

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX041323\
Data File : VX035047.D
Acq On : 12 Apr 2023 15:37
Operator : JC/MD
Sample : 02319-01
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E9074-PVSC-002

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:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M

Title : SW846 8260

Signal : TIC: VX035047.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	10.195	1483	1494	1500	rBV	2911852	3709131	2.39%	1.170%
2	10.988	1614	1624	1626	rBV3	64260754	155292349	100.00%	48.979%
3	11.659	1725	1734	1738	rBV2	71296172	142553331	91.80%	44.961%
4	11.726	1740	1745	1749	rBV	1803572	2225262	1.43%	0.702%
5	11.890	1761	1772	1780	rBV	3088602	4492451	2.89%	1.417%
6	11.982	1780	1787	1790	rVV2	1005469	1577491	1.02%	0.498%
7	12.799	1916	1921	1930	rBV	2812509	3631199	2.34%	1.145%
8	15.737	2397	2403	2412	rBV	1149194	1732530	1.12%	0.546%
9	15.835	2413	2419	2426	rVV	1166134	1844587	1.19%	0.582%

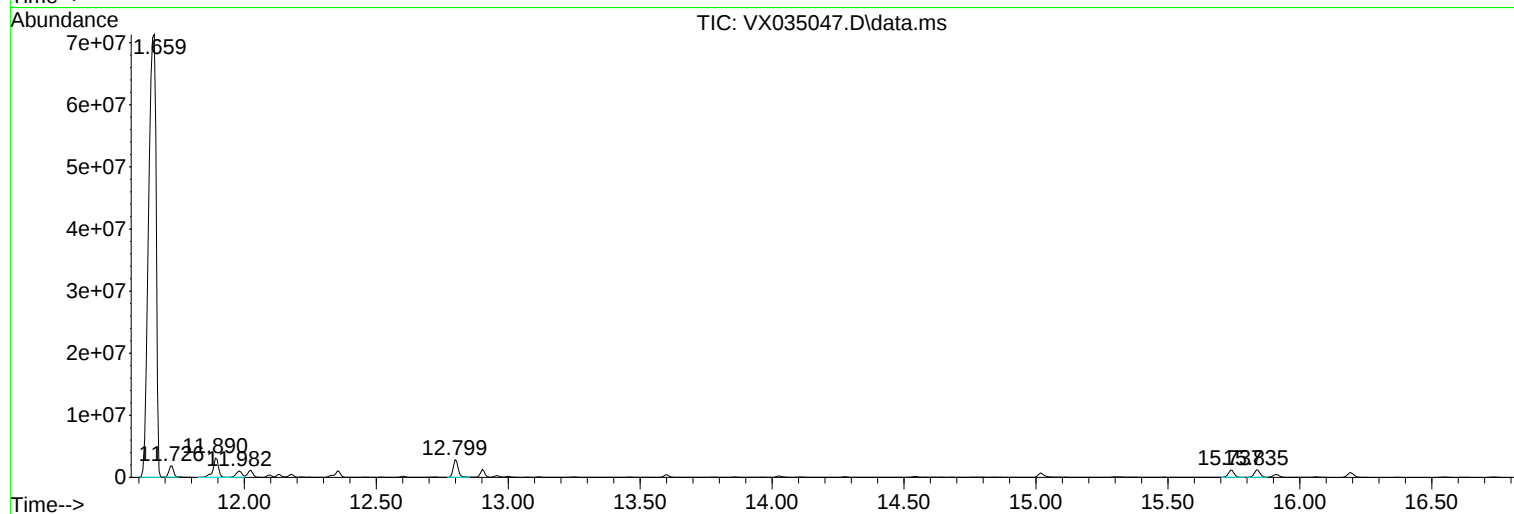
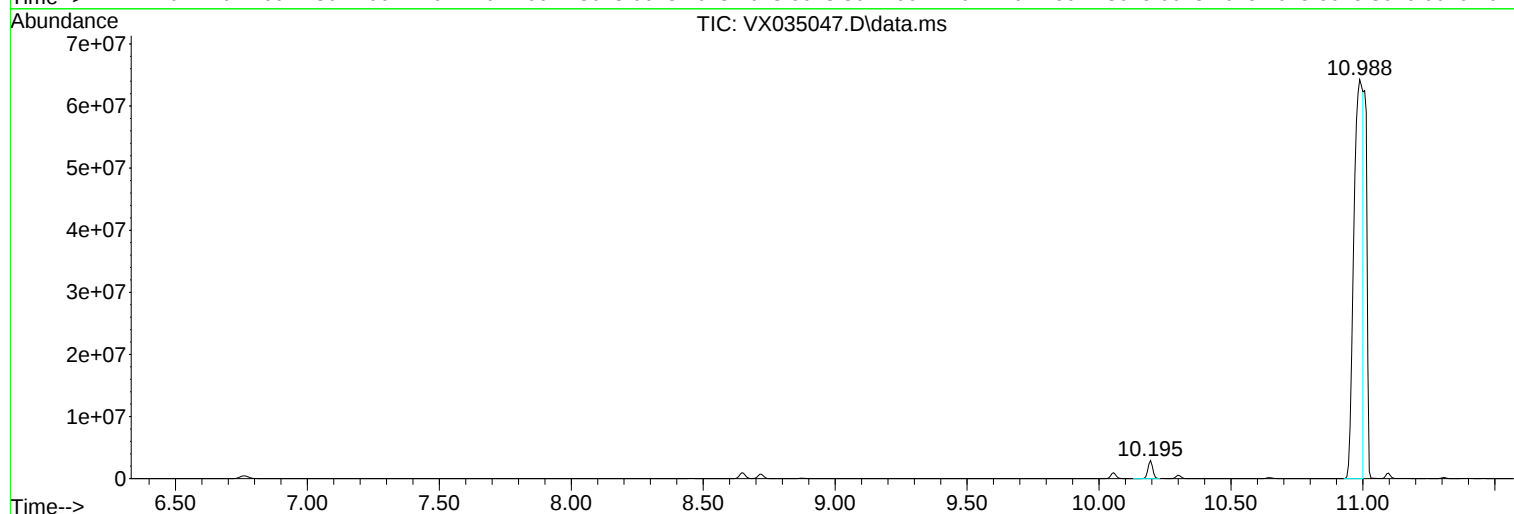
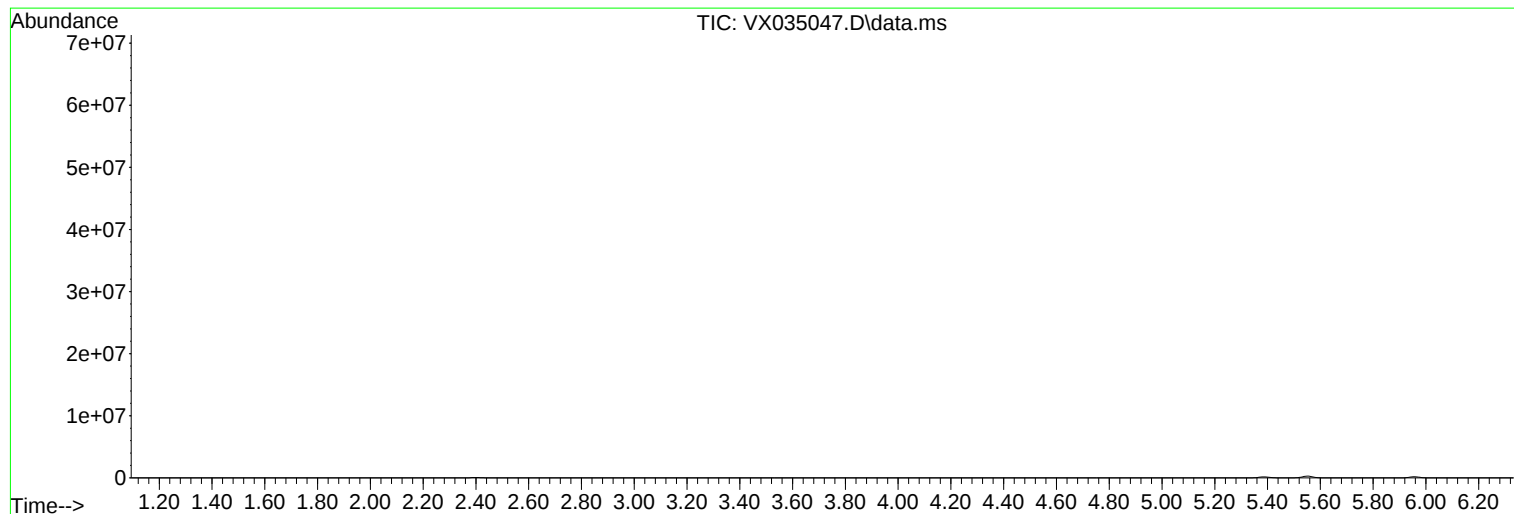
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TIC Library : C:\Database\NIST20.L
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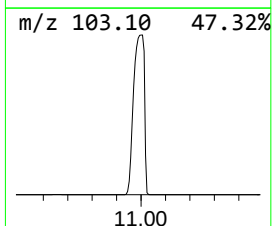
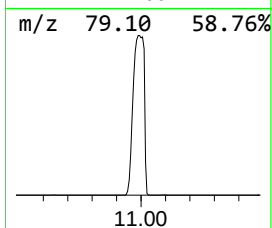
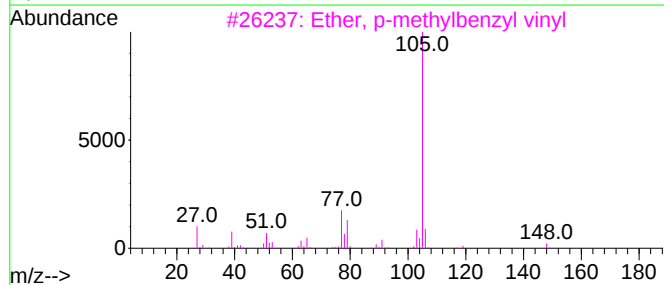
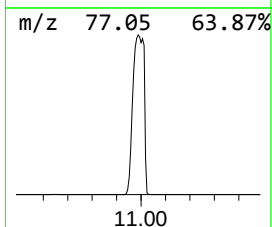
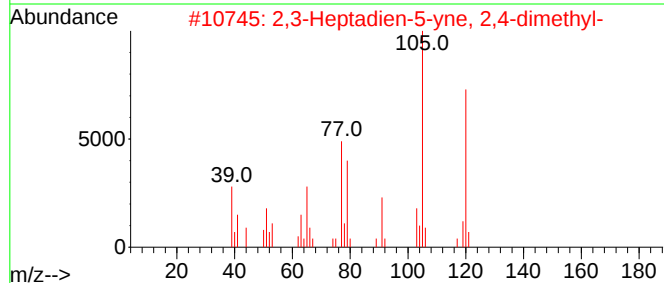
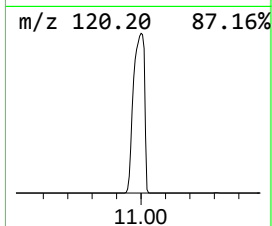
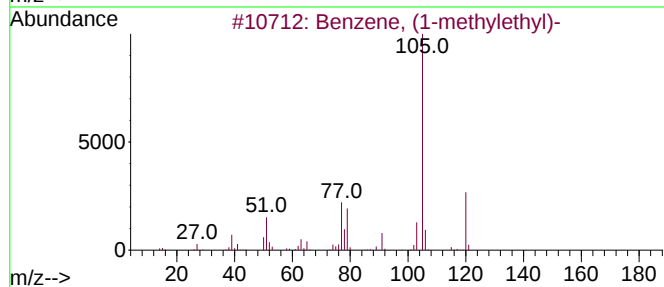
