

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
 Data File : BG022972.D
 Acq On : 9 Jul 2016 19:28
 Operator : UM/SJ
 Sample : H3840-01
 Misc :
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PZ-4

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-BG070816.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	5.699	479	487	497	rBV	1121381	1881967	16.34%	3.613%
2	7.303	749	760	770	rBV	865691	1524113	13.23%	2.926%
3	7.679	815	824	833	rBV	2014052	3623170	31.46%	6.956%
4	8.154	896	905	911	rVB	340084	590264	5.13%	1.133%
5	8.478	951	960	968	rBV	1536984	2747313	23.85%	5.275%
6	9.324	1096	1104	1116	rBV	1673350	3033452	26.34%	5.824%
7	10.029	1212	1224	1234	rBV7	70615	201179	1.75%	0.386%
8	10.981	1379	1386	1395	rVB	515366	938757	8.15%	1.802%
9	13.419	1791	1801	1815	rBV	4644170	7545452	65.52%	14.487%
10	14.236	1934	1940	1947	rBV	557243	816571	7.09%	1.568%
11	14.794	2029	2035	2042	rBV2	1010887	1660141	14.41%	3.187%
12	16.286	2279	2289	2302	rBV	4844848	7578786	65.80%	14.551%
13	17.549	2498	2504	2513	rBV2	1382043	2118003	18.39%	4.066%
14	18.131	2599	2603	2612	rVB	88806	143765	1.25%	0.276%
15	18.419	2647	2652	2662	rBV2	280351	431190	3.74%	0.828%
16	19.688	2863	2868	2876	rBV3	250559	398677	3.46%	0.765%
17	20.152	2941	2947	2954	rBV	8412596	11517068	100.00%	22.112%
18	21.033	3092	3097	3106	rVB	218176	313411	2.72%	0.602%
19	21.844	3229	3235	3242	rVB2	1356078	2328995	20.22%	4.472%
20	25.205	3797	3807	3822	rVB2	799945	2470796	21.45%	4.744%
21	26.374	4002	4006	4016	rVB8	86165	222082	1.93%	0.426%

