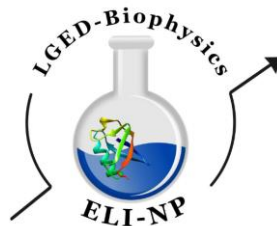


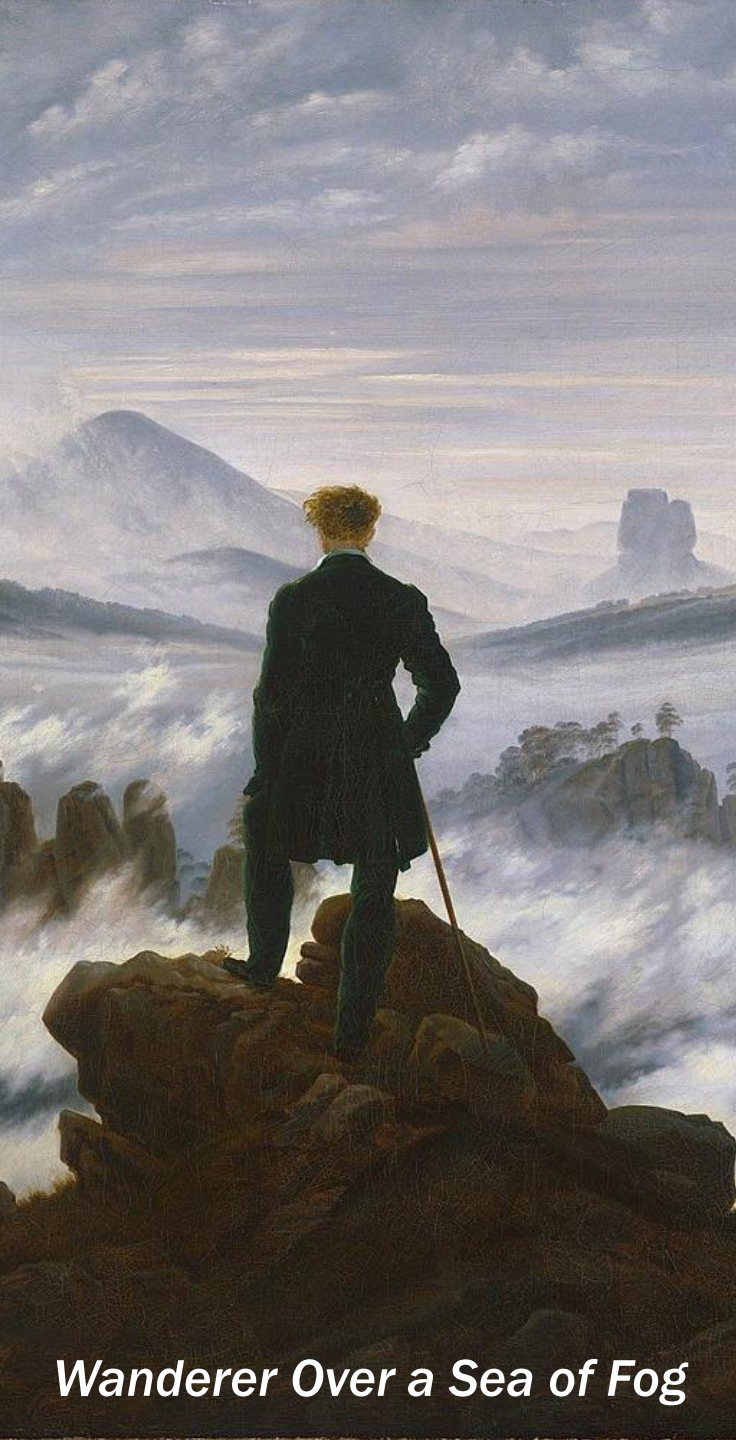
Proton Protein Paintings



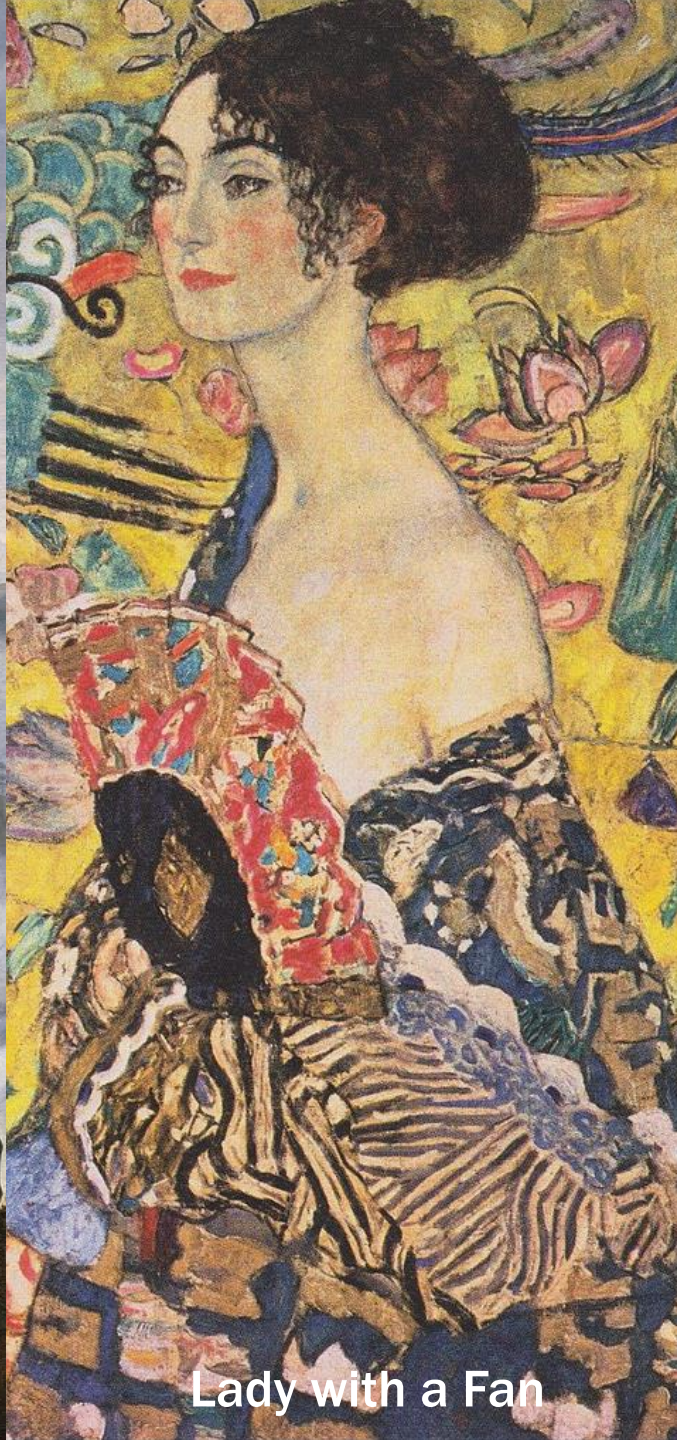
Octavian Ianc
Biophysics & Biomedical Applications
Laboratory @ ELI-NP
University of Bucharest