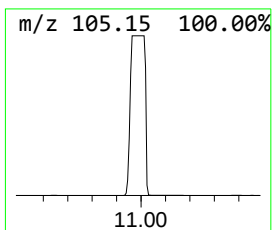
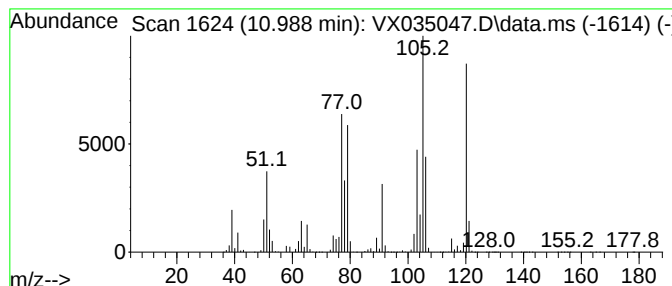
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Benzene, (1-methylethyl)- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.988	2093.38 ug/l	155292000	Chlorobenzene-d5	10.055

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, (1-methylethyl)-	120	C9H12	000098-82-8	81
2			2,3-Heptadien-5-yne, 2,4-dimethyl-	120	C9H12	041898-89-9	52
3			Ether, p-methylbenzyl vinyl	148	C10H12O	026437-10-5	47
4			Benzene, (1-nitroethyl)-	151	C8H9NO2	007214-61-1	43
5			Benzene, (1-bromoethyl)-	184	C8H9Br	000585-71-7	38



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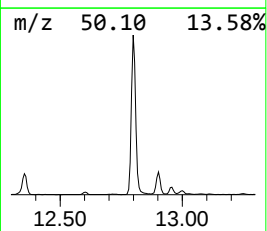
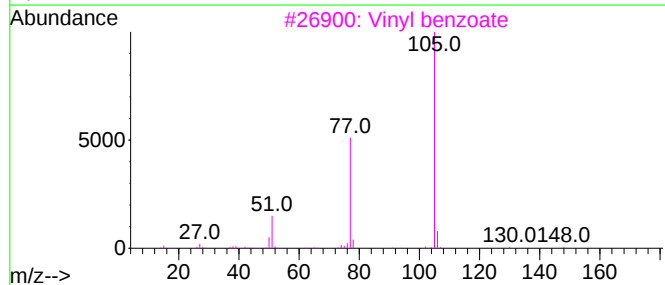
