

Supporting Information

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Synthesis, antimicrobial, and molecular docking studies of furan-based Schiff bases derived from 4 -nitrobenzene - 1, 2 - diamine

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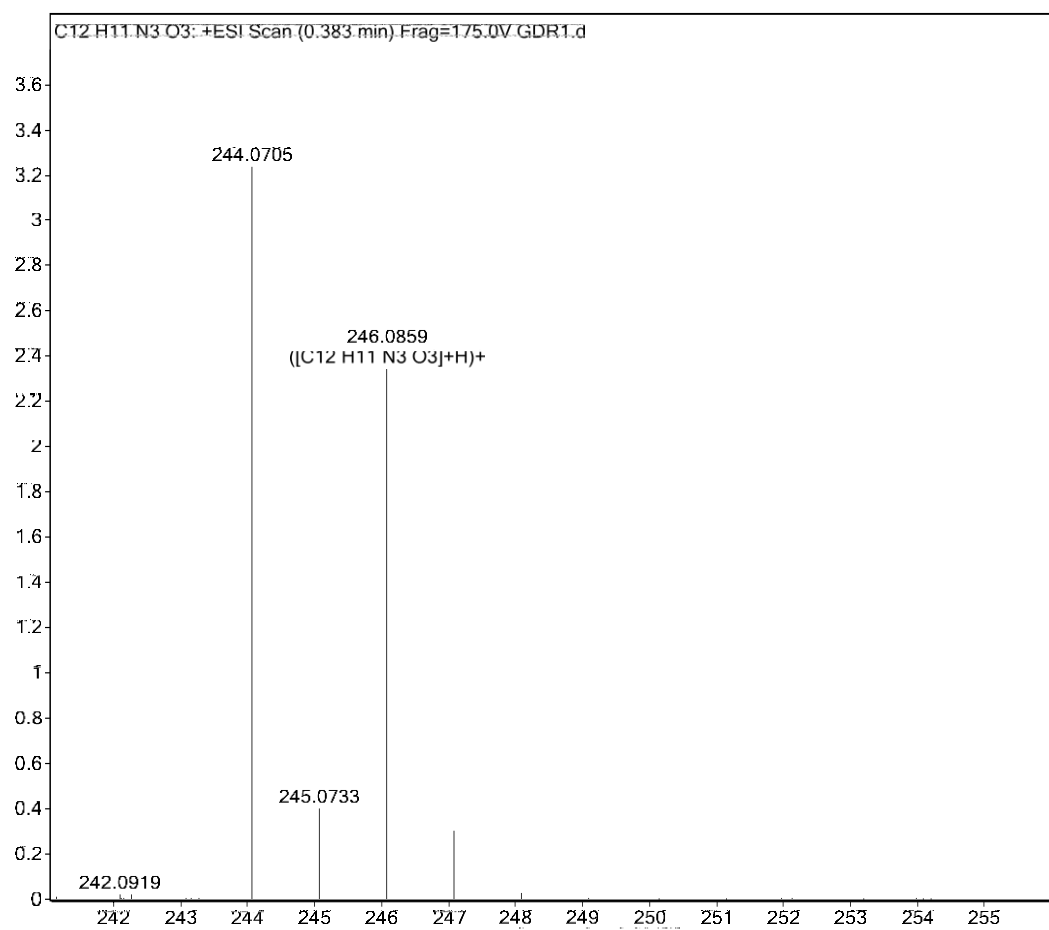


Figure S1: HRMS-ESI-MS Spectrum of Schiff base **3a**

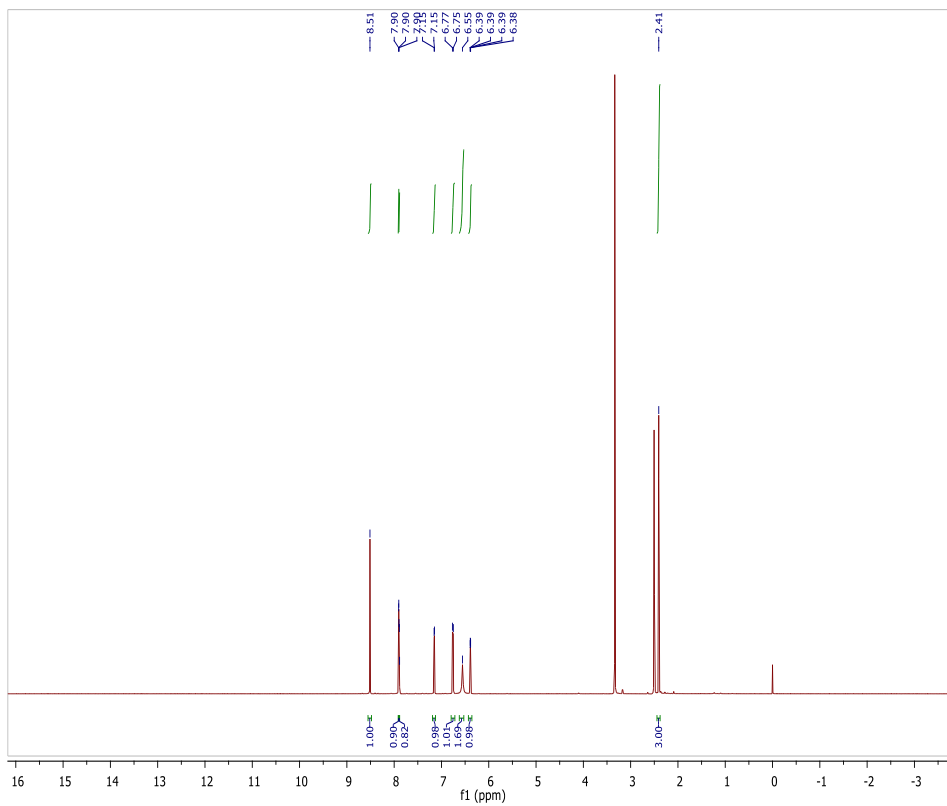


Figure S2: $^1\text{H-NMR}$ (500 MHz, $\text{DMSO-}d_6$) Spectrum of Schiff base **3a**

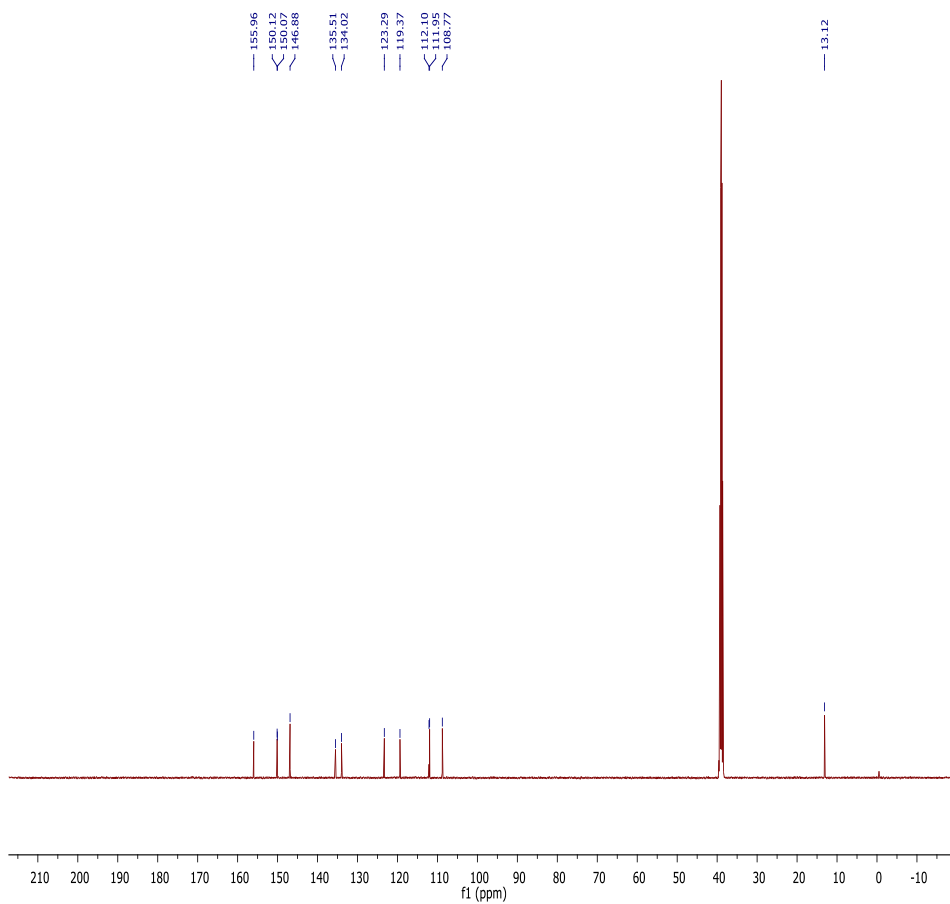
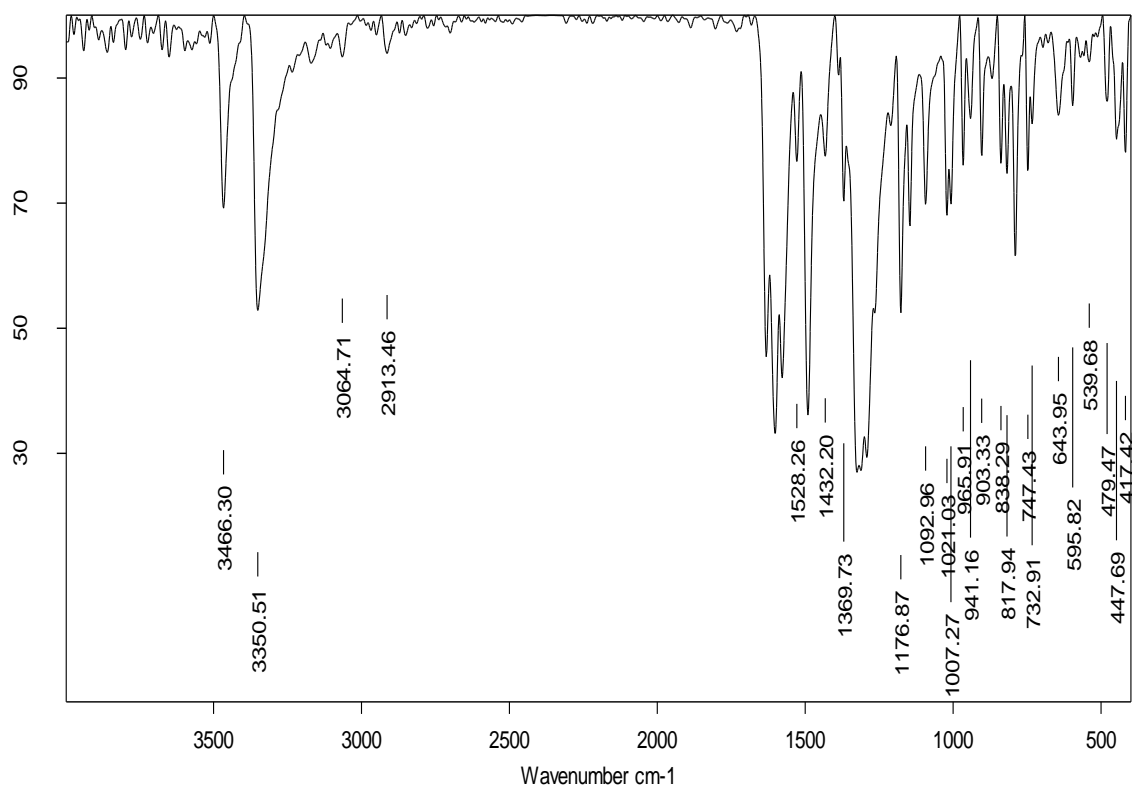


Figure S3: ^{13}C -NMR (125 MHz, DMSO d_6) Spectrum of Schiff base **3a**



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Figure S4: FTIR Spectrum (4000- 400 cm⁻¹) of Schiff base **3a**

