

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA_F\DATA\BF111317\
 Data File : BF100518.D
 Acq On : 13 Nov 2017 22:42
 Operator : SJ/JU
 Sample : I6389-15
 Misc :
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 3N-18

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	5.110	511	514	523	rBB	146474	166504	14.79%	1.611%
2	5.510	577	582	585	rBV	1100731	1040788	92.43%	10.071%
3	6.516	748	753	762	rBB	1054335	1126044	100.00%	10.896%
4	6.657	773	777	781	rBV	1223445	1098602	97.56%	10.631%
5	6.892	813	817	820	rBB	574958	443916	39.42%	4.296%
6	7.045	839	843	847	rBB	840654	730154	64.84%	7.065%
7	7.451	907	912	915	rBV	754232	615258	54.64%	5.954%
8	8.175	1031	1035	1038	rBV	684574	552814	49.09%	5.349%
9	8.722	1125	1128	1131	rBV	77206	63106	5.60%	0.611%
10	9.245	1213	1217	1220	rBV	1408962	1113099	98.85%	10.771%
11	9.633	1280	1283	1287	rBV	137158	118607	10.53%	1.148%
12	9.928	1329	1333	1337	rBB2	649555	529613	47.03%	5.125%
13	10.639	1450	1454	1457	rBV	226238	175855	15.62%	1.702%
14	10.716	1463	1467	1470	rBV	621070	519094	46.10%	5.023%
15	11.416	1582	1586	1589	rBV	523370	439449	39.03%	4.252%
16	11.927	1670	1673	1677	rBV2	17933	14545	1.29%	0.141%
17	12.998	1851	1855	1858	rBV	796120	715698	63.56%	6.925%
18	13.880	2002	2005	2014	rBV	87436	93634	8.32%	0.906%
19	14.051	2030	2034	2038	rBV	506920	433681	38.51%	4.197%
20	15.533	2281	2286	2294	rVB	251422	313250	27.82%	3.031%
21	16.686	2476	2482	2483	rBV5	18887	30567	2.71%	0.296%

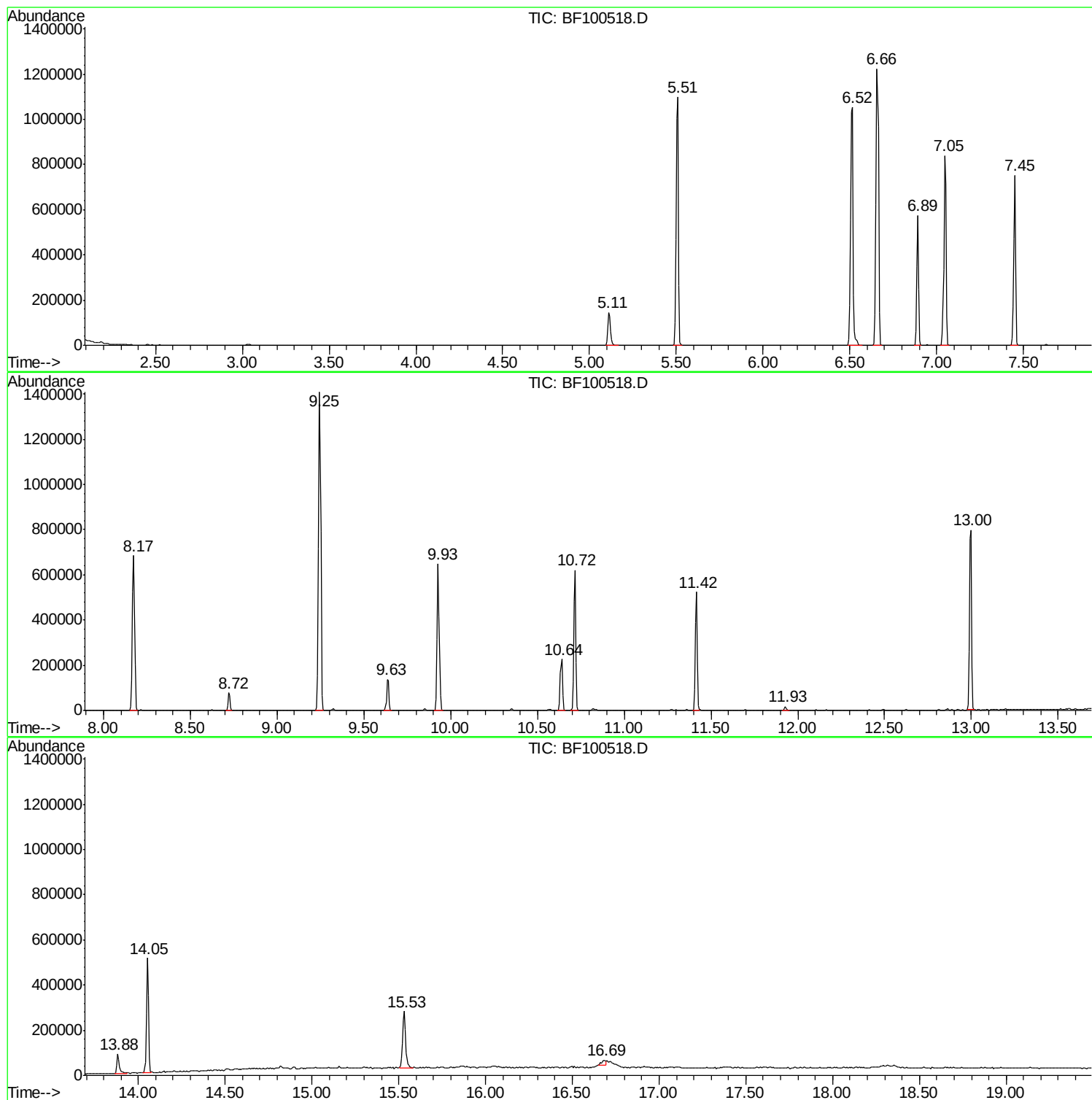
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Quant Title : ASP BNA STANDARDS FOR 5 POINT CALIBRATION

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



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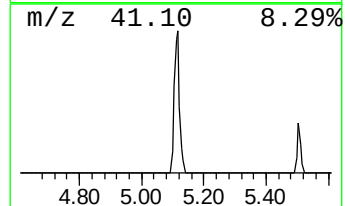
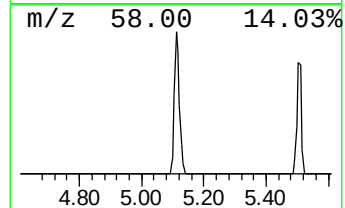