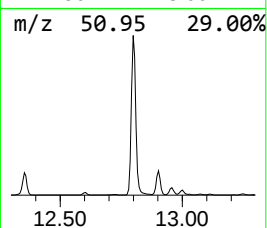
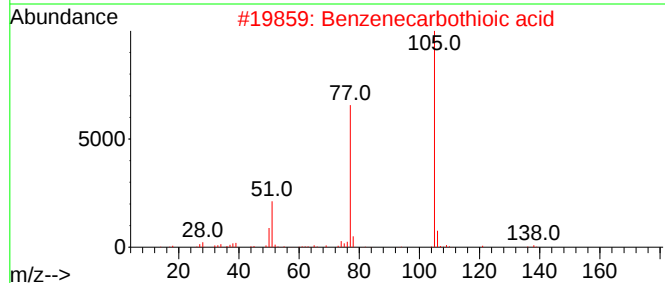
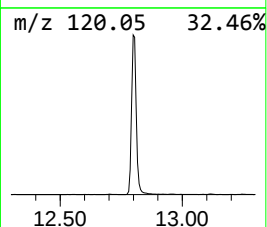
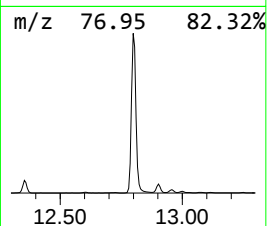
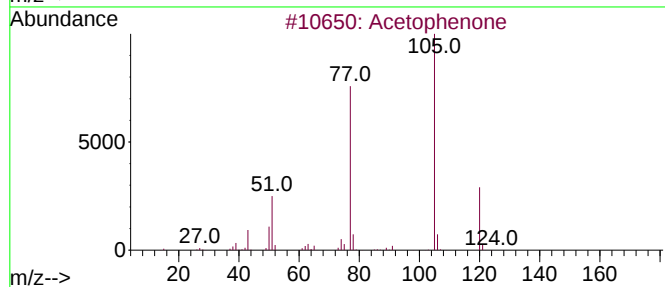
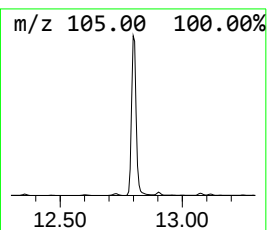
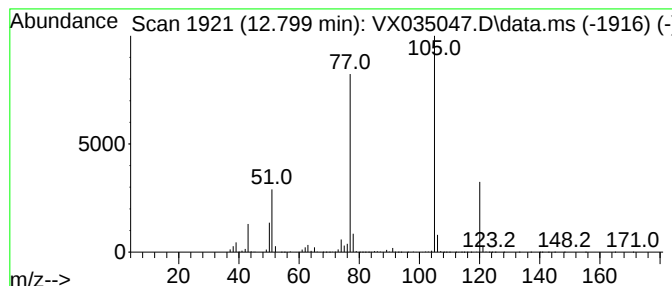
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Peak Number 3 Acetophenone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.799	115.09 ug/l	3631200	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetophenone	120	C8H8O	000098-86-2	97
2			Benzenecarbothioic acid	138	C7H6OS	000098-91-9	80
3			Vinyl benzoate	148	C9H8O2	000769-78-8	80
4			6-Benzoylhexanoic acid	220	C13H16O3	007472-43-7	72
5			Pentafluoroethyl phenyl ketone	224	C9H5F5O	000394-52-5	72



