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	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
2	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
3	Molecular basis of transport of surface functionalised gold nanoparticles to pulmonary surfactant. RSC Advances, 2022, 12, 18012-18021.	3.6	1
4	Structure and intermolecular interactions in spheroidal high-density lipoprotein subpopulations. Journal of Structural Biology: X, 2021, 5, 100042.	1.3	5
5	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
6	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
7	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
8	Elevating CDCA3 levels in non-small cell lung cancer enhances sensitivity to platinum-based chemotherapy. Communications Biology, 2021, 4, 638.	4.4	12
9	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
10	From Cancer to COVIDâ€19: A Perspective on Targeting Heparan Sulfateâ€Protein Interactions. Chemical Record, 2021, 21, 3087-3101.	5.8	24
11	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
12	Integrative Transcriptome-Wide Analyses Uncover Novel Risk-Associated MicroRNAs in Hormone-Dependent Cancers. Frontiers in Genetics, 2021, 12, 716236.	2.3	3
13	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
14	Identifying Complex lncRNA/Pseudogeneâ€“miRNAâ€“mRNA Crosstalk in Hormone-Dependent Cancers. Biology, 2021, 10, 1014.	2.8	5
15	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
16	Assessing Molecular Docking Tools to Guide Targeted Drug Discovery of CD38 Inhibitors. International Journal of Molecular Sciences, 2020, 21, 5183.	4.1	47
17	GlycoTorch Vina: Docking Designed and Tested for Glycosaminoglycans. Journal of Chemical Information and Modeling, 2020, 60, 6328-6343.	5.4	21
18	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

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19	Effect of hydroxylysine-O-glycosylation on the structure of type I collagen molecule: A computational study. Glycobiology, 2020, 30, 830-843.	2.5	10
20	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
21	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
22	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
23	Computational insights into the active structure of SGK1 and its implication for ligand design. Biochimie, 2019, 165, 57-66.	2.6	4
24	Analysis of crystallization phenomenon in Indian honey using molecular dynamics simulations and artificial neural network. Food Chemistry, 2019, 300, 125182.	8.2	13
25	Computational Modelling of the Interaction of Gold Nanoparticle with Lung Surfactant Monolayer. MRS Advances, 2019, 4, 1177-1185.	0.9	8
26	Interaction of gold nanosurfaces/nanoparticles with collagen-like peptides. Physical Chemistry Chemical Physics, 2019, 21, 3701-3711.	2.8	24
27	Dual targeting of dengue virus virions and NS1 protein with the heparan sulfate mimic PG545. Antiviral Research, 2019, 168, 121-127.	4.1	27
28	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
29	Novel analogs of sulfasalazine as system x‹sub›c‹/sub›‹sup›â^'‹/sup› antiporter inhibitors: Insights from the molecular modeling studies. Drug Development Research, 2019, 80, 758-777.	2.9	23
30	Adsorption of Collagen-like Peptides onto Gold Nanosurfaces. Langmuir, 2019, 35, 4435-4444.	3.5	20
31	Cross-Species Analysis of Glycosaminoglycan Binding Proteins Reveals Some Animal Models Are â€œMore Equalâ€•than Others. Molecules, 2019, 24, 924.	3.8	9
32	Heparanase: A Challenging Cancer Drug Target. Frontiers in Oncology, 2019, 9, 1316.	2.8	53
33	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
34	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
35	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
36	Atomistic molecular dynamics simulations of bioactive engrailed 1 interference peptides (EN1-iPeps). Oncotarget, 2018, 9, 22383-22397.	1.8	9

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37	Heterogeneous nanomechanical properties of type I collagen in longitudinal direction. Biomechanics and Modeling in Mechanobiology, 2017, 16, 1023-1033.	2.8	20
38	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
39	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
40	NMR Meets Tau: Insights into Its Function and Pathology. Biomolecules, 2016, 6, 28.	4.0	25
41	Adsorption and Unfolding of Lysozyme at a Polarized Aqueousâ€“Organic Liquid Interface. Journal of Physical Chemistry B, 2016, 120, 3100-3112.	2.6	16
42	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
43	Development and application of site mapping methods for the design of glycosaminoglycans. Glycobiology, 2014, 24, 840-851.	2.5	24
44	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
45	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
46	Prediction of heparin binding sites in bone morphogenetic proteins (BMPs). Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 1374-1381.	2.3	80
47	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
48	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
49	Developing Drugs from Sugars. , 2012, , 259-296.		0
50	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
51	Heparin/heparan sulphate-based drugs. Drug Discovery Today, 2010, 15, 1058-1069.	6.4	98
52	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
53	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
54	Free energy calculations of glycosaminoglycanâ€“protein interactions. Glycobiology, 2009, 19, 1103-1115.	2.5	56

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55	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
56	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
57	The Structure of Glycosaminoglycans and their Interactions with Proteins. Chemical Biology and Drug Design, 2008, 72, 455-482.	3.2	820
58	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
59	Platelet Endothelial Cell Adhesion Molecule 1 (PECAM-1) and Its Interactions with Glycosaminoglycans: 2. Biochemical Analyses. Biochemistry, 2008, 47, 4863-4875.	2.5	29
60	Computational Methods for the Prediction of the Structure and Interactions of Coiled-Coil Peptides. Current Bioinformatics, 2008, 3, 149-161.	1.5	3
61	A Comparative Structural Bioinformatics Analysis of the Insulin Receptor Family Ectodomain Based on Phylogenetic Information. PLoS ONE, 2008, 3, e3667.	2.5	45
62	Characterization of sequence and structural features of the Candida krusei enolase. In Silico Biology, 2008, 8, 449-60.	0.9	5
63	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
64	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
65	Oxazolidine-2-thiones: a molecular modeling study. Tetrahedron Letters, 2004, 45, 6269-6272.	1.4	19
66	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