

Data Path : Z:\HPCHEM1\BNA G\DATA\BG101315\
 Data File : BG019167.D
 Acq On : 12 Oct 2015 21:06
 Operator : UM/NP
 Sample : PB85643BL
 Misc :
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 BNA_G
 ClientSampleId :
 PB85643BL

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-BG101015.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	3.000	22	27	46	rBV	1429847	1722537	94.00%	16.308%
2	3.217	59	64	68	rBV	30117	35886	1.96%	0.340%
3	5.138	385	391	402	rVB	182179	262775	14.34%	2.488%
4	5.608	465	471	480	rBV	333125	526208	28.72%	4.982%
5	7.201	731	742	751	rBV	369738	614336	33.53%	5.816%
6	7.571	797	805	812	rBV	333713	565752	30.87%	5.356%
7	8.029	877	883	890	rBV	64195	108847	5.94%	1.031%
8	8.358	932	939	947	rVB	235759	403642	22.03%	3.821%
9	9.193	1073	1081	1093	rBV	225528	391165	21.35%	3.703%
10	10.838	1354	1361	1370	rVB	99283	172616	9.42%	1.634%
11	13.288	1771	1778	1785	rBV	622581	979019	53.43%	9.269%
12	14.663	2005	2012	2021	rVB2	171945	281334	15.35%	2.664%
13	16.149	2258	2265	2278	rBV	631952	950908	51.89%	9.003%
14	17.406	2472	2479	2485	rBV	260938	387580	21.15%	3.669%
