

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU060922\
 Data File : VU048981.D
 Acq On : 09 Jun 2022 17:18
 Operator : SY/MD
 Sample : N3248-06
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXYX6

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\SFAMULM051622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048981.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	102	rBV2	448262	544316	14.77%	2.841%
2	1.925	167	182	210	rVB2	477683	795080	21.57%	4.149%
3	2.565	366	381	395	rBV2	261079	452958	12.29%	2.364%
4	2.690	417	420	424	rVB2	624	435	0.01%	0.002%
5	2.864	469	474	479	rBV2	451	558	0.02%	0.003%
6	3.041	520	529	539	rBV6	2508	4586	0.12%	0.024%
7	3.137	553	559	560	rBV2	884	763	0.02%	0.004%
8	3.186	561	574	592	rVB3	12157	29068	0.79%	0.152%
9	3.353	609	626	646	rBV2	56081	111521	3.03%	0.582%
10	3.523	670	679	682	rVB2	352	379	0.01%	0.002%
11	3.729	739	743	747	rVB	382	363	0.01%	0.002%
12	3.751	747	750	756	rBV2	383	470	0.01%	0.002%
13	3.867	766	786	814	rBV	1259158	2996902	81.30%	15.639%
14	4.092	853	856	862	rVB2	680	473	0.01%	0.002%
15	4.137	862	870	876	rBV4	606	789	0.02%	0.004%
16	4.272	906	912	916	rBV2	490	533	0.01%	0.003%
17	4.404	949	953	956	rBV2	484	350	0.01%	0.002%
18	4.571	997	1005	1008	rBV4	425	601	0.02%	0.003%
19	4.665	1008	1034	1063	rBV2	1496021	3686225	100.00%	19.237%
20	4.973	1126	1130	1134	rBV4	767	778	0.02%	0.004%
