

# Ricky B Nellas

## List of Publications by Year in descending order

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22  
papers

276  
citations

933447

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940533

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23  
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23  
docs citations

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times ranked

317  
citing authors

#	ARTICLE	IF	CITATIONS
1	Potential Inhibitors of Galactofuranosyltransferase 2 (GfT2): Molecular Docking, 3D-QSAR, and In Silico ADMETox Studies. <i>Scientific Reports</i> , 2019, 9, 17096.	3.3	47
2	Machine Learning for Predicting Electron Transfer Coupling. <i>Journal of Physical Chemistry A</i> , 2019, 123, 7792-7802.	2.5	42
3	Mapping Allostery through Computational Glycine Scanning and Correlation Analysis of Residue-Residue Contacts. <i>Biochemistry</i> , 2015, 54, 1534-1541.	2.5	35
4	Pressure-Induced conformational switch of an interfacial protein. <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 820-827.	2.6	21
5	The Promiscuity of Allosteric Regulation of Nuclear Receptors by Retinoid X Receptor. <i>Journal of Physical Chemistry B</i> , 2016, 120, 8338-8345.	2.6	18
6	Solvent-Dependent Gating Motions of an Extremophilic Lipase from <i>Pseudomonas aeruginosa</i> . <i>Biochemistry</i> , 2012, 51, 6238-6245.	2.5	17
7	Solvent-Induced $\alpha$ - to $3_{10}$ -Helix Transition of an Amphiphilic Peptide. <i>Biochemistry</i> , 2013, 52, 7137-7144.	2.5	15
8	Ligand-Induced Conformational Dynamics of A Tyramine Receptor from <i>Sitophilus oryzae</i> . <i>Scientific Reports</i> , 2019, 9, 16275.	3.3	15
9	Effects of truncation of the peptide chain on the secondary structure and bioactivities of palmitoylated anoplin. <i>Peptides</i> , 2018, 104, 7-14.	2.4	12
10	The interaction and mechanism of monoterpenes with tyramine receptor (SoTyrR) of rice weevil ( <i>Sitophilus oryzae</i> ). <i>SN Applied Sciences</i> , 2020, 2, 1.	2.9	10
11	Structural Dynamics of Neighboring Water Molecules of N-Isopropylacrylamide Pentamer. <i>ACS Omega</i> , 2020, 5, 1408-1413.	3.5	10
12	Molecular Affinity of Mabolo Extracts to an Octopamine Receptor of a Fruit Fly. <i>Molecules</i> , 2017, 22, 1677.	3.8	8
13	The effect of ligand affinity to the contact dynamics of the ligand binding domain of thyroid hormone receptor - retinoid X receptor. <i>Journal of Molecular Graphics and Modelling</i> , 2021, 104, 107829.	2.4	5
14	Computational reverse engineering of the lipase from <i>Pseudomonas aeruginosa</i> PAO1: $\alpha$ -helices. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 100, 107657.	2.4	4
15	DMSO enhanced conformational switch of an interfacial enzyme. <i>Biopolymers</i> , 2016, 105, 864-872.	2.4	3
16	In Silico insights on enhancing thermostability and activity of a plant Fructosyltransferase from <i>Pachysandra terminalis</i> via introduction of disulfide bridges. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 89, 250-260.	2.4	3
17	Identification of Conomorphin Variants in the <i>Conus eburneus</i> Venom and the Effect of Sequence and PTM Variations on Conomorphin Conformations. <i>Marine Drugs</i> , 2020, 18, 503.	4.6	3
18	Conformational dynamics of $\alpha$ -conotoxin PnIB in complex solvent systems. <i>Molecular Diversity</i> , 2020, 24, 1291-1299.	3.9	2

#	ARTICLE	IF	CITATIONS
19	Small in size, big on taste: Metabolomics analysis of flavor compounds from Philippine garlic. PLoS ONE, 2021, 16, e0247289.	2.5	2
20	pH-Dependent Conformations of an Antimicrobial Spider Venom Peptide, Cupiennin 1a, from Unbiased HREMD Simulations. ACS Omega, 2021, 6, 24166-24175.	3.5	2
21	Sustainable Hues: Exploring the Molecular Palette of Biowaste Dyes through LC-MS Metabolomics. Molecules, 2021, 26, 6645.	3.8	2
22	Surface tension data of n-propane, n-octane and n-dodecane from nucleation simulations. Tellus, Series B: Chemical and Physical Meteorology, 2018, 70, 1-5.	1.6	0