

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100607.D
 Acq On : 16 Nov 2017 00:46
 Operator : SJ/JU
 Sample : I6426-05
 Misc :
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110917-SIDI-E-D-B

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	2.181	13	16	33	rVB2	49061	110248	3.18%	0.537%
2	5.098	509	512	520	rBV	252443	258423	7.45%	1.260%
3	5.498	575	580	583	rBV	1184406	1104527	31.85%	5.384%
4	6.498	746	750	757	rBV	860815	710017	20.47%	3.461%
5	6.651	771	776	779	rBV	1980585	1889599	54.49%	9.210%
6	6.881	811	815	819	rBB	881261	694682	20.03%	3.386%
7	7.039	837	842	845	rBV	2714631	2529635	72.94%	12.330%
8	7.445	905	911	914	rBV	1969327	2087725	60.20%	10.176%
9	8.163	1029	1033	1036	rBV	1087616	882652	25.45%	4.302%
10	8.716	1123	1127	1130	rBV	111155	89591	2.58%	0.437%
11	9.239	1210	1216	1219	rBV	3629303	3467960	100.00%	16.903%
12	9.916	1325	1331	1335	rBV	1010729	900458	25.97%	4.389%
13	10.627	1448	1452	1455	rBV	218131	169487	4.89%	0.826%
14	10.704	1461	1465	1468	rBV	1361332	1211703	34.94%	5.906%
15	11.404	1580	1584	1587	rBV	834987	720729	20.78%	3.513%
16	12.986	1848	1853	1856	rBV	2495462	2344178	67.60%	11.426%
17	13.868	2000	2003	2012	rBV	49324	59569	1.72%	0.290%
18	14.039	2028	2032	2035	rBV	738011	630426	18.18%	3.073%
19	15.509	2277	2282	2290	rBV	502323	655038	18.89%	3.193%

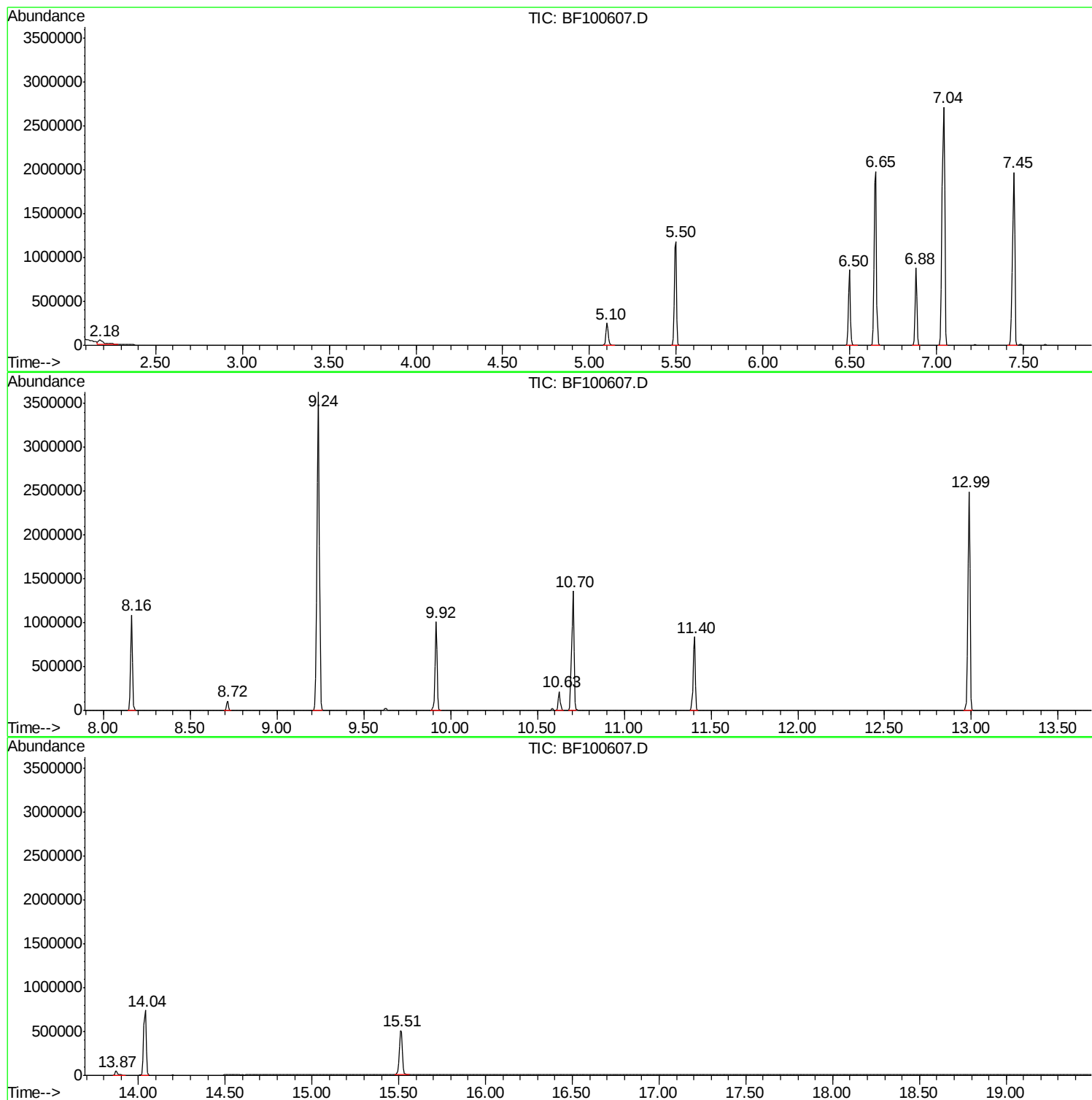
Sum of corrected areas: 20516647

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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



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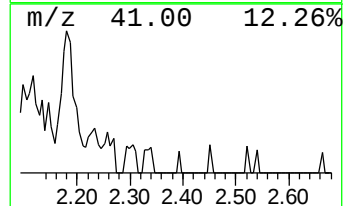
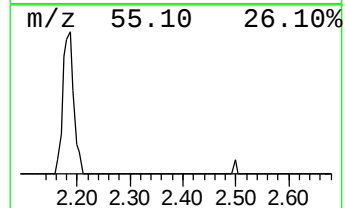
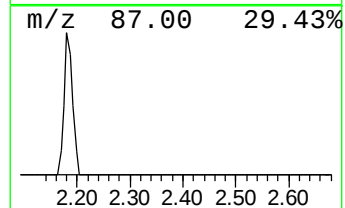
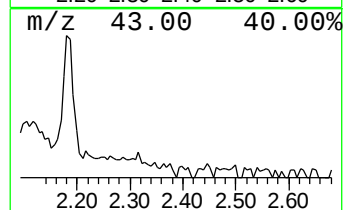
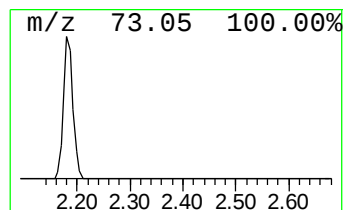
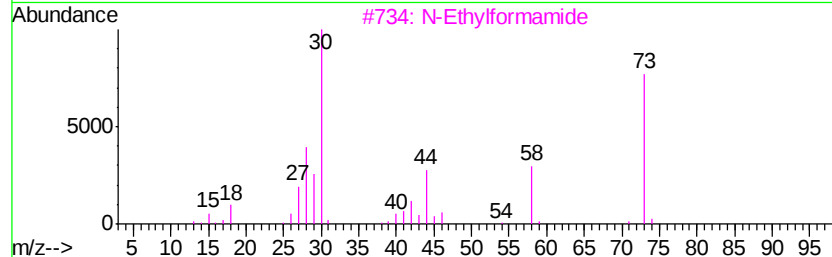
