

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074809.D
 Acq On : 07 Oct 2022 14:19
 Operator : JC\MD
 Sample : N4998-01
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 506D-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\82N100522W.M
 Title : SW846 8260

Signal : TIC: VN074809.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.312	38	44	52	rBV	309514	575222	18.72%	4.287%
2	2.430	55	64	65	rBV3	44767	105619	3.44%	0.787%
3	2.771	118	122	126	rBV2	90459	154249	5.02%	1.149%
4	2.830	128	132	134	rBV2	92652	142537	4.64%	1.062%
5	4.753	452	459	464	rBV3	15786	42329	1.38%	0.315%
6	7.447	909	917	925	rBV	27088	74599	2.43%	0.556%
7	8.182	1031	1042	1046	rBV	390549	954076	31.04%	7.110%
8	8.235	1046	1051	1062	rVB	401498	906435	29.49%	6.755%
9	8.588	1101	1111	1122	rBV	497870	1137451	37.01%	8.476%
10	9.106	1191	1199	1209	rBV	583548	1242772	40.43%	9.261%
11	10.570	1438	1448	1460	rBV	1637751	3073518	100.00%	22.904%
12	11.870	1660	1669	1679	rBV	927952	1672871	54.43%	12.466%
13	12.853	1827	1836	1844	rBV	931059	1605451	52.23%	11.964%
14	13.794	1987	1996	2007	rBV	1021244	1731965	56.35%	12.907%

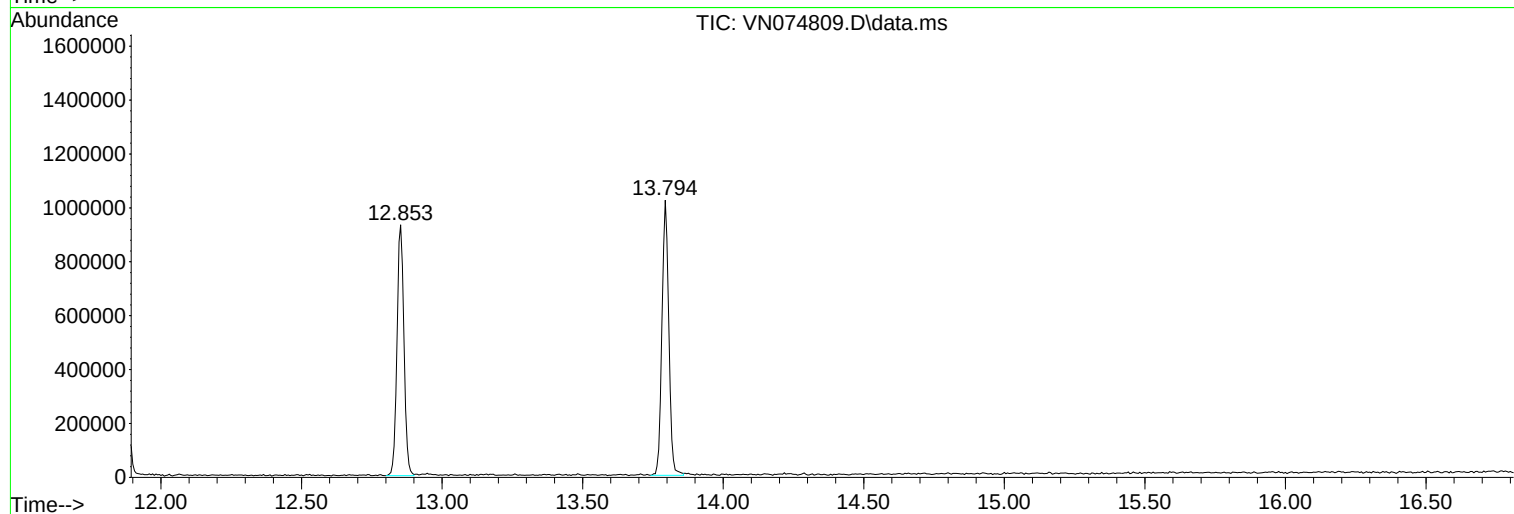
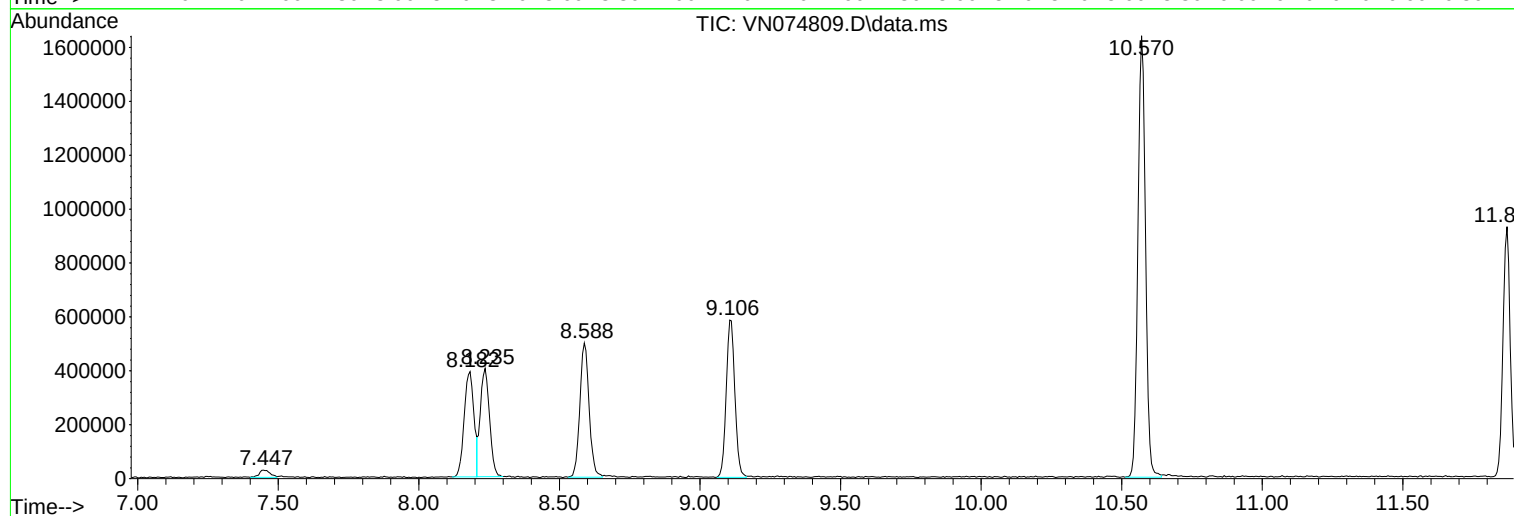
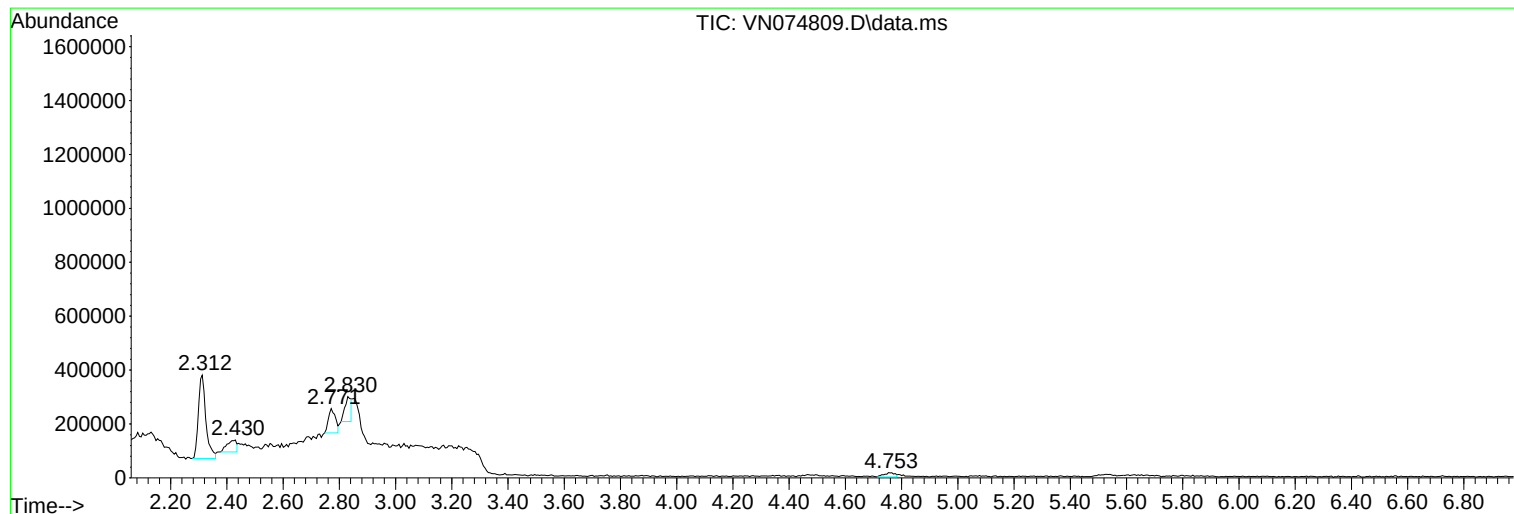
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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



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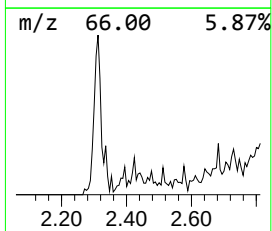
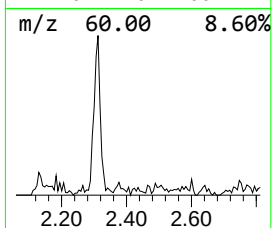
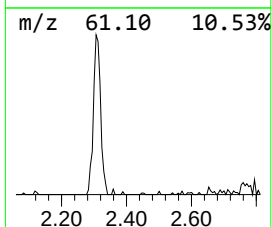
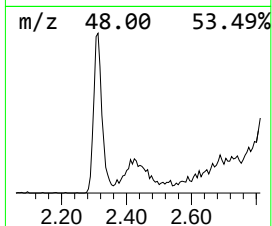
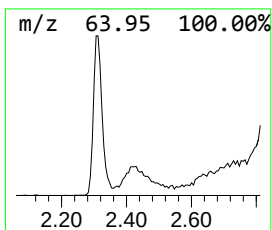
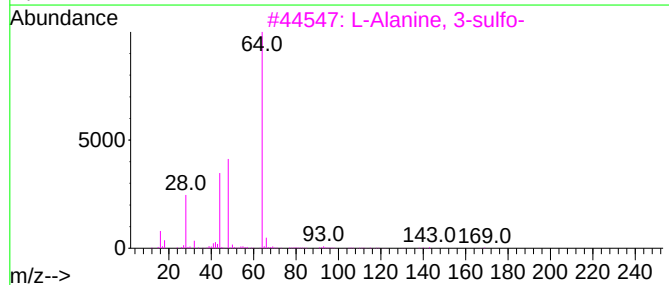
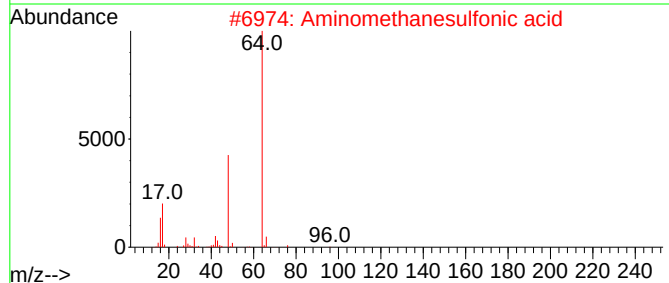
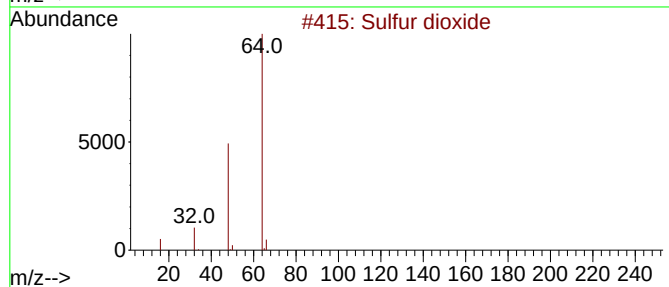
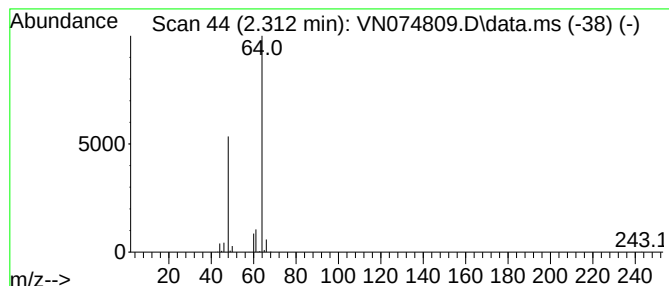
