Anil K Saxena

List of Publications by Year
in descending order

96 papers	1,891 citations	236925 25 h-index	315739 38 g-index
100 all docs	100 docs citations	100 times ranked	2522 citing authors

#	Article	IF	Citations
1	Computer-Aided Discovery of Anti-Inflammatory Thiazolidinones with Dual Cyclooxygenase/Lipoxygenase Inhibition. Journal of Medicinal Chemistry, 2008, 51, 1601-1609.	6.4	161
2	Novel Carbamates as Orally Active Acetylcholinesterase Inhibitors Found to Improve Scopolamine-Induced Cognition Impairment: Pharmacophore-Based Virtual Screening, Synthesis, and Pharmacology. Journal of Medicinal Chemistry, 2010, 53, 6490-6505.	6.4	80
3	Fragment-based design, docking, synthesis, biological evaluation and structureâ€“activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors. European Journal of Medicinal Chemistry, 2012, 47, 111-124.	5.5	72
4	Drug/drug interaction of common NSAIDs with antiplatelet effect of aspirin in human platelets. European Journal of Pharmacology, 2013, 721, 215-224.	3.5	69
5	Room Temperature Palladiumâ€Catalyzed Decarboxylative Acyl/Aroylation using [Fe(III)(EDTA)(Î·²â€Ó₂)]^{3â^'} as Oxidant at Biological pH. Advanced Synthesis and Catalysis, 2013, 355, 673-678.	4.3	58
6	Consensus Superiority of the Pharmacophore-Based Alignment, Over Maximum Common Substructure (MCS): 3D-QSAR Studies on Carbamates as Acetylcholinesterase Inhibitors. Journal of Chemical Information and Modeling, 2009, 49, 1590-1601.	5.4	54
7	Synthesis and biological evaluation of substituted 4-arylthiazol-2-amino derivatives as potent growth inhibitors of replicating Mycobacterium tuberculosis H37RV. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5589-5593.	2.2	48
8	An investigation of structurally diverse carbamates for acetylcholinesterase (AChE) inhibition using 3D-QSAR analysis. Journal of Molecular Graphics and Modelling, 2008, 27, 197-208.	2.4	45
9	Novel, potent, orally bioavailable and selective mycobacterial ATP synthase inhibitors that demonstrated activity against both replicating and non-replicating M. tuberculosis. Bioorganic and Medicinal Chemistry, 2015, 23, 742-752.	3.0	45
10	Agents acting on the central nervous system. 15. 2-Substituted 1,2,3,4,6,7,12,12a-octahydropyrazino [2',1':6,1]pyrido[3,4-b]indoles. New class of central nervous system depressants. Journal of Medicinal Chemistry, 1973, 16, 560-564.	6.4	44
11	Pharmacophore modelling, molecular docking and virtual screening for EGFR (HER 1) tyrosine kinase inhibitors. SAR and QSAR in Environmental Research, 2011, 22, 239-263.	2.2	41
12	Computer-Aided Drug Design: Integration of Structure-Based and Ligand-Based Approaches in Drug Design. Current Computer-Aided Drug Design, 2007, 3, 133-148.	1.2	40
13	Identification of novel PTP1B inhibitors by pharmacophore based virtual screening, scaffold hopping and docking. European Journal of Medicinal Chemistry, 2014, 87, 578-594.	5.5	40
14	Metal-Free, Mild, Nonepimerizing, Chemo- and Enantio- or Diastereoselective N-Alkylation of Amines by Alcohols via Oxidation/Imineâ€“Iminium Formation/Reductive Amination: A Pragmatic Synthesis of Octahydropyrazinopyridoindoles and Higher Ring Analogues. Journal of Organic Chemistry, 2013, 78, 11656-11669.	3.2	33
