

Supporting Information

The Synthesis, Characterization, Molecular docking, and In Vitro Antitumour Activity of Benzothiazole Aniline (BTA) Conjugated Metal-Salen Complexes as Non-Platinum Chemotherapeutic Agents

Md. Kamrul Islam ¹, Seongmin Ha ¹, Ah-Rum Baek ¹, Byeong-Woo Yang ¹, Yeoun-Hee Kim ², Hyun-Jin Park ², Minsup Kim ³, Sung-Wook Nam ⁴, Gang-Ho Lee ⁵ and Yongmin Chang ^{4,6,7,*}

¹ Institute of Biomedical Engineering Research, Kyungpook National University, 680, Gukchaebosang-ro, Jung-gu, Daegu 41944, Republic of Korea

² R&D Center, Etnova Therapeutics Corp., 124, Sagimakgol-ro, Jungwon-gu, Gyeonggi-do 13207, Republic of Korea

³ InCerebro Drug Discovery Institute, Seoul 01811, Republic of Korea

⁴ Department of Medical & Biological Engineering, Kyungpook National University, 80, Daehak-ro, Buk-gu, Daegu 41566, Republic of Korea

⁵ Department of Chemistry, Kyungpook National University, 80, Daehak-ro, Buk-gu, Daegu 41566, Republic of Korea

⁶ Department of Molecular Medicine, School of Medicine, Kyungpook National University, 680, Gukchaebosang-ro, Jung-gu, Daegu 41944, Republic of Korea

⁷ Department of Radiology, Kyungpook National University Hospital, 130 Dongdeok-ro, Jung-gu, Daegu 41944, Republic of Korea

* Correspondence: ychang@knu.ac.kr; Tel.: (+) 82-53-420-5471

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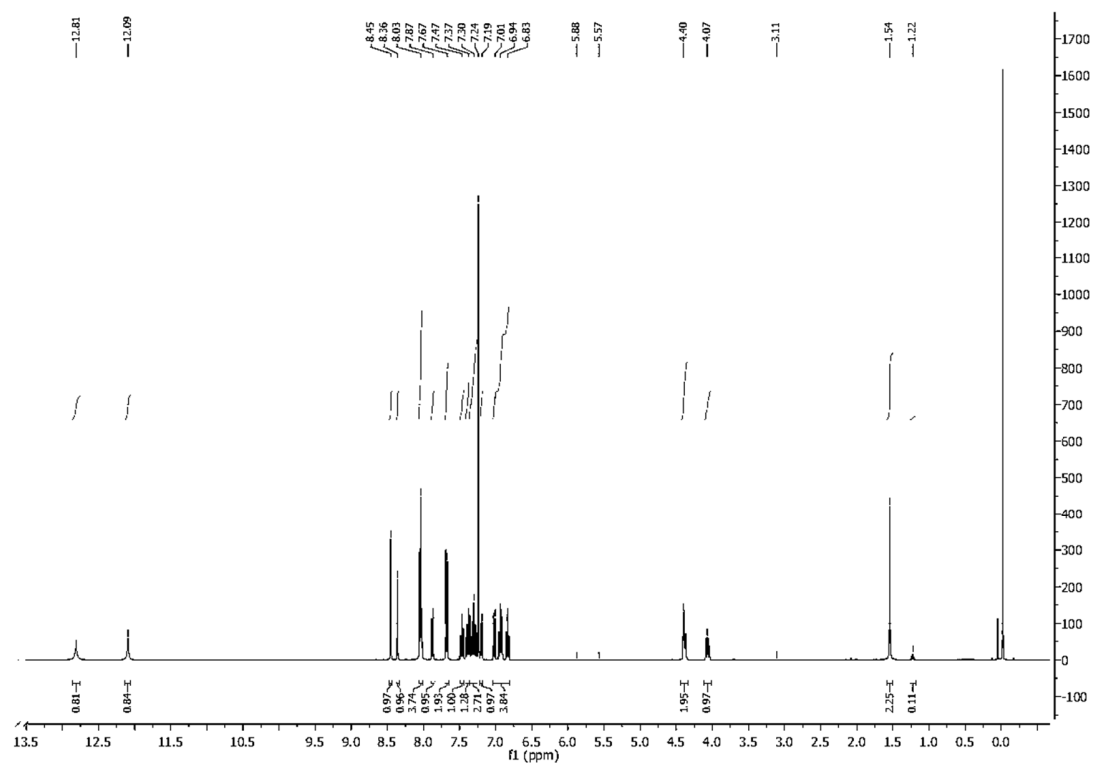


Figure S1. ¹H NMR spectrum of compound L.

