

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050522\
 Data File : VU048436.D
 Acq On : 05 May 2022 14:46
 Operator : SY/MD
 Sample : N2710-01
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXL83

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\SFAMULM042522WMA.M
 Title : VOC Analysis

Signal : TIC: VU048436.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.481	41	44	51	rVB2	3681	3171	0.20%	0.027%
2	1.600	73	81	96	rBV	182059	253757	16.28%	2.144%
3	1.903	167	175	192	rVB	126335	182417	11.70%	1.541%
4	2.565	368	381	396	rBV	322125	525916	33.75%	4.443%
5	2.684	410	418	429	rVB2	5255	9041	0.58%	0.076%
6	2.742	430	436	438	rBV2	540	420	0.03%	0.004%
7	2.796	438	453	467	rVV2	7076	15365	0.99%	0.130%
8	2.899	482	485	486	rBV2	328	206	0.01%	0.002%
9	3.189	563	575	601	rVB	16231	46137	2.96%	0.390%
10	3.279	601	603	607	rBV2	480	366	0.02%	0.003%
11	3.369	620	631	642	rVB4	6488	13019	0.84%	0.110%
12	3.571	690	694	695	rBV2	402	256	0.02%	0.002%
13	3.809	762	768	771	rVV2	163	183	0.01%	0.002%
14	3.861	771	784	795	rVV5	2053	4997	0.32%	0.042%
15	4.147	866	873	876	rVB2	161	183	0.01%	0.002%
16	4.501	980	983	986	rBV	170	146	0.01%	0.001%
17	4.623	1004	1021	1061	rBV	170866	433109	27.79%	3.659%
18	4.835	1085	1087	1095	rVB4	456	500	0.03%	0.004%
19	4.886	1101	1103	1107	rBV3	275	174	0.01%	0.001%
20	5.063	1138	1158	1179	rBV	267974	590784	37.91%	4.990%
21	5.179	1193	1194	1200	rVB2	486	163	0.01%	0.001%
22	5.292	1223	1229	1232	rBV3	679	760	0.05%	0.006%
23	5.346	1243	1246	1251	rVB2	315	207	0.01%	0.002%
24	5.372	1251	1254	1257	rVB2	377	151	0.01%	0.001%
25	5.411	1261	1266	1268	rBV	149	148	0.01%	0.001%
26	5.446	1273	1277	1282	rVB2	245	206	0.01%	0.002%
27	5.481	1282	1288	1291	rBV2	236	253	0.02%	0.002%
28	5.726	1342	1364	1396	rBV2	586166	1558456	100.00%	13.165%
29	5.970	1436	1440	1441	rBV2	501	407	0.03%	0.003%
30	5.996	1446	1448	1453	rVB3	249	159	0.01%	0.001%
31	6.128	1479	1489	1491	rBV4	445	592	0.04%	0.005%
32	6.166	1498	1501	1505	rVB2	257	172	0.01%	0.001%
33	6.250	1510	1527	1546	rBV	406283	767590	49.25%	6.484%
34	6.449	1587	1589	1592	rVB	390	147	0.01%	0.001%
35	6.529	1604	1614	1622	rBV6	1769	3438	0.22%	0.029%
36	6.584	1627	1631	1633	rBV3	405	347	0.02%	0.003%

