

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051981.D
 Acq On : 20 Nov 2022 18:14
 Operator : JC/MD
 Sample : N5710-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0KY4

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\SFAMULM111522WMA.M
 Title : VOC Analysis

Signal : TIC: VU051981.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	74	81	93	rBV	106733	124964	10.09%	1.158%
2	1.906	169	176	199	rVB	106153	161594	13.05%	1.498%
3	2.565	370	381	391	rBV	174307	281072	22.70%	2.605%
4	2.620	391	398	420	rVB	88602	153548	12.40%	1.423%
5	3.047	524	531	538	rVB6	1080	1632	0.13%	0.015%
6	3.173	556	570	589	rBV3	14377	35684	2.88%	0.331%
7	3.356	623	627	632	rBV3	231	256	0.02%	0.002%
8	3.420	644	647	648	rBV	141	80	0.01%	0.001%
9	3.616	705	708	711	rBV2	205	134	0.01%	0.001%
10	3.639	711	715	720	rVB2	341	308	0.02%	0.003%
11	3.665	720	723	724	rBV2	147	91	0.01%	0.001%
12	3.703	730	735	738	rBV3	334	268	0.02%	0.002%
13	3.774	754	757	762	rVB2	395	246	0.02%	0.002%
14	3.806	763	767	770	rBV	457	344	0.03%	0.003%
15	3.925	799	804	807	rBV	263	313	0.03%	0.003%
16	4.009	827	830	831	rBV	259	133	0.01%	0.001%
17	4.089	853	855	858	rBV2	214	112	0.01%	0.001%
18	4.108	858	861	863	rBV	145	97	0.01%	0.001%
19	4.157	872	876	880	rBV2	452	410	0.03%	0.004%
20	4.195	883	888	890	rBV2	271	271	0.02%	0.003%
21	4.237	899	901	904	rBV2	149	82	0.01%	0.001%
22	4.340	926	933	936	rBV3	417	457	0.04%	0.004%
23	4.417	954	957	960	rVB2	332	205	0.02%	0.002%
24	4.436	960	963	966	rBV	189	102	0.01%	0.001%
25	4.462	966	971	973	rVV2	154	134	0.01%	0.001%
26	4.478	973	976	979	rVB	187	119	0.01%	0.001%
27	4.510	984	986	988	rVB	264	102	0.01%	0.001%
28	4.565	1000	1003	1005	rBV	291	184	0.01%	0.002%
29	4.616	1007	1019	1040	rBV	158249	398280	32.16%	3.692%
30	5.060	1141	1157	1181	rBV	252826	556014	44.90%	5.154%
31	5.202	1199	1201	1205	rVB3	573	420	0.03%	0.004%
32	5.288	1221	1228	1239	rVB2	1411	2144	0.17%	0.020%
33	5.433	1269	1273	1274	rBV2	183	145	0.01%	0.001%
34	5.462	1279	1282	1288	rVB	406	326	0.03%	0.003%
35	5.494	1288	1292	1294	rBV	252	157	0.01%	0.001%
36	5.568	1311	1315	1316	rBV2	232	169	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051981.D
 Acq On : 20 Nov 2022 18:14
 Operator : JC/MD
 Sample : N5710-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0KY4

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\SFAMULM111522WMA.M
 Title : VOC Analysis

