

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100609.D
 Acq On : 16 Nov 2017 1:39
 Operator : SJ/JU
 Sample : I6426-07
 Misc :
 ALS Vial : 31 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110917-SIDI-E-U-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	2.187	14	17	27	rVB2	39759	70680	2.06%	0.354%
2	5.098	509	512	524	rVB	207311	227260	6.62%	1.138%
3	5.498	575	580	583	rBV	1262095	1104924	32.20%	5.533%
4	6.498	746	750	757	rVB	872308	732869	21.36%	3.670%
5	6.651	771	776	779	rBV	1942727	1831114	53.37%	9.170%
6	6.881	811	815	819	rVB	818348	656876	19.14%	3.290%
7	7.039	837	842	845	rBV	2662207	2418126	70.48%	12.110%
8	7.445	905	911	914	rBV	1982243	1993068	58.09%	9.981%
9	8.163	1029	1033	1036	rBV	1010605	843903	24.60%	4.226%
10	8.716	1123	1127	1130	rBV	108695	85111	2.48%	0.426%
11	9.239	1210	1216	1219	rBV	3576549	3431182	100.00%	17.183%
12	9.627	1279	1282	1285	rVB	67295	52457	1.53%	0.263%
13	9.916	1325	1331	1335	rBV2	993510	883371	25.75%	4.424%
14	10.627	1448	1452	1455	rBV	239374	181909	5.30%	0.911%
15	10.704	1461	1465	1468	rBV	1371269	1196894	34.88%	5.994%
16	11.404	1580	1584	1587	rBV	783527	707750	20.63%	3.544%
17	12.986	1848	1853	1856	rBV	2420504	2297976	66.97%	11.508%
18	13.868	2000	2003	2010	rBV	34995	43365	1.26%	0.217%
19	14.039	2028	2032	2035	rVB	619840	573642	16.72%	2.873%
20	15.509	2277	2282	2291	rBV	520482	635442	18.52%	3.182%

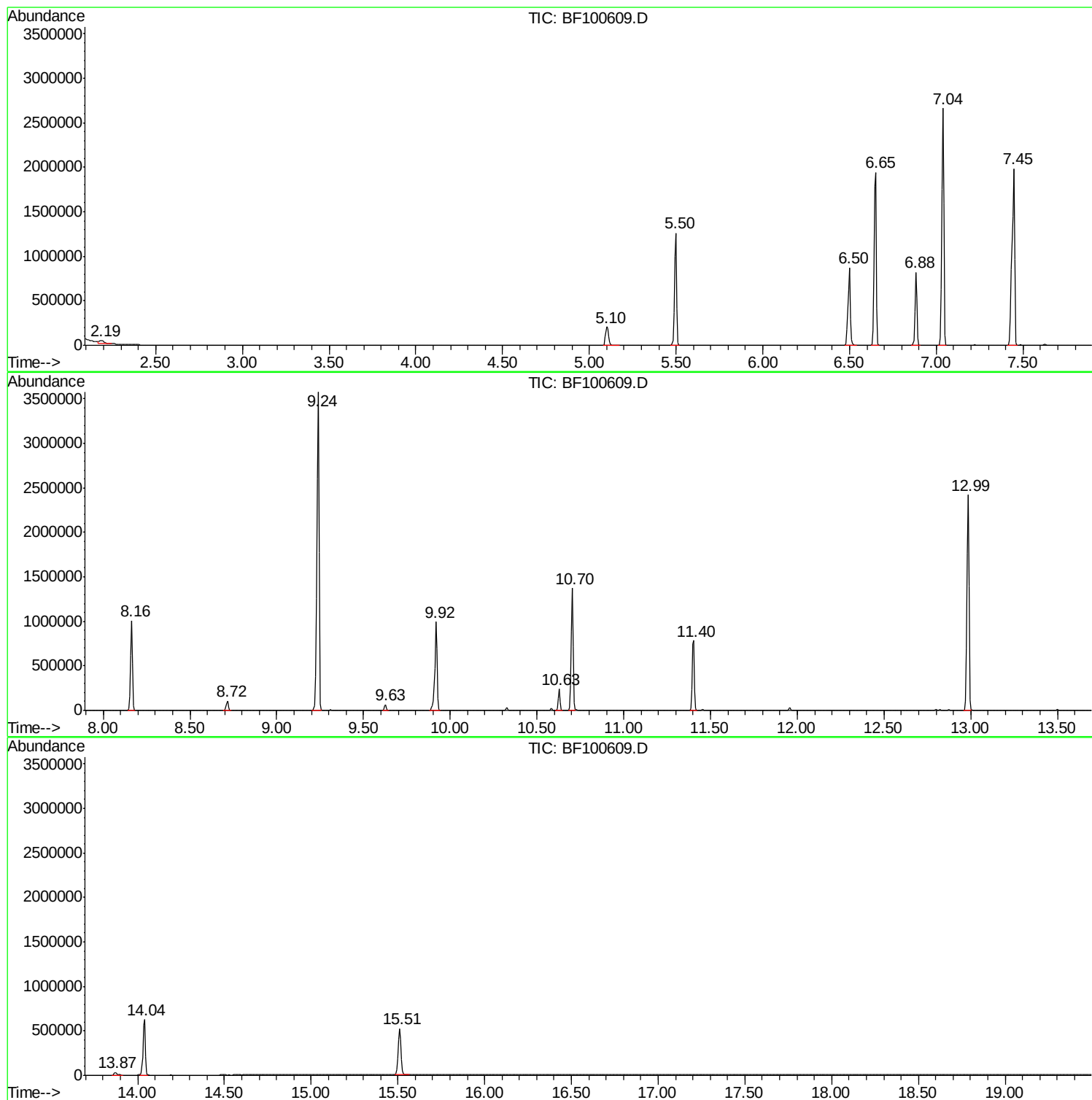
Sum of corrected areas: 19967919

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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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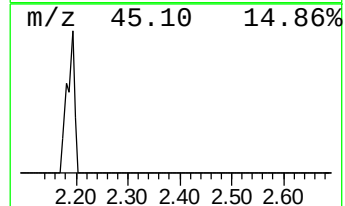
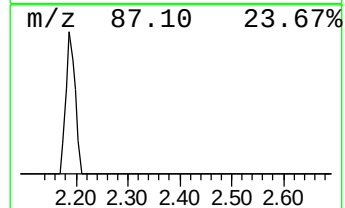
