

*Supplementary Materials*

# **In Silico Studies on Zinc Oxide based Nanostructured Oil Carriers with Seed Extracts of *Nigella sativa* and *Pimpinella anisum* as Potential Inhibitors of 3CL Protease of SARS-CoV-2**

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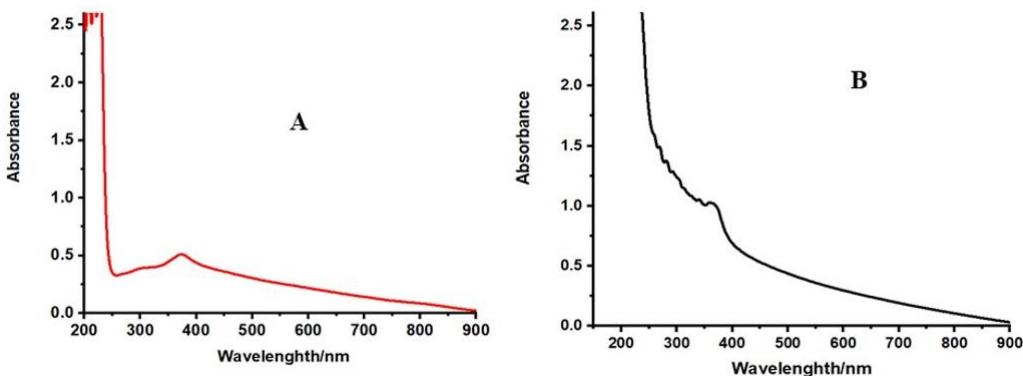
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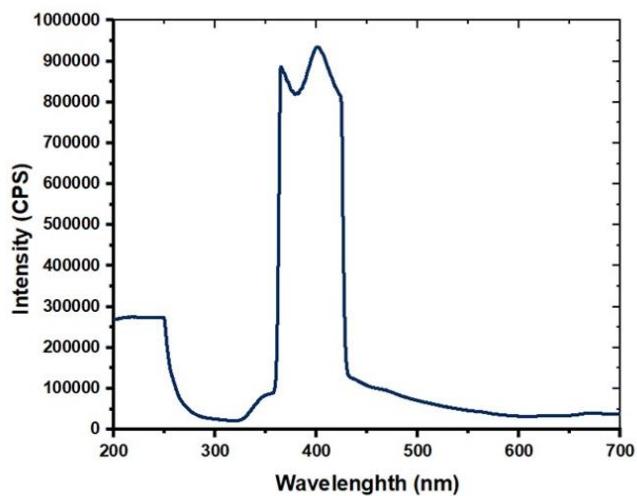
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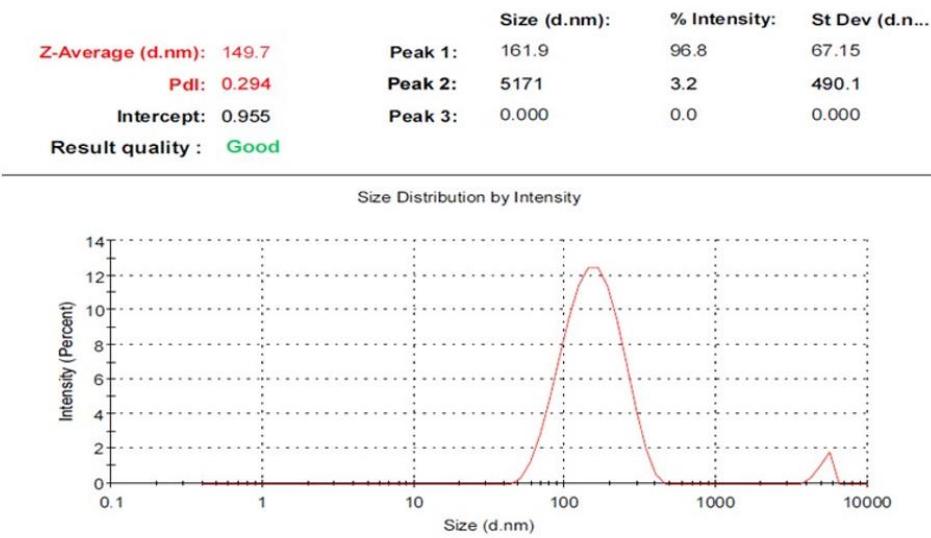
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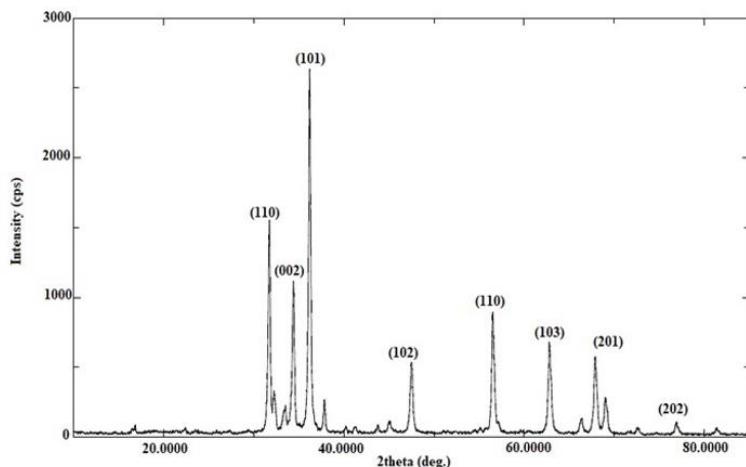
**Figure S1.** The UV–visible absorption spectra of synthesized (A) ZnO NPs (B) ZnO NPs–NLC.



