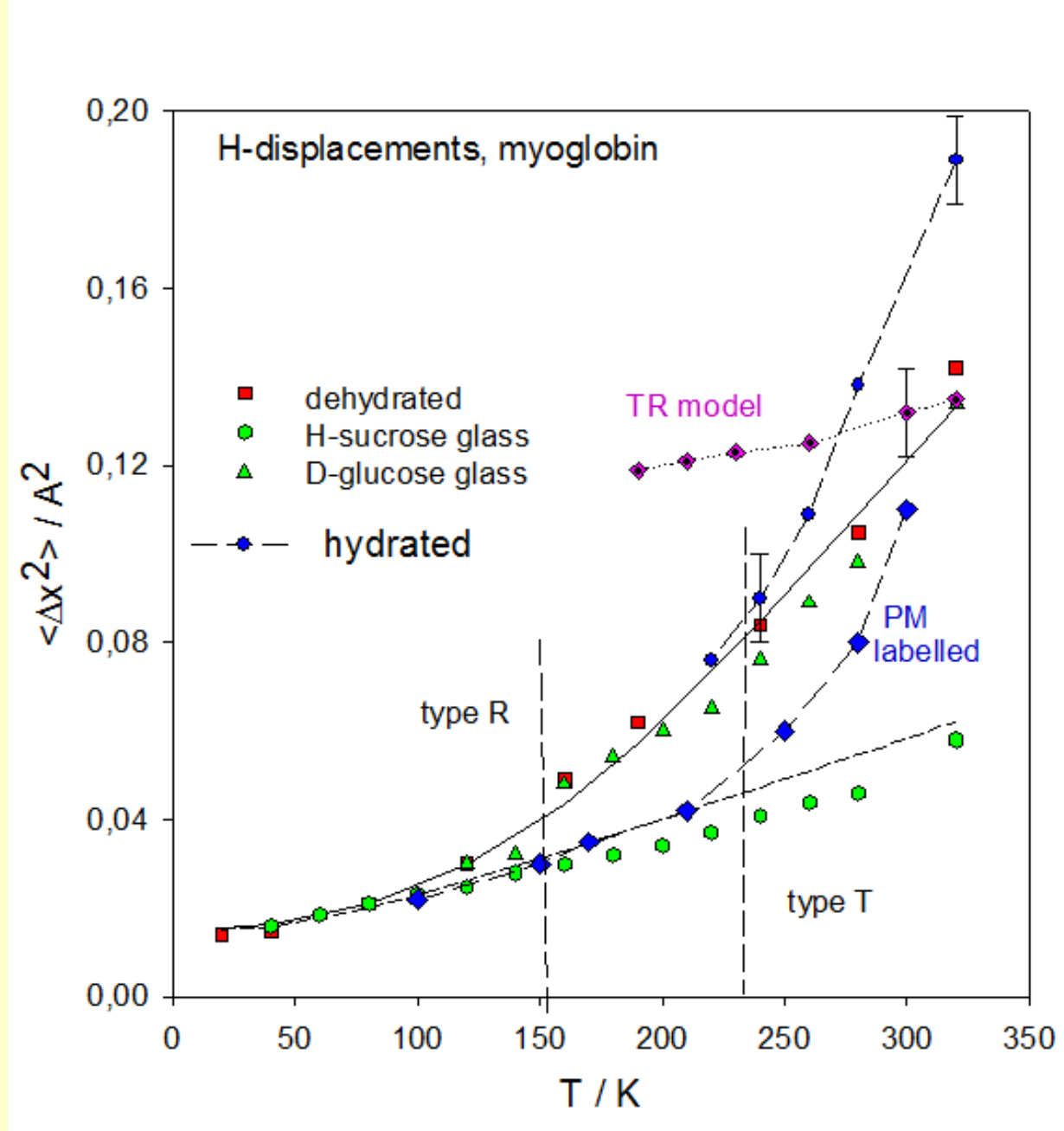


A rotation-translation model versus energy landscapes, combining elastic, time domain and multiple scattering of hydrated proteins

Beyond common phenomenological energy landscape models, we propose a two component analytical model of the neutron intermediate scattering function of dry and hydrated proteins: **rotational transitions of side chains** (methyl groups) and **local translational diffusion of non-methyl residues**. Spectra of three spectrometers with overlapping range are Fourier transformed to the time domain based on an exceptionally wide time and Q-range.

