Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Imine Ligands Based on Ferrocene: Synthesis, Structural and Mössbauer Characterization and Evaluation as Chromogenic and Electrochemical Sensors for Hg^{+2}†

Vitor Rosa,[a] Ana P. S. Gaspari,[a,d] Filipe Folgosa,[b,c] Cristina M. Cordas,[a] Pedro Tavares,[b] Teresa Santos-Silva,[b] Sónia Barroso,[b] and Teresa Avilés.[a*]

[a]*LAQV,REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, 2829-516, Portugal.*

[b]*UCIBIO,REQUIMTE, Departamento de Química, Faculdade de Ciências e Tecnologia, Universidade Nova de Lisboa, Caparica, 2829-516, Portugal.*

[c]*Current address: Instituto de Tecnologia Química e Biológica António Xavier, ITQB NOVA, Av. da República, 2780-157 Oeiras, Portugal.*

[d]*Current address: Departamento de Química, Faculdade de Filosofia, Ciências e Letras de Ribeirão Preto, Universidade de São Paulo, Avenida Bandeirantes, 3900 – Zip Code 14040-901, Ribeirão Preto/SP, Brasil.*

† Electronic supplementary information (ESI) available: Crystal data and structure refinements for ligands **1**, and **2** (Table 3); CCDC reference numbers 1579093-1579094. NMR spectra for all compounds (Fig. S1-S10), representative cyclic voltammograms of compounds **1** and **2** (Fig. S11), comparison of the behavior of **1** and **2** with and without Hg^{2+}, SWV spectra (Fig. 12), UV-Visible spectrum of compound **1** in ACN and DCM (Fig. S13), Packing diagrams of compounds **1** and **2** (Fig.S14).

* Corresponding Author. E-mail : teresa.aviles@fct.unl.pt

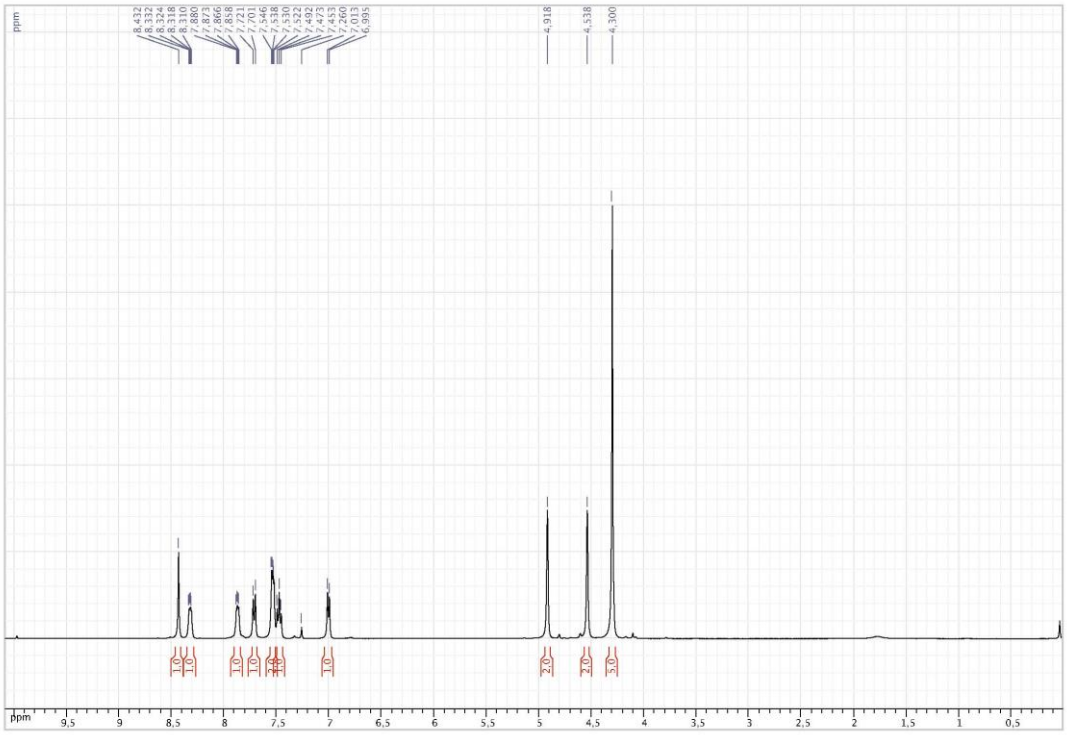

Figure S1: ^{1}H NMR of 1-naphthyliminoferrocene (compound **1**).

