Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplementary Information

1 Statistics of drug-target profiles and composite model:

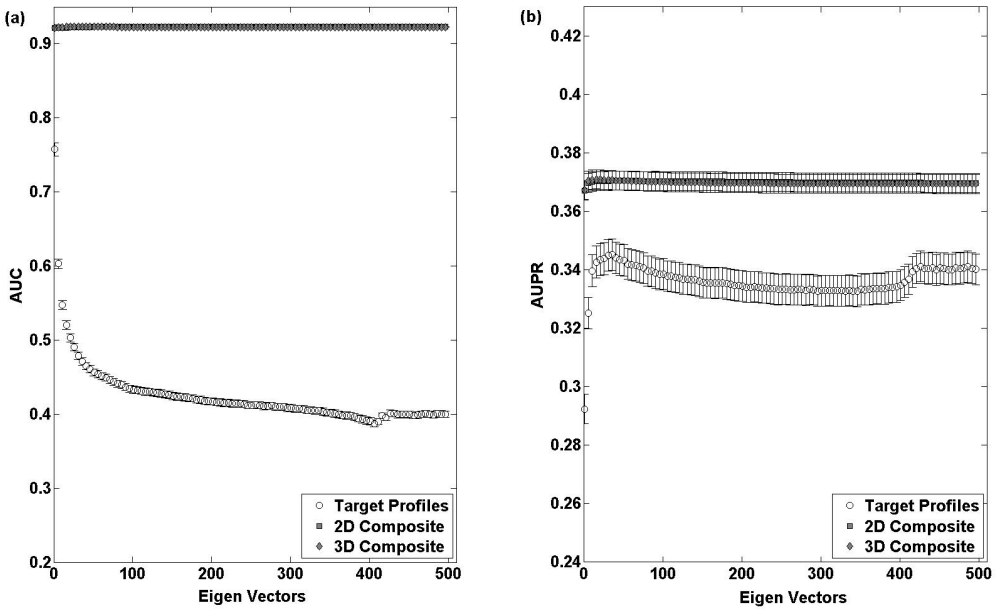

Figure 1: AUC (a) and AUPR (b) measured using increasing number of eigen vectors of drug-target profiles matrix only (○) and including those of 2D (■) and 3D (♦) drug-chemical eigen vectors. The error bars indicate standard error of data for 10 cross validation for test drug sets of size 83 each.

