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Supporting information for article:

A revisited version of the apo structure of the ligand-binding domain of the human nuclear receptor RXRα

Jérôme Eberhardt, Alastair G, McEwen, William Bourguet, Dino Moras and Annick Dejaegere

Supplementary Information: A revisited version of the apo structure of the ligand-binding domain of the human nuclear receptor RXRα

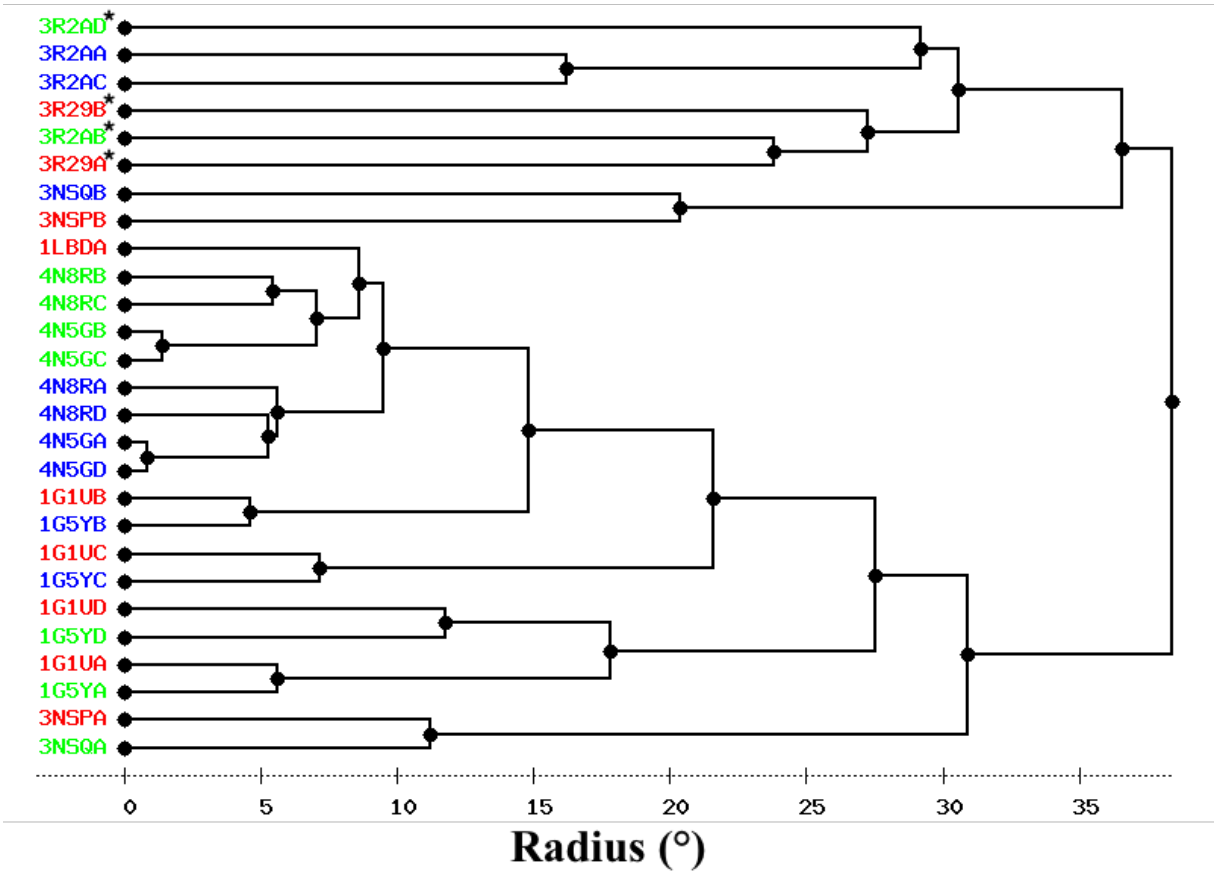

Fig. S1. Cluster analysis, using PSS (Gaillard et al, 2013), of all the RXR*α* LBD structures containing at least one chain where the RXR*α* LBD is indicated as being in the apo form. The tree is obtained from hierarchical clustering with the maximum-linkage method. Variables taken into account are all the common Φ and Ψ backbone dihedral angles in the RXR*α* LBD structures. Apo RXR*α* LBDs dimerized with an apo RXR*α* LBD are shown in red (however see text for discussion of 1G1U and 3NSP), apo RXR*α* LBDs dimerized with a holo RXR*α* LBDs in green and holo RXR*α* LBD chains (dimerized with an apo RXR*α* LBDs) in blue. The first four letters correspond to the structures PDB IDs and the last letter to the chain ID. The asterisk indicates the presence of a co-repressor peptide in interaction with the RXR*α* LBD. The clustering analysis shows that apo 1G1U (chains B and C) and 3NSP (chain B) are closer to holo 1G5Y (chains B and C) and holo 3NSQ (chain B) than to apo structures. As discussed in the text, density is visible in the ligand binding pocket for these structures, in agreement with the clustering. Likewise, apo RXR*α* LBDs 3NSP (chain A) is structurally similar to apo RXR*α* LBDs dimerized to holo RXR*α* LBDs 3NSQ (chain A). The clustering indicates that the structures closest to apo 1LBD are apo RXR*α* LBDs dimerized with ligand bound RXR*α*: 4N8R (chain B & C) and 4N5G (chains B and C) while the most distant structures from apo 1LBD are 3R2A, 3R29, 3NSQ (chain B) and 3NSP (chain B), due to their open conformation.

