

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074534.D
 Acq On : 17 Sep 2022 01:43
 Operator : JC\MD
 Sample : N4549-06
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 40 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-50D

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: VN074534.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	60	rBV	234770	443490	22.18%	3.592%
2	2.693	132	137	141	rBV3	48807	103893	5.20%	0.841%
3	3.169	216	218	228	rVB5	34453	73306	3.67%	0.594%
4	5.534	606	620	633	rBV3	111506	418029	20.91%	3.385%
5	7.234	900	909	918	rBV2	44704	124534	6.23%	1.009%
6	7.951	1021	1031	1036	rBV2	271872	655645	32.79%	5.310%
7	8.016	1036	1042	1054	rVB	405619	948191	47.43%	7.679%
8	8.369	1091	1102	1115	rBV	314509	711082	35.57%	5.759%
9	8.569	1128	1136	1141	rBV6	8378	20840	1.04%	0.169%
10	8.904	1184	1193	1208	rBV	690546	1427871	71.42%	11.564%
11	10.380	1436	1444	1455	rBV	1110348	1999272	100.00%	16.191%
12	10.586	1469	1479	1484	rBV2	91737	161383	8.07%	1.307%
13	10.657	1484	1491	1497	rVB	94357	166393	8.32%	1.348%
14	11.686	1657	1666	1677	rBV	1099477	1899924	95.03%	15.387%
15	12.674	1826	1834	1845	rBV	885469	1462693	73.16%	11.846%
16	13.615	1985	1994	2009	rBV	1053371	1731428	86.60%	14.022%

