Andrea Danani

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Solution of the tunneling-percolation problem in the nanocomposite regime. Physical Review B, 2010, 81, .	3.2	203
2	Modeling the Multivalent Recognition between Dendritic Molecules and DNA: Understanding How Ligand "Sacrifice―and Screening Can Enhance Binding. Journal of the American Chemical Society, 2009, 131, 9686-9694.	13.7	118
3	Lattice-Gas Theory of Collective Diffusion in Adsorbed Layers. International Journal of Modern Physics B, 1997, 11, 2217-2279.	2.0	101
4	Ability to Adapt: Different Generations of PAMAM Dendrimers Show Different Behaviors in Binding siRNA. Journal of Physical Chemistry B, 2010, 114, 2667-2675.	2.6	101
5	PAMAM Dendrimers for siRNA Delivery: Computational and Experimental Insights. Chemistry - A European Journal, 2010, 16, 7781-7795.	3.3	91
6	Validation of a Novel Molecular Dynamics Simulation Approach for Lipophilic Drug Incorporation into Polymer Micelles. Journal of Physical Chemistry B, 2012, 116, 4338-4345.	2.6	84
7	Targeting the Blind Spot of Polycationic Nanocarrier-Based siRNA Delivery. ACS Nano, 2012, 6, 9447-9454.	14.6	83
8	Elucidating the molecular mechanism of PAMAM–siRNA dendriplex self-assembly: Effect of dendrimer charge density. International Journal of Pharmaceutics, 2011, 416, 410-418.	5.2	77
9	Computational Insights into the Interactions between DNA and siRNA with "Rigid―and "Flexible― Triazine Dendrimers. Biomacromolecules, 2010, 11, 721-730.	5.4	76
10	Quantifying the Effect of Surface Ligands on Dendron–DNA Interactions: Insights into Multivalency through a Combined Experimental and Theoretical Approach. Chemistry - A European Journal, 2010, 16, 4519-4532.	3.3	63
11	Percolative properties of hard oblate ellipsoids of revolution with a soft shell. Physical Review E, 2008, 78, 061126.	2.1	60
12	Catalytic Chameleon Dendrimers. Journal of the American Chemical Society, 2011, 133, 14359-14367.	13.7	52
13	Ion-Selective Controlled Assembly of Dendrimer-Based Functional Nanofibers and Their Ionic-Competitive Disassembly. Journal of the American Chemical Society, 2012, 134, 3349-3357.	13.7	50
14	To the nanoscale, and beyond!. Fluid Phase Equilibria, 2007, 261, 366-374.	2.5	48
15	Molecular modeling and in vivo imaging can identify successful flexible triazine dendrimer-based siRNA delivery systems. Journal of Controlled Release, 2011, 153, 23-33.	9.9	47
16	The Extent of Human Apolipoprotein A-I Lipidation Strongly Affects the β-Amyloid Efflux Across the Blood-Brain Barrier in vitro. Frontiers in Neuroscience, 2019, 13, 419.	2.8	42
17	Cell penetrating peptide modulation of membrane biomechanics by Molecular dynamics. Journal of Biomechanics, 2018, 73, 137-144.	2.1	40
18	Computational Approach for Understanding the Interactions of UV-Degradable Dendrons with DNA and siRNA. Journal of Physical Chemistry B, 2010, 114, 5686-5693.	2.6	38

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19	Generation-Dependent Molecular Recognition Controls Self-Assembly in Supramolecular Dendronâ~`Virus Complexes. Nano Letters, 2011, 11, 723-728.	9.1	36
20	Cell Penetrating Peptide Adsorption on Magnetite and Silica Surfaces: A Computational Investigation. Journal of Physical Chemistry B, 2015, 119, 8239-8246.	2.6	33
21	Electron tunneling in conductor-insulator composites with spherical fillers. Journal of Applied Physics, 2009, 106, .	2.5	31
22	Genetic, cellular, and structural characterization of the membrane potential-dependent cell-penetrating peptide translocation pore. ELife, 2021, 10, .	6.0	31
23	Conformational fluctuations of the AXH monomer of Ataxin-1. Proteins: Structure, Function and Bioinformatics, 2016, 84, 52-59.	2.6	30
24	Conformational Dynamics and Stability of U-Shaped and S-Shaped Amyloid β Assemblies. International Journal of Molecular Sciences, 2018, 19, 571.	4.1	30
