

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
 Data File : VU048592.D
 Acq On : 16 May 2022 19:57
 Operator : SY/MD
 Sample : N2849-04
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXW9

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: VU048592.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	74	81	97	rVB	88219	100103	11.04%	1.261%
2	1.684	103	107	117	rVB	5132	5903	0.65%	0.074%
3	1.912	170	178	192	rBV	70391	90247	9.95%	1.137%
4	2.205	262	269	276	rVB3	2865	4137	0.46%	0.052%
5	2.485	353	356	358	rBV3	434	249	0.03%	0.003%
6	2.568	366	382	395	rBV	191776	317505	35.02%	4.000%
7	2.755	437	440	441	rBV	469	194	0.02%	0.002%
8	2.909	483	488	491	rBV2	418	326	0.04%	0.004%
9	2.932	491	495	498	rBV2	239	201	0.02%	0.003%
10	2.986	507	512	513	rBV	265	165	0.02%	0.002%
11	3.057	528	534	536	rBB2	556	425	0.05%	0.005%
12	3.266	597	599	604	rBV	263	225	0.02%	0.003%
13	3.408	640	643	645	rBV	301	171	0.02%	0.002%
14	3.584	695	698	701	rVV3	507	400	0.04%	0.005%
15	3.678	724	727	729	rBV	224	168	0.02%	0.002%
16	4.131	863	868	870	rBB	191	173	0.02%	0.002%
17	4.147	871	873	880	rBB	191	204	0.02%	0.003%
18	4.256	904	907	911	rBV2	260	249	0.03%	0.003%
19	4.453	960	968	981	rBV5	3066	7053	0.78%	0.089%
20	4.575	1003	1006	1008	rBV	412	301	0.03%	0.004%
21	4.620	1008	1020	1047	rVV	89764	214655	23.68%	2.705%
22	4.909	1107	1110	1115	rVB	359	284	0.03%	0.004%
23	4.935	1115	1118	1123	rVB	265	197	0.02%	0.002%
24	4.990	1133	1135	1137	rBV	391	231	0.03%	0.003%
25	5.067	1142	1159	1187	rVV2	187364	467558	51.57%	5.891%
26	5.199	1198	1200	1204	rVB2	420	228	0.03%	0.003%
27	5.285	1223	1227	1229	rBV	395	274	0.03%	0.003%
28	5.346	1243	1246	1249	rBV	193	170	0.02%	0.002%
29	5.385	1256	1258	1260	rBV	314	179	0.02%	0.002%
30	5.533	1300	1304	1307	rBV2	279	214	0.02%	0.003%
31	5.591	1319	1322	1325	rBB	299	221	0.02%	0.003%
32	5.726	1343	1364	1391	rBV2	326221	906655	100.00%	11.423%
33	5.903	1416	1419	1421	rBV3	535	310	0.03%	0.004%
34	5.970	1437	1440	1444	rVB3	508	377	0.04%	0.005%
35	6.025	1454	1457	1460	rVB	403	229	0.03%	0.003%
36	6.115	1476	1485	1488	rBB3	389	467	0.05%	0.006%

