

Competitive binding of natural amphiphiles with graphene derivatives

Radic, Slaven; Geitner, Nicholas K.; Podila, Ramakrishna; **Käkinen, Aleksandr**; Chen, Pengyu; Ke, Pu Chun; Ding, Feng Scientific reports 2013 / art. 2273 <https://doi.org/10.1038/srep02273> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

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> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

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

Sternberg, Ulrich; **Witter, Raiker** Magnetic resonance in chemistry 2024 / p. 125-144 <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 <https://doi.org/10.1002/cctc.201400019> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)