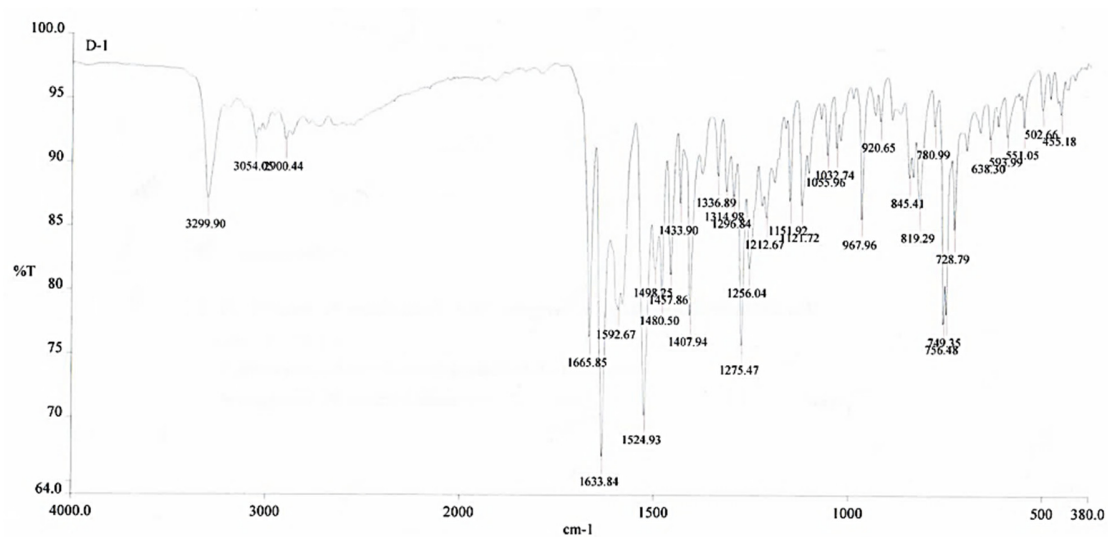


Figure S2. FT-IR spectrum of compound L.

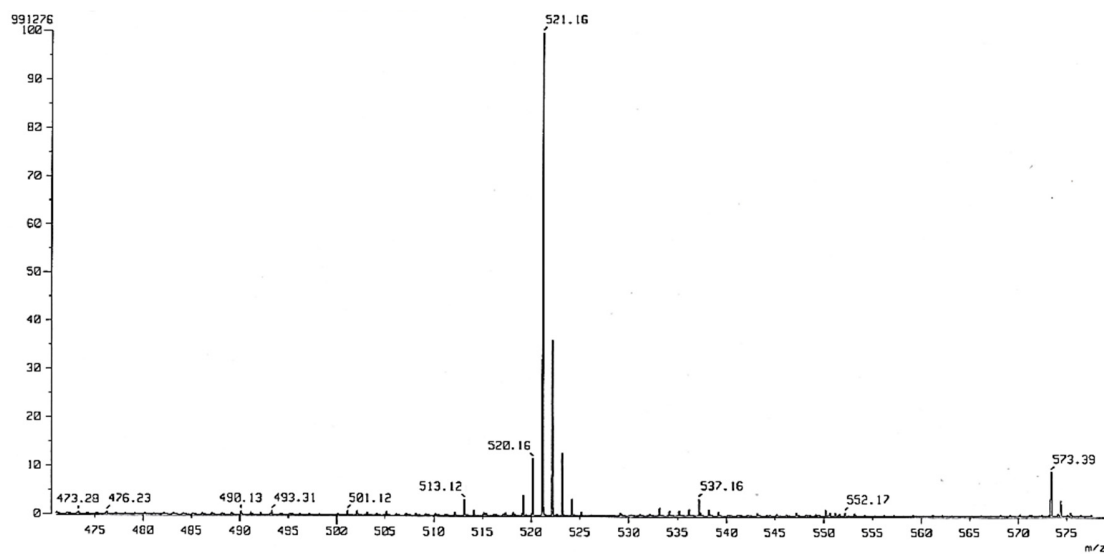


Figure S3. High-resolution FAB mass spectrum of compound **L**. Mass spectrum of main peak display parent ion (m/z): calcd, 521.1647 $[M+H]^+$; found, 521.1649 $[M+H]^+$.

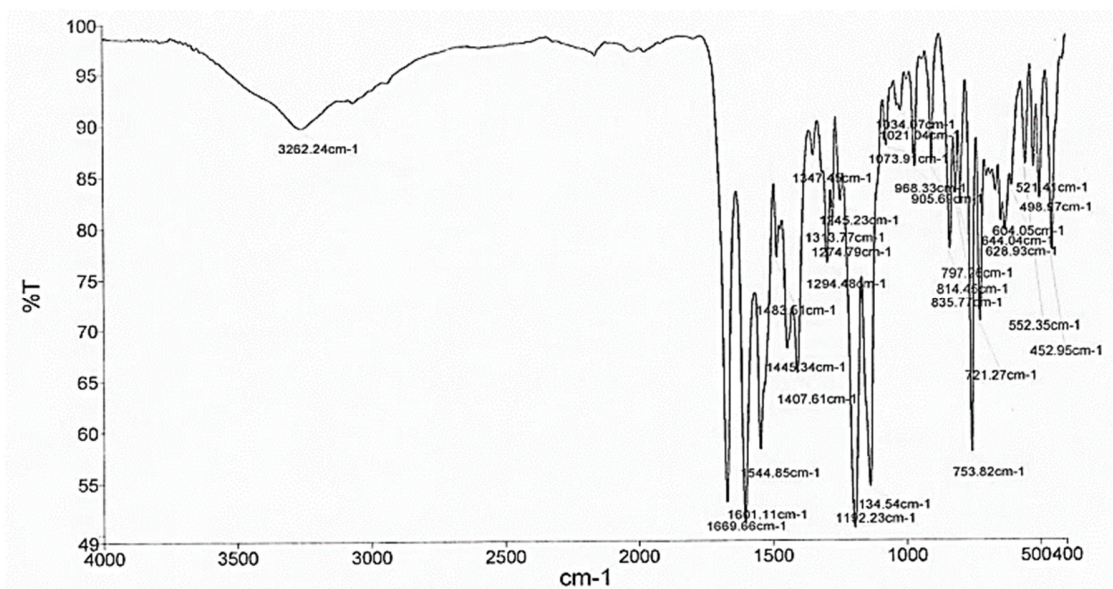


Figure S4. FTIR spectrum of compound **MnL**.

