

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN112923\
 Data File : VN080307.D
 Acq On : 29 Nov 2023 14:10
 Operator : JC\MD
 Sample : 05470-01
 Misc : 5.01g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 SB-1

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\82N111623W.M

Title : SW846 8260

Signal : TIC: VN080307.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.283	49	56	65	rBV2	29355	62156	5.89%	1.052%
2	2.889	137	159	160	rBV5	42031	148552	14.07%	2.515%
3	8.165	1043	1056	1060	rBV2	162268	384212	36.39%	6.504%
4	8.218	1060	1065	1078	rVB	236634	534328	50.61%	9.045%
5	8.577	1117	1126	1140	rBV	157460	359771	34.08%	6.090%
6	9.100	1205	1215	1224	rBV	355120	727413	68.90%	12.314%
7	10.565	1455	1464	1479	rBV	578300	1055803	100.00%	17.873%
8	11.865	1676	1685	1698	rBV	526511	959570	90.89%	16.244%
9	12.853	1842	1853	1865	rBV	431319	752467	71.27%	12.738%
10	13.794	2006	2013	2022	rBV	535321	896536	84.92%	15.177%
11	15.500	2300	2303	2309	rBV6	6623	10737	1.02%	0.182%
12	15.641	2322	2327	2334	rVB3	8796	15656	1.48%	0.265%

