

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
 Data File : BG022442.D
 Acq On : 19 Jun 2016 3:18
 Operator : UM/SJ
 Sample : H3489-01
 Misc :
 ALS Vial : 51 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S6-B1(0-8)C

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-BG060616.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	2.872	3	6	26	rVB	1489257	2370761	100.00%	15.443%
2	5.105	379	386	396	rBV	33717	67966	2.87%	0.443%
3	5.604	462	471	489	rBV	533087	1052230	44.38%	6.854%
4	7.238	741	749	762	rBV	591028	1191184	50.24%	7.759%
5	7.584	797	808	824	rBV	668646	1332158	56.19%	8.678%
6	8.049	879	887	896	rVB	112728	214622	9.05%	1.398%
7	8.372	934	942	953	rBV	530344	1019382	43.00%	6.640%
8	9.224	1079	1087	1101	rBV	365965	750619	31.66%	4.889%
9	9.382	1109	1114	1128	rVB5	8368	23766	1.00%	0.155%
10	10.869	1359	1367	1378	rBV	171808	355606	15.00%	2.316%
11	13.307	1774	1782	1796	rBV	1134156	1911905	80.65%	12.454%
12	14.130	1914	1922	1931	rBV	118071	197867	8.35%	1.289%
13	14.688	2010	2017	2026	rBV2	260145	458415	19.34%	2.986%
14	15.499	2151	2155	2160	rVB	24177	33207	1.40%	0.216%
15	16.180	2264	2271	2281	rBV	639833	1087233	45.86%	7.082%
16	16.357	2297	2301	2310	rBV2	19837	42111	1.78%	0.274%
17	17.432	2478	2484	2488	rBV	255668	429496	18.12%	2.798%
18	17.473	2488	2491	2499	rVV	94058	153800	6.49%	1.002%
19	17.567	2503	2507	2514	rVB	17092	33213	1.40%	0.216%
20	18.354	2639	2641	2647	rVB2	18804	27548	1.16%	0.179%
21	18.501	2661	2666	2670	rBV3	24264	50052	2.11%	0.326%
22	19.476	2828	2832	2839	rBV	119093	191823	8.09%	1.250%
23	19.700	2867	2870	2874	rBV2	62017	72974	3.08%	0.475%
24	19.841	2890	2894	2902	rVB	126344	200344	8.45%	1.305%
25	20.029	2920	2926	2933	rBV	1211740	1660233	70.03%	10.815%
26	21.697	3204	3210	3216	rBV2	210902	423302	17.86%	2.757%

