

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091317\
 Data File : BF098509.D
 Acq On : 14 Sep 2017 00:29
 Operator : SJ/JU
 Sample : I5202-01
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A5972-OT

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-BF091117.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	4.828	463	466	473	rBV	139958	190219	1.99%	0.426%
2	5.263	537	540	555	rVB	1649171	1698843	17.74%	3.807%
3	5.963	647	659	669	rBV6	32184	112502	1.17%	0.252%
4	6.310	713	718	734	rBV2	951836	1425560	14.89%	3.195%
5	6.428	734	738	743	rBV	3161380	2922235	30.51%	6.549%
6	6.657	768	777	783	rBV	1301293	1248881	13.04%	2.799%
7	6.757	783	794	796	rBV	5132804	9576508	100.00%	21.462%
8	6.816	799	804	807	rBV	3530964	3186687	33.28%	7.142%
9	7.069	844	847	851	rBV	273183	225496	2.35%	0.505%
10	7.128	851	857	862	rVB2	104993	122307	1.28%	0.274%
11	7.228	866	874	877	rBV	2547802	2383991	24.89%	5.343%
12	7.410	899	905	911	rVB2	108480	171544	1.79%	0.384%
13	7.816	971	974	977	rBV	183121	161758	1.69%	0.363%
14	7.851	977	980	987	rVB	110057	109706	1.15%	0.246%
15	7.939	992	995	1003	rVB	1561460	1327390	13.86%	2.975%
16	8.057	1007	1015	1016	rBV	1404679	1907847	19.92%	4.276%
17	8.086	1016	1020	1023	rVB	1849924	2406582	25.13%	5.393%
18	8.222	1039	1043	1050	rVB	396671	373307	3.90%	0.837%
19	8.363	1063	1067	1072	rBV2	92961	110836	1.16%	0.248%
20	8.533	1089	1096	1100	rBV	1042899	1029073	10.75%	2.306%
21	8.692	1116	1123	1127	rBV	636915	860929	8.99%	1.929%
22	9.016	1173	1178	1181	rBV	4647010	4250342	44.38%	9.525%
23	9.051	1181	1184	1190	rVB2	134786	124818	1.30%	0.280%
24	9.416	1241	1246	1252	rVB2	96562	136485	1.43%	0.306%
25	9.522	1258	1264	1266	rBV3	48338	96765	1.01%	0.217%
26	9.557	1267	1270	1276	rVB2	116597	152417	1.59%	0.342%
27	9.686	1288	1292	1296	rVV2	1337781	1180901	12.33%	2.647%
28	10.480	1422	1427	1435	rBV	1525883	1476702	15.42%	3.309%
29	11.168	1540	1544	1550	rBV	1149759	951432	9.94%	2.132%
30	12.751	1809	1813	1817	rBV	2886551	2832276	29.58%	6.347%
31	13.651	1962	1966	1971	rBV7	65259	95959	1.00%	0.215%
32	13.804	1988	1992	1998	rVB	1077226	982876	10.26%	2.203%
33	15.198	2225	2229	2237	rVB	619544	787675	8.23%	1.765%

LSC Area Percent Report

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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-BF091117.M
Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

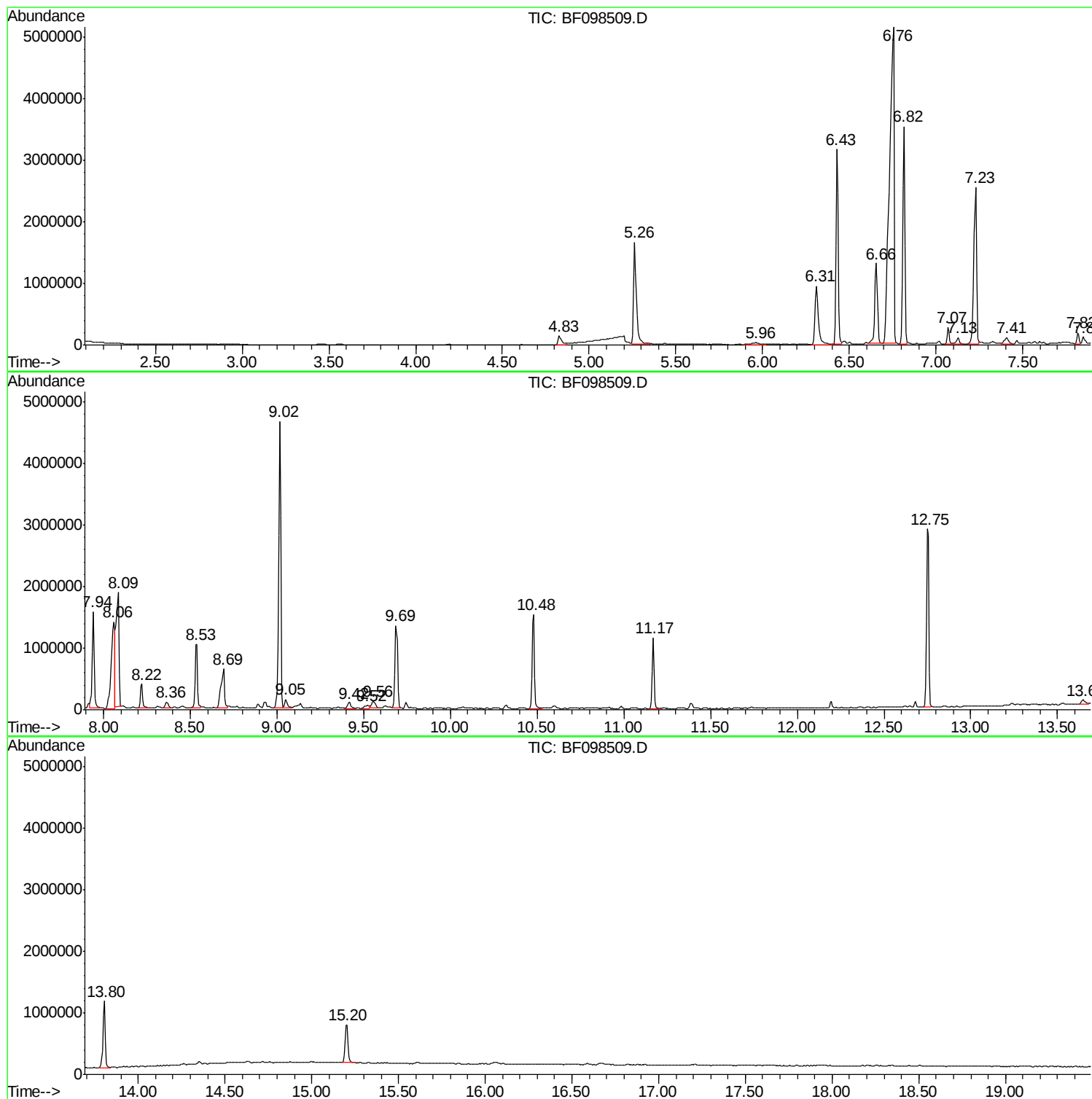
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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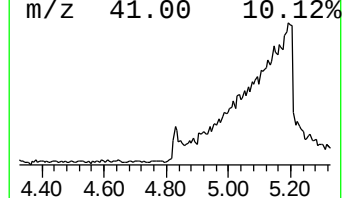
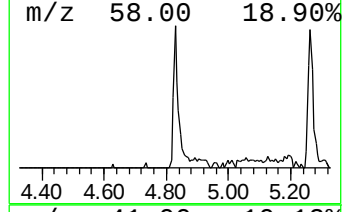
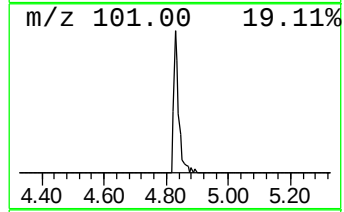
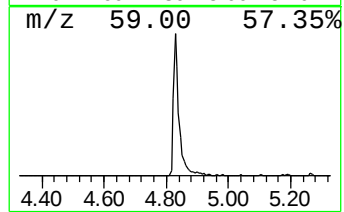
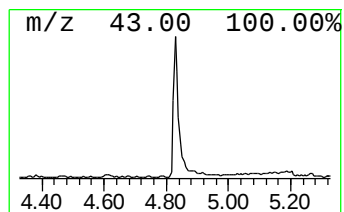
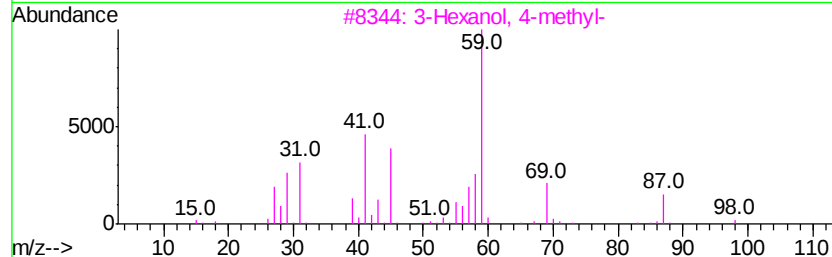
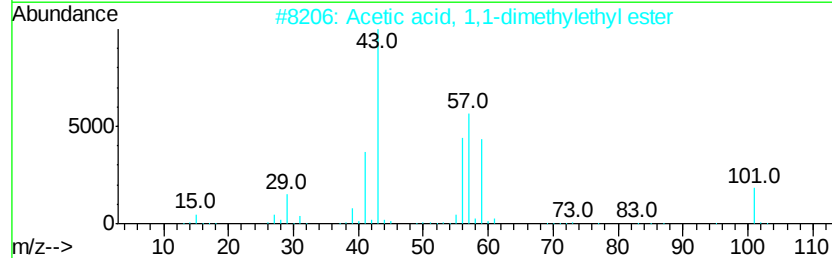
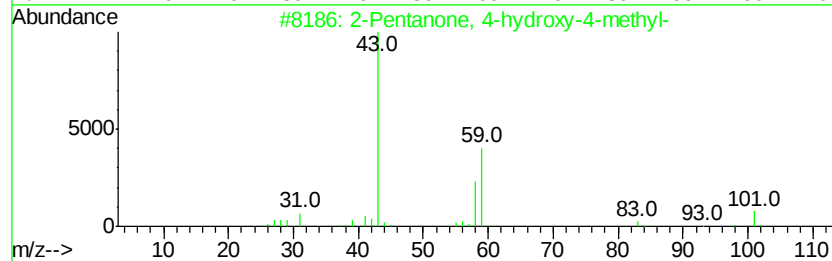
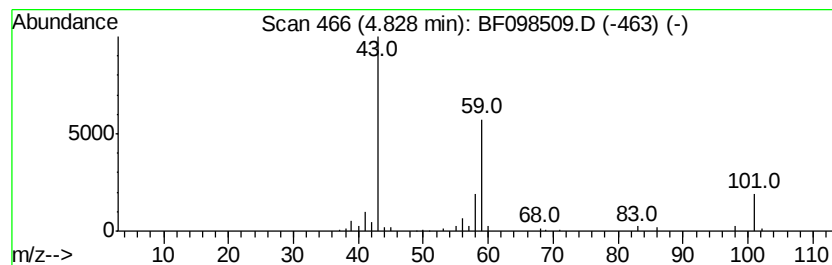
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.83	3.05 ng	190219	1,4-Dichlorobenzene-d4	6.66

