# Martiniano Bello

## List of Publications by Citations

**Source:** https://exaly.com/author-pdf/7030451/martiniano-bello-publications-by-citations.pdf
**Version:** 2024-04-23

This document has been generated based on the publications and citations recorded by exaly.com. For the latest version of this publication list, visit the link given above.
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 | Automated docking for novel drug discovery. *Expert Opinion on Drug Discovery*, **2013**, 8, 821-34 | 6.2 | 48 |
| 74 | Energetics of protein homodimerization: effects of water sequestering on the formation of beta-lactoglobulin dimer. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 1475-87 | 4.2 | 46 |
| 73 | Ligand binding and self-association cooperativity of β-lactoglobulin. *Journal of Molecular Recognition*, **2013**, 26, 67-75 | 2.6 | 45 |
| 72 | Energetics of ligand recognition and self-association of bovine β-lactoglobulin: differences between variants A and B. *Biochemistry*, **2011**, 50, 151-61 | 3.2 | 40 |
| 71 | Structure and dynamics of β-lactoglobulin in complex with dodecyl sulfate and laurate: a molecular dynamics study. *Biophysical Chemistry*, **2012**, 165-166, 79-86 | 3.5 | 33 |
| 70 | Identification of saquinavir as a potent inhibitor of dimeric SARS-CoV2 main protease through MM/GBSA. *Journal of Molecular Modeling*, **2020**, 26, 340 | 2 | 33 |
| 69 | Insights into structural features of HDAC1 and its selectivity inhibition elucidated by Molecular dynamic simulation and Molecular Docking. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 584-610 | 3.6 | 30 |
| 68 | Molecular dynamics of a thermostable multicopper oxidase from Thermus thermophilus HB27: structural differences between the apo and holo forms. *PLoS ONE*, **2012**, 7, e40700 | 3.7 | 27 |
| 67 | Ligand entry into the calyx of β-lactoglobulin. *Biopolymers*, **2014**, 101, 744-57 | 2.2 | 26 |
| 66 | Searching the conformational complexity and binding properties of HDAC6 through docking and molecular dynamic simulations. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2794-2814 | 3.6 | 23 |
| 65 | Molecular dynamics simulations to provide insights into epitopes coupled to the soluble and membrane-bound MHC-II complexes. *PLoS ONE*, **2013**, 8, e72575 | 3.7 | 22 |
| 64 | Folding and homodimerization of wheat germ agglutinin. *Biophysical Journal*, **2011**, 101, 1423-31 | 2.9 | 19 |
| 63 | Structural and energetic basis for the molecular recognition of dual synthetic vs. natural inhibitors of EGFR/HER2. *International Journal of Biological Macromolecules*, **2018**, 111, 569-586 | 7.9 | 18 |
| 62 | Understanding the molecular basis of agonist/antagonist mechanism of GPER1/GPR30 through structural and energetic analyses. *Journal of Steroid Biochemistry and Molecular Biology*, **2016**, 158, 104-116 | 5.1 | 18 |
| 61 | Predicting peptide vaccine candidates against H1N1 influenza virus through theoretical approaches. *Immunologic Research*, **2015**, 62, 3-15 | 4.3 | 16 |
| 60 | Molecular recognition between potential natural inhibitors of the Keap1-Nrf2 complex. *International Journal of Biological Macromolecules*, **2017**, 105, 981-992 | 7.9 | 16 |
| 59 | Structural and energetic basis for the inhibitory selectivity of both catalytic domains of dimeric HDAC6. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4701-4720 | 3.6 | 16 |

