

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX033123\
 Data File : VX034879.D
 Acq On : 31 Mar 2023 15:35
 Operator : JC/MD
 Sample : 02048-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-6

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: VX034879.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.270	25	30	45	rBV	32635	90773	6.94%	1.182%
2	3.111	322	332	347	rVB	104477	237448	18.16%	3.091%
3	5.385	694	705	721	rBV	143949	418440	32.00%	5.447%
4	5.550	721	732	747	rVV2	245671	702893	53.76%	9.150%
5	5.952	788	798	814	rBV	170524	458237	35.05%	5.965%
6	6.251	832	847	856	rBV	51155	159050	12.16%	2.071%
7	6.763	921	931	945	rBV	398458	957701	73.25%	12.467%
8	7.982	1123	1131	1143	rVB	47331	91281	6.98%	1.188%
9	8.104	1143	1151	1159	rBV2	11411	23621	1.81%	0.307%
10	8.647	1233	1240	1258	rBV	834770	1307517	100.00%	17.021%
11	10.055	1465	1471	1486	rBV	831084	1134887	86.80%	14.774%
12	11.079	1634	1639	1654	rBV	782441	981402	75.06%	12.776%
13	12.024	1788	1794	1804	rBV	872231	1118405	85.54%	14.559%

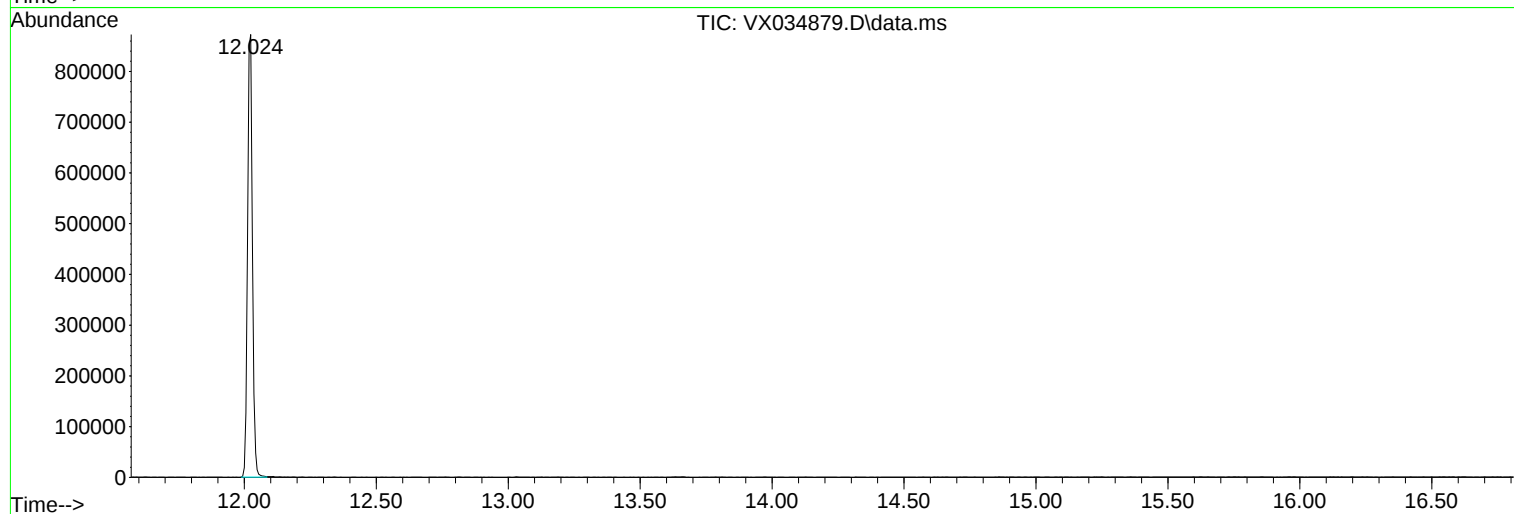
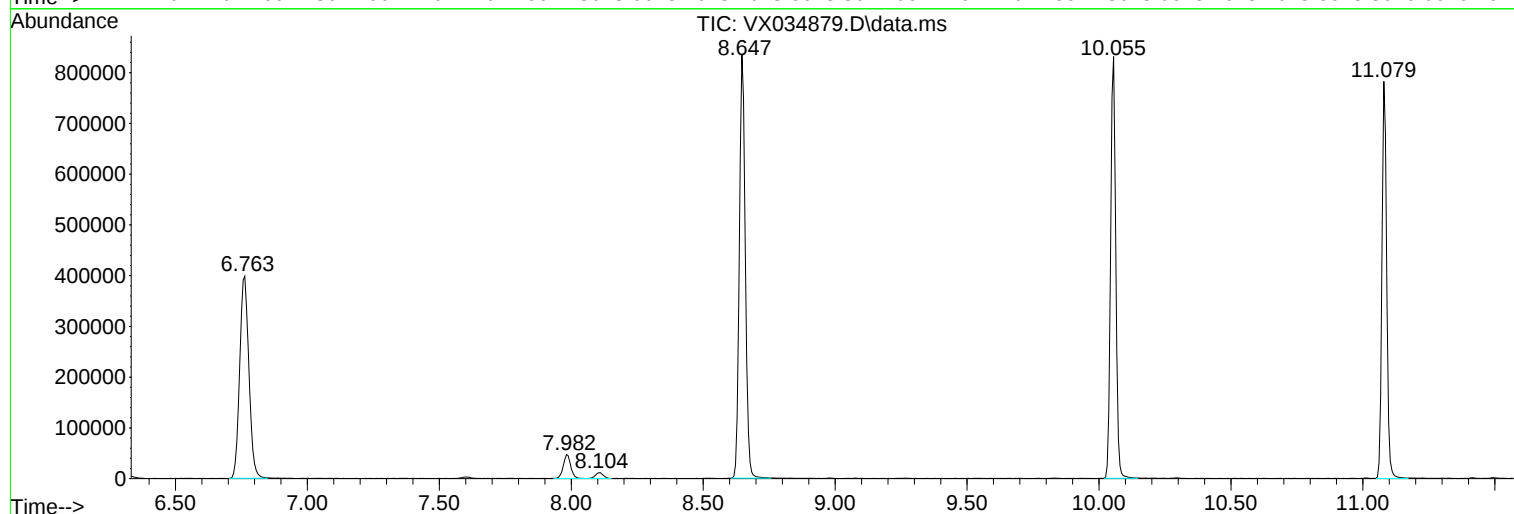
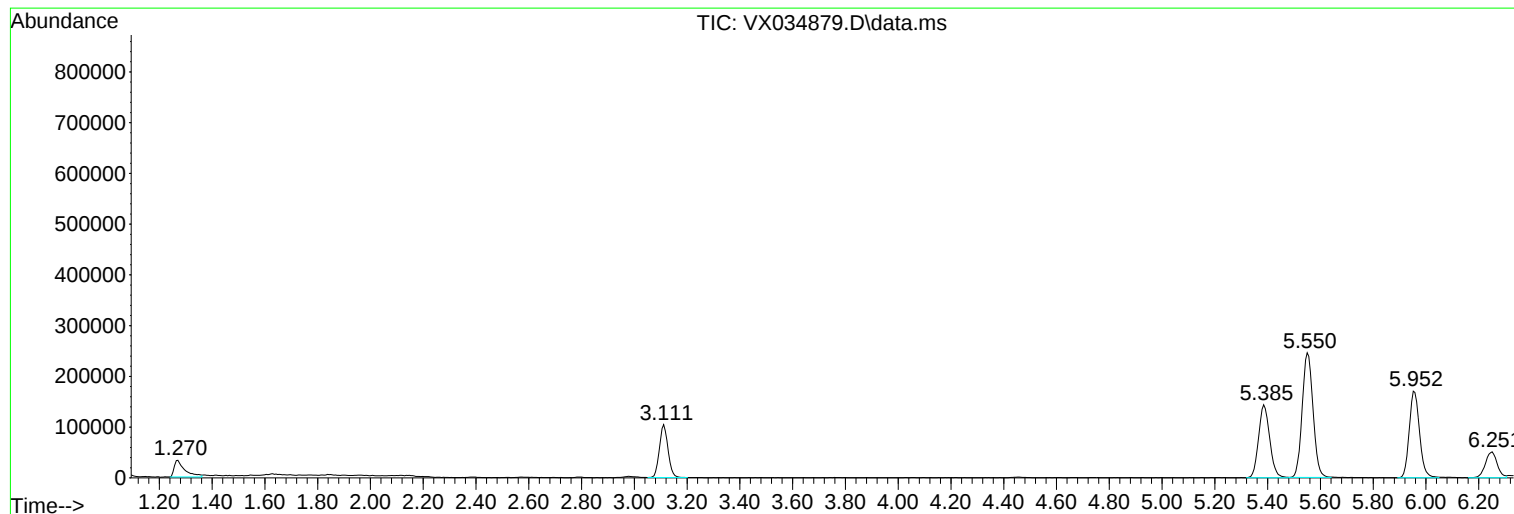
Sum of corrected areas: 7681655

