

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
 Data File : BF077944.D
 Acq On : 25 Mar 2015 8:51
 Operator : TP/IZ
 Sample : G1615-02
 Misc :
 ALS Vial : 35 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-15-2

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_F\METHODS\8270-BF031115.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	1.264	31	33	36	rVB	1447991	1753357	100.00%	13.502%
2	1.390	41	44	47	rVB	66314	105085	5.99%	0.809%
3	1.550	56	58	62	rVB	42598	66542	3.80%	0.512%
4	1.653	65	67	74	rVV	51150	82666	4.71%	0.637%
5	1.767	74	77	93	rVB	383678	719161	41.02%	5.538%
6	4.864	346	348	354	rVB	78186	103322	5.89%	0.796%
7	5.402	393	395	398	rBV	606757	784304	44.73%	6.040%
8	6.693	506	508	511	rBV	603197	835443	47.65%	6.433%
9	6.830	518	520	523	rBV	924007	873901	49.84%	6.729%
10	7.116	543	545	548	rVB	271355	251432	14.34%	1.936%
11	7.299	559	561	564	rBV	579089	682231	38.91%	5.254%
12	7.813	603	606	608	rBV	600152	516313	29.45%	3.976%
13	8.693	681	683	686	rBV	388295	350080	19.97%	2.696%
14	9.402	744	745	748	rBV	16741	20934	1.19%	0.161%
15	10.042	798	801	804	rBV	1332527	1162092	66.28%	8.949%
16	10.545	844	845	848	rBV	36217	48107	2.74%	0.370%
17	10.865	871	873	876	rBV	434013	409417	23.35%	3.153%
18	11.768	950	952	954	rBV	106163	98400	5.61%	0.758%
19	11.848	956	959	961	rBV	463379	635339	36.24%	4.892%
20	12.705	1031	1034	1036	rBV	363278	424882	24.23%	3.272%
21	14.694	1205	1208	1211	rBV	1421167	1384678	78.97%	10.663%
22	15.871	1308	1311	1318	rBV	117487	279354	15.93%	2.151%
23	15.974	1318	1320	1323	rVB	399035	503692	28.73%	3.879%
24	16.146	1333	1335	1337	rBV2	17895	19916	1.14%	0.153%
25	16.706	1380	1384	1389	rVV6	8634	34339	1.96%	0.264%
26	17.071	1414	1416	1421	rVB2	13367	21852	1.25%	0.168%
27	17.151	1421	1423	1427	rBV3	17189	39242	2.24%	0.302%
28	17.654	1465	1467	1470	rBV2	16764	23783	1.36%	0.183%
29	17.711	1470	1472	1475	rBV	361659	541272	30.87%	4.168%
30	17.860	1483	1485	1488	rBV3	20314	38703	2.21%	0.298%
31	18.134	1506	1509	1513	rBV3	23924	54572	3.11%	0.420%
32	18.672	1554	1556	1560	rVV	18772	41861	2.39%	0.322%
33	18.774	1563	1565	1570	rVB	42345	79869	4.56%	0.615%

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Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-2

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-BF031115.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

