

Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
 Data File : BG016883.D
 Acq On : 6 May 2015 3:13
 Operator : TP/IZ
 Sample : G2114-17
 Misc :
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 GRID-6(6-12)

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-BG050515.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	2.790	13	17	26	rVB	532529	643461	18.93%	2.504%
2	2.925	35	40	50	rBV	175865	327115	9.62%	1.273%
3	3.002	50	53	58	rVV	167351	223910	6.59%	0.871%
4	3.049	59	61	66	rVB5	33257	39101	1.15%	0.152%
5	4.330	274	279	284	rBV	112487	156026	4.59%	0.607%
6	4.923	375	380	386	rBV	304803	413333	12.16%	1.609%
7	5.381	451	458	466	rBV	992148	1463932	43.07%	5.698%
8	5.540	480	485	490	rBV	23375	38307	1.13%	0.149%
9	6.327	614	619	625	rBV2	21622	39292	1.16%	0.153%
10	6.968	721	728	740	rVB	1094308	1722761	50.69%	6.705%
11	7.332	783	790	799	rBV	1009019	1598282	47.02%	6.221%
12	7.802	863	870	878	rBV	328562	518756	15.26%	2.019%
13	8.125	918	925	933	rBV	649483	1059090	31.16%	4.122%
14	8.959	1059	1067	1074	rVB	615307	1010750	29.74%	3.934%
15	10.593	1339	1345	1353	rBV	449671	751172	22.10%	2.924%
16	11.909	1564	1569	1575	rBV2	35320	59073	1.74%	0.230%
17	12.802	1713	1721	1727	rVB	47989	75714	2.23%	0.295%
18	13.066	1758	1766	1772	rVB	1508469	2257479	66.42%	8.786%
19	13.895	1902	1907	1913	rVB	71512	100447	2.96%	0.391%
20	14.441	1993	2000	2008	rBV2	703571	1077368	31.70%	4.193%
21	15.798	2223	2231	2238	rBV	143705	190911	5.62%	0.743%
22	15.928	2247	2253	2259	rBV	1310558	1860356	54.73%	7.241%
23	17.185	2461	2467	2473	rBV	972714	1367168	40.22%	5.321%
24	17.955	2594	2598	2604	rBV6	20943	34661	1.02%	0.135%
25	18.084	2615	2620	2631	rBV	267431	412208	12.13%	1.604%
26	19.241	2810	2817	2826	rBV	106467	183926	5.41%	0.716%
27	19.365	2835	2838	2846	rBV2	135791	202053	5.94%	0.786%
28	19.606	2875	2879	2887	rVB3	78334	159746	4.70%	0.622%
29	19.811	2908	2914	2922	rVB	2765860	3398858	100.00%	13.229%
30	20.505	3028	3032	3038	rBV3	62085	103825	3.05%	0.404%
31	21.080	3126	3130	3137	rBV	251349	311850	9.18%	1.214%
32	21.286	3161	3165	3168	rBV	41460	47454	1.40%	0.185%
33	21.363	3171	3178	3182	rVV	1231537	1533499	45.12%	5.969%
34	21.398	3182	3184	3190	rVB	55602	69072	2.03%	0.269%

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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-BG050515.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	22.179	3314	3317	3321	rVB	47332	60978	1.79%	0.237%
36	22.585	3382	3386	3392	rVB	130020	181080	5.33%	0.705%
37	22.967	3446	3451	3456	rBV2	79270	174542	5.14%	0.679%
38	23.572	3548	3554	3563	rVB3	53439	116963	3.44%	0.455%
39	23.666	3563	3570	3582	rVB	676690	1393965	41.01%	5.426%
40	24.347	3681	3686	3692	rVB9	27290	53689	1.58%	0.209%
41	26.022	3965	3971	3981	rVB6	57422	179823	5.29%	0.700%
42	26.750	4087	4095	4102	rVB6	26278	80748	2.38%	0.314%

