

Data Path : Z:\HPCHEM1\BNA_F\DATA\BF111517\
 Data File : BF100594.D
 Acq On : 15 Nov 2017 17:59
 Operator : SJ/JU
 Sample : I6429-01
 Misc :
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 SP-1

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	2.193	15	18	23	rVB3	20380	30812	1.16%	0.136%
2	5.110	510	514	523	rVB	394602	491875	18.54%	2.170%
3	5.504	576	581	584	rBV	2425327	2413216	90.95%	10.648%
4	6.510	746	752	756	rBV	2287907	2504249	94.38%	11.050%
5	6.651	771	776	779	rBV	2506733	2454554	92.50%	10.830%
6	6.881	812	815	819	rVB	838516	712197	26.84%	3.142%
7	7.040	838	842	845	rBV	2221399	1940167	73.12%	8.561%
8	7.445	905	911	914	rBV	1693410	1536379	57.90%	6.779%
9	8.163	1029	1033	1037	rBV	1107004	918594	34.62%	4.053%
10	8.716	1123	1127	1130	rBV	236932	175316	6.61%	0.774%
11	9.239	1210	1216	1219	rBV	3026673	2653486	100.00%	11.708%
12	9.628	1278	1282	1285	rBV	414556	308450	11.62%	1.361%
