COX-1/COX-2 inhibition activities and molecular docking study of newly designed and synthesized pyrrolo[3,4-c]pyrrole Mannich bases.

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Rok wydania

2019

Czasopismo

Bioorganic and Medicinal Chemistry

Numer woluminu

27

Strony

3918-3928

DOI

10.1016/j.bmc.2019.07.033

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In the present paper we describe the biological activity of newly designed and synthesized series of pyrrolo[3,4-*c*]pyrrole Mannich bases (**7a**-**n**). The Mannich bases were obtained in good yields by one-pot, three-component condensation of pyrrolo[3,4–*c*]pyrrole scaffold (**6a**-**c**) with secondary amines and an excess of formaldehyde solution in C_2H_5OH. The chemical structures of the compounds were characterized by ^1H NMR, ^{13}C NMR, FT-IR, and elemental analysis. Moreover, single crystal X-ray diffraction has been recorded for compound **7l**. All synthesized derivatives were investigated for their potencies to inhibit COX-1 and COX-2 enzymes by colorimetric inhibitor screening assay. In order to analyse the intermolecular interactions between the ligands and cyclooxygenase, experimental data were supported with the results of molecular docking simulations. According to the results, all of the tested compounds inhibited the activity of COX-1 and COX-2.

Słowa kluczowe

Pyrrolo[3,4-c]pyrrole, Cyclooxygenase inhibition, COX-1/COX-2, Molecular docking, Mannich bases

Adres publiczny

http://dx.doi.org/10.1016/j.bmc.2019.07.033

Strona internetowa wydawcy

http://www.elsevier.com