| | | | |
|---|---|---|---|
| 58 | Binding free energy calculations between bovine β-lactoglobulin and four fatty acids using the MMGBSA method. *Biopolymers*, **2014**, 101, 1010-8 | 2.2 | 15 |
| 57 | Energetic and conformational features linked to the monomeric and dimeric states of bovine BLG. *International Journal of Biological Macromolecules*, **2016**, 92, 625-636 | 7.9 | 15 |
| 56 | Molecular recognition between pancreatic lipase and natural and synthetic inhibitors. *International Journal of Biological Macromolecules*, **2017**, 98, 855-868 | 7.9 | 14 |
| 55 | Binding mechanism of kinase inhibitors to EGFR and T790M, L858R and L858R/T790M mutants through structural and energetic analysis. *International Journal of Biological Macromolecules*, **2018**, 118, 1948-1962 | 7.9 | 14 |
| 54 | Theoretical analysis of the neuraminidase epitope of the Mexican A H1N1 influenza strain, and experimental studies on its interaction with rabbit and human hosts. *Immunologic Research*, **2013**, 56, 44-60 | 4.3 | 14 |
| 53 | Binding free energy calculations using MMPB/GBSA approaches for PAMAM-G4-drug complexes at neutral, basic and acid pH conditions. *Journal of Molecular Graphics and Modelling*, **2017**, 76, 330-341 | 2.8 | 14 |
| 52 | Prediction of potential inhibitors of the dimeric SARS-CoV2 main proteinase through the MM/GBSA approach. *Journal of Molecular Graphics and Modelling*, **2020**, 101, 107762 | 2.8 | 14 |
| 51 | 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. *Colloids and Surfaces B: Biointerfaces*, **2019**, 177, 77-93 | 6 | 13 |
| 50 | Hydroxamic acid derivatives as HDAC1, HDAC6 and HDAC8 inhibitors with antiproliferative activity in cancer cell lines. *Scientific Reports*, **2020**, 10, 10462 | 4.9 | 13 |
| 49 | Study of new interactions of glitazone's stereoisomers and the endogenous ligand 15d-PGJ2 on six different PPAR gamma proteins. *Biochemical Pharmacology*, **2017**, 142, 168-193 | 6 | 13 |
| 48 | Targeting quorum sensing by designing azoline derivatives to inhibit the N-hexanoyl homoserine lactone-receptor CviR: Synthesis as well as biological and theoretical evaluations. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 7565-77 | 3.4 | 13 |
| 47 | Structural insight into the binding mechanism of ATP to EGFR and L858R, and T790M and L858R/T790 mutants. *Journal of Biomolecular Structure and Dynamics*, **2019**, 37, 4671-4684 | 3.6 | 13 |
| 46 | Structural insights into SARS-CoV-2 spike protein and its natural mutants found in Mexican population. *Scientific Reports*, **2021**, 11, 4659 | 4.9 | 13 |
| 45 | Exploring the inhibitory activity of valproic acid against the HDAC family using an MMGBSA approach. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 857-878 | 4.2 | 12 |
| 44 | Structural and energetic analysis to provide insight residues of CYP2C9, 2C11 and 2E1 involved in valproic acid dehydrogenation selectivity. *Biochemical Pharmacology*, **2014**, 90, 145-58 | 6 | 12 |
| 43 | Exploring the conformational and binding properties of unphosphorylated/phosphorylated monomeric and trimeric Bcl-2 through docking and molecular dynamics simulations. *Biopolymers*, **2016**, 105, 393-413 | 2.2 | 10 |
| 42 | KRas4B-PDE6δ complex stabilization by small molecules obtained by virtual screening affects Ras signaling in pancreatic cancer. *BMC Cancer*, **2018**, 18, 1299 | 4.8 | 10 |
| 41 | Several effects of boron are induced by uncoupling steroid hormones from their transporters in blood. *Medical Hypotheses*, **2018**, 118, 78-83 | 3.8 | 10 |

