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## ACCEPTED MANUSCRIPT

Structural and Quantum Mechanical Computations to Elucidate the Altered Binding Mechanism of Metal and Drug with Pyrazinamidase from *Mycobacterium tuberculosis* due to Mutagenicity

**Short title:** Quantum mechanics of mutagenicity in *Mycobacterium tuberculosis* Nouman Rasool<sup>1\*</sup>, Saima Iftikhar<sup>2</sup>, Waqar Hussain<sup>3</sup>

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### **Graphical Abstract**



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