Neha S Gandhi

List of Publications by Year
in descending order

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66 papers	2,559 citations	279798 23 h-index	206112 48 g-index
73 all docs	73 docs citations	73 times ranked	3965 citing authors

#	Article	IF	Citations
1	The Structure of Glycosaminoglycans and their Interactions with Proteins. Chemical Biology and Drug Design, 2008, 72, 455-482.	3.2	820
2	Heparin Inhibits Cellular Invasion by SARS-CoV-2: Structural Dependence of the Interaction of the Spike S1 Receptor-Binding Domain with Heparin. Thrombosis and Haemostasis, 2020, 120, 1700-1715.	3.4	228
3	Heparin/heparan sulphate-based drugs. Drug Discovery Today, 2010, 15, 1058-1069.	6.4	98
4	Prediction of heparin binding sites in bone morphogenetic proteins (BMPs). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 1374-1381.	2.3	80
5	Metal-doped graphitic carbon nitride (g-C3N4) as selective NO2 sensors: A first-principles study. Applied Surface Science, 2018, 455, 1116-1122.	6.1	71
6	Synthetic Heparan Sulfate Mimetic Pixatimod (PG545) Potently Inhibits SARS-CoV-2 by Disrupting the Spikeâ€“ACE2 Interaction. ACS Central Science, 2022, 8, 527-545.	11.3	62
7	Diaryl Dihydropyrazole-3-carboxamides with Significant In Vivo Antiobesity Activity Related to CB1 Receptor Antagonism:â€‰ Synthesis, Biological Evaluation, and Molecular Modeling in the Homology Model. Journal of Medicinal Chemistry, 2007, 50, 5951-5966.	6.4	58
8	Free energy calculations of glycosaminoglycanâ€“protein interactions. Glycobiology, 2009, 19, 1103-1115.	2.5	56
9	Heparanase: A Challenging Cancer Drug Target. Frontiers in Oncology, 2019, 9, 1316.	2.8	53
10	Assessing Molecular Docking Tools to Guide Targeted Drug Discovery of CD38 Inhibitors. International Journal of Molecular Sciences, 2020, 21, 5183.	4.1	47
11	A Comparative Structural Bioinformatics Analysis of the Insulin Receptor Family Ectodomain Based on Phylogenetic Information. PLoS ONE, 2008, 3, e3667.	2.5	45
12	Computational analyses of the catalytic and heparin-binding sites and their interactions with glycosaminoglycans in glycoside hydrolase family 79 endo-Î²-d-glucuronidase (heparanase). Glycobiology, 2012, 22, 35-55.	2.5	44
13	A Phosphorylationâ€Induced Turn Defines the Alzheimerâ€™s Disease AT8 Antibody Epitope on the Tau Protein. Angewandte Chemie - International Edition, 2015, 54, 6819-6823.	13.8	41
14	Barrier-to-autointegration factor 1 (Banf1) regulates poly [ADP-ribose] polymerase 1 (PARP1) activity following oxidative DNA damage. Nature Communications, 2019, 10, 5501.	12.8	40
15	Platelet Endothelial Cell Adhesion Molecule 1 (PECAM-1) and Its Interactions with Glycosaminoglycans: 1. Molecular Modeling Studies. Biochemistry, 2008, 47, 4851-4862.	2.5	37
16	Understanding Insulin Endocrinology in Decapod Crustacea: Molecular Modelling Characterization of an Insulin-Binding Protein and Insulin-Like Peptides in the Eastern Spiny Lobster, Sagmariasus verreauxi. International Journal of Molecular Sciences, 2017, 18, 1832.	4.1	37
17	Can current force fields reproduce ring puckering in 2-O-sulfo-Î±-l-iduronic acid? A molecular dynamics simulation study. Carbohydrate Research, 2010, 345, 689-695.	2.3	33
18	Evidence of a putative glycosaminoglycan binding site on the glycosylated SARS-CoV-2 spike protein N-terminal domain. Computational and Structural Biotechnology Journal, 2021, 19, 2806-2818.	4.1	33

