

Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
 Data File : BG016167.D
 Acq On : 27 Mar 2015 7:57
 Operator : TP/IZ
 Sample : G1654-03
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 MW-5-3-24-15

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-BG032515.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	2.932	36	41	50	rBV	177140	283220	8.77%	1.615%
2	3.008	50	54	64	rVB	242767	290353	8.99%	1.655%
3	4.917	374	379	386	rVB	36539	51623	1.60%	0.294%
4	5.381	451	458	466	rBV	358077	511131	15.82%	2.914%
5	6.961	719	727	741	rBV2	219060	422158	13.07%	2.407%
6	7.326	779	789	796	rBV	721666	1133244	35.07%	6.461%
7	7.790	862	868	874	rBV	185495	278744	8.63%	1.589%
8	8.113	916	923	930	rBV	662339	1067504	33.04%	6.087%
9	8.947	1058	1065	1072	rBV	556415	892382	27.62%	5.088%
10	9.023	1073	1078	1087	rVB	28495	47736	1.48%	0.272%
11	9.646	1177	1184	1190	rBV3	21464	39794	1.23%	0.227%
12	9.993	1237	1243	1251	rVB2	81528	141162	4.37%	0.805%
13	10.351	1298	1304	1310	rBV2	26128	44341	1.37%	0.253%
14	10.574	1335	1342	1348	rBV	278392	454568	14.07%	2.592%
15	10.933	1398	1403	1411	rBV	32259	52977	1.64%	0.302%
16	13.041	1751	1762	1768	rBV	1557570	2342431	72.50%	13.356%
17	13.329	1804	1811	1817	rBV	25817	41063	1.27%	0.234%
18	14.416	1989	1996	2002	rVB2	420345	648726	20.08%	3.699%
19	14.839	2064	2068	2073	rBV	39628	58340	1.81%	0.333%
20	15.902	2242	2249	2256	rBV	1154586	1664074	51.50%	9.488%
21	17.154	2456	2462	2474	rBV	540317	795009	24.60%	4.533%
22	18.046	2610	2614	2625	rBV2	174371	348001	10.77%	1.984%
23	19.327	2828	2832	2839	rBV	133364	189463	5.86%	1.080%
24	19.486	2854	2859	2871	rBV	129896	215233	6.66%	1.227%
25	19.586	2873	2876	2882	rVB	86933	114355	3.54%	0.652%
26	19.774	2902	2908	2914	rBV	2629082	3231161	100.00%	18.423%
27	21.019	3115	3120	3133	rBV2	275638	563801	17.45%	3.215%
28	21.324	3167	3172	3178	rVB	632923	809236	25.04%	4.614%
29	23.604	3554	3560	3569	rVB2	418748	807045	24.98%	4.601%

