

**Development and validation of an *in situ* and real-time quantification
method for bicarbonate, carbonate and orthophosphate ions by ATR
FT-IR spectroscopy in aqueous solutions**

Supplementary Material

Analyst

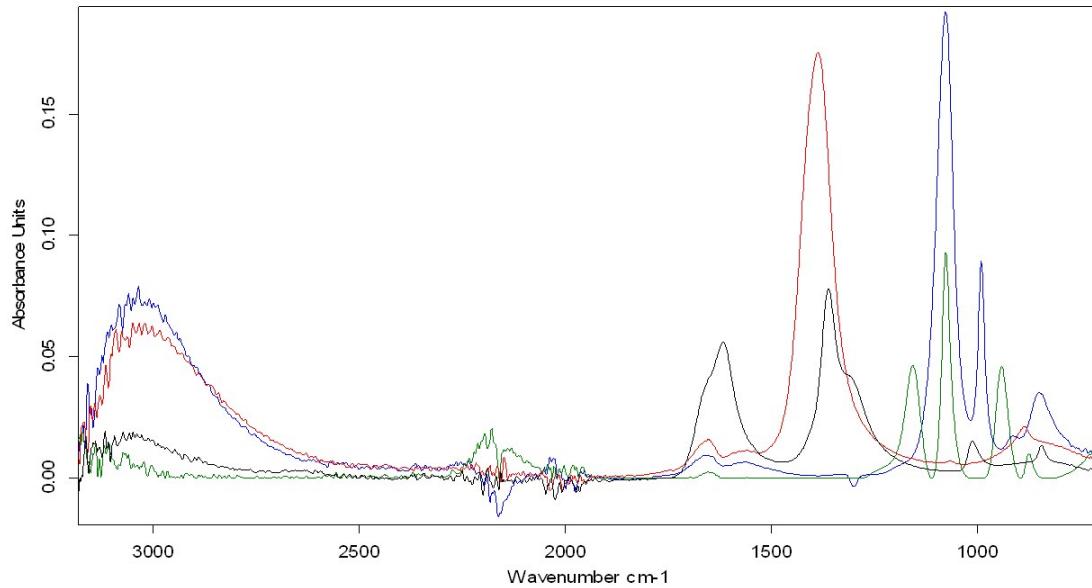
Pierre-Olivier Morisset¹, Jonathan Gagnon², Réjean Tremblay³, Jean-Sébastien Deschênes^{1*}

1. Département de mathématiques, informatique et génie, Université du Québec à Rimouski, 300 Allée des Ursulines, Rimouski, Québec, G5L 3A1, Canada

(Tel: +1-418-723-1986 Ext. 1997; e-mail: jean-sebastien_deschenes@uqar.ca)

2. Département de Biologie, chimie et géographie, Université du Québec à Rimouski, 300 Allée des Ursulines, Rimouski, Québec, G5L 3A1, Canada

3. Institut des sciences de la mer, Université du Québec à Rimouski, 310 Allée des Ursulines, Rimouski, Québec, G5L 3A1, Canada



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Page 1/1

Figure S1 ATR FT-IR absorption spectra for bicarbonate (black), carbonate (red), dihydrogenophosphate (green) and hydrogenophosphate (blue line)

