

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122223\
 Data File : VX039451.D
 Acq On : 22 Dec 2023 19:30
 Operator : JC/MD
 Sample : 05975-06
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 FB01-122023

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\82X121323W.M

Title : SW846 8260

Signal : TIC: VX039451.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	22	26	47	rBV	75554	184293	23.53%	4.010%
2	2.940	295	304	312	rBV	3974	8917	1.14%	0.194%
3	4.562	560	570	581	rBV2	3359	11917	1.52%	0.259%
4	5.385	694	705	720	rBV	83335	245328	31.32%	5.338%
5	5.550	720	732	748	rVV	121139	344370	43.97%	7.493%
6	5.952	786	798	813	rBV2	100013	264412	33.76%	5.753%
7	6.757	920	930	948	rBV	228104	550166	70.25%	11.971%
8	8.647	1234	1240	1252	rBV	495205	770891	98.43%	16.774%
9	10.055	1465	1471	1489	rBV	532249	751577	95.96%	16.353%
10	11.079	1634	1639	1650	rBV	456811	583918	74.56%	12.705%
11	12.018	1788	1793	1806	rBV	607287	783204	100.00%	17.042%
12	16.182	2467	2476	2494	rBV3	40427	96848	12.37%	2.107%

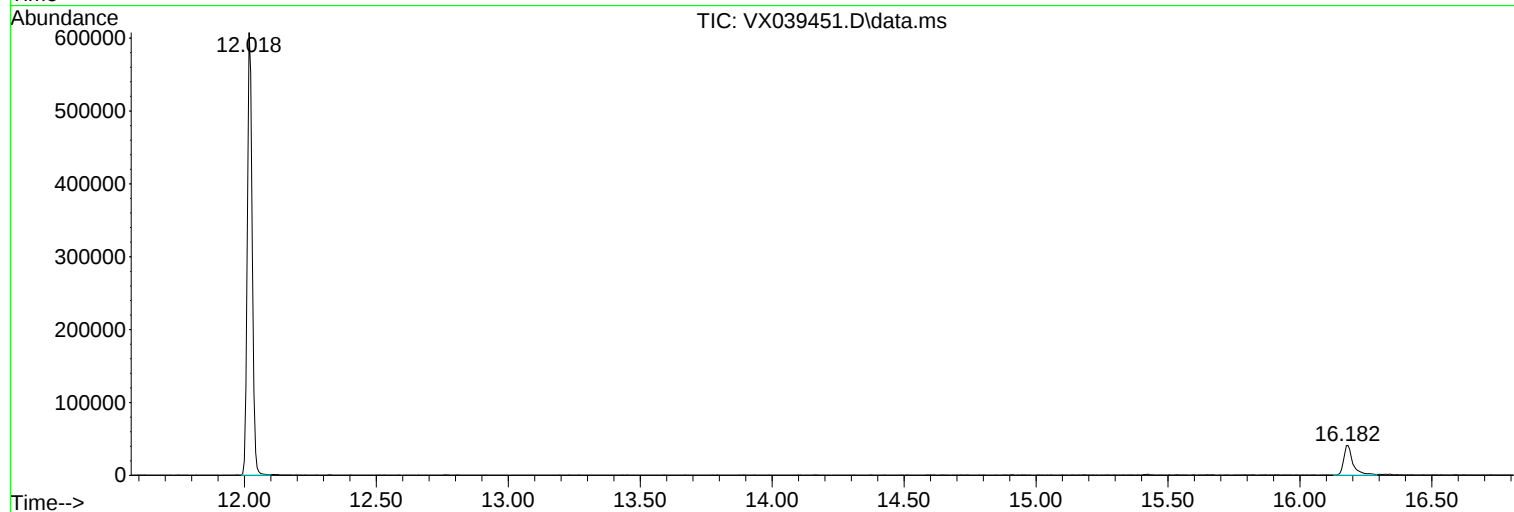
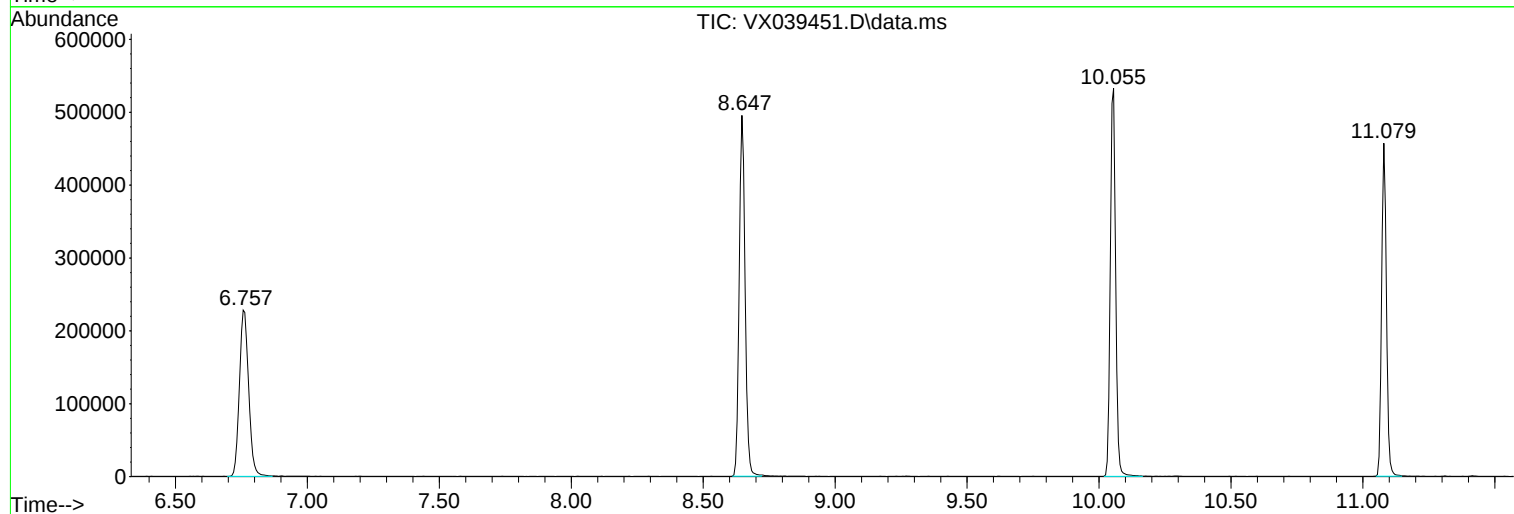
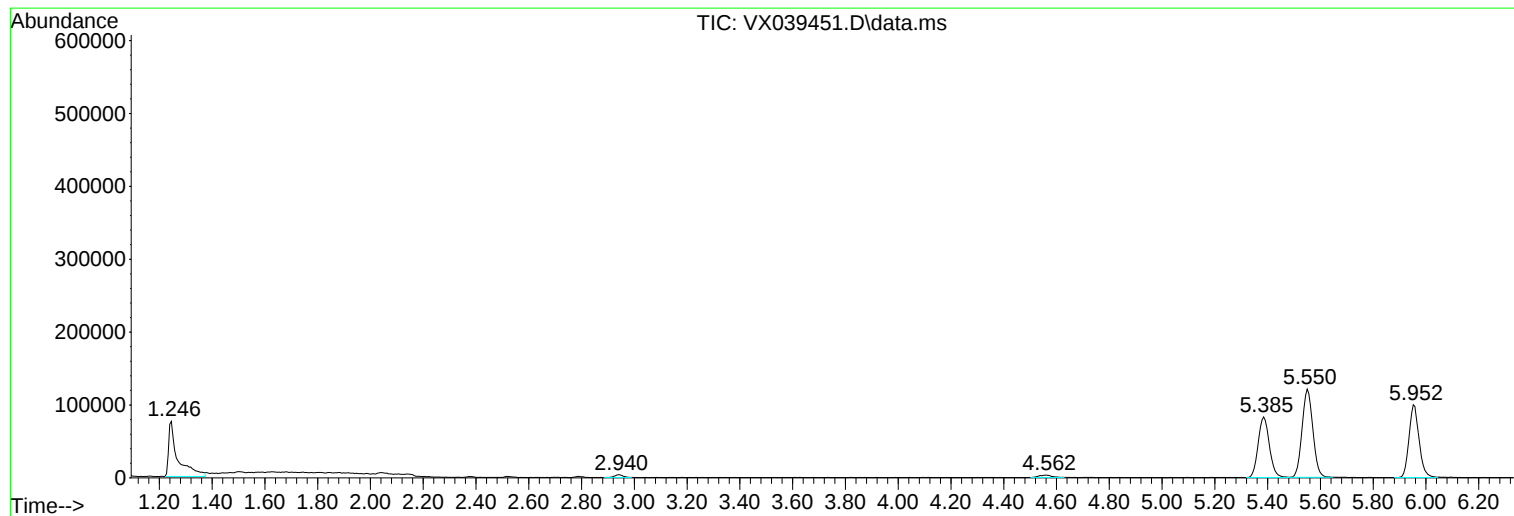
Sum of corrected areas: 4595841