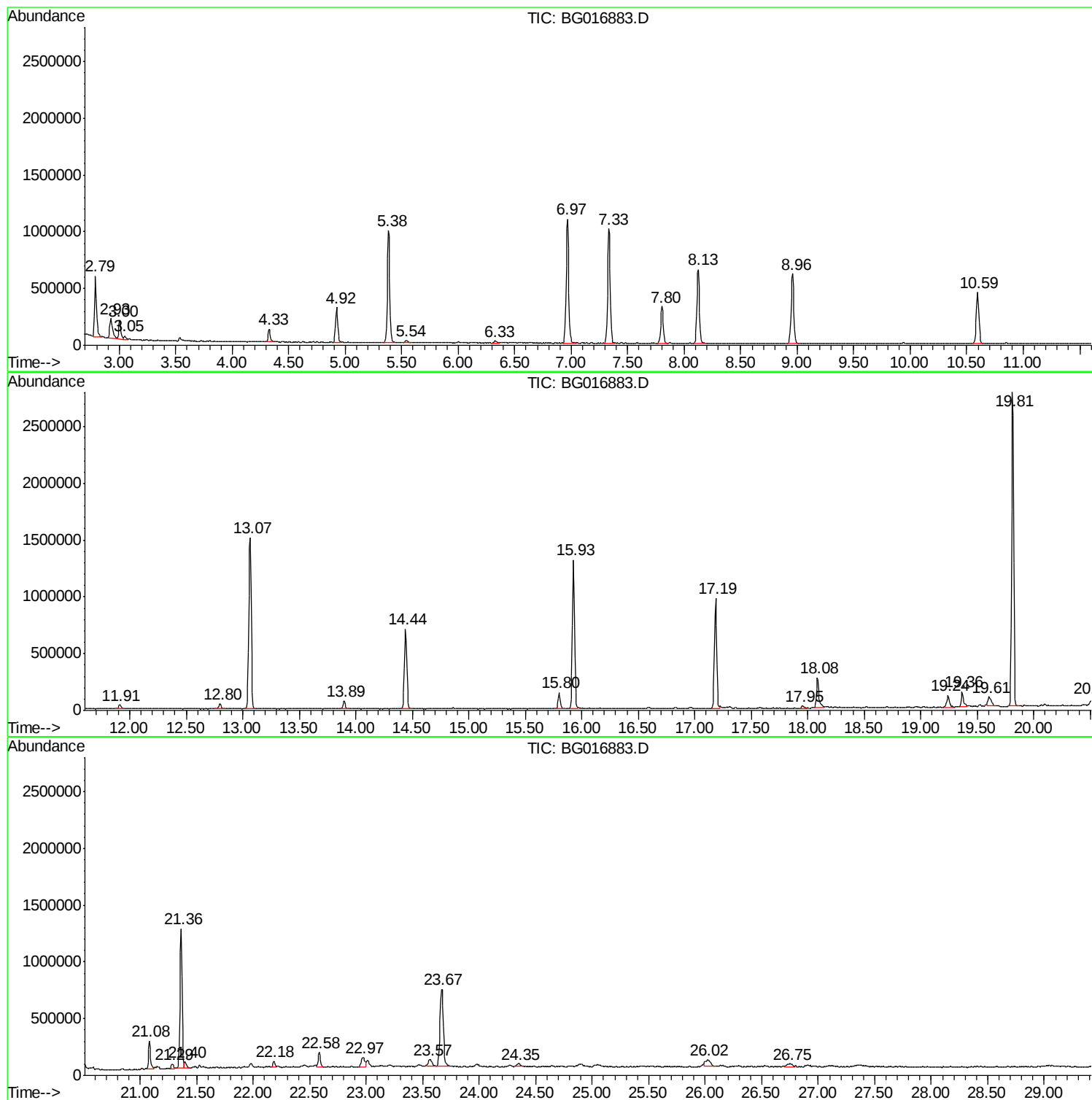
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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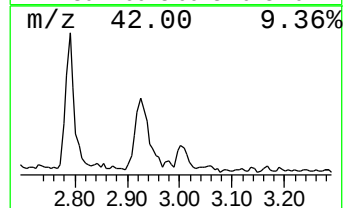
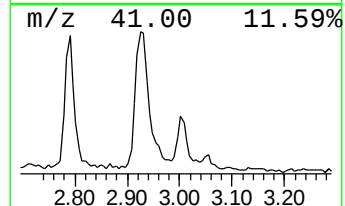
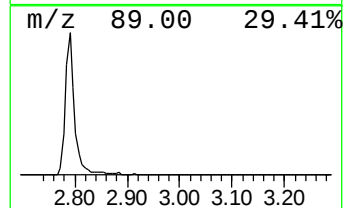
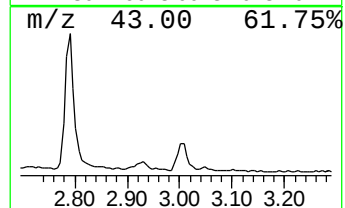
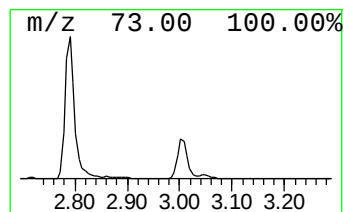
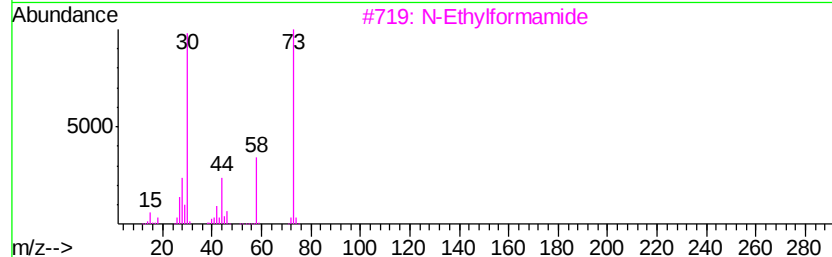
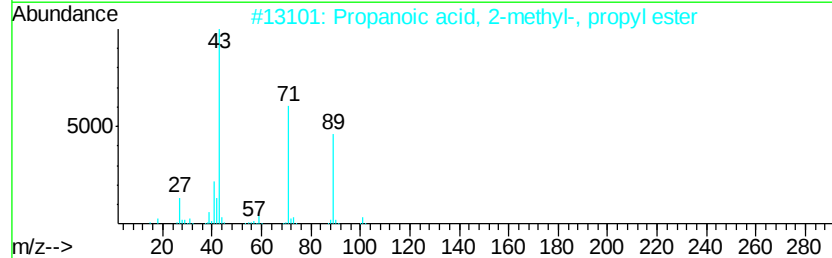
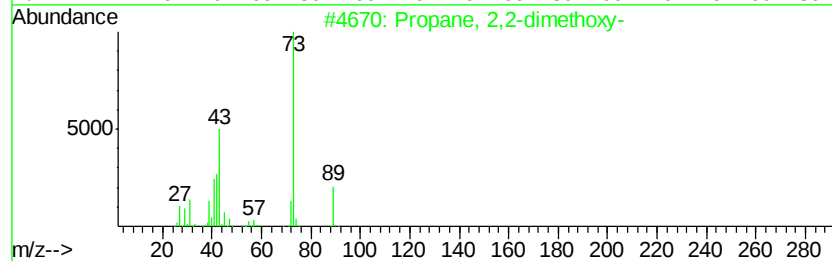
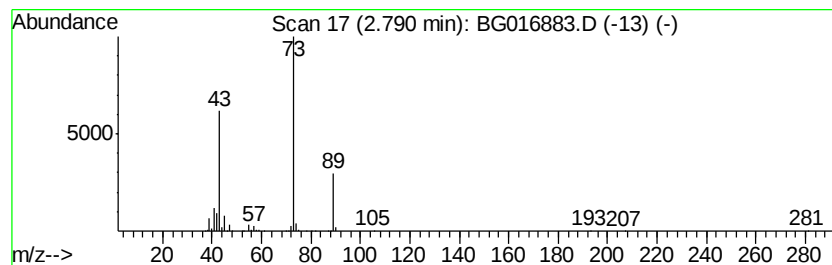
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown2.79 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.79	24.81 ng	643461	1,4-Dichlorobenzene-d4	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	28
3		N-Ethylformamide	73	C3H7NO	000627-45-2	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		Propanoic acid, 2-methyl-, penty...	158	C9H18O2	002445-72-9	9