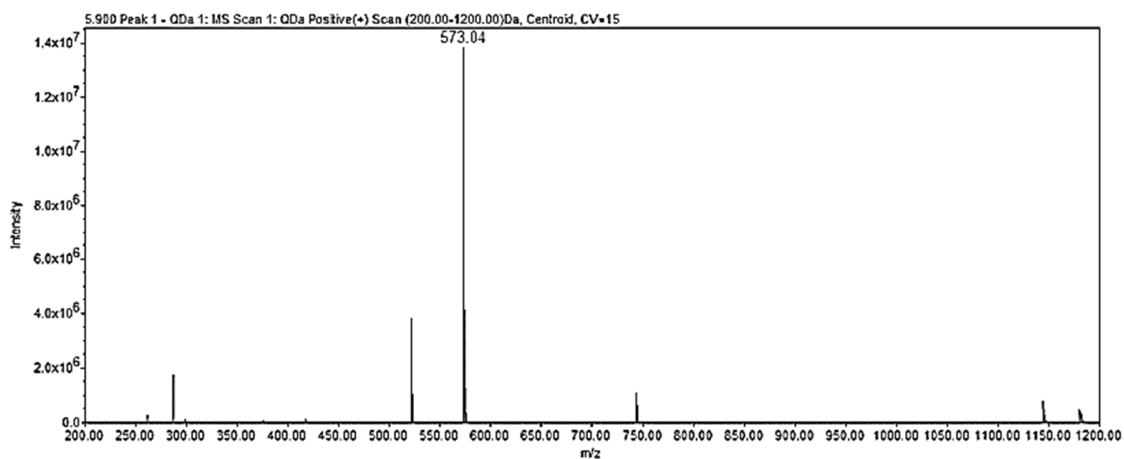


Figure S5. ESI-MS spectrum of compound **MnL**. Mass spectrum of main peak display parent ion (m/z): calcd, 573.07 [M]⁺; found, 573.04 [M]⁺.

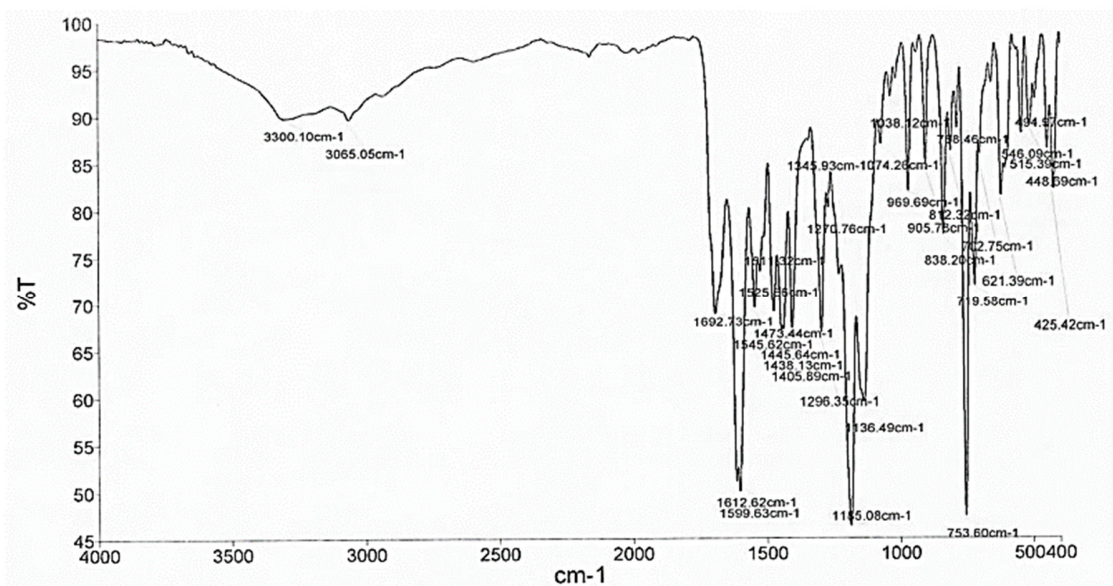


Figure S6. FTIR spectrum of compound **FeL**.