13	9.916	1327	1331	1335	rBV	977192	893732	33.68%	3.943%
14	10.628	1448	1452	1455	rBV	574241	437142	16.47%	1.929%
15	10.704	1461	1465	1468	rBV	1382395	1218987	45.94%	5.379%
16	11.404	1580	1584	1587	rBV	871752	701869	26.45%	3.097%
17	12.986	1849	1853	1856	rBV	1918076	1678303	63.25%	7.405%
18	13.868	2000	2003	2015	rBV	175901	199724	7.53%	0.881%
19	14.039	2028	2032	2036	rVB	773441	663728	25.01%	2.929%
20	14.504	2107	2111	2117	rBV4	19998	29961	1.13%	0.132%
21	15.515	2277	2283	2291	rBV	510472	665509	25.08%	2.936%
22	15.968	2356	2360	2364	rVB2	25449	35207	1.33%	0.155%

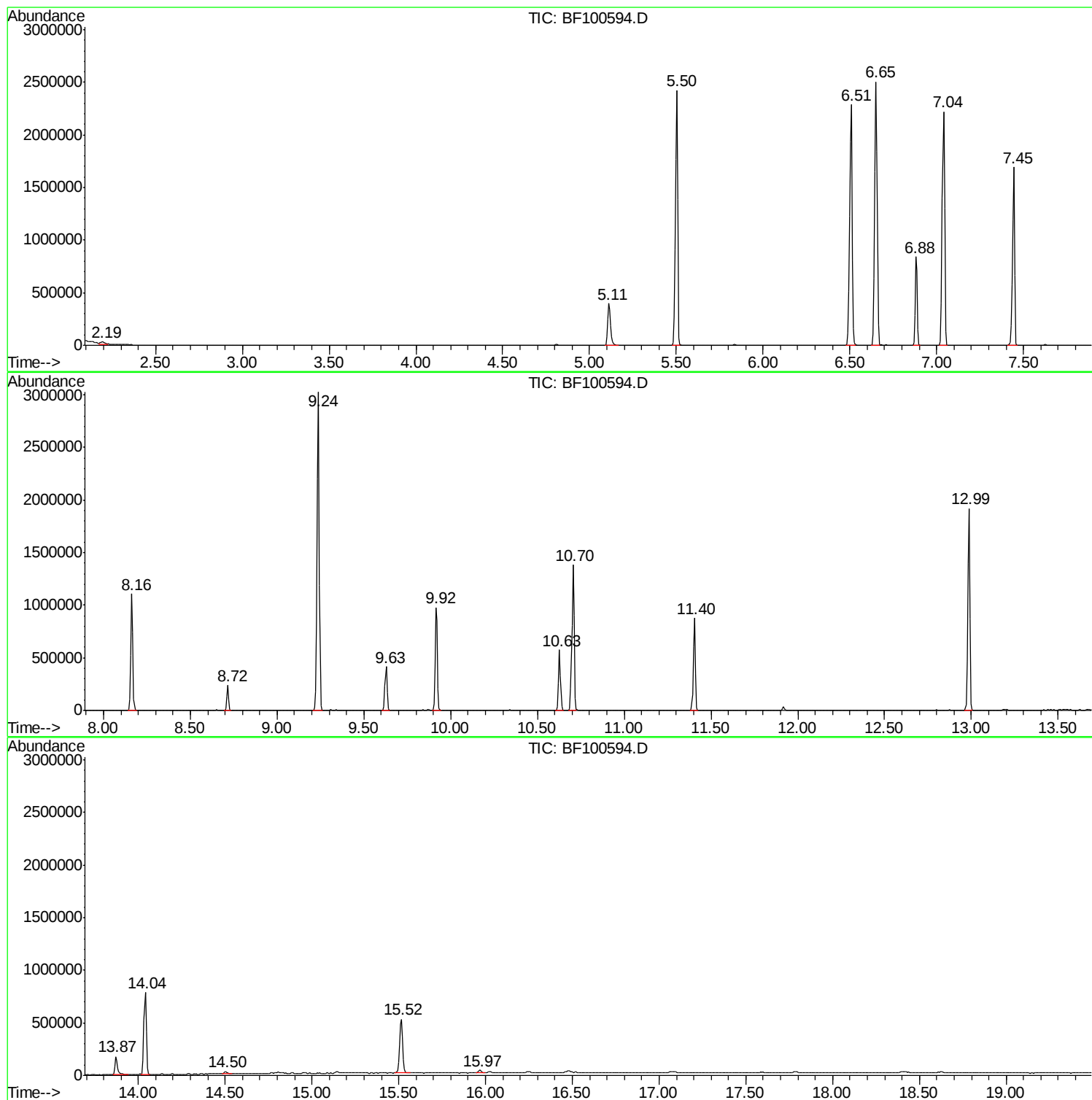
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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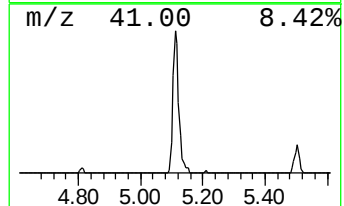
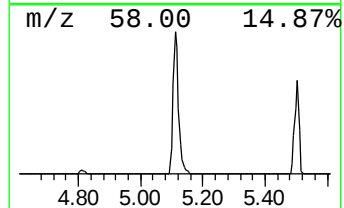
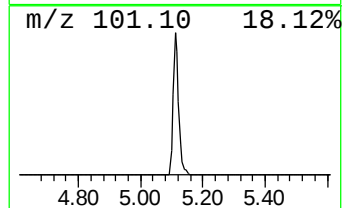
