

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN100722\
 Data File : VN074799.D
 Acq On : 07 Oct 2022 09:58
 Operator : JC\MD
 Sample : VN1007MBL01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_N/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 VN1007MBL01

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: VN074799.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.306	38	43	53	rBV	127495	268049	9.71%	2.167%
2	2.853	125	136	147	rVB4	198988	930747	33.71%	7.523%
3	7.447	909	917	919	rBV2	21413	38751	1.40%	0.313%
4	8.177	1031	1041	1046	rBV2	355028	853636	30.92%	6.900%
5	8.235	1046	1051	1064	rVB	362628	810345	29.35%	6.550%
6	8.588	1102	1111	1123	rBV2	416889	985254	35.69%	7.964%
7	9.106	1190	1199	1208	rBV2	536273	1118955	40.53%	9.044%
8	10.571	1440	1448	1462	rBV	1484704	2760677	100.00%	22.314%
9	11.870	1661	1669	1678	rBV	823587	1533241	55.54%	12.393%
10	12.853	1829	1836	1845	rBV	851961	1448524	52.47%	11.708%
11	13.794	1989	1996	2007	rVV	915587	1572078	56.95%	12.707%
12	15.641	2304	2310	2318	rBV3	26999	51435	1.86%	0.416%

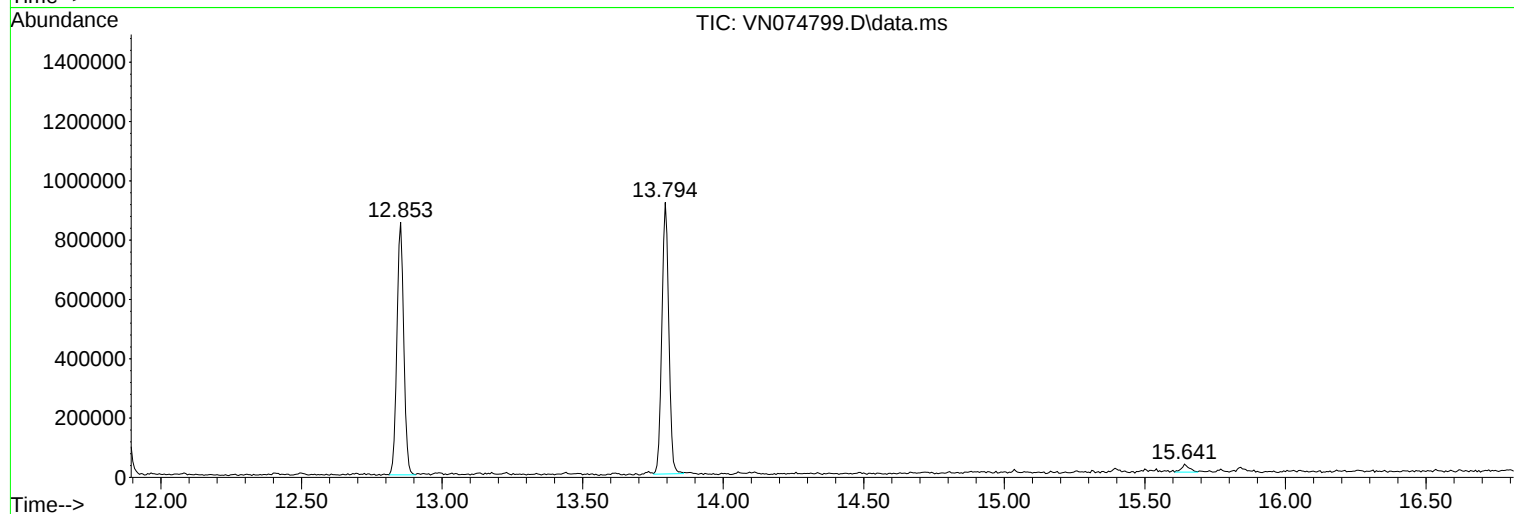
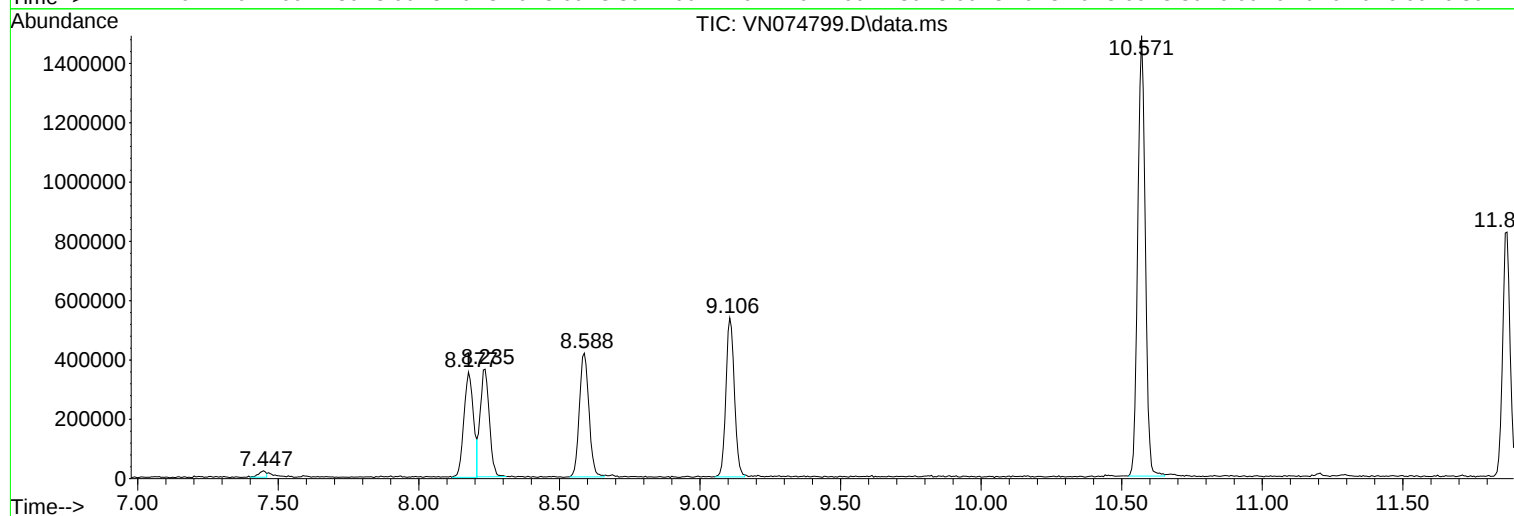
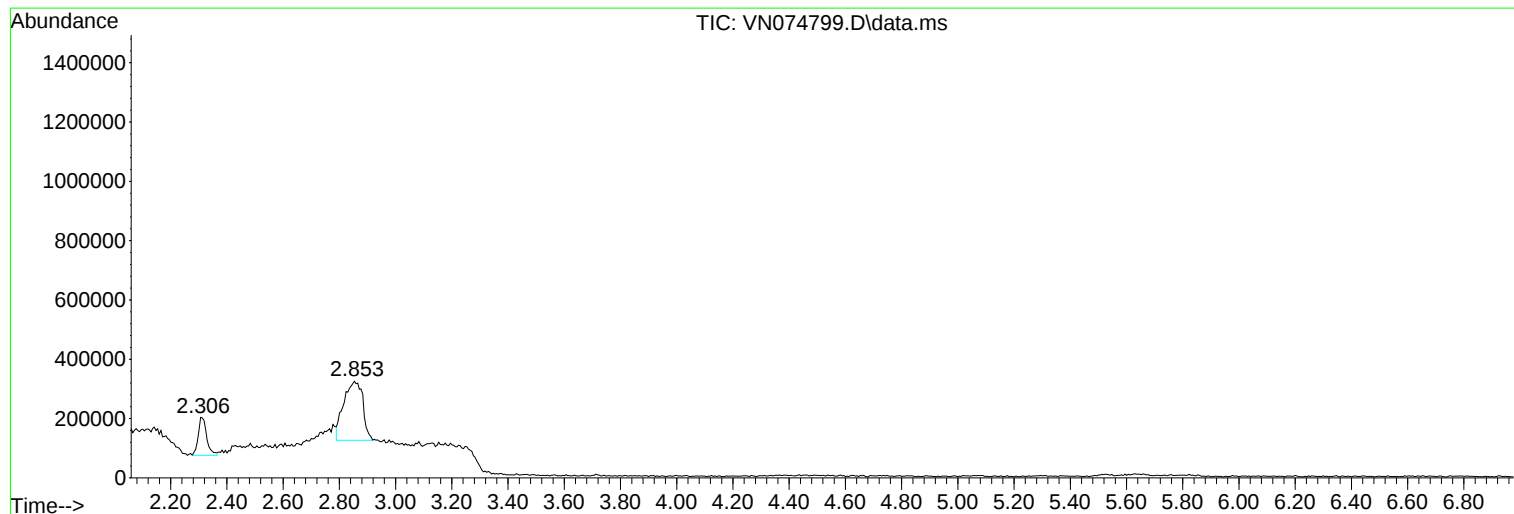
Sum of corrected areas: 12371692

