Khaled H Barakat

List of Publications by Year
in descending order

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86 papers	2,372 citations	201385 27 h-index	233125 45 g-index
88 all docs	88 docs citations	88 times ranked	3285 citing authors

#	Article	IF	Citations
1	Molecular dynamics-driven drug discovery: leaping forward with confidence. Drug Discovery Today, 2017, 22, 249-269.	3.2	243
2	Discovery and Characterization of the Laulimalide-Microtubule Binding Mode by Mass Shift Perturbation Mapping. Chemistry and Biology, 2010, 17, 725-734.	6.2	111
3	IL-28B is a Key Regulator of B- and T-Cell Vaccine Responses against Influenza. PLoS Pathogens, 2014, 10, e1004556.	2.1	108
4	Cardiac Late Sodium Channel Current Is a Molecular Target for the Sodium/Glucose Cotransporter 2 Inhibitor Empagliflozin. Circulation, 2021, 143, 2188-2204.	1.6	105
5	Development of Safe Drugs: The hERG Challenge. Medicinal Research Reviews, 2018, 38, 525-555.	5.0	96
6	Comprehensive in vitro characterization of PD-L1 small molecule inhibitors. Scientific Reports, 2019, 9, 12392.	1.6	88
7	Small Molecule Inhibitors of ERCC1-XPF Protein-Protein Interaction Synergize Alkylating Agents in Cancer Cells. Molecular Pharmacology, 2013, 84, 12-24.	1.0	80
8	Coinhibitory Receptor Expression and Immune Checkpoint Blockade: Maintaining a Balance in CD8+ T Cell Responses to Chronic Viral Infections and Cancer. Frontiers in Immunology, 2017, 8, 1215.	2.2	80
9	Immunomodulatory Function of Interleukin 28B During Primary Infection With Cytomegalovirus. Journal of Infectious Diseases, 2014, 210, 717-727.	1.9	68
10	Virtual Screening and Biological Evaluation of Inhibitors Targeting the XPA-ERCC1 Interaction. PLoS ONE, 2012, 7, e51329.	1.1	60
11	Ensemble-based virtual screening reveals dual-inhibitors for the p53â€“MDM2/MDMX interactions. Journal of Molecular Graphics and Modelling, 2010, 28, 555-568.	1.3	54
12	Computational Predictions of Volatile Anesthetic Interactions with the Microtubule Cytoskeleton: Implications for Side Effects of General Anesthesia. PLoS ONE, 2012, 7, e37251.	1.1	52
13	DNA polymerase beta (pol Î²) inhibitors: A comprehensive overview. Drug Discovery Today, 2012, 17, 913-920.	3.2	50
14	A human ether-Ã¡-go-go-related (hERG) ion channel atomistic model generated by long supercomputer molecular dynamics simulations and its use in predicting drug cardiotoxicity. Toxicology Letters, 2014, 230, 382-392.	0.4	47
15	Human PD-1 binds differently to its human ligands: A comprehensive modeling study. Journal of Molecular Graphics and Modelling, 2015, 57, 131-142.	1.3	45
16	Applications of computer-aided approaches in the development of hepatitis C antiviral agents. Expert Opinion on Drug Discovery, 2017, 12, 407-425.	2.5	45
17	Targeting B7â€‘1 in immunotherapy. Medicinal Research Reviews, 2020, 40, 654-682.	5.0	44
18	DNA Repair Inhibitors: The Next Major Step to Improve Cancer Therapy. Current Topics in Medicinal Chemistry, 2012, 12, 1376-1390.	1.0	40

