

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051622\
 Data File : VU048593.D
 Acq On : 16 May 2022 20:21
 Operator : SY/MD
 Sample : N2849-05
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXX0

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: VU048593.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	73	81	98	rVB	90910	99417	11.02%	1.259%
2	1.684	103	107	114	rVB2	4944	4925	0.55%	0.062%
3	1.912	170	178	194	rVB	68729	88610	9.82%	1.122%
4	2.208	262	270	278	rVB4	3461	4944	0.55%	0.063%
5	2.568	364	382	396	rBV	190040	315469	34.97%	3.995%
6	2.691	416	420	424	rBV	188	232	0.03%	0.003%
7	2.784	444	449	451	rBV	308	299	0.03%	0.004%
8	2.973	504	508	510	rBV	328	256	0.03%	0.003%
9	3.047	526	531	536	rBB3	687	600	0.07%	0.008%
10	3.092	542	545	551	rBB	192	253	0.03%	0.003%
11	3.154	563	564	567	rBV	272	155	0.02%	0.002%
12	3.182	567	573	575	rBV3	734	806	0.09%	0.010%
13	3.420	645	647	652	rBB	187	188	0.02%	0.002%
14	3.588	694	699	703	rBV4	560	541	0.06%	0.007%
15	3.665	720	723	725	rBV2	268	170	0.02%	0.002%
16	3.690	730	731	735	rBV	235	167	0.02%	0.002%
17	3.771	753	756	760	rBB	194	175	0.02%	0.002%
18	3.864	781	785	788	rBV	216	204	0.02%	0.003%
19	3.906	795	798	800	rBB	290	167	0.02%	0.002%
20	3.922	800	803	807	rBV	242	195	0.02%	0.002%
21	4.134	865	869	870	rBV	300	223	0.02%	0.003%
22	4.231	895	899	902	rBB	193	177	0.02%	0.002%
23	4.260	903	908	911	rBB	203	202	0.02%	0.003%
24	4.305	918	922	925	rBB	188	156	0.02%	0.002%
25	4.456	960	969	970	rBV3	2761	3554	0.39%	0.045%
26	4.620	1006	1020	1043	rBV	92483	217804	24.14%	2.758%
27	4.919	1108	1113	1115	rBV2	191	200	0.02%	0.003%
28	4.948	1119	1122	1124	rBV	288	184	0.02%	0.002%
29	4.964	1124	1127	1132	rVB2	278	233	0.03%	0.003%
30	4.996	1133	1137	1139	rBV	262	226	0.03%	0.003%
31	5.067	1142	1159	1185	rBV2	185475	464681	51.51%	5.884%
32	5.285	1224	1227	1231	rBV2	499	436	0.05%	0.006%
33	5.391	1258	1260	1264	rVB	382	235	0.03%	0.003%
34	5.440	1272	1275	1278	rVB	258	225	0.02%	0.003%
35	5.478	1284	1287	1294	rBV	273	273	0.03%	0.003%
36	5.578	1312	1318	1320	rBV	207	234	0.03%	0.003%

