Journal of Biomolecular Structure and Dynamics
Publication details, including instructions for authors and subscription information:
http://www.tandfonline.com/loi/tbsd20

196 Antiinflamatory activity of phenolic compounds extracted from Uruguayan propolis and grape

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Published online: 23 Jun 2015.

To cite this article: Elena Alvareda, Pablo Miranda, Victoria Espinosa, Helena Pardo, Sara Aguilera & Margot Paulino Zunini (2015) 196 Antiinflamatory activity of phenolic compounds extracted from Uruguayan propolis and grape, Journal of Biomolecular Structure and Dynamics, 33:sup1, 129-129, DOI: 10.1080/07391102.2015.1032833

To link to this article: http://dx.doi.org/10.1080/07391102.2015.1032833

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196 Antiinflamatory activity of phenolic compounds extracted from Uruguayan propolis and grape

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Propolis and grape pomace have significant amounts of phenols that can take part in antiinflammatory mechanisms (Paulino Zunini et al., 2010).

As the cyclooxygenases 2 and 1 (COX-2 and COX-1) are involved in them, the ability of phenolic extracts to inhibit these enzymes was analyzed in vitroand in silico. Samples of propolis and grape pomace from 2 grape species collected between 2008 and 2013 from different places of Uruguay and in different seasons were used (Rimon et al., 2010; Wang et al., 2010).

Based on phenols previously identified, and taking as reference a crystallographic structure of COX-2 (3LN1) and COX-1 (3KK6) bound to celecoxib, a molecular docking procedure was adjusted to reproduce the celecoxib position in the cristal and then used with the phenolic molecular models. The docking was performed with the MOE 2009.10 (Molecular Operating Environment) (ChemComp Co.) with the Affinity dG function for Scoring and Re-scoring, the MMFF94x force field to refinement and the Alpha Triangle as the placement algorithm.

When phenols were docked to COX-2, the most common binding aminoacids were Tyr341, Tyr101, Val74, Pro71, Arg106, Glu510, Leu109 and Ser105. In the case of COX-1, they were Glu524, Pro86 and Arg120. From best docked phenol-COXs complexes, 10 ns of Molecular Dynamics simulations were performed by triplicate, using Amber99 force field. The interaction energy phenol-environment was averaged and compared with the docking binding energies (Score) for COX-2 and COX-1 respectively and with those of in vitroassays that showed an inhibition range of 5,0–43,5% of COX-2 and 6,1–46,0% of COX-1.

We thank PEDECIBA QUÍMICA for the economic support, and Urimpex and Castel Pujol for the propolis and grape pomace samples respectively.

References

Paulino Zunini, M., Rojas, C., Depaula, S., Elingold, I., Alvareda, E., Casanova, … Dubin, M. (2010). Phenolic contents and antioxidant activity in central southern Uruguayan propolis extracts. *Journal of Chilean Chemical Society, 55*, 141–146.

Rimon, G., Sidhu, R. S., Lauver, D. A., Lee, J. Y., Sharma, N. P., Yuan, C., … Smith, W. L. (2010). Coxibs interfere with the action of aspirin by binding tightly to one monomer of cyclooxygenase-1. *Proceedings of the National Academy of Sciences, 107*, 28–33.

Wang, J. L., Limburg, D., Graneto, M. J., Springer, J., Hamper, J. R., Liao, S., … Carter, J. (2010). The novel benzopyran class of selective cyclooxygenase-2 inhibitors. Part 2: The second clinical candidate having a shorter and favorable human half-life. *Bioorganic & Medicinal Chemistry Letters,* 7159–7163.

197 Combination of e-pharmacophore modeling, multiple docking strategies and molecular dynamic simulations to discover of novel antagonists of BACE1

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Beta-site amyloid precursor protein cleaving enzyme (BACE1 or β-secretase), an aspartic protease responsible for ramping up of Aβ-40/42 peptide fragments by cleaving APP that conciliate for the production of senile plaques and neurofibrillary tangles. Thus it leads to the non-specific road blocks for physical transport and neuro transmitters elevating the hippocampal neuronal damage which eases the memory deficits in Alzheimer's disease (AD). Imparted fundamental role of β-secretase in the formation of Aβ peptide leading to AD, it has been a major therapeutic target for AD intervention, hence was targeted in the present work. One hundred and twenty-nine crystal structures were refined with respective co-crystal ligands to generate 129 e-pharmacophore models based on the interaction energy (Ravichand et al.,