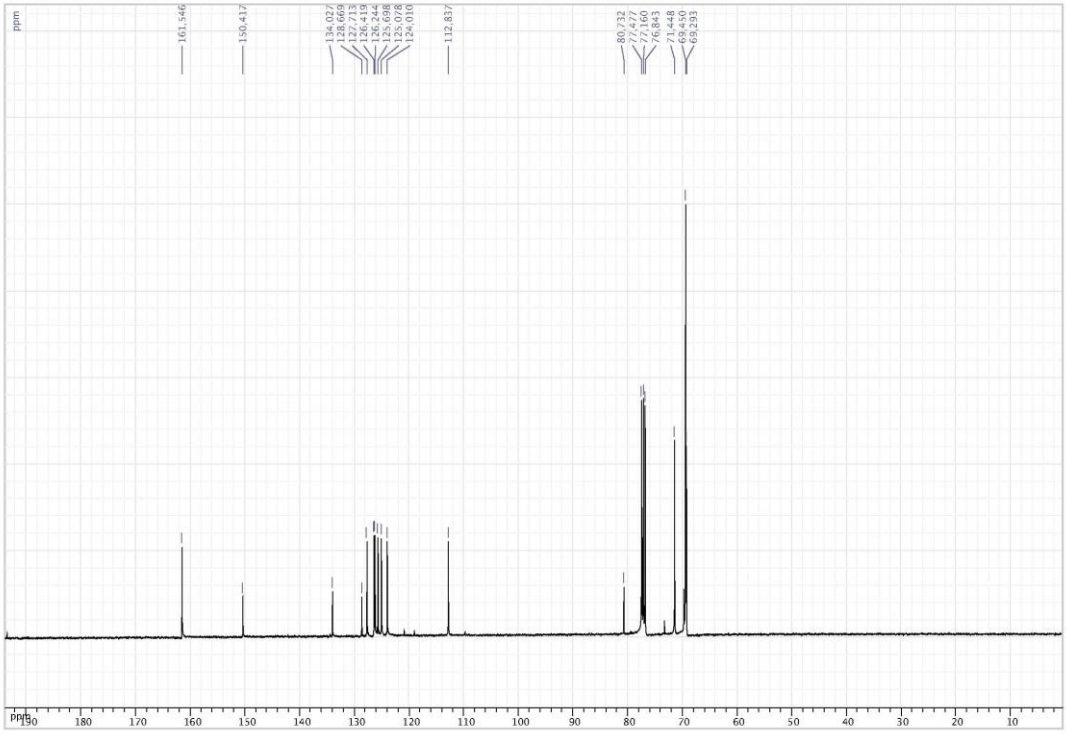

Figure S2: ^{13}C NMR of 1-naphthyliminoferrocene (compound **1**).

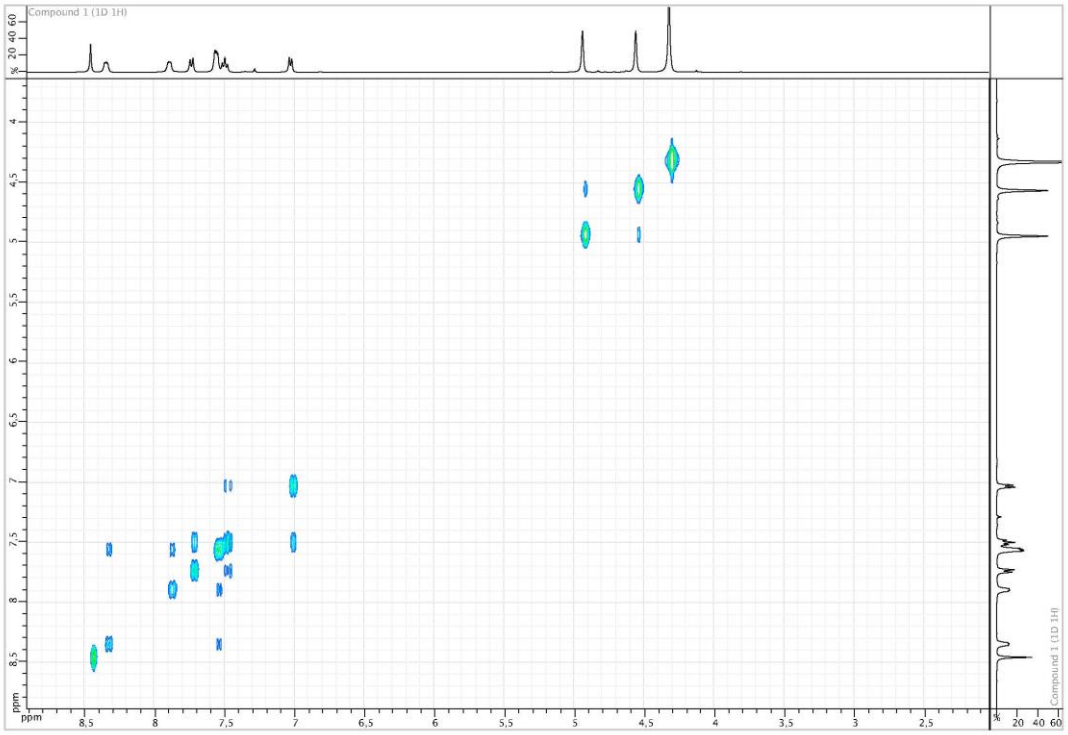

Figure S3: $^{1}H/^{1}H$ COSY of 1-naphthyliminoferrocene (compound **1**).

