

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046191.D
 Acq On : 08 Dec 2021 21:28
 Operator : SY/MD
 Sample : M4983-02
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW5N0

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046191.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.604	74	82	98	rVB2	189417	227688	11.64%	2.078%
2	1.938	171	186	202	rBV2	253692	403900	20.64%	3.686%
3	2.173	254	259	266	rVB4	2179	2993	0.15%	0.027%
4	2.208	266	270	275	rVV2	539	665	0.03%	0.006%
5	2.372	318	321	324	rBV2	437	342	0.02%	0.003%
6	2.398	324	329	337	rVB2	358	520	0.03%	0.005%
7	2.456	343	347	352	rBV2	557	690	0.04%	0.006%
8	2.501	357	361	369	rBV2	425	596	0.03%	0.005%
9	2.575	369	384	409	rBV2	154368	279713	14.30%	2.553%
10	2.803	452	455	461	rVB3	337	360	0.02%	0.003%
11	2.903	482	486	491	rBV2	324	428	0.02%	0.004%
12	2.958	496	503	505	rBV2	388	408	0.02%	0.004%
13	3.044	525	530	532	rBV3	786	775	0.04%	0.007%
14	3.160	562	566	569	rBV2	666	479	0.02%	0.004%
15	3.192	569	576	584	rVV4	1658	2442	0.12%	0.022%
16	3.360	616	628	643	rVB	29087	56286	2.88%	0.514%
17	3.472	658	663	670	rVB	410	456	0.02%	0.004%
18	3.543	679	685	688	rBV2	511	512	0.03%	0.005%
19	3.569	688	693	696	rBV	393	378	0.02%	0.003%
20	3.787	757	761	765	rBV	445	444	0.02%	0.004%
21	3.877	769	789	816	rBV	644880	1536033	78.51%	14.018%
22	4.205	887	891	895	rBV2	469	467	0.02%	0.004%
23	4.671	1010	1036	1063	rBV2	800216	1956524	100.00%	17.855%
24	5.067	1143	1159	1181	rBV	126561	290861	14.87%	2.654%
25	5.199	1196	1200	1202	rBV2	716	628	0.03%	0.006%
26	5.321	1220	1238	1259	rVV	370241	829501	42.40%	7.570%
27	5.652	1335	1341	1344	rBV3	522	441	0.02%	0.004%
28	5.729	1344	1365	1379	rBV2	267237	725131	37.06%	6.618%
29	6.102	1477	1481	1485	rBV2	404	381	0.02%	0.003%
30	6.250	1514	1527	1547	rBV	246391	465547	23.79%	4.249%
31	6.546	1606	1619	1633	rVB2	44230	84914	4.34%	0.775%
32	6.597	1633	1635	1641	rVB	472	377	0.02%	0.003%
33	6.636	1641	1647	1649	rBV	384	330	0.02%	0.003%
34	6.694	1651	1665	1682	rBV	167818	323133	16.52%	2.949%
35	6.877	1719	1722	1728	rBV2	399	470	0.02%	0.004%
36	6.957	1744	1747	1751	rVB	620	474	0.02%	0.004%

