Table S2. Comparisons of the hydrogen bonds of five compounds between the dengue E protein and TetR protein

| | DV E protein [a] | | | | TetR protein[b] |
|---|---|---|---|---|---|
| | Tetracycline | Oxytetracycline | Rolitetracycline | Doxycycline | Chlortetracycline |
| Number of Hydrogen Bonds | 7 | 9 | 8 | 8 | 6 |
| Backbone | 4 | 5 | 6 | 5 | 1 |
| Side chain | 3 | 4 | 2 | 3 | 5 |
| Hydrogen Bonding to Backbone | Ala50O[c]-4N[d], 3.59[e]<br>Phe279O-10OH, 2.61<br>Phe279O-11O, 3.46<br>Thr48O-12αOH, 2.37 | Thr48O-4N, 3.62<br>Ala50N-4αOH, 3.01<br>Thr48O-4αOH, 3.14<br>Thr48O-12OH, 2.33<br>Phe279O-11O, 2.62 | Ala50N-1O, 2.77<br>Thr48O-2N, 3.17<br>Ala50O-10OH, 3.49<br>Ala50O-11O, 3.22<br>Ala50O-12OH, 2.97<br>Ala50N-12O, 3.16 | Thr48O-1O, 3.62<br>Ala50N-1O, 2.76<br>Ala50N-12OH, 3.20<br>Ala50N-12αOH, 3.09<br>Thr48O-12αOH, 3.29 | Thr103O-10OH, 3.64 |
| Hydrogen Bonding to Side Chain | Gln271OE-2N, 2.62<br>Gln200NE-3OH, 2.67<br>Thr280OG-11O, 2.68 | Gln271OE-2N, 2.89<br>Gln200NE-3OH, 3.33<br>Thr280OG-11O, 3.01<br>Thr280OG-12OH, 2.92 | Gln200NE-6OH, 3.06<br>Glu49OE2-12αOH, 3.20 | Gln200NE-6OH, 3.14<br>Glu49OE2-10OH, 3.14<br>Glu49OE2-11O, 3.57 | Gln116NE2-2O, 3.27<br>His64NE2-3OH, 2.71<br>Asn82ND2-3OH, 2.82<br>Asn82OD2-4N, 2.70<br>His100NE2-12OH, 2.92 |

[a] The docked conformations against DV E protein (PDB entry 1OKE[3]).

[b] Tet-repressor protein (PDB entry is 2TRT [33]).

[c] Atom name of a residue and the number denotes the residue number in the target protein.

[d] Atom name of a compound and the number denotes the atom number in a compound.

[e] Distance of a pair of atoms forming a hydrogen bond between the protein and ligand.