Xanthone Derivatives: Conformational Study and Development of Force Field

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Xanthone derivatives extracted from herbs are important components of homeopatic antibacterial, mycotoxic and cytotoxic medicines. Synthetic substituted xanthones tested against broad spectrum of biological activities revealed: antiinflammatory, cytostatic, antimycotic, and cardiovascular activities. In a series of newly synthesized substituted xanthones, two constitutional isomers, 2-methyl-2[2-(methyl)-6-xanthonoxy]-propionic acid, 2-methyl-2[4-(methyl)-6-xanthonoxy]-propionic acid, and racemic (RS)-2-[2-(methyl)-6-xanthonoxy]-propionic acid have shown differentiated antiinflammatory action.

The crystal structures of xanthone derivatives were solved using both single-crystal diffraction and HRPD data recorded with synchrotron radiation. In order to find the native, optimal structures of xanthone derivatives in their natural environment of lipid bilayer, additional force field parameters were obtained using X-ray diffraction data and *ab-initio* calculations.

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