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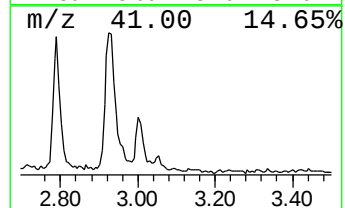
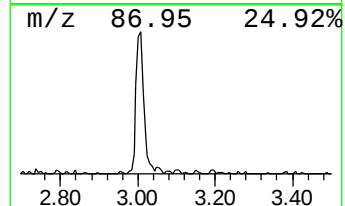
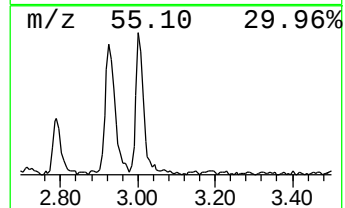
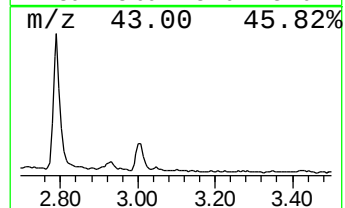
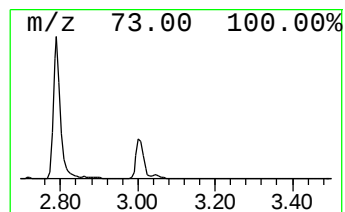
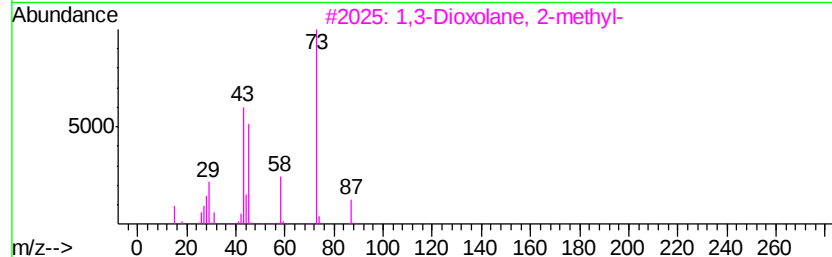
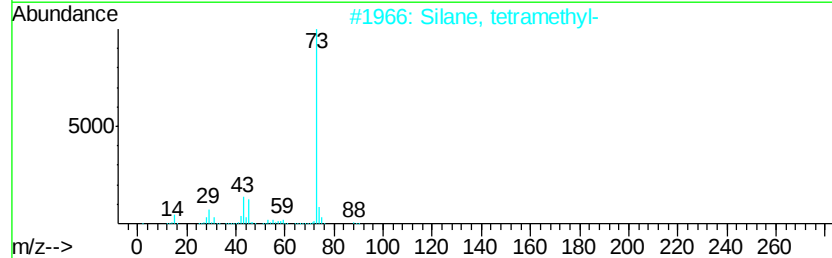
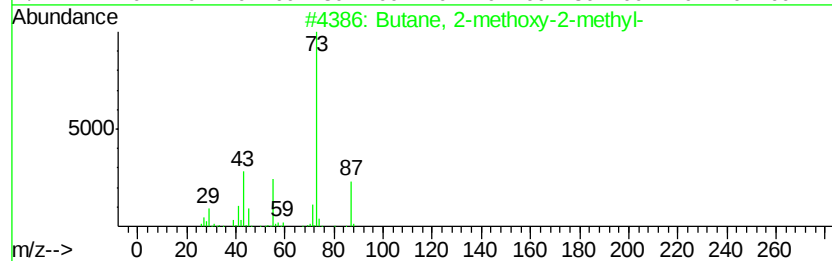
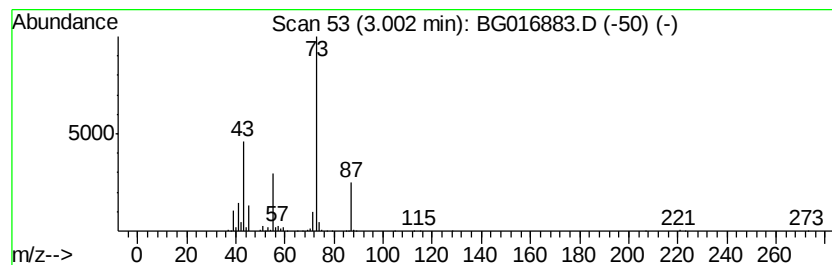
Instrument :
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
3.00	8.63 ng	223910	1,4-Dichlorobenzene-d4	7.80	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2	Silane, tetramethyl-	88	C4H12Si	000075-76-3	35
3	1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	25
4	1-Propene-1-thiol	74	C3H6S	000925-89-3	9
5	2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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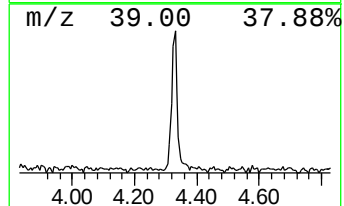
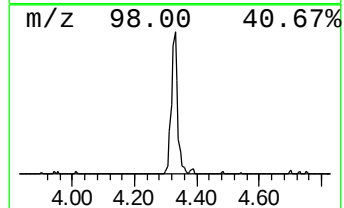
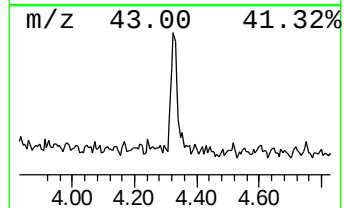
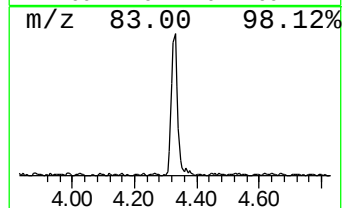
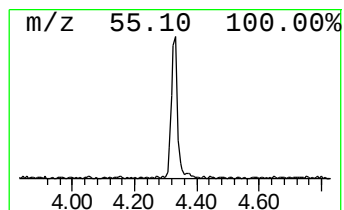
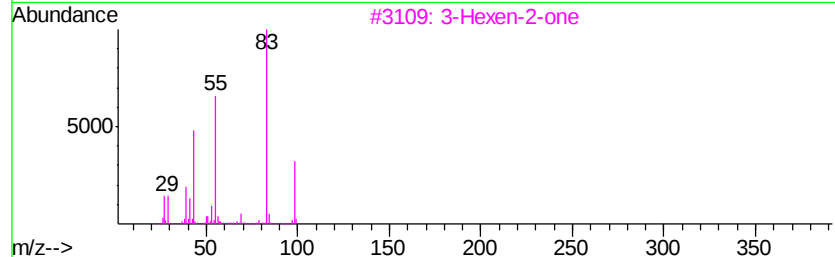
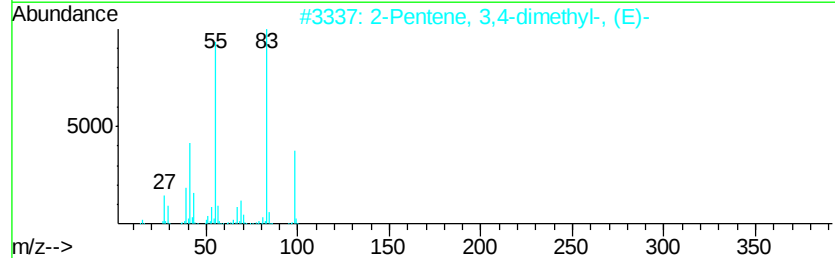
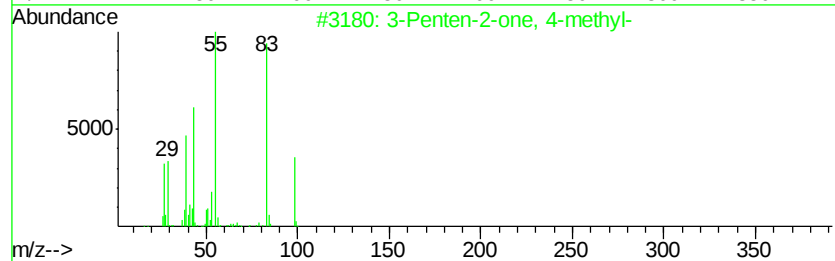
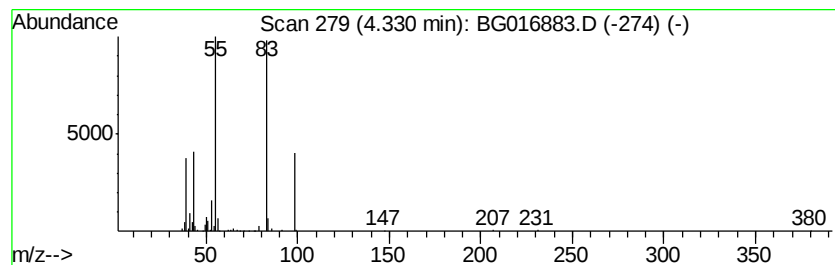
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 3-Penten-2-one, 4-methyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.33	6.02 ng	156026	1,4-Dichlorobenzene-d4	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2		2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	80
3		3-Hexen-2-one	98	C6H10O	000763-93-9	80
4		2-Pentene, 4,4-dimethyl-, (Z)-	98	C7H14	000762-63-0	78
5		2-Pentene, 2,3-dimethyl-	98	C7H14	010574-37-5	78



