

Martiniano Bello

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

75
papers

858
citations

16
h-index

25
g-index

82
ext. papers

1,034
ext. citations

3.7
avg, IF

5.13
L-index

#	Paper	IF	Citations
75	CDK4 as a phytochemical based anticancer drug target. <i>Informatics in Medicine Unlocked</i> , 2022 , 28, 1008236,	3.6	2
74	Dihydropyrazole-Carbohydrazide Derivatives with Dual Activity as Antioxidant and Anti-Proliferative Drugs on Breast Cancer Targeting the HDAC6. <i>Pharmaceuticals</i> , 2022 , 15, 690	5.2	1
73	In silico design of HDAC6 inhibitors with neuroprotective effects. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-19	3.6	0
72	Molecular recognition of tak-285 and lapatinib by inactive, active, and middle active-inactive HER2. <i>Journal of Molecular Modeling</i> , 2021 , 27, 105	2	0
71	Structural analogues of existing anti-viral drugs inhibit SARS-CoV-2 RNA dependent RNA polymerase: A computational hierarchical investigation. <i>Heliyon</i> , 2021 , 7, e06435	3.6	5
70	Elucidation of the inhibitory activity of ivermectin with host nuclear importin β and several SARS-CoV-2 targets. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-9	3.6	5
69	Energetic and structural basis for the differences in infectivity between the wild-type and mutant spike proteins of SARS-CoV-2 in the Mexican population. <i>Journal of Molecular Graphics and Modelling</i> , 2021 , 107, 107970	2.8	0
68	Elucidation of the inhibitory activity of plant-derived SARS-CoV inhibitors and their potential as SARS-CoV-2 inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-13	3.6	0
67	Fucosterol from as an amyloid-beta (A β) aggregation inhibitor: and studies. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 1271-1283	3.6	4
66	Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. <i>Pharmaceuticals</i> , 2021 , 14,	5.2	3
65	Structural insights into SARS-CoV-2 spike protein and its natural mutants found in Mexican population. <i>Scientific Reports</i> , 2021 , 11, 4659	4.9	13
64	Repurposing FDA Drug Compounds against Breast Cancer by Targeting EGFR/HER2. <i>Pharmaceuticals</i> , 2021 , 14,	5.2	4
63	Exploring the inhibitory activity of valproic acid against the HDAC family using an MMGBSA approach. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 857-878	4.2	12
62	and studies of gp120-HIV-derived peptides in complex with G4-PAMAM dendrimers.. <i>RSC Advances</i> , 2020 , 10, 20414-20426	3.7	3
61	Hydroxamic acid derivatives as HDAC1, HDAC6 and HDAC8 inhibitors with antiproliferative activity in cancer cell lines. <i>Scientific Reports</i> , 2020 , 10, 10462	4.9	13
60	Exploring the biotransformation of N-(2-hydroxyphenyl)-2-propylpentanamide (an aryl valproic acid derivative) by CYP2C11, using in silico predictions and in vitro studies. <i>Journal of Pharmacy and Pharmacology</i> , 2020 , 72, 938-955	4.8	2
59	Targeting Breast Cancer Cells with G4 PAMAM Dendrimers and Valproic Acid Derivative Complexes. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2020 , 20, 1857-1872	2.2	3