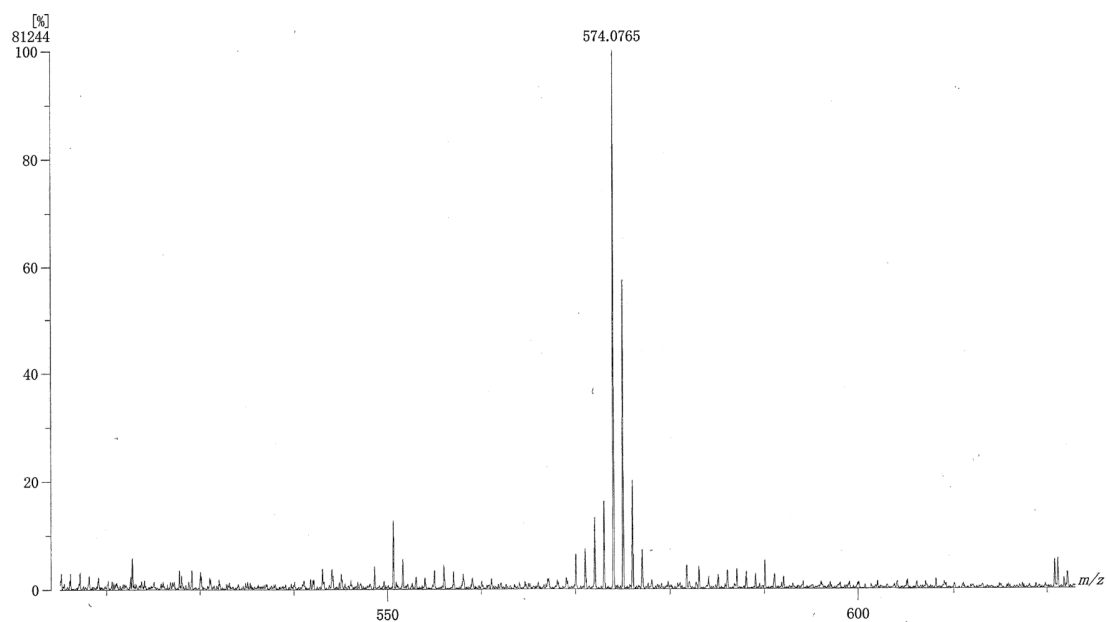


Figure S7. High-resolution FAB mass spectrum of compound FeL. Mass spectrum of main peak display parent ion (m/z): calcd, 521.1647 $[M+H]^+$; found, 574.0765 $[M+H]^+$.

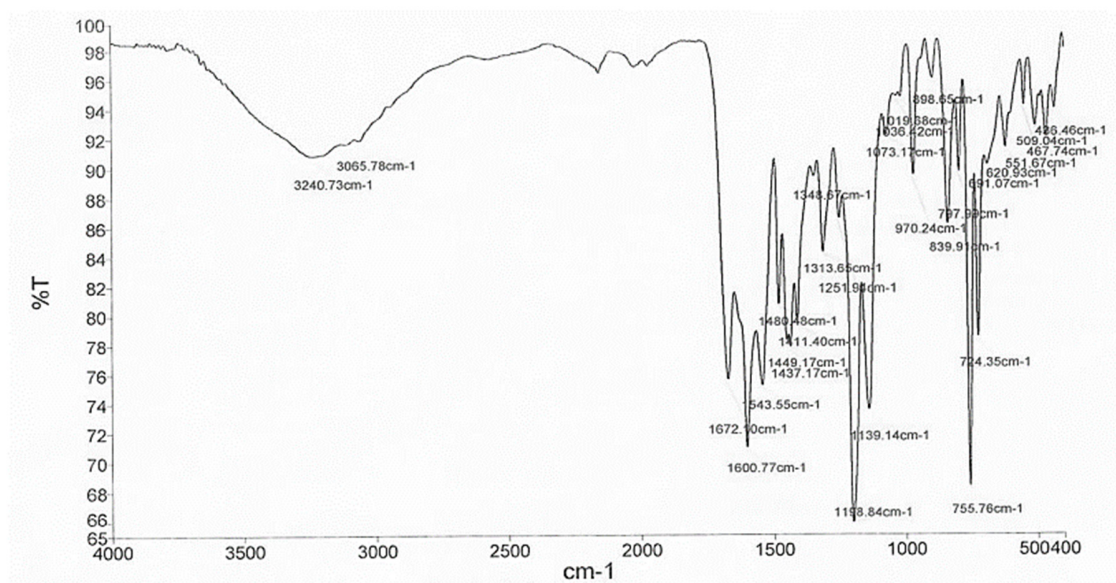


Figure S8. FTIR spectrum of compound CoL.

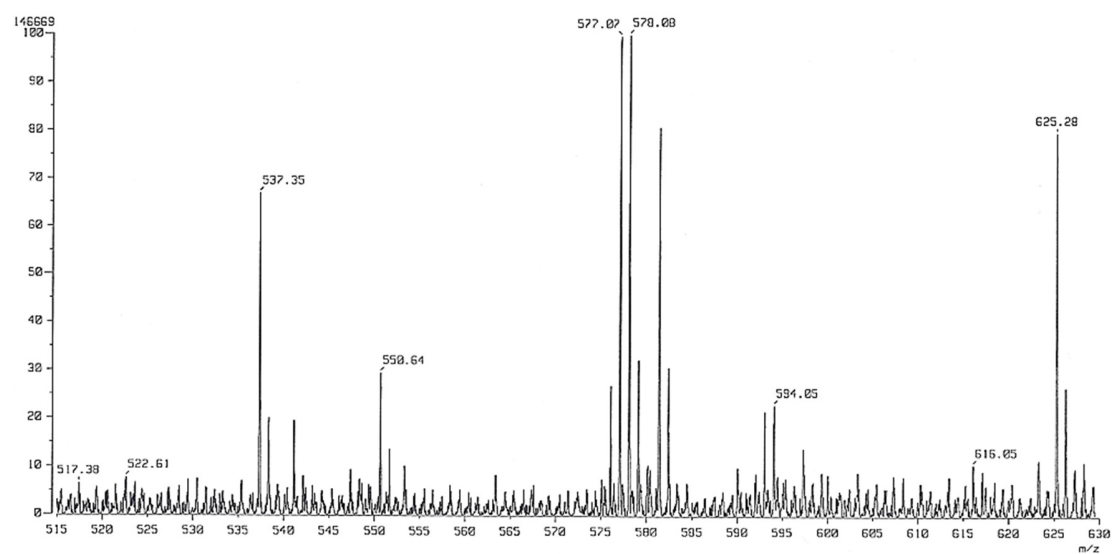


Figure S9. High-resolution FAB mass spectrum of compound CoL. Mass spectrum of main peak display parent ion (m/z): calcd, 577.0745 [M]⁺ and 578.0823 [M+H]⁺; found, 577.0749 [M]⁺ and 578.0820 [M+H]⁺.

