

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016420.D
 Acq On : 15 Apr 2015 13:31
 Operator : TP/IZ
 Sample : G1848-06
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 TE-PMW-2-26

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-BG040615.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	2.759	7	12	21	rBV	381957	630634	14.96%	2.309%
2	2.841	21	26	40	rVB	345409	463468	11.00%	1.697%
3	4.780	350	356	363	rVB	47536	69536	1.65%	0.255%
4	5.256	431	437	447	rVB	516305	751403	17.83%	2.751%
5	5.714	508	515	523	rVB	133350	198119	4.70%	0.725%
6	6.848	702	708	721	rVB	329360	526505	12.49%	1.928%
7	7.201	761	768	778	rBV	1044658	1601079	37.98%	5.862%
8	7.665	837	847	853	rBV	231099	352761	8.37%	1.292%
9	7.982	895	901	909	rVB	902209	1459092	34.62%	5.342%
10	8.822	1037	1044	1056	rVB	766873	1220338	28.95%	4.468%
11	10.450	1313	1321	1329	rBV	332514	544492	12.92%	1.994%
12	12.718	1701	1707	1719	rBV	101436	182676	4.33%	0.669%
13	12.847	1724	1729	1736	rVV2	43130	69537	1.65%	0.255%
14	12.929	1736	1743	1753	rVB	1965807	2810175	66.67%	10.289%
15	13.769	1880	1886	1895	rVB	46766	65077	1.54%	0.238%
16	14.310	1969	1978	1988	rVB2	492968	742599	17.62%	2.719%
17	15.673	2204	2210	2215	rBV	47695	67014	1.59%	0.245%
18	15.796	2225	2231	2242	rBV	1307874	1898304	45.04%	6.950%
19	16.255	2304	2309	2315	rBV3	34356	54492	1.29%	0.200%
20	16.460	2339	2344	2352	rBV4	25037	46390	1.10%	0.170%
21	17.048	2438	2444	2451	rBV2	667216	934979	22.18%	3.423%
22	17.953	2593	2598	2607	rBV	350246	497268	11.80%	1.821%
23	19.116	2788	2796	2800	rBV8	36257	87853	2.08%	0.322%
24	19.234	2812	2816	2827	rBV	236216	333588	7.91%	1.221%
25	19.680	2886	2892	2901	rBV	2830683	3450039	81.85%	12.631%
26	20.479	3026	3028	3033	rVB3	35935	42786	1.02%	0.157%
27	20.867	3090	3094	3098	rBV	977733	1178728	27.96%	4.316%
28	20.914	3098	3102	3105	rVV	3858329	4215158	100.00%	15.433%
29	20.943	3105	3107	3119	rVB	538037	636436	15.10%	2.330%
30	21.149	3138	3142	3145	rBV	201792	229235	5.44%	0.839%
31	21.231	3151	3156	3162	rBV	801322	983772	23.34%	3.602%
32	23.464	3529	3536	3553	rVB	502040	969578	23.00%	3.550%

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Integrator: RTE
Smoothing : ON Filtering: 5
Sampling : 1 Min Area: 3 % of largest Peak
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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-BG040615.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

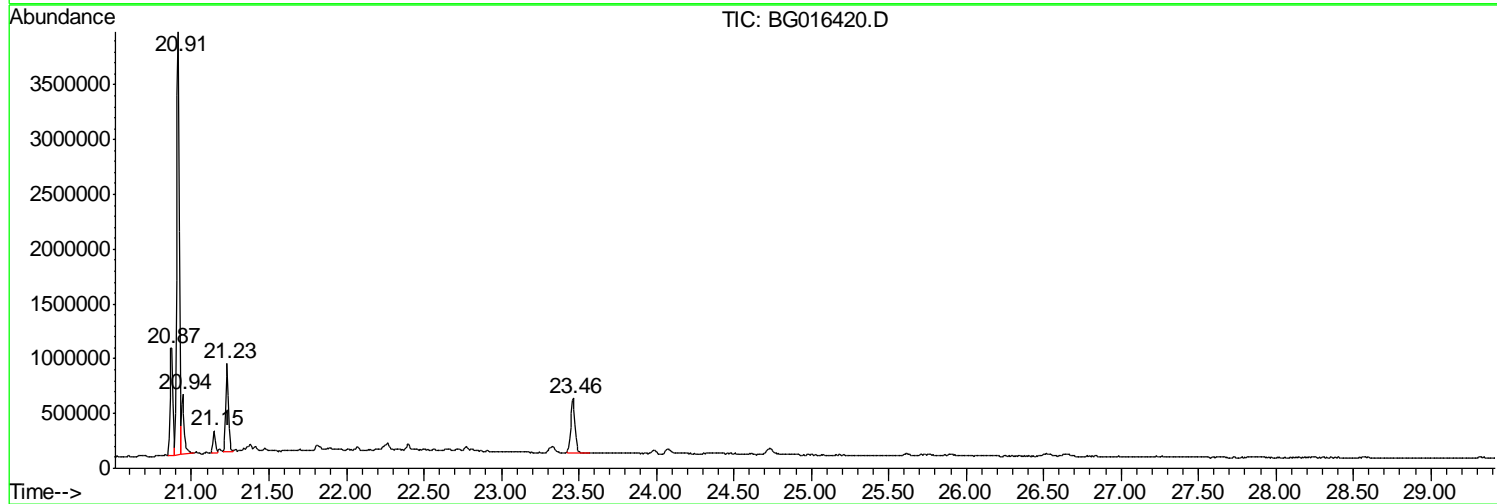
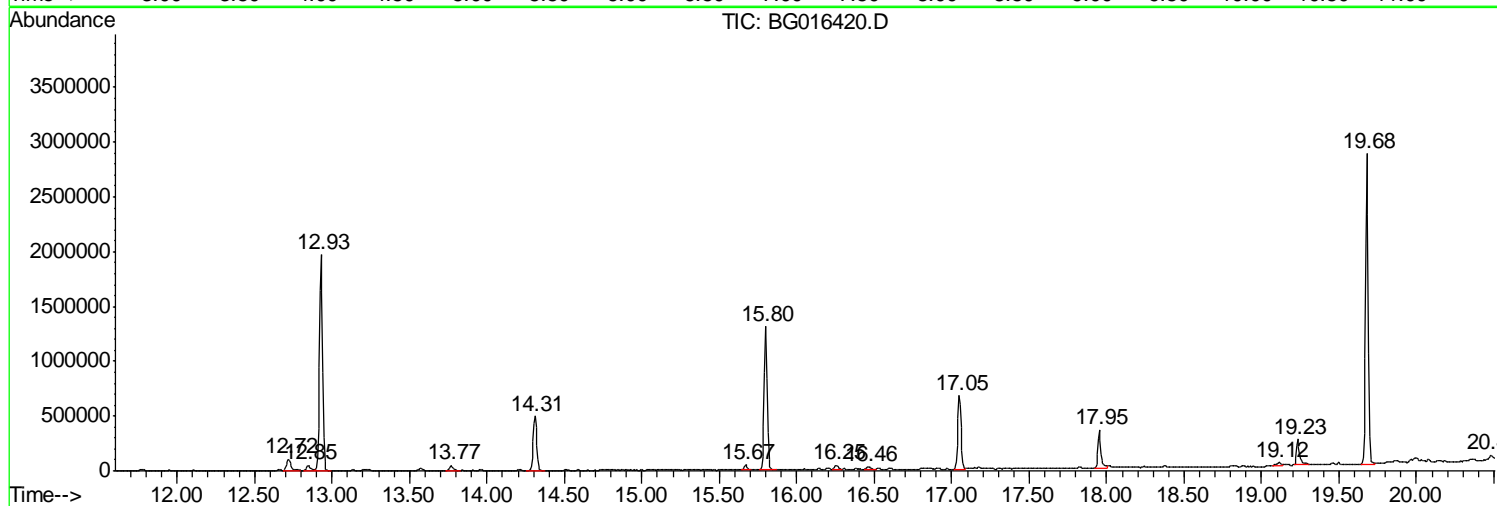
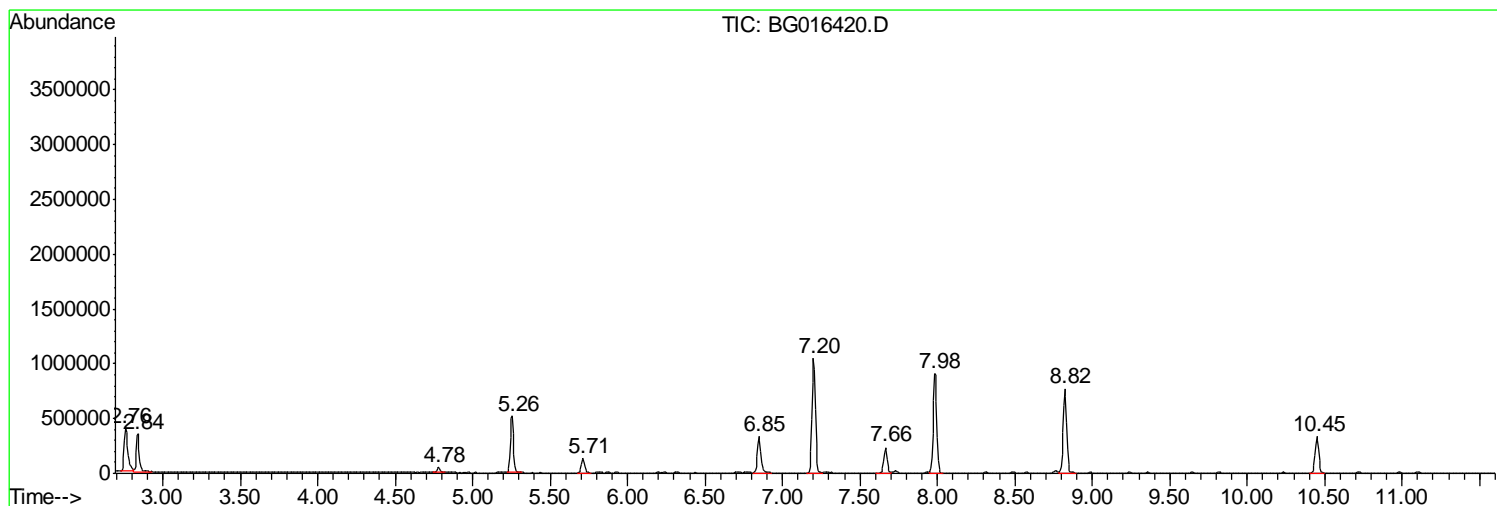
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.M
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P



