

Data Path : Z:\voasrv\HPCHEM1\MSVOA_N\Data\VN091622\
 Data File : VN074537.D
 Acq On : 17 Sep 2022 02:56
 Operator : JC\MD
 Sample : N4549-09
 Misc : 5.0mL/MSVOA_N/WATER
 ALS Vial : 43 Sample Multiplier: 1

Instrument :
 MSVOA_N
 ClientSampleId :
 MW-53

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\82N091522W.M

Title : SW846 8260

Signal : TIC: VN074537.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.199	47	53	62	rBV2	252868	599148	31.62%	4.270%
2	2.405	84	88	92	rBV	77908	110132	5.81%	0.785%
3	2.687	131	136	143	rBV4	65966	202237	10.67%	1.441%
4	5.275	561	576	592	rBV2	344148	1216807	64.22%	8.673%
5	5.528	606	619	635	rBV2	189017	648176	34.21%	4.620%
6	6.410	757	769	781	rBV3	36324	115889	6.12%	0.826%
7	7.951	1022	1031	1036	rBV2	253046	617247	32.58%	4.399%
8	8.016	1036	1042	1054	rVB2	409330	912297	48.15%	6.502%
9	8.369	1091	1102	1111	rBV3	313853	781986	41.27%	5.573%
10	8.463	1111	1118	1129	rVB2	288708	664252	35.06%	4.734%
11	8.904	1184	1193	1207	rBV	669205	1370427	72.33%	9.767%
12	10.133	1396	1402	1408	rBV3	22467	48702	2.57%	0.347%
13	10.380	1434	1444	1458	rBV	1052995	1894605	100.00%	13.503%
14	10.892	1524	1531	1535	rVB4	11562	19423	1.03%	0.138%
15	11.686	1656	1666	1677	rBV	1068349	1832111	96.70%	13.058%
16	11.904	1696	1703	1705	rBV5	9499	19394	1.02%	0.138%
17	12.674	1826	1834	1843	rBV	827070	1373624	72.50%	9.790%
18	13.616	1987	1994	2003	rBV	957653	1604064	84.66%	11.433%

