

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101215\
 Data File : BF082230.D
 Acq On : 12 Oct 2015 20:13
 Operator : UM/IZ
 Sample : G3990-10
 Misc :
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 TE-PMW(2-26)

Integration Parameters: rteint.p
 Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0
 Filtering: 5
 Min Area: 1 % 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_F\METHODS\8270-BF101015.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	4.994	248	250	260	rBV	326747	371139	13.69%	2.257%
2	5.417	285	287	290	rBV	717856	749342	27.63%	4.557%
3	6.457	377	378	381	rBV	369447	451728	16.66%	2.747%
4	6.594	388	390	393	rBV	1480359	1448585	53.42%	8.809%
5	6.834	409	411	413	rBV	309300	347086	12.80%	2.111%
6	6.983	422	424	427	rBV	1365920	1462243	53.93%	8.892%
7	7.406	458	461	463	rBV	1009008	1219350	44.97%	7.415%
8	8.115	521	523	526	rBV	502607	481950	17.77%	2.931%
9	9.200	615	618	620	rBV	2618418	2569040	94.74%	15.623%
10	9.589	650	652	654	rBV	126231	123950	4.57%	0.754%
11	9.875	674	677	679	rBV	677418	601745	22.19%	3.659%
12	10.252	708	710	713	rBV2	51715	68996	2.54%	0.420%
13	10.663	744	746	749	rBV	1418422	1486768	54.83%	9.041%
14	10.778	754	756	760	rVB	21994	36800	1.36%	0.224%
15	10.881	763	765	766	rVV2	21154	28844	1.06%	0.175%
16	10.915	766	768	771	rVB	18797	31739	1.17%	0.193%
17	11.018	776	777	779	rVB2	28482	32188	1.19%	0.196%
18	11.063	779	781	783	rBV	21799	27316	1.01%	0.166%
19	11.361	805	807	809	rBV	669670	604371	22.29%	3.675%
20	11.886	850	853	855	rBV	31202	33583	1.24%	0.204%
21	12.949	943	946	949	rBV	2394971	2711612	100.00%	16.490%
22	13.784	1016	1019	1020	rBV	59079	91971	3.39%	0.559%
23	13.807	1020	1021	1023	rVV	236877	190037	7.01%	1.156%
24	13.841	1023	1024	1031	rVB	33927	43560	1.61%	0.265%
25	14.001	1034	1038	1048	rBV	669545	708402	26.12%	4.308%
26	15.430	1160	1163	1169	rBV	308348	492860	18.18%	2.997%
27	16.104	1219	1222	1226	rVB	17186	28947	1.07%	0.176%

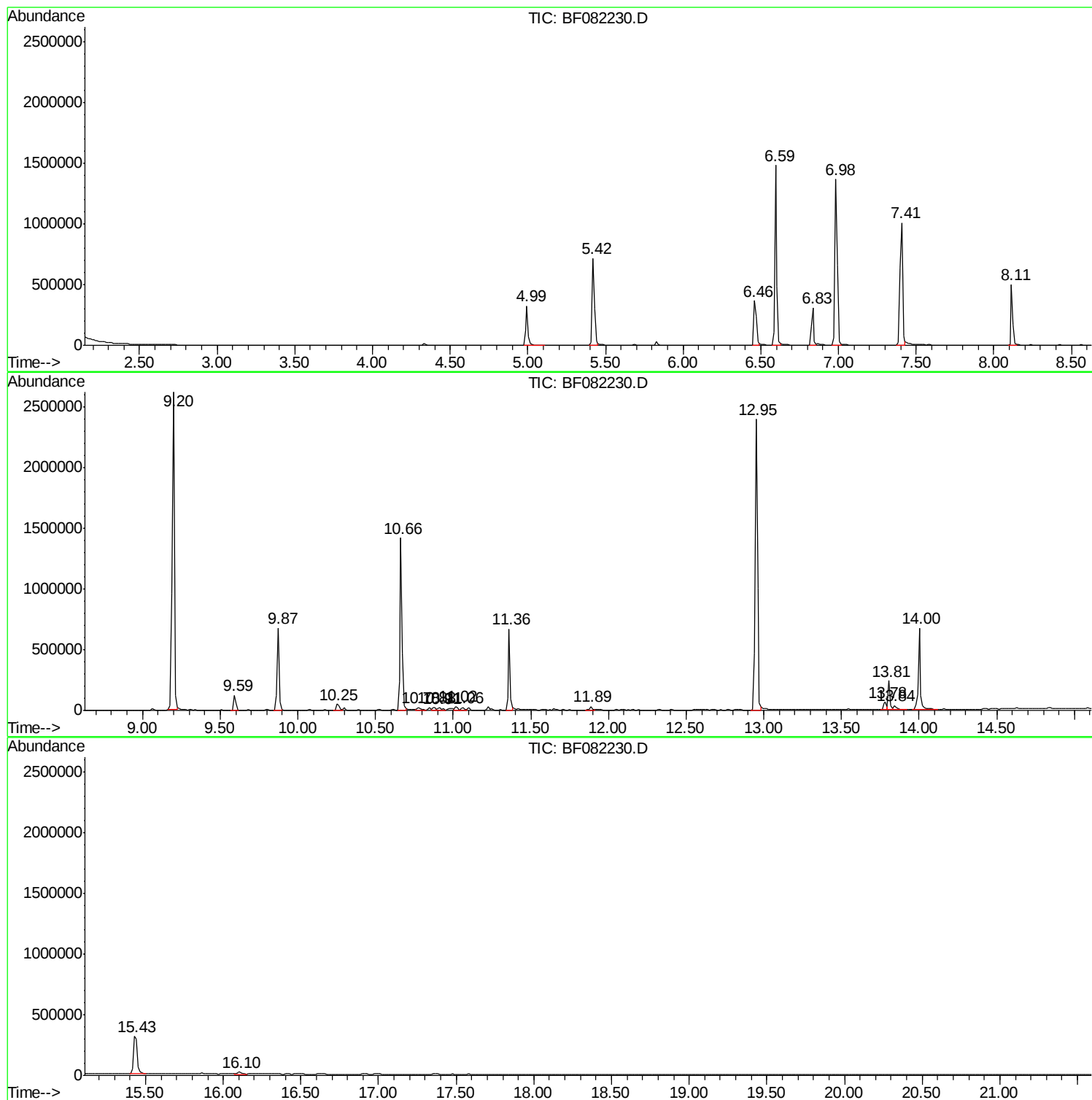
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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Instrument :
