

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU082922\
 Data File : VU050490.D
 Acq On : 29 Aug 2022 17:33
 Operator : SY/MD
 Sample : N4399-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVC9

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_U\Method\SFAMULM082422WMA.M
 Title : VOC Analysis

Signal : TIC: VU050490.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.903	167	175	196	rVB	135139	183782	12.64%	1.911%
2	2.562	370	380	392	rVB2	17656	28994	1.99%	0.301%
3	2.636	392	403	418	rBV	12810	23396	1.61%	0.243%
4	2.732	429	433	434	rBV2	362	223	0.02%	0.002%
5	2.784	443	449	459	rVB4	1179	1952	0.13%	0.020%
6	2.951	497	501	503	rBV2	640	474	0.03%	0.005%
7	3.041	523	529	530	rBV2	1326	1232	0.08%	0.013%
8	3.141	556	560	563	rBV	260	193	0.01%	0.002%
9	3.173	568	570	571	rBV2	453	209	0.01%	0.002%
10	3.182	571	573	576	rVV2	260	185	0.01%	0.002%
11	3.549	682	687	692	rVB	189	174	0.01%	0.002%
12	3.575	692	695	697	rBV2	515	373	0.03%	0.004%
13	3.674	721	726	730	rBV2	179	167	0.01%	0.002%
14	3.825	768	773	777	rBV2	202	204	0.01%	0.002%
15	4.311	920	924	931	rVB2	225	243	0.02%	0.003%
16	4.539	993	995	1000	rVB2	233	177	0.01%	0.002%
17	4.629	1000	1023	1063	rBV	147429	417517	28.72%	4.340%
18	5.063	1141	1158	1179	rBV	236562	526976	36.25%	5.478%
19	5.247	1213	1215	1219	rVB2	432	252	0.02%	0.003%
20	5.292	1219	1229	1238	rBV2	1713	2970	0.20%	0.031%
21	5.369	1248	1253	1267	rVB3	996	1547	0.11%	0.016%
22	5.616	1327	1330	1334	rBV	435	352	0.02%	0.004%
23	5.726	1342	1364	1395	rBV2	476651	1289142	88.67%	13.402%
24	5.912	1420	1422	1426	rVB2	281	180	0.01%	0.002%
25	5.967	1435	1439	1441	rBV2	512	374	0.03%	0.004%
26	6.031	1456	1459	1464	rVV2	295	195	0.01%	0.002%
27	6.067	1464	1470	1474	rVB3	253	251	0.02%	0.003%
28	6.121	1483	1487	1488	rBV2	442	335	0.02%	0.003%
29	6.150	1493	1496	1498	rBV3	296	167	0.01%	0.002%
30	6.250	1513	1527	1553	rBV	322746	621000	42.72%	6.456%
31	6.530	1606	1614	1615	rBV3	844	890	0.06%	0.009%
32	6.597	1630	1635	1638	rBV3	419	352	0.02%	0.004%
33	6.690	1649	1664	1683	rBV	309673	599897	41.26%	6.236%
34	6.787	1692	1694	1697	rBV3	417	211	0.01%	0.002%
35	6.886	1722	1725	1727	rVV2	289	217	0.01%	0.002%
36	6.903	1727	1730	1731	rVV	431	239	0.02%	0.002%