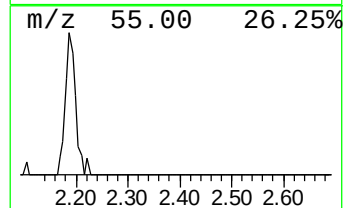
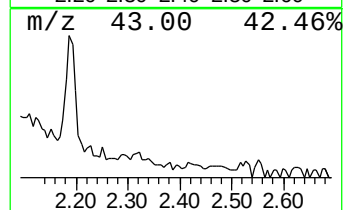
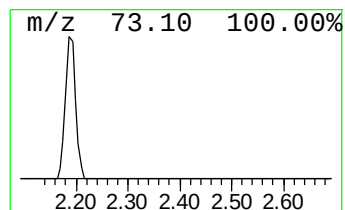
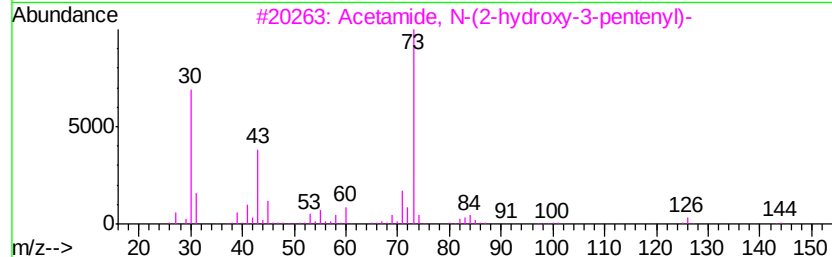
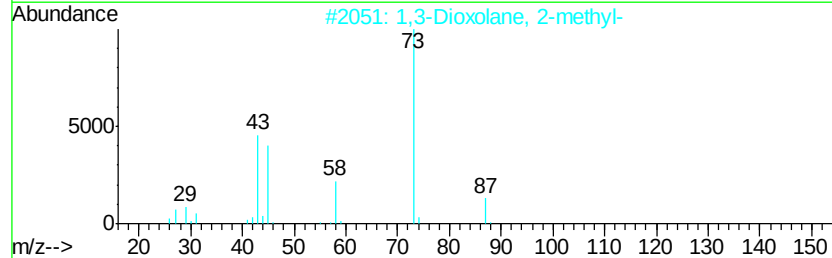
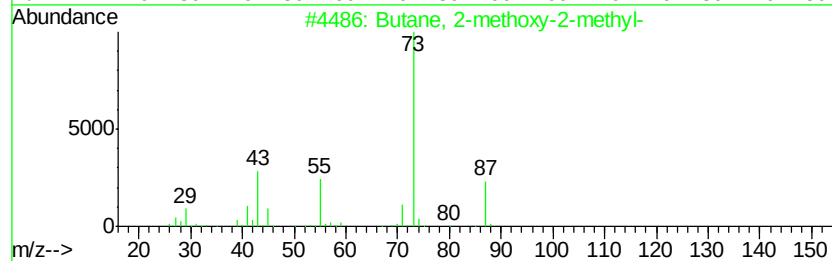
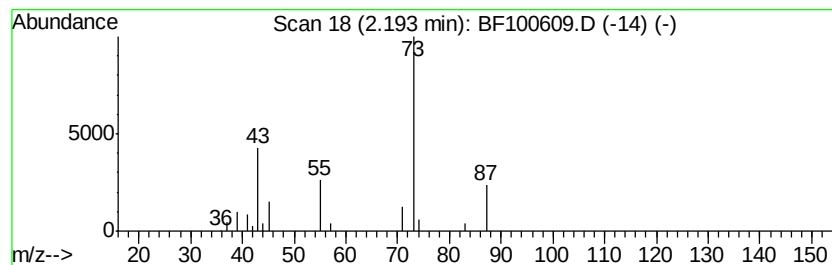
Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.19	2.15 ng	70680	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	72
2		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	9
3		Acetamide, N-(2-hydroxy-3-penten...	143	C7H13NO2	093393-95-4	9
4		3-Pentanol, 2,4-dimethyl-	116	C7H16O	000600-36-2	9
5		Propane, 2-methoxy-2-methyl-	88	C5H12O	001634-04-4	9



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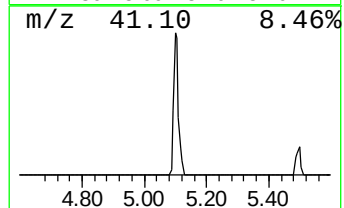
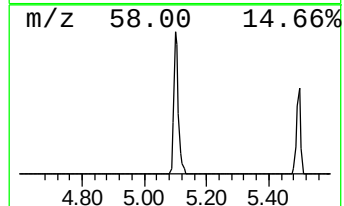
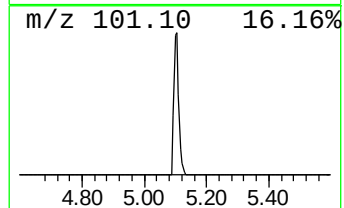
