

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX071521\
 Data File : VX023311.D
 Acq On : 15 Jul 2021 19:57
 Operator : JC/MD
 Sample : M3061-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PB-2021-WW-000-08

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\82X070221W.M

Title : SW846 8260

Signal : TIC: VX023311.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.117	321	333	349	rBV3	287734	775335	6.16%	3.581%
2	3.446	378	387	403	rBV	330882	749774	5.96%	3.463%
3	3.867	447	456	471	rBV2	61289	158647	1.26%	0.733%
4	4.306	508	528	543	rBV	266196	784747	6.24%	3.624%
5	5.397	696	707	719	rBV	142259	422521	3.36%	1.951%
6	5.562	725	734	749	rVB	255540	715000	5.68%	3.302%
7	5.964	786	800	817	rBV	155895	423771	3.37%	1.957%
8	6.769	922	932	944	rBV	379646	904206	7.19%	4.176%
9	8.653	1234	1241	1250	rBV	798642	1226768	9.75%	5.666%
10	9.281	1334	1344	1366	rBV	8586568	12582375	100.00%	58.111%
11	10.055	1465	1471	1480	rBV	773334	1073872	8.53%	4.960%
12	11.085	1634	1640	1651	rBV	675617	849805	6.75%	3.925%
13	12.024	1789	1794	1803	rBV	820532	985536	7.83%	4.552%

