

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
 Data File : VU048586.D
 Acq On : 16 May 2022 17:36
 Operator : SY/MD
 Sample : N2821-21
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXLE7

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: VU048586.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	71	80	98	rVB	96353	118906	12.77%	1.552%
2	1.912	170	178	194	rVB	70343	92820	9.97%	1.212%
3	2.257	283	285	286	rBV	461	181	0.02%	0.002%
4	2.568	365	382	394	rBV	193183	316570	33.99%	4.133%
5	2.752	431	439	449	rBV	4891	8264	0.89%	0.108%
6	2.832	461	464	467	rVB	242	184	0.02%	0.002%
7	2.900	482	485	488	rVV2	437	310	0.03%	0.004%
8	2.961	496	504	511	rVB2	546	825	0.09%	0.011%
9	3.038	526	528	533	rVB2	347	246	0.03%	0.003%
10	3.138	556	559	560	rVV	305	211	0.02%	0.003%
11	3.179	560	572	593	rVB3	13103	31077	3.34%	0.406%
12	3.324	613	617	621	rVB	321	291	0.03%	0.004%
13	3.366	626	630	635	rBB2	353	378	0.04%	0.005%
14	3.401	639	641	645	rVB2	270	172	0.02%	0.002%
15	3.437	649	652	655	rVV	240	160	0.02%	0.002%
16	3.588	696	699	701	rBV2	389	299	0.03%	0.004%
17	3.758	746	752	755	rBB	274	259	0.03%	0.003%
18	3.793	756	763	764	rBV	179	226	0.02%	0.003%
19	3.957	812	814	818	rBB	265	161	0.02%	0.002%
20	3.986	821	823	828	rBB	264	183	0.02%	0.002%
21	4.051	839	843	845	rBV	297	229	0.02%	0.003%
22	4.089	852	855	858	rBV	185	163	0.02%	0.002%
23	4.134	865	869	874	rBB	216	260	0.03%	0.003%
24	4.205	887	891	895	rBB2	313	244	0.03%	0.003%
25	4.359	936	939	941	rBV	267	161	0.02%	0.002%
26	4.449	951	967	977	rBV6	4005	10735	1.15%	0.140%
27	4.549	994	998	1000	rBV	257	174	0.02%	0.002%
28	4.620	1006	1020	1048	rBV2	99380	244609	26.26%	3.194%
29	5.063	1139	1158	1183	rBV	182712	400178	42.96%	5.225%
30	5.208	1198	1203	1208	rBV2	325	353	0.04%	0.005%
31	5.234	1208	1211	1215	rVB2	364	334	0.04%	0.004%
32	5.295	1226	1230	1232	rBV	496	477	0.05%	0.006%
33	5.337	1241	1243	1247	rVB	267	157	0.02%	0.002%
34	5.382	1254	1257	1260	rBV	568	376	0.04%	0.005%
35	5.469	1279	1284	1286	rBV	161	194	0.02%	0.003%
36	5.485	1287	1289	1293	rVB	313	215	0.02%	0.003%