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.312	31.73 ug/l	575222	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	78
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	5
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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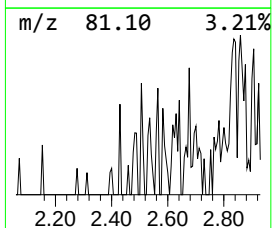
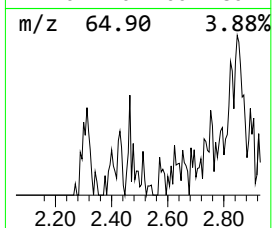
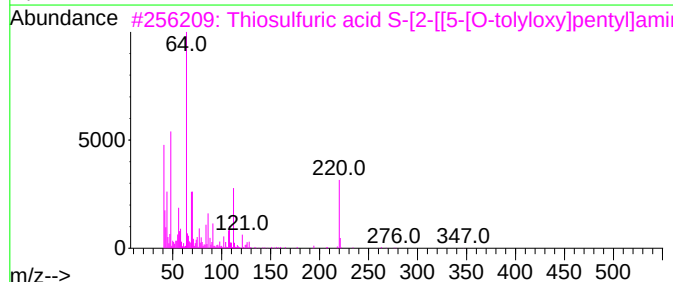
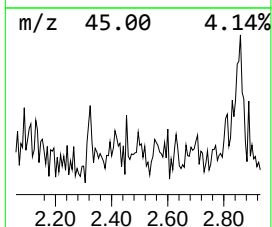
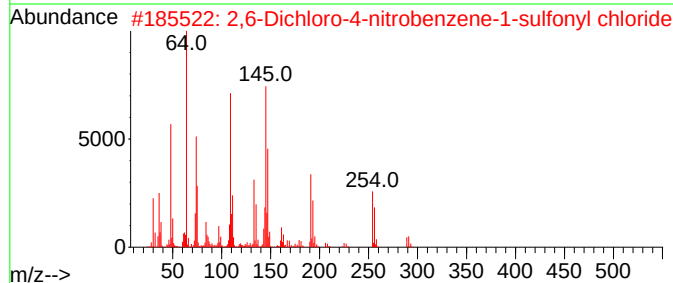
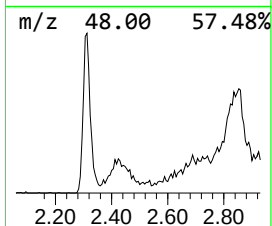
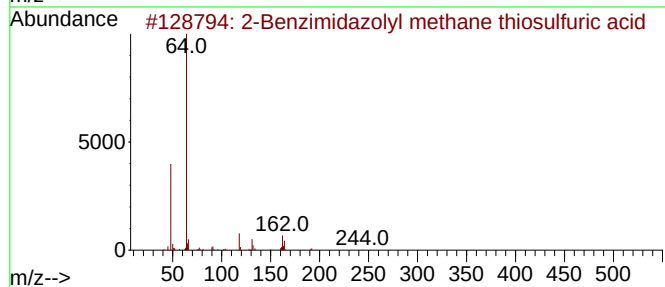
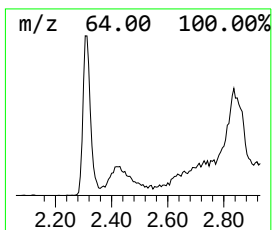
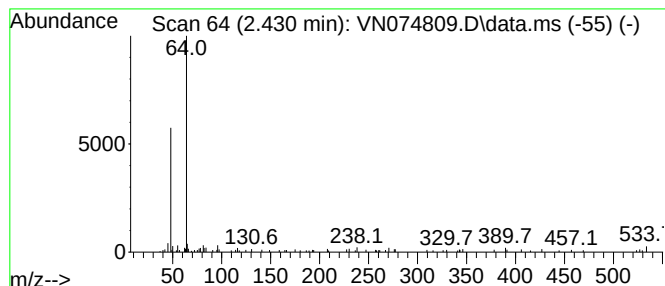
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Quant Title : SW846 8260

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