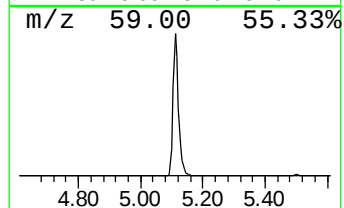
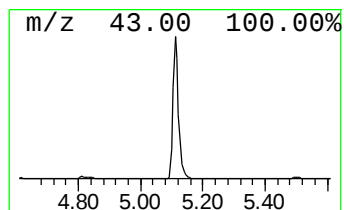
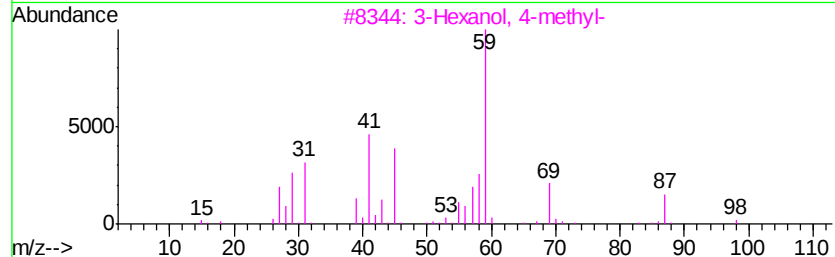
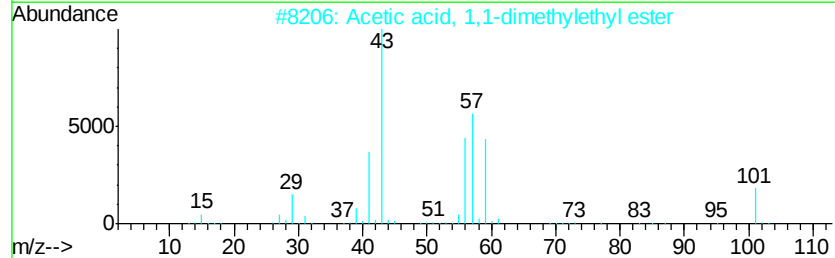
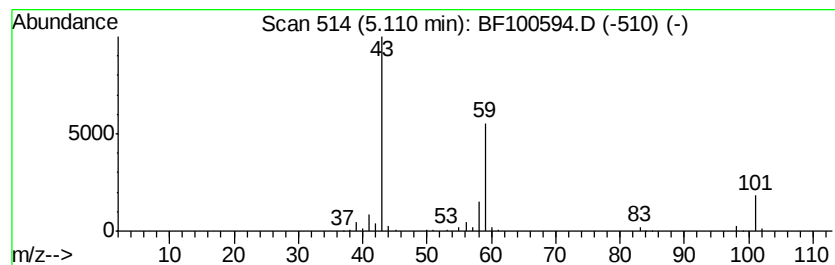
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Peak Number 1 2-Pentanone, 4-hydroxy-4-me... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.11	13.81 ng	491875	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			Acetic acid, 1,1-dimethylethyl e...	116	C6H12O2	000540-88-5	39
3			3-Hexanol, 4-methyl-	116	C7H16O	000615-29-2	33
4			3-Hexanol	102	C6H14O	000623-37-0	33
5			Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	33



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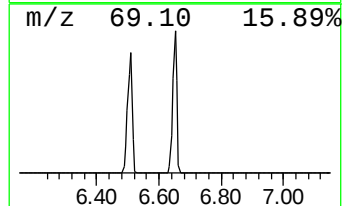
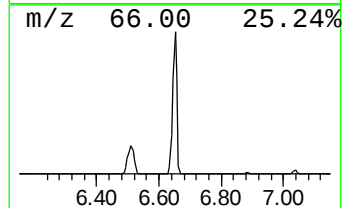
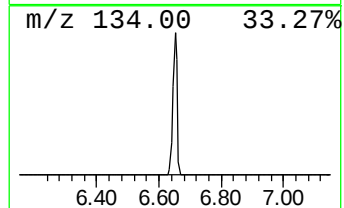
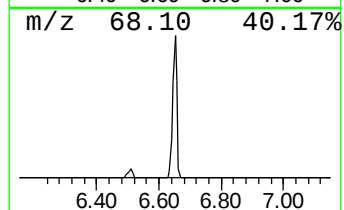
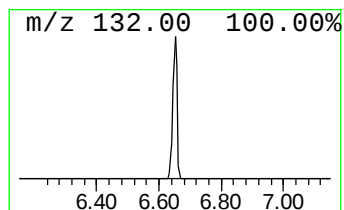
