

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX032023\
 Data File : VX034626.D
 Acq On : 20 Mar 2023 14:35
 Operator : JC/MD
 Sample : 01828-01
 Misc : 5.06g/10mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 AVENEL-60

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\82X031023W.M
 Title : SW846 8260

Signal : TIC: VX034626.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.624	67	88	95	rBV	39819	169671	12.75%	2.212%
2	2.715	261	267	274	rBV	116186	198853	14.94%	2.592%
3	2.776	274	277	293	rVB2	6720	14469	1.09%	0.189%
4	5.385	694	705	719	rVV2	133680	389122	29.24%	5.073%
5	5.544	719	731	747	rVB	250280	707995	53.19%	9.230%
6	5.952	788	798	808	rBV	167491	444206	33.37%	5.791%
7	6.031	808	811	821	rVB3	10256	22798	1.71%	0.297%
8	6.757	920	930	942	rBV	445091	1060424	79.67%	13.824%
9	8.647	1233	1240	1247	rBV	869731	1330994	100.00%	17.351%
10	8.720	1247	1252	1261	rVB	20205	39277	2.95%	0.512%
11	10.055	1465	1471	1479	rBV	774893	1071475	80.50%	13.968%
12	11.085	1634	1640	1651	rBV	615400	836474	62.85%	10.905%
13	12.024	1789	1794	1800	rBV	842230	1032212	77.55%	13.456%
14	12.908	1935	1939	1943	rBV	18403	25752	1.93%	0.336%
15	13.774	2078	2081	2086	rVB	38876	48331	3.63%	0.630%
16	14.755	2239	2242	2245	rBV	38929	43995	3.31%	0.574%
17	15.213	2313	2317	2322	rVB2	29723	42363	3.18%	0.552%
18	15.353	2336	2340	2346	rVB2	30231	43546	3.27%	0.568%
19	15.493	2359	2363	2370	rVB2	37232	62807	4.72%	0.819%
20	16.097	2457	2462	2468	rVB10	15375	32073	2.41%	0.418%
21	16.255	2483	2488	2492	rBV6	15090	31544	2.37%	0.411%
22	16.371	2504	2507	2518	rVB9	10445	22421	1.68%	0.292%

