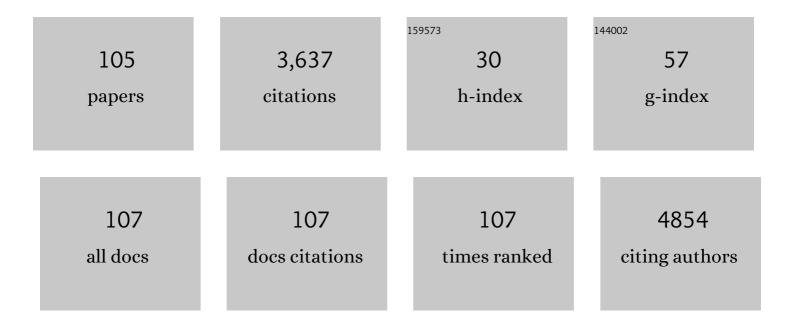
List of Publications by Year in descending order

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EMILIO PADISINI

#	Article	IF	CITATIONS
1	In Silico Engineering of Enzyme Access Tunnels. Methods in Molecular Biology, 2022, 2397, 203-225.	0.9	5
2	Anticancer Activity of the Choline Kinase Inhibitor PL48 Is Due to Selective Disruption of Choline Metabolism and Transport Systems in Cancer Cell Lines. Pharmaceutics, 2022, 14, 426.	4.5	3
3	Biological Evaluation of New Thienopyridinium and Thienopyrimidinium Derivatives as Human Choline Kinase Inhibitors. Pharmaceutics, 2022, 14, 715.	4.5	2
4	Hierarchical TiN‣upported TsFDH Nanobiocatalyst for CO ₂ Reduction to Formate. ChemElectroChem, 2021, 8, 2846-2857.	3.4	6
5	Design, synthesis, biological evaluation and structural characterization of novel GEBR library PDE4D inhibitors. European Journal of Medicinal Chemistry, 2021, 223, 113638.	5.5	8
6	New Compounds with Bioisosteric Replacement of Classic Choline Kinase Inhibitors Show Potent Antiplasmodial Activity. Pharmaceutics, 2021, 13, 1842.	4.5	1
7	Crystal Structure of the Apo and the ADP-Bound Form of Choline Kinase from Plasmodium falciparum. Crystals, 2020, 10, 613.	2.2	4
8	Rational backbone redesign of a fructosyl peptide oxidase to widen its active site access tunnel. Biotechnology and Bioengineering, 2020, 117, 3688-3698.	3.3	8
9	Insight into GEBR-32a: Chiral Resolution, Absolute Configuration and Enantiopreference in PDE4D Inhibition. Molecules, 2020, 25, 935.	3.8	8
10	Micro- and Nanopatterned Silk Substrates for Antifouling Applications. ACS Applied Materials & Interfaces, 2020, 12, 5437-5446.	8.0	27
11	Front Cover Image, Volume 117, Number 12, December 2020. Biotechnology and Bioengineering, 2020, 117, i.	3.3	Ο
12	Hybrid One-Dimensional Plasmonic–Photonic Crystals for Optical Detection of Bacterial Contaminants. Journal of Physical Chemistry Letters, 2019, 10, 4980-4986.	4.6	50
13	Structure-Based Virtual Screening Allows the Identification of Efficient Modulators of E-Cadherin-Mediated Cell–Cell Adhesion. International Journal of Molecular Sciences, 2019, 20, 3404.	4.1	20
14	Biohybrid Electrospun Membrane for the Filtration of Ketoprofen Drug from Water. ACS Omega, 2019, 4, 13270-13278.	3.5	29
15	Exploring E-cadherin-peptidomimetics interaction using NMR and computational studies. PLoS Computational Biology, 2019, 15, e1007041.	3.2	5
16	Thermal stabilization of the deglycating enzyme Amadoriase I by rational design. Scientific Reports, 2018, 8, 3042.	3.3	19
17	Synthesis, structure and behavior of vanadium(III) diphosphine complexes in the homo- and co-polymerization of ethylene with norbornene: the ligand donor strength and bite angle make the difference. Journal of Organometallic Chemistry, 2018, 861, 142-150.	1.8	14
18	Molecular Bases of PDE4D Inhibition by Memory-Enhancing GEBR Library Compounds. Biochemistry, 2018, 57, 2876-2888.	2.5	10

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19	Chain-Walking Polymerization of α-Olefins by α-Diimine Ni(II) Complexes: Effect of Reducing the Steric Hindrance of <i>Ortho-</i> and <i>Para-</i> Aryl Substituents on the Catalytic Behavior, Monomer Enchainment, and Polymer Properties. Macromolecules, 2018, 51, 801-814.	4.8	55
