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WELCOME

“Thinking Organic and Medicinal Chemistry in an inspiring atmosphere”

The Organic and Medicinal Chemistry divisions of the Portuguese Chemical Society (SPQ) would like to express a warm welcome to the 11th ENQO, taking place from december 1-3 in Porto, Portugal. For the first time under the auspices of SPQ, the competences of these two important fields of Chemistry are brought together into a single event, to highlight complementarities and to promote new synergies.

The Scientific Committee has put high expectations on the excellence of the scientific program, which includes plenary/keynote lectures from renowned scientists whose work has been an inspiration for researchers in Organic and Medicinal Chemistry. Oral communications will focus on topics from the following main research fields:

Organic Synthesis
Spectroscopic Methods (in Organic Chemistry)
Organic Natural Compounds
Drug Metabolism and Disposition
Beyond Small Molecules
Computational Methods and Drug Design
Antitumor and Anti-infective Drugs
Industrial Applications

This meeting is expected to bring together researchers with different expertise and perspectives, from senior to young scientists, to discuss and share their latest achievements in a stimulating environment, taking advantage of the inspiring atmosphere of “Teatro Municipal Campo Alegre”, a theatre that is a cultural landmark of Porto.

We warmly invite you to come and enjoy the meeting and our beautiful city!

VICTOR DE FREITAS

Conference Chairman

**11º ENCONTRO NACIONAL DE QUÍMICA ORGÂNICA
4º ENCONTRO DE QUÍMICA TERAPÊUTICA
1 A 3 DEZEMBRO DE 2015**

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Following the removal of fluoroquinolones of the environment: an HPLC-FD method

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Antibiotic residues have been detected in various environmental matrices, such as surface water and even drinking water. Although present at low levels ($\mu\text{g/L}$, ng/L), many antibiotics are bioaccumulative, pseudo-persistent and can promote resistance/alterations in bacterial populations.¹

In this work we present the biosorption of three widely used fluoroquinolones (FQ) - ofloxacin (OFL), norfloxacin (NOR) and ciprofloxacin (CPF) to activated sludge (AS) and aerobic granular sludge (AGS). A High Performance Liquid Chromatography with Fluorescence Detection (HPLC-FD) method was validated and optimized to follow the biosorption of the targeted FQ.²

The HPLC-FD method was validated according to Q2B ICH guideline.³ The validated method demonstrated good selectivity, linearity ($r^2 > 0.999$), intra-day and inter-day precisions ($\text{RSD} < 3\%$) and accuracy. The detection limits were 0.6 ng/mL for NOR and CPF and 0.7 ng/mL for OFL and quantification limits were 1 ng/mL for three FQs.

Several parameters that can affect FQ biosorption kinetics, namely contact time, pH, biosorption mass were studied. At pH 7 AS showed better performance to biosorb OFL, NOR and CPF than AGS. The higher biosorption capacity of AS was probably due to the negative charge on its surface, evaluated by a zeta potential of -25.65 mV , at pH 7. OFL was the less biosorbed antibiotic, both onto AS and AGS, because at pH 7 this FQ is mainly present in its anionic form. The equilibrium data for AS showed a better fit to the Langmuir model, while the model that presented better fit for AGS was the Freundlich model. The FQ could be desorbed from AGS at pH 3, pH 8 and pH 9 whereas at pH 4 the biosorption process was promoted.

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References:

1. Doorslaer V.X.; Dewulf J.; Langenhove H.V.; Demeestere K. *Science of the Total Environment*. **2014**, 500 (501), 250-269.
2. Maia A.S.; Ribeiro A.R.; Amorim C.L.; Barreiro J.C.; Cass Q.B.; Castro P.M.; Tiritan, M.E. *Journal of chromatography A*. **2014**, 1333, 87-98.
3. ICH. Q2B. Validation of Analytical Procedures: Methodology: International Conference on Harmonization Expert Working Group. **1996**.