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

37	6.179	1503	1505	1512	rVB	293	291	0.03%	0.004%
38	6.250	1513	1527	1549	rBV	290214	548335	60.48%	6.909%
39	6.430	1580	1583	1587	rVB2	282	175	0.02%	0.002%
40	6.497	1602	1604	1607	rBV	363	250	0.03%	0.003%
41	6.530	1607	1614	1629	rVB3	3000	5366	0.59%	0.068%
42	6.633	1642	1646	1651	rBV2	369	360	0.04%	0.005%
43	6.690	1651	1664	1682	rBV2	200857	395617	43.63%	4.985%
44	6.800	1694	1698	1699	rBV	301	247	0.03%	0.003%
45	6.813	1699	1702	1707	rVB4	906	768	0.08%	0.010%
46	6.880	1714	1723	1739	rBV4	15977	28215	3.11%	0.355%
47	6.964	1745	1749	1754	rBV	265	240	0.03%	0.003%
48	7.105	1782	1793	1808	rVB2	19552	35468	3.91%	0.447%
49	7.182	1808	1817	1821	rBV4	1244	1611	0.18%	0.020%
50	7.565	1923	1936	1952	rBV2	122162	217898	24.03%	2.745%
51	7.784	2000	2004	2006	rVV	354	290	0.03%	0.004%
52	7.851	2022	2025	2026	rBV	298	177	0.02%	0.002%
53	7.899	2026	2040	2057	rBV	429684	733612	80.91%	9.243%
54	8.128	2109	2111	2115	rVB	334	233	0.03%	0.003%
55	8.179	2115	2127	2143	rBV	93973	160494	17.70%	2.022%
56	8.375	2185	2188	2191	rBV2	374	263	0.03%	0.003%
57	8.475	2209	2219	2228	rBV4	2062	3508	0.39%	0.044%
58	8.584	2251	2253	2256	rBV	234	169	0.02%	0.002%
59	8.632	2256	2268	2304	rVV	276061	513146	56.60%	6.465%
60	8.787	2305	2316	2341	rVB2	220541	392743	43.32%	4.948%
61	8.986	2375	2378	2381	rBV2	270	168	0.02%	0.002%
62	9.140	2422	2426	2429	rBV2	299	232	0.03%	0.003%
63	9.160	2429	2432	2434	rBV	289	190	0.02%	0.002%
64	9.263	2455	2464	2468	rBB	361	404	0.04%	0.005%
65	9.417	2499	2512	2545	rBV	419424	706741	77.95%	8.905%
66	9.642	2579	2582	2586	rBV2	245	210	0.02%	0.003%
67	9.700	2592	2600	2612	rVB5	1038	1717	0.19%	0.022%
68	10.298	2779	2786	2792	rVV4	591	694	0.08%	0.009%
69	10.346	2793	2801	2811	rVV5	5350	8220	0.91%	0.104%
70	10.449	2830	2833	2836	rBV	310	170	0.02%	0.002%
71	10.555	2862	2866	2868	rBV	334	252	0.03%	0.003%
72	10.671	2894	2902	2908	rBV3	1071	1108	0.12%	0.014%
73	10.758	2916	2929	2947	rBV	306268	501776	55.34%	6.322%
74	10.893	2961	2971	2981	rVB3	2991	5014	0.55%	0.063%
75	11.137	3045	3047	3052	rVB2	328	208	0.02%	0.003%
76	11.256	3079	3084	3092	rBV2	1210	1558	0.17%	0.020%

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Peak Location: TOP

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

77	11.308	3092	3100	3108	rBV6	4223	6163	0.68%	0.078%
78	11.378	3118	3122	3123	rBV	533	268	0.03%	0.003%
79	11.410	3130	3132	3136	rVB2	346	228	0.03%	0.003%
80	11.452	3144	3145	3146	rBB	199	186	0.02%	0.002%
81	11.578	3182	3184	3185	rBV2	461	201	0.02%	0.003%
82	11.693	3212	3220	3230	rBV4	7362	10884	1.20%	0.137%
83	11.812	3244	3257	3275	rBV	476715	756065	83.39%	9.526%
84	11.912	3285	3288	3291	rBV	513	393	0.04%	0.005%
85	12.012	3316	3319	3322	rBV	203	197	0.02%	0.002%
86	12.044	3326	3329	3331	rVV	253	170	0.02%	0.002%
87	12.099	3343	3346	3351	rVB	320	278	0.03%	0.004%
88	12.124	3351	3354	3357	rBV2	429	306	0.03%	0.004%
89	12.150	3360	3362	3363	rVV	470	239	0.03%	0.003%
90	12.195	3363	3376	3398	rVB	461318	758733	83.68%	9.560%
91	12.533	3478	3481	3483	rBV2	293	194	0.02%	0.002%
92	12.558	3485	3489	3496	rVB4	1283	1417	0.16%	0.018%
93	12.893	3585	3593	3602	rBV5	6468	9213	1.02%	0.116%
94	13.144	3667	3671	3676	rBV	440	390	0.04%	0.005%
95	13.221	3692	3695	3696	rBV	629	320	0.04%	0.004%
96	13.304	3718	3721	3724	rVB	431	267	0.03%	0.003%
97	13.327	3724	3728	3730	rBV2	354	255	0.03%	0.003%
98	13.571	3801	3804	3807	rBV2	386	262	0.03%	0.003%
99	13.844	3886	3889	3899	rVB5	937	1093	0.12%	0.014%
100	14.182	3990	3994	3996	rBV2	437	360	0.04%	0.005%