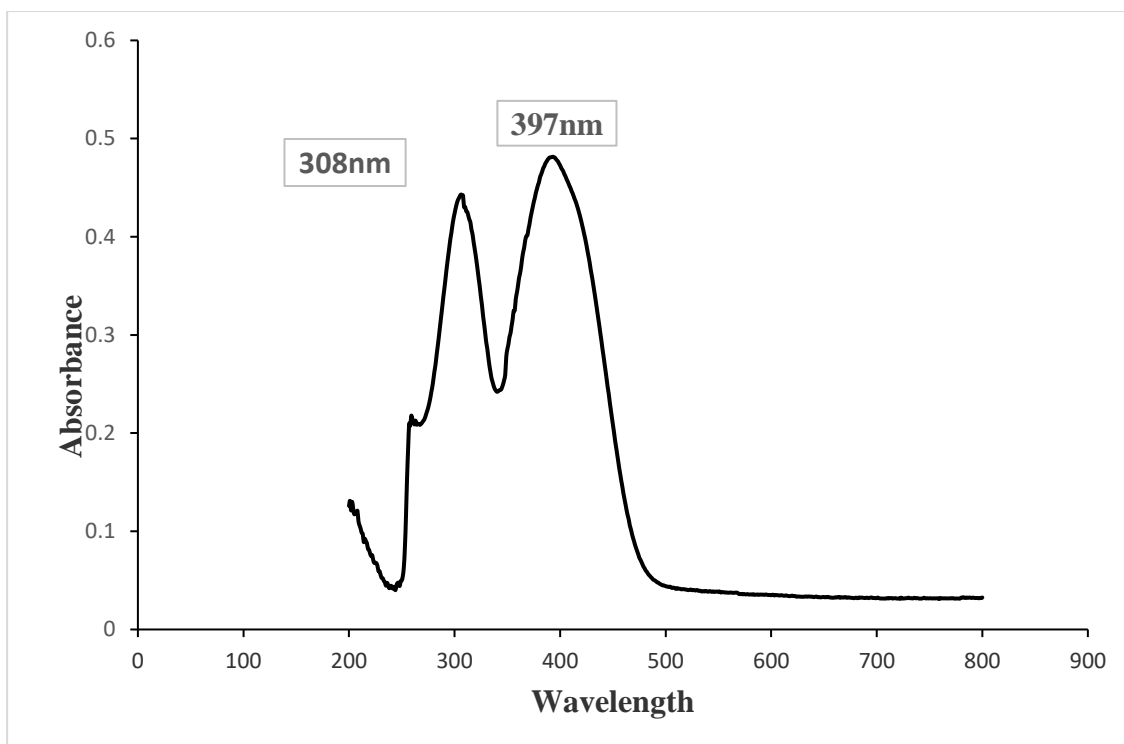


Figure S5: UV – Visible Spectrum of Schiff base **3a**

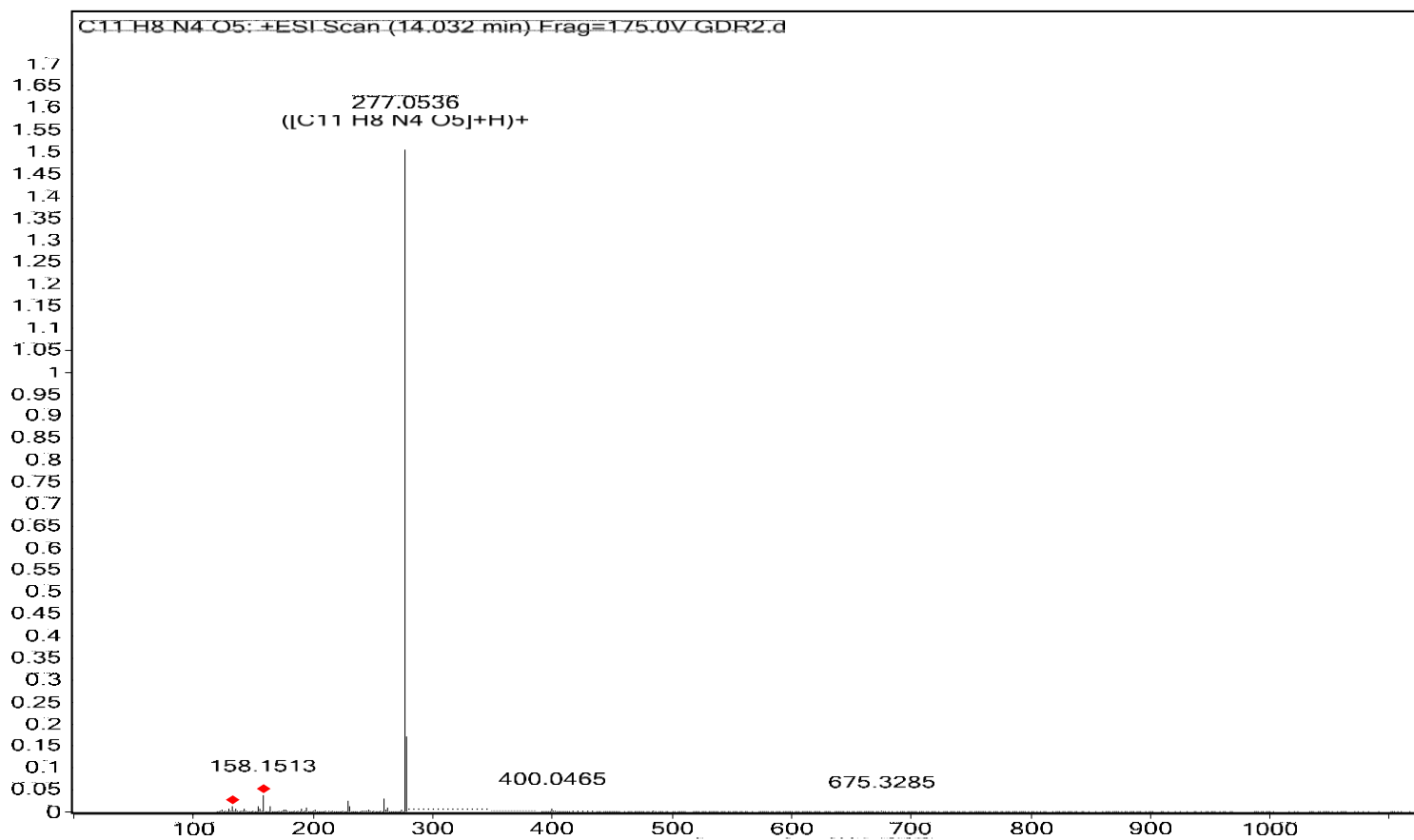


Figure S6: HRMS-ESI-MS Spectrum of Schiff base **3b**

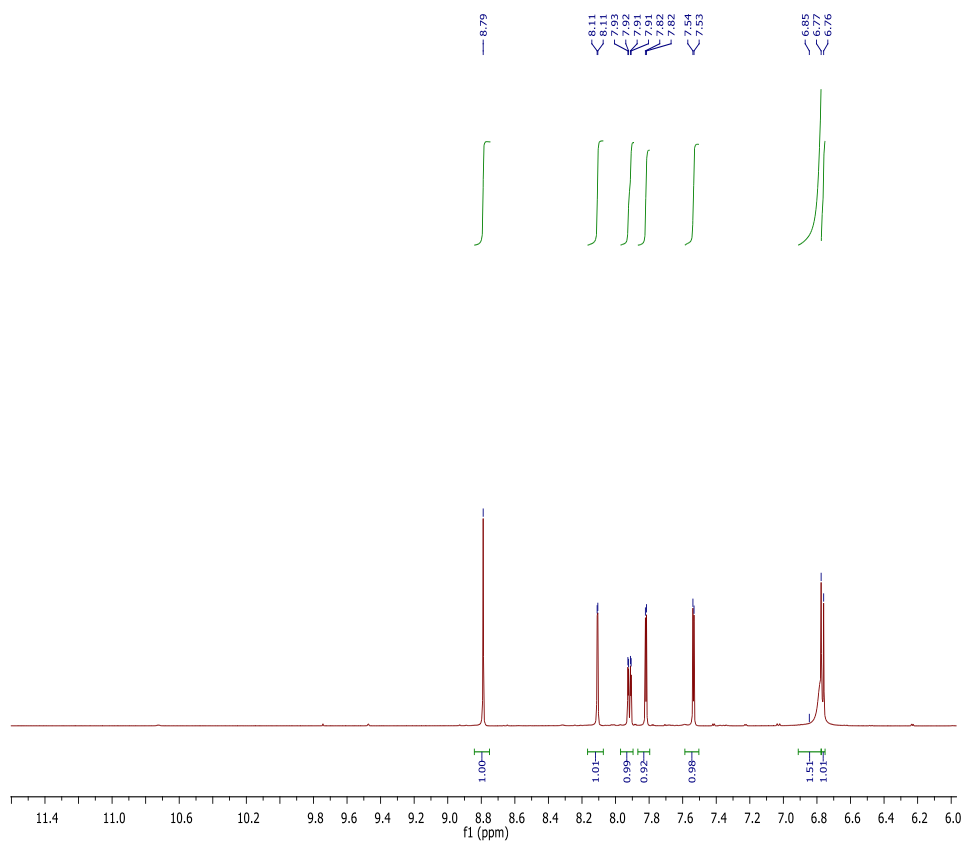


Figure S7: $^1\text{H-NMR}$ (500 MHz, DMSO-d_6) Spectrum of Schiff base **3b**

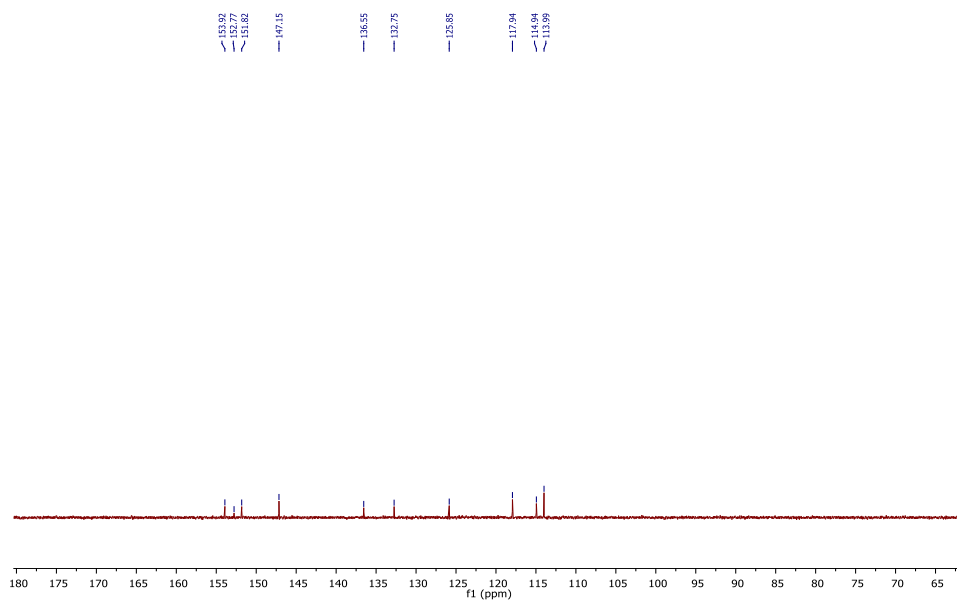
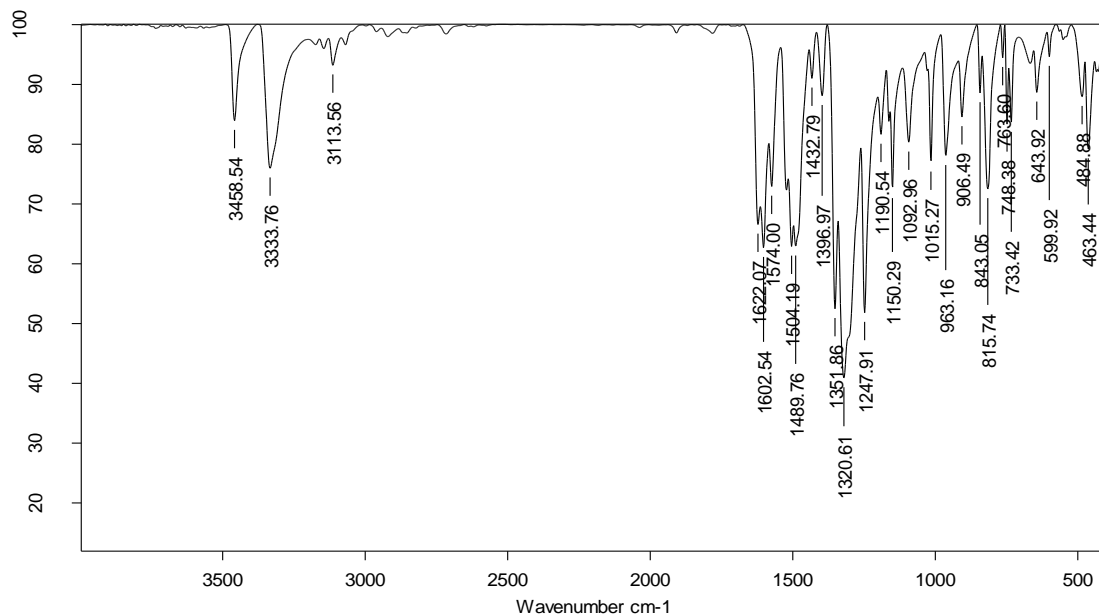


Figure S8: ^{13}C -NMR (125 MHz, DMSO d_6) Spectrum of Schiff base **3b**



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Figure S9: FTIR Spectrum (4000- 400 cm⁻¹) of Schiff base **3b**

