

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
 Data File : VN074691.D
 Acq On : 01 Oct 2022 05:37
 Operator : JC\MD
 Sample : N4882-03
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-105

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\82N092922W.M

Title : SW846 8260

Signal : TIC: VN074691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.152	40	45	51	rBV	441273	771982	13.83%	3.071%
2	2.234	53	59	61	rBV3	86598	172259	3.09%	0.685%
3	4.898	502	512	513	rBV2	90696	171178	3.07%	0.681%
4	7.869	1005	1017	1023	rBV	765888	1884136	33.77%	7.496%
5	7.934	1023	1028	1042	rVB	714069	1597237	28.62%	6.355%
6	8.286	1077	1088	1101	rBV2	880339	2018277	36.17%	8.030%
7	8.828	1170	1180	1190	rBV	1184989	2429622	43.54%	9.667%
8	10.310	1424	1432	1444	rBV	3049190	5580033	100.00%	22.201%
9	11.622	1647	1655	1662	rBV	1954264	3379767	60.57%	13.447%
10	12.604	1814	1822	1832	rBV	2276147	3847080	68.94%	15.306%
11	13.551	1975	1983	1992	rBV	1982079	3282360	58.82%	13.059%

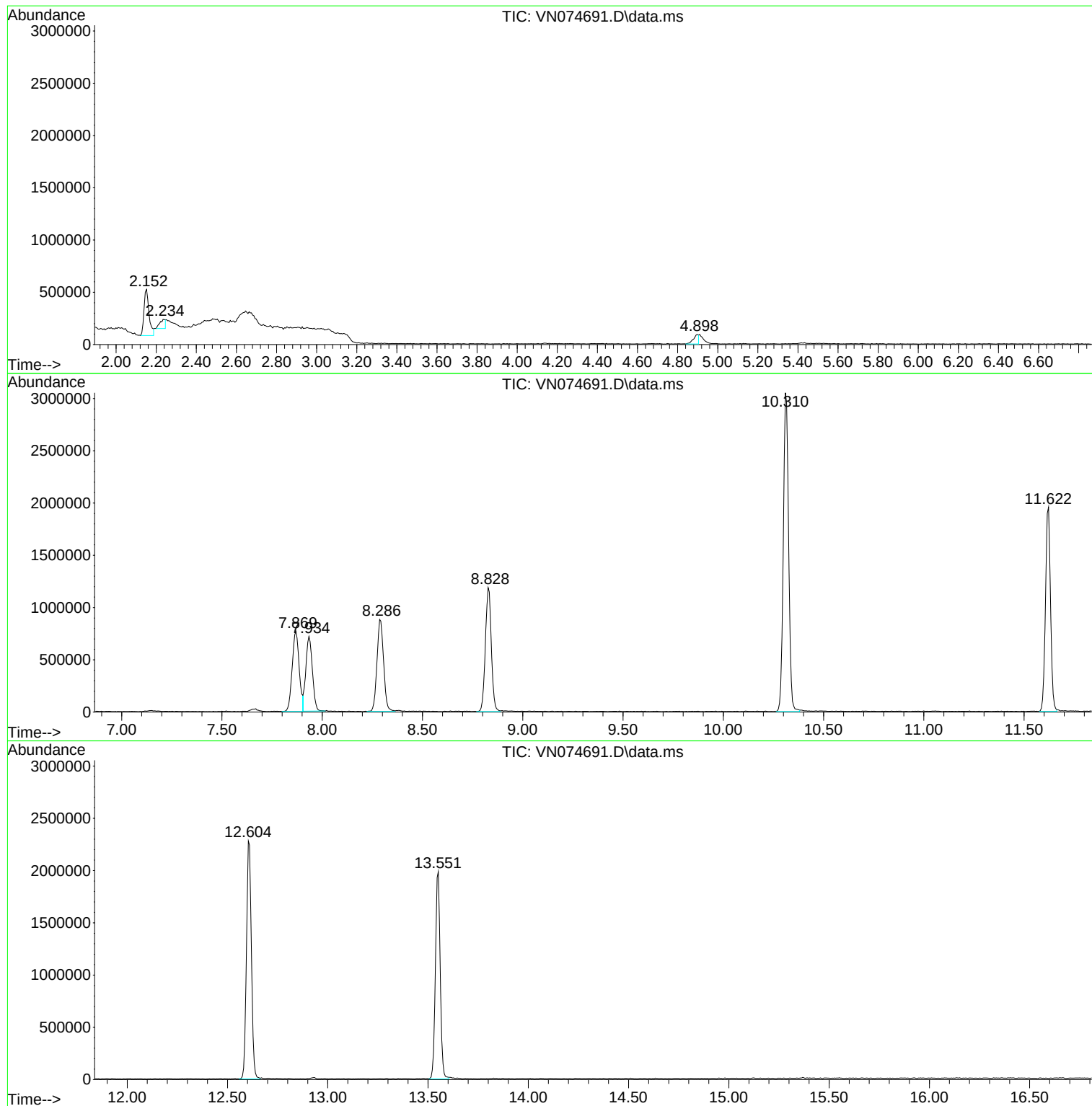
Sum of corrected areas: 25133931

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074691.D
Acq On : 01 Oct 2022 05:37
Operator : JC\MD
Sample : N4882-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-105

