

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN102122\
 Data File : VN074973.D
 Acq On : 21 Oct 2022 19:49
 Operator : JC\MD
 Sample : N5222-19
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-17

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\82N102022W.M
 Title : SW846 8260

Signal : TIC: VN074973.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.301	34	42	50	rBV	156477	388907	5.59%	1.170%
2	2.830	125	132	141	rVB2	102279	283186	4.07%	0.852%
3	7.453	907	918	924	rBV2	28131	84104	1.21%	0.253%
4	7.977	996	1007	1021	rVB2	359439	887706	12.76%	2.670%
5	8.177	1029	1041	1045	rBV	881583	2103545	30.23%	6.327%
6	8.230	1045	1050	1059	rVB	1025602	2262946	32.52%	6.807%
7	8.588	1100	1111	1122	rBV	1007482	2299041	33.03%	6.915%
8	9.106	1190	1199	1210	rBV	1425274	2858923	41.08%	8.599%
9	10.571	1437	1448	1465	rBV	3868380	6959474	100.00%	20.933%
10	11.106	1532	1539	1546	rVB3	62749	117852	1.69%	0.354%
11	11.865	1660	1668	1681	rBV	2262654	4084755	58.69%	12.286%
12	12.853	1827	1836	1845	rBV	2852895	4917722	70.66%	14.792%
13	13.488	1936	1944	1949	rBV2	40533	70710	1.02%	0.213%
14	13.794	1988	1996	2006	rVB	3080750	5158050	74.12%	15.514%
15	15.541	2279	2293	2301	rBV6	61591	212091	3.05%	0.638%
16	15.641	2303	2310	2320	rVB	223550	469738	6.75%	1.413%
17	16.776	2497	2503	2505	rBV4	54910	88055	1.27%	0.265%

