# Daniel J V A Dos Santos

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1340474/publications.pdf

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| 53 | 1,509 | 318942 | 371746 |
|---|---|---|---|
| papers | citations | 23 h-index | 37 g-index |

| 59 | 59 | 59 | 2465 |
|---|---|---|---|
| all docs | docs citations | times ranked | citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Alkylated monoterpene indole alkaloid derivatives as potent P-glycoprotein inhibitors in resistant cancer cells. European Journal of Medicinal Chemistry, 2021, 210, 112985. | 2.6 | 13 |
| 2 | Exploring the Monoterpene Indole Alkaloid Scaffold for Reversing P-Glycoprotein-Mediated Multidrug Resistance in Cancer. Pharmaceuticals, 2021, 14, 862. | 1.7 | 8 |
| 3 | Pedrolane, a Polycyclic Diterpene Scaffold Containing a Bicyclo[2.2.1]heptane System, from Euphorbia pedroi. Organic Letters, 2021, 23, 274-278. | 2.4 | 16 |
| 4 | Nitrogen-containing naringenin derivatives for reversing multidrug resistance in cancer. Bioorganic and Medicinal Chemistry, 2020, 28, 115798. | 1.4 | 16 |
| 5 | Activity to Breast Cancer Cell Lines of Different Malignancy and Predicted Interaction with Protein Kinase C Isoforms of Royleanones. International Journal of Molecular Sciences, 2020, 21, 3671. | 1.8 | 7 |
| 6 | Molecular Docking Studies of Royleanone Diterpenoids from Plectranthus spp. as P-Glycoprotein Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 839-845. | 1.3 | 19 |
| 7 | Theoretical insights on helix repacking as the origin of P-glycoprotein promiscuity. Scientific Reports, 2020, 10, 9823. | 1.6 | 15 |
| 8 | Identification of tetracyclic lactams as NMDA receptor antagonists with potential application in neurological disorders. European Journal of Medicinal Chemistry, 2020, 194, 112242. | 2.6 | 2 |
| 9 | Combining 1,3â€Ditriazolylbenzene and Quinoline to Discover a New Gâ€Quadruplexâ€Interactive Small Molecule Active against Cancer Stemâ€Like Cells. ChemMedChem, 2019, 14, 1325-1328. | 1.6 | 13 |
| 10 | Discovery of a small-molecule protein kinase CÎ´-selective activator with promising application in colon cancer therapy. Cell Death and Disease, 2018, 9, 23. | 2.7 | 25 |
| 11 | Optimizing the flavanone core toward new selective nitrogen-containing modulators of ABC transporters. Future Medicinal Chemistry, 2018, 10, 725-741. | 1.1 | 28 |
| 12 | Terpenoids from Euphorbia pedroi as Multidrug-Resistance Reversers. Journal of Natural Products, 2018, 81, 2032-2040. | 1.5 | 37 |
| 13 | About Pâ€glycoprotein: a new drugable domain is emerging from structural data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1316. | 6.2 | 15 |
| 14 | Structure-function relationships in ABCG2: insights from molecular dynamics simulations and molecular docking studies. Scientific Reports, 2017, 7, 15534. | 1.6 | 48 |
| 15 | Optimizing the macrocyclic diterpenic core toward the reversal of multidrug resistance in cancer. Future Medicinal Chemistry, 2016, 8, 629-645. | 1.1 | 12 |
| 16 | Probing the Azaaurone Scaffold against the Hepatic and Erythrocytic Stages of Malaria Parasites. ChemMedChem, 2016, 11, 2194-2204. | 1.6 | 23 |
| 17 | Effect of replacing [NTf<sub>2</sub>] by [PF<sub>6</sub>] anion on the [BMIm][NTf<sub>2</sub>] ionic liquid confined by gold. Molecular Simulation, 2015, 41, 455-462. | 0.9 | 17 |
| 18 | Do adsorbed drugs onto P-glycoprotein influence its efflux capability?. Physical Chemistry Chemical Physics, 2015, 17, 22023-22034. | 1.3 | 14 |