Starry Night



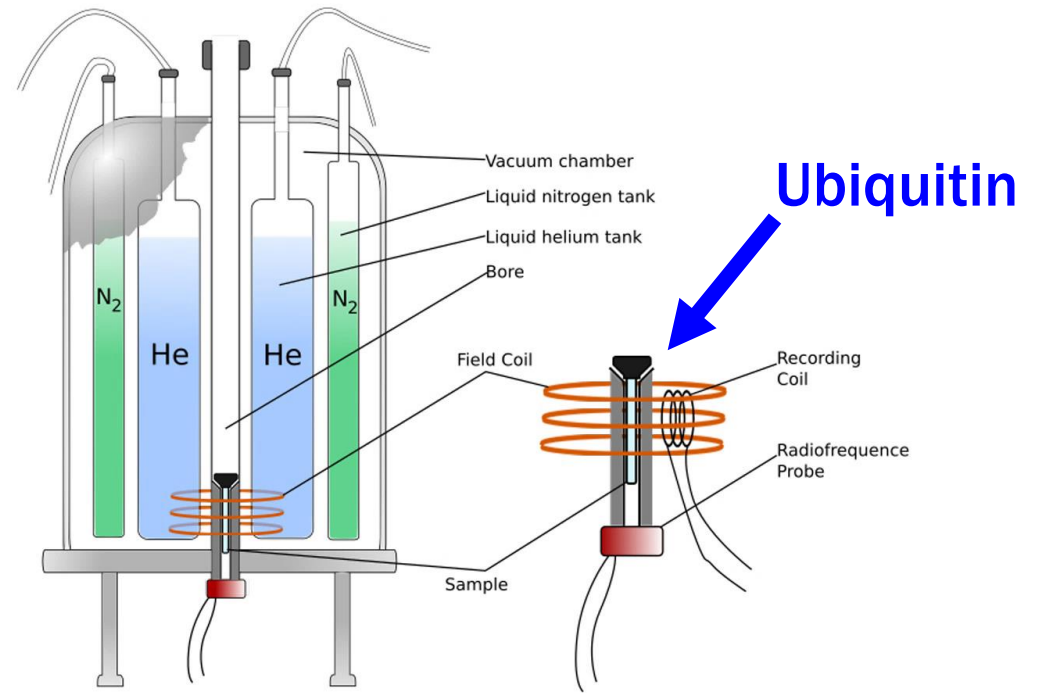
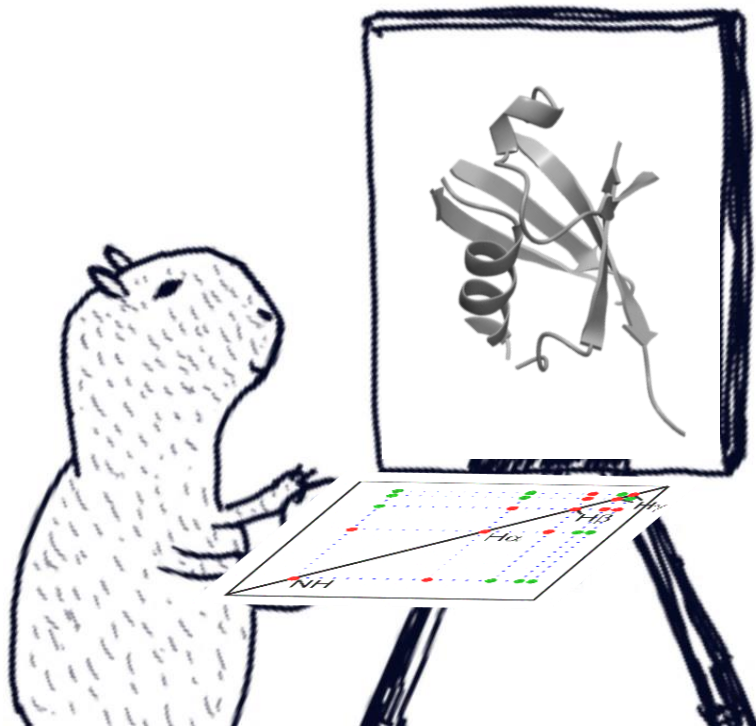
Wanderer Over a Sea of Fog



Lady with a Fan

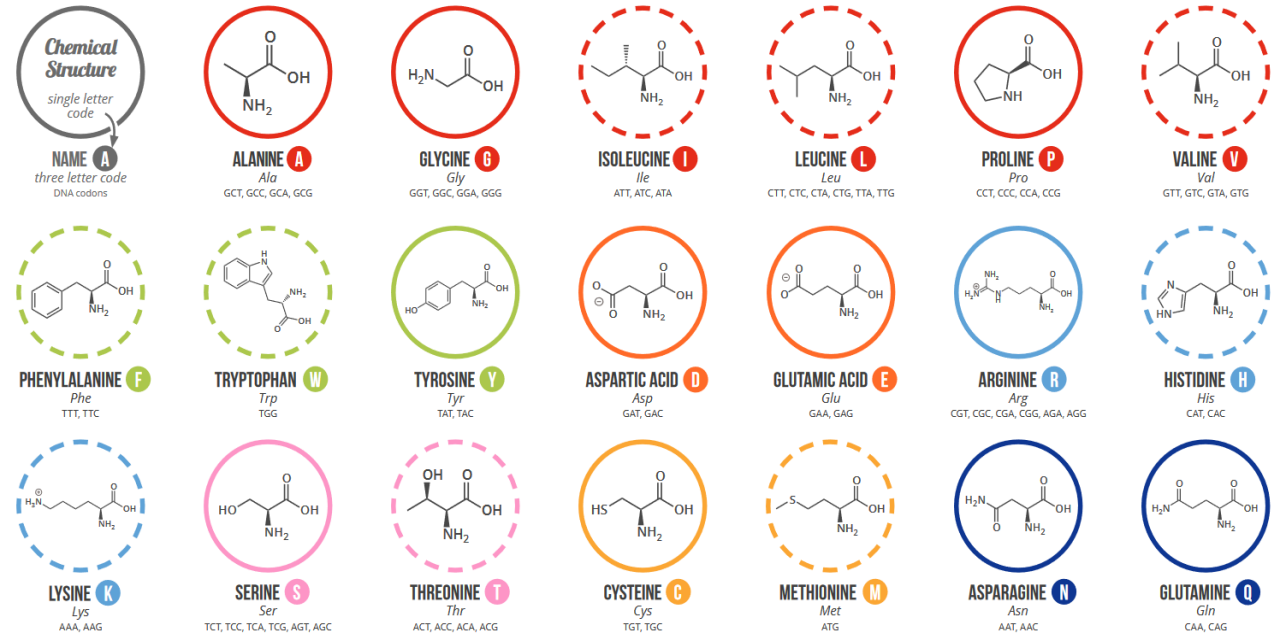
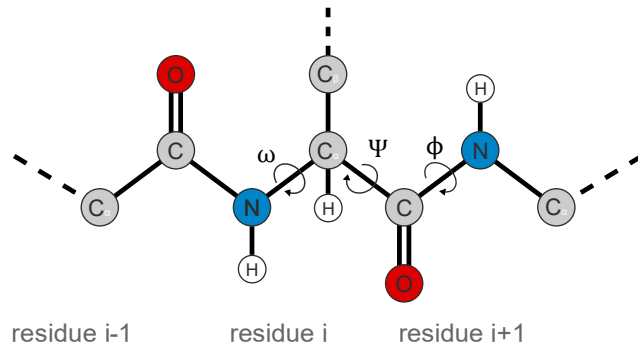


