

Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
 Data File : BF091563.D
 Acq On : 13 Dec 2016 19:30
 Operator : UM/SJ
 Sample : H5961-02
 Misc :
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 QNWP8-MW27S-GW

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-BF120916.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	2.418	27	29	38	rVB	33490	78894	1.07%	0.144%
2	4.978	250	253	256	rBV	746193	772868	10.49%	1.410%
3	5.413	289	291	294	rBV	3128813	2864819	38.87%	5.225%
4	6.453	379	382	384	rBV	1264016	1791676	24.31%	3.268%
5	6.578	391	393	396	rBV	5227803	5069351	68.79%	9.245%
6	6.807	411	413	416	rBV	1568768	1757655	23.85%	3.205%
7	6.967	425	427	430	rBV	5164421	4890160	66.36%	8.918%
8	7.379	460	463	465	rBV	4539270	4587433	62.25%	8.366%
9	7.516	472	475	477	rBV2	70424	121400	1.65%	0.221%
10	8.099	523	526	528	rBV	2779391	2443462	33.16%	4.456%
11	8.167	529	532	534	rVB	97644	103921	1.41%	0.190%
12	8.476	556	559	561	rVB	126583	126114	1.71%	0.230%
13	8.910	594	597	599	rVB2	108291	121506	1.65%	0.222%
14	9.104	613	614	617	rVB3	81065	79699	1.08%	0.145%
15	9.173	617	620	623	rBV	6821679	7369400	100.00%	13.440%
16	9.276	624	629	631	rBV4	45275	112586	1.53%	0.205%
17	9.379	636	638	640	rBV	745616	868359	11.78%	1.584%
18	9.413	640	641	644	rVV	433694	383951	5.21%	0.700%
19	9.470	644	646	648	rVB	1488163	1239324	16.82%	2.260%
20	9.573	653	655	656	rBV	72924	85246	1.16%	0.155%
21	9.699	664	666	670	rVB2	64420	86803	1.18%	0.158%
22	9.790	670	674	677	rBV2	102425	183706	2.49%	0.335%
23	9.847	677	679	681	rVV	2734525	2388962	32.42%	4.357%
24	9.882	681	682	684	rVV2	190563	184952	2.51%	0.337%
25	9.916	684	685	689	rVB2	71865	112320	1.52%	0.205%
26	9.996	689	692	693	rBV3	57146	90451	1.23%	0.165%
27	10.053	693	697	700	rVV2	92551	160506	2.18%	0.293%
28	10.122	700	703	704	rVV	223201	228465	3.10%	0.417%
29	10.179	704	708	713	rVV5	75120	204589	2.78%	0.373%
30	10.293	716	718	719	rVB	87813	94214	1.28%	0.172%
31	10.396	725	727	730	rVB	77488	95575	1.30%	0.174%
32	10.510	734	737	743	rVB6	56024	114777	1.56%	0.209%
33	10.636	745	748	750	rBV	4165613	4053179	55.00%	7.392%
34	10.762	756	759	764	rVB2	179824	285109	3.87%	0.520%

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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-BF120916.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

35	10.876	765	769	770	rBV2	32406	84225	1.14%	0.154%
36	11.070	784	786	790	rVB2	80379	124012	1.68%	0.226%
37	11.208	796	798	799	rBV	121138	95120	1.29%	0.173%
38	11.333	806	809	811	rVB	1789333	1971827	26.76%	3.596%
39	11.390	812	814	817	rBV3	49368	87129	1.18%	0.159%
40	11.562	824	829	831	rBV2	88166	134337	1.82%	0.245%
41	11.870	853	856	858	rBV2	108425	150246	2.04%	0.274%
42	12.133	877	879	887	rVB6	31005	106044	1.44%	0.193%
43	12.648	922	924	927	rBV	60393	90203	1.22%	0.165%
44	12.911	945	947	950	rBV	4051785	5362913	72.77%	9.781%
45	13.813	1024	1026	1029	rBV	104082	126348	1.71%	0.230%
46	13.962	1036	1039	1041	rBV	1656104	1696550	23.02%	3.094%
47	15.379	1160	1163	1165	rBV	1175822	1652178	22.42%	3.013%

