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Synthesis and biological evaluation of novel triazole-biscoumarin conjugates as potential antitubercular and anti-oxidant agents

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Abstract The synthesis of a new series of triazole-biscoumarin conjugates by using a molecular hybridization approach is described. The newly synthesized compounds **6a–k** were evaluated for their in vitro antitubercular activity against active and dormant *Mtb* H37Ra and anti-oxidant activity against DPPH radical scavenging. Molecular docking simulations for the antitubercular activity showed that the conjugates **6a–k** bind in the pocket of the DprE1 enzyme. Most of the conjugates displayed good antitubercular activity against both the active and dormant *Mtb* H37Ra strain. The compound **6h** displayed very good antitubercular activity against dormant *Mtb* H37Ra with an IC_{50} value of 1.44 μg/mL. Most of the synthesized conjugates exhibit excellent anti-oxidant activity with an IC_{50} of less than the standard BHT. Compound **6b** is the most active among all the conjugates with an IC_{50} value of 08.17 ± 0.11 μg/mL. The molecular docking study shows good agreement between the observed antitubercular activity and the binding affinity.

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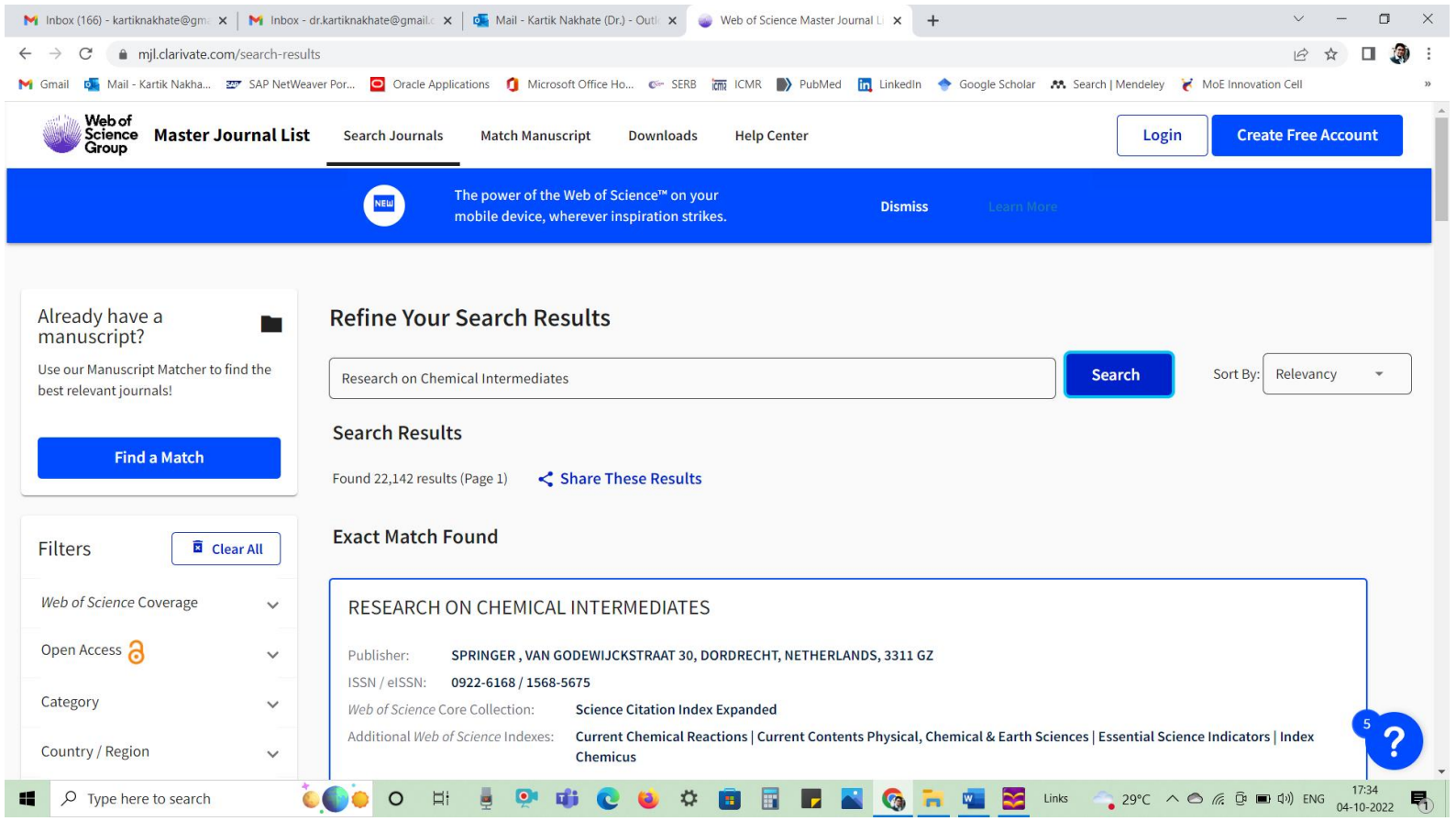
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