

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
 Data File : BF086893.D
 Acq On : 11 May 2016 10:53
 Operator : UM/SJ
 Sample : H2945-01
 Misc :
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 HSR-WC-43-050616

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_F\METHODS\8270-BF050916.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	2.430	28	30	36	rVB	80817	125459	2.70%	0.319%
2	4.156	179	181	186	rBV	432433	707435	15.21%	1.800%
3	4.396	199	202	205	rBV	30938	52416	1.13%	0.133%
4	4.853	240	242	251	rBV	833820	1297730	27.90%	3.302%
5	5.127	264	266	275	rVB	72144	106246	2.28%	0.270%
6	5.299	279	281	295	rBV	4269957	4585151	98.58%	11.665%
7	6.350	370	373	375	rBV	4037341	4359123	93.72%	11.090%
8	6.465	380	383	385	rBV	3344451	4651035	100.00%	11.833%
9	6.682	400	402	404	rBV	1157162	1017807	21.88%	2.589%
10	6.842	413	416	418	rBV	3452786	3877510	83.37%	9.865%
11	7.253	449	452	455	rBV	2765205	3081023	66.24%	7.838%
12	7.973	512	515	517	rBV	910426	1217232	26.17%	3.097%
13	9.048	606	609	612	rBV	4241975	4467619	96.06%	11.366%
14	9.722	665	668	670	rBV	1008112	1104954	23.76%	2.811%
15	10.511	734	737	739	rBV	2304347	2508108	53.93%	6.381%
16	11.196	794	797	799	rBV	1079518	940988	20.23%	2.394%
17	12.785	933	936	938	rBV	3223429	3651000	78.50%	9.288%
18	13.825	1025	1027	1029	rBV	794047	808424	17.38%	2.057%
19	15.197	1144	1147	1153	rVB	568603	678408	14.59%	1.726%
20	16.580	1262	1268	1274	rBV5	18738	69282	1.49%	0.176%

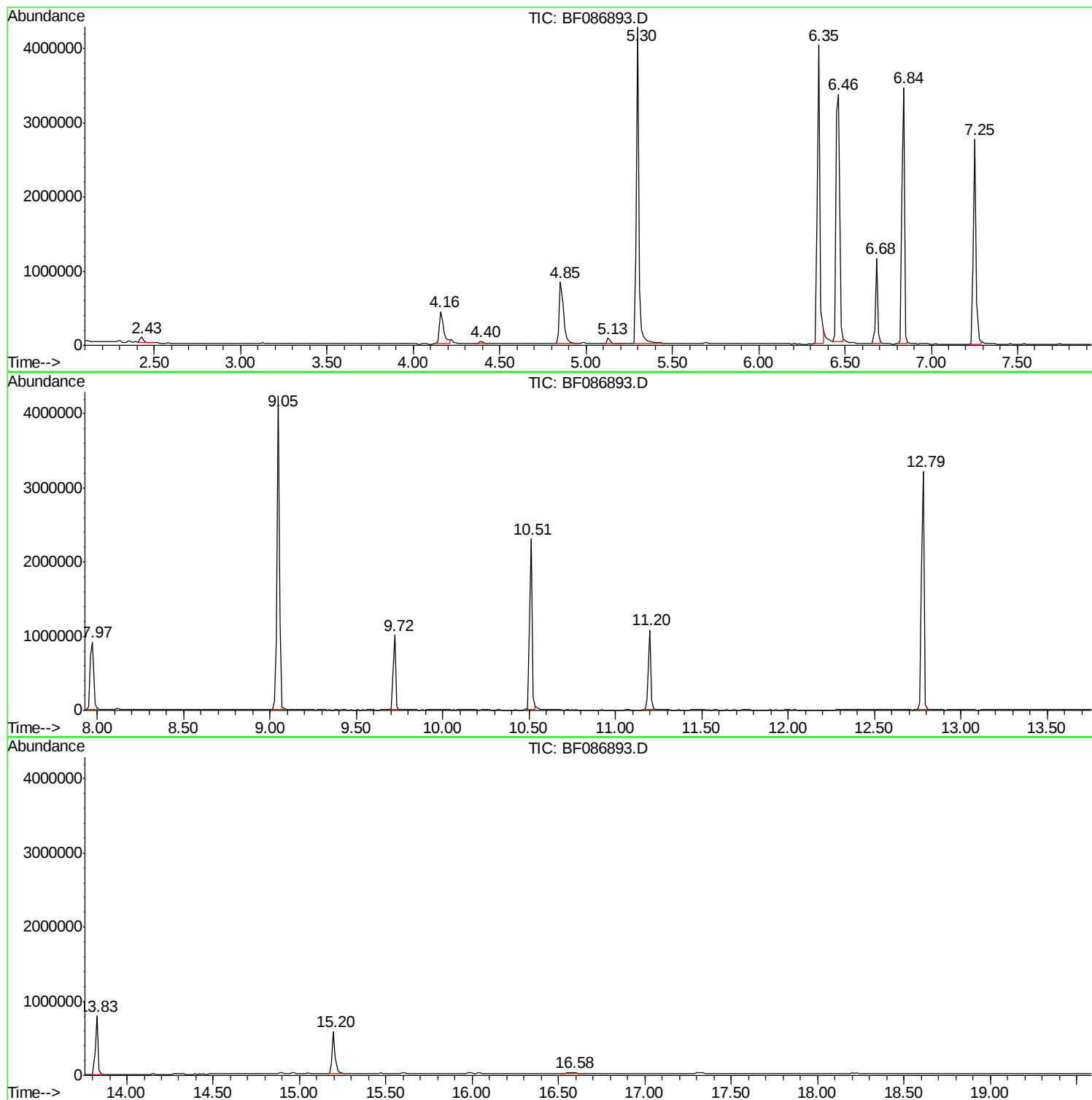
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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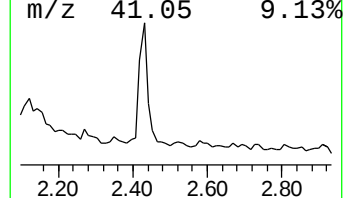
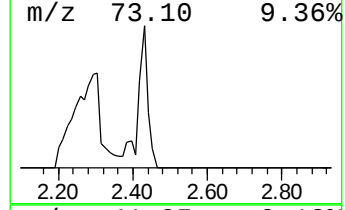
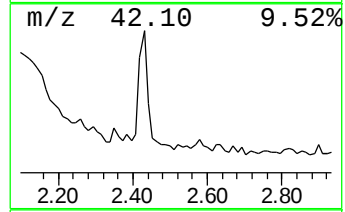
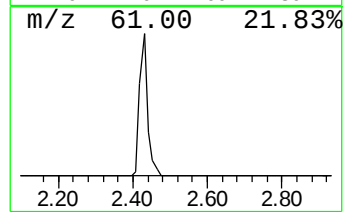
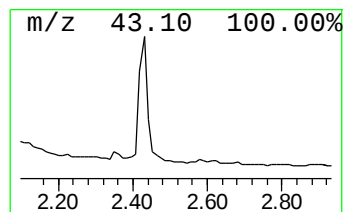
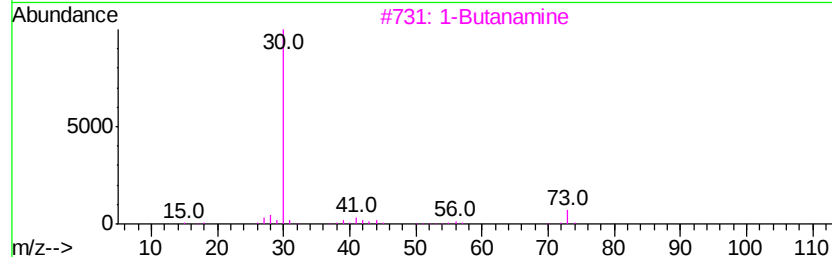
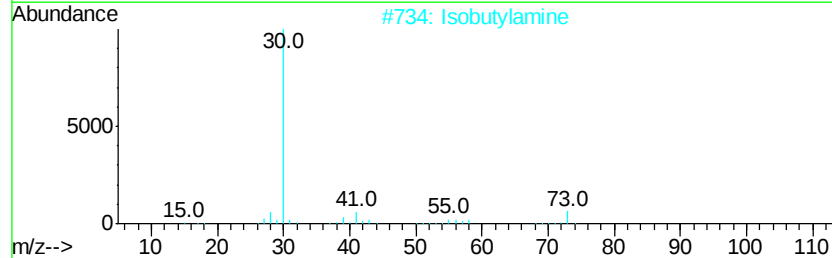
