

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
 Data File : BG023430.D
 Acq On : 3 Aug 2016 18:03
 Operator : UM/SJ
 Sample : H4287-13
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 SB-61-19.0-20.0

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-BG080116.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	2.993	21	26	45	rVB	4283759	6242812	59.58%	9.426%
2	4.250	235	240	249	rVB	299396	453136	4.32%	0.684%
3	5.190	394	400	410	rBV	644046	986620	9.42%	1.490%
4	5.666	474	481	491	rBV	2389743	4024503	38.41%	6.077%
5	7.287	749	757	774	rBV	2538826	4638047	44.26%	7.003%
6	7.657	812	820	830	rBV	2478343	4283929	40.88%	6.469%
7	8.127	892	900	909	rBV	395114	691613	6.60%	1.044%
8	8.456	948	956	964	rBV	1628483	2876676	27.45%	4.344%
9	9.308	1093	1101	1110	rBV	1505618	2737663	26.13%	4.134%
10	10.959	1375	1382	1392	rBV	584900	1060635	10.12%	1.602%
11	13.402	1789	1798	1807	rBV	3857657	6268600	59.83%	9.465%
12	14.231	1932	1939	1946	rBV	1757369	2603589	24.85%	3.931%
13	14.789	2027	2034	2042	rBV2	1033049	1729660	16.51%	2.612%
14	15.611	2170	2174	2178	rVB2	93244	123517	1.18%	0.187%
15	16.287	2282	2289	2299	rBV	4282868	6799167	64.89%	10.267%
16	16.475	2317	2321	2333	rBV2	106093	195342	1.86%	0.295%
17	17.550	2497	2504	2512	rBV	1667924	2548889	24.33%	3.849%
18	18.419	2647	2652	2662	rBV2	444781	666553	6.36%	1.006%
19	19.688	2863	2868	2877	rBV	314156	504568	4.82%	0.762%
20	19.829	2888	2892	2897	rVB2	225487	270865	2.59%	0.409%
21	20.158	2941	2948	2954	rBV	7867005	10478186	100.00%	15.822%
22	20.833	3056	3063	3066	rBV5	64829	114795	1.10%	0.173%
23	20.875	3066	3070	3074	rVB2	159654	195309	1.86%	0.295%
24	21.468	3167	3171	3184	rBV10	78582	207259	1.98%	0.313%
25	21.861	3231	3238	3245	rBV	1641052	2823561	26.95%	4.263%
26	25.239	3801	3813	3826	rBV	894146	2701211	25.78%	4.079%

