

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090622\
 Data File : VU050646.D
 Acq On : 06 Sep 2022 20:06
 Operator : SY/MD
 Sample : N4483-10ME
 Misc : 2.57g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW358ME

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\SFAMULM090222WMA.M
 Title : VOC Analysis

Signal : TIC: VU050646.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.488	42	46	52	rVB4	1864	1761	0.21%	0.029%
2	1.597	71	80	101	rBV	55511	70072	8.45%	1.150%
3	1.816	128	148	149	rBV8	5100	11354	1.37%	0.186%
4	1.861	160	162	166	rVB3	395	256	0.03%	0.004%
5	1.903	166	175	192	rBV	54352	73012	8.80%	1.198%
6	2.012	206	209	210	rBV	313	158	0.02%	0.003%
7	2.089	229	233	237	rBV2	328	281	0.03%	0.005%
8	2.147	249	251	255	rBV2	443	352	0.04%	0.006%
9	2.240	277	280	283	rBV3	275	272	0.03%	0.004%
10	2.292	294	296	298	rBV2	267	170	0.02%	0.003%
11	2.565	369	381	393	rBV	127629	205304	24.75%	3.369%
12	2.629	394	401	414	rVB	6408	11508	1.39%	0.189%
13	2.787	444	450	452	rBV	653	640	0.08%	0.011%
14	2.896	476	484	497	rBV2	1668	3013	0.36%	0.049%
15	3.044	526	530	535	rVB2	526	494	0.06%	0.008%
16	3.112	549	551	556	rVB	254	171	0.02%	0.003%
17	3.189	567	575	589	rVB3	1444	2941	0.35%	0.048%
18	3.272	598	601	605	rBV	146	163	0.02%	0.003%
19	3.491	664	669	673	rBV	201	197	0.02%	0.003%
20	3.668	721	724	728	rBV	245	295	0.04%	0.005%
21	3.829	770	774	778	rVB2	220	201	0.02%	0.003%
22	3.867	780	786	789	rBV2	194	243	0.03%	0.004%
23	3.989	820	824	827	rVB3	251	192	0.02%	0.003%
24	4.076	845	851	855	rVB2	154	159	0.02%	0.003%
25	4.108	857	861	864	rBV2	190	162	0.02%	0.003%
26	4.417	953	957	960	rBV	274	187	0.02%	0.003%
27	4.623	1009	1021	1063	rBV	79491	232304	28.00%	3.812%
28	5.063	1141	1158	1178	rVV	153937	341330	41.14%	5.601%
29	5.214	1202	1205	1209	rVB4	455	317	0.04%	0.005%
30	5.282	1222	1226	1227	rBV2	467	396	0.05%	0.006%
31	5.375	1251	1255	1256	rBV	297	202	0.02%	0.003%
32	5.449	1275	1278	1282	rVV2	182	168	0.02%	0.003%
33	5.722	1341	1363	1390	rBV2	299291	829652	100.00%	13.614%
34	5.989	1443	1446	1450	rVB3	220	193	0.02%	0.003%
35	6.021	1450	1456	1459	rBV2	373	397	0.05%	0.007%
36	6.147	1490	1495	1499	rBV2	131	138	0.02%	0.002%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