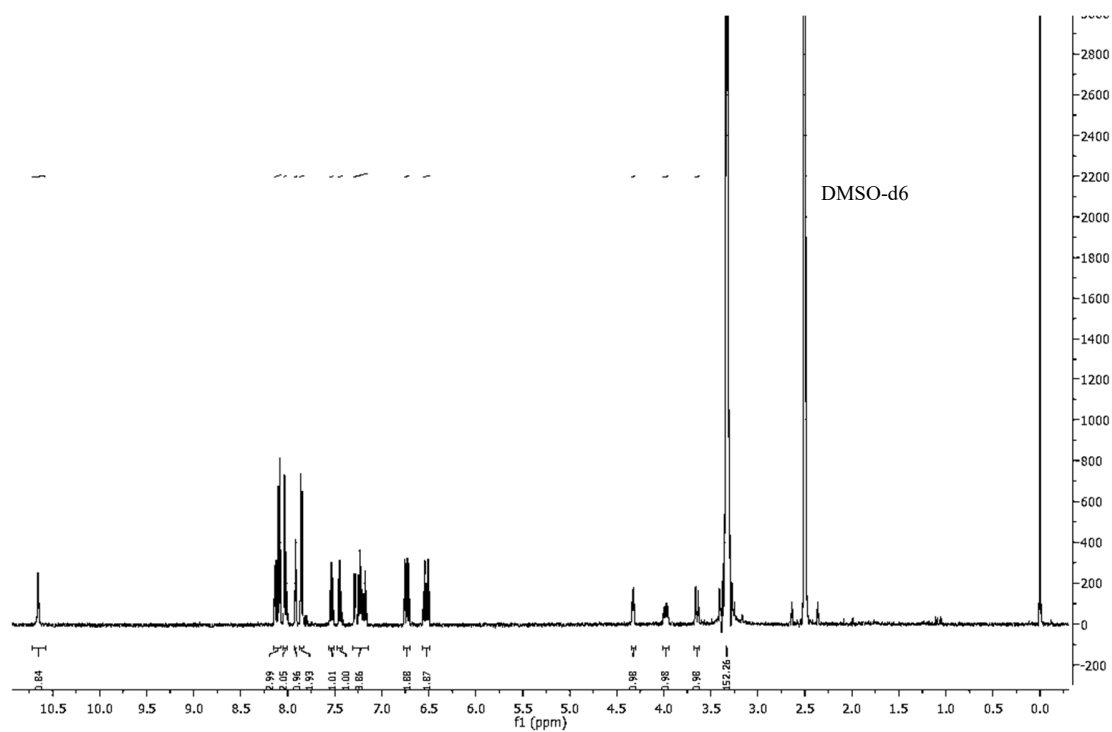


Figure S10. ¹H NMR spectrum of compound NiL.

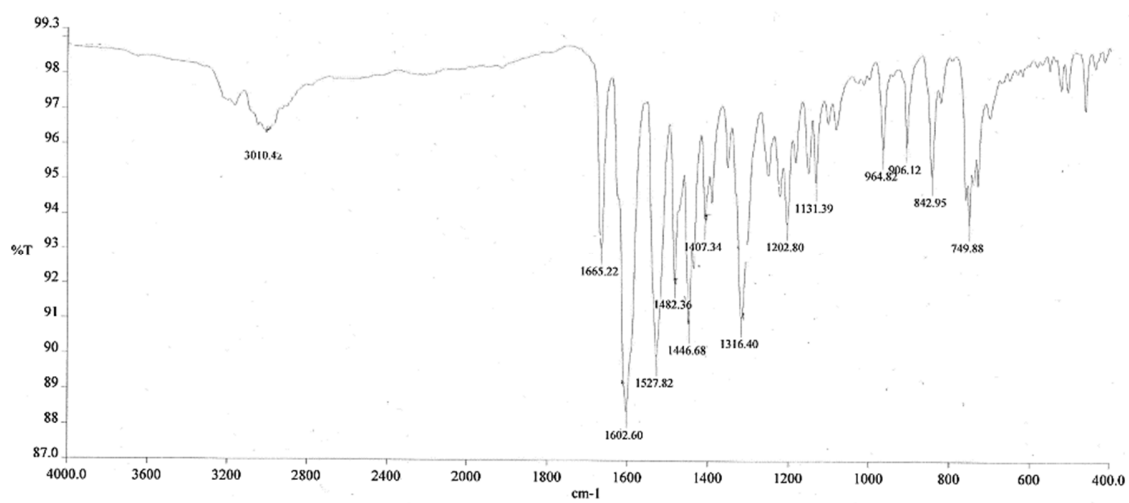


Figure S11. FTIR spectrum of compound NiL.