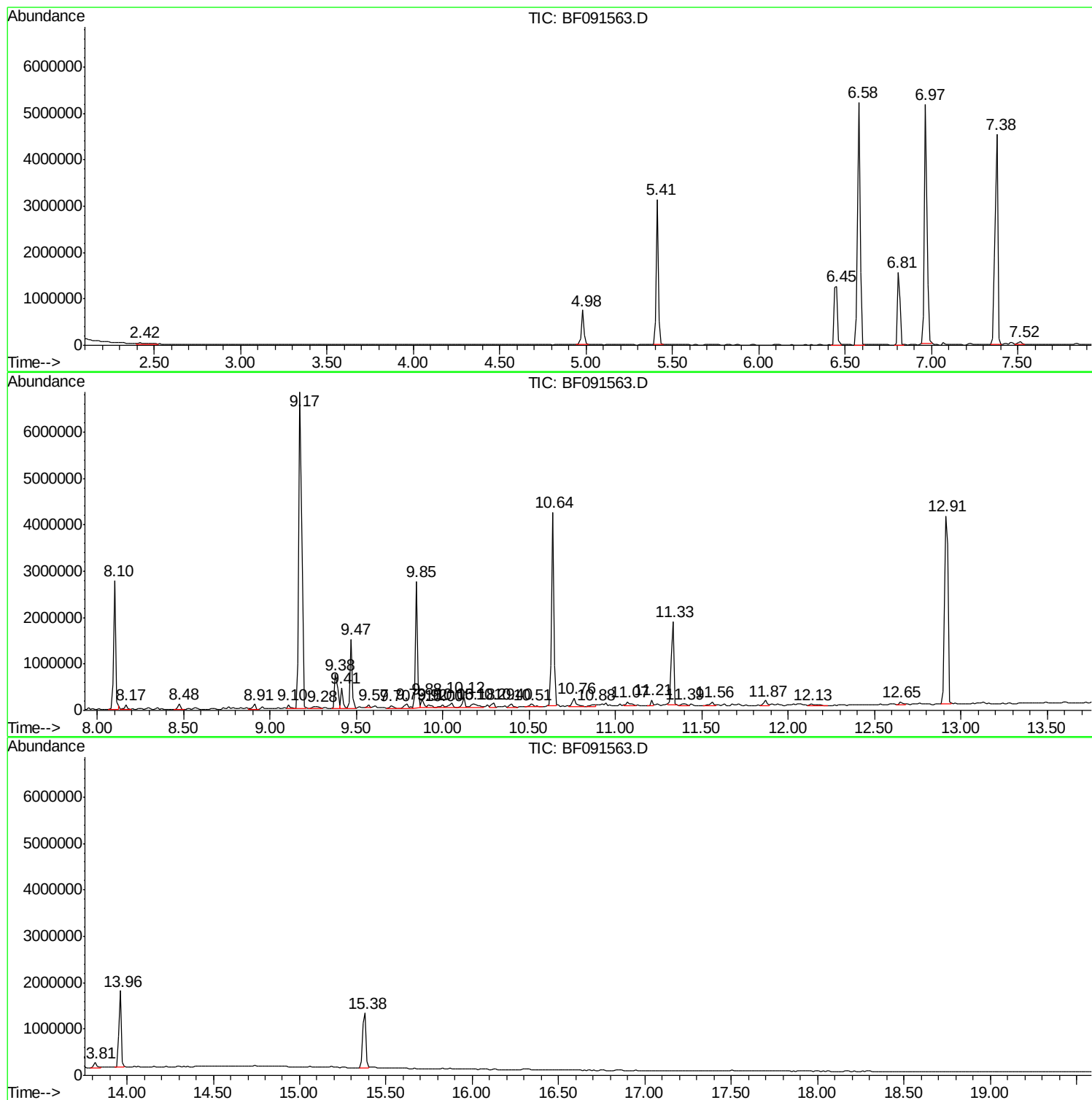
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Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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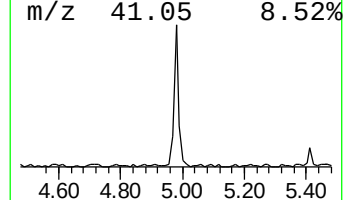
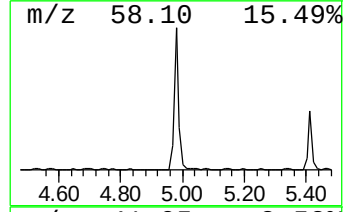
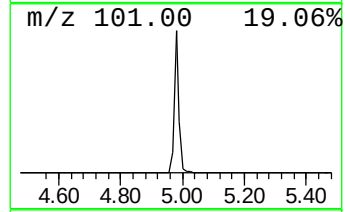
