LSC Area Percent Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU100818\
Data File : VU027493.D
Acq On : 08 Oct 2018 12:32
Operator : MD/SY
Sample : J5250-03
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0911

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\SOMULM100518WMA.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	1.399	63	70	85	rBV	103639	103440	13.47%	1.703%
2	1.682	151	158	171	rVB	77070	96924	12.62%	1.596%
3	2.273	332	342	354	rBV	160090	240626	31.33%	3.962%
4	2.447	387	396	420	rVB2	24332	43854	5.71%	0.722%
5	2.611	445	447	449	rBV	242	144	0.02%	0.002%
6	2.736	484	486	489	rBV	171	59	0.01%	0.001%
7	2.836	510	517	536	rVB3	2955	6295	0.82%	0.104%
8	2.910	536	540	543	rBV	233	179	0.02%	0.003%
9	2.929	543	546	548	rBV	262	161	0.02%	0.003%
10	3.019	572	574	578	rBV2	186	129	0.02%	0.002%
11	3.193	618	628	639	rVB4	1237	2337	0.30%	0.038%
12	3.254	644	647	650	rBV2	191	139	0.02%	0.002%
13	3.325	667	669	671	rVB	140	72	0.01%	0.001%
14	3.415	692	697	700	rBV	143	141	0.02%	0.002%
15	3.457	707	710	715	rBV2	190	208	0.03%	0.003%
16	3.489	718	720	721	rBV2	117	52	0.01%	0.001%
17	3.576	744	747	748	rBV2	195	93	0.01%	0.002%
18	3.653	770	771	773	rVB2	138	52	0.01%	0.001%
19	3.688	780	782	786	rVB	249	124	0.02%	0.002%
20	3.711	786	789	791	rBV2	173	106	0.01%	0.002%
21	3.733	791	796	799	rVV	140	134	0.02%	0.002%
22	3.762	802	805	807	rVV	92	71	0.01%	0.001%
23	3.785	810	812	815	rVB	176	77	0.01%	0.001%
24	3.826	822	825	826	rBV	107	59	0.01%	0.001%
25	3.871	837	839	842	rVB	147	66	0.01%	0.001%
26	3.897	843	847	850	rVB	194	146	0.02%	0.002%
27	3.977	867	872	876	rVB2	173	149	0.02%	0.002%
28	4.000	877	879	883	rVB	155	59	0.01%	0.001%
29	4.022	883	886	887	rBV	178	63	0.01%	0.001%
30	4.084	903	905	908	rVB	101	56	0.01%	0.001%
31	4.183	921	936	964	rBV3	92410	269263	35.06%	4.434%
32	4.547	1047	1049	1054	rBV2	265	215	0.03%	0.004%
33	4.592	1057	1063	1065	rBV	47	57	0.01%	0.001%
34	4.653	1065	1082	1106	rBV	127389	317345	41.32%	5.225%

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ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0911

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

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Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Title : VOC Analysis