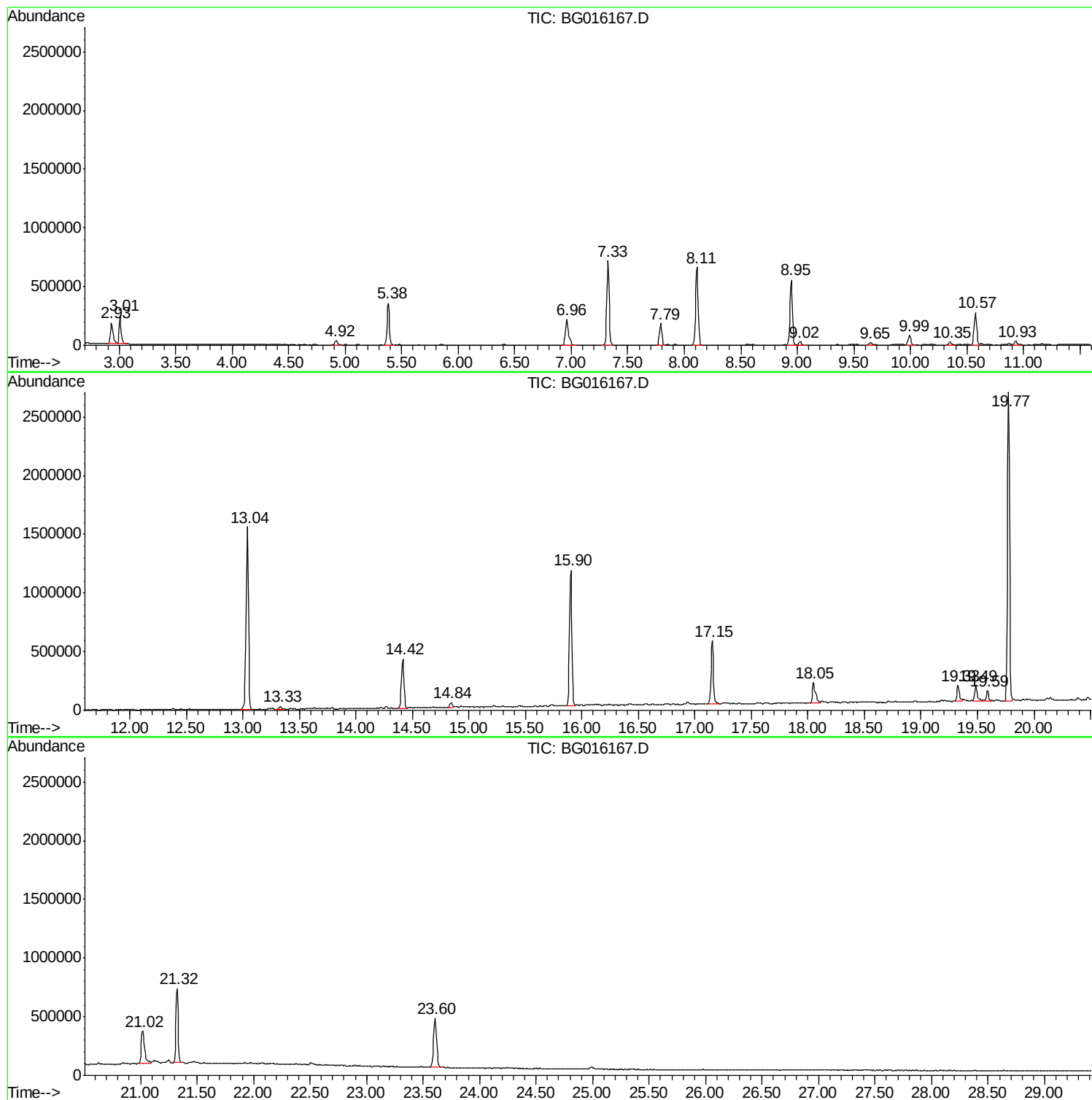
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Instrument :
BNA_G
ClientSampleId :
MW-5-3-24-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.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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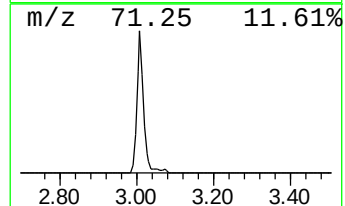
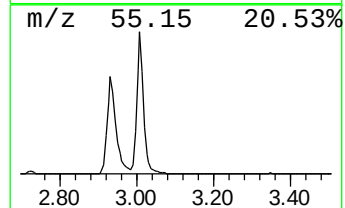
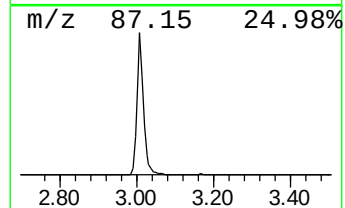
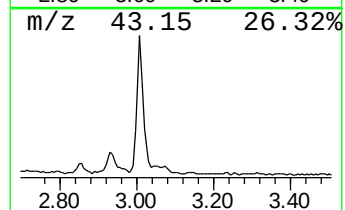
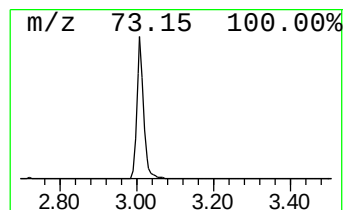
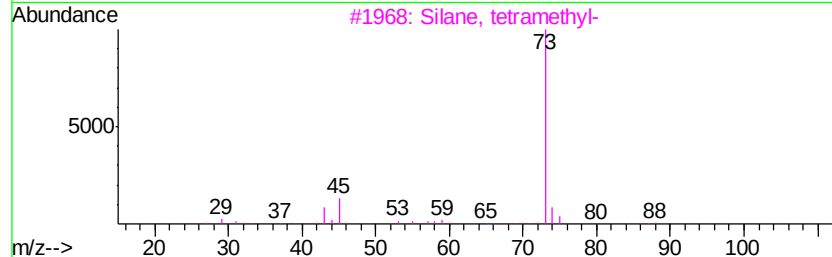
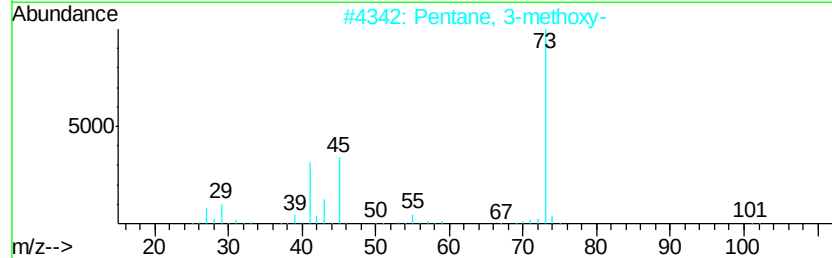
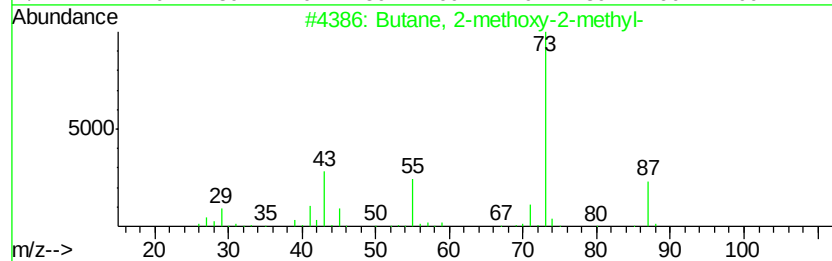
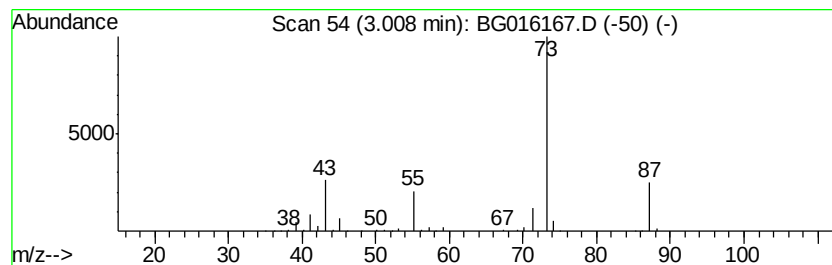
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.01	20.83 ng	290353	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	83
2		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	23
3		Silane, tetramethyl-	88	C4H12Si	000075-76-3	9
4		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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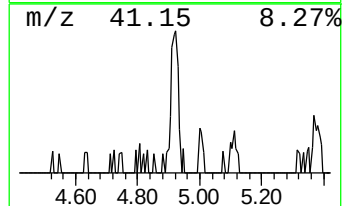
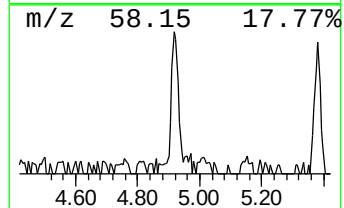
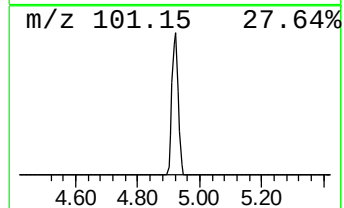
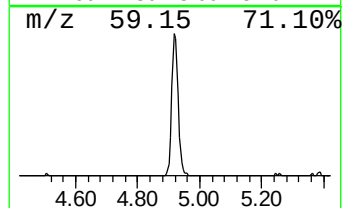
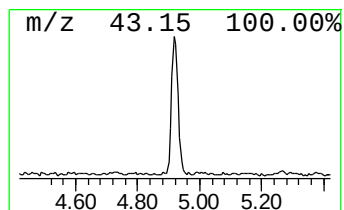
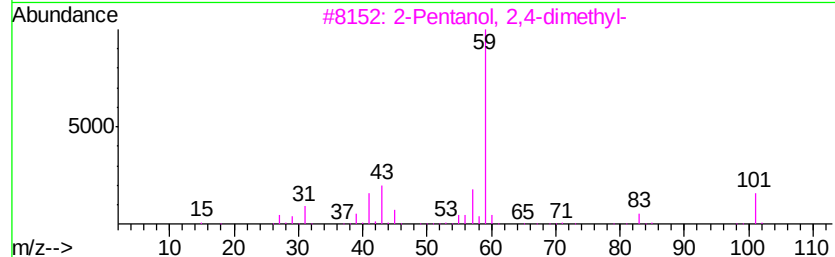
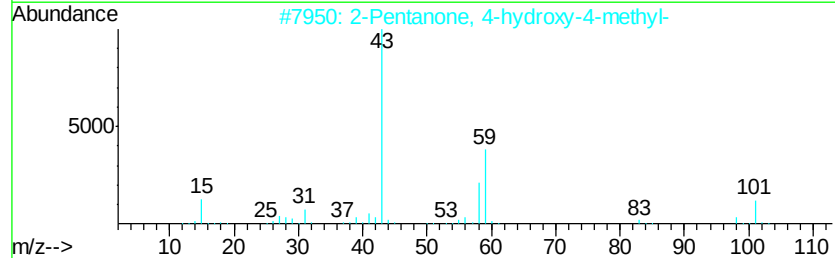
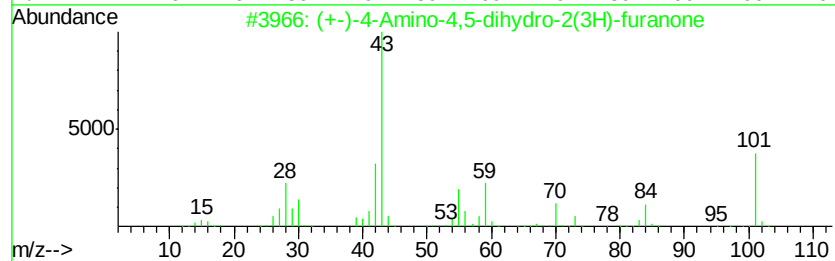
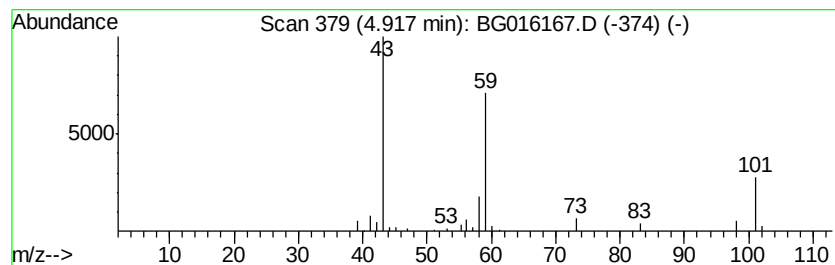
Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 3 unknown4.92 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.92	3.70 ng	51623	1,4-Dichlorobenzene-d4	7.79

