

PyModSim

FASTA sequence

1.

Structure Prediction
AlphaFold

PDB AlphaFold DB

AlphaFold Model

2.

Model Refinement
MODELLER

PDB External

Refined Model

3.

Membrane Positioning
PPM

Homology Model

PyMemDyn

Protein Model(s)

PDB Ligands

PDB Cofactors

PDB Model

1.

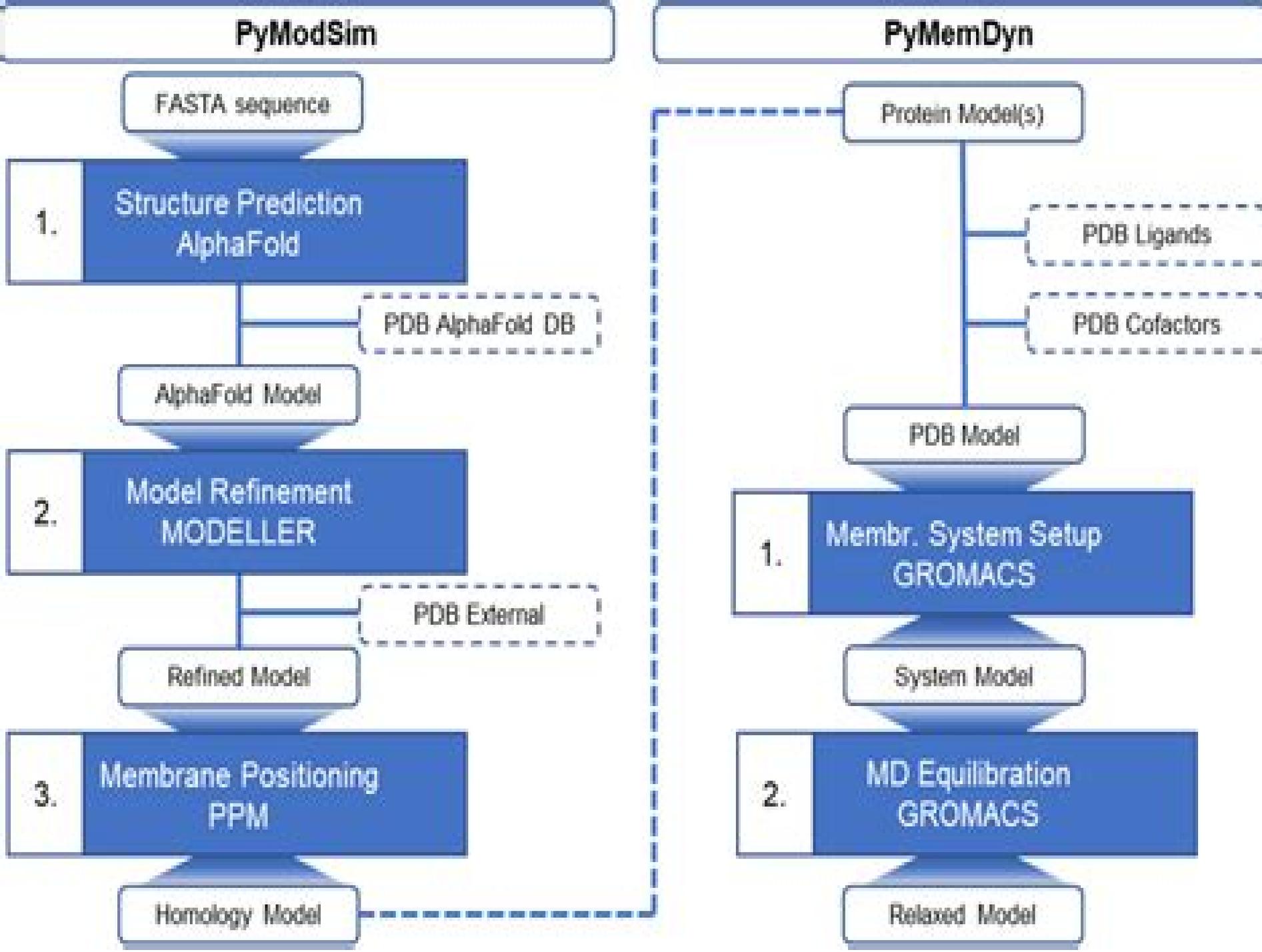
Membr. System Setup
GROMACS

System Model

2.

MD Equilibration
GROMACS

Relaxed Model



Modsim Iii A Tutorial

LM Reder



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