35	4.794	1124	1126	1127	rBV	115	49	0.01%	0.001%
36	4.871	1146	1150	1151	rBV	337	219	0.03%	0.004%
37	5.003	1189	1191	1194	rVB	176	74	0.01%	0.001%
38	5.061	1207	1209	1212	rVB	188	89	0.01%	0.001%
39	5.080	1212	1215	1219	rVB	187	131	0.02%	0.002%
40	5.112	1219	1225	1229	rBV	107	144	0.02%	0.002%
41	5.344	1273	1297	1330	rBV2	252055	768013	100.00%	12.646%
42	5.530	1351	1355	1358	rBV2	199	210	0.03%	0.003%
43	5.563	1364	1365	1368	rVB	147	77	0.01%	0.001%
44	5.582	1368	1371	1375	rBV	97	78	0.01%	0.001%
45	5.604	1375	1378	1382	rVB	80	58	0.01%	0.001%
46	5.646	1387	1391	1392	rBV	122	51	0.01%	0.001%
47	5.682	1398	1402	1410	rBV2	585	677	0.09%	0.011%
48	5.887	1452	1466	1500	rBV	243450	486166	63.30%	8.005%
49	6.106	1529	1534	1535	rBV	70	61	0.01%	0.001%
50	6.116	1536	1537	1539	rVB	157	52	0.01%	0.001%
51	6.135	1539	1543	1545	rBV	151	90	0.01%	0.001%
52	6.148	1545	1547	1549	rBV	145	68	0.01%	0.001%
53	6.206	1563	1565	1566	rBV	145	60	0.01%	0.001%
54	6.270	1580	1585	1587	rBV	149	137	0.02%	0.002%
55	6.334	1591	1605	1630	rBV	179443	363988	47.39%	5.993%
56	6.456	1638	1643	1646	rBV2	399	453	0.06%	0.007%
57	6.518	1659	1662	1667	rVB2	164	173	0.02%	0.003%
58	6.546	1667	1671	1674	rBV	260	144	0.02%	0.002%
59	6.575	1678	1680	1684	rVB	142	72	0.01%	0.001%
60	6.617	1691	1693	1696	rVB	192	72	0.01%	0.001%
61	6.636	1696	1699	1704	rBV	107	106	0.01%	0.002%
62	6.662	1704	1707	1710	rBV	137	87	0.01%	0.001%
63	6.829	1754	1759	1762	rBV	300	296	0.04%	0.005%
64	6.862	1762	1769	1774	rVV4	698	806	0.10%	0.013%
65	6.884	1774	1776	1781	rVV	307	133	0.02%	0.002%
66	6.919	1785	1787	1789	rVB	175	67	0.01%	0.001%
67	6.958	1796	1799	1801	rVB	191	129	0.02%	0.002%
68	6.977	1801	1805	1808	rBV2	190	147	0.02%	0.002%
69	7.016	1814	1817	1821	rBV	91	98	0.01%	0.002%
70	7.228	1871	1883	1906	rBV	96068	175978	22.91%	2.898%
71	7.344	1918	1919	1921	rVB	134	49	0.01%	0.001%

LSC Area Percent Report

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Instrument : MSVOA_U
ClientSampleId : C0911

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\SOMULM100518WMA.M
Title : VOC Analysis

72	7.366	1924	1926	1927	rVV	145	79	0.01%	0.001%
73	7.392	1928	1934	1943	rVB4	2510	3885	0.51%	0.064%
74	7.463	1952	1956	1958	rBV	72	62	0.01%	0.001%
75	7.479	1958	1961	1962	rBV	156	89	0.01%	0.001%
76	7.566	1974	1988	2020	rBV	323768	573859	74.72%	9.449%
77	7.775	2051	2053	2055	rBV	132	62	0.01%	0.001%
78	7.852	2065	2077	2099	rBV	70406	120657	15.71%	1.987%
79	7.990	2116	2120	2123	rBV3	218	200	0.03%	0.003%
80	8.035	2132	2134	2135	rBV	202	98	0.01%	0.002%
81	8.183	2167	2180	2188	rBV2	3275	7255	0.94%	0.119%
82	8.312	2210	2220	2249	rVB	256316	441926	57.54%	7.277%
83	8.726	2346	2349	2352	rBV2	316	212	0.03%	0.003%
84	8.948	2416	2418	2419	rBV	168	52	0.01%	0.001%
85	9.032	2441	2444	2447	rVB	199	123	0.02%	0.002%
86	9.090	2448	2462	2487	rBV	355485	598596	77.94%	9.856%
87	9.228	2502	2505	2507	rBV	272	190	0.02%	0.003%
88	9.283	2519	2522	2523	rBV	161	93	0.01%	0.002%
89	9.328	2534	2536	2539	rBV	193	139	0.02%	0.002%
90	9.906	2713	2716	2720	rBV2	159	176	0.02%	0.003%
91	9.951	2726	2730	2732	rBV	273	225	0.03%	0.004%
92	9.984	2736	2740	2742	rVV	250	186	0.02%	0.003%
93	10.051	2759	2761	2767	rBV2	211	157	0.02%	0.003%
94	10.434	2868	2880	2903	rVB	230059	368642	48.00%	6.070%
95	10.614	2929	2936	2951	rVB5	2707	5035	0.66%	0.083%
96	11.131	3094	3097	3099	rBV	173	109	0.01%	0.002%
97	11.151	3100	3103	3105	rVV	264	170	0.02%	0.003%
98	11.485	3195	3207	3224	rBV	354401	550890	71.73%	9.071%
99	11.678	3263	3267	3270	rBV2	296	293	0.04%	0.005%
100	11.861	3312	3324	3345	rBV	323848	517625	67.40%	8.523%

