

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
 Data File : VV024371.D
 Acq On : 17 Jan 2022 11:37
 Operator : SY/MD
 Sample : VV0117MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK299

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

Signal : TIC: VV024370.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.201	45	50	59	rBV	32029	28688	2.36%	0.317%
2	1.307	76	83	97	rVB	175465	175780	14.49%	1.945%
3	1.568	157	164	176	rVB	135239	148503	12.24%	1.643%
4	2.108	321	332	359	rVB	289681	429801	35.43%	4.756%
5	2.246	373	375	376	rBV	258	90	0.01%	0.001%
6	2.609	484	488	489	rBV3	436	285	0.02%	0.003%
7	2.680	508	510	512	rVB	236	51	0.00%	0.001%
8	2.822	552	554	556	rBV	287	121	0.01%	0.001%
9	2.838	556	559	563	rVV2	159	158	0.01%	0.002%
10	3.114	642	645	649	rBV	223	211	0.02%	0.002%
11	3.137	650	652	657	rVB2	398	213	0.02%	0.002%
12	3.169	657	662	665	rBV	266	240	0.02%	0.003%
13	3.272	691	694	696	rBV2	208	144	0.01%	0.002%
14	3.397	730	733	734	rBV2	201	121	0.01%	0.001%
15	3.571	784	787	791	rBV2	193	210	0.02%	0.002%
16	3.625	802	804	807	rVB2	366	248	0.02%	0.003%
17	3.658	810	814	816	rBV2	322	304	0.03%	0.003%
18	3.728	833	836	837	rBV	264	185	0.02%	0.002%
19	3.757	842	845	848	rBV2	159	142	0.01%	0.002%
20	3.876	872	882	918	rBV	69050	209451	17.27%	2.318%
21	4.342	1012	1027	1054	rBV	200680	491236	40.50%	5.435%
22	4.542	1086	1089	1092	rBV3	647	457	0.04%	0.005%
23	4.622	1111	1114	1117	rBV2	388	307	0.03%	0.003%
24	4.657	1120	1125	1127	rBV3	416	342	0.03%	0.004%
25	4.786	1162	1165	1169	rVB2	193	131	0.01%	0.001%
26	4.812	1169	1173	1176	rBV2	362	286	0.02%	0.003%
27	5.040	1227	1244	1278	rBV2	467766	1213039	100.00%	13.422%
28	5.506	1387	1389	1394	rVB	642	321	0.03%	0.004%
29	5.529	1394	1396	1399	rVB2	290	181	0.01%	0.002%
30	5.551	1399	1403	1404	rBV2	334	202	0.02%	0.002%
31	5.609	1409	1421	1456	rBV	345572	701981	57.87%	7.767%
32	5.902	1502	1512	1533	rVB4	16369	35240	2.91%	0.390%
33	6.063	1546	1562	1595	rBV	259841	536552	44.23%	5.937%
34	6.603	1728	1730	1734	rVB2	483	274	0.02%	0.003%
35	6.677	1751	1753	1754	rBV	369	146	0.01%	0.002%
36	6.706	1758	1762	1763	rBV	418	268	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
 Data File : VV024371.D
 Acq On : 17 Jan 2022 11:37
 Operator : SY/MD
 Sample : VV0117MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 VBLK299

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\SFAMVLM123121WMA.M
 Title : VOC Analysis

