

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011121\
 Data File : VV019969.D
 Acq On : 11 Jan 2021 16:18
 Operator : SY/MD
 Sample : M1064-01 2X
 Misc : 5.0mL/MSVOA_V/WATER
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 BG4X2

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\SOMVLM011121WMA.M

Title : VOC Analysis

Signal : TIC: VV019969.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.110	3	6	14	rVB	68374	55236	1.98%	0.295%
2	1.309	60	68	80	rVB	296318	308491	11.06%	1.646%
3	1.570	142	149	158	rBV	237537	255927	9.17%	1.366%
4	2.110	308	317	346	rVB	469022	724764	25.98%	3.868%
5	2.393	403	405	409	rBV3	972	511	0.02%	0.003%
6	2.701	495	501	504	rBV4	887	874	0.03%	0.005%
7	2.730	507	510	512	rBV	872	506	0.02%	0.003%
8	3.087	619	621	623	rBV3	668	395	0.01%	0.002%
9	3.270	675	678	680	rBV3	845	583	0.02%	0.003%
10	3.399	713	718	719	rBV3	489	371	0.01%	0.002%
11	3.447	729	733	736	rBV4	663	547	0.02%	0.003%
12	3.576	766	773	774	rBV3	746	597	0.02%	0.003%
13	3.598	777	780	781	rBV3	362	233	0.01%	0.001%
14	3.663	799	800	803	rVB	927	303	0.01%	0.002%
15	3.676	803	804	805	rBV	434	149	0.01%	0.001%
16	3.692	805	809	810	rVV2	485	314	0.01%	0.002%
17	3.785	836	838	841	rVB3	530	265	0.01%	0.001%
18	3.888	859	870	898	rBV	122042	377125	13.52%	2.012%
19	4.354	999	1015	1042	rBV	287054	708808	25.40%	3.782%
20	4.585	1084	1087	1092	rBV4	685	573	0.02%	0.003%
21	4.669	1110	1113	1115	rBV2	899	746	0.03%	0.004%
22	4.759	1136	1141	1144	rVB4	1166	833	0.03%	0.004%
23	4.775	1144	1146	1149	rVB2	844	321	0.01%	0.002%
24	4.811	1149	1157	1160	rBV7	726	975	0.03%	0.005%
25	4.823	1160	1161	1163	rBV2	885	243	0.01%	0.001%
26	4.840	1163	1166	1170	rBV3	527	471	0.02%	0.003%
27	4.875	1173	1177	1179	rBV4	741	580	0.02%	0.003%
28	4.978	1206	1209	1212	rVB4	800	503	0.02%	0.003%
29	5.052	1212	1232	1271	rBV2	672959	1783135	63.91%	9.515%
30	5.508	1372	1374	1378	rBV3	763	595	0.02%	0.003%
31	5.621	1397	1409	1437	rBV	510758	1025401	36.75%	5.472%
32	5.917	1487	1501	1532	rBV	1424413	2790235	100.00%	14.890%
33	6.074	1539	1550	1571	rVB	386289	778395	27.90%	4.154%
34	6.434	1659	1662	1667	rVB4	670	411	0.01%	0.002%
35	6.473	1672	1674	1676	rBV2	549	276	0.01%	0.001%
36	6.492	1678	1680	1684	rVB3	568	252	0.01%	0.001%