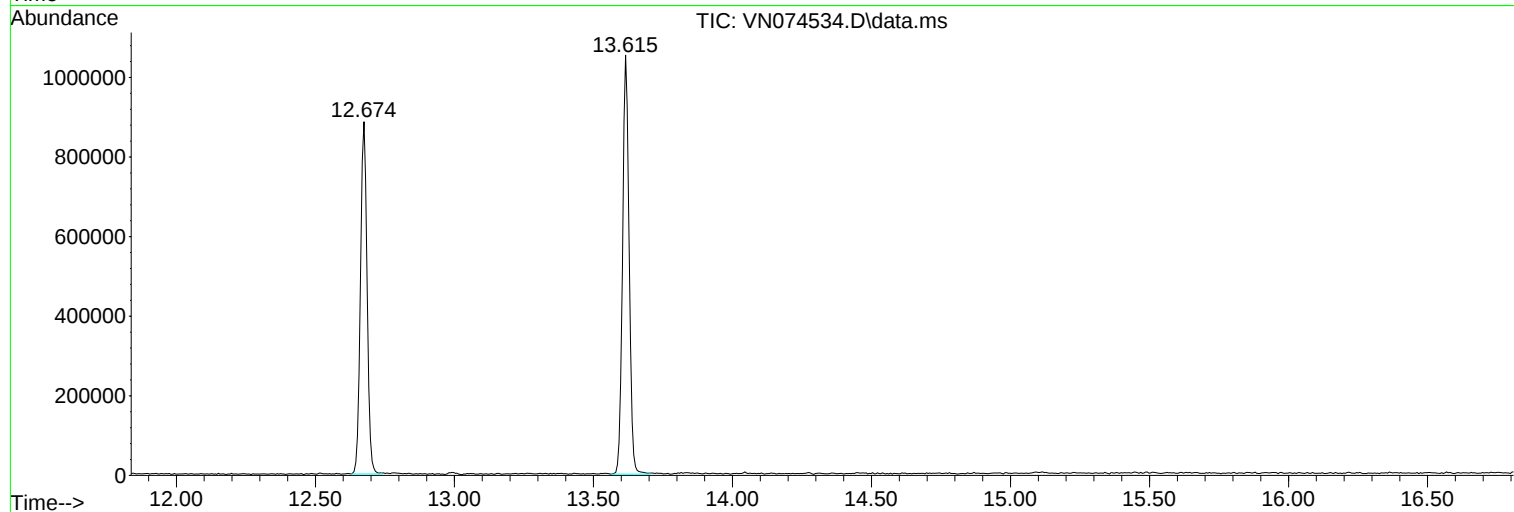
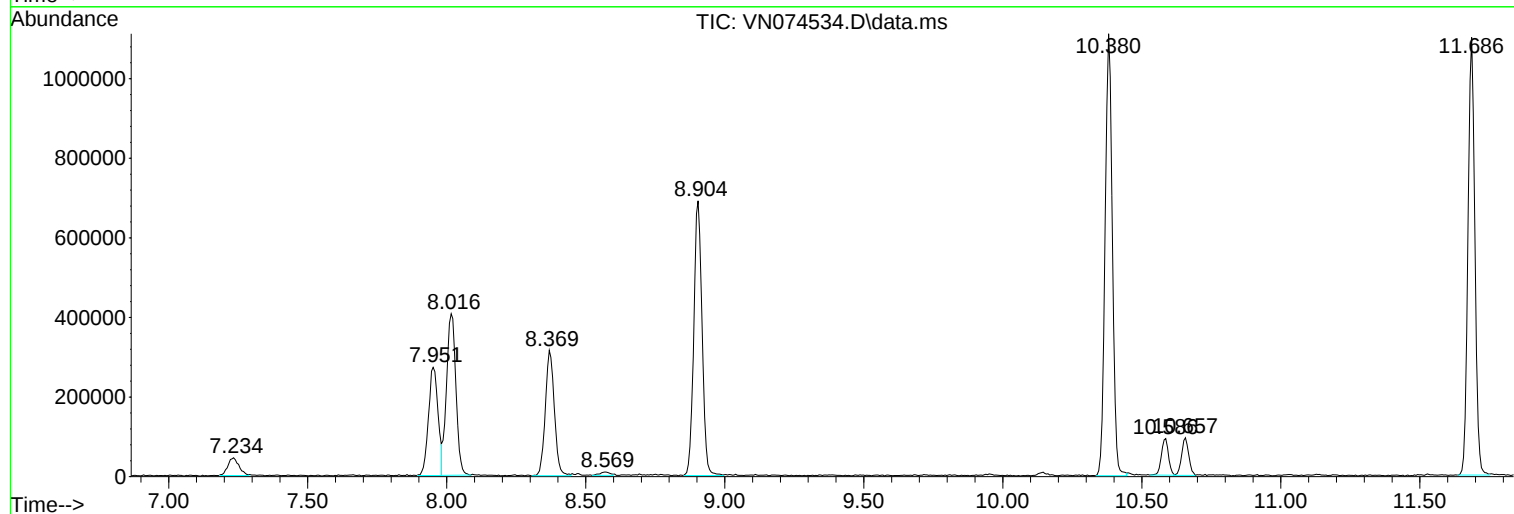
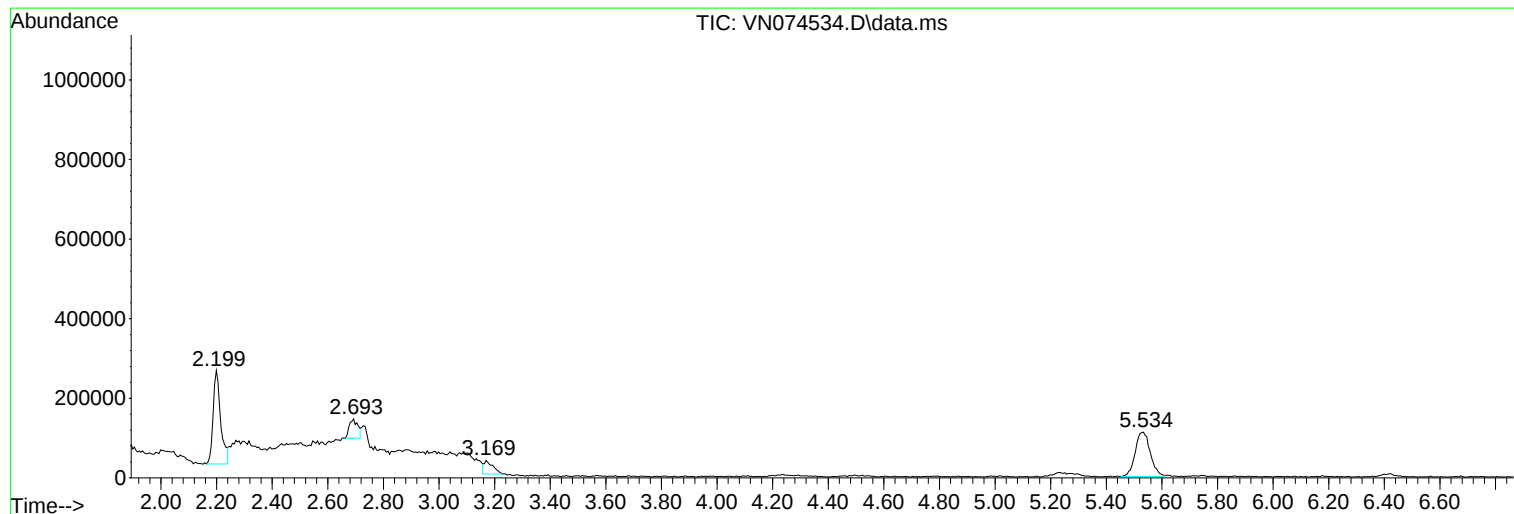
Sum of corrected areas: 12347974

