SUPPLEMENTARY MATERIALS

Cobalt(II) and Silver(I) Complexes with 2-Amino-4-Thiazolinone: Synthesis, Structural Characterization, and Antibacterial Potential

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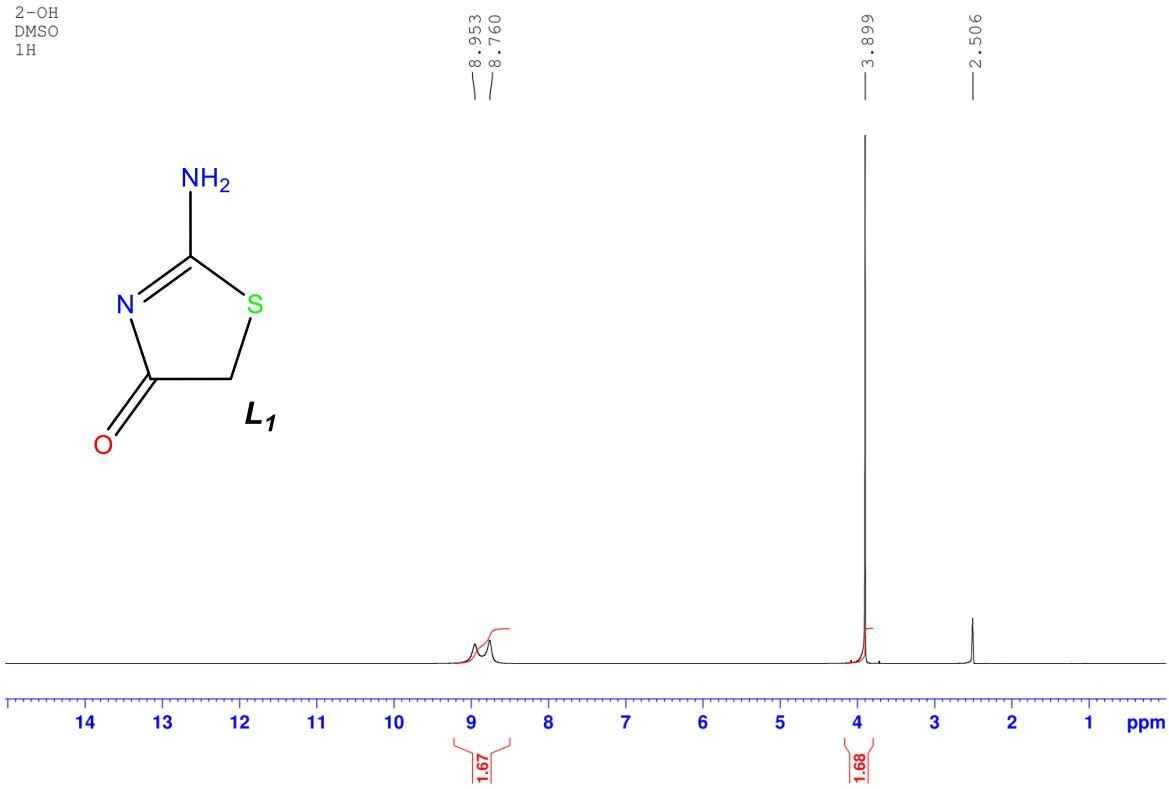


Figure S1. ^{1}H NMR spectrum of 2-Amino-4-thiazolinone (**L$_1$**)

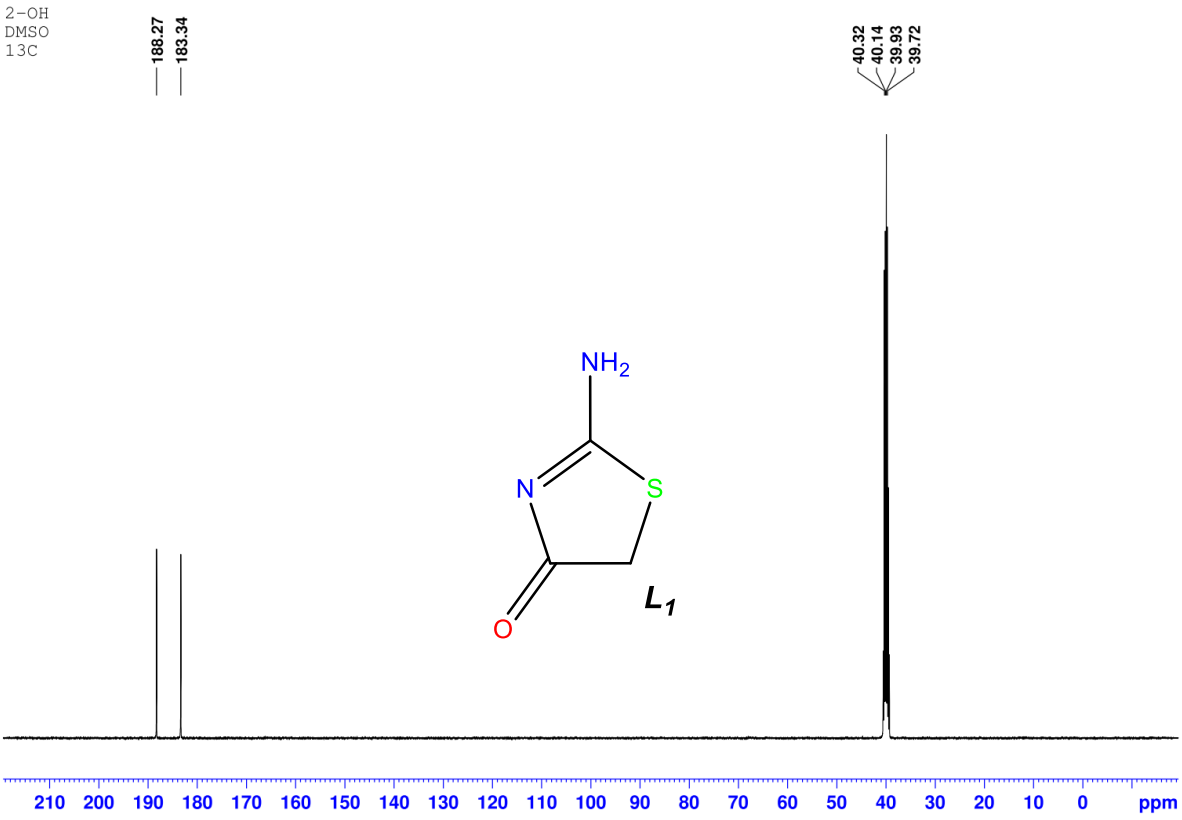


Figure S2. ^{13}C NMR spectrum of 2-Amino-4-thiazolinone (**L$_1$**)

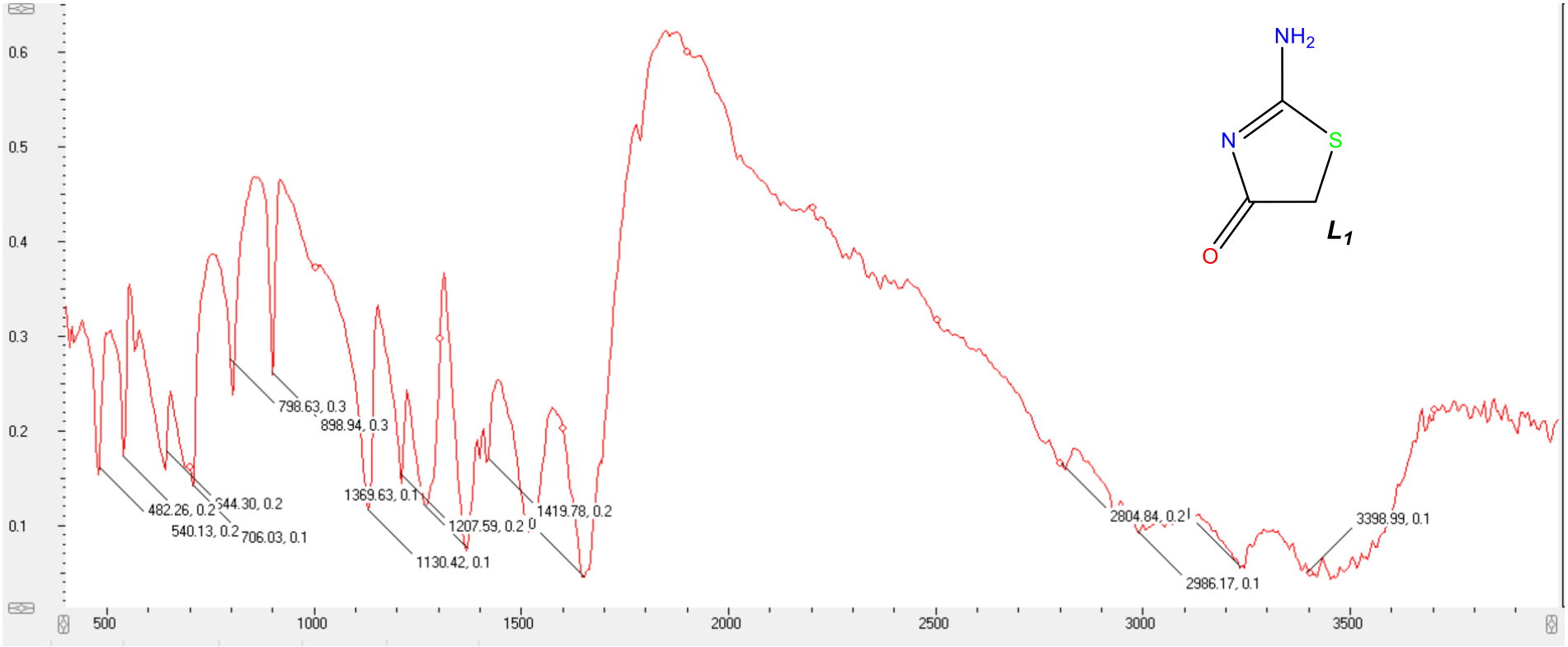


Figure S3. IR spectrum of 2-Amino-4-thiazolinone (**L_1**)

