
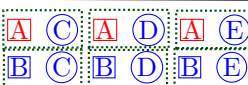
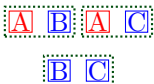
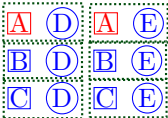


## Additional Ligands Set:

Example Congeneric Series: 

# of Additional	Training Set	Test Set
①		
②		
⋮	⋮	⋮

## BindingDB Congeneric Series

1082 congeneric series

943 unique receptor structures

## External Datasets:

Mobley et al.

1 congeneric series

Wang et al.

8 congeneric series

Schindler et al.

8 congeneric series

## External Datasets Evaluation:

Siamese Network  
Trained on All  
BindingDB Data

no finetune  
(no-shot)

2 ligands

3 ligands

⋮

7 ligands

3 Epoch Finetune Stratified with  
BindingDB Data

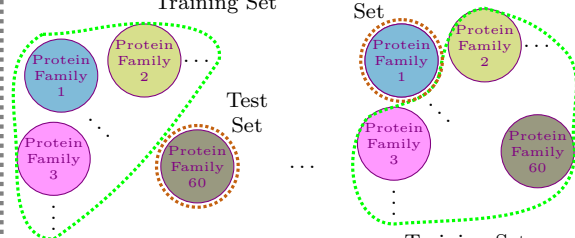
Evaluate on  
congeneric  
series  
remaining after  
removing 7  
ligands

## Leave One Protein Family Out CV:

### No-shot:

Training Set

Test Set



### Few-shot: (1 Additional Ligand Example)

Training Set

Test Set

