

S1 Text

Structure generation

The coordinates for the orphan human nuclear receptor subfamily 4 group A member 1 (NR4A1), also denoted as nuclear hormone receptor NUR77 or orphan nuclear receptor TR3, are available from the protein database as entry 2QW4.pdb.¹ The underlying sequence has the UniProt identifier P22736.² The structure contains 233 residues and is resolved at 2.8 Å resolution. Three amino acids (EPQ) comprising the surface-loop region of a helix-turn-helix motif are not structurally resolved. The missing amino acids were added by the loop-modeling functionality provided within the SwissModel web service available at <http://swissmodel.expasy.org>.^{3,4,5,6}

Ligands **1**⁷ and **2**⁸ were constructed employing standard fragments within UCSF Chimera,⁹ charged using the AM1-BCC Hamiltonian,¹⁰ and minimized to a final gradient of 0.05 kcal mol⁻¹Å⁻¹ applying the GAFF force field.¹¹

References and Notes

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