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Supplementary Data (for electronic supplementary information only)

Appendix-A

Biological activity study of complexes **1**-**5** *vs*. that of *Amphotericin B* (AmB).

Compound	Dose (μg/disk)	Diameter of clear zone (mm)			
		A. niger	*A. flavus*	*C. albicans*	*S. cerevisiae*
1	200	0	0	0	0
2	200	0	0	0	0
3	200	0	0	0	0
4	200	0	0	0	0
5	200	0	0	0	0
AmB	100	14	9	9.5	8

Appendix-B

Calculation of the Diamagnetic Correction for **1**

Using the values of χ_D and λ_i found in [1], the value of χ_D for **1** was calculated as:

$$\chi_D = \Sigma_i \chi_{Di} + \Sigma_i \lambda_i$$

χ_D (atom contributions) $= 9\,\chi_D(C_{ring}) + \chi_D(N_{ring}) + 14\chi_D(H) + 2\chi_D(C) + \chi_D(N_{open}) + \chi_D(O)$
$= [9(-6.24) + (-4.61) + 14(-2.93) + 2(-6.00) + (-5.57) + (-4.6)] \times 10^{-6}$ emu·mol^{-1}
$= -123.96 \times 10^{-6}$ emu·mol^{-1}

λ (bond contributions) $= \lambda_i(benzene) + \lambda_i(N{=}C) + \lambda_i(Ar\text{-}NR_2)$
$= [(-1.4) + (+8.15) + (+1)] \times 10^{-6}$ emu·mol^{-1}
$= +7.75 \times 10^{-6}$ emu·mol^{-1}

$\therefore \chi_D$ (**1**) $= \chi_D + \lambda$
$= [(-123.96) + (+7.75)] \times 10^{-6}$ emu·mol^{-1}
$= -116.2 \times 10^{-6}$ emu·mol^{-1}

The 'estimated' value of χ_D, based on the simpler formula using only molar mass (FW) considerations, results in:

χ_D (est.) $= -(FW / 2) \times 10^{-6}$ emu·mol^{-1}
$=[(-190.25) / 2] \times 10^{-6}$ emu·mol^{-1}
$= -95.1 \times 10^{-6}$ emu·mol^{-1}

In our calculations of μ_{eff}, we have employed the more accurate value above in addition to the tabulated values of χ_D for the other ligands and atoms involved [1].

Reference

[1] G. A. Bain, J. F. Berry, *J. Chem. Ed*. **2008**, *85*, 532.

Appendix-C

PM3(tm) Calculations of the Isomers of Complex **5**

The data refer to the relative energies calculated using Spartan Version 8.0 at the PM3(tm) level of theory. The corresponding isomer labelling numbers are shown in Figure 2.

Isomer	Calculated Relative Energy (kJ/mol)	Calculated Dipole Moment (debye)
I	-6883.63	13.04
II	-6891.56	5.10
III	-6803.33	8.81
IV	-6859.15	13.68
V	-6883.22	16.28