Elastic scattering: two dynamical transitions, R (rot) and T:



Results for various solvents:

- Hydrated: 2 transitions R (180 K) and T (240 K)
 - Dehydrated: a single transition R (180 K)
 - D-vitrified: a single transition R (180 K)
 - H-vitrified: no transition, only glassy matrix
 - Deuterated methyl groups: a single transition: T 240 K
 - Data corrected for resolution: TR model: no transition
- Two solvent dependent components R, T

Rotation-Translation Model

$$\Phi_s(Q, t) = \sigma_R \cdot \Phi_R(Q, t) + (1 - \sigma_R) \cdot \Phi_T(Q, t)$$

σ_R denotes the fractional cross section of the type R sites.

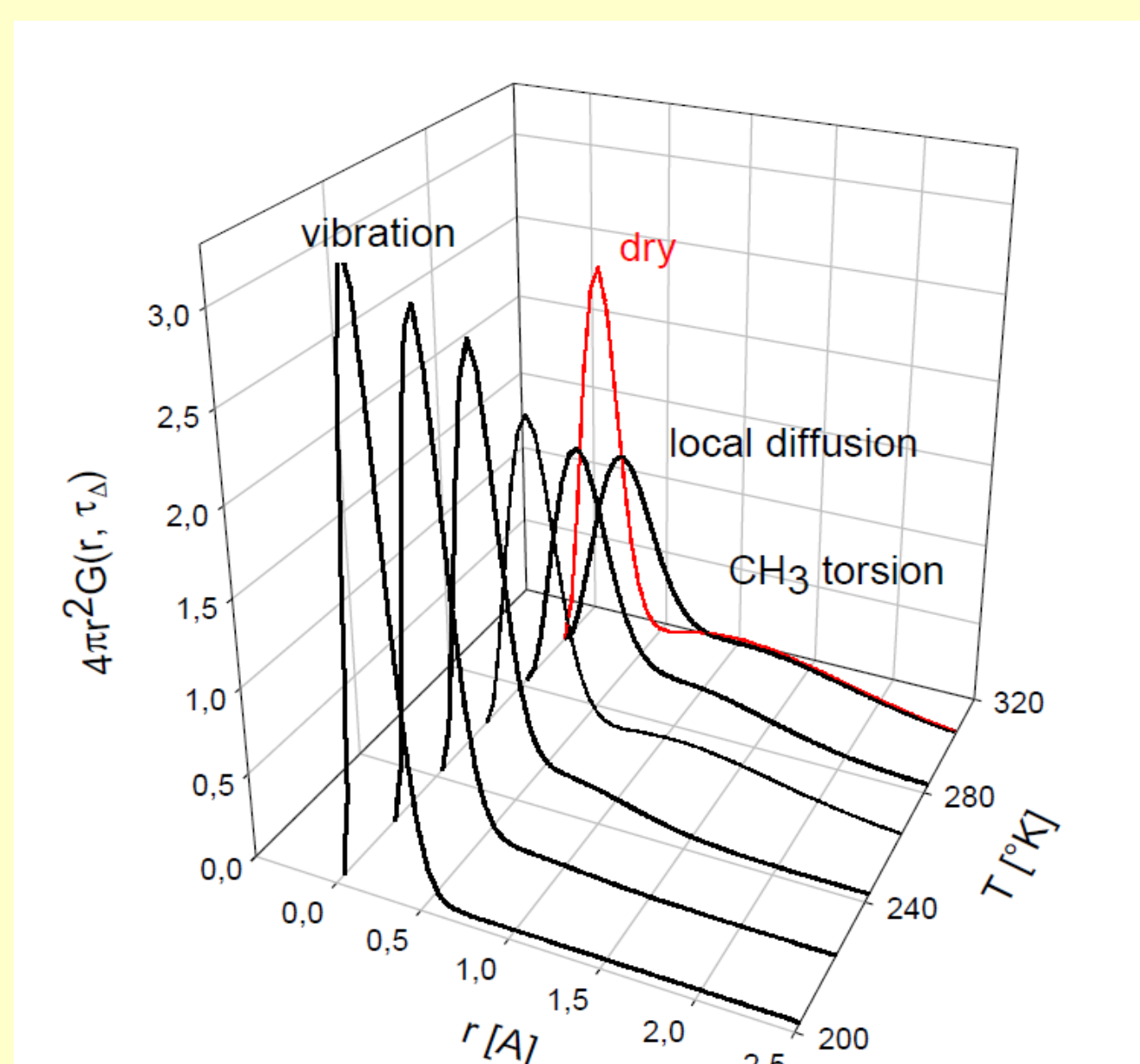
$$\Phi_R(Q, t) = \frac{1}{3} \{ 1 + 2j_0(Q) + 2 \cdot (1 - j_0(Q)) \cdot \exp(-t/\tau_{rot}) \}$$