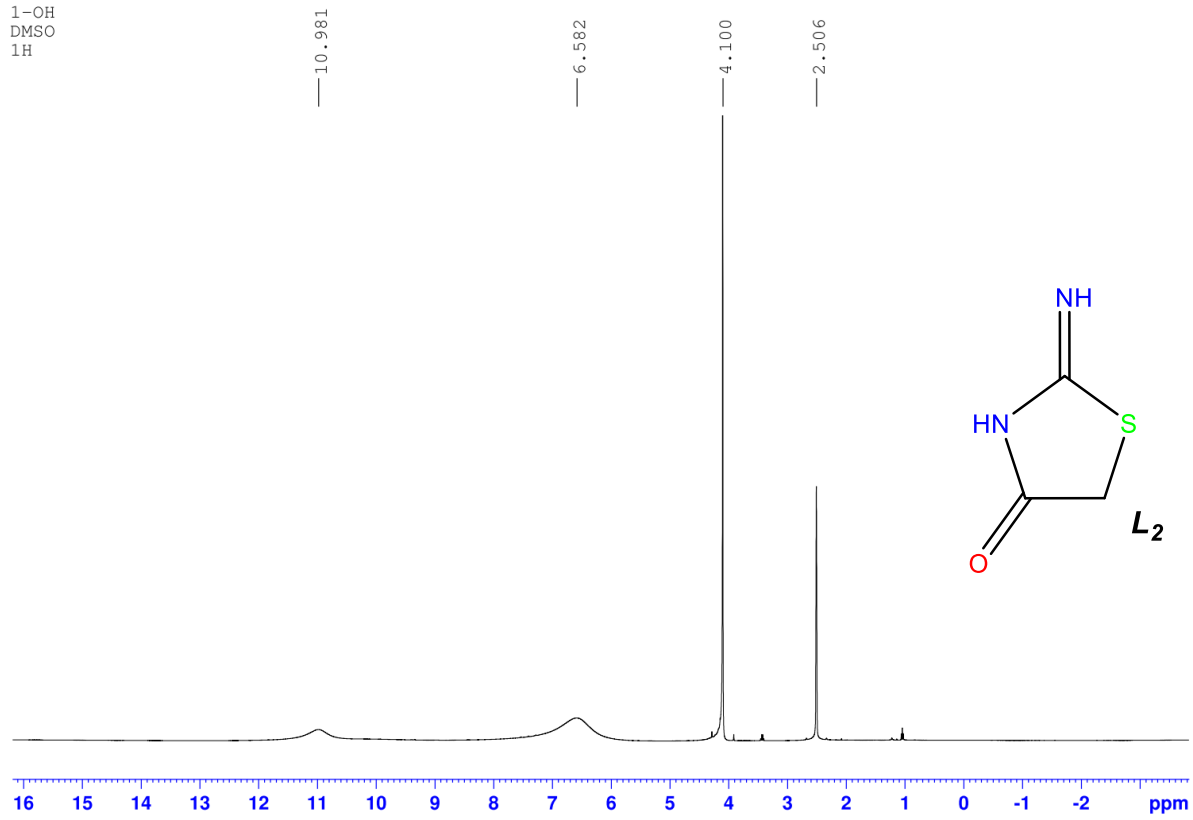


Figure S4. ^{1}H NMR spectrum of 2-Imino-4-thiazolidinone (**L2**)

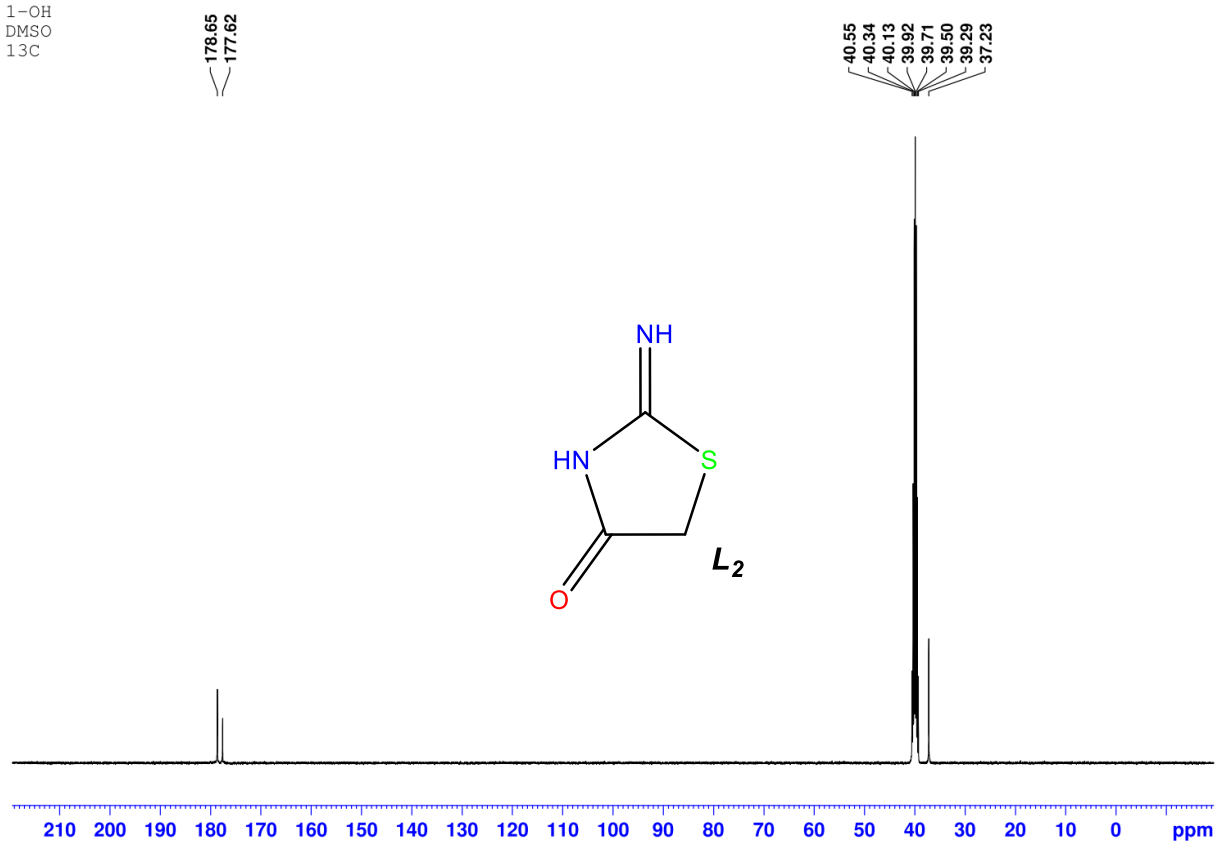


Figure S5. ^{13}C NMR spectrum of 2-Imino-4-thiazolidinone (**L2**)

