

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074811.D
 Acq On : 07 Oct 2022 15:07
 Operator : JC\MD
 Sample : N5002-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 5486-3

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_N\methods\82N100522W.M
 Title : SW846 8260

Signal : TIC: VN074811.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	38	44	52	rBV	289932	499063	20.07%	4.667%
2	2.777	118	123	127	rBV2	93686	173802	6.99%	1.625%
3	4.747	452	458	469	rBV4	18821	57699	2.32%	0.540%
4	7.453	909	918	927	rBV	36800	93428	3.76%	0.874%
5	8.177	1030	1041	1046	rBV3	327173	790157	31.78%	7.388%
6	8.235	1046	1051	1060	rVB2	309787	695204	27.96%	6.501%
7	8.588	1101	1111	1122	rBV2	395622	911521	36.66%	8.523%
8	9.112	1191	1200	1210	rBV	489241	1008230	40.55%	9.428%
9	10.571	1440	1448	1457	rBV	1330590	2486113	100.00%	23.247%
10	11.870	1661	1669	1679	rBV	733233	1363355	54.84%	12.748%
11	12.853	1828	1836	1847	rBV	718774	1283326	51.62%	12.000%
12	13.794	1989	1996	2003	rBV	759356	1332600	53.60%	12.461%

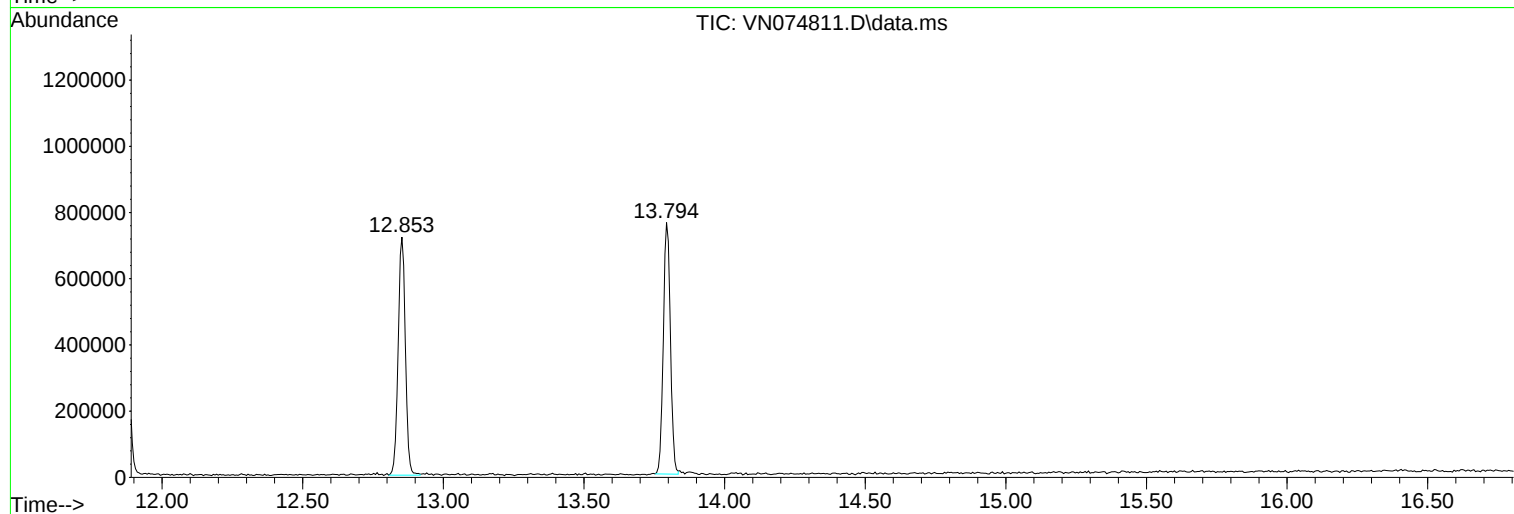
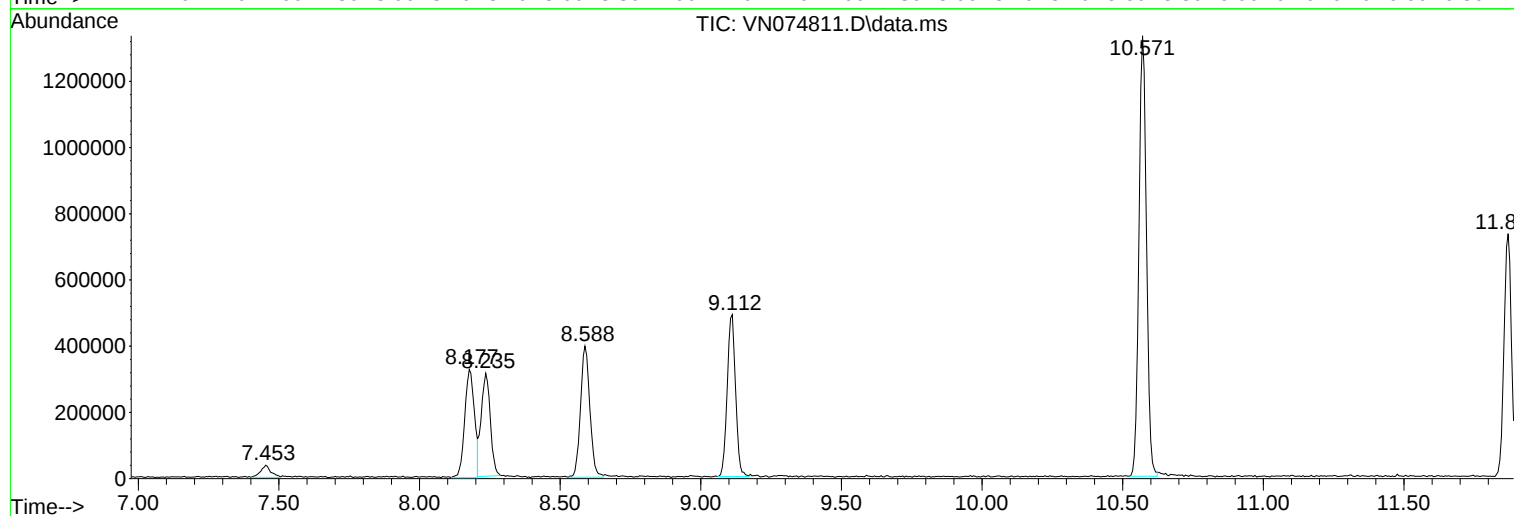
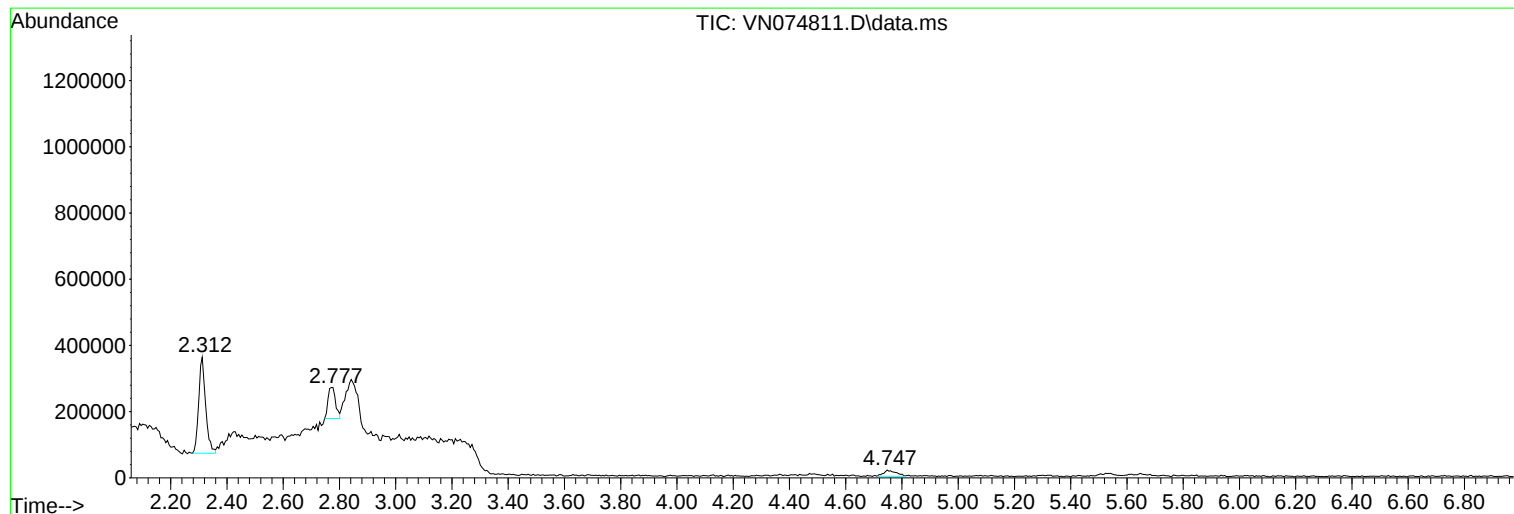
Sum of corrected areas: 10694498