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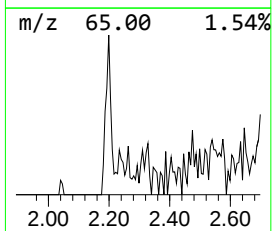
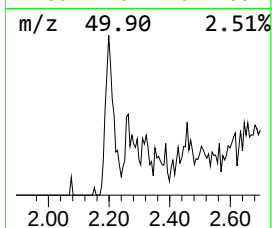
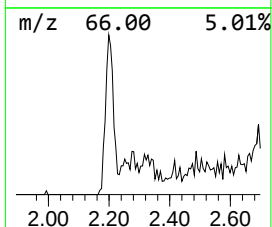
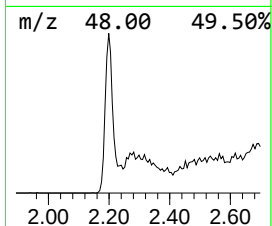
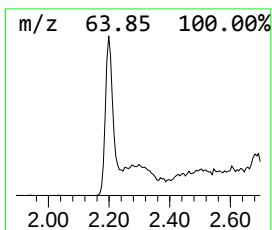
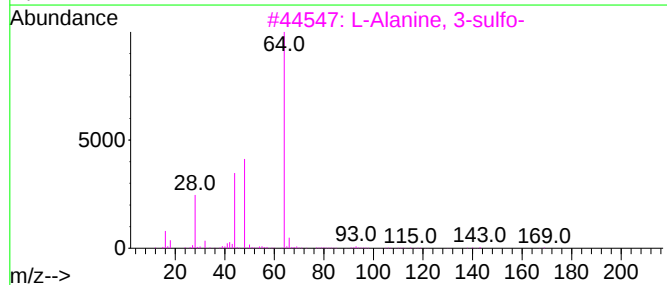
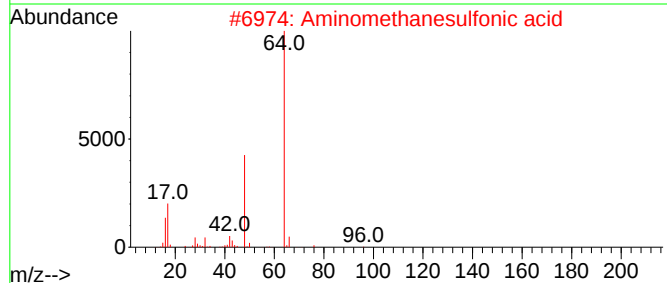
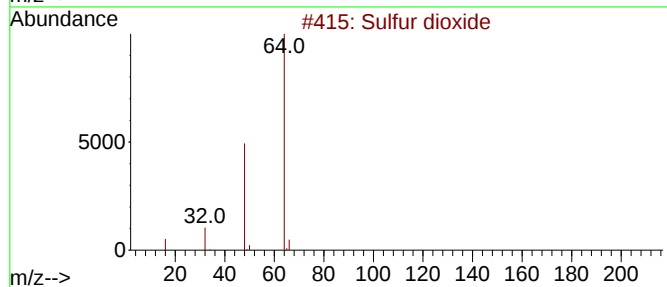
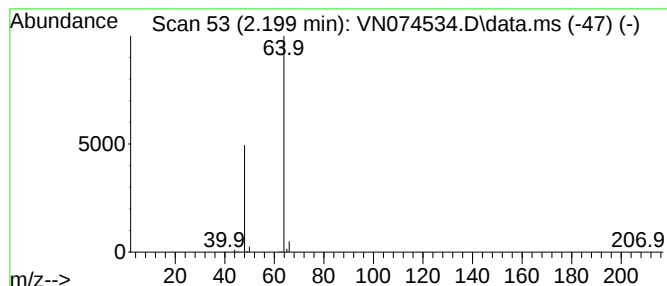
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
Quant Title : SW846 8260

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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.
2.199	23.39 ug/l	443490	Pentafluorobenzene	8.022

