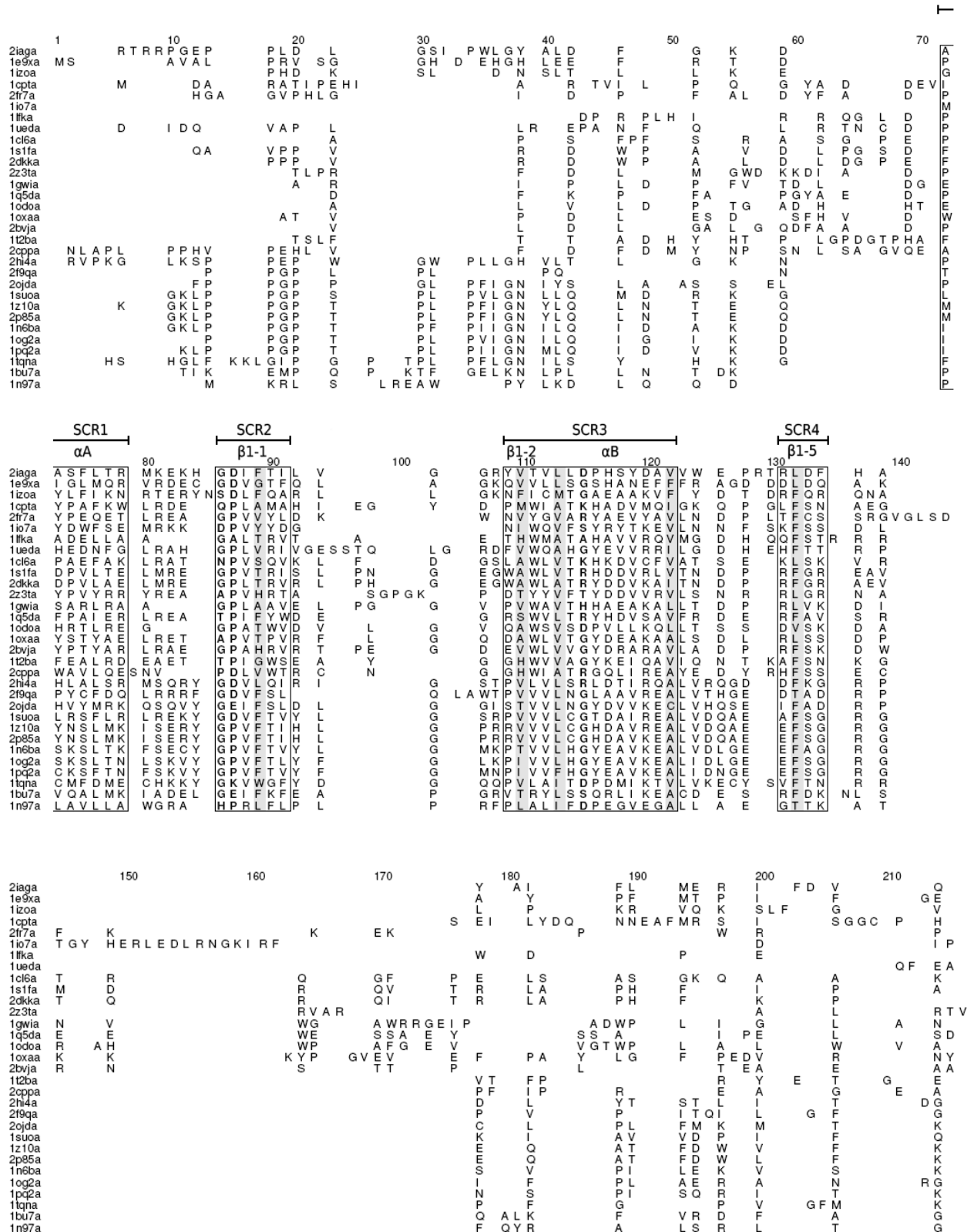


Prediction and analysis of the modular structure of cytochrome P450 monooxygenases

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Supplementary material



[illegible]

