Jana Sopkova-de Oliveira Santos

List of Publications by Year
in descending order

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	Pleiotropic prodrugs: Design of a dual butyrylcholinesterase inhibitor and 5-HT6 receptor antagonist with therapeutic interest in Alzheimerâ€™s disease. European Journal of Medicinal Chemistry, 2021, 210, 113059.	5.5	20
2	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. Biomolecules, 2021, 11, 1460.	4.0	1
3	Cryptic Pockets Repository through Pocket Dynamics Tracking and Metadynamics on Essential Dynamics Space: Applications to Mcl-1. Journal of Chemical Information and Modeling, 2021, 61, 5581-5588.	5.4	3
4	Drug Repurposing: Deferasirox Inhibits the Anti-Apoptotic Activity of Mcl-1. Drug Design, Development and Therapy, 2021, Volume 15, 5035-5059.	4.3	2
5	Selecting the first chemical molecule inhibitor of HSP110 for colorectal cancer therapy. Cell Death and Differentiation, 2020, 27, 117-129.	11.2	31
6	Hot-Spots of Mcl-1 Protein. Journal of Medicinal Chemistry, 2020, 63, 928-943.	6.4	57
7	Binding mode of Pyridoclax to myeloid cell leukemia-1 (Mcl-1) revealed by nuclear magnetic resonance spectroscopy, docking and molecular dynamics approaches. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4162-4178.	3.5	4
8	Insights into Mcl-1 Conformational States and Allosteric Inhibition Mechanism from Molecular Dynamics Simulations, Enhanced Sampling, and Pocket Crosstalk Analysis. Journal of Chemical Information and Modeling, 2020, 60, 3172-3187.	5.4	9
9	In silico chemical library screening and experimental validation of novel compounds with potential varroacide activities. Pesticide Biochemistry and Physiology, 2019, 160, 11-19.	3.6	11
10	Effect of oral exposure to the acaricide pirimicarb, a new varroacide candidate, on Apis mellifera feeding rate. Pest Management Science, 2018, 74, 1790-1797.	3.4	6
11	Novel donepezil-like N -benzylpyridinium salt derivatives as AChE inhibitors and their corresponding dihydropyridine â€œbio-oxidizableâ€•prodrugs: Synthesis, biological evaluation and structure-activity relationship. European Journal of Medicinal Chemistry, 2018, 145, 165-190.	5.5	29
12	Structure-guided design of pyridoclax derivatives based on Noxa / Mcl-1 interaction mode. European Journal of Medicinal Chemistry, 2018, 159, 357-380.	5.5	12
13	Design, Synthesis, Molecular Dynamics Simulation, and Functional Evaluation of a Novel Series of 26RFa Peptide Analogues Containing a Mono- or Polyalkyl Guanidino Arginine Derivative. Journal of Medicinal Chemistry, 2018, 61, 10185-10197.	6.4	5
14	Conformation and Dynamics of Human Urotensin II and Urotensin Related Peptide in Aqueous Solution. Journal of Chemical Information and Modeling, 2017, 57, 298-310.	5.4	12
15	Donepezil-Based Central Acetylcholinesterase Inhibitors by Means of a â€œBio-Oxidizableâ€•Prodrug Strategy: Design, Synthesis, and in Vitro Biological Evaluation. Journal of Medicinal Chemistry, 2017, 60, 5909-5926.	6.4	67
16	Benzylphenylpyrrolizinones with Antiâ€amyloid and Radical Scavenging Effects, Potentially Useful in Alzheimer's Disease Treatment. ChemMedChem, 2017, 12, 913-916.	3.2	10
17	Toward Understanding Mcl-1 Promiscuous and Specific Binding Mode. Journal of Chemical Information and Modeling, 2017, 57, 2885-2895.	5.4	13
18	Sequential one pot double C H heteroarylation of thiophene using bromopyridines to synthesize unsymmetrical 2,5-bipyridylthiophenes. Tetrahedron, 2017, 73, 5509-5516.	1.9	10

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19	A Threeâ€Site Mechanism for Agonist/Antagonist Selective Binding to Vasopressin Receptors. Angewandte Chemie - International Edition, 2016, 55, 8008-8012.	13.8	38
20	Î²â€Strand Mimicry: Exploring Oligothienylpyridine Foldamers. European Journal of Organic Chemistry, 2016, 2016, 5686-5696.	2.4	6
21	Novel benzylidenephenylpyrrolizinones with pleiotropic activities potentially useful in Alzheimer's disease treatment. European Journal of Medicinal Chemistry, 2016, 114, 365-379.	5.5	12
