

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032123\
 Data File : VX034651.D
 Acq On : 21 Mar 2023 13:53
 Operator : JC/MD
 Sample : 02013-02
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 31993

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\82X031023W.M

Title : SW846 8260

Signal : TIC: VX034651.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.447	55	59	72	rBV	2331400	2765860	3.91%	2.842%
2	2.300	187	199	204	rBV3	22228536	70746744	100.00%	72.705%
3	3.879	443	458	485	rBV	2794801	8349605	11.80%	8.581%
4	4.550	560	568	586	rVB	276557	763927	1.08%	0.785%
5	5.550	722	732	745	rVB	309281	861842	1.22%	0.886%
6	6.037	805	812	822	rVB	271917	710972	1.00%	0.731%
7	6.757	920	930	949	rBV	474827	1183372	1.67%	1.216%
8	8.647	1234	1240	1246	rBV	1074280	1678862	2.37%	1.725%
9	10.055	1463	1471	1473	rBV	1133213	1570329	2.22%	1.614%
10	10.085	1473	1476	1485	rVB	802669	1289507	1.82%	1.325%
11	11.079	1632	1639	1645	rBV	785037	1009145	1.43%	1.037%
12	11.152	1645	1651	1659	rVV	4250526	5214422	7.37%	5.359%
13	12.024	1789	1794	1801	rVB	897024	1162327	1.64%	1.194%