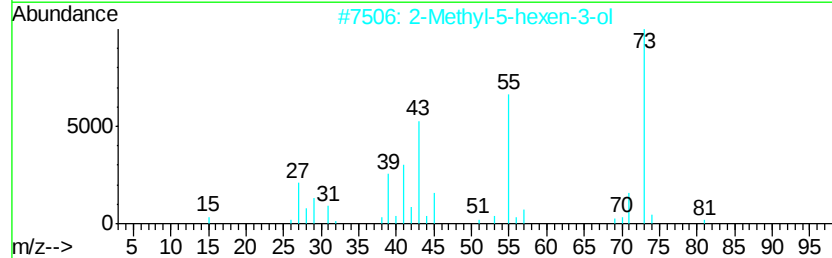
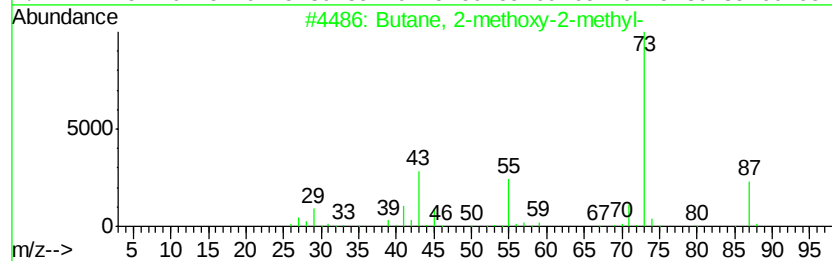
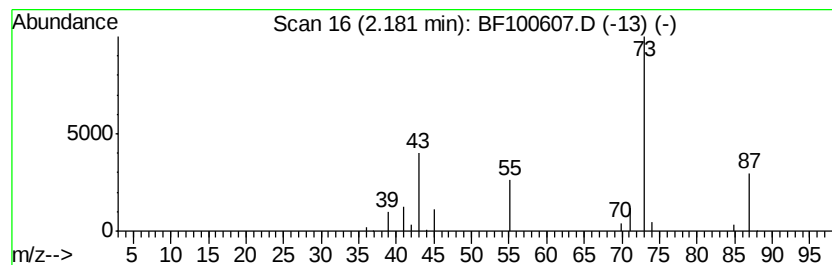
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.18	3.17 ng	110248	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	78
2		2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	38
3		N-Ethylformamide	73	C3H7NO	000627-45-2	5
4		Isobutylamine	73	C4H11N	000078-81-9	5
5		1,4-Butanediamine	88	C4H12N2	000110-60-1	5



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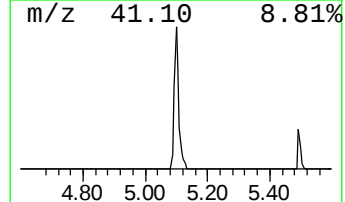
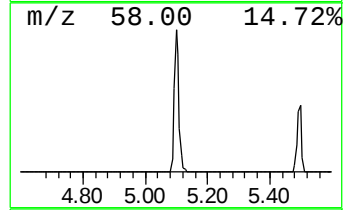
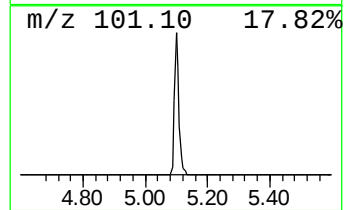
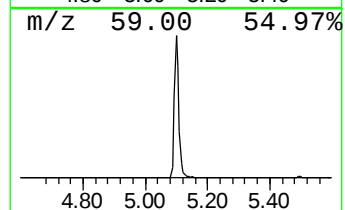
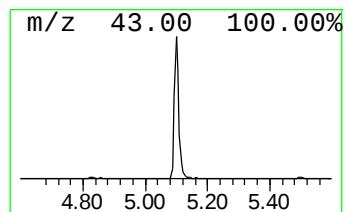
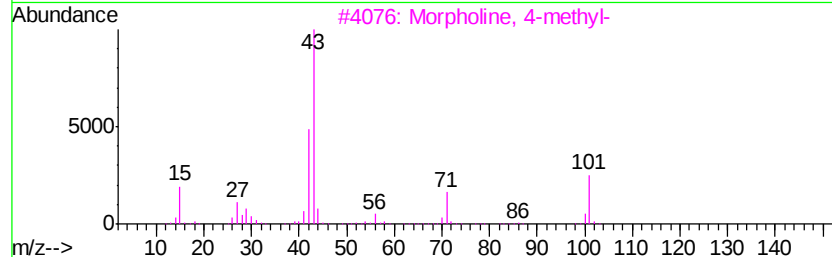
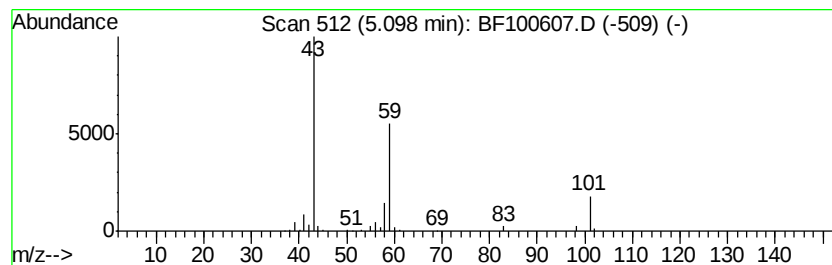
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	7.44 ng	258423	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	50
