

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX021925\
 Data File : VX045005.D
 Acq On : 19 Feb 2025 15:28
 Operator : JC/MD
 Sample : Q1393-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 PURGE-WATER-COMP

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\82X021025W.M
 Title : SW846 8260

Signal : TIC: VX045005.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	21	25	34	rBV	71565	107046	18.62%	3.112%
2	1.666	92	95	102	rVB	14980	20775	3.61%	0.604%
3	2.374	206	211	221	rBV	34385	55962	9.73%	1.627%
4	2.965	296	308	321	rBV2	17274	53492	9.30%	1.555%
5	3.099	321	330	339	rVB6	3363	9351	1.63%	0.272%
6	3.428	377	384	393	rBV2	4902	12008	2.09%	0.349%
7	4.282	513	524	539	rBV3	9006	27458	4.78%	0.798%
8	5.373	693	703	719	rBV	64815	193963	33.73%	5.640%
9	5.538	719	730	746	rBV	88339	264302	45.96%	7.685%
10	5.940	784	796	814	rBV	75620	204049	35.49%	5.933%
11	6.745	919	928	949	rBV	165473	415625	72.28%	12.085%
12	7.409	1029	1037	1045	rBV2	9728	21185	3.68%	0.616%
13	8.641	1233	1239	1248	rBV	355890	575015	100.00%	16.719%
14	8.708	1248	1250	1257	rVB2	7119	13651	2.37%	0.397%
15	10.049	1464	1470	1488	rBV	366084	517963	90.08%	15.060%
16	10.195	1490	1494	1500	rVB	4997	7547	1.31%	0.219%
17	10.299	1505	1511	1522	rBV	21560	33785	5.88%	0.982%
18	10.640	1562	1567	1573	rBV	10914	14929	2.60%	0.434%
19	11.079	1633	1639	1652	rBV	286850	389621	67.76%	11.329%
20	11.750	1742	1749	1756	rBV	6733	9508	1.65%	0.276%
21	12.018	1788	1793	1802	rBV	390644	492004	85.56%	14.306%

