

Regioselective Diels-Alder reaction using hydrogen bonding of amides

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In the Diels-Alder reaction of a diene with an electron-donating group and a dienophile with an electron-withdrawing group, one of the two possible regioisomers is formed selectively because the overlap of frontier molecular orbitals controls the regioselectivity. Therefore, the regioselective Diels-Alder reaction of diene **1** with dienophile **2** is difficult because ester and amide functional groups in **2** exhibit similar electronic effects. When the Diels-Alder reaction is carried out in the presence of xanthene derivative **3**, a regioselective formation of **4** is expected because **1** and **2** will be aligned on **3** by the hydrogen bonding between amides. Formamide **1** was synthesized from **6** by the reductive amidation using formamide in the pressure of formic acid. Diacylhydrazine **2** was synthesized by the acylation of formhydrazide with the half ester derived from **7**. Cu(I)-catalyzed condensation of **8** and uracil **9** afforded **3**. While direct Diels-Alder reaction of **1** and **2** did not occur, regio-selective Diels-Alder reaction of **1** and **2** was investigated in the presence of **3**.