Peak Number 2 2-Benzimidazolyl methane th... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.430	5.83 ug/l	105619	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	83
2			2,6-Dichloro-4-nitrobenzene-1-su...	289	C6H2Cl3NO4S	074875-17-5	64
3			Thiosulfuric acid S-[2-[5-[O-to...	347	C15H25NO4S2	038920-47-7	64
4			Sulfur dioxide	64	O2S	007446-09-5	64
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9



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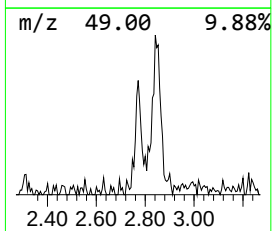
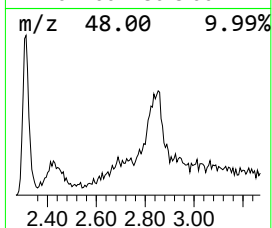
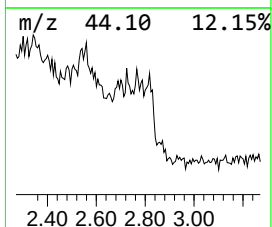
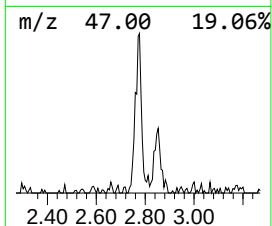
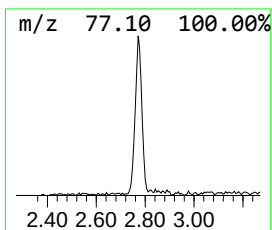
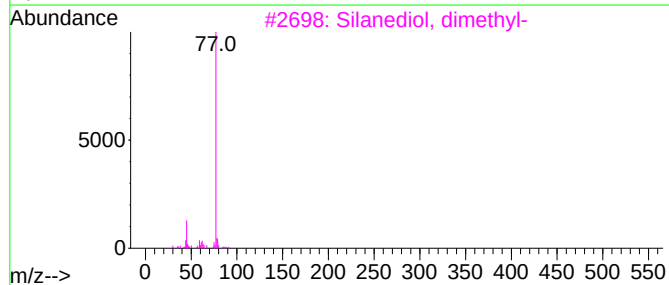
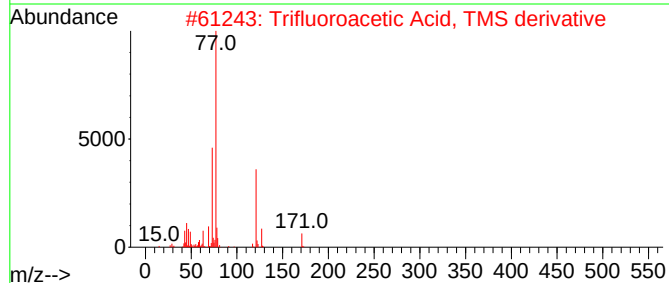
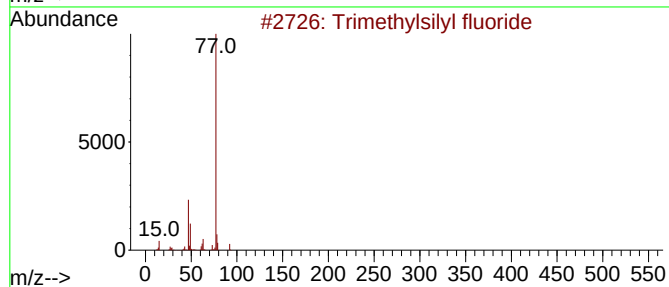
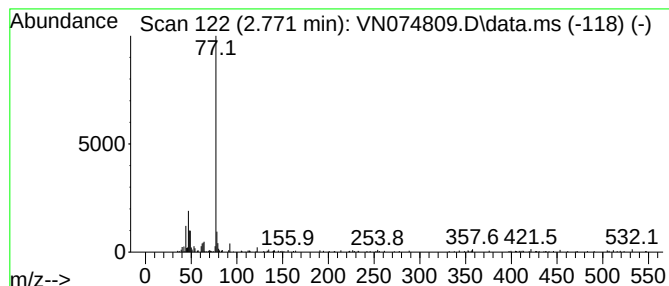