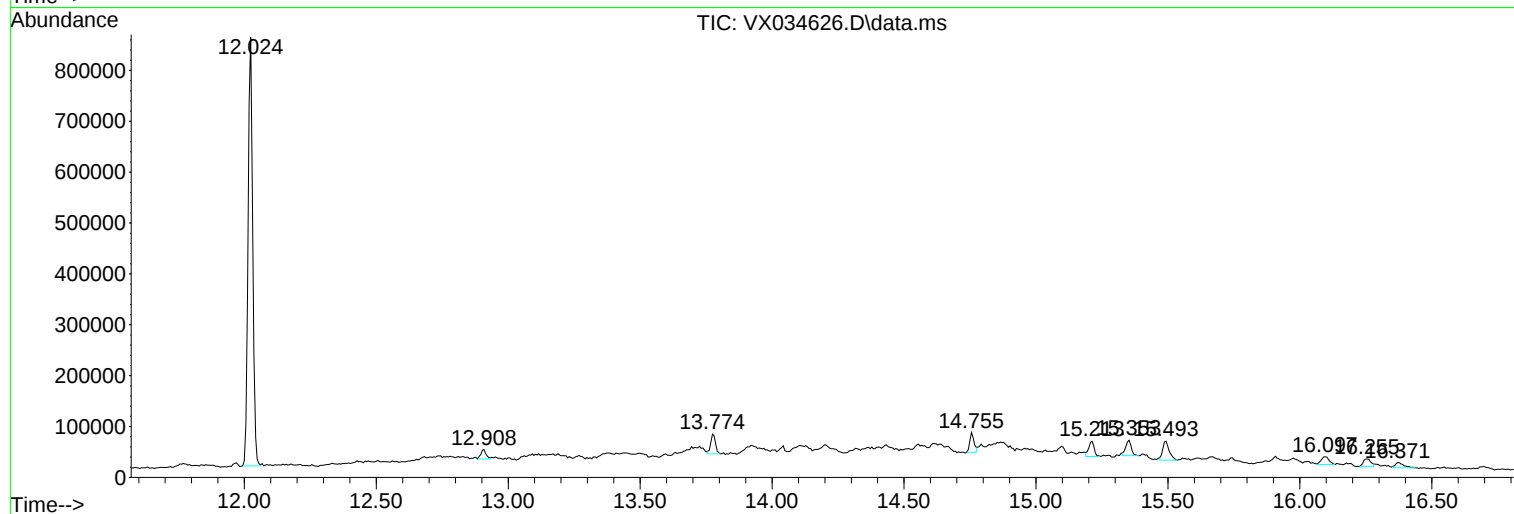
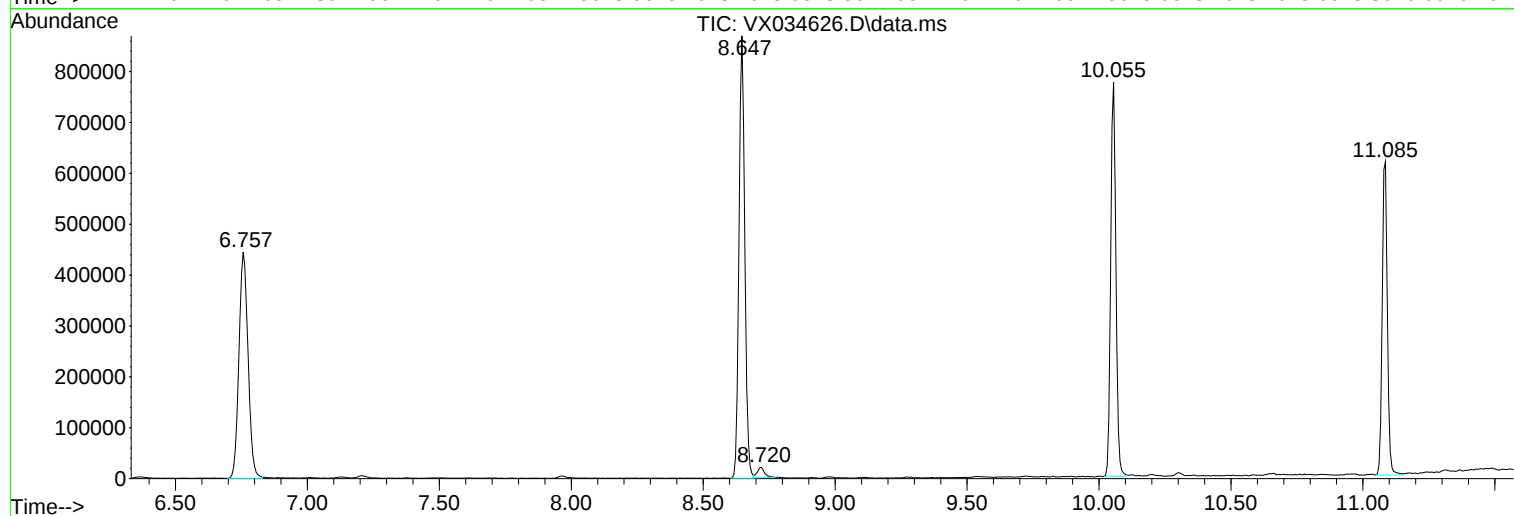
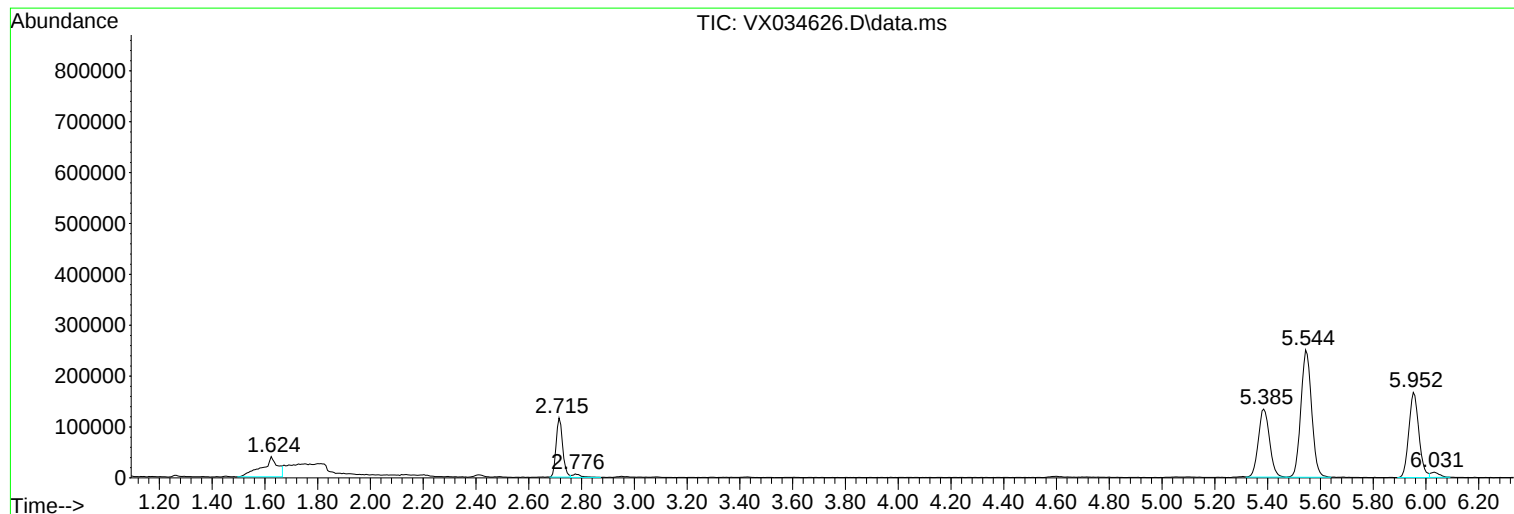
Sum of corrected areas: 7670802

