

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU102023\
 Data File : VU055829.D
 Acq On : 20 Oct 2023 13:50
 Operator : MD/SY
 Sample : 04922-04ME
 Misc : 4.33g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EOAR2ME

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_U\Method\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.483	55	60	66	rVB4	5357	5578	0.26%	0.033%
2	1.596	86	95	116	rVB	181845	279747	12.98%	1.672%
3	1.821	136	165	167	rBV	32540	115447	5.36%	0.690%
4	1.878	178	183	199	rVB	65624	95073	4.41%	0.568%
5	2.544	377	390	407	rBV	421751	689864	32.00%	4.122%
6	2.631	411	417	430	rVB2	4443	8704	0.40%	0.052%
7	2.727	445	447	453	rVB4	691	441	0.02%	0.003%
8	2.753	453	455	458	rBV4	780	434	0.02%	0.003%
9	2.833	475	480	483	rBV2	427	435	0.02%	0.003%
10	2.920	503	507	509	rBV4	763	468	0.02%	0.003%
11	3.033	527	542	560	rBV8	11911	32372	1.50%	0.193%
12	3.174	572	586	603	rVB2	5788	14429	0.67%	0.086%
13	3.258	609	612	614	rBV3	487	329	0.02%	0.002%
14	3.303	624	626	629	rBV	550	416	0.02%	0.002%
15	3.335	629	636	637	rBV2	2410	2212	0.10%	0.013%
16	3.444	666	670	673	rVB	715	573	0.03%	0.003%
17	3.499	683	687	690	rVB2	535	377	0.02%	0.002%
18	3.550	697	703	707	rBV3	746	845	0.04%	0.005%
19	3.676	732	742	744	rBV5	3720	4693	0.22%	0.028%
20	3.959	828	830	834	rVB4	619	415	0.02%	0.002%
21	3.981	834	837	840	rBV	740	660	0.03%	0.004%
22	4.075	862	866	867	rBV	625	431	0.02%	0.003%
23	4.402	961	968	970	rBV3	583	607	0.03%	0.004%
24	4.521	989	1005	1012	rVB6	2255	4995	0.23%	0.030%
25	4.624	1025	1037	1079	rBV	130311	459054	21.29%	2.743%
26	5.055	1154	1171	1200	rBV	367792	861253	39.95%	5.146%
27	5.200	1213	1216	1221	rVB5	975	760	0.04%	0.005%
28	5.309	1242	1250	1252	rBV5	1141	1124	0.05%	0.007%
29	5.444	1283	1292	1293	rBV4	2221	2518	0.12%	0.015%
30	5.557	1322	1327	1328	rBV2	450	345	0.02%	0.002%
31	5.579	1328	1334	1346	rVB6	1781	2997	0.14%	0.018%
32	5.714	1355	1376	1409	rBV2	809723	2155834	100.00%	12.882%
33	5.891	1423	1431	1446	rVB3	6566	14156	0.66%	0.085%
34	5.972	1446	1456	1466	rBV9	4120	8830	0.41%	0.053%
35	6.029	1472	1474	1477	rBV3	568	451	0.02%	0.003%
36	6.116	1496	1501	1502	rBV3	860	664	0.03%	0.004%