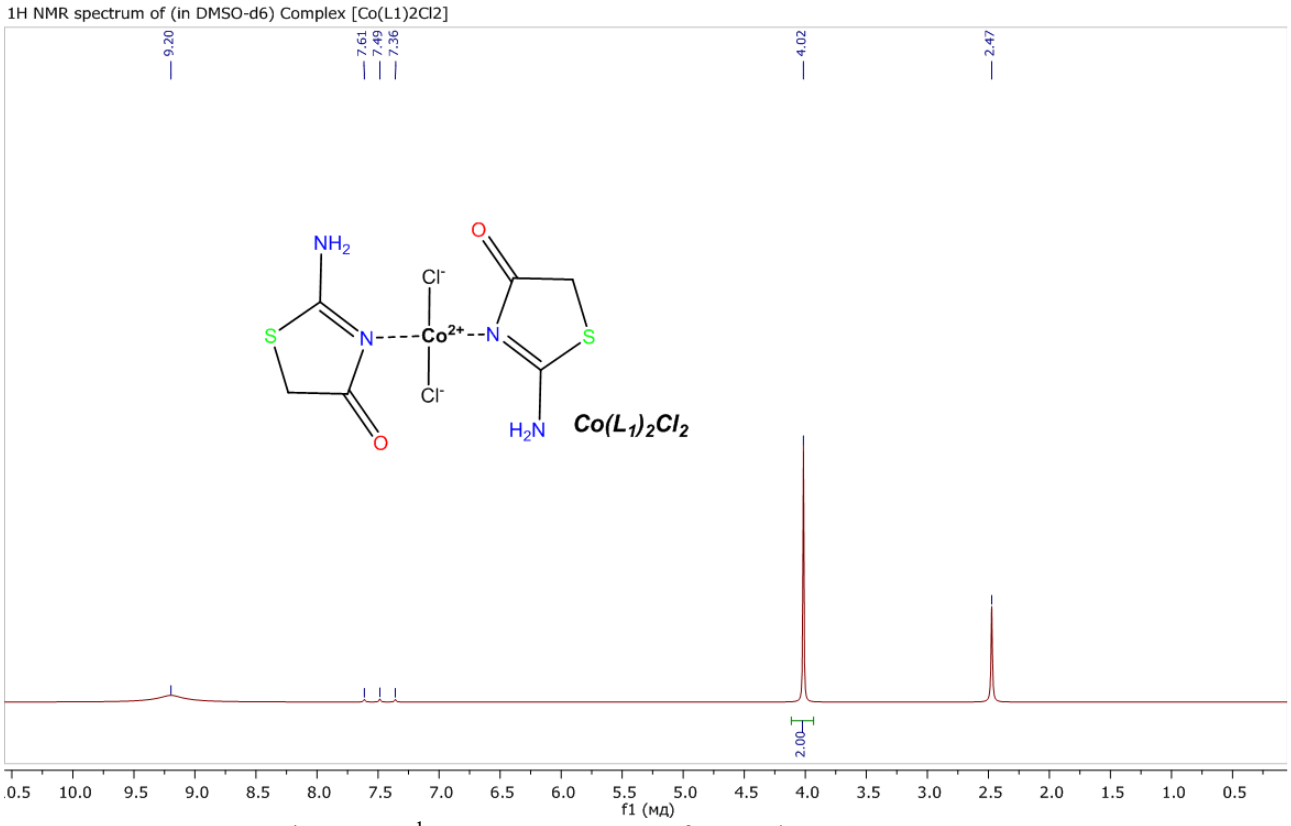


Figure S6. ^{1}H NMR spectrum of Complex **[Co(L$_1$)$_2$Cl$_2$]**



Figure S7. IR spectrum of Complex **[Co(L1)2Cl2]**

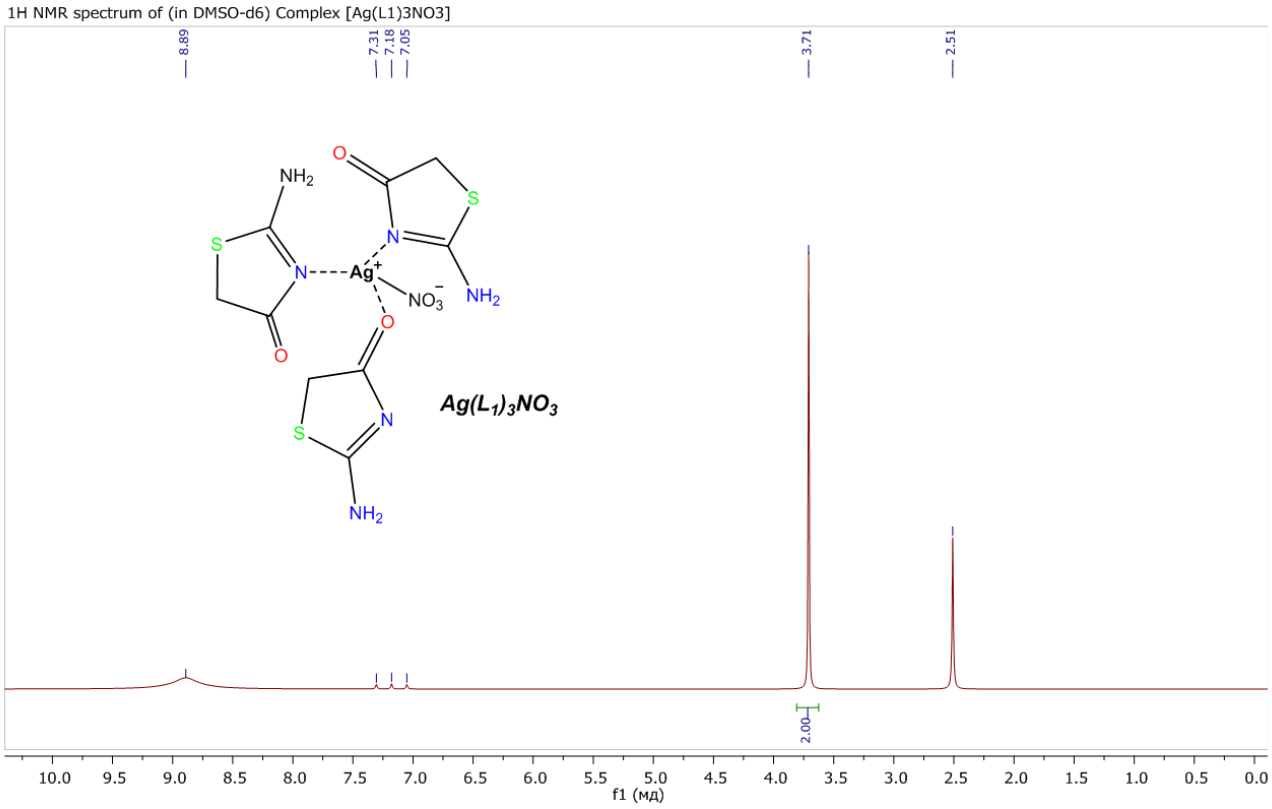


Figure S8. ^{1}H NMR spectrum of Complex **[Ag(L$_1$)$_3$NO$_3$]**



Figure S9. IR spectrum of Complex **[Ag(L₁)₃NO₃]**

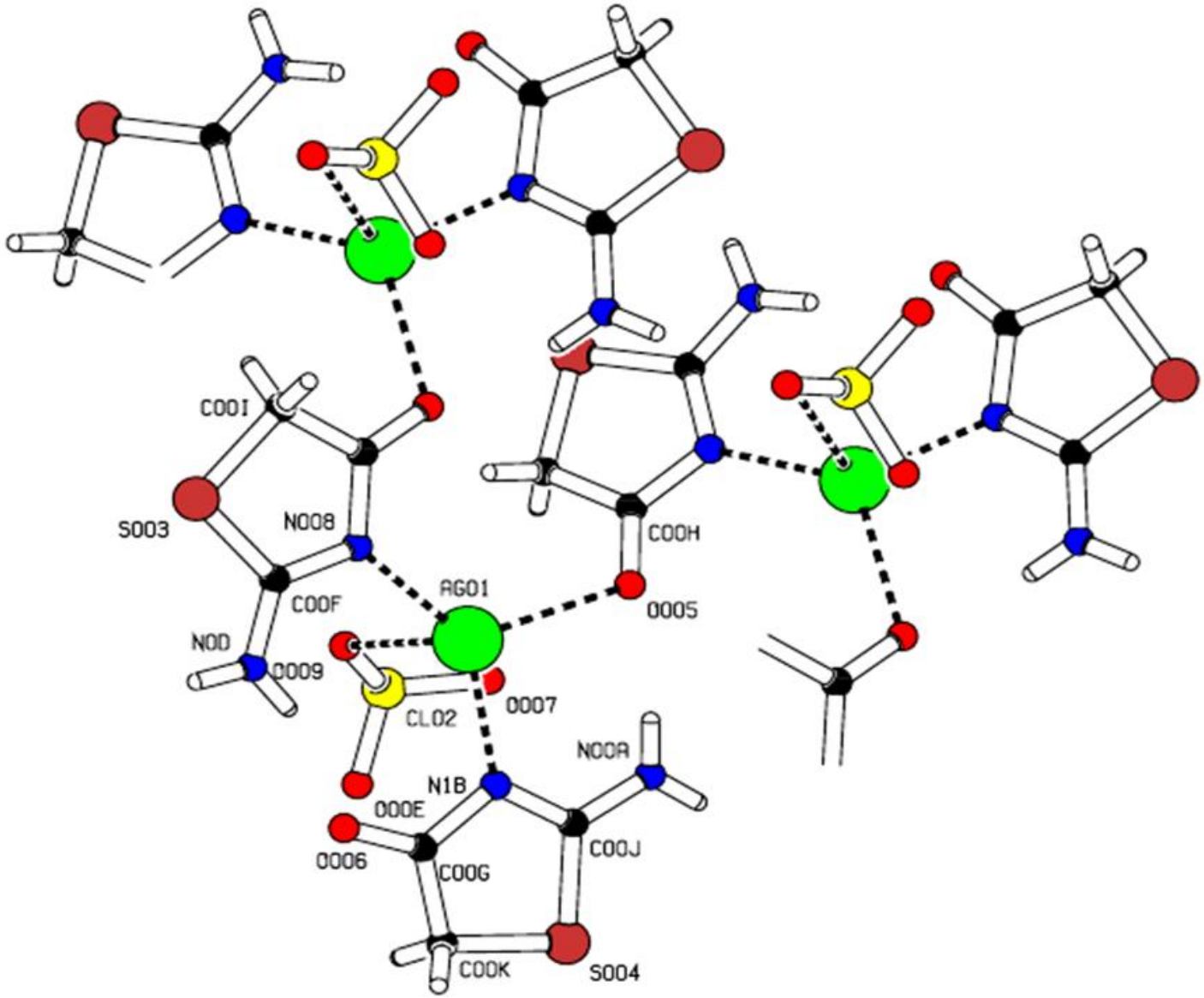
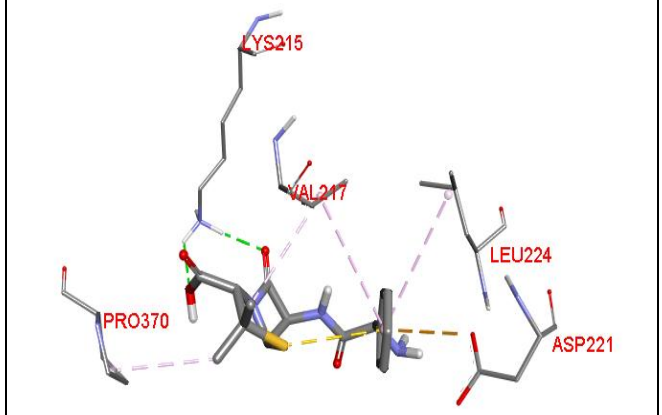
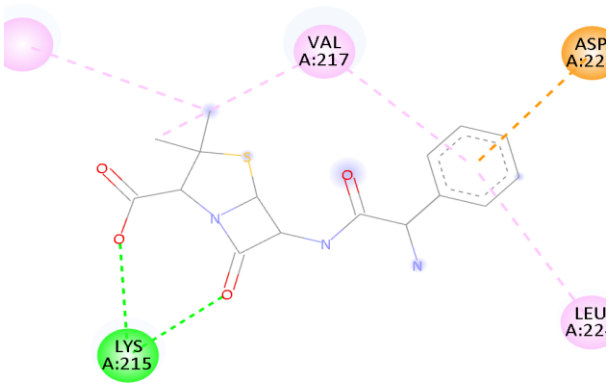


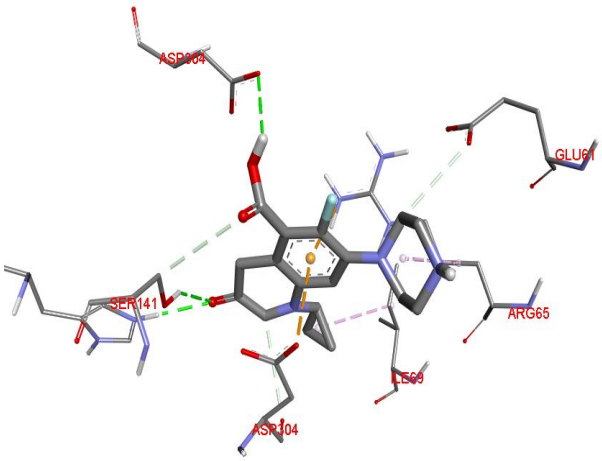
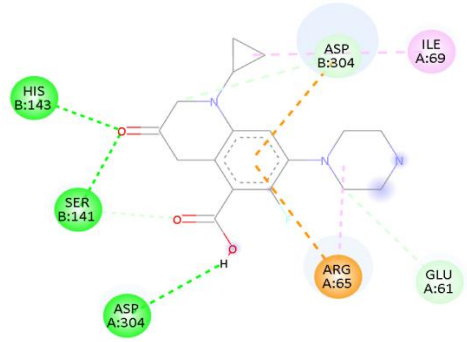
Figure S10. The crystal packing of Complex **[Ag(L$_1$)$_3$NO$_3$]**

Figures S11. 2D and 3D visualizations of key active-site amino acid interactions between ligands (L_1, metal complexes, and reference drugs) and target proteins (PDB IDs: 6RKS, 2XCT, 2EXB, 1VQQ, and 4WMZ)

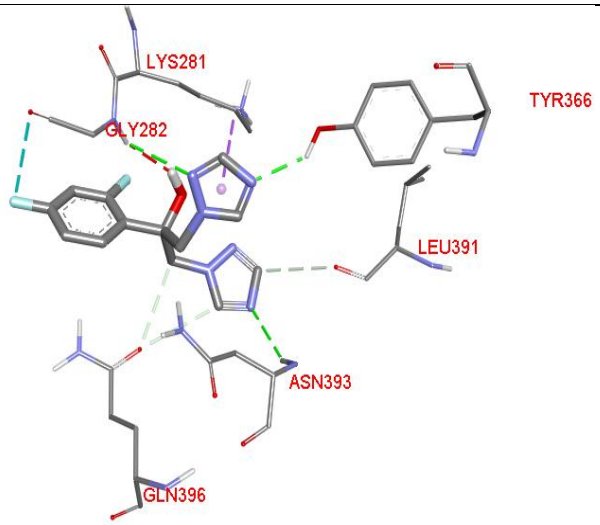
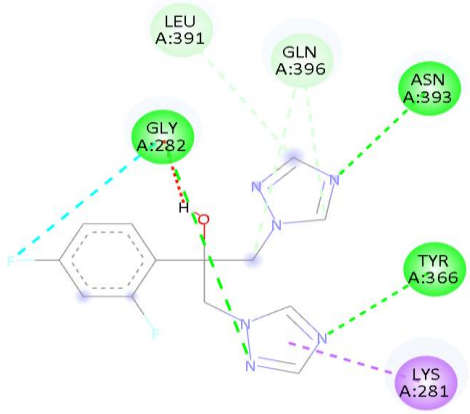
Ampicillin - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

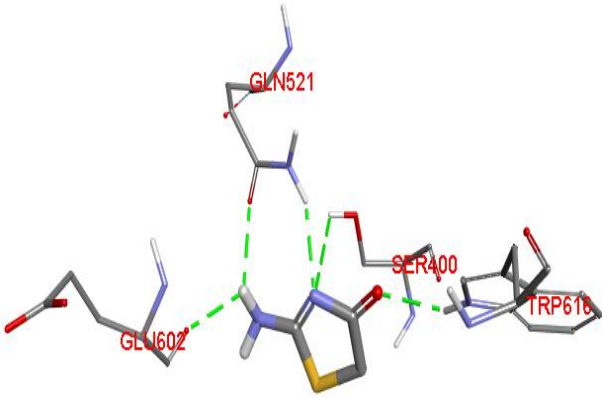
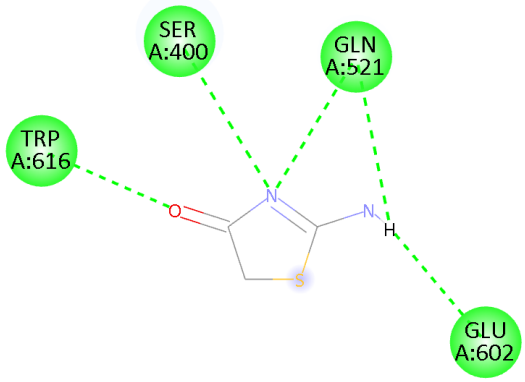
Ciprofloxacin - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

