

Data Path : Z:\voasrv\HPCHEM1\MSVOA_V\Data\VV011822\
 Data File : VV024394.D
 Acq On : 18 Jan 2022 15:21
 Operator : SY/MD
 Sample : N1129-06ME
 Misc : 6.14g/5.0mL/100uL/5.0mL/MSVOA_V/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_V
 ClientSampleId :
 DBLZ9ME

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: VV024394.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.214	50	54	59	rBV2	11682	9935	0.72%	0.101%
2	1.307	76	83	98	rVB	142178	166156	11.96%	1.686%
3	1.571	157	165	180	rBV	96556	144518	10.41%	1.466%
4	2.092	317	327	342	rBV	304680	431056	31.04%	4.373%
5	2.317	395	397	398	rBV2	569	226	0.02%	0.002%
6	2.436	428	434	436	rBV3	1083	1198	0.09%	0.012%
7	2.748	530	531	533	rBV	374	186	0.01%	0.002%
8	2.780	537	541	547	rBV3	312	378	0.03%	0.004%
9	2.818	550	553	559	rBV2	447	405	0.03%	0.004%
10	2.941	583	591	592	rBV3	2145	2101	0.15%	0.021%
11	3.127	647	649	653	rBV2	329	257	0.02%	0.003%
12	3.265	689	692	696	rVB	319	263	0.02%	0.003%
13	3.294	697	701	705	rBV2	345	311	0.02%	0.003%
14	3.365	721	723	726	rBV	267	179	0.01%	0.002%
15	3.429	741	743	746	rBV2	351	173	0.01%	0.002%
16	3.510	765	768	771	rBV2	415	311	0.02%	0.003%
17	3.645	807	810	813	rBV2	357	257	0.02%	0.003%
18	3.731	835	837	842	rVB2	288	224	0.02%	0.002%
19	3.760	842	846	850	rVB2	322	325	0.02%	0.003%
20	3.789	850	855	858	rBV	417	477	0.03%	0.005%
21	3.802	858	859	862	rBV	233	114	0.01%	0.001%
22	3.847	870	873	875	rBV2	311	234	0.02%	0.002%
23	3.902	879	890	916	rBV2	59092	222021	15.99%	2.252%
24	4.346	1015	1028	1058	rVB	226219	560131	40.33%	5.682%
25	4.686	1130	1134	1136	rBV3	503	380	0.03%	0.004%
26	4.783	1162	1164	1170	rBV3	242	283	0.02%	0.003%
27	4.883	1191	1195	1198	rBV	358	339	0.02%	0.003%
28	4.918	1203	1206	1210	rBV2	400	329	0.02%	0.003%
29	4.940	1211	1213	1215	rBV	324	154	0.01%	0.002%
30	5.040	1227	1244	1276	rBV2	555780	1388701	100.00%	14.088%
31	5.336	1326	1336	1348	rBV5	5301	12699	0.91%	0.129%
32	5.612	1410	1422	1462	rBV	366062	746690	53.77%	7.575%
33	5.905	1500	1513	1533	rBV2	22595	50494	3.64%	0.512%
34	6.066	1551	1563	1594	rVB	295433	620209	44.66%	6.292%
35	6.506	1698	1700	1702	rBV3	470	275	0.02%	0.003%
36	6.609	1728	1732	1733	rBV2	467	293	0.02%	0.003%