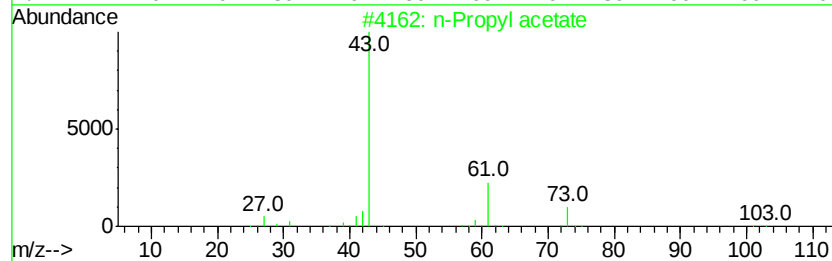
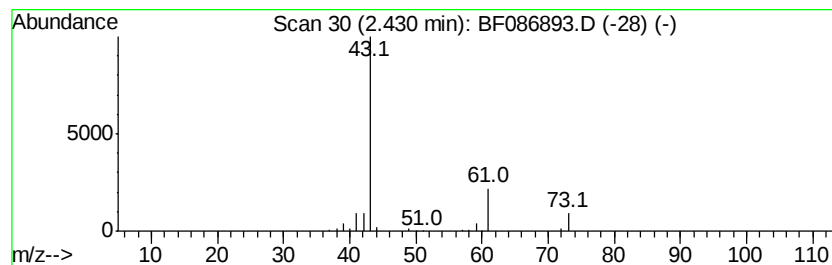
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 n-Propyl acetate Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.43	2.47 ng	125459	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	n-Propyl acetate	102	C5H10O2	000109-60-4	78
2		Isobutylamine	73	C4H11N	000078-81-9	5
3		1-Butanamine	73	C4H11N	000109-73-9	5
4		Butane, 2-methyl-	72	C5H12	000078-78-4	4
5		1,4-Butanediol, diacetate	174	C8H14O4	000628-67-1	4



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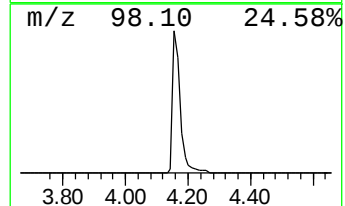
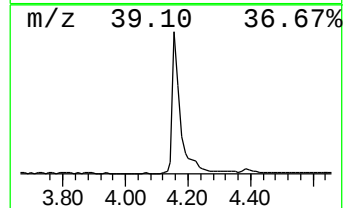
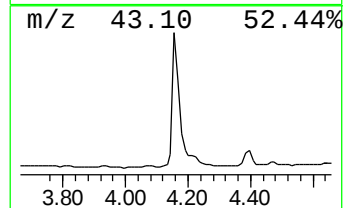
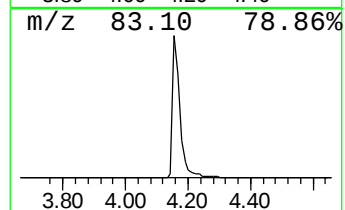
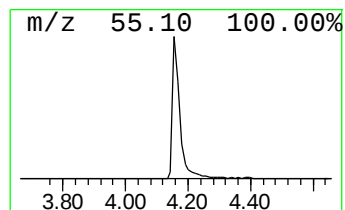
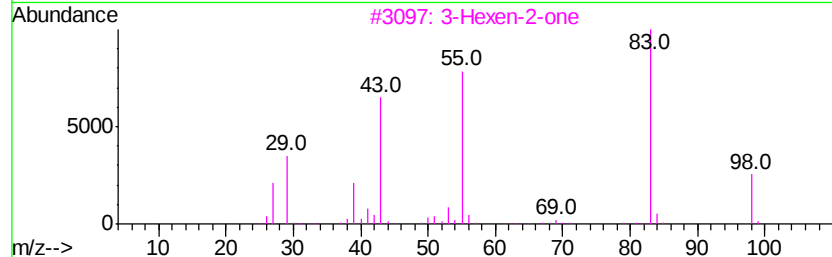
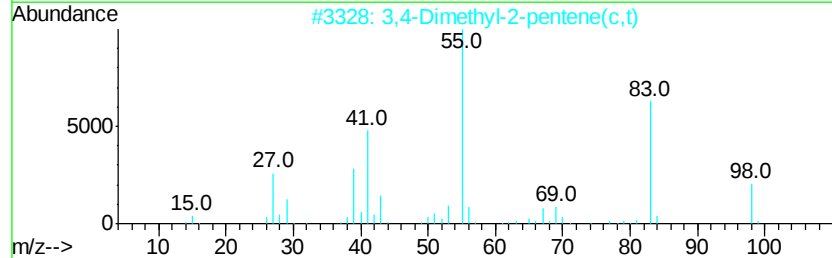
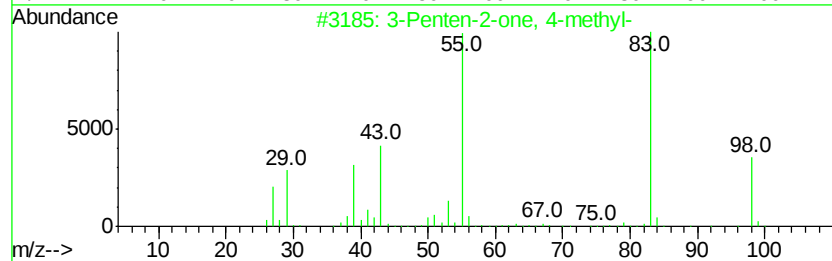
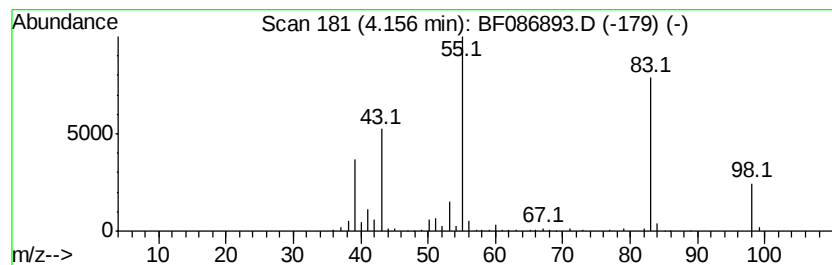
