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## PS184

### Quantitative structure-property relationship (QSPR) of thiazolidin-4-one derivitives as RTIs of HIV virus

N. Moussavi Harami*, A. Almasi Rad

*Department of Medicinal Chemistry, Faculty of Pharmacy, Islamic Azad University, Iran*
*E-mail address:* moussavi.nasim@gmail.com
(N. Moussavi Harami).

**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 log *P*.

**Introduction:** Performing computational drug design is an important step for their synthesis and properties characterizations. 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 act as non-nucleoside reversed transcriptase inhibitors of HIV.

**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.

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## PS185

### Lung branching morphogenesis, in the chicken model, is accompanied by temporal metabolic changes

H. Fernandes-Silva[1,2,*], M.G. Alves[3,4], J. Correia-Pinto[1,2,5], P.F. Oliveira[3,4,6,7], R.S. Moura[1,2]

[1] *Life and Health Sciences Research Institute (ICVS), School of Medicine, University of Minho, 4710-057 Braga, Portugal*
[2] *ICVS/3B's – PT Government Associate Laboratory, 4710-057 Braga/Guimarães, Portugal*
[3] *Unit for Multidisciplinary Research in Biomedicine (UMIB), Institute of Biomedical Sciences Abel Salazar (ICBAS), University of Porto, 4050-313 Porto, Portugal*
[4] *Department of Microscopy, Institute of Biomedical Sciences Abel Salazar (ICBAS), University of Porto, 4050-313 Porto, Portugal*
[5] *Department of Pediatric Surgery, Hospital de Braga, 4710-243 Braga, Portugal*
[6] *i3S - Instituto de Inovação e Investigação em Saúde, University of Porto, 4050-313 Porto, Portugal*
[7] *Department of Genetics, Faculty of Medicine (FMUP), University of Porto*
*E-mail address:* hugomiguelfsilva@gmail.com
(H. Fernandes-Silva).

**Aim:** In this work, we characterized, for the first time, the metabolic profile of chick lung branching in early stages of development: b1, b2 and b3 (1, 2 or 3 secondary bronchi, respectively).

**Introduction:** Pulmonary development is a complex process that depends on the activation of conserved signaling pathways that regulate cellular processes such as proliferation, differentiation and migration.[1–3] These cellular processes require high amounts of energy and nutrients to form new biomass.[4,5] However, the metabolic changes that occur during lung branching morphogenesis have not been described so far.

**Methods:** Ex vivo lung explant culture was performed and the medium collected to analyze the production/consumption of metabolic intermediates associated with glucose catabolism (lactate, acetate, alanine), by 1H-NMR. qPCR was performed to assess the expression levels of key enzymes and transporters from the correspondent metabolic pathways.

**Results:** The results showed that the major variations occur from stage b1 to stage b3. In b3 there is an increase in lactate and acetate production. Still, glucose consumption is maintained from b1 to b3 stage, with a concurrent decrease of glucose transporter 3 (glut3) transcript levels. Hexokinase 1 (hk1) levels also decrease in b3 stage (as compared to b2). This phenomenon suggests an increase in the glycolytic efficiency and a shift to lactic acid production (in detriment of mitochondrial respiration). In fact, we observed a decrease on pyruvate dehydrogenase B (pdhB) and an increase in lactate dehydrogenase A (ldhA) expression levels in b3 stage (as compared to b2), while lactate dehydrogenase B (ldhB) levels decrease.

**Conclusion:** This study describes, for the first time, the temporal metabolic changes associated with chick pulmonary branching. It seems that glycolytic efficiency is increased and Krebs cycle metabolism shifts to lactate production along development. Furthermore, acetate and lactate are potentially seen as metabolic biomarkers of lung development.