

Dalton Transactions

**Synthesis and biological activity of cymantrene and cyrhetrene
4-aminoquinoline conjugates against malaria, leishmaniasis,
and trypanosomiasis†**

SUPPLEMENTARY MATERIAL

Lotta Glans^a, Wanning Hu^b, Christian Jöst^a, Carmen de Kock^c, Peter J. Smith^c, Matti Haukka^d, Heike Bruhn^e, Ulrich Schatzschneider^{b*}, and Ebbe Nordlander^{a*}

^a *Inorganic Chemistry Research Group, Chemical Physics, Center for Chemistry and Chemical Engineering, Lund University, Box 124, SE-221 00 Lund, Sweden*

^b *Institut für Anorganische Chemie, Julius-Maximilians-Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany*

^c *Division of Pharmacology, Department of Medicine, University of Cape Town Medical School, Observatory 7925, South Africa*

^d *Department of Chemistry, University of Eastern Finland, Box 111, FIN-80101 Joensuu, Finland*

^e *Institut für Molekulare Infektionsbiologie, Julius-Maximilians-Universität Würzburg, Josef-Schneider-Str. 2 D15, D-97080 Würzburg, Germany*

* Corresponding authors: E-mail: Ebbe.Nordlander@chemphys.lu.se; Tel: +46 46 222 8118; Fax: +46 46 222 4119; ulrich.schatzschneider@uni-wuerzburg.de; Tel: +49 931 31 83636; Fax: +49 931 31 84605.

Table S1. Crystallographic parameters for *N*-(7-chloroquinolin-4-yl)-*N'*-(cymantrenylmethyl)ethane-1,2-diamine·2H₂O (**6**·2H₂O).

6	
Empirical formula	C ₂₀ H ₂₁ ClMnN ₃ O ₅
Formula weight	473.79
temp (K)	100(2)
λ (Å)	0.71073
cryst syst	Monoclinic
space group	P2 ₁ /n
<i>a</i> (Å)	14.7914(2)
<i>b</i> (Å)	6.80990(10)
<i>c</i> (Å)	20.2659(3)
β (°)	99.1560(10)
<i>V</i> (Å ³)	2015.33(5)
<i>Z</i>	4
ρ_{calc} (Mg/m ³)	1.562
μ (Mo K α) (mm ⁻¹)	0.826
No. reflections	62133
Unique reflections	4990
GOOF (F ²)	1.024
R _{int}	0.0410
R1 ^a (<i>I</i> ≥ 2 σ)	0.0310
wR2 ^b (<i>I</i> ≥ 2 σ)	0.0783

^a $R1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$. ^b $wR2 = [\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]]^{1/2}$.