

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100608.D
 Acq On : 16 Nov 2017 1:13
 Operator : SJ/JU
 Sample : I6426-06
 Misc :
 ALS Vial : 30 Sample Multiplier: 1

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

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-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	2.175	12	15	21	rVB2	42323	67966	2.02%	0.344%
2	5.098	508	512	521	rBV	274909	276442	8.23%	1.399%
3	5.492	575	579	583	rBV	1168675	1086556	32.34%	5.498%
4	6.498	746	750	754	rBV	891802	734226	21.85%	3.715%
5	6.645	771	775	779	rBV	1808644	1762830	52.46%	8.920%
6	6.881	811	815	819	rBB	835009	672898	20.03%	3.405%
7	7.039	837	842	845	rBV	2587654	2376473	70.73%	12.026%
8	7.445	905	911	914	rBV	1905593	1967435	58.55%	9.956%
9	8.163	1029	1033	1036	rBV	1050993	857127	25.51%	4.337%
10	8.716	1123	1127	1130	rBV	159369	121412	3.61%	0.614%
11	9.239	1210	1216	1219	rBV	3551593	3360063	100.00%	17.003%
12	9.627	1279	1282	1286	rBV	50703	41379	1.23%	0.209%
13	9.916	1325	1331	1335	rBV2	1004833	888656	26.45%	4.497%
14	10.627	1448	1452	1455	rBV	361967	277299	8.25%	1.403%
15	10.704	1461	1465	1468	rBV	1312729	1131082	33.66%	5.724%
16	11.404	1580	1584	1587	rVB	851283	729424	21.71%	3.691%
17	12.986	1849	1853	1856	rBV	2424269	2232222	66.43%	11.296%
18	14.039	2028	2032	2035	rBV	605345	553514	16.47%	2.801%
19	15.509	2277	2282	2292	rVB	484933	624580	18.59%	3.161%

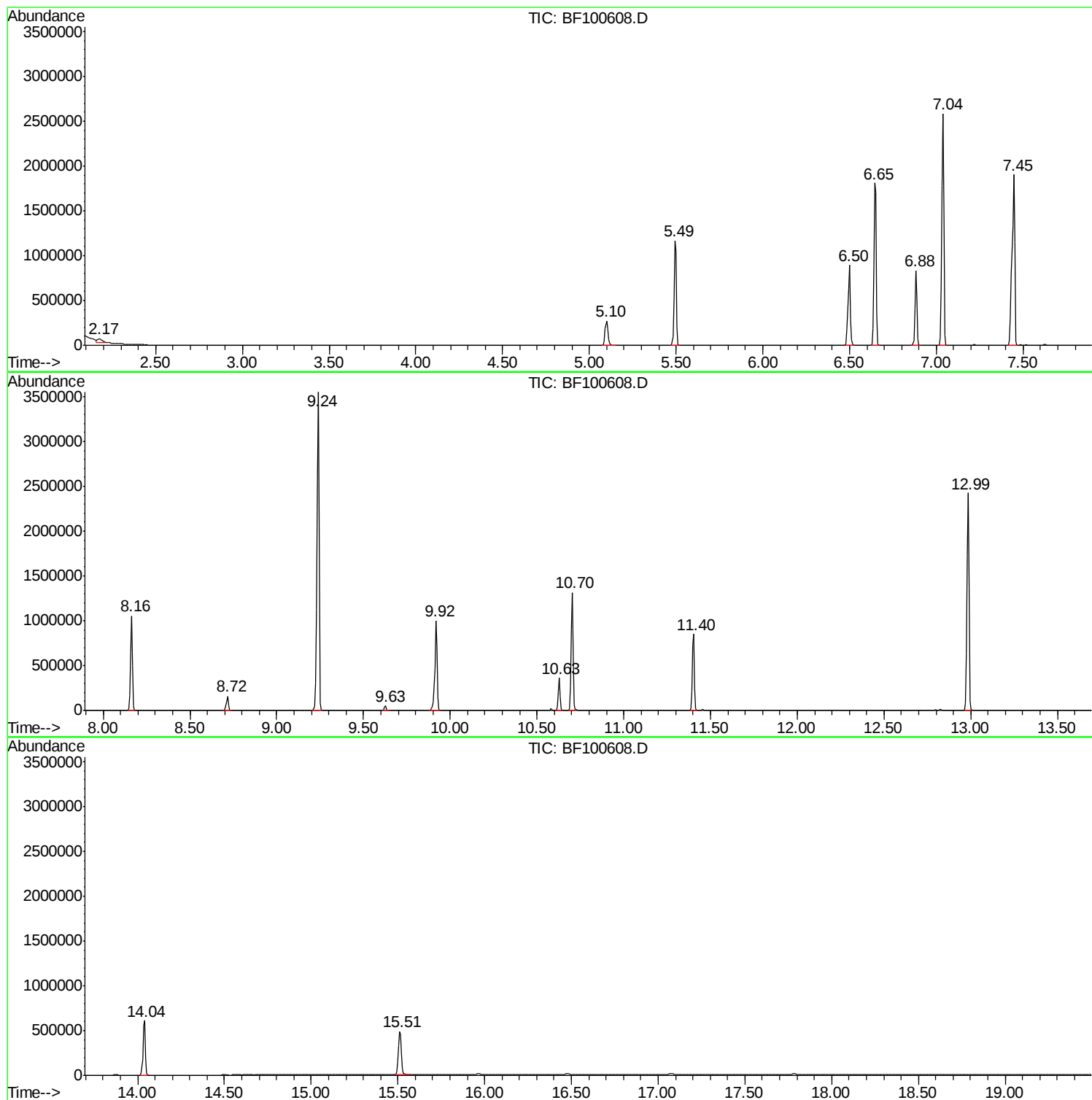
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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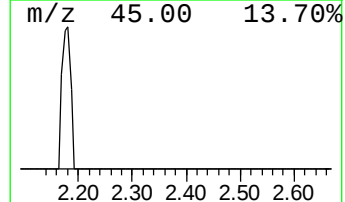
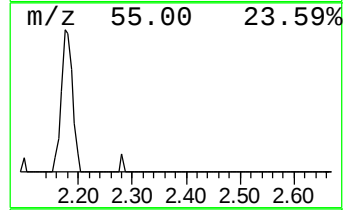