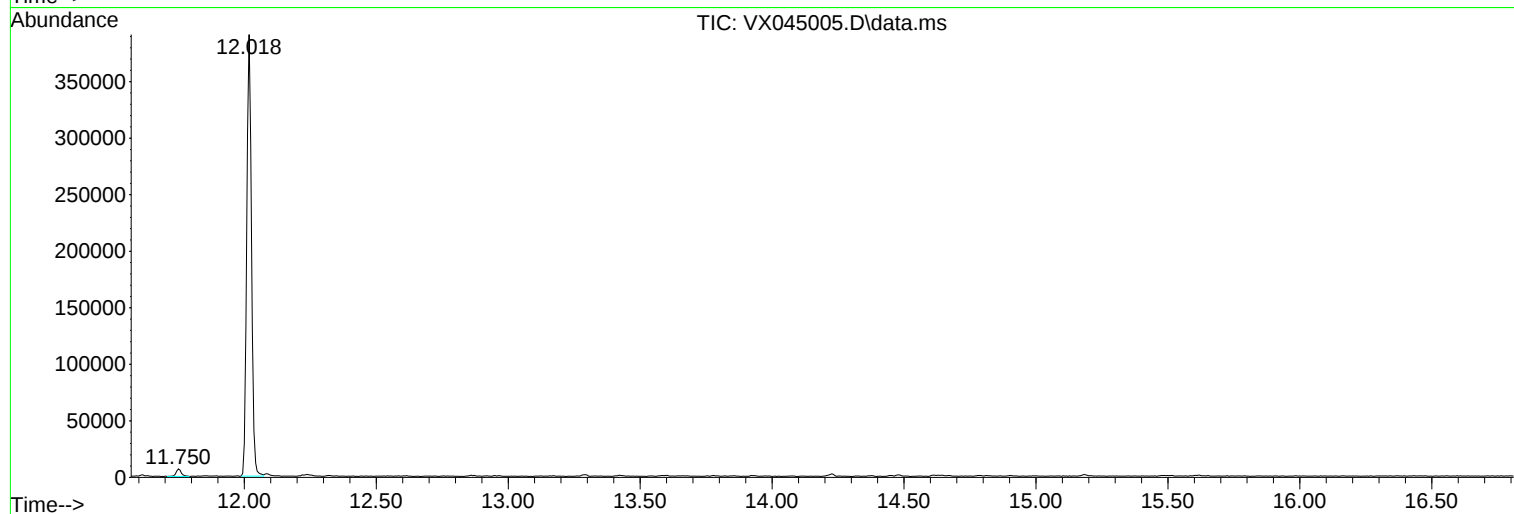
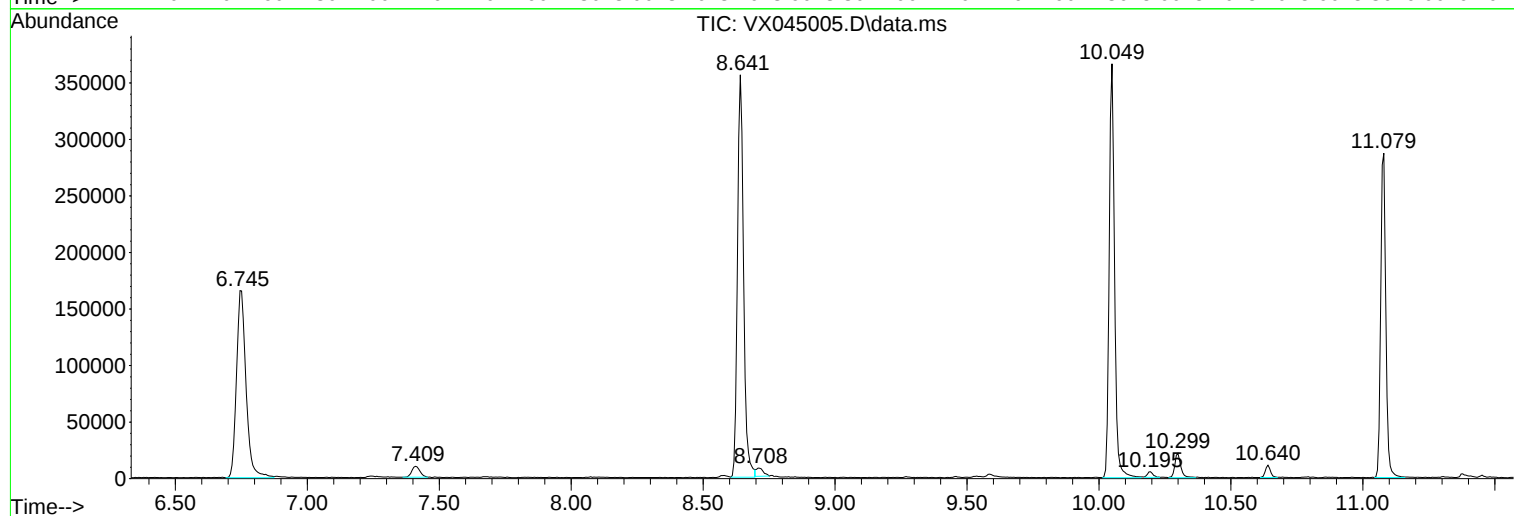
