

Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
 Data File : BG023016.D
 Acq On : 12 Jul 2016 1:18
 Operator : UM/SJ
 Sample : H3967-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S22-0008

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : ON Filtering: 5
 Sampling : 1 Min Area: 3 % of largest Peak
 Start Thrs: 0.2 Max Peaks: 100
 Stop Thrs : 0 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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	5.223	400	406	415	rBV	125092	203794	1.93%	0.384%
2	5.699	480	487	497	rVB	1092095	1811315	17.19%	3.410%
3	7.303	750	760	772	rBV	820029	1514425	14.37%	2.851%
4	7.532	793	799	807	rBV	281162	492431	4.67%	0.927%
5	7.685	816	825	832	rBV	2025424	3590650	34.08%	6.761%
6	8.155	897	905	917	rVV	407511	771567	7.32%	1.453%
7	8.266	917	924	930	rVB	269147	465679	4.42%	0.877%
8	8.478	954	960	967	rVB	1629332	2856017	27.11%	5.378%
9	9.177	1071	1079	1082	rBV3	120345	236400	2.24%	0.445%
10	9.330	1097	1105	1116	rVB	1685406	3237098	30.72%	6.095%
11	10.370	1277	1282	1290	rVB2	138146	247437	2.35%	0.466%
12	10.981	1377	1386	1393	rBV	664068	1231068	11.68%	2.318%
13	11.592	1487	1490	1497	rVB4	104154	179610	1.70%	0.338%
14	11.686	1500	1506	1513	rVB7	67498	139646	1.33%	0.263%
15	11.821	1522	1529	1535	rBV2	60211	133662	1.27%	0.252%
16	12.356	1613	1620	1625	rBV3	88501	167061	1.59%	0.315%
17	12.914	1708	1715	1724	rVB2	149659	316417	3.00%	0.596%
18	13.419	1794	1801	1808	rBV	4671554	7386671	70.11%	13.908%
19	13.648	1836	1840	1849	rVB9	52782	107253	1.02%	0.202%
20	14.242	1936	1941	1949	rBV	175455	281108	2.67%	0.529%
21	14.800	2026	2036	2043	rBV2	1183995	1955876	18.56%	3.683%
22	16.292	2283	2290	2301	rBV	4361409	6893155	65.42%	12.979%
23	17.555	2499	2505	2517	rBV2	1480272	2298937	21.82%	4.329%
24	18.425	2649	2653	2661	rBV	341441	515275	4.89%	0.970%
25	19.694	2865	2869	2876	rBV2	274544	377923	3.59%	0.712%
26	20.164	2943	2949	2955	rBV	7701052	10536555	100.00%	19.839%
27	21.868	3233	3239	3248	rVB2	1490836	2617729	24.84%	4.929%
28	25.252	3805	3815	3828	rVB2	812752	2545404	24.16%	4.793%

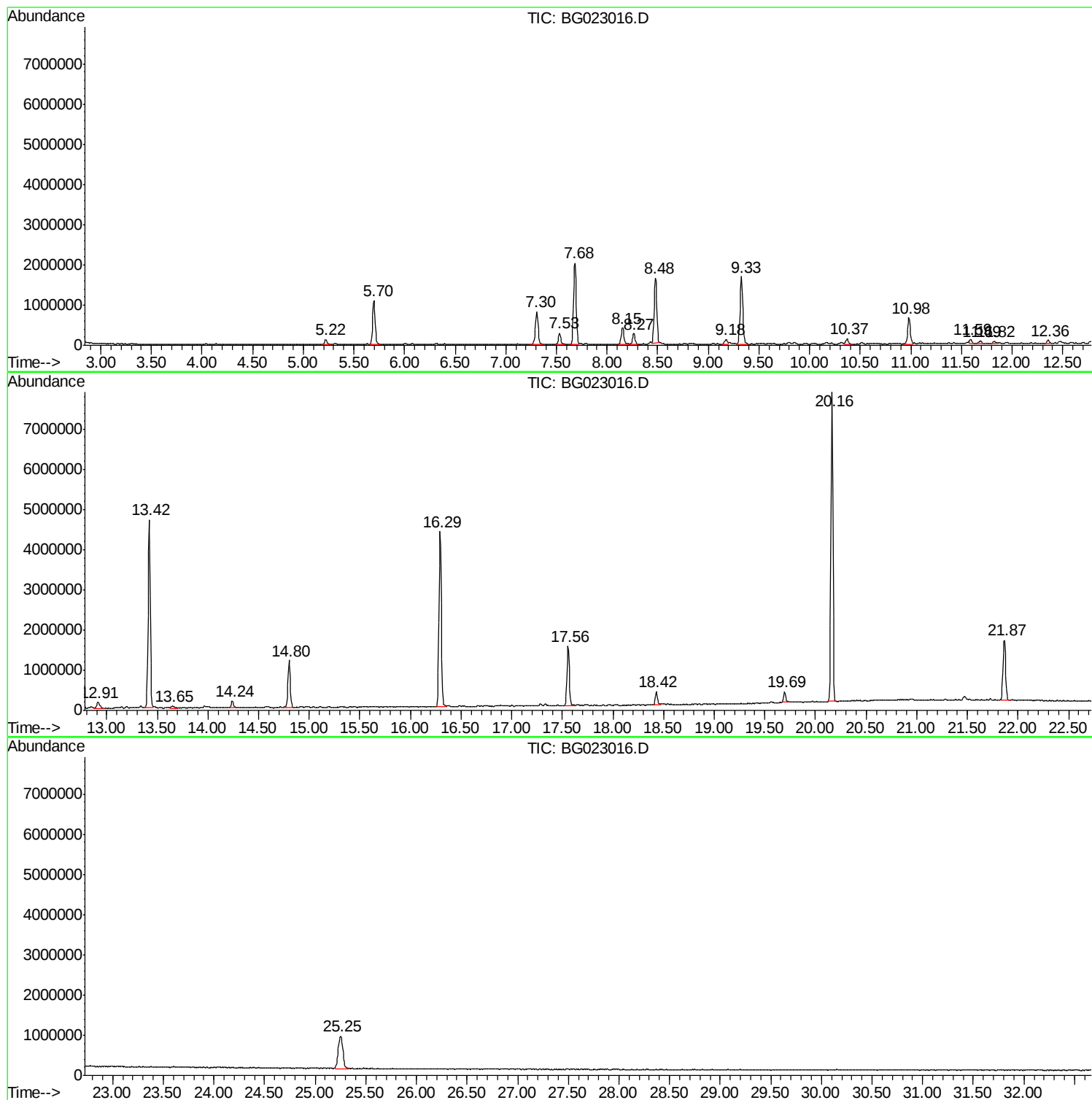
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ClientSampleId :
S22-0008

Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.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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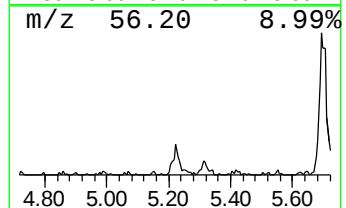
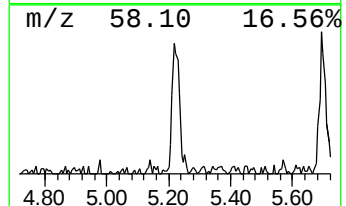
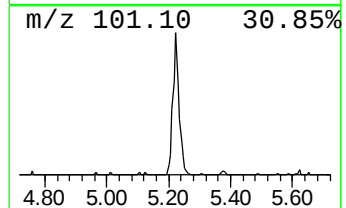
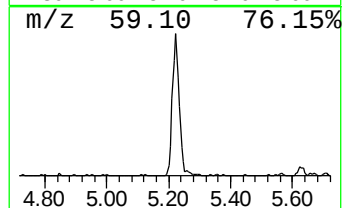
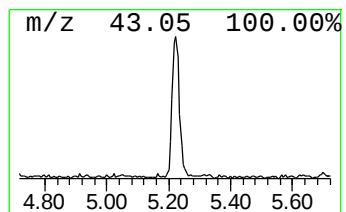
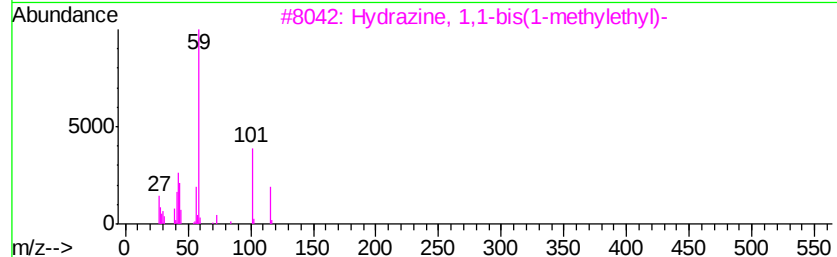
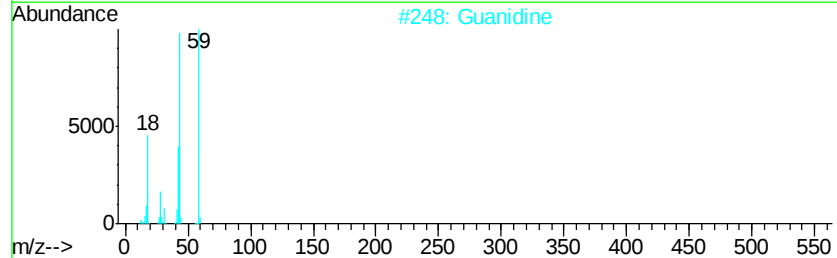
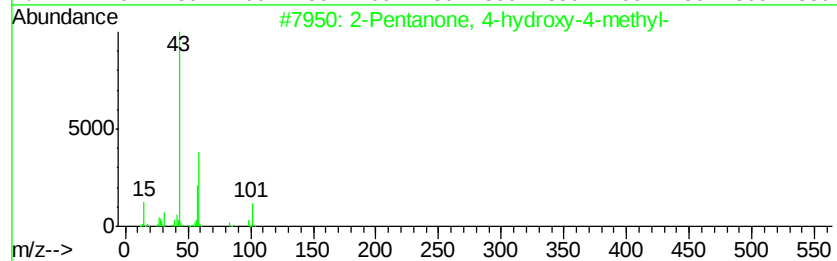
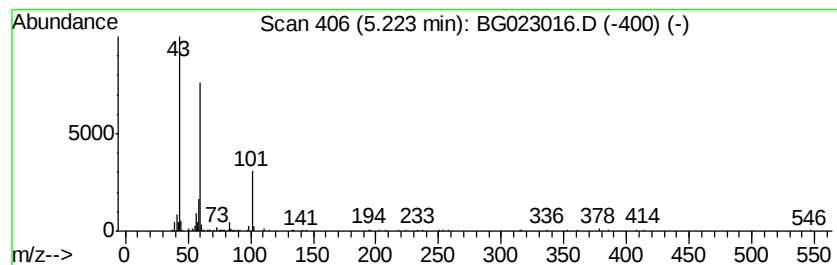
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.22	5.28 ng	203794	1,4-Dichlorobenzene-d4	8.15

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	72
2			Guanidine	59	CH5N3	000113-00-8	53
3			Hydrazine, 1,1-bis(1-methylethyl)-	116	C6H16N2	000921-14-2	45
4			Acetic acid, 10,11-dihydroxy-3,7...	298	C17H30O4	1000194-28-5	40
5			1,8-Nonanediol, 8-methyl-	174	C10H22O2	054725-73-4	38



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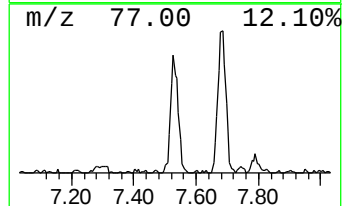
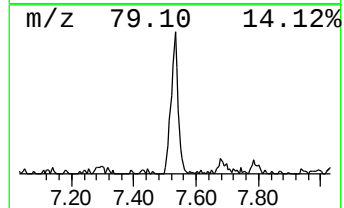
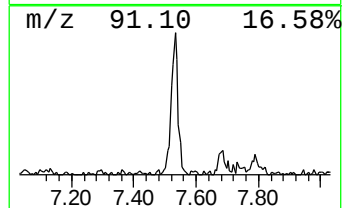
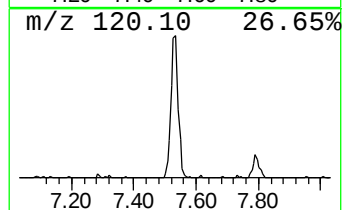
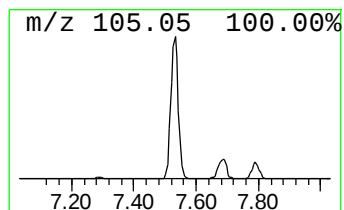
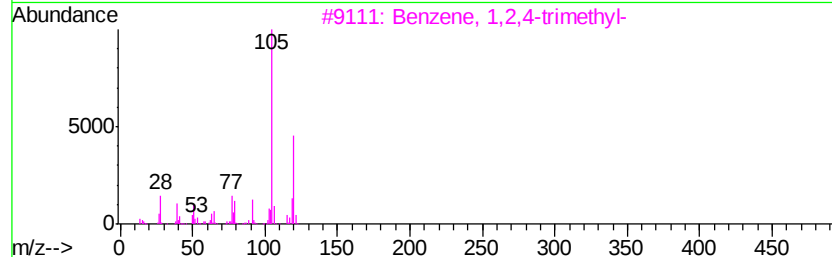
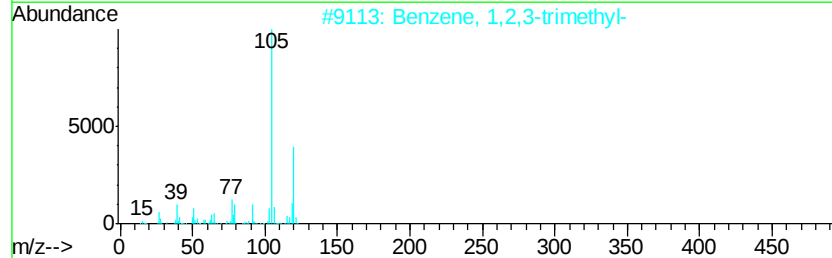
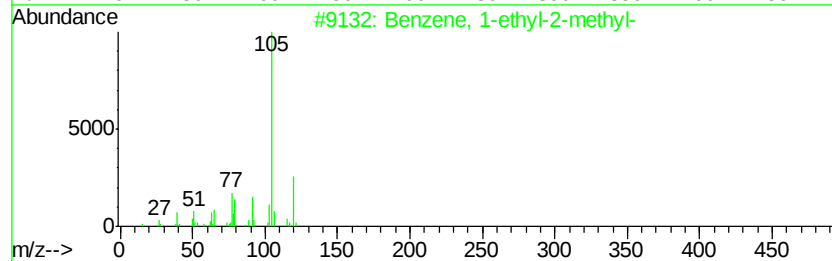
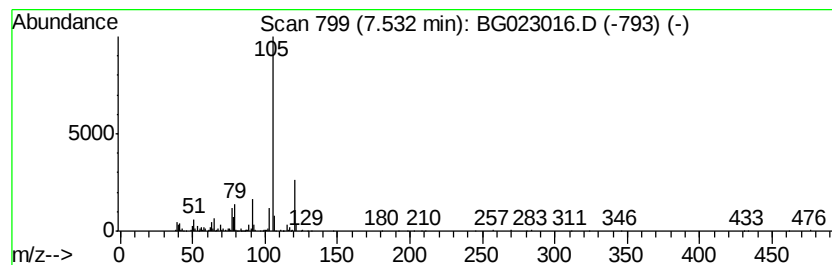
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Peak Number 2 Benzene, 1-ethyl-2-methyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.53	12.76 ng	492431	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	90
3		Benzene, 1,2,4-trimethyl-	120	C9H12	000095-63-6	90
4		Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	87
5		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	86