37	6.250	1513	1527	1551	rVV	256213	491399	59.23%	8.063%
38	6.407	1573	1576	1579	rVB2	327	253	0.03%	0.004%
39	6.484	1597	1600	1605	rVB2	352	261	0.03%	0.004%
40	6.523	1607	1612	1613	rBV2	765	588	0.07%	0.010%
41	6.607	1633	1638	1644	rBV2	340	331	0.04%	0.005%
42	6.632	1644	1646	1650	rVB	224	142	0.02%	0.002%
43	6.690	1650	1664	1685	rBV	196623	390112	47.02%	6.401%
44	6.816	1697	1703	1708	rVB4	798	783	0.09%	0.013%
45	6.851	1708	1714	1719	rVB2	180	264	0.03%	0.004%
46	7.163	1801	1811	1812	rBV2	999	1183	0.14%	0.019%
47	7.291	1849	1851	1856	rVB2	209	149	0.02%	0.002%
48	7.565	1924	1936	1959	rBV	99678	176125	21.23%	2.890%
49	7.693	1971	1976	1983	rBV2	725	626	0.08%	0.010%
50	7.748	1990	1993	2002	rVB3	289	340	0.04%	0.006%
51	7.790	2003	2006	2010	rBV2	389	315	0.04%	0.005%
52	7.899	2025	2040	2061	rBV	327412	580143	69.93%	9.519%
53	8.179	2116	2127	2146	rBV	68085	117577	14.17%	1.929%
54	8.555	2241	2244	2250	rVB2	423	292	0.04%	0.005%
55	8.635	2257	2269	2278	rBV3	155777	327269	39.45%	5.370%
56	8.896	2347	2350	2354	rBV2	170	169	0.02%	0.003%
57	8.941	2361	2364	2370	rVB2	227	215	0.03%	0.004%
58	9.012	2382	2386	2389	rBV2	202	146	0.02%	0.002%
59	9.176	2433	2437	2439	rBV2	179	141	0.02%	0.002%
60	9.417	2499	2512	2546	rBV	360112	612740	73.86%	10.054%
61	9.571	2557	2560	2571	rVB4	734	903	0.11%	0.015%
62	9.697	2593	2599	2606	rVB5	715	1006	0.12%	0.017%
63	9.941	2672	2675	2680	rBV2	285	250	0.03%	0.004%
64	10.102	2723	2725	2728	rVB	353	181	0.02%	0.003%
65	10.407	2817	2820	2826	rVB	282	272	0.03%	0.004%
66	10.487	2837	2845	2851	rBV3	468	631	0.08%	0.010%
67	10.754	2916	2928	2950	rBV	316362	519669	62.64%	8.527%
68	10.992	2999	3002	3006	rVB2	254	171	0.02%	0.003%
69	11.092	3028	3033	3038	rVV2	453	456	0.05%	0.007%
70	11.471	3145	3151	3152	rBV4	629	621	0.07%	0.010%
71	11.526	3165	3168	3177	rVB	436	567	0.07%	0.009%
72	11.568	3177	3181	3184	rBV2	376	395	0.05%	0.006%
73	11.745	3231	3236	3243	rVB4	743	907	0.11%	0.015%
74	11.812	3244	3257	3278	rBV	300264	484374	58.38%	7.948%
75	12.063	3326	3335	3349	rBV3	21204	39942	4.81%	0.655%
76	12.192	3362	3375	3393	rBV	323075	539483	65.03%	8.852%

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Integrator: RTE

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
 Title : VOC Analysis

77	12.298	3405	3408	3411	rVB2	591	416	0.05%	0.007%
78	12.391	3435	3437	3440	rVB3	285	161	0.02%	0.003%
79	12.465	3454	3460	3464	rBV	228	313	0.04%	0.005%
80	12.629	3508	3511	3516	rBV2	285	225	0.03%	0.004%
81	13.047	3637	3641	3646	rVB3	366	397	0.05%	0.007%
82	13.076	3646	3650	3652	rBV2	277	202	0.02%	0.003%
83	13.134	3665	3668	3670	rBV	203	146	0.02%	0.002%
84	13.220	3689	3695	3705	rBV3	1193	1684	0.20%	0.028%
85	13.288	3714	3716	3719	rBV	236	213	0.03%	0.003%
86	13.339	3730	3732	3740	rVB2	269	317	0.04%	0.005%
87	13.417	3753	3756	3760	rBV2	374	233	0.03%	0.004%
88	13.439	3760	3763	3765	rBV	377	258	0.03%	0.004%
89	13.600	3809	3813	3818	rBV3	394	503	0.06%	0.008%
90	13.751	3856	3860	3862	rBV2	398	353	0.04%	0.006%
91	13.844	3884	3889	3895	rBV5	1390	1481	0.18%	0.024%
92	14.098	3962	3968	3978	rBV5	1559	2105	0.25%	0.035%
93	14.195	3996	3998	4002	rVB2	333	235	0.03%	0.004%
94	14.333	4033	4041	4049	rBV5	1966	2519	0.30%	0.041%
95	14.423	4067	4069	4074	rBV2	306	169	0.02%	0.003%
96	14.696	4152	4154	4158	rVB2	482	221	0.03%	0.004%
97	14.719	4159	4161	4165	rVB3	360	212	0.03%	0.003%
98	14.870	4206	4208	4212	rVB2	639	366	0.04%	0.006%
99	15.021	4252	4255	4258	rBV3	481	330	0.04%	0.005%
100	16.227	4627	4630	4634	rBV3	1090	1183	0.14%	0.019%