2 Statistics of drug-chemical profiles and composite models:

2.1 3D Chemical properties

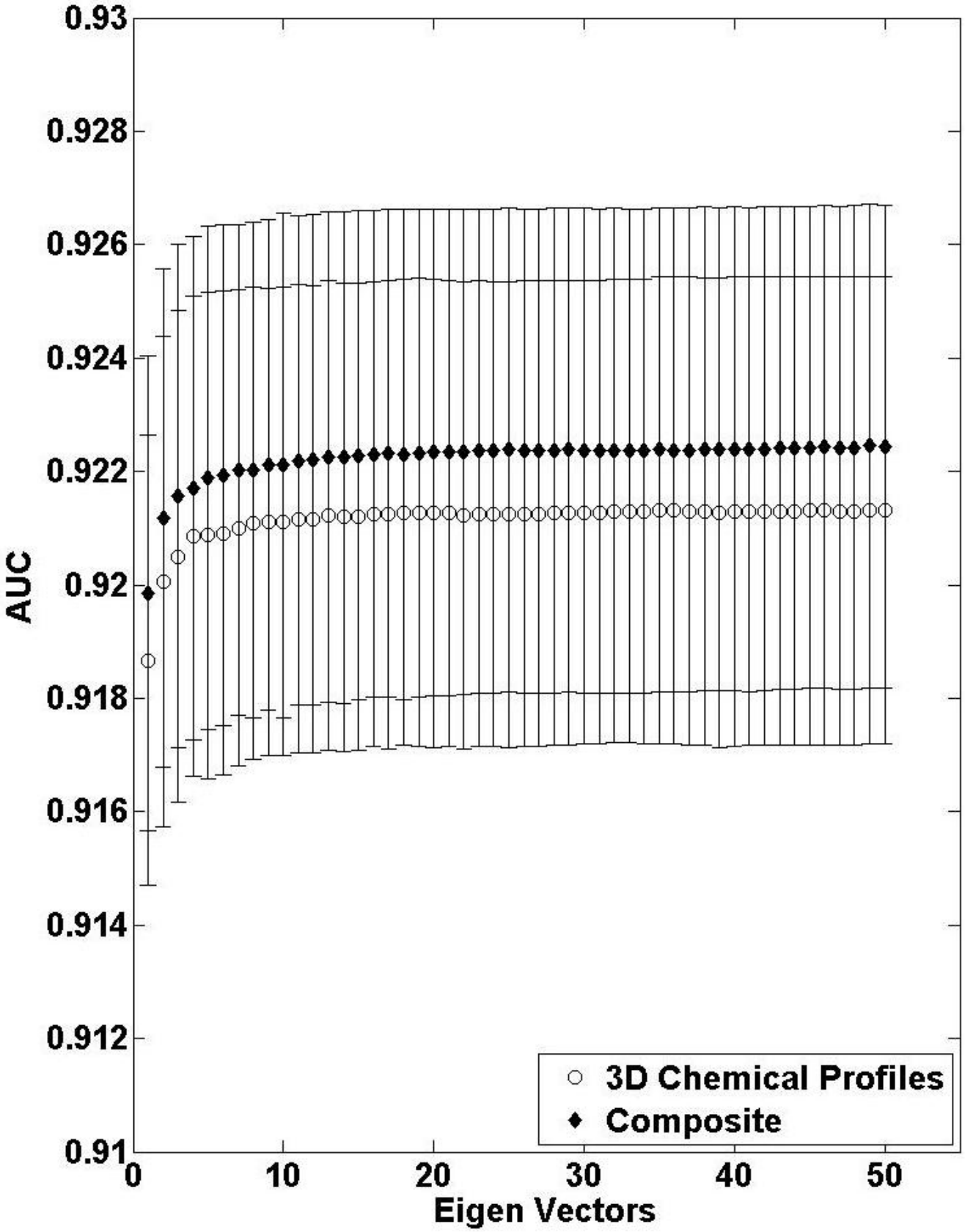

Figure 2: AUC (a) and AUPR (b) measured using increasing number of eigen vectors of 3D drug-chemical profiles matrix, in the absence (◇) and presence (⧫) of drug-target eigen vectors. The error bars indicate standard error of data for 10 cross validation for test drug sets of size 83 each.