| | | | |
|---|---|---|---|
| 40 | Heterodimerization of the Entamoeba histolytica EhCPADH virulence complex through molecular dynamics and protein-protein docking. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 486-503 | 3.6 | 9 |
| 39 | Simulation of the cavity-binding site of three bacterial multicopper oxidases upon complex stabilization: interactional profile and electron transference pathways. *Journal of Biomolecular Structure and Dynamics*, **2014**, 32, 1303-17 | 3.6 | 8 |
| 38 | Theoretical Studies for Dendrimer-Based Drug Delivery. *Current Pharmaceutical Design*, **2017**, 23, 3048-3061 | 3.4 | 8 |
| 37 | The small organic molecule C19 binds and strengthens the KRAS4b-PDE□complex and inhibits growth of colorectal cancer cells in vitro and in vivo. *BMC Cancer*, **2018**, 18, 1056 | 4.8 | 8 |
| 36 | Structural and energetic basis for novel epicatechin derivatives acting as GPER agonists through the MMGBSA method. *Journal of Steroid Biochemistry and Molecular Biology*, **2019**, 189, 176-186 | 5.1 | 7 |
| 35 | QSAR, DFT and molecular modeling studies of peptides from HIV-1 to describe their recognition properties by MHC-I. *Journal of Biomolecular Structure and Dynamics*, **2018**, 36, 2312-2330 | 3.6 | 7 |
| 34 | Energetic and flexibility properties captured by long molecular dynamics simulations of a membrane-embedded pMHCII-TCR complex. *Molecular BioSystems*, **2016**, 12, 1350-66 | | 7 |
| 33 | Structural and energetic requirements for a second binding site at the dimeric □lactoglobulin interface. *Journal of Biomolecular Structure and Dynamics*, **2016**, 34, 1884-902 | 3.6 | 7 |
| 32 | Synthesis and In Vitro Evaluation of Tetrahydroquinoline Derivatives as Antiproliferative Compounds of Breast Cancer via Targeting the GPER. *Anti-Cancer Agents in Medicinal Chemistry*, **2019**, 19, 760-771 | 2.2 | 7 |
| 31 | Advances in Theoretical Studies on the Design of Single Boron Atom Compounds. *Current Pharmaceutical Design*, **2018**, 24, 3466-3475 | 3.3 | 6 |
| 30 | Selection of a GPER1 Ligand via Ligand-based Virtual Screening Coupled to Molecular Dynamics Simulations and Its Anti-proliferative Effects on Breast Cancer Cells. *Anti-Cancer Agents in Medicinal Chemistry*, **2018**, 18, 1629-1638 | 2.2 | 6 |
| 29 | Seeking potential anticonvulsant agents that target GABAA receptors using experimental and theoretical procedures. *Journal of Computer-Aided Molecular Design*, **2014**, 28, 1217-32 | 4.2 | 5 |
| 28 | Structural analogues of existing anti-viral drugs inhibit SARS-CoV-2 RNA dependent RNA polymerase: A computational hierarchical investigation. *Heliyon*, **2021**, 7, e06435 | 3.6 | 5 |
| 27 | Elucidation of the inhibitory activity of ivermectin with host nuclear importin □and several SARS-CoV-2 targets. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-9 | 3.6 | 5 |
| 26 | Cell-based assays and molecular dynamics analysis of a boron-containing agonist with different profiles of binding to human and guinea pig beta2 adrenoceptors. *European Biophysics Journal*, **2019**, 48, 83-97 | 1.9 | 5 |
| 25 | Complexation of methotrexate via ligand diffusion molecular dynamic simulations under neutral, basic, and acidic conditions. *Journal of Molecular Graphics and Modelling*, **2019**, 93, 107443 | 2.8 | 4 |
| 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. *Anti-Cancer Agents in Medicinal Chemistry*, **2017**, 17, 1441-1454 | 2.2 | 4 |
| 23 | Dissecting the molecular recognition of dual lapatinib derivatives for EGFR/HER2. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 293-303 | 4.2 | 4 |