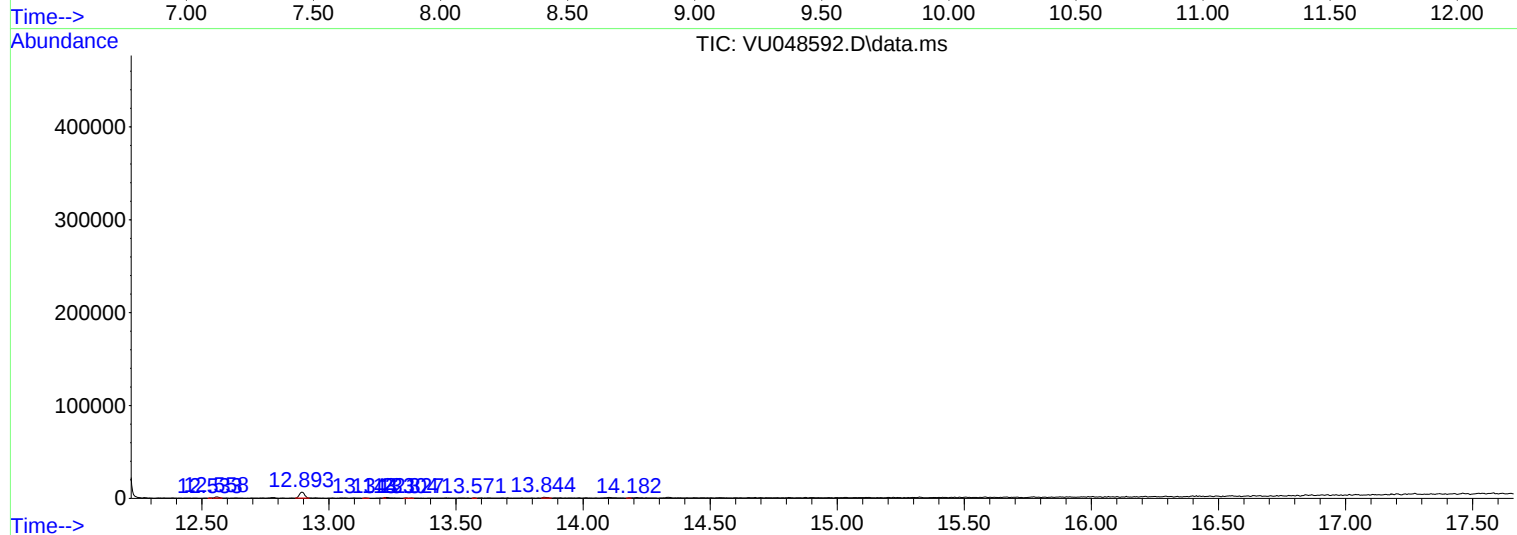
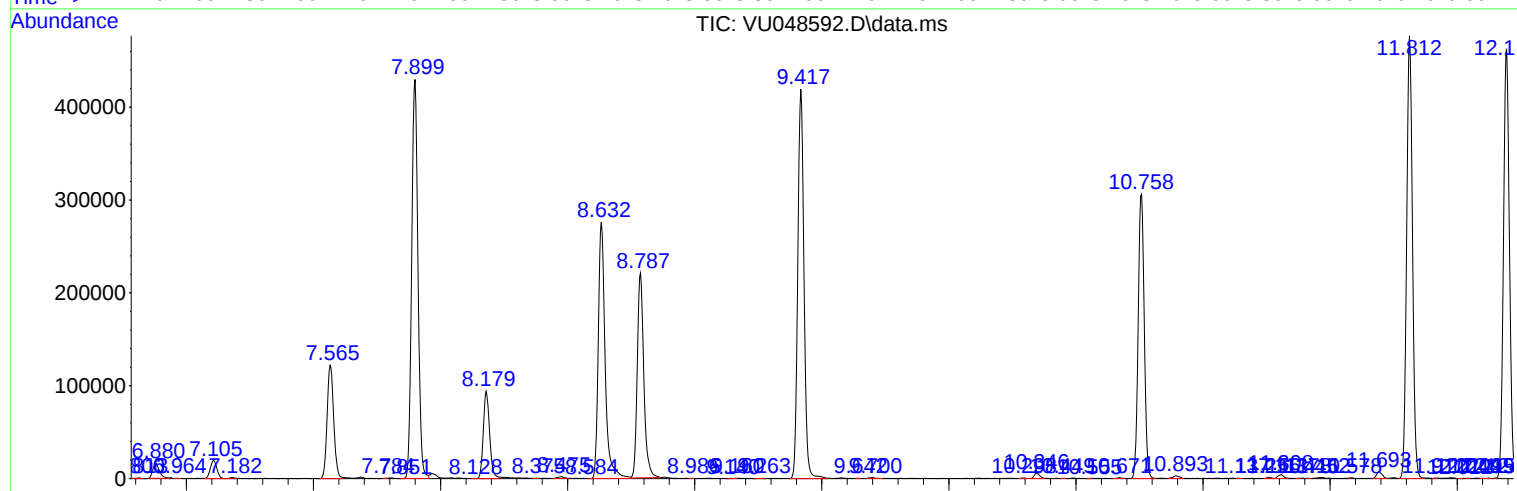