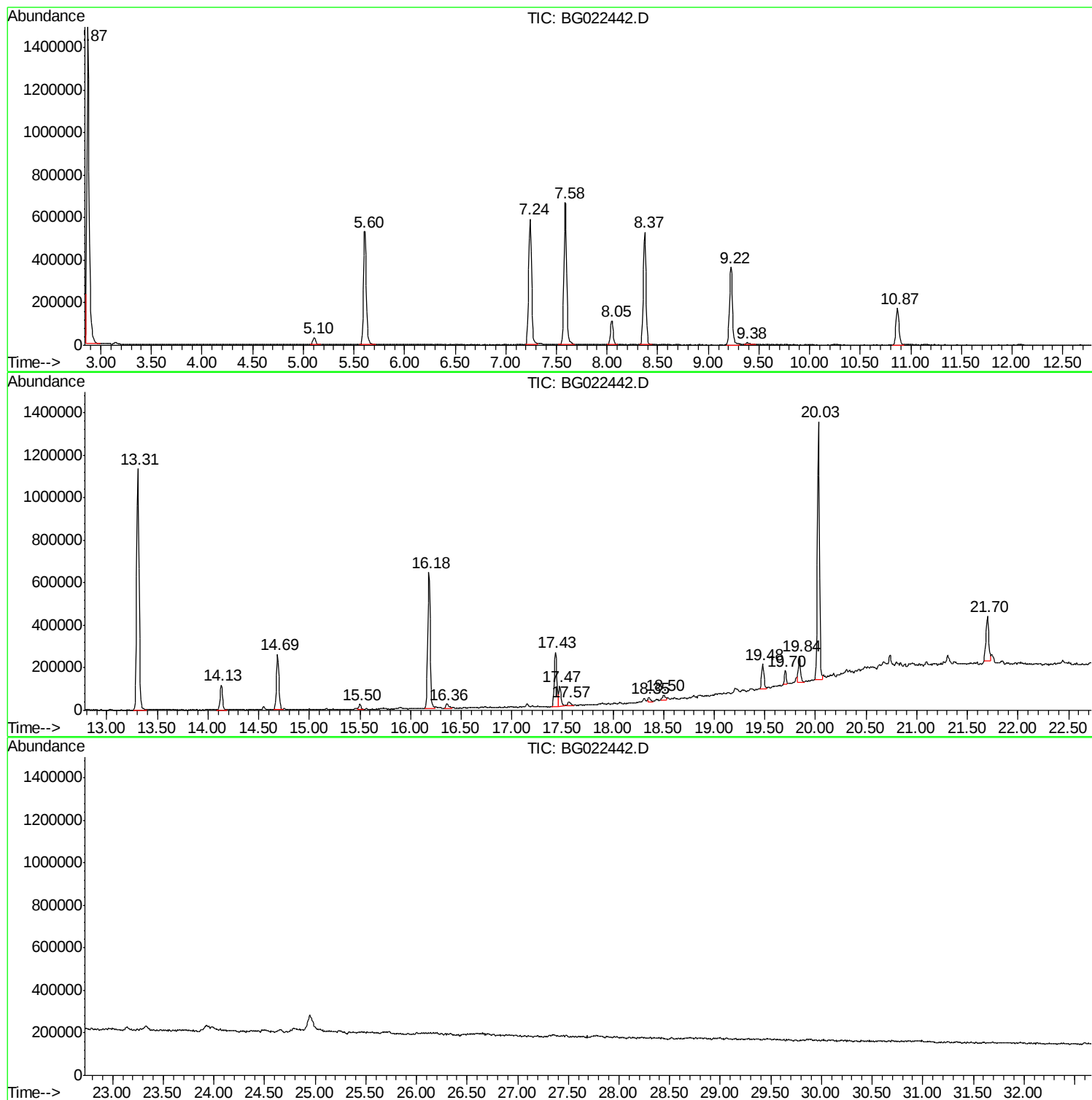
Sum of corrected areas: 15351817

Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.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\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

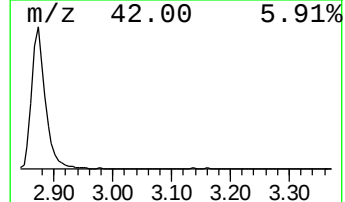
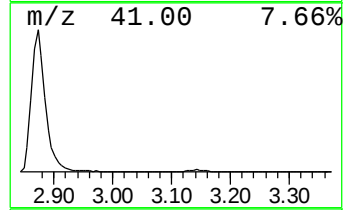
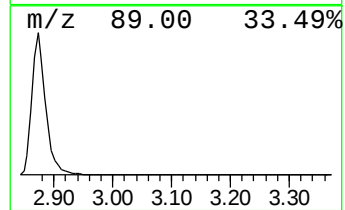
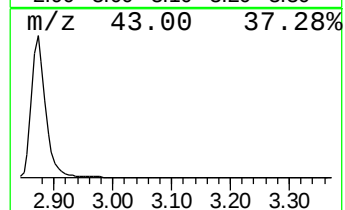
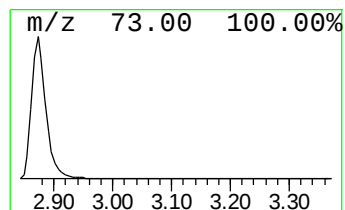
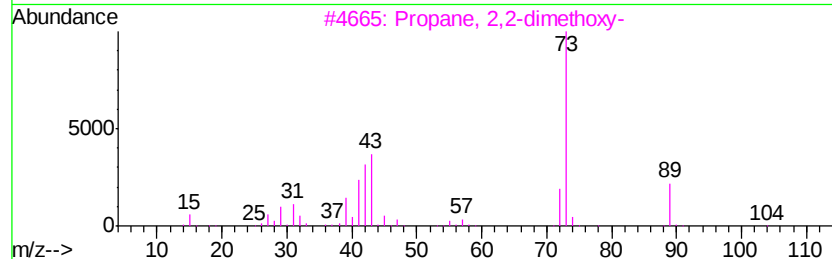