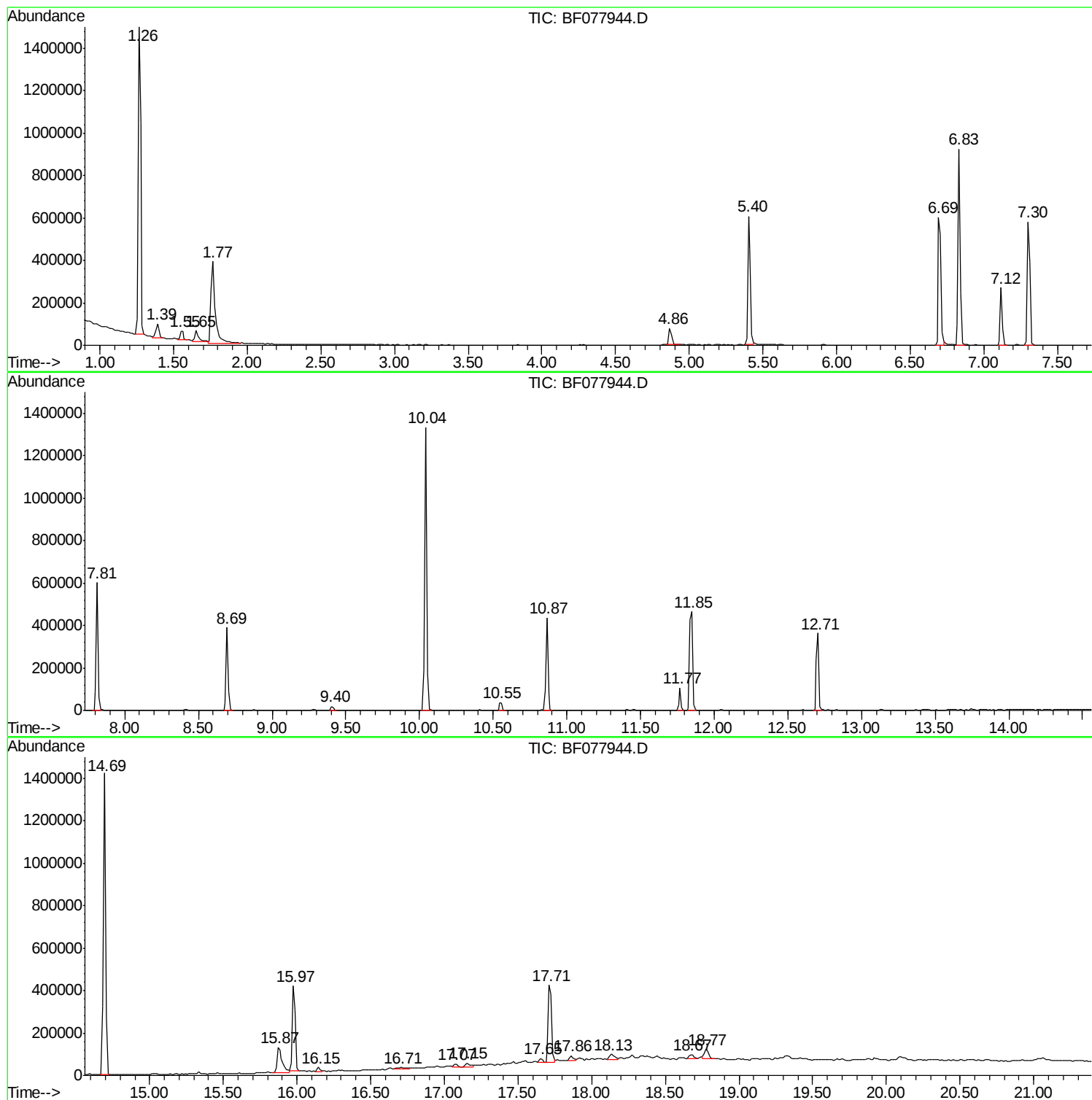
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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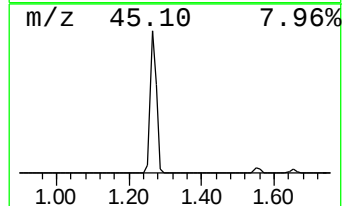
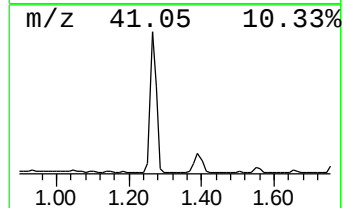
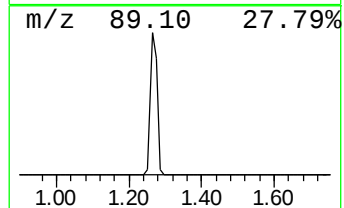
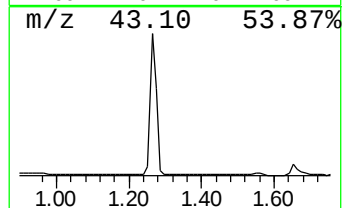
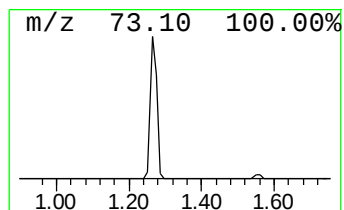
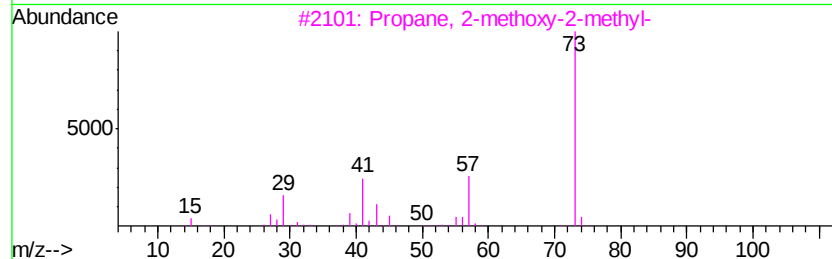
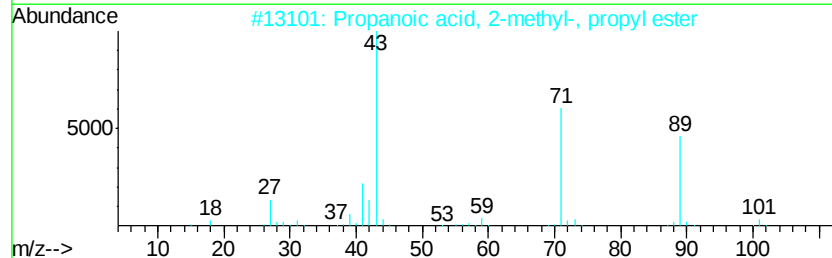
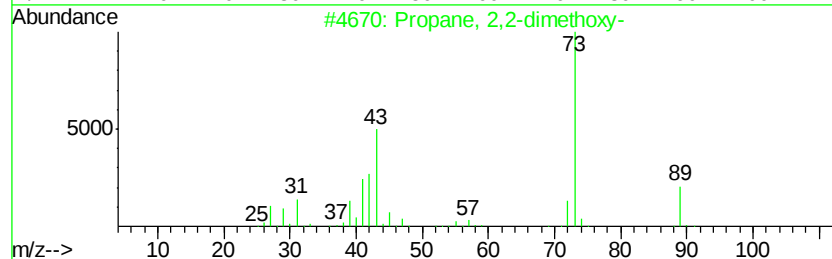
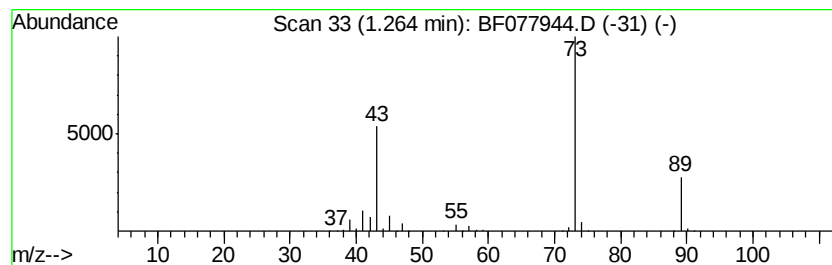
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.26 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.26	139.47 ng	1753360	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2,2-dimethoxy-	104	C5H12O2	000077-76-9	38
2		Propanoic acid, 2-methyl-, propy...	130	C7H14O2	000644-49-5	9
3		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9
4		1-Hexen-4-ol, 1-chloro-3,5-dimet...	162	C8H15ClO	100244-09-5	9
5		2-Hydroxy-2-methylbutyric acid	118	C5H10O3	003739-30-8	9



