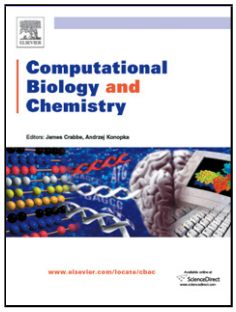

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PII: S1476-9271(17)30412-7
DOI: https://doi.org/10.1016/j.compbiolchem.2017.09.007
Reference: CBAC 6732

To appear in: *Computational Biology and Chemistry*

Received date: 18-6-2017
Revised date: 4-9-2017
Accepted date: 21-9-2017

Please cite this article as: Aryapour, Hassan, Dehdab, Maryam, Sohraby, Farzin, Bargahi, Afshar, Prediction of new chromene-based inhibitors of tubulin using structure-based virtual screening and molecular dynamics simulation methods.Computational Biology and Chemistry https://doi.org/10.1016/j.compbiolchem.2017.09.007

Prediction of new chromene-based inhibitors of tubulin using structure-based virtual screening and molecular dynamics simulation methods

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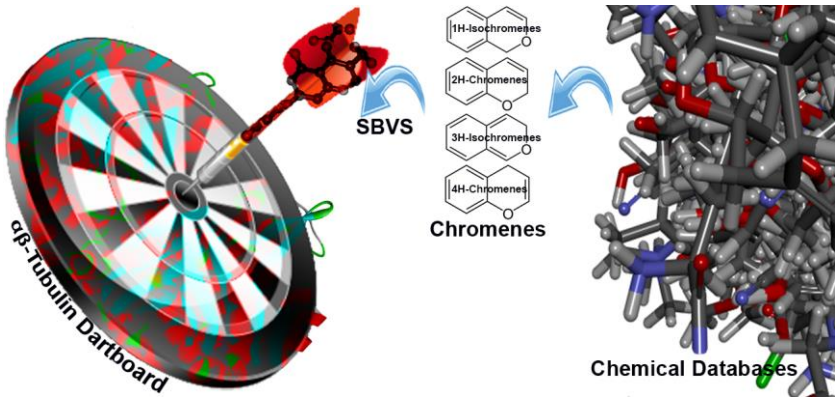
Graphical abstract



Highlights

- . A computational method based on physicochemical, ADMET properties and molecular docking and molecular dynamics were carried out to identify chromene-based inhibitors of tubulin.
- . After the virtual screening, the hit compounds were identified: PubChem CID: 16814409, 17594471, 57367244 and 69899719.
- . Using RMSD, RMSF, MMPBSA binding free energy values and total energy of the simulated protein-ligand complexes, we confirmed that our identified hit compounds show identical and even better activity than the reference ligand (Colchicine) and therefore can be potential inhibitors of tubulin polymerization.