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 Title : VOC Analysis

37	6.511	1684	1686	1689	rBV3	652	474	0.02%	0.003%
38	6.553	1694	1699	1701	rBV3	544	464	0.02%	0.002%
39	6.592	1710	1711	1712	rBV	394	141	0.01%	0.001%
40	6.701	1743	1745	1747	rBV2	683	341	0.01%	0.002%
41	6.749	1758	1760	1765	rVB3	757	583	0.02%	0.003%
42	6.782	1768	1770	1774	rBV2	461	310	0.01%	0.002%
43	6.814	1778	1780	1783	rBV3	462	346	0.01%	0.002%
44	6.868	1795	1797	1798	rVB	482	156	0.01%	0.001%
45	6.888	1798	1803	1804	rBV2	748	339	0.01%	0.002%
46	6.926	1811	1815	1817	rVB3	480	326	0.01%	0.002%
47	6.936	1817	1818	1821	rVB	466	187	0.01%	0.001%
48	6.991	1823	1835	1865	rBV	222322	403220	14.45%	2.152%
49	7.248	1911	1915	1920	rBV3	1129	1098	0.04%	0.006%
50	7.322	1925	1938	1960	rBV	768788	1340585	48.05%	7.154%
51	7.627	2023	2033	2057	rBV	150340	266559	9.55%	1.422%
52	7.827	2094	2095	2099	rBV3	643	497	0.02%	0.003%
53	7.900	2116	2118	2120	rBV3	420	191	0.01%	0.001%
54	7.981	2129	2143	2162	rBV	1515436	2517908	90.24%	13.437%
55	8.093	2168	2178	2211	rBV2	393674	750102	26.88%	4.003%
56	8.476	2294	2297	2299	rBV2	480	310	0.01%	0.002%
57	8.717	2370	2372	2374	rVB2	543	173	0.01%	0.001%
58	8.769	2386	2388	2391	rBV3	686	414	0.01%	0.002%
59	8.859	2403	2416	2439	rBV	789505	1282289	45.96%	6.843%
60	9.142	2498	2504	2509	rBV4	1620	2032	0.07%	0.011%
61	9.325	2559	2561	2562	rBV	466	180	0.01%	0.001%
62	9.338	2562	2565	2568	rVB4	695	416	0.01%	0.002%
63	9.412	2585	2588	2591	rBV3	619	528	0.02%	0.003%
64	9.437	2594	2596	2598	rBV	523	374	0.01%	0.002%
65	9.486	2609	2611	2615	rVB2	584	356	0.01%	0.002%
66	9.502	2615	2616	2618	rBV	520	210	0.01%	0.001%
67	9.746	2690	2692	2694	rBV	474	290	0.01%	0.002%
68	9.778	2699	2702	2704	rBV2	722	481	0.02%	0.003%
69	10.113	2802	2806	2808	rBV2	490	443	0.02%	0.002%
70	10.222	2826	2840	2867	rBV	476949	748036	26.81%	3.992%
71	10.392	2890	2893	2894	rBV2	438	217	0.01%	0.001%
72	10.482	2919	2921	2924	rBV	410	239	0.01%	0.001%
73	10.515	2929	2931	2932	rBV	798	253	0.01%	0.001%
74	10.569	2947	2948	2949	rBV	608	200	0.01%	0.001%
75	10.650	2969	2973	2974	rBV2	668	372	0.01%	0.002%
76	10.736	2997	3000	3002	rBV2	354	289	0.01%	0.002%

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 Title : VOC Analysis

77	10.756	3004	3006	3008	rBV3	425	183	0.01%	0.001%
78	10.878	3042	3044	3045	rBV	545	247	0.01%	0.001%
79	11.068	3098	3103	3104	rBV3	637	499	0.02%	0.003%
80	11.254	3150	3161	3184	rBV	838588	1294389	46.39%	6.907%
81	11.518	3241	3243	3246	rVB2	696	320	0.01%	0.002%
82	11.630	3267	3278	3300	rBV	825775	1289371	46.21%	6.881%
83	11.871	3351	3353	3354	rBV	955	408	0.01%	0.002%
84	11.997	3390	3392	3394	rBV2	526	239	0.01%	0.001%
85	12.010	3394	3396	3398	rVV2	584	192	0.01%	0.001%
86	12.077	3413	3417	3419	rBV2	706	508	0.02%	0.003%
87	12.219	3458	3461	3463	rBV2	900	490	0.02%	0.003%
88	12.296	3482	3485	3487	rBV3	685	480	0.02%	0.003%
89	12.341	3497	3499	3500	rBV	1022	411	0.01%	0.002%
90	12.495	3545	3547	3550	rBV3	686	464	0.02%	0.002%
91	12.627	3582	3588	3591	rBV5	853	852	0.03%	0.005%
92	12.656	3591	3597	3603	rBV7	2246	2954	0.11%	0.016%
93	12.723	3617	3618	3622	rVB2	668	350	0.01%	0.002%
94	12.746	3622	3625	3628	rBV2	952	811	0.03%	0.004%
95	12.842	3653	3655	3656	rBV	696	272	0.01%	0.001%
96	12.878	3664	3666	3667	rBV	858	383	0.01%	0.002%
97	13.032	3712	3714	3717	rBV2	840	346	0.01%	0.002%
98	13.061	3719	3723	3726	rVB3	1224	881	0.03%	0.005%
99	13.579	3881	3884	3886	rBV	756	468	0.02%	0.002%
100	13.752	3935	3938	3946	rVB7	1611	1914	0.07%	0.010%

