Addition/Correction

Refinement of the Conformation of UDP–Galactose Bound to Galactosyltransferase Using the STD NMR Intensity-Restrained CORCEMA Optimization [*J. Am. Chem. Soc.* 2004, *126*, 8610–8611].

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ADDITIONS AND CORRECTIONS

Refinement of the Conformation of UDP−Galactose Bound to Galactosyltransferase Using the STD NMR Intensity-Restrained CORCEMA Optimization [*J. Am. Chem. Soc.* **2004**, *126*, 8610−8611]. V. Jayalakshmi, Thorsten Biet, Thomas Peters,* and N. Rama Krishna*

We also performed additional calculations by retaining the χ_1 torsion angle for V253 side chain in the gauche+ conformation as in the energy-minimized crystal structure. We assumed saturation of the methyls of I186 (this residue was not included in the previous calculations as it was just outside the 5 Å cutoff used), along with the L255 methyls. We also made the reasonable assumption that the V253 methyls escape saturation (due to low-field shifts induced by proximal aromatic rings). This resulted in an *R*-factor of 0.306 (and a protein correlation time of 23.5 ns) for the SICO structure with the ligand torsion angles $\alpha = 145.51°$, $\beta = 103.73°$, $\gamma = -91.60°$, $\phi = 83.60°$, $\psi = -131.88°$, and $\omega = 130.85°$. This *R*-factor is significantly lower than the corresponding *R*-factors for the energy-minimized crystal structure (0.428) and the original crystal structure (0.587). Most importantly, the SICO optimized ligand conformation in this case (see Figure 1 below) is essentially identical to the one we reported (ligand torsion angles differ by less than 4°), while the V253 side-chain orientation remains the same as in the crystal structure.

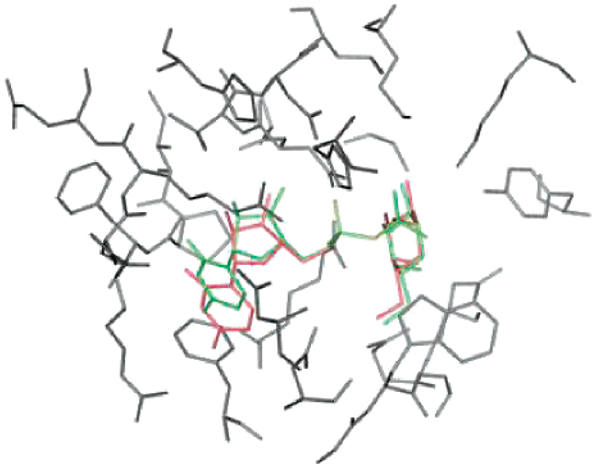

Figure 1.

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