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Computational study of binding of oseltamivir to neuraminidase mutants of influenza A virus

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Supporting Information

Computational Study of Binding of Oseltamivir to Neuraminidase Mutants of Influenza A Virus

Table and Figure Legends

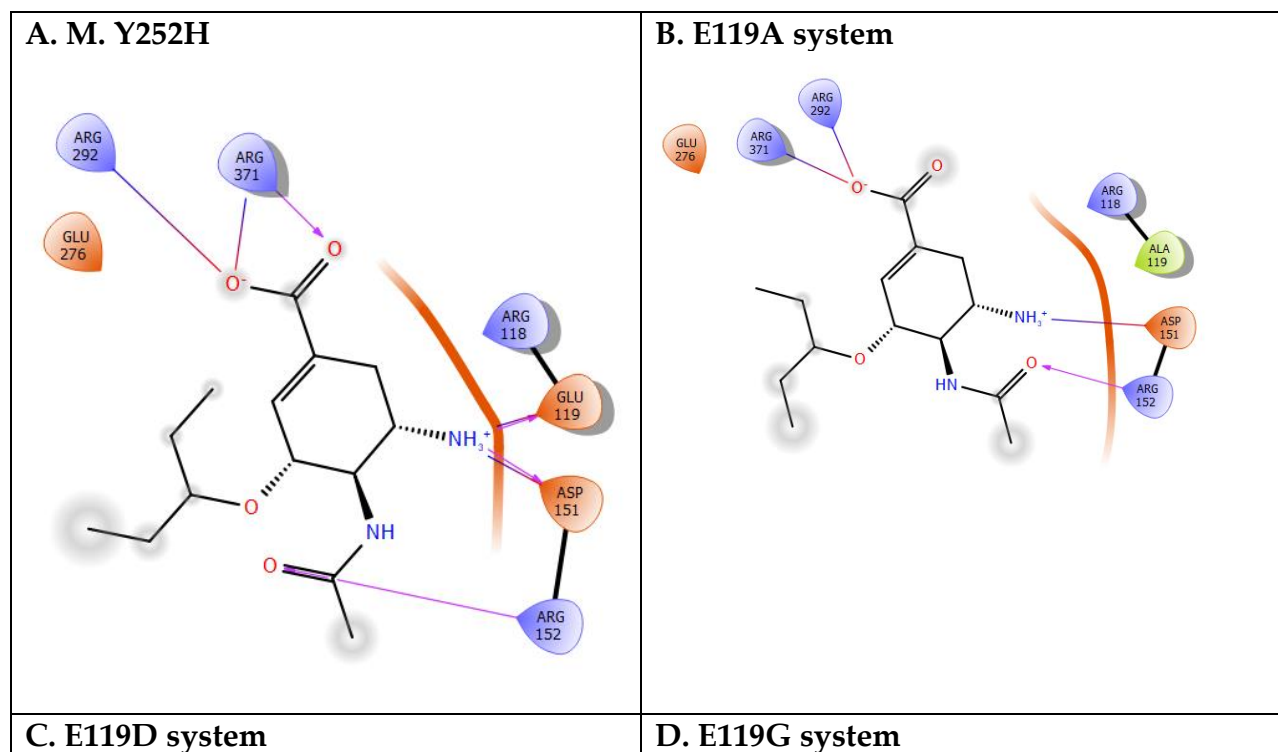
Table S1. The XP-docked energy of Oseltamivir to WT and mutants systems.

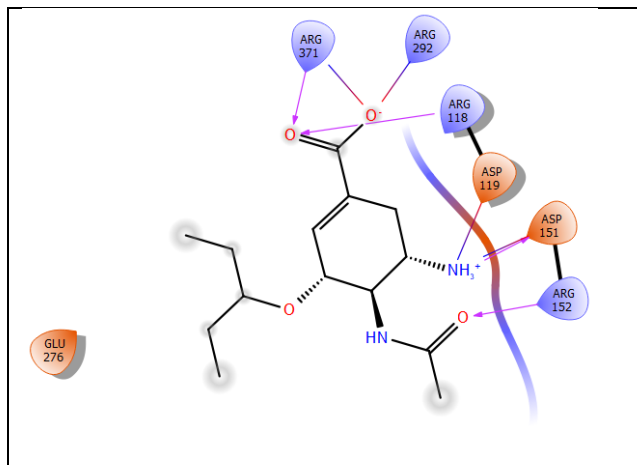
Figure S1. The 2D interaction of Oseltamivir in mutant systems.

Figure S2. The active site conformation and 2D interactions of E119A-OTV (B), E119D-OTV (C), E119G-OTV (D), H274Y-OTV (E), I117T-OTV (F), I117V-OTV (G), I117V-E119A-OTV (H), K150N-OTV (I), N294S-OTV (J), R292K-OTV (K), V116A-OTV (L), Y252H-OTV (M) systems taken from most populated cluster.