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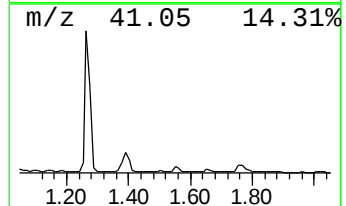
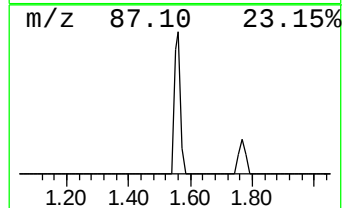
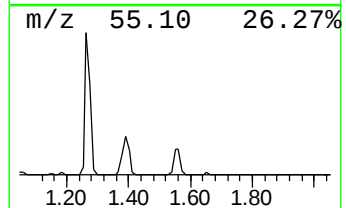
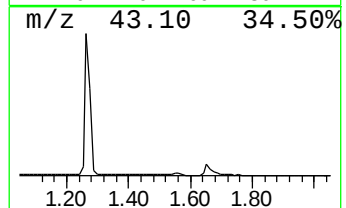
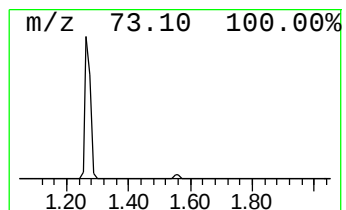
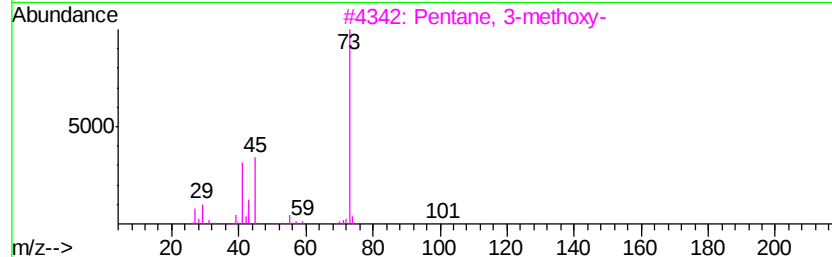
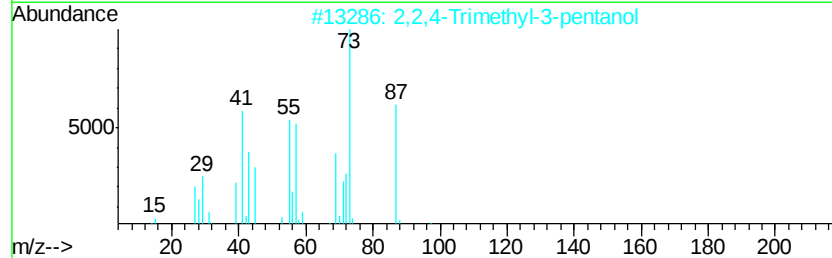
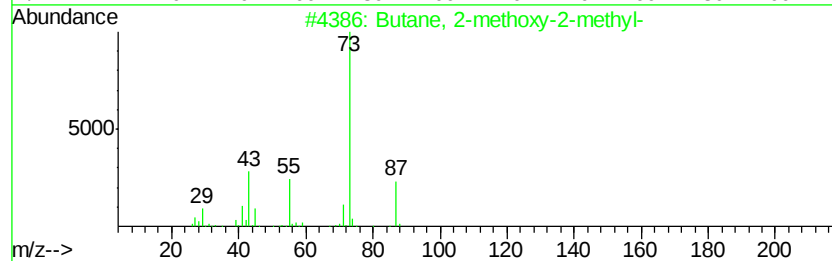
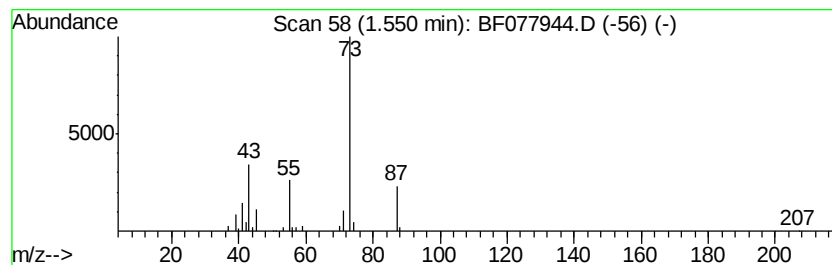
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Butane, 2-methoxy-2-methyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.55	5.29 ng	66542	1,4-Dichlorobenzene-d4	7.12

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	40
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	17
4		N-Ethylformamide	73	C3H7NO	000627-45-2	9
5		Acetamide, N-ethyl-	87	C4H9NO	000625-50-3	9



