

Electronic Supporting Information

Curcumin-nicotinoyl derivative and its transitional metal complexes: synthesis, characterization, *in silico* and *in vitro* selective anticancer, and anti-bacterial behaviors

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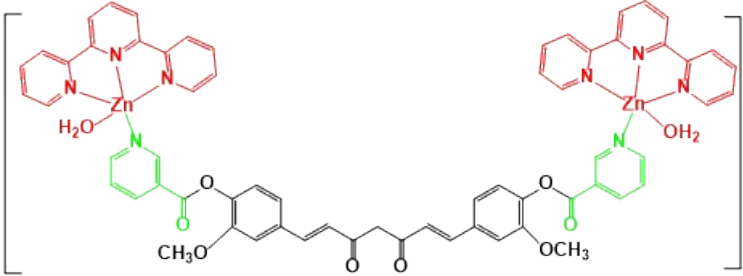
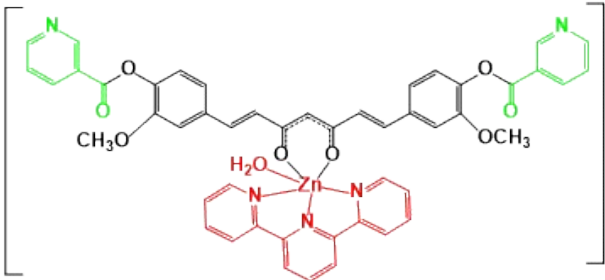
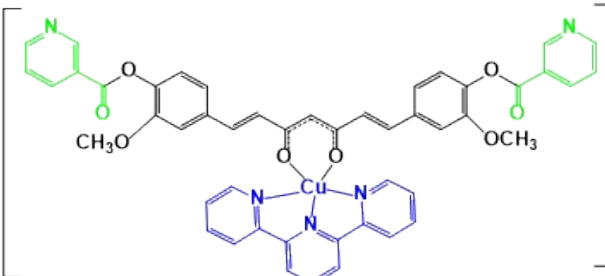
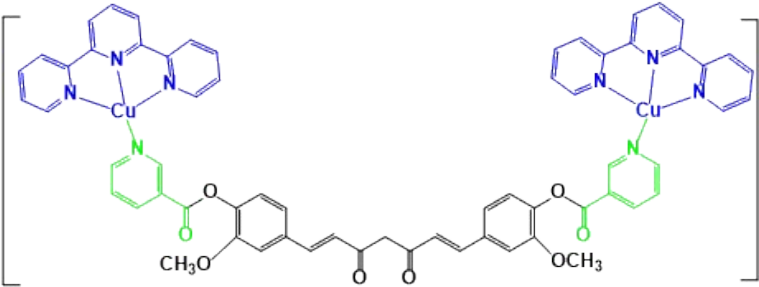
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- Table S1 DFT analysis of the most probable structures of Cu(II) and Zn(II) complexes.
- Fig. S1 FT-IR spectra of (a) curcumin, (b) Cur-Nic, (c) Cu(II) complex, and (d) Zn(II) complex.
- Fig. S2 MS spectrum of Cur-Nic.
- Scheme S1 Proposed fragmentation pathways of (A) curcumin and (B) Cur-Nic.
- Fig. S3 optimized structure of (A) Cur-Nic, (B) Cu(II) complex, and (C) Zn(II) complex.

Table S1 DFT analysis of the most probable structures of Cu(II) and Zn(II) complexes

Energy (kcal/mol)	Structure
-3.171×10^{-19}	
-2.654×10^{-19}	
-1.735×10^{-16}	
-1.247×10^{-16}	

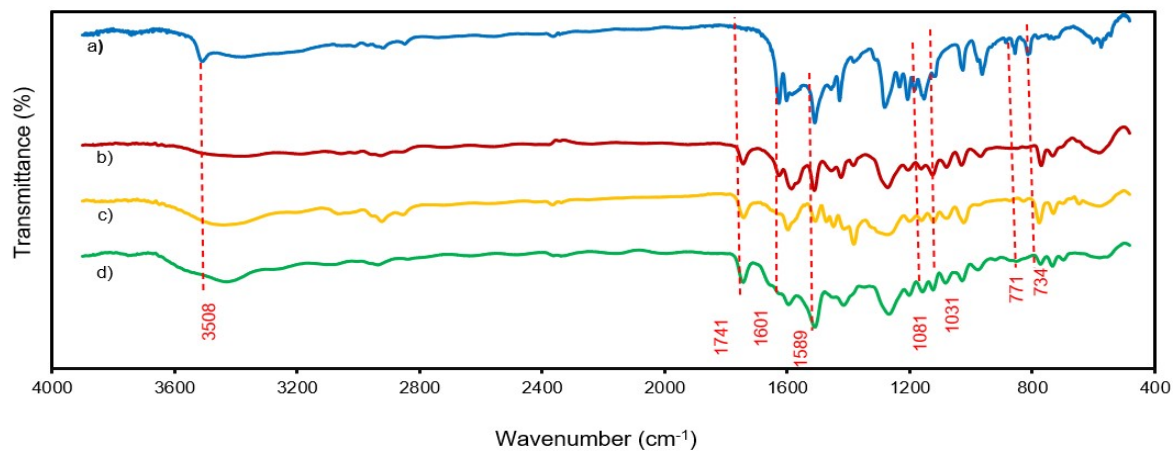


Fig. S1 FT-IR spectra of (a) curcumin, (b) Cur-Nic, (c) Cu(II) complex, and (d) Zn(II) complex.

