

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
 Data File : BG024674.D
 Acq On : 4 Nov 2016 9:31
 Operator : UM/SJ
 Sample : H5509-20
 Misc :
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GW-90-8.15-18.0

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-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	3.598	124	129	138	rBV	304201	562642	5.66%	1.155%
2	5.325	418	423	430	rBV	187928	315405	3.17%	0.648%
3	5.795	496	503	513	rBV	1277175	2130545	21.43%	4.374%
4	7.399	769	776	784	rBV	876910	1522527	15.32%	3.126%
5	7.793	833	843	851	rBV	2034797	3704391	37.26%	7.605%
6	8.263	916	923	932	rBV2	396253	738437	7.43%	1.516%
7	8.592	969	979	988	rBV	1765619	3245060	32.64%	6.662%
8	9.444	1114	1124	1132	rBV	1582465	3019140	30.37%	6.198%
9	9.573	1140	1146	1152	rVB3	165885	274096	2.76%	0.563%
10	11.089	1393	1404	1412	rBV	533681	1063362	10.70%	2.183%
11	11.847	1528	1533	1538	rBV5	121693	255534	2.57%	0.525%
12	11.894	1538	1541	1546	rVB3	80010	122835	1.24%	0.252%
13	13.510	1808	1816	1823	rBV	4002586	6537978	65.77%	13.423%
14	14.450	1969	1976	1980	rBV8	59233	114470	1.15%	0.235%
15	14.884	2040	2050	2056	rBV	872596	1472798	14.81%	3.024%
16	15.255	2109	2113	2122	rBV6	65394	118725	1.19%	0.244%
17	16.365	2294	2302	2312	rBV	3940784	6178661	62.15%	12.685%
18	16.976	2402	2406	2413	rVB7	90135	138555	1.39%	0.284%
19	17.622	2510	2516	2522	rBV	1186550	1886638	18.98%	3.873%
20	17.664	2522	2523	2530	rVB2	96973	100800	1.01%	0.207%
21	18.469	2656	2660	2669	rBV3	145055	273054	2.75%	0.561%
22	19.726	2871	2874	2881	rBV6	124473	162955	1.64%	0.335%
23	20.208	2950	2956	2961	rBV	7346779	9941400	100.00%	20.410%
24	21.917	3241	3247	3254	rVB	1329501	2384376	23.98%	4.895%
25	25.349	3821	3831	3844	rVB3	776479	2444577	24.59%	5.019%

