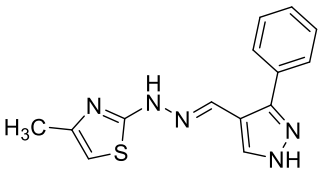
DESIGN, SYNTHESIS, AND EVALUATION OF ANTIBACTERIAL POTENTIAL OF HYDRAZONE-TETHERED PYRAZOLE-THIAZOLE DERİVATİVES

HİDRAZON BAĞLI PİRAZOL-TİYAZOL TÜREVLERİNİN TASARIMI, SENTEZİ VE ANTİBAKTERİYEL POTANSİYELİNİN DEĞERLENDİRİLMESİ

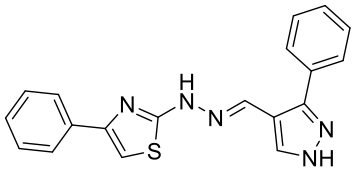
Supporting Information

Table of Contents **Page**

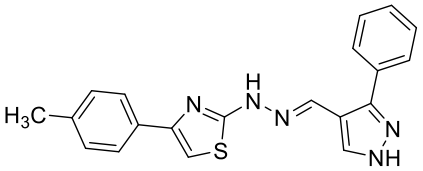
The designed compounds:



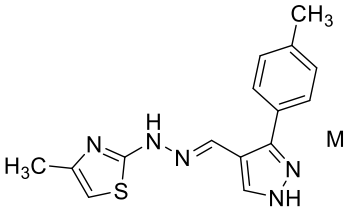
a



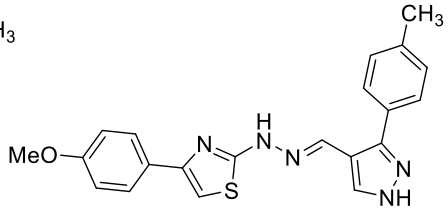
b



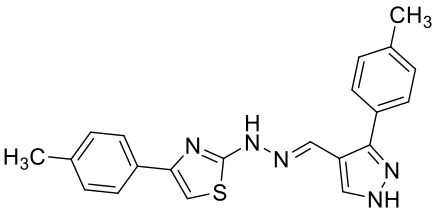
c



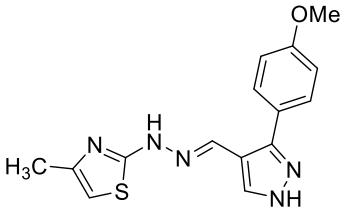
d



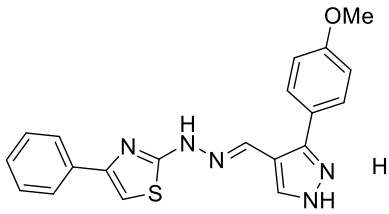
e



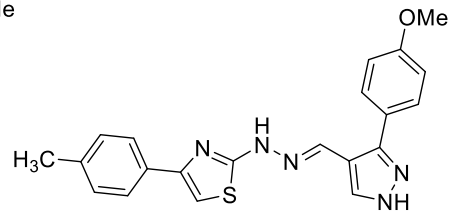
f



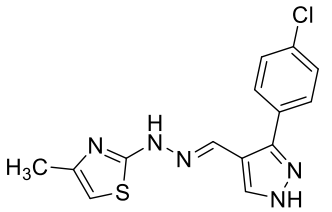
17a



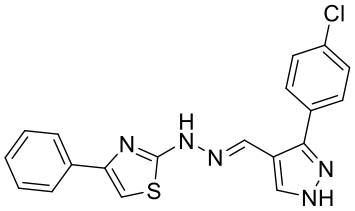
17b



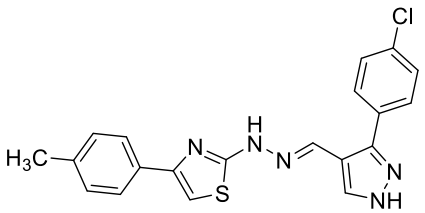
17c



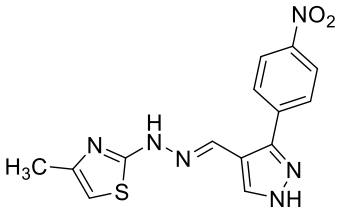
g



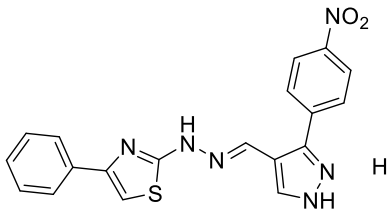
h



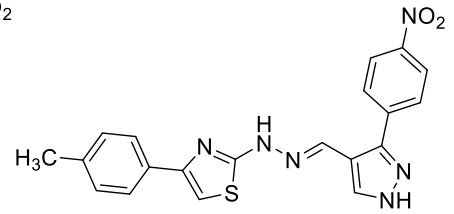
i



j



k



l

Table S1. Predicted LD_{50} Values of the Compounds

Compounds	SMILES	LD_{50} (mg/kg) (ProTox-3.0)
a	CC1=CSC(N\N=C\C2=CNN=C2C2=CC=CC=C2)=N1	300
b	N(\N=C\C1=CNN=C1C1=CC=CC=C1)C1=NC(=CS1)C1=CC=CC=C1	300
c	CC1=CC=C(C=C1)C1=CSC(N\N=C\C2=CNN=C2C2=CC=CC=C2)=N1	300
d	CC1=CSC(N\N=C\C2=CNN=C2C2=CC=C(C)C=C2)=N1	300
e	CC1=CC=C(C=C1)C1=NNC=C1\C=N\NC1=NC(=CS1)C1=CC=CC=C1	300
f	CC1=CC=C(C=C1)C1=CSC(N\N=C\C2=CNN=C2C2=CC=C(C)C=C2)=N1	300
g	CC1=CSC(N\N=C\C2=CNN=C2C2=CC=C(Cl)C=C2)=N1	300
h	ClC1=CC=C(C=C1)C1=NNC=C1\C=N\NC1=NC(=CS1)C1=CC=CC=C1	300
i	CC1=CC=C(C=C1)C1=CSC(N\N=C\C2=CNN=C2C2=CC=C(Cl)C=C2)=N1	300
j	CC1=CSC(N\N=C\C2=CNN=C2C2=CC=C(C=C2)[N+]([O-])=O)=N1	300
k	[O-][N+](=O)C1=CC=C(C=C1)C1=NNC=C1\C=N\NC1=NC(=CS1)C1=CC=CC=C1	300
l	CC1=CC=C(C=C1)C1=CSC(N\N=C\C2=CNN=C2C2=CC=C(C=C2)[N+]([O-])=O)=N1	300

All compounds have an LD_{50} of 300 mg/kg, which means these compounds fall under "Class III: toxic if swallowed ($50 < LD_{50} \leq 300$ mg/kg)".