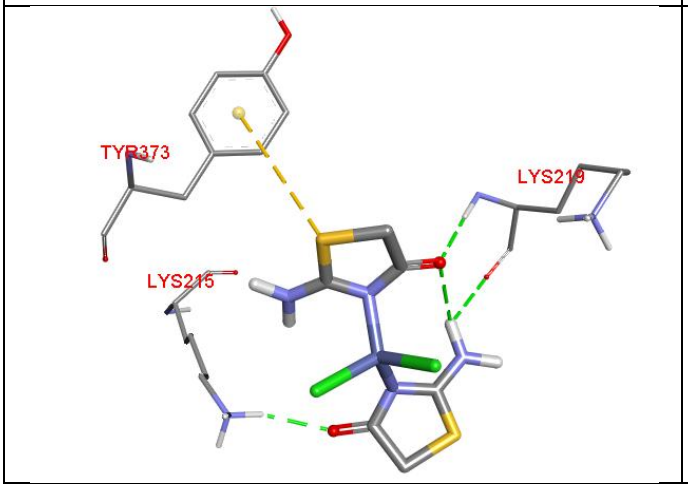
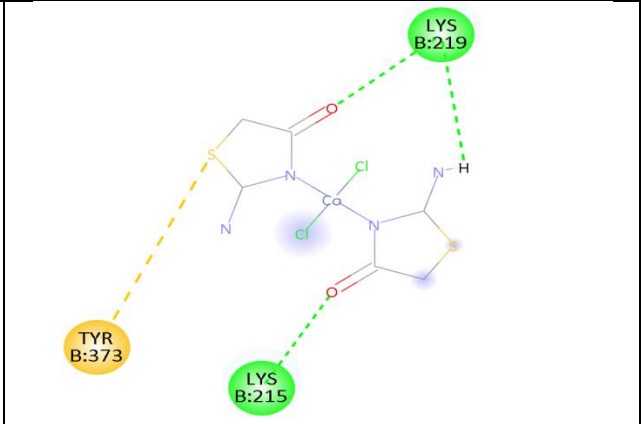
Fluconazole - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

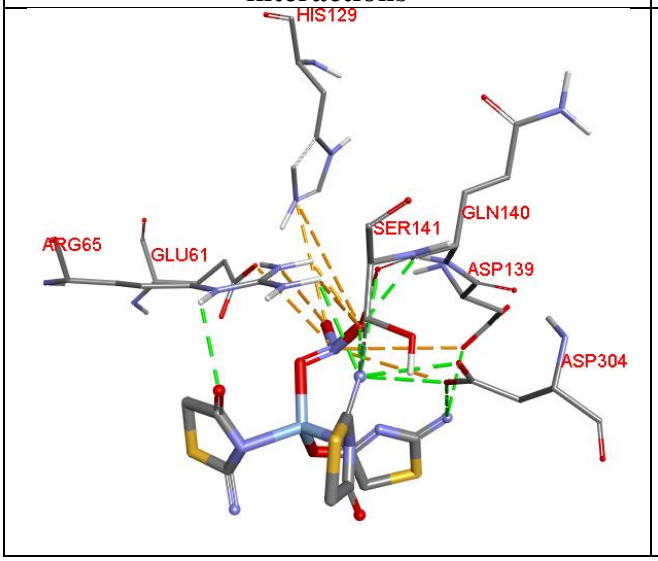
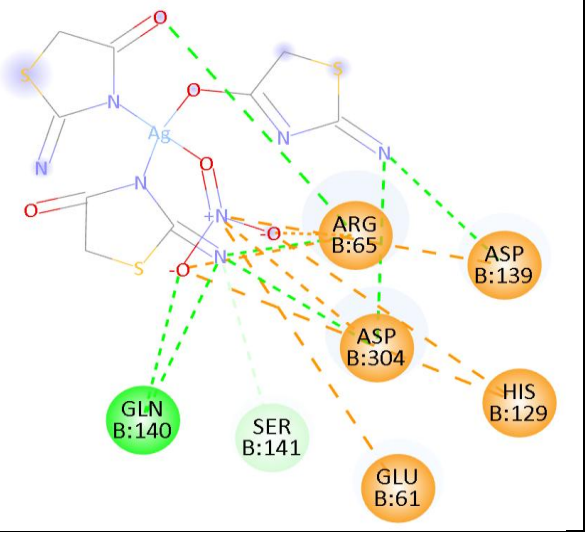
2-Amino-4-thiazolinone (L_1) - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

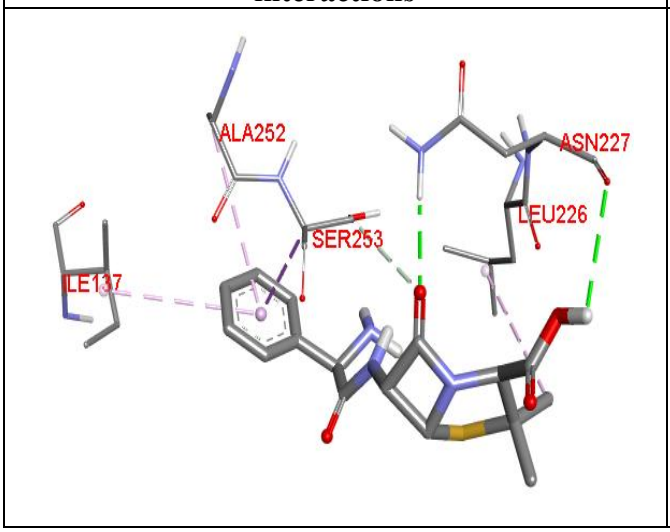
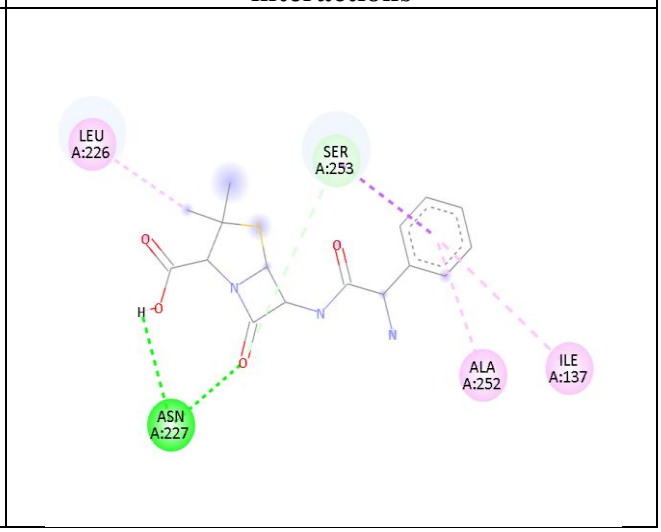
Complex 1 - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

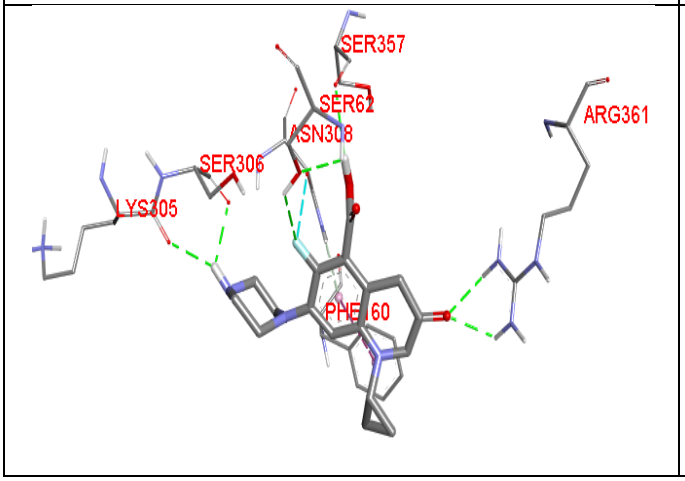
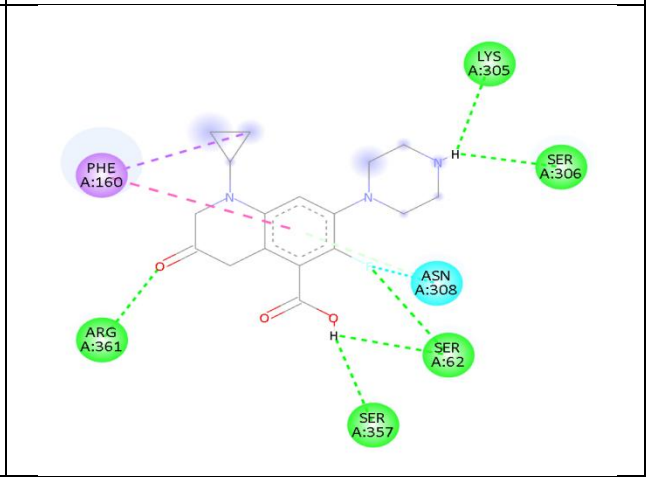
Complex 2 - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

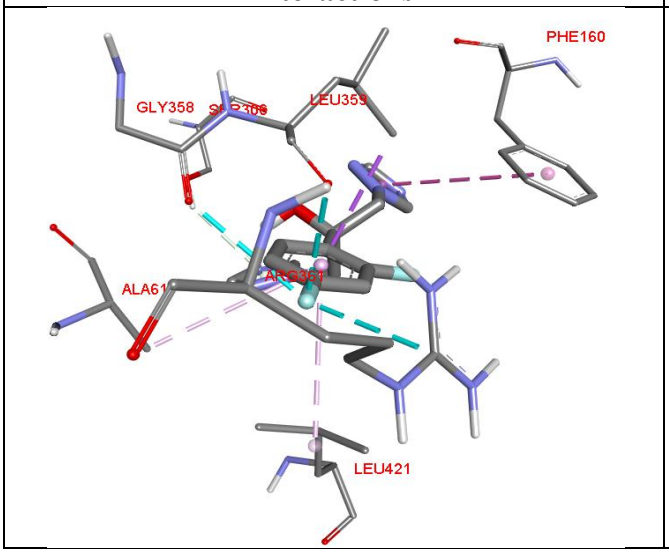
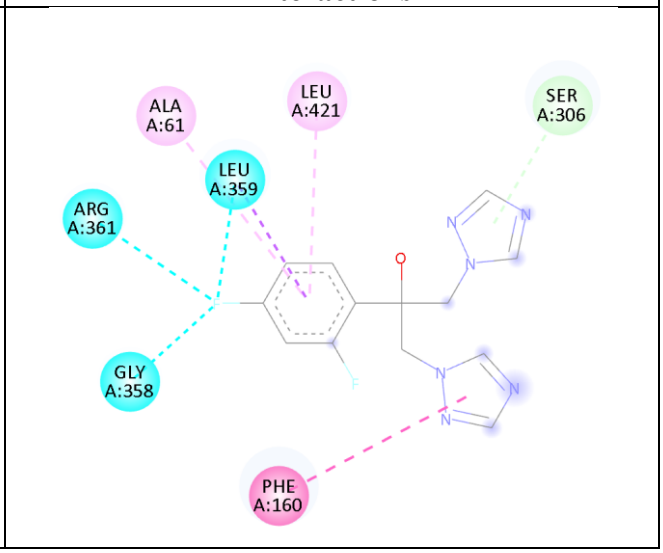
Ampicillin – **2EXB**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