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	56
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	38
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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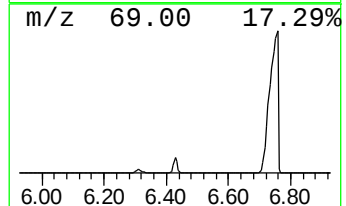
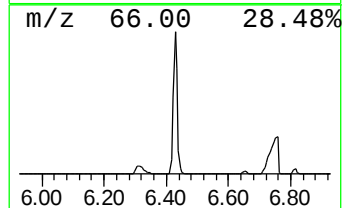
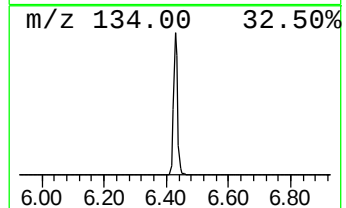
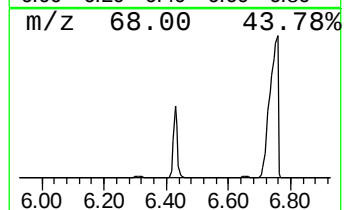
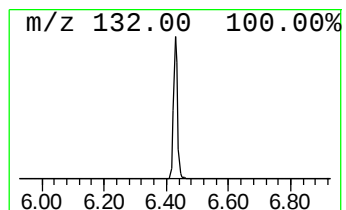
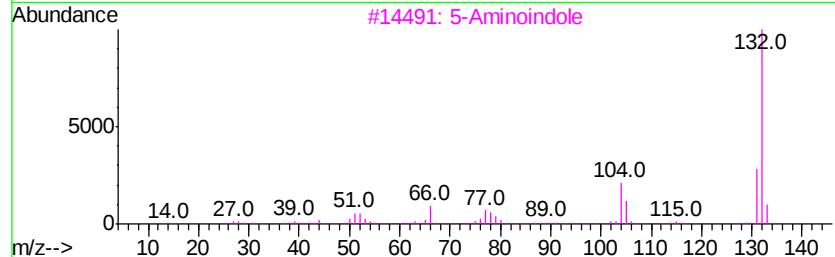
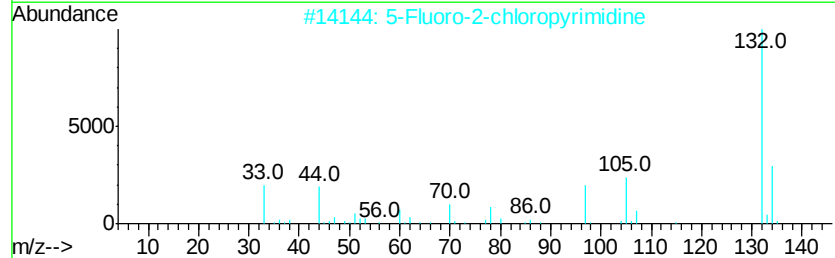
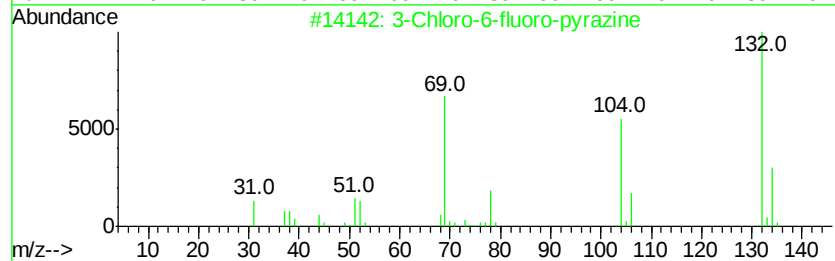
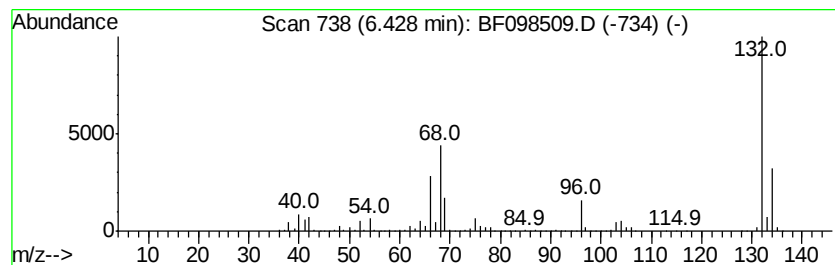
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.43 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.43	46.80 ng	2922240	1,4-Dichlorobenzene-d4	6.66