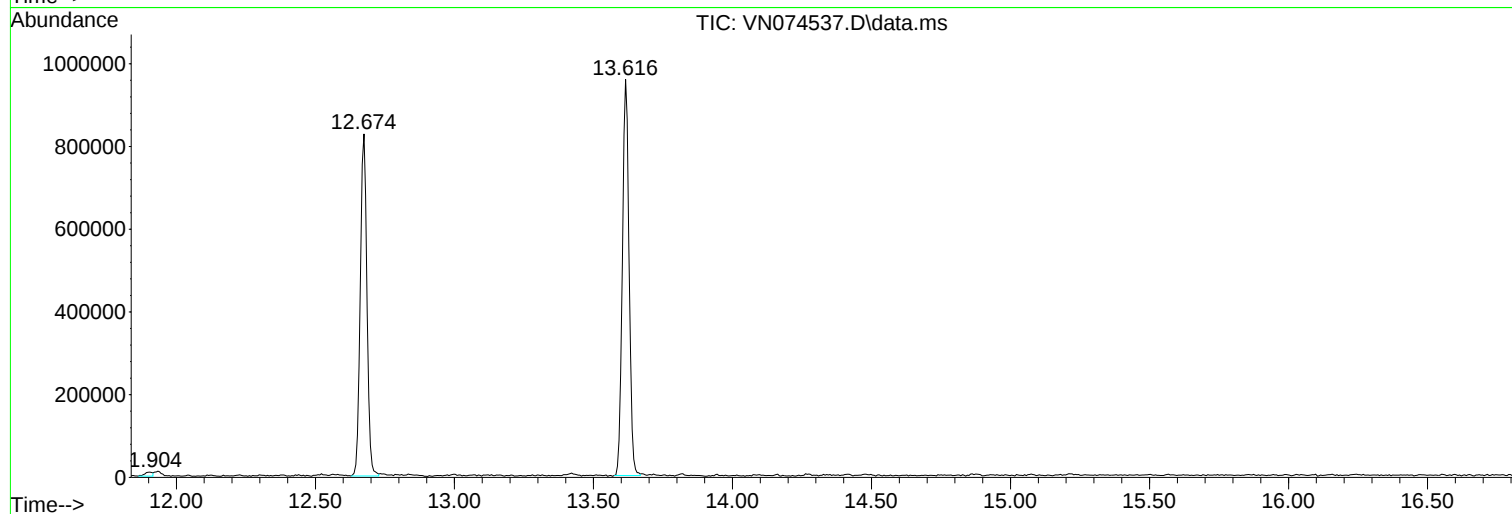
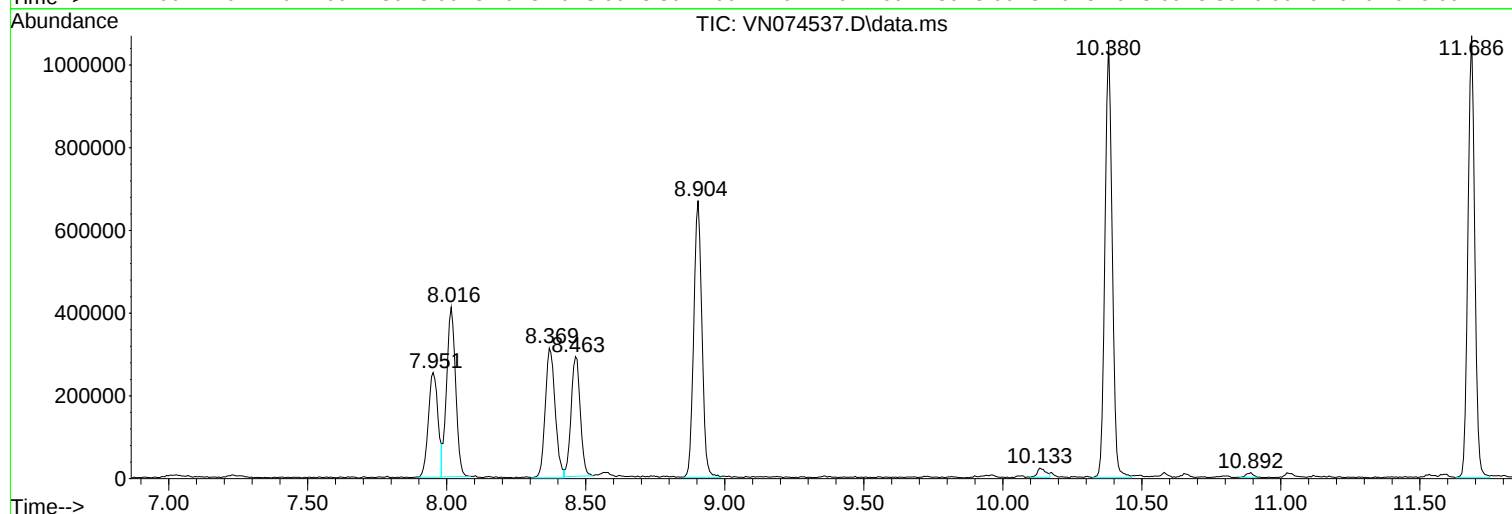
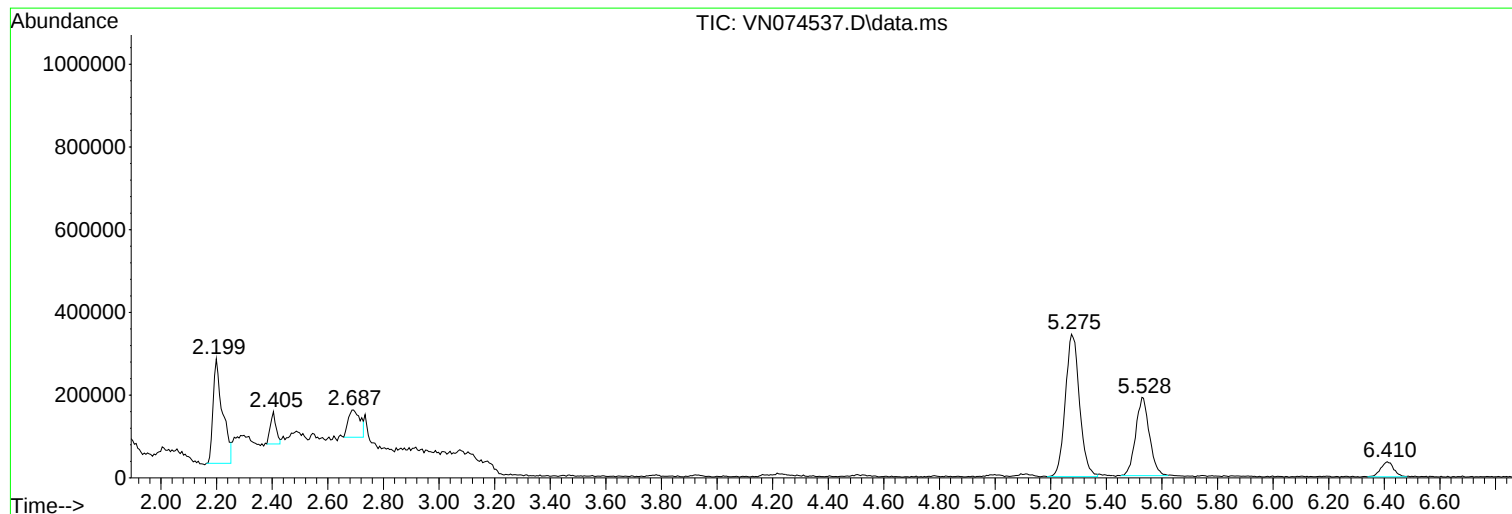
Sum of corrected areas: 14030521