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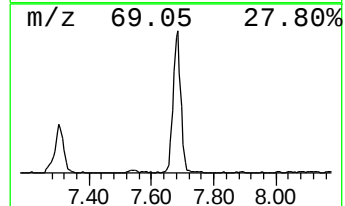
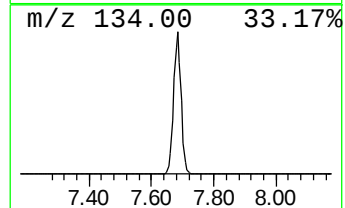
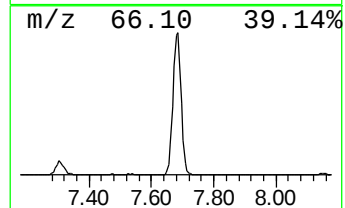
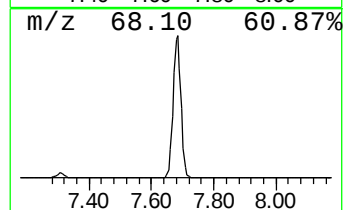
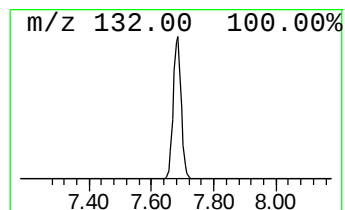
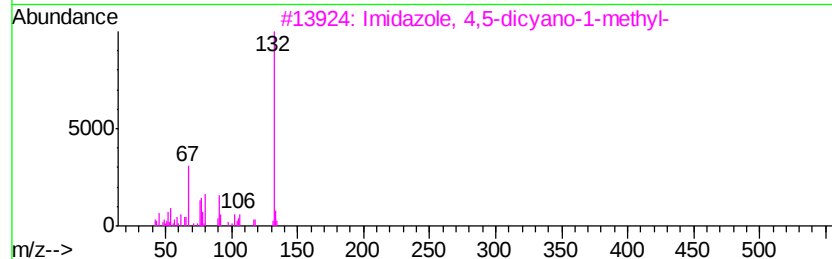
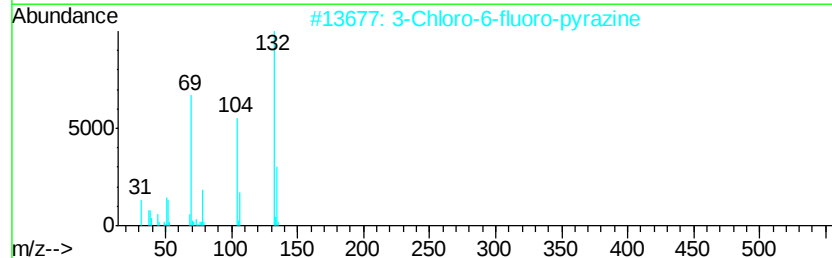
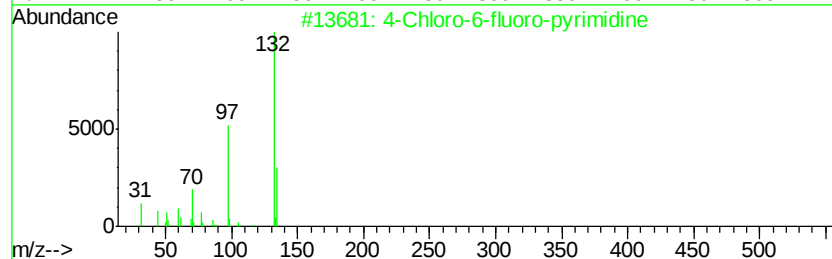
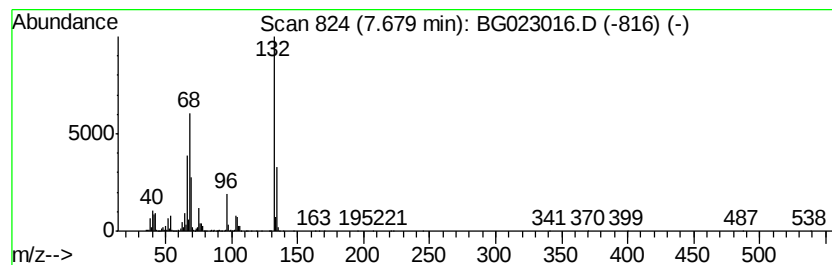
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 3 unknown7.68 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.68	93.07 ng	3590650	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	14
2		3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	14
3		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	11
4		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	10
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	10



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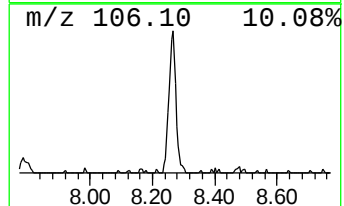
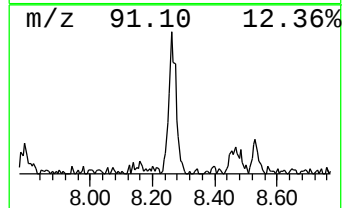
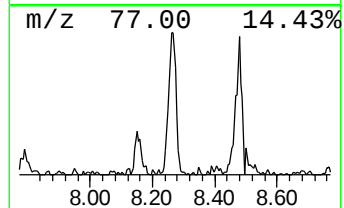
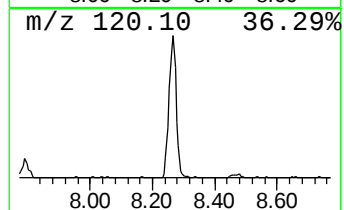
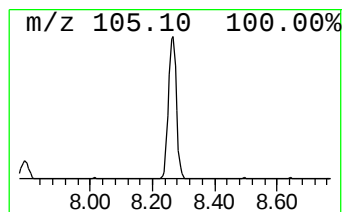
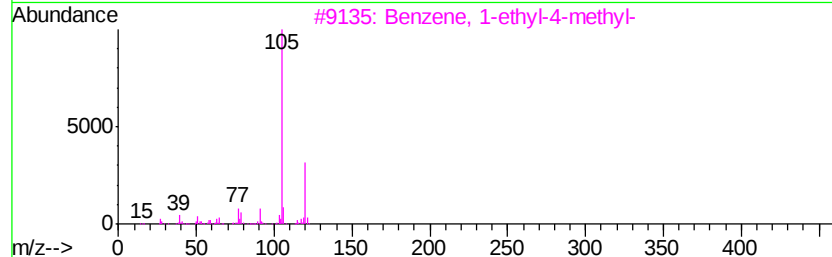
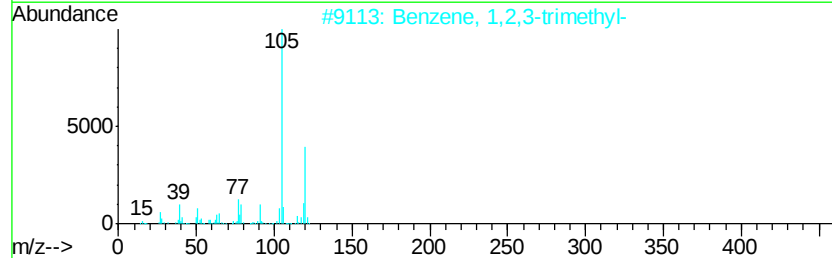
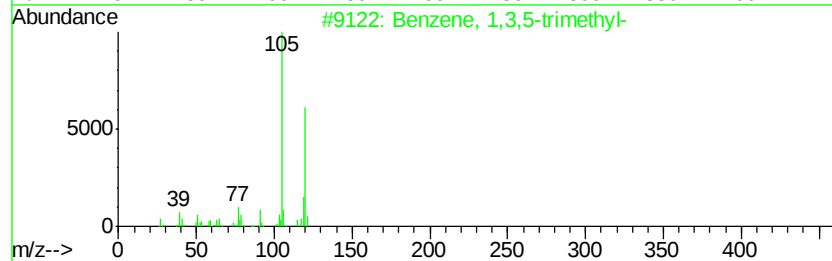
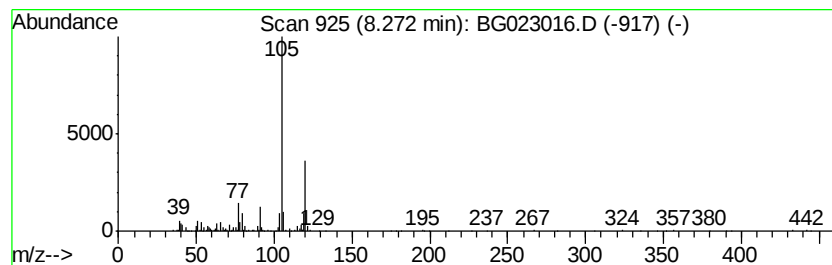
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Peak Number 4 Benzene, 1,3,5-trimethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.27	12.07 ng	465679	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1,3,5-trimethyl-	120	C9H12	000108-67-8	94
2		Benzene, 1,2,3-trimethyl-	120	C9H12	000526-73-8	93
3		Benzene, 1-ethyl-4-methyl-	120	C9H12	000622-96-8	91
4		Benzene, 1-ethyl-2-methyl-	120	C9H12	000611-14-3	91
5		Benzene, 1-ethyl-3-methyl-	120	C9H12	000620-14-4	91



