

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074536.D
 Acq On : 17 Sep 2022 02:31
 Operator : JC\MD
 Sample : N4549-08
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-52

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: VN074536.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.198	47	53	59	rBV	257721	473403	24.51%	4.103%
2	2.687	132	136	141	rBV4	47639	129490	6.70%	1.122%
3	2.728	141	143	149	rVB2	80441	97363	5.04%	0.844%
4	3.187	219	221	229	rVB3	33341	53690	2.78%	0.465%
5	5.234	556	569	576	rBV4	10924	41161	2.13%	0.357%
6	7.228	901	908	916	rBV2	42261	114649	5.93%	0.994%
7	7.951	1020	1031	1036	rBV	268707	637963	33.02%	5.530%
8	8.016	1036	1042	1057	rVB	407584	939607	48.64%	8.144%
9	8.369	1093	1102	1112	rBV2	308251	703050	36.39%	6.094%
10	8.904	1184	1193	1206	rBV	678649	1385939	71.74%	12.013%
11	10.380	1435	1444	1458	rBV	1079978	1931815	100.00%	16.745%
12	11.686	1658	1666	1680	rBV	1080354	1872838	96.95%	16.234%
13	12.674	1827	1834	1844	rBV	873537	1435457	74.31%	12.442%
14	13.615	1987	1994	2006	rBV	1046587	1720363	89.05%	14.912%

