

## BindingDB Congeneric Series

1082 congeneric series

943 unique receptor structures

### Leave One Protein Family Out CV:

No-shot:

Training Set

Test Set

Test Set

Training Set

### Additional Ligands Set:

Example Congeneric Series: A B C D E F

Reference  
Ligand

# of  
Additional

Training Set

Test Set

①

A B

<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span>	<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span>	<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>
<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>

②

A B A C  
B C

<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span>	<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>
<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>
<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>

③

A B A C  
A D B C  
B D C D

<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid red; border-radius: 50%; padding: 2px;">A</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">B</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>
<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">C</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">E</span>	<span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">D</span> <span style="border: 1px solid blue; border-radius: 50%; padding: 2px;">F</span>