

## Supplementary Materials

**Table S1.** Hydrogen bonds for **1** (Å, °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N2A-H2A...O34 <sup>i</sup>	0.88	2.19	2.958(5)	146
N2A-H2A...O2 <sup>ii</sup>	0.88	2.37	3.079(5)	138
N2B-H2B...O1S	0.88	1.96	2.811(5)	161
N2C-H2C...O33 <sup>iii</sup>	0.88	2.13	2.890(5)	145
N2D-H2D...O14 <sup>iv</sup>	0.88	2.02	2.894(6)	177
N2E-H2E...O24 <sup>v</sup>	0.88	2.03	2.893(5)	166
N2F-H2F...O2W	0.88	1.96	2.818(6)	164
O1S-H1S...O1W	0.84	1.92	2.740(7)	165

Symmetry transformations used to generate equivalent atoms: (i):  $x, y, z + 1$ ; (ii):  $-x + 1, -y + 1, -z + 2$ ; (iii):  $x - 1, y, z$ ; (iv):  $-x + 1, -y + 1, -z + 1$ ; (v):  $-x + 1, -y, -z + 1$ .

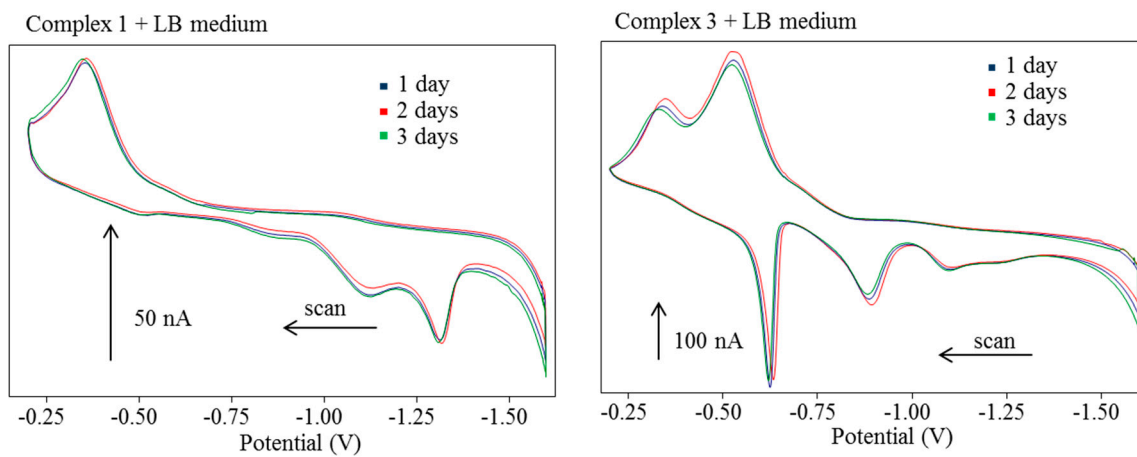
**Table S2.** Hydrogen bonds for **2** (Å, °).

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)
N1A-H1A...N3D	0.88	1.85	2.719(4)	169
N2A-H2A...O1	0.88	1.97	2.818(4)	160
N1B-H1B...N1E	0.88	2.46	3.160(4)	136
N1B-H1B...S1E	0.88	2.48	3.295(3)	154
N2B-H2B...S2E <sup>i</sup>	0.88	2.48	3.274(3)	151
N2B-H2B...N1E <sup>i</sup>	0.88	2.57	3.125(4)	122
N1C-H1C...S2E <sup>ii</sup>	0.88	2.42	3.273(3)	164
N2C-H2C...S1E <sup>iii</sup>	0.88	2.40	3.274(3)	172
N3C-H3C...O1	0.88	2.10	2.952(4)	162
N1D-H1D...S1D <sup>iv</sup>	0.88	2.49	3.359(3)	168
N2D-H2D...S3D <sup>v</sup>	0.88	2.43	3.306(3)	174
N2E-H2E...S1C <sup>vi</sup>	0.88	2.42	3.287(3)	170
N3E-H3E...S3C <sup>vii</sup>	0.88	2.45	3.330(3)	175
O1-H1...S3D <sup>viii</sup>	0.80(5)	2.53(5)	3.302(3)	164
O1-H2...S1C	0.83(5)	2.88(5)	3.344(3)	117

Symmetry transformations used to generate equivalent atoms: (i):  $-x, -y + 2, -z + 2$ ; (ii):  $x, y - 1, z + 1$ ; (iii):  $x, y, z + 1$ ; (iv):  $-x + 1, -y + 2, -z + 1$ ; (v):  $-x + 1, -y + 1, -z + 1$ ; (vi):  $x, y + 1, z - 1$ ; (vii):  $x, y, z - 1$ ; (viii):  $-x + 1, -y + 1, -z + 2$ .

Electrochemical behaviour of the prepared complexes was studied in water solution using cyclic voltammetry. Electrochemical measurements were performed with an AUTOLAB Analyzer (Metrohm, Herisau, Switzerland) connected to a VA-Stand 663 (Metrohm), using a standard cell with three electrodes. The three-electrode cell used a reference  $\text{Li}^+/\text{Li}$  electrode (E0 of the ferrocene/ferrocenium couple +470 mV) with a Luggine capillary and a Pt wire sealed in glass (0.5 mm diameter, 0.00196 cm<sup>2</sup>). For smoothing and baseline correction the software GPES 4.9 supplied by EcoChemie (Utrecht, Netherlands) was employed. The analysed samples were deoxygenated prior to measurements by purging with argon (99.999%) for 120 s. All experiments were carried out at room temperature 20 °C. Tetramethylammonium perchlorate (TMAP, 0.1 M) was used as supporting electrolyte and the solutions were  $1 \times 10^{-3}$  M in complex. All the potentials are referred against

reference electrode used in this work. The CV studies were also performed in the presence of serum as a function of time and also in a growth medium which contained 10 g/L of glucose, 10 g/L of tryptone (mixture of aminoacids) and 5 g/L of yeast extract at pH 7. The result of the study shows on the stability of the complexes (see Figure S1).



**Figure S1.** Cyclic voltammograms of the complexes **1** and **3** measured in LB medium.