20	Concerted Electron Transfer in Iminopyridine Chromium Complexes: Ligand Effects on the Polymerization of Various (Di)olefins. Organometallics, 2018, 37, 4827-4840.	2.3	10
21	Cover Image, Volume 84, Issue 6. Proteins: Structure, Function and Bioinformatics, 2016, 84, C1-C1.	2.6	0
22	The interplay of soft-hard substituents in photochromic diarylethenes. Journal of Photochemistry and Photobiology A: Chemistry, 2016, 325, 45-54.	3.9	4
23	Crystal Structure of Human E-Cadherin-EC1EC2 in Complex with a Peptidomimetic Competitive Inhibitor of Cadherin Homophilic Interaction. Journal of Medicinal Chemistry, 2016, 59, 5089-5094.	6.4	17
24	Crystal structure of the deglycating enzyme Amadoriase I in its free form and substrateâ€bound complex. Proteins: Structure, Function and Bioinformatics, 2016, 84, 744-758.	2.6	17
25	Molecular dynamics simulations provide insights into the substrate specificity of FAOX family members. Molecular BioSystems, 2016, 12, 2622-2633.	2.9	14
26	Meeting the Challenging Magnetic and Electronic Structure of Thiophene-Based Heterophenoquinones. Journal of Physical Chemistry C, 2016, 120, 5732-5740.	3.1	10
27	Synthesis and Structural Properties of Aza[<i>n</i>]helicene Platinum Complexes: Control of Cis and Trans Stereochemistry. Inorganic Chemistry, 2016, 55, 2009-2017.	4.0	13
28	Synthesis and Characterization of Farâ€Red/NIRâ€Fluorescent BODIPY Dyes, Solidâ€State Fluorescence, and Application as Fluorescent Tags Attached to Carbon Nanoâ€onions. Chemistry - A European Journal, 2015, 21, 9727-9732.	3.3	49
29	Outside rules inside: the role of electron-active substituents in thiophene-based heterophenoquinones. Physical Chemistry Chemical Physics, 2015, 17, 10426-10437.	2.8	12
30	The X-ray structure of human P-cadherin EC1-EC2 in a closed conformation provides insight into the type I cadherin dimerization pathway. Acta Crystallographica Section F, Structural Biology Communications, 2015, 71, 371-380.	0.8	10
31	Computational design of novel peptidomimetic inhibitors of cadherin homophilic interactions. Organic and Biomolecular Chemistry, 2015, 13, 2570-2573.	2.8	16
32	Mycobacterium tuberculosis Low Molecular Weight Phosphatases (MPtpA and MPtpB): From Biological Insight to Inhibitors. Current Medicinal Chemistry, 2015, 22, 3110-3132.	2.4	31
33	Salvage combination antifungal therapy for acute invasive aspergillosis may improve outcomes: a systematic review and meta-analysis. International Journal of Infectious Diseases, 2014, 28, 80-94.	3.3	50
34	Time-Dependent Structure and Solubilization Kinetics of Graphene Oxide in Methanol and Water Dispersions. Journal of Physical Chemistry C, 2014, 118, 28162-28169.	3.1	24
35	Boron dipyrromethene (BODIPY) functionalized carbon nano-onions for high resolution cellular imaging. Nanoscale, 2014, 6, 13761-13769.	5.6	72
36	Structure–Photoluminescence Correlation for Two Crystalline Polymorphs of a Thiophene–Phenylene Co-Oligomer with Bulky Terminal Substituents. Journal of Physical Chemistry Letters, 2014, 5, 2171-2176.	4.6	37

