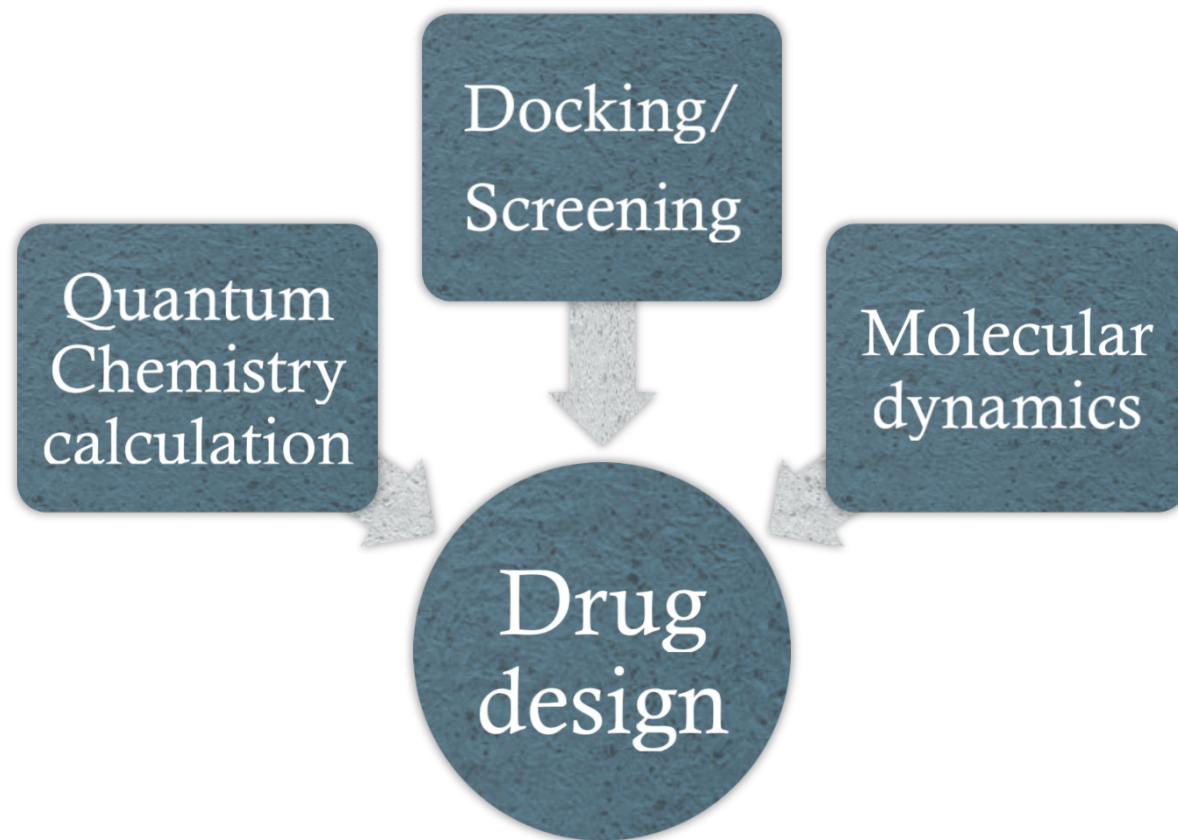