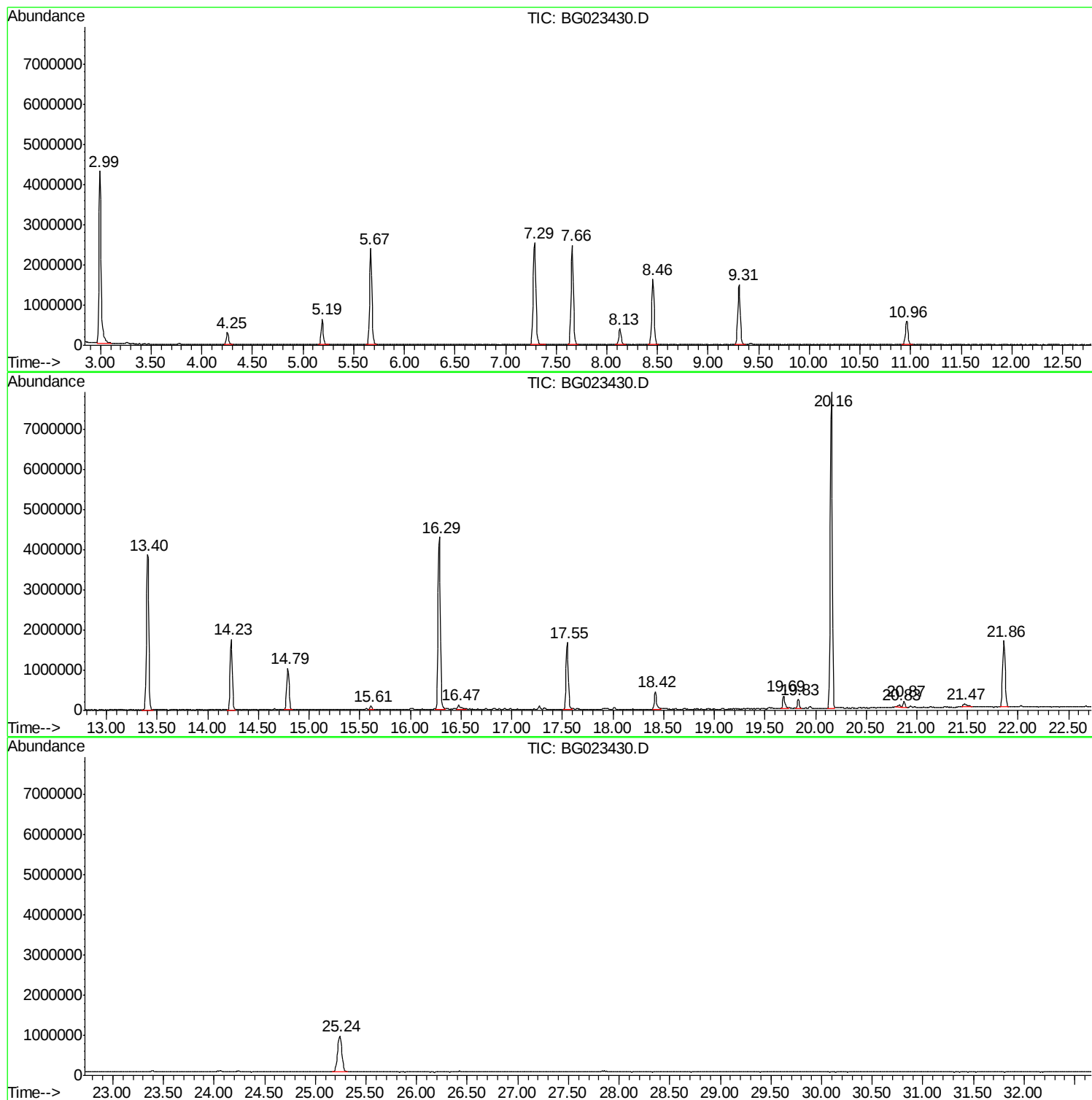
Sum of corrected areas: 66226705

Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.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\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

