

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100610.D
 Acq On : 16 Nov 2017 2:06
 Operator : SJ/JU
 Sample : I6426-08
 Misc :
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 110917-SIDI-E-U-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	2.181	12	16	21	rVB2	36683	50357	1.43%	0.240%
2	5.098	509	512	520	rBV	232544	234898	6.69%	1.120%
3	5.492	575	579	583	rBV	1180555	1141093	32.49%	5.442%
4	6.498	746	750	760	rBB	913524	761071	21.67%	3.630%
5	6.651	771	776	779	rBV	1936169	1883520	53.62%	8.983%
6	6.881	811	815	819	rVB	847202	673788	19.18%	3.214%
7	7.039	837	842	845	rBV	2708175	2452948	69.83%	11.699%
8	7.445	905	911	914	rBV	1981162	2053485	58.46%	9.794%
9	8.163	1029	1033	1036	rBV	1053994	858791	24.45%	4.096%
10	8.716	1123	1127	1130	rBV	122514	100366	2.86%	0.479%
11	9.239	1210	1216	1219	rBV	3688131	3512618	100.00%	16.753%
12	9.627	1279	1282	1285	rVB	63286	50888	1.45%	0.243%
13	9.916	1325	1331	1335	rBV2	1058780	927681	26.41%	4.424%
14	10.627	1448	1452	1455	rBV	288549	220678	6.28%	1.052%
15	10.704	1461	1465	1468	rBV	1528558	1336170	38.04%	6.373%
16	11.404	1580	1584	1587	rVB	903854	806567	22.96%	3.847%
17	12.986	1848	1853	1856	rBV	2665099	2618823	74.55%	12.490%
18	13.868	2000	2003	2012	rBV2	48088	64893	1.85%	0.309%
19	14.039	2028	2032	2035	rVB	637672	592137	16.86%	2.824%
20	15.509	2276	2282	2291	rBV	507135	626282	17.83%	2.987%

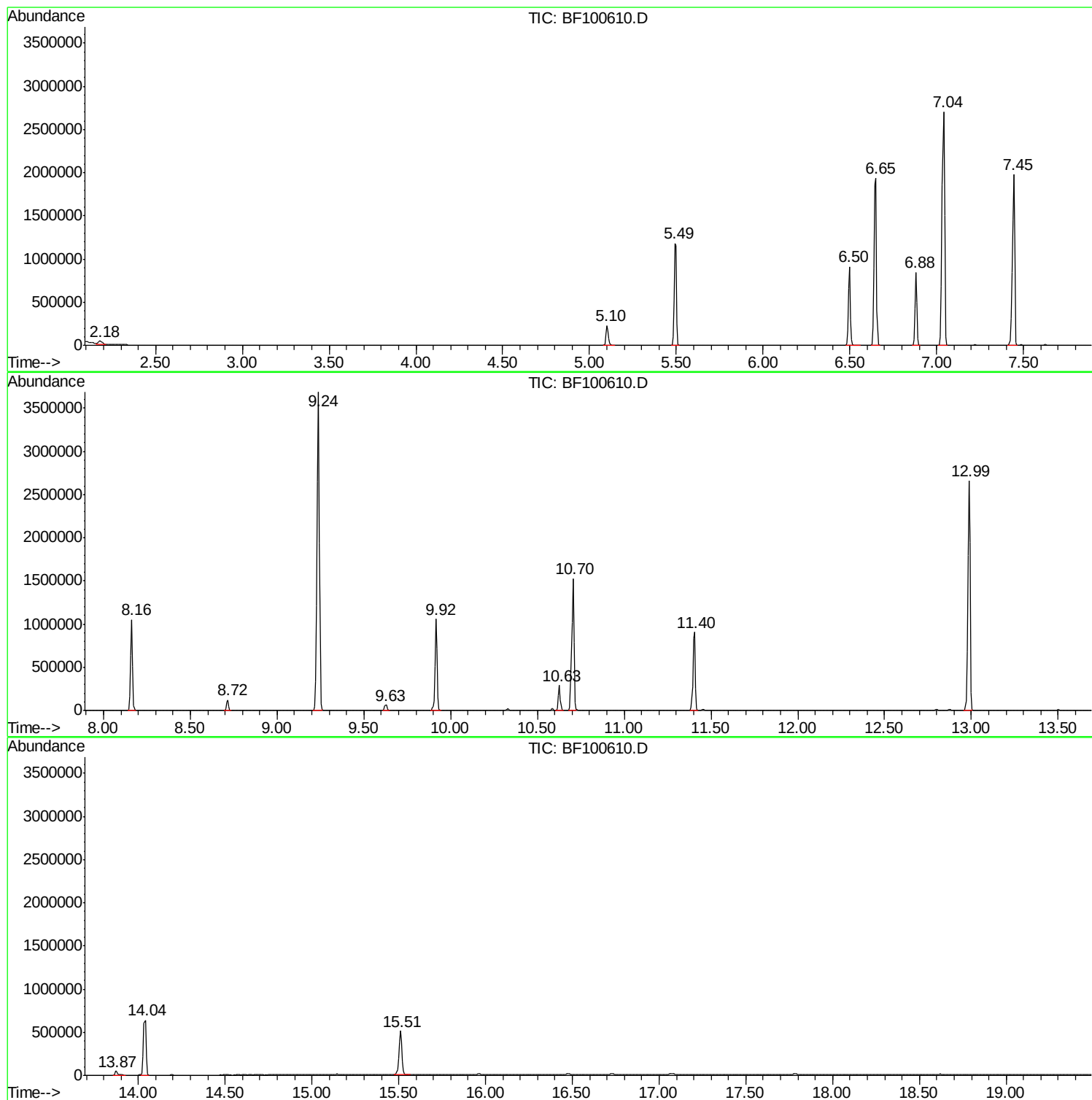
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF110817.M
Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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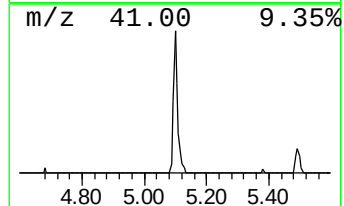