37	5.722	1340	1363	1391	rBV2	429132	1238475	100.00%	11.479%
38	6.002	1448	1450	1452	rBV	206	98	0.01%	0.001%
39	6.105	1480	1482	1483	rBV	216	115	0.01%	0.001%
40	6.147	1493	1495	1497	rVB	277	124	0.01%	0.001%
41	6.163	1497	1500	1501	rBV2	345	223	0.02%	0.002%
42	6.247	1512	1526	1567	rBV	511693	984820	79.52%	9.128%
43	6.542	1606	1618	1631	rVB4	14512	27707	2.24%	0.257%
44	6.616	1640	1641	1647	rBV2	285	177	0.01%	0.002%
45	6.687	1648	1663	1685	rBV	320107	627155	50.64%	5.813%
46	6.890	1723	1726	1729	rBV2	427	261	0.02%	0.002%
47	6.931	1732	1739	1748	rVV3	1121	1878	0.15%	0.017%
48	7.034	1767	1771	1773	rBV	252	177	0.01%	0.002%
49	7.086	1784	1787	1789	rBV2	175	88	0.01%	0.001%
50	7.115	1793	1796	1799	rBV2	184	125	0.01%	0.001%
51	7.176	1801	1815	1833	rVV5	8171	23271	1.88%	0.216%
52	7.269	1842	1844	1851	rBV2	186	187	0.02%	0.002%
53	7.369	1872	1875	1877	rBV	200	102	0.01%	0.001%
54	7.385	1877	1880	1882	rBV2	181	124	0.01%	0.001%
55	7.420	1889	1891	1894	rVB2	144	74	0.01%	0.001%
56	7.449	1897	1900	1901	rBV	137	76	0.01%	0.001%
57	7.565	1920	1936	1958	rBV	130581	232717	18.79%	2.157%
58	7.690	1968	1975	1986	rBV3	3561	5536	0.45%	0.051%
59	7.800	2002	2009	2014	rBV3	1030	1358	0.11%	0.013%
60	7.896	2025	2039	2059	rBV	434467	755519	61.00%	7.003%
61	8.134	2110	2113	2114	rBV	149	96	0.01%	0.001%
62	8.176	2115	2126	2149	rVV	92367	160500	12.96%	1.488%
63	8.552	2231	2243	2256	rBV3	53746	90118	7.28%	0.835%
64	8.629	2256	2267	2302	rBV2	443288	871386	70.36%	8.077%
65	8.931	2358	2361	2363	rBV3	507	276	0.02%	0.003%
66	8.986	2376	2378	2380	rBV	315	114	0.01%	0.001%
67	8.999	2380	2382	2383	rBV	262	112	0.01%	0.001%
68	9.182	2434	2439	2440	rBV	222	223	0.02%	0.002%
69	9.227	2451	2453	2458	rBV	164	122	0.01%	0.001%
70	9.266	2459	2465	2466	rBV2	379	326	0.03%	0.003%
71	9.291	2470	2473	2482	rVB2	372	447	0.04%	0.004%
72	9.327	2482	2484	2485	rBV2	239	94	0.01%	0.001%
73	9.365	2493	2496	2498	rBV	187	137	0.01%	0.001%
74	9.414	2498	2511	2534	rBV	733747	1232400	99.51%	11.423%
75	9.648	2581	2584	2586	rVB	204	106	0.01%	0.001%
76	9.664	2586	2589	2593	rVB2	299	199	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051981.D
 Acq On : 20 Nov 2022 18:14
 Operator : JC/MD
 Sample : N5710-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0KY4

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\SFAMULM111522WMA.M
 Title : VOC Analysis

77	9.693	2596	2598	2601	rBV2	464	334	0.03%	0.003%
78	9.799	2628	2631	2639	rBV2	327	422	0.03%	0.004%
79	9.838	2641	2643	2646	rVB2	325	176	0.01%	0.002%
80	9.877	2653	2655	2660	rVB3	487	223	0.02%	0.002%
81	9.980	2683	2687	2689	rBV2	253	209	0.02%	0.002%
82	10.053	2707	2710	2712	rBV2	212	117	0.01%	0.001%
83	10.391	2813	2815	2818	rBV	295	160	0.01%	0.001%
84	10.491	2841	2846	2850	rBV5	686	737	0.06%	0.007%
85	10.610	2878	2883	2887	rVB3	674	609	0.05%	0.006%
86	10.674	2900	2903	2906	rBV	273	207	0.02%	0.002%
87	10.754	2914	2928	2950	rBV	580275	941684	76.04%	8.729%
88	11.034	3012	3015	3017	rBV2	308	201	0.02%	0.002%
89	11.352	3109	3114	3117	rBV	369	327	0.03%	0.003%
90	11.513	3161	3164	3167	rBV3	305	185	0.01%	0.002%
91	11.703	3220	3223	3225	rBV2	247	167	0.01%	0.002%
92	11.809	3243	3256	3277	rBV	556237	887549	71.66%	8.227%
93	12.005	3314	3317	3319	rBV3	478	291	0.02%	0.003%
94	12.060	3323	3334	3351	rBV	52926	96387	7.78%	0.893%
95	12.188	3363	3374	3397	rBV	534514	879455	71.01%	8.152%
96	12.584	3492	3497	3500	rBV3	668	602	0.05%	0.006%
97	12.931	3603	3605	3607	rVB	415	164	0.01%	0.002%
98	13.092	3652	3655	3657	rBV2	425	278	0.02%	0.003%
99	13.272	3709	3711	3714	rBV	321	222	0.02%	0.002%
100	13.327	3725	3728	3730	rBV2	399	254	0.02%	0.002%

