

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU091318\
 Data File : VU026706.D
 Acq On : 12 Sep 2018 16:55
 Operator : MD/SY
 Sample : J4860-03
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VHBLK01

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.395	63	69	85	rVB	86720	87583	11.64%	1.517%
2	1.678	149	157	171	rVB	75105	96525	12.83%	1.672%
3	2.270	330	341	354	rVB	147405	219278	29.15%	3.797%
4	2.450	387	397	411	rBV	14364	26101	3.47%	0.452%
5	2.694	467	473	474	rBV	770	461	0.06%	0.008%
6	2.765	490	495	496	rBV2	215	136	0.02%	0.002%
7	2.842	509	519	529	rBV3	1361	3028	0.40%	0.052%
8	2.903	536	538	542	rVB2	170	123	0.02%	0.002%
9	2.948	549	552	555	rVB2	141	102	0.01%	0.002%
10	3.022	572	575	579	rVB	253	182	0.02%	0.003%
11	3.048	579	583	585	rBV	173	186	0.02%	0.003%
12	3.196	627	629	636	rVB2	177	190	0.03%	0.003%
13	3.283	653	656	657	rBV2	133	71	0.01%	0.001%
14	3.292	657	659	660	rBV	348	146	0.02%	0.003%
15	3.427	691	701	704	rBV2	217	373	0.05%	0.006%
16	3.447	705	707	710	rVV2	156	98	0.01%	0.002%
17	3.472	713	715	719	rVV2	202	152	0.02%	0.003%
18	3.511	724	727	733	rBV2	193	168	0.02%	0.003%
19	3.588	748	751	753	rVV	127	96	0.01%	0.002%
20	3.617	757	760	765	rBV	74	70	0.01%	0.001%
21	3.646	765	769	773	rBV2	211	185	0.02%	0.003%
22	3.742	797	799	807	rVB2	152	175	0.02%	0.003%
23	3.784	810	812	815	rVB2	203	113	0.02%	0.002%
24	3.839	826	829	835	rVB	198	182	0.02%	0.003%
25	3.903	847	849	853	rBV2	123	127	0.02%	0.002%
26	3.929	854	857	860	rVB3	302	220	0.03%	0.004%
27	4.032	887	889	894	rVB	153	91	0.01%	0.002%
28	4.054	894	896	899	rVB2	149	100	0.01%	0.002%
29	4.180	920	935	965	rBV	76252	202685	26.94%	3.510%
30	4.443	1014	1017	1018	rBV	121	65	0.01%	0.001%
31	4.546	1047	1049	1052	rVB	170	74	0.01%	0.001%
32	4.649	1064	1081	1106	rBV2	126052	293402	39.00%	5.081%
33	4.768	1116	1118	1121	rBV	243	121	0.02%	0.002%
34	4.839	1139	1140	1146	rVB	298	238	0.03%	0.004%

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Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
 Title : VOC Analysis