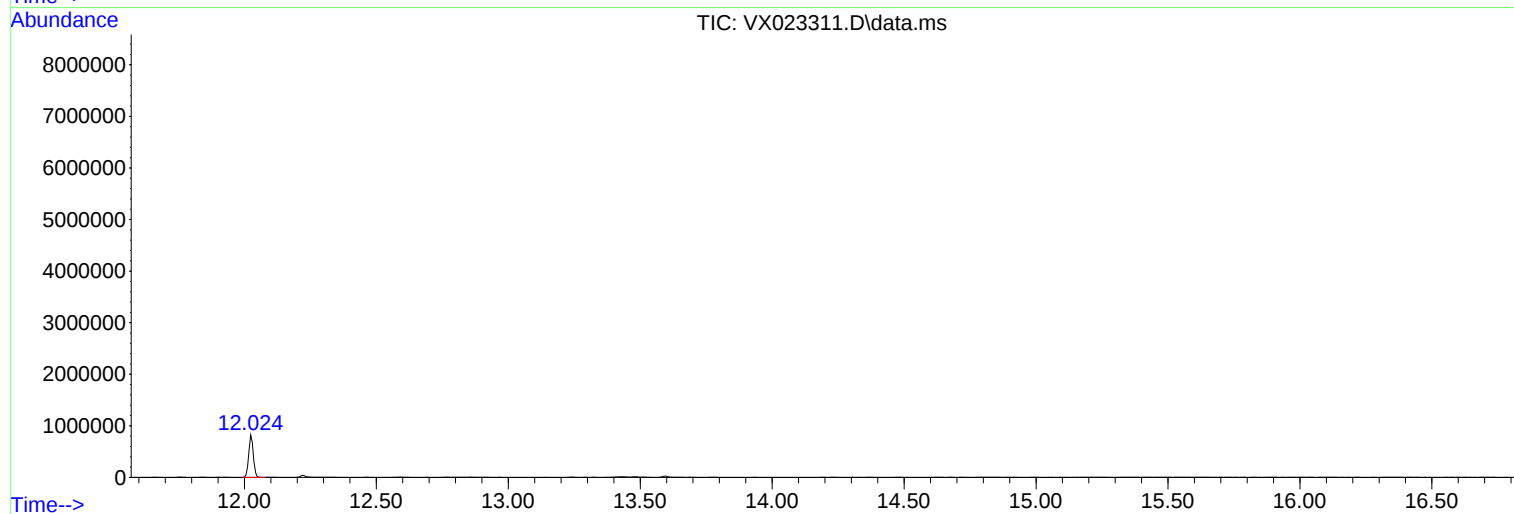
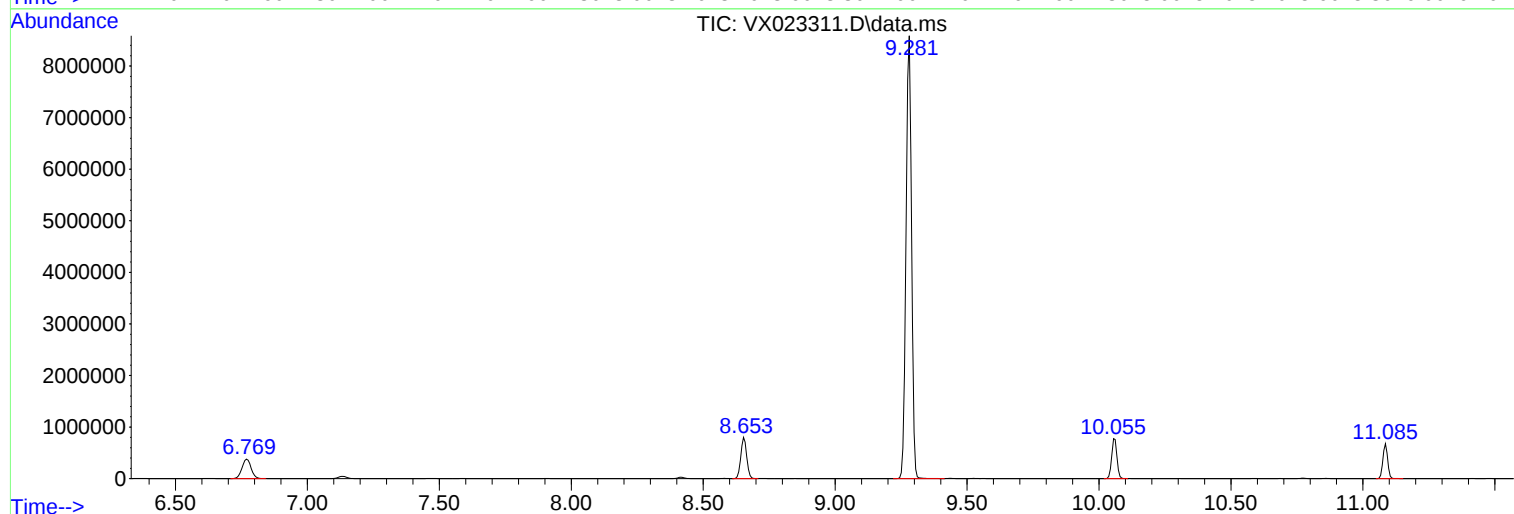
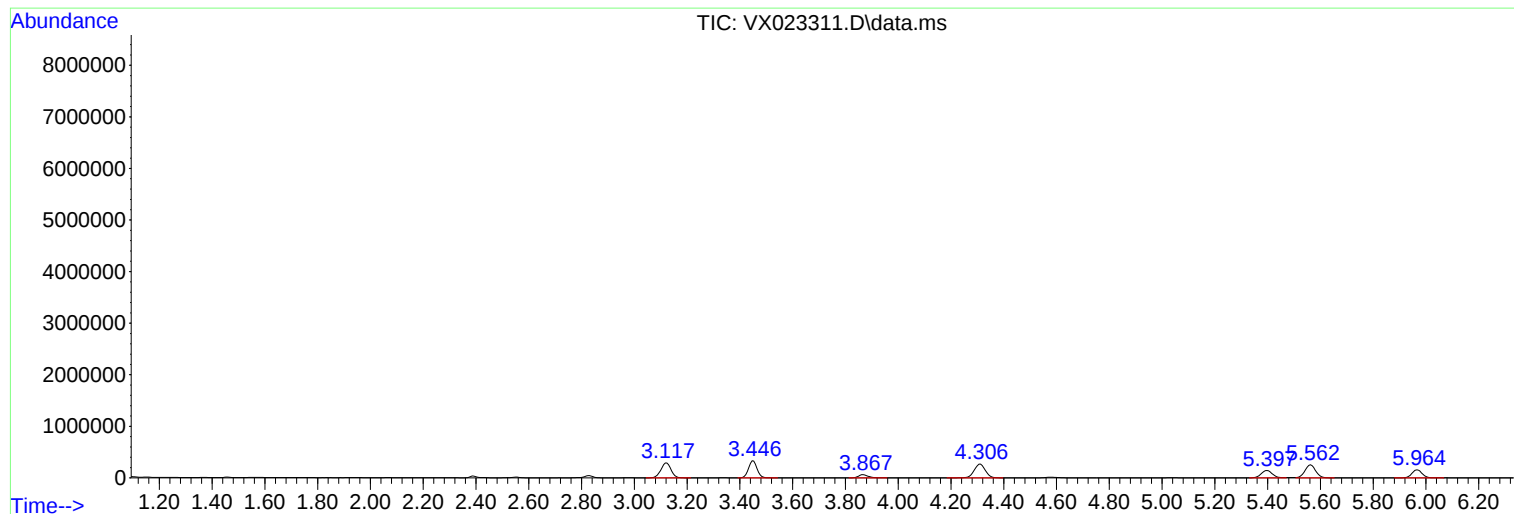
Sum of corrected areas: 21652357

