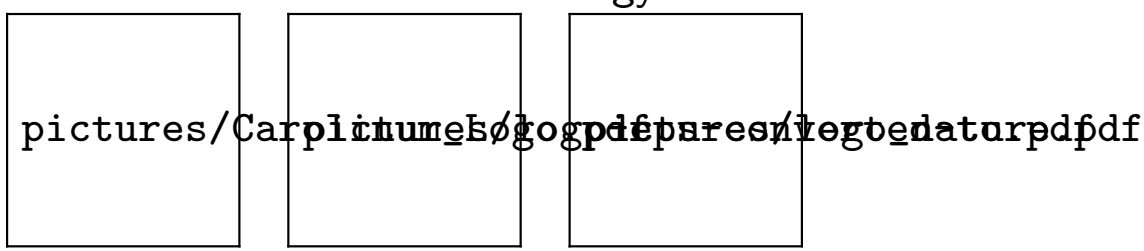
Dynamics of membrane bound peptides from NMR experiments and MD simulations

Ricky Nencini
Supervisor: Samuli Ollila

Faculty of Science, University of Helsinki
Institute of Biotechnology



ricky.nencini@helsinki.fi

June 14, 2022

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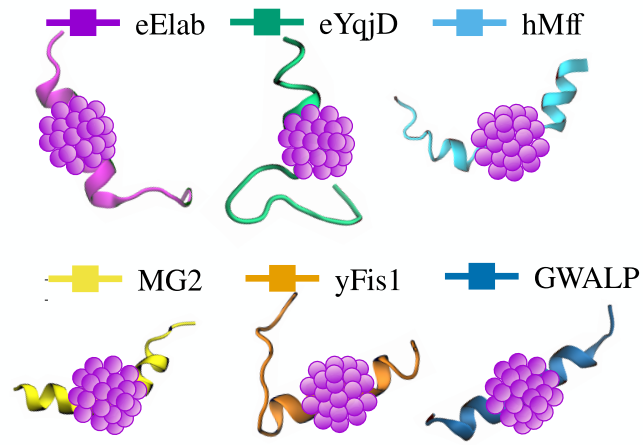

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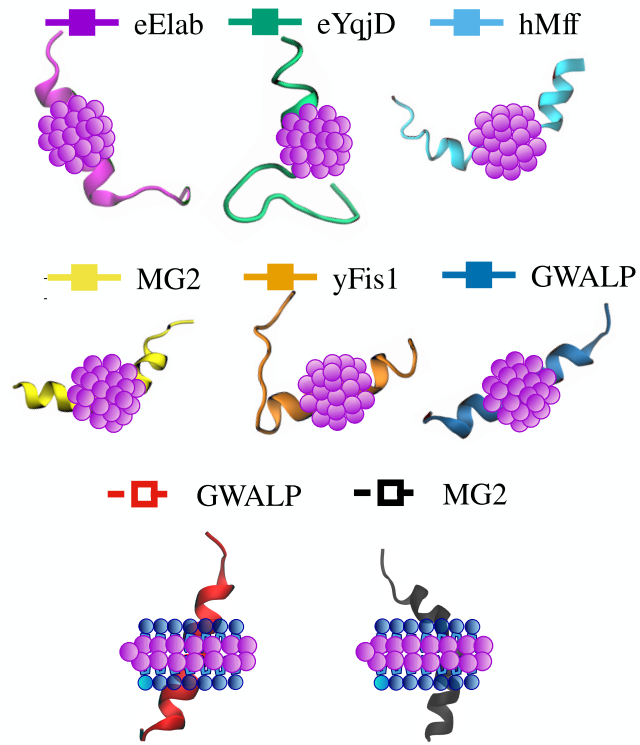

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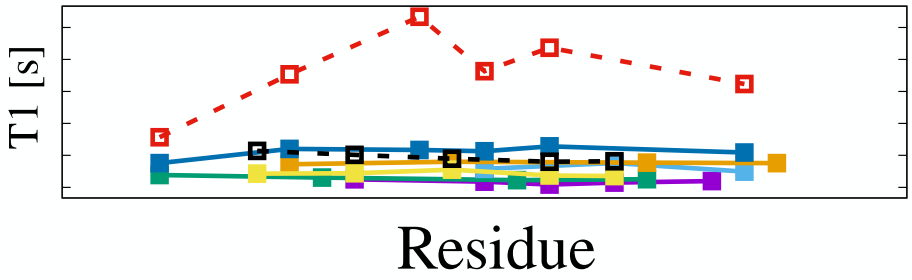

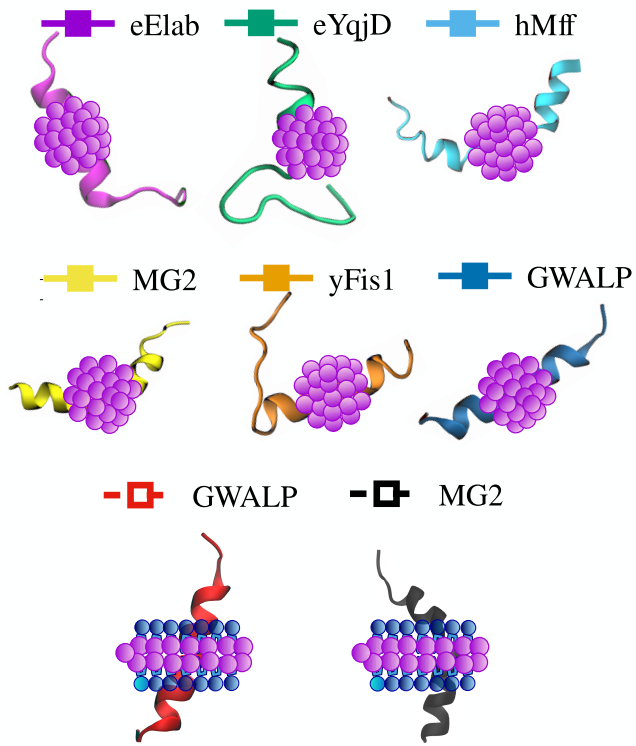

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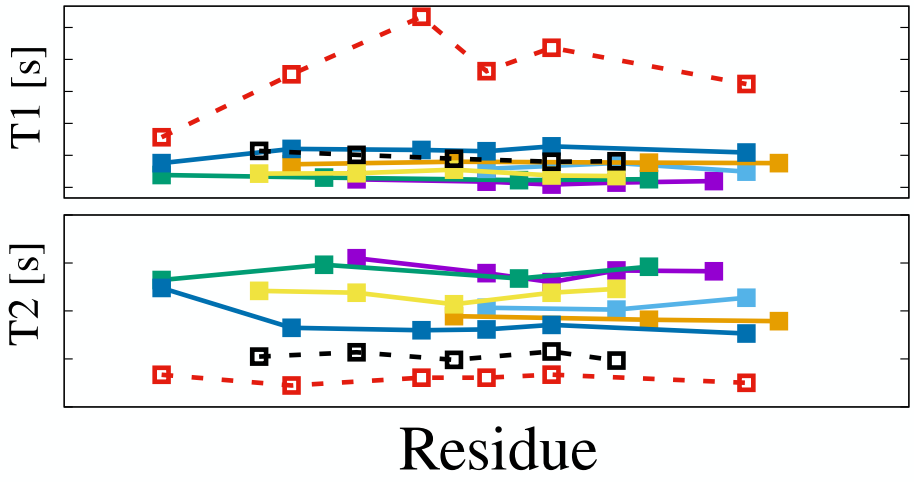

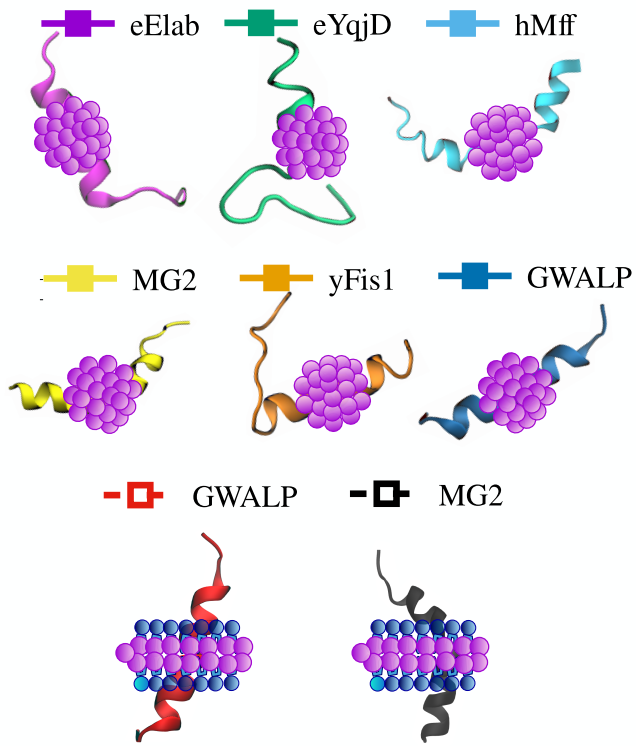

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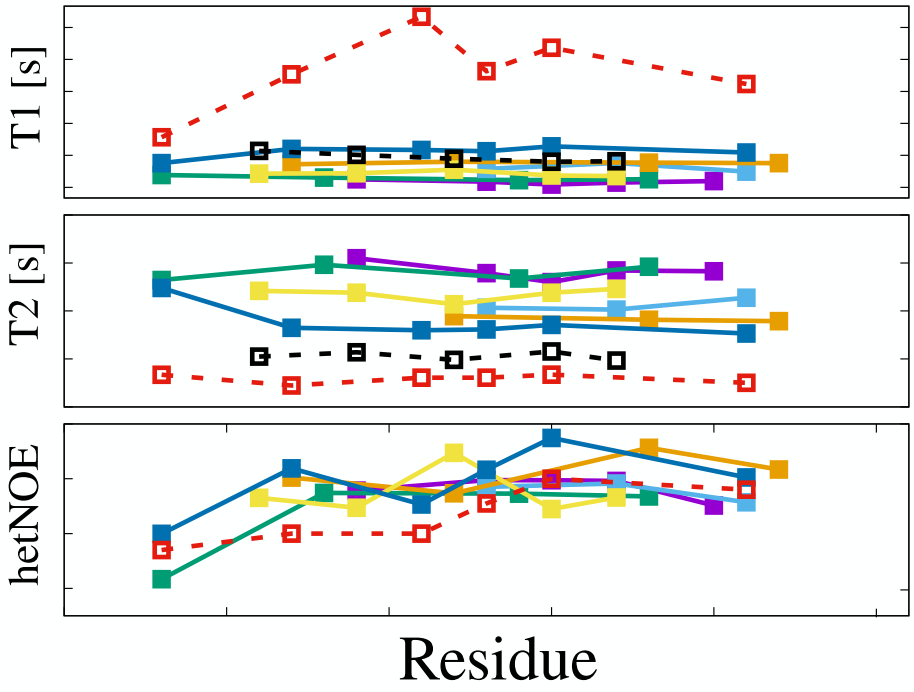

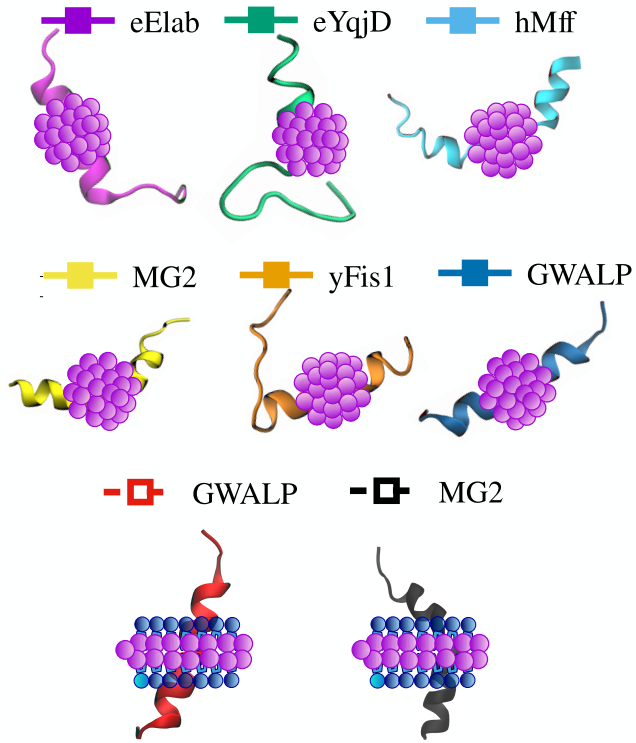

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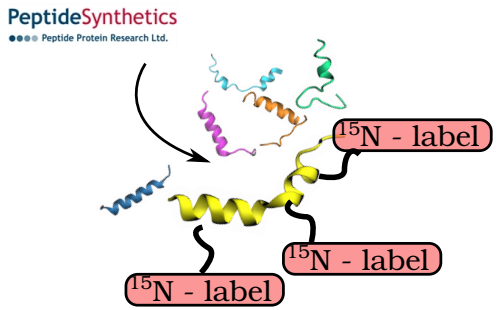

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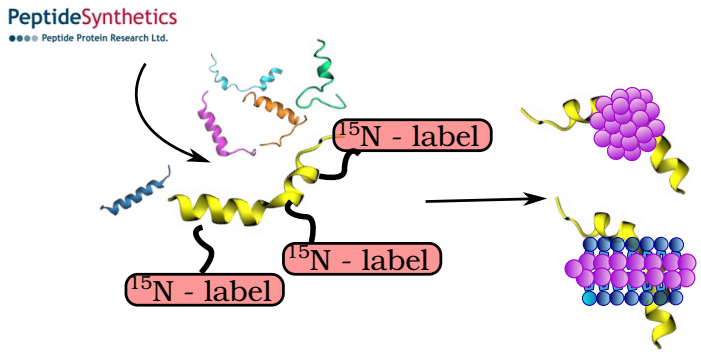

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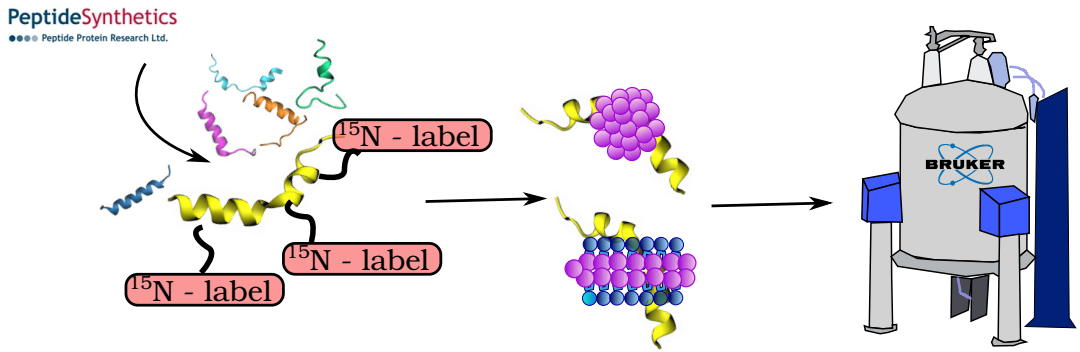

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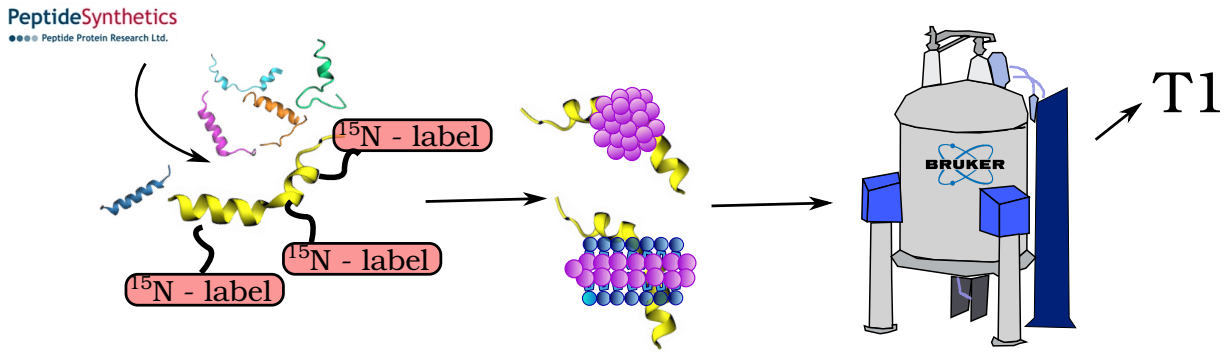

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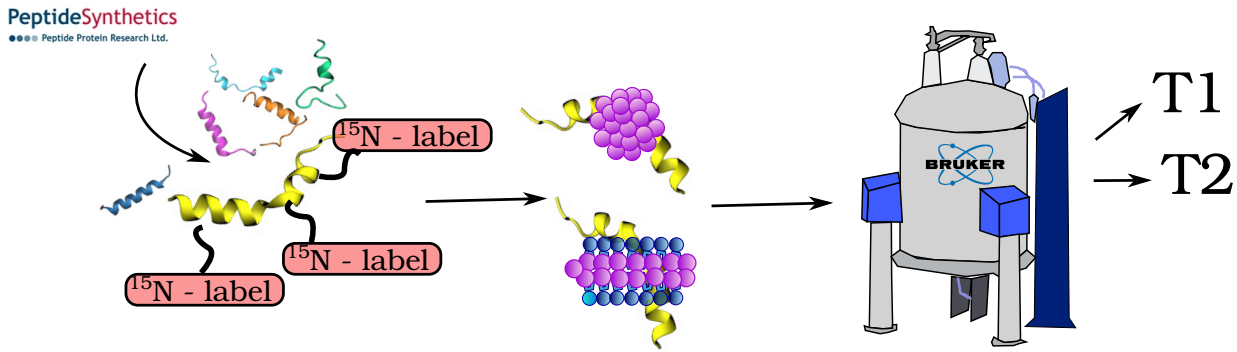

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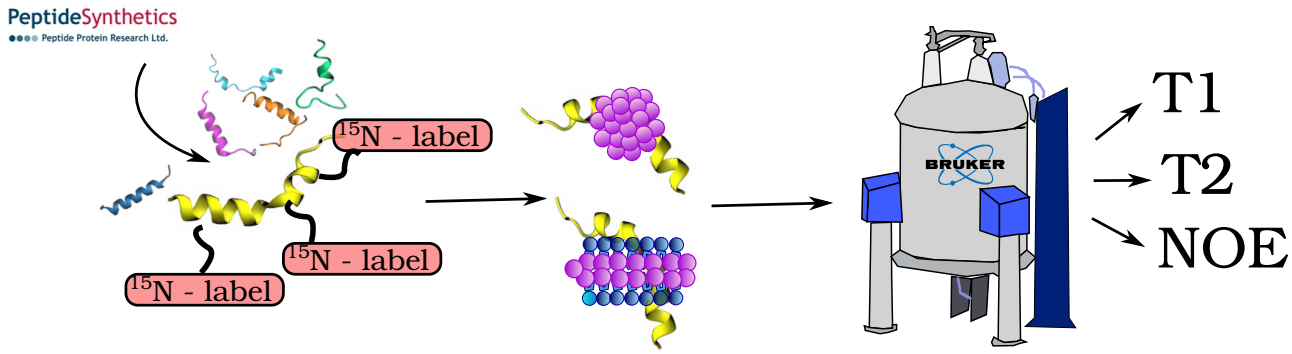

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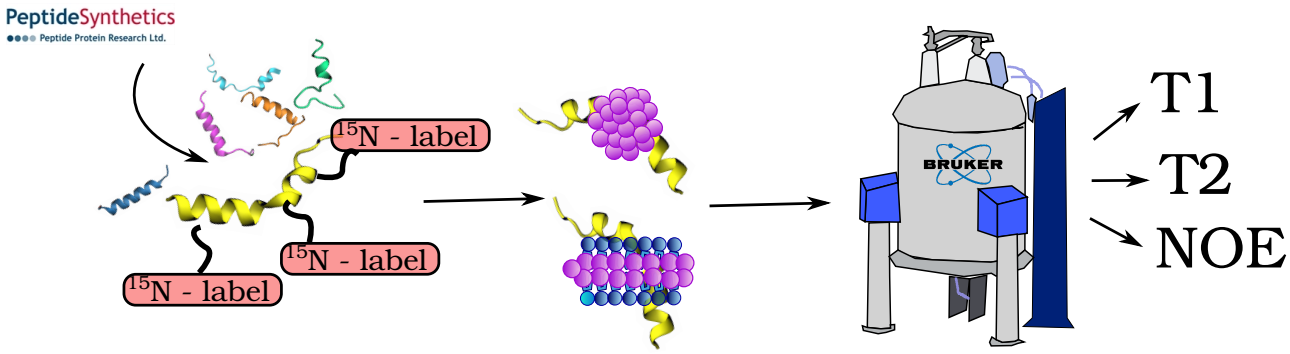

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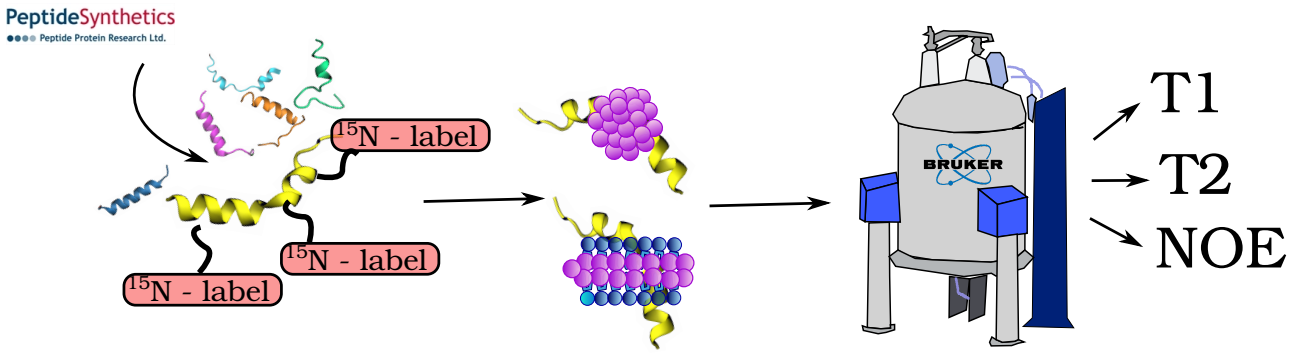