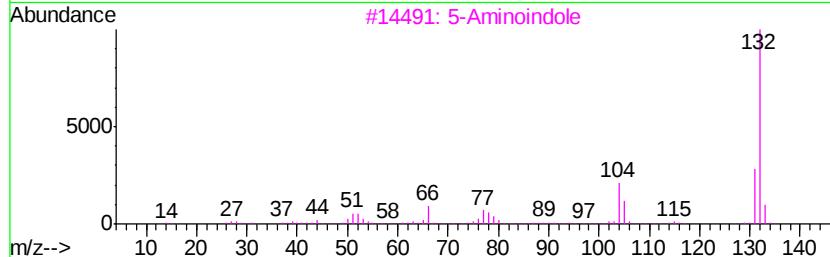
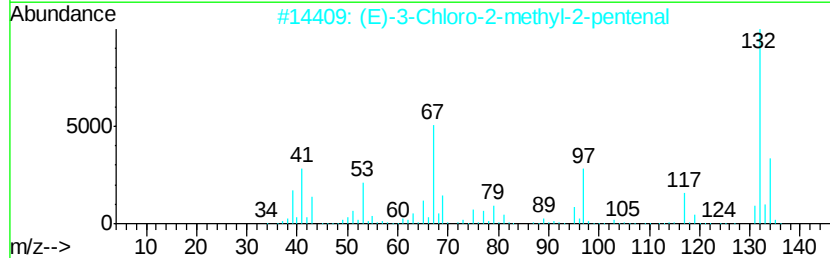
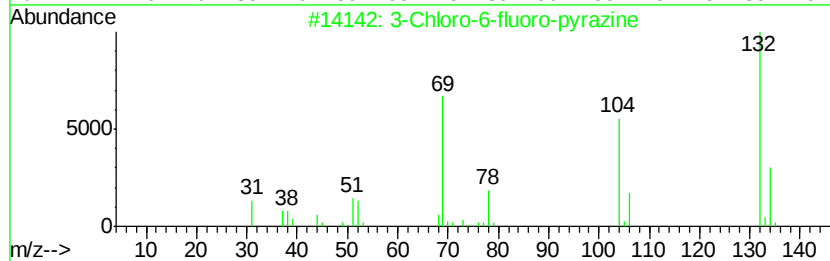
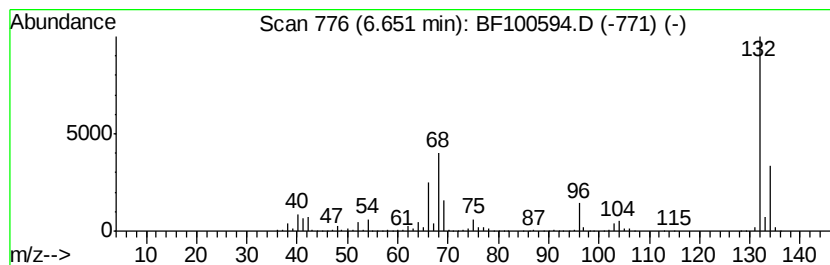
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TIC Library : C:\DATABASE\NIST11.L
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Peak Number 2 unknown6.65 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.65	68.93 ng	2454550	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	27
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	16
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	10
5		5-Fluoro-2-chloropyrimidine	132	C4H2ClFN2	062802-42-0	9



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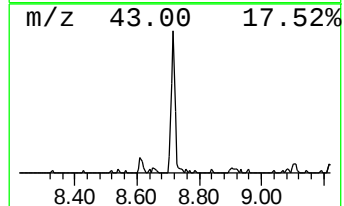
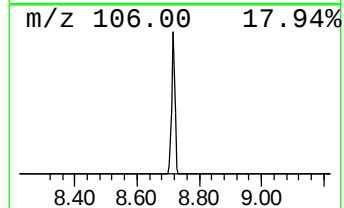
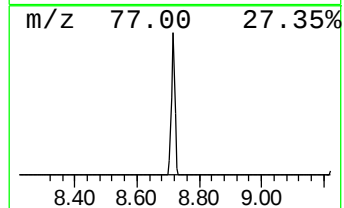
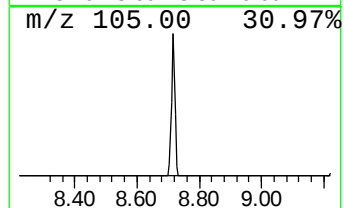
