

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX042723\
 Data File : VX035365.D
 Acq On : 28 Apr 2023 04:59
 Operator : JC/MD
 Sample : 02522-08
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 42 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-10D

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\82X042523W.M
 Title : SW846 8260

Signal : TIC: VX035365.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.252	23	27	43	rBV	78643	180565	15.08%	2.558%
2	5.099	648	658	671	rVB2	6636	20320	1.70%	0.288%
3	5.385	693	705	720	rBV2	132581	387264	32.35%	5.485%
4	5.550	720	732	748	rVB	236368	676047	56.46%	9.576%
5	5.952	787	798	810	rBV	141929	385073	32.16%	5.454%
6	6.763	921	931	949	rBV	365256	882226	73.69%	12.496%
7	8.647	1232	1240	1250	rBV	788517	1197290	100.00%	16.959%
8	9.275	1336	1343	1354	rVB	45392	68010	5.68%	0.963%
9	10.055	1465	1471	1488	rBV	758818	1059231	88.47%	15.003%
10	10.195	1488	1494	1500	rBV	10470	15315	1.28%	0.217%
11	10.299	1506	1511	1520	rVB	54259	80120	6.69%	1.135%
12	10.640	1562	1567	1577	rBV	24324	34830	2.91%	0.493%
13	11.079	1634	1639	1655	rBV	654646	838361	70.02%	11.875%
14	11.378	1684	1688	1691	rBV3	7832	12484	1.04%	0.177%
15	11.750	1744	1749	1758	rVB	29426	38636	3.23%	0.547%
16	12.018	1788	1793	1801	rBV	766046	1014492	84.73%	14.370%
17	12.085	1801	1804	1815	rVB	13549	18268	1.53%	0.259%
18	12.244	1823	1830	1838	rVB2	11492	16693	1.39%	0.236%
19	13.774	2076	2081	2092	rBV	81528	107253	8.96%	1.519%
20	14.640	2219	2223	2228	rBV	9947	12656	1.06%	0.179%
21	14.780	2241	2246	2252	rBV2	11064	14841	1.24%	0.210%