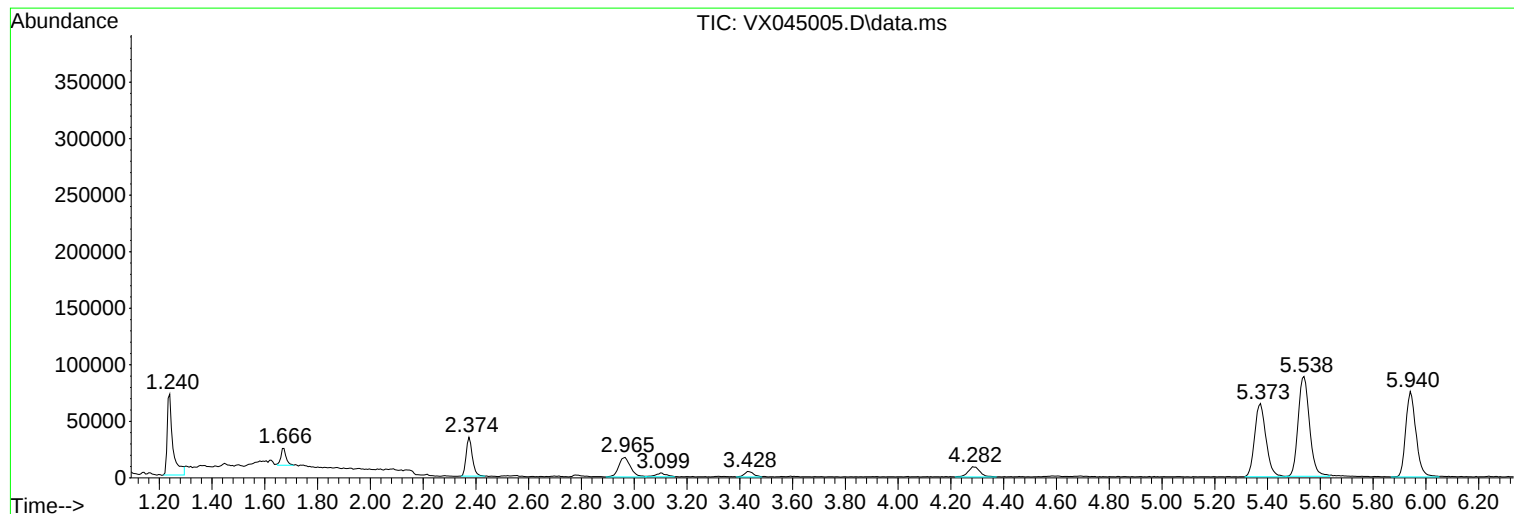
Sum of corrected areas: 3439239