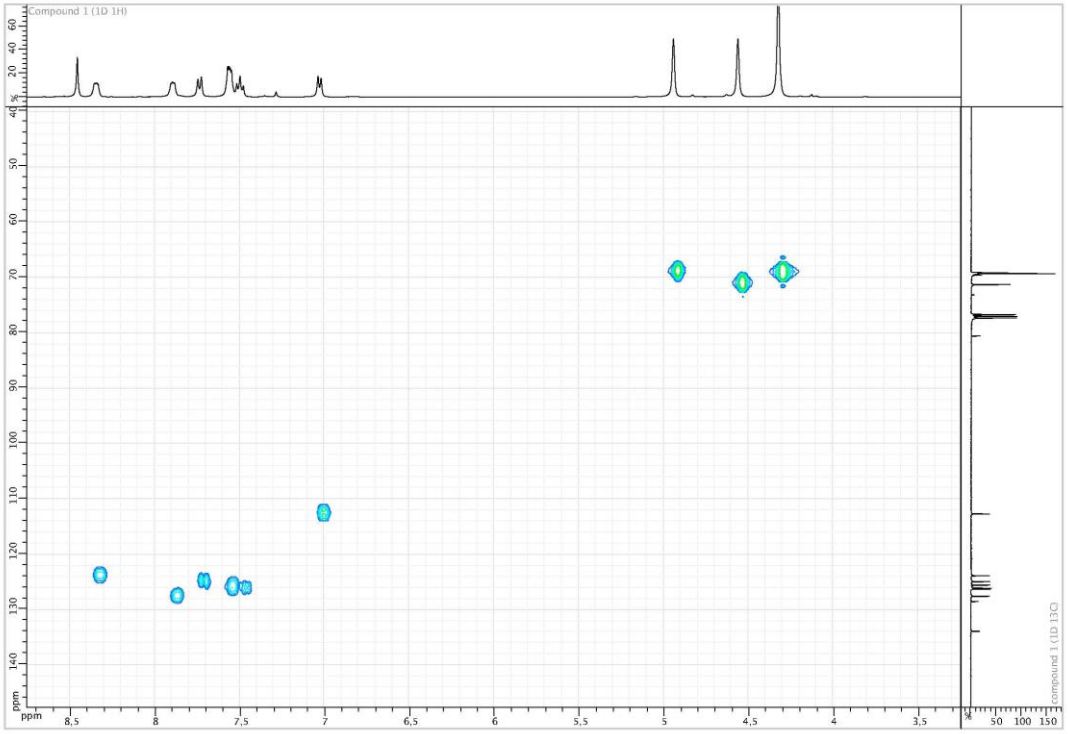

Figure S4: $^{1}H/^{13}C$ HSQC of 1-naphthyliminoferrocene (compound **1**).

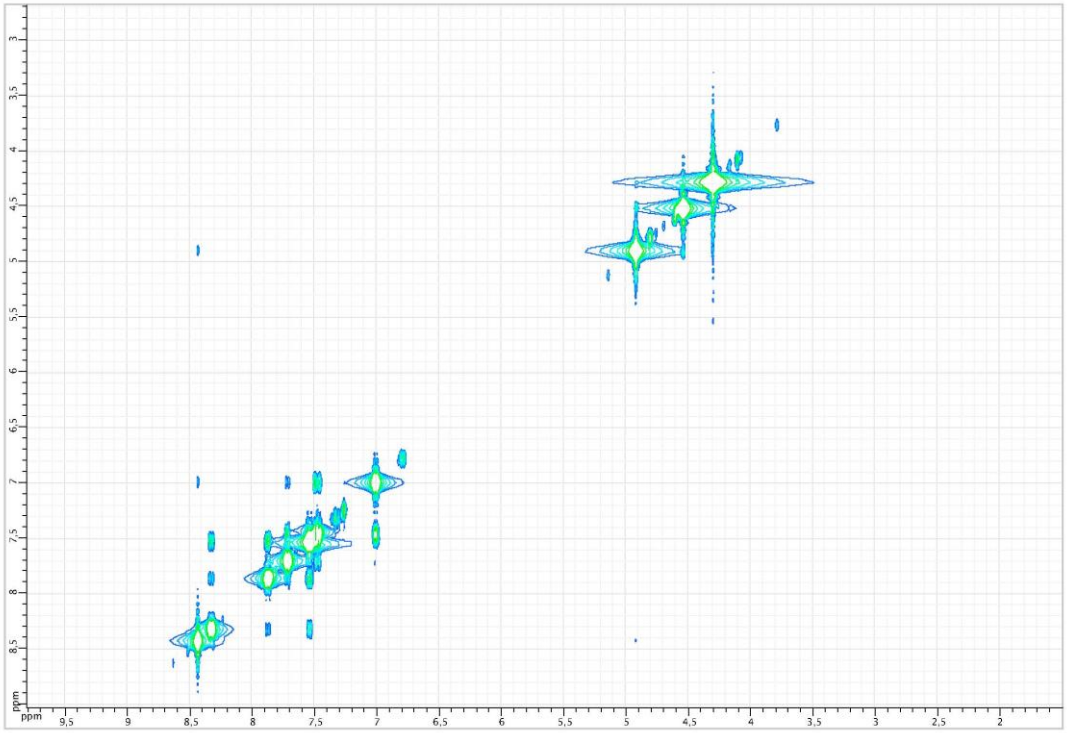

Figure S5: NOESY of 1-naphthyliminoferrocene (compound **1**).

