Optical NMR for spin- & photochemistry

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The group aims for understanding the **spin- and photochemistry** of natural and artificial photosynthetic systems, of photoreceptors and materials as well as for development and application of **optical NMR methods**. Furthermore, being aware of the rising global problem of **microplastics**, we identify, analyse and optimise enzymes able to degenerate PET.

Signal enhancement above 20000

Photochemically induced dynamic nuclear polarization (photo-CIDNP) in solids allows for enhancement of NMR intensities by induction of ***non-Boltzmann nuclear spin states***. The best enhancement is achieved at 2.4 T (Fig. 1).

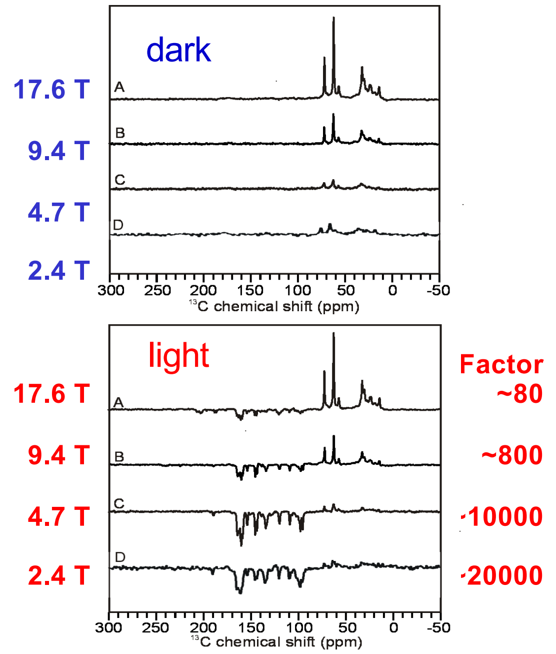

Fig. 1. ^{13}C photo-CIDNP MAS NMR spectra of reaction centers of a photosynthetic purple bacterium in dark (A) and light (B).

Leaves of plants are not too big

The strong signal increase allows detecting the chlorophyll cofactors involved in photo-CIDNP in isolated reaction centers (Fig. 1), and even in entire ***plants*** (Fig. 2).

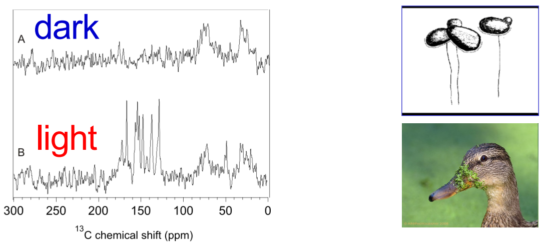

Fig. 2. ^{13}C photo-CIDNP MAS NMR spectra of intact leaves of *Spirodela* (duckweed) at 4.7 T in dark (A) and light (B).

Functional relevance?

The effect occurs in all families of photosynthetic organisms which were tested (Fig. 3) appearing to be ***conserved in evolution***.

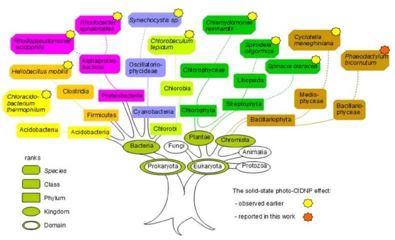

Fig. 3. The tree of life. Yellow stars indicate where the effect has been observed.

Biological photo-switch

In plants and many microorganisms, phytochromes regulate a numerous light-dependent processes. All phytochromes switch photochromically between two states, ***Pr*** and ***Pfr***. The phototransformation is triggered by a double-bond isomerization of an open-chain ***tetrapyrrole chromophore*** (Fig. 4).

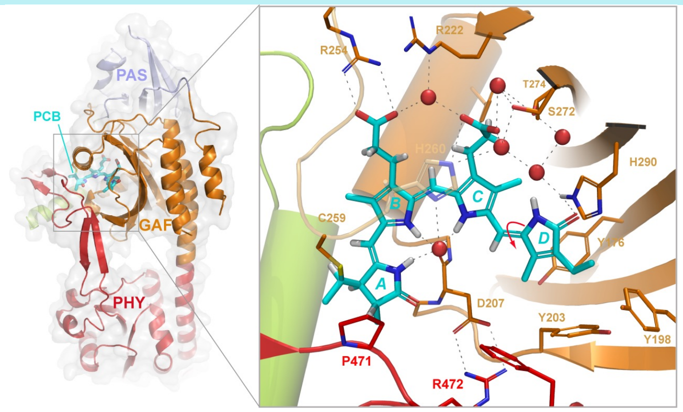

Fig. 4. Structure of cyanobacterial phytochrome Cph1 in its ***Pr*** state.

PET-degrading enzymes

The biocatalytic degradation of PET by microbial enzymes (Fig. 5) has recently emerged as attractive option for a future eco-friendly recycling process for plastic waste. Biophysical and bioanalytical methods to study structural and functional relationships of these enzymes provide a better understanding of the degradation mechanism at the molecular level.

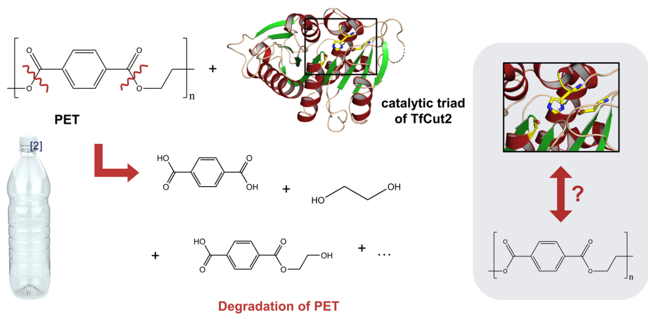

Fig. 5. Schematic representation of the enzymatic PET degradation. The aim of ongoing research is to elucidate the molecular degradation mechanism.

Metabolomics studies

HR-MAS NMR applied to intact zebrafish (*Danio rerio*) embryos, as a model of vertebrate development, to elucidate toxicity effects and changes in metabolic profiles associated with PET nanoparticles exposure (Fig. 6)

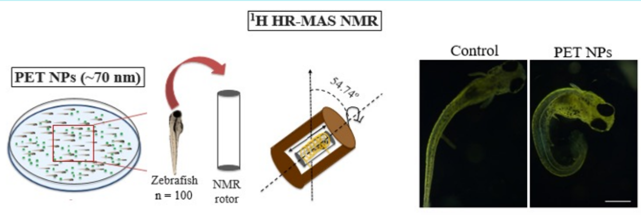

Fig. 6. HR-MAS NMR used to elucidate toxicity of PET NPs on intact zebrafish