LSC Area Percent Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV072021\
Data File : VV021691.D
Acq On : 20 Jul 2021 16:36
Operator : SY/MD
Sample : M3034-02ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AT4ME

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\SFAMVLM071921WMA.M
Title : VOC Analysis

Signal : TIC: VV021691.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.301	75	81	113	rVB	174481	289075	13.56%	1.933%
2	2.066	310	319	334	rBV	448160	653142	30.63%	4.368%
3	2.651	498	501	503	rBV3	468	293	0.01%	0.002%
4	2.706	513	518	522	rBV2	675	562	0.03%	0.004%
5	2.735	524	527	531	rVV3	323	269	0.01%	0.002%
6	2.786	541	543	544	rBV2	326	86	0.00%	0.001%
7	2.799	545	547	553	rVV4	381	336	0.02%	0.002%
8	2.873	569	570	575	rBV2	300	182	0.01%	0.001%
9	3.111	643	644	645	rBV2	319	118	0.01%	0.001%
10	3.146	653	655	657	rVV	296	109	0.01%	0.001%
11	3.162	657	660	663	rVB2	469	306	0.01%	0.002%
12	3.278	692	696	697	rBV	359	237	0.01%	0.002%
13	3.317	705	708	714	rVB3	368	263	0.01%	0.002%
14	3.371	722	725	727	rBV2	598	379	0.02%	0.003%
15	3.432	739	744	748	rBV3	504	373	0.02%	0.002%
16	3.461	751	753	758	rVB2	540	431	0.02%	0.003%
17	3.526	770	773	774	rBV	308	153	0.01%	0.001%
18	3.571	785	787	788	rBV	324	145	0.01%	0.001%
19	3.693	823	825	830	rVB2	455	265	0.01%	0.002%
20	3.719	830	833	834	rBV2	286	153	0.01%	0.001%
21	3.780	850	852	854	rBV	191	84	0.00%	0.001%
22	3.793	854	856	858	rVB	340	158	0.01%	0.001%
23	3.841	868	871	873	rBV2	262	116	0.01%	0.001%
24	3.892	876	887	943	rBV	112422	449525	21.08%	3.006%
25	4.346	1010	1028	1055	rBV	306879	824956	38.69%	5.516%
26	4.780	1161	1163	1166	rBV2	447	204	0.01%	0.001%
27	4.818	1173	1175	1178	rBV3	272	110	0.01%	0.001%
28	4.850	1181	1185	1187	rVB2	280	166	0.01%	0.001%
29	4.860	1187	1188	1189	rBV2	202	65	0.00%	0.000%
30	4.879	1193	1194	1195	rBV2	171	39	0.00%	0.000%
31	4.924	1207	1208	1210	rBV	234	108	0.01%	0.001%
32	5.037	1226	1243	1276	rBV2	861563	2132435	100.00%	14.259%
33	5.535	1395	1398	1399	rBV	311	194	0.01%	0.001%
34	5.612	1409	1422	1463	rBV	531324	1145235	53.71%	7.658%
35	5.902	1501	1512	1528	rBV2	32149	71054	3.33%	0.475%
36	6.069	1551	1564	1601	rVB	432684	952074	44.65%	6.366%

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Operator : SY/MD
Sample : M3034-02ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AT4ME

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\SFAMVLM071921WMA.M
Title : VOC Analysis