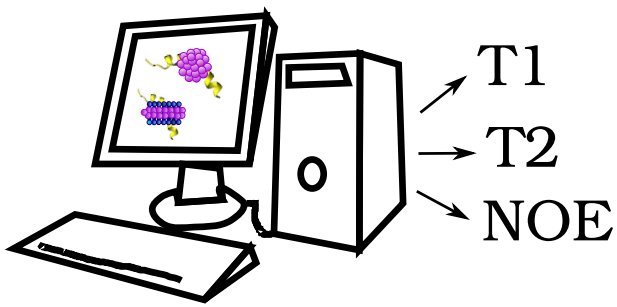

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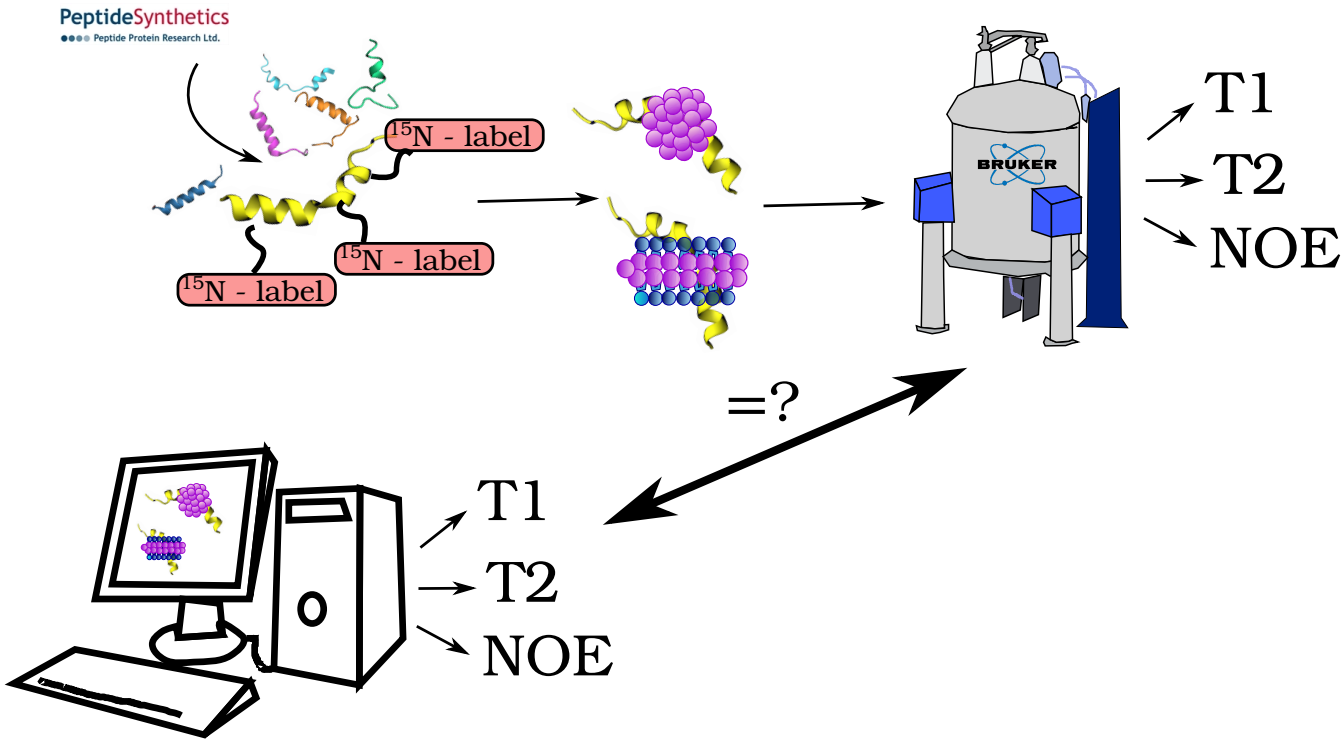

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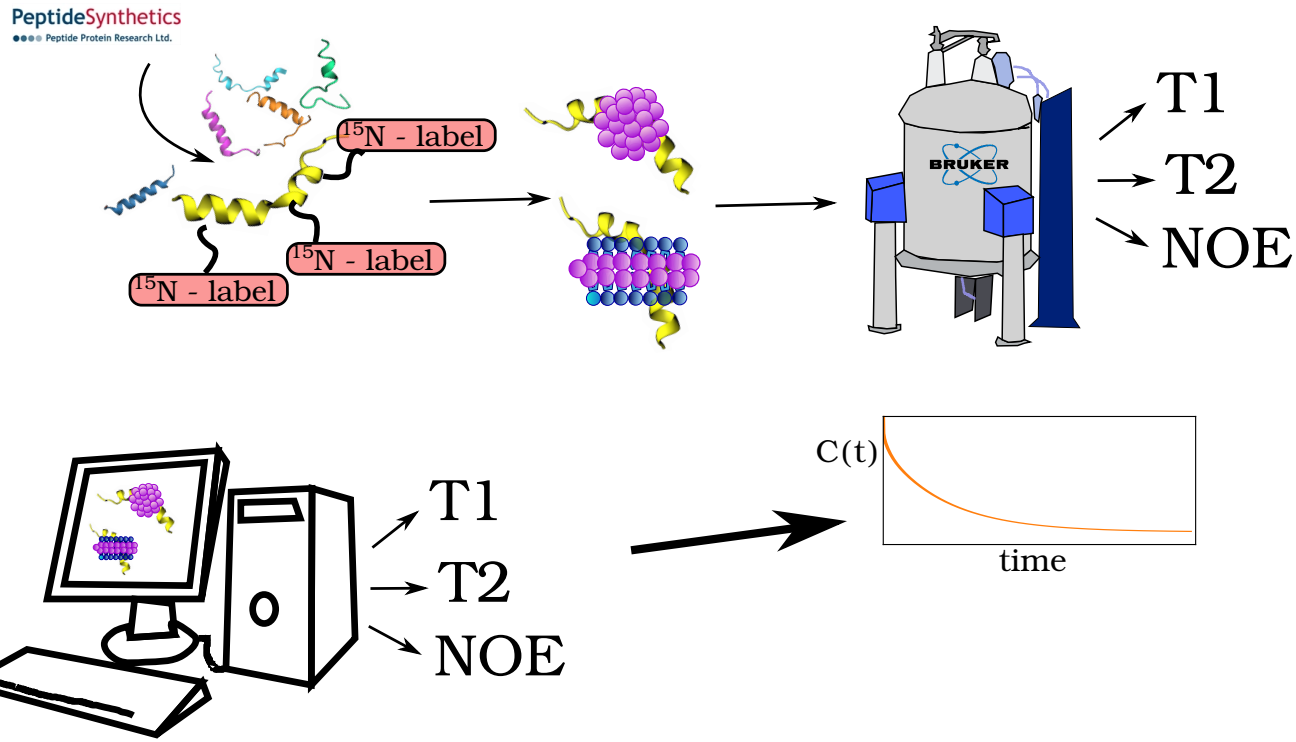

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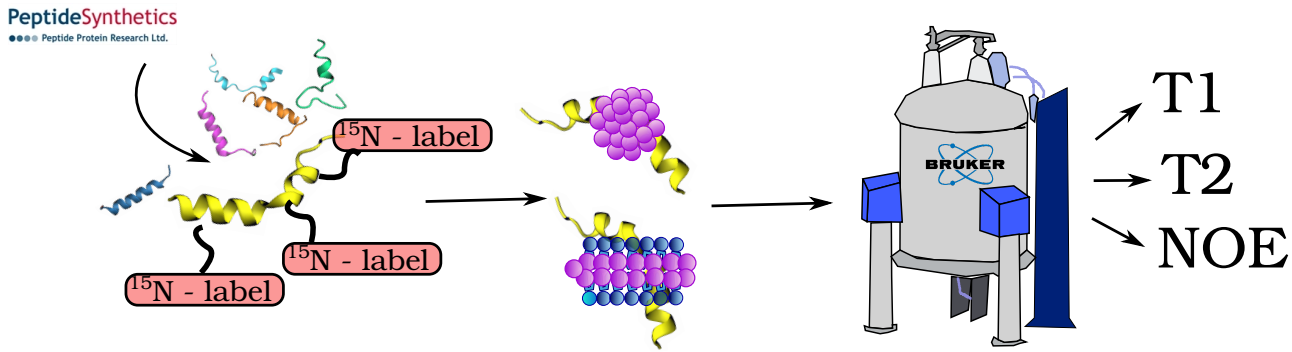

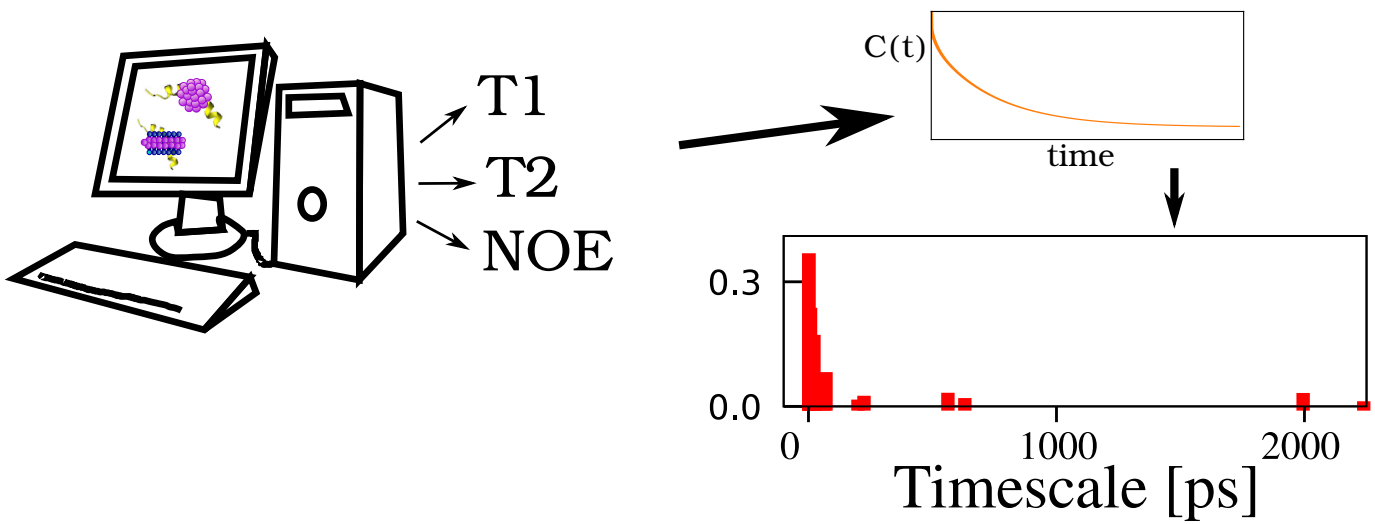

Succesfull case: TonB

Yet to be done - Our approach shad a light on the conformational ensamble of the protein

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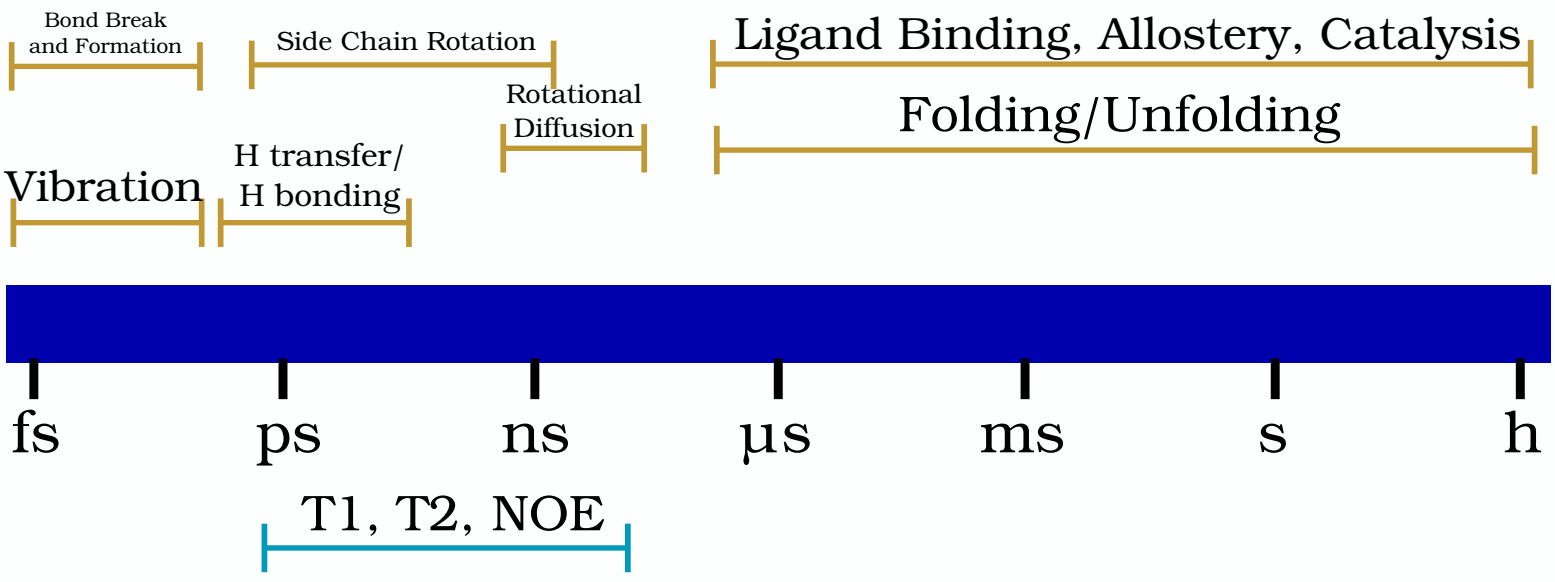

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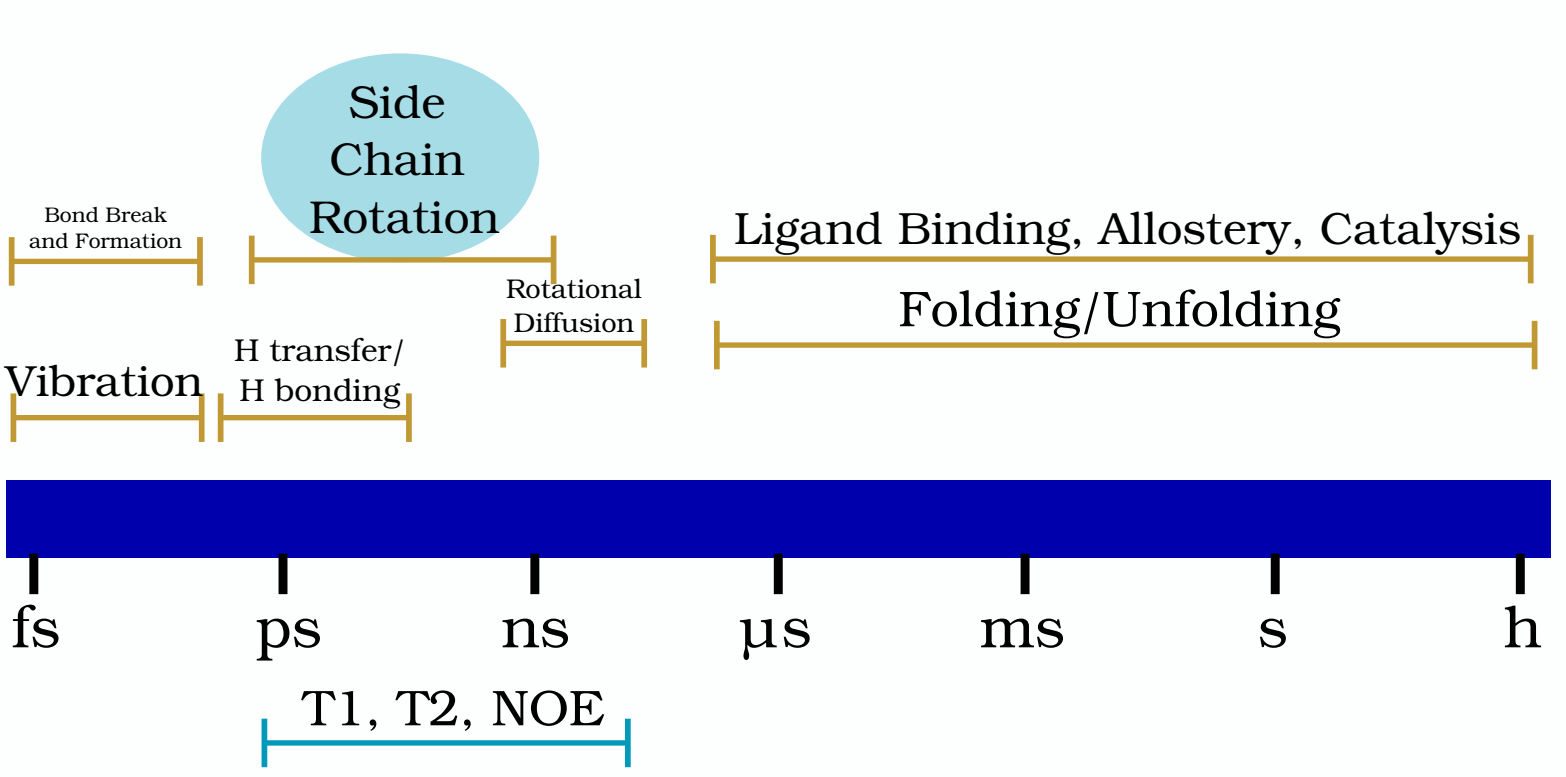

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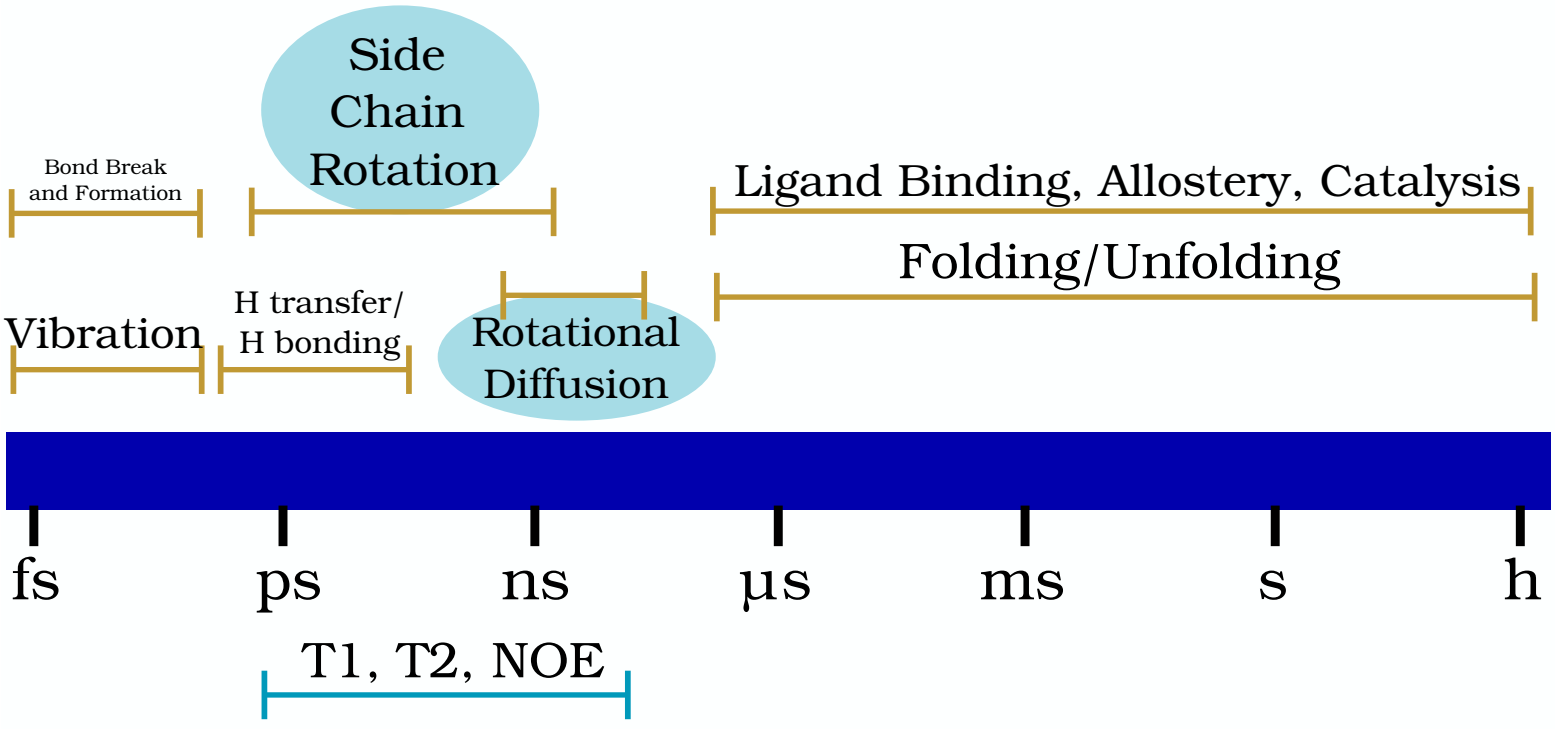

