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)	<i>S. -β- haemolyticus</i>	<i>K. pneumoniae</i>	<i>E. coli</i>
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**)

FTIR2014 - 1-55 - Chemistry_RUET1.ispd

Operator: Al-Amin

	Item	Value
2	Sample name	Mumit ML1
3	Sample ID	19.11.2014(1)
4	Option	
5	Intensity Mode	%Transmittance
6	Apodization	Happ-Genzel
9	No. of Scans	15

Figure 8S: Solid state IR spectrum of ligand **1** as KBr Pellet

FTIR2014 - 1-56 - Chemistry_RUET2.ispd

Operator: Al-Amin

	Item	Value
2	Sample name	Mumit_ML1_Ni
3	Sample ID	19.11.2014(2)
4	Option	
5	Intensity Mode	%Transmittance
6	Apodization	Happ-Genzel
9	No. of Scans	15

Figure 9S: Solid state IR spectrum of nickel(II) complex **2** as KBr Pellet

FTIR2014 - 1-59 - Chemistry_RUET5.ispd

Operator: Al-Amin

	Item	Value
2	Sample name	Mumit ML1 Zn
3	Sample ID	19.11.2014(4)
4	Option	
5	Intensity Mode	%Transmittance
6	Apodization	Happ-Genzel
9	No. of Scans	15

Figure 10S: Solid state IR spectrum of zinc(II) complex **3** as KBr Pellet

FTIR2014 - 1-61 - Chemistry_RUET7.ispd

Operator: Al-Amin

	Item	Value
2	Sample name	Mumit ML1 Pd
3	Sample ID	19.11.2014(6)
4	Option	
5	Intensity Mode	%Transmittance
6	Apodization	Happ-Genzel
9	No. of Scans	15

Figure 11S: IR spectrum of palladium(II) complex **4** as KBr Pellet

FTIR2014 - 1-57 - Chemistry_RUET3.ispd

Operator: Al-Amin

	Item	Value
2	Sample name	Mumit ML1 Cu
3	Sample ID	19.11.2014(3)
4	Option	
5	Intensity Mode	%Transmittance
6	Apodization	Happ-Genzel
9	No. of Scans	15

Figure 12S: Solid state IR spectrum of copper(II) complex **5** as KBr Pellet

[Mass Spectrum]
 Data : ML1002 Date : 26-Jun-2015 13:53
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.67 min Scan# : 5 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 13.93 (146033)
 Output m/z range : 10 to 403 Cut Level : 0.00 %

Figure 13S: Low Resolution Mass spectrum of ligand **1** by FAB⁺ method.

[Mass Spectrum]
 Data : ML1002 Date : 26-Jun-2015 13:53
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.67 min Scan# : 5 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 13.93 (146033)
 Output m/z range : 364 to 391 Cut Level : 0.00 %

Figure 14S: Low Resolution Mass spectrum of ligand **1** by FAB⁺ method.

Data : ML1H004 Date : 10-Jul-2015 15:40
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 0.34 min Scan# : 5
Elements : C 18/0, H 21/0, N 2/0, O 3/0, S 2/0
Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 - 20.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1 377.0990	30.11	-1.0 / -0.4	11.5 C18 H21 N2 O3 S2

Figure 15S: High Resolution Mass spectrum of ligand **1** by FAB⁺ method.

Figure 16S: Low Resolution Mass spectrum of Nickel(II) complex **2** by FAB⁺ method.

[Mass Spectrum]
 Data : ML1C1-N008 Date : 26-Jun-2015 14:35
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.67 min Scan# : 5 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 4.21 (44186)
 Output m/z range : 10 to 886 Cut Level : 0.00 %

Figure 17S: Low Resolution Mass spectrum of Nickel(II) complex **2** by FAB⁺ method.

