

**Table1 Supplementary Data2** – Abundances of molecular water, hydroxyl group and total water by NIR Spectroscopy.

Run#	<i>(TT)</i> “area”			“height”			<i>(GG)</i> “area”			“height”		
	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>
<b>1</b>	0.36	0.64	1.01	0.33	0.73	1.06	0.28	0.72	1.01	0.30	0.76	1.06
<b>2</b>	1.04	1.35	2.39	0.96	1.45	2.41	0.85	1.46	2.31	0.89	1.49	2.38
<b>3</b>	2.52	1.45	3.97	2.25	1.73	3.98	2.32	1.90	4.22	2.22	1.89	4.12
<b>4</b>	4.44	1.48	5.91	3.97	1.78	5.75	3.82	2.05	5.87	3.77	2.02	5.78
<b>5</b>	4.26	1.34	5.60	3.90	1.68	5.58	3.63	2.01	5.64	3.66	1.99	5.65
<b>6</b>	3.64	1.14	4.78	3.41	1.75	5.16	3.18	1.69	4.87	3.23	1.80	5.03
<b>7</b>	5.16	1.77	6.93	4.56	2.17	6.73	4.68	2.34	7.02	4.32	2.35	6.68
<b>9</b>	4.30	1.31	5.61	3.90	1.66	5.56	3.69	2.12	5.81	3.68	2.05	5.73
<b>10</b>	3.61	1.81	5.42	3.26	1.90	5.16	3.05	2.20	5.25	3.03	2.05	5.08
<b>11</b>	4.87	1.51	6.38	4.47	2.18	6.65	4.49	2.14	6.62	4.25	2.19	6.43
<b>12</b>	0.68	0.92	1.60	0.54	1.09	1.63	0.55	0.92	1.47	0.51	1.09	1.60
<b>13</b>	1.90	1.47	3.37	1.58	1.68	3.26	1.74	1.67	3.41	1.49	1.83	3.32
<b>14</b>	1.62	1.52	3.14	1.39	1.64	3.03	1.41	1.59	3.00	1.35	1.72	3.07

**Table 2 Supplementary Data 2** – Errors on molecular water, hydroxyl group and total water contents by NIR Spectroscopy.

Run#	<i>(TT)</i> “area”			“height”			<i>(GG)</i> “area”			“height”		
	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>	H <sub>2</sub> O <sub>mol</sub>	OH	H <sub>2</sub> O <sub>tot</sub>
<b>1</b>	0.04	0.06	0.14	0.03	0.08	0.16	0.03	0.07	0.14	0.03	0.08	0.16
<b>2</b>	0.10	0.14	0.34	0.10	0.16	0.36	0.09	0.15	0.33	0.09	0.16	0.35
<b>3</b>	0.25	0.15	0.56	0.23	0.19	0.59	0.23	0.19	0.60	0.22	0.20	0.61
<b>4</b>	0.44	0.15	0.84	0.40	0.19	0.85	0.38	0.21	0.83	0.38	0.22	0.85
<b>5</b>	0.43	0.13	0.79	0.39	0.18	0.83	0.36	0.20	0.80	0.37	0.22	0.83
<b>6</b>	0.38	0.12	0.71	0.36	0.20	0.80	0.34	0.18	0.73	0.34	0.20	0.78
<b>7</b>	0.53	0.18	1.00	0.47	0.24	1.01	0.48	0.24	1.01	0.44	0.26	1.00
<b>9</b>	0.43	0.13	0.79	0.39	0.18	0.82	0.37	0.21	0.82	0.37	0.22	0.84
<b>10</b>	0.36	0.18	0.77	0.33	0.21	0.76	0.31	0.22	0.74	0.31	0.22	0.75
<b>11</b>	0.49	0.15	0.91	0.45	0.24	0.99	0.45	0.22	0.95	0.43	0.24	0.96
<b>12</b>	0.07	0.09	0.23	0.06	0.12	0.24	0.06	0.09	0.21	0.05	0.12	0.24
<b>13</b>	0.20	0.15	0.49	0.16	0.19	0.50	0.18	0.17	0.50	0.15	0.20	0.50
<b>14</b>	0.17	0.15	0.45	0.14	0.18	0.46	0.14	0.16	0.43	0.14	0.19	0.46

Errors are defined taking into account all the different uncertainties related to the variables present in Equation 1 of the text: absorbance uncertainty, sample thickness and glass density errors and molar absorptivities errors.