37	6.352	1650	1652	1655	rVB2	720	335	0.02%	0.002%
38	6.368	1655	1657	1659	rBV2	260	174	0.01%	0.001%
39	6.387	1661	1663	1666	rVV2	360	223	0.01%	0.001%
40	6.419	1670	1673	1677	rBV2	468	351	0.02%	0.002%
41	6.442	1678	1680	1683	rBV2	322	142	0.01%	0.001%
42	6.513	1695	1702	1703	rBV	396	404	0.02%	0.003%
43	6.519	1703	1704	1708	rVV	416	327	0.02%	0.002%
44	6.638	1732	1741	1742	rBV5	2140	2654	0.12%	0.018%
45	6.741	1771	1773	1776	rVB3	302	122	0.01%	0.001%
46	6.815	1795	1796	1798	rBV	108	39	0.00%	0.000%
47	6.834	1801	1802	1805	rVB	347	106	0.00%	0.001%
48	6.853	1805	1808	1809	rBV2	369	176	0.01%	0.001%
49	6.870	1809	1813	1816	rBV3	227	130	0.01%	0.001%
50	6.908	1822	1825	1826	rBV2	422	211	0.01%	0.001%
51	6.985	1838	1849	1878	rBV	261933	521106	24.44%	3.485%
52	7.146	1897	1899	1904	rBV2	417	220	0.01%	0.001%
53	7.313	1939	1951	1970	rBV	989666	1791181	84.00%	11.978%
54	7.622	2037	2047	2085	rBV	169421	340107	15.95%	2.274%
55	7.796	2099	2101	2103	rBV2	598	308	0.01%	0.002%
56	7.992	2156	2162	2168	rVB3	416	502	0.02%	0.003%
57	8.021	2168	2171	2173	rBV2	209	151	0.01%	0.001%
58	8.037	2174	2176	2181	rVB3	518	308	0.01%	0.002%
59	8.101	2184	2196	2198	rBV2	278183	413537	19.39%	2.765%
60	8.538	2329	2332	2336	rBV3	447	407	0.02%	0.003%
61	8.667	2370	2372	2375	rBV2	330	182	0.01%	0.001%
62	8.718	2386	2388	2389	rBV2	249	114	0.01%	0.001%
63	8.751	2396	2398	2404	rBV3	211	234	0.01%	0.002%
64	8.796	2409	2412	2418	rBV3	324	295	0.01%	0.002%
65	8.857	2418	2431	2462	rBV	746950	1383950	64.90%	9.254%
66	9.201	2536	2538	2539	rBV	334	139	0.01%	0.001%
67	9.294	2564	2567	2570	rBV2	289	195	0.01%	0.001%
68	9.349	2582	2584	2586	rBV2	427	264	0.01%	0.002%
69	9.513	2633	2635	2640	rVB3	258	224	0.01%	0.001%
70	9.541	2641	2644	2645	rBV2	370	151	0.01%	0.001%
71	9.702	2692	2694	2697	rVB2	350	180	0.01%	0.001%
72	9.725	2699	2701	2706	rVB2	233	121	0.01%	0.001%
73	9.757	2709	2711	2713	rBV	230	89	0.00%	0.001%
74	9.828	2729	2733	2736	rBV2	375	321	0.02%	0.002%
75	9.853	2739	2741	2744	rBV2	347	180	0.01%	0.001%
76	9.873	2745	2747	2753	rVB2	441	287	0.01%	0.002%

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Acq On : 20 Jul 2021 16:36
Operator : SY/MD
Sample : M3034-02ME
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AT4ME

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\SFAMVLM071921WMA.M
Title : VOC Analysis

77	9.902	2753	2756	2758	rBV2	315	132	0.01%	0.001%
78	9.918	2758	2761	2762	rBV2	192	85	0.00%	0.001%
79	9.979	2779	2780	2781	rBV2	312	63	0.00%	0.000%
80	10.008	2786	2789	2791	rBV3	430	258	0.01%	0.002%
81	10.037	2796	2798	2800	rBV2	316	148	0.01%	0.001%
82	10.130	2818	2827	2842	rBV4	7925	14185	0.67%	0.095%
83	10.223	2843	2856	2878	rBV	544045	973739	45.66%	6.511%
84	10.715	3007	3009	3014	rVB2	483	266	0.01%	0.002%
85	10.741	3014	3017	3022	rBV2	605	555	0.03%	0.004%
86	10.767	3022	3025	3027	rBV3	540	435	0.02%	0.003%
87	10.924	3066	3074	3083	rVB5	7093	11139	0.52%	0.074%
88	11.149	3138	3144	3151	rVB5	3954	5234	0.25%	0.035%
89	11.255	3165	3177	3198	rBV	877339	1367261	64.12%	9.143%
90	11.631	3282	3294	3316	rBV	1002601	1594938	74.79%	10.665%
91	11.959	3394	3396	3398	rBV2	300	111	0.01%	0.001%
92	12.426	3537	3541	3546	rBV5	794	868	0.04%	0.006%
93	12.532	3569	3574	3575	rBV3	772	660	0.03%	0.004%
94	12.657	3611	3613	3615	rBV2	400	155	0.01%	0.001%
95	12.728	3633	3635	3637	rBV	327	172	0.01%	0.001%
96	12.741	3637	3639	3644	rVB2	377	285	0.01%	0.002%
97	13.011	3721	3723	3725	rBV	596	279	0.01%	0.002%