21	5.063	1143	1158	1182	rVB	231529	501601	13.61%	2.618%
22	5.211	1202	1204	1209	rVB3	503	451	0.01%	0.002%
23	5.314	1213	1236	1256	rBV	598553	1359929	36.89%	7.097%
24	5.478	1282	1287	1290	rBV	475	400	0.01%	0.002%
25	5.726	1343	1364	1378	rBV2	449511	1222368	33.16%	6.379%
26	5.964	1433	1438	1441	rBV3	732	663	0.02%	0.003%
27	6.009	1447	1452	1454	rBV3	340	323	0.01%	0.002%
28	6.112	1481	1484	1492	rVB3	278	349	0.01%	0.002%
29	6.173	1499	1503	1511	rVB2	574	415	0.01%	0.002%
30	6.250	1511	1527	1555	rBV	400509	763879	20.72%	3.986%
31	6.542	1604	1618	1637	rVB2	69676	133727	3.63%	0.698%
32	6.690	1647	1664	1683	rBV	293880	572619	15.53%	2.988%
33	6.964	1739	1749	1765	rBV3	13183	27024	0.73%	0.141%
34	7.050	1773	1776	1780	rBV3	490	414	0.01%	0.002%
35	7.108	1790	1794	1805	rVB3	524	924	0.03%	0.005%
36	7.176	1807	1815	1818	rBV5	1637	2152	0.06%	0.011%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
 Title : VOC Analysis

37	7.568	1924	1937	1952	rBV	162107	285686	7.75%	1.491%
38	7.697	1975	1977	1984	rVB3	837	785	0.02%	0.004%
39	7.793	2004	2007	2014	rVB4	641	748	0.02%	0.004%
40	7.899	2024	2040	2058	rBV	561511	965316	26.19%	5.038%
41	8.041	2081	2084	2088	rBV3	430	355	0.01%	0.002%
42	8.179	2112	2127	2143	rBV	114229	196258	5.32%	1.024%
43	8.404	2190	2197	2204	rVB7	2490	3895	0.11%	0.020%
44	8.472	2207	2218	2228	rBV3	8907	16256	0.44%	0.085%