25	Collective surface diffusion on triangular and square interacting lattice gases. Surface Science, 1998, 409, 117-129.	1.9	29
26	Investigation of the Josephin Domain Protein-Protein Interaction by Molecular Dynamics. PLoS ONE, 2014, 9, e108677.	2.5	28
27	Structure Based Modeling of Small Molecules Binding to the TLR7 by Atomistic Level Simulations. Molecules, 2015, 20, 8316-8340.	3.8	27
28	Multivalent interacting glycodendrimer to prevent amyloid-peptide fibril formation induced by Cu(II): A multidisciplinary approach. Nano Research, 2018, 11, 1204-1226.	10.4	27
29	Energetics of fcc and decahedral nanowires of Ag, Cu, Ni, andC60:A quenched molecular dynamics study. Physical Review B, 2004, 69, .	3.2	26
30	Free energy landscape of siRNA-polycation complexation: Elucidating the effect of molecular geometry, polymer flexibility, and charge neutralization. PLoS ONE, 2017, 12, e0186816.	2.5	25
31	Role of Generation, Architecture, pH and Ionic Strength on Successful siRNA Delivery and Transfection by Hybrid PPV-PAMAM Dendrimers. Current Medicinal Chemistry, 2012, 19, 4929-4941.	2.4	24
32	Josephin Domain Structural Conformations Explored by Metadynamics in Essential Coordinates. PLoS Computational Biology, 2016, 12, e1004699.	3.2	22
33	TAT-RasGAP ₃₁₇₋₃₂₆ kills cells by targeting inner-leaflet–enriched phospholipids. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 31871-31881.	7.1	22
34	The influence of dendron's architecture on the "rigid―and "flexible―behaviour in binding DNA—a modelling study. Physical Chemistry Chemical Physics, 2010, 12, 13914.	2.8	21
35	Characterization of the <scp>AXH</scp> domain of Ataxinâ€1 using enhanced sampling and functional mode analysis. Proteins: Structure, Function and Bioinformatics, 2016, 84, 666-673.	2.6	21
36	The Role of Structural Polymorphism in Driving the Mechanical Performance of the Alzheimer's Beta Amyloid Fibrils. Frontiers in Bioengineering and Biotechnology, 2019, 7, 83.	4.1	21

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37	Elucidating the role of surface chemistry on cationic phosphorus dendrimer–siRNA complexation. Nanoscale, 2018, 10, 10952-10962.	5.6	20
38	The synergistic effect of chlorotoxin-mApoE in boosting drug-loaded liposomes across the BBB. Journal of Nanobiotechnology, 2019, 17, 115.	9.1	20
39	Steroid identification via deep learning retention time predictions and two-dimensional gas chromatography-high resolution mass spectrometry. Journal of Chromatography A, 2020, 1612, 460661.	3.7	19
40	Iron oxide/PAMAM nanostructured hybrids: combined computational and experimental studies. Journal of Materials Science, 2016, 51, 1996-2007.	3.7	18
41	The Impact of Natural Compounds on S-Shaped Aβ42 Fibril: From Molecular Docking to Biophysical Characterization. International Journal of Molecular Sciences, 2020, 21, 2017.	4.1	18
42	Fludarabine-Specific Molecular Interactions with Maltose-Modified Poly(propyleneimine) Dendrimer Enable Effective Cell Entry of the Active Drug Form: Comparison with Clofarabine. Biomacromolecules, 2019, 20, 1429-1442.	5.4	16
43	Molecular simulations of amyloid beta assemblies. Advances in Physics: X, 2020, 5, 1770627.	4.1	16
44	Making biological membrane resistant to the toxicity of misfolded protein oligomers: a lesson from trodusquemine. Nanoscale, 2020, 12, 22596-22614.	5.6	16
45	Biophysical Insights into Cancer Transformation and Treatment. Scientific World Journal, The, 2013, 2013, 1-11.	2.1	15
46	Thermodynamic and kinetic stability of the Josephin Domain closed arrangement: evidences from replica exchange molecular dynamics. Biology Direct, 2017, 12, 2.	4.6	15
47	Biofunctionalization of Silica Nanoparticles with Cell-Penetrating Peptides: Adsorption Mechanism and Binding Energy Estimation. Journal of Physical Chemistry B, 2019, 123, 10622-10630.	2.6	15