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 Title : VOC Analysis

37	6.985	1838	1849	1887	rBV	171264	335900	24.19%	3.408%
38	7.313	1935	1951	1970	rBV	650759	1167743	84.09%	11.847%
39	7.580	2032	2034	2036	rBV	459	220	0.02%	0.002%
40	7.622	2037	2047	2077	rVV2	107455	223348	16.08%	2.266%
41	7.902	2131	2134	2136	rVB3	478	253	0.02%	0.003%
42	7.918	2136	2139	2140	rBV3	335	183	0.01%	0.002%
43	7.953	2148	2150	2152	rBV2	817	293	0.02%	0.003%
44	7.976	2152	2157	2166	rVV5	2474	3874	0.28%	0.039%
45	8.046	2177	2179	2182	rVB	269	119	0.01%	0.001%
46	8.059	2182	2183	2184	rBV	281	104	0.01%	0.001%
47	8.098	2185	2195	2197	rBV	93201	126483	9.11%	1.283%
48	8.712	2383	2386	2387	rBV	322	174	0.01%	0.002%
49	8.770	2402	2404	2405	rBV	258	104	0.01%	0.001%
50	8.853	2418	2430	2457	rBV	451397	897315	64.62%	9.103%
51	9.281	2561	2563	2565	rBV	243	90	0.01%	0.001%
52	9.661	2678	2681	2683	rBV2	192	130	0.01%	0.001%
53	9.828	2731	2733	2736	rBV2	450	322	0.02%	0.003%
54	9.844	2736	2738	2739	rBV2	682	241	0.02%	0.002%
55	9.905	2746	2757	2775	rVB3	57579	96400	6.94%	0.978%
56	9.998	2783	2786	2788	rVB2	334	143	0.01%	0.001%
57	10.098	2814	2817	2818	rBV2	362	205	0.01%	0.002%
58	10.127	2819	2826	2837	rVB4	4200	6651	0.48%	0.067%
59	10.226	2839	2857	2877	rBV	350825	626550	45.12%	6.356%
60	10.577	2957	2966	2973	rBV7	4465	7419	0.53%	0.075%
61	10.831	3039	3045	3050	rBV4	634	965	0.07%	0.010%
62	10.918	3064	3072	3083	rVB5	3562	5799	0.42%	0.059%
63	11.088	3124	3125	3128	rBV5	309	124	0.01%	0.001%
64	11.146	3137	3143	3152	rVB4	1996	3266	0.24%	0.033%
65	11.252	3164	3176	3202	rBV	558393	884264	63.68%	8.971%
66	11.513	3255	3257	3260	rBV2	377	231	0.02%	0.002%
67	11.628	3281	3293	3318	rBV	690092	1086478	78.24%	11.022%
68	11.789	3336	3343	3352	rVB2	9865	14065	1.01%	0.143%
69	12.352	3511	3518	3526	rBV9	2870	4231	0.30%	0.043%
70	12.525	3570	3572	3575	rBV	407	233	0.02%	0.002%
71	12.586	3590	3591	3592	rBV	614	212	0.02%	0.002%
72	12.654	3610	3612	3615	rBV	304	201	0.01%	0.002%
73	13.088	3746	3747	3750	rBV2	394	180	0.01%	0.002%
74	13.233	3788	3792	3795	rBV2	393	351	0.03%	0.004%
75	13.757	3954	3955	3958	rBV	244	130	0.01%	0.001%

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Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M

