Supporting information

Novel antitrypanosomal agents based on palladium nitrofurylthiosemicarbazone complexes: DNA and redox metabolism as potential therapeutic targets

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Table S1. Crystal data and structure solution methods and refinement results for [Pd(**L5**)$_2$]·3DMSO

Empirical formula	$C_{22}H_{32}N_8O_9PdS_5$
Formula weight	819.26
Temperature (K)	293(2)
Wavelength	0.71073 Å
Crystal system	triclinic
Space group	P-1
Unit cell dimensions[a)]	a= 9.5720(5) Å α=78.497(4)º b=12.0590(9) Å β=77.746(4)º c=16.613(1) Å γ=66.717(4)º
Volume(Å^3)	1707.0(2)
Z	2
Calculated density (Mg/m^3)	1.594
Absorption coefficient μ (mm^{-1})	0.907
F(000)	836
Crystal size (mm)	0.20 x 0.11 x 0.06
Crystal color/shape	red/prismatic
Diffractometer/scan	KappaCCD/φ and ω
Radiation / graphite monochromator	MoK$_\alpha$ / λ=0.71073 Å
ϑ range for data collection	2.94 to 25.00º deg.
Limiting indices	-11≤h≤10, -14≤k≤14, -19≤l≤19
Reflections collected/unique	17315 / 5974 [R(int)=0.0533]
Completeness to ϑ=25.00º	99.3%
Reflections observed [I>2σ(I)]	4227
Absorption correction	PLATON [1]
Max. and min. transm.	0.945 and 0.840
Data reduction and correction[b)]	DENZO and SCALEPACK [2]
and structure solution[c)] and	SHELXS-97 [3]
refinement[d)] programs	SHELXL-97 [4]
Refinement method	Full-matrix least-squares on F^2
Weights, w	$[\sigma^2(F_o^2)+(0.1465P)^2+4.10P]^{-1}$ $P=[Max(F_o^2,0)+2F_c^2]/3$
Data/restraints/param.	5974 / 0 / 398
Goodness-of-fit on F^2	1.040
Final R indices [I>2σ(I)]	R1=0.0779, wR2=0.2151
R indices (all data)[e)]	R1=0.1081, wR2=0.2472
Largest diff. peak and hole (e.Å^{-3})	1.998 and -1.504

[a] Least-squares refinement of the angular settings for 16315 reflections in the 2.94<ϑ<25.00° range.

[b] Corrections: Lorentz, polarization and absorption.

[c] Neutral scattering factors and anomalous dispersion corrections.

[d] Structure solved by Patterson and Fourier methods. The final molecular model obtained by anisotropic full-matrix least-squares refinement of the non-hydrogen atoms.

[e] R indices defined as: $R1=\Sigma\left|\left|F_o\right|-\left|F_c\right|\right|/\Sigma\left|F_o\right|$, $wR_2=[\Sigma w(F_o^2-F_c^2)^2/\Sigma w(F_o^2)^2]^{1/2}$.

(1) Spek, A. L. *Acta Cryst.* **1990**, , A46-C34.

(2) Otwinowski, Z. & Minor, W. in *Methods in Enzymology* (eds. Carter, C. W. & Sweet, R. M.) 307-326 (Academic Press, New York, 1997).

(3) Sheldrick, G. M. (Univ. of Göttingen, Göttingen, Germany, 1997).

(4) Sheldrick, G. M. (Univ. of Göttingen, Göttingen, Germany, 1997).

Table S2. Microanalytical results

Compound	% C found (calcd.)	% H found (calcd.)	% N found (calcd.)	% S found (calcd.)
9	18.8(18.4)	1.48(1.54)	14.5(14.3)	7.91(8.19)
10	21.0(20.7)	2.05(1.97)	14.0(13.8)	7.81(7.89)
11	23.0(22.9)	2.60(2.38)	13.7(13.4)	7.77(7.63)
12	31.2(30.8)	1.95(2.14)	12.0(12.0)	6.82(6.85)
13	23.2(23.0)	1.74(1.92)	13.6(13.4)	7.53(7.67)
14	24.7(25.0)	2.27(2.31)	12.7(13.0)	7.66(7.42)
15	26.9(26.9)	2.79(2.69)	12.3(12.6)	7.44(7.18)
16	35.1(34.8)	2.66(2.43)	11.6(11.3)	6.29(6.49)
17·**DMSO**	27.3(27.5)	2.48(2.62)	18.5(18.3)	15.4(15.7)
18	30.5(30.0)	2.16(2.50)	19.7(20.0)	11.2(11.4)
19	31.2(31.2)	2.95(3.06)	18.9(19.0)	10.7(10.9)
20	42.2(42.1)	2.66(2.63)	16.1(16.4)	9.00(9.35)
21·**3DMSO**	32.5(32.3)	3.58(3.91)	13.7(13.7)	19.3(19.6)
22	35.6(35.3)	2.94(2.93)	18.5(18.3)	10.3(10.4)
23	37.0(37.5)	3.39(3.44)	17.5(17.5)	9.66(9.99)
24· **2DMSO**	42.8(43.0)	4.00(3.81)	12.7(12.6)	13.9(14.3)