BNA_F
ClientSampled :
TE-PMW(2-26)

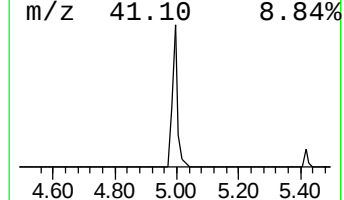
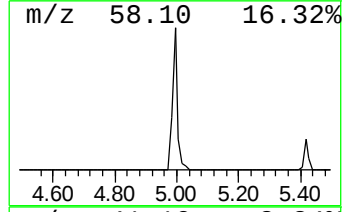
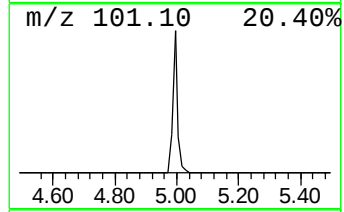
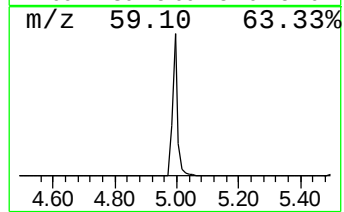
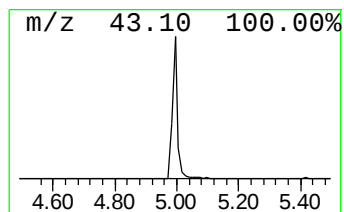
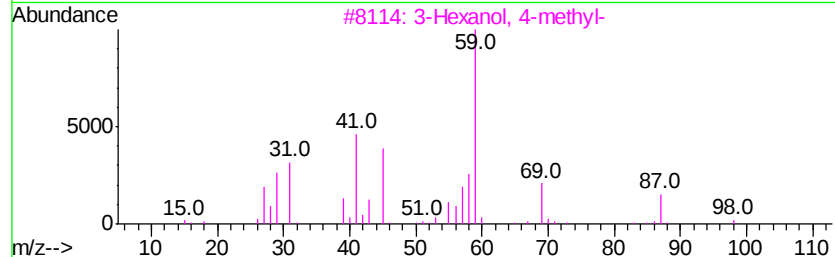
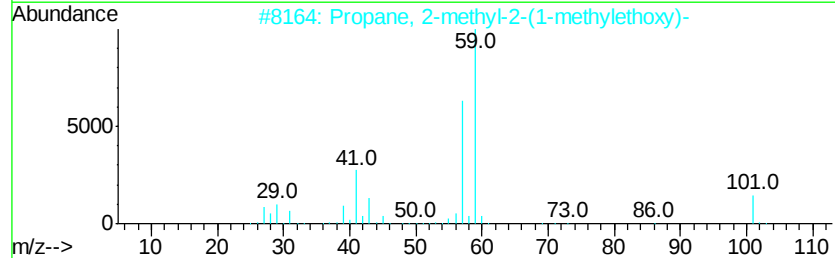
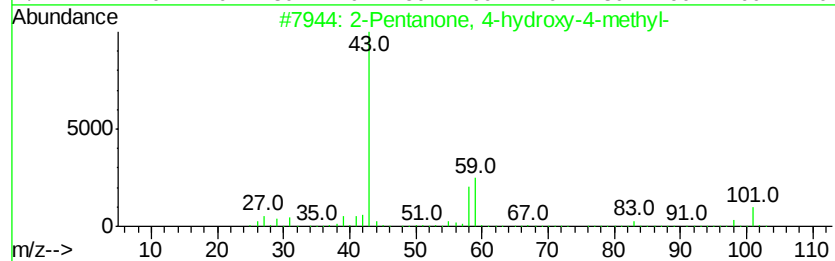
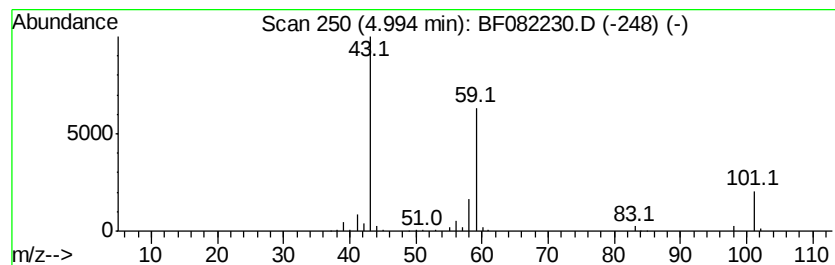
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.99	21.39 ng	371139	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	42
3		3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	28
4		Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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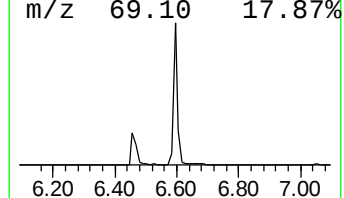
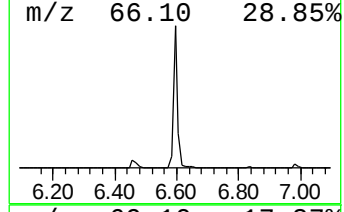
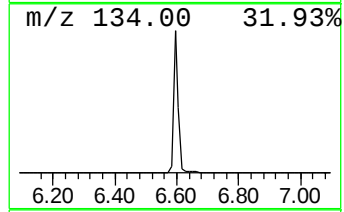
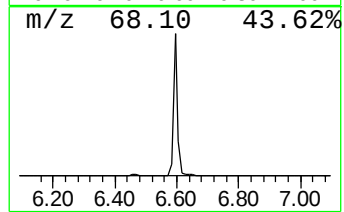
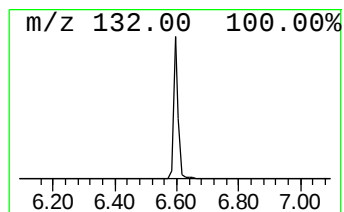
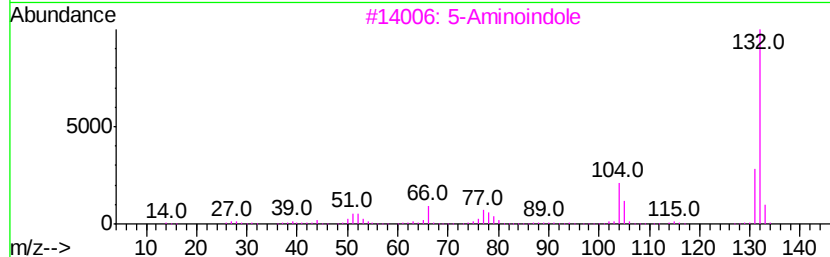