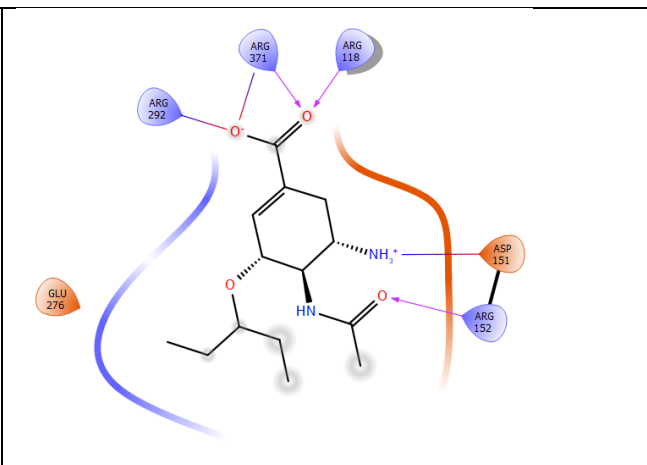
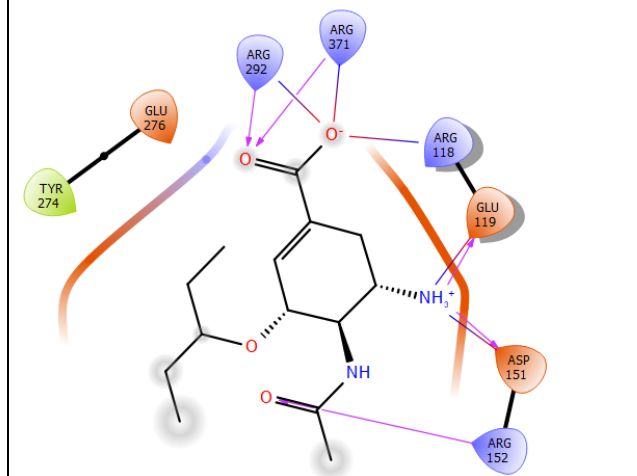
Table S1. The XP-docked energy of Oseltamivir to WT and mutants systems.

No.	System	XP (kcal/mol)
1.	WT	-12.857
2.	E119A	-7.760
3.	E119D	-11.683
4.	E119G	-7.860
5.	H274Y	-10.575
6.	I117T	-10.887
7.	I117V	-10.898
8.	I117V-E119A	-7.647
9.	K150N	-10.999
10.	N294S	-10.947
11.	R292K	-10.534
12.	V116A	-10.825
13.	Y252H	-11.080