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Peak Number 2 3-Penten-2-one, 4-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.16	13.90 ng	707435	1,4-Dichlorobenzene-d4	6.68

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Penten-2-one, 4-methyl-	98	C6H10O	000141-79-7	91
2			3,4-Dimethyl-2-pentene(c,t)	98	C7H14	1000118-16-5	86
3			3-Hexen-2-one	98	C6H10O	000763-93-9	80
4			2-Pentene, 2,4-dimethyl-	98	C7H14	000625-65-0	72
5			2-Pentene, 3,4-dimethyl-, (E)-	98	C7H14	004914-92-5	72



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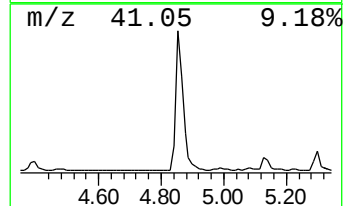
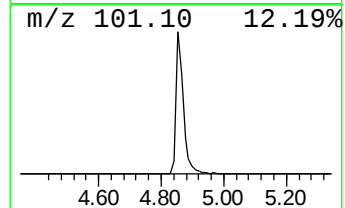
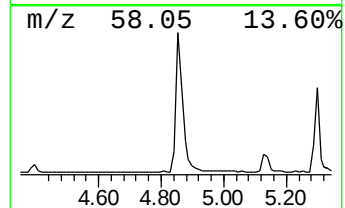
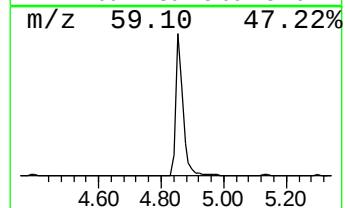
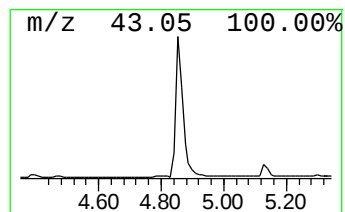
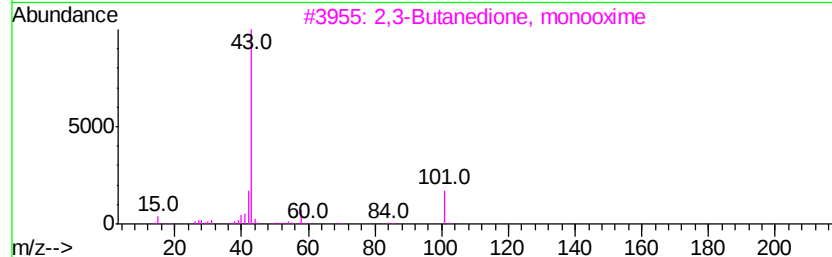
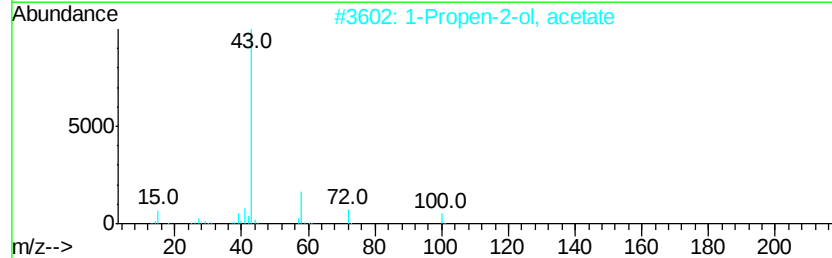
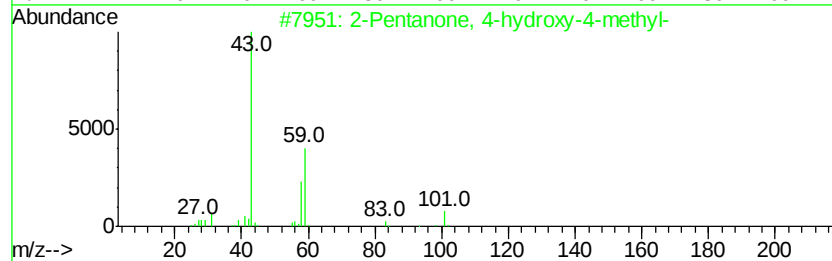
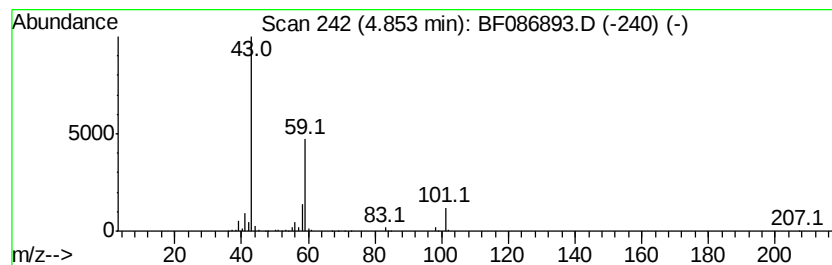