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|---|---|---|---|
| 19 | Molecular Dynamics Study of the Gold/Ionic Liquids Interface. Journal of Physical Chemistry B, 2015, 119, 9883-9892. | 1.2 | 35 |
| 20 | A tryptophanol-derived oxazolopiperidone lactam is cytotoxic against tumors via inhibition of p53 interaction with murine double minute proteins. Pharmacological Research, 2015, 95-96, 42-52. | 3.1 | 37 |
| 21 | Indolo[3,2â€c]quinoline Gâ€Quadruplex Stabilizers: a Structural Analysis of Binding to the Human Telomeric Gâ€Quadruplex. ChemMedChem, 2015, 10, 836-849. | 1.6 | 24 |
| 22 | Do Drugs Have Access to the P-Glycoprotein Drug-Binding Pocket through Gates?. Journal of Chemical Theory and Computation, 2015, 11, 4525-4529. | 2.3 | 23 |
| 23 | P-glycoprotein and membrane roles in multidrug resistance. Future Medicinal Chemistry, 2015, 7, 929-946. | 1.1 | 64 |
| 24 | Reversing cancer multidrug resistance: insights into the efflux by <scp>ABC</scp> transports from in silico studies. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 27-55. | 6.2 | 26 |
| 25 | Oxazoloisoindolinones with in vitro antitumor activity selectively activate a p53-pathway through potential inhibition of the p53â€“MDM2 interaction. European Journal of Pharmaceutical Sciences, 2015, 66, 138-147. | 1.9 | 41 |
| 26 | Probing the aurone scaffold against Plasmodium falciparum: Design, synthesis and antimalarial activity. European Journal of Medicinal Chemistry, 2014, 80, 523-534. | 2.6 | 64 |
| 27 | Exploring the Molecular Basis of Q<sub>o</sub>bc<sub>1</sub> Complex Inhibitors Activity to Find Novel Antimalarials Hits. Molecular Informatics, 2013, 32, 659-670. | 1.4 | 11 |
| 28 | Synthesis, Gâ€Quadruplex Stabilisation, Docking Studies, and Effect on Cancer Cells of Indolo[3,2â€b]quinolines with One, Two, or Three Basic Side Chains. ChemMedChem, 2013, 8, 1648-1661. | 1.6 | 39 |
| 29 | Molecular Docking Characterizes Substrate-Binding Sites and Efflux Modulation Mechanisms within P-Glycoprotein.. Journal of Chemical Information and Modeling, 2013, 53, 1747-1760. | 2.5 | 136 |
| 30 | Flavones as isosteres of 4(1H)-quinolones: Discovery of ligand efficient and dual stage antimalarial lead compounds. European Journal of Medicinal Chemistry, 2013, 69, 872-880. | 2.6 | 13 |
| 31 | Enhancing Macrocyclic Diterpenes as Multidrug-Resistance Reversers: Structureâ€“Activity Studies on Jolkinol D Derivatives. Journal of Medicinal Chemistry, 2013, 56, 748-760. | 2.9 | 61 |
| 32 | Assessing the Stabilization of Pâ€Glycoproteinâ€™s Nucleotideâ€Binding Domains by the Linker, Using Molecular Dynamics. Molecular Informatics, 2013, 32, 529-540. | 1.4 | 17 |
| 33 | Colon Adenocarcinoma Multidrug Resistance Reverted by Euphorbia Diterpenes: Structure-Activity Relationships and Pharmacophore Modeling. Anti-Cancer Agents in Medicinal Chemistry, 2012, 12, 1015-1024. | 0.9 | 22 |
| 34 | Insights on P-Glycoproteinâ€™s Efflux Mechanism Obtained by Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2012, 8, 1853-1864. | 2.3 | 102 |
| 35 | Properties and behaviour of tetracyclic allopsoralen derivatives inside a DPPC lipid bilayer model. Physical Chemistry Chemical Physics, 2011, 13, 10174. | 1.3 | 5 |
| 36 | Incorporation of Basic Side Chains into Cryptolepine Scaffold: Structureâ^'Antimalarial Activity Relationships and Mechanistic Studies. Journal of Medicinal Chemistry, 2011, 54, 734-750. | 2.9 | 57 |

