

Paola Posocco

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93
papers

3,190
citations

34
h-index

54
g-index

95
ext. papers

3,451
ext. citations

6.3
avg, IF

4.86
L-index

#	Paper	IF	Citations
93	Anticancer drug nanomicelles formed by self-assembling amphiphilic dendrimer to combat cancer drug resistance. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015 , 112, 2978-83	11.5	274
92	Degradable self-assembling dendrons for gene delivery: experimental and theoretical insights into the barriers to cellular uptake. <i>Journal of the American Chemical Society</i> , 2011 , 133, 20288-300	16.4	156
91	Adaptive amphiphilic dendrimer-based nanoassemblies as robust and versatile siRNA delivery systems. <i>Angewandte Chemie - International Edition</i> , 2014 , 53, 11822-7	16.4	144
90	Sodium montmorillonite silylation: unexpected effect of the aminosilane chain length. <i>Journal of Colloid and Interface Science</i> , 2010 , 351, 108-15	9.3	124
89	Polymer-clay nanocomposites: a multiscale molecular modeling approach. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 2143-51	3.4	110
88	Efficient delivery of sticky siRNA and potent gene silencing in a prostate cancer model using a generation 5 triethanolamine-core PAMAM dendrimer. <i>Molecular Pharmaceutics</i> , 2012 , 9, 470-81	5.6	92
87	Mallard blue: a high-affinity selective heparin sensor that operates in highly competitive media. <i>Journal of the American Chemical Society</i> , 2013 , 135, 2911-4	16.4	92
86	PAMAM dendrimers for siRNA delivery: computational and experimental insights. <i>Chemistry - A European Journal</i> , 2010 , 16, 7781-95	4.8	83
85	Homology Model and Docking-Based Virtual Screening for Ligands of the μ Receptor. <i>ACS Medicinal Chemistry Letters</i> , 2011 , 2, 834-9	4.3	75
84	Interfacial tension of oil/water emulsions with mixed non-ionic surfactants: comparison between experiments and molecular simulations. <i>RSC Advances</i> , 2016 , 6, 4723-4729	3.7	71
83	Less is more [multiscale modelling of self-assembling multivalency and its impact on DNA binding and gene delivery. <i>Chemical Science</i> , 2010 , 1, 393	9.4	71
82	Hydrophobically modified dendrons: developing structure-activity relationships for DNA binding and gene transfection. <i>Molecular Pharmaceutics</i> , 2011 , 8, 416-29	5.6	70
81	Synthesis, biological evaluation, and three-dimensional in silico pharmacophore model for sigma(1) receptor ligands based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives. <i>Journal of Medicinal Chemistry</i> , 2009 , 52, 5380-93	8.3	68
80	Molecular dynamics reveal BCR-ABL1 polymutants as a unique mechanism of resistance to PAN-BCR-ABL1 kinase inhibitor therapy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 3550-5	11.5	65
79	Antiviral and cytotoxic activities of aminoaryloxo compounds and aryltriazene derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2009 , 17, 4425-40	3.4	61
78	Mastering Dendrimer Self-Assembly for Efficient siRNA Delivery: From Conceptual Design to In Vivo Efficient Gene Silencing. <i>Small</i> , 2016 , 12, 3667-76	11	61
77	Poly(amidoamine)-based dendrimer/siRNA complexation studied by computer simulations: effects of pH and generation on dendrimer structure and siRNA binding. <i>Macromolecular Bioscience</i> , 2012 , 12, 225-40	5.5	58