37	6.757	1775	1778	1780	rBV	384	236	0.02%	0.003%
38	6.828	1799	1800	1801	rBV	217	67	0.01%	0.001%
39	6.902	1819	1823	1824	rBV2	273	183	0.02%	0.002%
40	6.982	1837	1848	1871	rBV	159772	288590	23.79%	3.193%
41	7.310	1939	1950	1968	rBV	576038	1004498	82.81%	11.115%
42	7.616	2034	2045	2066	rBV	109430	193073	15.92%	2.136%
43	7.902	2132	2134	2136	rVB2	358	121	0.01%	0.001%
44	7.937	2136	2145	2156	rBV3	2891	4902	0.40%	0.054%
45	8.085	2181	2191	2226	rBV	238655	468296	38.61%	5.182%
46	8.480	2312	2314	2315	rVB2	542	164	0.01%	0.002%
47	8.612	2352	2355	2357	rBV3	280	179	0.01%	0.002%
48	8.641	2362	2364	2366	rBV	351	228	0.02%	0.003%
49	8.683	2374	2377	2378	rBV	363	190	0.02%	0.002%
50	8.722	2387	2389	2392	rVB2	199	119	0.01%	0.001%
51	8.763	2399	2402	2403	rBV	287	194	0.02%	0.002%
52	8.847	2416	2428	2456	rBV	509457	832235	68.61%	9.209%
53	9.152	2515	2523	2533	rBV5	1347	2148	0.18%	0.024%
54	9.226	2544	2546	2547	rBV	240	90	0.01%	0.001%
55	9.271	2557	2560	2564	rBV	239	278	0.02%	0.003%
56	9.493	2627	2629	2631	rBV2	195	109	0.01%	0.001%
57	9.548	2644	2646	2656	rVB3	685	736	0.06%	0.008%
58	9.590	2656	2659	2661	rBV2	288	159	0.01%	0.002%
59	9.799	2720	2724	2726	rBV	445	322	0.03%	0.004%
60	10.059	2802	2805	2806	rBV	191	111	0.01%	0.001%
61	10.127	2818	2826	2835	rVB4	3260	4581	0.38%	0.051%
62	10.214	2841	2853	2878	rBV	331019	519332	42.81%	5.746%
63	10.574	2959	2965	2971	rBV6	1198	2056	0.17%	0.023%
64	10.914	3060	3071	3082	rVB7	3200	5201	0.43%	0.058%
65	10.963	3084	3086	3087	rBV	172	55	0.00%	0.001%
66	11.140	3137	3141	3151	rBV3	1349	1764	0.15%	0.020%
67	11.246	3163	3174	3195	rBV	515517	798810	65.85%	8.839%
68	11.622	3279	3291	3312	rBV	590979	921513	75.97%	10.196%
69	11.947	3385	3392	3393	rBV2	370	380	0.03%	0.004%
70	12.297	3499	3501	3505	rBV	287	128	0.01%	0.001%
71	12.464	3549	3553	3556	rVB2	383	305	0.03%	0.003%
72	12.651	3609	3611	3617	rVB3	595	545	0.04%	0.006%
73	12.853	3672	3674	3681	rVB2	381	394	0.03%	0.004%
74	12.882	3681	3683	3685	rBV	238	110	0.01%	0.001%
75	13.001	3718	3720	3721	rBV	384	150	0.01%	0.002%
76	13.262	3798	3801	3803	rBV	713	480	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
Data File : VV024371.D
Acq On : 17 Jan 2022 11:37
Operator : SY/MD
Sample : VV0117MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK299

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\SFAMVLM123121WMA.M

Title : VOC Analysis

77	13.483	3867	3870	3871	rBV	541	322	0.03%	0.004%
78	13.509	3871	3878	3887	rVV	4483	6637	0.55%	0.073%
79	13.599	3903	3906	3909	rBV2	427	397	0.03%	0.004%
80	13.734	3945	3948	3949	rBV	749	417	0.03%	0.005%
81	13.811	3970	3972	3975	rVB2	632	276	0.02%	0.003%
82	14.709	4245	4251	4254	rBV2	529	640	0.05%	0.007%