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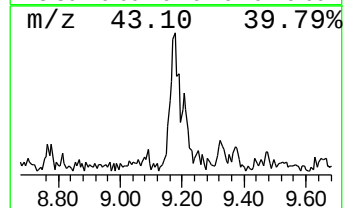
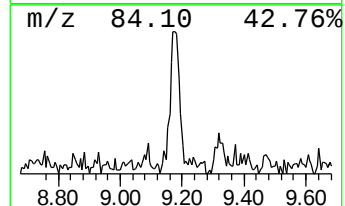
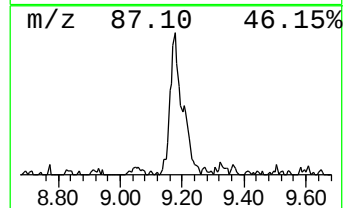
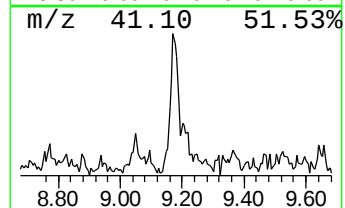
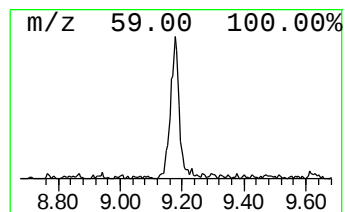
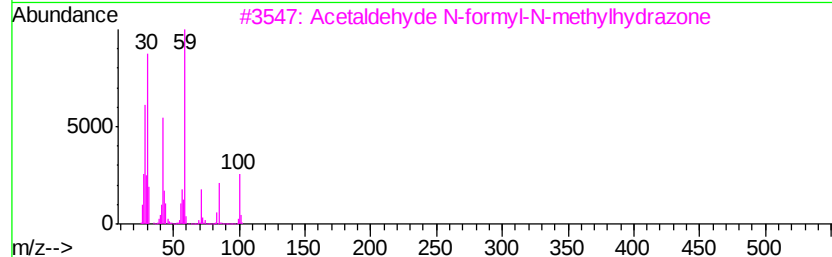
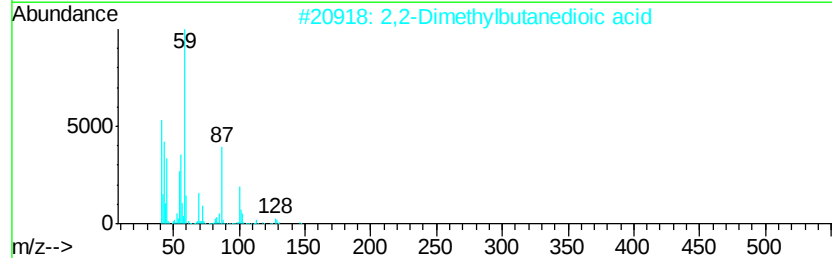
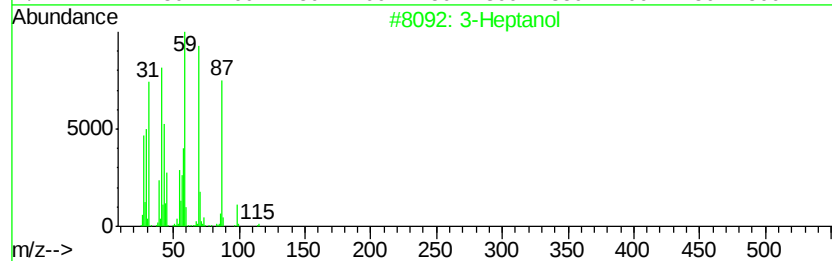
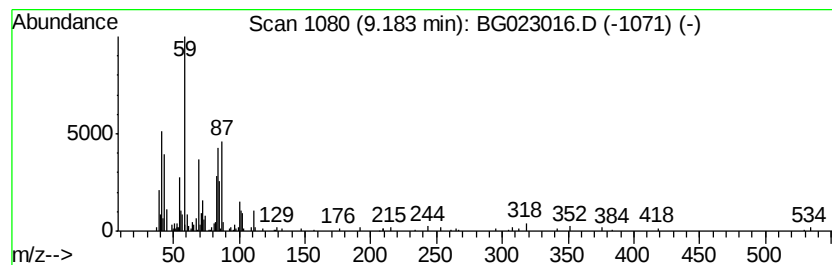
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Peak Number 6 unknown9.18 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.18	6.13 ng	236400	1,4-Dichlorobenzene-d4	8.15

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Heptanol	116	C7H16O	000589-82-2	43
2		2,2-Dimethylbutanedioic acid	146	C6H10O4	000597-43-3	40
3		Acetaldehyde N-formyl-N-methylhydrazone	100	C4H8N2O	016568-02-8	32
4		Pentan-2-ol, 4-allyloxy-2-methyl-	158	C9H18O2	102840-52-8	32
5		1-Butene, 4-ethoxy-	100	C6H12O	044611-46-3	25



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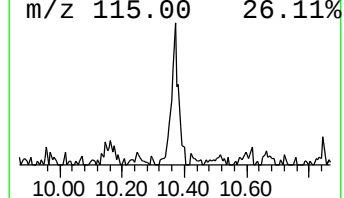
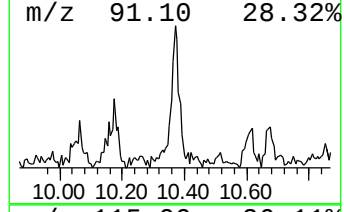
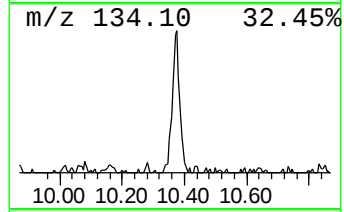
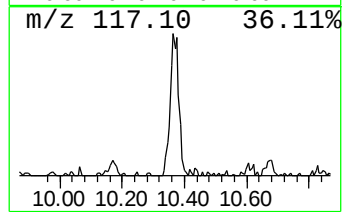
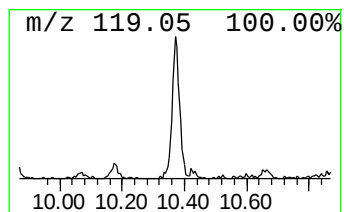
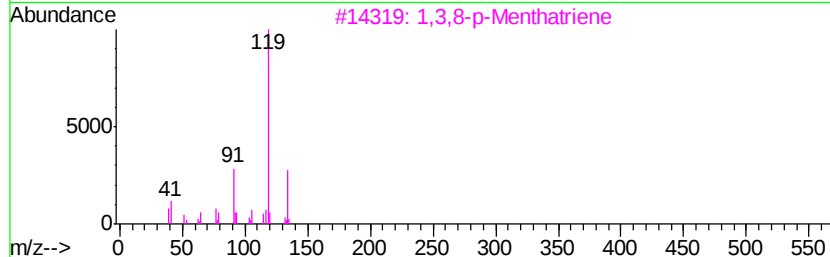
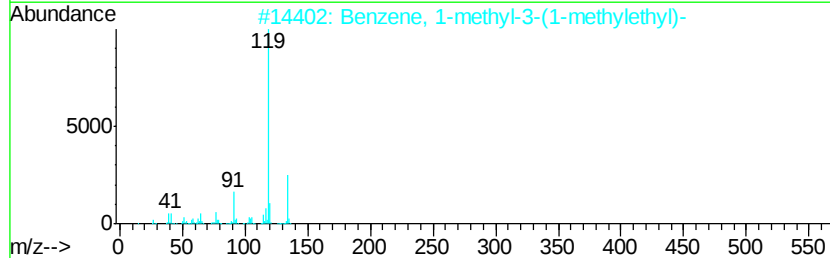
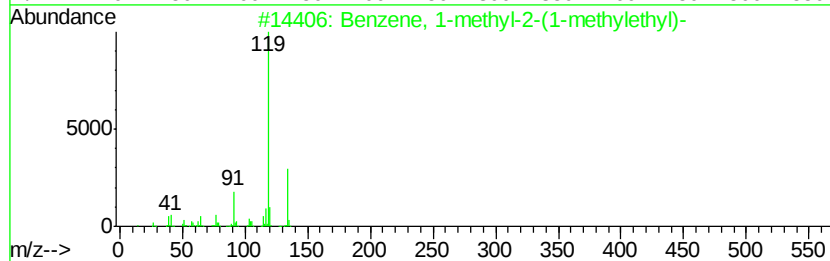
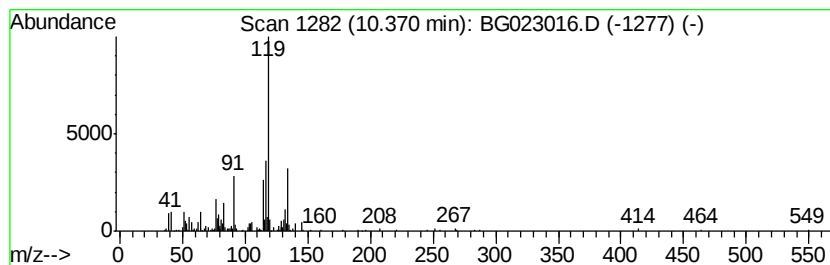
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Benzene, 1-methyl-2-(1-meth... Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.37	4.02 ng	247437	Naphthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-methyl-2-(1-methyleth...	134	C10H14	000527-84-4	58
2		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	58
3		1,3,8-p-Menthatriene	134	C10H14	021195-59-5	58
4		Benzene, 1-methyl-4-(1-methyleth...	134	C10H14	000099-87-6	52
5		Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
Operator : UM/SJ
Sample : H3967-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S22-0008