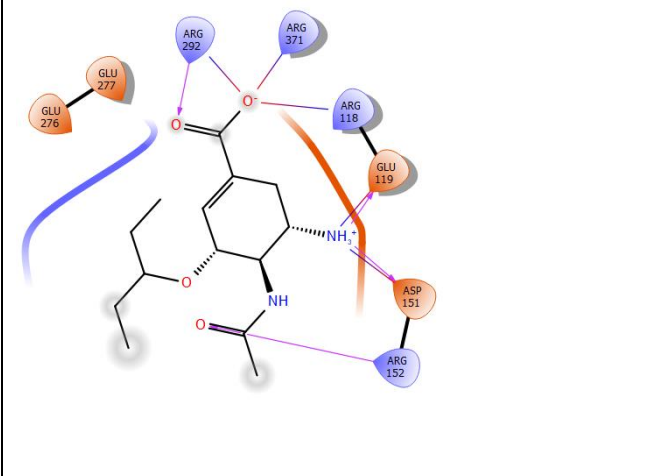




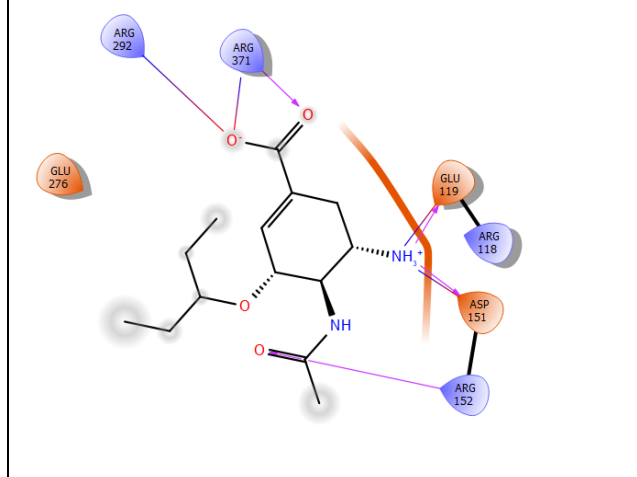
E. H274Y system



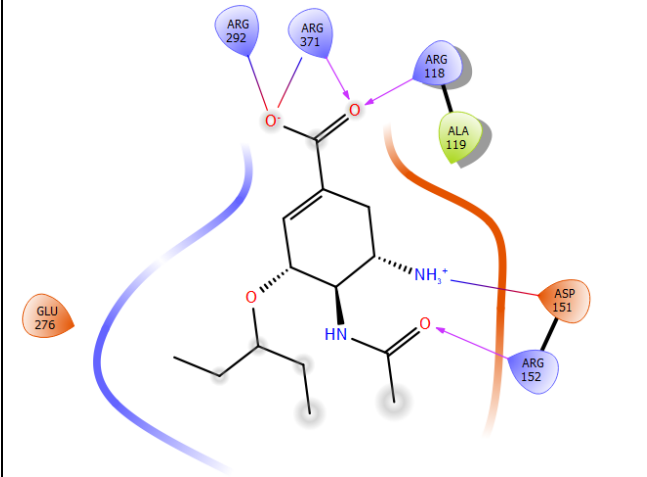
F. I117T system



G. I117V



H. I117V-E119A



I. K150N system

