

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
 Data File : VU044867.D
 Acq On : 26 Sep 2021 03:54
 Operator : SY/MD
 Sample : M3888-03
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 20894

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_U\Method\82U092421W.M

Title : SW846 8260

Signal : TIC: VU044867.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.633	85	91	136	rBV2	39695754	147861291	100.00%	60.800%
2	2.337	282	310	365	rBV	6350778	22149190	14.98%	9.108%
3	5.587	1303	1321	1344	rBV	869246	1875346	1.27%	0.771%
4	5.777	1365	1380	1412	rVB	6032454	12181659	8.24%	5.009%
5	7.973	2050	2063	2091	rVB	10206898	17042503	11.53%	7.008%
6	8.796	2308	2319	2342	rVB	1754873	3038267	2.05%	1.249%
7	9.468	2520	2528	2546	rVV	1117520	1924466	1.30%	0.791%
8	9.693	2579	2598	2622	rBV2	6449568	11003944	7.44%	4.525%
9	10.105	2714	2726	2741	rVB2	3755428	6292212	4.26%	2.587%
10	12.314	3401	3413	3427	rVB	2140275	3418843	2.31%	1.406%
11	14.092	3952	3966	3982	rBV	9087345	14722176	9.96%	6.054%
12	15.224	4307	4318	4334	rBV	1051755	1684904	1.14%	0.693%