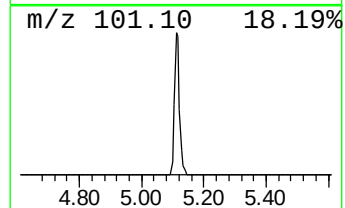
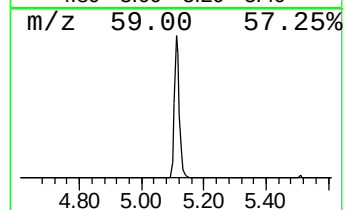
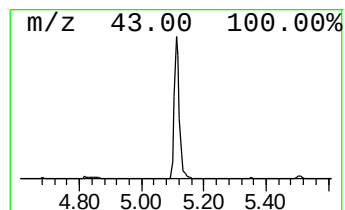
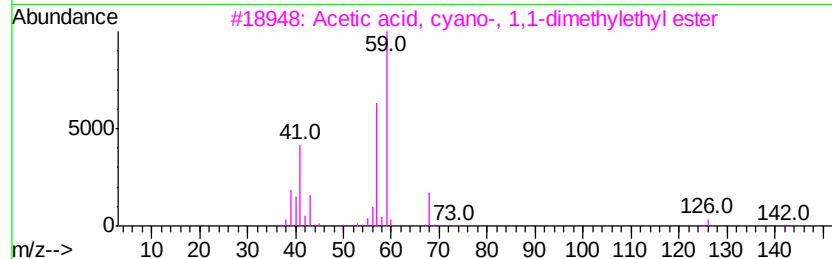
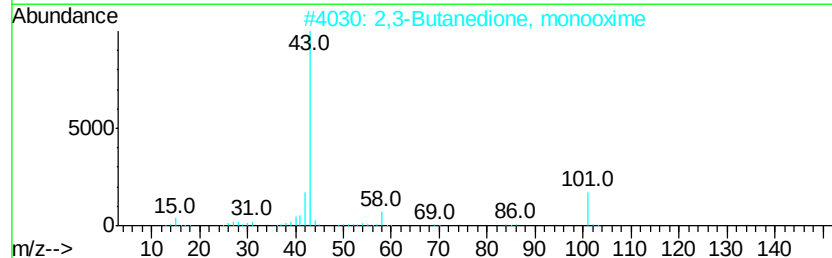
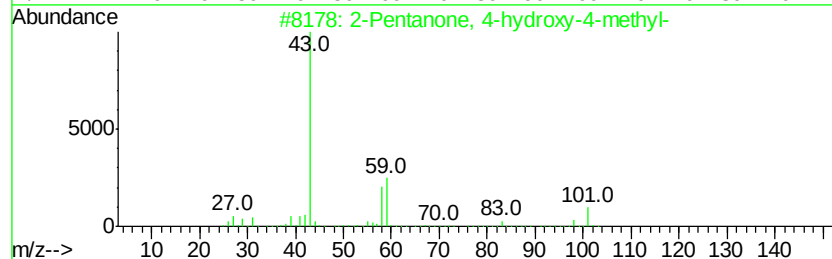
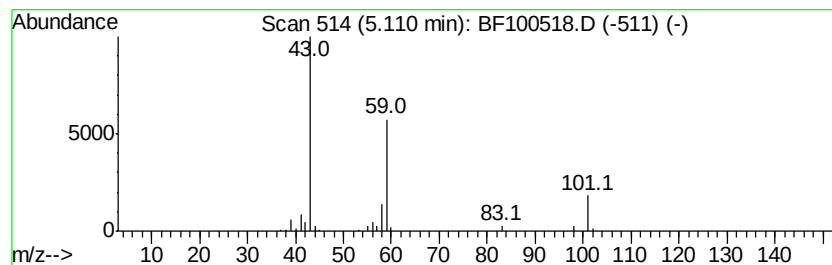
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	7.50 ng	166504	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			2,3-Butanedione, monooxime	101	C4H7NO2	000057-71-6	27
3			Acetic acid, cyano-, 1,1-dimethyl...	141	C7H11NO2	001116-98-9	23
4			1-Propen-2-ol, acetate	100	C5H8O2	000108-22-5	10
5			Butane	58	C4H10	000106-97-8	9



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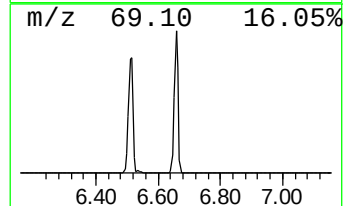
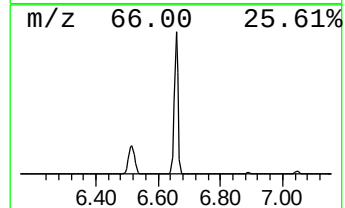
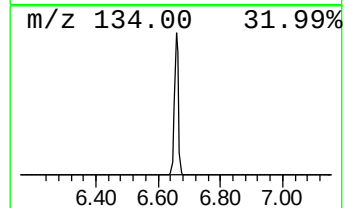
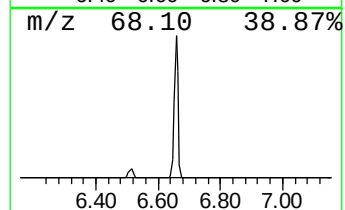
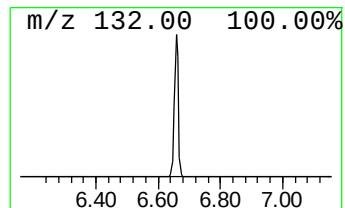
