

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111417\
 Data File : BF100551.D
 Acq On : 14 Nov 2017 19:09
 Operator : SJ/JU
 Sample : I6388-07
 Misc :
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-4

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	2.198	16	19	27	rVB	22831	36034	1.51%	0.172%
2	5.110	510	514	523	rBV	366954	457006	19.09%	2.175%
3	5.504	576	581	584	rBV	2313571	2337571	97.64%	11.127%
4	6.510	746	752	761	rBV	2336680	2393959	100.00%	11.395%
5	6.651	772	776	780	rBV	2401209	2315026	96.70%	11.019%
6	6.886	812	816	819	rBV	907478	763310	31.88%	3.633%
7	7.039	838	842	846	rVB	2056132	1828128	76.36%	8.702%
8	7.445	906	911	914	rBV	1582718	1447110	60.45%	6.888%
9	8.169	1029	1034	1037	rBV	1032421	957818	40.01%	4.559%
10	8.716	1123	1127	1131	rBV	134756	104116	4.35%	0.496%
11	9.239	1211	1216	1219	rBV	2721569	2338804	97.70%	11.133%
12	9.627	1279	1282	1286	rBV	236095	175939	7.35%	0.837%
13	9.922	1328	1332	1335	rBV	1040878	864861	36.13%	4.117%
14	10.627	1449	1452	1456	rVB	312390	254286	10.62%	1.210%
15	10.704	1461	1465	1469	rBV	1060983	978555	40.88%	4.658%
16	11.404	1581	1584	1587	rBV	836714	729911	30.49%	3.474%
17	11.427	1587	1588	1591	rVB	46774	27853	1.16%	0.133%
18	12.615	1787	1790	1793	rBV	45895	36163	1.51%	0.172%
19	12.845	1824	1829	1833	rBV	34352	37249	1.56%	0.177%
20	12.986	1849	1853	1857	rBV	1744963	1524452	63.68%	7.256%
21	13.874	2000	2004	2014	rBV2	70767	96261	4.02%	0.458%
22	14.045	2029	2033	2036	rBV	813146	759089	31.71%	3.613%
23	15.515	2278	2283	2290	rBV2	413095	545221	22.77%	2.595%

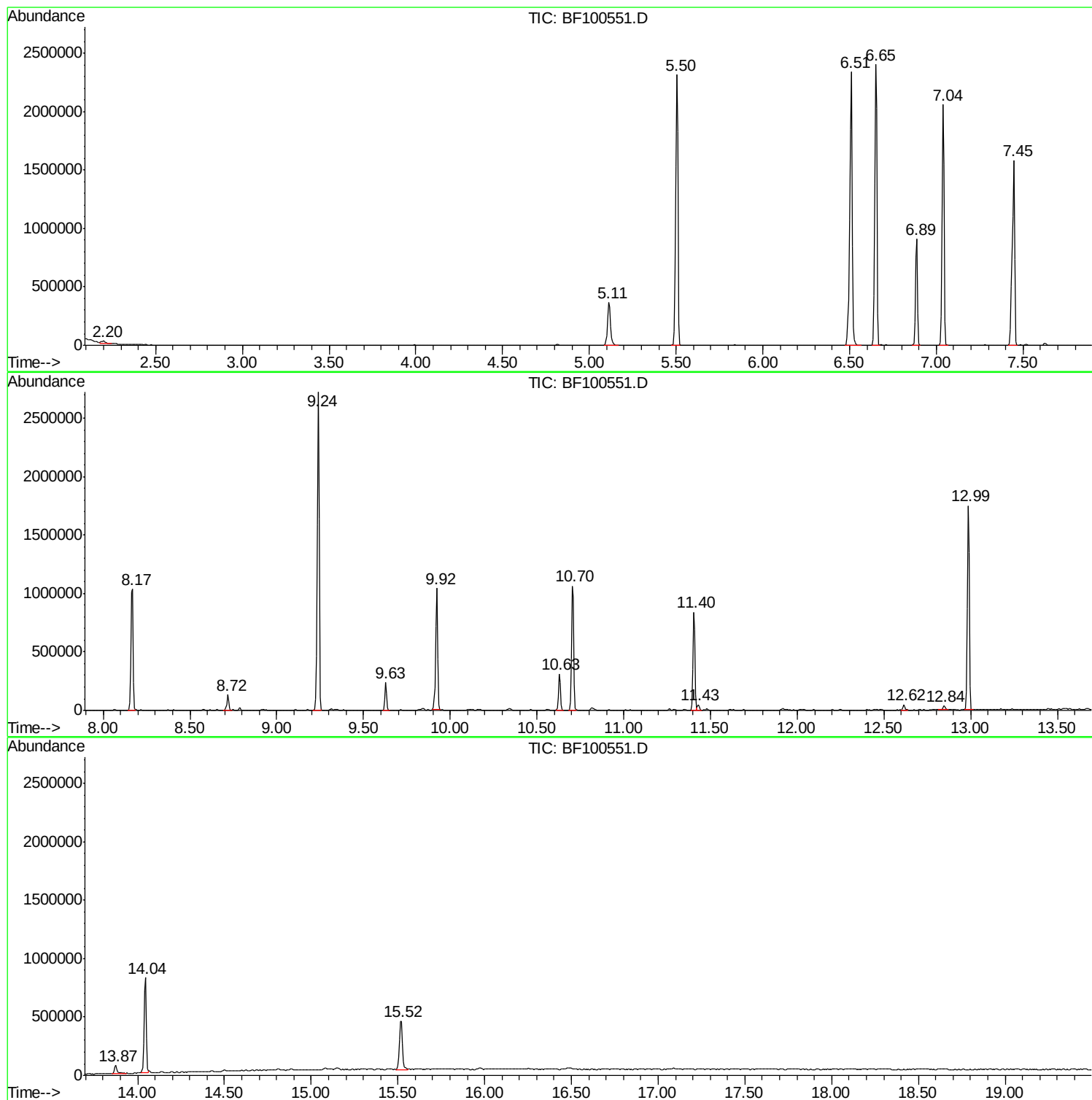