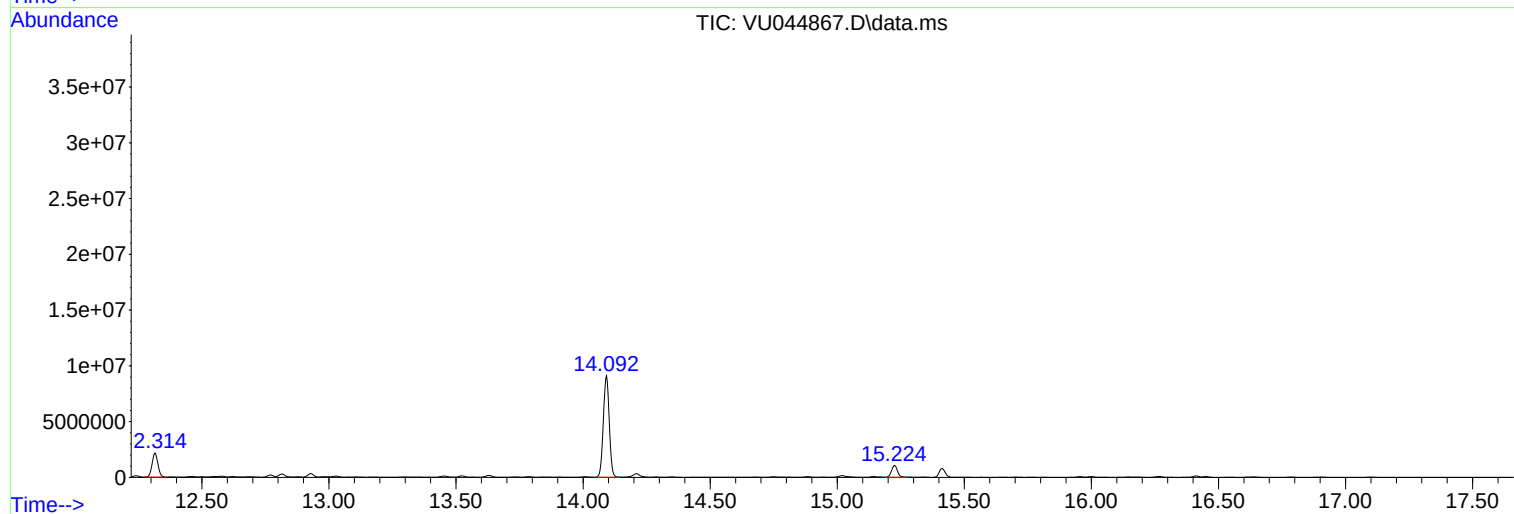
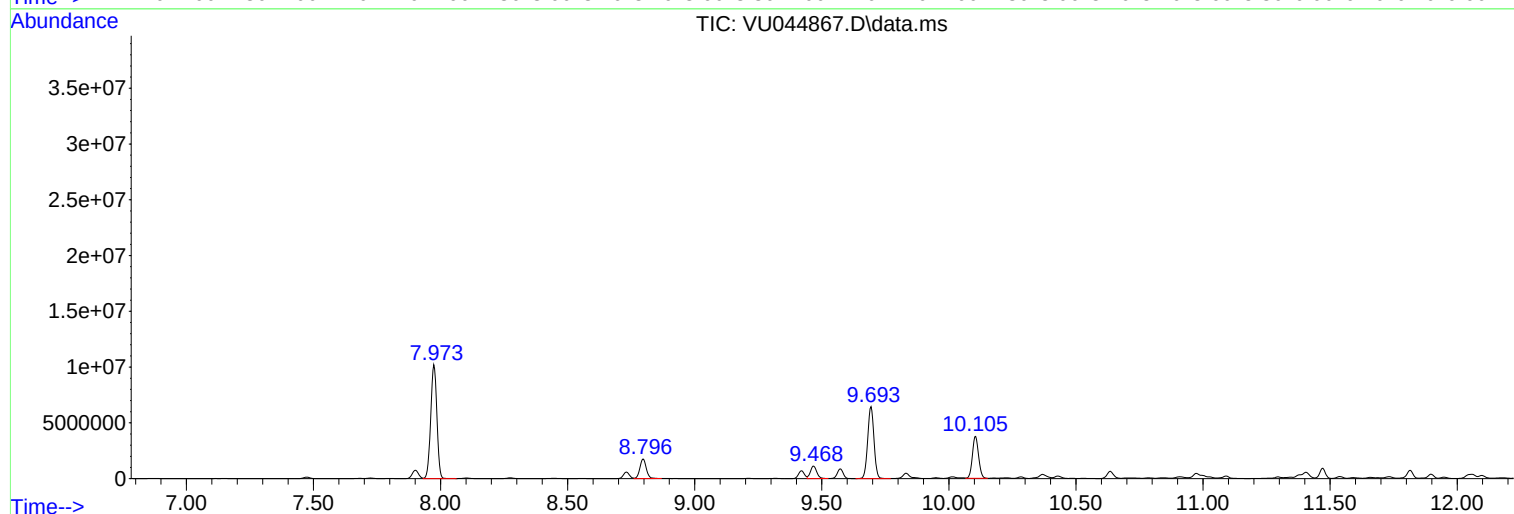
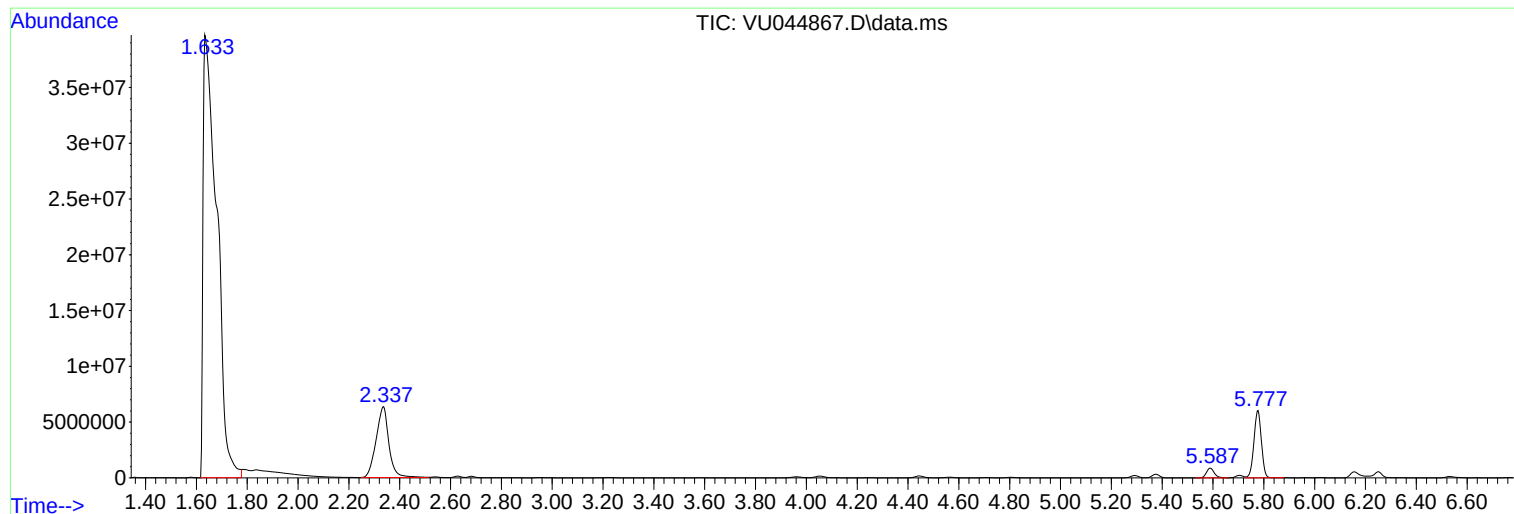
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Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092521\
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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