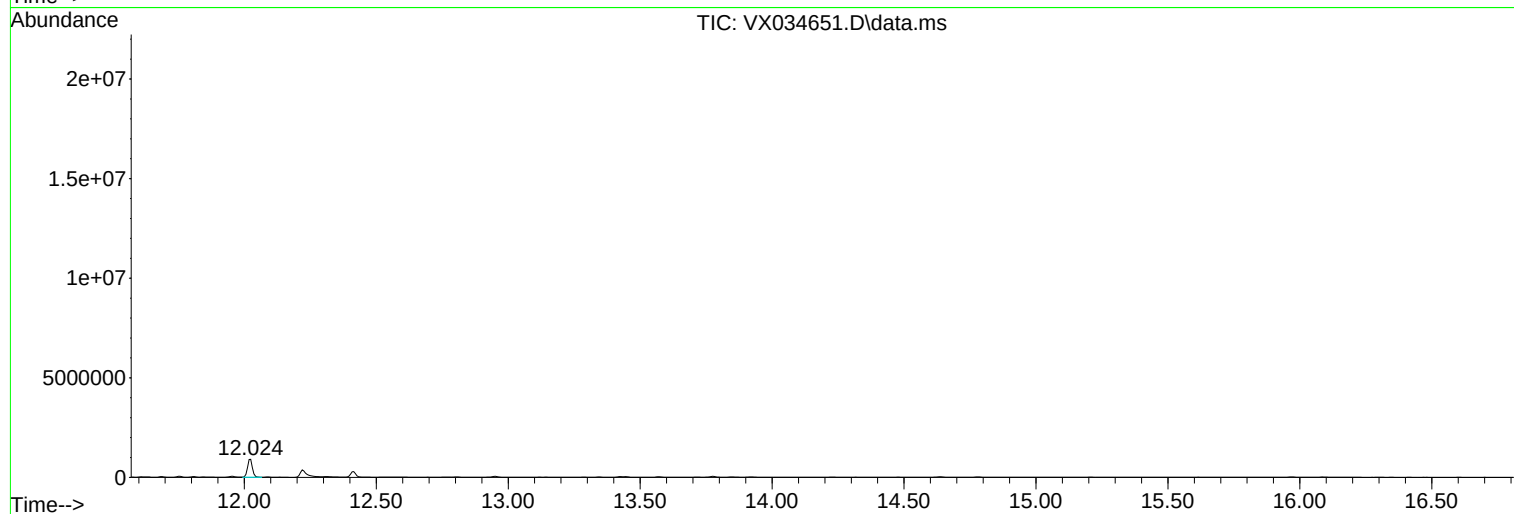
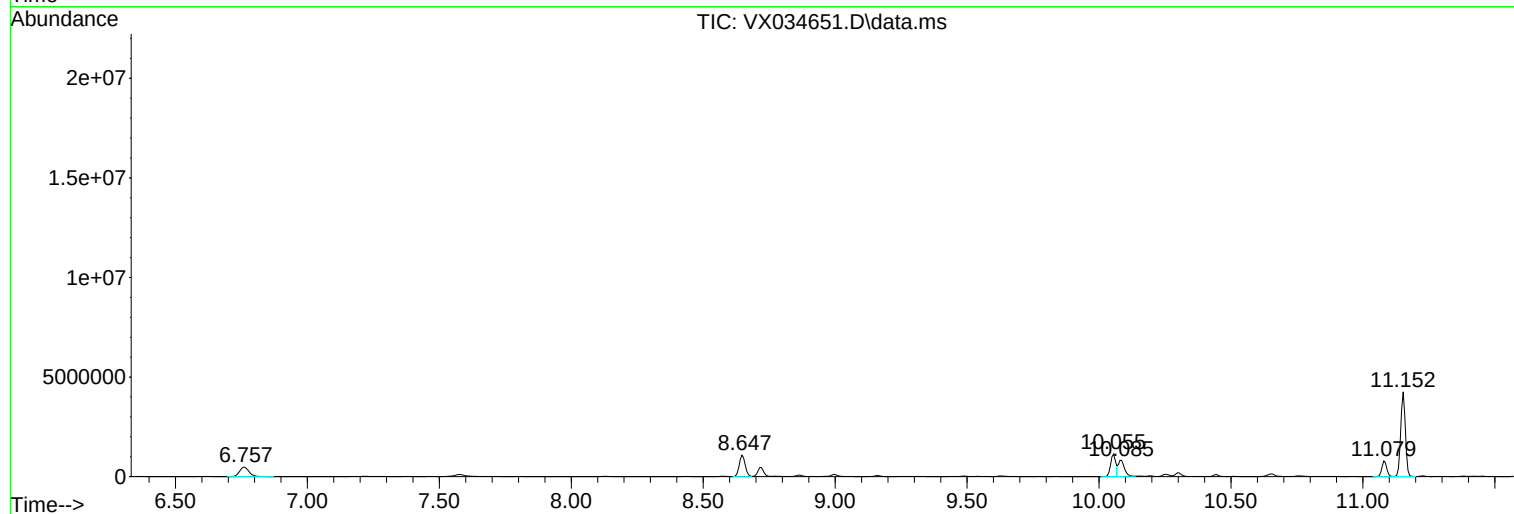
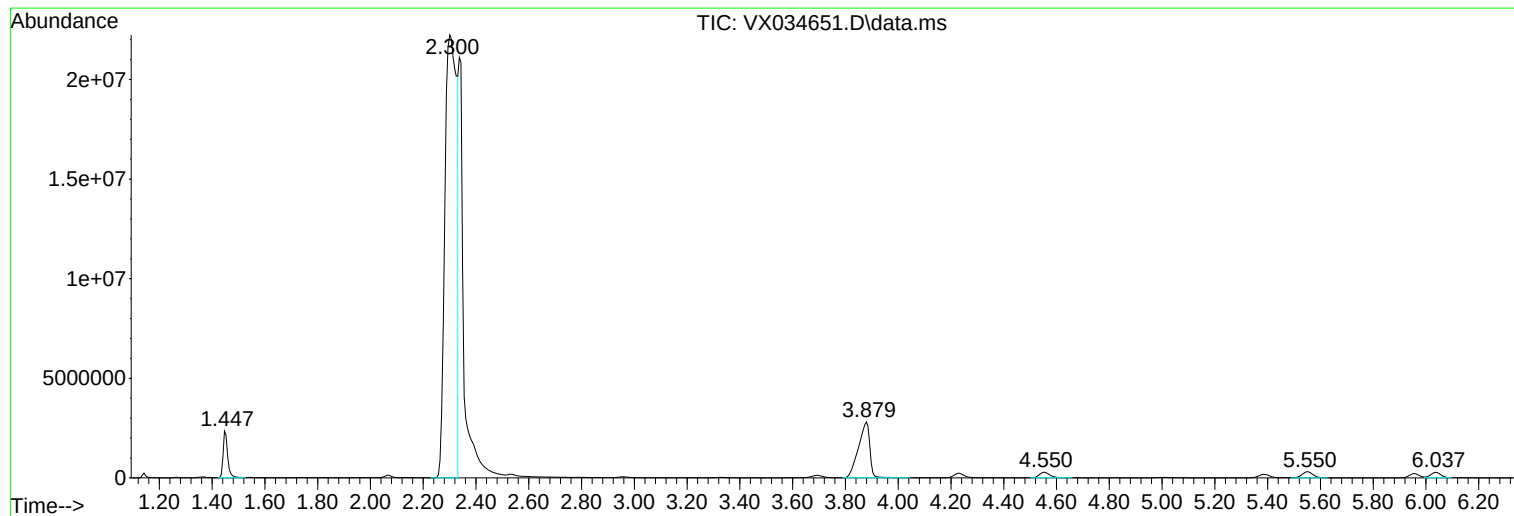
Sum of corrected areas: 97306914