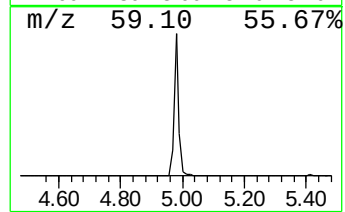
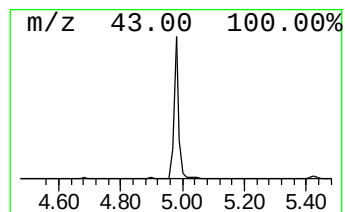
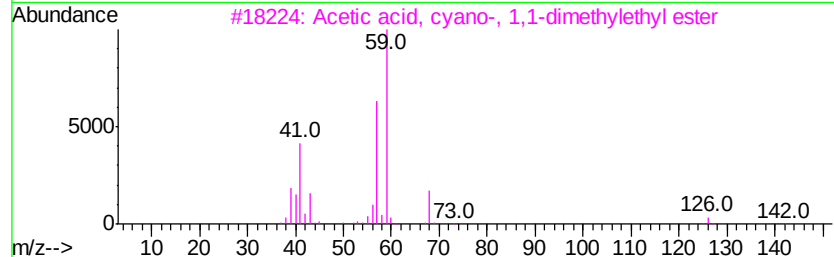
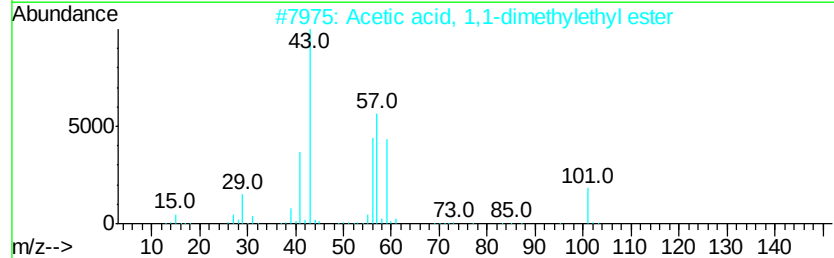
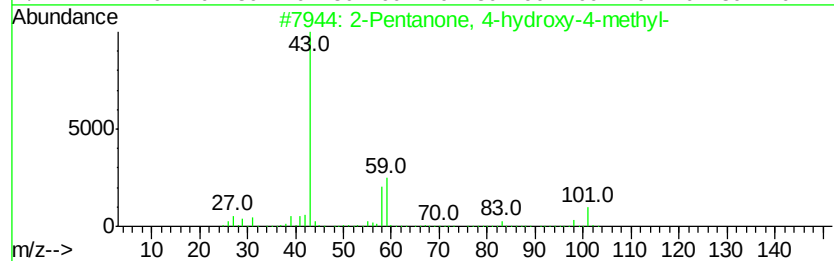
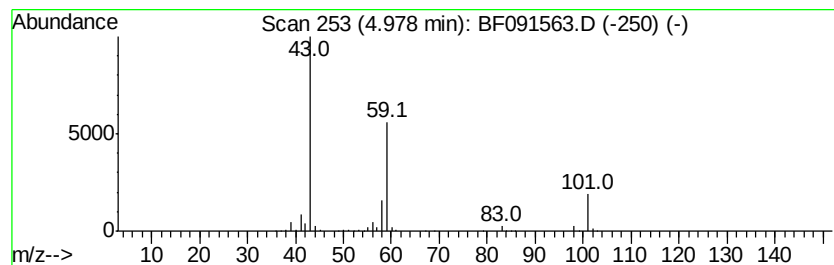
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.98	8.79 ng	772868	1,4-Dichlorobenzene-d4	6.81

