

Rakesh Gupta

List of Publications by Citations

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

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	Effect of Size and Surface Charge of Gold Nanoparticles on their Skin Permeability: A Molecular Dynamics Study. <i>Scientific Reports</i> , 2017 , 7, 45292	4.9	105
29	Molecular Dynamics Simulation Study of Permeation of Molecules through Skin Lipid Bilayer. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 8987-96	3.4	64
28	Effect of Chemical Permeation Enhancers on Skin Permeability: In silico screening using Molecular Dynamics simulations. <i>Scientific Reports</i> , 2019 , 9, 1456	4.9	51
27	Penetration of Gold Nanoparticles through Human Skin: Unraveling Its Mechanisms at the Molecular Scale. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 7133-42	3.4	50
26	Molecular Dynamics Simulation Study of Skin Lipids: Effects of the Molar Ratio of Individual Components over a Wide Temperature Range. <i>Journal of Physical Chemistry B</i> , 2015 , 119, 11643-55	3.4	49
25	Molecular dynamics simulation study of translocation of fullerene C through skin bilayer: effect of concentration on barrier properties. <i>Nanoscale</i> , 2017 , 9, 4114-4127	7.7	39
24	Molecular Dynamics Simulation of Skin Lipids: Effect of Ceramide Chain Lengths on Bilayer Properties. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 12536-12546	3.4	37
23	Transdermal cellular membrane penetration of proteins with gold nanoparticles: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 7537-7545	3.6	33
22	In-silico design of nanoparticles for transdermal drug delivery application. <i>Nanoscale</i> , 2018 , 10, 4940-4951	7.7	31
21	Permeation of nanoparticles across the intestinal lipid membrane: dependence on shape and surface chemistry studied through molecular simulations. <i>Nanoscale</i> , 2020 , 12, 6318-6333	7.7	25
20	In-Silico Skin Model: A Multiscale Simulation Study of Drug Transport. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 2027-2034	6.1	22
19	Electroporation of Skin Stratum Corneum Lipid Bilayer and Molecular Mechanism of Drug Transport: A Molecular Dynamics Study. <i>Langmuir</i> , 2018 , 34, 5860-5870	4	19
18	Effect of surface coverage and chemistry on self-assembly of monolayer protected gold nanoparticles: a molecular dynamics simulation study. <i>Physical Chemistry Chemical Physics</i> , 2018 , 20, 25883-25891	3.6	19
17	In-silico prediction of sweetness using structure-activity relationship models. <i>Food Chemistry</i> , 2018 , 253, 127-131	8.5	17
16	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]. <i>Chemistry and Physics of Lipids</i> , 2018 , 214, 58-68	3.7	14
15	Molecular mechanism of the skin permeation enhancing effect of ethanol: a molecular dynamics study.. <i>RSC Advances</i> , 2020 , 10, 12234-12248	3.7	13
14	Molecular mechanism of transdermal co-delivery of interferon-alpha protein with gold nanoparticle via molecular dynamics study. <i>Molecular Simulation</i> , 2018 , 44, 274-284	2	8

13	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.. <i>RSC Advances</i> , 2021 , 11, 3816-3826	3.7	8
12	Structural and barrier properties of the skin ceramide lipid bilayer: a molecular dynamics simulation study. <i>Journal of Molecular Modeling</i> , 2019 , 25, 140	2	7
11	In-silico screening of database for finding potential sweet molecules: A combined data and structure based modeling approach. <i>Food Chemistry</i> , 2021 , 343, 128538	8.5	6
10	Interfacial structure in the liquid-liquid extraction of rare earth elements by phosphoric acid ligands: a molecular dynamics study. <i>Physical Chemistry Chemical Physics</i> , 2020 , 22, 4177-4192	3.6	5
9	Applied machine learning for predicting the lanthanide-ligand binding affinities. <i>Scientific Reports</i> , 2020 , 10, 14322	4.9	5
8	Differential Stabilization of the Metal-Ligand Complexes between Organic and Aqueous Phases Drives the Selectivity of Phosphoric Acid Ligands toward Heavier Rare Earth Elements. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 17209-17217	3.9	4
7	Coronavirus: a comparative analysis of detection technologies in the wake of emerging variants.. <i>Infection</i> , 2022 , 1	5.8	3
6	Generate and Test for Formulated Product Variants With Information Extraction and an In-Silico Model. <i>Advances in E-Business Research Series</i> , 2020 , 223-250	0.4	2
5	Computer-Aided Design of Nanoparticles for Transdermal Drug Delivery. <i>Methods in Molecular Biology</i> , 2020 , 2059, 225-237	1.4	2
4	Multiscale Modeling of Skin Electroporation. <i>Langmuir</i> , 2020 , 36, 6651-6660	4	1
3	Development and application of coarse-grained MARTINI model of skin lipid ceramide [AP]. <i>Journal of Molecular Modeling</i> , 2020 , 26, 182	2	1
2	Integrated Generate, Make, and Test for Formulated Products using Knowledge Graphs. <i>Data Intelligence</i> , 2021 , 3, 340-375	3	1
1	Materials Design in Digital Era: Challenges and Opportunities. <i>Transactions of the Indian Institute of Metals</i> , 2019 , 72, 2199-2208	1.2	0