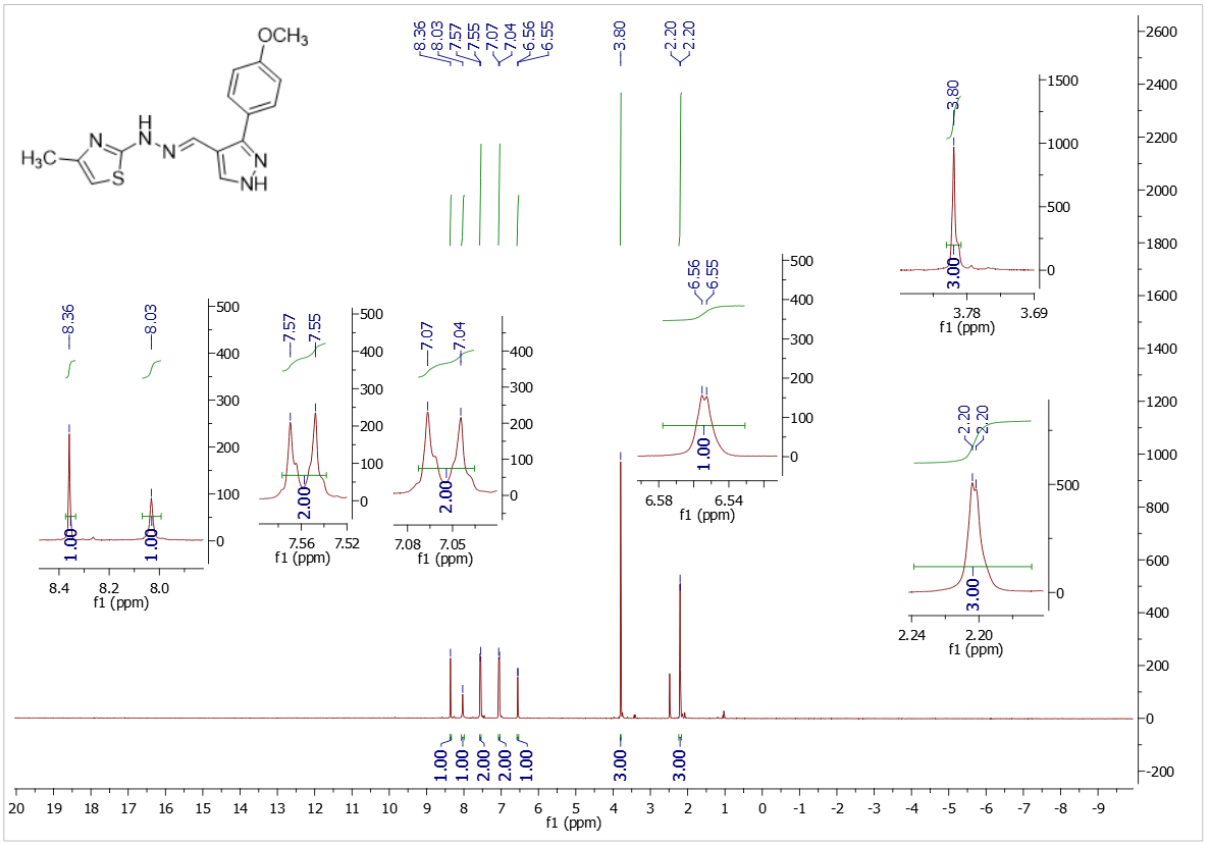


Figure S1. ^{1}H NMR spectrum of **17a**

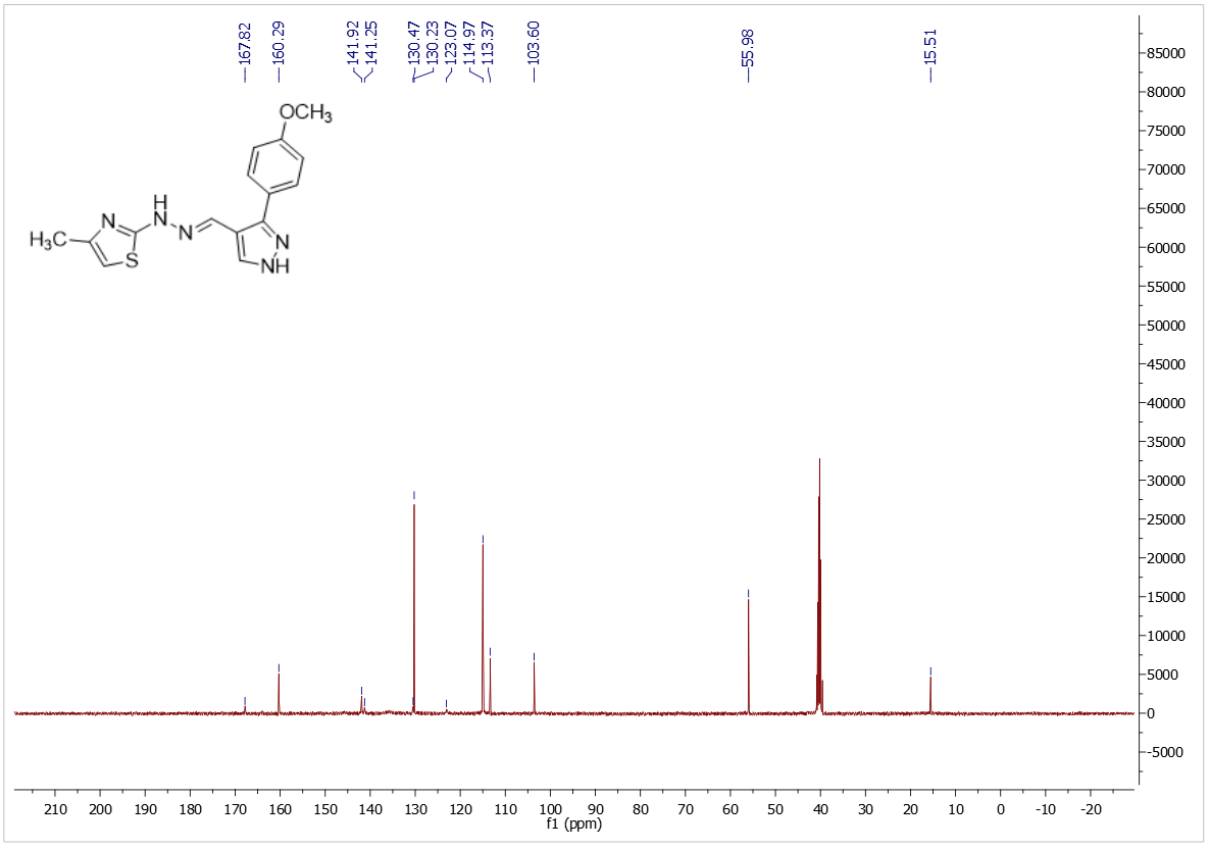


Figure S2. ^{13}C NMR spectrum of **17a**

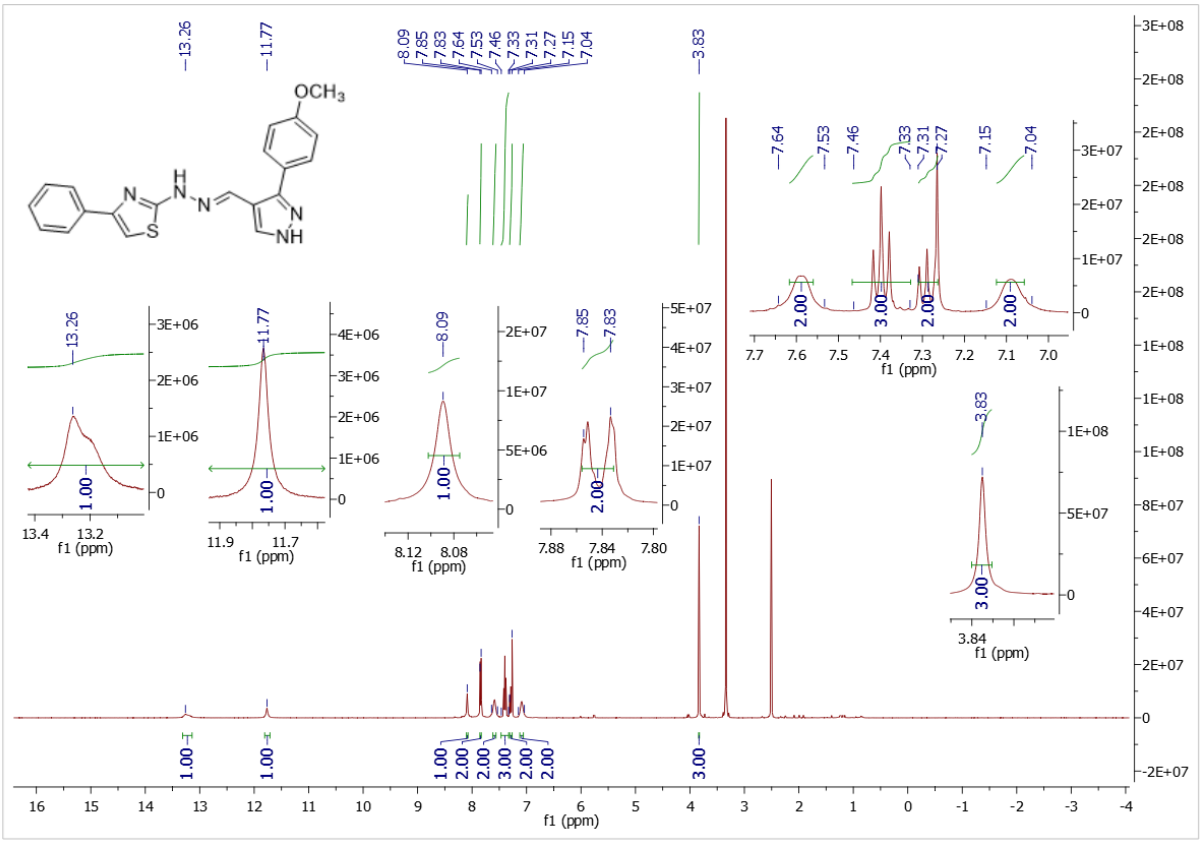


Figure S3. ^{1}H NMR spectrum of **17b**

