University of Zabol
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Department of Chemistry

The Thesis Submitted for The Degree of Master of sciences (In the field of Analytical Chemistry)

Applying some cheminformatics methods to find effective predictors on physicochemical properties of a set of radiopharmaceuticals

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Abstract

The utilization of radiopharmaceuticals has seen remarkable expansion in their application for therapeutic purposes and non-invasive disease diagnosis through diagnostic imaging. The rising durations and expenses involved with the discovery and development of novel radiopharmaceuticals have led to the creation of better ways to do this job faster and cheaper. We present a quantitative structure-property relationship (QSPR) model for a group of 121 PET tracers, which is based on their lipophilicity or LogP values. To create this model, we used CORAL software to randomly divide the dataset into three sets: a training set (50%), a calibration set (25%), and a validation set (25%). The hybrid optimal descriptor is computed using a combination of SMILES and Hydrogen- Suppressed Graph (HSG) molecular descriptors, and the QSPR models are generated through the Monte Carlo algorithm. The constructed models exhibited strong stability in relation to statistical metrics. In conclusion, the structural details extracted from the model descriptors provide valuable insight for the increase/decrease of LogP.

Keywords: CORAL, SMILES, Radiopharmaceuticals, PET tracers