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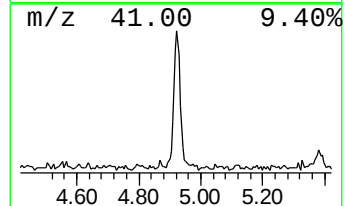
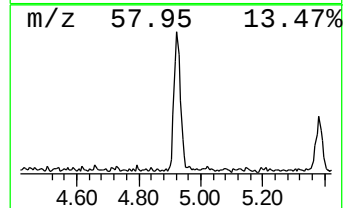
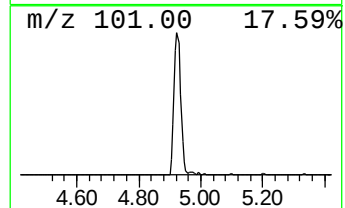
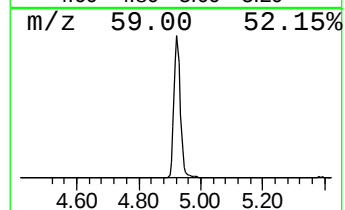
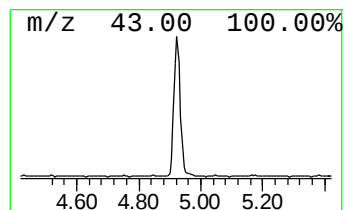
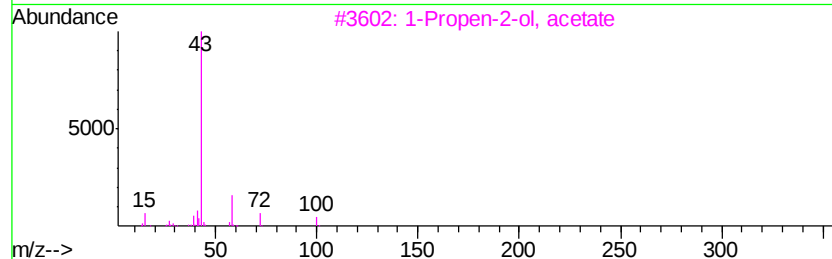
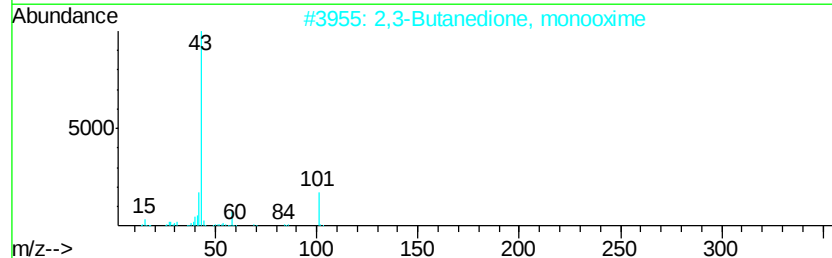
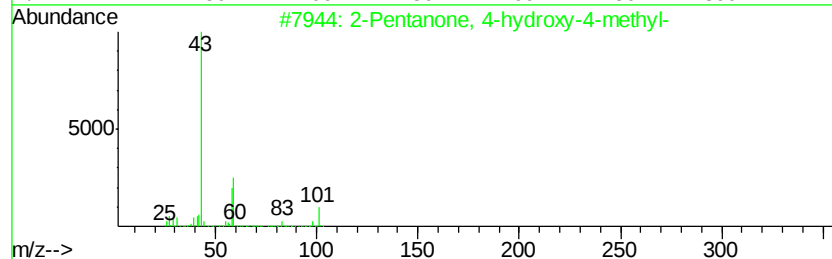
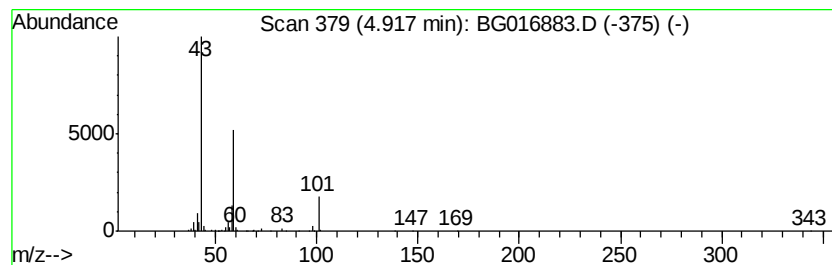
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	15.94 ng	413333	1,4-Dichlorobenzene-d4	7.80

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64		
2	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16		
3	1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10		
4	Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	10		
5	2-Butanol, 1-methoxy-	104	C5H12O2	053778-73-7	9		