Sum of corrected areas: 14954515

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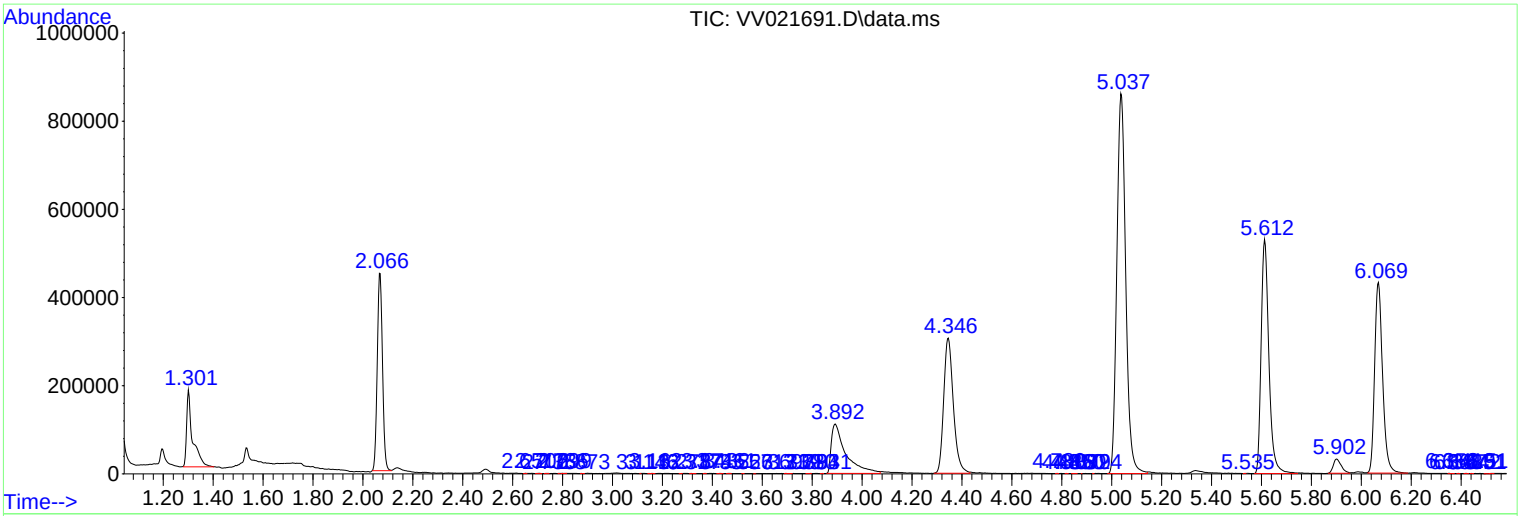
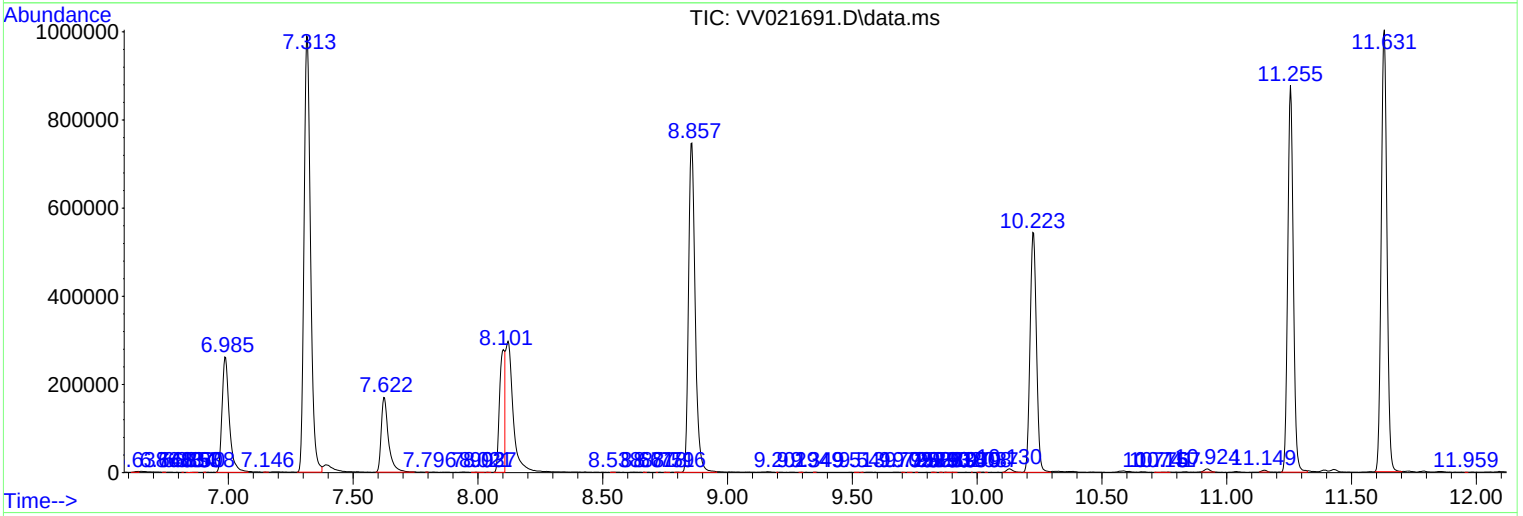
Misc : 5.06g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 8 Sample Multiplier: 1