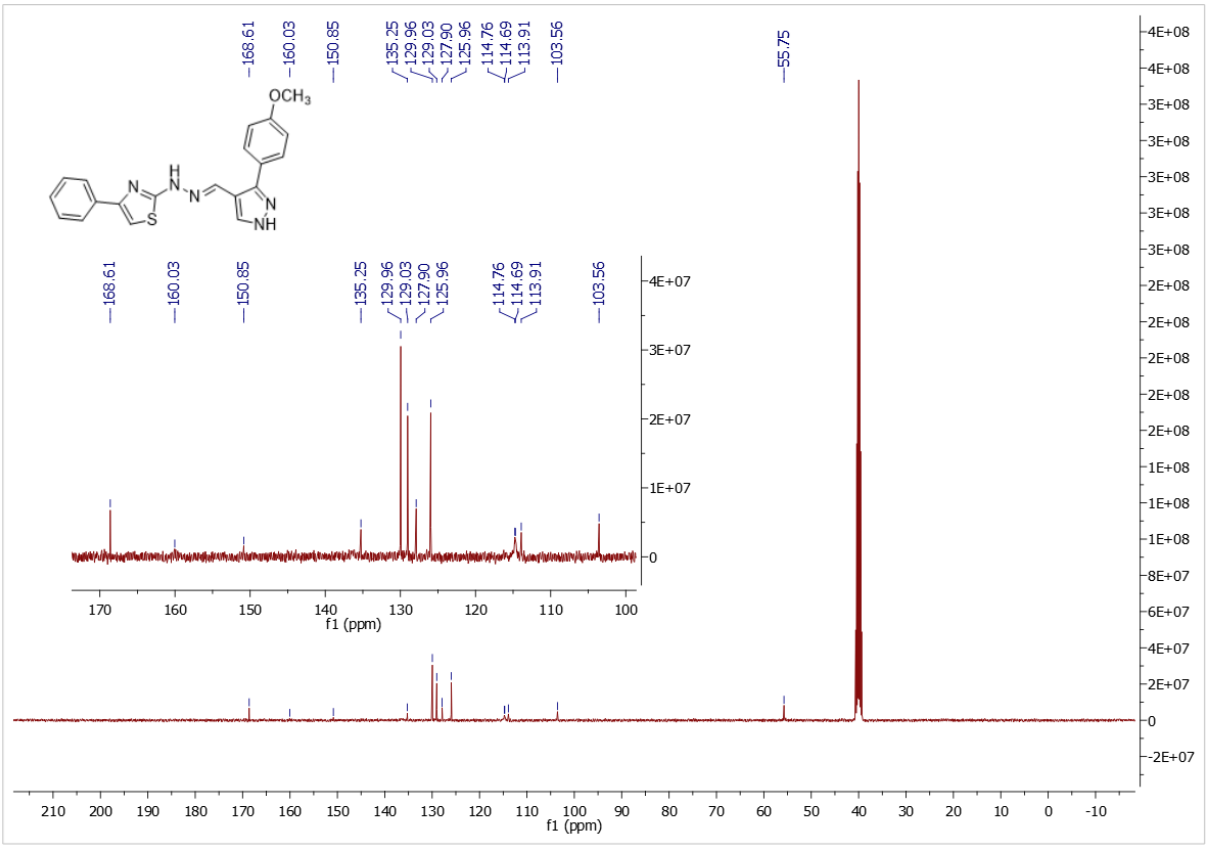


Figure S4. ^{13}C NMR spectrum of **17b**

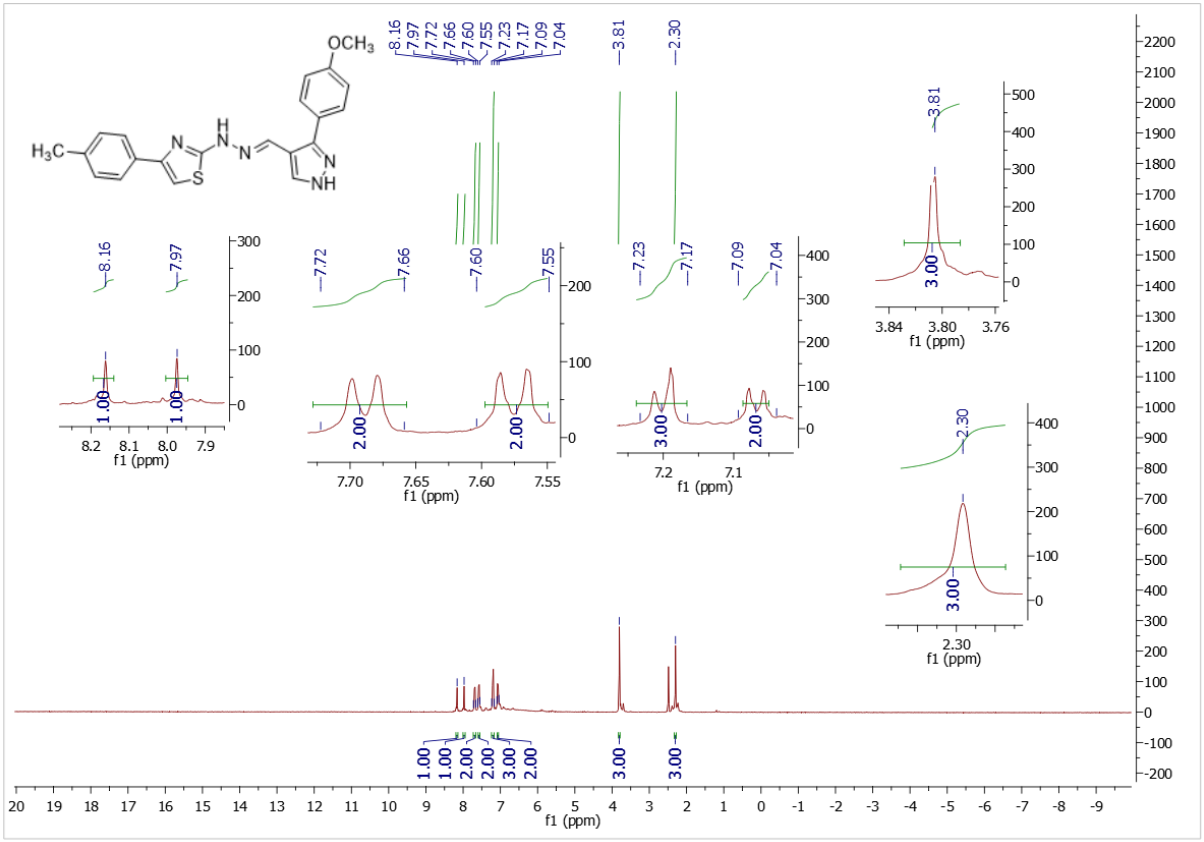


Figure S5. ^{1}H NMR spectrum of **17c**

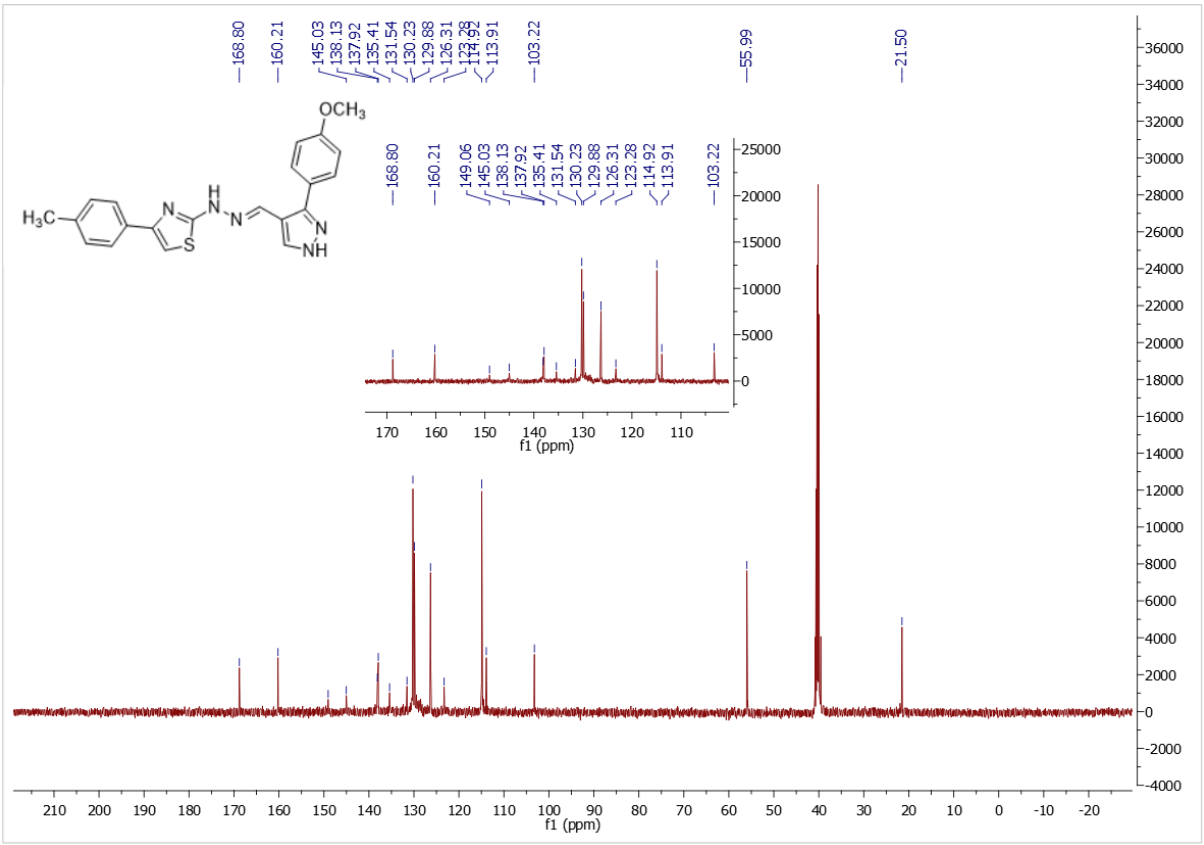