45	8.555	2233	2244	2256	rBV	47853	79902	2.17%	0.417%
46	8.632	2256	2268	2309	rBV	413000	765312	20.76%	3.994%
47	8.992	2375	2380	2383	rVB2	396	340	0.01%	0.002%
48	9.089	2406	2410	2414	rBV2	418	319	0.01%	0.002%
49	9.163	2429	2433	2437	rVB3	576	527	0.01%	0.003%
50	9.208	2443	2447	2450	rBV2	428	342	0.01%	0.002%
51	9.285	2466	2471	2475	rBV2	353	455	0.01%	0.002%
52	9.420	2498	2513	2530	rBV	545862	905065	24.55%	4.723%
53	9.571	2552	2560	2570	rVB2	8728	13658	0.37%	0.071%
54	9.700	2592	2600	2606	rVB3	1398	2091	0.06%	0.011%
55	10.031	2699	2703	2706	rBV2	504	415	0.01%	0.002%
56	10.102	2716	2725	2736	rBV4	2420	4235	0.11%	0.022%
57	10.311	2786	2790	2795	rVB	359	347	0.01%	0.002%
58	10.484	2834	2844	2854	rBV5	2010	2980	0.08%	0.016%
59	10.642	2889	2893	2896	rBV3	549	413	0.01%	0.002%
60	10.758	2913	2929	2949	rVV	434905	701551	19.03%	3.661%
61	10.838	2951	2954	2958	rVB4	480	328	0.01%	0.002%
62	10.896	2958	2972	2988	rVB5	15971	26936	0.73%	0.141%
63	10.989	2997	3001	3002	rBV2	615	392	0.01%	0.002%
64	11.025	3009	3012	3021	rVB2	791	865	0.02%	0.005%
65	11.092	3024	3033	3040	rBV3	1855	2754	0.07%	0.014%
66	11.182	3055	3061	3067	rBV2	417	656	0.02%	0.003%
67	11.237	3067	3078	3082	rBV3	907	1442	0.04%	0.008%
68	11.295	3087	3096	3107	rVV	9749	14400	0.39%	0.075%
69	11.356	3112	3115	3118	rVV2	506	352	0.01%	0.002%
70	11.378	3119	3122	3125	rVB	496	325	0.01%	0.002%
71	11.407	3130	3131	3135	rVV	510	369	0.01%	0.002%
