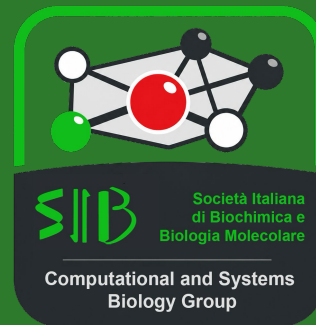


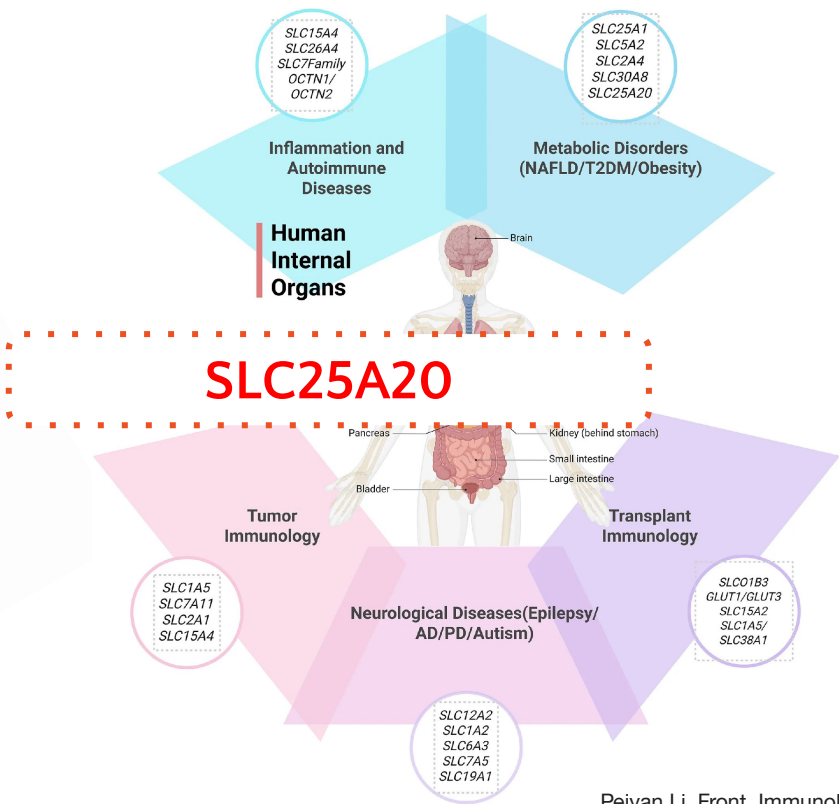
S2 · 12:10–12:25

Combined Computational Modeling and Proteoliposome Nanotechnology to Accelerate Ligand Discovery for Solute Carriers (SLC)

