

Paola Posocco

List of Publications by Year in descending order

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papers

3,686
citations

101496

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95
docs citations

95
times ranked

4842
citing authors

#	ARTICLE	IF	CITATIONS
1	Anticancer drug nanomicelles formed by self-assembling amphiphilic dendrimer to combat cancer drug resistance. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2978-2983.	3.3	318
2	Adaptive Amphiphilic Dendrimer-Based Nanoassemblies as Robust and Versatile siRNA Delivery Systems. Angewandte Chemie - International Edition, 2014, 53, 11822-11827.	7.2	181
3	Degradable Self-Assembling Dendrons for Gene Delivery: Experimental and Theoretical Insights into the Barriers to Cellular Uptake. Journal of the American Chemical Society, 2011, 133, 20288-20300.	6.6	166
4	Sodium montmorillonite silylation: Unexpected effect of the aminosilane chain length. Journal of Colloid and Interface Science, 2010, 351, 108-115.	5.0	149
5	Polymer-Clay Nanocomposites: A Multiscale Molecular Modeling Approach. Journal of Physical Chemistry B, 2007, 111, 2143-2151.	1.2	120
6	Mallard Blue: A High-Affinity Selective Heparin Sensor That Operates in Highly Competitive Media. Journal of the American Chemical Society, 2013, 135, 2911-2914.	6.6	107
7	Efficient Delivery of Sticky siRNA and Potent Gene Silencing in a Prostate Cancer Model Using a Generation 5 Triethanolamine-Core PAMAM Dendrimer. Molecular Pharmaceutics, 2012, 9, 470-481.	2.3	102
8	Interfacial tension of oil/water emulsions with mixed non-ionic surfactants: comparison between experiments and molecular simulations. RSC Advances, 2016, 6, 4723-4729.	1.7	95
9	PAMAM Dendrimers for siRNA Delivery: Computational and Experimental Insights. Chemistry - A European Journal, 2010, 16, 7781-7795.	1.7	91
10	Homology Model and Docking-Based Virtual Screening for Ligands of the β_1 Receptor. ACS Medicinal Chemistry Letters, 2011, 2, 834-839.	1.3	80
11	Mastering Dendrimer Self-Assembly for Efficient siRNA Delivery: From Conceptual Design to In Vivo Efficient Gene Silencing. Small, 2016, 12, 3667-3676.	5.2	78
12	Synthesis, Biological Evaluation, and Three-Dimensional in Silico Pharmacophore Model for β_1 Receptor Ligands Based on a Series of Substituted Benzo[<i>d</i>]oxazol-2(3 <i>H</i>)-one Derivatives. Journal of Medicinal Chemistry, 2009, 52, 5380-5393.	2.9	77
13	Less is more – multiscale modelling of self-assembling multivalency and its impact on DNA binding and gene delivery. Chemical Science, 2010, 1, 393.	3.7	76
14	Hydrophobically Modified Dendrons: Developing Structure-Activity Relationships for DNA Binding and Gene Transfection. Molecular Pharmaceutics, 2011, 8, 416-429.	2.3	74
15	Molecular dynamics reveal BCR-ABL1 polymutants as a unique mechanism of resistance to PAN-BCR-ABL1 kinase inhibitor therapy. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3550-3555.	3.3	74
16	Antiviral and cytotoxic activities of aminoaryloxo compounds and aryltriazene derivatives. Bioorganic and Medicinal Chemistry, 2009, 17, 4425-4440.	1.4	69
17	Structurally Flexible Triethanolamine Core PAMAM Dendrimers Are Effective Nanovectors for DNA Transfection in Vitro and in Vivo to the Mouse Thymus. Bioconjugate Chemistry, 2011, 22, 2461-2473.	1.8	65
18	Gold nanoparticles with patterned surface monolayers for nanomedicine: current perspectives. European Biophysics Journal, 2017, 46, 749-771.	1.2	64

