

## Supplementary Material

### Selectivity mechanism of BCL-XL/2 inhibition through *in silico* investigation

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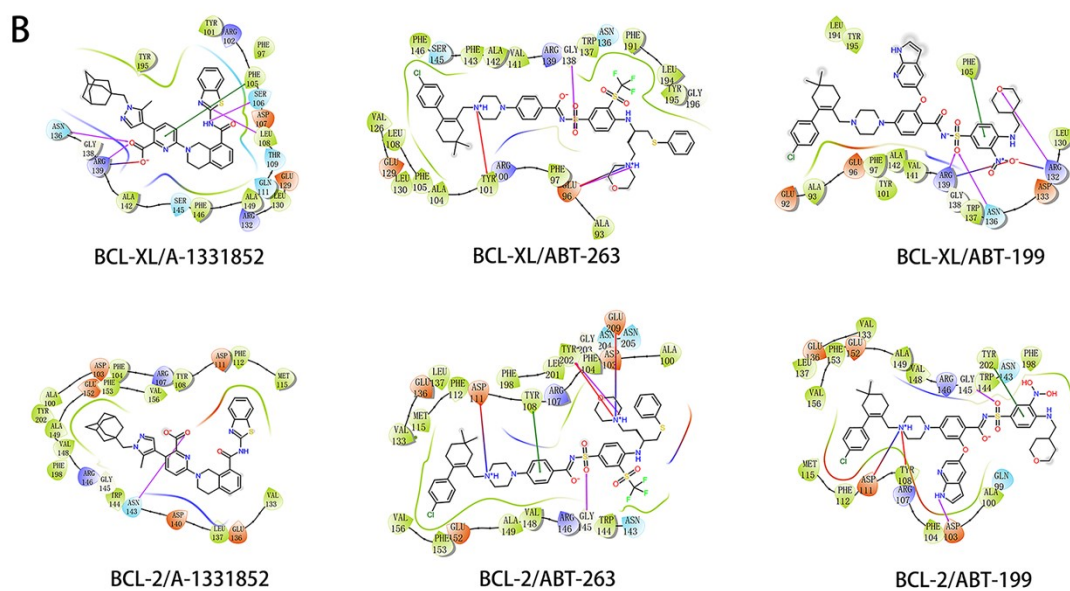
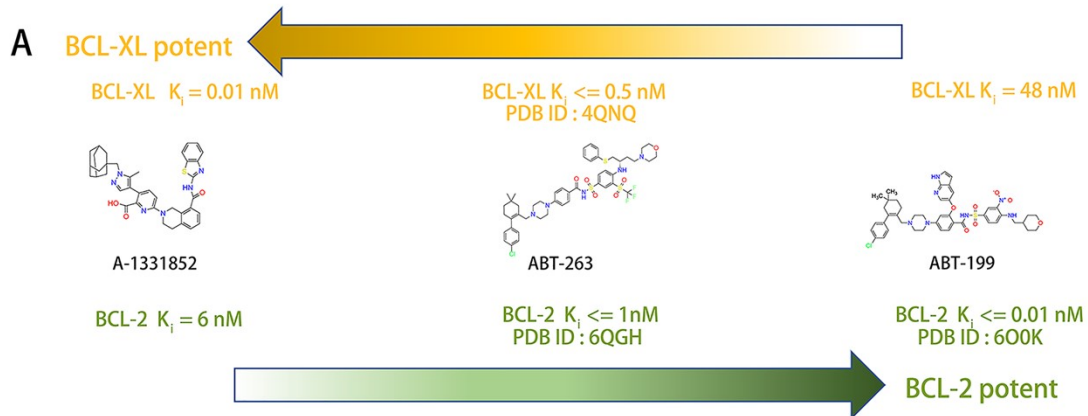
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**Figure S1** Comparison of proteins and inhibitors. (A) Structures of BCL-XL and BCL-2 inhibitors. (B) Ligand interaction diagram.