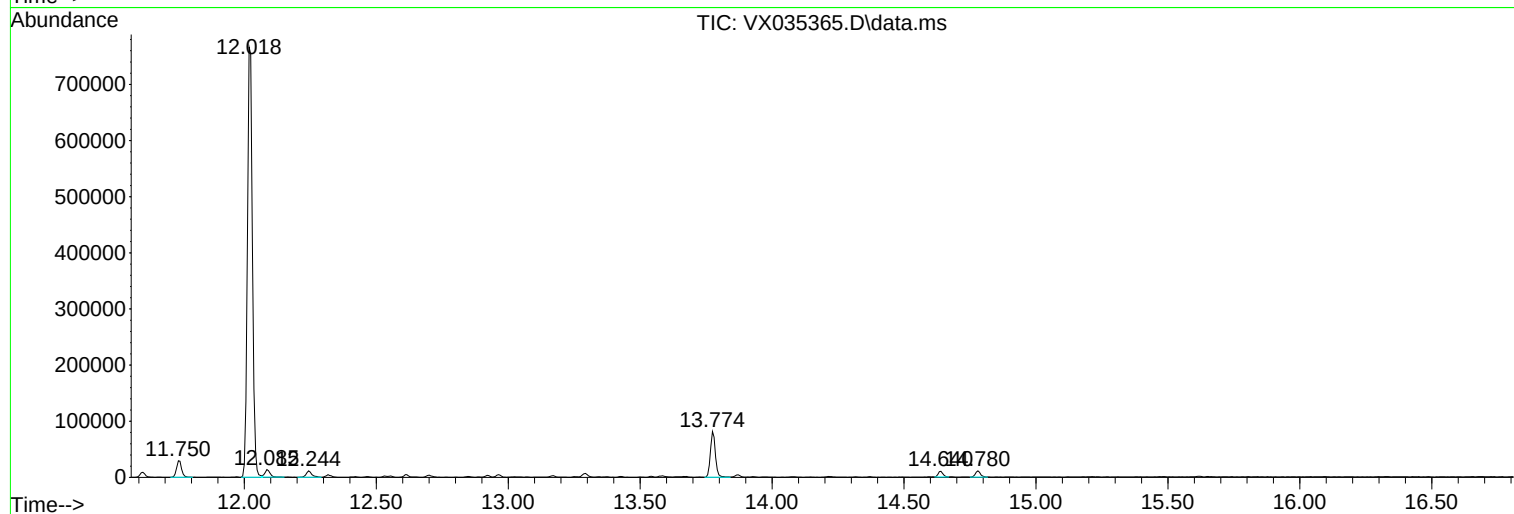
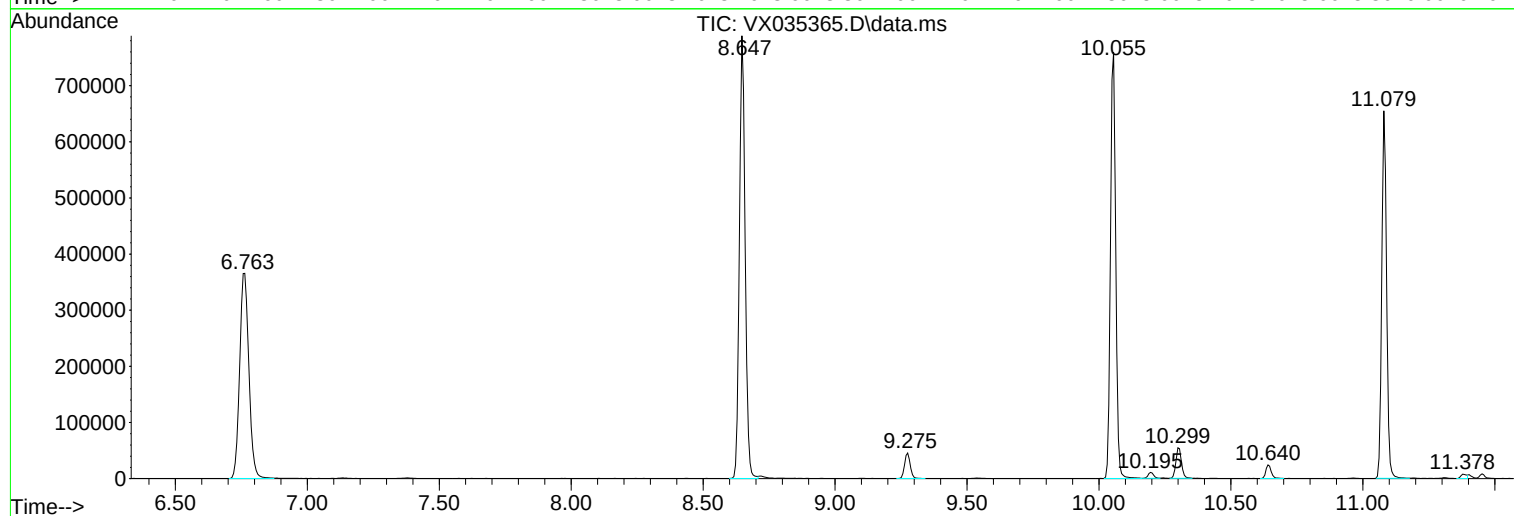
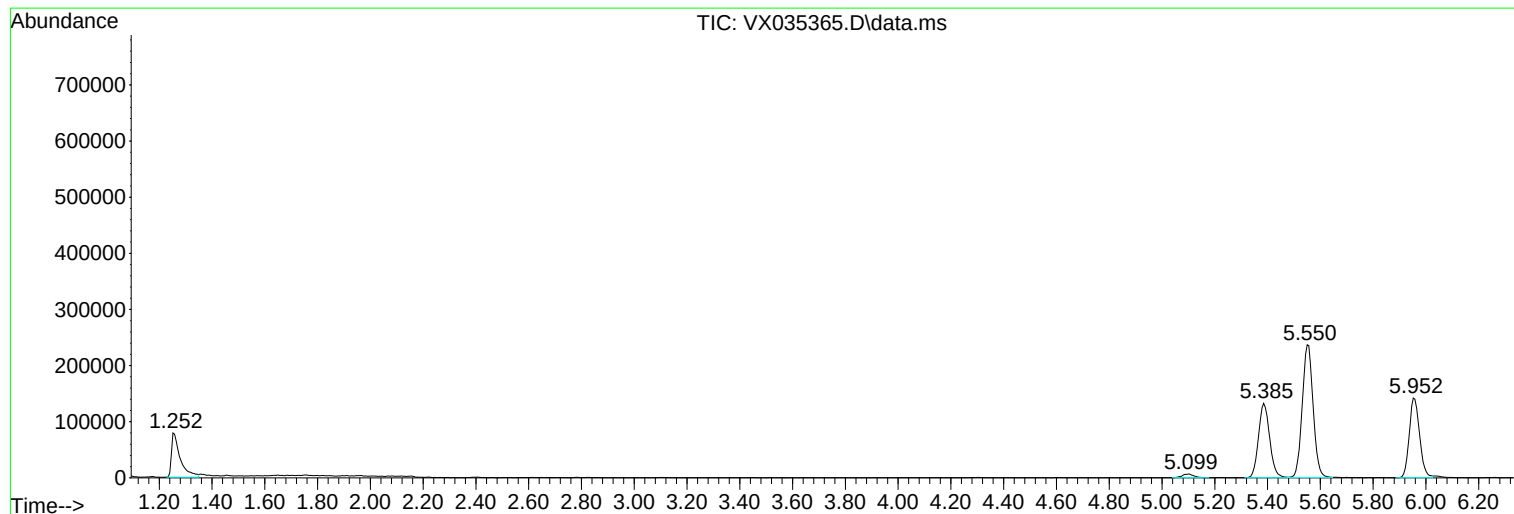
Sum of corrected areas: 7059975

