

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN122123\
 Data File : VN080589.D
 Acq On : 21 Dec 2023 21:23
 Operator : JC\MD
 Sample : 05978-01 20X
 Misc : 1.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 27 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 N41547

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\82N121223W.M
 Title : SW846 8260

Signal : TIC: VN080589.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.289	47	57	67	rBV	181464	387538	21.91%	3.749%
2	2.442	72	83	86	rBV2	30191	95508	5.40%	0.924%
3	7.424	920	930	940	rBV2	14001	38967	2.20%	0.377%
4	8.165	1046	1056	1061	rBV	260178	622890	35.22%	6.025%
5	8.224	1061	1066	1079	rVB	401228	870470	49.22%	8.420%
6	8.577	1117	1126	1138	rBV	239351	548043	30.99%	5.301%
7	9.100	1205	1215	1232	rBV	638105	1323441	74.83%	12.801%
8	10.571	1453	1465	1474	rBV	942170	1755439	99.25%	16.980%
9	11.865	1677	1685	1696	rBV	993801	1768653	100.00%	17.108%
10	12.847	1845	1852	1862	rBV	698890	1207628	68.28%	11.681%
11	13.729	1997	2002	2006	rBV2	16191	26919	1.52%	0.260%
12	13.794	2006	2013	2023	rVB	931217	1572525	88.91%	15.211%
13	14.059	2049	2058	2062	rBV2	15223	25579	1.45%	0.247%
14	15.394	2280	2285	2291	rVB4	11588	22801	1.29%	0.221%
15	15.500	2297	2303	2309	rVB5	14615	24824	1.40%	0.240%
16	15.635	2320	2326	2334	rBV	11405	23913	1.35%	0.231%
17	15.841	2353	2361	2369	rVB7	12090	23273	1.32%	0.225%

