Retro Diels Alder protocol for regioselective synthesis of novel [1,2,4]triazolo[4,3-a]pyrimidin-7(1H)-ones

Said, A.I., Palko, M., Haukka, M., Fülöp, F.

Abstract:

Reactions of diastereochemically varied norbornene-condensed 2-thioxopyrimidin-4-ones6and10with variously functionalized hydrazonoyl chlorides2a-hgave regioselectively angular norbornene-based [1,2,4]triazolo[4,3-a]pyrimidin-7(1H)-ones7a-hand11a,c-e, respectively. Thermal retro Diels-Alder (RDA) reaction of7a-hand11a,c-eresulted in the target compounds4a-has single products. On the other hand, reactions of thiouracil1and hydrazonoyl chlorides2a-egave regioselectively [1,2,4]triazolo[4,3-a]pyrimidinone-5(1H)-ones3a-e. The opposite regioselectivity of thiouracil1and norbornene-condensed 2-thioxopyrimidin-4-ones6and10was attributed to electronic factors according to DFT calculations. The angular structure of norbornene based [1,2,4]triazolo[4,3-a]pyrimidin-7(1H)-ones was confirmed by single crystal X-ray crystallography.

Published In:

RSC Advances, Volume 10, Issue 56, , 33937-33943