2		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
3		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9
4		Butane, 1-ethoxy-	102	C6H14O	000628-81-9	9
5		2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9



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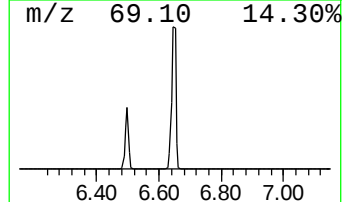
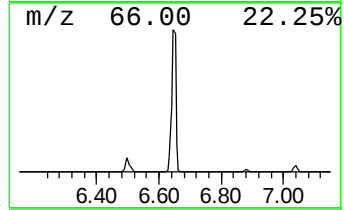
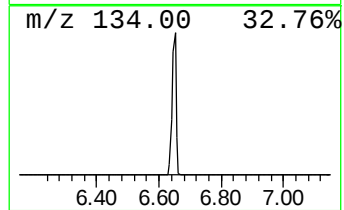
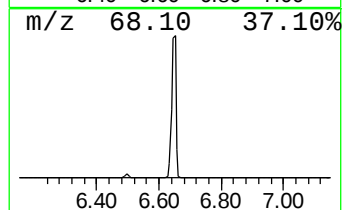
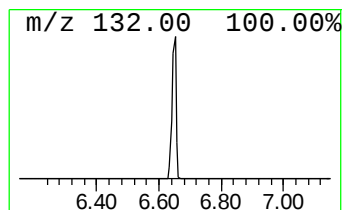
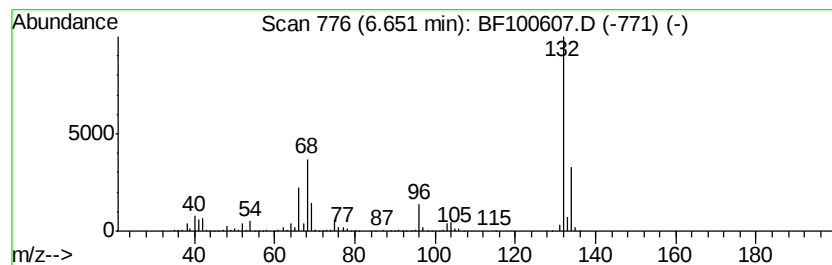
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	54.40 ng	1889600	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	35
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	17
3		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
4		5-Aminoindole	132	C8H8N2	005192-03-0	12
5		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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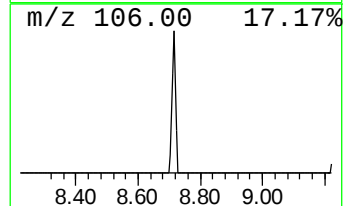
