Supporting Information

Ruthenium(II) arene complexes with chelating chloroquine analogue ligands: Synthesis, characterization and *in vitro* antimalarial activity

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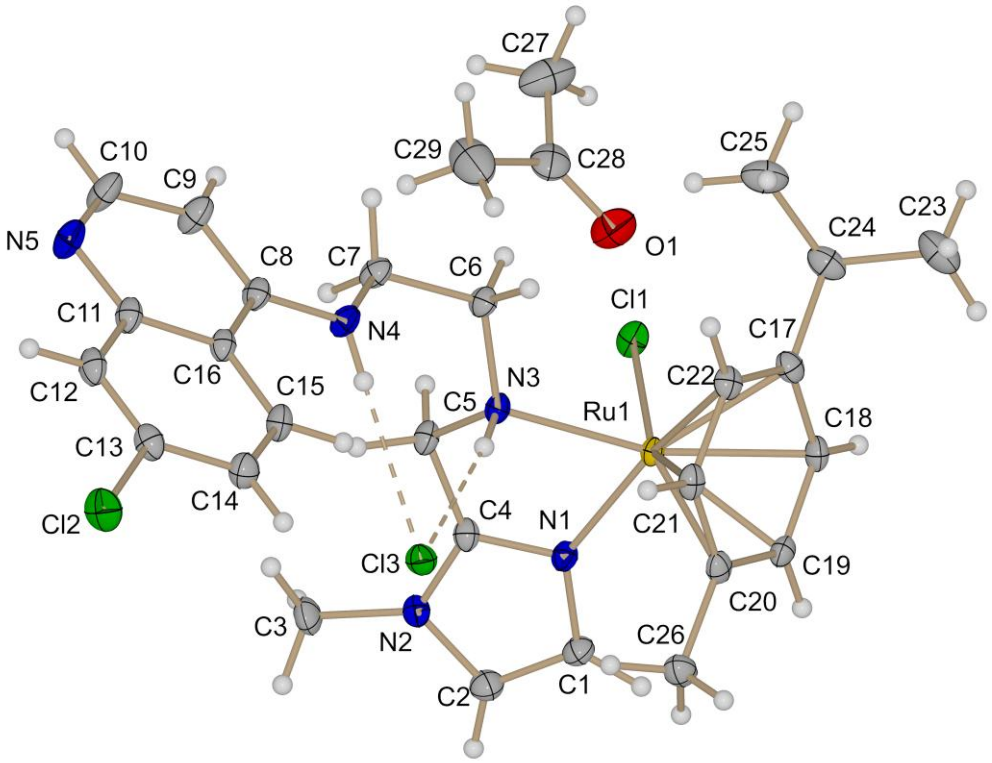

Figure S1. Molecular structure of **2**·$(CH_3)_2CO$, showing the atom numbering scheme. Hydrogen bonding to the chloride counter ion is indicated by dashed lines. Relevant bond lengths, d(D...A): N(3)-H(3N)...Cl(3) 3.099(1) Å; N(4)-H(4N)...Cl(3) 3.293(1) Å.

