

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV031122\
 Data File : VV024958.D
 Acq On : 11 Mar 2022 12:36
 Operator : SY/MD
 Sample : N1816-05ME
 Misc : 4.55g/5.0mL/100uL/5mL/MSVOA_V/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBSD2ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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_V\Method\SFAMVLM022822WMA.M
 Title : VOC Analysis

Signal : TIC: VV024958.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.211	50	53	58	rVV	4122	3078	0.18%	0.025%
2	1.240	59	62	69	rVB	4014	3263	0.19%	0.026%
3	1.304	75	82	99	rBV	197532	238601	13.65%	1.902%
4	1.568	156	164	182	rVB	127806	174833	10.00%	1.394%
5	2.085	314	325	338	rBV	392322	557350	31.88%	4.444%
6	2.275	374	384	397	rVB	9898	16056	0.92%	0.128%
7	2.388	417	419	424	rVB	454	315	0.02%	0.003%
8	2.500	443	454	463	rVB6	1972	3546	0.20%	0.028%
9	2.616	484	490	493	rBV2	350	508	0.03%	0.004%
10	2.954	591	595	599	rVB2	428	369	0.02%	0.003%
11	3.224	674	679	682	rBV	350	363	0.02%	0.003%
12	3.278	692	696	699	rBV	344	238	0.01%	0.002%
13	3.323	707	710	717	rVB2	313	305	0.02%	0.002%
14	3.362	717	722	724	rBV	281	246	0.01%	0.002%
15	3.429	736	743	746	rVB2	219	253	0.01%	0.002%
16	3.638	804	808	813	rBV2	329	370	0.02%	0.003%
17	3.780	849	852	856	rVB2	393	288	0.02%	0.002%
18	3.909	880	892	953	rBV	63936	336294	19.24%	2.681%
19	4.343	1011	1027	1055	rBV	264644	676106	38.67%	5.391%
20	4.693	1133	1136	1141	rBV3	376	273	0.02%	0.002%
21	4.722	1141	1145	1150	rBV3	277	352	0.02%	0.003%
22	4.854	1183	1186	1191	rVB2	284	250	0.01%	0.002%
23	5.040	1226	1244	1284	rBV2	704732	1748342	100.00%	13.940%
24	5.339	1328	1337	1356	rBV6	4421	13425	0.77%	0.107%
25	5.497	1384	1386	1391	rVB3	595	422	0.02%	0.003%
26	5.535	1391	1398	1399	rBV	289	299	0.02%	0.002%
27	5.613	1409	1422	1455	rBV	424899	890522	50.94%	7.100%
28	5.902	1502	1512	1530	rBV2	29577	63800	3.65%	0.509%
29	6.066	1549	1563	1605	rVB	363828	780840	44.66%	6.226%
30	6.211	1605	1608	1610	rBV2	806	588	0.03%	0.005%
31	6.262	1622	1624	1629	rVB3	422	281	0.02%	0.002%
32	6.307	1633	1638	1646	rVB2	315	358	0.02%	0.003%
33	6.548	1709	1713	1717	rBV2	290	294	0.02%	0.002%
34	6.642	1733	1742	1745	rBV6	2055	2824	0.16%	0.023%
35	6.777	1781	1784	1788	rVB4	368	276	0.02%	0.002%
36	6.896	1816	1821	1825	rBV	200	238	0.01%	0.002%

