

# A DR/NIR Hybrid Polymeric Tool for Functional Bio-Coatings: Theoretical Study, Cytotoxicity, and Antimicrobial Activity

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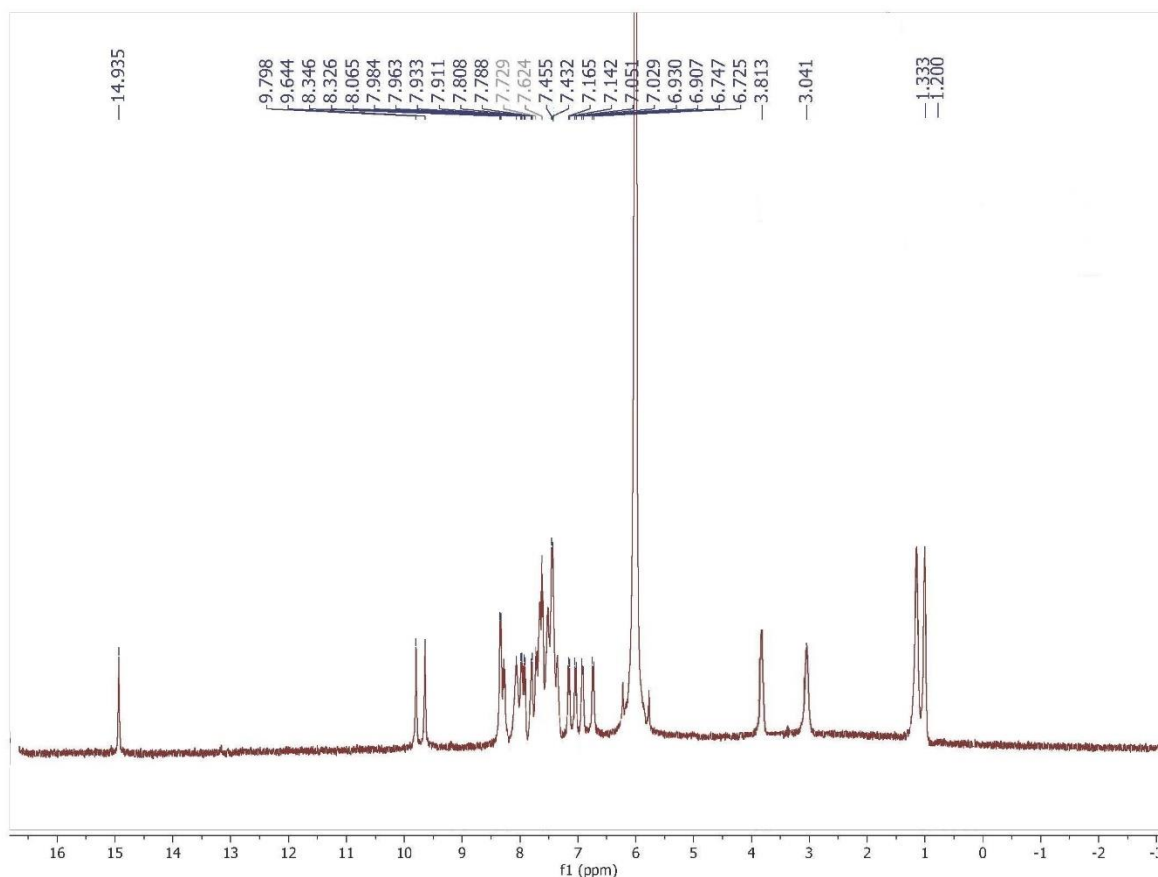
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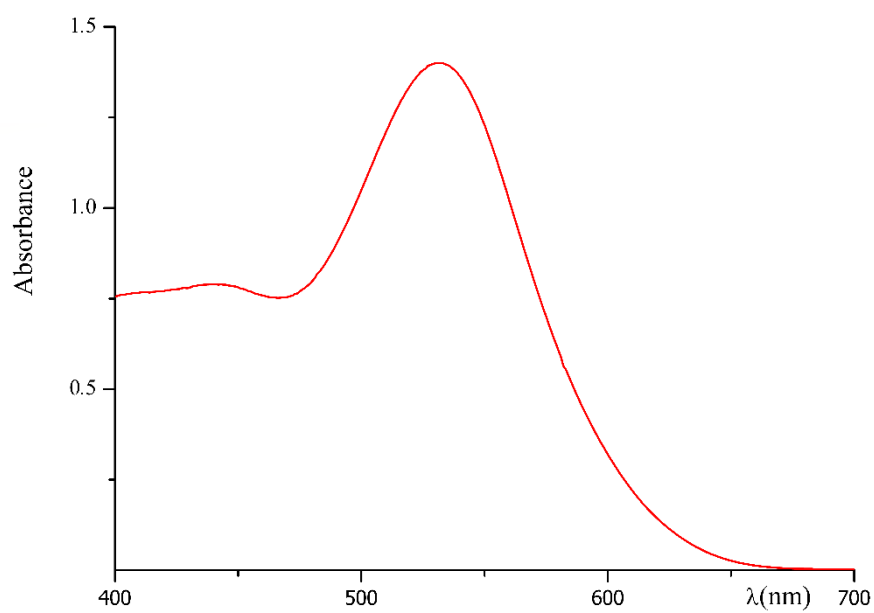
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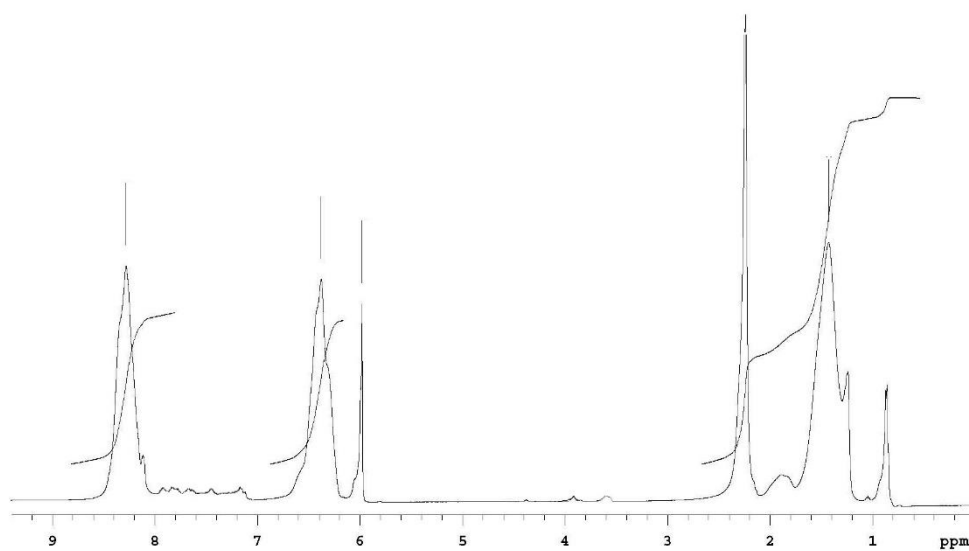
## SUPPLEMENTARY MATERIAL



