Electronic supplementary information:

Substituted bidentate and ancillary ligands modulate bioimaging properties of classical Re (I) tricarbonyl core with yeasts and bacteria

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† Electronic supplementary information (ESI) available.

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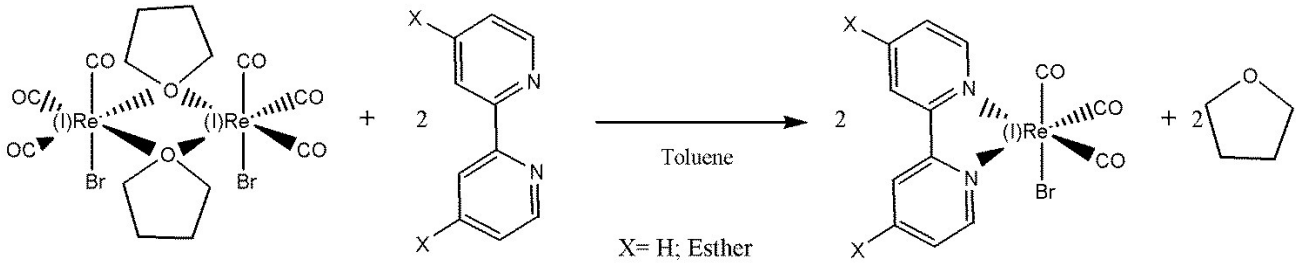


Scheme S1. Alternative route to obtained classical rhenium complexes (**C1** to **C5**).

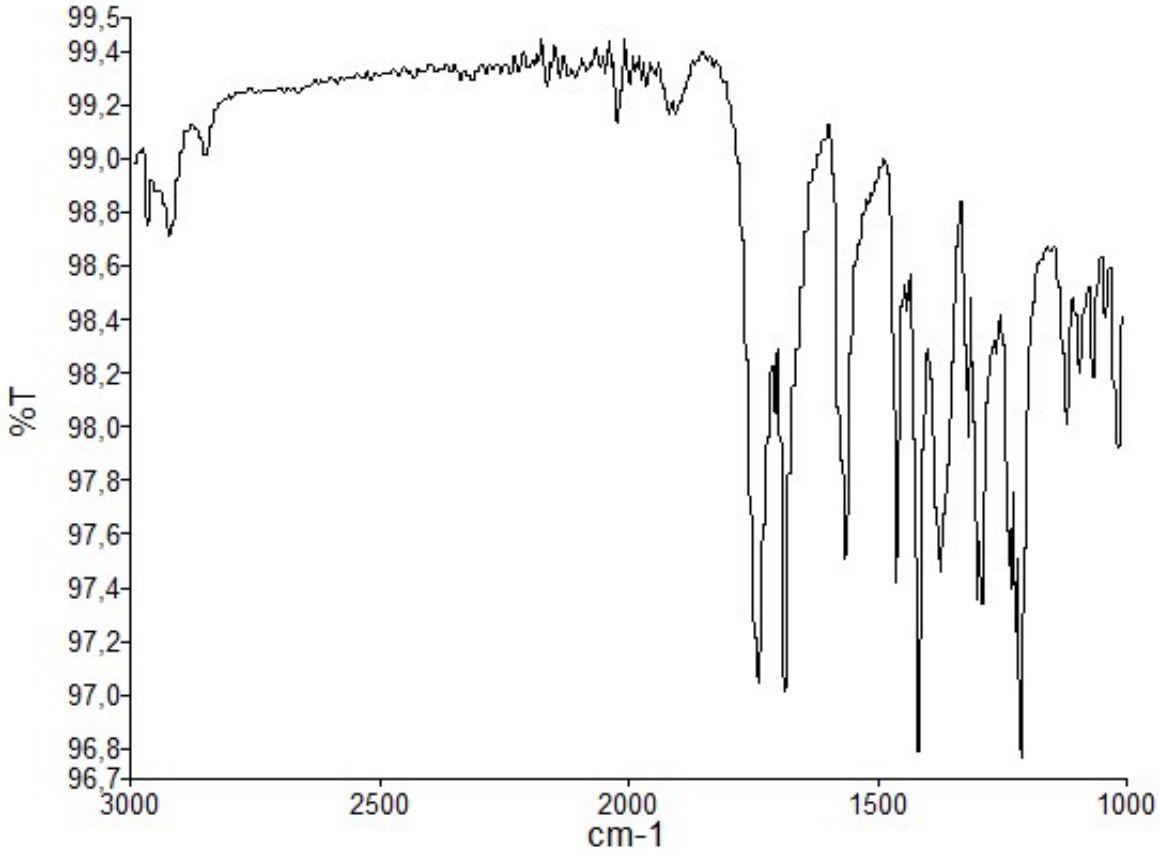


Figure S1. FTIR spectrum for 1,10-phenantroline-5,6-dione (**dione)**.

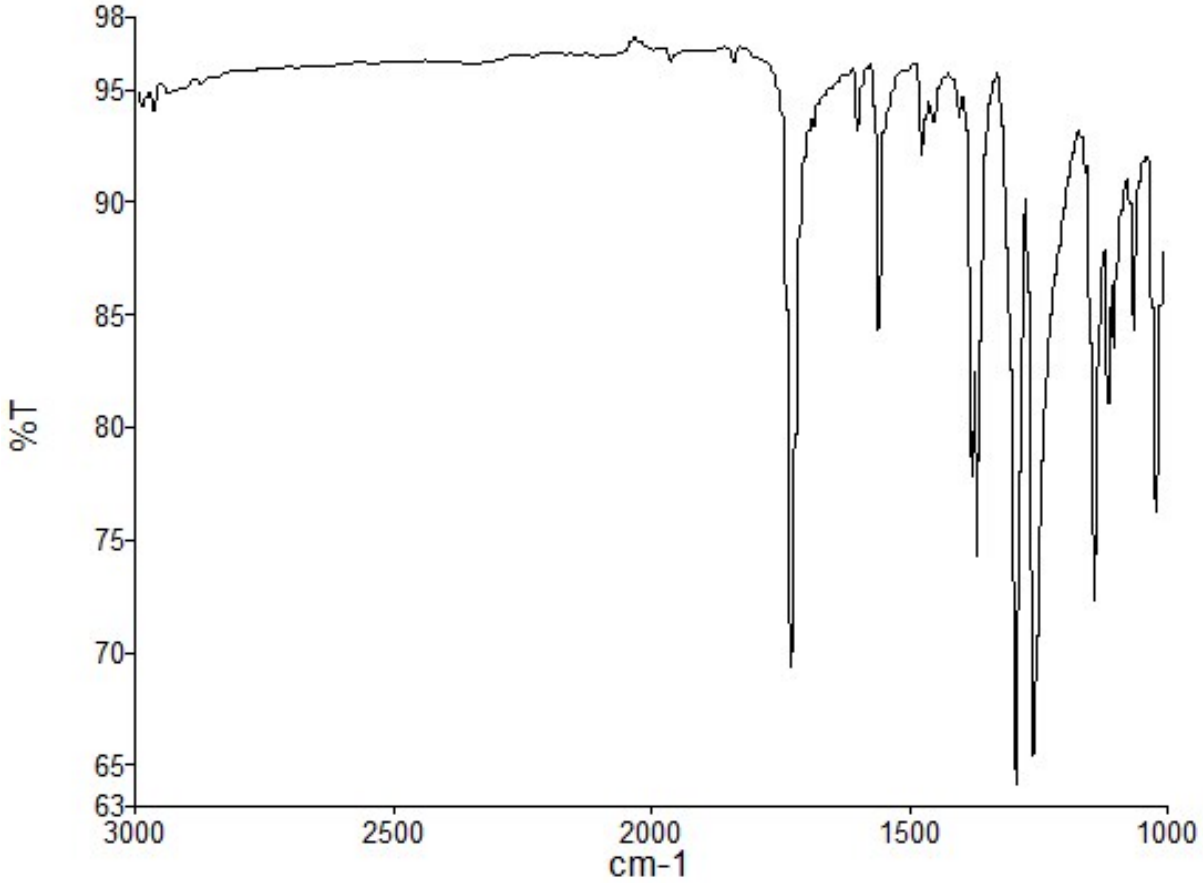


Figure S2. FTIR spectrum for 4,4'-diethanoate-2,2'-bpy (**deeb)**.