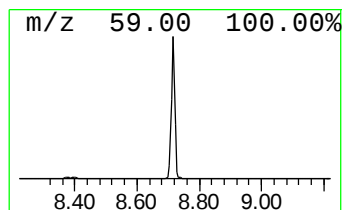
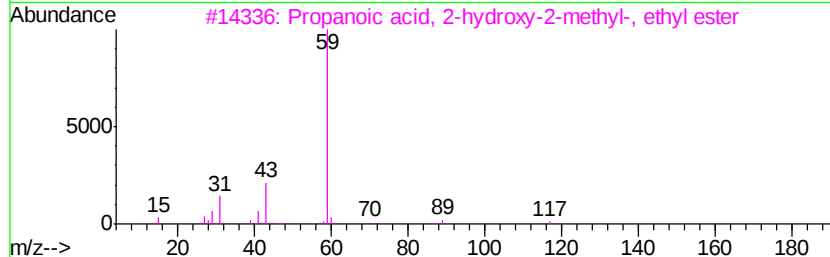
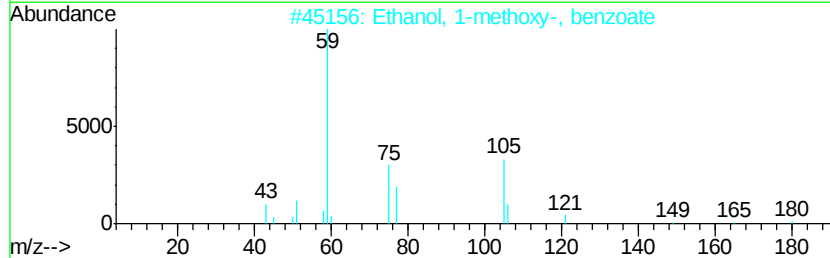
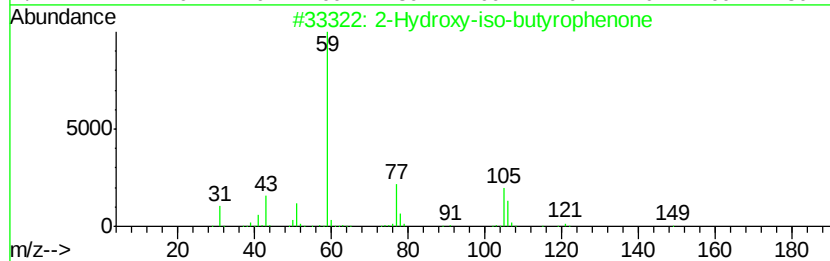
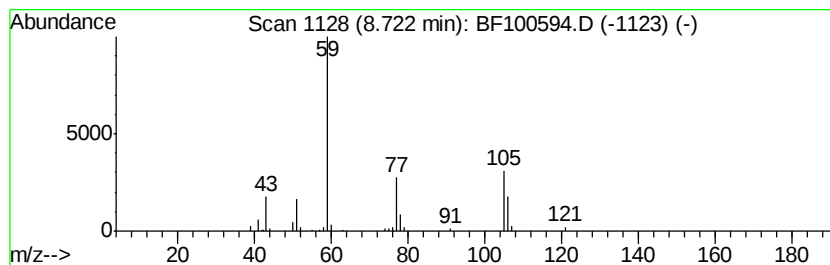
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.72	3.82 ng	175316	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		Propanoic acid, 2-hydroxy-2-meth...	132	C6H12O3	000080-55-7	9
4		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
5		Formamide, N-methyl-	59	C2H5NO	000123-39-7	7



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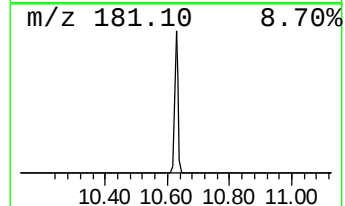
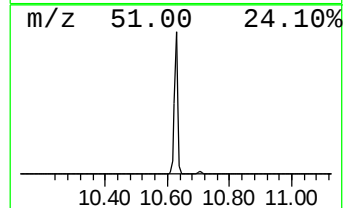
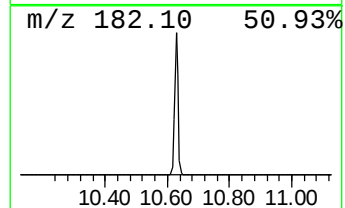
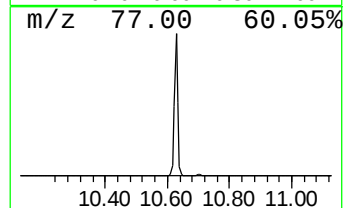
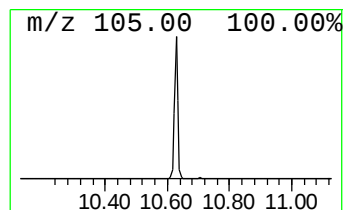
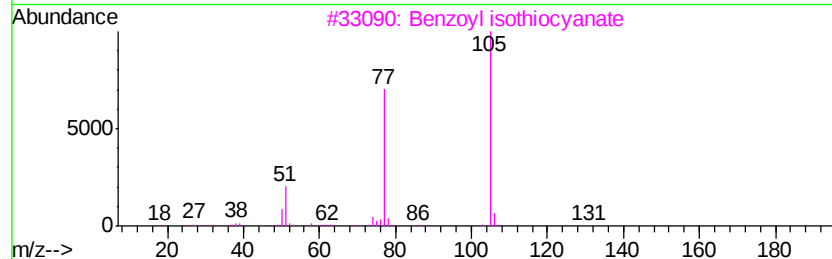
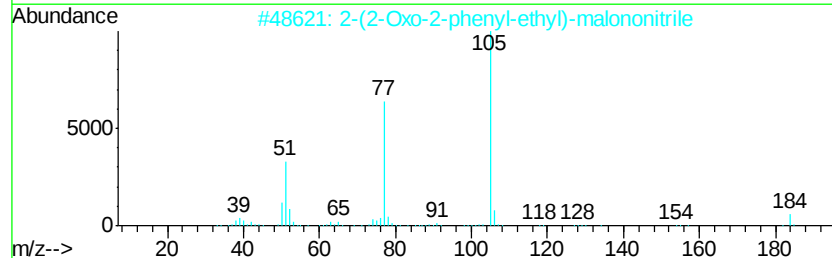
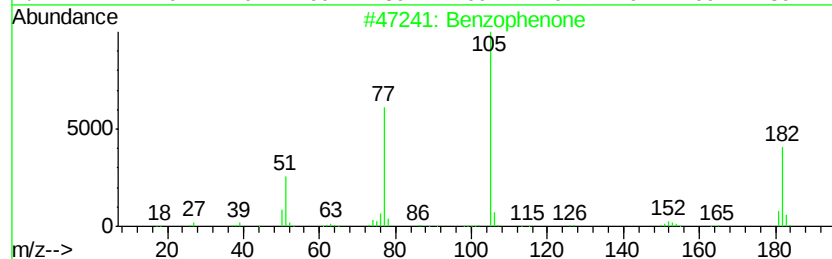