15	20.021	2917	2924	2929	rBV	1386204	1832459	100.00%	17.349%
16	21.678	3199	3206	3219	rBV	301426	488297	26.65%	4.623%
17	23.364	3486	3493	3502	rBV7	10396	22875	1.25%	0.217%
18	24.433	3669	3675	3681	rBV7	15843	37431	2.04%	0.354%
19	24.909	3744	3756	3773	rBV2	154035	451361	24.63%	4.273%
20	25.755	3891	3900	3913	rVB6	21743	70567	3.85%	0.668%
21	27.401	4167	4180	4190	rBV6	24040	92848	5.07%	0.879%
22	29.469	4520	4532	4545	rVB9	22330	99722	5.44%	0.944%
23	32.083	4961	4977	4980	rBV8	15889	64284	3.51%	0.609%

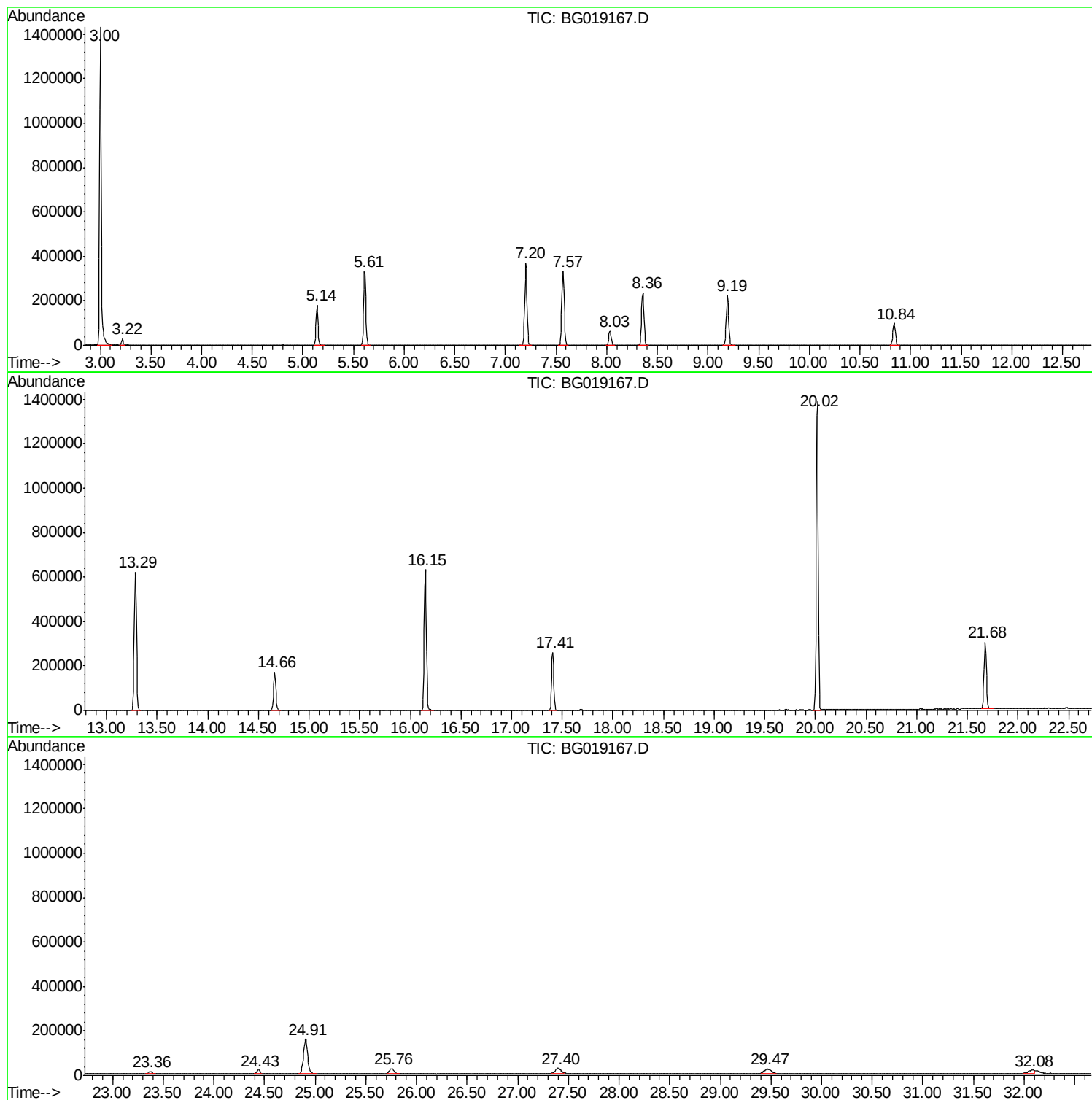
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Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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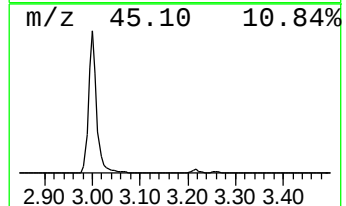
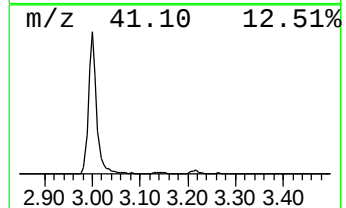
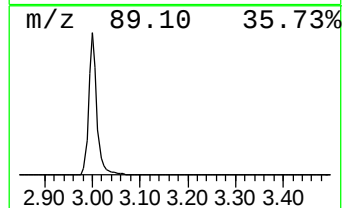
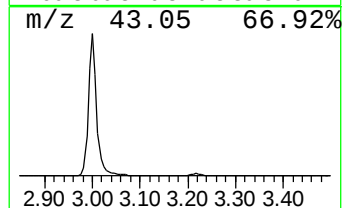
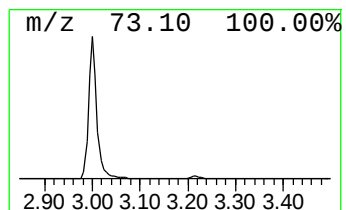
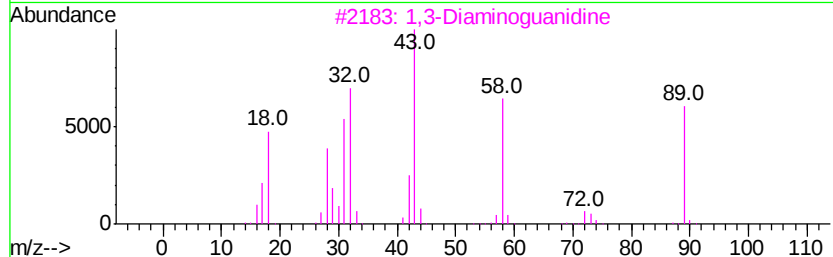
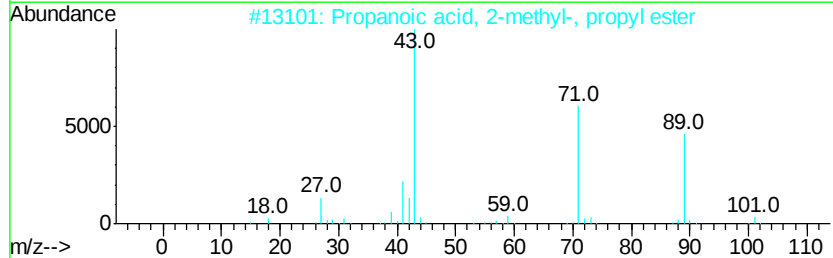
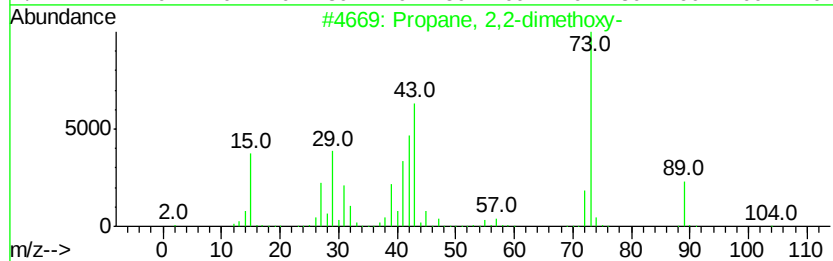
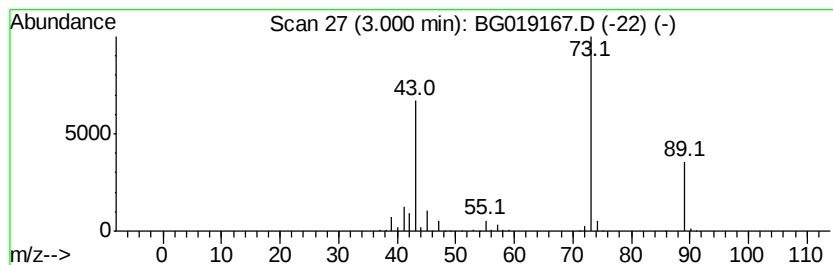