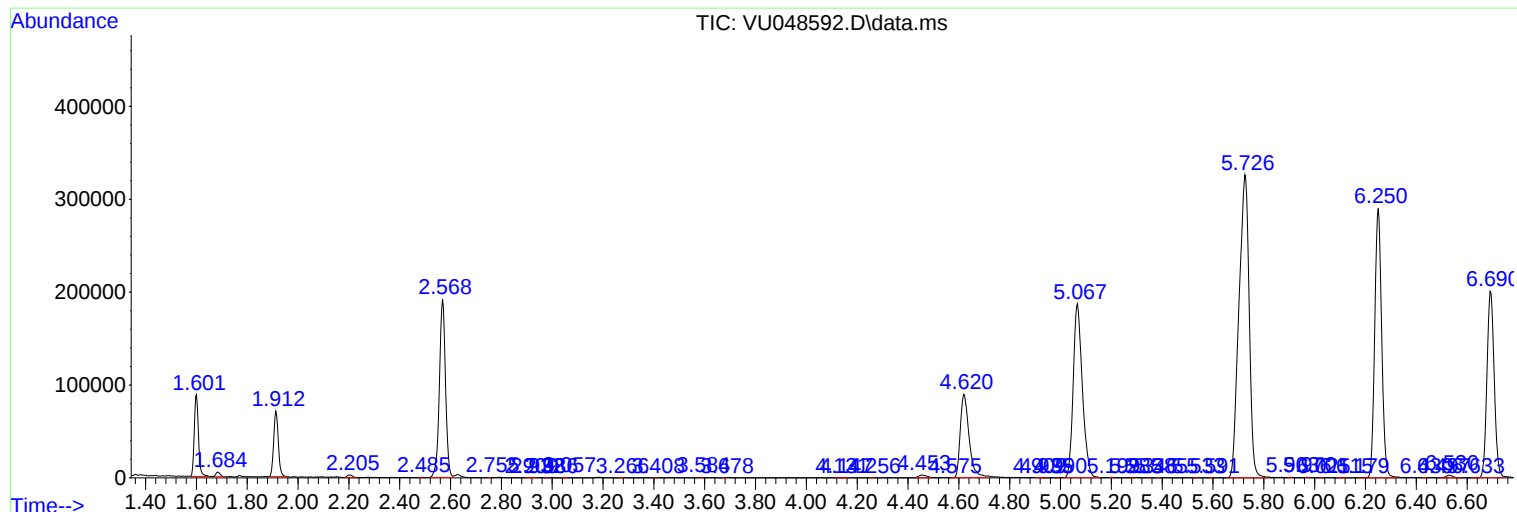
Sum of corrected areas: 7936868