76	Structurally flexible triethanolamine core PAMAM dendrimers are effective nanovectors for DNA transfection in vitro and in vivo to the mouse thymus. <i>Bioconjugate Chemistry</i> , 2011 , 22, 2461-73	6.3	57
75	Multiscale Computer Simulation Studies of Water-Based Montmorillonite/Poly(ethylene oxide) Nanocomposites. <i>Macromolecules</i> , 2009 , 42, 8260-8270	5.5	54
74	Combination of dendrimer-nanovector-mediated small interfering RNA delivery to target Akt with the clinical anticancer drug paclitaxel for effective and potent anticancer activity in treating ovarian cancer. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 2634-42	8.3	48
73	Morphology prediction of block copolymers for drug delivery by mesoscale simulations. <i>Journal of Materials Chemistry</i> , 2010 , 20, 7742		47
72	Gold nanoparticles with patterned surface monolayers for nanomedicine: current perspectives. <i>European Biophysics Journal</i> , 2017 , 46, 749-771	1.9	46
71	To the nanoscale, and beyond!: Multiscale molecular modeling of polymer-clay nanocomposites. <i>Fluid Phase Equilibria</i> , 2007 , 261, 366-374	2.5	46
70	Patchy and Janus Nanoparticles by Self-Organization of Mixtures of Fluorinated and Hydrogenated Alkanethiolates on the Surface of a Gold Core. <i>ACS Nano</i> , 2016 , 10, 9316-9325	16.7	45
69	Nanoscale self-assembled multivalent (SAMul) heparin binders in highly competitive, biologically relevant, aqueous media. <i>Chemical Science</i> , 2014 , 5, 1484	9.4	40
68	Self-Assembly of Nanoparticle Mixtures in Diblock Copolymers: Multiscale Molecular Modeling. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 5023-5038	3.9	40
67	Impact of siRNA overhangs for dendrimer-mediated siRNA delivery and gene silencing. <i>Molecular Pharmaceutics</i> , 2013 , 10, 3262-73	5.6	39
66	A complete multiscale modelling approach for polymer-clay nanocomposites. <i>Chemistry - A European Journal</i> , 2009 , 15, 7586-92	4.8	38
65	Self-organization of mixtures of fluorocarbon and hydrocarbon amphiphilic thiolates on the surface of gold nanoparticles. <i>ACS Nano</i> , 2012 , 6, 7243-53	16.7	37
64	A simple new competition assay for heparin binding in serum applied to multivalent PAMAM dendrimers. <i>Chemical Communications</i> , 2013 , 49, 4830-2	5.8	36
63	Size and shape matter! A multiscale molecular simulation approach to polymer nanocomposites. <i>Journal of Materials Chemistry</i> , 2012 , 22, 5398		35
62	Pharmacophore modeling, resistant mutant isolation, docking, and MM-PBSA analysis: Combined experimental/computer-assisted approaches to identify new inhibitors of the bovine viral diarrhea virus (BVDV). <i>Bioorganic and Medicinal Chemistry</i> , 2010 , 18, 2304-2316	3.4	35
61	A 3D-pharmacophore model for sigma2 receptors based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010 , 20, 2954-7	2.9	35
60	Adaptive Amphiphilic Dendrimer-Based Nanoassemblies as Robust and Versatile siRNA Delivery Systems. <i>Angewandte Chemie</i> , 2014 , 126, 12016-12021	3.6	34
59	Antimycobacterial activity of new 3,5-disubstituted 1,3,4-oxadiazol-2(3H)-one derivatives. Molecular modeling investigations. <i>Bioorganic and Medicinal Chemistry</i> , 2009 , 17, 4693-707	3.4	34

58	A molecular simulation approach to the prediction of the morphology of self-assembled nanoparticles in diblock copolymers. <i>Journal of Materials Chemistry</i> , 2010 , 20, 10511		33
57	Quantitative 3D determination of self-assembled structures on nanoparticles using small angle neutron scattering. <i>Nature Communications</i> , 2018 , 9, 1343	17.4	32
56	3-Aryl-2-[1H-benzotriazol-1-yl]acrylonitriles: a novel class of potent tubulin inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2011 , 46, 4151-67	6.8	31
55	Self-assembled multivalent RGD-peptide arrays--morphological control and integrin binding. <i>Organic and Biomolecular Chemistry</i> , 2013 , 11, 3177-86	3.9	30
54	Synergistic experimental/computational studies on arylazoenamine derivatives that target the bovine viral diarrhoea virus RNA-dependent RNA polymerase. <i>Bioorganic and Medicinal Chemistry</i> , 2010 , 18, 6055-68	3.4	29
53	Binding at the Core. Computational Study of Structural and Ligand Binding Properties of Naphthyridine-Based Dendrimers. <i>Macromolecules</i> , 2007 , 40, 2257-2266	5.5	29
52	Tell me something I do not know. Multiscale molecular modeling of dendrimer/ dendron organization and self-assembly in gene therapy. <i>Current Medicinal Chemistry</i> , 2012 , 19, 5062-87	4.3	28
51	Double-degradable responsive self-assembled multivalent arrays--temporary nanoscale recognition between dendrons and DNA. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 446-55	3.9	27
50	Electrostatic binding of polyanions using self-assembled multivalent (SAMul) ligand displays - structure-activity effects on DNA/heparin binding. <i>Chemical Science</i> , 2016 , 7, 4653-4659	9.4	26
49	Through the open door: Preferential binding of dasatinib to the active form of BCR-ABL unveiled by in silico experiments. <i>Molecular Oncology</i> , 2013 , 7, 968-75	7.9	23
48	Highly grafted polystyrene/polyvinylpyridine polymer gold nanoparticles in a good solvent: effects of chain length and composition. <i>Soft Matter</i> , 2016 , 12, 3600-11	3.6	22
47	Modeling hierarchically structured nanoparticle/diblock copolymer systems. <i>Soft Matter</i> , 2013 , 9, 2936	3.6	21
46	Simple, fast, and accurate in silico estimations of contact angle, surface tension, and work of adhesion of water and oil nanodroplets on amorphous polypropylene surfaces. <i>ACS Applied Materials & Interfaces</i> , 2012 , 4, 2855-9	9.5	20
45	Emergence of highly-ordered hierarchical nanoscale aggregates on electrostatic binding of self-assembled multivalent (SAMul) cationic micelles with polyanionic heparin. <i>Journal of Materials Chemistry B</i> , 2017 , 5, 341-347	7.3	19
44	Copper(II) binding to flexible triethanolamine-core PAMAM dendrimers: a combined experimental/in silico approach. <i>Physical Chemistry Chemical Physics</i> , 2014 , 16, 685-94	3.6	19
43	Shape-persistent and adaptive multivalency: rigid transgeden (TGD) and flexible PAMAM dendrimers for heparin binding. <i>Chemistry - A European Journal</i> , 2014 , 20, 9666-74	4.8	19
42	Graphene oxide as a 2D platform for complexation and intracellular delivery of siRNA. <i>Nanoscale</i> , 2019 , 11, 13863-13877	7.7	18
41	MULTISCALE MODELING OF POLYMER/CLAY NANOCOMPOSITES. <i>Journal of Multiscale Modeling</i> , 2011 , 03, 151-176	0.8	18

