

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX100322\
 Data File : VX031846.D
 Acq On : 03 Oct 2022 20:12
 Operator : JC/MD
 Sample : N4864-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-13

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\82X100322W.M
 Title : SW846 8260

Signal : TIC: VX031846.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	40	rBV	10512	29315	4.47%	0.897%
2	5.385	694	705	721	rBV	83737	240616	36.65%	7.366%
3	5.550	721	732	749	rVB	85899	238896	36.39%	7.313%
4	5.952	789	798	812	rBV	79297	211597	32.23%	6.478%
5	6.763	920	931	944	rBV	115664	272377	41.49%	8.338%
6	8.647	1232	1240	1251	rBV	420791	656510	100.00%	20.098%
7	10.055	1465	1471	1481	rBV	286492	385300	58.69%	11.795%
8	11.079	1634	1639	1651	rBV	345347	440587	67.11%	13.488%
9	12.024	1788	1794	1801	rBV	420666	530341	80.78%	16.235%
10	12.250	1821	1831	1835	rBV	19500	30828	4.70%	0.944%
11	12.311	1838	1841	1850	rVB6	4323	8606	1.31%	0.263%
12	13.164	1965	1981	1992	rBV5	19726	92134	14.03%	2.820%
13	13.292	1999	2002	2007	rVB	24112	27858	4.24%	0.853%
14	13.658	2056	2062	2068	rVB2	8342	17990	2.74%	0.551%
15	14.091	2124	2133	2141	rVB2	8210	25425	3.87%	0.778%
16	14.213	2148	2153	2159	rVB8	3149	7479	1.14%	0.229%
17	14.621	2212	2220	2221	rBV4	7303	15469	2.36%	0.474%
18	14.908	2260	2267	2277	rBV6	5992	16787	2.56%	0.514%
19	15.383	2338	2345	2354	rBV8	6445	18483	2.82%	0.566%