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 Title : VOC Analysis

37	6.690	1649	1664	1686	rBV	355976	695778	44.65%	5.877%
38	6.780	1691	1692	1694	rBV2	311	151	0.01%	0.001%
39	6.796	1694	1697	1699	rBV3	384	212	0.01%	0.002%
40	7.047	1767	1775	1780	rVV2	307	484	0.03%	0.004%
41	7.185	1806	1818	1829	rBV4	4522	8809	0.57%	0.074%
42	7.391	1879	1882	1885	rBV2	277	241	0.02%	0.002%
43	7.565	1918	1936	1956	rBV	185147	321756	20.65%	2.718%
44	7.687	1967	1974	1982	rBV5	2042	3318	0.21%	0.028%
45	7.735	1986	1989	1991	rVB3	298	148	0.01%	0.001%
46	7.783	2001	2004	2006	rBV	321	211	0.01%	0.002%
47	7.803	2006	2010	2016	rVB4	537	591	0.04%	0.005%
48	7.851	2021	2025	2026	rBV2	237	161	0.01%	0.001%
49	7.899	2026	2040	2056	rBV	713361	1239053	79.51%	10.466%
50	8.179	2114	2127	2147	rBV	125598	209903	13.47%	1.773%
51	8.394	2191	2194	2199	rBV2	325	222	0.01%	0.002%
52	8.472	2209	2218	2229	rVB2	4285	7678	0.49%	0.065%
53	8.552	2239	2243	2247	rVB4	478	493	0.03%	0.004%
54	8.635	2255	2269	2303	rBV2	511360	935766	60.04%	7.905%
55	8.873	2340	2343	2344	rBV2	294	162	0.01%	0.001%
56	9.034	2390	2393	2398	rBV	302	281	0.02%	0.002%
57	9.169	2432	2435	2438	rVB2	302	221	0.01%	0.002%
58	9.275	2464	2468	2473	rBV2	276	270	0.02%	0.002%
59	9.320	2478	2482	2488	rBV2	236	256	0.02%	0.002%
60	9.356	2488	2493	2494	rBV	230	205	0.01%	0.002%
61	9.417	2499	2512	2534	rBV	572570	935748	60.04%	7.904%
62	9.561	2555	2557	2561	rBV	188	159	0.01%	0.001%
63	9.642	2578	2582	2585	rVB2	265	212	0.01%	0.002%
64	9.697	2592	2599	2611	rVB5	1229	2090	0.13%	0.018%
65	9.761	2613	2619	2624	rVB3	511	558	0.04%	0.005%
66	9.918	2657	2668	2684	rBV	32077	51446	3.30%	0.435%
67	10.102	2720	2725	2726	rBV2	435	391	0.03%	0.003%
68	10.188	2743	2752	2761	rBV3	2499	4041	0.26%	0.034%
69	10.558	2864	2867	2872	rBV	198	194	0.01%	0.002%
70	10.619	2884	2886	2892	rVV2	211	155	0.01%	0.001%
71	10.671	2893	2902	2911	rVB5	2458	3814	0.24%	0.032%
72	10.758	2911	2929	2950	rBV	564822	898765	57.67%	7.592%
73	10.893	2962	2971	2984	rVB2	10365	17862	1.15%	0.151%
74	10.970	2992	2995	2998	rVB2	326	195	0.01%	0.002%
75	11.089	3030	3032	3035	rBV2	329	218	0.01%	0.002%
76	11.121	3035	3042	3048	rVV4	992	1375	0.09%	0.012%

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 Title : VOC Analysis

77	11.356	3111	3115	3119	rBV	248	208	0.01%	0.002%
78	11.410	3130	3132	3138	rVB4	508	427	0.03%	0.004%
79	11.462	3138	3148	3155	rBV6	1970	3460	0.22%	0.029%
80	11.629	3196	3200	3201	rBV2	558	358	0.02%	0.003%
81	11.664	3209	3211	3213	rBV2	405	208	0.01%	0.002%
82	11.693	3217	3220	3228	rVB3	1427	1562	0.10%	0.013%
83	11.748	3233	3237	3241	rVB3	574	537	0.03%	0.005%
84	11.812	3244	3257	3274	rBV	580095	916003	58.78%	7.738%
85	11.970	3304	3306	3321	rVB5	1963	2852	0.18%	0.024%
86	12.063	3326	3335	3346	rBV4	10996	19714	1.26%	0.167%
87	12.192	3362	3375	3395	rBV	681678	1108654	71.14%	9.365%
88	12.327	3411	3417	3426	rVB7	1989	2832	0.18%	0.024%
89	12.394	3435	3438	3440	rBV2	410	262	0.02%	0.002%
90	12.420	3444	3446	3447	rBV2	334	159	0.01%	0.001%
91	12.639	3511	3514	3517	rBV	311	184	0.01%	0.002%
92	12.770	3546	3555	3565	rBV2	4499	7326	0.47%	0.062%
93	13.140	3668	3670	3673	rBV	424	257	0.02%	0.002%
94	13.224	3693	3696	3700	rVB4	467	318	0.02%	0.003%
95	13.433	3753	3761	3767	rBV4	3253	4093	0.26%	0.035%
96	14.095	3961	3967	3972	rBV4	1506	1854	0.12%	0.016%
97	14.288	4025	4027	4030	rBV	373	223	0.01%	0.002%
98	14.449	4068	4077	4087	rBV3	5714	7970	0.51%	0.067%
99	15.066	4267	4269	4272	rBV2	811	570	0.04%	0.005%
100	15.204	4309	4312	4318	rBV6	1126	1320	0.08%	0.011%