Sum of corrected areas: 6073282

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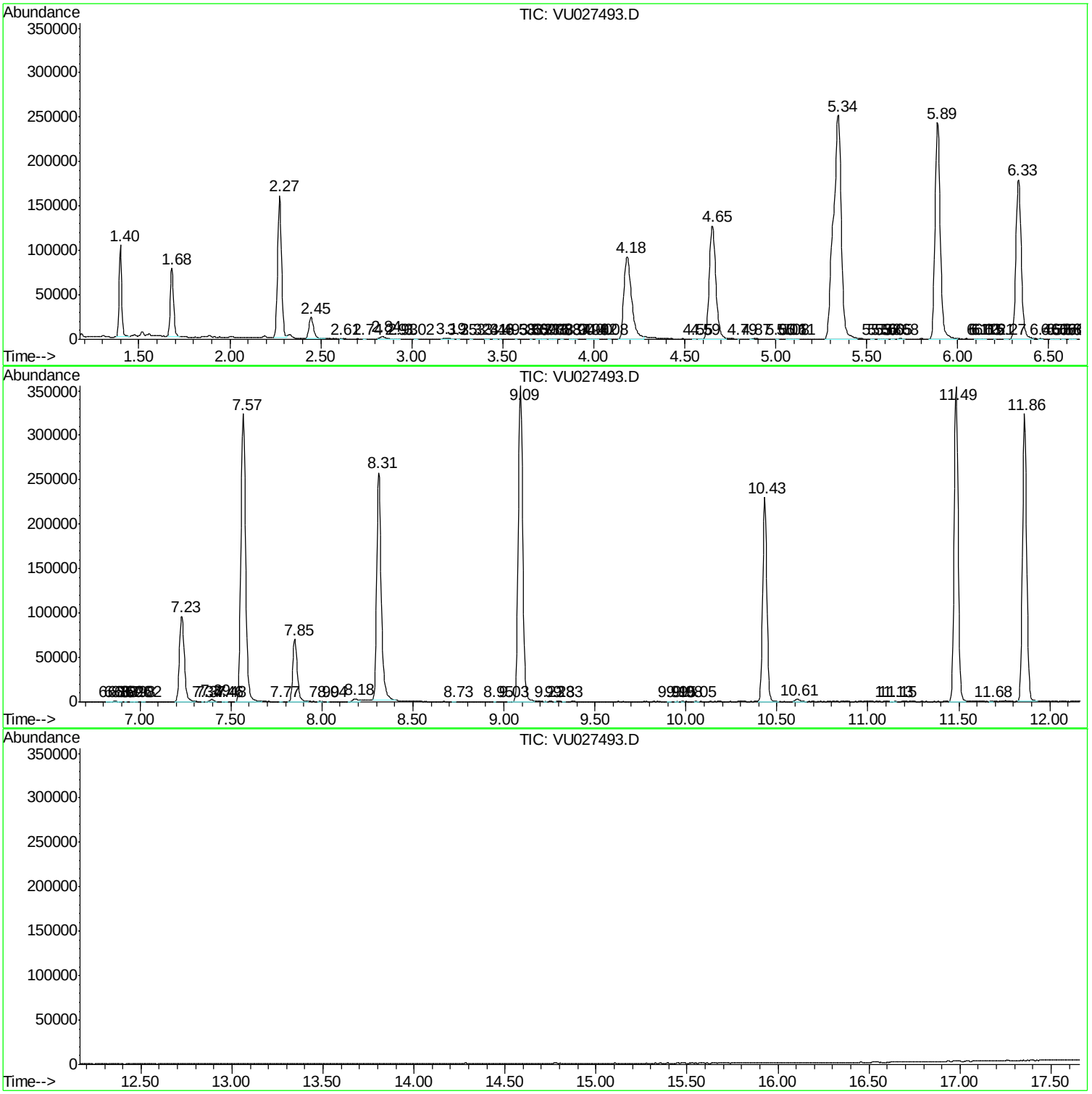
ClientSampleId : C0911

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\VOASRV\HPCHEM1\MSVOA_U\DATA\VU100818\
Data File : VU027493.D
Acq On : 08 Oct 2018 12:32
Operator : MD/SY
Sample : J5250-03
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 8 Sample Multiplier: 1

Instrument : MSVOA_U
ClientSampleId : C0911

Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.M
Quant Title : VOC Analysis

