Paola Posocco

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/1499204/publications.pdf Version: 2024-02-01



#	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.	7.1	318
2	Adaptive Amphiphilic Dendrimerâ€Based Nanoassemblies as Robust and Versatile siRNA Delivery Systems. Angewandte Chemie - International Edition, 2014, 53, 11822-11827.	13.8	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.	13.7	166
4	Sodium montmorillonite silylation: Unexpected effect of the aminosilane chain length. Journal of Colloid and Interface Science, 2010, 351, 108-115.	9.4	149
5	Polymerâ^'Clay Nanocomposites:Â A Multiscale Molecular Modeling Approach. Journal of Physical Chemistry B, 2007, 111, 2143-2151.	2.6	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.	13.7	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.	4.6	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.	3.6	95
9	PAMAM Dendrimers for siRNA Delivery: Computational and Experimental Insights. Chemistry - A European Journal, 2010, 16, 7781-7795.	3.3	91
10	Homology Model and Docking-Based Virtual Screening for Ligands of the σ ₁ Receptor. ACS Medicinal Chemistry Letters, 2011, 2, 834-839.	2.8	80
11	Mastering Dendrimer Selfâ€Assembly for Efficient siRNA Delivery: From Conceptual Design to In Vivo Efficient Gene Silencing. Small, 2016, 12, 3667-3676.	10.0	78
12	Synthesis, Biological Evaluation, and Three-Dimensional in Silico Pharmacophore Model for Ïf 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.	6.4	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.	7.4	76
14	Hydrophobically Modified Dendrons: Developing Structureâ^'Activity Relationships for DNA Binding and Gene Transfection. Molecular Pharmaceutics, 2011, 8, 416-429.	4.6	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.	7.1	74
16	Antiviral and cytotoxic activities of aminoarylazo compounds and aryltriazene derivatives. Bioorganic and Medicinal Chemistry, 2009, 17, 4425-4440.	3.0	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.	3.6	65
18	Gold nanoparticles with patterned surface monolayers for nanomedicine: current perspectives. European Biophysics Journal, 2017, 46, 749-771.	2.2	64

PAOLA POSOCCO

#	Article	IF	CITATIONS
19	Poly(amidoamine)â€based Dendrimer/siRNA Complexation Studied by Computer Simulations: Effects of pH and Generation on Dendrimer Structure and siRNA Binding. Macromolecular Bioscience, 2012, 12, 225-240.	4.1	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. Journal of Medicinal Chemistry, 2014, 57, 2634-2642.	6.4	59
21	Multiscale Computer Simulation Studies of Water-Based Montmorillonite/Poly(ethylene oxide) Nanocomposites. Macromolecules, 2009, 42, 8260-8270.	4.8	58
22	Morphology prediction of block copolymers for drug delivery by mesoscale simulations. Journal of Materials Chemistry, 2010, 20, 7742.	6.7	55
23	Quantitative 3D determination of self-assembled structures on nanoparticles using small angle neutron scattering. Nature Communications, 2018, 9, 1343.	12.8	54
24	To the nanoscale, and beyond!. Fluid Phase Equilibria, 2007, 261, 366-374.	2.5	48
25	Patchy and Janus Nanoparticles by Self-Organization of Mixtures of Fluorinated and Hydrogenated Alkanethiolates on the Surface of a Gold Core. ACS Nano, 2016, 10, 9316-9325.	14.6	48
26	A Complete Multiscale Modelling Approach for Polymer–Clay Nanocomposites. Chemistry - A European Journal, 2009, 15, 7586-7592.	3.3	43
27	Impact of siRNA Overhangs for Dendrimer-Mediated siRNA Delivery and Gene Silencing. Molecular Pharmaceutics, 2013, 10, 3262-3273.	4.6	43
28	Self-Assembly of Nanoparticle Mixtures in Diblock Copolymers: Multiscale Molecular Modeling. Industrial & Engineering Chemistry Research, 2008, 47, 5023-5038.	3.7	42
29	Nanoscale self-assembled multivalent (SAMul) heparin binders in highly competitive, biologically relevant, aqueous media. Chemical Science, 2014, 5, 1484.	7.4	42
30	3-Aryl-2-[1H-benzotriazol-1-yl]acrylonitriles: A novel class of potent tubulin inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 4151-4167.	5.5	40
31	Self-Organization of Mixtures of Fluorocarbon and Hydrocarbon Amphiphilic Thiolates on the Surface of Gold Nanoparticles. ACS Nano, 2012, 6, 7243-7253.	14.6	40
32	A simple new competition assay for heparin binding in serum applied to multivalent PAMAM dendrimers. Chemical Communications, 2013, 49, 4830.	4.1	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). Bioorganic and Medicinal Chemistry, 2010, 18, 2304-2316.	3.0	38
34	Size and shape matter! A multiscale molecular simulation approach to polymer nanocomposites. Journal of Materials Chemistry, 2012, 22, 5398.	6.7	38
35	A 3D-pharmacophore model for Ïf2 receptors based on a series of substituted benzo[d]oxazol-2(3H)-one derivatives. Bioorganic and Medicinal Chemistry Letters, 2010, 20, 2954-2957.	2.2	37
36	A molecular simulation approach to the prediction of the morphology of self-assembled nanoparticles in diblock copolymers. Journal of Materials Chemistry, 2010, 20, 10511.	6.7	36