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ClientSampleId :
AVENEL-60

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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



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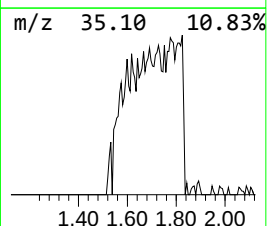
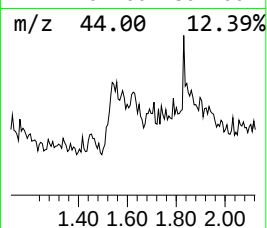
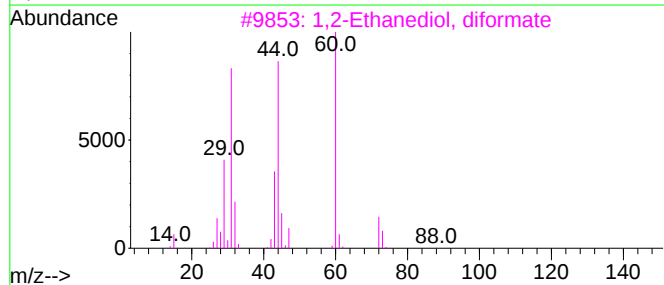
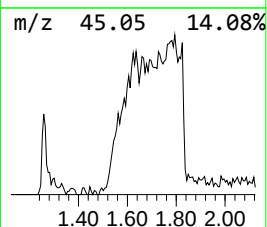
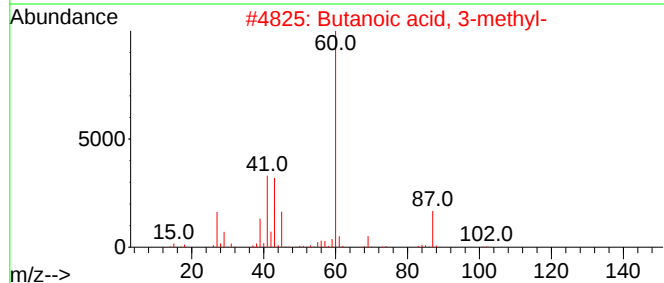
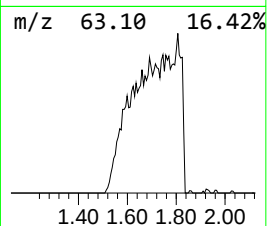
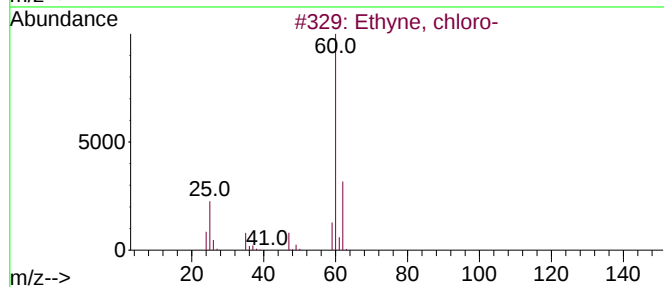
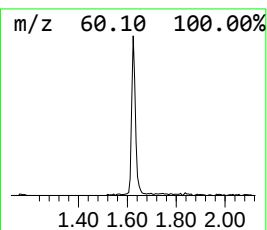
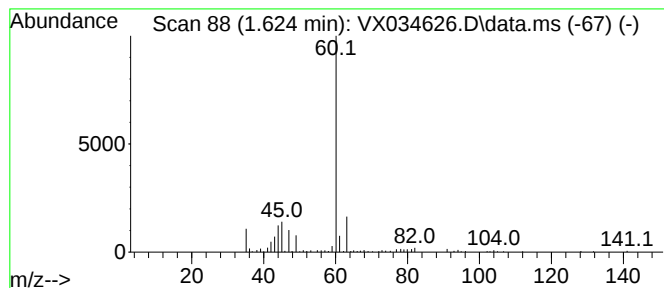
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\82X031023W.M
Quant Title : SW846 8260

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

Peak Number 1 Ethyne, chloro- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.624	11.98 ug/l	169671	Pentafluorobenzene	5.544

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyne, chloro-	60	C2HCl	000593-63-5	59
2			Butanoic acid, 3-methyl-	102	C5H10O2	000503-74-2	38
3			1,2-Ethanediol, diformate	118	C4H6O4	000629-15-2	36
4			Hexanoic acid	116	C6H12O2	000142-62-1	9
5			2-Amino-1,3-propanediol	91	C3H9NO2	000534-03-2	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Ethyne, chloro-	1.624	12.0	ug/l	169671	1	5.544	707995	50.0