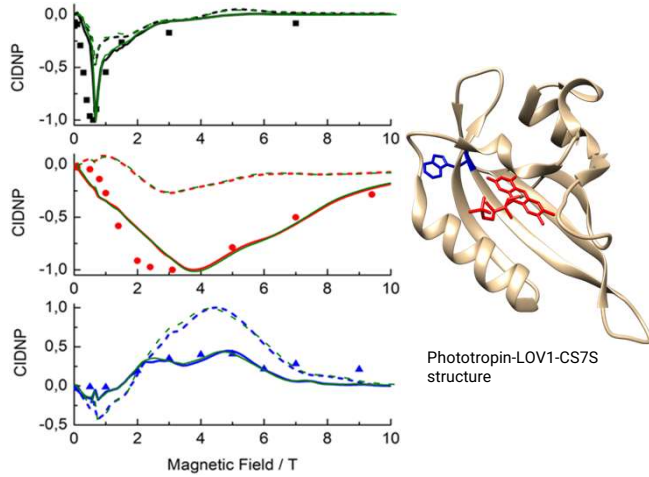




MAGNETIC RESONANCE SPECTROSCOPY SIMULATIONS

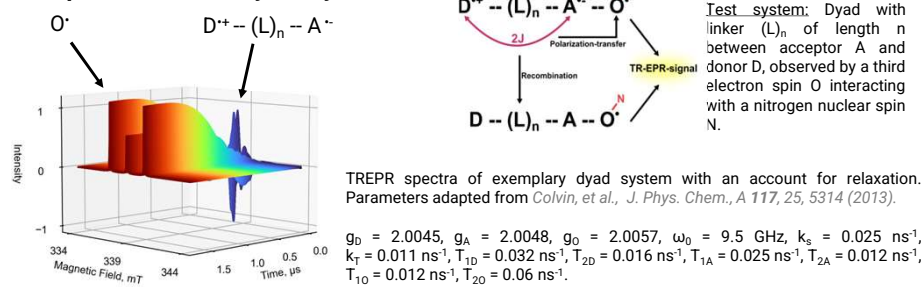
Versatile theories:	Applications:	Integration and Linking:
Analytic propagation for $t \rightarrow \infty$. Numerical propagation on a time grid.	CW-AQEPR/NMR. Complex pulse sequence.	Combining electronic structure and spin dynamics.
Rotating frame approximation. Pulse sequences.	CIDNP/CIDEP	Multiscale approaches.
Arbitrary spin states. Thermal ensembles. Chiral states.	Correlation methods DEER COSY etc.	Graphical and intuitive user interface.
Multiple spin relaxation terms. Multi-spin systems.		