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Peak Number 3 Trimethylsilyl fluoride Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.771	8.51 ug/l	154249	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Trimethylsilyl fluoride	92	C3H9FSi	000420-56-4	72
2			Trifluoroacetic Acid, TMS deriva...	186	C5H9F3O2Si	000400-53-3	36
3			Silanediol, dimethyl-	92	C2H8O2Si	001066-42-8	28
4			2-Propanone, 1,1,3-trichloro-	160	C3H3Cl3O	000921-03-9	9
5			Propane, 1,2-dichloro-2-methyl-	126	C4H8Cl2	000594-37-6	9



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MSVOA_N
ClientSampleId :
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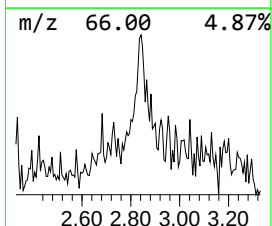
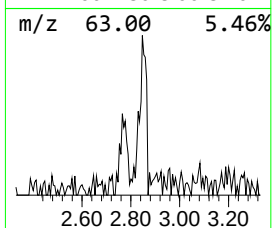
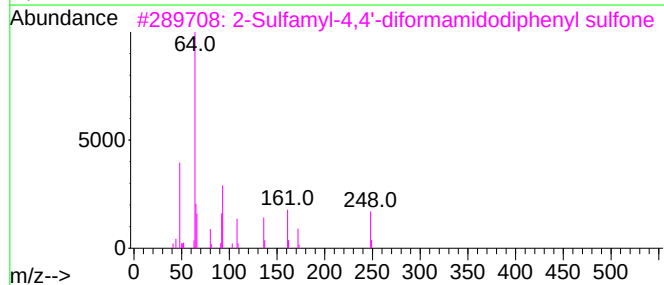
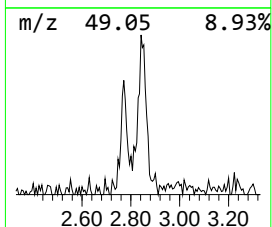
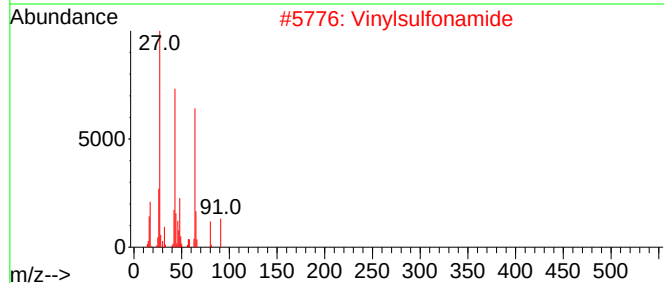
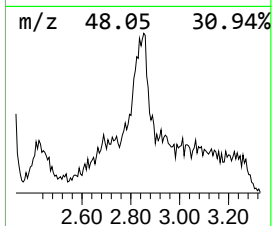
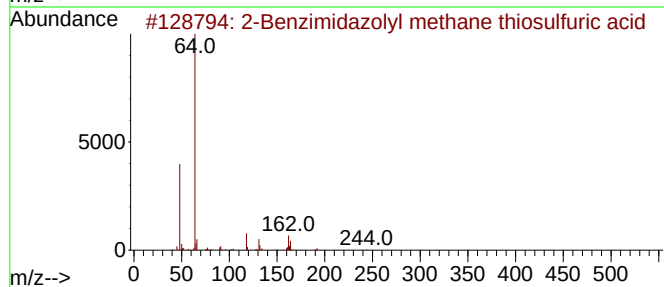
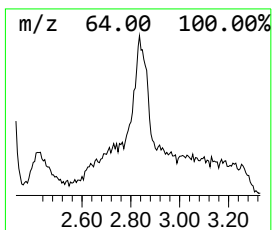
