

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051822\
 Data File : VU048620.D
 Acq On : 18 May 2022 17:42
 Operator : SY/MD
 Sample : N2849-13
 Misc : 5.0mL/MSVOA_U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EXXX6

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: VU048620.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	94	rVB	77903	86472	10.12%	1.168%
2	1.684	103	107	114	rVB2	4474	4694	0.55%	0.063%
3	1.912	170	178	190	rBV	63984	80575	9.43%	1.088%
4	2.205	264	269	276	rVB4	1321	1894	0.22%	0.026%
5	2.366	315	319	323	rBV2	443	330	0.04%	0.004%
6	2.481	352	355	358	rVB2	348	209	0.02%	0.003%
7	2.568	366	382	395	rBV	174341	286618	33.56%	3.870%
8	2.774	443	446	449	rBV	210	194	0.02%	0.003%
9	2.793	449	452	454	rVV	238	168	0.02%	0.002%
10	2.887	479	481	483	rBV2	454	299	0.04%	0.004%
11	3.012	518	520	523	rVB2	318	186	0.02%	0.003%
12	3.035	523	527	528	rBV	500	313	0.04%	0.004%
13	3.182	568	573	574	rBV	430	342	0.04%	0.005%
14	3.244	589	592	596	rBV	279	229	0.03%	0.003%
15	3.317	610	615	618	rBB	181	196	0.02%	0.003%
16	3.588	691	699	701	rBV3	950	1083	0.13%	0.015%
17	3.771	754	756	760	rBV	192	196	0.02%	0.003%
18	3.967	814	817	820	rVB2	289	205	0.02%	0.003%
19	4.449	956	967	985	rBV3	11435	26921	3.15%	0.364%
20	4.539	993	995	999	rVB2	339	253	0.03%	0.003%
21	4.620	1006	1020	1044	rBV2	90218	209176	24.49%	2.825%
22	4.906	1105	1109	1112	rVB2	430	304	0.04%	0.004%
23	4.938	1115	1119	1121	rBB	312	201	0.02%	0.003%
24	4.993	1134	1136	1139	rVB2	329	191	0.02%	0.003%
25	5.067	1140	1159	1185	rBV2	176054	441337	51.67%	5.959%
26	5.179	1191	1194	1199	rVB2	374	290	0.03%	0.004%
27	5.221	1203	1207	1210	rBB2	234	183	0.02%	0.002%
28	5.282	1224	1226	1230	rVV3	396	273	0.03%	0.004%
29	5.427	1269	1271	1276	rBB	393	282	0.03%	0.004%
30	5.726	1342	1364	1388	rBV2	311870	854070	100.00%	11.533%
31	5.899	1414	1418	1420	rBB2	346	225	0.03%	0.003%
32	5.967	1431	1439	1444	rBV4	1213	1555	0.18%	0.021%
33	6.009	1449	1452	1454	rVV	257	192	0.02%	0.003%
34	6.034	1456	1460	1463	rVV2	581	446	0.05%	0.006%
35	6.047	1463	1464	1469	rVV2	343	236	0.03%	0.003%
36	6.128	1487	1489	1491	rBV	289	194	0.02%	0.003%

