These cellular processes require high lipophilicity in chemical molecules. These group of compounds act as non-nucleoside reverse transcriptase inhibitors of HIV. 

Aim: The aim of this study is to build a quantitative structure-property relationship (QSPR) of 66 thiazolidin-4-one derivatives in order to predict their logP.

Introduction: Performing computational drug design is an important step for their synthesis and properties characterization. In this work, quantitative structure-property relationship (QSPR) of 66 thiazolidin-4-one derivatives was examined in order to predict their logP which is the most commonly used measure of lipophilicity in chemical molecules. These group of compounds were optimized by DFT method showed better correlation than HF. Morever, acetate and lactate are potentially seen as metabolic biomarkers of lung development.

Methods: Two different quantum mechanics approaches including HF and DFT were applied for energy minimization of structures and different classes of molecular descriptors including quantum chemical descriptors were generated for prediction of their logP. Numbers of descriptors which showed high correlation with each other were removed by MATLAB software. The model between structures and their LogP was built for both methods with performing Multiple Linear Regression (MLR) in Spss package.

Results: Statistical results and application of developed model to the test set demonstrates that the DFT model is reliable with good predictive accuracy. (R2cal = 0.90, R2cv = 0.88) The lack of significant difference between the original and modeled values of logP reveals the validity of the built model which was built with 2D and 3D descriptors. The coefficients of model are statistically significant.

Conclusion: QSPR models can be used to predict molecular properties such as LogP. That will be beneficial in drug design processes. In this research, MLR model was built in order to correlate structure of 66 compounds with their LogP. Molecules that were optimized by DFT method showed better correlation than HF method that indicates the accuracy of the built model with 2D and 3D descriptors.