Electronic Supplementary Information

for

Thermodynamic study of lanthanide(III) complexes with bifunctional monophosphinic acid analogues of H₄dota and comparative kinetic study of yttrium(III) complexes with H₄dota-like ligands

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Figure S1 Dependence of ¹H (A) and ³¹P (B) NMR chemical shift on pH.

Figure S2 An example of the data obtained for the formation of yttrium(III)-macrocycle complexes in the presence of Arsenazo III (c₇ = 7.8×10⁻⁷ mol dm⁻³, c₅ = 1.7×10⁻⁵ mol dm⁻³, pH 6.07).

Figure S3 An example of the experimental data obtained for the formation of the yttrium(III) complex of H₅do₃apPrA in presence of Arsenazo III (c₇ = 7.8×10⁻⁷ mol dm⁻³, c₅ = 1.7×10⁻⁵ mol dm⁻³) at different pH values.

Figure S4 Correlation of rate constant k₂ for dissociation of the yttrium(III) complexes with the first protonation constant of the ligands. The solid line was fitted for all the studied ligands and the dotted line was fitted only through three the most similar ligands (H₄dota, H₅do₃apPrA and H₆do₃apAbn).
Figure S1

Dependence of $^1$H (A) and $^{31}$P (B) NMR chemical shift on pH.

A

B
Figure S2
An example of the data obtained for the formation of yttrium(III)-macrocycle complexes in the presence of Arsenazo III ($c_Y = 7.8 \times 10^{-7}$ mol dm$^{-3}$, $c_{\text{Lig}} = 1.7 \times 10^{-5}$ mol dm$^{-3}$, pH 6.07).
Figure S3

An example of the experimental data obtained for the formation of the yttrium(III) complex of H₅do3apPrA in presence of Arsenazo III ($c_Y = 7.8 \times 10^{-7}$ mol dm$^{-3}$, $c_{Lig} = 1.7 \times 10^{-5}$ mol dm$^{-3}$) at different pH values.
Correlation of rate constant $k_\text{H}$ for dissociation of the yttrium(III) complexes with the first protonation constant of the ligands. The solid line was fitted for all the studied ligands and the dotted line was fitted only through three the most similar ligands ($\text{H}_4\text{dota}$, $\text{H}_5\text{do3ap}^{\text{PrA}}$ and $\text{H}_4\text{do3ap}^{\text{Abn}}$).