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

37	5.559	1308	1312	1313	rBV	190	156	0.02%	0.002%
38	5.626	1330	1333	1334	rBV	250	160	0.02%	0.002%
39	5.726	1342	1364	1388	rBV2	337673	931417	100.00%	12.160%
40	5.944	1429	1432	1436	rVB2	306	229	0.02%	0.003%
41	6.041	1459	1462	1463	rBV	409	238	0.03%	0.003%
42	6.073	1467	1472	1474	rBV	301	223	0.02%	0.003%
43	6.186	1504	1507	1510	rBV2	290	282	0.03%	0.004%
44	6.250	1513	1527	1547	rBV	296417	554774	59.56%	7.243%
45	6.465	1588	1594	1599	rBV3	238	302	0.03%	0.004%
46	6.533	1606	1615	1625	rBB7	2345	5050	0.54%	0.066%
47	6.690	1650	1664	1684	rBV	210270	411910	44.22%	5.378%
48	6.887	1722	1725	1728	rBV	513	317	0.03%	0.004%
49	6.957	1744	1747	1756	rBB2	298	363	0.04%	0.005%
50	7.038	1767	1772	1774	rBV	290	289	0.03%	0.004%
51	7.128	1789	1800	1804	rBV6	1961	3283	0.35%	0.043%
52	7.565	1925	1936	1958	rVV	127025	225551	24.22%	2.945%
53	7.687	1969	1974	1976	rBV2	1064	931	0.10%	0.012%
54	7.732	1986	1988	1992	rVB2	319	216	0.02%	0.003%
55	7.803	2002	2010	2014	rBV2	520	637	0.07%	0.008%
56	7.899	2026	2040	2055	rBV	444161	758932	81.48%	9.908%
57	8.096	2099	2101	2104	rVB	369	202	0.02%	0.003%
58	8.179	2115	2127	2143	rBV	92540	163290	17.53%	2.132%
59	8.472	2206	2218	2229	rBV2	9841	18428	1.98%	0.241%
60	8.632	2255	2268	2303	rBV	290829	539762	57.95%	7.047%
61	8.829	2326	2329	2333	rVB	292	188	0.02%	0.002%
62	9.102	2410	2414	2416	rBV	202	190	0.02%	0.002%
63	9.163	2432	2433	2436	rVB2	475	204	0.02%	0.003%
64	9.182	2436	2439	2442	rBV	245	204	0.02%	0.003%
65	9.205	2443	2446	2449	rVV2	220	154	0.02%	0.002%
66	9.372	2494	2498	2499	rBV	232	175	0.02%	0.002%
67	9.417	2500	2512	2532	rBV	428582	707745	75.99%	9.240%
68	9.655	2583	2586	2589	rVB2	261	155	0.02%	0.002%
69	9.694	2592	2598	2602	rBV4	953	1129	0.12%	0.015%
70	10.031	2700	2703	2707	rVB	322	188	0.02%	0.002%
71	10.092	2717	2722	2724	rBV2	542	518	0.06%	0.007%
72	10.105	2724	2726	2728	rBV2	327	196	0.02%	0.003%
73	10.202	2753	2756	2759	rVB2	310	227	0.02%	0.003%
74	10.266	2772	2776	2778	rBV	327	304	0.03%	0.004%
75	10.324	2790	2794	2795	rBV	334	166	0.02%	0.002%
76	10.349	2796	2802	2808	rVV3	1668	1605	0.17%	0.021%

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77	10.391	2812	2815	2822	rVB	257	188	0.02%	0.002%
78	10.671	2896	2902	2904	rBV3	1067	1006	0.11%	0.013%
79	10.758	2916	2929	2949	rBV	321227	517413	55.55%	6.755%
80	10.893	2963	2971	2986	rVB3	11002	18490	1.99%	0.241%
81	11.021	3008	3011	3015	rVB	207	148	0.02%	0.002%
82	11.092	3029	3033	3039	rBV2	435	426	0.05%	0.006%
83	11.327	3102	3106	3109	rBV2	373	268	0.03%	0.003%
84	11.462	3143	3148	3150	rBV3	1324	1223	0.13%	0.016%
85	11.619	3188	3197	3199	rBV	403	541	0.06%	0.007%
86	11.693	3216	3220	3224	rBV3	723	558	0.06%	0.007%
87	11.751	3231	3238	3243	rBV3	1412	1574	0.17%	0.021%
88	11.812	3245	3257	3273	rBV	475948	767350	82.39%	10.018%
89	11.973	3304	3307	3313	rVB2	958	837	0.09%	0.011%
90	12.076	3334	3339	3342	rBV	269	280	0.03%	0.004%
91	12.195	3362	3376	3397	rBV	471932	779990	83.74%	10.183%
92	12.587	3495	3498	3501	rBV	361	216	0.02%	0.003%
93	12.742	3543	3546	3550	rBV3	447	354	0.04%	0.005%
94	13.086	3650	3653	3656	rBV2	390	195	0.02%	0.003%
95	13.224	3690	3696	3698	rBV2	1142	1088	0.12%	0.014%
96	13.526	3786	3790	3793	rBV2	381	302	0.03%	0.004%
97	13.848	3882	3890	3899	rBV4	2235	3297	0.35%	0.043%
98	13.960	3922	3925	3928	rBV2	351	316	0.03%	0.004%
99	14.092	3962	3966	3974	rBV3	2118	2235	0.24%	0.029%
100	14.224	4004	4007	4008	rBV	478	305	0.03%	0.004%