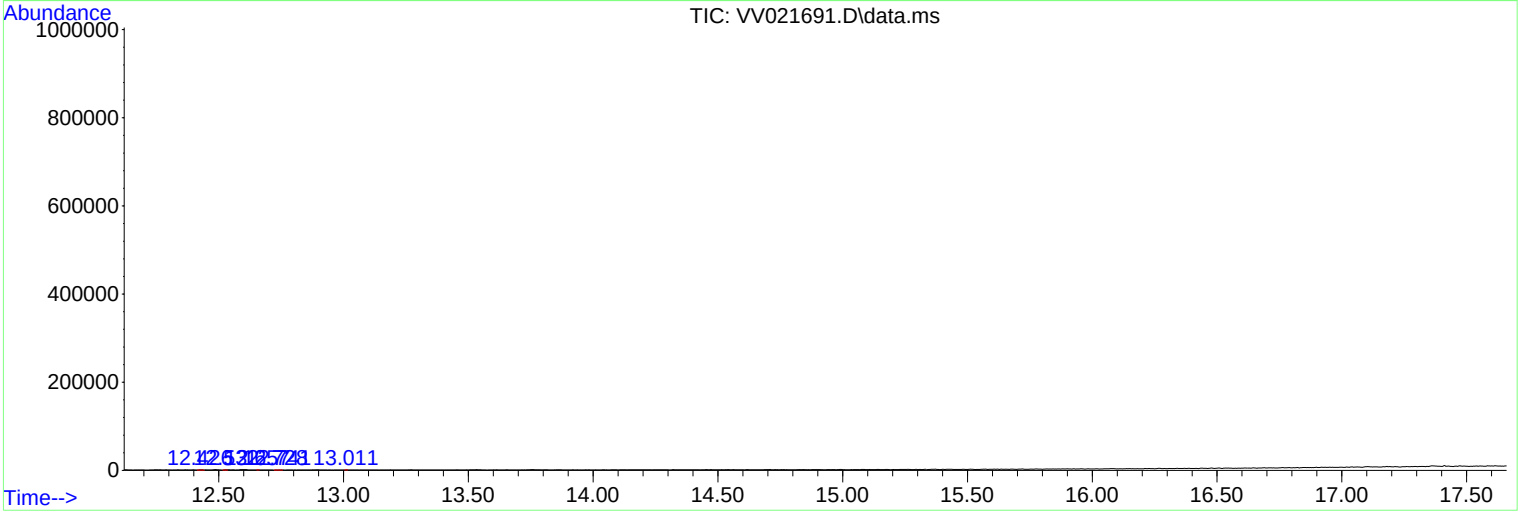
Instrument :
MSVOA_V
ClientSampleId :
C0AT4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