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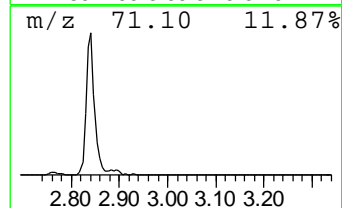
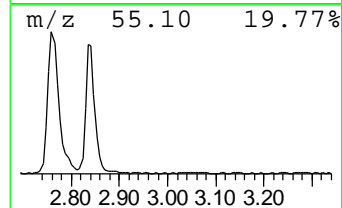
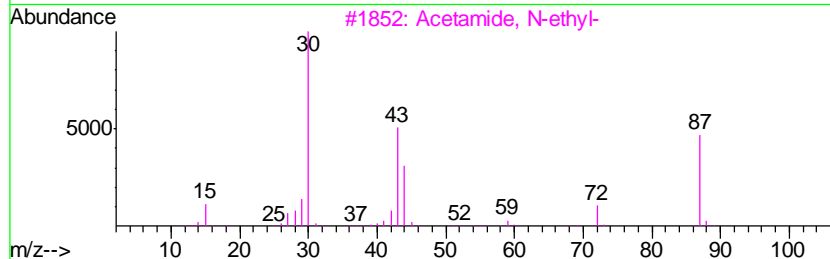
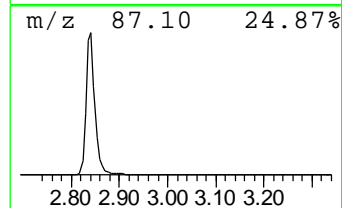
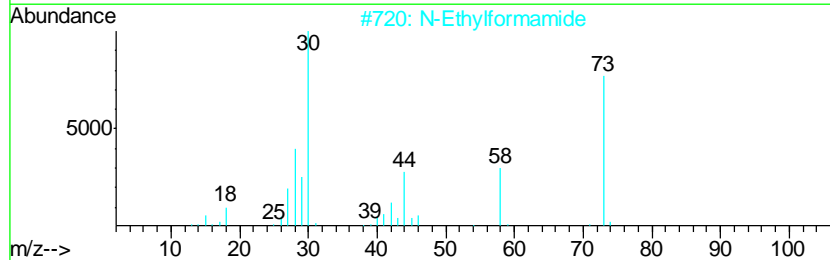
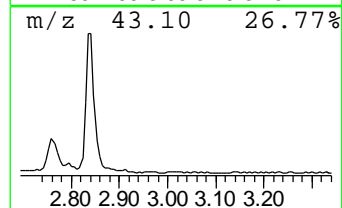
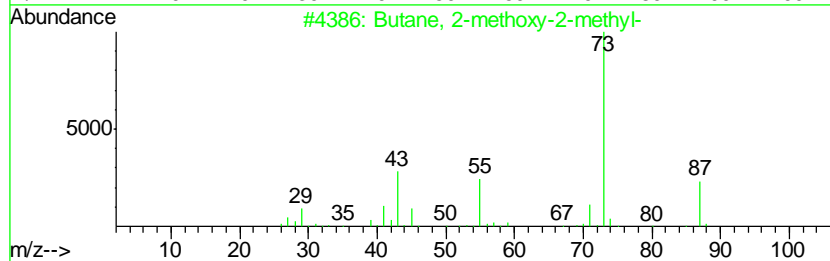
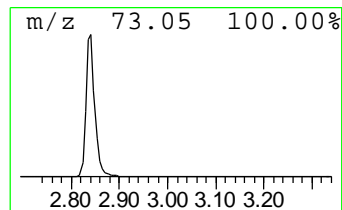
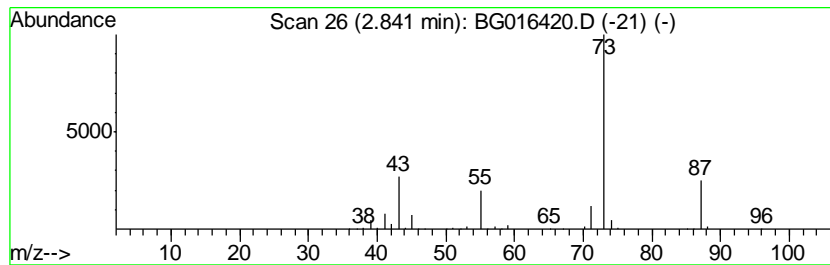
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 2 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.84	26.28 ng	463468	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		N-Ethylformamide	73	C3H7NO	000627-45-2	9
3		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
4		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	9
5		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9



