Supplementary Materials

New azolyl-derivatives as multitargeting agents against breast cancer and fungal infections: synthesis, biological evaluation and docking study

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Figure S1. The binding interactions (panel A) and binding energy (panel B) of compound 4-androstene-3-17-dione with the hCYP19A1 active site during the 50 ns MD simulation. Hydrophobic amino acids are indicated in green and cationic amino acids are indicated in purple.
Figure S2. The binding interactions (panel A) and binding energy (panel B) of compound ethylisothiourea with the iNOS active site during the 50 ns MD simulation. Hydrophobic amino acids are indicated in green and anionic amino acids are indicated in red.
**Figure S3.** The binding interactions (panel A) and binding energy (panel B) of compound *itraconazole* with the CaCYP51 active site during the 50 ns MD simulation. Hydrophobic amino acids are indicated in green.

**Figure S4.** Compound 5 chemical stability in NaOH (pH=9): superimposition of selected chromatograms recorded after 5' (black), 1 h (blue) and 2 h (green) incubation time at 37° C.
Compound 7
Compound 7
Compound 8
Compound 14
Compound 15
Compound 17

Diagram showing various chemical shifts and intensities in the range of 150-2 ppm.
Compound 19
Compound 20
