

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
 Data File : VU055731.D
 Acq On : 10 Oct 2023 19:13
 Operator : MD/SY
 Sample : 04707-09ME
 Misc : 6.76g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EY1A8ME

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: VU055731.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.480	55	59	66	rVB3	4967	5063	0.05%	0.018%
2	1.596	86	95	120	rBV	167995	341190	3.49%	1.210%
3	1.817	133	164	165	rBV9	47508	178600	1.83%	0.634%
4	2.531	375	386	403	rVB	486512	799989	8.19%	2.838%
5	2.756	450	456	458	rBV6	1180	1343	0.01%	0.005%
6	2.798	466	469	471	rBV4	577	388	0.00%	0.001%
7	3.030	531	541	556	rBV3	9565	20292	0.21%	0.072%
8	3.171	570	585	603	rBV	30442	74540	0.76%	0.264%
9	3.332	633	635	641	rVB5	964	670	0.01%	0.002%
10	3.637	727	730	733	rBV2	521	390	0.00%	0.001%
11	3.669	733	740	741	rBV4	1664	1534	0.02%	0.005%
12	3.924	815	819	823	rBV2	443	467	0.00%	0.002%
13	3.988	836	839	841	rBV2	623	443	0.00%	0.002%
14	4.432	974	977	983	rVB2	501	541	0.01%	0.002%
15	4.631	1025	1039	1090	rBV	160280	647733	6.63%	2.298%
16	5.055	1154	1171	1200	rBV	407194	1003438	10.27%	3.560%
17	5.303	1245	1248	1249	rBV	1030	571	0.01%	0.002%
18	5.370	1267	1269	1274	rVB2	746	420	0.00%	0.001%
19	5.512	1295	1313	1333	rBV	164804	372553	3.81%	1.322%
20	5.602	1338	1341	1344	rVB2	1033	731	0.01%	0.003%
21	5.624	1344	1348	1350	rBV3	635	493	0.01%	0.002%
22	5.711	1354	1375	1408	rBV2	937603	2465611	25.24%	8.748%
23	5.981	1449	1459	1463	rBV6	3067	5717	0.06%	0.020%
24	6.139	1504	1508	1512	rBV	503	343	0.00%	0.001%
25	6.161	1513	1515	1520	rVB2	382	350	0.00%	0.001%
26	6.242	1526	1540	1565	rBV	510038	1089921	11.16%	3.867%
27	6.531	1617	1630	1643	rBV10	19741	44448	0.46%	0.158%
28	6.599	1643	1651	1663	rVV5	4731	9889	0.10%	0.035%
29	6.685	1663	1678	1701	rVV	520102	1106790	11.33%	3.927%
30	6.862	1730	1733	1738	rVB3	712	609	0.01%	0.002%
31	6.920	1748	1751	1755	rBV3	357	346	0.00%	0.001%
32	7.013	1771	1780	1783	rBV2	421	518	0.01%	0.002%
33	7.042	1786	1789	1794	rBV2	463	406	0.00%	0.001%
34	7.084	1797	1802	1805	rBV3	752	617	0.01%	0.002%
35	7.100	1805	1807	1815	rVB2	346	360	0.00%	0.001%
36	7.193	1827	1836	1838	rBV6	2903	3806	0.04%	0.014%