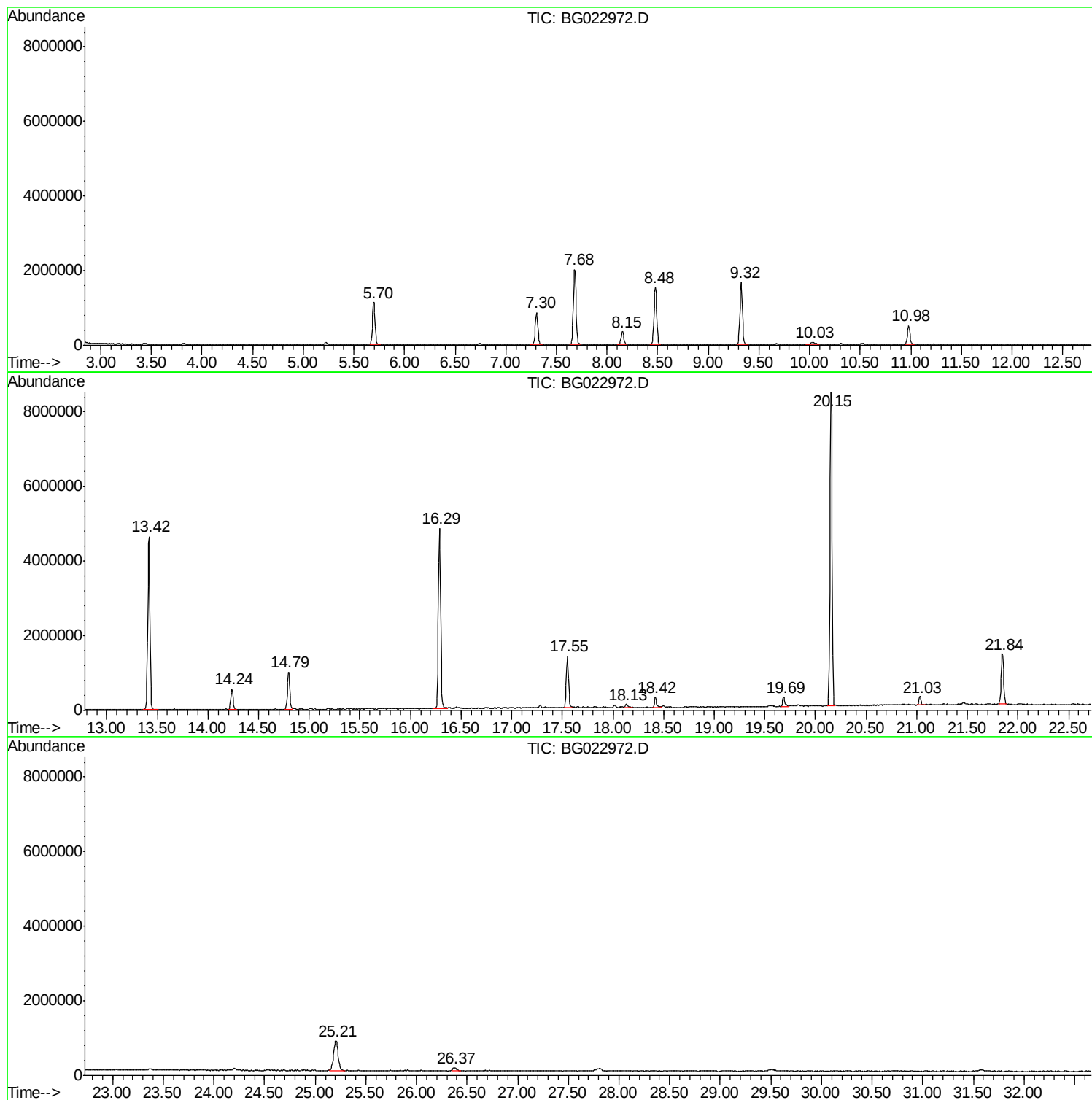
Sum of corrected areas: 52085152

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

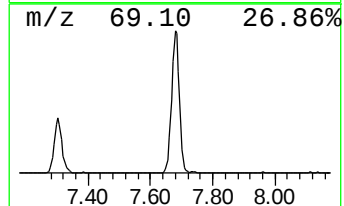
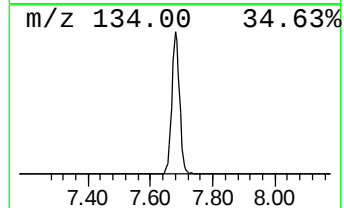
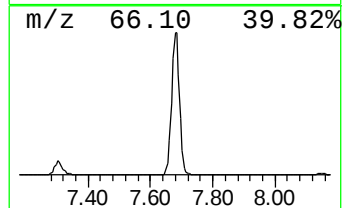
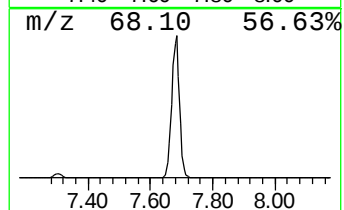
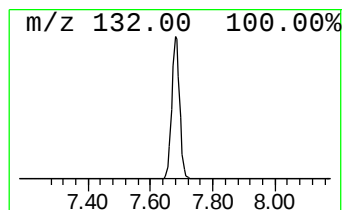