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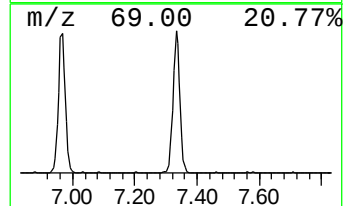
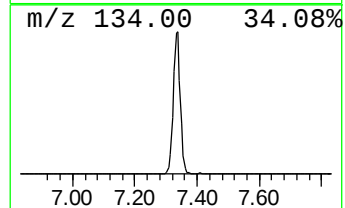
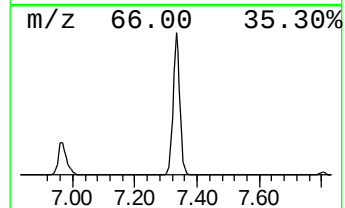
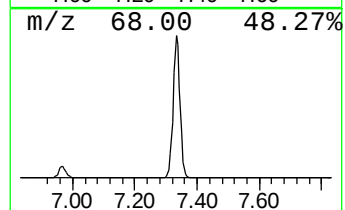
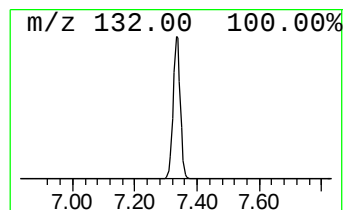
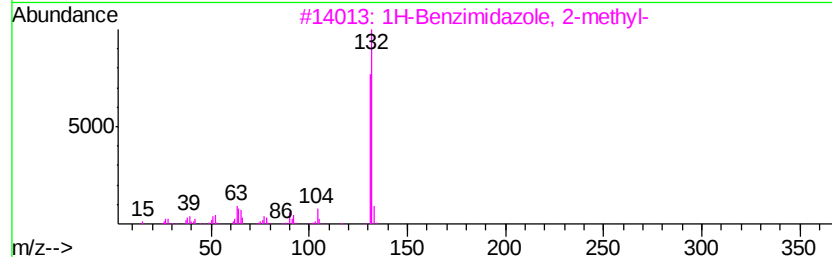
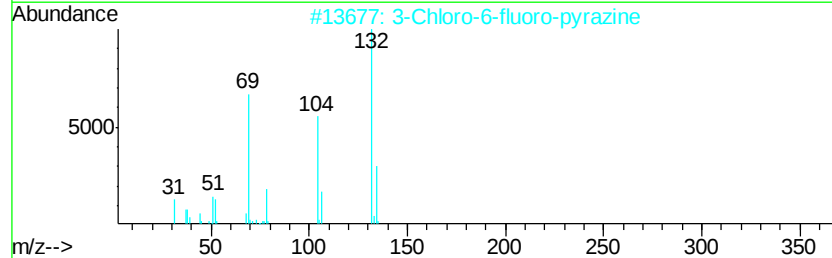
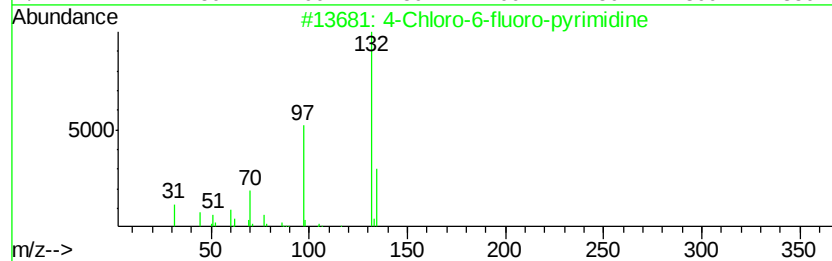
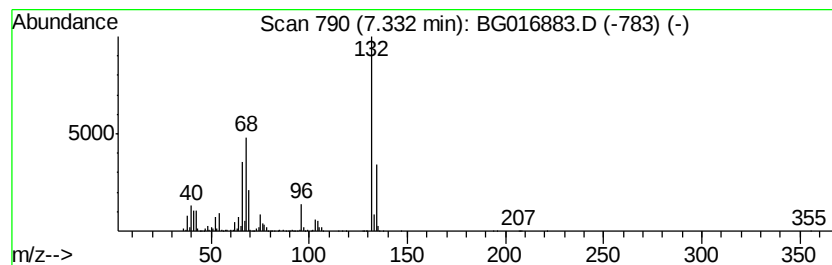
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 unknown7.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	61.62 ng	1598280	1,4-Dichlorobenzene-d4	7.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
3		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	12



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016883.D
Acq On : 6 May 2015 3:13
Operator : TP/IZ
Sample : G2114-17
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
GRID-6(6-12)

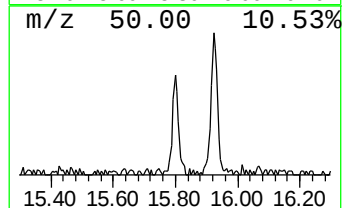
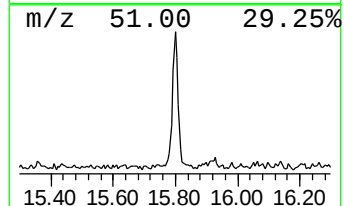
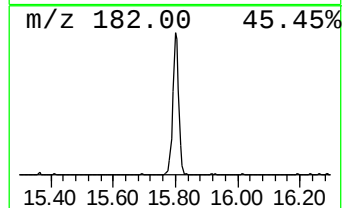
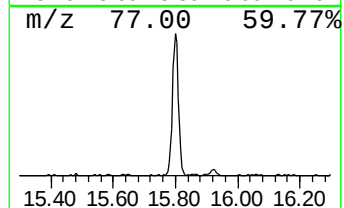
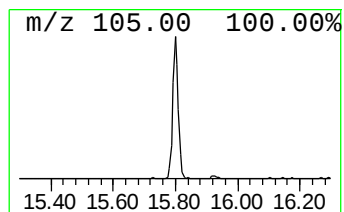
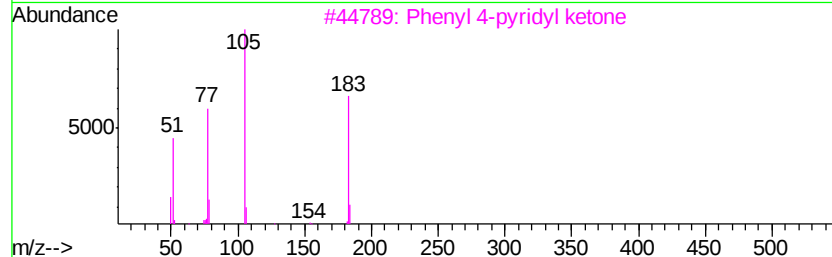
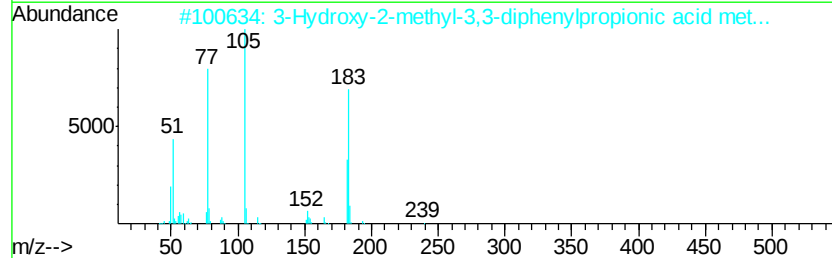
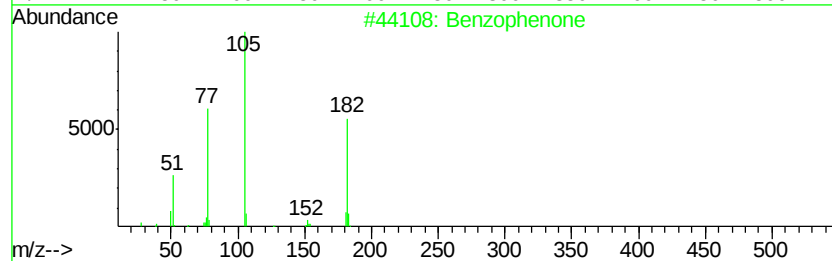
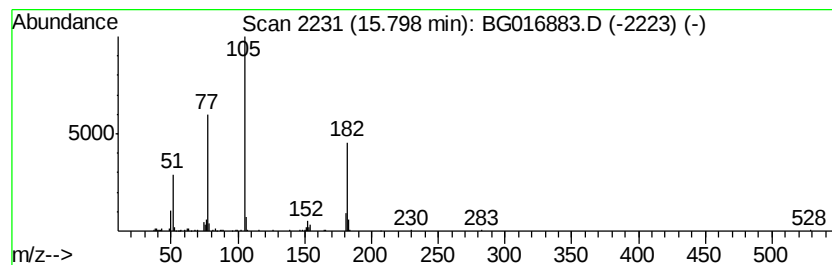
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.80	3.54 ng	190911	Acenaphthene-d10	14.44