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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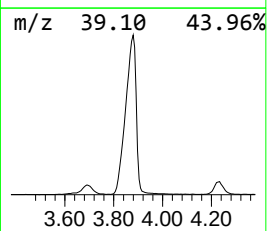
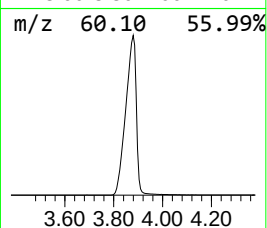
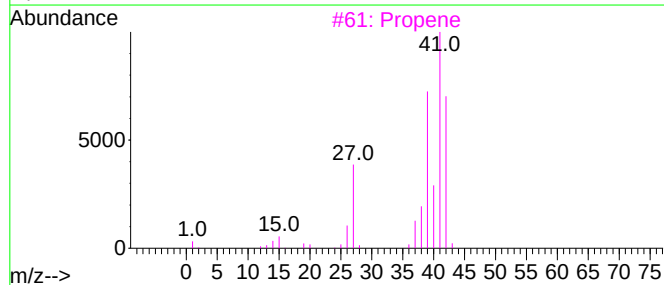
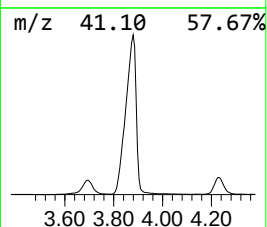
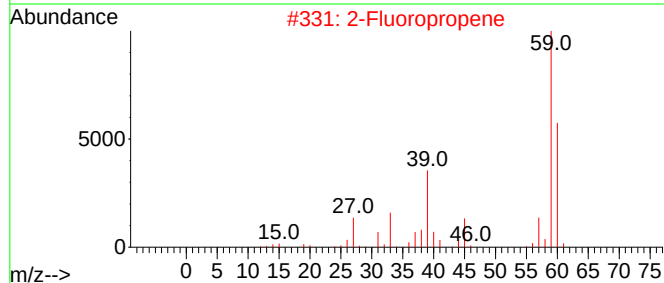
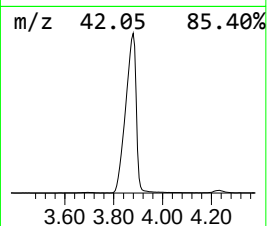
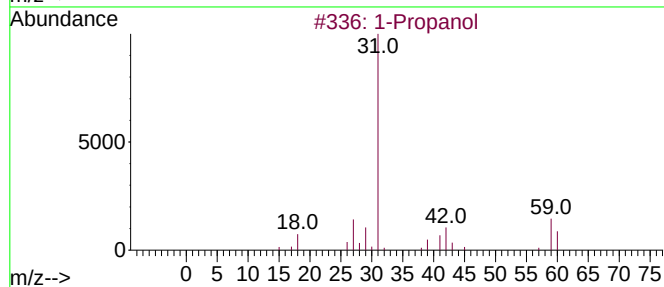
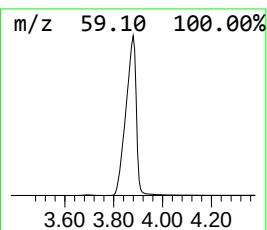
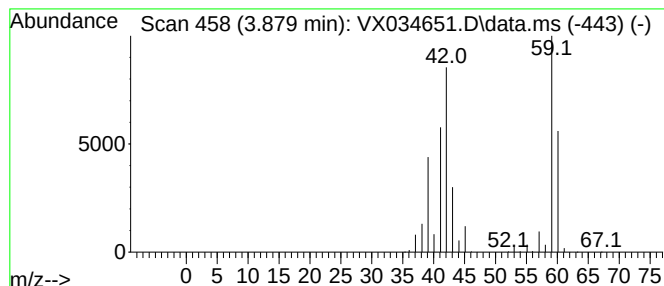
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Quant Title : SW846 8260

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TIC Integration Parameters: LSCINT.P

Peak Number 3 1-Propanol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.879	484.40 ug/l	8349610	Pentafluorobenzene	5.550

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	52
3			Propene	42	C3H6	000115-07-1	25
4			Cyclopropane	42	C3H6	000075-19-4	25
5			2-Butanol, 3-methoxy-	104	C5H12O2	053778-72-6	10