Figure S6. ^{13}C NMR spectrum of **17c**

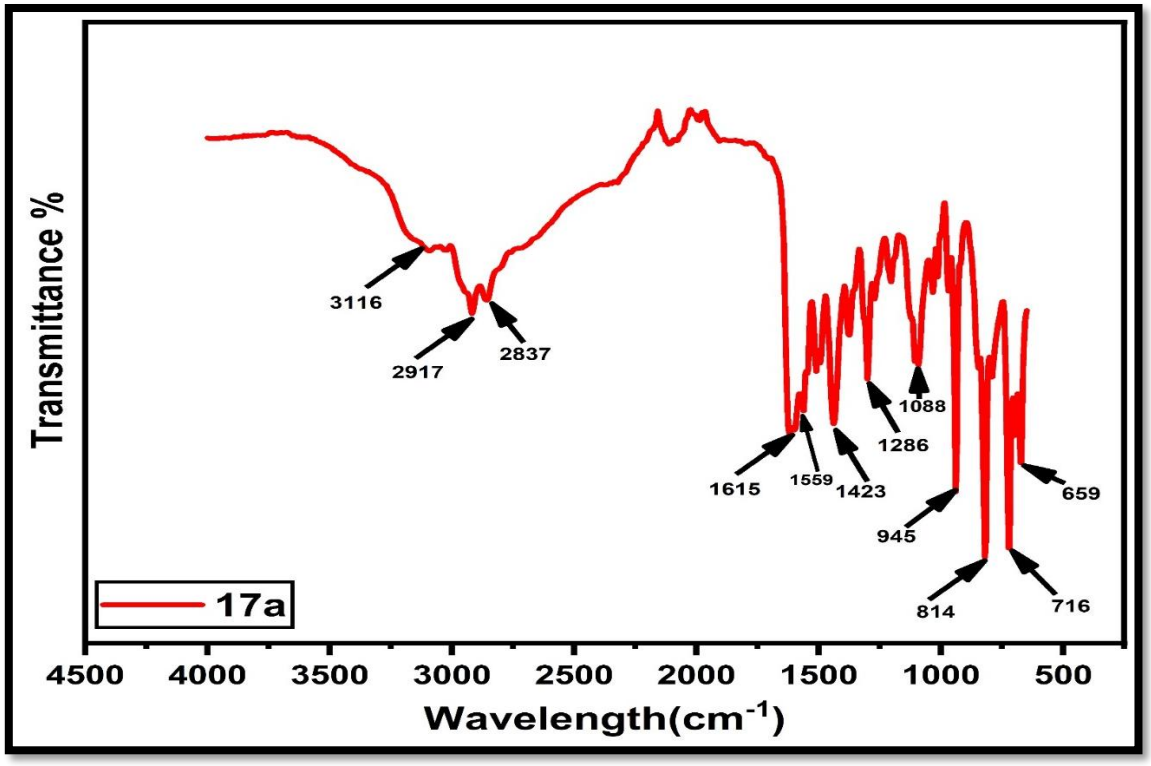


Figure S7. FT-IR spectrum of **17a**

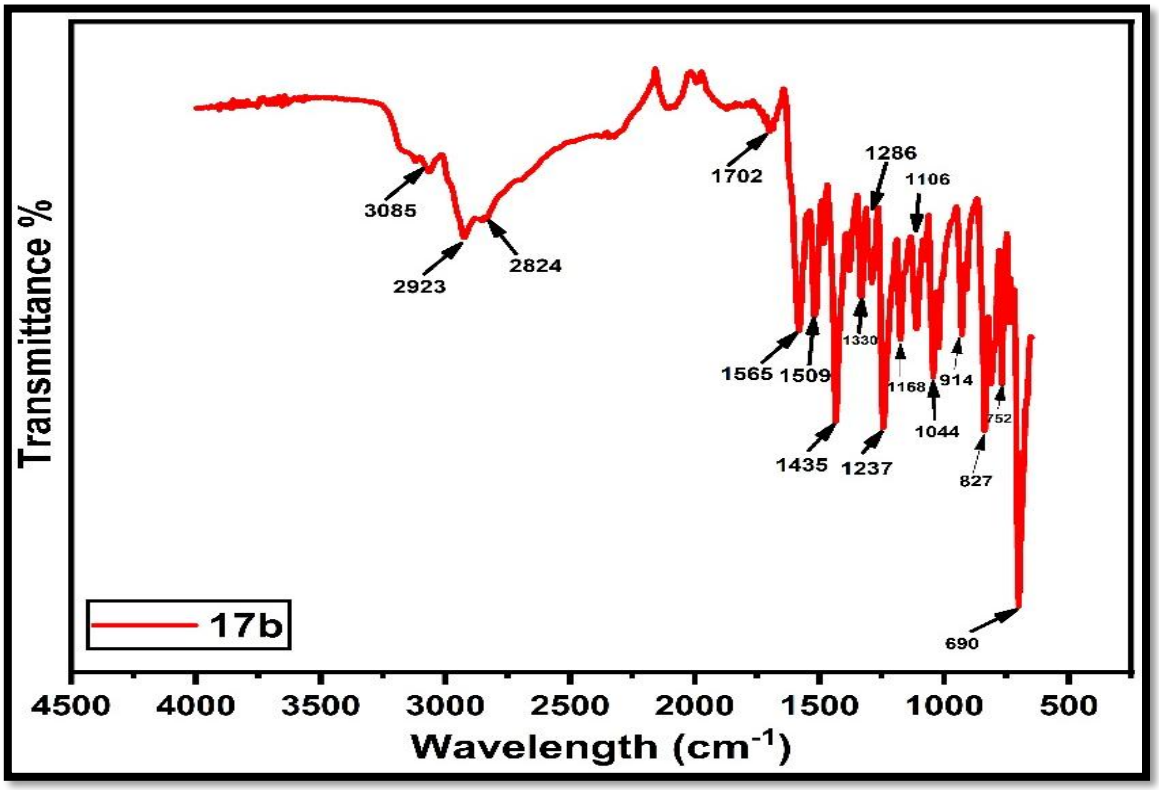


Figure S8. FT-IR spectrum of **17b**

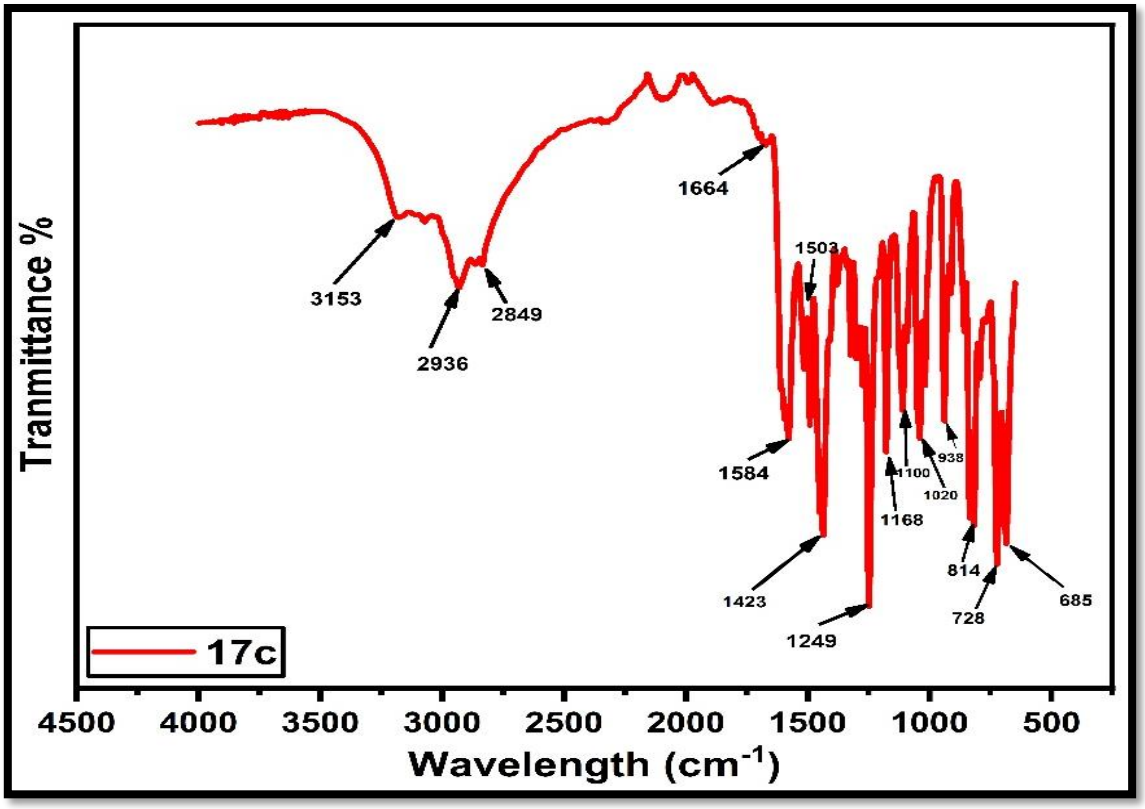


