

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

**Awatif A. Hendi ¹, Promy Virk ^{2,*}, Manal A. Awad ³, Mai Elobeid ², Khalid M. O. Ortashi ⁴,
Meznah M. Alanazi ¹, Fatemah H. Alkallas ¹, Maha Mohammad Almoneef ¹ and
Mohammed Aly Abdou ⁵**

¹ Department of Physics, College of Science, Princess Nourah Bint Abdulrahman University, P.O. Box 84428, Riyadh 11671, Saudi Arabia; aahindi@pnu.edu.sa (A.A.H.); mmalenazy@pnu.edu.sa (M.M.A.); fhalkallas@pnu.edu.sa (F.H.A.); mmalmoneef@pnu.edu.sa (M.M.A.)

² Department of Zoology, College of Sciences, King Saud University, P.O. Box: 2455, Riyadh, 11451, Saudi Arabia; melobeid@ksu.edu.sa

³ King Abdullah Institute for Nanotechnology, King Saud University, Riyadh 11451, Saudi Arabia; mawad@ksu.edu.sa

⁴ Department of Chemical Engineering, King Saud University, Riyadh 11421, Saudi Arabia; ortashi9@ksu.edu.sa

⁵ Department of Physics, College of Sciences, University of Bisha, P.O. Box 344, Bisha 61922, Saudi Arabia; m_abdou_eg@yahoo.com

* Correspondence: bvirk@ksu.edu.sa; Tel: +966-15-0220-5785

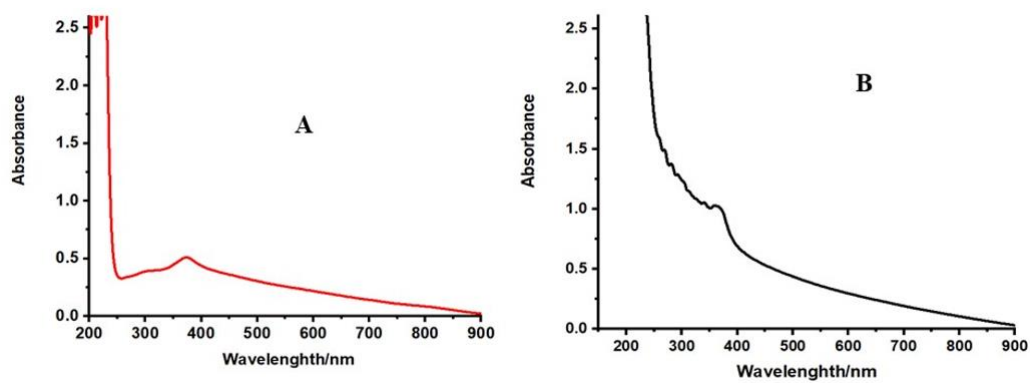


Figure S1. The UV-visible absorption spectra of synthesized (A) ZnO NPs (B) ZnO NPs-NLC.

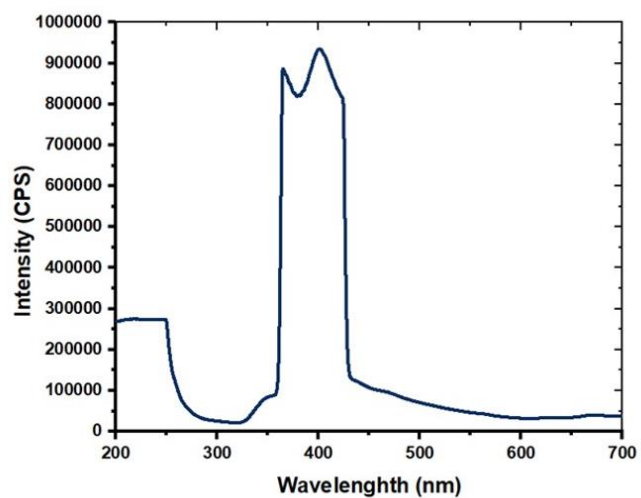


Figure S2. The emission spectrum of synthesized ZnO NPs.