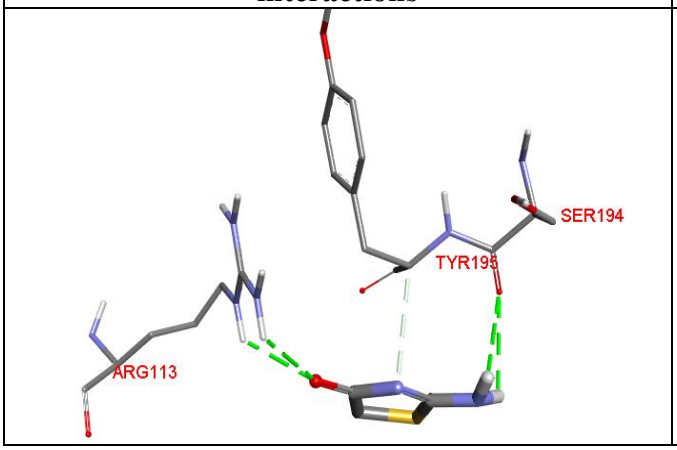
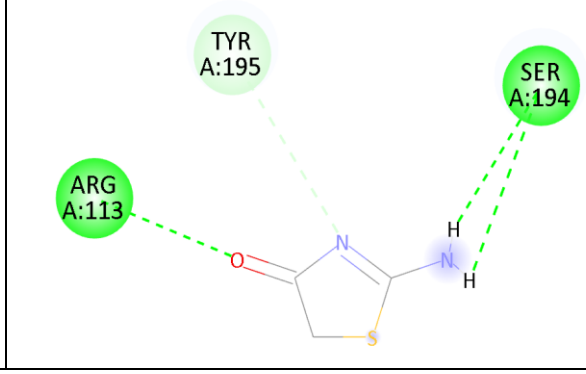
Ciprofloxacin - **2EXB**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

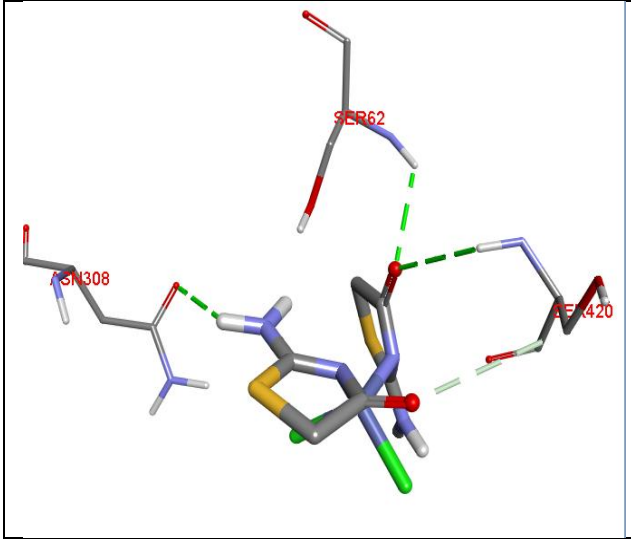
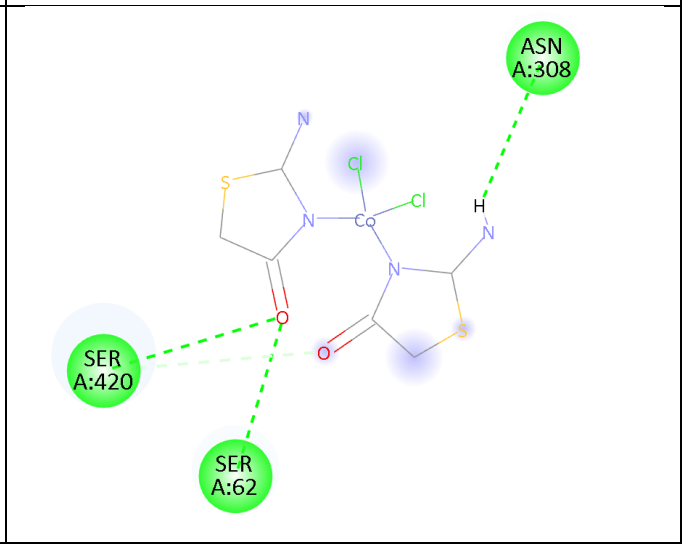
Fluconazole - **2EXB**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

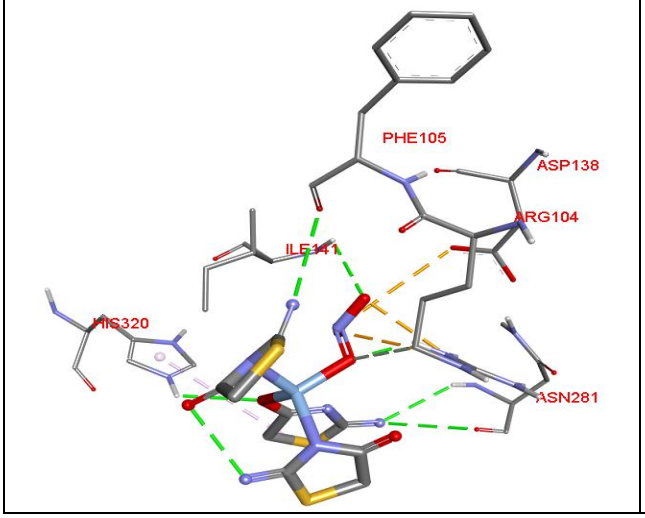
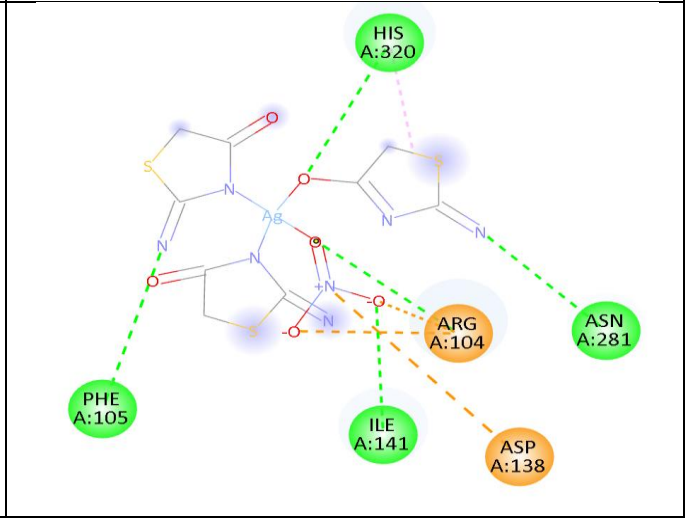
2-Amino-4-thiazolinone (L_1) - **2EXB**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

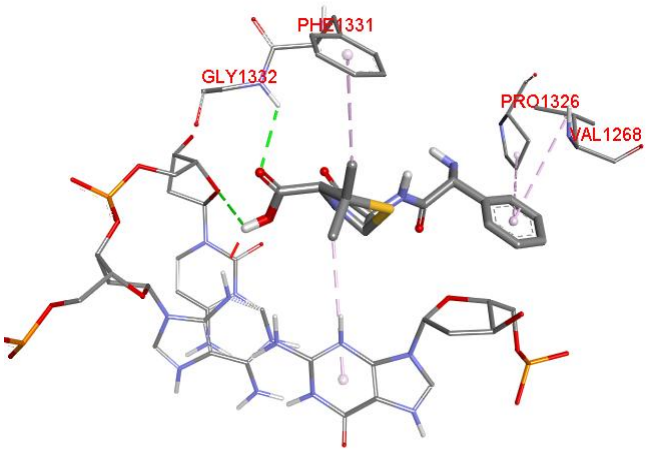
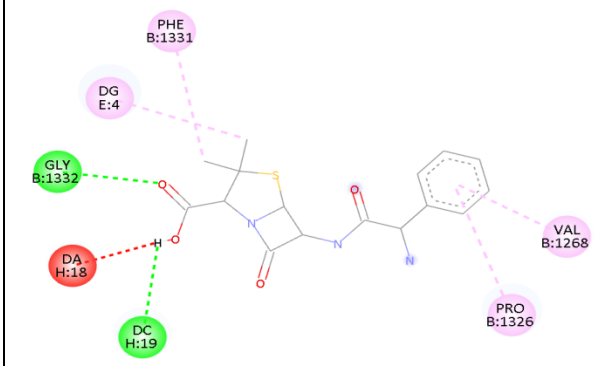
Complex 1 - **2EXB**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

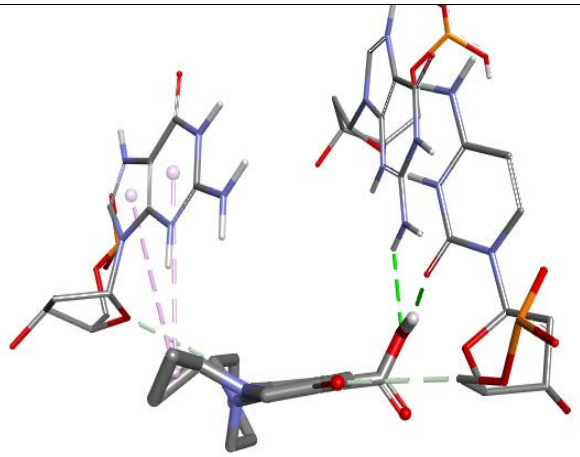
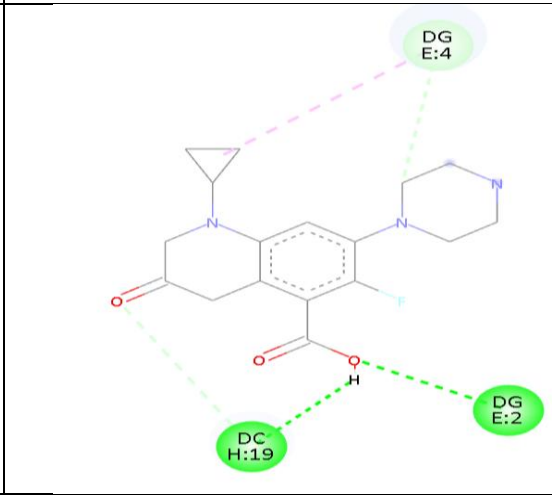
Complex 2 - **2EXB**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

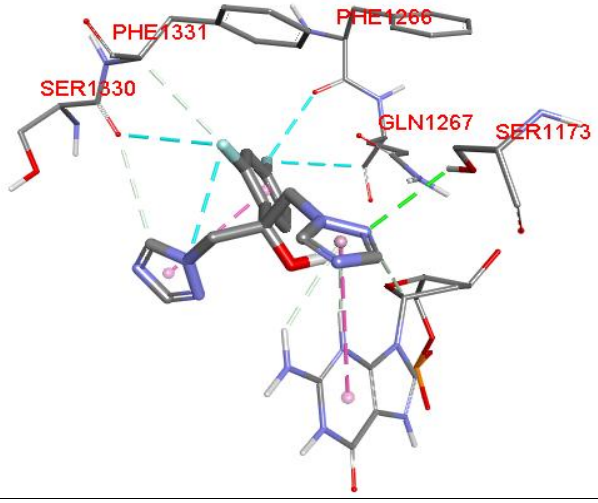
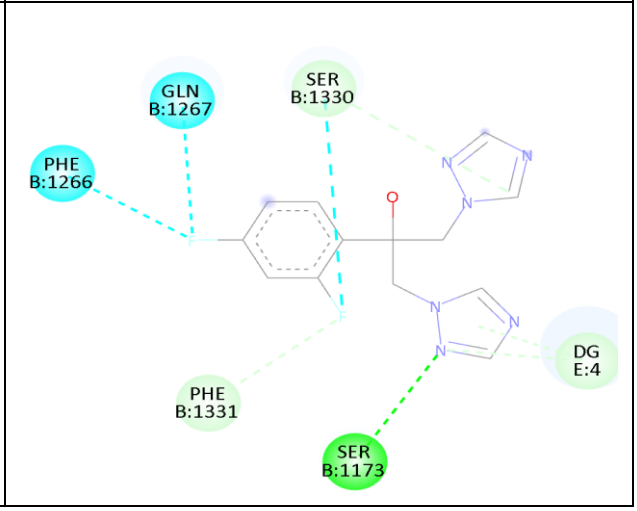
Ampicillin – **2XCT**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

