

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN010522\
 Data File : VN070499.D
 Acq On : 5 Jan 2022 19:19
 Operator : JC/MD
 Sample : N1012-16
 Misc : 5.00mL/MSVOA_N/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 31333

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\82N122721W.M
 Title : SW846 8260

Signal : TIC: VN070499.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.236	80	92	101	rBV3	138681	300557	5.81%	0.973%
2	3.687	623	633	659	rVB3	35081	95683	1.85%	0.310%
3	4.291	835	858	865	rBV2	147030	355662	6.88%	1.152%
4	4.358	867	883	923	rVB	980218	2878028	55.66%	9.322%
5	5.961	1457	1481	1515	rBV5	37260	120890	2.34%	0.392%
6	7.069	1873	1894	1911	rBV6	29045	92078	1.78%	0.298%
7	7.278	1955	1972	1982	rBV	26664	66283	1.28%	0.215%
8	7.340	1984	1995	2019	rVB2	44464	118536	2.29%	0.384%
9	7.694	2100	2127	2156	rBV5	42899	140276	2.71%	0.454%
10	8.021	2225	2249	2260	rBV2	633218	1535065	29.69%	4.972%
11	8.086	2261	2273	2303	rVB	1151565	2610410	50.49%	8.455%
12	8.437	2382	2404	2430	rBV	797382	1863844	36.05%	6.037%
13	8.968	2580	2602	2636	rBV	1737569	3658651	70.76%	11.850%
14	9.413	2752	2768	2784	rBV2	29969	63657	1.23%	0.206%
15	10.253	3065	3081	3097	rBV2	71464	150303	2.91%	0.487%
16	10.333	3097	3111	3129	rVB2	46782	89733	1.74%	0.291%
17	10.440	3132	3151	3166	rBV	2782280	5170376	100.00%	16.746%
18	10.505	3166	3175	3202	rVB	304516	615115	11.90%	1.992%
19	11.744	3618	3637	3662	rBV	2318037	4240231	82.01%	13.733%
20	12.277	3822	3836	3838	rBV2	38805	55045	1.06%	0.178%
21	12.358	3855	3866	3884	rVB2	27020	56405	1.09%	0.183%
22	12.731	3980	4005	4029	rBV	1918325	3389199	65.55%	10.977%
23	13.584	4303	4323	4332	rBV10	25293	65365	1.26%	0.212%
24	13.675	4341	4357	4380	rBV	1700547	3015389	58.32%	9.766%
25	13.769	4383	4392	4410	rVB3	72968	128332	2.48%	0.416%

