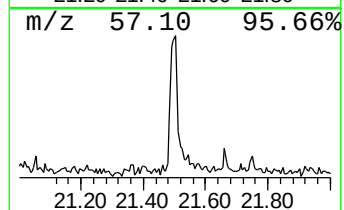
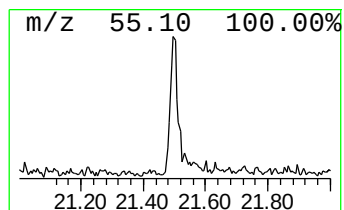
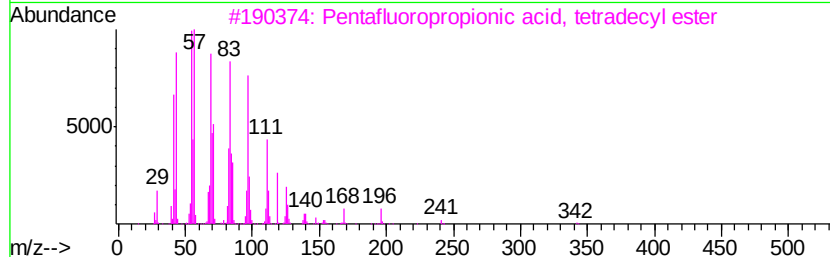
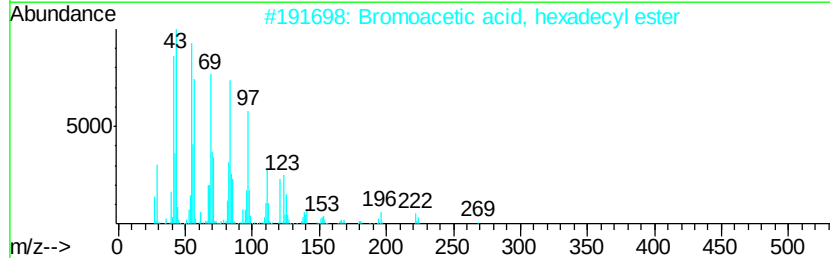
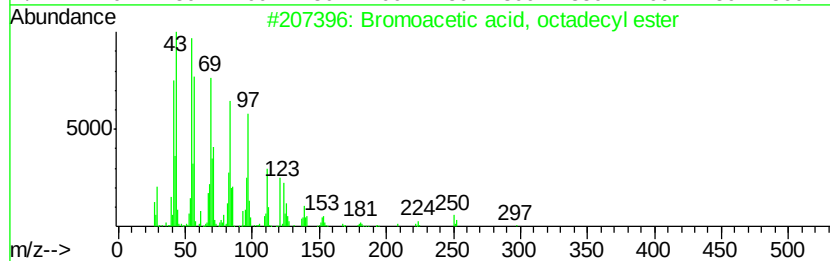
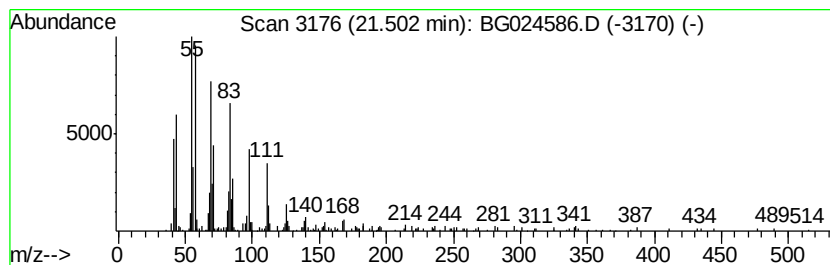
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 Bromoacetic acid, octadecyl... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.50	3.00 ng	400679	Chrysene-d12	21.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bromoacetic acid, octadecyl ester	390	C20H39BrO2	018992-03-5	91
2		Bromoacetic acid, hexadecyl ester	362	C18H35BrO2	005454-48-8	91
3		Pentafluoropropionic acid, tetra...	360	C17H29F5O2	006222-06-6	90
4		E-7-Octadecene	252	C18H36	1000130-92-0	89
5		n-Nonadecanol-1	284	C19H40O	001454-84-8	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

