

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX082223\
 Data File : VX037149.D
 Acq On : 22 Aug 2023 12:56
 Operator : JC/MD
 Sample : VX0822MBL01
 Misc : 5.00g/10mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0822MBL01

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_X\Method\82X081723W.M
 Title : SW846 8260

Signal : TIC: VX037149.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	24	29	50	rBV	14766	55895	8.16%	1.397%
2	5.385	692	705	721	rBV	78593	229356	33.50%	5.732%
3	5.550	721	732	746	rBV	145452	416498	60.84%	10.409%
4	5.958	787	799	817	rBV	83783	227178	33.18%	5.678%
5	6.757	921	930	954	rBV	213275	514668	75.18%	12.862%
6	8.647	1233	1240	1250	rBV	453555	684604	100.00%	17.109%
7	10.055	1465	1471	1484	rBV	442037	615845	89.96%	15.391%
8	11.079	1634	1639	1649	rBV	401685	503493	73.55%	12.583%
9	11.372	1680	1687	1689	rBV4	3690	7212	1.05%	0.180%
10	11.457	1698	1701	1715	rVB3	7649	18814	2.75%	0.470%
11	12.018	1788	1793	1805	rVB	509808	664329	97.04%	16.603%
12	12.335	1838	1845	1850	rBV2	8903	11532	1.68%	0.288%
13	13.140	1973	1977	1990	rVB2	5245	7797	1.14%	0.195%
14	13.591	2044	2051	2057	rBV	5760	7349	1.07%	0.184%
15	13.719	2068	2072	2077	rVB2	14283	17737	2.59%	0.443%
16	13.774	2077	2081	2089	rBV	8422	11912	1.74%	0.298%
17	13.963	2107	2112	2118	rVB2	5552	7131	1.04%	0.178%

