

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX063021\
 Data File : VX023040.D
 Acq On : 30 Jun 2021 17:41
 Operator : JC/MD
 Sample : M2892-05
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 MW-7

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\82X062321W.M

Title : SW846 8260

Signal : TIC: VX023040.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	23	26	35	rBV	21108	35267	1.39%	0.684%
2	2.971	299	309	320	rBV	231428	499776	19.70%	9.687%
3	3.123	323	334	347	rVB	1112177	2536747	100.00%	49.170%
4	3.770	430	440	454	rVB2	20722	53274	2.10%	1.033%
5	5.397	696	707	720	rBV3	41329	119469	4.71%	2.316%
6	5.562	724	734	750	rVB	69458	189957	7.49%	3.682%
7	5.964	790	800	812	rBV	57686	147181	5.80%	2.853%
8	6.257	837	848	856	rBV2	20780	62443	2.46%	1.210%
9	6.769	922	932	943	rBV	119742	283441	11.17%	5.494%
10	7.988	1124	1132	1140	rBV2	15125	29469	1.16%	0.571%
11	8.653	1234	1241	1251	rBV	254372	393718	15.52%	7.632%
12	10.055	1466	1471	1477	rBV	242796	327060	12.89%	6.339%
13	11.085	1635	1640	1649	rBV	175331	223970	8.83%	4.341%
14	12.024	1789	1794	1800	rBV	210816	257341	10.14%	4.988%