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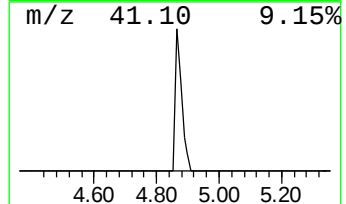
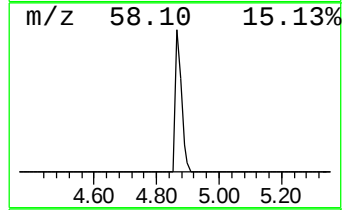
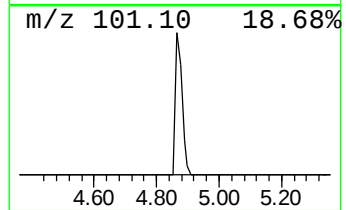
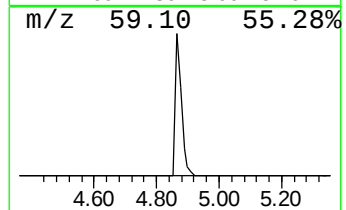
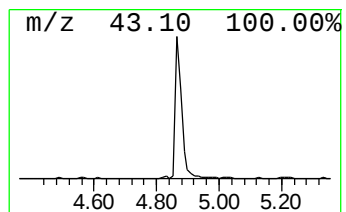
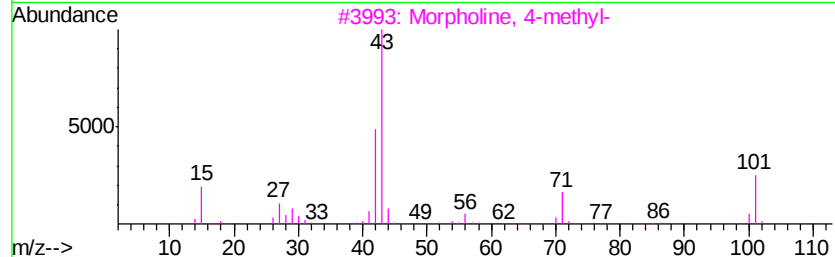
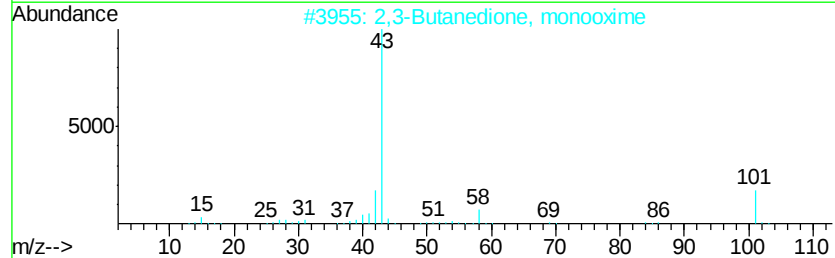
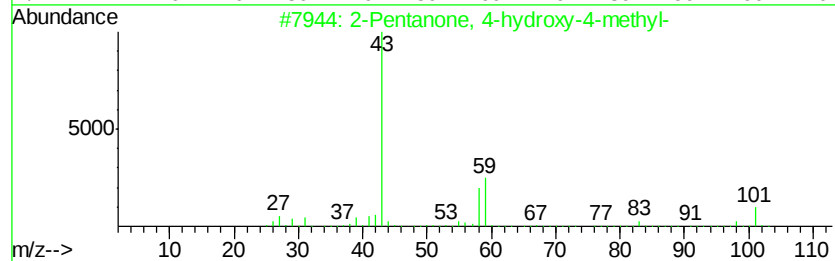
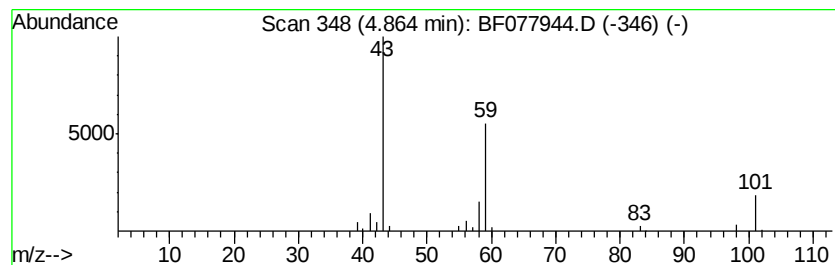
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.86	8.22 ng	103322	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	16
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		3-Hexanol	102	C6H14O	000623-37-0	9