15	Designing, synthesis of selective and high-affinity chalcone-benzothiazole hybrids as Brugia malayi thymidylate kinase inhibitors: InÂvitro validation and docking studies. European Journal of Medicinal Chemistry, 2015, 103, 418-428.	5.5	33
16	Identification and characterisation of small-molecule inhibitors of Rv3097c-encoded lipase (LipY) of Mycobacterium tuberculosis that selectively inhibit growth of bacilli in hypoxia. International Journal of Antimicrobial Agents, 2013, 42, 27-35.	2.5	31
17	Biological evaluation of novel substituted chloroquinolines targeting mycobacterial ATP synthase. International Journal of Antimicrobial Agents, 2013, 41, 41-46.	2.5	31
18	3D QSAR Studies on Protein Tyrosine Phosphatase 1B Inhibitors:â€‰ Comparison of the Quality and Predictivity among 3D QSAR Models Obtained from Different Conformer-Based Alignments. Journal of Chemical Information and Modeling, 2006, 46, 2579-2590.	5.4	30

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19	Lead optimization studies towards the discovery of novel carbamates as potent AChE inhibitors for the potential treatment of Alzheimerâ€™s disease. Bioorganic and Medicinal Chemistry, 2012, 20, 6313-6320.	3.0	30
20	Application of Docking Analysis in the Prediction and Biological Evaluation of the Lipoxygenase Inhibitory Action of Thiazolyl Derivatives of Mycophenolic Acid. Molecules, 2018, 23, 1621.	3.8	30
21	Synthesis of some substituted pyrazinopyridoindoles and 3D QSAR studies along with related compounds: Piperazines, piperidines, pyrazinoisoquinolines, and diphenhydramine, and its semi-rigid analogs as antihistamines (H1). Bioorganic and Medicinal Chemistry, 2006, 14, 8249-8258.	3.0	28
22	Profiling the Structural Determinants for the Selectivity of Representative Factor-Xa and Thrombin Inhibitors Using Combined Ligand-Based and Structure-Based Approaches. Journal of Chemical Information and Modeling, 2011, 51, 1966-1985.	5.4	28
23	Characterization of Î²3-adrenergic receptor: determination of pharmacophore and 3D QSAR model for Î²3 adrenergic receptor agonism. Journal of Computer-Aided Molecular Design, 2005, 19, 93-110.	2.9	27
24	Synthesis, biological evaluation, and quantitative structure-activity relationship analysis of [.beta.-(aroylamino)ethyl]piperazines and -piperidines and [2-[(arylamino)carbonyl]ethyl]piperazines, -piperidines, -pyrazinopyridoindoles, and -pyrazinoisoquinolines. A new class of potent H1 antagonists. Journal of Medicinal Chemistry, 1990, 33, 2970-2976.	6.4	25
25	CoMFA and Docking Studies on Glycogen PhosphorylaseaInhibitors as Antidiabetic Agents#. Journal of Chemical Information and Modeling, 2005, 45, 136-145.	5.4	25
26	Substituted 1,2,3,4-tetrahydroquinolin-6-yloxypropanes as Î²3-adrenergic receptor agonists: Design, synthesis, biological evaluation and pharmacophore modeling. Bioorganic and Medicinal Chemistry, 2009, 17, 830-847.	3.0	25
27	Design, synthesis and biological evaluation of new substituted 5-benzylideno-2-adamantylthiazol[3,2-b][1,2,4]triazol-6(5 H)ones. Pharmacophore models for antifungal activity. Arabian Journal of Chemistry, 2018, 11, 573-590.	4.9	25
28	Synthesis and QSAR Studies in 2-(N-aryl-N-aroyl)amino-4,5-dihydrothiazole Derivatives as Potential Antithrombotic Agents. Bioorganic and Medicinal Chemistry, 2001, 9, 2025-2034.	3.0	24