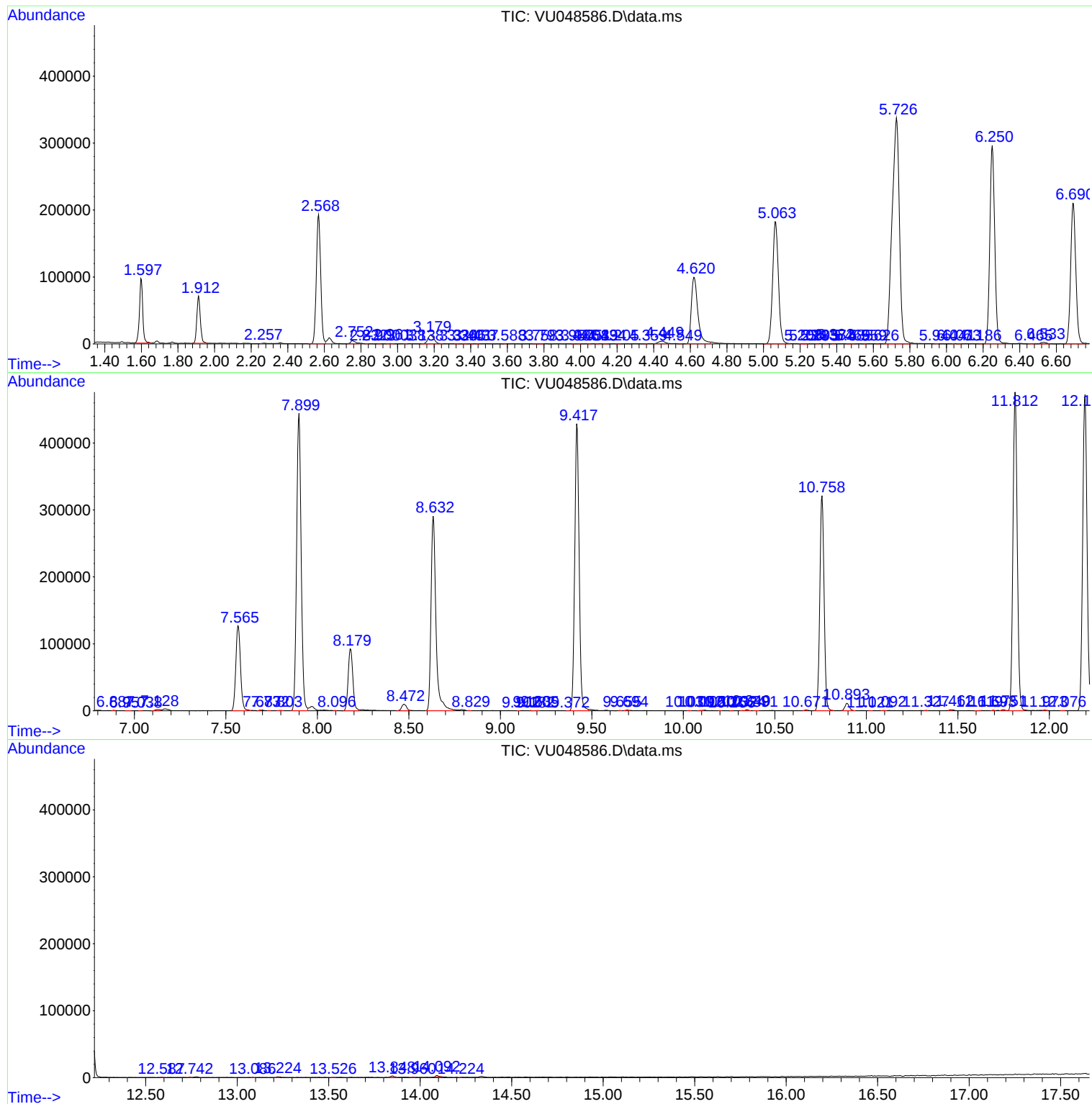
Sum of corrected areas: 7659472

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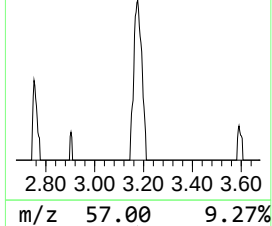
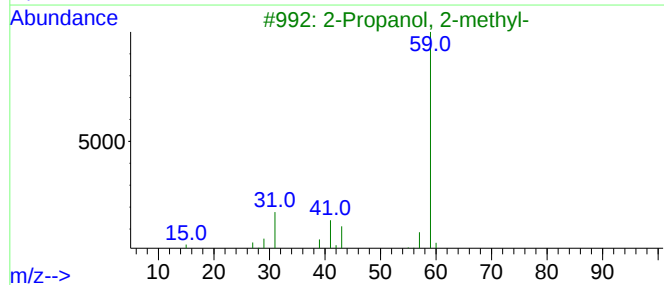
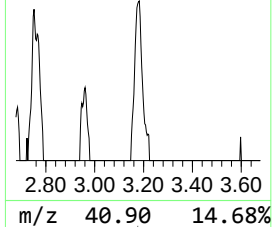
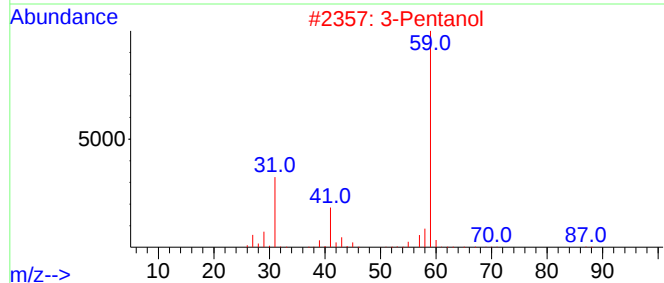
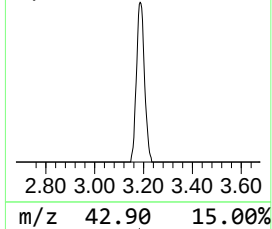
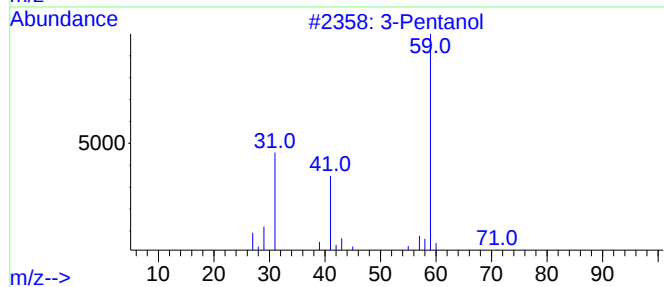
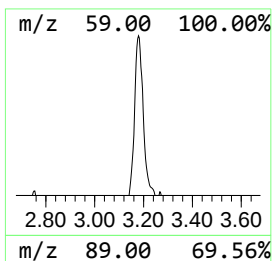
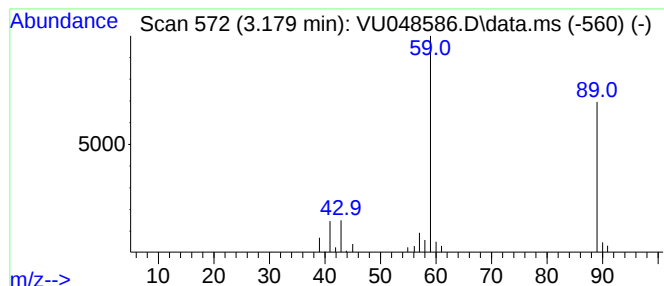
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.179	2.80 ug/L	31077	1,4-Difluorobenzene	6.250

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Pentanol	88	C5H12O	000584-02-1	40
2		3-Pentanol	88	C5H12O	000584-02-1	38
3		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
4		2-Propanol, 2-methyl-	74	C4H10O	000075-65-0	38
5		3-Pentanol	88	C5H12O	000584-02-1	38



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	3.179	2.8	ug/L	31077	1	6.250	554774	50.0