LSC Area Percent Report

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050218\
Data File : VU023585.D
Acq On : 02 May 2018 18:19
Operator : MD/SY
Sample : J2660-13RE
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.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	0.626	9	11	15	rVB2	198	129	0.01%	0.001%
2	0.648	15	18	25	rVB	151	132	0.01%	0.001%
3	0.847	76	80	85	rBV2	143	149	0.01%	0.002%
4	1.060	135	146	147	rBV	1584	1615	0.14%	0.018%
5	1.089	147	155	179	rBV	436312	500505	44.30%	5.546%
6	1.182	180	184	193	rVV2	9840	11614	1.03%	0.129%
7	1.397	245	251	262	rVB	139997	146214	12.94%	1.620%
8	1.680	331	339	352	rVB	106015	131031	11.60%	1.452%
9	2.272	511	523	534	rBV	231868	350341	31.01%	3.882%
10	2.449	568	578	596	rBV	16439	31376	2.78%	0.348%
11	2.542	605	607	608	rBV	322	138	0.01%	0.002%
12	2.558	609	612	621	rVB4	707	779	0.07%	0.009%
13	2.625	624	633	640	rBV2	863	1314	0.12%	0.015%
14	2.699	651	656	657	rBV2	646	470	0.04%	0.005%
15	2.793	683	685	688	rVV2	250	156	0.01%	0.002%
16	2.841	688	700	711	rVV3	4700	9403	0.83%	0.104%
17	2.982	741	744	750	rVB3	473	543	0.05%	0.006%
18	3.024	755	757	762	rBV	131	118	0.01%	0.001%
19	3.198	806	811	816	rVB5	553	517	0.05%	0.006%
20	3.233	819	822	827	rVB	192	150	0.01%	0.002%
21	3.272	827	834	835	rBV	133	117	0.01%	0.001%
22	3.301	840	843	846	rBV2	140	127	0.01%	0.001%
23	3.384	867	869	871	rBV2	177	116	0.01%	0.001%
24	3.400	871	874	876	rVV	211	147	0.01%	0.002%
25	3.449	886	889	893	rBV	143	135	0.01%	0.001%
26	3.767	984	988	991	rBV2	201	154	0.01%	0.002%
27	3.966	1046	1050	1054	rVB2	196	190	0.02%	0.002%
28	3.998	1054	1060	1064	rBV2	234	317	0.03%	0.004%
29	4.182	1100	1117	1150	rBV	126679	347730	30.78%	3.853%
30	4.513	1216	1220	1223	rBV2	274	208	0.02%	0.002%
31	4.558	1230	1234	1238	rBV	362	338	0.03%	0.004%
32	4.580	1238	1241	1244	rVB2	200	127	0.01%	0.001%
33	4.651	1244	1263	1286	rBV	187075	440657	39.01%	4.882%
34	4.889	1331	1337	1346	rVB2	744	1465	0.13%	0.016%

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ALS Vial : 19 Sample Multiplier: 1

Integration Parameters: LSCINT.P
Integrator: RTE
Smoothing : OFF Filtering: 5
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Peak separation: 5

Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Title : VOC Analysis

35	4.989	1362	1368	1371	rBV4	544	599	0.05%	0.007%
36	5.050	1384	1387	1392	rVB	211	156	0.01%	0.002%
37	5.082	1392	1397	1402	rBV2	163	219	0.02%	0.002%
38	5.204	1431	1435	1440	rVB2	138	122	0.01%	0.001%
39	5.342	1453	1478	1515	rBV2	373929	1129702	100.00%	12.517%
40	5.571	1547	1549	1554	rVB2	201	116	0.01%	0.001%
41	5.629	1563	1567	1570	rVB	193	164	0.01%	0.002%
42	5.670	1576	1580	1585	rVB3	351	248	0.02%	0.003%
43	5.693	1585	1587	1594	rVB2	144	150	0.01%	0.002%
44	5.741	1594	1602	1605	rBV2	333	354	0.03%	0.004%
45	5.892	1610	1649	1666	rBV	273958	598135	52.95%	6.627%
46	6.336	1773	1787	1815	rBV	259782	525328	46.50%	5.821%
47	6.551	1852	1854	1859	rBV4	252	227	0.02%	0.003%
48	6.709	1898	1903	1905	rBV2	318	277	0.02%	0.003%
49	6.738	1909	1912	1919	rVB3	287	345	0.03%	0.004%
50	6.786	1924	1927	1929	rBV	169	130	0.01%	0.001%
51	6.821	1935	1938	1941	rVB3	403	277	0.02%	0.003%
52	6.860	1941	1950	1951	rBV4	757	1156	0.10%	0.013%
53	6.918	1966	1968	1974	rVB3	309	294	0.03%	0.003%
54	6.976	1982	1986	1989	rBV	382	340	0.03%	0.004%
55	7.021	1996	2000	2001	rBV	242	119	0.01%	0.001%
56	7.030	2001	2003	2008	rVB2	247	191	0.02%	0.002%
57	7.178	2045	2049	2052	rVB	213	171	0.02%	0.002%
58	7.233	2052	2066	2097	rBV	138011	254785	22.55%	2.823%
59	7.394	2113	2116	2121	rVB3	637	543	0.05%	0.006%
60	7.468	2135	2139	2141	rVV2	448	354	0.03%	0.004%
61	7.522	2152	2156	2157	rBV2	238	148	0.01%	0.002%
62	7.571	2157	2171	2208	rVV	496279	886875	78.51%	9.827%
63	7.854	2247	2259	2277	rBV	97979	168882	14.95%	1.871%
64	8.034	2313	2315	2319	rVB3	237	161	0.01%	0.002%
65	8.095	2330	2334	2337	rBV	237	172	0.02%	0.002%
66	8.120	2337	2342	2344	rBV	262	166	0.01%	0.002%
67	8.149	2347	2351	2352	rBV	272	161	0.01%	0.002%
68	8.181	2358	2361	2372	rVB5	1136	1583	0.14%	0.018%
69	8.230	2373	2376	2378	rBV2	508	297	0.03%	0.003%
70	8.243	2378	2380	2382	rVB	441	136	0.01%	0.002%
71	8.313	2390	2402	2433	rBV	410006	702961	62.23%	7.789%

LSC Area Percent Report

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ALS Vial : 19 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Title : VOC Analysis

72	8.571	2479	2482	2487	rVB	228	164	0.01%	0.002%
73	8.664	2509	2511	2518	rVB	246	193	0.02%	0.002%
74	8.773	2543	2545	2551	rVB2	161	143	0.01%	0.002%
75	9.095	2632	2645	2677	rBV	390596	654589	57.94%	7.253%
76	9.259	2690	2696	2703	rVB3	1412	1805	0.16%	0.020%
77	9.381	2725	2734	2749	rBV2	5239	8071	0.71%	0.089%
78	9.542	2781	2784	2790	rVB2	156	149	0.01%	0.002%
79	9.667	2820	2823	2828	rBV	221	166	0.01%	0.002%
80	9.702	2830	2834	2844	rVV2	639	807	0.07%	0.009%
81	9.786	2851	2860	2869	rBV	4915	6731	0.60%	0.075%
82	9.882	2888	2890	2897	rBV2	146	139	0.01%	0.002%
83	10.011	2928	2930	2936	rBV	137	128	0.01%	0.001%
84	10.056	2941	2944	2953	rVB	304	345	0.03%	0.004%
85	10.435	3049	3062	3085	rBV	375893	600871	53.19%	6.658%
86	10.570	3095	3104	3129	rBV3	11011	24501	2.17%	0.271%
87	10.792	3170	3173	3176	rBV	235	165	0.01%	0.002%
88	10.821	3179	3182	3185	rVV2	317	240	0.02%	0.003%
89	10.850	3189	3191	3196	rVB	509	260	0.02%	0.003%
90	11.046	3249	3252	3260	rVB2	244	241	0.02%	0.003%
91	11.143	3280	3282	3284	rBV	231	142	0.01%	0.002%
92	11.284	3323	3326	3329	rBV2	199	140	0.01%	0.002%
93	11.423	3365	3369	3377	rVB3	988	1157	0.10%	0.013%
94	11.490	3377	3390	3406	rBV	391589	623597	55.20%	6.909%
95	11.622	3429	3431	3434	rBV2	257	181	0.02%	0.002%
96	11.728	3461	3464	3468	rVB2	222	126	0.01%	0.001%
97	11.763	3468	3475	3477	rBV3	466	543	0.05%	0.006%
98	11.866	3494	3507	3526	rBV	522741	844554	74.76%	9.358%
99	12.336	3650	3653	3656	rBV2	292	223	0.02%	0.002%
100	14.853	4434	4436	4440	rVB	477	308	0.03%	0.003%

