

A total conformational analysis of diastereomeric esters and calculation of their conformational shielding models
Tamp, Sven; Danilas, Kady; Kreen, Malle; Vares, Lauri; Kiirend, Ene; Vija, Sirje; Pehk, Tõnis; Parve, Omar; Metsala, Andrus
Journal of molecular structure : THEOCHEM 2008 / 1/3, p. 84-91 : ill
https://www.researchgate.net/publication/244272489_A_total_conformational_analysis_of_diastereomeric_esters_and_calculation_of_their_conformational_shielding_models

An assessment of alternative low level calculation methods for the initial selection of conformers of diastereomeric esters
Metsala, Andrus; Tamp, Sven; Danilas, Kady; Lille, Ülo; Villo, Ly; Vija, Sirje; Pehk, Tõnis; Parve, Omar Journal of theoretical chemistry 2014 / p. 1-10 : ill

An NMR and MD modeling insight into nucleation of 1,2-alkanediols : selective crystallization of lipase-catalytically resolved enantiomers from the reaction mixtures
Parve, Omar; Reile, Indrek; Parve, Jaan; Kasvandik, Sergio; Kudrjašova, Marina; Tamp, Sven; Metsala, Andrus; Villo, Ly; Pehk, Tõnis; Jarvet, Jüri; Vares, Lauri Journal of organic chemistry 2013 / p. 12795-12801 : ill <https://doi.org/10.1021/jo402189e> [Journal metrics at Scopus](#) [Article at Scopus](#) [Article at WOS](#) [Journal metrics at WOS](#)

Assignment of configuration of chiral cyclic compounds by modelled spin-spin couplings and vibrational circular dichroism spectra
Aav, Riina; Suun, Silver; Tamp, Sven; Ausmees, Kerti; Kriis, Kadri; Metsala, Andrus; Peterson, Anna; Öeren, Mario 2nd Polish-Taiwanese Conference : From Molecular Modeling to Nano- and Biotechnology : 26-28 August 2015, Opole, Poland 2015 / [1] p. : ill

Asymmetric organocatalytic aza-Michael reactions of isatin derivatives
Žari, Sergei; Metsala, Andrus; Kudrjašova, Marina; Kaabel, Sandra; Järving, Ivar; Kanger, Tõnis Synthesis 2015 / p. 875-886 : ill <https://doi.org/10.1055/s-0034-1379956> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Aza-Michael reactions of isatin imines : deeper insight and origin of the stereoselectivity
Metsala, Andrus; Žari, Sergei; Kanger, Tõnis ChemCatChem 2016 / p. 2961-2967 : ill <https://doi.org/10.1002/cctc.201600584> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Aza-Michael reactions of isatin imines : role of S- π interactions
Metsala, Andrus; Žari, Sergei; Lopp, Margus; Kanger, Tõnis Balticum Organicum Syntheticum : 3-6 July 2016, Riga, Latvia : program and abstracts 2016 / p. 116 : ill http://www.boschem.eu/public/BOS2016/BOS-2016_Anstract-Book_Final.pdf

Chemical versus enzymatic acetylation of [alfa]-bromo-[omega]-hydroxyaldehydes : decyclization of hemiacetals by lipase
Villo, Ly; Metsala, Andrus; Parve, Omar; Pehk, Tõnis Tetrahedron letters 2002 / p. 3203-3207
https://www.academia.edu/17112413/Chemical_versus_enzymatic_acetylation_of_%CE%B1_bromo_%CF%89_hydroxyaldehydes_decyclization_of_hemiacetals_by_lipase

A chemoenzymatic synthesis of a deoxy sugar ester of N-Boc-protected L-tyrosine
Villo, Ly; Kreen, Malle; Kudrjašova, Marina; Metsala, Andrus; Tamp, Sven; Lille, Ülo; Pehk, Tõnis; Parve, Omar Practical methods for biocatalysis and biotransformations. 2 2012 / p. 335-339
<https://www.sciencedirect.com/science/article/pii/S1381117710002511>