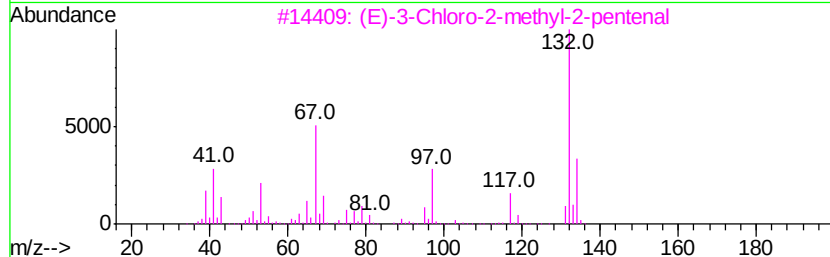
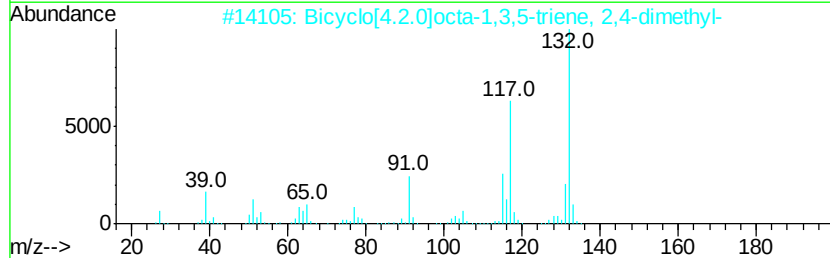
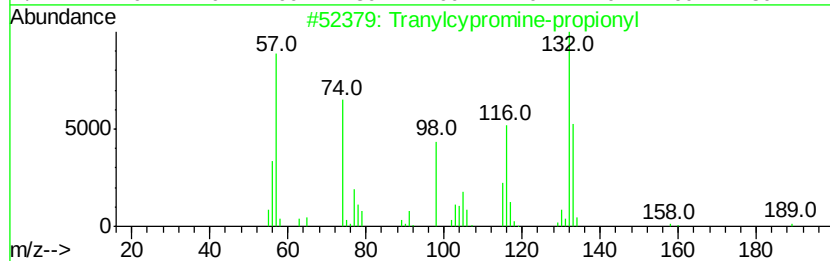
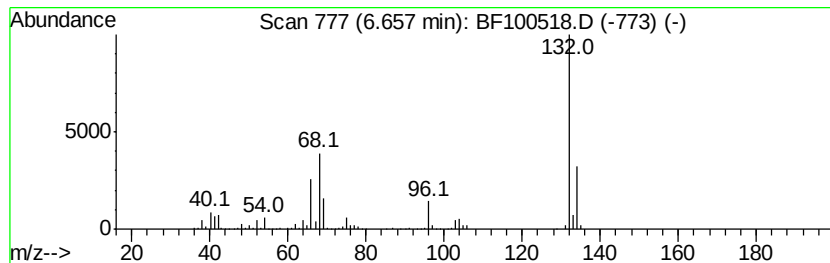
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Peak Number 2 unknown6.66 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.66	49.50 ng	1098600	1,4-Dichlorobenzene-d4	6.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Tranlylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
2		Bicyclo[4.2.0]octa-1,3,5-triene,...	132	C10H12	028749-81-7	9
3		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	9
4		4-Chloro-2-fluoro-pyrimidine	132	C4H2ClFN2	051422-00-5	9
5		1-Methylpyrrolo[1,2-a]pyrazine	132	C8H8N2	064608-59-9	9



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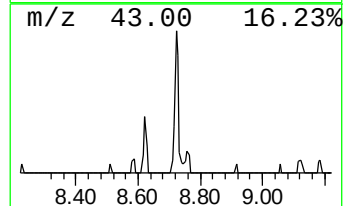
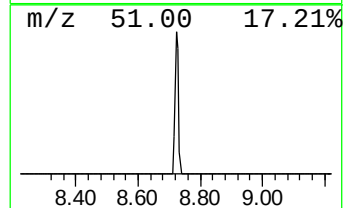
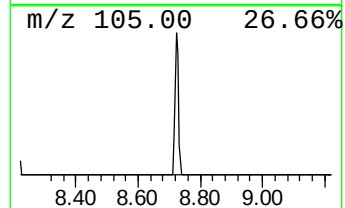
