

**POS-15**

**Binding characteristics of a photochromic calcium-chelating naphthopyran**

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Calcium ion is an important second messenger in the signal transduction pathway. The photochromic 2,2'-(3,3-diphenyl-3H-benzo[f]chromen-5-ylazanediyl)diacetic acid (**1**) is designed to mimic the intracellular calcium concentration changes observed during certain cell signaling processes. Compound **1** undergoes light-induced ring-opening and thermal closure in the dark in aqueous buffered solution. The binding affinity of calcium and magnesium ion to the closed and open forms of **1** was measured via NMR titration and kinetic analysis, respectively. The binding constants of **1** for calcium at pH 7.6 were found to be  $30.0 \text{ M}^{-1}$  in the closed form and  $2.04 \times 10^3 \text{ M}^{-1}$  in the open form. Fatigue studies were also performed in order to test the efficiency of the photoreversibility of **1**. The fatigue of **1** was determined in different buffers (HEPES, Phosphate, Tris), and at different pH's Tris (pH 7.6, 8.7, 9.8). The fatigue of **1** with metal present was also determined. Neither pH nor buffer salt had much influence on fatigue, but metal ions influenced the steady-state concentration of ring-opened product. Compound **1** represents a good step towards the creation of a mimic of physiological calcium signals, however binding affinities must be increased and thermal fading rates must be increased through further structural modifications.