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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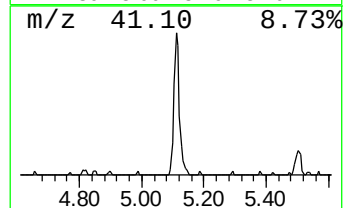
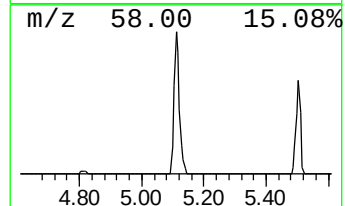
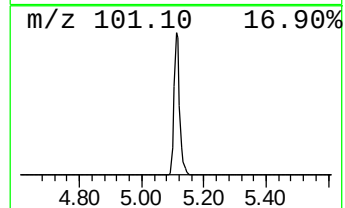
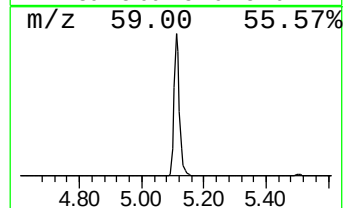
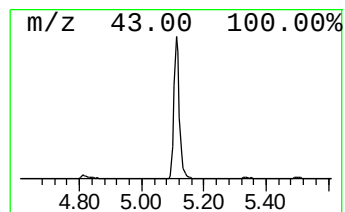
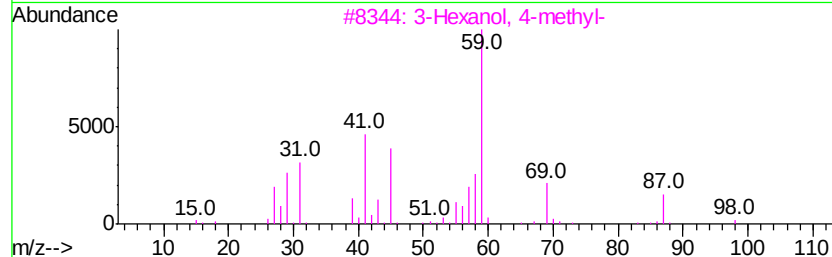
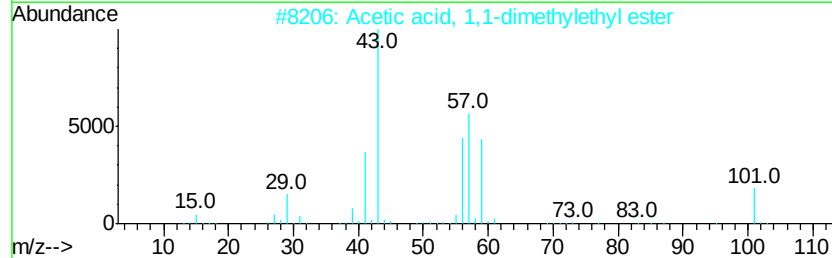
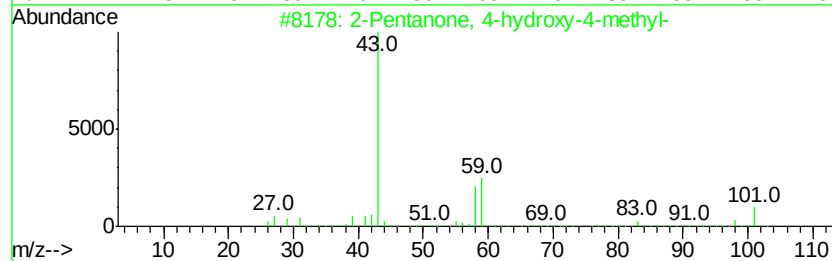
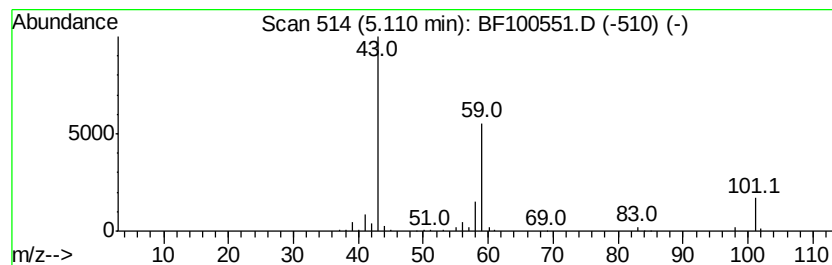
Quant Method : Z:\HPCHEM1\BNA F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	11.97 ng	457006	1,4-Dichlorobenzene-d4	6.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	59
2			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	23
5			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10



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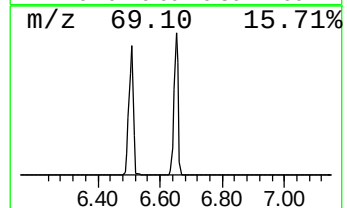