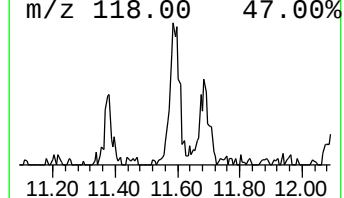
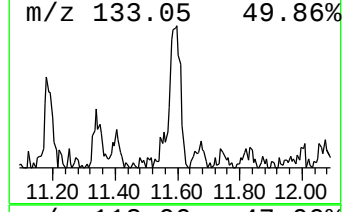
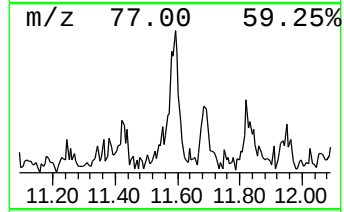
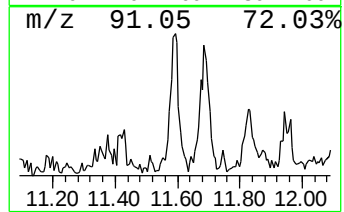
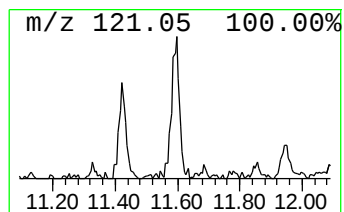
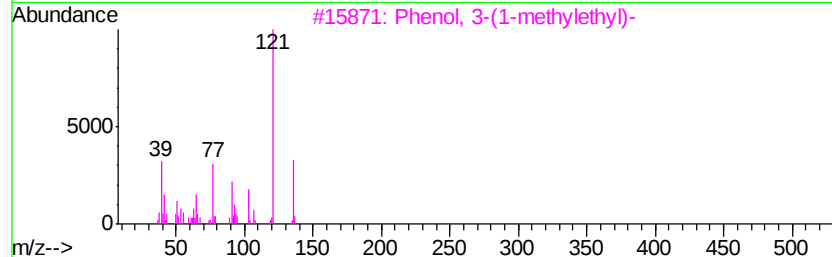
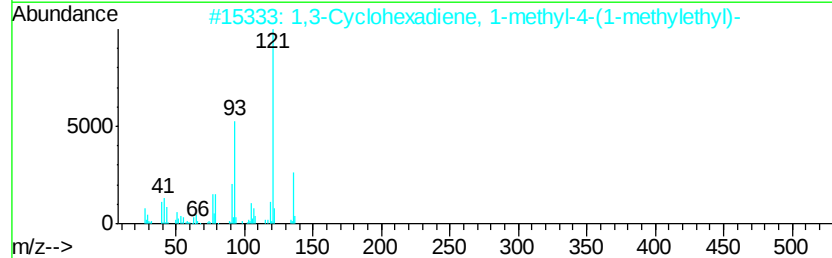
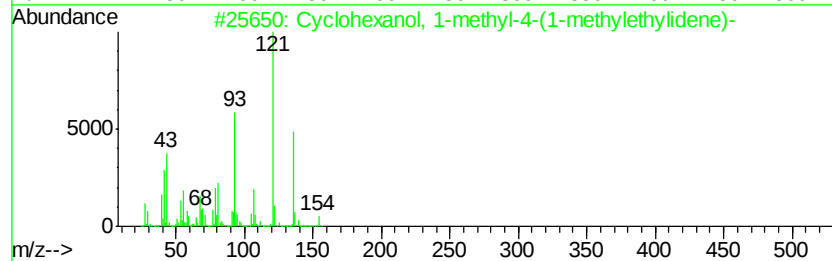
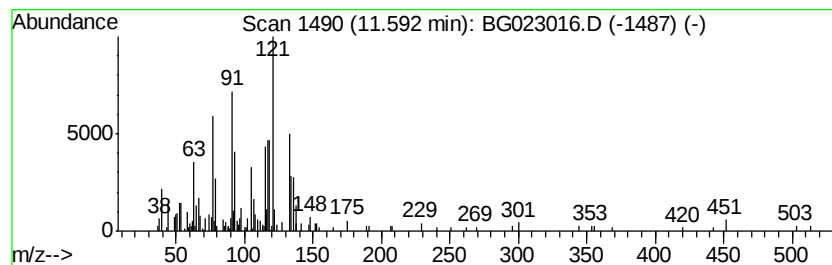
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown11.59 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.59	2.92 ng	179610	Napthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclohexanol, 1-methyl-4-(1-meth...	154	C10H18O	000586-81-2	30
2		1,3-Cyclohexadiene, 1-methyl-4-(...	136	C10H16	000099-86-5	25
3		Phenol, 3-(1-methylethyl)-	136	C9H12O	000618-45-1	25
4		Benzene, 1-ethyl-4-methoxy-	136	C9H12O	001515-95-3	25
5		Benzenemethanol, .alpha.,4-dimet...	136	C9H12O	000536-50-5	25



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
Operator : UM/SJ
Sample : H3967-05
Misc :
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Instrument :
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ClientSampleId :
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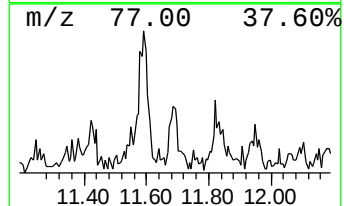
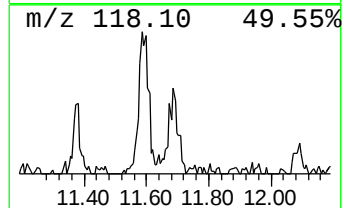
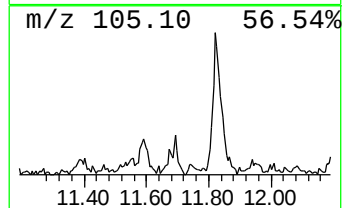
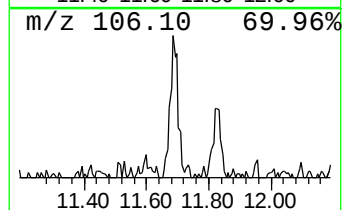
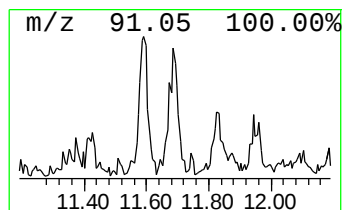
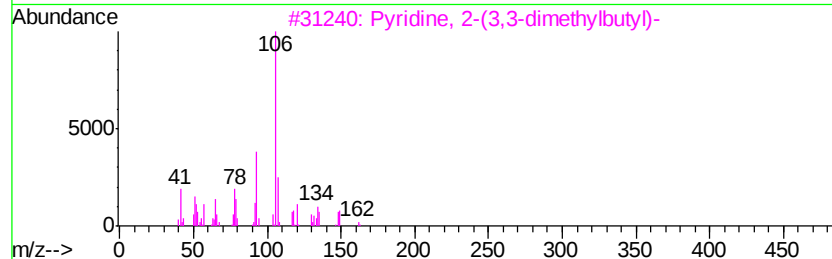
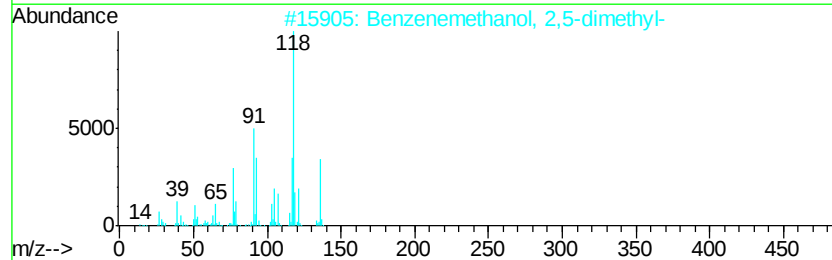
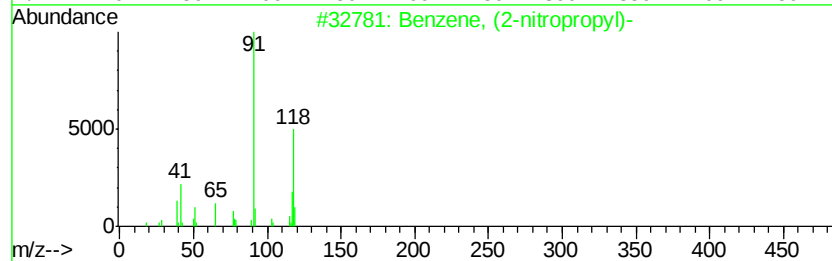
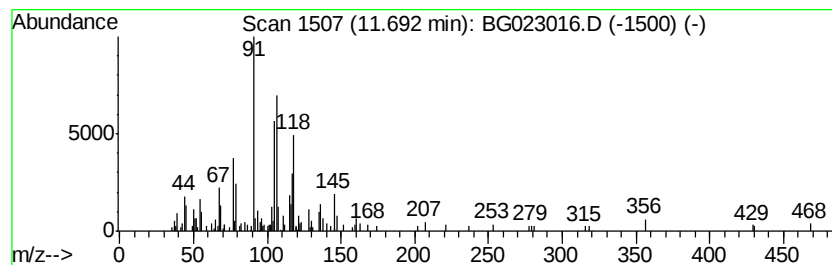
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown11.69 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.69	2.27 ng	139646	Naphthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, (2-nitropropyl)-	165	C9H11NO2	017322-34-8	27
2		Benzenemethanol, 2,5-dimethyl-	136	C9H12O	053957-33-8	27
3		Pyridine, 2-(3,3-dimethylbutyl)-	163	C11H17N	060263-44-7	22
4		p-Xylene	106	C8H10	000106-42-3	11
5		o-Xylene	106	C8H10	000095-47-6	11