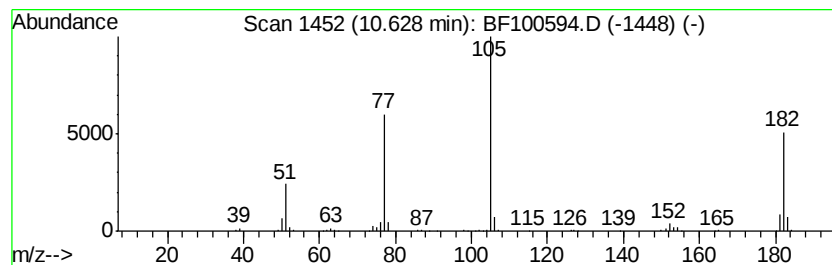
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Peak Number 5 Benzophenone Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.63	9.78 ng	437142	Acenaphthene-d10	9.92
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1		Benzophenone	182 C13H10O	000119-61-9 97
2		2-(2-Oxo-2-phenyl-ethyl)-malonon...	184 C11H8N2O	1000296-76-9 47
3		Benzoyl isothiocyanate	163 C8H5NOS	000532-55-8 47
4		1,2-Propanedione, 1-phenyl-	148 C9H8O2	000579-07-7 47
5		Benzenebutanoic acid, .gamma.-oxo-	178 C10H10O3	002051-95-8 47



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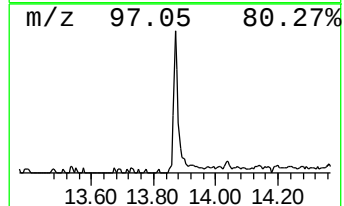
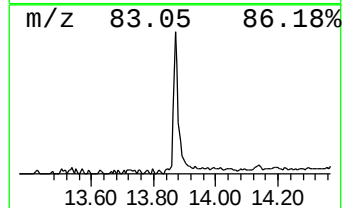
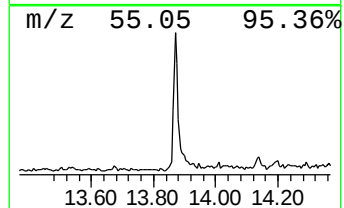
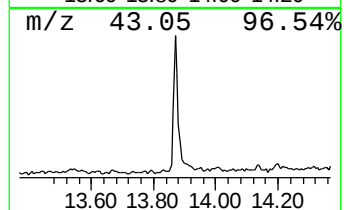
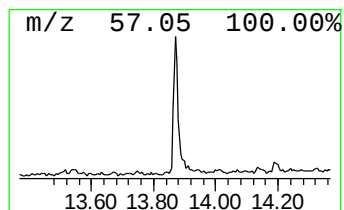
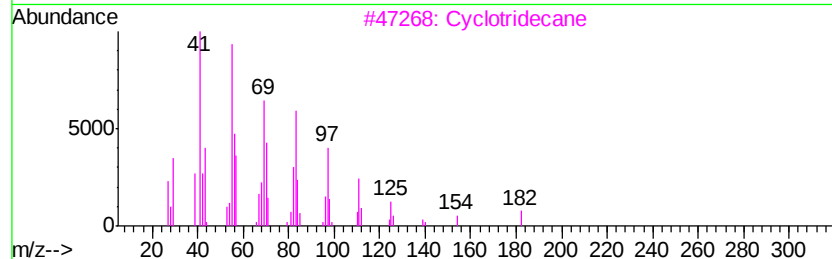
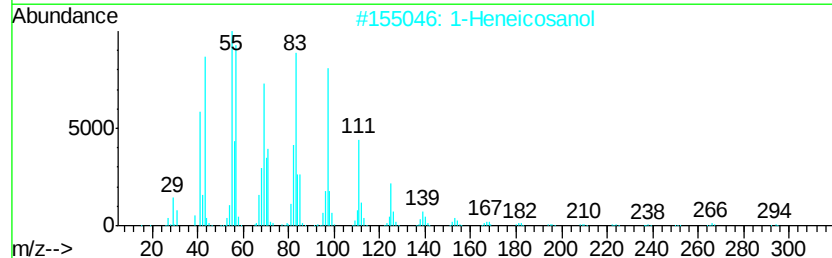
