



UNIVERSITÉ DE  
**SHERBROOKE**

Institut de Pharmacologie de Sherbrooke  
3001, 12<sup>e</sup> Avenue Nord  
Sherbrooke (Québec)  
CANADA J1H 5N4

Éric MARSAULT, Ph.D.  
Director  
Institut de Pharmacologie de Sherbrooke  
Telephone: (819) 821.8000 ext72433  
Fax: (819) 564-5400  
e.mail: eric.marsault@usherbrooke.ca

Sherbrooke, September 30, 2019

### **Post-doctoral Position in Molecular modeling**

*Subject: homology modeling and docking in bacterial ATP synthase*

Our group has identified that tomatidine, a steroid alkaloid, possesses antibiotic properties against Small Colony Variants of *S. aureus* and potentiates the action of aminoglycoside antibiotics. We further identified the bacterial ATP synthase as the target of the molecule and a series of analogues. With the goal to further characterize the mechanism of action and optimize novel antibiotics targeting different pathogens, we now aim to build homology models of several bacterial ATP synthases and perform docking of a series of molecules in these targets. Additional projects in medicinal chemistry with other types of targets will also require this expertise.

#### *Candidate profile*

Master or Ph.D. in computational chemistry, bioinformatics, biochemistry or another relevant field with strong proficiency in molecular modeling, homology model building and curating, docking, virtual high throughput screening and associated know-how. Excellent track record demonstrated by a solid publication profile. Autonomy, resourcefulness, ability to work in a multidisciplinary environment and to interact productively with a team of medicinal chemists.

Knowledge of MOE software (from CCG) would be considered an asset.

#### *Location :*

Medicinal chemistry laboratory, Institut de Pharmacologie de Sherbrooke, Sherbrooke (Qc, Canada).

*Start date:* January 2020, or depending on availability.

For inquiries, please send CV, letter of motivation and synopsis of research experience to date to:  
Pr Éric Marsault ([eric.marsault@usherbrooke.ca](mailto:eric.marsault@usherbrooke.ca))

*(NB: only candidates whose application is further considered will be contacted within two weeks of application)*

#### Key references:

Lamontagne Boulet *et al*, *Antimicrob. Ag. Chemother.* **2018**, e02197.

Boulamnger *et al*, *Antimicrob. Ag. Chemother.* **2015**, 7458.

Mitchell *et al*, *Antimicrob. Ag. Chemother.* **2011**, 1937.

Hahn *et al*, *Science* **2018**, 360.

Preiss *et al*, *Sci. Adv.* **2015**, e1500106.