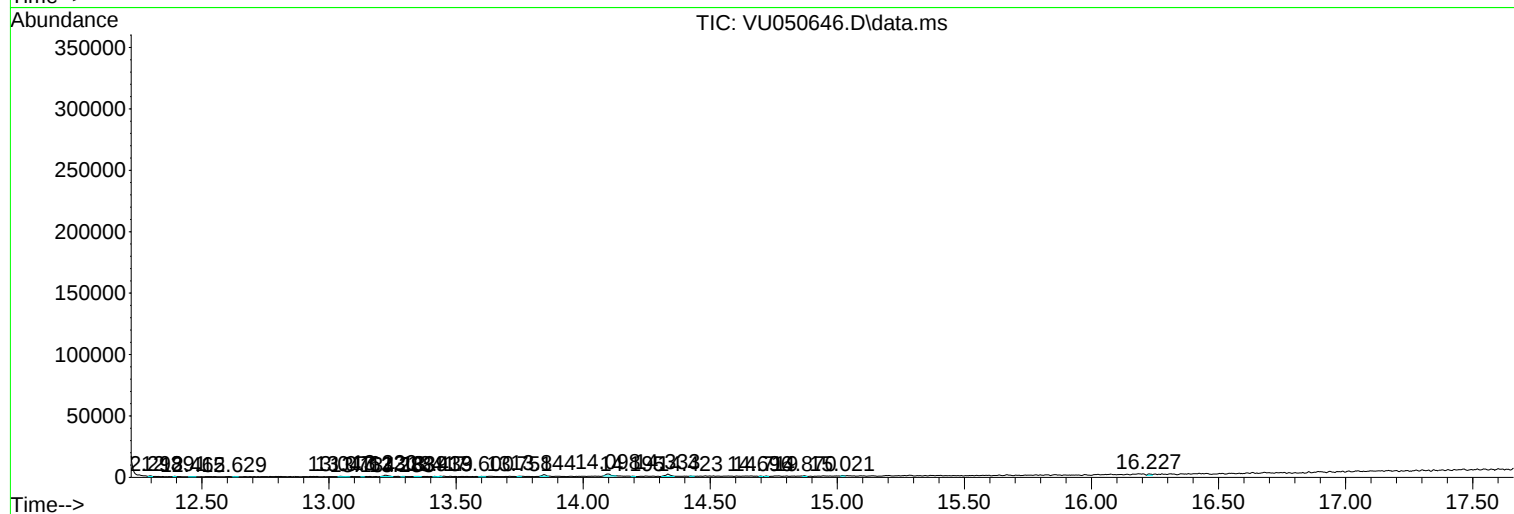
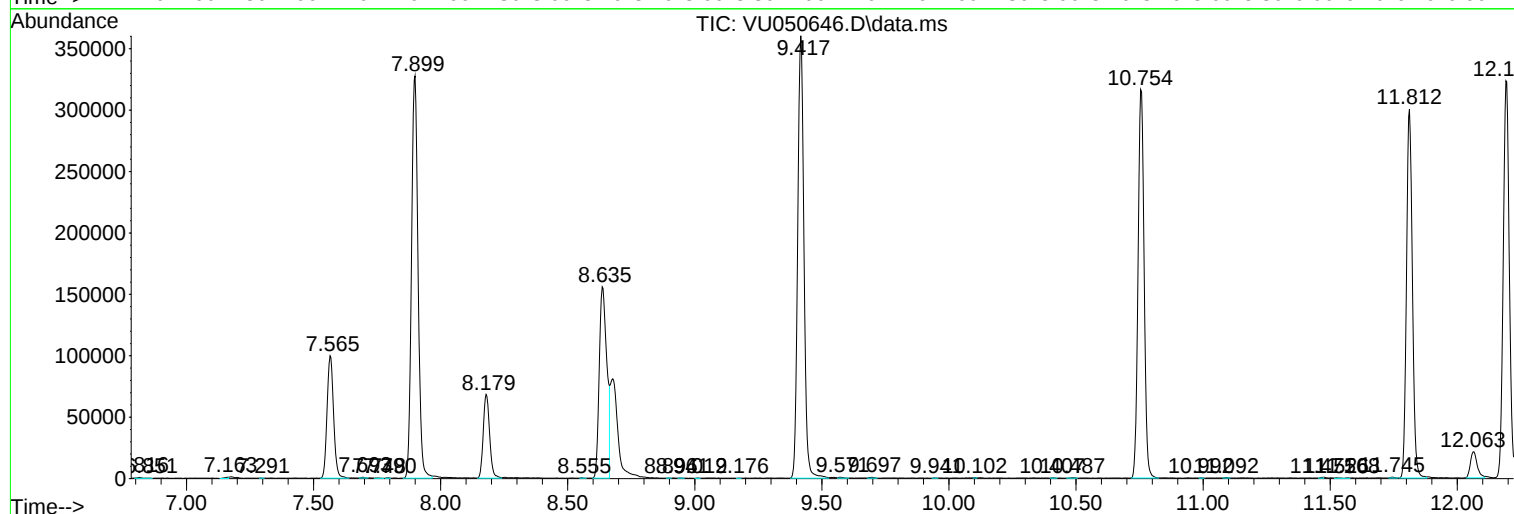