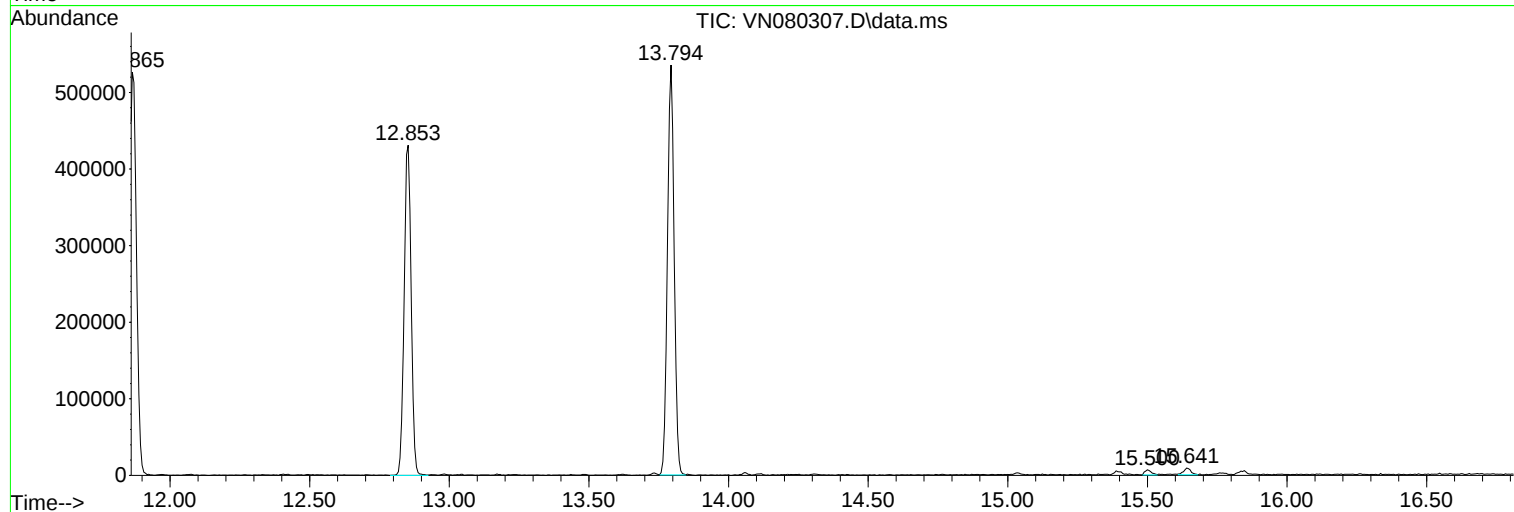
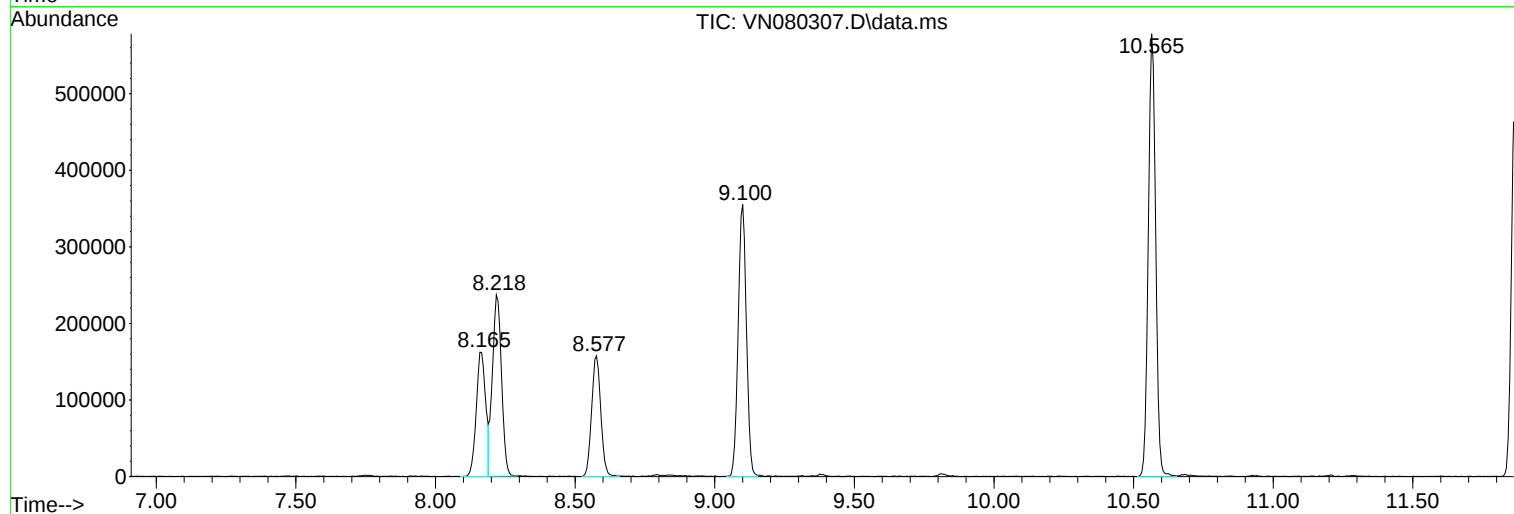
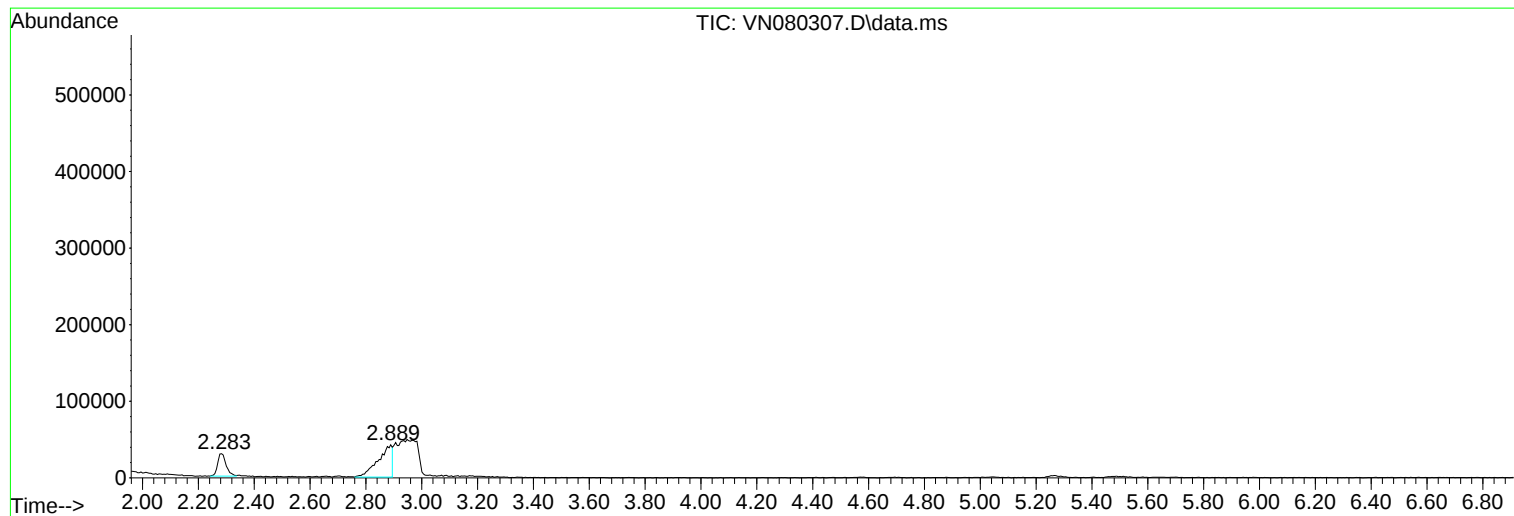
Sum of corrected areas: 5907201