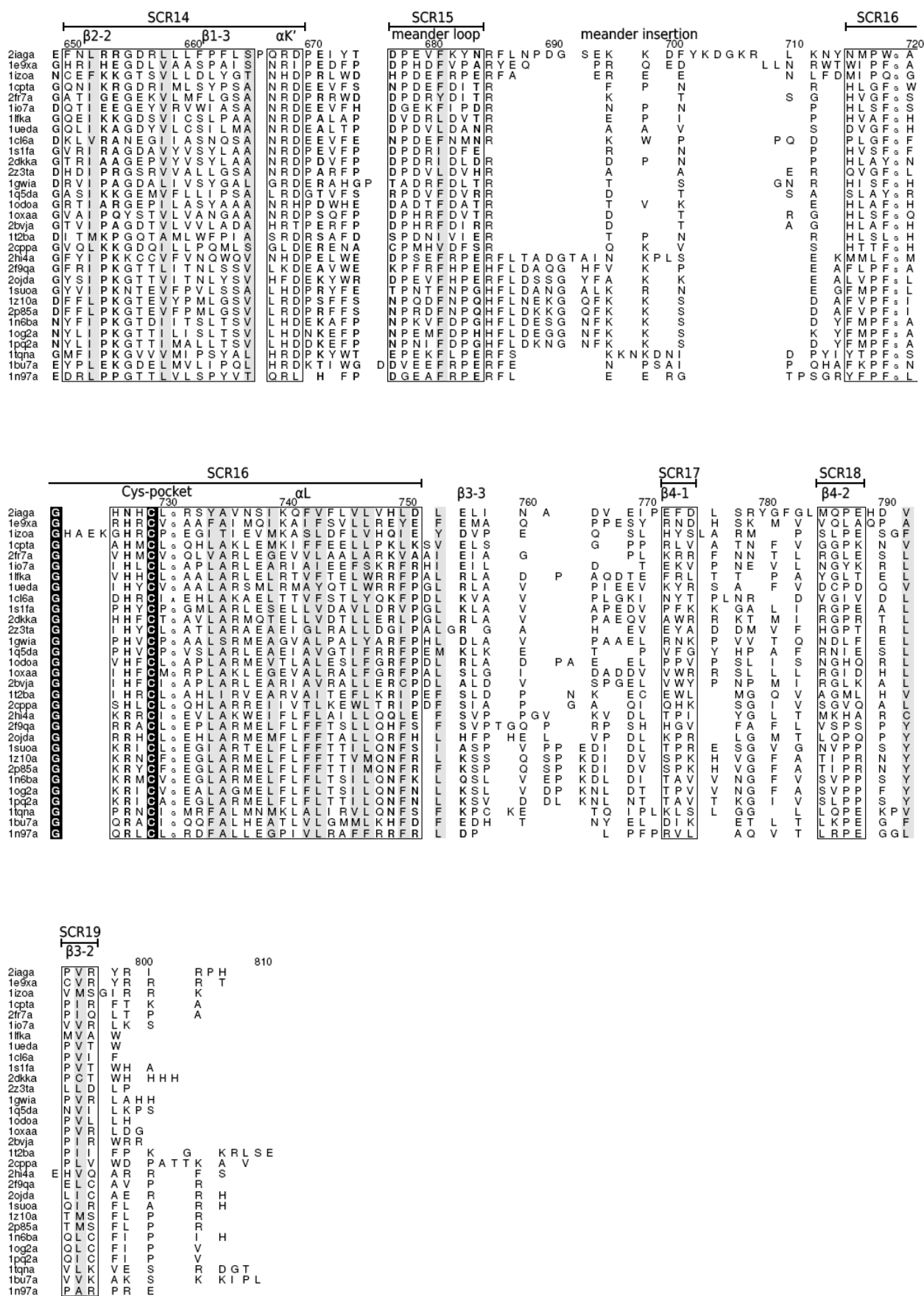


Figure S1 - Structure-based multisequence alignment of 31 CYP structures.

Regions marked by black boxes in the alignment have high P'_{ij} and imply regions of conserved secondary structure. Pos87 and the corresponding residues are highlighted in red.