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

37	5.726	1342	1364	1386	rBV2	324947	902195	100.00%	11.424%
38	5.906	1418	1420	1423	rBV2	351	231	0.03%	0.003%
39	5.983	1442	1444	1448	rBV	365	216	0.02%	0.003%
40	6.038	1458	1461	1464	rBV3	323	266	0.03%	0.003%
41	6.121	1484	1487	1489	rBV2	309	171	0.02%	0.002%
42	6.137	1490	1492	1497	rVB3	280	171	0.02%	0.002%
43	6.250	1513	1527	1547	rVV	289814	544738	60.38%	6.898%
44	6.446	1584	1588	1592	rVB2	217	201	0.02%	0.003%
45	6.530	1604	1614	1625	rBV6	2709	5504	0.61%	0.070%
46	6.690	1650	1664	1684	rBV	201557	394265	43.70%	4.992%
47	6.880	1713	1723	1738	rBV2	14941	27331	3.03%	0.346%
48	6.996	1756	1759	1762	rBV2	337	261	0.03%	0.003%
49	7.108	1783	1794	1805	rBV3	19056	34032	3.77%	0.431%
50	7.179	1811	1816	1817	rBV2	719	676	0.07%	0.009%
51	7.369	1871	1875	1881	rBV	280	298	0.03%	0.004%
52	7.520	1918	1922	1924	rBV	175	161	0.02%	0.002%
53	7.565	1924	1936	1952	rBV	122998	215849	23.92%	2.733%
54	7.722	1982	1985	1988	rBV2	429	337	0.04%	0.004%
55	7.793	1999	2007	2009	rBV3	1006	935	0.10%	0.012%
56	7.838	2018	2021	2025	rVB2	419	303	0.03%	0.004%
57	7.899	2026	2040	2056	rBV	425252	724816	80.34%	9.178%
58	8.179	2113	2127	2143	rBV	90576	157577	17.47%	1.995%
59	8.417	2198	2201	2204	rVB2	387	230	0.03%	0.003%
60	8.475	2209	2219	2225	rBV4	1856	3121	0.35%	0.040%
61	8.558	2243	2245	2249	rVB	466	266	0.03%	0.003%
62	8.632	2256	2268	2303	rBV	279746	518593	57.48%	6.567%
63	8.787	2305	2316	2340	rVB	218974	383828	42.54%	4.860%
64	9.163	2431	2433	2435	rBV	366	201	0.02%	0.003%
65	9.173	2435	2436	2439	rVV2	458	230	0.03%	0.003%
66	9.202	2442	2445	2448	rBV	165	160	0.02%	0.002%
67	9.417	2499	2512	2534	rBV	412371	693768	76.90%	8.785%
68	9.565	2554	2558	2559	rBV2	469	281	0.03%	0.004%
69	9.578	2559	2562	2565	rVB2	743	493	0.05%	0.006%
70	9.639	2579	2581	2584	rBV	350	213	0.02%	0.003%
71	9.693	2593	2598	2606	rVB3	1179	1631	0.18%	0.021%
72	9.787	2625	2627	2631	rBV	365	252	0.03%	0.003%
73	10.092	2719	2722	2724	rBV	353	232	0.03%	0.003%
74	10.237	2765	2767	2774	rVB4	550	537	0.06%	0.007%
75	10.292	2780	2784	2786	rBV2	367	329	0.04%	0.004%
76	10.343	2793	2800	2816	rVB5	5045	7979	0.88%	0.101%

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Peak Location: TOP

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

77	10.500	2844	2849	2853	rVV3	261	256	0.03%	0.003%
78	10.668	2897	2901	2903	rBV	798	641	0.07%	0.008%
79	10.758	2916	2929	2946	rBV	313535	510918	56.63%	6.470%
80	10.893	2963	2971	2980	rBV4	3804	5477	0.61%	0.069%
81	11.044	3016	3018	3021	rBV2	349	181	0.02%	0.002%
82	11.259	3079	3085	3092	rBV2	1186	1531	0.17%	0.019%
83	11.301	3092	3098	3107	rVV9	3707	5783	0.64%	0.073%
84	11.462	3137	3148	3151	rBV4	1352	1771	0.20%	0.022%
85	11.497	3157	3159	3163	rVB	381	187	0.02%	0.002%
86	11.587	3181	3187	3191	rBV3	566	645	0.07%	0.008%
87	11.629	3197	3200	3203	rBV2	305	249	0.03%	0.003%
88	11.690	3212	3219	3230	rVB4	6658	10396	1.15%	0.132%
89	11.812	3244	3257	3275	rBV	481331	757413	83.95%	9.591%
90	12.073	3329	3338	3348	rBV5	2343	3987	0.44%	0.050%
91	12.195	3362	3376	3391	rBV	454801	752763	83.44%	9.532%
92	12.327	3415	3417	3419	rBV	405	235	0.03%	0.003%
93	12.404	3439	3441	3448	rVB2	426	368	0.04%	0.005%
94	12.558	3483	3489	3498	rVB6	1862	2801	0.31%	0.035%
95	12.893	3586	3593	3601	rBV4	7184	9712	1.08%	0.123%
96	13.008	3626	3629	3632	rBV	397	271	0.03%	0.003%
97	13.057	3641	3644	3647	rBV2	395	218	0.02%	0.003%
98	13.330	3726	3729	3732	rBV2	334	213	0.02%	0.003%
99	13.799	3872	3875	3877	rBV2	386	233	0.03%	0.003%
100	13.841	3884	3888	3894	rBV3	1146	1314	0.15%	0.017%

