Supplementary Information

Ga[(NO2A-*N*-(α-amino)propionate)] chelates: synthesis and evaluation as potential tracers for ^{68}Ga PET

Miguel F. Ferreira,[a] Goretti Pereira,[a] João P. André, [a] M. I. M. Prata,[b] Paula M. T. Ferreira,[a] José A. Martins,[a*] Carlos F. G. C. Geraldes[c,d]

[a]Centro de Química (CQ-UM), Universidade do Minho, Campus de Gualtar, 4710-057 Braga, Portugal

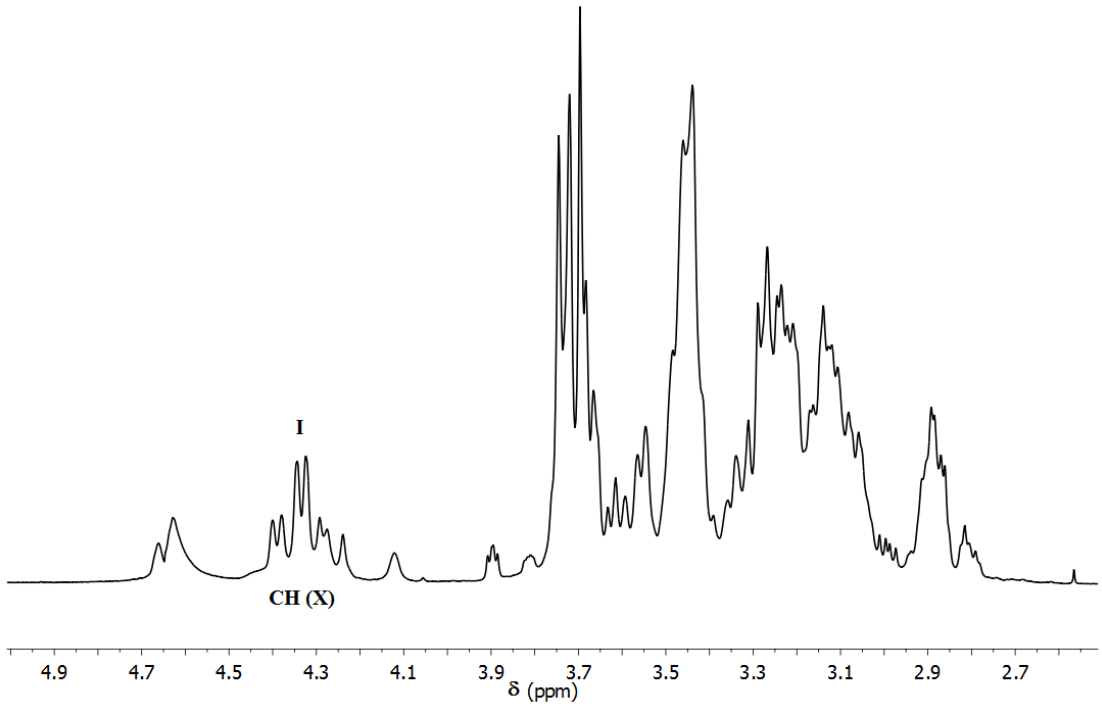
[b]ICNAS and IBILI, Faculty of Medicine, University of Coimbra, 3000-548 Coimbra, Portugal

[c]Department of Life Sciences, Faculty of Science and Technology, University of Coimbra, P.O. Box 3046, 3001-401 Coimbra, Portugal

[d]Chemistry Centre, Universityof Coimbra, Rua Larga, 3004-535 Coimbra, Portugal

Corresponding author: José A. Martins, Centro de Química, Campus de Gualtar, Universidade do Minho, 4710-057 Braga, Portugal.jmartins@quimica.uminho.pt

A)



B)

