## Dibyendu Mondal

List of Publications by Year in descending order

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1040056 1199594 12 187 9 12 citations g-index h-index papers 12 12 12 297 docs citations times ranked citing authors all docs

| #  | Article   | lF   | CITATIONS |
|----|---|------|-----------|
| 1  | Exploring the Mechanism of Covalent Inhibition: Simulating the Binding Free Energy of α-Ketoamide Inhibitors of the Main Protease of SARS-CoV-2. Biochemistry, 2020, 59, 4601-4608.   | 2.5  | 45        |
| 2  | EF-Tu and EF-G are activated by allosteric effects. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 3386-3391.  | 7.1  | 18        |
| 3  | Exploring alternative catalytic mechanisms of the Cas9 HNH domain. Proteins: Structure, Function and Bioinformatics, 2020, 88, 260-264.   | 2.6  | 17        |
| 4  | Exploring the Effectiveness of Binding Free Energy Calculations. Journal of Physical Chemistry B, 2019, 123, 8910-8915.   | 2.6  | 16        |
| 5  | Combinatorial Approach for Exploring Conformational Space and Activation Barriers in Computer-Aided Enzyme Design. ACS Catalysis, 2020, 10, 6002-6012.  | 11.2 | 16        |
| 6  | Exploring the activation pathway and G $<$ sub $>isub>-coupling specificity of the \hat{l}^{1}\!\!/\!\!4-opioid receptor. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 26218-26225.$ | 7.1  | 15        |
| 7  | Exploring the Activation Process of the Î <sup>2</sup> 2AR-G <sub>s</sub> Complex. Journal of the American Chemical Society, 2021, 143, 11044-11051.  | 13.7 | 14        |
| 8  | Soluble TREM2 inhibits secondary nucleation of $\hat{Al^2}$ fibrillization and enhances cellular uptake of fibrillar $\hat{Al^2}$ . Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .   | 7.1  | 14        |
| 9  | Exploring the Proteolysis Mechanism of the Proteasomes. Journal of Physical Chemistry B, 2020, 124, 5626-5635.  | 2.6  | 12        |
| 10 | Solvent Thermodynamic Driving Force Controls Stacking Interactions between Polyaromatics. Journal of Physical Chemistry C, 2016, 120, 23858-23869.  | 3.1  | 10        |
| 11 | Exploring the Drug Resistance of HCV Protease. Journal of Physical Chemistry B, 2017, 121, 6831-6840.   | 2.6  | 8         |
| 12 | Histidine protonation states are key in the LigI catalytic reaction mechanism. Proteins: Structure, Function and Bioinformatics, 2021, , .  | 2.6  | 2         |