

Electronic Supplementary Information for:

Detection of hydrogen bonding in solution: A ^2H nuclear magnetic resonance method based on rotational motion of a donor/acceptor complex

Nathaniel K. Szymczak, Alan B. Oelkers, and David R. Tyler^a

a: Department of Chemistry, 1253 University of Oregon, Eugene OR, USA Fax: 541-346-0487; Tel: 541-346-4649; E-mail: dtyler@uoregon.edu

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Table S1: Estimated length of axes, shape, axial ratios, friction and shape factors for the modeled probe/solvent complexes.

Figure S1: Rotational correlation time calibration curve

Table S1. Estimated length of axes, shape, axial ratios, friction and shape factors for the modeled probe/solvent complexes.

Solvent	x-axis	y-axis	z-axis	Shape	Axial Ratio	C	f
MeOH	11.1	7.3	7.3	Prolate	0.66	0.44	1.02
EtOH	11.9	7.3	7.3	Prolate	0.61	0.53	1.02
n-propanol	13.4	7.3	7.3	Prolate	0.55	0.63	1.03
n-butanol	14.4	7.3	7.3	Prolate	0.51	0.72	1.04
isobutanol	13.4	7.3	7.3	Prolate	0.55	0.63	1.03
isoamyl alcohol	14.4	7.3	7.3	Prolate	0.52	0.72	1.04
p-isopropyl benzyl alcohol	13.9	7.3	7.3	Prolate	0.53	0.72	1.04

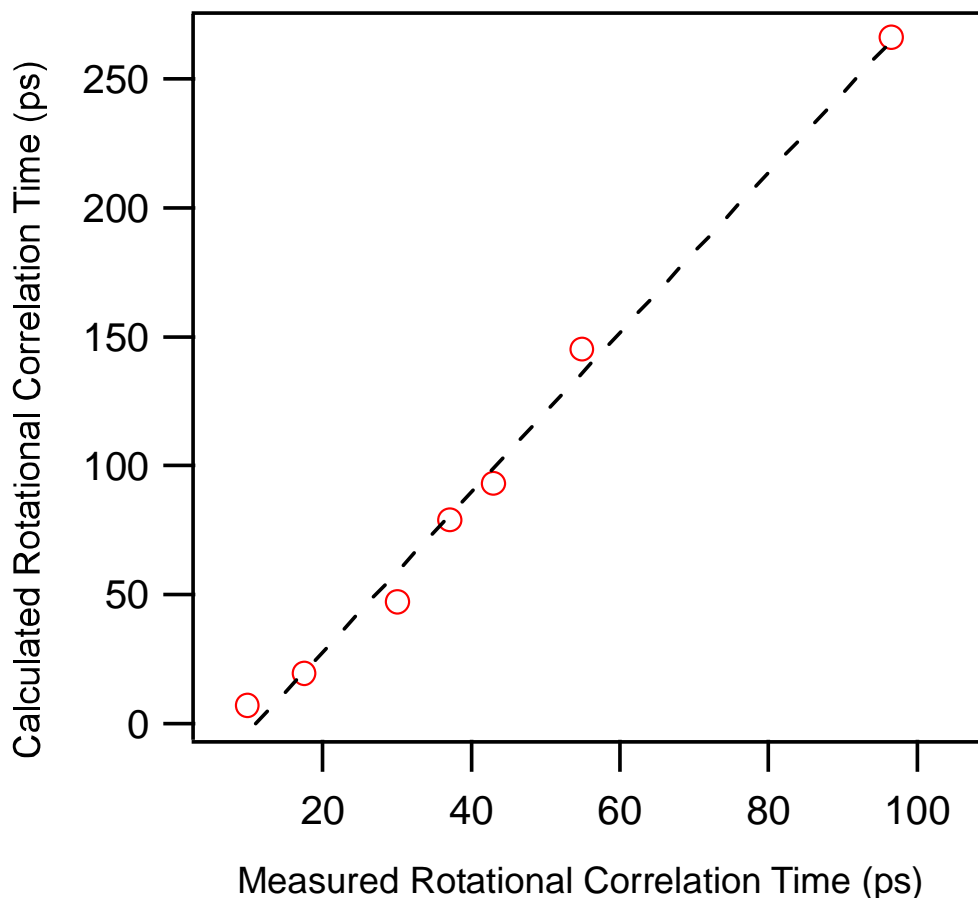


Figure S1. A comparison of the empirically measured rotational correlation times vs. those predicted from the SED model of probe/solvent complex. A linear relationship was found, and used to estimate the predicted correlation time (and hence hydrodynamic volume) of the probe/cholesterol complex. The linear equation derived from figure S1 is

$$\tau_{calc} = 3.1 \times \tau_{measured} - 35.$$