35	4.887	1146	1155	1162	rBV3	675	1386	0.18%	0.024%
36	4.948	1171	1174	1177	rVB	289	145	0.02%	0.003%
37	4.980	1177	1184	1185	rBV2	445	253	0.03%	0.004%
38	5.344	1273	1297	1319	rBV2	252477	752324	100.00%	13.028%
39	5.485	1338	1341	1342	rBV	198	120	0.02%	0.002%
40	5.617	1378	1382	1384	rBV	130	96	0.01%	0.002%
41	5.717	1410	1413	1416	rBV	106	77	0.01%	0.001%
42	5.890	1452	1467	1488	rBV	237337	461571	61.35%	7.993%
43	6.176	1551	1556	1564	rVB4	759	992	0.13%	0.017%
44	6.276	1584	1587	1590	rVB	171	82	0.01%	0.001%
45	6.334	1590	1605	1627	rBV	179987	355521	47.26%	6.156%
46	6.498	1653	1656	1658	rBV	232	105	0.01%	0.002%
47	6.610	1688	1691	1693	rBV	98	64	0.01%	0.001%
48	6.813	1750	1754	1757	rBV	89	88	0.01%	0.002%
49	6.868	1764	1771	1774	rBV2	251	369	0.05%	0.006%
50	6.919	1783	1787	1790	rBV	101	87	0.01%	0.002%
51	6.958	1790	1799	1802	rBV	162	212	0.03%	0.004%
52	7.083	1836	1838	1840	rBV	165	91	0.01%	0.002%
53	7.144	1855	1857	1860	rVV	173	68	0.01%	0.001%
54	7.176	1864	1867	1869	rVV	190	120	0.02%	0.002%
55	7.231	1872	1884	1912	rVV	99171	173883	23.11%	3.011%
56	7.363	1920	1925	1927	rBV	163	98	0.01%	0.002%
57	7.389	1927	1933	1939	rVB	303	333	0.04%	0.006%
58	7.414	1939	1941	1944	rBV	132	88	0.01%	0.002%
59	7.440	1947	1949	1952	rVV	181	108	0.01%	0.002%
60	7.459	1952	1955	1957	rVV	189	147	0.02%	0.003%
61	7.472	1957	1959	1962	rVB	208	98	0.01%	0.002%
62	7.569	1973	1989	2009	rBV	329290	566415	75.29%	9.808%
63	7.733	2038	2040	2041	rBV	222	95	0.01%	0.002%
64	7.765	2046	2050	2053	rVB2	237	212	0.03%	0.004%
65	7.790	2053	2058	2063	rBV2	256	272	0.04%	0.005%
66	7.852	2066	2077	2097	rVV	70586	117603	15.63%	2.037%
67	7.996	2118	2122	2123	rVB2	226	119	0.02%	0.002%
68	8.032	2126	2133	2138	rBV3	507	695	0.09%	0.012%
69	8.186	2167	2181	2191	rBV3	4663	10779	1.43%	0.187%
70	8.315	2210	2221	2249	rVB	251088	422096	56.11%	7.309%
71	8.536	2288	2290	2292	rBV2	208	136	0.02%	0.002%

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 Title : VOC Analysis

72	8.623	2309	2317	2327	rVB5	1780	3213	0.43%	0.056%
73	8.671	2329	2332	2336	rBV	214	170	0.02%	0.003%
74	8.691	2336	2338	2342	rVB2	290	157	0.02%	0.003%
75	8.716	2342	2346	2349	rBV	235	194	0.03%	0.003%
76	8.887	2393	2399	2402	rBV2	165	199	0.03%	0.003%
77	8.909	2402	2406	2409	rVB2	181	113	0.02%	0.002%
78	8.925	2409	2411	2413	rBV2	239	123	0.02%	0.002%
79	8.987	2424	2430	2431	rBV	228	228	0.03%	0.004%
80	9.038	2443	2446	2450	rVB2	299	264	0.04%	0.005%
81	9.093	2450	2463	2487	rBV	341810	555329	73.82%	9.617%
82	9.382	2549	2553	2557	rBV2	330	263	0.03%	0.005%
83	9.443	2569	2572	2577	rVB3	313	263	0.03%	0.005%
84	9.475	2577	2582	2585	rBV	334	341	0.05%	0.006%
85	9.652	2634	2637	2638	rBV	315	167	0.02%	0.003%
86	9.675	2642	2644	2647	rVB2	293	135	0.02%	0.002%
87	9.697	2647	2651	2654	rBV2	174	181	0.02%	0.003%
88	9.832	2690	2693	2696	rBV	208	180	0.02%	0.003%
89	9.980	2736	2739	2741	rBV	264	179	0.02%	0.003%
90	10.012	2744	2749	2753	rBV2	207	231	0.03%	0.004%
91	10.070	2765	2767	2773	rBV2	187	177	0.02%	0.003%
92	10.433	2868	2880	2900	rBV	256677	405195	53.86%	7.017%
93	10.578	2922	2925	2928	rBV2	229	178	0.02%	0.003%
94	10.610	2928	2935	2946	rVB5	1386	2574	0.34%	0.045%
95	10.749	2975	2978	2981	rBV	208	164	0.02%	0.003%
96	11.035	3065	3067	3070	rVB	274	101	0.01%	0.002%
97	11.485	3196	3207	3224	rBV	311313	485418	64.52%	8.406%
98	11.610	3244	3246	3248	rBV2	212	124	0.02%	0.002%
99	11.861	3312	3324	3349	rBV	322012	518137	68.87%	8.972%
100	12.478	3511	3516	3523	rBV3	630	956	0.13%	0.017%

