S3 Table

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| --- | --- | --- |
| **Energy component** | **DiCDD** | **TCDD** |
| **pCYP1A1** | **pCYP1A2** | **pCYP1B1** | **pCYP1A1** | **pCYP1A2** | **pCYP1B1** |
| $$ΔG\_{elec+vdw+rest}^{prot}$$ | -16.300±0.073 | -22.369±0.022 | -19.325±0.082 | -21.809±0.063 | -23.335±0.013 | -20.141±0.071 |
| $$ΔG\_{elec+vdw}^{solv}$$ | 2.611±0.014 | 2.611±0.014 | 2.611±0.014 | 2.497±0.016 | 2.497±0.016 | 2.497±0.016 |
| $$ΔG\_{rest}^{solv}$$ | 6.906 | 6.980 | 7.092 | 7.055 | 6.894 | 7.167 |
| $$ΔG\_{binding}^{0}$$ | **-6.783±0.074** | **-12.778±0.026** | **-9.622±0.083** | **-12.145±0.065** | **-13.671±0.02** | **-10.477±0.073** |

$ΔG\_{elec+vdw+rest}^{prot}$– ligand decoupling from complex; $ΔG\_{elec+vdw}^{solv}$ – ligand decoupling from solution; $ΔG\_{rest}^{solv}$– ligand restraints added to decoupled ligand; $ΔG\_{binding}^{0}$– absolute binding free energy, $ΔG\_{binding}^{o}=ΔG\_{elec+vdw+rest}^{prot}+ΔG\_{elec+vdw}^{solv}+ΔG\_{rest}^{solv}$

DiCDD – 2,7-dichlorodibenzo-*p*-dioxin, TCDD – 2,3,7,8-tetrachlorodibenzo-*p*-dioxin