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 Title : VOC Analysis

37	6.126	1502	1504	1510	rVB5	864	1021	0.05%	0.006%
38	6.171	1515	1518	1521	rBV2	559	366	0.02%	0.002%
39	6.242	1525	1540	1575	rBV	645135	1319478	61.20%	7.885%
40	6.399	1586	1589	1591	rBV2	799	411	0.02%	0.002%
41	6.444	1600	1603	1607	rBV3	473	425	0.02%	0.003%
42	6.531	1613	1630	1643	rBV10	24799	61446	2.85%	0.367%
43	6.599	1643	1651	1662	rVV6	5505	12727	0.59%	0.076%
44	6.685	1663	1678	1708	rVV	465881	968427	44.92%	5.787%
45	6.859	1729	1732	1737	rVB4	1517	1112	0.05%	0.007%
46	6.920	1748	1751	1756	rVB3	736	572	0.03%	0.003%
47	6.946	1756	1759	1763	rVB3	449	391	0.02%	0.002%
48	6.991	1763	1773	1777	rBV4	728	1111	0.05%	0.007%
49	7.049	1786	1791	1792	rBV	614	479	0.02%	0.003%
50	7.190	1823	1835	1839	rBV3	7492	12349	0.57%	0.074%
51	7.341	1875	1882	1883	rBV6	1144	1075	0.05%	0.006%
52	7.418	1903	1906	1907	rBV2	689	358	0.02%	0.002%
53	7.492	1925	1929	1931	rBV3	987	782	0.04%	0.005%
54	7.563	1937	1951	1972	rBV	233085	465557	21.60%	2.782%
55	7.698	1986	1993	1995	rBV5	2982	3464	0.16%	0.021%
56	7.788	2018	2021	2025	rBV3	516	424	0.02%	0.003%
57	7.836	2025	2036	2040	rBV7	1882	3166	0.15%	0.019%
58	7.894	2041	2054	2076	rBV	937221	1710191	79.33%	10.219%
59	8.087	2112	2114	2120	rVB3	1047	644	0.03%	0.004%
60	8.129	2120	2127	2131	rBV5	1268	1263	0.06%	0.008%
61	8.177	2131	2142	2172	rVV	152002	322752	14.97%	1.929%
62	8.344	2189	2194	2196	rBV4	1107	1115	0.05%	0.007%
63	8.370	2199	2202	2205	rVB3	1261	832	0.04%	0.005%
64	8.454	2225	2228	2230	rBV3	475	347	0.02%	0.002%
65	8.470	2230	2233	2234	rBV3	1015	633	0.03%	0.004%
66	8.550	2248	2258	2270	rVB4	30073	54702	2.54%	0.327%
67	8.650	2274	2289	2321	rBV3	371090	929628	43.12%	5.555%
68	8.920	2364	2373	2374	rBV6	2395	2913	0.14%	0.017%
69	9.010	2399	2401	2405	rVB3	719	384	0.02%	0.002%
70	9.049	2411	2413	2416	rBV3	825	461	0.02%	0.003%
71	9.116	2431	2434	2437	rBV3	1097	803	0.04%	0.005%
72	9.152	2442	2445	2446	rBV3	1967	1264	0.06%	0.008%
73	9.213	2456	2464	2472	rVB9	2908	5603	0.26%	0.033%
74	9.280	2483	2485	2489	rVB2	589	358	0.02%	0.002%
75	9.328	2494	2500	2502	rBV4	2686	2669	0.12%	0.016%
76	9.418	2512	2528	2549	rBV	859560	1662160	77.10%	9.932%

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 Title : VOC Analysis

77	9.560	2563	2572	2573	rBV5	3153	3137	0.15%	0.019%
78	9.637	2594	2596	2599	rVB4	899	437	0.02%	0.003%
79	9.656	2599	2602	2603	rBV2	1205	629	0.03%	0.004%
80	9.833	2652	2657	2663	rBV4	615	767	0.04%	0.005%
81	9.875	2668	2670	2674	rVB3	592	405	0.02%	0.002%
82	9.946	2687	2692	2693	rBV2	633	488	0.02%	0.003%
83	9.978	2699	2702	2706	rBB4	949	583	0.03%	0.003%
84	10.023	2706	2716	2722	rBV9	4973	8747	0.41%	0.052%
85	10.113	2736	2744	2754	rBV9	4427	8128	0.38%	0.049%
86	10.174	2761	2763	2768	rVB2	1509	911	0.04%	0.005%
87	10.251	2768	2787	2791	rBV6	6700	13215	0.61%	0.079%
88	10.460	2848	2852	2858	rBV4	2333	2376	0.11%	0.014%
89	10.550	2869	2880	2890	rBV9	4456	9028	0.42%	0.054%
90	10.759	2931	2945	2973	rBV	708173	1184101	54.93%	7.076%
91	11.007	3017	3022	3027	rBV8	3122	4379	0.20%	0.026%
92	11.058	3035	3038	3044	rBV5	4662	4946	0.23%	0.030%
93	11.113	3049	3055	3073	rVB5	20303	37500	1.74%	0.224%
94	11.238	3090	3094	3096	rBV5	1902	1383	0.06%	0.008%
95	11.306	3109	3115	3128	rVB5	8373	16216	0.75%	0.097%
96	11.415	3142	3149	3156	rBV4	15371	21405	0.99%	0.128%
97	11.573	3189	3198	3202	rBV7	5432	8552	0.40%	0.051%
98	11.814	3261	3273	3287	rBV	956922	1545154	71.67%	9.233%
99	12.193	3379	3391	3407	rBV	898651	1488355	69.04%	8.894%
100	12.325	3426	3432	3442	rVB4	37064	52691	2.44%	0.315%