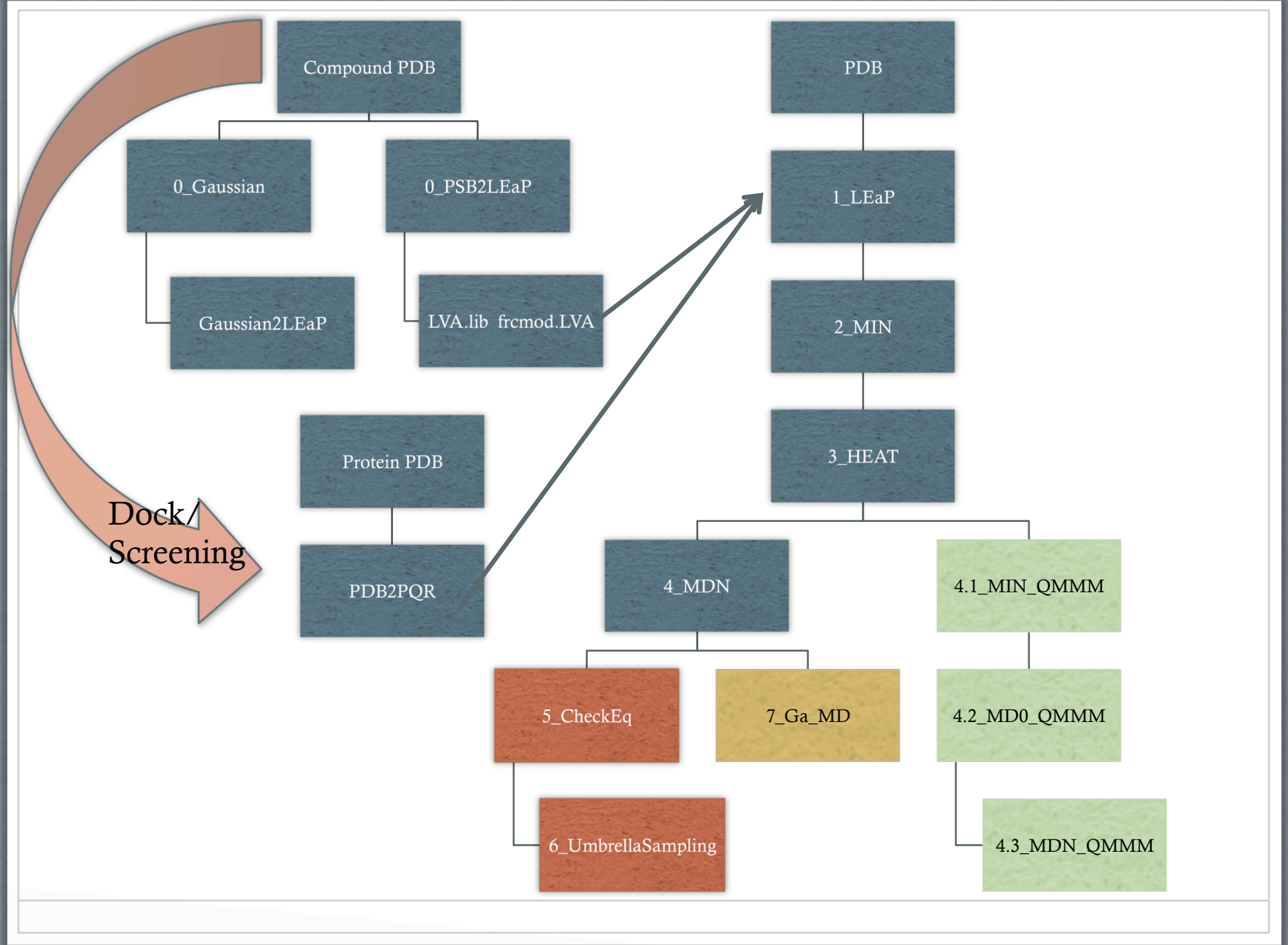


