

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051986.D
 Acq On : 20 Nov 2022 20:24
 Operator : JC/MD
 Sample : N5710-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COKZ0

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: VU051986.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.359	3	6	22	rVB	191546	197118	2.20%	0.465%
2	1.494	41	48	53	rBV2	19633	22354	0.25%	0.053%
3	1.604	71	82	96	rBV	4417071	5211060	58.26%	12.283%
4	1.729	117	121	127	rVB	29486	27042	0.30%	0.064%
5	1.906	167	176	194	rVB	107045	163434	1.83%	0.385%
6	2.150	246	252	261	rVV3	11216	14444	0.16%	0.034%
7	2.198	262	267	274	rVV	7046	9075	0.10%	0.021%
8	2.240	274	280	289	rVB	18214	23587	0.26%	0.056%
9	2.578	366	385	415	rBV	2157000	3681900	41.17%	8.679%
10	2.890	477	482	490	rBV5	503	724	0.01%	0.002%
11	2.977	505	509	518	rVB6	1764	2108	0.02%	0.005%
12	3.047	521	531	547	rVB5	5222	11183	0.13%	0.026%
13	3.131	552	557	560	rBV3	636	627	0.01%	0.001%
14	3.176	564	571	584	rVB4	3690	7305	0.08%	0.017%
15	3.353	614	626	647	rVB2	24763	49775	0.56%	0.117%
16	3.510	672	675	680	rBV3	812	770	0.01%	0.002%
17	3.578	694	696	701	rVB4	520	388	0.00%	0.001%
18	3.636	710	714	717	rBV3	247	261	0.00%	0.001%
19	3.694	730	732	735	rVV2	459	404	0.00%	0.001%
20	3.726	739	742	745	rBV2	334	253	0.00%	0.001%
21	3.761	751	753	758	rVB2	427	262	0.00%	0.001%
22	3.867	768	786	816	rBV2	238356	565978	6.33%	1.334%
23	3.989	820	824	828	rBV2	434	404	0.00%	0.001%
24	4.047	836	842	845	rBV3	375	394	0.00%	0.001%
25	4.137	867	870	877	rVB3	296	300	0.00%	0.001%
26	4.356	935	938	942	rVB2	363	248	0.00%	0.001%
27	4.440	959	964	967	rBV4	529	421	0.00%	0.001%
28	4.517	984	988	992	rBV3	751	663	0.01%	0.002%
29	4.562	997	1002	1003	rBV2	642	481	0.01%	0.001%
30	4.661	1007	1033	1063	rBV2	1565929	3914935	43.77%	9.228%
31	5.060	1141	1157	1181	rBV	261482	577529	6.46%	1.361%
32	5.259	1216	1219	1221	rVB3	481	254	0.00%	0.001%
33	5.314	1221	1236	1255	rBV2	69878	159705	1.79%	0.376%
34	5.620	1322	1331	1337	rBV3	575	887	0.01%	0.002%
35	5.722	1342	1363	1412	rBV2	458800	1368224	15.30%	3.225%
36	6.021	1442	1456	1476	rVB2	35451	72523	0.81%	0.171%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051986.D
 Acq On : 20 Nov 2022 20:24
 Operator : JC/MD
 Sample : N5710-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 COKZ0