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19	A Refined Model of the HCV NS5A Protein Bound to Daclatasvir Explains Drug-Resistant Mutations and Activity against Divergent Genotypes. Journal of Chemical Information and Modeling, 2015, 55, 362-373.	2.5	39
20	Effects of Temperature on the p53-DNA Binding Interactions and Their Dynamical Behavior: Comparing the Wild Type to the R248Q Mutant. PLoS ONE, 2011, 6, e27651.	1.1	39
21	Human structural proteome-wide characterization of Cyclosporine A targets. Bioinformatics, 2014, 30, 3561-3566.	1.8	38
22	Relaxed complex scheme suggests novel inhibitors for the lyase activity of DNA polymerase beta. Journal of Molecular Graphics and Modelling, 2011, 29, 702-716.	1.3	37
23	Characterization of an inhibitory dynamic pharmacophore for the ERCC1â€“XPA interaction using a combined molecular dynamics and virtual screening approach. Journal of Molecular Graphics and Modelling, 2009, 28, 113-130.	1.3	36
24	New design of nucleotide excision repair (NER) inhibitors for combination cancer therapy. Journal of Molecular Graphics and Modelling, 2016, 65, 71-82.	1.3	36
25	Discovery of Small Molecule Inhibitors that Interact with Î³â€Tubulin. Chemical Biology and Drug Design, 2012, 79, 639-652.	1.5	33
26	Design, synthesis, biological evaluation and dynamics simulation of indazole derivatives with antiangiogenic and antiproliferative anticancer activity. Bioorganic Chemistry, 2019, 82, 340-359.	2.0	33
27	Entropy in bimolecular simulations: A comprehensive review of atomic fluctuations-based methods. Journal of Molecular Graphics and Modelling, 2015, 62, 105-117.	1.3	29
28	Modeling the human Na_v1.5 sodium channel: structural and mechanistic insights of ion permeation and drug blockade. Drug Design, Development and Therapy, 2017, Volume 11, 2301-2324.	2.0	28
29	Detailed Computational Study of the Active Site of the Hepatitis C Viral RNA Polymerase to Aid Novel Drug Design. Journal of Chemical Information and Modeling, 2013, 53, 3031-3043.	2.5	27
30	Revealing the atomistic details behind the binding of B7â€“1 to CD28 and CTLA-4: A comprehensive protein-protein modelling study. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 2764-2778.	1.1	26
31	Reversing T-cell exhaustion in immunotherapy: a review on current approaches and limitations. Expert Opinion on Therapeutic Targets, 2021, 25, 347-363.	1.5	25
32	Vaccine adjuvants â€“ understanding molecular mechanisms to improve vaccines. Swiss Medical Weekly, 2014, 144, w13940.	0.8	24
33	The Too Many Faces of PD-L1: A Comprehensive Conformational Analysis Study. Biochemistry, 2017, 56, 5428-5439.	1.2	23
34	Binding modes of hERG blockers: an unsolved mystery in the drug design arena. Expert Opinion on Drug Discovery, 2018, 13, 207-210.	2.5	23
35	Targeting the Achilles heel of the hepatitis B virus: a review of current treatments against covalently closed circular DNA. Drug Discovery Today, 2015, 20, 548-561.	3.2	22
36	An ELISA Based Binding and Competition Method to Rapidly Determine Ligand-receptor Interactions. Journal of Visualized Experiments, 2016, , .	0.2	22