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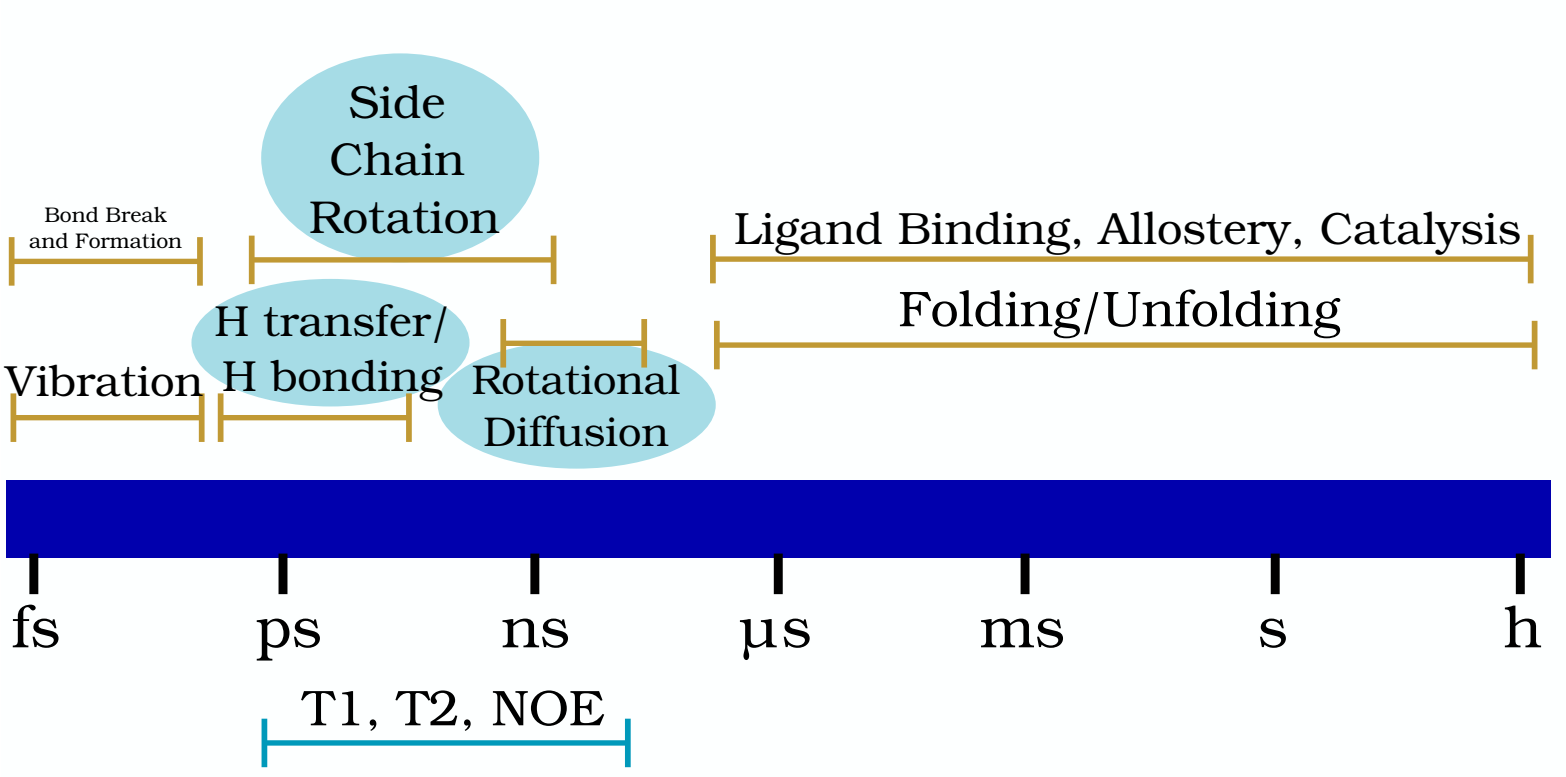

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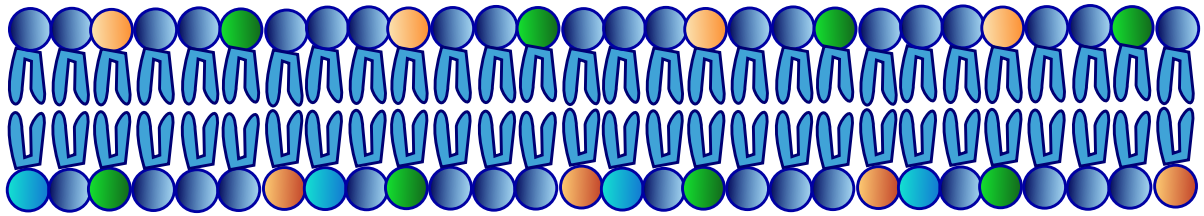
Solid state NMR - lipid bilayer



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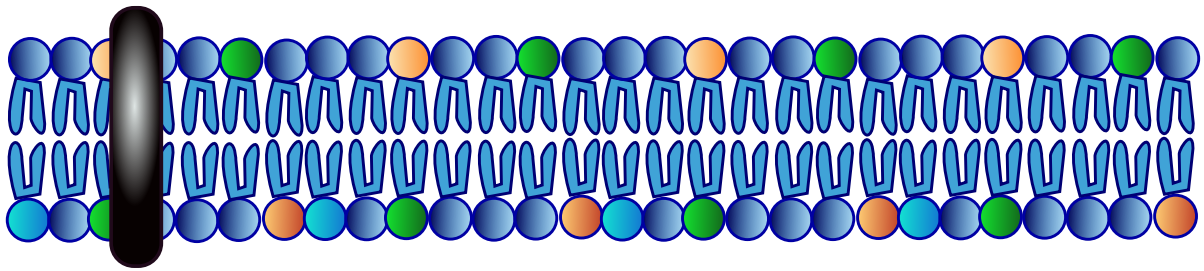

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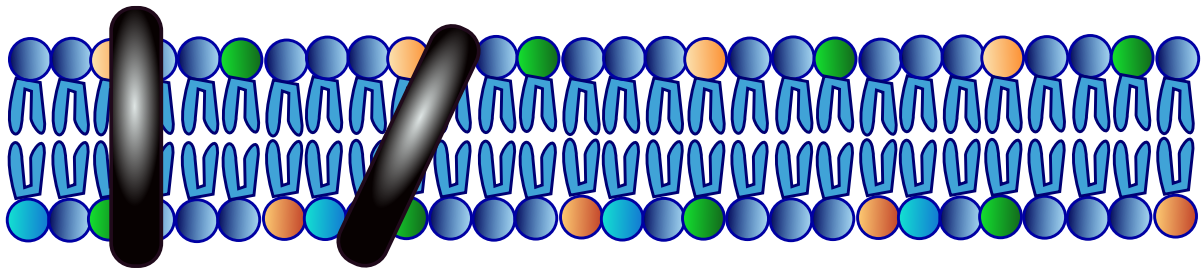

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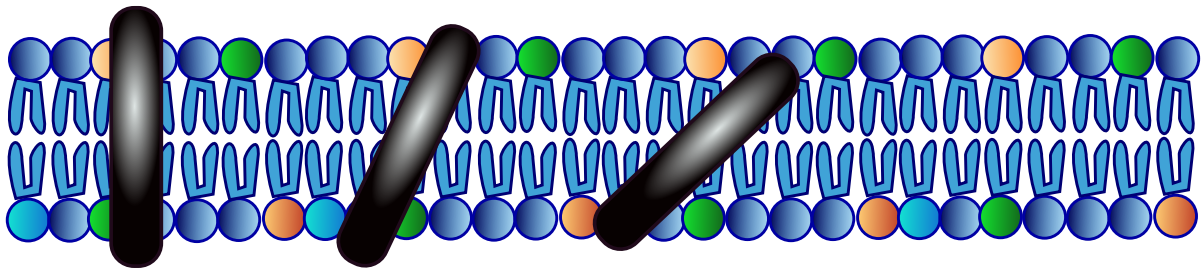

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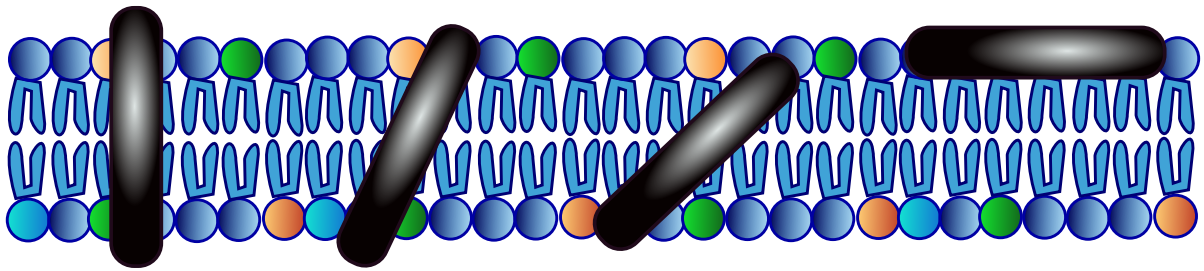

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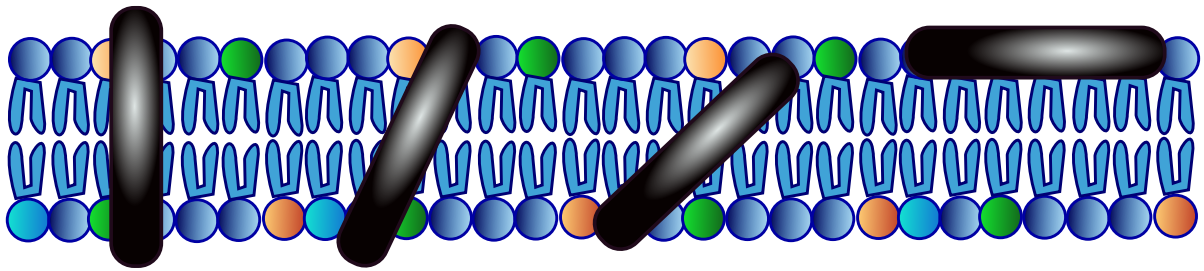

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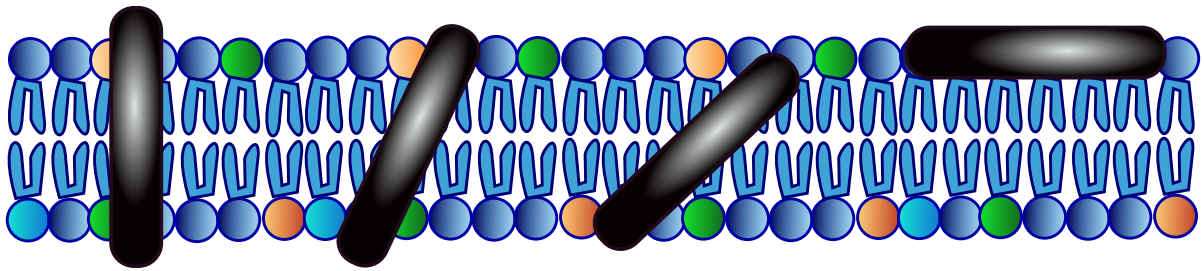

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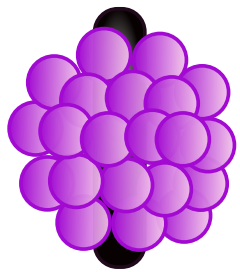

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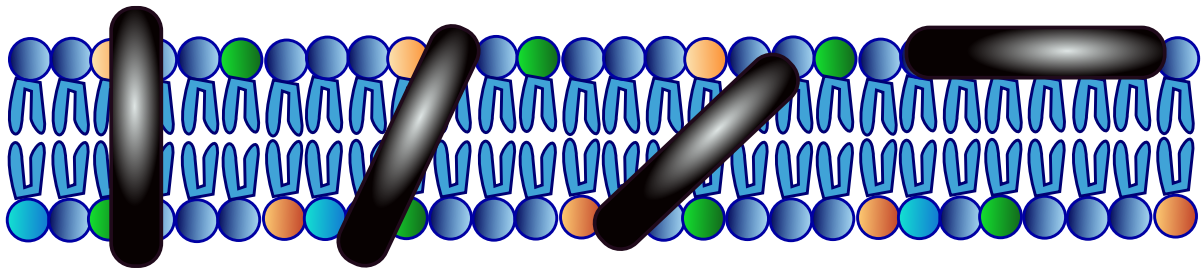

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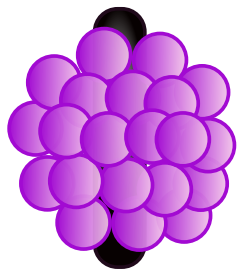
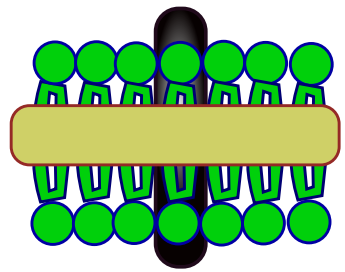


Nanodisk



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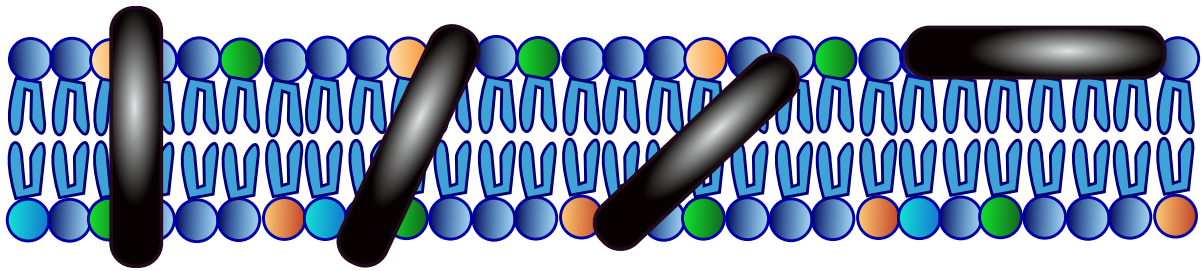

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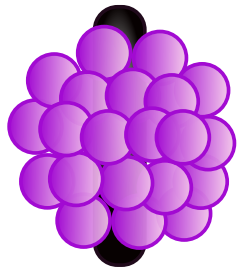

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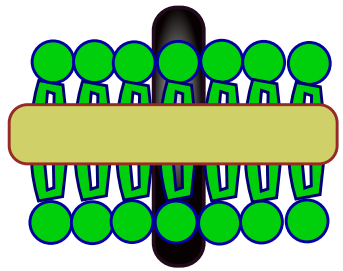
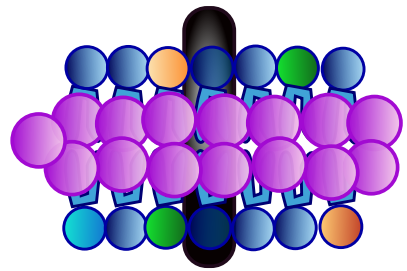
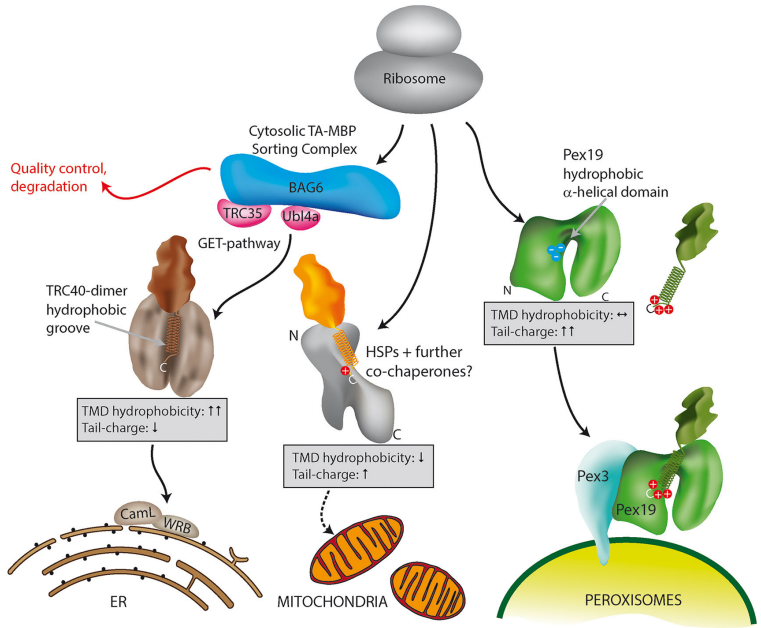


Bicelle



Case study: Tail anchored mitochondria targeted peptides

to be developed



Studied peptides

E.coli - ElaB	PWQGIGVGAAVGLVLGLLLARR
E.coli - YqjD	WTGVGIGAAIGVVLGVLLSRR
human - Mff	AKREMVMISITVAFWLLNSWLWFRR
yeast - Fis1	LKGVVVAGGVLAGAVAVASFFLRNKRR
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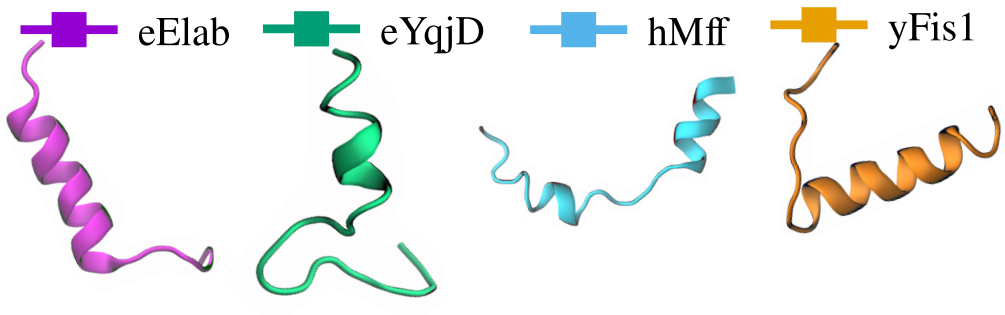

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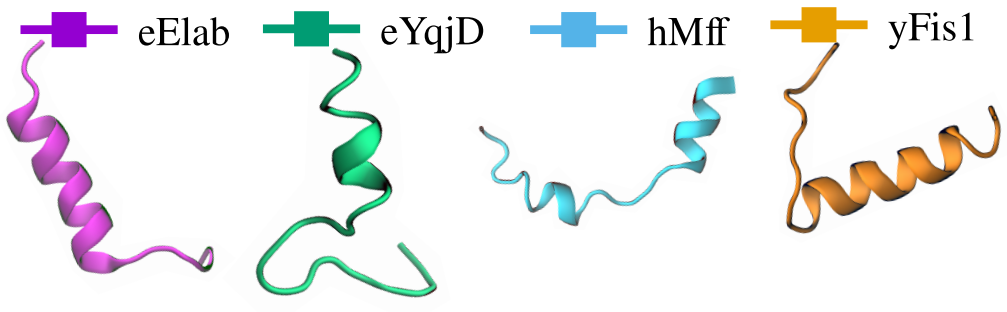

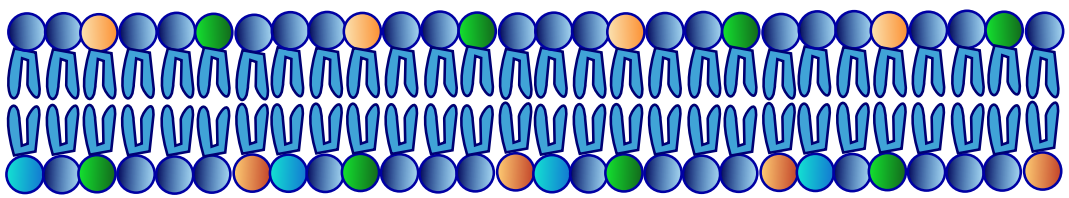

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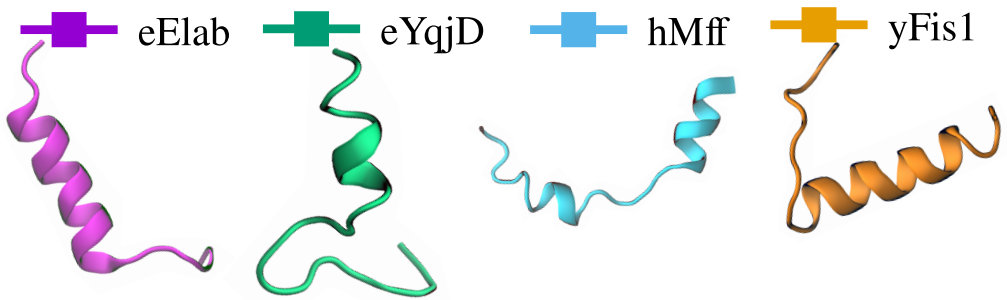

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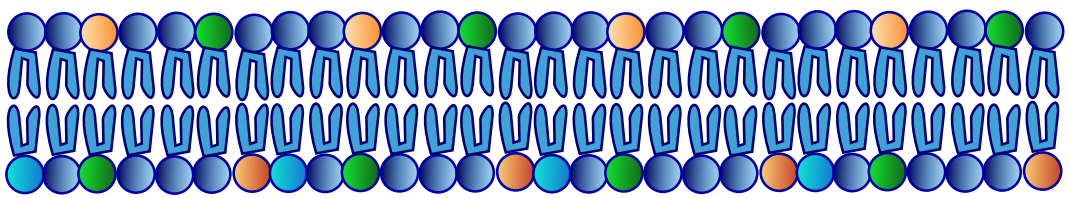

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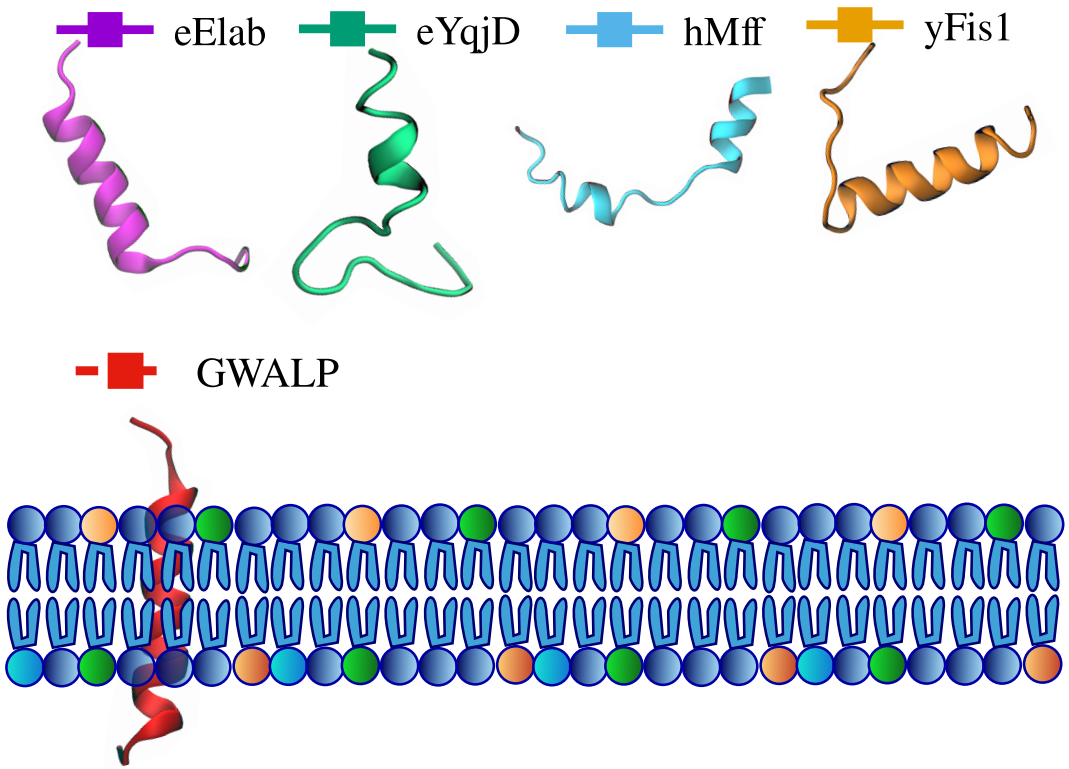