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	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		2H-Cyclopenta[d]pyridazine, 2-me...	132	C8H8N2	022291-85-6	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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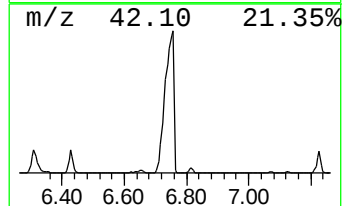
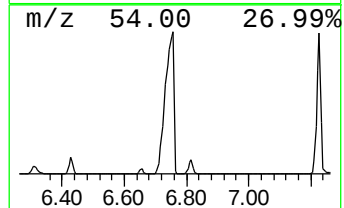
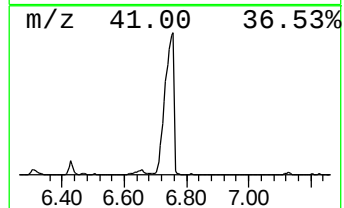
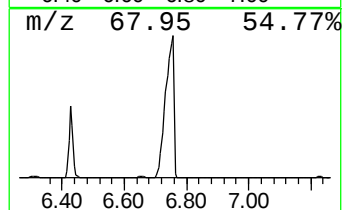
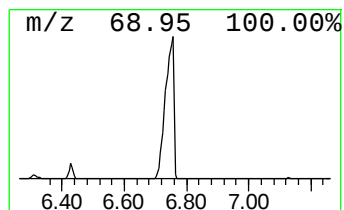
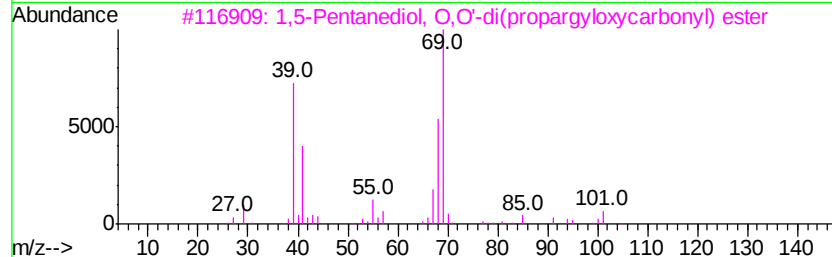
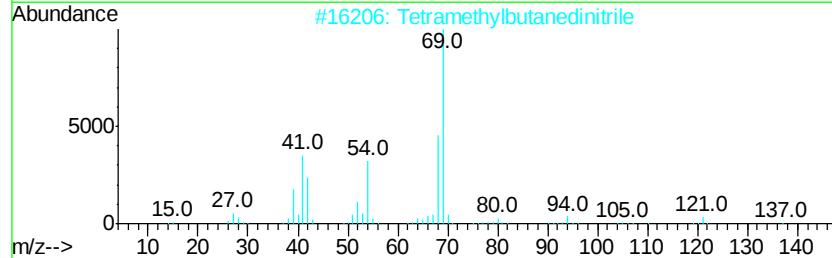
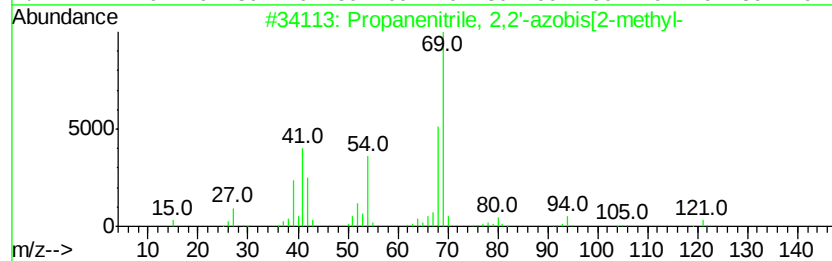
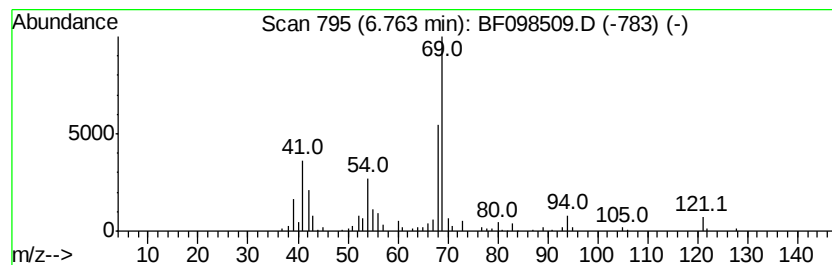
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Propanenitrile, 2,2'-azobis... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.76	153.36 ng	9576510	1,4-Dichlorobenzene-d4	6.66

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propanenitrile, 2,2'-azobis[2-me...	164	C8H12N4	000078-67-1	90
2		Tetramethylbutanedinitrile	136	C8H12N2	003333-52-6	90
3		1,5-Pentanediol, 0,0'-di(proparg...	268	C13H16O6	1000331-35-4	53
4		Trifluoroacetic acid, cyclopentyl...	182	C7H9F3O2	000703-13-9	38
5		Isoxazole	69	C3H3NO	000288-14-2	36



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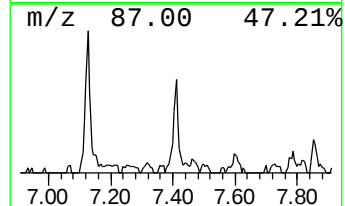
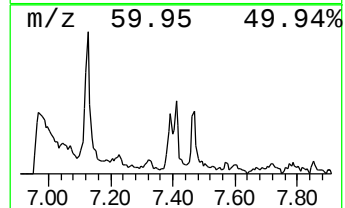
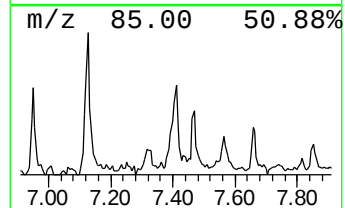
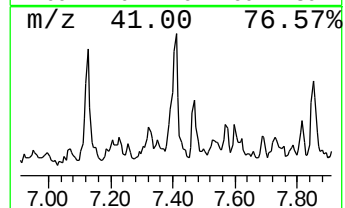
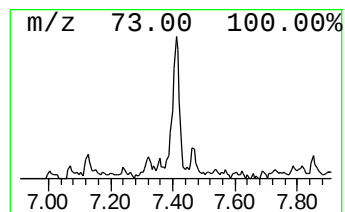
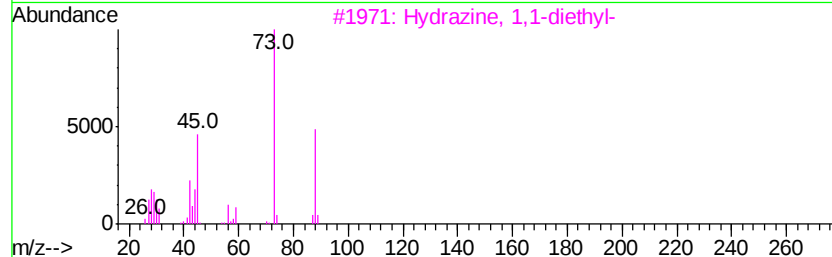
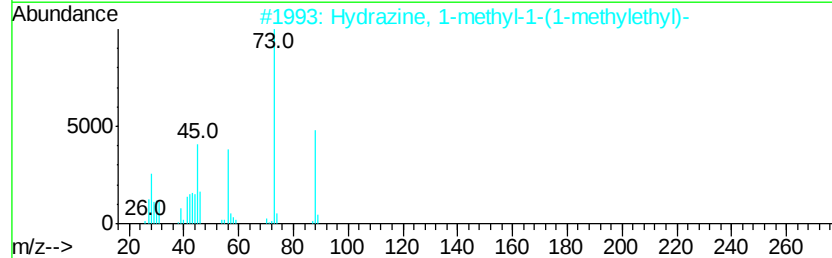
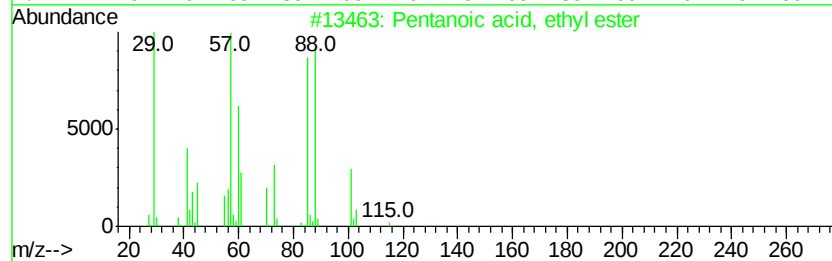
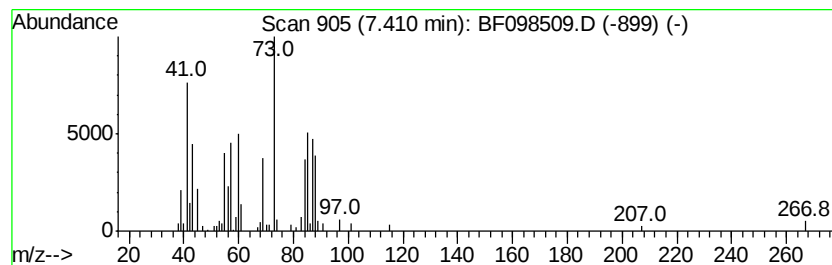
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Peak Number 5 unknown7.41 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.41	2.58 ng	171544	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentanoic acid, ethyl ester	130	C7H14O2	000539-82-2	32
2		Hydrazine, 1-methyl-1-(1-methyle...	88	C4H12N2	033668-54-1	27
3		Hydrazine, 1,1-diethyl-	88	C4H12N2	000616-40-0	22
4		Malonic acid, isobutyl 3-methylp...	244	C13H24O4	1000348-67-2	22
5		Dimethylmalonic acid, di(2-methy...	300	C17H32O4	1000361-80-4	16



