Analytical and environmental chemistry

S1_P_08

INFLUENCE OF FLUOROQUINOLONE ANTIBIOTICS ON BIOSPECIATION OF CALCIUM(II) ION IN HUMAN BLOOD PLASMA BY COMPUTER SIMULATION

LJUBINKA JOKSOVIC[1], BILJANA SMIT[1], IVAN JAKOVLJEVIC[1], NEVENA MIHAILOVIC[1], DJORDJE PETROVIC[2]

Abstract. Fluoroquinolones (FQs) are therapeutic agents which, based on chemical structure, can act as complexing agents for metal ions. The relative ability of FQs to compete with plasma metal ions and with other low molecular weight (LMW) ligands can be expressed as plasma mobilization index (PMI). This is a useful tool to carry out preliminary in vitro assessment of mobilizing influence of chelating agent using computer modeling based on the thermodynamic data.

The effect of fluoroquinolones (levofloxacin, ciprofloxacin and moxifloxacin) on calcium biospeciation in blood plasma was studied by computer simulation. Results obtained from HySS2009 calculation indicate that below therapeutic concentration (10^{-5} mol·L^{-1}) FQs are dominantly bound into the calcium and magnesium complexes. On the basis of PMI it could be concluded that mobilization of calcium ions is the most significant with levofloxacin while other FQs show the order levofloxacin > ciprofloxacin > moksifloxacin. This results indicate that fluoroquinolones at therapeutic concentration does not affect the biospeciation of calcium ion in blood plasma.

Keywords: fluoroquinolone; human blood plasma; biospeciation.

[1] *University of Kragujevac, Faculty of Science, 34000, Serbia and Montenegro. E-mail: ljubinka@kg.ac.rs.*

[2] *Institute of Nuclear Science Vinca, 11001, Serbia and Montenegro.*