Federica Moraca

List of Publications by Year
in descending order

40 papers	1,015 citations	361045 20 h-index	433756 31 g-index
42 all docs	42 docs citations	42 times ranked	1708 citing authors

#	Article	IF	Citations
1	Ligand binding to telomeric G-quadruplex DNA investigated by funnel-metadynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E2136-E2145.	3.3	91
2	Identification and Characterization of New DNA G-Quadruplex Binders Selected by a Combination of Ligand and Structure-Based Virtual Screening Approaches. Journal of Medicinal Chemistry, 2013, 56, 843-855.	2.9	81
3	Hijacking SARS-CoV-2/ACE2 Receptor Interaction by Natural and Semi-synthetic Steroidal Agents Acting on Functional Pockets on the Receptor Binding Domain. Frontiers in Chemistry, 2020, 8, 572885.	1.8	76
4	Mediterranean products as promising source of multi-target agents in the treatment of metabolic syndrome. European Journal of Medicinal Chemistry, 2020, 186, 111903.	2.6	66
5	The Mediterranean Diet as source of bioactive compounds with multi-targeting anti-cancer profile. European Journal of Medicinal Chemistry, 2019, 181, 111579.	2.6	51
6	Structureâ€“activity relationships of novel substituted naphthalene diimides as anticancer agents. European Journal of Medicinal Chemistry, 2012, 57, 417-428.	2.6	44
7	GRID-Based Three-Dimensional Pharmacophores II: PharmBench, a Benchmark Data Set for Evaluating Pharmacophore Elucidation Methods. Journal of Chemical Information and Modeling, 2012, 52, 2599-2608.	2.5	36
8	Macrocyclic naphthalene diimides as G-quadruplex binders. Bioorganic and Medicinal Chemistry, 2015, 23, 3819-3830.	1.4	34
9	Identification of G-quadruplex DNA/RNA binders: Structure-based virtual screening and biophysical characterization. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 1329-1340.	1.1	33
10	Targeting unimolecular G-quadruplex nucleic acids: a new paradigm for the drug discovery?. Expert Opinion on Drug Discovery, 2014, 9, 1167-1187.	2.5	31
11	Novel natural non-nucleoside inhibitors of HIV-1 reverse transcriptase identified by shape- and structure-based virtual screening techniques. European Journal of Medicinal Chemistry, 2019, 161, 1-10.	2.6	31
12	Feedback inhibition of cAMP effector signaling by a chaperone-assisted ubiquitin system. Nature Communications, 2019, 10, 2572.	5.8	29
13	Structure-Based Virtual Screening of Novel Natural Alkaloid Derivatives as Potential Binders of h-telo and c-myc DNA G-Quadruplex Conformations. Molecules, 2015, 20, 206-223.	1.7	25
14	Molecular recognition of a carboxy pyridostatin toward Gâ€quadruplex structures: Why does it prefer <scp>RNA</scp>?. Chemical Biology and Drug Design, 2017, 90, 919-925.	1.5	25
15	C-6Î±- vs C-7Î±-Substituted Steroidal Aromatase Inhibitors: Which Is Better? Synthesis, Biochemical Evaluation, Docking Studies, and Structureâ€“Activity Relationships. Journal of Medicinal Chemistry, 2019, 62, 3636-3657.	2.9	25
16	The Polymorphisms of DNA G-Quadruplex Investigated by Docking Experiments with Telomestatin Enantiomers. Current Pharmaceutical Design, 2012, 18, 1873-1879.	0.9	23
17	Toward the design of new DNA G-quadruplex ligands through rational analysis of polymorphism and binding data. European Journal of Medicinal Chemistry, 2013, 68, 139-149.	2.6	23
18	A computer-assisted discovery of novel potential anti-obesity compounds as selective carbonic anhydrase VA inhibitors. European Journal of Medicinal Chemistry, 2019, 181, 111565.	2.6	23