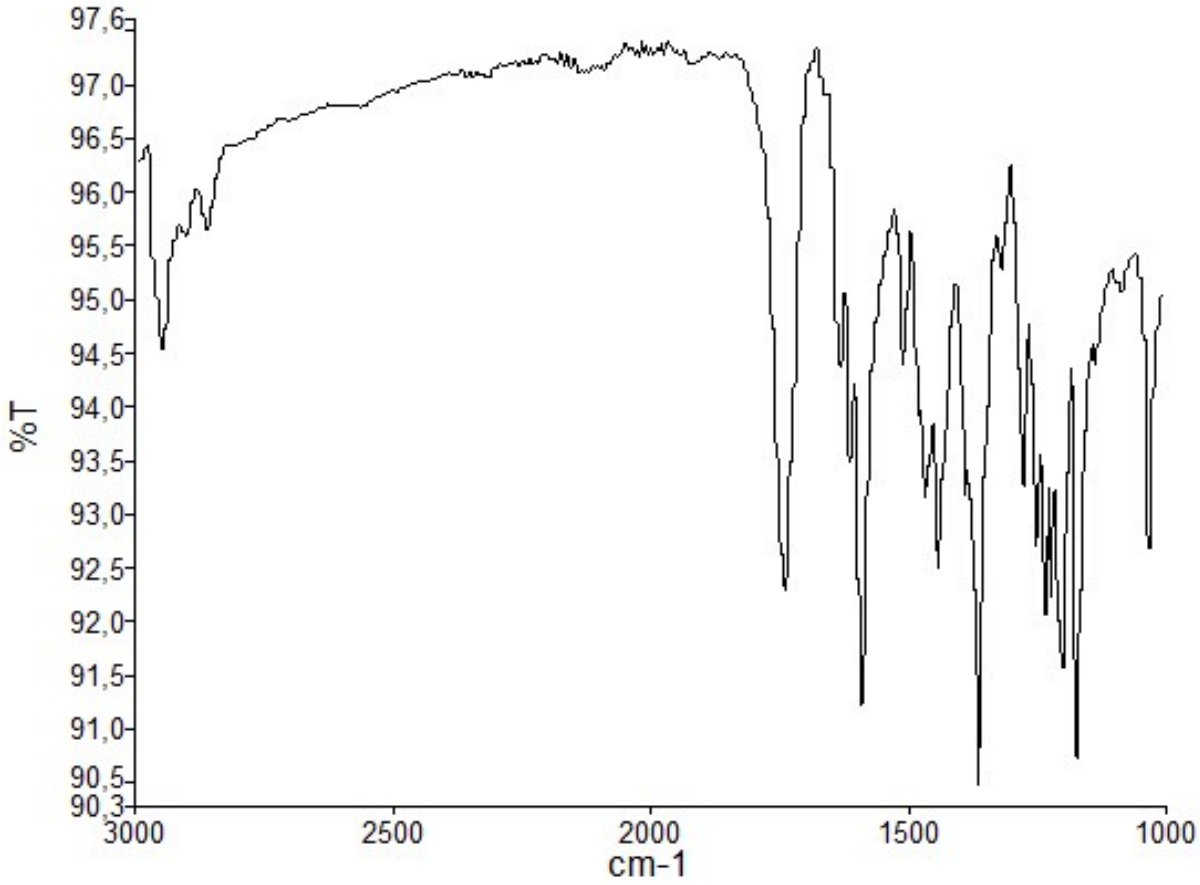


Figure S3. FTIR spectrum for (*E*)-2-{[(3-aminopyridin-4-yl)imino]-methyl}-4,6-di-tert-butyl-phenol (**L**).

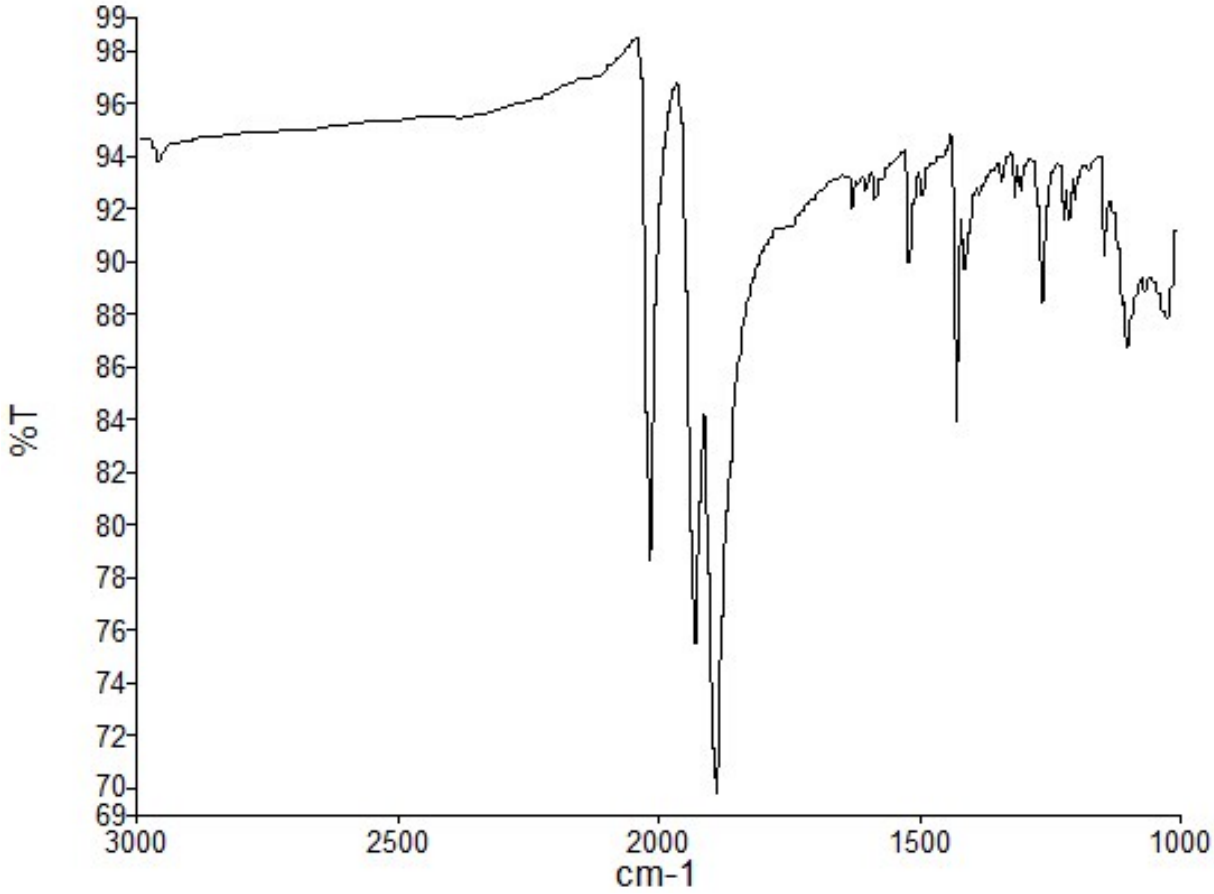


Figure S4. FTIR spectrum for **C1**.

