SUPPLEMENTARY FILE

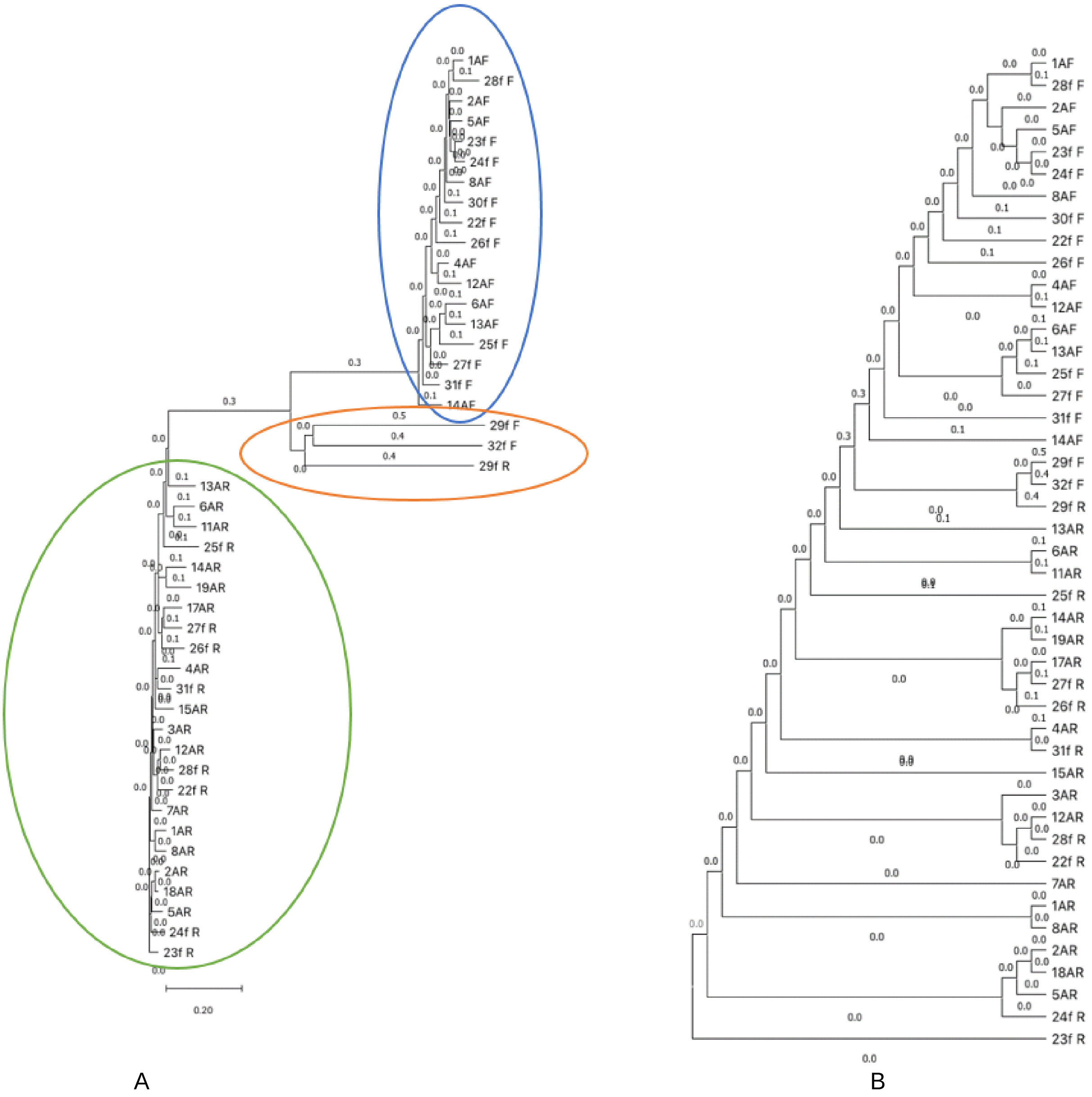


Figure 1. The phylogenetic trees of the *gyrA* gene sequences of the patients. A) the standard clustering tree, and the colored circles show the distinct variants of the *gyrA gene*. B) The time cohort trees