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

37	7.460	1915	1919	1922	rBV2	516	457	0.00%	0.002%
38	7.492	1927	1929	1938	rBV6	765	1104	0.01%	0.004%
39	7.563	1938	1951	1979	rBV	269594	561322	5.75%	1.991%
40	7.660	1979	1981	1987	rVB4	825	684	0.01%	0.002%
41	7.695	1987	1992	1993	rBV3	1544	1133	0.01%	0.004%
42	7.782	2013	2019	2022	rBV4	1319	1543	0.02%	0.005%
43	7.894	2039	2054	2082	rBV	1034038	1988871	20.36%	7.056%
44	8.181	2130	2143	2168	rBV2	166371	384673	3.94%	1.365%
45	8.306	2180	2182	2186	rVB3	538	352	0.00%	0.001%
46	8.345	2191	2194	2198	rVV4	1294	1142	0.01%	0.004%
47	8.550	2242	2258	2276	rBV	5575189	9767309	100.00%	34.653%
48	8.660	2276	2292	2322	rVB2	590168	1519722	15.56%	5.392%
49	8.878	2358	2360	2365	rVB3	1053	785	0.01%	0.003%
50	8.904	2365	2368	2371	rBV3	803	569	0.01%	0.002%
51	8.923	2371	2374	2378	rBV4	784	534	0.01%	0.002%
52	9.055	2412	2415	2421	rVB2	692	554	0.01%	0.002%
53	9.107	2429	2431	2440	rVB5	867	1004	0.01%	0.004%
54	9.213	2459	2464	2469	rVB4	856	791	0.01%	0.003%
55	9.293	2483	2489	2494	rBV4	873	803	0.01%	0.003%
56	9.322	2494	2498	2501	rBV2	563	597	0.01%	0.002%
57	9.418	2513	2528	2553	rBV	653291	1414103	14.48%	5.017%
58	9.550	2565	2569	2570	rBV4	762	470	0.00%	0.002%
59	9.666	2601	2605	2607	rBV2	680	434	0.00%	0.002%
60	9.695	2610	2614	2615	rBV2	591	455	0.00%	0.002%
61	9.730	2622	2625	2629	rVB3	649	428	0.00%	0.002%
62	9.820	2648	2653	2657	rBV	604	550	0.01%	0.002%
63	9.885	2669	2673	2676	rVB2	585	435	0.00%	0.002%
64	9.943	2687	2691	2695	rBV2	544	468	0.00%	0.002%
65	9.991	2702	2706	2709	rBV3	477	355	0.00%	0.001%
66	10.029	2714	2718	2723	rVB3	647	684	0.01%	0.002%
67	10.065	2723	2729	2731	rBV2	702	597	0.01%	0.002%
68	10.103	2737	2741	2742	rBV2	666	409	0.00%	0.001%
69	10.197	2765	2770	2776	rBV2	523	543	0.01%	0.002%
70	10.762	2932	2946	2963	rBV	846679	1405394	14.39%	4.986%
71	10.872	2978	2980	2983	rVB	670	350	0.00%	0.001%
72	10.894	2983	2987	2991	rVB4	644	604	0.01%	0.002%
73	11.058	3036	3038	3042	rVB2	593	383	0.00%	0.001%
74	11.258	3098	3100	3107	rVB4	397	384	0.00%	0.001%
75	11.312	3111	3117	3124	rVB5	1033	1326	0.01%	0.005%
76	11.348	3124	3128	3130	rBV	737	543	0.01%	0.002%

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 Title : VOC Analysis

77	11.418	3143	3150	3153	rBV3	963	1175	0.01%	0.004%
78	11.470	3163	3166	3169	rBV	659	537	0.01%	0.002%
79	11.698	3234	3237	3243	rBV3	516	479	0.00%	0.002%
80	11.750	3249	3253	3258	rBV4	619	547	0.01%	0.002%
81	11.814	3261	3273	3302	rBV	775100	1262346	12.92%	4.479%
82	12.039	3339	3343	3350	rBV6	847	908	0.01%	0.003%
83	12.193	3378	3391	3416	rBV	1017313	1665541	17.05%	5.909%
84	12.338	3434	3436	3440	rVB2	720	428	0.00%	0.002%
85	12.502	3483	3487	3491	rBV2	452	366	0.00%	0.001%
86	12.695	3545	3547	3552	rVB	402	340	0.00%	0.001%
87	12.721	3552	3555	3558	rBV3	616	444	0.00%	0.002%
88	13.077	3662	3666	3670	rBV2	912	849	0.01%	0.003%
89	13.245	3712	3718	3724	rVB3	977	1277	0.01%	0.005%
90	13.283	3724	3730	3734	rBV3	651	737	0.01%	0.003%
91	13.335	3741	3746	3747	rBV2	596	443	0.00%	0.002%
92	13.422	3769	3773	3776	rBV3	687	548	0.01%	0.002%
93	13.441	3776	3779	3783	rBV	584	525	0.01%	0.002%
94	13.489	3787	3794	3798	rVB3	959	1142	0.01%	0.004%
95	13.512	3798	3801	3802	rBV2	658	343	0.00%	0.001%
96	13.650	3839	3844	3847	rBV3	754	924	0.01%	0.003%
97	13.749	3872	3875	3878	rBV	517	339	0.00%	0.001%
98	13.775	3880	3883	3885	rBV2	778	558	0.01%	0.002%
99	13.952	3933	3938	3941	rBV4	659	760	0.01%	0.003%
100	14.727	4177	4179	4182	rVB3	1227	555	0.01%	0.002%