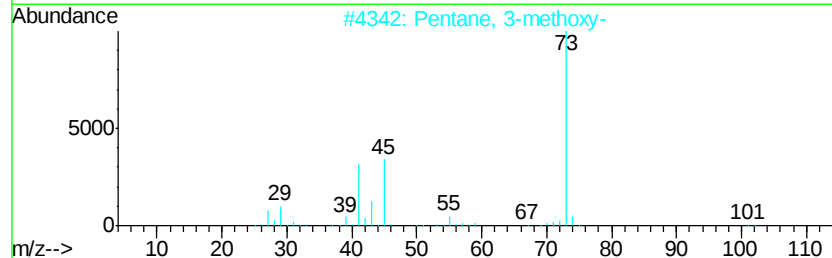
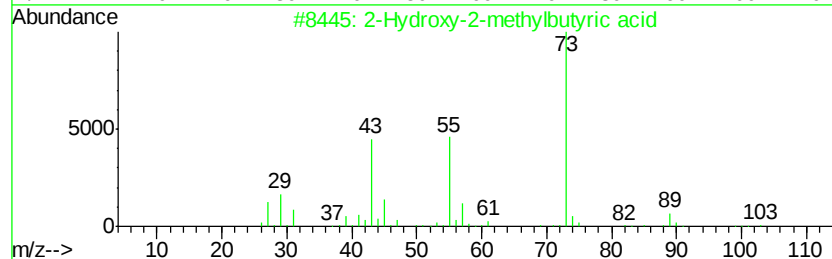
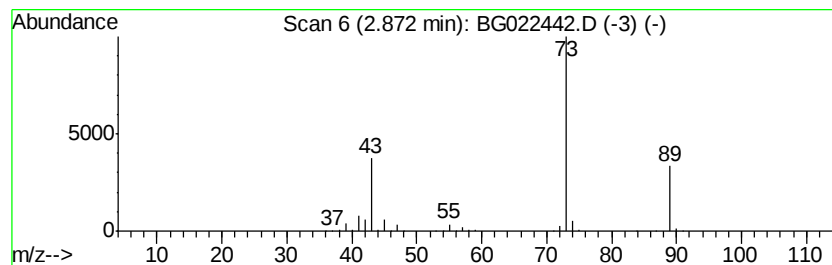
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.87 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.87	220.92 ng	2370760	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	28
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	9
4		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
5		Methane, isothiocyanato-	73	C2H3NS	000556-61-6	7