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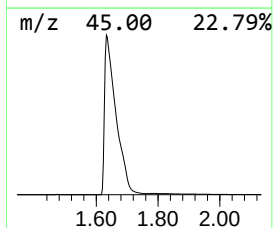
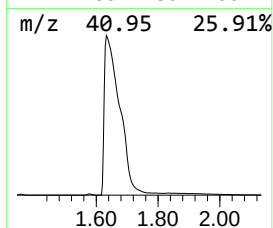
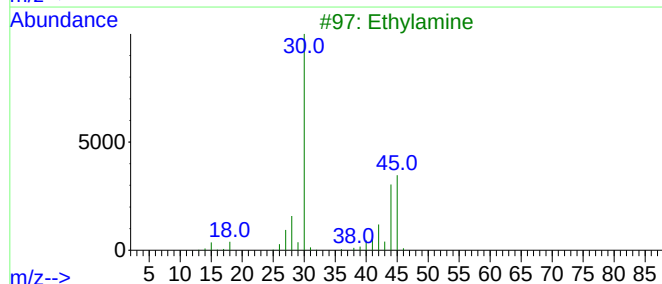
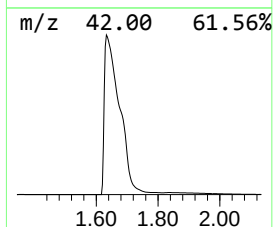
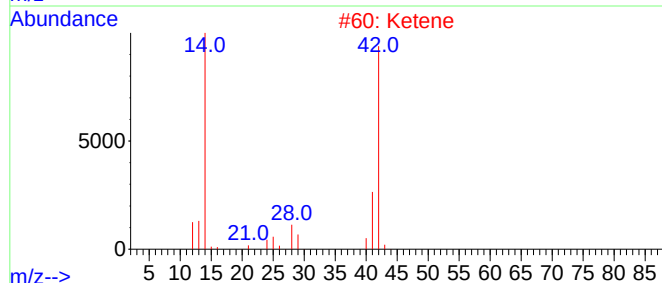
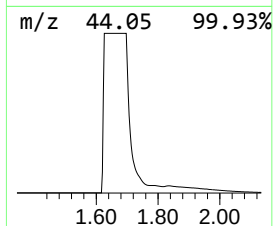
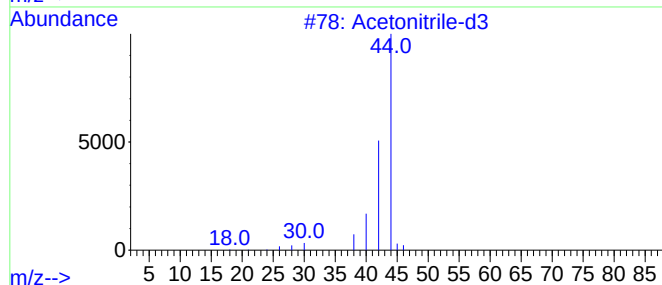
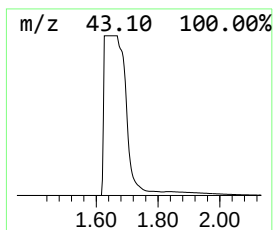
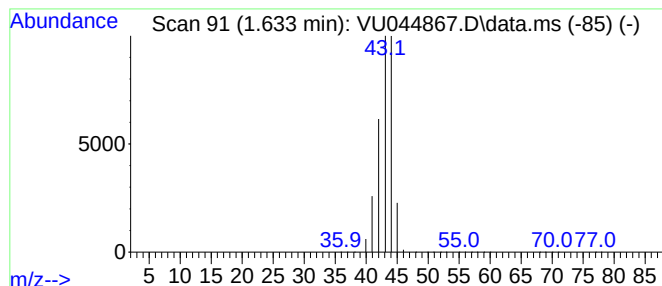
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown1.633 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.633	3942.24 ug/l	147861000	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetonitrile-d3	44	C2D3N	002206-26-0	4
2			Ketene	42	C2H2O	000463-51-4	4
3			Ethylamine	45	C2H7N	000075-04-7	4
4			Ethylene oxide	44	C2H4O	000075-21-8	3
5			Dimethylamine	45	C2H7N	000124-40-3	3