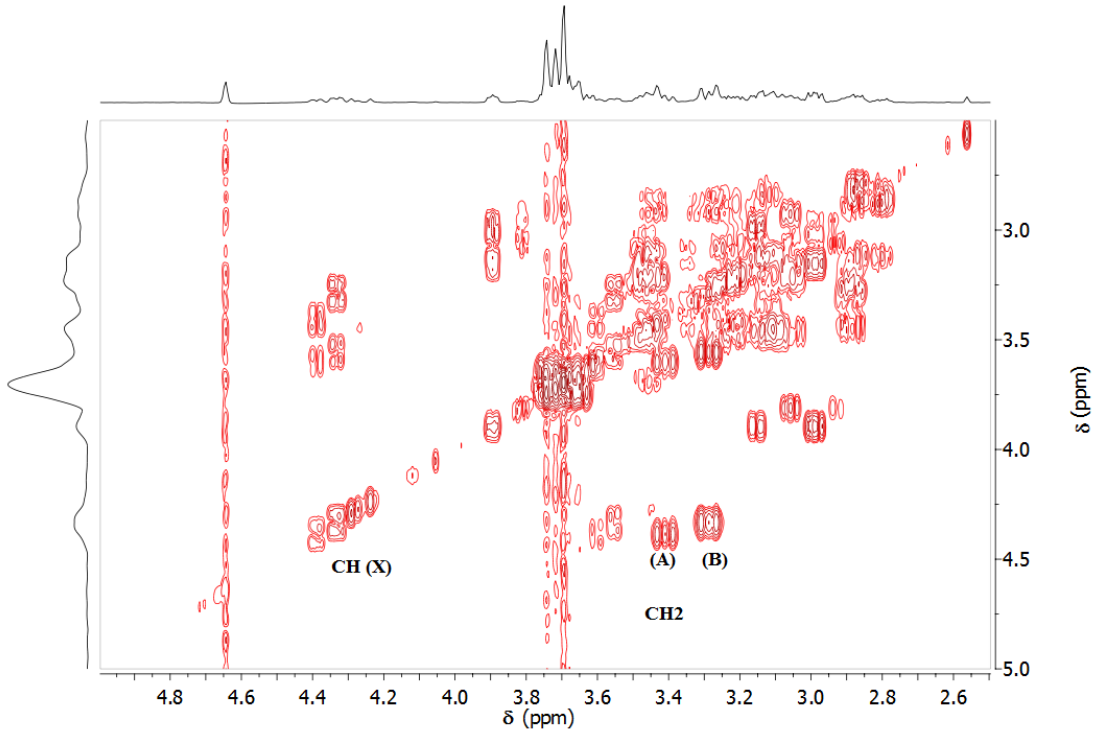
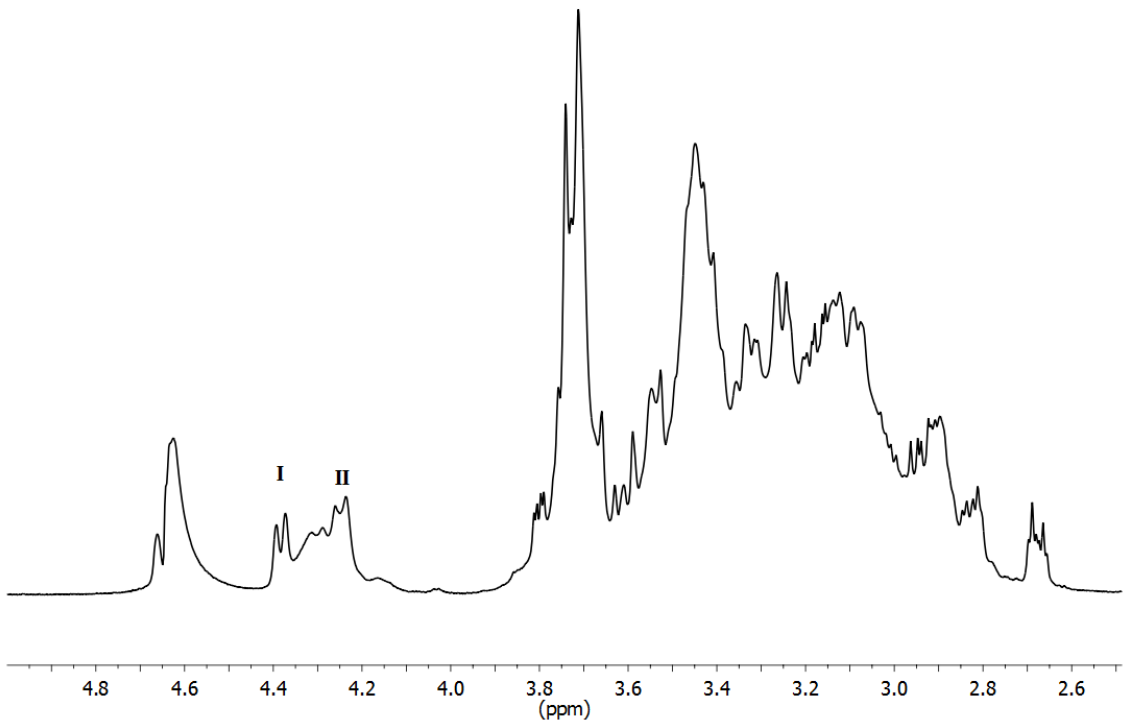


Figure S1. A) 1D proton and B) 2D COSY NMR spectrum of Ga**L**$_1$ at pH 3.0 (600 MHz, 20 mM in D_2O, 25 ºC).