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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



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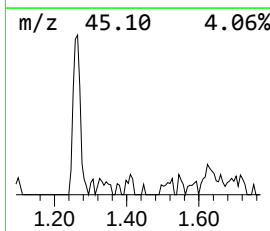
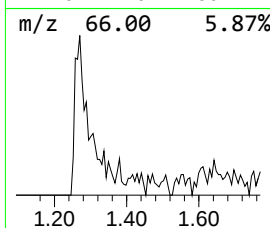
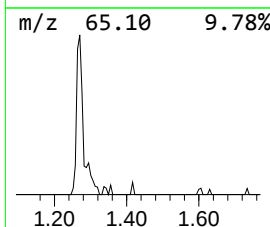
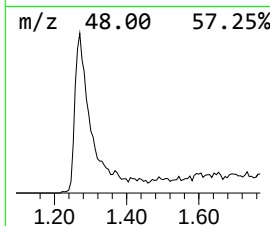
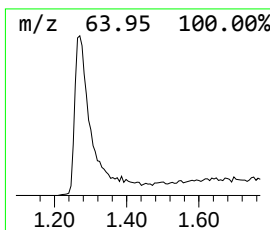
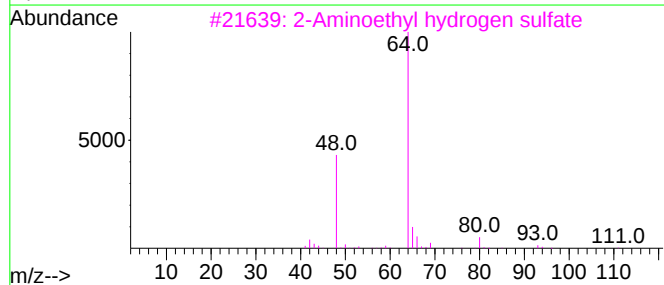
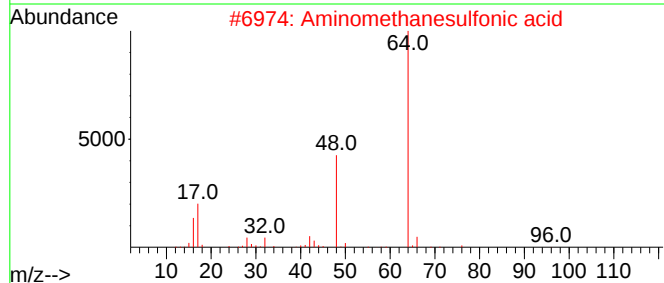
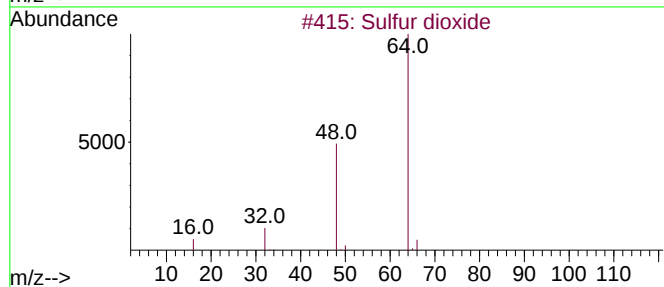
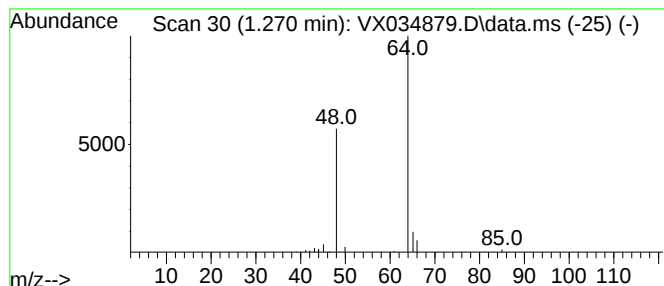
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X032923W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.270	6.46 ug/l	90773	Pentafluorobenzene	5.556

