

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU092322\
 Data File : VU050917.D
 Acq On : 23 Sep 2022 14:08
 Operator : JC/MD
 Sample : N4650-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXYZ6

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\SFAMULM092022WMA.M

Title : VOC Analysis

Signal : TIC: VU050917.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	73	82	101	rBV2	603315	761601	16.97%	3.102%
2	1.928	169	183	207	rVB2	812186	1319743	29.41%	5.376%
3	2.568	369	382	398	rBV2	364249	632005	14.09%	2.575%
4	2.781	438	448	449	rBV4	1589	1779	0.04%	0.007%
5	2.790	449	451	456	rVV5	982	942	0.02%	0.004%
6	2.938	493	497	500	rBV2	451	403	0.01%	0.002%
7	3.047	521	531	540	rVB3	5516	9273	0.21%	0.038%
8	3.195	565	577	605	rVB4	6558	22008	0.49%	0.090%
9	3.356	614	627	647	rBV	59387	115934	2.58%	0.472%
10	3.436	651	652	656	rVB2	564	284	0.01%	0.001%
11	3.472	656	663	666	rBV3	642	685	0.02%	0.003%
12	3.533	679	682	685	rVB	516	266	0.01%	0.001%
13	3.562	685	691	694	rBV3	330	325	0.01%	0.001%
14	3.697	729	733	737	rBV2	324	304	0.01%	0.001%
15	3.768	751	755	760	rBV2	322	313	0.01%	0.001%
16	3.867	765	786	813	rBV	1627409	3832180	85.41%	15.611%
17	4.362	937	940	948	rVB4	541	649	0.01%	0.003%
18	4.417	950	957	960	rBV3	440	385	0.01%	0.002%
19	4.443	962	965	969	rVB3	321	253	0.01%	0.001%
20	4.520	987	989	993	rBV4	384	255	0.01%	0.001%
21	4.568	999	1004	1007	rBV4	562	372	0.01%	0.002%
22	4.665	1007	1034	1070	rBV2	1812146	4486990	100.00%	18.278%
23	5.063	1141	1158	1187	rVB	318760	697594	15.55%	2.842%
24	5.317	1216	1237	1258	rBV	701801	1574644	35.09%	6.414%
25	5.475	1283	1286	1288	rBV	584	282	0.01%	0.001%
26	5.555	1309	1311	1315	rVB2	642	363	0.01%	0.001%
27	5.600	1322	1325	1328	rVB3	686	409	0.01%	0.002%
28	5.639	1332	1337	1341	rVB3	526	545	0.01%	0.002%
29	5.726	1341	1364	1378	rBV2	649310	1748561	38.97%	7.123%
30	6.134	1486	1491	1499	rVB3	681	840	0.02%	0.003%
31	6.250	1512	1527	1552	rBV	506253	962552	21.45%	3.921%
32	6.542	1603	1618	1634	rBV4	82991	168025	3.74%	0.684%
33	6.690	1649	1664	1684	rBV	412267	809918	18.05%	3.299%
34	6.935	1733	1740	1742	rBV3	446	465	0.01%	0.002%
35	6.986	1744	1756	1780	rVV2	10897	29062	0.65%	0.118%
36	7.189	1809	1819	1832	rVB6	2519	4465	0.10%	0.018%