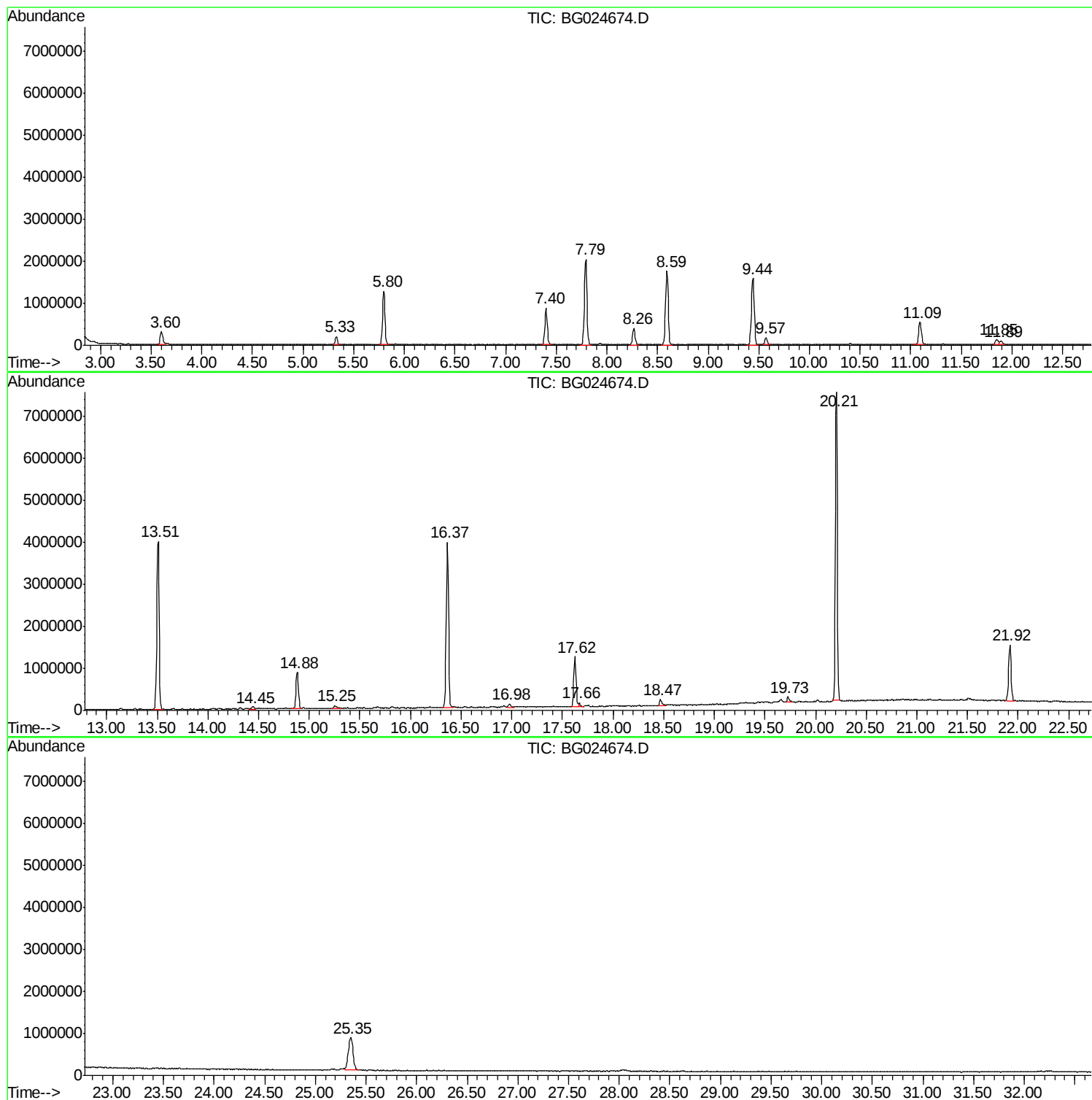
Sum of corrected areas: 48708961

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

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\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

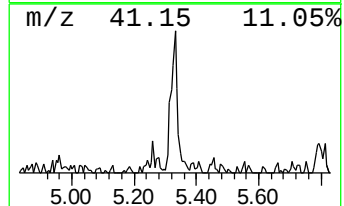
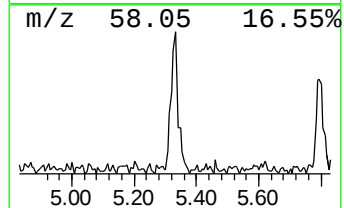
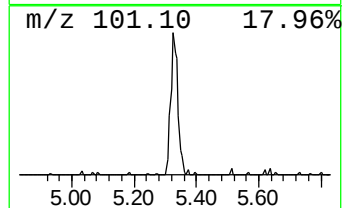
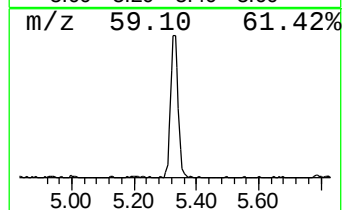
