

# Jana Sopkova-de Oliveira Santos

## List of Publications by Year in descending order

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90  
papers

1,672  
citations

279798

23  
h-index

361022

35  
g-index

92  
all docs

92  
docs citations

92  
times ranked

2320  
citing authors

#	ARTICLE	IF	CITATIONS
1	Protein Crystallography under Xenon and Nitrous Oxide Pressure: Comparison with In Vivo Pharmacology Studies and Implications for the Mechanism of Inhaled Anesthetic Action. <i>Biophysical Journal</i> , 2007, 92, 217-224.	0.5	80
2	Design, Synthesis, and Evaluation of Novel Thienopyrrolizinones as Antitubulin Agents. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 1448-1464.	6.4	79
3	Toward Safer Thrombolytic Agents in Stroke: Molecular Requirements for NMDA Receptor-Mediated Neurotoxicity. <i>Journal of Cerebral Blood Flow and Metabolism</i> , 2008, 28, 1212-1221.	4.3	74
4	Donepezil-Based Central Acetylcholinesterase Inhibitors by Means of a "Bio-Oxidizable" Prodrug Strategy: Design, Synthesis, and in Vitro Biological Evaluation. <i>Journal of Medicinal Chemistry</i> , 2017, 60, 5909-5926.	6.4	67
5	Oxygen Pressurized X-Ray Crystallography: Probing the Dioxxygen Binding Site in Cofactorless Urate Oxidase and Implications for Its Catalytic Mechanism. <i>Biophysical Journal</i> , 2008, 95, 2415-2422.	0.5	65
6	Hot-Spots of Mcl-1 Protein. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 928-943.	6.4	57
7	Room-Temperature ortho-Alkoxylation and Halogenation of N-Tosylbenzamides by Using Palladium(II)-Catalyzed C-H Activation. <i>Chemistry - A European Journal</i> , 2014, 20, 7507-7513.	3.3	50
8	Synthesis, Crystal Structure and Thermal Properties of Phosphorylated Cyclotriphosphazenes. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 138-143.	2.0	44
9	First Evidence That Oligopyridines, $\alpha$ -Helix Foldamers, Inhibit Mcl-1 and Sensitize Ovarian Carcinoma Cells to Bcl-2-Targeting Strategies. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 1644-1668.	6.4	40
10	A Three-Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 8008-8012.	13.8	38
11	Synthesis and biological evaluation as AChE inhibitors of new indanones and thiaindanones related to donepezil. <i>European Journal of Medicinal Chemistry</i> , 2005, 40, 1222-1245.	5.5	36
12	Pressure-response analysis of anesthetic gases xenon and nitrous oxide on urate oxidase: a crystallographic study. <i>FASEB Journal</i> , 2011, 25, 2266-2275.	0.5	31
13	Selecting the first chemical molecule inhibitor of HSP110 for colorectal cancer therapy. <i>Cell Death and Differentiation</i> , 2020, 27, 117-129.	11.2	31
14	3D-QSAR and Docking Studies of Selective GSK-3 $\beta$ Inhibitors. Comparison with a Thieno[2,3-b]pyrrolizinone Derivative, a New Potential Lead for GSK-3 $\beta$ Ligands. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 708-715.	5.4	29
15	An Efficient and Straightforward Access to Sulfur Substituted [2.2]Paracyclophanes: Application to Stereoselective Sulfenate Salt Alkylation. <i>Organic Letters</i> , 2008, 10, 1271-1274.	4.6	29
16	Novel donepezil-like N-benzylpyridinium salt derivatives as AChE inhibitors and their corresponding dihydropyridine "bio-oxidizable" prodrugs: Synthesis, biological evaluation and structure-activity relationship. <i>European Journal of Medicinal Chemistry</i> , 2018, 145, 165-190.	5.5	29
17	Synthesis and biological evaluation of new 5-benzylated 4-oxo-3,4-dihydro-5H-pyridazino[4,5-b]indoles as PI3K $\alpha$ inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2012, 57, 225-233.	5.5	27
18	Pathway for Large-Scale Conformational Change in Annexin V. <i>Biochemistry</i> , 2000, 39, 14065-14074.	2.5	26