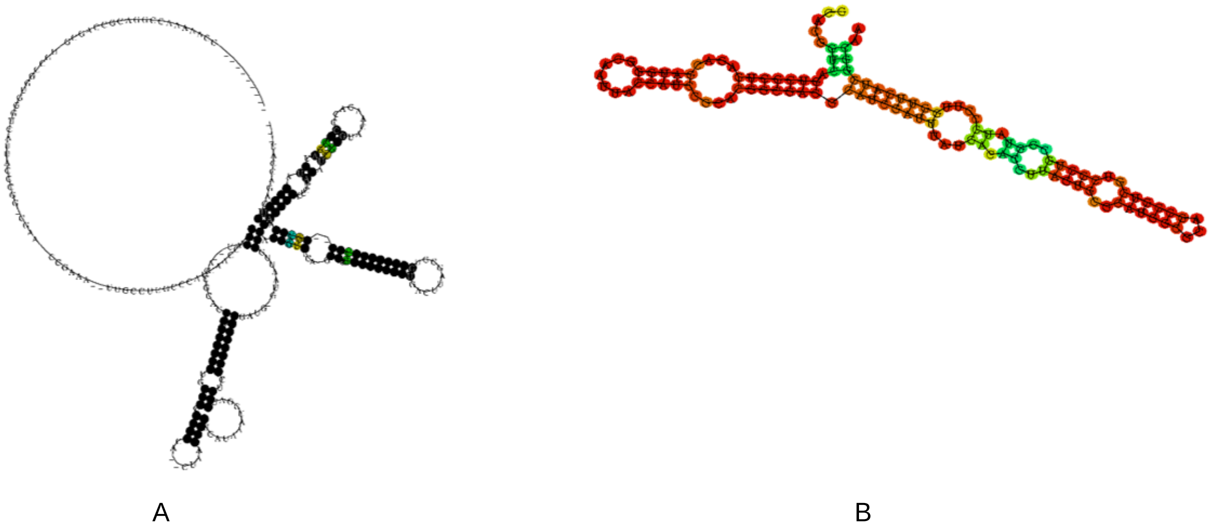
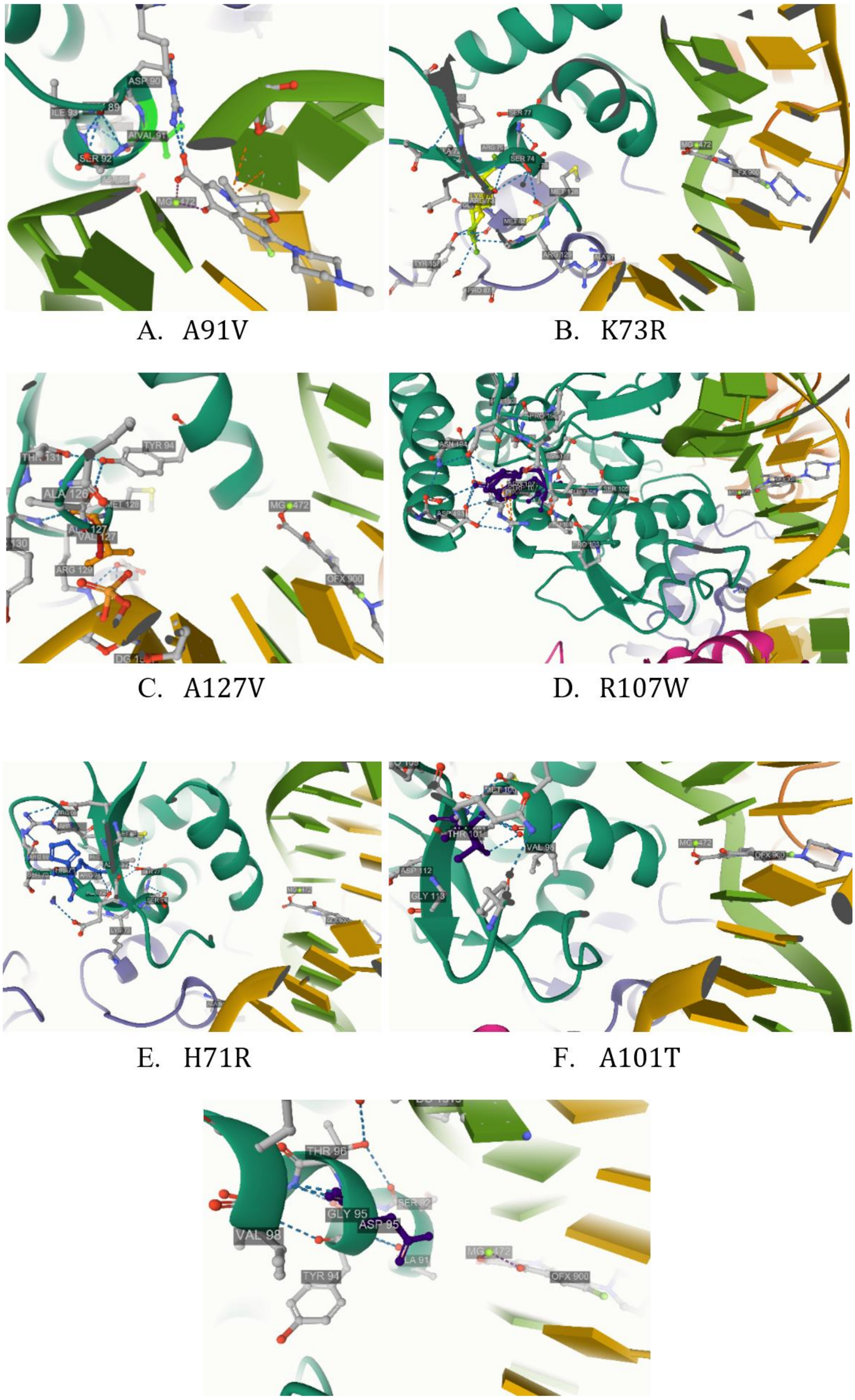