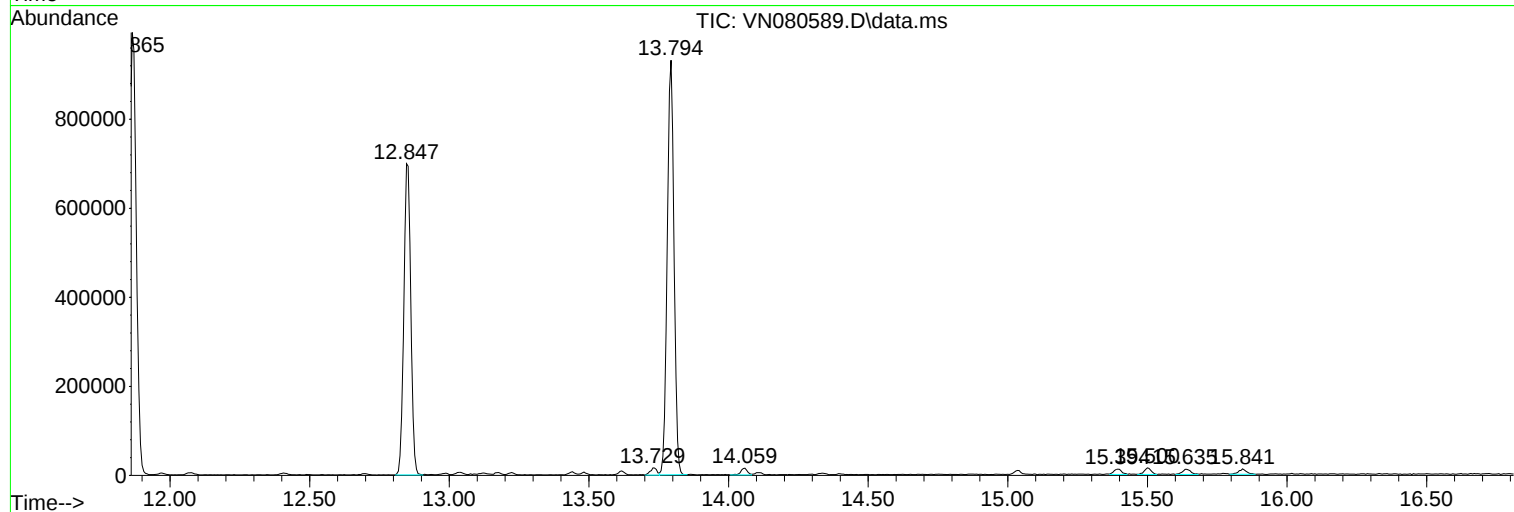
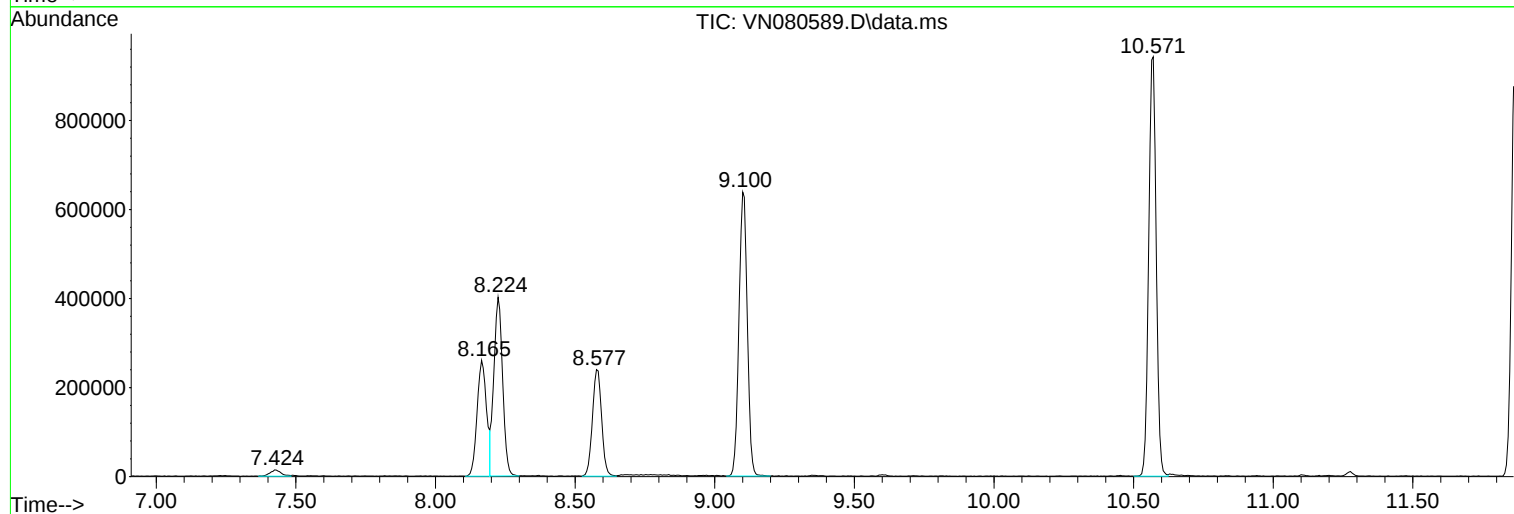
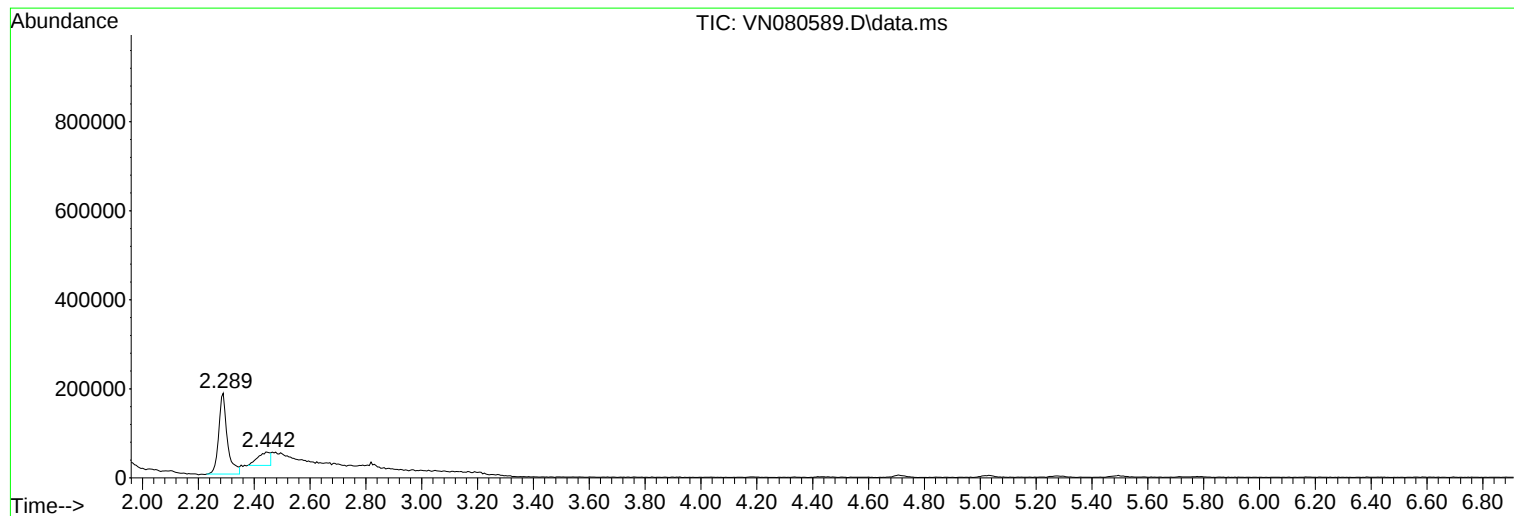
Sum of corrected areas: 10338411