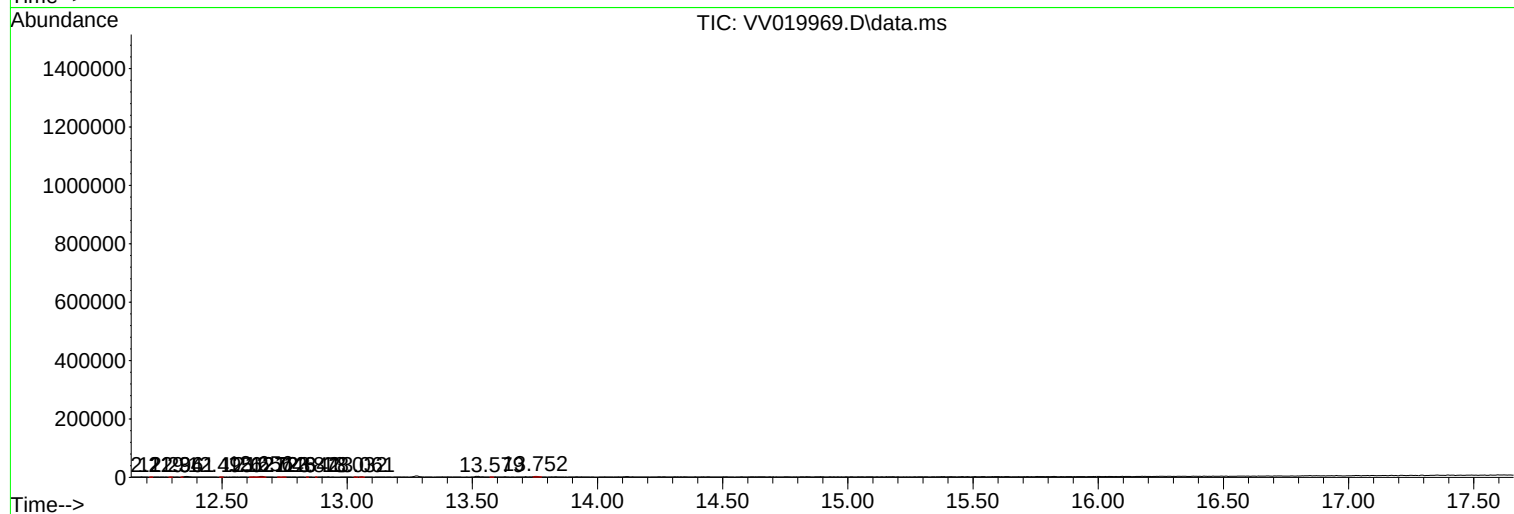
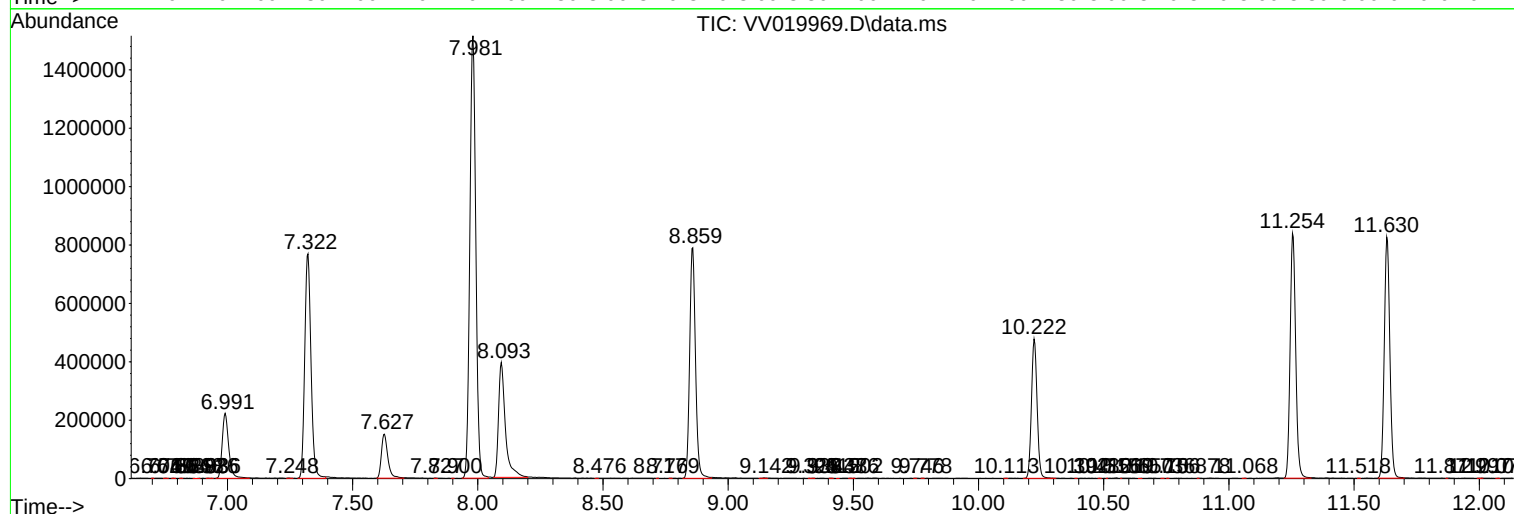