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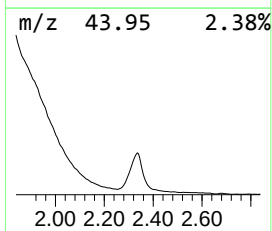
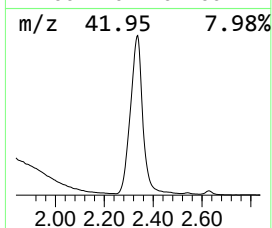
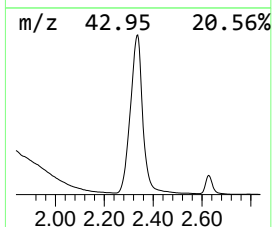
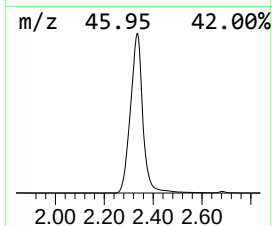
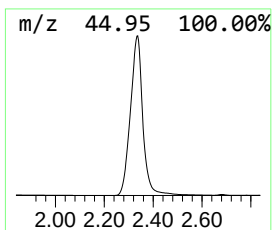
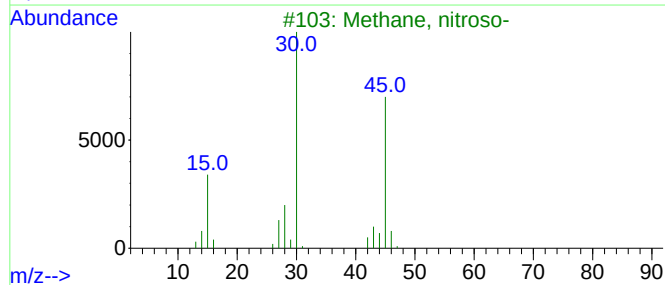
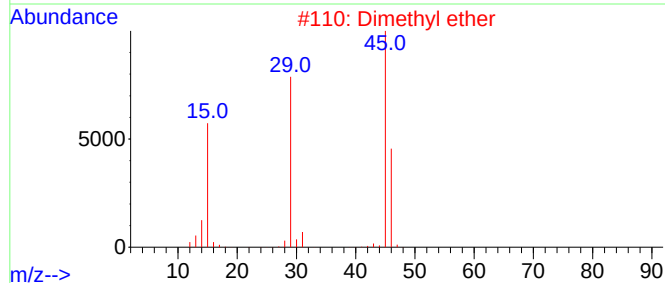
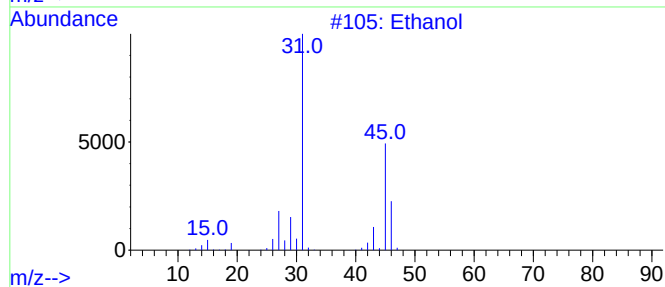
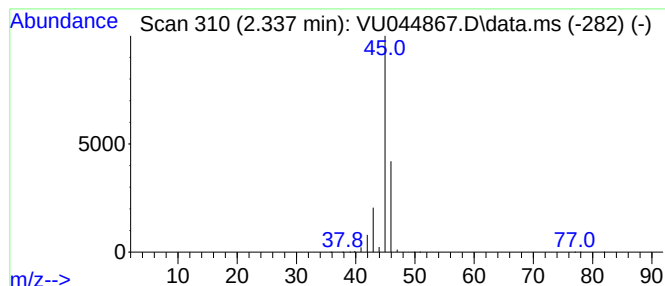
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Quant Title : SW846 8260

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

Peak Number 2 Ethanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.337	590.54 ug/l	22149200	Pentafluorobenzene	5.375

