

Binding Affinity via Docking: Fact and Fiction

Molecules

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Pyridinylimidazoles as GSK3 ^{Î²} Inhibitors: The Impact of Tautomerism on Compound Activity via Water Networks. ACS Medicinal Chemistry Letters, 2019, 10, 1407-1414.	2.8	12
2	Molecular modeling of four Dermaseptin-related peptides of the gliding tree frog <i>Agalychnis spurrelli</i> . Journal of Molecular Modeling, 2019, 25, 260.	1.8	3
3	Molecular Docking: Shifting Paradigms in Drug Discovery. International Journal of Molecular Sciences, 2019, 20, 4331.	4.1	890
4	Molecular Modeling in Drug Design. Molecules, 2019, 24, 321.	3.8	11
5	Increasing the Potential of the Auristatin Cancer-Drug Family by Shifting the Conformational Equilibrium. Molecular Pharmaceutics, 2019, 16, 3600-3608.	4.6	7
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7	The effects of bioactive compounds from blueberry and blackcurrant powders on the inhibitory activities of oat bran pastes against Î±-amylase and Î±-glucosidase linked to type 2 diabetes. Food Research International, 2020, 138, 109756.	6.2	40
8	In silico drug discovery of major metabolites from spices as SARS-CoV-2 main protease inhibitors. Computers in Biology and Medicine, 2020, 126, 104046.	7.0	98
9	Alkaloids from <i>Cryptolepis sanguinolenta</i> as Potential Inhibitors of SARS-CoV-2 Viral Proteins: An <i>In Silico</i> Study. BioMed Research International, 2020, 2020, 1-14.	1.9	54
10	<i>In-silico</i> drug repurposing and molecular dynamics puzzled out potential SARS-CoV-2 main protease inhibitors. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5756-5767.	3.5	48
11	<i>In silico</i> drug design and molecular docking studies targeting Akt1 (RAC-alpha) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 357 Td (ser investigation of CYP (cytochrome P450) inhibitors against MAOB (monoamine oxidase B) for OSCC (oral squamous cell carcinoma) treatment. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6467-6479.	3.5	19
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13	Rigorous Computational Study Reveals What Docking Overlooks: Double Trouble from Membrane Association in Protein Kinase C Modulators. Journal of Chemical Information and Modeling, 2020, 60, 5624-5633.	5.4	6
14	Making NSCLC Crystal Clear: How Kinase Structures Revolutionized Lung Cancer Treatment. Crystals, 2020, 10, 725.	2.2	4
15	An in silico approach to analyze HCV genotype-specific binding-site variation and its effect on drug-protein interaction. Scientific Reports, 2020, 10, 20885.	3.3	2
16	Synthesis, Molecular Docking Screening and Anti-Proliferative Potency Evaluation of Some New Imidazo[2,1-b]Thiazole Linked Thiadiazole Conjugates. Molecules, 2020, 25, 4997.	3.8	30
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18	Identification and immunogenic properties of recombinant ZnuD protein loops of <i>Acinetobacter baumannii</i> . Informatics in Medicine Unlocked, 2020, 19, 100342.	3.4	3

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