

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111017\
 Data File : BF100426.D
 Acq On : 11 Nov 2017 7:30
 Operator : SJ/JU
 Sample : I6355-16
 Misc :
 ALS Vial : 44 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110317-SIDI-E-D-S

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-BF110817.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	2.204	16	20	37	rVB	73293	131834	3.05%	0.485%
2	5.122	512	516	525	rVB	236003	246281	5.70%	0.906%
3	5.516	578	583	586	rBV	1644149	1441458	33.35%	5.301%
4	6.516	749	753	756	rBV	1255383	1007807	23.32%	3.706%
5	6.545	756	758	763	rVB	58017	48285	1.12%	0.178%
6	6.669	774	779	782	rBV	2767440	2468505	57.11%	9.078%
7	6.898	815	818	822	rVB	1153315	1005534	23.26%	3.698%
8	7.057	841	845	849	rVB	3268104	3144201	72.74%	11.562%
9	7.463	909	914	917	rBV	2407405	2687952	62.19%	9.885%
10	8.181	1032	1036	1040	rBV	1416996	1232192	28.51%	4.531%
11	8.733	1127	1130	1133	rBV	173168	131970	3.05%	0.485%
12	9.257	1214	1219	1223	rBV	4123266	4322326	100.00%	15.895%
13	9.939	1329	1335	1344	rVB	1353450	1245199	28.81%	4.579%
14	10.604	1445	1448	1451	rBV	87969	59314	1.37%	0.218%
15	10.651	1452	1456	1459	rBV	561301	506394	11.72%	1.862%
16	10.722	1464	1468	1472	rBV	1561086	1502201	34.75%	5.524%
17	11.421	1581	1587	1591	rBV	1232072	1033463	23.91%	3.800%
18	12.821	1822	1825	1828	rBV	76548	55160	1.28%	0.203%
19	13.010	1852	1857	1860	rBV	3411670	3310194	76.58%	12.173%
20	14.062	2032	2036	2042	rVB	959406	906570	20.97%	3.334%
21	15.545	2282	2288	2299	rVB	518100	706699	16.35%	2.599%

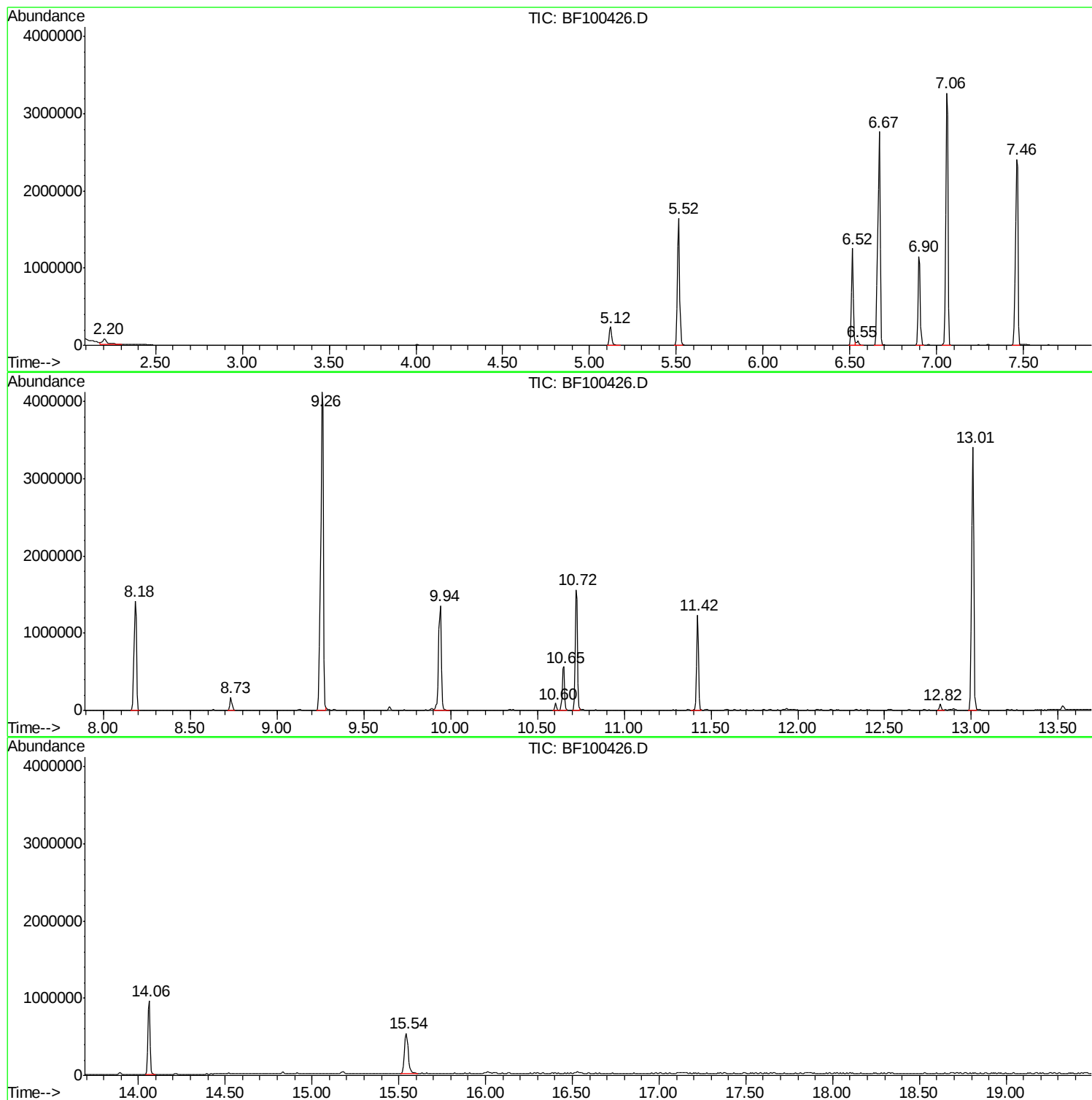