Creation of Adam

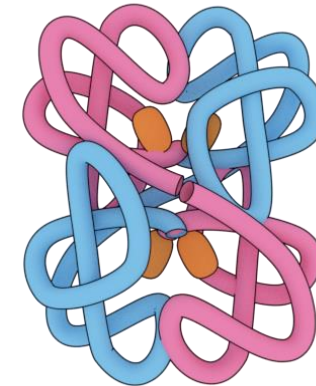
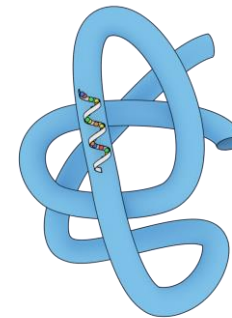
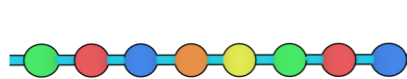


Adapted from Ana Lupoaie's drawing

The Subject: Proteins



Adapted from compoundchem.com

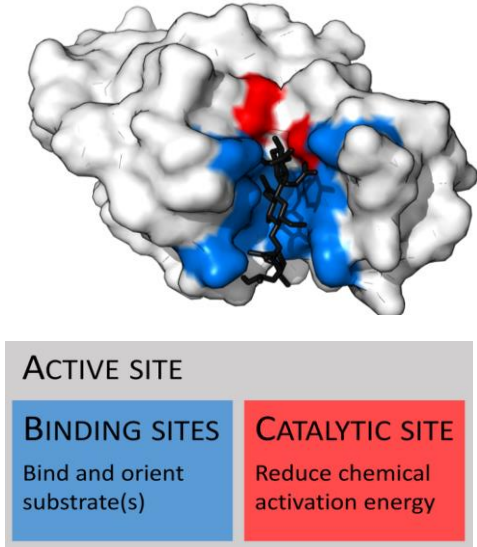
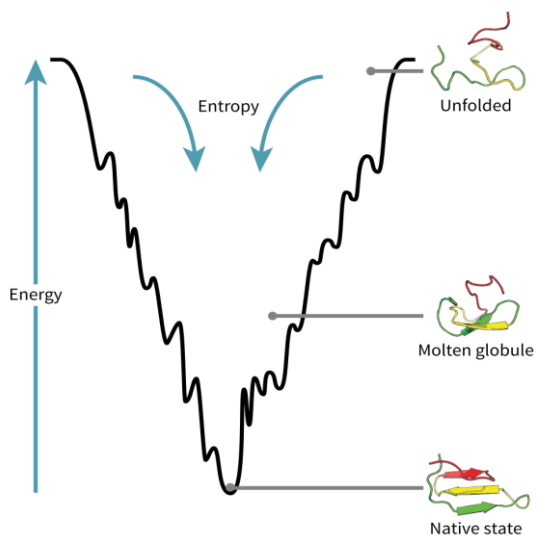


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Structure

Function

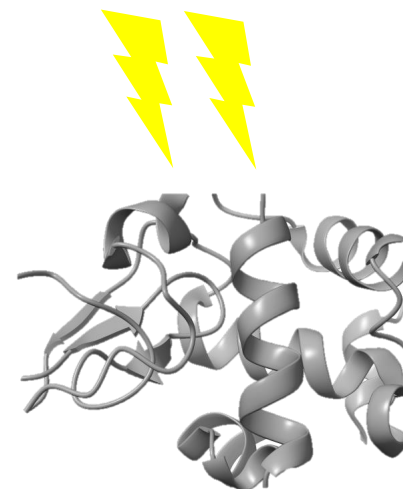


Thomas Splettstoesser

Adapted from Thomas Shafee

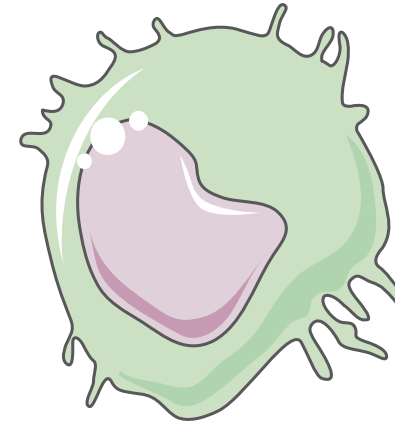
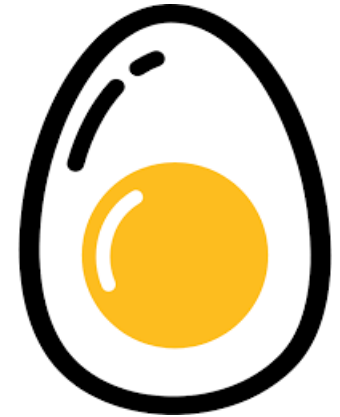
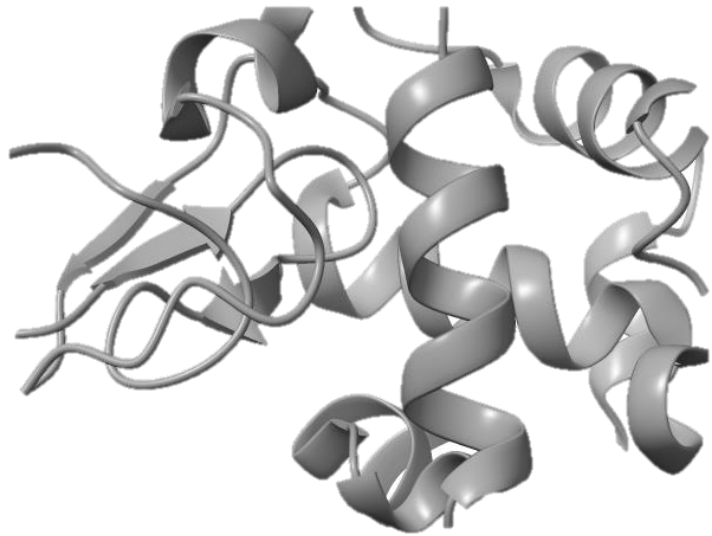
Biological response to radiation