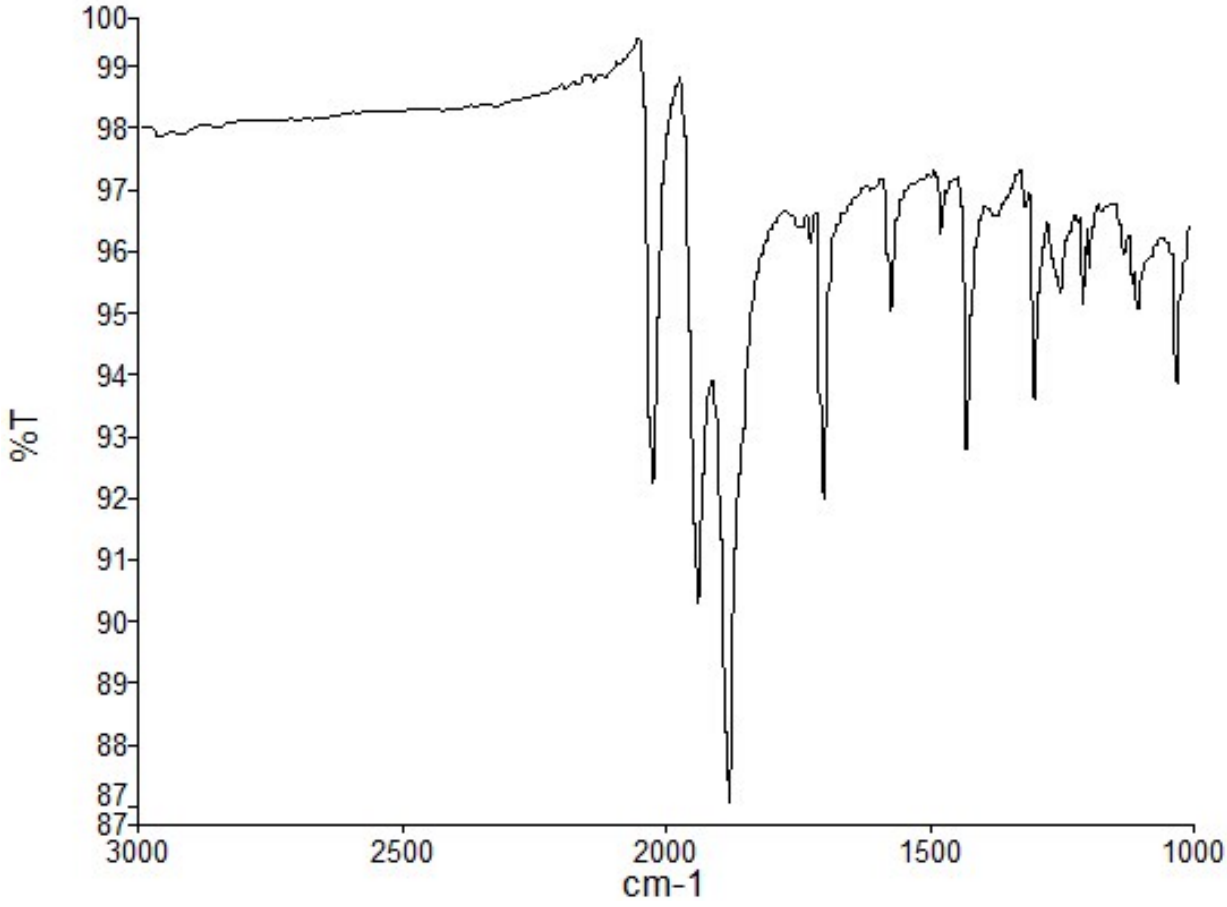


Figure S5. FTIR spectrum for **C2**.

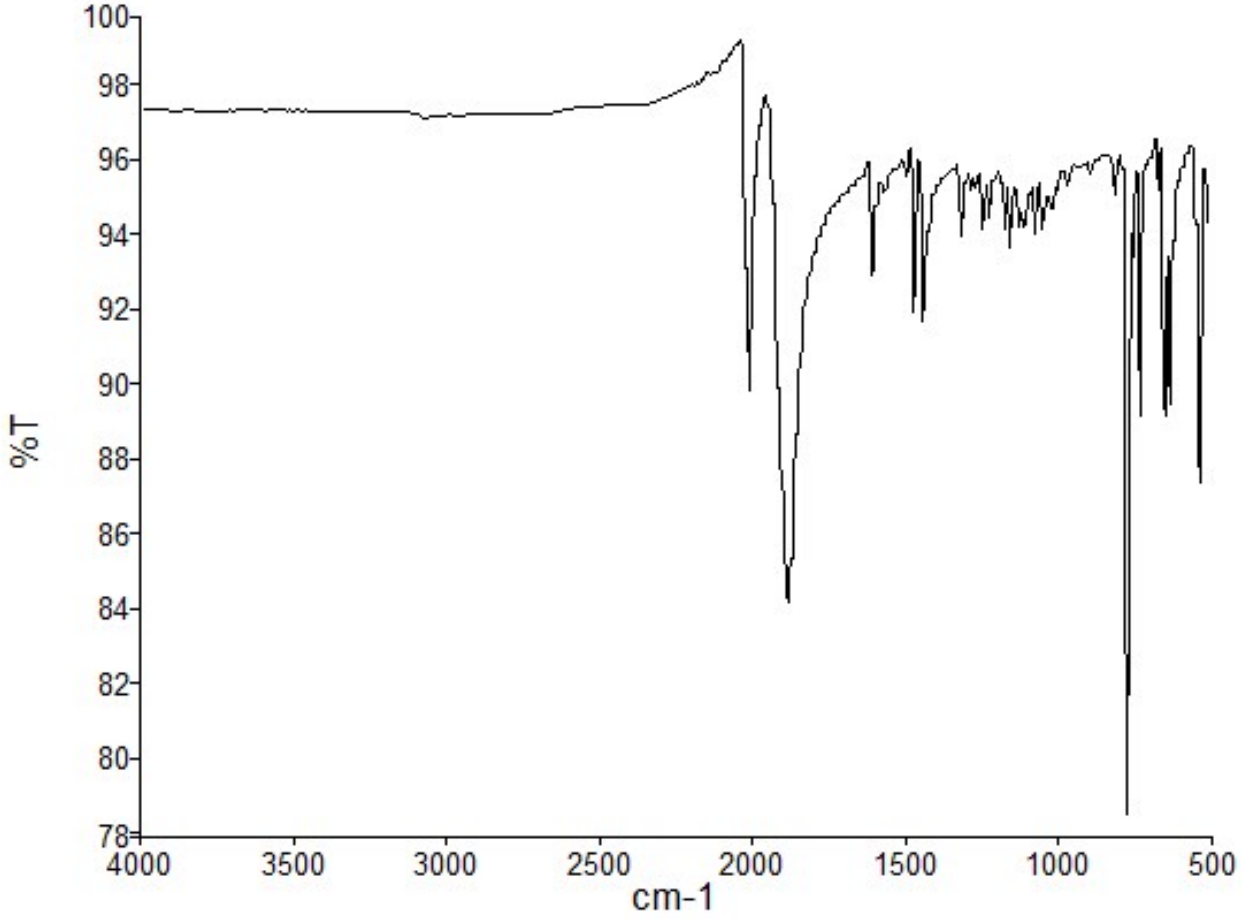


Figure S6. FTIR spectrum for **C3**.

