Francesca Moraca

List of Publications by Year
in descending order

16	326	1040056 9	888059 17
papers	citations	h-index	g-index

17	17	17	722
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	In Vitro and In Vivo Inhibition of the Mycobacterium tuberculosis Phosphopantetheinyl Transferase PptT by Amidinoureas. Journal of Medicinal Chemistry, 2022, 65, 1996-2022.	6.4	10
2	Exploring the Activity Profile of TbrPDEB1 and hPDE4 Inhibitors Using Free Energy Perturbation. ACS Medicinal Chemistry Letters, 2022, 13, 904-910.	2.8	1
3	Macrocyclic Peptides that Selectively Inhibit the Mycobacterium tuberculosis Proteasome. Journal of Medicinal Chemistry, 2021, 64, 6262-6272.	6.4	9
4	Identification of gp120 Residue His105 as a Novel Target for HIV-1 Neutralization by Small-Molecule CD4-Mimics. ACS Medicinal Chemistry Letters, 2021, 12, 1824-1831.	2.8	8
5	Application of Free Energy Perturbation (FEP+) to Understanding Ligand Selectivity: A Case Study to Assess Selectivity Between Pairs of Phosphodiesterases (PDEâ€™s). Journal of Chemical Information and Modeling, 2019, 59, 2729-2740.	5.4	20
6	Specific Noncovalent Interactions Determine Optimal Structure of a Buried Ligand Moiety: QM/MM and Pure QM Modeling of Complexes of the Smallâ€Molecule CD4 Mimetics and HIVâ€1 gp120. ChemMedChem, 2018, 13, 627-633.	3.2	4
7	Recognition of HIV-inactivating peptide triazoles by the recombinant soluble Env trimer, BG505 SOSIP.664. Proteins: Structure, Function and Bioinformatics, 2017, 85, 843-851.	2.6	7
8	The Î²20â€“Î²21 of gp120 is a regulatory switch for HIV-1 Env conformational transitions. Nature Communications, 2017, 8, 1049.	12.8	88
9	Binding Mode and Selectivity of Steroids towards Glucose-6-phosphate Dehydrogenase from the Pathogen Trypanosoma cruzi. Molecules, 2016, 21, 368.	3.8	16
10	Computational Evaluation of HIV-1 gp120 Conformations of Soluble Trimeric gp140 Structures as Targets for de Novo Docking of First- and Second-Generation Small-Molecule CD4 Mimics. Journal of Chemical Information and Modeling, 2016, 56, 2069-2079.	5.4	9
11	InÂvitro screening of 2-(1H-imidazol-1-yl)-1-phenylethanol derivatives as antiprotozoal agents and docking studies on Trypanosoma cruzi CYP51. European Journal of Medicinal Chemistry, 2016, 113, 28-33.	5.5	18
12	Synthesis, biological evaluation and structureâ€“activity correlation study of a series of imidazol-based compounds as Candida albicans inhibitors. European Journal of Medicinal Chemistry, 2014, 83, 665-673.	5.5	15
13	Discovery of the first potent and selective Mycobacterium tuberculosis Zmp1 inhibitor. Bioorganic and Medicinal Chemistry Letters, 2014, 24, 2508-2511.	2.2	22
14	Inhibition of Leishmania infantum Trypanothione Reductase by Azoleâ€Based Compounds: a Comparative Analysis with Its Physiological Substrate by Xâ€ray Crystallography. ChemMedChem, 2013, 8, 1175-1183.	3.2	63
15	New Promising Compounds with in Vitro Nanomolar Activity against Trypanosoma cruzi. ACS Medicinal Chemistry Letters, 2013, 4, 538-541.	2.8	14
16	A fast virtual screening approach to identify structurally diverse inhibitors of trypanothione reductase. Bioorganic and Medicinal Chemistry Letters, 2011, 21, 5255-5258.	2.2	19