

Supplementary Information for:

Do mammalian cytochrome P450s exhibit multiple ligand access pathways and ligand channelling?

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The supplementary information consists of three movies supplied in MPEG format showing two trajectories of the substrate DMZ leaving the active site of CYP2C5 by pathway 2c.

The first 2 movies are shown viewed down the I-helix with exit via pw2c towards the viewer.

The third movie shows the same trajectory as movie 2 but with the view rotated ca. 90 degrees to the left about the vertical axis showing exit via pw2c to the left.

The heme is shown in white, the substrate in yellow and the protein ribbon trace in magenta.

In movies 2 and 3, four protein side-chains (V106: green; K241: cyan, K108: cyan, E:282, pink) are shown so that the disruption of hydrogen bonds between the BC loop and the G and I helices during ligand egress can be observed.

The parameters used for the simulations are: movie1: $A = 0.25$, $N = 40$, $r_{\min} = 0.005$; movie 2 and 3 $A = 0.25$, $N = 80$, $r_{\min} = 0.005$. The variation in the K241-V108 hydrogen bond length is shown for these two trajectories in Figure 4 (trajectory ** corresponds to movie 1; trajectory * to movies 2 and 3).

File sizes: Movie1: 3.2 MB, Movies 2 and 3: 2.1MB each.