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

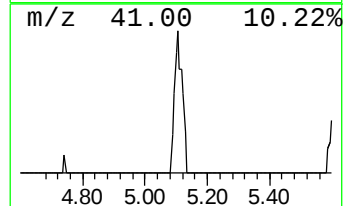
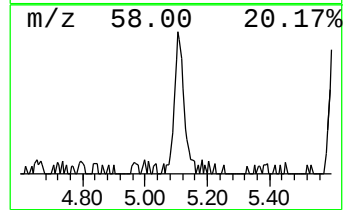
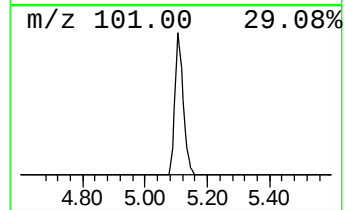
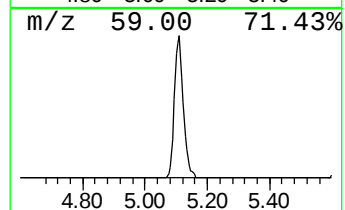
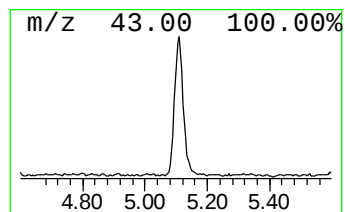
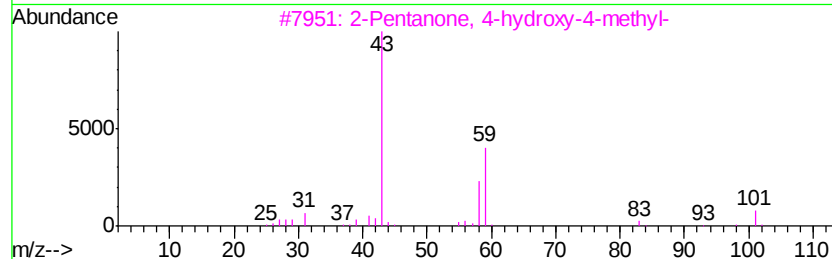
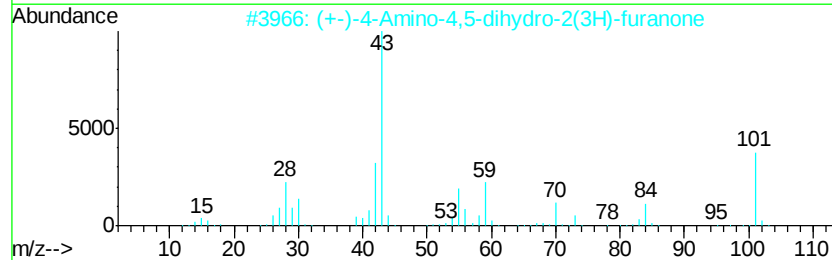
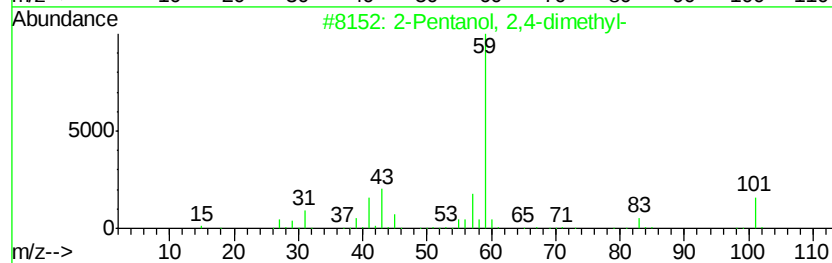
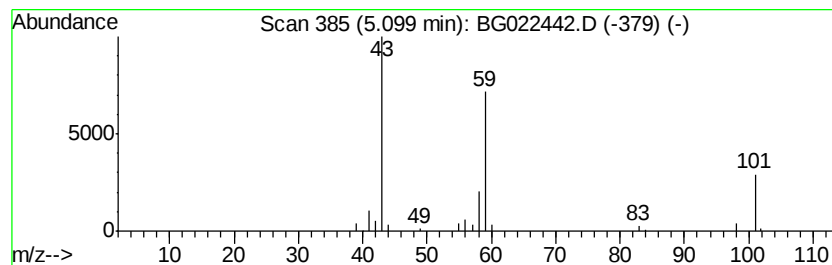
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 unknown5.10 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.33 ng	67966	1,4-Dichlorobenzene-d4	8.05