22	First Evidence That Oligopyridines, Î±-Helix Foldamers, Inhibit Mcl-1 and Sensitize Ovarian Carcinoma Cells to Bcl-x_L-Targeting Strategies. Journal of Medicinal Chemistry, 2015, 58, 1644-1668.	6.4	40
23	Protective effects of caffeic acid against hypothalamic neuropeptides alterations induced by malathion in rat. Environmental Science and Pollution Research, 2015, 22, 6198-6207.	5.3	8
24	Molecular basis of agonist docking in a human <scp>GPR</scp>103 homology model by siteâ€directed mutagenesis and structureâ€“activity relationship studies. British Journal of Pharmacology, 2014, 171, 4425-4439.	5.4	13
25	Poly[[chlorido(1,10-phenanthroline-Î²²N,Nâ€²)copper(II)]-Î¼₃-1,1,3,3-tetracyano-2-ethoxypro coordination polymer sheets linked into bilayers by hydrogen bonds. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 19-22.	0.5	20
26	Roomâ€Temperature orthoâ€Alkoxylation and â€Halogenation of Nâ€Tosylbenzamides by Using Palladium(II)â€Catalyzed Cï£¿H Activation. Chemistry - A European Journal, 2014, 20, 7507-7513.	3.3	50
27	Design, synthesis and biological evaluation of novel indano- and thiaindano-pyrazoles with potential interest for Alzheimer's disease. MedChemComm, 2013, 4, 925.	3.4	20
28	Conformation Control of Abiotic Î±-Helical Foldamers. Journal of Chemical Information and Modeling, 2013, 53, 2671-2680.	5.4	7
29	New hypotheses for the binding mode of 4- and 7-substituted indazoles in the active site of neuronal nitric oxide synthase. Bioorganic and Medicinal Chemistry, 2012, 20, 5296-5304.	3.0	15
30	Synthesis and biological evaluation of new 5-benzylated 4-oxo-3,4-dihydro-5H-pyridazino[4,5-b]indoles as PI3KÎ± inhibitors. European Journal of Medicinal Chemistry, 2012, 57, 225-233.	5.5	27
31	Synthesis of dual AChE/5-HT4 receptor multi-target directed ligands. MedChemComm, 2012, 3, 627.	3.4	14
32	Interpretation of honeybees contact toxicity associated to acetylcholinesterase inhibitors. Ecotoxicology and Environmental Safety, 2012, 79, 13-21.	6.0	20
33	Structural Characterizations of Oligopyridyl Foldamers, Î±-Helix Mimetics. Journal of Chemical Information and Modeling, 2012, 52, 429-439.	5.4	15
34	Synthesis of novel 7-oxo and 7-hydroxy trifluoroallocolchicinoids with cytotoxic effect. Bioorganic and Medicinal Chemistry, 2012, 20, 2614-2623.	3.0	9
35	Synthesis of new linear poly(phenylpyridyl) chains. Tetrahedron, 2012, 68, 1910-1917.	1.9	14
36	Aromatic garlands, as new foldamers, to mimic protein secondary structure. Tetrahedron, 2012, 68, 4381-4389.	1.9	7

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37	One-pot synthesis of new aza- and diaza-aminophenanthrenes. Tetrahedron, 2011, 67, 5806-5810.	1.9	9
38	Design and synthesis of thienylpyridyl garlands as non-peptidic alpha helix mimetics and potential proteinâ€“protein interactions disruptors. Tetrahedron, 2011, 67, 6145-6154.	1.9	24
39	Pressureâ€response analysis of anesthetic gases xenon and nitrous oxide on urate oxidase: a crystallographic study. FASEB Journal, 2011, 25, 2266-2275.	0.5	31
40	Receptor- and Ligand-Based Study on Novel 2,2â€²-Bithienyl Derivatives as Non-Peptidic AANAT Inhibitors. Journal of Chemical Information and Modeling, 2010, 50, 446-460.	5.4	3
41	One-pot synthesis of novel poly-substituted phenanthrenes. Tetrahedron, 2010, 66, 2803-2808.	1.9	12
42	Synthesis of new phenylpyridyl scaffolds using the Garlanding approach. Tetrahedron, 2010, 66, 8000-8005.	1.9	24
43	Hydrogenative desulphurization of thienopyrrolizinones: An easy and selective access to (Z)-phenethylidenepyrrolizinones with in vitro cytotoxic activity. European Journal of Medicinal Chemistry, 2010, 45, 1146-1150.	5.5	18
44	Synthesis of New [2,3â€²:6â€²,3â€²â€²]Terpyridines Using Iterative Cross-Coupling Reactions. Synthesis, 2010, 2010, 2804-2810.	2.3	4
45	Virtual Screening Discovery of New Acetylcholinesterase Inhibitors Issued from CERMN Chemical Library. Journal of Chemical Information and Modeling, 2010, 50, 422-428.	5.4	24