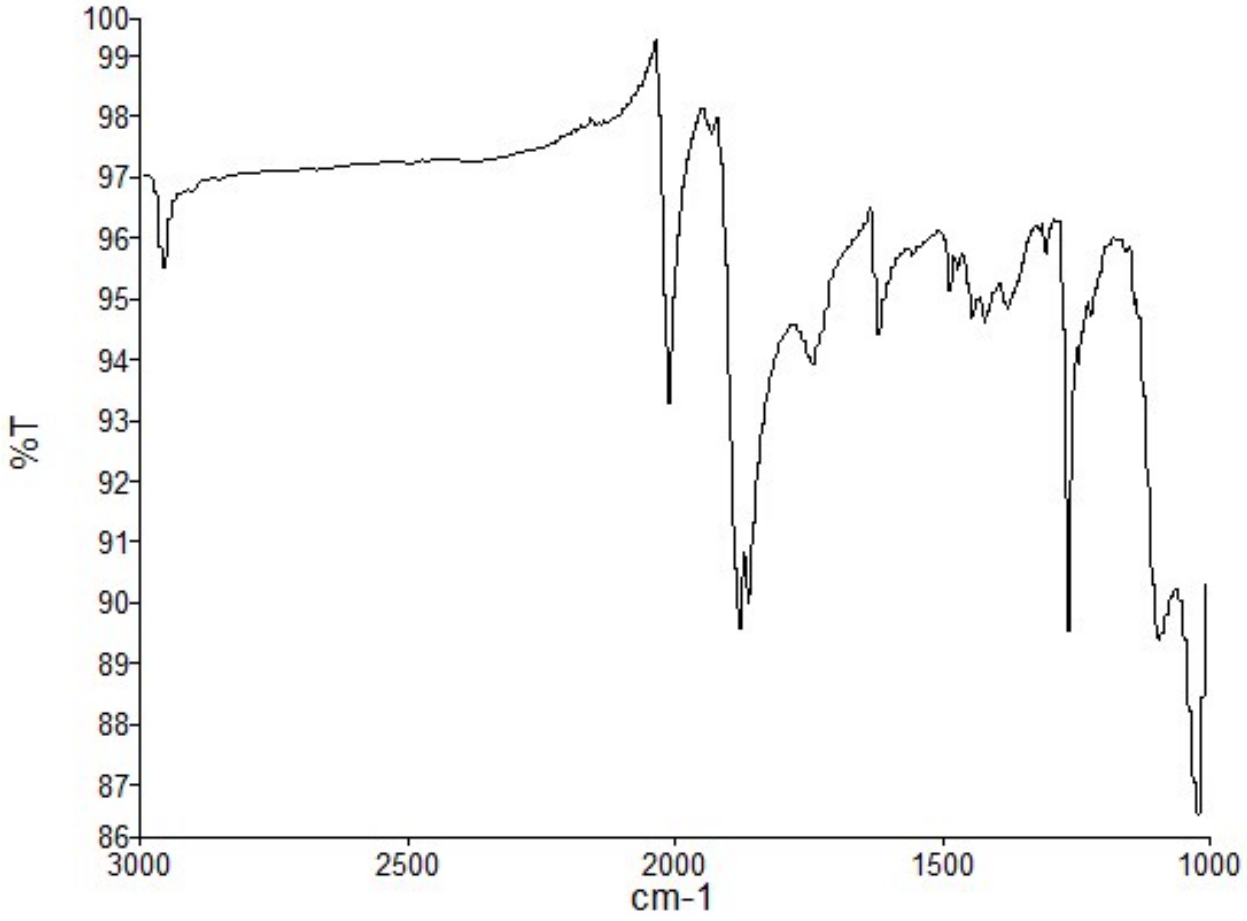


Figure S7. FTIR spectrum for **C4**.

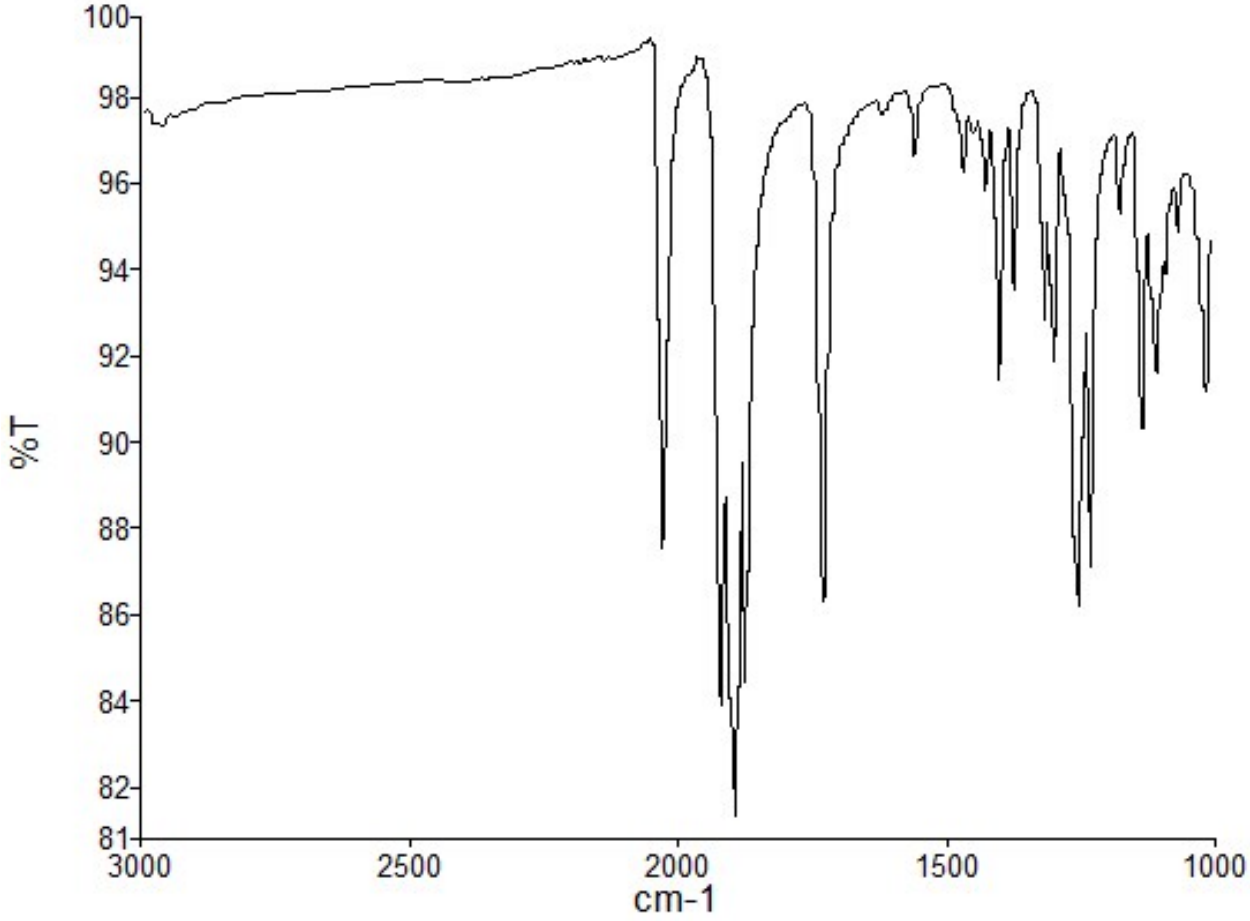


Figure S8. FTIR spectrum for **C5**.