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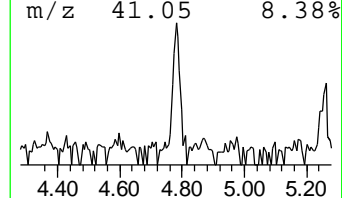
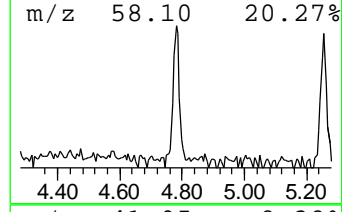
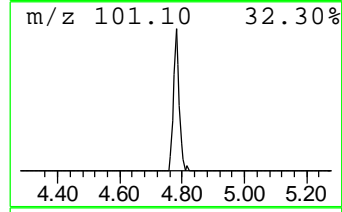
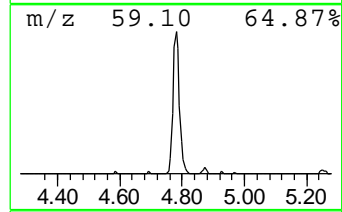
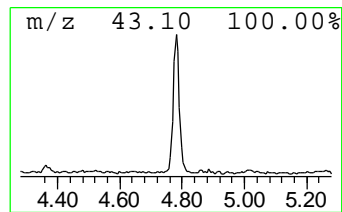
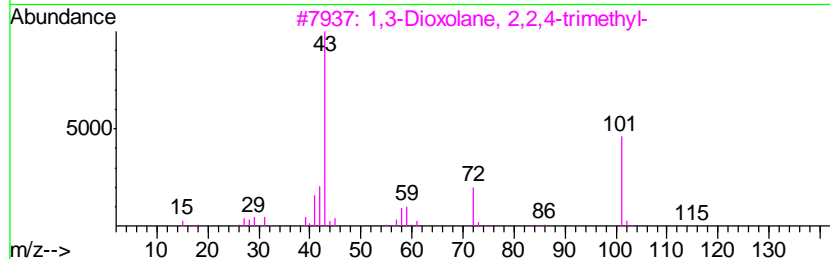
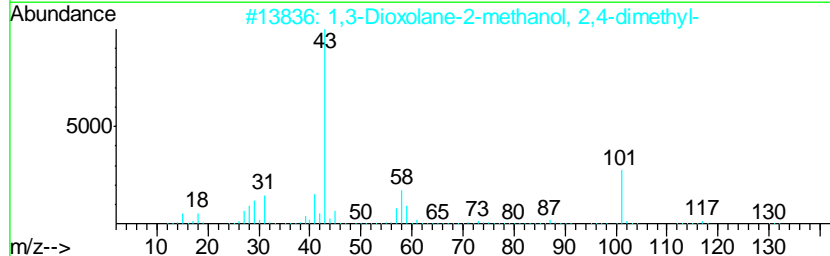
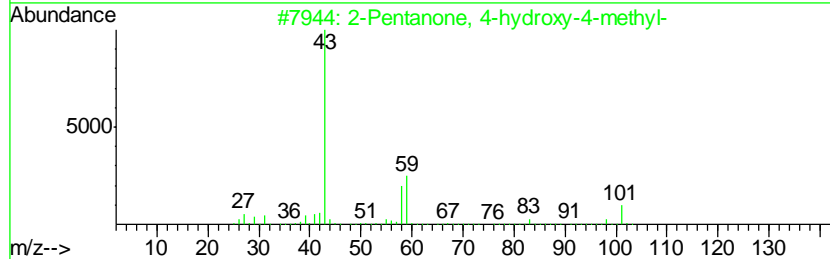
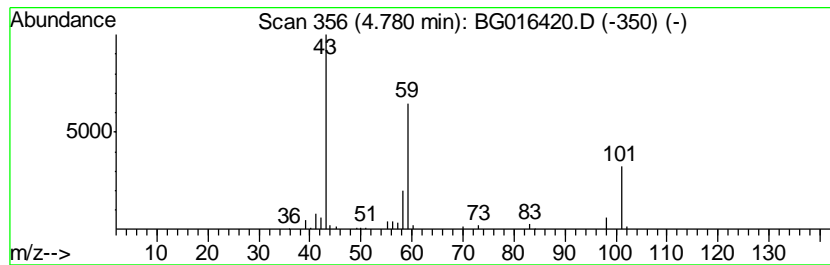
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TIC Library : C:\DATABASE\NIST02.L
 TIC Integration Parameters: LSCINT.P

 Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.78	3.94 ng	69536	1,4-Dichlorobenzene-d4	7.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
2		1,3-Dioxolane-2-methanol, 2,4-di...	132	C6H12O3	053951-43-2	28
3		1,3-Dioxolane, 2,2,4-trimethyl-	116	C6H12O2	001193-11-9	25
4		4-Hydroxy-3-hexanone	116	C6H12O2	004984-85-4	25
5		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	23