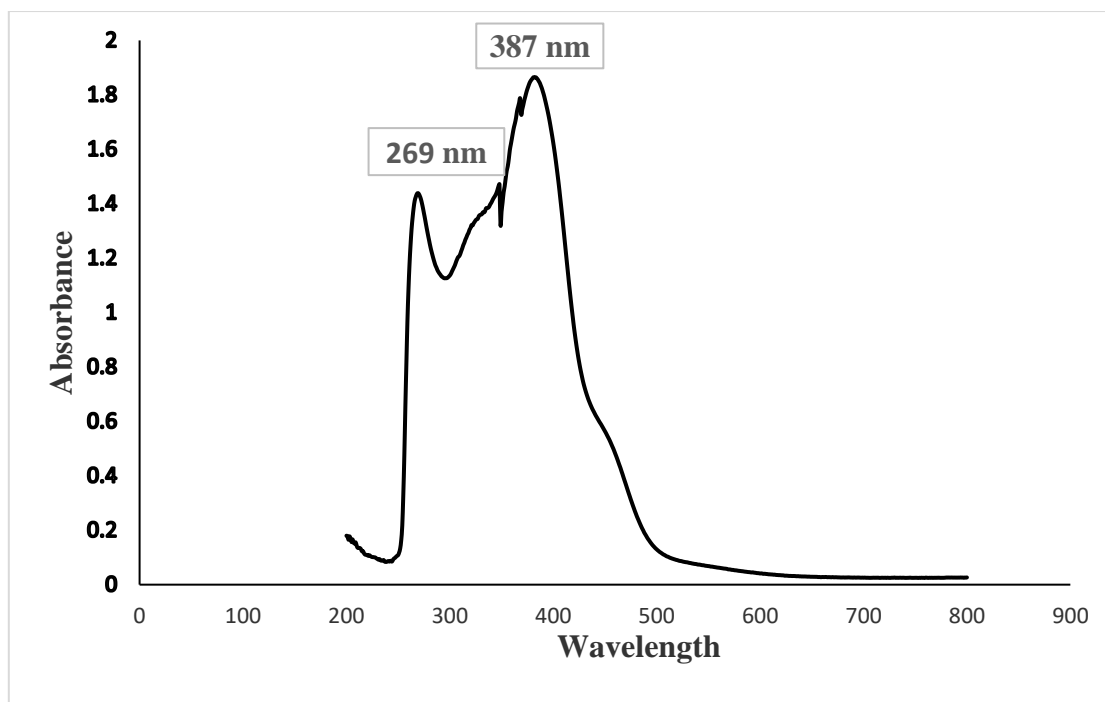


Figure S10: UV – Visible Spectrum of Schiff base **3b**

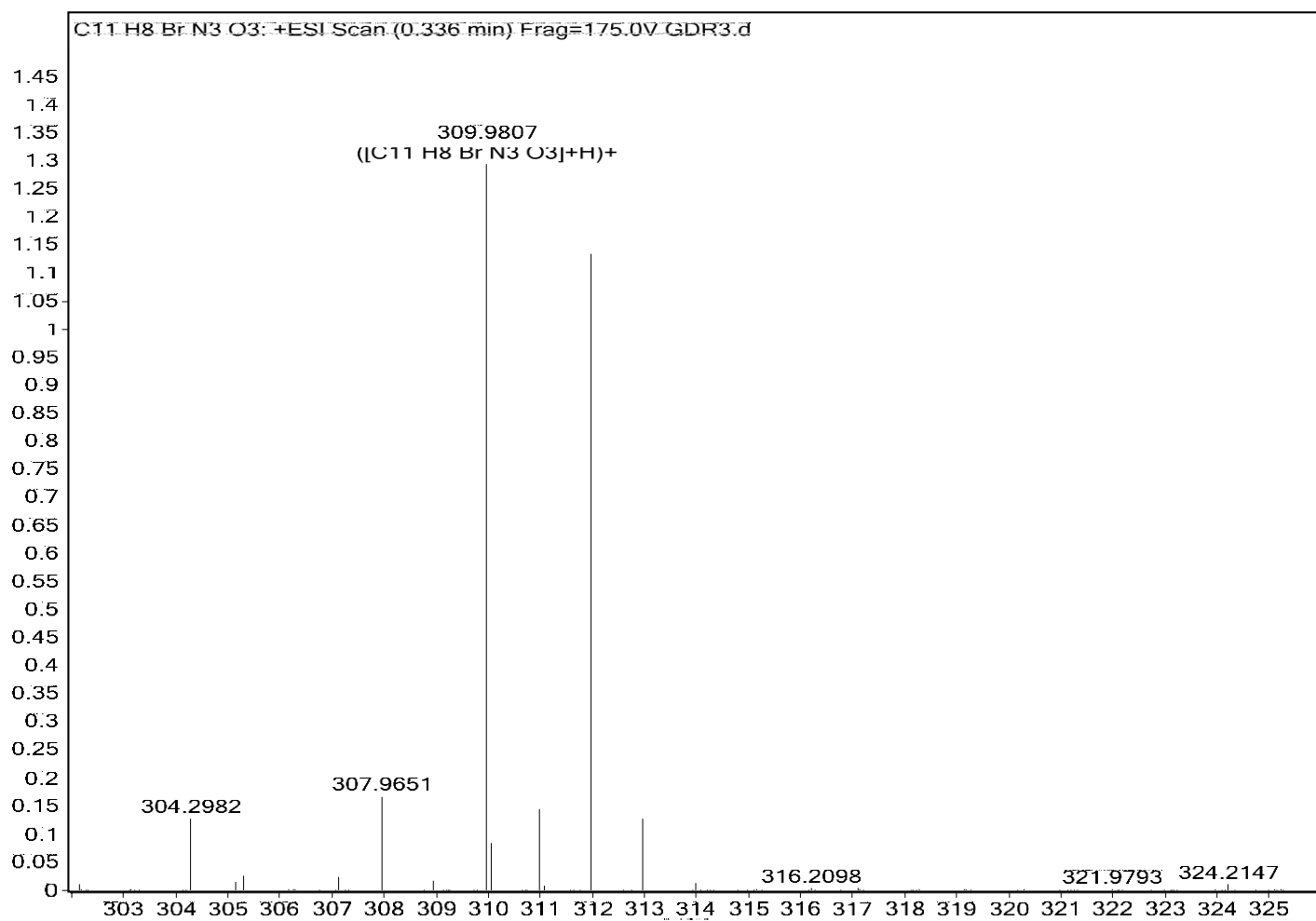


Figure S11: HRMS-ESI-MS Spectrum of Schiff base **3c**

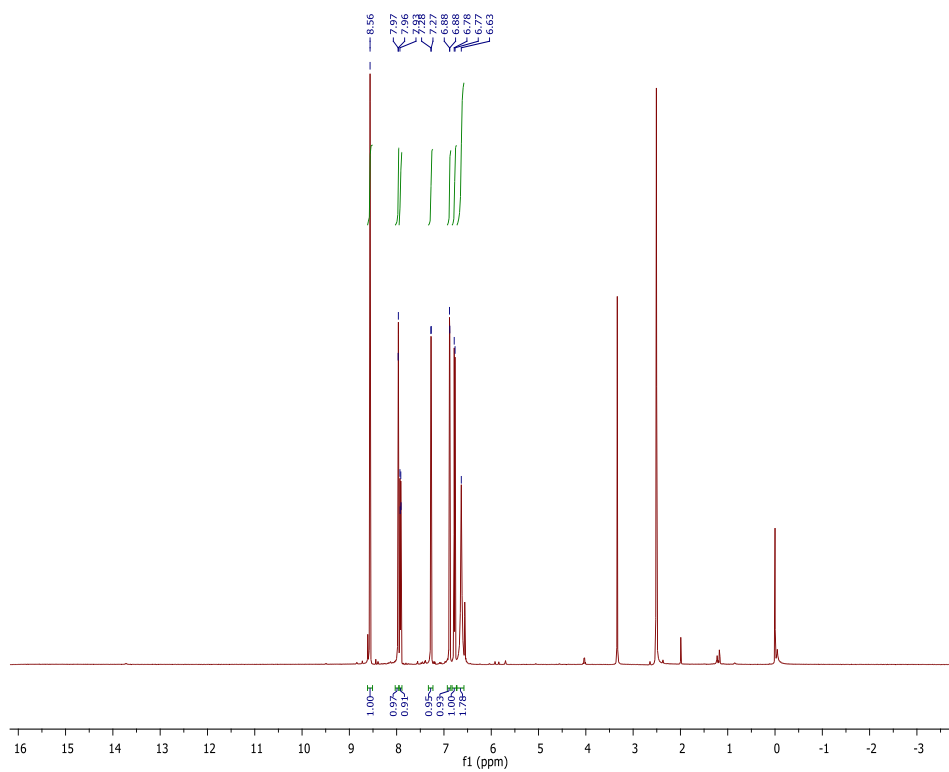


Figure S12: ¹H-NMR (500 MHz, DMSO d₆) Spectrum of Schiff base **3c**

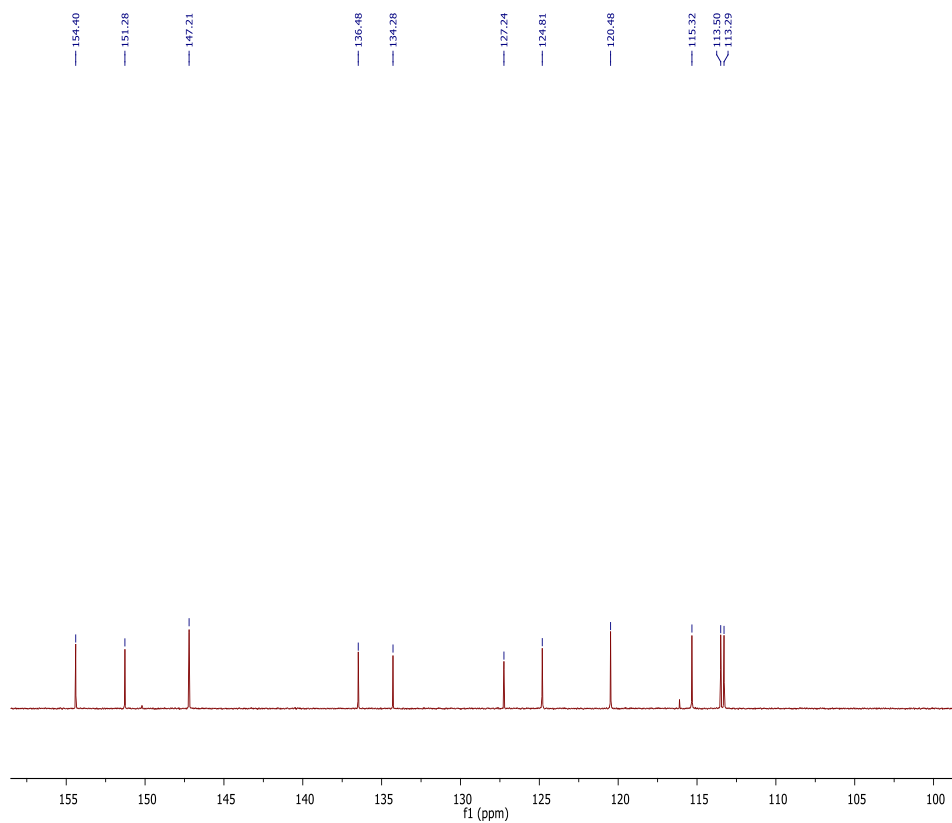
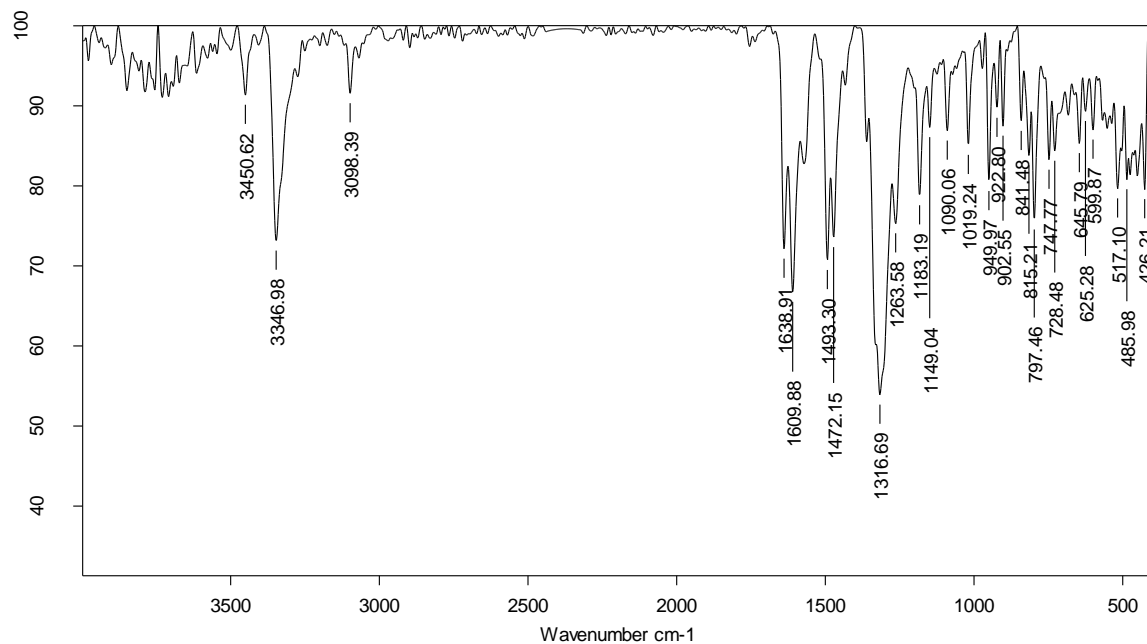


Figure S13: ^{13}C -NMR (125 MHz, DMSO d_6) Spectrum of Schiff base **3c**

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Figure S14: FTIR Spectrum (4000- 400 cm⁻¹) of Schiff base **3c**