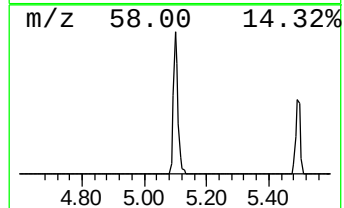
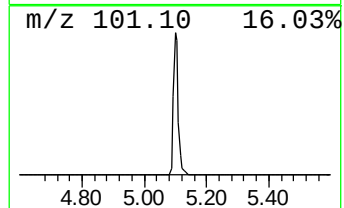
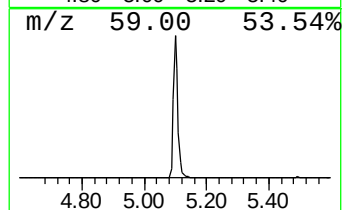
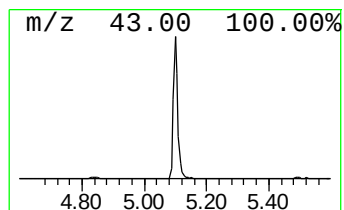
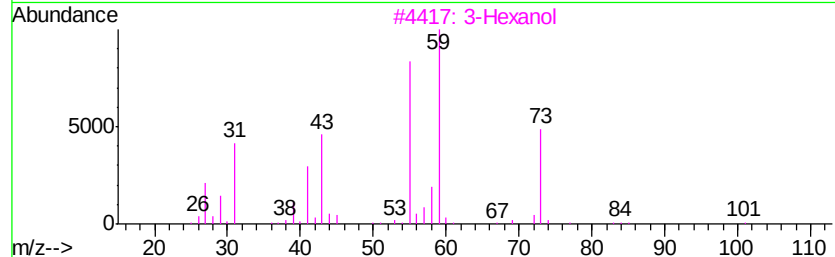
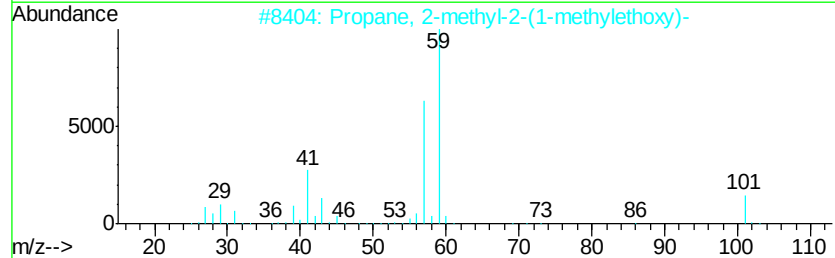
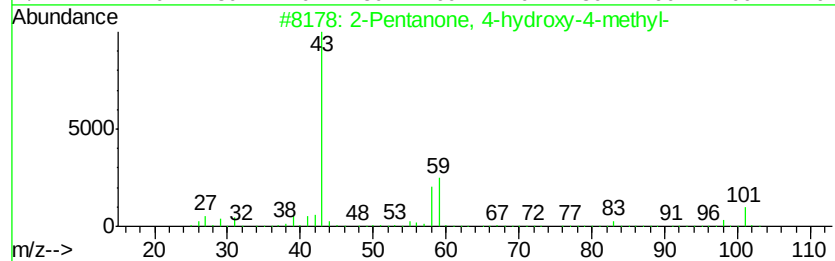
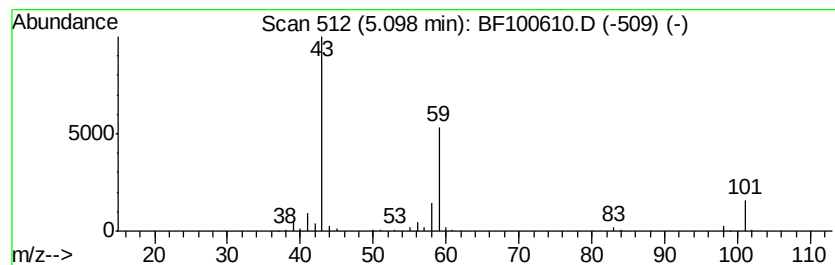
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.10	6.97 ng	234898	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	59
2		Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	36
3		3-Hexanol	102	C6H14O	000623-37-0	33
4		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
5		3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	9



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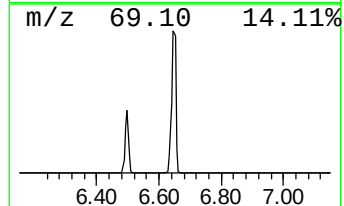