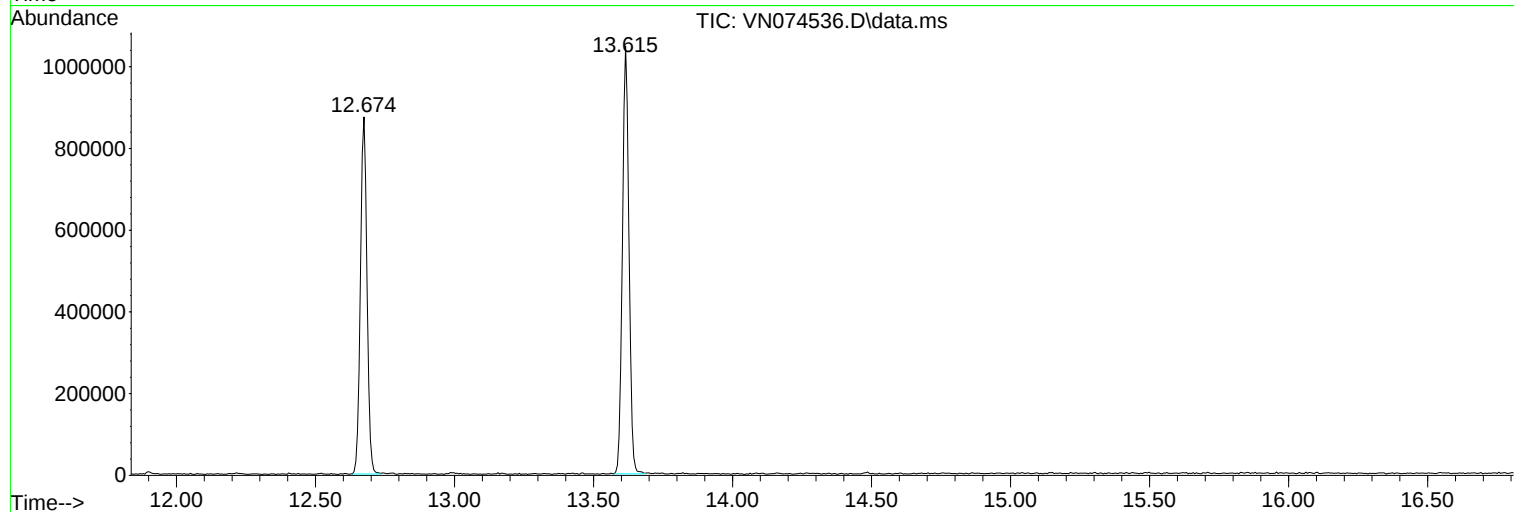
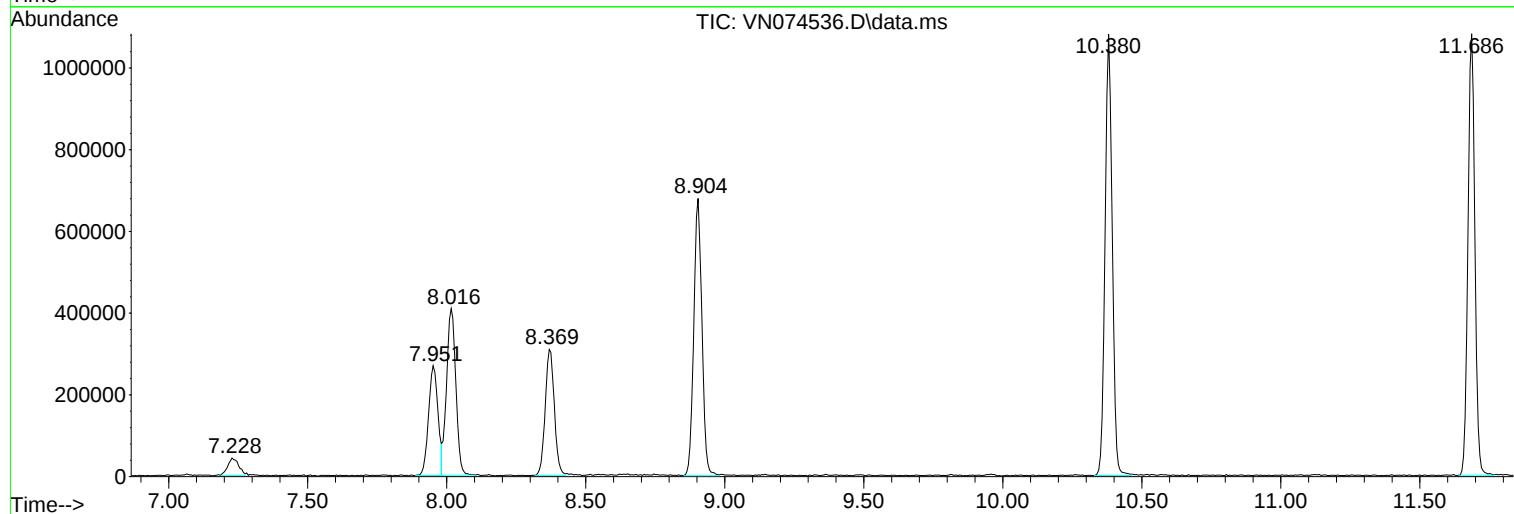
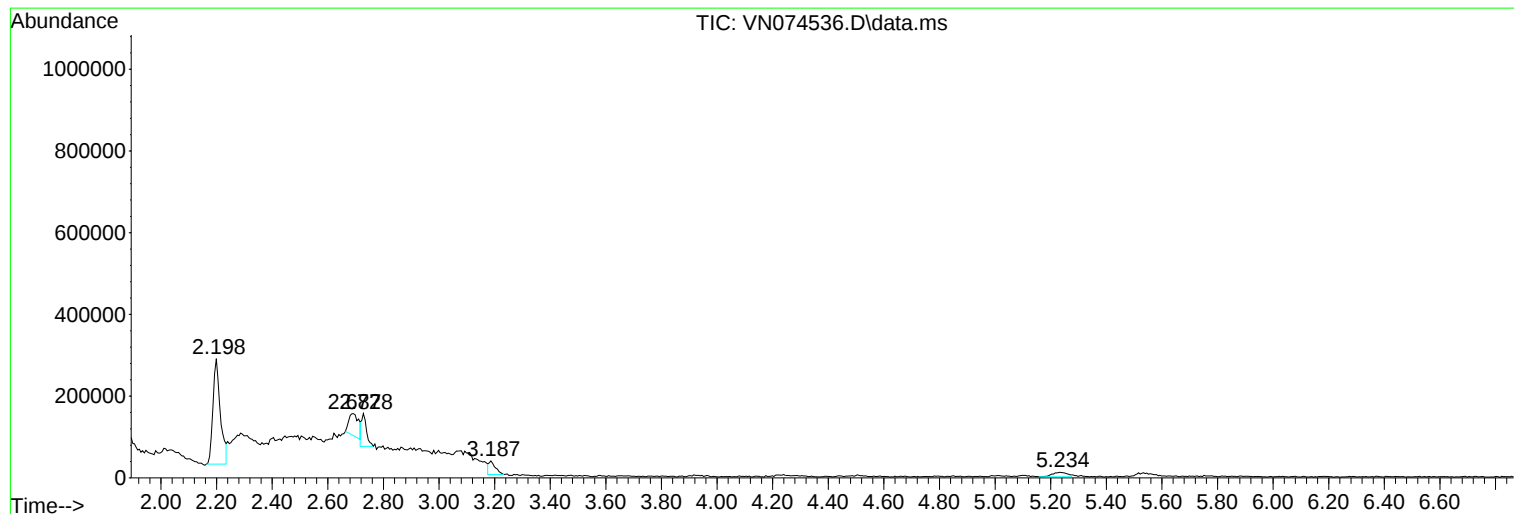
Sum of corrected areas: 11536788

