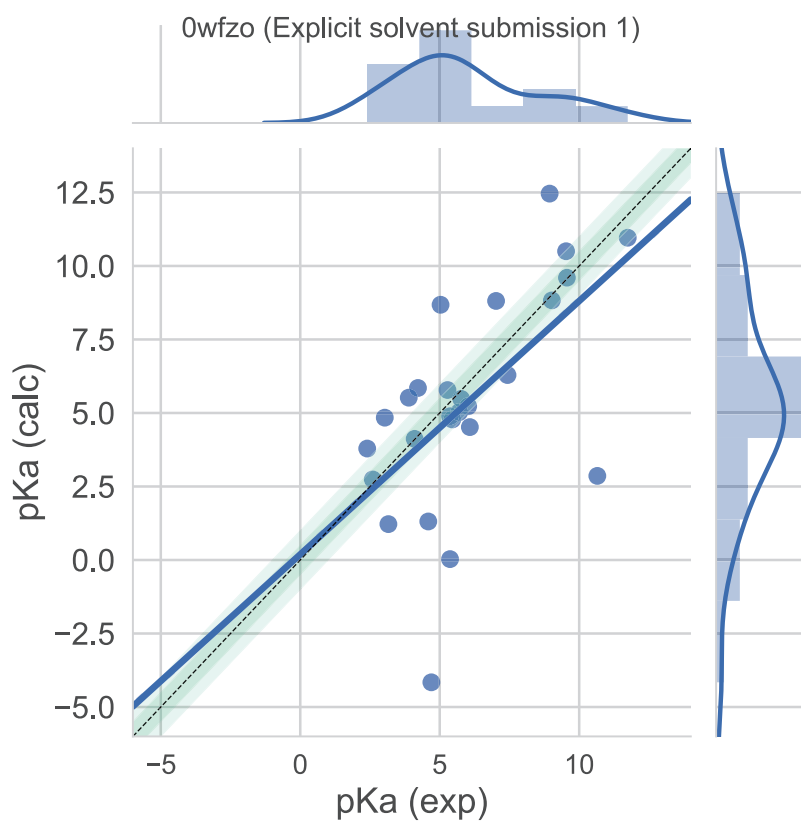
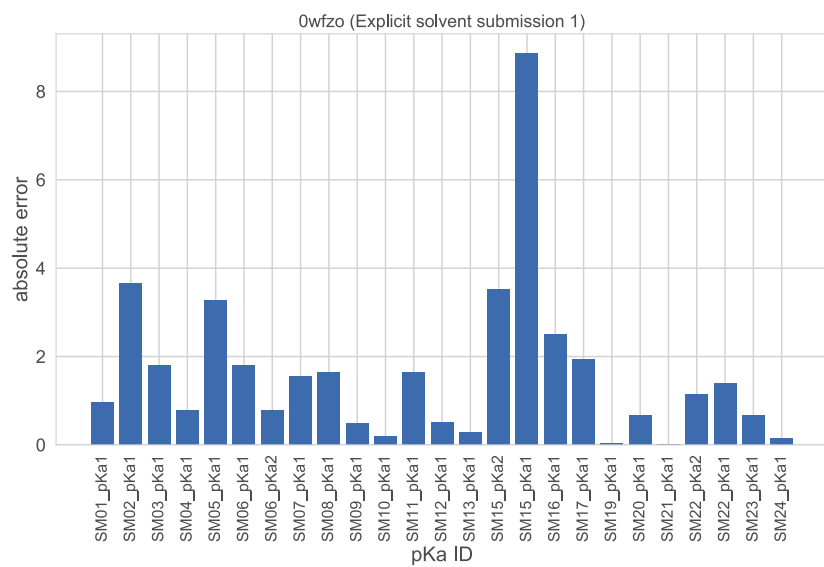


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Supplementary Information



**Fig. 1** Supplementary Figure. Plot of the hungarian analysis scheme and experimental pKa values. Plot courtesy of the organizers [https://github.com/MobleyLab/SAMPL6/blob/master/physical\\_properties/pKa/analysis/analysis\\_of\\_typeI\\_predictions/analysis\\_outputs\\_hungarian/pKaCorrelationPlots/0wfzo.pdf](https://github.com/MobleyLab/SAMPL6/blob/master/physical_properties/pKa/analysis/analysis_of_typeI_predictions/analysis_outputs_hungarian/pKaCorrelationPlots/0wfzo.pdf)



**Fig. 2** Supplementary Figure. Plot of the absolute error for each macroscopic pKa being considered. Picture courtesy of the organizers [https://github.com/MobleyLab/SAMPL6/blob/master/physical\\_properties/pKa/analysis/analysis\\_of\\_typeI\\_predictions/analysis\\_outputs\\_closest/AbsoluteErrorPlots/0wfzo.pdf](https://github.com/MobleyLab/SAMPL6/blob/master/physical_properties/pKa/analysis/analysis_of_typeI_predictions/analysis_outputs_closest/AbsoluteErrorPlots/0wfzo.pdf)

**Table 1** Supplementary Table. Calculated pKa and  $\Delta G$  (kcal/mol) for all the microstate pairs considered. Attached csv file