2.2 2D Chemical properties

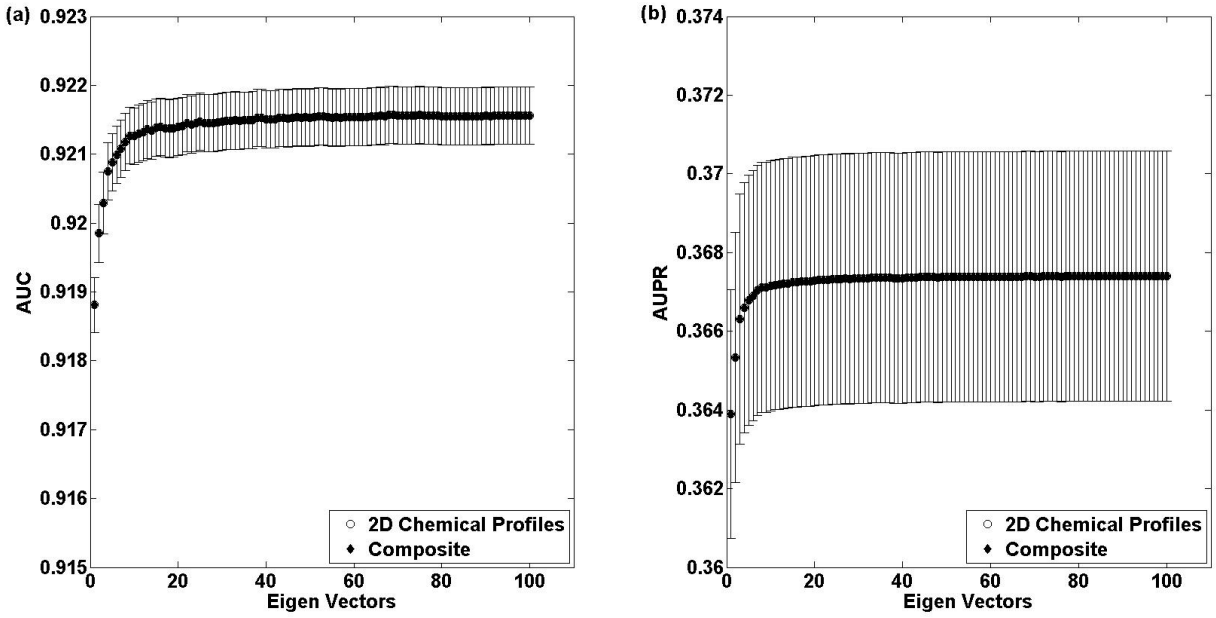

Figure 3: AUC (a) and AUPR (b) measured using increasing number of eigen vectors of 3D drug-chemical profiles matrix, in the absence (◇) and presence (⧫) of drug-target eigen vectors. The error bars indicate standard error of data for 10 cross validation for test drug sets of size 83 each.

3 3D Chemical Properties

Following are the 62 3D chemical properties that were used for the analysis: Dipole_mag (1), Dipole_X (2), Dipole_Y (3), Dipole_Z (4), Clean Energy (5), Energy (6), Minimized_Energy (7), Strain_Energy (8), Jurs_DPSA_1 (9), Jurs_DPSA_2 (10), Jurs_DPSA_3 (11), Jurs_FNSA_1 (12), Jurs_FNSA_2 (13), Jurs_FNSA_3 (14), Jurs_FPSA_1 (15), Jurs_FPSA_2 (16), Jurs_FPSA_3 (17), Jurs_PNSA_1 (18), Jurs_PNSA_2 (19), Jurs_PNSA_3 (20), Jurs_PPSA_1 (21), Jurs_PPSA_2 (22), Jurs_PPSA_3 (23), Jurs_RASA (24), Jurs_RNCG (25), Jurs_RNCS (26), Jurs_RPCG (27), Jurs_RPCS (28), Jurs_RPSA (29), Jurs_SASA (30), Jurs_TASA (31), Jurs_TPSA (32), Jurs_WNSA_1 (33), Jurs_WNSA_2 (34), Jurs_WNSA_3 (35), Jurs_WPSA_1 (36), Jurs_WPSA_2 (37), Jurs_WPSA_3 (38), PMI_mag (39), PMI_X (40), PMI_Y (41), PMI_Z (42), Shadow_nu (43), Shadow_Xlength (44), Shadow_XY (45), Shadow_XYfrac (46), Shadow_XZ (47), Shadow_XZfrac (48), Shadow_Ylength (49), Shadow_YZ (50), Shadow_YZfrac (51), Shadow_Zlength (52), Molecular_3D_PolarSASA (53), Molecular_3D_SASA (54), Molecular_3D_SAVol (55), Molecular_Volume (56), Number of Atoms (57), Exact Mol. Weight (58), Net Formal Charge (59), AverageBondLength (60), RadOfGyration (61).