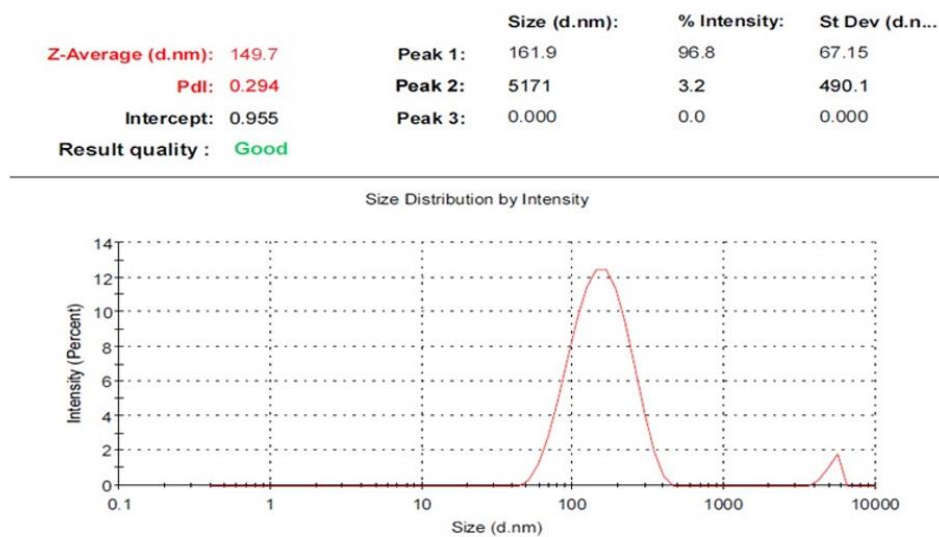


Figure S3. Particle size and polydispersity index of the ZnNPs.

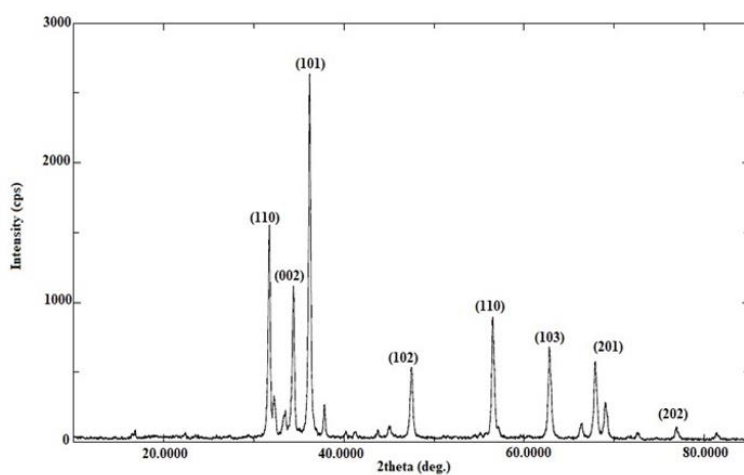


Figure S4. X-Ray diffraction pattern and diffraction angles peaks of synthesized ZnO NPs–NLC.

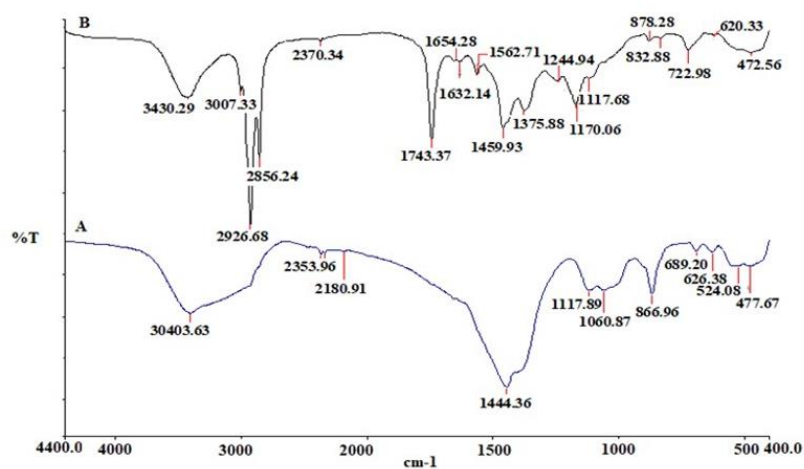


Figure S5. FT-IR spectra of synthesized (A) ZnO NPs (B) ZnO NPs-NLC.