A)



B)

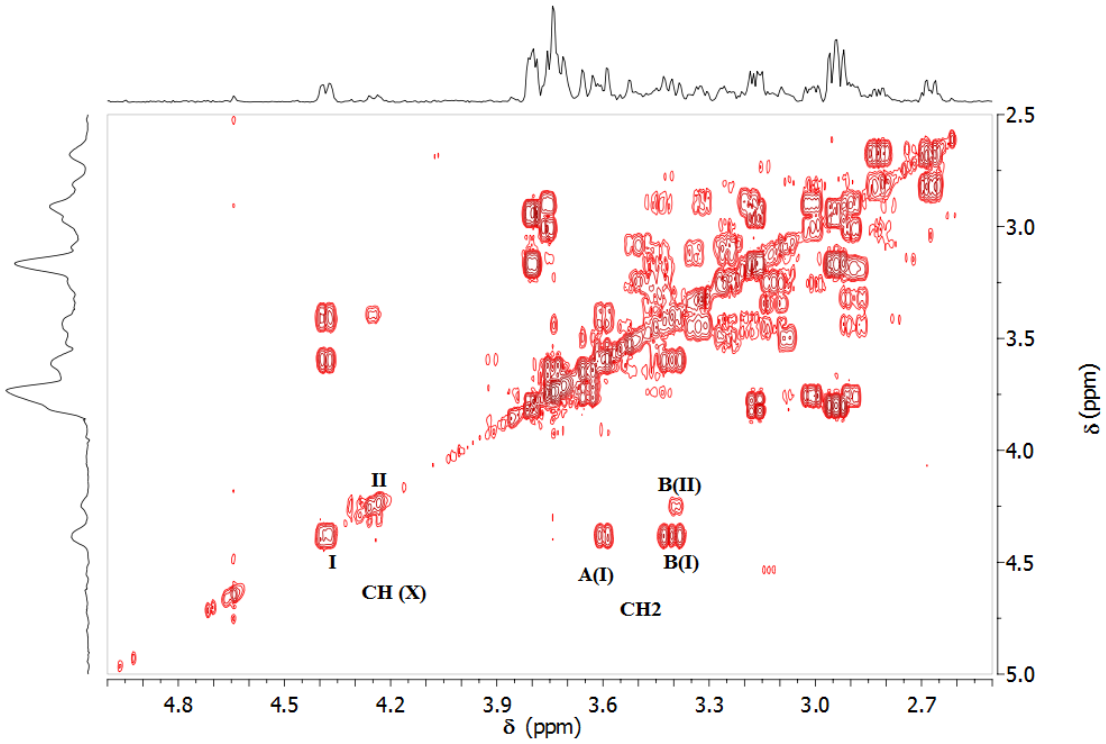


Figure S2. A) 1D proton and B) 2D COSY NMR spectrum of Ga**L**$_1$ at pH 4.0 (600 MHz, 20 mM in D_2O, 25 ºC).

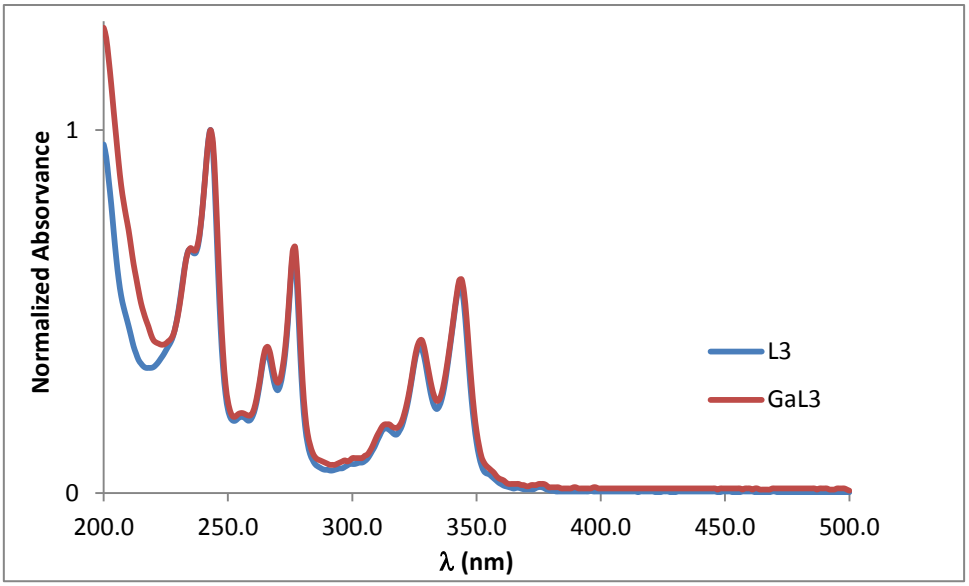


Figure S3. UV-Vis spectra for the free ligand $\mathbf{L_3}$ and for the Ga$\mathbf{L_3}$ complex ($1.0x10^{-5}$ M).

