LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA V\DATA\VV092420\
Data File : VV018418.D
Acq On : 24 Sep 2020 11:01
Operator : SY/MD
Sample : VV0924MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK78

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\SOMVLM090920WMA.M
Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.315	63	70	87	rVB	138095	141347	12.84%	1.597%
2	1.579	144	152	162	rVB	120269	136201	12.37%	1.539%
3	2.119	310	320	333	rBV	249405	364392	33.10%	4.118%
4	2.306	371	378	387	rVB	2545	3842	0.35%	0.043%
5	2.428	412	416	418	rBV2	217	144	0.01%	0.002%
6	2.460	424	426	429	rVB2	272	133	0.01%	0.002%
7	2.479	429	432	434	rBV3	301	226	0.02%	0.003%
8	2.524	439	446	454	rVB3	1877	3080	0.28%	0.035%
9	2.579	460	463	466	rVB2	210	129	0.01%	0.001%
10	2.598	466	469	471	rBV	228	169	0.02%	0.002%
11	2.637	479	481	486	rVB2	200	101	0.01%	0.001%
12	2.663	486	489	492	rBV2	126	100	0.01%	0.001%
13	2.704	500	502	505	rVB2	215	98	0.01%	0.001%
14	2.785	519	527	535	rVB5	1311	2101	0.19%	0.024%
15	2.888	556	559	564	rBV2	144	124	0.01%	0.001%
16	3.071	613	616	619	rBV	219	122	0.01%	0.001%
17	3.209	656	659	662	rBV3	213	201	0.02%	0.002%
18	3.319	690	693	695	rBV2	193	152	0.01%	0.002%
19	3.341	695	700	702	rBV	123	117	0.01%	0.001%
20	3.418	718	724	731	rVB2	177	276	0.03%	0.003%
21	3.614	780	785	790	rVB2	148	135	0.01%	0.002%
22	3.814	841	847	850	rBV2	211	217	0.02%	0.002%
23	3.923	868	881	927	rBV	69223	255902	23.25%	2.892%
24	4.370	1004	1020	1050	rBV	175689	432862	39.32%	4.891%
25	4.495	1057	1059	1068	rVB3	408	491	0.04%	0.006%
26	4.560	1077	1079	1082	rVB	246	118	0.01%	0.001%
27	4.643	1101	1105	1110	rVB3	402	329	0.03%	0.004%
28	4.695	1116	1121	1125	rBV3	461	537	0.05%	0.006%
29	4.846	1162	1168	1169	rBV2	244	175	0.02%	0.002%
30	4.859	1169	1172	1173	rVV	300	193	0.02%	0.002%
31	4.868	1173	1175	1181	rVB2	332	157	0.01%	0.002%
32	4.997	1213	1215	1218	rVB2	175	97	0.01%	0.001%
33	5.068	1219	1237	1272	rBV2	431967	1100807	100.00%	12.439%
34	5.302	1307	1310	1311	rBV	177	104	0.01%	0.001%

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ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK78

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\SOMVLM090920WMA.M
Title : VOC Analysis

