

Data Path : \\74.0.250.170\SV0ASRV\HPCHEM1\BNA F\DATA\BF101517\
 Data File : BF099524.D
 Acq On : 15 Oct 2017 20:11
 Operator : SJ/JU
 Sample : I5821-02
 Misc :
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 BNA_F
 ClientSampleId :
 WPSB-5B-23.5-24-BGS

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-BF092317.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	5.069	504	507	520	rBV	263815	322495	16.85%	1.959%
2	5.469	571	575	596	rBV	2002846	1903675	99.46%	11.563%
3	6.481	743	747	760	rBV	1833626	1900367	99.28%	11.542%
4	6.616	766	770	773	rBV	2212659	1914097	100.00%	11.626%
5	6.845	806	809	816	rBB	592967	476532	24.90%	2.894%
6	6.998	831	835	839	rBV	1731452	1496352	78.18%	9.089%
7	7.410	900	905	908	rBV	1229841	1099518	57.44%	6.678%
8	8.127	1023	1027	1034	rBV	654456	582491	30.43%	3.538%
9	8.680	1118	1121	1129	rBV	136416	109649	5.73%	0.666%
10	9.198	1205	1209	1212	rBV	2212314	1851215	96.71%	11.244%
11	9.592	1273	1276	1285	rBV	327733	252722	13.20%	1.535%
12	9.880	1321	1325	1333	rVB	610906	509519	26.62%	3.095%
13	10.592	1443	1446	1450	rBV	479902	355640	18.58%	2.160%
14	10.669	1456	1459	1470	rBV	821205	791099	41.33%	4.805%
15	11.368	1575	1578	1586	rVB	517882	422848	22.09%	2.568%
16	12.951	1843	1847	1850	rBV	1641236	1409372	73.63%	8.560%
17	13.833	1994	1997	2005	rBV	54931	74917	3.91%	0.455%
18	14.015	2024	2028	2035	rVB	524898	521536	27.25%	3.168%
19	15.486	2273	2278	2284	rBV	388905	470107	24.56%	2.855%

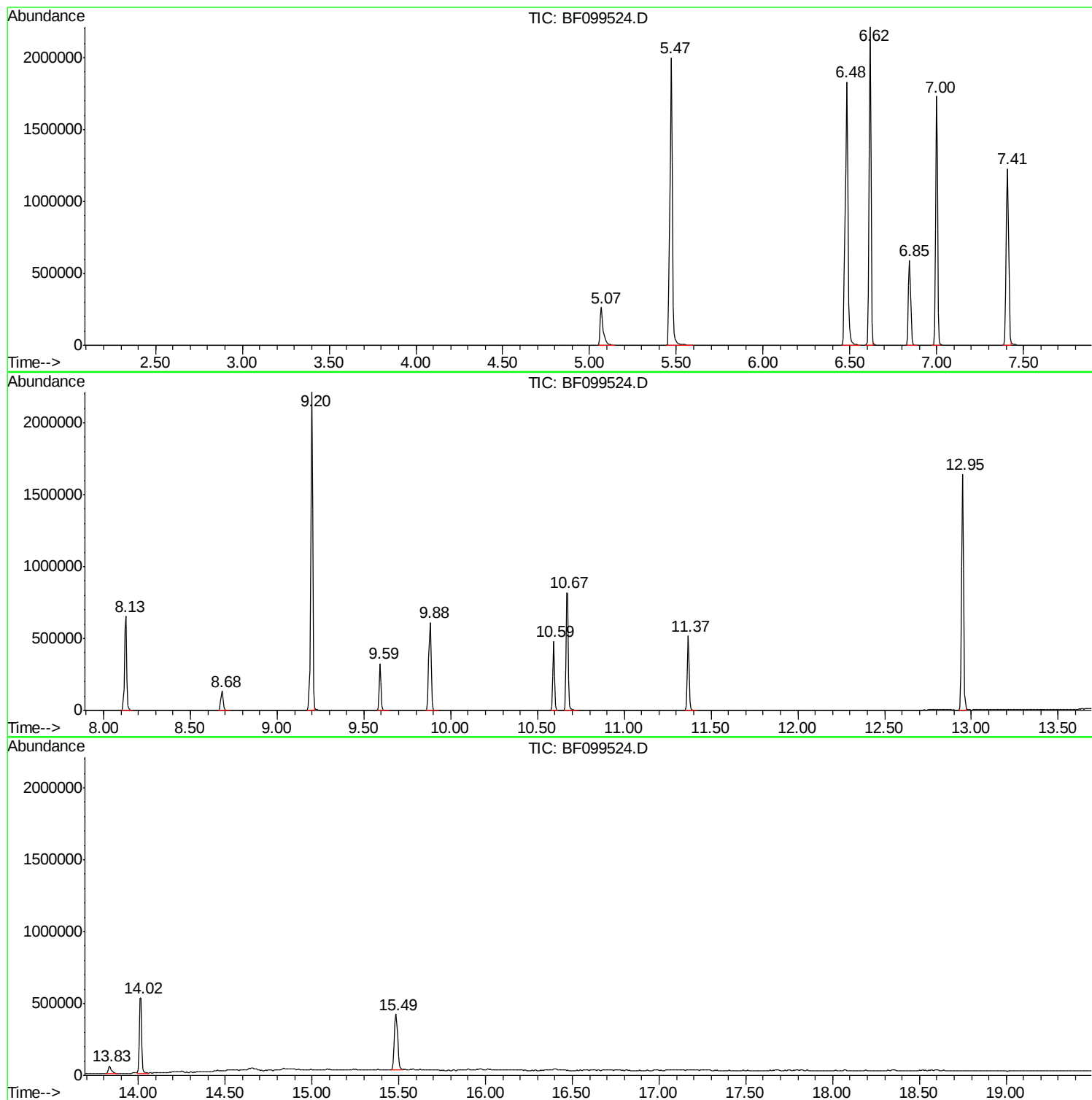
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Quant Method : Z:\HPCHEM1\BNA_F\METHODS\8270-BF092317.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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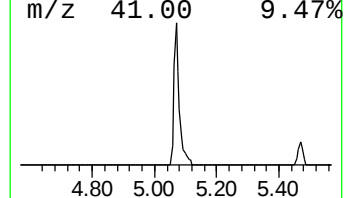
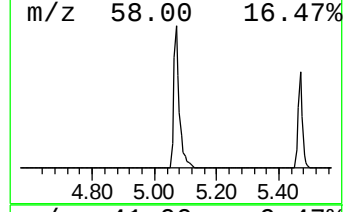
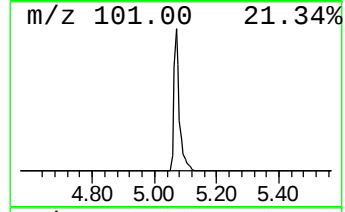