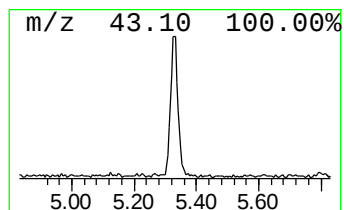
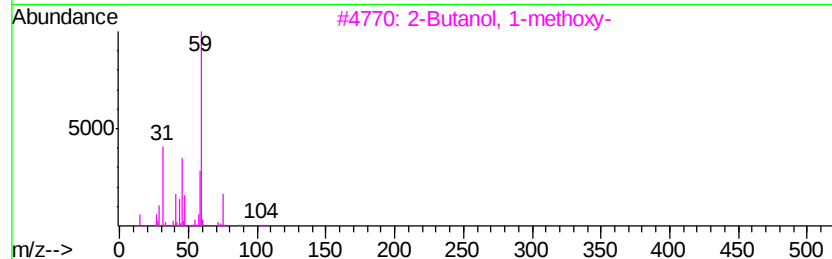
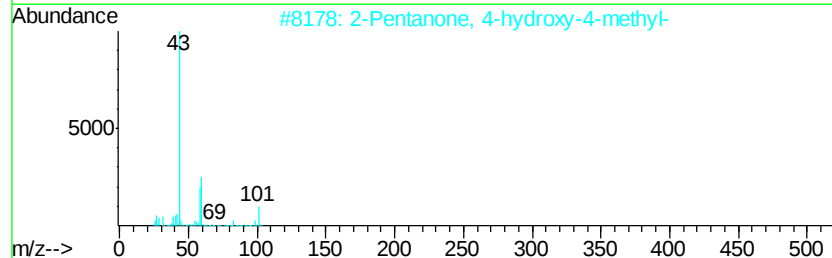
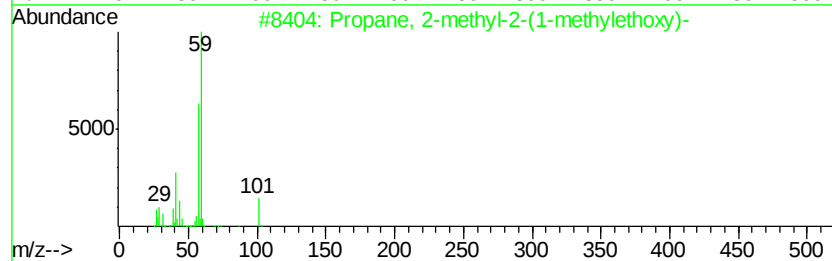
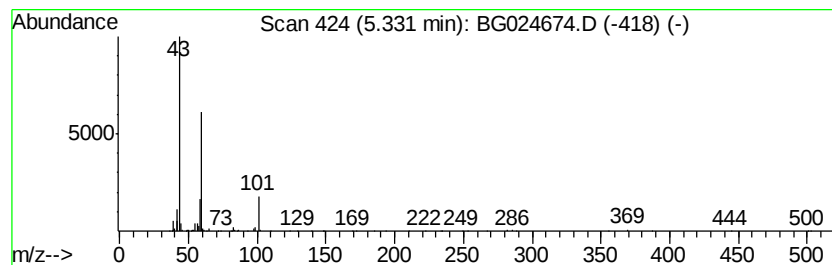
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 Propane, 2-methyl-2-(1-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.33	8.54 ng	315405	1,4-Dichlorobenzene-d4	8.27