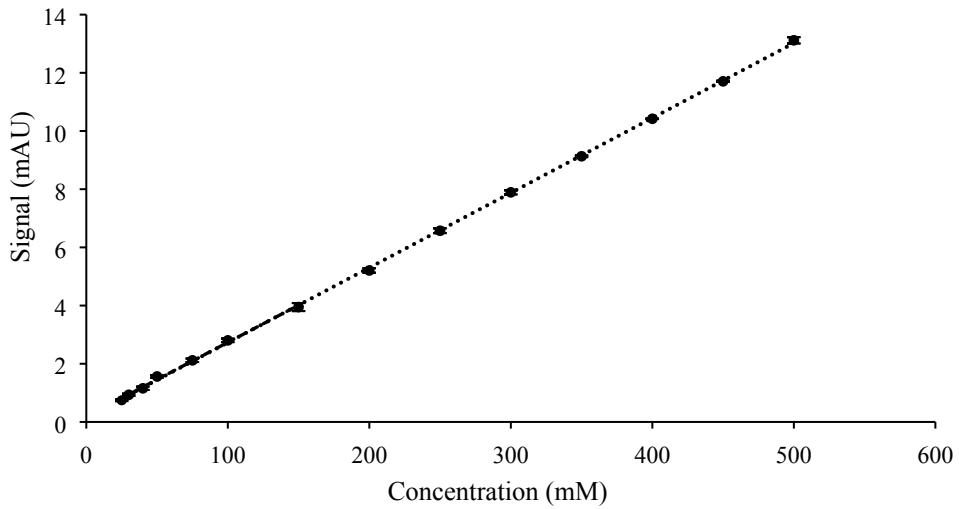


Figure S2 Univariate calibration curve and linearity for bicarbonate

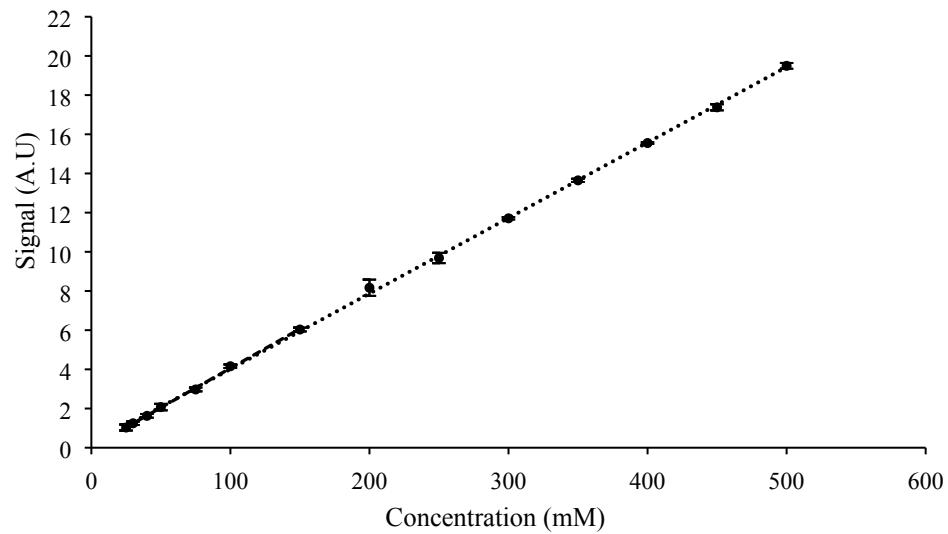


Figure S3 Univariate calibration curve and linearity for carbonate

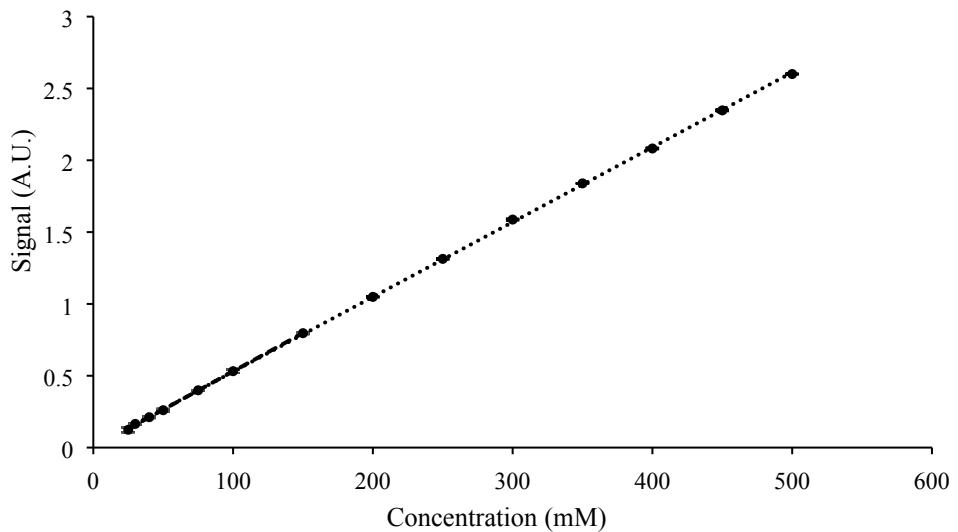


Figure S4 Univariate calibration curve and linearity for dihydrogenophosphate

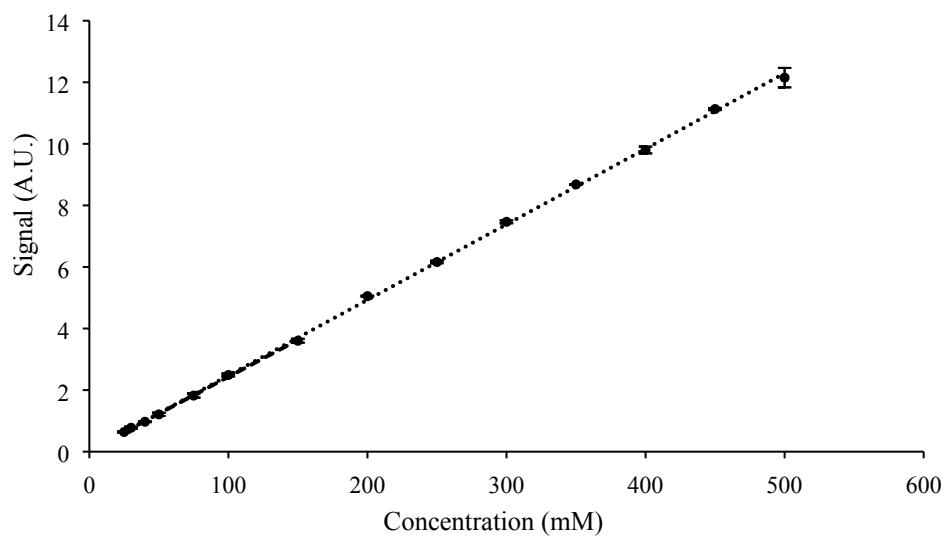


Figure S5 Univariate calibration curve and linearity for hydrogenophosphate

