

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF100416\
 Data File : BF090366.D
 Acq On : 5 Oct 2016 2:23
 Operator : UM/SJ
 Sample : H5065-02 10X
 Misc :
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SB-BC-2-10032016

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-BF100416.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	5.194	248	250	253	rVB	98707	122312	8.27%	0.922%
2	5.606	284	286	289	rBV	418917	565721	38.26%	4.266%
3	5.823	303	305	309	rBV	62312	65388	4.42%	0.493%
4	6.623	373	375	377	rBV	695397	563444	38.10%	4.249%
5	6.772	386	388	391	rVB	632078	557909	37.73%	4.207%
6	7.012	407	409	411	rBV	1455483	1149250	77.72%	8.666%
7	7.172	420	423	425	rVB	358332	387713	26.22%	2.924%
8	7.572	455	458	460	rBV	245013	292389	19.77%	2.205%
9	8.303	519	522	524	rBV	1351328	1330608	89.98%	10.034%
10	9.046	583	587	591	rVB3	6285	16673	1.13%	0.126%
11	9.378	613	616	618	rBV	521707	486483	32.90%	3.669%
12	9.766	648	650	652	rBV	170001	131163	8.87%	0.989%
13	10.063	673	676	678	rBV	1069246	1297124	87.72%	9.782%
14	10.841	742	744	746	rBV2	290089	288029	19.48%	2.172%
15	10.966	753	755	757	rBV2	14141	17466	1.18%	0.132%
16	11.412	793	794	798	rVB2	11072	17086	1.16%	0.129%
17	11.549	803	806	808	rVV	1719529	1402564	94.85%	10.577%
18	11.606	808	811	813	rVB4	12357	19974	1.35%	0.151%
19	11.766	824	825	828	rBV	25401	27557	1.86%	0.208%
20	12.075	850	852	853	rBV	35480	55682	3.77%	0.420%
21	12.589	895	897	899	rBV	84847	82951	5.61%	0.626%
22	12.761	910	912	915	rBV3	17721	44359	3.00%	0.335%
23	12.807	915	916	918	rVB2	19647	21752	1.47%	0.164%
24	13.069	937	939	940	rBV2	18702	17437	1.18%	0.131%
25	13.138	943	945	947	rBV	569111	510348	34.51%	3.849%
26	14.007	1018	1021	1022	rBV	158646	177657	12.01%	1.340%
27	14.041	1022	1024	1026	rVB	56791	88599	5.99%	0.668%
28	14.201	1035	1038	1040	rBV	1207824	1478788	100.00%	11.152%
29	14.670	1077	1079	1082	rBV	87699	109692	7.42%	0.827%
30	14.967	1104	1105	1109	rVB2	57581	87160	5.89%	0.657%
31	15.070	1112	1114	1118	rVV2	82071	117707	7.96%	0.888%
32	15.138	1118	1120	1123	rVB2	70910	92132	6.23%	0.695%
33	15.367	1136	1140	1151	rVB2	115085	317089	21.44%	2.391%
34	15.710	1167	1170	1172	rBV	770553	1184971	80.13%	8.936%

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Misc :
ALS Vial : 21 Sample Multiplier: 1

Instrument :
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ClientSampleId :
SB-BC-2-10032016

