

17 February 2026

Kenno Vanommeslaeghe, Ph.D.

<https://kenno.org/pro/>

Professional and research experience

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| Associate Professor
Vrije Universiteit Brussel, Faculty of Medicine and Pharmacy | 2020-2026 |
| <ul style="list-style-type: none">• Research topics:<ul style="list-style-type: none">- Simulation and drug discovery projects targeting proteins of biomedical and pharmaceutical interest: Cystine/Glutamate Antiporter System x_c^- (Sxc⁻), the serotonin 2A (5-HT_{2A}) receptor and the glucocorticoid receptor- Molecular Dynamics studies and development of chiral molecular descriptors to understand and predict chromatographic separations on chiral stationary phases- Improved potentials for nonbonded interaction- Adaptive Biasing Force variant for efficiently driving conformational changes in Molecular Dynamics simulations of biomolecules- Advanced Replica Exchange-based Molecular Dynamics methodology for quantifying adsorption equilibria on conformationally disordered adsorbants | |
| Tenure-Track Assistant Professor
Vrije Universiteit Brussel, Faculty of Medicine and Pharmacy | 2015-2020 |
| <ul style="list-style-type: none">• Research topics: first three items listed above | |
| Research Specialist, Department of Pharmaceutical Sciences,
University of Maryland, Baltimore (Baltimore, MD, USA) | 2011-2015 |
| <ul style="list-style-type: none">• Mentor: Alexander D. MacKerell Jr.• Research topics:<ul style="list-style-type: none">- Parametrization and automation of the CHARMM General Force Field (CGenFF)- Cyberenvironment for Molecular Mechanics and Semi-Empirical parameter optimization: https://www.paramchem.org/- Computer-aided design of foldamer-based α-helix and β-sheet mimetic inhibitors of oncoproteins such as BCL-x_L and Mcl-1 | |
| Post Doctoral Fellow, University of Maryland, Baltimore (Baltimore, MD, USA) | 2006-2010 |
| <ul style="list-style-type: none">• Mentor: Alexander D. MacKerell Jr.• Research topics:<ul style="list-style-type: none">- Parametrization and automation of the CHARMM General Force Field (CGenFF)- Cyberenvironment for Molecular Mechanics and Semi-Empirical parameter optimization: https://www.paramchem.org/- Target-based design of inhibitors of the oncoprotein BCL-6 | |
| Post Doctoral Research Assistant, Vrije Universiteit Brussel (Brussels, Belgium) | 2005-2006 |
| <ul style="list-style-type: none">• Mentor: Paul Geerlings• Research topics:<ul style="list-style-type: none">- Interplay between stacking interactions and hydrogen bonding in nucleic acids- Accurate dispersion interactions with post-DFT methods | |
| Ph.D. in Sciences, Vrije Universiteit Brussel (Brussels, Belgium), summa cum laude | 2000-2005 |
| <ul style="list-style-type: none">• Advisors: Dirk Tourwé, Paul Geerlings• Dissertation: Theoretical study of the catalytic mechanism and inhibition of Histone Deacetylase | |

Education

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| Master's in Chemistry, Vrije Universiteit Brussel (Brussels, Belgium), magna cum laude | 1998-2000 |
| <ul style="list-style-type: none">• Advisor: Dirk Tourwé• Thesis: Synthesis and molecular modeling of a Trichostatin A analogue as a potential Histone Deacetylase inhibitor | |
| Bachelor's in Chemistry, Vrije Universiteit Brussel (Brussels, Belgium), magna cum laude | 1996-1998 |

Formal teaching

- As a course director ("titularis")
 - General and Inorganic Chemistry (8 ECTS credits) 1st year Pharmacy 2018-2025
 - Advanced Chemistry (5 ECTS credits) 1st year Pharmaceutical Sciences 2018-2025
 - Biomedical Chemistry (12 ECTS credits) 1st year Biomedical Sciences 2015-2018
 - Chemistry (12 ECTS credits) 1st year Pharmaceutical Sciences 2015-2018
 - Chemistry – Practicals (9 ECTS credits) 1st year Pharmaceutical Sciences 2015-2018
- As a lecturer ("co-titularis")
 - Biomedical Chemistry (12 ECTS credits) 1st year Biomedical Sciences 2018-2025
- In a formal advisory role ("co-titularis")
 - General and Inorganic Chemistry Practicals (3 ECTS credits) 1st year Pharmacy 2018-2025
 - Organic Chemistry – Theory and Practicals (5 ECTS credits) 1st year Pharmacy 2018-2025
- As an assistant
 - Exercises Organic Structure Analysis for Master in Bioengineering - option Chemistry 2003-2006

Mentoring activities

- PhD students
 - F. Ameli (supervisors [K. Vanommeslaeghe](#), D. Mangelings, Y. Vander Heyden); tentative title: *Molecular Dynamics approaches to elucidate enantioselective retention mechanisms on polysaccharide and antibiotic based chiral selectors* 2022-2026
 - P. De Gauquier (supervisors D. Mangelings, [K. Vanommeslaeghe](#), Y. Vander Heyden); tentative title: *Development of Quantitative Structure Enantioselective Retention Relationship (QSERR) models to predict enantioseparations on polysaccharide-based chiral stationary phases* 2019-2026
 - J. Peeters (supervisor [K. Vanommeslaeghe](#)); tentative title: *Principles and applications of Molecular Dynamics: innovations in nonbonded potentials, quantification of chirality and the molecular understanding of the 5-HT_{2A} serotonin receptor* 2018-2025
- Mentored 7 Ma students Pharmaceutical Sciences 2018-2025
- Initial tutoring and mentoring a majority of the new people at Alexander D. MacKerell Jr.'s lab, specifically 3 graduate students, 11 postdocs and 3 visiting junior faculty members 2008-2015