35	5.386	1330	1336	1342	rBV3	262	412	0.04%	0.005%
36	5.515	1372	1376	1378	rBV3	188	139	0.01%	0.002%
37	5.637	1401	1414	1442	rBV	377231	746787	67.84%	8.439%
38	5.926	1493	1504	1527	rVB2	19788	41667	3.79%	0.471%
39	6.016	1527	1532	1535	rBV3	164	135	0.01%	0.002%
40	6.090	1540	1555	1583	rBV	244828	498525	45.29%	5.633%
41	6.238	1599	1601	1604	rVB3	379	159	0.01%	0.002%
42	6.254	1604	1606	1613	rVB4	504	431	0.04%	0.005%
43	6.286	1613	1616	1619	rBV2	196	117	0.01%	0.001%
44	6.360	1636	1639	1644	rBV	123	98	0.01%	0.001%
45	6.498	1679	1682	1686	rVB2	115	92	0.01%	0.001%
46	6.543	1691	1696	1702	rVB3	225	310	0.03%	0.004%
47	6.852	1787	1792	1794	rBV	164	144	0.01%	0.002%
48	7.006	1829	1840	1866	rBV	141710	255929	23.25%	2.892%
49	7.109	1870	1872	1876	rVV4	677	446	0.04%	0.005%
50	7.129	1876	1878	1881	rVB2	207	106	0.01%	0.001%
51	7.164	1887	1889	1892	rVB2	521	272	0.02%	0.003%
52	7.225	1907	1908	1913	rVB	162	93	0.01%	0.001%
53	7.254	1913	1917	1918	rBV2	389	223	0.02%	0.003%
54	7.334	1929	1942	1965	rBV	527371	894537	81.26%	10.108%
55	7.640	2027	2037	2062	rBV	99449	176260	16.01%	1.992%
56	7.868	2105	2108	2110	rBV	178	122	0.01%	0.001%
57	7.958	2132	2136	2139	rBV2	189	129	0.01%	0.001%
58	8.003	2145	2150	2155	rVB2	746	794	0.07%	0.009%
59	8.106	2172	2182	2227	rVV	267571	504070	45.79%	5.696%
60	8.379	2264	2267	2273	rVB4	513	574	0.05%	0.006%
61	8.412	2273	2277	2280	rBV3	242	246	0.02%	0.003%
62	8.437	2282	2285	2288	rBV3	395	359	0.03%	0.004%
63	8.871	2408	2420	2454	rBV	593407	932689	84.73%	10.539%
64	9.035	2466	2471	2484	rVB2	1059	1757	0.16%	0.020%
65	9.170	2506	2513	2523	rVB2	794	1244	0.11%	0.014%
66	9.354	2568	2570	2575	rBV	173	99	0.01%	0.001%
67	9.473	2604	2607	2610	rBV2	148	98	0.01%	0.001%
68	9.527	2621	2624	2629	rVB2	143	130	0.01%	0.001%
69	9.572	2632	2638	2642	rVV2	705	1071	0.10%	0.012%
70	9.595	2642	2645	2651	rVV3	1095	1145	0.10%	0.013%
71	9.646	2655	2661	2664	rBV2	168	179	0.02%	0.002%

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ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK78

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\SOMVLM090920WMA.M
Title : VOC Analysis

72	9.756	2692	2695	2699	rVB	197	113	0.01%	0.001%
73	9.820	2712	2715	2719	rVB2	140	104	0.01%	0.001%
74	9.955	2751	2757	2766	rVB3	943	1275	0.12%	0.014%
75	10.238	2832	2845	2862	rBV	313544	491252	44.63%	5.551%
76	10.563	2940	2946	2952	rBV2	792	1107	0.10%	0.013%
77	10.817	3022	3025	3028	rBV	172	119	0.01%	0.001%
78	10.907	3050	3053	3055	rBV	127	94	0.01%	0.001%
79	10.942	3058	3064	3072	rVB2	922	1339	0.12%	0.015%
80	11.209	3138	3147	3154	rBV3	1658	2399	0.22%	0.027%
81	11.270	3154	3166	3187	rBV	608834	933813	84.83%	10.552%
82	11.473	3226	3229	3230	rBV	213	110	0.01%	0.001%
83	11.646	3270	3283	3308	rBV	566815	891964	81.03%	10.079%
84	11.791	3326	3328	3331	rBV2	215	113	0.01%	0.001%
85	11.817	3333	3336	3338	rBV	296	174	0.02%	0.002%
86	11.887	3355	3358	3362	rBV2	154	133	0.01%	0.002%
87	11.913	3362	3366	3369	rVV	153	137	0.01%	0.002%
88	11.977	3384	3386	3391	rVB2	257	127	0.01%	0.001%
89	12.228	3461	3464	3469	rBV2	152	120	0.01%	0.001%
90	12.675	3596	3603	3614	rVB5	2094	3065	0.28%	0.035%
91	13.289	3786	3794	3803	rBV4	2893	4177	0.38%	0.047%
92	13.350	3810	3813	3816	rBV2	171	109	0.01%	0.001%
93	13.431	3837	3838	3841	rVB	184	94	0.01%	0.001%
94	13.492	3854	3857	3861	rBV	167	152	0.01%	0.002%
95	13.537	3861	3871	3886	rVB2	3103	5438	0.49%	0.061%
96	13.772	3936	3944	3955	rBV4	2978	4123	0.37%	0.047%
97	14.048	4027	4030	4033	rBV2	187	129	0.01%	0.001%
98	14.189	4070	4074	4082	rVB2	468	641	0.06%	0.007%
99	14.225	4082	4085	4087	rBV2	186	125	0.01%	0.001%
100	14.280	4097	4102	4105	rBV2	257	291	0.03%	0.003%