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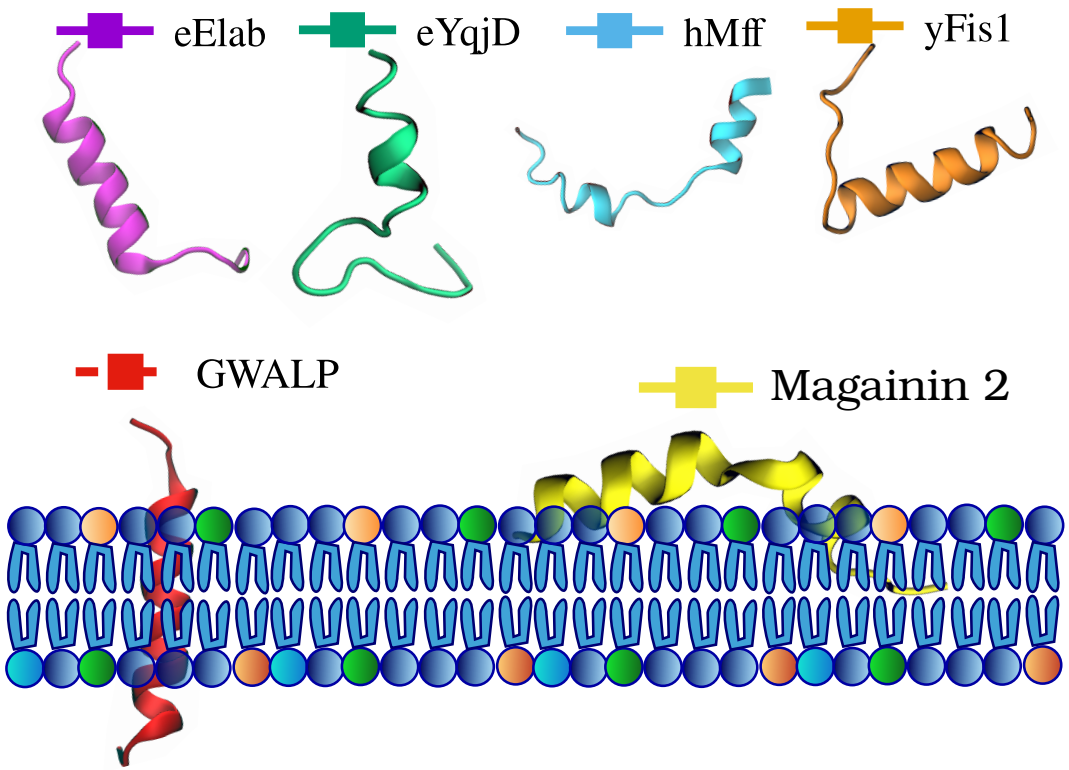

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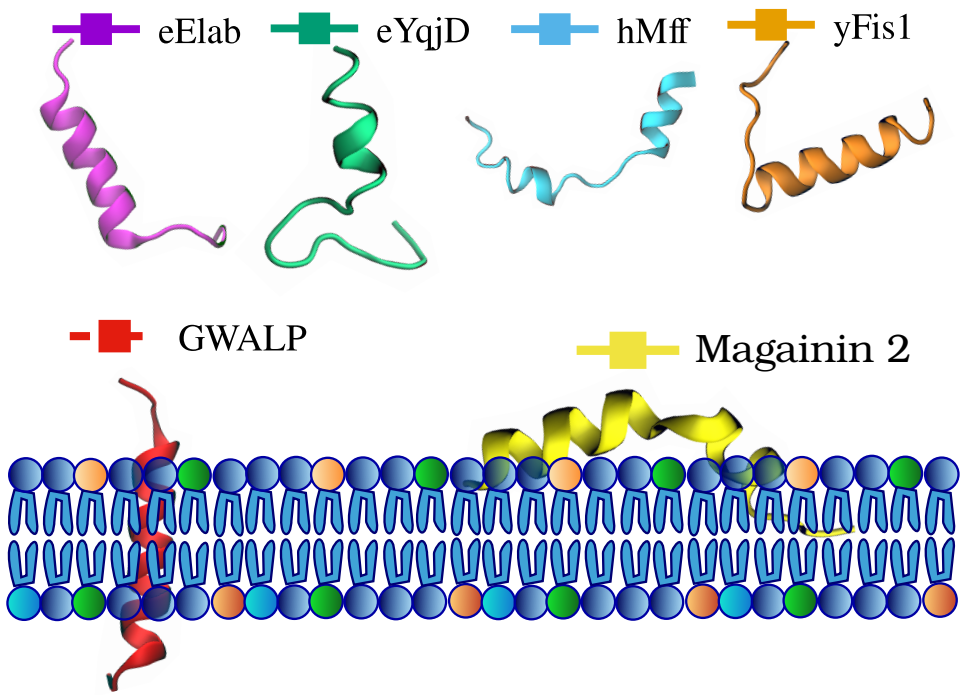
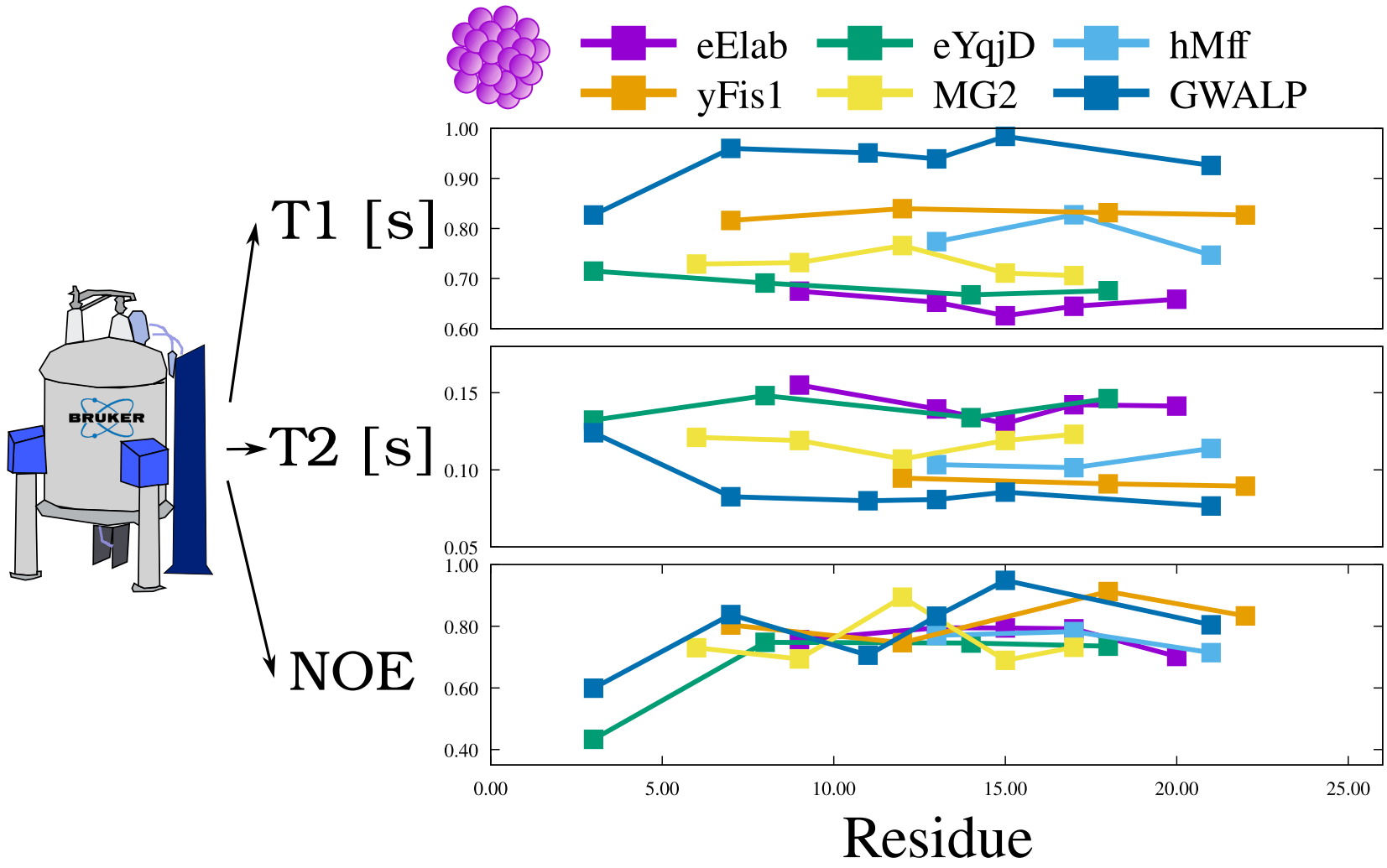
		Hydrobphobic	Acid	Basic	Neutral
E.coli - ElaB	PWQGIGVGAAVGLVLGLLLARR	63.64%	0.0%	9.09%	27.27%
E.coli - YqjD	WTGVGIGAAIGVVLGVLLSRR	57.14%	0.0%	9.52%	33.33%
human - Mff	AKREMVMISITVAFWLLNSWLWFRR	60.00%	4.0%	16.00%	20.00%
yeast - Fis1	LKGVVVAGGVLAGAVAVASFFLRNKRR	59.26%	0.0%	18.52%	22.22%
Model - GWALP	Ac-GGALWLALALALALALALWLAGA-NH-CH_2-CH_2OH	100.00%	0.0%	0.00%	0.00%
Model - Magainin 2	GIGKFLHSAKKFGKAFVGEIMNS	43.48%	4.4%	21.74%	30.43%

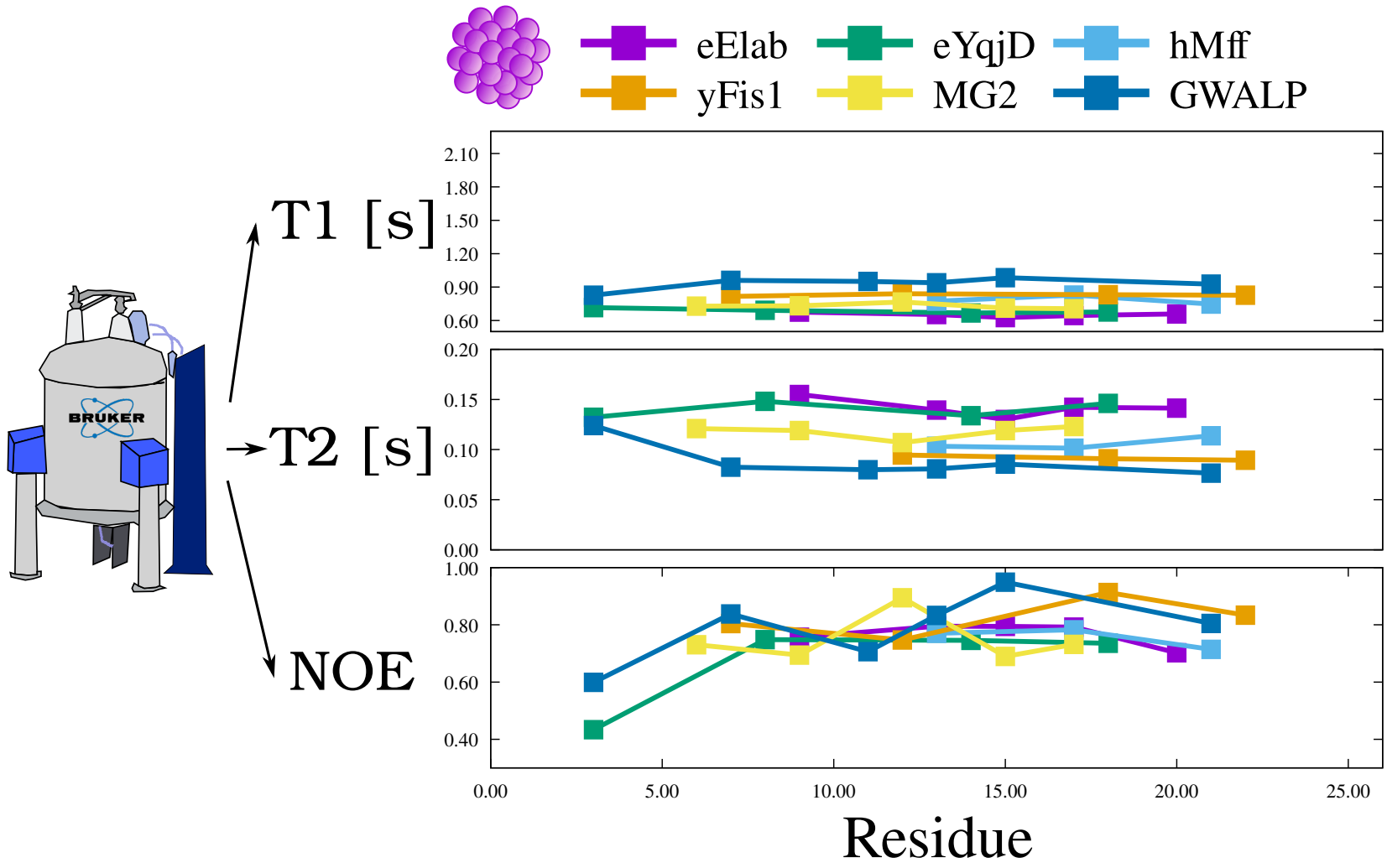
https://www.peptide2.com/N_peptide_hydrophobicity_hydrophilicity.php



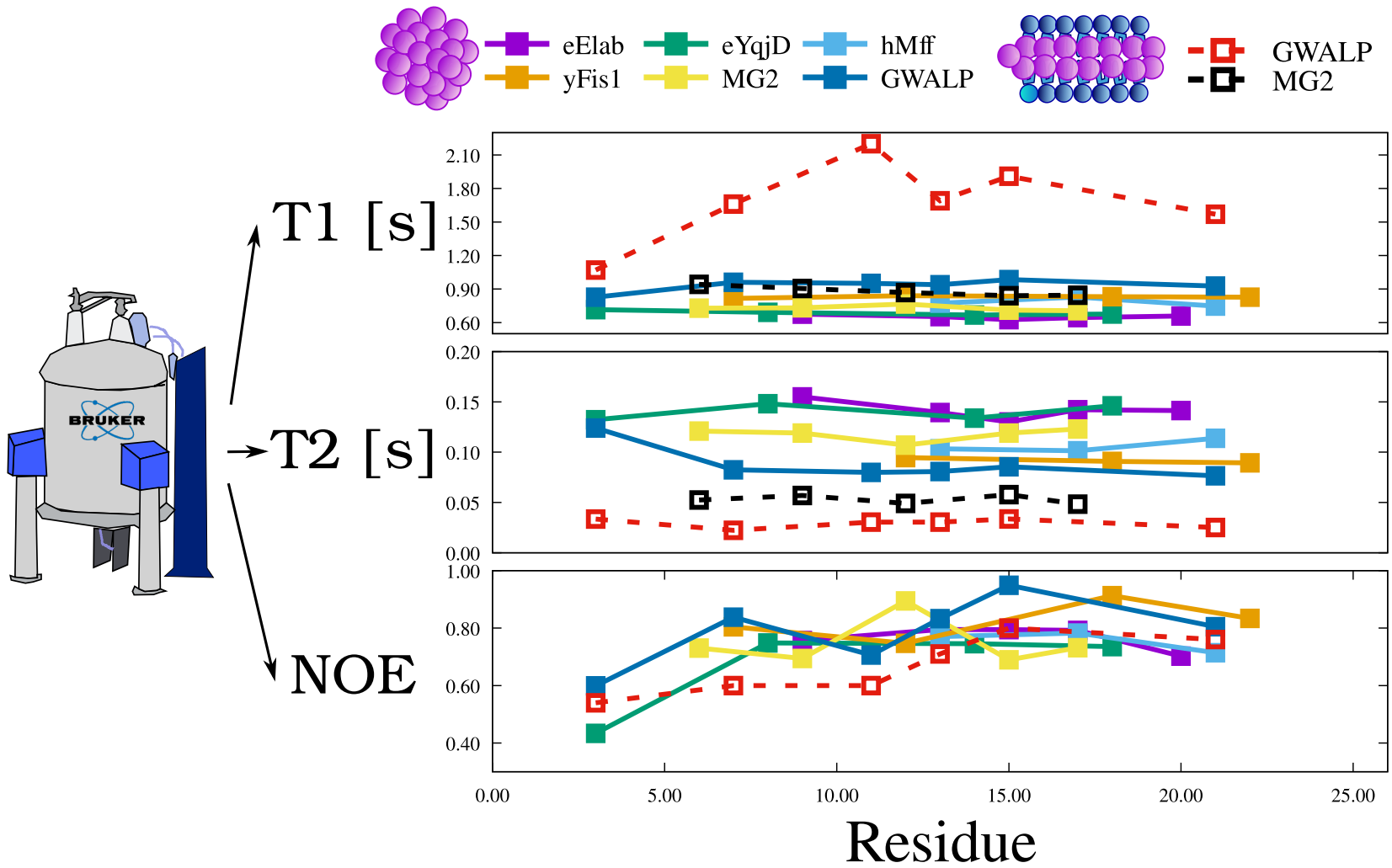
Results


eElab
eYqjD
hMff
yFis1
MG2
GWALP
T1 [s]
T2 [s]
NOE
BRUKER
1.00
0.90
0.80
0.70
0.60
0.15
0.10
0.05
1.00
0.80
0.60
0.40
0.00
5.00
10.00
15.00
20.00
25.00
Residue

Results

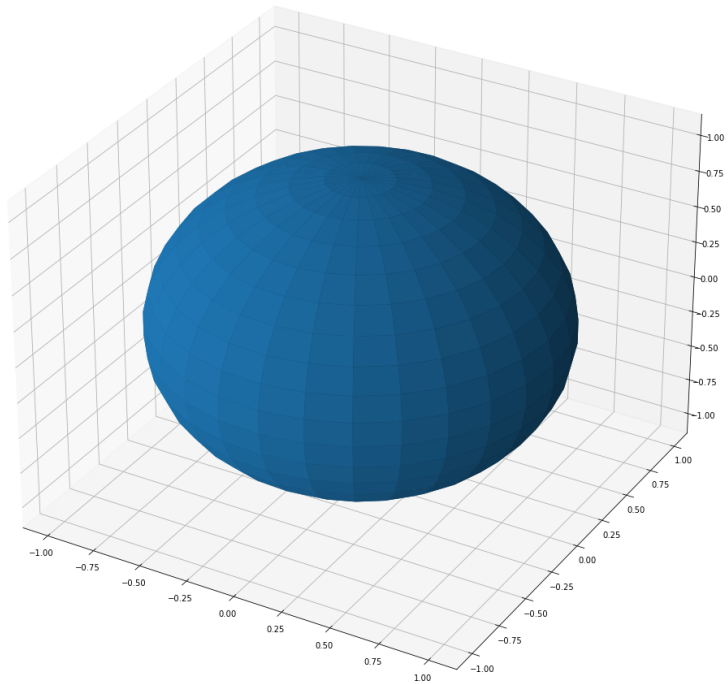

eElab
eYqjD
hMff
yFis1
MG2
GWALP
T1 [s]
T2 [s]
NOE
BRUKER
2.10
1.80
1.50
1.20
0.90
0.60
0.20
0.15
0.10
0.05
0.00
1.00
0.80
0.60
0.40
0.00
5.00
10.00
15.00
20.00
25.00
Residue

Results


eElab
yFis1
eYqjD
MG2
hMff
GWALP
GWALP
MG2
BRUKER
T1 [s]
T2 [s]
NOE
2.10
1.80
1.50
1.20
0.90
0.60
0.20
0.15
0.10
0.05
0.00
1.00
0.80
0.60
0.40
0.00
5.00
10.00
15.00
20.00
25.00
Residue

How can we interpret experimental NMR spin relaxation times?

To be developed or deleted, comment on what people do otherwise...



How can we interpret experimental NMR spin relaxation times?

Redfield equations

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$

How can we interpret experimental NMR spin relaxation times?

Redfield equations

Dipolar coupling constant

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

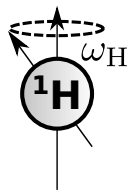
$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$

How can we interpret experimental NMR spin relaxation times?

Redfield equations

Dipolar coupling constant



Larmor angular frequency

$$\frac{1}{T_1} = \frac{d_{NH}^2}{20}[J(\omega_H - \omega_N) + 3J(\omega_N) + 6J(\omega_H + \omega_N)]$$

$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{NH}^2}{20}[4J(0) + J(\omega_H - \omega_N) + 3J(\omega_N) + 3J(\omega_H) + 6J(\omega_H + \omega_N)]$$

$$\mathrm{NOE} = 1 + \frac{d_{NH}^2}{20}[J(\omega_H + 6J(\omega_H + \omega_N)]\frac{\gamma_H T_1}{\gamma_N}$$

How can we interpret experimental NMR spin relaxation times?

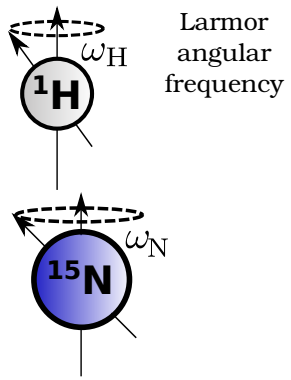
Redfield equations

Dipolar coupling constant

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$



Larmor angular frequency

How can we interpret experimental NMR spin relaxation times?

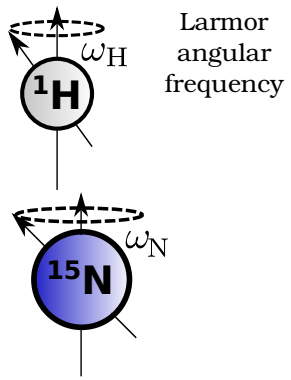
Redfield equations

Dipolar coupling constant

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$



Larmor angular frequency

spectral density

$$J(\omega) = 2\int_0^\infty C(t)cos(\omega t)\mathrm{d}t$$

How can we interpret experimental NMR spin relaxation times?

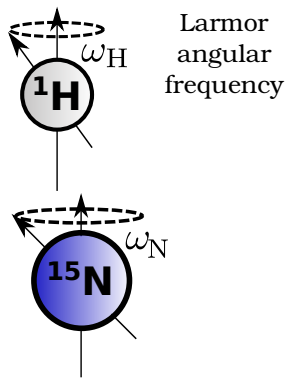
Redfield equations

Dipolar coupling constant

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

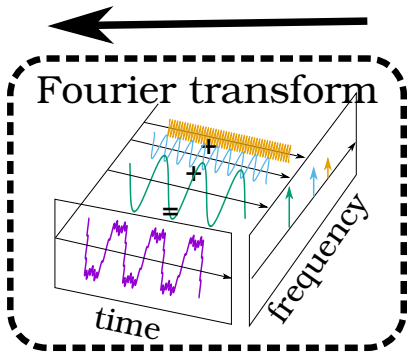
$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$



Larmor angular frequency

spectral density

$$J(\omega) = 2\int_0^\infty C(t)cos(\omega t)\mathrm{d}t$$



How can we interpret experimental NMR spin relaxation times?