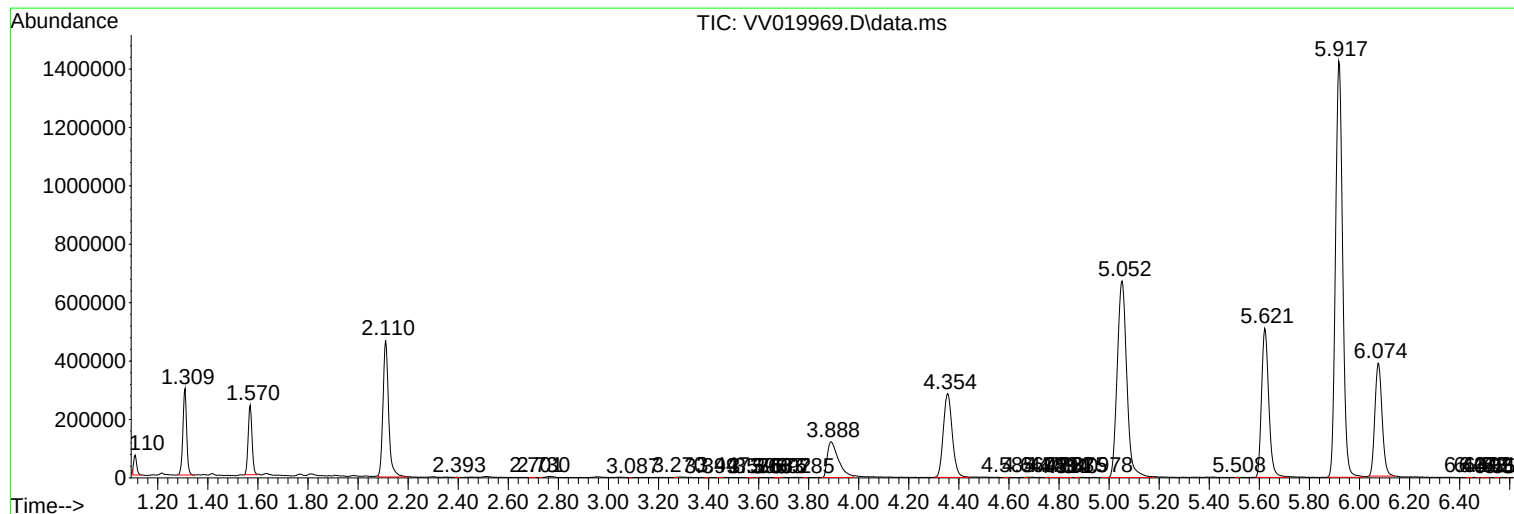
Sum of corrected areas: 18739305