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 unknown3.00 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.00	316.51 ng	1722540	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	28
2		Propanoic acid, 2-methyl-, propyl...	130	C7H14O2	000644-49-5	27
3		1,3-Diaminoquanidine	89	CH7N5	004364-78-7	9
4		Acetamide, N-methyl-	73	C3H7NO	000079-16-3	9
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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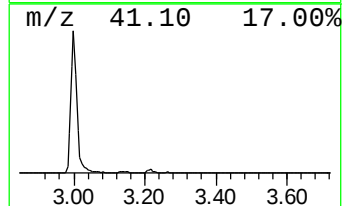
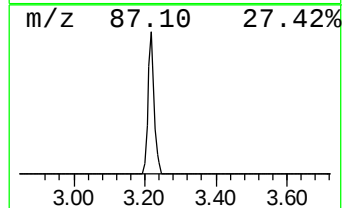
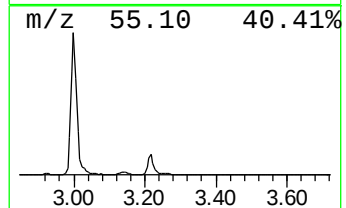
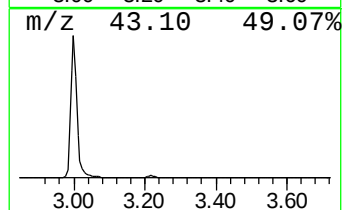
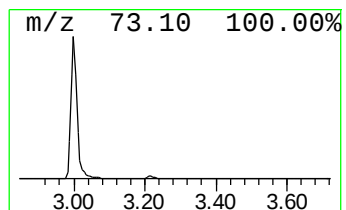
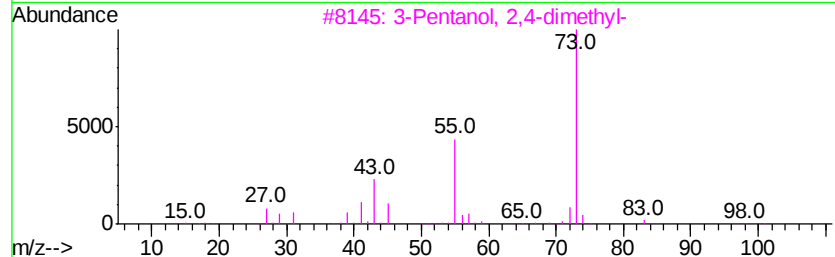
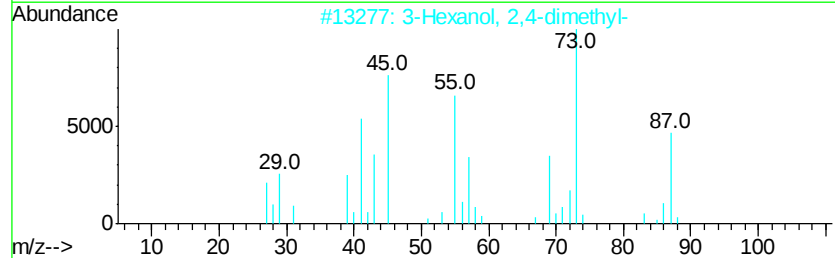
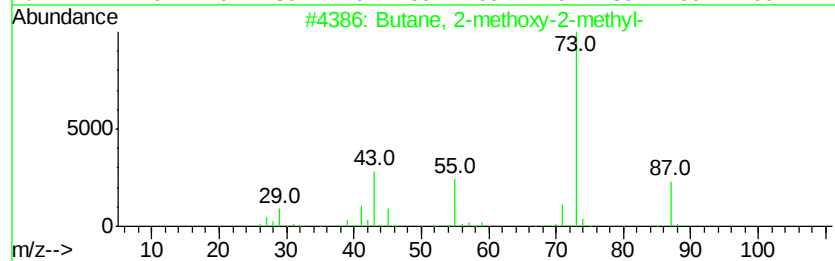
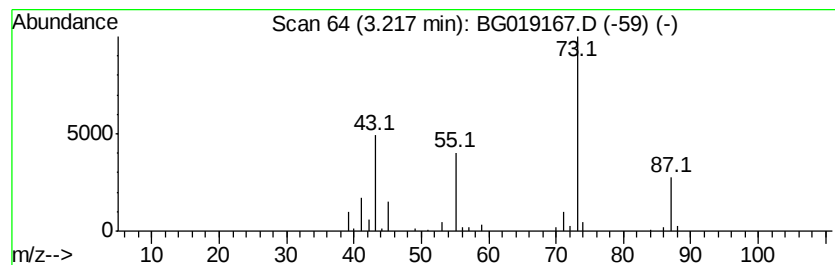
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.22	6.59 ng	35886	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		3-Hexanol, 2,4-dimethyl-	130	C8H18O	013432-25-2	30
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	25