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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



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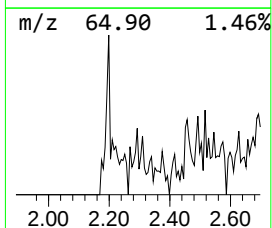
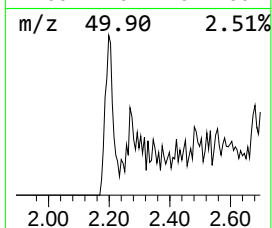
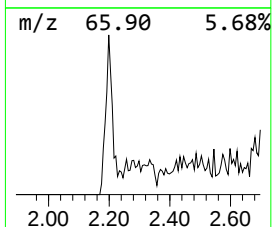
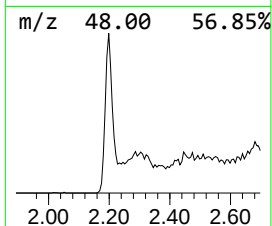
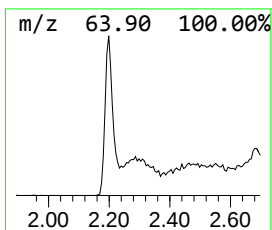
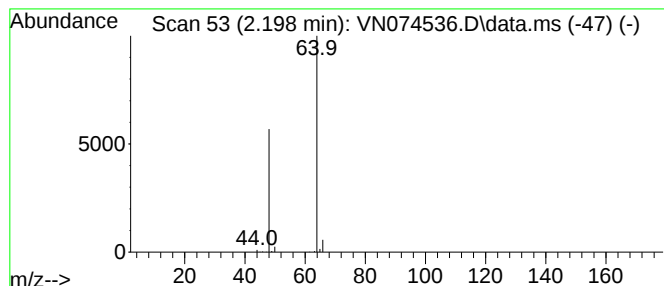
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.198	25.19 ug/l	473403	Pentafluorobenzene	8.016