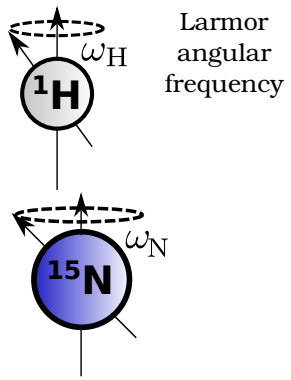
Redfield equations

Dipolar coupling constant

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

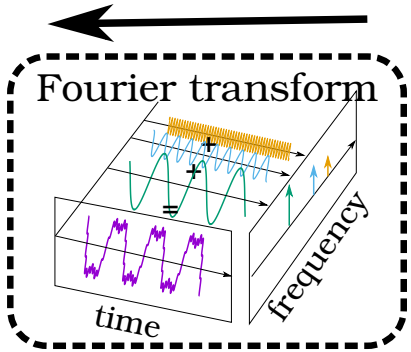
$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$



spectral density

$$J(\omega) = 2\int_0^\infty C(t)cos(\omega t)\mathrm{d}t$$



second-order rotational correlation function of N-H bond vector

$$C(t) = \left\langle \frac{3}{2}\cos^2\theta_{t'+t} - \frac{1}{2} \right\rangle_{t'}$$

How can we interpret experimental NMR spin relaxation times?

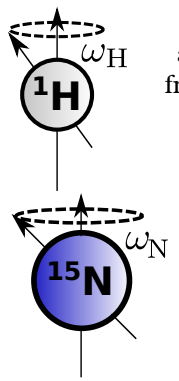
Redfield equations

Dipolar coupling constant

$$\frac{1}{T_1} = \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\frac{1}{T_2} = \frac{1}{2}\frac{d_{\mathrm{NH}}^2}{20}[4J(0) + J(\omega_{\mathrm{H}} - \omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{N}}) + 3J(\omega_{\mathrm{H}}) + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]$$

$$\mathrm{NOE} = 1 + \frac{d_{\mathrm{NH}}^2}{20}[J(\omega_{\mathrm{H}} + 6J(\omega_{\mathrm{H}} + \omega_{\mathrm{N}})]\frac{\gamma_{\mathrm{H}} T_1}{\gamma_{\mathrm{N}}}$$



Larmor angular frequency

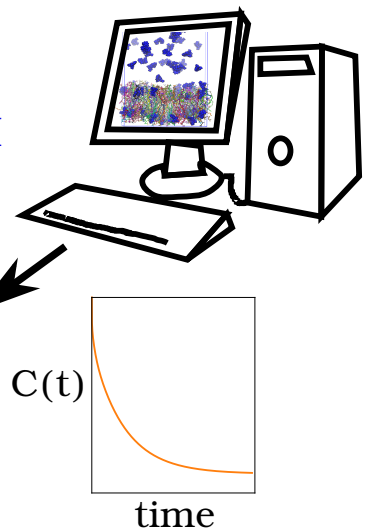
second-order rotational correlation function of N-H bond vector

$$C(t) = \left\langle \frac{3}{2}\cos^2\theta_{t'+t} - \frac{1}{2} \right\rangle_{t'}$$