58	Molecular insights into how SHBG dimerization exerts changes on ligand molecular recognition. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2020 , 197, 105502	5.1	0
57	Complexation of peptide epitopes with G4-PAMAM dendrimer through ligand diffusion molecular dynamic simulations. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 96, 107514	2.8	1
56	Dissecting the molecular recognition of dual lapatinib derivatives for EGFR/HER2. <i>Journal of Computer-Aided Molecular Design</i> , 2020 , 34, 293-303	4.2	4
55	Prediction of potential inhibitors of the dimeric SARS-CoV2 main proteinase through the MM/GBSA approach. <i>Journal of Molecular Graphics and Modelling</i> , 2020 , 101, 107762	2.8	14
54	Identification of saquinavir as a potent inhibitor of dimeric SARS-CoV2 main protease through MM/GBSA. <i>Journal of Molecular Modeling</i> , 2020 , 26, 340	2	33
53	Structural mechanism of the Tanford transition of bovine β lactoglobulin through microsecond molecular dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-13	3.6	1
52	Binding of Folate-G4-PAMAM dendrimer conjugate with indomethacin via ligand diffusion MD simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-11	3.6	
51	Complexation of methotrexate via ligand diffusion molecular dynamic simulations under neutral, basic, and acidic conditions. <i>Journal of Molecular Graphics and Modelling</i> , 2019 , 93, 107443	2.8	4
50	Impact of tetramerization on the ligand recognition of N1 influenza neuraminidase via MMGBSA approach. <i>Biopolymers</i> , 2019 , 110, e23251	2.2	1
49	Structural and energetic basis for novel epicatechin derivatives acting as GPER agonists through the MMGBSA method. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2019 , 189, 176-186	5.1	7
48	In silico search, chemical characterization and immunogenic evaluation of amino-terminated G4-PAMAM-HIV peptide complexes using three-dimensional models of the HIV-1 gp120 protein. <i>Colloids and Surfaces B: Biointerfaces</i> , 2019 , 177, 77-93	6	13
47	Molecular mechanism of the association and dissociation of Deltarasin from the heterodimeric KRas4B-PDE1 α complex. <i>Biopolymers</i> , 2019 , 110, e23333	2.2	1
46	Synthesis and In Vitro Evaluation of Tetrahydroquinoline Derivatives as Antiproliferative Compounds of Breast Cancer via Targeting the GPER. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2019 , 19, 760-771	2.2	7
45	Structural and energetic basis for the inhibitory selectivity of both catalytic domains of dimeric HDAC6. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 4701-4720	3.6	16
44	Structural insight into the binding mechanism of ATP to EGFR and L858R, and T790M and L858R/T790 mutants. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 4671-4684	3.6	13
43	Cell-based assays and molecular dynamics analysis of a boron-containing agonist with different profiles of binding to human and guinea pig beta2 adrenoceptors. <i>European Biophysics Journal</i> , 2019 , 48, 83-97	1.9	5
42	Insights into structural features of HDAC1 and its selectivity inhibition elucidated by Molecular dynamic simulation and Molecular Docking. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 584-610	3.6	30
41	Structural and energetic basis for the molecular recognition of dual synthetic vs. natural inhibitors of EGFR/HER2. <i>International Journal of Biological Macromolecules</i> , 2018 , 111, 569-586	7.9	18

40	QSAR, DFT and molecular modeling studies of peptides from HIV-1 to describe their recognition properties by MHC-I. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 2312-2330	3.6	7
39	Design of Drugs by Filtering Through ADMET, Physicochemical and Ligand-Target Flexibility Properties. <i>Methods in Molecular Biology</i> , 2018 , 1824, 403-416	1.4	2
38	Binding mechanism of kinase inhibitors to EGFR and T790M, L858R and L858R/T790M mutants through structural and energetic analysis. <i>International Journal of Biological Macromolecules</i> , 2018 , 118, 1948-1962	7.9	14
37	Advances in Theoretical Studies on the Design of Single Boron Atom Compounds. <i>Current Pharmaceutical Design</i> , 2018 , 24, 3466-3475	3.3	6
36	Selection of a GPER1 Ligand via Ligand-based Virtual Screening Coupled to Molecular Dynamics Simulations and Its Anti-proliferative Effects on Breast Cancer Cells. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2018 , 18, 1629-1638	2.2	6
35	KRas4B-PDE6 β complex stabilization by small molecules obtained by virtual screening affects Ras signaling in pancreatic cancer. <i>BMC Cancer</i> , 2018 , 18, 1299	4.8	10
34	The small organic molecule C19 binds and strengthens the KRAS4b-PDE6 β complex and inhibits growth of colorectal cancer cells in vitro and in vivo. <i>BMC Cancer</i> , 2018 , 18, 1056	4.8	8
33	Several effects of boron are induced by uncoupling steroid hormones from their transporters in blood. <i>Medical Hypotheses</i> , 2018 , 118, 78-83	3.8	10
32	Heterodimerization of the Entamoeba histolytica EhCPADH virulence complex through molecular dynamics and protein-protein docking. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 486-503	3.6	9
31	Molecular recognition between pancreatic lipase and natural and synthetic inhibitors. <i>International Journal of Biological Macromolecules</i> , 2017 , 98, 855-868	7.9	14
30	Study of new interactions of glitazone's stereoisomers and the endogenous ligand 15d-PGJ2 on six different PPAR gamma proteins. <i>Biochemical Pharmacology</i> , 2017 , 142, 168-193	6	13
29	Binding free energy calculations using MMPB/GBSA approaches for PAMAM-G4-drug complexes at neutral, basic and acid pH conditions. <i>Journal of Molecular Graphics and Modelling</i> , 2017 , 76, 330-341	2.8	14
28	Molecular recognition between potential natural inhibitors of the Keap1-Nrf2 complex. <i>International Journal of Biological Macromolecules</i> , 2017 , 105, 981-992	7.9	16
27	Searching the conformational complexity and binding properties of HDAC6 through docking and molecular dynamic simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 2794-2814	3.6	23
26	Conformational changes associated with L16P and T118M mutations in the membrane-embedded PMP22 protein, consequential in CMT-1A. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 2880-2894	3.6	3
25	Theoretical Studies for Dendrimer-Based Drug Delivery. <i>Current Pharmaceutical Design</i> , 2017 , 23, 3048-3061	3.5	8
24	Design, Synthesis and Biological Evaluation of a Phenyl Butyric Acid Derivative, N-(4-chlorophenyl)-4-phenylbutanamide: A HDAC6 Inhibitor with Anti-proliferative Activity on Cervix Cancer and Leukemia Cells. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2017 , 17, 1441-1454	2.2	4
23	Exploring the conformational and binding properties of unphosphorylated/phosphorylated monomeric and trimeric Bcl-2 through docking and molecular dynamics simulations. <i>Biopolymers</i> , 2016 , 105, 393-413	2.2	10