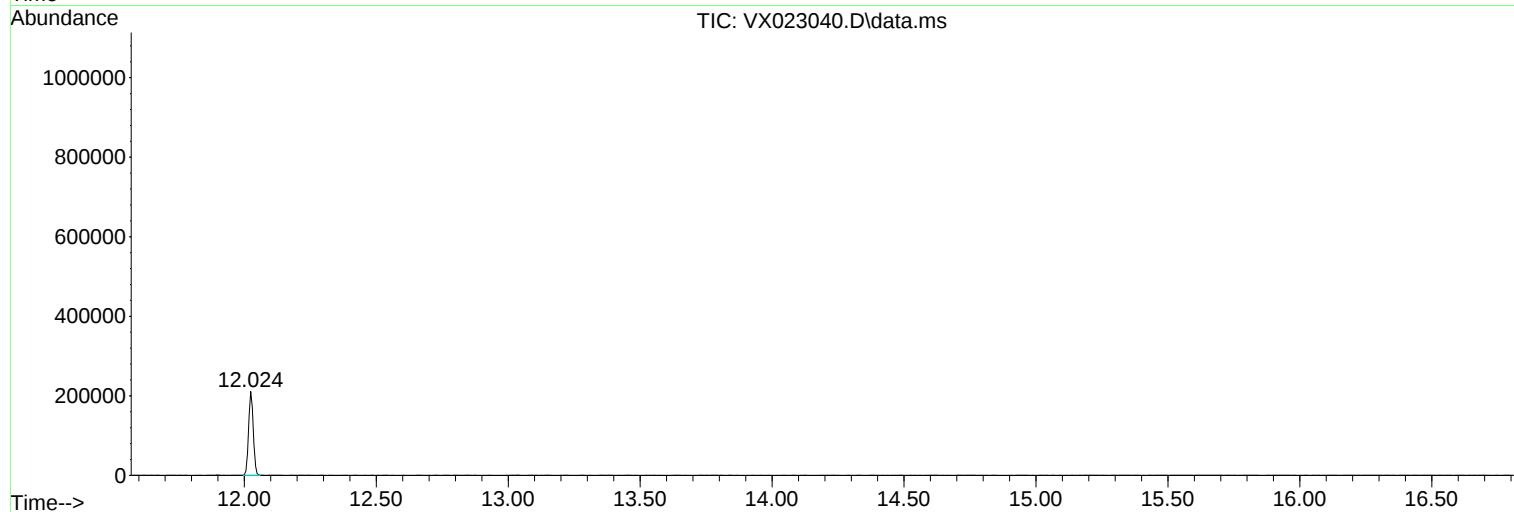
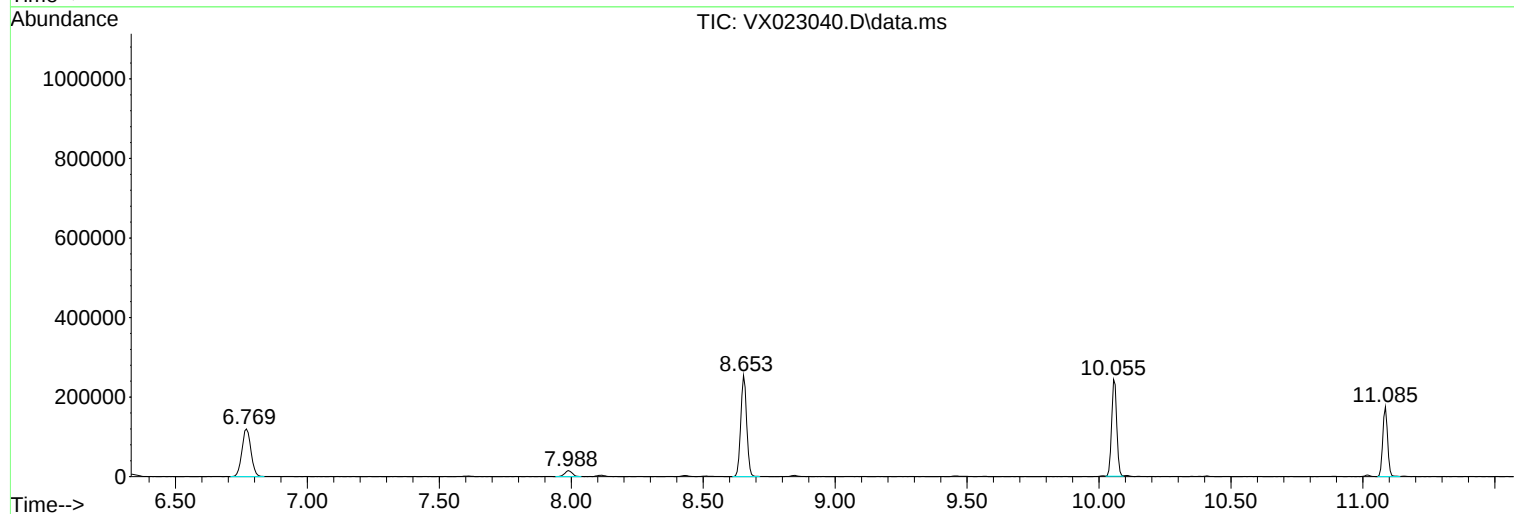
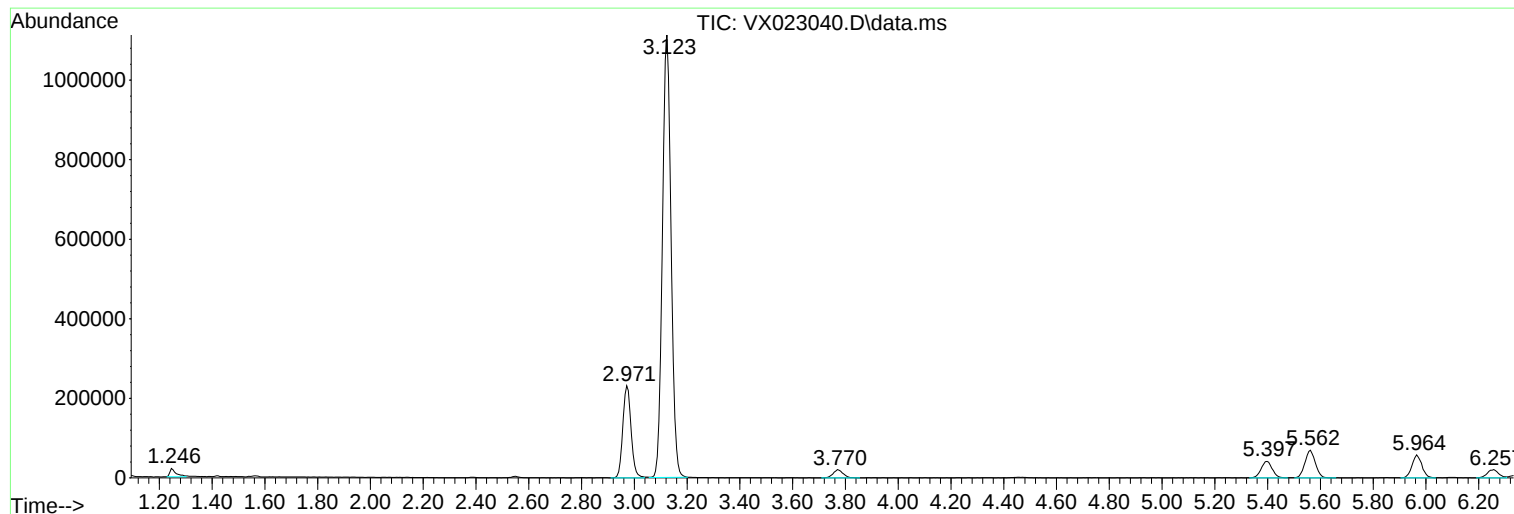
Sum of corrected areas: 5159113