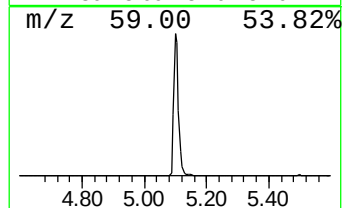
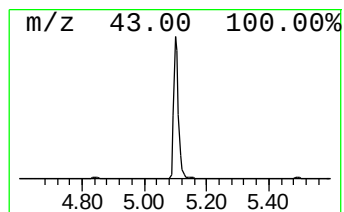
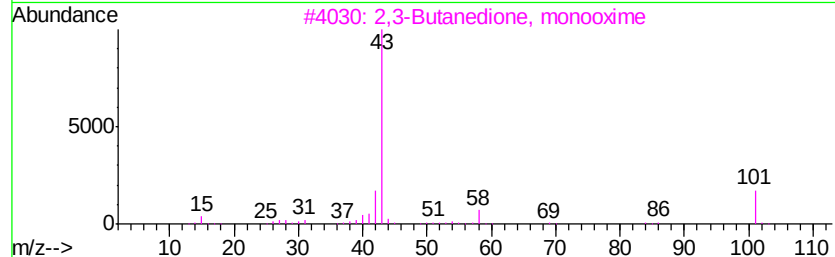
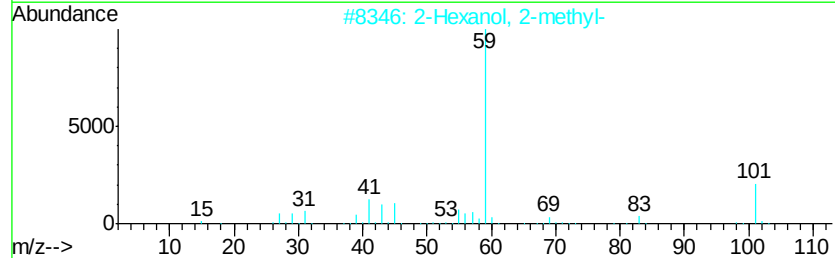
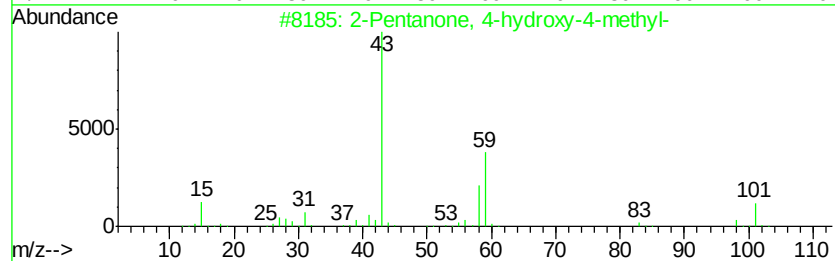
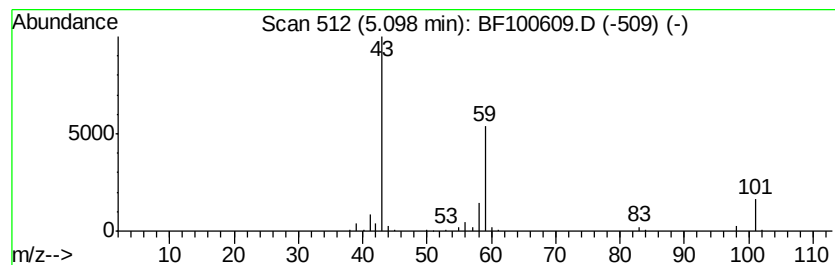
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Peak Number 2 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.92 ng	227260	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	64
2			2-Hexanol, 2-methyl-	116	C7H16O	000625-23-0	28
3			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	9
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	9
5			Propane, 1-ethoxy-2-methyl-	102	C6H14O	000627-02-1	9



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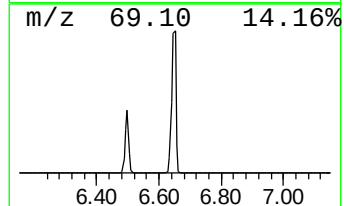
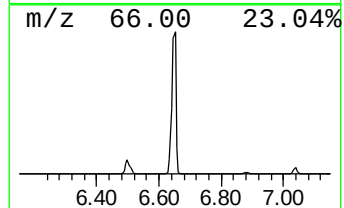
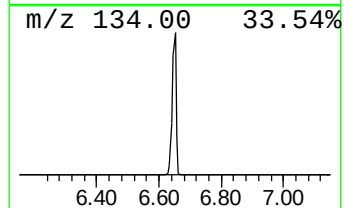