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 Title : VOC Analysis

37	6.919	1731	1735	1741	rVB2	887	941	0.06%	0.010%
38	6.989	1750	1757	1760	rBV	160	216	0.01%	0.002%
39	7.102	1788	1792	1796	rVB2	287	269	0.02%	0.003%
40	7.163	1805	1811	1813	rBV2	292	280	0.02%	0.003%
41	7.343	1864	1867	1872	rVB	285	221	0.02%	0.002%
42	7.411	1882	1888	1891	rBV2	198	252	0.02%	0.003%
43	7.439	1894	1897	1899	rVV2	286	229	0.02%	0.002%
44	7.452	1899	1901	1908	rVB2	492	300	0.02%	0.003%
45	7.594	1942	1945	1950	rVB2	207	172	0.01%	0.002%
46	7.780	2000	2003	2007	rVB2	297	163	0.01%	0.002%
47	7.812	2007	2013	2018	rBV3	401	468	0.03%	0.005%
48	7.899	2026	2040	2062	rBV	370202	650884	44.77%	6.767%
49	8.218	2136	2139	2142	rBV3	214	172	0.01%	0.002%
50	8.398	2192	2195	2199	rVB2	365	298	0.02%	0.003%
51	8.430	2199	2205	2208	rBV2	330	359	0.02%	0.004%
52	8.552	2230	2243	2258	rBV	857403	1453799	100.00%	15.114%
53	8.636	2258	2269	2311	rVB2	360217	799544	55.00%	8.312%
54	8.947	2364	2366	2369	rVB2	555	278	0.02%	0.003%
55	8.970	2369	2373	2381	rVV	325	382	0.03%	0.004%
56	9.044	2393	2396	2398	rBV2	359	189	0.01%	0.002%
57	9.118	2417	2419	2425	rVB2	469	305	0.02%	0.003%
58	9.295	2470	2474	2476	rBV2	282	220	0.02%	0.002%
59	9.417	2499	2512	2541	rBV	459447	771756	53.09%	8.023%
60	9.533	2541	2548	2557	rVB9	3316	5626	0.39%	0.058%
61	9.722	2601	2607	2614	rVB5	1588	2132	0.15%	0.022%
62	9.864	2648	2651	2655	rVB2	242	164	0.01%	0.002%
63	9.906	2662	2664	2670	rVB2	245	184	0.01%	0.002%
64	9.941	2670	2675	2676	rBV	193	183	0.01%	0.002%
65	9.976	2682	2686	2689	rBV2	185	197	0.01%	0.002%
66	10.134	2729	2735	2736	rBV4	882	799	0.05%	0.008%
67	10.291	2772	2784	2796	rBV	40875	67153	4.62%	0.698%
68	10.349	2796	2802	2811	rVB4	1853	3032	0.21%	0.032%
69	10.555	2863	2866	2869	rBV2	413	212	0.01%	0.002%
70	10.590	2874	2877	2881	rBV	304	220	0.02%	0.002%
71	10.758	2915	2929	2955	rBV	458798	742899	51.10%	7.723%
72	10.931	2975	2983	2994	rVB2	5555	9027	0.62%	0.094%
73	11.002	3000	3005	3007	rBV2	201	201	0.01%	0.002%
74	11.057	3013	3022	3029	rBV5	1489	2255	0.16%	0.023%
75	11.214	3066	3071	3074	rBV2	231	275	0.02%	0.003%
76	11.311	3097	3101	3104	rBV2	261	235	0.02%	0.002%

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 Title : VOC Analysis

77	11.481	3150	3154	3156	rBV2	697	642	0.04%	0.007%
78	11.687	3216	3218	3224	rVB3	501	456	0.03%	0.005%
79	11.748	3234	3237	3239	rBV2	234	174	0.01%	0.002%
80	11.812	3244	3257	3273	rBV	339150	545212	37.50%	5.668%
81	12.066	3327	3336	3343	rBV3	10093	17071	1.17%	0.177%
82	12.115	3343	3351	3362	rVB2	33434	53604	3.69%	0.557%
83	12.192	3362	3375	3401	rBV2	419982	775718	53.36%	8.064%
84	12.401	3438	3440	3445	rVB3	400	296	0.02%	0.003%
85	12.449	3452	3455	3458	rVB2	316	245	0.02%	0.003%
86	12.468	3458	3461	3464	rVB2	301	179	0.01%	0.002%
87	12.574	3491	3494	3495	rBV	268	171	0.01%	0.002%
88	12.629	3509	3511	3516	rVB3	329	254	0.02%	0.003%
89	12.680	3522	3527	3530	rBV2	376	370	0.03%	0.004%
90	12.700	3530	3533	3535	rVV2	405	185	0.01%	0.002%
91	12.754	3546	3550	3553	rBV2	552	442	0.03%	0.005%
92	12.796	3560	3563	3564	rBV	331	208	0.01%	0.002%
93	12.886	3588	3591	3592	rBV	351	224	0.02%	0.002%
94	12.899	3592	3595	3597	rVV2	671	462	0.03%	0.005%
95	13.295	3715	3718	3722	rBV	361	205	0.01%	0.002%
96	13.571	3802	3804	3808	rBV2	301	215	0.01%	0.002%
97	13.825	3880	3883	3885	rBV2	466	334	0.02%	0.003%
98	14.111	3970	3972	3977	rBV	394	327	0.02%	0.003%
99	15.526	4410	4412	4414	rBV2	645	382	0.03%	0.004%
100	15.577	4426	4428	4429	rBV2	602	233	0.02%	0.002%