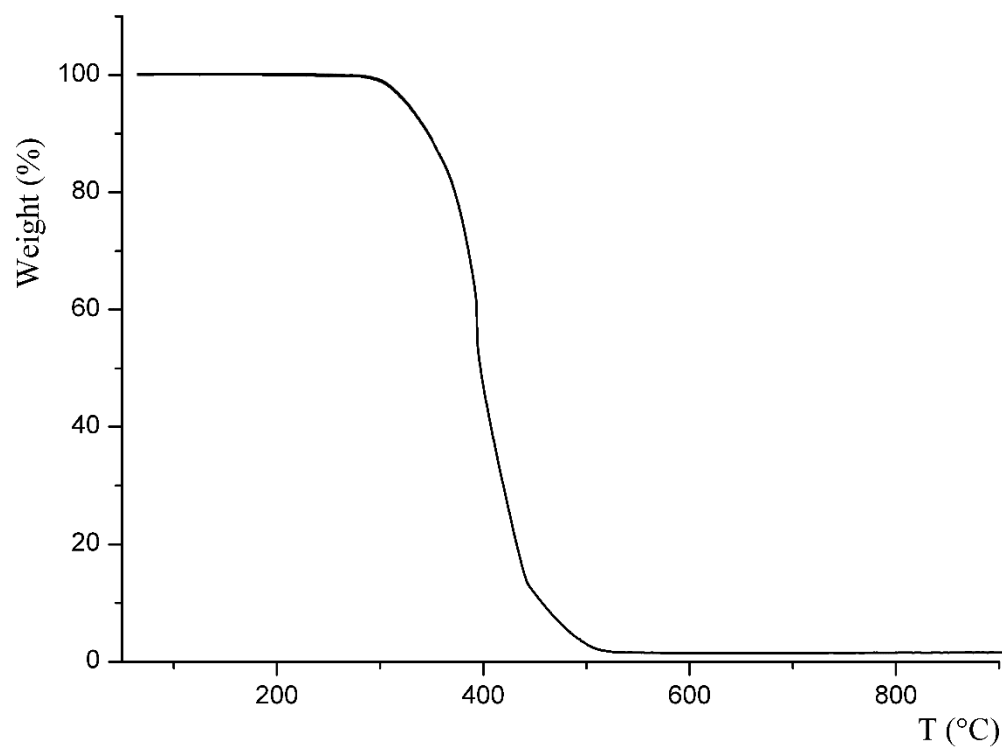
**Figure S1.** Hard copy <sup>1</sup>H NMR (500 MHz, TCE-d<sub>2</sub>, 25 °C, ppm) of ZnNB.