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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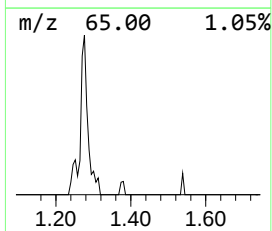
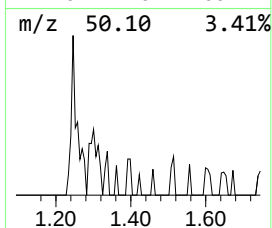
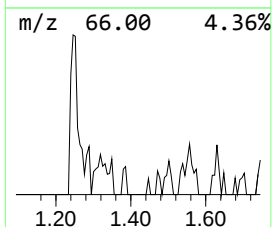
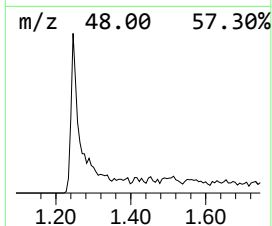
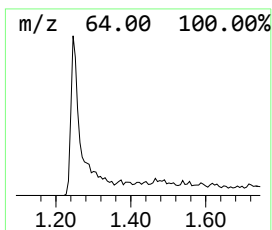
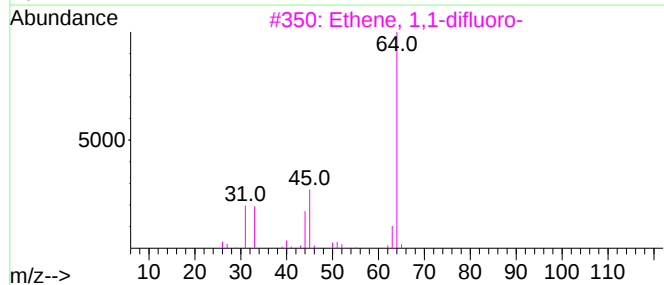
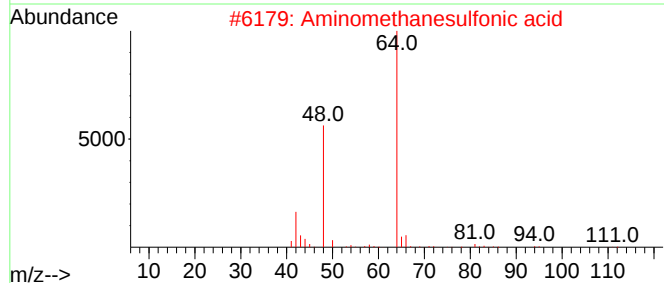
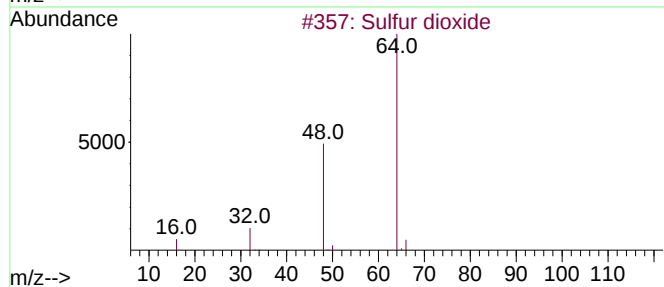
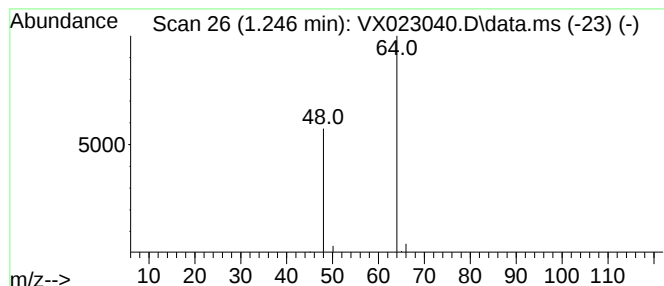
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X062321W.M
Quant Title : SW846 8260