Radiation



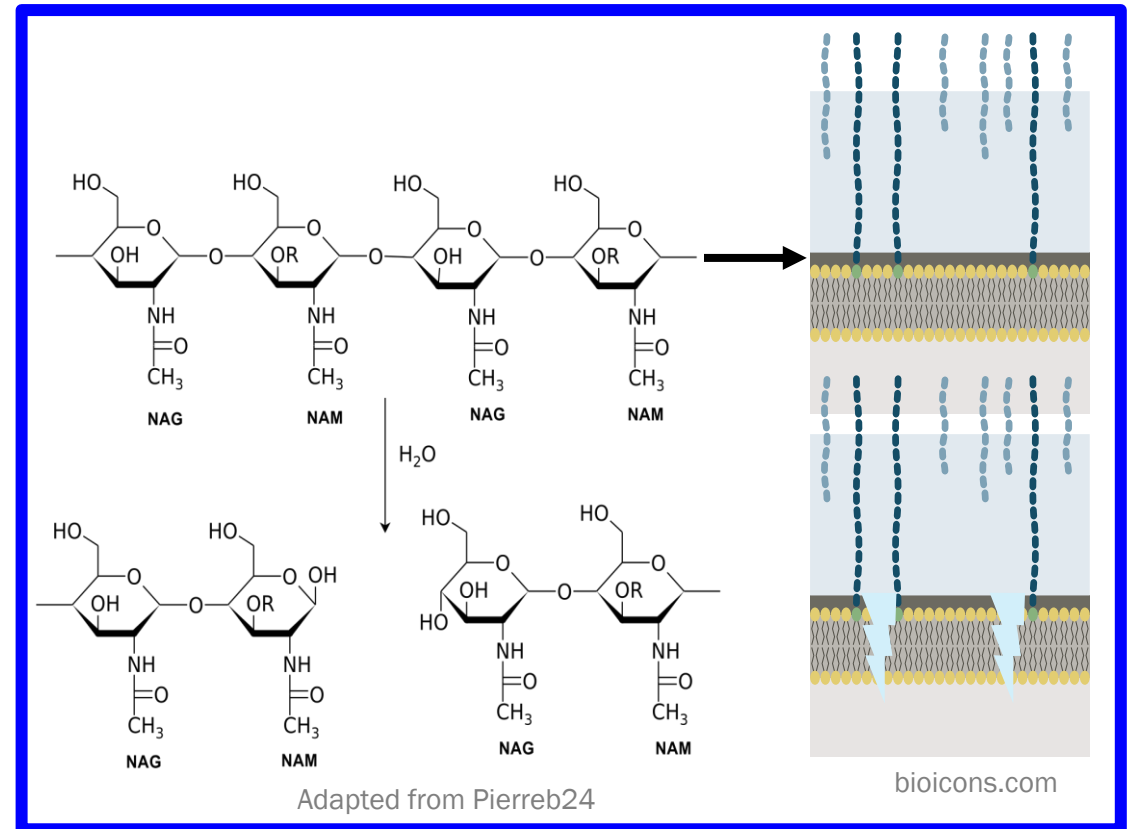
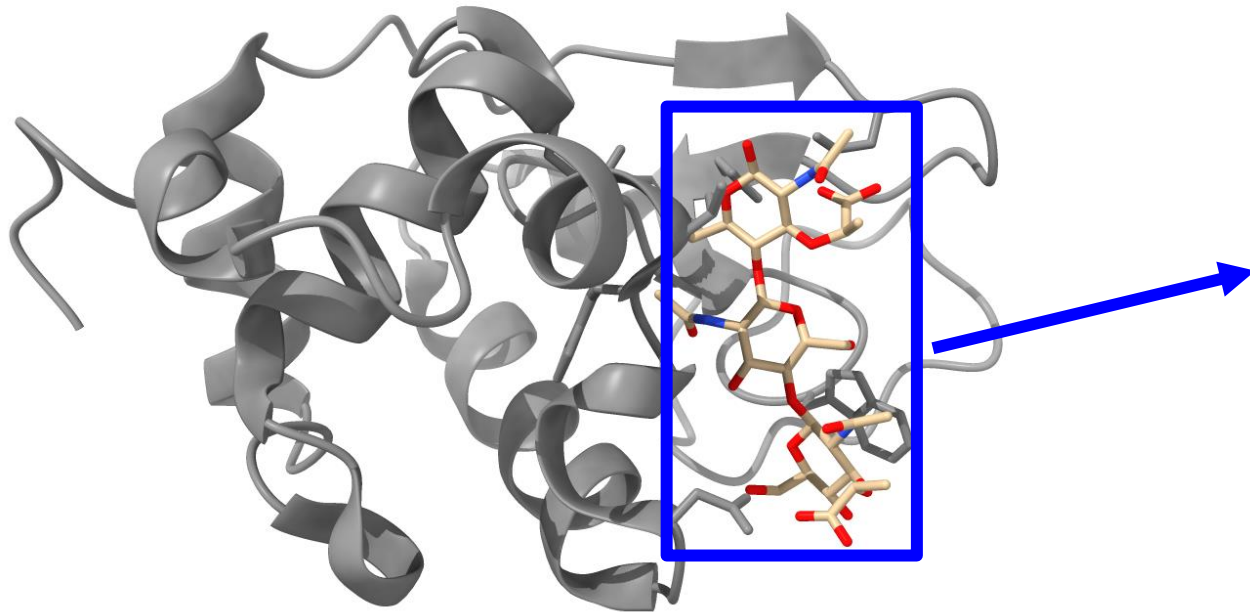
Lysozyme