PAOLA POSOCCO

#	Article	IF	CITATIONS
37	Antimycobacterial activity of new 3,5-disubstituted 1,3,4-oxadiazol-2(3H)-one derivatives. Molecular modeling investigations. Bioorganic and Medicinal Chemistry, 2009, 17, 4693-4707.	3.0	35
38	Graphene oxide as a 2D platform for complexation and intracellular delivery of siRNA. Nanoscale, 2019, 11, 13863-13877.	5.6	35
39	Double-degradable responsive self-assembled multivalent arrays – temporary nanoscale recognition between dendrons and DNA. Organic and Biomolecular Chemistry, 2014, 12, 446-455.	2.8	33
40	Self-assembled multivalent RGD-peptide arrays – morphological control and integrin binding. Organic and Biomolecular Chemistry, 2013, 11, 3177.	2.8	32
41	Synergistic experimental/computational studies on arylazoenamine derivatives that target the bovine viral diarrhea virus RNA-dependent RNA polymerase. Bioorganic and Medicinal Chemistry, 2010, 18, 6055-6068.	3.0	31
42	Electrostatic binding of polyanions using self-assembled multivalent (SAMul) ligand displays – structure–activity effects on DNA/heparin binding. Chemical Science, 2016, 7, 4653-4659.	7.4	31
43	Binding at the Core. Computational Study of Structural and Ligand Binding Properties of Naphthyridine-Based Dendrimers. Macromolecules, 2007, 40, 2257-2266.	4.8	30
44	Supramolecular Tripeptide Hydrogel Assembly with 5-Fluorouracil. Gels, 2019, 5, 5.	4.5	30
45	Through the open door: Preferential binding of dasatinib toÂthe active form of BCRâ€ABL unveiled by <i>in silico</i> experiments. Molecular Oncology, 2013, 7, 968-975.	4.6	28
46	Tell Me Something I Do Not Know. Multiscale Molecular Modeling of Dendrimer/ Dendron Organization and Self-Assembly In Gene Therapy. Current Medicinal Chemistry, 2012, 19, 5062-5087.	2.4	28
47	Highly grafted polystyrene/polyvinylpyridine polymer gold nanoparticles in a good solvent: effects of chain length and composition. Soft Matter, 2016, 12, 3600-3611.	2.7	25
48	Modeling hierarchically structured nanoparticle/diblock copolymer systems. Soft Matter, 2013, 9, 2936.	2.7	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. ACS Applied Materials & Interfaces, 2012, 4, 2855-2859.	8.0	21
50	Shapeâ€Persistent and Adaptive Multivalency: Rigid Transgeden (TGD) and Flexible PAMAM Dendrimers for Heparin Binding. Chemistry - A European Journal, 2014, 20, 9666-9674.	3.3	21
51	MULTISCALE MODELING OF POLYMER/CLAY NANOCOMPOSITES. Journal of Multiscale Modeling, 2011, 03, 151-176.	1.1	20
52	Copper(ii) binding to flexible triethanolamine-core PAMAM dendrimers: a combined experimental/in silico approach. Physical Chemistry Chemical Physics, 2014, 16, 685-694.	2.8	20
53	Emergence of highly-ordered hierarchical nanoscale aggregates on electrostatic binding of self-assembled multivalent (SAMul) cationic micelles with polyanionic heparin. Journal of Materials Chemistry B, 2017, 5, 341-347.	5.8	20
54	Imatinib response in two GIST patients carrying two hitherto functionally uncharacterized PDGFRA mutations: An imaging, biochemical and molecular modeling study. International Journal of Cancer, 2011, 128, 983-990.	5.1	18