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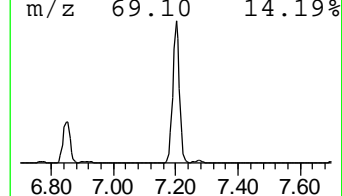
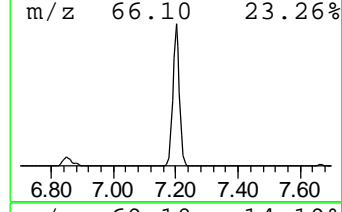
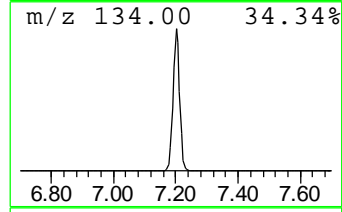
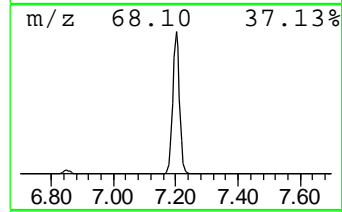
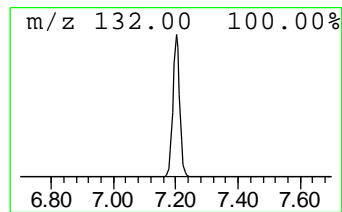
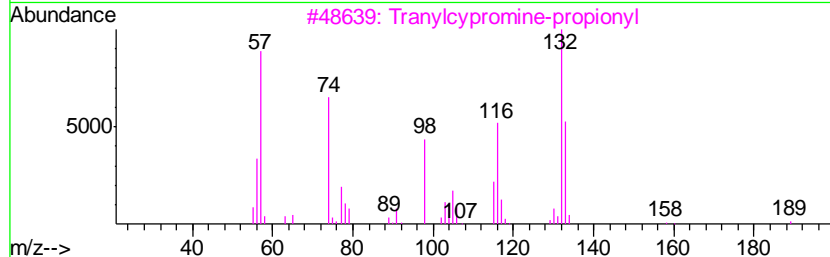
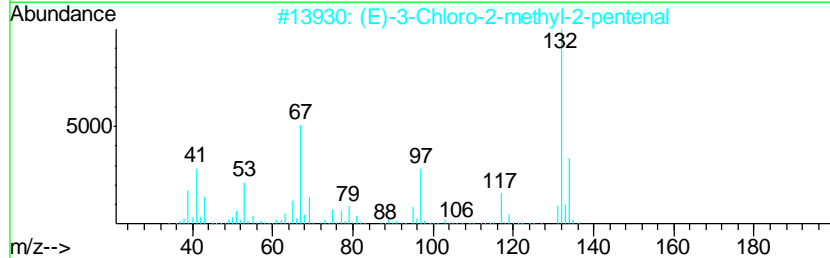
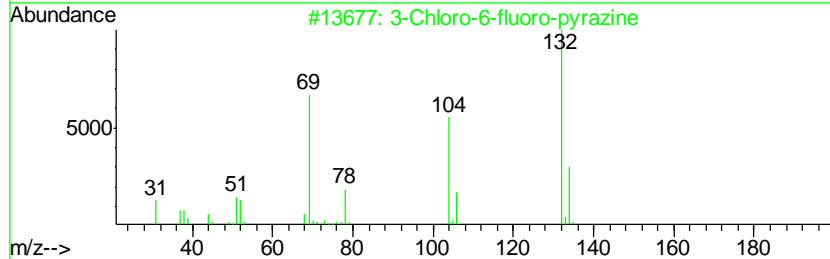
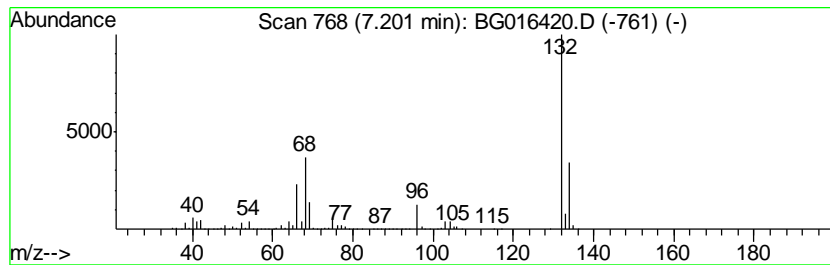
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 TIC Integration Parameters: LSCINT.P

 Peak Number 5 unknown7.20 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.20	90.77 ng	1601080	1,4-Dichlorobenzene-d4	7.66

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	35
3		Tranylcyromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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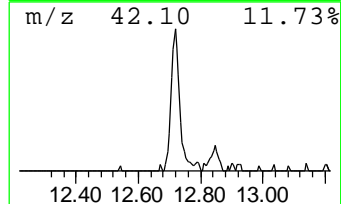
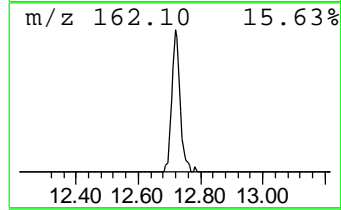
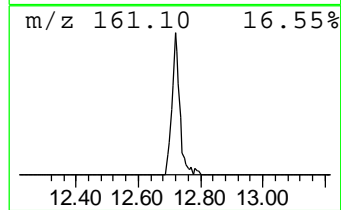
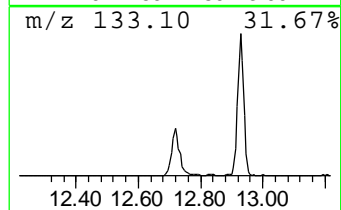
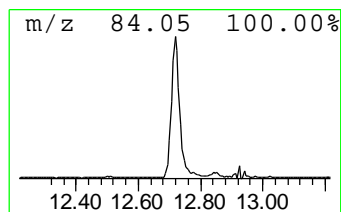
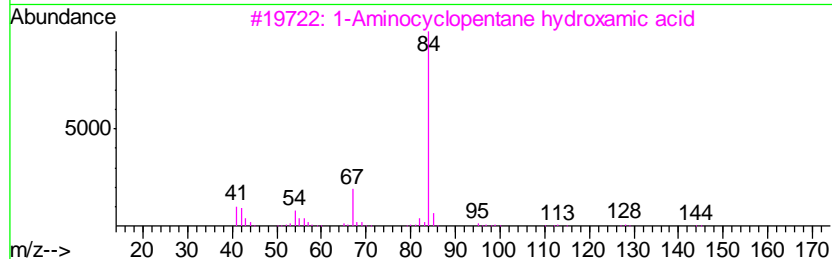
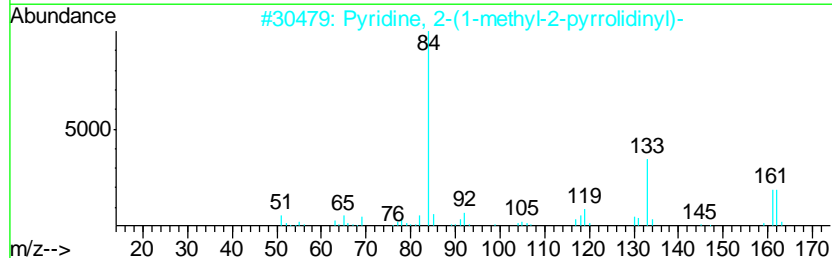
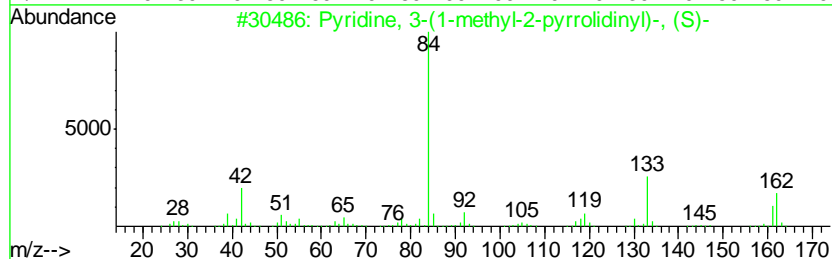
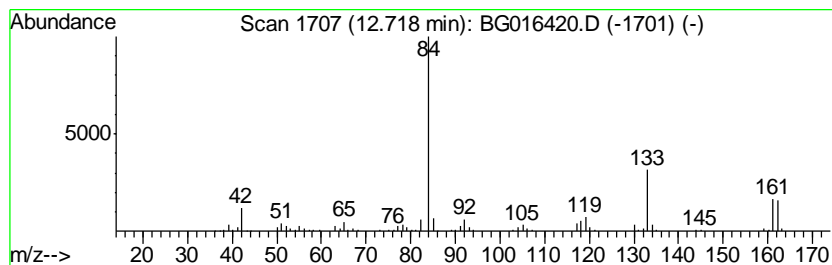
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 Peak Number 7 Pyridine, 3-(1-methyl-2-pyr... Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.72	4.92 ng	182676	Acenaphthene-d10	14.31