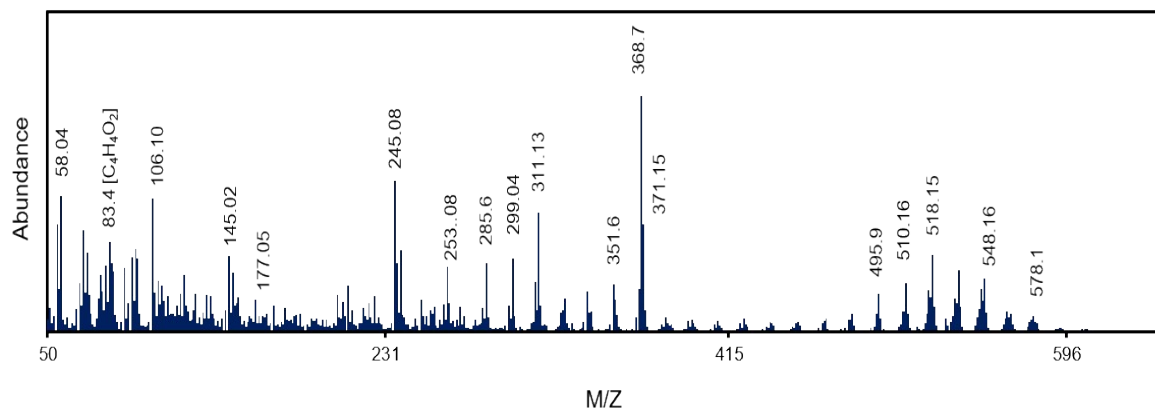
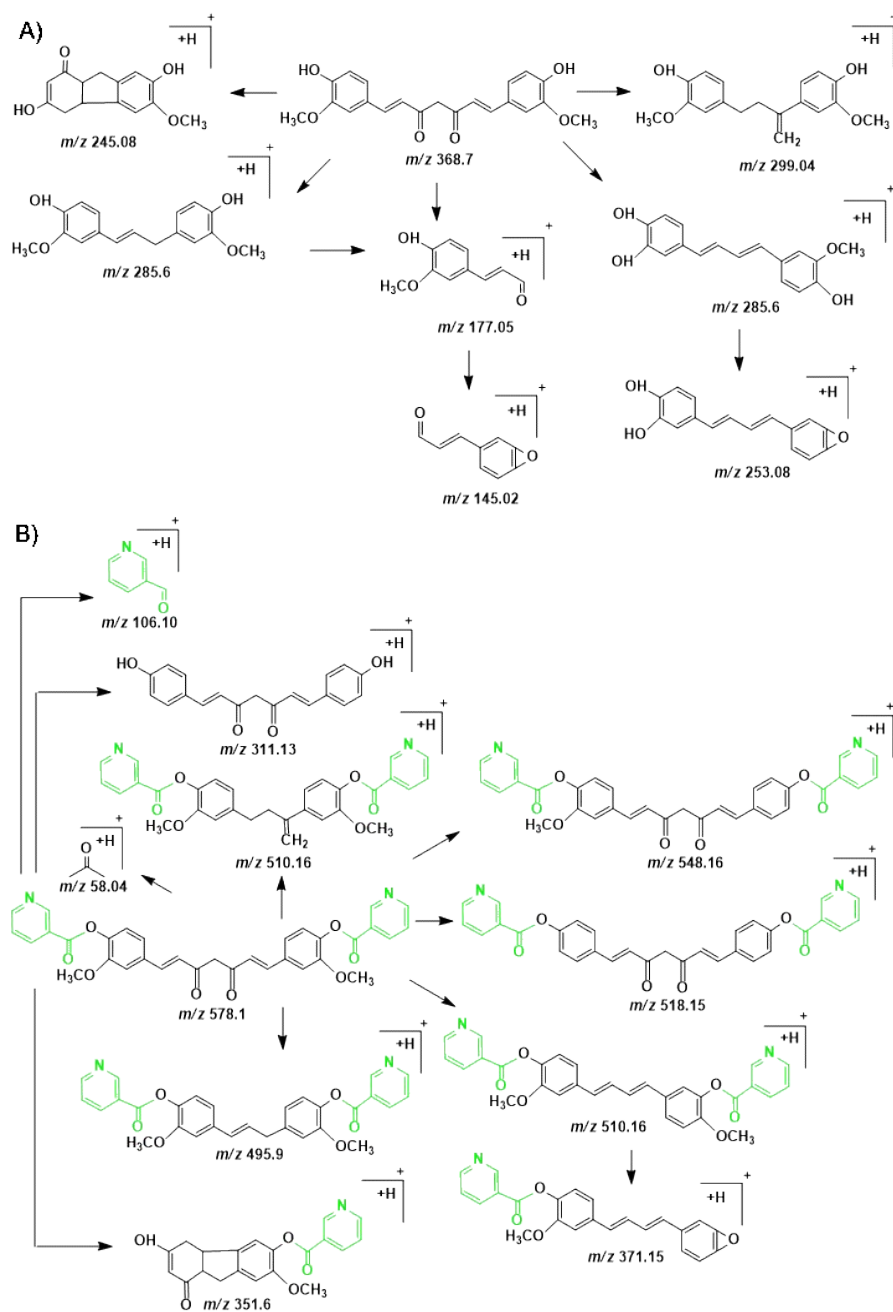