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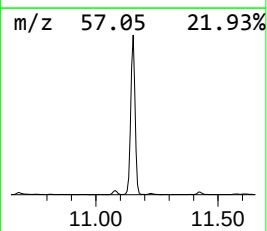
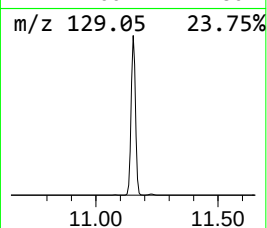
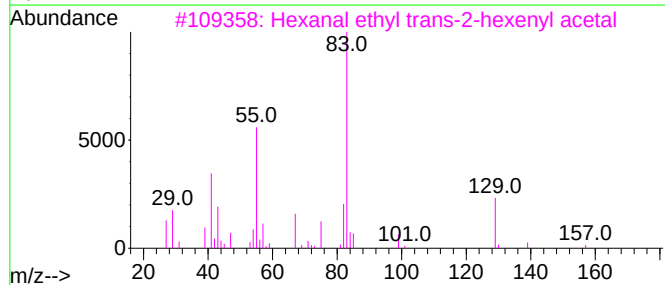
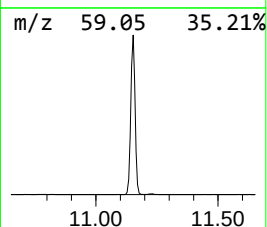
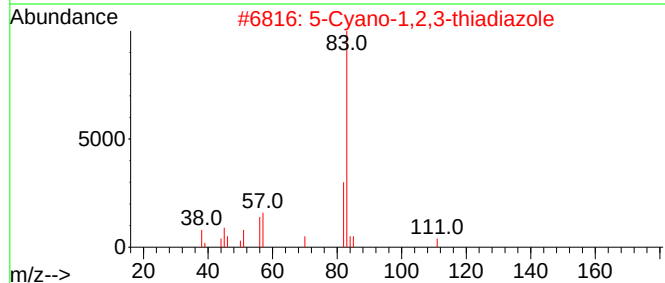
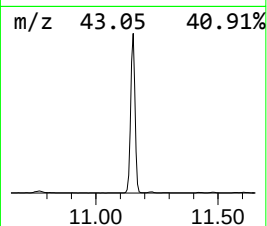
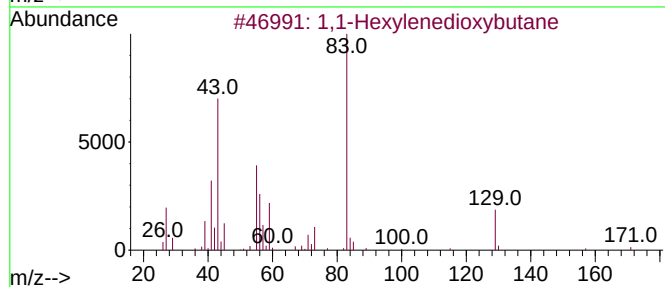
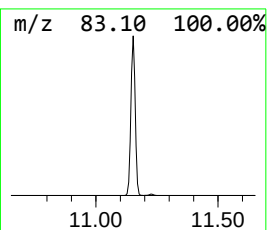
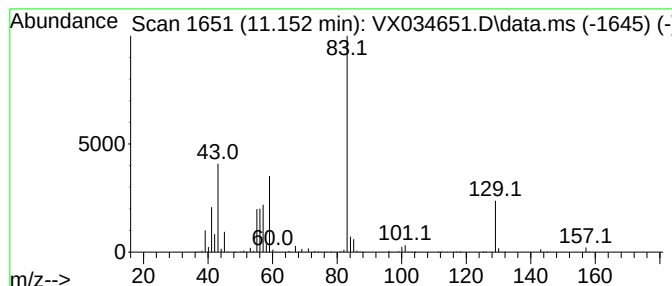
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Peak Number 4 1,1-Hexylenedioxybutane Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.152	224.31 ug/l	5214420	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1-Hexylenedioxybutane	172	C10H20O2	1000249-77-4	78
2			5-Cyano-1,2,3-thiadiazole	111	C3HN3S	057352-02-0	42
3			Hexanal ethyl trans-2-hexenyl ac...	228	C14H28O2	1000431-42-6	42
4			Oxalic acid, cyclohexyl isohexyl...	256	C14H24O4	1010309-30-7	37
5			Oxalic acid, cyclohexyl nonyl ester	298	C17H30O4	1000309-31-1	37



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Propanol	3.879	484.4	ug/l	8349610	1	5.550	861842	50.0
1,1-Hexylenedio...	11.152	224.3	ug/l	5214420	4	12.024	1162330	50.0