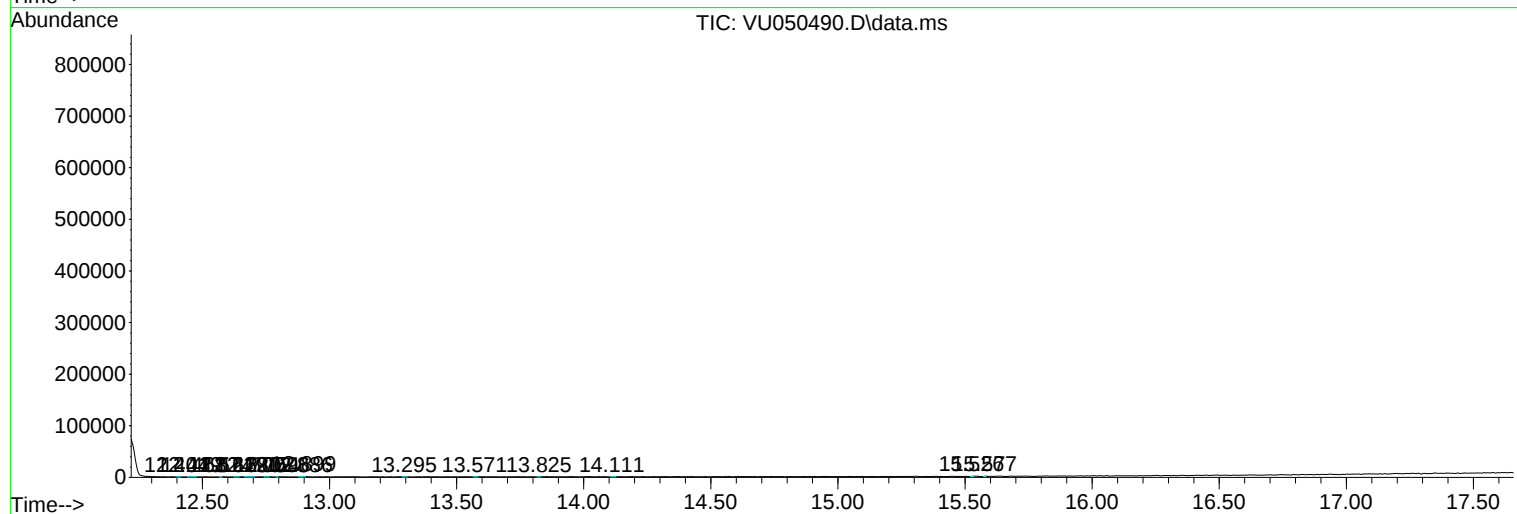
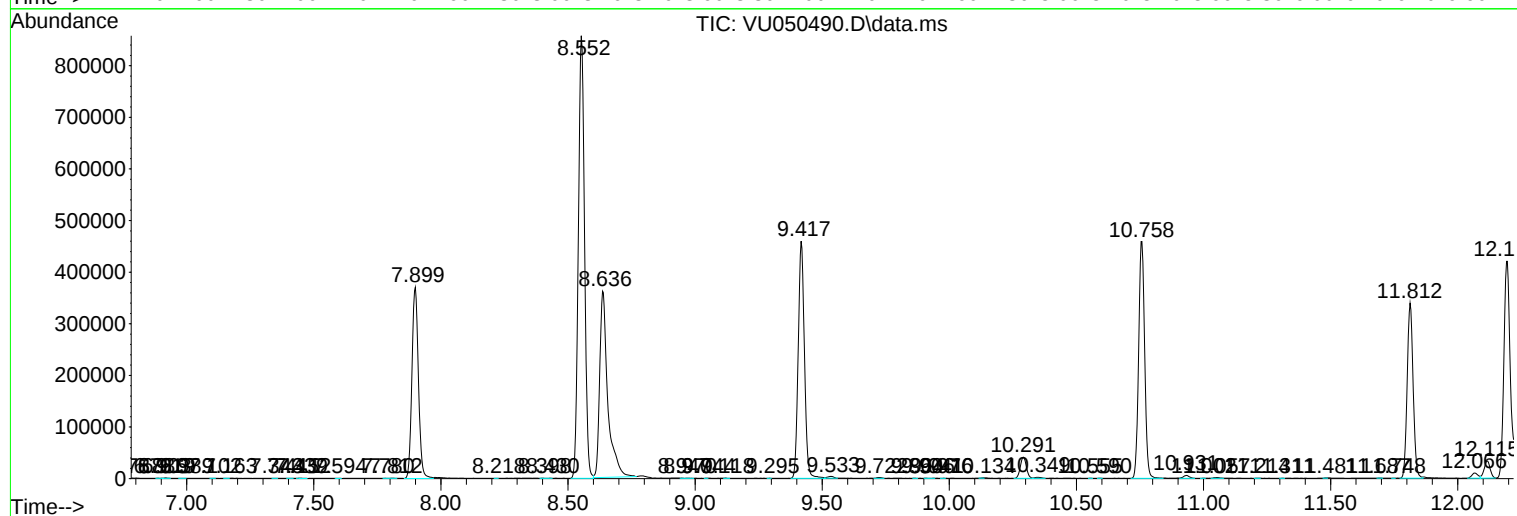