Figure S9. FT-IR spectrum of **17c**

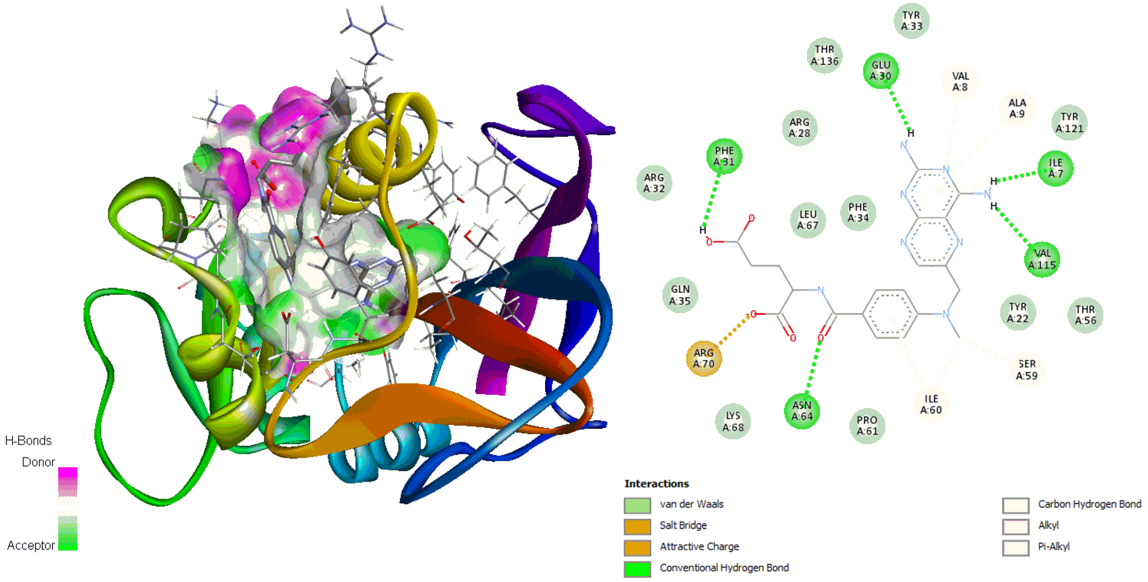


Figure S10. 3D and 2D interactions of **Methotrexate** with DHFR enzyme

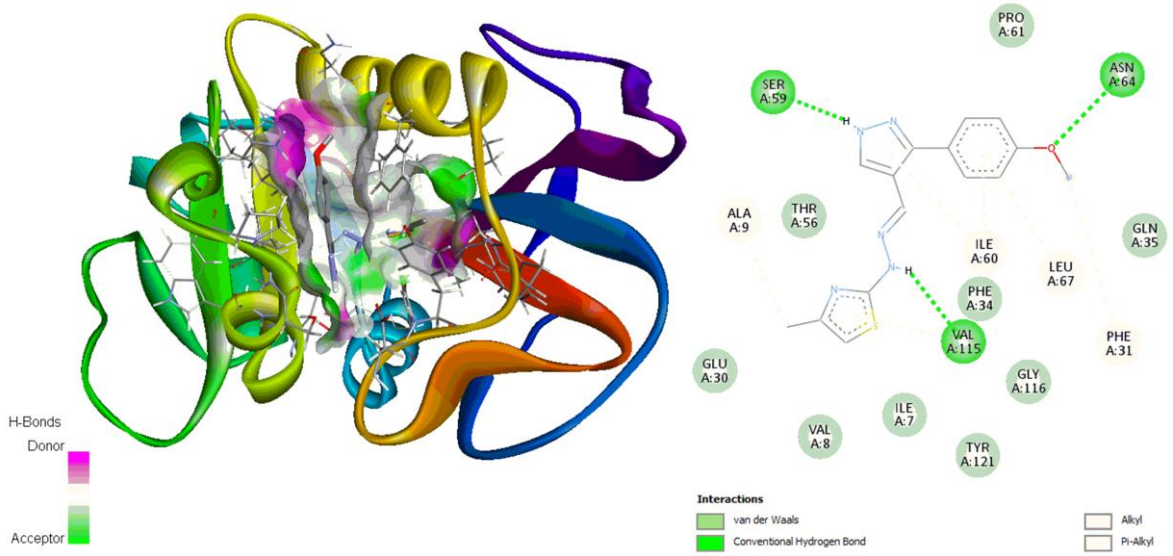