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Peak Number 3 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.85	25.50 ng	1297730	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2		1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4		2-Propanone, 1-(1-methylethoxy)-	116	C6H12O2	042781-12-4	9
5		Acetic acid, 2-propenyl ester	100	C5H8O2	000591-87-7	9



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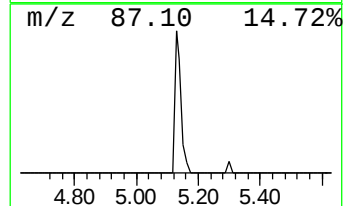
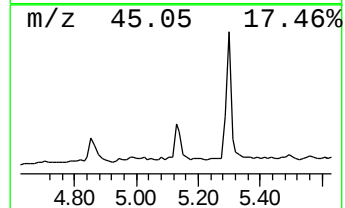
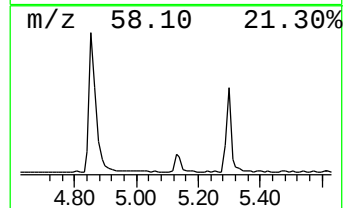
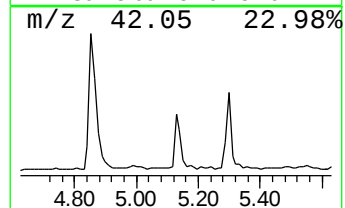
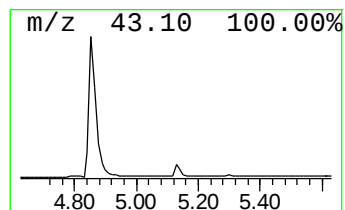
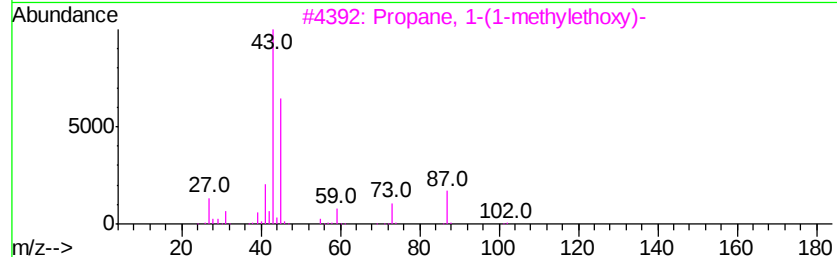
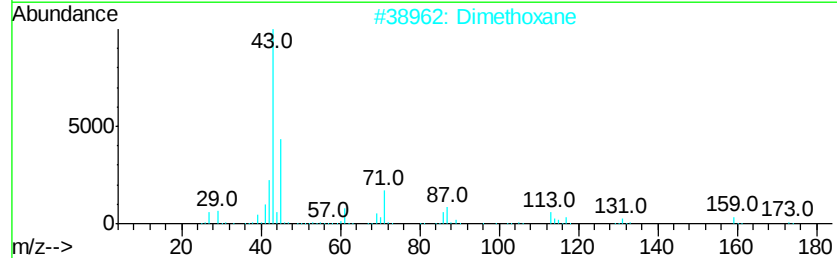
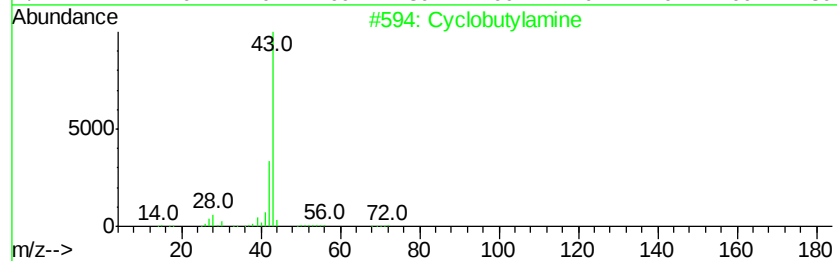
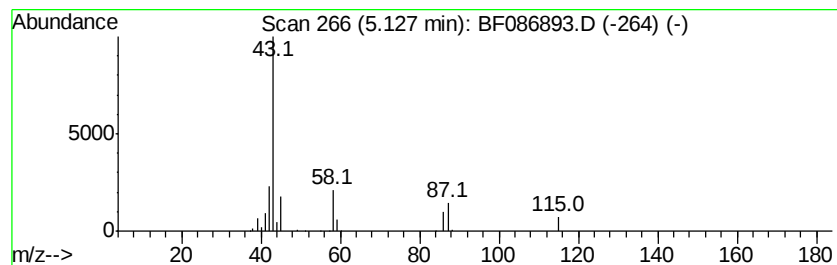
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Peak Number 4 unknown5.13 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.13	2.09 ng	106246	1,4-Dichlorobenzene-d4	6.68