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Quant Title : SW846 8260

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



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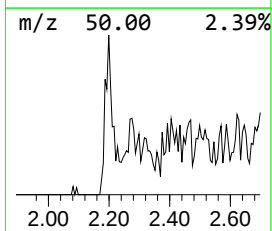
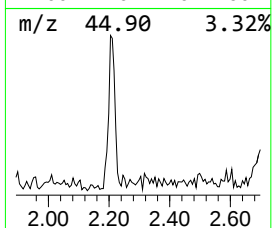
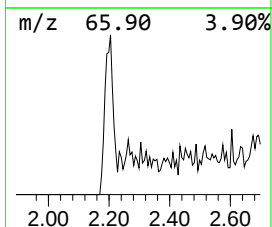
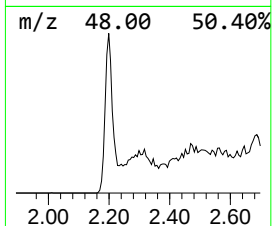
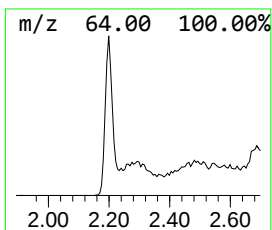
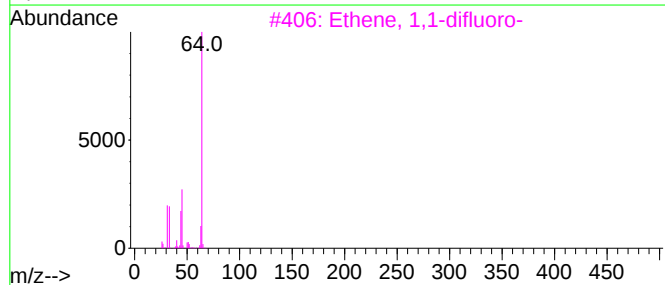
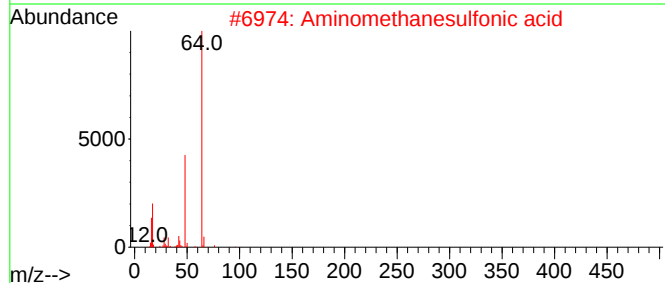
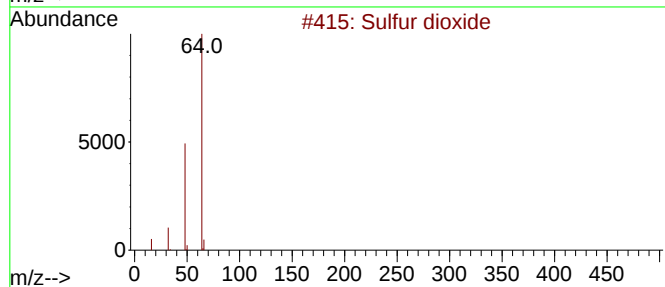
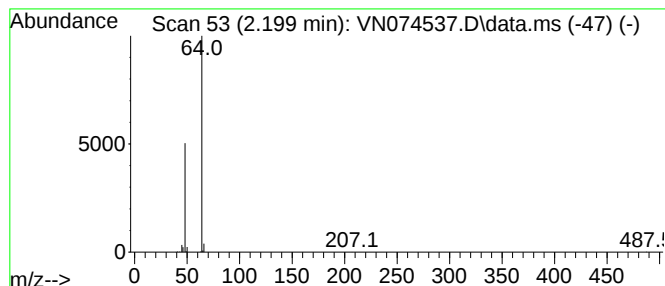
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_N\methods\82N091522W.M
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TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.199	32.84 ug/l	599148	Pentafluorobenzene	8.016