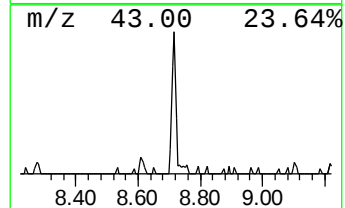
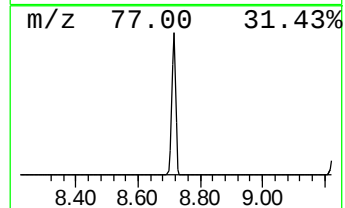
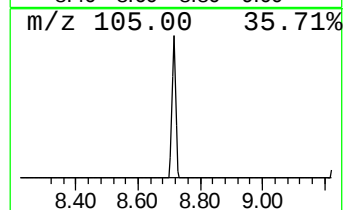
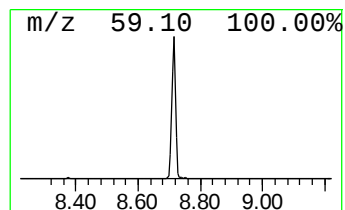
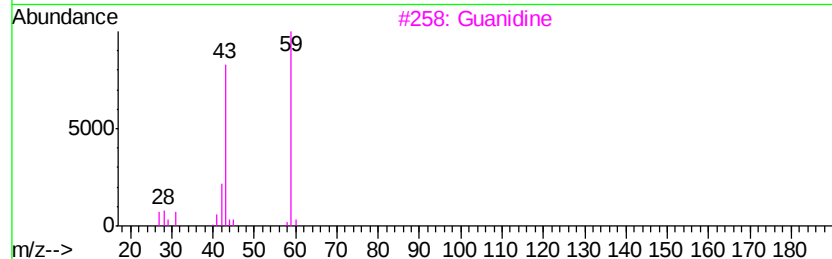
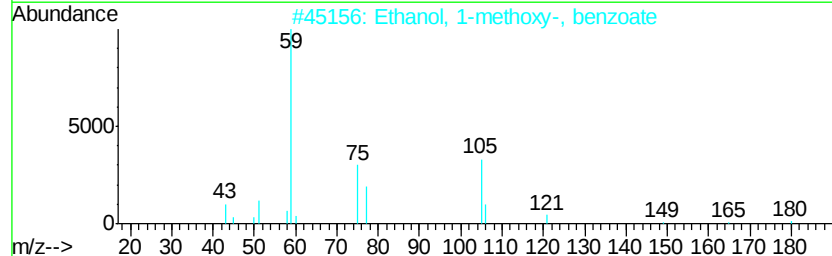
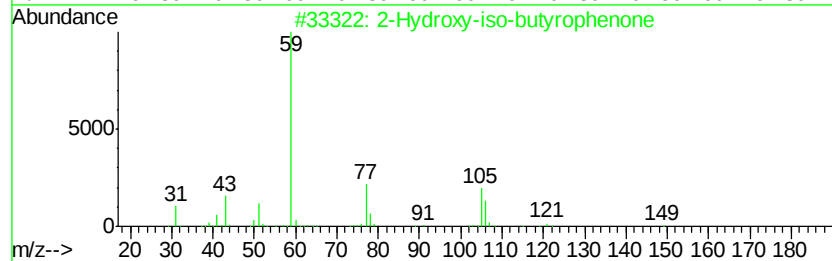
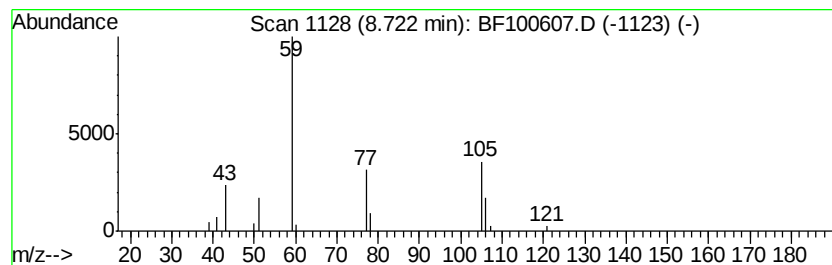
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Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.03 ng	89591	Napthalene-d8	8.16

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		Guanidine	59	CH5N3	000113-00-8	7
4		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
5		Acetamide	59	C2H5NO	000060-35-5	5



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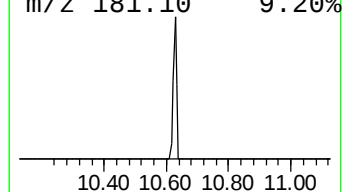
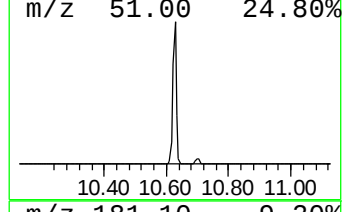
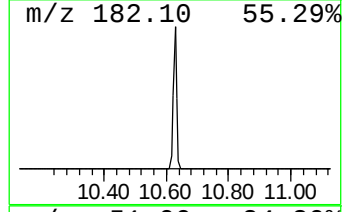
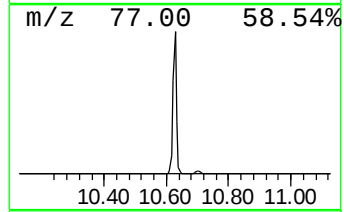