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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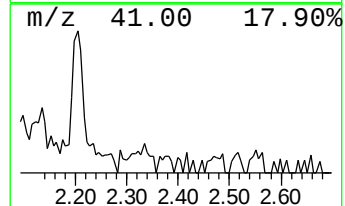
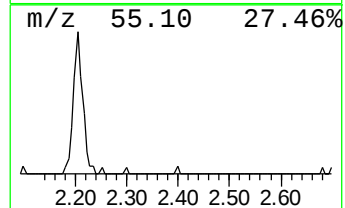
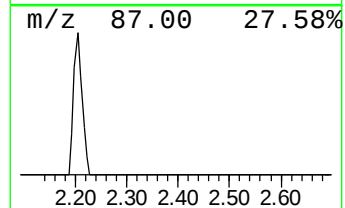
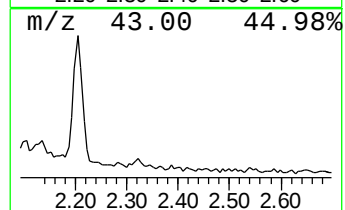
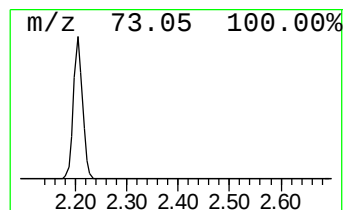
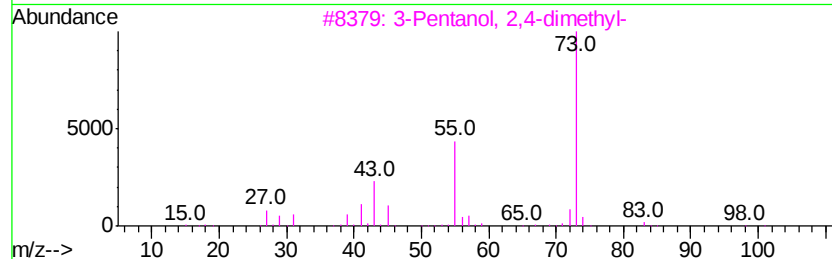
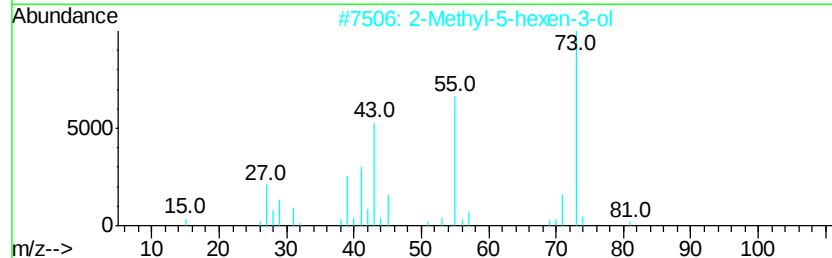
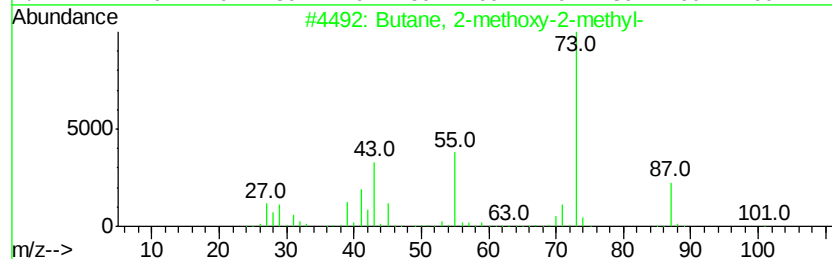
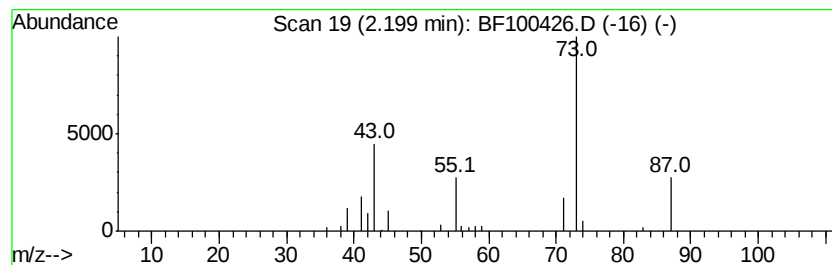
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.20	2.62 ng	131834	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	42
3		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	23
4		Boronic acid, ethyl-, dimethyl e...	102	C4H11BO2	007318-82-3	12
5		N-Ethylformamide	73	C3H7NO	000627-45-2	9