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(+)-	4-Amino-4,5-dihydro-2(3H)-f...	101	C4H7NO2	016504-58-8	38	
2	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	38		
3	2-Pentanol, 2,4-dimethyl-	116	C7H16O	000625-06-9	37		
4	Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	35		
5	Butane, 1-ethoxy-	102	C6H14O	000628-81-9	25		



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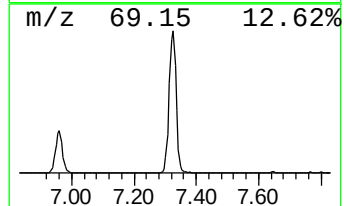
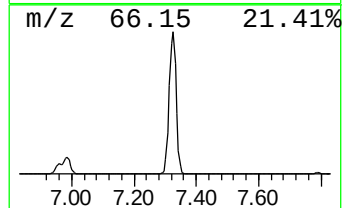
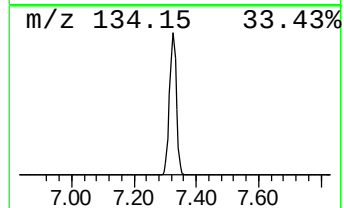
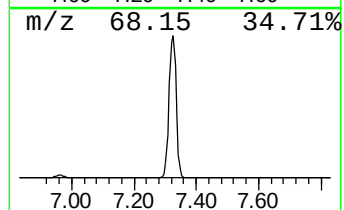
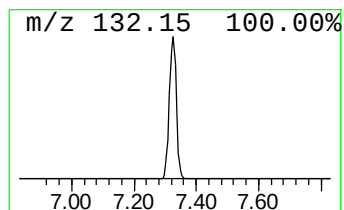
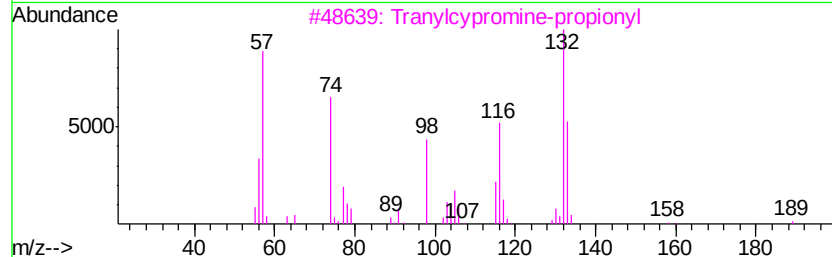
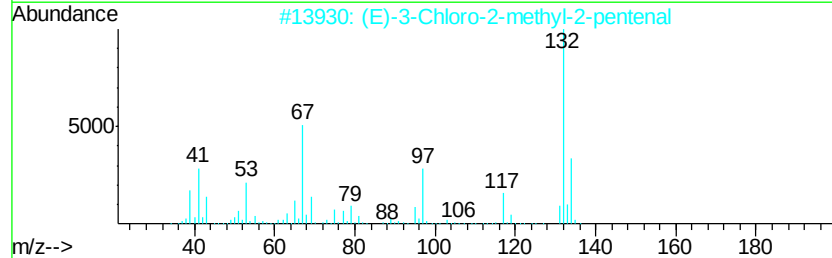
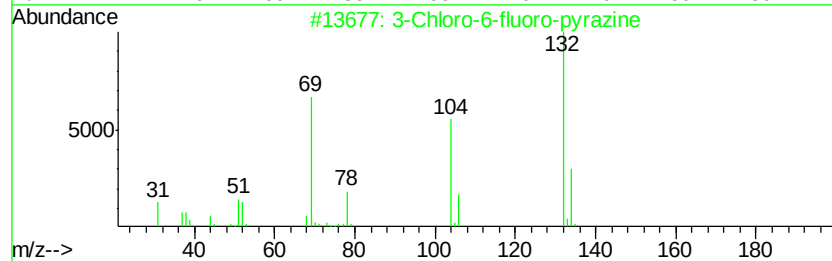
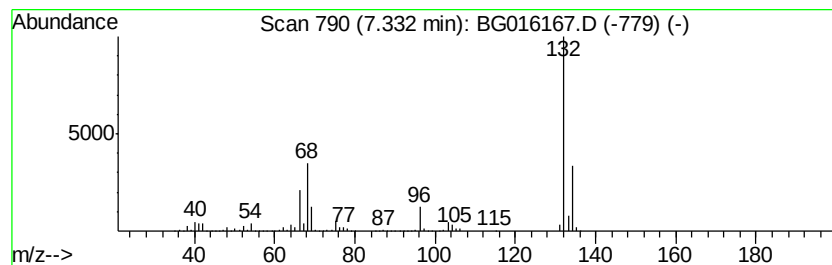
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown7.33 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.33	81.31 ng	1133240	1,4-Dichlorobenzene-d4	7.79

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		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		4-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-60-2	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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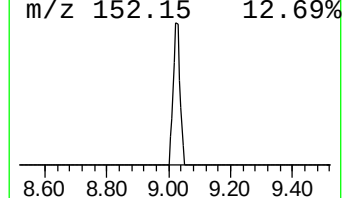
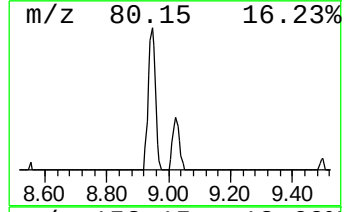
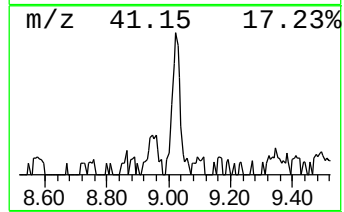
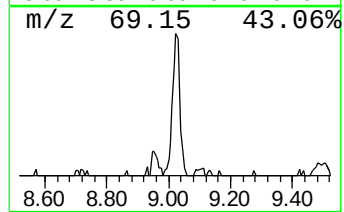
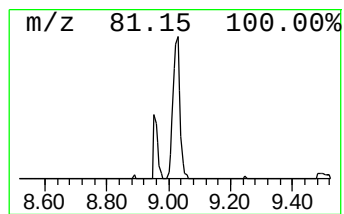
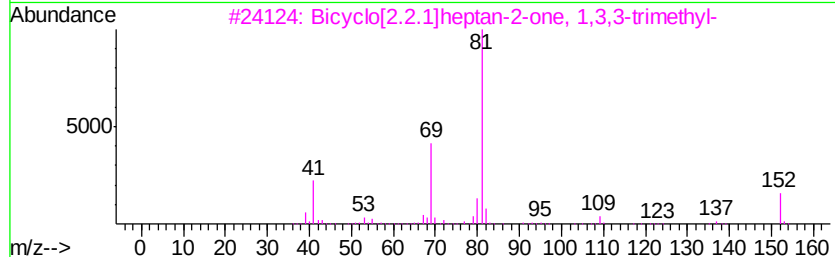
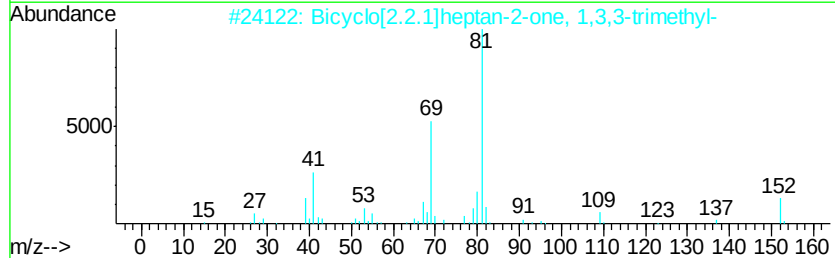
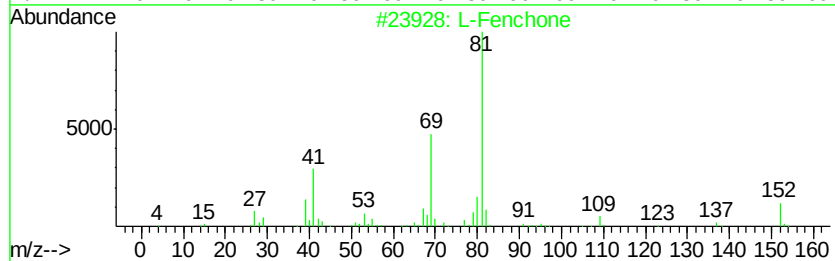
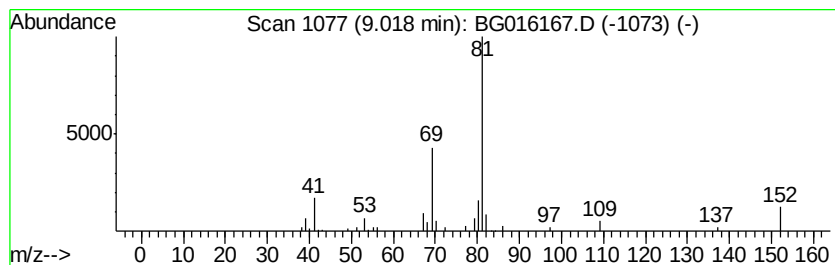
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 L-Fenchone Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.02	3.43 ng	47736	1,4-Dichlorobenzene-d4	7.79