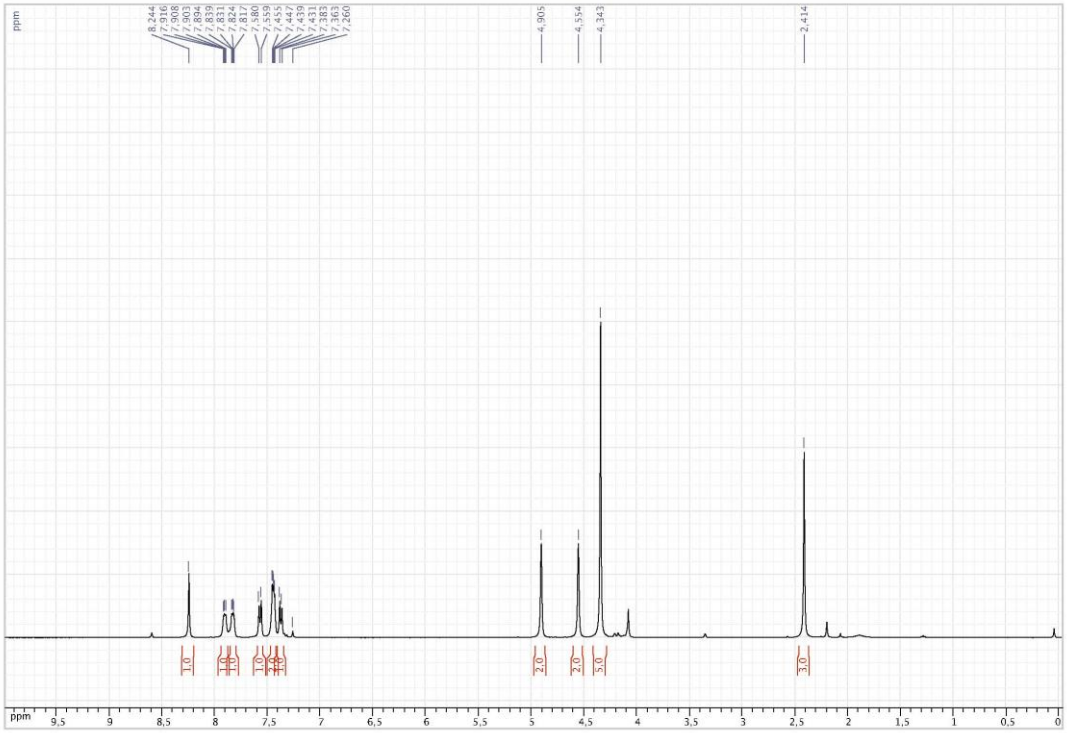

Figure S6: ^{1}H NMR of 2-methyl-1-naphthyliminoferrocene (compound **2**).