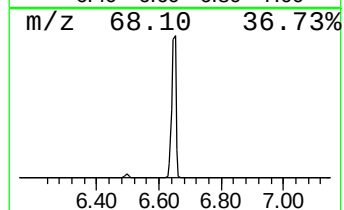
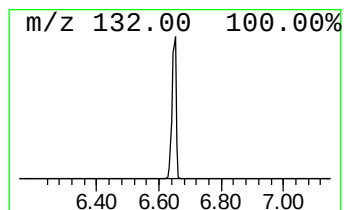
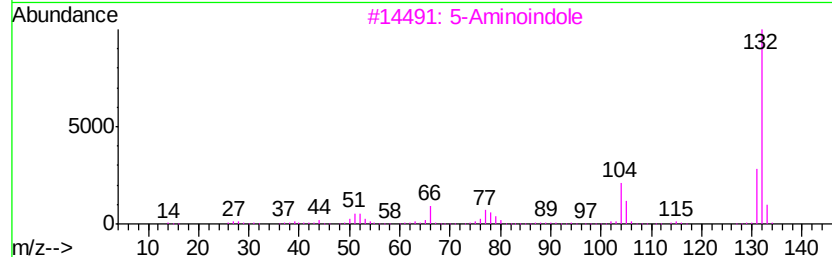
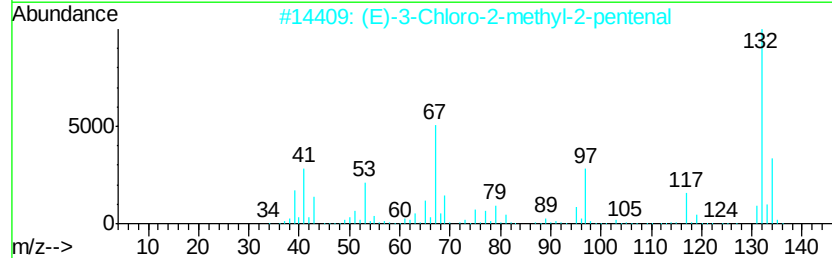
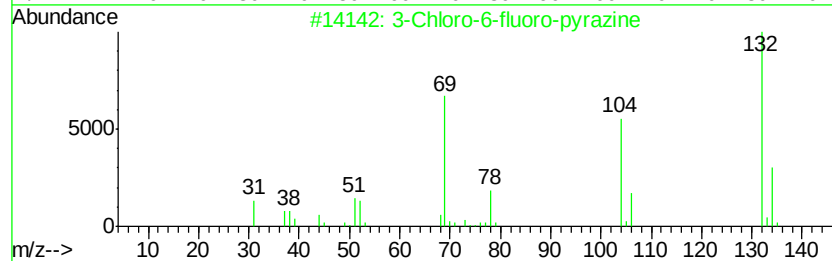
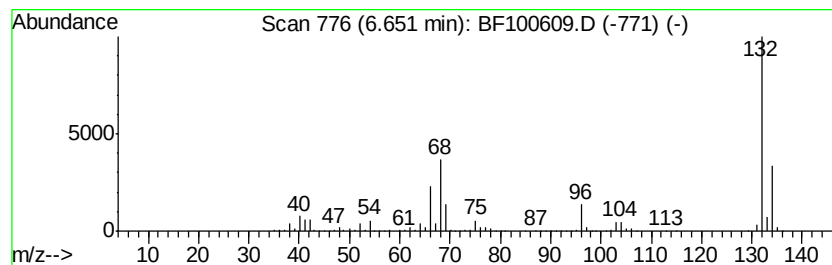
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Peak Number 3 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	55.75 ng	1831110	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		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		Imidazole, 4,5-dicyano-1-methyl-	132	C6H4N4	019485-35-9	9



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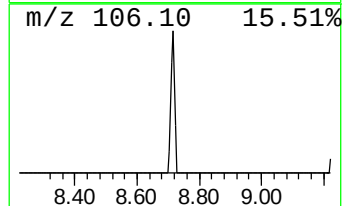
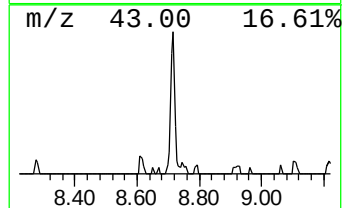
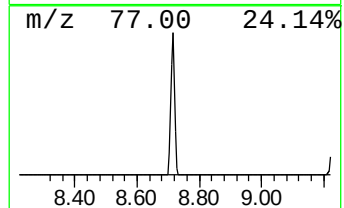
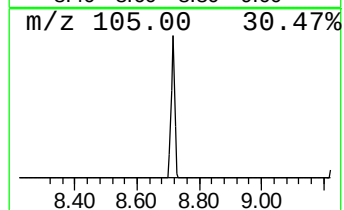
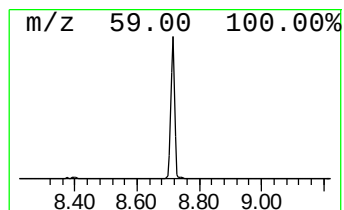
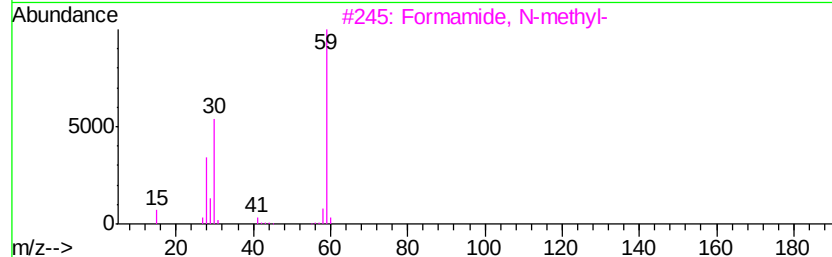