72	11.468	3142	3150	3162	rVB2	15495	23303	0.63%	0.122%
73	11.648	3204	3206	3211	rVB	500	336	0.01%	0.002%
74	11.754	3237	3239	3243	rVB2	525	357	0.01%	0.002%
75	11.815	3245	3258	3276	rVV	536351	861872	23.38%	4.498%
76	11.899	3276	3284	3295	rVB3	8185	13223	0.36%	0.069%

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 Title : VOC Analysis

77	12.095	3334	3345	3354	rBV4	5669	9066	0.25%	0.047%
78	12.195	3363	3376	3400	rBV	543459	892445	24.21%	4.657%
79	12.375	3430	3432	3435	rBV2	558	351	0.01%	0.002%
80	12.487	3454	3467	3482	rBV3	70150	134269	3.64%	0.701%
81	12.574	3492	3494	3500	rVB2	1212	963	0.03%	0.005%
82	12.610	3500	3505	3508	rBV3	525	531	0.01%	0.003%
83	12.770	3547	3555	3556	rBV2	4566	3895	0.11%	0.020%
84	12.925	3600	3603	3611	rVB2	337	408	0.01%	0.002%
85	13.458	3766	3769	3773	rVB3	607	494	0.01%	0.003%
86	13.555	3795	3799	3802	rBV2	561	465	0.01%	0.002%
87	13.822	3877	3882	3884	rBV2	488	439	0.01%	0.002%
88	13.841	3884	3888	3889	rBV2	444	323	0.01%	0.002%
89	14.057	3951	3955	3959	rBV3	772	631	0.02%	0.003%
90	14.095	3964	3967	3980	rVB6	1811	2696	0.07%	0.014%
91	14.529	4097	4102	4107	rBV2	520	744	0.02%	0.004%
92	14.796	4182	4185	4191	rBV3	424	480	0.01%	0.003%
93	14.825	4191	4194	4199	rBV2	756	656	0.02%	0.003%
94	15.079	4269	4273	4274	rBV2	623	472	0.01%	0.002%
95	15.163	4297	4299	4302	rBV	656	427	0.01%	0.002%