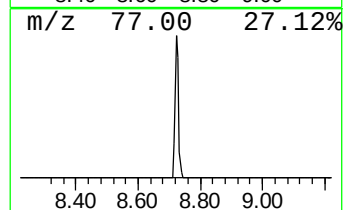
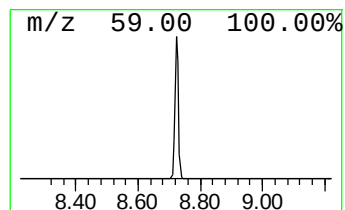
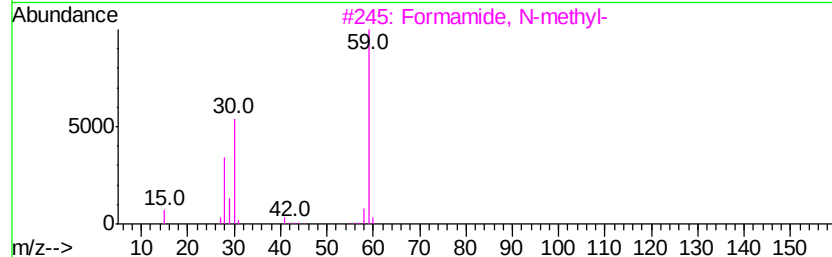
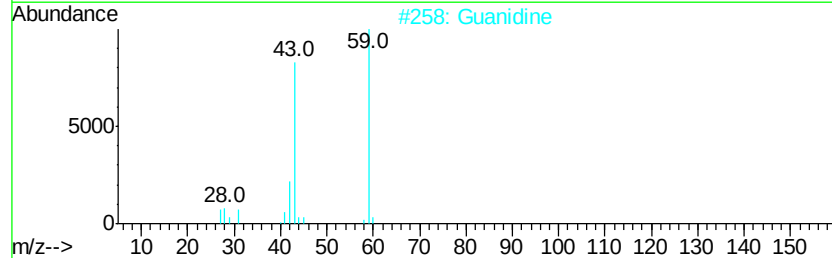
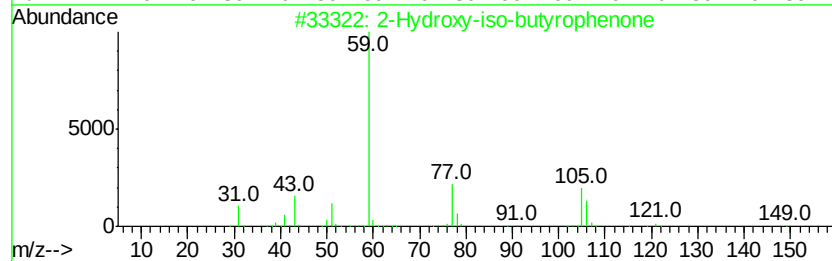
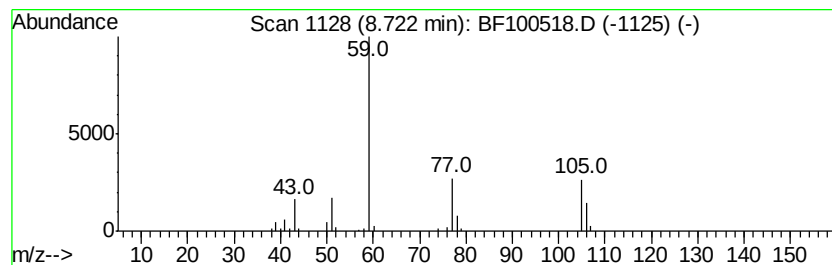
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	2.28 ng	63106	Napthalene-d8	8.17

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	72
2		Guanidine	59	CH5N3	000113-00-8	9
3		Formamide, N-methyl-	59	C2H5NO	000123-39-7	5
4		Acetamide	59	C2H5NO	000060-35-5	5
5		Hydrazine, 1-methyl-1-propyl-	88	C4H12N2	004986-49-6	4



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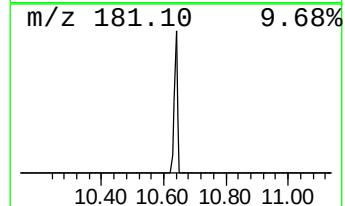
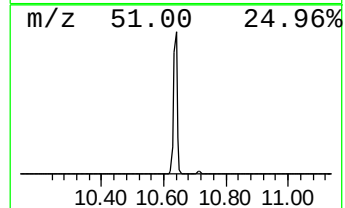
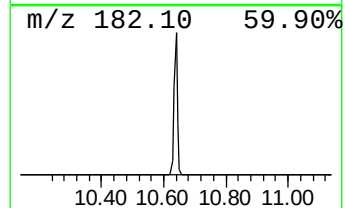
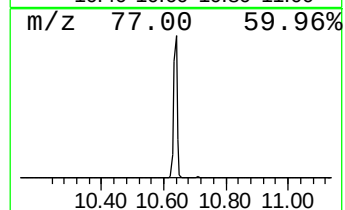
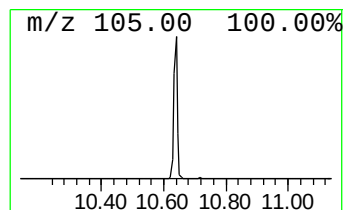
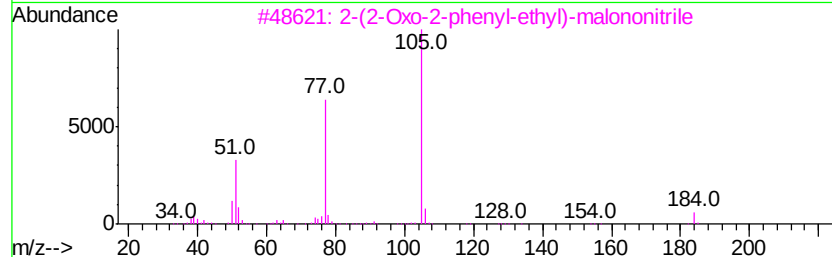