40	Combined Mesoscale/Experimental Study of Selective Placement of Magnetic Nanoparticles in Diblock Copolymer Films via Solvent Vapor Annealing. <i>Journal of Physical Chemistry C</i> , 2016 , 120, 7403-7411	3.8	17
39	In vitro and in silico studies of MDM2/MDMX isoforms predict Nutlin-3A sensitivity in well/de-differentiated liposarcomas. <i>Laboratory Investigation</i> , 2013 , 93, 1232-40	5.9	17
38	Imatinib response in two GIST patients carrying two hitherto functionally uncharacterized PDGFRA mutations: an imaging, biochemical and molecular modeling study. <i>International Journal of Cancer</i> , 2011 , 128, 983-90	7.5	17
37	Conformational sensitivity of conjugated poly(ethylene oxide)-poly(amidoamine) molecules to cations adducted upon electrospray ionization - a mass spectrometry, ion mobility and molecular modeling study. <i>Analytica Chimica Acta</i> , 2014 , 808, 163-74	6.6	16
36	2-difluoromethylene-4-methylenepentanoic acid, a paradoxical probe able to mimic the signaling role of 2-oxoglutaric acid in cyanobacteria. <i>Organic Letters</i> , 2011 , 13, 2924-7	6.2	16
35	Chiral recognition at self-assembled multivalent (SAMul) nanoscale interfaces - enantioselectivity in polyanion binding. <i>Chemical Communications</i> , 2016 , 52, 10540-3	5.8	16
34	Mix and Match: Coassembly of Amphiphilic Dendrimers and Phospholipids Creates Robust, Modular, and Controllable Interfaces. <i>ACS Applied Materials & Interfaces</i> , 2017 , 9, 1029-1035	9.5	15
33	Supramolecular Tripeptide Hydrogel Assembly with 5-Fluorouracil. <i>Gels</i> , 2019 , 5,	4.2	15
32	Exploring the Shape Influence on Melting Temperature, Enthalpy, and Solubility of Organic Drug Nanocrystals by a Thermodynamic Model. <i>Crystal Growth and Design</i> , 2017 , 17, 4072-4083	3.5	15
31	Mixed Fluorinated/Hydrogenated Self-Assembled Monolayer-Protected Gold Nanoparticles: In Silico and In Vitro Behavior. <i>Small</i> , 2019 , 15, e1900323	11	14
30	Structure-Activity relationship study of dendritic polyglycerolamines for efficient siRNA transfection. <i>RSC Advances</i> , 2015 , 5, 78760-78770	3.7	14
29	Rationalizing the F _{118S} interaction discovered within a tetrafluorophenylazido-containing bola-phospholipid. <i>Chemical Communications</i> , 2012 , 48, 4284-6	5.8	14
28	Morphological control of self-assembled multivalent (SAMul) heparin binding in highly competitive media. <i>Chemical Communications</i> , 2017 , 53, 6335-6338	5.8	13
27	Self-Assembled Multivalent (SAMul) Polyanion Binding-Impact of Hydrophobic Modifications in the Micellar Core on DNA and Heparin Binding at the Peripheral Cationic Ligands. <i>Chemistry - A European Journal</i> , 2017 , 23, 6391-6397	4.8	13
26	Cationic carbosilane dendrimers and oligonucleotide binding: an energetic affair. <i>Nanoscale</i> , 2015 , 7, 3876-87	7.7	12
25	Structural requirements of 2-oxoglutaric acid analogues to mimic its signaling function. <i>Organic Letters</i> , 2013 , 15, 4662-5	6.2	12
24	Scripting approach in hybrid organic/inorganic condensation simulation: the GPTMS proof-of-concept. <i>Molecular Simulation</i> , 2008 , 34, 1215-1236	2	12
23	MoDeNa Nanotools: An integrated multiscale simulation workflow to predict thermophysical properties of thermoplastic polyurethanes. <i>Journal of Computational Science</i> , 2016 , 15, 24-33	3.4	9