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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



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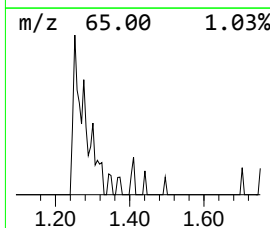
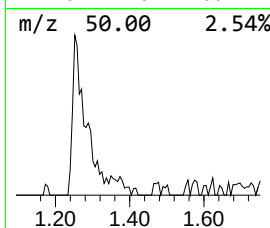
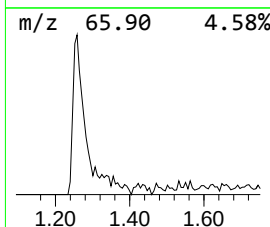
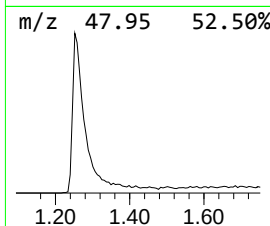
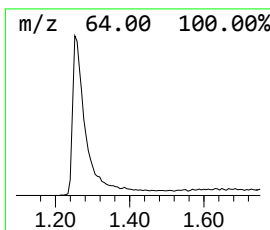
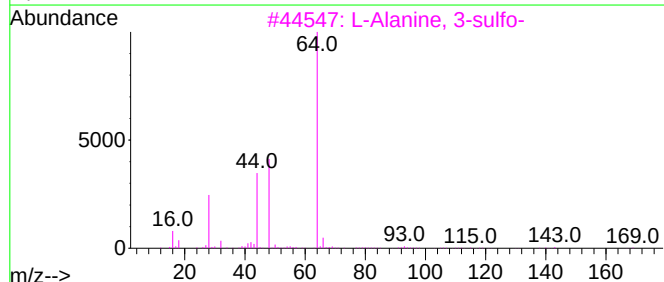
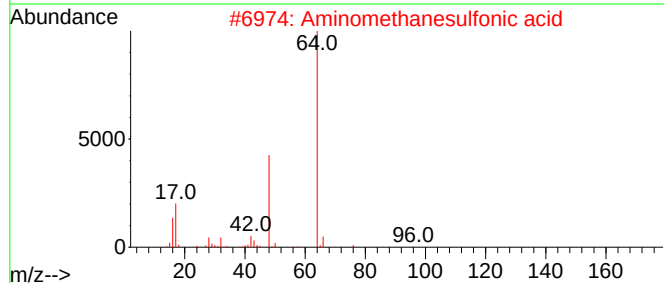
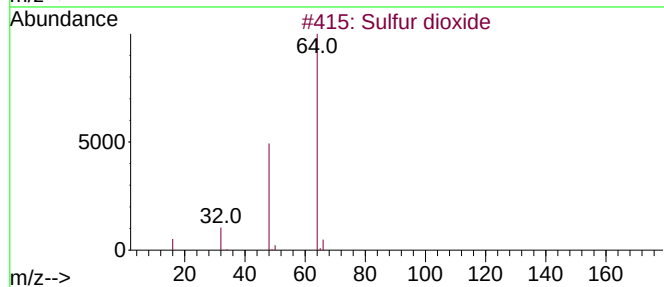
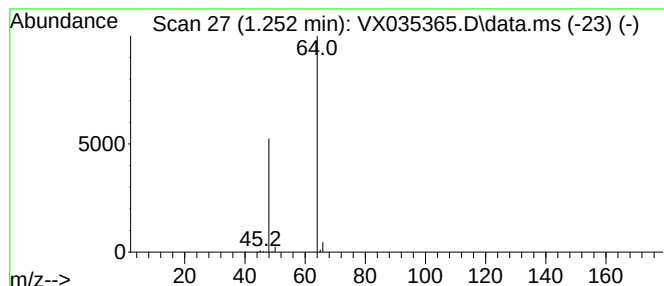
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X042523W.M
Quant Title : SW846 8260

