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Synthesis and *in vitro* antifungal activity of selenium-containing chitin derivatives

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In this study, we used crab shell chitin with a viscosity-average molecular weight (MW) of 3.5×10^4, 7.1×10^4, 17.2×10^4 and a degree of acetylation of 100% (Sigma Aldrich, USA).

3-(Chloromethyl)[1,2,4]selenadiazolo[4,5-*a*]pyridin-4-ium bromide was prepared as described [S1]. Other chemicals, solvents and materials were obtained from commercial sources and were used as received.

The ^{1}H NMR spectra were recorded on a Bruker Avance II spectrometer (Germany) at operating frequencies of 400 MHz and 100 MHz, respectively.

Antifungal activities were investigated as described elsewhere drug [S2,S3]. Briefly, a homogeneous mixture of glucose–peptone–agar (40:10:15) was sterilized by autoclaving at 121 ºC and 15 lb cm^{-2} for 20 min. The sterilized solution (25 ml) was poured in each sterilized Petri dish in laminar flow and left for 20 min to form the solidified Sabouraud dextrose agar plate. These plates were inverted and kept at 30 ºC in incubator to remove the moisture and to check for any contamination. Fungal strain was grown in 5 ml Sabouraud dextrose broth (glucose/peptone, 40:10) for 3–4 days to achieve 10^5 CFU/ml cells. The fungal culture (0.1 ml) was spread out uniformly on the Sabouraud dextrose agar plates by sterilized triangular folded glass rod. Plates were left for 5–10 min so that culture is properly adsorbed on the surface of Sabouraud dextrose agar plates. Now small wells of size (4 mm × 2 mm) were cut into the plates with the help of well cutter and bottom of the wells were sealed with 0.8% soft agar to prevent the flow of test sample at the bottom of the well. The test solutions 50, 100, 200, 400 μl of stock solution (10 mg ml^{-1}) were loaded into the wells of the plates. DMF was loaded as control. The plates were kept for incubation at 30 ºC for 3–4 days and then the plates were examined for the formation of zone of inhibition.

Toxicity was studied as described elsewhere [S4,S5].

Synthesis of selenium-containing derivatives of chitin

Chitin samples (0.5 g) were dispersed in water (10 ml), then 3-(chloromethyl)-[1,2,4]selenadiazolo[4,5-*a*]pyridin-4-ium bromide (2.3, 3.5 or 6.1 g, 3, 5 or 8 equiv., respectively) were added, and the reaction mixtures were sonicated at 90 kHz, 250 W for 25 min at 25 °C. The formed polymers were precipitated by addition of acetone (25 ml). The precipitated polymers were dissolved in water, dialyzed against distilled water and freeze-dried.

Degree of substitution (or general degree of N- and O-substitution) was calculated according to the formula DS = $DS_{N,O}$ = (*I*(***2***,***3***,***4***,***5***,***6***,***7***) – 6)/2, while *I*(***1***) + *I*(***1'***) = 1. The degree of *N*-substitution was calculated as DS_N = *I*(***1'***), where *I*(***1***) + *I*(***1'***) = 1 [S6,S7]. Parameters *I* stand for integral intensities of the corresponding signals (see also Figure 1 of the main text).

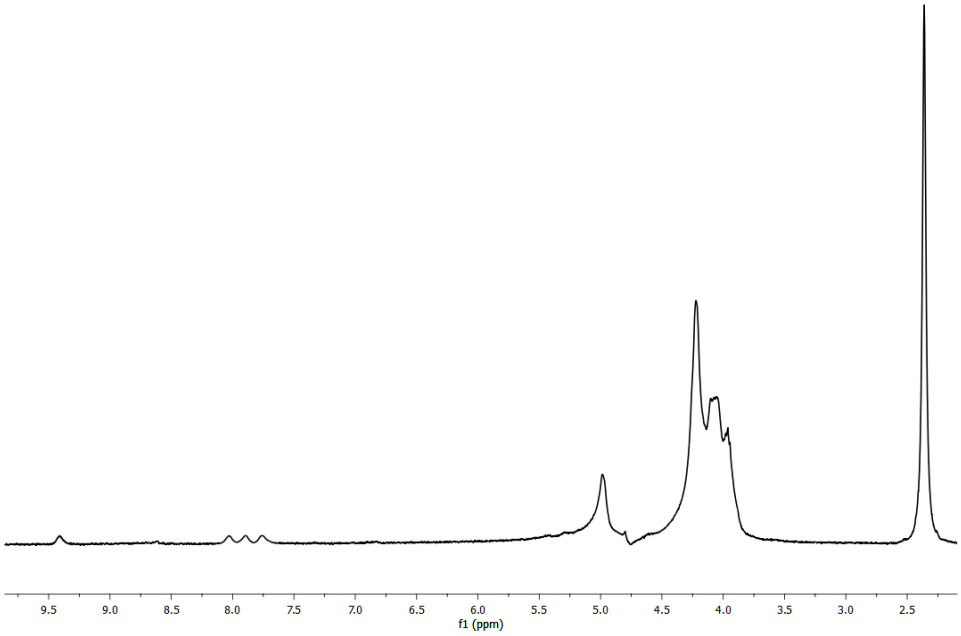

Figure S1. ^{1}H NMR spectrum of the selenium congaing derivative **3**.

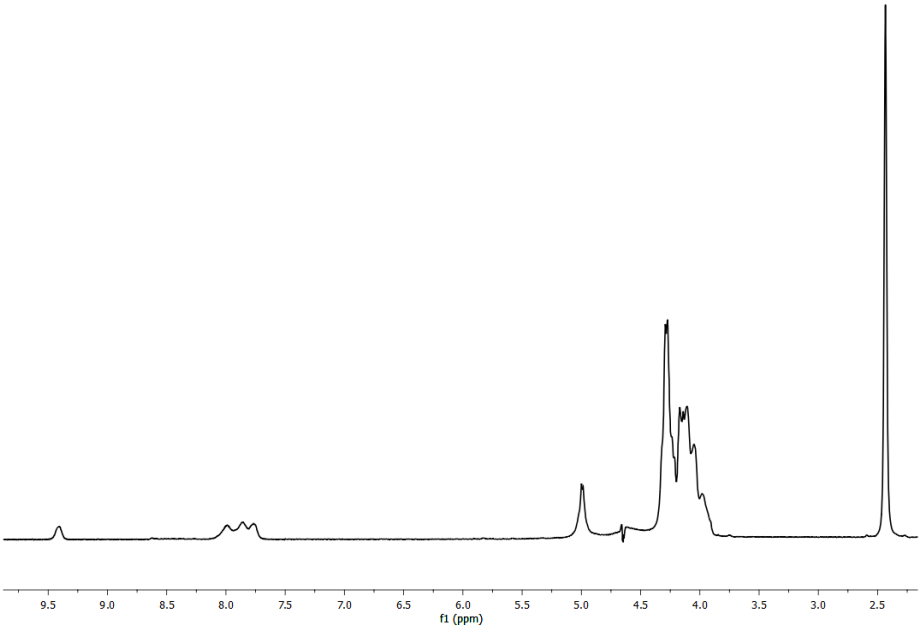

Figure 2 ^{1}H NMR spectrum of the selenium congaing derivative **3'**.

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