

Supplementary Information for

**Assessing the Role of Residue Phe108 of Cytochrome P450 3A4 in
Allosteric Effects of Midazolam Metabolism**

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Fig. S3. Complex models and residue structures. The complex models constructed in this study: (A) the CYP3A4-MDZ-MDZ complex; (B) the CYP3A4-MDZ-TST complex. (C) Structures of F108 and mutant residues A108, M108, and W108. The S-MDZ, E-MDZ, and TST are shown in orange, yellow, and cyan, respectively.

Table S1. The length of 2a and 2f channels in the wild-type and mutation systems (Å).

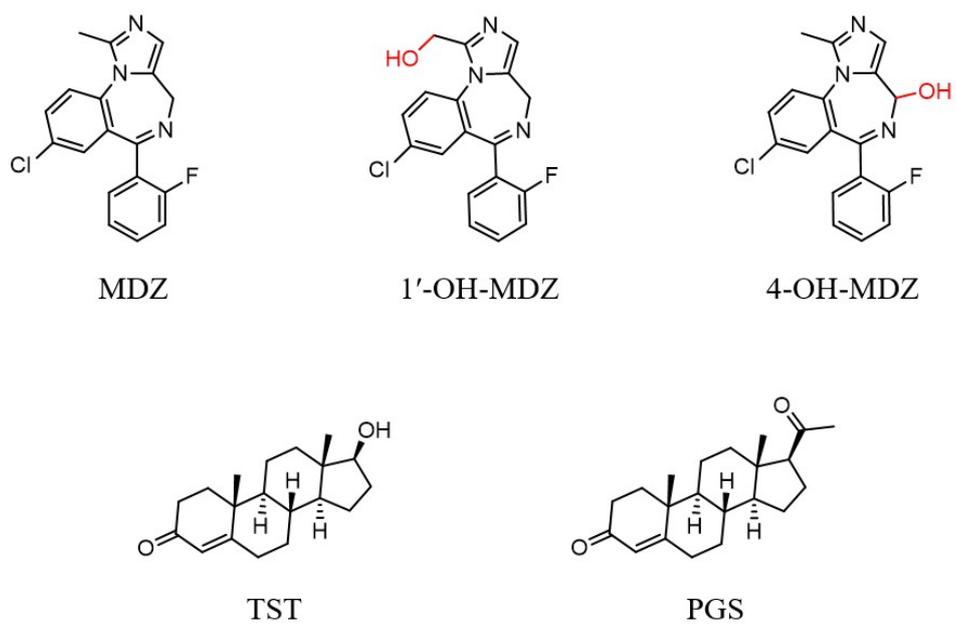


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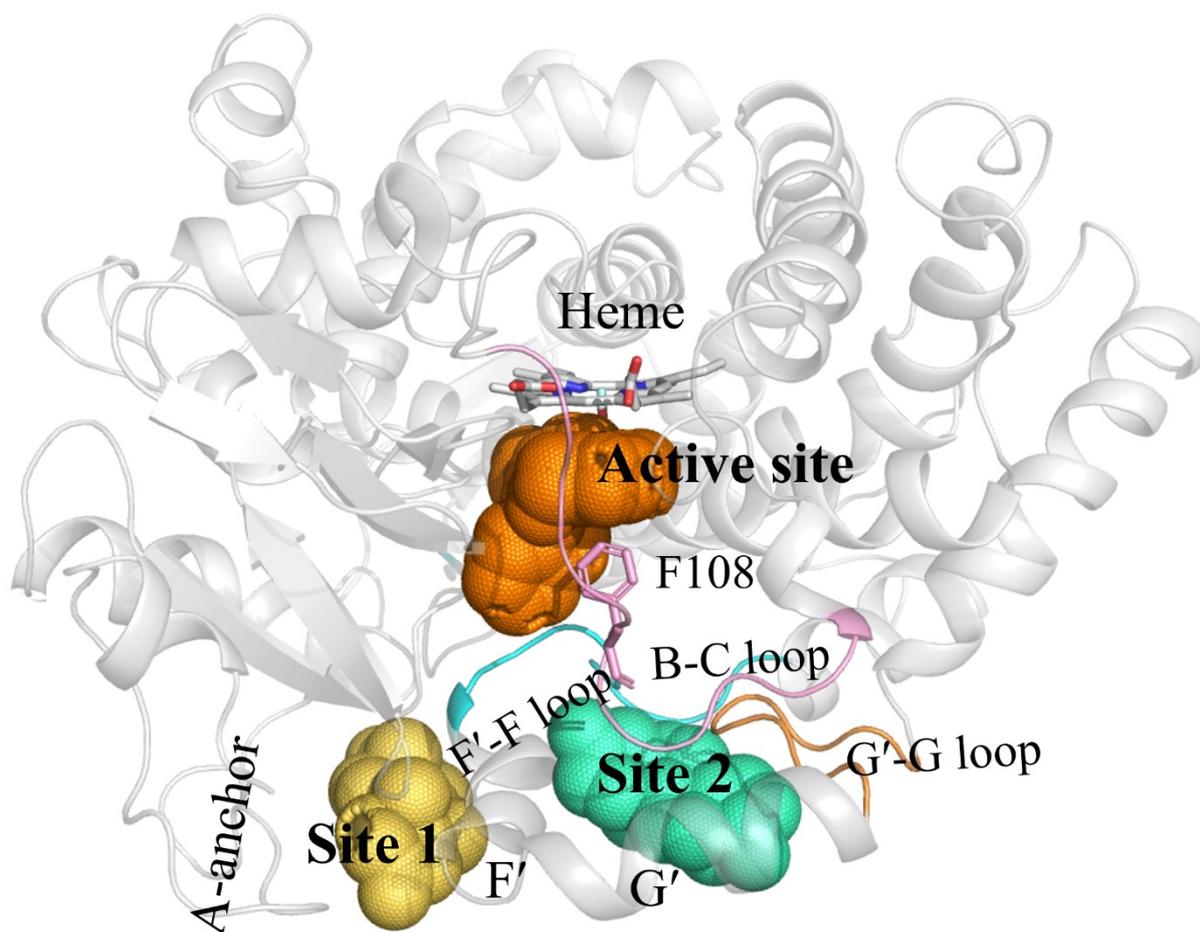