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Sulfur dioxide Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.246	9.28 ug/l	35267	Pentafluorobenzene	5.562

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	9
3			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	4
4			Ethyl Chloride	64	C2H5Cl	000075-00-3	3
5			Ethene, 1,2-difluoro-	64	C2H2F2	001691-13-0	3



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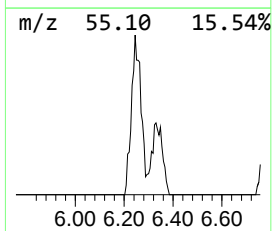
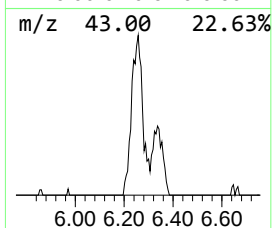
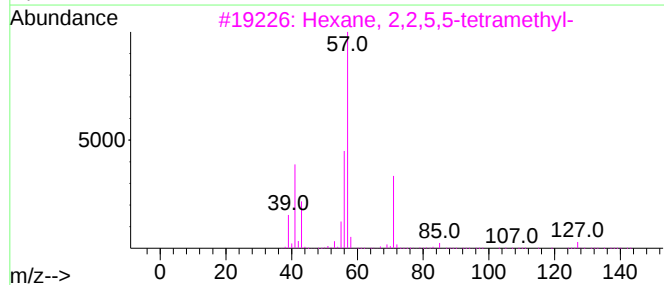
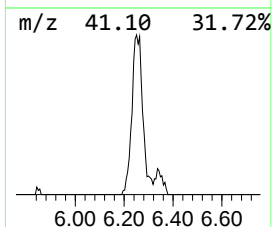
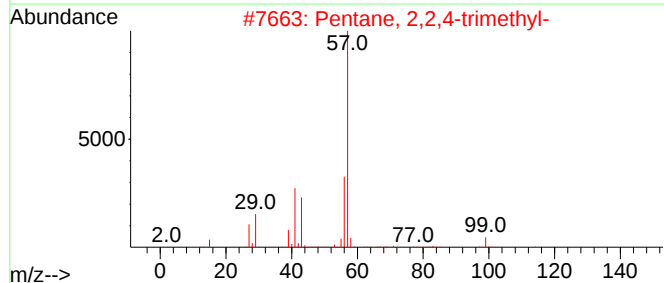
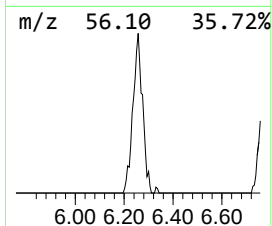
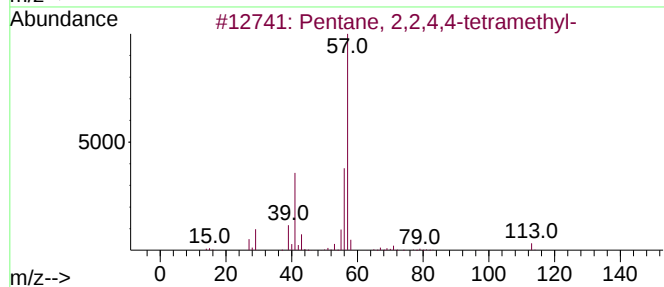
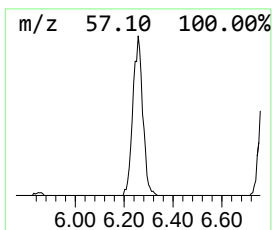
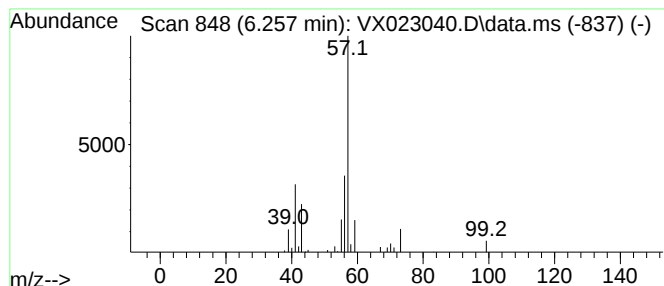
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Peak Number 2 unknown6.257 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.257	11.02 ug/l	62443	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,4,4-tetramethyl-	128	C9H20	001070-87-7	47
2			Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	47
3			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	43
4			Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	38
5			Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	38