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	64
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	17
4			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
5			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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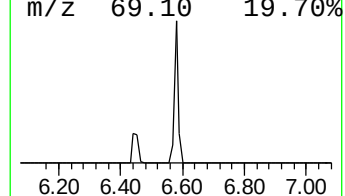
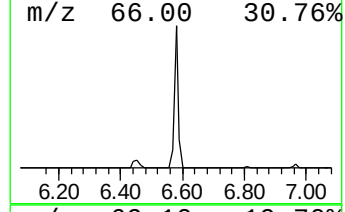
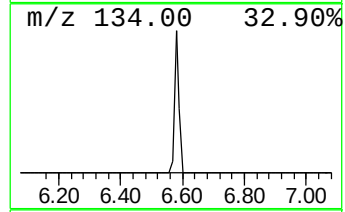
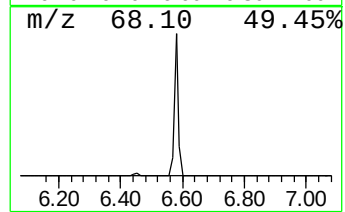
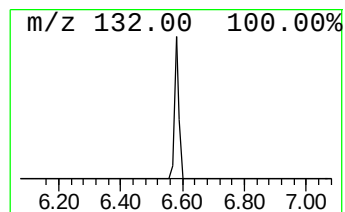
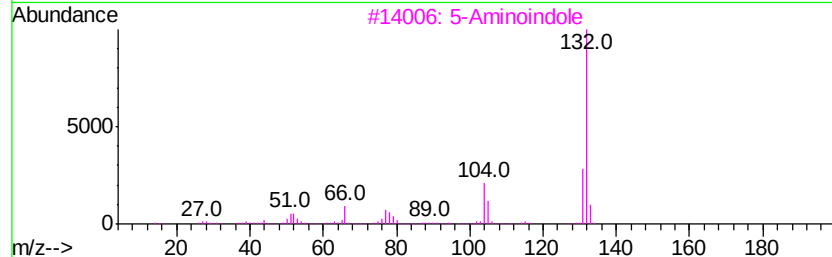
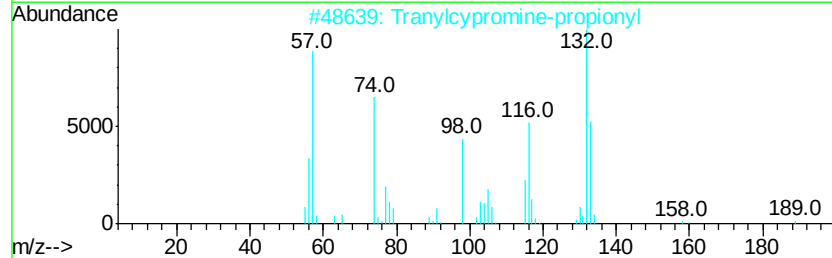
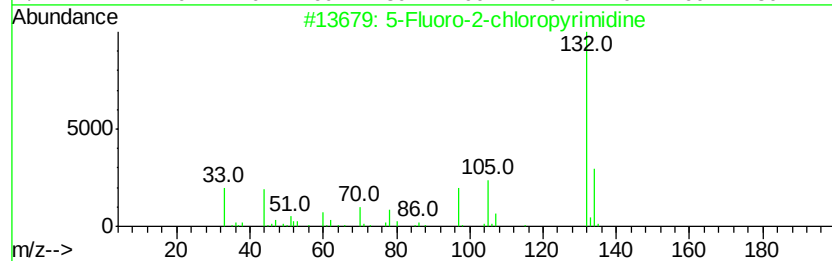
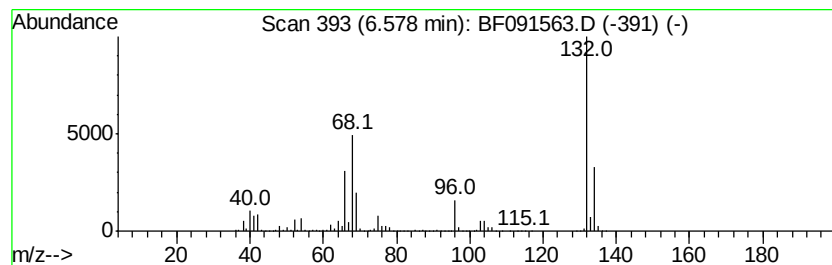
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TIC Library : C:\DATABASE\NIST02.L
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Peak Number 2 unknown6.58 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.58	57.68 ng	5069350	1,4-Dichlorobenzene-d4	6.81