46	Synthesis of 3-amino-thiochromanes from 4-benzyl 2-thiazolines, via an unprecedented intramolecular electrophilic aromatic substitution. Organic and Biomolecular Chemistry, 2010, 8, 2520.	2.8	6
47	An intermolecular dative Bâ†N bond in 5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)-1,3-thiazole. Acta Crystallographica Section E: Structure Reports Online, 2010, 66, o156-o156.	0.2	0
48	Synthesis of dihalo bi- and terpyridines by regioselective Suzukiâ€“Miyaura cross-coupling reactions. Tetrahedron, 2009, 65, 5413-5417.	1.9	26
49	1,2,3-Trimethoxy-4-[(E)-2-phenylvinyl]benzene and (E,E)-1,4-bis(2,3,4-trimethoxyphenyl)buta-1,3-diene. Acta Crystallographica Section C: Crystal Structure Communications, 2009, 65, o311-o313.	0.4	2
50	Synthesis of new dipyrrolo- and furopyrrolopyrazinones related to tripentones and their biological evaluation as potential kinases (CDKs1â€“5, GSK-3) inhibitors. European Journal of Medicinal Chemistry, 2009, 44, 708-716.	5.5	22
51	Fluoride Ion and Phosphines as Nucleophilic Catalysts: Synthesis of 1,4-Benzothiazepines from Cyclic Sulfenamides. Journal of Organic Chemistry, 2009, 74, 3936-3939.	3.2	23
52	Ethane-1,1,2-trisphosphonic acid hemihydrate. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o47-o49.	0.4	5
53	Nitrated isomers of 2-(trichloromethyl)quinoline. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o441-o444.	0.4	1
54	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. Acta Crystallographica Section C: Crystal Structure Communications, 2008, 64, o453-o455.	0.4	6

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55	Threeâ€dimensional model of the human urotensinâ€II receptor: Docking of human urotensinâ€II and nonpeptide antagonists in the binding site and comparison with an antagonist pharmacophore model. Proteins: Structure, Function and Bioinformatics, 2008, 73, 173-184.	2.6	10
56	Synthesis, Crystal Structure and Thermal Properties of Phosphorylated Cyclotriphosphazenes. European Journal of Inorganic Chemistry, 2008, 2008, 138-143.	2.0	44
57	X-ray structure of floridoside isolated from the marine red algae Dilsea carnosa. Carbohydrate Research, 2008, 343, 2697-2698.	2.3	4
58	A new boronic-acid based strategy to synthesize 4(5)-(het)aryl-1H-imidazoles. Tetrahedron, 2008, 64, 4596-4601.	1.9	21
59	Toward Safer Thrombolytic Agents in Stroke: Molecular Requirements for NMDA Receptor-Mediated Neurotoxicity. Journal of Cerebral Blood Flow and Metabolism, 2008, 28, 1212-1221.	4.3	74
60	Oxygen Pressurized X-Ray Crystallography: Probing the Dioxygen Binding Site in Cofactorless Urate Oxidase and Implications for Its Catalytic Mechanism. Biophysical Journal, 2008, 95, 2415-2422.	0.5	65
61	An Efficient and Straightforward Access to Sulfur Substituted [2.2]Paracyclophanes:â€‰ Application to Stereoselective Sulfenate Salt Alkylation. Organic Letters, 2008, 10, 1271-1274.	4.6	29
62	A straightforward asymmetric synthesis of 1,2-disubstituted ferrocenylalkyl amines with the unusual (SFc,S) configuration. Chemical Communications, 2007, , 4875.	4.1	14
63	trans-(Â±)-2-tert-Butyl-3-phenyloxaziridine:â€‰ A Unique Reagent for the Oxidation of Thiolates into Sulfenates. Journal of Organic Chemistry, 2007, 72, 5403-5406.	3.2	21
64	Definition of New Pharmacophores for Nonpeptide Antagonists of Human Urotensin-II. Comparison with the 3D-structure of Human Urotensin-II and URP. Journal of Chemical Information and Modeling, 2007, 47, 602-612.	5.4	25
65	Protein Crystallography under Xenon and Nitrous Oxide Pressure: Comparison with In Vivo Pharmacology Studies and Implications for the Mechanism of Inhaled Anesthetic Action. Biophysical Journal, 2007, 92, 217-224.	0.5	80
66	New practical access to 2-azatryptophans and dehydro derivatives via the Wittigâ€“Horner reaction. Tetrahedron Letters, 2007, 48, 2457-2460.	1.4	17
67	Quinoline derivatives: potential antiparasitic and antiviral agents. Acta Crystallographica Section C: Crystal Structure Communications, 2007, 63, o643-o645.	0.4	9
