Rakesh Gupta

List of Publications by Year in Descending Order

30 papers	642 citations	14 h-index	25 g-index
36 ext. papers	808 ext. citations	4 avg, IF	5 L-index

#	Paper	IF	Citations
30	Coronavirus: a comparative analysis of detection technologies in the wake of emerging variants.. *Infection*, **2022**, 1	5.8	3
29	In-silico screening of database for finding potential sweet molecules: A combined data and structure based modeling approach. *Food Chemistry*, **2021**, 343, 128538	8.5	6
28	design of peptides with binding to the receptor binding domain (RBD) of the SARS-CoV-2 and their utility in bio-sensor development for SARS-CoV-2 detection.. *RSC Advances*, **2021**, 11, 3816-3826	3.7	8
27	Integrated Generate, Make, and Test for Formulated Products using Knowledge Graphs. *Data Intelligence*, **2021**, 3, 340-375	3	1
26	Multiscale Modeling of Skin Electroporation. *Langmuir*, **2020**, 36, 6651-6660	4	1
25	Molecular mechanism of the skin permeation enhancing effect of ethanol: a molecular dynamics study.. *RSC Advances*, **2020**, 10, 12234-12248	3.7	13
24	Development and application of coarse-grained MARTINI model of skin lipid ceramide [AP]. *Journal of Molecular Modeling*, **2020**, 26, 182	2	1
23	Permeation of nanoparticles across the intestinal lipid membrane: dependence on shape and surface chemistry studied through molecular simulations. *Nanoscale*, **2020**, 12, 6318-6333	7.7	25
22	Interfacial structure in the liquid-liquid extraction of rare earth elements by phosphoric acid ligands: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2020**, 22, 4177-4192	3.6	5
21	Generate and Test for Formulated Product Variants With Information Extraction and an In-Silico Model. *Advances in E-Business Research Series*, **2020**, 223-250	0.4	2
20	Applied machine learning for predicting the lanthanide-ligand binding affinities. *Scientific Reports*, **2020**, 10, 14322	4.9	5
19	Computer-Aided Design of Nanoparticles for Transdermal Drug Delivery. *Methods in Molecular Biology*, **2020**, 2059, 225-237	1.4	2
18	Materials Design in Digital Era: Challenges and Opportunities. *Transactions of the Indian Institute of Metals*, **2019**, 72, 2199-2208	1.2	0
17	Structural and barrier properties of the skin ceramide lipid bilayer: a molecular dynamics simulation study. *Journal of Molecular Modeling*, **2019**, 25, 140	2	7
16	Effect of Chemical Permeation Enhancers on Skin Permeability: In silico screening using Molecular Dynamics simulations. *Scientific Reports*, **2019**, 9, 1456	4.9	51
15	In-silico prediction of sweetness using structure-activity relationship models. *Food Chemistry*, **2018**, 253, 127-131	8.5	17
14	In-silico design of nanoparticles for transdermal drug delivery application. *Nanoscale*, **2018**, 10, 4940-4951	7.7	31

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13	Electroporation of Skin Stratum Corneum Lipid Bilayer and Molecular Mechanism of Drug Transport: A Molecular Dynamics Study. *Langmuir*, **2018**, 34, 5860-5870	4	19
12	Molecular mechanism of transdermal co-delivery of interferon-alpha protein with gold nanoparticle a molecular dynamics study. *Molecular Simulation*, **2018**, 44, 274-284	2	8
11	Differential Stabilization of the Metal Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. *Industrial & Engineering Chemistry Research*, **2018**, 57, 17209-17217	3.9	4
10	Effect of surface coverage and chemistry on self-assembly of monolayer protected gold nanoparticles: a molecular dynamics simulation study. *Physical Chemistry Chemical Physics*, **2018**, 20, 25883-25891	3.6	19
9	Impact of the ceramide subspecies on the nanostructure of stratum corneum lipids using neutron scattering and molecular dynamics simulations. Part I: impact of CER[NS]. *Chemistry and Physics of Lipids*, **2018**, 214, 58-68	3.7	14
8	Molecular dynamics simulation study of translocation of fullerene C through skin bilayer: effect of concentration on barrier properties. *Nanoscale*, **2017**, 9, 4114-4127	7.7	39
7	Transdermal cellular membrane penetration of proteins with gold nanoparticles: a molecular dynamics study. *Physical Chemistry Chemical Physics*, **2017**, 19, 7537-7545	3.6	33
6	Effect of Size and Surface Charge of Gold Nanoparticles on their Skin Permeability: A Molecular Dynamics Study. *Scientific Reports*, **2017**, 7, 45292	4.9	105
5	In-Silico Skin Model: A Multiscale Simulation Study of Drug Transport. *Journal of Chemical Information and Modeling*, **2017**, 57, 2027-2034	6.1	22
4	Molecular Dynamics Simulation Study of Permeation of Molecules through Skin Lipid Bilayer. *Journal of Physical Chemistry B*, **2016**, 120, 8987-96	3.4	64
3	Molecular Dynamics Simulation of Skin Lipids: Effect of Ceramide Chain Lengths on Bilayer Properties. *Journal of Physical Chemistry B*, **2016**, 120, 12536-12546	3.4	37
2	Penetration of Gold Nanoparticles through Human Skin: Unraveling Its Mechanisms at the Molecular Scale. *Journal of Physical Chemistry B*, **2016**, 120, 7133-42	3.4	50
1	Molecular Dynamics Simulation Study of Skin Lipids: Effects of the Molar Ratio of Individual Components over a Wide Temperature Range. *Journal of Physical Chemistry B*, **2015**, 119, 11643-55	3.4	49