29	Structural Basis for the Î²-Adrenergic Receptor Subtype Selectivity of the Representative Agonists and Antagonists. Journal of Chemical Information and Modeling, 2011, 51, 1405-1422.	5.4	24
30	Novel Glycoprotein VI Antagonists as Antithrombotics: Synthesis, Biological Evaluation, and Molecular Modeling Studies on 2,3-Disubstituted Tetrahydropyrido(3,4-b)indoles. Journal of Medicinal Chemistry, 2017, 60, 322-337.	6.4	23
31	Pharmacophore Modeling of Substituted 1,2,4-Trioxanes for Quantitative Prediction of their Antimalarial Activity. Journal of Chemical Information and Modeling, 2010, 50, 1510-1520.	5.4	22
32	Pharmacophore-based virtual screening and docking studies on Hsp90 inhibitors. SAR and QSAR in Environmental Research, 2010, 21, 445-462.	2.2	21
33	Identification of Novel 2-((1-(Benzyl(2-hydroxy-2-phenylethyl)amino)-1-oxo-3-phenylpropan-2-yl)carbamoyl)benzoic Acid Analogues as BMP-2 Stimulators. Journal of Medicinal Chemistry, 2012, 55, 8248-8259.	6.4	19
34	Substituted hydrazinecarbothioamide as potent antitubercular agents: Synthesis and quantitative structureâ€“activity relationship (QSAR). Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2597-2600.	2.2	18
35	Novel Glycoconjugate of 8â€Fluoro Norfloxacin Derivatives as Gentamicinâ€resistant Staphylococcus aureus Inhibitors: Synthesis and Molecular Modelling Studies. Chemical Biology and Drug Design, 2015, 86, 440-446.	3.2	18
36	Physicochemical Significance of Topological Parameters: Molecular Connectivity Index and Information Content: Part 2. Correlation Studies With Molar Refractivity and Lipophylicity. QSAR and Combinatorial Science, 1995, 14, 142-148.	1.2	17

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37	Synthesis of protein tyrosine phosphatase 1B inhibitors: Model validation and docking studies. Bioorganic and Medicinal Chemistry Letters, 2009, 19, 2320-2323.	2.2	17
38	Synthesis and anti-tubercular activity of conformationally-constrained and bisquinoline analogs of TMC207. MedChemComm, 2015, 6, 1554-1563.	3.4	17
39	Identification of NovelS-Adenosyl-l-Homocysteine Hydrolase Inhibitors through Homology-Model-Based Virtual Screening, Synthesis, and Biological Evaluation. Journal of Chemical Information and Modeling, 2012, 52, 777-791.	5.4	16
40	Synthesis, Structureâ€“Activity Relationship and Docking Studies of Substituted Aryl Thiazolyl Phenylsulfonamides as Potential Protein Tyrosine Phosphataseâ€…1B Inhibitors. ChemMedChem, 2012, 7, 1185-1190.	3.2	16
41	Identification of Novel Amino Acid Derived CCK-2R Antagonists As Potential Antiulcer Agent: Homology Modeling, Design, Synthesis, and Pharmacology. Journal of Chemical Information and Modeling, 2013, 53, 176-187.	5.4	16
42	Synthesis of primaquine glycoâ€conjugates as potential tissue schizontocidal antimalarial agents. Chemical Biology and Drug Design, 2017, 90, 254-261.	3.2	16
43	Design, synthesis and docking studies on phenoxy-3-piperazin-1-yl-propan-2-ol derivatives as protein tyrosine phosphatase 1B inhibitors. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 5732-5734.	2.2	15