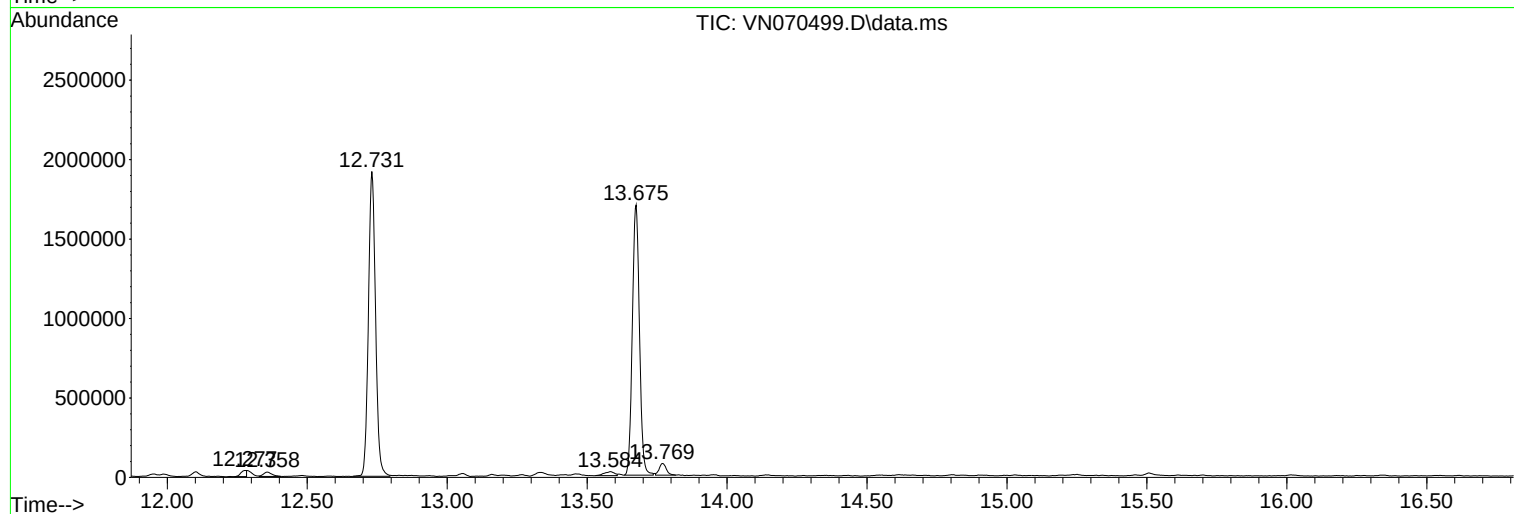
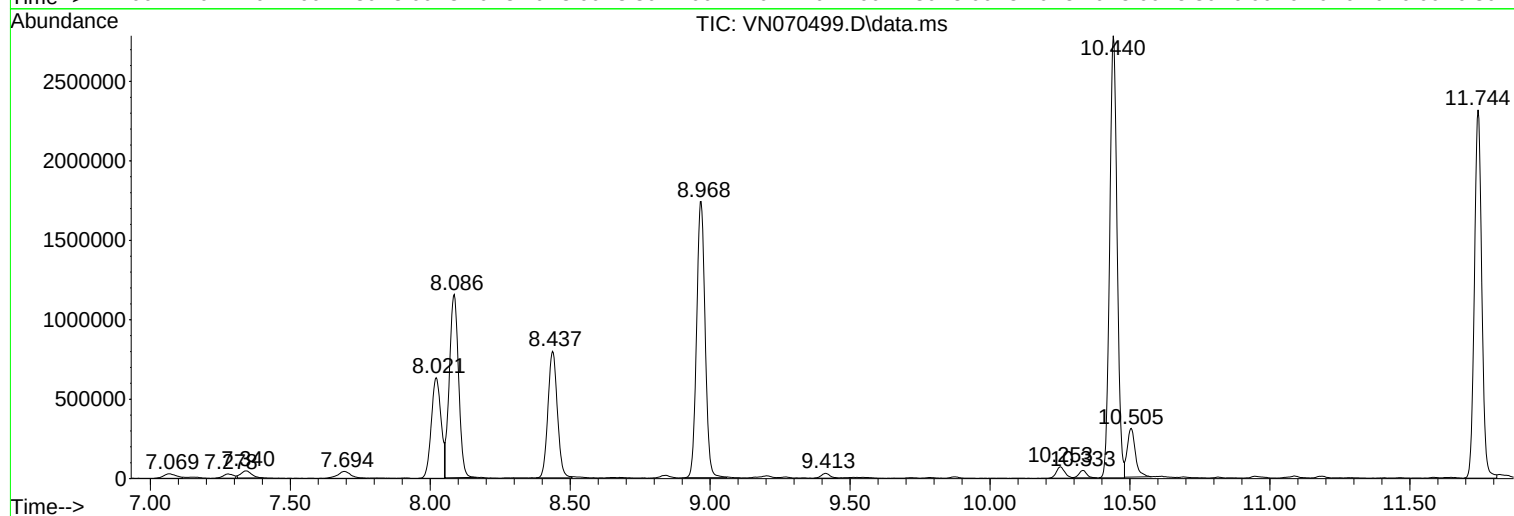
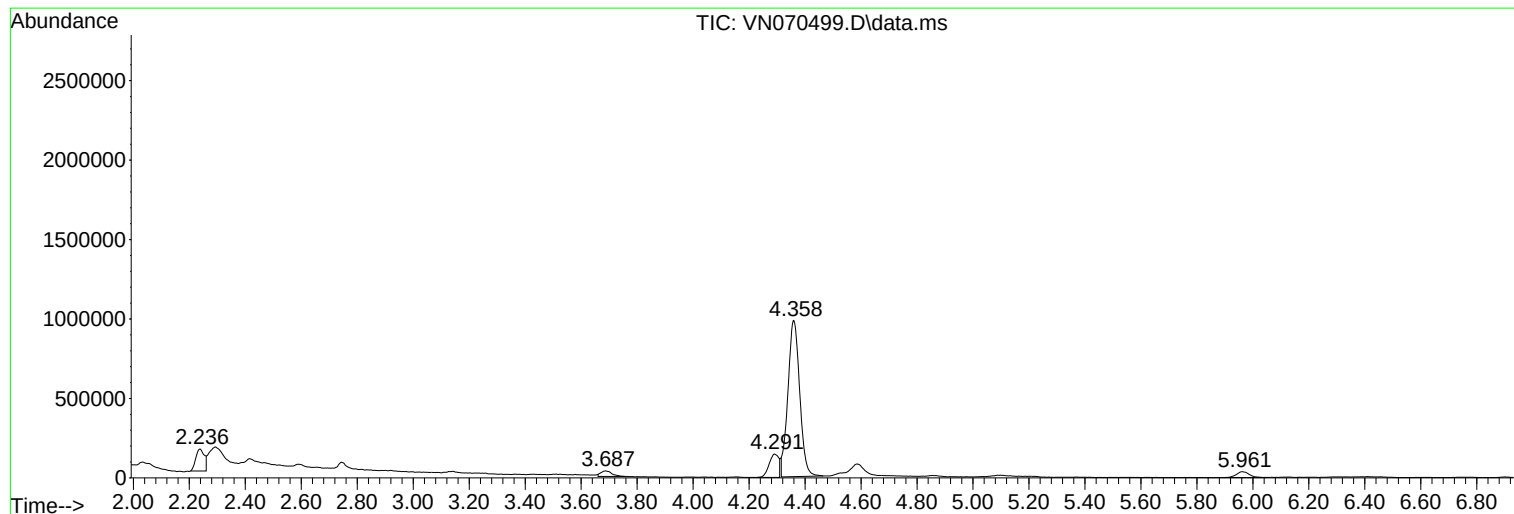
Sum of corrected areas: 30875113