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 Title : VOC Analysis

37	6.986	1751	1756	1759	rBV2	416	426	0.02%	0.004%
38	7.015	1761	1765	1767	rBV3	816	599	0.03%	0.005%
39	7.035	1768	1771	1773	rBV3	885	680	0.03%	0.006%
40	7.510	1915	1919	1923	rBV	439	435	0.02%	0.004%
41	7.568	1923	1937	1951	rBV	96966	166819	8.53%	1.522%
42	7.620	1951	1953	1956	rVB2	693	385	0.02%	0.004%
43	7.835	2013	2020	2027	rBV2	461	560	0.03%	0.005%
44	7.900	2027	2040	2057	rBV	334292	588360	30.07%	5.369%
45	8.083	2090	2097	2099	rVB3	341	357	0.02%	0.003%
46	8.099	2099	2102	2107	rBV2	376	381	0.02%	0.003%
47	8.179	2116	2127	2143	rBV	66939	111125	5.68%	1.014%
48	8.318	2165	2170	2173	rBV2	386	388	0.02%	0.004%
49	8.353	2178	2181	2184	rBV2	403	337	0.02%	0.003%
50	8.404	2193	2197	2202	rVB4	1104	1114	0.06%	0.010%
51	8.472	2207	2218	2230	rBV2	5802	10868	0.56%	0.099%
52	8.555	2233	2244	2256	rVB3	29533	50454	2.58%	0.460%
53	8.633	2256	2268	2304	rBV	238766	438152	22.39%	3.999%
54	8.964	2367	2371	2374	rBV2	432	346	0.02%	0.003%
55	9.041	2391	2395	2404	rBV	482	709	0.04%	0.006%
56	9.276	2465	2468	2474	rVB	497	397	0.02%	0.004%
57	9.417	2500	2512	2536	rBV	350832	591582	30.24%	5.399%
58	9.571	2548	2560	2572	rBV	5073	7806	0.40%	0.071%
59	9.633	2575	2579	2584	rBV2	358	403	0.02%	0.004%
60	9.694	2591	2598	2606	rVB3	892	1463	0.07%	0.013%
61	10.025	2697	2701	2705	rBV	465	374	0.02%	0.003%
62	10.102	2718	2725	2734	rVB4	1114	1701	0.09%	0.016%
63	10.485	2839	2844	2851	rVB	728	917	0.05%	0.008%
64	10.571	2868	2871	2874	rBV	407	322	0.02%	0.003%
65	10.591	2874	2877	2885	rVB2	422	437	0.02%	0.004%
66	10.671	2895	2902	2908	rBV3	1049	1451	0.07%	0.013%
67	10.758	2916	2929	2949	rBV	260050	419234	21.43%	3.826%
68	10.893	2957	2971	2983	rBV2	8577	14525	0.74%	0.133%
69	11.031	3009	3014	3018	rVB2	339	362	0.02%	0.003%
70	11.079	3025	3029	3030	rBV	532	356	0.02%	0.003%
71	11.231	3069	3076	3078	rBV3	586	684	0.03%	0.006%
72	11.295	3085	3096	3104	rBV2	5138	7444	0.38%	0.068%
73	11.369	3116	3119	3124	rVB	486	479	0.02%	0.004%
74	11.395	3124	3127	3130	rBV	494	430	0.02%	0.004%
75	11.469	3140	3150	3160	rBV3	9131	13511	0.69%	0.123%
76	11.726	3227	3230	3236	rVB	539	492	0.03%	0.004%

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77	11.758	3236	3240	3245	rBV2	388	393	0.02%	0.004%
78	11.813	3245	3257	3272	rBV	404732	639336	32.68%	5.835%
79	11.896	3276	3283	3292	rVB2	3683	5386	0.28%	0.049%
80	11.967	3300	3305	3306	rBV	553	439	0.02%	0.004%
81	12.041	3325	3328	3331	rVV	436	367	0.02%	0.003%
82	12.067	3331	3336	3337	rVV4	1102	1053	0.05%	0.010%
83	12.096	3340	3345	3354	rVB3	3188	4418	0.23%	0.040%
84	12.192	3363	3375	3394	rVB	373900	603923	30.87%	5.511%
85	12.327	3414	3417	3422	rVV2	525	415	0.02%	0.004%
86	12.481	3453	3465	3478	rBV	33833	55212	2.82%	0.504%
87	12.559	3485	3489	3496	rVB2	341	467	0.02%	0.004%
88	12.623	3504	3509	3513	rBV2	279	331	0.02%	0.003%
89	12.774	3546	3556	3565	rVB	4050	6197	0.32%	0.057%
90	12.813	3565	3568	3573	rBV	253	324	0.02%	0.003%
91	12.874	3582	3587	3590	rBV	371	373	0.02%	0.003%
92	13.108	3656	3660	3663	rVB	553	422	0.02%	0.004%
93	13.327	3725	3728	3737	rVB2	543	597	0.03%	0.005%
94	13.600	3809	3813	3819	rBV2	395	483	0.02%	0.004%
95	13.857	3889	3893	3896	rBV	432	372	0.02%	0.003%
96	14.211	3999	4003	4008	rVB2	380	370	0.02%	0.003%
97	14.356	4045	4048	4054	rBV2	549	518	0.03%	0.005%
98	14.472	4079	4084	4089	rBV2	516	732	0.04%	0.007%
99	14.575	4108	4116	4124	rBV3	1811	3124	0.16%	0.029%
100	16.475	4705	4707	4710	rBV3	643	342	0.02%	0.003%