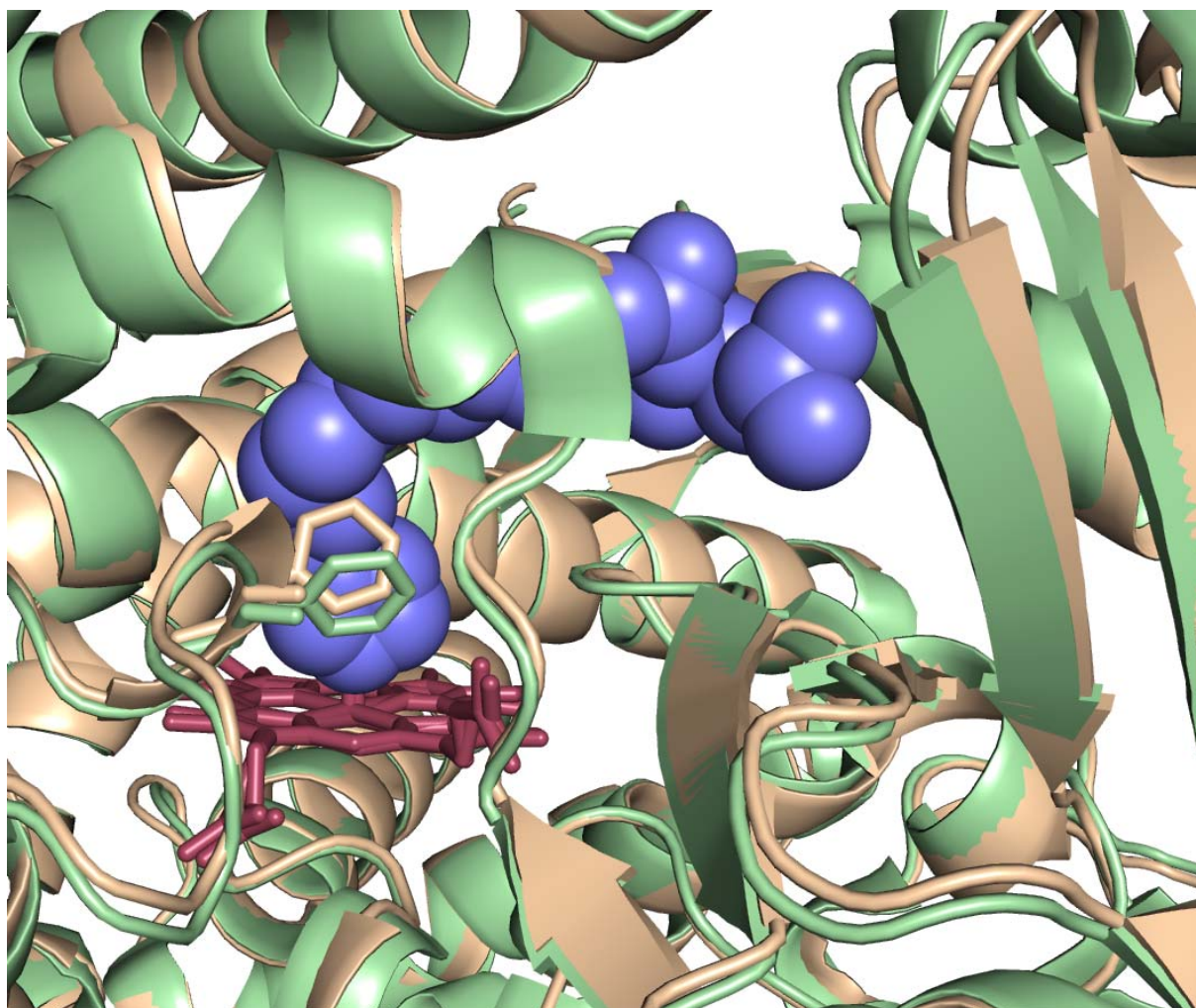


Figure S2 - Comparison of substrate-bound and substrate-free structure of CYP102A1 (P450 BM-3)

The substrate free structure is shown in wheat [PDB: 1BU7]. The substrate-bound structure [PDB: 3BEN] in green (with bound inhibitor N-[12-(1H-imidazol-1-yl)dodecanoyl]-L-leucine in blue). The phenylalanines at positions 87 are represented as sticks.