J. N294S

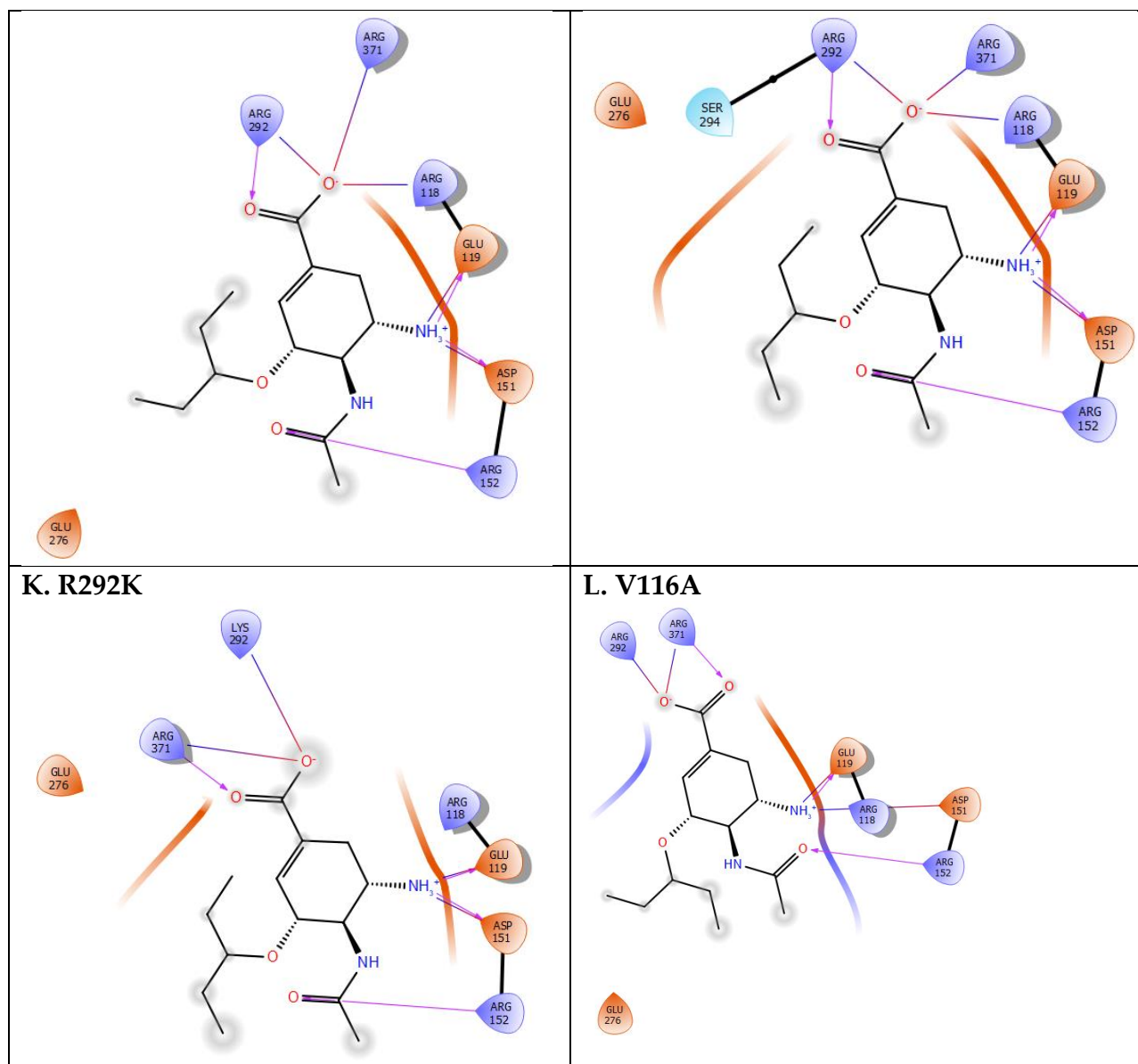
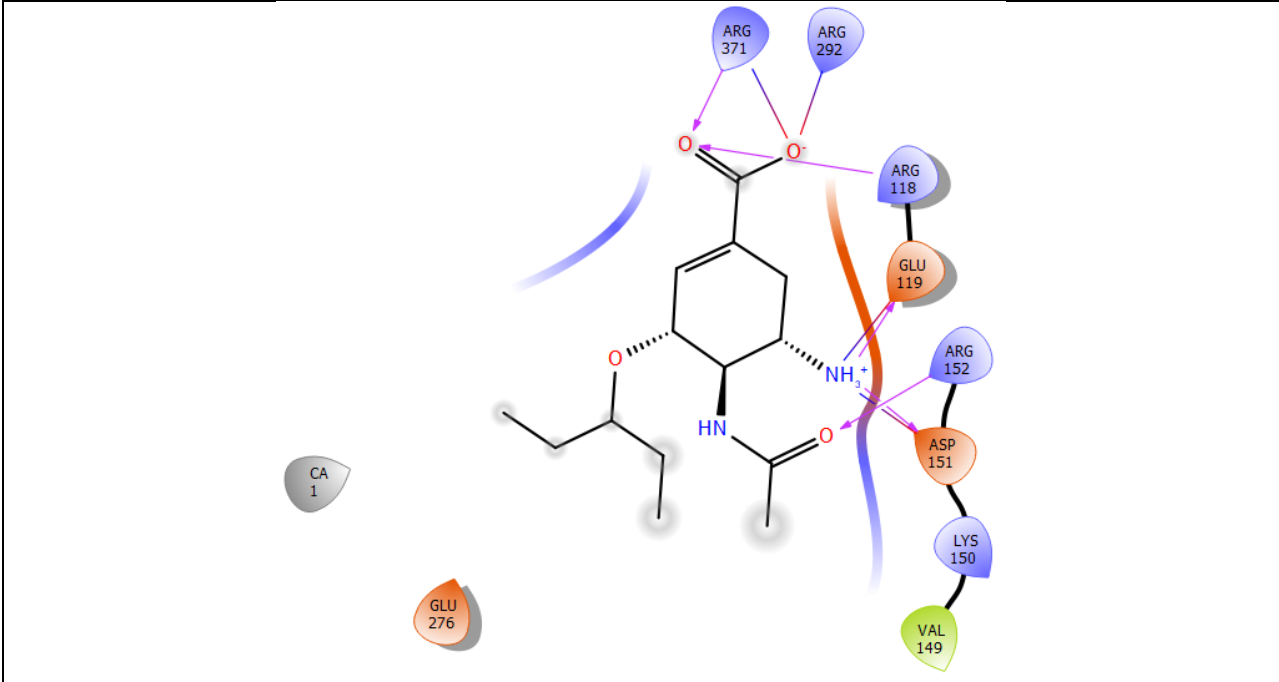
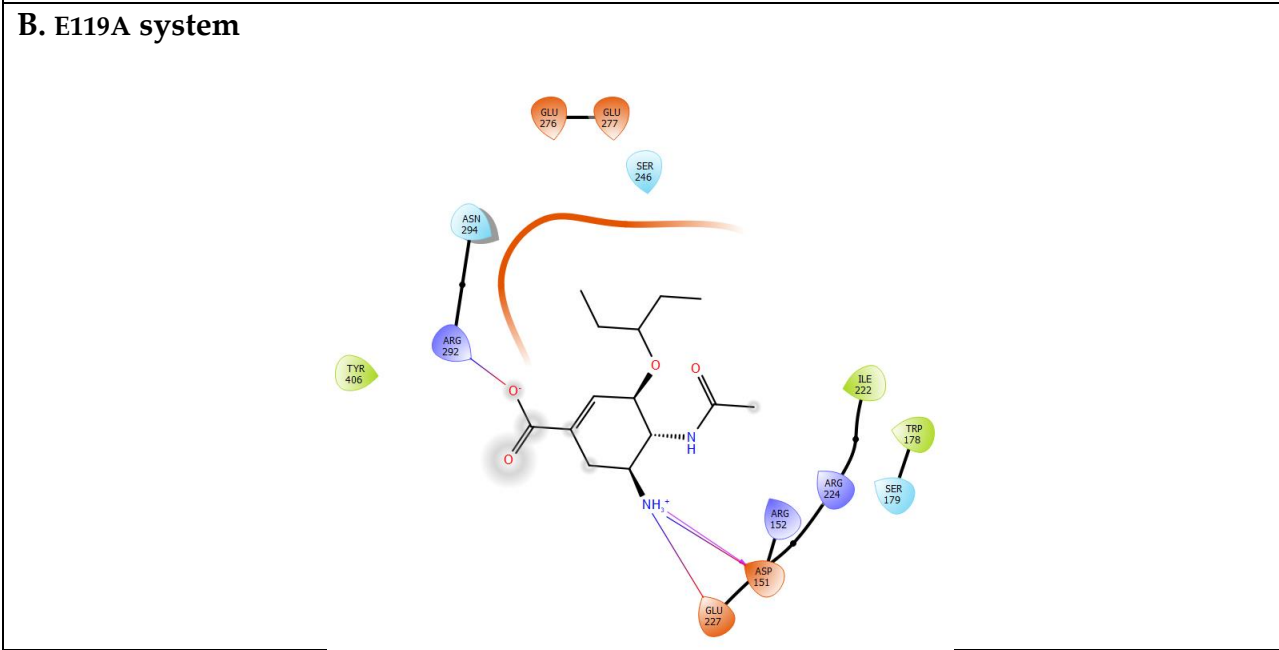


Figure S1. The 2D interaction of Oseltamivir in mutant systems.

