

**Reaction path scans : Aza-Michael reactions of isatin imines**

**Metsala, Andrus; Žari, Sergei; Kanger, Tõnis** Computational and theoretical chemistry 2017 / p. 30-40 : ill

<https://doi.org/10.1016/j.comptc.2017.07.014>

**Simulation of oriented NMR spectra : combining molecular dynamics and chemical shift tensor calculations**

Sternberg, Ulrich; Witter, Raiker Magnetic resonance in chemistry 2023 <https://doi.org/10.1002/mrc.5403>

**Thermomyces lanuginosus lipase with closed lid catalyzes elimination of acetic acid from 11-acetyl-prostaglandin E2**

Villo, Ly; Metsala, Andrus; Tamp, Sven; Parve, Jaan; Vallikivi, Imre; Järving, Ivar; Nigulas, Samel; Lille, Ülo; Pehk, Tõnis;

Parve, Omar ChemCatChem 2014 / p. 1998-2010 : ill