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37	Modeling the Yew Tree Tubulin and a Comparison of its Interaction with Paclitaxel to Human Tubulin. Pharmaceutical Research, 2012, 29, 3007-3021.	1.7	20
38	Antibodies to Cryptic Epitopes in Distant Homologues Underpin a Mechanism of Heterologous Immunity betweenPlasmodium vivaxPvDBP andPlasmodium falciparumVAR2CSA. MBio, 2019, 10, .	1.8	20
39	Discovery of Novel Peptidomimetics as Irreversible <scp>CHIKV</scp> Ns<scp>P</scp>2 Protease Inhibitors Using Quantum Mechanicalâ€Based Ligand Descriptors. Chemical Biology and Drug Design, 2015, 86, 1518-1527.	1.5	18
40	Targeting DNA Repair in Tumor Cells via Inhibition of ERCC1â€“XPF. Journal of Medicinal Chemistry, 2019, 62, 7684-7696.	2.9	18
41	Effects of protein-protein interactions and ligand binding on the ion permeation in KCNQ1 potassium channel. PLoS ONE, 2018, 13, e0191905.	1.1	17
42	Phase transitions of methane using molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 124517.	1.2	16
43	Cyclosporine A binding to COX-2 reveals a novel signaling pathway that activates the IRE1Î± unfolded protein response sensor. Scientific Reports, 2018, 8, 16678.	1.6	16
44	Computational Characterization of Small Molecules Binding to the Human XPF Active Site and Virtual Screening to Identify Potential New DNA Repair Inhibitors Targeting the ERCC1-XPF Endonuclease. International Journal of Molecular Sciences, 2018, 19, 1328.	1.8	16
45	Computerâ€aided drug design of small molecule inhibitors of the ERCC1â€XPF proteinâ€“protein interaction. Chemical Biology and Drug Design, 2020, 95, 460-471.	1.5	15
46	A structure-based computational workflow to predict liability and binding modes of small molecules to hERG. Scientific Reports, 2020, 10, 16262.	1.6	15
47	A Computational Model for Overcoming Drug Resistance Using Selective Dual-Inhibitors for Aurora Kinase A and Its T217D Variant. Molecular Pharmaceutics, 2013, 10, 4572-4589.	2.3	14
48	GRP78: A possible relationship of COVID-19 and the mucormycosis; in silico perspective. Computers in Biology and Medicine, 2021, 139, 104956.	3.9	14
49	Interactions of laulimalide, peloruside, and their derivatives with the isoforms of Î²-tubulin. Canadian Journal of Chemistry, 2013, 91, 511-517.	0.6	13
50	Atomistic modeling and molecular dynamics analysis of human CaV1.2 channel using external electric field and ion pulling simulations. Biochimica Et Biophysica Acta - General Subjects, 2019, 1863, 1116-1126.	1.1	13
51	Î²-Caryophyllene Induces Apoptosis and Inhibits Angiogenesis in Colorectal Cancer Models. International Journal of Molecular Sciences, 2021, 22, 10550.	1.8	13
52	Novel Allosteric Pathway of Eg5 Regulation Identified through Multivariate Statistical Analysis of Hydrogen-Exchange Mass Spectrometry (HX-MS) Ligand Screening Data. Molecular and Cellular Proteomics, 2017, 16, 428-437.	2.5	12
53	L-Type Calcium Channels: Structure and Functions. , 0, , .		12
54	Molecular â€˜timeâ€machinesâ€™ to unravel key biological events for drug design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1306.	6.2	11