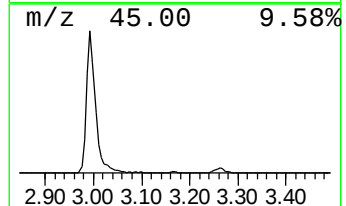
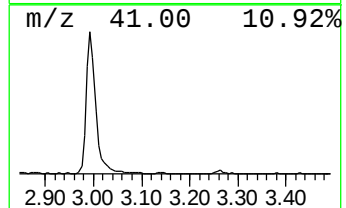
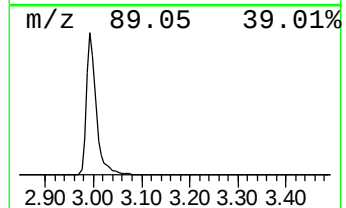
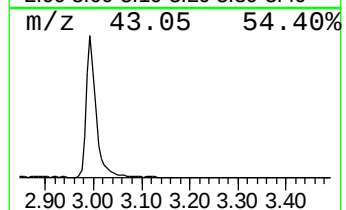
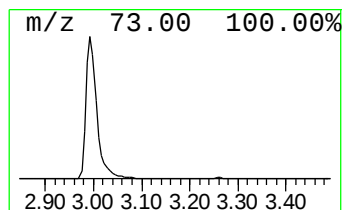
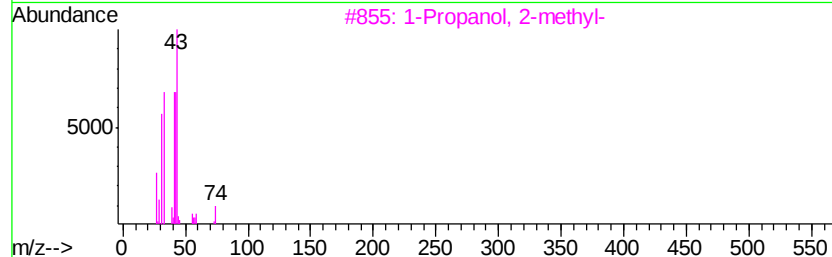
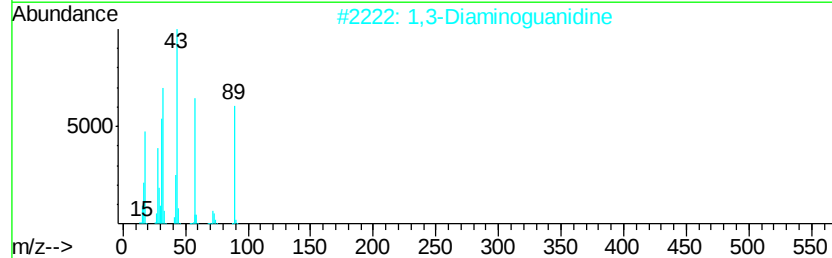
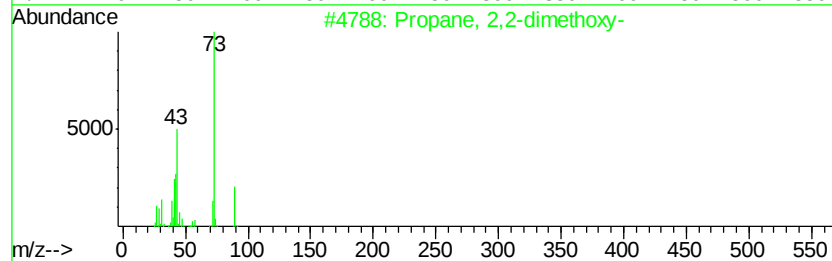
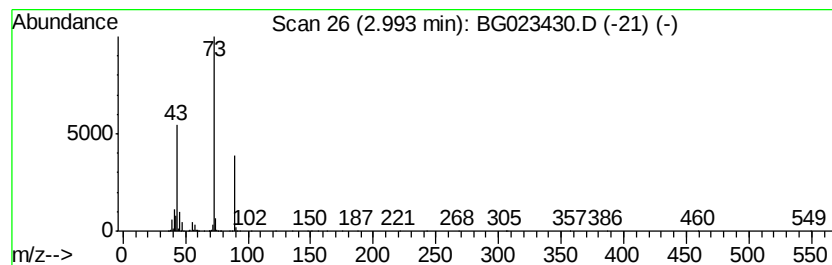
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Propane, 2,2-dimethoxy- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.99	180.53 ng	6242810	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	72
2		1,3-Diaminoguanidine	89	CH7N5	004364-78-7	25
3		1-Propanol, 2-methyl-	74	C4H10O	000078-83-1	9
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		1-(2-Methoxyethoxy)-2-methyl-2-p...	162	C8H18O3	1000364-24-4	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

