

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX091323\
 Data File : VX037684.D
 Acq On : 13 Sep 2023 10:48
 Operator : JC/MD
 Sample : VX0913MBL01
 Misc : 5.00g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VX0913MBL01

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\82X091123W.M
 Title : SW846 8260

Signal : TIC: VX037684.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.575	68	80	82	rBV5	16927	55723	6.06%	1.118%
2	2.788	273	279	286	rBV3	5091	10266	1.12%	0.206%
3	2.947	297	305	318	rVB2	7895	20800	2.26%	0.417%
4	4.580	561	573	584	rBV2	13093	42960	4.67%	0.862%
5	5.385	693	705	721	rBV2	104385	308175	33.49%	6.183%
6	5.550	721	732	750	rVB	187888	532977	57.92%	10.694%
7	5.952	789	798	810	rBV	114313	310581	33.75%	6.231%
8	6.763	920	931	947	rBV	277460	676254	73.49%	13.568%
9	8.647	1234	1240	1251	rBV	587339	920206	100.00%	18.463%
10	10.055	1465	1471	1486	rBV	585931	798241	86.75%	16.016%
11	11.079	1634	1639	1651	rBV	447670	573277	62.30%	11.502%
12	12.024	1788	1794	1809	rVB	529350	693306	75.34%	13.910%
13	12.335	1841	1845	1852	rBV2	6666	9470	1.03%	0.190%
14	13.591	2046	2051	2056	rBV	6902	9304	1.01%	0.187%
15	13.780	2076	2082	2088	rBV	8576	11344	1.23%	0.228%
16	13.963	2107	2112	2118	rVB	8748	11207	1.22%	0.225%

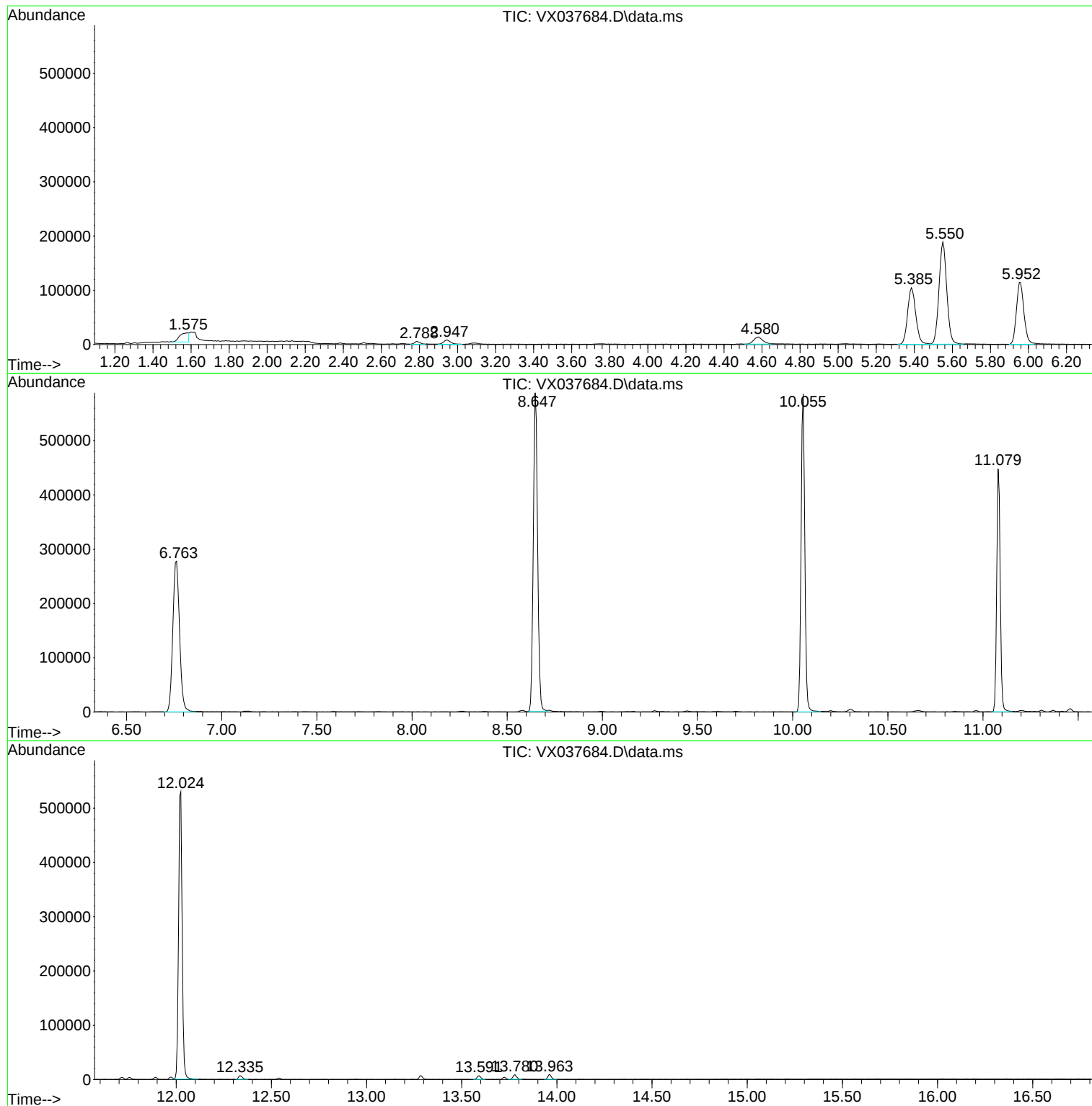
Sum of corrected areas: 4984091

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091123W.M
Quant Title : SW846 8260