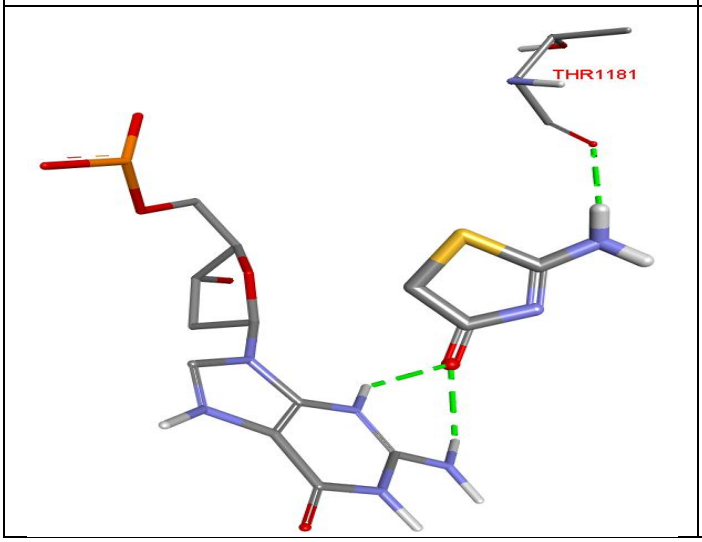
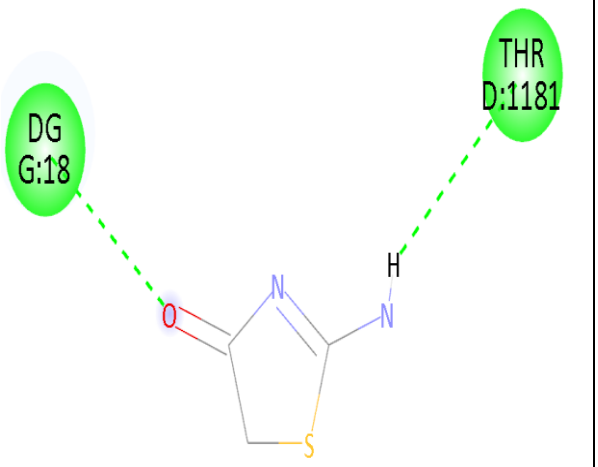
Ciprofloxacin - **2XCT**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

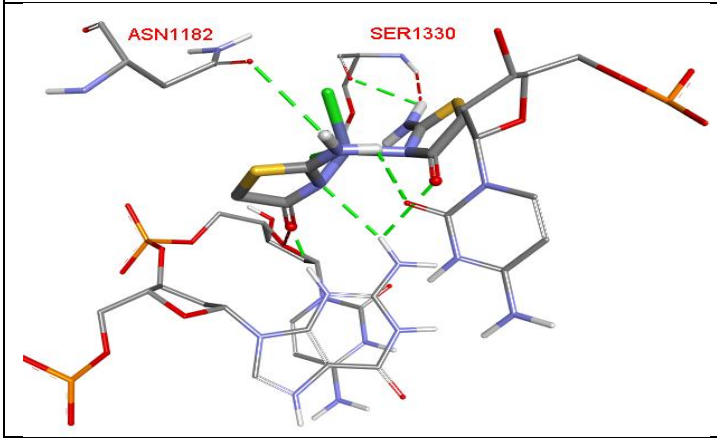
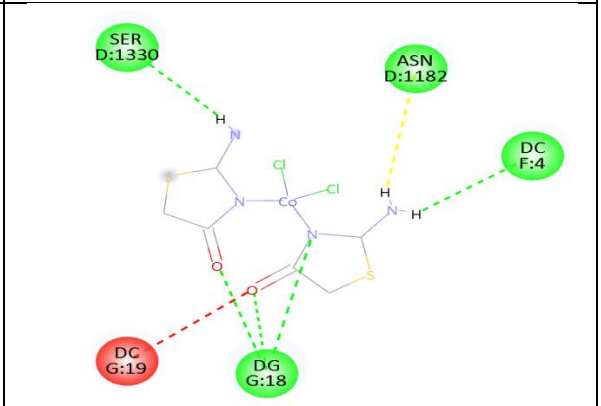
Fluconazole - **2XCT**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

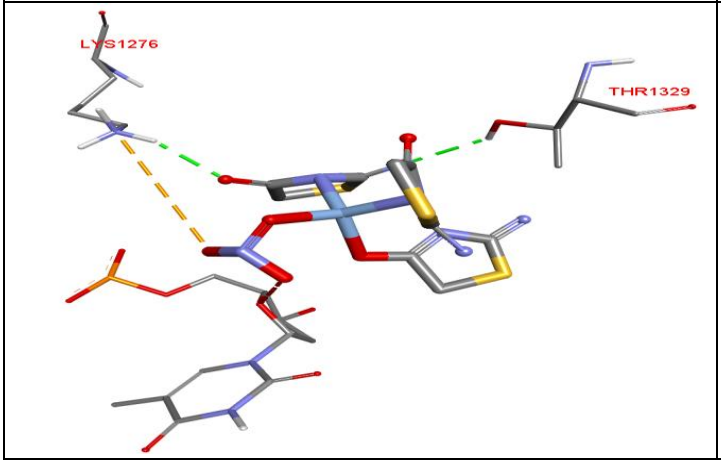
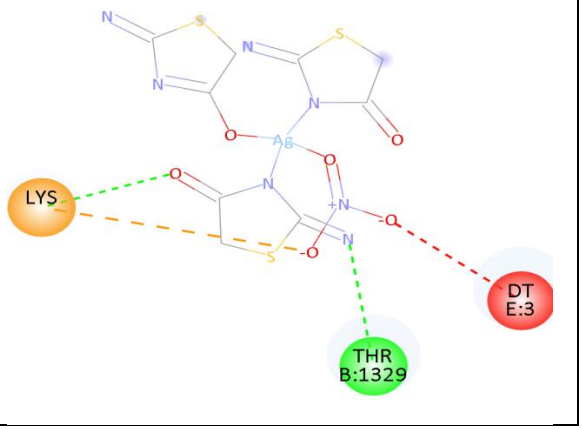
2-Amino-4-thiazolinone (L_1) - **2XCT**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

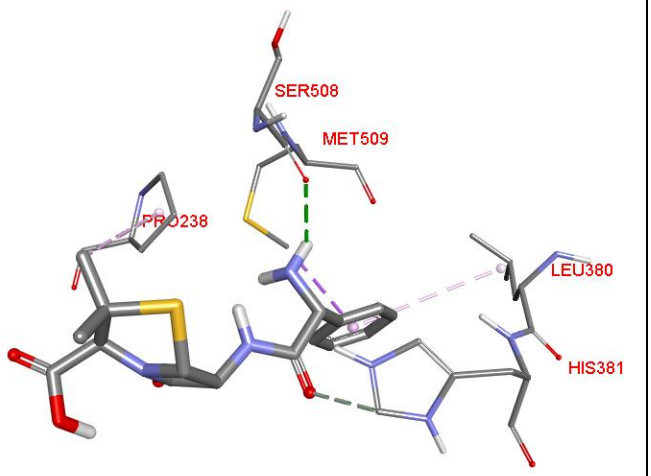
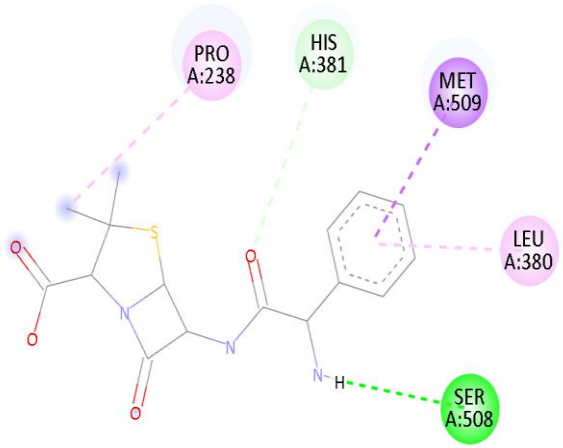
Complex 1 - **2XCT**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

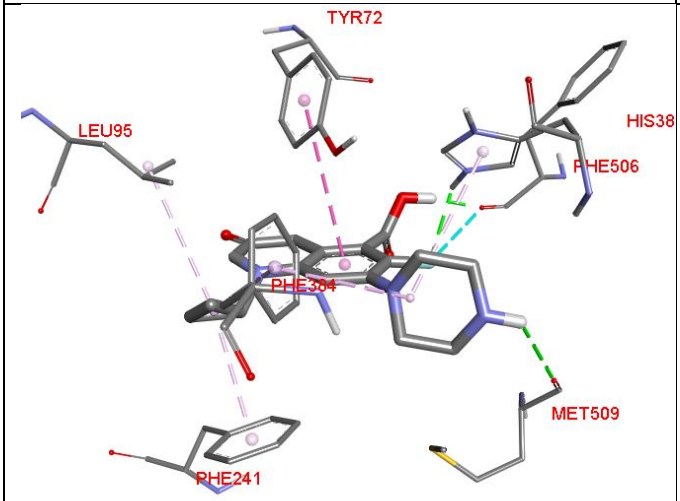
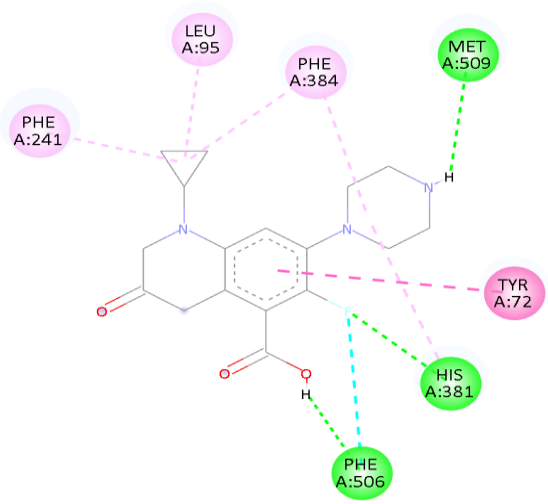
Complex 2 - **2XCT**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

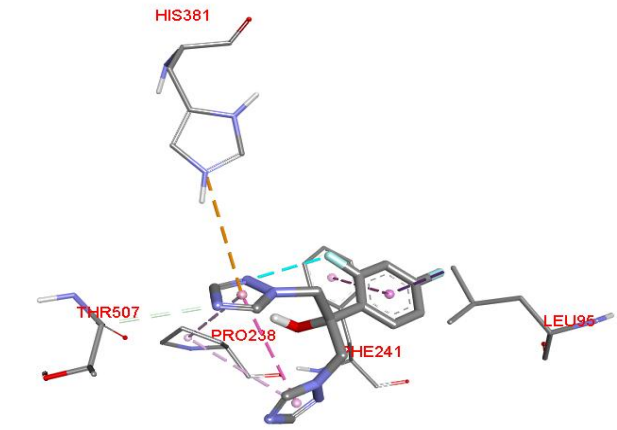
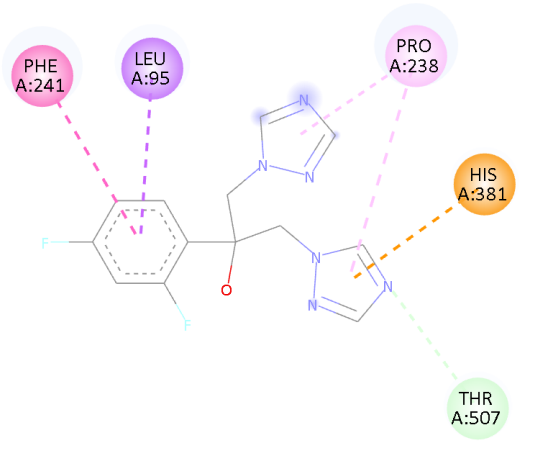
Ampicillin – **4WMZ**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