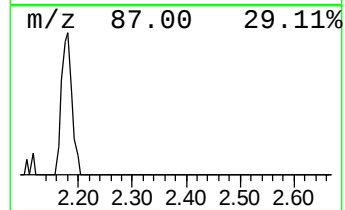
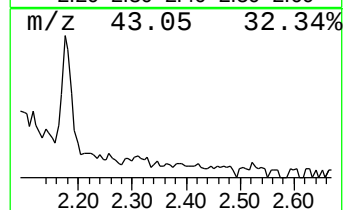
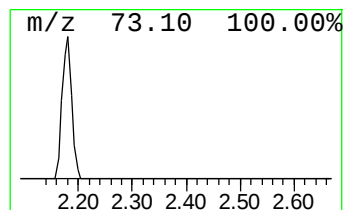
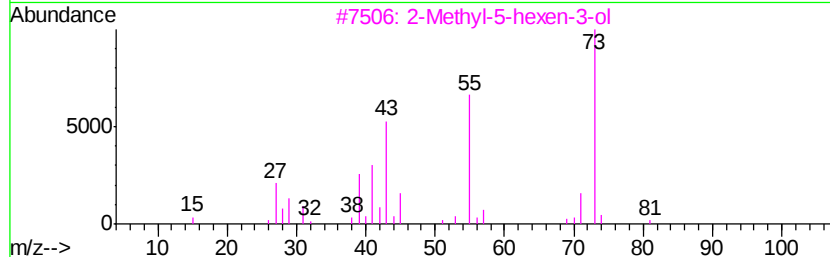
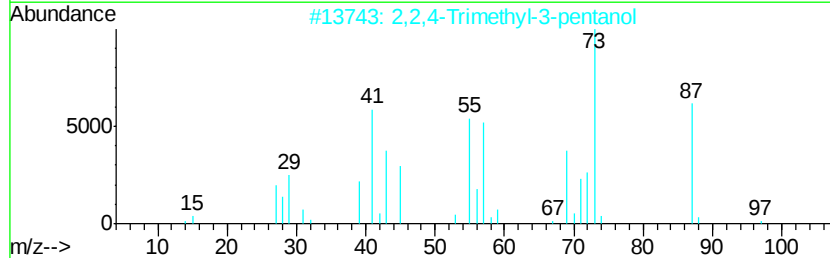
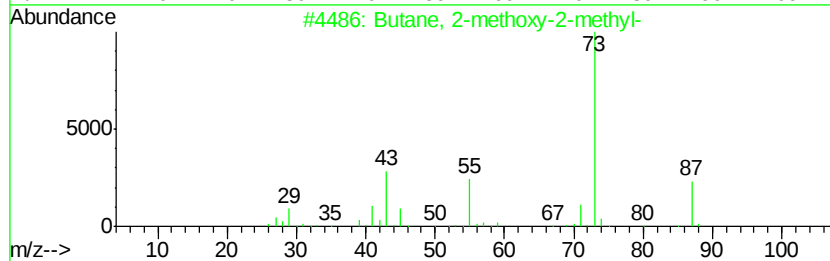
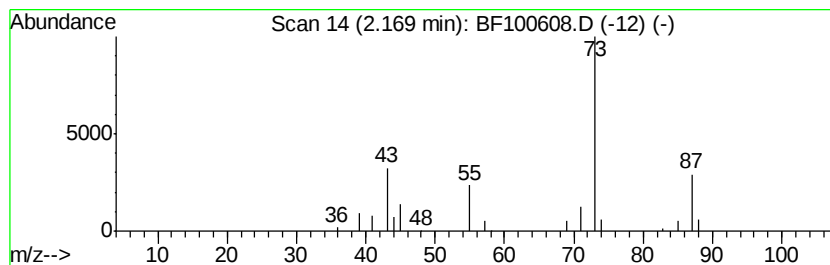
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 Butane, 2-methoxy-2-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.17	2.02 ng	67966	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butane, 2-methoxy-2-methyl-	102	C6H14O	000994-05-8	72
2			2,2,4-Trimethyl-3-pentanol	130	C8H18O	005162-48-1	36
3			2-Methyl-5-hexen-3-ol	114	C7H14O	032815-70-6	28
4			1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
5			Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9