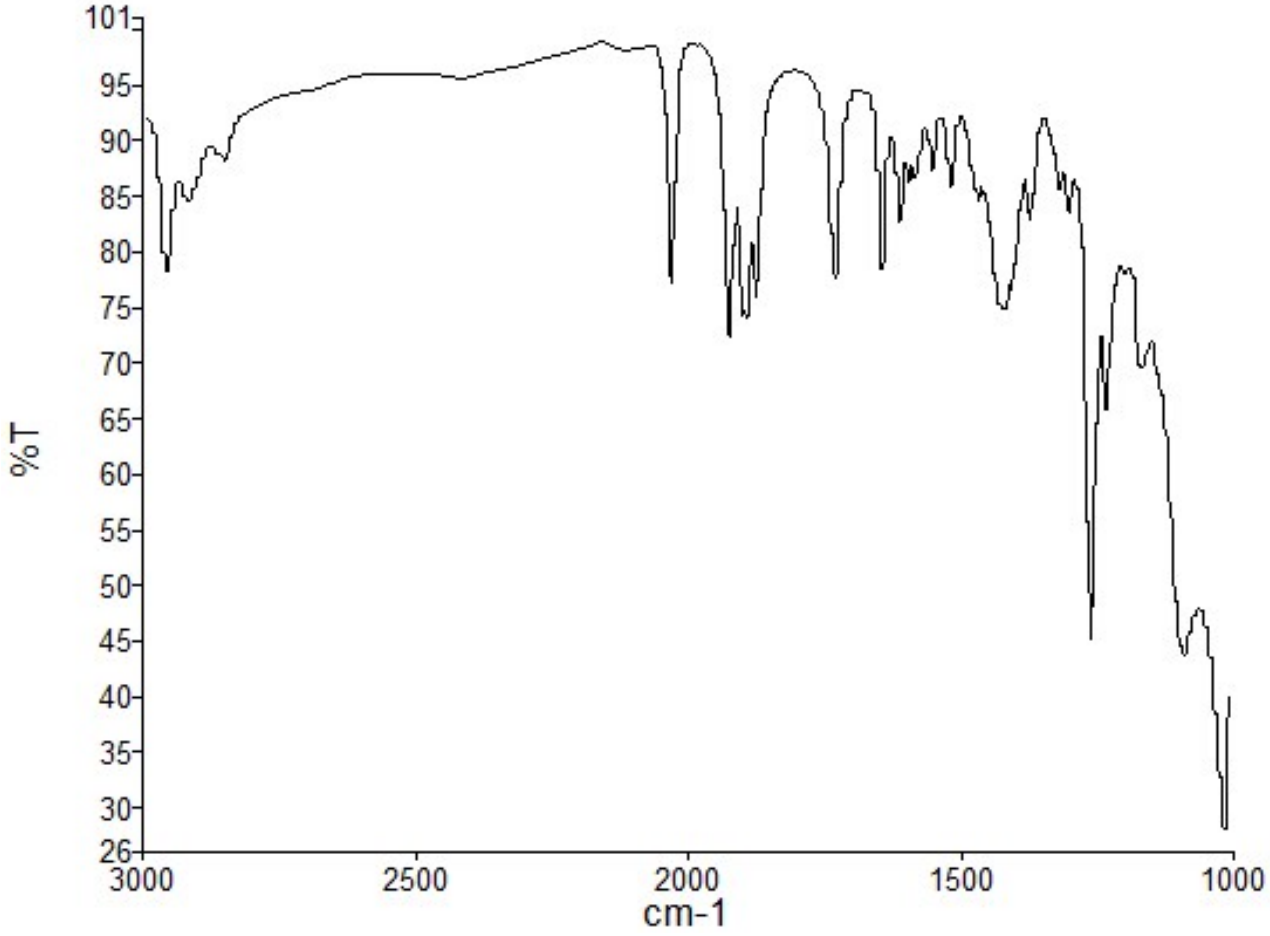


Figure S9. FTIR spectrum for **C6**.

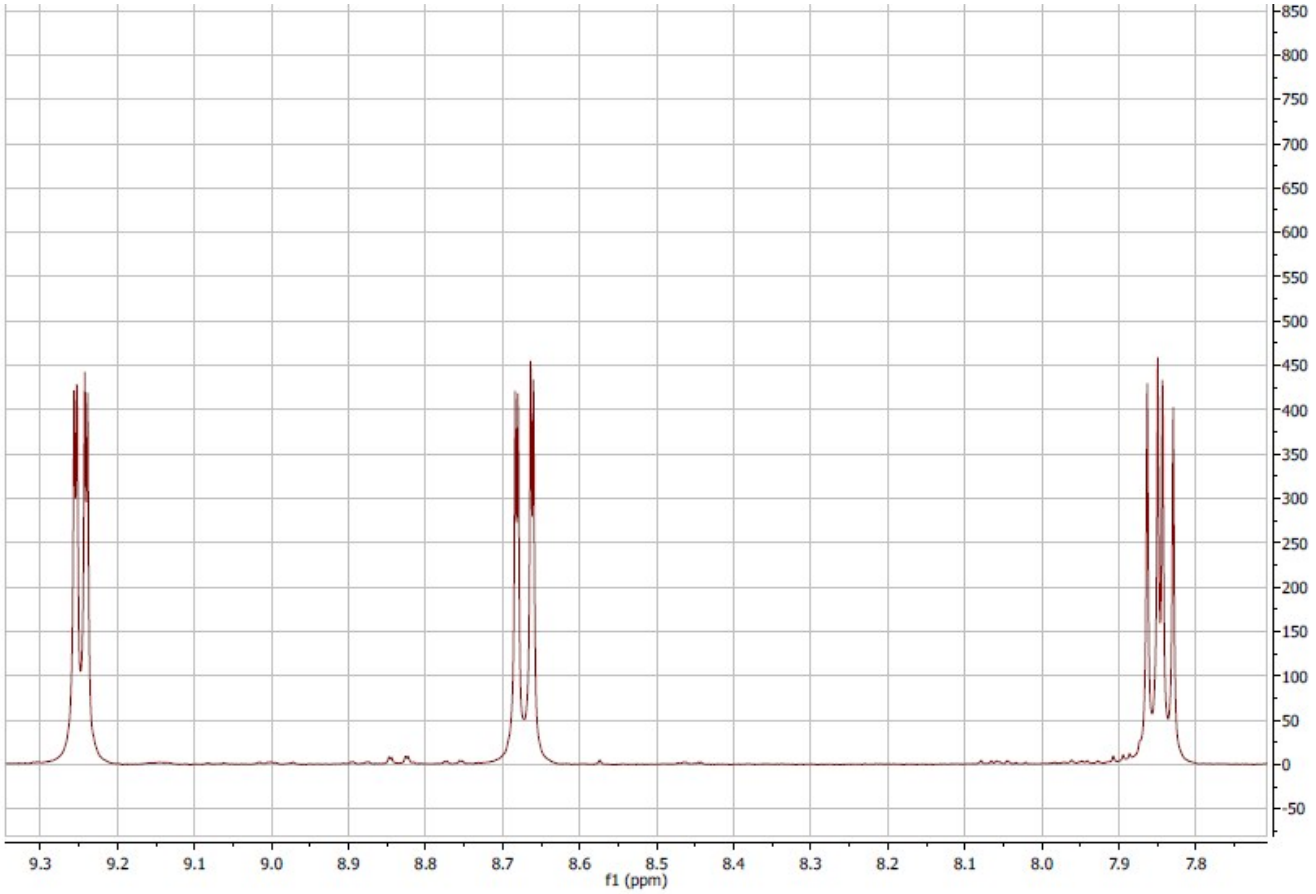


Figure S10. ^{1}H NMR spectrum of **C2** (CD_3CN)

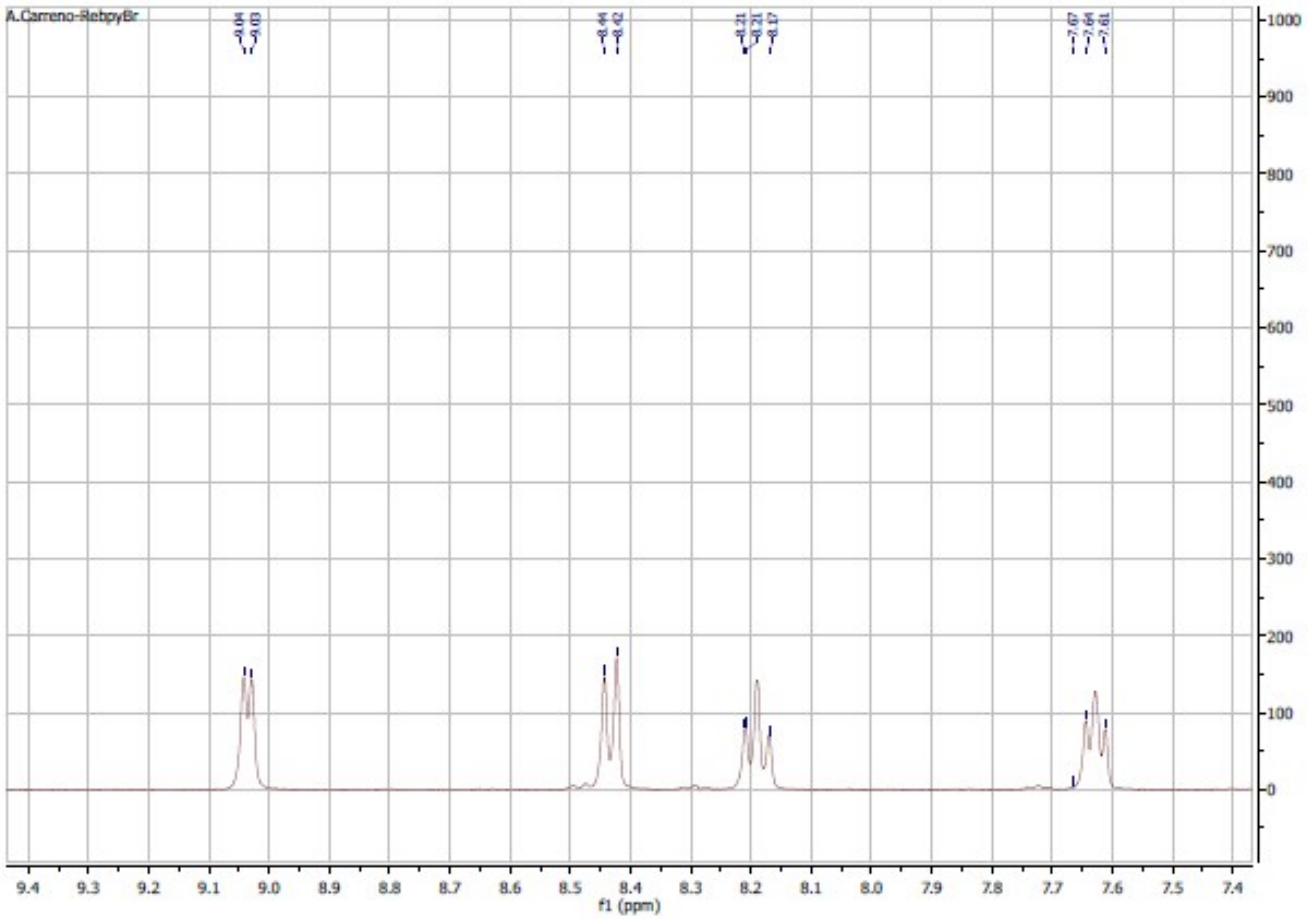


Figure S11. ^{1}H NMR spectrum of **C3** (CD_3CN)

