Electronic Supplementary Material (ESI) for Molecular BioSystems. This journal is © The Royal Society of Chemistry 2015

PLS regression results (complete model).

	R ² X cum.	R ² y cum.	Q ² cum.
1st component	10.4%	56.3%	31.1%
2nd component	25.6%	66.7%	45.6%
3rd component	33.5%	76.3%	47.3%