#	Article	IF	CITATIONS
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. Analytica Chimica Acta, 2014, 808, 163-174.	5.4	18
56	Combined Mesoscale/Experimental Study of Selective Placement of Magnetic Nanoparticles in Diblock Copolymer Films via Solvent Vapor Annealing. Journal of Physical Chemistry C, 2016, 120, 7403-7411.	3.1	18
57	Exploring the Shape Influence on Melting Temperature, Enthalpy, and Solubility of Organic Drug Nanocrystals by a Thermodynamic Model. Crystal Growth and Design, 2017, 17, 4072-4083.	3.0	18
58	Mixed Fluorinated/Hydrogenated Selfâ€Assembled Monolayerâ€Protected Gold Nanoparticles: In Silico and In Vitro Behavior. Small, 2019, 15, e1900323.	10.0	18
59	In vitro and in silico studies of MDM2/MDMX isoforms predict Nutlin-3A sensitivity in well/de-differentiated liposarcomas. Laboratory Investigation, 2013, 93, 1232-1240.	3.7	17
60	Chiral recognition at self-assembled multivalent (SAMul) nanoscale interfaces – enantioselectivity in polyanion binding. Chemical Communications, 2016, 52, 10540-10543.	4.1	17
61	Mix and Match: Coassembly of Amphiphilic Dendrimers and Phospholipids Creates Robust, Modular, and Controllable Interfaces. ACS Applied Materials & amp; Interfaces, 2017, 9, 1029-1035.	8.0	17
62	2-Difluoromethylene-4-methylenepentanoic Acid, A Paradoxical Probe Able To Mimic the Signaling Role of 2-Oxoglutaric Acid in Cyanobacteria. Organic Letters, 2011, 13, 2924-2927.	4.6	16
63	Iron-mediated interaction of alpha synuclein with lipid raft model membranes. Nanoscale, 2020, 12, 7631-7640.	5.6	16
64	Selfâ€Assembled Multivalent (SAMul) Polyanion Binding—Impact of Hydrophobic Modifications in the Micellar Core on DNA and Heparin Binding at the Peripheral Cationic Ligands. Chemistry - A European Journal, 2017, 23, 6391-6397.	3.3	15
65	Scripting approach in hybrid organic–inorganic condensation simulation: the GPTMS proof-of-concept. Molecular Simulation, 2008, 34, 1215-1236.	2.0	14
66	Rationalizing the Fâ<⁻S interaction discovered within a tetrafluorophenylazido-containing bola-phospholipid. Chemical Communications, 2012, 48, 4284.	4.1	14
67	Structure–activity relationship study of dendritic polyglycerolamines for efficient siRNA transfection. RSC Advances, 2015, 5, 78760-78770.	3.6	14
68	Morphological control of self-assembled multivalent (SAMul) heparin binding in highly competitive media. Chemical Communications, 2017, 53, 6335-6338.	4.1	14
69	Structural Requirements of 2-Oxoglutaric Acid Analogues To Mimic Its Signaling Function. Organic Letters, 2013, 15, 4662-4665.	4.6	13
70	Cationic carbosilane dendrimers and oligonucleotide binding: an energetic affair. Nanoscale, 2015, 7, 3876-3887.	5.6	12
71	Effect of surface decoration on properties and drug release ability of nanogels. Colloids and Surfaces A: Physicochemical and Engineering Aspects, 2021, 614, 126164.	4.7	12
72	MoDeNa Nanotools: An integrated multiscale simulation workflow to predict thermophysical properties of thermoplastic polyurethapes, Journal of Computational Science, 2016, 15, 24-33	2.9	10

PAOLA POSOCCO

#	Article	IF	CITATIONS
73	Probing Multiscale Factors Affecting the Reactivity of Nanoparticle-Bound Molecules. ACS Nano, 2021, 15, 8295-8305.	14.6	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.	2.5	7
75	The interaction of β2-microglobulin with gold nanoparticles: impact of coating, charge and size. Journal of Materials Chemistry B, 2018, 6, 5964-5974.	5.8	7
76	Effects of primary amine-based coatings on microglia internalization of nanogels. Colloids and Surfaces B: Biointerfaces, 2020, 185, 110574.	5.0	7
77	Phase Behavior of Gradient Copolymer Melts with Different Gradient Strengths Revealed by Mesoscale Simulations. Polymers, 2020, 12, 2462.	4.5	6
78	Nano tools for macro problems: multiscale molecular modeling of nanostructured polymer systems. Composite Interfaces, 2013, 20, 379-394.	2.3	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.	2.8	5
80	Theoretical Importance of PVP-Alginate Hydrogels Structure on Drug Release Kinetics. Gels, 2019, 5, 22.	4.5	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.	4.1	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.	9.4	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.	10.0	3
85	Fluorescent Imprinted Nanoparticles for the Effective Monitoring of Irinotecan in Human Plasma. Nanomaterials, 2020, 10, 1707.	4.1	3
86	Molecular Features for Probing Small Amphiphilic Molecules with Self-Assembled Monolayer-Protected Nanoparticles. Langmuir, 2020, 36, 5671-5679.	3.5	3
87	The importance of molecular structure and functionalization of oxo-graphene sheets for gene silencing. Carbon, 2022, , .	10.3	3
88	Anomerization of Acrylated Clucose During Traveling Wave Ion Mobility Spectrometry. Journal of the American Society for Mass Spectrometry, 2015, 26, 1483-1493.	2.8	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.	4.1	2

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