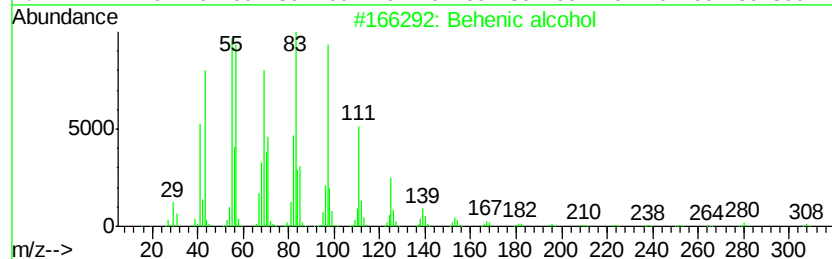
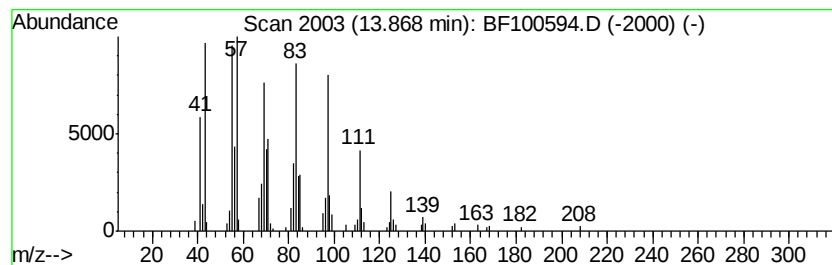
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Peak Number 6 Behenic alcohol Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.87	6.02 ng	199724	Chrysene-d12	14.04

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Behenic alcohol	326	C22H46O	000661-19-8	95
2		1-Heneicosanol	312	C21H44O	015594-90-8	95
3		Cyclotridecane	182	C13H26	000295-02-3	95
4		n-Tetracosanol-1	354	C24H50O	000506-51-4	94
5		Trifluoroacetoxy hexadecane	338	C18H33F3O2	006222-03-3	94



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
2-Pentanone, 4-hy...	5.11	13.8	ng	491875	1	6.88	712197	20.0
unknown6.65	6.65	68.9	ng	2454550	1	6.88	712197	20.0
2-Hydroxy-iso-but...	8.72	3.8	ng	175316	2	8.16	918594	20.0
Benzophenone	10.63	9.8	ng	437142	3	9.92	893732	20.0
Behenic alcohol	13.87	6.0	ng	199724	5	14.04	663728	20.0