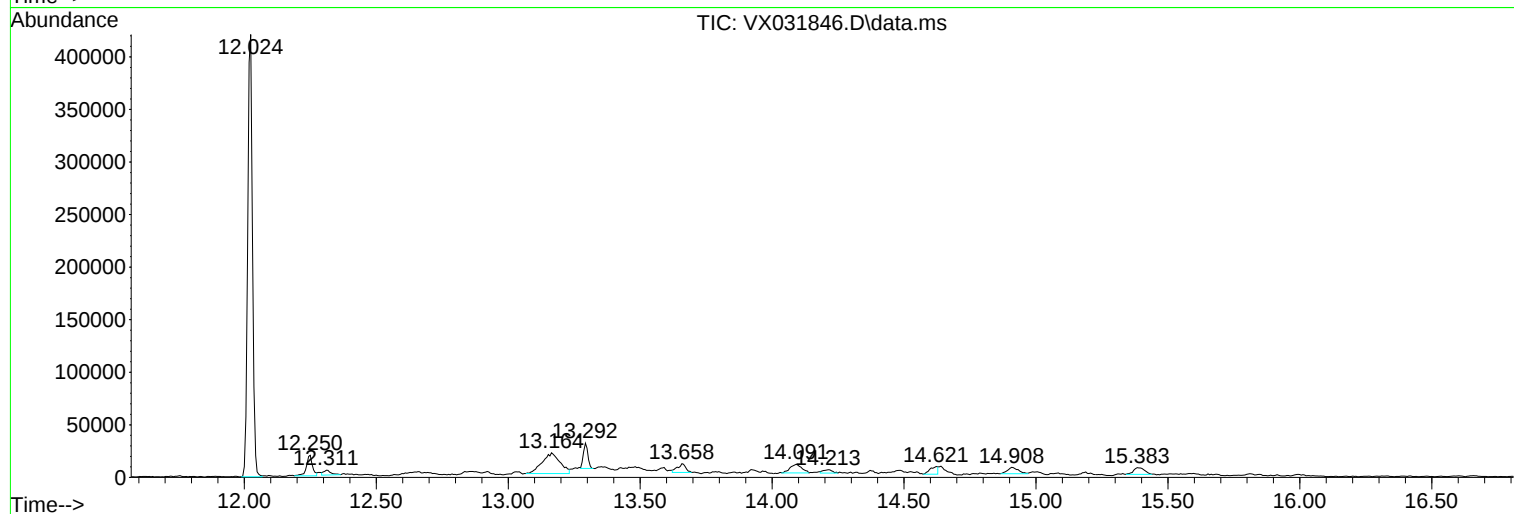
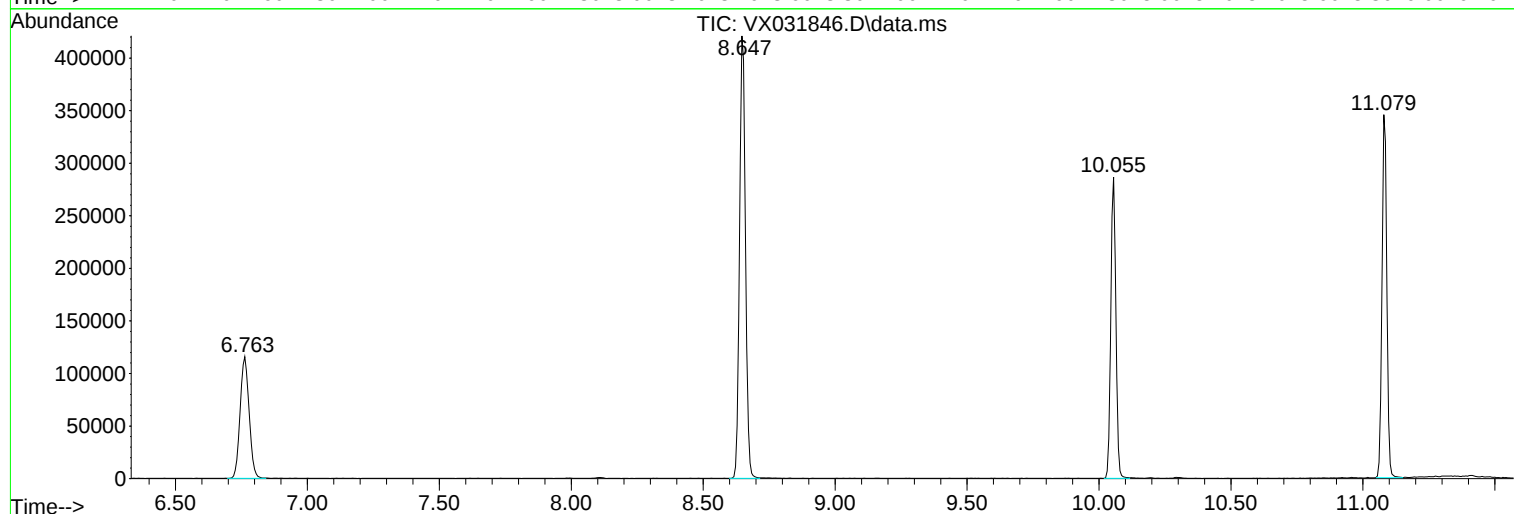
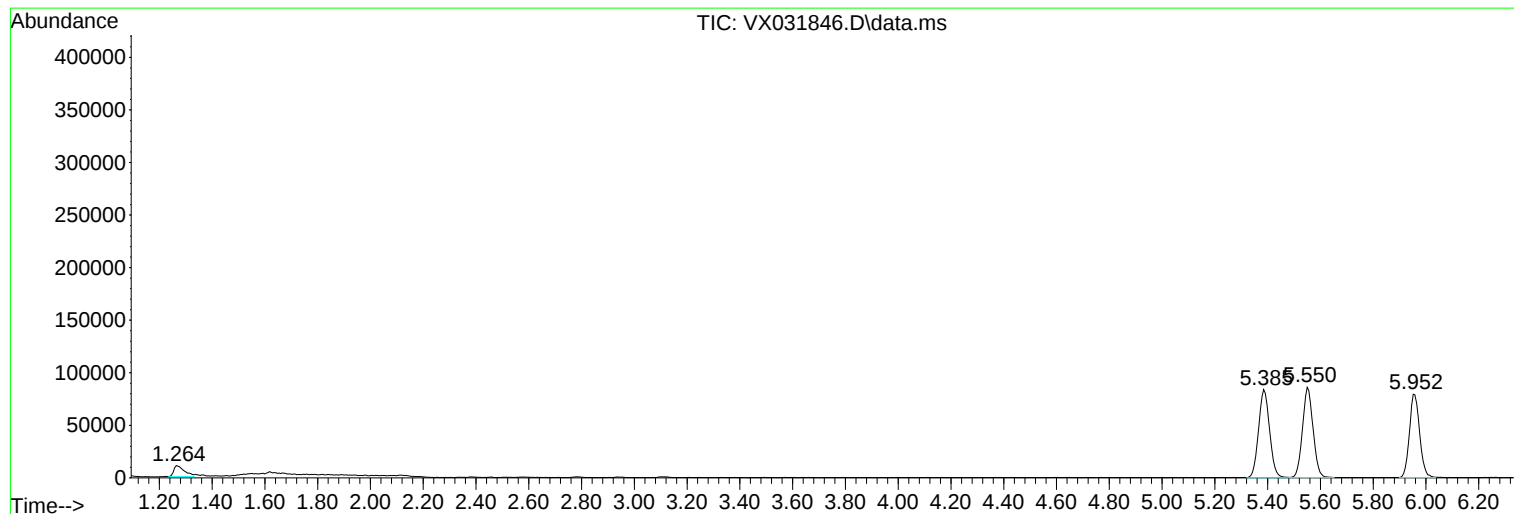
Sum of corrected areas: 3266598

