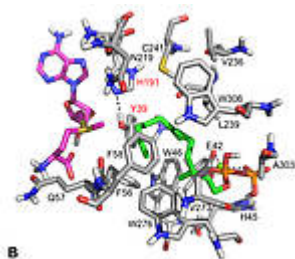


Protein Models

The project group Applied Modelling (formerly research group [Computer Chemistry](#)) is working on protein structures based on both *de-novo* molecular dynamics and homology modelling.

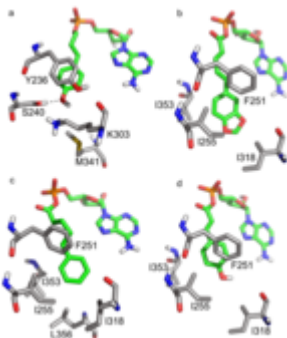
2020: Marie Chantal Lemfack, Wolfgang Brandt, Katja Krüger, Alexandra Gurowietz, Jacky Djifack, Philip Jung, Marius Hopf, Heiko Noack, Björn Junker, Stephan von Reuß, Birgit Piechulla. Reaction mechanism of the SAM-dependent FPP C-methyltransferase toward the formation of pre-sodorifen pyrphopshapte by *Serratia plymuthica* 4Rx13, submitted



Active site of the SAM-dependent FPP C-methyltransferase from *Serratia plymuthica* 4Rx13

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2019: W. Brandt. 2019. A piperic acid CoA ligase produces a putative precursor of piperine, the pungent principle from black pepper fruits. *Plant Journal* in press



PipCoA ligase with docked piperoyl-AMP (b)

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PipCoA ligase with docked 5-phenylpentanoyl-AMP (c)

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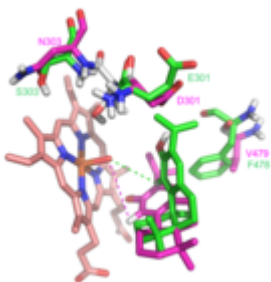
PipCoA ligase with docked 4-coumaroyl-AMP (d)
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2018: D. Eisenschmidt-Bönn, N. Schneegans, A. Backenköhler, U. Wittstock, W. Brandt. 2018. A Structural diversification during glucosinolate breakdown: mechanisms of thiocyanate, epithionitrile and simple nitrile formation. *The Plant Journal* 99(2):329-343



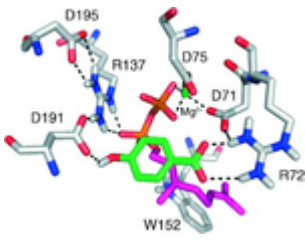
Arabidopsis thaliana nitrile-specifier protein 3 (AtNSP3)
[Model Download](#)

2016: U. Scheler, W. Brandt, A. Porzel, K. Rothe, D. Manzano, D. Bozic, D. Papaefthimiou, G. U. Balcke, A. Henning, S. Lohse, S. Marillonnet, A. K. Kanellis, A. Ferrer, A. Tissier. 2016. Elucidation of the biosynthesis of carnosic acid and its reconstitution in yeast. *Nature Communications*, 7.



3D-model of CYP76AH1
[Model Download](#)

2008: L. Bräuer, W. Brandt, D. Schulze, S. Zakharova, and L. Wessjohann. 2008. A Structural Model of the Membrane-Bound Aromatic Prenyltransferase UbiA from *E. coli*. *Chembiochem* 9:982-992.



Membrane-Bound Aromatic Prenyltransferase UbiA from *E. coli*
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