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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 ± 5.36 µM for hCA I, 1.82 ± 0.30–27.94 ± 4.74 µM for hCA II, and 48.94 ± 9.63–116.05 ± 14.95 µM 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.