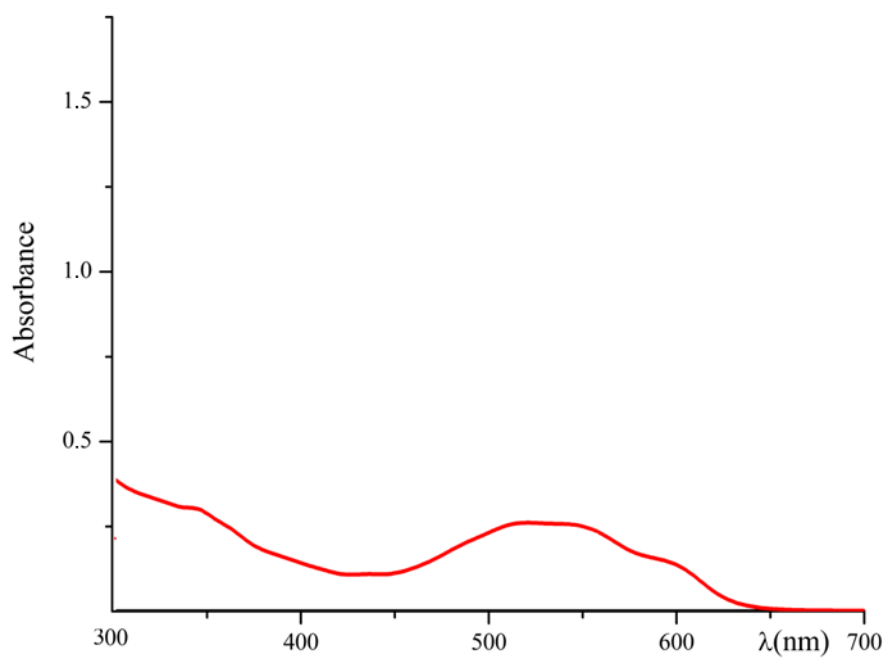
**Figure S2.** Absorbance spectrum of ZnNB deposited as powder crystals onto a quartz slide.



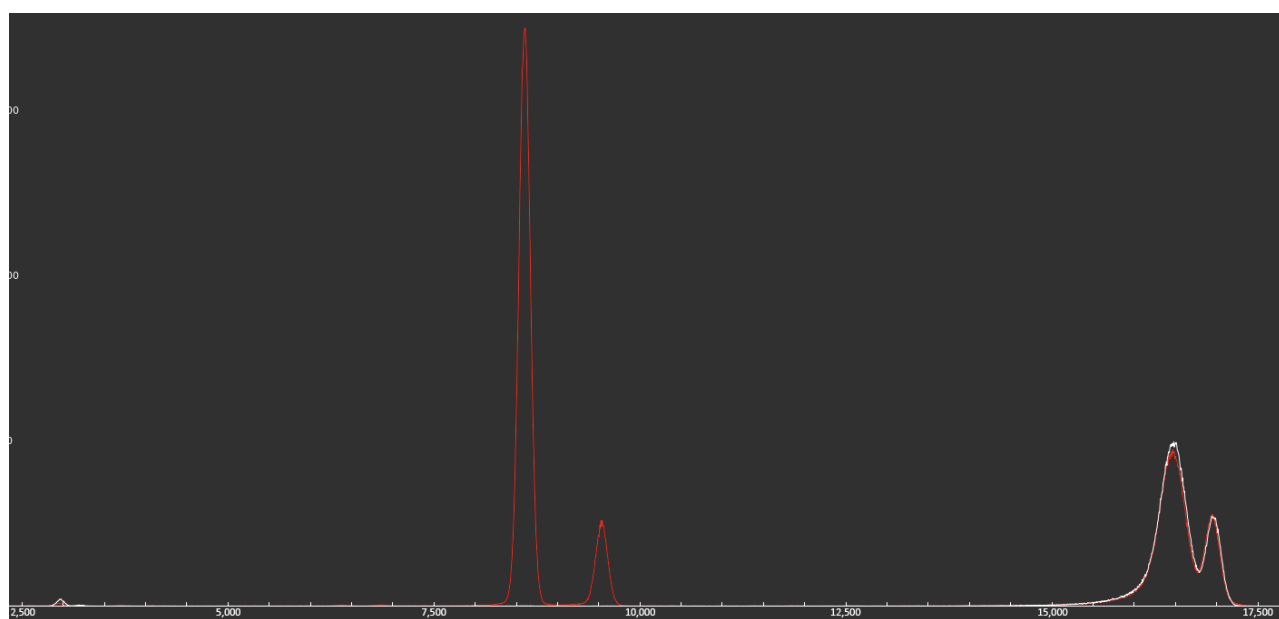
**Figure S3.** Hard copy  $^1\text{H}$  NMR (500 MHz, TCE- $d_2$ , 25  $^\circ\text{C}$ , ppm) of P4VP-ZnNB 20%.



