

Supplementary Materials: Improved Homology Model of Human *all-trans* Retinoic Acid Metabolizing Enzyme CYP26A1

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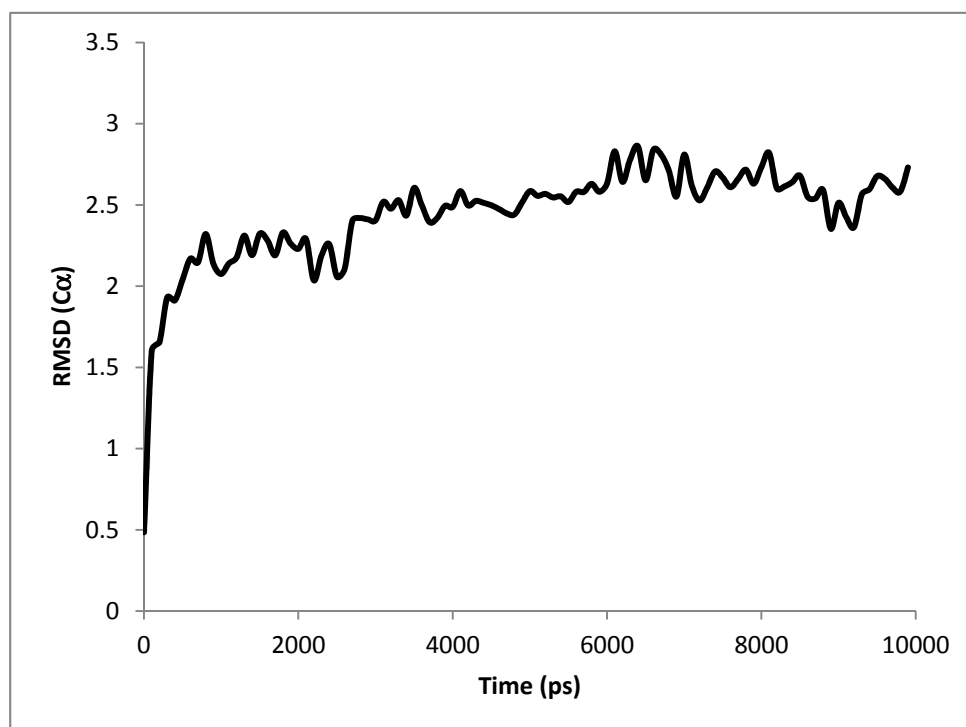


Figure S1. RMSD values of the positions of the C α atoms versus time, of the homology model obtained.

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Query  41  ALPLPPGTMGFPFFGETLQMVLQRRKFLQMKRRKYGFIYKTHLFGRPVVRVMGADNVRRI 100
      +LP+PPG  G P+ GETL  L  F + +++++G I+KT LFG+  + + GA  R +
Sbjct  10  SLPIPPGDFGLPWLGETLNF-LNDGDFGKKRQQQFGPIFKTRLFGKNVIFISGALANRFL 68

Query  101 LLGEHRLVSVHWPASVRTILGSGCLSNLHDSHKKQKKVIMRAFSREALECYVPVITEEV 160
      E      WP S R +LG  L+      H+ R+K++ +AF  L+ Y+P +  V
Sbjct  69  FTKEQETFQATWPLSTRILLGPNALATQMGEIHRSRKILYQAFLPRTLDSYLPKMDGIV 128

Query  161  GSSLEQWLSCGERGLLVYPEVKRMLFRIAMRILLGCEPQLAGDGDSEQQIVEAFEEMTRN 220
      LEQW  E  ++ YP+++R+ F +A  + +G +      QL  FE  +
Sbjct  129  QGYLEQWKGKANE--VIWYPQLRRMTFDVAATLFMGEK-----VSQNPQLFPWFETYIQG 180

Query  221  LFSLPIDVPFSGLYRGMKARNLIHARIEQNIRAKICGLRASEAGQGCKDALQLLIEHSWE 280
      LFSLP I +P +  + +AR L+ A +E+ I+A+      +      +DAL +L+  +
Sbjct  181  LFSLP IPIPLNTLFGKSQRARALLLALEKIIKAR-----QQQPPSEEDALGILLAARD 234

Query  281  RGERLDMQALKQSSTELLFGGHETTASAATSLITYLGlyphVLQKVREELKSKGLLCKSN 340
      + L +  LK      LLF GHET  SA +S  LG +  + ++VR+E  L
Sbjct  235  NNQPLSLPELKDQILLLLFAGHETLTSALSSFCLLLGQHS DIRERVVRQE QNKLQL----- 289

Query  341  QDNKLDMEILEQLKYIGCVIKETLRLNPPVPGGFRVALKTFELNGYQIPKGWNVISICD 400
      +L  E L+++ Y+  V++E LRL PPV GGFR  ++  +  G+  PKGW V Y I
Sbjct  290  -SQELTAETLKKMPYLDQVLQEVLRLLIPPVGGGFREL IQDCQFQGFHFPKGWLVSYQISQ 348

Query  401  THDVAEIFTNKEEFNPDRFMLPHPEDASR----FSFIPFGGGLRSCVGKEFAKILLKIFT 456
      TH  +++ + E+F+P+RF  P+ ++  F+ +PFGGGLR C+GKEFA++ +K+F
Sbjct  349  THADPDLYPDPEKFDPERFT---PDGSATHNPPFAHVFPFGGGLRECLGKEFARLEMKLFA 405

Query  457  VELARHCDWQLLNGPP-TMKTSPVYFVDNL 486
      L +  DW LL G  +  +P+  P DNL
Sbjct  406  TRLIQQFDWTLLPGQNLELVVTPSPRPKDNL 436

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Figure S2. CYP26A1 (Query) and CYP120A1 (Template; “Sbjct”) sequence alignment.