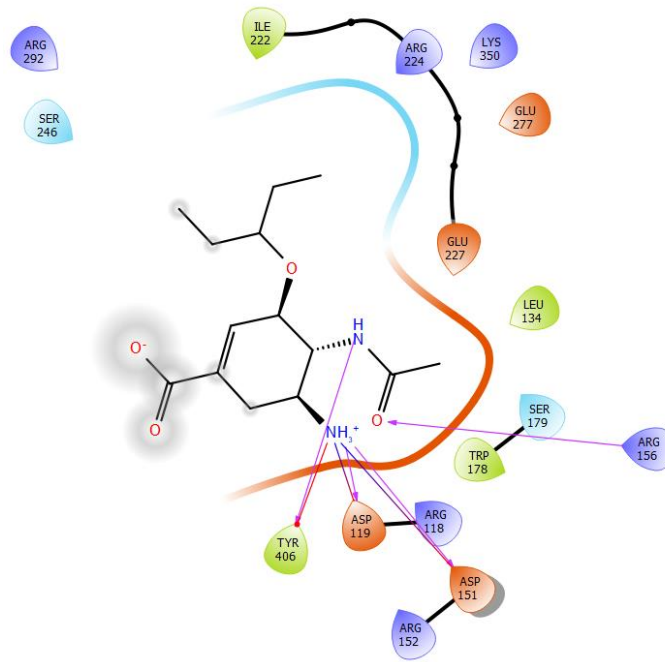
A. WT system



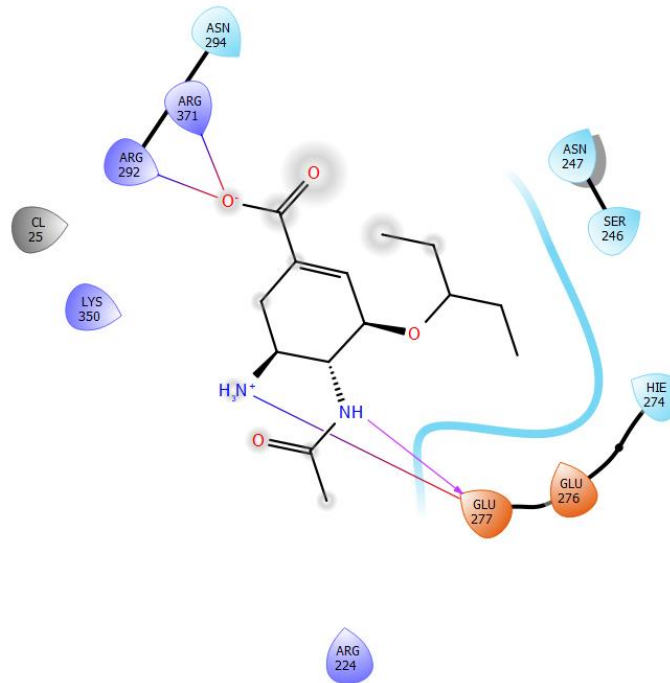
B. E119A system



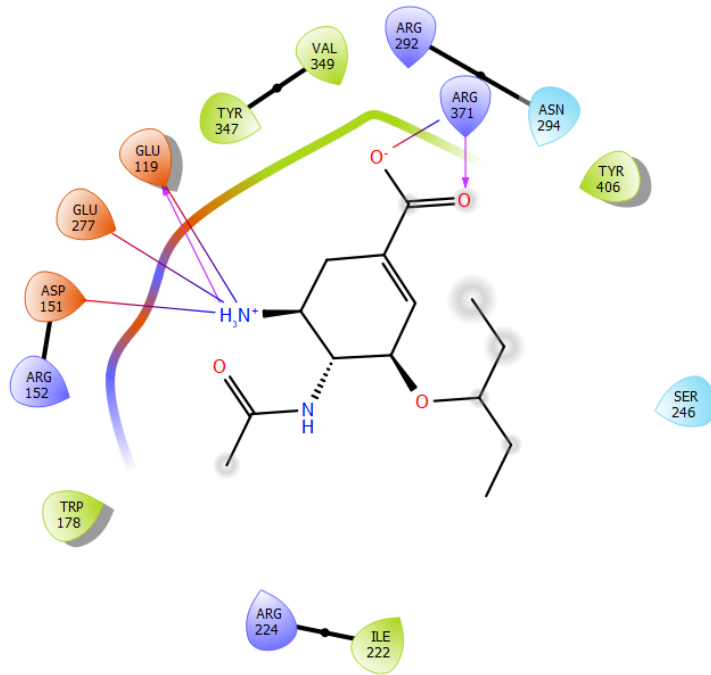
B. E119D system