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cyclobutylamine	71	C4H9N	002516-34-9	9
2		Dimethoxane	174	C8H14O4	000828-00-2	9
3		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	9
4		Acetone	58	C3H6O	000067-64-1	7
5		3-Pyrrolidinol	87	C4H9NO	040499-83-0	7



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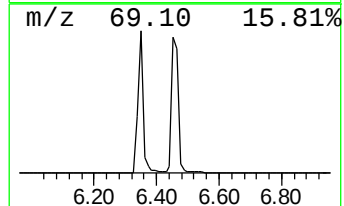
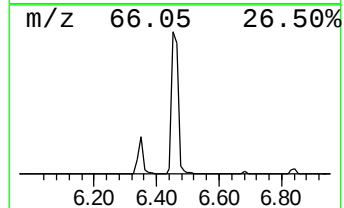
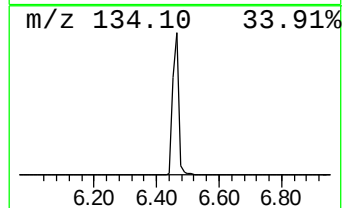
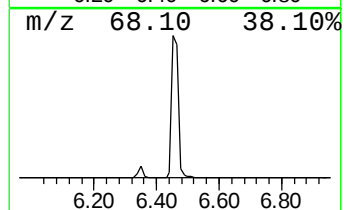
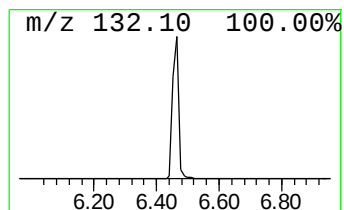
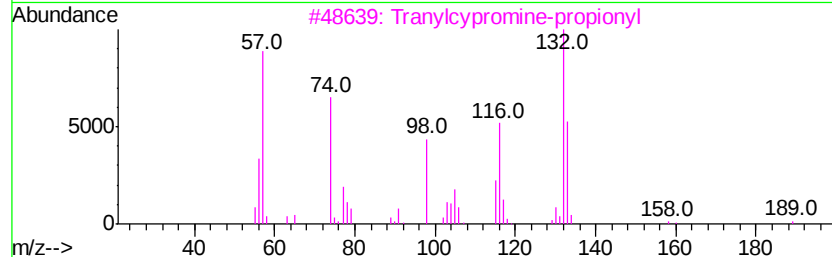
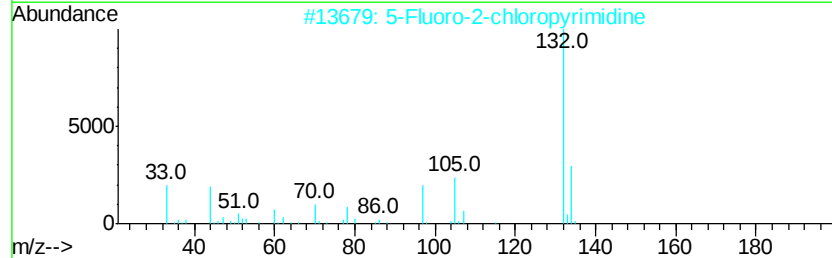
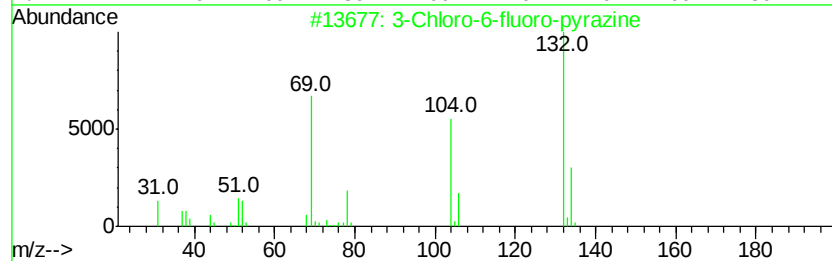
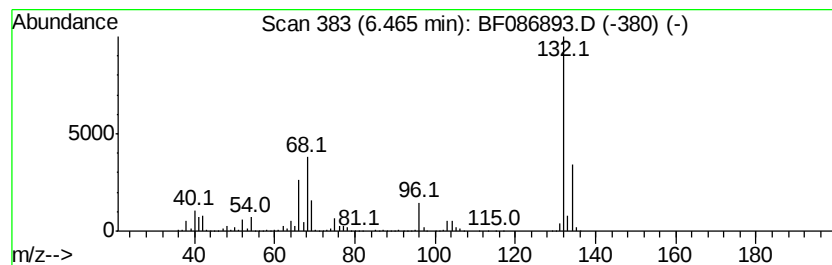
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 5 unknown6.46 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.46	91.39 ng	4651040	1,4-Dichlorobenzene-d4	6.68