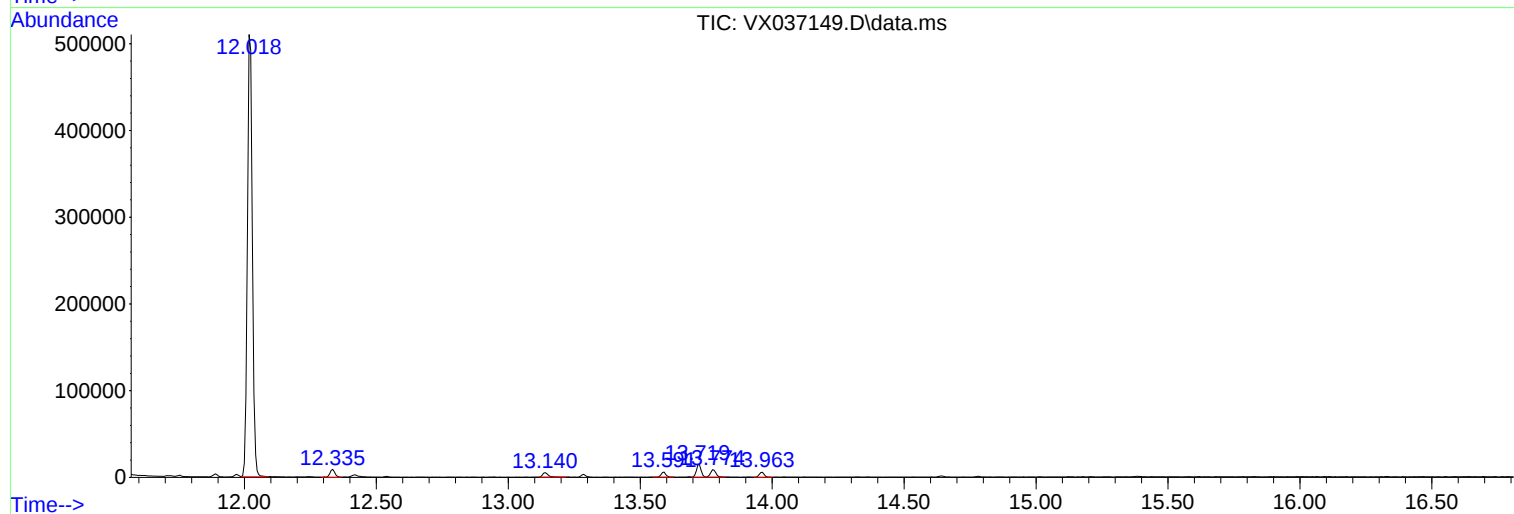
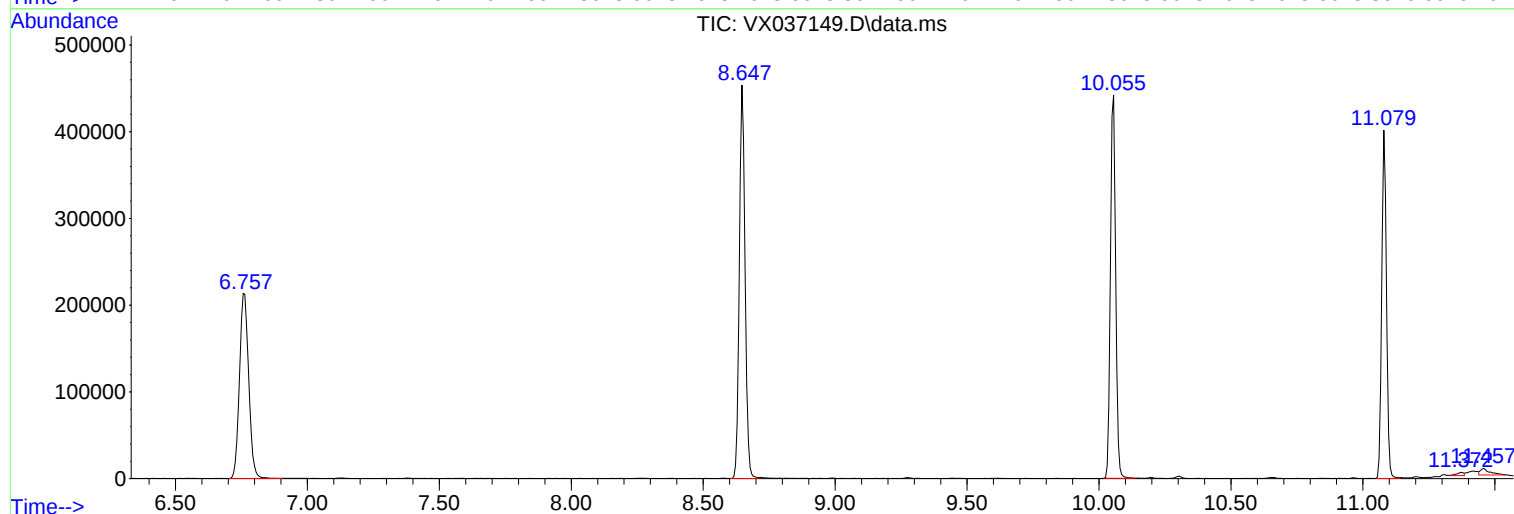
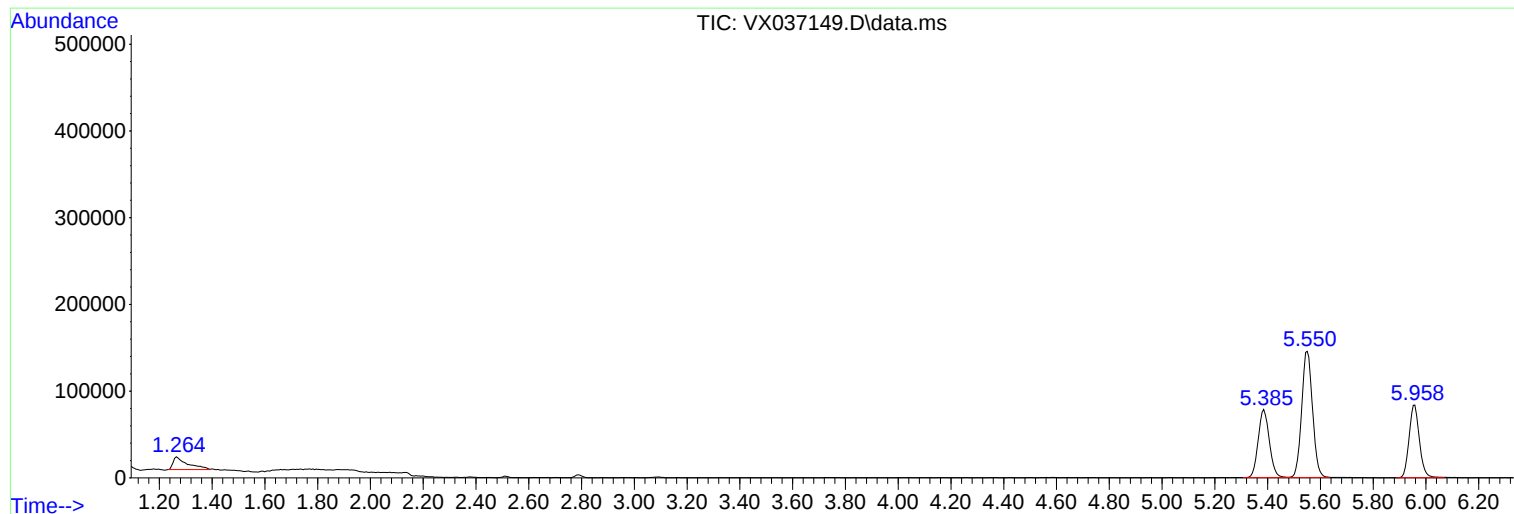
Sum of corrected areas: 4001350