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
Quant Title : SW846 8260

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



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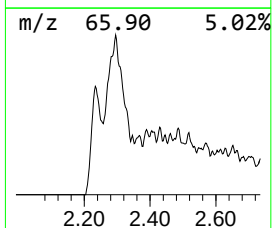
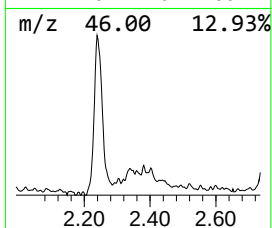
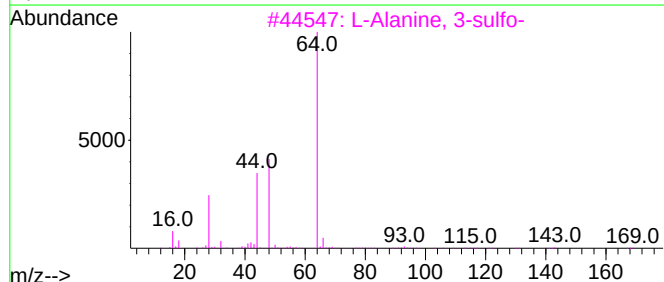
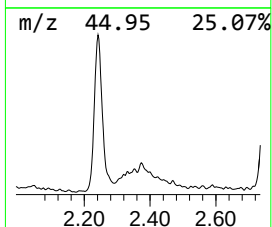
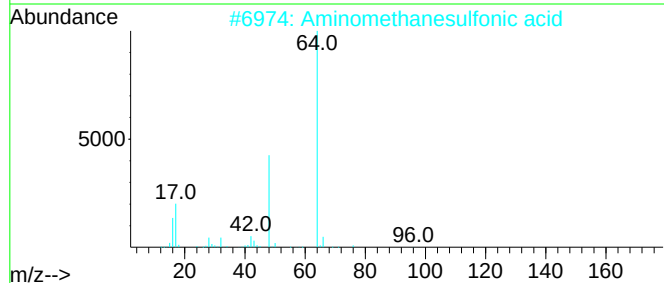
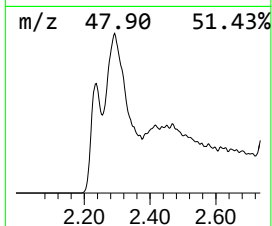
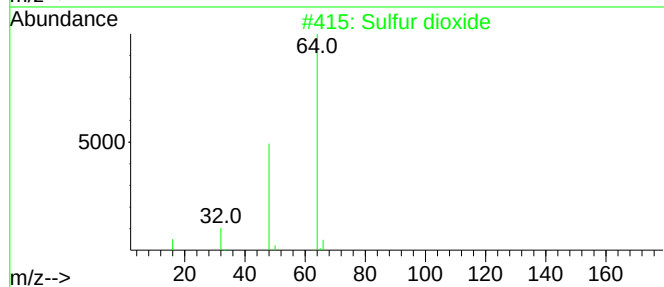
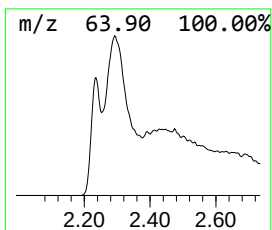
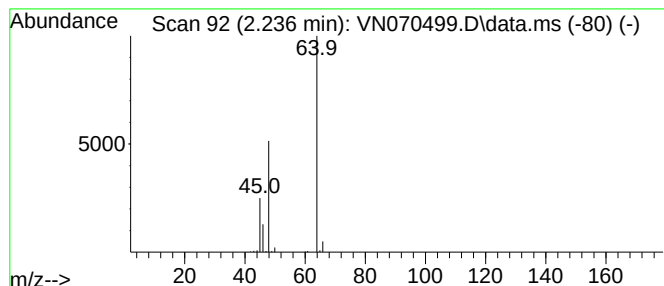
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N122721W.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.236	5.76 ug/l	300557	Pentafluorobenzene	8.086