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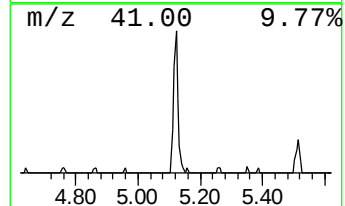
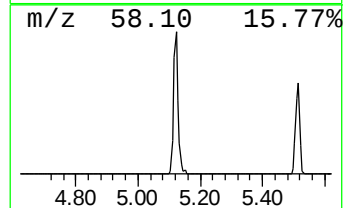
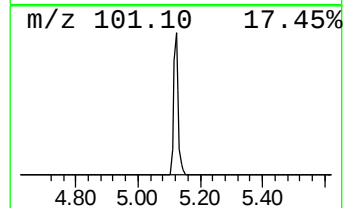
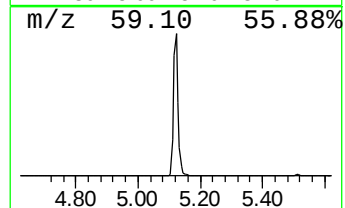
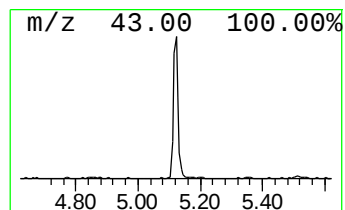
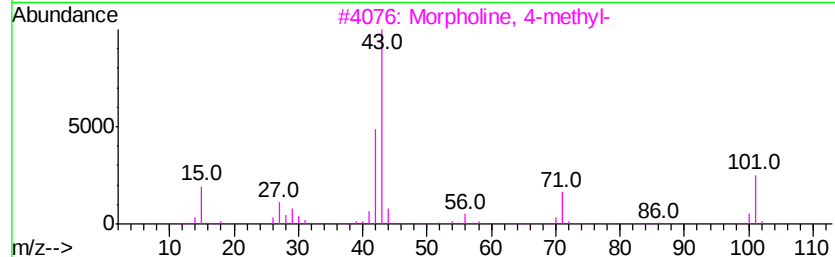
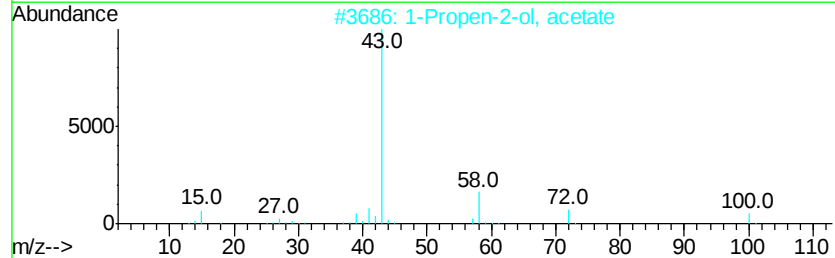
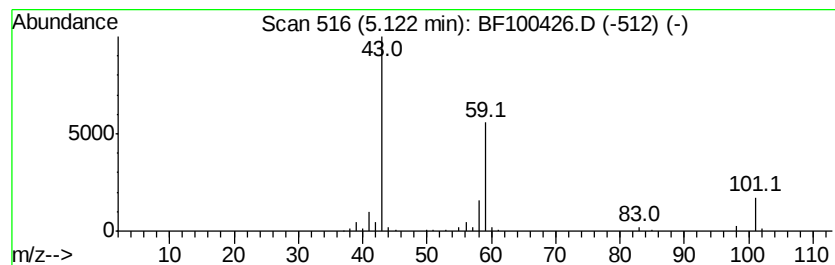
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.12	4.90 ng	246281	1,4-Dichlorobenzene-d4	6.90

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
3			Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9



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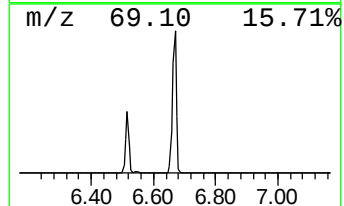
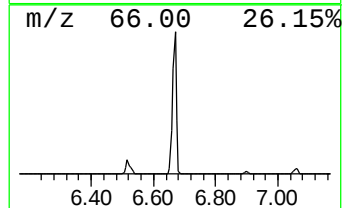
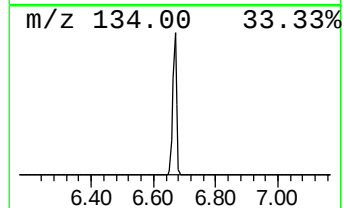
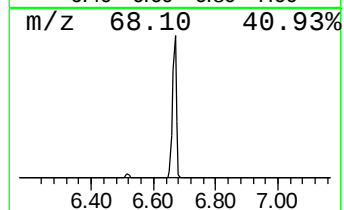