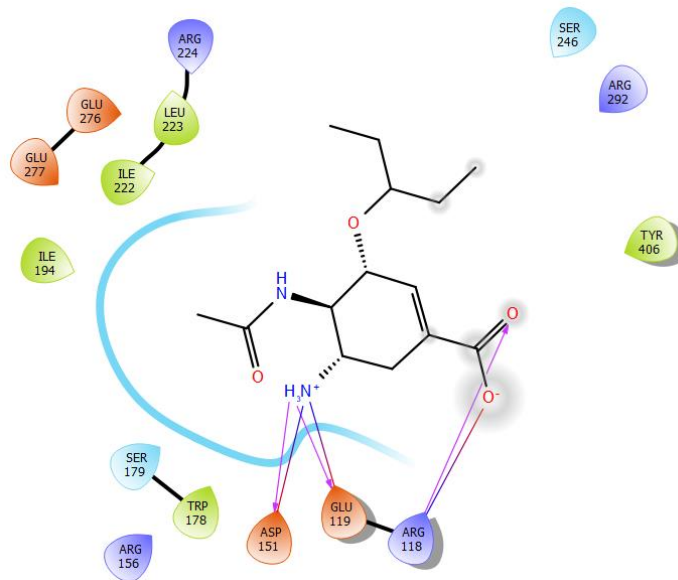
C. E119G system



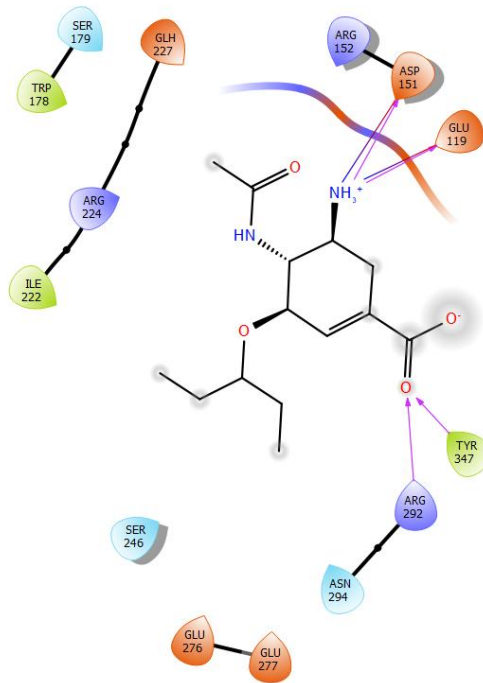
D. H274Y system



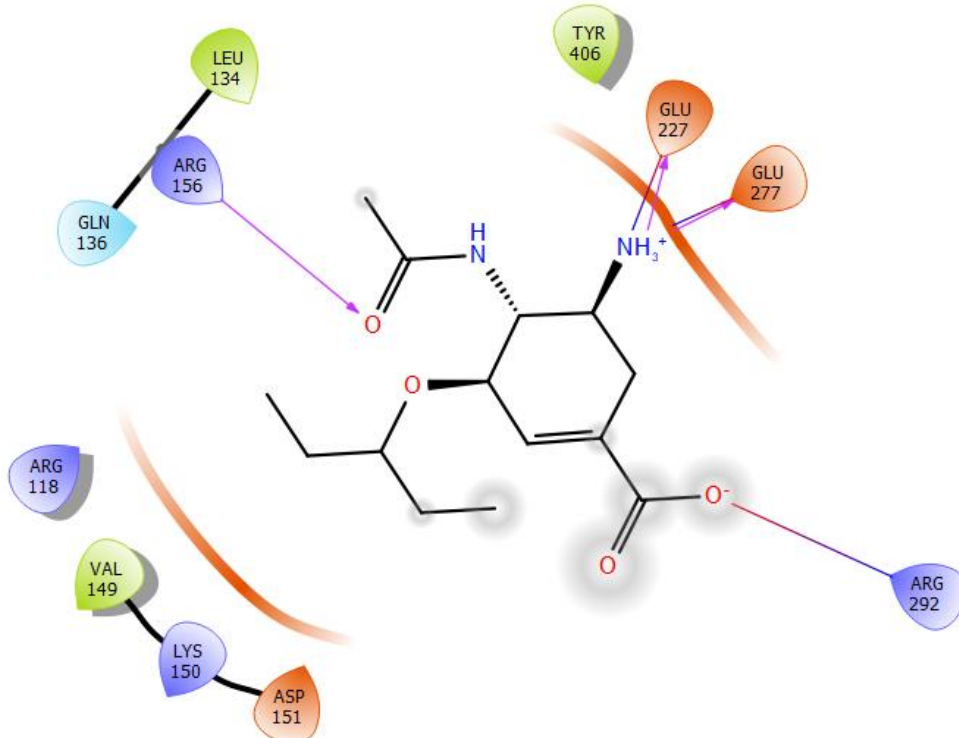
E. I117T system



