TU-32

QUANTIFICATION OF PHARMACEUTICALS CONTAMINANTS IN WASTEWATERS BY NIR SPECTROSCOPY

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Emerging contaminants, as pharmaceuticals, are compounds of special concern due to the widespread usage and growing presence in aqueous systems. The traditional techniques used for the determination of pharmaceuticals are time or reagent consuming and faster, and labour and environmental friendly methods are welcome. In this context, this work presents a very simple, non-destructive, inexpensive and green strategy applied to the determination of ibuprofen (IBU), carbamazepine (CRB), β-estradiol (E2), ethinylestradiol (EE2), and sulfamethoxazole (SMX) concentrations using FT-NIR spectroscopy, in aqueous solutions.

The Y dataset employed in the chemometric analyses consisted of pharmaceuticals concentrations, monitored throughout the time length of the different experiments in this work, whilst the X dataset consisted of the collected FT-NIR spectra (ranging from 14000 to 200 cm^{-1}). Kolmogorov–Smirnov test and boxplot analysis were used for normal distribution check and outliers' rejection, followed by principal component analysis (PCA) for cluster analysis and outliers' rejection, and partial least squares (PLS) regression for the pharmaceuticals concentrations prediction. For all, except for EE2, the overall (tr+val) R^2 was above 0.94, RPD above 4 and RMSE around or below 6% (Table 1).

Table 1 – Main results of the PLS analysis

	Eq. (tr+val)	R^2 (tr+val)	RMSE (tr+val)	RMSE (val)	RPD (tr+val)	RPD (val)	n
IBU	**y = 1.022x**	**0.943**	**5.47**	**9.17**	**4.26**	**2.54**	**6**
SMX	**y = 1.001x**	**0.948**	**4.91**	**7.90**	**4.41**	**2.74**	**11**
E2	**y = 0.987x**	**0.951**	**6.16**	**10.72**	**4.69**	**2.70**	**12**
EE2	**y = 0.981x**	**0.858**	**10.12**	**17.50**	**2.83**	**1.64**	**16**
CRB	**y = x**	**0.963**	**5.10**	**8.79**	**5.44**	**3.16**	**17**

tr – training; val – validation; R^2 – coefficient of determination; RMSE – root mean square error; RPD – residual predictive deviation; n – number of PLS components

Acknowledgement

The authors thank the Portuguese Foundation for Science and Technology (FCT) under the scope of the strategic funding of UID/BIO/04469 unit, COMPETE 2020 (POCI-01-0145-FEDER-006684) and BioTecNorte operation (NORTE-01-0145-FEDER-000004) funded by the European Regional Development Fund under the scope of Norte2020 - Programa Operacional Regional do Norte. The authors also acknowledge the financial support to Cristina Quintelas through the postdoctoral grant (SFRH/BPD/101338/2014) provided by FCT – Portugal.