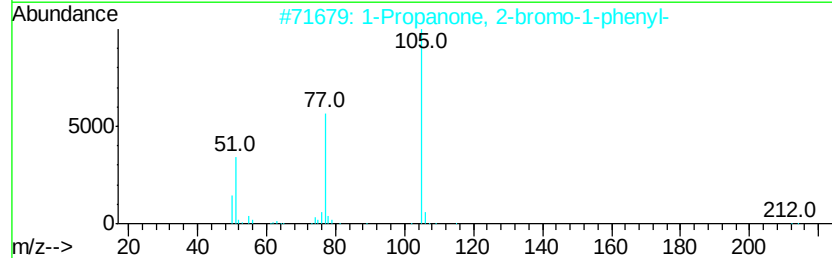
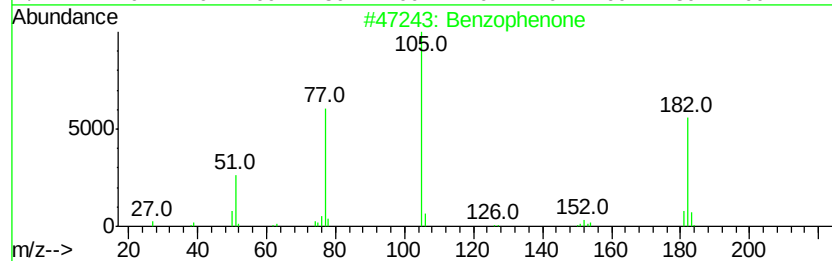
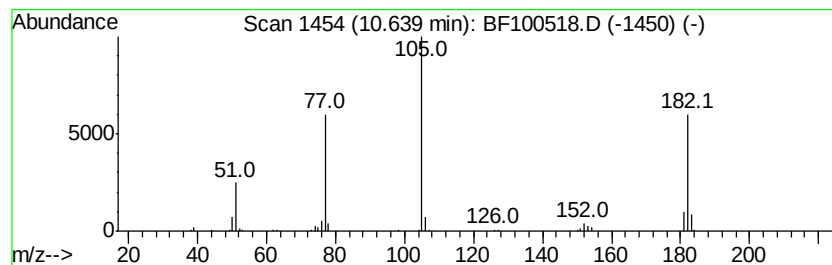
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.64	6.64 ng	175855	Acenaphthene-d10	9.93

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzophenone	182	C13H10O	000119-61-9	96
2		1-Propanone, 2-bromo-1-phenyl-	212	C9H9BrO	002114-00-3	47
3		2-(2-Oxo-2-phenyl-ethyl)-malononitrile	184	C11H8N2O	1000296-76-9	47
4		Benzenebutanoic acid, .gamma.-oxo-	178	C10H10O3	002051-95-8	47
5		Benzoyl bromide	184	C7H5BrO	000618-32-6	47



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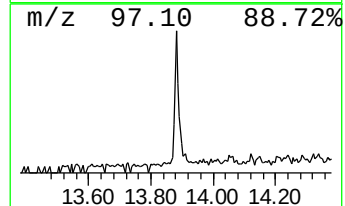
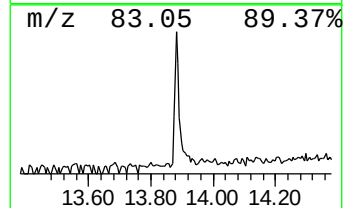
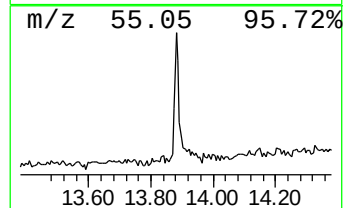
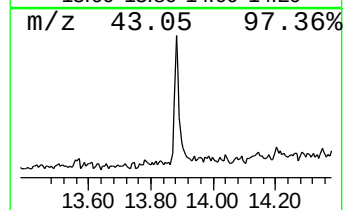
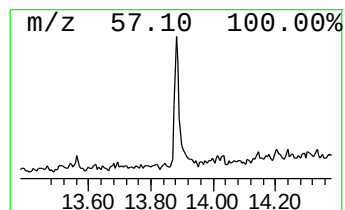
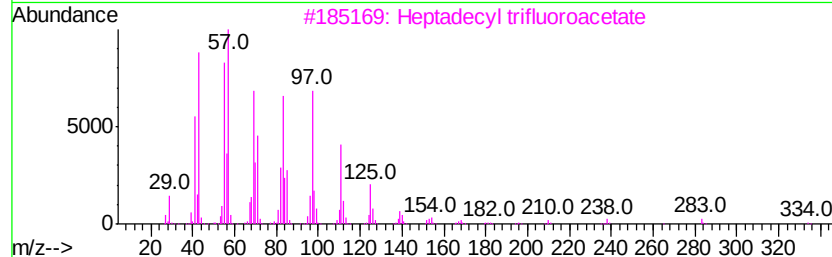
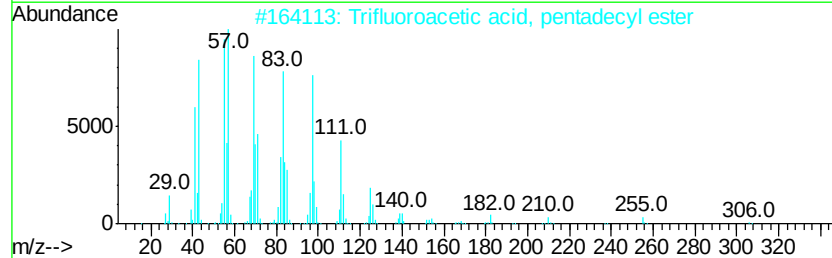
