J|A|C|S
ADDITIONS & CORRECTIONS

Unexpected Binding Modes of Nitric Oxide Synthase Inhibitors Effective in the Prevention of a Cerebral Palsy Phenotype in an Animal Model [*J. Am. Chem. Soc.* **2010,** *132,* 5437–5442]. Silvia L Delker, Haitao Ji, Huiying Li, Joumana Jamal, Jianguo Fang, Fengtian Xue, Richard B. Silverman,* and Thomas L. Poulos*

Supporting Information. Figure S2 was mistakenly omitted.

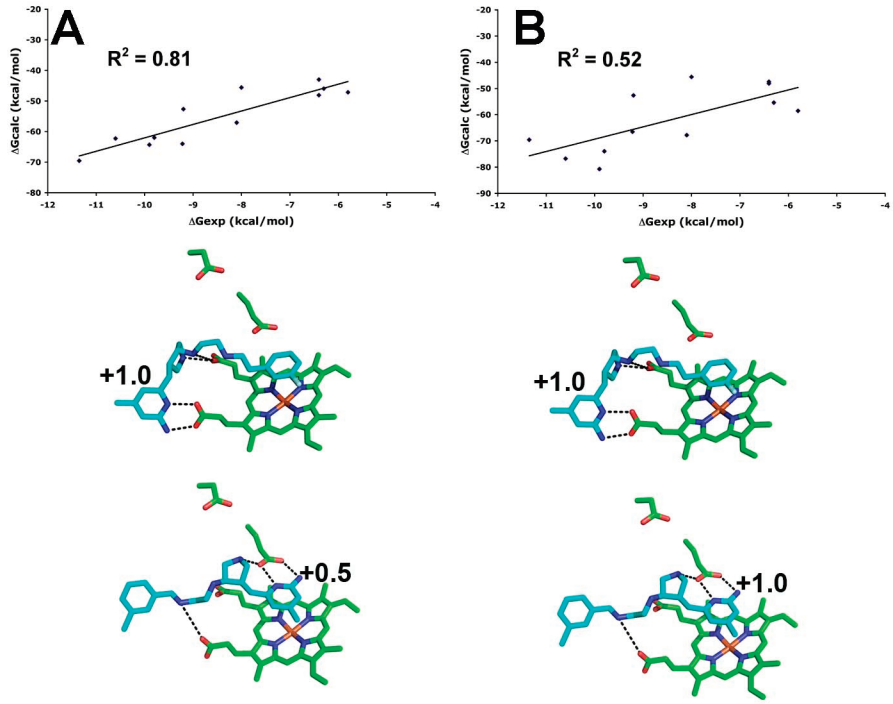

Figure S2. Plots of the calculated binding free energy (ΔG_{calc}) vs the experimental binding free energy (ΔG_{exp}) using two different models. In panel A it is assumed that the aminopyridine carries a net +0.5 charge when the aminopyridine is oriented over the heme and a net +1.0 charge in the flipped orientation. In panel B the aminopyridine is assumed to carry a net +1.0 charge independent of orientation. The crystal structures used for the calculations were (3′*S*,4′*S*)-**2** (eNOS and nNOS), (3′*R*,4′*R*)-**2** (eNOS, nNOS, nNOS D597N, nNOS D597N/M366V, nNOS D597N/M336V/Y706A), and (±)-N^1-{*cis*-4′-[(6″-amino-4″-methylpyridin-2″-yl)methyl]pyrrolidin-3′-yl}-N^2-(4′-chlorobenzyl)ethane-1,2-diamine tetrahydrochloride (nNOS, eNOS).

JA107808U

10.1021/ja107808u
Published on Web 09/21/2010

10.1021/ja107808u