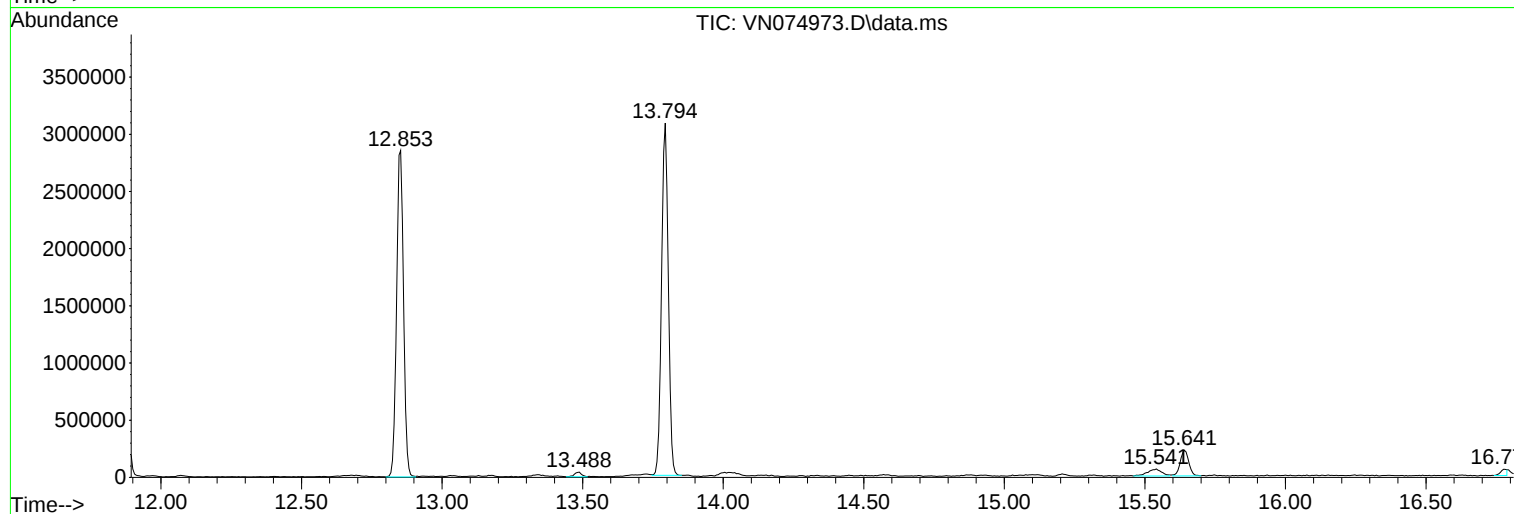
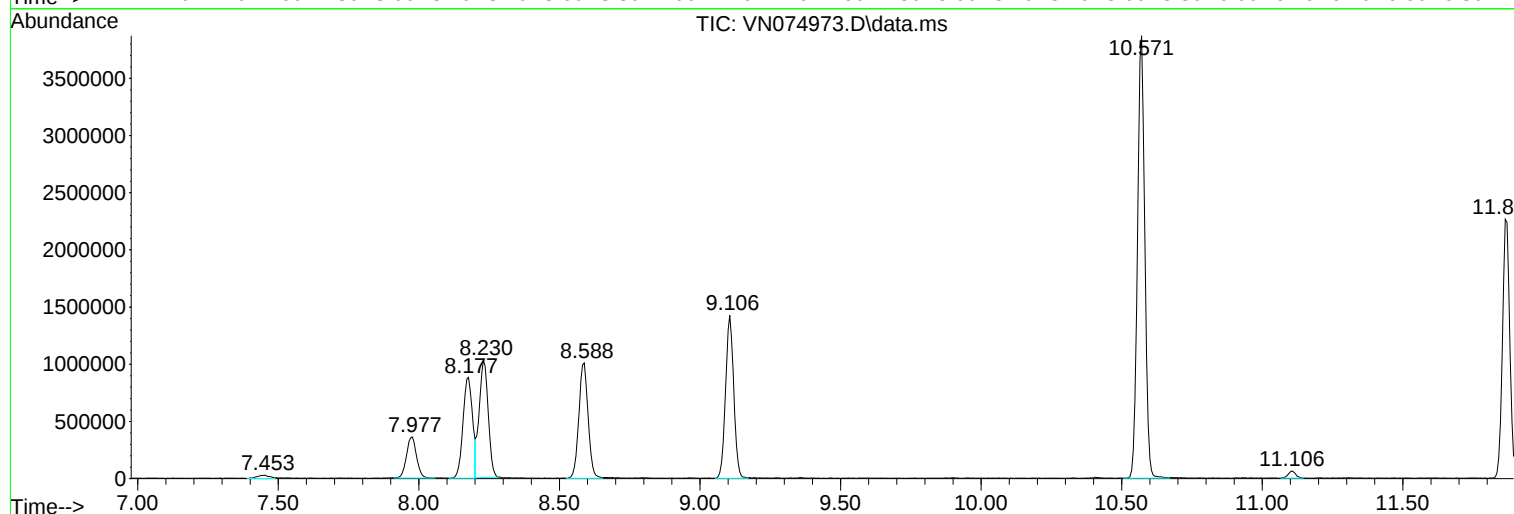
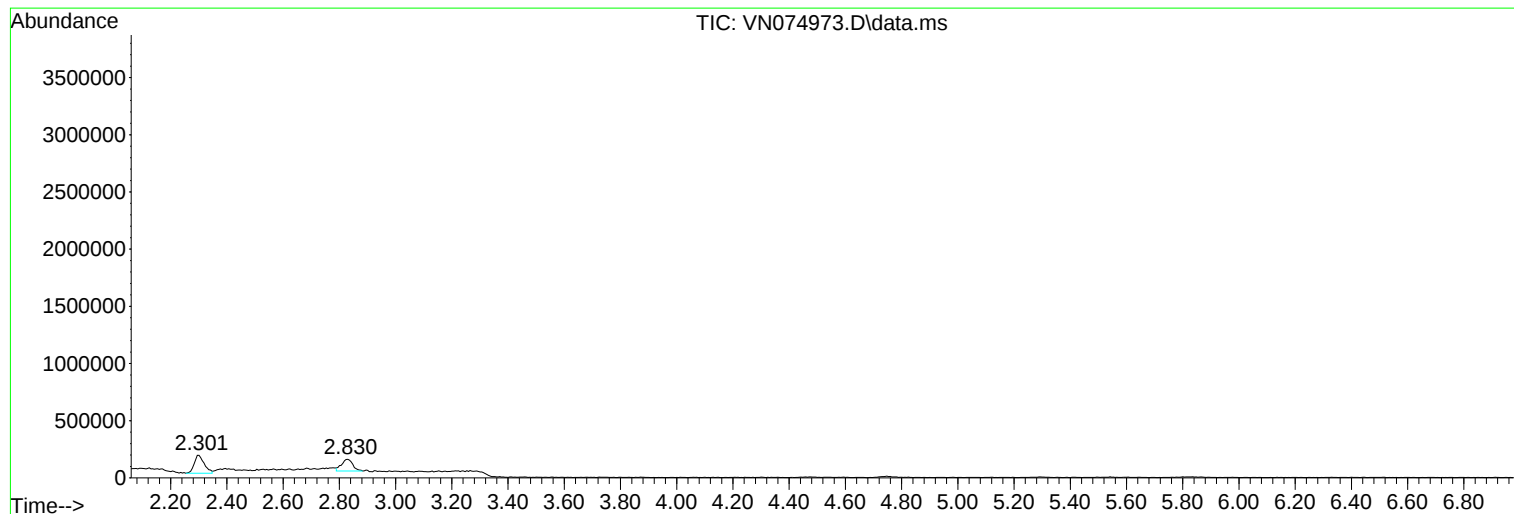
Sum of corrected areas: 33246805

