

- 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](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
- 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
- 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 <http://dx.doi.org/10.1002/cctc.201600584>
- 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](http://www.boschem.eu/public/BOS2016/BOS-2016_Anstract-Book_Final.pdf)
- Chemical versus enzymatic acetylation of [α]-bromo-[ω]-hydroxyaldehydes : decyclization of hemiacetals by lipase**  
**Villo, Ly; Metsala, Andrus; Parve, Omar; Pehk, Tõnis** Tetrahedron letters 2002 / p. 3203-3207
- 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 physikalische Chemie 2007 / 5, p. 723-749  
<https://www.degruyter.com/document/doi/10.1524/zpch.2007.221.5.723/html>
- Enantioselective Henry reaction catalyzed by Cull salt and biperidine**  
**Noole, Artur; Lippur, Kristin; Metsala, Andrus; Lopp, Margus; Kanger, Tõnis** The journal of organic chemistry 2010 / p. 1313-1316
- Enantioselective Michael addition to vinyl phosphonates via hydrogen bond-enhanced halogen bond catalysis**  
**Kaasik, Mik; Martõnova, Jevgenia; 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, Jevgenia; 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](#)
- 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 :

**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](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

**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

**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

**Mittestatistilisus 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>

**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://fntdk.ut.ee/wp-content/uploads/2020/01/GSFMT2020.pdf>

**The dipeptide cyclic(glycyltryptophanyl) in the gas phase : astat 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

**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

**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  $\alpha$ -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](#)