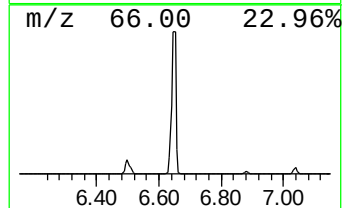
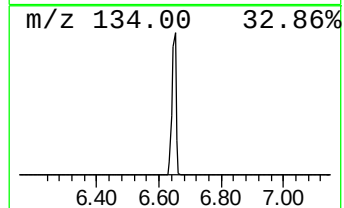
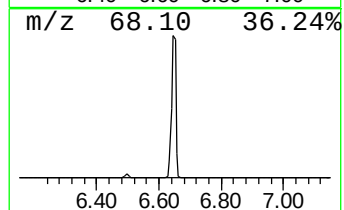
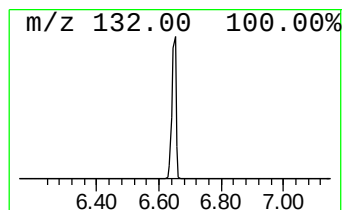
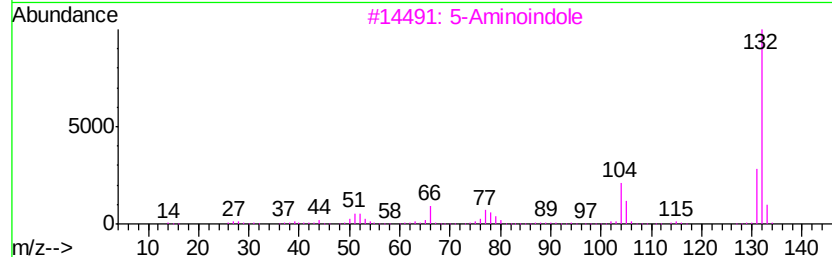
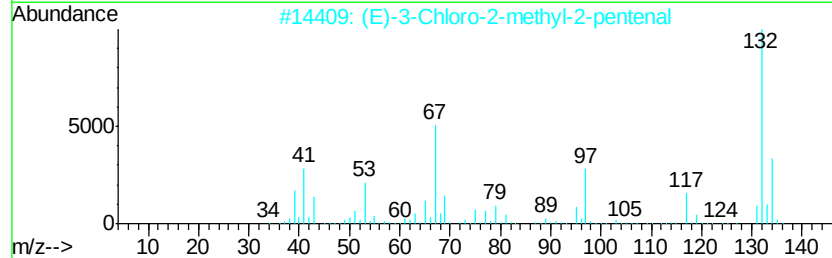
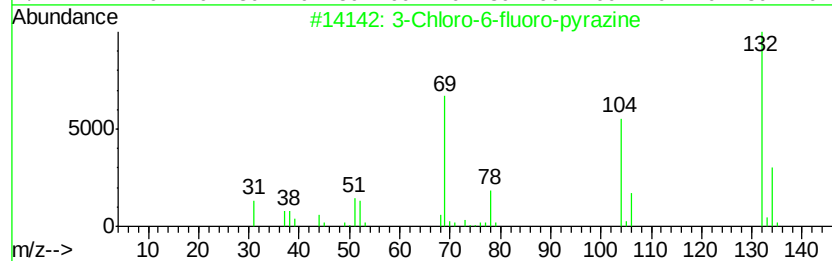
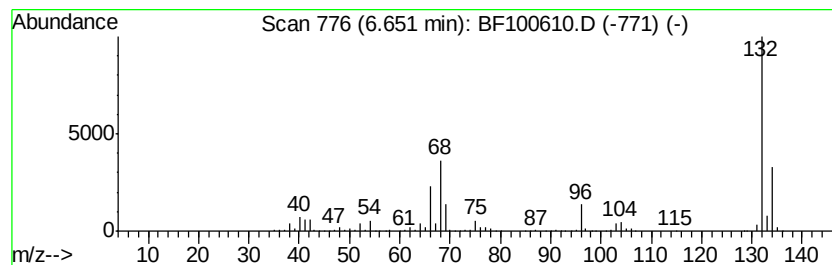
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Peak Number 2 unknown6.65 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	55.91 ng	1883520	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		1,3,5-Trifluorobenzene	132	C6H3F3	000372-38-3	9



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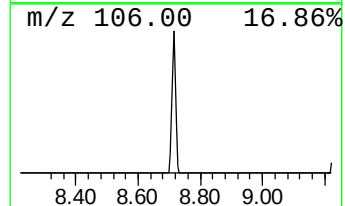
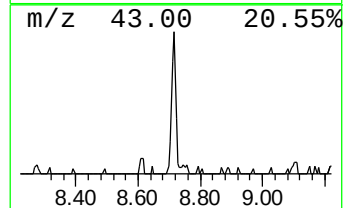
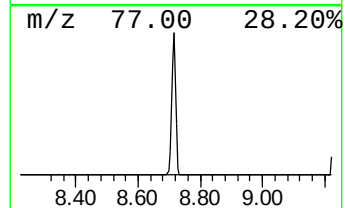
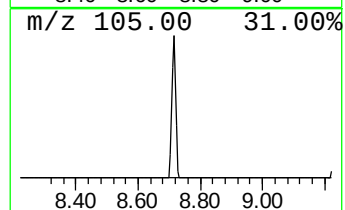