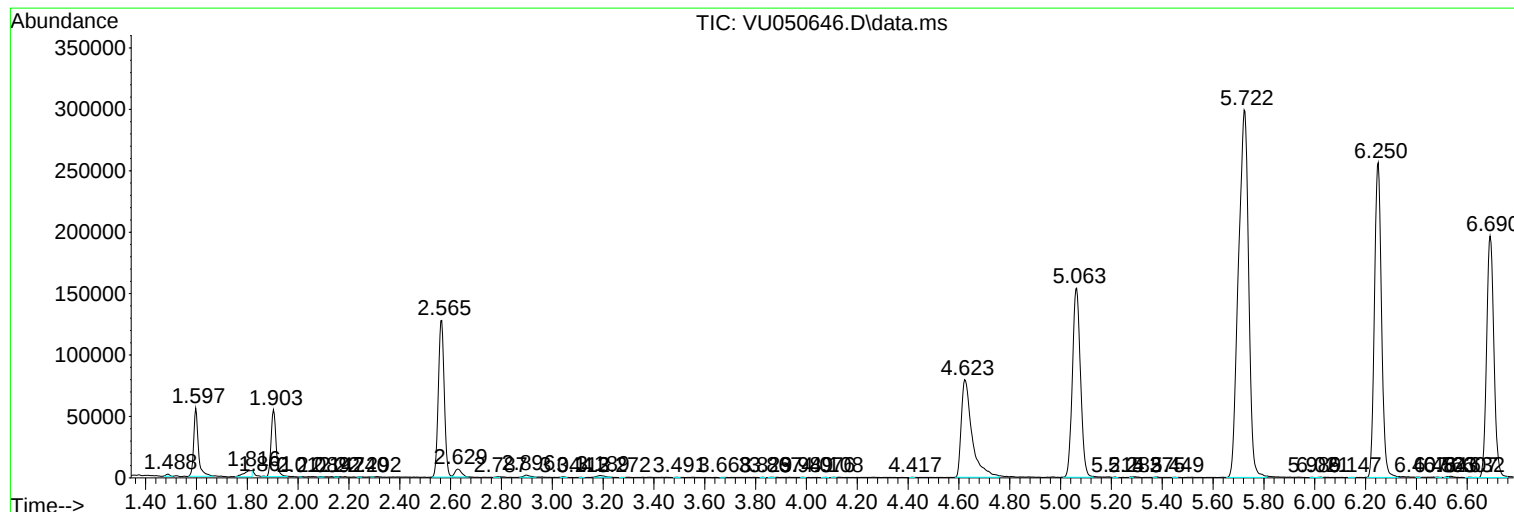
Sum of corrected areas: 6094288