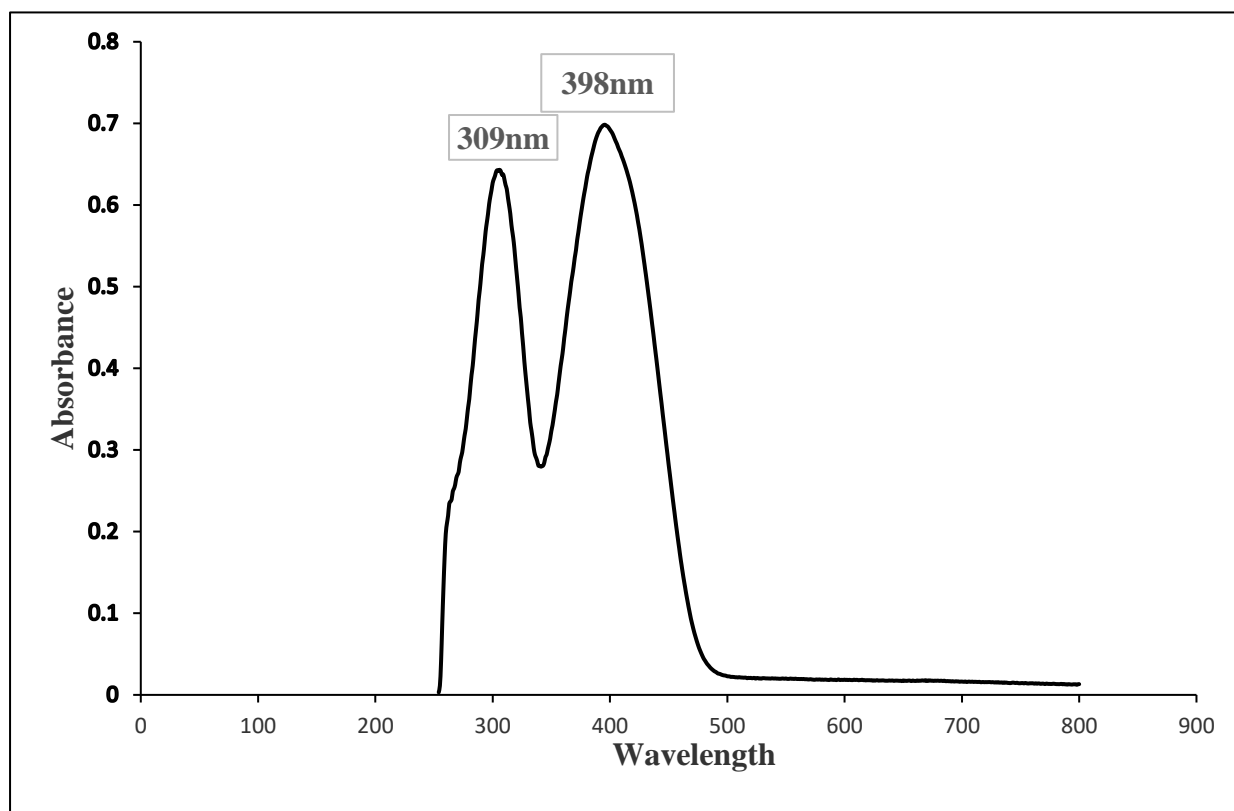


Figure S15: UV – Visible Spectrum of Schiff base **3c**

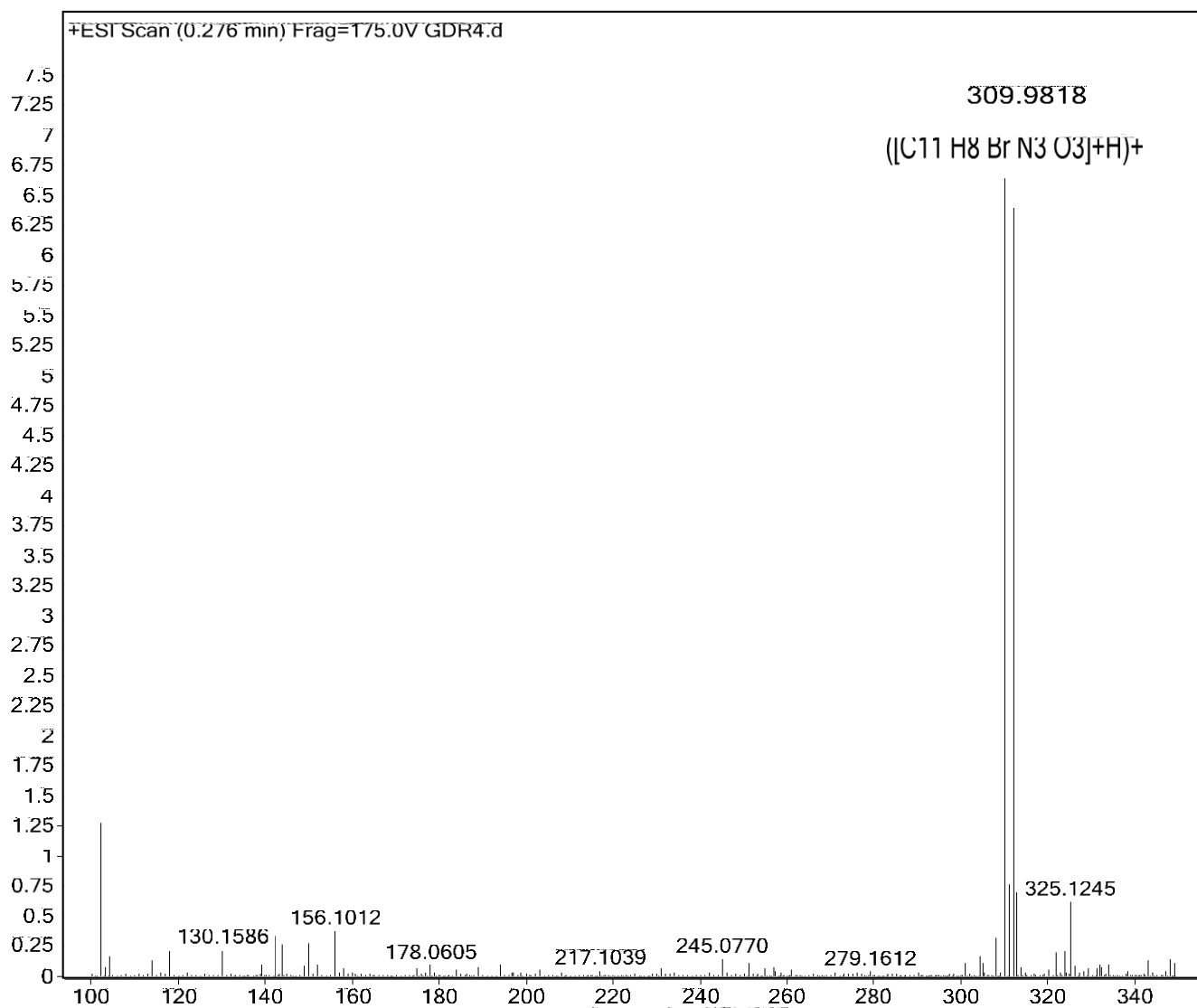


Figure S16: HRMS-ESI-MS Spectrum of Schiff base **3d**

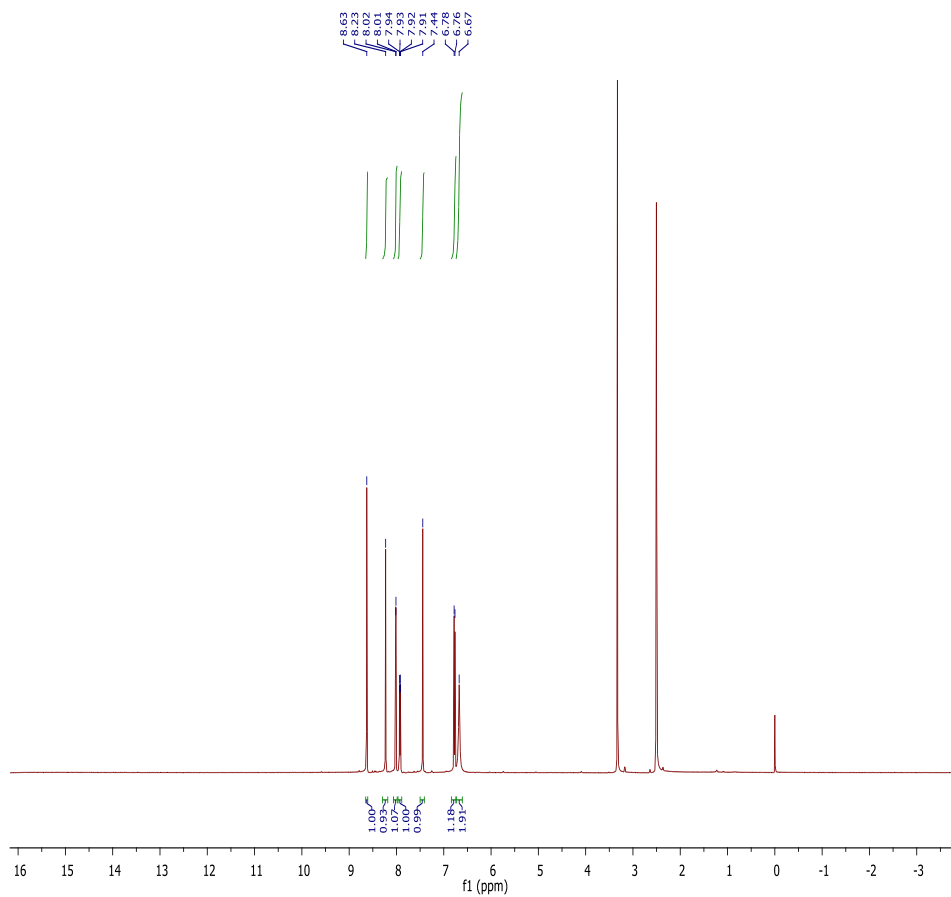


Figure S17: $^1\text{H-NMR}$ (500 MHz, DMSO-d_6) Spectrum of Schiff base **3d**

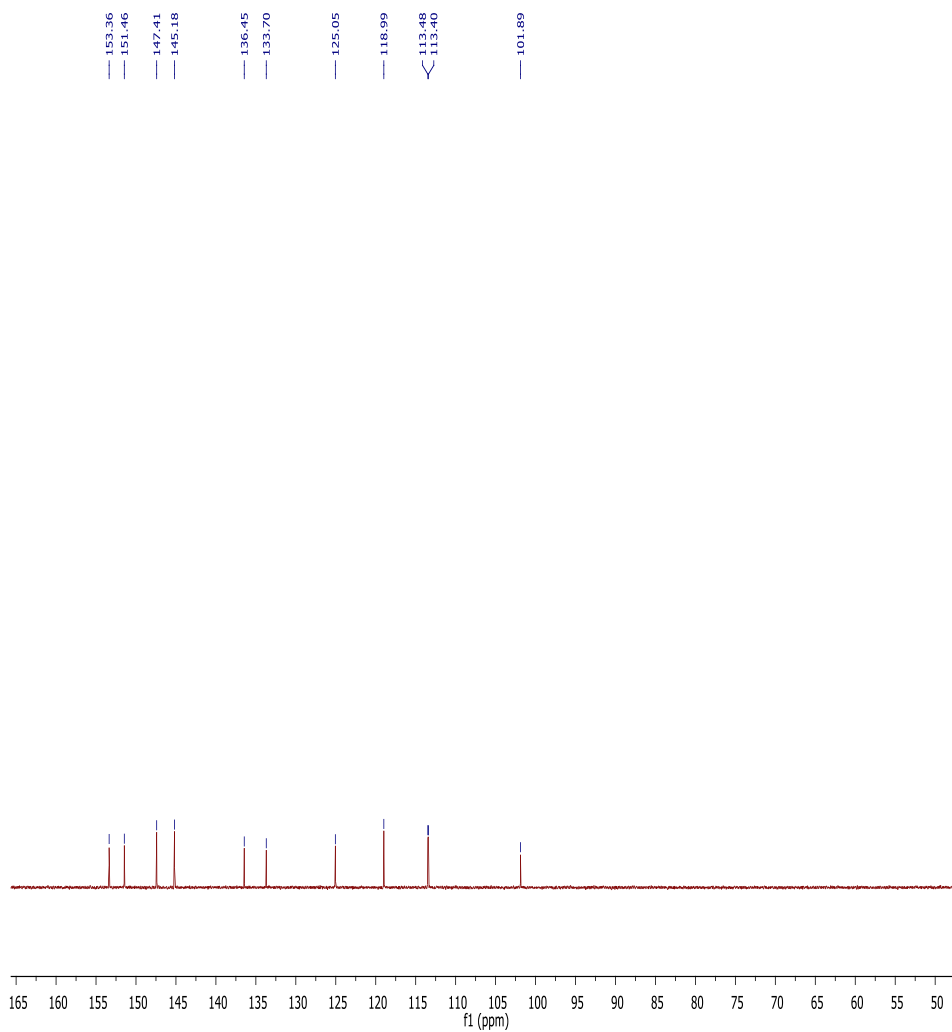
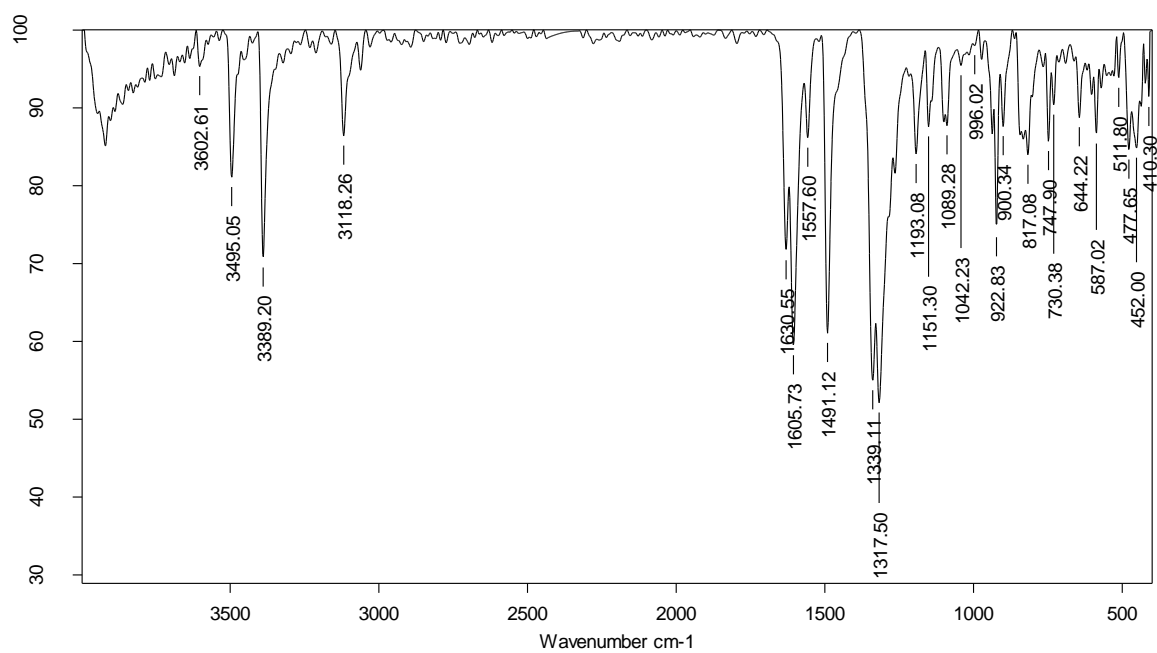


Figure S18: ^{13}C -NMR (125 MHz, DMSO d_6) Spectrum of Schiff base **3d**

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Figure S19: FTIR Spectrum (4000- 400 cm⁻¹) of Schiff base **3d**