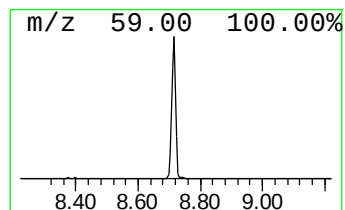
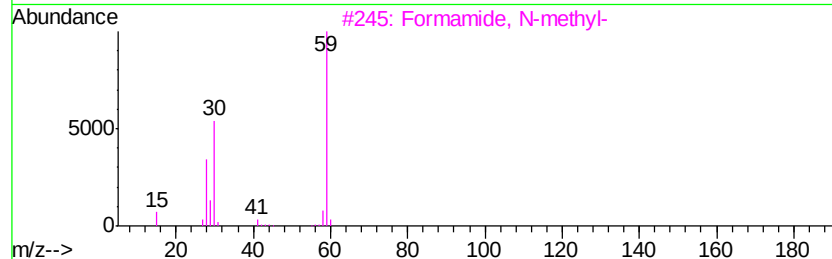
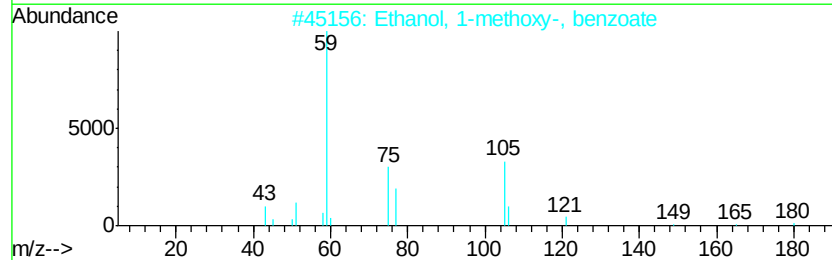
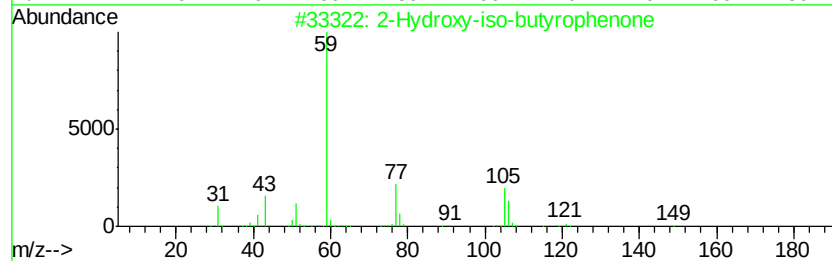
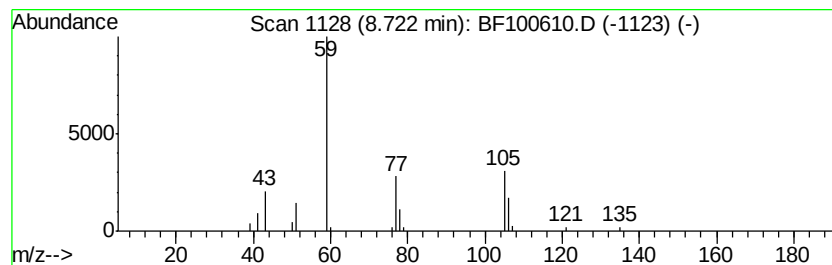
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.34 ng	100366	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	56
3		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
4		Guanidine	59	CH5N3	000113-00-8	5
5		Acetamide	59	C2H5NO	000060-35-5	5



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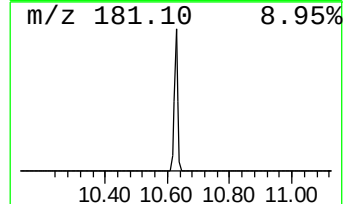
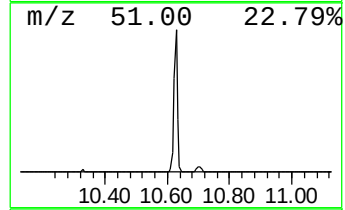
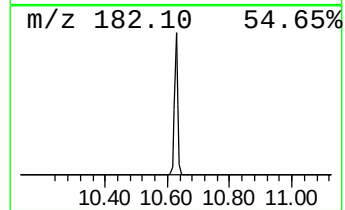
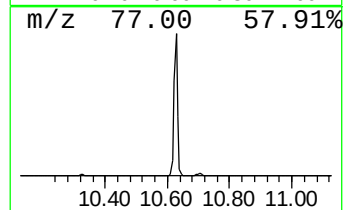
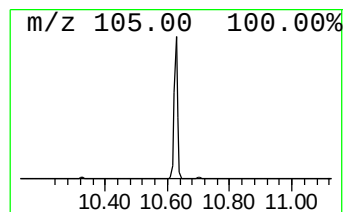
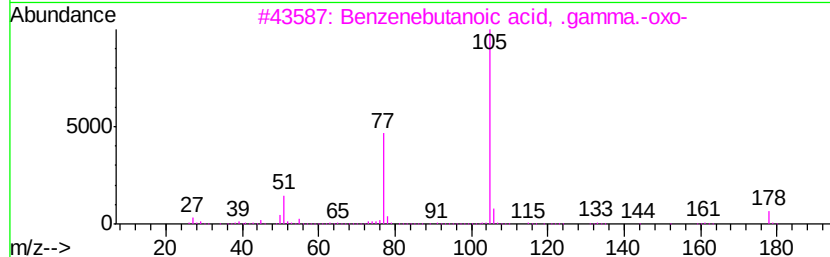
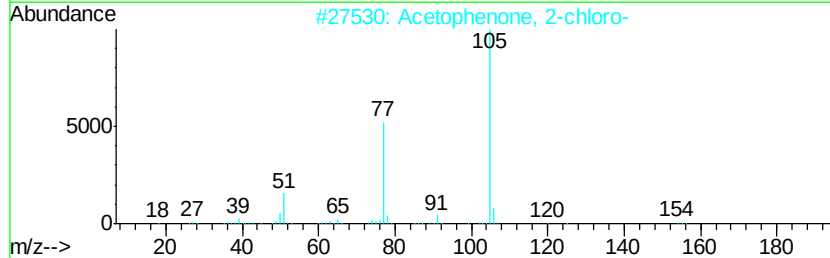
