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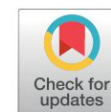
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Synthesis, biological evaluation and molecular docking of novel pyrazole derivatives as potent carbonic anhydrase and acetylcholinesterase inhibitors



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ABSTRACT

A series of substituted pyrazole compounds (**1–8** and **9a, b**) were synthesized and their structure was characterized by IR, NMR, and Mass analysis. These obtained novel pyrazole derivatives (**1–8** and **9a, b**) were emerged as effective inhibitors of the cytosolic carbonic anhydrase I and II isoforms (hCA I and II) and acetylcholinesterase (AChE) enzymes with K_i values in the range of 1.03 ± 0.23 – $22.65 \pm 5.36 \mu\text{M}$ for hCA I, 1.82 ± 0.30 – $27.94 \pm 4.74 \mu\text{M}$ for hCA II, and 48.94 ± 9.63 – $116.05 \pm 14.95 \mu\text{M}$ for AChE, respectively. Docking studies were performed for the most active compounds, **2** and **5**, and binding mode between the compounds and the receptors were determined.