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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



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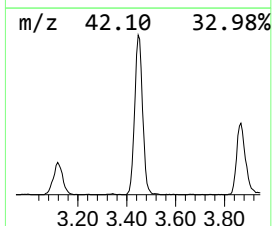
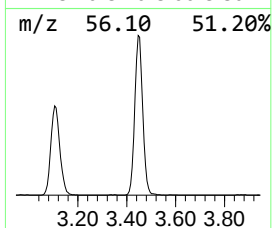
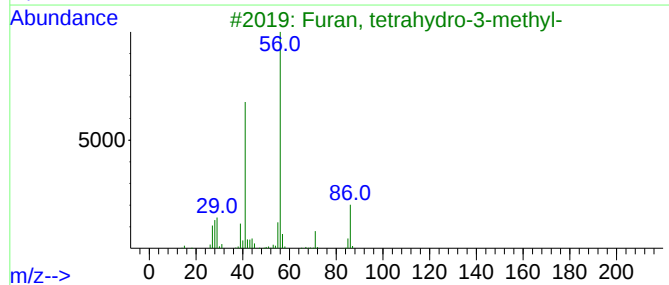
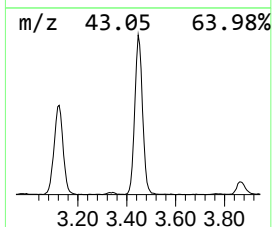
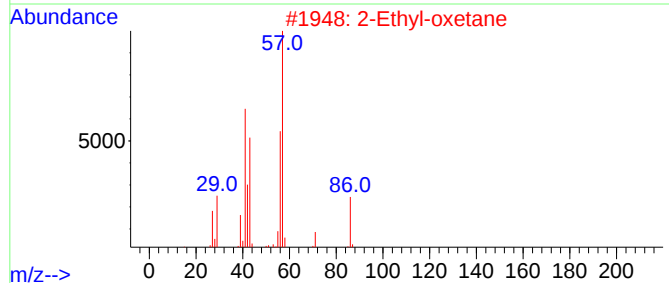
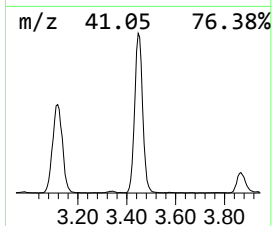
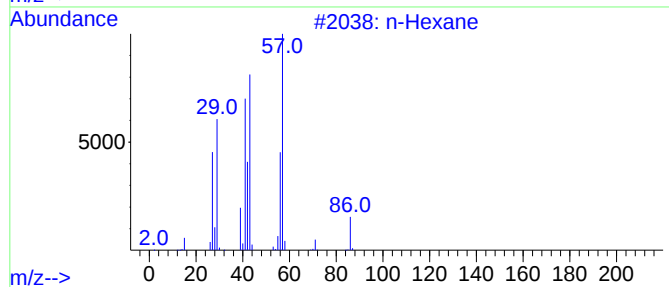
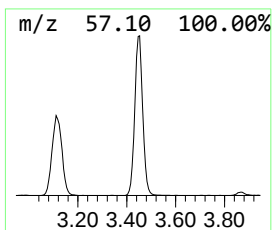
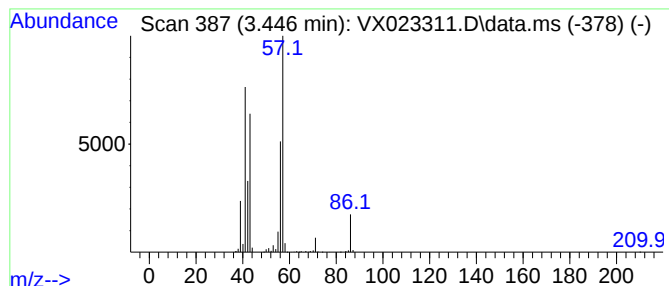
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X070221W.M
Quant Title : SW846 8260