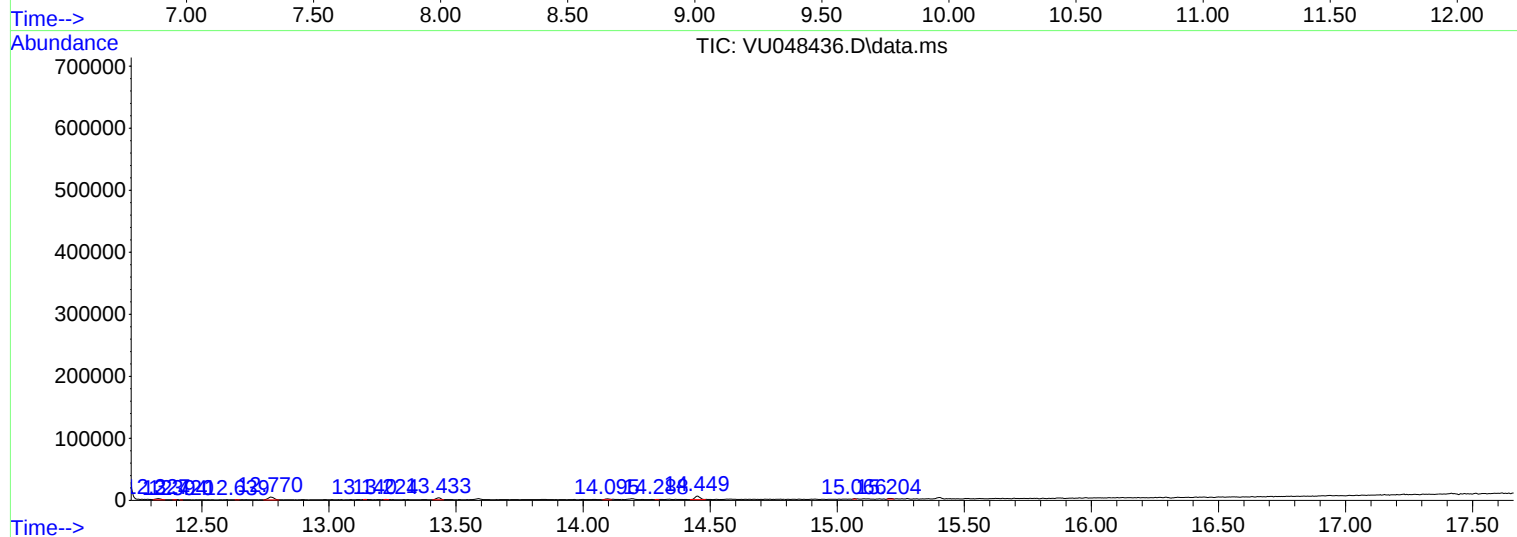
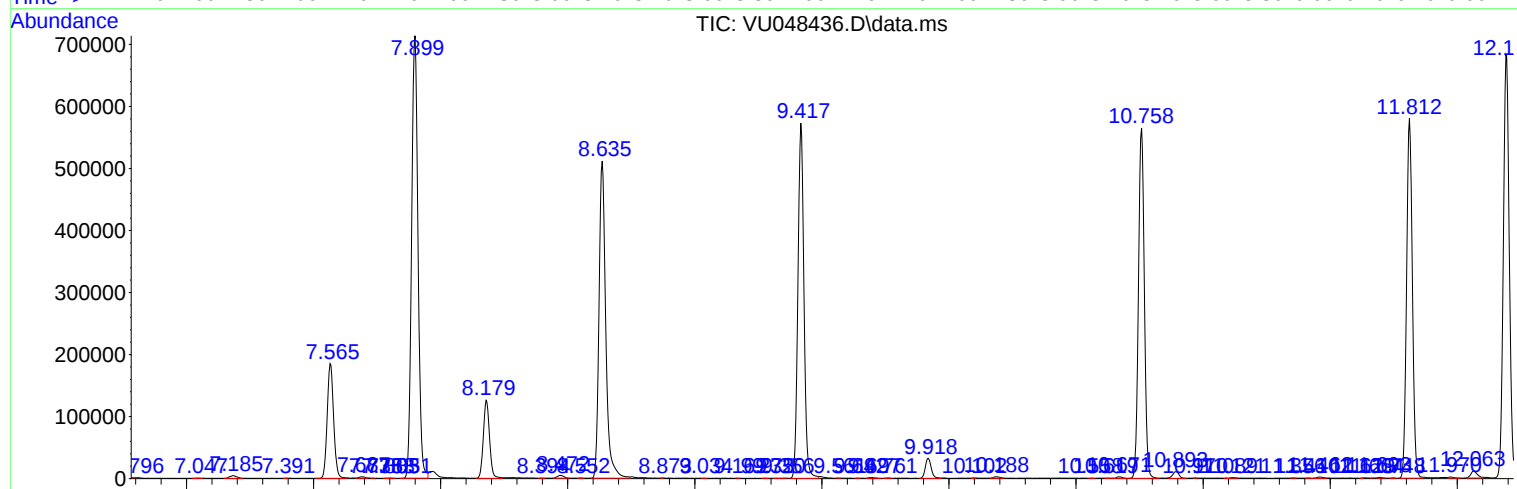