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	6.108	1481	1483	1486	rBV3	366	294	0.00%	0.001%
38	6.137	1489	1492	1495	rBV2	463	328	0.00%	0.001%
39	6.247	1512	1526	1559	rBV	545671	1052216	11.76%	2.480%
40	6.539	1596	1617	1650	rBV	4867436	8943900	100.00%	21.082%
41	6.687	1652	1663	1681	rVB	340659	658316	7.36%	1.552%
42	6.957	1735	1747	1769	rVV	90107	177702	1.99%	0.419%
43	7.182	1802	1817	1832	rBV5	7286	15582	0.17%	0.037%
44	7.250	1832	1838	1847	rVB6	2442	3715	0.04%	0.009%
45	7.391	1879	1882	1884	rBV2	492	303	0.00%	0.001%
46	7.565	1922	1936	1957	rBV	143578	259267	2.90%	0.611%
47	7.693	1968	1976	1986	rVB5	4005	7139	0.08%	0.017%
48	7.803	2006	2010	2018	rVB5	691	897	0.01%	0.002%
49	7.896	2026	2039	2055	rBV	475897	820461	9.17%	1.934%
50	7.967	2056	2061	2075	rVB	11943	20946	0.23%	0.049%
51	8.099	2092	2102	2115	rBV	11918	19703	0.22%	0.046%
52	8.176	2115	2126	2143	rBV	99936	168507	1.88%	0.397%
53	8.269	2149	2155	2167	rVB2	4538	7204	0.08%	0.017%
54	8.398	2189	2195	2206	rVB7	2583	4853	0.05%	0.011%
55	8.484	2206	2222	2229	rBV	25699	45427	0.51%	0.107%
56	8.552	2229	2243	2258	rVV	5183605	8761768	97.96%	20.653%
57	8.629	2258	2267	2305	rVB2	508427	991941	11.09%	2.338%
58	8.938	2360	2363	2367	rBV5	633	647	0.01%	0.002%
59	9.037	2387	2394	2403	rVB4	5294	8026	0.09%	0.019%
60	9.076	2403	2406	2409	rBV3	351	250	0.00%	0.001%
61	9.282	2465	2470	2480	rVB3	3914	5666	0.06%	0.013%
62	9.414	2497	2511	2540	rBV	775339	1305908	14.60%	3.078%
63	9.664	2582	2589	2594	rBV5	1883	2404	0.03%	0.006%
64	9.758	2609	2618	2630	rVB3	8103	12981	0.15%	0.031%
65	9.809	2630	2634	2636	rBV3	329	295	0.00%	0.001%
66	9.828	2636	2640	2643	rBV3	443	349	0.00%	0.001%
67	9.867	2649	2652	2654	rBV3	639	418	0.00%	0.001%
68	10.102	2722	2725	2730	rVB3	576	512	0.01%	0.001%
69	10.282	2779	2781	2786	rVB3	408	287	0.00%	0.001%
70	10.555	2864	2866	2872	rVB4	510	430	0.00%	0.001%
71	10.655	2895	2897	2903	rVB3	409	295	0.00%	0.001%
72	10.754	2914	2928	2951	rBV	608674	976423	10.92%	2.302%
73	11.134	3042	3046	3050	rVB4	643	458	0.01%	0.001%
74	11.410	3129	3132	3134	rBV2	558	410	0.00%	0.001%
75	11.471	3148	3151	3158	rVB3	400	449	0.01%	0.001%
76	11.526	3158	3168	3177	rVB6	4700	7599	0.08%	0.018%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
 Data File : VU051986.D
 Acq On : 20 Nov 2022 20:24
 Operator : JC/MD
 Sample : N5710-11
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0KZ0

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	11.568	3177	3181	3186	rBV4	358	346	0.00%	0.001%
78	11.661	3207	3210	3213	rBV3	433	298	0.00%	0.001%
79	11.693	3214	3220	3223	rBV6	1771	1952	0.02%	0.005%
80	11.809	3244	3256	3285	rBV	606970	967575	10.82%	2.281%
81	12.057	3324	3333	3359	rBV3	58872	110519	1.24%	0.261%
82	12.192	3362	3375	3396	rVB	582375	957420	10.70%	2.257%
83	12.555	3486	3488	3491	rVV2	435	249	0.00%	0.001%
84	12.616	3496	3507	3510	rBV2	454	756	0.01%	0.002%
85	12.677	3522	3526	3533	rVB2	647	673	0.01%	0.002%
86	12.828	3570	3573	3581	rVB2	388	440	0.00%	0.001%
87	12.893	3583	3593	3601	rBV8	4119	6458	0.07%	0.015%
88	13.262	3703	3708	3709	rBV	361	363	0.00%	0.001%
89	13.385	3743	3746	3750	rBV3	386	350	0.00%	0.001%
90	13.716	3846	3849	3851	rBV	581	445	0.00%	0.001%
91	13.809	3875	3878	3880	rBV	491	376	0.00%	0.001%
92	14.134	3976	3979	3984	rVB3	465	287	0.00%	0.001%
93	14.166	3984	3989	3993	rBV3	795	957	0.01%	0.002%
94	14.388	4054	4058	4064	rVB2	463	486	0.01%	0.001%
95	14.417	4064	4067	4069	rBV3	459	358	0.00%	0.001%
96	14.995	4244	4247	4252	rBV3	542	567	0.01%	0.001%
97	15.330	4348	4351	4352	rBV	525	301	0.00%	0.001%
98	15.429	4378	4382	4384	rBV4	754	579	0.01%	0.001%
99	15.587	4429	4431	4434	rBV2	564	331	0.00%	0.001%
100	15.815	4498	4502	4506	rBV4	693	652	0.01%	0.002%