$$j_0(Q) = \frac{\sin(Q\sqrt{3} \cdot r)}{Q\sqrt{3} \cdot r}$$

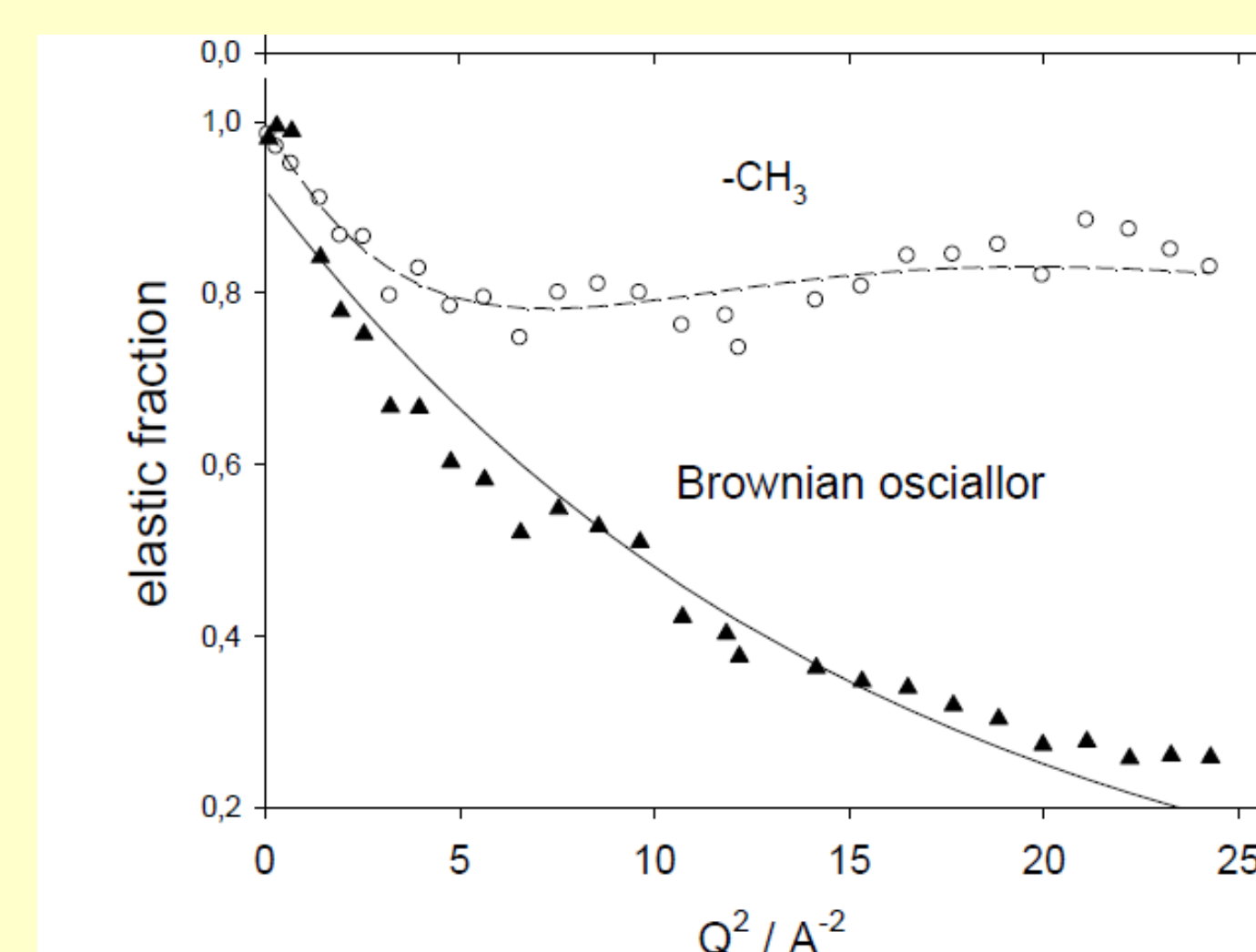
Side chain torsion
Brownian oscillator
(6)