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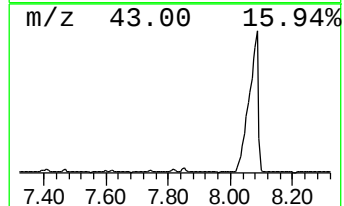
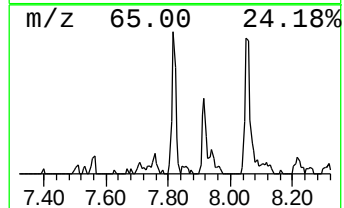
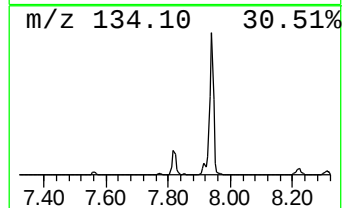
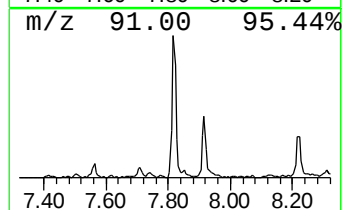
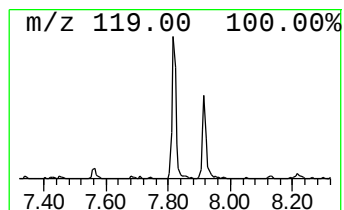
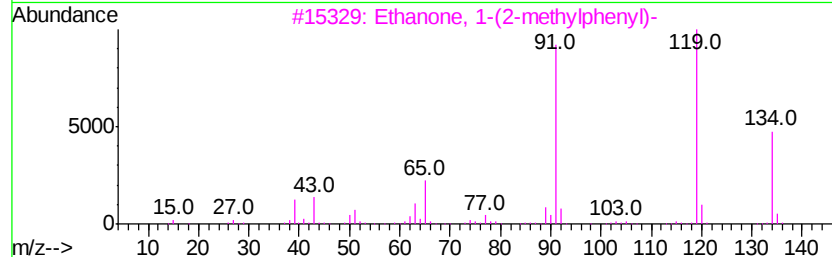
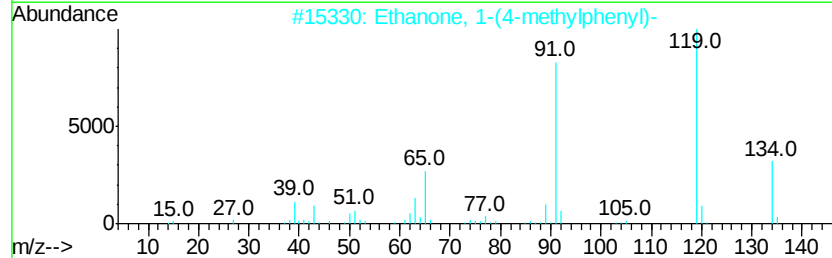
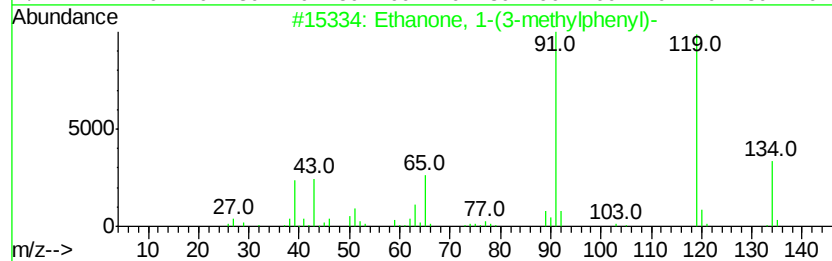
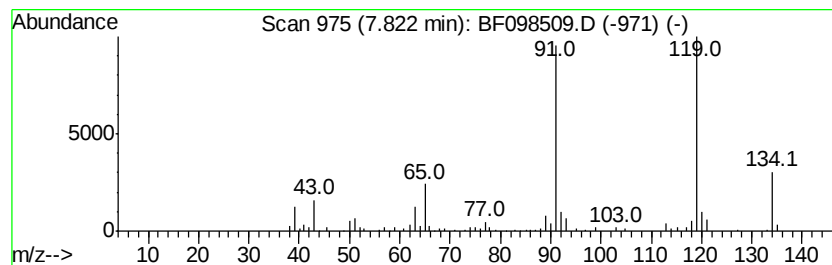
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Peak Number 6 Ethanone, 1-(3-methylphenyl)- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.82	2.44 ng	161758	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Ethanone, 1-(3-methylphenyl)-	134	C9H10O	000585-74-0	95
2		Ethanone, 1-(4-methylphenyl)-	134	C9H10O	000122-00-9	95
3		Ethanone, 1-(2-methylphenyl)-	134	C9H10O	000577-16-2	87
4		Benzene, 1-methyl-3-(1-methyleth...	134	C10H14	000535-77-3	72
5		Benzaldehyde, 4-methyl-	120	C8H8O	000104-87-0	64



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Data File : BF098509.D
Acq On : 14 Sep 2017 00:29
Operator : SJ/JU
Sample : I5202-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

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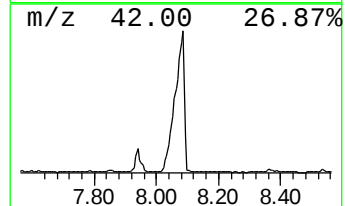
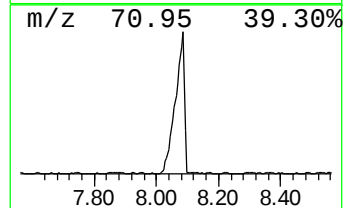
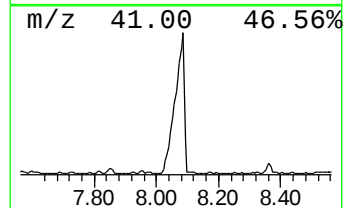
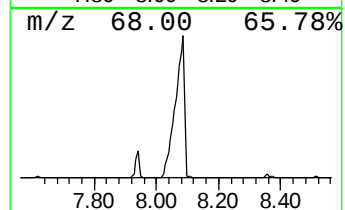
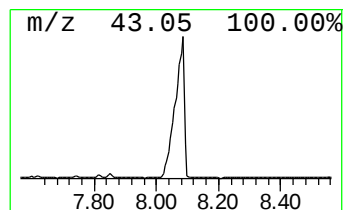
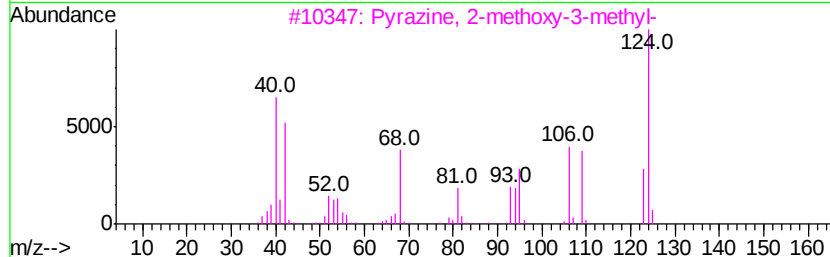
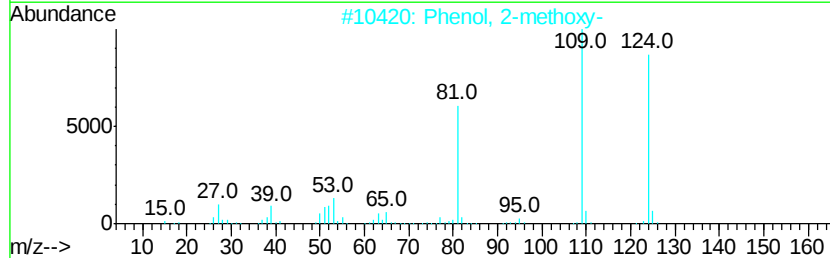
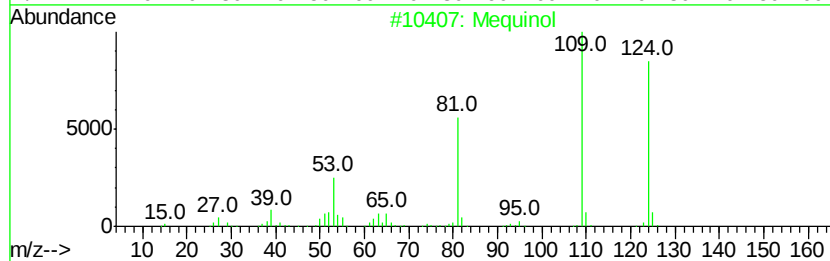
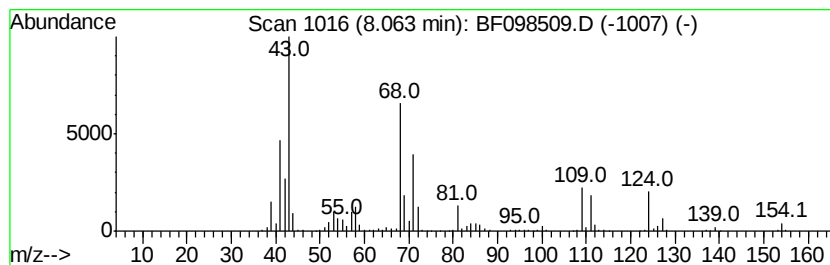
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 7 Mequinol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.06	28.75 ng	1907850	Naphthalene-d8	7.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Mequinol	124	C7H8O2	000150-76-5	83
2		Phenol, 2-methoxy-	124	C7H8O2	000090-05-1	70
3		Pvrazine, 2-methoxy-3-methyl-	124	C6H8N2O	002847-30-5	35
4		Ethanone, 1-(1-cyclohexen-1-yl)-	124	C8H12O	000932-66-1	27
5		2-Acetyl-5-methylfuran	124	C7H8O2	001193-79-9	22