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
Operator : UM/SJ
Sample : H3967-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

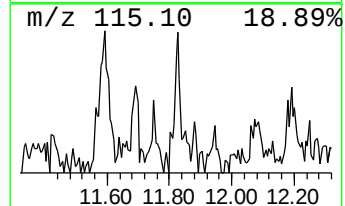
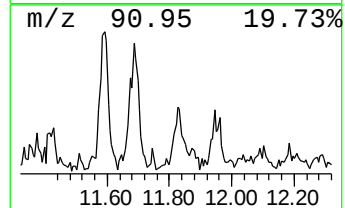
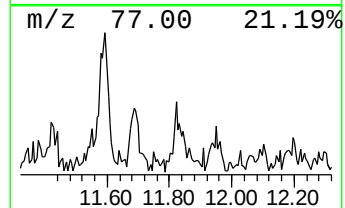
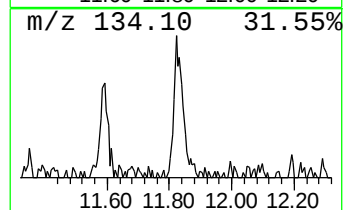
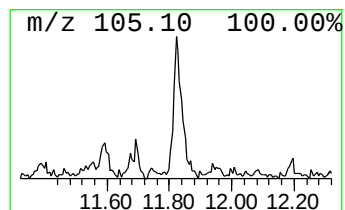
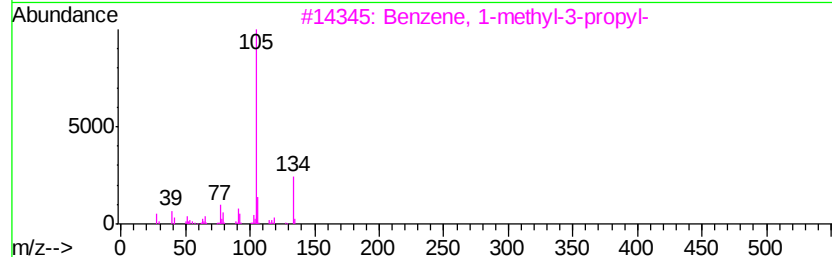
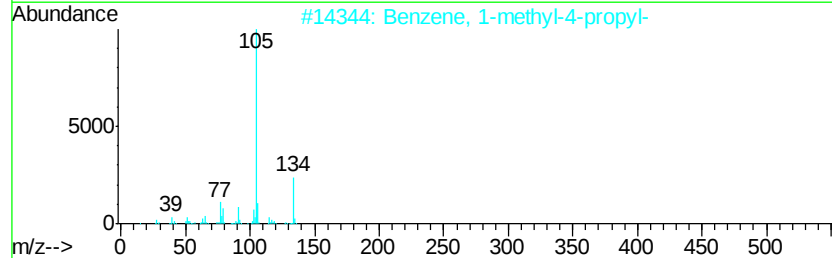
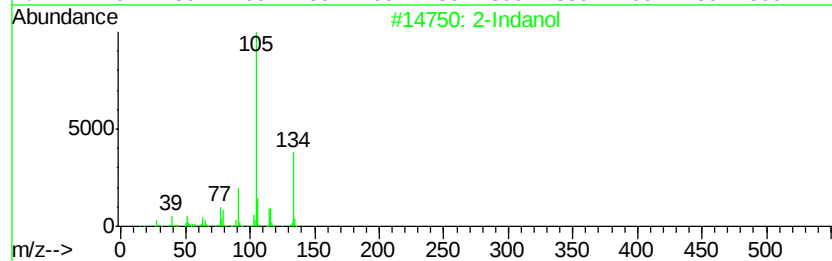
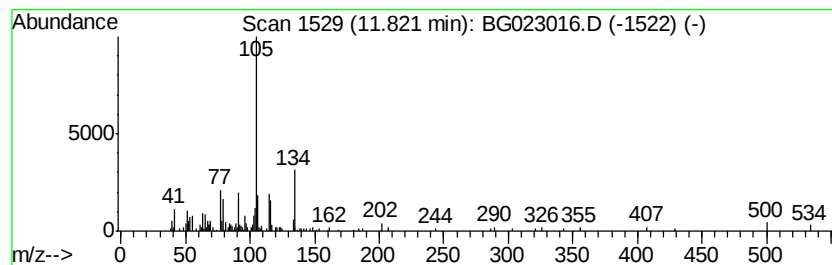
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ClientSampleId :
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG070816.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 2-Indanol Concentration Rank 14

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.82	2.17 ng	133662	Napthalene-d8	10.98
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Indanol		134 C9H10O	004254-29-9 52
2	Benzene, 1-methyl-4-propyl-		134 C10H14	001074-55-1 49
3	Benzene, 1-methyl-3-propyl-		134 C10H14	001074-43-7 47
4	Oxirane, 2-methyl-2-phenyl-		134 C9H10O	002085-88-3 43
5	Benzene, 1-(bromomethyl)-3-methyl-		184 C8H9Br	000620-13-3 43



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
Operator : UM/SJ
Sample : H3967-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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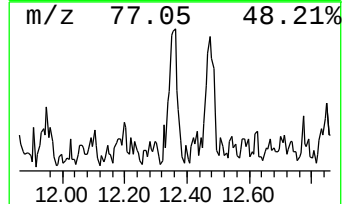
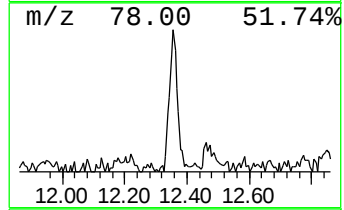
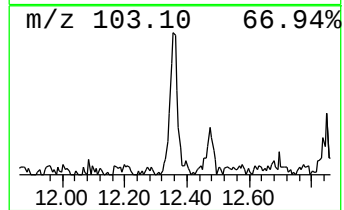
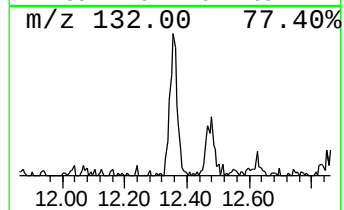
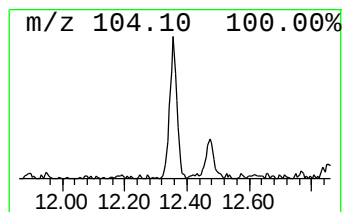
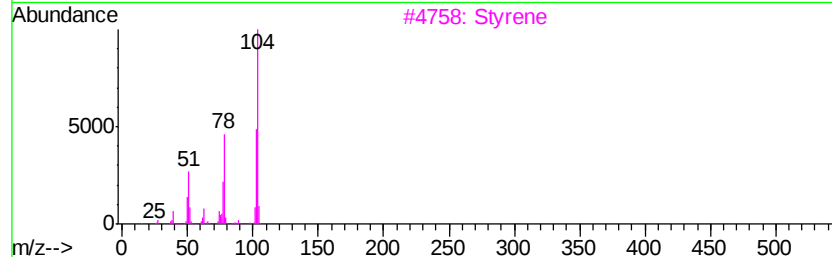
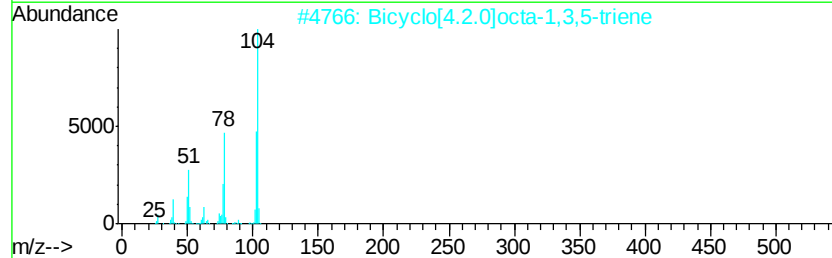
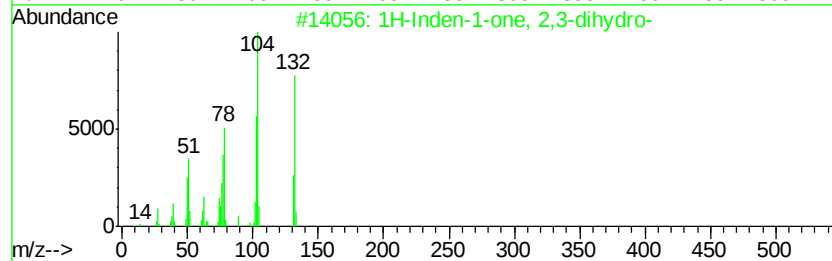
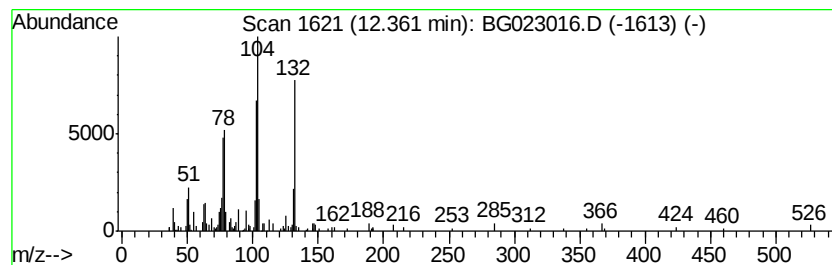
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	2.71 ng	167061	Napthalene-d8	10.98