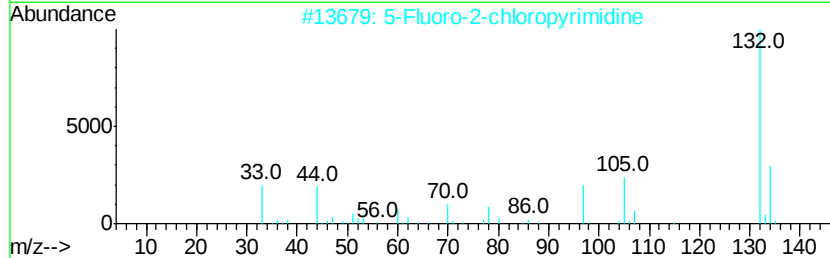
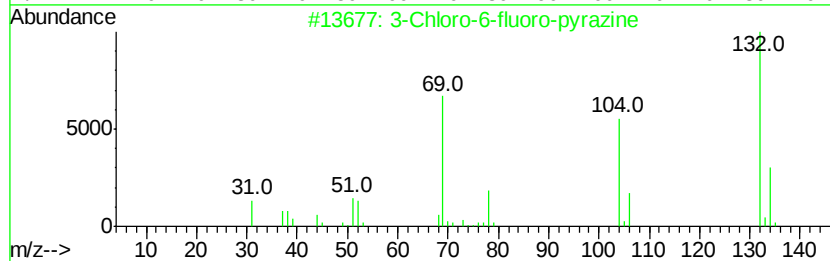
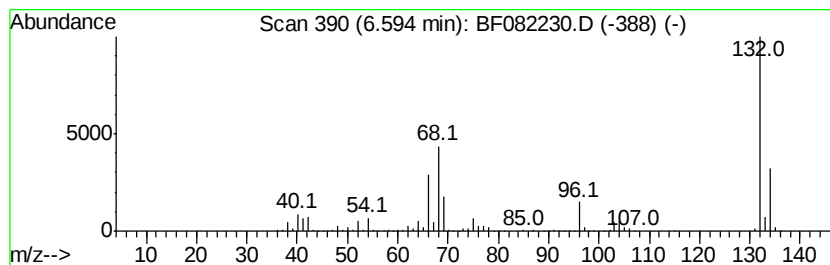
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 3-Chloro-6-fluoro-pyrazine Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.59	83.47 ng	1448590	1,4-Dichlorobenzene-d4	6.83

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	16
3			5-Aminoindole	132	C8H8N2	005192-03-0	12
4			Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5			Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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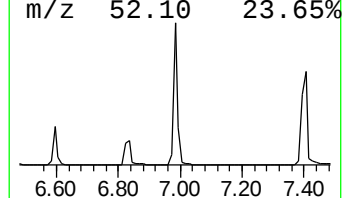
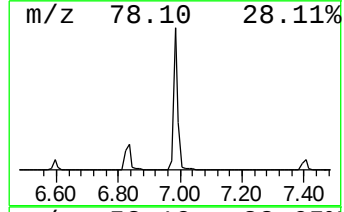
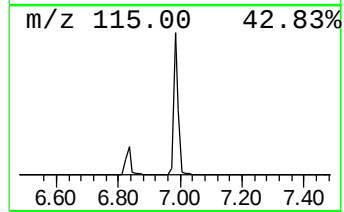
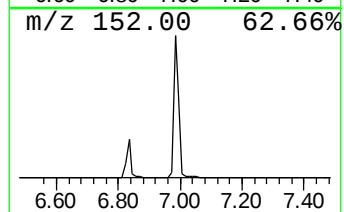
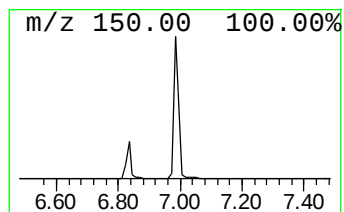
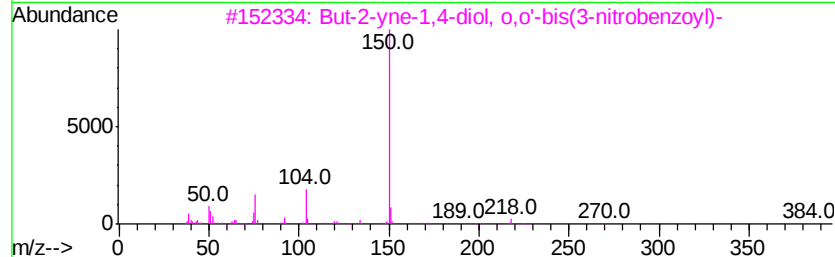
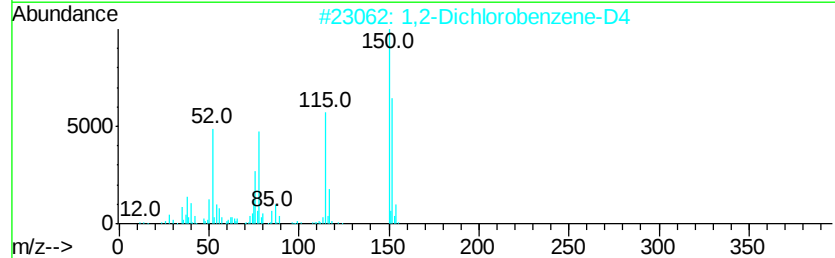
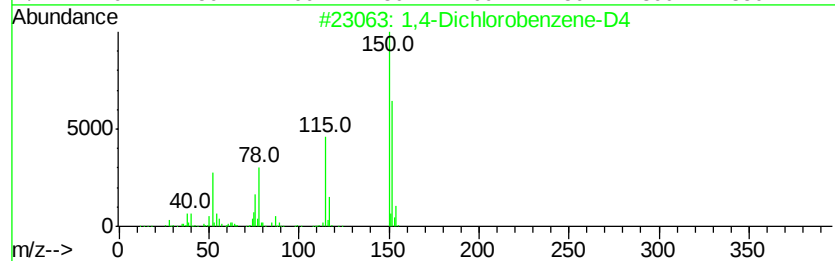
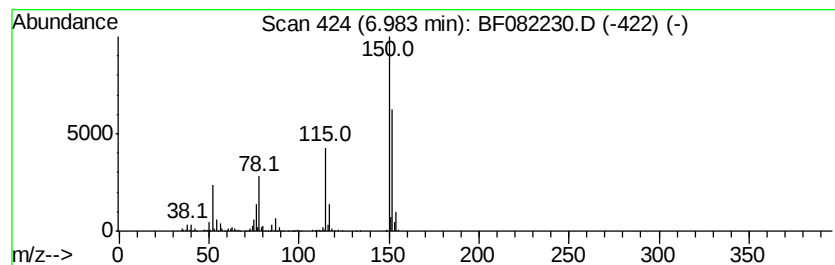
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 1,4-Dichlorobenzene-D4 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.98	84.26 ng	1462240	1,4-Dichlorobenzene-d4	6.83

