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**Master Thesis Defense**

Entitled

*ESTIMATION OF THE REMOVAL OF CHIRAL PHARMACEUTICAL DRUGS FROM DOMESTIC WASTEWATER USING UPLC-MS/MS*

by

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Abstract

This thesis is concerned with the assessment of the removal of chiral pharmaceutical compounds (PCs) from domestic wastewater in Al Ain using UPLC-MS/MS. PCs are classified into many classes such as hormones, antibiotics, analgesics,  $\beta$ -blockers, and anti-inflammatory drugs. PCs do not have a guideline to describe their concentrations in treated domestic wastewater. Additionally, there is a very high demand for using PCs around the world, which results in their discharge to wastewater at relatively high masses which could be harmful to the environment. Moreover, very limited work has been reported on the estimation of the removal of chiral PCs from wastewater, and the removal mechanisms of every enantiomer alone at wastewater treatment plants (WWTPs). This study aimed to develop a chiral separation and determination method for 16 chiral PCs. It intended to study PCs levels and removal selectivity at different locations at Al Saad WWTP in Al Ain city using ultra-performance liquid chromatography-tandem mass spectrometry (LC-MS/MS). Four batches of wastewater and sludge samples have been grabbed from different locations at Al Saad WWTP, followed by solid-phase extraction (SPE). 15 out of 16 chiral PCs were successfully chirally separated except for tramadol drug. Calibration curves, instrument limit of detection, instrument limit of quantification, and method limit of detection were successfully determined. Results show tramadol, atenolol, and o-desmethylfenlaxine occur at relatively high concentrations compared to others ( $>2 \mu\text{g/L}$ ). In general, the removal efficiency exceeded 90% for most of the tested PCs with exception of metoprolol, terbutaline, and fluoxetine (between 30% and 70%), while a low removal was indicated for atenolol (25.9%). Moreover, the treatment process was more selective for the removal of the second enantiomer of bupivacaine and fluoxetine. In general, results indicate that filtration and disinfection play the main role in the removal of the target PCs. A change in the PCs behavior at the Return Activated Sludge (RAS), Anaerobic Digester (AD), and Filter Press (FP) units was indicated. Propranolol preferably sorbed to RAS more than the other tested PCs, while citalopram and tolperisone preferably sorbed to the AD sludge surface more than other operational units. In addition, E2 of propranolol and mianserin was at the higher concentration on the sludge than their antipode in the RAS. While RAS was enriched with the first enantiomer of bupivacaine, terbutaline, citalopram, and fluoxetine.

**Keywords:** Chiral pharmaceutical compounds, Enantiomers, Wastewater, Al-Saad WWTP, sludge, LC-MS/MS, mass balance, internal standard, removal efficiency, Al Ain, UAE.