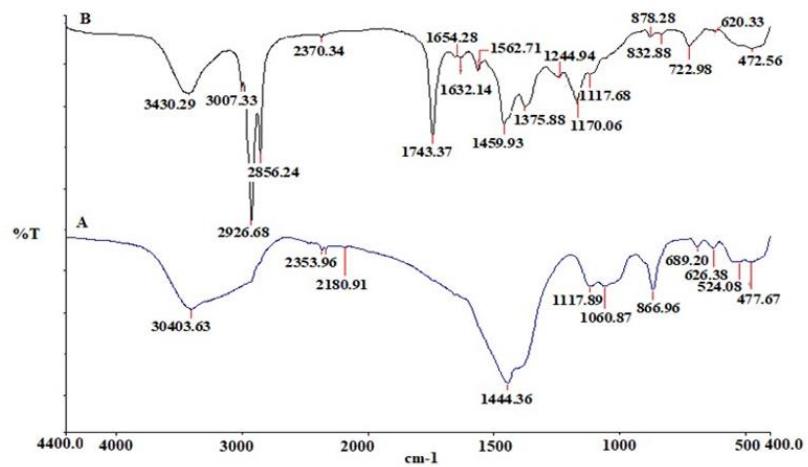
**Figure S2.** The emission spectrum of synthesized ZnO NPs.



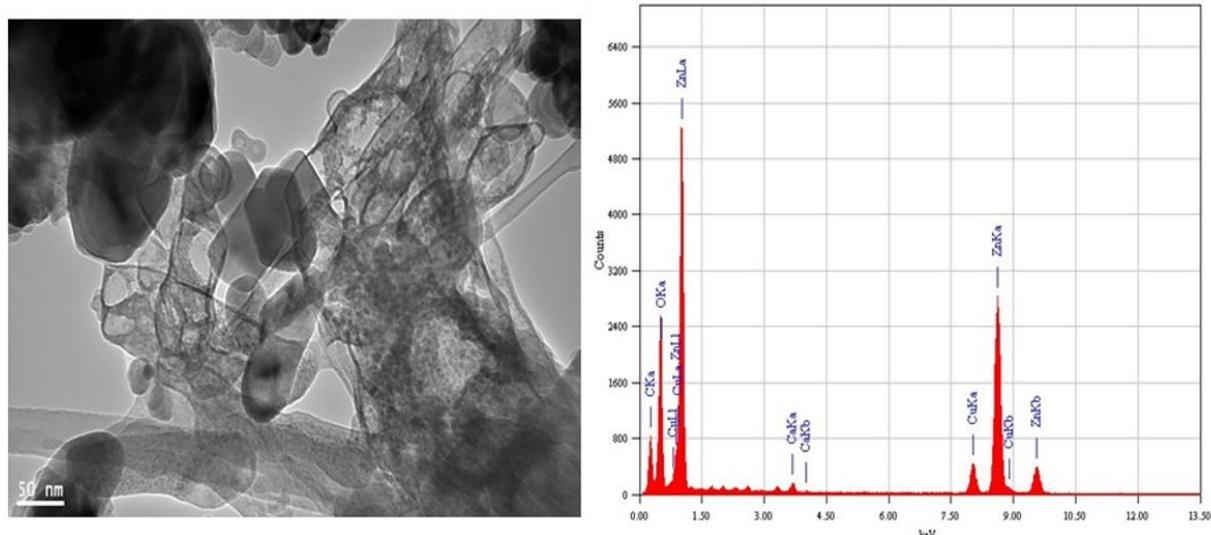
**Figure S3.** Particle size and polydispersity index of the ZnNPs.