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X121323W.M
Quant Title : SW846 8260

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



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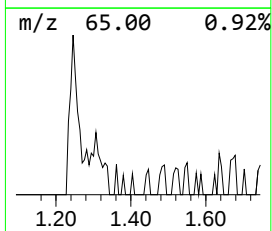
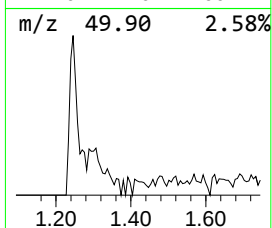
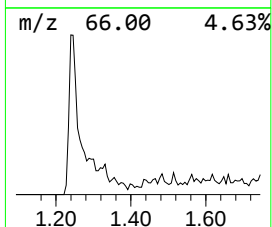
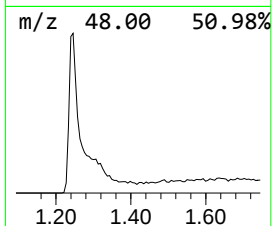
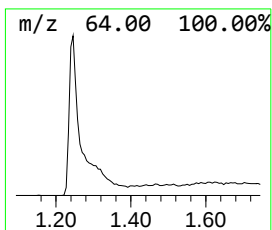
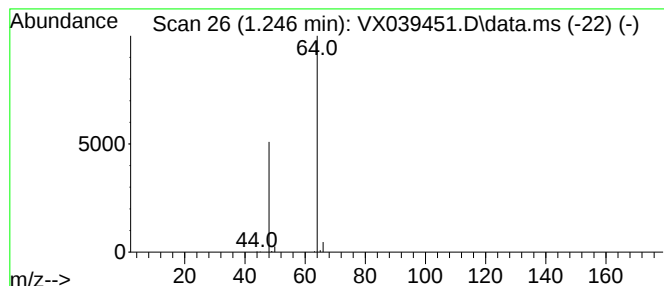
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Peak Number 1 Sulfur dioxide Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	26.76 ug/l	184293	Pentafluorobenzene	5.550

