

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091922\
 Data File : VN074590.D
 Acq On : 19 Sep 2022 16:52
 Operator : JC\MD
 Sample : N4680-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 5869-2

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\82N091522W.M

Title : SW846 8260

Signal : TIC: VN074590.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	59	rBV	162851	317486	18.29%	3.162%
2	2.622	122	125	127	rBV4	24311	33685	1.94%	0.335%
3	2.693	131	137	140	rBV4	51099	110010	6.34%	1.096%
4	7.951	1020	1031	1036	rBV2	244097	594248	34.23%	5.918%
5	8.016	1036	1042	1053	rVB	363212	845914	48.72%	8.424%
6	8.369	1092	1102	1115	rBV2	281708	641270	36.94%	6.386%
7	8.904	1184	1193	1203	rBV	613733	1257148	72.41%	12.519%
8	10.380	1436	1444	1460	rBV	967471	1736201	100.00%	17.290%
9	11.686	1657	1666	1678	rBV	979802	1673745	96.40%	16.668%
10	12.674	1827	1834	1844	rVB	778359	1273889	73.37%	12.686%
11	13.616	1985	1994	2005	rBV	912581	1505748	86.73%	14.995%
12	13.716	2005	2011	2017	rVB4	30822	52458	3.02%	0.522%

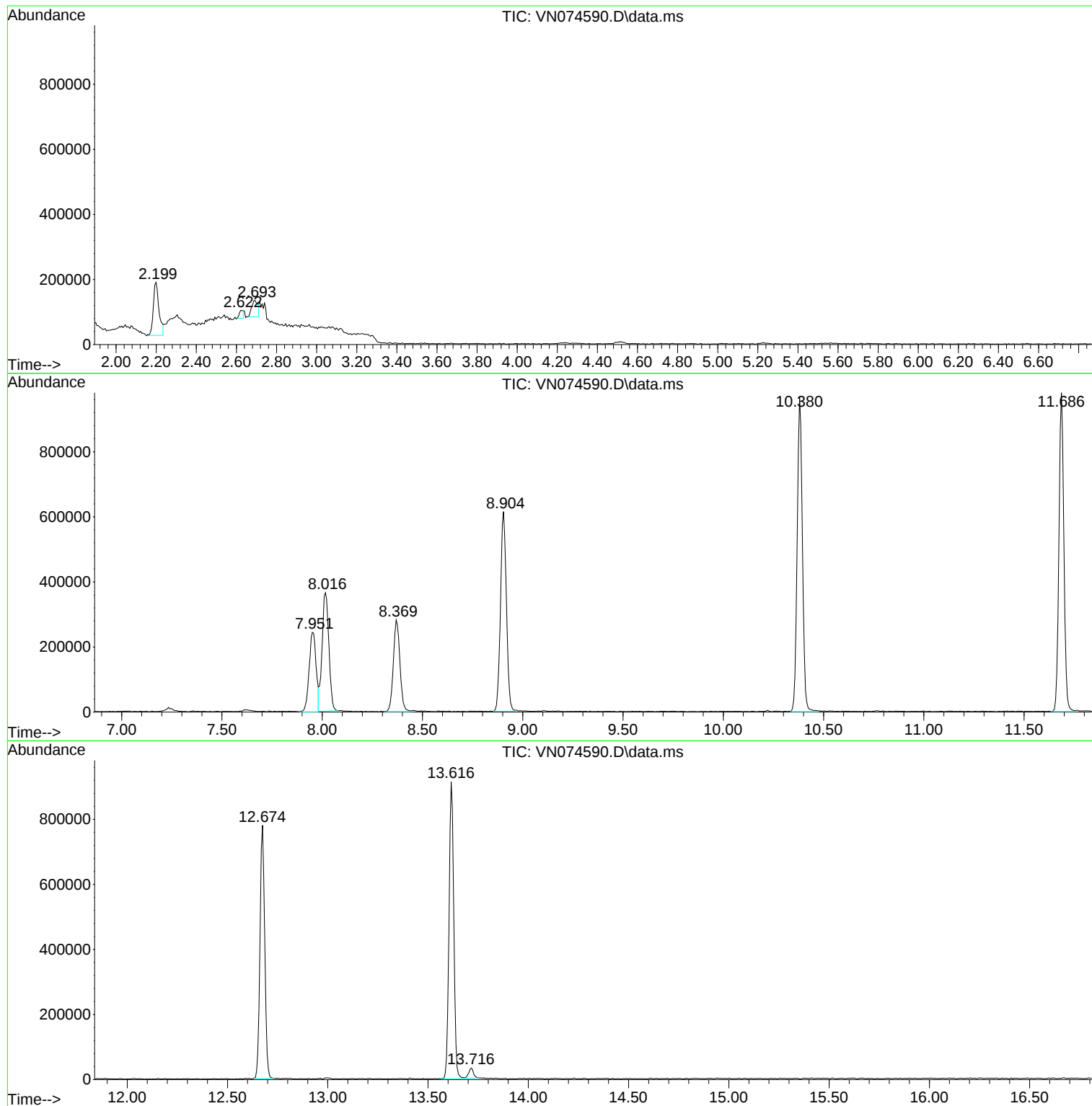
Sum of corrected areas: 10041802

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



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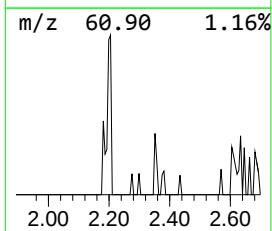
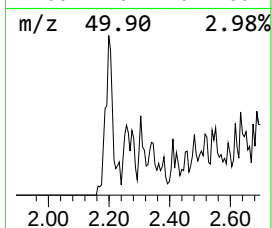
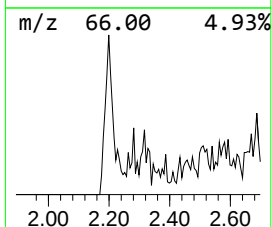
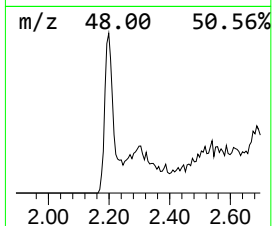
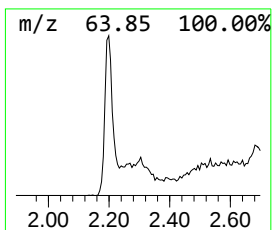
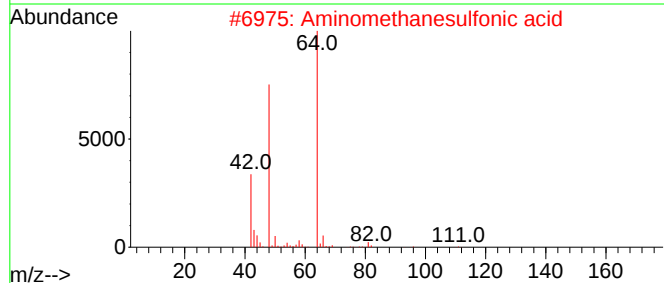
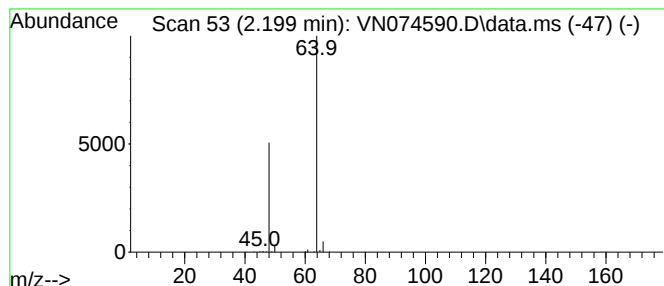
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Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	18.77 ug/l	317486	Pentafluorobenzene	8.016

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	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	4