Fourier transform

spectral density

$$J(\omega) = 2\int_0^\infty C(t)cos(\omega t)\mathrm{d}t$$

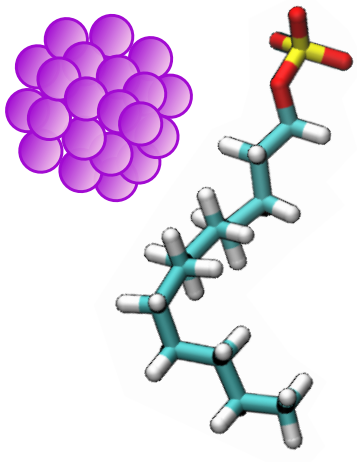


Results

Empty SDS micelles

SDS

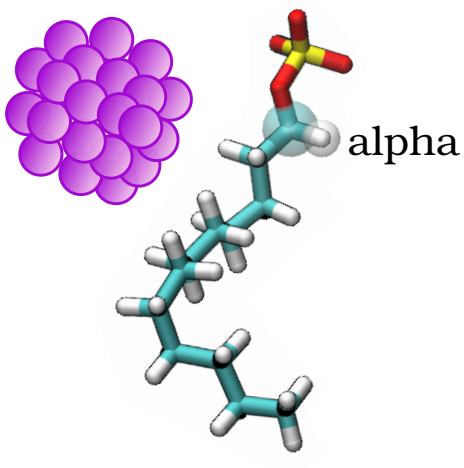
sodium dodecyl sulfate



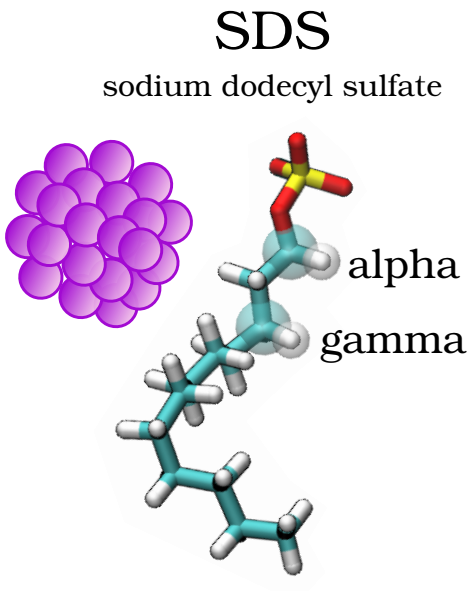
Empty SDS micelles

SDS

sodium dodecyl sulfate



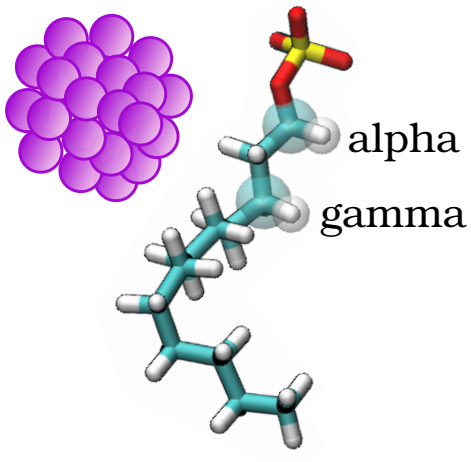
Empty SDS micelles

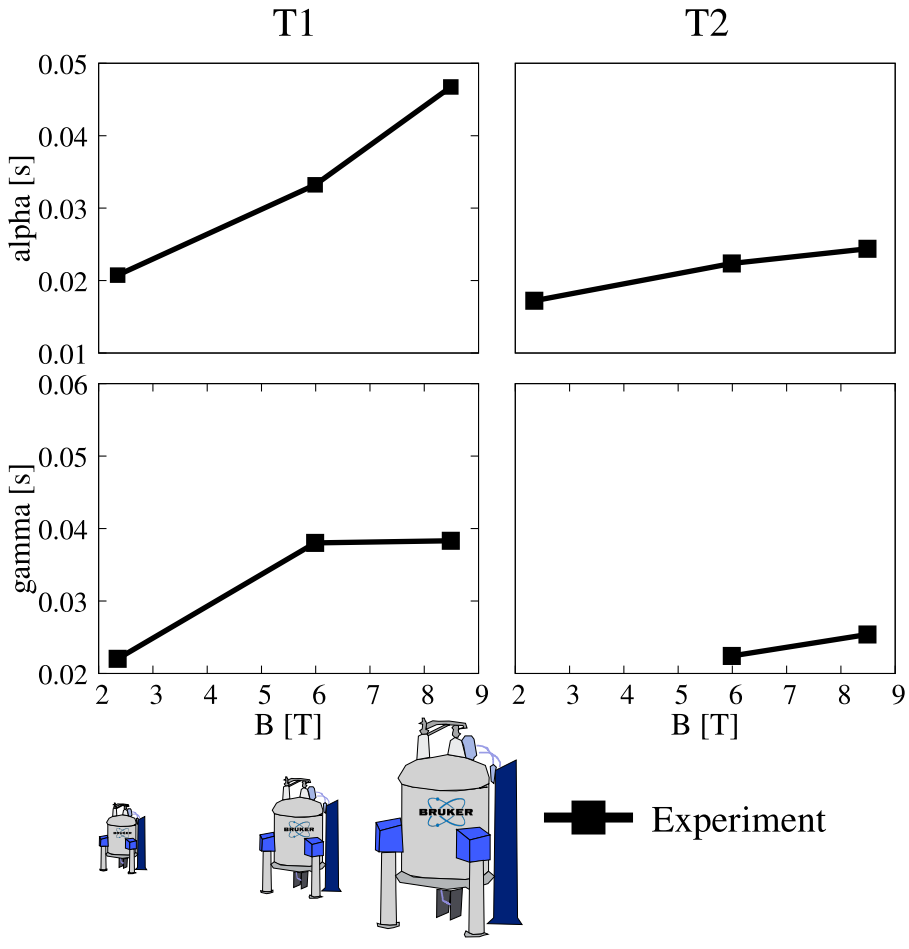


Empty SDS micelles

SDS

sodium dodecyl sulfate

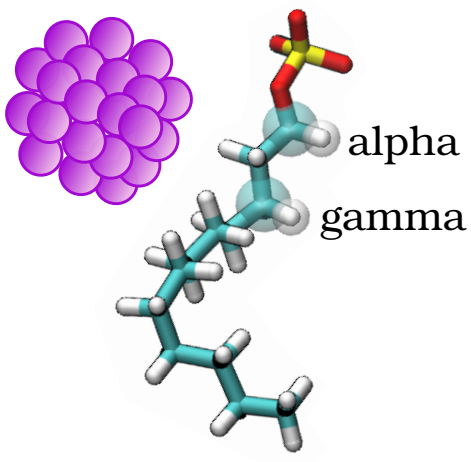


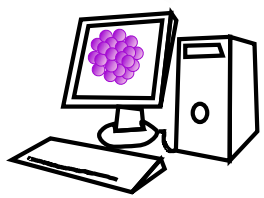


Empty SDS micelles

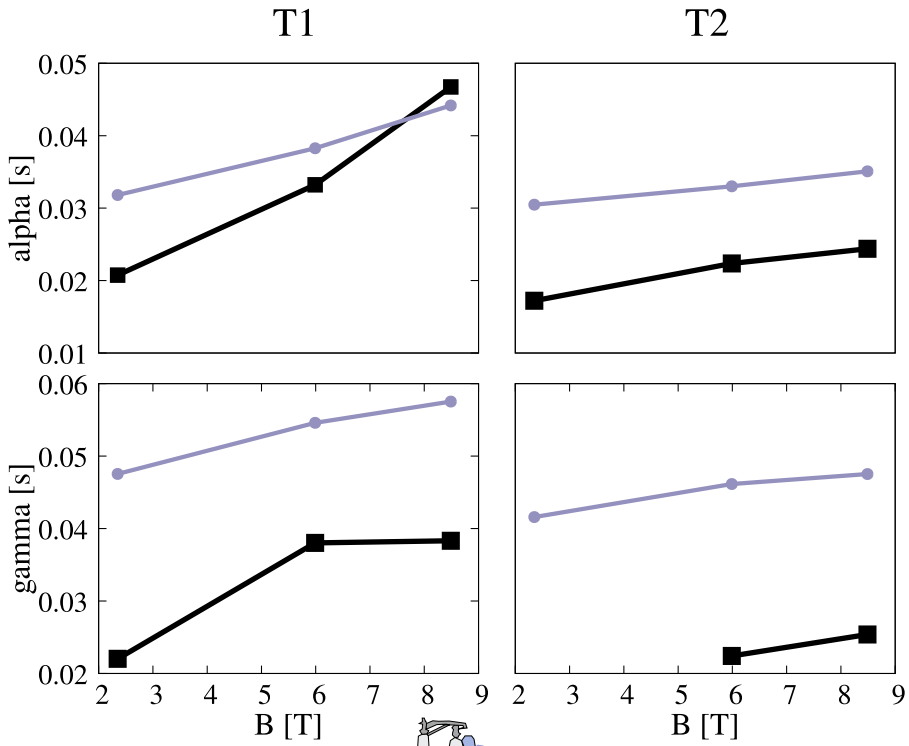
SDS

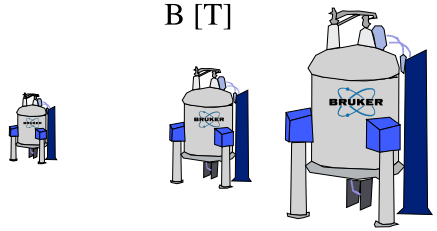
sodium dodecyl sulfate





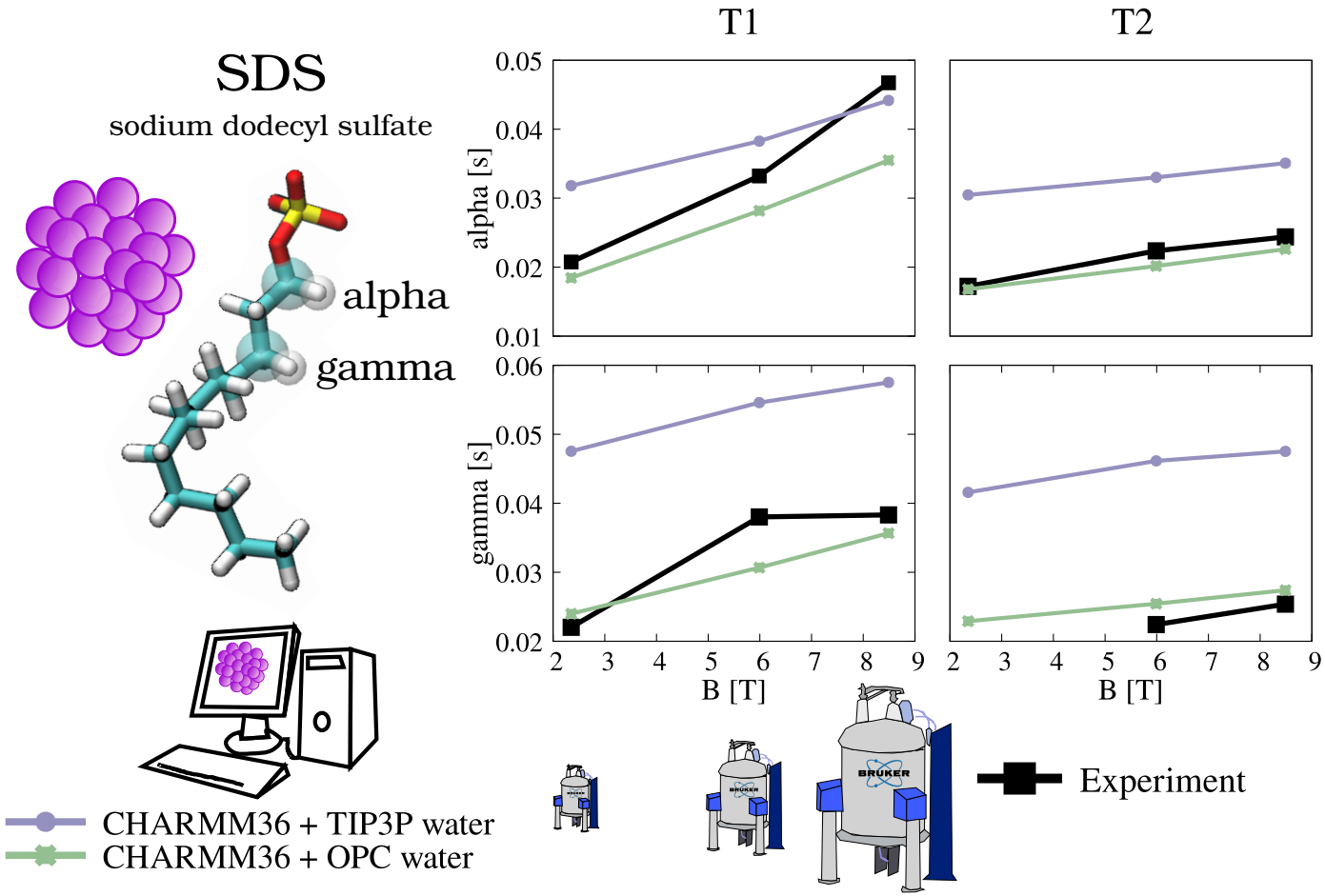
CHARMM36 + TIP3P water



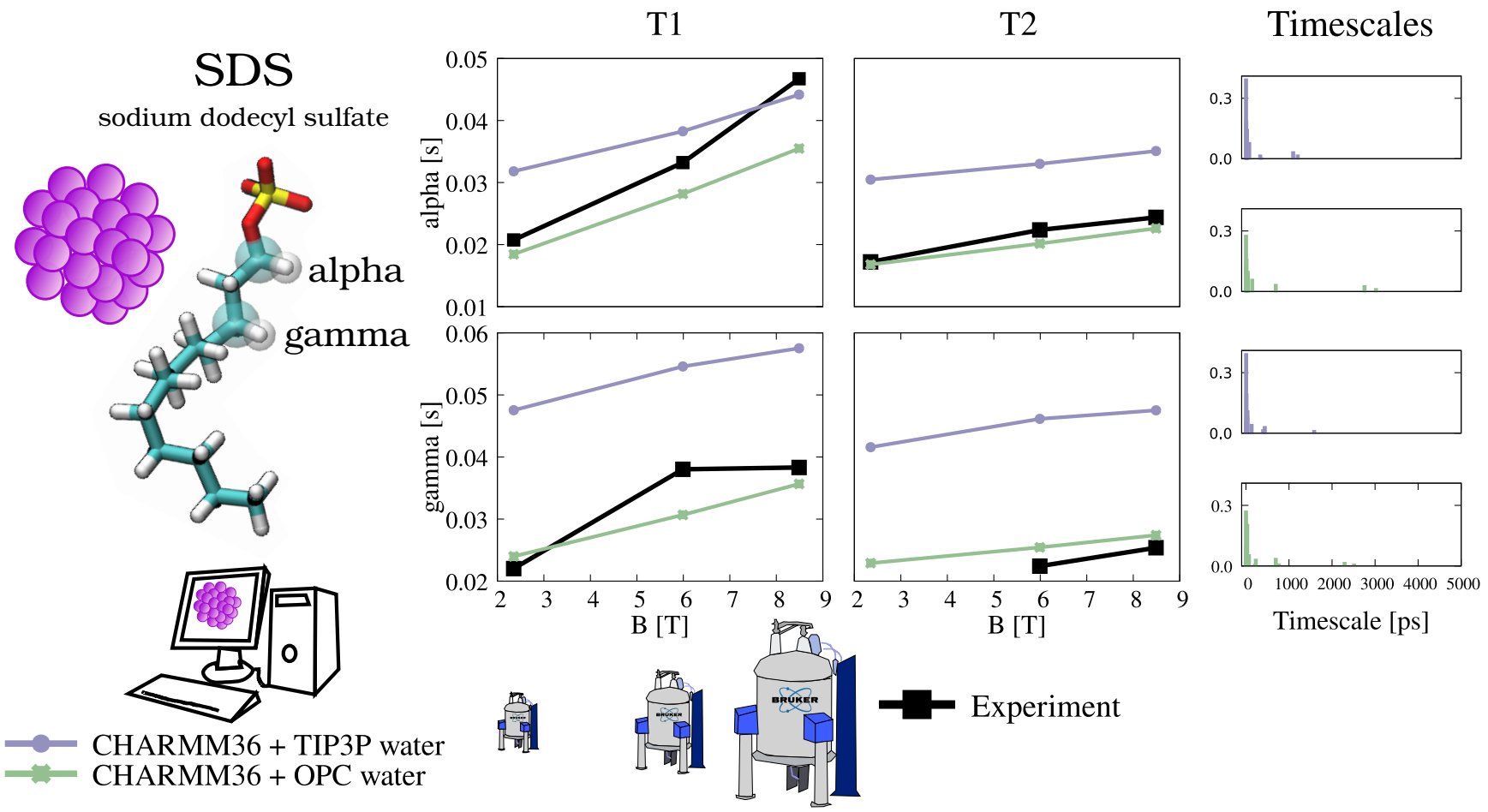


Experiment

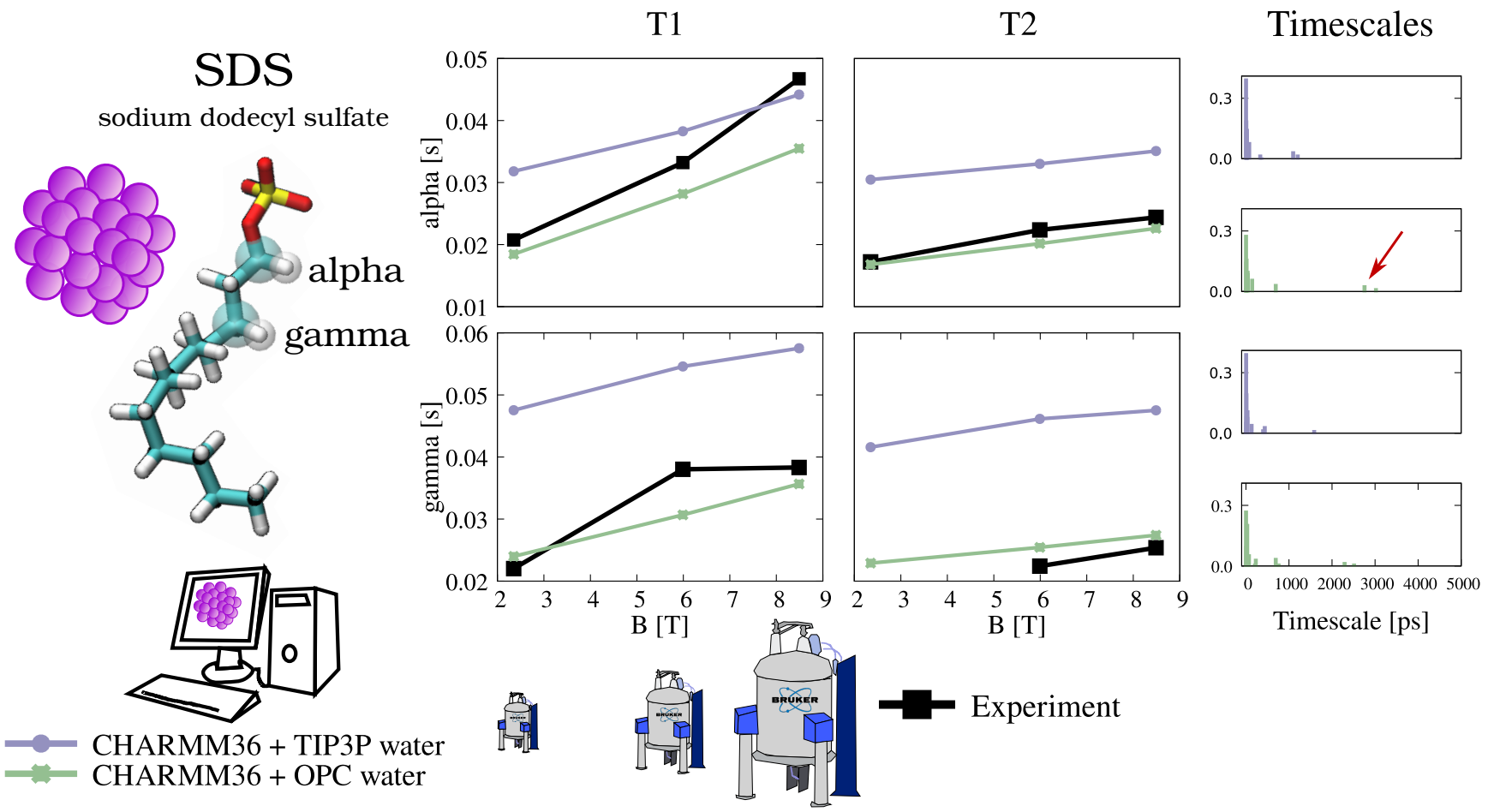
Empty SDS micelles



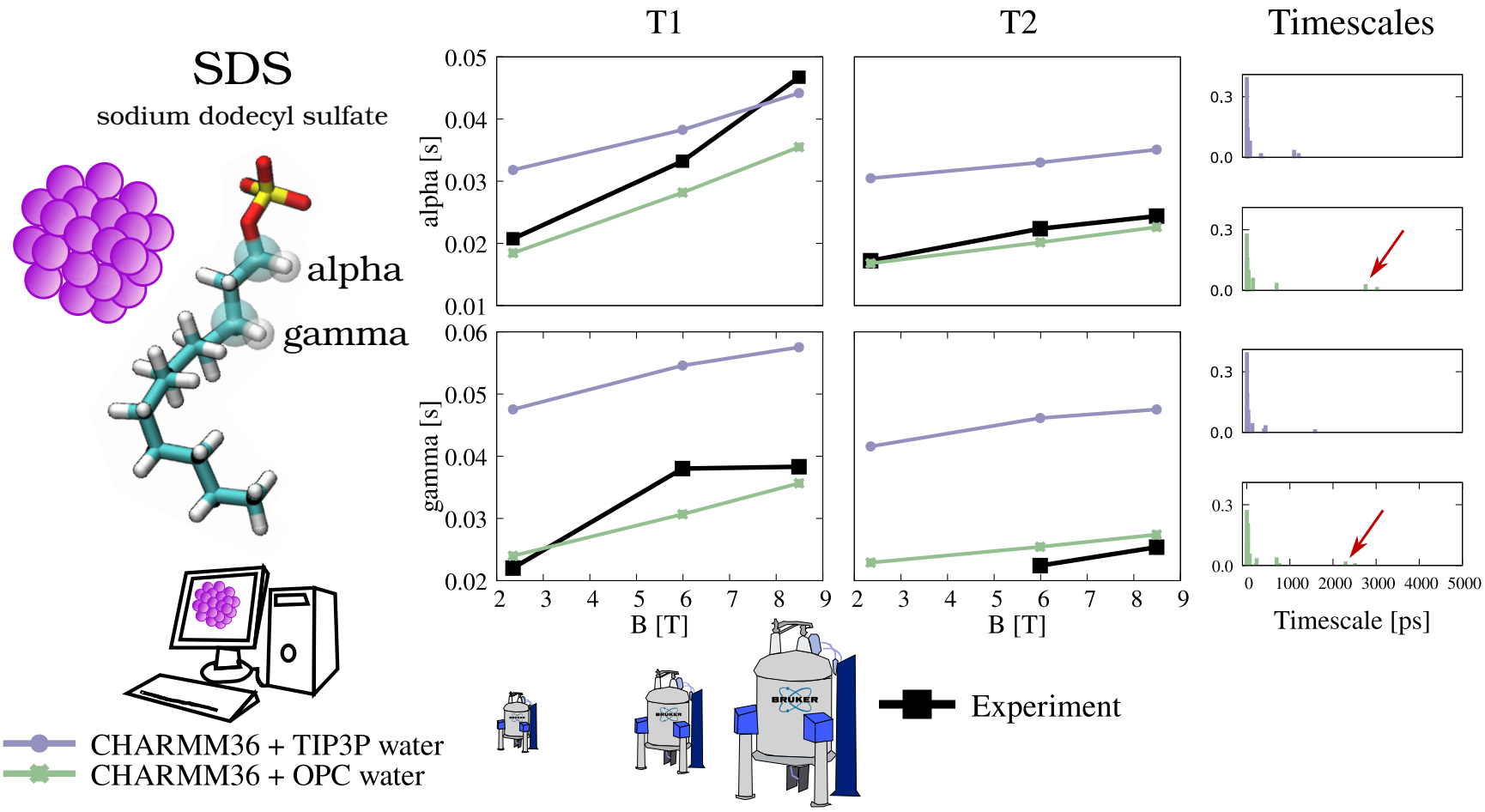
Empty SDS micelles



Empty SDS micelles

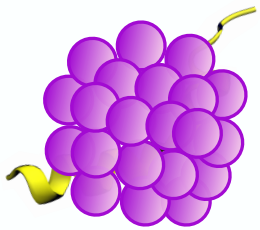


Empty SDS micelles



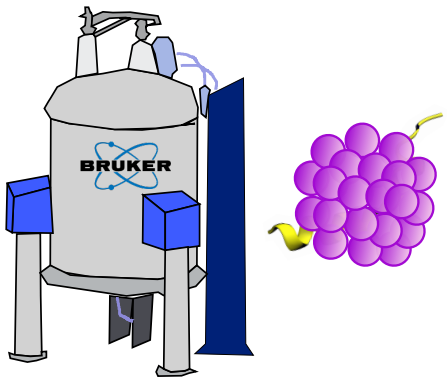
Optimization of simulations

- Magainin 2

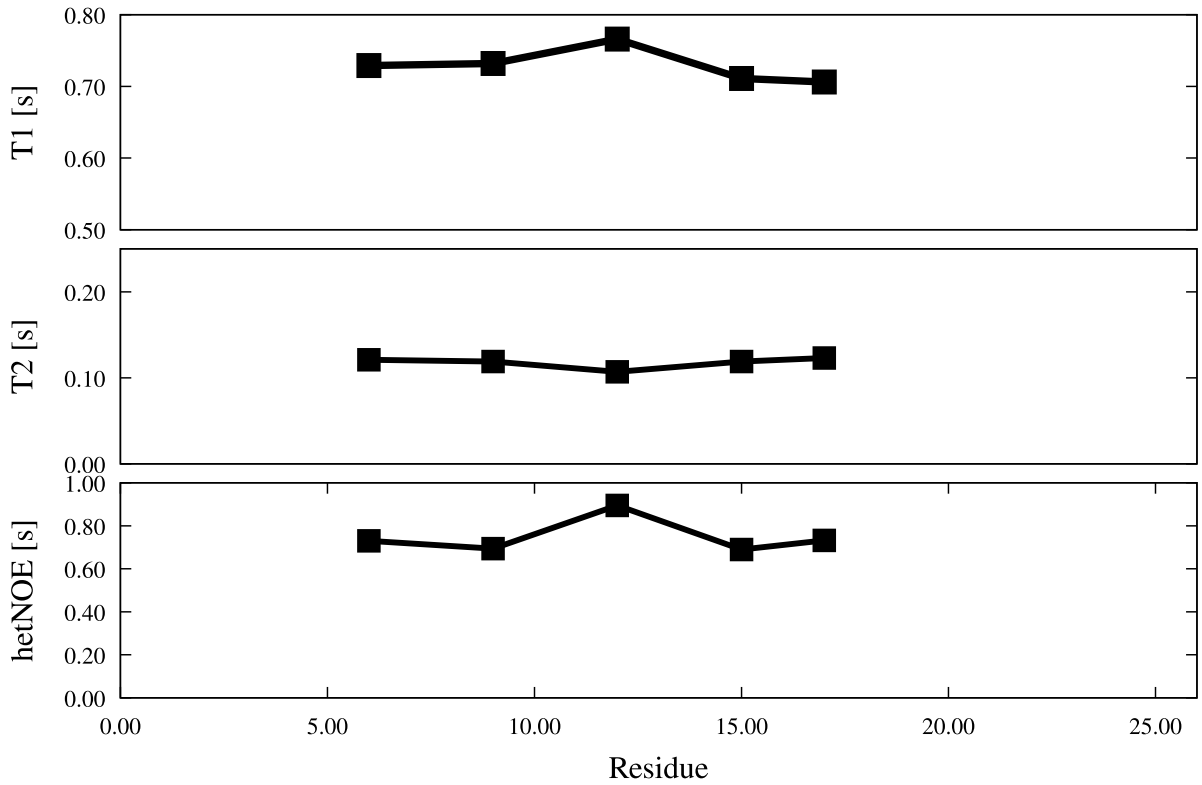


Optimization of simulations

Magainin 2

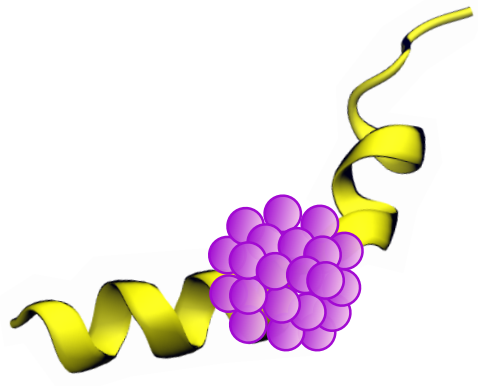


Experiment

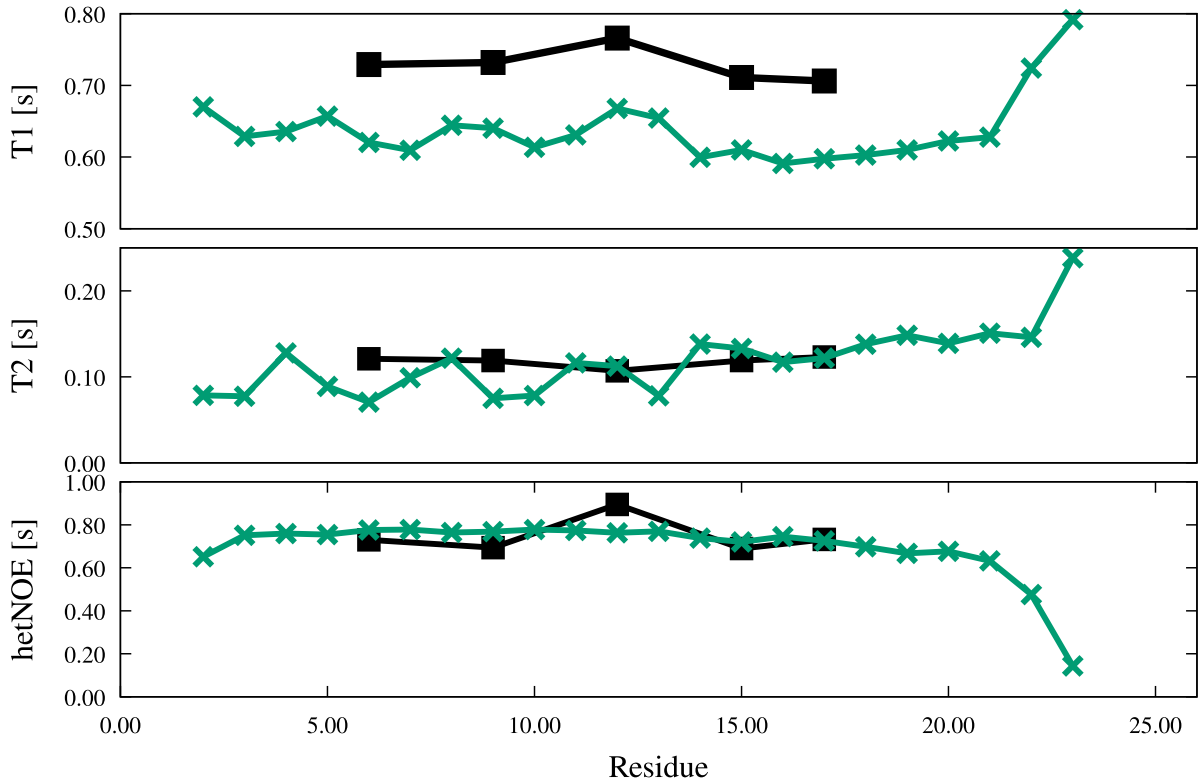


Optimization of simulations

Magainin 2

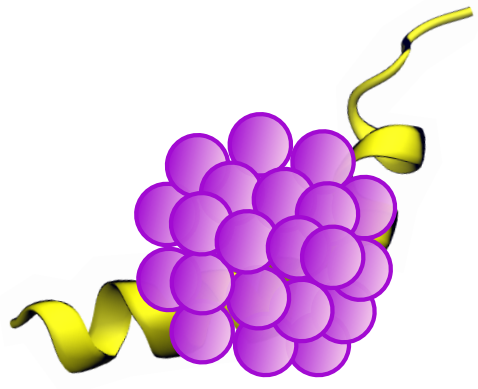


Experiment
Simulation, 40 SDS

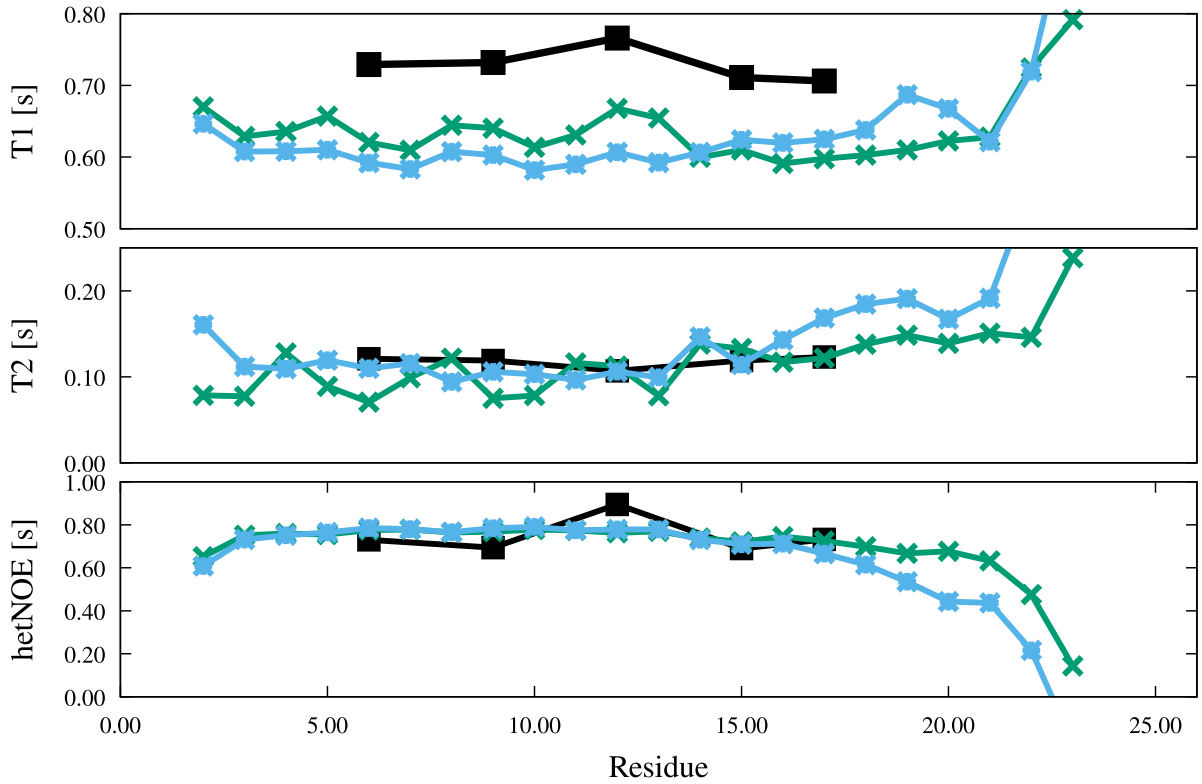


Optimization of simulations

Magainin 2

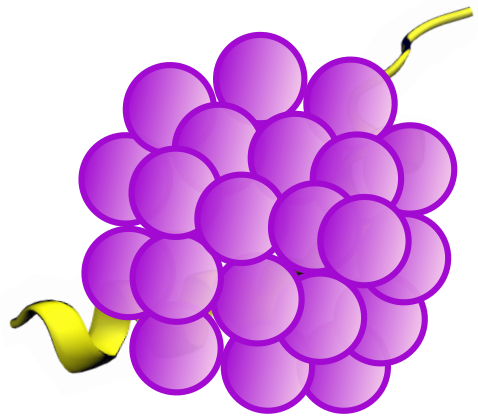


Experiment
Simulation, 40 SDS
Simulation, 45 SDS

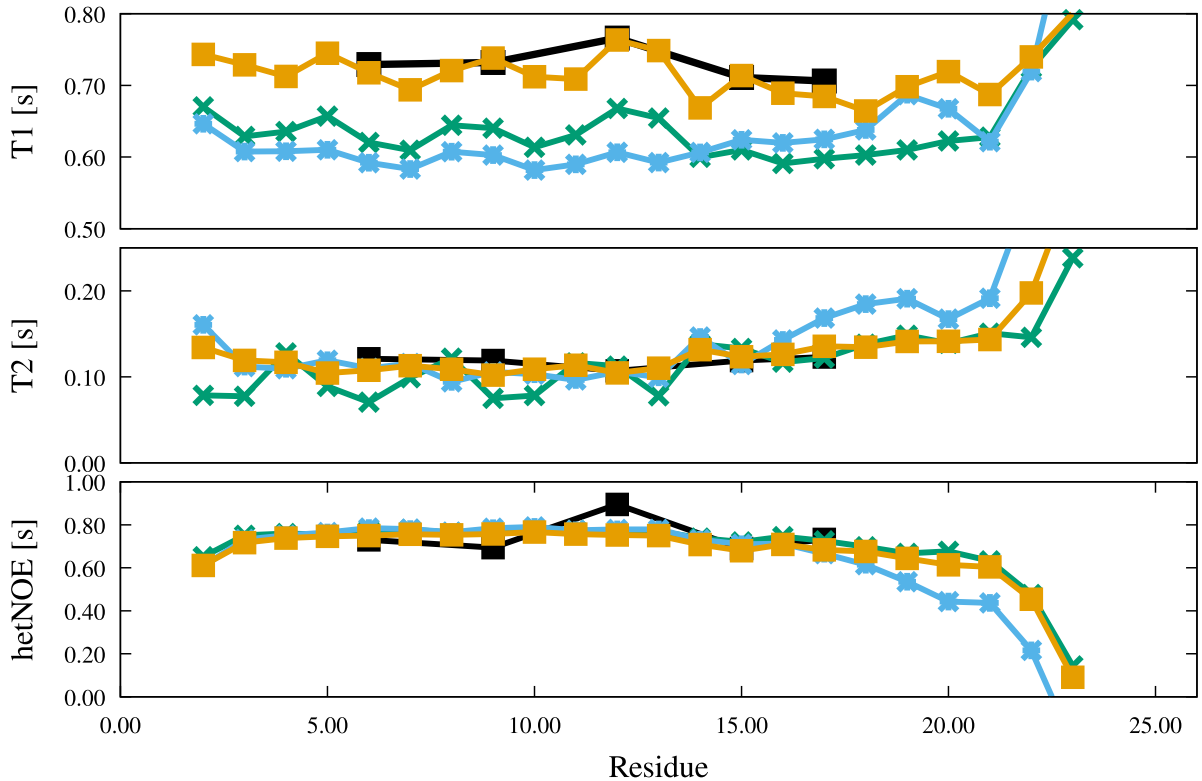


Optimization of simulations

Magainin 2

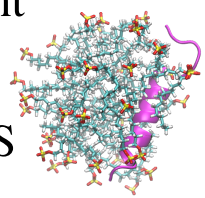


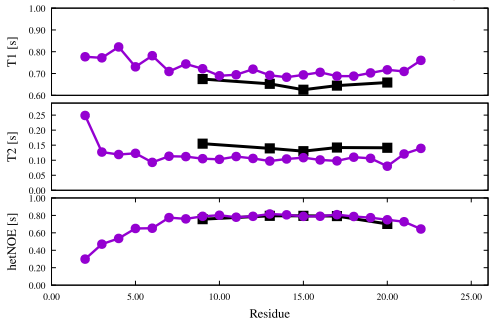
Experiment
Simulation, 40 SDS
Simulation, 45 SDS
Simulation, 50 SDS