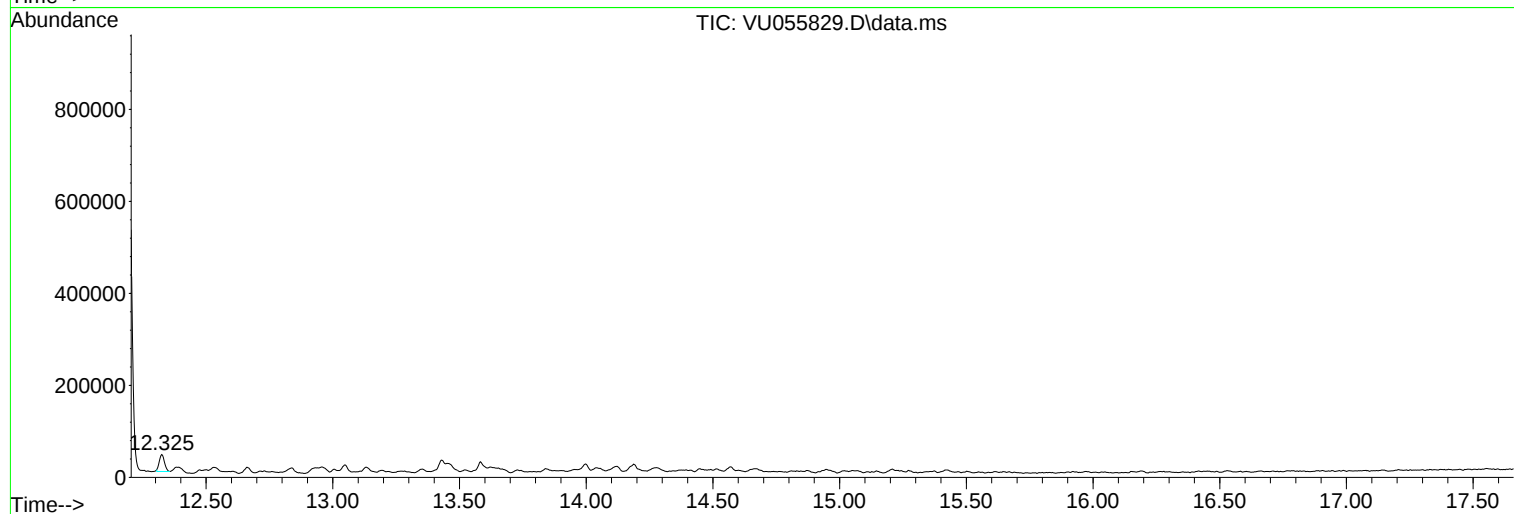
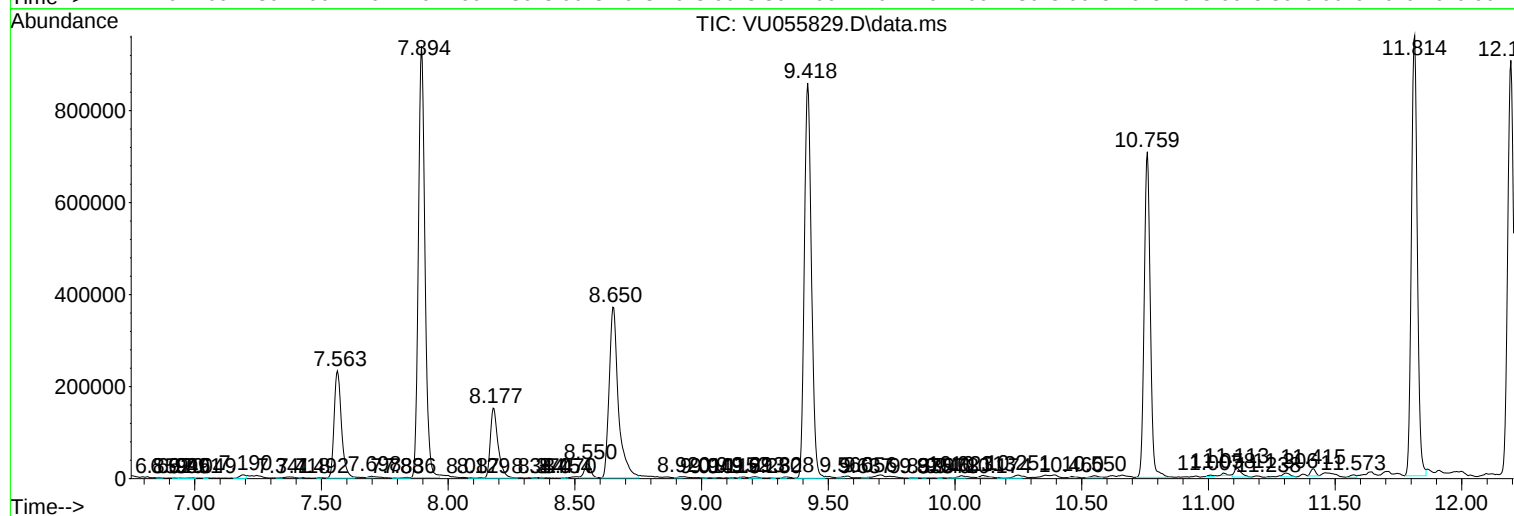