| | | | |
|---|---|---|---|
| 22 | Mapping the intrinsically disordered properties of the flexible loop domain of Bcl-2: a molecular dynamics simulation study. *Journal of Molecular Modeling*, **2016**, 22, 98 | 2 | 4 |
| 21 | Fucosterol from as an amyloid-beta (A) aggregation inhibitor: and studies. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 1271-1283 | 3.6 | 4 |
| 20 | Repurposing FDA Drug Compounds against Breast Cancer by Targeting EGFR/HER2. *Pharmaceuticals*, **2021**, 14, | 5.2 | 4 |
| 19 | and studies of gp120-HIV-derived peptides in complex with G4-PAMAM dendrimers.. *RSC Advances*, **2020**, 10, 20414-20426 | 3.7 | 3 |
| 18 | Conformational changes associated with L16P and T118M mutations in the membrane-embedded PMP22 protein, consequential in CMT-1A. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 2880-2894 | 3.6 | 3 |
| 17 | Targeting Breast Cancer Cells with G4 PAMAM Dendrimers and Valproic Acid Derivative Complexes. *Anti-Cancer Agents in Medicinal Chemistry*, **2020**, 20, 1857-1872 | 2.2 | 3 |
| 16 | Modifications on the Tetrahydroquinoline Scaffold Targeting a Phenylalanine Cluster on GPER as Antiproliferative Compounds against Renal, Liver and Pancreatic Cancer Cells. *Pharmaceuticals*, **2021**, 14, | 5.2 | 3 |
| 15 | Exploring the biotransformation of N-(2-hydroxyphenyl)-2-propylpentanamide (an aryl valproic acid derivative) by CYP2C11, using in silico predictions and in vitro studies. *Journal of Pharmacy and Pharmacology*, **2020**, 72, 938-955 | 4.8 | 2 |
| 14 | Design of Drugs by Filtering Through ADMET, Physicochemical and Ligand-Target Flexibility Properties. *Methods in Molecular Biology*, **2018**, 1824, 403-416 | 1.4 | 2 |
| 13 | CDK4 as a phytochemical based anticancer drug target. *Informatics in Medicine Unlocked*, **2022**, 28, 100826 | 3.3 | 2 |
| 12 | Impact of tetramerization on the ligand recognition of N1 influenza neuraminidase via MMGBSA approach. *Biopolymers*, **2019**, 110, e23251 | 2.2 | 1 |
| 11 | Molecular mechanism of the association and dissociation of Deltarasin from the heterodimeric KRas4B-PDE complex. *Biopolymers*, **2019**, 110, e23333 | 2.2 | 1 |
| 10 | Complexation of peptide epitopes with G4-PAMAM dendrimer through ligand diffusion molecular dynamic simulations. *Journal of Molecular Graphics and Modelling*, **2020**, 96, 107514 | 2.8 | 1 |
| 9 | Structural mechanism of the Tanford transition of bovine lactoglobulin through microsecond molecular dynamics simulations. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-13 | 3.6 | 1 |
| 8 | Structural Insight of the Anticancer Properties of Doxazosin on Overexpressing EGFR/HER2 Cell Lines | | 1 |
| 7 | Dihydropyrazole-Carbohydrazide Derivatives with Dual Activity as Antioxidant and Anti-Proliferative Drugs on Breast Cancer Targeting the HDAC6. *Pharmaceuticals*, **2022**, 15, 690 | 5.2 | 1 |
| 6 | In silico design of HDAC6 inhibitors with neuroprotective effects. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-19 | 3.6 | 0 |
| 5 | Molecular insights into how SHBG dimerization exerts changes on ligand molecular recognition. *Journal of Steroid Biochemistry and Molecular Biology*, **2020**, 197, 105502 | 5.1 | 0 |

| | | | |
|---|---|---|---|
| 4 | Molecular recognition of tak-285 and lapatinib by inactive, active, and middle active-inactive HER2. *Journal of Molecular Modeling*, **2021**, 27, 105 | 2 | 0 |
| 3 | 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. *Journal of Molecular Graphics and Modelling*, **2021**, 107, 107970 | 2.8 | 0 |
| 2 | Elucidation of the inhibitory activity of plant-derived SARS-CoV inhibitors and their potential as SARS-CoV-2 inhibitors. *Journal of Biomolecular Structure and Dynamics*, **2021**, 1-13 | 3.6 | 0 |
| 1 | Binding of Folate-G4-PAMAM dendrimer conjugate with indomethacin via ligand diffusion MD simulations. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-11 | 3.6 | |