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N111623W.M
Quant Title : SW846 8260

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



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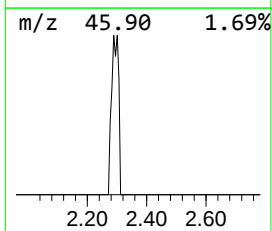
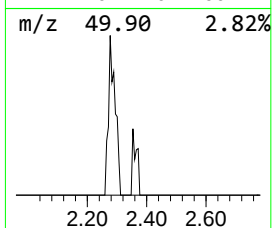
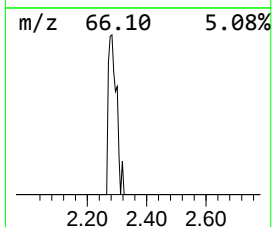
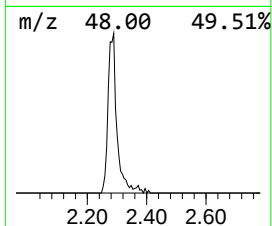
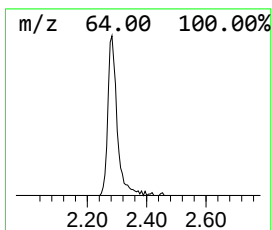
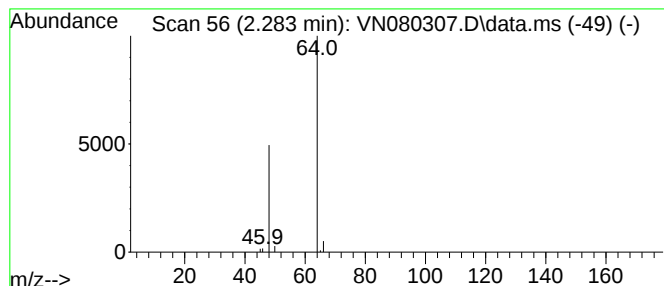
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Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.283	5.82 ug/l	62156	Pentafluorobenzene	8.218

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			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3