4		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	23
5		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	12



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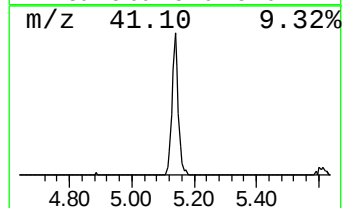
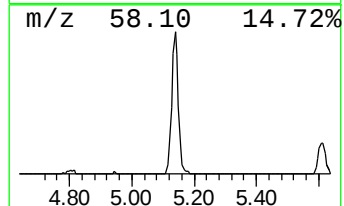
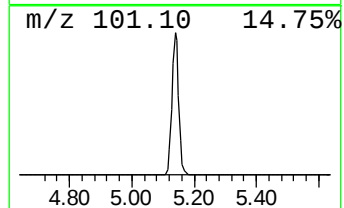
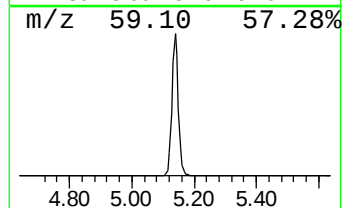
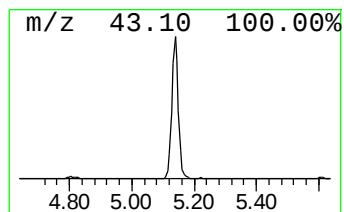
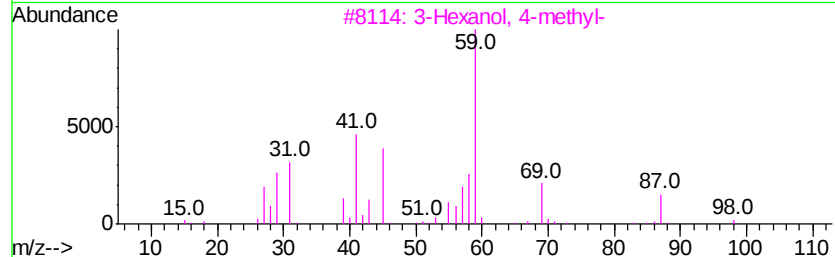
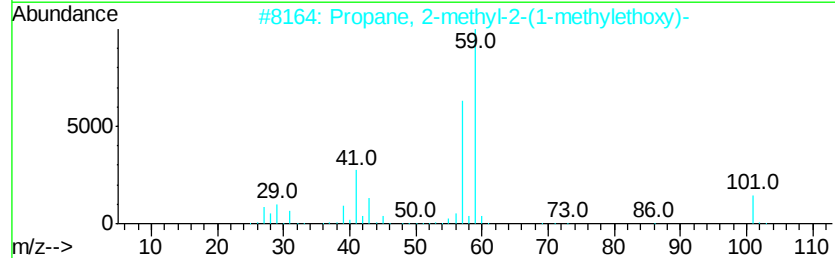
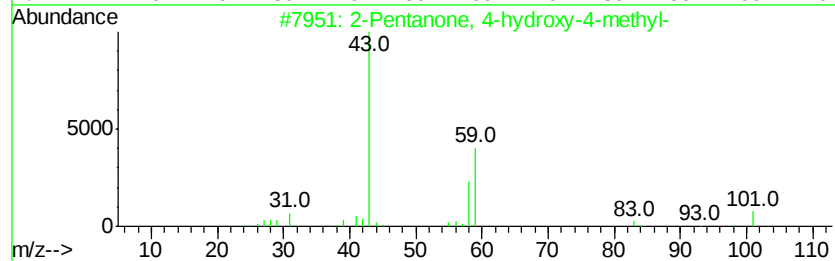
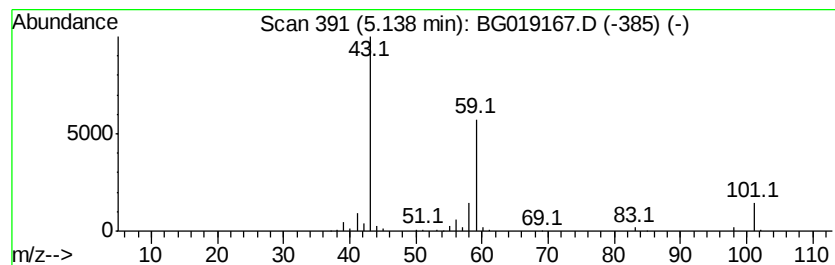
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TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.14	48.28 ng	262775	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4		2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
5		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25



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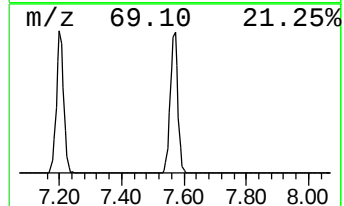
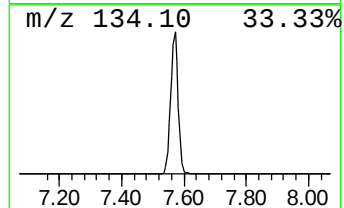
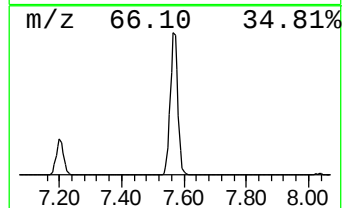
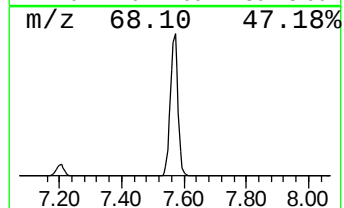