44	Docking studies of novel pyrazinopyridoindoles class of antihistamines with the homology modelled H1-receptor. SAR and QSAR in Environmental Research, 2012, 23, 311-325.	2.2	15
45	An updated patent review on drugs for the treatment of tuberculosis (2018-present). Expert Opinion on Therapeutic Patents, 2022, 32, 243-260.	5.0	15
46	Integration-mediated prediction enrichment of quantitative model for Hsp90 inhibitors as anti-cancer agents: 3D-QSAR study. Molecular Diversity, 2011, 15, 477-489.	3.9	14
47	3D-QSAR CoMFA and CoMSIA studies on a set of diverse Î±1a-adrenergic receptor antagonists. Medicinal Chemistry Research, 2011, 20, 1455-1464.	2.4	14
48	Physicochemical Significance of Topological Parameters, Connectivity Indices and Information Content. Part 1: Correlation Studies in the Sets with Aromatic and Aliphatic Substituents. QSAR and Combinatorial Science, 1995, 14, 31-38.	1.2	13
49	Operative conversions of 3-carboxy-4-quinolones into 3-nitro-4-quinolones via ipso-nitration: potential antifilarial agents as inhibitors of Brugia malayi thymidylate kinase. RSC Advances, 2015, 5, 82208-82214.	3.6	13
50	Design, synthesis and evaluation of benzofuran-acetamide scaffold as potential anticonvulsant agent. Acta Pharmaceutica, 2016, 66, 353-372.	2.0	13
51	Collection and preparation of molecular databases for virtual screening. SAR and QSAR in Environmental Research, 2006, 17, 371-392.	2.2	12
52	Hierarchical virtual screening: identification of potential high-affinity and selective Î²3-adrenergic receptor agonists. SAR and QSAR in Environmental Research, 2012, 23, 389-407.	2.2	12
53	Synthesis and Characterization of Chalconeâ€Pyridinium Hybrids as Potential Antiâ€Cancer and Antiâ€Microbial Agents. ChemistrySelect, 2018, 3, 1424-1431.	1.5	12
54	QSAR studies in substituted 1,2,3,4,6,7,12,12a-octa-hydropyrazino[2â€²,1â€²:6,1]pyrido[3,4-b]indolesâ€”a potent class of neuroleptics. Bioorganic and Medicinal Chemistry, 2003, 11, 2085-2090.	3.0	11

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55	SYNTHESIS, ANOREXIGENIC ACTIVITY AND QSAR OF SUBSTITUTED ARYLOXYPROPANOLAMINES. Medicinal Chemistry Research, 2004, 13, 631-642.	2.4	11
56	Identification and optimization of novel pyrimido-isoxazolidine and oxazine as selective hydride donors. Tetrahedron, 2012, 68, 10122-10129.	1.9	11
57	Molecular modelling and docking studies on heat shock protein 90 (Hsp90) inhibitors. SAR and QSAR in Environmental Research, 2010, 21, 1-20.	2.2	10
58	CoMFA, CoMSIA, and Docking Studies on Thiolactoneâ€Class of Potent Antiâ€malarials: Identification of Essential Structural Features Modulating Antiâ€malarial Activity. Chemical Biology and Drug Design, 2011, 78, 483-493.	3.2	10
59	Pharmacokinetic and metabolism studies of rohitukine in rats by high performance liquid-chromatography with tandem mass spectrometry. FÃ¬toterapÃ¬Ã¢, 2014, 97, 34-42.	2.2	10
60	Enantioselective inhibition of Cytochrome P450-mediated drug metabolism by a novel antithrombotic agent, S002-333: Major effect on CYP2B6. Chemico-Biological Interactions, 2016, 256, 257-265.	4.0	10
61	Advances in chemotherapy of malaria. , 1986, 30, 221-280.		10
62	Pharmacokinetics, dose proportionality and permeability of S002-333 and its enantiomers, a potent antithrombotic agent, in rabbits. Xenobiotica, 2015, 45, 1016-1023.	1.1	9