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
2		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
3		5-Aminoindole	132	C8H8N2	005192-03-0	10
4		Xenon	132	Xe	007440-63-3	9
5		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9



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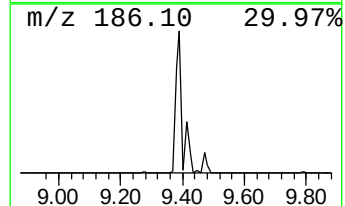
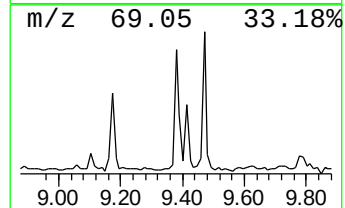
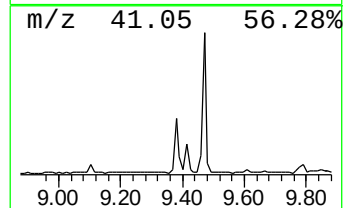
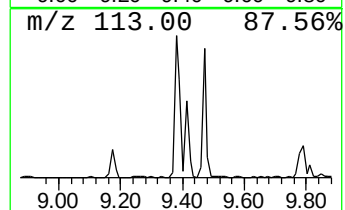
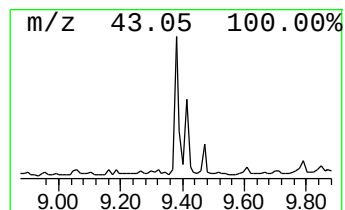
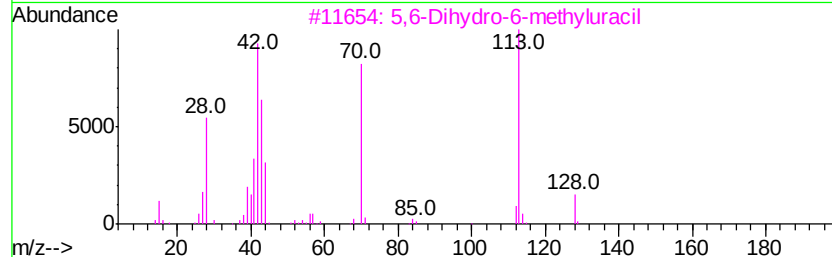
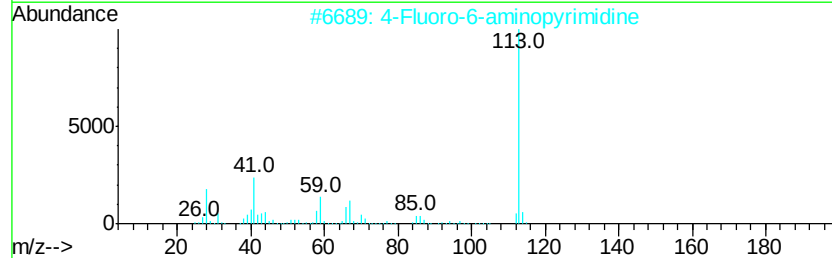
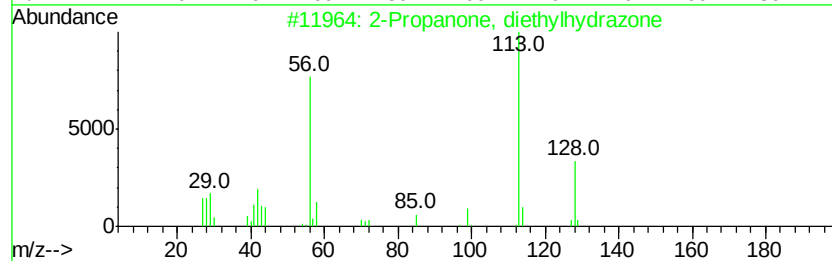
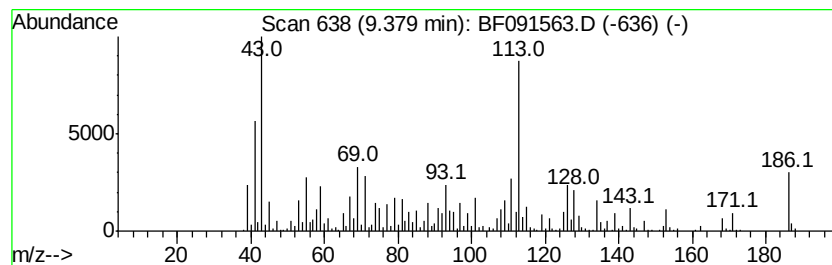
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 4 unknown9.38 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.38	7.27 ng	868359	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propanone, diethylhydrazone	128	C7H16N2	016713-36-3	35
2		4-Fluoro-6-aminopyrimidine	113	C4H4FN3	051421-96-6	35
3		5,6-Dihydro-6-methyluracil	128	C5H8N2O2	002434-49-3	35
4		1-Amino-2,6-dimethylpiperidine	128	C7H16N2	039135-39-2	35
5		N'-tert-Butyl-N,N-dimethylformam...	128	C7H16N2	023314-06-9	35