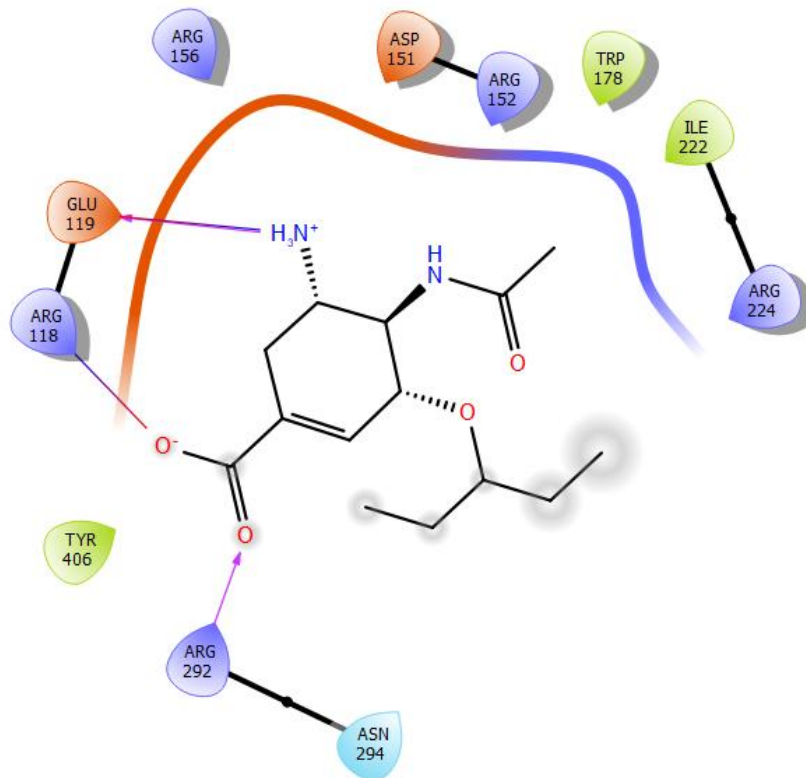
E. I117V



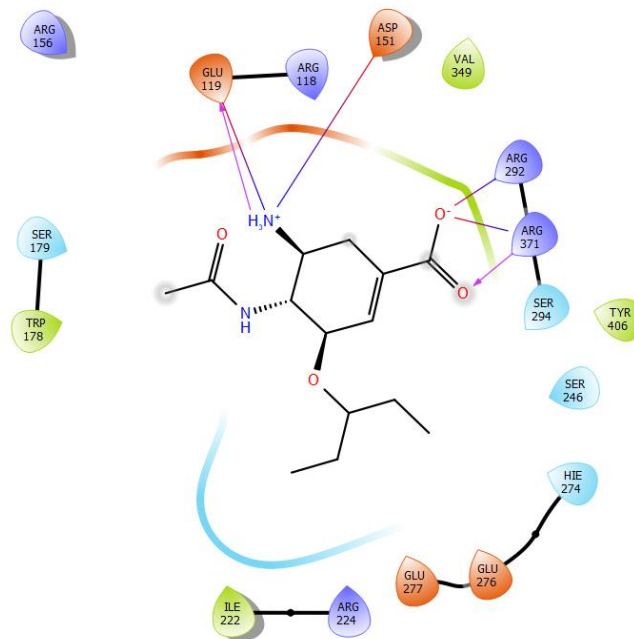
G. I117V-E119A



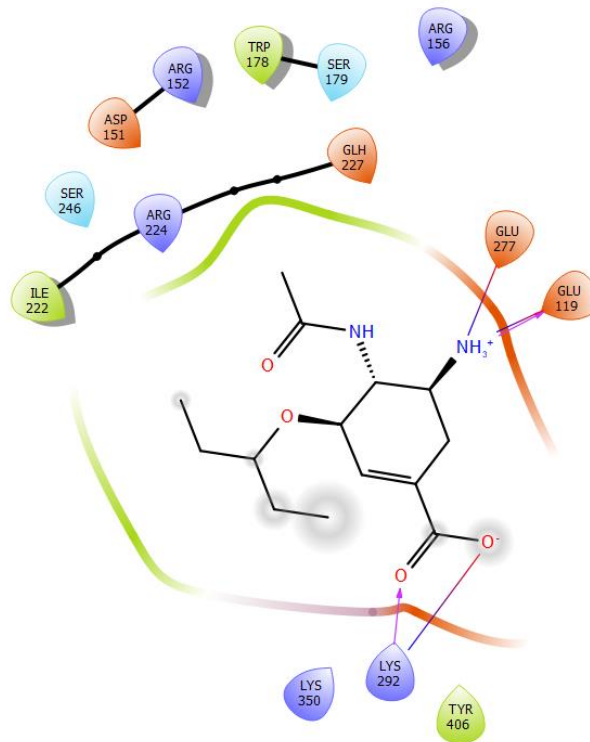
H. K150N