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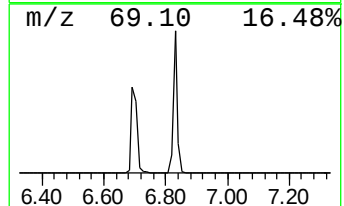
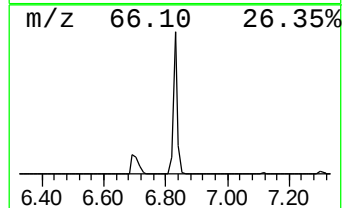
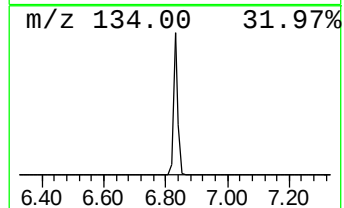
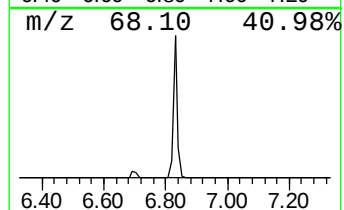
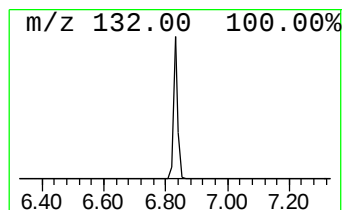
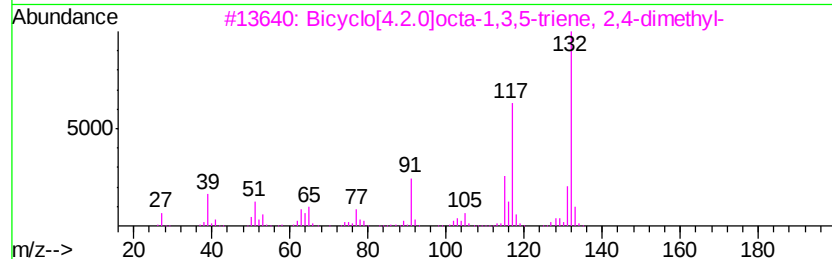
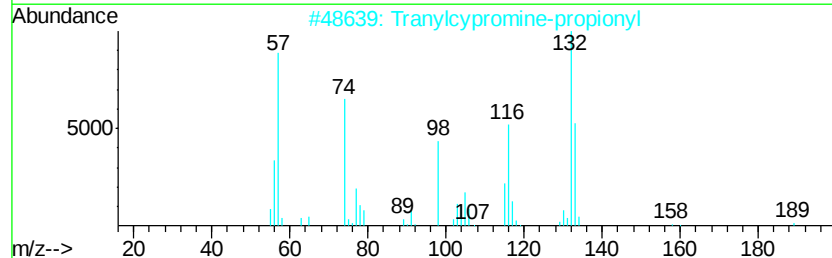
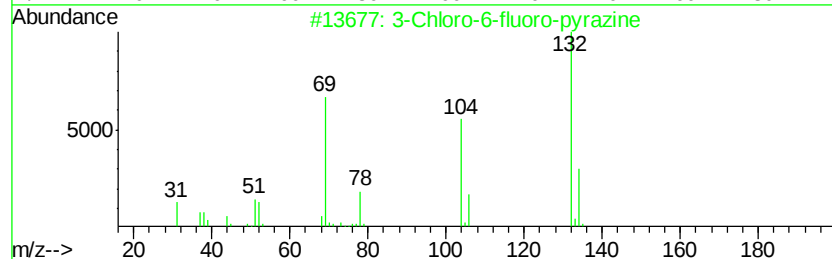
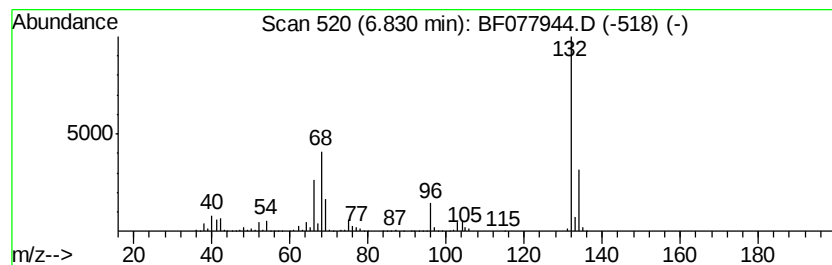
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 unknown6.83 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.83	69.51 ng	873901	1,4-Dichlorobenzene-d4	7.12

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	16
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9



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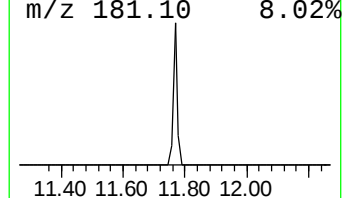
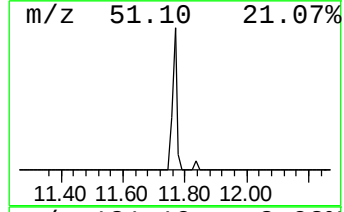
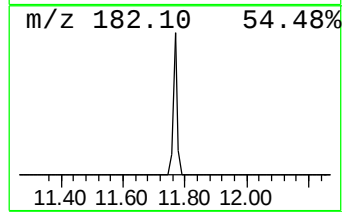
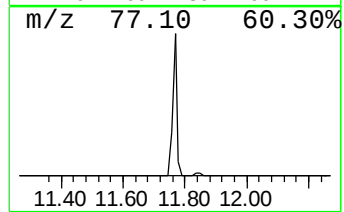
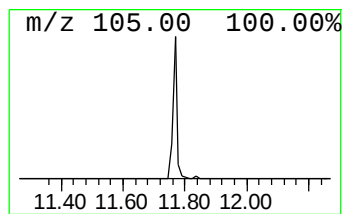
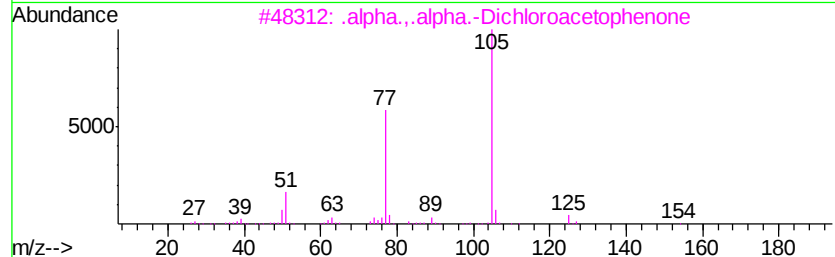
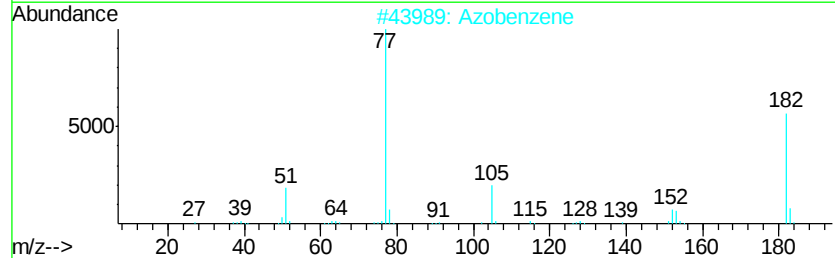
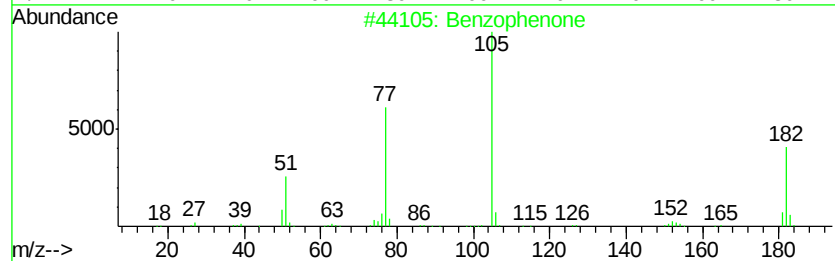
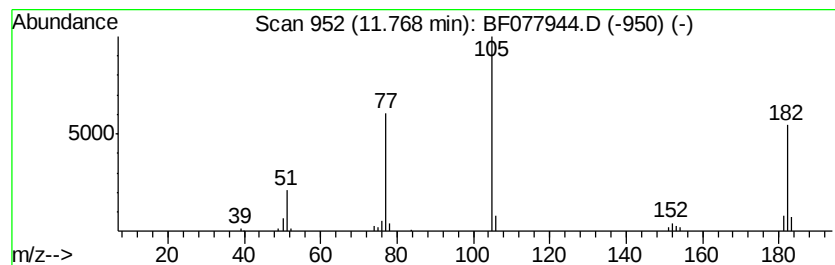
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 9 Benzophenone Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD		R.T.
11.77	4.81 ng	98400	Acenaphthene-d10		10.87
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	96
2	Azobenzene	182	C12H10N2	000103-33-3	59
3	.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
4	1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
5	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47