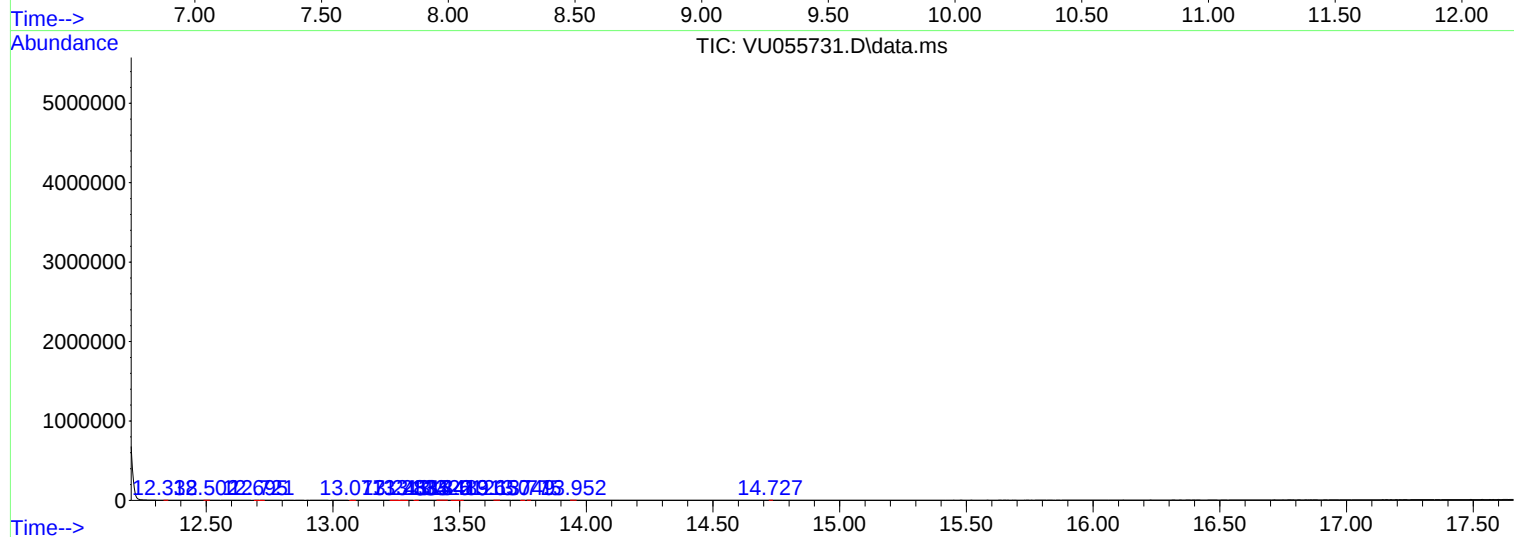
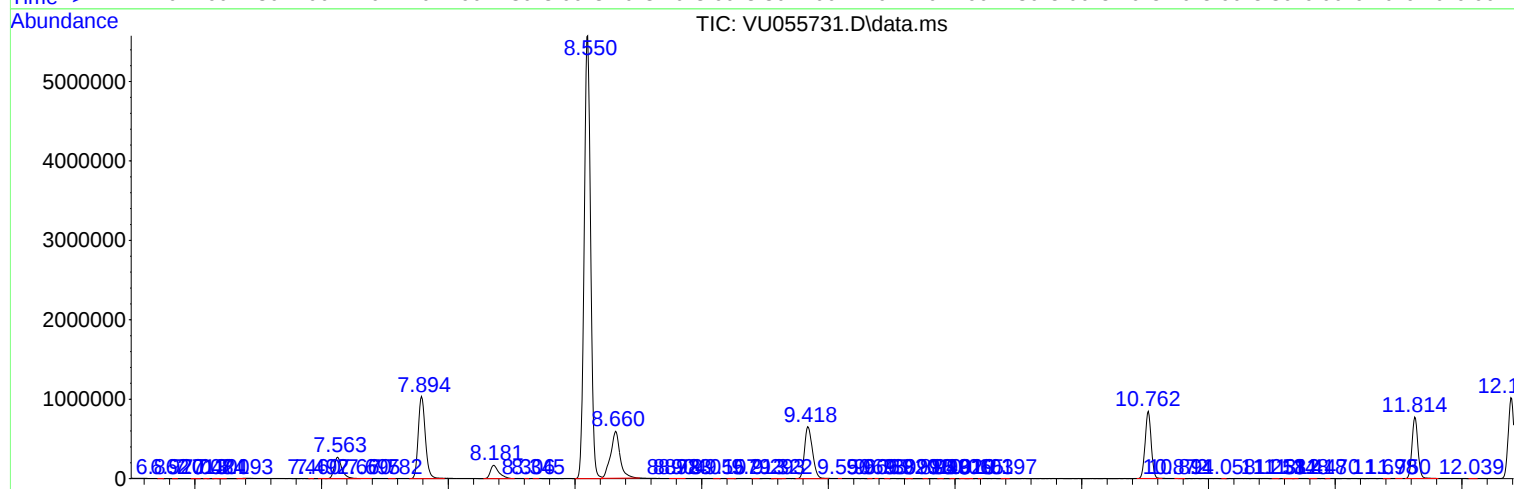