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

Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.252	13.35 ug/l	180565	Pentafluorobenzene	5.556

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			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
5			Ethyl Chloride	64	C2H5Cl	000075-00-3	3



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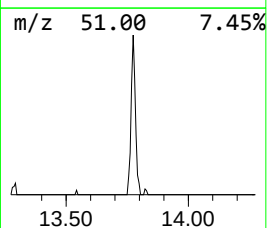
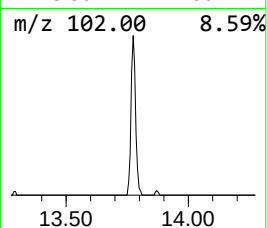
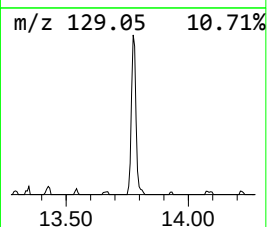
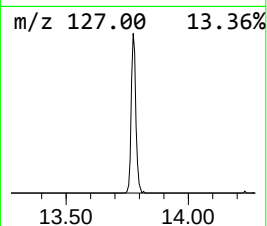
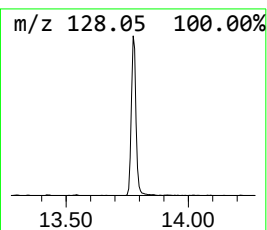
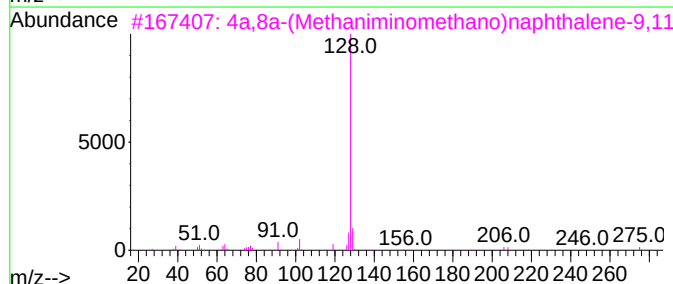
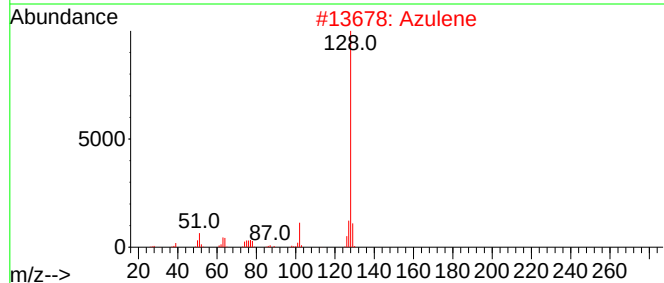
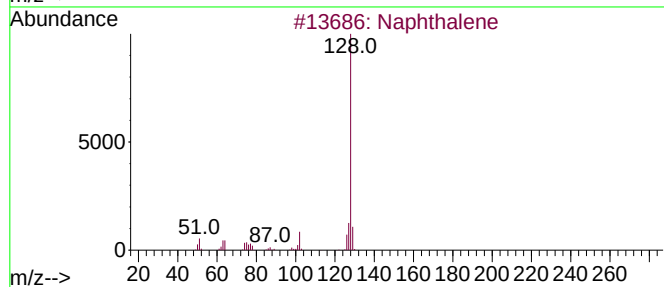
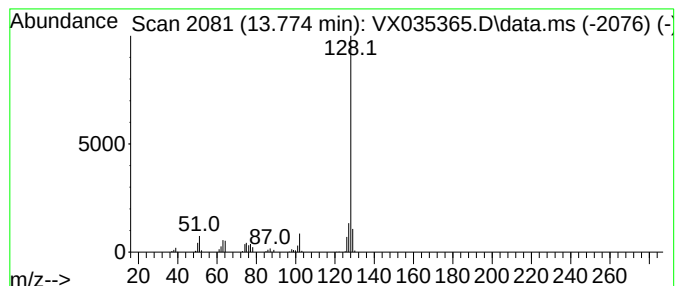
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Quant Title : SW846 8260

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

Peak Number 2 Azulene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.774	5.29 ug/l	107253	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	93
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
4			1H-Indene, 1-methylene-	128	C10H8	002471-84-3	72
5			1,4-Benzenedicarbonitrile	128	C8H4N2	000623-26-7	64



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TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.252	13.4	ug/l	180565	1	5.556	676047	50.0
Azulene	13.774	5.3	ug/l	107253	4	12.024	1014490	50.0