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19	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, 225-240.	2.1	61
20	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, 2634-2642.	2.9	59
21	Multiscale Computer Simulation Studies of Water-Based Montmorillonite/Poly(ethylene oxide) Nanocomposites. <i>Macromolecules</i> , 2009, 42, 8260-8270.	2.2	58
22	Morphology prediction of block copolymers for drug delivery by mesoscale simulations. <i>Journal of Materials Chemistry</i> , 2010, 20, 7742.	6.7	55
23	Quantitative 3D determination of self-assembled structures on nanoparticles using small angle neutron scattering. <i>Nature Communications</i> , 2018, 9, 1343.	5.8	54
24	To the nanoscale, and beyond!. <i>Fluid Phase Equilibria</i> , 2007, 261, 366-374.	1.4	48
25	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.	7.3	48
26	A Complete Multiscale Modelling Approach for Polymer-Clay Nanocomposites. <i>Chemistry - A European Journal</i> , 2009, 15, 7586-7592.	1.7	43
27	Impact of siRNA Overhangs for Dendrimer-Mediated siRNA Delivery and Gene Silencing. <i>Molecular Pharmaceutics</i> , 2013, 10, 3262-3273.	2.3	43
28	Self-Assembly of Nanoparticle Mixtures in Diblock Copolymers: Multiscale Molecular Modeling. <i>Industrial & Engineering Chemistry Research</i> , 2008, 47, 5023-5038.	1.8	42
29	Nanoscale self-assembled multivalent (SAMul) heparin binders in highly competitive, biologically relevant, aqueous media. <i>Chemical Science</i> , 2014, 5, 1484.	3.7	42
30	3-Aryl-2-[1H-benzotriazol-1-yl]acrylonitriles: A novel class of potent tubulin inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 4151-4167.	2.6	40
31	Self-Organization of Mixtures of Fluorocarbon and Hydrocarbon Amphiphilic Thiolates on the Surface of Gold Nanoparticles. <i>ACS Nano</i> , 2012, 6, 7243-7253.	7.3	40
32	A simple new competition assay for heparin binding in serum applied to multivalent PAMAM dendrimers. <i>Chemical Communications</i> , 2013, 49, 4830.	2.2	39
33	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.	1.4	38
34	Size and shape matter! A multiscale molecular simulation approach to polymer nanocomposites. <i>Journal of Materials Chemistry</i> , 2012, 22, 5398.	6.7	38
35	A 3D-pharmacophore model for β_2 receptors based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 2954-2957.	1.0	37
36	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.	6.7	36

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37	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, 4693-4707.	1.4	35
38	Graphene oxide as a 2D platform for complexation and intracellular delivery of siRNA. <i>Nanoscale</i> , 2019, 11, 13863-13877.	2.8	35
39	Double-degradable responsive self-assembled multivalent arrays " temporary nanoscale recognition between dendrons and DNA. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 446-455.	1.5	33
40	Self-assembled multivalent RGD-peptide arrays " morphological control and integrin binding. <i>Organic and Biomolecular Chemistry</i> , 2013, 11, 3177.	1.5	32
41	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, 6055-6068.	1.4	31
42	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.	3.7	31
43	Binding at the Core. Computational Study of Structural and Ligand Binding Properties of Naphthyridine-Based Dendrimers. <i>Macromolecules</i> , 2007, 40, 2257-2266.	2.2	30
44	Supramolecular Tripeptide Hydrogel Assembly with 5-Fluorouracil. <i>Gels</i> , 2019, 5, 5.	2.1	30
45	Through the open door: Preferential binding of dasatinib to the active form of BCR"ABL unveiled by <i>in silico</i> experiments. <i>Molecular Oncology</i> , 2013, 7, 968-975.	2.1	28
46	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, 5062-5087.	1.2	28
47	Highly grafted polystyrene/polyvinylpyridine polymer gold nanoparticles in a good solvent: effects of chain length and composition. <i>Soft Matter</i> , 2016, 12, 3600-3611.	1.2	25
48	Modeling hierarchically structured nanoparticle/diblock copolymer systems. <i>Soft Matter</i> , 2013, 9, 2936.	1.2	22
49	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, 2855-2859.	4.0	21
50	Shape"Persistent and Adaptive Multivalency: Rigid Transgeden (TGD) and Flexible PAMAM Dendrimers for Heparin Binding. <i>Chemistry - A European Journal</i> , 2014, 20, 9666-9674.	1.7	21
51	MULTISCALE MODELING OF POLYMER/CLAY NANOCOMPOSITES. <i>Journal of Multiscale Modeling</i> , 2011, 03, 151-176.	1.0	20
52	Copper(ii) binding to flexible triethanolamine-core PAMAM dendrimers: a combined experimental/in silico approach. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 685-694.	1.3	20
53	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.	2.9	20
54	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, 983-990.	2.3	18

