

Computer-aided drug discovery of DNA repair inhibitors

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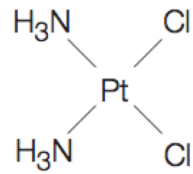
DNA repair and cancer drugs

CANCER CELL DNA

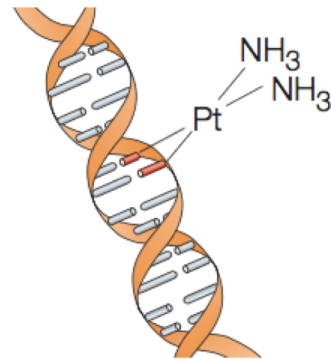


Wang et al. (2005)

CISPLATIN



DNA ADDUCT



APOPTOSIS



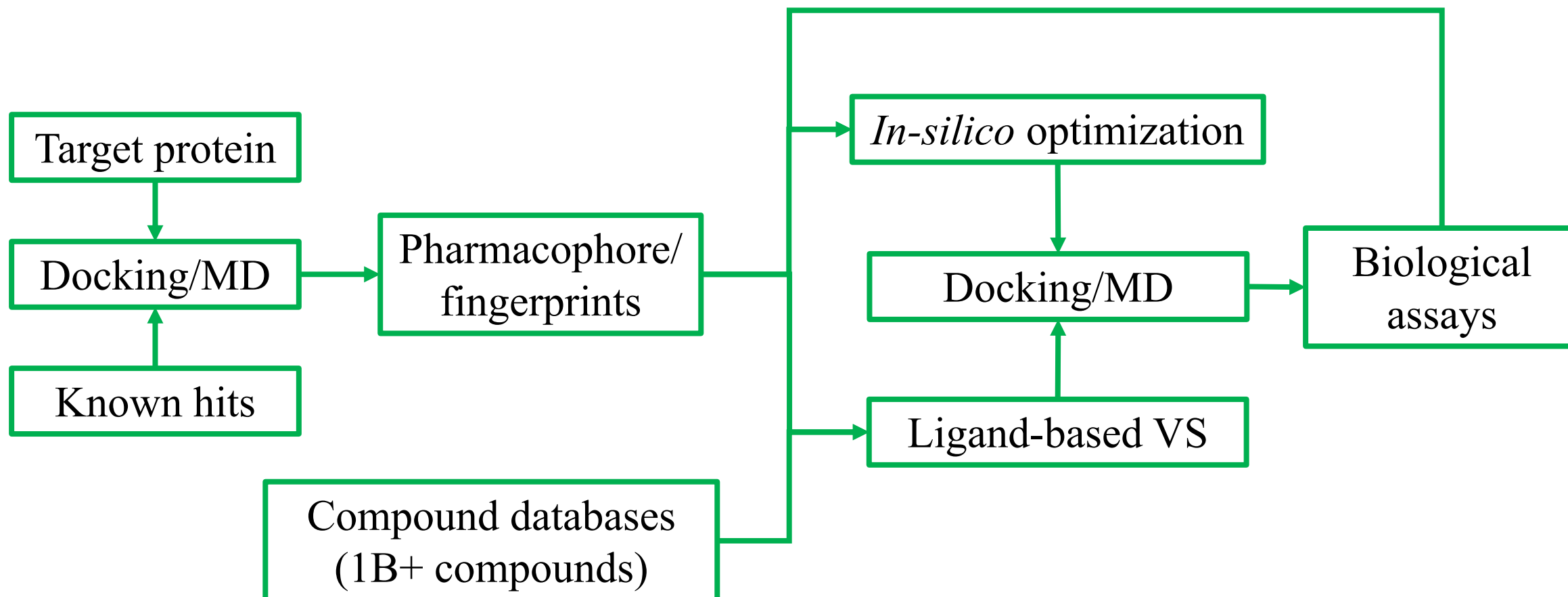
DNA REPAIR



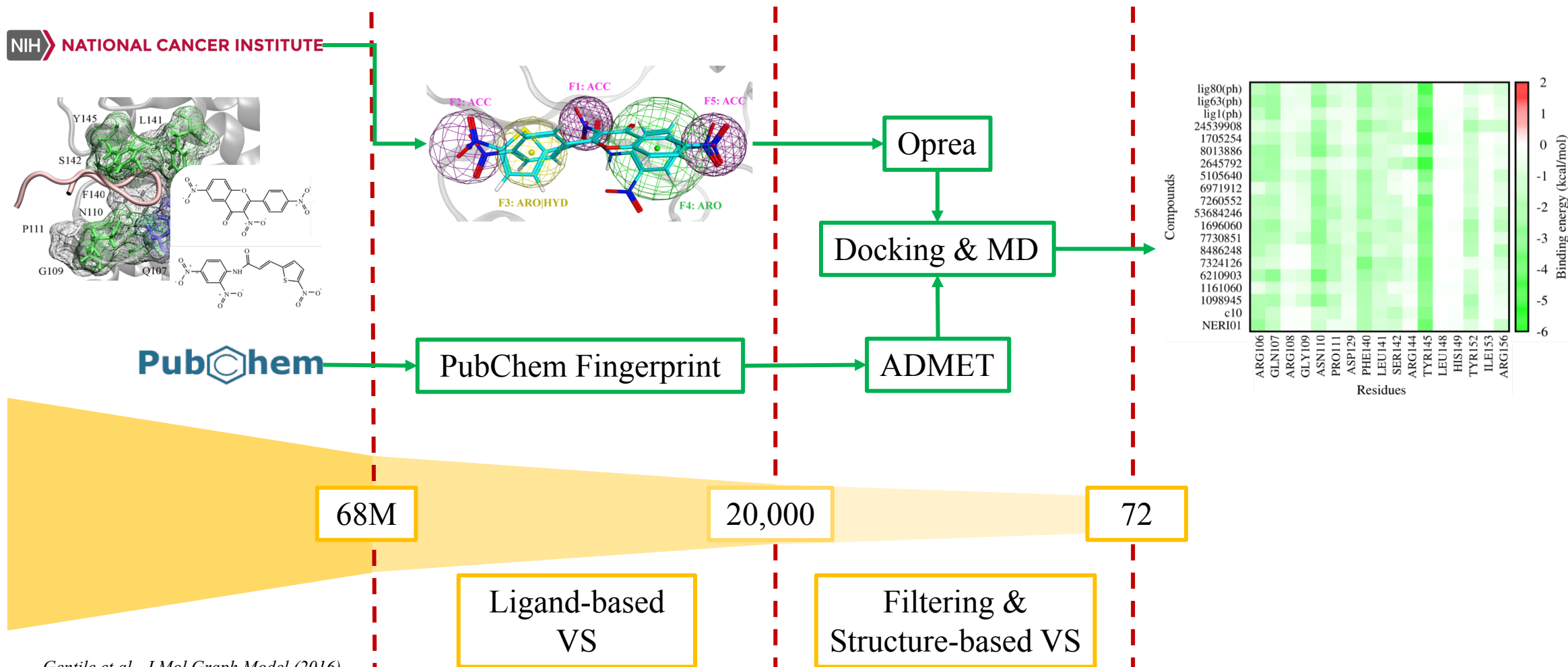
DNA REPAIR INHIBITOR



The drug discovery pipeline

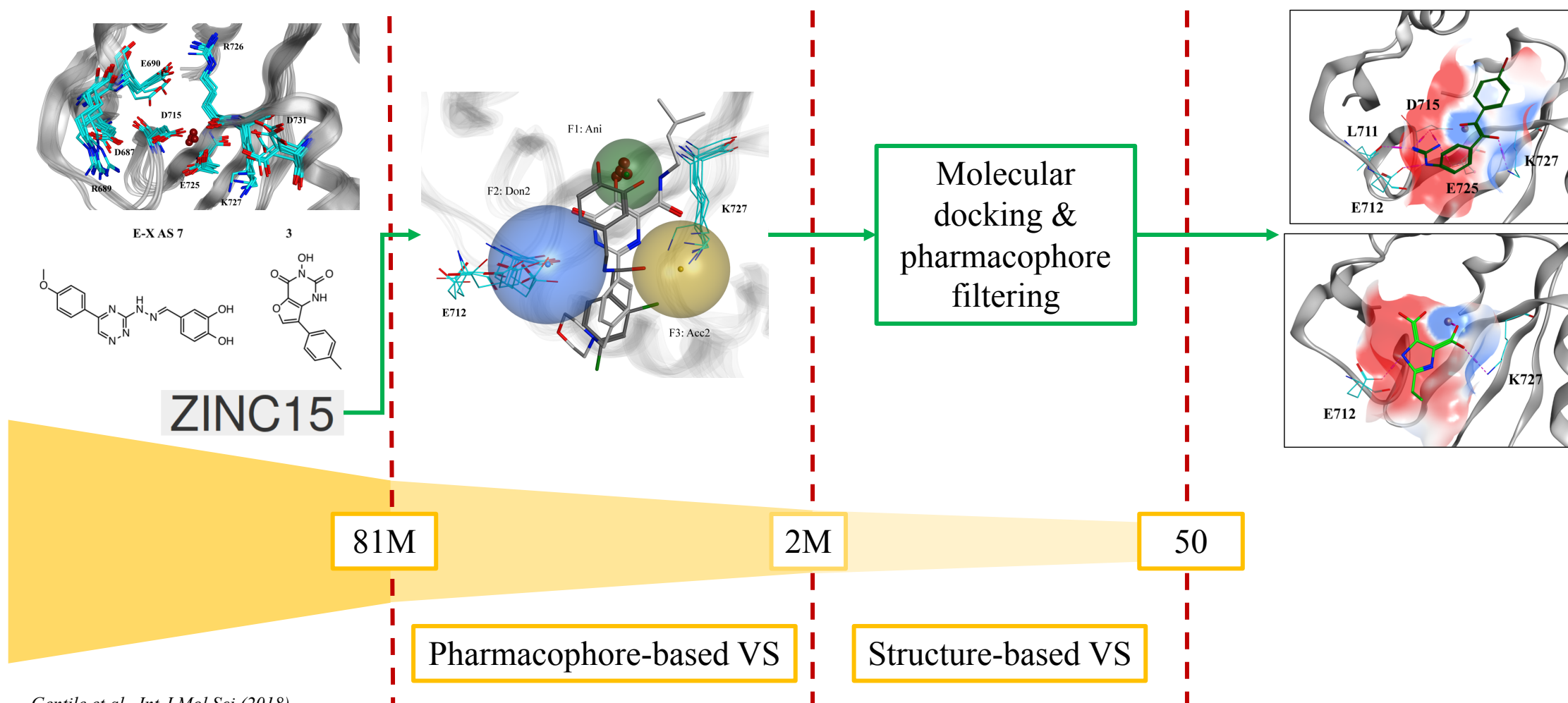


Application I: XPA-ERCC1



Gentile et al., J Mol Graph Model (2016)

Application II: XPF active site



Application II: ERCC1-XPF dimer