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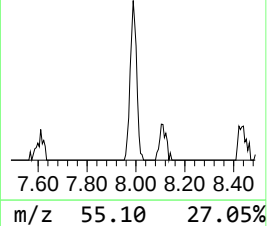
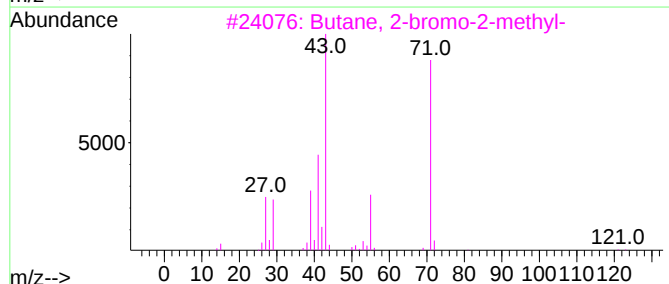
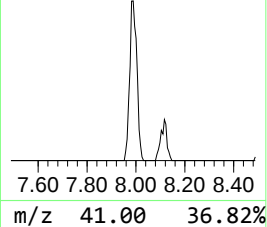
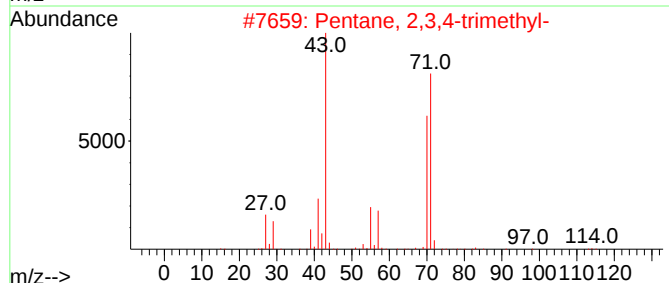
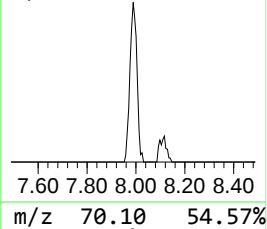
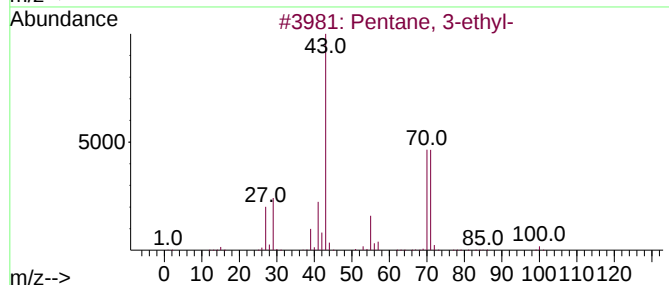
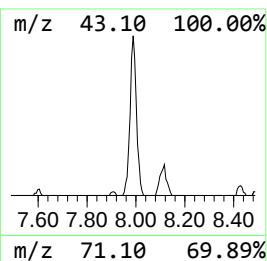
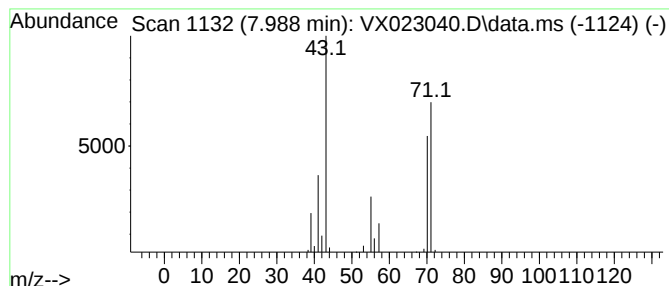
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Peak Number 3 Pentane, 3-ethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.988	5.20 ug/l	29469	1,4-Difluorobenzene	6.769

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 3-ethyl-	100	C7H16	000617-78-7	83
2			Pentane, 2,3,4-trimethyl-	114	C8H18	000565-75-3	83
3			Butane, 2-bromo-2-methyl-	150	C5H11Br	000507-36-8	38
4			1,6-Heptadien-4-ol	112	C7H12O	002883-45-6	37
5			Ethanedioic acid, bis(3-methylbu...	230	C12H22O4	002051-00-5	36



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.246	9.3	ug/l	35267	1	5.562	189957	50.0
unknown6.257	6.257	11.0	ug/l	62443	2	6.769	283441	50.0
Pentane, 3-ethyl-	7.988	5.2	ug/l	29469	2	6.769	283441	50.0