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ClientSampleId :
SB-15-2

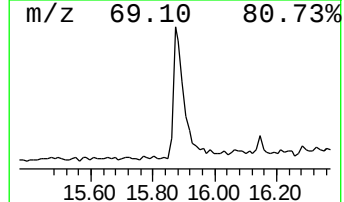
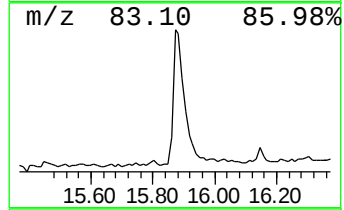
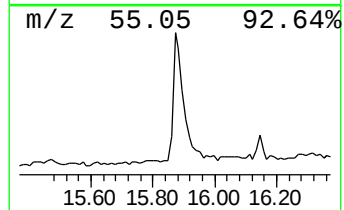
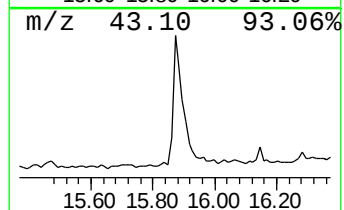
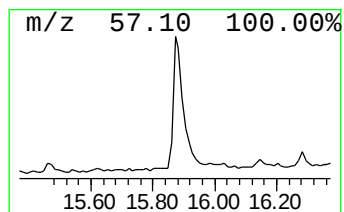
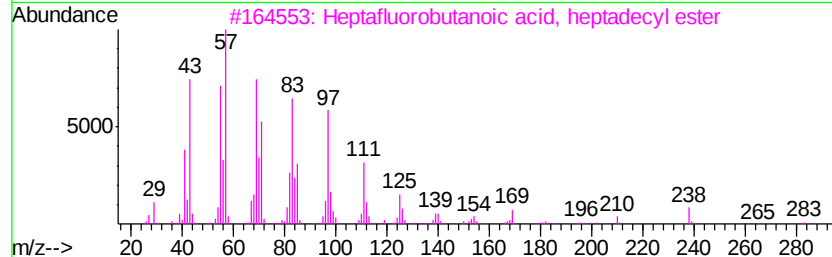
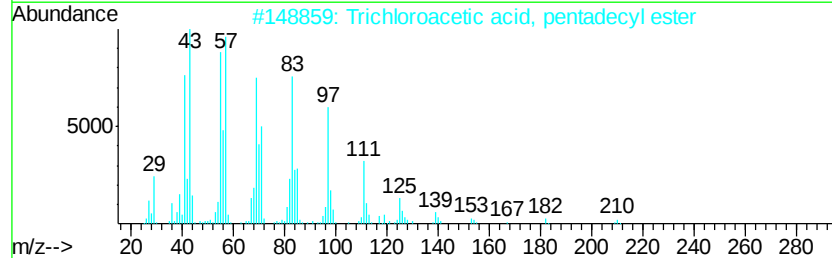
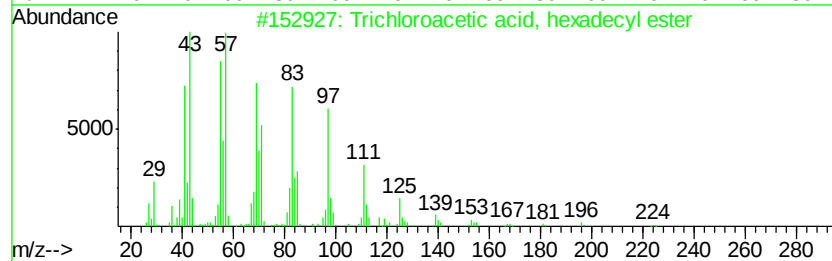
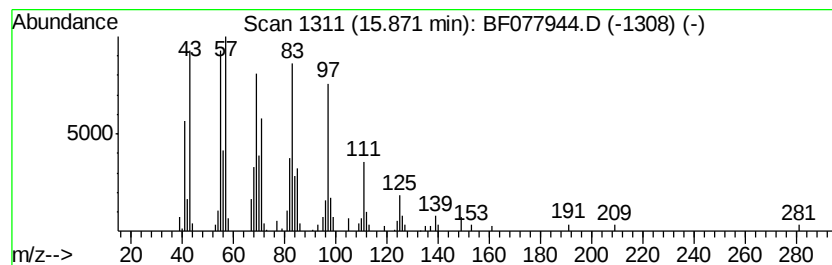
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 Trichloroacetic acid, hexadecyl... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.87	11.09 ng	279354	Chrysene-d12	15.97