Title : VOC Analysis

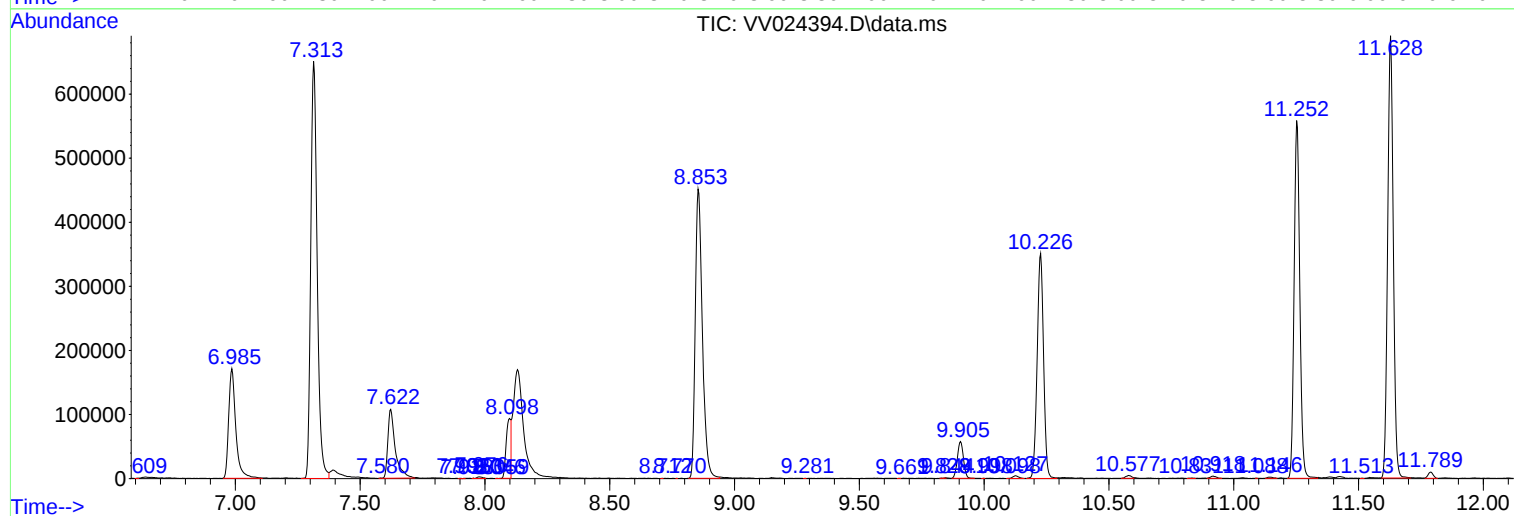
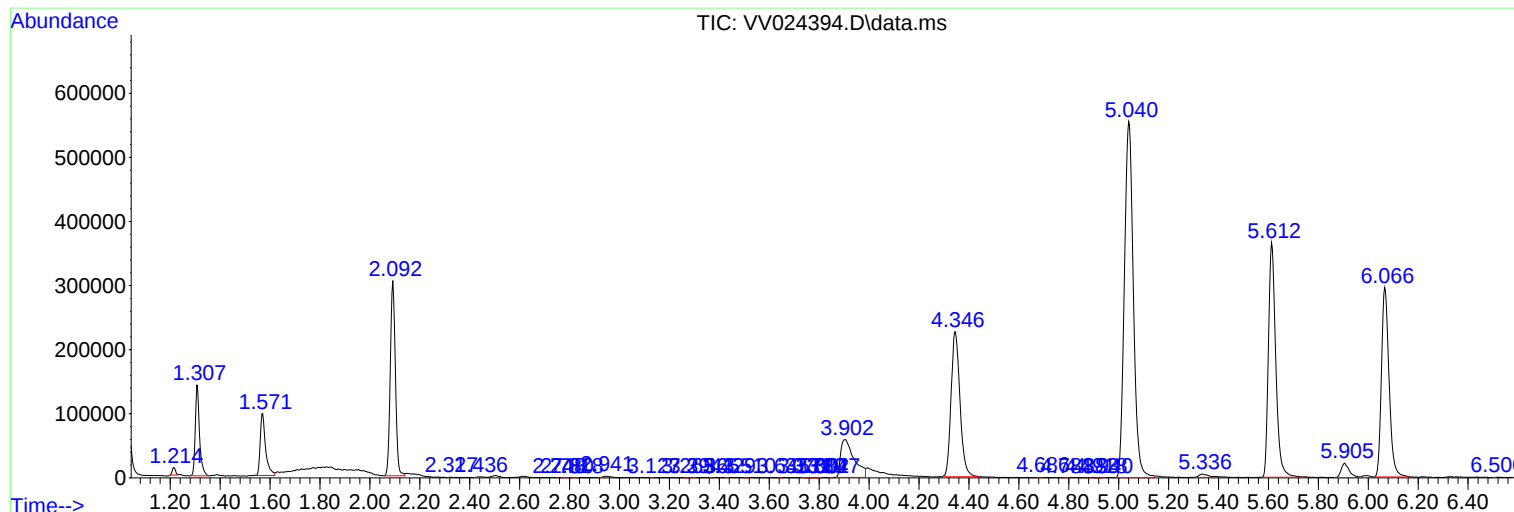
Sum of corrected areas: 9857276

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ClientSampleId :
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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



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ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_V
ClientSampleId :
DBLZ9ME