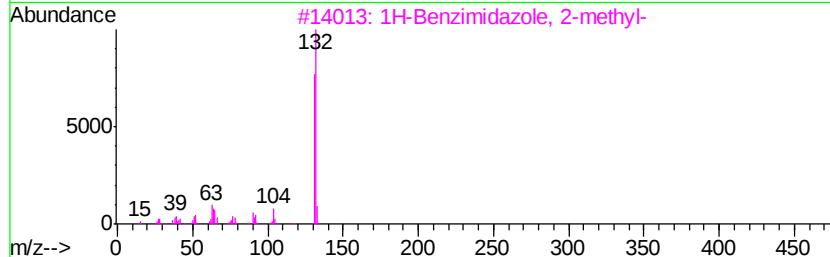
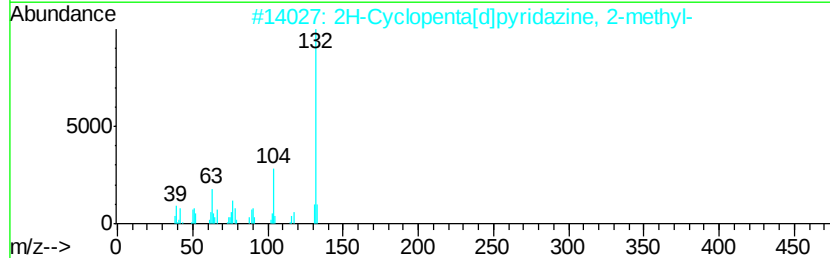
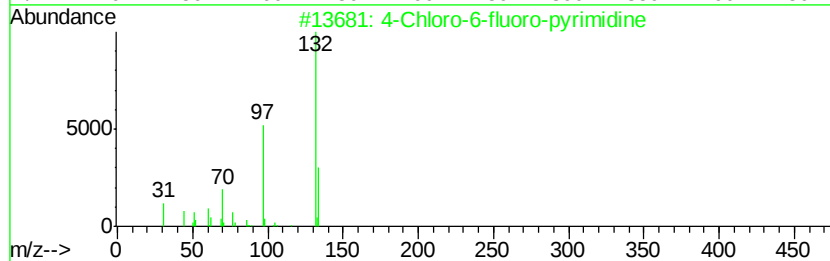
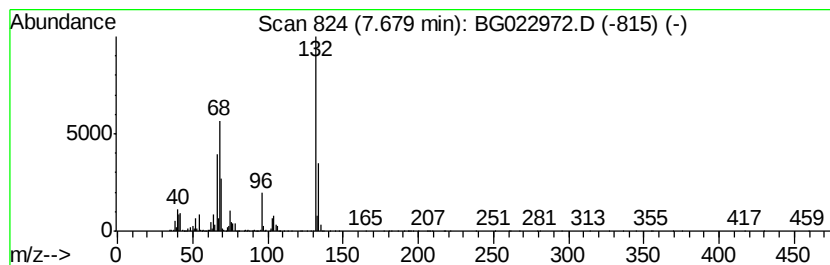
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	122.76 ng	3623170	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	10
4		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