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O		017348-59-3	53
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2		000123-42-2	50
3	2-Butanol, 1-methoxy-	104	C5H12O2		053778-73-7	37
4	Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2		000921-14-2	36
5	Propane, 1,2-dimethoxy-	104	C5H12O2		007778-85-0	32



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

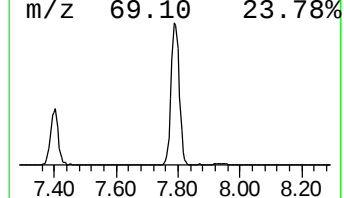
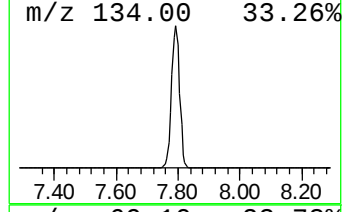
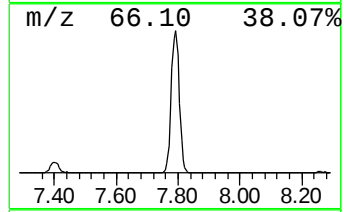
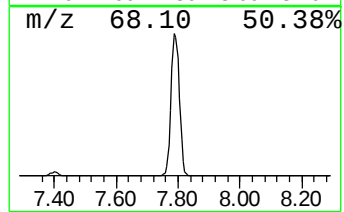
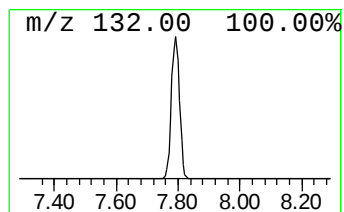
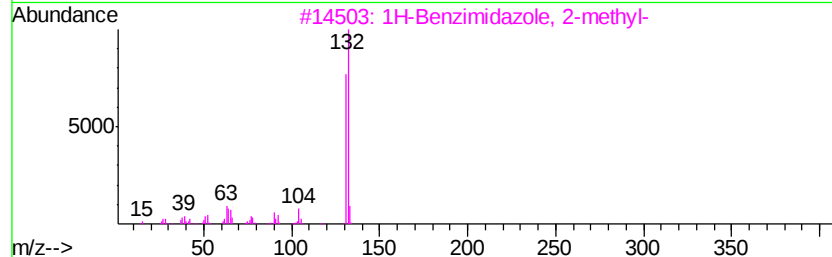
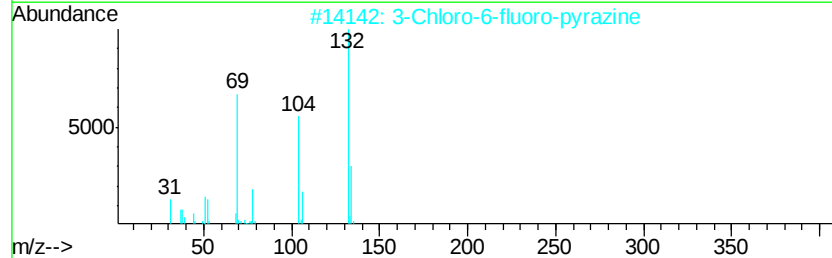
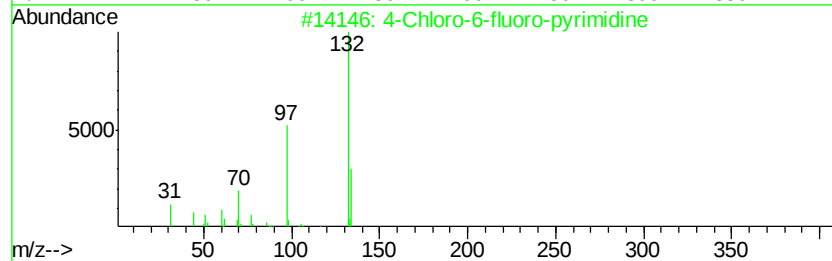
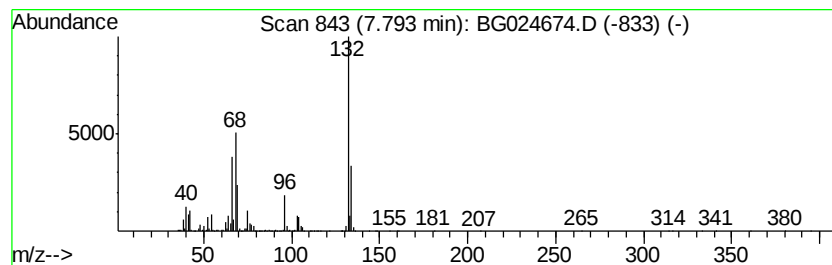
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.79 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.79	100.33 ng	3704390	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	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	14
4		5-Aminoindole	132	C8H8N2	005192-03-0	14
5		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