Experiment

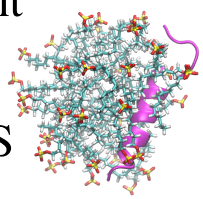
eElab, 40 SDS

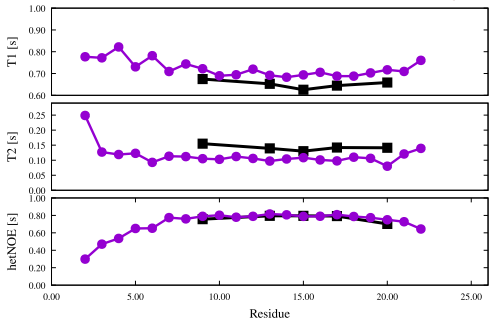




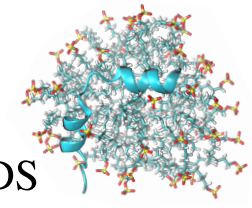
Experiment

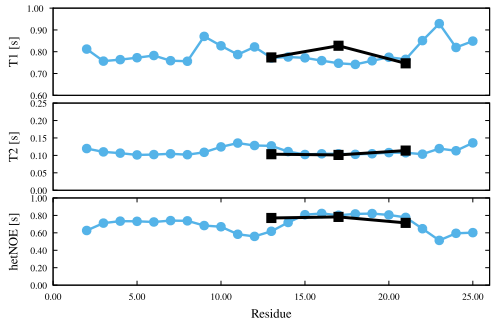
eElab, 40 SDS





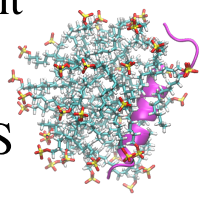
hMff, 50 SDS

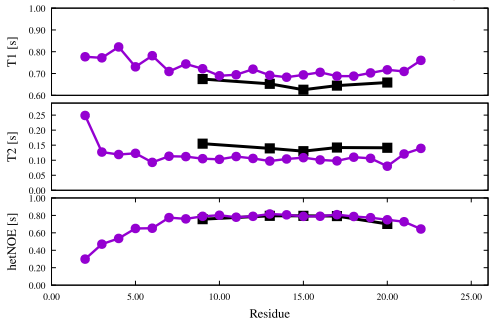




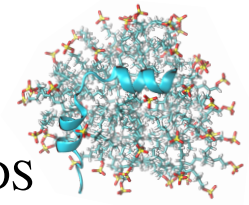
Experiment

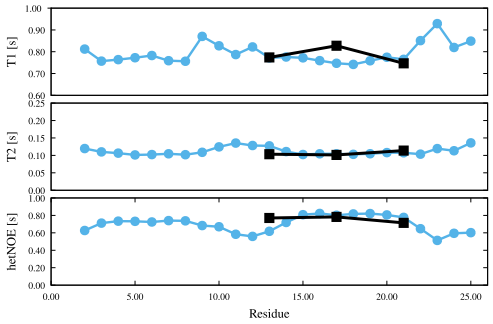
eElab, 40 SDS



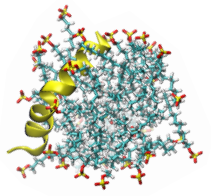


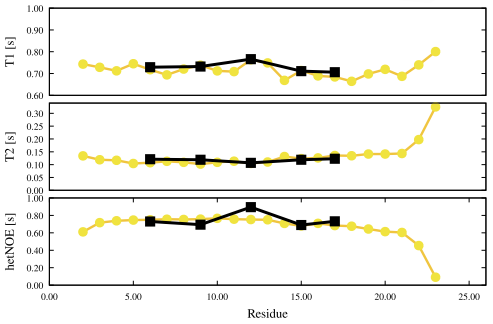
hMff, 50 SDS





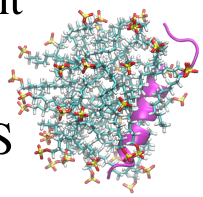
Magainin 2, 50 SDS

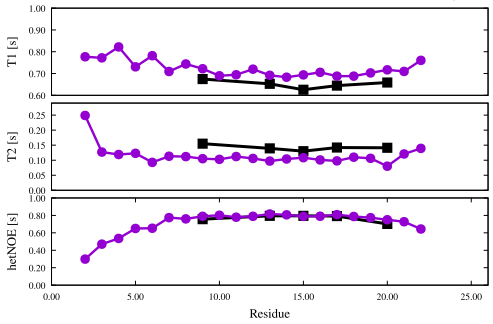




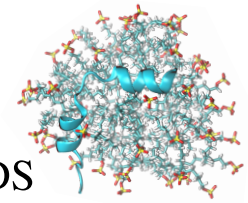
Experiment

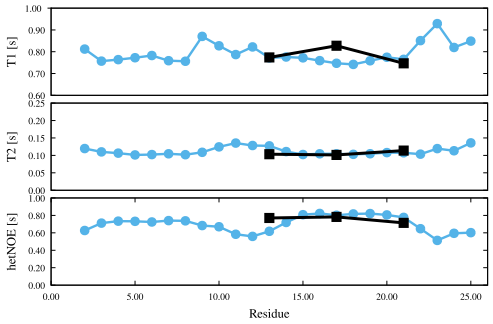
eElab, 40 SDS



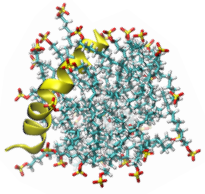


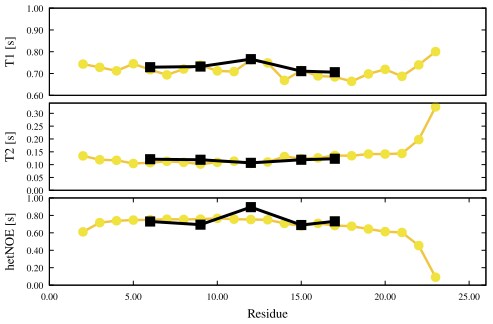
hMff, 50 SDS



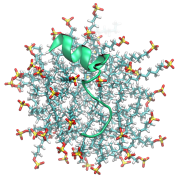


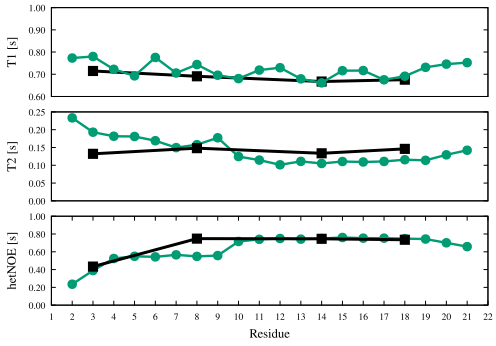
Magainin 2, 50 SDS





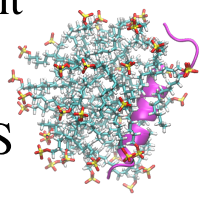
eYqjD, 50 SDS

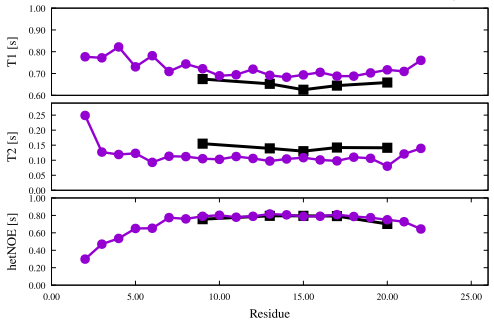




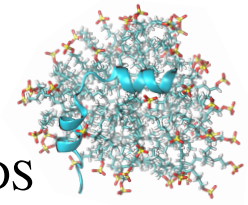
Experiment

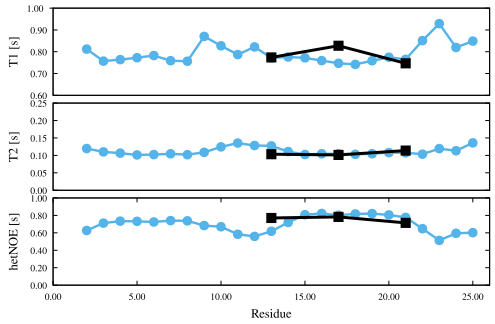
eElab, 40 SDS



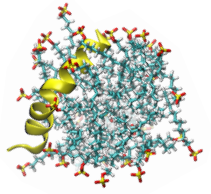


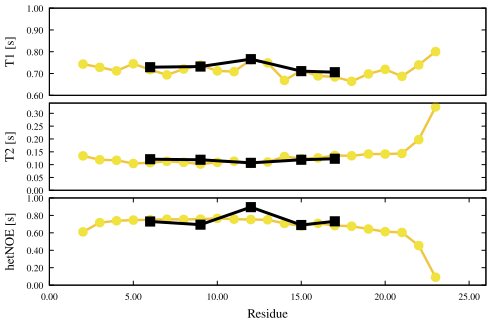
hMff, 50 SDS



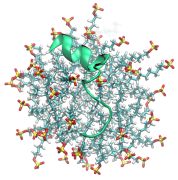


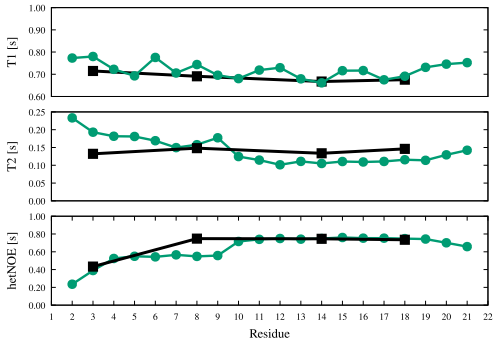
Magainin 2, 50 SDS



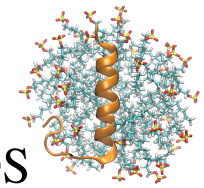


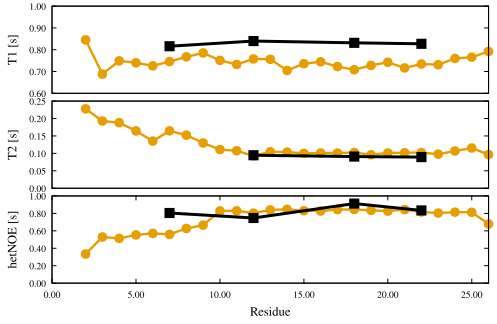
eYqjD, 50 SDS





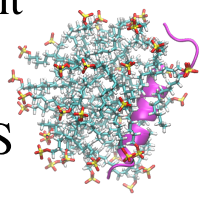
yFis1, 50 SDS

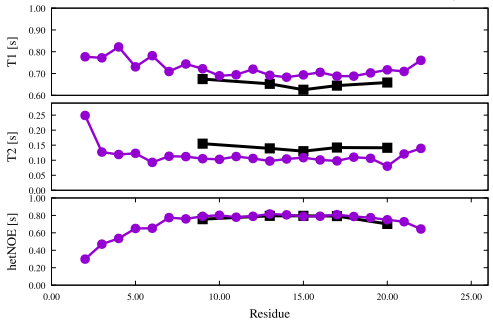




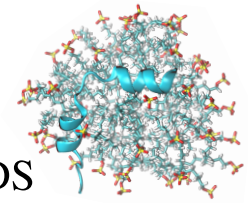
Experiment

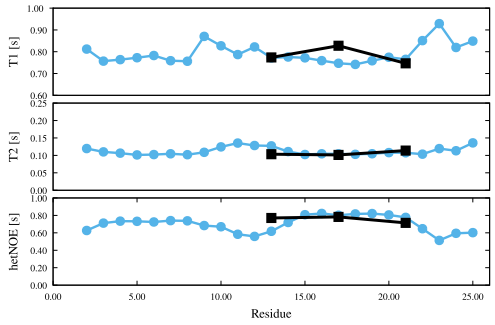
eElab, 40 SDS



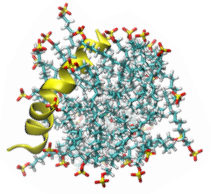


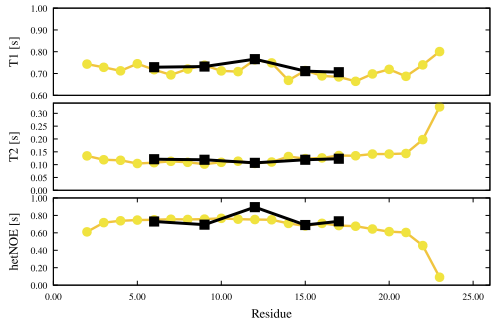
hMff, 50 SDS



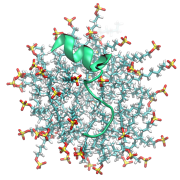


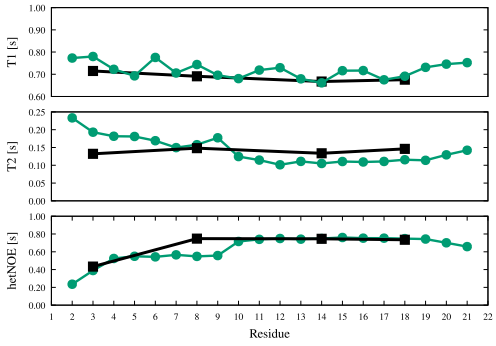
Magainin 2, 50 SDS



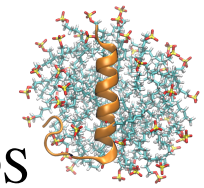


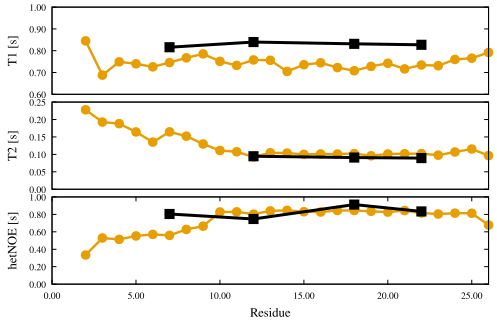
eYqjD, 50 SDS



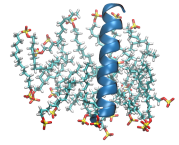


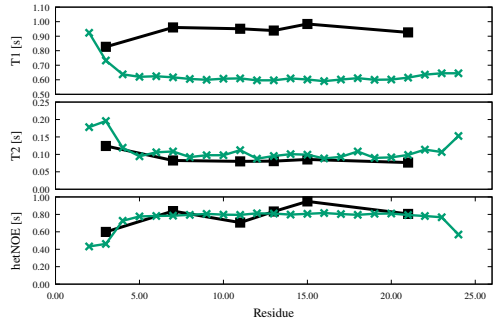
yFis1, 50 SDS





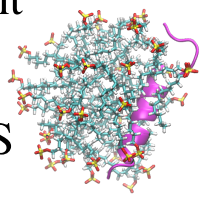
GWALP, 40 SDS

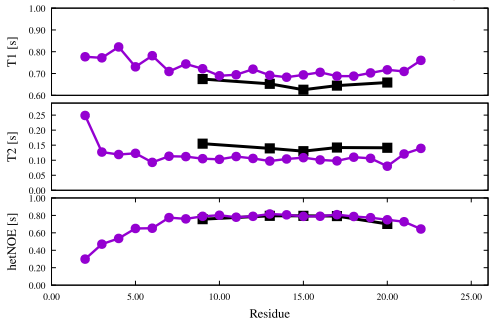




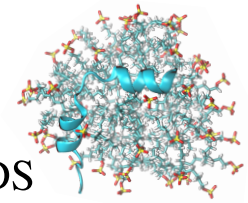
Experiment

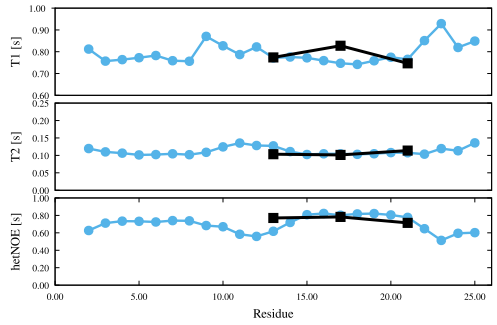
eElab, 40 SDS



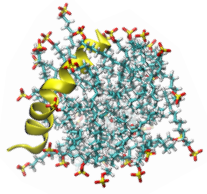


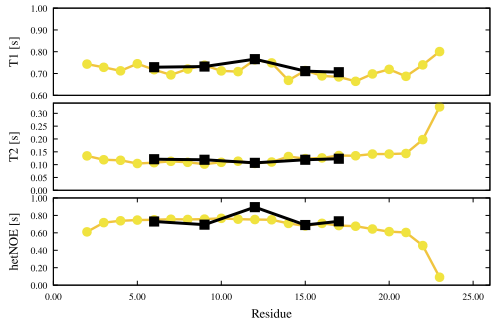
hMff, 50 SDS



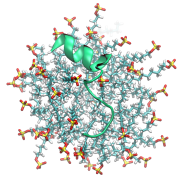


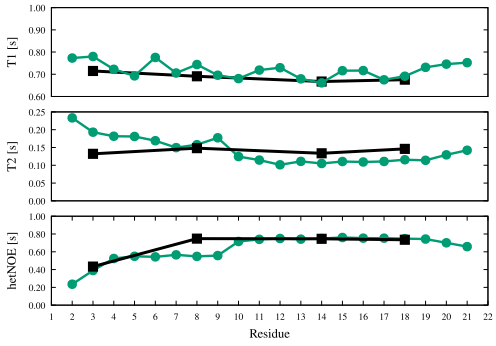
Magainin 2, 50 SDS



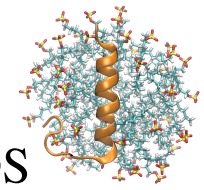


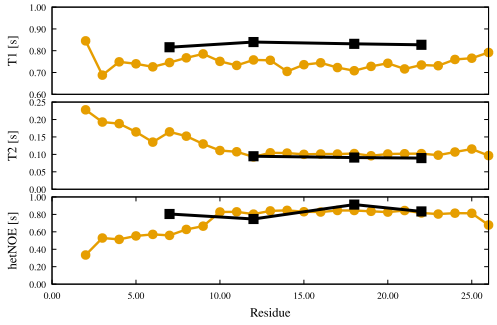
eYqjD, 50 SDS



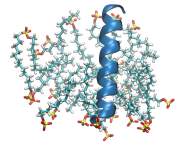


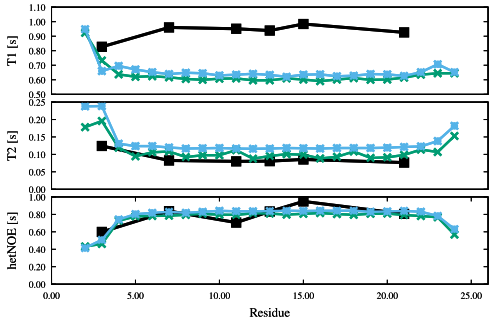
yFis1, 50 SDS





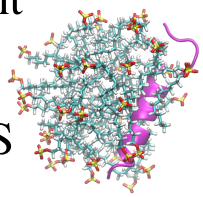
GWALP, 40 SDS
GWALP 45 SDS

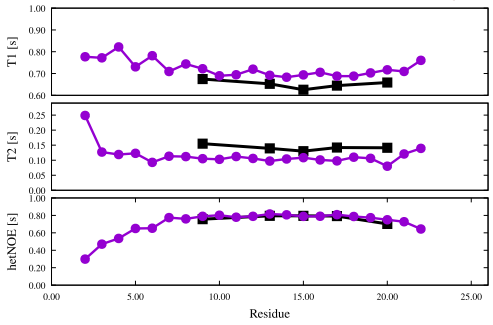




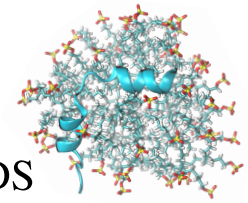
Experiment

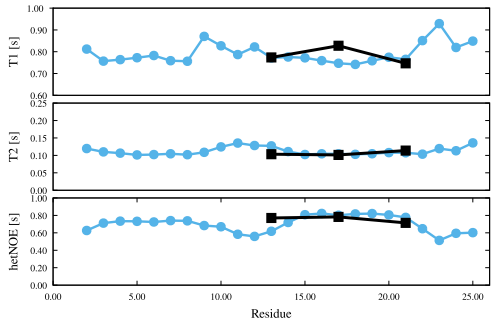
eElab, 40 SDS



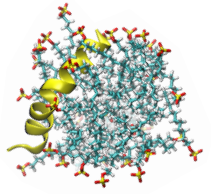


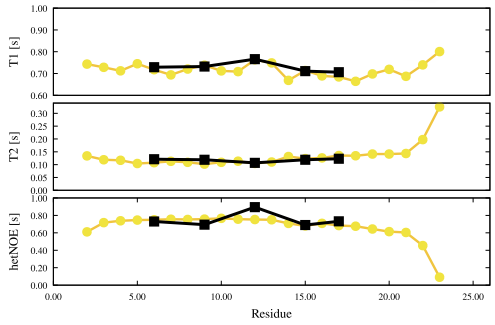
hMff, 50 SDS



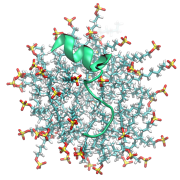


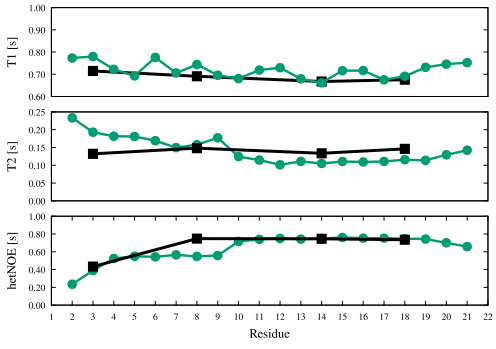
Magainin 2, 50 SDS



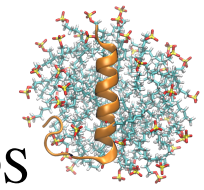


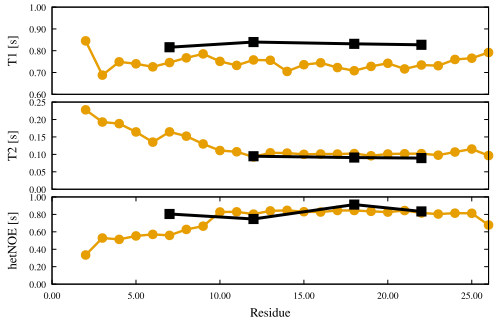
eYqjD, 50 SDS



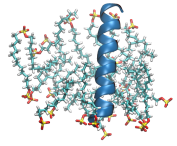


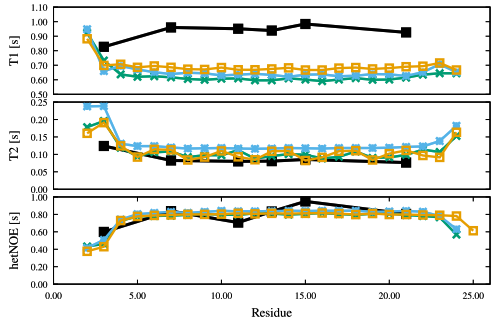
yFis1, 50 SDS





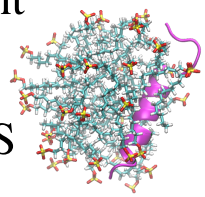
GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS