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19	Synthesis of dihalo bi- and terpyridines by regioselective Suzuki-Miyaura cross-coupling reactions. <i>Tetrahedron</i> , 2009, 65, 5413-5417.	1.9	26
20	S100 protein-annexin interactions: a model of the (Anx2-p11) <sub>2</sub> heterotetramer complex. <i>Biochimica Et Biophysica Acta - Molecular Cell Research</i> , 2000, 1498, 181-191.	4.1	25
21	One pot diastereoselective synthesis of new chiral spiro[1,3,4]thiadiazoles and 1,4,2-oxathiazoles from (1 <i>R</i> ,2 <i>R</i> )-thiocamphor. <i>Journal of Heterocyclic Chemistry</i> , 2004, 41, 731-735.	2.6	25
22	Definition of New Pharmacophores for Nonpeptide Antagonists of Human Urotensin-II. Comparison with the 3D-structure of Human Urotensin-II and URP. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 602-612.	5.4	25
23	Synthesis of new phenylpyridyl scaffolds using the Garlanding approach. <i>Tetrahedron</i> , 2010, 66, 8000-8005.	1.9	24
24	Virtual Screening Discovery of New Acetylcholinesterase Inhibitors Issued from CERMN Chemical Library. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 422-428.	5.4	24
25	Design and synthesis of thienylpyridyl garlands as non-peptidic alpha helix mimetics and potential protein-protein interactions disruptors. <i>Tetrahedron</i> , 2011, 67, 6145-6154.	1.9	24
26	Fluoride Ion and Phosphines as Nucleophilic Catalysts: Synthesis of 1,4-Benzothiazepines from Cyclic Sulfenamides. <i>Journal of Organic Chemistry</i> , 2009, 74, 3936-3939.	3.2	23
27	Diastereoselective Addition of Enantiopure Lithiumtert-Butylsulfinylferrocene to Imines. <i>Journal of Organic Chemistry</i> , 2006, 71, 9572-9579.	3.2	22
28	Synthesis of new dipyrrolo- and fuopyrrolopyrazinones related to triptones and their biological evaluation as potential kinases (CDKs1 <sup>5</sup> , GSK-3) inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2009, 44, 708-716.	5.5	22
29	trans-(±)-2-tert-Butyl-3-phenyloxaziridine: A Unique Reagent for the Oxidation of Thiolates into Sulfenates. <i>Journal of Organic Chemistry</i> , 2007, 72, 5403-5406.	3.2	21
30	A new boronic-acid based strategy to synthesize 4(5)-(het)aryl-1H-imidazoles. <i>Tetrahedron</i> , 2008, 64, 4596-4601.	1.9	21
31	Interpretation of honeybees contact toxicity associated to acetylcholinesterase inhibitors. <i>Ecotoxicology and Environmental Safety</i> , 2012, 79, 13-21.	6.0	20
32	Design, synthesis and biological evaluation of novel indano- and thiaindano-pyrazoles with potential interest for Alzheimer's disease. <i>MedChemComm</i> , 2013, 4, 925.	3.4	20
33	Poly[[chlorido(1,10-phenanthroline-1,2-dicyano)copper(II)]-1,3,3-tetracyano-2-ethoxypropyl] coordination polymer sheets linked into bilayers by hydrogen bonds. <i>Acta Crystallographica Section C, Structural Chemistry</i> , 2014, 70, 19-22.	0.5	20
34	Pleiotropic prodrugs: Design of a dual butyrylcholinesterase inhibitor and 5-HT <sub>6</sub> receptor antagonist with therapeutic interest in Alzheimer's disease. <i>European Journal of Medicinal Chemistry</i> , 2021, 210, 113059.	5.5	20
35	Hydrogenative desulphurization of thienopyrrolizinones: An easy and selective access to (Z)-phenethylidenepyrrolizinones with in vitro cytotoxic activity. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 1146-1150.	5.5	18
36	Association of Two 3D QSAR Analyses. Application to the Study of Partial Agonist Serotonin-3 Ligands. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 815-823.	2.8	17