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

Peak Number 1 n-Hexane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.446	52.43 ug/l	749774	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			n-Hexane	86	C6H14	000110-54-3	91
2			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	72
3			Furan, tetrahydro-3-methyl-	86	C5H10O	013423-15-9	50
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	40
5			Butanal, 2-methyl-	86	C5H10O	000096-17-3	35



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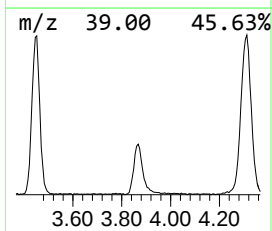
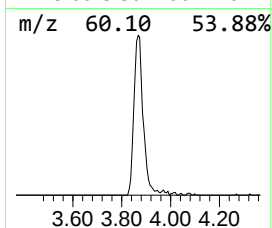
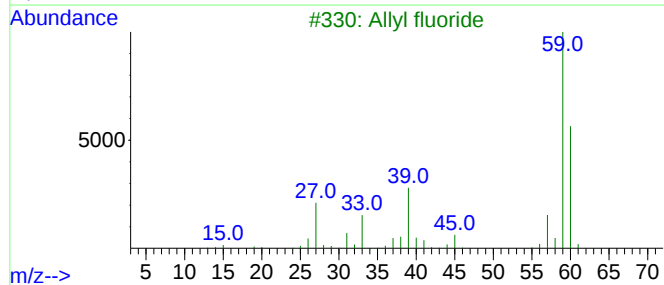
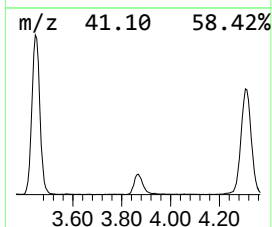
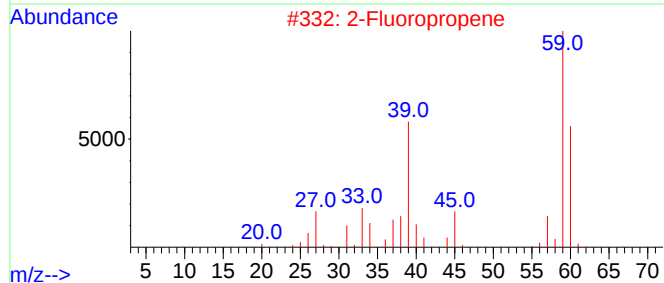
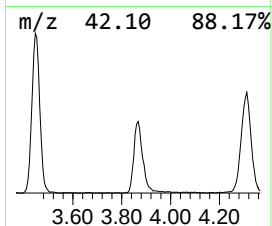
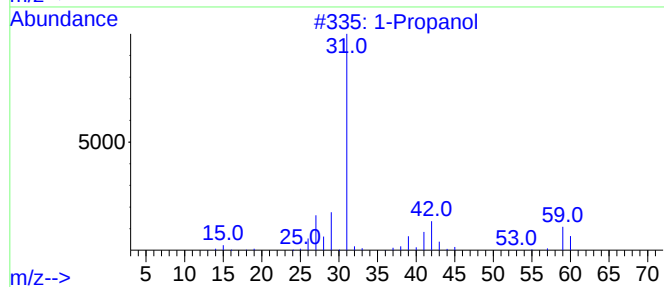
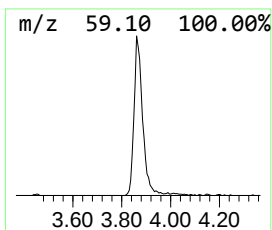
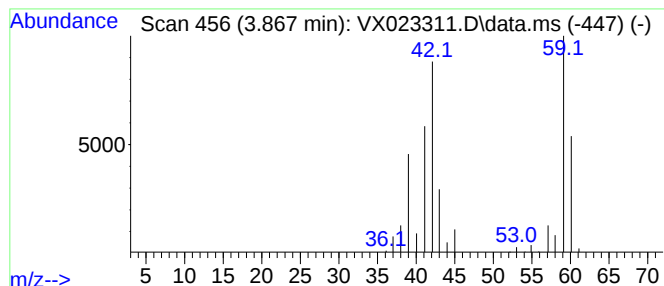
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Peak Number 2 1-Propanol Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.867	11.09 ug/l	158647	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol	60	C3H8O	000071-23-8	59
2			2-Fluoropropene	60	C3H5F	001184-60-7	46
3			Allyl fluoride	60	C3H5F	000818-92-8	38
4			Cyclopropane	42	C3H6	000075-19-4	25
5			Propene	42	C3H6	000115-07-1	17



