

Research Article

Predicting experimental yields as an index to rank synthetic routes II: application to the Curtius rearrangement

K. Yoshimura, K. Okano, R. Ishikawa, H. Yamamoto, M. Sumimoto and K. Hori

We tried to predict the yields observed for the Curtius rearrangement using the $E_a(\text{calc})$ values from DFT calculations, together with the reaction conditions. In order to construct a good model equation for the experimental yields of the Curtius reaction, we have to use those obtained from the reaction within 90 min for the PLS regression.