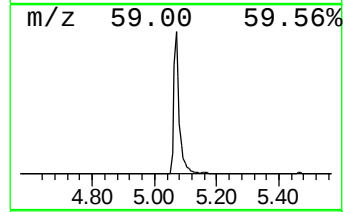
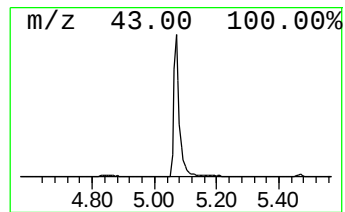
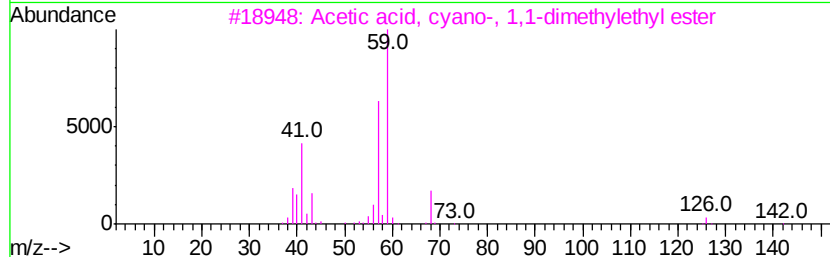
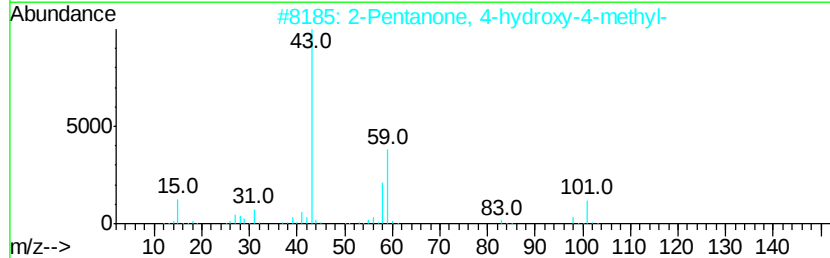
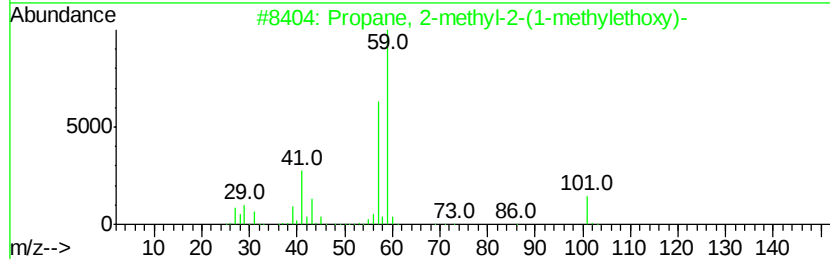
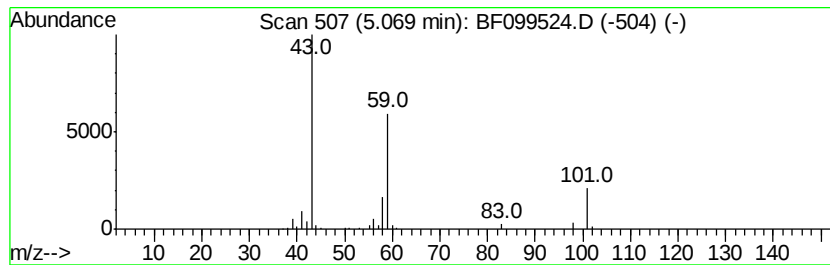
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Propane, 2-methyl-2-(1-meth... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.07	13.54 ng	322495	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Propane, 2-methyl-2-(1-methyleth...	116	C7H16O	017348-59-3	53
2		2-Pentanone, 4-hydroxy-4-methyl-	116	C6H12O2	000123-42-2	53
3		Acetic acid, cyano-, 1,1-dimethy...	141	C7H11NO2	001116-98-9	25
4		5-Hexen-2-one	98	C6H10O	000109-49-9	9
5		Morpholine, 4-methyl-	101	C5H11NO	000109-02-4	9



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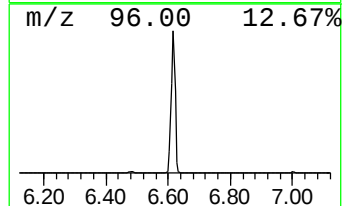
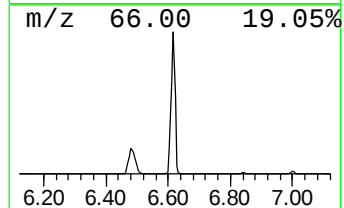
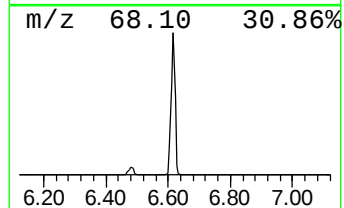