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	L-Fenchone	152	C10H16O	000126-21-6	91
2		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	001195-79-5	91
3		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	004695-62-9	91
4		Bicyclo[2.2.1]heptan-2-one, 1,3,...	152	C10H16O	007787-20-4	91
5		Ethanone, 1-(2-methyl-2-cyclopen...	124	C8H12O	001767-84-6	42



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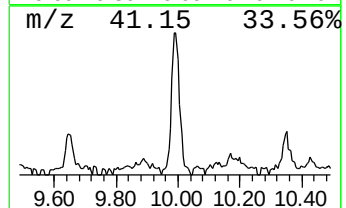
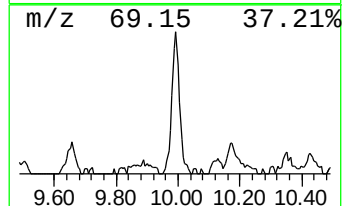
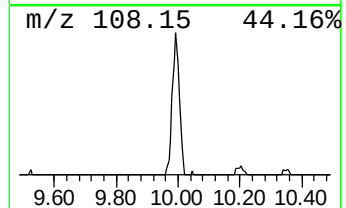
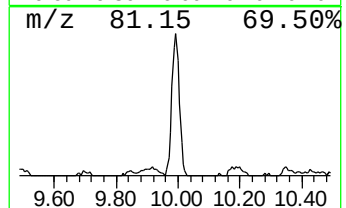
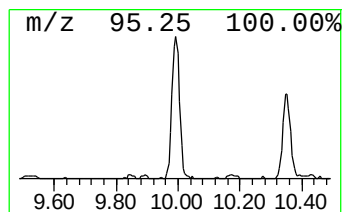
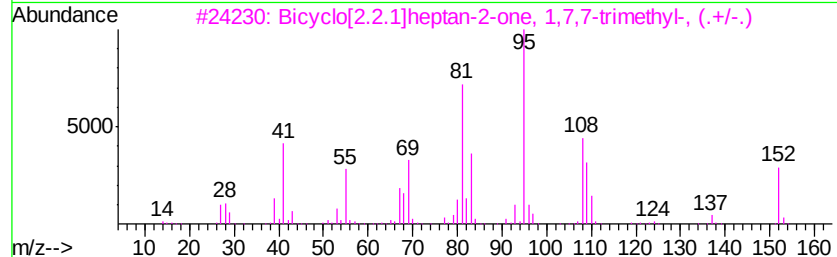
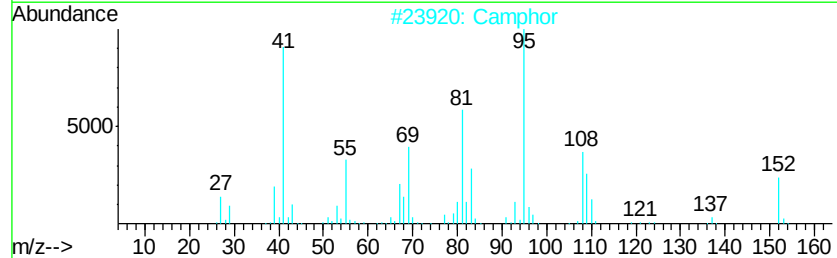
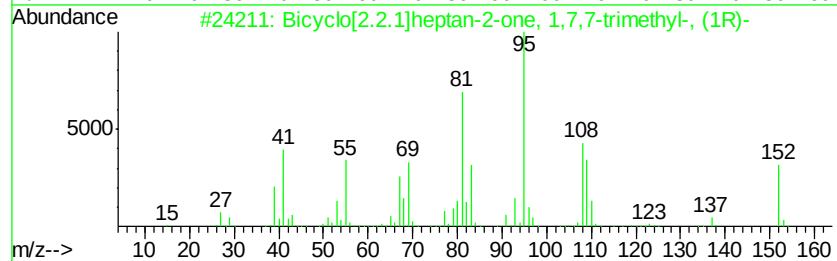
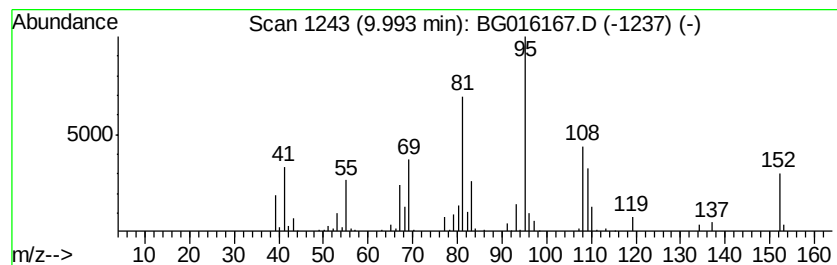
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 7 Bicyclo[2.2.1]heptan-2-one,... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.99	6.21 ng	141162	Naphthalene-d8	10.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-49-3	98
2		Camphor	152	C10H16O	000076-22-2	98
3		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	021368-68-3	96
4		Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	96
5		2-Butanone, 4-(5-methyl-2-furanyl)-	152	C9H12O2	013679-56-6	46