peptidoglycan *N*-acetylmuramoylhydrolase
m = 14kDa

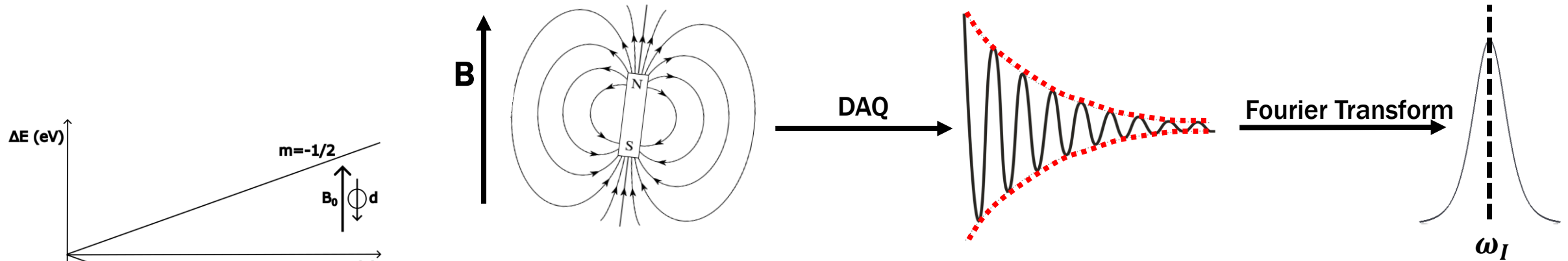


Lysozyme

peptidoglycan *N*-acetylmuramoylhydrolase



The Painter: NMR



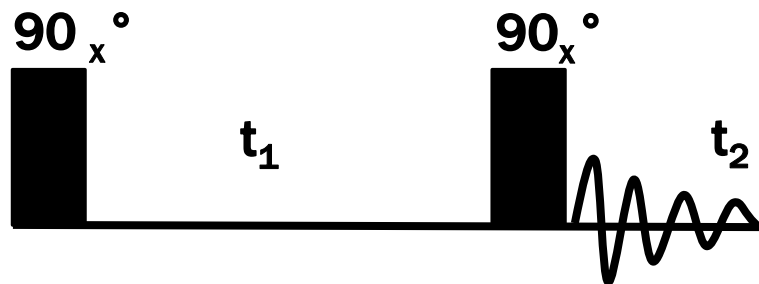
$$\rho = |\psi\rangle\langle\psi|$$

$$i\hbar \frac{d\rho}{dt} = [H, \rho]$$

$$H = H_0 + \overset{\text{Relaxation}}{iR}$$

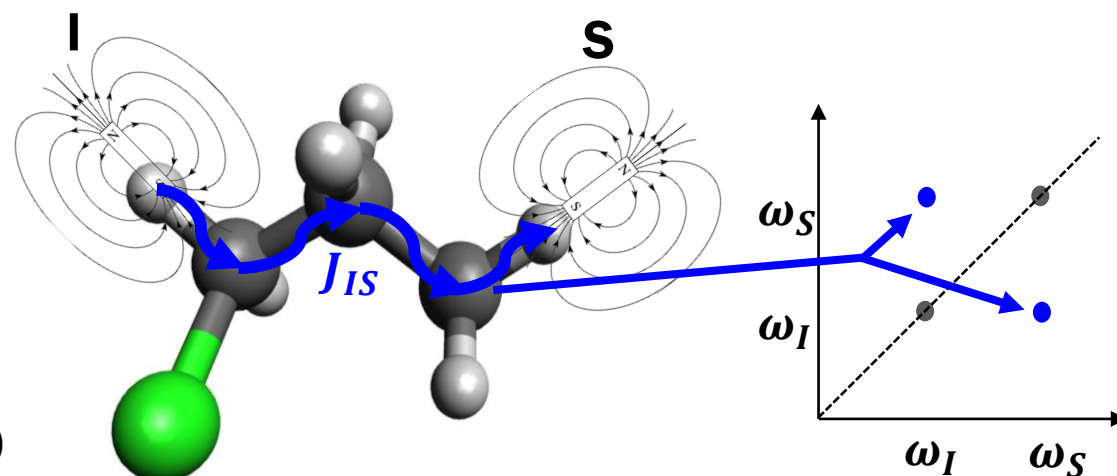
Zeeman splitting
Couplings
etc.

COSY



$$\begin{aligned}
 I_z &\xrightarrow{90_x^\circ} -I_y \\
 &\xrightarrow{t_1} -I_y \cos(\omega_I t_1) \cos(\pi J t_1) + 2I_x S_z \cos(\Omega_I t_1) \sin(\pi J t_1) \\
 &\quad + I_x \sin(\Omega_I t_1) \cos(\pi J t_1) + 2I_y S_z \sin(\Omega_I t_1) \sin(\pi J t_1) \\
 &\xrightarrow{90_x^\circ} -I_z \cos(\omega_I t_1) \cos(\pi J t_1) - 2I_x S_y \cos(\omega_I t_1) \sin(\pi J t_1) \\
 &\quad + I_x \sin(\omega_I t_1) \cos(\pi J t_1) - 2I_z S_y \sin(\omega_I t_1) \sin(\pi J t_1)
 \end{aligned}$$

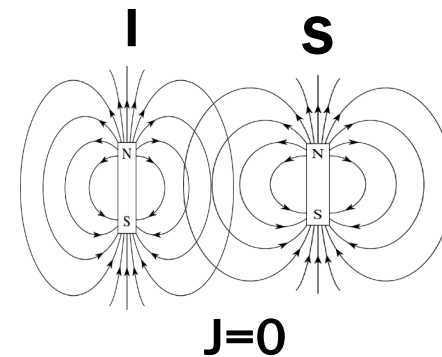
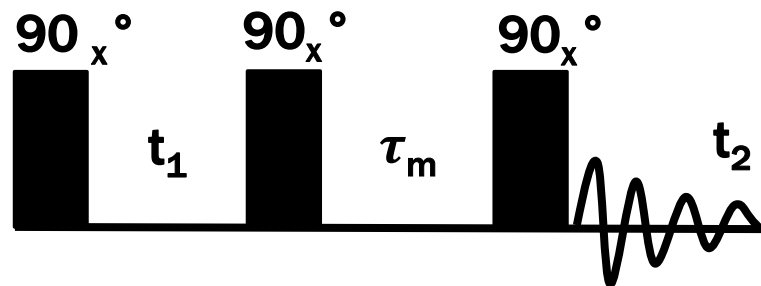
$$\begin{array}{l}
 I \rightarrow S \quad \left[\begin{array}{l} \sin(\omega_I t_1) \cos(\pi J t_1) \cos(\pi J t_2) \exp(i\omega_I t_2) \\ \sin(\omega_I t_1) \sin(\pi J t_1) \sin(\pi J t_2) \exp(i\omega_S t_2) \end{array} \right. \quad \begin{array}{l} (\omega_I, \omega_I) \\ (\omega_I, \omega_S) \end{array} \\
 S \rightarrow I \quad \left[\begin{array}{l} \sin(\omega_S t_1) \cos(\pi J t_1) \cos(\pi J t_2) \exp(i\omega_S t_2) \\ \sin(\omega_S t_1) \sin(\pi J t_1) \sin(\pi J t_2) \exp(i\omega_I t_2) \end{array} \right. \quad \begin{array}{l} (\omega_S, \omega_S) \\ (\omega_S, \omega_I) \end{array}
 \end{array}$$



$$H = J_{IS} \mathbf{I} \cdot \mathbf{S}$$

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NOESY



$$H = -\frac{\mu_0}{4\pi|\mathbf{r}|^3} [3(\mathbf{m}_1 \cdot \hat{\mathbf{r}})(\mathbf{m}_2 \cdot \hat{\mathbf{r}}) - \mathbf{m}_1 \cdot \mathbf{m}_2] - \mu_0 \frac{2}{3} \mathbf{m}_1 \cdot \mathbf{m}_2 \delta(\mathbf{r})$$