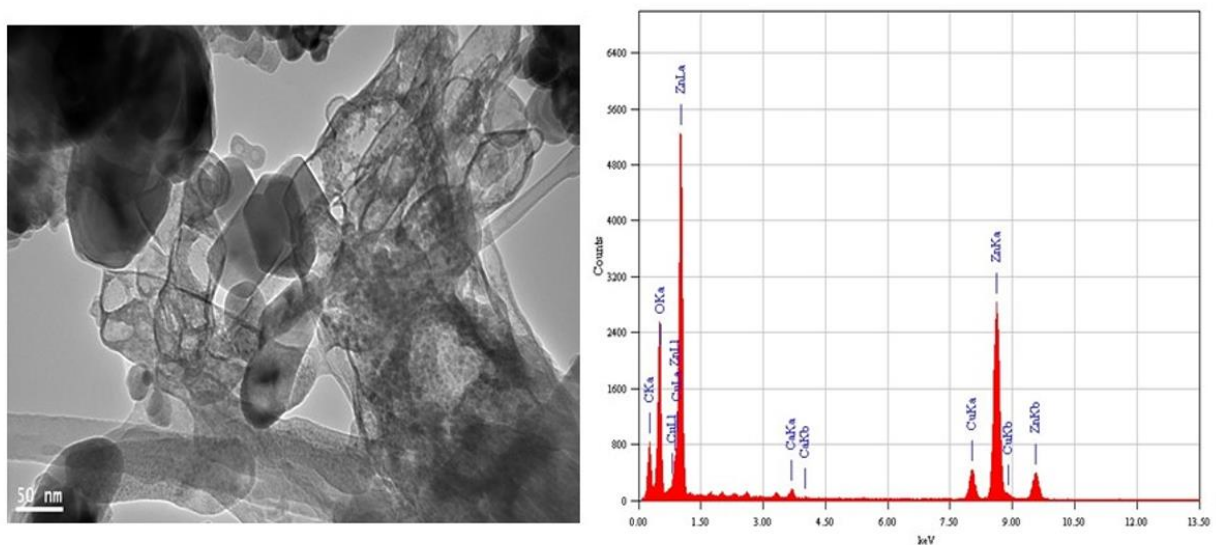
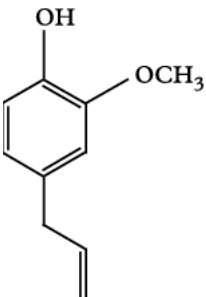
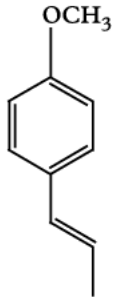
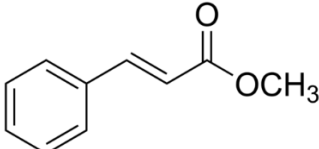
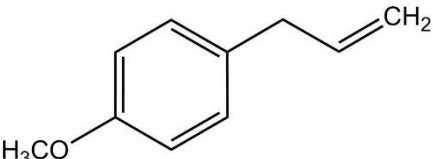
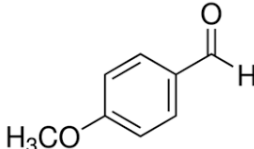
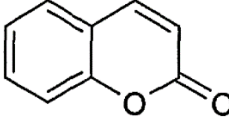
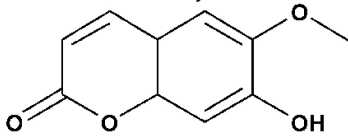
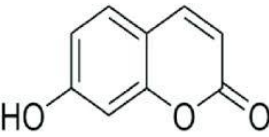
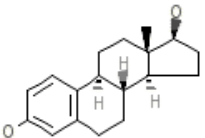
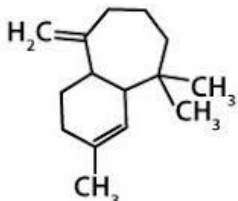
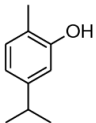
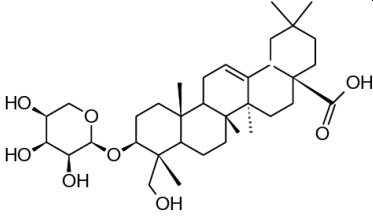
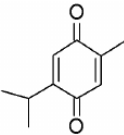
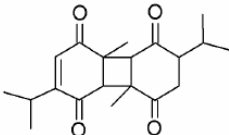
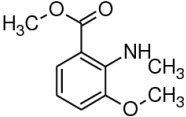
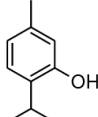
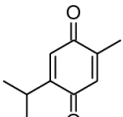
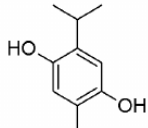
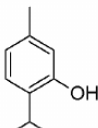
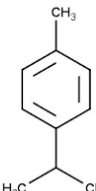
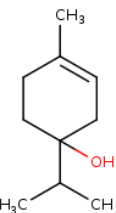
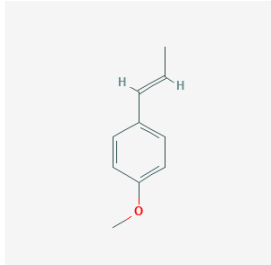
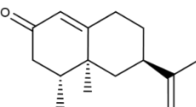
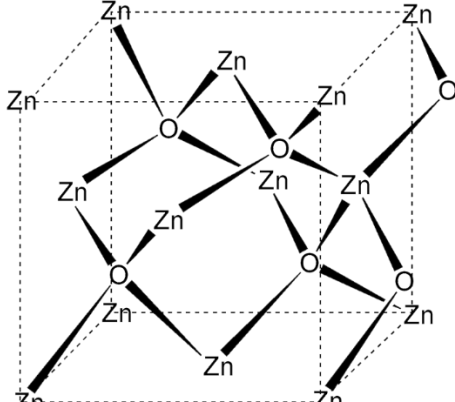