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,4-Dichlorobenzene-D4	150	C6D4Cl2	003855-82-1	95
2		1,2-Dichlorobenzene-D4	150	C6D4Cl2	002199-69-1	94
3		But-2-yne-1,4-diol, o,o'-bis(3-n...	384	C18H12N2O8	055709-58-5	10
4		3-(4-Nitrobenzoyl)-2-thioxo-4-th...	431	C17H9N3O7S2	329218-74-8	10
5		2-Bromo-2'-nitroacetophenone	243	C8H6BrNO3	006851-99-6	10



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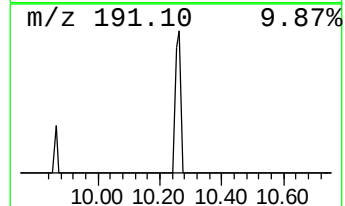
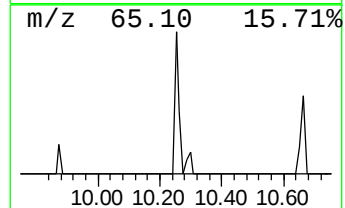
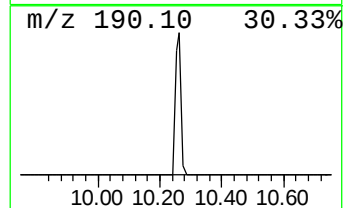
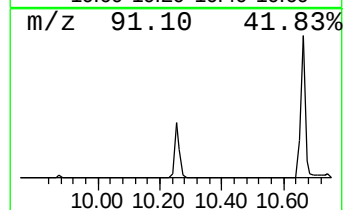
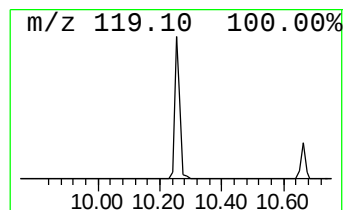
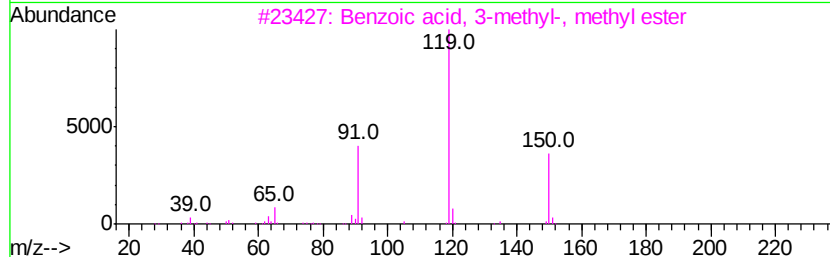
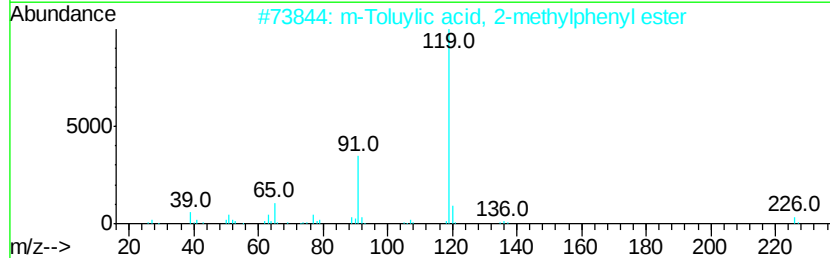
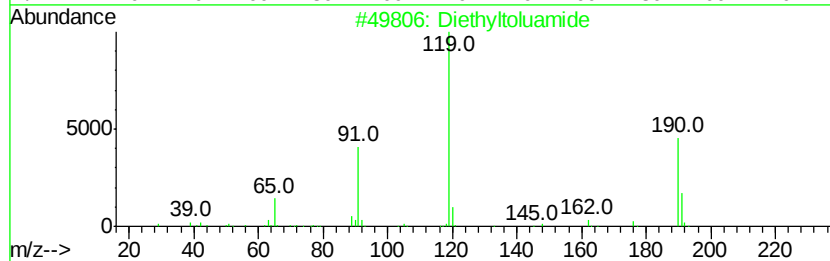
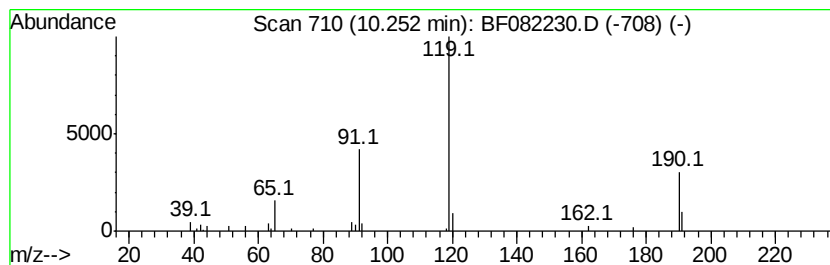
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Diethyltoluamide Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.25	2.29 ng	68996	Acenaphthene-d10	9.87