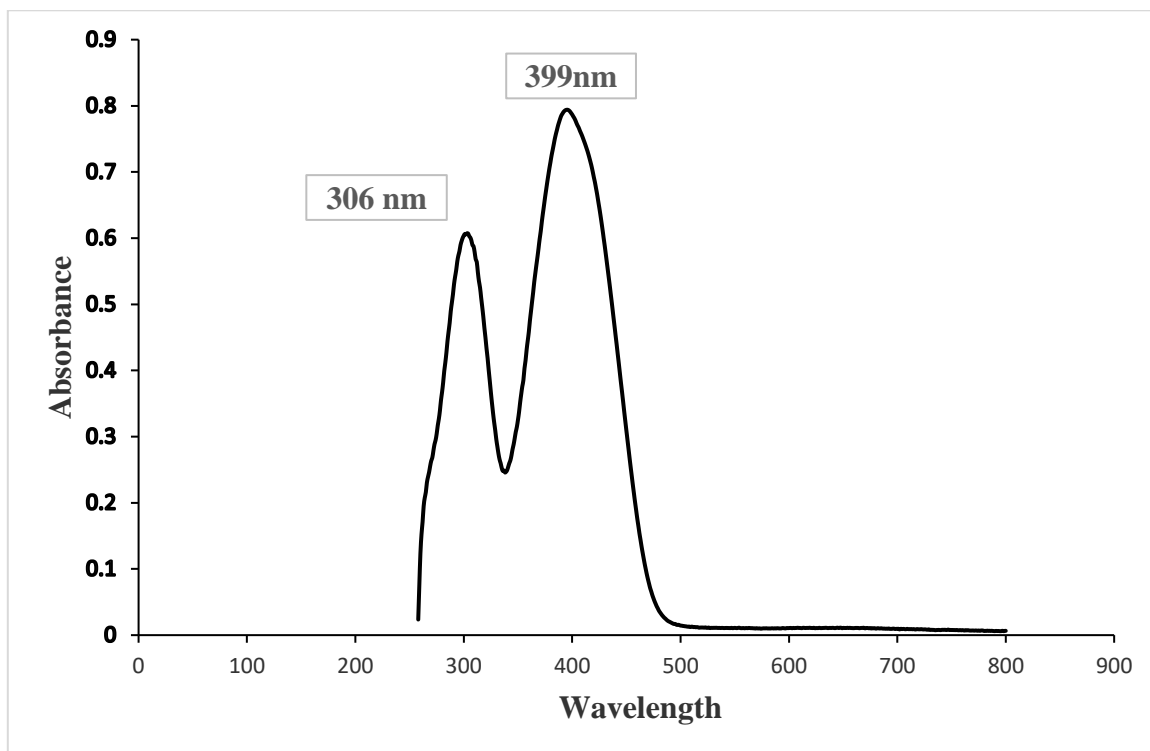


Figure S20: UV – Visible Spectrum of Schiff base **3d**

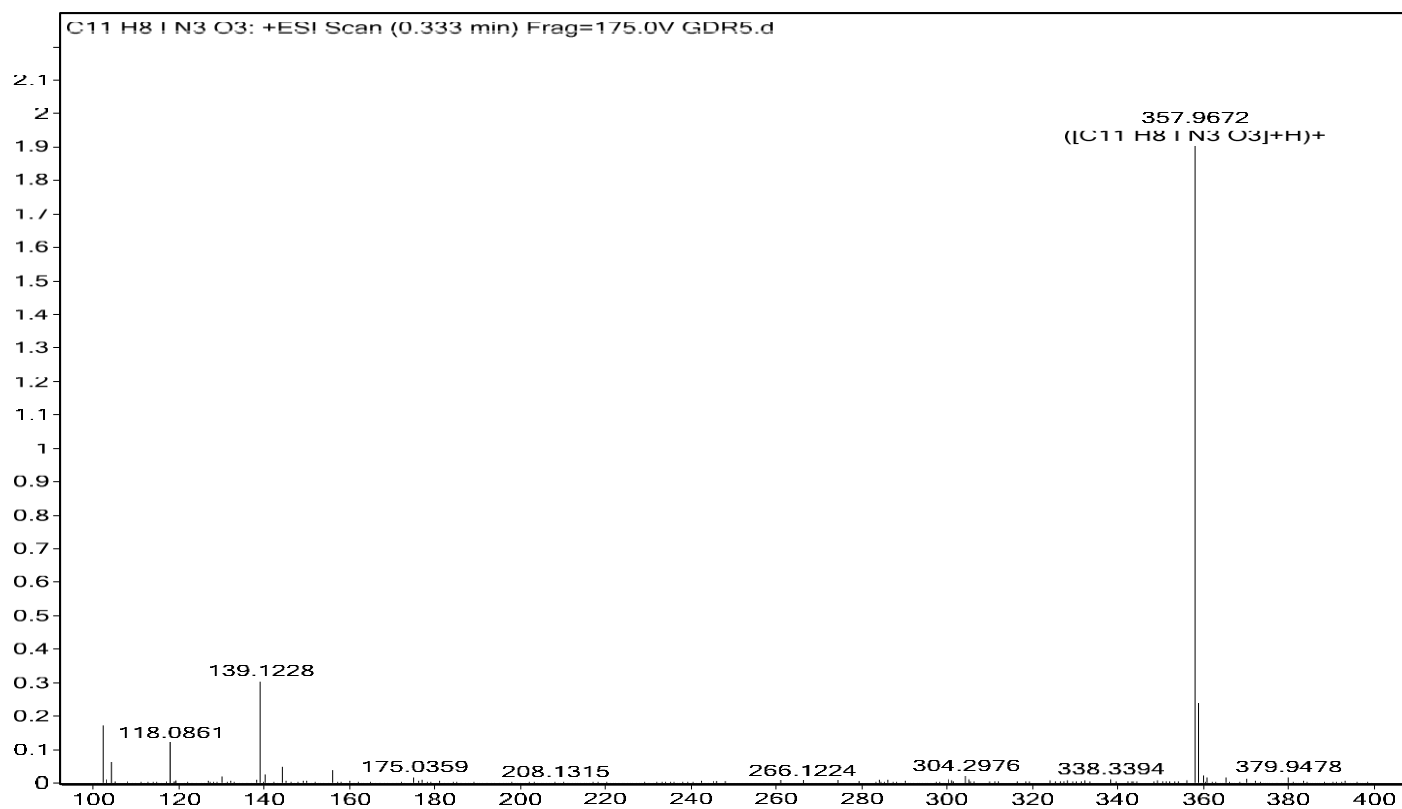


Figure S21: HRMS-ESI-MS Spectrum of Schiff base **3e**

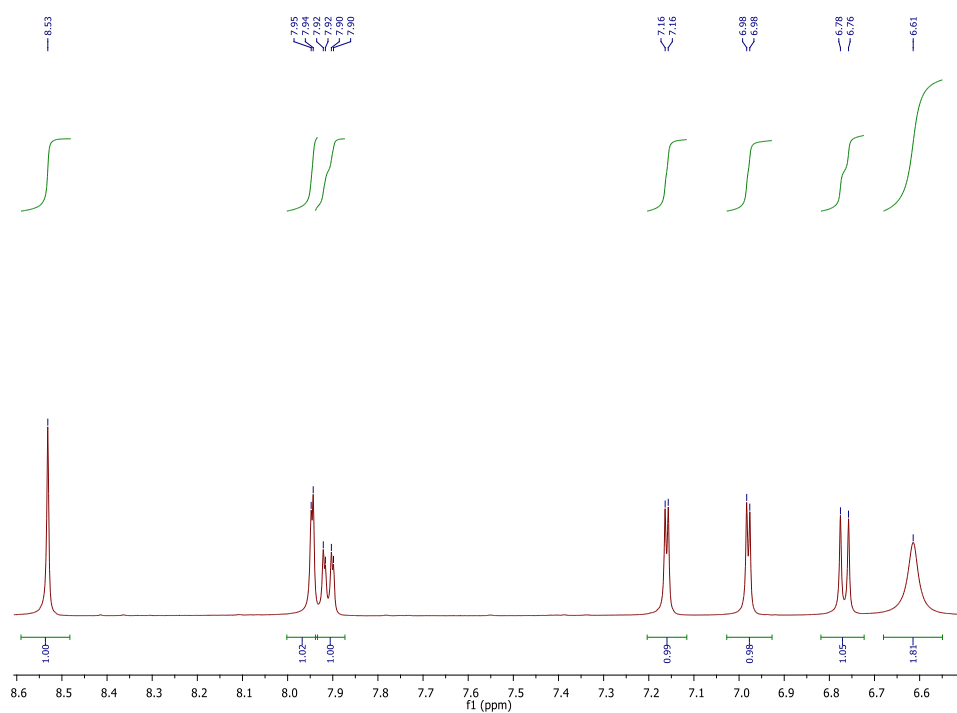


Figure S22: ¹H-NMR (500 MHz, DMSO d₆) Spectrum of Schiff base **3e**

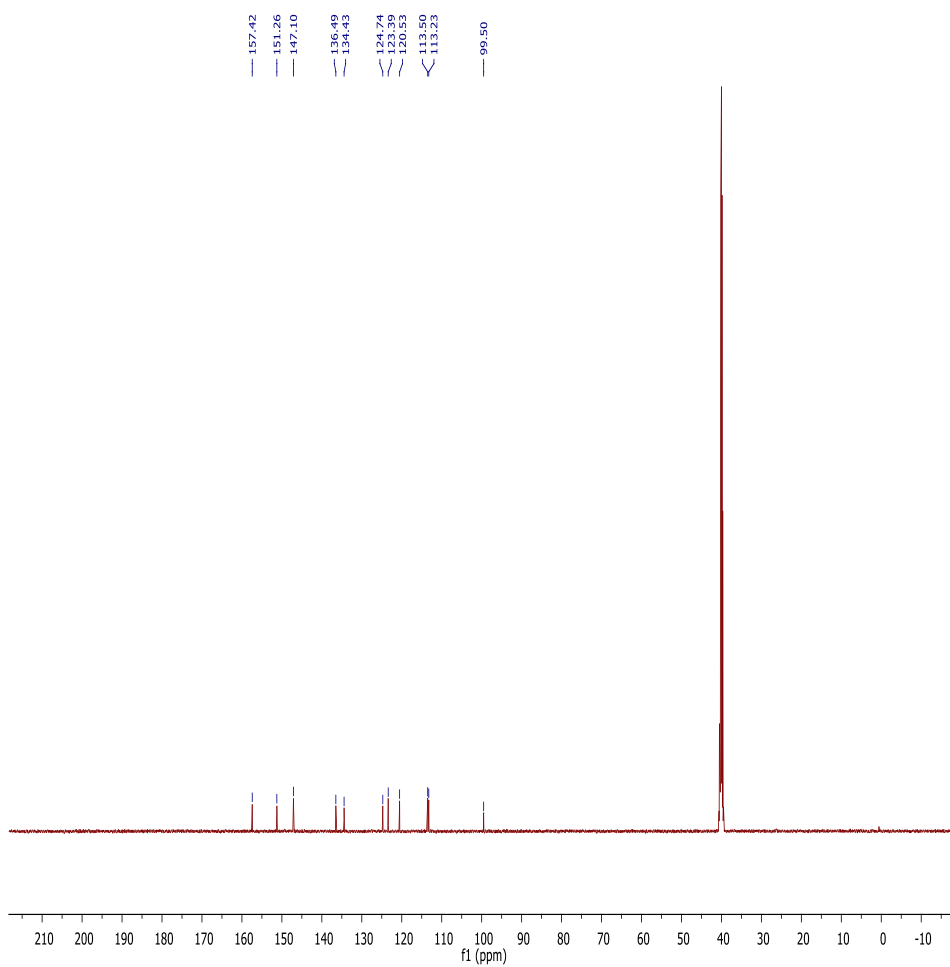


Figure S23: ^{13}C -NMR (125 MHz, DMSO d6) Spectrum of Schiff base **3e**

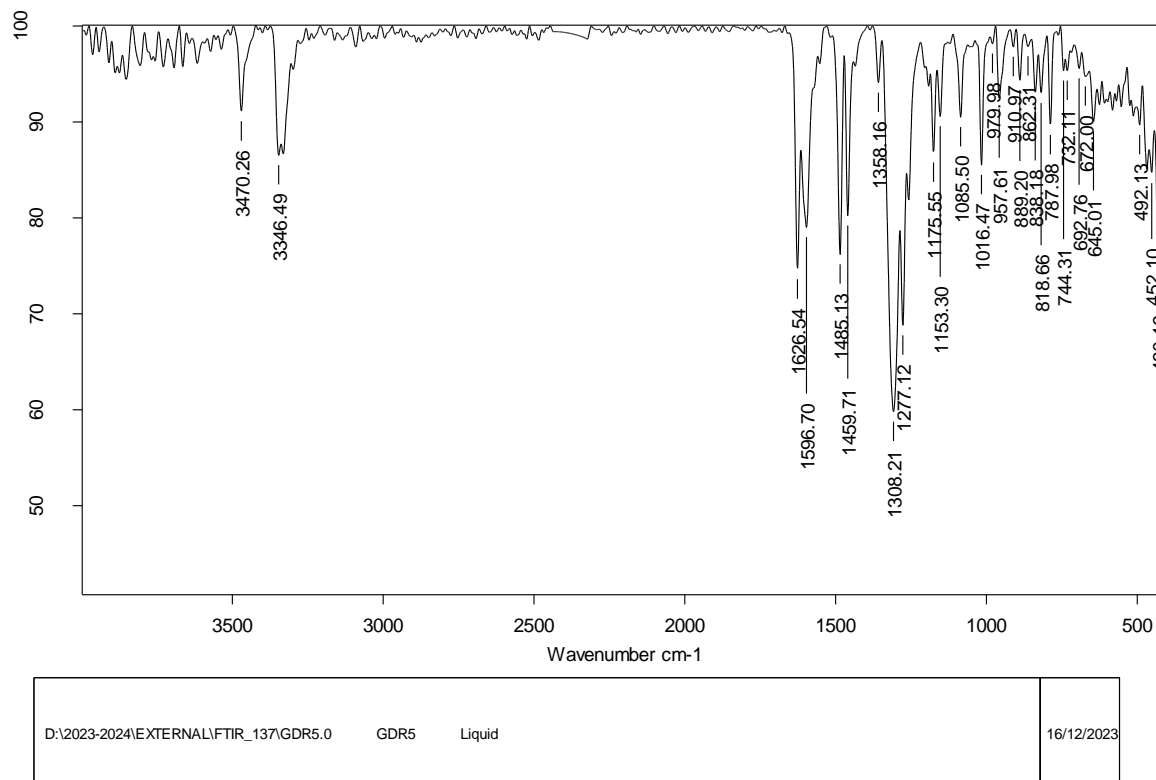


Figure S24: FTIR Spectrum (4000- 400 cm⁻¹) of Schiff base 3e

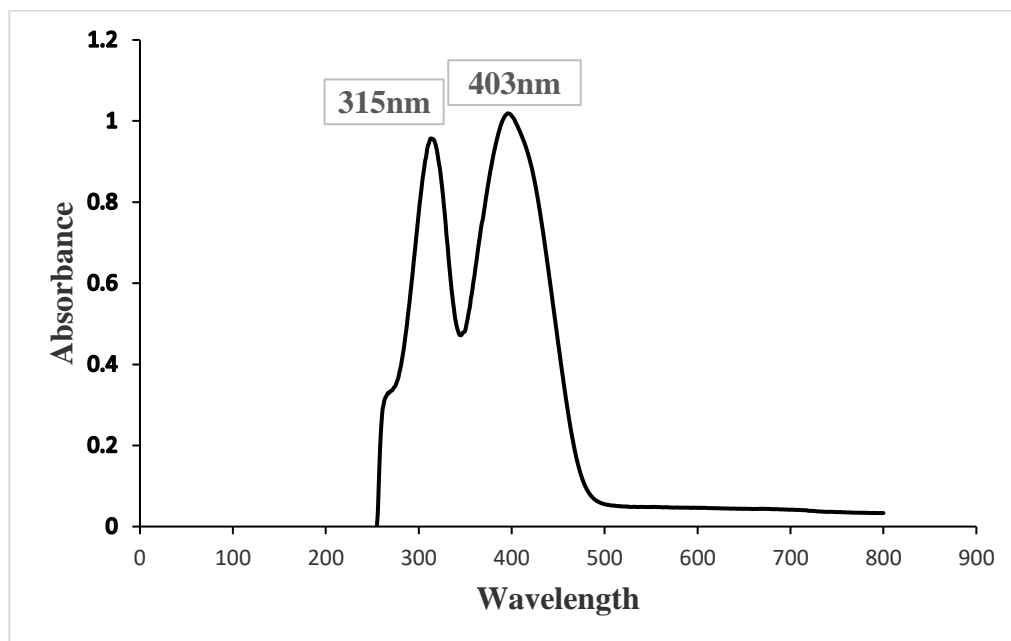


Figure S25: UV – Visible Spectrum of Schiff base **3e**

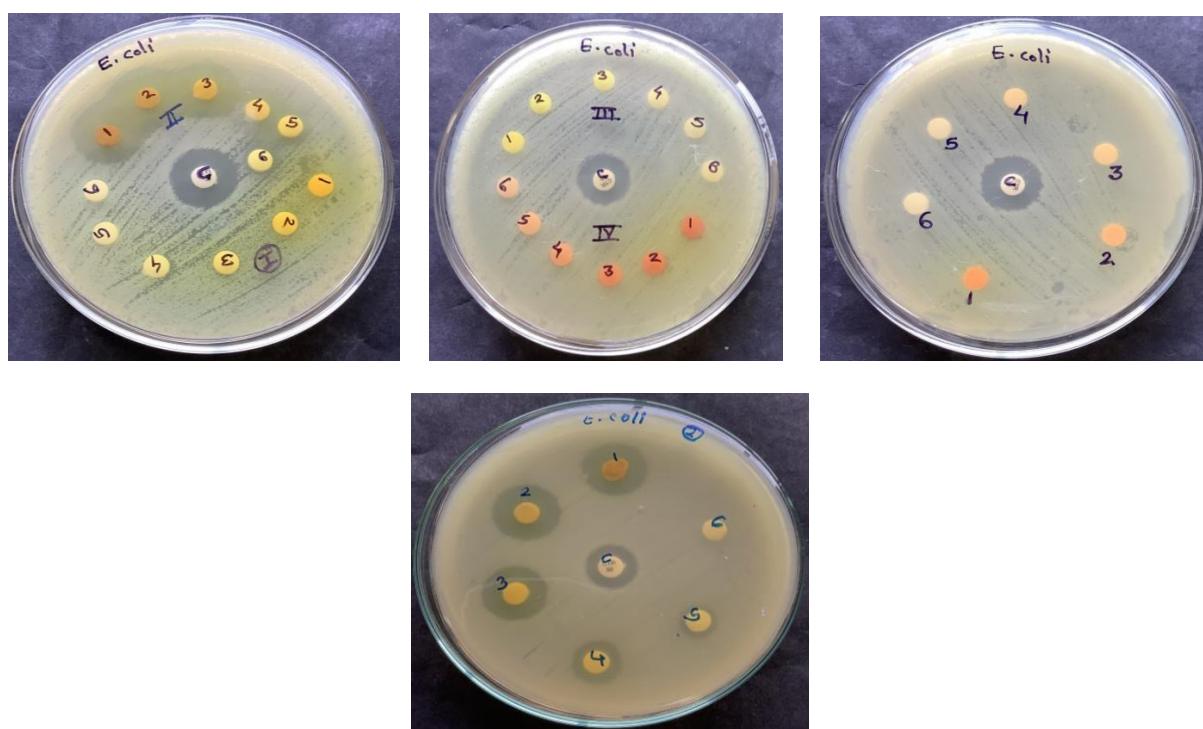


Figure S26: Antimicrobial activities of Schiff bases(3a-3e) against *E. coli*

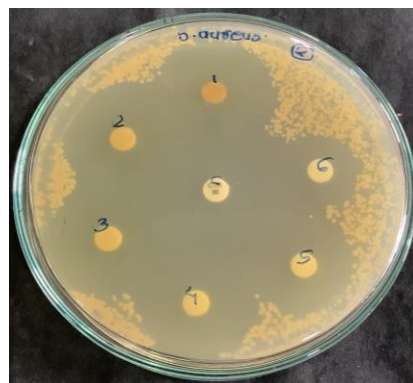
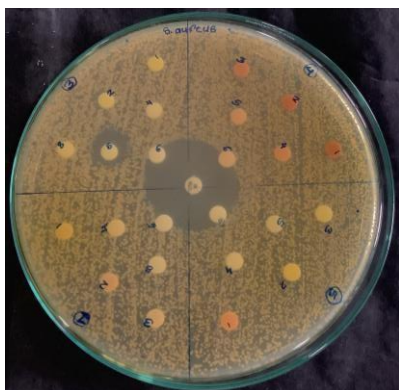


Figure S27: Antimicrobial activities of Schiff bases(3a-3e) against *S. aureus*

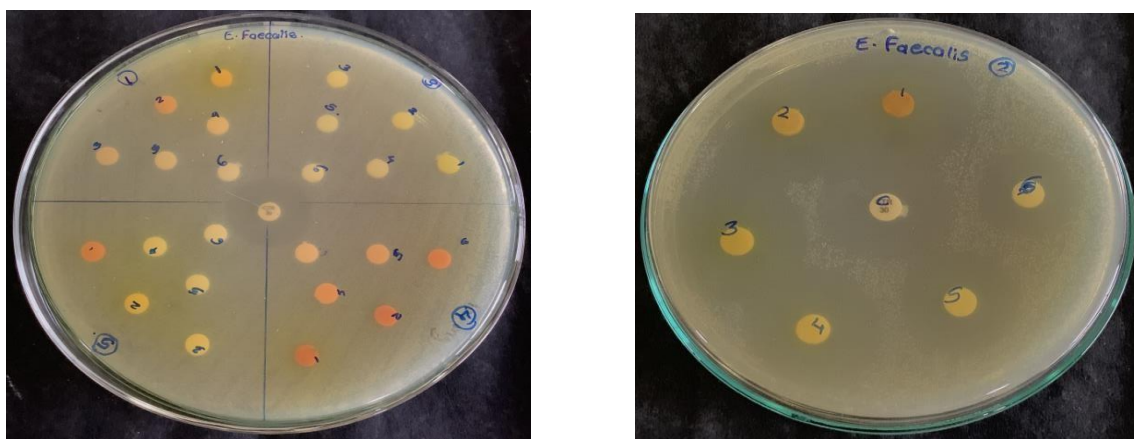


Figure S28: Antimicrobial activities of Schiff bases(**3a-3e**) against *E.faecalis*

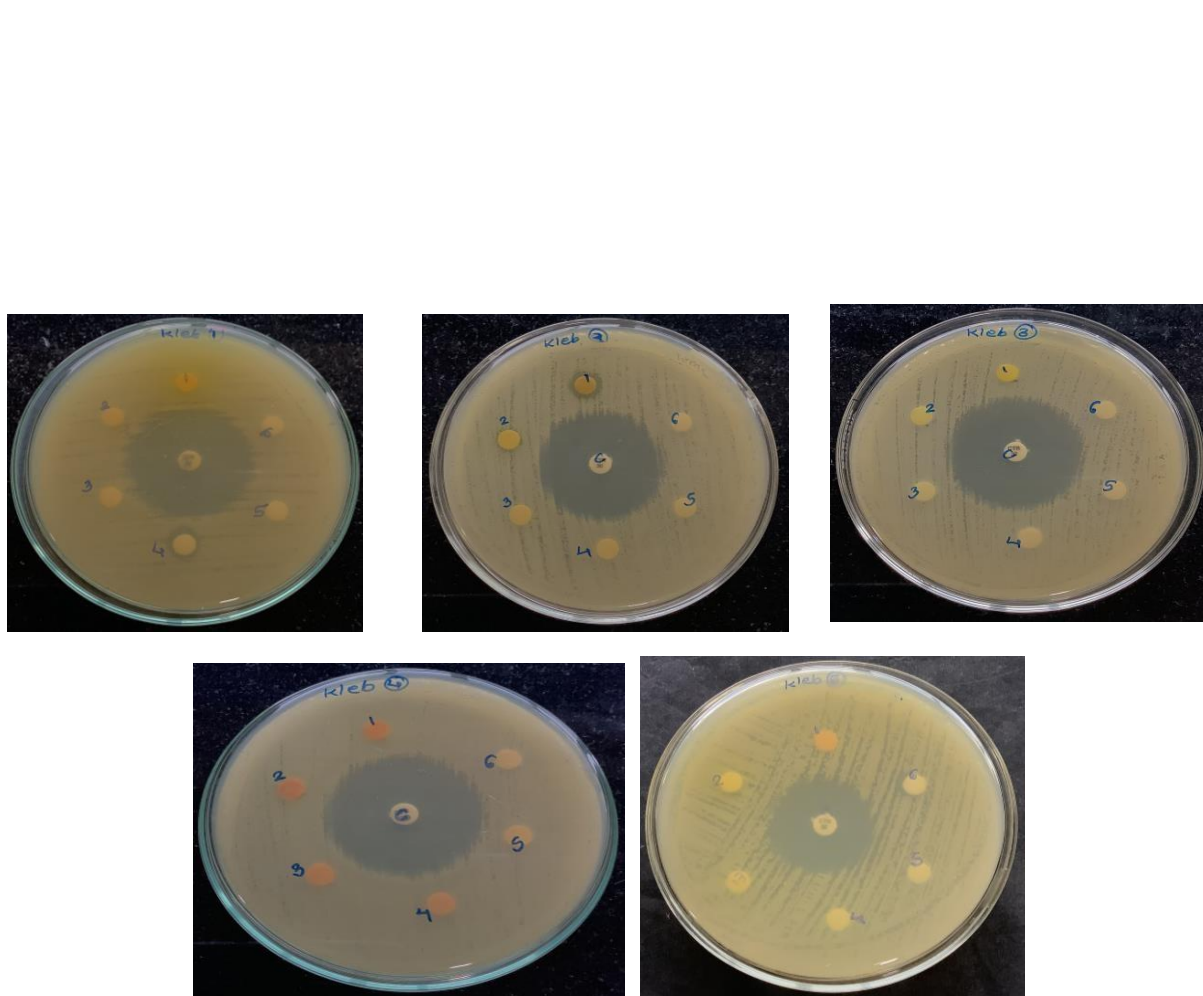


Figure S29: Antimicrobial activities of Schiff bases(3a-3e) against *K. pneumoniae*