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 Title : VOC Analysis

37	6.141	1491	1493	1496	rVV	441	256	0.03%	0.003%
38	6.250	1509	1527	1556	rBV	283321	531292	62.21%	7.174%
39	6.452	1585	1590	1594	rBB2	330	314	0.04%	0.004%
40	6.530	1606	1614	1624	rBV2	3694	5678	0.66%	0.077%
41	6.690	1651	1664	1686	rBV	193810	371606	43.51%	5.018%
42	6.790	1693	1695	1697	rBV	637	298	0.03%	0.004%
43	6.809	1697	1701	1709	rVB3	709	705	0.08%	0.010%
44	6.880	1713	1723	1737	rBV3	11295	21304	2.49%	0.288%
45	7.047	1769	1775	1779	rBV	510	598	0.07%	0.008%
46	7.108	1784	1794	1805	rVB2	12437	21632	2.53%	0.292%
47	7.185	1809	1818	1824	rBV4	1427	2133	0.25%	0.029%
48	7.462	1900	1904	1907	rBB2	279	226	0.03%	0.003%
49	7.568	1924	1937	1962	rBV	114723	204092	23.90%	2.756%
50	7.690	1970	1975	1980	rVB4	790	865	0.10%	0.012%
51	7.796	2001	2008	2014	rBV3	1121	1501	0.18%	0.020%
52	7.899	2026	2040	2054	rBV	401600	686271	80.35%	9.267%
53	8.047	2084	2086	2089	rBV2	284	162	0.02%	0.002%
54	8.179	2114	2127	2146	rBV2	83884	146932	17.20%	1.984%
55	8.475	2205	2219	2221	rBV4	1459	1790	0.21%	0.024%
56	8.542	2237	2240	2242	rBV	306	209	0.02%	0.003%
57	8.632	2256	2268	2303	rBV	265323	489025	57.26%	6.603%
58	8.787	2305	2316	2334	rVB2	146097	250654	29.35%	3.385%
59	8.970	2370	2373	2376	rVB	401	263	0.03%	0.004%
60	8.992	2376	2380	2382	rBV	223	217	0.03%	0.003%
61	9.031	2389	2392	2397	rBV	173	210	0.02%	0.003%
62	9.417	2498	2512	2529	rBV	404702	668446	78.27%	9.026%
63	9.571	2557	2560	2570	rVB3	825	900	0.11%	0.012%
64	9.693	2591	2598	2605	rBV4	1359	1812	0.21%	0.024%
65	9.790	2625	2628	2630	rBV	194	163	0.02%	0.002%
66	9.883	2653	2657	2660	rBV	231	236	0.03%	0.003%
67	9.960	2678	2681	2683	rBV	194	167	0.02%	0.002%
68	10.012	2693	2697	2699	rBV	284	208	0.02%	0.003%
69	10.050	2706	2709	2712	rBV	235	189	0.02%	0.003%
70	10.346	2794	2801	2811	rVB6	3753	5617	0.66%	0.076%
71	10.443	2829	2831	2835	rVV	317	190	0.02%	0.003%
72	10.758	2916	2929	2952	rVB	294394	480933	56.31%	6.494%
73	10.893	2960	2971	2982	rVB4	2126	3246	0.38%	0.044%
74	10.967	2992	2994	2999	rVB	321	227	0.03%	0.003%
75	10.999	3002	3004	3006	rBV2	431	229	0.03%	0.003%
76	11.259	3081	3085	3087	rBV2	604	494	0.06%	0.007%

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Min Area: 0 % of largest Peak

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Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

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

77	11.301	3093	3098	3100	rBV4	1900	1695	0.20%	0.023%
78	11.391	3122	3126	3131	rBV2	431	412	0.05%	0.006%
79	11.449	3141	3144	3145	rBV2	617	296	0.03%	0.004%
80	11.697	3212	3221	3230	rVB5	5052	7911	0.93%	0.107%
81	11.738	3230	3234	3235	rBV	349	273	0.03%	0.004%
82	11.812	3244	3257	3274	rBV	468886	742136	86.89%	10.021%
83	11.976	3303	3308	3313	rVB2	524	568	0.07%	0.008%
84	12.066	3328	3336	3345	rBV3	5553	8879	1.04%	0.120%
85	12.195	3360	3376	3392	rBV	450180	725344	84.93%	9.794%
86	12.359	3425	3427	3431	rBV	347	297	0.03%	0.004%
87	12.529	3478	3480	3483	rBV2	317	237	0.03%	0.003%
88	12.552	3483	3487	3490	rBV4	920	807	0.09%	0.011%
89	12.767	3549	3554	3557	rBV2	483	438	0.05%	0.006%
90	12.838	3571	3576	3580	rBV4	656	551	0.06%	0.007%
91	12.893	3585	3593	3603	rBV7	7676	11770	1.38%	0.159%
92	13.172	3677	3680	3684	rBV	293	231	0.03%	0.003%
93	13.394	3746	3749	3751	rBV	373	205	0.02%	0.003%
94	13.426	3756	3759	3763	rBV4	602	407	0.05%	0.005%
95	13.468	3769	3772	3775	rBV2	313	180	0.02%	0.002%
96	13.578	3803	3806	3808	rBV	281	180	0.02%	0.002%
97	13.616	3816	3818	3823	rVB	312	210	0.02%	0.003%
98	13.851	3889	3891	3894	rBV2	372	236	0.03%	0.003%
99	13.896	3899	3905	3907	rBV	390	387	0.05%	0.005%
100	14.217	4002	4005	4008	rVB	387	233	0.03%	0.003%