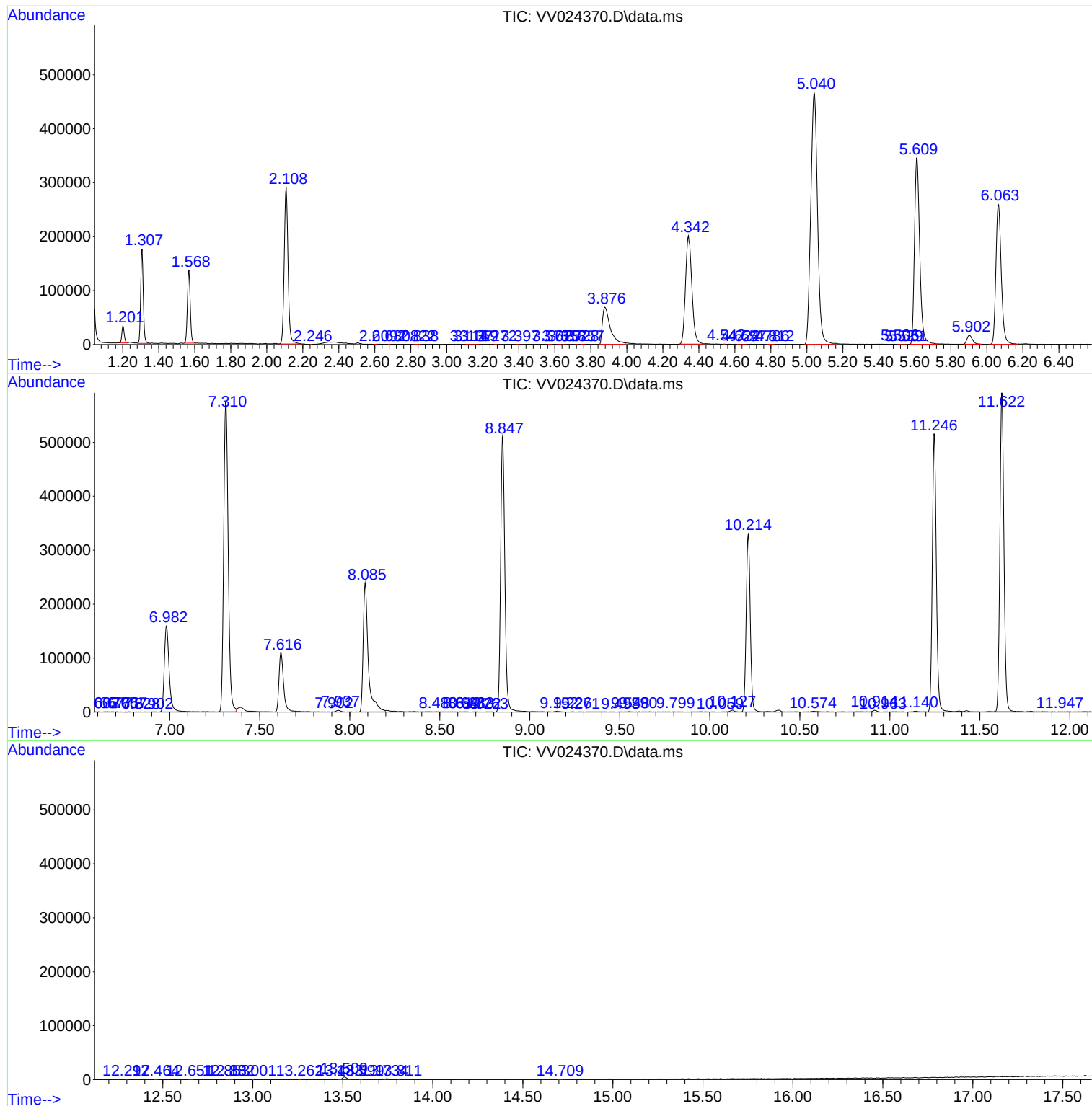
Sum of corrected areas: 9037630

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
Data File : VV024371.D
Acq On : 17 Jan 2022 11:37
Operator : SY/MD
Sample : VV0117MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK299

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
Data File : VV024371.D
Acq On : 17 Jan 2022 11:37
Operator : SY/MD
Sample : VV0117MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK299