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

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35	16.453	1232	1235	1236	rBV2	69485	135696	9.18%	1.023%
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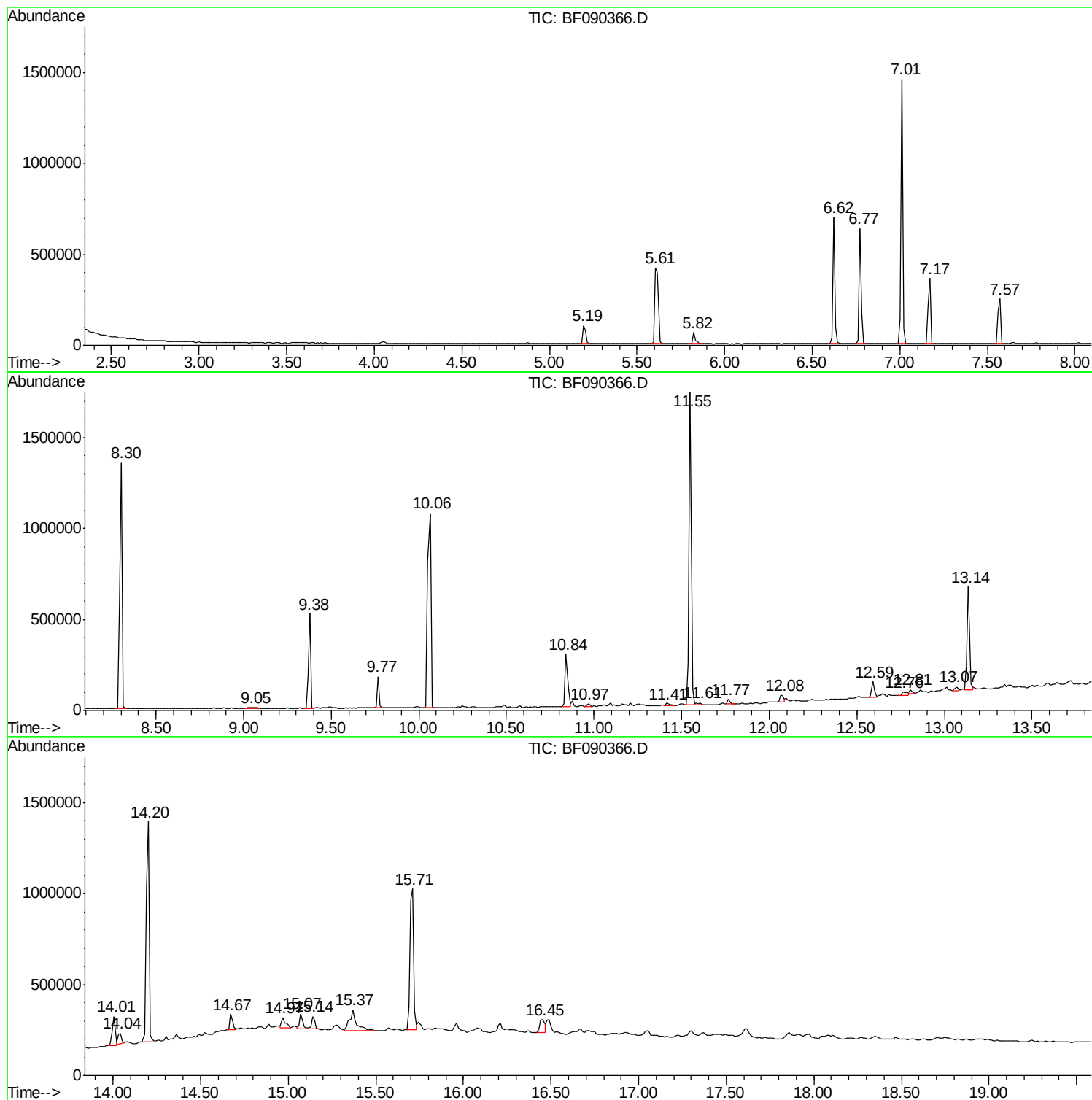
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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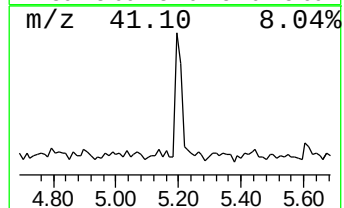