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19	Chemoinformatic Database Building and in Silico Hit-Identification of Potential Multi-Targeting Bioactive Compounds Extracted from Mushroom Species. Molecules, 2017, 22, 1571.	1.7	22
20	Folding intermediate states of the parallel human telomeric G-quadruplex DNA explored using Well-Tempered Metadynamics. Scientific Reports, 2020, 10, 3176.	1.6	21
21	Review about the multi-target profile of resveratrol and its implication in the SGK1 inhibition. European Journal of Medicinal Chemistry, 2019, 183, 111675.	2.6	20
22	In Silico Identification of Piperidinyl-amine Derivatives as Novel Dual Binders of Oncogene c-myc/c-Kit G-quadruplexes. ACS Medicinal Chemistry Letters, 2018, 9, 848-853.	1.3	19
23	Naphthalene diimide-polyamine hybrids as antiproliferative agents: Focus on the architecture of the polyamine chains. European Journal of Medicinal Chemistry, 2017, 128, 107-122.	2.6	17
24	Molecular modelling of epitopes recognized by neoplastic B lymphocytes in Chronic Lymphocytic Leukemia. European Journal of Medicinal Chemistry, 2020, 185, 111838.	2.6	17
25	Computer-based techniques for lead identification and optimization I: Basics. Physical Sciences Reviews, 2019, 4, .	0.8	16
26	A Comparative Docking Strategy to Identify Polyphenolic Derivatives as Promising Antineoplastic Binders of Gâ€quadruplex DNA câ€myc and bclâ€2 Sequences. Molecular Informatics, 2016, 35, 391-402.	1.4	15
27	Targeting multiple G-quadruplexâ€"forming DNA sequences: Design, biophysical and biological evaluations of indolo-naphthyridine scaffold derivatives. European Journal of Medicinal Chemistry, 2019, 182, 111627.	2.6	15
28	The TBC1D31/praja2 complex controls primary ciliogenesis through PKAâ€directed OFD1 ubiquitylation. EMBO Journal, 2021, 40, e106503.	3.5	15
29	Discovery of Bile Acid Derivatives as Potent ACE2 Activators by Virtual Screening and Essential Dynamics. Journal of Chemical Information and Modeling, 2022, 62, 196-209.	2.5	15
30	Hit Identification of a Novel Dual Binder for hâ€telo/câ€myc Gâ€Quadruplex by a Combination of Pharmacophore Structureâ€Based Virtual Screening and Docking Refinement. ChemMedChem, 2016, 11, 1721-1733.	1.6	14
31	Multi-Targeting Bioactive Compounds Extracted from Essential Oils as Kinase Inhibitors. Molecules, 2020, 25, 2174.	1.7	10
32	Exploring the fatty acid amide hydrolase and cyclooxygenase inhibitory properties of novel amide derivatives of ibuprofen. Journal of Enzyme Inhibition and Medicinal Chemistry, 2020, 35, 815-823.	2.5	9
33	Computer-based techniques for lead identification and optimization II: Advanced search methods. Physical Sciences Reviews, 2020, 5, .	0.8	8
34	Extended Naphthalene Diimides with Donor/Acceptor Hydrogenâ€Bonding Properties Targeting Gâ€Quadruplex Nucleic Acids. European Journal of Organic Chemistry, 2016, 2016, 4824-4833.	1.2	7
35	Chromene Derivatives as Selective TERRA G-Quadruplex RNA Binders with Antiproliferative Properties. Pharmaceuticals, 2022, 15, 548.	1.7	7
36	Benzylamides and piperazinoarylamides of ibuprofen as fatty acid amide hydrolase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 562-576.	2.5	6

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37	State-of-the-art and dissemination of computational tools for drug-design purposes: a survey among Italian academics and industrial institutions. Future Medicinal Chemistry, 2013, 5, 907-927.	1.1	5
38	Design, synthesis and inÂvitro and inÂvivo biological evaluation of flurbiprofen amides as new fatty acid amide hydrolase/cyclooxygenase-2 dual inhibitory potential analgesic agents. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 940-953.	2.5	3
39	12. Computer-based techniques for lead identification and optimization I: Basics. , 2020, , 311-332.		2
40	13. Computer-based techniques for lead identification and optimization II: Advanced search methods. , 2020, , 333-360.		0