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pyridine, 3-(1-methyl-2-pyrrolid...	162	C10H14N2	000054-11-5	95
2		Pyridine, 2-(1-methyl-2-pyrrolid...	162	C10H14N2	023950-04-1	78
3		1-Aminocyclopentane hydroxamic acid	144	C6H12N2O2	062104-33-0	43
4		Rolicyprine	244	C14H16N2O2	002829-19-8	40
5		Pyridine-D5-	84	C5D5N	007291-22-7	37



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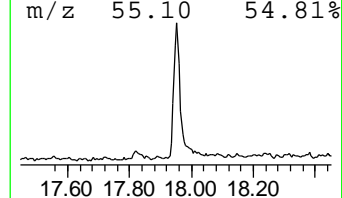
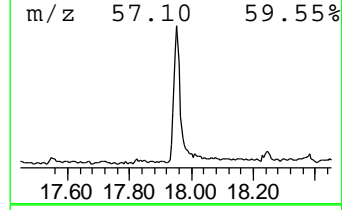
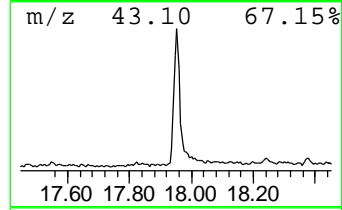
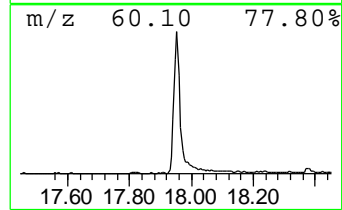
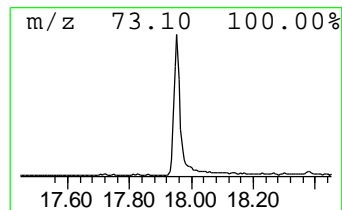
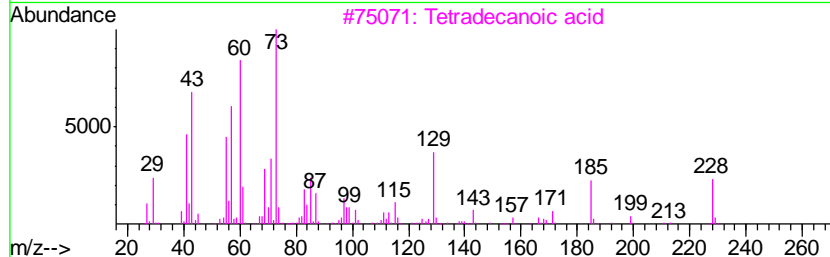
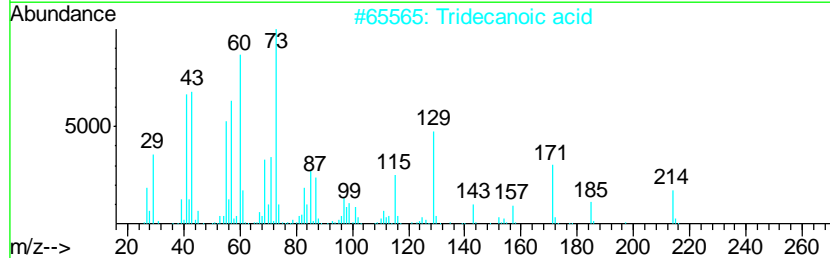
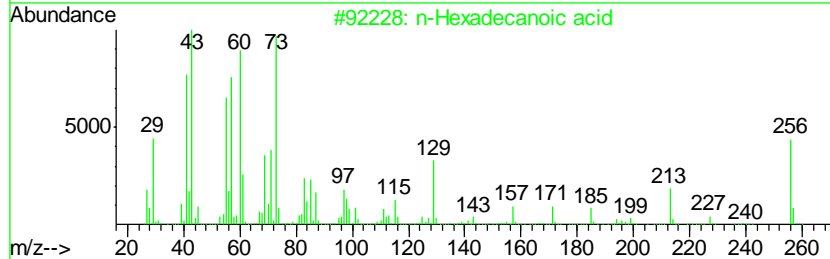
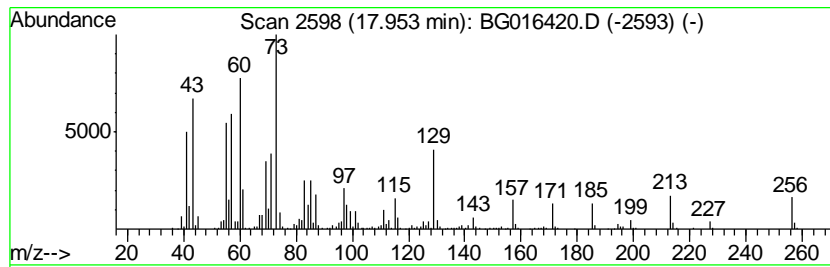
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 Peak Number 8 n-Hexadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
17.95	10.64 ng	497268	Phenanthrene-d10	17.05