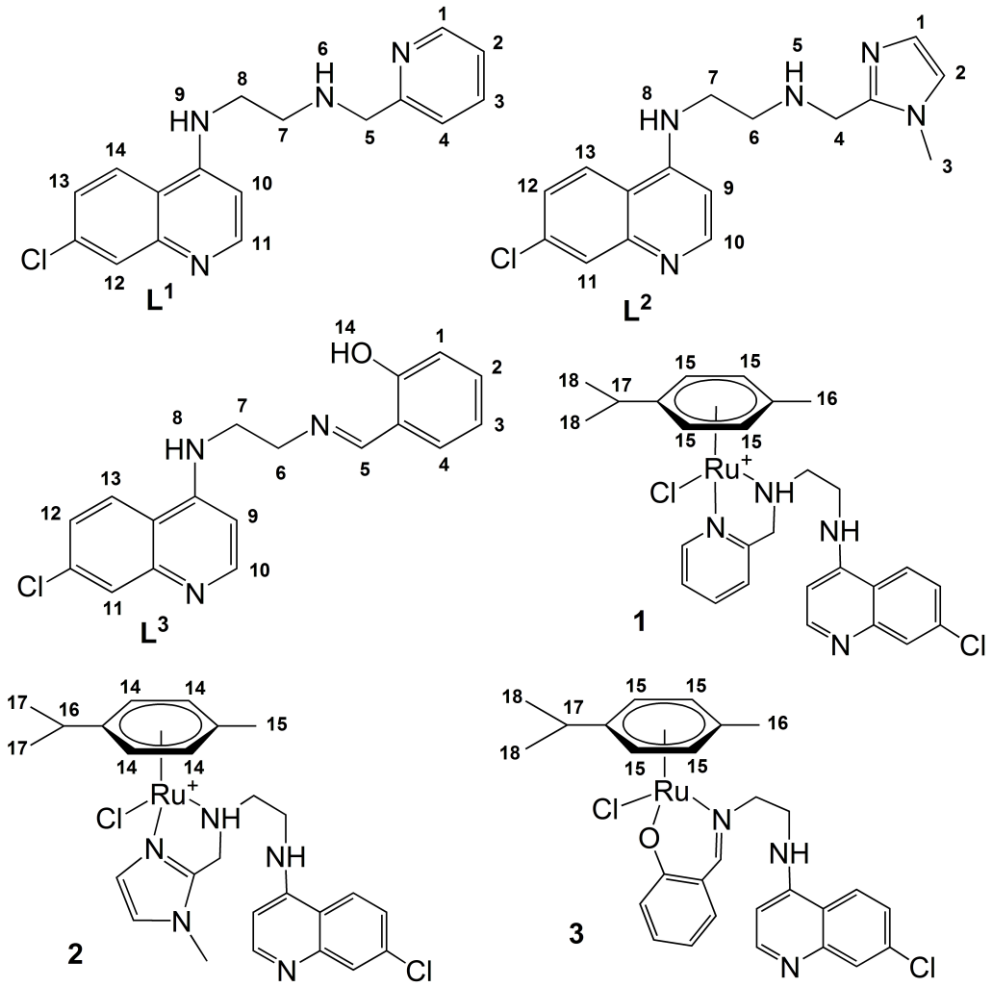

Figure S2. Numbering scheme for the assignment of ^{1}H NMR signals for **L**^{1}-**L**^{3} and complexes **1**-**3**.