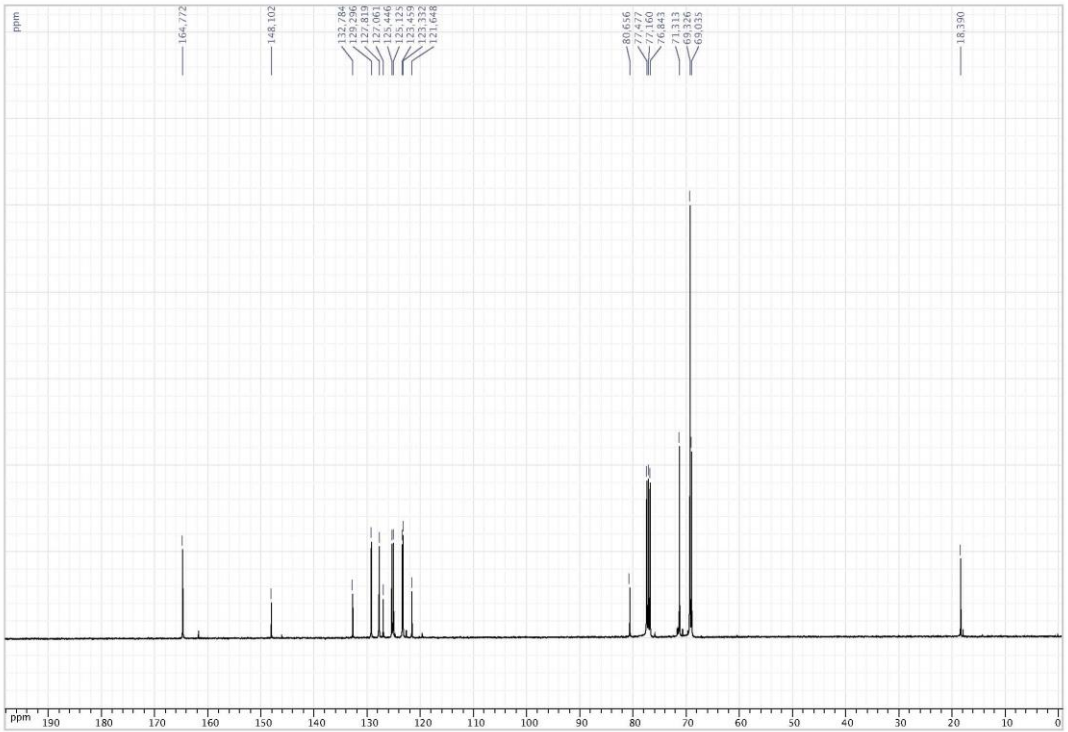

Figure S7: ^{13}C NMR of 2-methyl-1-naphthyliminoferrocene (compound **2**).

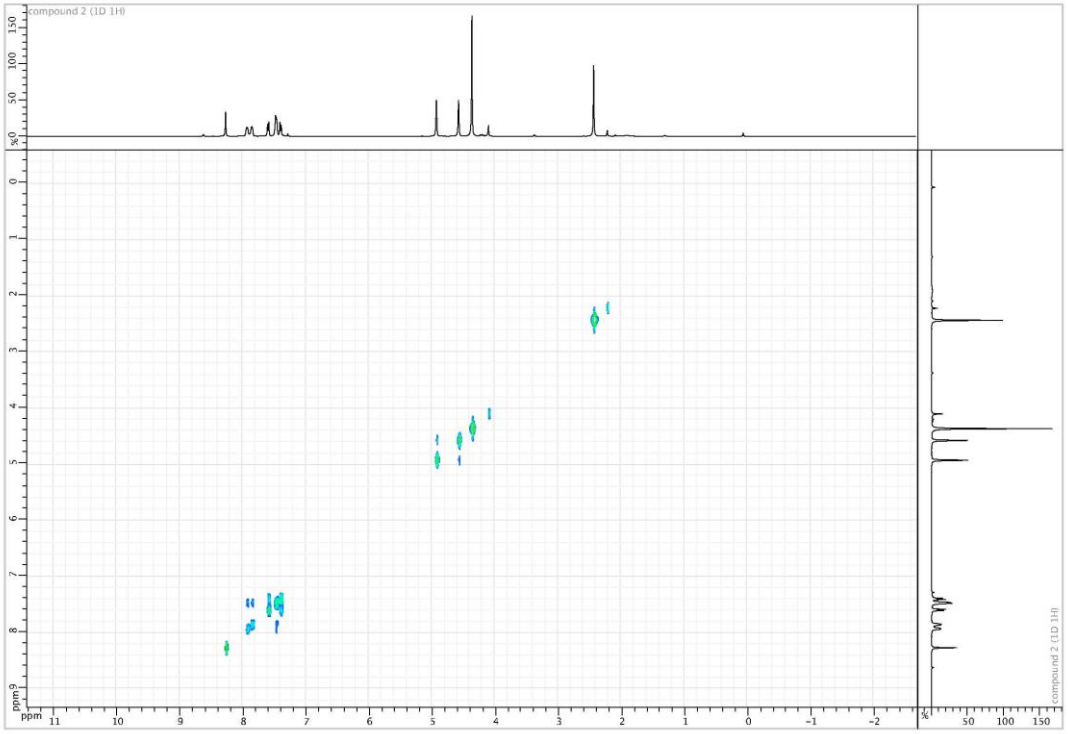

Figure S8: $^{1}H/^{1}H$ NMR COSY of 2-methyl-1-naphthyliminoferrocene (compound **2**).