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55	Molecular Dynamics Simulation and Prediction of Druggable Binding Sites. Methods in Molecular Biology, 2018, 1762, 87-103.	0.4	11
56	Homology Modeling: an Overview of Fundamentals and Tools. International Review on Modelling and Simulations, 2017, 10, 129.	0.2	11
57	A Comprehensive Computational Analysis for the Binding Modes of Hepatitis C Virus NS5A Inhibitors: The Question of Symmetry. ACS Infectious Diseases, 2016, 2, 872-881.	1.8	10
58	A comprehensive structural model for the human KCNQ1/KCNE1 ion channel. Journal of Molecular Graphics and Modelling, 2017, 78, 26-47.	1.3	10
59	Towards discovery of novel scaffold with potent antiangiogenic activity; design, synthesis of pyridazine based compounds, impact of hinge interaction, and accessibility of their bioactive conformation on VEGFR-2 activities. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 1573-1589.	2.5	10
60	Tackling Immune Targets for Breast Cancer: Beyond PD-1/PD-L1 Axis. Frontiers in Oncology, 2021, 11, 628138.	1.3	9
61	GPCR_LigandClassify.py; a rigorous machine learning classifier for GPCR targeting compounds. Scientific Reports, 2021, 11, 9510.	1.6	7
62	Modelling DNA Repair Pathways: Recent Advances and Future Directions. Current Pharmaceutical Design, 2016, 22, 3527-3546.	0.9	7
63	Virtual Screening. , 2011, , 28-60.		7
64	A â€˜deep diveâ€™ into the SARS-Cov-2 polymerase assembly: identifying novel allosteric sites and analyzing the hydrogen bond networks and correlated dynamics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9443-9463.	2.0	6
65	Modulation of ERCC1-XPF Heterodimerization Inhibition via Structural Modification of Small Molecule Inhibitor Side-Chains. Frontiers in Oncology, 2022, 12, 819172.	1.3	6
66	Do We Need Small Molecule Inhibitors for the Immune Checkpoints?. Journal of Pharmaceutical Care & Health Systems, 2014, 01, .	0.1	5
67	Rational Drug Design. International Journal of Computational Models and Algorithms in Medicine, 2014, 4, 59-85.	0.4	5
68	A mathematical modelling tool for unravelling the antibody-mediated effects on CTLA-4 interactions. BMC Medical Informatics and Decision Making, 2018, 18, 37.	1.5	5
69	When theory meets experiment: the PD-1 challenge. Journal of Molecular Modeling, 2017, 23, 308.	0.8	4
70	Protein-Protein Docking. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 173-195.	0.3	4
71	A Novel Interaction Between the TLR7 and a Colchicine Derivative Revealed Through a Computational and Experimental Study. Pharmaceuticals, 2018, 11, 22.	1.7	3
72	Structure-based screening and validation of potential dengue virus inhibitors through classical and QM/MM affinity estimation. Journal of Molecular Graphics and Modelling, 2019, 90, 128-143.	1.3	3

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73	Effects of selective calcium channel blockers on ionsâ€™ permeation through the human Cav1.2 ion channel: A computational study. Journal of Molecular Graphics and Modelling, 2021, 102, 107776.	1.3	3
74	Solubility: A Speed-Breaker on the Drug Discovery Highway. MOJ Bioequivalence & Bioavailability, 2017, 3, .	0.1	3
75	Leveraging structural and 2D-QSAR to investigate the role of functional group substitutions, conserved surface residues and desolvation in triggering the small molecule-induced dimerization of hPD-L1. BMC Chemistry, 2022, 16, .	1.6	3
76	Phase transitions of carbon tetra-fluoride using raman spectroscopy and molecular dynamics simulations. High Pressure Research, 2006, 26, 383-386.	0.4	2
77	Electrostatic Contributions to Colchicine Binding within Tubulin Isotypes. Electromagnetic Biology and Medicine, 2009, 28, 355-364.	0.7	2
78	A multi-compartment pharmacokinetic model of the interaction between paclitaxel and doxorubicin. EPJ Nonlinear Biomedical Physics, 2014, 2, .	0.8	2
79	Modelling Off-target Interactions (I): Cardiotoxicity. Journal of Pharmaceutical Care & Health Systems, 2015, 02, .	0.1	1
80	Immune Checkpoints: The Search for a Single Antiviral-Anticancer Magic Bullet. Journal of Pharmaceutical Care & Health Systems, 2015, 02, .	0.1	1
81	Targeting the Aryl Hydrocarbon Receptor (AhR): A Review of the In-Silico Screening Approaches to Identify AhR Modulators. , 0, , .		1
82	Immune Checkpoints Inhibitors: A Single Antiviral and Anticancer Magic Bullet. Journal of Pharmaceutical Care & Health Systems, 2015, 02, .	0.1	0
83	Inside Cover Image, Volume 7, Issue 4. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1325.	6.2	0
84	Rational Drug Design Rational Drug Design. , 2017, , 1144-1174.		0
85	Protein-Protein Docking. , 2017, , 1092-1114.		0
86	DNA Repair Inhibitors: Our Last Disposal to Improve Cancer Therapy. Current Topics in Medicinal Chemistry, 2012, , .	1.0	0