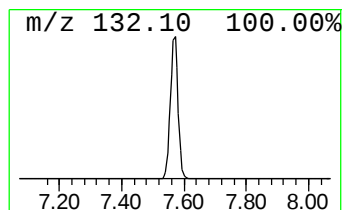
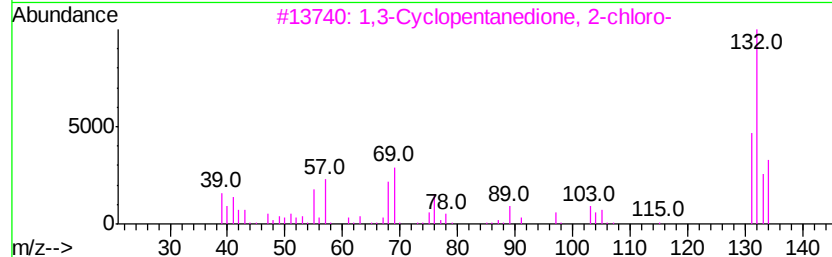
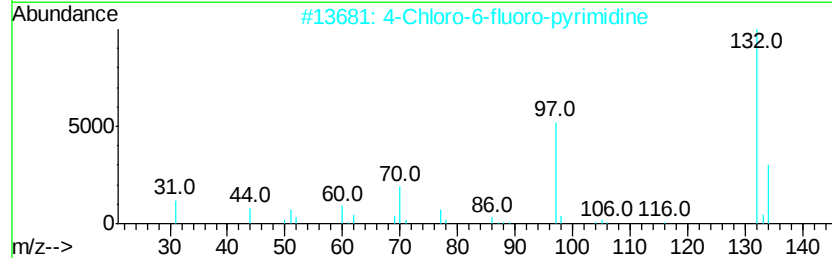
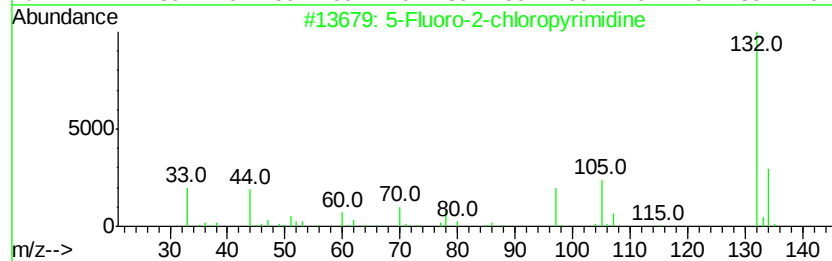
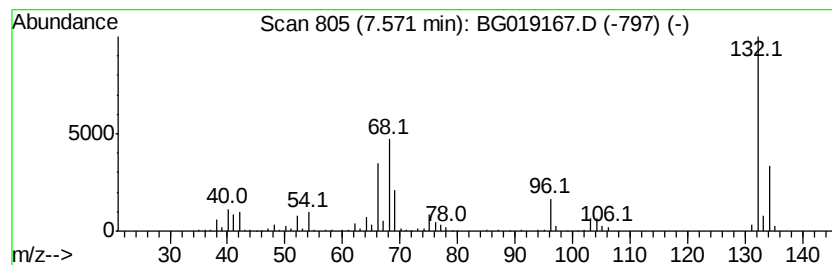
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Peak Number 4 unknown7.57 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.57	103.95 ng	565752	1,4-Dichlorobenzene-d4	8.03

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	27
2		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	27
3		1,3-Cyclopentanedione, 2-chloro-	132	C5H5ClO2	014203-19-1	25
4		5-Aminoindole	132	C8H8N2	005192-03-0	22
5		1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22



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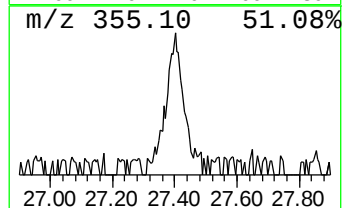
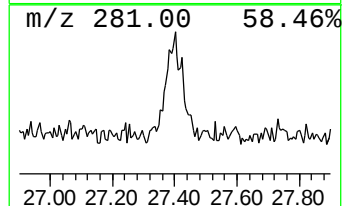
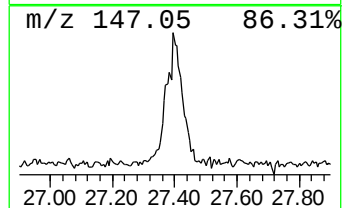
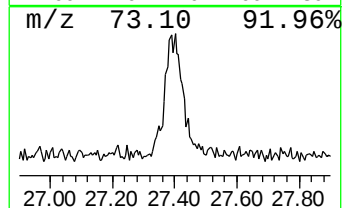
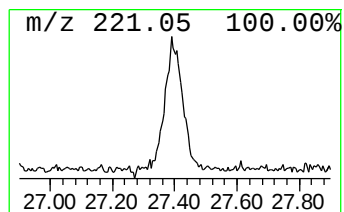
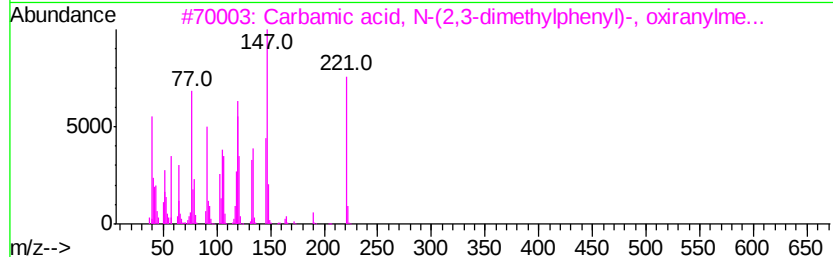
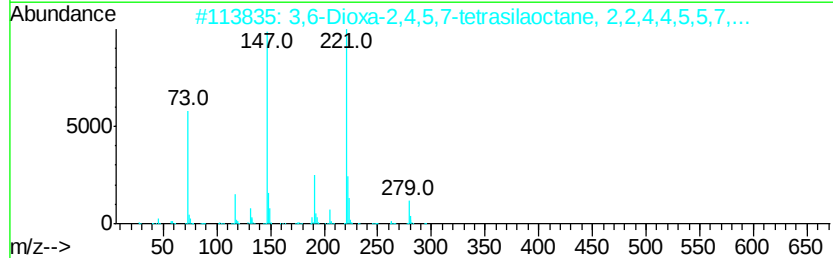
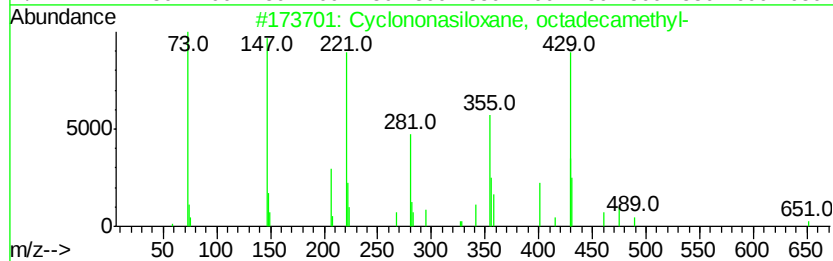
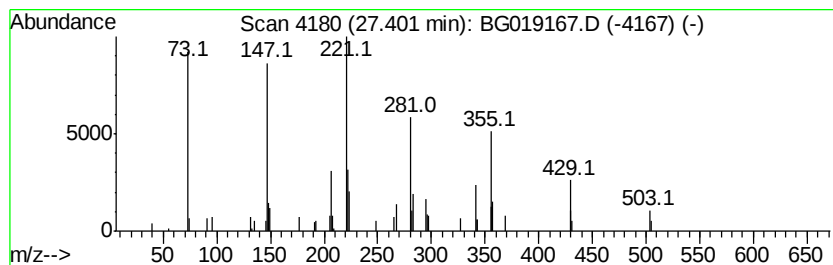