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	47
2			(+)-4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	43
3			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	42
4			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	25
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	10



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

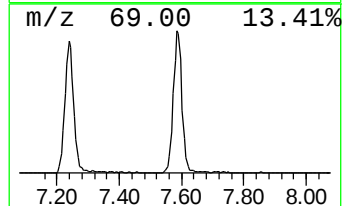
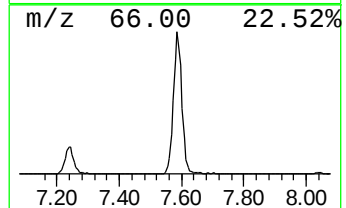
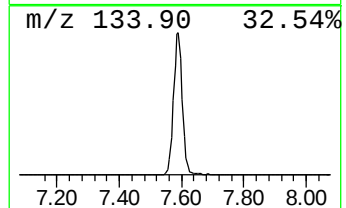
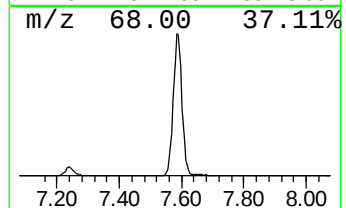
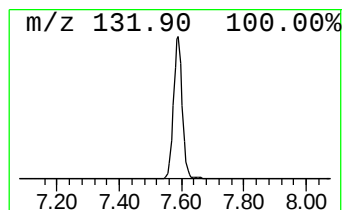
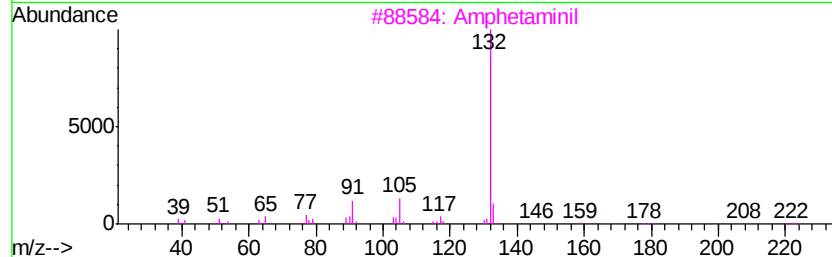
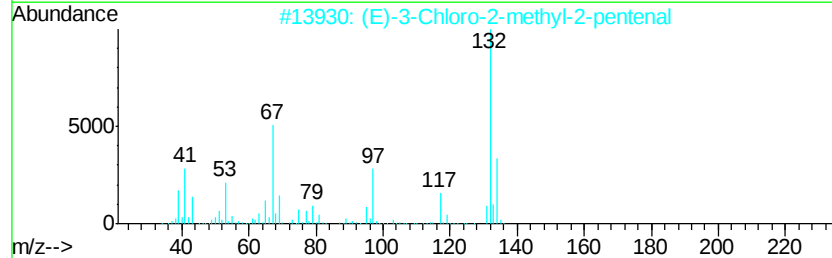
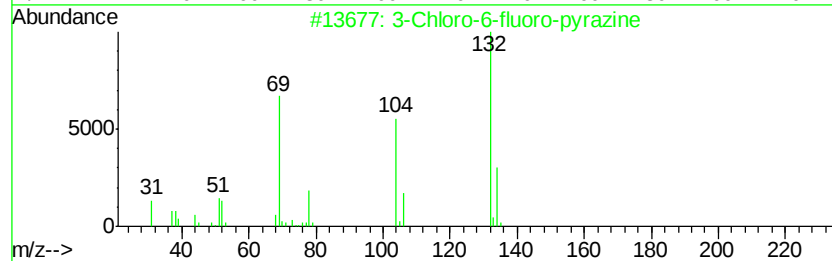
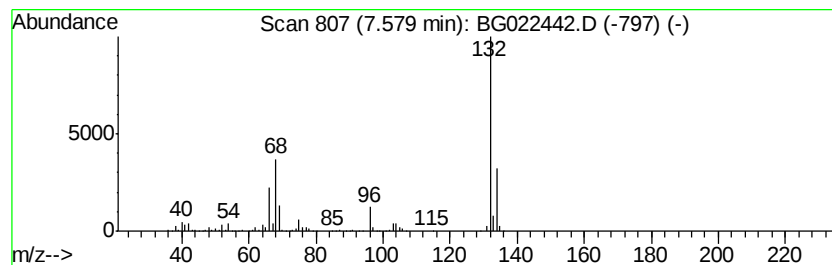
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown7.58 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.58	124.14 ng	1332160	1,4-Dichlorobenzene-d4	8.05