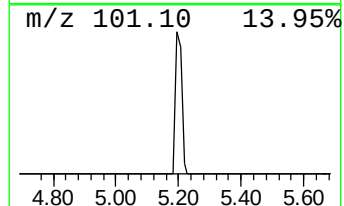
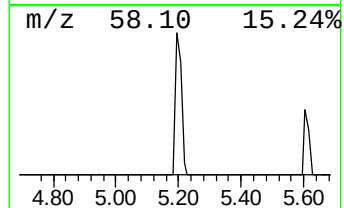
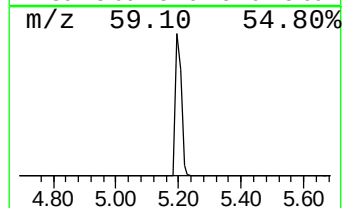
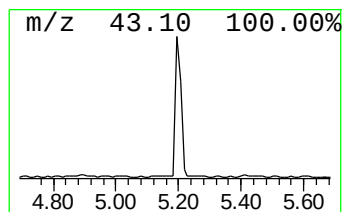
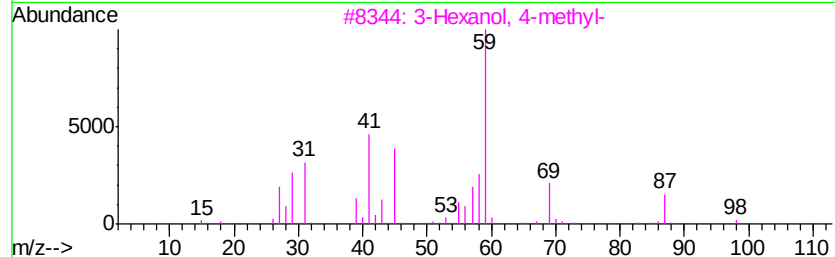
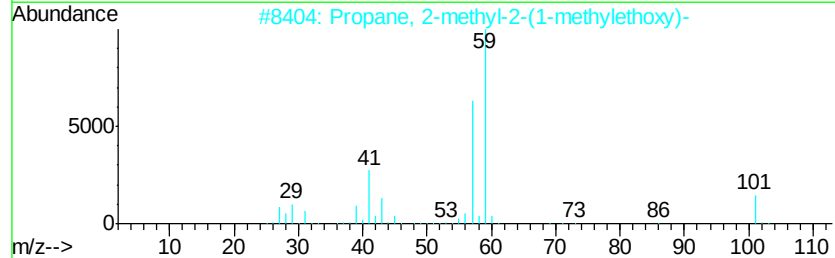
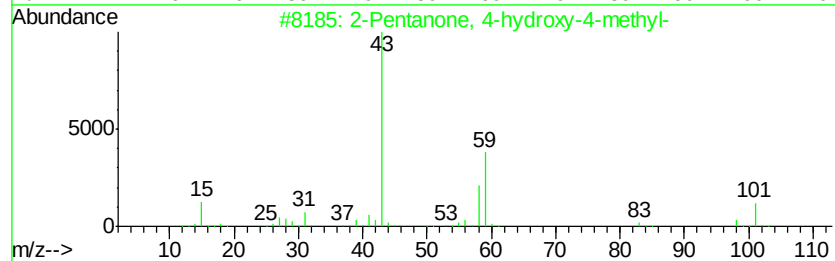
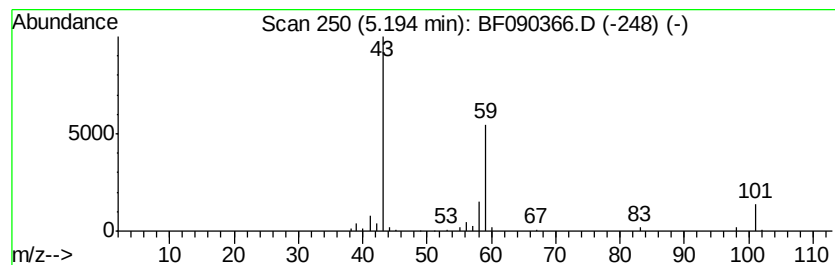
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.19	2.13 ng	122312	1,4-Dichlorobenzene-d4	7.01