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Peak Number 7 unknown27.40 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
27.40	4.11 ng	92848	Perylene-d12	24.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	72
2			3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
3			Carbamic acid, N-(2,3-dimethylph...	221	C12H15N03	339273-79-9	32
4			Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	27
5			N-Benzyl-N-ethyl-p-isopropylbenz...	281	C19H23NO	015089-22-2	22



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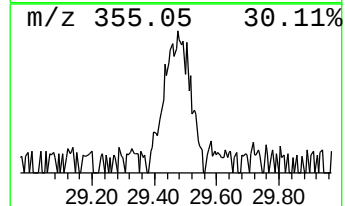
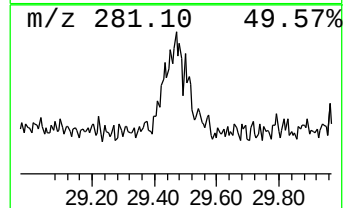
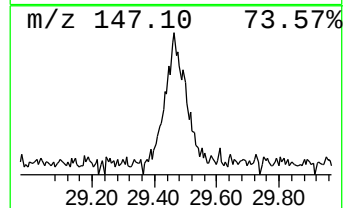
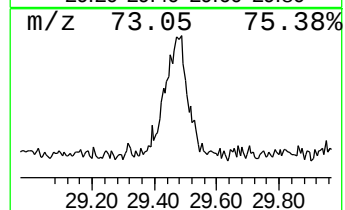
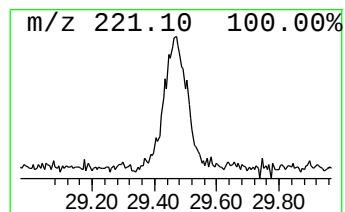
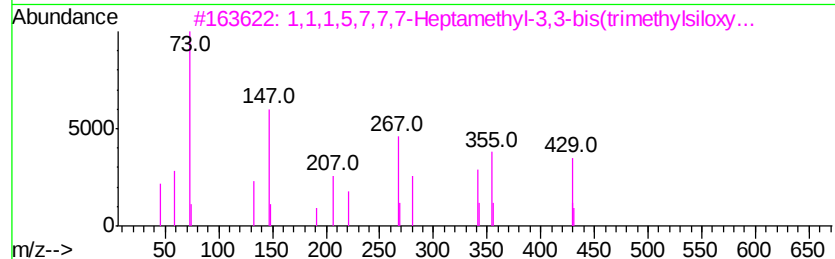
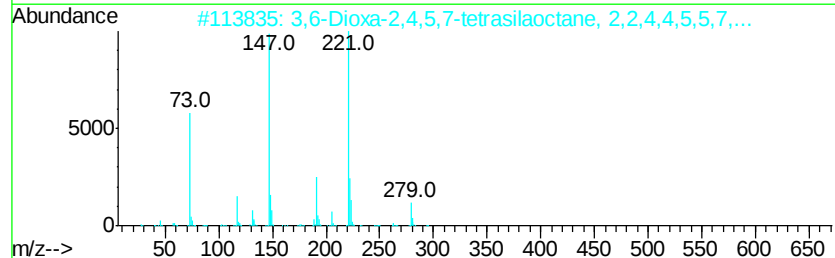
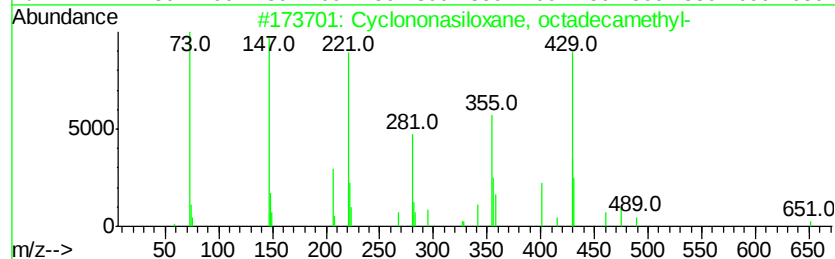
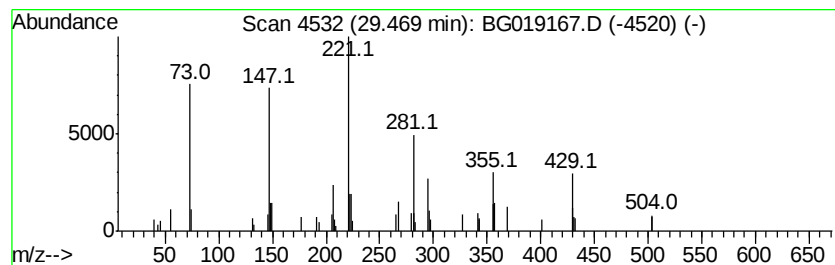
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 unknown29.47 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