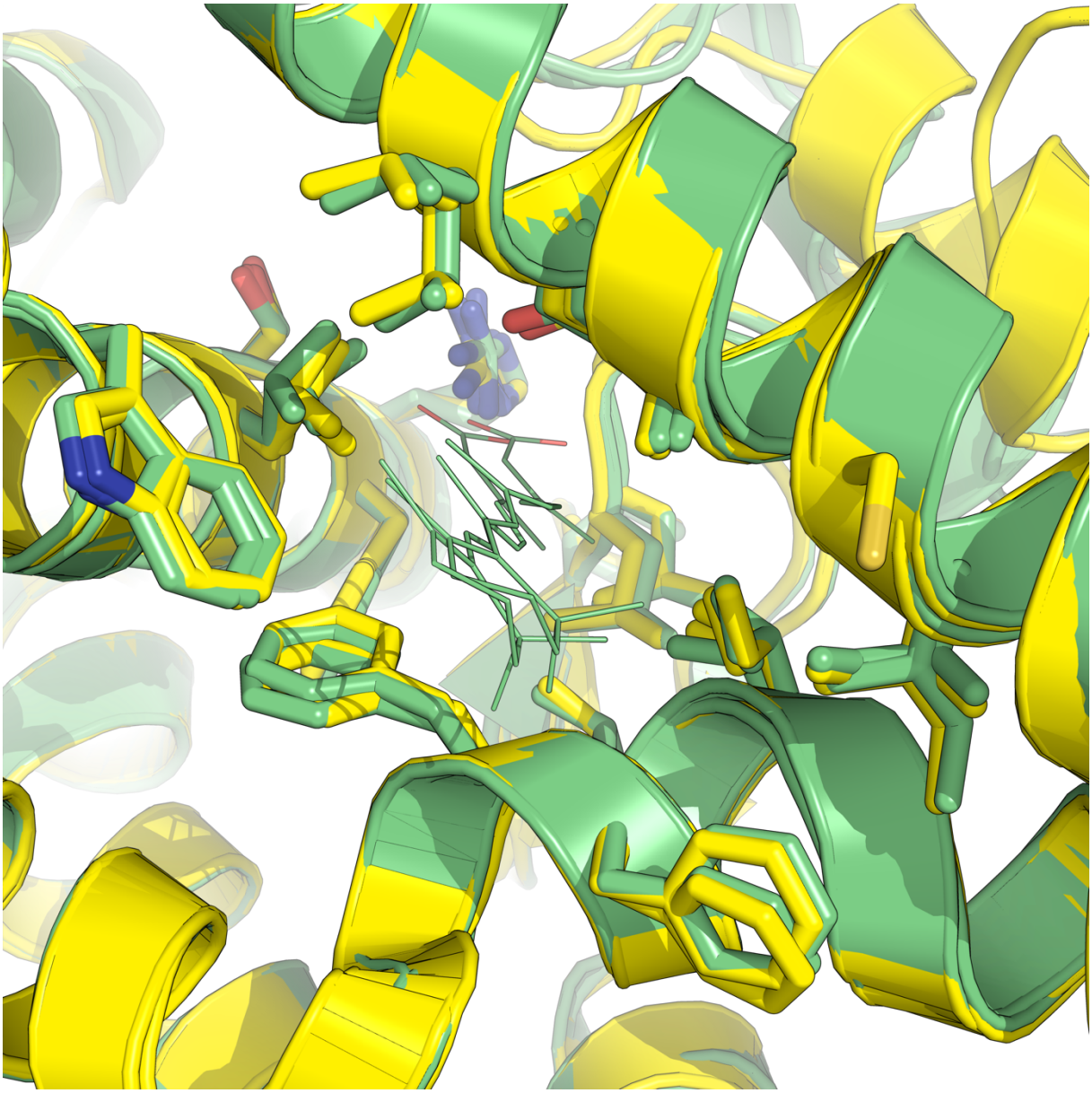

Fig. S2. Sidechain positions of residues, represented in sticks, in the ligand binding pocket of the RXRα LBD of 1G5Y (chains B and C; in green) and 1G1U (chains B and C; in yellow). The non-activating retinoic acid ligands present in the RXRα LBD of 1G5Y (chains B and C) are represented in lines.