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098509.D
Acq On : 14 Sep 2017 00:29
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ClientSampleId :
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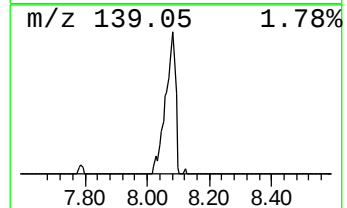
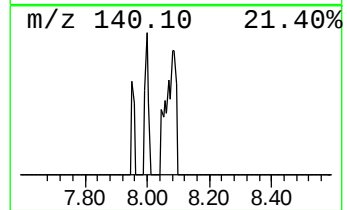
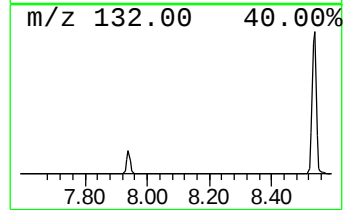
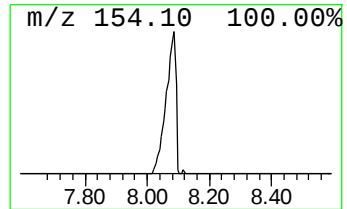
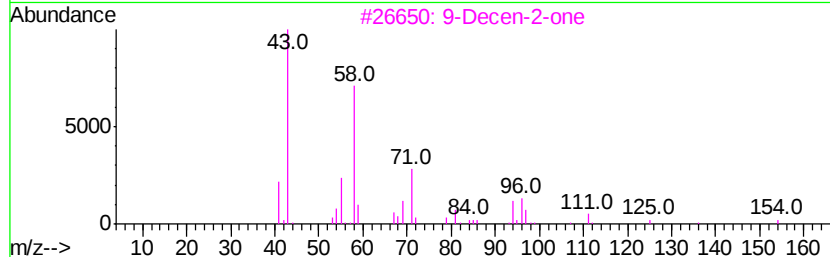
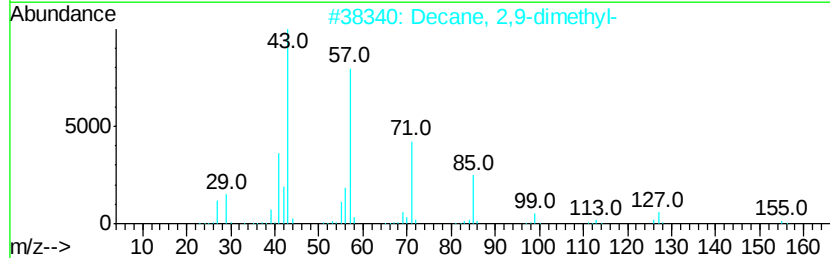
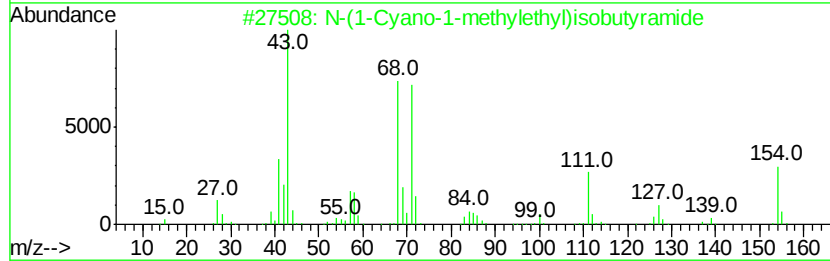
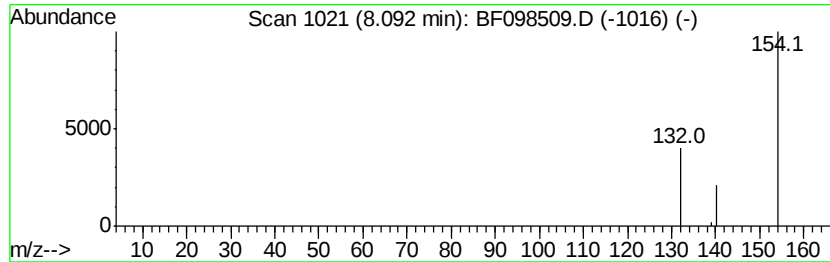
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 8 N-(1-Cyano-1-methylethyl)is... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.09	36.26 ng	2406580	Napthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	N-(1-Cyano-1-methylethyl)isobuty...	154	C8H14N2O	084213-57-0	64
2		Decane, 2,9-dimethyl-	170	C12H26	001002-17-1	25
3		9-Decen-2-one	154	C10H18O	035194-30-0	12
4		Glycine, N-(trifluoroacetyl)-, 1...	241	C9H14F3NO3	057983-43-4	12
5		Hexane, 3-methyl-	100	C7H16	000589-34-4	12



