



SMART Teams 2013-2014 Research and Design Phase

Wisconsin Virtual Learning SMART Team

Jenna Amro, Noah Amro, Chenoah Gad, Elizabeth Merkel, Catherine Minter,
Sylvia Stuebs, Holly Van Gorden

Teacher: Karen O'Donnell

Mentors:

Allie Reeme, Ph.D Candidate, Microbiology and Molecular Genetics, Medical College of Wisconsin
Richard Robinson, Ph.D. Microbiology and Molecular Genetics, Medical College of Wisconsin

Vitamin D Receptor: An Underrated Hero

PDB: 1DB1

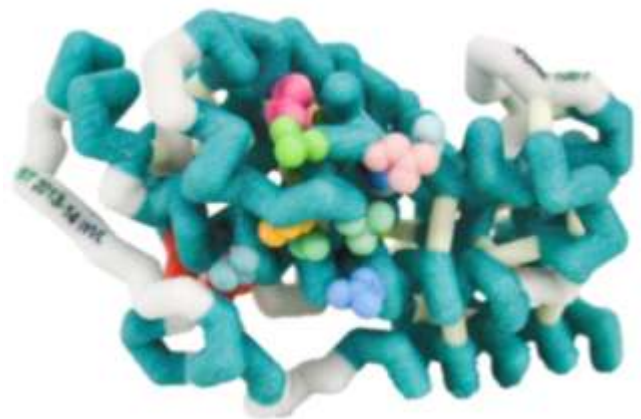
Primary Citation: Rochel, N., Wurtz, J.M., Mitschler, A., Klaholz, B., Moras, D. (2000). The crystal structure of the nuclear receptor for vitamin D bound to its natural ligand. *Molecular Cell* 5: 173-179.

Format: Alpha carbon backbone

RP: Zcorp with plaster

Description:

For over a century, vitamin D (vit. D) has been used as therapy for the bacteria *Mycobacterium tuberculosis* (*Mtb*) due to its effects on the immune system. Interest has risen for vit. D's ability to modulate immune responses by signaling through the vitamin D receptor (VDR). Vit. D is obtained through dietary sources, like seafood, or exposure to sun's UVB rays. Vit. D in its active form can passively diffuse into multiple cell types, such as lymphocytes, while the VDR, a transcription factor for vit. D regulated genes, can regulate the effects of the hormone in these cells. Vit. D has been shown to modulate the immune response during *Mtb* infection by controlling production of cytokines and antimicrobial peptides and its interactions with the VDR is critical for these effects. In order to recognize VDR's role during the immune response to *Mtb*, the Wisconsin Virtual learning SMART Team (Students Modeling A Research Topic) is using 3D printing technology to model the structure, primarily highlighting amino acids Arg274 and His305 which are required for ligand binding to the VDR. Scientists, recognizing vit. D's positive role during an immune response, will continue to investigate vit. D as a therapeutic agent to treat this significant plight.



Specific Model Information:

- Alpha helices are highlighted in dark cyan.
- Beta sheets are highlighted in crimson.
- The alpha carbon backbone is colored white.
- Hydrogen bonds are colored linen.
- Structural supports are colored light yellow.
- Amino acids in the active site are displayed in ball and stick and colored according to the following scheme:
 - Thr 415 – orange
 - Leu 417 – dark sea green
 - Val 418 – dark khaki
 - Leu 419 – green yellow
 - Val 421 – medium slate blue
 - Phe 422 – olive drab
 - Asp 232 – slate gray
 - Val 234 – aquamarine
 - Ser 235 – spring green
 - Ile 238 – dark goldenrod
 - Gln 239 – dodger blue
 - Ala 267 – honey dew
 - Ile 268 – gray
 - His 397 – indian red
 - Tyr 401 – deep pink
- Polar interactions involve the conserved salt bridge between Lys 264 and Glu 420, displayed in ball and stick and colored light blue and pale violet red respectively.
- A hydrogen bond is located between Ser 235 and Thr 415, displayed in ball and stick and colored spring green and orange respectively.

<http://cbm.msoe.edu/smartTeams/>

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