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



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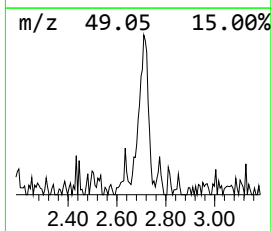
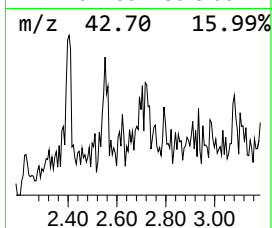
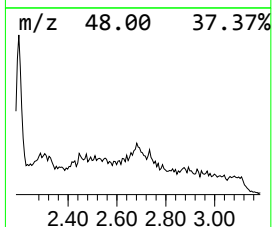
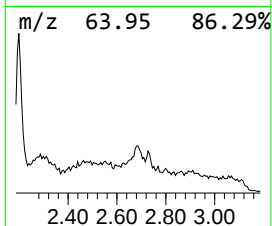
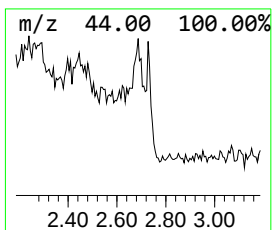
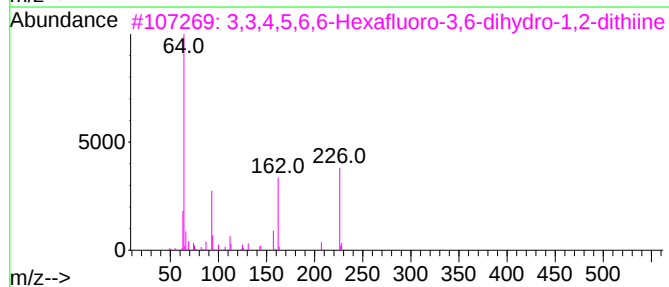
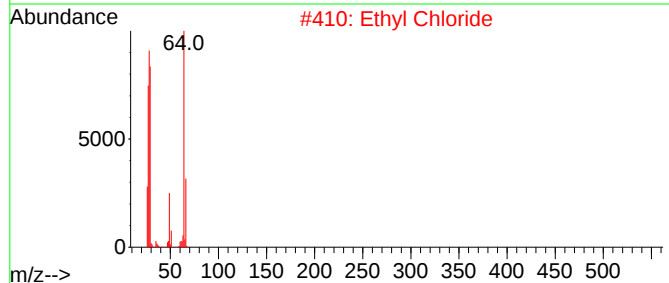
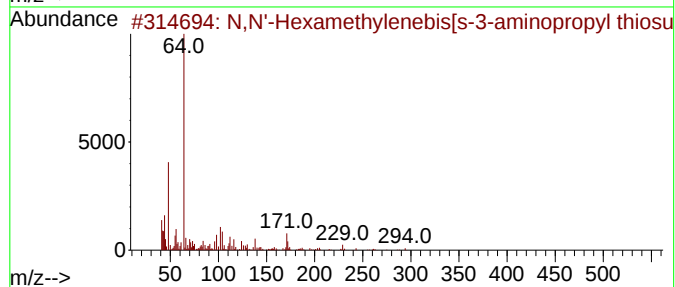
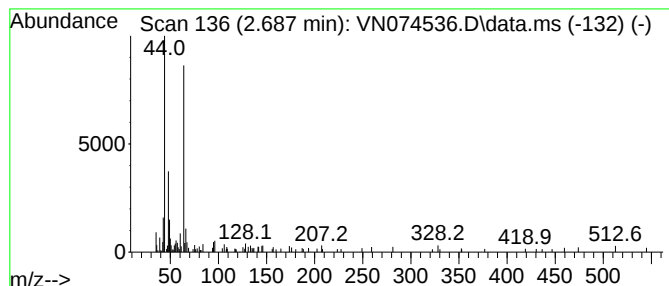
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Peak Number 2 N,N'-Hexamethylenebis[s-3-a... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
2.687	6.89 ug/l	129490	Pentafluorobenzene	8.016	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	N,N'-Hexamethylenebis[s-3-aminop...	424	C12H28N2O6S4	035871-55-7	50
2	Ethyl Chloride	64	C2H5Cl	000075-00-3	45
3	3,3,4,5,6,6-Hexafluoro-3,6-dihyd...	226	C4F6S2	1000461-21-0	43
4	L-Cysteine sulfinic acid	153	C3H7NO4S	001115-65-7	43
5	N,N'-Nonamethylenebis[-S-3-amino...	466	C15H34N2O6S4	035871-58-0	39



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.198	25.2	ug/l	473403	1	8.016	939607	50.0
N,N'-Hexamethyl...	2.687	6.9	ug/l	129490	1	8.016	939607	50.0