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



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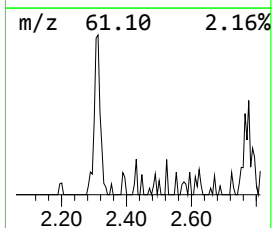
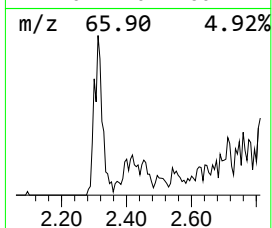
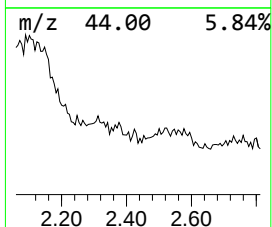
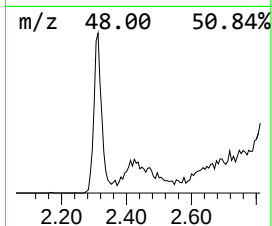
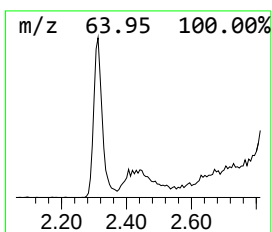
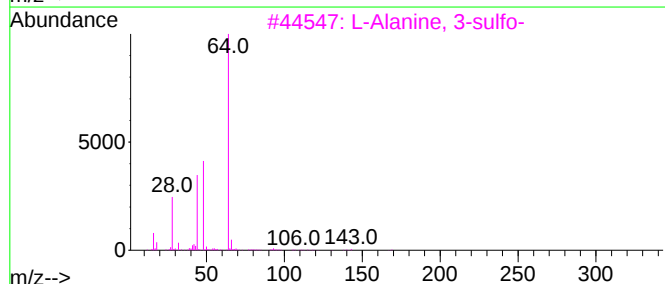
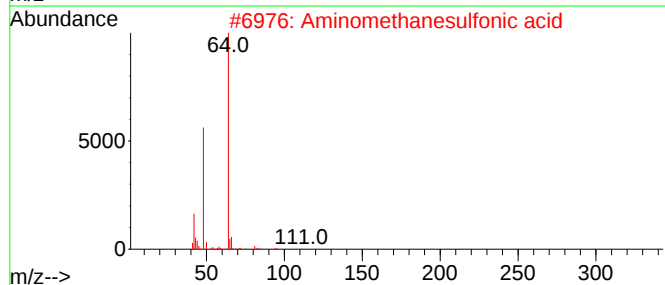
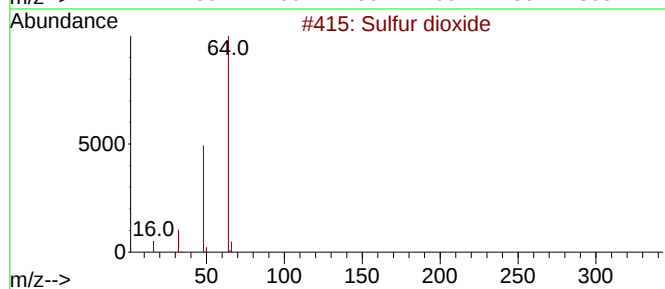
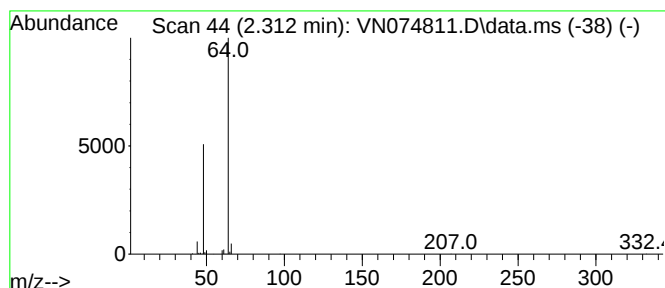
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	35.89 ug/l	499063	Pentafluorobenzene	8.235

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	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	7
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	3