Sum of corrected areas: 42424034

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051986.D
Acq On : 20 Nov 2022 20:24
Operator : JC/MD
Sample : N5710-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COKZ0

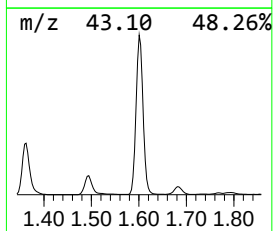
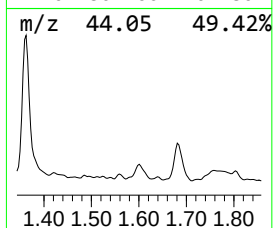
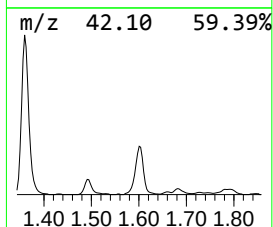
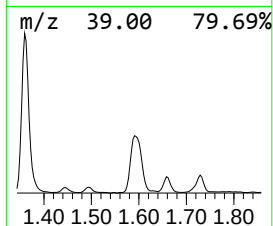
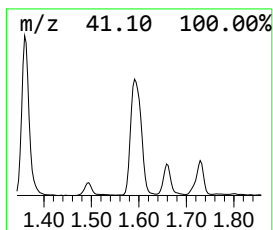
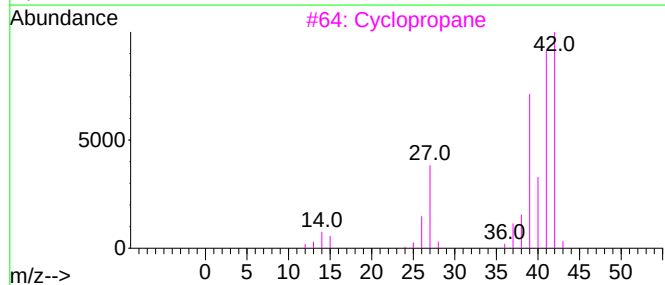
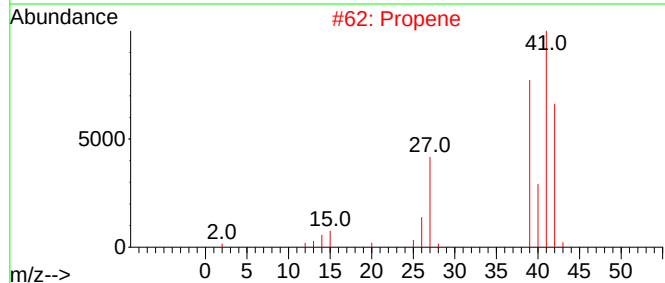
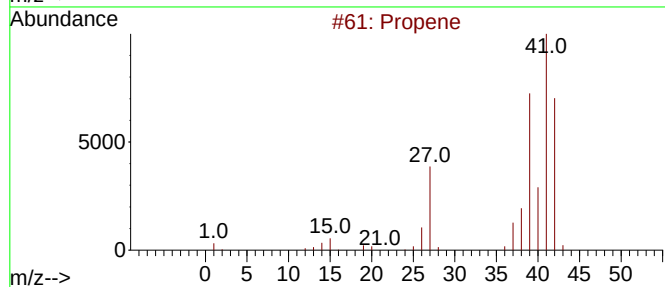
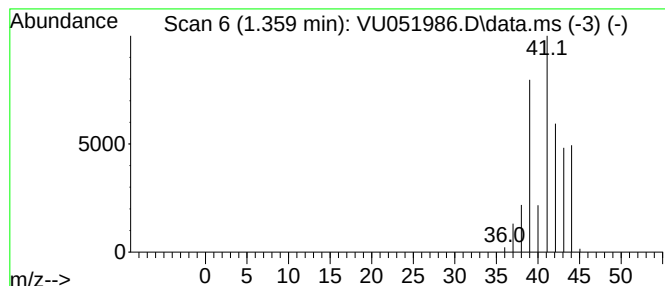
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.359	9.37 ug/L	197118	1,4-Difluorobenzene	6.247

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		Propene	42	C3H6	000115-07-1	72
2		Propene	42	C3H6	000115-07-1	42
3		Cyclopropane	42	C3H6	000075-19-4	9
4		Cyclopropene	40	C3H4	002781-85-3	9
5		Cyclopropane	42	C3H6	000075-19-4	7