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ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW358ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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



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Instrument :
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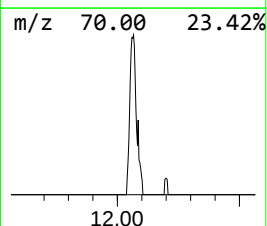
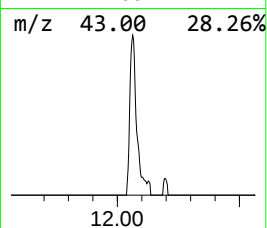
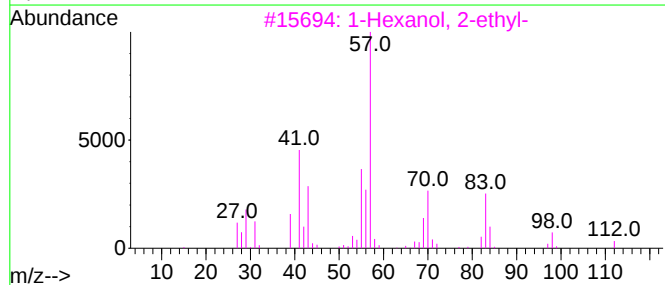
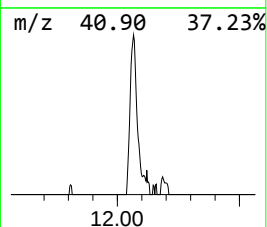
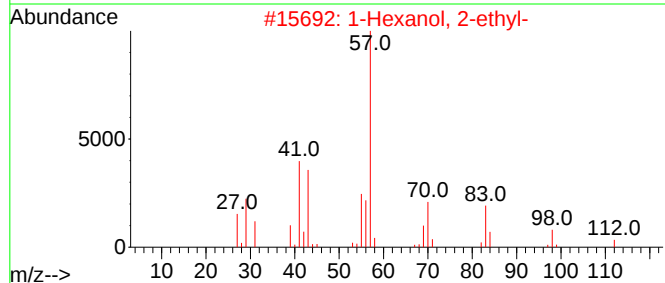
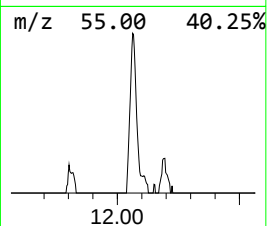
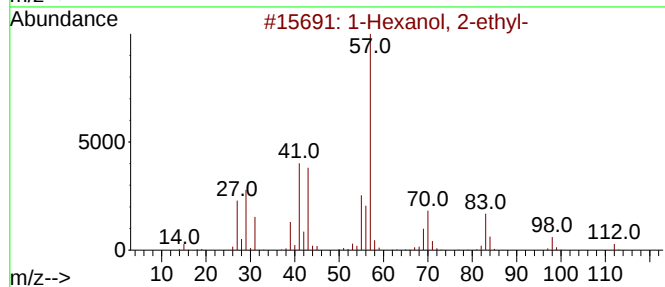
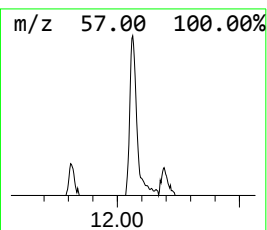
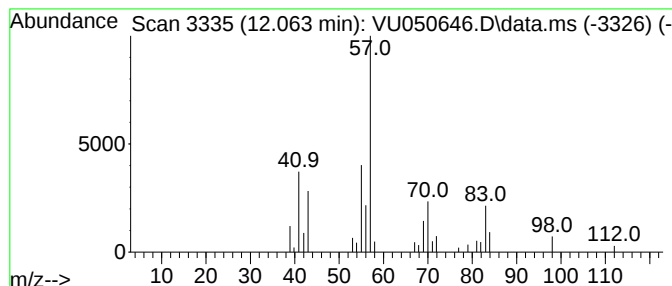
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM090222WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 1-Hexanol, 2-ethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.063	4.12 ug/L	39942	1,4-Dichlorobenzene-d4	11.812

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
4			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.063	4.1	ug/L	39942	3	11.812	484374	50.0