Giovanni M Pavan

List of Publications by Citations

102 papers	3,232 citations	34 h-index	52 g-index
129 ext. papers	3,844 ext. citations	9 avg, IF	5.56 L-index

#	Paper	IF	Citations
102	Activity of dasatinib against L576P KIT mutant melanoma: molecular, cellular, and clinical correlates. *Molecular Cancer Therapeutics*, **2009**, 8, 2079-85	6.1	163
101	The key role of the scaffold on the efficiency of dendrimer nanodrugs. *Nature Communications*, **2015**, 6, 7722	17.4	116
100	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, 9686-94	16.4	110
99	Consequences of chirality on the dynamics of a water-soluble supramolecular polymer. *Nature Communications*, **2015**, 6, 6234	17.4	94
98	Ability to adapt: different generations of PAMAM dendrimers show different behaviors in binding siRNA. *Journal of Physical Chemistry B*, **2010**, 114, 2667-75	3.4	90
97	Self-assembled poly-catenanes from supramolecular toroidal building blocks. *Nature*, **2020**, 583, 400-405	50.4	85
96	PAMAM dendrimers for siRNA delivery: computational and experimental insights. *Chemistry - A European Journal*, **2010**, 16, 7781-95	4.8	83
95	Self-Sorted, Random, and Block Supramolecular Copolymers via Sequence Controlled, Multicomponent Self-Assembly. *Journal of the American Chemical Society*, **2020**, 142, 7606-7617	16.4	75
94	Effect of H-Bonding on Order Amplification in the Growth of a Supramolecular Polymer in Water. *Journal of the American Chemical Society*, **2016**, 138, 13985-13995	16.4	75
93	Into the Dynamics of a Supramolecular Polymer at Submolecular Resolution. *Nature Communications*, **2017**, 8, 147	17.4	74
92	Validation of a novel molecular dynamics simulation approach for lipophilic drug incorporation into polymer micelles. *Journal of Physical Chemistry B*, **2012**, 116, 4338-45	3.4	73
91	A Block Supramolecular Polymer and Its Kinetically Enhanced Stability. *Journal of the American Chemical Society*, **2018**, 140, 10570-10577	16.4	71
90	Targeting the blind spot of polycationic nanocarrier-based siRNA delivery. *ACS Nano*, **2012**, 6, 9447-54	16.7	71
89	Elucidating the molecular mechanism of PAMAM-siRNA dendriplex self-assembly: effect of dendrimer charge density. *International Journal of Pharmaceutics*, **2011**, 416, 410-8	6.5	71
88	Molecular characterization of the interaction between siRNA and PAMAM G7 dendrimers by SAXS, ITC, and molecular dynamics simulations. *Biomacromolecules*, **2010**, 11, 3571-7	6.9	70
87	Computational insights into the interactions between DNA and siRNA with "rigid" and "flexible" triazine dendrimers. *Biomacromolecules*, **2010**, 11, 721-30	6.9	68
86	Synthesis of large dendrimers with the dimensions of small viruses. *Journal of the American Chemical Society*, **2013**, 135, 4660-3	16.4	59