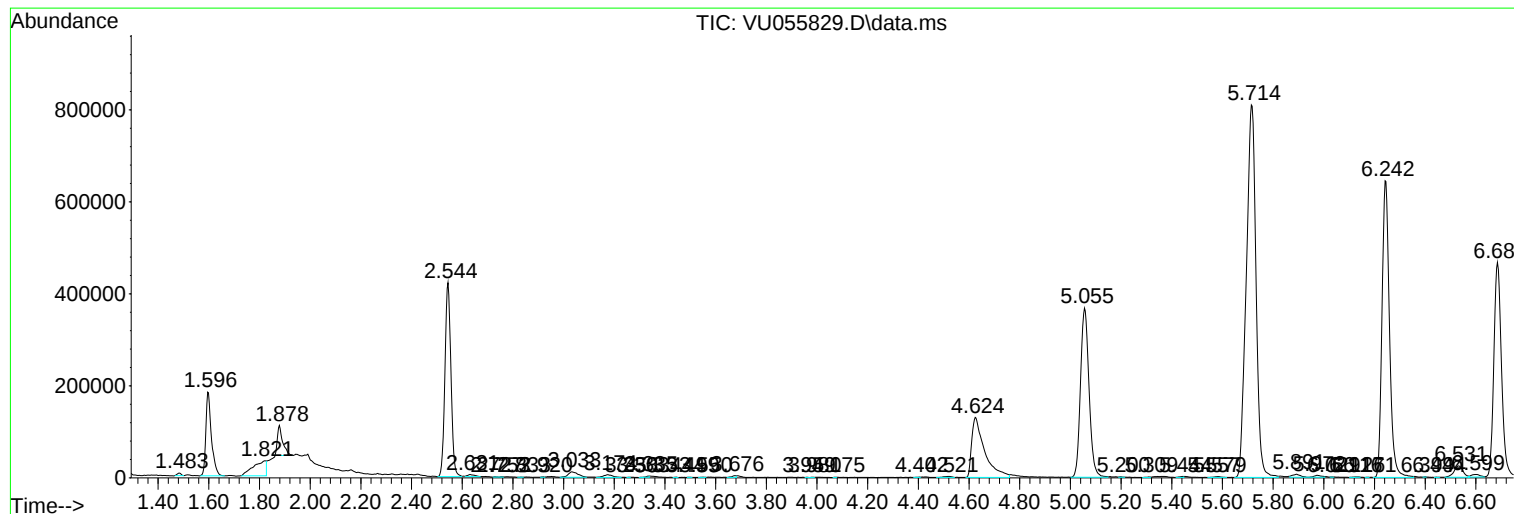
Sum of corrected areas: 16734927