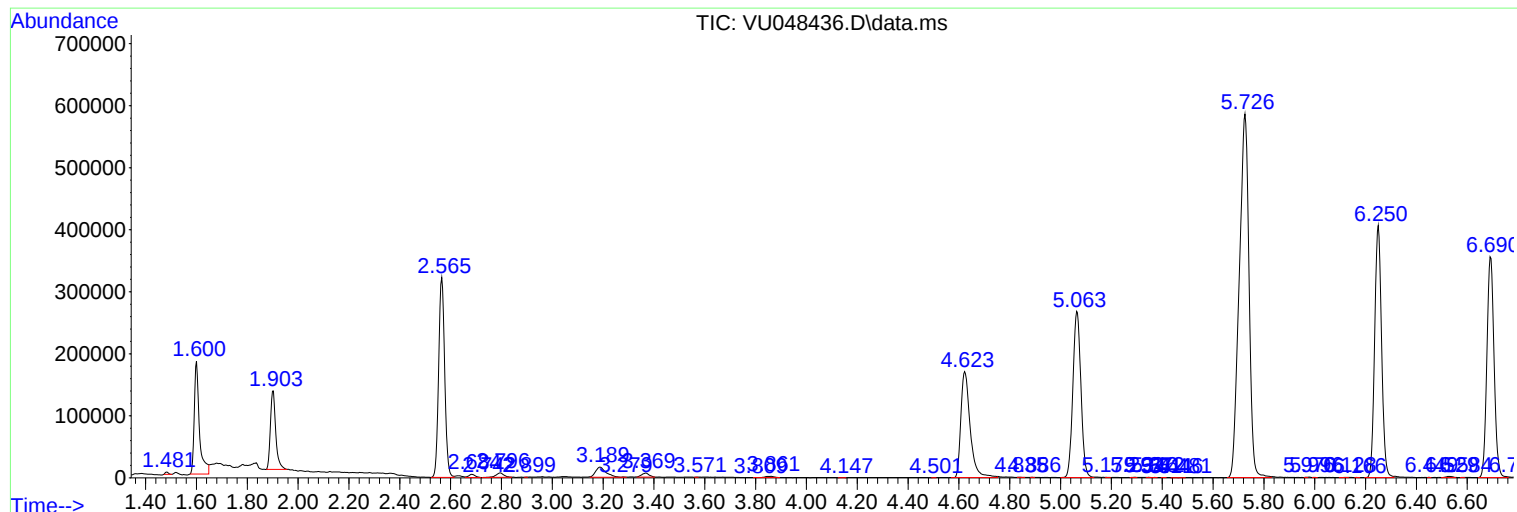
Sum of corrected areas: 11838287