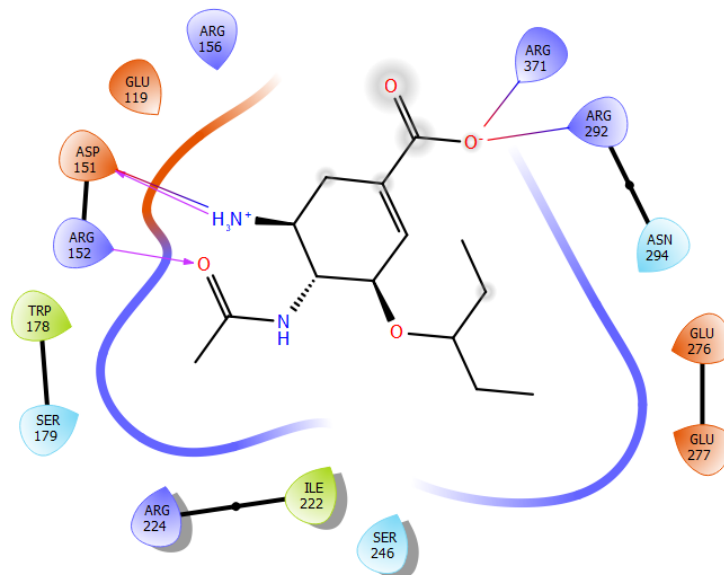
I. N294S



J. R292K



K. V116A



L. Y252H

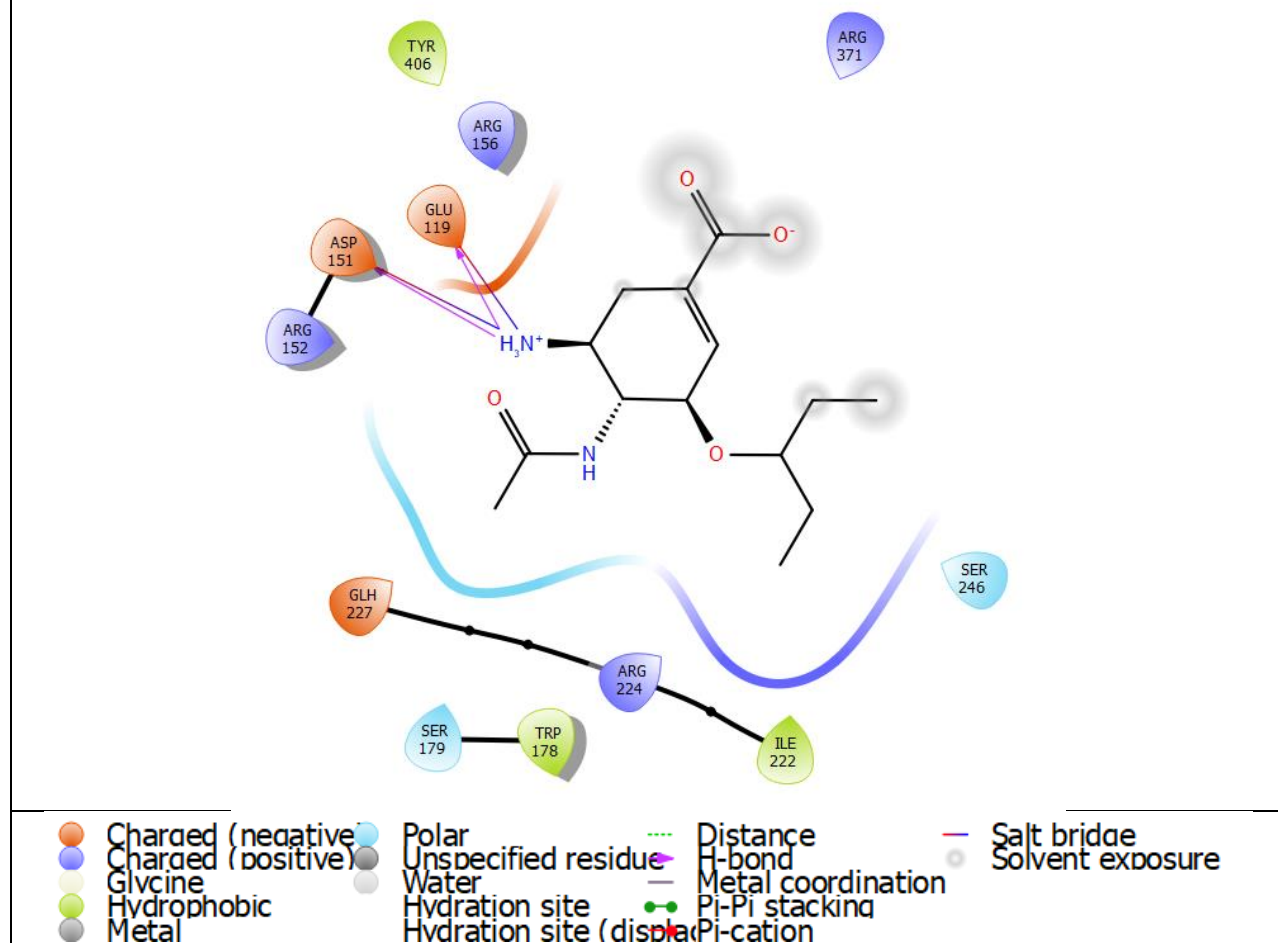


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