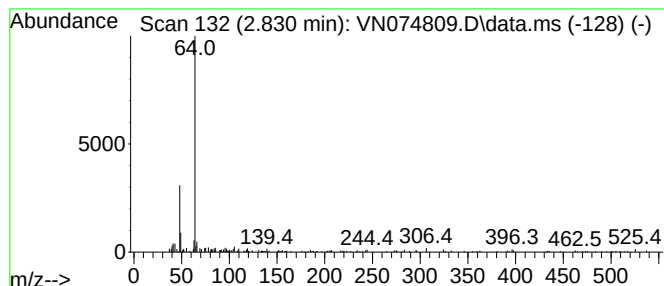
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TIC Integration Parameters: LSCINT.P

Peak Number 4 Vinylsulfonamide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.830	7.86 ug/l	142537	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Benzimidazolyl methane thiosul...	244	C8H8N2O3S2	1010256-39-2	83
2			Vinylsulfonamide	107	C2H5NO2S	002386-58-5	64
3			2-Sulfamyl-4,4'-diformamidodiphe...	383	C14H13N3O6S2	1000256-33-9	64
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
5			2,2,3,3-Tetrafluorocyclobutane-1...	153	C5H3F4N	1000487-04-1	9



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.312	31.7	ug/l	575222	1	8.235	906435	50.0
2-Benzimidazoly...	2.430	5.8	ug/l	105619	1	8.235	906435	50.0
Trimethylsilyl ...	2.771	8.5	ug/l	154249	1	8.235	906435	50.0
Vinylsulfonamide	2.830	7.9	ug/l	142537	1	8.235	906435	50.0