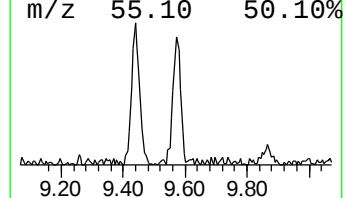
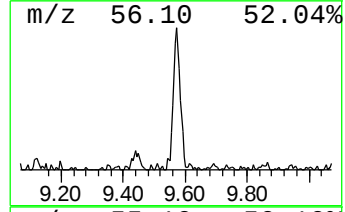
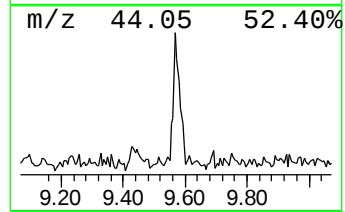
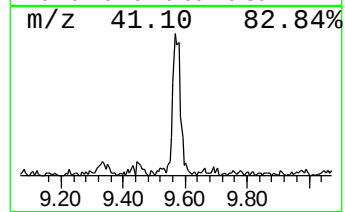
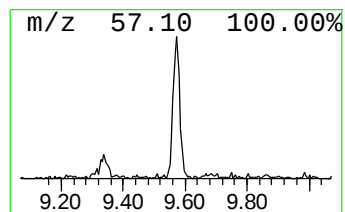
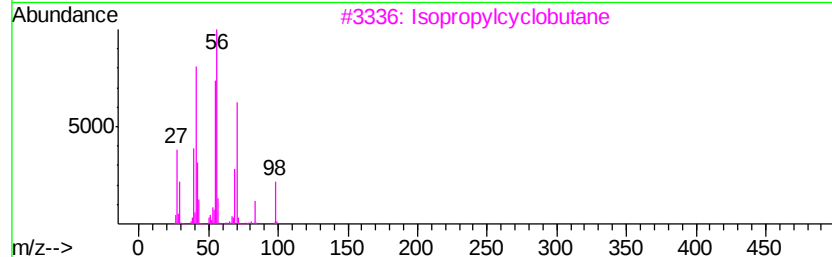
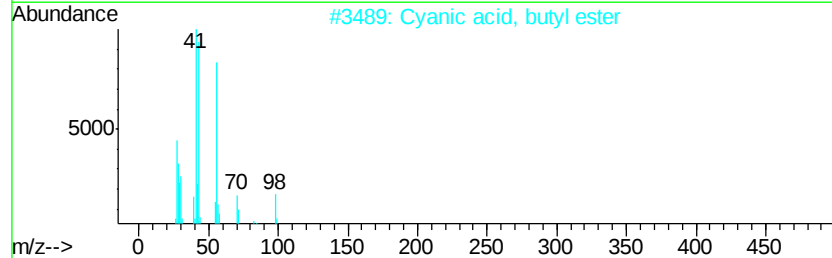
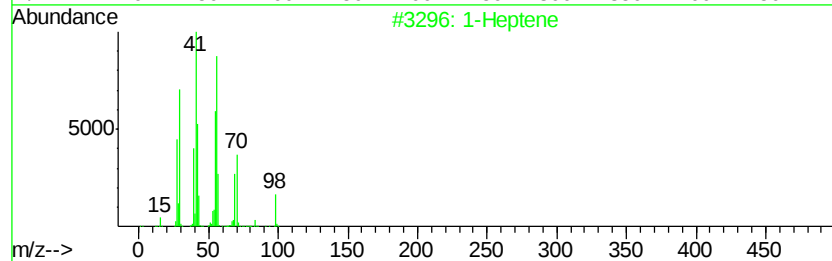
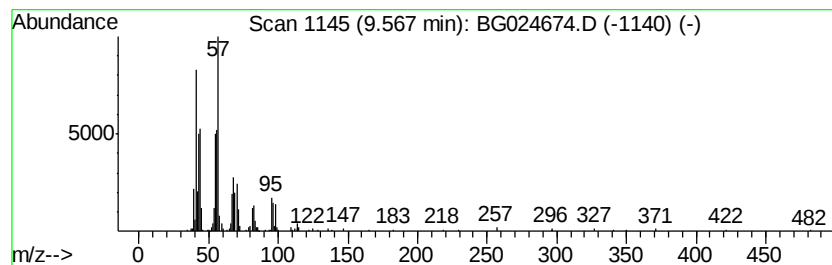
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 unknown9.57 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.57	7.42 ng	274096	1,4-Dichlorobenzene-d4	8.27

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heptene	98	C7H14	000592-76-7	46
2		Cyanoic acid, butyl ester	99	C5H9NO	001768-24-7	45
3		Isopropylcyclobutane	98	C7H14	000872-56-0	43
4		2-Hexene, 5-methyl-, (E)-	98	C7H14	007385-82-2	38
5		(Z)-Hex-2-ene, 5-methyl-	98	C7H14	013151-17-2	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