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|---|---|---|---|
| 37 | Toward a Better Pharmacophore Description of P-Glycoprotein Modulators, Based on Macrocyclic Diterpenes from Euphorbia Species. Journal of Chemical Information and Modeling, 2011, 51, 1315-1324. | 2.5 | 59 |
| 38 | Identification of new antimalarial leads by use of virtual screening against cytochrome bc1. Bioorganic and Medicinal Chemistry, 2011, 19, 6302-6308. | 1.4 | 10 |
| 39 | A quantum mechanical study of novel potential inhibitors of cytochrome bc<sub>1</sub> as antimalarial compounds. International Journal of Quantum Chemistry, 2011, 111, 1196-1207. | 1.0 | 16 |
| 40 | Synthesis and evaluation of vinyl sulfones as caspase-3 inhibitors. AÂstructureâ€“activity study. European Journal of Medicinal Chemistry, 2010, 45, 3858-3863. | 2.6 | 34 |
| 41 | Interfacial Excess Free Energies of Solidâ€“Liquid Interfaces by Molecular Dynamics Simulation and Thermodynamic Integration. Macromolecular Rapid Communications, 2009, 30, 864-870. | 2.0 | 73 |
| 42 | Design, synthesis and structureâ€“activity relationships of (1H-pyridin-4-ylidene)amines as potential antimalarials. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 3476-3480. | 1.0 | 29 |
| 43 | Properties and Permeability of Hypericin and Brominated Hypericin in Lipid Membranes. Journal of Chemical Theory and Computation, 2009, 5, 3139-3149. | 2.3 | 32 |
| 44 | Substituent effects on Oâ€“H and Sâ€“H bond dissociation enthalpies of disubstituted phenols and thiophenols. International Journal of Quantum Chemistry, 2008, 108, 754-761. | 1.0 | 12 |
| 45 | Modelling the behavior of 5-aminolevulinic acid and its alkyl esters in a lipid bilayer. Chemical Physics Letters, 2008, 463, 178-182. | 1.2 | 17 |
| 46 | Consistency of Ion Adsorption and Excess Surface Tension in Molecular Dynamics Simulations of Aqueous Salt Solutions. Journal of Physical Chemistry C, 2008, 112, 19431-19442. | 1.5 | 43 |
| 47 | Theoretical Study of Sequence Selectivity and Preferred Binding Mode of Psoralen with DNA. Research Letters in Physical Chemistry, 2007, 2007, 1-5. | 0.3 | 3 |
| 48 | Theoretical prediction of binding modes and hot sequences for allopsoralenâ€“DNA interaction. Chemical Physics Letters, 2007, 450, 127-131. | 1.2 | 3 |
| 49 | Permeability of Psoralen Derivatives in Lipid Membranes. Biophysical Journal, 2006, 91, 2464-2474. | 0.2 | 27 |
| 50 | Structure and Properties of Hexadecyltrimethylammonium Chloride Monolayers in Contact with Oil Films with Different Thicknesses. Journal of Physical Chemistry B, 2004, 108, 17153-17159. | 1.2 | 2 |
| 51 | Molecular Dynamics Study of a Hexadecyltrimethylammonium Chloride Monolayer at the Interface between Two Immiscible Liquids. Langmuir, 2003, 19, 958-966. | 1.6 | 6 |
| 52 | Molecular Dynamics Study of the Calcium Ion Transfer across the Water/Nitrobenzene Interface. ChemPhysChem, 2002, 3, 946-951. | 1.0 | 29 |
| 53 | Application of the hypervolume Monte Carlo methods to a molten ionic system. Computational and Theoretical Chemistry, 1999, 463, 191-196. | 1.5 | 1 |