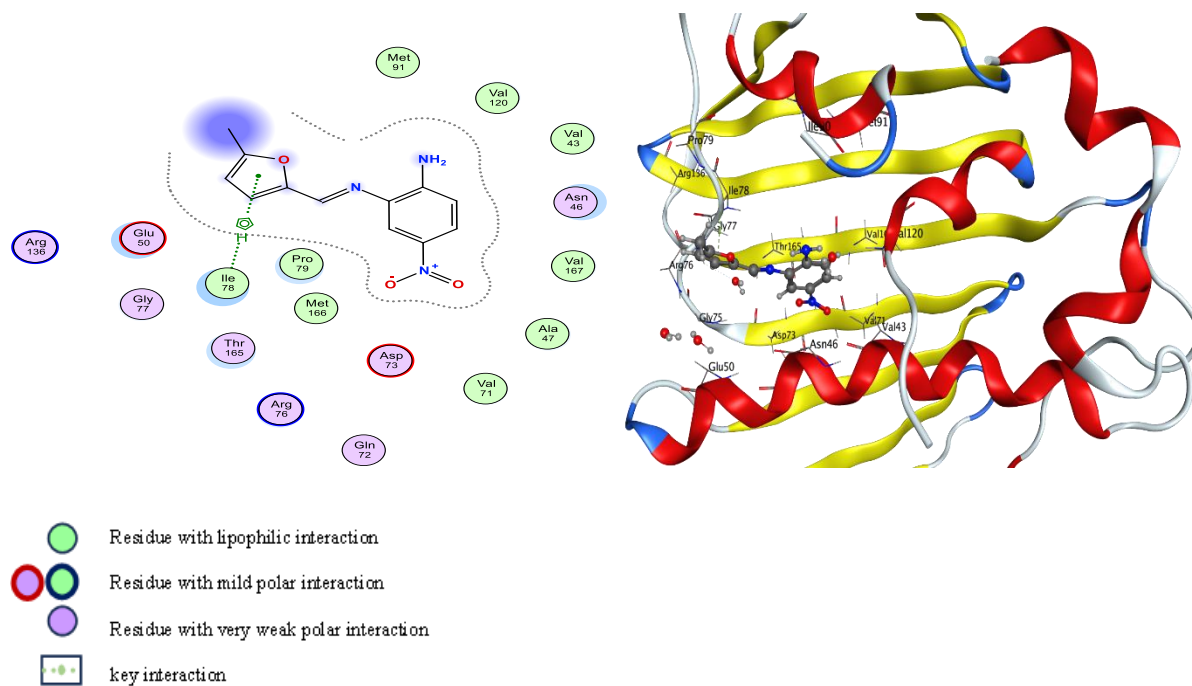


Figure S30: 2D and 3D interaction of Schiff bases **3a** against DNA Gyrase

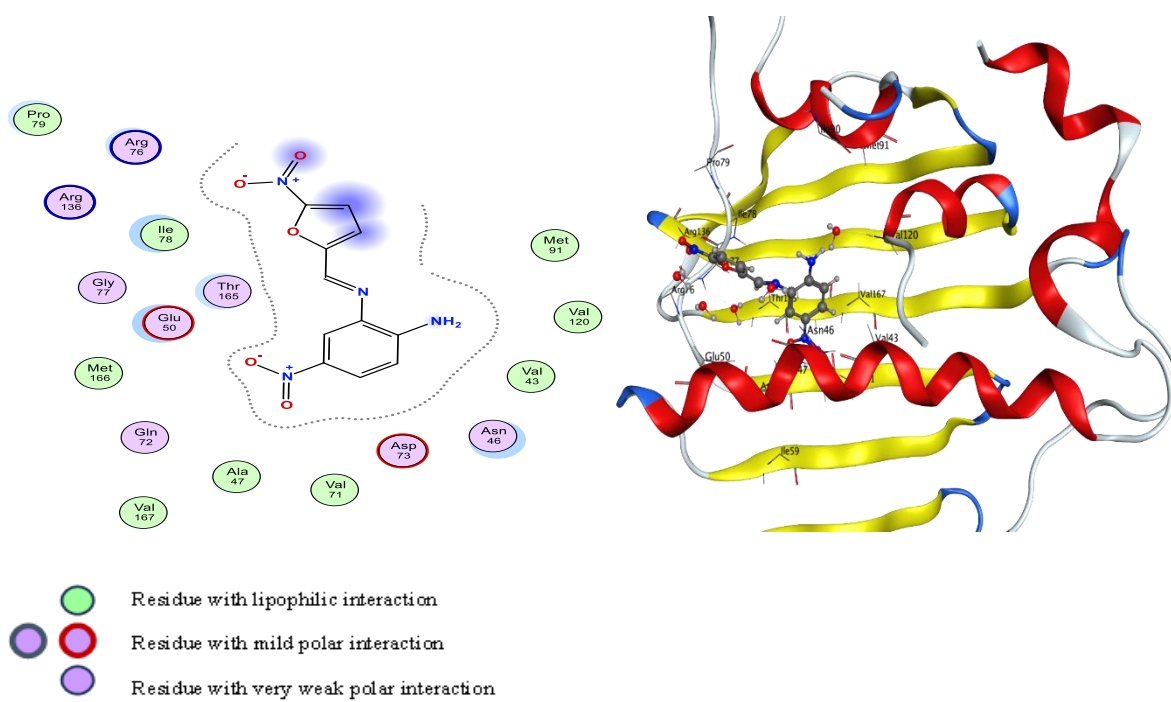


Figure S31: 2D and 3D interaction of Schiff base **3b** against DNA Gyrase

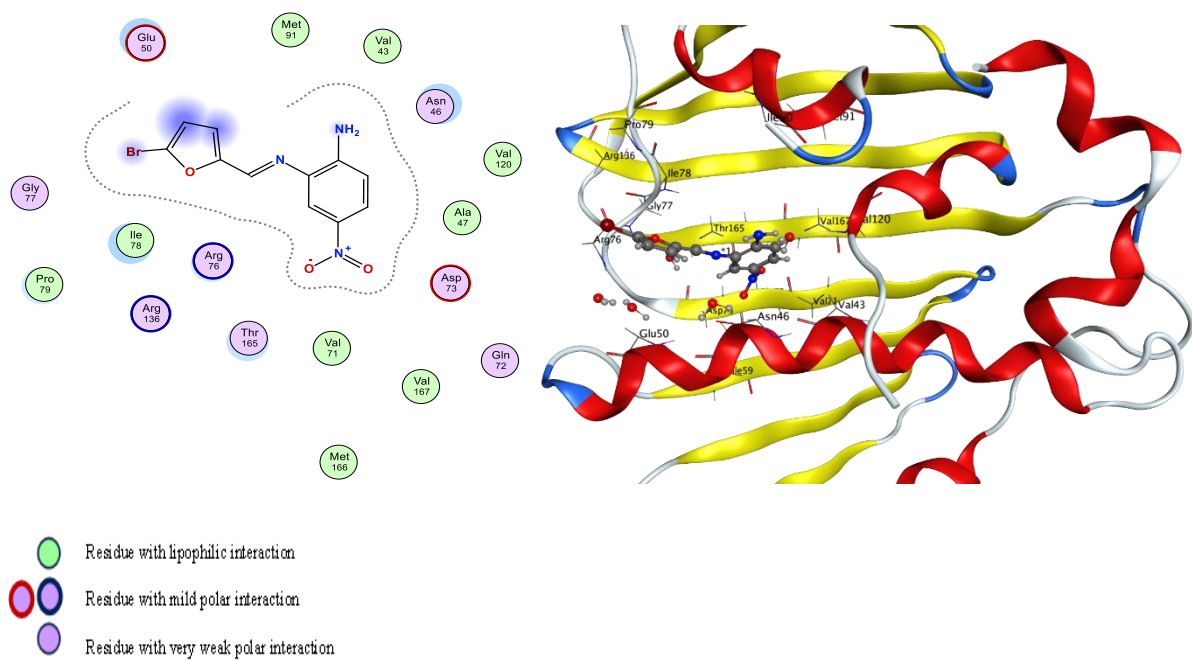


Figure S32: 2D and 3D interaction of Schiff base **3c** against DNA Gyrase

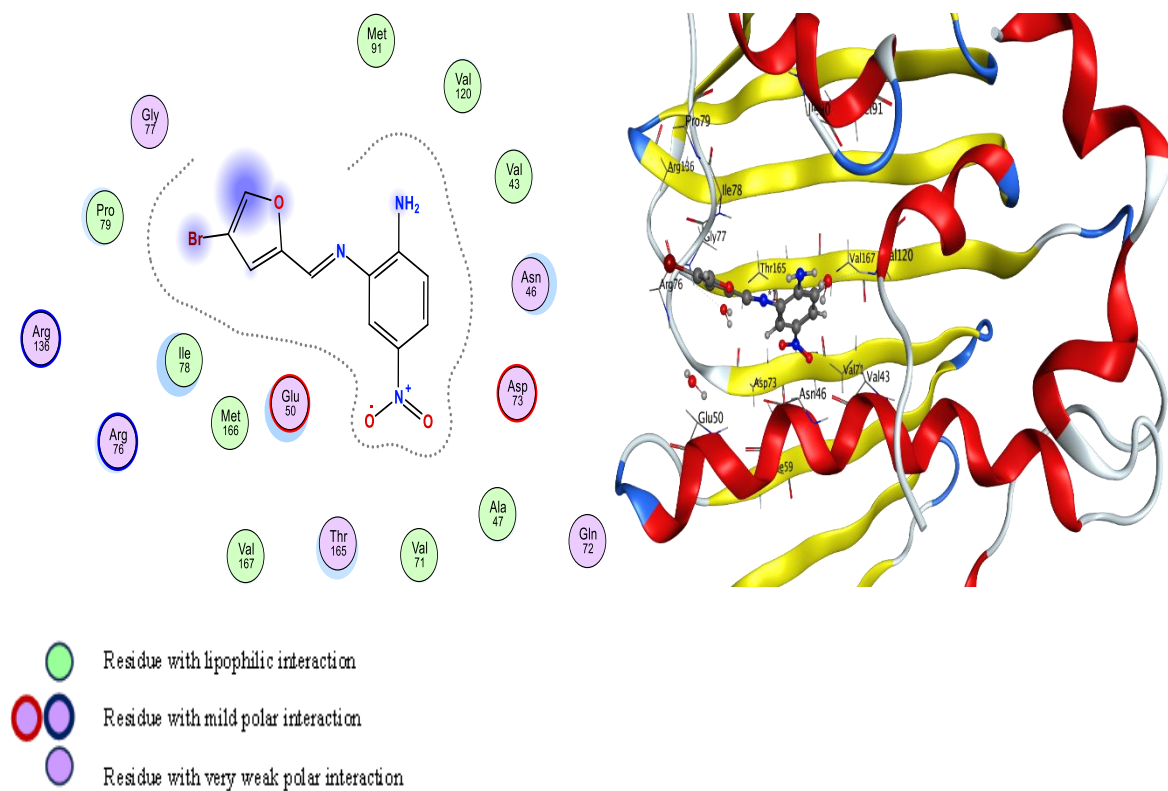


Figure S33: 2D and 3D interaction of Schiff base **3d** against DNA Gyrase

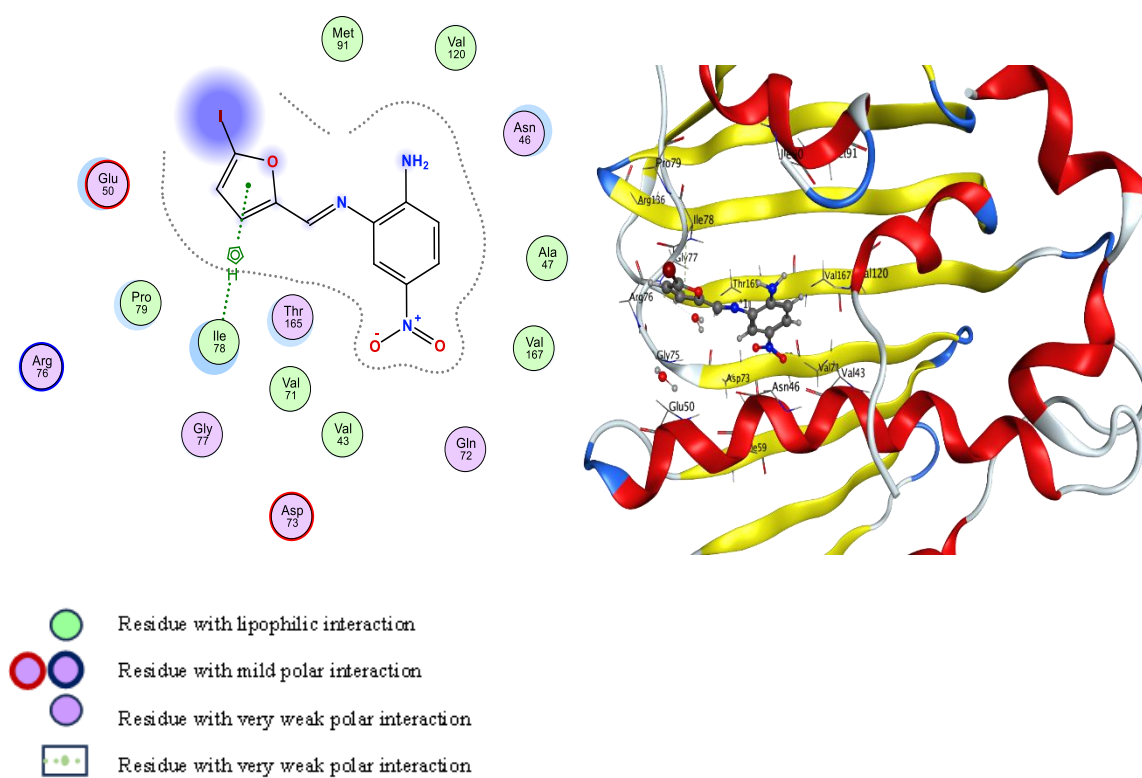


Figure S34: 2D and 3D interaction of Schiff base **3e** against DNA Gyrase

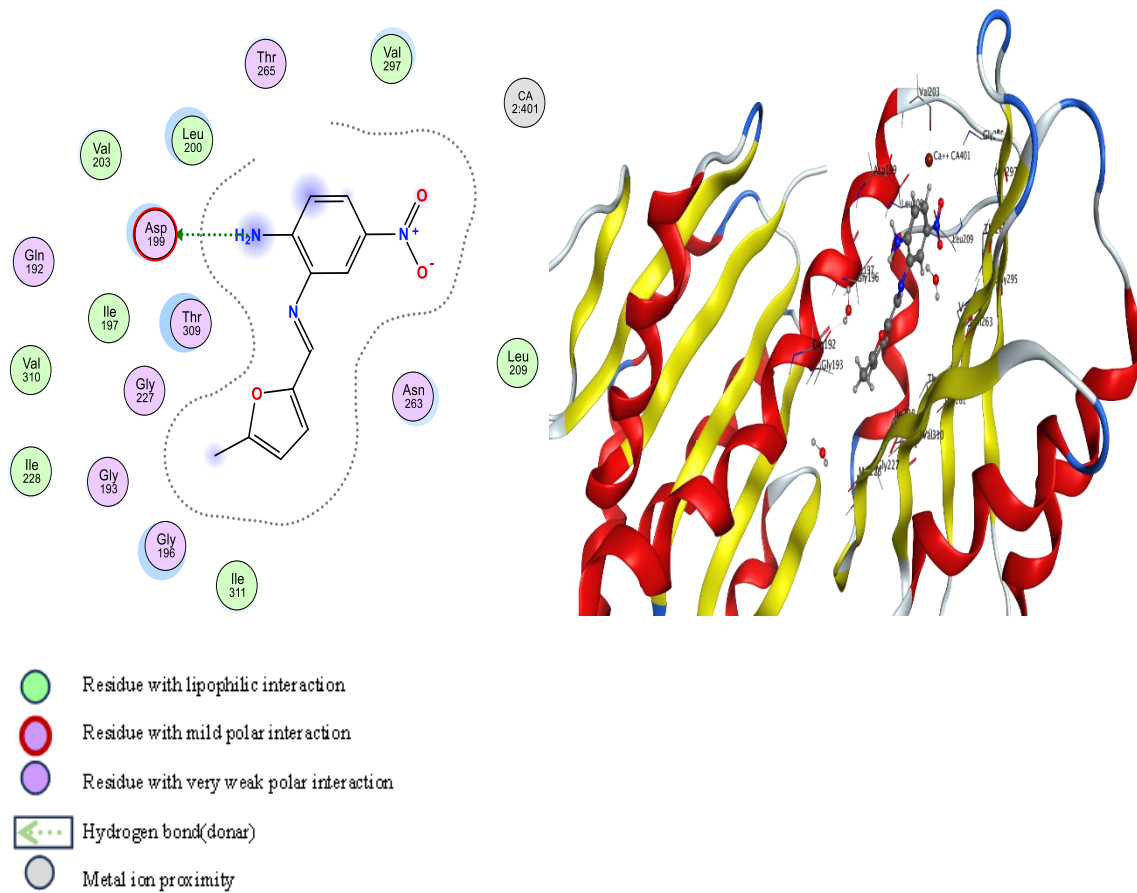


Figure S35: 2D and 3D interaction of Schiff base **3a** against cell division protein FtsZ