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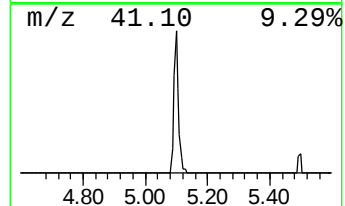
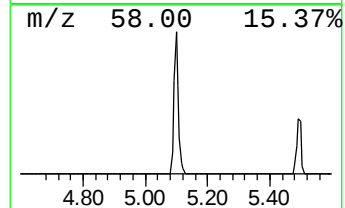
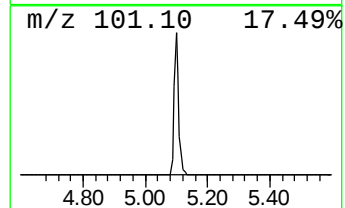
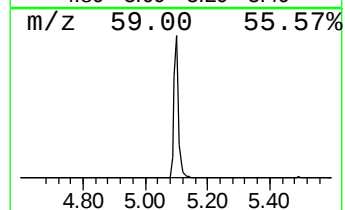
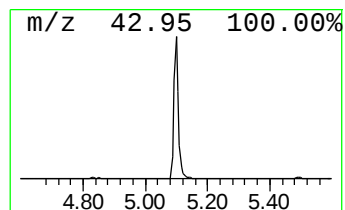
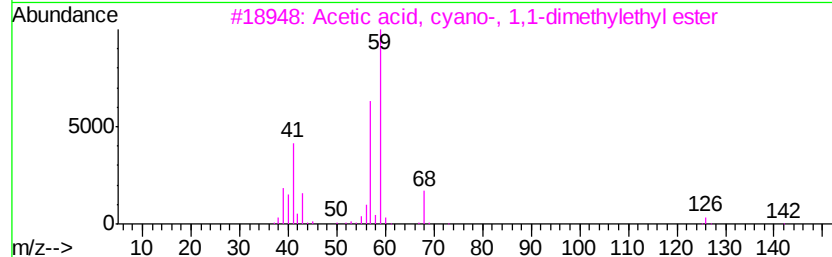
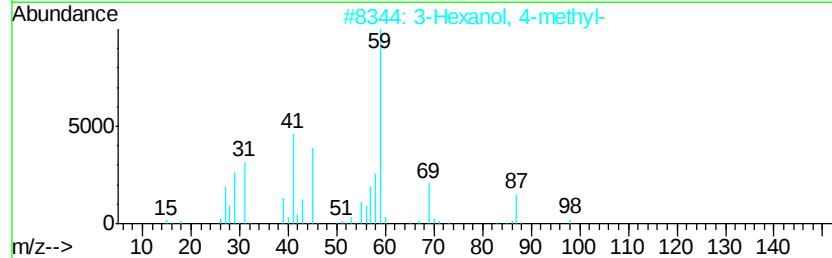
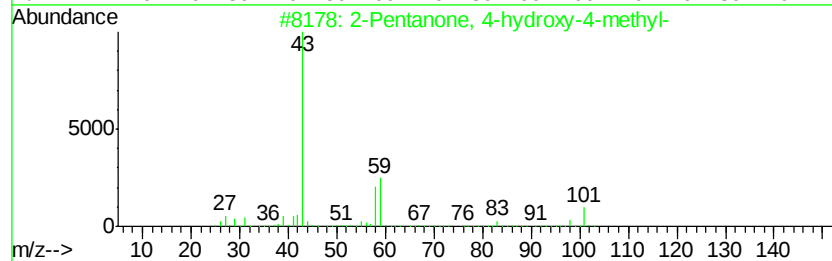
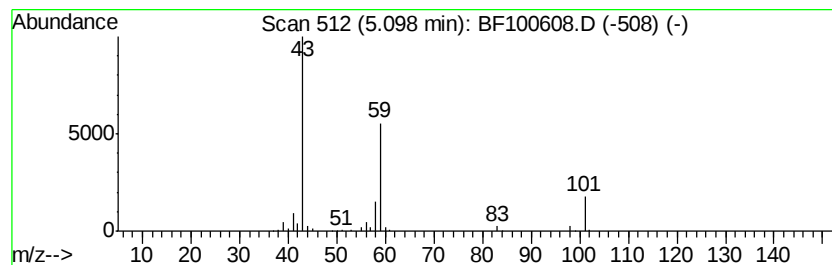
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	8.22 ng	276442	1,4-Dichlorobenzene-d4	6.88

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
3			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
4			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
5			Ethanol, pentamethyl-	116	C7H16O	000594-83-2	9



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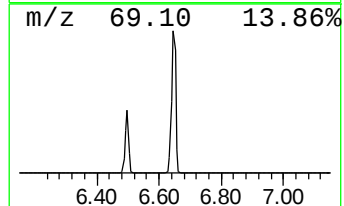