[Mass Spectrum]
 Data : ML1C1-N008 Date : 26-Jun-2015 14:35
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.67 min Scan# : 5 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 4.21 (44186)
 Output m/z range : 775 to 847 Cut Level : 0.00 %

Figure 18S: Low Resolution Mass spectrum of Nickel(II) complex **2** by FAB⁺ method.

Data : ML1-NHR004 Date : 15-Nov-2014 11:55
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 RT : 1.40 min Scan# : 15
 Elements : C 36/36, H 39/39, N 4/4, O 5/5, S 4/4, 58Ni 1/0, 60Ni 1/0
 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
 Unsaturation (U.S.) : -0.5 - 30.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1 809.1100	4.76	-0.7 / -0.6	24.0 C36 H39 N4 O5 S4 58Ni

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.

[Mass Spectrum]
 Data : ML1C3-Zn010 Date : 25-Jun-2015 14:53
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 1.17 min Scan# : 8 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 10.79 (113123)
 Output m/z range : 10 to 892 Cut Level : 0.00 %

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

[Mass Spectrum]
 Data : ML1C3-Zn010 Date : 25-Jun-2015 14:53
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 1.17 min Scan# : 8 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 10.79 (113123)
 Output m/z range : 799 to 835 Cut Level : 0.00 %

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

Data : ML1-ZnH005 Date : 15-Nov-2014 12:08
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 RT : 1.40 min Scan# : 15
 Elements : C 36/36, H 39/39, N 4/4, O 5/5, S 4/4, 64Zn 1/0, 66Zn 1/0, 68Zn 1/0
 Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
 Unsaturation (U.S.) : -0.5 - 30.0

Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1 815.1040	47.50	-0.5 / -0.4	23.5 C36 H39 N4 O5 S4 64Zn

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.

[Mass Spectrum]
 Data : ML1C5-P0011 Date : 26-Jun-2015 15:02
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.84 min Scan# : 6 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 8.14 (85313)
 Output m/z range : 10 to 917 Cut Level : 0.00 %

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

[Mass Spectrum]
 Data : ML1C5-P0011 Date : 26-Jun-2015 15:02
 Instrument : MStation
 Sample : -
 Note : -
 Inlet : Direct Ion Mode : FAB+
 Spectrum Type : Normal Ion [MF-Linear]
 RT : 0.84 min Scan# : 6 Temp : 3276.7 deg.C
 BP : m/z 154.1000 Int. : 8.14 (85313)
 Output m/z range : 839 to 873 Cut Level : 0.00 %

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

Data : ML1C5-PdH017 Date : 10-Jul-2015 19:29
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : FAB+
RT : 1.14 min Scan# : 18
Elements : C 35/36, H 39/39, N 4/4, O 6/6, S 4/4, 104Pd 1/0, 105Pd 1/0,
106Pd 1/0, 108Pd 1/0, 110Pd 1/0
Mass Tolerance : 1000ppm, 5mmu if m/z < 5, 50mmu if m/z > 50
Unsaturation (U.S.) : -0.5 ~ 25.0
Unsaturation (U.S.) : -0.5 ~ 25.0

	Observed m/z	Int%	Err [ppm / mmu]	U.S. Composition
1	857.0786	39.12	-0.1 / -0.1	23.5 C36 H39 N4 O6 S4 106Pd

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

[Mass Spectrum]
Data : ML1C2-Cu009 Date : 26-Jun-2015 14:43
Instrument : MStation
Sample : -
Note : -
Inlet : Direct Ion Mode : FAB+
Spectrum Type : Normal Ion [MF-Linear]
RT : 1.17 min Scan# : 8 Temp : 3276.7 deg.C
BP : m/z 154.1000 Int. : 20.28 (212619)
Output m/z range : 265 to 845 Cut Level : 0.00 %

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: ¹H-NMR spectrum of ligand **1** in CDCl₃

Figure 32S: ¹H-NMR spectrum of ligand **1** in CDCl₃

Figure 33S: ¹H-NMR spectrum of ligand **1** in CDCl₃

Figure 34S: ¹H-NMR spectrum of nickel(II) complex **2** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C1-Ni in CDCl₃, Mumit,RUET