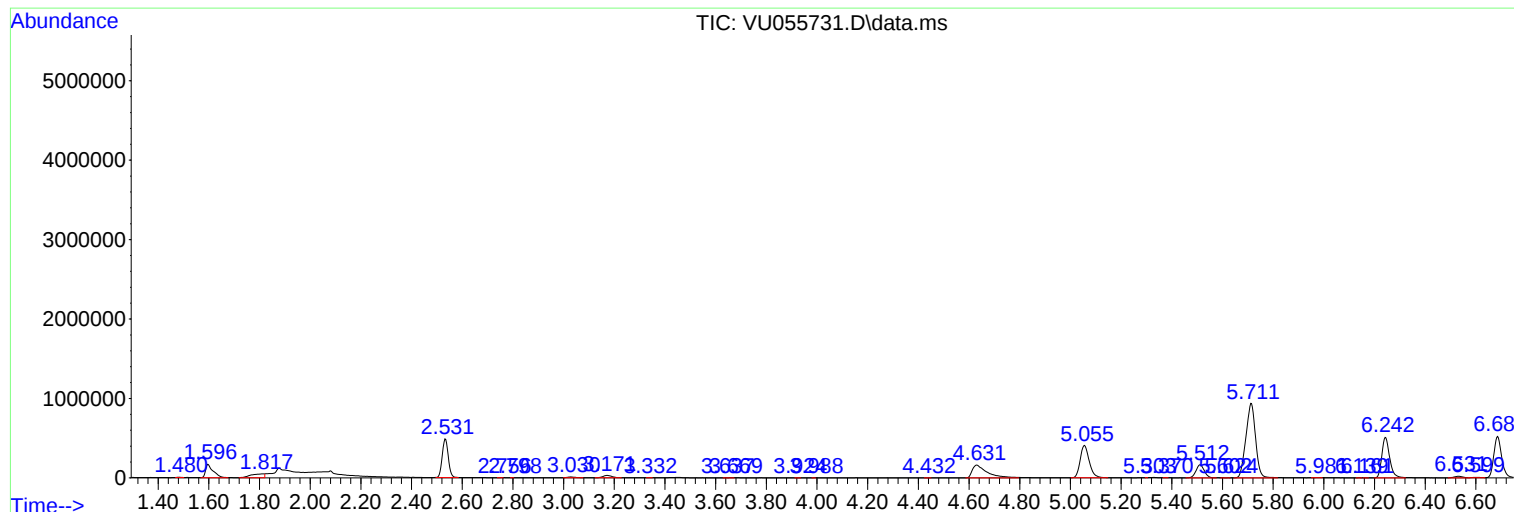
Sum of corrected areas: 28186095