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

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



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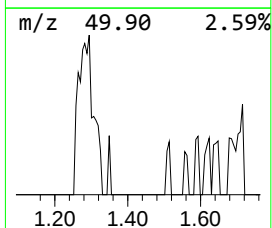
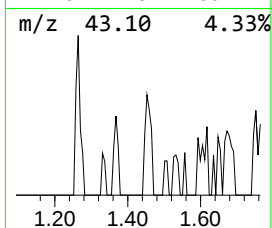
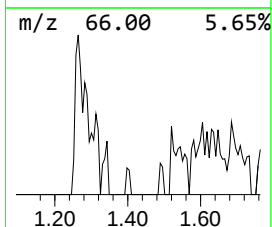
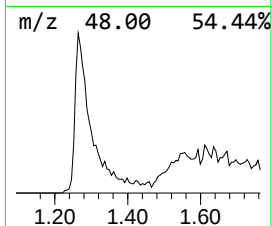
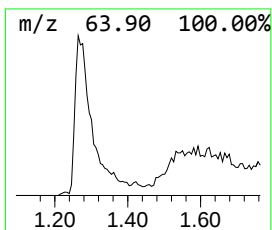
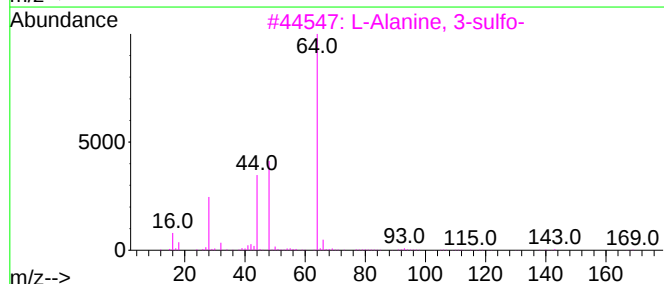
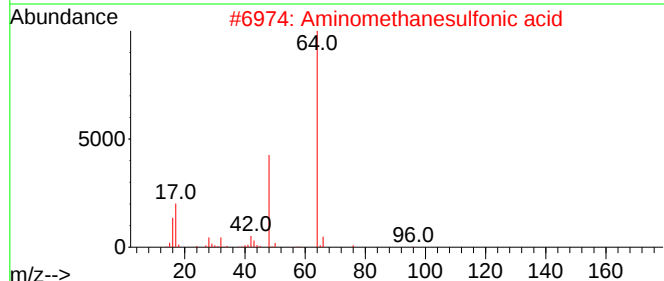
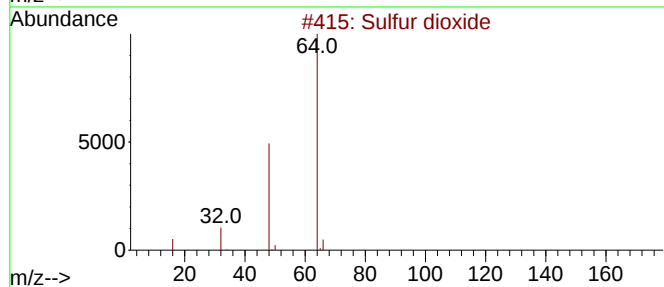
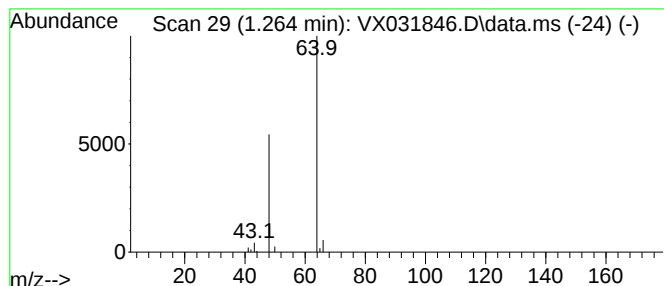
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X100322W.M
Quant Title : SW846 8260