A chemoenzymatic synthesis of deoxy sugar esters involving stereoselective acetylation of hemiacetals catalyzed by CALB
Villo, Ly; Kreen, Malle; Metsala, Andrus; Tamp, Sven; Lille, Ülo; Pehk, Tõnis; Parve, Omar; Kudrjašova, Marina Journal of molecular catalysis B : enzymatic 2011 / p. 44-51 <https://www.sciencedirect.com/science/article/abs/pii/S1381117710002511>

Comparison of photoelectron-spectroscopy results to ab-initio and density functional calculations : the ethylbenzene cation
Lehrer, F.; Weinkauff, R.; Metsala, Andrus Zeitschrift für physicalische Chemie 2007 / 5, p. 723-749
<https://www.degruyter.com/document/doi/10.1524/zpch.2007.221.5.723/html>

A DFT study of an organocatalytic enantioselective Mannich Reaction reveals that the enantiodetermining step is associated with the torsional degrees of freedom
Metsala, Andrus; Kriis, Kadri; Kaasik, Mikk; Kanger, Tõnis Balticum Organicum Syntheticum (BOS 2024) : Book of Abstracts 2024 / art. P83, p. 102 https://boschem.eu/bos2024/wp-content/uploads/sites/5/2024/07/BOS2024_Abstract-Book.pdf

A DFT study of an organocatalytic enantioselective Mannich reaction under the sway of noncovalent interactions
Metsala, Andrus; Kriis, Kadri; Kanger, Tõnis Journal of computational chemistry 2025 / art. e70159 <https://doi.org/10.1002/jcc.70159>

Enantioselective Henry reaction catalyzed by Cull salt and bipiperidine
Noole, Artur; Lippur, Kristin; Metsala, Andrus; Lopp, Margus; Kanger, Tõnis The journal of organic chemistry 2010 / p. 1313-1316 <https://pubmed.ncbi.nlm.nih.gov/20095538/>

Enantioselective Michael addition to vinyl phosphonates via hydrogen bond-enhanced halogen bond catalysis

Kaasik, Mikk; Martõnova, Jevgenija; Erkman, Kristin; Metsala, Andrus; Järving, Ivar; Kanger, Tõnis Chemical science 2021 / p. 7561-7568 <https://doi.org/10.1039/D1SC01029H> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Enantioselective N-Alkylation of Nitroindoles under Phase-Transfer Catalysis

Trubitsõn, Dmitri; Martõnova, Jevgenija; Erkman, Kristin; Metsala, Andrus; Saame, Jaan; Köster, Kristjan; Järving, Ivar; Leito, Ivo; Kanger, Tõnis Synthesis 2020 / p. 1047-1059 <https://doi.org/10.1055/s-0039-1690751> [Journal metrics at Scopus](#) [Article at WOS](#) [Journal metrics at WOS](#) [Article at WOS](#)

Estrite lipaaskatalüütiline enantioselektiivne hüdroolüüs : kineetiliste mõõtmiste tulemuste interpretatsioon

Parve, Omar; Metsala, Andrus; **Lille, Ülo** XXIII Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid 1997 / lk. 99

Extending traditional area of lipases' application for prostanoid and hemiacetal chemistry

Parve, Omar; Metsala, Andrus; Tamp, Sven; Villo, Ly BIT's 1st Annual World Congress of Catalytic Asymmetric Synthesis : Beijing, China, 19.-21.05.2010 2010

Halo-1,2,3-triazolium salts as halogen bond donors for the activation of imines in dihydropyridinone synthesis

Kaasik, Mikk; Metsala, Andrus; Kaabel, Sandra; Kriis, Kadri; Järving, Ivar; Kanger, Tõnis Journal of organic chemistry 2019 / p. 4294-4303 : ill <https://doi.org/10.1021/acs.joc.9b00248> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

Halogeenside võib võimendada kaugete aatomite interaktsioone

Metsala, Andrus; Kaasik, Mikk; Kanger, Tõnis; Lopp, Margus XXXIV Eesti keemiapäevad : 100. aastapäeva teaduskonverentsi teesid 2019 / lk. 28 https://www.ester.ee/record=b5208044*est