96	15.204	4309	4312	4317	rVB3	550	360	0.01%	0.002%
97	15.282	4333	4336	4340	rBV2	540	394	0.01%	0.002%
98	15.375	4359	4365	4367	rBV2	882	990	0.03%	0.005%
99	15.841	4507	4510	4513	rBV3	943	652	0.02%	0.003%
100	16.465	4702	4704	4706	rBV2	1269	695	0.02%	0.004%

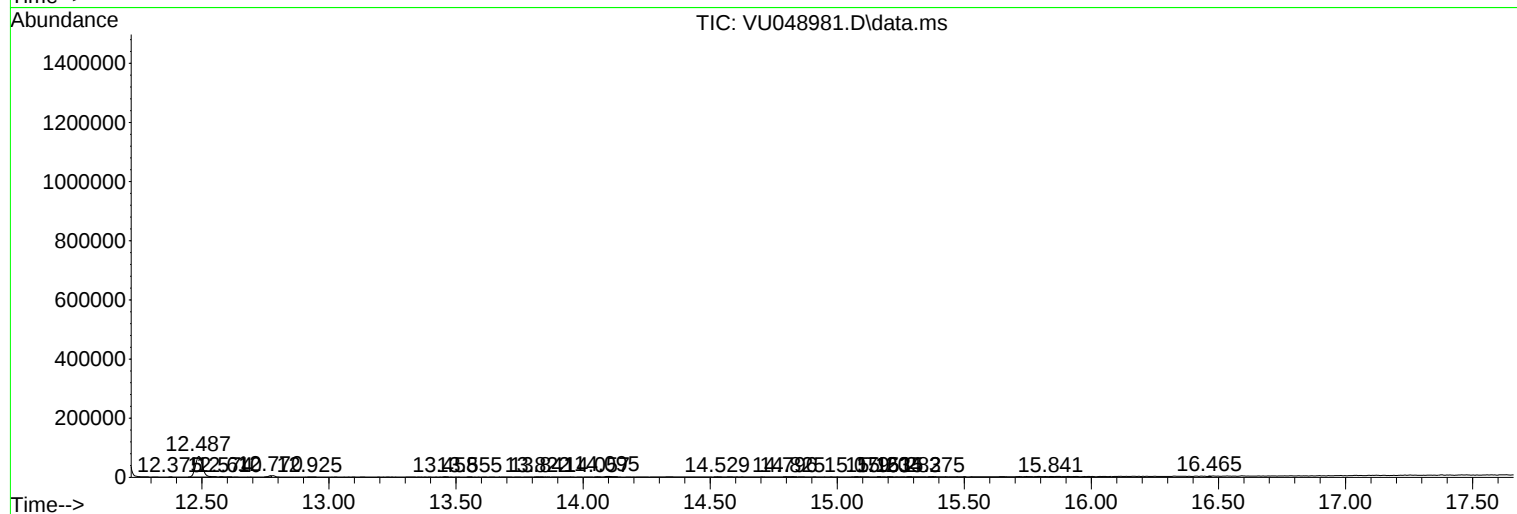
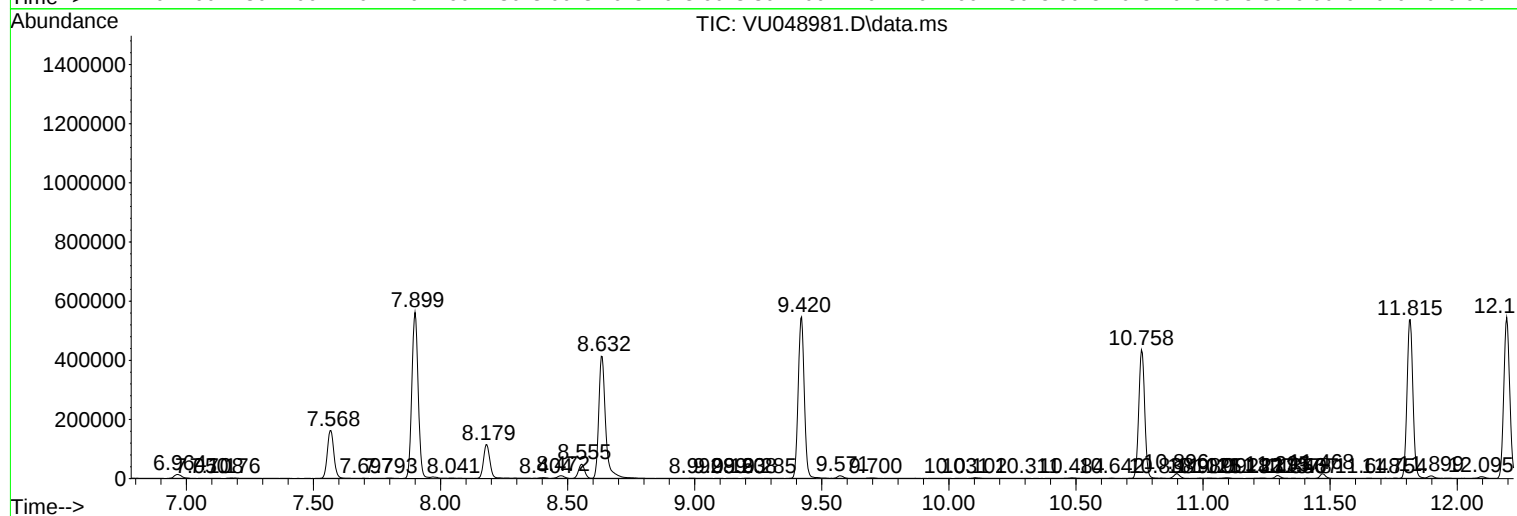
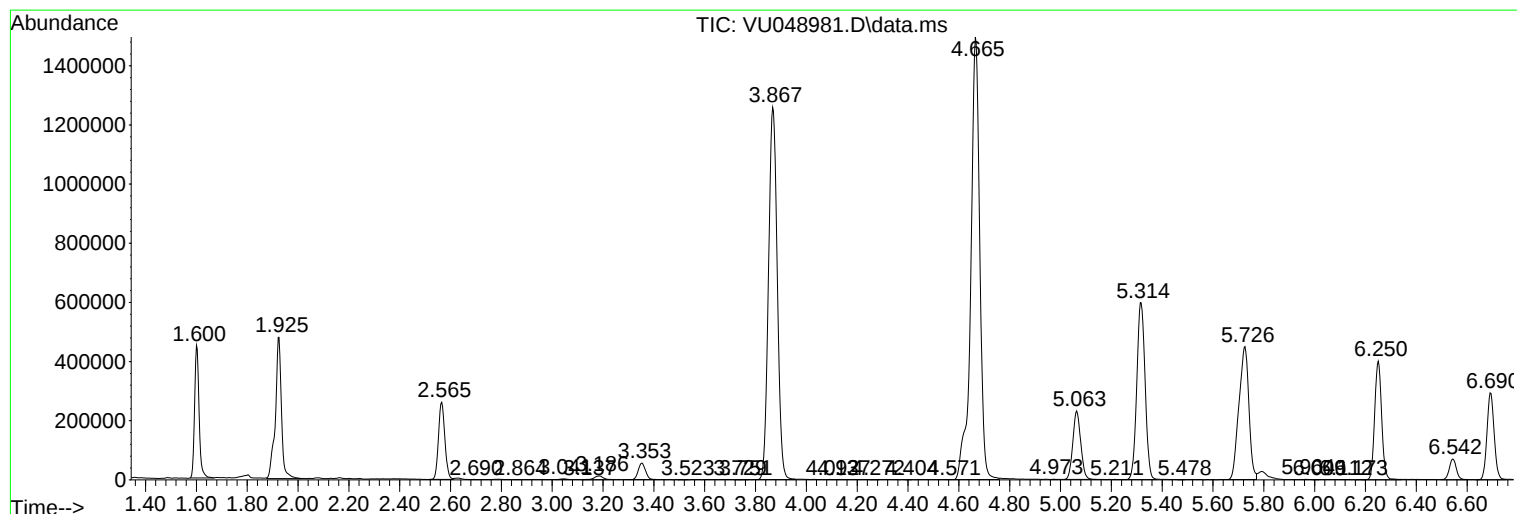
Sum of corrected areas: 19162393

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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



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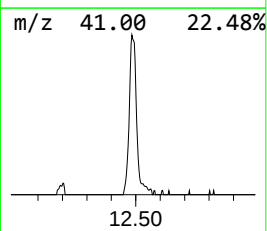
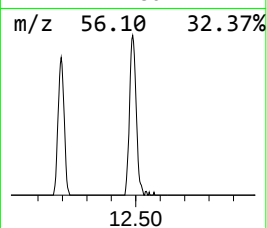
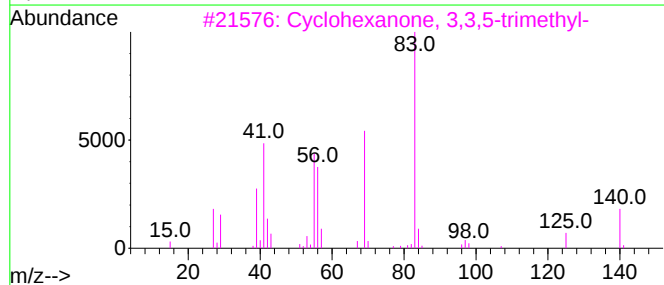
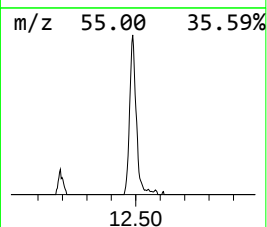
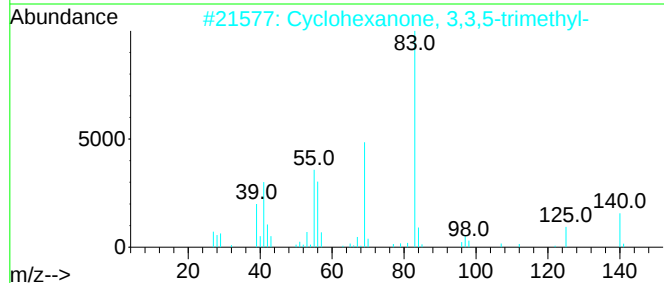
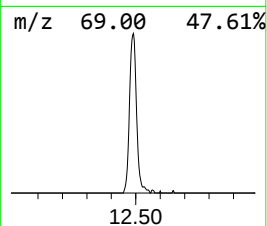
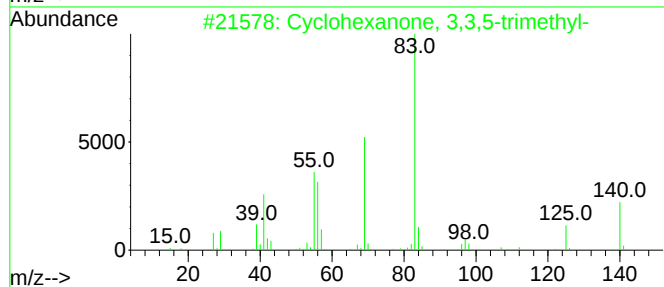
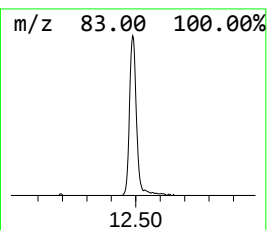
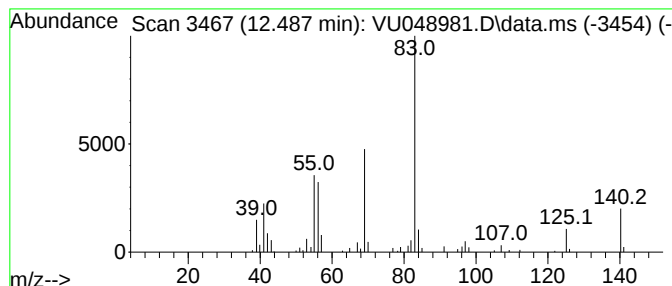
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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.
12.488	7.79 ug/L	134269	1,4-Dichlorobenzene-d4			11.816
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	91
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	Cyclohexane, butyl-		140	C10H20	001678-93-9	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Cyclohexanone, ...	12.488	7.8	ug/L	134269	3	11.816	861872	50.0