Lara Console

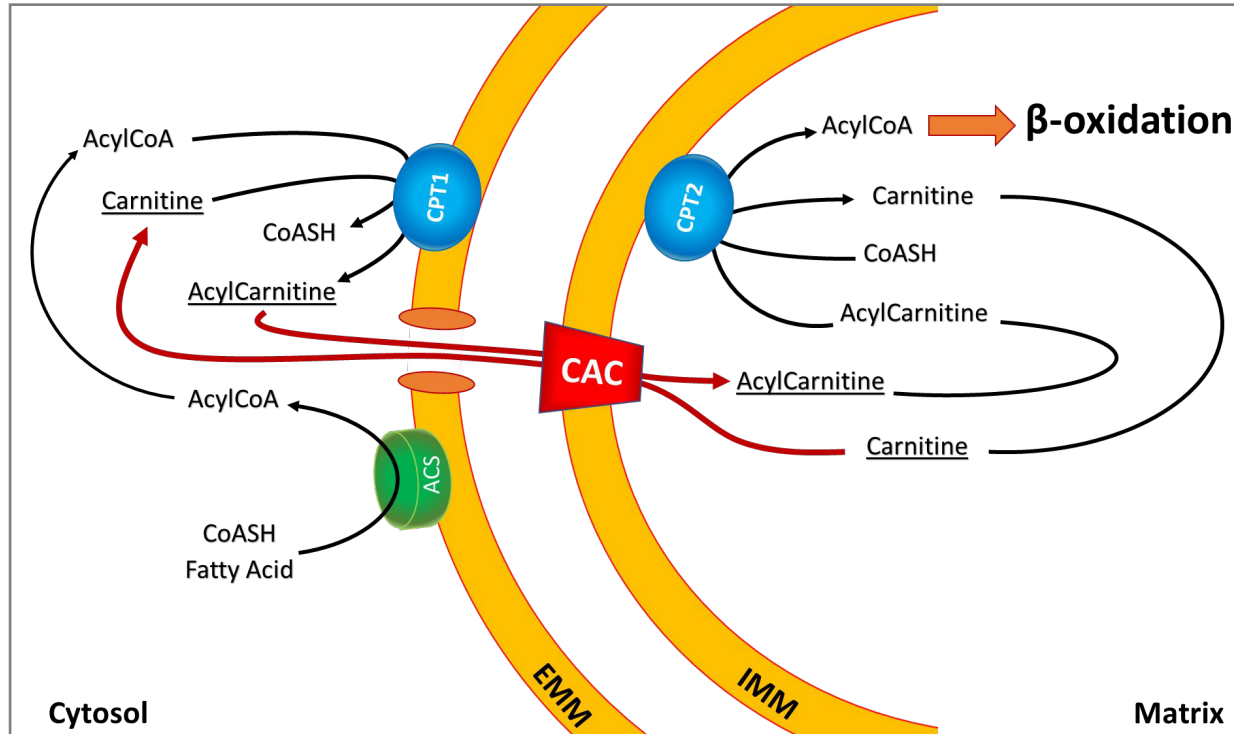
University of Calabria





The Mitochondrial Carnitine/Acylcarnitine Carrier (CAC)