22	Iron-mediated interaction of alpha synuclein with lipid raft model membranes. <i>Nanoscale</i> , 2020 , 12, 7631-7640	1.7	8
21	Effect of surface decoration on properties and drug release ability of nanogels. <i>Colloids and Surfaces A: Physicochemical and Engineering Aspects</i> , 2021 , 614, 126164	5.1	8
20	The interaction of α -microglobulin with gold nanoparticles: impact of coating, charge and size. <i>Journal of Materials Chemistry B</i> , 2018 , 6, 5964-5974	7.3	7
19	Structure and binding thermodynamics of viologen-phosphorous dendrimers to human serum albumin: A combined computational/experimental investigation. <i>Fluid Phase Equilibria</i> , 2016 , 422, 18-31	2.5	6
18	Effects of primary amine-based coatings on microglia internalization of nanogels. <i>Colloids and Surfaces B: Biointerfaces</i> , 2020 , 185, 110574	6	6
17	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems. <i>Composite Interfaces</i> , 2013 , 20, 379-394	2.3	5
16	Mimicking the 2-oxoglutaric acid signalling function using molecular probes: insights from structural and functional investigations. <i>Organic and Biomolecular Chemistry</i> , 2014 , 12, 4723-9	3.9	5
15	Theoretical Importance of PVP-Alginate Hydrogels Structure on Drug Release Kinetics. <i>Gels</i> , 2019 , 5,	4.2	4
14	Multiscale Molecular Modeling of Clay/Polymer Nanocomposites 2017 , 83-112		3
13	Phase Behavior of Gradient Copolymer Melts with Different Gradient Strengths Revealed by Mesoscale Simulations. <i>Polymers</i> , 2020 , 12,	4.5	2
12	siRNA Delivery: Mastering Dendrimer Self-Assembly for Efficient siRNA Delivery: From Conceptual Design to In Vivo Efficient Gene Silencing (Small 27/2016). <i>Small</i> , 2016 , 12, 3604-3604	11	2
11	Fluorescent Imprinted Nanoparticles for the Effective Monitoring of Irinotecan in Human Plasma. <i>Nanomaterials</i> , 2020 , 10,	5.4	2
10	Tuning the Properties of Nanogel Surfaces by Grafting Charged Alkylamine Brushes. <i>Nanomaterials</i> , 2019 , 9,	5.4	2
9	Noble metal nanoparticles with anisotropy in shape and surface functionality for biomedical applications 2018 , 313-333		2
8	Molecular Features for Probing Small Amphiphilic Molecules with Self-Assembled Monolayer-Protected Nanoparticles. <i>Langmuir</i> , 2020 , 36, 5671-5679	4	1
7	Modelling and Simulation of Sol-Gel Nanocomposites 2014 , 21-49		1
6	Multiscale Molecular Modeling of Hybrid Organic-Inorganic Nanocomposites of Type I and II. <i>Advances in Science and Technology</i> , 2008 , 54, 265-269	0.1	1
5	Base Invaders. Coupling Experiments and Multiscale Modeling of Dendrimer-Based siRNA Delivery Agents. <i>Advances in Science and Technology</i> , 2008 , 57, 154-159	0.1	1

- 4 Anomerization of Acrylated Glucose During Traveling Wave Ion Mobility Spectrometry. *Journal of the American Society for Mass Spectrometry*, **2015**, 26, 1483-93 3.5 ○
- 3 Probing Multiscale Factors Affecting the Reactivity of Nanoparticle-Bound Molecules. *ACS Nano*, **2021**, 15, 8295-8305 16.7 ○
- 2 Thiolate end-group regulates ligand arrangement, hydration and affinity for small compounds in monolayer-protected gold nanoparticles. *Journal of Colloid and Interface Science*, **2022**, 607, 1373-1381 9.3 ○
- 1 Multiscale Modeling Approach for Polymeric Nanocomposites **2013**, 95-128