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N102022W.M
Quant Title : SW846 8260

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



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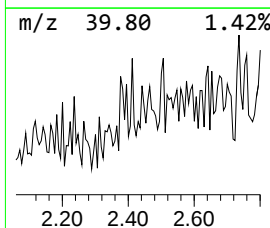
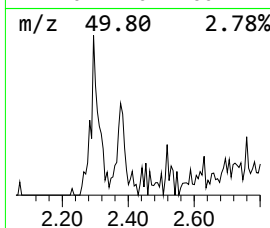
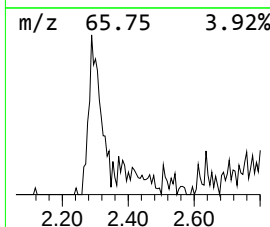
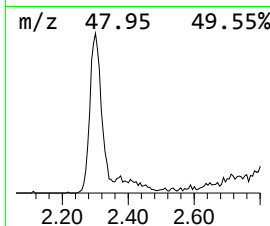
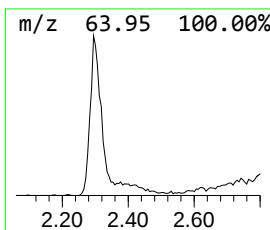
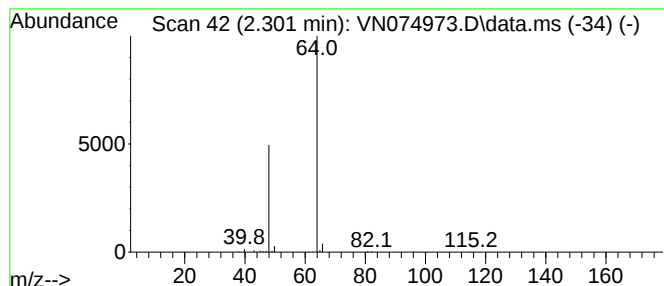
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Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.301	8.59 ug/l	388907	Pentafluorobenzene	8.230

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	64
4			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9
5			(N-(-2-Acetamido))-2-aminoethane...	182	C4H10N2O4S	007365-82-4	9