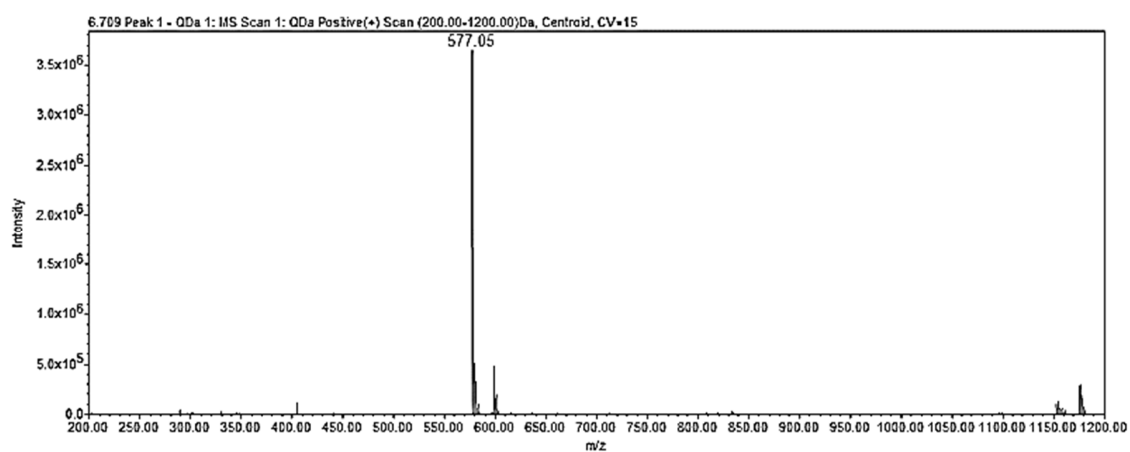


Figure S12. ESI-MS spectrum of compound NiL. Mass spectrum of main peak display parent ion (m/z): calcd, 577.08 [M+H]⁺; found, 577.05 [M+H]⁺.

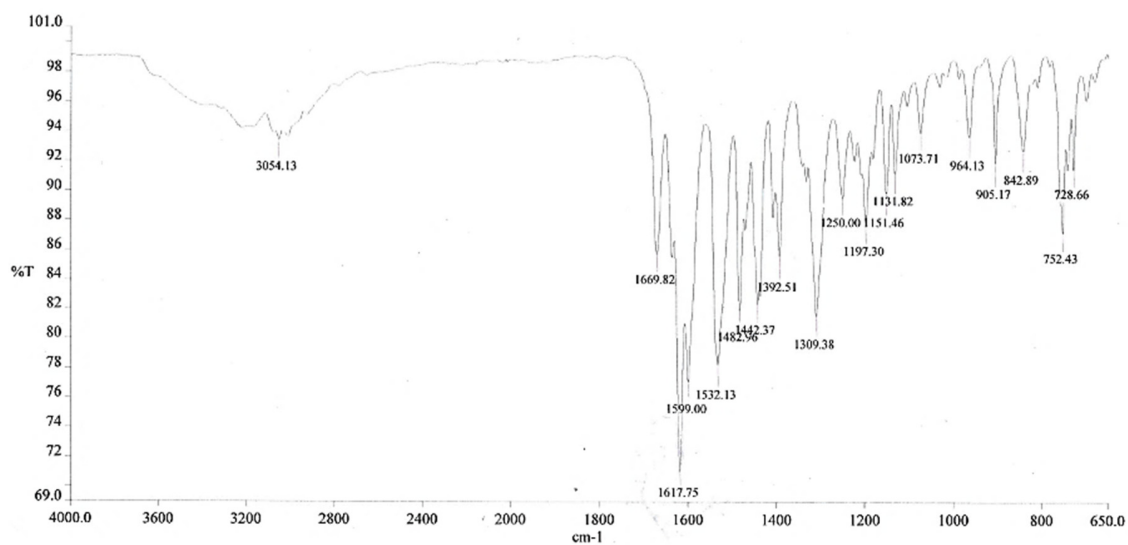


Figure S13. FTIR spectrum of compound CuL.

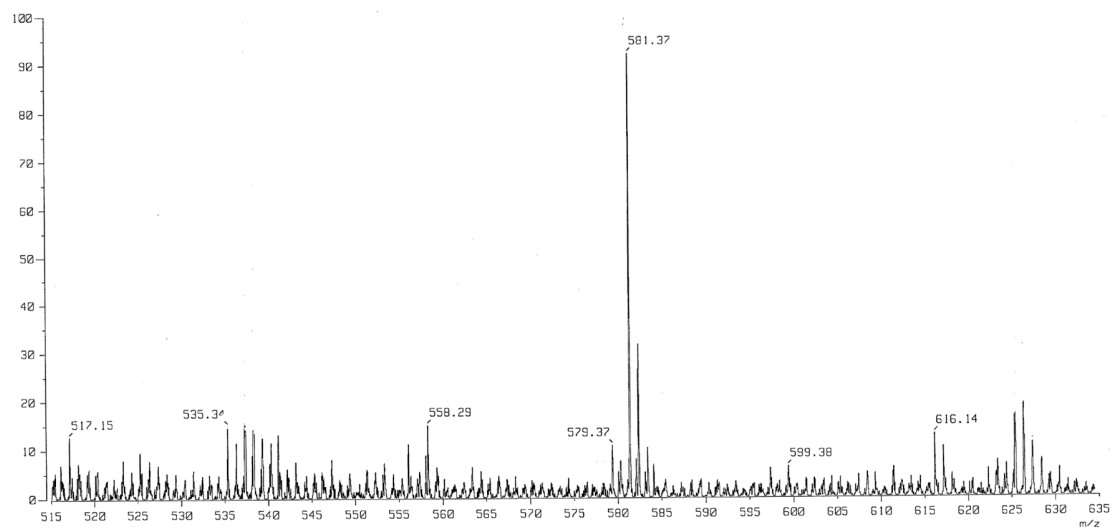


Figure S14. High-resolution FAB mass spectrum of compound CuL. Mass spectrum of main peak display parent ion (m/z): calcd, 581.0809 [M]⁺; found, 581.0709 [M]⁺.