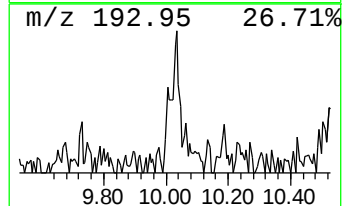
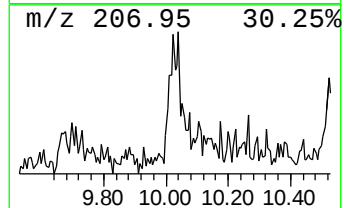
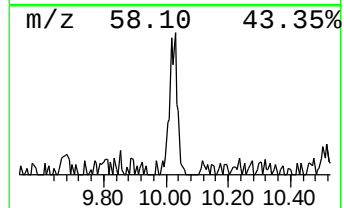
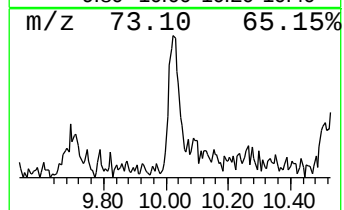
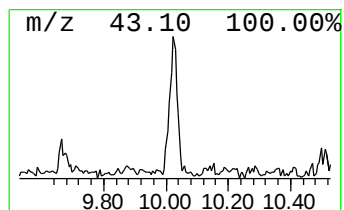
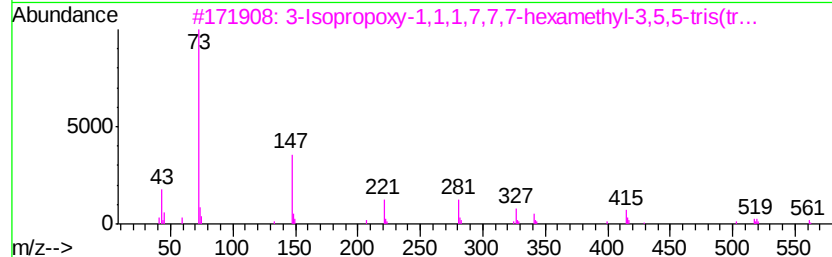
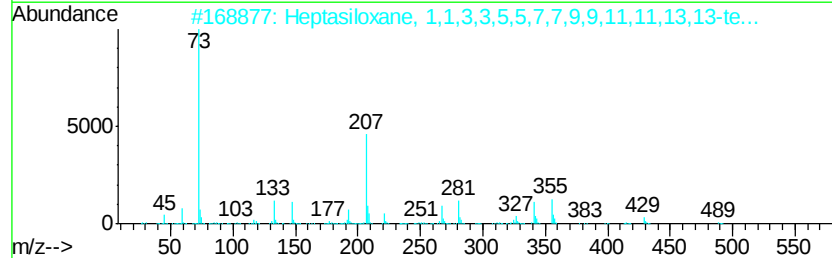
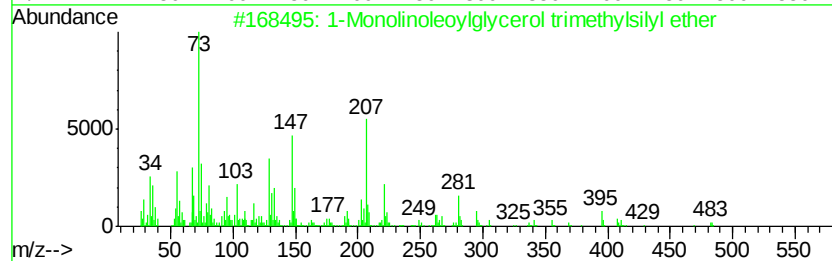
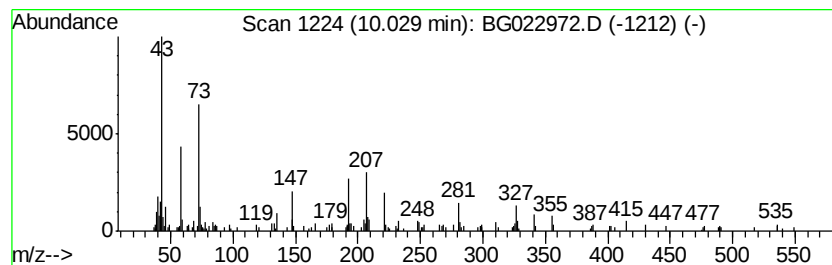
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown10.03 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.03	4.29 ng	201179	Naphthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Monolinoleoylglycerol trimethy...	498	C27H54O4Si2	054284-45-6	32
2		Heptasiloxane, 1,1,3,3,5,5,7,7,9...	504	C14H44O6Si7	019095-23-9	27
3		3-Isopropoxy-1,1,1,7,7,7-hexamet...	576	C18H52O7Si7	071579-69-6	22
4		1,1,1,3,5,7,9,11,11,11-Decamethy...	490	C13H42O6Si7	050694-26-3	16
5		Octasiloxane, 1,1,3,3,5,5,7,7,9,...	578	C16H50O7Si8	019095-24-0	16