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098509.D
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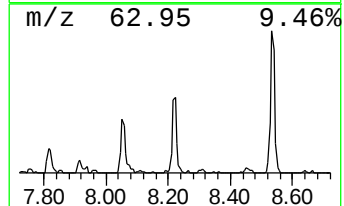
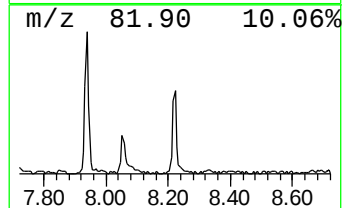
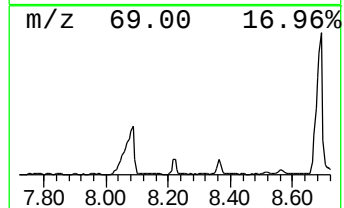
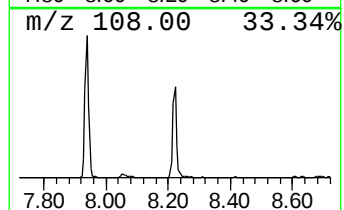
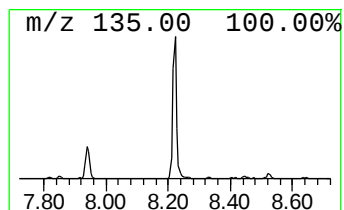
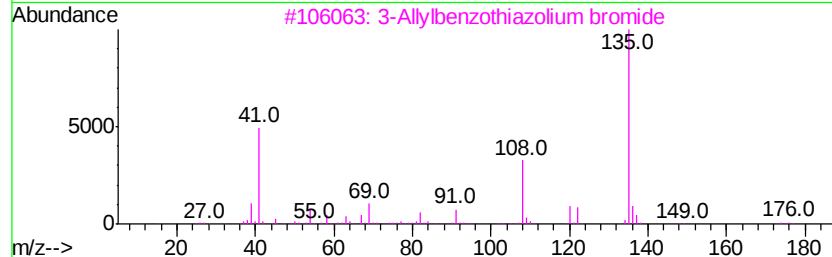
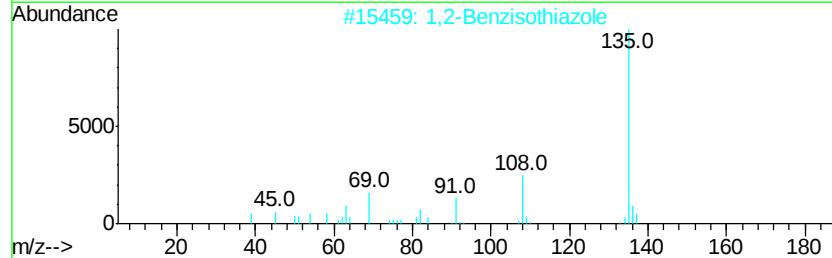
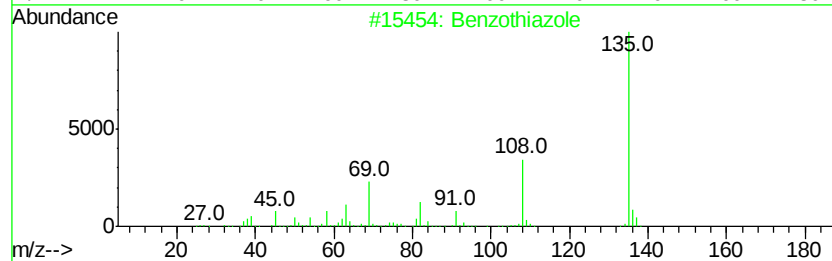
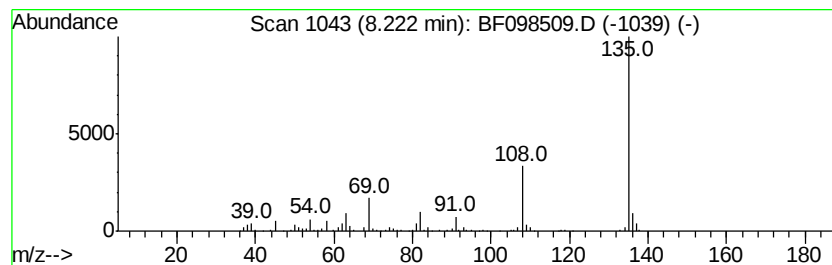
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 9 Benzothiazole Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.22	5.62 ng	373307	Naphthalene-d8	7.94

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzothiazole	135	C7H5NS	000095-16-9	95
2		1,2-Benzisothiazole	135	C7H5NS	000272-16-2	87
3		3-Allylbenzothiazolium bromide	255	C10H10BrNS	016407-55-9	72
4		2-Fluoro-4-cyanotoluene	135	C8H6FN	170572-49-3	64
5		Thieno[2,3-c]pyridine	135	C7H5NS	000272-12-8	64



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098509.D
Acq On : 14 Sep 2017 00:29
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Sample : I5202-01
Misc :
ALS Vial : 27 Sample Multiplier: 1

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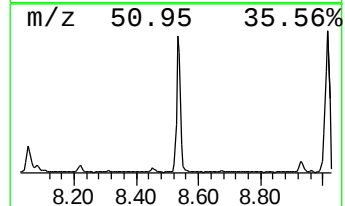
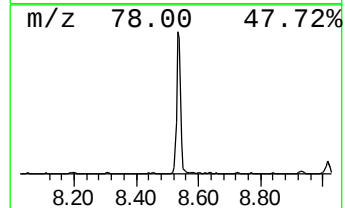
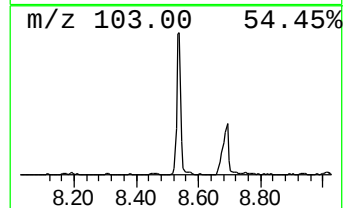
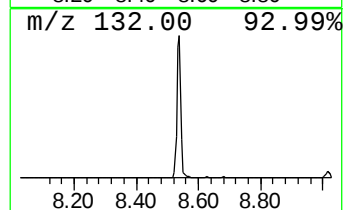
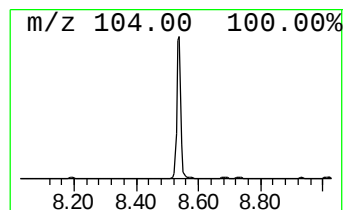
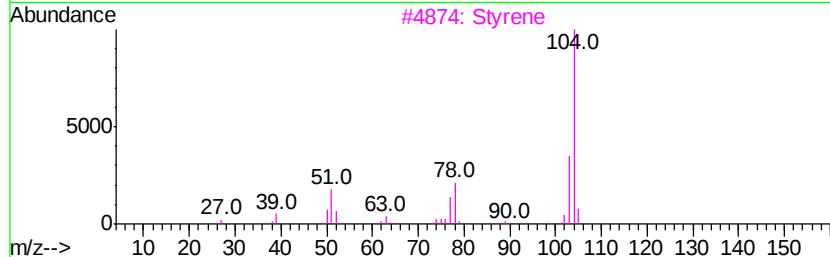
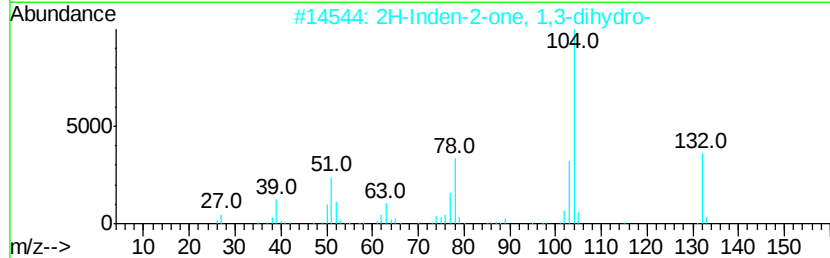
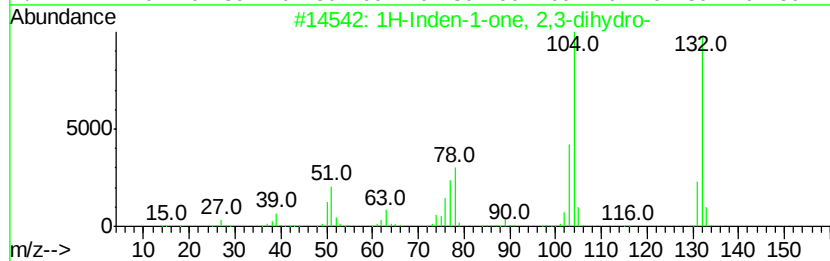
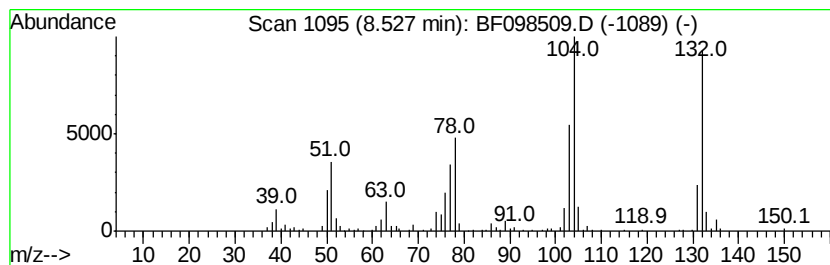
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 10 1H-Inden-1-one, 2,3-dihydro- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.53	15.51 ng	1029070	Napthalene-d8	7.94