**Figure S4.** X-Ray diffraction pattern and diffraction angles peaks of synthesized ZnO NPs–NLC.

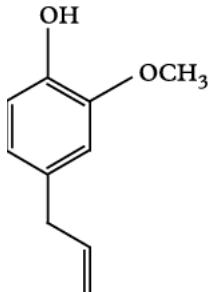
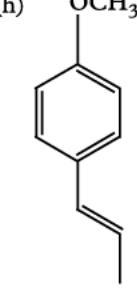
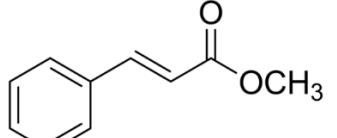
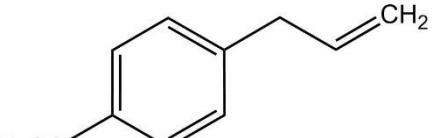
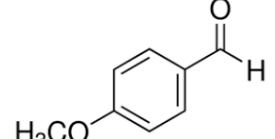
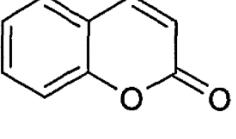
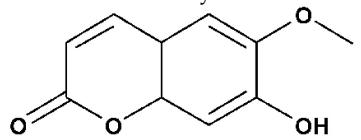
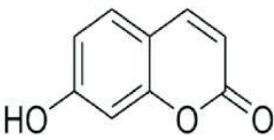
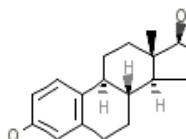
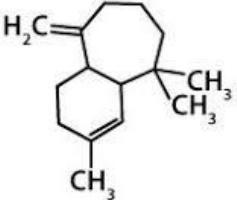


**Figure S5.** FT-IR spectra of synthesized (A) ZnO NPs (B) ZnO NPs–NLC.



**Figure S6.** TEM micrograph and EDX spectrum of synthesized ZnO NPs.

**Table S1:** Structures of constituent compounds.

	Bioactive compounds
<i>Pimpinella anisum</i>	eugenol, <i>trans</i> -anethole, methylchavicol, anisaldehyde, estragole, coumarins, scopoletin, umbelliferone, estrols, terpene hydrocarbons, polyenes, and polyacetylenes
	 <p>eugenol</p>
	 <p>(h) <i>trans</i>-anethole</p>
	 <p>methylchavicol</p>
	 <p>estragole</p>
	 <p>anisaldehyde</p>
	 <p>coumarin</p>
	 <p>Scopoletin</p>
	 <p>Umbelliferone</p>
	 <p>estrol</p>
	 <p>Sesquiterpene: Himachalene</p>

<i>Nigella Sativa</i>	thymoquinone (30%-48%), thymohydroquinone, dithymoquinone, <i>p</i> -cymene (7%-15%), carvacrol (6%-12%), 4-terpineol (2%-7%), <i>t</i> -anethole (1%-4%), sesquiterpene longifolene (1%-8%) $\alpha$ -pinene and thymol
Zinc Oxide	<p>The diagram shows the chemical structures of several compounds:</p> <ul style="list-style-type: none"> <li><b>Carvacrol:</b> A monoterpenoid phenol with a hydroxyl group at the para position of a substituted benzene ring.</li> <li><b><math>\delta</math>-Hederin:</b> A triterpenoid saponin with multiple hydroxyl groups and a complex carbon skeleton.</li> <li><b>Nigellone:</b> A substituted benzene ring with a carbonyl group and two methyl groups attached to the same carbon atom.</li> <li><b>Thymol:</b> A monoterpenoid phenol with a hydroxyl group at the para position of a substituted benzene ring.</li> <li><b>Thymoquinone:</b> A quinone derivative with two methyl groups and a hydroxyl group.</li> <li><b>Thymohydroquinone:</b> A hydroquinone derivative with two methyl groups and a hydroxyl group.</li> <li><b><i>p</i>-cymene:</b> A monoterpenoid hydrocarbon with two methyl groups at the para positions of a benzene ring.</li> <li><b>4-terpineol:</b> A monoterpenoid alcohol with a hydroxyl group and a double bond.</li> <li><b><i>t</i>-anethole:</b> A monoterpenoid alcohol with a double bond and a hydroxyl group.</li> <li><b>sesquiterpene longifolene:</b> A complex tricyclic sesquiterpene with a double bond.</li> </ul>

Olive Oil

