Evaluation of the unbinding kinetics of Mineralocorticoid (MR) receptor steroid agonist Cortisol (COL) , Aldosterone (AS4), and Progesteron (STR) ligands using Molecular Dynamics (MD) and Monte Carlo (MC) simulations

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Abstract

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I Introduction

Is wildly known the important role of the mineralocorticoid hormone aldosterone in the cardiovascular system, in particular in the effects that have in the kidney. Nevertheless, several researches have demonstrated the importance of this hormone [1, 2]

[3]

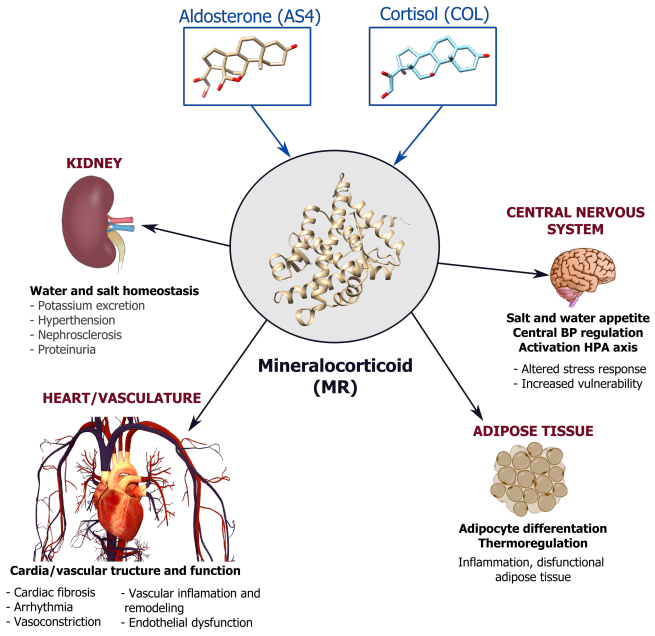

Figure 1: Mineralocorticoid/aldosterone receptor impact on health. *Image adapted from [1]*

II Methods

Selection of the best method to simulate the system, description of the simulation methods and how are we analyzing the date, since the MD simulations have a sense of time while the MC simulations does not, pyEMMA.

LiBEla [4]

Amber and LiGaMD [5]

[6, 7]

[8]

why MC and MD, what software are we using?

III Results and Discussion

Select images of interest and explain them

IV Conclusion

What is possible to conclude from each simulation and how can it be explain from chemistry and physics

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