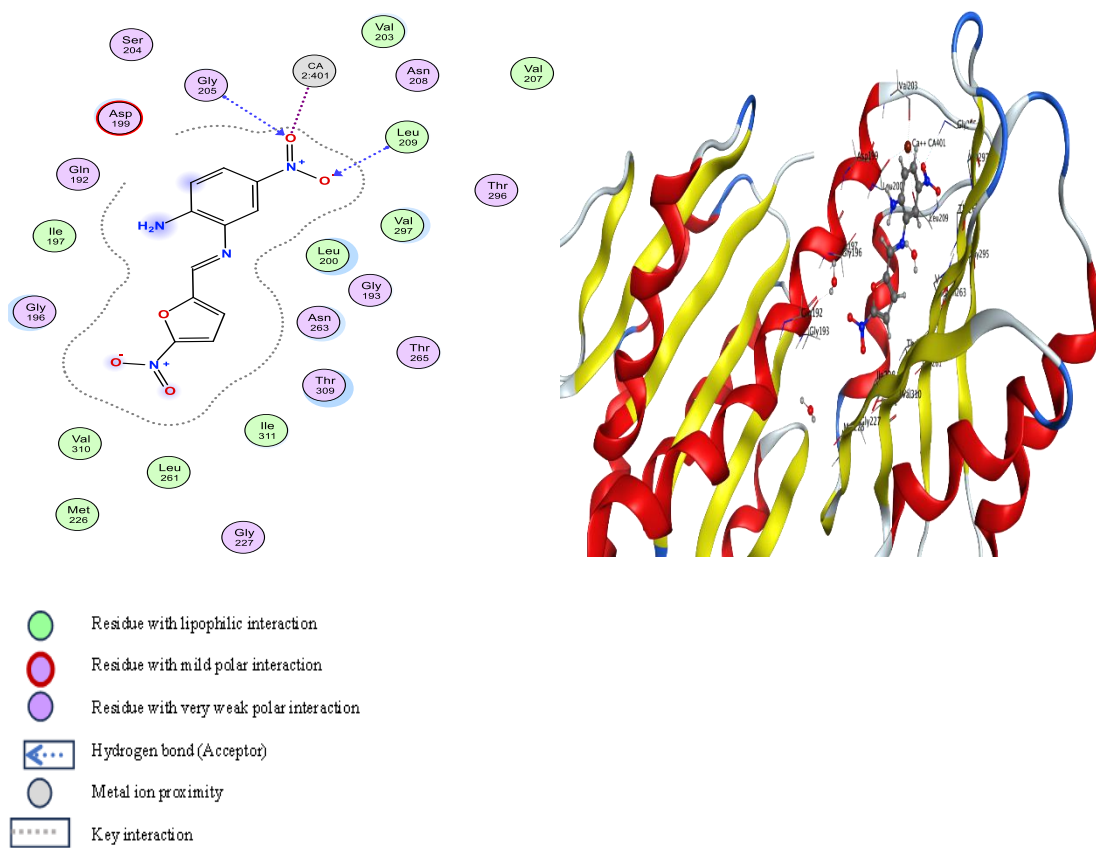


Figure S36: 2D and 3D interaction of Schiff base **3b** against cell division protein FtsZ

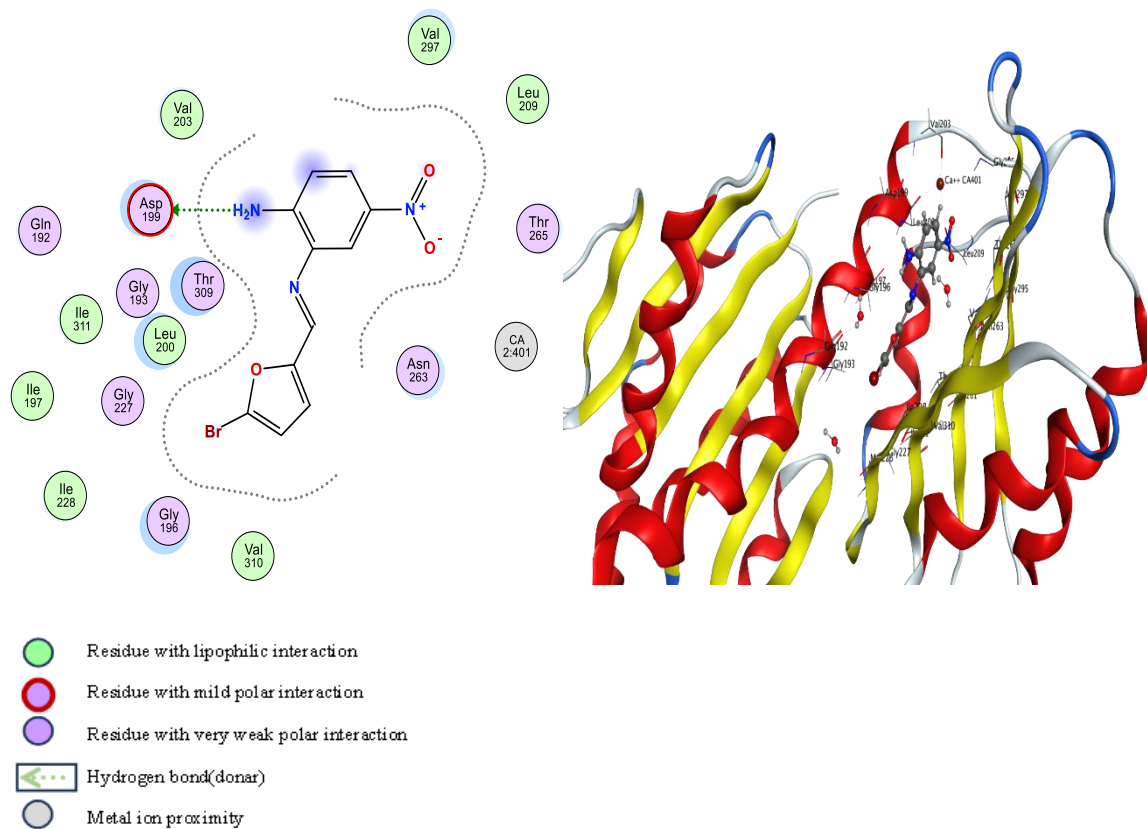


Figure S37: 2D and 3D interaction of Schiff base **3c** against cell division protein FtsZ

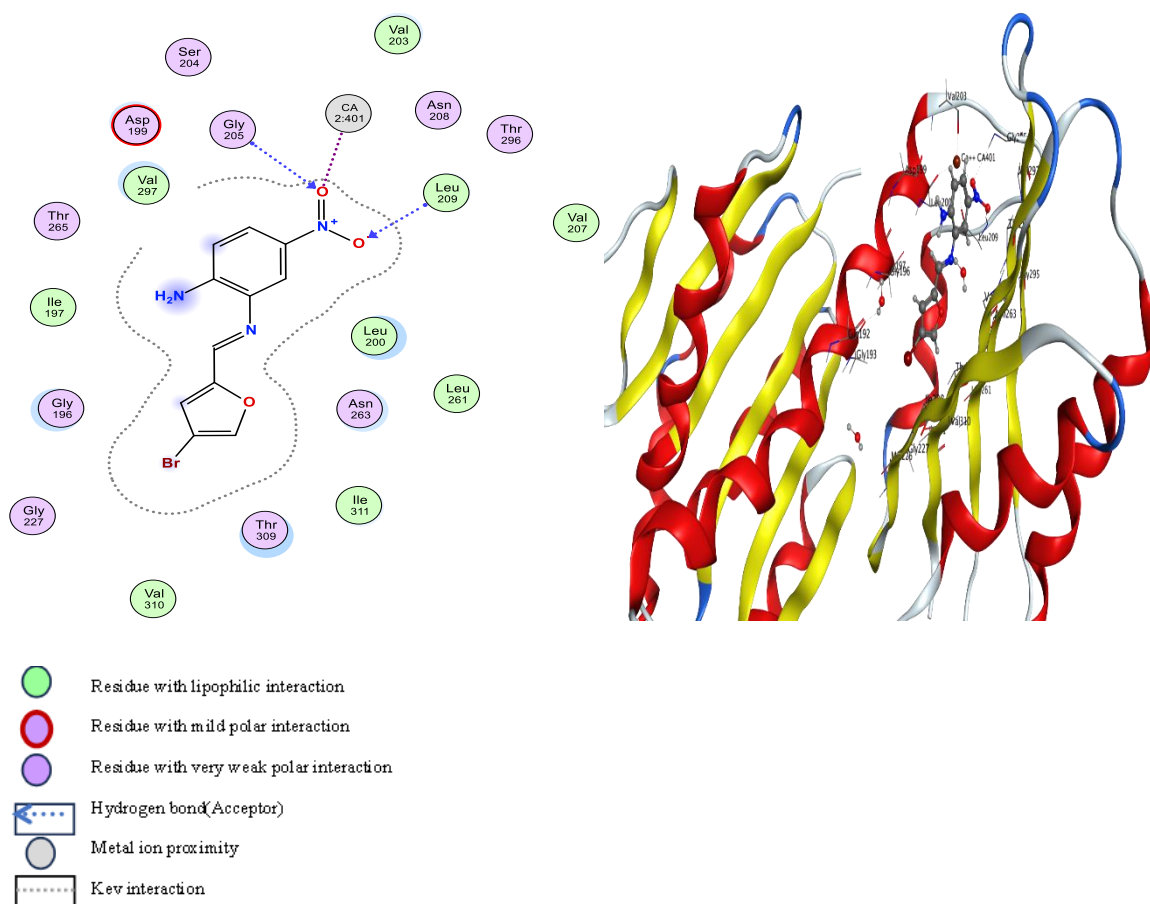


Figure S38: 2D and 3D interaction of Schiff base **3d** against cell division protein FtsZ

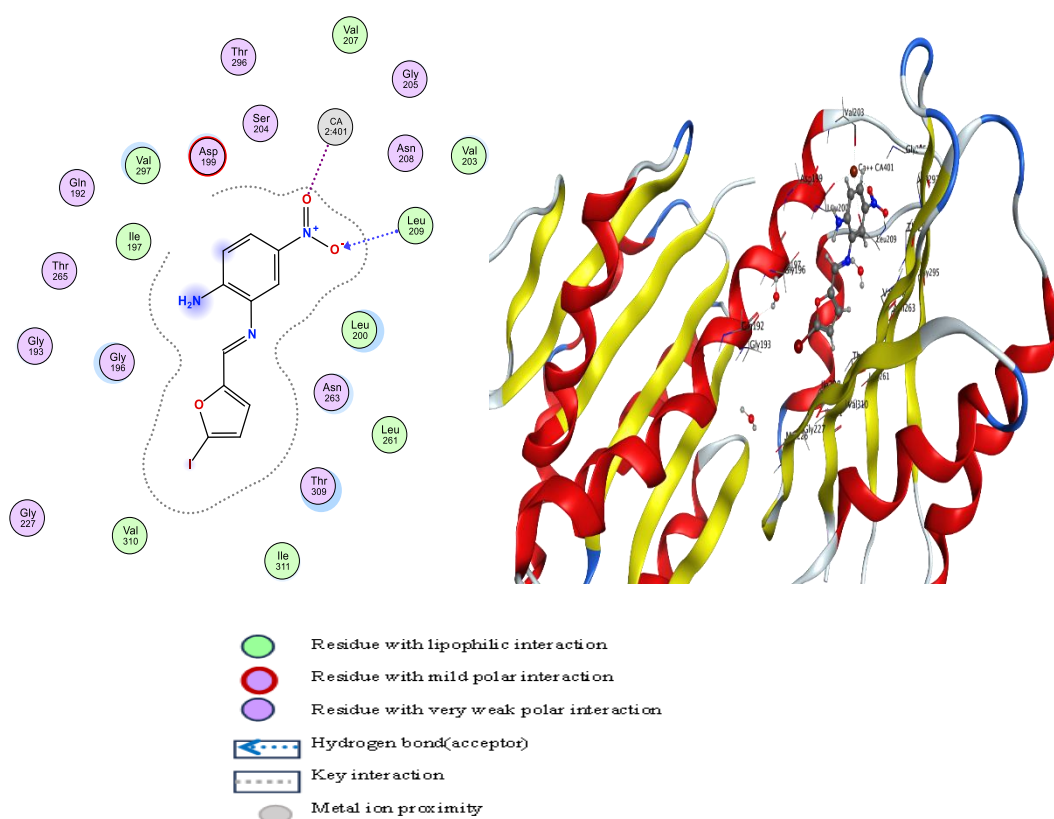


Figure S39: 2D and 3D interaction of Schiff base **3e** against cell division protein FtsZ

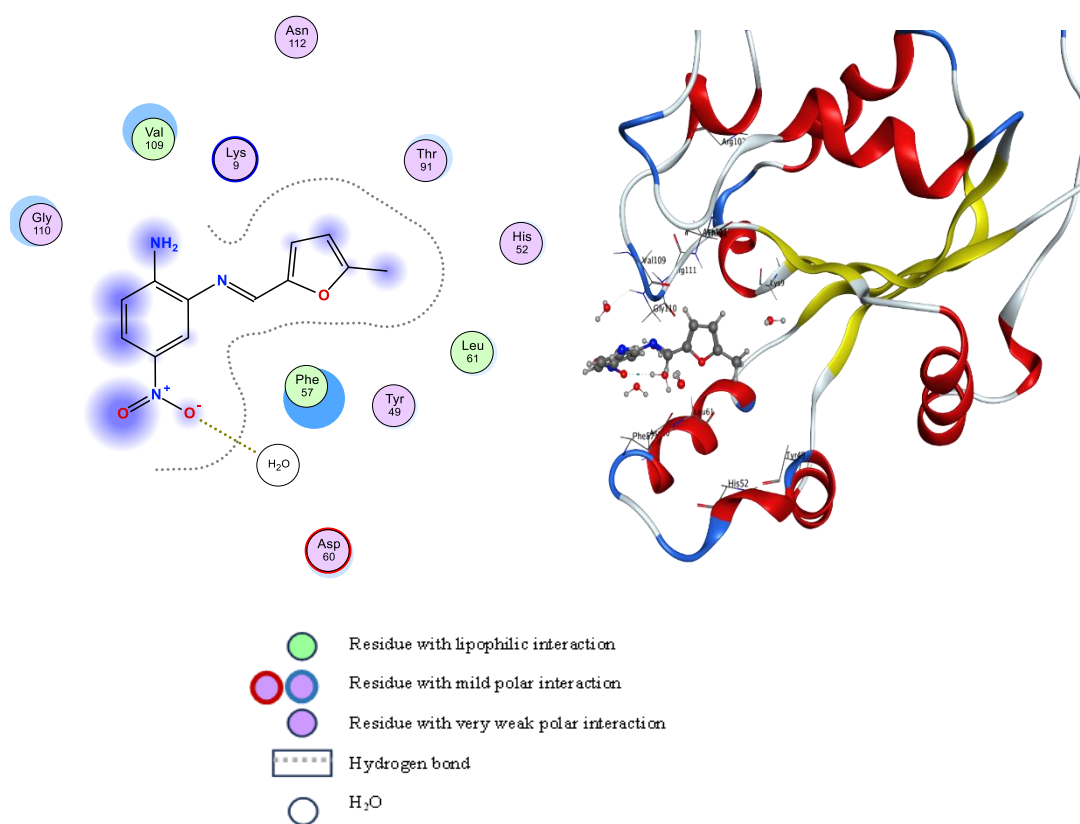


Figure S40: 2D and 3D interaction of Schiff base **3a** against protein nucleoside diphosphate kinase