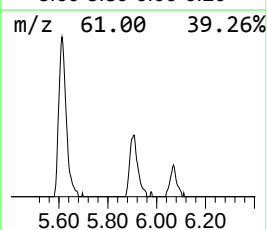
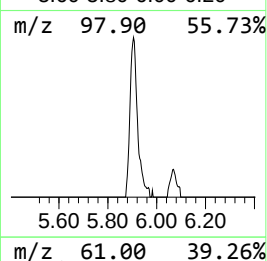
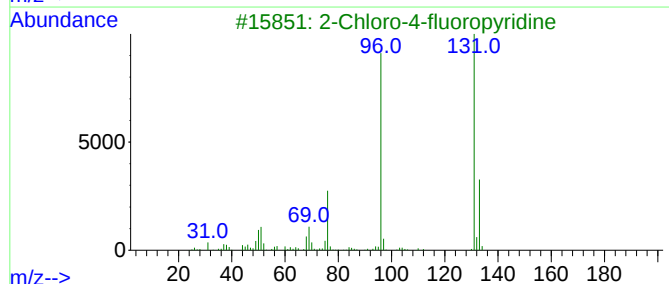
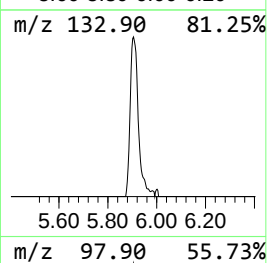
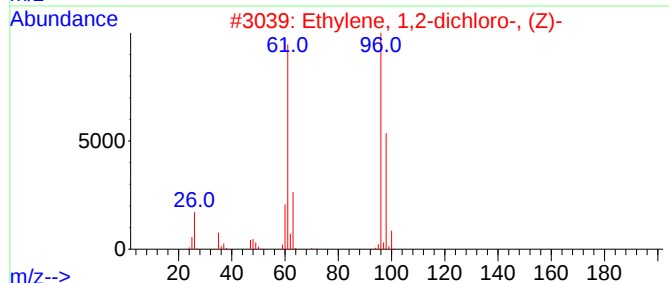
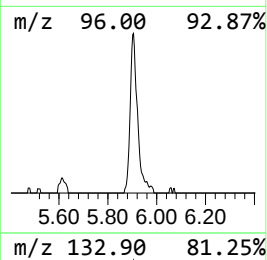
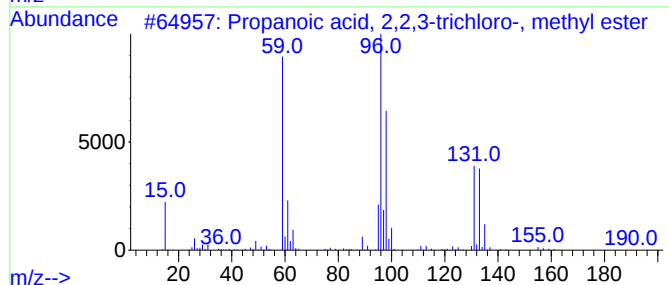
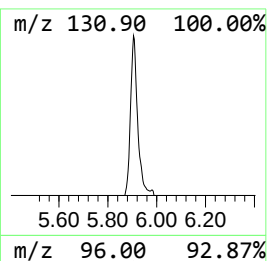
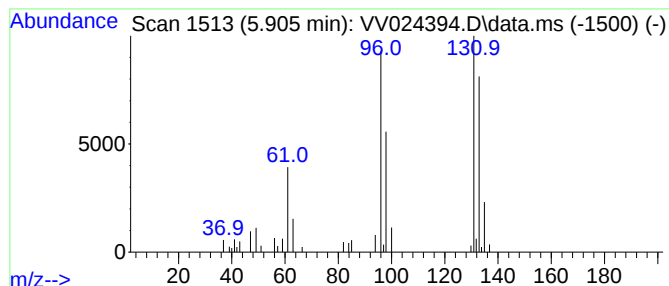
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_V\Method\SFAMVLM123121WMA.M
Quant Title : VOC Analysis

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

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.905	3.38 ug/L	50494	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			Ethylene, 1,2-dichloro-, (Z)-	96	C2H2Cl2	000156-59-2	35
3			2-Chloro-4-fluoropyridine	131	C5H3ClFN	1000484-44-8	23
4			4-Chloro-3-fluoropyridine	131	C5H3ClFN	002546-56-7	22
5			Ethane, 1,1,1,2-tetrachloro-	166	C2H2Cl4	000630-20-6	17