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	90
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	74
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5



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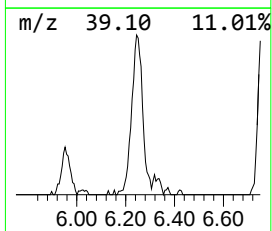
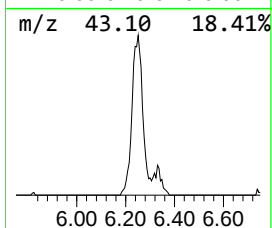
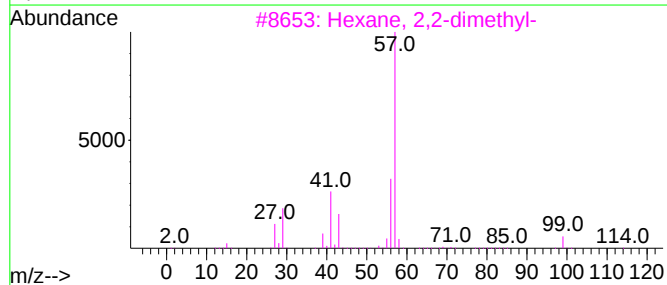
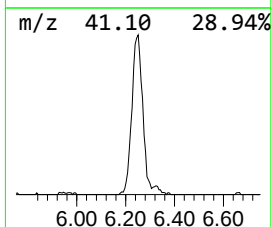
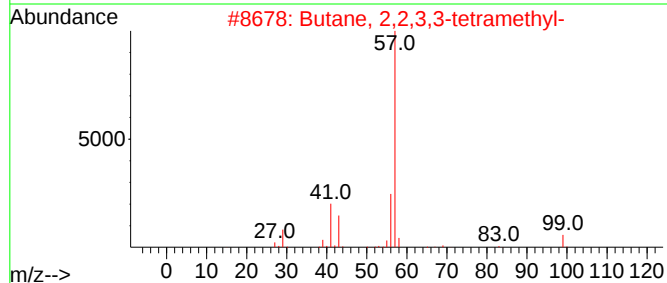
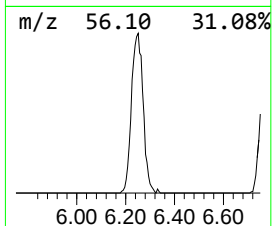
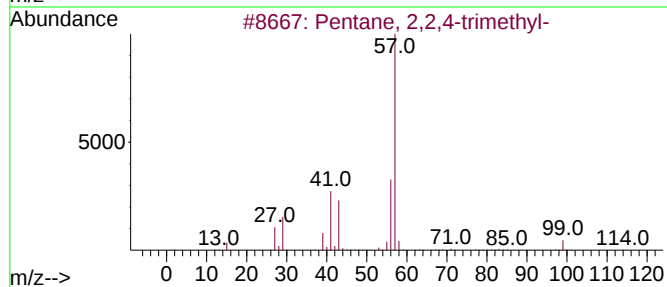
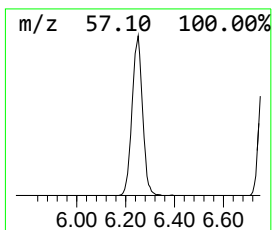
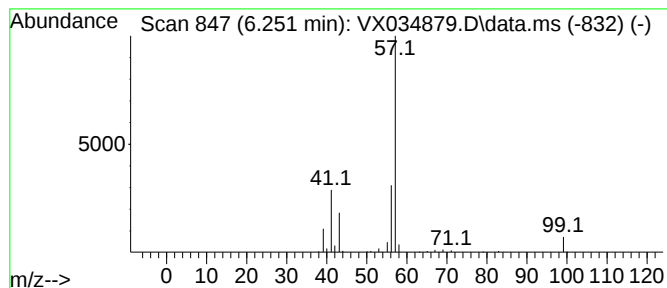
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Pentane, 2,2,4-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.251	8.30 ug/l	159050	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	72
2			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	72
3			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	72
4			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
5			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.270	6.5	ug/l	90773	1	5.556	702893	50.0
Pentane, 2,2,4-...	6.251	8.3	ug/l	159050	2	6.763	957701	50.0