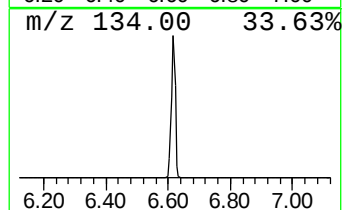
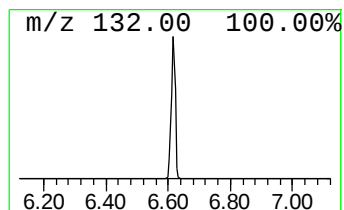
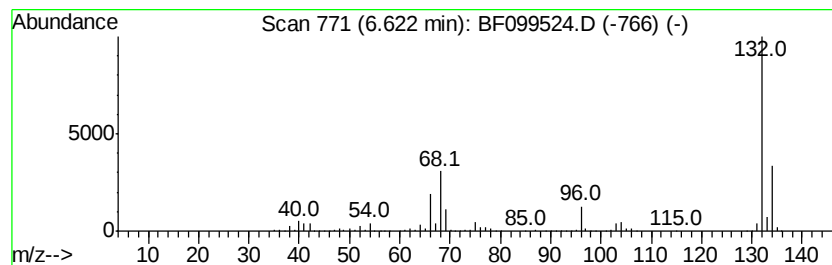
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 unknown6.62 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.62	80.33 ng	1914100	1,4-Dichlorobenzene-d4	6.85

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	3-Chloro-6-fluoro-pyrazine	132	C4H2ClFN2	1000146-10-7	38
2		(E)-3-Chloro-2-methyl-2-pentenal	132	C6H9ClO	031357-76-3	25
3		5-Aminoindole	132	C8H8N2	005192-03-0	12
4		Tranylcypromine-propionyl	189	C12H15NO	1000123-86-3	12
5		4-Chloro-6-fluoro-pyrimidine	132	C4H2ClFN2	051422-01-6	9



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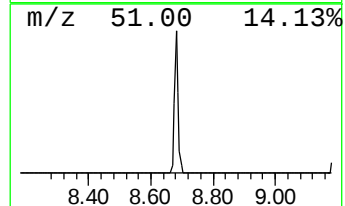
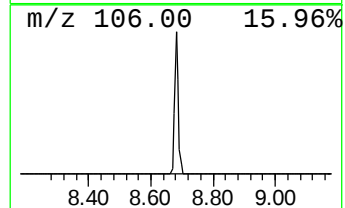
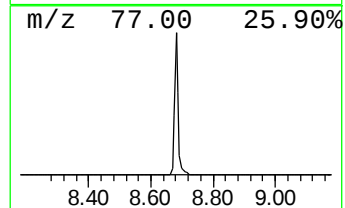
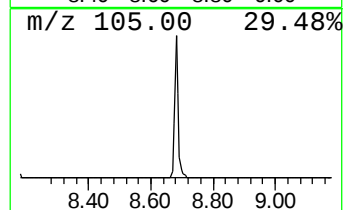
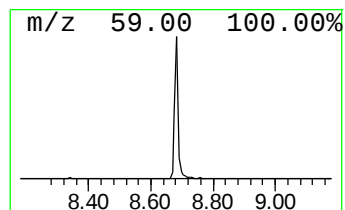