Figure 2. The 2D structures of the mRNA for the gyrA gene. A) The conserved structure of the gyrAfrom the patients. B) The refseq structure from the gene bank (Accession ID: X87124.1)



A. A91V

B. K73R

C. A127V

D. R107W

E. H71R

F. A101T

G. D95G

Figure 3. Comparison of the positions of wild type and mutant residues in the 3D structure of M. leprae gyrase DNA. The A91V mutant was used as a comparison against the mutants obtained

Table. I Impact of each mutant on *M. leprae* gyrase DNA

No	**Mutation**	**Distance from Ofloxacin**	**mCSM ($\Delta\Delta G$)**		**Encom $\Delta\Delta S_{Vib}$ Prediction:**		**Overall Impact of the Mutation**	**PUBMED Reference for the Mutation (PMID):**
			Result (Kcal/mol)	**Impact**	**Result (Kcal/mol/K)**	**Impact**		
1	A91V	**3.5 Å**	**-0.322**	Destabilizing	0.068	Increase in Molecular Flexibility	High Impact	23356028
2	K73R	**18.1 Å**	**-0.281**	Destabilizing	**-0.391**	Decrease in Molecular Flexibility	Moderate Impact	No
3	A127V	**12.3 Å**	-0.288	Destabilizing	-0.006	Decrease in Molecular Flexibility	Moderate Impact	No
4	R107W	**23.6 Å**	**-0.589**	Destabilizing	**-0.316**	Decrease in Molecular Flexibility	Moderate Impact	No
5	H71R	**23.4 Å**	**-0.717**	Destabilizing	**0.18**	Increase in Molecular Flexibility	High Impact	No
6	A101T	**17.3 Å**	**-1.445**	Destabilizing	**-0.27**	Decrease in Molecular Flexibility	Moderate Impact	No
7	D95G	**4.8 Å**	**-0.993**	Destabilizing	**0.146**	Increase in Molecular Flexibility	High Impact	No