Sum of corrected areas: 8849604

LSC Report - Integrated Chromatogram

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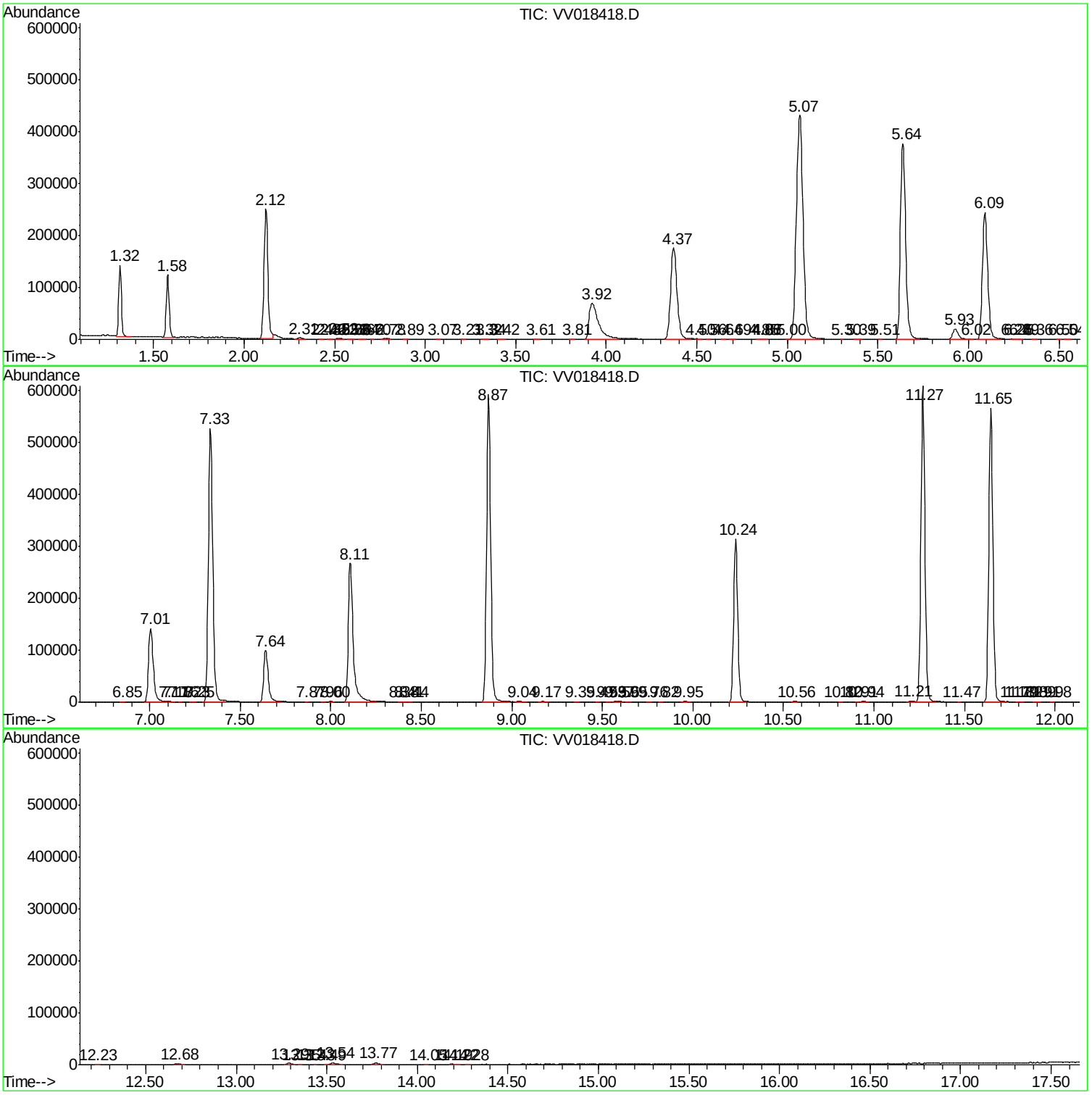
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK78

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM090920WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV092420\
Data File : VV018418.D
Acq On : 24 Sep 2020 11:01
Operator : SY/MD
Sample : VV0924MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument : MSVOA_V
ClientSampleId : VBLK78

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM090920WMA.M
Quant Title : VOC Analysis