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



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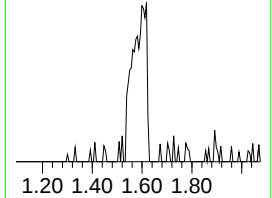
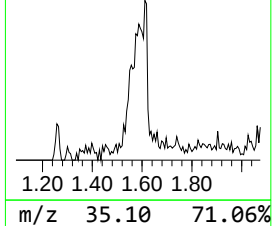
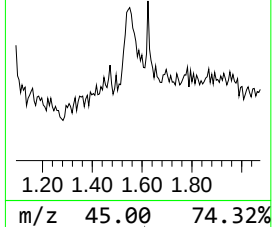
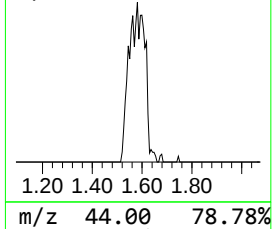
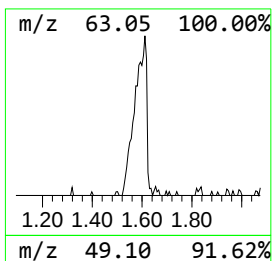
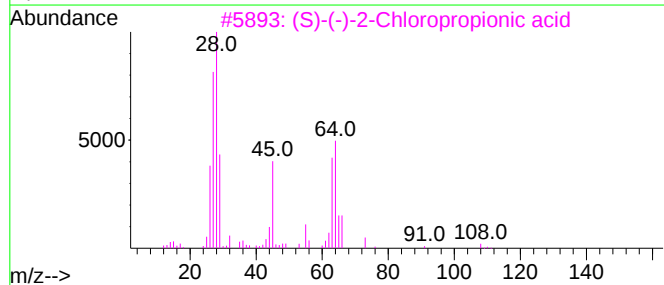
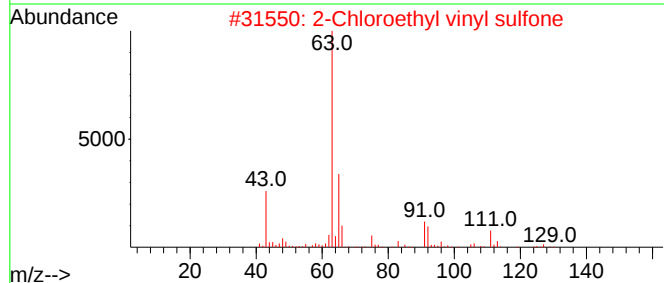
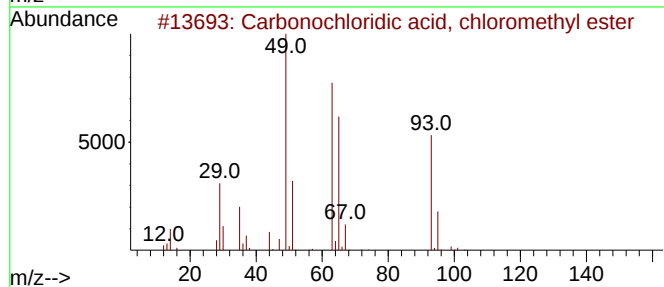
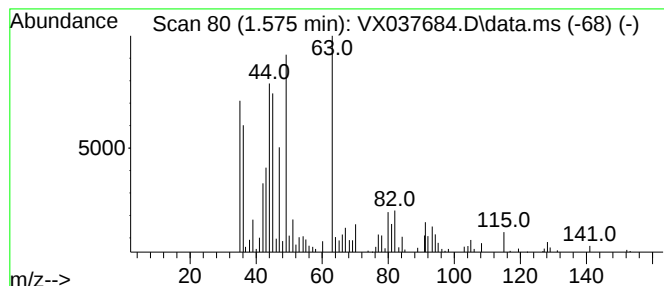
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X091123W.M
Quant Title : SW846 8260

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Peak Number 1 unknown1.575 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.575	5.23 ug/l	55723	Pentafluorobenzene	5.550

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Carbonochloridic acid, chloromet...	128	C2H2Cl2O2	022128-62-7	28
2			2-Chloroethyl vinyl sulfone	154	C4H7ClO2S	007327-58-4	10
3			(S)-(-)-2-Chloropropionic acid	108	C3H5ClO2	029617-66-1	10
4			Propanoic acid, 2-chloro-	108	C3H5ClO2	000598-78-7	9
5			2-Chloroethyl methyl sulfoxide	126	C3H7ClOS	005331-57-7	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown1.575	1.575	5.2	ug/l	55723	1	5.550	532977	50.0