Sum of corrected areas: 7897257

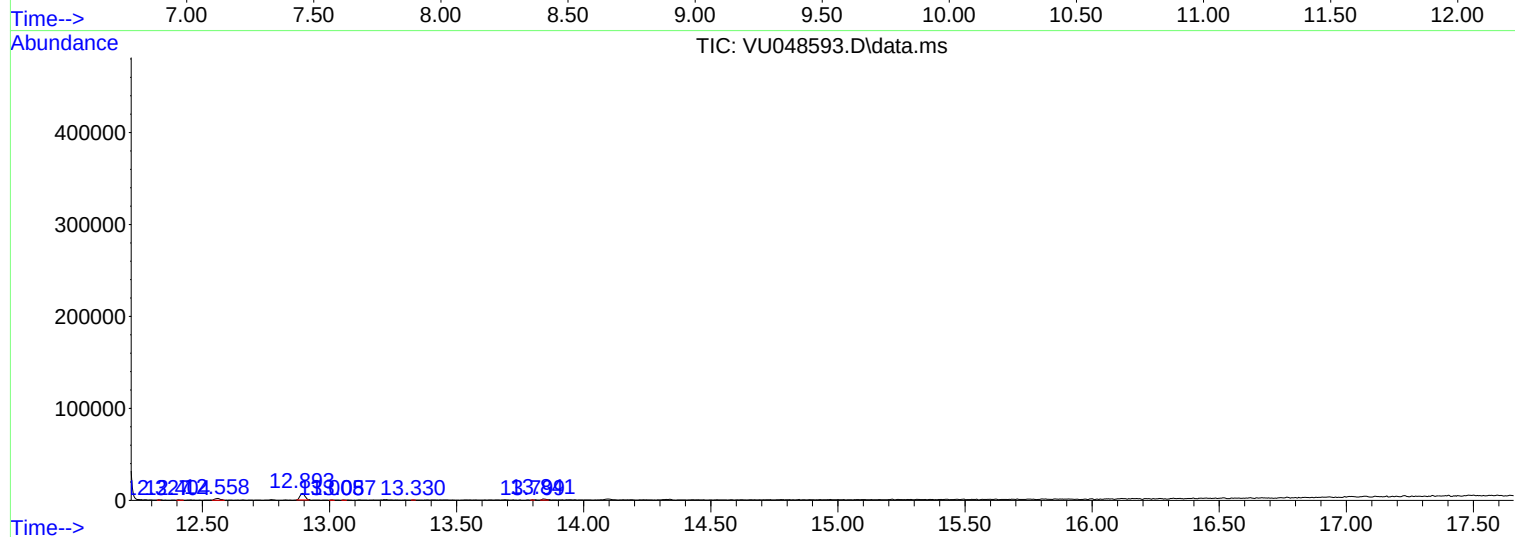
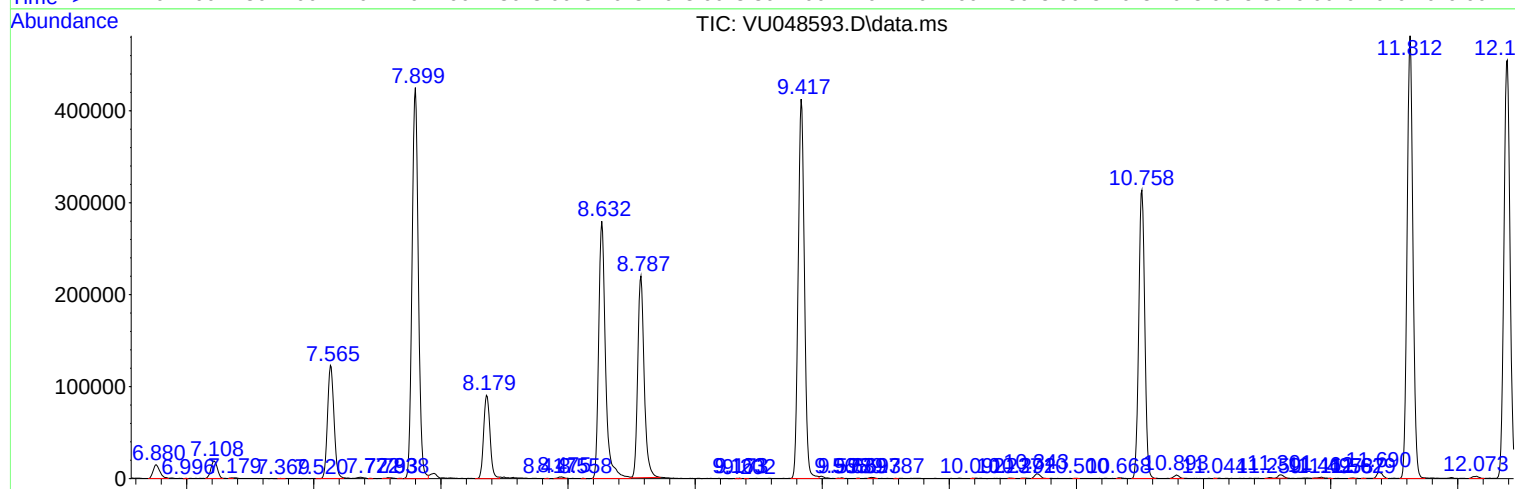