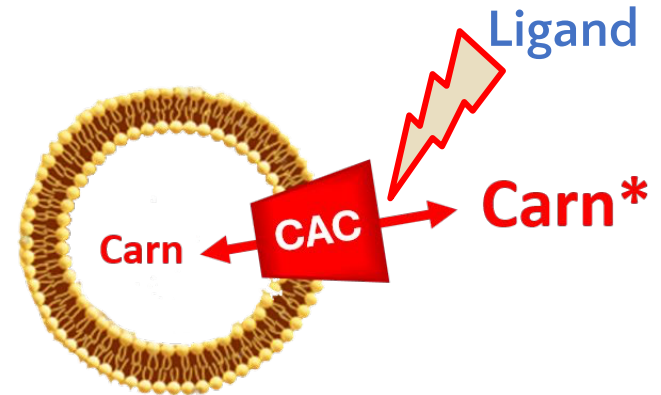
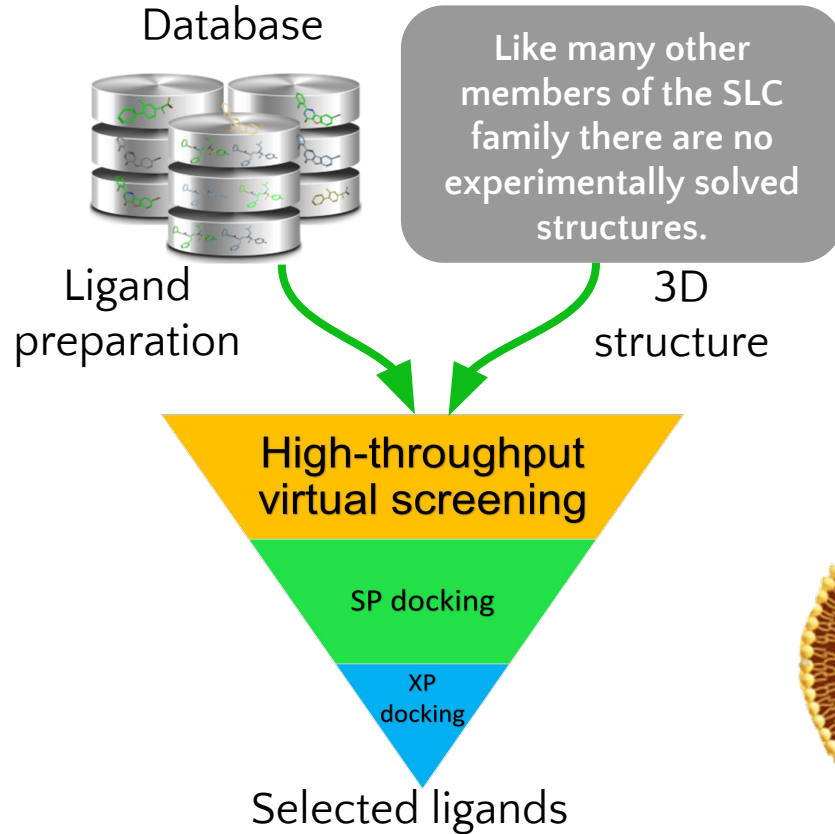
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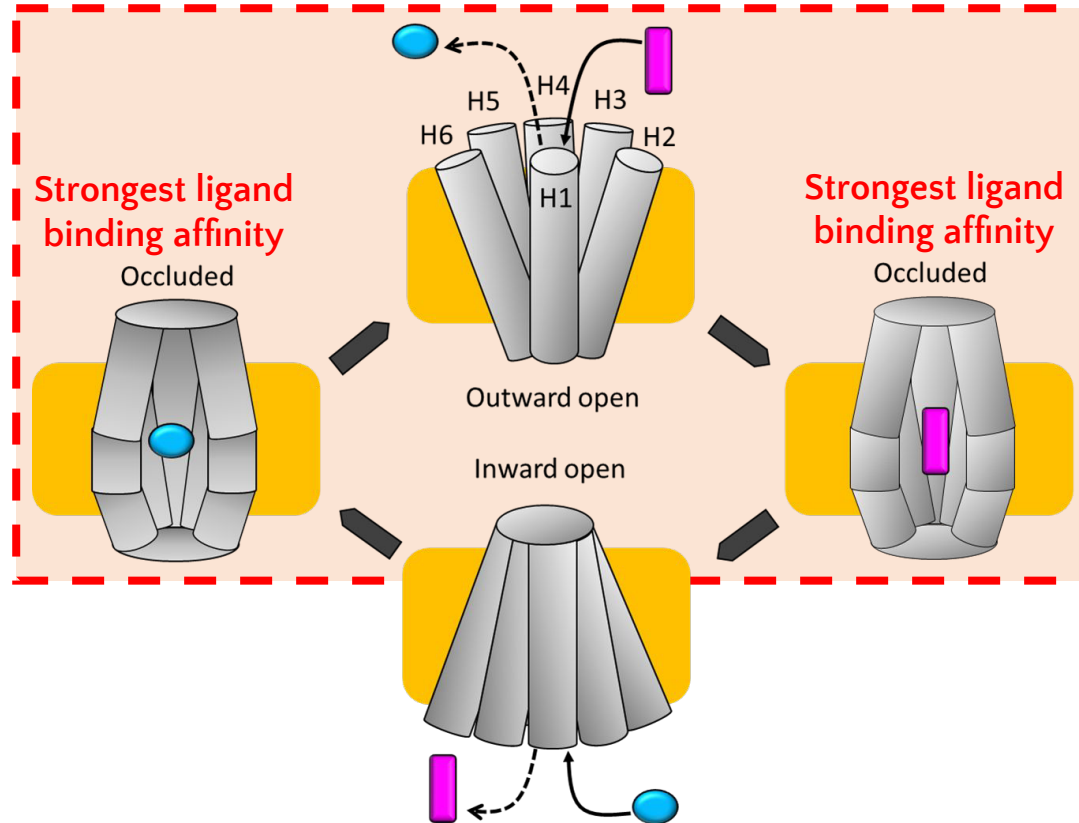




