

Synthesis, Characterization, and Antioxidant Activity of a New Copper(II)-imidazole Derivative Complex

Ariel Colaço de Oliveira¹, Ana Claudia Pedrozo da Silva², Antonio Gustavo Sampaio de Oliveira-Filho³, Lilian Tatiani Dusman Tonin², André Luiz Tessaro^{2*}, Rafael Block Samulewski^{2*}

Supplementary data

Table 1S. ¹H-NMR data for *cis/trans* 3NIMDZ-H.

	<i>cis</i>	<i>trans</i>
H	δ _H (mult., J=Hz)	δ _H (multi., J=Hz)
2	7,32 (s)	7,47 (s)
4	5,06 (s)	5,14 (s)
6	3,26 (dd, 3,0; 9,0)	3,11 (dd, 3,0; 9,0)
7α	2,72-2,83 (m)	2,72-2,83 (m)
7β	2,55-2,64 (m)	2,55-2,64 (m)
2'	8,17 (d, 3,0)	8,17 (d, 3,0)
4'	8,09-8,12 (m)	8,09-8,12 (m)
5'	7,60 (t, 7,0)	7,59 (t, 7,0)
6'	7,84 (d, 6,0)	7,84 (d, 6,0)

Figure 1S. ¹H-NMR (300 MHz) spectra at DMSO-d₆ for 3-NIMDZ-H ligand.

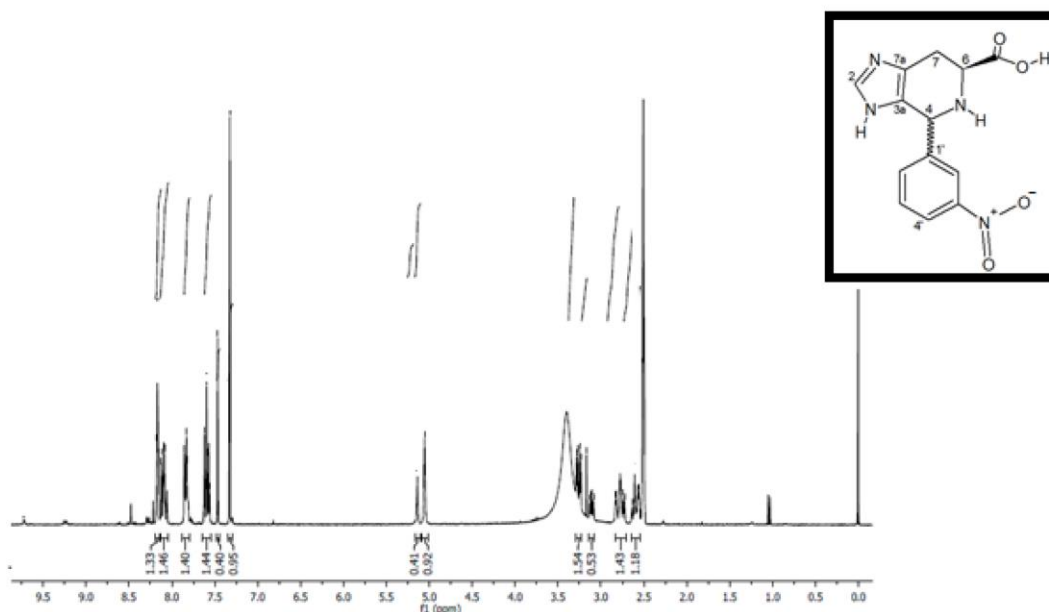
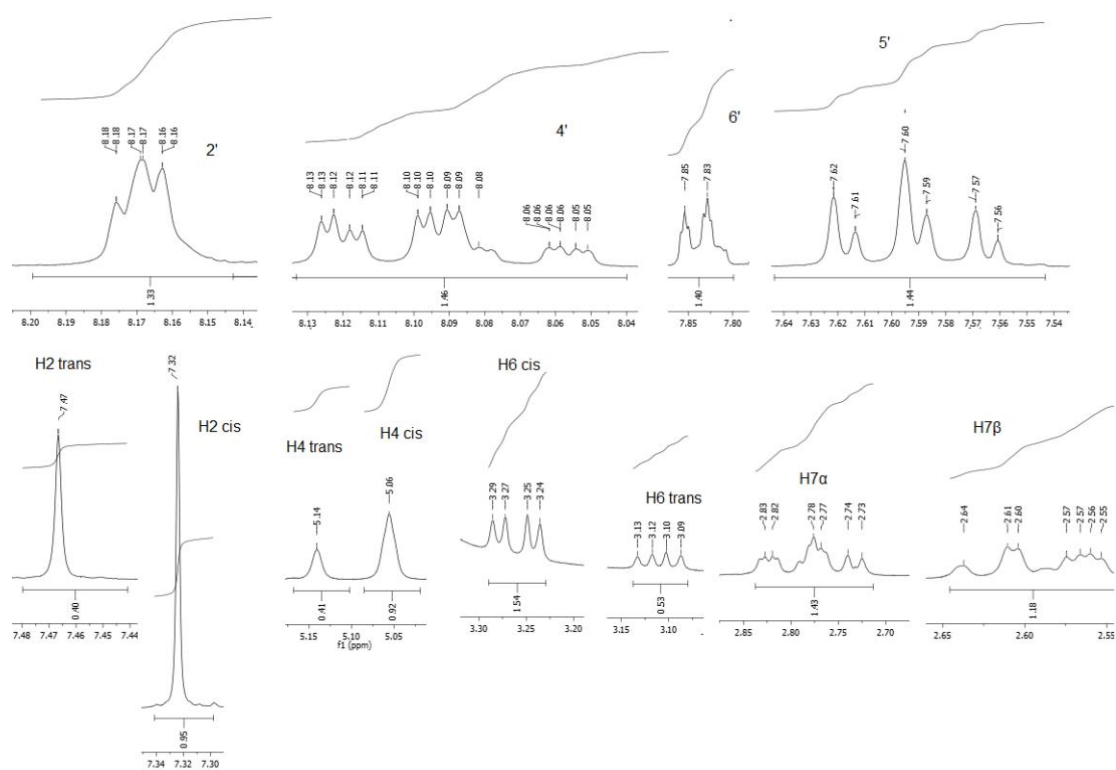