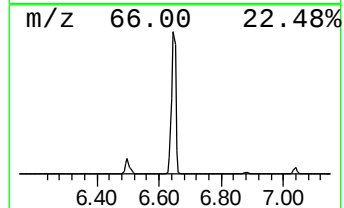
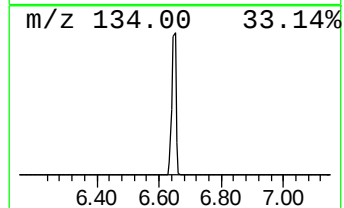
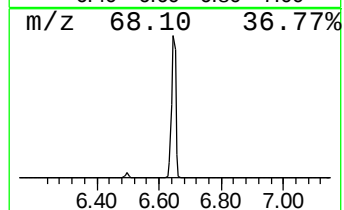
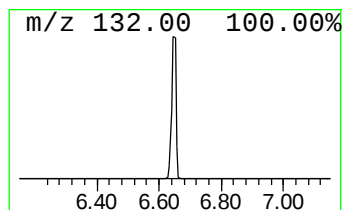
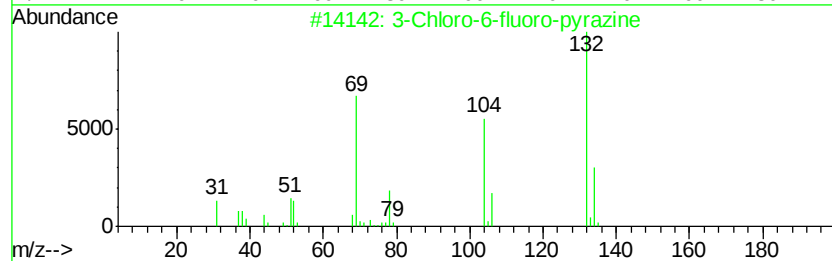
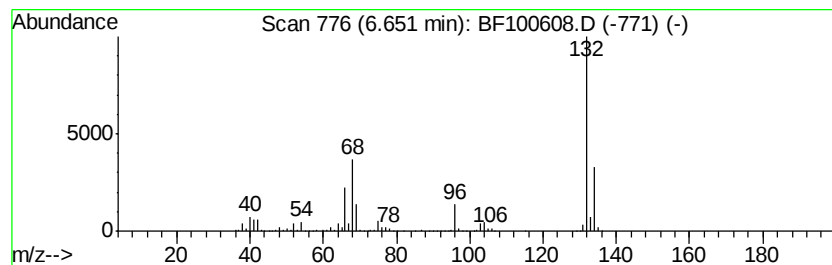
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Peak Number 3 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	52.40 ng	1762830	1,4-Dichlorobenzene-d4	6.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	27	
2	5-Aminoindole	132	C8H8N2	005192-03-0	12	
3	Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10	
4	(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9	
5	1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9	



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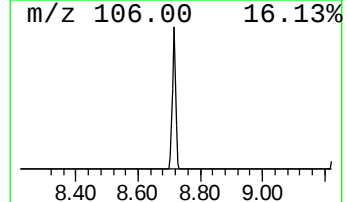
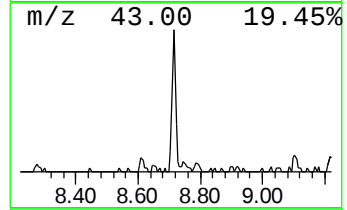