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 Title : VOC Analysis

37	7.327	1858	1862	1865	rVV2	299	260	0.01%	0.001%
38	7.362	1869	1873	1876	rVB2	296	266	0.01%	0.001%
39	7.385	1876	1880	1883	rBV2	465	265	0.01%	0.001%
40	7.565	1923	1936	1963	rBV	205205	366712	8.17%	1.494%
41	7.697	1972	1977	1982	rVB5	1498	1693	0.04%	0.007%
42	7.745	1989	1992	1996	rVB2	430	385	0.01%	0.002%
43	7.806	2007	2011	2014	rVB3	640	516	0.01%	0.002%
44	7.896	2026	2039	2055	rBV	731651	1259782	28.08%	5.132%
45	8.089	2096	2099	2105	rBV3	416	345	0.01%	0.001%
46	8.179	2114	2127	2150	rBV	145660	252362	5.62%	1.028%
47	8.401	2188	2196	2209	rVB3	2696	4471	0.10%	0.018%
48	8.472	2209	2218	2229	rBV3	2633	4501	0.10%	0.018%
49	8.552	2233	2243	2255	rVB3	49539	82588	1.84%	0.336%
50	8.636	2255	2269	2304	rBV2	499212	1026278	22.87%	4.181%
51	8.861	2336	2339	2343	rVB3	639	564	0.01%	0.002%
52	8.999	2372	2382	2388	rBV5	718	1211	0.03%	0.005%
53	9.057	2396	2400	2403	rBV3	516	458	0.01%	0.002%
54	9.169	2432	2435	2438	rVB3	493	276	0.01%	0.001%
55	9.227	2448	2453	2455	rBV2	295	269	0.01%	0.001%
56	9.417	2499	2512	2536	rBV	709807	1168914	26.05%	4.762%
57	9.571	2552	2560	2575	rVB2	10367	16112	0.36%	0.066%
58	9.655	2581	2586	2588	rVB4	502	321	0.01%	0.001%
59	9.700	2593	2600	2603	rBV2	1458	1850	0.04%	0.008%
60	9.973	2681	2685	2688	rBV2	364	294	0.01%	0.001%
61	10.099	2716	2724	2733	rVB5	1828	2979	0.07%	0.012%
62	10.327	2792	2795	2800	rBV3	474	379	0.01%	0.002%
63	10.484	2836	2844	2859	rVB7	1906	3016	0.07%	0.012%
64	10.668	2897	2901	2908	rVB4	1783	2031	0.05%	0.008%
65	10.754	2914	2928	2948	rBV	591948	952194	21.22%	3.879%
66	10.896	2964	2972	2982	rVB5	3900	7026	0.16%	0.029%
67	11.005	3002	3006	3009	rBV3	320	316	0.01%	0.001%
68	11.092	3029	3033	3036	rVV4	991	748	0.02%	0.003%
69	11.208	3064	3069	3070	rVV	342	304	0.01%	0.001%
70	11.234	3071	3077	3084	rVB5	1084	1533	0.03%	0.006%
71	11.291	3085	3095	3103	rBV3	7079	10601	0.24%	0.043%
72	11.468	3139	3150	3164	rBV3	13480	21388	0.48%	0.087%
73	11.578	3179	3184	3188	rVB2	385	342	0.01%	0.001%
74	11.603	3189	3192	3197	rVB	453	361	0.01%	0.001%
75	11.693	3214	3220	3222	rBV4	879	934	0.02%	0.004%
76	11.742	3231	3235	3236	rBV	779	414	0.01%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
 Title : VOC Analysis

77	11.812	3244	3257	3274	rBV	558544	894766	19.94%	3.645%
78	11.893	3278	3282	3292	rVV4	6644	10066	0.22%	0.041%
79	11.941	3294	3297	3300	rVB5	1046	806	0.02%	0.003%
80	12.092	3330	3344	3357	rBV4	6047	11358	0.25%	0.046%
81	12.192	3360	3375	3401	rBV	631816	1027731	22.90%	4.187%
82	12.324	3413	3416	3418	rBV4	778	501	0.01%	0.002%
83	12.478	3452	3464	3486	rBV	122804	214062	4.77%	0.872%
84	12.574	3492	3494	3497	rBV2	710	462	0.01%	0.002%
85	12.934	3601	3606	3609	rBV3	485	521	0.01%	0.002%
86	13.195	3683	3687	3689	rBV2	520	426	0.01%	0.002%
87	13.224	3692	3696	3699	rVV2	613	543	0.01%	0.002%
88	13.301	3717	3720	3725	rBV3	347	303	0.01%	0.001%
89	13.327	3725	3728	3731	rBV	591	406	0.01%	0.002%
90	13.426	3756	3759	3763	rVB	666	480	0.01%	0.002%
91	13.520	3785	3788	3791	rBV3	571	418	0.01%	0.002%
92	13.619	3814	3819	3821	rBV3	467	328	0.01%	0.001%
93	13.729	3851	3853	3856	rBV2	415	280	0.01%	0.001%
94	13.822	3877	3882	3885	rBV3	512	572	0.01%	0.002%
95	13.851	3885	3891	3896	rVV5	1058	1254	0.03%	0.005%
96	14.050	3950	3953	3956	rBV	461	378	0.01%	0.002%
97	14.086	3960	3964	3967	rBV3	1171	1281	0.03%	0.005%
98	14.288	4023	4027	4029	rBV3	663	406	0.01%	0.002%
99	14.407	4061	4064	4068	rVB3	850	661	0.01%	0.003%
100	14.430	4068	4071	4072	rBV	528	321	0.01%	0.001%

