

Supplementary

Table S.1. Division of the sample set and results of the prediction within the calibration and validation data sets along with their deviation (predicted STDE for calibration and SD for validation set).

Data set	Sample	ORO	Predicted	SD
Calibration	<i>Sample 1</i>	7,86	11,45	2,16
	<i>Sample 2</i>	2,33	1,04	2,31
	<i>Sample 3</i>	16,37	18,67	2,13
	<i>Sample 4</i>	42,37	41,05	2,40
	<i>Sample 5</i>	4,07	1,04	2,31
	<i>Sample 6</i>	16,29	17,10	2,13
	<i>Sample 7</i>	19,64	19,46	2,42
Validation	<i>Sample 8</i>	5,35	6,49	1,91
	<i>Sample 9</i>	11,87	11,09	4,81
	<i>Sample 10</i>	40,9	39,47	2,21
	<i>Sample 11</i>	30,37	35,70	2,77
	<i>Sample 12</i>	25,69	29,71	2,01
	<i>Sample 13</i>	15,7	15,14	1,90