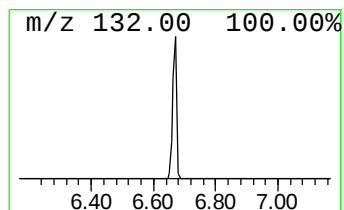
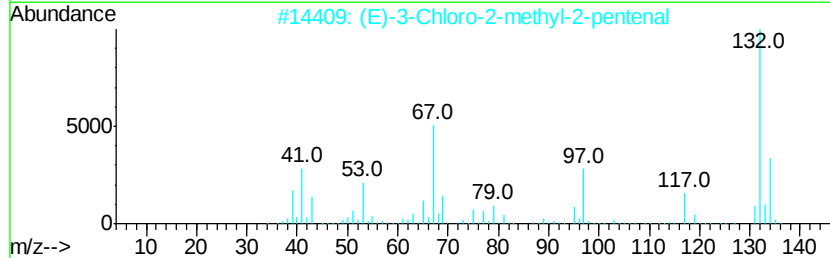
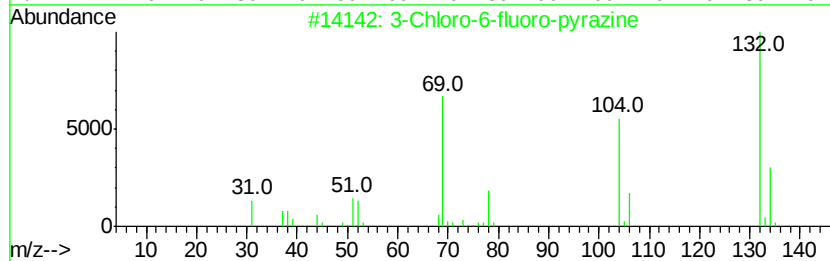
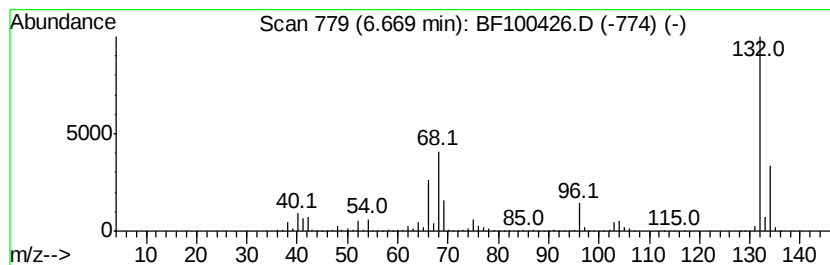
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Peak Number 3 unknown6.67 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.67	49.10 ng	2468510	1,4-Dichlorobenzene-d4	6.90

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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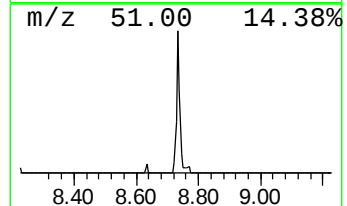
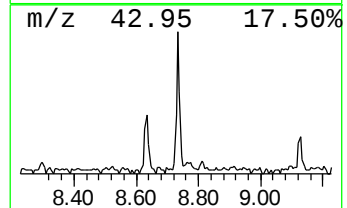
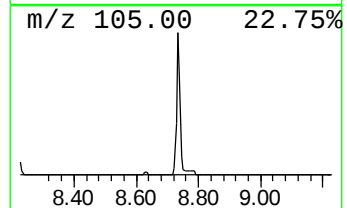
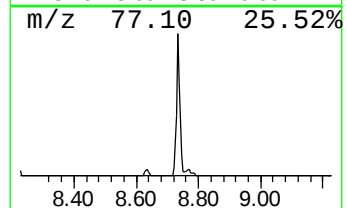
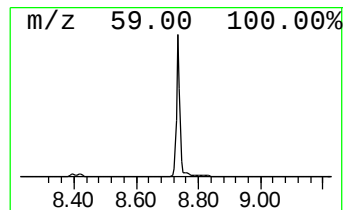
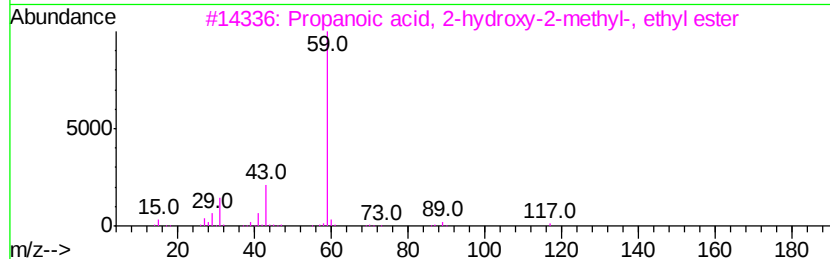
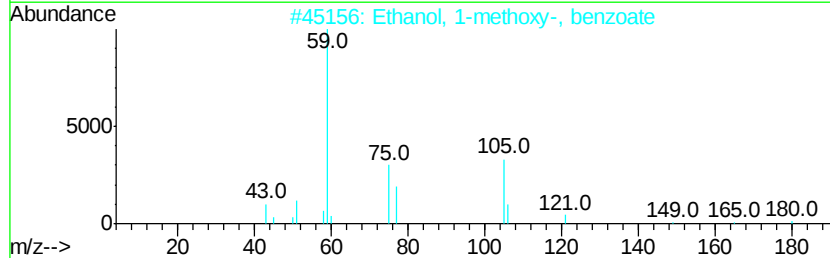
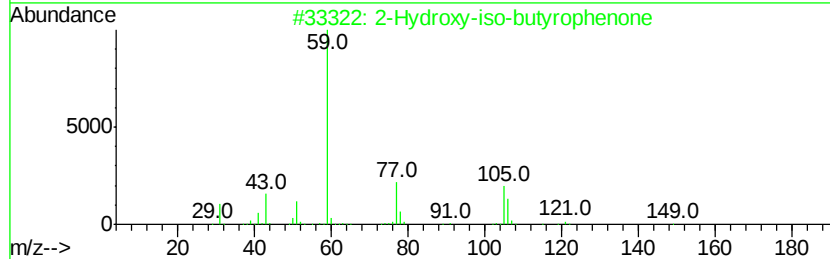
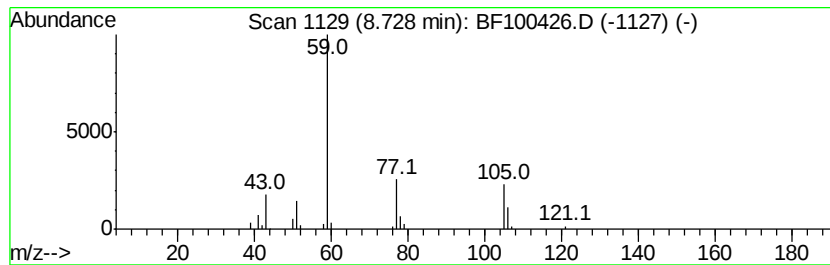