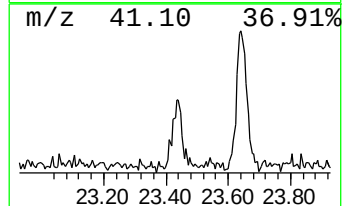
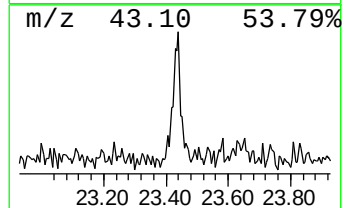
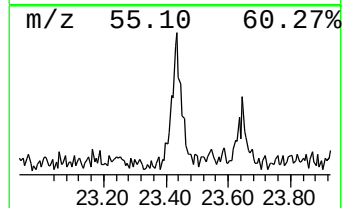
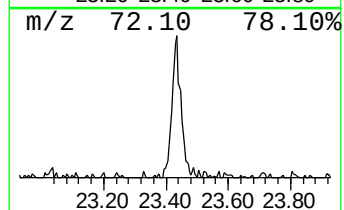
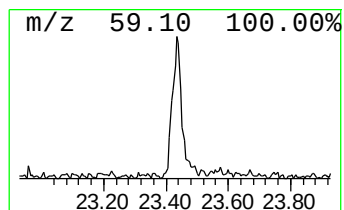
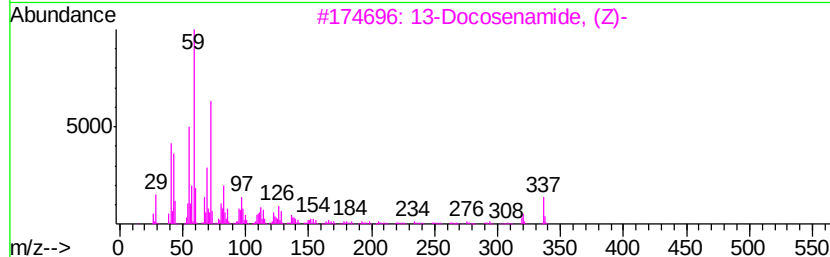
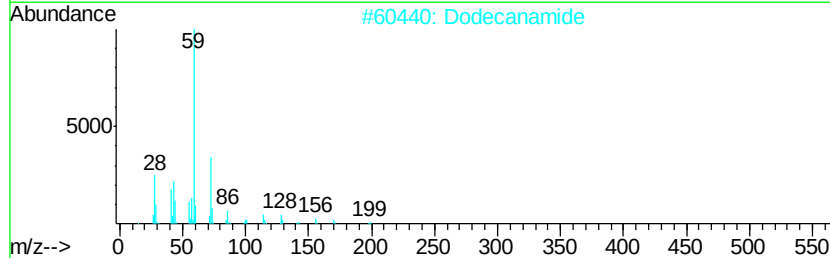
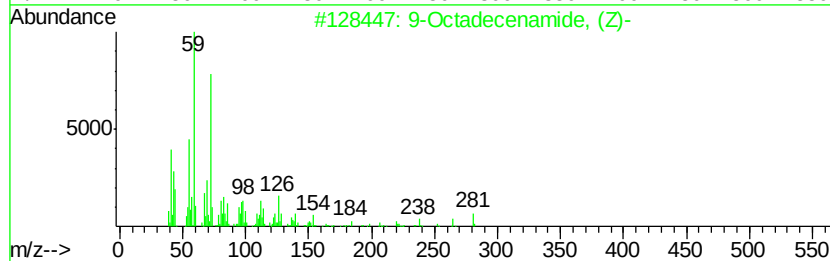
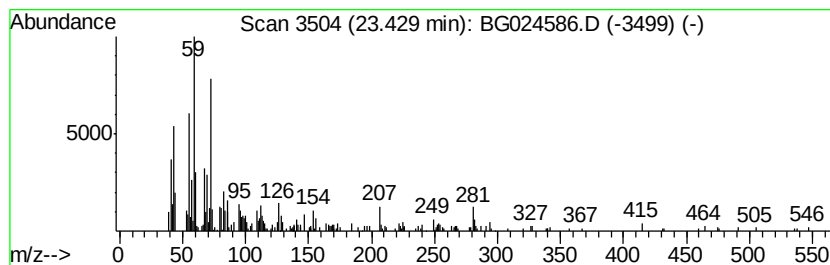
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 9-Octadecenamide, (Z)- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.43	2.23 ng	297836	Chrysene-d12	21.92

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	9-Octadecenamide, (Z)-	281	C18H35NO	000301-02-0	89
2		Dodecanamide	199	C12H25NO	001120-16-7	68
3		13-Docosenamide, (Z)-	337	C22H43NO	000112-84-5	68
4		Hexadecanamide	255	C16H33NO	000629-54-9	59
5		Octadecanamide	283	C18H37NO	000124-26-5	58