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 Title : VOC Analysis

37	6.986	1836	1849	1888	rBV	188092	383236	21.92%	3.056%
38	7.314	1938	1951	1970	rBV	800638	1441459	82.45%	11.493%
39	7.622	2036	2047	2077	rBV2	111792	247877	14.18%	1.976%
40	7.802	2100	2103	2106	rBV3	354	259	0.01%	0.002%
41	7.899	2129	2133	2137	rVB2	317	224	0.01%	0.002%
42	7.928	2137	2142	2146	rBV	272	315	0.02%	0.003%
43	7.995	2160	2163	2168	rVV2	275	275	0.02%	0.002%
44	8.124	2184	2203	2239	rBV	196297	703726	40.25%	5.611%
45	8.410	2289	2292	2295	rBV3	357	272	0.02%	0.002%
46	8.629	2356	2360	2363	rBV3	434	364	0.02%	0.003%
47	8.776	2401	2406	2412	rBV2	248	301	0.02%	0.002%
48	8.854	2417	2430	2455	rBV	579474	1126798	64.45%	8.984%
49	9.024	2478	2483	2485	rBV2	302	307	0.02%	0.002%
50	9.075	2493	2499	2501	rVB2	339	290	0.02%	0.002%
51	9.140	2515	2519	2520	rBV2	380	289	0.02%	0.002%
52	9.149	2520	2522	2526	rVV2	368	312	0.02%	0.002%
53	9.272	2556	2560	2566	rBV2	225	259	0.01%	0.002%
54	9.539	2634	2643	2648	rBV2	333	608	0.03%	0.005%
55	9.786	2714	2720	2722	rBV	345	345	0.02%	0.003%
56	9.841	2733	2737	2739	rBV	284	223	0.01%	0.002%
57	9.976	2772	2779	2782	rBV2	295	358	0.02%	0.003%
58	10.127	2816	2826	2836	rVV3	5270	8199	0.47%	0.065%
59	10.223	2842	2856	2875	rBV	427871	747095	42.73%	5.957%
60	10.384	2903	2906	2913	rVB3	758	681	0.04%	0.005%
61	10.458	2925	2929	2933	rBV2	257	294	0.02%	0.002%
62	10.577	2958	2966	2981	rVB5	4024	7426	0.42%	0.059%
63	10.661	2986	2992	2997	rVB2	797	716	0.04%	0.006%
64	10.709	3003	3007	3010	rBV	335	285	0.02%	0.002%
65	10.780	3024	3029	3034	rBV3	512	593	0.03%	0.005%
66	10.831	3041	3045	3053	rVB4	688	827	0.05%	0.007%
67	10.870	3053	3057	3059	rBV2	328	233	0.01%	0.002%
68	10.915	3062	3071	3082	rVB4	4126	6812	0.39%	0.054%
69	11.034	3101	3108	3116	rVB2	1003	1289	0.07%	0.010%
70	11.146	3133	3143	3150	rVB5	2801	4100	0.23%	0.033%
71	11.249	3164	3175	3193	rBV	704463	1097134	62.75%	8.748%
72	11.387	3214	3218	3224	rVB4	1718	1774	0.10%	0.014%
73	11.423	3225	3229	3239	rVB4	4082	5697	0.33%	0.045%
74	11.458	3239	3240	3246	rVB3	424	287	0.02%	0.002%
75	11.487	3246	3249	3254	rVB3	292	254	0.01%	0.002%
76	11.625	3279	3292	3313	rBV	785462	1224216	70.02%	9.761%

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 Title : VOC Analysis

77	11.783	3336	3341	3348	rVB5	1279	1774	0.10%	0.014%
78	11.831	3351	3356	3358	rBV3	703	568	0.03%	0.005%
79	12.014	3408	3413	3417	rBV2	354	434	0.02%	0.003%
80	12.053	3422	3425	3429	rVB3	322	234	0.01%	0.002%
81	12.082	3431	3434	3437	rBV2	653	515	0.03%	0.004%
82	12.249	3483	3486	3495	rVB2	514	570	0.03%	0.005%
83	12.288	3495	3498	3503	rVB	277	246	0.01%	0.002%
84	12.706	3624	3628	3635	rBV2	279	323	0.02%	0.003%
85	12.818	3659	3663	3666	rBV	243	228	0.01%	0.002%
86	13.525	3875	3883	3888	rBV4	488	714	0.04%	0.006%
87	13.767	3952	3958	3961	rBV3	319	319	0.02%	0.003%
88	13.847	3980	3983	3989	rVB3	362	331	0.02%	0.003%
89	13.982	4021	4025	4031	rBV3	274	251	0.01%	0.002%
90	14.072	4049	4053	4061	rVV3	349	471	0.03%	0.004%
91	14.275	4113	4116	4120	rVV2	384	274	0.02%	0.002%
92	14.304	4121	4125	4129	rVV2	410	398	0.02%	0.003%
93	14.361	4141	4143	4149	rVB2	287	246	0.01%	0.002%
94	14.403	4152	4156	4158	rBV3	354	297	0.02%	0.002%
95	14.509	4185	4189	4193	rBV3	264	324	0.02%	0.003%
96	14.783	4272	4274	4277	rBV2	437	255	0.01%	0.002%
97	14.802	4277	4280	4284	rVB2	308	218	0.01%	0.002%
98	15.667	4546	4549	4550	rBV	418	253	0.01%	0.002%
99	15.805	4590	4592	4596	rVB2	503	253	0.01%	0.002%
100	16.011	4650	4656	4659	rBV4	639	756	0.04%	0.006%