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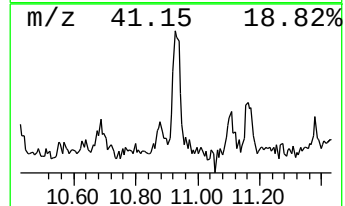
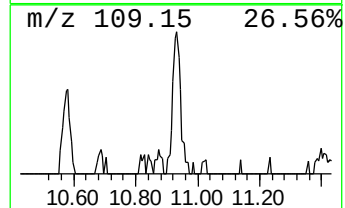
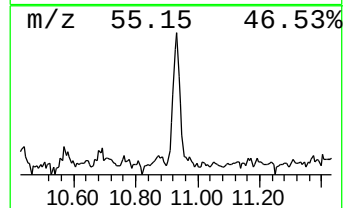
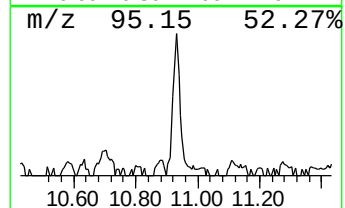
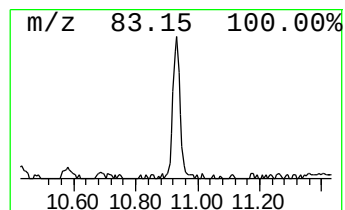
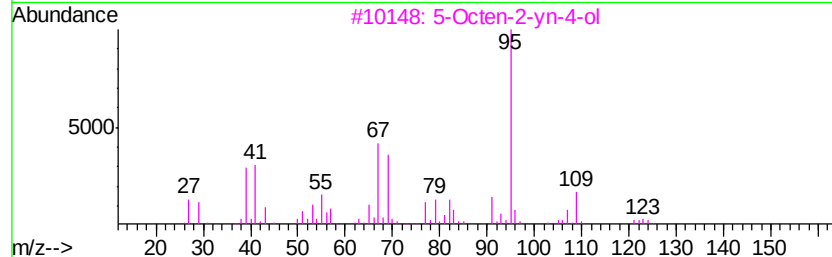
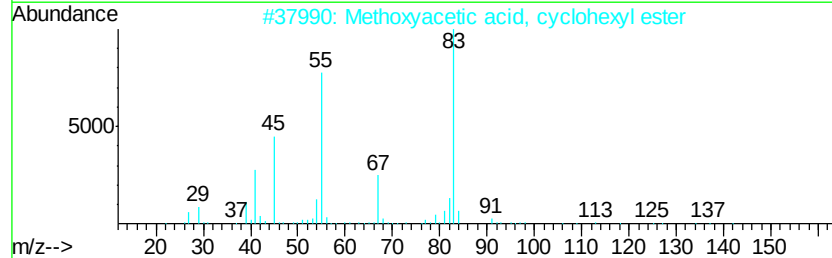
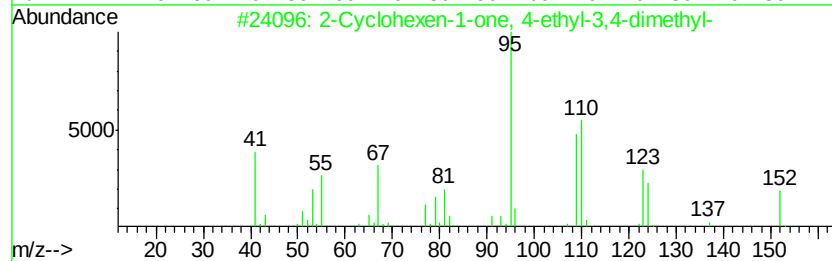
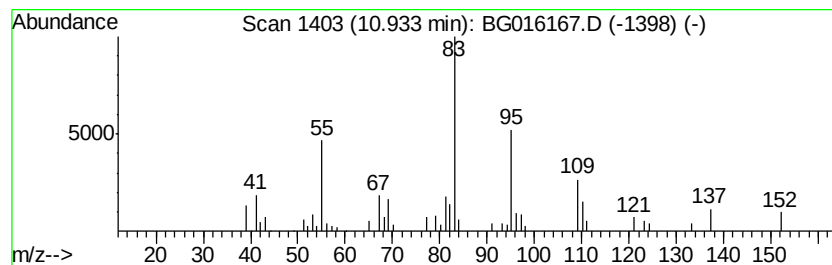
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown10.93 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.93	2.33 ng	52977	Napthalene-d8	10.57

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Cyclohexen-1-one, 4-ethyl-3,4-dimethyl-	152	C10H16O	017622-46-7	30
2		Methoxyacetic acid, cyclohexyl ester	172	C9H16O3	1000282-69-4	27
3		5-Octen-2-yn-4-ol	124	C8H12O	1000196-87-1	22
4		1,3-Dimethyl-1-cyclohexene	110	C8H14	002808-76-6	18
5		Furan, 2-ethyl-5-methyl-	110	C7H10O	001703-52-2	18



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016167.D
Acq On : 27 Mar 2015 7:57
Operator : TP/IZ
Sample : G1654-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-5-3-24-15

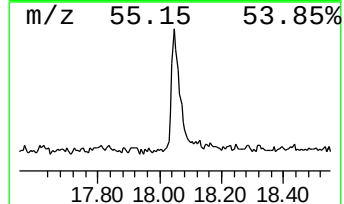
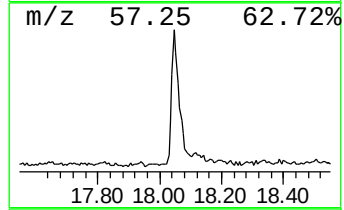
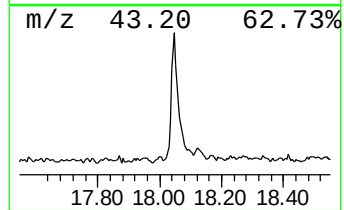
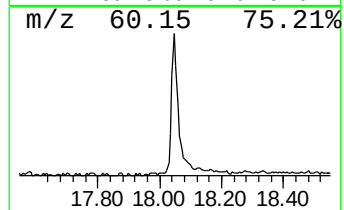
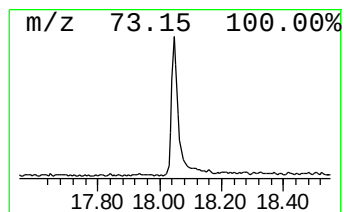
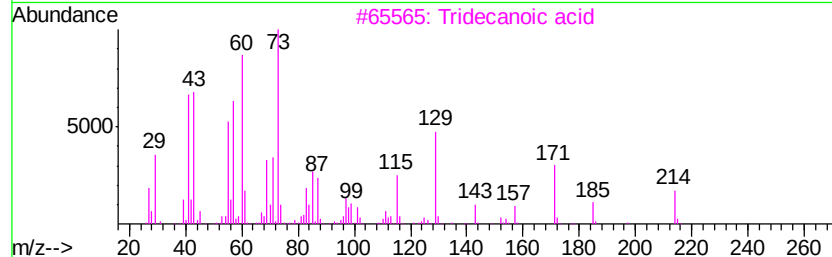
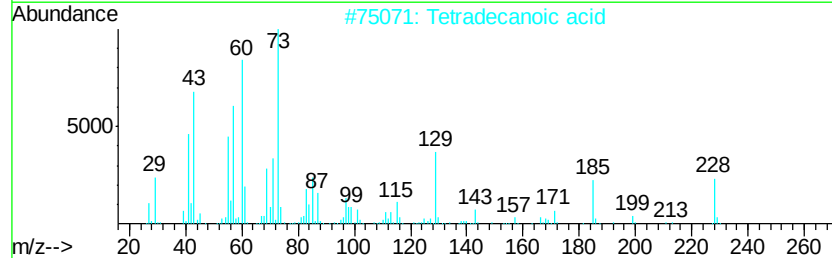
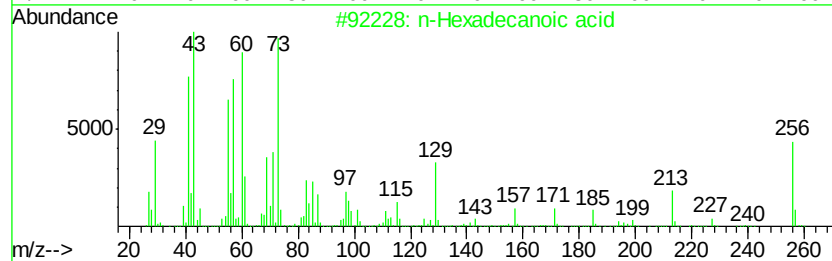
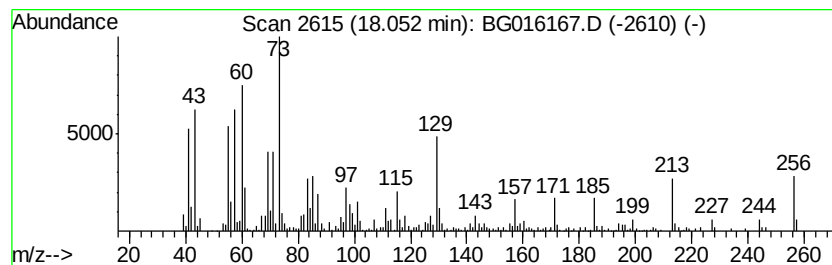
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 n-Hexadecanoic acid Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.05	8.75 ng	348001	Phenanthrene-d10	17.15