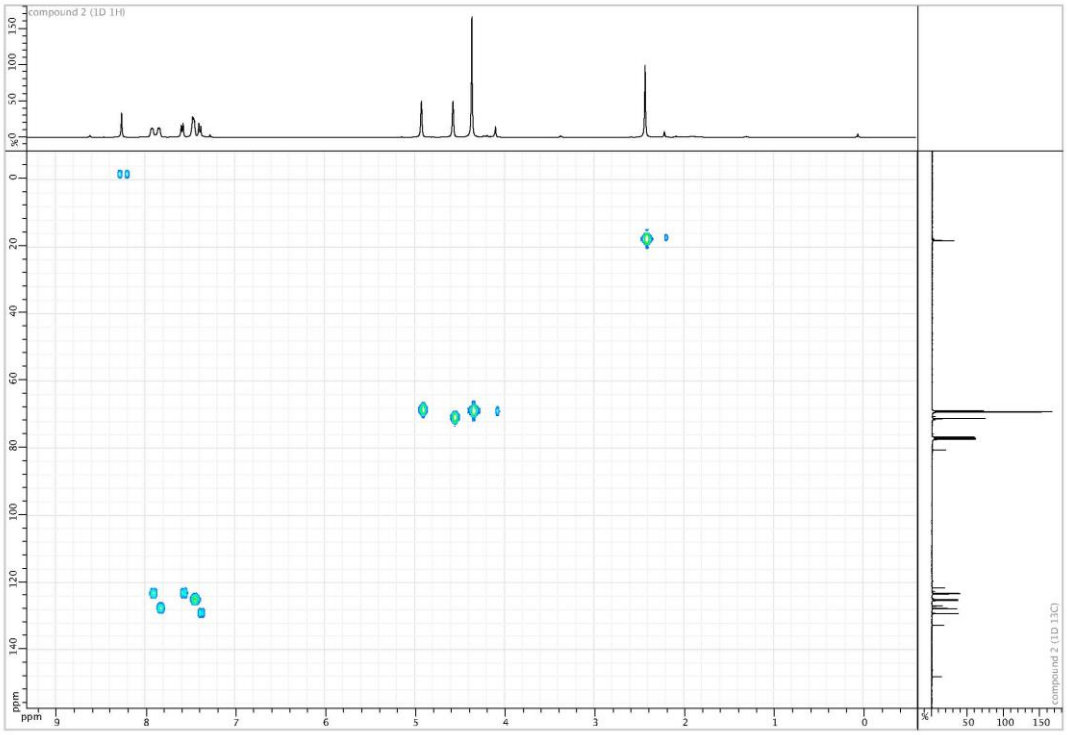

Figure S9: $^{1}H/^{13}C$ HSQC of 2-methyl-1-naphthyliminoferrocene (compound **2**).

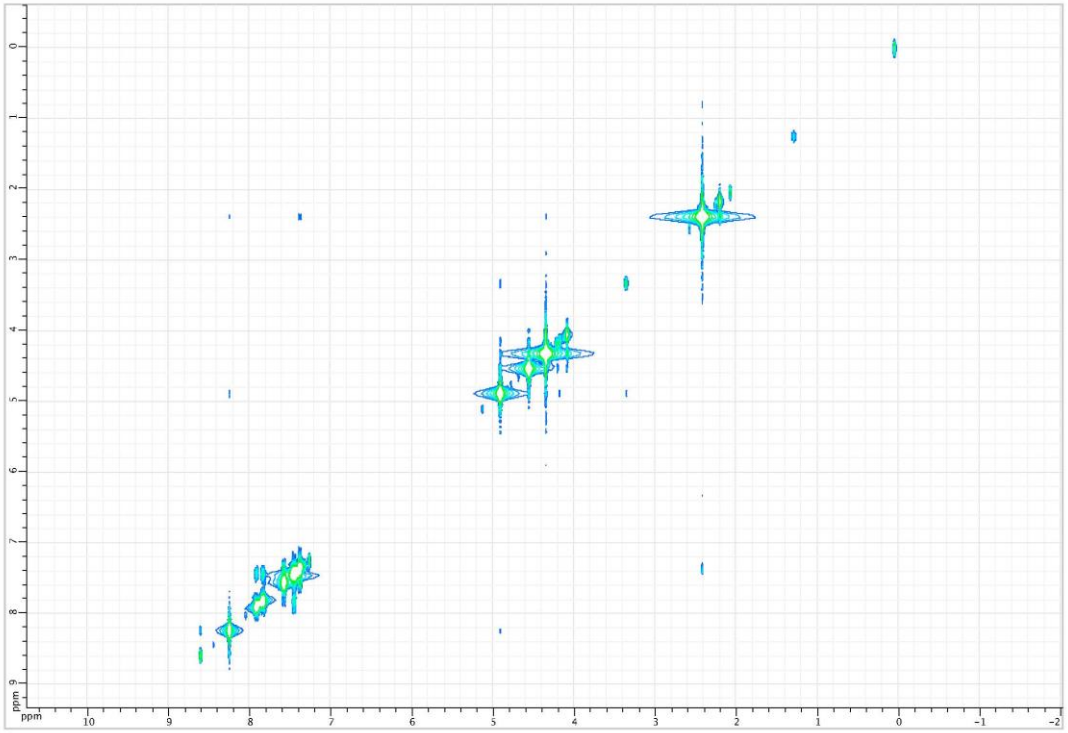

Figure S10: NOESY of 2-methyl-1-naphthyliminoferrocene (compound **2**).