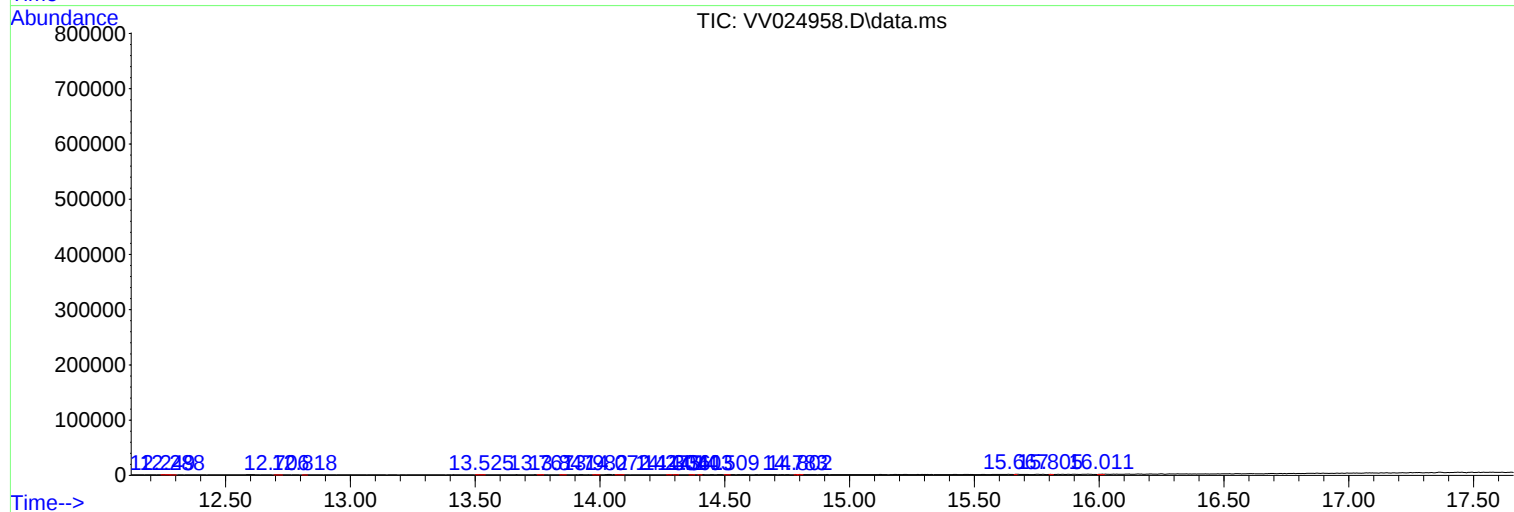
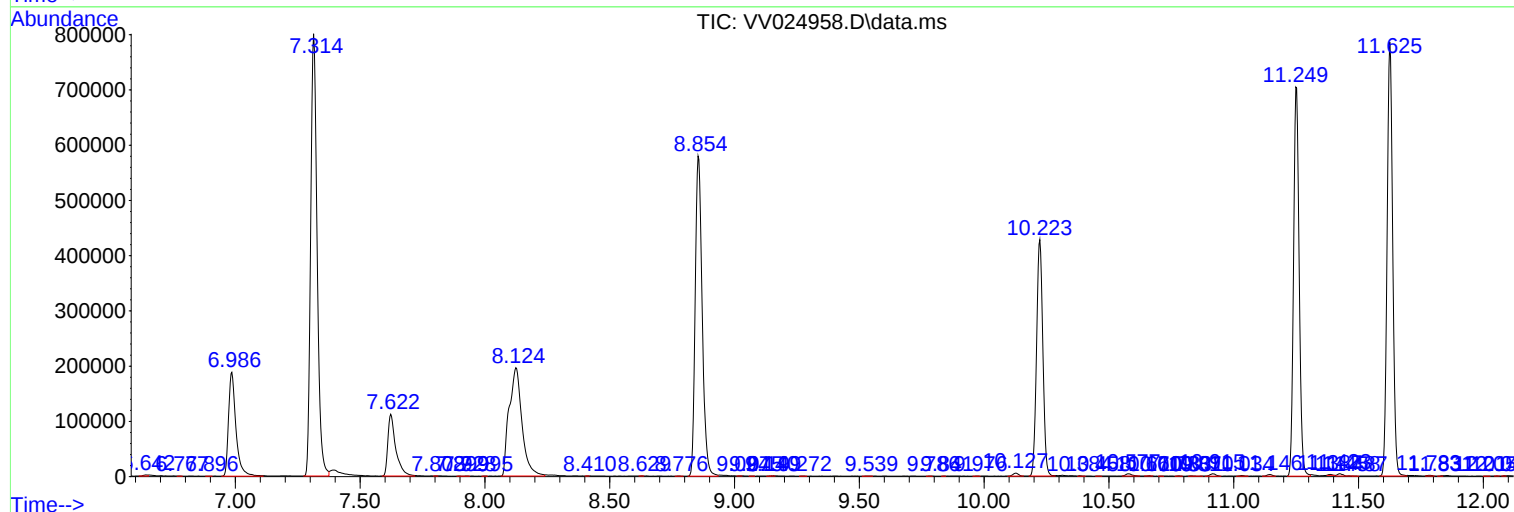