$$\Phi_T(Q, t) = \exp\{-Q^2 \delta^2 \cdot (1 - \exp(-t/\tau_{trans}))\}$$

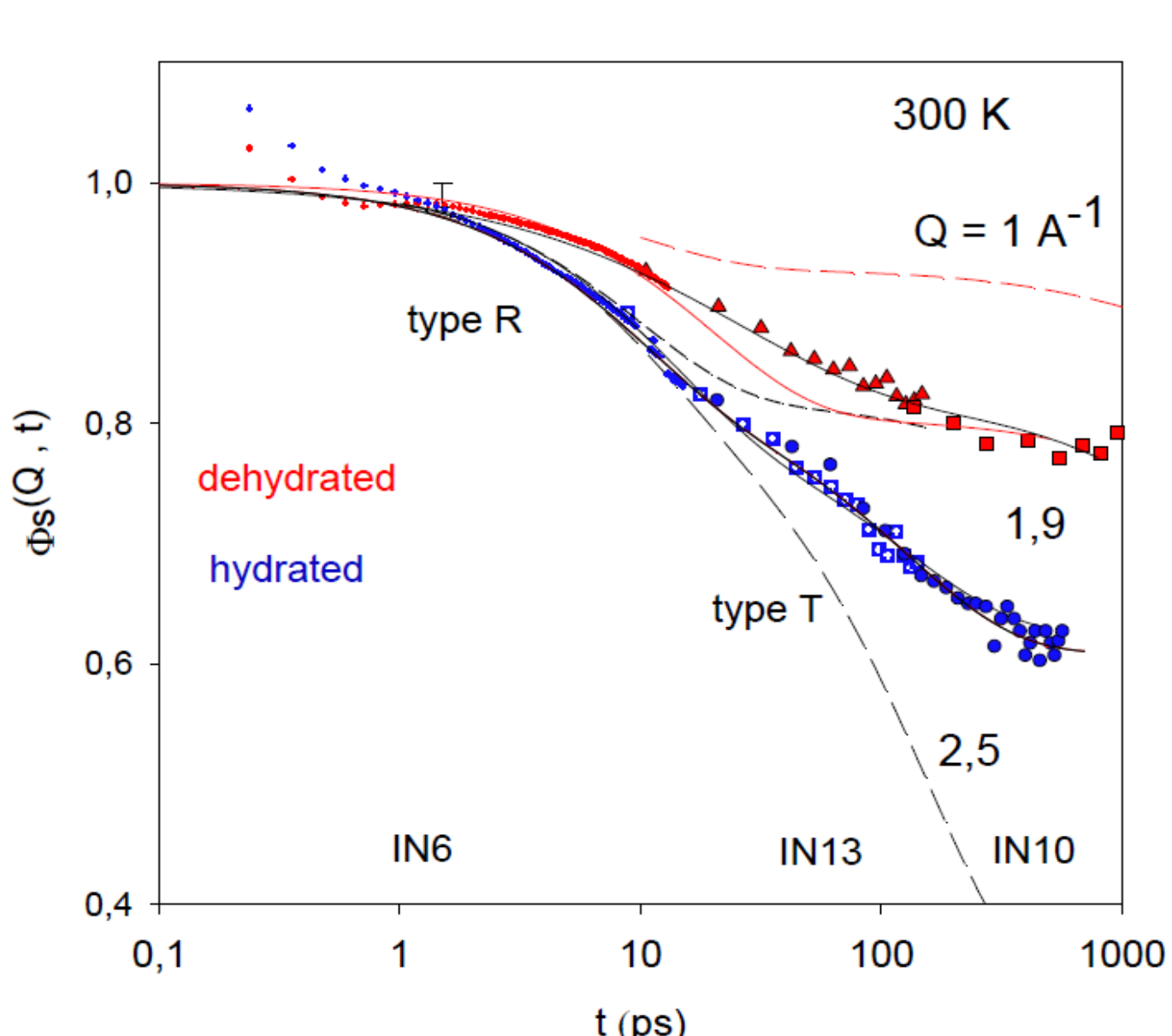
$\delta^2 = \langle \Delta x^2 \rangle$ denotes the translational mean square displacement of local diffusion