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Diethyltoluamide	191	C12H17NO	000134-62-3	94
2		m-Toluylic acid, 2-methylphenyl ...	226	C15H14O2	021121-93-7	59
3		Benzoic acid, 3-methyl-, methyl ...	150	C9H10O2	000099-36-5	59
4		N-Isopropyl-p-toluamide	177	C11H15NO	002144-17-4	59
5		p-Toluylic acid, 3,5-difluorophe...	248	C14H10F2O2	1000292-64-0	59



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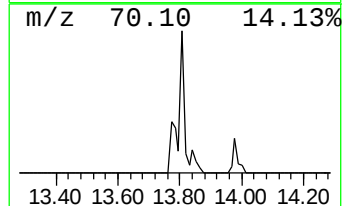
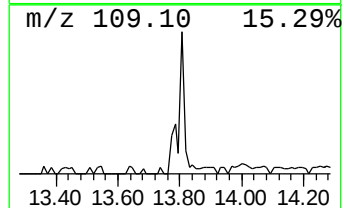
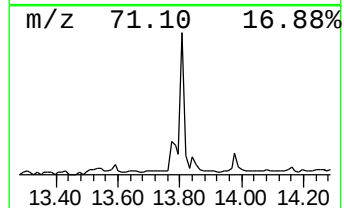
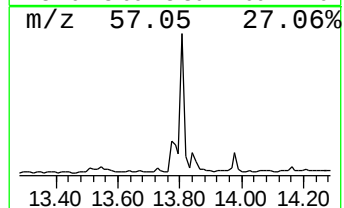
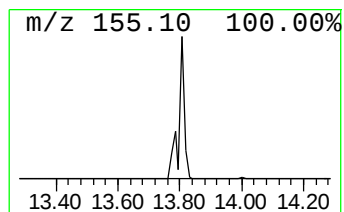
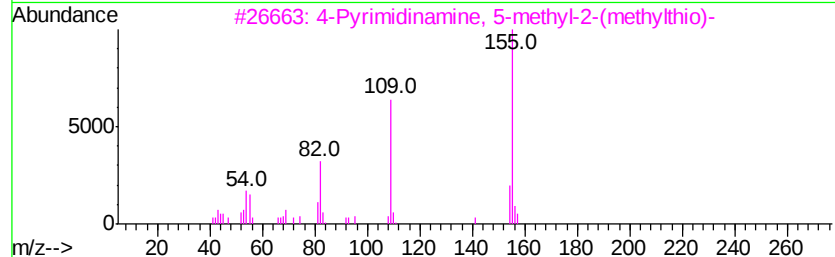
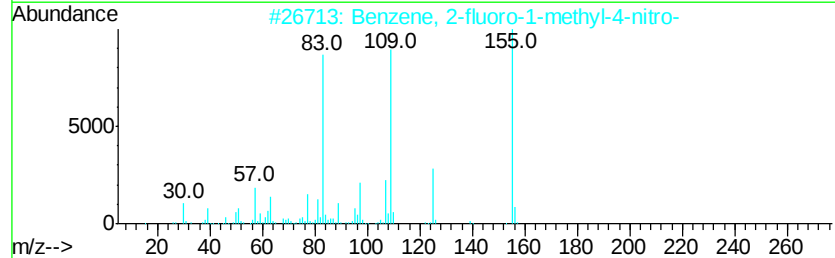
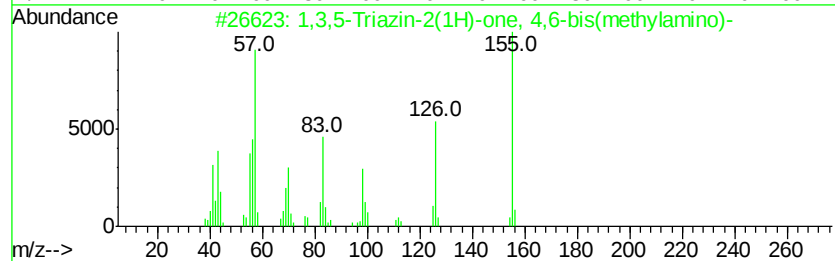
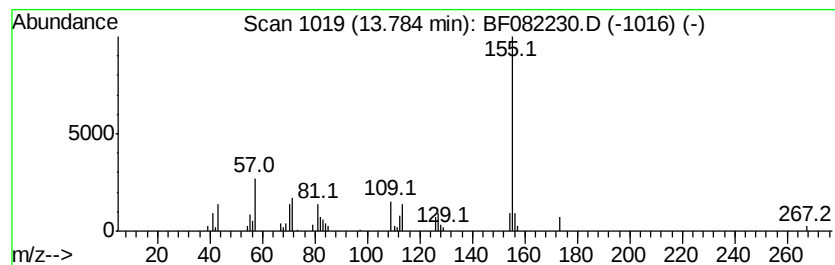
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 1,3,5-Triazin-2(1H)-one, 4,... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.78	2.60 ng	91971	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3,5-Triazin-2(1H)-one, 4,6-bis...	155	C5H9N5O	055702-52-8	59