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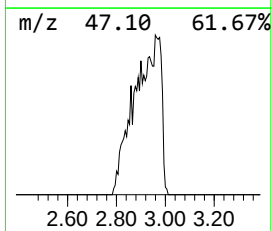
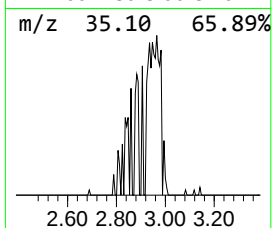
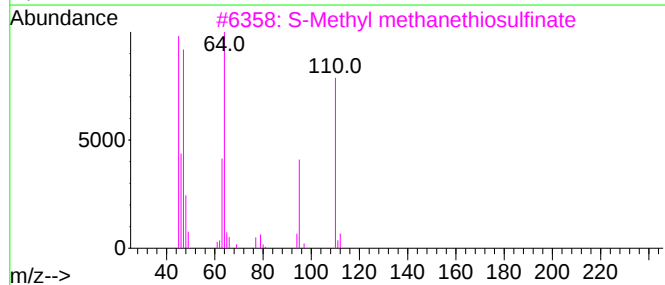
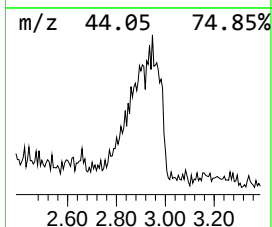
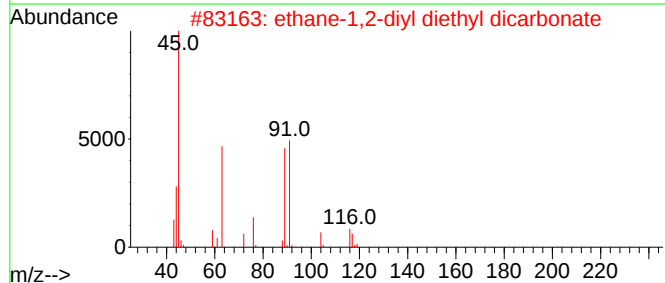
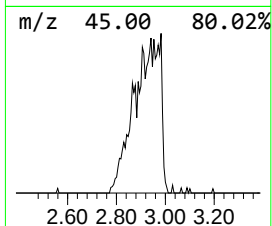
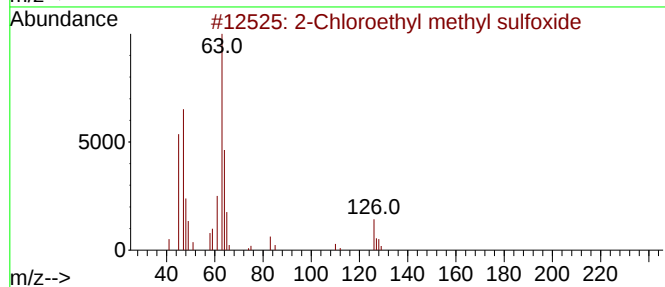
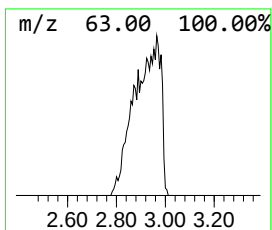
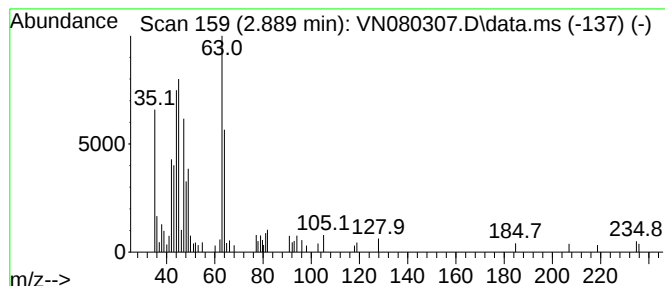
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Peak Number 2 unknown2.889 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.889	13.90 ug/l	148552	Pentafluorobenzene	8.218

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	40
2			ethane-1,2-diyl diethyl dicarbonate	206	C8H14O6	1000456-16-7	17
3			S-Methyl methanethiosulfinate	110	C2H6OS2	013882-12-7	16
4			Ethene, (methylsulfonyl)-	106	C3H6O2S	003680-02-2	10
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.283	5.8	ug/l	62156	1	8.218	534328	50.0
unknown2.889	2.889	13.9	ug/l	148552	1	8.218	534328	50.0