Vibrational Spectroscopy and Chemometrics for Rapid, Quantitative Analysis of Bitter Acids in Hops (*Humulus lupulus*)

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*S Supporting Information

Table S1. PLS-R model summaries (all models)

	PLS-R Parameters	UV Analyses			HPLC Analyses							
		α-acids	β-acids	Total	α-acids	β-acids	Total	Cohumulone	Hum/AdHum[a]	Colupulone	Lup/AdLup[b]	Xanthohumol
IR	r^2 (RMSEC)[c]	0.92 (1.2)	0.79 (0.7)	0.90 (1.6)	0.86 (1.4)	0.49 (1.1)	0.90 (1.5)	0.92 (0.3)	0.84 (1.2)	0.85 (0.3)	0.71 (0.3)	0.85 (0.09)
	r^2 (RMSEP)[d]	0.91 (1.3)	0.80 (0.7)	0.91 (1.8)	0.89 (1.4)	0.56 (1.0)	0.89 (1.8)	0.91 (0.4)	0.87 (1.1)	0.83 (0.4)	0.71 (0.4)	0.88 (0.07)
	LVs used	5	5	5	3	1	5	5	3	5	5	5
	RPD[e]	**3.4**	2.2	**3.3**	2.9	1.0	3.0	**3.4**	2.8	2.4	1.8	2.9
Raman	r^2 (RMSEC)[c]	0.88 (1.5)	0.75 (0.8)	0.87 (1.9)	0.86 (1.5)	0.67 (0.7)	0.84 (1.9)	0.90 (0.4)	0.84 (1.2)	0.83 (0.4)	0.71 (0.3)	0.87 (0.08)
	r^2 (RMSEP)[d]	0.91 (1.3)	0.80 (0.7)	0.90 (1.8)	0.90 (1.3)	0.62 (1.1)	0.90 (1.7)	0.91 (0.4)	0.84 (1.2)	0.82 (0.4)	0.5 (0.4)	0.87 (0.08)
	LVs used	4	4	4	4	4	4	7	4	6	6	4
	RPD[e]	**3.3**	2.2	**3.1**	**3.2**	1.8	**3.1**	**3.3**	2.5	2.4	1.5	2.8
NIR DRIFT	r^2 (RMSEC)[c]	0.87 (1.5)	0.76 (0.7)	0.91 (1.6)	0.86 (1.4)	0.53 (0.9)	0.89 (1.6)	0.82 (0.5)	0.87 (1.0)	0.64 (0.5)	0.58 (0.4)	0.85 (0.09)
	r^2 (RMSEP)[d]	0.91 (1.4)	0.66 (1.0)	0.93 (1.5)	0.91 (1.2)	0.64 (0.9)	0.92 (1.5)	0.82 (0.5)	0.88 (1.0)	0.63 (0.6)	0.44 (0.5)	0.78 (0.10)
	LVs used	4	6	4	4	3	4	5	6	5	5	6
	RPD[e]	**3.3**	1.7	**3.7**	**3.3**	1.7	**3.6**	2.4	2.9	1.7	1.3	2.1
MicroNIR®	r^2 (RMSEC)[c]	0.82 (1.8)	0.71 (0.8)	0.85 (2.0)	0.81 (1.7)	0.68 (0.7)	0.82 (2.0)	0.76 (0.6)	0.76 (1.4)	0.68 (0.5)	0.44 (0.5)	0.77 (0.10)
	r^2 (RMSEP)[d]	0.88 (1.5)	0.77 (0.8)	0.90 (1.8)	0.90 (1.3)	0.75 (0.7)	0.91 (1.6)	0.76 (0.6)	0.88 (1.0)	0.70 (0.5)	0.52 (0.4)	0.63 (0.13)
	LVs used	7	7	7	7	7	7	7	7	7	7	6
	RPD[e]	3.0	2.1	**3.3**	**3.2**	2.1	**3.5**	2.0	3.0	1.9	1.5	1.5

[a] Humulone and adhumulone. [b] Lupulone and adlupulone. [c] Root mean square error of calibration. [d] Root mean square error of prediction. [e] Ratio of prediction to deviation.