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Tetradecanoic acid	228	C14H28O2	000544-63-8	94
3		Tridecanoic acid	214	C13H26O2	000638-53-9	90
4		n-Decanoic acid	172	C10H20O2	000334-48-5	76
5		Pentadecanoic acid	242	C15H30O2	001002-84-2	74



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
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Acq On : 27 Mar 2015 7:57
Operator : TP/IZ
Sample : G1654-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

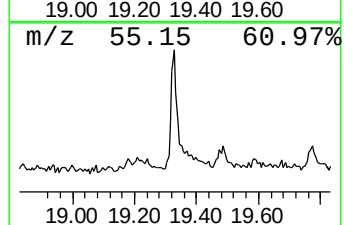
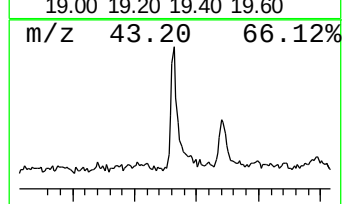
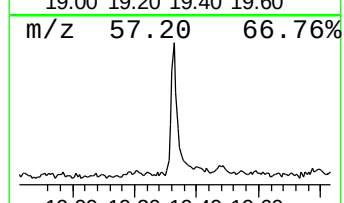
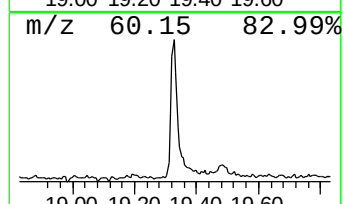
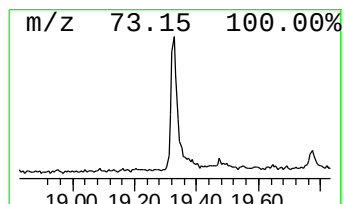
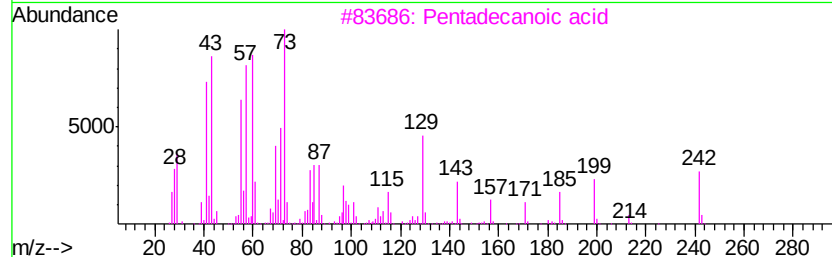
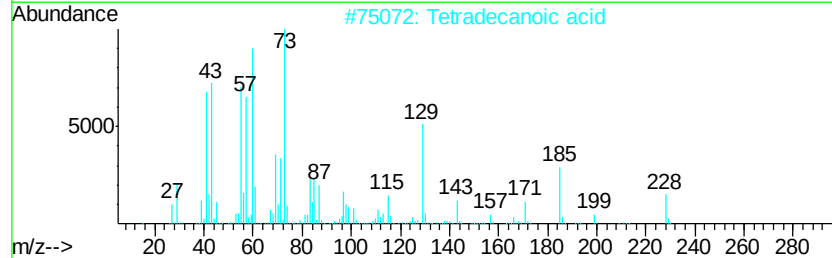
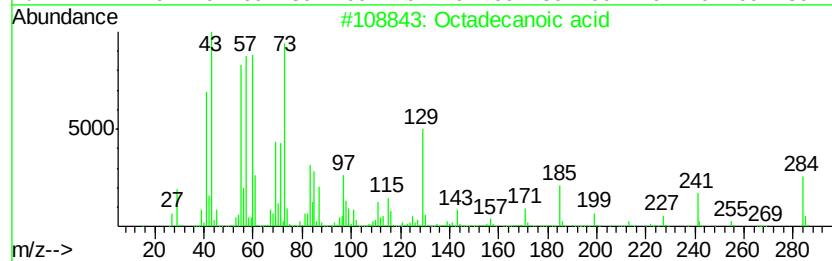
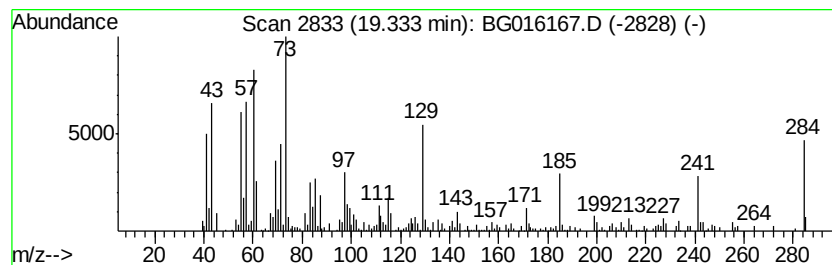
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ClientSampleId :
MW-5-3-24-15

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD		R.T.
19.33	4.68 ng	189463	Chrysene-d12		21.32
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Octadecanoic acid	284	C18H36O2	000057-11-4	99
2	Tetradecanoic acid	228	C14H28O2	000544-63-8	93
3	Pentadecanoic acid	242	C15H30O2	001002-84-2	83
4	Tridecanoic acid	214	C13H26O2	000638-53-9	64
5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	60



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016167.D
Acq On : 27 Mar 2015 7:57
Operator : TP/IZ
Sample : G1654-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