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.
1.264	6.14 ug/l	29315	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	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	5
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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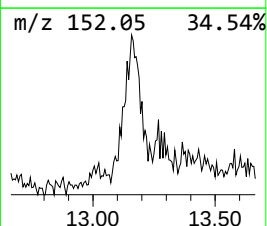
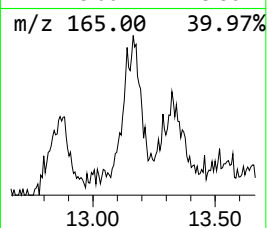
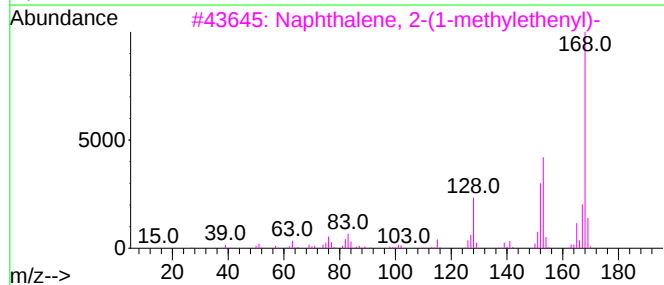
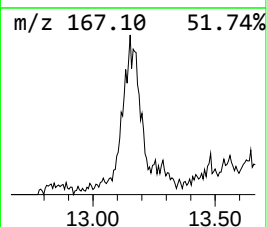
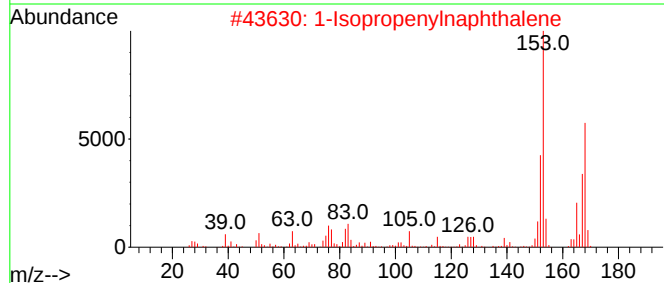
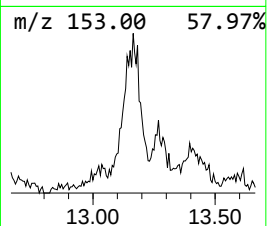
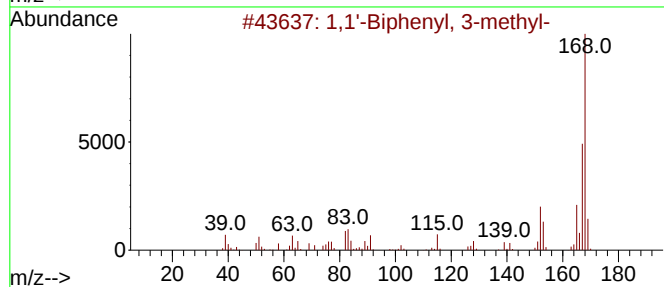
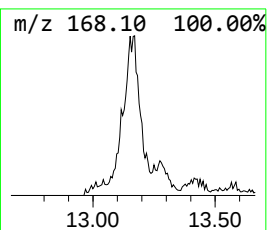
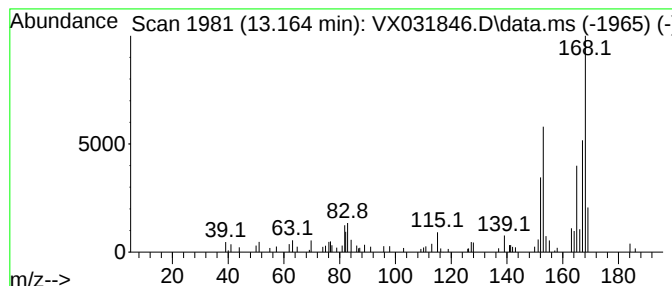
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TIC Integration Parameters: LSCINT.P

Peak Number 2 1,1'-Biphenyl, 3-methyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.164	8.69 ug/l	92134	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,1'-Biphenyl, 3-methyl-	168	C13H12	000643-93-6	64
2			1-Isopropenylnaphthalene	168	C13H12	001855-47-6	62
3			Naphthalene, 2-(1-methylethenyl)-	168	C13H12	003710-23-4	53
4			Benzene, [1-(2,4-cyclopentadien-...	168	C13H12	002320-32-3	49
5			1,1'-Biphenyl, 4-methyl-	168	C13H12	000644-08-6	49



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.264	6.1	ug/l	29315	1	5.550	238896	50.0
1,1'-Biphenyl, ...	13.164	8.7	ug/l	92134	4	12.024	530341	50.0