Sum of corrected areas: 9025245

LSC Report - Integrated Chromatogram

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Data File : VU023585.D
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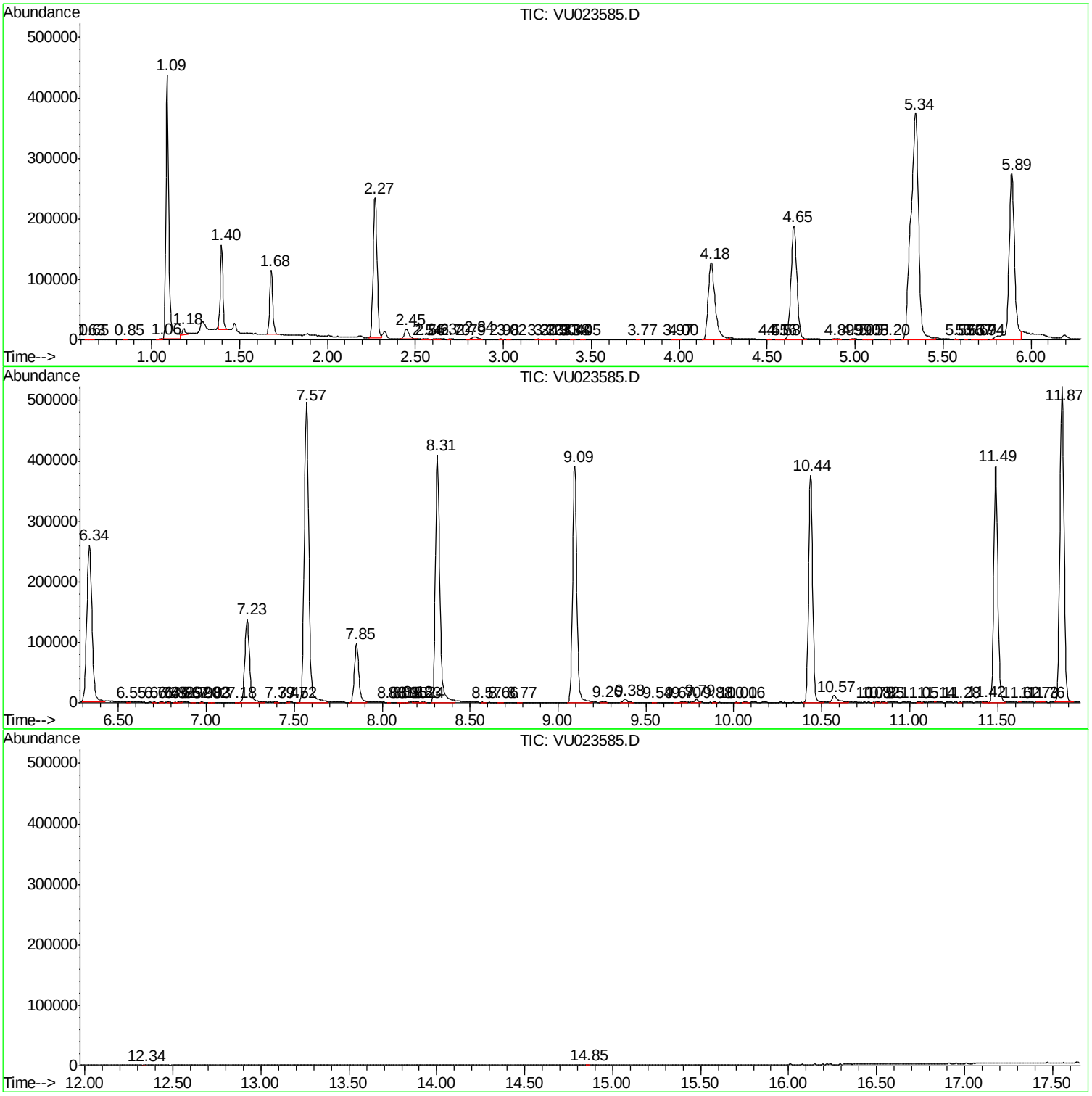
Operator : MD/SY
Sample : J2660-13RE
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050218\
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Acq On : 02 May 2018 18:19
Operator : MD/SY
Sample : J2660-13RE
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ALS Vial : 19 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

