

Supporting Table 1. Experimental and calculated nOe ratios( $\eta$ ), and  $T_1$  relaxation data for isotropic and anisotropic models of diffusion.

|                            | 14.1T         |                |             |               | 18.1T         |                |             |               | 21.1T         |                |             |               |
|----------------------------|---------------|----------------|-------------|---------------|---------------|----------------|-------------|---------------|---------------|----------------|-------------|---------------|
|                            | $\eta_{exp.}$ | $\eta_{calc.}$ | $T_1 (exp)$ | $T_1 (calc.)$ | $\eta_{exp.}$ | $\eta_{calc.}$ | $T_1 (exp)$ | $T_1 (calc.)$ | $\eta_{exp.}$ | $\eta_{calc.}$ | $T_1 (exp)$ | $T_1 (calc.)$ |
| <b>Tetrasaccharide (1)</b> |               |                |             |               |               |                |             |               |               |                |             |               |
| ISOTROPIC                  |               |                |             |               |               |                |             |               |               |                |             |               |
| $\alpha$                   | -1.35         | -1.70          | 1.79        | 1.65          | -1.23         | -1.13          | 1.62        | 1.69          | -0.42         | -0.81          | 1.53        | 1.68          |
| $\beta$                    | -1.63         | -1.65          | 1.61        | 1.54          | -1.22         | -1.07          | 1.52        | 1.59          | -0.56         | -0.75          | 1.45        | 1.57          |
| $\omega$                   | -1.89         | -1.51          | 1.26        | 1.22          | -0.95         | -0.89          | 1.18        | 1.26          | -0.39         | -0.55          | 1.12        | 1.25          |
| ANISOTROPIC                |               |                |             |               |               |                |             |               |               |                |             |               |
| $\alpha$                   | -1.35         | -1.47          | 1.79        | 1.67          | -1.23         | -0.96          | 1.62        | 1.70          | -0.42         | -0.68          | 1.53        | 1.68          |
| $\beta$                    | -1.63         | -1.67          | 1.61        | 1.54          | -1.22         | -1.09          | 1.52        | 1.59          | -0.56         | -0.77          | 1.45        | 1.57          |
| $\omega$                   | -1.89         | -1.69          | 1.26        | 1.21          | -0.95         | -1.05          | 1.18        | 1.26          | -0.39         | -0.68          | 1.12        | 1.25          |
| <b>Hexasaccharide (2)</b>  |               |                |             |               |               |                |             |               |               |                |             |               |
| ISOTROPIC                  |               |                |             |               |               |                |             |               |               |                |             |               |
| $\alpha$                   | -0.96         | -1.22          | 1.61        | 1.43          | -0.85         | -0.72          | 1.47        | 1.45          | -0.28         | -0.46          | 1.40        | 1.44          |
| $\beta$                    | -1.12         | -1.19          | 1.46        | 1.37          | -0.79         | -0.68          | 1.37        | 1.40          | -0.34         | -0.42          | 1.31        | 1.39          |
| $\gamma$                   | -1.07         | -0.95          | 1.00        | 0.92          | -0.33         | -0.39          | 0.94        | 0.94          | 0.14          | -0.11          | 0.89        | 0.93          |
| $\omega$                   | -1.17         | -0.98          | 1.05        | 0.98          | -0.38         | -0.43          | 0.98        | 1.01          | -0.01         | -0.16          | 0.94        | 1.00          |
| ANISOTROPIC                |               |                |             |               |               |                |             |               |               |                |             |               |
| $\alpha$                   | -0.96         | -1.09          | 1.61        | 1.49          | -0.85         | -0.65          | 1.47        | 1.52          | -0.28         | -0.42          | 1.40        | 1.50          |
| $\beta$                    | -1.12         | -1.18          | 1.46        | 1.38          | -0.79         | -0.68          | 1.37        | 1.40          | -0.34         | -0.42          | 1.31        | 1.39          |
| $\gamma$                   | -1.07         | -0.97          | 1.00        | 0.90          | -0.33         | -0.41          | 0.94        | 0.92          | 0.14          | -0.12          | 0.89        | 0.92          |
| $\omega$                   | -1.17         | -1.07          | 1.05        | 0.93          | -0.38         | -0.48          | 0.98        | 0.96          | -0.01         | -0.18          | 0.94        | 0.95          |
| <b>Octasaccharide (3)</b>  |               |                |             |               |               |                |             |               |               |                |             |               |
| ISOTROPIC                  |               |                |             |               |               |                |             |               |               |                |             |               |
| $\alpha$                   | -0.81         | -1.17          | 1.44        | 1.49          | -0.84         | -0.70          | 1.36        | 1.51          | -0.14         | -0.45          | 1.34        | 1.49          |
| $\beta$                    | -0.99         | -1.12          | 1.32        | 1.40          | -0.75         | -0.64          | 1.28        | 1.42          | -0.33         | -0.39          | 1.25        | 1.41          |
| $\gamma$                   | -0.58         | -0.70          | 0.76        | 0.64          | 0.04          | -0.15          | 0.80        | 0.66          | 0.50          | 0.13           | 0.80        | 0.66          |
| $\psi$                     | -0.77         | -0.72          | 0.83        | 0.68          | -0.17         | -0.17          | 0.82        | 0.70          | 0.40          | 0.10           | 0.80        | 0.69          |
| $\omega$                   | -0.92         | -0.79          | 0.95        | 0.81          | -0.18         | -0.26          | 0.91        | 0.83          | 0.25          | 0.01           | 0.91        | 0.82          |
| ANISOTROPIC                |               |                |             |               |               |                |             |               |               |                |             |               |
| $\alpha$                   | -0.81         | -1.36          | 1.44        | 1.36          | -0.84         | -0.83          | 1.36        | 1.40          | -0.14         | -0.54          | 1.34        | 1.39          |
| $\beta$                    | -0.99         | -1.27          | 1.32        | 1.29          | -0.75         | -0.74          | 1.28        | 1.32          | -0.33         | -0.46          | 1.25        | 1.31          |
| $\gamma$                   | -0.58         | -0.29          | 0.76        | 0.72          | 0.04          | 0.10           | 0.80        | 0.74          | 0.50          | 0.27           | 0.80        | 0.74          |
| $\psi$                     | -0.77         | -0.43          | 0.83        | 0.74          | -0.17         | 0.00           | 0.82        | 0.76          | 0.40          | 0.20           | 0.80        | 0.76          |
| $\omega$                   | -0.92         | -0.63          | 0.95        | 0.91          | -0.18         | -0.18          | 0.91        | 0.93          | 0.25          | 0.04           | 0.91        | 0.93          |