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Molecular modeling studies of atorvastatin analogues as HMGR inhibitors using 3D-QSAR, molecular docking and molecular dynamics simulations

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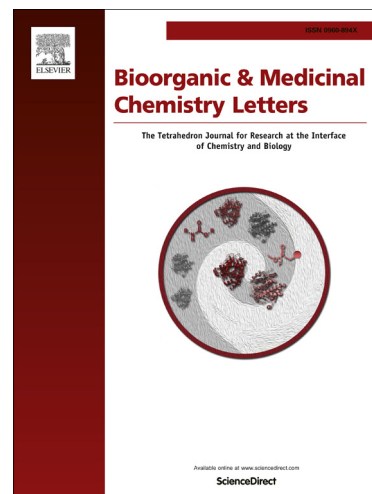
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## Graphical Abstract

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(A) MD conformation derived for compound **20** with HMG the binding site of HMGR (PDB entry code: **2Q1L**). (B) The “scorpion” conformation of compound **20** at the binding site of MHGR.

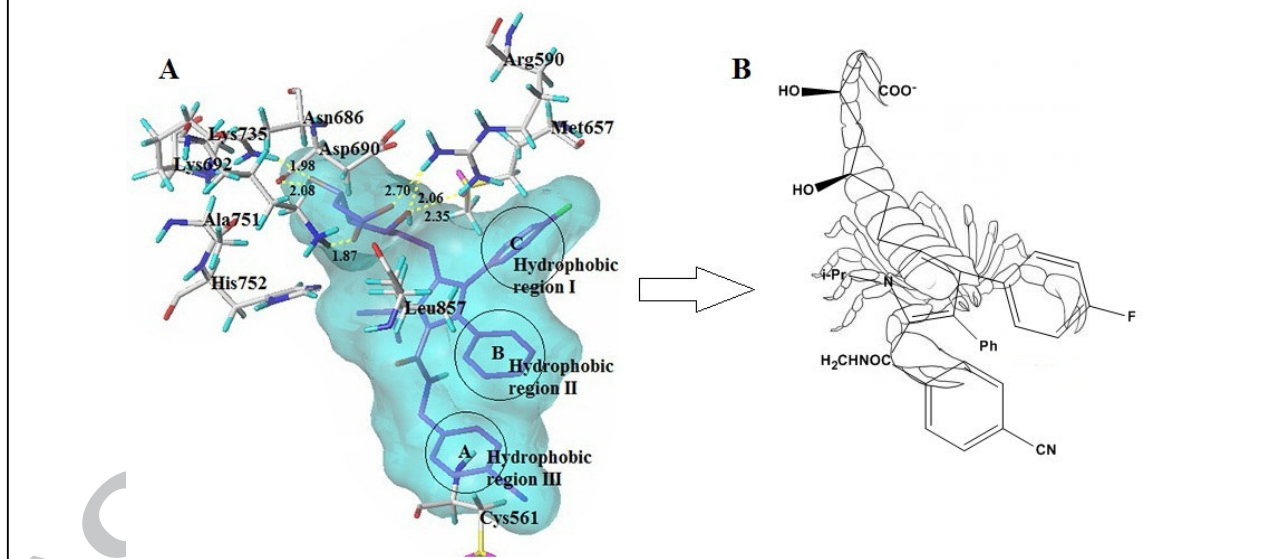
## Molecular modeling studies of atorvastatin analogues as HMGR inhibitors using 3D-QSAR, molecular docking and molecular dynamics simulations

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