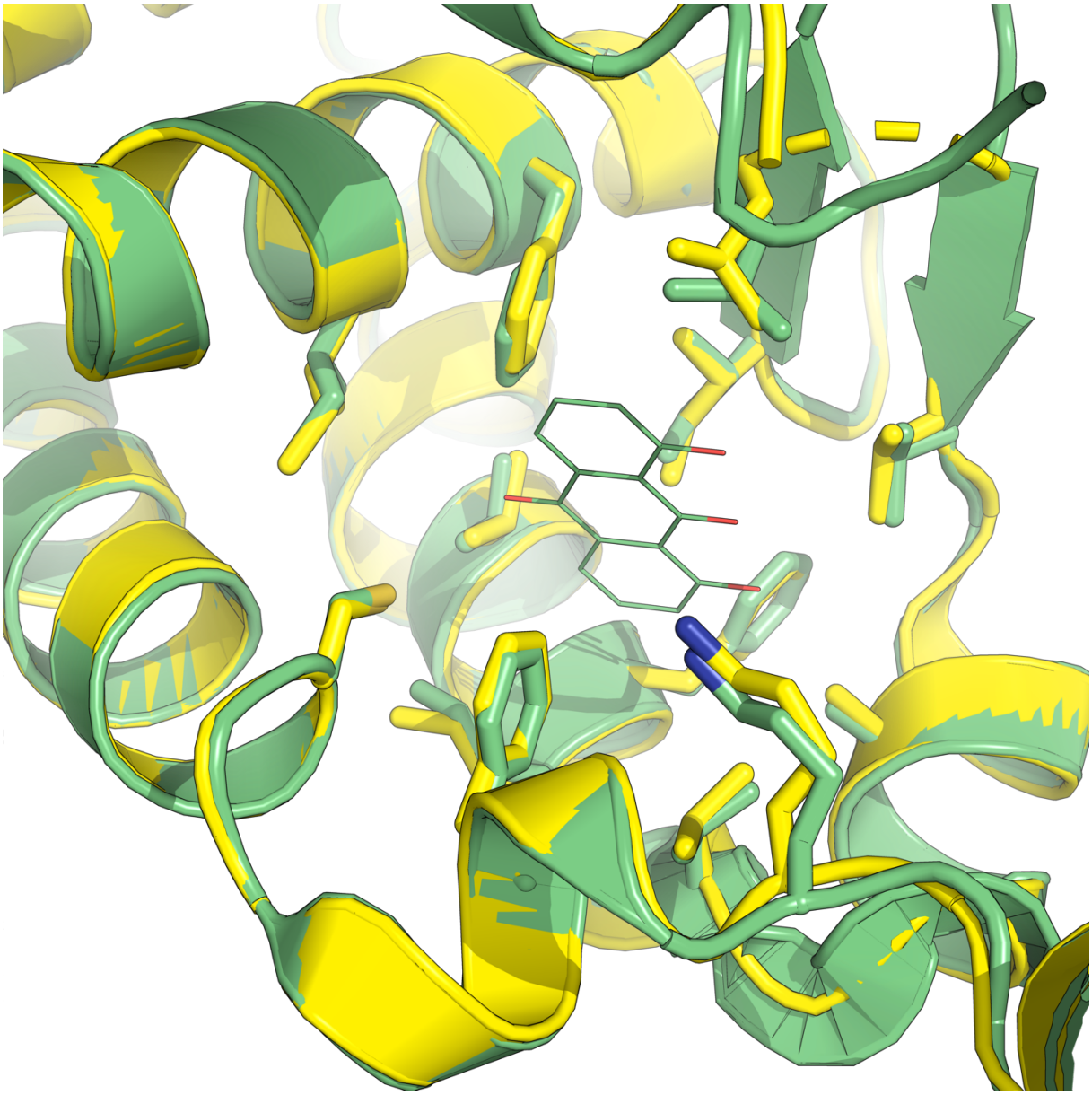

Fig. S3. Sidechain positions of residues, represented in sticks, in the ligand binding pocket of the RXRα LBD of 3NSQ (chain B; in green) and 3NSP (chain B; in yellow). The ligand danthron in the RXRα LBD of 3NSQ (chain B) is represented in lines.

Bibliography of Supplementary Material

Gaillard, T., Schwarz, B. B., Chebaro, Y., Stote, R. H. & Dejaegere, A. (2013). *Journal of chemical information and modeling* **53**, 2471-2482.