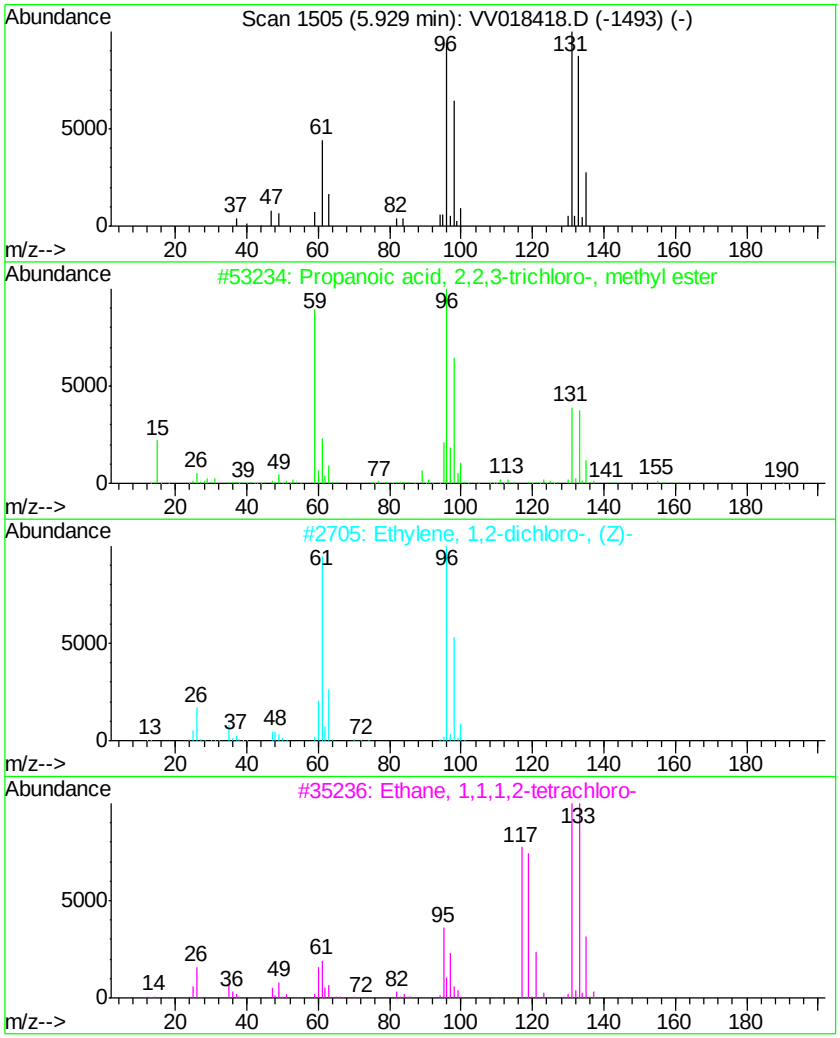
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

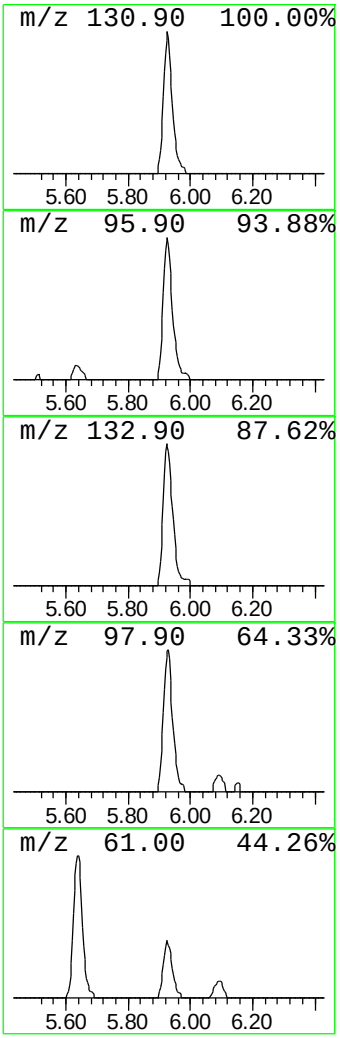
****

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.93	2.79 ug/L	41667	1,4-Difluorobenzene	5.64

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	56
2	Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	38
3	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	37
4	Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	32
5	Dihydro-4,5-dichloro-2(3H)furanone	154	C4H4Cl2O2	114434-99-0	25





Tentatively Identified Compound (LSC) summary

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_V\DATA\VV092420\
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_V\METHOD\SOMVLM090920WMA.M
Quant Title : VOC Analysis

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

					Internal Standard			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
Propanoic acid, 2...	5.93	2.8	ug/L	41667	1	5.64	746787	50.0