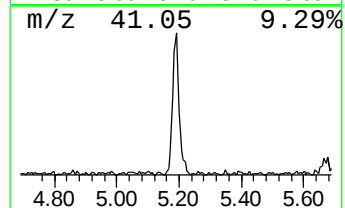
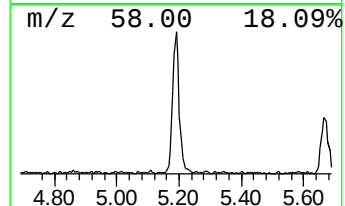
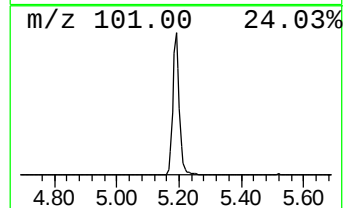
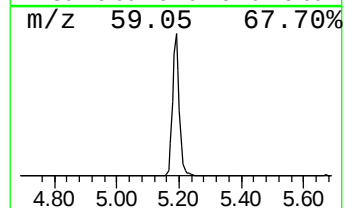
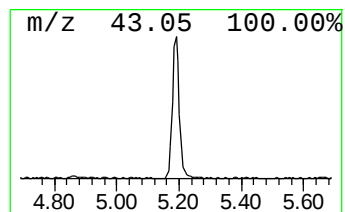
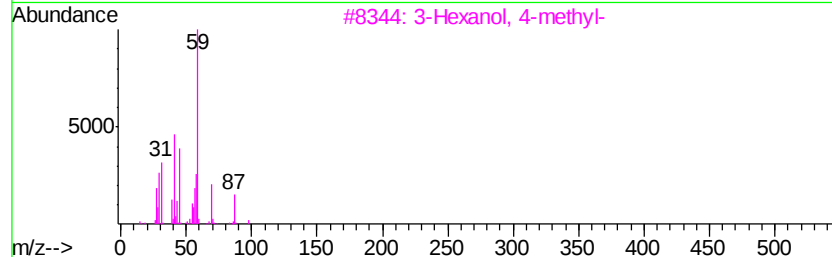
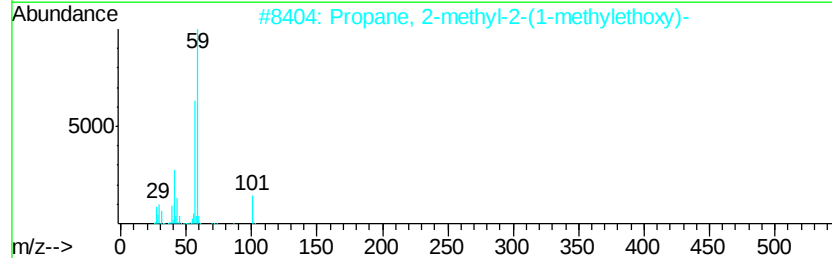
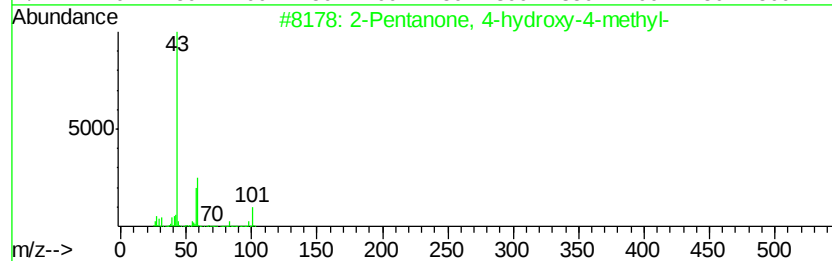
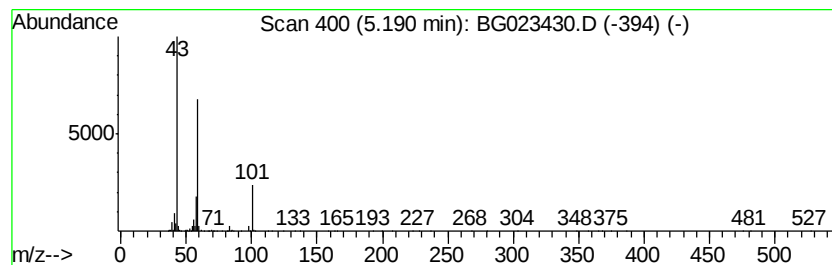
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	28.53 ng	986620	1,4-Dichlorobenzene-d4	8.13

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	28		
3	3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28		
4	1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	25		
5	Acetone	58	C3H6O	000067-64-1	9		