85	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, 4519-32	4.8	57
84	From Cooperative Self-Assembly to Water-Soluble Supramolecular Polymers Using Coarse-Grained Simulations. *ACS Nano*, **2017**, 11, 1000-1011	16.7	56
83	Experimental and theoretical investigations in stimuli responsive dendrimer-based assemblies. *Nanoscale*, **2015**, 7, 3817-37	7.7	56
82	Molecular photoswitches mediating the strain-driven disassembly of supramolecular tubules. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 11850-11855	11.5	55
81	Cooperative Supramolecular Block Copolymerization for the Synthesis of Functional Axial Organic Heterostructures. *Journal of the American Chemical Society*, **2020**, 142, 11528-11539	16.4	51
80	Enhanced bioactivity of internally functionalized cationic dendrimers with PEG cores. *Biomacromolecules*, **2012**, 13, 4089-97	6.9	50
79	Catalytic chameleon dendrimers. *Journal of the American Chemical Society*, **2011**, 133, 14359-67	16.4	49
78	Protein-triggered supramolecular disassembly: insights based on variations in ligand location in amphiphilic dendrons. *Journal of the American Chemical Society*, **2014**, 136, 5385-99	16.4	48
77	Antitumor activity and molecular dynamics simulations of paclitaxel-laden triazine dendrimers. *Molecular Pharmaceutics*, **2012**, 9, 404-12	5.6	46
76	Ion-selective controlled assembly of dendrimer-based functional nanofibers and their ionic-competitive disassembly. *Journal of the American Chemical Society*, **2012**, 134, 3349-57	16.4	43
75	Molecular modeling and in vivo imaging can identify successful flexible triazine dendrimer-based siRNA delivery systems. *Journal of Controlled Release*, **2011**, 153, 23-33	11.7	42
74	Gadolinium MRI contrast agents based on triazine dendrimers: relaxivity and in vivo pharmacokinetics. *Bioconjugate Chemistry*, **2012**, 23, 2291-9	6.3	41
73	Experimental and computational evidence for an inversion in guest capacity in high-generation triazine dendrimer hosts. *Journal of the American Chemical Society*, **2012**, 134, 1942-5	16.4	40
72	Molecular Factors Controlling the Isomerization of Azobenzenes in the Cavity of a Flexible Coordination Cage. *Journal of the American Chemical Society*, **2020**, 142, 9792-9802	16.4	38
71	How Defects Control the Out-of-Equilibrium Dissipative Evolution of a Supramolecular Tubule. *ACS Nano*, **2019**, 13, 4322-4334	16.7	36
70	Computational approach for understanding the interactions of UV-degradable dendrons with DNA and siRNA. *Journal of Physical Chemistry B*, **2010**, 114, 5686-93	3.4	35
69	Self-organization of star-shaped columnar liquid crystals with a coaxial nanophase segregation revealed by a combined experimental and simulation approach. *Chemical Communications*, **2015**, 51, 1811-4	5.8	34
68	Supramolecular Copolymerization as a Strategy to Control the Stability of Self-Assembled Nanofibers. *Angewandte Chemie - International Edition*, **2018**, 57, 6843-6847	16.4	34

67	Combining metadynamics simulation and experiments to characterize dendrimers in solution. *Soft Matter*, **2013**, 9, 2593	3.6	34
66	Interaction studies reveal specific recognition of an anti-inflammatory polyphosphorhydrazone dendrimer by human monocytes. *Nanoscale*, **2015**, 7, 17672-84	7.7	33
65	Biomimetic Synthesis of Sub-20 nm Covalent Organic Frameworks in Water. *Journal of the American Chemical Society*, **2020**, 142, 3540-3547	16.4	33
64	Design, synthesis and biological assessment of a triazine dendrimer with approximately 16 Paclitaxel groups and 8 PEG groups. *Molecular Pharmaceutics*, **2013**, 10, 4452-61	5.6	33
63	Structure and shape effects of molecular glue on supramolecular tubulin assemblies. *ACS Nano*, **2014**, 8, 904-14	16.7	32
62	Generation-dependent molecular recognition controls self-assembly in supramolecular dendron-virus complexes. *Nano Letters*, **2011**, 11, 723-8	11.5	32
61	Molecular modelling of supramolecular polymers. *Advances in Physics: X*, **2018**, 3, 1436408	5.1	31
60	Activate and resist: L576P-KIT in GIST. *Molecular Cancer Therapeutics*, **2009**, 8, 2491-5	6.1	30
59	From isodesmic to highly cooperative: reverting the supramolecular polymerization mechanism in water by fine monomer design. *Chemical Communications*, **2018**, 54, 4112-4115	5.8	28
58	Crystalline Cyclophane-Protein Cage Frameworks. *ACS Nano*, **2018**, 12, 8029-8036	16.7	27
57	Dendrimer-based fluorescent indicators: in vitro and in vivo applications. *PLoS ONE*, **2011**, 6, e28450	3.7	27
56	Modeling the interaction between dendrimers and nucleic acids: a molecular perspective through hierarchical scales. *ChemMedChem*, **2014**, 9, 2623-31	3.7	25
55	Identifying and Tracking Defects in Dynamic Supramolecular Polymers. *Journal of Physical Chemistry B*, **2020**, 124, 589-599	3.4	25
54	Role of Aromatic Interactions in Temperature-Sensitive Amphiphilic Supramolecular Assemblies. *Langmuir*, **2016**, 32, 2874-81	4	24
53	Consequences of a cosolvent on the structure and molecular dynamics of supramolecular polymers in water. *Chemical Science*, **2018**, 9, 6199-6209	9.4	24
52	Optically degradable dendrons for temporary adhesion of proteins to DNA. *Chemistry - A European Journal*, **2010**, 16, 6912-8	4.8	23
51	Role of generation, architecture, pH and ionic strength on successful siRNA delivery and transfection by hybrid PPV-PAMAM dendrimers. *Current Medicinal Chemistry*, **2012**, 19, 4929-41	4.3	23
50	Effect of Concentration on the Supramolecular Polymerization Mechanism via Implicit-Solvent Coarse-Grained Simulations of Water-Soluble 1,3,5-Benzenetricarboxamide. *Journal of Physical Chemistry Letters*, **2017**, 8, 3813-3819	6.4	21