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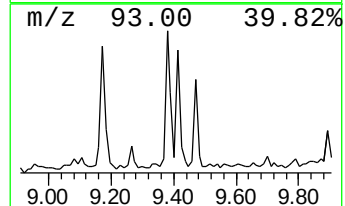
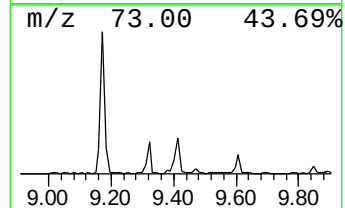
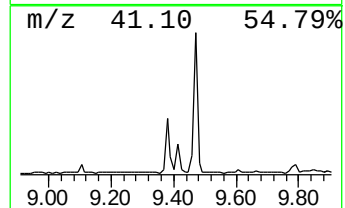
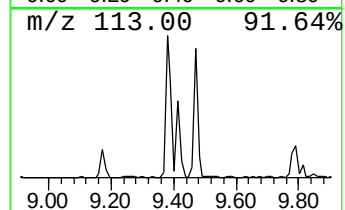
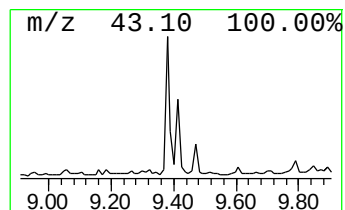
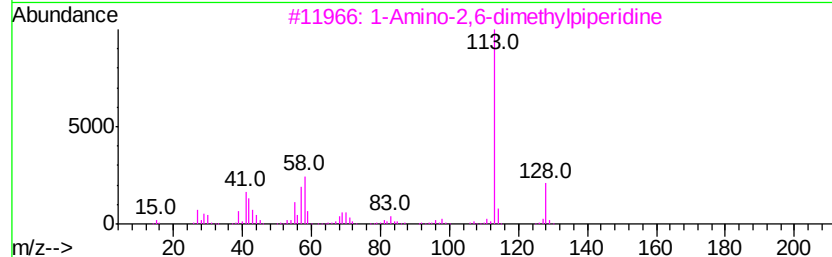
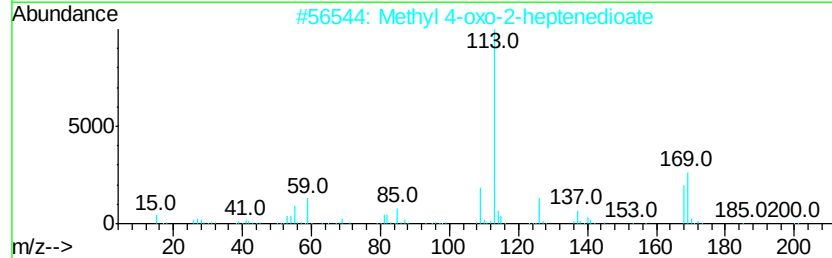
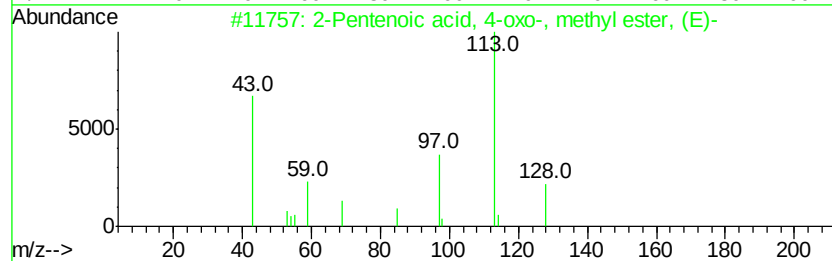
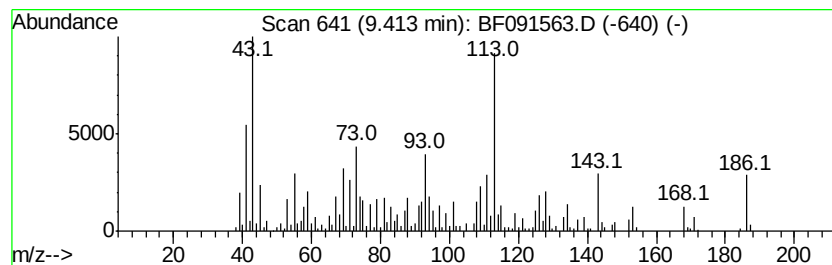
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 unknown9.41 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.41	3.21 ng	383951	Acenaphthene-d10	9.85

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Pentenoic acid, 4-oxo-, methyl...	128	C6H8O3	002833-24-1	35		
2	Methyl 4-oxo-2-heptenedioate	200	C9H12O5	022503-69-1	35		
3	1-Amino-2,6-dimethylpiperidine	128	C7H16N2	039135-39-2	27		
4	2-Chloromethylcyclopropanecarbox...	148	C6H9ClO2	064583-96-6	22		
5	Maleic monoacid chloride, methyl...	148	C5H5ClO3	1000152-93-6	22		