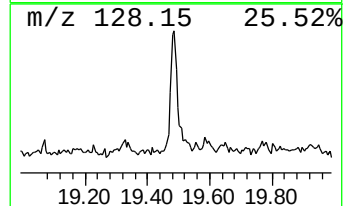
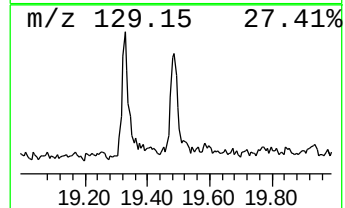
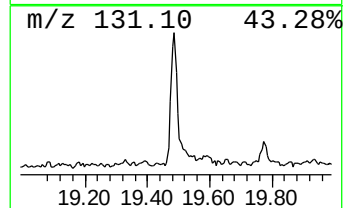
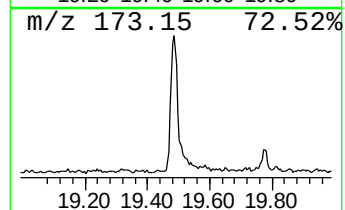
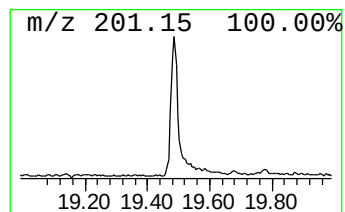
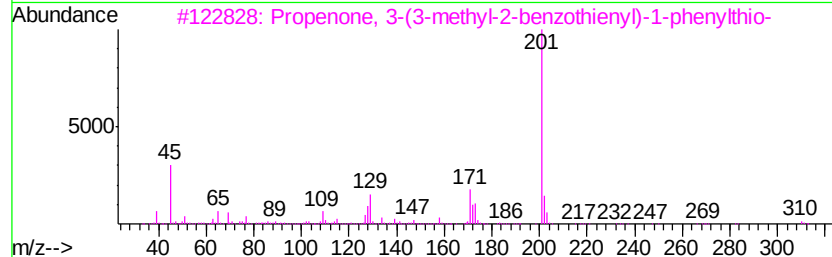
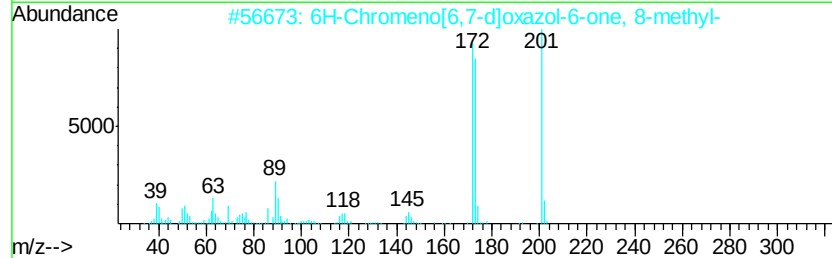
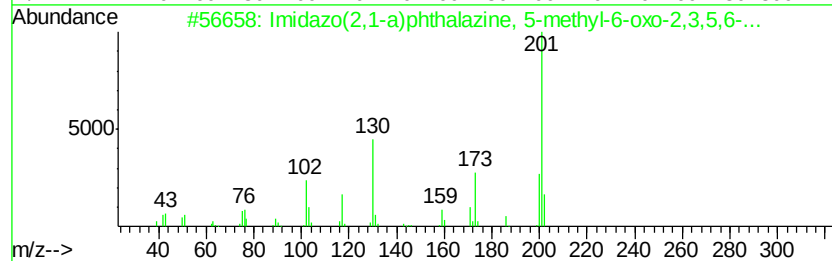
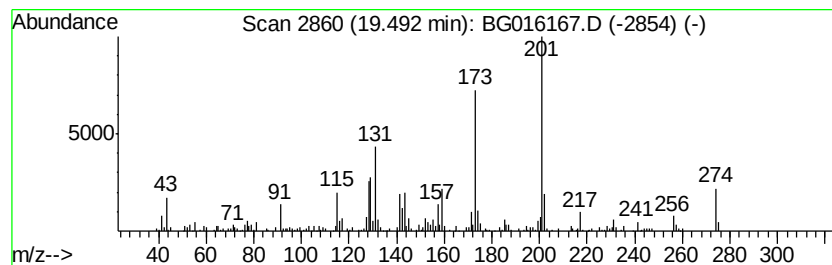
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown19.49 Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.49	5.32 ng	215233	Chrysene-d12	21.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Imidazo(2,1-a)phthalazine, 5-met...	201	C11H11N3O	057100-17-1	35
2	6H-Chromeno[6,7-d]oxazol-6-one, ...	201	C11H7NO3	1000272-31-8	27
3	Propenone, 3-(3-methyl-2-benzoth...	310	C18H14OS2	1000272-96-7	27
4	Methyl p-(1-pyrrolyl)benzoate	201	C12H11NO2	023351-08-8	22
5	2-Benzyl-3-(4-fluoro-phenylamino...	331	C21H18FN3	1000287-81-2	22



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016167.D
Acq On : 27 Mar 2015 7:57
Operator : TP/IZ
Sample : G1654-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

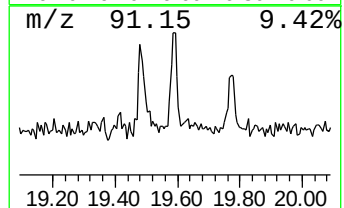
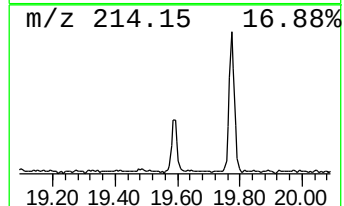
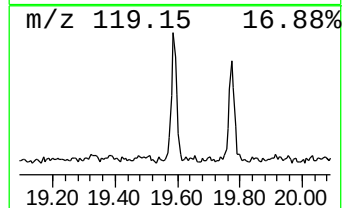
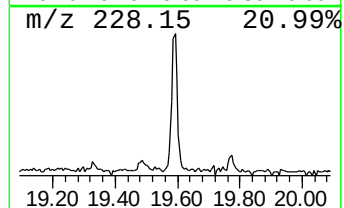
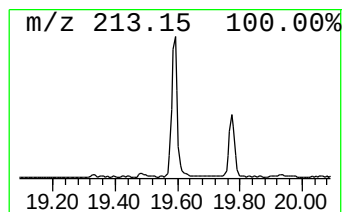
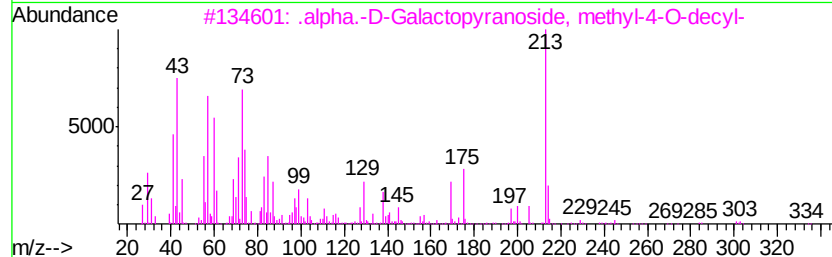
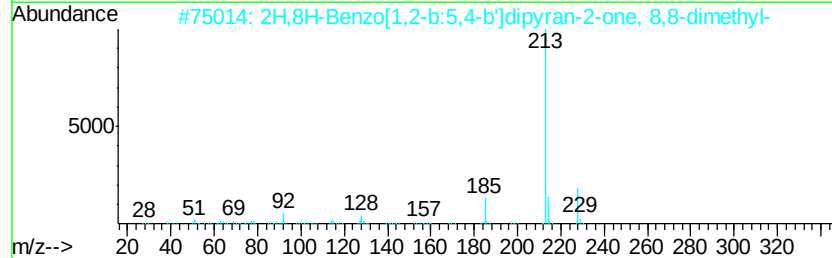
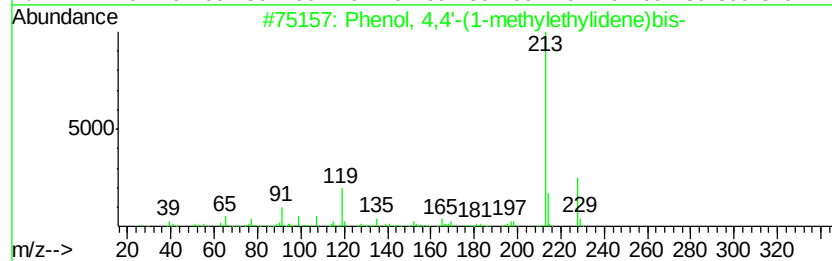
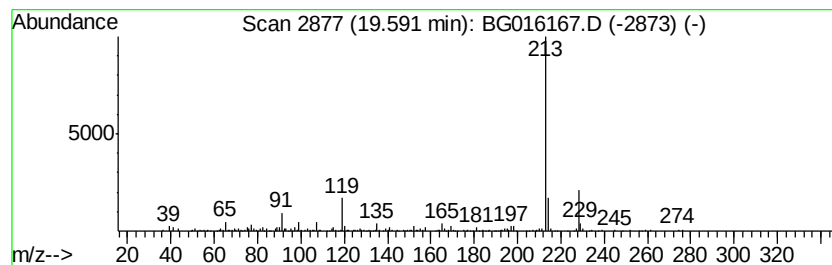
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Phenol, 4,4'-(1-methylethyl... Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.	
19.59	2.83 ng	114355	Chrysene-d12	21.32	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Phenol, 4,4'-(1-methylethylidene...	228	C15H16O2	000080-05-7	98
2	2H,8H-Benzo[1,2-b:5,4-b']dipyran...	228	C14H12O3	000553-19-5	59
3	.alpha.-D-Galactopyranoside, met...	334	C17H34O6	1000157-55-9	49
4	Decanedioic acid, diethyl ester	258	C14H26O4	000110-40-7	47
5	9-Propanoyl-1,2,3,4,5,6,7,8-octa...	242	C17H22O	1000255-01-4	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
Data File : BG016167.D
Acq On : 27 Mar 2015 7:57
Operator : TP/IZ
Sample : G1654-03
Misc :
ALS Vial : 29 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
MW-5-3-24-15