# Workshop on Frontiers in Computational Drug Discovery

16. March. 2018 ~ 19. March. 2018

# Computational Drug Discovery





Compound PDB

PDB

0\_Gaussian

0\_PSB2LEaP

1\_LEaP

Gaussian2LEaP

LVA.lib frcmod.LVA

2\_MIN

Protein PDB

3\_HEAT

Dock/  
Screening

PDB2PQR

4\_MDN

4.1\_MIN\_QMMM

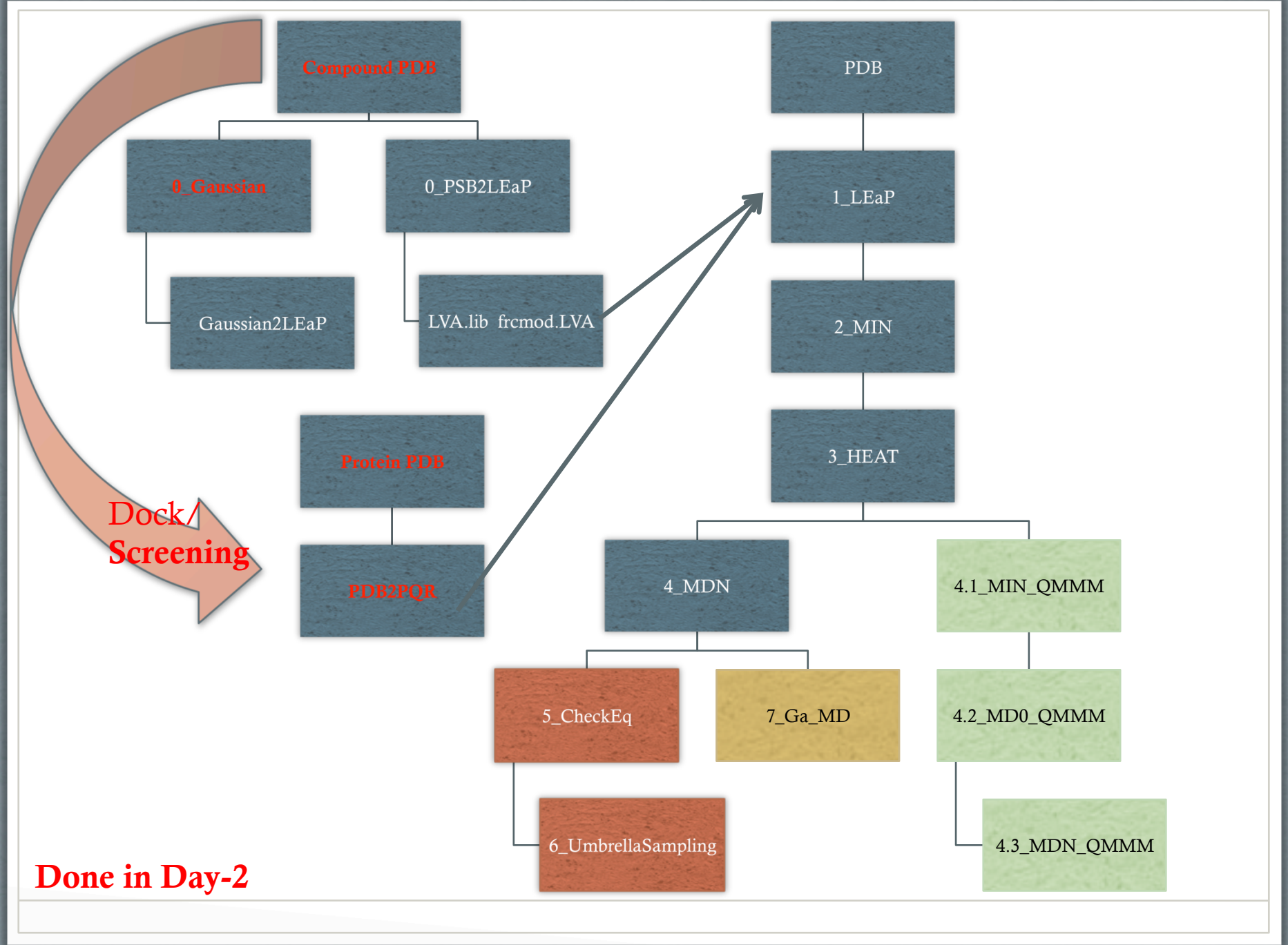
5\_CheckEq

7\_Ga\_MD

4.2\_MD0\_QMMM