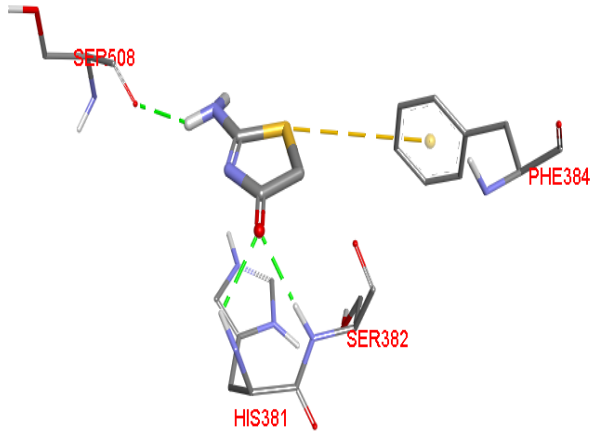
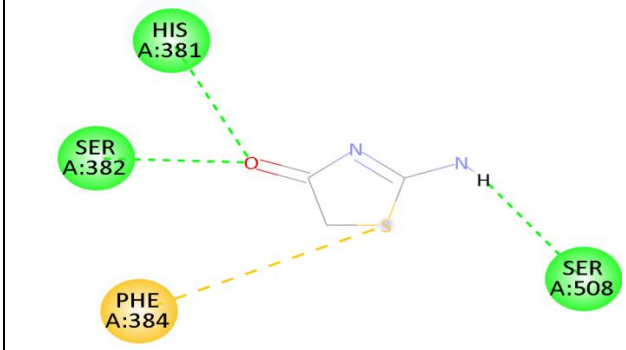
Ciprofloxacin - **4WMZ**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

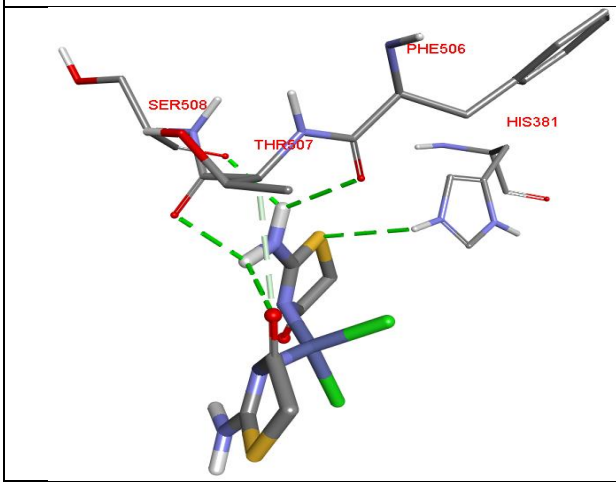
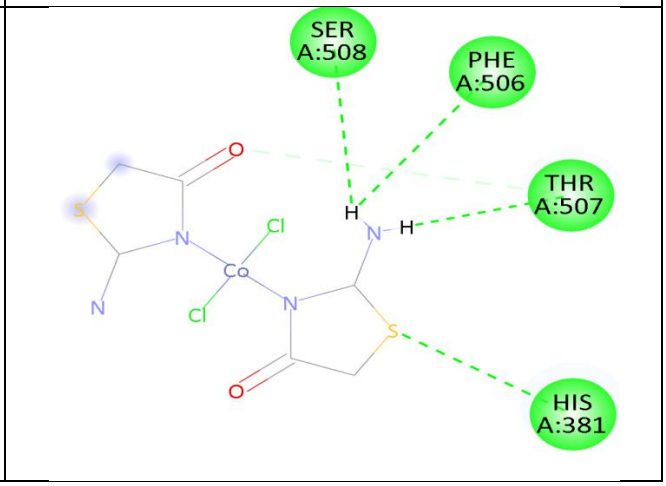
Fluconazole - **4WMZ**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

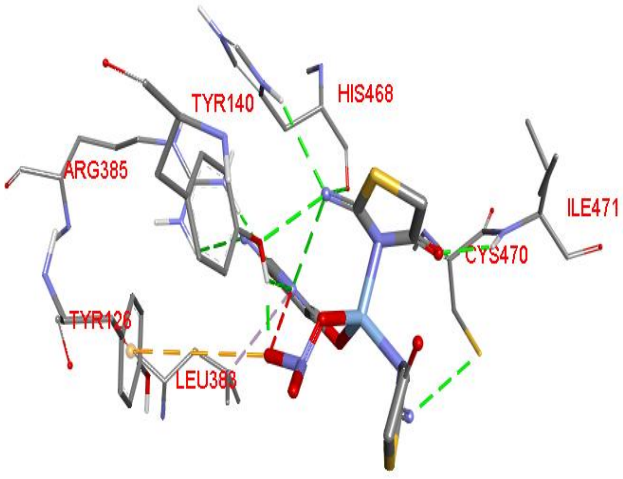
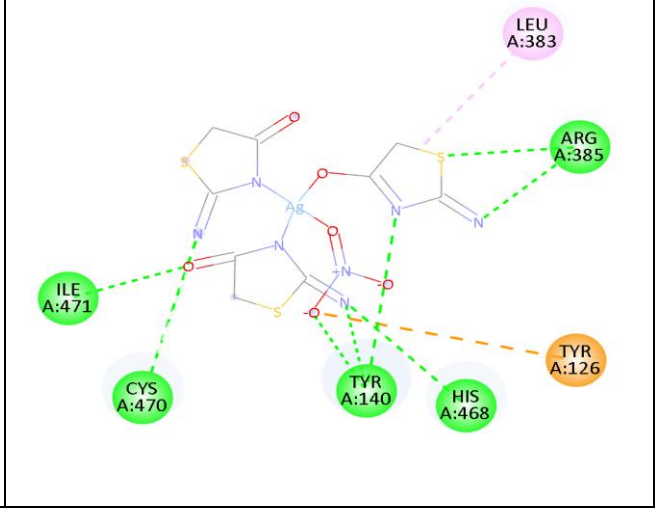
2-Amino-4-thiazolinone (L_1) - **4WMZ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

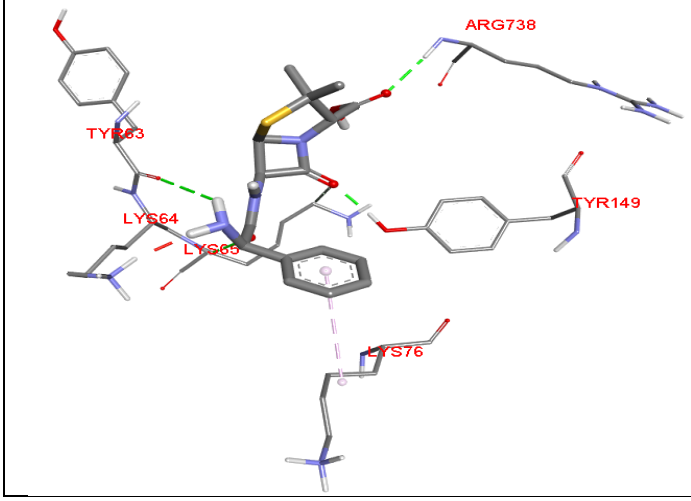
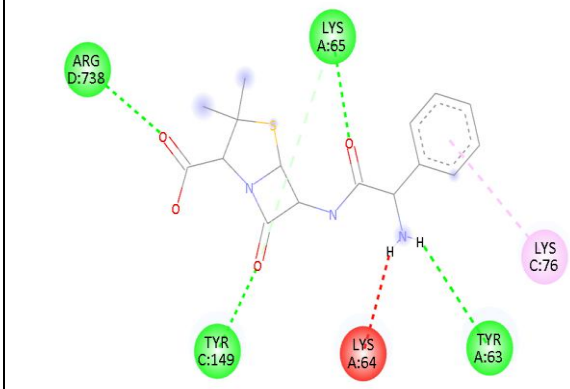
Complex 1 - **4WMZ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

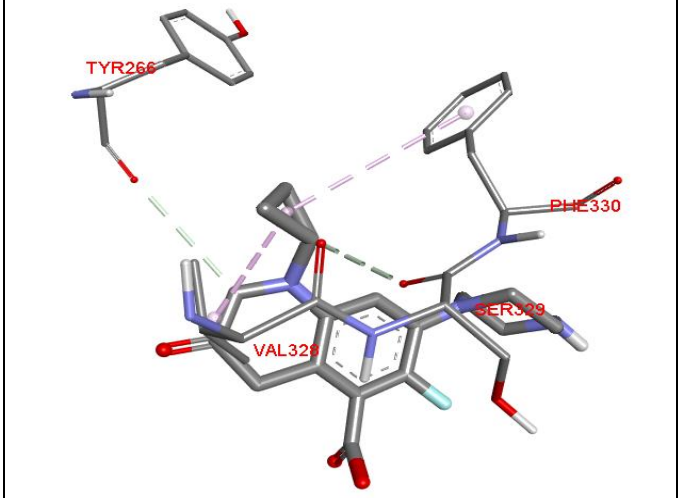
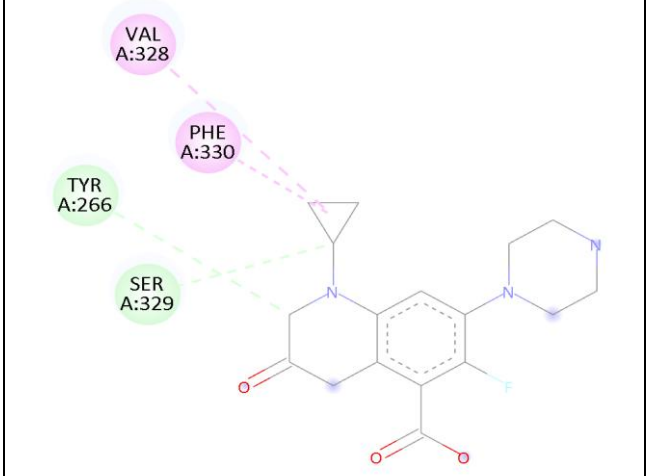
Complex 2 - **4WMZ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