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37	New practical access to 2-azatryptophans and dehydro derivatives via the Wittigâ€“Horner reaction. <i>Tetrahedron Letters</i> , 2007, 48, 2457-2460.	1.4	17
38	New hypotheses for the binding mode of 4- and 7-substituted indazoles in the active site of neuronal nitric oxide synthase. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 5296-5304.	3.0	15
39	Structural Characterizations of Oligopyridyl Foldamers, $\hat{1}\pm$ -Helix Mimetics. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 429-439.	5.4	15
40	Annexin A5 D226K structure and dynamics: identification of a molecular switch for the large-scale conformational change of domain III. <i>FEBS Letters</i> , 2001, 493, 122-128.	2.8	14
41	A straightforward asymmetric synthesis of 1,2-disubstituted ferrocenylalkyl amines with the unusual (S <sub>Fc</sub> ,S) configuration. <i>Chemical Communications</i> , 2007, , 4875.	4.1	14
42	Synthesis of dual AChE/5-HT4 receptor multi-target directed ligands. <i>MedChemComm</i> , 2012, 3, 627.	3.4	14
43	Synthesis of new linear poly(phenylpyridyl) chains. <i>Tetrahedron</i> , 2012, 68, 1910-1917.	1.9	14
44	Assembly of benzene-1,3,5-tris(methylenephosphonic acid) and guanidinium salt: Single crystal-X-ray characterisation and <sup>31</sup> P solid state NMR investigations. <i>New Journal of Chemistry</i> , 2004, 28, 1244-1249.	2.8	13
45	Molecular basis of agonist docking in a human <sc>GPR</sc> 103 homology model by siteâ€“directed mutagenesis and structureâ€“activity relationship studies. <i>British Journal of Pharmacology</i> , 2014, 171, 4425-4439.	5.4	13
46	Toward Understanding Mcl-1 Promiscuous and Specific Binding Mode. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2885-2895.	5.4	13
47	One-pot synthesis of novel poly-substituted phenanthrenes. <i>Tetrahedron</i> , 2010, 66, 2803-2808.	1.9	12
48	Novel benzyldenephénylpyrrolizinones with pleiotropic activities potentially useful in Alzheimer's disease treatment. <i>European Journal of Medicinal Chemistry</i> , 2016, 114, 365-379.	5.5	12
49	Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 298-310.	5.4	12
50	Structure-guided design of pyridoclox derivatives based on Noxa / Mcl-1 interaction mode. <i>European Journal of Medicinal Chemistry</i> , 2018, 159, 357-380.	5.5	12
51	The Crystal Structure of Annexin A8 is Similar to that of Annexin A3. <i>Journal of Molecular Biology</i> , 2005, 345, 1131-1139.	4.2	11
52	In silico chemical library screening and experimental validation of novel compounds with potential varroacide activities. <i>Pesticide Biochemistry and Physiology</i> , 2019, 160, 11-19.	3.6	11
53	Synthesis of novel benzo[ <i>h</i> ] [1,6]naphthyridines <i>via</i> a rearrangement of hexahydroâ€“ <i>h</i> â€“pyrrolo [2,1- <i>c</i> ] [1,4]benzodiazepines. <i>Journal of Heterocyclic Chemistry</i> , 2003, 40, 255-259.	2.6	10
54	2-(6-Bromopyridin-3-yl)-4,4,5,5-tetramethyl-1,3,2-dioxaborolane and (6-bromopyridin-3-yl)boronic acid, new bifunctional building blocks for combinatorial chemistry. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2003, 59, o111-o113.	0.4	10

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55	Three-dimensional model of the human urotensin receptor: Docking of human urotensin and nonpeptide antagonists in the binding site and comparison with an antagonist pharmacophore model. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 73, 173-184.	2.6	10
56	Benzylphenylpyrrolizinones with Anti-amyloid and Radical Scavenging Effects, Potentially Useful in Alzheimer's Disease Treatment. <i>ChemMedChem</i> , 2017, 12, 913-916.	3.2	10
57	Sequential one pot double C H heteroarylation of thiophene using bromopyridines to synthesize unsymmetrical 2,5-bipyridylthiophenes. <i>Tetrahedron</i> , 2017, 73, 5509-5516.	1.9	10
58	7-Methoxy-1H-indazole, a new inhibitor of neuronal nitric oxide synthase. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2002, 58, o688-o690.	0.4	9
59	Quinoline derivatives: potential antiparasitic and antiviral agents. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2007, 63, o643-o645.	0.4	9
60	One-pot synthesis of new aza- and diaza-aminophenanthrenes. <i>Tetrahedron</i> , 2011, 67, 5806-5810.	1.9	9
61	Synthesis of novel 7-oxo and 7-hydroxy trifluoroalcolchicinoids with cytotoxic effect. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 2614-2623.	3.0	9
62	Insights into Mcl-1 Conformational States and Allosteric Inhibition Mechanism from Molecular Dynamics Simulations, Enhanced Sampling, and Pocket Crosstalk Analysis. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3172-3187.	5.4	9
63	An expedient route to aromatic pyrrolo[2,1-c][1,4]benzodiazepines and a study of their reactivity. <i>Tetrahedron Letters</i> , 2001, 42, 5183-5185.	1.4	8
64	Synthesis, Pharmacological Study and Modeling of 7-Methoxyindazole and Related Substituted Indazoles as Neuronal Nitric Oxide Synthase Inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2003, 18, 195-199.	5.2	8
65	Synthesis and Biological Evaluation of Thienopyrrolizines, a New Family of CDK/GSK-3 Inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2004, 19, 585-593.	5.2	8
66	Synthesis of Novel Pyrazolopyrrolizinones as Prospective Anticancer Agents. <i>Heterocycles</i> , 2006, 68, 2063.	0.7	8
67	Protective effects of caffeic acid against hypothalamic neuropeptides alterations induced by malathion in rat. <i>Environmental Science and Pollution Research</i> , 2015, 22, 6198-6207.	5.3	8
68	2-Bromo-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine, a new unexpected bifunctional building block for combinatorial chemistry. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2003, 59, o596-o597.	0.4	7
69	Aromatic garlands, as new foldamers, to mimic protein secondary structure. <i>Tetrahedron</i> , 2012, 68, 4381-4389.	1.9	7
70	Conformation Control of Abiotic $\beta$ -Helical Foldamers. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2671-2680.	5.4	7
71	7-Nitro-1H-indazole, an inhibitor of nitric oxide synthase. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2000, 56, 1503-1504.	0.4	6
72	9-Ethyl-1,4-dimethyl-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-9H-carbazole and 6-bromo-9-ethyl-1,4-dimethyl-9H-carbazole. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008, 64, o453-o455.	0.4	6