Lipase action on some non-triglyceride substrates

Vallikivi, Imre; Lille, Ülo; Lõokene, Aivar; Metsala, Andrus; Sikk, Peeter; Tõugu, Vello; Vija, Heiki; Villo, Ly; Parve, Omar Journal of molecular catalysis B : enzymatic 2003 / 5/6, p. 279-298 : ill <https://www.sciencedirect.com/science/article/abs/pii/S1381117703000432>

Lipase-catalysed acyl transfer in deoxysugars : a computational study

Kaevand, Toomas; Villo, Ly; Metsala, Andrus; Parve, Omar; Lille, Ülo International journal of engineering and applied sciences (EAAS) 2015 / p. 1-7 : ill

Lipase-catalysed acylation of prostanoids

Parve, Omar; **Järving, Ivar; Martin, Ivar; Metsala, Andrus; Vallikivi, Imre; Aidnik, Madis; Pehk, Tõnis**; Samel, Nigulas Bioorganic & medicinal chemistry letters 1999 / p. 1853-1858: ill

Lipase-catalysed enantioselective hydrolysis : interpretation of the kinetic results in terms of frontier orbital localisation

Parve, Omar; **Vallikivi, Imre**; Metsala, Andrus; **Lille, Ülo**; Tõugu, Vello; Sikk, Peeter; **Käämbre, Tuuli**; Vija, Heiki; **Pehk, Tõnis** Tetrahedron 1997 / 13, p. 4889-4900

Lipase-catalysed enantioselective hydrolysis of bicyclo[3.2.0]heptanol esters in supercritical carbon dioxide

Parve, Omar; **Vallikivi, Imre**; Lahe, Liija; Metsala, Andrus; **Lille, Ülo**; Tõugu, Vello; Vija, Heiki; **Pehk, Tõnis** Bioorganic & medicinal chemistry letters 1997 / 7, p. 811-816

Lipase-catalysed enantioselective hydrolysis of esters : interpretation of the kinetic results

Parve, Omar; Metsala, Andrus; **Lille, Ülo** 23rd Estonian Chemistry Days : abstracts of scientific conference 1997 / p. 109

Lipase-catalysed regioselective acylation/deacylation of prostanoids

Vallikivi, Imre; Järving, Ivar; Metsala, Andrus; **Pehk, Tõnis**; Parve, Omar International Conference on Organic Synthesis : Vilnius, 2000, June 26-29 : program and abstracts 2000 / p. [82]

"Lipolase" allub sekundaarsete alkoholide enantioeelistuse üldisele reeglile nii vesi kui ka superkriitilise SKCO₂ keskkonnas = "Lipolase" obeys the general enantiopreference rule of secondary alcohols in water and supercritical (SC)CO₂ media as well

Lille, Ülo; Metsala, Andrus; Parve, Omar; Tõugu, Vello; Vija, Heiki XVII Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid = 17th Estonian Chemistry Days : abstracts of scientific conference 1996 / lk. 101-102

Local ionization in 2-phenylethyl-N,N-dimethylamine : charge transfer and dissociation directly after ionization

Weinkauff, R.; Lehr, L.; **Metsala, Andrus** Journal of physical chemistry A 2003 / p. 2787-2799 <https://pubs.acs.org/doi/full/10.1021/jp021092c>

Microcanonical rate constant in case of intramolecular large amplitude vibrations

Metsala, Andrus 23rd Estonian Chemistry Days : abstracts of scientific conference 1997 / p. 92

Mikrokanooniline kiiruskonstant suureamplituudiliste molekulisestest võnkumiste korral
Metsala, Andrus XXIII Eesti keemiapäevad : teaduskonverentsi ettekannete referaadid 1997 / lk. 83

Mittestatistilises vinüülbromiidi molekulis

Metsala, Andrus XXVIII Eesti keemiapäevad : teaduskonverentsi ettekannete teesid = 28th Estonian Chemistry Days : abstracts of scientific conference 2002 / lk. 86

