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Supplementary Information

Stability and Toxicity of Heteroleptic Organometallic Bi(V) Complexes towards Leishmania major

Yih Ching Ong,¹ Victoria L. Blair,¹ Lukasz Kedzierski,², Philip C. Andrews^{*1}

¹School of Chemistry, Monash University, Clayton, Melbourne, VIC 3800, Australia ²Walter and Eliza Institute of Medical Research, Parkville, Melbourne, VIC 3800, Australia

Email: phil.andrews@monash.edu

Crystallography Section



Figure S1 Molecular structure of $[Bi(C_6H_5)_3(O_2CC_6H_3(m-CH_3)_2))_2]$ **1B**, showing thermal ellipsoids at 50 % probability. Hydrogen atoms have been omitted for clarity. Symmetry operator -x, -y, -z+1/2. Selected bond lengths (Å) and angles (°): Bi(1)-O(1), 2.7737(19); Bi(1)-O(2), 2.284(3); Bi(1)-C(10), 2.191(3); Bi(1)-C(16), 2.206(3); Bi(1)-C(10)', 2.191(3); O(1)-Bi(1)-O(2), 50.95(6); C(10)-Bi(1)-C(16), 102.91 (7); C(10)-Bi(1)-C(10)', 154.19(15);



Figure S2 Molecular structure of $[Bi(C_6H_5)_3(O_2CC_6H_4-o-OCH_2CH_3)_2]$ **4B** showing thermal ellipsoids at 50 % probability. Hydrogen atoms have been omitted for clarity. Symmetry operator: -x, y, 1/2-z. Selected bond lengths (Å) and angles (°): Bi(1)-O(1), 2.270(2); Bi(1)-O(2), 2.8666(18); Bi(1)-C(14), 2.198(3); Bi(1)-C(10), 2.204(3); O(1)-Bi(1)-O(2), 49.63(6); C(14)-Bi(1)-C(14)', 150.11(13); C(14)-Bi(1)-C(10)', 104.95(6).



Figure S3 Molecular structure of $[Bi(C_6H_5)_3(O_2CC_6H_4-p-NO_2)_2]$ **5B** showing thermal ellipsoids at 50 % probability. Hydrogen atoms have been omitted for clarity. Symmetry operator, -x+1, -y, z. Selected bond lengths (Å) and angles (°): Bi(1)-O(2), 2.280(3); Bi(1)-O(4), 2.902(3); Bi(1)-C(8), 2.180(4); Bi(1)-C(14), 2.198(6); O(2)-Bi(1)-O(4), 49.05(9); C(8)-Bi(1)-C(14), 109.21(11); C(8)'-Bi(1)-C(8), 141.6(2).



Figure S4 Molecular structure of $[Bi(C_6H_5)_3(O_2CC_6H_3-2-OH-5-Br)_2]$ **7B** showing thermal ellipsoids at 50 % probability. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Bi(1)-O(1), 2.282(3); Bi(1)-O(4), 2.282(3); Bi(1)-O(5), 3.002(3); Bi(1)-C(15), 2.177(4); Bi(1)-C(21), 2.184(4); Bi-C(27), 2.188(4); O(4)-Bi(1)-O(5), 47.44(9); O(1)-Bi(1)-O(2), 47.31; C(15)-Bi(1)-C(21), 134.33(14); C(15)-Bi(1)-C(27), 114.59(15); C(21)-Bi(1)-C(27), 111.08(16).



Figure S5 Molecular structure of $[Bi(C_6H_5)_3(O_2CC_6H_3-2-OH-5-C_6H_3(2,4-F)_2)_2]$ **8B** showing thermal ellipsoids at 50 % probability. Hydrogen atoms have been omitted for clarity. Symmetry operator: -x+1, y, 5/2-z. Selected bond lengths (Å) and angles (°): Bi(1)-O(1), 2.253(6); Bi(1)-O(2), 3.041(7); Bi(1)-C(5), 2.204(8); Bi(1)-C(1), 2.217(12); O(1)-Bi(1)-O(2), 46.30(19); C(5)-Bi(1)-C(5)', 148.2(5); C(5)-Bi(1)-C(1), 105.9(2).

Table S1 Deviation angles between the axial and equatorial plane for solid state structures found

Complexes	Deviation angle between axial & equatorial plane
1B	86.44 (0.08)
3B	88.76 (0.07)
4B	86.97 (0.08)
5B	88.29 (0.14)
6B	88.42 (0.06)
7B	89.73 (0.07)
8B	85.26 (0.24)
10B	89.15 (0.14)
Average angle of deviation	87.88





Figure S7 ¹³C NMR of Complex 1B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S9 ¹³C NMR of Complex 2B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S11 ¹³C NMR of Complex 3B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S13 ¹³C NMR of Complex 4B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S15¹³C NMR of Complex 5B in CDCl₃ at 25 °C, 400 MHz



Figure S17 ¹³C NMR of Complex 6B in CDCl₃ at 25 °C, 400 MHz



Figure S19 ¹³C NMR of Complex 7B in CDCl₃ at 25 °C, 400 MHz



Figure S21 ¹³C NMR of Complex 8B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S23 ¹³C NMR of Complex 9B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S24 ¹³C NMR of Complex 10B in CDCl₃ at 25 °C, 400 MHz



Figure S25 ¹³C NMR of Complex 10B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S27 ¹³C NMR of Complex 11B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S31 ³¹P NMR of 3B in DMEM culture, at 25 °C, 400 MHz in (CD₃)₂SO



Figure S35 ³¹P NMR of 8B in DMEM culture, at 25 °C, 400 MHz in (CD₃)₂SO



Figure S37 ³¹P NMR of 11B in DMEM culture, at 25 °C, 400 MHz in (CD₃)₂SO

¹H NMR of complexes 1B-11B in DMSO after 48 hours



Figure S38 ¹H NMR of Complex 1B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S40 ¹H NMR of Complex 3B in (CD₃)₂SO at 25°C, 400 MHz



Figure S42 ¹H NMR of Complex 5B in CDCl₃ at 25 °C, 400 MHz



Figure S44 ¹H NMR of Complex 7B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S46 ¹H NMR of Complex 9B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S48 1 H NMR of Complex 11B in (CD₃)₂SO at 25 °C, 400 MHz



Figure S52 ³¹P NMR of 4B in DMEM culture, at 25 °C, 400 MHz in (CD₃)₂SO



Figure S56 ³¹P NMR of 9B in DMEM culture, at 25 °C, 400 MHz in (CD₃)₂SO



Figure S57 ³¹P NMR of 11B in DMEM culture, at 25 °C, 400 MHz in (CD₃)₂SO

Stability studies of Complex 2B



Figure S58 ¹H NMR of 2B in D₂O at t = 0 hours and t = 24 h at 25 °C, 400 MHz



Figure S59 ¹H NMR of 2B and DL-Lysine.HCl in D_2O at t = 0 hours and t = 20 hours at 25 °C, 400 MHz

Mass Spectrometry



Figure S60 Mass spectrometry of unknown precipitate compared with spectra of BiPh₃