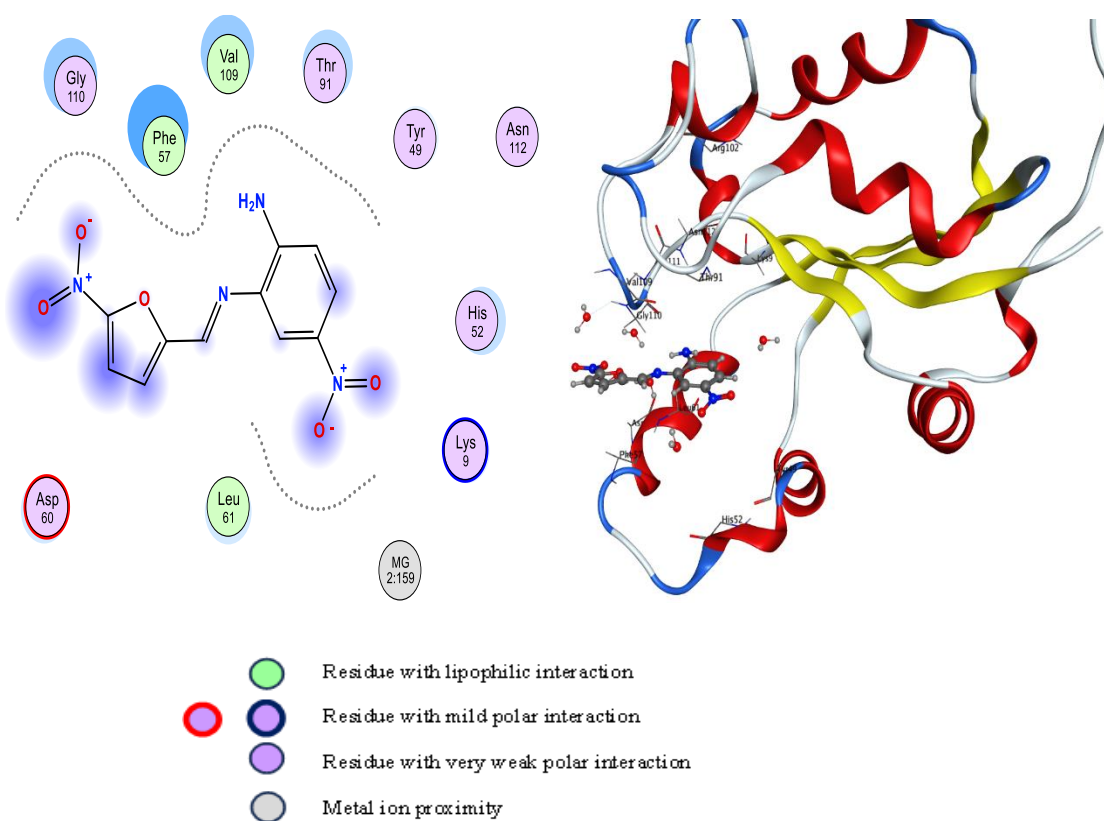


Figure S41: 2D and 3D interaction of Schiff base **3b** against protein nucleoside diphosphate kinase

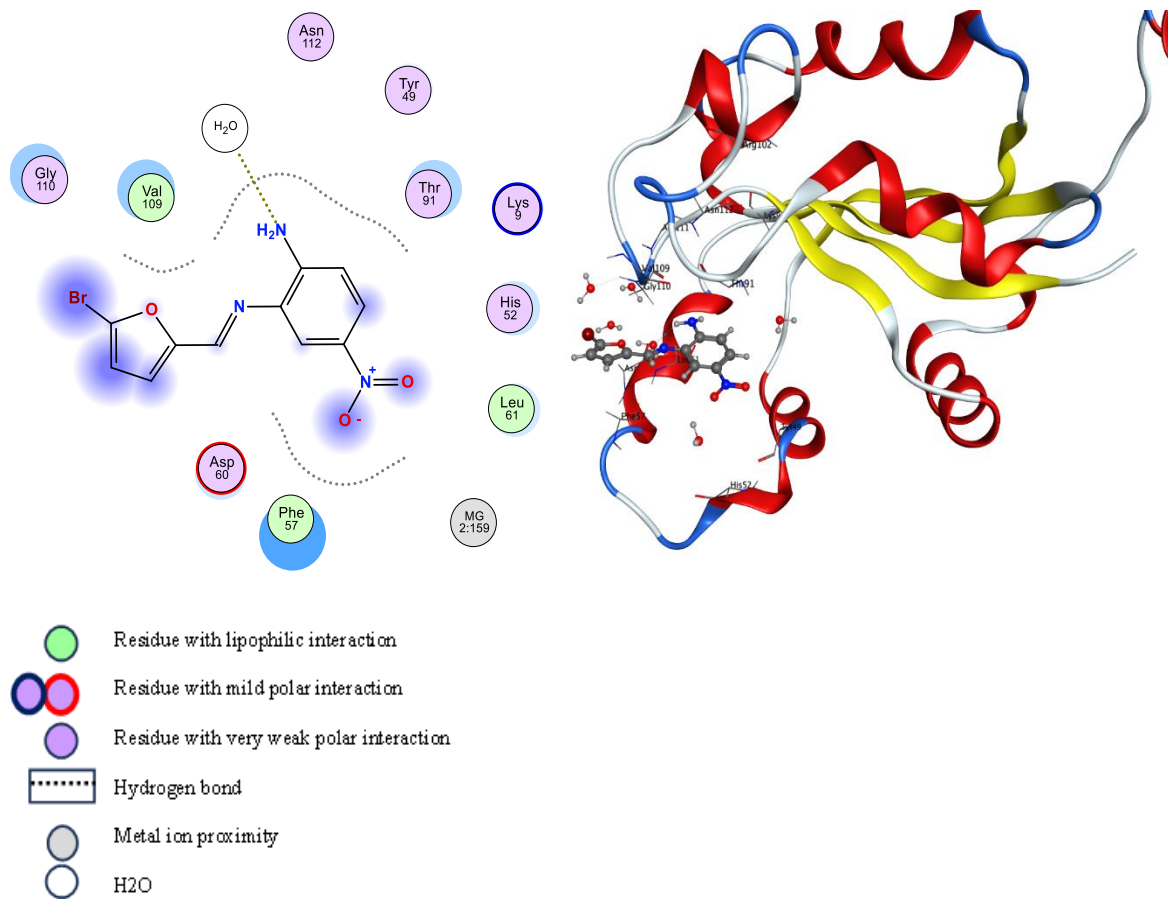


Figure S42: 2D and 3D interaction of Schiff base **3c** against protein nucleoside diphosphate kinase

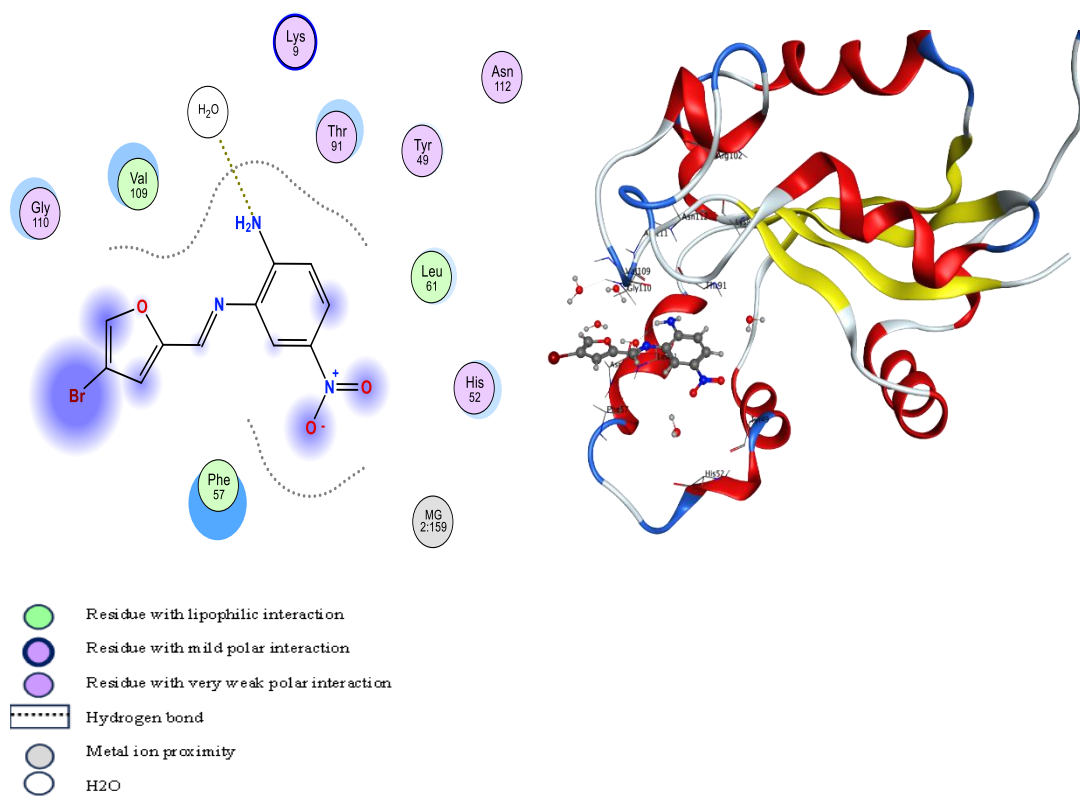


Figure S43: 2D and 3D interaction of Schiff base **3d** against protein nucleoside diphosphate kinase

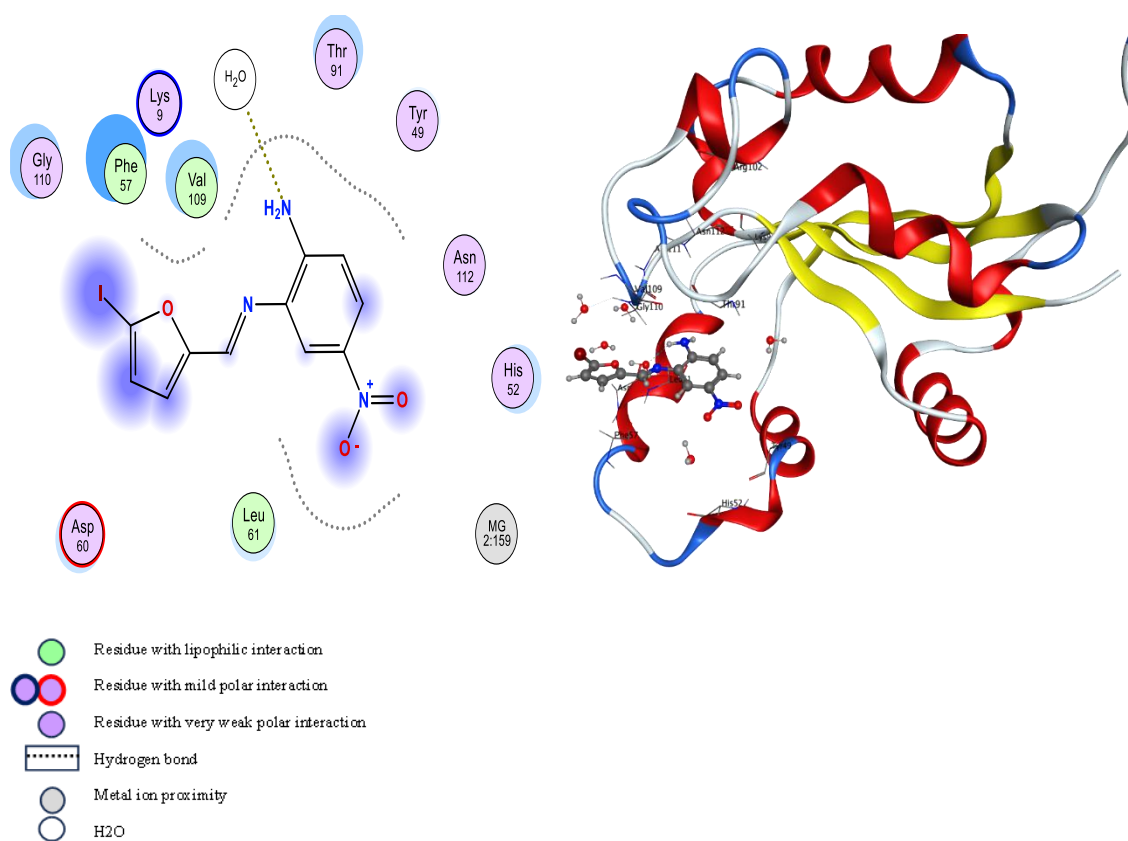
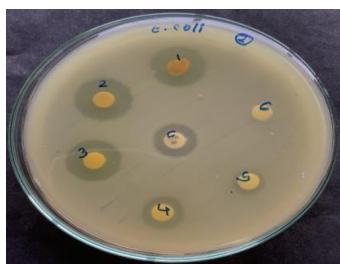


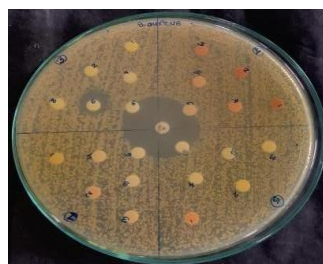
Figure S44: 2D and 3D interaction of Schiff base **3e** against protein nucleoside diphosphate kinase

Table S1 : Antimicrobial activities of Schiff base against *Escherichia coli*, *Staphylococcus aureus*, *Enterococcus faecalis*, and *Klebsiella pneumoniae*.

Microorganism		10 mg/m L	5 mg/ mL	2.5 mg/ mL	1.25 mg/ mL	0.625 mg/mL	0.313 mg/mL	Control Ceftriaxone	MIC	IC50
Zone of Inhibition (mm)										
Escherichia coli	3a	-	-	-	-	-	-	17	-	-
	3b	17	16	15	13	10		18	0.625	0.5618
	3c	-	-	-	-	-	-	18	-	-
	3d	-	-	-	-	-	-	17	-	-
	3e	-	-	-	-	-	-	16	-	-
Staphylococcus aureus	3a	-	-	-	-	-	-	34	-	-
	3b	32	30	28	28	26	21	31	0.313	0.0395
	3c	-	-	-	-	15	-	34	-	-
	3d	-	-	-	-	-	-	34	-	-
	3e	-	-	-	-	-	-	34	-	-
Enterococcus faecalis	3a	-	-	-	-	-	-	20	-	-
	3b	30	28	27	25	23	20	22	0.313	0.0727
	3c	-	-	-	-	-	-	20	-	-
	3d	-	-	-	-	-	-	20	-	-
	3e	-	-	-	-	-	-	20	-	-
Klebsiella pneumoniae	3a	-	-	-	-	-	-	33	-	-
	3b	-	-	-	-	-	-	33	-	-
	3c	-	-	-	-	-	-	33	-	-
	3d	-	-	-	-	-	-	33	-	-
	3e	-	-	-	-	-	-	33	-	-
	Control	Ceftriaxone								
	(-)	No zone of inhibition								



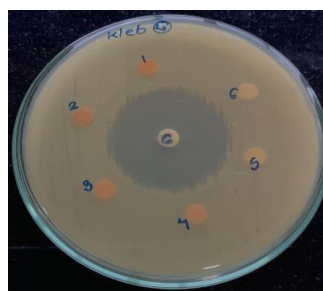
3b Against
Escherichia coli



3b Against
Staphylococcus aureus



3b Against
Enterococcus faecalis



3b Against
Klebsiella pneumoniae

Figure S45 : Antimicrobial activity of Schiff base **3b** against *Escherichia coli*, *Staphylococcus aureus*, *Enterococcus faecalis*, and *Klebsiella pneumoniae*.

