

Identification by NMR Spectroscopy of Residues at Contact Surfaces in Large, Slowly Exchanging Macromolecular Complexes

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Supporting Information

Chemical exchange between two states has been well studied using NMR and the line shapes during exchange has been simulated using eq 1, which is derived from principles previously outlined^{10,11}:

$$I(\omega) = \text{re} \int_0^{\infty} \mathbf{W} \cdot \exp\{i(\Omega - \omega \mathbf{E})t - \mathbf{K}t + \mathbf{R}t\} \cdot \mathbf{1} \, dt \quad (1)$$

where

$$\mathbf{E} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \quad \mathbf{1} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \quad \mathbf{W} = (a, \quad 1-a)$$

$$\Omega = \begin{pmatrix} \omega_f & 0 \\ 0 & \omega_b \end{pmatrix} \quad \mathbf{K} = \begin{pmatrix} -k & k \\ k & -k \end{pmatrix} \quad \mathbf{R} = \begin{pmatrix} R_f & 0 \\ 0 & R_b \end{pmatrix}$$

Matrix **R** contains the transverse relaxation rates in s⁻¹ for the free (*R_f*) and bound (*R_b*) states, where a single exponential describes the relaxation rates. Matrices **K** and **Ω** contain the chemical exchange rate (*k*) and chemical shifts for the free (*ω_f*) and bound states (*ω_b*), respectively. **W** is a matrix containing the probability of occurrence for the

free (a) and bound (1-a) frequencies. This equation can be simplified if ω_f is set equal to $-\omega_b$ to produce eq 2:

$$I(\omega) = \frac{(-\omega + \omega_1 - 2a\omega_1)\{-2k\omega - (R_f + R_b)\omega + (-R_f + R_b)\omega_1\} + \{2k + (1-a)R_f + aR_b\}(R_f R_b + k(R_f + R_b) - \omega^2 + \omega_1^2)}{\{-2k\omega - (R_f + R_b)\omega + (-R_f + R_b)\omega_1\}^2 + \{R_f R_b + k(R_f + R_b) - \omega^2 + \omega_1^2\}^2} \quad (2)$$

where $\omega_1 = \omega_f = -\omega_b$.