

(E)-2-cyano-3-(indol-3-yl)-N-phenylacrylamide, a Hybrid Compound Derived from Indomethacin and Paracetamol: Design, Synthesis and Evaluation of Anti-inflammatory Potential

Pablo Silva, Maria de Almeida, Jamire Silva, Sonaly Albino, Renan Espirito-Santo, Maria Lima, Cristiane Villarreal, Ricardo Moura, Vanda Santos.

Supplementary data

Supplementary data captions

Figure S1 FT-IR spectrum of ICMD-01

Figure S2 ^1H NMR spectrum of ICMD-01

Figure S3 ^{13}C NMR spectrum of ICMD-01

Figure S4 HRMS m/z [$\text{M}^+ + \text{Na}$] of ICMD-01

Figure S5 3D crystallographic pose of co-crystallized ligand indomethacin (yellow) and redocked ligand (gray) on binding site of cyclooxygenase-2 (4COX)

Figure S1. FT-IR spectrum of ICMD-01

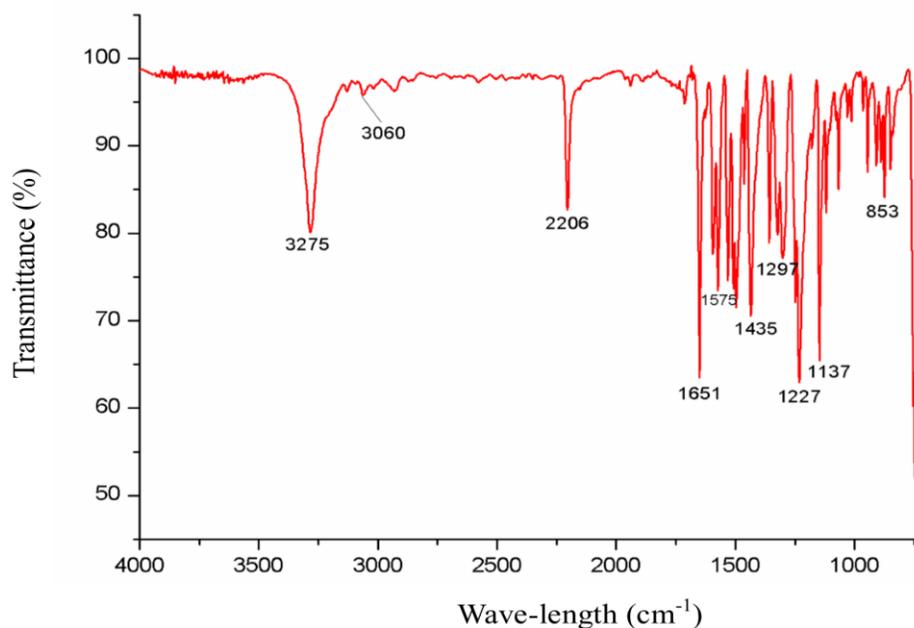