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37	Ly6 family proteins in neutrophil biology. Journal of Leukocyte Biology, 2013, 94, 585-594.	3.3	227
38	Vasopressin and terlipressin in adult vasodilatory shock. Critical Care, 2012, 16, 470.	5.8	2
39	Collective evidence supports neutrality of BRCA1 V1687I, a novel sequence variant in the conserved THV motif of the first BRCT repeat. Breast Cancer Research and Treatment, 2012, 134, 435-441.	2.5	1
40	Vasopressin for treatment of vasodilatory shock: an ESICM systematic review and meta-analysis. Intensive Care Medicine, 2012, 38, 9-19.	8.2	88
41	Halogen bonding in halocarbon–protein complexes: a structural survey. Chemical Society Reviews, 2011, 40, 2267.	38.1	399
42	NSAID Exposure and Risk of Nonunion: A Meta-Analysis of Case–Control and Cohort Studies. Calcified Tissue International, 2010, 87, 193-202.	3.1	197
43	Comparison of Web-Versus Classroom-Based Basic Ultrasonographic and EFAST Training in 2 European Hospitals. Annals of Emergency Medicine, 2010, 56, 660-667.e1.	0.6	55
44	Multimodal Assessment of Protein Functional Deficiency Supports Pathogenicity of BRCA1 p.V1688del. Cancer Research, 2009, 69, 7030-7037.	0.9	16
45	Meta-analysis: Travel and Risk for Venous Thromboembolism. Annals of Internal Medicine, 2009, 151, 180.	3.9	159
46	pH-Dependent Interdomain Tethers of CD1b Regulate Its Antigen Capture. Immunity, 2008, 28, 774-786.	14.3	47
47	Distinct Structural Requirements of GATA-3 for the Regulation of Thymocyte and Th2 Cell Differentiation. Journal of Immunology, 2008, 180, 1050-1059.	0.8	11
48	The Crystal Structure of Human E-cadherin Domains 1 and 2, and Comparison with other Cadherins in the Context of Adhesion Mechanism. Journal of Molecular Biology, 2007, 373, 401-411.	4.2	112
49	From The Cover: Characterization of two avian MHC-like genes reveals an ancient origin of the CD1 family. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 8674-8679.	7.1	98
50	Structural and Mutational Analyses of a CD8αβ Heterodimer and Comparison with the CD8αα Homodimer. Immunity, 2005, 23, 661-671.	14.3	39
51	Structure of the regulatory subunit of CK2 in the presence of a p21WAF1peptide demonstrates flexibility of the acidic loop. Acta Crystallographica Section D: Biological Crystallography, 2004, 60, 1698-1704.	2.5	6
52	Disparate peptide-dependent thymic selection outcomes in β2M-deficient mice versus TAP-1-deficient mice: implications for repertoire formation. European Journal of Immunology, 2003, 33, 368-380.	2.9	2
53	A New Strategy for the Stereoselective Synthesis of 1,2,3-Trisubstituted Cyclopropanes. European Journal of Organic Chemistry, 2000, 2000, 2955-2965.	2.4	67
54	Protein-Protein Interactions in Receptor Activation and Intracellular Signalling. Biological Chemistry, 2000, 381, 955-9.	2.5	51

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55	Ab initio solution and refinement of two high-potential iron protein structures at atomic resolution. Acta Crystallographica Section D: Biological Crystallography, 1999, 55, 1773-1784.	2.5	36