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	93
2		Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	58
3		Styrene	104	C8H8	000100-42-5	58
4		1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	52
5		2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	50



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
Operator : UM/SJ
Sample : H3967-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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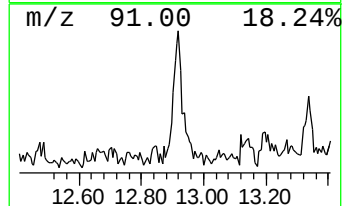
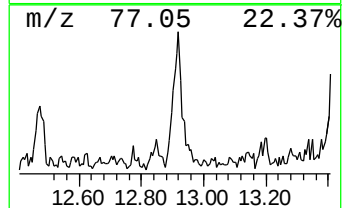
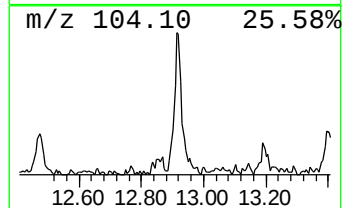
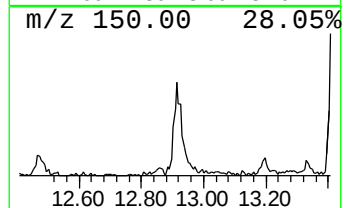
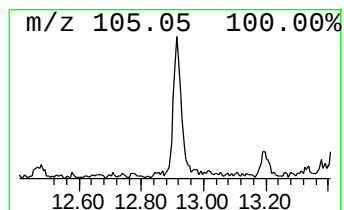
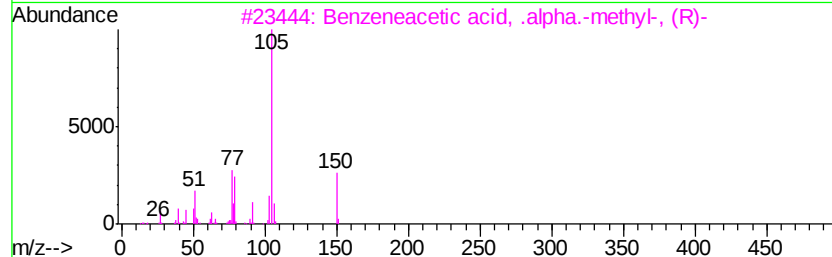
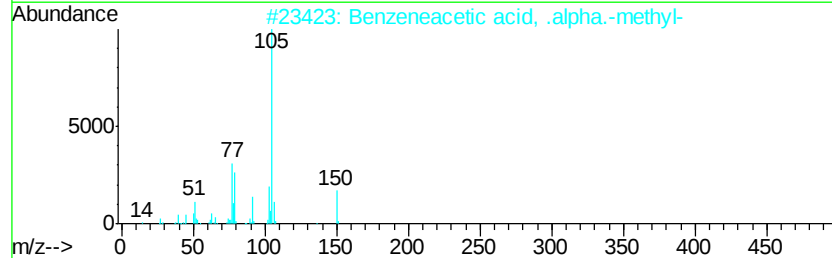
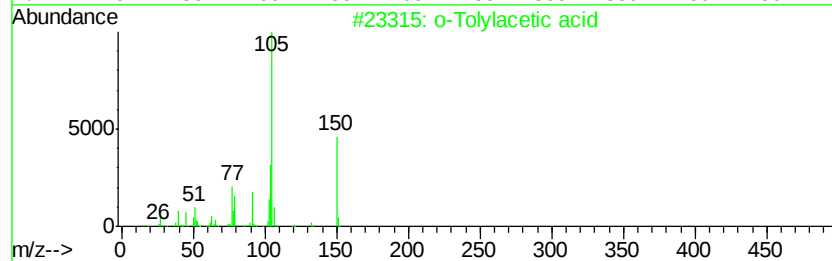
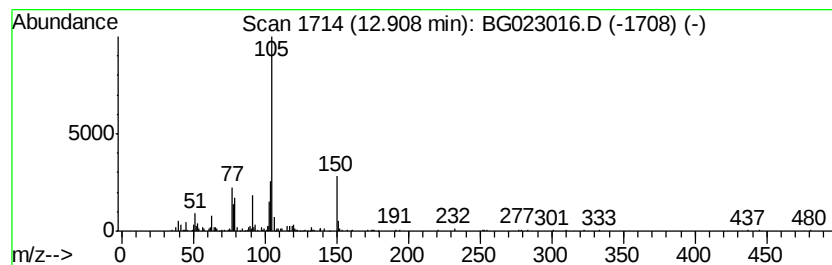
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 o-Tolylacetic acid Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.91	3.24 ng	316417	Acenaphthene-d10	14.80

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	o-Tolylacetic acid	150	C9H10O2	000644-36-0	91
2		Benzeneacetic acid, .alpha.-methyl-	150	C9H10O2	000492-37-5	68
3		Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-26-5	60
4		m-Tolylacetic acid	150	C9H10O2	000621-36-3	60
5		Benzeneacetic acid, .alpha.-meth...	150	C9H10O2	007782-24-3	60



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
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Misc :
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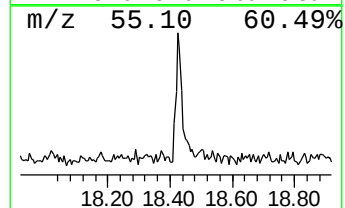
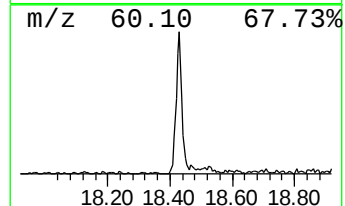
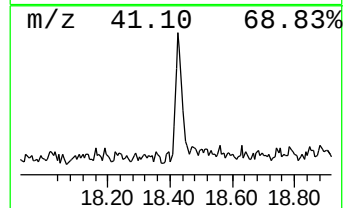
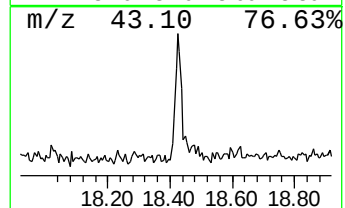
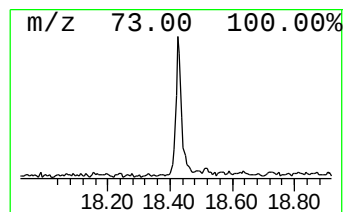
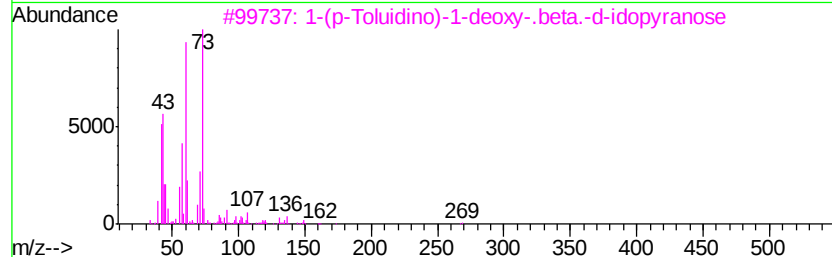
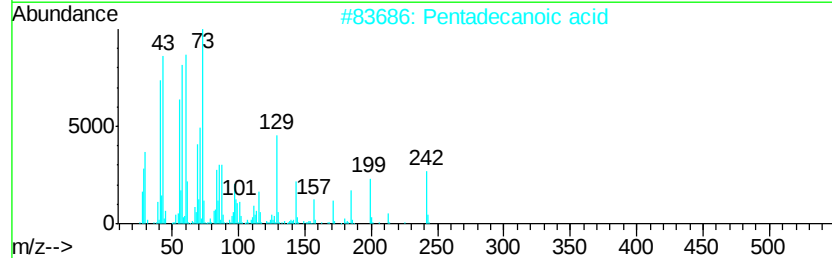
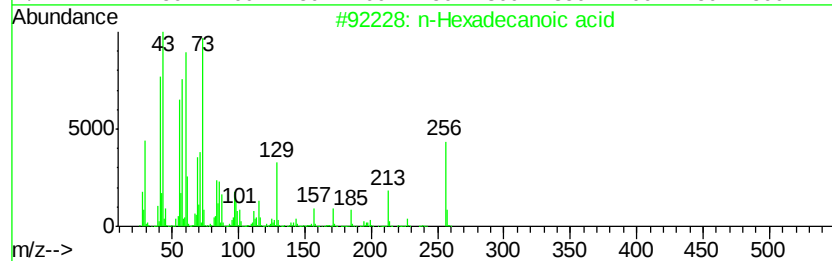
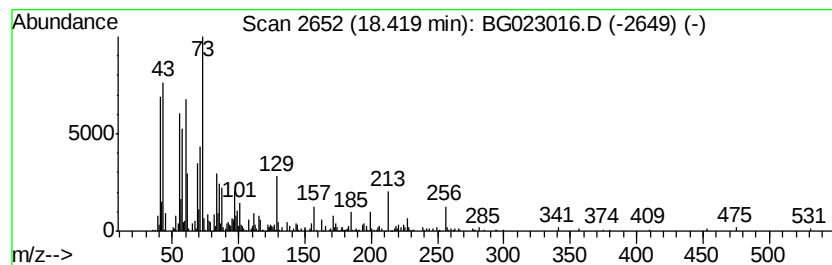
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 n-Hexadecanoic acid Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.42	4.48 ng	515275	Phenanthrene-d10	17.56