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Instrument :
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM011121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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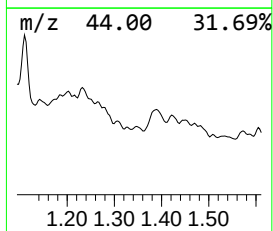
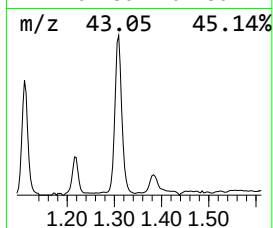
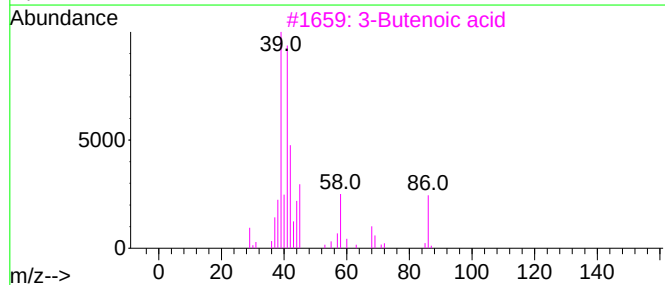
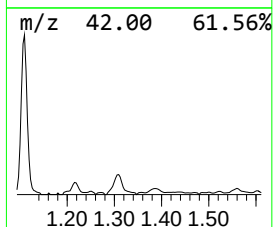
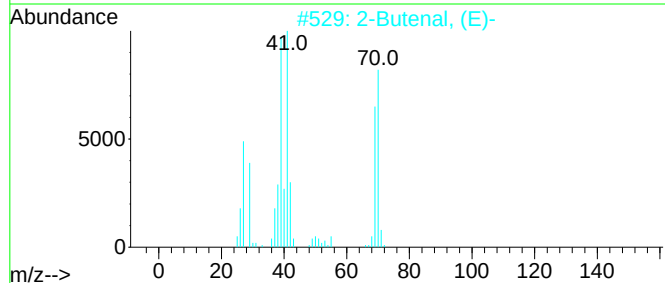
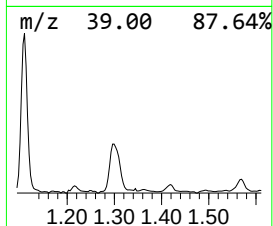
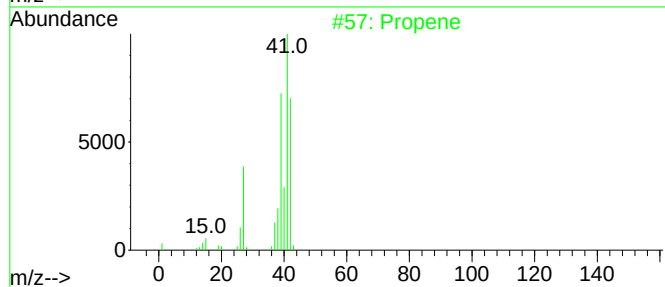
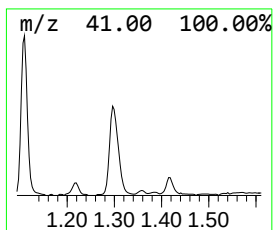
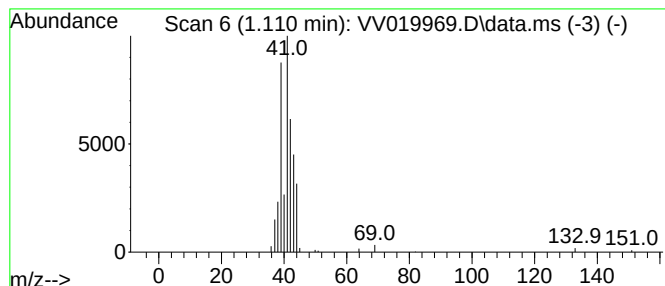
Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM011121WMA.M
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.110	2.69 ug/L	55236	1,4-Difluorobenzene	5.621

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	86
2			2-Butenal, (E)-	70	C4H6O	000123-73-9	78
3			3-Butenoic acid	86	C4H6O2	000625-38-7	78
4			Pyrimidin-4(3H)-one, 3-amino-2,6...	139	C6H9N3O	093098-74-9	78
5			Cyclopropanecarboxylic acid	86	C4H6O2	001759-53-1	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.110	2.7	ug/L	55236	1	5.621	1025400	50.0