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X081723W.M
Quant Title : SW846 8260

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



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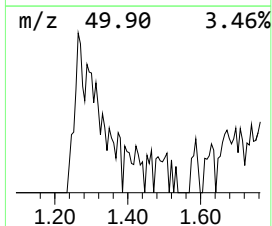
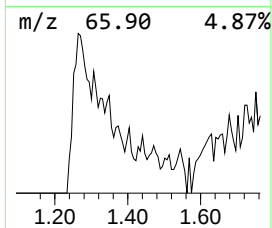
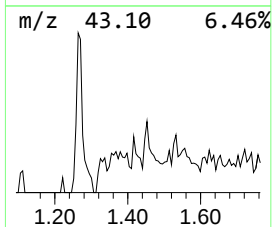
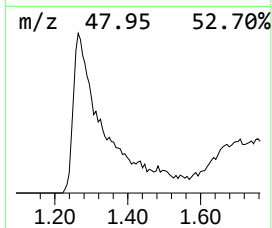
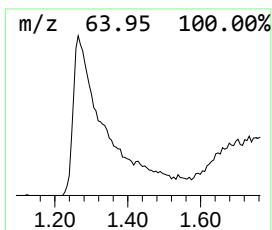
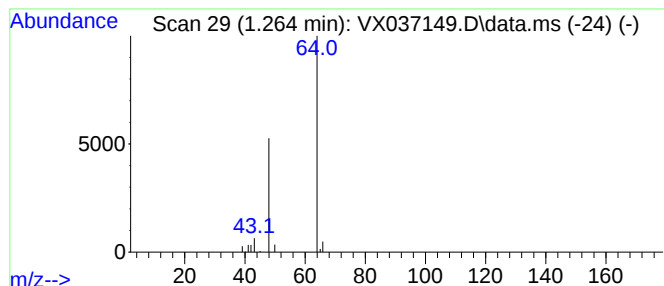
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.264	6.71 ug/l	55895	Pentafluorobenzene	5.550

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	74
3			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	64
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.264	6.7	ug/l	55895	1	5.550	416498	50.0