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051986.D
Acq On : 20 Nov 2022 20:24
Operator : JC/MD
Sample : N5710-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
COKZ0

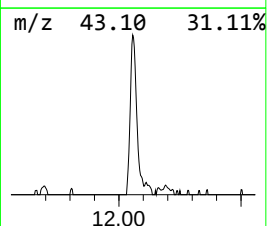
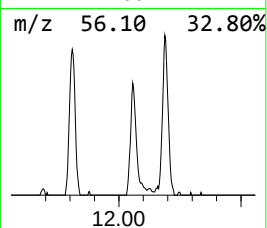
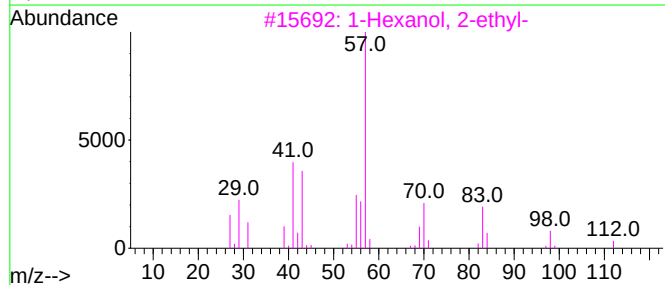
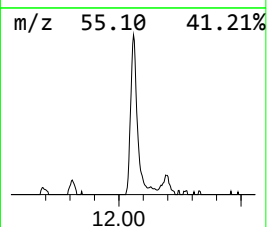
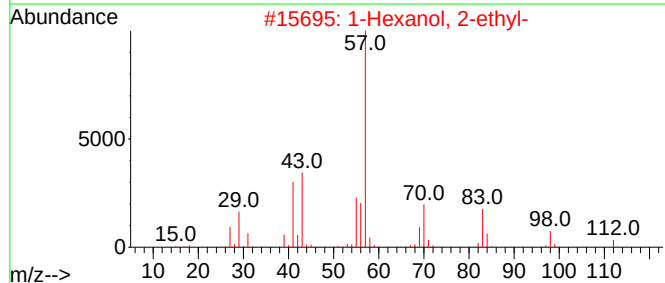
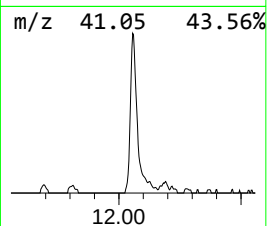
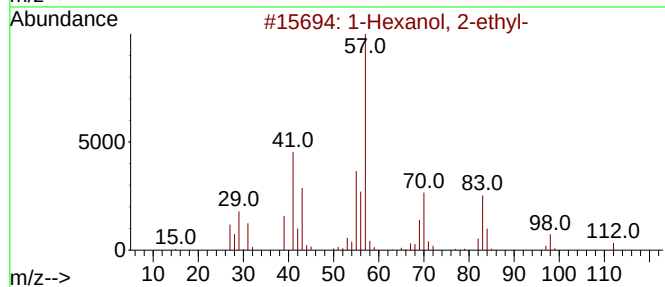
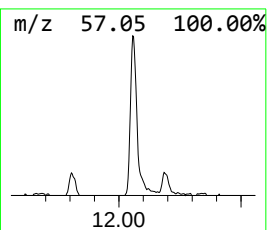
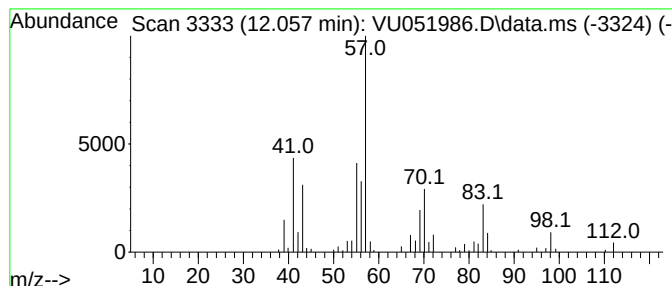
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM111522WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 1-Hexanol, 2-ethyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.057	5.71 ug/L	110519	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	78
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	78
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	64
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	64
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU112022\
Data File : VU051986.D
Acq On : 20 Nov 2022 20:24
Operator : JC/MD
Sample : N5710-11
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
C0KZ0

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
(DEL) Alkane: S...	1.359	9.4	ug/L	197118	1	6.247	1052220	50.0
1-Hexanol, 2-et...	12.057	5.7	ug/L	110519	3	11.809	967575	50.0