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	99
2		Tridecanoic acid	214	C13H26O2	000638-53-9	94
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	91
4		n-Decanoic acid	172	C10H20O2	000334-48-5	52
5		.alpha.-D-Glucopyranoside, .alph...	342	C12H22O11	000099-20-7	35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016420.D
 Acq On : 15 Apr 2015 13:31
 Operator : TP/IZ
 Sample : G1848-06
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleID :
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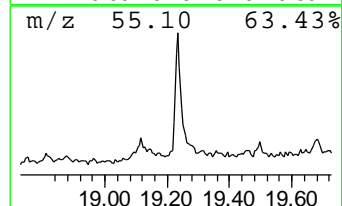
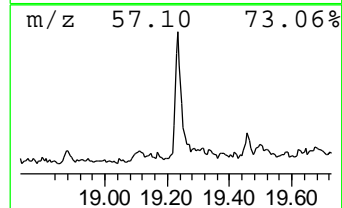
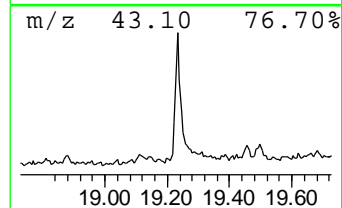
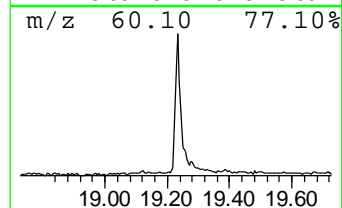
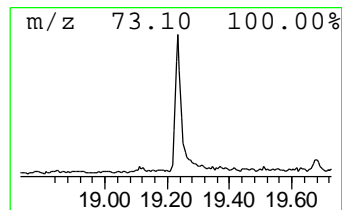
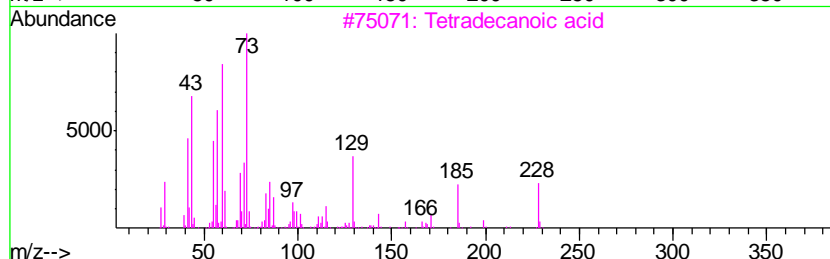
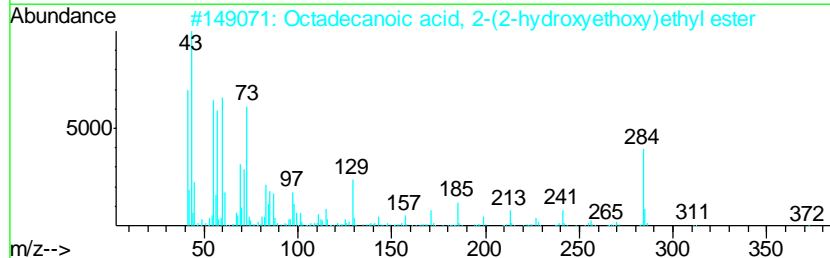
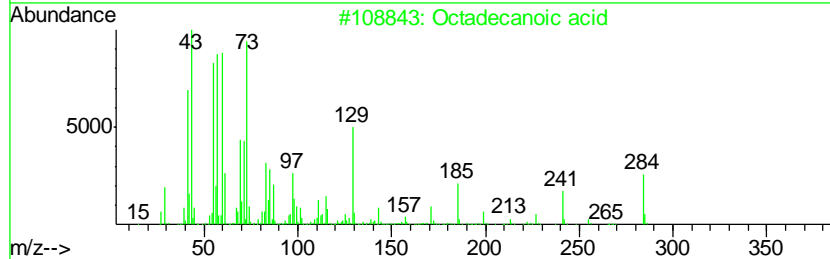
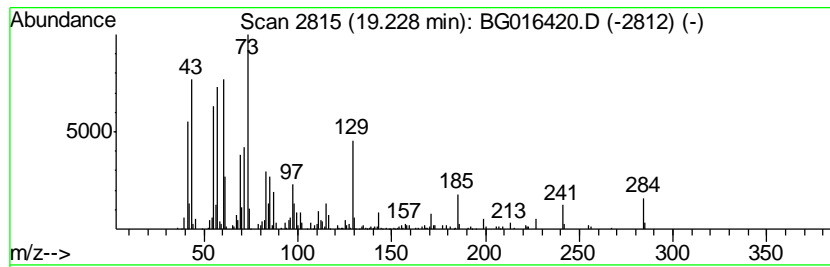
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 9 Octadecanoic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.23	6.78 ng	333588	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2		Octadecanoic acid, 2-(2-hydroxye...	372	C22H44O4	000106-11-6	91
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	83
4		Pentadecanoic acid	242	C15H30O2	001002-84-2	72
5		n-Decanoic acid	172	C10H20O2	000334-48-5	62



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016420.D
 Acq On : 15 Apr 2015 13:31
 Operator : TP/IZ
 Sample : G1848-06
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
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 ClientSampleID :
 TE-PMW-2-26