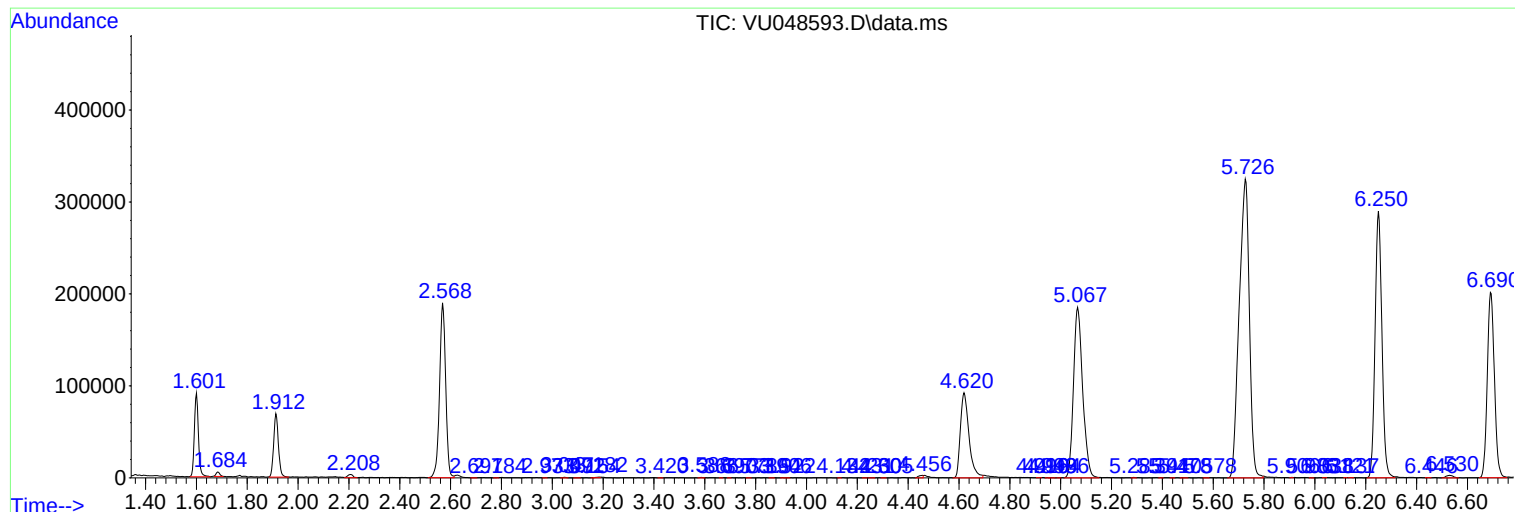
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EXXX0