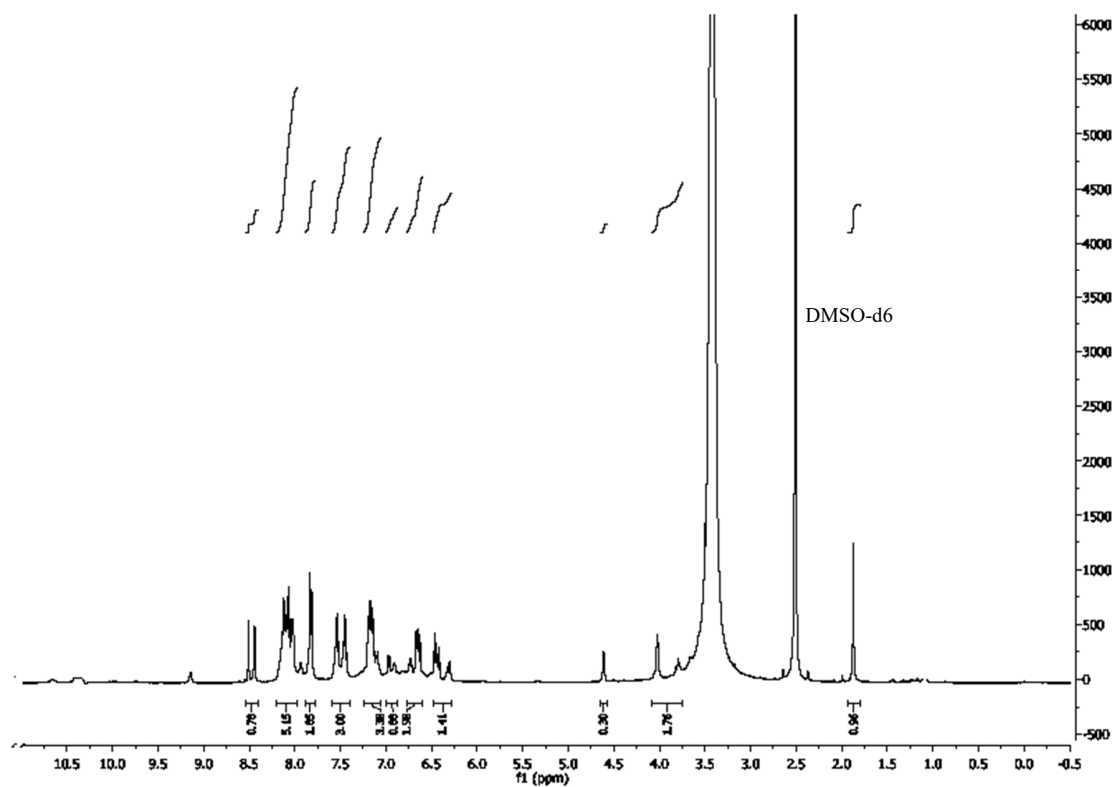


Figure S15. ^1H NMR spectrum of compound ZnL.

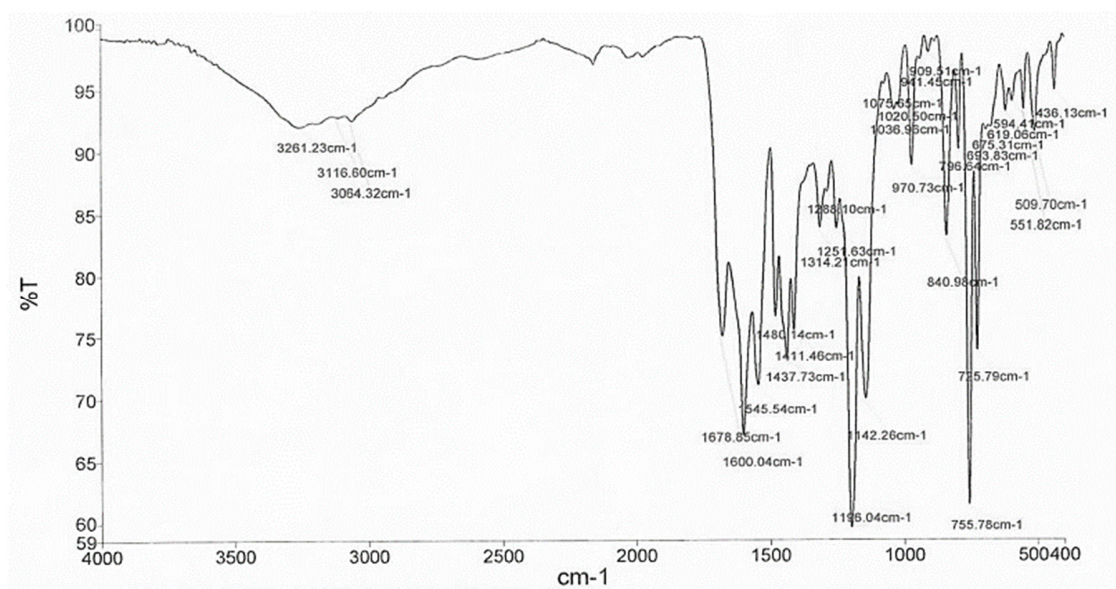


Figure S16. FTIR spectrum of compound ZnL.