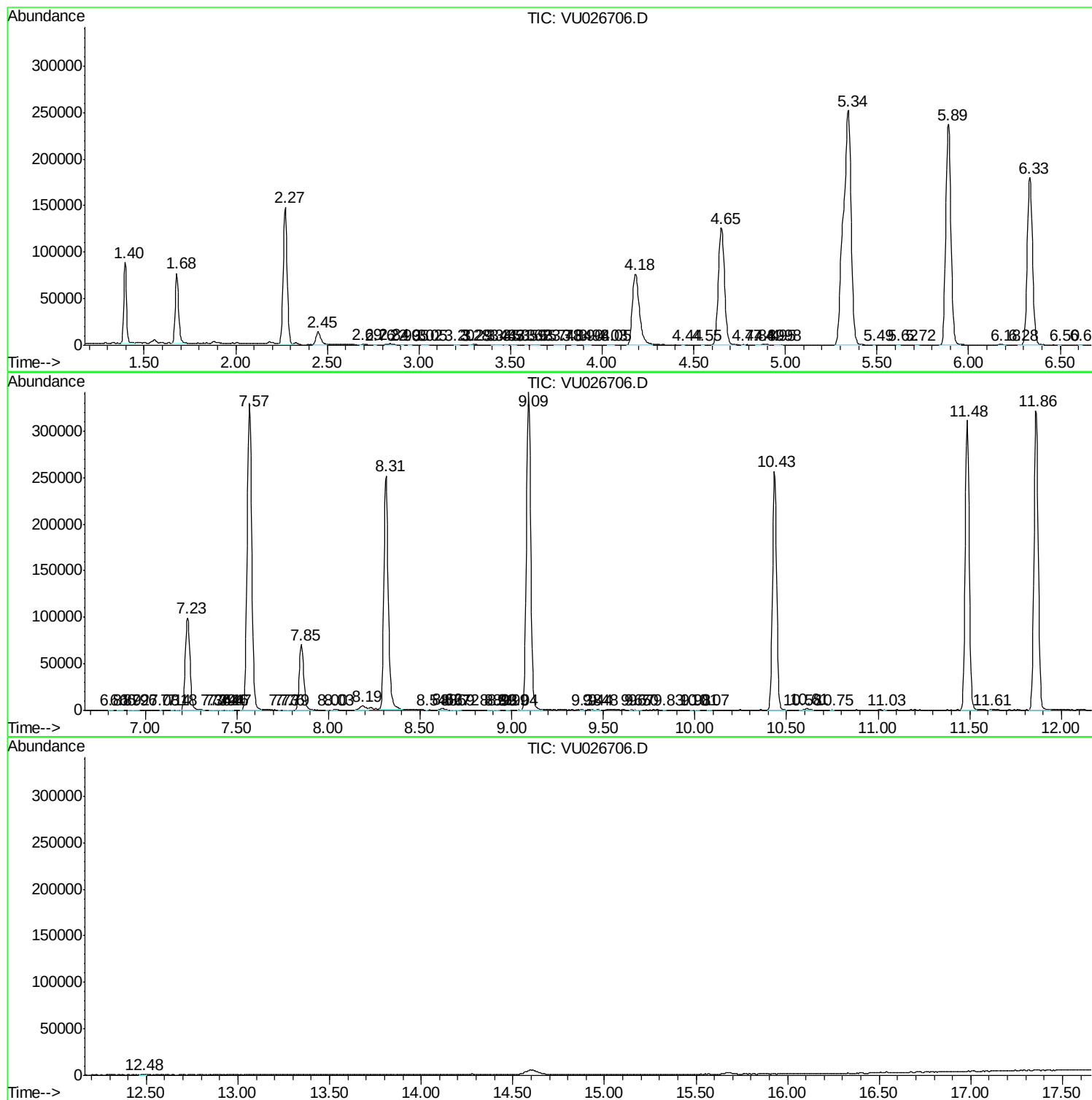
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P