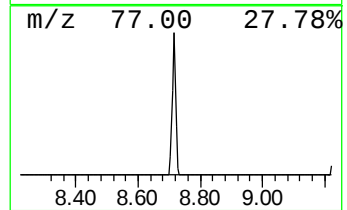
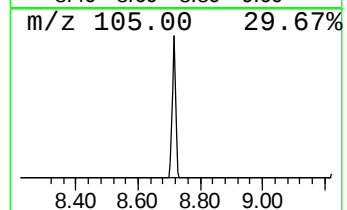
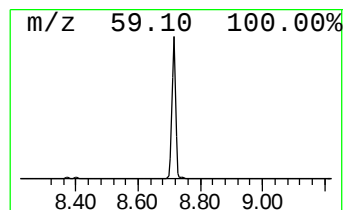
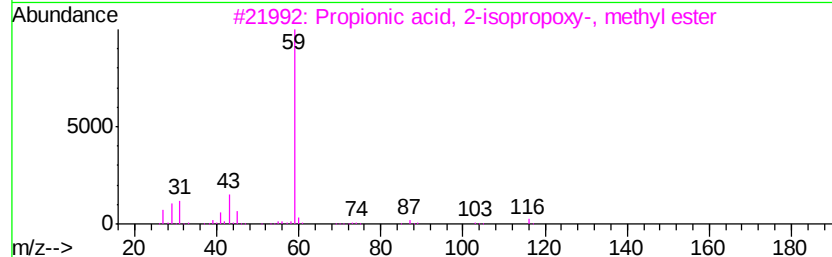
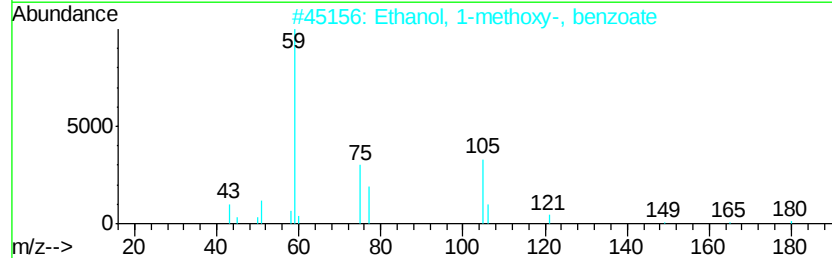
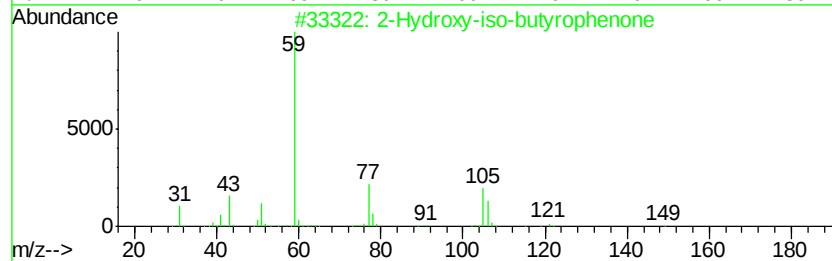
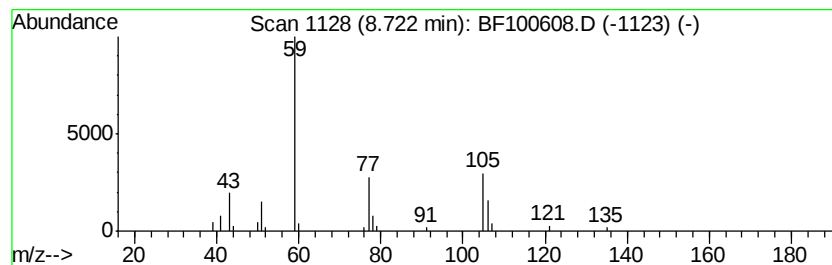
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Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.83 ng	121412	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	64
3		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
4		Ethane, 1,1-dimethoxy-	90	C4H10O2	000534-15-6	9
5		Propanoic acid, 2-nitro-, methyl...	133	C4H7NO4	006118-50-9	9



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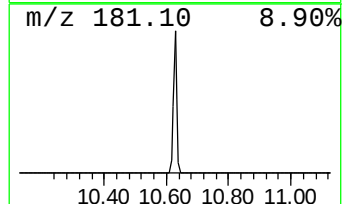
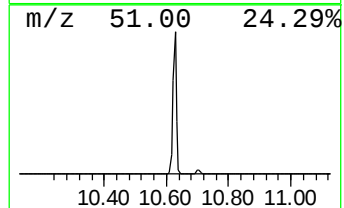