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	17
3		Amphetaminil	250	C17H18N2	017590-01-1	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Benzene, 1,3,5-trifluoro-	132	C6H3F3	000372-38-3	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

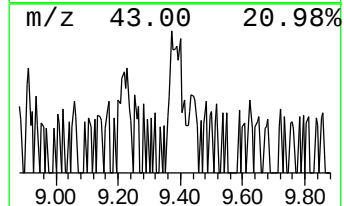
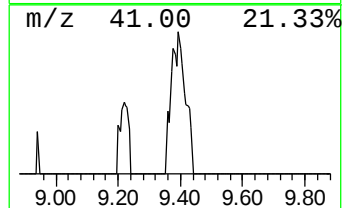
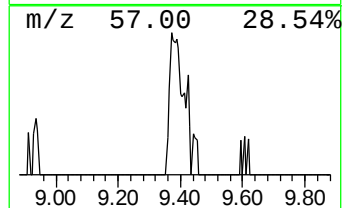
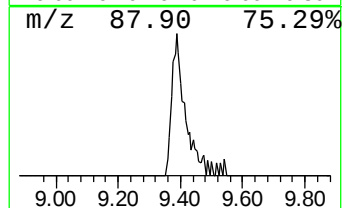
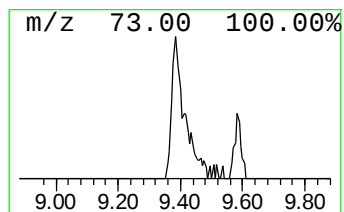
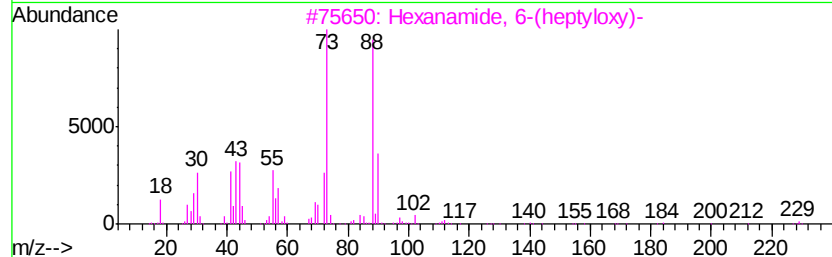
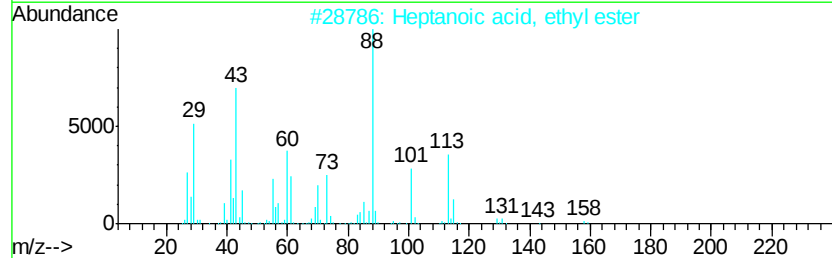
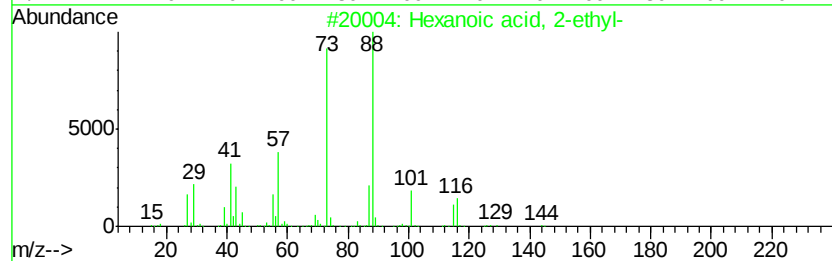
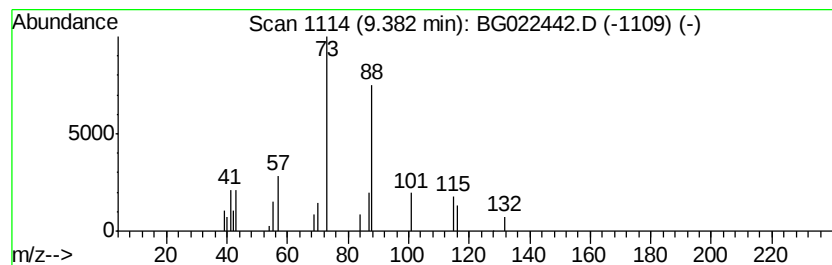
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 5 Hexanoic acid, 2-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.38	2.21 ng	23766	1,4-Dichlorobenzene-d4	8.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexanoic acid, 2-ethyl-	144	C8H16O2	000149-57-5	72
2		Heptanoic acid, ethyl ester	158	C9H18O2	000106-30-9	36
3		Hexanamide, 6-(heptyloxy)-	229	C13H27NO2	055191-08-7	33
4		.alpha.-D-Mannofuranoside, 1-O-d...	320	C16H32O6	1000160-04-7	10
5		2-Ethylbutylamine	101	C6H15N	000617-79-8	9



