Supplementary Material

Synthesis, characterization and antimicrobial activity of a bidentate NS Schiff base of S-benzyl dithiocarbazate and its divalent complexes

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Table 1S: Minimum inhibitory concentrations (MICs) against test bacteria for complex 2.

| Test tube No. | Nutrient broth medium added (mL) | compound-2 (μg/mL) | Inoculum added (μL) | S. -β-haemolyticus | K. pneumonia | E. coli |
|---------------|---------------------------------|-------------------|---------------------|---------------------|--------------|--------|
| 1             | 1                               | 512               | 10                  | -                   | -            | -      |
| 2             | 1                               | 256               | 10                  | -                   | -            | -      |
| 3             | 1                               | 128               | 10                  | -                   | 128          | -      |
| 4             | 1                               | 64                | 10                  | -                   | -            | +      |
| 5             | 1                               | 32                | 10                  | +                   | -            | +      |
| 6             | 1                               | 16                | 10                  | +                   | +            | +      |
| 7             | 1                               | 8                 | 10                  | +                   | +            | +      |
| 8             | 1                               | 4                 | 10                  | +                   | +            | +      |
| 9             | 1                               | 2                 | 10                  | +                   | +            | +      |
| 10            | 1                               | 1                 | 10                  | +                   | +            | +      |
| Cm            | 1                               | 0                 | 0                   | -                   | -            | -      |
| Cs            | 1                               | 512               | 0                   | -                   | -            | -      |
| Ci            | 1                               | 0                 | 10                  | +                   | +            | +      |

Results of MIC values in (μg/ml) 64 32 128

“+” = Growth “-” = No growth
Figure 1S. Crystal packing of 1 showing pair of molecules connected by N-H…S interactions (dashed line). The C-H---π interactions are shown as green lines.
Figure 2S. Crystal packing viewed down axis b of the CuL₂ complex 5; H atoms not shown for clarity.)
Figure 3S: Solution UV-visible spectrum of the ligand in chloroform (1)

Figure 4S: Solution UV-visible spectrum of nickel(II) complex in chloroform (2)
Figure 5S: Solution UV-visible spectrum of zinc(II) complex in chloroform (3)

Figure 6S: Solution UV-visible spectrum of palladium(II) complex in chloroform (4)
Figure 7S: Solution UV-visible spectrum of copper(II) complex in chloroform (5)
Figure 8S: Solid state IR spectrum of ligand 1 as KBr Pellet
Figure 9S: Solid state IR spectrum of nickel(II) complex 2 as KBr Pellet
Figure 10S: Solid state IR spectrum of zinc(II) complex 3 as KBr Pellet
Figure 11S: IR spectrum of palladium(II) complex 4 as KBr Pellet
Figure 12S: Solid state IR spectrum of copper(II) complex 5 as KBr Pellet
Figure 13S: Low Resolution Mass spectrum of ligand 1 by FAB\(^+\) method.

Figure 14S: Low Resolution Mass spectrum of ligand 1 by FAB\(^+\) method.
Figure 15S: High Resolution Mass spectrum of ligand 1 by FAB<sup>+</sup> method.

Figure 16S: Low Resolution Mass spectrum of Nickel(II) complex 2 by FAB<sup>+</sup> method.
Figure 17S: Low Resolution Mass spectrum of Nickel(II) complex 2 by FAB<sup>+</sup> method.

Figure 18S: Low Resolution Mass spectrum of Nickel(II) complex 2 by FAB<sup>−</sup> method.
Figure 19S: High Resolution Mass spectrum of Nickel(II) complex 2 by FAB\(^+\) method.

Figure 20S: Low Resolution Mass spectrum of zinc(II) complex 3 by FAB\(^+\) method.
Figure 21S: Low Resolution Mass spectrum of zinc(II) complex 3 by FAB⁻ method.

Figure 22S: Low Resolution Mass spectrum of zinc(II) complex 3 by FAB⁺ method.
Figure 23S: High Resolution Mass spectrum of zinc(II) complex 3 by FAB\(^+\) method.

Figure 24S: Low Resolution Mass spectrum of palladium(II) complex 4 by FAB\(^+\) method.
Figure 25S: Low Resolution Mass spectrum of palladium(II) complex 4 by FAB$^+$ method.

Figure 26S: Low Resolution Mass spectrum of palladium(II) complex 4 by FAB$^+$ method.
Figure 27S: High Resolution Mass spectrum of palladium(II) complex 4 by FAB⁺ method.

Figure 28S: Low Resolution Mass spectrum of copper(II) complex 5 by FAB⁻ method.
Figure 29S: Low Resolution Mass spectrum of copper(II) complex 5 by FAB$^+$ method.

Figure 30S: Low Resolution Mass spectrum of copper(II) complex 5 by FAB$^+$ method.
Figure 31S: $^1$H-NMR spectrum of ligand 1 in CDCl$_3$

Figure 32S: $^1$H-NMR spectrum of ligand 1 in CDCl$_3$
Figure 33S: $^1$H-NMR spectrum of ligand 1 in CDCl$_3$

Figure 34S: $^1$H-NMR spectrum of nickel(II) complex 2 in CDCl$_3$
Figure 35S: $^1$H-NMR spectrum of nickel(II) complex 2 in CDCl$_3$

Figure 36S: $^1$H-NMR spectrum of zinc(II) complex 3 in CDCl$_3$
Figure 37S: $^1$H-NMR spectrum of zinc(II) complex 3 in CDCl$_3$

Figure 38S: $^1$H-NMR spectrum of zinc(II) complex 3 in CDCl$_3$
Figure 39S: $^1$H-NMR spectrum of zinc(II) complex 3 in CDCl$_3$

Figure 40S: $^1$H-NMR spectrum of zinc(II) complex 3 in CDCl$_3$
Figure 41S: $^1$H-NMR spectrum of palladium(II) complex 4 in CDCl$_3$

Figure 42S: $^1$H-NMR spectrum of palladium(II) complex 4 in CDCl$_3$
Figure 43S: $^1$H-NMR spectrum of palladium(II) complex 4 in CDCl$_3$

Figure 44S: $^1$H-NMR spectrum of palladium(II) complex 4 in CDCl$_3$
Figure 45S: $^1$H-NMR spectrum of palladium(II) complex 4 in CDCl$_3$