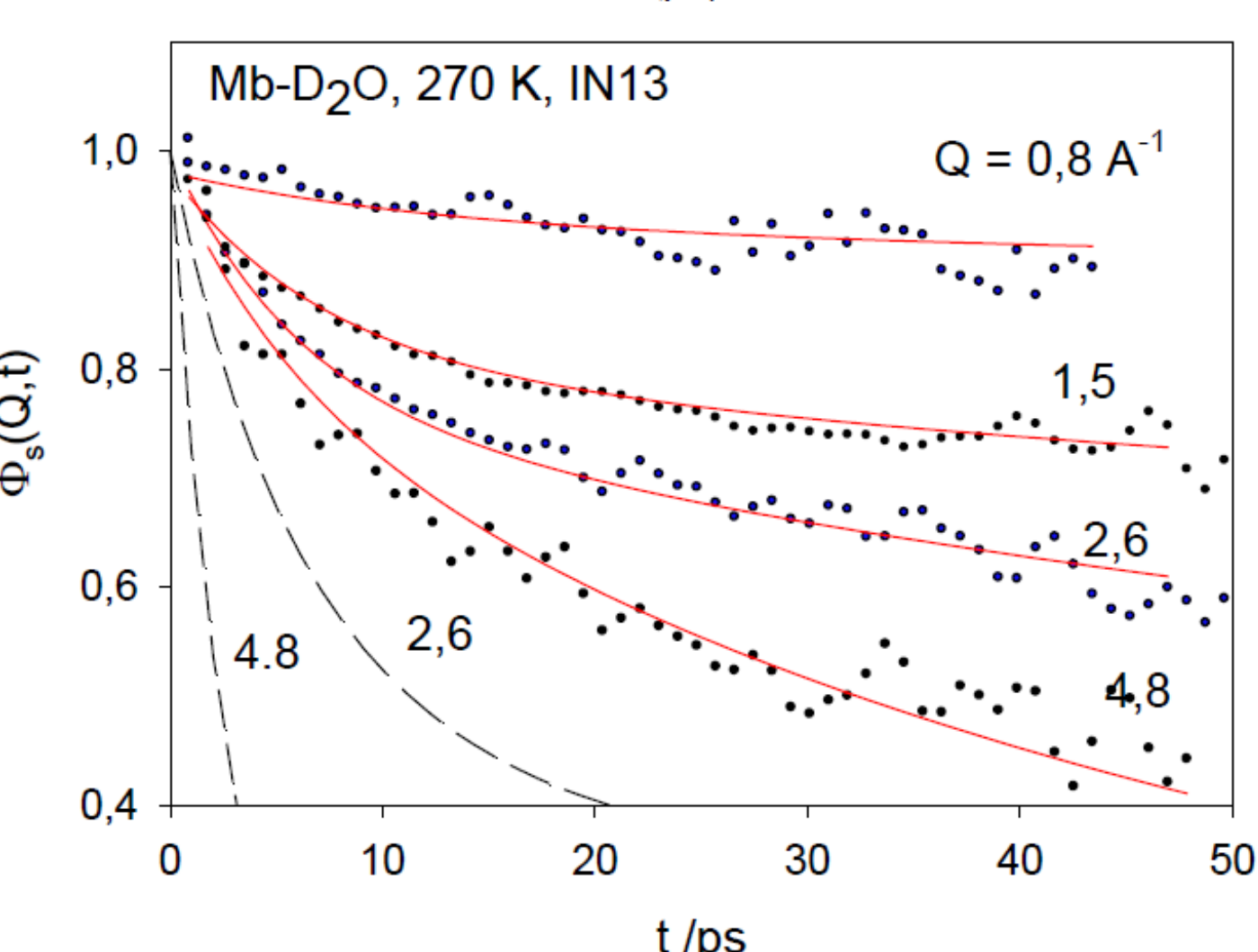
Displacement Distribution
at 150 ps versus temperature
Vibration +
- two dynamical components
above 180 K: Rot, Trans
- A single component in the
dry state: R : CH₃ -torsion