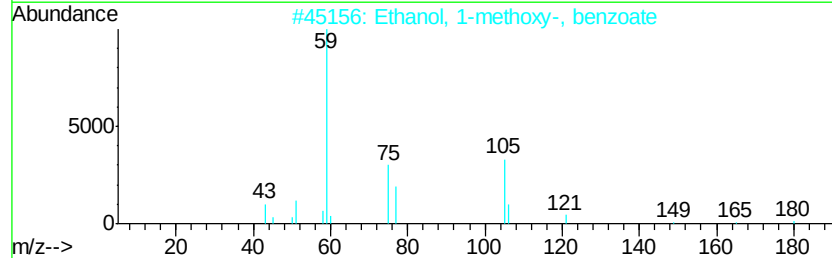
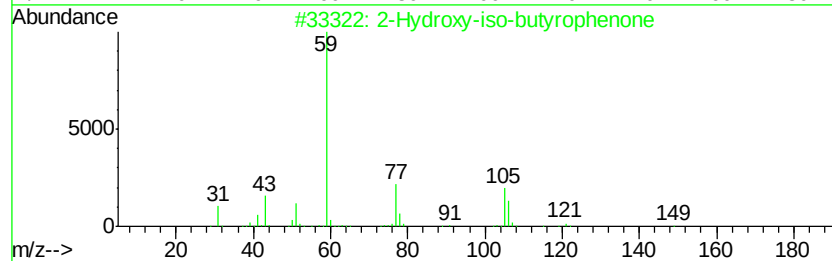
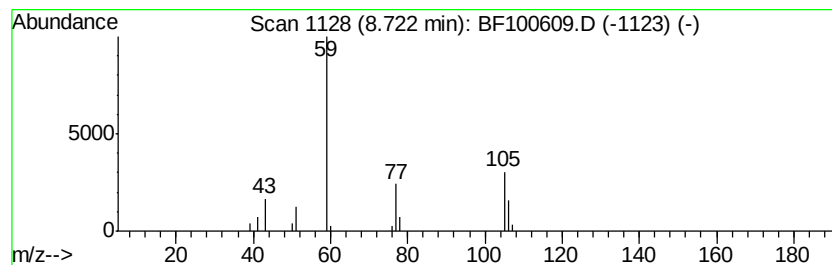
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Peak Number 5 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.02 ng	85111	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		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7
4		Guanidine	59	CH5N3	000113-00-8	5
5		Acetamide	59	C2H5NO	000060-35-5	5



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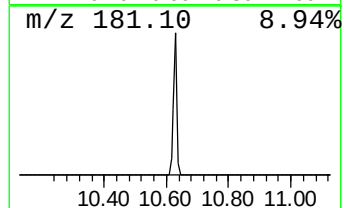
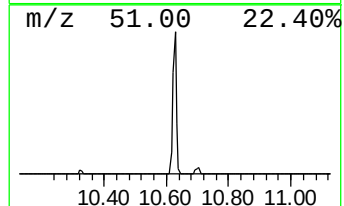
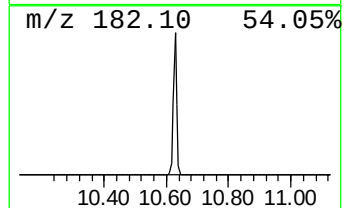
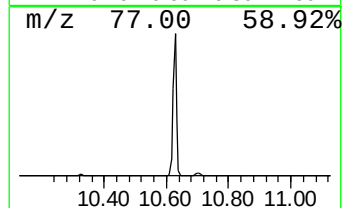
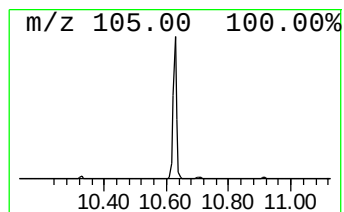
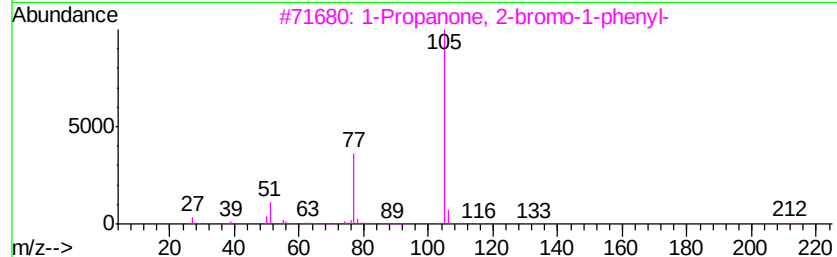
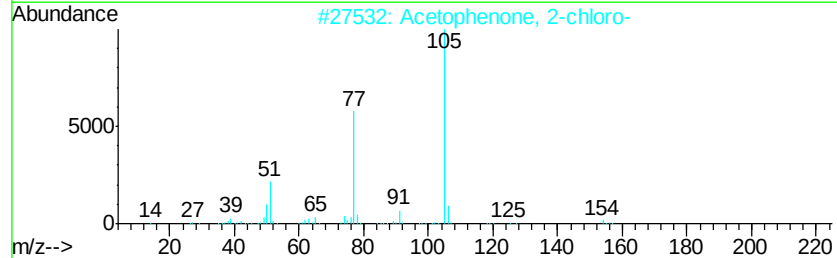
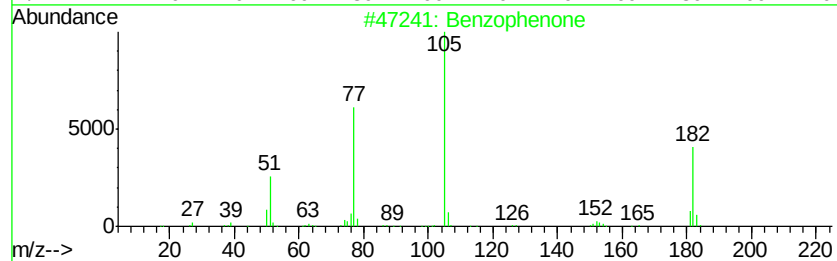
