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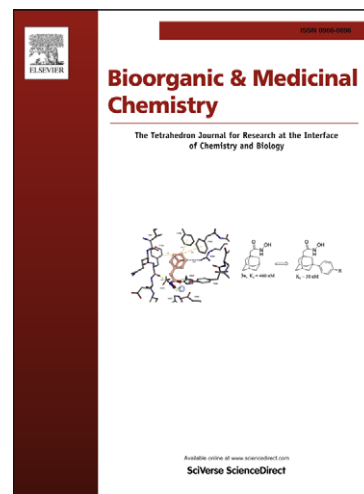
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The systematic structure-activity relationship to predict how flavones bind to human androgen receptor for their antagonistic activity

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ABSTRACT

Although flavones act as potent androgen receptor (AR) antagonists, it remains unclear how flavones interact with AR. The aim of this *in silico* study was to investigate the molecular recognition processes of newly synthesized 5,4'-difluoroflavone with the highest activity (IC_{50} value = 0.19 μ M) in the AR-ligand binding domain (AR-LBD). The results demonstrated that at its 4'-position of 5,4'-difluoroflavone the substituents may face Arg752 and that in AR-LBD, the submolecular bulk of substituents is unfavorable for AR antagonists and the negative electrostatic interaction site prefers the

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