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	94
2		Trichloroacetic acid, pentadecyl...	372	C17H31Cl3O2	074339-53-0	91
3		Heptafluorobutanoic acid, heptad...	452	C21H35F7O2	1000282-97-3	91
4		2- Chloropropionic acid, hexadec...	332	C19H37ClO2	086711-81-1	91
5		Trifluoroacetic acid, n-octadecy...	366	C20H37F3O2	079392-43-1	91



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077944.D
Acq On : 25 Mar 2015 8:51
Operator : TP/IZ
Sample : G1615-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-2

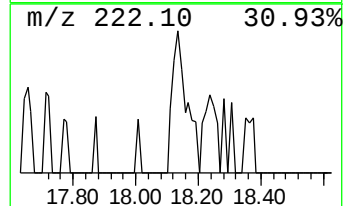
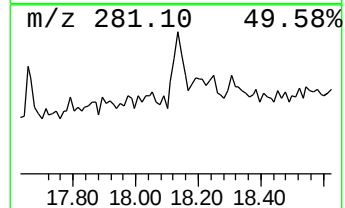
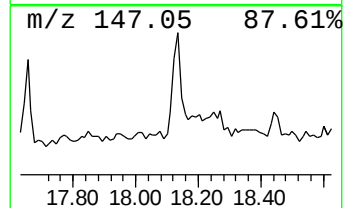
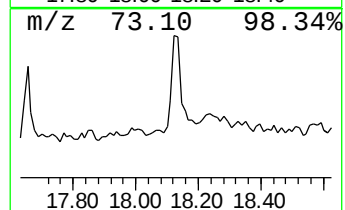
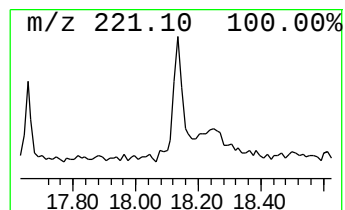
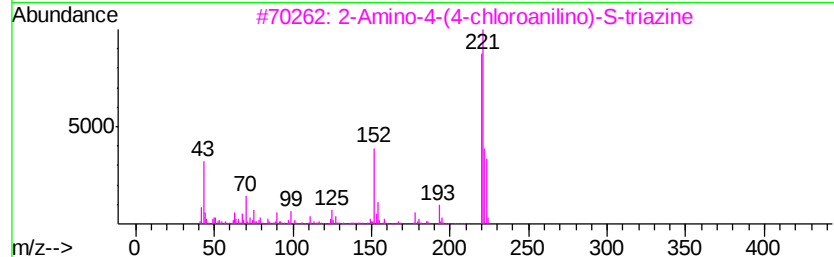
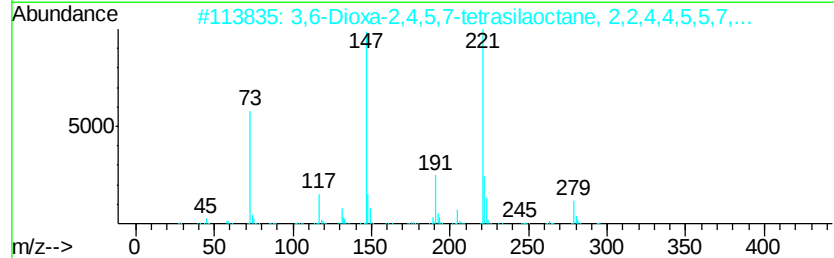
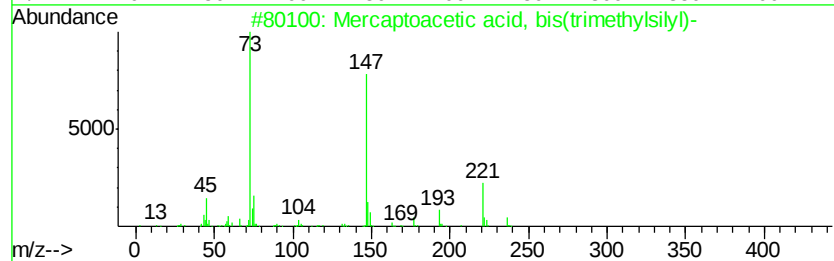
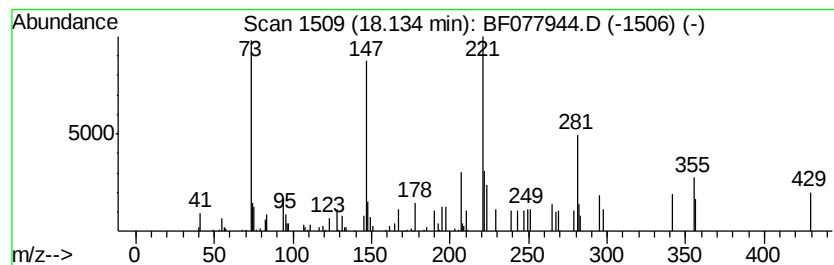
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 11 unknown18.13 Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.13	2.02 ng	54572	Perylene-d12	17.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Mercaptoacetic acid, bis(trimeth...	236	C8H20O2SSi2	006398-62-5	43
2		3,6-Dioxa-2,4,5,7-tetrasilaoctan...	294	C10H30O2Si4	004342-25-0	43
3		2-Amino-4-(4-chloroanilino)-S-tr...	221	C9H8ClN5	000500-42-5	14
4		Pyridazin-3(2H)-one, 4-amino-5-c...	221	C10H8ClN3O	001698-61-9	14
5		Trisiloxane, 1,1,1,5,5,5-hexamet...	384	C12H36O4Si5	003555-47-3	12



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077944.D
Acq On : 25 Mar 2015 8:51
Operator : TP/IZ
Sample : G1615-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-2