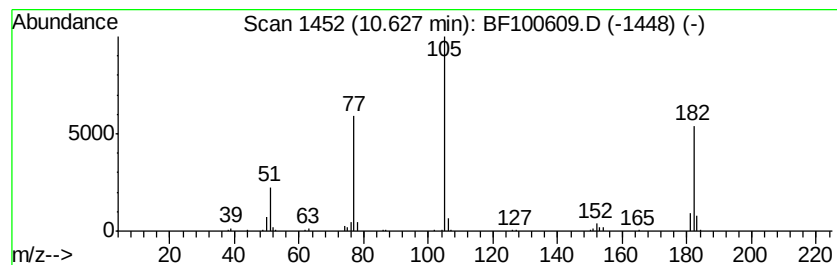
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Peak Number 6 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.	
10.63	4.12 ng	181909	Acenaphthene-d10	9.92	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Benzophenone	182	C13H10O	000119-61-9	97
2	Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3	1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
4	Benzoyl isothiocyanate	163	C8H5NOS	000532-55-8	47
5	1-Propanone, 3-chloro-1-phenyl-	168	C9H9ClO	000936-59-4	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Butane, 2-methoxy...	2.19	2.1	ng	70680	1	6.88	656876	20.0
2-Pentanone, 4-hy...	5.10	6.9	ng	227260	1	6.88	656876	20.0
unknown6.65	6.65	55.8	ng	1831110	1	6.88	656876	20.0
2-Hydroxy-iso-but...	8.72	2.0	ng	85111	2	8.16	843903	20.0
Benzophenone	10.63	4.1	ng	181909	3	9.92	883371	20.0