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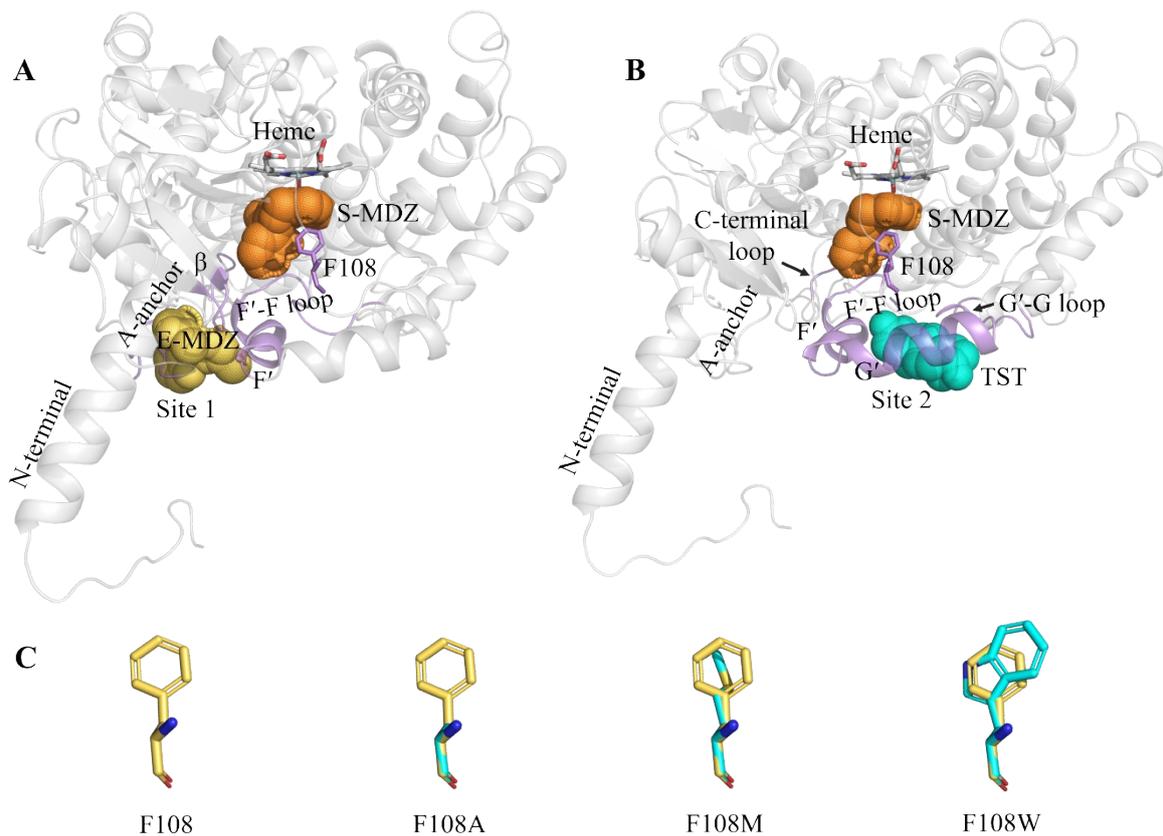


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Systems	2a	2f
CYP3A4-MDZ-TST	31.19	32.25
F108A-MDZ-TST	19.63	
F108M-MDZ-TST	28.47	23.24
F108W-MDZ-TST	16.31	27.16