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Inden-1-one, 2,3-dihydro-	132	C9H8O	000083-33-0	96
2			2H-Inden-2-one, 1,3-dihydro-	132	C9H8O	000615-13-4	68
3			Styrene	104	C8H8	000100-42-5	64
4			1,3,5,7-Cyclooctatetraene	104	C8H8	000629-20-9	64
5			Bicyclo[4.2.0]octa-1,3,5-triene	104	C8H8	000694-87-1	60



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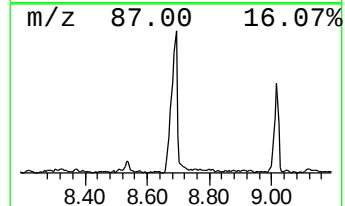
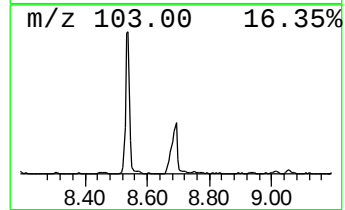
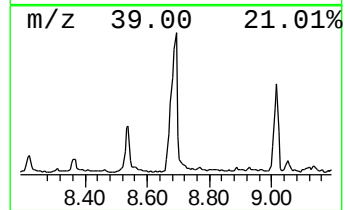
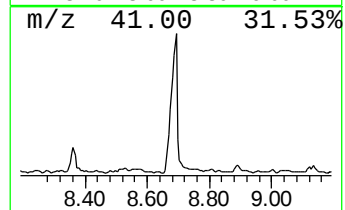
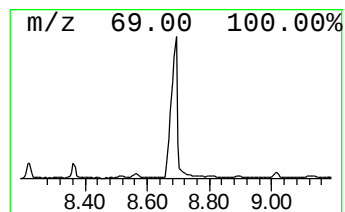
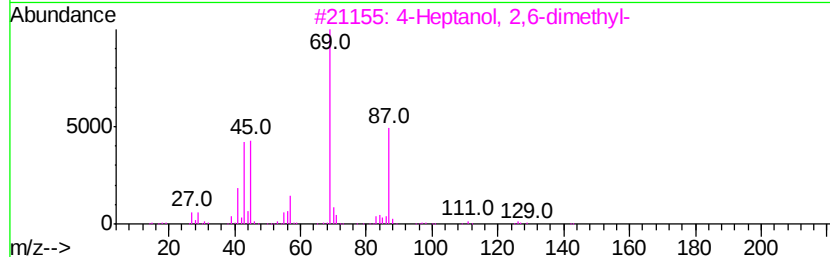
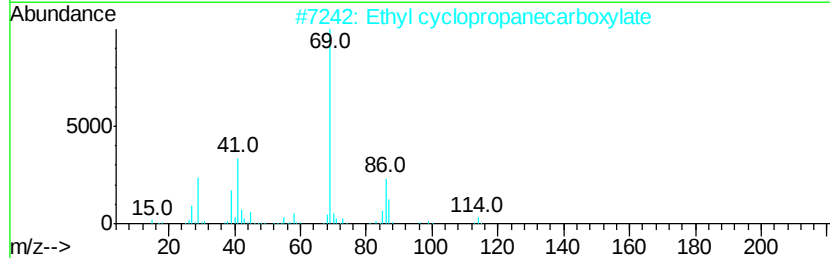
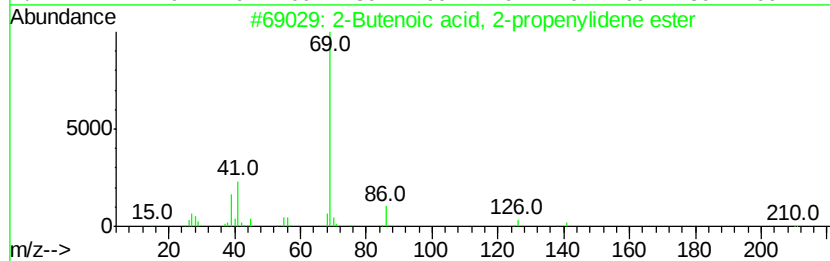
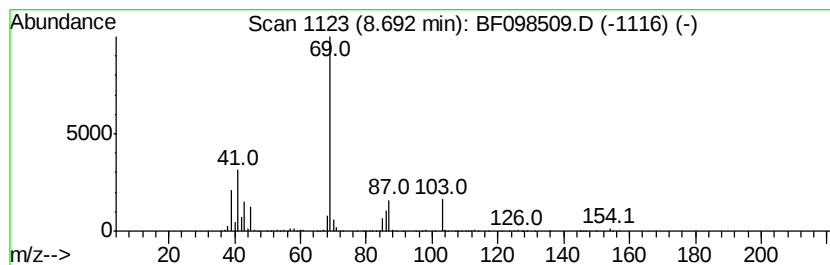
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 Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

 Peak Number 11 unknown8.69 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.69	12.97 ng	860929	Naphthalene-d8	7.94

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Butenoic acid, 2-propenylidene...	210	C11H14O4	055030-70-1	45
2		Ethyl cyclopropanecarboxylate	114	C6H10O2	004606-07-9	39
3		4-Heptanol, 2,6-dimethyl-	144	C9H20O	000108-82-7	9
4		meso-5,6-Decanediol	174	C10H22O2	003266-25-9	9
5		Cyclopropanecarboxylic acid, buty...	142	C8H14O2	054947-39-6	9



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
Data File : BF098509.D
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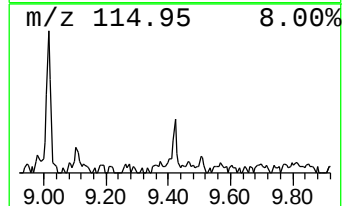
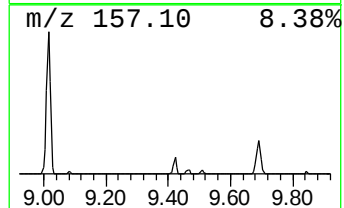
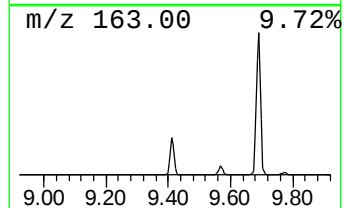
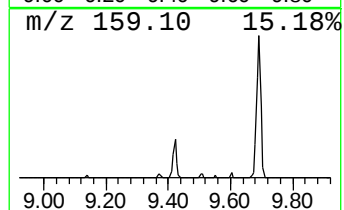
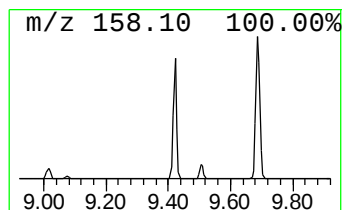
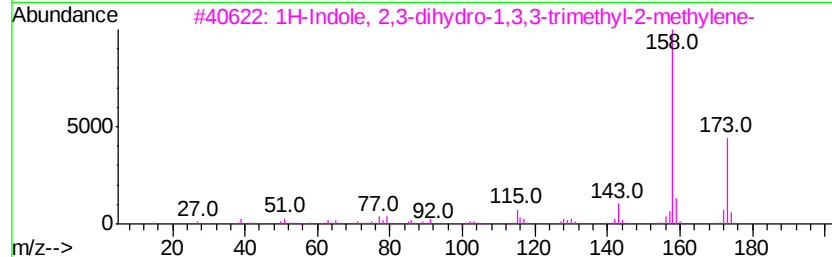
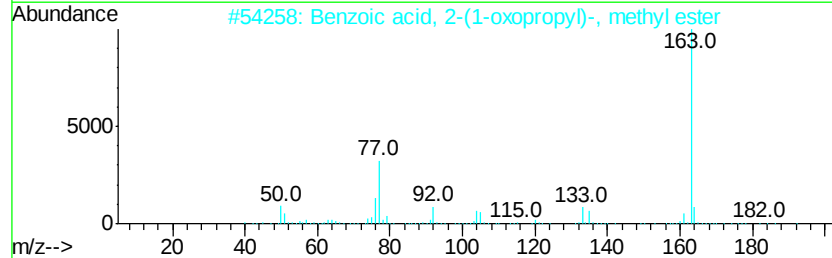
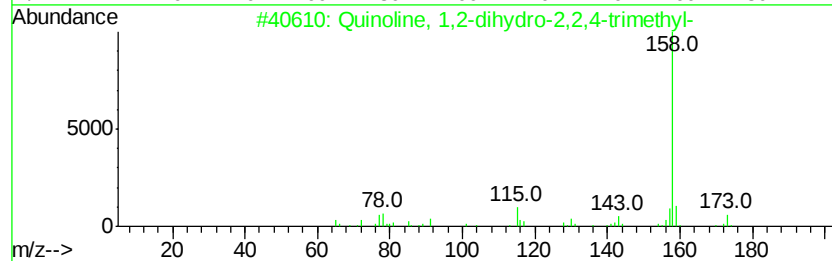
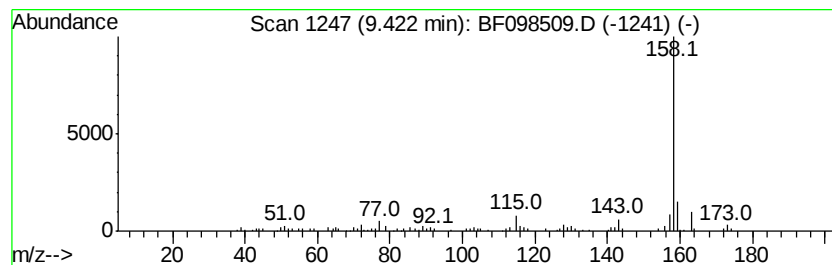
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 12 unknown9.42 Concentration Rank 13