Fig. S2 MS spectrum of Cur-Nic.



Scheme S1 Proposed fragmentation pathways of (A) curcumin and (B) Cur-Nic.

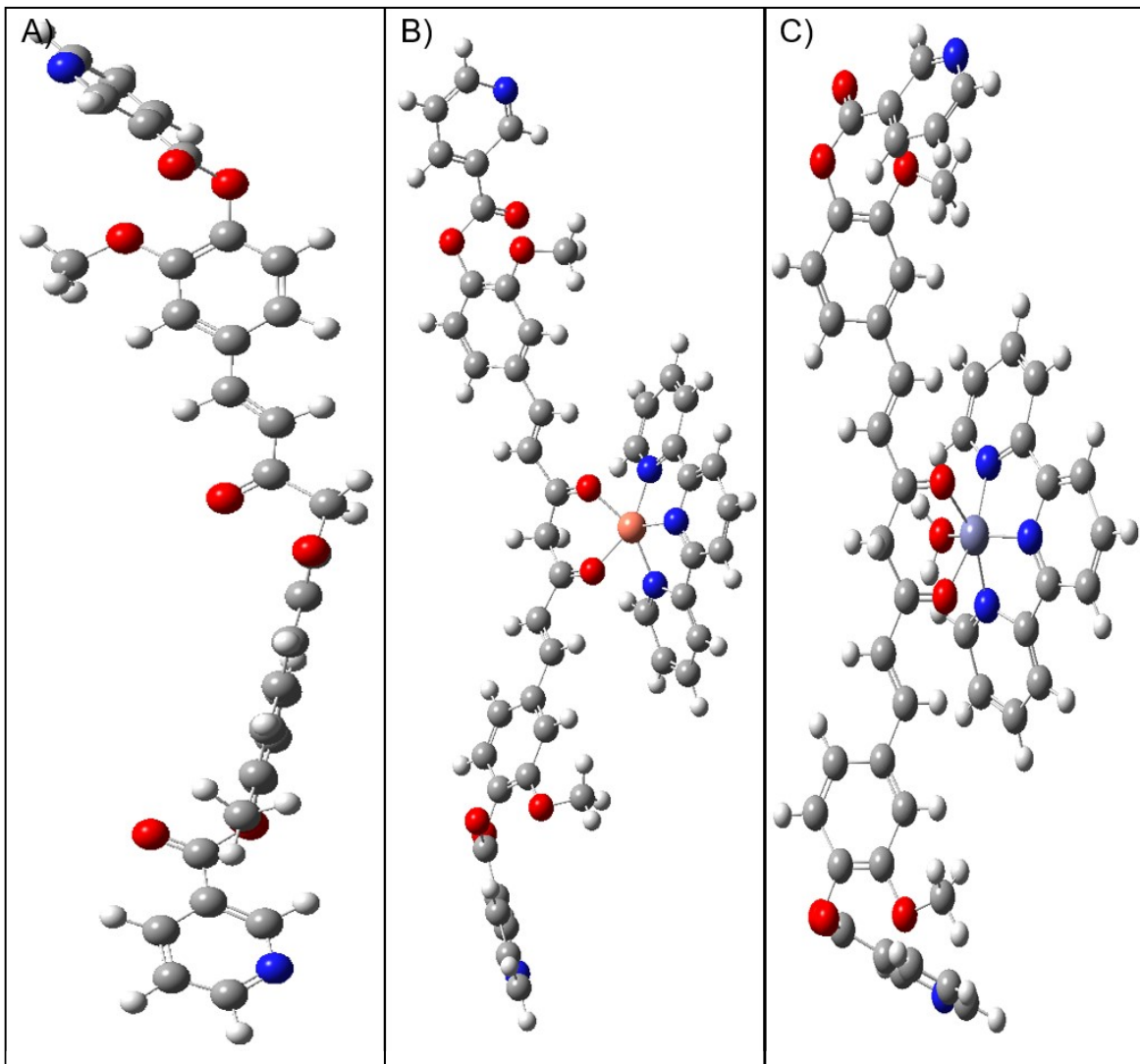


Fig. S3 optimized structure of (A) Cur-Nic, (B) Cu(II) complex, and (C) Zn(II) complex.