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074691.D
Acq On : 01 Oct 2022 05:37
Operator : JC\MD
Sample : N4882-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-105

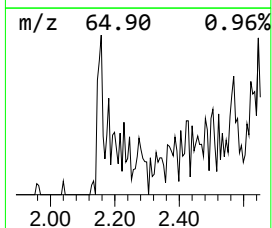
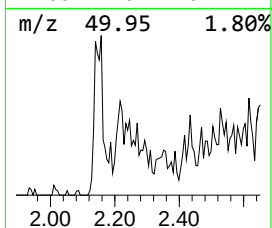
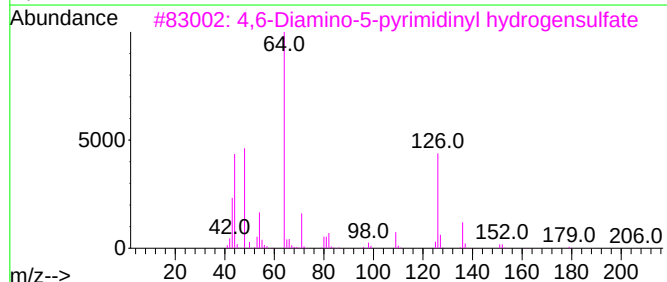
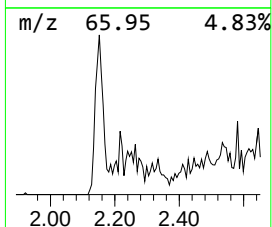
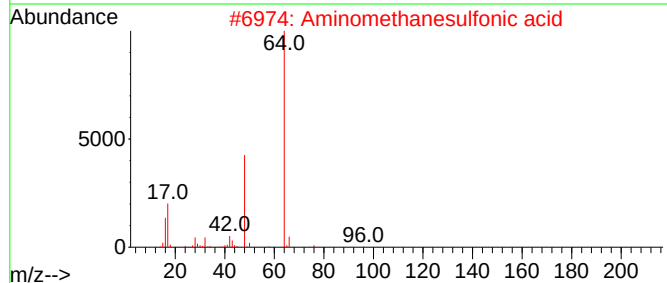
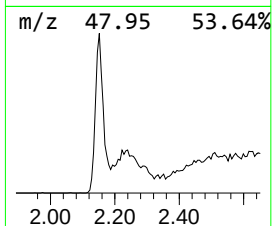
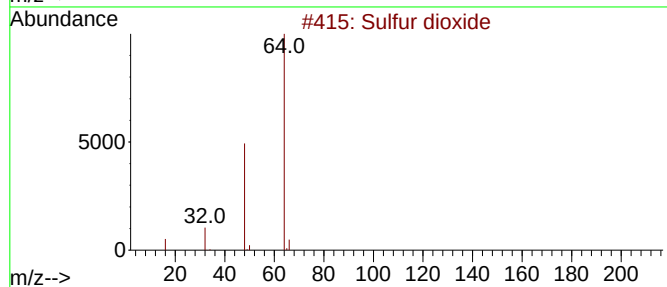
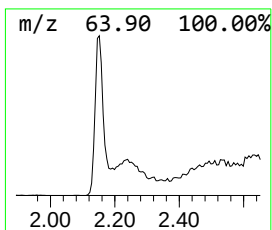
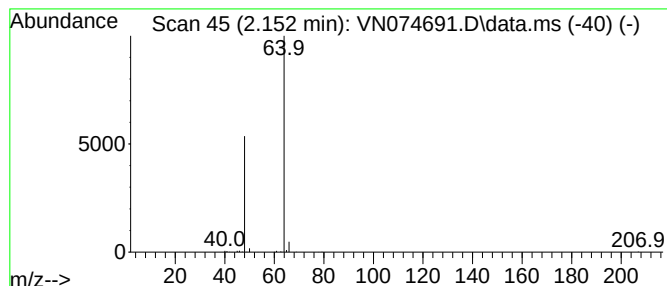
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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.
2.152	24.17 ug/l	771982	Pentafluorobenzene	7.934

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			4,6-Diamino-5-pyrimidinyl hydrog...	206	C4H6N4O4S	071525-41-2	9
4			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	9
5			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074691.D
Acq On : 01 Oct 2022 05:37
Operator : JC\MD
Sample : N4882-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-105

