Khaled H Barakat

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4103859/publications.pdf

Version: 2024-02-01

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	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
2	Modulation of ERCC1-XPF Heterodimerization Inhibition via Structural Modification of Small Molecule Inhibitor Side-Chains. Frontiers in Oncology, 2022, 12, 819172.	1.3	6
3	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
4	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
5	Tackling Immune Targets for Breast Cancer: Beyond PD-1/PD-L1 Axis. Frontiers in Oncology, 2021, 11, 628138.	1.3	9
6	GPCR_LigandClassify.py; a rigorous machine learning classifier for GPCR targeting compounds. Scientific Reports, 2021, 11, 9510.	1.6	7
7	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
8	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
9	Î²-Caryophyllene Induces Apoptosis and Inhibits Angiogenesis in Colorectal Cancer Models. International Journal of Molecular Sciences, 2021, 22, 10550.	1.8	13
10	GRP78: A possible relationship of COVID-19 and the mucormycosis; in silico perspective. Computers in Biology and Medicine, 2021, 139, 104956.	3.9	14
11	Targeting B7â€1 in immunotherapy. Medicinal Research Reviews, 2020, 40, 654-682.	5.0	44
12	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
13	A structure-based computational workflow to predict liability and binding modes of small molecules to hERG. Scientific Reports, 2020, 10, 16262.	1.6	15
14	Targeting DNA Repair in Tumor Cells via Inhibition of ERCC1â€“XPF. Journal of Medicinal Chemistry, 2019, 62, 7684-7696.	2.9	18
15	Comprehensive in vitro characterization of PD-L1 small molecule inhibitors. Scientific Reports, 2019, 9, 12392.	1.6	88
16	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
17	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
18	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

#	Article	IF	Citations
19	Antibodies to Cryptic Epitopes in Distant Homologues Underpin a Mechanism of Heterologous Immunity betweenPlasmodium vivaxPvDBP andPlasmodium falciparumVAR2CSA. MBio, 2019, 10, .	1.8	20
20	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
21	Molecular Dynamics Simulation and Prediction of Druggable Binding Sites. Methods in Molecular Biology, 2018, 1762, 87-103.	0.4	11
22	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
23	Development of Safe Drugs: The hERG Challenge. Medicinal Research Reviews, 2018, 38, 525-555.	5.0	96
24	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
25	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
26	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
27	A Novel Interaction Between the TLR7 and a Colchicine Derivative Revealed Through a Computational and Experimental Study. Pharmaceuticals, 2018, 11, 22.	1.7	3
28	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
29	Effects of protein-protein interactions and ligand binding on the ion permeation in KCNQ1 potassium channel. PLoS ONE, 2018, 13, e0191905.	1.1	17
30	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
31	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
32	Molecular â€˜timeâ€machinesâ€™ to unravel key biological events for drug design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1306.	6.2	11
33	A comprehensive structural model for the human KCNQ1/KCNE1 ion channel. Journal of Molecular Graphics and Modelling, 2017, 78, 26-47.	1.3	10
34	When theory meets experiment: the PD-1 challenge. Journal of Molecular Modeling, 2017, 23, 308.	0.8	4
35	The Too Many Faces of PD-L1: A Comprehensive Conformational Analysis Study. Biochemistry, 2017, 56, 5428-5439.	1.2	23
36	Inside Cover Image, Volume 7, Issue 4. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1325.	6.2	0

#	Article	IF	Citations
37	Molecular dynamics-driven drug discovery: leaping forward with confidence. Drug Discovery Today, 2017, 22, 249-269.	3.2	243
38	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
39	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
40	Solubility: A Speed-Breaker on the Drug Discovery Highway. MOJ Bioequivalence & Bioavailability, 2017, 3, .	0.1	3
41	Homology Modeling: an Overview of Fundamentals and Tools. International Review on Modelling and Simulations, 2017, 10, 129.	0.2	11
42	Rational Drug Design Rational Drug Design. , 2017, , 1144-1174.		0
43	Protein-Protein Docking. , 2017, , 1092-1114.		0
44	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
45	An ELISA Based Binding and Competition Method to Rapidly Determine Ligand-receptor Interactions. Journal of Visualized Experiments, 2016, , .	0.2	22
46	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
47	Modelling DNA Repair Pathways: Recent Advances and Future Directions. Current Pharmaceutical Design, 2016, 22, 3527-3546.	0.9	7
48	Protein-Protein Docking. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 173-195.	0.3	4
49	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
50	Modelling Off-target Interactions (I): Cardiotoxicity. Journal of Pharmaceutical Care & Health Systems, 2015, 02, .	0.1	1
51	Immune Checkpoints Inhibitors: A Single Antiviral and Anticancer Magic Bullet. Journal of Pharmaceutical Care & Health Systems, 2015, 02, .	0.1	0
52	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
53	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
54	Immune Checkpoints: The Search for a Single Antiviral-Anticancer Magic Bullet. Journal of Pharmaceutical Care & Health Systems, 2015, 02, .	0.1	1