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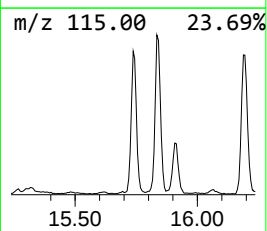
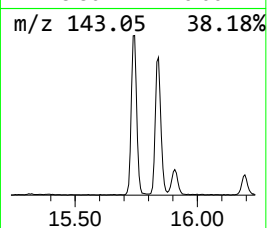
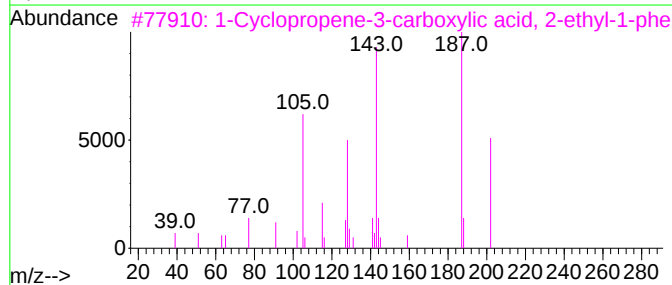
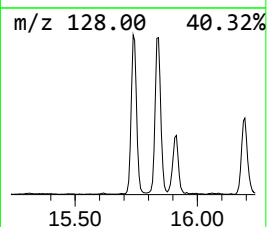
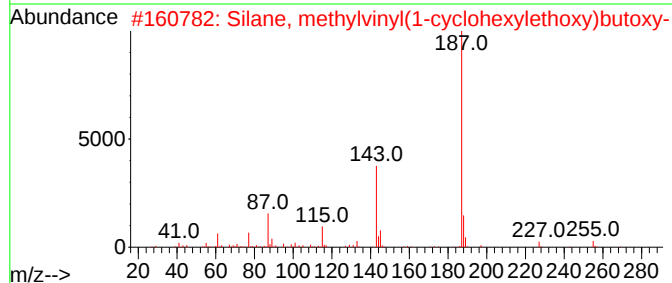
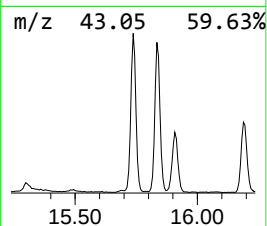
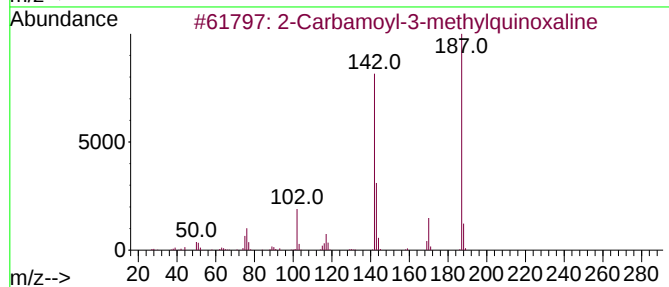
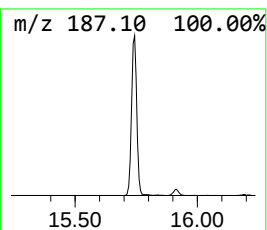
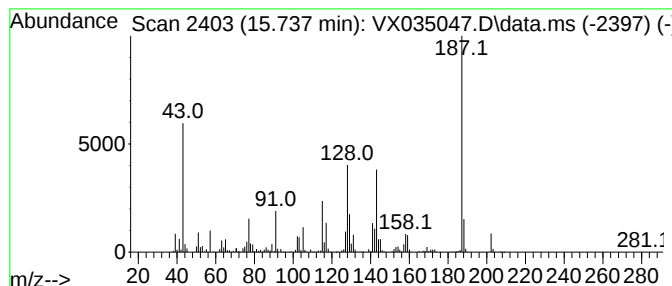
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Peak Number 4 unknown15.737 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.737	54.91 ug/l	1732530	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Carbamoyl-3-methylquinoxaline	187	C10H9N3O	017357-92-5	43
2			Silane, methylvinyl(1-cyclohexyl...)	270	C15H30O2Si	1000421-14-3	38