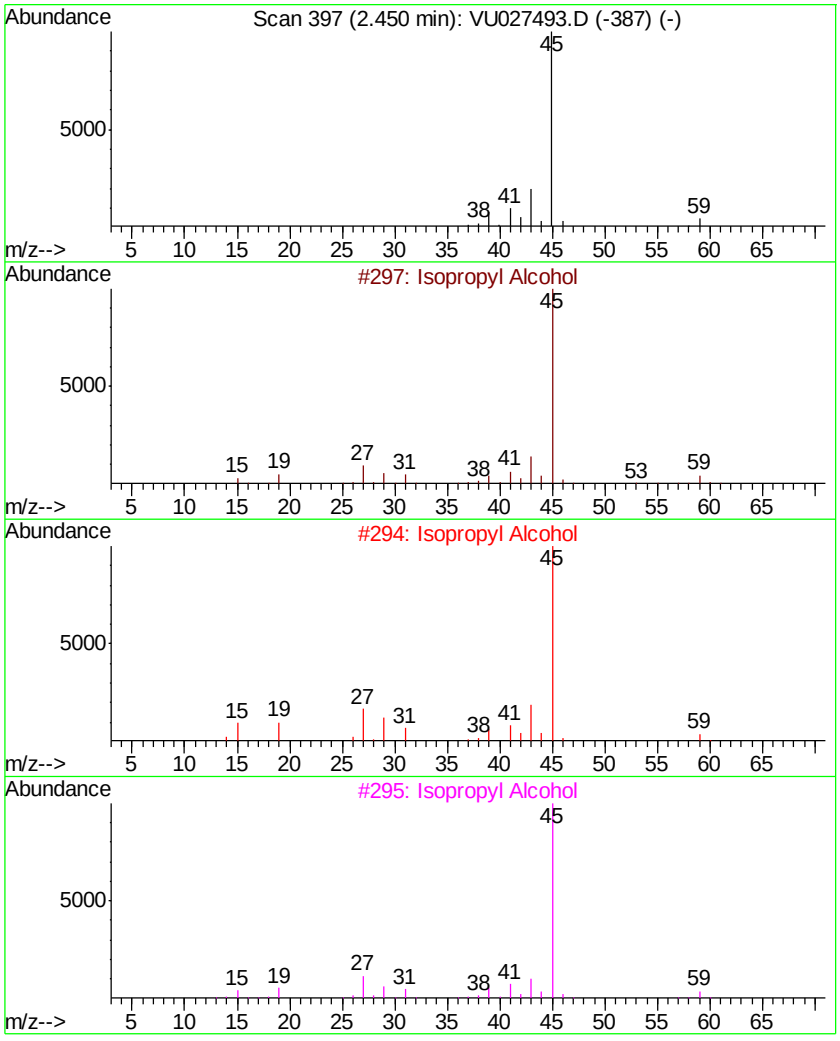
TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

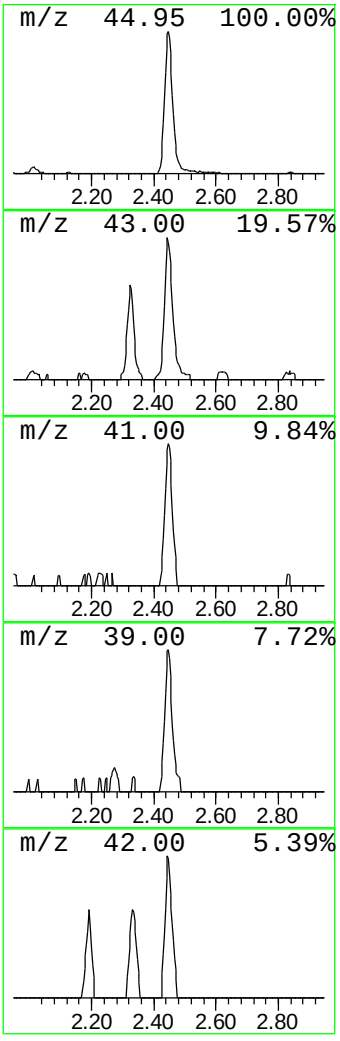
****

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.45	4.51 ug/L	43854	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	43
3	Isopropyl Alcohol	60	C3H8O	000067-63-0	9
4	4-Penten-2-ol	86	C5H10O	000625-31-0	9
5	L-Lactic acid	90	C3H6O3	000079-33-4	4





Tentatively Identified Compound (LSC) summary

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Instrument : MSVOA_U
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Quant Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM100518WMA.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	4.5	ug/L	43854	1	5.89	486166	50.0