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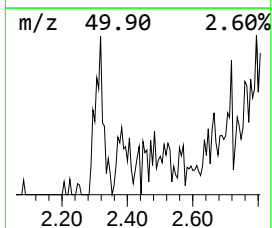
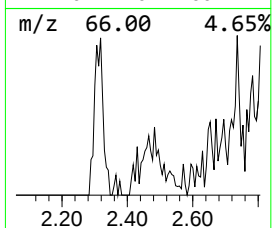
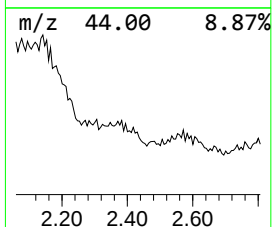
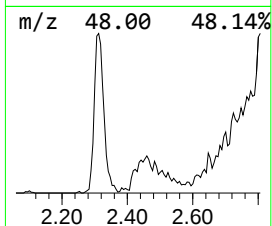
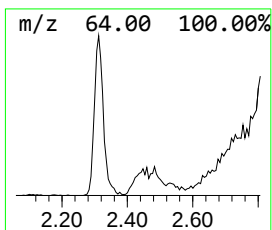
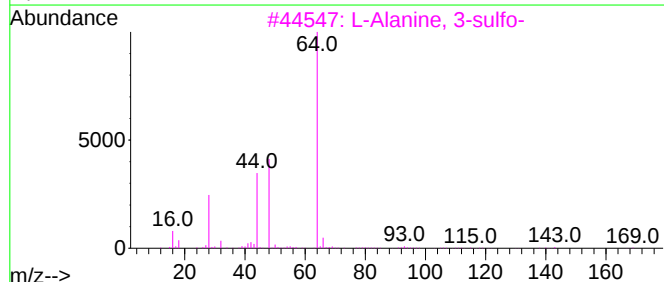
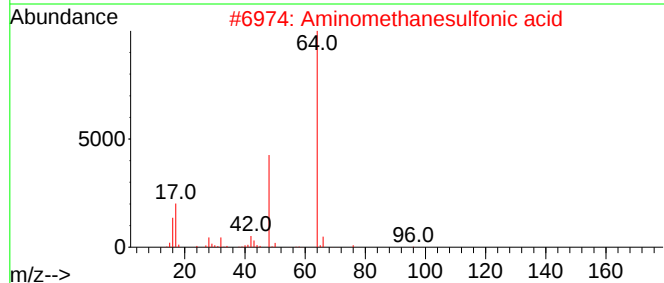
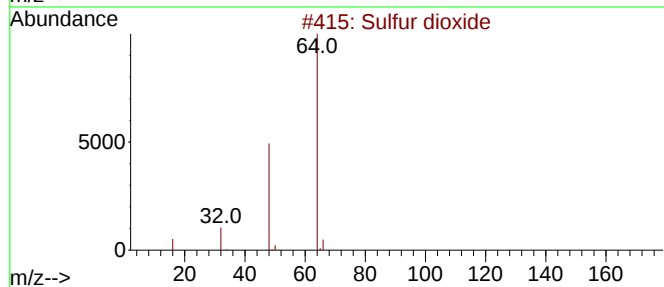
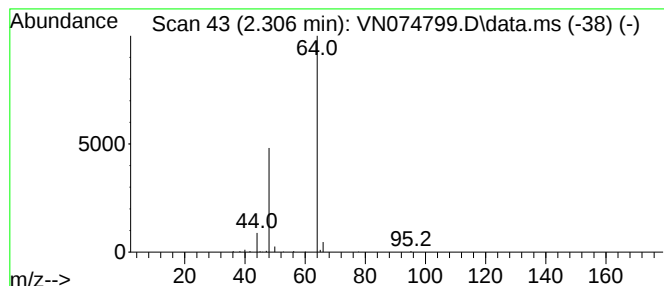
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N100522W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.306	16.54 ug/l	268049	Pentafluorobenzene	8.235

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			2-Aminoethyl hydrogen sulfate	141	C2H7NO4S	000926-39-6	9
5			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4