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol	46	C2H6O	000064-17-5	83
2			Dimethyl ether	46	C2H6O	000115-10-6	9
3			Methane, nitroso-	45	CH3NO	000865-40-7	4
4			Formic acid	46	CH2O2	000064-18-6	4
5			Oxalic acid	90	C2H2O4	000144-62-7	4



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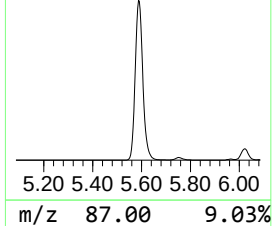
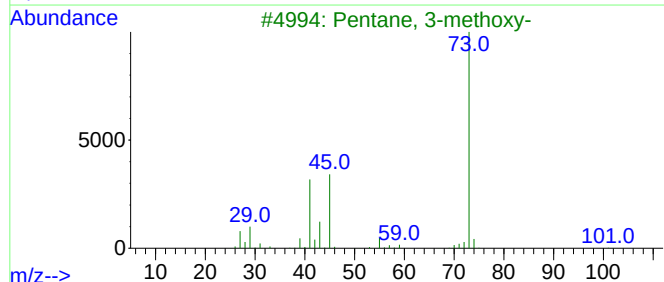
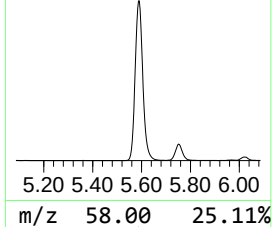
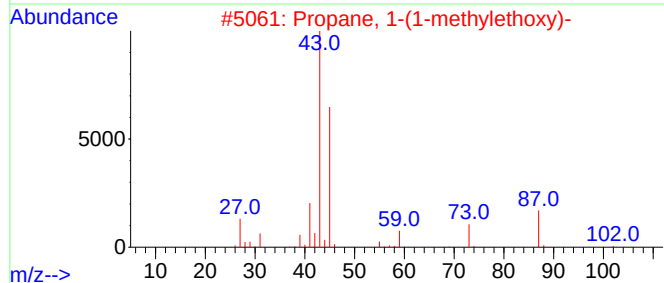
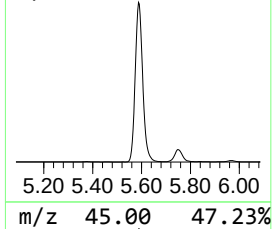
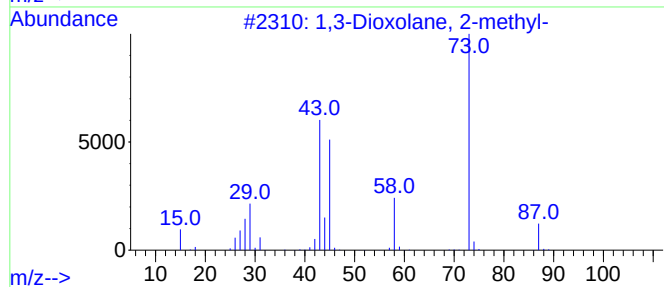
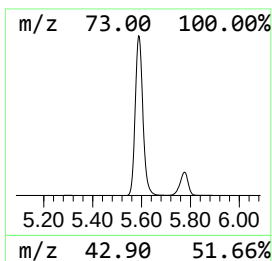
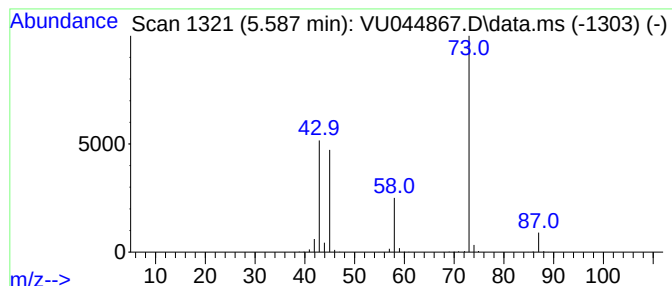
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 3 1,3-Dioxolane, 2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.587	50.00 ug/l	1875350	Pentafluorobenzene	5.375

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		1,3-Dioxolane, 2-methyl-	88	C4H8O2	000497-26-7	91
2		Propane, 1-(1-methylethoxy)-	102	C6H14O	000627-08-7	33
3		Pentane, 3-methoxy-	102	C6H14O	036839-67-5	28
4		2-Acetamido-N-methylacetamide	130	C5H10N2O2	007606-79-3	17
5		Silane, tetramethyl-	88	C4H12Si	000075-76-3	16



