Supporting Information

Efficient estimation of MMGBSA based binding energies for DNA and aromatic furan amidino derivatives

Hemant Kumar Srivastava* and G. Narahari Sastry*

Molecular Modelling Group, Indian Institute of Chemical Technology,

Uppal Road, Taranaka, Hyderabad 500 607, INDIA

Phone- +91 40 2719 3016, Fax- +91 40 2716 0512,

Email- hemantkrsri@gmail.com (HKS); gnsastry@gmail.com (GNS)

Key words: MMGBSA based binding energies, Molecular dynamics simulations, ΔT_m values, *Pneumocystis carinii* agents, DNA ligand complexes, DFT based QSAR studies

1

2

3

Fig. S1. Separate RMSD plot for complex, DNA and ligand for all thirty derivatives