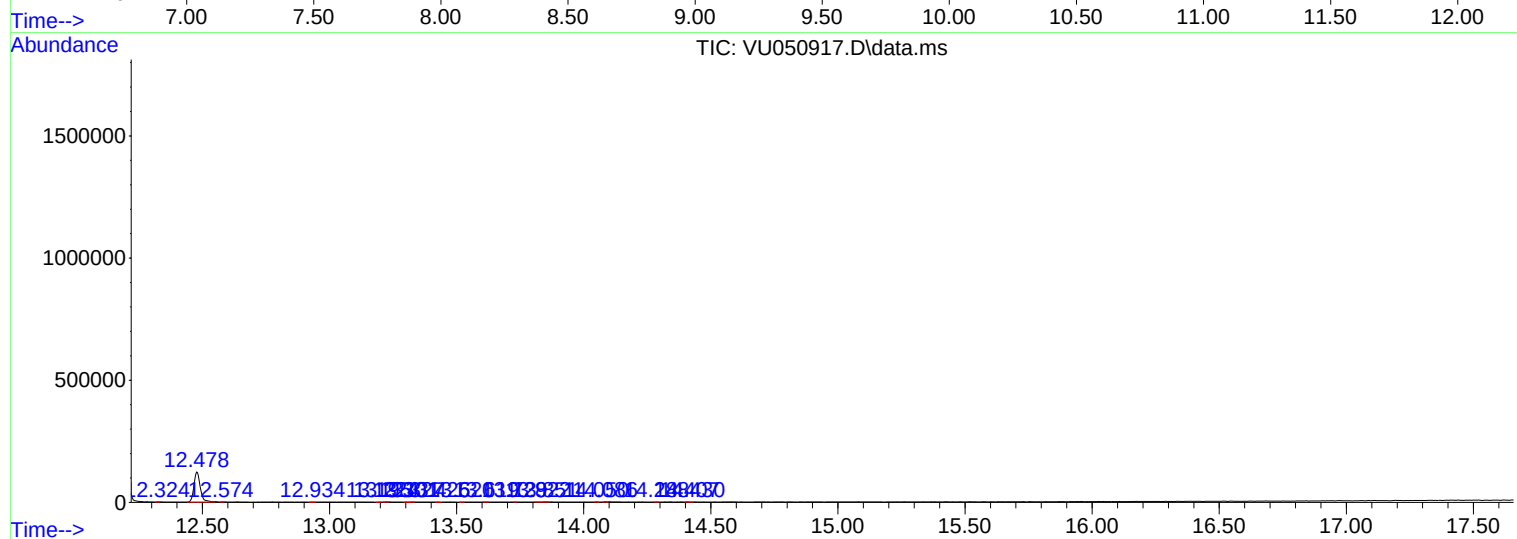
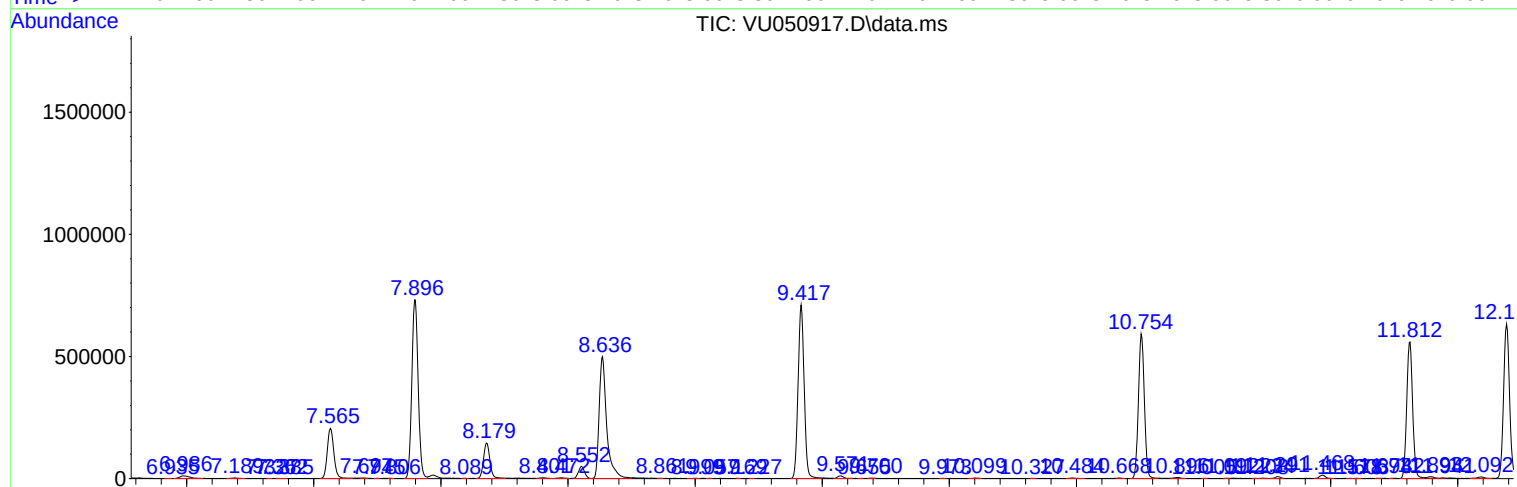