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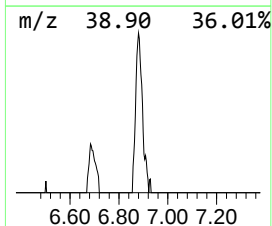
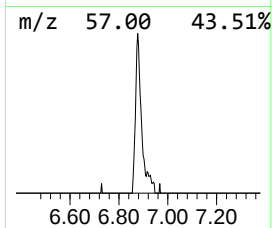
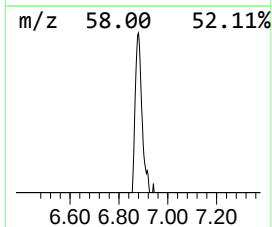
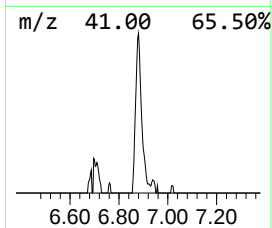
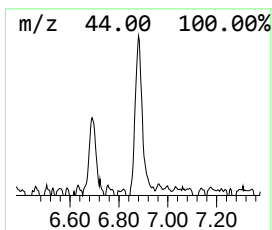
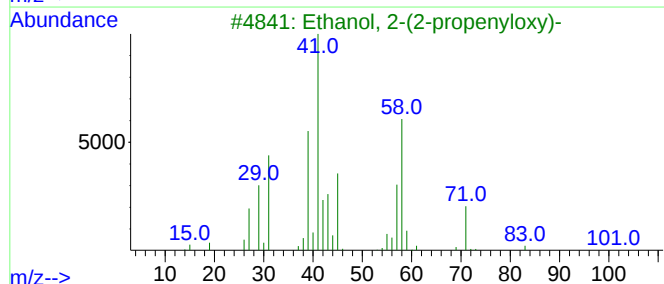
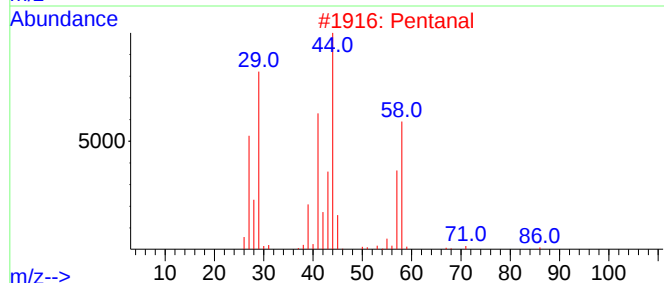
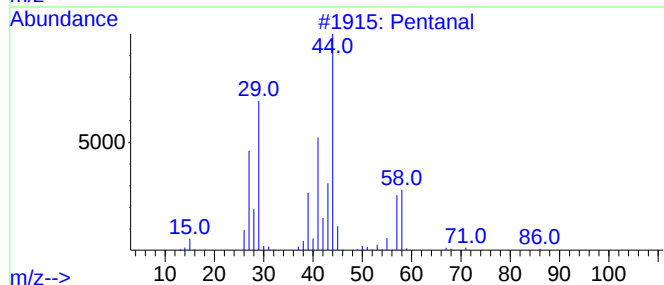
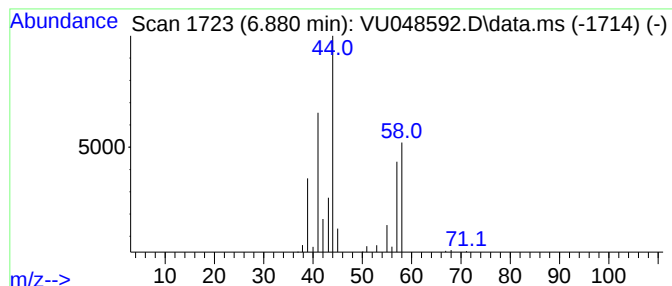
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Pentanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.880	2.57 ug/L	28215	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentanal			86	C5H10O	000110-62-3	56
2	Pentanal			86	C5H10O	000110-62-3	56
3	Ethanol, 2-(2-propenyloxy)-			102	C5H10O2	000111-45-5	10
4	Cyclopropyl carbinol			72	C4H8O	002516-33-8	9
5	Cyclopropyl carbinol			72	C4H8O	002516-33-8	9



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentanal	6.880	2.6	ug/L	28215	1	6.250	548335	50.0