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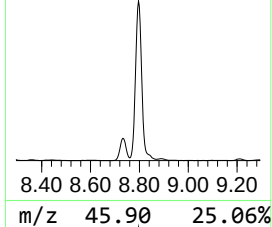
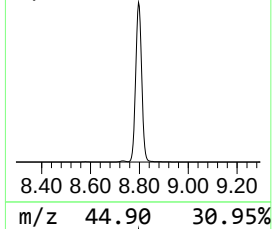
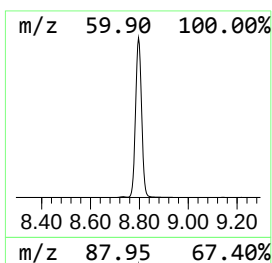
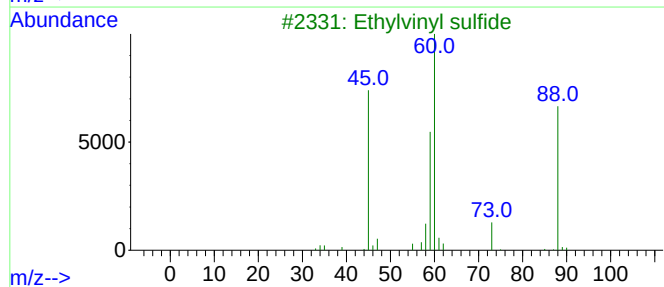
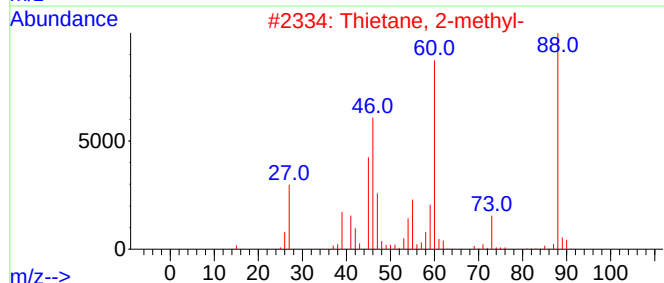
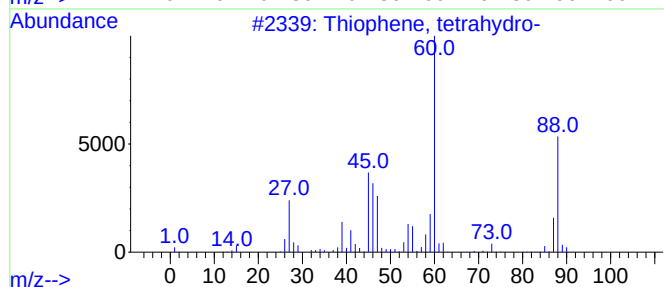
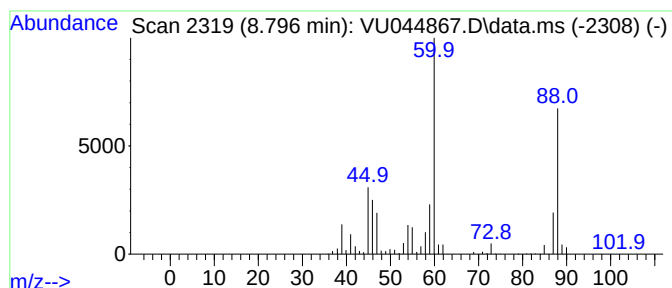
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\82U092421W.M
Quant Title : SW846 8260

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

Peak Number 4 Thiophene, tetrahydro- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.796	78.94 ug/l	3038270	Chlorobenzene-d5	9.420

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Thiophene, tetrahydro-	88	C4H8S	000110-01-0	97
2		Thietane, 2-methyl-	88	C4H8S	017837-41-1	74
3		Ethylvinyl sulfide	88	C4H8S	000627-50-9	38
4		4-Bromobutyric acid	166	C4H7BrO2	002623-87-2	23
5		Ethanol, 2-mercapto-	78	C2H6OS	000060-24-2	23