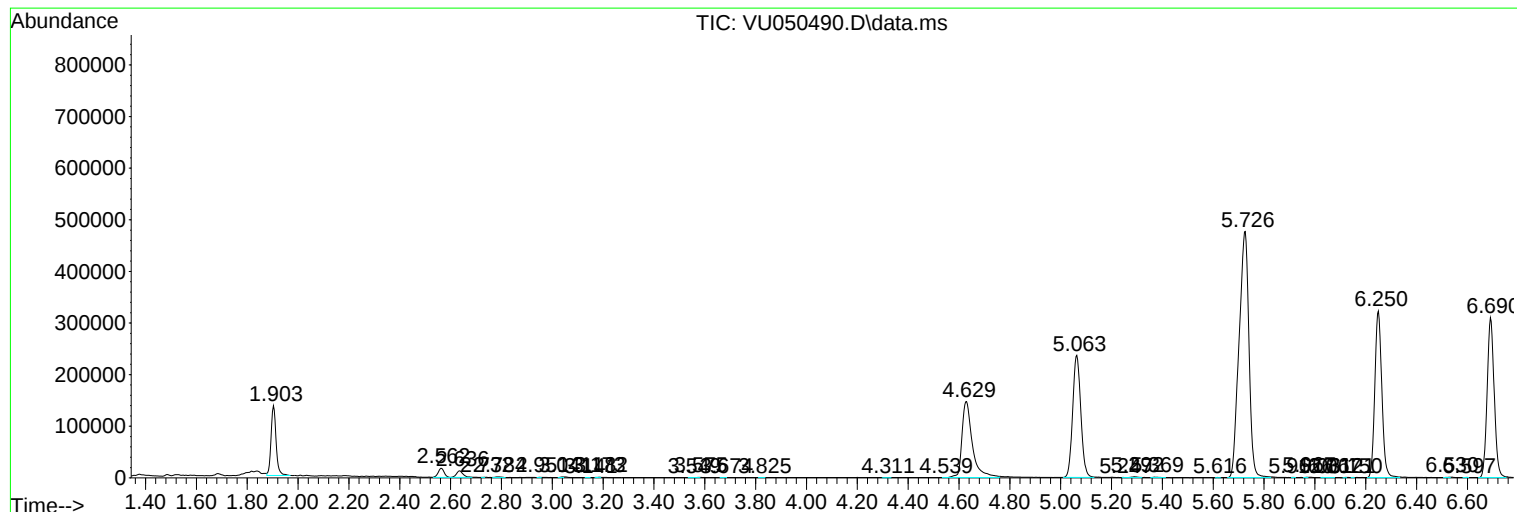
Sum of corrected areas: 9619142