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Instrument :
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ClientSampleId :
EY1A8ME

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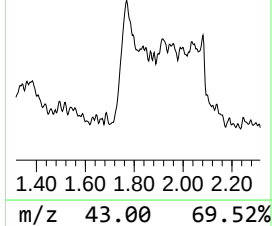
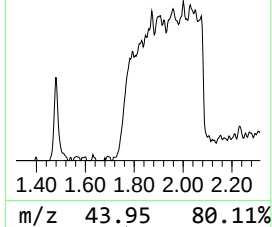
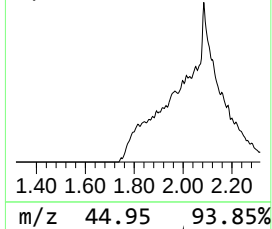
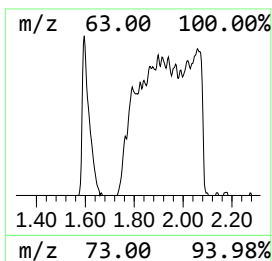
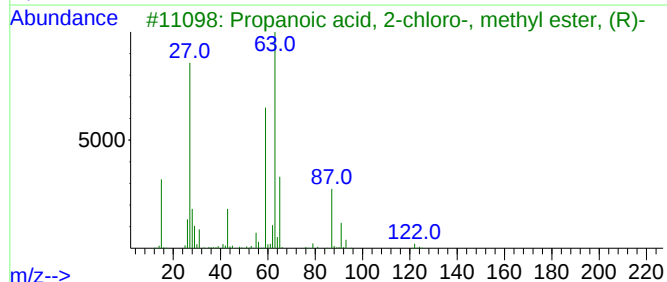
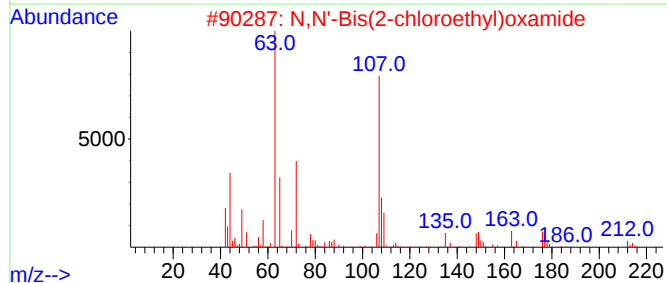
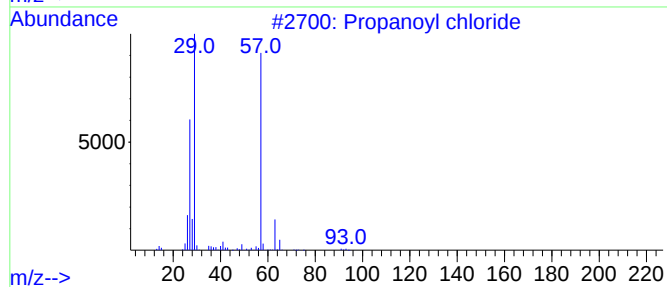
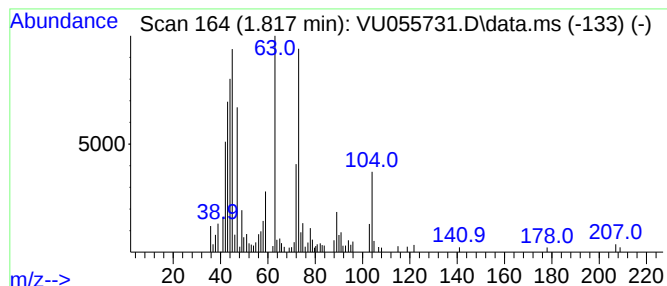
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM101023WMA.M
Quant Title : VOC Analysis

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.
1.817	8.19 ug/L	178600	1,4-Difluorobenzene	6.242

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoyl chloride	92	C3H5ClO	000079-03-8	37
2			N,N'-Bis(2-chloroethyl)oxamide	212	C6H10Cl2N2O2	016813-43-7	28
3			Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	077287-29-7	12
4			Propanoic acid, 2-chloro-, methy...	122	C4H7ClO2	073246-45-4	12
5			Silane, diethylmethyl-	102	C5H14Si	000760-32-7	10



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.817	8.2	ug/L	178600	1	6.242	1089920	50.0