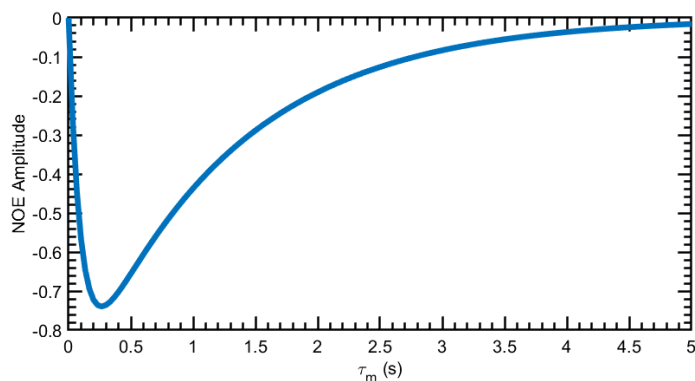
$$I_Z \xrightarrow{90_x^\circ} -I_Y$$

$$\xrightarrow{t_1} -I_Y \cos(\omega_I t_1) + I_X \sin(\Omega_I t_1) \cos(\pi/t_1)$$

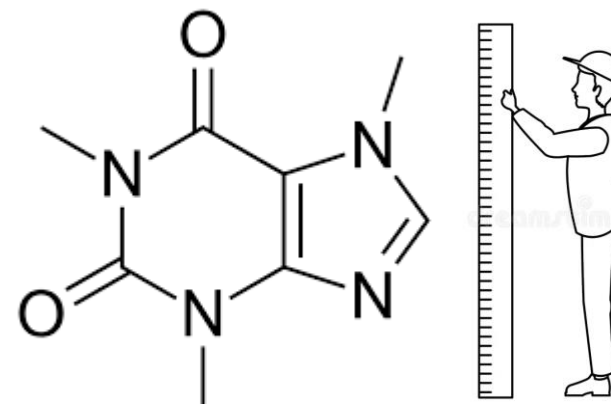
$$\xrightarrow{90_x^\circ} -I_Z \cos(\omega_I t_1) + \cancel{I_X \sin(\omega_I t_1)}$$

$$I_{NOE} = \frac{c}{r^6}$$

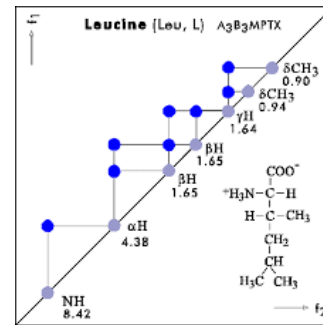
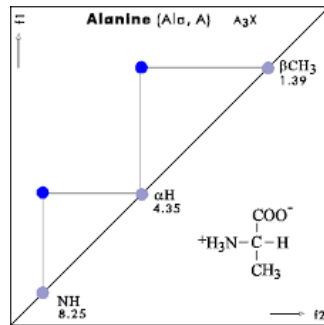
$$-I_Z \cos(\omega_I t_1) \xrightarrow{\tau_m} -I_Z \cos(\omega_I t_1) a_{II}(\tau_m) - \underline{S_Z \cos(\omega_I t_1) a_{IS}(\tau_m)}$$



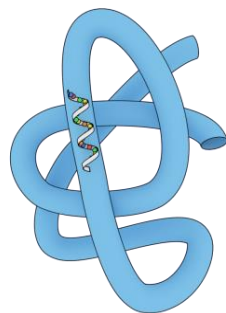
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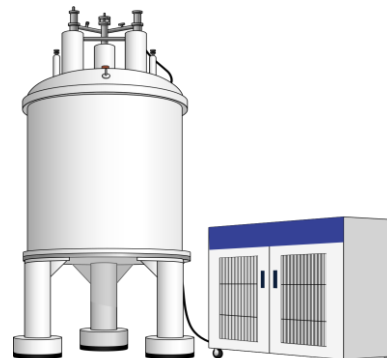
2D NMR Spectroscopy