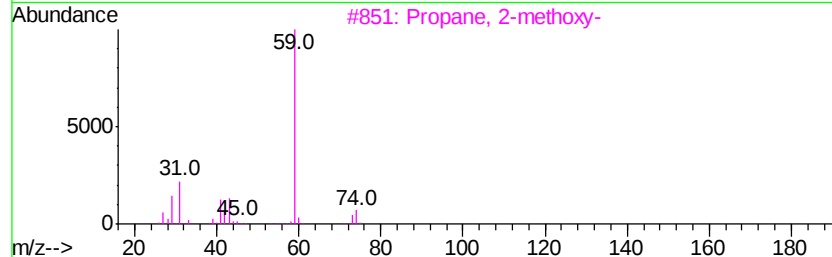
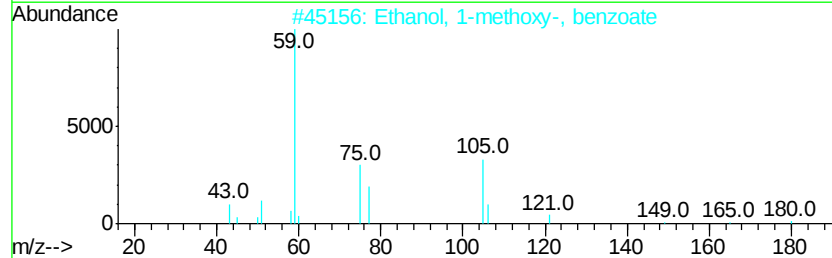
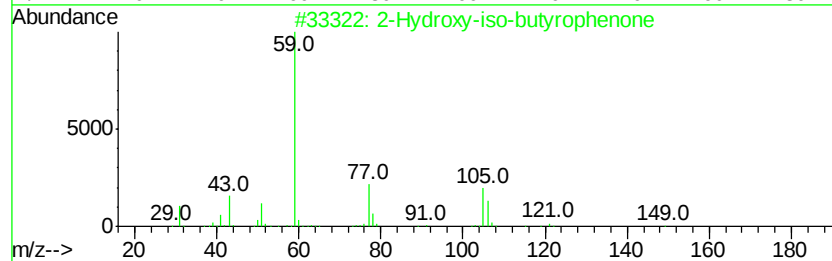
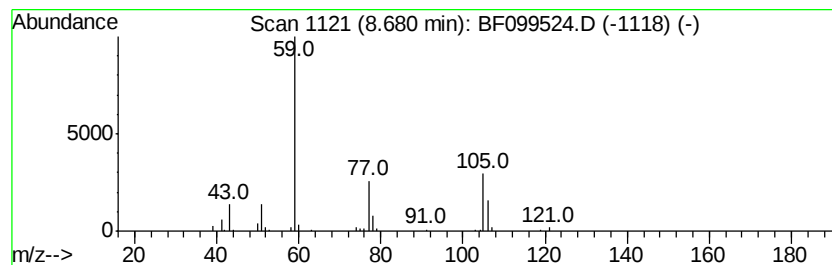
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Peak Number 4 2-Hydroxy-iso-butyrophenone Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.68	3.76 ng	109649	Napthalene-d8	8.13

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Hydroxy-iso-butyrophenone	164	C10H12O2	007473-98-5	86
2		Ethanol, 1-methoxy-, benzoate	180	C10H12O3	051835-44-0	56
3		Propane, 2-methoxy-	74	C4H10O	000598-53-8	9
4		Propionic acid, 2-isopropoxy-, m...	146	C7H14O3	1000151-15-1	9
5		Guanidine	59	CH5N3	000113-00-8	7



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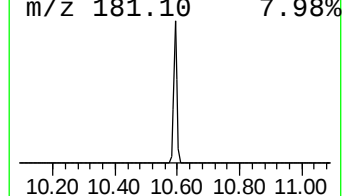
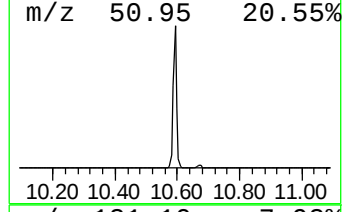
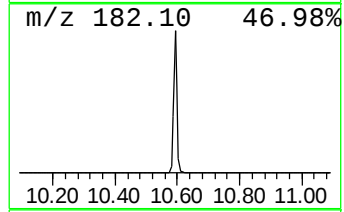
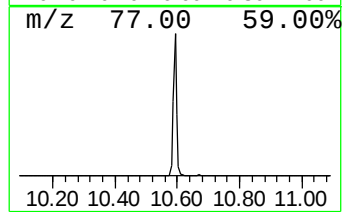
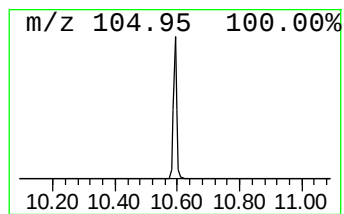