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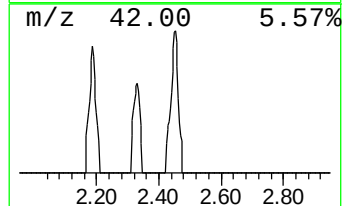
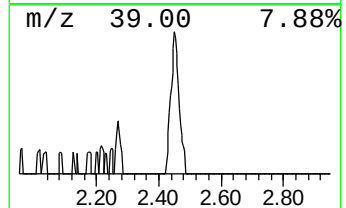
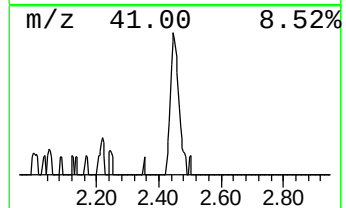
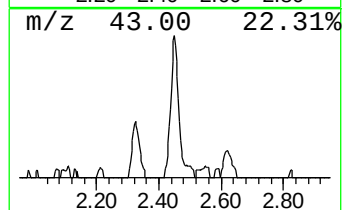
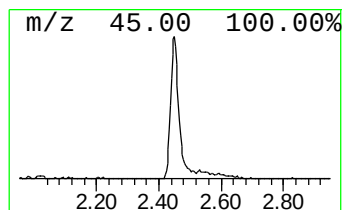
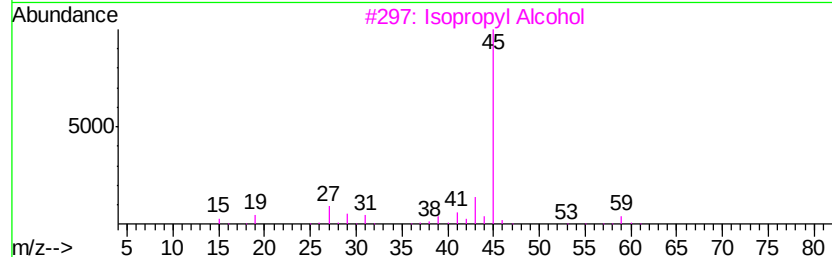
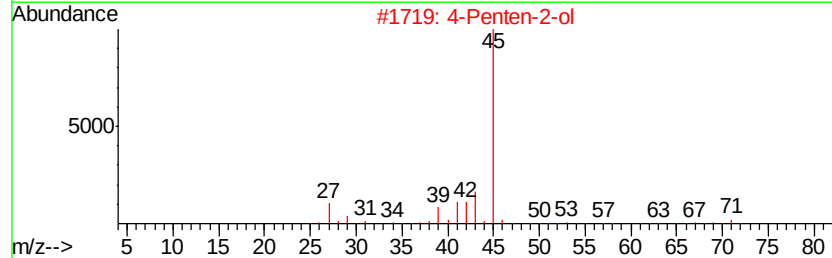
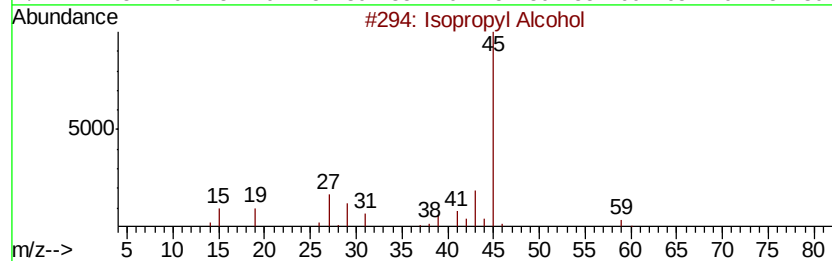
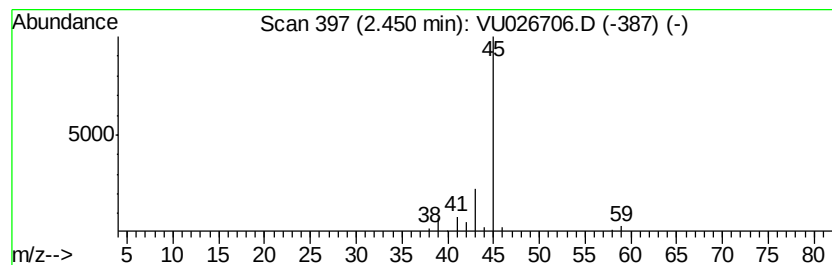
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM091018WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Isopropyl Alcohol Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	2.83 ug/L	26101	1,4-Difluorobenzene	5.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isopropyl Alcohol	60	C3H8O	000067-63-0	74
2			4-Penten-2-ol	86	C5H10O	000625-31-0	9
3			Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4			Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4
5			Formamide	45	CH3NO	000075-12-7	4



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TIC Library : C:\DATABASE\NIST11.L
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TIC Top Hit name	RT	EstConc	Units	Response	---Internal Standard---			
					#	RT	Resp	Conc
Isopropyl Alcohol	2.45	2.8	ug/L	26101	1	5.89	461571	50.0