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Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.73	2.14 ng	131970	Napthalene-d8	8.18

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	90
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	72
3		Propanoic acid, 2-hydroxy-2-methoxy-, ethyl ester	132	C6H12O3	000080-55-7	9
4		Guanidine	59	CH5N3	000113-00-8	7
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5



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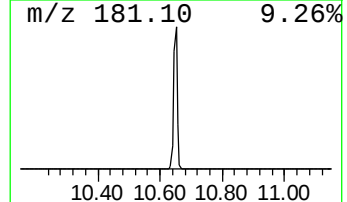
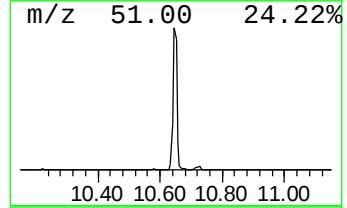
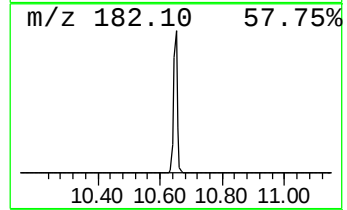
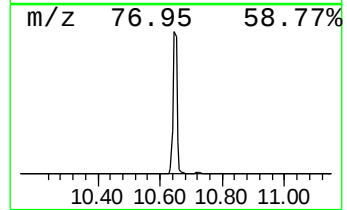
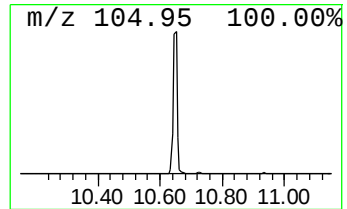
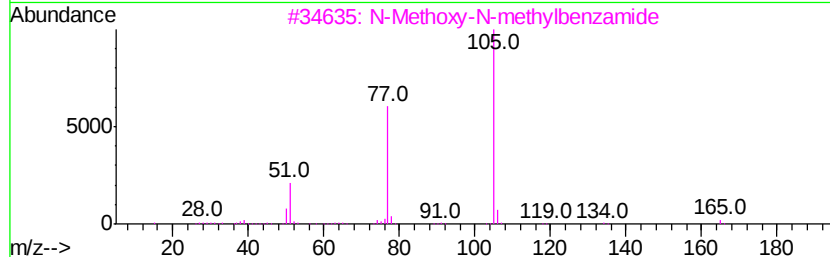
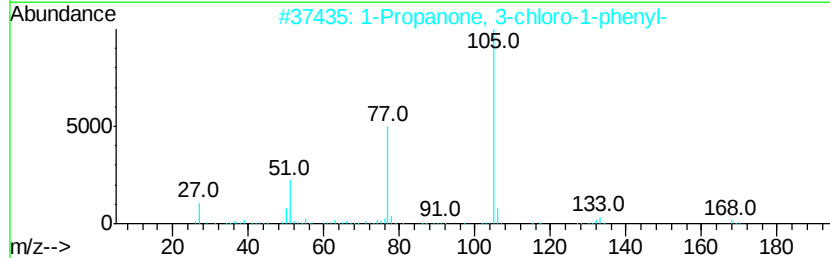