2		Benzene, 2-fluoro-1-methyl-4-nitro-	155	C7H6FN02	001427-07-2	52
3		4-Pyrimidinamine, 5-methyl-2-(me...	155	C6H9N3S	054308-64-4	40
4		3-Pyridinol, 6-methyl-2-(methylt...	155	C7H9NOS	023003-25-0	40
5		6-Amino-1,3-dimethyluracil	155	C6H9N3O2	006642-31-5	40



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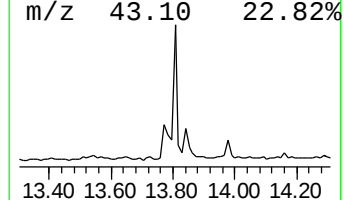
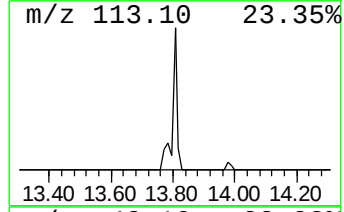
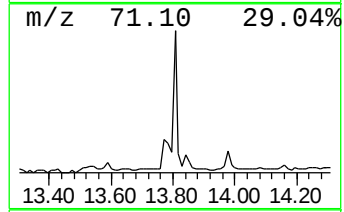
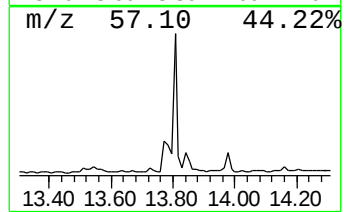
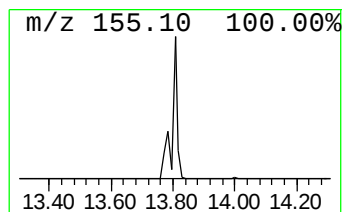
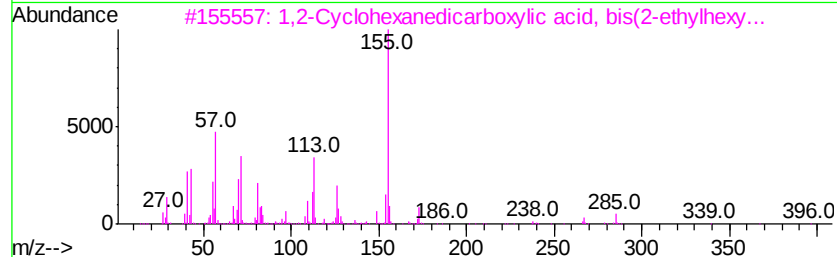
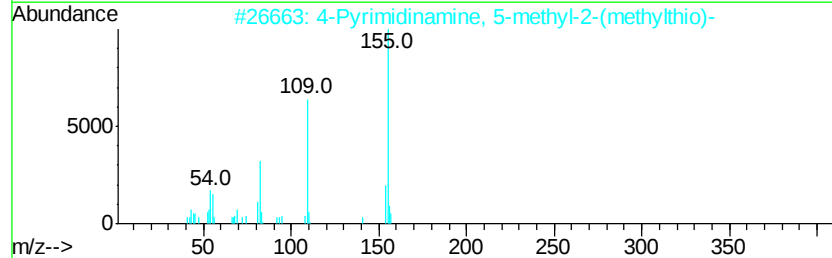
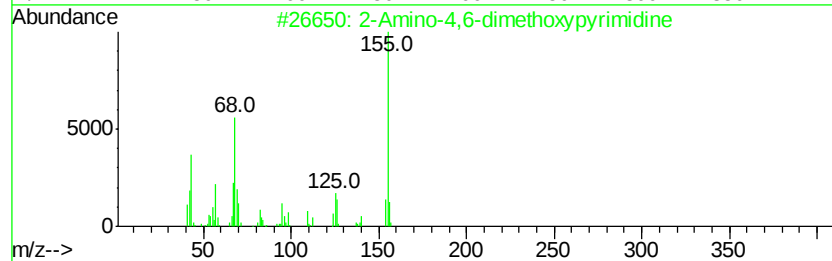
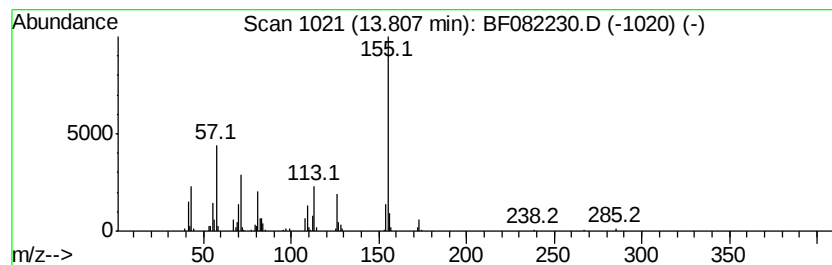
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF101015.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 6 2-Amino-4,6-dimethoxypyrimi... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.81	5.37 ng	190037	Chrysene-d12	14.00