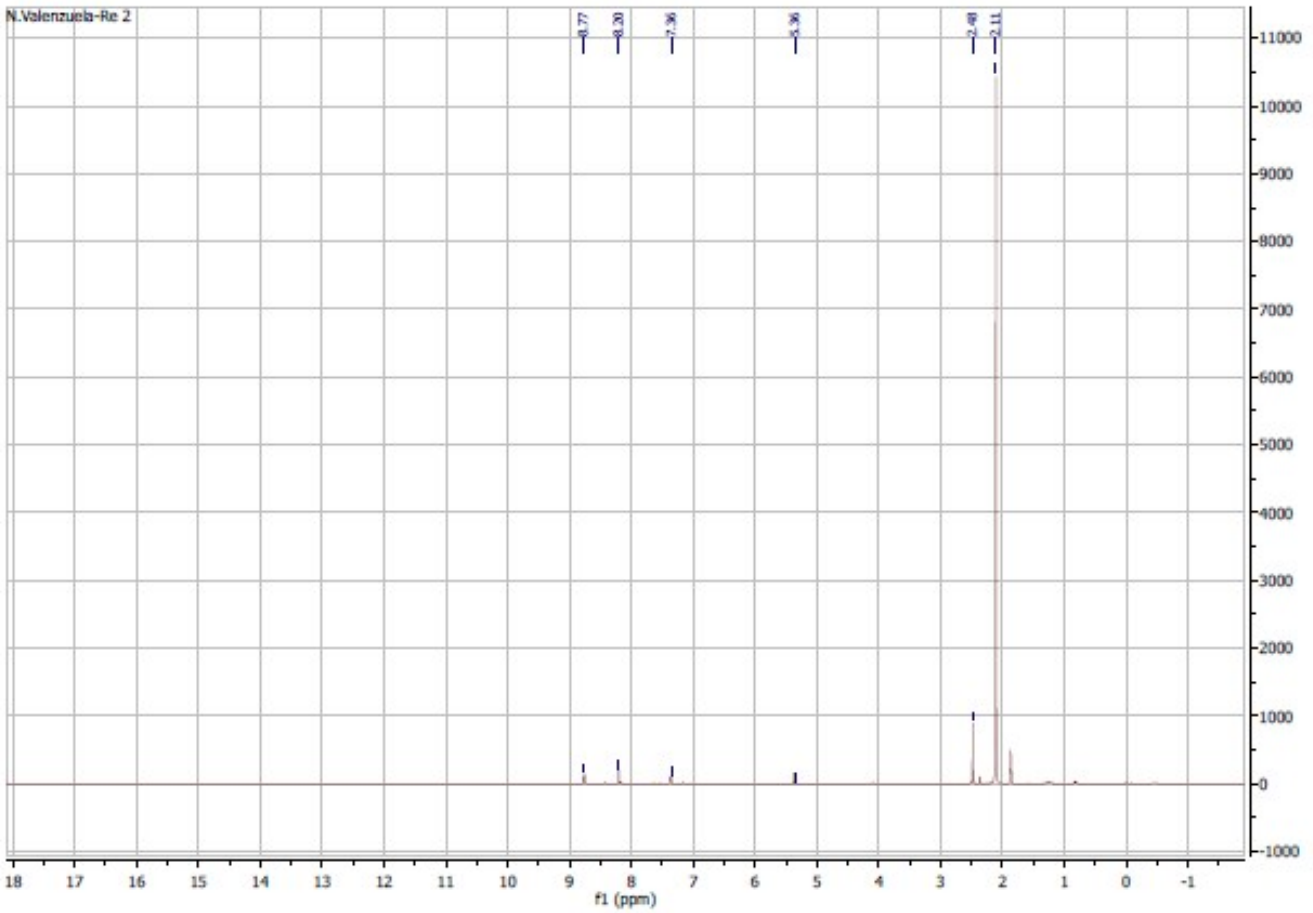


Figure S12. ^{1}H NMR spectrum of **C4** (CD_3CN)

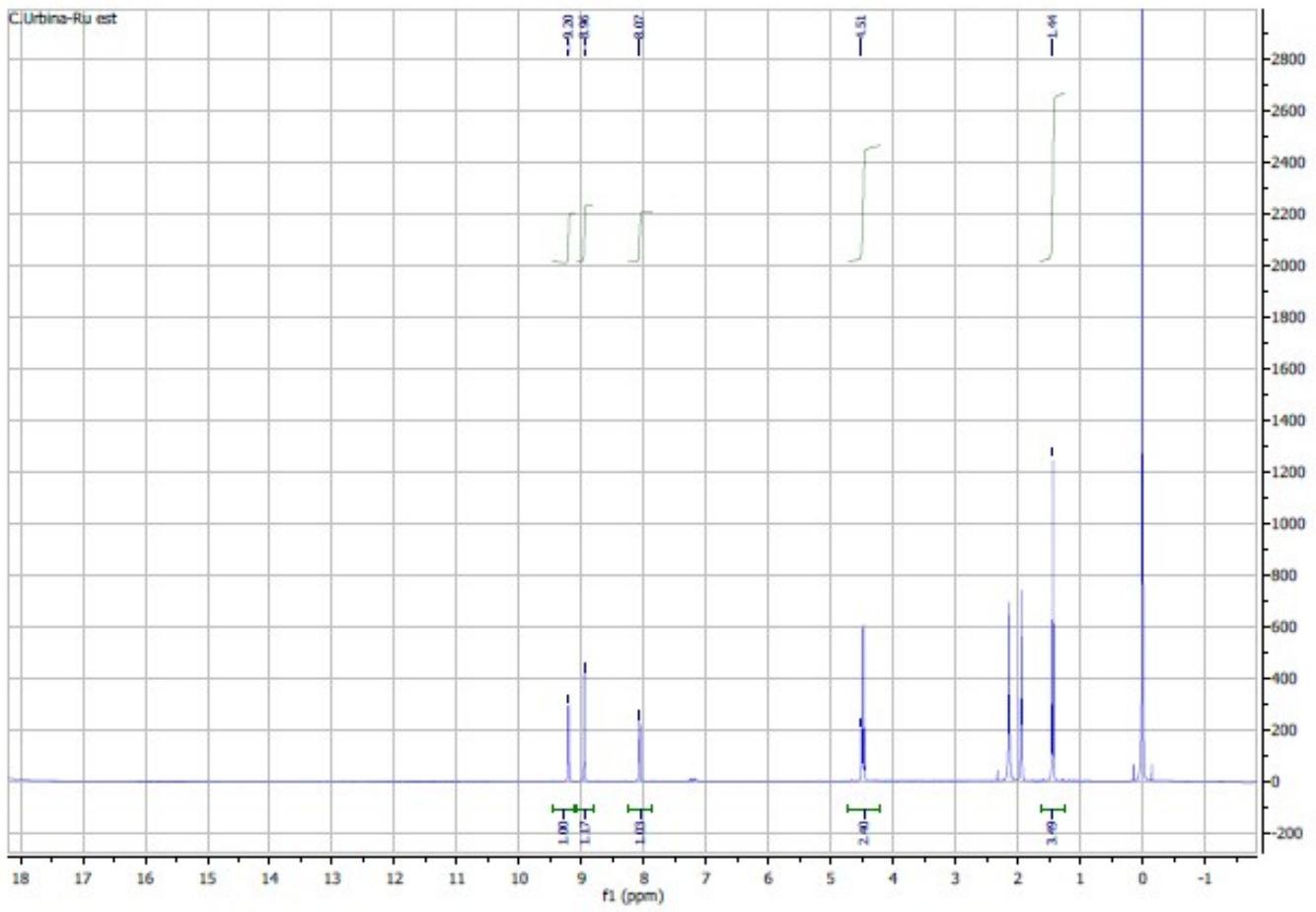


Figure S13. ^{1}H NMR spectrum of **C5** (CD_3CN)