#	Article	IF	Citations
55	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
56	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
57	IL-28B is a Key Regulator of B- and T-Cell Vaccine Responses against Influenza. PLoS Pathogens, 2014, 10, e1004556.	2.1	108
58	Immunomodulatory Function of Interleukin 28B During Primary Infection With Cytomegalovirus. Journal of Infectious Diseases, 2014, 210, 717-727.	1.9	68
59	Do We Need Small Molecule Inhibitors for the Immune Checkpoints?. Journal of Pharmaceutical Care & Health Systems, 2014, 01, .	0.1	5
60	A multi-compartment pharmacokinetic model of the interaction between paclitaxel and doxorubicin. EPJ Nonlinear Biomedical Physics, 2014, 2, .	0.8	2
61	Vaccine adjuvants â€“ understanding molecular mechanisms to improve vaccines. Swiss Medical Weekly, 2014, 144, w13940.	0.8	24
62	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
63	Human structural proteome-wide characterization of Cyclosporine A targets. Bioinformatics, 2014, 30, 3561-3566.	1.8	38
64	Rational Drug Design. International Journal of Computational Models and Algorithms in Medicine, 2014, 4, 59-85.	0.4	5
65	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
66	Small Molecule Inhibitors of ERCC1-XPF Protein-Protein Interaction Synergize Alkylating Agents in Cancer Cells. Molecular Pharmacology, 2013, 84, 12-24.	1.0	80
67	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
68	Interactions of laulimalide, peloruside, and their derivatives with the isoforms of Î²-tubulin. Canadian Journal of Chemistry, 2013, 91, 511-517.	0.6	13
69	DNA Repair Inhibitors: The Next Major Step to Improve Cancer Therapy. Current Topics in Medicinal Chemistry, 2012, 12, 1376-1390.	1.0	40
70	Virtual Screening and Biological Evaluation of Inhibitors Targeting the XPA-ERCC1 Interaction. PLoS ONE, 2012, 7, e51329.	1.1	60
71	DNA polymerase beta (pol Î²) inhibitors: A comprehensive overview. Drug Discovery Today, 2012, 17, 913-920.	3.2	50
72	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

#	Article	IF	Citations
73	Discovery of Small Molecule Inhibitors that Interact with Î³â€Tubulin. Chemical Biology and Drug Design, 2012, 79, 639-652.	1.5	33
74	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
75	DNA Repair Inhibitors: Our Last Disposal to Improve Cancer Therapy. Current Topics in Medicinal Chemistry, 2012, , .	1.0	0
76	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
77	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
78	Virtual Screening. , 2011, , 28-60.		7
79	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
80	Discovery and Characterization of the Laulimalide-Microtubule Binding Mode by Mass Shift Perturbation Mapping. Chemistry and Biology, 2010, 17, 725-734.	6.2	111
81	Electrostatic Contributions to Colchicine Binding within Tubulin Isotypes. Electromagnetic Biology and Medicine, 2009, 28, 355-364.	0.7	2
82	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
83	Phase transitions of carbon tetra-fluoride using raman spectroscopy and molecular dynamics simulations. High Pressure Research, 2006, 26, 383-386.	0.4	2
84	Phase transitions of methane using molecular dynamics simulations. Journal of Chemical Physics, 2006, 124, 124517.	1.2	16
85	L-Type Calcium Channels: Structure and Functions. , 0, , .		12
86	Targeting the Aryl Hydrocarbon Receptor (AhR): A Review of the In-Silico Screening Approaches to Identify AhR Modulators. , 0, , .		1