Figure S6. TEM micrograph and EDX spectrum of synthesized ZnO NPs.

Table S1: Structures of constituent compounds.

	Bioactive compounds
<i>Pimpinella anisum</i>	<p>eugenol, <i>trans</i>-anethole, methylchavicol, anisaldehyde, estragole, coumarins, scopoletin, umbelliferone, estrols, terpene hydrocarbons, polyenes, and polyacetylenes</p> <div style="display: flex; flex-wrap: wrap; justify-content: space-around;"> <div style="text-align: center;">  <p>eugenol</p> </div> <div style="text-align: center;"> <p>(h)</p>  <p><i>trans</i>-anethole</p> </div> <div style="text-align: center;">  <p>methylchavicol</p> </div> <div style="text-align: center;">  <p>estragole</p> </div> <div style="text-align: center;">  <p>anisaldehyde</p> </div> <div style="text-align: center;">  <p>coumarin</p> </div> <div style="text-align: center;">  <p>Scopoletin</p> </div> <div style="text-align: center;">  <p>Umbelliferone</p> </div> <div style="text-align: center;">  <p>estrol</p> </div> <div style="text-align: center;">  <p>Sesquiterpene: Himachalene</p> </div> </div>

<p><i>Nigella Sativa</i></p>	<p>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 α-pinene and thymol</p>
	<div style="display: flex; flex-wrap: wrap; justify-content: space-around;"> <div style="text-align: center;">  <p>Carvacrol</p> </div> <div style="text-align: center;">  <p>δ-Hederin</p> </div> <div style="text-align: center;">  <p>Thymoquinone</p> </div> <div style="text-align: center;">  <p>Dithymoquinone</p> </div> <div style="text-align: center;">  <p>Nigellone</p> </div> <div style="text-align: center;">  <p>Thymol</p> </div> <div style="text-align: center;">  <p>Thymoquinone</p> </div> <div style="text-align: center;">  <p>Thymohydroquinone</p> </div> <div style="text-align: center;">  <p>Thymol</p> </div> <div style="text-align: center;">  <p><i>p</i>-cymene</p> </div> <div style="text-align: center;">  <p>4-terpineol</p> </div> <div style="text-align: center;">  <p><i>t</i>-anethole</p> </div> <div style="text-align: center;">  <p>sesquiterpene longifolene</p> </div> </div>
<p>Zinc Oxide</p>	

Olive Oil