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	83
2			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	74
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	7
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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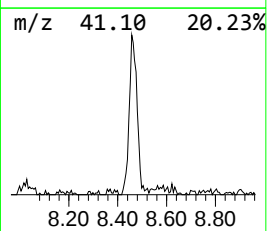
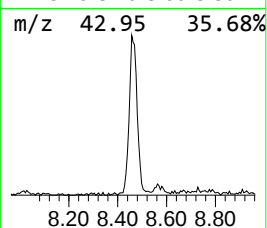
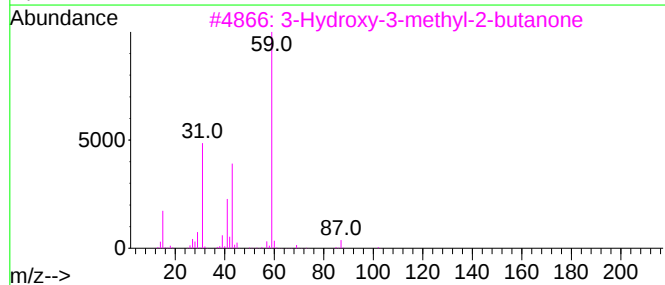
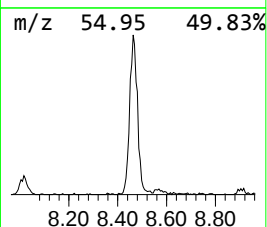
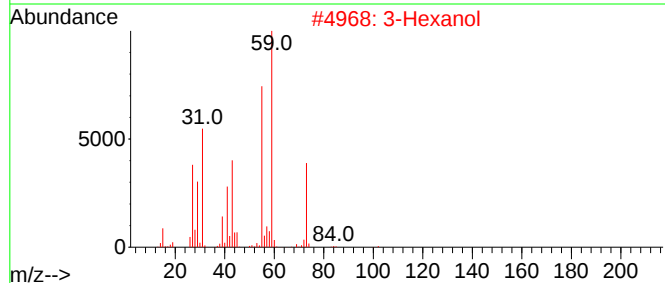
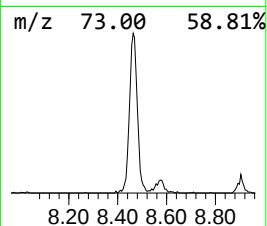
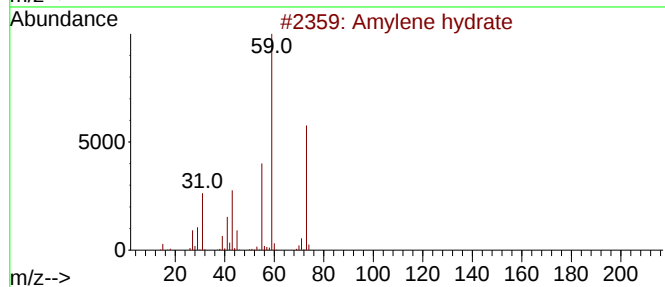
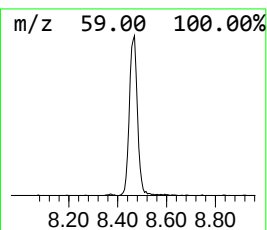
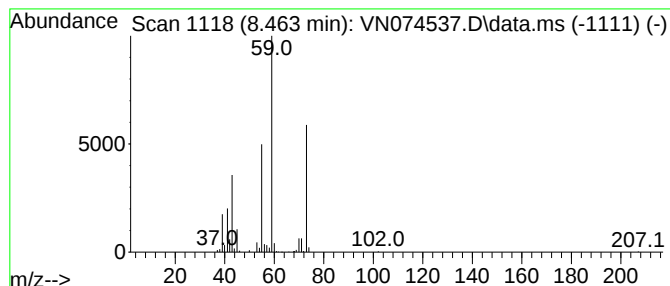
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Peak Number 4 Amylene hydrate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
8.463	24.24 ug/l	664252	1,4-Difluorobenzene	8.904

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Amylene hydrate	88	C5H12O	000075-85-4	78
2			3-Hexanol	102	C6H14O	000623-37-0	64
3			3-Hydroxy-3-methyl-2-butanone	102	C5H10O2	000115-22-0	49
4			Propanoic acid, 2-hydroxy-2-methyl-	104	C4H8O3	000594-61-6	40
5			3-Pentanol, 2-methyl-	102	C6H14O	000565-67-3	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	2.199	32.8	ug/l	599148	1	8.016	912297	50.0
2,4,6-Triamino-...	2.687	11.1	ug/l	202237	1	8.016	912297	50.0
Amylene hydrate	8.463	24.2	ug/l	664252	2	8.904	1370430	50.0