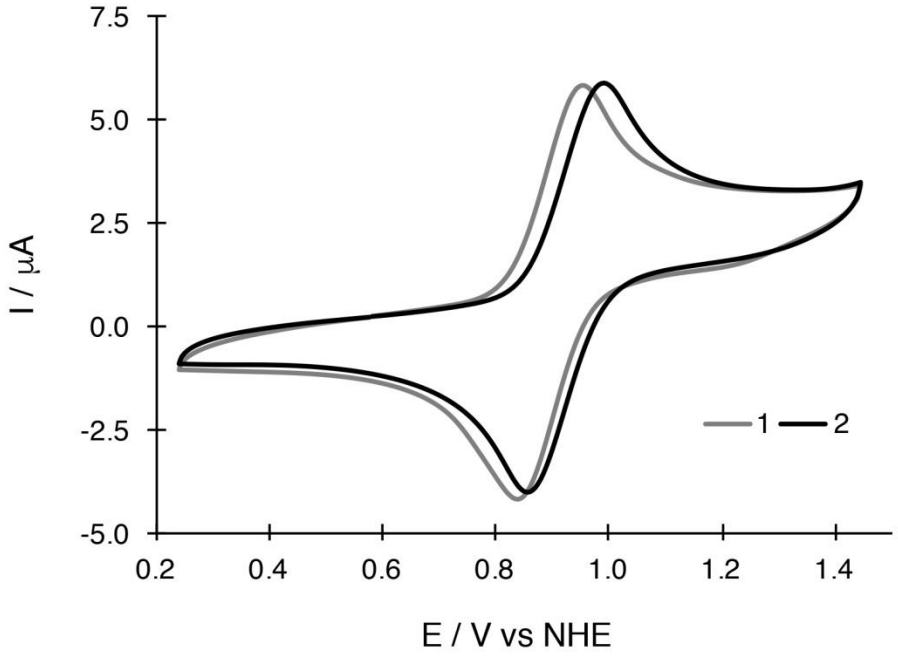

Figure S11: Representative cyclic voltammograms of compounds **1** and **2** both 1mM in 0.1 M TBAP/DCM, at 75 mVs^{-1} (for comparison with Figure 1 panel A) in the paper main text).

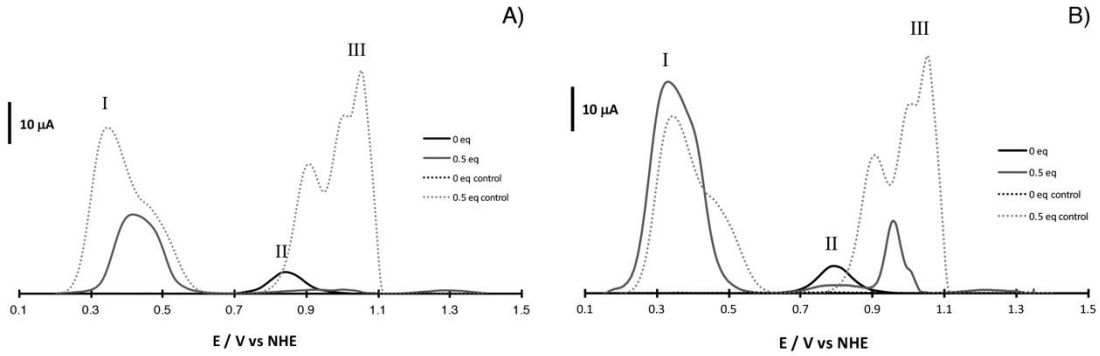

Figure S12: Comparison of the behavior of **1** and **2** with and without Hg^{2+} addition and controls (Hg^{2+} addition in the absence of compounds **1** and **2**), A) for compound **1** and B) for compound **2**; Potential window: 0.24 to 1.44 V vs NHE; SWV parameters: 100 Hz frequency, step potential: 50 V, amplitude 25 mV, scan rate 0.5 Vs^{-1}. Note: the 0 eq control, corresponds to the electrolyte (in the absence of compounds or mercury) and since there are any significant signals, in the figures scales it is observed as a flat line close to the xx axes (and not observable).

In the presence of **1**, the free mercury ions process I increase its current intensities from 0 to 0.7 eq of added Hg^{2+}, decreasing from 0.8 to 1 eq of Hg^{2+}, and remaining approximately constant until the maximum 2.0 eq added. For processes III associated with free Hg^{2+}, the current increase occurs from 0 to 0.4 eq, diminishing continuously until the maximum added 2.0 eq.