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	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	3-Octanol	130	C8H18O	000589-98-0	33	
5	2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27	



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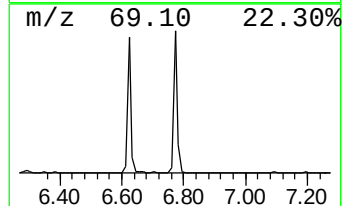
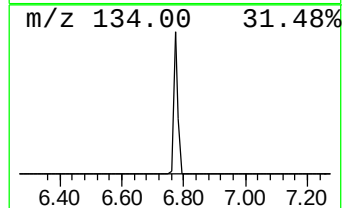
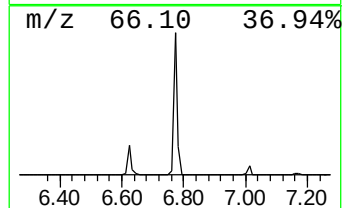
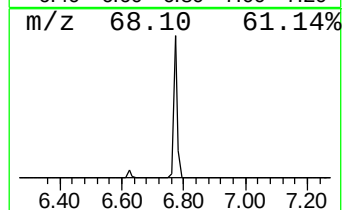
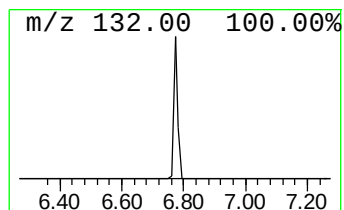
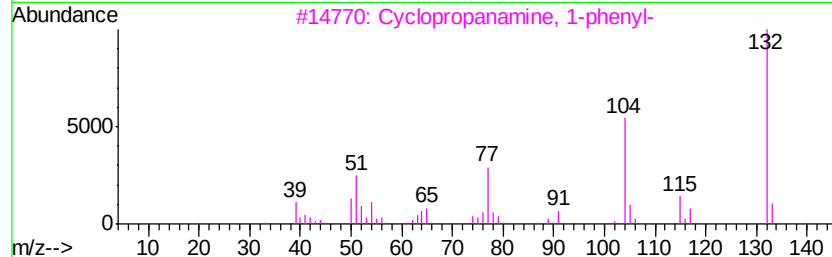
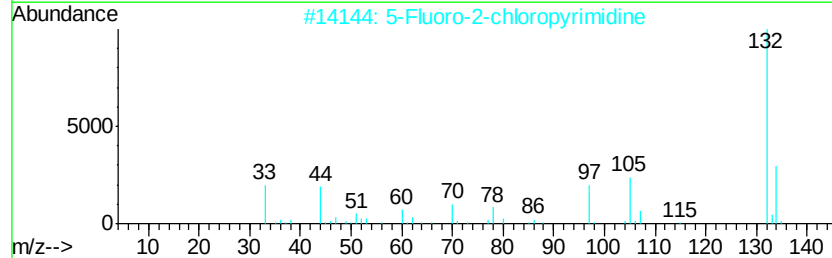
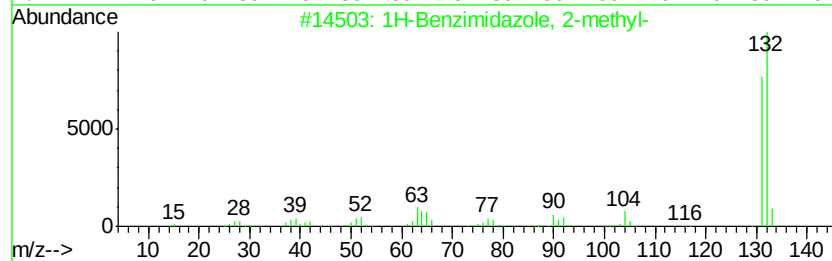
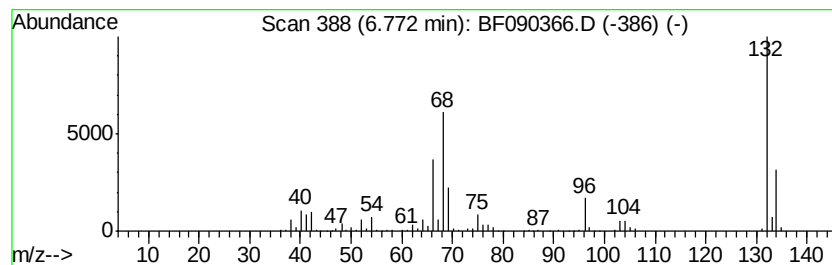
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.77 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.77	9.71 ng	557909	1,4-Dichlorobenzene-d4	7.01