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

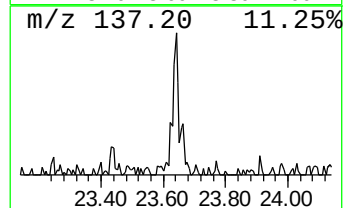
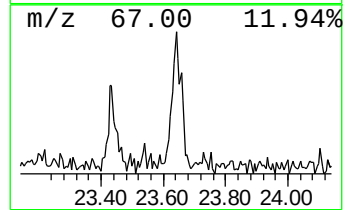
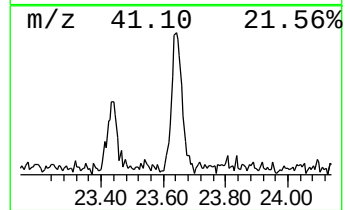
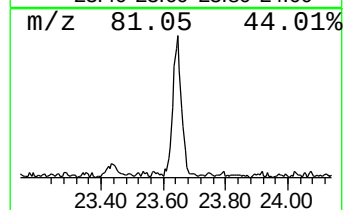
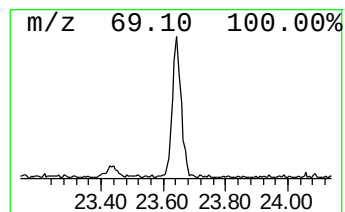
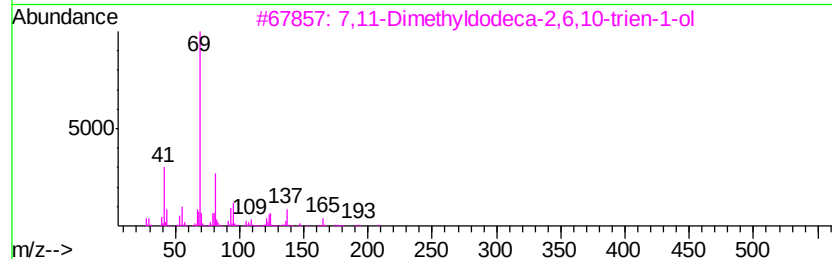
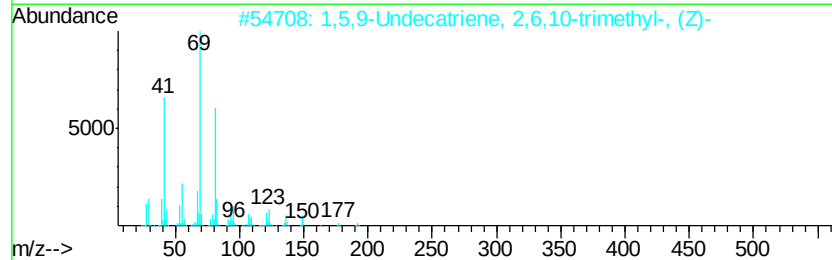
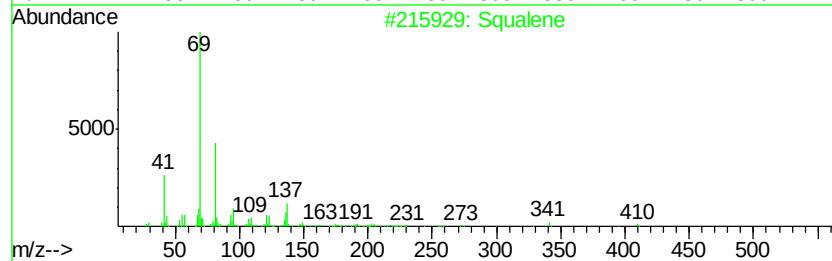
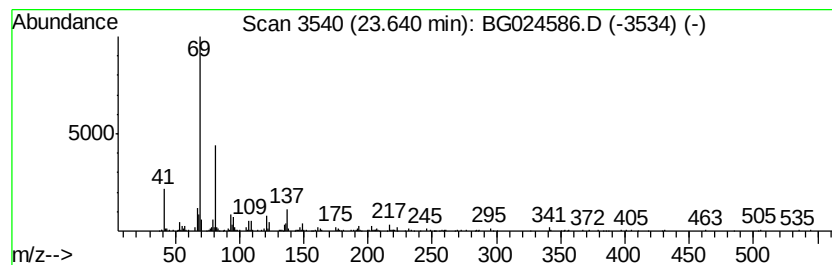
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Squalene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
23.64	3.60 ng	489308	Perylene-d12	25.35

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Squalene	410	C30H50	000111-02-4	72
2		1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	70
3		7,11-Dimethyldodeca-2,6,10-trien...	208	C14H24O	125529-10-4	64
4		1-(3,5-Dinitrophenoxy)-3,7,11-tr...	388	C21H28N2O5	1000187-44-2	64
5		3,7,11-Tridecatrienitrile, 4,8...	231	C16H25N	006006-01-5	64



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG103116\
Data File : BG024586.D
Acq On : 1 Nov 2016 10:50
Operator : UM/SJ
Sample : H5447-06
Misc :
ALS Vial : 28 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
RPC-B3

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.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
unknown3.13	3.13	408.0	ng	16789900	1	8.27	823000	20.0
2-Pentanone, 4-hy...	5.33	21.4	ng	880589	1	8.27	823000	20.0
unknown7.79	7.79	100.0	ng	4113460	1	8.27	823000	20.0
n-Hexadecanoic acid	18.47	2.5	ng	244773	4	17.62	1996510	20.0
Bromoacetic acid,...	21.50	3.0	ng	400679	5	21.92	2671300	20.0
9-Octadecenamide,...	23.43	2.2	ng	297836	5	21.92	2671300	20.0
Squalene	23.64	3.6	ng	489308	6	25.35	2719050	20.0