

Additional Ligands Set:

Example Congeneric Series: (A) (B) (C) (D) (E)

Reference
Ligand

# 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

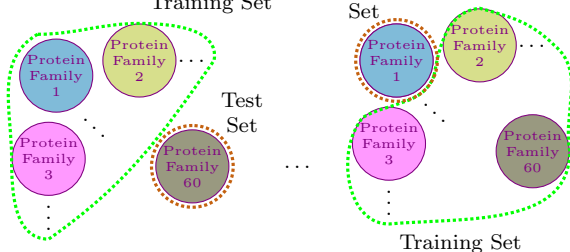
Evaluate on
congeneric
series
remaining after
removing 7
ligands

Leave One Protein Family Out CV:

No-shot:

Training Set

Test
Set



Few-shot: (2 Ligand Example)

Training Set

Test
Set