63	Recent Breakthroughs in Various Antimicrobial Resistance Induced Quorum Sensing Biosynthetic Pathway Mediated Targets and Design of their Inhibitors. Combinatorial Chemistry and High Throughput Screening, 2020, 23, 458-476.	1.1	9
64	Pharmacophore Modeling, Docking and Molecular Dynamics Studies on Caspase-3 Activators Binding at Î²-Tubulin Site. Current Computer-Aided Drug Design, 2015, 11, 72-83.	1.2	9
65	Internet resources in GPCR modelling. SAR and QSAR in Environmental Research, 2008, 19, 11-25.	2.2	8
66	Identification of novel urea derivatives as PTP1B inhibitors: synthesis, biological evaluation and structureâ€“activity relationships. MedChemComm, 2013, 4, 1382.	3.4	8
67	Ligand- and Structure-Based Virtual Screening in Drug Discovery. Topics in Medicinal Chemistry, 2021, , 281-339.	0.8	8
68	(R/S)â€BINOLâ€±â€Phosphoryloxy Enecarbamateâ€Mediated and (R/S)â€Titanium(IV) BINOLatesâ€Catalyzed Enantioselective Intramolecular Heck/Azaâ€Dielsâ€“Alder Cycloaddition (IHADA): An Expedient Methodology. Advanced Synthesis and Catalysis, 2013, 355, 2617-2626.	4.3	7
69	In vitro metabolism of a novel antithrombotic compound, S002-333, and its enantiomers: quantitative cytochrome P450 phenotyping, metabolic profiling and enzyme kinetic studies. Xenobiotica, 2014, 44, 295-308.	1.1	7
70	Pre-clinical investigation of plasma pharmacokinetics and biodistribution of a novel antithrombotic agent S002-333 in mice using LCâ€“MS/MS. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2016, 1031, 154-162.	2.3	7
71	Pharmacological evaluation of the efficacy of Dysoxylum binectariferum stem bark and its active constituent rohitukine in regulation of dyslipidemia in rats. Journal of Natural Medicines, 2018, 72, 837-845.	2.3	7
72	QSAR and molecular docking studies of lethal factor protease inhibitors against Bacillus anthracis. SAR and QSAR in Environmental Research, 2019, 30, 715-731.	2.2	7

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73	Efficiency of Homology Modeling Assisted Molecular Docking in G-protein Coupled Receptors. Current Topics in Medicinal Chemistry, 2021, 21, 269-294.	2.1	7
74	Rational design, synthesis and evaluation of (6aRâˆ—,11bSâˆ—)-1-(4-fluorophenyl)-4-{7-[4-(4-fluorophenyl)-4-oxobutyl]1,2,3,4,6,6a,7,11b,12,12a(RS)-decahydropyrazino[2â€²,1â€²: as a potential neuroleptic agent. Bioorganic and Medicinal Chemistry, 2007, 15, 7361-7367.	3	
75	ATP Synthase Inhibitors as Anti-tubercular Agents: QSAR Studies in Novel Substituted Quinolines. Current Topics in Medicinal Chemistry, 2020, 20, 2723-2734.	2.1	6
76	Syntheses and Biological Activities of 1,4-Disubstituted Piperidines. Archiv Der Pharmazie, 1984, 317, 1010-1017.	4.1	5
77	CoMFA AND CoMSIA STUDIES ON A SET OF BENZYL PIPERAZINES, PIPERADINES, PYRAZINOPYRIDOINDOLES, PYRAZINOISOQUINOLINES AND SEMI RIGID ANALOGS OF DIPHENHYDRAMINE. Medicinal Chemistry Research, 2004, 13, 746-757.	2.4	5
78	QSAR AND MOLECULAR MODELING STUDIES IN IMIDAZOPYRIDINETHIAZOLIDINE-2,4-DIONES: PPARÎ³ AGONISTS. Medicinal Chemistry Research, 2004, 13, 770-780.	2.4	5
79	Synthesis and QSAR studies on hypotensive 1-[3-(4-substituted phenylthio) propyl]-4-(substituted) Tj ETQq1 1 0.784314 rgBT /Overlo	2.2	5
