Design, characterization and quantum chemical computations of a novel series of pyrazoles derivatives with potential anti-proinflammatory response

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The synthesis and characterization of the full family of 11 pyrazoles were performed by means of UV?Vis, FTIR, 1H NMR, 13C NMR, two-dimensional NMR experiments and DFT simulations. As pyrazoles are known for showing diverse biological actions, they were also tested in the NCI-60 cancer cell line panel, showing moderate to good activity against different cell lines. Furthermore, the anti-proinflammatory activity test of a set of pyrazoles of the form (E)-4-((4-bromophenyl)diazenyl)-3,5-dimethyl-1-R-phenyl-1H-pyrazole was performed, this is based on the study of the blockage of the increase in intracellular [Ca2+] observed in response to platelet-activating factor (PAF) treatment of four pyrazoles (i.e. 6, 8, 9 and 10), which successfully displayed [Ca2+] channel inhibition. Therefore, the obtained intracellular [Ca2+] signal results indicate that the pyrazole family characterized in this study, in particular compounds 6 and 10, are potent blockers of the PAF-initiated Ca2+ signaling that mediates the hyperpermeability typically observed during the development of inflammation.

Anti-proinflammatory

DFT

NCI-60

Platelet-activating factor

Pyrazoles

Cell culture

Design for testability

Nuclear magnetic resonance spectroscopy

Phospholipids

Biological actions

Cancer cell lines

Platelet-activating factors

Proinflammatory

Proinflammatory response

Quantum chemical computations

Synthesis and characterizations

Two-dimensional NMR

Quantum chemistry