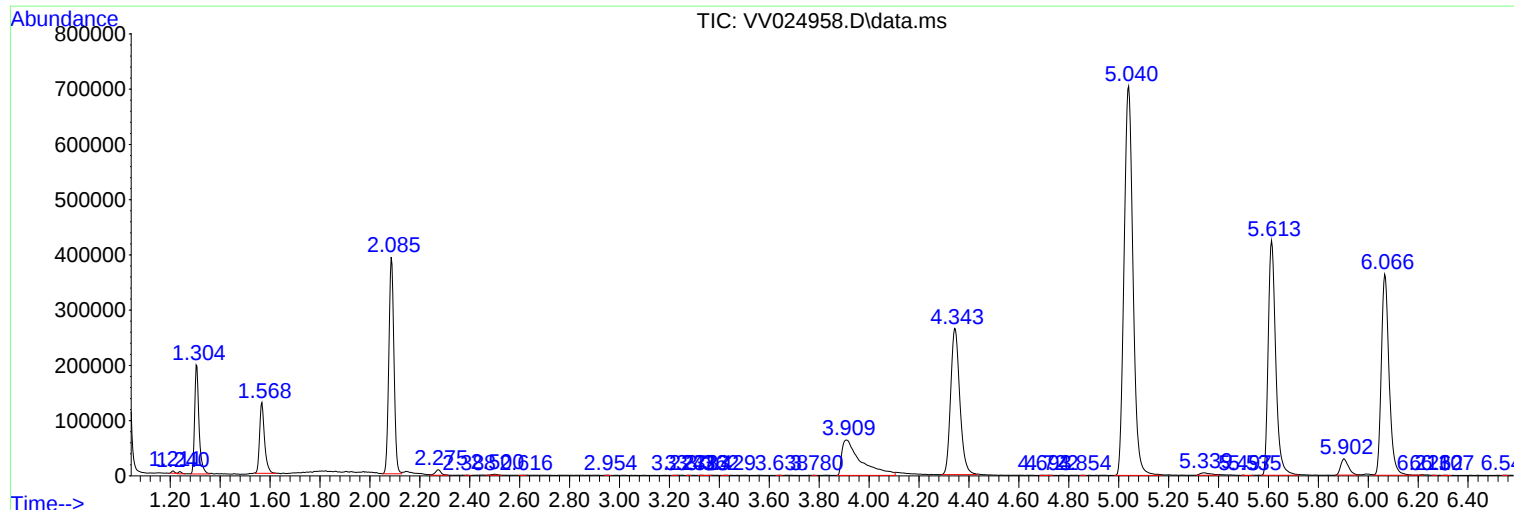
Sum of corrected areas: 12542027