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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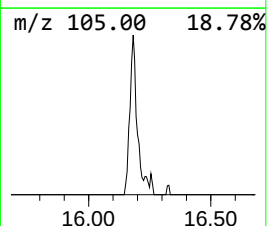
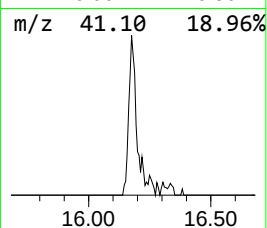
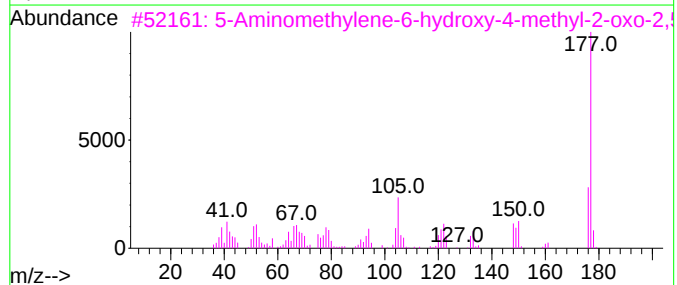
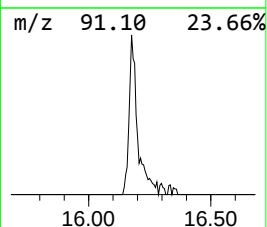
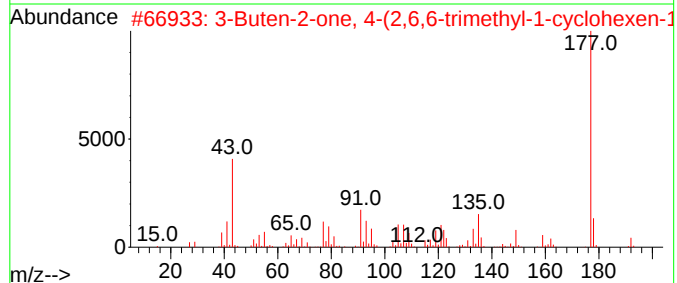
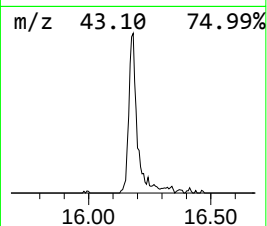
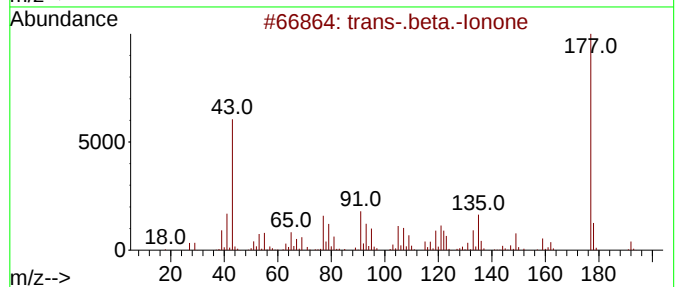
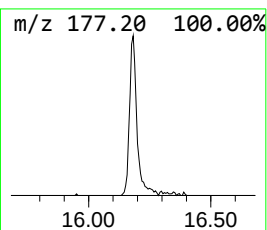
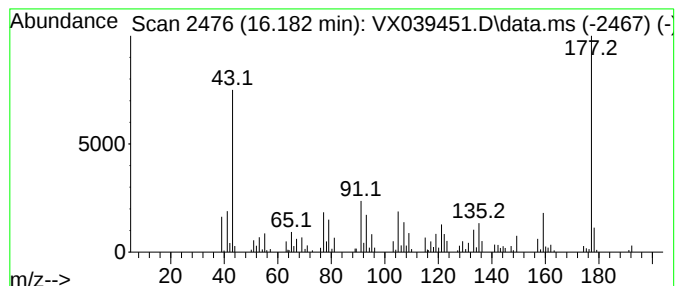
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Peak Number 2 trans-.beta.-Ionone Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.182	6.18 ug/l	96848	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-.beta.-Ionone	192	C13H20O	000079-77-6	97
2			3-Buten-2-one, 4-(2,6,6-trimethy...	192	C13H20O	014901-07-6	96
3			5-Aminomethylene-6-hydroxy-4-met...	177	C8H7N3O2	1000223-27-4	64
4			1,3-di-n-Propyladamantane	220	C16H28	040002-47-9	59
5			4(1H)-Pteridinone, 2-amino-7-met...	177	C7H7N5O	013040-58-9	59



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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	1.246	26.8	ug/l	184293	1	5.550	344370	50.0
trans-.beta.-Io...	16.182	6.2	ug/l	96848	4	12.024	783204	50.0