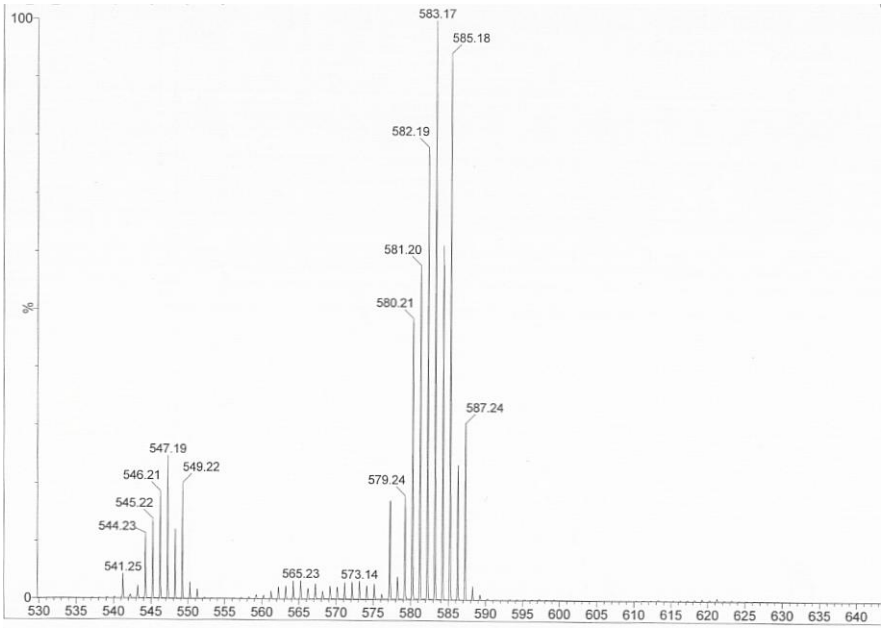

Figure S3. ESI-MS spectrum of complex **1**, showing fragments corresponding to [Ru^{II}Cl(*p*-cymene)($\mathbf{L^1}$)]$^+$ and [Ru^{II}Cl(*p*-cymene)($\mathbf{L^1}$)]-HCl. Details on the measurements are given in the experimental part of the paper.

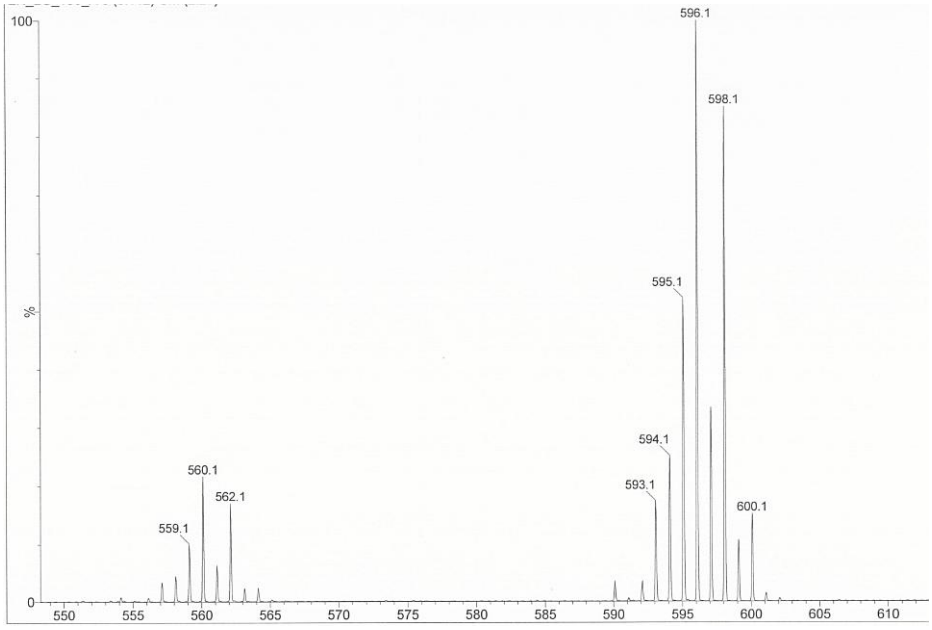

Figure S4. ESI-MS spectrum of complex **3**, showing fragments corresponding to [Ru^{II}Cl(*p*-cymene)($\mathbf{L^3}$)]+H and [Ru^{II}(*p*-cymene)($\mathbf{L^3}$)]. Details on the measurements are given in the experimental part of the paper.

Table S2. Assigned ^{1}H NMR signals for $\mathbf{L^1}$ and **1**, solvent given in parenthesis. Numbering scheme given in Fig. S2.

^{1}H[a]	$\mathbf{L^1}$ ($CDCl_3$)	**1** ($CDCl_3$)
1	8.58 (d, 4.4)	8.89 (d, 5.2)
2	7.29 (d, 8.0)	7.30 (d, 7.7)
3	7.65 (dt, 1.7, 7.7)	7.83 (dt, 1.4, 7.8)
4	7.19 (dd, 5.1, 6.7)	7.40 (t, 6.9)
5[b]	3.99 (s)	4.62 (dd, 6.1, 16.1)
		3.93 (dd, 5.4, 16.2)
6	2.05 (br s)	9.56 (br s)
7[b]	3.08 (m)	3.56 (m)
		3.13 (m)
8	3.37 (m)	3.62 (m)
9	6.09 (br s)	8.34 (br s)
10	6.38 (d, 5.4)	6.33 (d, 5.4)
11	8.52 (d, 5.4)	8.52 (d, 5.4)
12	7.95 (d, 2.1)	7.95 (d, 0.8)
13	7.36 (dd, 2.1, 8.9)	7.52 (dd, 2.1, 9.0)
14	7.81 (d, 8.9)	8.98 (d, 9.1)
15[b]		5.98 (d, 5.9)
		5.91 (d, 6.1)
		5.55 (d, 6.0)
		5.39 (d, 6.1)
16		2.04 (s)
17		2.78 (hept, 6.9)
18[b]		1.08 (d, 7.0)
		1.02 (d, 6.9)