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

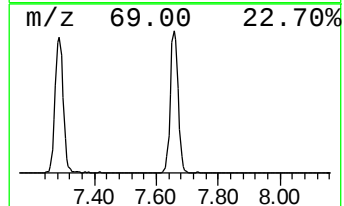
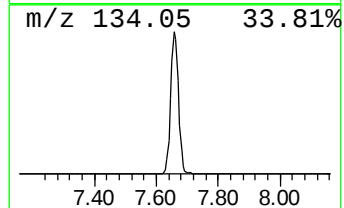
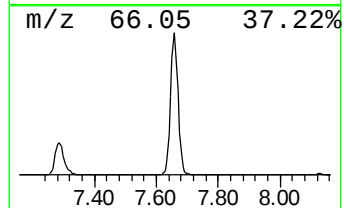
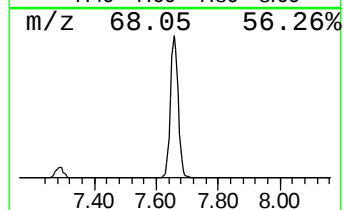
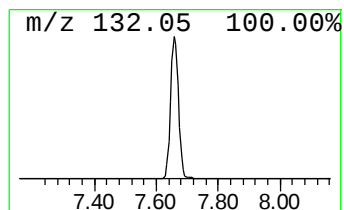
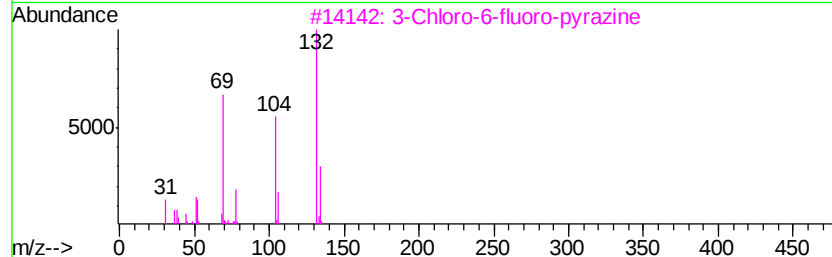
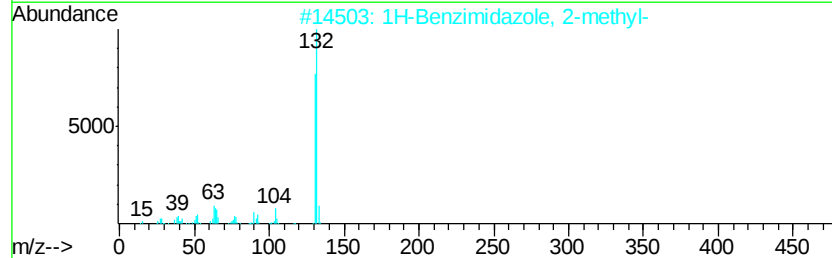
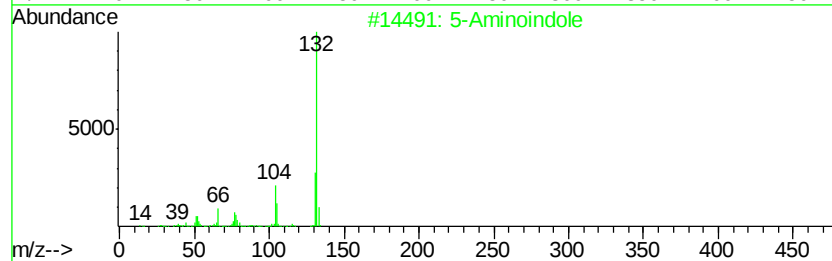
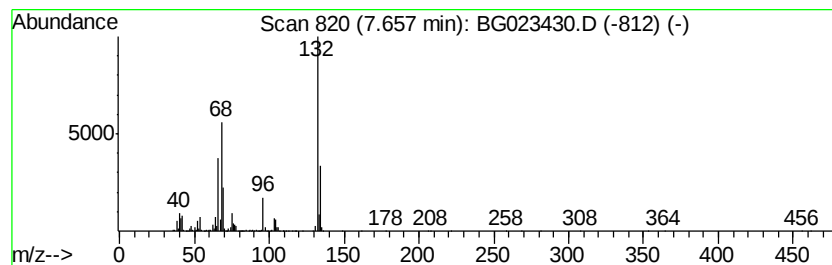
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown7.66 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.66	123.88 ng	4283930	1,4-Dichlorobenzene-d4	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Aminoindole	132	C8H8N2	005192-03-0	22
2		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
3		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		N-(-3,4-Methylenedioxyphenyl)isop...	267	C17H17NO2	1000378-96-6	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