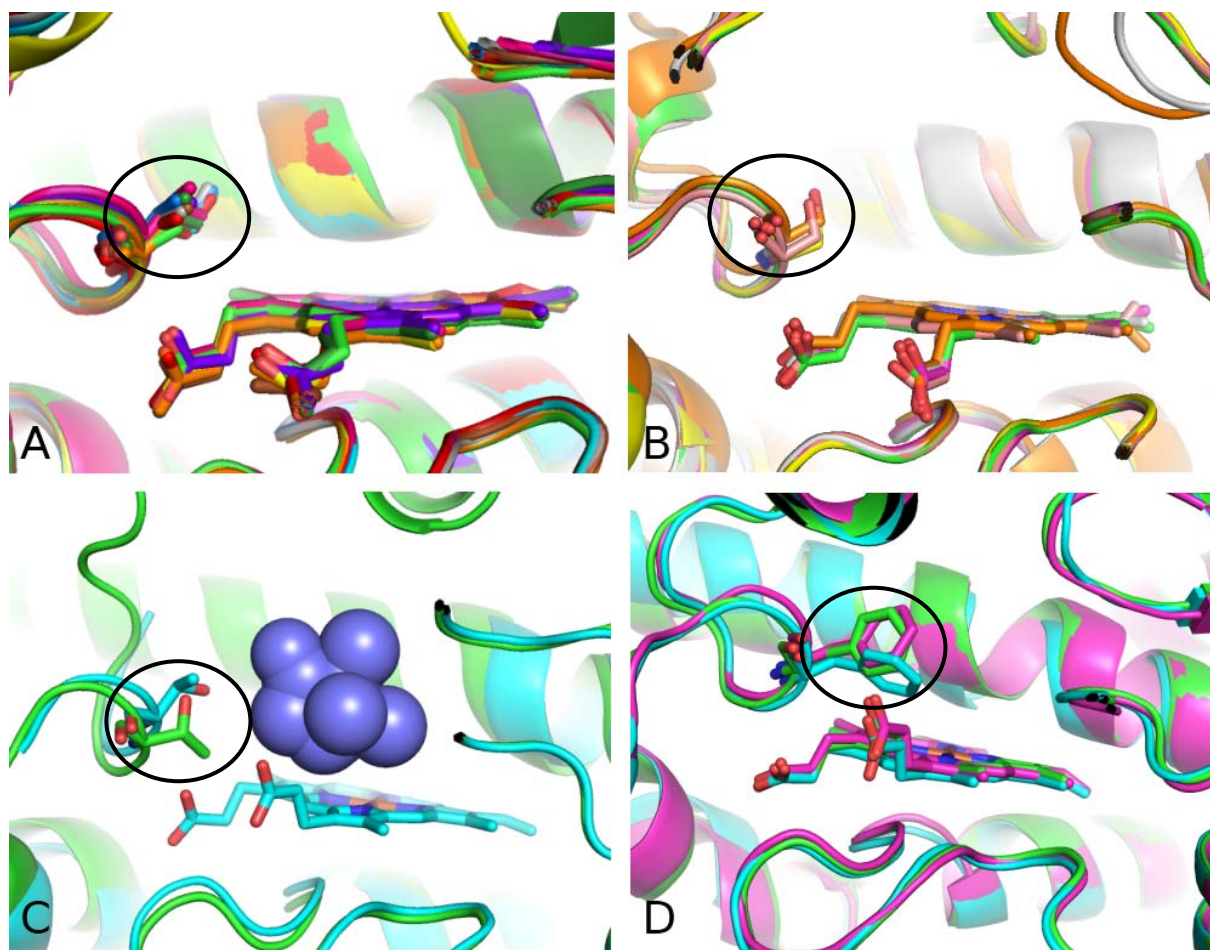


Figure S3 - Comparison of the F87 corresponding residues indicated (black circle) in multiple structures of the CYP2C family, CYP3A4, CYP101D (P450_{cam}) and CYP102A1 (P450 BM-3)

(A) Structures of the homologous family CYP2C were superimposed. A113 in CYP2C5 [PDBs: 1DT6 (light green), 1N6B (orange), 1NR6 (yellow)], I113 in CYP2C8 [PDBs: 2VN0 (cyan), 1PQ2 (brown), 2NNH (red), 2NNI (grey), 2NNJ (blue)] and V113 in CYP2C2 [PDBs: 1OG2 (dark green), 1OG5 (purple), 1R9O (magenta)] point in the direction of the heme. **(B)** Multiple structures of CYP3A4 were superimposed. For S119 it could be shown for all structures that it points towards the heme [PDBs: 1TQN (light green), 1W0E (pink), 1W0F (magenta), 1W0G (pink), 1J0D (grey), 2V0M (orange)]. **(C)** Open, substrate-free [PDB: 3L61] and closed, substrate-bound [PDB: 2CPP] CYP101D (P450_{cam}) both have T101 pointing towards the heme. Bound camphor is shown in blue. **(D)** F87 of CYP102A1 in points towards the heme in multiple structures [PDBs: 1BU7 (light green), 1FAG (cyan), 1BVY (magenta)].