Figure 2S. Expanded ^1H -NMR (300 MHz) spectra at DMSO- d_6 for 3-NIMDZ-H ligand.**Table 2S** – ^{13}C -NMR data for *cis/trans* 3NIMDZ-H.

C	<i>cis</i>	<i>trans</i>
	δ_{C}	δ_{C}
2	134,0 (CH)	134,3 (CH)
3a	147,1 (C)	147,6 (C)
4	59,0 (CH)	58,3 (CH)
6	53,7 (CH)	54,3 (CH)
7	27,3 (CH ₂)	27,3 (CH ₂)
1'	134,9 (C)	134,9 (C)
2'	122,5 (CH)	121,8 (CH)
3'	148,0 (C)	148,0 (C)
4'	123,2 (CH)	122,3 (CH)
5'	129,7 (CH)	129,7 (CH)
6'	135,9 (CH)	135,9 (CH)

Figure 3S. ^{13}C -NMR (75.5 MHz) spectra at DMSO- d_6 for 3-NIMDZ-H ligand.

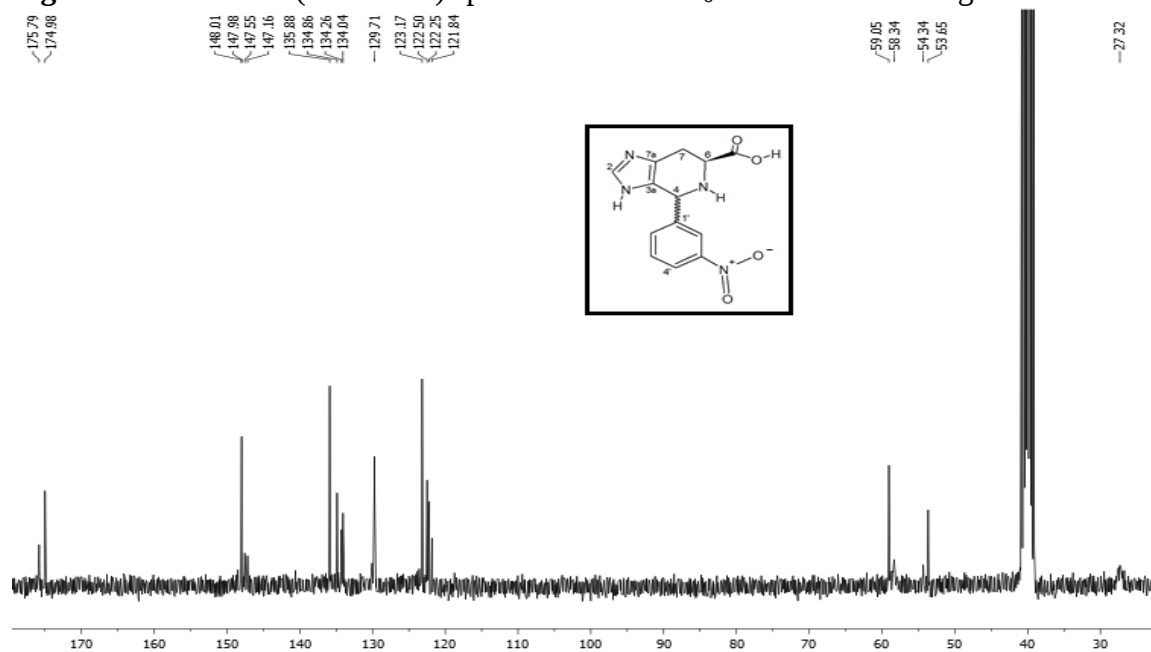


Figure 4S. Expanded ^{13}C -NMR (75.5 MHz) spectra at DMSO- d_6 for 3-NIMDZ-H ligand.