[a] Multiplicity of the resonances and the corresponding *J* coupling constants in Hz are given in parenthesis.
[b] Not individually assigned, cf. Figure S2.

Table S3. Assigned ^{1}H NMR signals for $\mathbf{L^2}$ and **2**, solvent given in parenthesis. Numbering scheme given in Fig. S2.

^{1}H[a]	$\mathbf{L^2}$ (CD_3OD)	**2** ($CDCl_3$)
1	6.98 (d, 1.3)	7.20 (d, 1.6)
2	6.86 (d, 1.3)	6.91 (d, 1.5)
3	3.68 (s)	3.57 (s)
4[c]	3.90 (s)	4.27 (m)
		3.45 (m)
5	NO[b]	9.09 (br s)
6[c]	2.96 (t, 6.3)	3.91 (m)
		3.65 (m)
7	3.46 (t, 6.3)	3.65 (m)
8	NO[b]	8.34 (br s)
9	6.52 (d, 5.6)	6.36 (d, 5.5)
10	8.34 (d, 5.6)	8.54 (d, 5.4)
11	7.77 (d, 2.1)	7.96 (d, 2.1)
12	7.39 (dd, 2.2, 9.0)	7.50 (dd, 2.2, 9.0)
13	8.09 (d, 9.0)	8.99 (d, 9.0)
14[c]		5.87 (d, 5.6)
		5.55 (d, 6.0)
		5.36 (d, 6.1)
		5.28 (d, 5.7)
15		2.14 (s)
16		2.89 (hept, 6.9)
17[c]		1.19 (d, 6.9)
		1.16 (d, 7.0)

[a] Multiplicity of the resonances and the corresponding *J* coupling constants in Hz are given in parenthesis.
[b] Not observed.
[c] Not individually assigned, cf. Figure S2.

Table S4. Assigned ^{1}H NMR signals for $\mathbf{L^3}$ and **3**, solvent given in parenthesis. Numbering scheme given in Fig. S2.

^{1}H[a]	$\mathbf{L^3}$ ($CDCl_3$)	**3** ($CDCl_3$)
1	6.98 (d, 8.3)	6.91 (d, 8.5)
2	7.36 (m)	7.15 (m)
3	6.89 (t, 7.5)	6.27 (t, 7.3)
4	7.22 (d, 7.5)	6.48 (d, 7.7)
5	8.37 (s)	7.39 (s)
6[b]	3.74 (m)	4.57 (m)
		3.97 (m)
7	3.95 (m)	4.27 (m)
8	5.20 (br s)	7.51 (br s)
9	6.51 (d, 5.3)	6.55 (d, 3.9)
10	8.58 (d, 5.3)	8.37 (d, 4.3)
11	7.97 (d, 0.9)	8.02 (d, 1.5)
12	7.36 (m)	7.22 (dd, 1.5, 9.0)
13	7.60 (d, 8.9)	7.85 (d, 9.0)
14	12.99 (br s)	-
15[b]		5.57 (d, 6.2)
		5.52 (d, 6.2)
		5.46 (d, 5.4)
		5.09 (d, 5.4)
16		2.29 (s)
17		2.75 (hept, 6.9)
18[b]		1.24 (d, 6.9)
		1.14 (d, 6.9)

[a] Multiplicity of the resonances and the corresponding *J* coupling constants in Hz are given in parenthesis.
[b] Not individually assigned, cf. Figure S2.