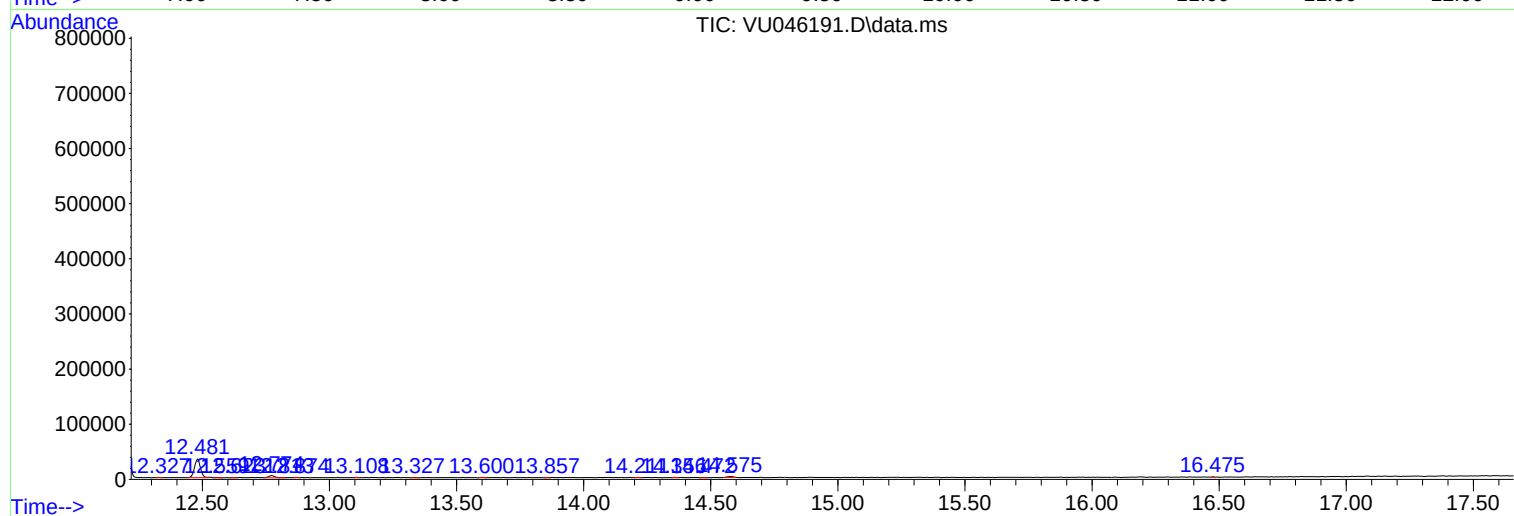
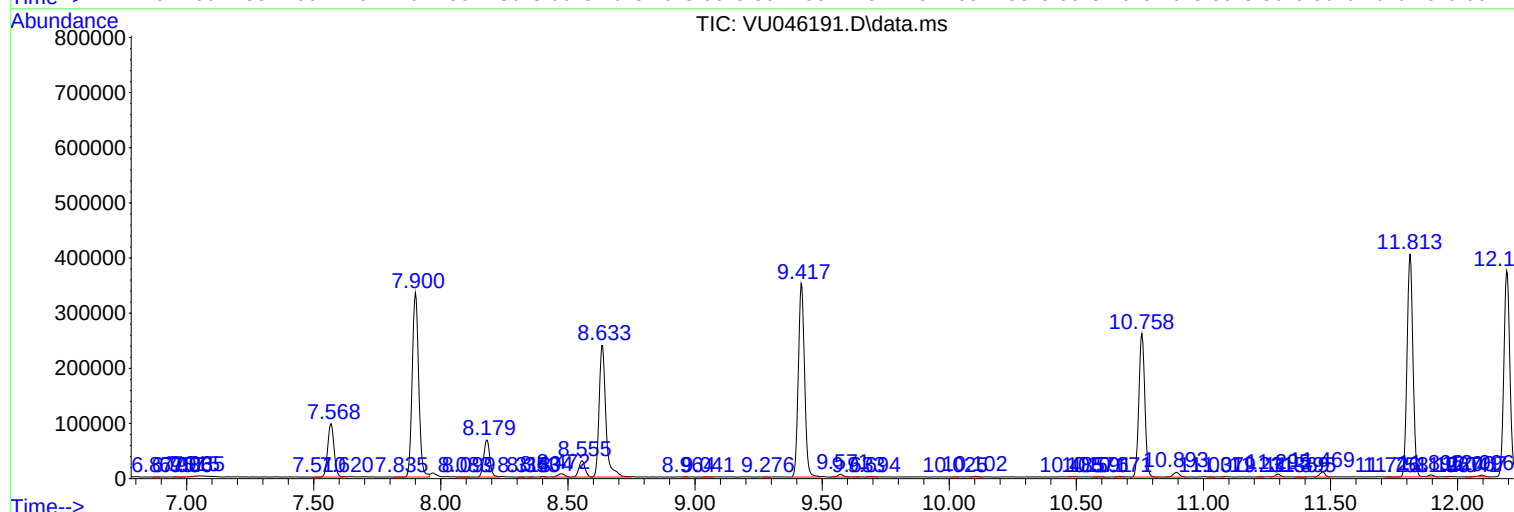
