Table S1. Expanded side-by-side comparison of manual versus automated homology model creation for the Col α1(XI) NPP protein.

I: BLAST		
Method	Manual	DockoMatic
Time	5 minutes	1 minute
Steps	1) Select a saved .txt file of the sequence or copy and paste the entire sequence into the box labeled "Enter ascension number(s), gi(s), or FASTA sequence(s)." 2) In the "Choose Search Set" section, select "Protein Data Bank proteins (pdb)" from the "Database" dropdown. 3) Click the BLAST button located at the lower left side of the webpage. The process is initiated and takes less than a minute to generate a list of sequences. 4) Under the "Descriptions" section select the protein link from the "Accession column" that has the lowest "E value". 5) On the right side of the web page under "Protein 3D Structure", select the link to the protein, e.g. "N-Terminal Nc4 Domain Of Collagen IX." 6) In the "View or Save 3D Structure" box, select "PDB" from the "File Format" dropdown followed by "Save file" from the "Display as" dropdown and click the "View structure" button to initiate the PDB file download, which enables the user to save the structure to their computer.	1) Select the "Output Directory" box in the TIM wizard, choose the "Project" file from the drop down to specify the homology model output directory. 2) Copy and paste the 223 amino acids for the Col α1(XI) NPP protein into the box below the "Sequence" tab. Alternatively, select the "Sequence" tab and browse to the location of a saved .txt file containing the protein sequence. Provide a name for the homology model structure file by entering HM Col XI NPP in the "Name" tab. Select the "Next" button at the bottom of the Wizard.
II: MODELLER		

Method	Manual	DockoMatic
Time	45 minutes	4 minutes
Steps	1) Download the ".tar.gz format (for Unix/Linux)" link in the first line of the tutorial page and unzip the file. 2) Open the "TvLDH.ali", from the "basic-example" file, in a text editor and modify the script to NPP sequence. Rename the TvLDH sections to NPP and save in the .ali format in your project folder. 3) Open the "align2d.py", from the "basic-example" file, in a text editor and change the '1bdm' labels to 2UUR; the structure of the Nc4 domain of Col IX, i.e. the template. Update all TvLDH labels to NPP, the desired protein sequence name. 4) Open terminal program and enter the "Project" file directory. Run the align code, "mod9.9 align2d.py" in MODEL-LER. A new .ali file and .pap file will be generated in the "Project" file (e.g. NPP-2UUR.ali and NPP-2UUR.pap). 5) Open the "model-single.py", from the "basic-example" file, in a text editor and change the 'TvLDH-1bdma.ali' label to the NPP-2UUR.ali file created by MOD-ELLER. Update 1bdm and TvLDH labels as done in previous steps, respectively. Save the updated file as model-single.py in the Project file 6) Return to terminal in the "Project" file directory and type "mod9.9 model-single.py" and press enter.	1) Once a list of models is generated in the TIM wizard, select the homologous protein from the top of the list and select the "Next" button. 2) Highlight the homology model file in the TIM wizard window, and then select the "Next" button. 3) Protein sequence data will appear in the wizard window showing the 5 homology versions of the target protein. Select the "Next" button to initiate creation of homology models for NPP. 4) Once DockoMatic creates the homology models, select the top Homology model from the list and click the finish button in the lower right side of the Wizard window.

For table of content use only

DockoMatic 2.0: High Throughput Inverse Virtual Screening and Homology Modeling

Casey Bullock, Nic Cornia, Reed B. Jacob, Andrew Remm, Thomas Peavey, Ken Weekes, Chris Mallory, Julia Thom Oxford, Owen M. McDougal, Tim Andersen