Figure S11. 3D and 2D interactions of **17a** with DHFR enzyme

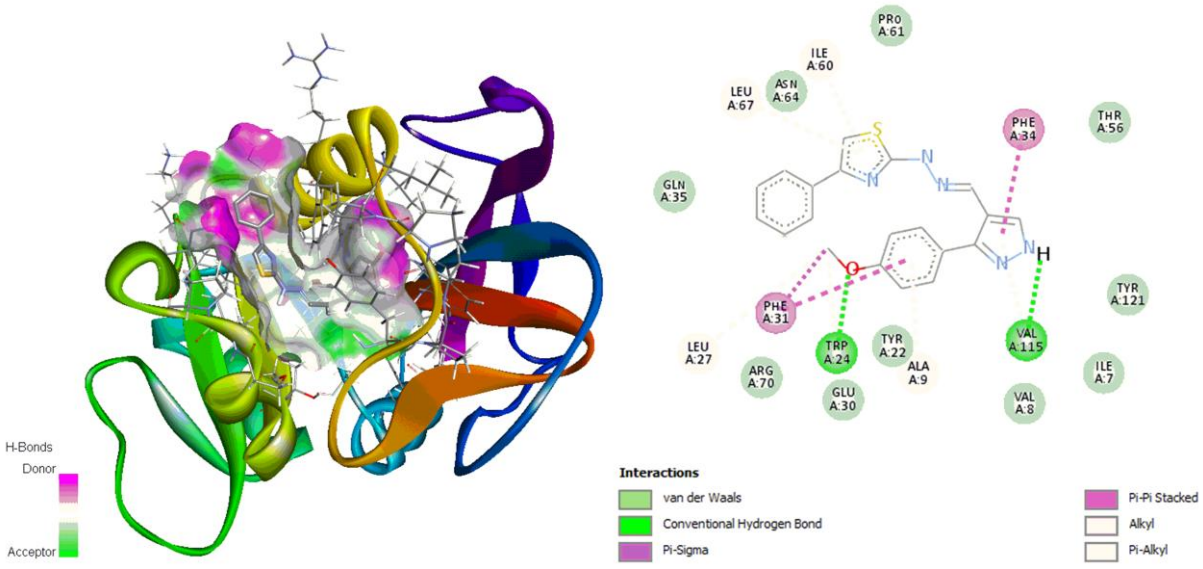


Figure S12. 3D and 2D interactions of **17b** with DHFR enzyme

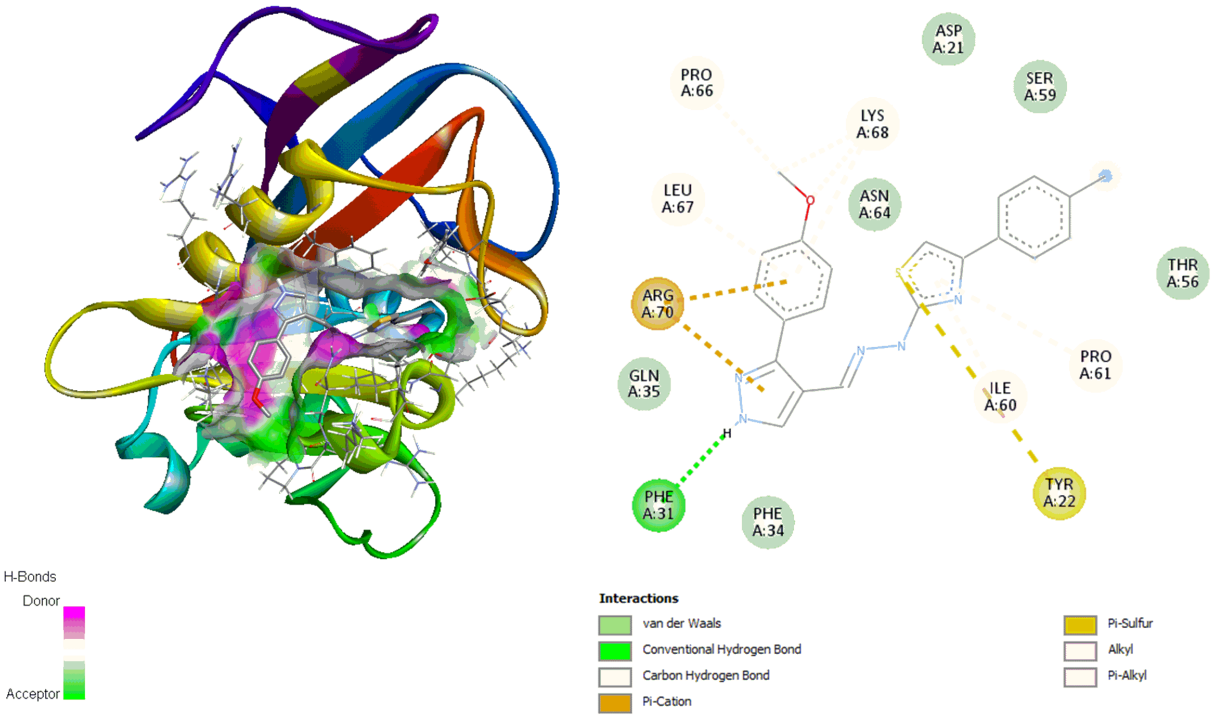


Figure S13. 3D and 2D interactions of **17c** with DHFR enzyme