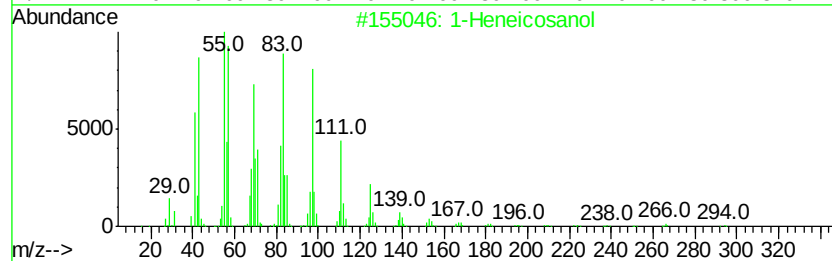
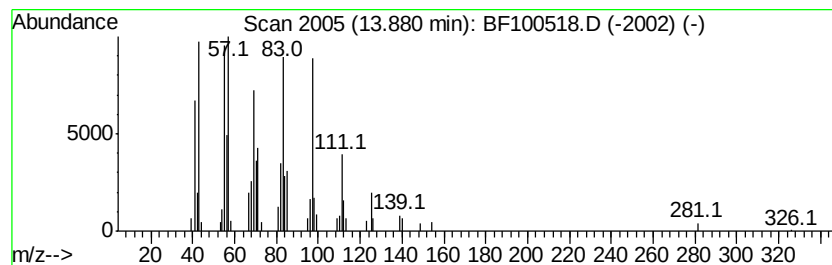
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Peak Number 6 1-Heneicosanol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.88	4.32 ng	93634	Chrysene-d12	14.05	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Heneicosanol	312	C21H44O	015594-90-8	95
2	Trifluoroacetic acid, pentadecyl...	324	C17H31F3O2	959010-23-2	94
3	Heptadecyl trifluoroacetate	352	C19H35F3O2	1000351-87-0	94
4	Pentafluoropropionic acid, penta...	374	C18H31F5O2	959092-08-1	94
5	n-Tetracosanol-1	354	C24H50O	000506-51-4	93



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	7.5	ng	166504	1	6.89	443916	20.0
unknown6.66	6.66	49.5	ng	1098600	1	6.89	443916	20.0
2-Hydroxy-iso-but...	8.72	2.3	ng	63106	2	8.17	552814	20.0
Benzophenone	10.64	6.6	ng	175855	3	9.93	529613	20.0
1-Heneicosanol	13.88	4.3	ng	93634	5	14.05	433681	20.0