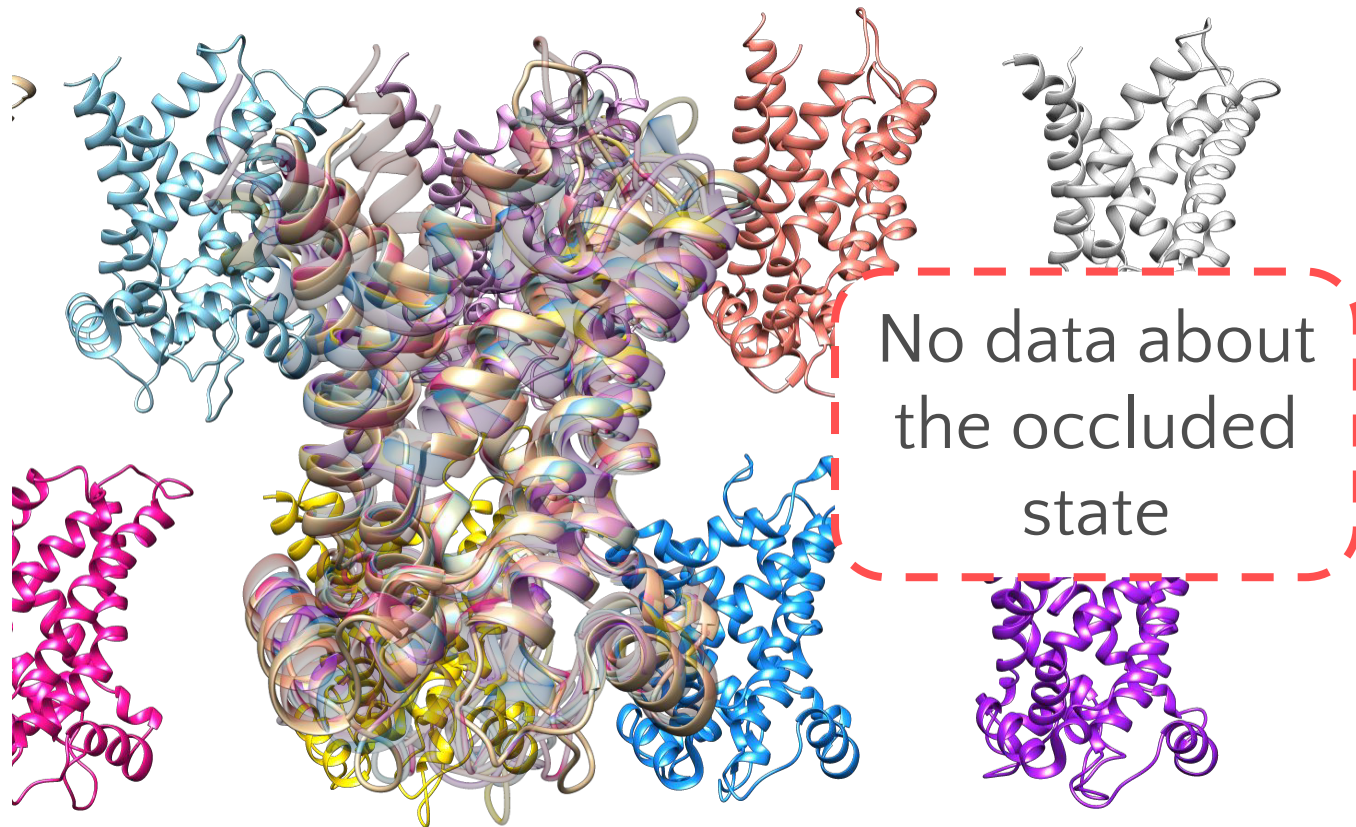
Accurate models must be built using homology modeling or AI

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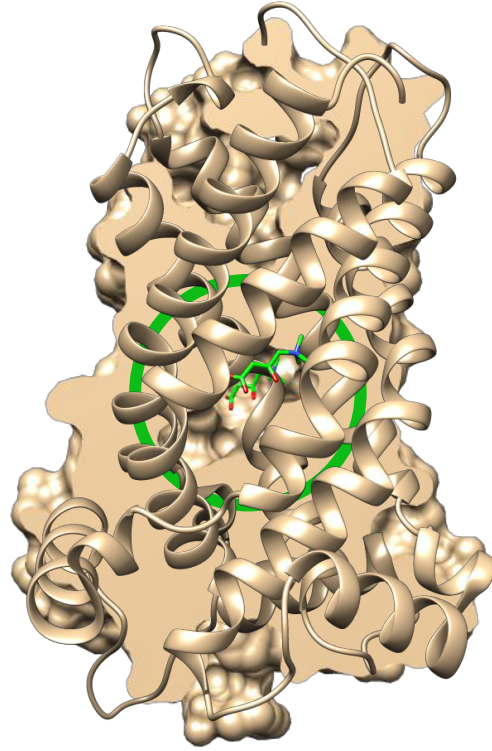


Are these
different steps
of the transport
cycle?