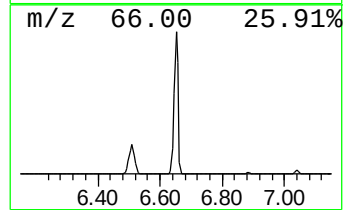
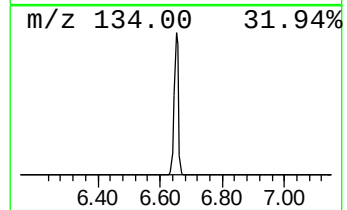
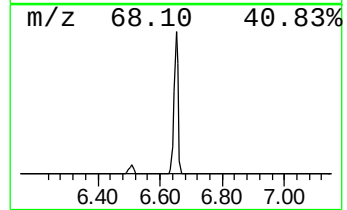
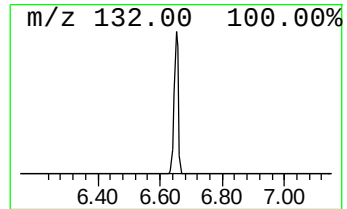
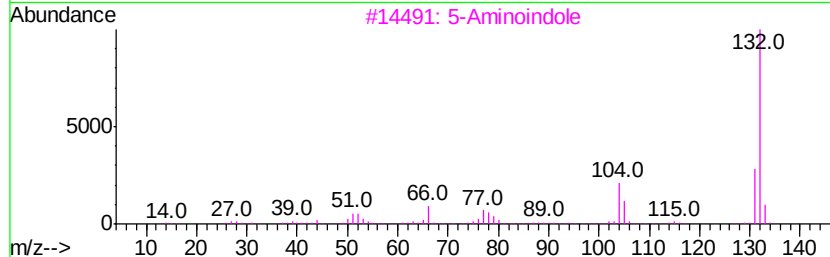
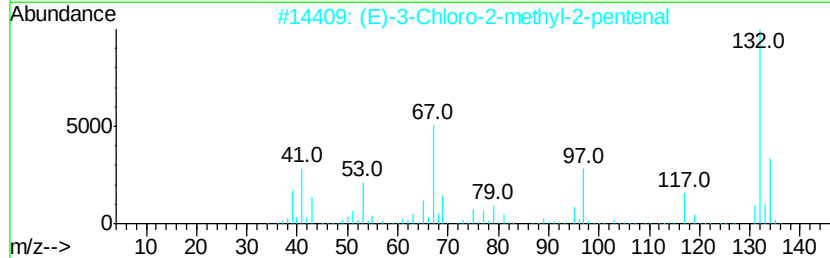
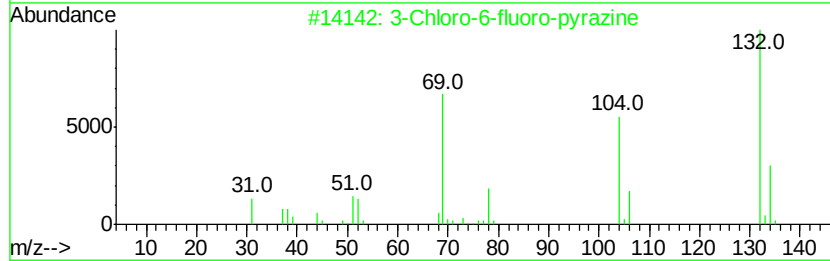
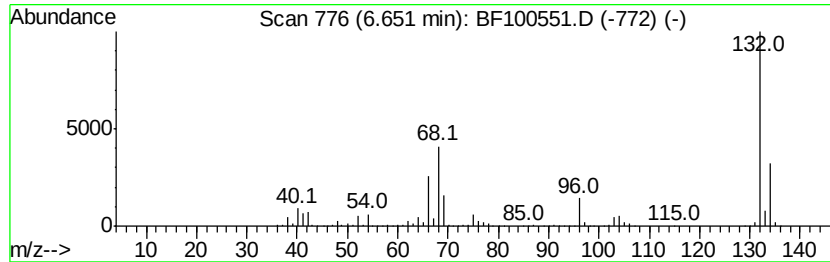
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	60.66 ng	2315030	1,4-Dichlorobenzene-d4	6.89

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		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9



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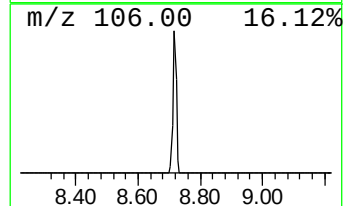
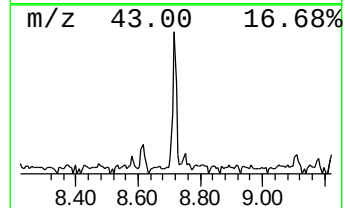
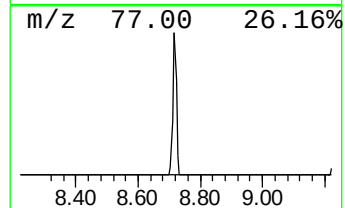
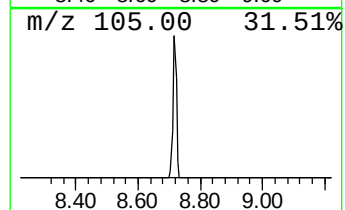
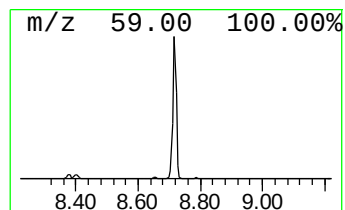