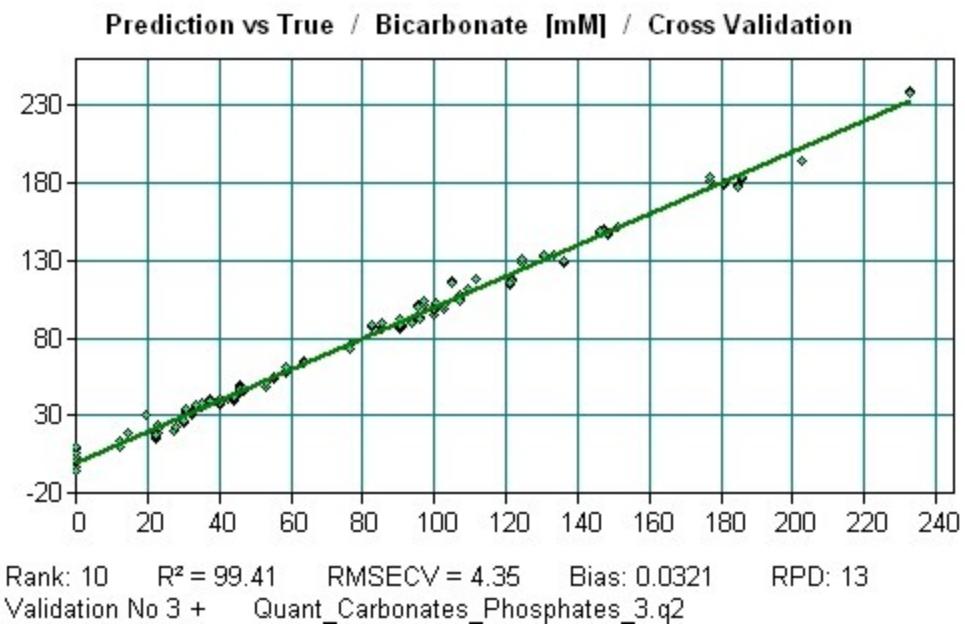


Figure S6 Multivariate model cross-validation curve and data for bicarbonate

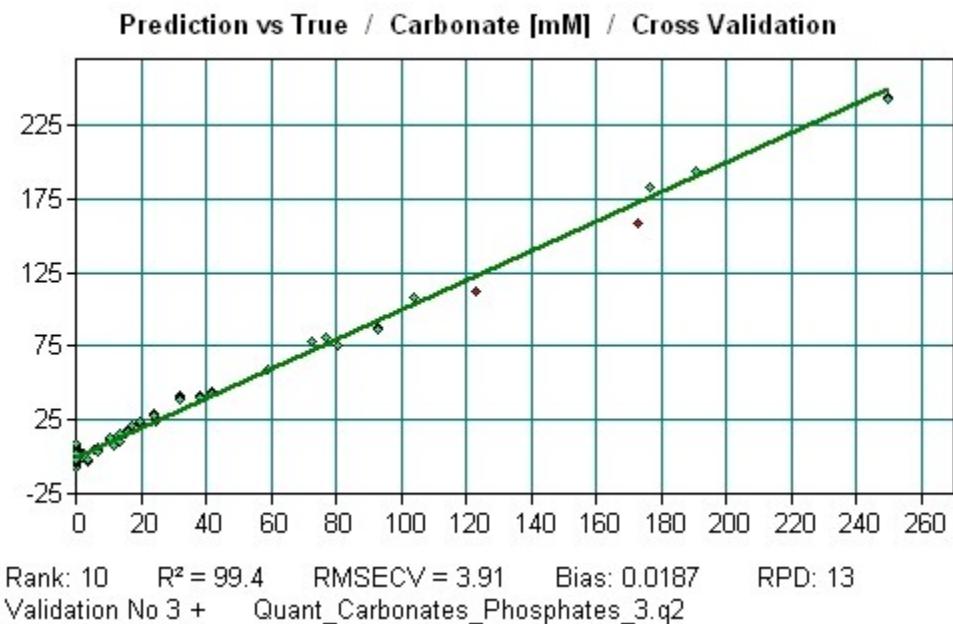
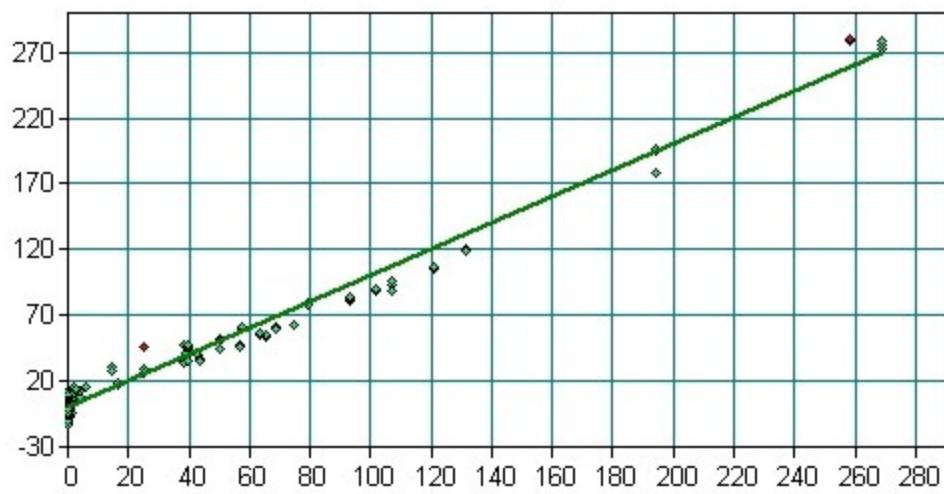


Figure S7 Multivariate model cross-validation curve and data for carbonate

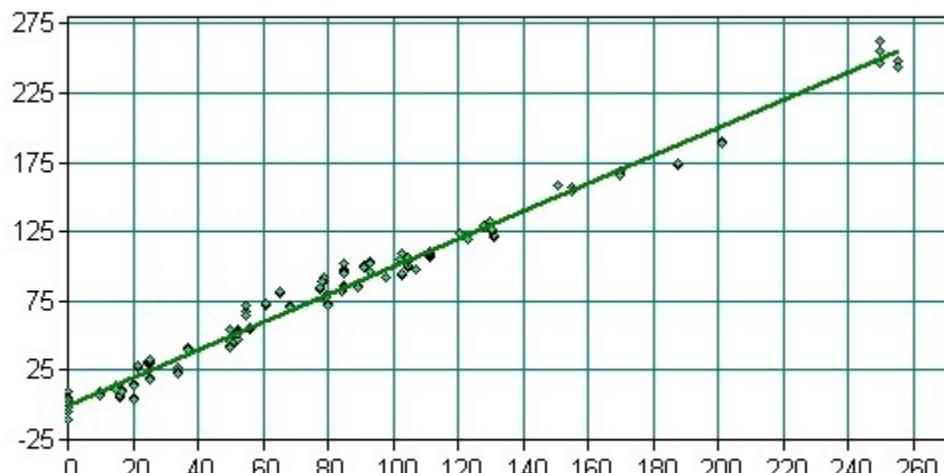
Prediction vs True / H₂PO₄- [mM] / Cross Validation



Rank: 10 R² = 98.04 RMSECV = 8.09 Bias: 0.0499 RPD: 7.15
Validation No 3 + Quant_Carbonates_Phosphates_3.q2

Figure S8 Multivariate model cross-validation curve and data for dihydrogenophosphate

Prediction vs True / HP04 2- [mM] / Cross Validation



Rank: 10 R² = 98.41 RMSECV = 7.23 Bias: -0.0671 RPD: 7.94
Validation No 3 + Quant_Carbonates_Phosphates_3.q2

Figure S9 Multivariate model cross-validation curve and data for hydrogenophosphate