48	Collective surface diffusion on a triangular lattice in presence of ordered phases. Surface Science, 1998, 402-404, 281-285.	1.9	14
49	Highly Organized Self-Assembled Dendriplexes Based on Poly(propylene imine) Glycodendrimer and Anti-HIV Oligodeoxynucleotides. Current Medicinal Chemistry, 2012, 19, 4708-4719.	2.4	14
50	Destabilizing the AXH Tetramer by Mutations: Mechanisms and Potential Antiaggregation Strategies. Biophysical Journal, 2018, 114, 323-330.	0.5	14
51	Elucidating the Effect of Static Electric Field on Amyloid Beta 1–42 Supramolecular Assembly. Journal of Molecular Graphics and Modelling, 2020, 96, 107535.	2.4	14
52	Lattice-gas model of diffusion of NH3 on Re(0001). Chemical Physics Letters, 1995, 236, 533-537.	2.6	13
53	Homology and Molecular Dynamics Models of Tollâ€Like Receptor 7 Protein and Its Dimerization. Chemical Biology and Drug Design, 2014, 83, 656-665.	3.2	12
54	Preparation and characterization of new hybrid nanostructured thin films for biosensors design. Materials Letters, 2011, 65, 2032-2035.	2.6	11

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55	Molecular and Coarse-Grained Modeling to Characterize and Optimize Dendrimer-Based Nanocarriers for Short Interfering RNA Delivery. ACS Omega, 2020, 5, 2978-2986.	3.5	10
56	In situ functionalization of self-assembled dendrimer nanofibers with cadmium sulfide quantum dots through simple ionic-substitution. New Journal of Chemistry, 2016, 40, 6325-6331.	2.8	9
57	Wavelets as basis functions to represent the coarse-graining potential in multiscale coarse graining approach. Journal of Computational Physics, 2015, 300, 592-604.	3.8	8
58	Aminoacid substitutions in the glycine zipper affect the conformational stability of amyloid beta fibrils. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3908-3915.	3.5	8
59	Fragmented blind docking: a novel protein–ligand binding prediction protocol. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13472-13481.	3.5	8
60	Combined EPR and Molecular Modeling Study of PPI Dendrimers Interacting with Copper Ions: Effect of Generation and Maltose Decoration. Journal of Physical Chemistry B, 2014, 118, 12098-12111.	2.6	7
61	Explaining the Microtubule Energy Balance: Contributions Due to Dipole Moments, Charges, van der Waals and Solvation Energy. International Journal of Molecular Sciences, 2017, 18, 2042.	4.1	7
62	Supporting the Design of Efficient Dendritic DNA and siRNA Nano-Carriers with Molecular Modeling. Current Drug Discovery Technologies, 2011, 8, 314-328.	1.2	7
63	Protein–dendron conjugates for DNA binding: understanding the effect of the protein core on multivalency. RSC Advances, 2011, 1, 1677.	3.6	6
64	Self-Assembled Ligands Targeting TLR7: A Molecular Level Investigation. Langmuir, 2017, 33, 14460-14471.	3.5	5
65	Effect of Lactose Pseudopolymorphic Transition on the Aerosolization Performance of Drug/Carrier Mixtures. Pharmaceutics, 2019, 11, 576.	4.5	5
66	Spin probe analysis of microtubules structure and formation. Archives of Biochemistry and Biophysics, 2012, 522, 1-8.	3.0	3
67	A Novel Interaction Between the TLR7 and a Colchicine Derivative Revealed Through a Computational and Experimental Study. Pharmaceuticals, 2018, 11, 22.	3.8	3
68	Multi-site correlation functions in two-dimensional lattice gases. Physica A: Statistical Mechanics and Its Applications, 1996, 223, 149-166.	2.6	2
69	Base Invaders. Coupling Experiments and Multiscale Modeling of Dendrimer-Based siRNA Delivery Agents. Advances in Science and Technology, 0, , .	0.2	1
70	Extended diffusion theory: Recovering dynamics from biased/accelerated molecular simulations. Journal of Computational Chemistry, 2021, 42, 586-599.	3.3	1