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







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ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : C0AT4ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

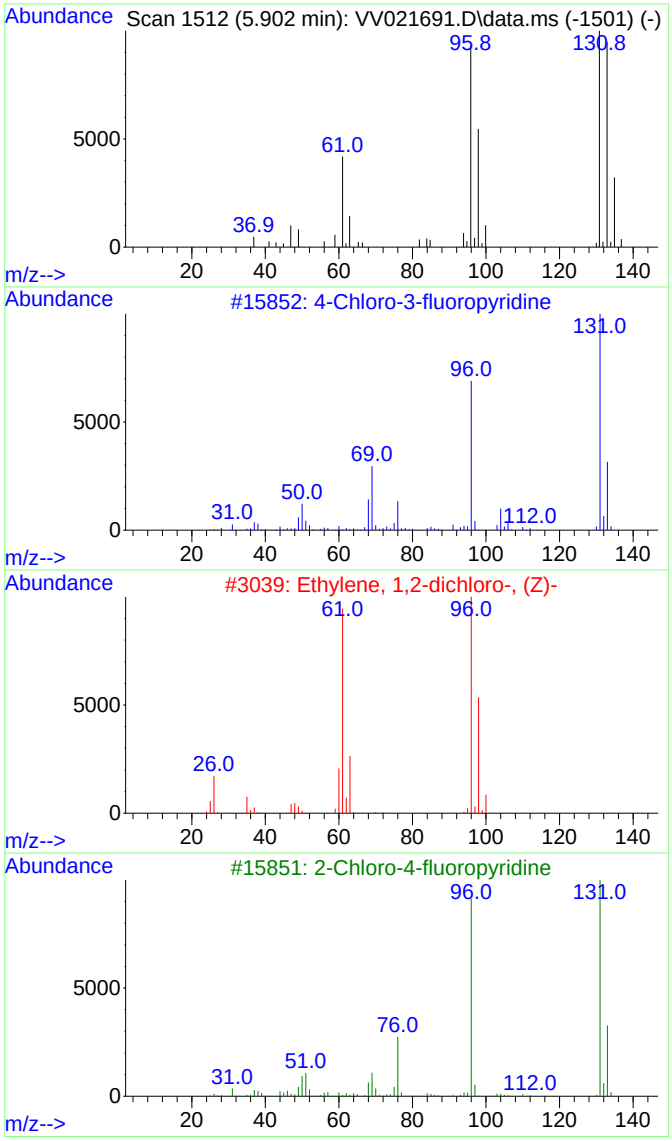
TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

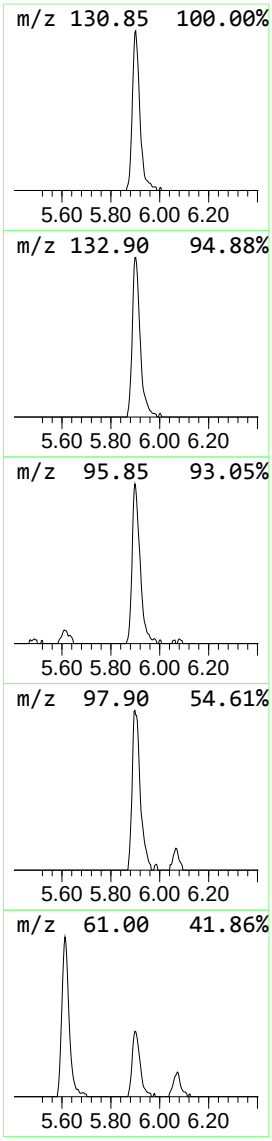
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.902	3.10 ug/L	71054	1,4-Difluorobenzene	5.612

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	38
2	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3	2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
4	1H-Pyrazole, 1,3-dimethyl-	96	C5H8N2	000694-48-4	9
5	m-Methoxybenzontrile	133	C8H7NO	001527-89-5	9





Tentatively Identified Compound (LSC) summary

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM071921WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	5.902	3.1	ug/L	71054	1	5.612	1145240	50.0