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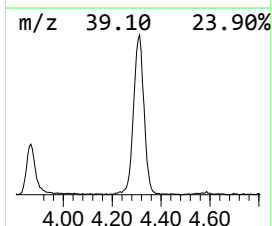
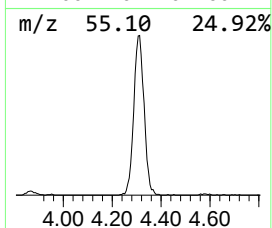
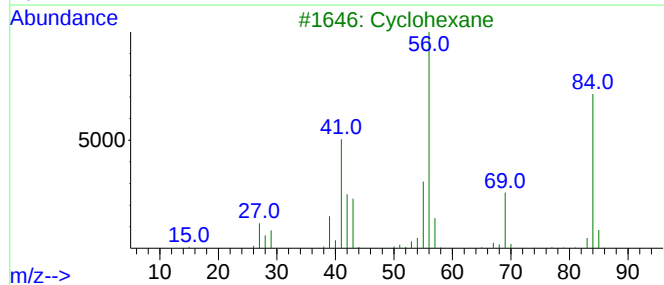
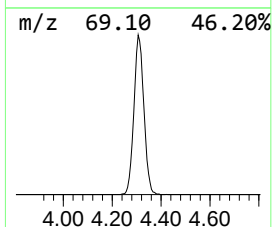
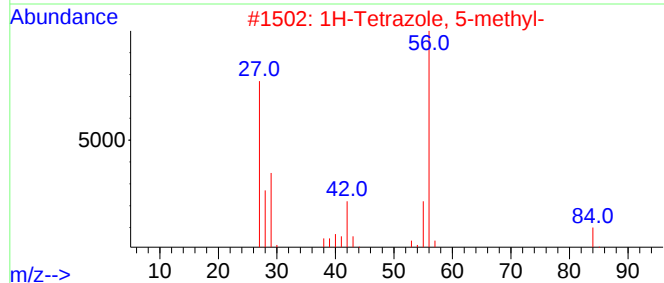
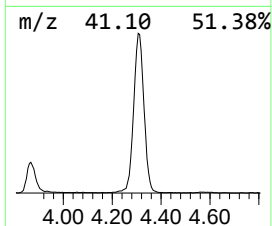
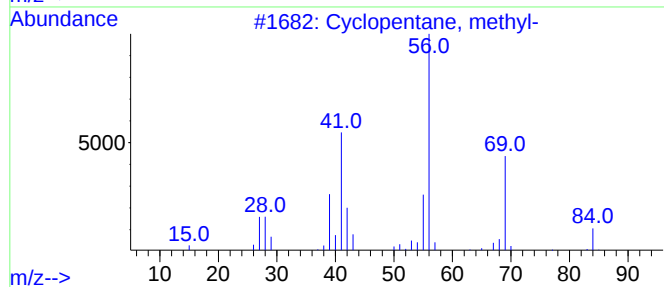
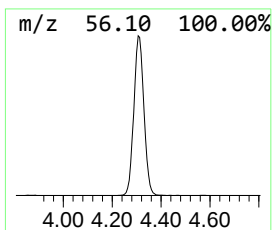
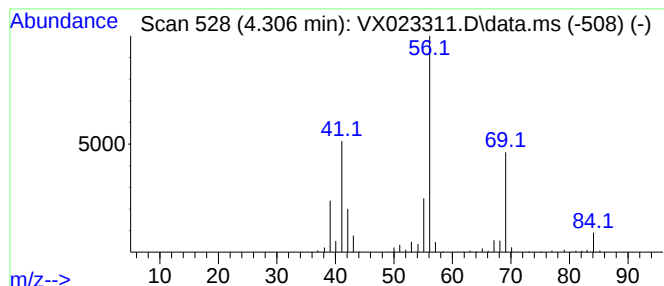
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Peak Number 3 Cyclopentane, methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.306	54.88 ug/l	784747	Pentafluorobenzene	5.562

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	94
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	80
3			Cyclohexane	84	C6H12	000110-82-7	78
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	72
5			Cyclobutane, butyl-	112	C8H16	013152-44-8	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
n-Hexane	3.446	52.4	ug/l	749774	1	5.562	715000	50.0
1-Propanol	3.867	11.1	ug/l	158647	1	5.562	715000	50.0
Cyclopentane, m...	4.306	54.9	ug/l	784747	1	5.562	715000	50.0