MUE: 1.41 [1.04, 1.77] MSE: -1.39 [-1.67, -0.95] ρ: 0.98 [0.96, 0.99] τ: 0.88 [0.76, 0.99]  $(\Delta G_{vac \rightarrow sol}^{ML/MM} - \Delta G_{vac \rightarrow sol}^{EXP})^2$  [kcal.mol<sup>-1</sup>] 5.0 thioanisole 1-propanethiol benzamide 2.5 aniline pyridine 0.0 acetonitrile  $\Delta G_{vac o so/}^{ML/MM}$  [kcal.mol<sup>-1</sup>] m-hydroxybenzaldehyde -2.5 ethylphenylether 2-pentanone -5.0 methylbenzoate methylpentanoate 1 4-dioxane -7.5 aceticacid o-cresol -10.0 methanol water -12.5naphthalene benzene n-octane -15.0 n-pentane 0.7 8.0 -15 -10 -5 1.0 0 0.9  $arepsilon^{-1}$  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>] Patched Model ( $\varepsilon^{-1} = 0.9$ ) Patched Model ( $\varepsilon^{-1} = 0.8$ ) R<sup>2</sup>: 0.95 [0.88, 0.98] R<sup>2</sup>: 0.95 [0.90, 0.98] RMSE: 0.97 [0.74, 1.21] RMSE: 1.26 [0.94, 1.55] MUE: 1.11 [0.87, 1.42] MUE: 0.83 [0.61, 1.11] MSE: -0.99 [-1.36, -0.56] MSE: -0.62 [-0.92, -0.22] ρ: 0.98 [0.94, 0.99] ρ: 0.98 [0.95, 0.99] τ: 0.86 [0.73, 0.97] τ: 0.87 [0.76, 0.98] 5.0 5.0 2.5 2.5 0.0 0.0  $\Delta G_{vac o sol}^{ML/MM}$  [kcal.mol<sup>-1</sup>] -2.5 -2.5-5.0-5.0-7.5 -7.5-10.0 -10.0-12.5-12.5-10 -10-5 -15  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>]  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>] Patched Model ( $\varepsilon^{-1} = 0.7$ ) Patched Model ( $\varepsilon^{-1} = 0.6$ ) R<sup>2</sup>: 0.95 [0.89, 0.98] R<sup>2</sup>: 0.95 [0.91, 0.98] RMSE: 0.78 [0.60, 0.93] RMSE: 0.74 [0.55, 0.91] MUE: 0.58 [0.38, 0.80] MUE: 0.66 [0.47, 0.82] MSE: -0.27 [-0.54, 0.05] MSE: 0.04 [-0.21, 0.49] ρ: 0.98 [0.94, 0.99] ρ: 0.97 [0.95, 0.99]  $\tau$ : 0.87 [0.76, 0.97]  $\tau$ : 0.88 [0.77, 0.99] 5.0 5.0 2.5 2.5 0.0 0.0 -2.5-2.5-5.0-5.0-7.5-7.5-10.0-10.0-12.5-12.5-15.0-15.0 -15 -10 -5 -15 -10 -5 0 0 5  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>]  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>] Patched Model ( $\varepsilon^{-1} = 0.4$ ) Patched Model ( $\varepsilon^{-1} = 0.5$ ) R<sup>2</sup>: 0.95 [0.88, 0.98] R<sup>2</sup>: 0.95 [0.87, 0.98] RMSE: 0.82 [0.56, 1.06] RMSE: 1.00 [0.75, 1.22] MUE: 0.66 [0.47, 0.85] MUE: 0.81 [0.59, 1.07] MSE: 0.36 [0.01, 0.69] MSE: 0.66 [0.29, 1.00] ρ: 0.97 [0.94, 0.99] ρ: 0.97 [0.95, 0.99]  $\tau$ : 0.88 [0.75, 0.99]  $\tau$ : 0.88 [0.72, 0.99] 5.0 5.0 2.5 2.5 0.0 0.0 -2.5-2.5-5.0-5.0-7.5-7.5-10.0 -10.0 -12.5 -12.5 -15.0 -15.0 -10 -15 -10 -155  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>]  $\Delta G_{vac \rightarrow sol}^{EXP}$  [kcal.mol<sup>-1</sup>]

Patched Model ( $\varepsilon^{-1} = 1.0$ )

R<sup>2</sup>: 0.95 [0.90, 0.98] RMSE: 1.63 [1.31, 1.89]