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

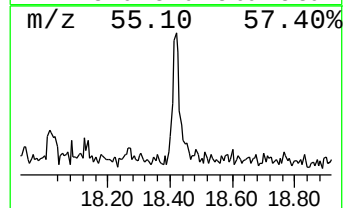
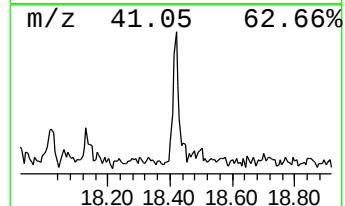
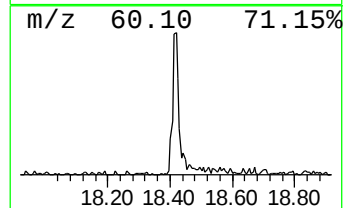
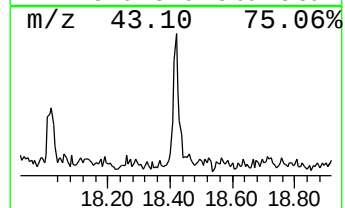
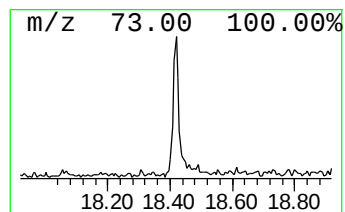
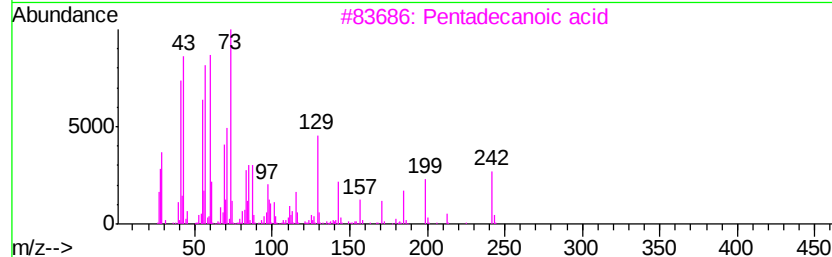
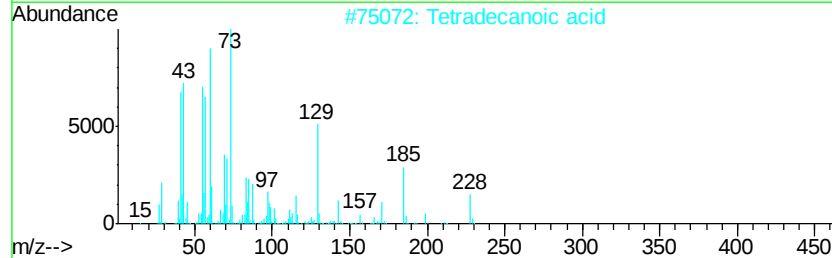
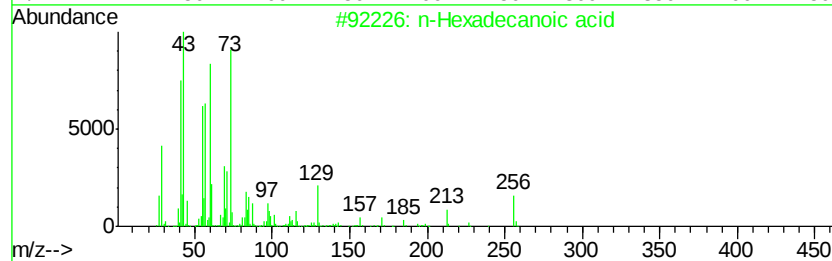
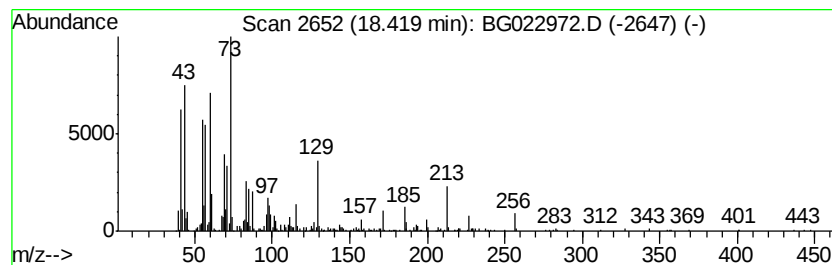
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 n-Hexadecanoic acid Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.07 ng	431190	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	96
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	74
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	58
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Undecanoic acid	186	C11H22O2	000112-37-8	53