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19	Molecular Dynamics Simulations of CXCL-8 and Its Interactions with a Receptor Peptide, Heparin Fragments, and Sulfated Linked Cyclitols. Journal of Chemical Information and Modeling, 2011, 51, 335-358.	5.4	32
20	Molecular dynamics simulation of the phosphorylation-induced conformational changes of a tau peptide fragment. Proteins: Structure, Function and Bioinformatics, 2014, 82, 1907-1923.	2.6	31
21	Phosphorylation and O-GlcNAcylation of the PHF-1 Epitope of Tau Protein Induce Local Conformational Changes of the C-Terminus and Modulate Tau Self-Assembly Into Fibrillar Aggregates. Frontiers in Molecular Neuroscience, 2021, 14, 661368.	2.9	30
22	Platelet Endothelial Cell Adhesion Molecule 1 (PECAM-1) and Its Interactions with Glycosaminoglycans: 2. Biochemical Analyses. Biochemistry, 2008, 47, 4863-4875.	2.5	29
23	3D QSAR studies of N-4-arylacryloylpiperazin-1-yl-phenyl-oxazolidinones: A novel class of antibacterial agents. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 3817-3823.	2.2	27
24	Dual targeting of dengue virus virions and NS1 protein with the heparan sulfate mimic PG545. Antiviral Research, 2019, 168, 121-127.	4.1	27
25	NMR Meets Tau: Insights into Its Function and Pathology. Biomolecules, 2016, 6, 28.	4.0	25
26	Development and application of site mapping methods for the design of glycosaminoglycans. Glycobiology, 2014, 24, 840-851.	2.5	24
27	Interaction of gold nanosurfaces/nanoparticles with collagen-like peptides. Physical Chemistry Chemical Physics, 2019, 21, 3701-3711.	2.8	24
28	From Cancer to COVIDâ€19: A Perspective on Targeting Heparan Sulfateâ€Protein Interactions. Chemical Record, 2021, 21, 3087-3101.	5.8	24
29	Novel analogs of sulfasalazine as system x_c^{â^’} antiporter inhibitors: Insights from the molecular modeling studies. Drug Development Research, 2019, 80, 758-777.	2.9	23
30	GlycoTorch Vina: Docking Designed and Tested for Glycosaminoglycans. Journal of Chemical Information and Modeling, 2020, 60, 6328-6343.	5.4	21
31	Heterogeneous nanomechanical properties of type I collagen in longitudinal direction. Biomechanics and Modeling in Mechanobiology, 2017, 16, 1023-1033.	2.8	20
32	Steered molecular dynamics characterization of the elastic modulus and deformation mechanisms of single natural tropocollagen molecules. Journal of the Mechanical Behavior of Biomedical Materials, 2018, 86, 359-367.	3.1	20
33	Adsorption of Collagen-like Peptides onto Gold Nanosurfaces. Langmuir, 2019, 35, 4435-4444.	3.5	20
34	Oxazolidine-2-thiones: a molecular modeling study. Tetrahedron Letters, 2004, 45, 6269-6272.	1.4	19
35	Molecular modeling of Bt Cry1Ac (DIâ€“DII)â€“ASAL (Allium sativum lectin)â€“fusion protein and its interaction with aminopeptidase N (APN) receptor of Manduca sexta. Journal of Molecular Graphics and Modelling, 2012, 33, 61-76.	2.4	19
36	Adsorption and Unfolding of Lysozyme at a Polarized Aqueousâ€“Organic Liquid Interface. Journal of Physical Chemistry B, 2016, 120, 3100-3112.	2.6	16