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	3



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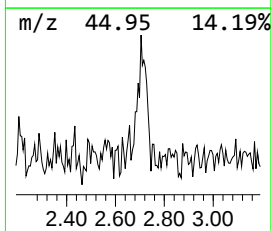
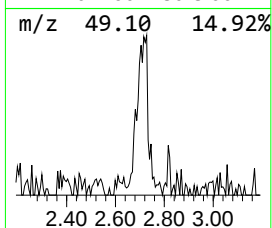
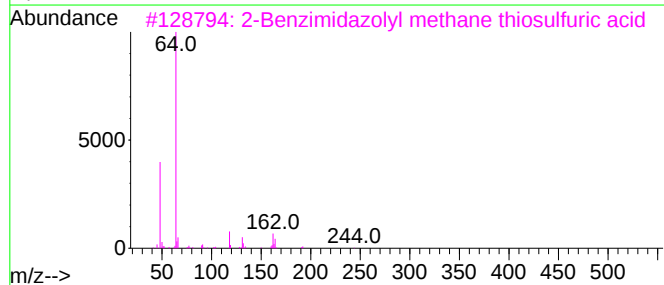
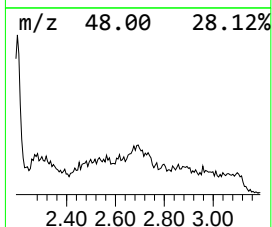
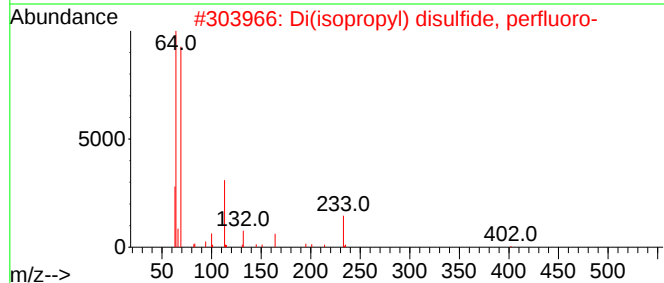
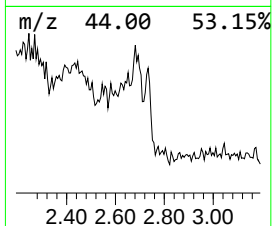
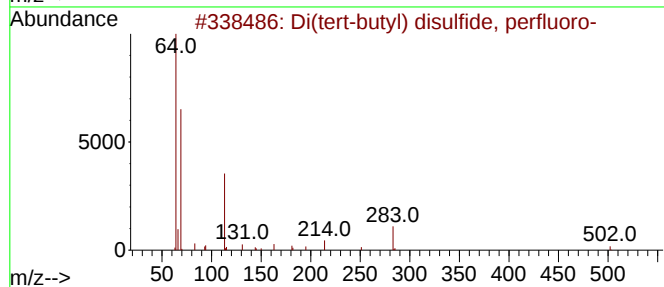
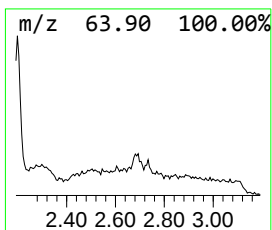
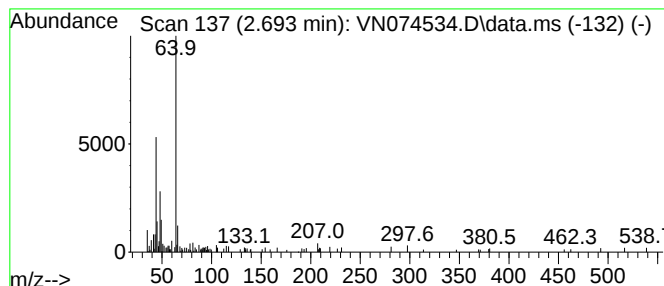
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Peak Number 2 Di(tert-butyl) disulfide, p... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD		R.T.	
2.693	5.48 ug/l	103893	Pentafluorobenzene		8.022	
Hit# of 5	Tentative ID		MW	MolForm	CAS#	Qual
1	Di(tert-butyl) disulfide, perflu...		502	C8F18S2	034880-30-3	74
2	Di(isopropyl) disulfide, perfluoro-		402	C6F14S2	000754-62-1	64
3	2-Benzimidazolyl methane thiosul...		244	C8H8N2O3S2	1010256-39-2	56
4	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	43
5	S-2-[3-Succinimidopropylamino]et...		296	C9H16N2O5S2	031701-75-4	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	23.4	ug/l	443490	1	8.022	948191	50.0
Di(tert-butyl) ...	2.693	5.5	ug/l	103893	1	8.022	948191	50.0