Jurica Novak

List of Publications by Year
in descending order

25	207	1163117 8	1125743 13
papers	citations	h-index	g-index

26	26	26	231
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Proposition of a new allosteric binding site for potential SARS-CoV-2 3CL protease inhibitors by utilizing molecular dynamics simulations and ensemble docking. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9347-9360.	3.5	18
2	Exploring potential inhibitors against Kyasanur forest disease by utilizing molecular dynamics simulations and ensemble docking. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13547-13563.	3.5	8
3	A new glimpse on the active site of SARS-CoV-2 3CLpro, coupled with drug repurposing study. Molecular Diversity, 2022, 26, 2631-2645.	3.9	3
4	On the propensity of formation of cyclobutane dimers in face-to-face and face-to-back uracil stacks in solution. Physical Chemistry Chemical Physics, 2022, 24, 14836-14845.	2.8	1
5	Fluorinated twist-bend nematogens: the role of intermolecular interaction. Liquid Crystals, 2021, 48, 756-766.	2.2	10
6	Simulation of UV absorption spectra and relaxation dynamics of uracil and uracilâ€“water clusters. Physical Chemistry Chemical Physics, 2021, 23, 2594-2604.	2.8	17
7	Can natural products stop the SARS-CoV-2 virus? A docking and molecular dynamics study of a natural product database. Future Medicinal Chemistry, 2021, 13, 363-378.	2.3	14
8	Design, synthesis, antibacterial evaluation, and computational studies of hybrid oxothiazolidinâ€“1,2,4â€triazole scaffolds. Archiv Der Pharmazie, 2021, 354, e2000473.	4.1	9
9	The Influence of Hydrogen Atoms on the Performance of Radial Distribution Function-Based Descriptors in the Chemoinformatic Studies of HIV-1 Protease Complexes with Inhibitors. Current Drug Discovery Technologies, 2021, 18, 414-422.	1.2	2
10	Anti-neoplastic phramacophore benzophenone-1 coumarin (BP-1C) targets JAK2 to induce apoptosis in lung cancer. Apoptosis: an International Journal on Programmed Cell Death, 2021, , 1.	4.9	3
11	Structural isomers of saligenin-based Î²2-agonists: synthesis and insight into the reaction mechanism. Organic and Biomolecular Chemistry, 2020, 18, 9675-9688.	2.8	2
12	Polyphenolic rich extract of Oroxylum indicum alleviate Î²-glucuronidase activity via down-regulate oxidative stress: Experimental and computational studies. Biocatalysis and Agricultural Biotechnology, 2020, 29, 101804.	3.1	8
13	Novel radial distribution function approach in the study of point mutations: the HIV-1 protease case study. Future Medicinal Chemistry, 2020, 12, 1025-1036.	2.3	2
14	Performance of radial distribution function-based descriptors in the chemoinformatic studies of HIV-1 protease. Future Medicinal Chemistry, 2020, 12, 299-309.	2.3	7
15	Electronic properties investigation of human dihydrofolate reductase complexes with ligands. Journal of Biomolecular Structure and Dynamics, 2020, , 1-16.	3.5	4
16	On the Possible Role of an Intermolecular Charge Transfer State in the Excitation of the Biologically Active Bond of the Retinal Chromophore-counterion Pair. Croatica Chemica Acta, 2020, 93, .	0.4	0
17	New Brush-Type Chiral Stationary Phases for Enantioseparation of Pharmaceutical Drugs. Molecules, 2019, 24, 823.	3.8	7
18	Determination of the Absolute Configuration of (S)â€Nâ€(1â€Arylâ€allyl)â€3,5â€dinitrobenzamides and Their Elution Order on Brushâ€Type Chiral Stationary Phases. European Journal of Organic Chemistry, 2018, 2018, 3982-3991.	2.4	5

#	Article	IF	Citations
19	Photochemistry of 1â€•and 2â€Naphthols and Their Water Clusters: The Role of ¹Ï€Ï€*(L_a) Mediated Hydrogen Transfer to Carbon Atoms. Chemistry - A European Journal, 2017, 23, 8244-8251.	3.3	18
20	Mechanism of ultrafast non-reactive deactivation of the retinal chromophore in non-polar solvents. Physical Chemistry Chemical Physics, 2017, 19, 25970-25978.	2.8	8
21	Photoinduced Dynamics of Formic Acid Monomers and Dimers: The Role of the Double Hydrogen Bond. Journal of Physical Chemistry A, 2012, 116, 11467-11475.	2.5	26
22	One catalyst for both enantiomers: uncovering the inversion of enantioselectivity in cinchona-mediated desymmetrization of glutaric meso-anhydrides. Tetrahedron, 2012, 68, 8311-8317.	1.9	11
23	Localization of the Counterion of the Protonated Schiff Base of n-butylretinal in Solution. Croatica Chemica Acta, 2011, 84, 221-231.	0.4	4
24	Shaping the infrared spectrum of the acetic acid dimer in the OH-stretching range: Multiple conformers and anharmonic coupling. Chemical Physics Letters, 2009, 474, 248-252.	2.6	14
25	Withasomniferol C, a new potential SARS-CoV-2 main protease inhibitor from the Withania somnifera plant proposed by in silico approaches. PeerJ, 0, 10, e13374.	2.0	4