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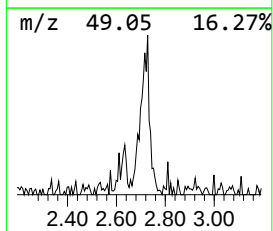
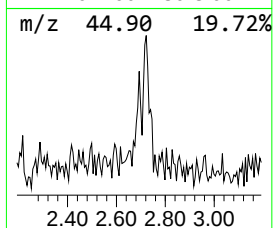
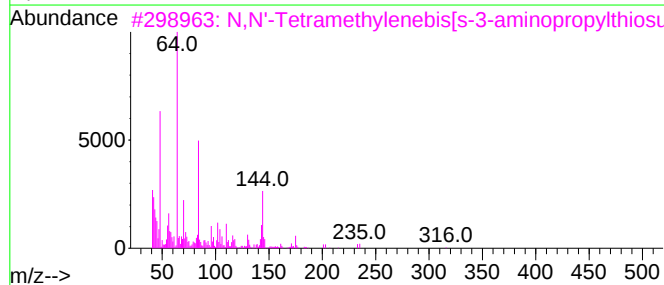
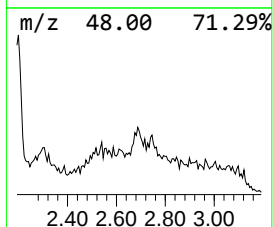
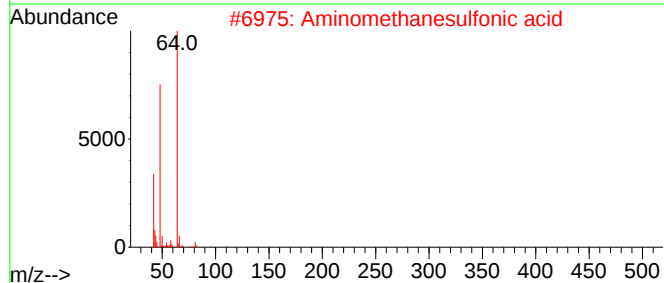
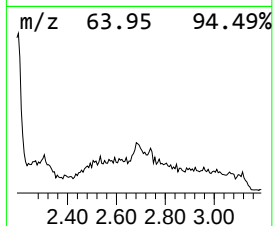
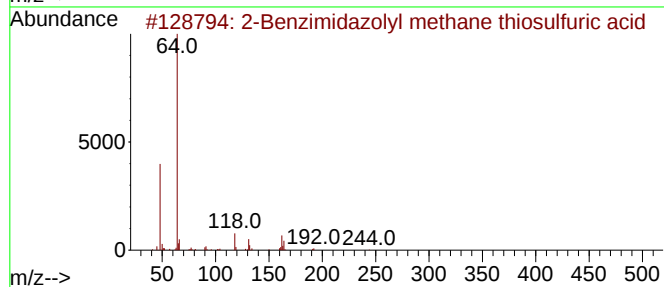
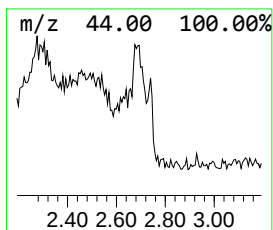
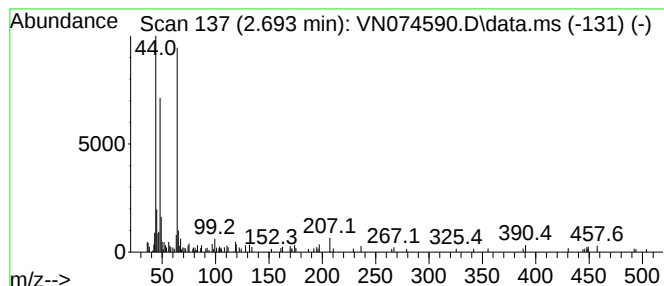
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Peak Number 2 unknown2.693 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.693	6.50 ug/l	110010	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	38		
2	Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	38		
3	N,N'-Tetramethylenebis[s-3-amino...	396	C10H24N2O6S4	035871-61-5	38		
4	Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	38		
5	Tetrazolo[1,5-b]pyridazine, 6-ch...	155	C4H2C1N5	021413-15-0	36		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	18.8	ug/l	317486	1	8.016	845914	50.0
unknown2.693	2.693	6.5	ug/l	110010	1	8.016	845914	50.0