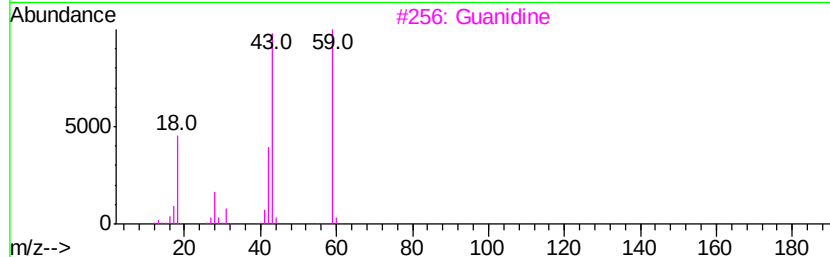
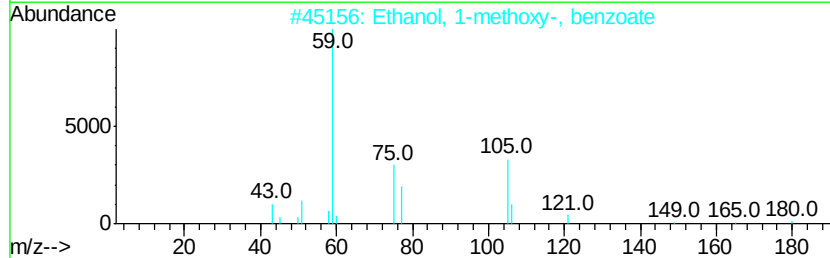
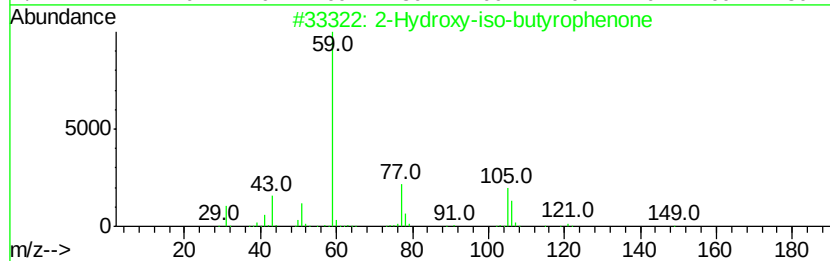
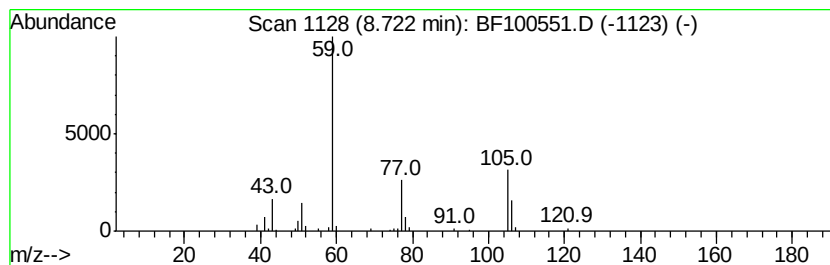
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.17 ng	104116	Napthalene-d8	8.17

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		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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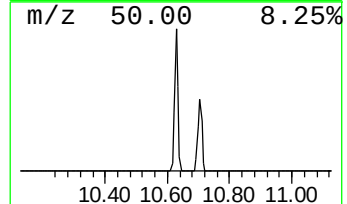
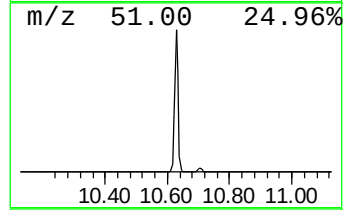
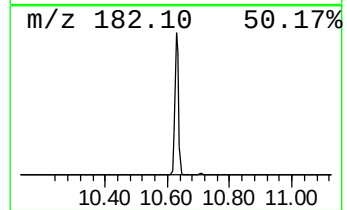
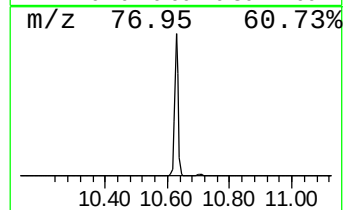
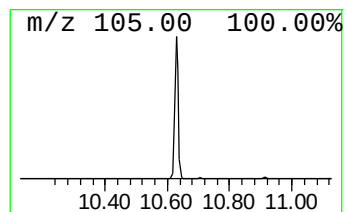
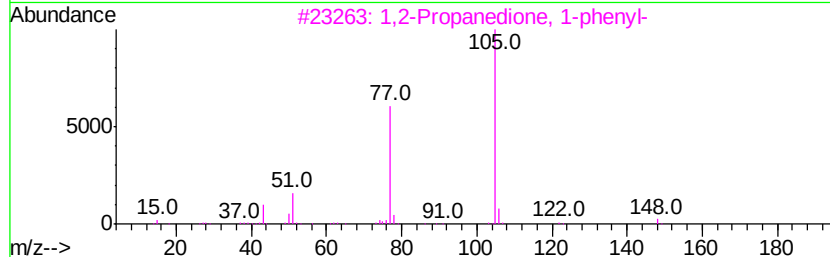
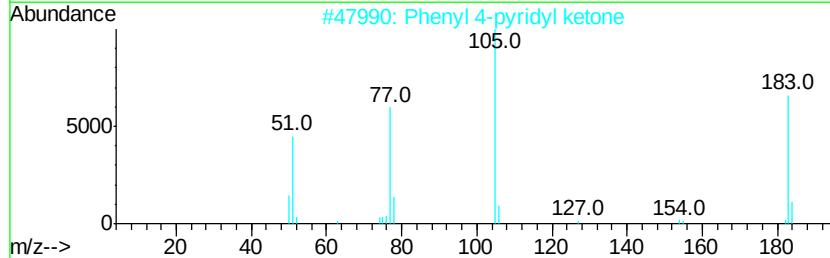
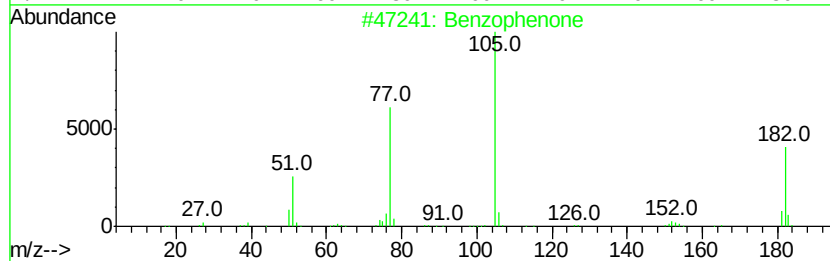
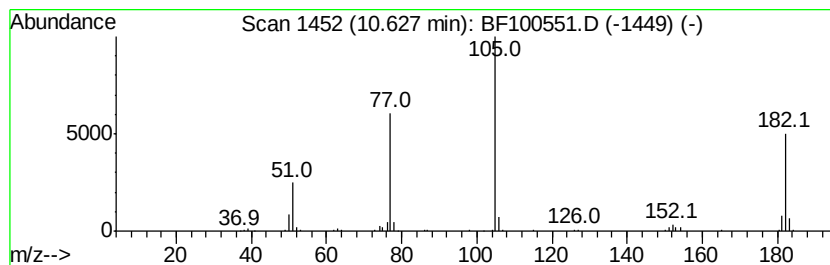