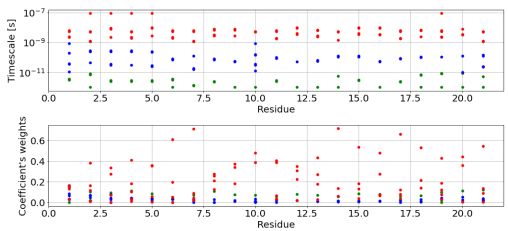




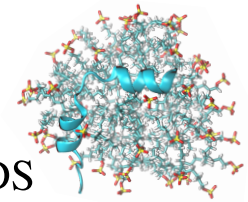
Experiment

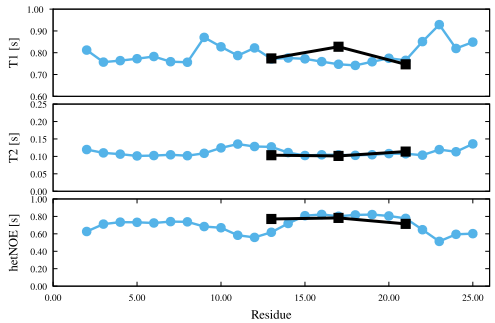
eElab, 40 SDS



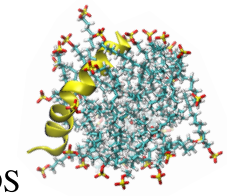


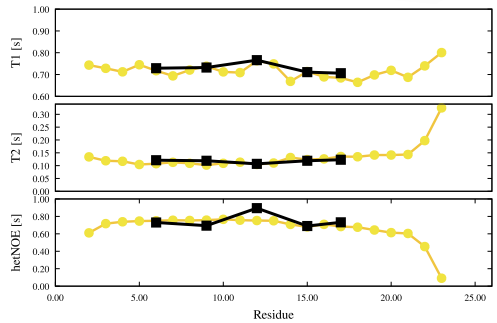
hMff, 50 SDS



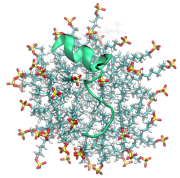


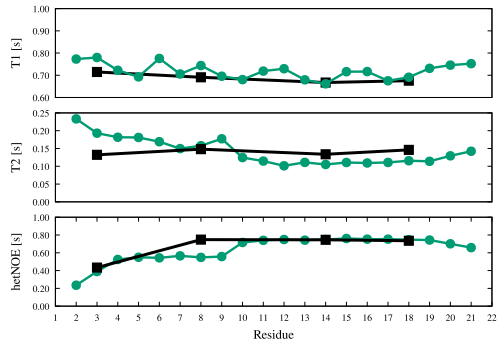
Magainin 2, 50 SDS



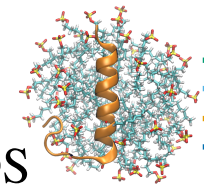


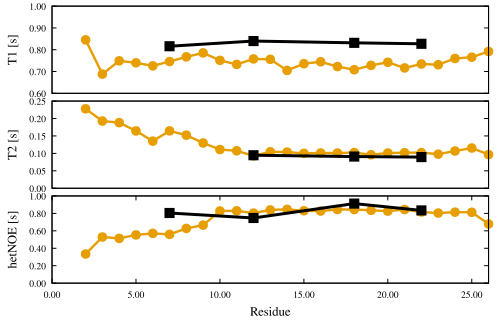
eYqjD, 50 SDS



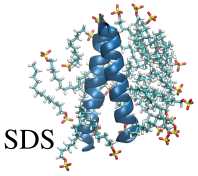


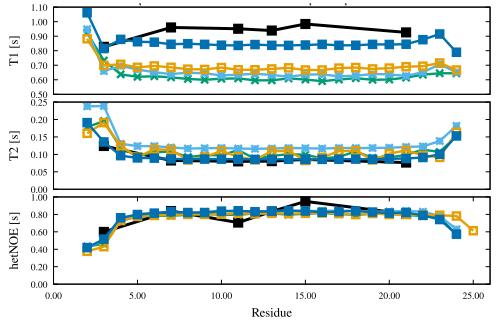
yFis1, 50 SDS





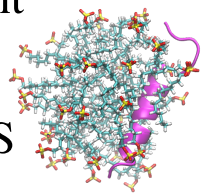
GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS
GWALP dimer 50 SDS

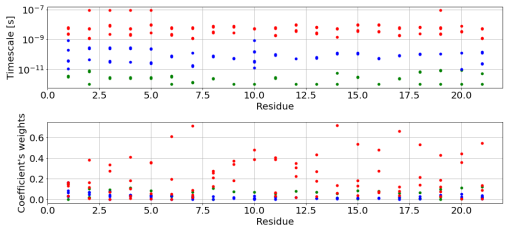




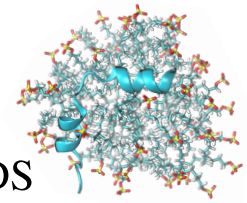
Experiment

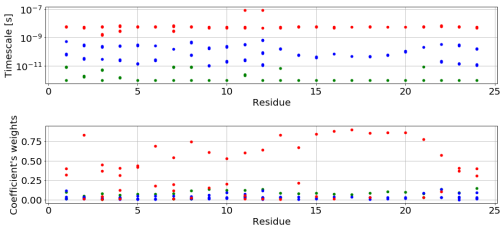
eElab, 40 SDS



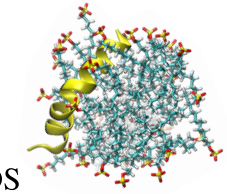


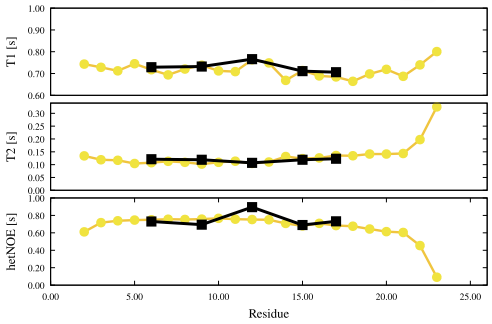
hMff, 50 SDS



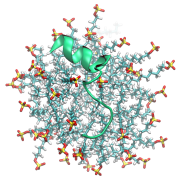


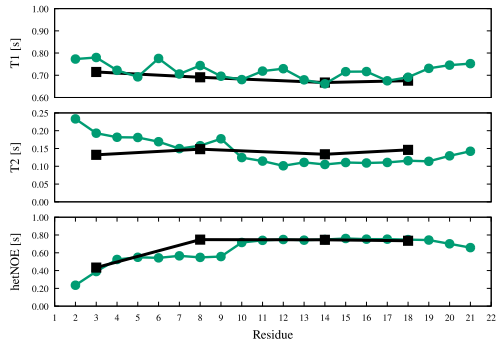
Magainin 2, 50 SDS



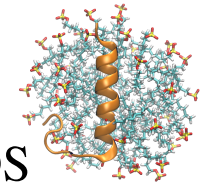


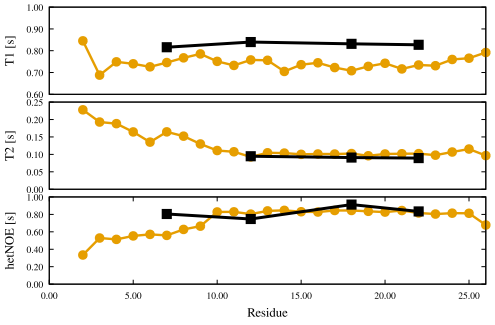
eYqjD, 50 SDS



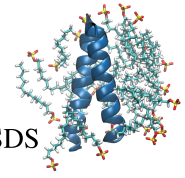


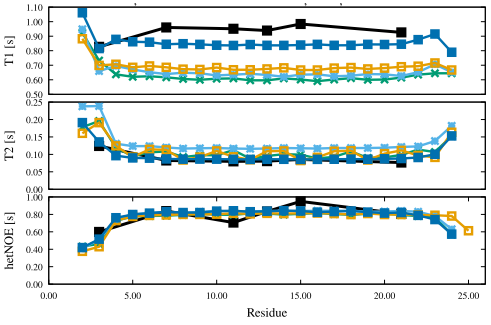
yFis1, 50 SDS





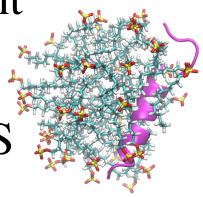
GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS
GWALP dimer 50 SDS



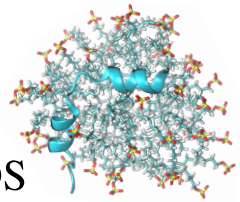


Experiment

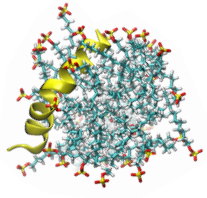
eElab, 40 SDS

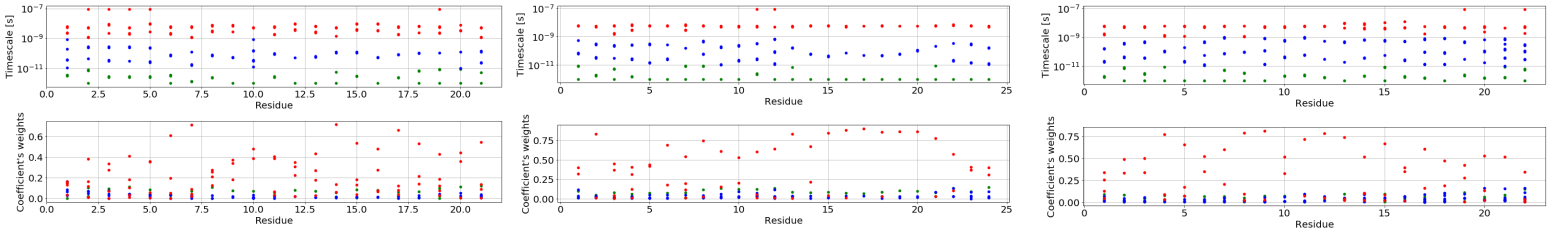


hMff, 50 SDS

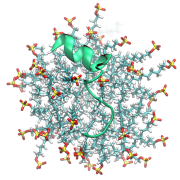


Magainin 2, 50 SDS

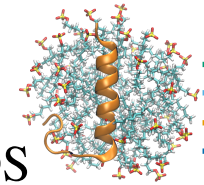




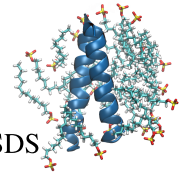
eYqjD, 50 SDS

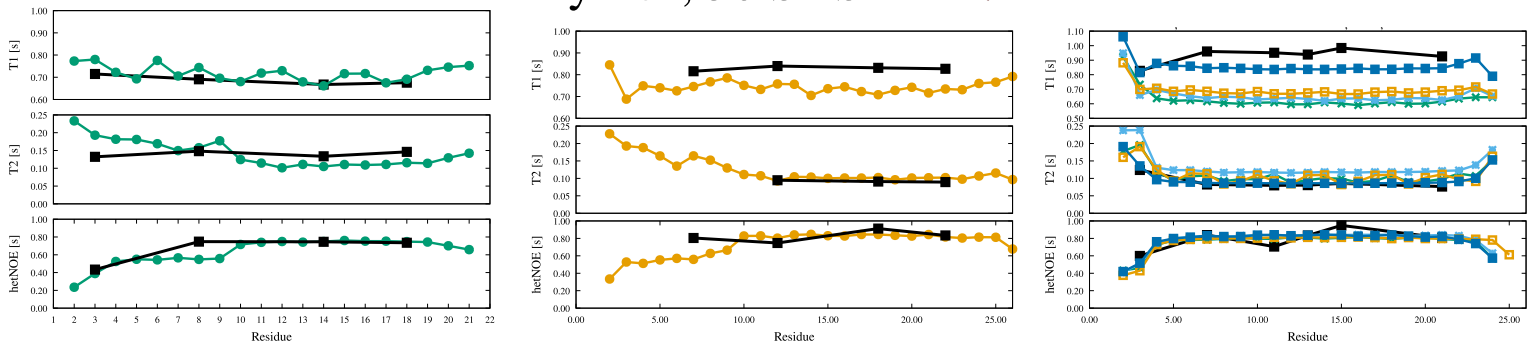


yFis1, 50 SDS



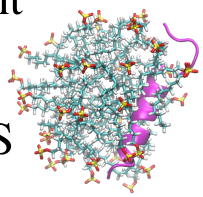
GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS
GWALP dimer 50 SDS



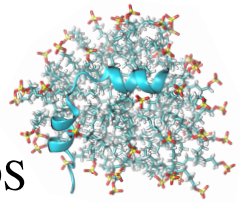


Experiment

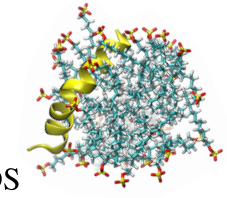
eElab, 40 SDS

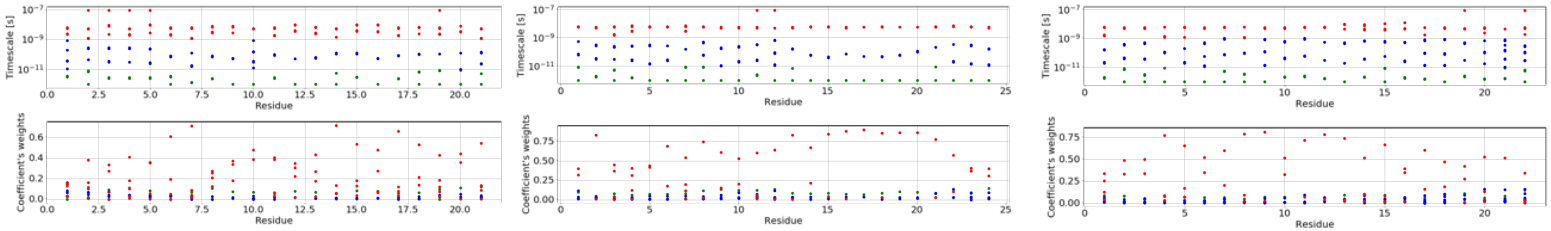


hMff, 50 SDS

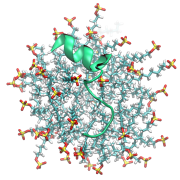


Magainin 2, 50 SDS

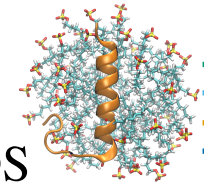




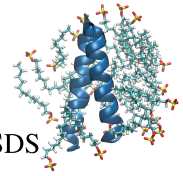
eYqjD, 50 SDS

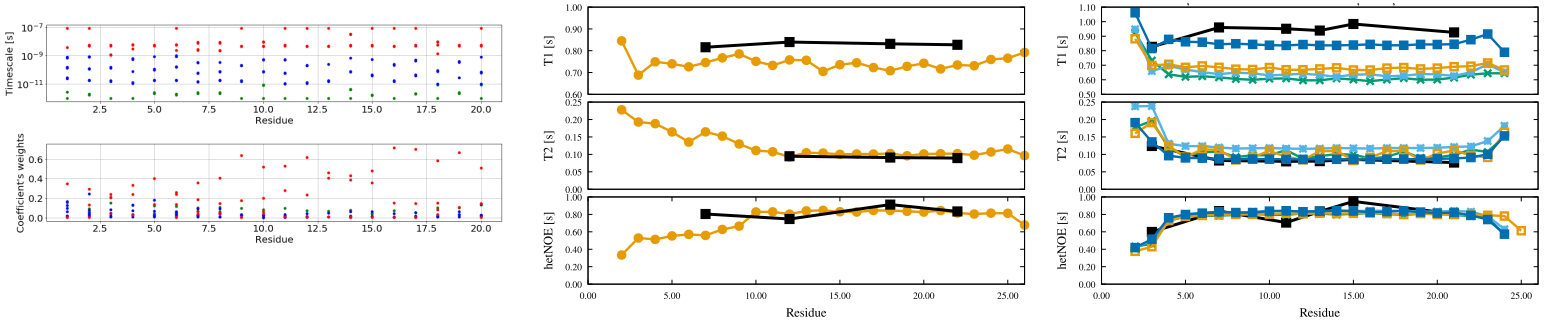


yFis1, 50 SDS



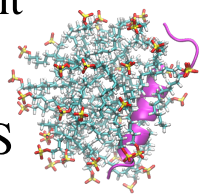
GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS
GWALP dimer 50 SDS



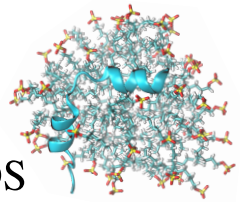


Experiment

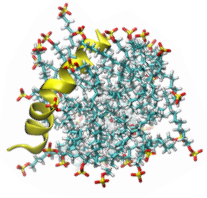
eElab, 40 SDS

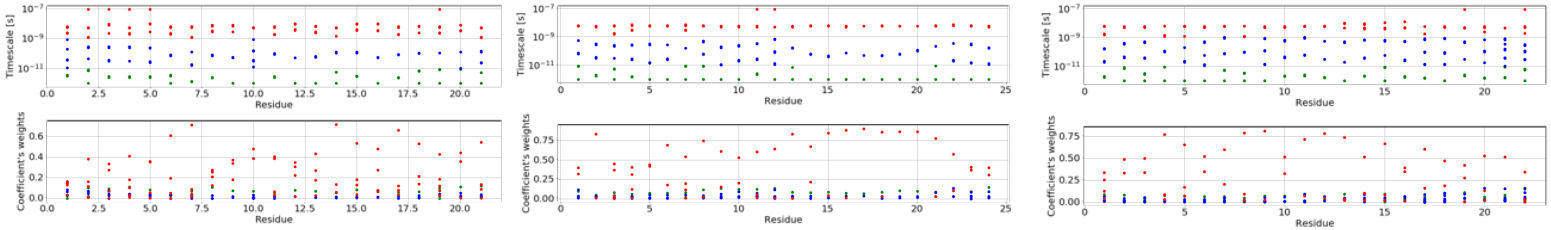


hMff, 50 SDS

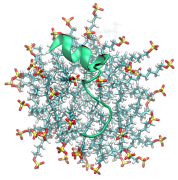


Magainin 2, 50 SDS

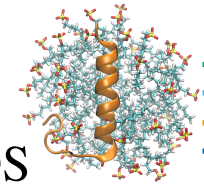




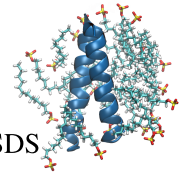
eYqjD, 50 SDS

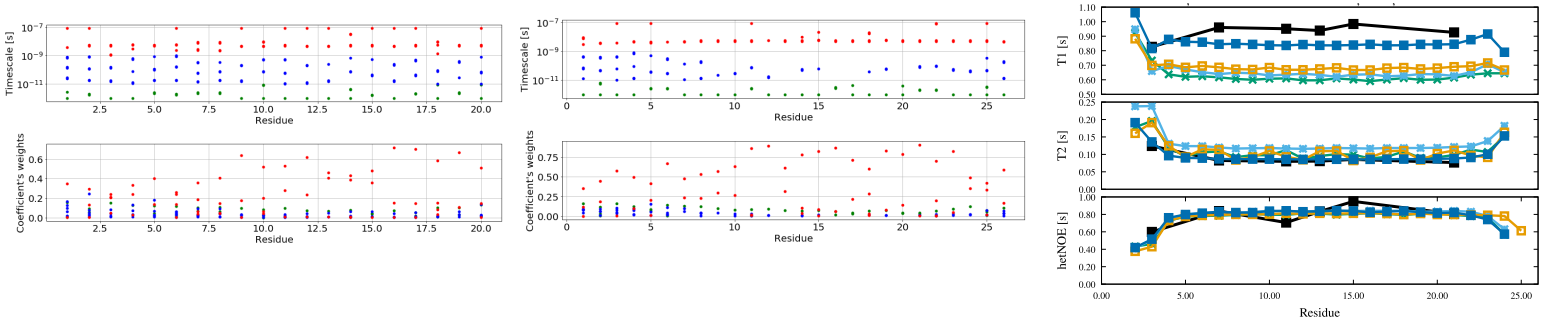


yFis1, 50 SDS



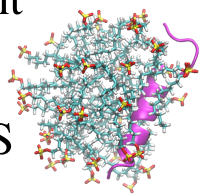
GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS
GWALP dimer 50 SDS



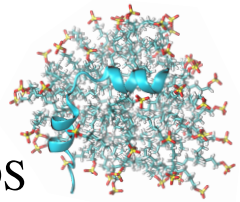


Experiment

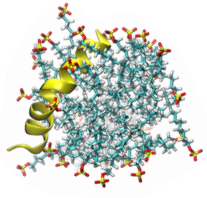
eElab, 40 SDS

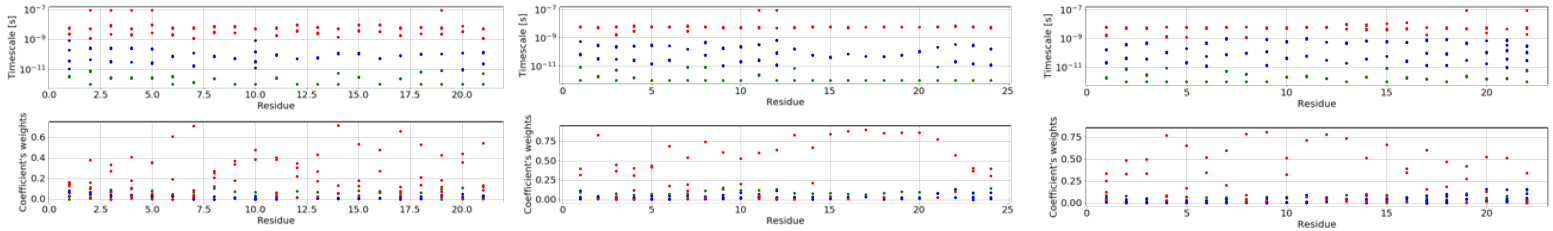


hMff, 50 SDS

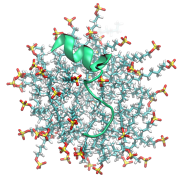


Magainin 2, 50 SDS

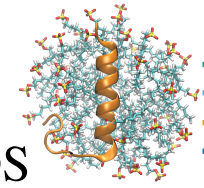




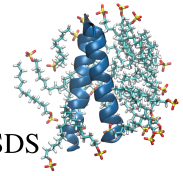
eYqjD, 50 SDS

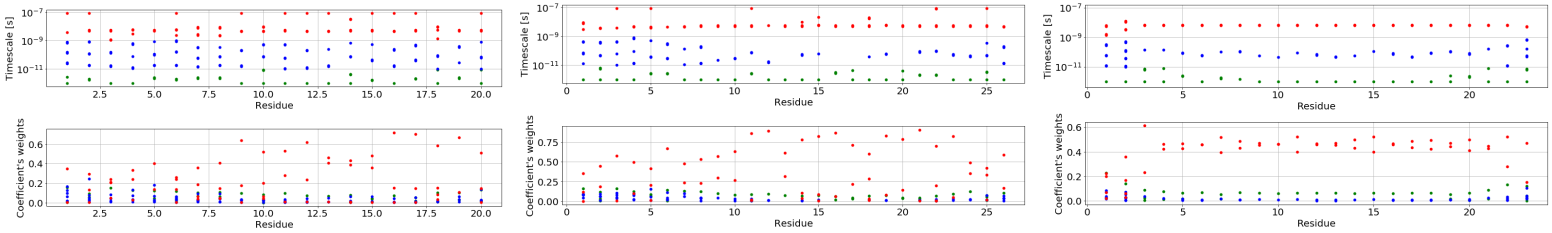


yFis1, 50 SDS



GWALP, 40 SDS
GWALP 45 SDS
GWALP, 50 SDS
GWALP dimer 50 SDS





Results in Micelles

Empty bicelles work with CHARMM36 and OPC water

Optimization of micelle size

GWALP fits better as dimer

to be developed

Results in Micelles

We can get time scales

Comment on helicity??

to be developed

Acknowledgmnents

to be developed