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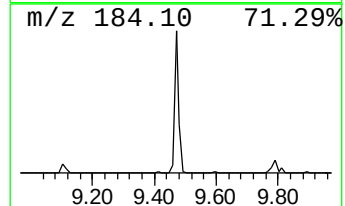
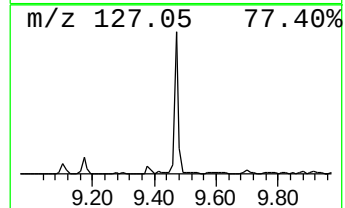
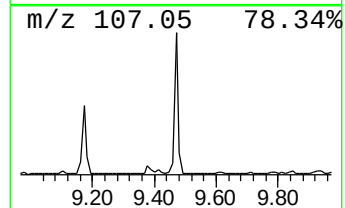
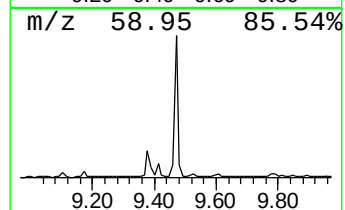
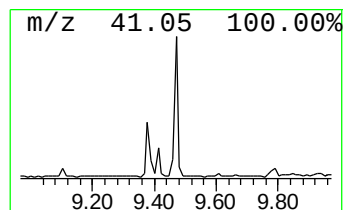
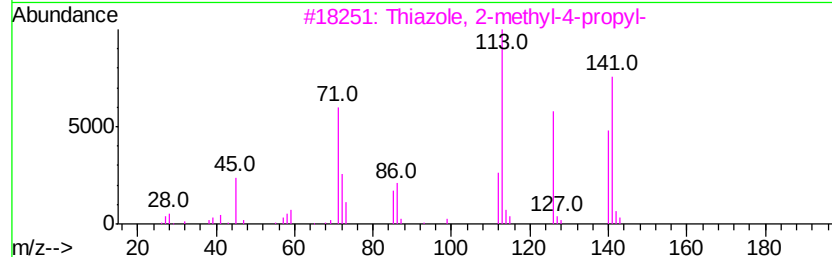
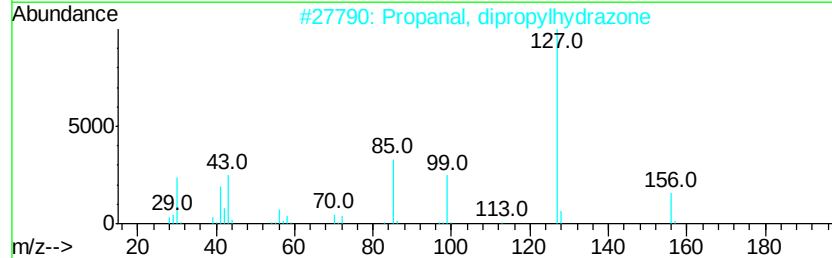
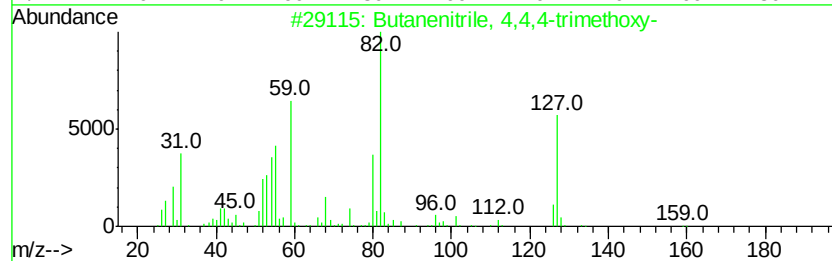
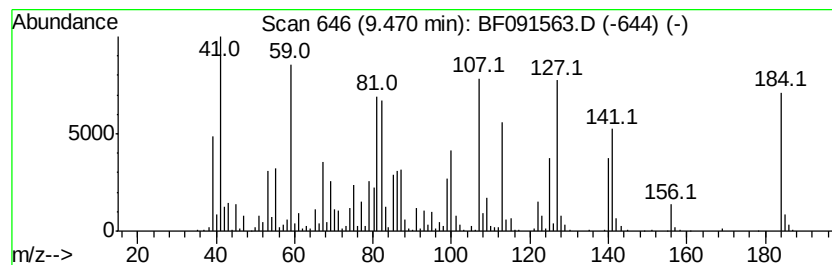
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TIC Library : C:\DATABASE\NIST02.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown9.47 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.47	10.38 ng	1239320	Acenaphthene-d10	9.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butanenitrile, 4,4,4-trimethoxy-	159	C7H13NO3	133871-50-8	12
2		Propanal, dipropylhydrazone	156	C9H20N2	034687-35-9	11
3		Thiazole, 2-methyl-4-propyl-	141	C7H11NS	041981-63-9	10
4		Phenol, 2-(methylsulfinyl)-	156	C7H8O2S	001074-02-8	10
5		1-[p-Chlorophenyl]-3-[4-[3-[1-p...	490	C18H22Cl4N8	110045-52-8	9



Data Path : Z:\HPCHEM1\BNA F\DATA\BF121316\
Data File : BF091563.D
Acq On : 13 Dec 2016 19:30
Operator : UM/SJ
Sample : H5961-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
QNWP8-MW27S-GW