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Benzimidazole, 2-methyl-	132	C8H8N2	000615-15-6	22
2			5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	12
3			Cyclopropanamine, 1-phenyl-	133	C9H11N	1000351-26-2	10
4			5-Aminoindole	132	C8H8N2	005192-03-0	10
5			2-Cyclohexen-1-one	96	C6H8O	000930-68-7	10



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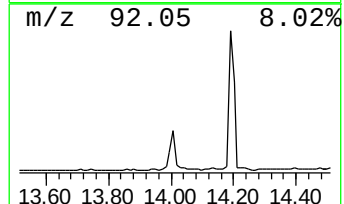
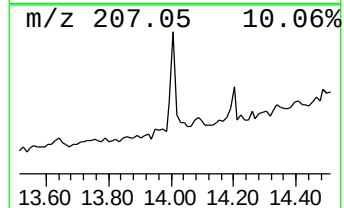
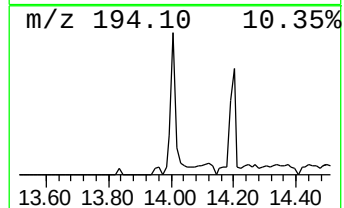
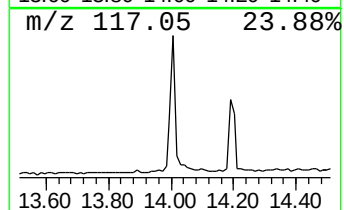
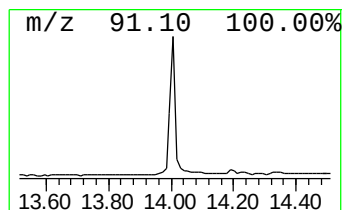
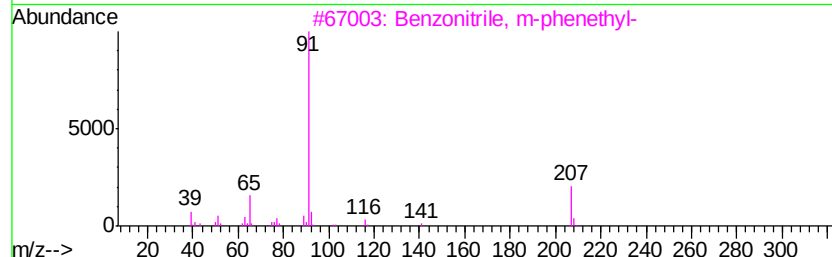
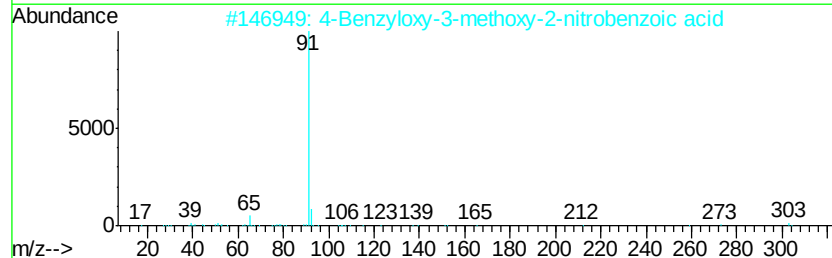
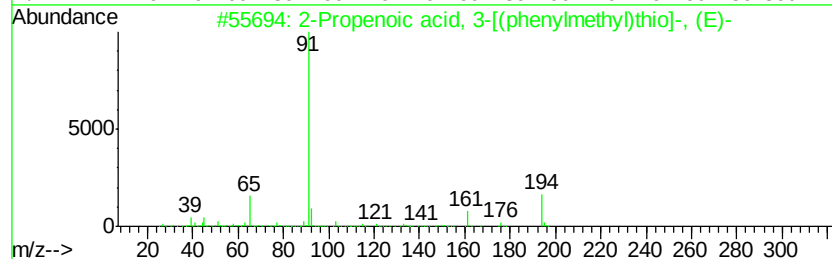
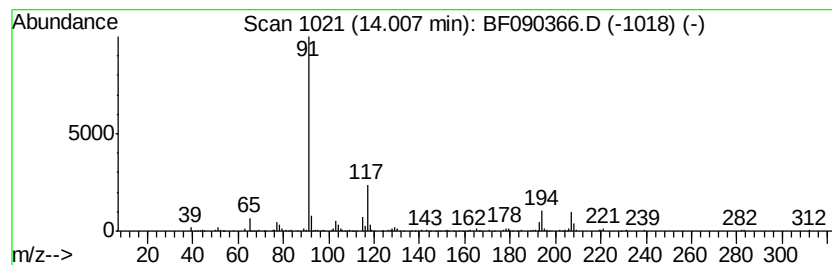
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	2.40 ng	177657	Chrysene-d12	14.20