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.		
10.63	5.88 ng	254286	Acenaphthene-d10	9.92		
Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	97
2		Phenyl 4-pyridyl ketone	183	C12H9NO	014548-46-0	58
3		1,2-Propanedione, 1-phenyl-	148	C9H8O2	000579-07-7	47
4		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
5		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184	C11H8N2O	1000296-76-9	47



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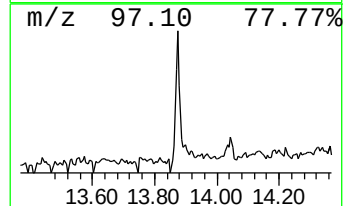
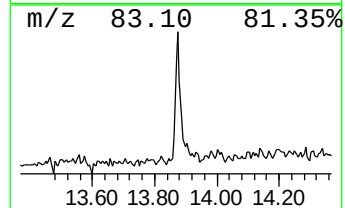
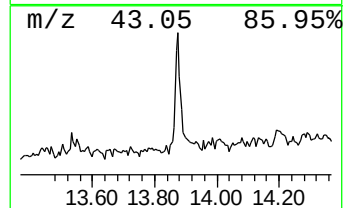
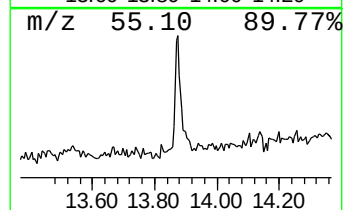
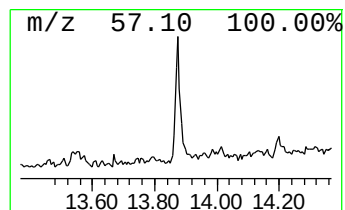
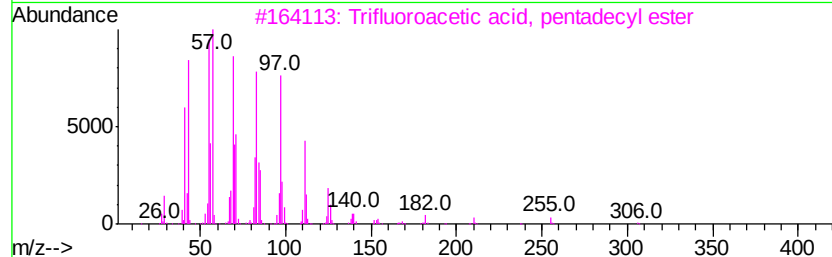
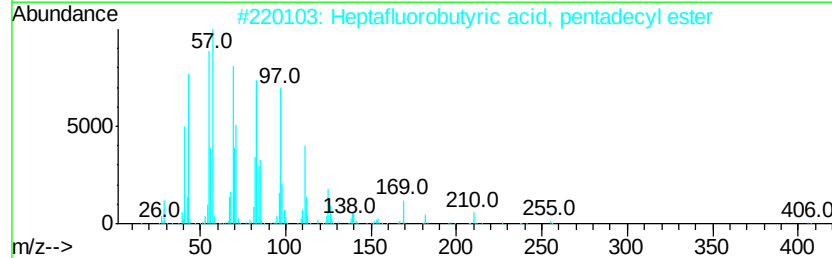
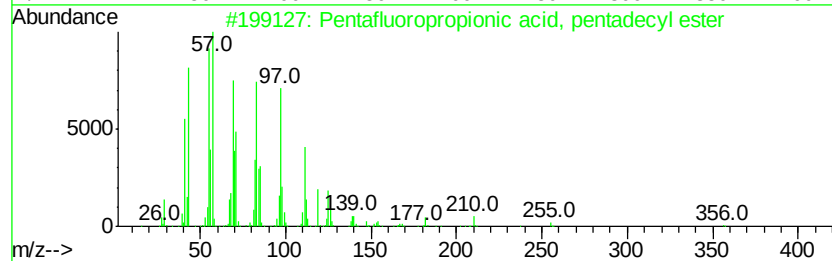