Figure S2. ¹H NMR spectrum of ICMD-01

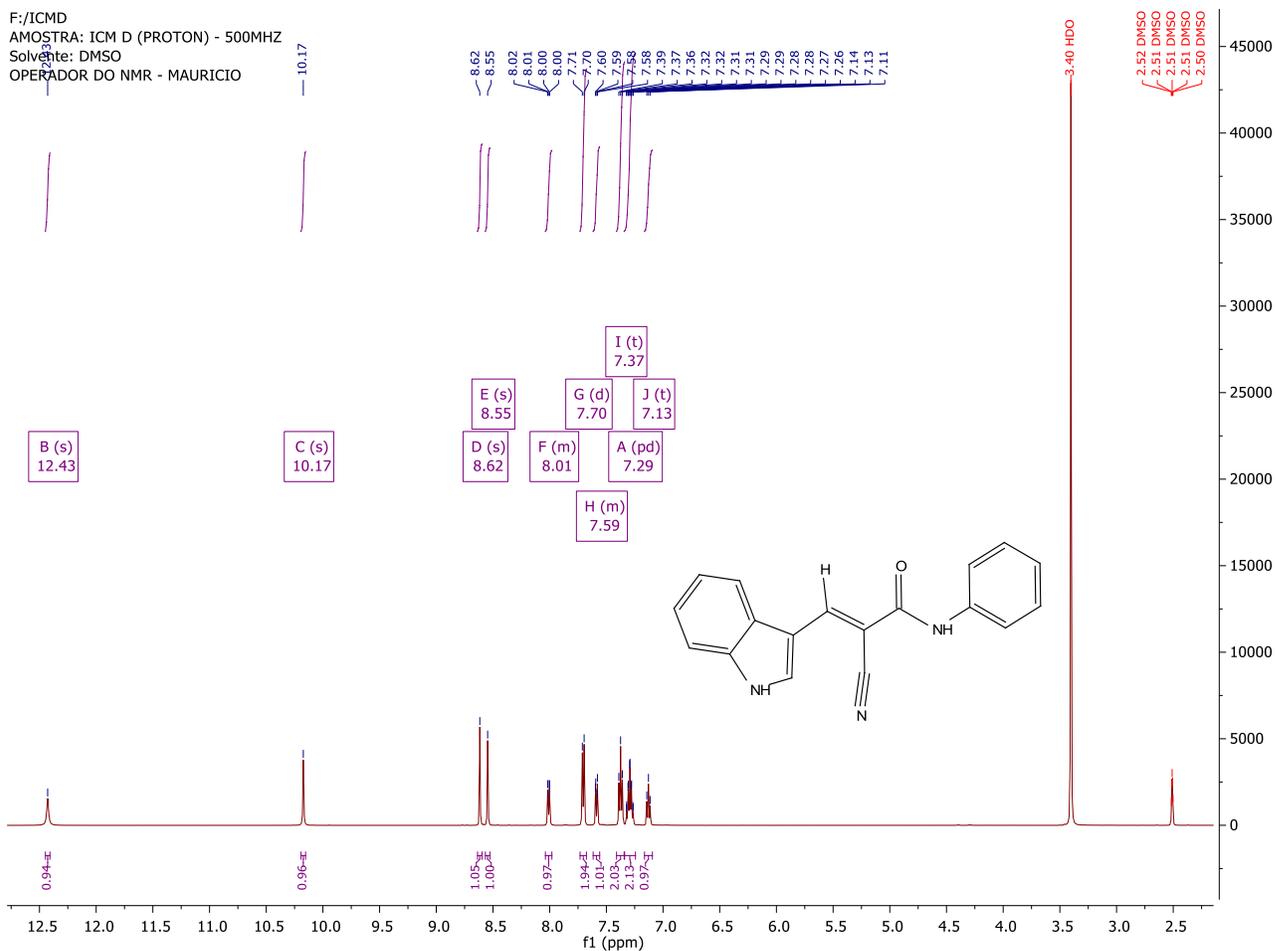


Figure S3. ¹³C NMR spectrum of ICMD-01

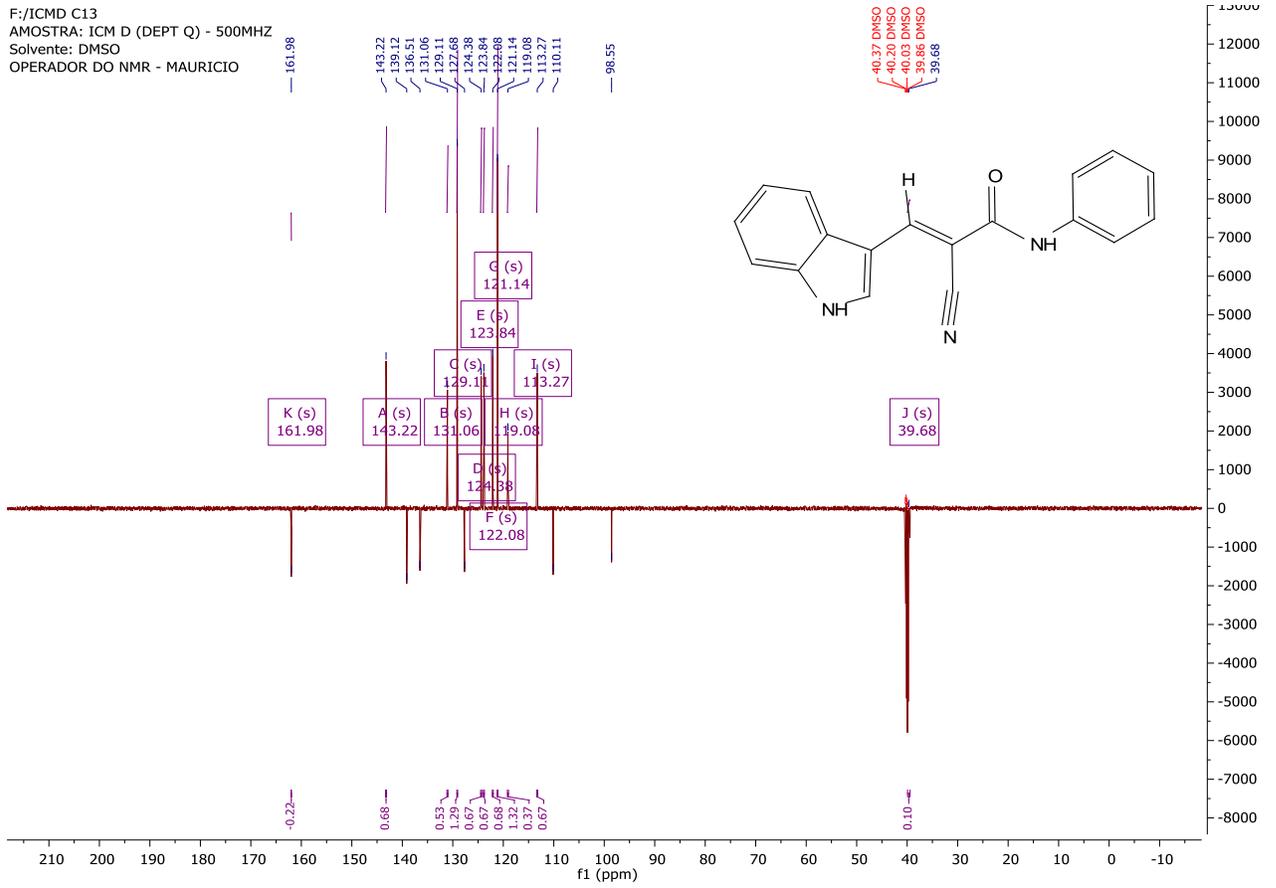


Figure S4. HRMS m/z [$M^+ + Na$] of ICMD-01

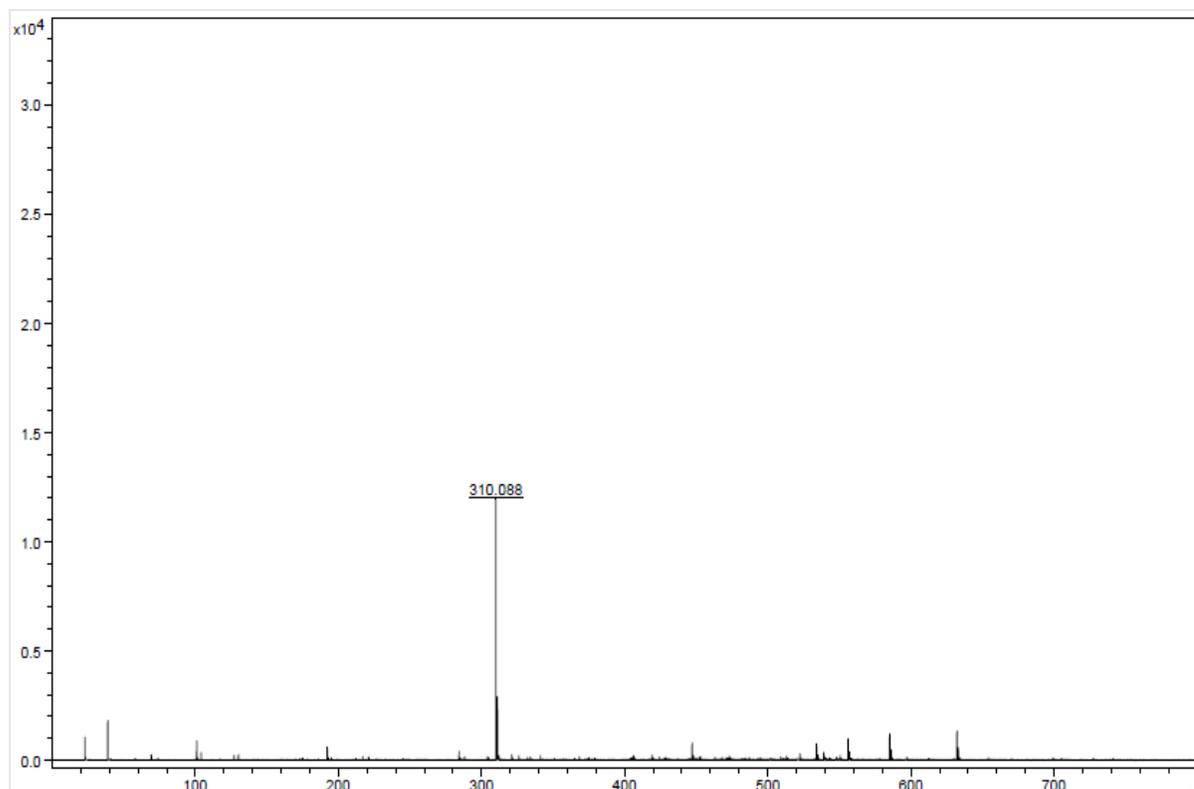


Figure S5. 3D crystallographic pose of co-crystallized ligand indomethacin (yellow) and redocked ligand (gray) on binding site of cyclooxygenase-2 (4COX)