80	Triple-layered QSAR studies on substituted 1,2,4-trioxanes as potential antimalarial agents: superiority of the quantitative pharmacophore-based alignment over common substructure-based alignment. SAR and QSAR in Environmental Research, 2013, 24, 119-134.	2.2	5
81	Metabolic profiling of a novel antithrombotic compound, S002â€333 and enantiomers: metabolic stability, species comparison and in vitroâ€“in vivo extrapolation. Biopharmaceutics and Drug Disposition, 2016, 37, 185-199.	1.9	5
82	Design, Synthesis, and Biological Evaluation of Novel 1,2,4â€Trioxanes as Potential Antimalarial Agents. Archiv Der Pharmazie, 2017, 350, 1600335.	4.1	5
83	Synthesis, <scp>SAR</scp> and docking studies of substituted aryl phenylthiazolyl phenylcarboxamide as potential protein tyrosine phosphatase 1B (<scp>PTP</scp>1B) inhibitors. Chemical Biology and Drug Design, 2019, 94, 1378-1389.	3.2	5
84	Naturally Sourced CDK Inhibitors and Current Trends in Structure-Based Synthetic Anticancer Drug Design by Crystallography. Anti-Cancer Agents in Medicinal Chemistry, 2022, 22, 485-498.	1.7	5
85	Molecular Modelling Based Target Identification for Endo-Peroxides Class of Antimalarials. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 199-207.	1.1	5
86	2D- QSAR studies on new stilbene derivatives of resveratrol as a new selective aryl hydrocarbon receptor. Medicinal Chemistry Research, 2008, 17, 212-218.	2.4	4
87	Synthesis and 2D QSAR of O-sulphonated Î²-aminols derivatives as novel antifungal and antibacterial agents. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 6476-6481.	2.2	4
88	Exploring Targets of Cell Wall Protein Synthesis and Overexpression Mediated Drug Resistance for the Discovery of Potential M. tb Inhibitors. Current Topics in Medicinal Chemistry, 2021, 21, 1922-1942.	2.1	4
89	Molecular docking-based interactions in QSAR studies on Mycobacterium tuberculosis ATP synthase inhibitors. SAR and QSAR in Environmental Research, 2022, 33, 289-305.	2.2	4
90	3D-QSAR STUDIES ON SUBSTITUTED DIHYDROPYRIDINES FOR THEIR Î±1A-ADRENERGIC RECEPTOR BINDING AFFINITY. Medicinal Chemistry Research, 2004, 13, 812-823.	2.4	2

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91	Insight into stereoselective disposition of enantiomers of a potent antithrombotic agent, S002-333 following administration of the racemic compound to mice. European Journal of Pharmaceutical Sciences, 2017, 101, 107-114.	4.0	2
92	Lipid Lowering Oxopropanylindole Hydrazone Derivatives with Antioxidant and Anti-hyperglycemic Activity. Current Topics in Medicinal Chemistry, 2019, 18, 2256-2265.	2.1	2
93	Integration on Ligand and Structure Based Approaches in GPCRs. Topics in Medicinal Chemistry, 2017, , 101-161.	0.8	1
94	A CONVENIENT ROUTE FOR THE SYNTHESIS OF CIS-1-SUBSTITUTED 1,2,3,4,4a,5,11,11a-OCTAHYDRO-6H-PYRIDO[3,2-b]CARBAZOLES AND 4-SUBSTITUTED 1,2,3,4,4a,5,6,11c-OCTAHYDRO-7H-PYRIDO[2,3-c] CARBAZOLES AS POTENT DOPAMINE AGONISTS. Medicinal Chemistry Research, 2004, 13, 758-769.	2.4	0
95	Crystal Structure of Daijisong. Analytical Sciences: X-ray Structure Analysis Online, 2004, 20, X105-X106.	0.1	0
96	Current trends in drug discovery research â€œCTDDR-2010â€• Medicinal Chemistry Research, 2011, 20, 1421-1421.	2.4	0