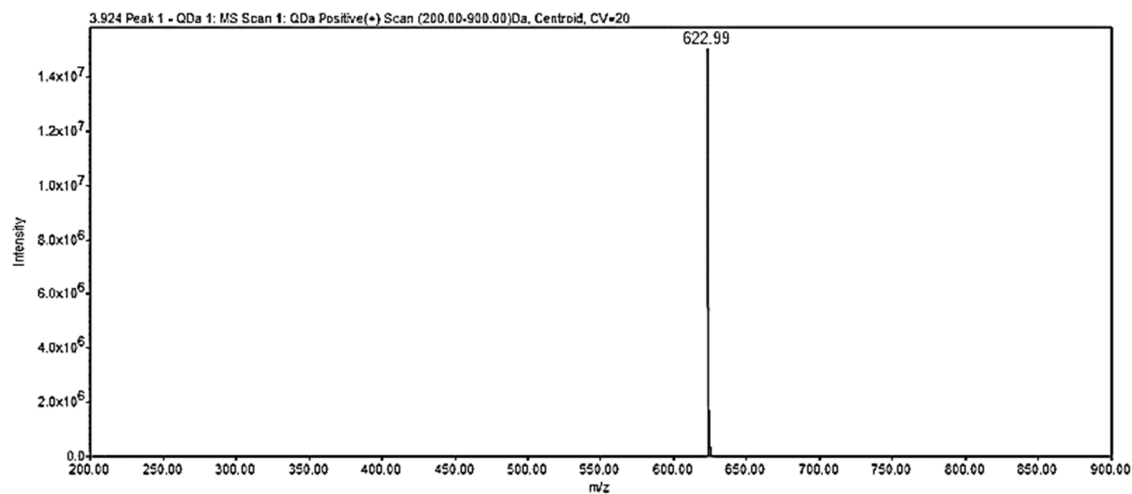


Figure S17. ESI-MS spectrum of compound **ZnL**. Mass spectrum of main peak display parent ion (m/z): calcd, 622.04 [M+K]⁺; found, 622.99 [M+K]⁺.

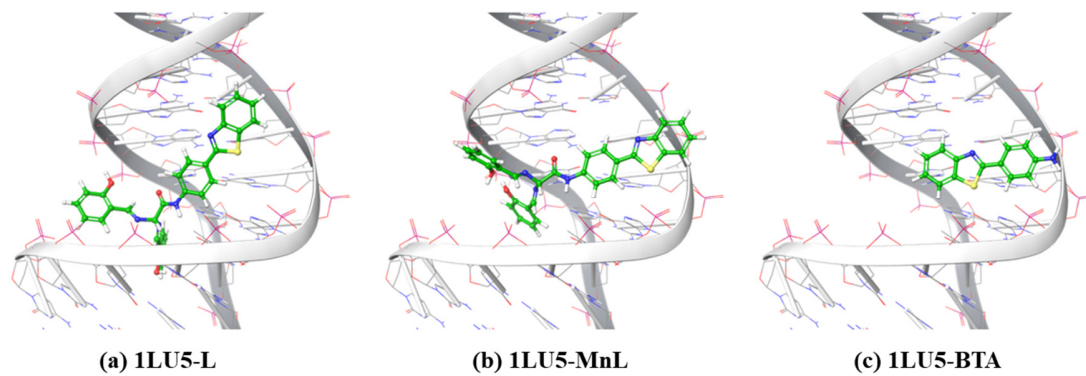


Figure S18. DNA binding configurations were predicted for the compounds (a) **L**, (b) **MnL**, and (c) **BTA** (PDB ID: 1LU5).

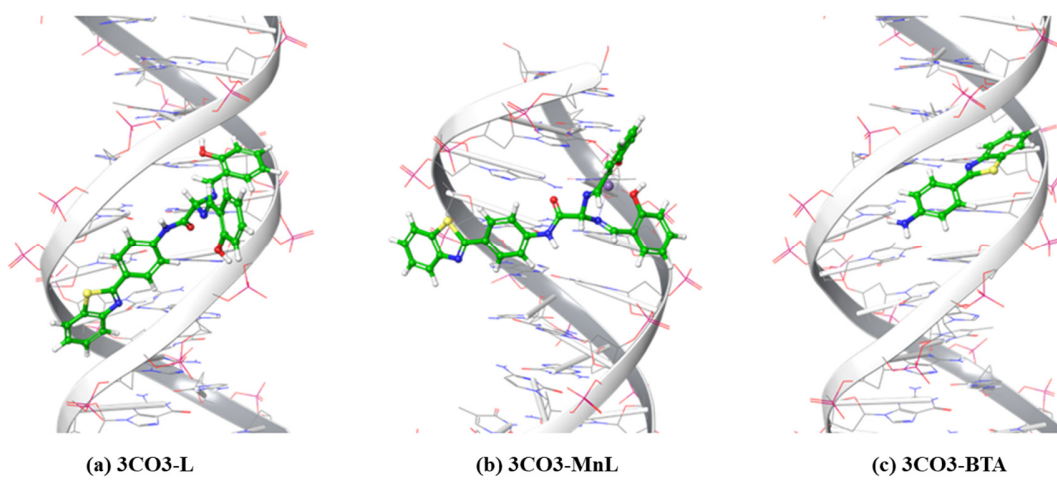


Figure S19. DNA binding configurations were predicted for the compounds (a) **L**, (b) **MnL**, and (c) **BTA** (PDB ID: 3CO3).