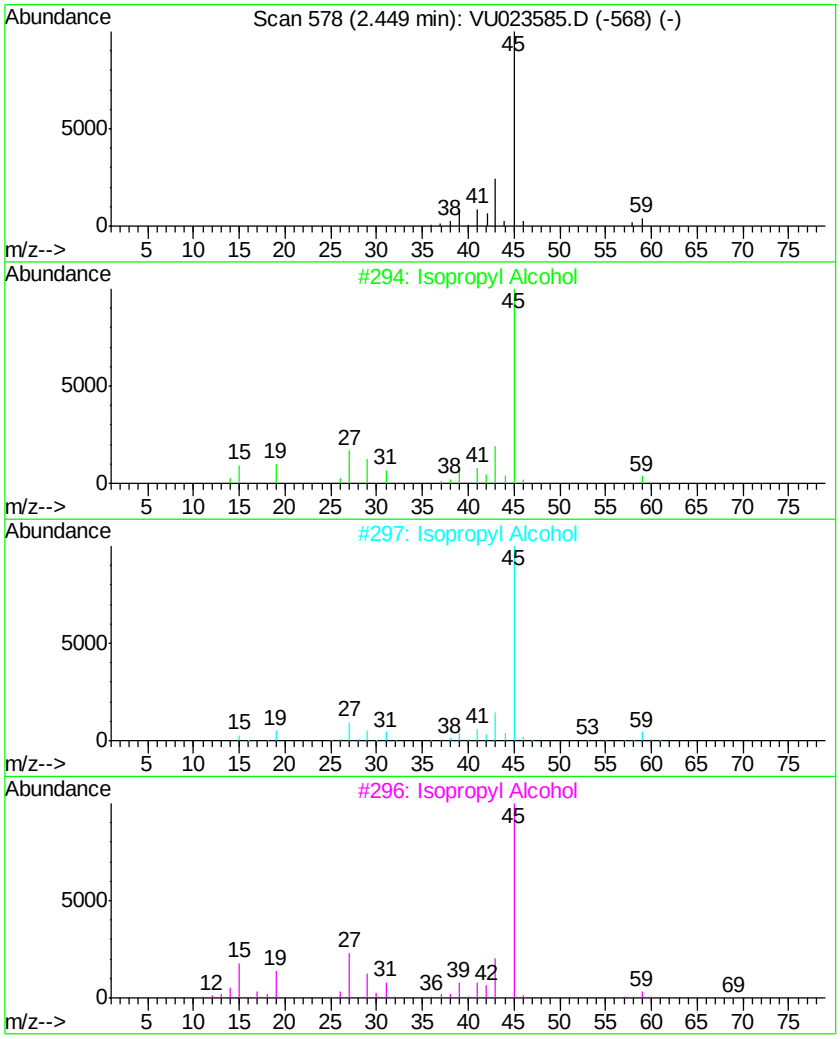
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

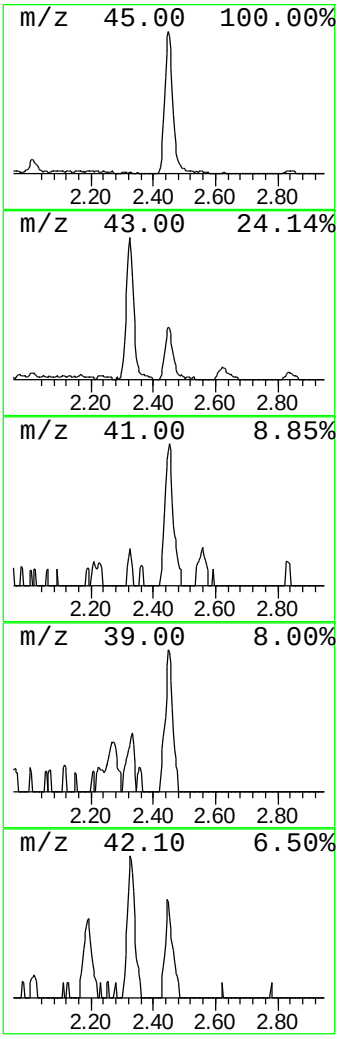
****

Peak Number 2 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	2.62 ug/L	31376	1,4-Difluorobenzene	5.89

Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Isopropyl Alcohol	60	C3H8O	000067-63-0	43
2	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	1-Butene, 4-methoxy	86	C5H10O	004696-30-4	4
5	Oxirane, (methoxymethyl)-	88	C4H8O2	000930-37-0	4





Tentatively Identified Compound (LSC) summary

Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050218\
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Acq On : 02 May 2018 18:19
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Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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

					--Internal Standard---			
TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
unknown-01	2.45	2.6	ug/L	31376	1	5.89	598135	50.0