29.47	4.42 ng	99722	Perylene-d12	24.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	50
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	47
3		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	27
4		Dithioerythritol, 0,0',S,S'-tetr...	442	C16H42O2S2Si4	1000079-30-7	25
5		Trisiloxane, octamethyl-	236	C8H24O2Si3	000107-51-7	22



Data Path : Z:\HPCHEM1\BNA G\DATA\BG101315\
Data File : BG019167.D
Acq On : 12 Oct 2015 21:06
Operator : UM/NP
Sample : PB85643BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB85643BL

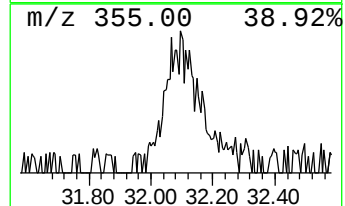
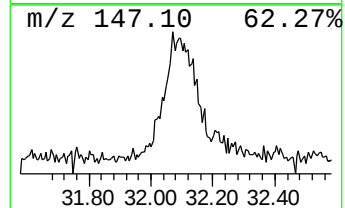
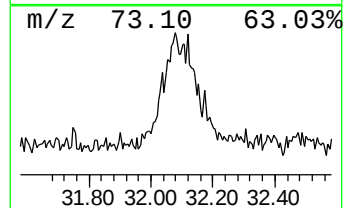
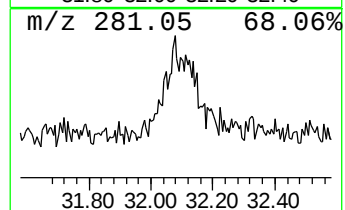
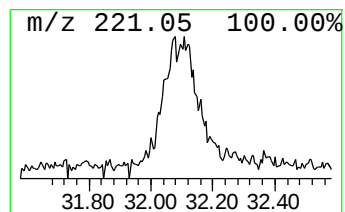
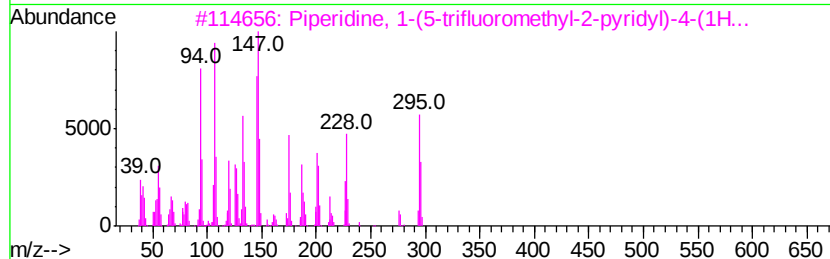
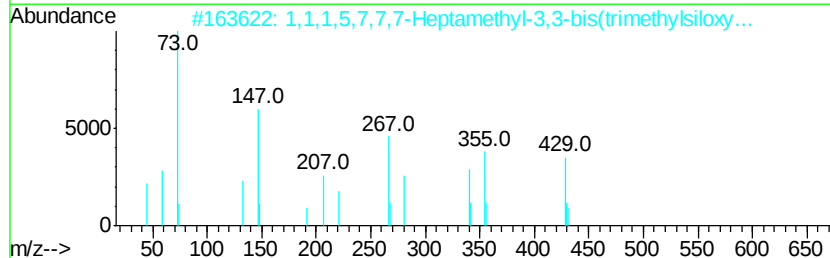
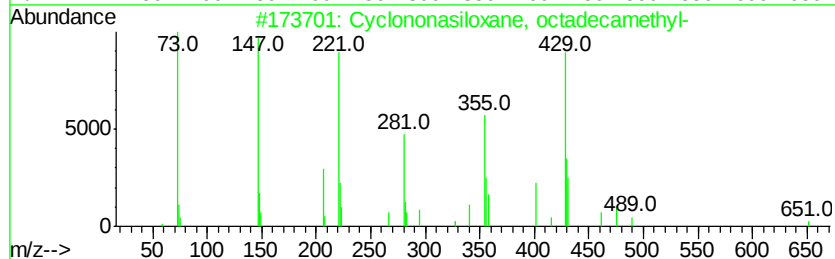
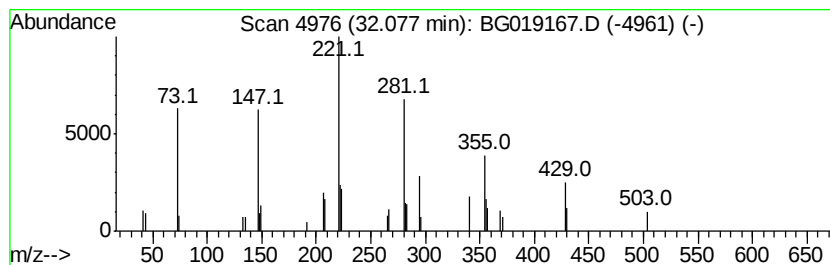
Quant Method : Z:\HPCHEM1\BNA G\METHODS\8270-BG101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 unknown32.08 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