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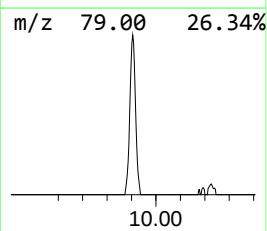
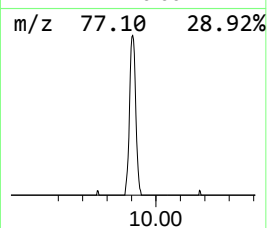
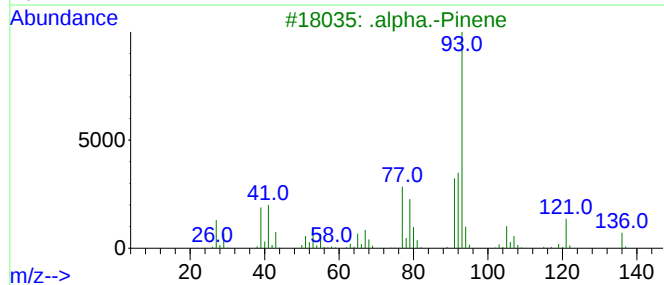
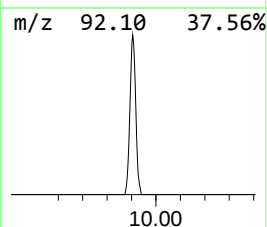
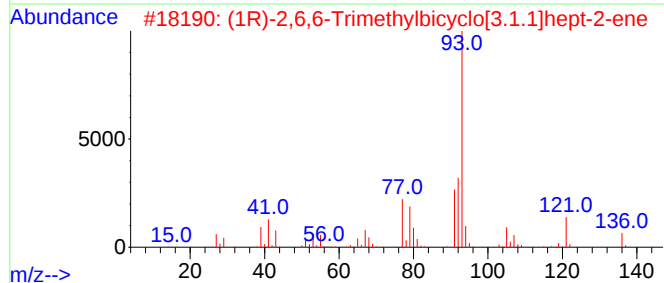
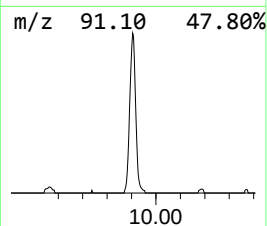
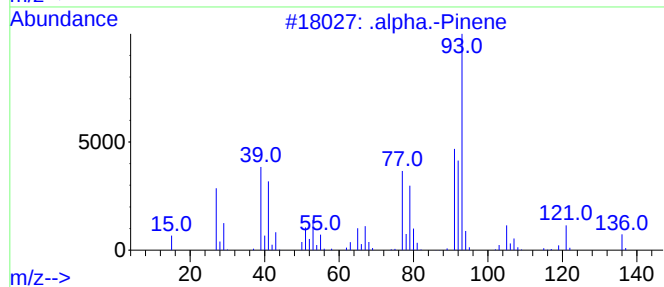
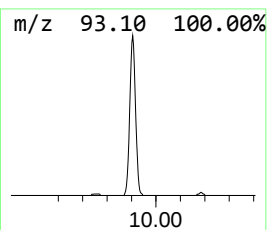
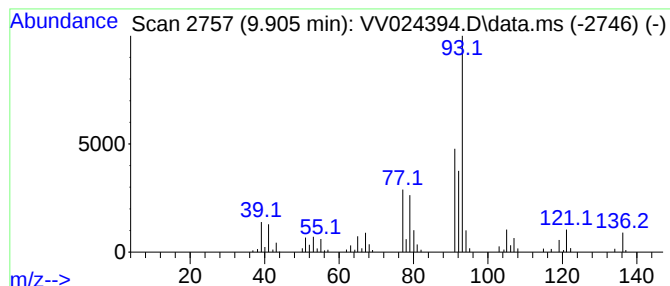
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 .alpha.-Pinene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.905	5.37 ug/L	96400	Chlorobenzene-d5	8.853

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.		.alpha.-Pinene	136	C10H16	000080-56-8	95
2	(1R)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-70-8	94
3	.		.alpha.-Pinene	136	C10H16	000080-56-8	93
4	.		.beta.-Pinene	136	C10H16	000127-91-3	90
5	(1S)-2,6,6-Trimethylbicyclo[3.1....			136	C10H16	007785-26-4	90



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Propanoic acid,...	5.905	3.4	ug/L	50494	1	5.612	746690	50.0
.alpha.-Pinene	9.905	5.4	ug/L	96400	2	8.853	897315	50.0