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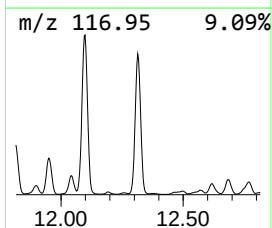
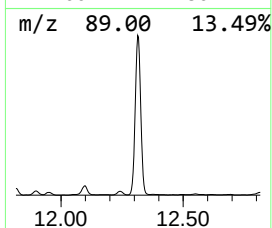
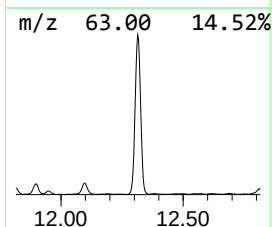
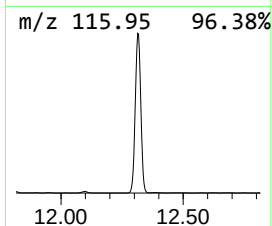
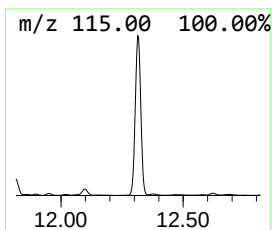
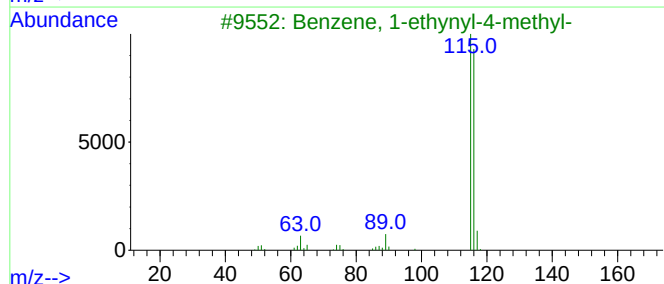
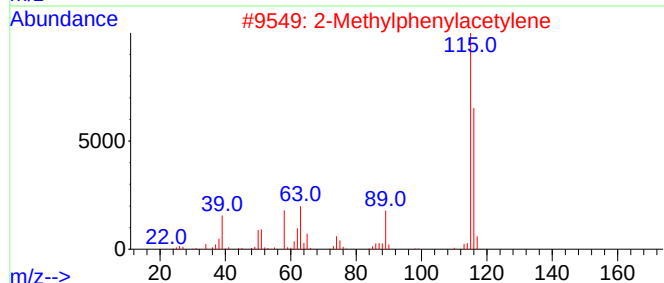
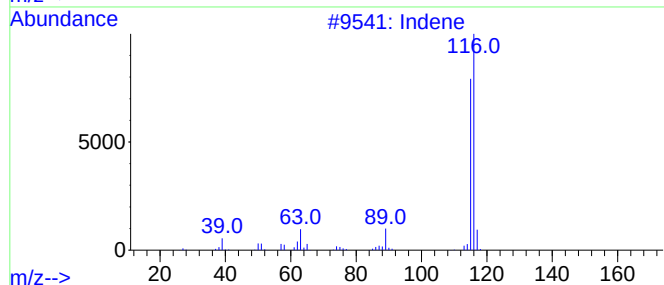
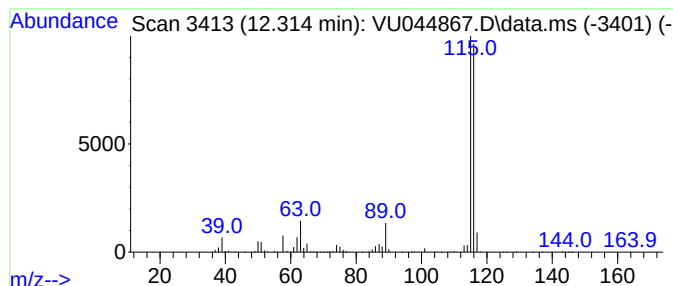
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Peak Number 5 Indene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.314	50.00 ug/l	3418840	1,4-Dichlorobenzene-d4	11.816

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Indene	116	C9H8	000095-13-6	95
2	2-Methylphenylacetylene	116	C9H8	000766-47-2	91
3	Benzene, 1-ethynyl-4-methyl-	116	C9H8	000766-97-2	91
4	3-Methylphenylacetylene	116	C9H8	000766-82-5	91
5	Benzene, 1-propynyl-	116	C9H8	000673-32-5	91