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.42	2.31 ng	136485	Acenaphthene-d10	9.69

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Quinoline, 1,2-dihydro-2,2,4-tri...	173	C12H15N	000147-47-7	46
2		Benzoic acid, 2-(1-oxopropyl)-, ...	192	C11H12O3	032025-37-9	43
3		1H-Indole, 2,3-dihydro-1,3,3-tri...	173	C12H15N	000118-12-7	38
4		Methyl propyl phthalate	222	C12H14O4	1000373-89-2	35
5		Dimethyl phthalate	194	C10H10O4	000131-11-3	35



Data Path : \\74.0.250.170\SVOASRV\HPCHEM1\BNA F\DATA\BF091317\
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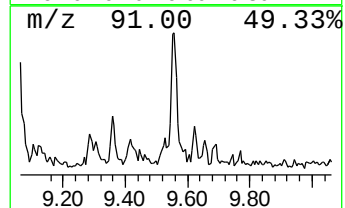
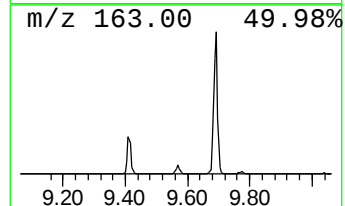
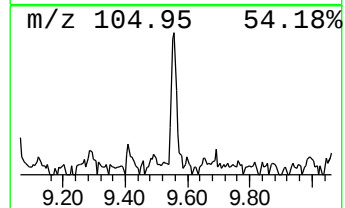
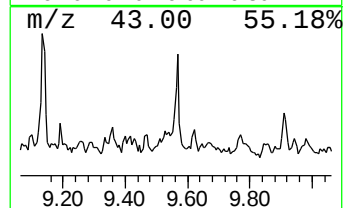
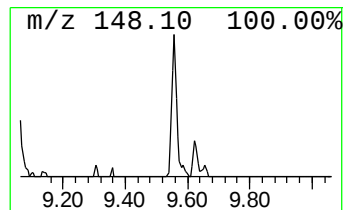
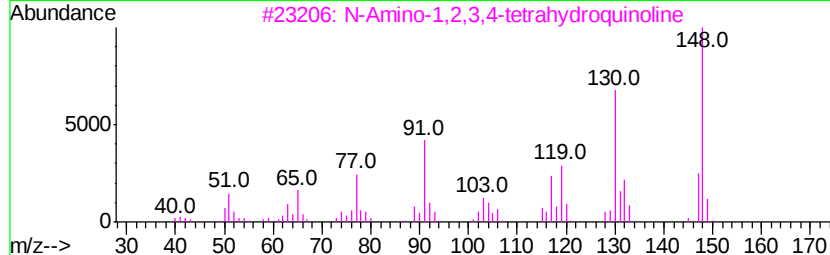
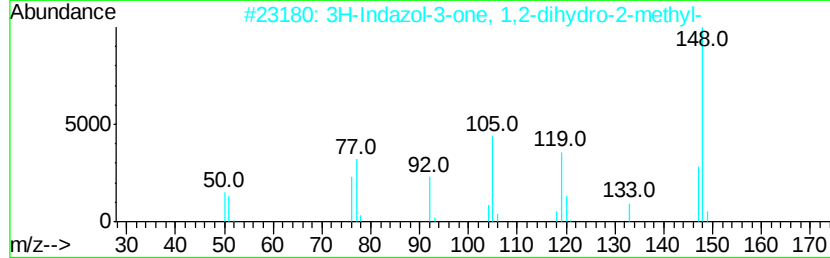
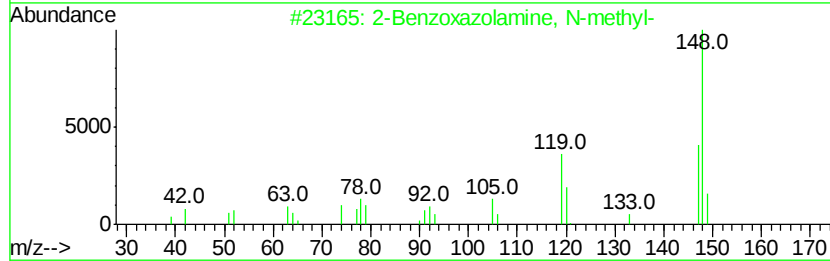
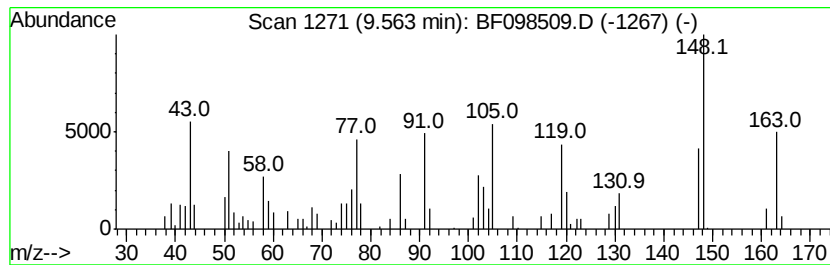
Instrument :
BNA_F
ClientSampleId :
A5972-OT

Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF091117.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 13 2-Benzoxazamine, N-methyl- Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.56	2.58 ng	152417	Acenaphthene-d10	9.69
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	2-Benzoxazamine, N-methyl-	148 C8H8N2O	019776-98-8	55
2	3H-Indazol-3-one, 1,2-dihydro-2-...	148 C8H8N2O	001848-40-4	49
3	N-Amino-1,2,3,4-tetrahydroquinoline	148 C9H12N2	1000305-92-6	47
4	Methanimidamide, N,N-dimethyl-N'...	148 C9H12N2	001783-25-1	47
5	trans-Cinnamic acid	148 C9H8O2	000140-10-3	46



Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF091317\
 Data File : BF098509.D
 Acq On : 14 Sep 2017 00:29
 Operator : SJ/JU
 Sample : I5202-01
 Misc :
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 A5972-OT

Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF091117.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...	4.83	3.0	ng	190219	1	6.66	1248880	20.0
unknown6.43	6.43	46.8	ng	2922240	1	6.66	1248880	20.0
Propanenitrile, 2...	6.76	153.4	ng	9576510	1	6.66	1248880	20.0
unknown7.41	7.41	2.6	ng	171544	2	7.94	1327390	20.0
Ethanone, 1-(3-me...	7.82	2.4	ng	161758	2	7.94	1327390	20.0
Mequinol	8.06	28.8	ng	1907850	2	7.94	1327390	20.0
N-(1-Cyano-1-meth...	8.09	36.3	ng	2406580	2	7.94	1327390	20.0
Benzothiazole	8.22	5.6	ng	373307	2	7.94	1327390	20.0
1H-Inden-1-one, 2...	8.53	15.5	ng	1029070	2	7.94	1327390	20.0
unknown8.69	8.69	13.0	ng	860929	2	7.94	1327390	20.0
unknown9.42	9.42	2.3	ng	136485	3	9.69	1180900	20.0
2-Benzoxazoline...	9.56	2.6	ng	152417	3	9.69	1180900	20.0