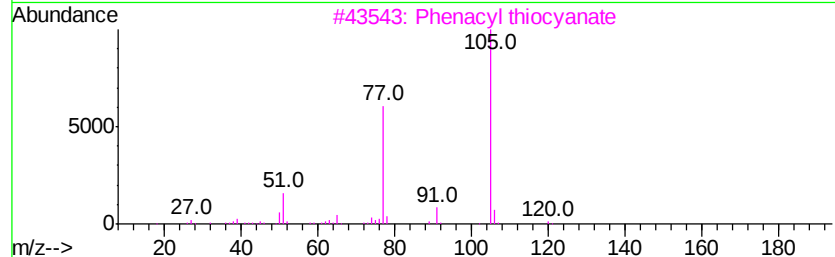
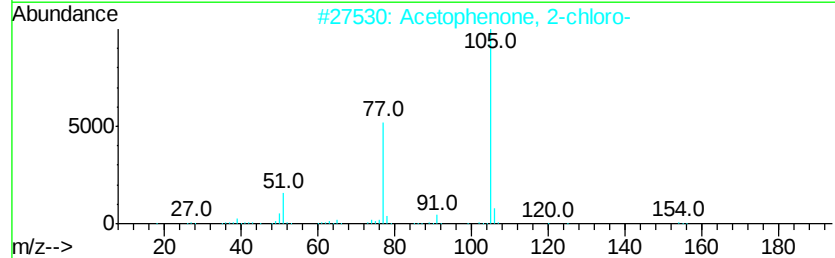
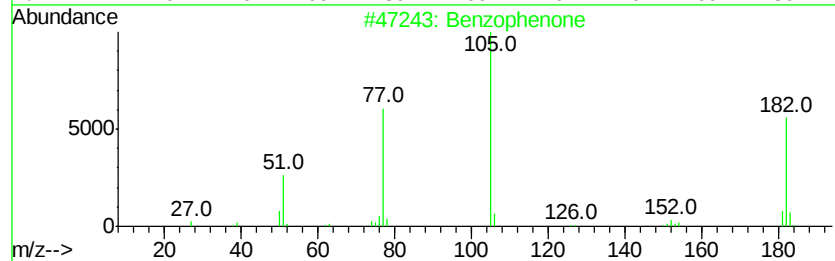
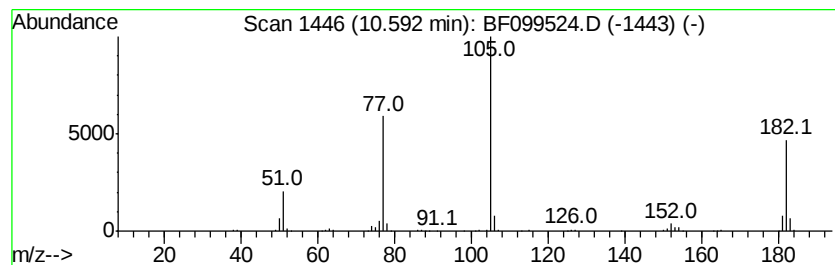
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Peak Number 5 Benzophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.59	13.96 ng	355640	Acenaphthene-d10	9.88

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzophenone	182	C13H10O	000119-61-9	96
2		Acetophenone, 2-chloro-	154	C8H7ClO	000532-27-4	49
3		Phenacyl thiocyanate	177	C9H7NOS	005399-30-4	47
4		.alpha.,.alpha.-Dichloroacetophe...	188	C8H6Cl2O	002648-61-5	47
5		S-Benzoyl(thiohydroxylamine)	153	C7H7NOS	025740-80-1	47



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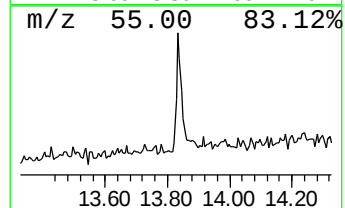
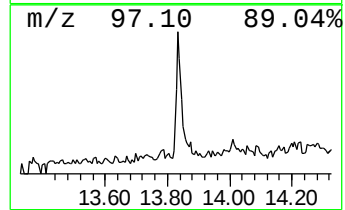
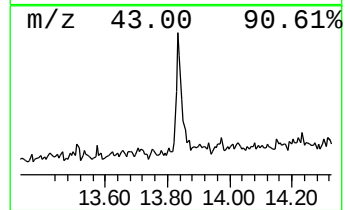
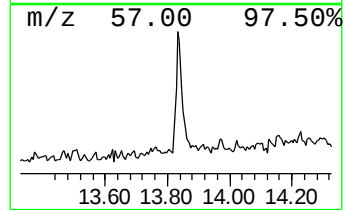
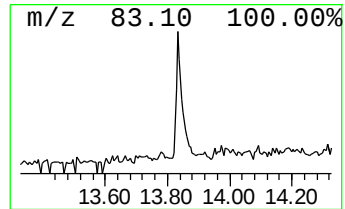