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
Quant Title : SW846 8260

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



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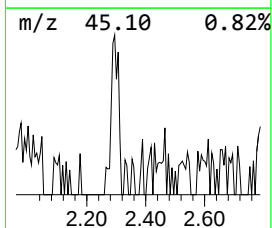
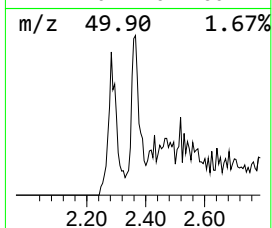
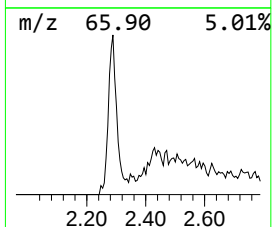
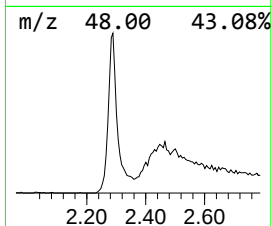
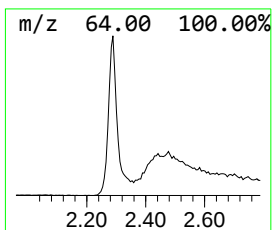
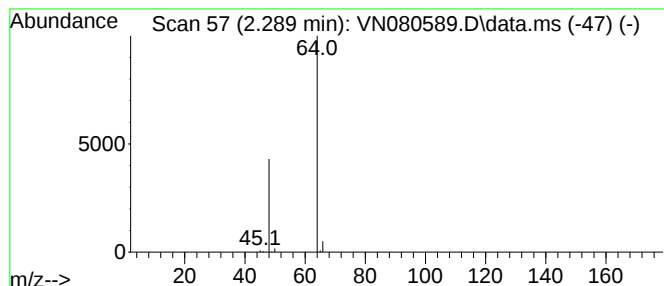
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N121223W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.289	22.26 ug/l	387538	Pentafluorobenzene	8.224

