Supplementary Table 1. Descriptors generated by PowerMV used for model generation

Pharmacophore Fingerprint	Weighted Burden Number	Property
NEG_01_NEG, NEG_02_NEG, NEG_03_NEG, NEG_04_NEG, NEG_05_NEG, NEG_06_NEG, NEG_07_NEG, NEG_03_POS, NEG_04_POS, NEG_05_POS, NEG_06_POS, NEG_07_POS, NEG_01_HBD, NEG_02_HBD, NEG_03_HBD, NEG_04_HBD, NEG_05_HBD, NEG_06_HBD, NEG_07_HBD, NEG_03_HBA, NEG_04_HBA, NEG_05_HBA, NEG_06_HBA, NEG_07_HBA, NEG_02_ARC, NEG_03_ARC, NEG_04_ARC, NEG_05_ARC, NEG_06_ARC, NEG_07_ARC, NEG_02_HYP, NEG_03_HYP, NEG_04_HYP, NEG_05_HYP, NEG_06_HYP, NEG_07_HYP, POS_03_POS, POS_04_POS, POS_05_POS, POS_06_POS, POS_07_POS, POS_02_HBD, POS_03_HBD, POS_04_HBD, POS_05_HBD, POS_06_HBD, POS_07_HBD, POS_03_HBA, POS_04_HBA, POS_05_HBA, POS_06_HBA, POS_07_HBA, POS_02_ARC, POS_03_ARC, POS_04_ARC, POS_05_ARC, POS_06_ARC, POS_07_ARC, POS_02_HYP, POS_03_HYP, POS_04_HYP, POS_05_HYP, POS_06_HYP, POS_07_HYP, HBD_03_HBD, HBD_04_HBD, HBD_05_HBD, HBD_06_HBD, HBD_07_HBD, HBD_03_HBA, HBD_04_HBA, HBD_05_HBA, HBD_06_HBA, HBD_07_HBA, HBD_02_ARC, HBD_03_ARC, HBD_04_ARC, HBD_05_ARC, HBD_06_ARC, HBD_07_ARC,	WBN_GC_L_0.25 WBN_GC_H_0.25 WBN_GC_L_0.50 WBN_GC_H_0.50 WBN_GC_L_0.75 WBN_GC_H_0.75 WBN_GC_L_1.00 WBN_GC_H_1.00 WBN_EN_L_0.25 WBN_EN_H_0.25 WBN_EN_L_0. 50 WBN_EN_H_0. 50 WBN_EN_L_0.75 WBN_EN_H_0.75 WBN_EN_L_1.00 WBN_EN_H_1.00 WBN_LP_L_0.25 WBN_ LP _H_0.25 WBN_ LP _L_0. 50	XLogP PSA, NumRot NumHBA NumHBD MW BBB BadGroup

HBD_02_HYP, HBD_03_HYP, HBD_04_HYP, HBD_05_HYP, HBD_06_HYP, HBD_07_HYP, HBA_03_HBA, HBA_04_HBA, HBA_05_HBA, HBA_06_HBA, HBA_07_HBA, HBA_03_ARC, HBA_04_ARC, HBA_05_ARC, HBA_06_ARC, HBA_07_ARC, HBA_02_HYP, HBA_03_HYP, HBA_04_HYP, HBA_05_HYP, HBA_06_HYP, HBA_07_HYP, ARC_01_ARC, ARC_02_ARC, ARC_03_ARC, ARC_04_ARC, ARC_05_ARC, ARC_06_ARC, ARC_07_ARC, ARC_02_HYP, ARC_03_HYP, ARC_04_HYP, ARC_05_HYP, ARC_06_HYP, ARC_07_HYP, HYP_01_HYP, HYP_02_HYP, HYP_03_HYP, HYP_04_HYP, HYP_05_HYP, HYP_06_HYP, HYP_07_HYP	WBN_ LP _H_0. 50 WBN_ LP _L_0.75 WBN_ LP _H_0.75 WBN_ LP _L_1.00 WBN_ LP _H_1.00	