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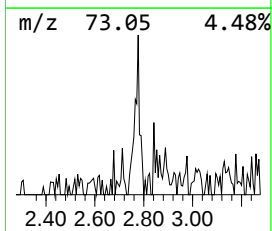
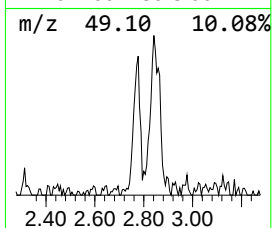
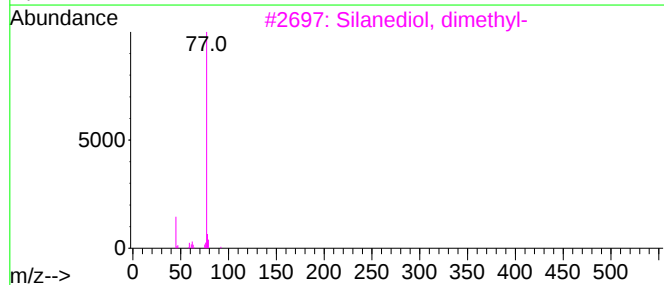
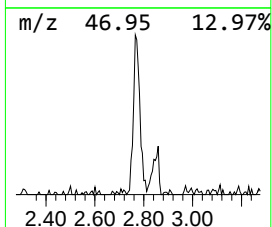
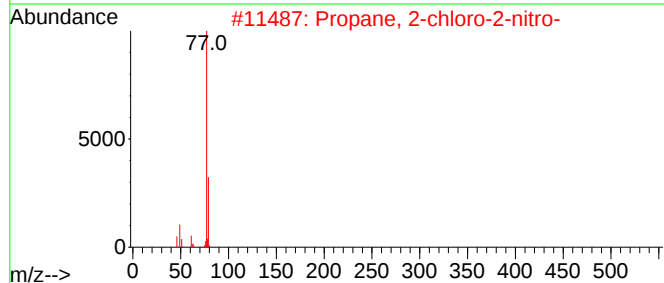
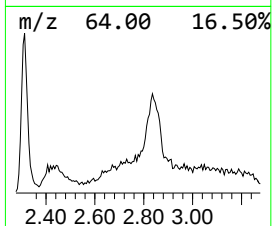
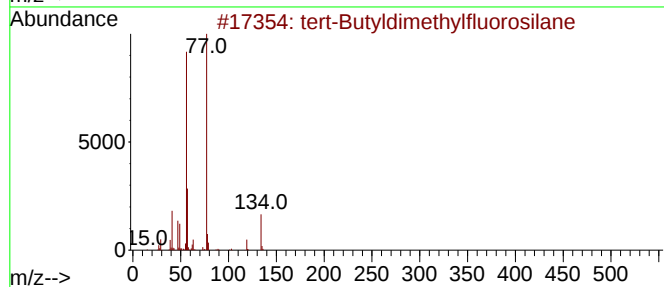
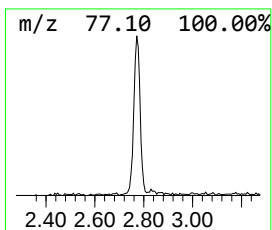
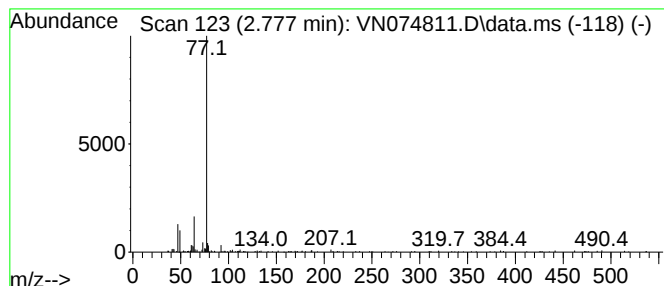
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Peak Number 2 unknown2.777 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.777	12.50 ug/l	173802	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			tert-Butyldimethylfluorosilane	134	C6H15FSi	1000366-62-3	39
2			Propane, 2-chloro-2-nitro-	123	C3H6ClNO2	000594-71-8	36
3			Silanediol, dimethyl-	92	C2H8O2Si	001066-42-8	33
4			Trimethylsilyl fluoride	92	C3H9FSi	000420-56-4	9
5			3,5-Hexadiyn-2-one	92	C6H4O	031097-80-0	9