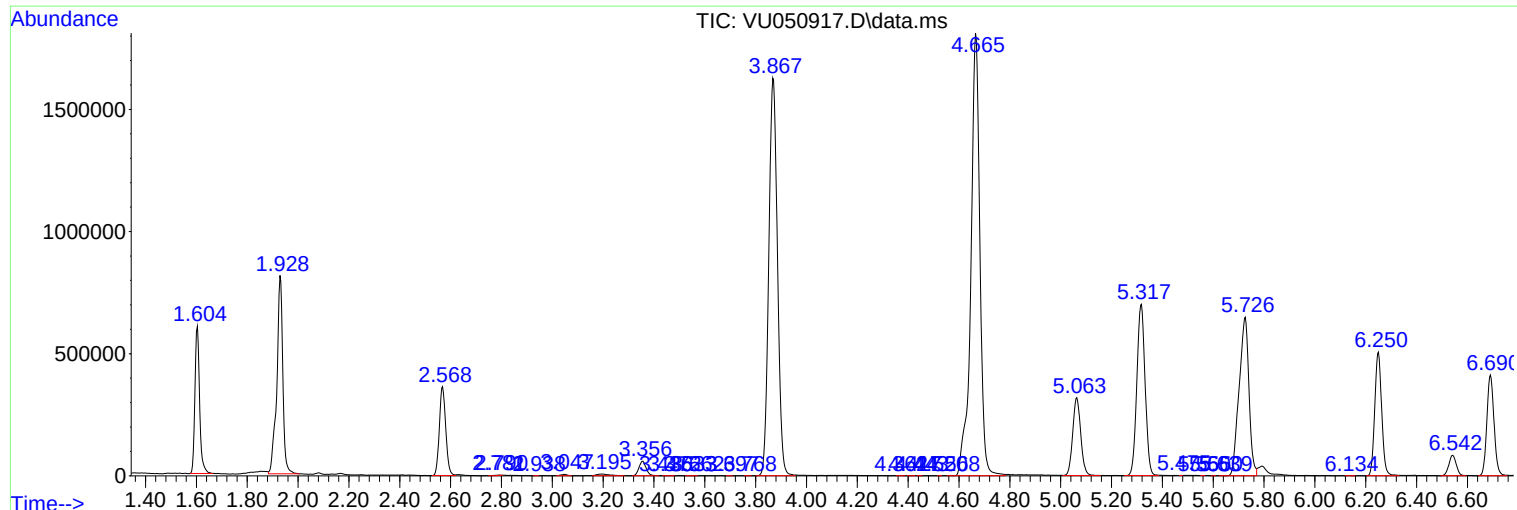
Sum of corrected areas: 24548263