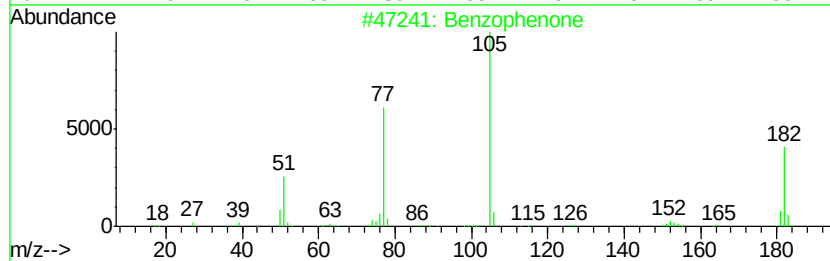
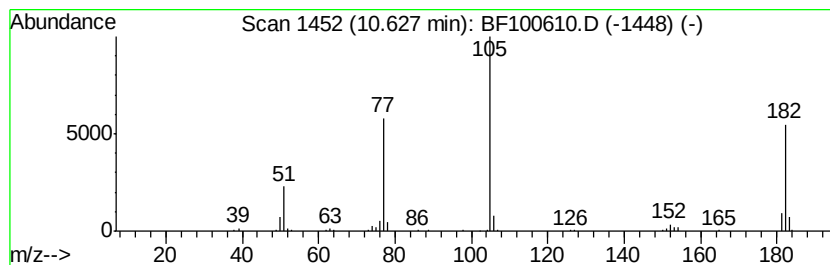
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	4.76 ng	220678	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		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47
4		1,2-Propanedione, 1-phenyl-	148 C9H8O2	000579-07-7 47
5		Phenacyl thiocyanate	177 C9H7NOS	005399-30-4 47



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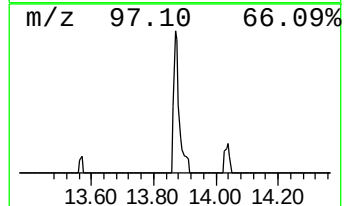
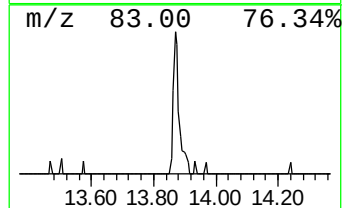
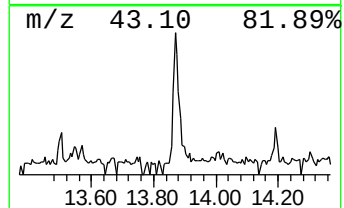
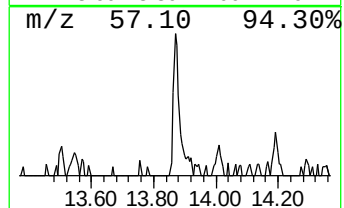
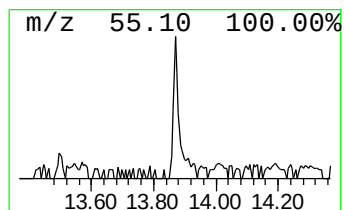
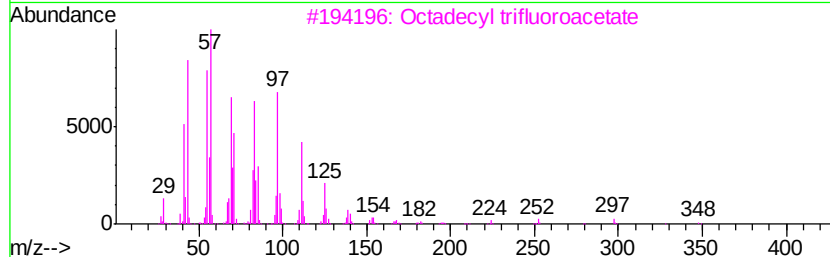
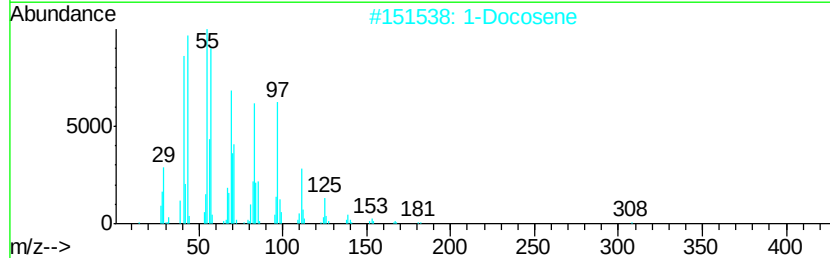
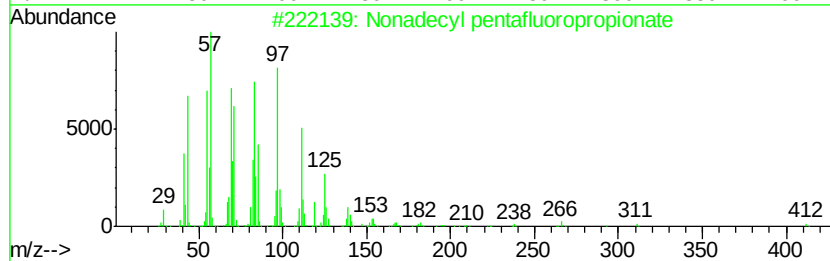
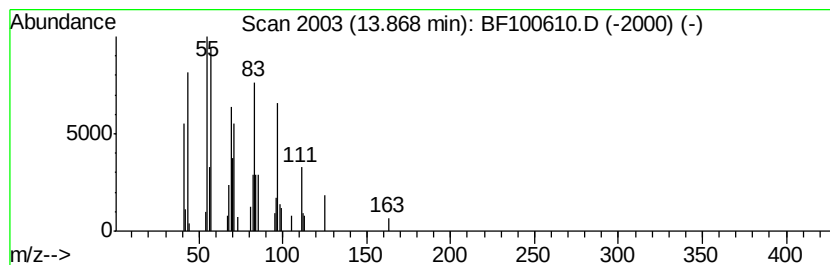
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 6 Nonadecyl pentafluoropropio... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	2.19 ng	64893	Chrysene-d12	14.04

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Nonadecyl pentafluoropropionate	430	C22H39F5O2	1000351-88-8	91
2		1-Docosene	308	C22H44	001599-67-3	91
3		Octadecyl trifluoroacetate	366	C20H37F3O2	079392-43-1	91
4		Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	91
5		Triacontyl acetate	480	C32H64O2	041755-58-2	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.10	7.0	ng	234898	1	6.88	673788	20.0
unknown6.65	6.65	55.9	ng	1883520	1	6.88	673788	20.0
2-Hydroxy-iso-but...	8.72	2.3	ng	100366	2	8.16	858791	20.0
Benzophenone	10.63	4.8	ng	220678	3	9.92	927681	20.0
Nonadecyl pentafl...	13.87	2.2	ng	64893	5	14.04	592137	20.0