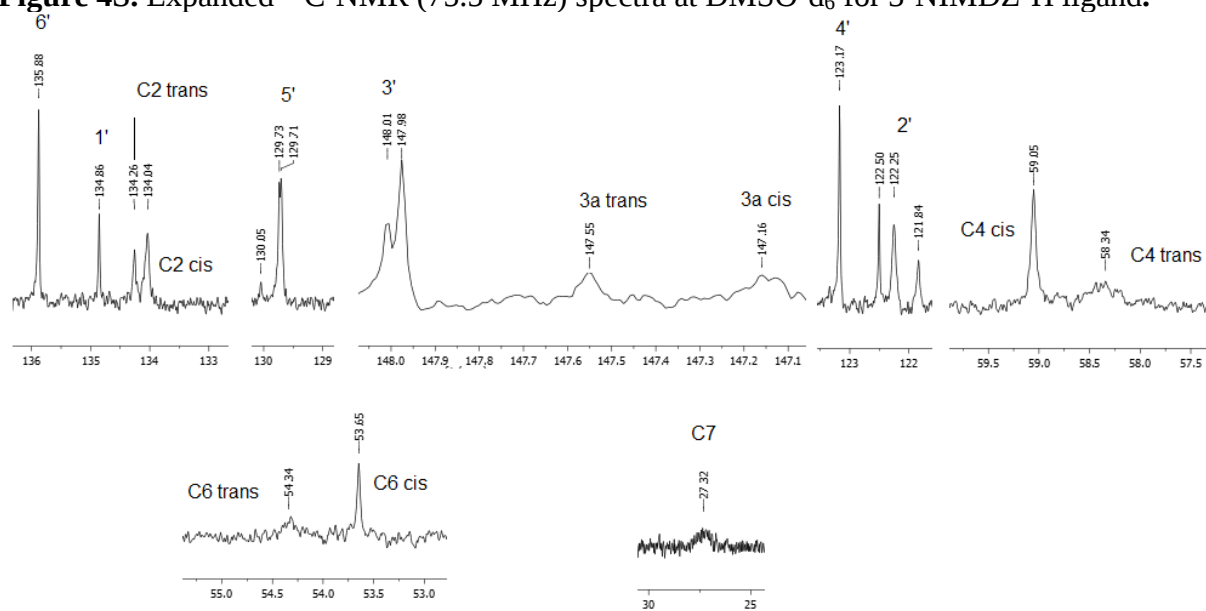


Figure 5S. Calculated vibrational spectra, at the B3LYP-D3(BJ) level of theory, for 3NIMDZ-H and $[\text{Cu}(\text{3NIMDZ-H})(\text{OH}_2)_5]^{2+}$.

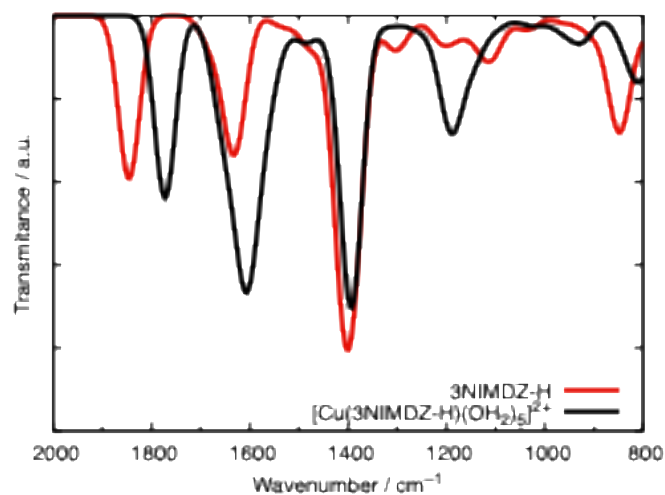


Figure 6S. Calculated electronic spectrum calculated with TDDFT, at the B3LYP-D3(BJ)/def2-TZVP level, for $[\text{Cu}(\text{3NIMDZ-H})(\text{OH}_2)_5]^{2+}$.

