

**Toward Optimized High-Relaxivity MRI Agents: Thermodynamic Selectivity of  
Hydroxypyridonate/Catecholate Ligands**

*Valérie C. Pierre, Marco Melchior, Dan M. J. Doble and Kenneth N. Raymond\**

Department of Chemistry, University of California, Berkeley, CA 94720-1460, USA

**Supporting Information**

**Figure 1.** Species distribution diagrams for ligands H<sub>3</sub>L1, H<sub>3</sub>L2 and H<sub>4</sub>L3 with Gd<sup>3+</sup>, Ca<sup>2+</sup>, Zn<sup>2+</sup> and Fe<sup>3+</sup>. Diagrams are calculated using the formation constants in Table 2 and the conditions of pH 7.4, [M]<sub>total</sub> = 1×10<sup>-6</sup> M and [L]<sub>total</sub> = 1×10<sup>-5</sup> M.