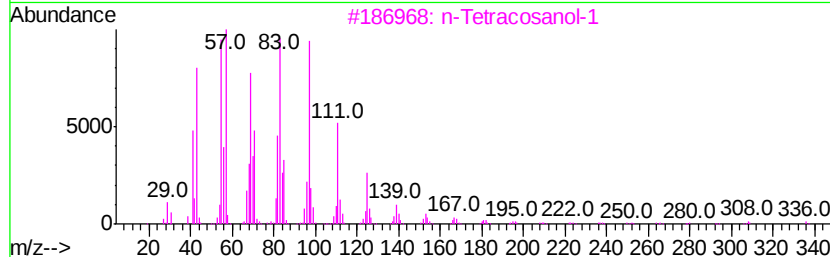
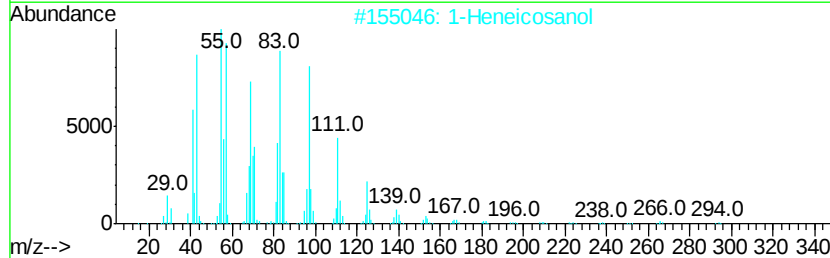
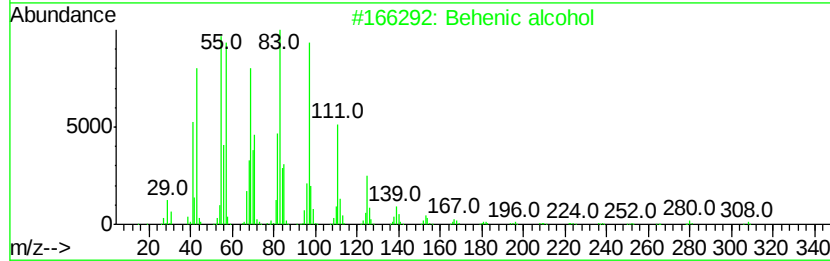
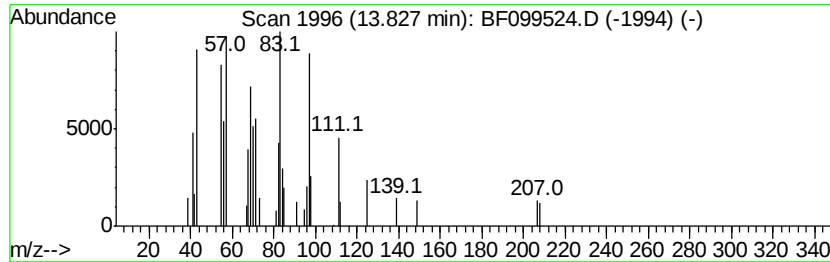
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Peak Number 6 Behenic alcohol Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
13.83	2.87 ng	74917	Chrysene-d12	14.02	
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	n-Tetracosanol-1	354	C24H50O	000506-51-4	95
4	Carbonic acid, octadecyl 2,2,2-t...	444	C21H39Cl3O3	1000314-56-3	93
5	n-Heptadecanol-1	256	C17H36O	001454-85-9	90



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propane, 2-methyl...	5.07	13.5	ng	322495	1	6.85	476532	20.0
unknown6.62	6.62	80.3	ng	1914100	1	6.85	476532	20.0
2-Hydroxy-iso-but...	8.68	3.8	ng	109649	2	8.13	582491	20.0
Benzophenone	10.59	14.0	ng	355640	3	9.88	509519	20.0
Behenic alcohol	13.83	2.9	ng	74917	5	14.02	521536	20.0