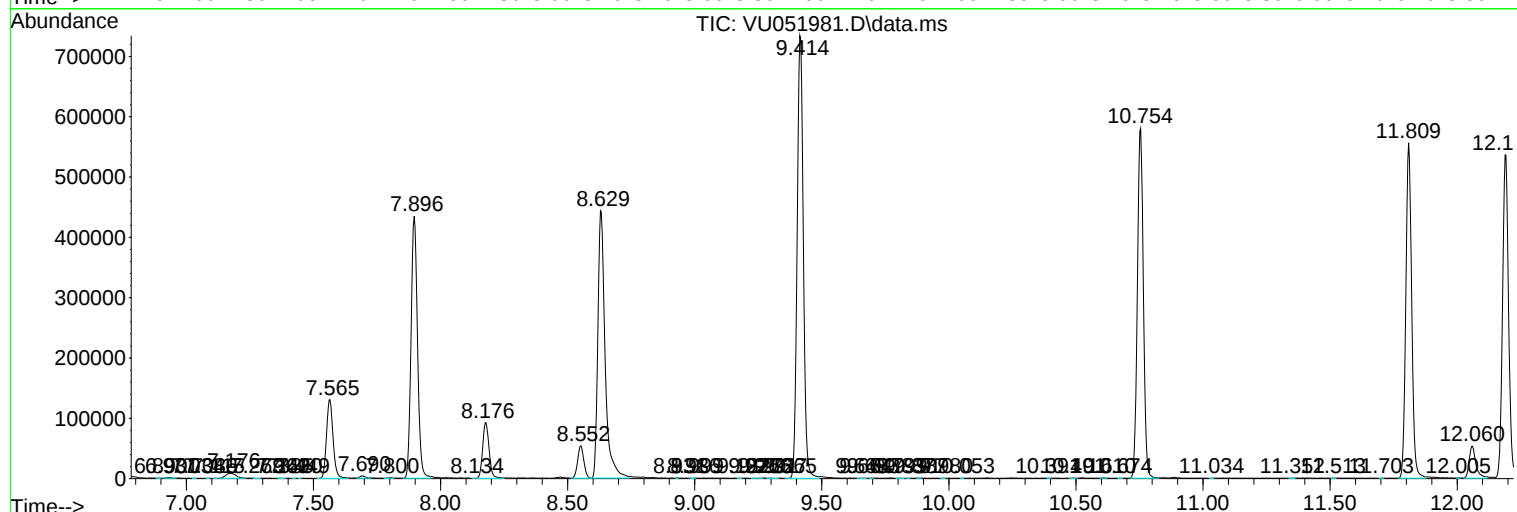
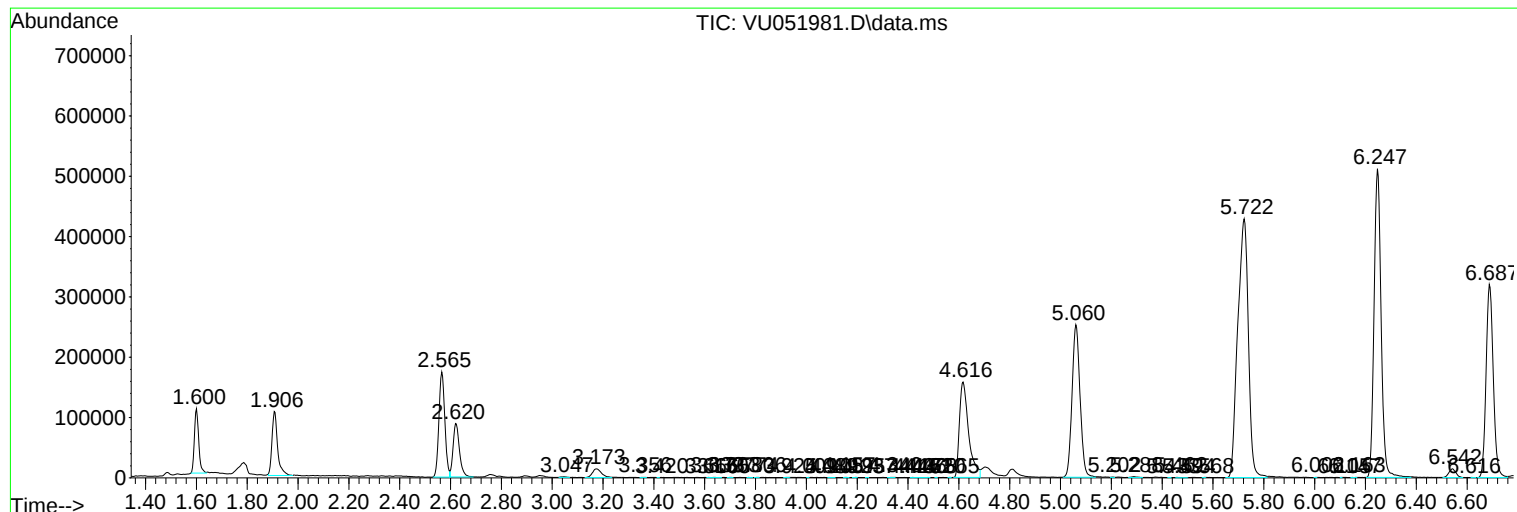
Sum of corrected areas: 10788600

