

Virtual screening approach to identifying influenza virus neuraminidase inhibitors using molecular docking combined with machine-learning-based scoring function

SUPPLEMENTARY MATERIALS

Supplementary Table 1: List of 67 neuraminidase-ligand complex used as the training set for scoring function building

See Supplementary File 1

Supplementary Table 2: Details of the 281 inhibitors and 322 non-inhibitors collected from literatures and bindingDB database

See Supplementary File 2