56	Crystal structure determination at 1.4 Ã resolution of ferredoxin from the green alga Chlorella fusca. Structure, 1999, 7, 1201-S2.	3.3	63
57	Crystal structure of the complex of the cyclin D-dependent kinase Cdk6 bound to the cell-cycle inhibitor p19INK4d. Nature, 1998, 396, 390-390.	27.8	0
58	Crystal structure of the complex of the cyclin D-dependent kinase Cdk6 bound to the cell-cycle inhibitor p19INK4d. Nature, 1998, 395, 244-250.	27.8	199
59	Reactions of Thioketones with a Fluorinated ThioneS-Imide. European Journal of Organic Chemistry, 1998, 1998, 459-465.	2.4	16
60	Synthesis and Characterization of Tris(trimethylsilyl)methyl Halide Derivatives of Aluminum:Â Potential Precursors for Low-Valent Aluminum Compounds. Crystal Structures of [{(Me3Si)3CAlF2}3], [(Me3Si)3CAlX2·THF] (X = Cl, Br, I), and [{(THF)2K(Me3Si)3CAlF2(μ-F)F2AlC(SiMe3)3}2]â€. Organometallics, 1998, 17, 2249-2257.	2.3	57
61	Synthesis and structure of an anionic aluminium–nitrogen compound containing a ladder-shaped core. Journal of the Chemical Society Dalton Transactions, 1997, , 2761-2764.	1.1	8
62	Synthesis and Characterization of (4-Fluorophenyl)amino-Based Amino- and Iminometallanes of Group 13. Crystal Structures of (MeAlNRf)4, (MeMNRf)6A·nTHF (M = Al,n= 2; M = Ga,n= 7), and (MeIn(THF)NRf)4(Rf= 4-C6H4F)â€. Organometallics, 1997, 16, 1197-1202.	2.3	32
63	Aminodimethylalanes (R1R2NAlMe2) as Useful Synthetic Precursors of Aminoalane Difluorides Using Trimethyltin Fluoride:Â Crystal Structures of (2,6-i-Pr2C6H3)N(SiMe3)AlMe2and (2,6-i-Pr2C6H3)N(SiMe3)AlF2â€. Organometallics, 1997, 16, 1260-1264.	2.3	55
64	Synthesis and characterisation of trifluoro(η5-n-propyltetramethylcyclopentadienyl) metal(IV)-compounds of the elements of group IV. Journal of Organometallic Chemistry, 1997, 536-537, 177-180.	1.8	6
65	Areneî—,alkyne derivatives of RU6C(CO)17: synthesis and structure of RU6C(CO)12 (η6-arene)(η3-C2Me2) (arene î—» C6H6â înMen, n = 0–3) and RU6C(CO)12(μ3-C16H16)(μ3-C2Me2). Journal of Organometallic Cl 1997, 532, 133-142.	ne ns istry,	13
66	Soluble Molecular Titanosilicates. Angewandte Chemie International Edition in English, 1997, 36, 1001-1003.	4.4	46
67	Organic-Soluble Neutral and Ionic Indium Siloxane Cages: Potential Precursors for Indium-Containing Silicates. Angewandte Chemie International Edition in English, 1997, 36, 2203-2205.	4.4	29
68	The Role of the 2,4,6â€Tris(trifluoromethyl)phenylamino Group in Stabilizing New Phosphorusâ€, Arsenicâ€, and Germaniumâ€Containing Mainâ€Group Compounds and Transitionâ€Metal Derivatives. Chemische Berichte, 1997, 130, 1113-1121.	0.2	51
69	Synthesis, Structure and Hydrolysis Studies of Dimethyltris(Trimethylsilyl)Methylmetallanes of Aluminium and Gallium. Chemistry - A European Journal, 1997, 3, 1783-1792.	3.3	70
70	Organometallic Fluorides of Zirconium and Hafnium in the Synthesis of Carboxylate Complexes:Â Molecular Structures of [{(Î-5-C5Me5)ZrF(OCOCF3)2}2] and [(Î-5-C5Me5)2Zr(OCOCF3)2]. Inorganic Chemistry, 1996, 35, 7181-7184.	4.0	18
71	Group 4 Metal Amido Fluorides and Chlorides:Â Molecular Structures and the First Comparison in Ethylene Polymerization Catalysis. Organometallics, 1996, 15, 3176-3181.	2.3	108