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Instrument :
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ClientSampleId :
DBSD2ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM022822WMA.M
Quant Title : VOC Analysis

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



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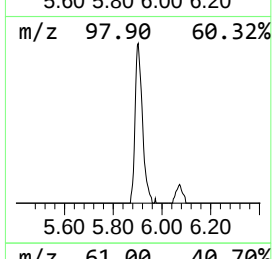
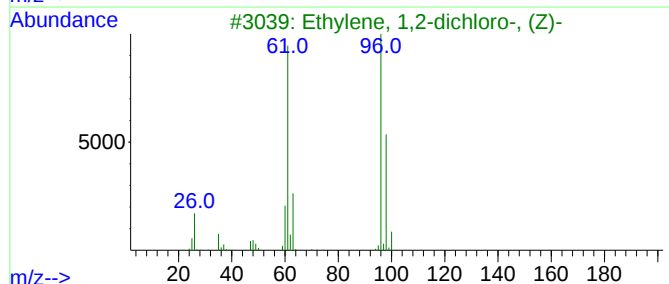
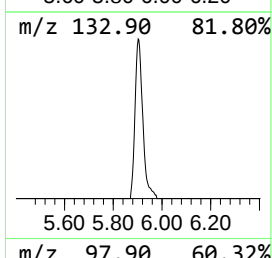
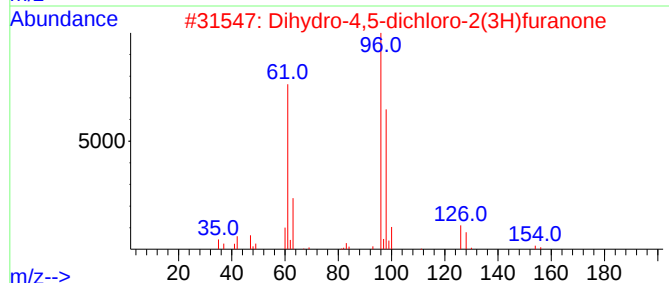
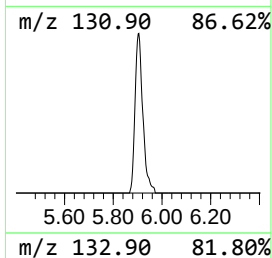
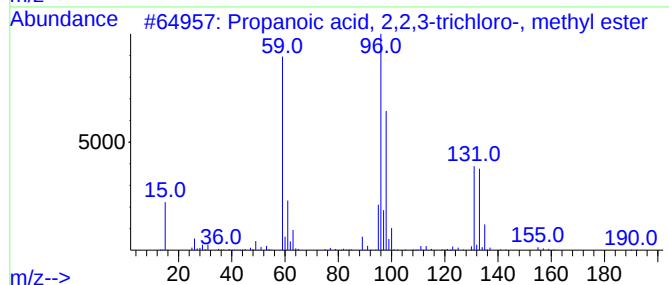
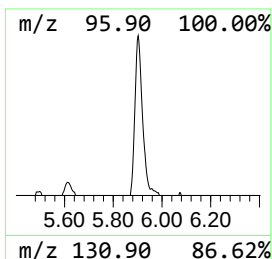
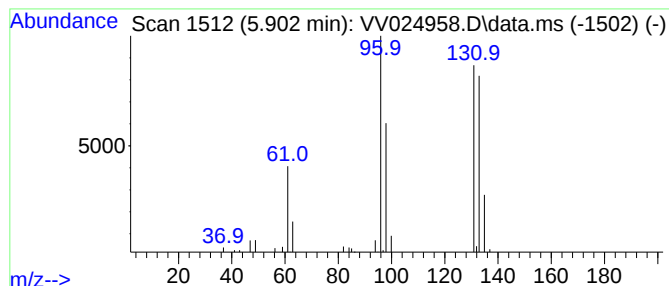
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Peak Number 1 Propanoic acid, 2,2,3-trich... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.58 ug/L	63800	1,4-Difluorobenzene	5.613

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2			Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	35
3			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	25
4			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	25
5			2-Chloro-5-methylthiazole	133	C4H4ClNS	033342-65-3	22



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.902	3.6	ug/L	63800	1	5.613	890522	50.0