6\_UmbrellaSampling

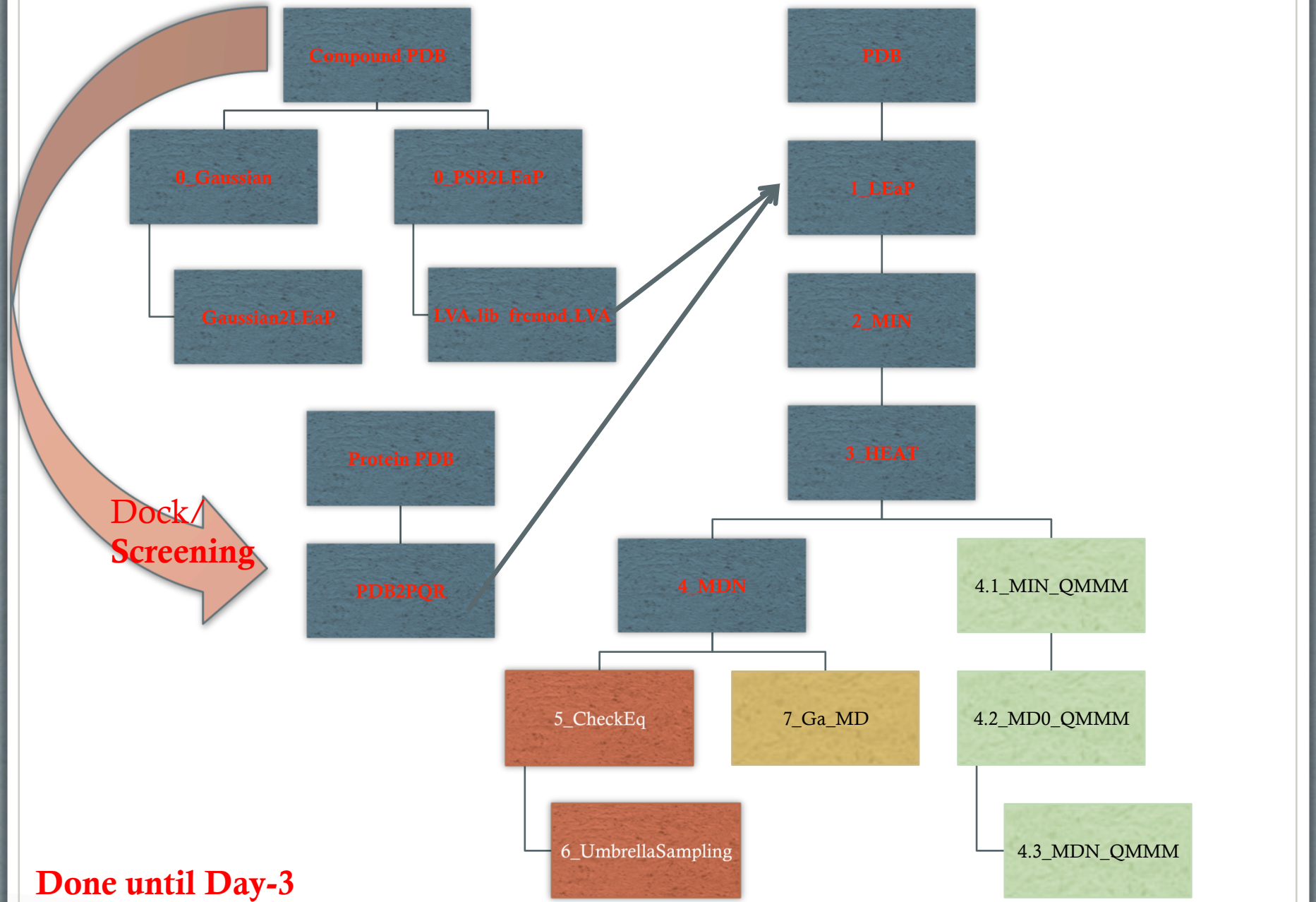
4.3\_MDN\_QMMM

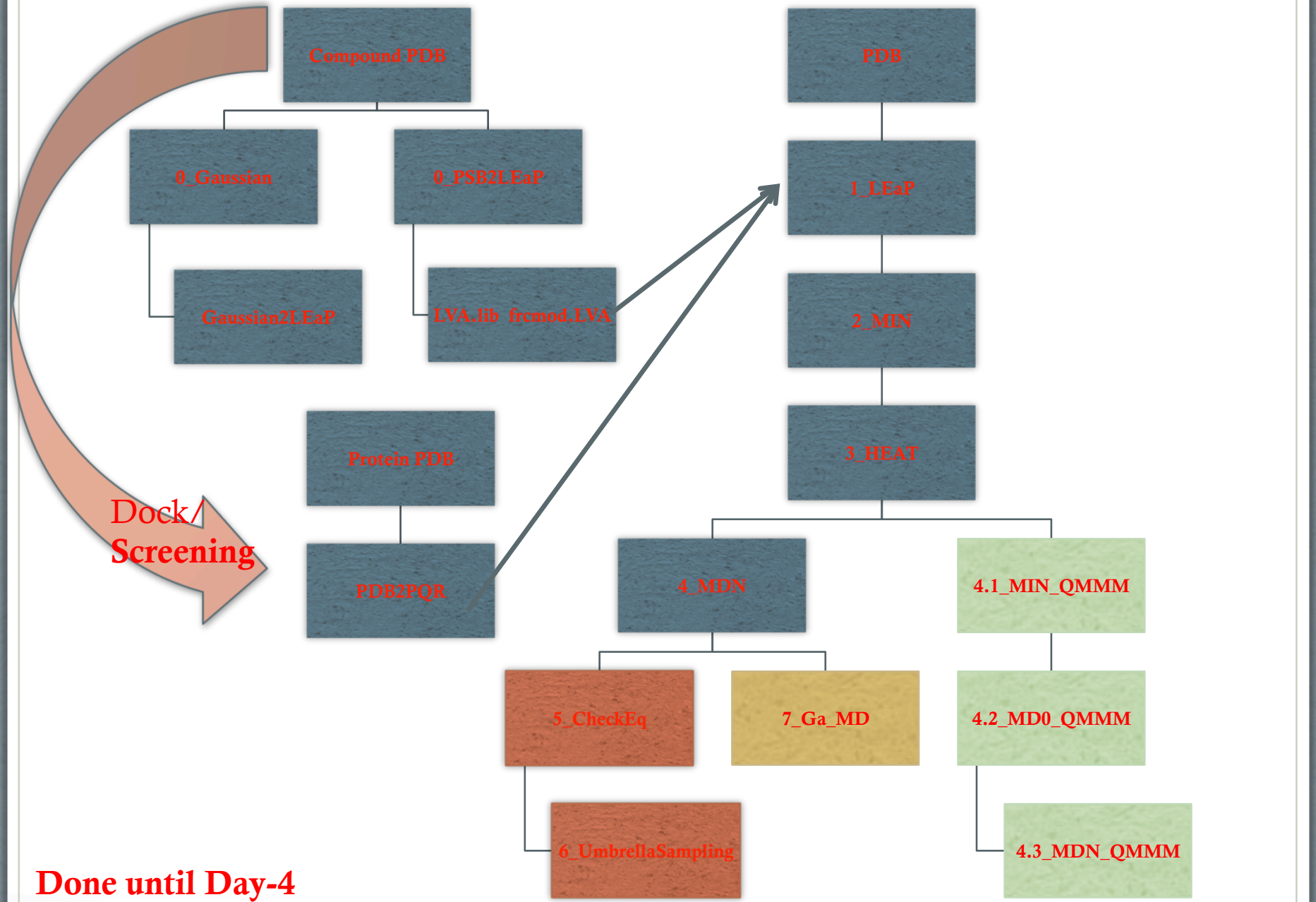


**Dock/  
Screening**

**Done in Day-2**







**Done until Day-4**