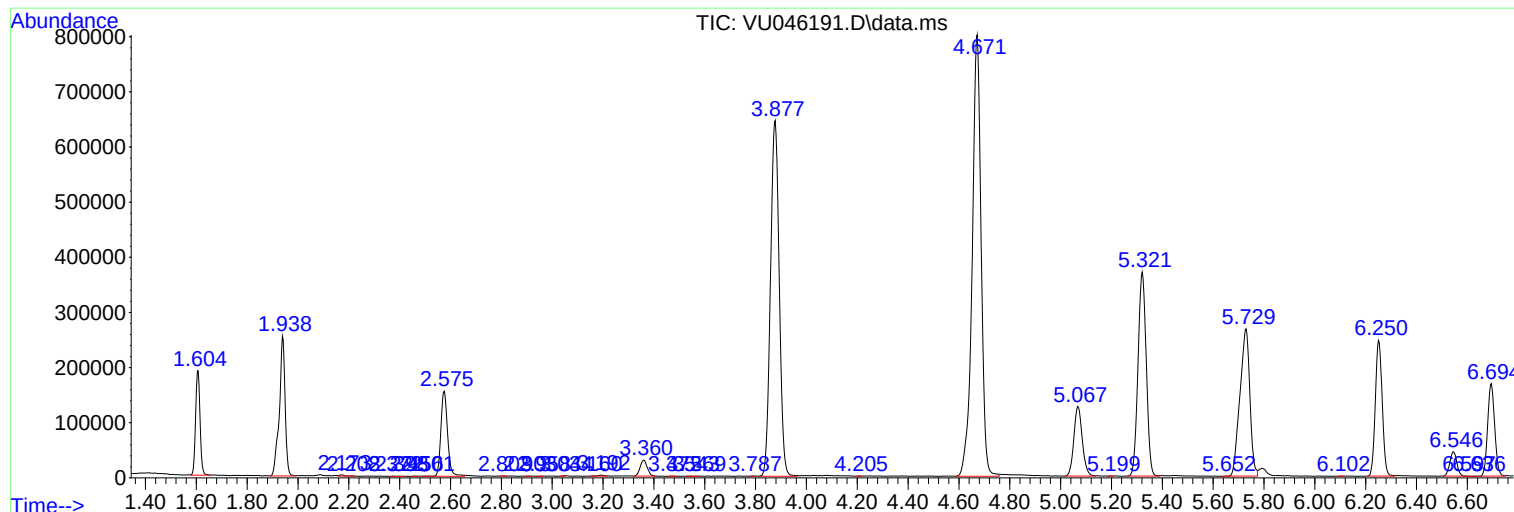
Sum of corrected areas: 10957746