Prootoni transport peptiidides

Metsala, Andrus; Schlag, E.W. XXIX Eesti keemiapäevad : teaduskonverentsi ettekannete teesid = 29th Estonian Chemistry Days : abstracts of scientific conference 2005 / lk. 64-65

Quantum chemical calculation procedure for the c-c bond forming reactions

Metsala, Andrus; Kaasik, Mikk; Kriis, Kadri; Kanger, Tõnis; Kimm, Mariliis Balticum Organicum Syntheticum (BOS 2022) : program and abstract book 2022 / p. 127 [Kogumik](#)

Quantum chemical evaluation of the yield of hydroxybenzophenones in the Fries rearrangement of hydroxyphenyl benzoates

Metsala, Andrus; Usin, Eve; Vallikivi, Imre; Villo, Ly; Pehk, Tõnis; Parve, Omar Journal of molecular structure : THEOCHEM 2004 / p. 215-221 : ill <https://www.sciencedirect.com/science/article/pii/S016612800400750X>

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](#)

Synthesis of 3,4-dideoxy ribose esters: a novel chemoenzymatic approach to synthesis of activated, extended-chain glycoconjugates

Villo, Ly; Danilas, Kady; Metsala, Andrus; Pehk, Tõnis; Parve, Omar International Conference on Organic Synthesis : Tallinn, Estonia, June 25-29, 2006 : program and abstracts 2006 / p. 164

Synthesis of deoxy sugar esters : a chemoenzymatic stereoselective approach affording deoxy sugar derivatives also in the form of aldehyde

Villo, Ly; Danilas, Kady; Metsala, Andrus; Kreen, Malle; Vallikivi, Imre; Vija, Sirje; Pehk, Tõnis; Luciano, Saso; Parve, Omar Journal of organic chemistry 2007 / p. 5813-5816 <https://pubs.acs.org/doi/10.1021/jo062640b>

A synthesis of deoxy sugar esters. Stereoselective acetylation of hemiacetals by CALB

Villo, Ly; Metsala, Andrus; Tamp, Sven; Pehk, Tõnis; Parve, Omar Biotrans 2011 : Itaalia, Giardini Naxos, 02.-05.10.2011 2011

Synthesis, characterization and catalytic activity of enantiopure triazole-based halogen bond donors

Kaasik, Mikk; Kaabel, Sandra; Metsala, Andrus; Peterson, Anna; Kriis, Kadri; Järving, Ivar; Aav, Riina; Rissanen, Kari; Adamson, Jasper; Kanger, Tõnis GSFMT Scientific Conference 2020 : Tallinn, February 4-5, 2020 : abstracts 2020 / p. 35 : ill <http://fmdk.ut.ee/wp-content/uploads/2020/01/GSFMT2020.pdf>

The dipeptide cyclic(glycyltryptophanyl) in the gas phase : a concerted action of density functional calculations, S-O-S-1 two-photon ionization, spectral UV/UV hole burning and laser photoelectron spectroscopy

Wiedemann, S.; **Metsala, Andrus;** Nolting, D. Physical chemistry chemical 2004 / 10, p. 2641-2649 <https://pubs.rsc.org/en/content/articlelanding/2004/cp/b316185d>

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](#)

Tunable chiral triazole-based halogen bond donors : assessment of donor strength in solution with nitrogen-containing acceptors

Peterson, Anna; Kaasik, Mikk; Metsala, Andrus; Järving, Ivar; Adamson, Jasper; Kanger, Tõnis RSC advances 2019 / p. 11718-11721 : ill <https://doi.org/10.1039/c9ra01692a> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)

[2,3]-Wittig rearrangement as a formal asymmetric alkylation of α -branched ketones

Kimm, Mariliis; Ošeka, Maksim; Kaabel, Sandra; Metsala, Andrus; Järving, Ivar; Kanger, Tõnis Organic letters 2019 / p. 4976-4980 <https://doi.org/10.1021/acs.orglett.9b01495> [Journal metrics at Scopus](#) [Article at Scopus](#) [Journal metrics at WOS](#) [Article at WOS](#)