

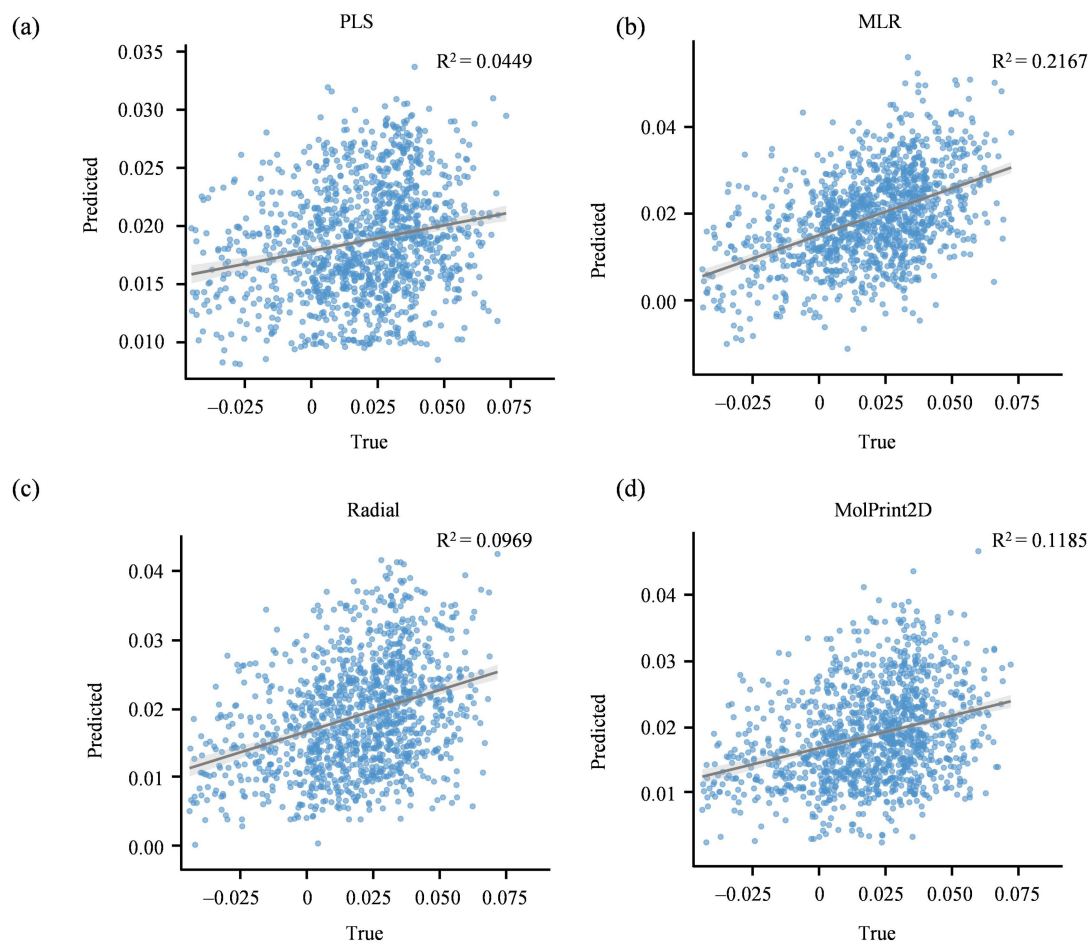


Fig. S5. Performance of DDN surpasses multiple QSAR models. a-d. Scatter plots showing the QSAR performance calculated by PLS (a) and MLR (b) in Discovery Studio, and Radial (c) and MolPrint2D (d) in Schrödinger.