22	Energetic and flexibility properties captured by long molecular dynamics simulations of a membrane-embedded pMHCII-TCR complex. <i>Molecular BioSystems</i> , 2016 , 12, 1350-66		7
21	Understanding the molecular basis of agonist/antagonist mechanism of GPER1/GPR30 through structural and energetic analyses. <i>Journal of Steroid Biochemistry and Molecular Biology</i> , 2016 , 158, 104-116	5.1	18
20	Structural and energetic requirements for a second binding site at the dimeric β -lactoglobulin interface. <i>Journal of Biomolecular Structure and Dynamics</i> , 2016 , 34, 1884-902	3.6	7
19	Mapping the intrinsically disordered properties of the flexible loop domain of Bcl-2: a molecular dynamics simulation study. <i>Journal of Molecular Modeling</i> , 2016 , 22, 98	2	4
18	Energetic and conformational features linked to the monomeric and dimeric states of bovine BLG. <i>International Journal of Biological Macromolecules</i> , 2016 , 92, 625-636	7.9	15
17	Predicting peptide vaccine candidates against H1N1 influenza virus through theoretical approaches. <i>Immunologic Research</i> , 2015 , 62, 3-15	4.3	16
16	Targeting quorum sensing by designing azoline derivatives to inhibit the N-hexanoyl homoserine lactone-receptor CviR: Synthesis as well as biological and theoretical evaluations. <i>Bioorganic and Medicinal Chemistry</i> , 2015 , 23, 7565-77	3.4	13
15	Binding free energy calculations between bovine β -lactoglobulin and four fatty acids using the MMGBSA method. <i>Biopolymers</i> , 2014 , 101, 1010-8	2.2	15
14	Ligand entry into the calyx of β -lactoglobulin. <i>Biopolymers</i> , 2014 , 101, 744-57	2.2	26
13	Seeking potential anticonvulsant agents that target GABAA receptors using experimental and theoretical procedures. <i>Journal of Computer-Aided Molecular Design</i> , 2014 , 28, 1217-32	4.2	5
12	Structural and energetic analysis to provide insight residues of CYP2C9, 2C11 and 2E1 involved in valproic acid dehydrogenation selectivity. <i>Biochemical Pharmacology</i> , 2014 , 90, 145-58	6	12
11	Simulation of the cavity-binding site of three bacterial multicopper oxidases upon complex stabilization: interactional profile and electron transference pathways. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014 , 32, 1303-17	3.6	8
10	Theoretical analysis of the neuraminidase epitope of the Mexican A H1N1 influenza strain, and experimental studies on its interaction with rabbit and human hosts. <i>Immunologic Research</i> , 2013 , 56, 44-60	4.3	14
9	Ligand binding and self-association cooperativity of β -lactoglobulin. <i>Journal of Molecular Recognition</i> , 2013 , 26, 67-75	2.6	45
8	Automated docking for novel drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2013 , 8, 821-34	6.2	48
7	Molecular dynamics simulations to provide insights into epitopes coupled to the soluble and membrane-bound MHC-II complexes. <i>PLoS ONE</i> , 2013 , 8, e72575	3.7	22
6	Structure and dynamics of β -lactoglobulin in complex with dodecyl sulfate and laurate: a molecular dynamics study. <i>Biophysical Chemistry</i> , 2012 , 165-166, 79-86	3.5	33
5	Molecular dynamics of a thermostable multicopper oxidase from <i>Thermus thermophilus</i> HB27: structural differences between the apo and holo forms. <i>PLoS ONE</i> , 2012 , 7, e40700	3.7	27

4	Folding and homodimerization of wheat germ agglutinin. <i>Biophysical Journal</i> , 2011 , 101, 1423-31	2.9	19
3	Energetics of ligand recognition and self-association of bovine β -lactoglobulin: differences between variants A and B. <i>Biochemistry</i> , 2011 , 50, 151-61	3.2	40
2	Energetics of protein homodimerization: effects of water sequestering on the formation of beta-lactoglobulin dimer. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 70, 1475-87	4.2	46
1	Structural Insight of the Anticancer Properties of Doxazosin on Overexpressing EGFR/HER2 Cell Lines		1