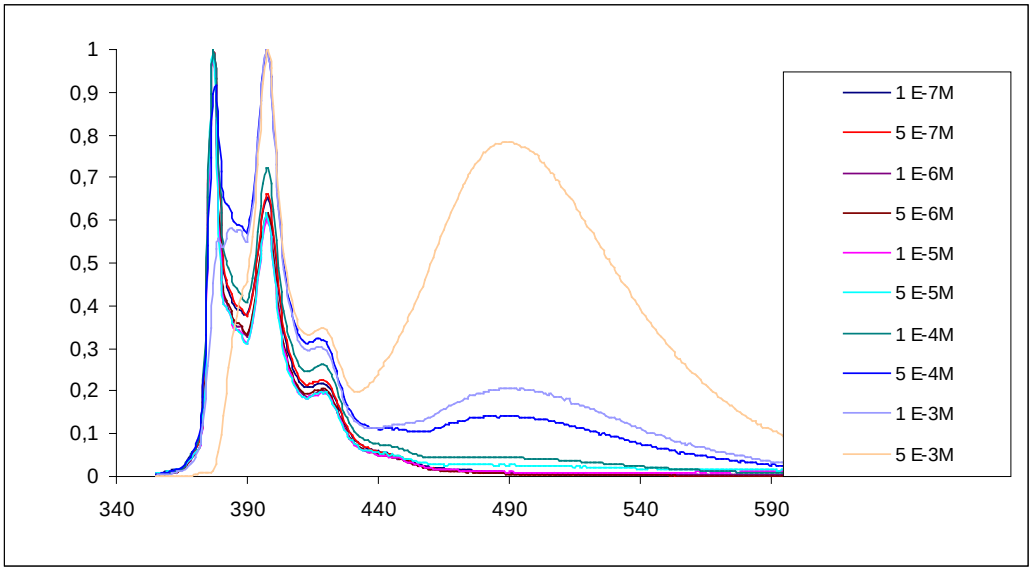


Figure S4. Fluorescence spectra for ligand $\mathbf{L_3}$ in non-deoxygenated water over the concentration range $1x10^{-7}$ - $5x10^{-3}$ mol.dm^{-3} (λ_{exc}=345 nm).

Table S1. Computed LogP values for the Ga**L**$_2$ and Ga**L**$_3$ complexes after structure optimization with Mopac PM6 COSMO, water implicit solvent.

	Calculated logP
Ga**L**$_2$	0.69
Ga**L**$_3$	3.31

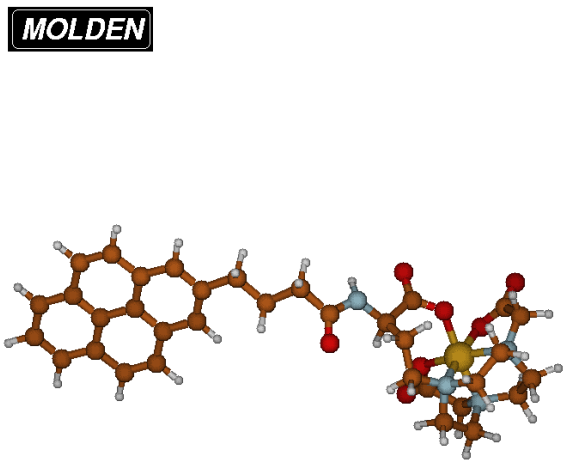


Figure S5. Optimized structure of Ga**L**$_3$ (Mopac PM6 COSMO, water implicit solvent).

Table S2. Biodistribution, stated as percentage of injected dose per gram of organ (%ID/g ±SD), of [^{67}Ga]**L**$_3$ in Wistar rats at 1 and 24 hours after *i.v.* injection. Results are the mean of 4 animals.

Organ	**1h %ID**	**24h %ID**
blood	0.10007	0.000406308
liver	0.350711	0.019477613
spleen	0.04807	0.010971577
kidney	0.817741	0.033667745
heart	0.028524	0.002091018
brain + cerebellum	0.002673	0.000355646
lung	0.101831	0.006952801
s. intestine	0.064156	0.004023468
l. intestine	0.04826	0.003821414
bone	0.027221	0.000864891
muscle	0.023675	0.000383012