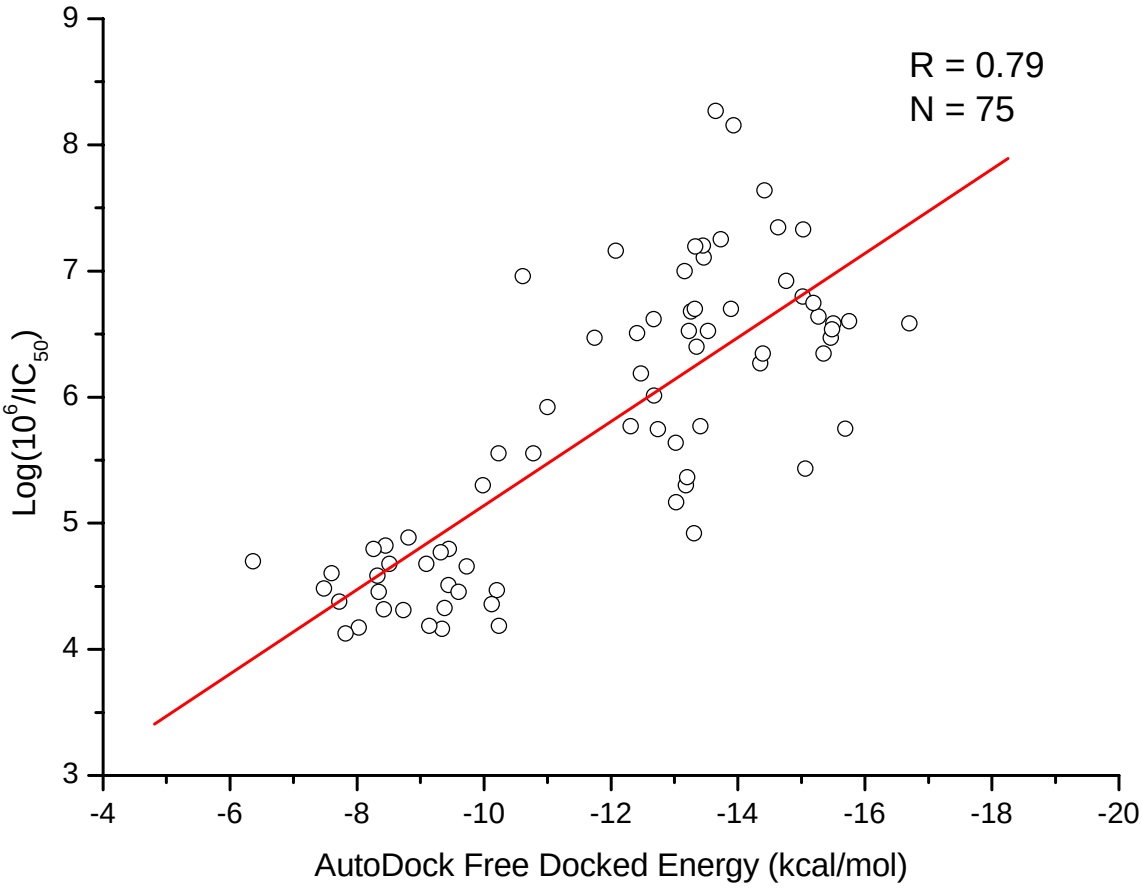
SUPPORTING INFORMATION

Insights into the Structural Basis of N2 and O6 Substituted Guanine Derivatives as Cyclin-Dependent Kinase 2 (CDK2) Inhibitors: Prediction of the Binding Modes and potency of the inhibitors by Docking and ONIOM Calculation

Jans H. Alzate-Morales*, Julio Caballero, Ariela Vergara and Fernando D. González Nilo

Figure SI1. Plot of the AutoDock3 docked energy versus the Log ($10^6/IC_{50}$) for the set of compounds studied.



Statistical data for linear regression equation:

$$Log(10^6/IC_{50}) = 1.8056 - 0.33 \times \Delta G_{AutoDock3}\ (kcal/mol) \qquad (1)$$

$$N = 75 \qquad r = 0.790 \qquad r^2 = 0.619 \qquad F_{(1,\ 73)} = 121.44 \qquad p < 10^{-4}$$