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Hexadecanoic acid	256	C16H32O2	000057-10-3	98
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	68
3		1-(p-Toluidino)-1-deoxv-.beta.-d...	269	C13H19NO5	1000226-06-4	43
4		n-Decanoic acid	172	C10H20O2	000334-48-5	43
5		Tridecanoic acid	214	C13H26O2	000638-53-9	42



Data Path : Z:\HPCHEM1\BNA G\DATA\BG071116\
Data File : BG023016.D
Acq On : 12 Jul 2016 1:18
Operator : UM/SJ
Sample : H3967-05
Misc :
ALS Vial : 14 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
S22-0008

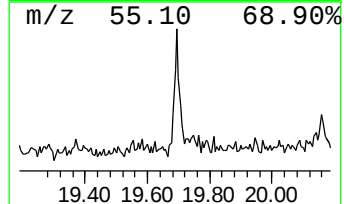
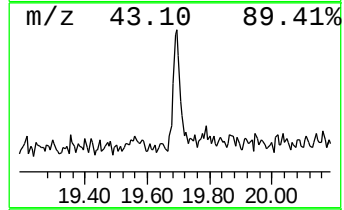
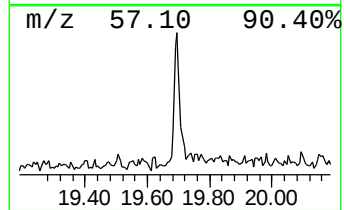
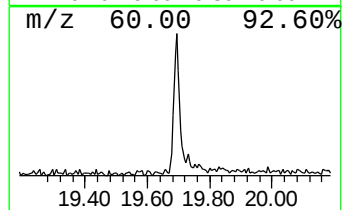
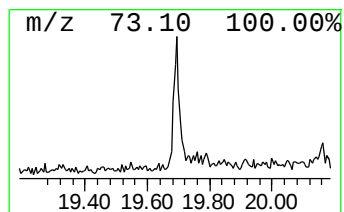
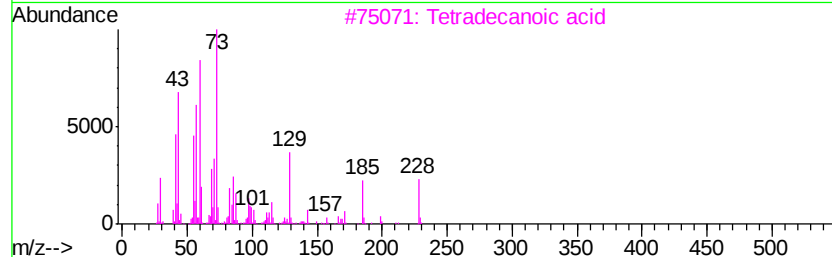
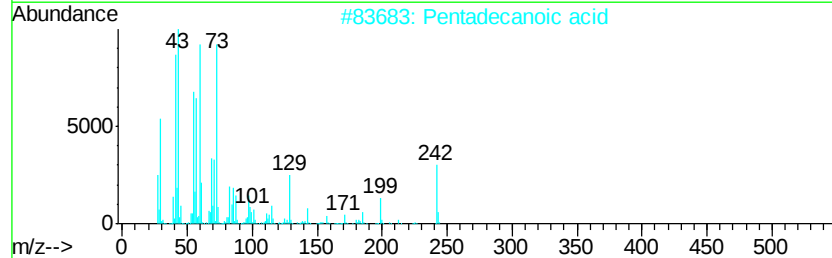
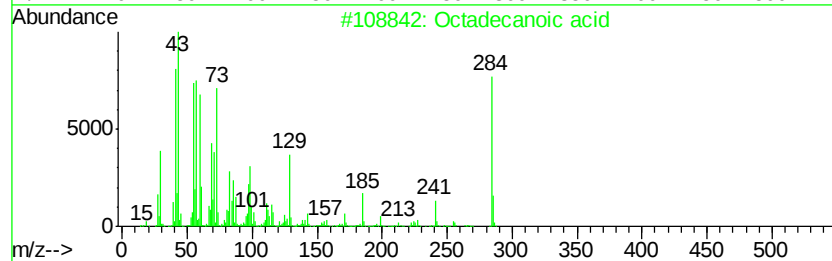
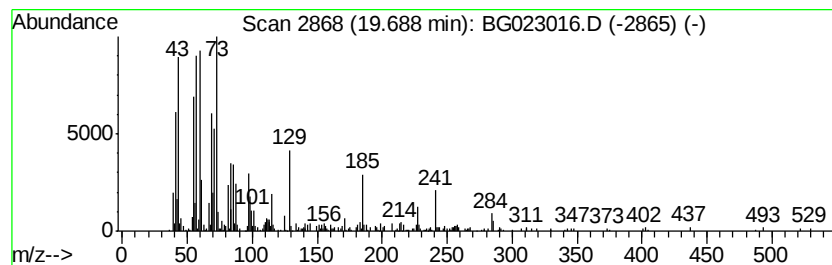
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 14 Octadecanoic acid Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
19.69	3.29 ng	377923	Phenanthrene-d10	17.56

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Octadecanoic acid	284	C18H36O2	000057-11-4	83
2		Pentadecanoic acid	242	C15H30O2	001002-84-2	81
3		Tetradecanoic acid	228	C14H28O2	000544-63-8	72
4		n-Decanoic acid	172	C10H20O2	000334-48-5	64
5		Lactose	342	C12H22O11	000063-42-3	47



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG071116\
 Data File : BG023016.D
 Acq On : 12 Jul 2016 1:18
 Operator : UM/SJ
 Sample : H3967-05
 Misc :
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 S22-0008

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG070816.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
2-Pentanone, 4-hy...	5.22	5.3	ng	203794	1	8.15	771567	20.0
Benzene, 1-ethyl-...	7.53	12.8	ng	492431	1	8.15	771567	20.0
unknown7.68	7.68	93.1	ng	3590650	1	8.15	771567	20.0
Benzene, 1,3,5-tr...	8.27	12.1	ng	465679	1	8.15	771567	20.0
unknown9.18	9.18	6.1	ng	236400	1	8.15	771567	20.0
Benzene, 1-methyl...	10.37	4.0	ng	247437	2	10.98	1231070	20.0
unknown11.59	11.59	2.9	ng	179610	2	10.98	1231070	20.0
unknown11.69	11.69	2.3	ng	139646	2	10.98	1231070	20.0
2-Indanol	11.82	2.2	ng	133662	2	10.98	1231070	20.0
1H-Inden-1-one, 2...	12.36	2.7	ng	167061	2	10.98	1231070	20.0
o-Tolylacetic acid	12.91	3.2	ng	316417	3	14.80	1955880	20.0
n-Hexadecanoic acid	18.42	4.5	ng	515275	4	17.56	2298940	20.0
Octadecanoic acid	19.69	3.3	ng	377923	4	17.56	2298940	20.0