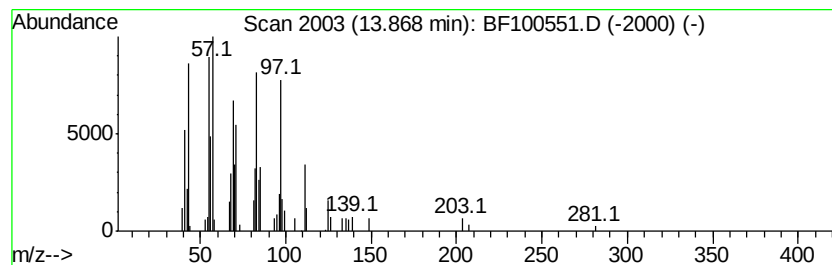
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Peak Number 6 Pentafluoropropionic acid, ... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.54 ng	96261	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	95
2		Heptafluorobutyric acid, pentade...	424	C19H31F7O2	959261-23-5	95
3		Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	95
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	95
5		Heptafluorobutyric acid, hexadec...	438	C20H33F7O2	006385-15-5	95



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	12.0	ng	457006	1	6.89	763310	20.0
unknown6.65	6.65	60.7	ng	2315030	1	6.89	763310	20.0
2-Hydroxy-iso-but...	8.72	2.2	ng	104116	2	8.17	957818	20.0
Benzophenone	10.63	5.9	ng	254286	3	9.92	864861	20.0
Pentafluoropropio...	13.87	2.5	ng	96261	5	14.04	759089	20.0