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051981.D
Acq On : 20 Nov 2022 18:14
Operator : JC/MD
Sample : N5710-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051981.D
Acq On : 20 Nov 2022 18:14
Operator : JC/MD
Sample : N5710-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY4

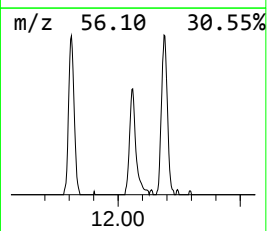
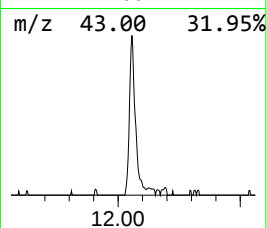
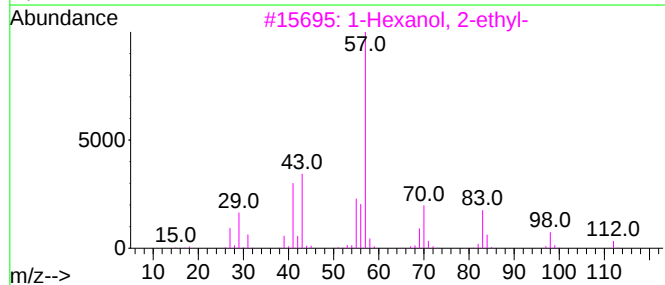
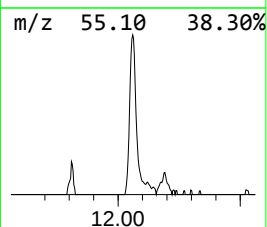
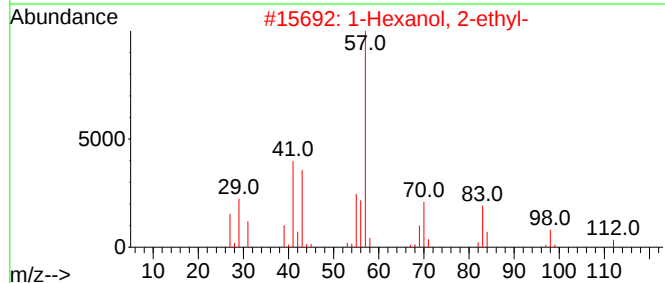
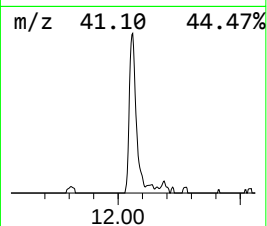
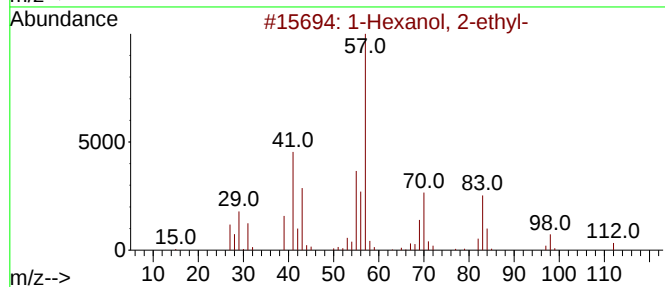
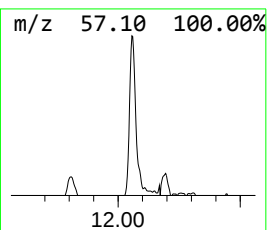
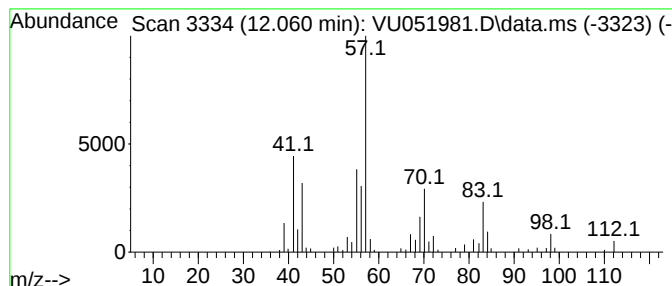
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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.
12.060	5.43 ug/L	96387	1,4-Dichlorobenzene-d4	11.809

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	86
2	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	78
3	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
4	1-Hexanol, 2-ethyl-			130	C8H18O	000104-76-7	64
5	2-Propyl-1-pentanol			130	C8H18O	058175-57-8	53



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051981.D
Acq On : 20 Nov 2022 18:14
Operator : JC/MD
Sample : N5710-05
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KY4

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
1-Hexanol, 2-et...	12.060	5.4	ug/L	96387	3	11.809	887549	50.0