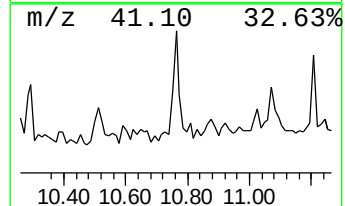
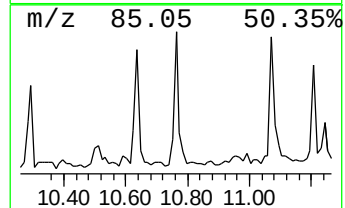
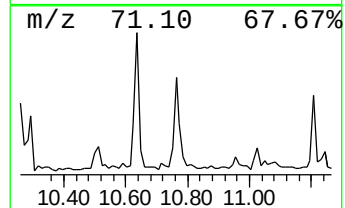
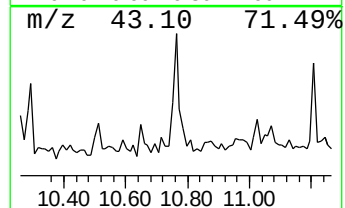
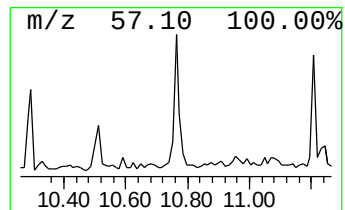
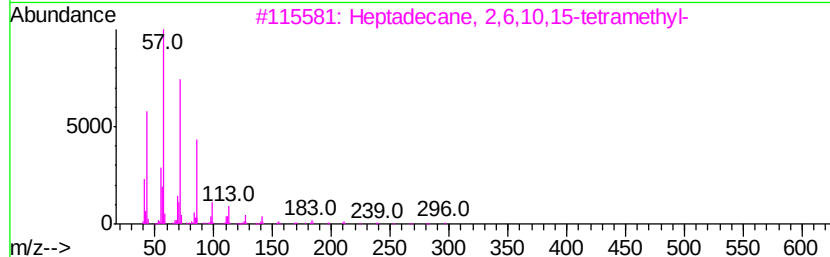
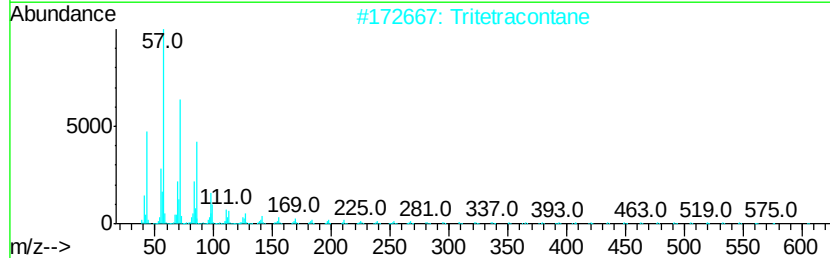
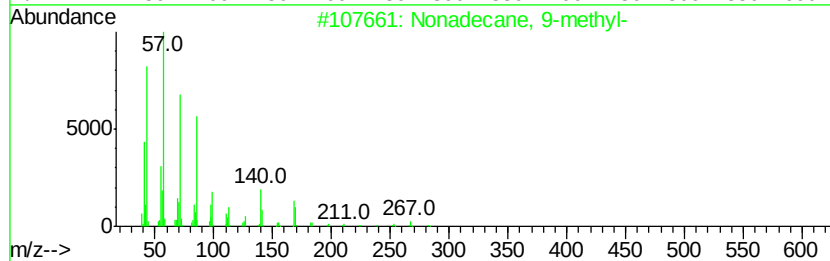
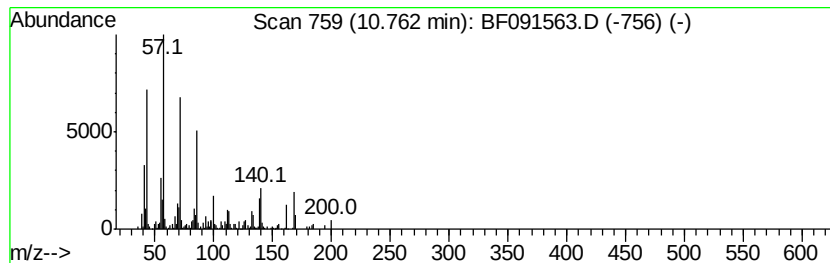
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Nonadecane, 9-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.76	2.89 ng	285109	Phenanthrene-d10	11.33

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Nonadecane, 9-methyl-	282	C20H42	013287-24-6	68
2			Tritetracontane	605	C43H88	007098-21-7	58
3			Heptadecane, 2,6,10,15-tetramethyl-	296	C21H44	054833-48-6	53
4			10-Methylnonadecane	282	C20H42	056862-62-5	52
5			Tridecane, 1-iodo-	310	C13H27I	035599-77-0	49



Data Path : Z:\HPCHEM1\BNA_F\DATA\BF121316\
Data File : BF091563.D
Acq On : 13 Dec 2016 19:30
Operator : UM/SJ
Sample : H5961-02
Misc :
ALS Vial : 19 Sample Multiplier: 1

Instrument :
BNA_F
ClientSampleId :
QNWP8-MW27S-GW

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF120916.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...	4.98	8.8	ng	772868	1	6.81	1757660	20.0
unknown6.58	6.58	57.7	ng	5069350	1	6.81	1757660	20.0
unknown9.38	9.38	7.3	ng	868359	3	9.85	2388960	20.0
unknown9.41	9.41	3.2	ng	383951	3	9.85	2388960	20.0
unknown9.47	9.47	10.4	ng	1239320	3	9.85	2388960	20.0
Nonadecane, 9-met...	10.76	2.9	ng	285109	4	11.33	1971830	20.0