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



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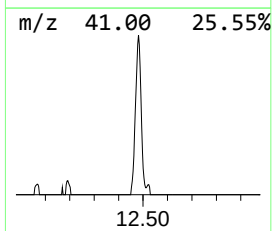
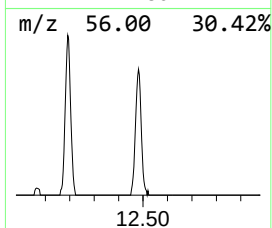
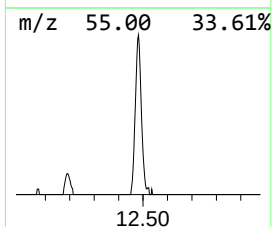
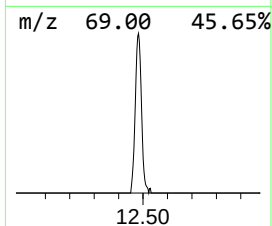
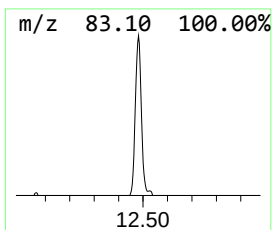
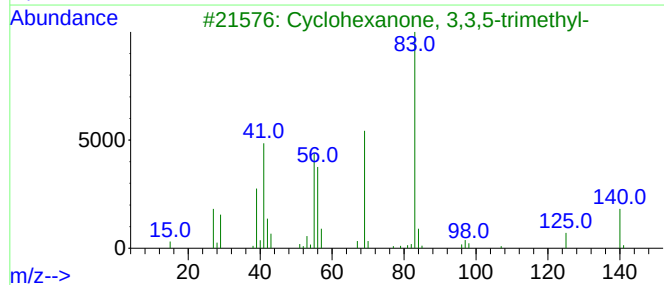
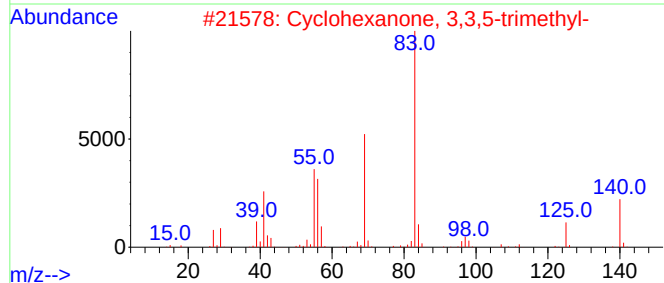
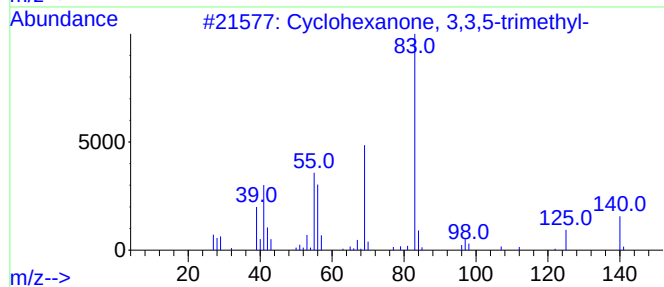
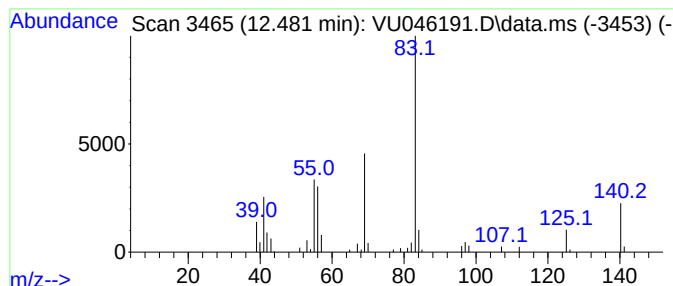
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Cyclohexanone, 3,3,5-trimet... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.481	4.32 ug/L	55212	1,4-Dichlorobenzene-d4	11.813

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	96
2			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	93
3			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
4			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	91
5			1H-1,2,4-Triazole, 3-(2-methylpr...	125	C6H11N3	040515-29-5	47



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone, ...	12.481	4.3	ug/L	55212	3	11.813	639336	50.0