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

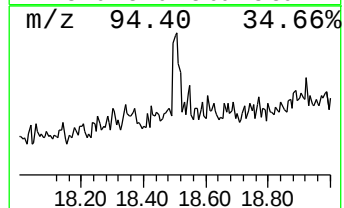
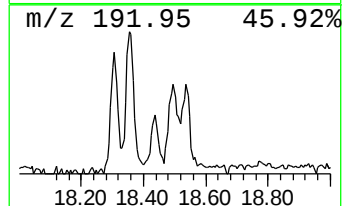
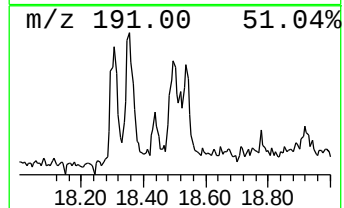
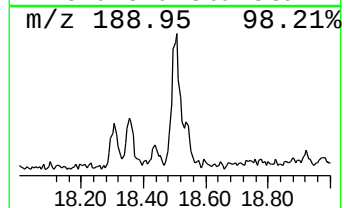
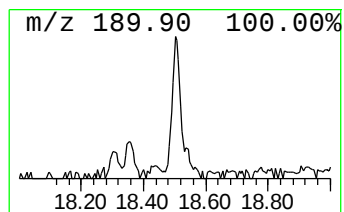
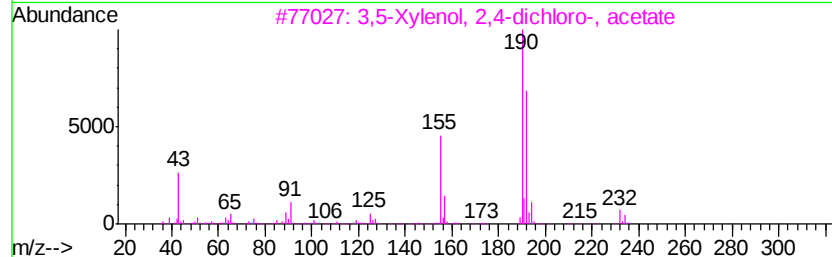
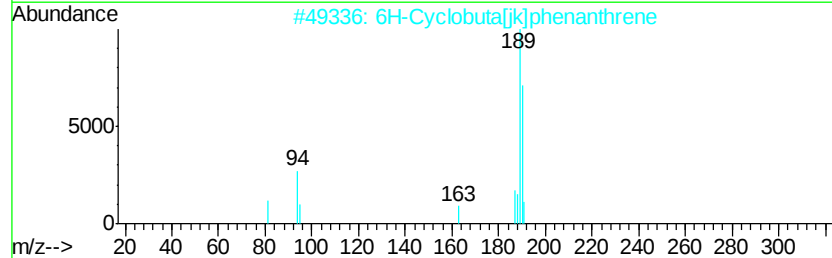
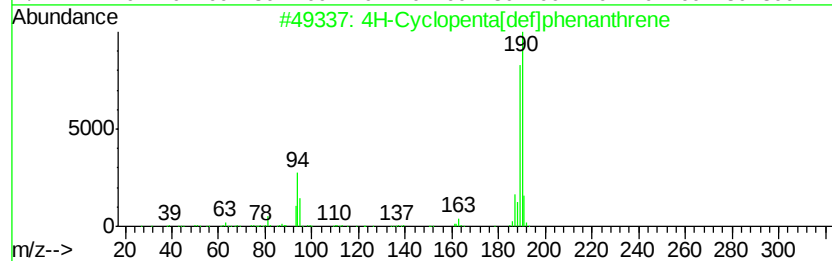
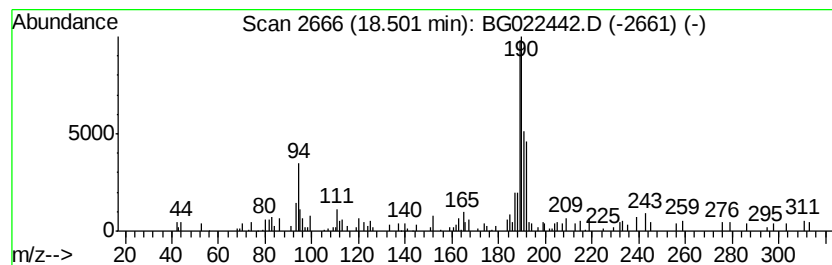
Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 4H-Cyclopenta[def]phenanthrene Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
18.50	2.33 ng	50052	Phenanthrene-d10	17.43	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4H-Cyclopenta[def]phenanthrene	190	C15H10	000203-64-5	70
2	6H-Cyclobuta[ik]phenanthrene	190	C15H10	083469-43-6	58
3	3,5-Xylenol, 2,4-dichloro-, acetate	232	C10H10Cl2O2	099421-62-2	27
4	3H-Indazole-3-carbonitrile, 3-(4...	253	C14H8ClN3	056630-97-8	25
5	.alpha.,.alpha.,.alpha.,6-Tetra...	189	C8H3F4N	133116-83-3	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