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzophenone	182	C13H10O	000119-61-9	96
2			3-Hydroxy-2-methyl-3,3-diphenylpropionic acid methyl ester	270	C17H18O3	119020-91-6	50
3			Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	47
4			Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	47
5			Benzoylformic acid	150	C8H6O3	000611-73-4	46



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
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Acq On : 6 May 2015 3:13
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Sample : G2114-17
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GRID-6(6-12)

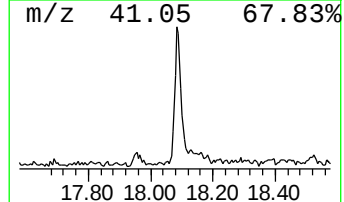
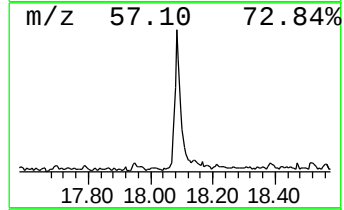
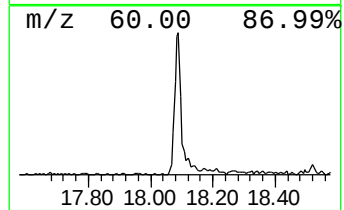
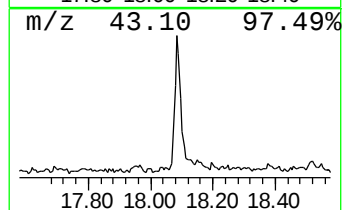
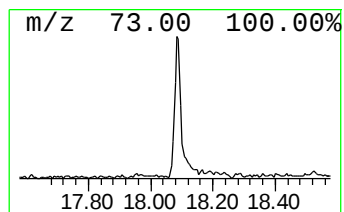
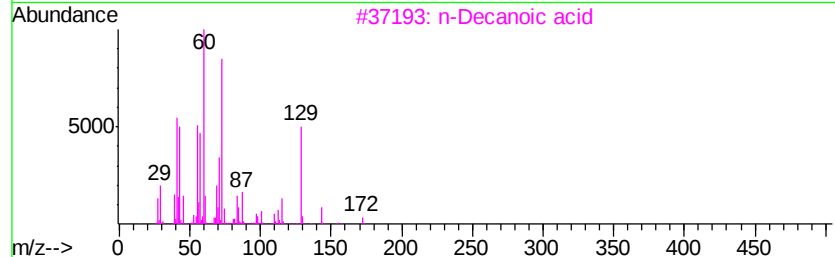
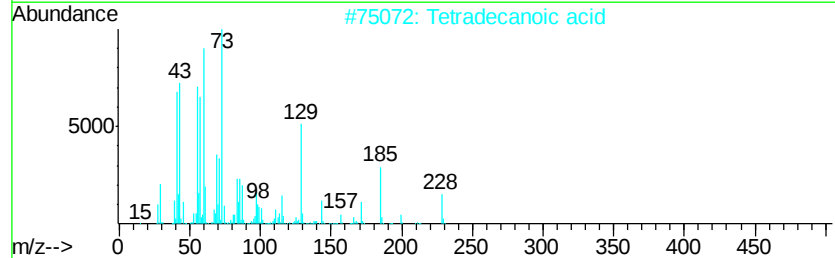
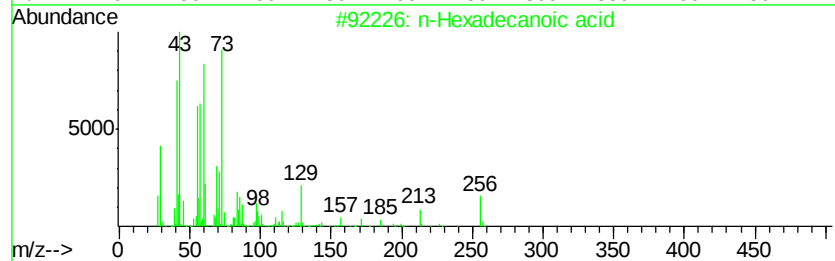
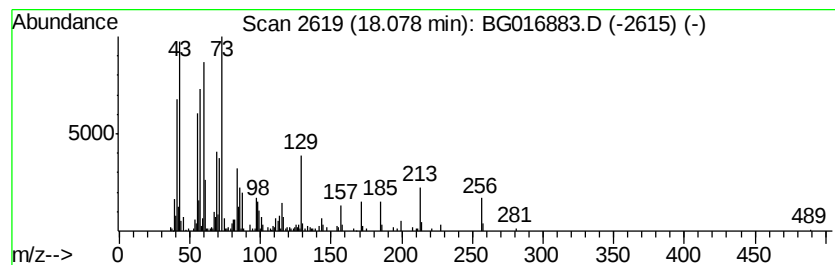
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.08	6.03 ng	412208	Phenanthrene-d10	17.19

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	95
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	92
3		n-Decanoic acid	172	C10H20O2	000334-48-5	60
4		Tridecanoic acid	214	C13H26O2	000638-53-9	53
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	52



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016883.D
Acq On : 6 May 2015 3:13
Operator : TP/IZ
Sample : G2114-17
Misc :
ALS Vial : 22 Sample Multiplier: 1