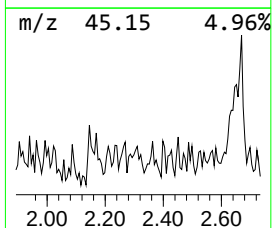
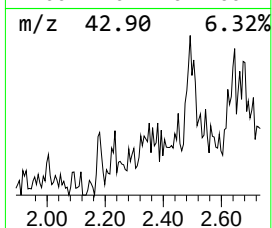
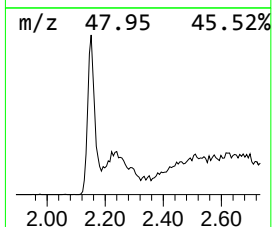
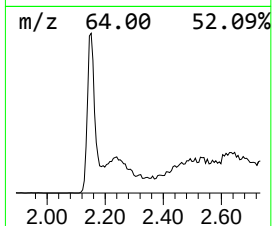
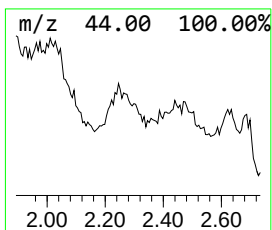
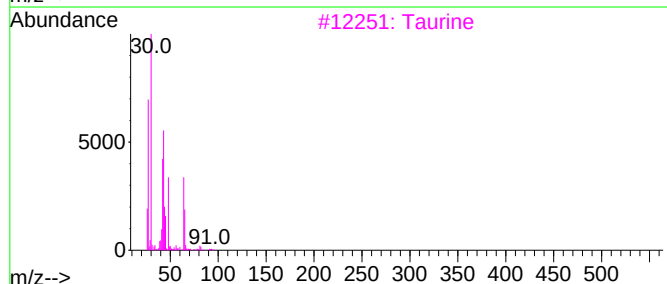
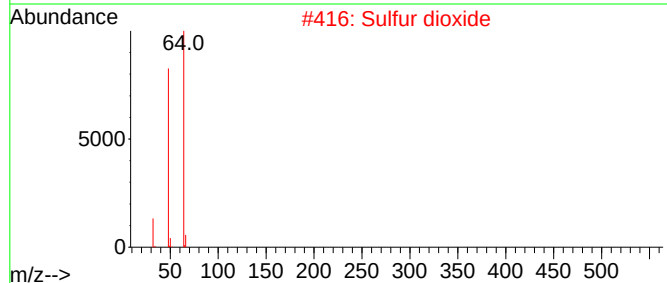
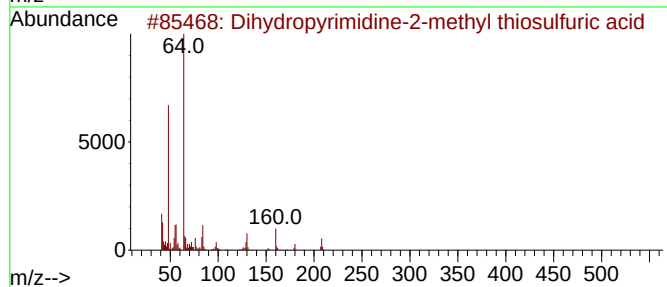
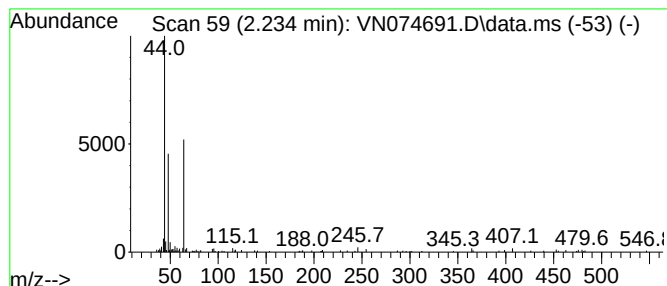
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
Quant Title : SW846 8260

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

Peak Number 2 unknown2.234 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.234	5.39 ug/l	172259	Pentafluorobenzene	7.934

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dihydropyrimidine-2-methyl thios...	208	C5H8N2O3S2	1000256-28-8	33
2			Sulfur dioxide	64	O2S	007446-09-5	9
3			Taurine	125	C2H7NO3S	000107-35-7	9
4			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5			Ethanethiol, 2-(5-phthalimidopen...	372	C15H20N2O5S2	031792-45-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN093022\
Data File : VN074691.D
Acq On : 01 Oct 2022 05:37
Operator : JC\MD
Sample : N4882-03
Misc : 5.0mL/MSVOA_N/WATER
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_N
ClientSampleId :
MW-105

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N092922W.M
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	2.152	24.2	ug/l	771982	1	7.934	1597240	50.0
unknown2.234	2.234	5.4	ug/l	172259	1	7.934	1597240	50.0