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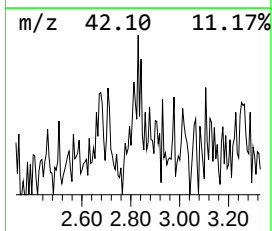
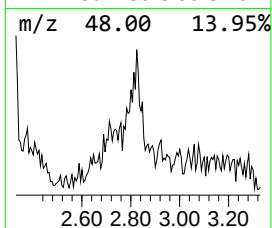
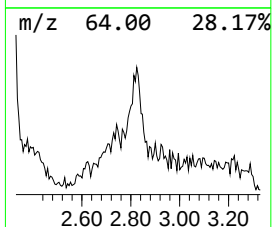
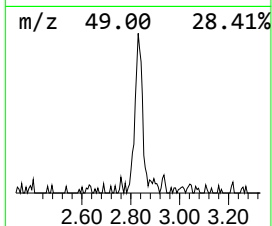
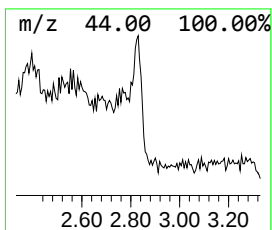
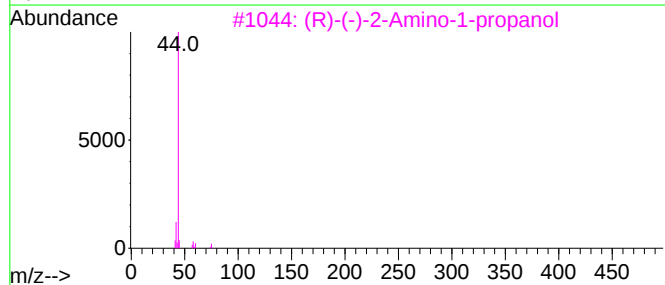
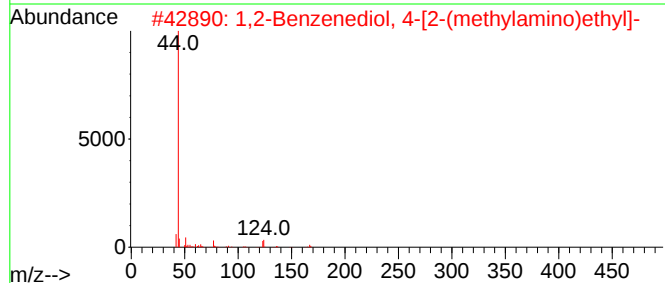
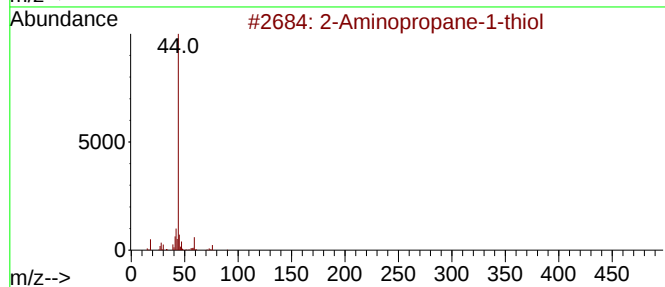
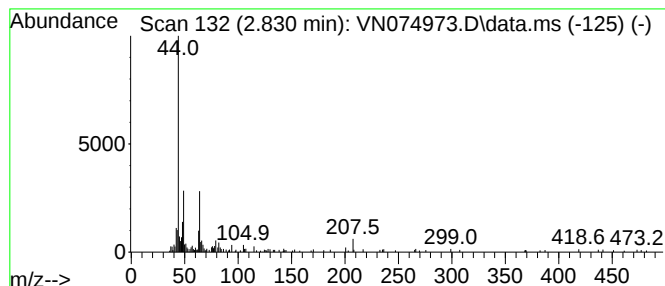
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Peak Number 2 unknown2.830 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.830	6.26 ug/l	283186	Pentafluorobenzene	8.230

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Aminopropane-1-thiol			91	C3H9NS	010229-29-5	27
2	1,2-Benzenediol, 4-[2-(methylami...			167	C9H13NO2	000501-15-5	22
3	(R)-(-)-2-Amino-1-propanol			75	C3H9NO	035320-23-1	22
4	Cyclohexanol, 2-(methylaminometh...			143	C8H17NO	077612-16-9	22
5	n-Hexylmethylaniline			115	C7H17N	035161-70-7	12



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.301	8.6	ug/l	388907	1	8.230	2262950	50.0
unknown2.830	2.830	6.3	ug/l	283186	1	8.230	2262950	50.0