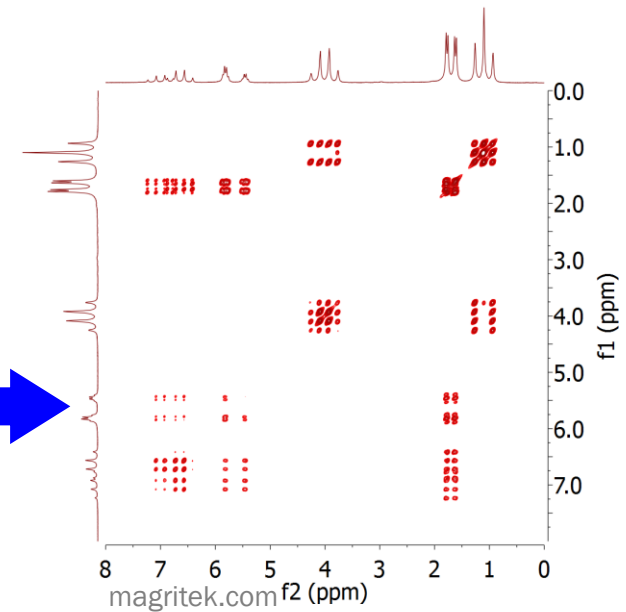
www.bp.uni-bayreuth.de



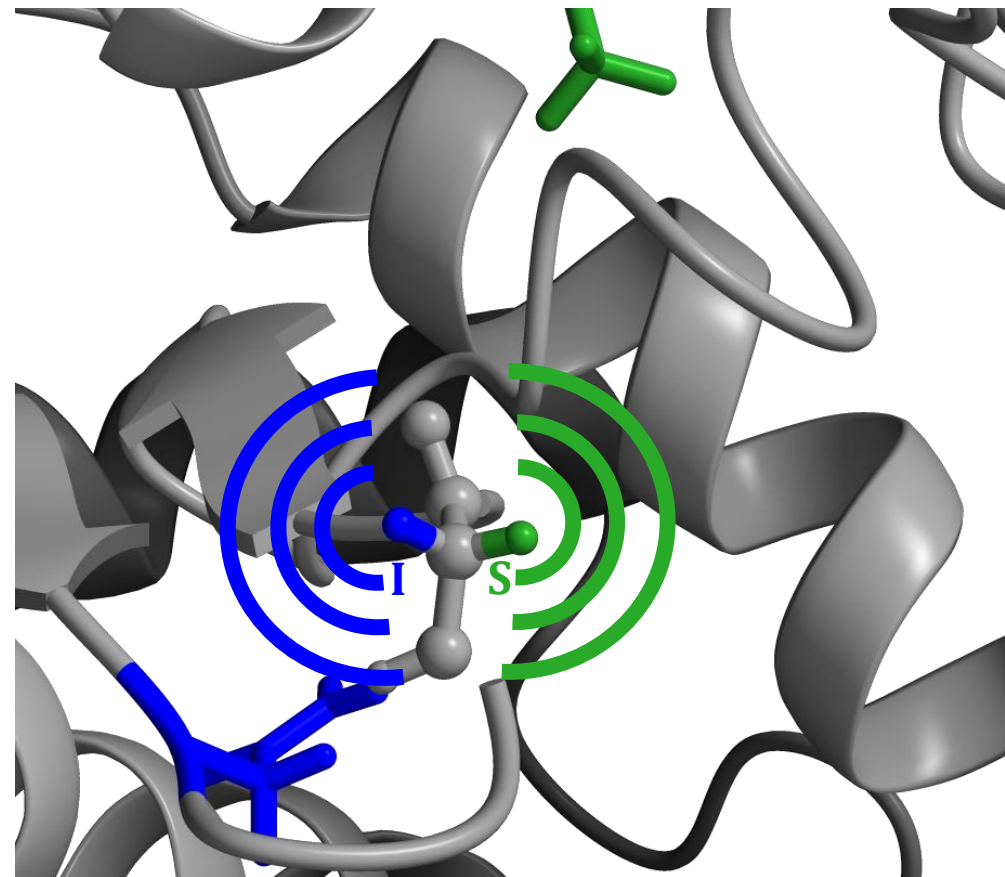
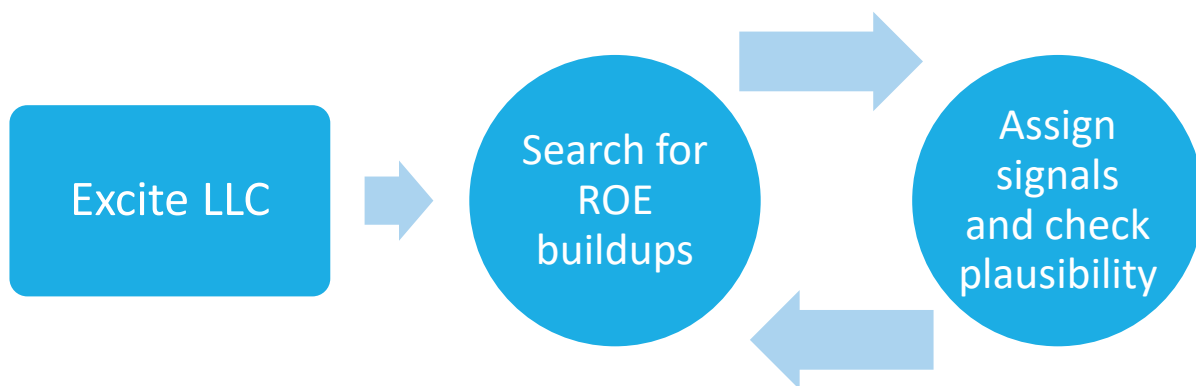
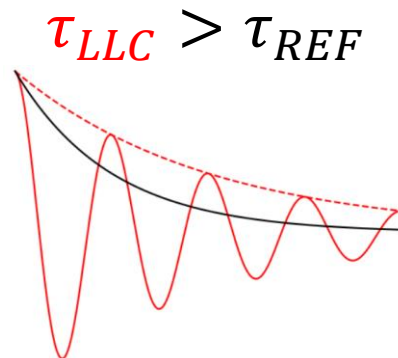
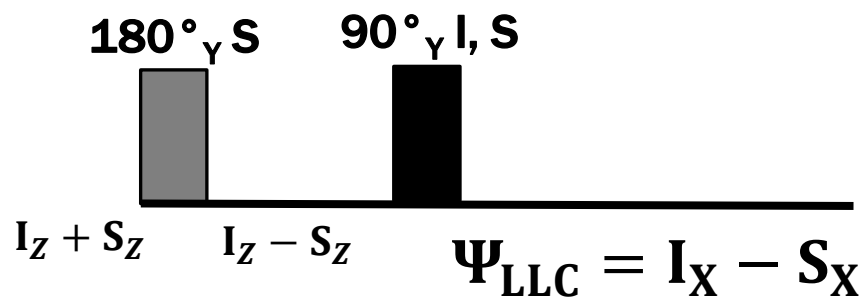
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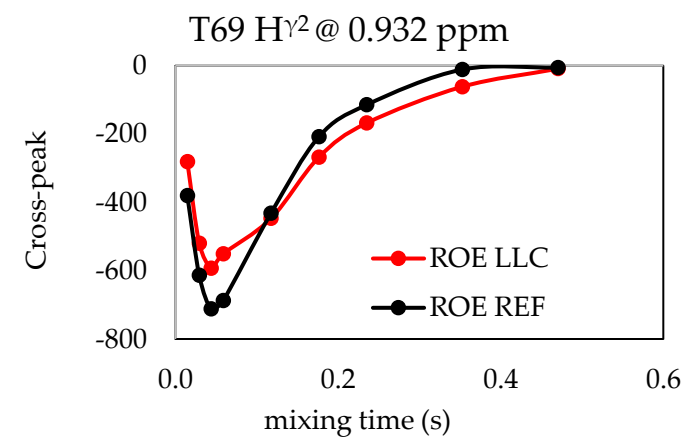
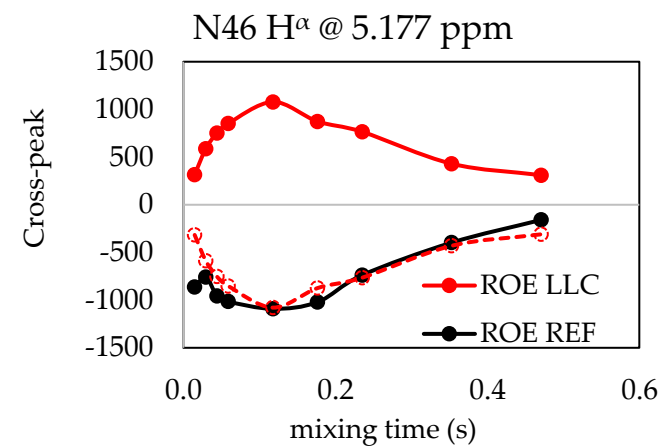
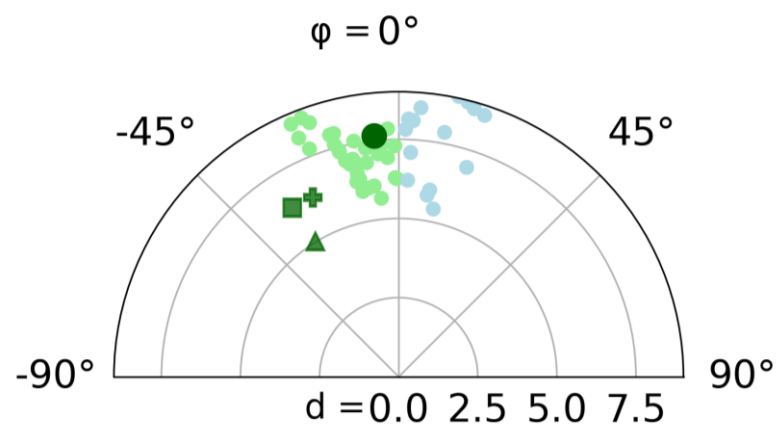
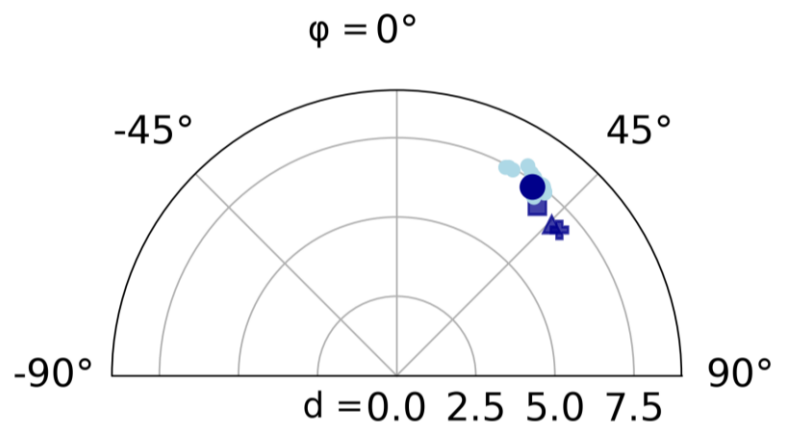
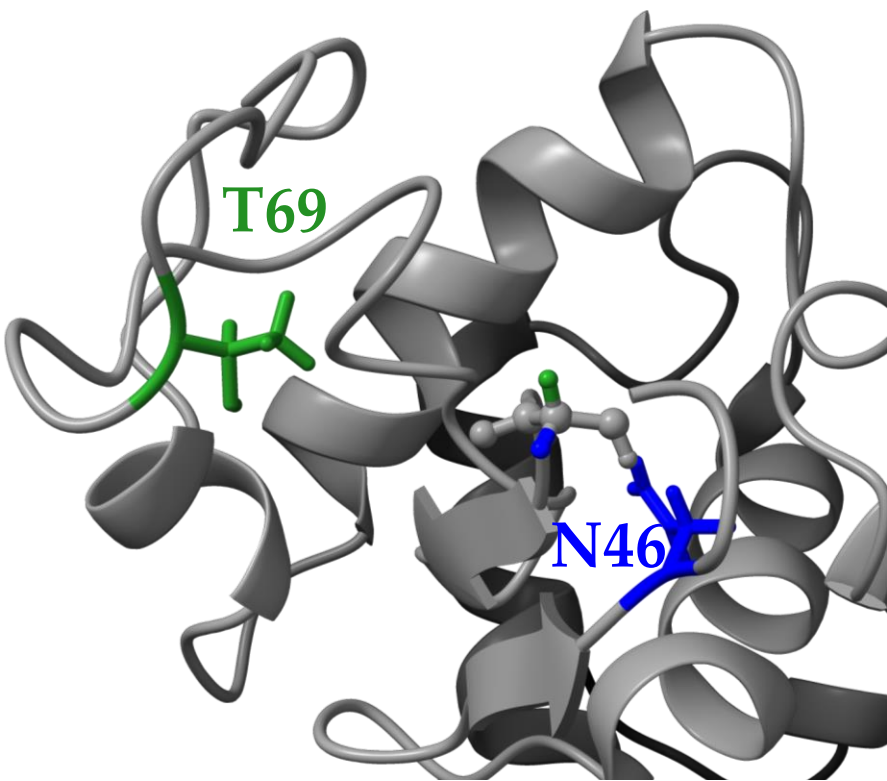
The Painting: Our Work