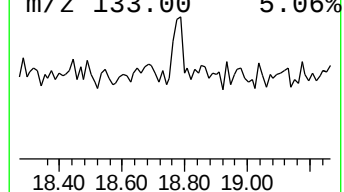
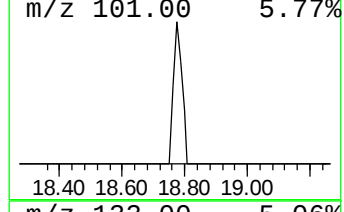
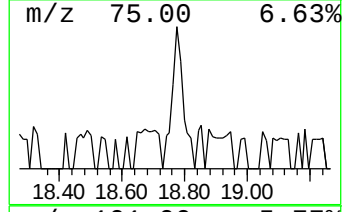
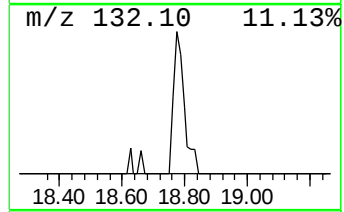
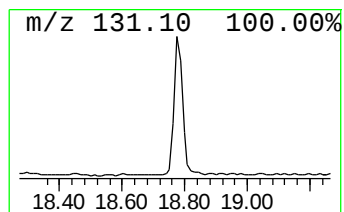
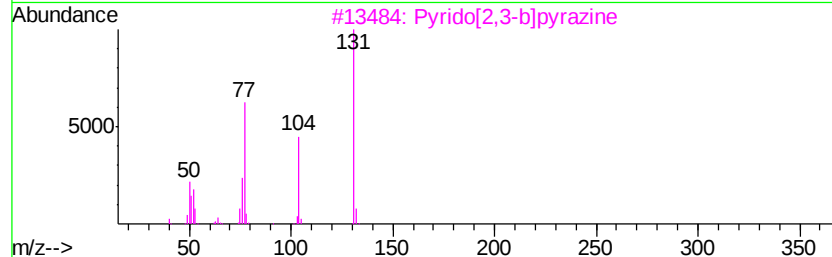
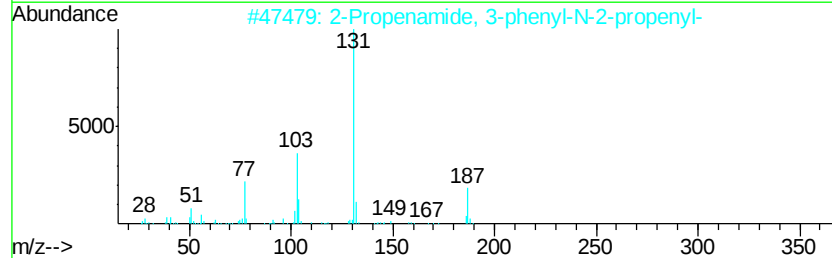
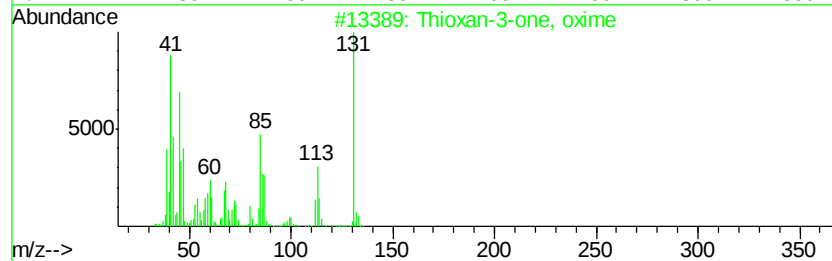
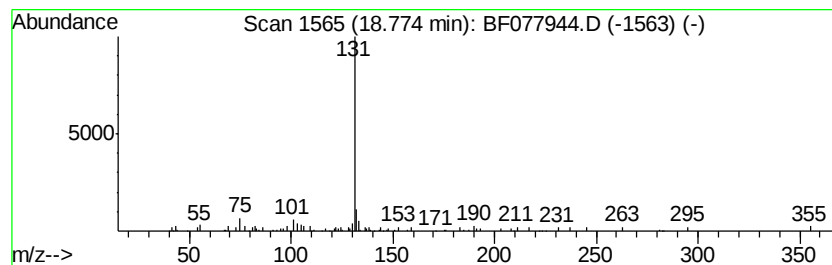
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 Thioxan-3-one, oxime Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
18.77	2.95 ng	79869	Perylene-d12	17.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Thioxan-3-one, oxime	131	C5H9NOS	058230-51-6	53
2		2-Propenamide, 3-phenyl-N-2-prop...	187	C12H13NO	041041-34-3	50
3		Pyrido[2,3-b]pyrazine	131	C7H5N3	000322-46-3	45
4		Silane, [1-(5-ethenyltetrahydro-...	242	C13H26O2Si	057397-14-5	40
5		1H-Indene, 2,3-dihydro-1-methyl-...	244	C18H28	029138-84-9	40



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF032415\
Data File : BF077944.D
Acq On : 25 Mar 2015 8:51
Operator : TP/IZ
Sample : G1615-02
Misc :
ALS Vial : 35 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
SB-15-2

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF031115.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
unknown1.26	1.26	139.5	ng	1753360	1	7.12	251432	20.0
Butane, 2-methoxy...	1.55	5.3	ng	66542	1	7.12	251432	20.0
2-Pentanone, 4-hy...	4.86	8.2	ng	103322	1	7.12	251432	20.0
unknown6.83	6.83	69.5	ng	873901	1	7.12	251432	20.0
Benzophenone	11.77	4.8	ng	98400	3	10.87	409417	20.0
Trichloroacetic a...	15.87	11.1	ng	279354	5	15.97	503692	20.0
unknown18.13	18.13	2.0	ng	54572	6	17.71	541272	20.0
Thioxan-3-one, oxime	18.77	3.0	ng	79869	6	17.71	541272	20.0