EISF(Q) of R-T Model
components
data and simulation

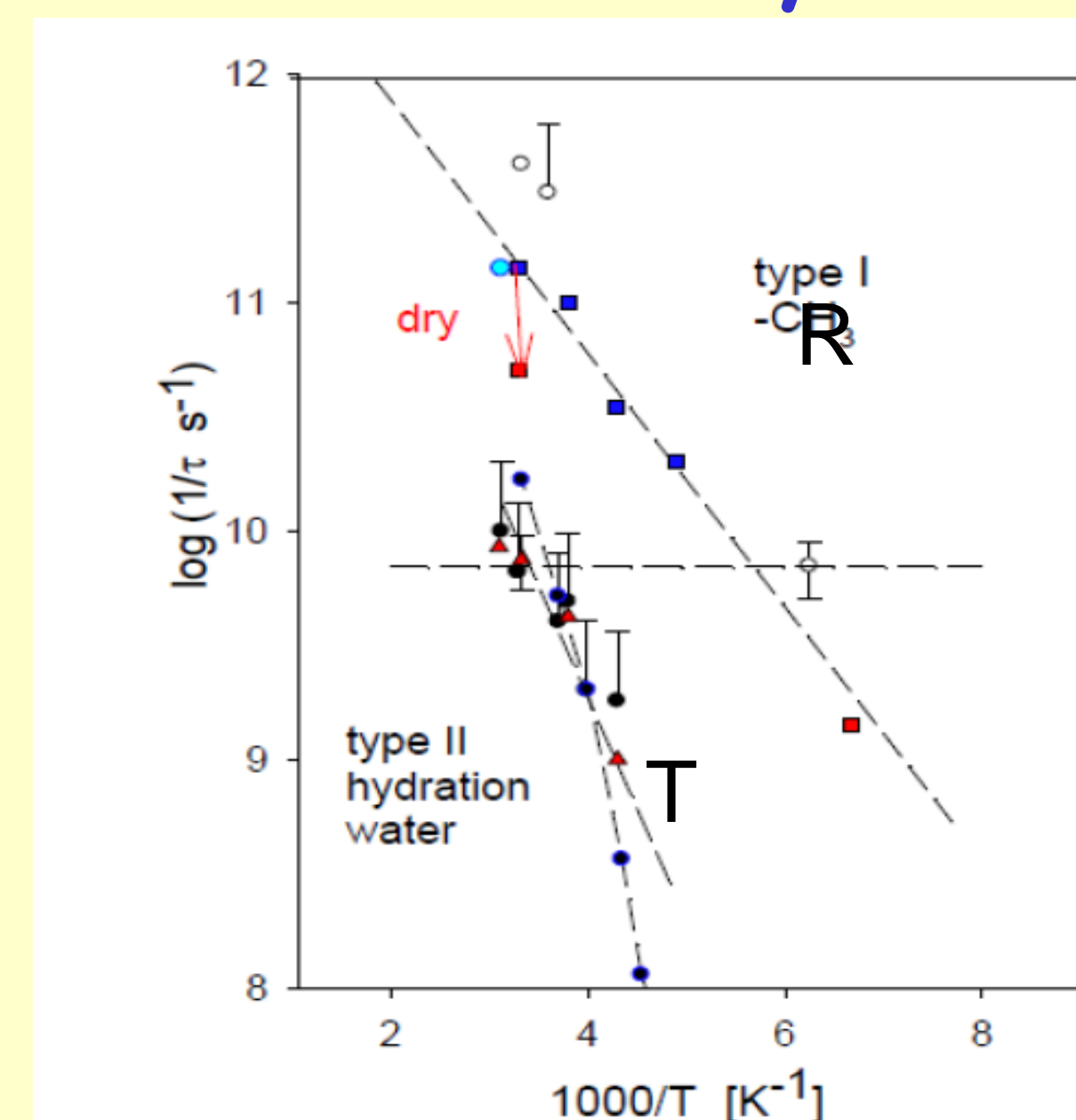


Intermediate scattering function
of dry and hydrated myoglobin
 $\Phi_s(Q, t)$ at 300 K and $Q = 1.9 \text{ Å}^{-1}$
R-T model fits versus Q
Methyl rotation is exponential in
the hydrated state but becomes
distributed upon dehydration, the
T-component disappears