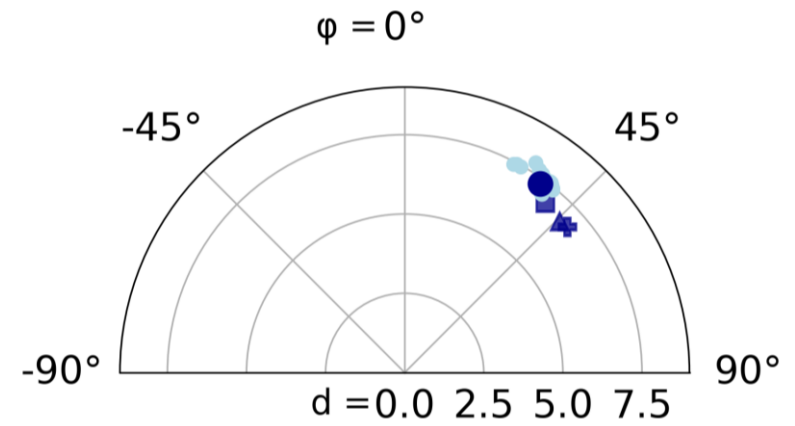
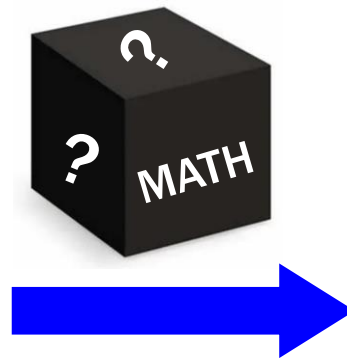
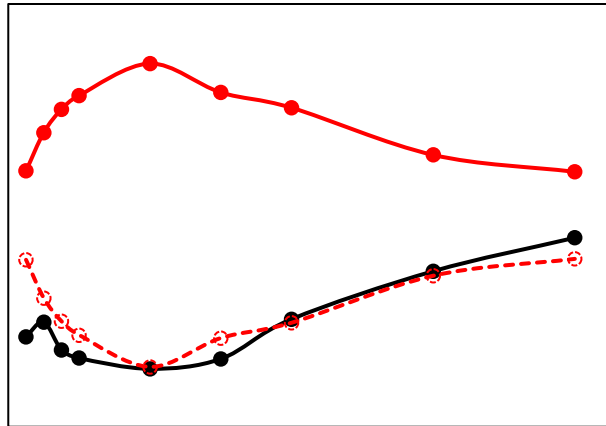
Long-lived coherences for magnetic interactions in proteins
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Preprint COMMSCHEM-24-0038-T

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What's next?



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Biophysics & Biomedical Applications Group – ELI-NP

Univ. Florence – NMR Time at 950MHz