

# Medicinal Chemistry & Computer Aided Drug Designing

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## Synthesis, characterization and evaluation of arylamines in a murine model of obesity

Christian F Hernández-Martínez, Marvin A Soriano-Ursúa and José G Trujillo-Ferrara  
Instituto Politécnico Nacional, Mexico

The human  $\beta_3$  adrenergic receptor ( $\beta_3$ AR) is mainly expressed in white and brown adipocyte tissue, its activation is associated with lipolysis and thermogenesis; therefore it has become an attractive target for the treatment of some metabolic diseases. The aim of this job is to perform rational design of dopamine derivatives with *in silico* study for getting good affinity and efficacy on  $\beta_3$ AR and then synthesize the most promising compounds for further evaluation in a murine model of obesity. Two compounds were chosen (Doprotec and Dop1) for their synthesis. The compounds were evaluated in a murine model of obesity using male C57BL/6 mice of which underwent low calorie diet or high calorie diet. The *in silico* study results of  $\beta_3$ AR demonstrate that the presence of boron promote affinity and voluminous substituents on the amino group enhance selectivity. Synthetic methods used are suitable for generating dopamine derivatives substituted at the amino group generating good yields thus, high purity. Doprotec compound has an action on the body weight and significantly lowers glucose levels, triglycerides and cholesterol in plasma, whereas only dop1 decreases triglycerides and cholesterol. The suggested mechanism by which Doprotec acts on body weight include: 1) Direct effects on adipose tissue by modifying the lipid metabolism through activation of  $\beta_3$ AR inducing lipolysis, and 2) Modifying the secretory pathway of other hormones that regulate metabolism.

### Biography

Christian F Hernández-Martínez is a Master's student in Pharmacology Science in the Escuela Superior de Medicina at Instituto Politécnico Nacional. He is a Pharmacist and currently has different research lines that include activating adrenergic receptors, obesity and synthesis of boron-containing compounds.

[cri16fhm@gmail.com](mailto:cri16fhm@gmail.com)

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