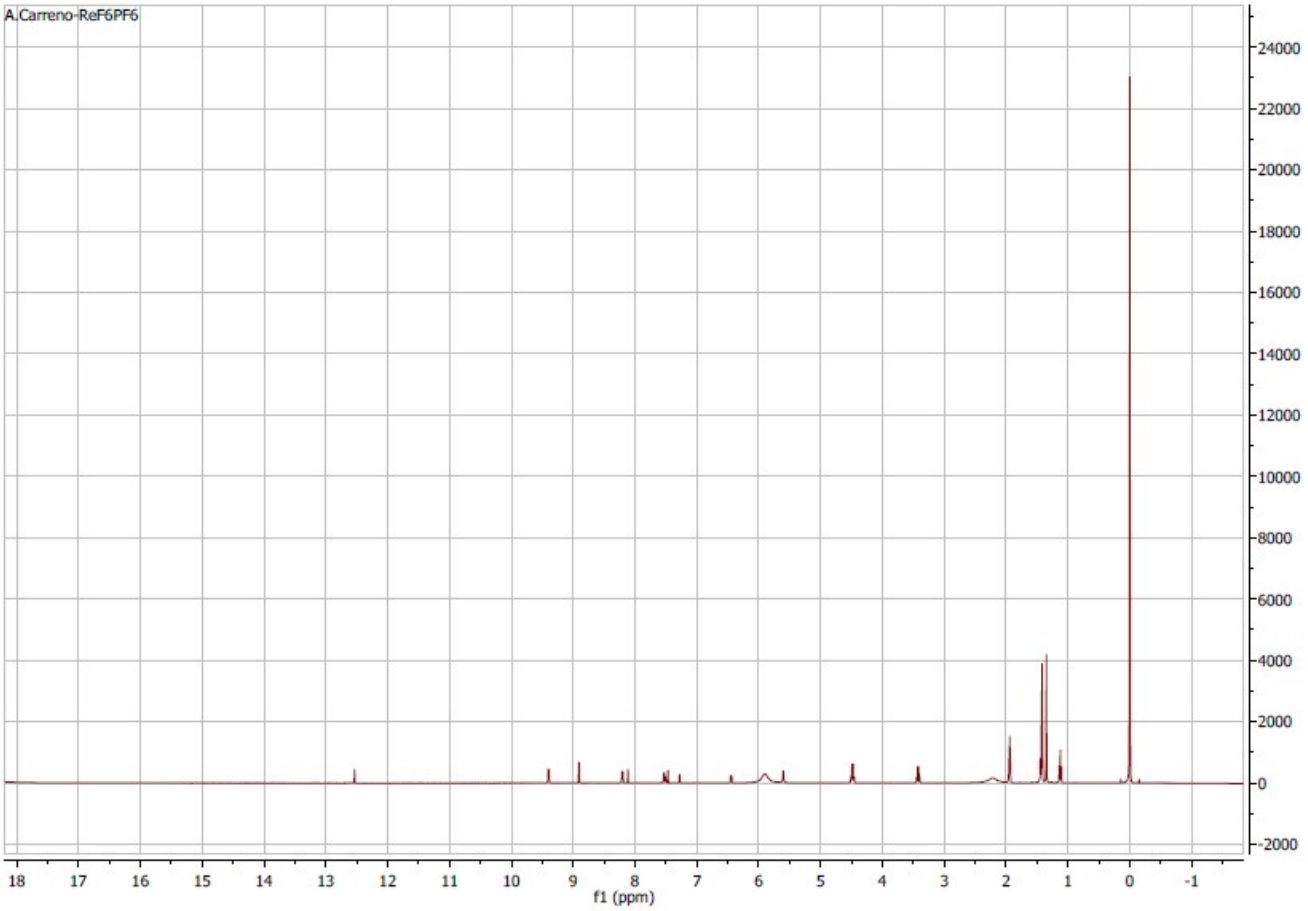


Figure S14. ^{1}H NMR spectrum of **C6** (CD_3CN)

S.3. Biological methods and Supplementary Results

S.3.1. Minimum inhibitory concentration (MIC): All the compounds were evaluated for their *in vitro* growth inhibitory activity against Gram-negative pathogen *Salmonella enterica* serovar Typhimurium ATCC14028s (*S. enterica*), and the clinical yeasts *Candida albicans* and *Cryptococcus* spp. obtained from the Hospital Clínico of the Universidad de Chile, Santiago, Chile. Minimum inhibitory concentration (MIC) was obtained by broth dilution. The MIC is defined as the lowest concentration of the tested compounds at which no growth of the strain was observed after incubation. *S. enterica* was previously grown in Luria-Bertani broth (Bacto peptone, 10 g/l; Bacto yeast extract, 5 g/l; NaCl, 5 g/l) at 37 °C with shaking to OD_{600} = 1.4 (stationary phase). Yeasts were previously cultured in Sabouraud agar (Bacto peptone, 10 g/L; glucose, 40 g/L; agar, 15 g/L; pH 5.6) at 30 °C. Further dilutions of microorganisms (bacteria and yeasts; 0.5 McFarland) were performed with Bacto Tryptic Soy broth (pancreatic digest casein 17.0 g/l, papaic digest of soybean 3.0 g/l, dextrose 2.5 g/l, sodium chloride 5.0 g/l, dipotassium phosphate 2.5 g/l). Stock solutions of the tested compounds were prepared in dimethyl sulfoxide (DMSO) for **C1**, **C2**, **C3**, **C4**, **C5**, **C6**, and **K1** (ketoconazole, control for yeasts); or in ethanol 95% for **Cam** (chloramphenicol, control for bacteria). The concentration range of the compounds tested was between 1.042 µg/ml and 133.33 µg/ml. The inoculated wells were then incubated at 37 °C for 24 h and 48 h (bacteria), or at 30 °C for 48 h and 72 h (yeasts). As control, DMSO or ethanol 95% without any tested compound, were included when necessary. Only when the inhibition effects of the tested compounds were distinguishable from DMSO alone (in the case of **C1**, **C2**, **C3**, **C4**, **C5**, **C6**, and **K1**), or from ethanol 95% alone (in the case of **Cam**), the compound was considered to exhibit antimicrobial activity. The MIC values of the tested compounds were obtained as µg/ml. All the experiments were performed in triplicate. Results are shown in Table S1.

S.3.2. MTT assay performed in HeLa cells: Cells were cultured in Dulbecco's Modified Eagle's Medium (DMEM) containing 10% fetal bovine serum (FBS), 2 mM L-glutamine, 100 units/mL penicillin and 100 μg/mL streptomycin. Cells were maintained in 75 cm^2 flasks in a 5% CO2-humidified atmosphere at 37 °C. Passage takes place every 2–3 days. All cell culture ingredients were purchased from Sigma-Aldrich. Toxicity of the respective complexes was determined using the 3-(4,5-dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide (MTT) cell viability assay after 24 h of incubation with **C1**, **C2**, **C3**, **C4**, **C5**, or **C6**. MTT is a yellow compound that, when reduced by functioning mitochondria, produces purple formazan crystals that can be measured spectrophotometrically. For this purpose, MTT (Sigma-Aldrich) was dissolved in phosphate buffered saline (PBS) to a concentration of 5 mg/mL and further diluted in culture medium (1:11). Cells were incubated with this MTT-solution for 3 h under normal culture conditions. Afterwards 155 μL of the solution were rejected and 90 μL of DMSO were added. To completely dissolve the formazan salts plates were incubated for 10 min on a shaker and afterwards quantified by measuring the absorbance at 535 nm with a ELISA microplate reader. Cell viability was calculated as percentage of surviving cells compared to untreated control cells. As shown in **Figure S16**, toxicity of complexes tested is undistinguishable from the vehicle (i.e. DMSO) alone.