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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



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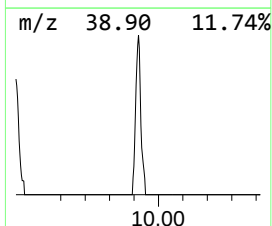
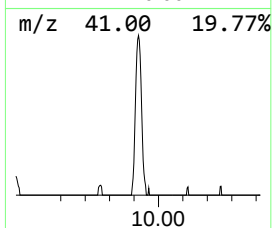
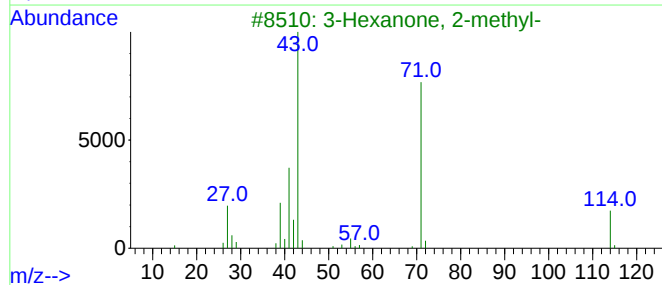
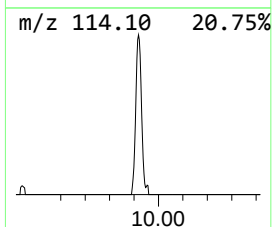
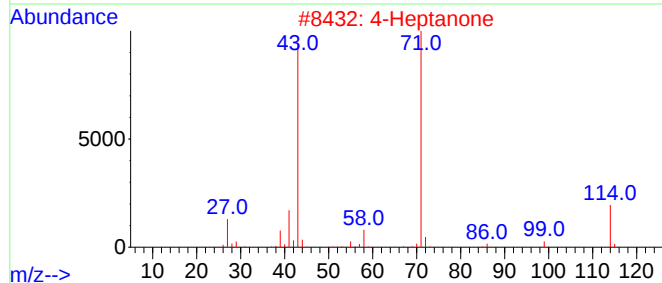
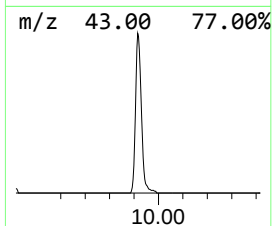
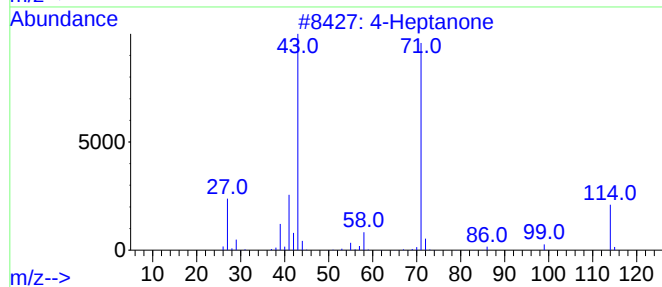
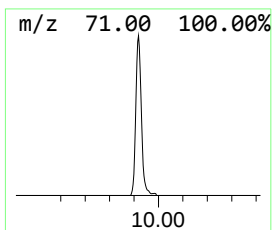
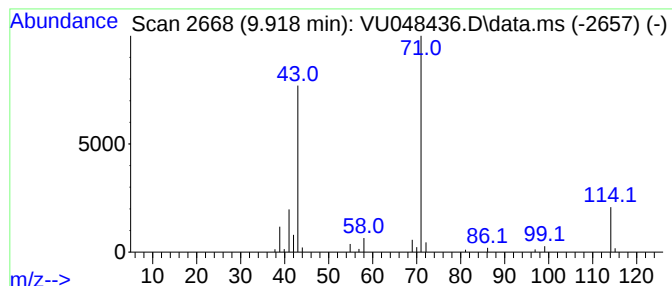
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 4-Heptanone Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.918	2.75 ug/L	51446	Chlorobenzene-d5	9.417

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Heptanone	114	C7H14O	000123-19-3	91
2			4-Heptanone	114	C7H14O	000123-19-3	90
3			3-Hexanone, 2-methyl-	114	C7H14O	007379-12-6	80
4			4-Heptanone	114	C7H14O	000123-19-3	78
5			3-Pentanone, 2,4-dimethyl-	114	C7H14O	000565-80-0	72



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
4-Heptanone	9.918	2.8	ug/L	51446	2	9.417	935748	50.0