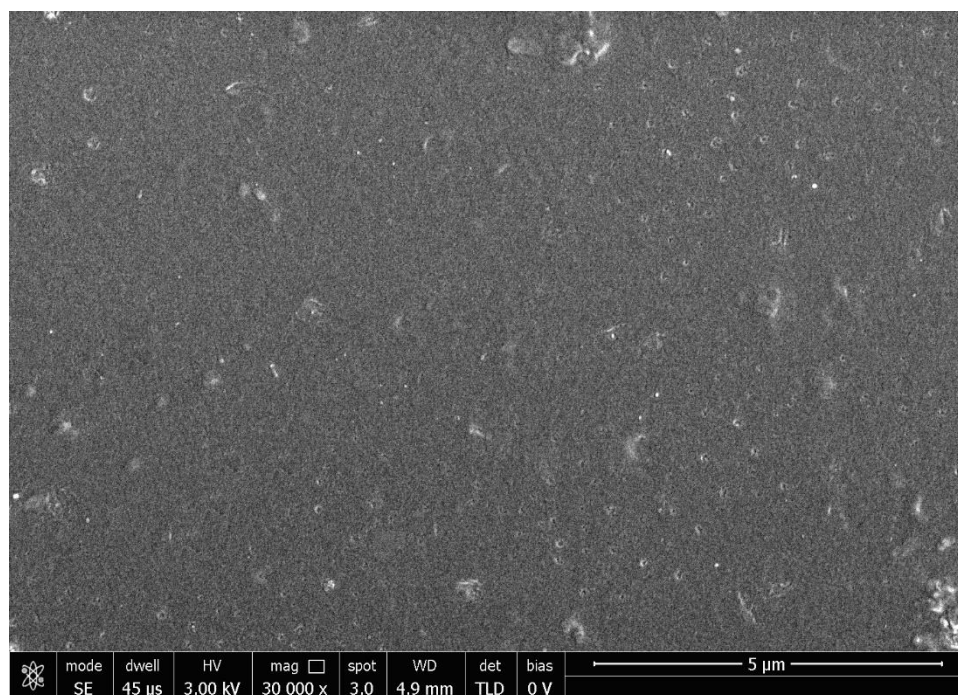
**Figure S4.** TGA curve of P4VP-ZnNB 20%.



**Figure S5.** Absorbance spectrum of a thin transparent film P4VP-ZnNB 20% spin-coated onto a quartz slide.



**Figure S6.** Energy spectrum obtained from X-ray fluorescence measurement of washed single crystal of ZnNB shows characteristic K edge (8.6 keV) and K peaks of zinc (red color). For comparison, the spectrum obtained for Kapton (shown in white color) is included. The material was used as support and a reference material.



**Figure S7.** SEM micrographs of P4VP-ZnNB 20% film deposited onto quartz slide and metalized by gold sputtering (about 5 nm)

**Table S1.** Data collection statistics for crystals of ZnNB

Color	Red
Temperature (K)	100
Wavelength (Å)	0.619
Crystal system	Monoclinic
Space group	$P 2_1/n$
$a$ (Å)	16.442 (7)
$b$ (Å)	4.790 (2)
$c$ (Å)	25.880 (9)
$\alpha$ (°)	90.00 (3)
$\beta$ (°)	91.24 (11)
$\gamma$ (°)	92.49 (3)
Resolution (Å)	2.32–0.78
R-merge	0.053
I/s(I) (highest shell)	14.14 (2.07)
Completeness (%)	99.4
Multiplicity	6.5 (5.5)
Mosaicity (°)	0.281
Volume	5628 Å <sup>3</sup>
Z	1