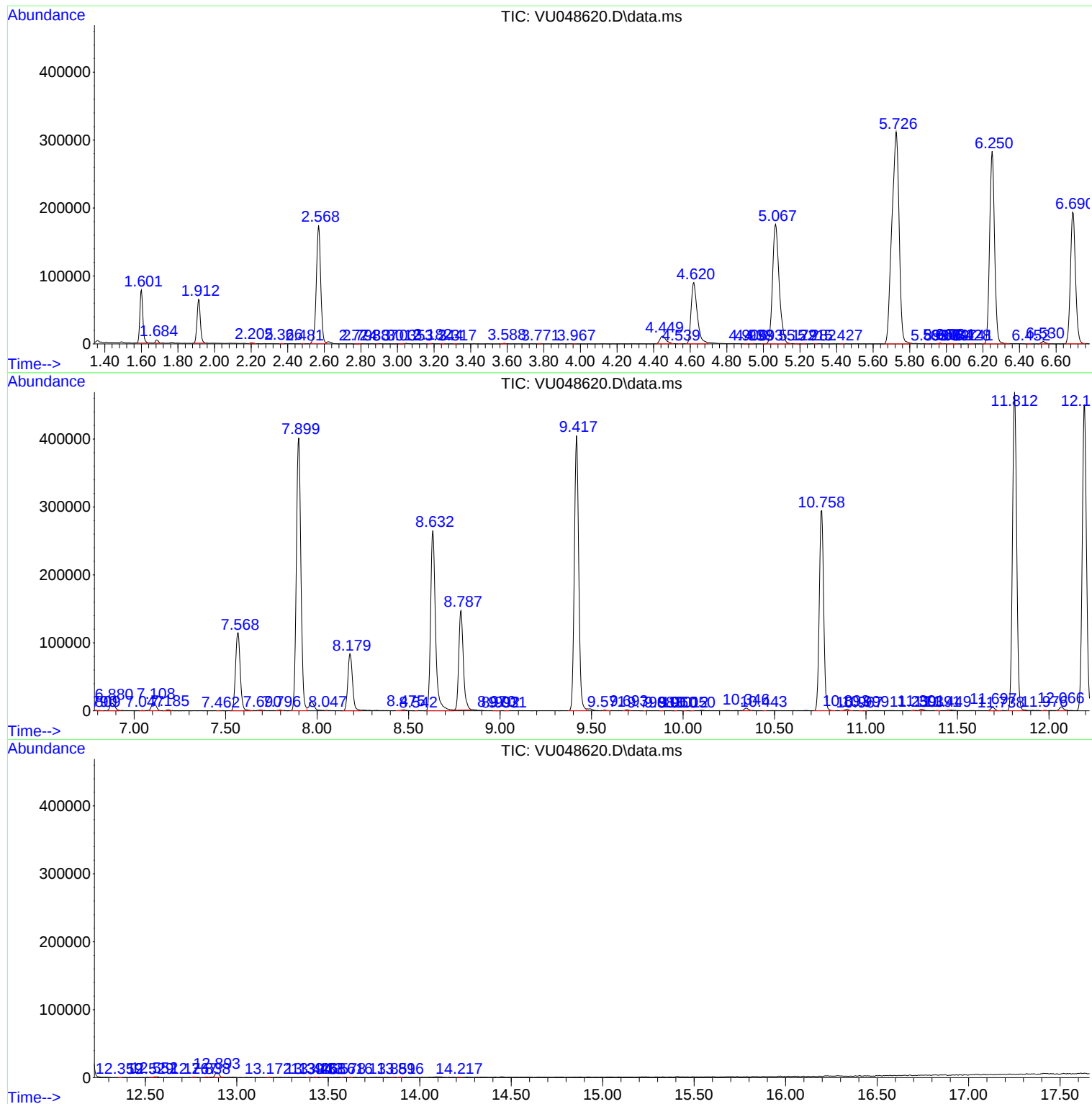
Sum of corrected areas: 7405705

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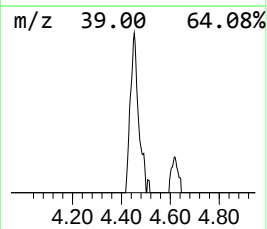
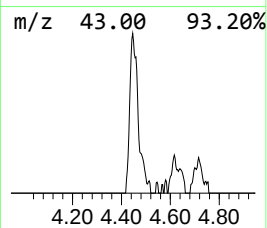
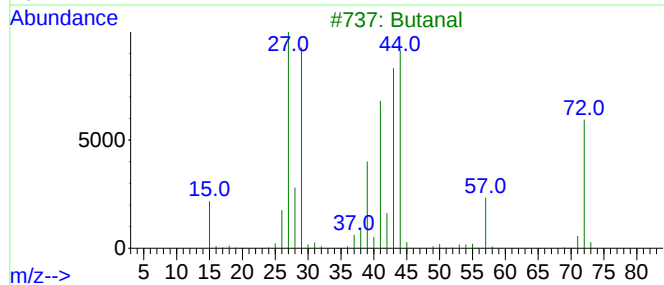
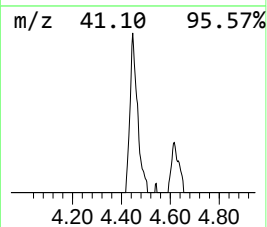
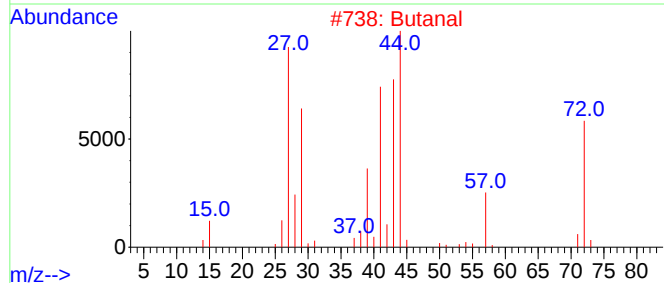
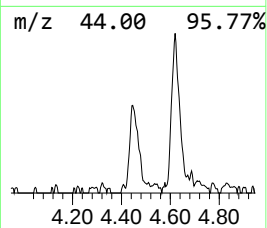
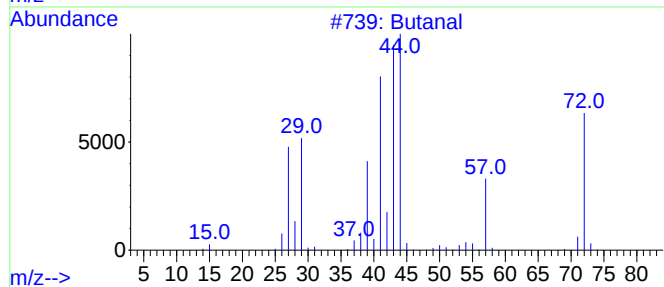
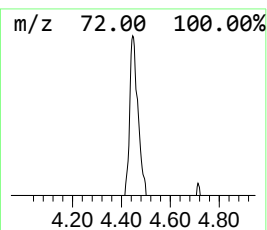
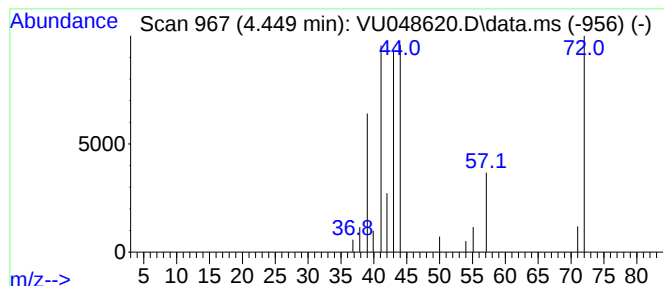
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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.
4.449	2.53 ug/L	26921	1,4-Difluorobenzene	6.250

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Butanal	72	C4H8O	000123-72-8	43
2			Butanal	72	C4H8O	000123-72-8	43
3			Butanal	72	C4H8O	000123-72-8	38
4			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	37
5			Butanal	72	C4H8O	000123-72-8	27



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	4.449	2.5	ug/L	26921	1	6.250	531292	50.0