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In silico Molecular Modelling of Selected Natural Ligands and their Binding Features with Estrogen Receptor Alpha

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Current Computer-Aided Drug Design, 2019, 15, 89-96.

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#	Paper	IF	Citations
17	Predicting estrogen receptor binding of chemicals using a suite of in silico methods - Complementary approaches of (Q)SAR, molecular docking and molecular dynamics. <i>Toxicology and Applied Pharmacology</i> , 2019 , 378, 114630	4.6	15
16	Molecular Targets of Genistein and Its Related Flavonoids to Exert Anticancer Effects. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	36
15	Design, synthesis and biological evaluation of 2-(phenoxyethyl)-5-phenyl-1,3,4-oxadiazole derivatives as anti-breast cancer agents. <i>European Journal of Medicinal Chemistry</i> , 2019 , 168, 1-10	6.8	21
14	Design, Synthesis, and Biological Evaluation of 2-(2-Bromo-3-nitrophenyl)-5-phenyl-1,3,4-oxadiazole Derivatives as Possible Anti-Breast Cancer Agents. <i>Chemistry and Biodiversity</i> , 2020 , 17, e1900659	2.5	10
13	Multifaceted targeting strategies in cancer against the human notch 3 protein: a computational study. <i>In Silico Pharmacology</i> , 2021 , 9, 53	4.3	
12	Potential of baicalein in the prevention and treatment of cancer: A scientometric analyses based review. <i>Journal of Functional Foods</i> , 2021 , 86, 104660	5.1	6
11	Design, synthesis, characterization, molecular docking and computational studies of 3-phenyl-2-thioxoimidazolidin-4-one derivatives. <i>Journal of Molecular Structure</i> , 2021 , 1246, 131212	3.4	18
10	Design and synthesis of 1,4-disubstituted 1,2,3-triazoles: Biological evaluation, in silico molecular docking and ADME screening. <i>Journal of Molecular Structure</i> , 2022 , 1247, 131344	3.4	6
9	In Silico Molecular Docking, Synthesis of 4-(4-benzoylamino-phenoxy) Phenol Derivatives as Androgen Receptor Antagonists. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2019 , 22, 307-316	1.3	2
8	Degradation product of curcumin restrain virulent protein L-asparaginase. <i>Journal of Complementary and Integrative Medicine</i> , 2021 ,	1.5	
7	Synthesis of isatin and its derivatives having antibacterial, antifungal and cytotoxic activities.. <i>Current Organic Synthesis</i> , 2022 ,	1.9	0
6	Modulation of TLR/NF- κ B/NLRP Signaling by Bioactive Phytocompounds: A Promising Strategy to Augment Cancer Chemotherapy and Immunotherapy.. <i>Frontiers in Oncology</i> , 2022 , 12, 834072	5.3	2
5	A molecular dynamics perspective into estrogen receptor inhibition by selective flavonoids as alternative therapeutic options.. <i>Journal of Biomolecular Structure and Dynamics</i> , 2022 , 1-13	3.6	1
4	STRIDER: Steric hindrance and metal coordination identifier.. <i>Computational Biology and Chemistry</i> , 2022 , 98, 107686	3.6	0
3	In silico Investigation and BSA Denaturation Inhibitory Activity of Ethyl Acetate and N-butanol Extracts of <i>Centaurea tougourensis</i> Boiss. and Reut.. 2022 , 18, 1296-1308		
2	Novel compounds from endophytic fungi of <i>Ceriops decandra</i> inhibit breast cancer cell growth through estrogen receptor alpha in in-silico study. 2022 , 32, 101046		2
1	Anti-tumor potential and mode of action of karanjin against breast cancer; an in-silico approach. 2023 , 16, 104778		0