Example 1: Photo-CIDNP effect in phototropin-LOV1-C57S



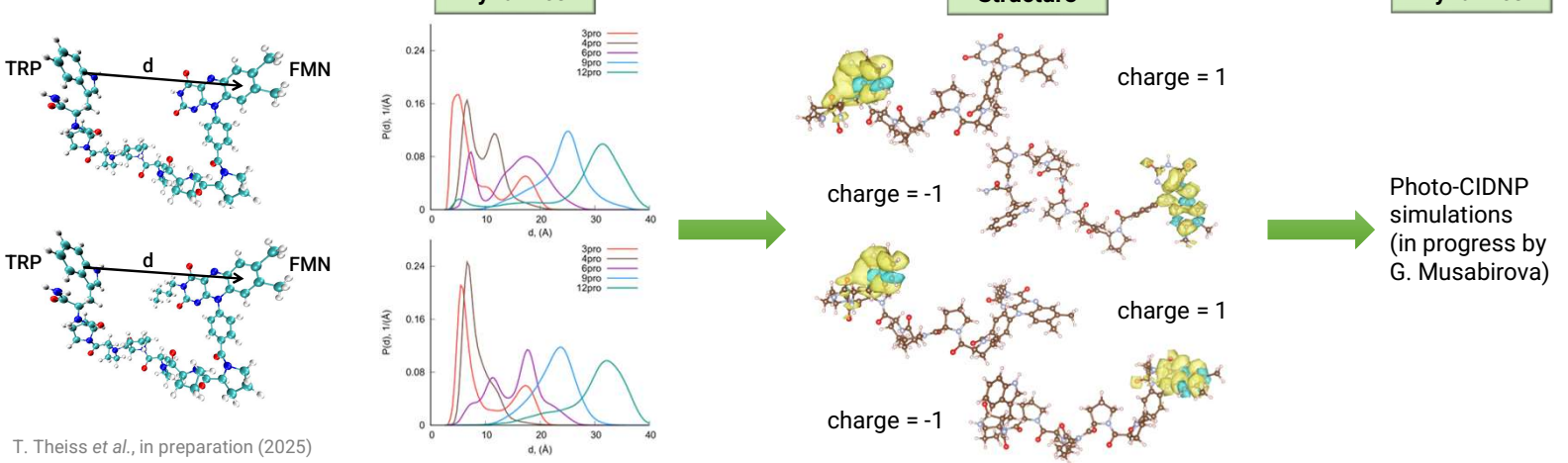
Comparison of the experimental (dots) and simulated (lines) CIDNP field dependencies for ^1H (top), ^{13}C (middle) and ^{15}N (bottom) nuclei taken from Ding et al., *Sci. Rep.*, 9, 18436 (2019). The green lines represent results of MolSpin simulations.

Example 2: TREPR of dyads system



SIMULATIONS FOR THE ARTIFICIAL DIADS

Jointly with T. Gulder, Ch. Tegenkamp, J. Matsysik, et al.

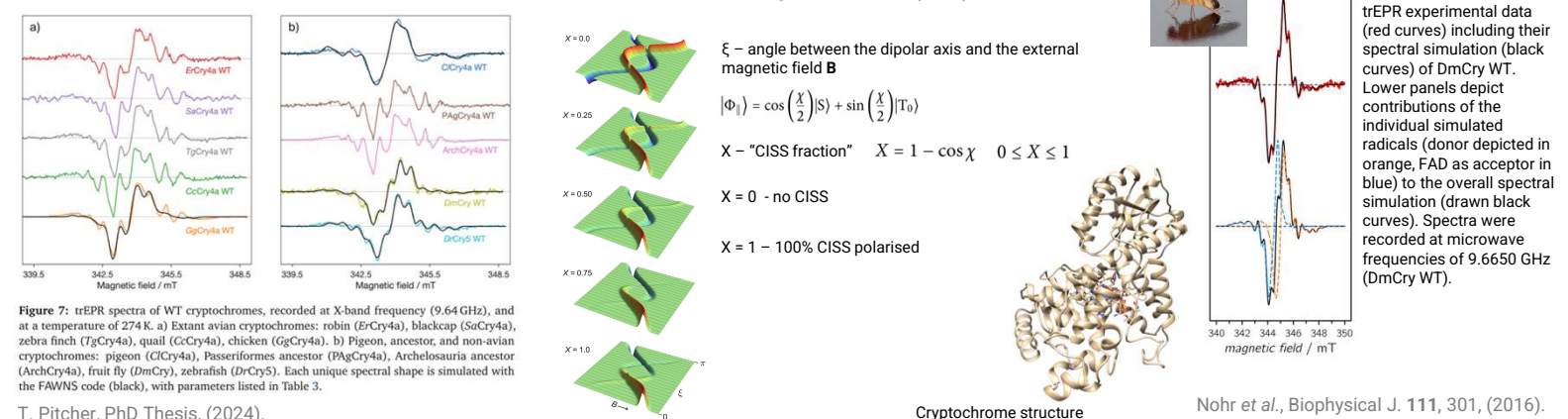


T. Theiss et al., in preparation (2025)

TREPR SIMULATIONS FOR THE DROSOPHILA CRYPTOCHROME

Jointly with P. Hore

Y. Ren, P.J. Hore, *J. Chem. Phys.* 159, 145104 (2023)



T. Pitcher, PhD Thesis, (2024).