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	Tranvlcvpromine-propionyl			189	C12H15NO	1000123-86-3	12
4	(E)-3-Chloro-2-methyl-2-pentenal			132	C6H9ClO	031357-76-3	12
5	Bicyclo[4.2.0]octa-1,3,5-triene, ...			132	C10H12	028749-81-7	9



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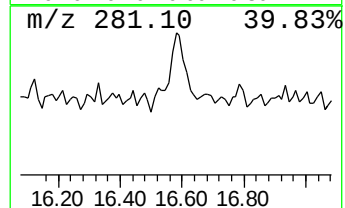
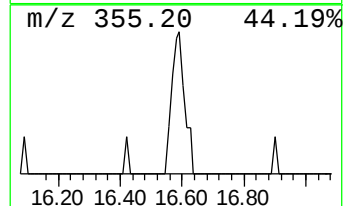
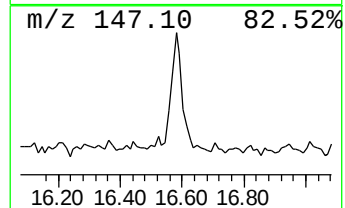
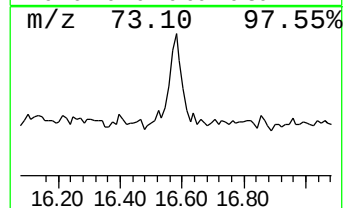
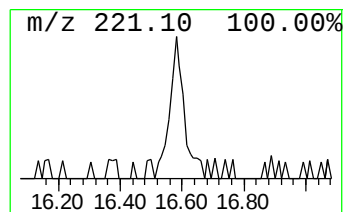
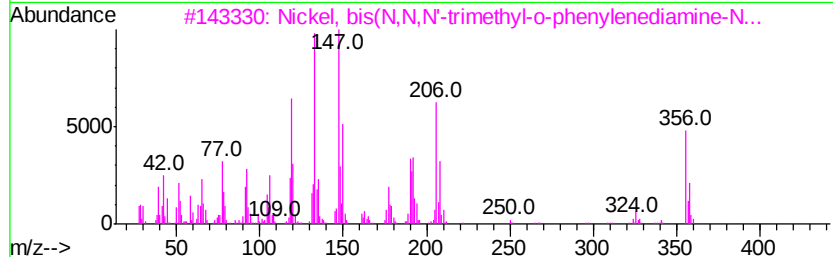
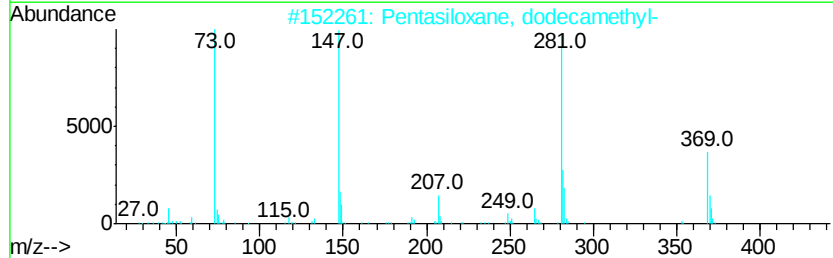
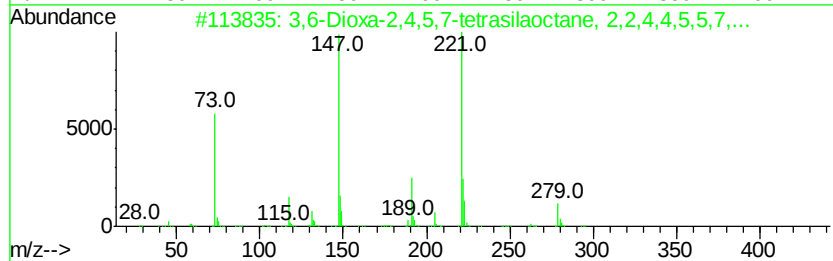
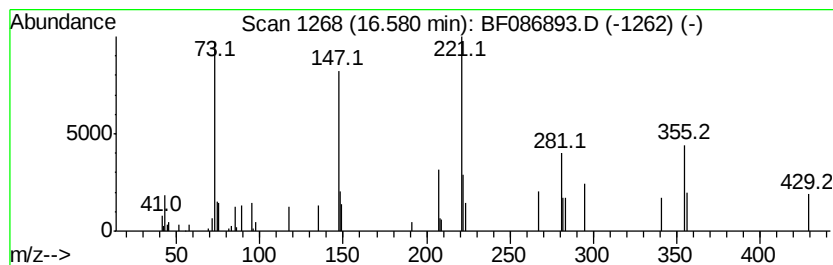
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF050916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown16.58 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.58	2.04 ng	69282	Perylene-d12	15.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	37
2		Pentasiloxane, dodecamethyl-	384	C12H36O4Si5	000141-63-9	22
3		Nickel, bis(N,N,N'-trimethyl-o-p...	356	C18H26N4Ni	1000153-51-1	18
4		Piperidine, 1-(5-trifluoromethyl...	295	C15H16F3N3	1000268-74-7	10
5		Isothiourea, 1-cyano-3-(4-methox...	221	C10H11N3OS	075565-12-7	9



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF051016\
Data File : BF086893.D
Acq On : 11 May 2016 10:53
Operator : UM/SJ
Sample : H2945-01
Misc :
ALS Vial : 4 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
HSR-WC-43-050616

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF050916.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
n-Propyl acetate	2.43	2.5	ng	125459	1	6.68	1017810	20.0
3-Penten-2-one, 4...	4.16	13.9	ng	707435	1	6.68	1017810	20.0
2-Pentanone, 4-hy...	4.85	25.5	ng	1297730	1	6.68	1017810	20.0
unknown5.13	5.13	2.1	ng	106246	1	6.68	1017810	20.0
unknown6.46	6.46	91.4	ng	4651040	1	6.68	1017810	20.0
unknown16.58	16.58	2.0	ng	69282	6	15.20	678408	20.0