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



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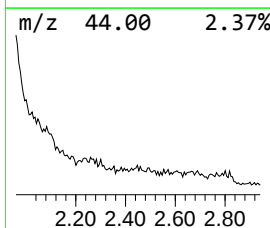
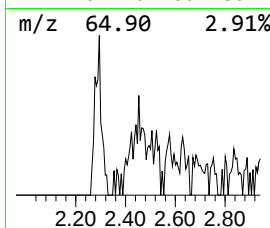
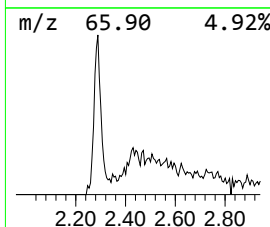
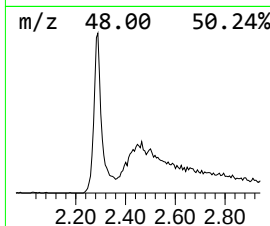
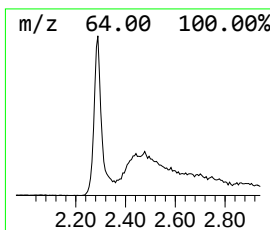
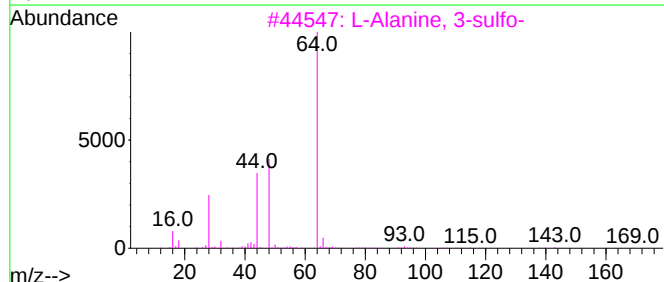
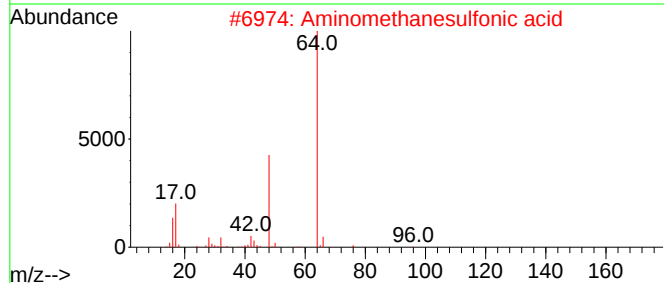
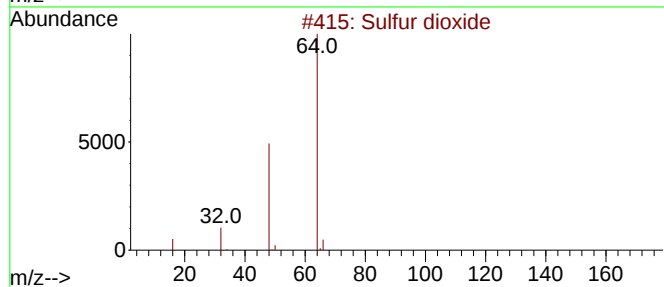
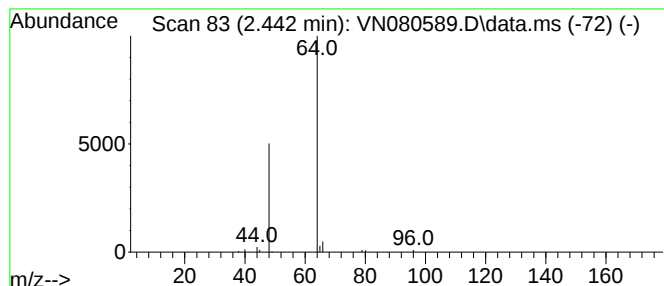
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Peak Number 2 Aminomethanesulfonic acid Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.442	5.49 ug/l	95508	Pentafluorobenzene	8.224

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			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9
5			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9



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TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.289	22.3	ug/l	387538	1	8.224	870470	50.0
Aminomethanesul...	2.442	5.5	ug/l	95508	1	8.224	870470	50.0