

Supplementary Materials: A Theoretical Study of the Relationship between the Electrophilicity ω Index and Hammett Constant σ_p in [3+2] Cycloaddition Reactions of Aryl Azide/Alkyne Derivatives

Hicham Ben El Ayouchia, Hafid Anan, Moulay Lahcen El Idrissi Moubtassim, Luis R. Domingo, Miguel Julve and Salah-Eddine Stiriba

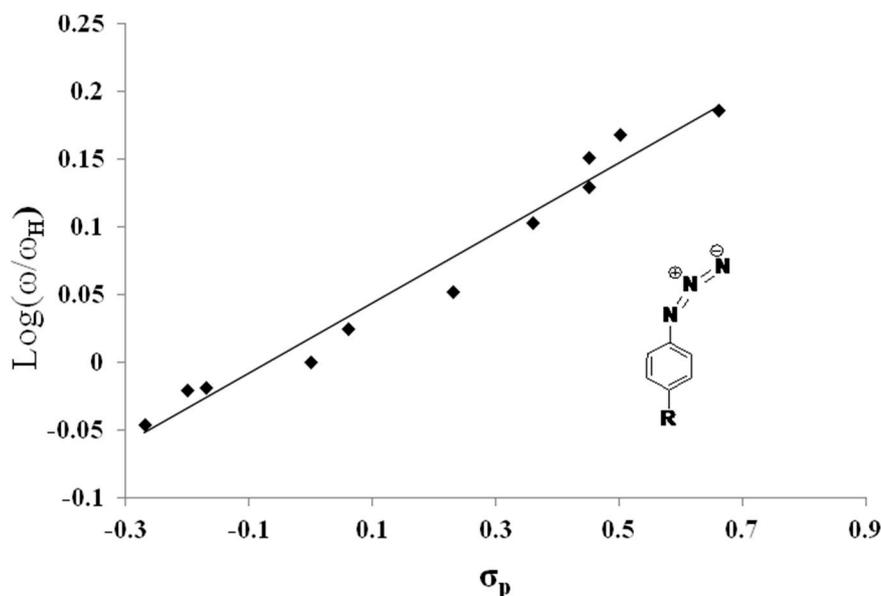


Figure S1. Plot of the logarithm of the global electrophilicity ratios of substituted azides versus the σ_p Hammett substituent constants. The value of the regression coefficient for the least-squares fit to a linear plot is $R^2 = 0.97$.

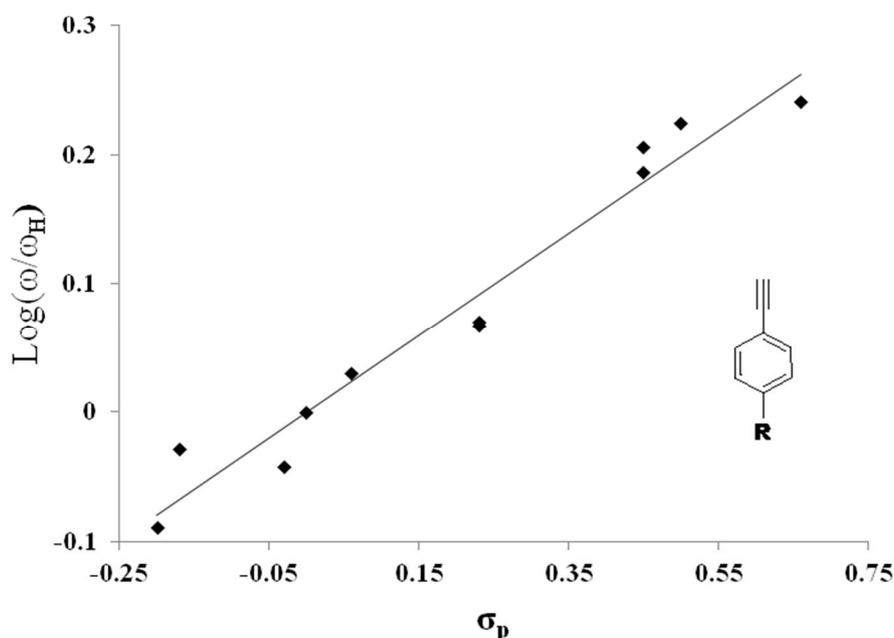


Figure S2. Plot of the logarithm of the global electrophilicity ratios of substituted alkynes versus the Hammett σ_p substituent constants. The value of the regression coefficient for the least-squares fit to a linear plot is $R^2 = 0.96$.