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, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
5			Ethanol, 2-fluoro-	64	C2H5FO	000371-62-0	5



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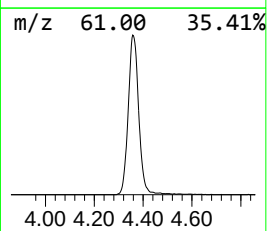
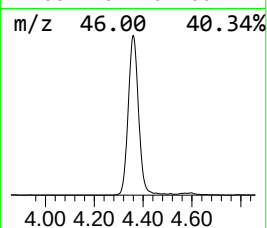
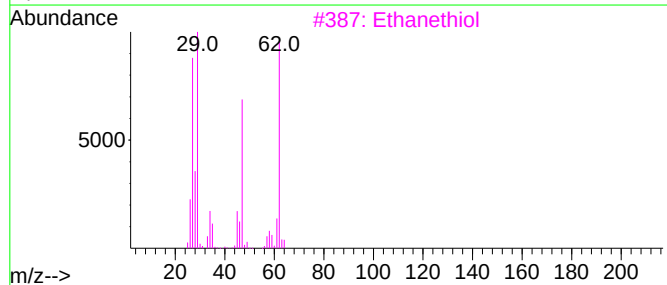
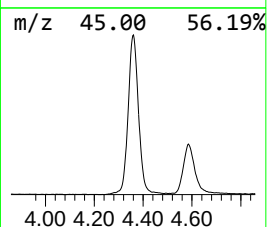
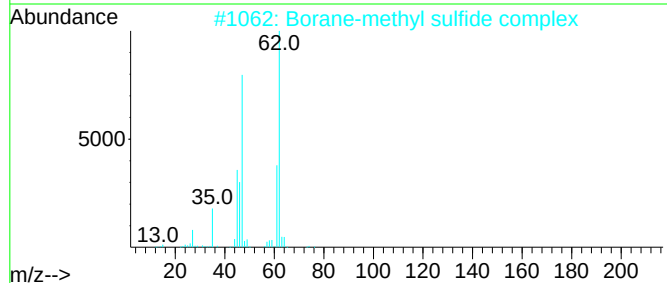
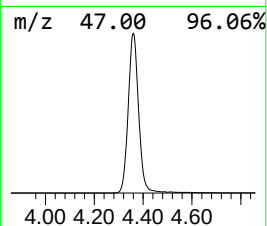
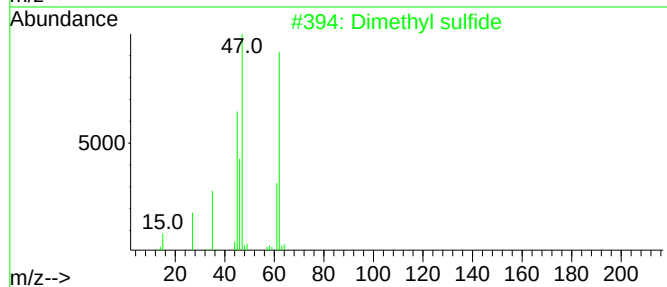
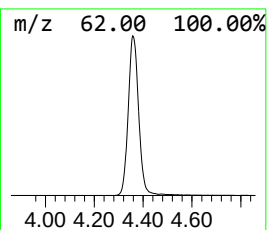
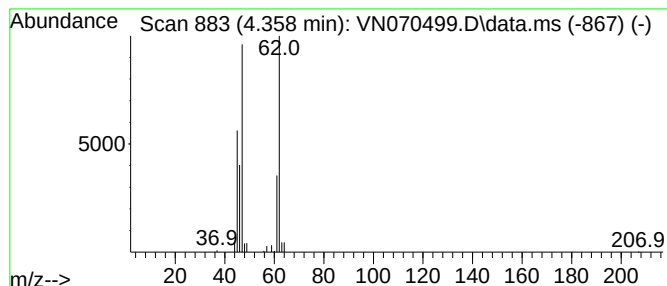
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TIC Integration Parameters: LSCINT.P

Peak Number 2 Dimethyl sulfide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
4.358	55.13 ug/l	2878030	Pentafluorobenzene	8.086

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Dimethyl sulfide	62	C2H6S	000075-18-3	94
2			Borane-methyl sulfide complex	76	C2H9BS	013292-87-0	90
3			Ethanethiol	62	C2H6S	000075-08-1	72
4			Ethene, chloro-	62	C2H3Cl	000075-01-4	9
5			Propane, 2-fluoro-	62	C3H7F	000420-26-8	7



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.236	5.8	ug/l	300557	1	8.086	2610410	50.0
Dimethyl sulfide	4.358	55.1	ug/l	2878030	1	8.086	2610410	50.0