

Molecular dynamics simulations of creatine kinase and adenine nucleotide translocase in mitochondrial membrane patch
Karo, Jaanus; Peterson, Pearu; Vendelin, Marko The journal of biological chemistry 2012 / p. 7467-7476 : ill
<https://www.ncbi.nlm.nih.gov/pmc/articles/PMC3293576/>

Molecular dynamics simulations on PGLa using NMR orientational constraints
Sternberg, Ulrich; Witter, Raiker Journal of biomolecular NMR 2015 / p. 265-274 : ill <http://dx.doi.org/10.1007/s10858-015-9983-y>

Molecular dynamics study of bending deformation in fivefold twinned silver nanowires
Jõgi, Jakob; Dorogin, Leonid; **Kalda, Jaan** TÜ ja TTÜ doktorikool "Funktsionaalsed materjalid ja tehnoloogiad" : 04.-05. märts 2014, Tartu 2014 / [1] p

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>