

UNIVERSITÀ DELLA CALABRIA



XXV Congresso Nazionale della Società Chimica Italiana

Arcavacata di Rende
07-12 Settembre 2014

ATTI DEL CONGRESSO

DA-Phen, a new dopamine aminoacid conjugate: *in vivo* testing and molecular modeling as dopaminergic modulator

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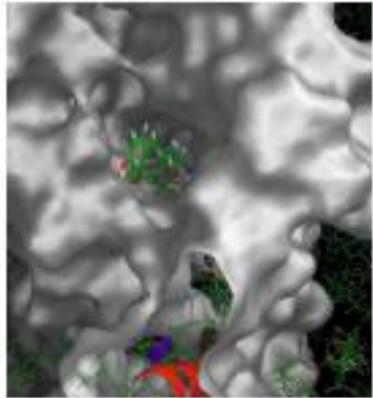
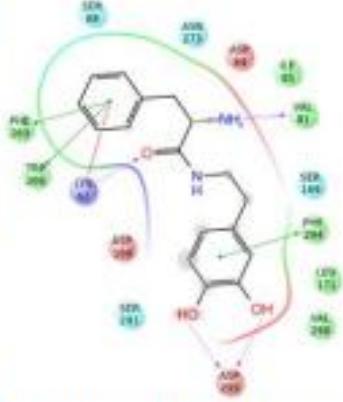
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DA-Phen [1] was designed potential dopaminergic active, depressive like-behavior. Spatial learning memory assessment protocols (Forced Swim Test and Morris Water Maze) were used in order investigate the *in vivo* potential behavioral pattern



DA-Phen on male Wistar rats. Our results strengthen the hypothesis that DA-Phen could induce adaptive responses to environmental challenges, probably due to the modulation of dopaminergic neurotransmission.

Homology modeling of GPCR D1 dopamine receptor was performed. The model, validated by means Ramachandran plot and q-mean score, was thereafter inserted in a double layer membrane. The surfaces of the binding pocket were mapped and used to perform a validated protocol of induced fit docking [2] with the aim to confirm the results obtained from the behavioral tests. DA-Phen showed docking capability higher than other known D1 agonists.

- [1] Giannola L.I. et al., *Pharmazie*, 2008, **63**, 704–710.
 [2] Almerico A. M. et al., *J. Mol. Mod.*, 2012, **18**, 2885–289.