3			1-Cyclopropene-3-carboxylic acid...	202	C13H14O2	107939-18-4	37
4			1-Indanone, 3,3,5,6,7-pentamethyl-	202	C14H18O	016204-69-6	37
5			(5R,6S)-1-Methyl-6-phenyl-5-(phe...	329	C18H19NO3S	1000482-58-6	35



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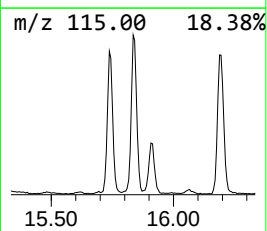
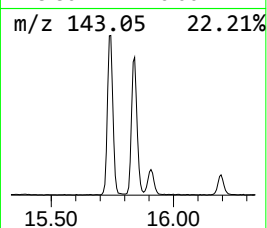
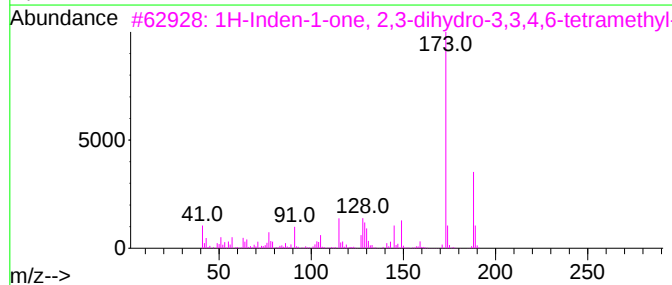
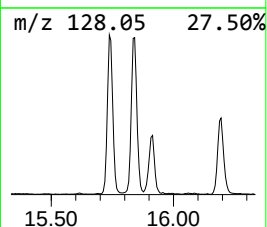
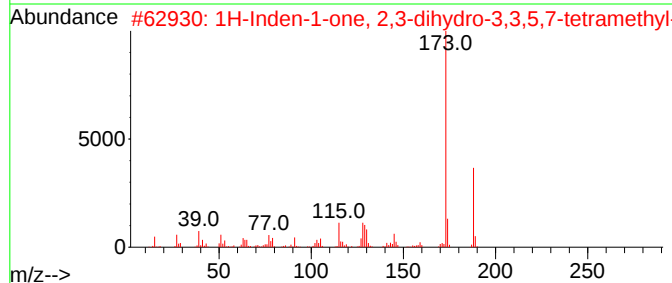
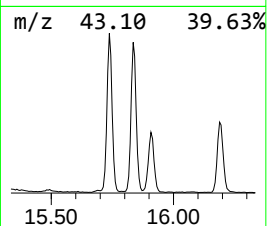
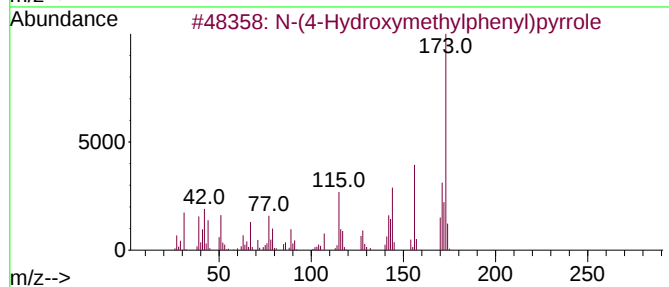
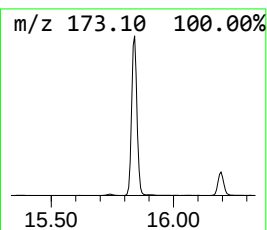
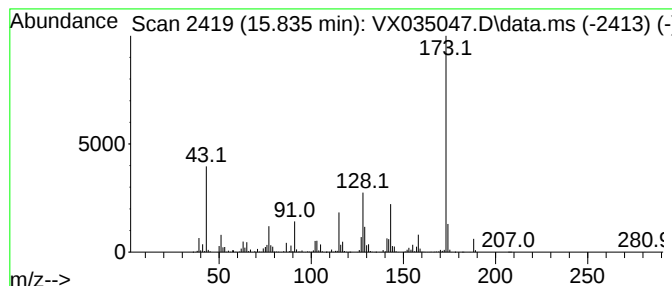
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Peak Number 5 N-(4-Hydroxymethylphenyl)py... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.835	58.47 ug/l	1844590	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			N-(4-Hydroxymethylphenyl)pyrrole	173	C11H11NO	143426-51-1	52
2			1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	054789-23-0	50
3			1H-Inden-1-one, 2,3-dihydro-3,3,...	188	C13H16O	055255-42-0	50
4			5,8-Dimethyl-4-quinolinol	173	C11H11NO	203626-57-7	50
5			2(1H)-Quinolinone, 4,8-dimethyl-	173	C11H11NO	005349-78-0	49



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Benzene, (1-met...	10.988	2093.4	ug/l	155292000	3	10.055	3709130	50.0
Acetophenone	12.799	115.1	ug/l	3631200	4	12.024	1577490	50.0
unknown15.737	15.737	54.9	ug/l	1732530	4	12.024	1577490	50.0
N-(4-Hydroxymet...	15.835	58.5	ug/l	1844590	4	12.024	1577490	50.0