BRUKER

Current Data Parameters
NAME A-96_D-110_Abdul Munit_RUET
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150309
Time_ 10.32
INSTRUM spect
PROBHD 5 mm F4000 BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 118
DS 1
SWH 6002.401 Hz
FIDRES 0.091589 Hz
AQ 5.4591489 sec
RG 142.89
DW 83.300 usec
DE 13.43 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 32768
SF 400.1700244 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 35S: ¹H-NMR spectrum of nickel(II) complex **2** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C3-Zn in CDCl₃, Mumit,RUET

BRUKER

Current Data Parameters
NAME A-96_D-110_Abdul Munit_RUET
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150309
Time_ 9.54
INSTRUM spect
PROBHD 5 mm F4000 BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 1
SWH 6002.401 Hz
FIDRES 0.091589 Hz
AQ 5.4591489 sec
RG 76.38
DW 83.300 usec
DE 13.43 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
NUC1 1H
P1 10.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 32768
SF 400.1700244 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 36S: ¹H-NMR spectrum of zinc(II) complex **3** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C3-Zn in CDCl₃, Munit,RUET

Figure 37S: ¹H-NMR spectrum of zinc(II) complex **3** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C3-Zn in CDCl₃, Munit,RUET

Figure 38S: ¹H-NMR spectrum of zinc(II) complex **3** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C3-Zn in CDCl3, Mumit,RUET

Figure 39S: ^1H -NMR spectrum of zinc(II) complex **3** in CDCl_3

INARS,BCSIR,1H spectrum, ML1 C3-Zn in CDCl3, Mumit,RUET

Figure 40S: ^1H -NMR spectrum of zinc(II) complex **3** in CDCl_3

INARS,BCSIR,1H spectrum, ML1 C5-Pd in CDCl3, Mumit,RUET

Figure 41S: ^1H -NMR spectrum of palladium(II) complex **4** in CDCl_3

INARS,BCSIR,1H spectrum, ML1 C5-Pd in CDCl3, Mumit,RUET

Figure 42S: ^1H -NMR spectrum of palladium(II) complex **4** in CDCl_3

INARS,BCSIR,1H spectrum, ML1 C5-Pd in CDCl₃, Mumit,RUET

Current Data Parameters
NAME A-94_D-110_Abdul Mumit_RUET
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150309
Time 10.56
INSTRUM spect
PROBHD 5 mm FANNO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 1
SWH 6002.401 Hz
FIDRES 0.001589 Hz
AQ 5.4591889 sec
RG 78.38
OW 83.300 usec
DE 13.43 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1724008 MHz
NUC1 1H
P1 10.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 32768
SF 400.1700244 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 43S: ¹H-NMR spectrum of palladium(II) complex **4** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C5-Pd in CDCl₃, Mumit,RUET

Current Data Parameters
NAME A-94_D-110_Abdul Mumit_RUET
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20150309
Time 10.56
INSTRUM spect
PROBHD 5 mm FANNO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl₃
NS 64
DS 1
SWH 6002.401 Hz
FIDRES 0.001589 Hz
AQ 5.4591889 sec
RG 78.38
OW 83.300 usec
DE 13.43 usec
TE 300.0 K
D1 1.00000000 sec
TD0 1

===== CHANNEL f1 =====
SFO1 400.1724008 MHz
NUC1 1H
P1 10.50 usec
PLW1 17.00000000 W

F2 - Processing parameters
SI 32768
SF 400.1700244 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

Figure 44S: ¹H-NMR spectrum of palladium(II) complex **4** in CDCl₃

INARS,BCSIR,1H spectrum, ML1 C5-Pd in CDCl3, Mumit,RUET

Figure 45S: ^1H -NMR spectrum of palladium(II) complex **4** in CDCl_3