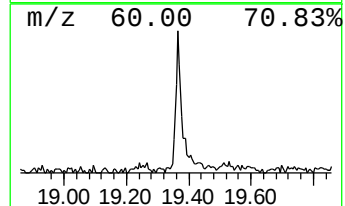
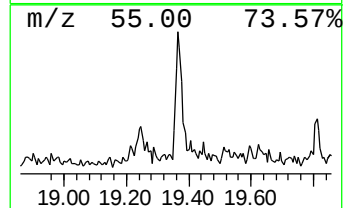
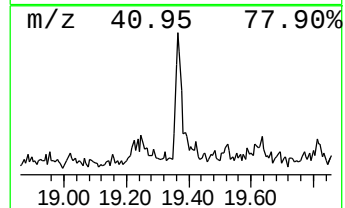
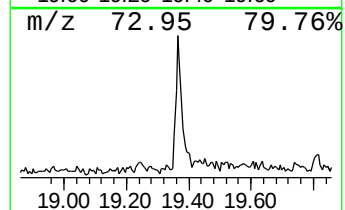
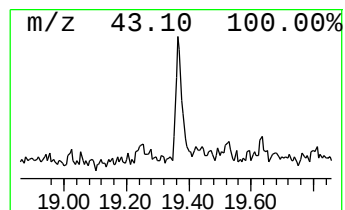
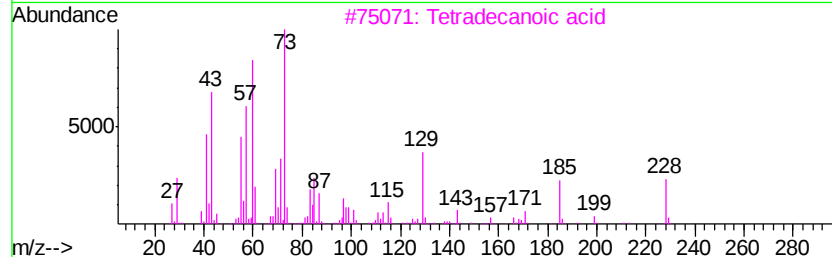
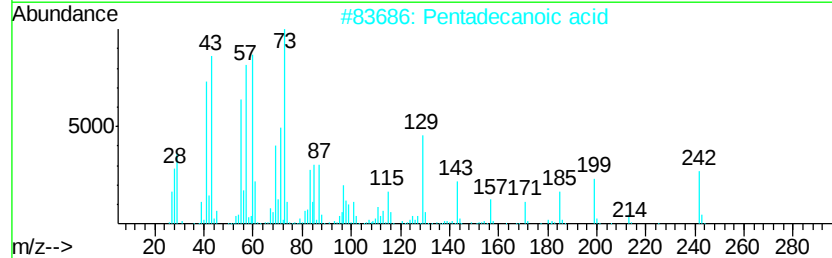
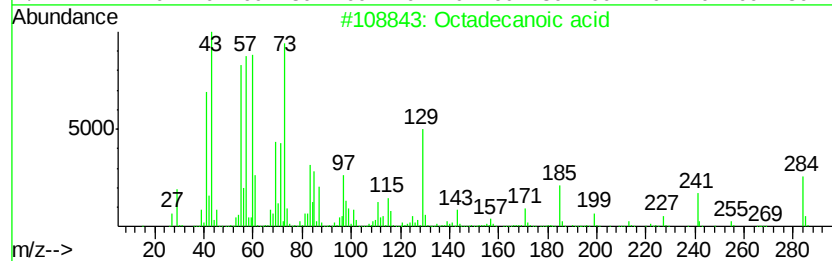
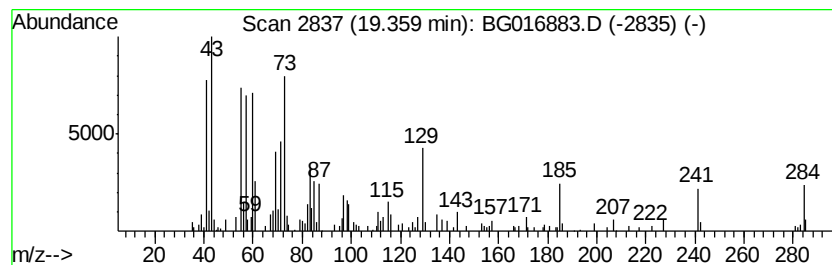
Instrument :
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ClientSampleId :
GRID-6(6-12)

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG050515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 Octadecanoic acid Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.36	2.64 ng	202053	Chrysene-d12		21.36
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	98
2	Pentadecanoic acid	242	C15H30O2	001002-84-2	89
3	Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4	Tridecanoic acid	214	C13H26O2	000638-53-9	62
5	Octadecanoic acid, 2-(2-hydroxy...	372	C22H44O4	000106-11-6	58



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016883.D
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Operator : TP/IZ
Sample : G2114-17
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GRID-6(6-12)

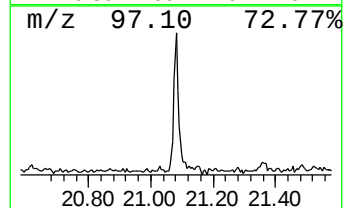
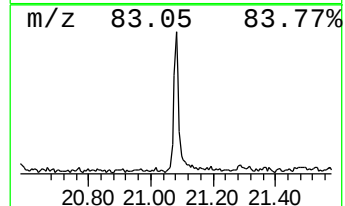
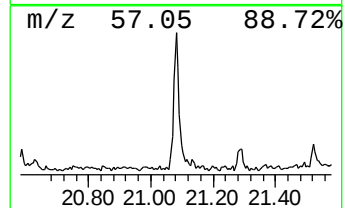
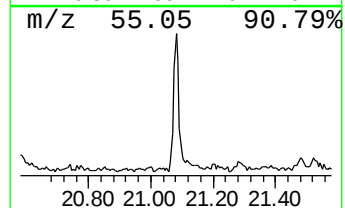
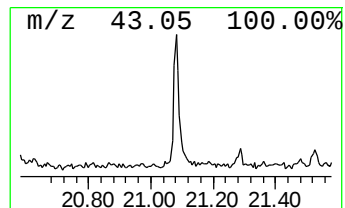
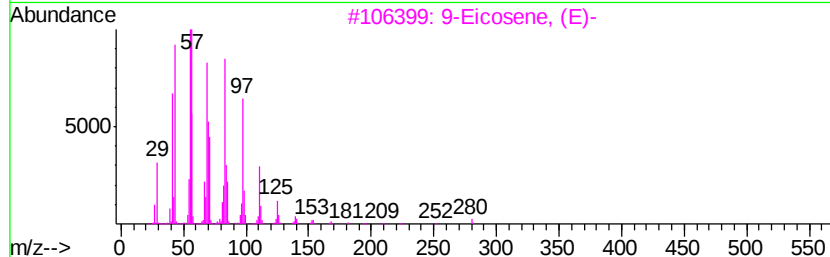
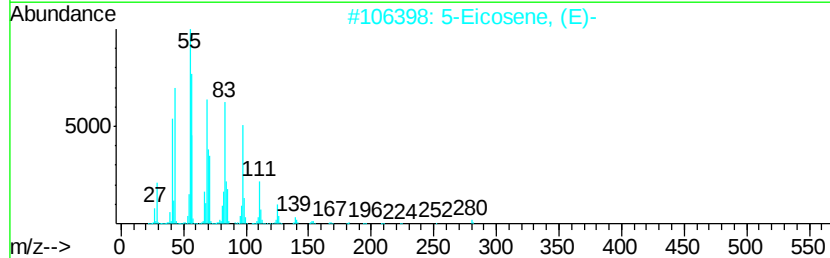
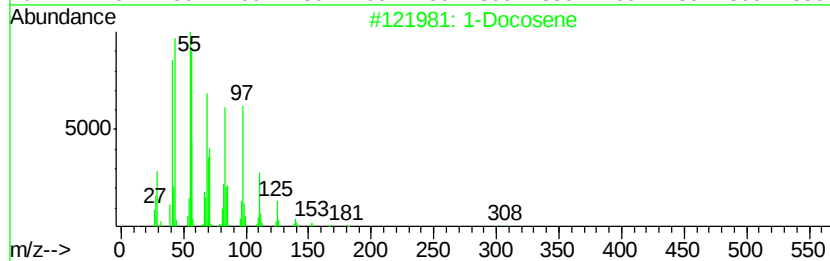
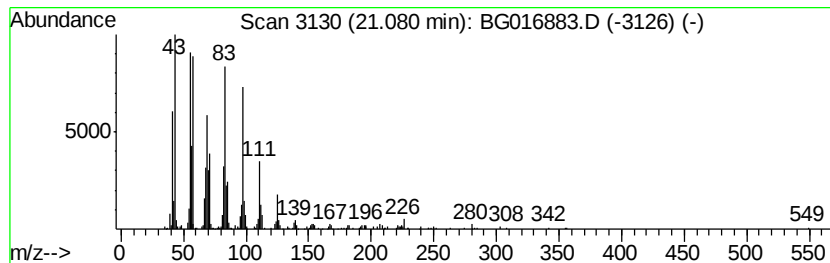
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Docosene Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.08	4.07 ng	311850	Chrysene-d12	21.36