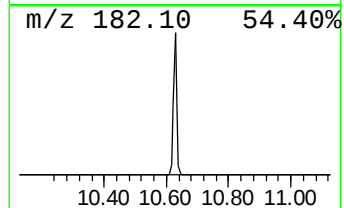
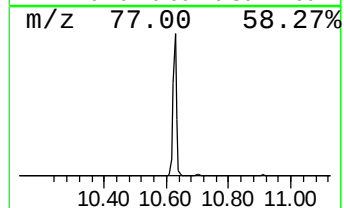
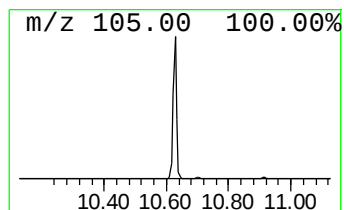
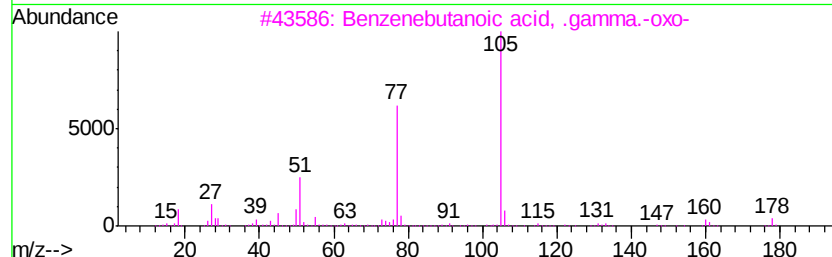
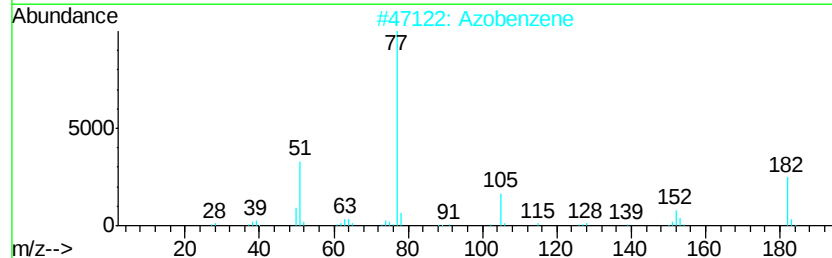
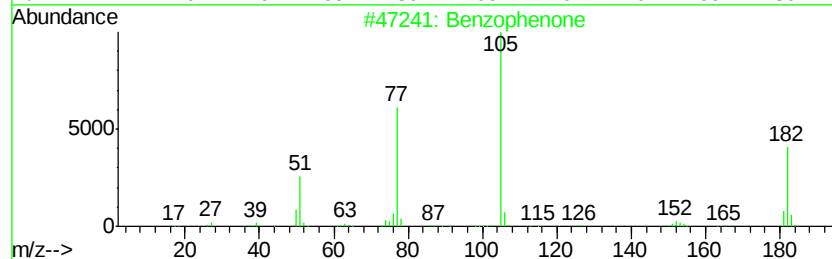
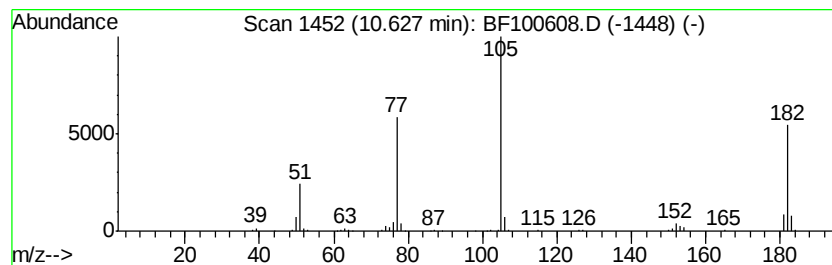
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Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	6.24 ng	277299	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		Benzilamide	227 C14H13N02	004746-87-6 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...	2.17	2.0	ng	67966	1	6.88	672898	20.0
2-Pentanone, 4-hy...	5.10	8.2	ng	276442	1	6.88	672898	20.0
unknown6.65	6.65	52.4	ng	1762830	1	6.88	672898	20.0
2-Hydroxy-iso-but...	8.72	2.8	ng	121412	2	8.16	857127	20.0
Benzophenone	10.63	6.2	ng	277299	3	9.92	888656	20.0