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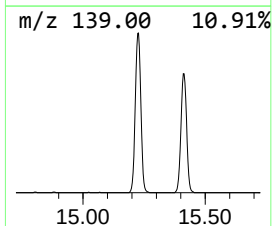
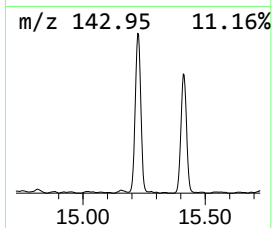
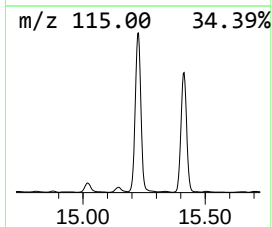
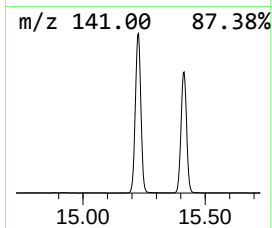
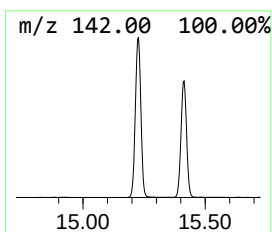
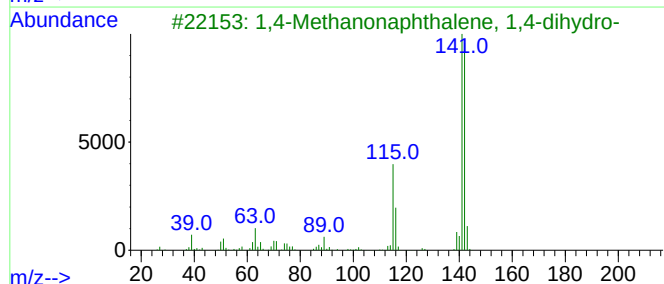
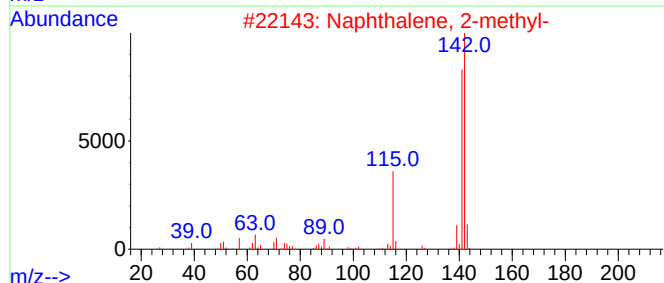
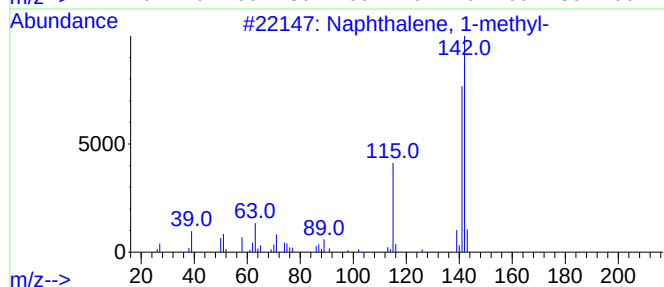
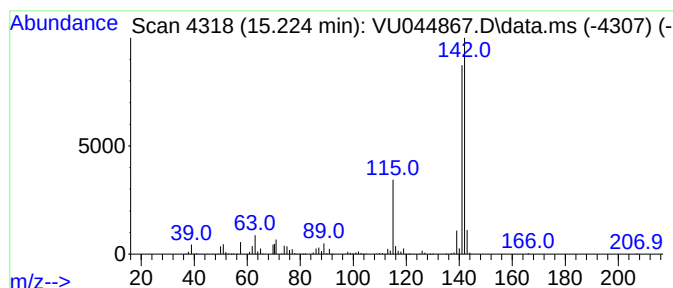
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Peak Number 6 Naphthalene, 1-methyl- Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.	
15.224	24.64 ug/l	1684900	1,4-Dichlorobenzene-d4	11.816	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
2	Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
3	1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	93
4	Benzocycloheptatriene	142	C11H10	000264-09-5	90
5	1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.633	1.633	3942.2	ug/l	147861000	1	5.375	1875350	50.0
Ethanol	2.337	590.5	ug/l	22149200	1	5.375	1875350	50.0
1,3-Dioxolane, ...	5.587	50.0	ug/l	1875350	1	5.375	1875350	50.0
Thiophene, tetr...	8.796	78.9	ug/l	3038270	3	9.420	1924470	50.0
Indene	12.314	50.0	ug/l	3418840	4	11.816	3418840	50.0
Naphthalene, 1-...	15.224	24.6	ug/l	1684900	4	11.816	3418840	50.0