S2 Table. The parameters used to do the fitting by Berkeley modenna (Up numbers) and the parameters observed after the fitting (Down number). The range of $k_{s\text{-}f}$ and $k_{f\text{-}s}$ used for fitting was board (Table 1, highlight), whereas the fitting showed closed value to the predicted, this indicated the conformational selection model was the most dominant process of CsA binding to Cyp18 in aqueous solution.

CsA/Cyp18	Cyp18 (nM)[a]	CsA (nM)[a]	$k_{on\text{-}fast}(nM^{-1}s^{-1})$[b]	koff(s^{-1})[b]	$k_{f\text{-}s}(s^{-1})$[c]	$k_{s\text{-}f}(s^{-1})$[c]
1.6	450 ~ 550 503.74	344.88 ~ 421.52 383.91	0.00792-0.00876 0.00833	0.0647-0.0715 0.0700	**0.000825-0.0825** **0.00794**	**0.000758-0.0758** **0.00709**
1.4	450 ~ 550 507.77	301.77 ~ 368.83 352.22				
1.2	450 ~ 550 520.11	258.66 ~ 316.44 315.00				
1.0	450 ~ 550 525.00	215.55 ~ 263.45 245.00				
0.8	450 ~ 550 503.30	172.44 ~ 210.76 200.91				
0.6	450 ~ 550 492.59	129.33 ~ 158.07 143.91				
0.4	450 ~ 550 504.58	86.22 ~ 105.38 104.78				

a. For Cyp18, the concentration range: 500 nM X 0.9 ~ 500 nM X 1.1.
   For CsA, the concentration range: 500 nM X ratio X 0.479 X 0.9 ~ 500 nM X ratio X 0.479 X 1.1
b. The range: the obtained value X 0.95 ~ the obtained value X 1.05
c. The range: the obtained value X 0.1 ~ the obtained value X 10