49	T670X KIT mutations in gastrointestinal stromal tumors: making sense of missense. *Journal of the National Cancer Institute*, **2009**, 101, 194-204	9.7	21
48	Electrostatic co-assembly of nanoparticles with oppositely charged small molecules into static and dynamic superstructures. *Nature Chemistry*, **2021**, 13, 940-949	17.6	21
47	Low generation polyamine dendrimers bearing flexible tetraethylene glycol as nanocarriers for plasmids and siRNA. *Nanoscale*, **2016**, 8, 5106-19	7.7	20
46	Solvent-Driven Supramolecular Wrapping of Self-Assembled Structures. *Angewandte Chemie - International Edition*, **2021**, 60, 5407-5413	16.4	20
45	How the Dynamics of a Supramolecular Polymer Determines Its Dynamic Adaptivity and Stimuli-Responsiveness: Structure-Dynamics-Property Relationships From Coarse-Grained Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 4169-4178	3.4	18
44	The influence of dendron architecture on the "rigid" and "flexible" behaviour in binding DNA--a modelling study. *Physical Chemistry Chemical Physics*, **2010**, 12, 13914-7	3.6	18
43	Facile synthesis of stable, water soluble, dendron-coated gold nanoparticles. *Nanoscale*, **2017**, 9, 3128-3132	7.7	17
42	Programmable Nanoassemblies from Non-Assembling Homopolymers Using Ad Hoc Electrostatic Interactions. *Angewandte Chemie - International Edition*, **2017**, 56, 4145-4149	16.4	16
41	Computational design principles for the discovery of bioactive dendrimers: [s]-triazines and other examples. *Expert Opinion on Drug Discovery*, **2013**, 8, 1057-69	6.2	16
40	Unlucky number 13? Differential effects of KIT exon 13 mutation in gastrointestinal stromal tumors. *Molecular Oncology*, **2008**, 2, 161-3	7.9	16
39	Intrinsic Fluorescence of Triazine Dendrimers Provides a New Approach to Study Dendrimer Structure and Conformational Dynamics. *Journal of Physical Chemistry C*, **2017**, 121, 6946-6954	3.8	15
38	Three-Dimensional Directionality Is a Pivotal Structural Feature for the Bioactivity of Azabisphosphonate-Capped Poly(PhosphorHydrazone) Nanodrug Dendrimers. *Biomacromolecules*, **2018**, 19, 712-720	6.9	15
37	Impact of the water-compatible periphery on the dynamic and structural properties of benzene-1,3,5-tricarboxamide based amphiphiles. *Chemical Communications*, **2018**, 54, 11128-11131	5.8	14
36	Improving Fatigue Resistance of Dihydropyrene by Encapsulation within a Coordination Cage. *Journal of the American Chemical Society*, **2020**, 142, 14557-14565	16.4	13
35	Influence of linker groups on the solubility of triazine dendrimers. *New Journal of Chemistry*, **2015**, 39, 1247-1252	3.6	12
34	Structural and energetic basis for hybridization limits in high-density DNA monolayers. *Nanoscale*, **2013**, 5, 9988-93	7.7	12
33	Living supramolecular polymerization of fluorinated cyclohexanes. *Nature Communications*, **2021**, 12, 3134	17.4	12
32	: Automatic Parametrization of Bonded Terms in MARTINI-Based Coarse-Grained Models of Simple to Complex Molecules Fuzzy Self-Tuning Particle Swarm Optimization. *ACS Omega*, **2020**, 5, 32823-32843	3.9	11