No data about
the occluded
state

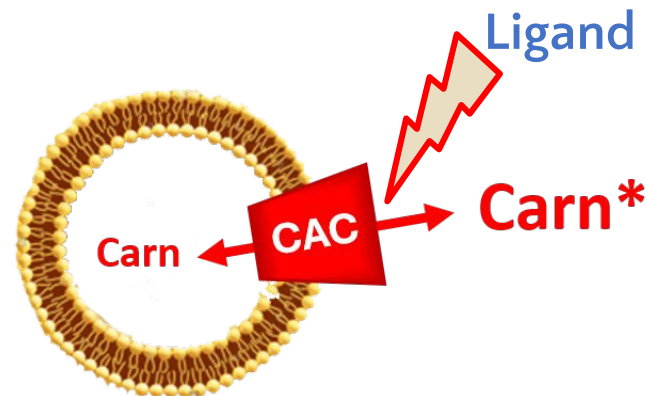
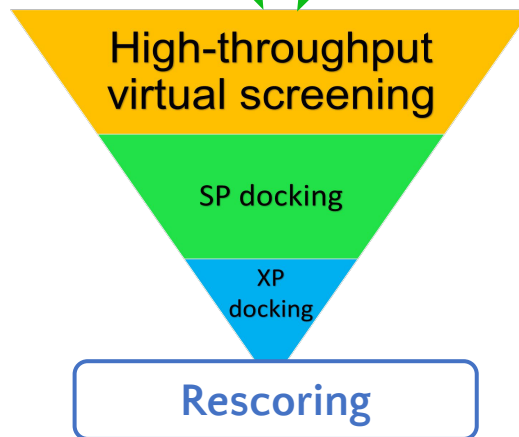
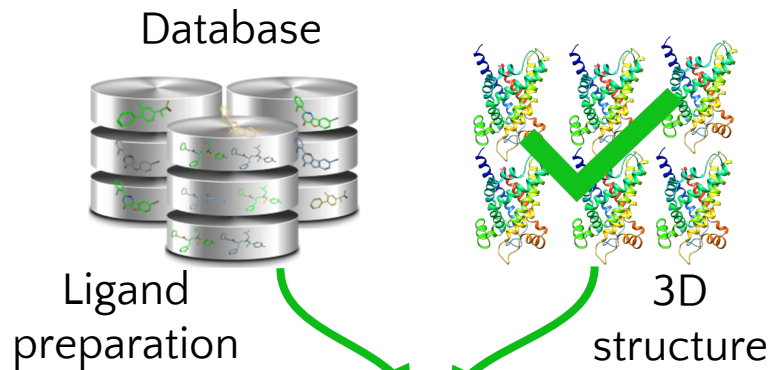
With carnitine