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

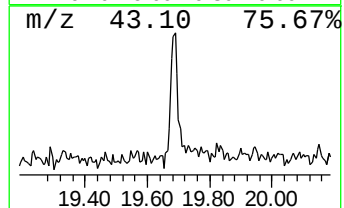
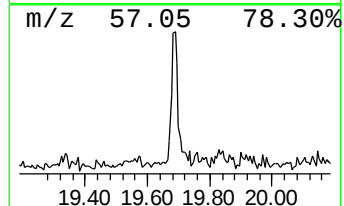
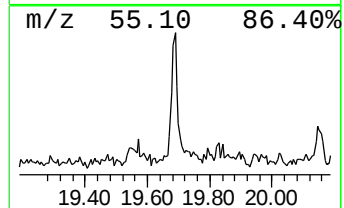
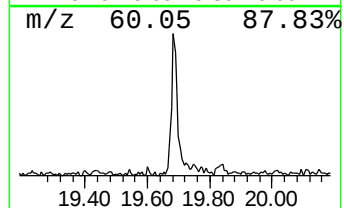
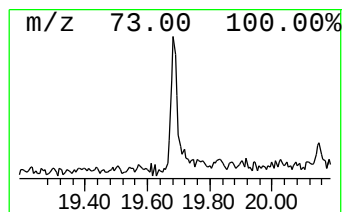
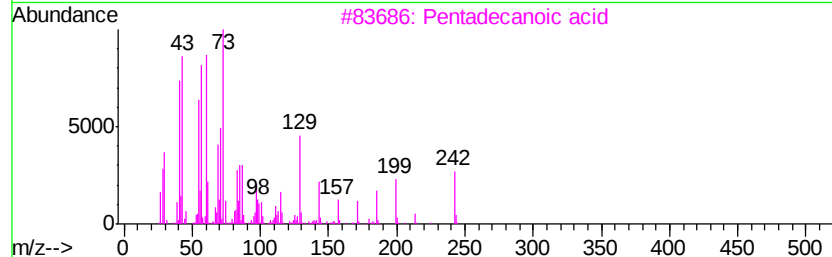
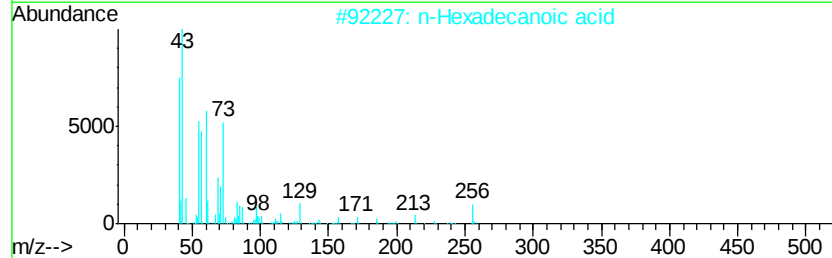
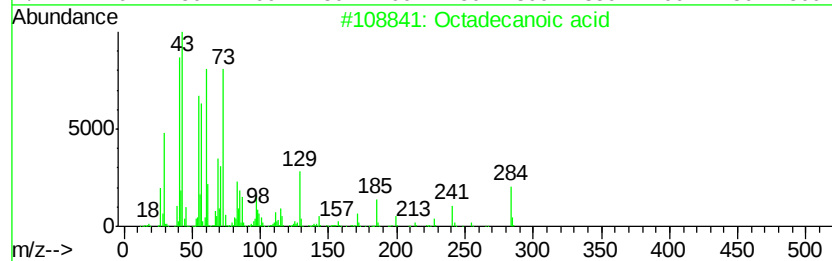
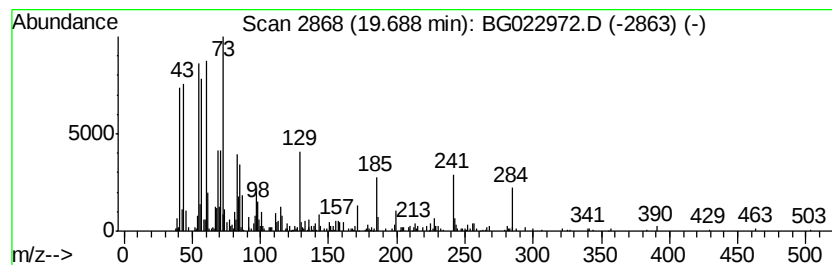
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Octadecanoic acid Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.76 ng	398677	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	93
2		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	86
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	70
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	62
5		Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	59



