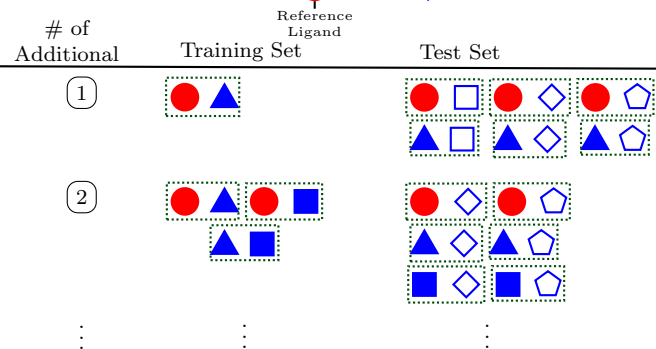


## Retrospective Lead Optimization:

Example Congeneric Series: 



### 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

⋮

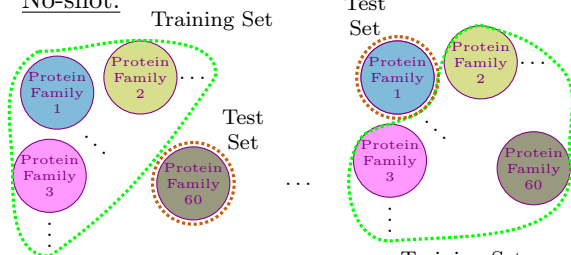
7 ligands

3 Epoch Finetune Stratified with  
BindingDB Data

Evaluate on  
congeneric  
series  
remaining after  
removing 7  
ligands

## Leave One Protein Family Out CV:

No-shot:



Few-shot: (1 Additional Ligand Example)