Time domain back-scattering
 $\Phi_s(Q, t)$ much wider Q-range
than ever published before
and RT model fits
work remarkably well

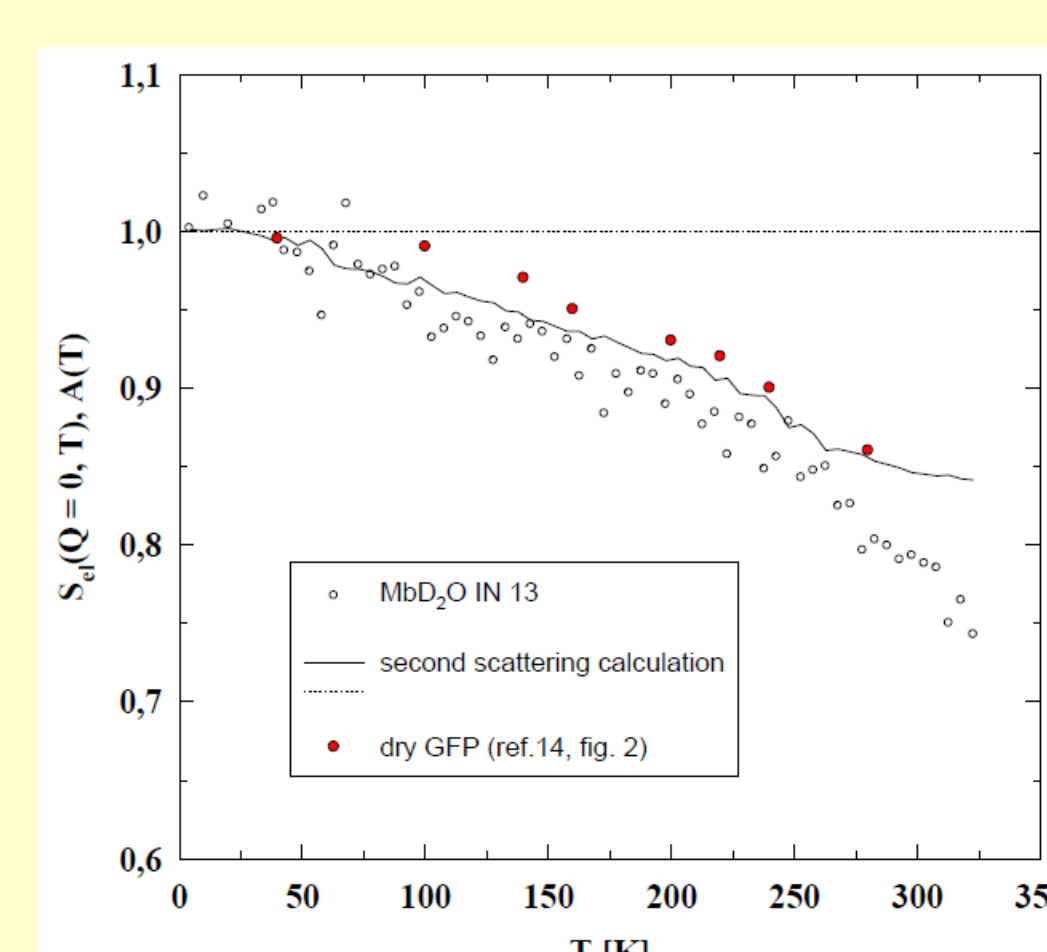
Arrhenius Analysis of R-T Model



Type R: coincides with methyl rotational
transitions

Type T: coincides with hydration water
relaxation times of
NMR and n-scattering

Multiple scattering decreases with temperature



We show temperature dependent
MS calculations (second scattering)
in comparison with IN13 data and the
Frauenfelder analysis (GFP, PNAS 2017)

MS explains the anomaly attributed
erraneously to energy landscapes

- Conclusions:**
- 1) The R-T model unifies the description of elastic and inelastic neutron scattering spectra of solvated proteins covering a wide range in time and momentum exchange. Accounting for resolution effects the „dynamical transition“ disappears. This result demonstrates the validity of scattering theory even for complex systems.
 - 2) Heterogeneity does not play a dominant role in protein dynamics, two slightly distributed components are sufficient within a wide parameter range.