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37	Molecular insights on the interference of simplified lung surfactant models by gold nanoparticle pollutants. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1458-1467.	2.6	16
38	Calculations of the Free Energy of Interaction of the c-Fosâ^'c-Jun Coiled Coil: Effects of the Solvation Model and the Inclusion of Polarization Effects. Journal of Chemical Information and Modeling, 2010, 50, 2201-2212.	5.4	15
39	Chitosan/graphene complex membrane for polymer electrolyte membrane fuel cell: A molecular dynamics simulation study. International Journal of Hydrogen Energy, 2020, 45, 25960-25969.	7.1	15
40	Analysis of crystallization phenomenon in Indian honey using molecular dynamics simulations and artificial neural network. Food Chemistry, 2019, 300, 125182.	8.2	13
41	Elevating CDCA3 levels in non-small cell lung cancer enhances sensitivity to platinum-based chemotherapy. Communications Biology, 2021, 4, 638.	4.4	12
42	Structural Insights into Pixatimod (PG545) Inhibition of Heparanase, a Key Enzyme in Cancer and Viral Infections. Chemistry - A European Journal, 2022, 28, .	3.3	11
43	Free energy calculations of the interactions of câ€Junâ€based synthetic peptides with the câ€Fos protein. Biopolymers, 2012, 97, 899-909.	2.4	10
44	Cyclophilin A allows the allosteric regulation of a structural motif in the disordered domain 2 of NS5A and thereby fine-tunes HCV RNA replication. Journal of Biological Chemistry, 2019, 294, 13171-13185.	3.4	10
45	Effect of hydroxylysine-O-glycosylation on the structure of type I collagen molecule: A computational study. Glycobiology, 2020, 30, 830-843.	2.5	10
46	Cross-Species Analysis of Glycosaminoglycan Binding Proteins Reveals Some Animal Models Are â€œMore Equalâ€•than Others. Molecules, 2019, 24, 924.	3.8	9
47	The role of SP-B‹sub›1â€“25‹/sub› peptides in lung surfactant monolayers exposed to gold nanoparticles. Physical Chemistry Chemical Physics, 2020, 22, 15231-15241.	2.8	9
48	Atomistic molecular dynamics simulations of bioactive engrailed 1 interference peptides (EN1-iPeps). Oncotarget, 2018, 9, 22383-22397.	1.8	9
49	Facile synthesis, ex-vivo and in vitro screening of 3-sulfonamide derivative of 5-(4-chlorophenyl)-1-(2,4-dichlorophenyl)-4-methyl-1H-pyrazole-3-carboxylic acid piperidin-1-ylamide (SR141716) a potent CB1 receptor antagonist. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3882-3886.	2.2	8
50	Computational Modelling of the Interaction of Gold Nanoparticle with Lung Surfactant Monolayer. MRS Advances, 2019, 4, 1177-1185.	0.9	8
51	COMMD4 functions with the histone H2A-H2B dimer for the timely repair of DNA double-strand breaks. Communications Biology, 2021, 4, 484.	4.4	8
52	The Impact of Rare Human Variants on Barrier-To-Auto-Integration Factor 1 (Banf1) Structure and Function. Frontiers in Cell and Developmental Biology, 2021, 9, 775441.	3.7	8
53	Design and synthesis of novel 3-hydroxy-cyclobut-3-ene-1,2-dione derivatives as thyroid hormone receptor Î² (TR-Î²) selective ligands. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 3919-3924.	2.2	7
54	Computational Studies of Lipid-Wrapped Gold Nanoparticle Transport Through Model Lung Surfactant Monolayers. Journal of Physical Chemistry B, 2021, 125, 1392-1401.	2.6	7

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55	Molecular Dynamics Simulation of Tau Peptides for the Investigation of Conformational Changes Induced by Specific Phosphorylation Patterns. Methods in Molecular Biology, 2017, 1523, 33-59.	0.9	6
56	Identification of Proteins Deregulated by Platinum-Based Chemotherapy as Novel Biomarkers and Therapeutic Targets in Non-Small Cell Lung Cancer. Frontiers in Oncology, 2021, 11, 615967.	2.8	6
57	Structure and intermolecular interactions in spheroidal high-density lipoprotein subpopulations. Journal of Structural Biology: X, 2021, 5, 100042.	1.3	5
58	Identifying Complex lncRNA/Pseudogeneâ€“miRNAâ€“mRNA Crosstalk in Hormone-Dependent Cancers. Biology, 2021, 10, 1014.	2.8	5
59	Characterization of sequence and structural features of the Candida krusei enolase. In Silico Biology, 2008, 8, 449-60.	0.9	5
60	Computational insights into the active structure of SGK1 and its implication for ligand design. Biochimie, 2019, 165, 57-66.	2.6	4
61	Design and Characterization of a Cell-Penetrating Peptide Derived from the SOX2 Transcription Factor. International Journal of Molecular Sciences, 2021, 22, 9354.	4.1	4
62	Computational Methods for the Prediction of the Structure and Interactions of Coiled-Coil Peptides. Current Bioinformatics, 2008, 3, 149-161.	1.5	3
63	Integrative Transcriptome-Wide Analyses Uncover Novel Risk-Associated MicroRNAs in Hormone-Dependent Cancers. Frontiers in Genetics, 2021, 12, 716236.	2.3	3
64	A supervised machine learning approach identifies geneâ€regulating factorâ€mediated competing endogenous RNA networks in hormoneâ€dependent cancers. Journal of Cellular Biochemistry, 0, , .	2.6	3
65	Molecular basis of transport of surface functionalised gold nanoparticles to pulmonary surfactant. RSC Advances, 2022, 12, 18012-18021.	3.6	1
66	Developing Drugs from Sugars. , 2012, , 259-296.		0