Table S1. Minimal inhibition concentration (µg/ml) of tested compounds determined after 48 and 72 h for yeasts, and after 24 and 48 h for bacteria.

	Yeasts				**Bacteria**	
	Candida albicans		***Cryptococcus* spp.**		***S. enterica*[a]**	
	48 h	**72 h**	**48 h**	**72 h**	**24 h**	**48 h**
C1	-	-	-	-	-	-
C2	-	-	-	-	-	-
C3	-	-	-	-	-	-
C4	-	-	-	-	-	-
C4	-	-	-	-	-	-
C5	-	-	-	-	-	-
C6	-	-	-	-	-	-
K1[b]	-[d]	-[d]	<1.042	<1.042	ND	ND
Cam[c]	ND	ND	ND	ND	3.125 ± 0.156	3.125 ± 0.156

- : The inhibition was indistinguishable from the vehicle alone (i.e. DMSO for **C1** to **C6**, and **K1**; Ethanol for **Cam**)

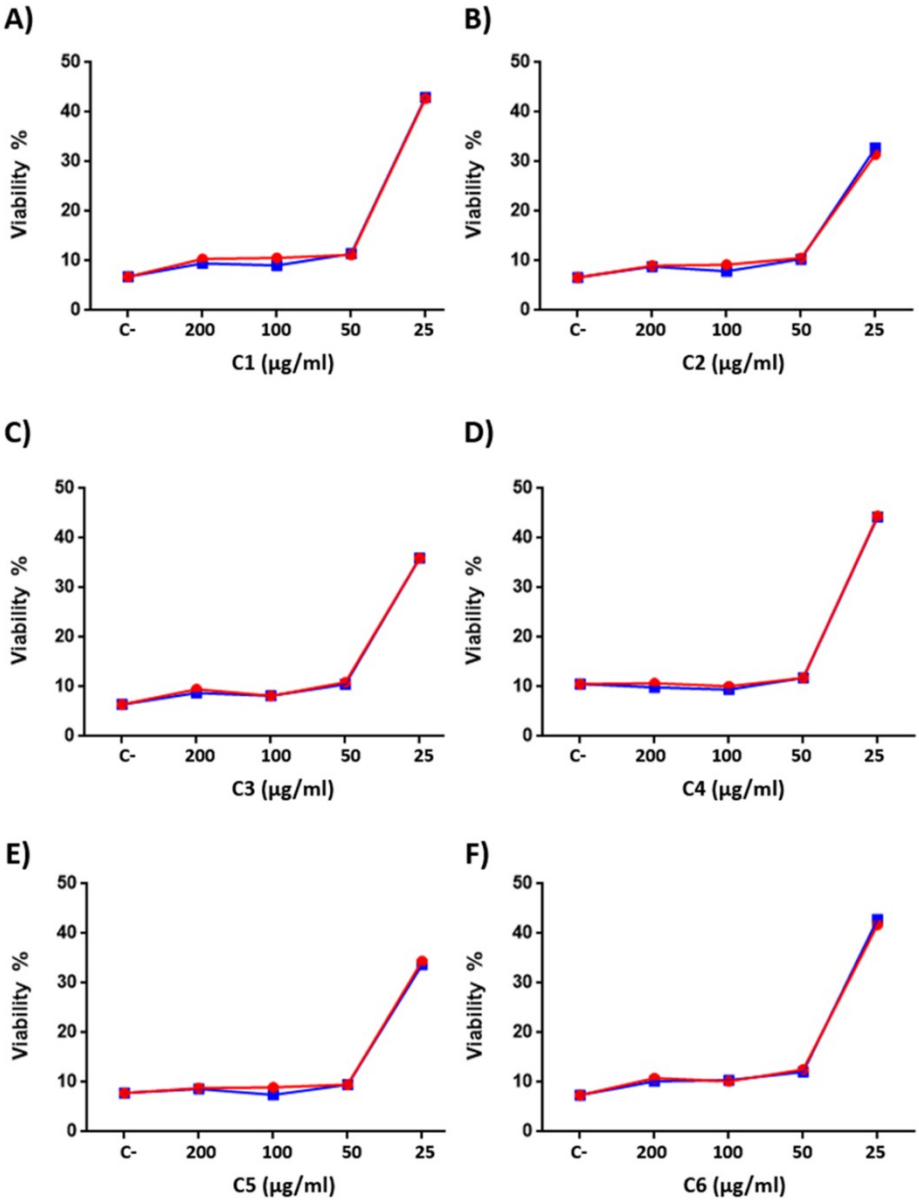
ND: Not determined

[a]: *Salmonella enterica* serovar Typhimurium ATCC14028s

[b]: Ketoconazole (antifungal compound)

[c]: Chloramphenicol (antibacterial/antibiotic)

[d]: The *Candida albicans* strain tested is resistant to ketoconazole



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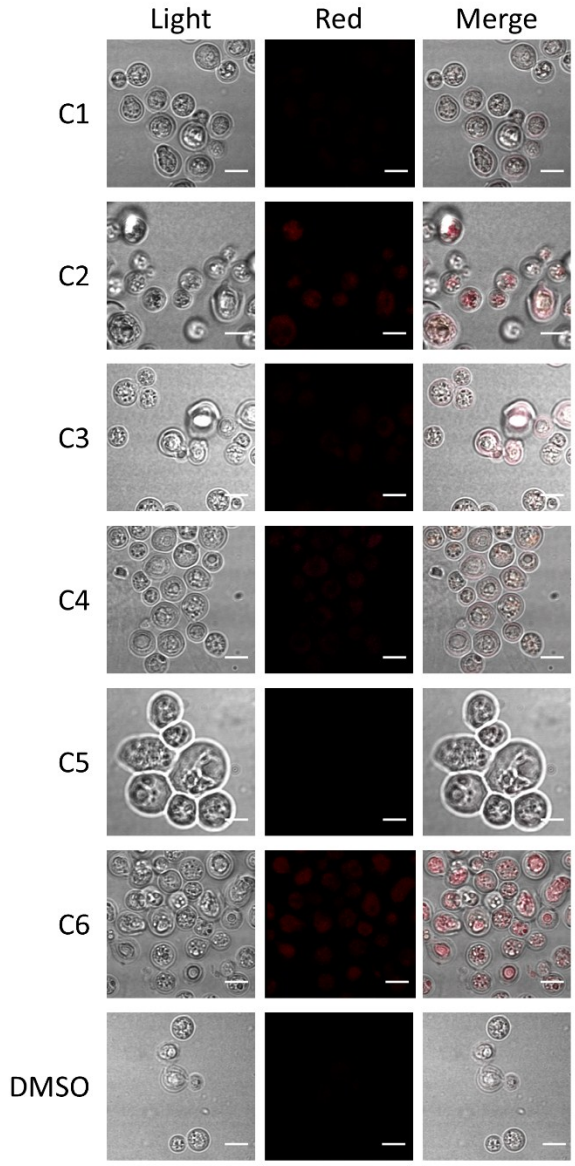
240 **Figure S15. MTT Assay in HeLa cells.** Cells were incubated 24 h with the complexes prior
241 to measuring cell viability. Red line: Rhenium complex **C1** (A), **C2** (B), **C3** (C), **C4** (D), **C5**
242 (E), or **C6** (F) (200 µg/ml + DMSO 50% v/v, 100 µg/ml + DMSO 25% v/v, 50 µg/ml +
243 DMSO 12.5% v/v, or 25 µg/ml + DMSO 6.3% v/v); Blue line: Vehicle alone (i.e. DMSO)
244 (50% v/v, 25% v/v, 12.5% v/v, or 6.3% v/v, respectively). Medium alone was used to set
245 100% viability. C- corresponded to DMSO 100% v/v. The figure shows a representative
246 experiment.



Cryptococcus spp.

Figure S16. Fluorescence confocal microscopy images showing *Cryptococcus spp.* (yeasts) under confocal microscopy. The "Red channel" corresponded to excitation of 405 nm and emission collected in a range of 555 to 625 nm. In all the cases, microorganisms were observed fresh, immobilized with 1% agarose, using a 100X objective. White bars represent 5 µm. DMSO alone was used to set the detection threshold.