31	Molecularly Defined Nanostructures Based on a Novel AAA-DDD Triple Hydrogen-Bonding Motif. *Angewandte Chemie - International Edition*, **2016**, 55, 1685-9	16.4	11
30	Exploring the Potential of Benzene-1,3,5-tricarboxamide Supramolecular Polymers as Biomaterials. *Biomacromolecules*, **2020**, 21, 4105-4115	6.9	11
29	A Data-Driven Dimensionality Reduction Approach to Compare and Classify Lipid Force Fields. *Journal of Physical Chemistry B*, **2021**, 125, 7785-7796	3.4	10
28	Theoretical and experimental characterization of amino-PEG-phosphonate-terminated Polyphosphorhydrazone dendrimers: Influence of size and PEG capping on cytotoxicity profiles. *Journal of Polymer Science Part A*, **2015**, 53, 761-774	2.5	9
27	Controlling the length of porphyrin supramolecular polymers via coupled equilibria and dilution-induced supramolecular polymerization.. *Nature Communications*, **2022**, 13, 248	17.4	9
26	Supramolecular Copolymerization as a Strategy to Control the Stability of Self-Assembled Nanofibers. *Angewandte Chemie*, **2018**, 130, 6959-6963	3.6	9
25	Insights into the Kinetics of Supramolecular Comonomer Incorporation in Water. *Macromolecules*, **2019**, 52, 3049-3055	5.5	8
24	Symbiotic Self-Assembly Strategy toward Lipid-Encased Cross-Linked Polymer Nanoparticles for Efficient Gene Silencing. *ACS Applied Materials & Interfaces*, **2019**, 11, 24971-24983	9.5	8
23	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	3.6	7
22	Solvent-Driven Supramolecular Wrapping of Self-Assembled Structures. *Angewandte Chemie*, **2021**, 133, 5467-5473	3.6	7
21	Protein□endron conjugates for DNA binding: understanding the effect of the protein core on multivalency. *RSC Advances*, **2011**, 1, 1677	3.7	6
20	Supporting the design of efficient dendritic DNA and siRNA nano-carriers with molecular modeling. *Current Drug Discovery Technologies*, **2011**, 8, 314-28	1.5	6
19	Synthesis of Dense and Chiral Dendritic Polyols Using Glyconanosynthon Scaffolds. *Molecules*, **2016**, 21, 448	4.8	6
18	Porous covalent organic nanotubes and their assembly in loops and toroids.. *Nature Chemistry*, **2022**,	17.6	6
17	Multiscale Molecular Modelling of ATP-Fueled Supramolecular Polymerisation and Depolymerisation**. *ChemSystemsChem*, **2021**, 3, e2000038	3.1	5
16	Understanding functional group and assembly dynamics in temperature responsive systems leads to design principles for enzyme responsive assemblies. *Nanoscale*, **2021**, 13, 11568-11575	7.7	5
15	Controlling Exchange Pathways in Dynamic Supramolecular Polymers by Controlling Defects. *ACS Nano*, **2021**, 15, 14229-14241	16.7	5
14	Nitrobenzoxadiazole-Appended Cell Membrane Modifiers for Efficient Optoporation with Noncoherent Light. *Bioconjugate Chemistry*, **2018**, 29, 2068-2073	6.3	4

13	Molecular communications in complex systems of dynamic supramolecular polymers.. *Nature Communications*, **2022**, 13, 2162	17.4	4
12	Programmable Nanoassemblies from Non-Assembling Homopolymers Using Ad Hoc Electrostatic Interactions. *Angewandte Chemie*, **2017**, 129, 4209-4213	3.6	3
11	Molecularly Defined Nanostructures Based on a Novel AAADDD Triple Hydrogen-Bonding Motif. *Angewandte Chemie*, **2016**, 128, 1717-1721	3.6	3
10	Toward Chemotactic Supramolecular Nanoparticles: From Autonomous Surface Motion Following Specific Chemical Gradients to Multivalency-Controlled Disassembly. *ACS Nano*, **2021**, 15, 16149-16161	16.7	3
9	Swarm-CG: Automatic Parametrization of Bonded Terms in Coarse-Grained Models of Simple to Complex Molecules via Fuzzy Self-Tuning Particle Swarm Optimization		2
8	Non-uniform Photoinduced Unfolding of Supramolecular Polymers Leading to Topological Block Nanofibers. *Angewandte Chemie - International Edition*, **2021**, 60, 26986	16.4	2
7	Site accessibility tailors DNA cleavage by restriction enzymes in DNA confined monolayers. *Nanoscale*, **2017**, 9, 6399-6405	7.7	1
6	Base Invaders. Coupling Experiments and Multiscale Modeling of Dendrimer-Based siRNA Delivery Agents. *Advances in Science and Technology*, **2008**, 57, 154-159	0.1	1
5	Automatic multi-objective optimization of coarse-grained lipid force fields using SwarmCG.. *Journal of Chemical Physics*, **2022**, 156, 024801	3.9	1
4	Understanding the Dynamics of Supramolecular Polymers. *Chimia*, **2020**, 74, 734	1.3	1
3	Solvent-driven chirality for luminescent self-assembled structures: experiments and theory. *Nanoscale*, **2020**, 12, 21359-21367	7.7	1
2	Discordant Supramolecular Fibres Reversibly Depolymerised by Temperature and Light. *Chemistry - A European Journal*, **2021**, 27, 1829-1838	4.8	0
1	Innentitelbild: Molecularly Defined Nanostructures Based on a Novel AAADDD Triple Hydrogen-Bonding Motif (Angew. Chem. 5/2016). *Angewandte Chemie*, **2016**, 128, 1594-1594	3.6	