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Amino-4,6-dimethoxypvrimidine	155	C6H9N3O2	036315-01-2	50
2		4-Pyrimidinamine, 5-methyl-2-(me...	155	C6H9N3S	054308-64-4	47
3		1,2-Cyclohexanedicarboxylic acid...	396	C24H44O4	000084-71-9	40
4		Butanal, dibutylhydrazine	198	C12H26N2	067660-51-9	38
5		2,3,4-Trimethylpentan-2-ol decan...	284	C18H36O2	1000130-74-2	38



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF101215\
Data File : BF082230.D
Acq On : 12 Oct 2015 20:13
Operator : UM/IZ
Sample : G3990-10
Misc :
ALS Vial : 15 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
TE-PMW(2-26)

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF101015.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...	4.99	21.4	ng	371139	1	6.83	347086	20.0
3-Chloro-6-fluoro...	6.59	83.5	ng	1448590	1	6.83	347086	20.0
1,4-Dichlorobenze...	6.98	84.3	ng	1462240	1	6.83	347086	20.0
Diethyltoluamide	10.25	2.3	ng	68996	3	9.87	601745	20.0
1,3,5-Triazin-2(1...	13.78	2.6	ng	91971	5	14.00	708402	20.0
2-Amino-4,6-dimet...	13.81	5.4	ng	190037	5	14.00	708402	20.0