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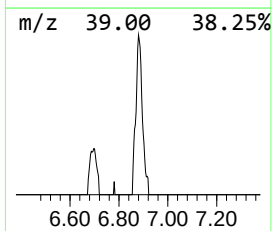
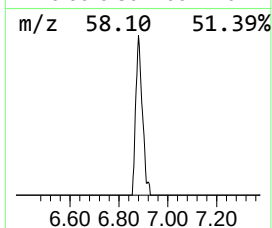
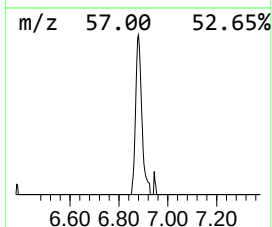
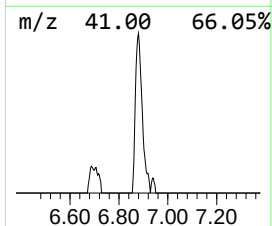
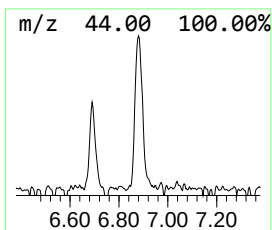
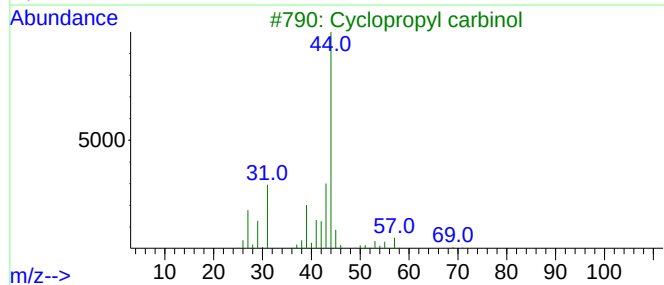
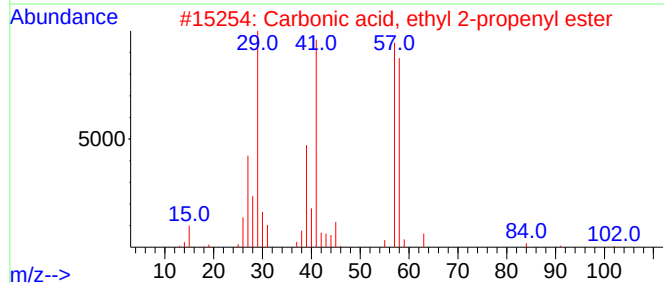
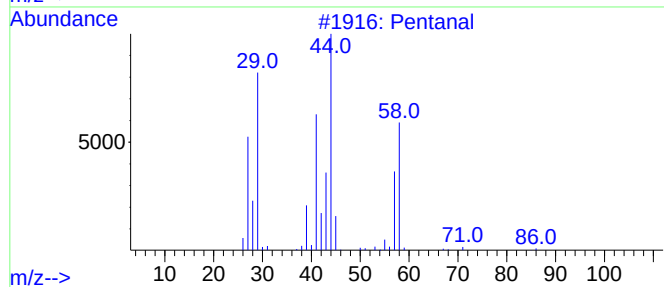
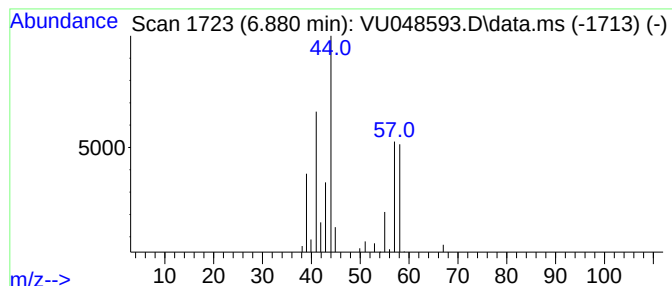
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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.
6.880	2.51 ug/L	27331	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentanal	86	C5H10O	000110-62-3	36
2			Carbonic acid, ethyl 2-propenyl ...	130	C6H10O3	001469-70-1	32
3			Cyclopropyl carbinol	72	C4H8O	002516-33-8	23
4			Cyclopropyl carbinol	72	C4H8O	002516-33-8	23
5			Cyclopropyl carbinol	72	C4H8O	002516-33-8	17



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TIC Library : C:\Database\NIST20.L
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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	6.880	2.5	ug/L	27331	1	6.250	544738	50.0