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73	Synthesis of 3-amino-thiochromanes from 4-benzyl 2-thiazolines, via an unprecedented intramolecular electrophilic aromatic substitution. <i>Organic and Biomolecular Chemistry</i> , 2010, 8, 2520.	2.8	6
74	β-Strand Mimicry: Exploring Oligothienylpyridine Foldamers. <i>European Journal of Organic Chemistry</i> , 2016, 2016, 5686-5696.	2.4	6
75	Effect of oral exposure to the acaricide pirimicarb, a new varroacide candidate, on <i>Apis mellifera</i> feeding rate. <i>Pest Management Science</i> , 2018, 74, 1790-1797.	3.4	6
76	2-(6-Bromopyridin-2-yl)-6-methyl-[1,3,6,2]dioxaborocane, a new stable (pyridin-2-yl)boronic acid derivative. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2004, 60, o582-o584.	0.4	5
77	Ethane-1,1,2-trisphosphonic acid hemihydrate. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008, 64, o47-o49.	0.4	5
78	Design, Synthesis, Molecular Dynamics Simulation, and Functional Evaluation of a Novel Series of 26RFa Peptide Analogues Containing a Mono- or Polyalkyl Guanidino Arginine Derivative. <i>Journal of Medicinal Chemistry</i> , 2018, 61, 10185-10197.	6.4	5
79	X-ray structure of floridoside isolated from the marine red algae <i>Dilsea carnosa</i> . <i>Carbohydrate Research</i> , 2008, 343, 2697-2698.	2.3	4
80	Synthesis of New [2,3,6-trisubstituted]Terpyridines Using Iterative Cross-Coupling Reactions. <i>Synthesis</i> , 2010, 2010, 2804-2810.	2.3	4
81	Binding mode of Pyridoclast to myeloid cell leukemia-1 (Mcl-1) revealed by nuclear magnetic resonance spectroscopy, docking and molecular dynamics approaches. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4162-4178.	3.5	4
82	YC-1, an activation inductor of soluble guanylyl cyclase. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2000, 56, 1035-1036.	0.4	3
83	1-Chloro-1,3,3,5,5-pentaphenoxycyclotriphosphazene: a precursor of functionalized cyclophosphazene derivatives. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2004, 60, o751-o753.	0.4	3
84	Receptor- and Ligand-Based Study on Novel 2,2-Bithienyl Derivatives as Non-Peptidic AANAT Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 446-460.	5.4	3
85	Cryptic Pockets Repository through Pocket Dynamics Tracking and Metadynamics on Essential Dynamics Space: Applications to Mcl-1. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5581-5588.	5.4	3
86	1,2,3-Trimethoxy-4-[(E)-2-phenylvinyl]benzene and (E,E)-1,4-bis(2,3,4-trimethoxyphenyl)buta-1,3-diene. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2009, 65, o311-o313.	0.4	2
87	Drug Repurposing: Deferasirox Inhibits the Anti-Apoptotic Activity of Mcl-1. <i>Drug Design, Development and Therapy</i> , 2021, Volume 15, 5035-5059.	4.3	2
88	Nitrated isomers of 2-(trichloromethyl)quinoline. <i>Acta Crystallographica Section C: Crystal Structure Communications</i> , 2008, 64, o441-o444.	0.4	1
89	Description of Joint Alterations Observed in a Family Carrying p.Asn453Ser COMP Variant: Clinical Phenotypes, In Silico Prediction of Functional Impact on COMP Protein and Stability, and Review of the Literature. <i>Biomolecules</i> , 2021, 11, 1460.	4.0	1
90	An intermolecular dative B $\rightarrow$ N bond in 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-thiazole. <i>Acta Crystallographica Section E: Structure Reports Online</i> , 2010, 66, o156-o156.	0.2	0