72	An efficient synthetic route to primary and secondary condensation products of silanetriols starting from (arylamino)trichlorosilanes. Chemical Communications, 1996, , 2417-2418.	4.1	27

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73	Derivatives of Group 4 metal amide chlorides and fluorides: synthesis, structure and characterization of novel dimethyl and fluoro–chloro complexes. Journal of the Chemical Society Dalton Transactions, 1996, , 4143-4146.	1.1	4
74	Synthesis and spectroscopic characterization of a series of substituted cyclopentadienyl Group 4 fluorides; crystal structure of the acetylacetonato complex [(acac)2(η-C5Me5)Zr(µ-F)SnMe3Cl]. Journal of the Chemical Society Dalton Transactions, 1996, , 1983-1987.	1.1	29
75	Synthesis and Structure of Gallium Siloxane Cages: Model Substances for Gallium-Containing Silicates. Angewandte Chemie International Edition in English, 1996, 35, 748-750.	4.4	40
76	The synthesis, molecular and crystal structure of the bis(arene) hexaruthenium carbido-carbonyl isomers Ru6C(CO)11(C6H4Me2-1,3)(C6H5Me). Inorganica Chimica Acta, 1995, 235, 413-420.	2.4	9
77	Crystal structures of salts of transition-metal halide clusters. Journal of the Chemical Society Dalton Transactions, 1995, , 287.	1.1	10
78	Synthesis and Characterization of Ru3 and Ru4 Clusters with Isopropenylbenzene and Diisopropenylbenzene Ligands. Organometallics, 1995, 14, 4892-4898.	2.3	14
79	Synthesis and molecular structure of tetraruthenium clusters carrying facial arene ligands. Journal of the Chemical Society Chemical Communications, 1995, , 537.	2.0	6
80	Synthesis and crystallographic characterisation of [Ru7C(CO)16(C9H8)] and [Ru7C(CO)16(C12H12)]: facial ? bonding and ? bonding from the same ring system. Journal of the Chemical Society Dalton Transactions, 1995, , 3431.	1.1	5
81	Synthesis and characterisation of guaiazulene derivatives of two ruthenium carbonyl clusters. Journal of the Chemical Society Dalton Transactions, 1995, , 3307.	1.1	14
82	Dynamics and molecular aggregation in crystalline [{M(C5H5)}3(µ3-η2: η2: η2-C6H5R)][M = Co, R = CH(Ph)Me, CH2CH2Ph or CHCHMe; M = Rh, R = H] clusters. Journal of the Chemical Society Dalton Transactions, 1995, , 1089-1093.	1.1	4
83	Solid-state studies into the possible rearrangement mechanisms for the fluxional behaviour of the tetranuclear carbonyls M4(CO)12 and their derivatives. Journal of Organometallic Chemistry, 1994, 478, 21-28.	1.8	9
84	The synthesis and characterisation of the octaruthenium–benzene cluster [Ru8H4(CO)18(η6-C6H6)]. Journal of the Chemical Society Chemical Communications, 1994, , 1253-1254.	2.0	9
85	Sequential synthesis of some tetraosmium–arene clusters. Journal of the Chemical Society Dalton Transactions, 1994, , 2167-2175.	1.1	11
86	Cocrystallization of Organometallic Clusters: Homo- and Heteromolecular Crystals of Ru6C(CO)14(.eta.6-C6H4Me2) and Ru6C(CO)11(.eta.6-C6H4Me2)2. Organometallics, 1994, 13, 2170-2177.	2.3	19
87	[2.2]Paracyclophane as a Face-Capping Ligand: Conformational Variability over the Ruthenium Triangle. Organometallics, 1994, 13, 2113-2117.	2.3	30