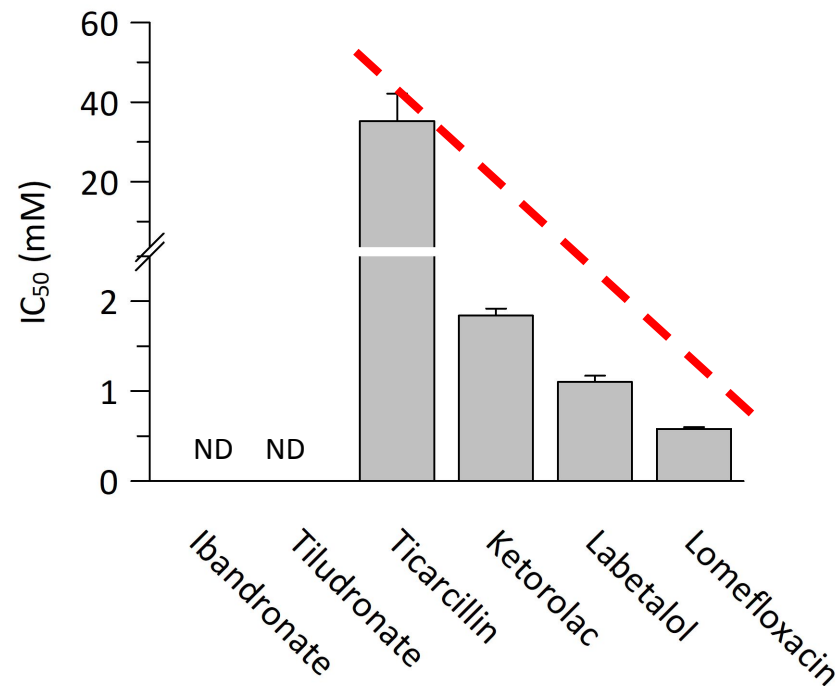
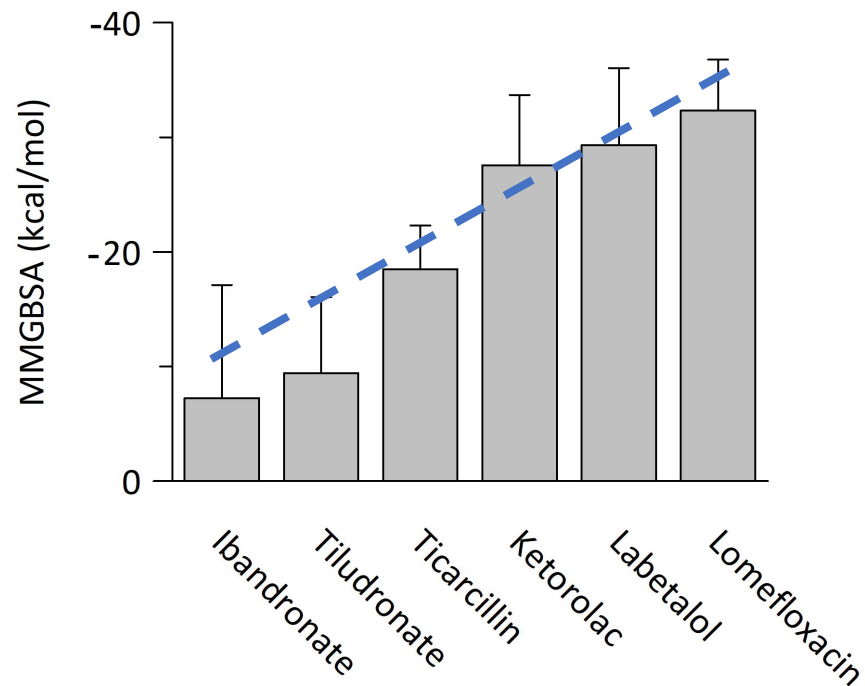


Occluded



Rescoring
MMGBSA?