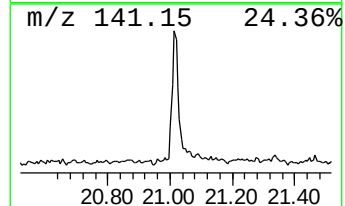
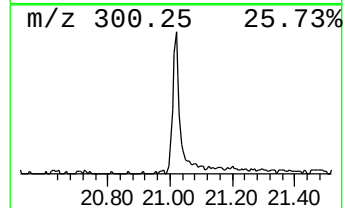
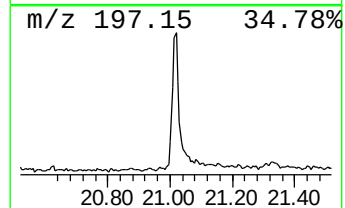
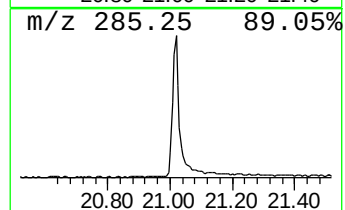
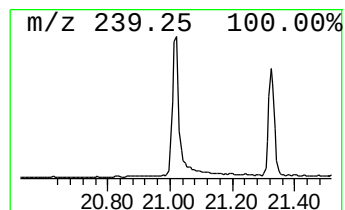
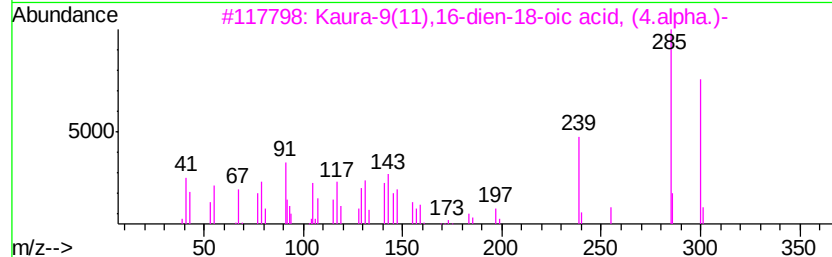
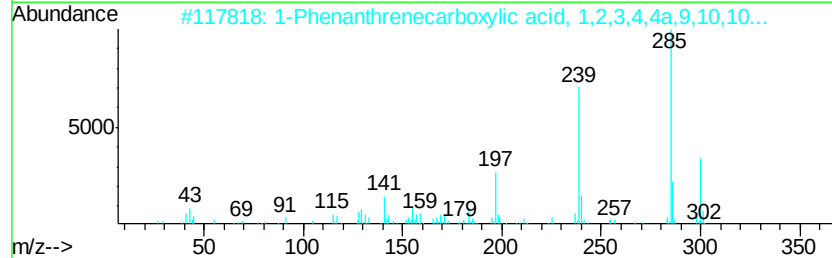
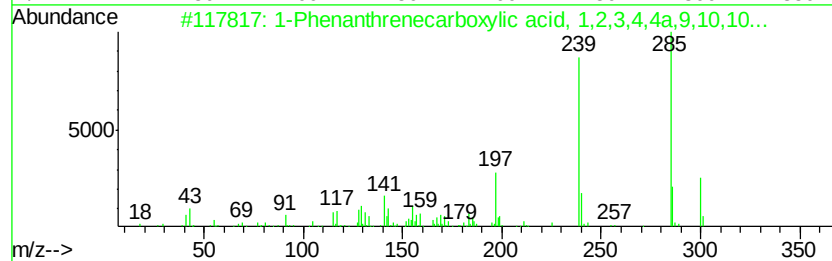
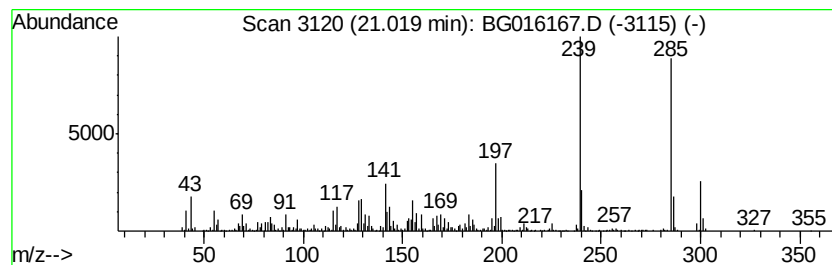
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 1-Phenanthrenecarboxylic ac... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
21.02	13.93 ng	563801	Chrysene-d12	21.32

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	001740-19-8	99
2		1-Phenanthrenecarboxylic acid, 1...	300	C20H28O2	005155-70-4	90
3		Kaura-9(11),16-dien-18-oic acid,...	300	C20H28O2	022338-67-6	80
4		Ethyl 4-hydroxy-7-trifluoromethy...	285	C13H10F3N03	000391-02-6	58
5		3-Quinolinecarboxylic acid, 4-hy...	285	C13H10F3N03	023851-84-5	53



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG032615\
 Data File : BG016167.D
 Acq On : 27 Mar 2015 7:57
 Operator : TP/IZ
 Sample : G1654-03
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
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 ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG032515.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
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unknown4.92	4.92	3.7	ng	51623	1	7.79	278744	20.0
unknown7.33	7.33	81.3	ng	1133240	1	7.79	278744	20.0
L-Fenchone	9.02	3.4	ng	47736	1	7.79	278744	20.0
Bicyclo[2.2.1]hep...	9.99	6.2	ng	141162	2	10.57	454568	20.0
unknown10.93	10.93	2.3	ng	52977	2	10.57	454568	20.0
n-Hexadecanoic acid	18.05	8.8	ng	348001	4	17.15	795009	20.0
Octadecanoic acid	19.33	4.7	ng	189463	5	21.32	809236	20.0
unknown19.49	19.49	5.3	ng	215233	5	21.32	809236	20.0
Phenol, 4,4'-(1-m...	19.59	2.8	ng	114355	5	21.32	809236	20.0
1-Phenanthrenecar...	21.02	13.9	ng	563801	5	21.32	809236	20.0