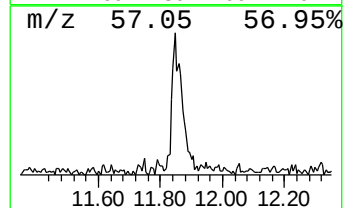
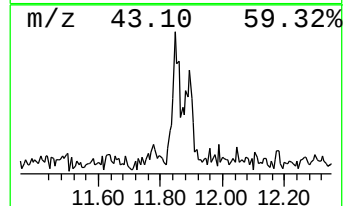
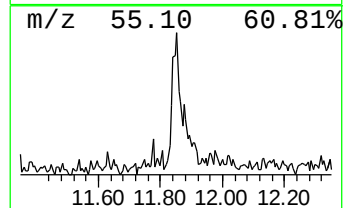
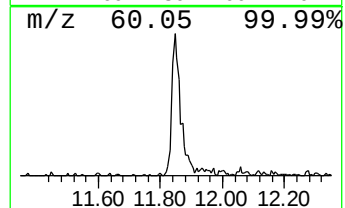
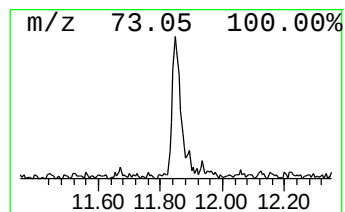
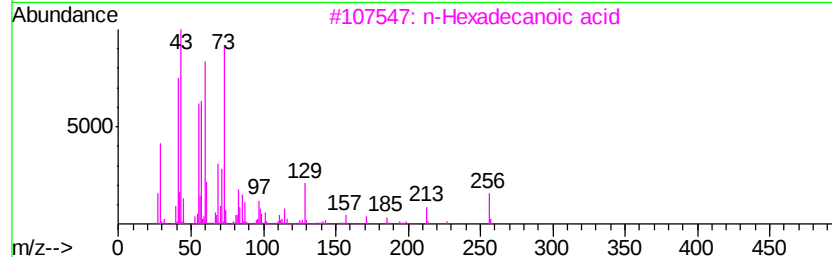
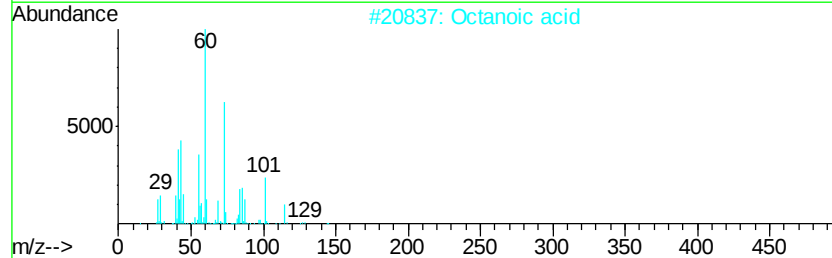
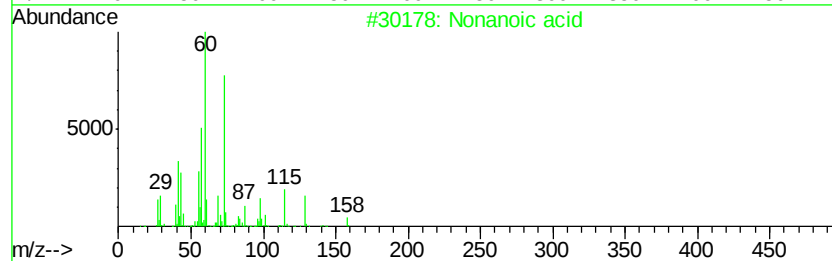
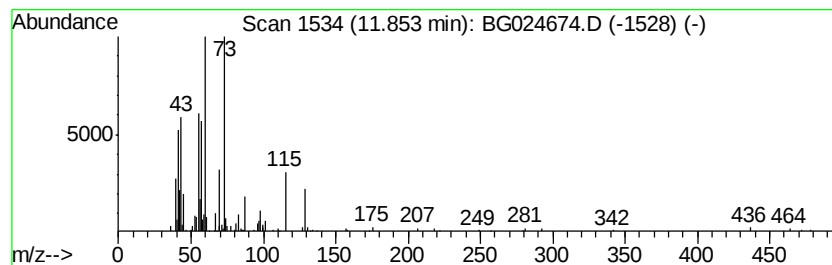
Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

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 Nonanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
11.85	4.81 ng	255534	Naphthalene-d8	11.09	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Nonanoic acid	158	C9H18O2	000112-05-0	64
2	Octanoic acid	144	C8H16O2	000124-07-2	53
3	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	50
4	n-Decanoic acid	172	C10H20O2	000334-48-5	50
5	12-Bromododecanoic acid	278	C12H23BrO2	073367-80-3	50