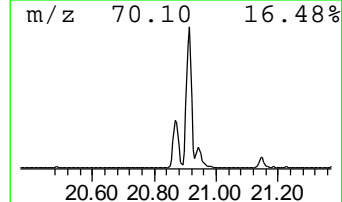
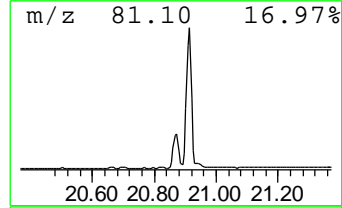
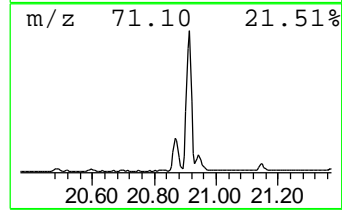
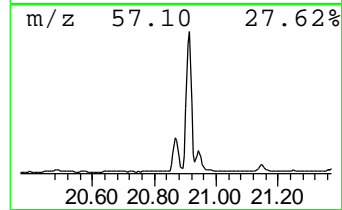
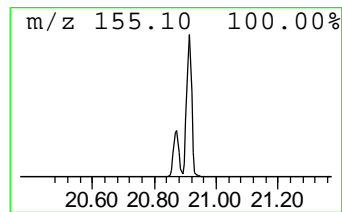
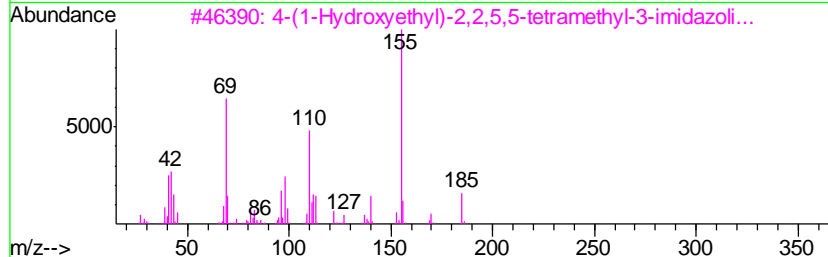
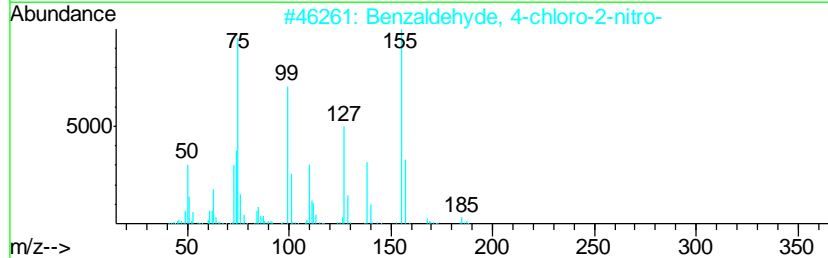
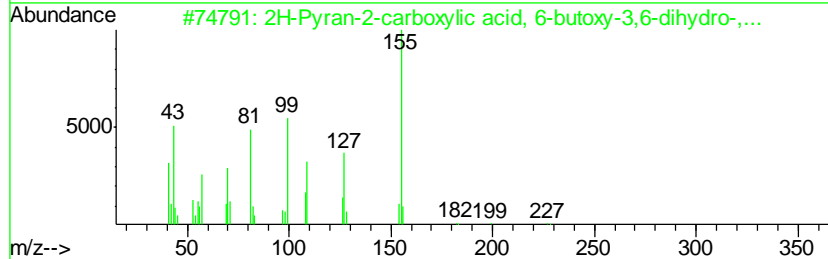
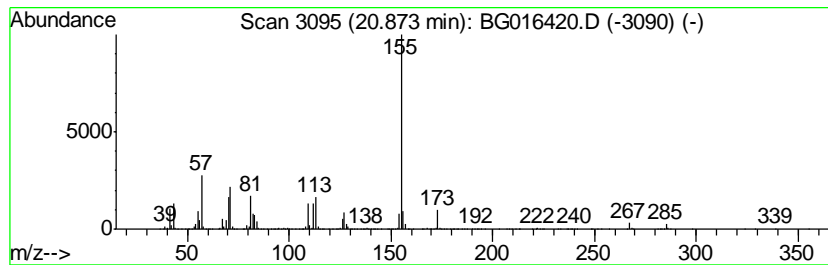
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 10 2H-Pyran-2-carboxylic acid,... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.87	23.96 ng	1178730	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2H-Pyran-2-carboxylic acid, 6-bu...	228	C12H20O4	026457-97-6	50
2		Benzaldehyde, 4-chloro-2-nitro-	185	C7H4ClNO3	005551-11-1	43
3		4-(1-Hydroxyethyl)-2,2,5,5-tetra...	185	C9H17N2O2	066250-75-7	42
4		1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	40
5		Pyridine, 4-phenyl-	155	C11H9N	000939-23-1	38



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016420.D
 Acq On : 15 Apr 2015 13:31
 Operator : TP/IZ
 Sample : G1848-06
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleID :
 TE-PMW-2-26

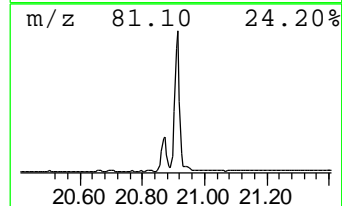
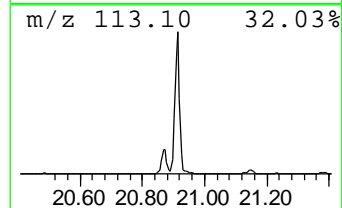
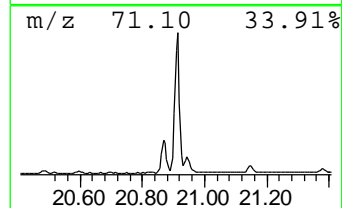
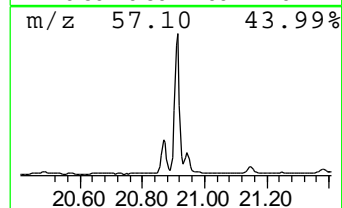
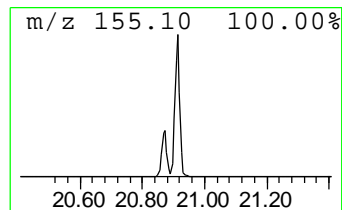
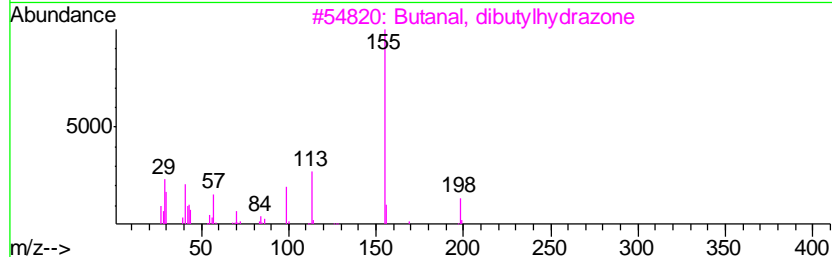
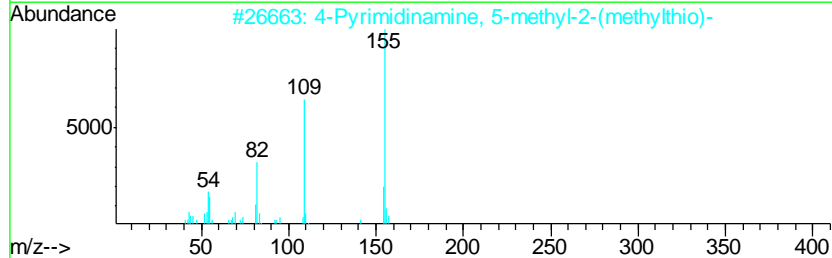
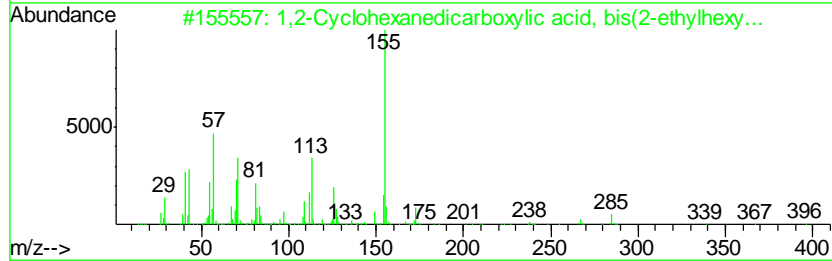
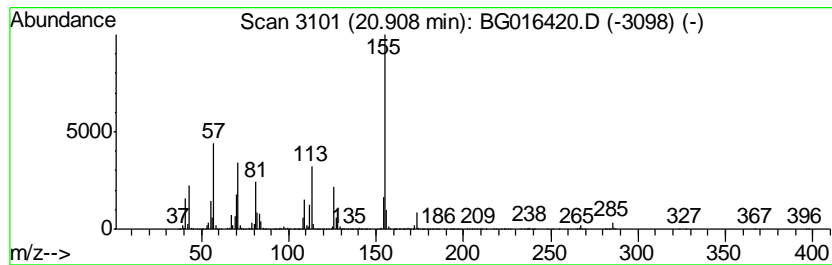
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 1,2-Cyclohexanedicarboxylic... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.91	85.69 ng	4215160	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	58
2		4-Pyrimidinamine, 5-methyl-2-(me...	155	C6H9N3S	054308-64-4	43
3		Butanal, dibutylhydrazone	198	C12H26N2	067660-51-9	43
4		2,3,4-Trimethylpentan-2-ol decan...	284	C18H36O2	1000130-74-2	43
5		Benzaldehyde, 4-chloro-2-nitro-	185	C7H4ClNO3	005551-11-1	35