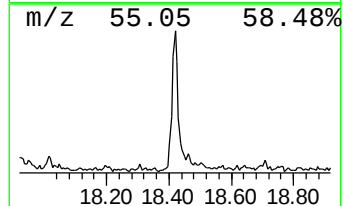
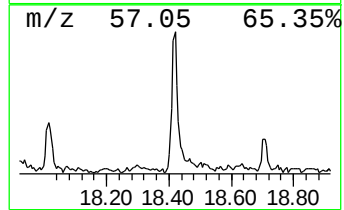
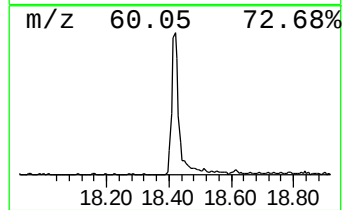
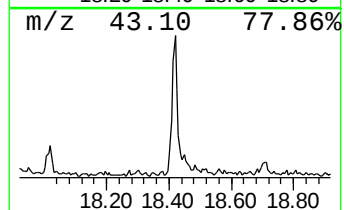
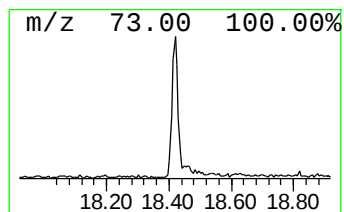
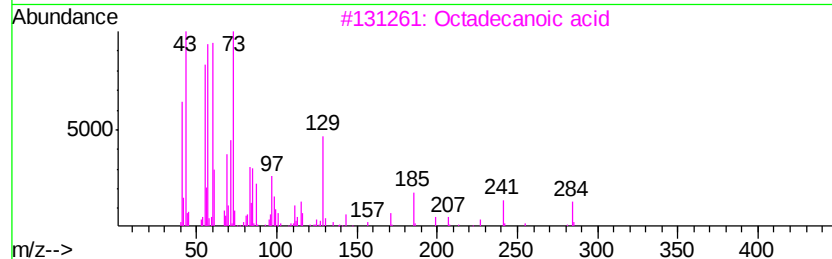
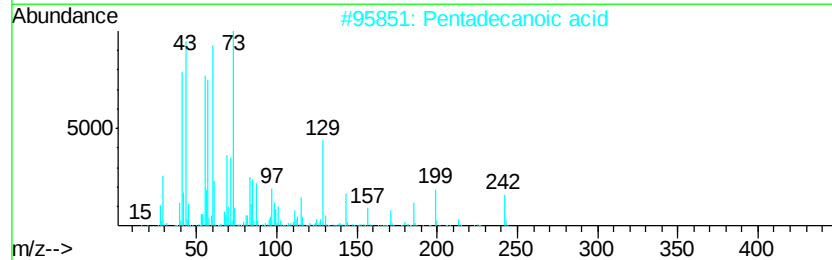
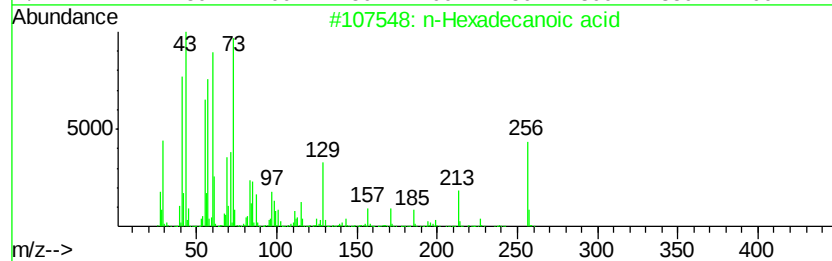
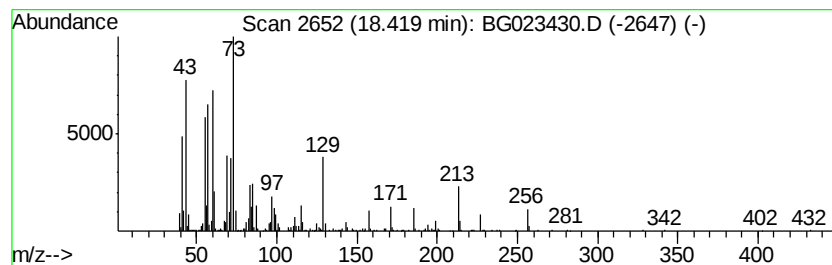
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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.
18.42	5.23 ng	666553	Phenanthrene-d10	17.55

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3		Octadecanoic acid	284	C18H36O2	000057-11-4	64
4		Tridecanoic acid	214	C13H26O2	000638-53-9	58
5		Tetradecanoic acid	228	C14H28O2	000544-63-8	47



Data Path : Z:\HPCHEM1\BNA G\DATA\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