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

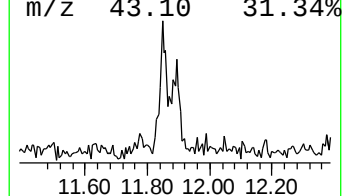
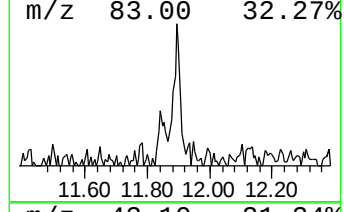
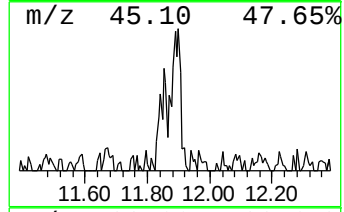
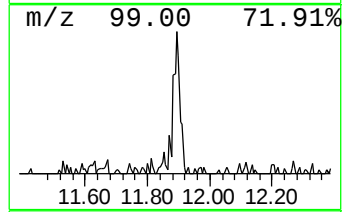
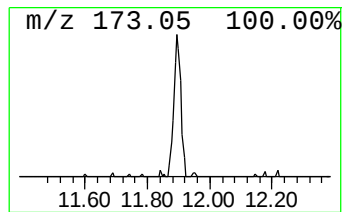
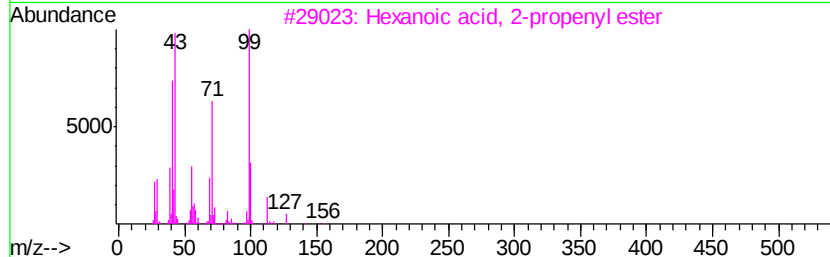
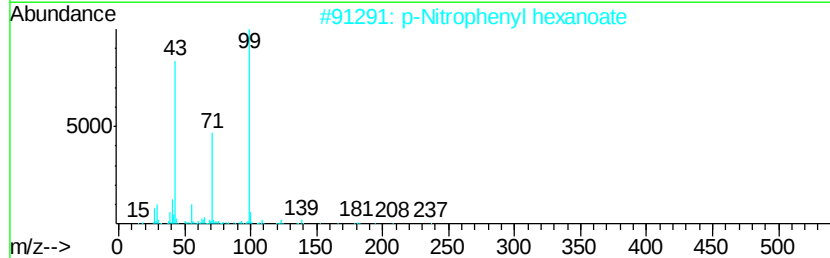
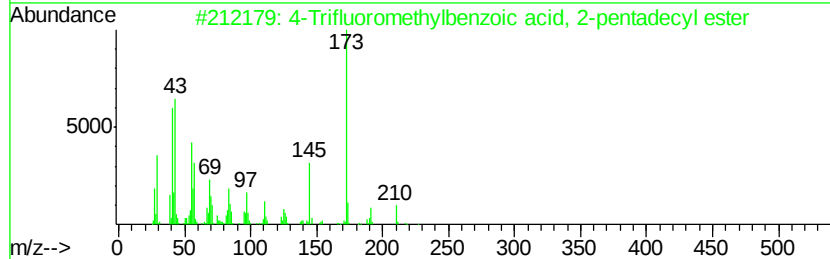
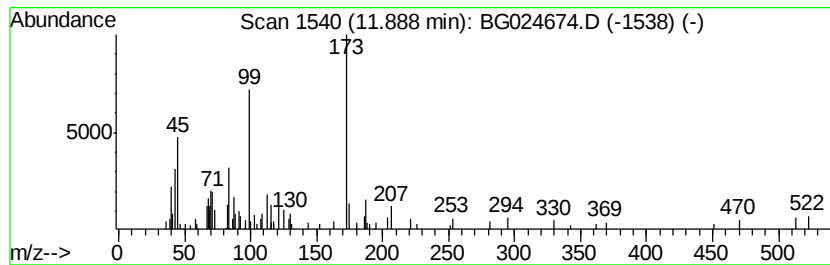
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown11.89 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.89	2.31 ng	122835	Naphthalene-d8	11.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Trifluoromethylbenzoic acid, 2...	400	C23H35F3O2	1000280-65-5	38
2		p-Nitrophenyl hexanoate	237	C12H15NO4	000956-75-2	25
3		Hexanoic acid, 2-propenyl ester	156	C9H16O2	000123-68-2	25
4		6-Hydroxycyclohepta(b)pyridin-7-one	173	C10H7NO2	026825-25-2	14
5		3-Trifluoromethylbenzoic acid, 3...	386	C22H33F3O2	1000281-99-8	14