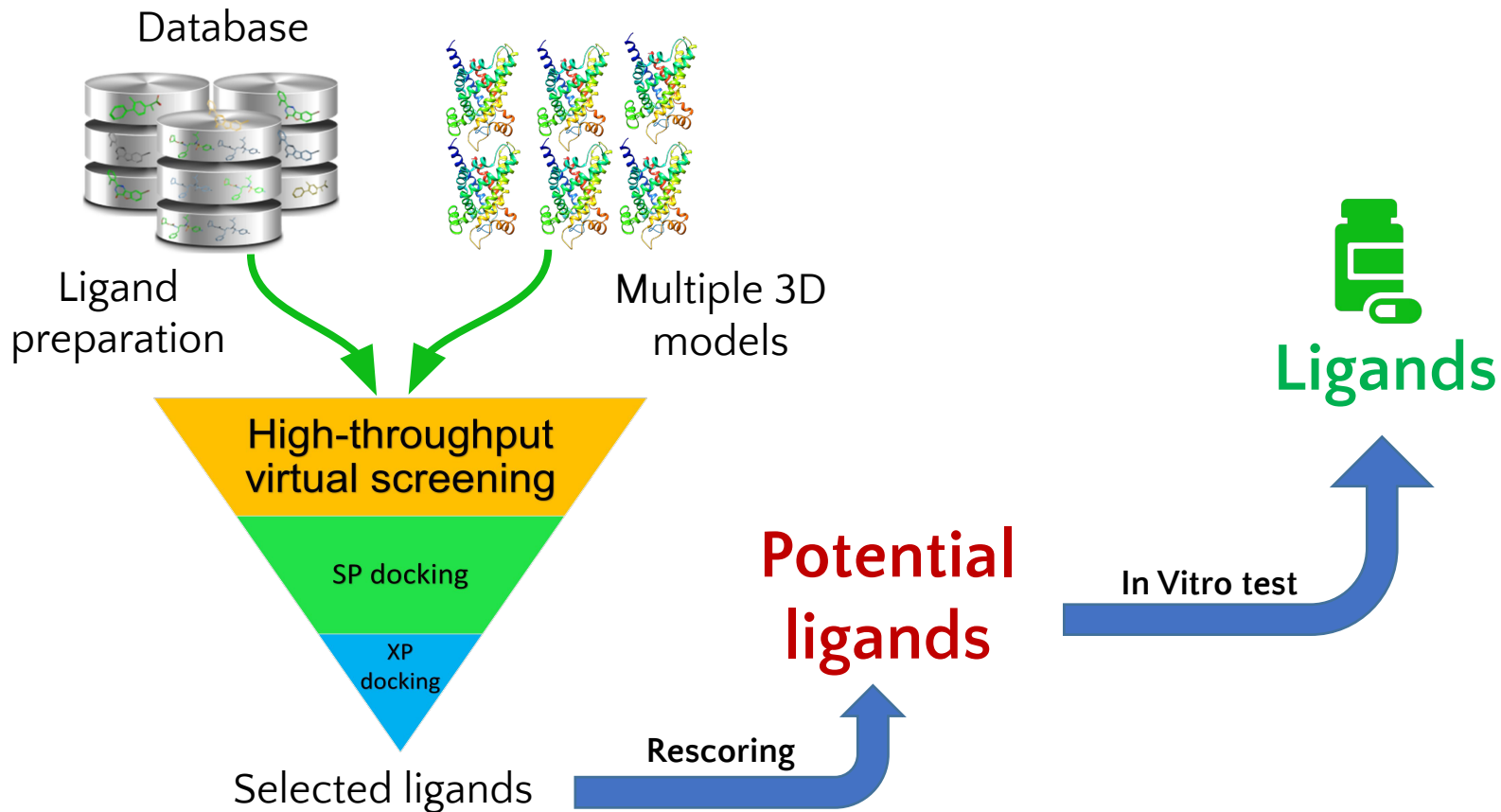


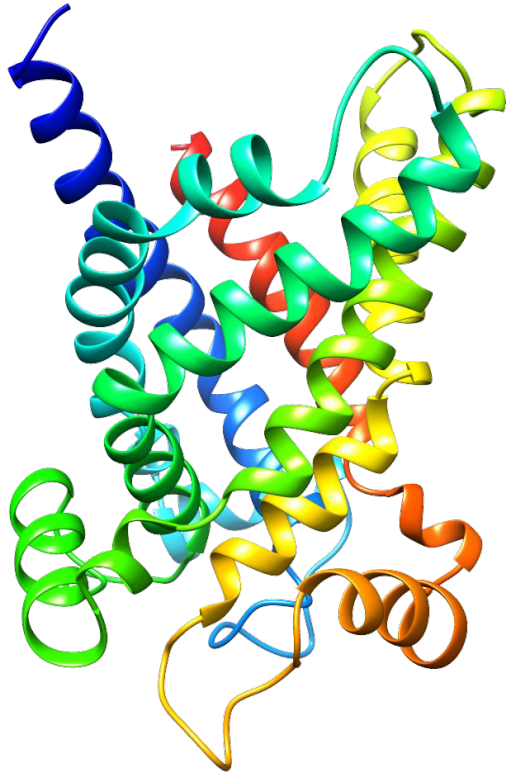




Final Virtual Screening workflow

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Cesare Indiveri
Sara Filice
Mattia di Sevo



Annamaria Tonazzi
Nicola Giangregorio

**Thanks
for your attention**