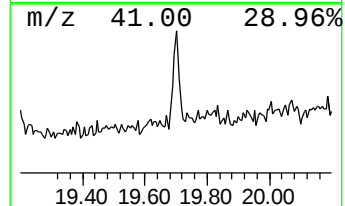
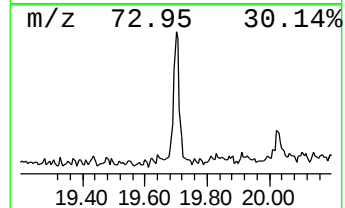
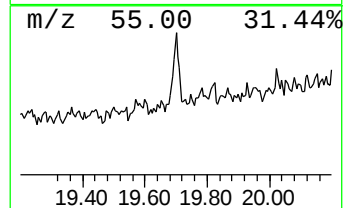
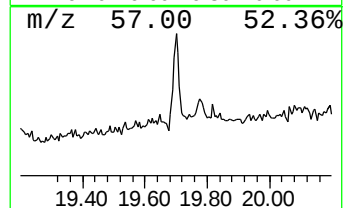
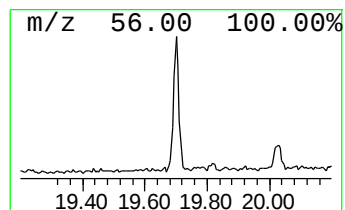
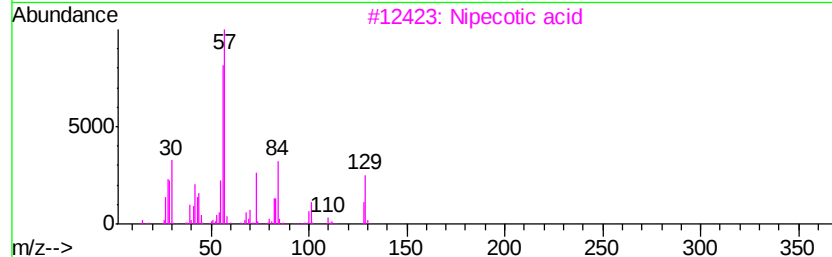
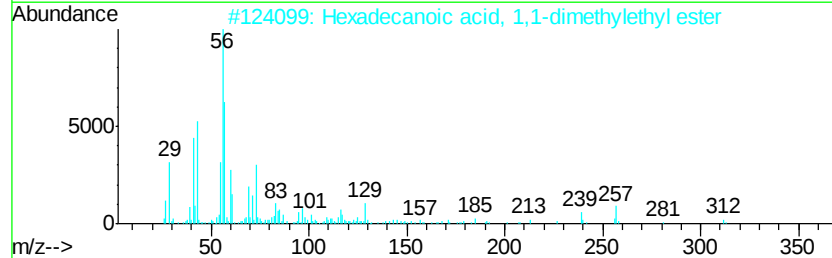
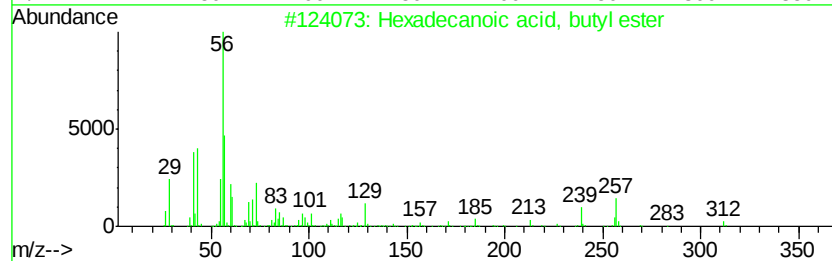
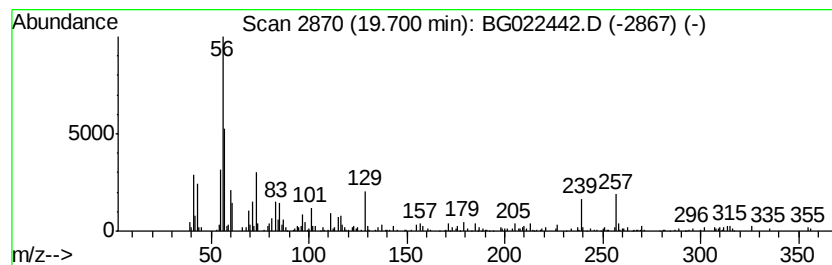
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG060616.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Hexadecanoic acid, butyl ester Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.70	3.45 ng	72974	Chrysene-d12	21.70

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Hexadecanoic acid, butyl ester	312	C20H40O2	000111-06-8	94
2		Hexadecanoic acid, 1,1-dimethyle...	312	C20H40O2	031158-91-5	50
3		Nipecotic acid	129	C6H11NO2	000498-95-3	50
4		Hexadecanoic acid, 2-methylpropyl...	312	C20H40O2	000110-34-9	45
5		Cyclobutane, 1,1-dimethyl-2-octyl-	196	C14H28	062338-30-1	35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG061716\
Data File : BG022442.D
Acq On : 19 Jun 2016 3:18
Operator : UM/SJ
Sample : H3489-01
Misc :
ALS Vial : 51 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S6-B1(0-8)C

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG060616.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
unknown2.87	2.87	220.9	ng	2370760	1	8.05	214622	20.0
unknown5.10	5.10	6.3	ng	67966	1	8.05	214622	20.0
unknown7.58	7.58	124.1	ng	1332160	1	8.05	214622	20.0
Hexanoic acid, 2-...	9.38	2.2	ng	23766	1	8.05	214622	20.0
4H-Cyclopenta[def...	18.50	2.3	ng	50052	4	17.43	429496	20.0
Hexadecanoic acid...	19.70	3.5	ng	72974	5	21.70	423302	20.0