Supplementary Material (ESI) for Chemical Communications

Supplementary materials for:

Dendrimeric Gd(III) complex of a monophosphinated DOTA analogue: optimizing relaxivity by reducing internal motion

Jakub Rudovský[a], Petr Hermann*[a], Mauro Botta[b], Silvio Aime*[c] and Ivan Lukeš[a]

[a] *Department of Inorganic Chemistry, Universita Karlova, Hlavova 2030, 128 40 Prague 2, Czech Republic. E-mail: petrh@natur.cuni.cz; Fax: +420-221951253; Tel: +420-21951263*

[b] *Dipartimento di Scienze dell'Ambiente e della Vita, Università del Piemonte Orientale "Amedeo Avogadro", Spalto Marengo 33, I-15100 Alessandria, Italy*

[c] *Dipartimento di Chimica I. F. M., Università di Torino, Via P. Giuria 7, I-10125 Torino, Italy. E-mail: silvio.aime@unito.it; Fax: +39-0116707855; Tel: +39-0116707520*

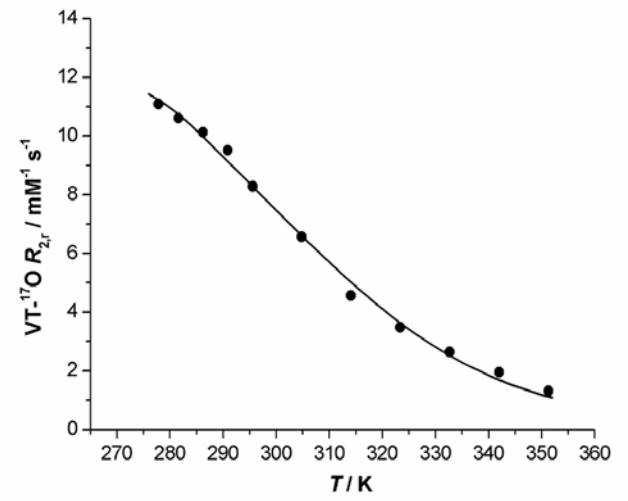

Fig. S1 Variable-temperature ^{17}O R_2 NMR data for G2-16Gd conjugate (2.1 T, 25 °C, pH 7).

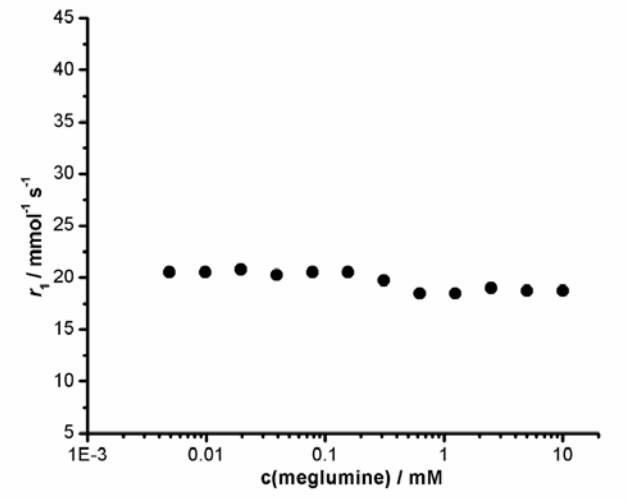

Fig. S2 Relaxometric titration of G2-16Gd (22 μM) with *N*-methyl-*D,L*-glucamine (meglumine) at 20 MHz, 25 °C and pH 7.

Equations S1:

Determination of binding constant

IndVars: c

DepVars: E

Params: Ct,Eb,K

// Variables and parameters

// c - total concentration of polyaminoacid

// E - enhancement factor

// Eb - maximal achievable relaxivity enhancement

// K – affinity constant

// Ct – total concentration of conjugate

// Equation

E=(((Eb-1)*(((K*Ct)+(K*c)+1)-(((K*Ct)+(K*c)+1)^2-(4*(K^2)*c*Ct))^0.5)/(2*K*Ct)))+1

// Initial conditions

K=1e6

Ct=0.03

Eb=2