4 2D Chemical Properties

Following are the 145 2D chemical properties that were used for the analysis: Molecular_FractionalPolarSASA (1), Molecular_FractionalPolarSurfaceArea (2), Molecular_PolarSASA (3), Molecular_PolarSurfaceArea (4), Molecular_SASA (5), Molecular_SAVol (6), Molecular_SurfaceArea (7), HBA_Count (8), HBD_Count (9), NPlusO_Count (10), Num_AliphaticDoubleBonds (11), Num_AliphaticSingleBonds (12), Num_AromaticBonds (13), Num_AromaticRings (14), Num_AtomClasses (15), Num_Atoms (16), Num_AtropisomerCenters (17), Num_AxialStereoCenters (18), Num_Bonds (19), Num_BridgeBonds (20), Num_BridgeHeadAtoms (21), Num_ChainAssemblies (22), Num_Chains (23), Num_ComplexedFragments (24), Num_DoubleBonds (25), Num_ExplicitAtoms (26), Num_ExplicitBonds (27), Num_ExplicitHydrogens (28), Num_Fragments (29), Num_H_Acceptors (30), Num_H_Acceptors_Lipinski (31), Num_H_Donors (32), Num_H_Donors_Lipinski (33), Num_Hydrogens (34), Num_MesoStereoAtoms (35), Num_MetalAtoms (36), Num_NegativeAtoms (37), Num_PositiveAtoms (38), Num_PseudoStereoAtoms (39), Num_QueryBonds (40), Num_RingAssemblies (41), Num_RingBonds (42), Num_RingFusionBonds (43), Num_Rings (44), Num_Rings3 (45), Num_Rings4 (46), Num_Rings5 (47), Num_Rings6 (48), Num_Rings7 (49), Num_Rings8 (50), Num_Rings9Plus (51), Num_RotatableBonds (52), Num_SingleBonds (53), Num_SpiroAtoms (54), Num_StereoAtoms (55), Num_StereoBonds (56), Num_TerminalRotomers (57), Num_TripleBonds (58), Num_TrueStereoAtoms (59), Num_UnknownPseudoStereoAtoms (60), Num_UnknownTrueStereoAtoms (61), Organic_Count (62), ES_Count_aaaC (63), ES_Count_aaCH (64), ES_Count_aaN (65), ES_Count_aaNH (66), ES_Count_aaO (67), ES_Count_aaS (68), ES_Count_aasC (69), ES_Count_aasN (70), ES_Count_dCH2 (71), ES_Count_ddsN (72), ES_Count_ddssS (73), ES_Count_dNH (74), ES_Count_dO (75), ES_Count_dS (76), ES_Count_dsCH (77), ES_Count_dsN (78), ES_Count_dssC (79), ES_Count_dssS (80), ES_Count_dsssP (81), ES_Count_sBr (82), ES_Count_sCH3 (83), ES_Count_sCl (84), ES_Count_sF (85), ES_Count_sI (86), ES_Count_sNH2 (87), ES_Count_sNH3 (88), ES_Count_sOH (89), ES_Count_ssCH2 (90), ES_Count_sSH (91), ES_Count_ssNH (92), ES_Count_ssO (93), ES_Count_ssS (94), ES_Count_sssAs (95), ES_Count_sssB (96), ES_Count_sssCH (97), ES_Count_sssN (98), ES_Count_ssssC (99), ES_Count_ssssN (100), ES_Count_tCH (101), ES_Count_tN (102), ES_Count_tsC (103), ES_Sum_aaaC (104), ES_Sum_aaCH (105), ES_Sum_aaN (106), ES_Sum_aaNH (107), ES_Sum_aaO (108), ES_Sum_aaS (109), ES_Sum_aasC (110), ES_Sum_aasN (111), ES_Sum_dCH2 (112), ES_Sum_ddsN (113), ES_Sum_ddssS (114), ES_Sum_dNH (115), ES_Sum_dO (116), ES_Sum_dS (117), ES_Sum_dsCH (118), ES_Sum_dsN (119), ES_Sum_dssC (120), ES_Sum_dssS (121), ES_Sum_dsssP (122), ES_Sum_sBr (123), ES_Sum_sCH3 (124), ES_Sum_sCl (125), ES_Sum_sF (126), ES_Sum_sI (127), ES_Sum_sNH2 (128), ES_Sum_sNH3 (129), ES_Sum_sOH (130), ES_Sum_ssCH2 (131), ES_Sum_sSH (132), ES_Sum_ssNH (133), ES_Sum_ssO (134), ES_Sum_ssS (135), ES_Sum_sssAs (136), ES_Sum_sssB (137), ES_Sum_sssCH (138), ES_Sum_sssN (139), ES_Sum_ssssC (140), ES_Sum_ssssN (141), ES_Sum_tCH (142), ES_Sum_tN (143), ES_Sum_tsC (144), and Estate_NumUnknown (145).