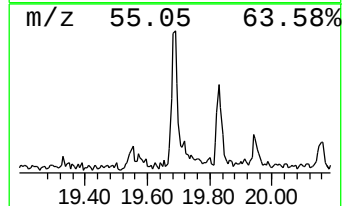
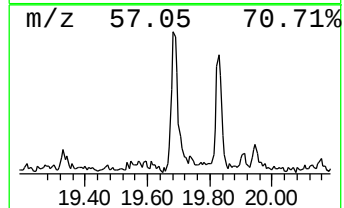
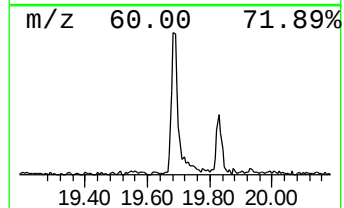
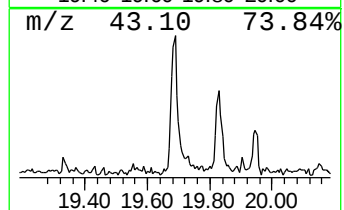
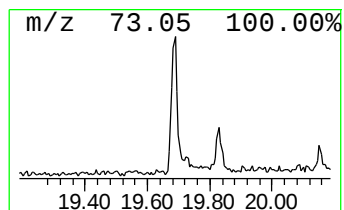
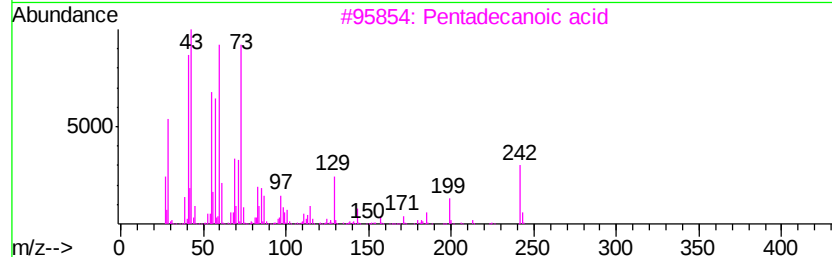
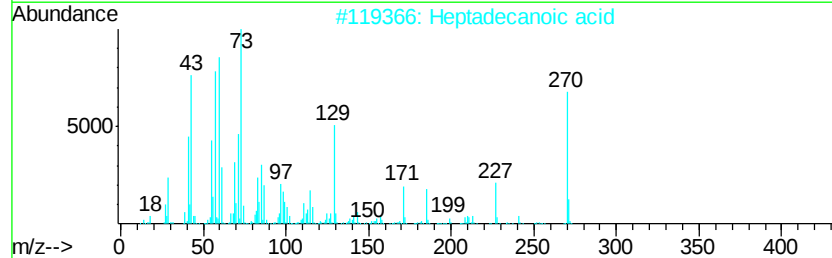
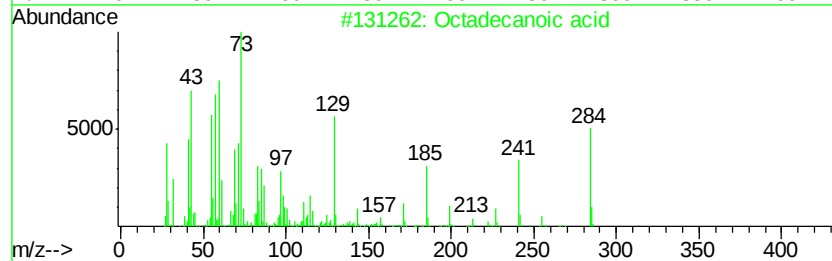
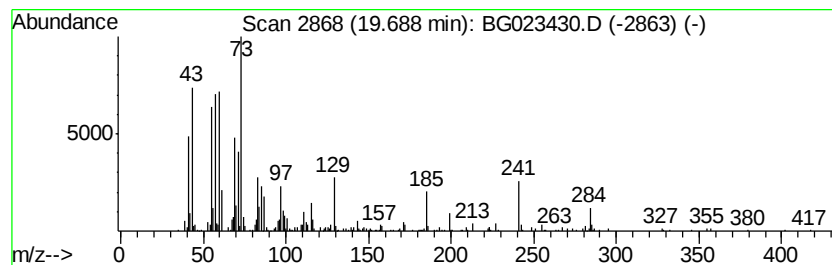
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG080116.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Octadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.96 ng	504568	Phenanthrene-d10	17.55

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	97
2		Heptadecanoic acid	270	C17H34O2	000506-12-7	93
3		Pentadecanoic acid	242	C15H30O2	001002-84-2	89
4		Tetradecanoic acid	228	C14H28O2	000544-63-8	58
5		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	58



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG080316\
Data File : BG023430.D
Acq On : 3 Aug 2016 18:03
Operator : UM/SJ
Sample : H4287-13
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
SB-61-19.0-20.0

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG080116.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
Propane, 2,2-dime...	2.99	180.5	ng	6242810	1	8.13	691613	20.0
2-Pentanone, 4-hy...	5.19	28.5	ng	986620	1	8.13	691613	20.0
unknown7.66	7.66	123.9	ng	4283930	1	8.13	691613	20.0
n-Hexadecanoic acid	18.42	5.2	ng	666553	4	17.55	2548890	20.0
Octadecanoic acid	19.69	4.0	ng	504568	4	17.55	2548890	20.0