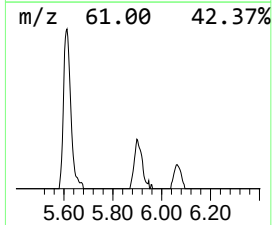
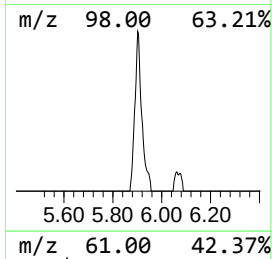
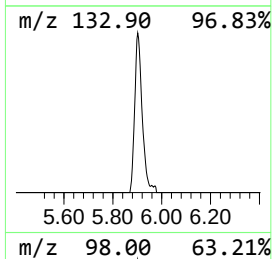
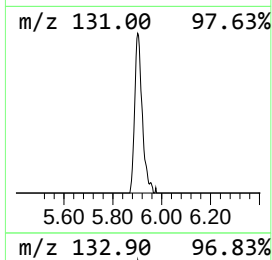
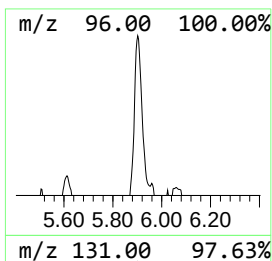
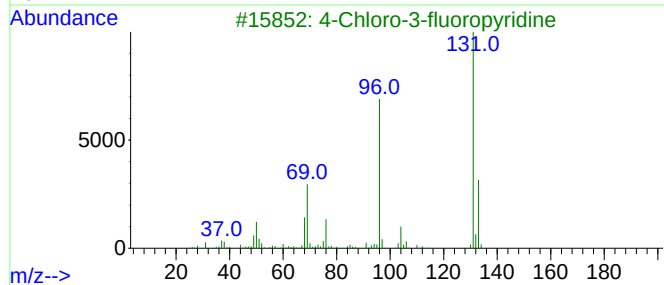
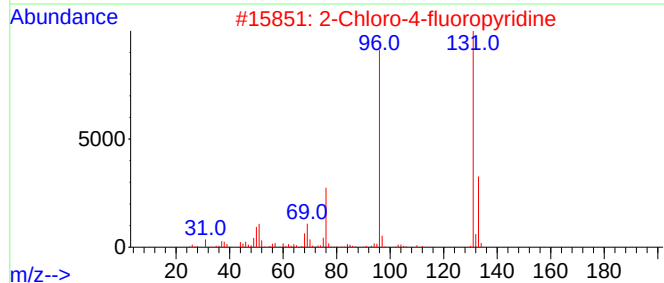
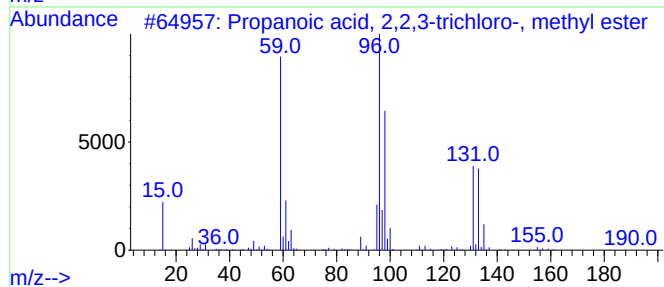
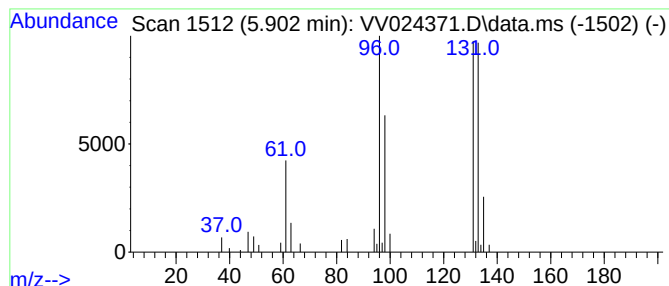
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.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.
5.902	2.51 ug/L	35240	1,4-Difluorobenzene	5.612

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propanoic acid, 2,2,3-trichloro-...	190	C4H5Cl3O2	004749-35-3	50
2			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	38
3			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	32
4			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	30
5			Heptanoic acid, heptyl ester	228	C14H28O2	000624-09-9	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011722\
Data File : VV024371.D
Acq On : 17 Jan 2022 11:37
Operator : SY/MD
Sample : VV0117MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
VBLK299

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.902	2.5	ug/L	35240	1	5.612	701981	50.0