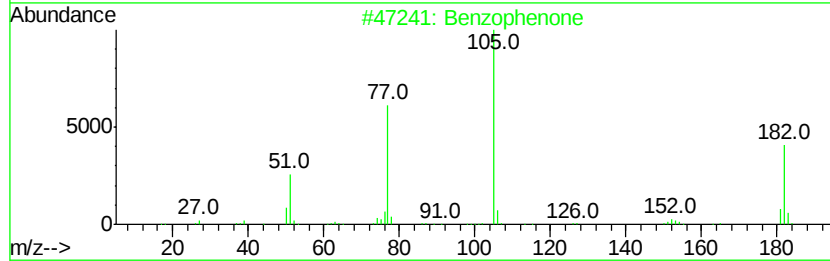
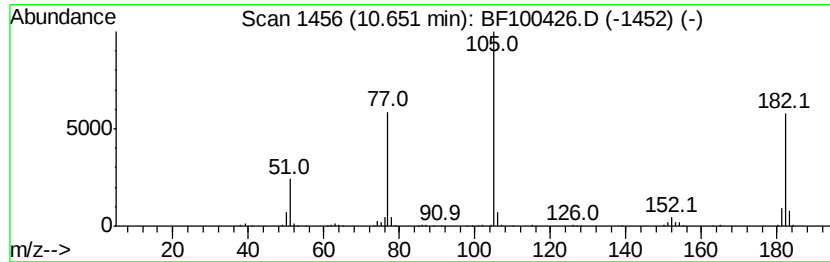
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Peak Number 6 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.65	8.13 ng	506394	Acenaphthene-d10	9.94
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		1-Propanone, 3-chloro-1-phenyl-	168 C9H9ClO	000936-59-4 47
3		N-Methoxy-N-methylbenzamide	165 C9H11NO2	006919-61-5 47
4		1-Propanone, 2-bromo-1-phenyl-	212 C9H9BrO	002114-00-3 47
5		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.20	2.6	ng	131834	1	6.90	1005530	20.0
2-Pentanone, 4-hy...	5.12	4.9	ng	246281	1	6.90	1005530	20.0
unknown6.67	6.67	49.1	ng	2468510	1	6.90	1005530	20.0
2-Hydroxy-iso-but...	8.73	2.1	ng	131970	2	8.18	1232190	20.0
Benzophenone	10.65	8.1	ng	506394	3	9.94	1245200	20.0