88	A new mechanism for the rearrangement of the icosahedral carboranes. Inorganica Chimica Acta, 1993, 211, 17-21.	2.4	15
89	The synthesis, characterization and molecular structures of two mixed metal octahedral carbido clusters, Ru5RhC(CO)14(ŀ5-C5Me5) and Ru5RhC(CO)9(ŀ5-C5Me5)(ŀ5-C5H5)2. Journal of Organometallic Chemistry, 1993, 452, 175-179.	1.8	29
90	The synthesis, structural characterisation and variable temperature 1H NMR study of the bis-toluene hexaruthenium carbidocarbonyl cluster [Ru6C(CO)11(η6C6H5Me)(ι⁄43-η2: η2: η2-C6H5Me)]. Journal of Organometallic Chemistry, 1993, 462, 301-308.	1.8	22

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91	Stereochemical changes in mononuclear complexes MLn (n = 10–12). Polyhedron, 1993, 12, 897-901.	2.2	2
92	Molecular salts of high nuclearity cluster anions: cation control on the crystal structure. Inorganica Chimica Acta, 1993, 213, 121-127.	2.4	7
93	Synthesis, molecular and crystal structures of arene derivatives of [Ru6C(CO)17]. Journal of the Chemical Society Dalton Transactions, 1993, , 2951.	1.1	30
94	Hexanuclear arene clusters of ruthenium. Journal of the Chemical Society Dalton Transactions, 1993, , 2817.	1.1	24
95	New synthetic routes to [M3(CO)9(µ3-η2:η2:Ĉ-C6H6)](M = Ru or Os). Journal of the Chemical Society Dalton Transactions, 1993, , 981-984.	1.1	27
96	Synthesis of [M3H(CO)9(µ3-σ:η2:η2-C6H7)](M = Ru or Os). Molecular and crystal structure of the ruthenium cluster. Journal of the Chemical Society Dalton Transactions, 1993, , 1891-1895.	1.1	32
97	Application of the ligand polyhedral model to the fluxionality of Fe3(CO)10(CNCF3)(L) (L = CO, PMe3,) Tj ETQq1	1 0.7843] 2.3	14.rgBT /0ve
98	Cation control on the crystal organization of hexanuclear carbonyl cluster anions. Journal of the American Chemical Society, 1993, 115, 5115-5122.	13.7	34
99	Synthesis and x-ray structure of the tetranuclear butterfly iridium cluster Ir4(CO)8L[.mu.3eta.3-Ph2PC(H)CPh](.muPPh2) (L = PCy3) and carbon-13, proton, and 13C{1H}, 1H, and 31P{1H} NMR studies of the compounds with L = CO, PCy3, and P(OMe)3, [carbon monoxide, tricvclohexvlphosphine. and trimethyl phosphite]. Organometallics. 1993. 12. 2955-2961.	2.3	16
100	Trinuclear benzene clusters of ruthenium and osmium. Journal of the Chemical Society Dalton Transactions, 1992, , 807.	1.1	27
101	Fluxional behaviour of the carbonyls [M3(CO)12](M = Fe, Ru or Os). Journal of the Chemical Society Dalton Transactions, 1992, , 2573.	1.1	19
102	Application of the ligand polyhedral model to dicobalt octacarbonyl. Inorganica Chimica Acta, 1992, 198-200, 345-349.	2.4	5
103	Reaction of [Os4(µ-H)4(CO)12] with cyclohexa-1,3-diene via chemical activation: synthesis and structural characterisation of [Os4(µ-H)2(CO)10(η6-C6H6)] and [Os4(CO)9(η6-C6H6)(η4-C6H8)] and their interconversion. Journal of the Chemical Society Dalton Transactions, 1991, , 215-219.	1.1	26
104	Dynamic processes in the solid state. Diene flip and ring reorientation in crystalline zirconocene complexes. Organometallics, 1991, 10, 3735-3739.	2.3	8
105	Dynamic processes in crystals of transition metal clusters. Materials Chemistry and Physics, 1991, 29, 165-173.	4.0	0