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenoic acid, 3-[(phenylmeth...	194	C10H10O2S	013831-01-1	10
2		4-Benzyloxy-3-methoxy-2-nitroben...	303	C15H13N06	003584-32-5	10
3		Benzonitrile, m-phenethyl-	207	C15H13N	034176-91-5	10
4		N-Benzyl-1H-benzimidazole	208	C14H12N2	004981-92-4	9
5		4-Benzyloxybenzonitrile	209	C14H11NO	052805-36-4	9



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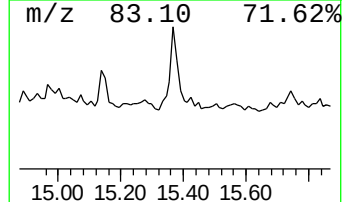
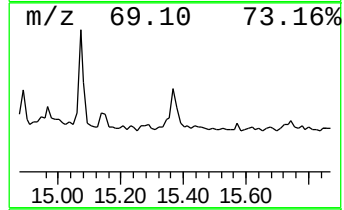
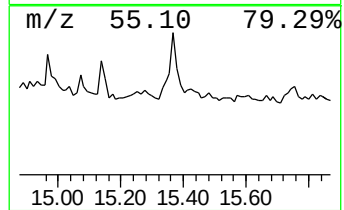
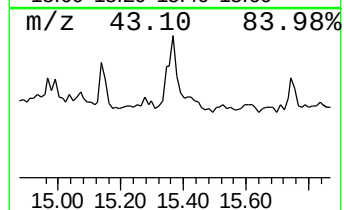
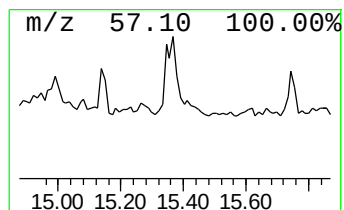
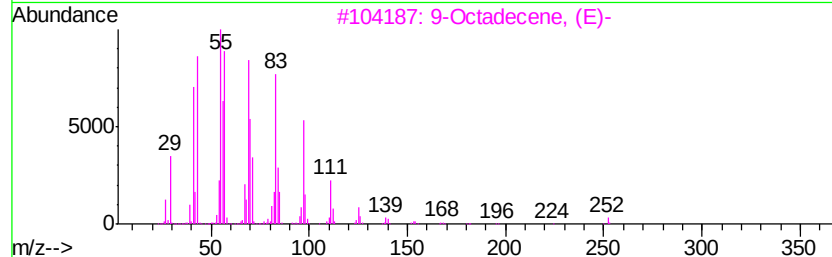
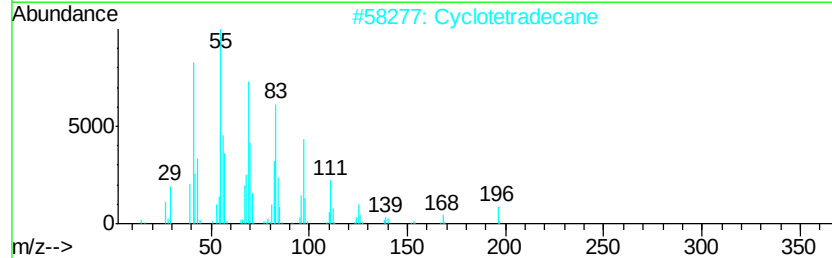
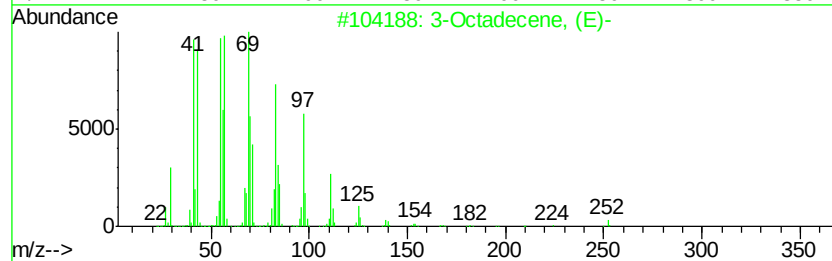
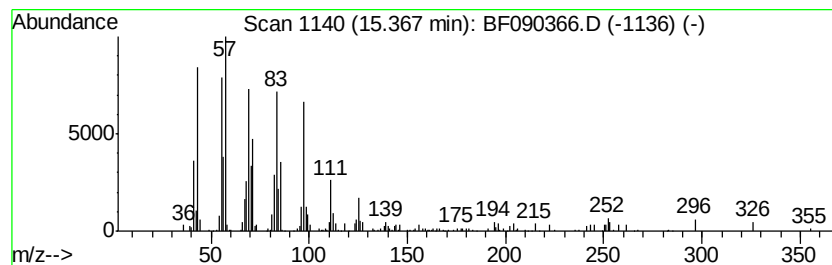
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 3-Octadecene, (E)- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.37	5.35 ng	317089	Perylene-d12	15.71