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

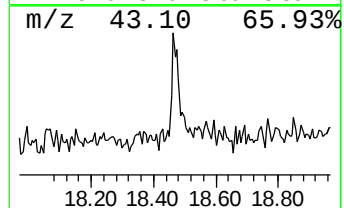
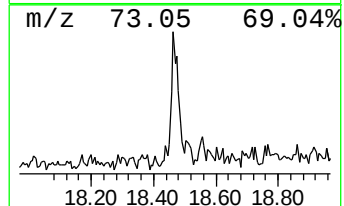
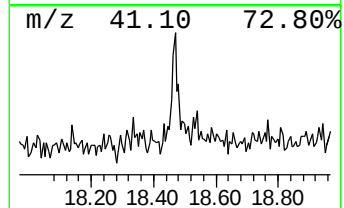
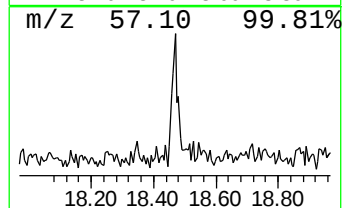
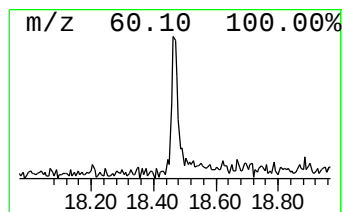
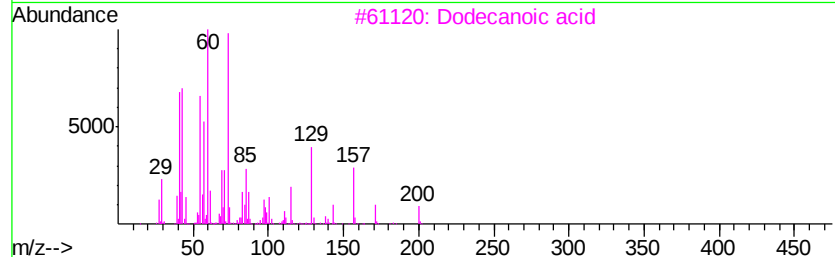
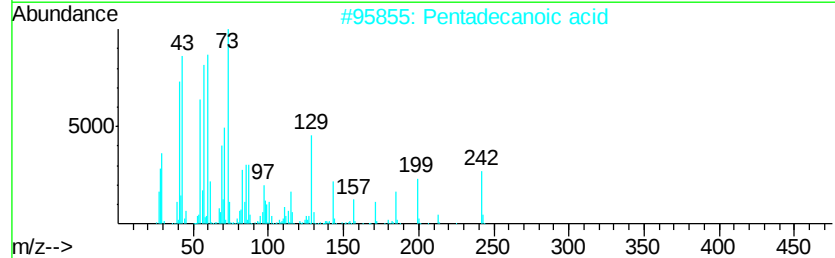
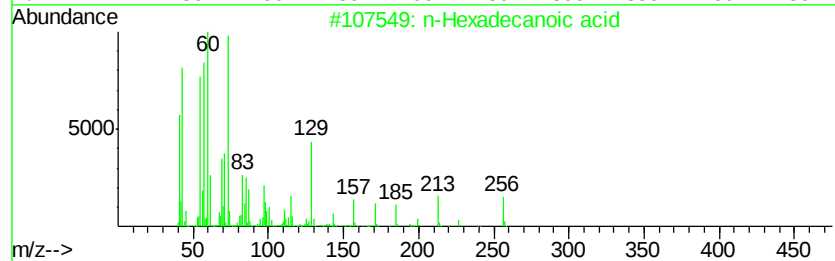
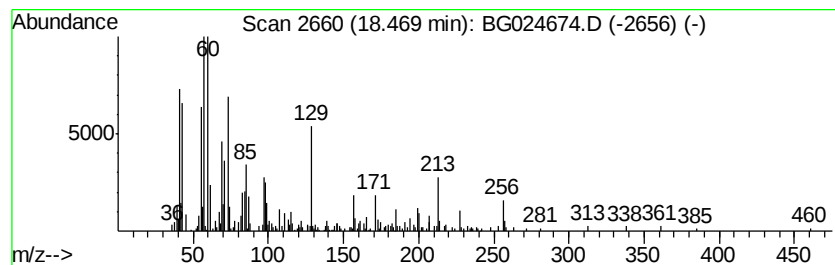
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG102516.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.47	2.89 ng	273054	Phenanthrene-d10	17.62

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	83
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	64
3		Dodecanoic acid	200	C12H24O2	000143-07-7	58
4		n-Decanoic acid	172	C10H20O2	000334-48-5	43
5		Octadecanoic acid	284	C18H36O2	000057-11-4	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG110316\
Data File : BG024674.D
Acq On : 4 Nov 2016 9:31
Operator : UM/SJ
Sample : H5509-20
Misc :
ALS Vial : 42 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GW-90-8.15-18.0

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
Propane, 2-methyl...	5.33	8.5	ng	315405	1	8.27	738437	20.0
unknown7.79	7.79	100.3	ng	3704390	1	8.27	738437	20.0
unknown9.57	9.57	7.4	ng	274096	1	8.27	738437	20.0
Nonanoic acid	11.85	4.8	ng	255534	2	11.09	1063360	20.0
unknown11.89	11.89	2.3	ng	122835	2	11.09	1063360	20.0
n-Hexadecanoic acid	18.47	2.9	ng	273054	4	17.62	1886640	20.0