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

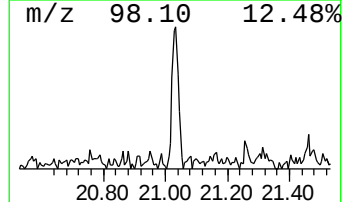
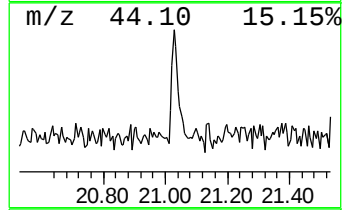
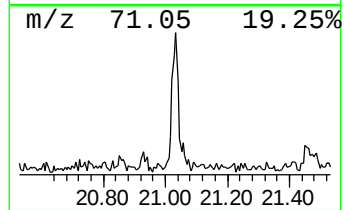
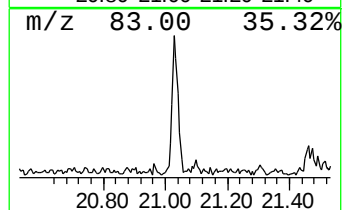
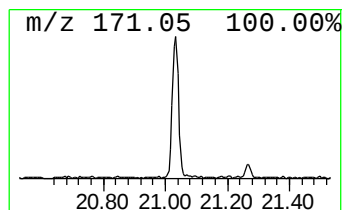
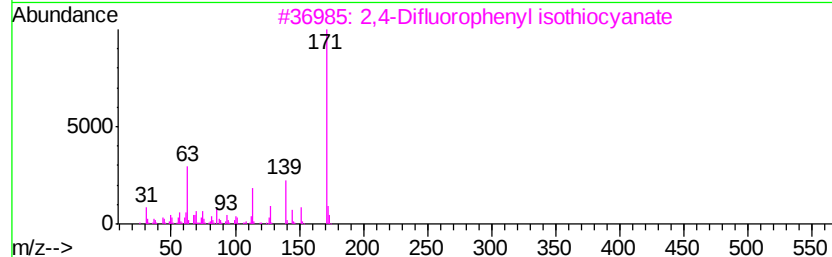
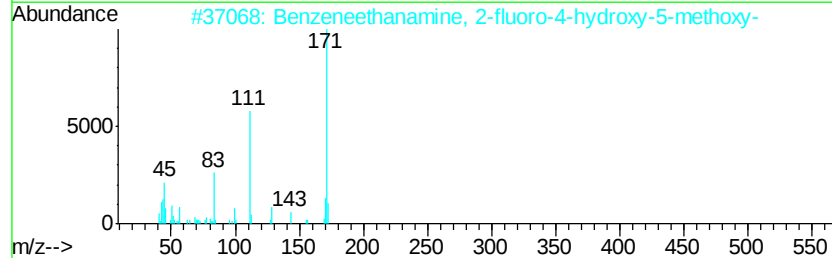
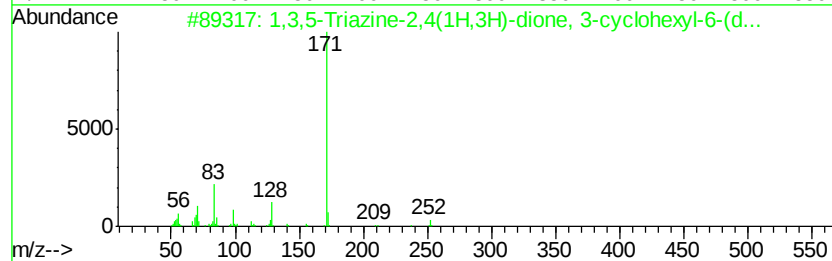
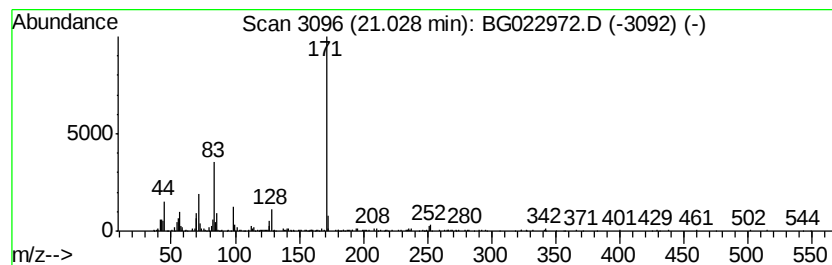
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 1,3,5-Triazine-2,4(1H,3H)-d... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.03	2.69 ng	313411	Chrysene-d12	21.84

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1,3,5-Triazine-2,4(1H,3H)-dione,...	252	C12H20N4O2	051235-04-2	96		
2	Benzeneethanamine, 2-fluoro-4-hy...	171	C8H10FN02	1000116-43-3	42		
3	2,4-Difluorophenyl isothiocyanate	171	C7H3F2NS	141106-52-7	37		
4	Thiazolo[5,4-d]pyrimidine, 5-chl...	171	C5H2ClN3S	013316-08-0	33		
5	Pyrimidine-2,4,6(1H,3H,5H)-trion...	334	C17H26N4O3	201928-46-3	28		



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071016\
Data File : BG022972.D
Acq On : 9 Jul 2016 19:28
Operator : UM/SJ
Sample : H3840-01
Misc :
ALS Vial : 8 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PZ-4

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown7.68	7.68	122.8	ng	3623170	1	8.15	590264	20.0
unknown10.03	10.03	4.3	ng	201179	2	10.98	938757	20.0
n-Hexadecanoic acid	18.42	4.1	ng	431190	4	17.55	2118000	20.0
Octadecanoic acid	19.69	3.8	ng	398677	4	17.55	2118000	20.0
1,3,5-Triazine-2,...	21.03	2.7	ng	313411	5	21.84	2329000	20.0