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Instrument :
MSVOA_U
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EXYZ6

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

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



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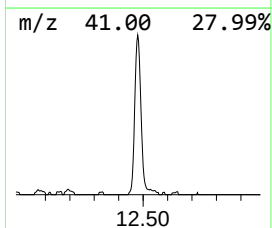
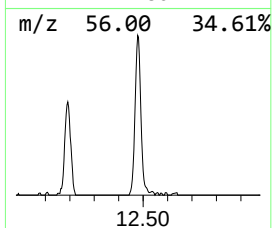
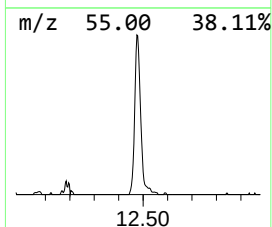
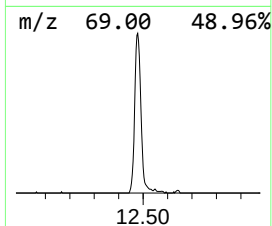
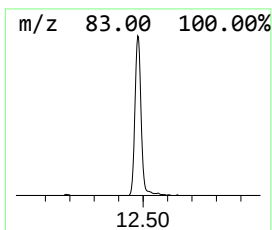
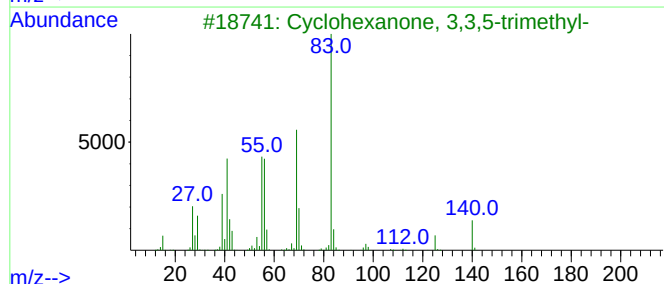
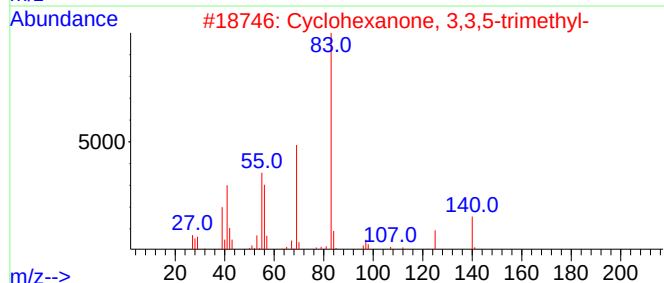
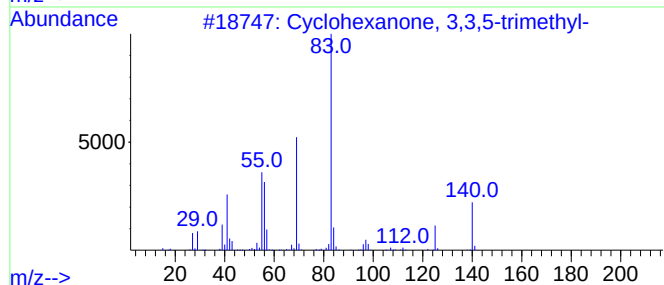
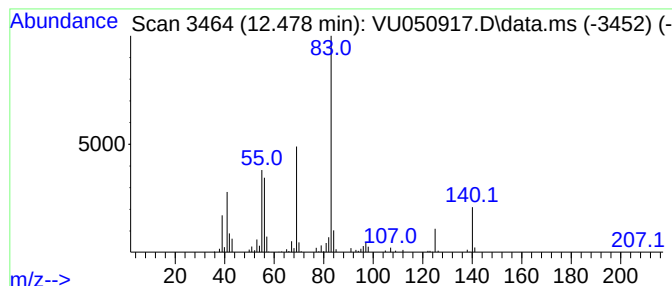
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM092022WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST11.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.
12.478	11.96 ug/L	214062	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 3,3,5-trimethyl-	140	C9H16O	000873-94-9	97
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	78
5			Cyclohexane, (2-methylpropyl)-	140	C10H20	001678-98-4	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone, ...	12.478	12.0	ug/L	214062	3	11.812	894766	50.0