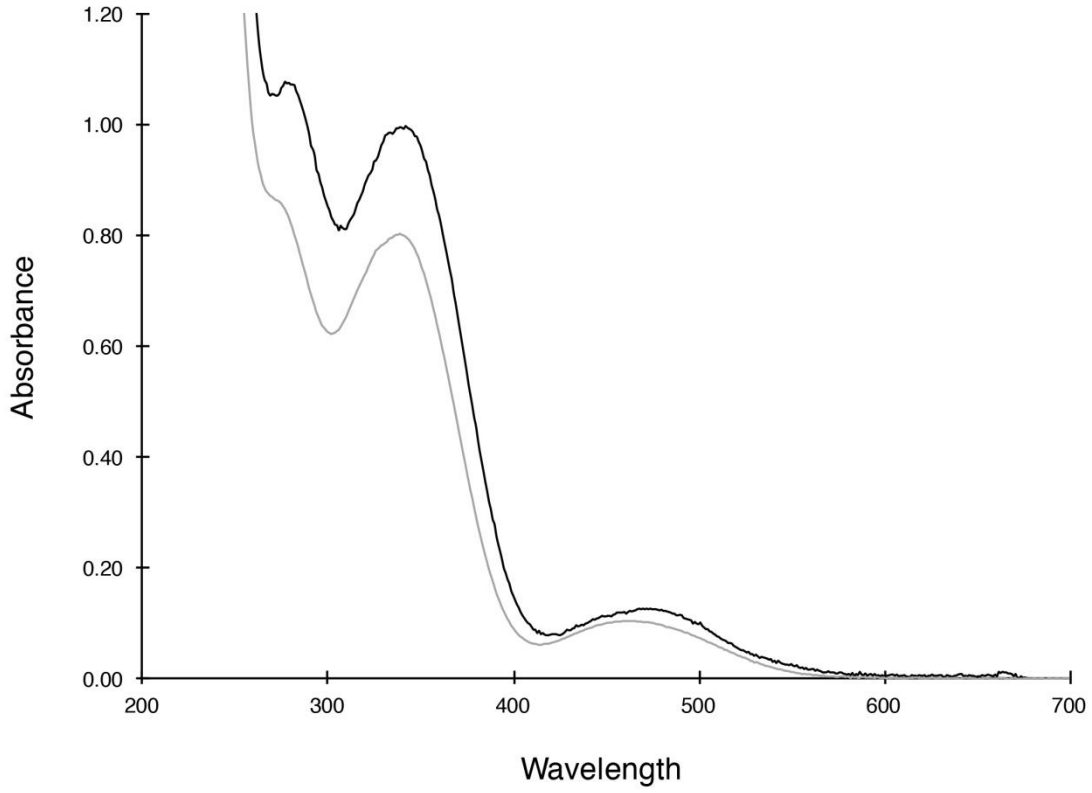

Figure S13: UV-Visible spectrum of compound **1**, $1x10^{-4}$M in Acetonitrile (dark grey line) and Dichloromethane (light grey line).

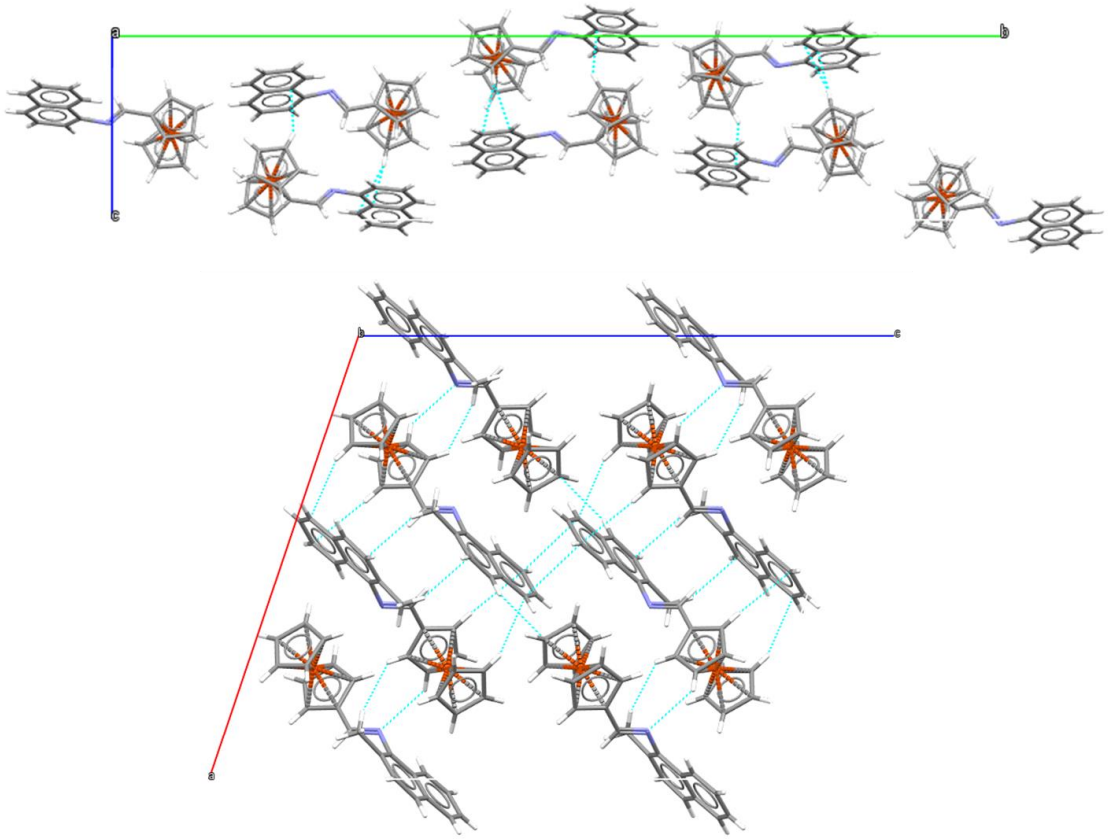

Figure S14: Packing diagrams of compounds **1** (top, view down the *a* axis) and **2** (bottom, view down the *b* axis) showing short contact interactions (dashed blue lines).