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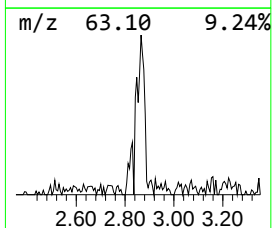
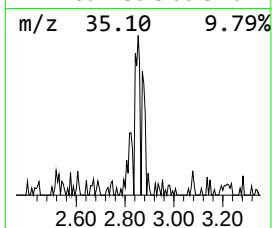
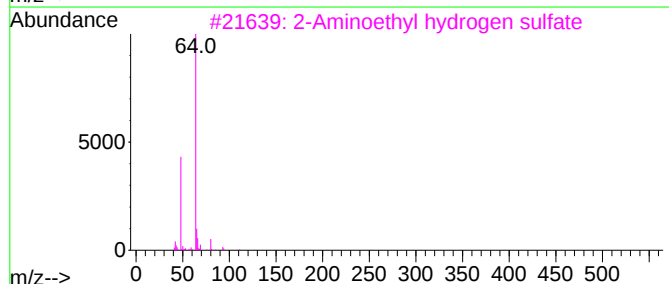
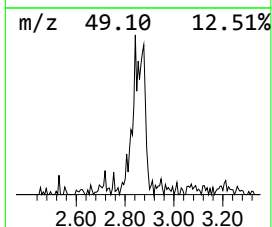
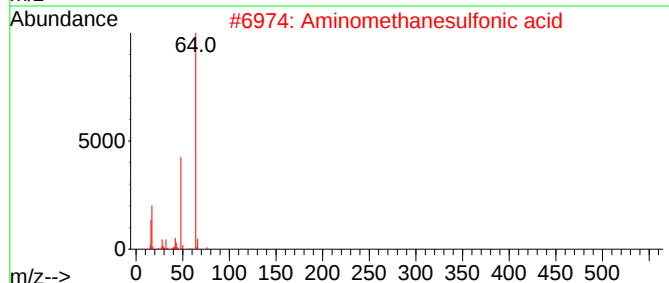
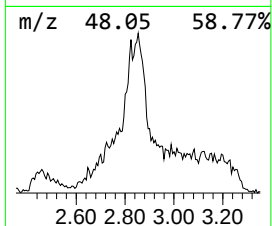
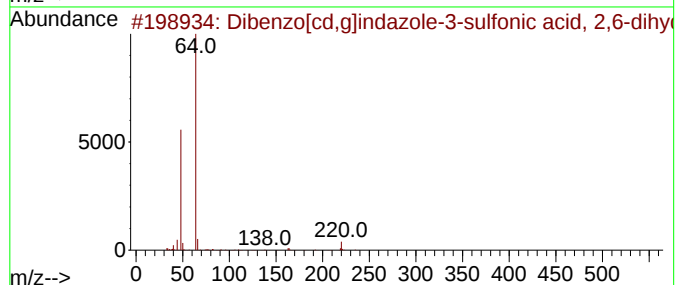
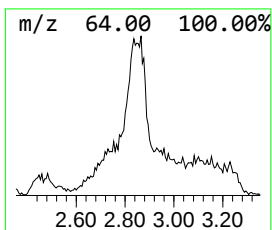
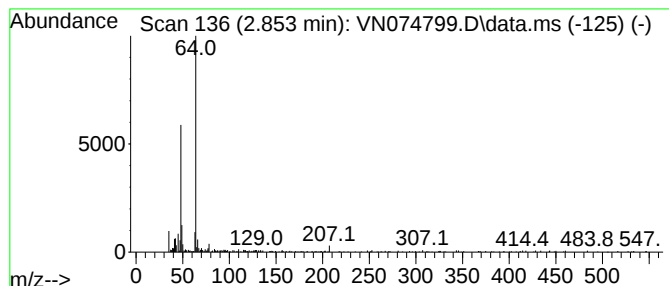
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Peak Number 2 Dibenzo[cd,g]indazole-3-sul... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.853	57.43 ug/l	930747	Pentafluorobenzene	8.235

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dibenzo[cd,g]indazole-3-sulfonic...	300	C14H8N2O4S	293765-87-4	78
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	78
3			2-Aminoethyl hydrogen sulfate	141	C2H7N04S	000926-39-6	64
4			Sulfur dioxide	64	O2S	007446-09-5	64
5			Thiosulfuric acid (H2S2O3), S-(2...	320	C11H16N2O3S3	040284-00-2	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.306	16.5	ug/l	268049	1	8.235	810345	50.0
Dibenzo[cd,g]in...	2.853	57.4	ug/l	930747	1	8.235	810345	50.0