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Octadecene, (E)-	252	C18H36	007206-19-1	95
2		Cyclotetradecane	196	C14H28	000295-17-0	93
3		9-Octadecene, (E)-	252	C18H36	007206-25-9	93
4		1-Heptacosanol	396	C27H56O	002004-39-9	91
5		Trichloroacetic acid, hexadecyl ...	386	C18H33Cl3O2	074339-54-1	91



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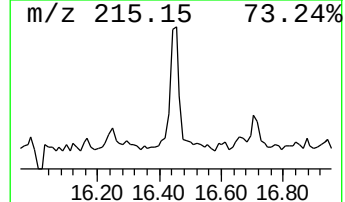
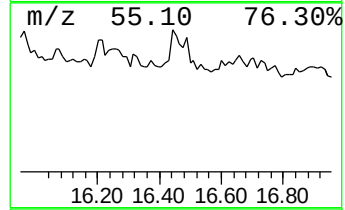
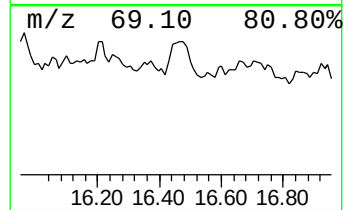
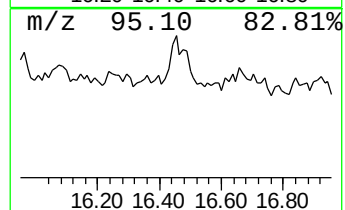
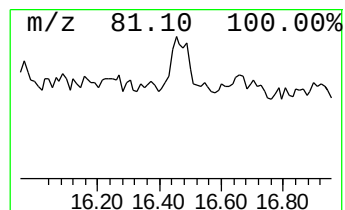
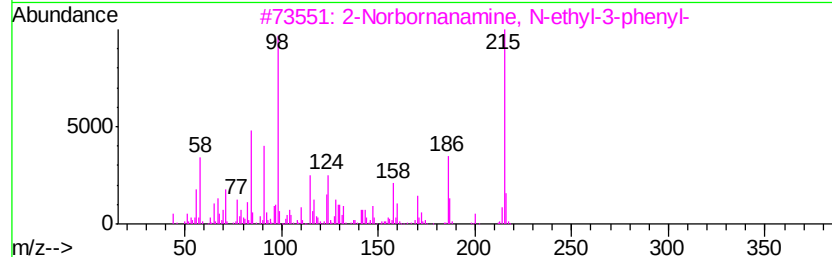
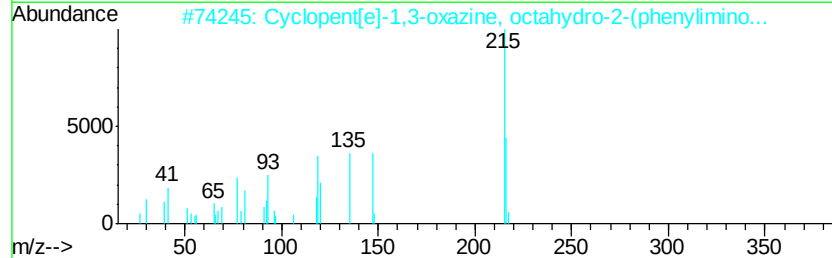
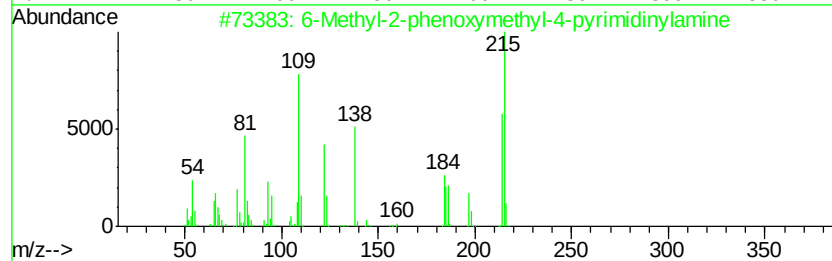
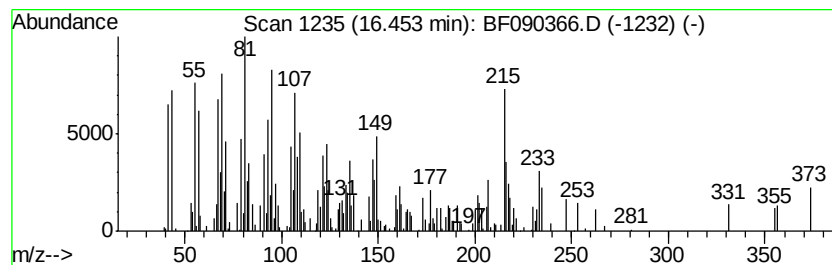
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Peak Number 6 unknown16.45 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.45	2.29 ng	135696	Perylene-d12	15.71

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	6-Methyl-2-phenoxyethyl-4-pyrim...	215	C12H13N3O	067386-50-9	30
2		Cyclopent[e]-1,3-oxazine, octahy...	216	C13H16N2O	1000138-92-2	25
3		2-Norbornanamine, N-ethyl-3-phenyl-	215	C15H21N	001209-98-9	11
4		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	11
5		Norbornane, carbanilide	215	C14H17NO	100717-55-3	11



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SB-BC-2-10032016

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF100416.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.19	2.1	ng	122312	1	7.01	1149250	20.0
unknown6.77	6.77	9.7	ng	557909	1	7.01	1149250	20.0
unknown14.01	14.01	2.4	ng	177657	5	14.20	1478790	20.0
3-Octadecene, (E)-	15.37	5.3	ng	317089	6	15.71	1184970	20.0
unknown16.45	16.45	2.3	ng	135696	6	15.71	1184970	20.0