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Instrument :
MSVOA_U
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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



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Instrument :
MSVOA_U
ClientSampleId :
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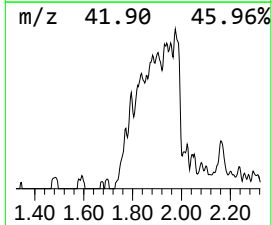
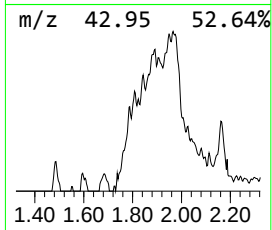
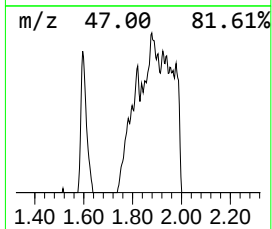
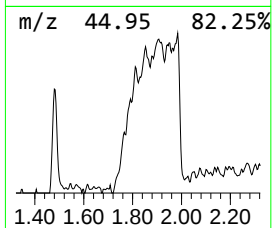
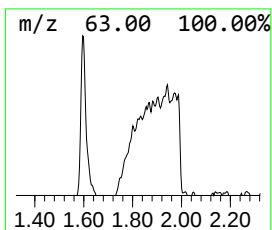
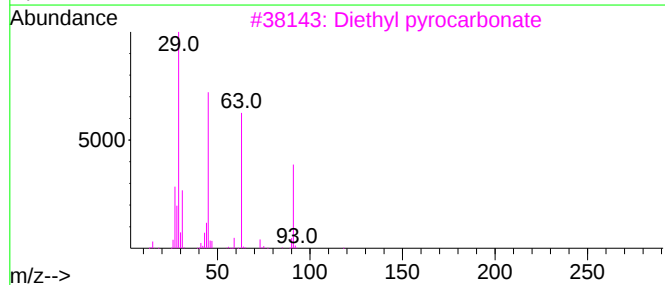
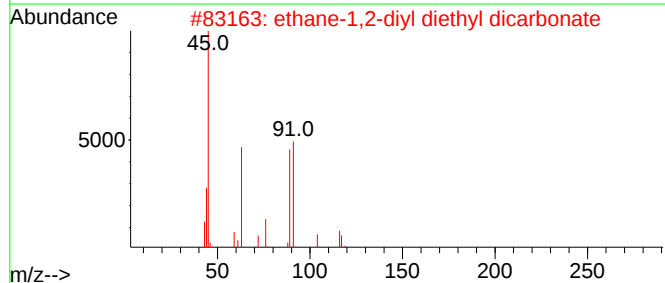
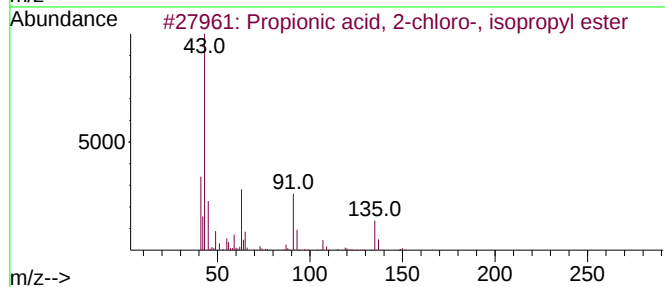
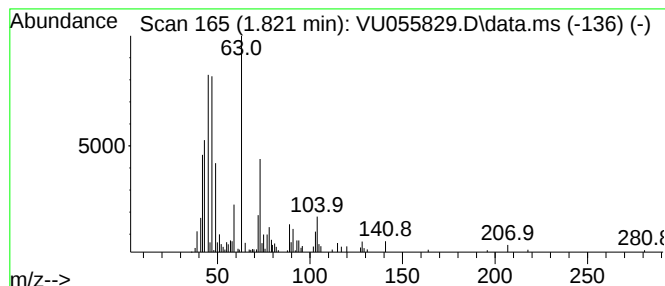
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.821	4.37 ug/L	115447	1,4-Difluorobenzene	6.245

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propionic acid, 2-chloro-, isopr...	150	C6H11ClO2	040058-87-5	36
2			ethane-1,2-diyl diethyl dicarbonate	206	C8H14O6	1000456-16-7	32
3			Diethyl pyrocarbonate	162	C6H10O5	001609-47-8	25
4			Bis(2-(2-chloroethoxy)ethyl) ether	230	C8H16Cl2O3	000638-56-2	25
5			Methyl 2,2,4-trichloro-3-oxopent...	232	C6H7Cl3O3	1000112-41-1	23



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.821	4.4	ug/L	115447	1	6.245	1319480	50.0