32.08	2.85 ng	64284	Perylene-d12	24.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclononasiloxane, octadecamethyl-	666	C18H54O9Si9	000556-71-8	78
2		1,1,1,5,7,7,7-Heptamethyl-3,3-bi...	444	C13H40O5Si6	038147-00-1	36
3		Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	25
4		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	12
5		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	12



Data Path : Z:\HPCHEM1\BNA_G\DATA\BG101315\
Data File : BG019167.D
Acq On : 12 Oct 2015 21:06
Operator : UM/NP
Sample : PB85643BL
Misc :
ALS Vial : 3 Sample Multiplier: 1

Instrument :
BNA_G
ClientSampleId :
PB85643BL

Quant Method : Z:\HPCHEM1\BNA_G\METHODS\8270-BG101015.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
unknown3.00	3.00	316.5	ng	1722540	1	8.03	108847	20.0
Butane, 2-methoxy...	3.22	6.6	ng	35886	1	8.03	108847	20.0
2-Pentanone, 4-hy...	5.14	48.3	ng	262775	1	8.03	108847	20.0
unknown7.57	7.57	104.0	ng	565752	1	8.03	108847	20.0
unknown27.40	27.40	4.1	ng	92848	6	24.90	451361	20.0
unknown29.47	29.47	4.4	ng	99722	6	24.90	451361	20.0
unknown32.08	32.08	2.9	ng	64284	6	24.90	451361	20.0