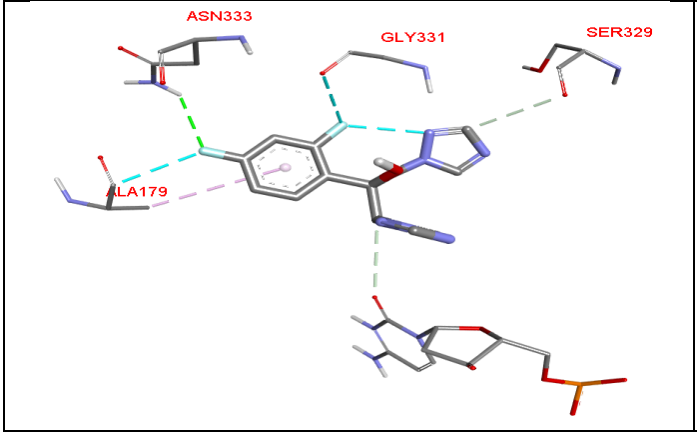
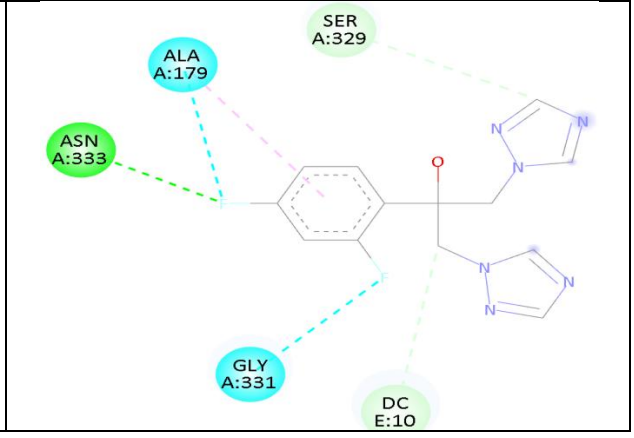
Ampicillin – **6RKS**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

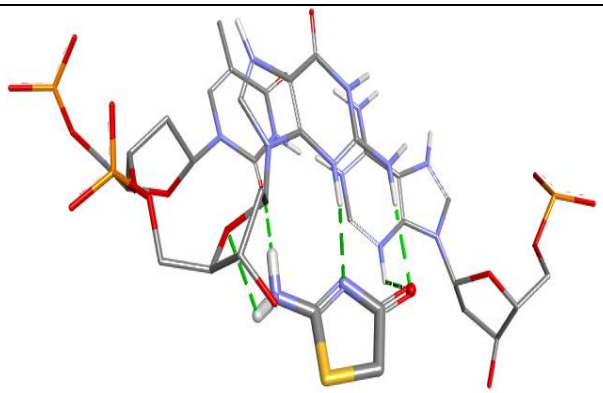
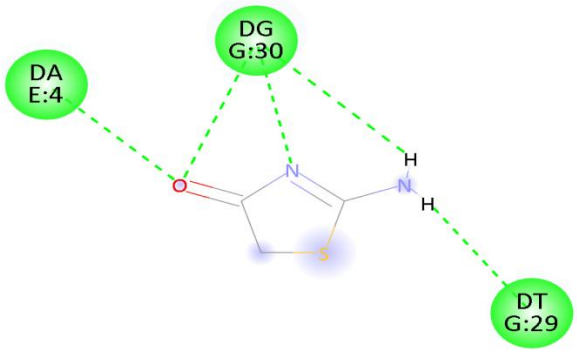
Ciprofloxacin - **6RKS**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

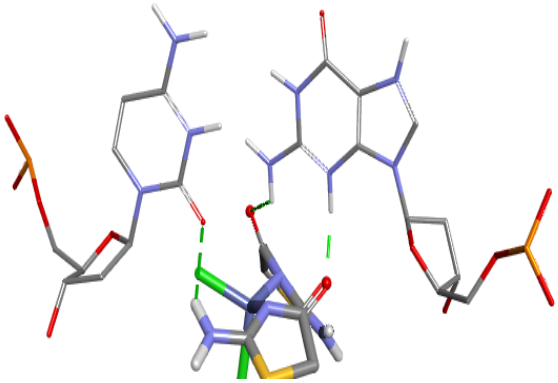
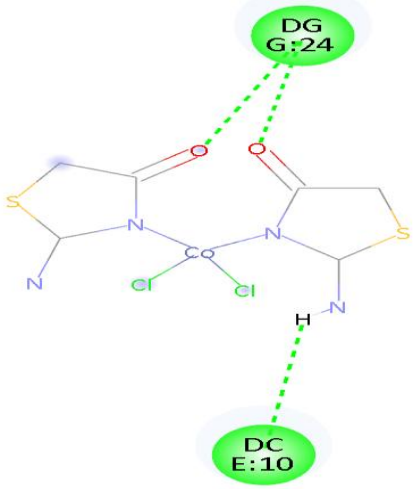
Fluconazole - **6RKS**

3D-visualizitaion of “ligand – amino acids” interactions	2D-visualizitaion of “ligand – amino acids” interactions
	

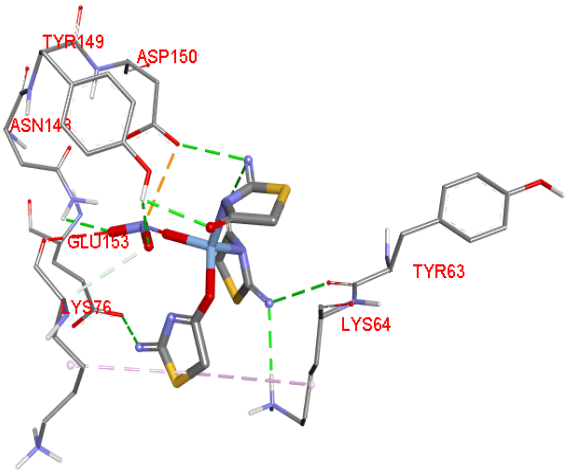
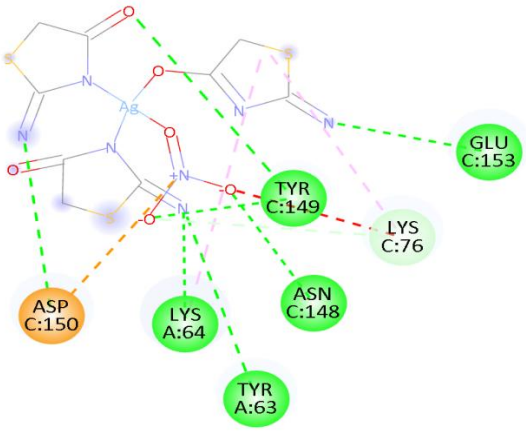
2-Amino-4-thiazolinone (L1) - **6RKS**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

Complex 1 - **6RKS**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

Complex 2 - **1VQQ**

3D-visualizitaion of "ligand – amino acids" interactions	**2D-visualizitaion of "ligand – amino acids" interactions**
	

T a b l e S1

Intermolecular interactions formed by ligand L_1, complexes $[Co(L_1)_2Cl_2]$ and $[Ag(L_1)_3NO_3]$, and reference drugs with target proteins (PDB IDs: 6RKS, 2XCT, 2EXB, 1VQQ, and 4WMZ)

Ligand	Receptor	Conventional Hydrogen Bond	Pi-Pi Stacked	Pi-sigma	Pi-Anion	Pi-Cation	Pi-Alkyl	Pi-Sulfur	Alkyl	Attractive Charge	Carbon Hydrogen Bond	Unfavorable Acceptor-Acceptor	Unfavorable Donor-Donor	Halogen
L_1	**6RKS**	-	-	-	-	-	-	-	-	-	-	-	-	-
Complex **[Co(L_1)$_2$Cl$_2$]**	**6RKS**	-	-	-	-	-	-	-	-	-	-	-	-	-
Complex **[Ag(L_1)$_3$NO$_3$]**	**6RKS**	TYR149,GLU153,ASN148,LYS64,TYR63	-	-	-	-	-	-	LYS64	ASP150	LYS76	LYS76	-	-
Ciprofloxacin	**6RKS**	-	-	-	-	-	VAL328,PHE330	-	-	-	TYR266,SER329	-	-	-
Ampicillin	**6RKS**	ARG738,TYR149,LYS65,TYR63	-	-	-	-	LYS76	-	-	-	LYS65	-	LYS64	-
Fluconazole	**6RKS**	ASN333	-	-	-	-	-	-	-	SER329	-	-	-	ALA179,GLY331
L_1	**2XCT**	THR1181	-	-	-	-	-	-	-	-	-	-	-	-
Complex **[Co(L_1)$_2$Cl$_2$]**	**2XCT**	SER1330,ASN1182	-	-	-	-	-	-	-	-	-	-	-	-
Complex **[Ag(L_1)$_3$NO$_3$]**	**2XCT**	THE1329	-	-	-	-	-	-	-	-	-	-	-	-
Ciprofloxacin	**2XCT**		-	-	-	-	-	-	-	-	-	-	-	-
Ampicillin	**2XCT**	GLY1332	-	-	-	-	PHE1331,VAL1268,PRO1326	-	-	-	PHE1331,SER1330	-	-	PHE1266,GLN1267
Fluconazole	**2XCT**	SER1173	-	-	-	-	-	-	-	-	-	-	-	-
L_1	**2EXB**	-	PHE160	LEU359	-	-	ALA61,LEU421	-	-	-	SER306	-	-	GLY358,ARG361,LEU359
Complex **[Co(L_1)$_2$Cl$_2$]**	**2EXB**	SER420,SER62,ASN308	-	-	-	-	-	-	-	-	SER420	-	-	-
Complex **[Ag(L_1)$_3$NO$_3$]**	**2EXB**	PHE105,ILE141,ASN281,HIS320	-	-	-	-	HIS320	-	-	ARG104,ASP138	-	-	-	-
Ciprofloxacin	**2EXB**	ARG361,SER357,SER62,SER306,LYS305	PHE160	PHE160	-	-	-	-	-	-	-	-	-	ASN308
Ampicillin	**2EXB**	ASN227	-	SER253	-	-	LEU226	-	ALA252,ILE137	-	SER253	-	-	-
Fluconazole	**2EXB**		PHE160	LEU359	-	-	LEU421,ALA61	-	-	-	SER306	-	-	LEU359,ARG361,GLY358

L_1	**1VQQ**	TRP616,SER400, GLN521,GLU602	-	-	-	-	-	-	-	-	-	-	-	-
Complex **[Co(L_1)$_2$Cl$_2$]**	**1VQQ**	LYS219, LYS215	-	-	-	-	-	TYR373	-	-	-	-	-	-
Complex **[Ag(L_1)$_3$NO$_3$]**	**1VQQ**	GLN140	-	-	-	-	-	-	-	ARG65, ASP139, ASP304, HIS129, GLU61	SER141	GLN140	-	-
Ciprofloxacin	**1VQQ**	HIS143, SER141, ASP304	-	-	ARG65	-	-	-	ILE69	-	ASP304, GLU61	-	-	-
Ampicillin	**1VQQ**	LYS215	-	-	A221	-	VAL217	-	PRO370, LEU224	-	-	-	-	-
Fluconazole	**1VQQ**	GLY282,ASN393, TYR366		LYS281	-	-	-	-	-	-	LEU391,GLN396	-	GLY282	-
L_1	**4WMZ**	HIS381,SER382, SER508	-	-	-	-	-	PHE384	-	-	-	-	-	-
Complex **[Co(L_1)$_2$Cl$_2$]**	**4WMZ**	SER508,PHE506, THR507,HIS381	-	-	-	-	-	-	-	-	-	-	-	-
Complex **[Ag(L_1)$_3$NO$_3$]**	**4WMZ**	ILE471,CYS470, TYR140,HIS468, ARG385	-	-	TYR126	-	-	-	LEU383	-	CYS470	-	-	-
Ciprofloxacin	**4WMZ**	MET509,HIS381, PHE506	TYR72	-	-	-	-	-	PHE241,LEU95,PHE384	-	-	-	-	PHE506
Ampicillin	**4WMZ**	SER508	-	MET509	-	-	-	-	PRO238, LEU380	-	HIS381	-	-	-
Fluconazole	**4WMZ**	-	PHE241	LEU95	-	HIS381	PRO238	-	-	-	THR507	-	-	-