

# A differentiable representation of solvent-solute interface

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## Abstract

The biophysical processes of protein, include ligand binding, protein folding, have attracted lots of interest for decades. Implicit solvent models are widely used to research these processes in silico, as the explicitly solvated protein model is too expensive to be simulated. A critical step of constituting an effective implicit solvent model is representing the solvent-solute interface properly. However, most current representations are based on specific geometric criteria, making the interface derivative hard to calculate. To overcome this difficulty, we introduced a Transformer-like neural network to represent the solvent-solute interface. This network is trained on a dataset containing 8000 all-atom solvated protein models and has a good generalization ability for the untrained protein structure.

## 1 Introduction

Since Max Perutz and John Kendrew resolved the Myoglobin’s structure in 1960<sup>[1;2;3]</sup>, the native structure of protein has attracted many scientists for over six decades, as this knowledge is germane for the advanced research in many area, for example: pharmaceuticals<sup>[4;5;6]</sup>, enzyme catalysis mechanism<sup>[7;8;9;10]</sup>,

## 2 Method

### 2.1 Dataset constitution

### 2.2 Model architecture

## 3 Result

## 4 Conclusion

## References

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