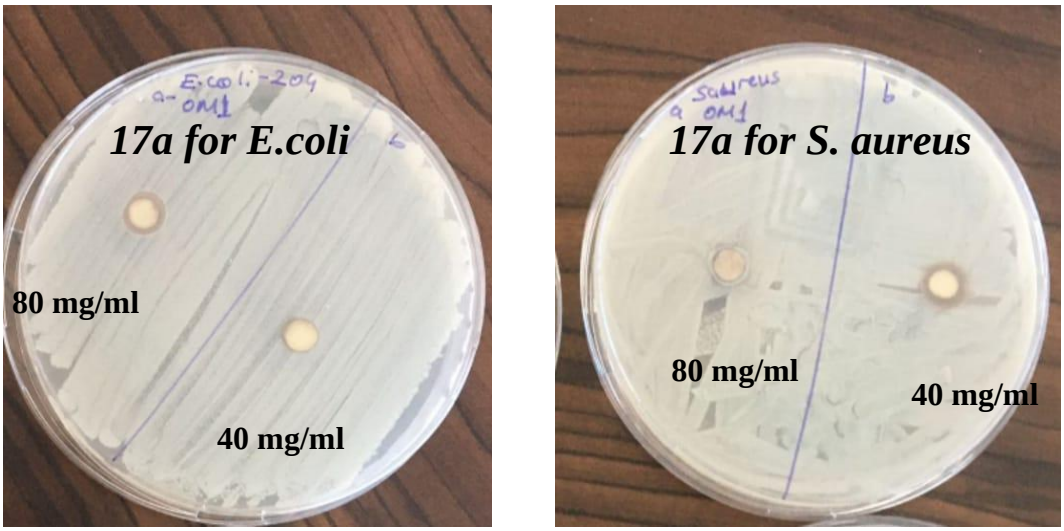


Figure S14. Antibacterial activity results of compounds **17a** tested against *E. coli* and *S. aureus* strains

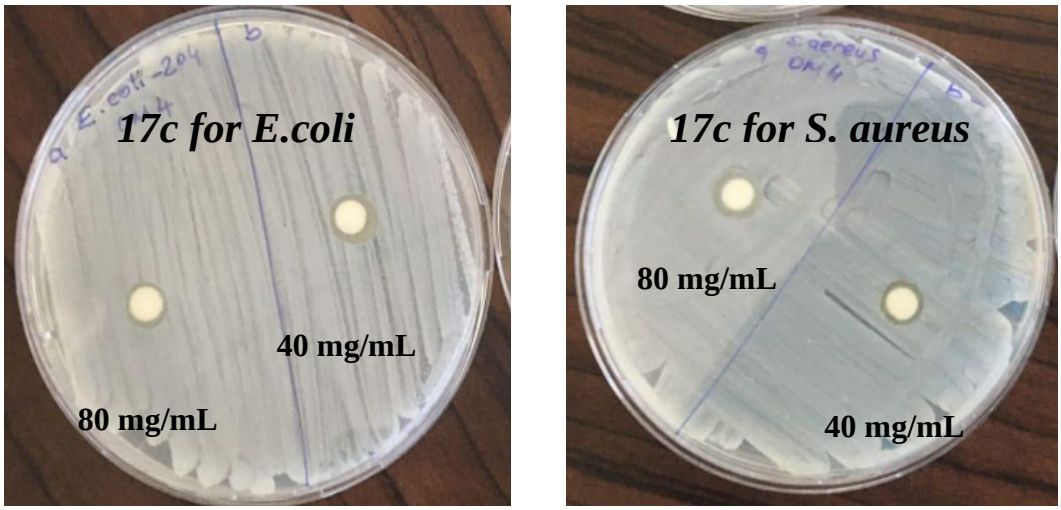


Figure S15. Antibacterial activity results of compounds **17c** tested against *E. coli* and *S. aureus* strains

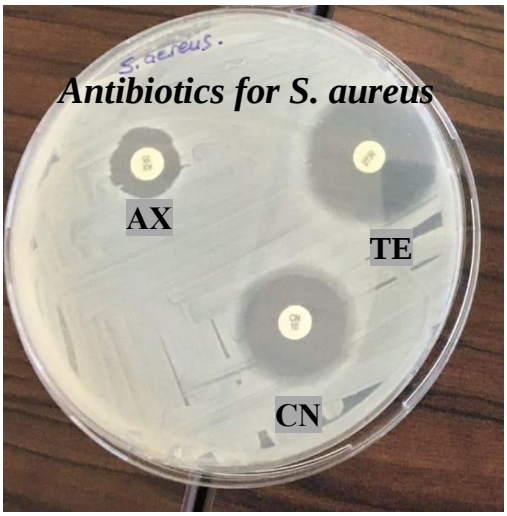


Figure S63. Antibacterial activity results of control compounds tested against *S. aureus* strains