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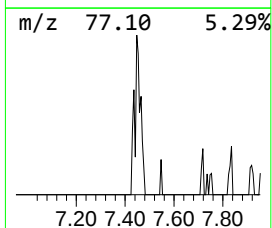
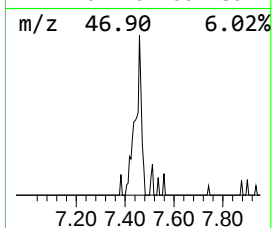
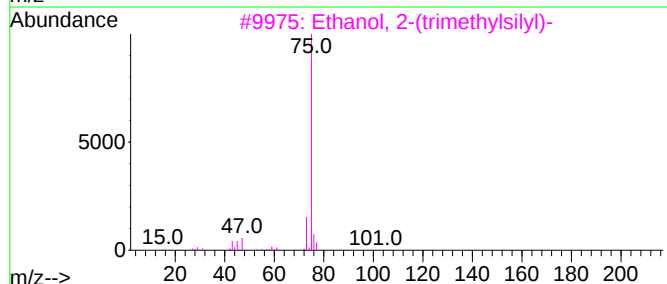
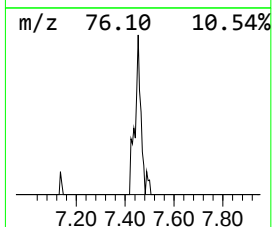
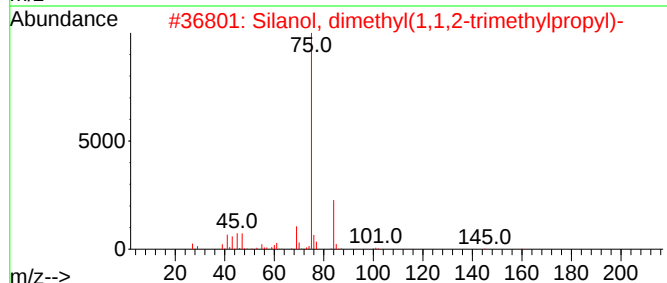
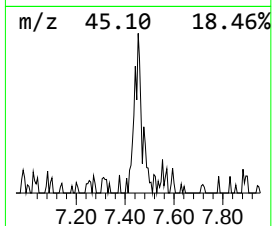
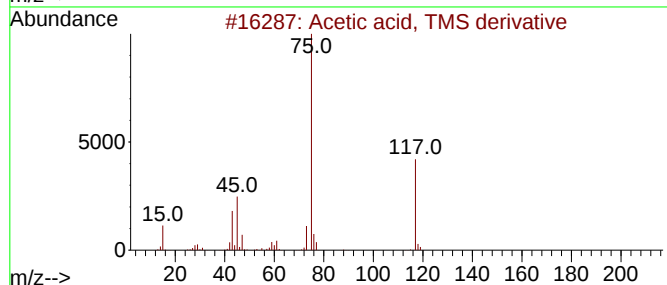
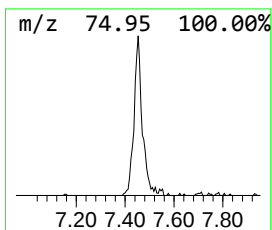
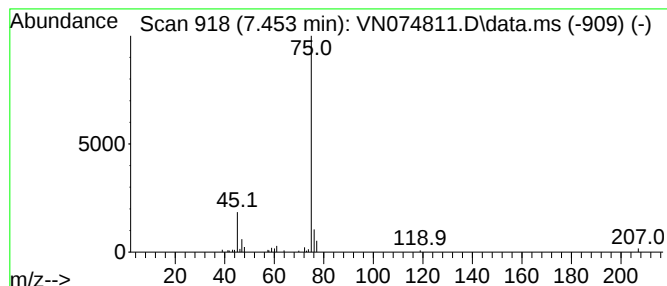
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Peak Number 3 Acetic acid, TMS derivative Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.453	6.72 ug/l	93428	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acetic acid, TMS derivative	132	C5H12O2Si	002754-27-0	64
2			Silanol, dimethyl(1,1,2-trimethylpropyl)-	160	C8H20OSi	055644-10-5	56
3			Ethanol, 2-(trimethylsilyl)-	118	C5H14OSi	002916-68-9	50
4			Propanoic acid, TMS derivative	146	C6H14O2Si	016844-98-7	43
5			2-Dimethyl(dichloromethyl)silylo...	214	C7H16Cl2OSi	1000280-00-3	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	35.9	ug/l	499063	1	8.235	695204	50.0
unknown2.777	2.777	12.5	ug/l	173802	1	8.235	695204	50.0
Acetic acid, TM...	7.453	6.7	ug/l	93428	1	8.235	695204	50.0