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55	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, 163-174.	2.6	18
56	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.	1.5	18
57	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.	1.4	18
58	Mixed Fluorinated/Hydrogenated Self-Assembled Monolayer-Protected Gold Nanoparticles: In Silico and In Vitro Behavior. <i>Small</i> , 2019, 15, e1900323.	5.2	18
59	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, 1232-1240.	1.7	17
60	Chiral recognition at self-assembled multivalent (SAMul) nanoscale interfaces – enantioselectivity in polyanion binding. <i>Chemical Communications</i> , 2016, 52, 10540-10543.	2.2	17
61	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.	4.0	17
62	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, 2924-2927.	2.4	16
63	Iron-mediated interaction of alpha synuclein with lipid raft model membranes. <i>Nanoscale</i> , 2020, 12, 7631-7640.	2.8	16
64	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.	1.7	15
65	Scripting approach in hybrid organic-inorganic condensation simulation: the GPTMS proof-of-concept. <i>Molecular Simulation</i> , 2008, 34, 1215-1236.	0.9	14
66	Rationalizing the F π -S interaction discovered within a tetrafluorophenylazido-containing bola-phospholipid. <i>Chemical Communications</i> , 2012, 48, 4284.	2.2	14
67	Structure-activity relationship study of dendritic polyglycerolamines for efficient siRNA transfection. <i>RSC Advances</i> , 2015, 5, 78760-78770.	1.7	14
68	Morphological control of self-assembled multivalent (SAMul) heparin binding in highly competitive media. <i>Chemical Communications</i> , 2017, 53, 6335-6338.	2.2	14
69	Structural Requirements of 2-Oxoglutaric Acid Analogues To Mimic Its Signaling Function. <i>Organic Letters</i> , 2013, 15, 4662-4665.	2.4	13
70	Cationic carbosilane dendrimers and oligonucleotide binding: an energetic affair. <i>Nanoscale</i> , 2015, 7, 3876-3887.	2.8	12
71	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.	2.3	12
72	MoDeNa Nanotools: An integrated multiscale simulation workflow to predict thermophysical properties of thermoplastic polyurethanes. <i>Journal of Computational Science</i> , 2016, 15, 24-33.	1.5	10

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73	Probing Multiscale Factors Affecting the Reactivity of Nanoparticle-Bound Molecules. ACS Nano, 2021, 15, 8295-8305.	7.3	8
74	Structure and binding thermodynamics of viologen-phosphorous dendrimers to human serum albumin: A combined computational/experimental investigation. Fluid Phase Equilibria, 2016, 422, 18-31.	1.4	7
75	The interaction of \hat{I}^{22} -microglobulin with gold nanoparticles: impact of coating, charge and size. Journal of Materials Chemistry B, 2018, 6, 5964-5974.	2.9	7
76	Effects of primary amine-based coatings on microglia internalization of nanogels. Colloids and Surfaces B: Biointerfaces, 2020, 185, 110574.	2.5	7
77	Phase Behavior of Gradient Copolymer Melts with Different Gradient Strengths Revealed by Mesoscale Simulations. Polymers, 2020, 12, 2462.	2.0	6
78	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems. Composite Interfaces, 2013, 20, 379-394.	1.3	5
79	Mimicking the 2-oxoglutaric acid signalling function using molecular probes: insights from structural and functional investigations. Organic and Biomolecular Chemistry, 2014, 12, 4723-4729.	1.5	5
80	Theoretical Importance of PVP-Alginate Hydrogels Structure on Drug Release Kinetics. Gels, 2019, 5, 22.	2.1	5
81	Multiscale Molecular Modeling of Clay-Polymer Nanocomposites. , 2017, , 83-112.		4
82	Tuning the Properties of Nanogel Surfaces by Grafting Charged Alkylamine Brushes. Nanomaterials, 2019, 9, 1514.	1.9	4
83	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.	5.0	4
84	siRNA Delivery: Mastering Dendrimer Self-Assembly for Efficient siRNA Delivery: From Conceptual Design to In Vivo Efficient Gene Silencing (Small 27/2016). Small, 2016, 12, 3604-3604.	5.2	3
85	Fluorescent Imprinted Nanoparticles for the Effective Monitoring of Irinotecan in Human Plasma. Nanomaterials, 2020, 10, 1707.	1.9	3
86	Molecular Features for Probing Small Amphiphilic Molecules with Self-Assembled Monolayer-Protected Nanoparticles. Langmuir, 2020, 36, 5671-5679.	1.6	3
87	The importance of molecular structure and functionalization of oxo-graphene sheets for gene silencing. Carbon, 2022, , .	5.4	3
88	Anomerization of Acrylated Glucose During Traveling Wave Ion Mobility Spectrometry. Journal of the American Society for Mass Spectrometry, 2015, 26, 1483-1493.	1.2	2
89	Noble metal nanoparticles with anisotropy in shape and surface functionality for biomedical applications. , 2018, , 313-333.		2
90	Label-Free, Rapid and Facile Gold-Nanoparticles-Based Assay as a Potential Spectroscopic Tool for Trastuzumab Quantification. Nanomaterials, 2021, 11, 3181.	1.9	2

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91	Multiscale Molecular Modeling of Hybrid Organic-Inorganic Nanocomposites of Type I and II. <i>Advances in Science and Technology</i> , 0, , .	0.2	1
92	Base Invaders. Coupling Experiments and Multiscale Modeling of Dendrimer-Based siRNA Delivery Agents. <i>Advances in Science and Technology</i> , 0, , .	0.2	1
93	Modelling and Simulation of Sol-Gel Nanocomposites. , 2014, , 21-49.		1