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016420.D
 Acq On : 15 Apr 2015 13:31
 Operator : TP/IZ
 Sample : G1848-06
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
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 ClientSampleID :
 TE-PMW-2-26

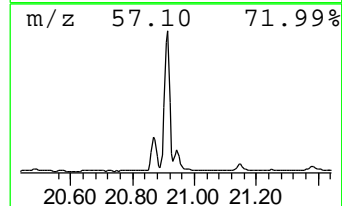
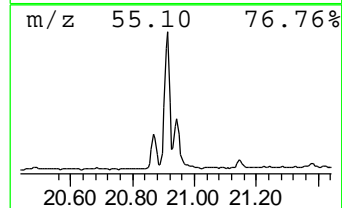
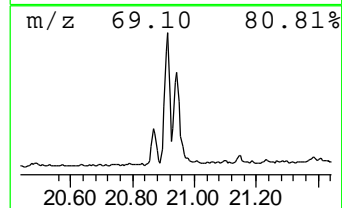
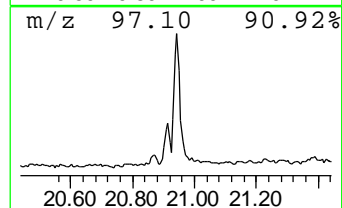
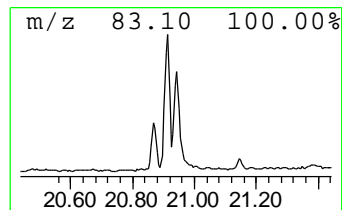
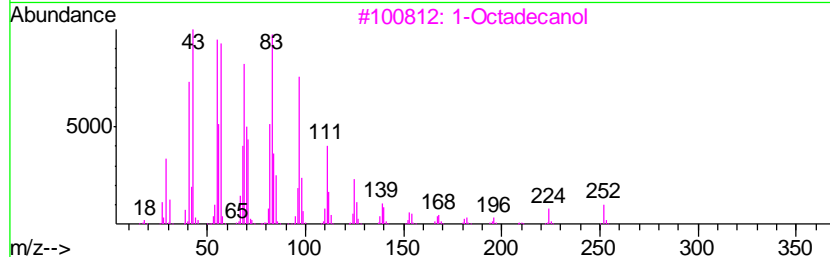
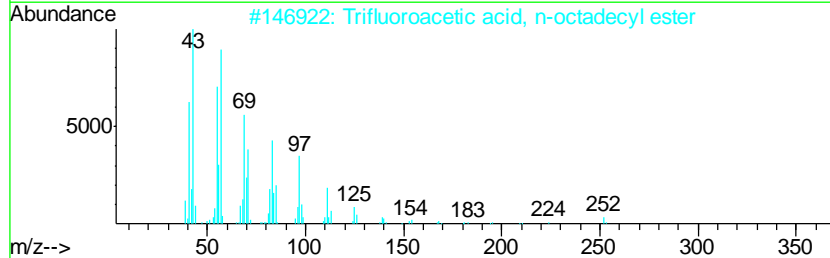
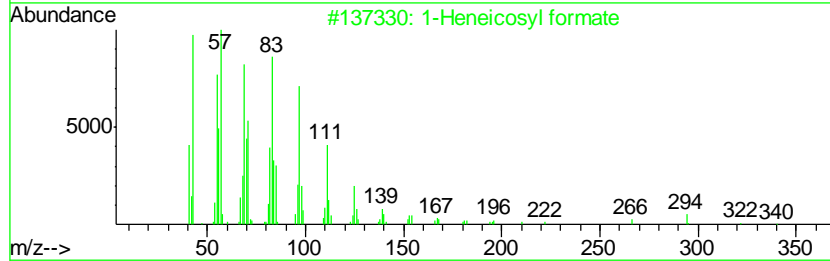
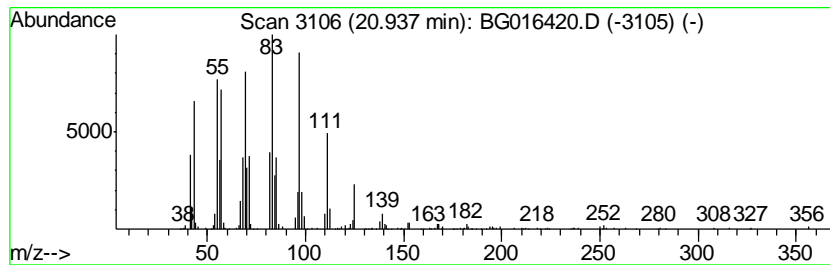
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 12 1-Heneicosyl formate Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
20.94	12.94 ng	636436	Chrysene-d12	21.23

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Heneicosyl formate	340	C22H44O2	077899-03-7	91
2		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91
3		1-Octadecanol	270	C18H38O	000112-92-5	91
4		Dichloroacetic acid, heptadecyl ...	366	C19H36Cl2O2	1000282-98-2	90
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	87



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG041515\
 Data File : BG016420.D
 Acq On : 15 Apr 2015 13:31
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 Sample : G1848-06
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG040615.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
Butane, 2-methoxy...	2.84	26.3	ng	463468	1	7.66	352761	20.0
2-Pentanone, 4-hy...	4.78	3.9	ng	69536	1	7.66	352761	20.0
unknown7.20	7.20	90.8	ng	1601080	1	7.66	352761	20.0
Pyridine, 3-(1-me...	12.72	4.9	ng	182676	3	14.31	742599	20.0
n-Hexadecanoic acid	17.95	10.6	ng	497268	4	17.05	934979	20.0
Octadecanoic acid	19.23	6.8	ng	333588	5	21.23	983772	20.0
2H-Pyran-2-carbox...	20.87	24.0	ng	1178730	5	21.23	983772	20.0
1,2-Cyclohexanedi...	20.91	85.7	ng	4215160	5	21.23	983772	20.0
1-Heneicosyl formate	20.94	12.9	ng	636436	5	21.23	983772	20.0