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
Quant Title : VOC Analysis

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



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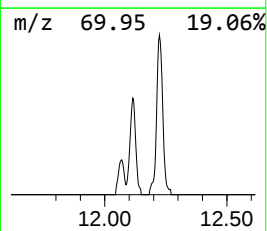
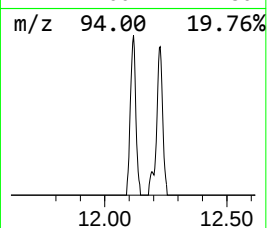
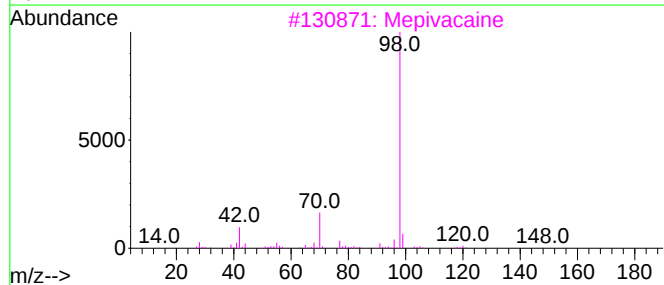
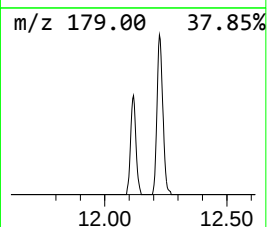
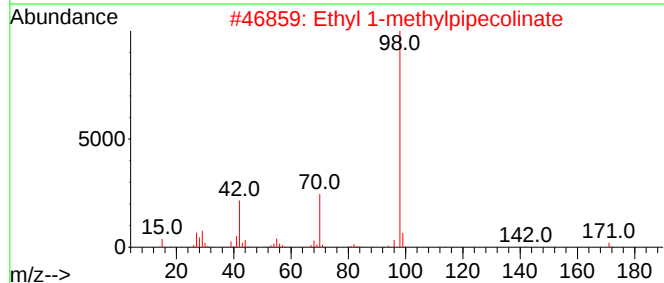
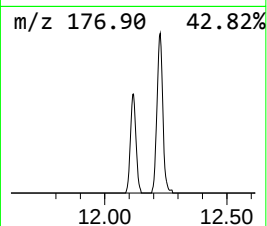
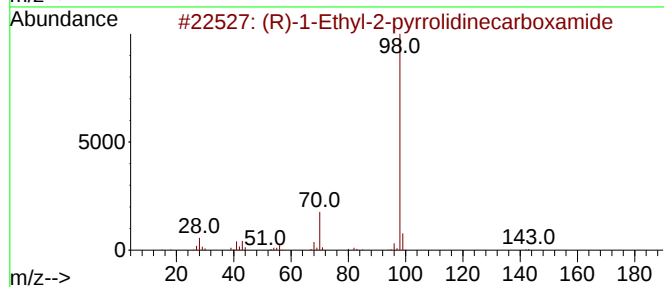
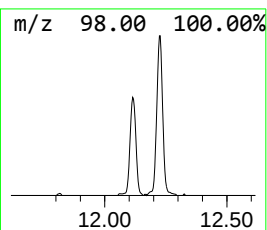
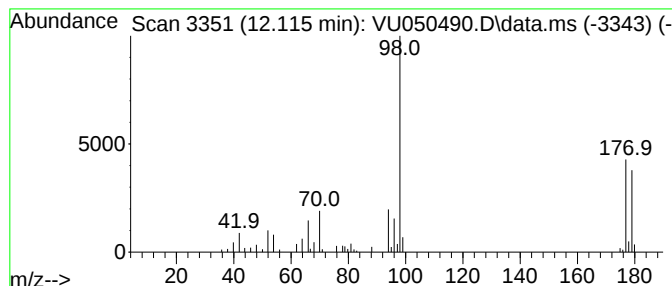
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM082422WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 unknown-01 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.115	4.92 ug/L	53604	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	(R)-1-Ethyl-2-pyrrolidinecarboxa...	142	C7H14N2O	1000237-69-9	25		
2	Ethyl 1-methylpipercolinate	171	C9H17N02	030727-18-5	25		
3	Mepivacaine	246	C15H22N2O	000096-88-8	25		
4	2-Sec-Butylcyclohexanone	154	C10H18O	014765-30-1	25		
5	[1,1'-Bicyclohexyl]-2-one	180	C12H20O	000090-42-6	25		



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	12.115	4.9	ug/L	53604	3	11.812	545212	50.0