68	Diastereoselective Addition of Enantiopure Lithiumtert-Butylsulfinylferrocene to Imines. Journal of Organic Chemistry, 2006, 71, 9572-9579.	3.2	22
69	Synthesis of Novel Pyrazolopyrrolizinones as Prospective Anticancer Agents. Heterocycles, 2006, 68, 2063.	0.7	8
70	Synthesis and biological evaluation as AChE inhibitors of new indanones and thiaindanones related to donepezil. European Journal of Medicinal Chemistry, 2005, 40, 1222-1245.	5.5	36
71	3D-QSAR and Docking Studies of Selective GSK-3Î² Inhibitors. Comparison with a Thieno[2,3-b]pyrrolizinone Derivative, a New Potential Lead for GSK-3Î² Ligands. Journal of Chemical Information and Modeling, 2005, 45, 708-715.	5.4	29
72	The Crystal Structure of Annexin A8 is Similar to that of Annexin A3. Journal of Molecular Biology, 2005, 345, 1131-1139.	4.2	11

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73	Design, Synthesis, and Evaluation of Novel Thienopyrrolizinones as Antitubulin Agents. Journal of Medicinal Chemistry, 2004, 47, 1448-1464.	6.4	79
74	2-(6-Bromopyridin-2-yl)-6-methyl-[1,3,6,2]dioxazaborocane, a new stable (pyridin-2-yl)boronic acid derivative. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o582-o584.	0.4	5
75	1-Chloro-1,3,3,5,5-pentaphenoxycyclotriphosphazene: a precursor of functionalized cyclophosphazene derivatives. Acta Crystallographica Section C: Crystal Structure Communications, 2004, 60, o751-o753.	0.4	3
76	One pot diastereoselective synthesis of new chiral spiroâ€1,3,4â€thiadiazoles and 1,4,2â€oxathiazoles from (1R)â€thiocamphor. Journal of Heterocyclic Chemistry, 2004, 41, 731-735.	2.6	25
77	Synthesis and Biological Evaluation of Thienopyrrolizines, a New Family of CDK/GSK-3 Inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2004, 19, 585-593.	5.2	8
78	Assembly of benzene-1,3,5-tris(methylenephosphonic acid) and guanidinium salt: Single crystal-X-ray characterisation and31P solid state NMR investigations. New Journal of Chemistry, 2004, 28, 1244-1249.	2.8	13
79	Synthesis of novel benzo[h] [1,6]naphthyridines via a rearrangement of hexahydroâ€5Hâ€pyrrolo [2,1 â€c] [1,4]benzodiazepines. Journal of Heterocyclic Chemistry, 2003, 40, 255-259.	2.6	10
80	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. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o111-o113.	0.4	10
81	2-Bromo-6-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pyridine, a new unexpected bifunctional building block for combinatorial chemistry. Acta Crystallographica Section C: Crystal Structure Communications, 2003, 59, o596-o597.	0.4	7
82	Synthesis, Pharmacological Study and Modeling of 7-Methoxyindazole and Related Substituted Indazoles as Neuronal Nitric Oxide Synthase Inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2003, 18, 195-199.	5.2	8
83	7-Methoxy-1H-indazole, a new inhibitor of neuronal nitric oxide synthase. Acta Crystallographica Section C: Crystal Structure Communications, 2002, 58, o688-o690.	0.4	9
84	Annexin A5 D226K structure and dynamics: identification of a molecular switch for the large-scale conformational change of domain III. FEBS Letters, 2001, 493, 122-128.	2.8	14
85	Association of Two 3D QSAR Analyses. Application to the Study of Partial Agonist Serotonin-3 Ligands. Journal of Chemical Information and Computer Sciences, 2001, 41, 815-823.	2.8	17
86	An expedient route to aromatic pyrrolo[2,1-c][1,4]benzodiazepines and a study of their reactivity. Tetrahedron Letters, 2001, 42, 5183-5185.	1.4	8
87	YC-1, an activation inductor of soluble guanylyl cyclase. Acta Crystallographica Section C: Crystal Structure Communications, 2000, 56, 1035-1036.	0.4	3
88	7-Nitro-1H-indazole, an inhibitor of nitric oxide synthase. Acta Crystallographica Section C: Crystal Structure Communications, 2000, 56, 1503-1504.	0.4	6
89	S100 proteinâ€“annexin interactions: a model of the (Anx2-p11)2 heterotetramer complex. Biochimica Et Biophysica Acta - Molecular Cell Research, 2000, 1498, 181-191.	4.1	25
90	Pathway for Large-Scale Conformational Change in Annexin V. Biochemistry, 2000, 39, 14065-14074.	2.5	26