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Docosene	308	C22H44	001599-67-3	96
2		5-Eicosene, (E)-	280	C20H40	074685-30-6	96
3		9-Eicosene, (E)-	280	C20H40	074685-29-3	94
4		3-Eicosene, (E)-	280	C20H40	074685-33-9	92
5		1-Tricosene	322	C23H46	018835-32-0	91



Data Path : Z:\HPCHEM1\BNA G\DATA\BG050515\
Data File : BG016883.D
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Sample : G2114-17
Misc :
ALS Vial : 22 Sample Multiplier: 1

Instrument :
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ClientSampleId :
GRID-6(6-12)

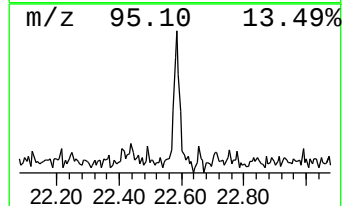
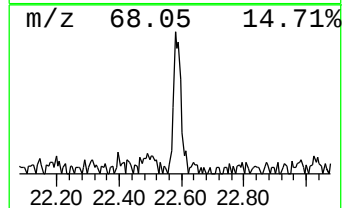
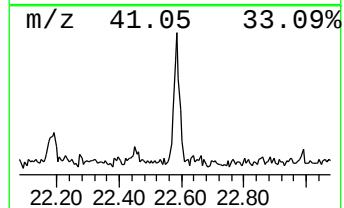
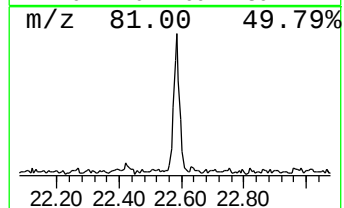
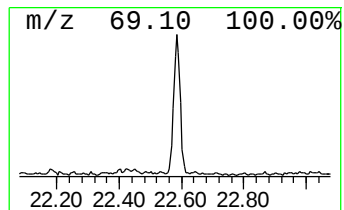
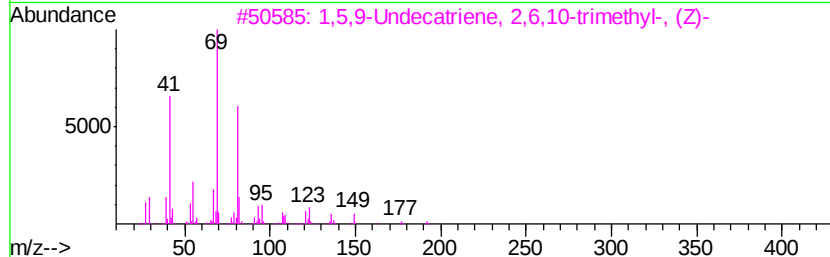
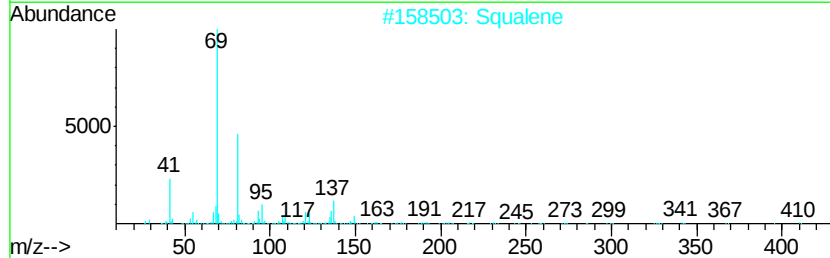
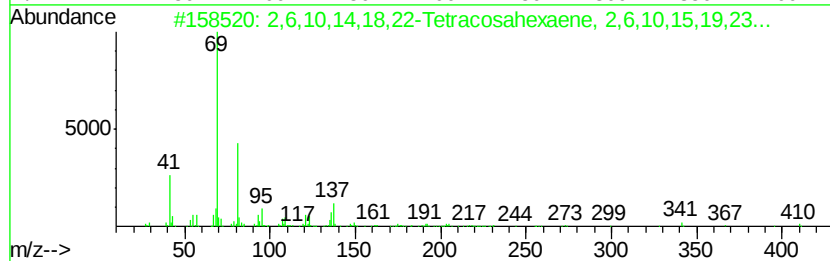
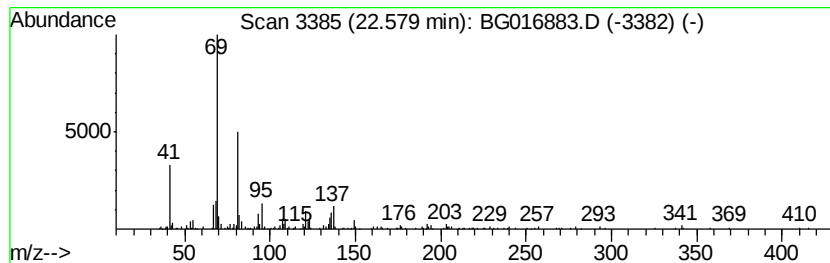
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 2,6,10,14,18,22-Tetracosahexaene... Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
22.58	2.60 ng	181080	Perylene-d12	23.67

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,6,10,14,18,22-Tetracosahexaene...	410	C30H50	000111-02-4	87		
2	Squalene	410	C30H50	007683-64-9	87		
3	1,5,9-Undecatriene, 2,6,10-trime...	192	C14H24	062951-96-6	83		
4	2,6,10-Dodecatrien-1-ol, 3,7,11-...	222	C15H26O	004602-84-0	59		
5	2,6,10-Dodecatrien-1-ol, 3,7,11-...	264	C17H28O2	004128-17-0	53		



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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
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Butane, 2-methoxy...	3.00	8.6	ng	223910	1	7.80	518756	20.0
3-Penten-2-one, 4...	4.33	6.0	ng	156026	1	7.80	518756	20.0
2-Pentanone, 4-hy...	4.92	15.9	ng	413333	1	7.80	518756	20.0
unknown7.33	7.33	61.6	ng	1598280	1	7.80	518756	20.0
Benzophenone	15.80	3.5	ng	190911	3	14.44	1077370	20.0
n-Hexadecanoic acid	18.08	6.0	ng	412208	4	17.19	1367170	20.0
Octadecanoic acid	19.36	2.6	ng	202053	5	21.36	1533500	20.0
1-Docosene	21.08	4.1	ng	311850	5	21.36	1533500	20.0
2,6,10,14,18,22-T...	22.58	2.6	ng	181080	6	23.67	1393970	20.0