Supplementary Material

Detection of a high-barrier conformational change in the active site of cytochrome P450$_{cam}$ upon binding of putidaredoxin

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1) AMBER 8 (D. Case et al., UCSF, 2004) script for dynamics run

2) Selected dynamics tracks

3) ^{1}H, ^{13}C HSQC of perdeuterated CYP101-CO-bound camphor

AMBER control file (sander script)

```
Minimization without Cartesian restraints
 &cntrl
   imin = 0,
   ntb = 0, igb = 0,
   ntpr = 100, ntwx=100, ntwv=100, ntwe=100, ntave=100,
ntwr=100, ntwr=500,
   ntt = 3, gamma_ln = 1.0,
   tempi = 300.0, temp0 = 300.0
   nstlim = 1000000000, nscm=500, dt = 0.002,
   cut = 12.0,
   nmropt=2, pencut=-0.001, ipnlty=1,
 /
 &ewald
     eedmeth=5,
 /

 &wt type='SHIFTS',
istep1=0,istep2=1000000000,value1=1.0,value2=1.0, /
 &wt type='END' /
```

LISTIN=POUT
LISTOUT=POUT
SHIFTS=./rel_camshf2

non-NMR constraint energy

RMSD all backbone

Ring current shift constraint violation, cam methyls

Fe-CO---H5(exo) CAM distance