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X021025W.M
Quant Title : SW846 8260

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



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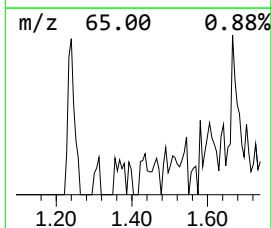
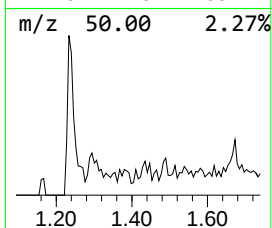
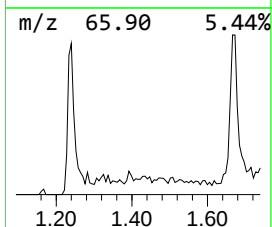
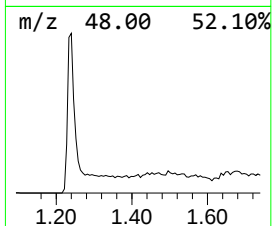
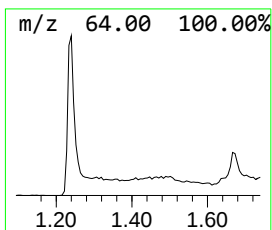
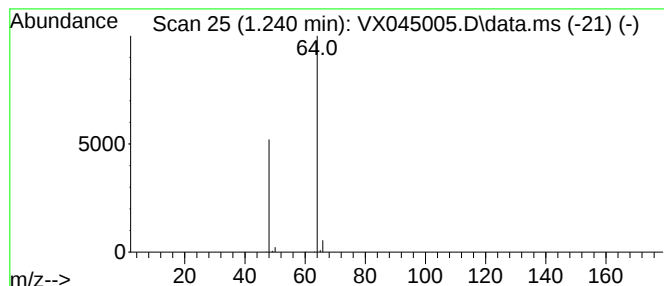
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.240	20.25 ug/l	107046	Pentafluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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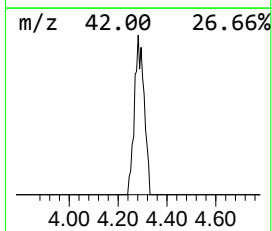
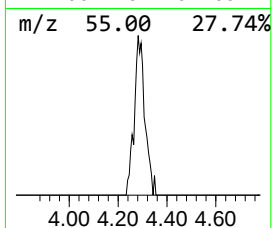
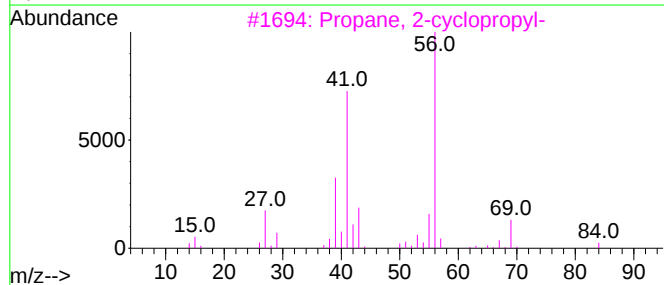
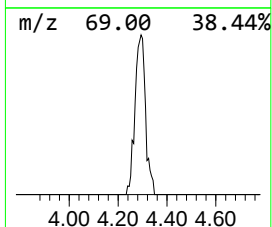
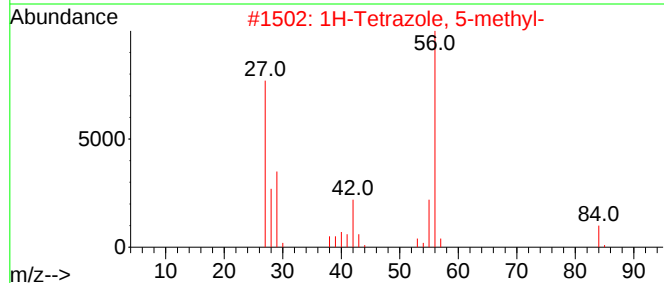
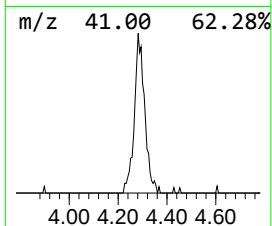
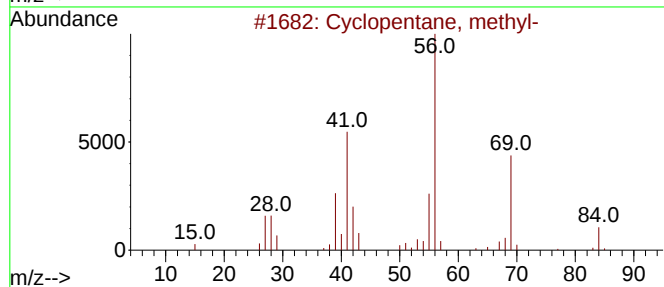
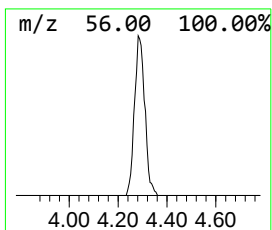
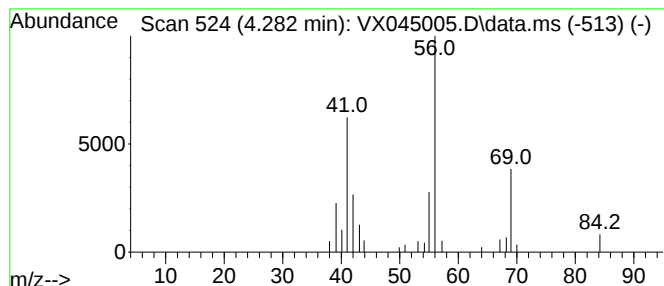
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Peak Number 2 Cyclopentane, methyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.282	5.19 ug/l	27458	Pentafluorobenzene	5.538

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, methyl-	84	C6H12	000096-37-7	91
2			1H-Tetrazole, 5-methyl-	84	C2H4N4	004076-36-2	59
3			Propane, 2-cyclopropyl-	84	C6H12	003638-35-5	59
4			Cyclobutane, ethyl-	84	C6H12	004806-61-5	59
5			1-Pentene, 2-methyl-	84	C6H12	000763-29-1	56



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.240	20.3	ug/l	107046	1	5.538	264302	50.0
Cyclopentane, m...	4.282	5.2	ug/l	27458	1	5.538	264302	50.0