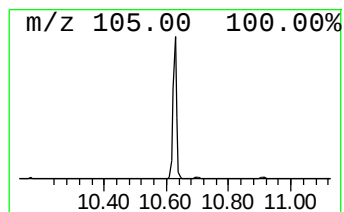
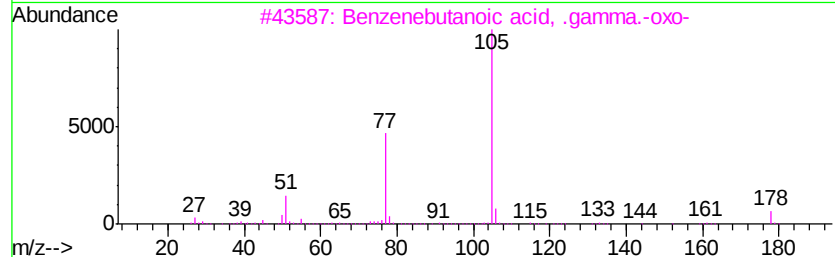
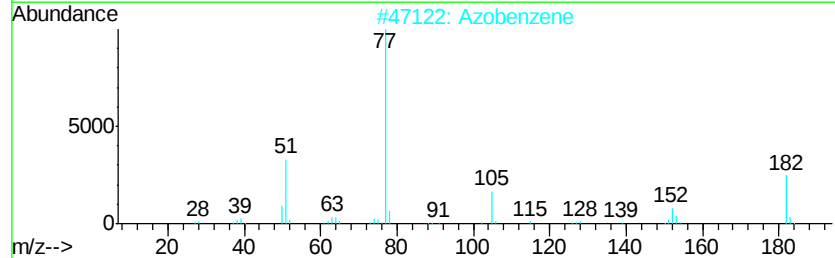
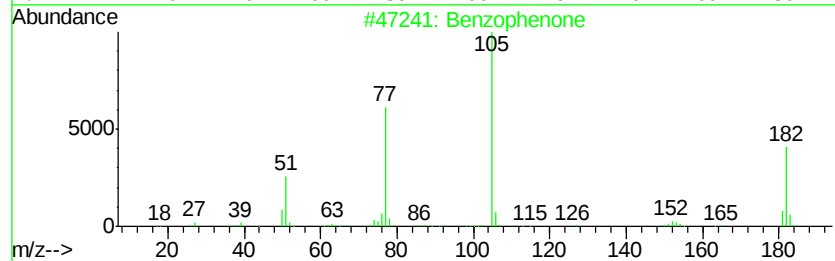
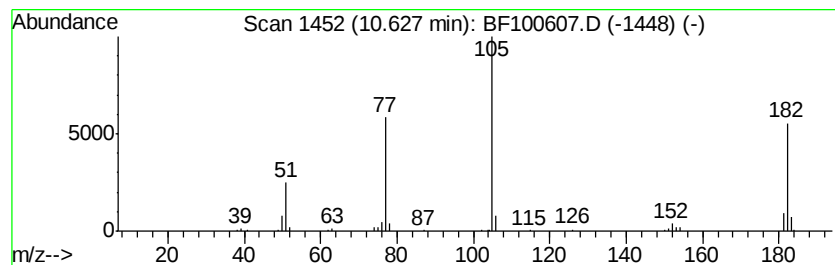
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Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	3.76 ng	169487	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		Azobenzene	182 C12H10N2	000103-33-3 59
3		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
4		Acetophenone, 2-chloro-	154 C8H7ClO	000532-27-4 47
5		Benzopinacol	366 C26H22O2	000464-72-2 47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.18	3.2	ng	110248	1	6.88	694682	20.0
2-Pentanone, 4-hy...	5.10	7.4	ng	258423	1	6.88	694682	20.0
unknown6.65	6.65	54.4	ng	1889600	1	6.88	694682	20.0
2-Hydroxy-iso-but...	8.72	2.0	ng	89591	2	8.16	882652	20.0
Benzophenone	10.63	3.8	ng	169487	3	9.92	900458	20.0