Fellowship & Grants

- FWOAL1041 (Senior research project): D. Mangelings, [K. Vanommeslaeghe](#), Y. Vander Heyden; *Combination of Molecular Dynamics and Quantitative Structure Enantioselective Relationships (QSER) models to elucidate enantioselective retention mechanisms on polysaccharide and antibiotic based chiral selectors* 2022-2025
- HERC53 (FWO & Hercules): A. Massie, J. Stiens, J. Van Ginderachter, [K. Vanommeslaeghe](#), M. Vinken, E. Menu, C. Spits, R. Njemini; *Seahorse platform: the Agilent Seahorse Flux Analyser with integrated normalization system* 2020-2024
- FWOTM983 (*as supervisor* of Junior postdoc): T. D. Hang; *Employing state-of-the-art simulation and drug design techniques in search for the structure, mechanism and small-molecule modulators of the Cystine/Glutamate Antiporter system xc⁻* 2019-2023
- Contributed to the writing of US NIH R01 grant 2R01GM070855 extension 2014
- Aspirant FWO (Research Foundation Flanders Ph.D. Scholarship) 2000-2004

Valorization

Contributions to spin-off: SilcsBio, LLC

- Creation of the CGenFF program, software distribution and web interface 2009-2015
- Early contributions in the development of the SILCS methodology 2008-2012

Scientific consulting

- Theoretical study of the configurational and conformational preference of BAL5788, an antibiotic, for the pharmaceutical company Johnson & Johnson 2006
- Theoretical study of a possible side reaction in the synthesis of TMC114, an HIV-1 protease inhibitor, for the pharmaceutical R&D company Tibotec 2002

PhD Committee membership

- Olivier Beyens, *Computational study of DPP8 and DPP9: fundamental insights and inhibitor design*, Universiteit Antwerpen (UAntwerpen, Belgium), the 29th of October 2024.
- Sameneh Davoudi, *Investigating the Effect of Curvature and Composition on Lipid Membrane Permeability Using Molecular Dynamics Simulations*, Universiteit Gent (UGent, Belgium), the 26th of June 2024.
- Thorben Fröhlking, *Machine learning RNA force fields from experimental data*, Scuola Internazionale Superiore di Studi Avanzati (SISSA, Italy), the 30th of September 2022.
- Abu Hanif Shaikh, *Wiener-Hammerstein System Identification Applied to Bio-impedance Spectroscopy*, Vrije Universiteit Brussel (VUB, Belgium), the 21st of September 2022.

Society memberships

- American Chemical Society (ACS)
- Biophysical Society
- Royal Flemish Chemical Society (KVCV)

Scientific community service

Reviewer for *ACS Chemical Biology*, *Australian Journal of Chemistry*, *Biophysical Journal*, *Current Medicinal Chemistry*, *European Journal of Medicinal Chemistry*, *Journal of Chemical Information and Modeling*, *Journal of Chemical Theory and Computation*, *Journal of Molecular Graphics and Modelling*, *Journal of Molecular Modeling*, *Journal of Physical Chemistry*, *PLOS ONE*, *Spectrochimica Acta A*.

Professional skills

- Languages:**
- Native Dutch
 - Close-to-native English
 - Moderate French
 - Notions of German

Usage of scientific software

- Expert-level skills in the CHARMM molecular simulation program and CHARMM force fields (lead developer of the CHARMM General Force Field and part of the community of developers of the CHARMM program)
- Proficiency in VMD, NAMD, GROMACS, Dock, Vina, Gaussian, GaussView, psi4
- Working knowledge of Sybyl, MOE, Macromodel/Maestro, Q-Chem, MolPro
- Basic knowledge of Discovery Studio, MODELLER, Spartan, Brabo, Molden

Programming experience

- CGenFF atom typing and assignment of parameters and charges (see publications): 8000 lines of C
- Restrained least-squares fitting of parameters in empirical force fields (see publications): 2000 lines of C
- Post-DFT dispersion correction (see publications): 1000 lines of Fortran
- MPI parallelization of an in-house modified version of Dock 4 in Alexander D. MacKerell Jr.'s lab
- Diverse sh and awk scripts to facilitate CADD in Alexander D. MacKerell Jr.'s lab
- Basic knowledge of Python

System administration experience

- Professional-level skills in set-up and maintenance of Rocks and Perceus-driven Linux supercomputing clusters running a variety of computational chemistry software under Sun/Oracle Gridengine
- Professional-level skills in set-up and maintenance of Linux workstations running a wide variety of computational chemistry software and utilities
- Proficiency in set-up and maintenance of Linux data storage clusters running Gluster
- Working knowledge of web design including HTML, CSS, Ajax, Flask framework

Miscellaneous

Delegate for Belgium at the 28th International Chemistry Olympiad (Moscow, Russian Federation, 1996)

Administrative Services

As a professor: active member of

- Study Program Committee (opleidingsraad) Biomedical Sciences 2015-2025
 - Exam commission (examencommissie) Biomedical sciences 2015-2025
- Study Program Committee (opleidingsraad) Pharmaceutical Sciences 2015-2025
 - Exam commission (examencommissie) Pharmaceutical Sciences 2015-2025
 - Subcommission Doctorates (doctoraatscommissie) 2015-2025
 - Task Group Study Program (werkgroep curriculum) 2015-2025
- Council of the Department (vakgroeppraad) 2015-2025
Pharmaceutical and Pharmacological Sciences (FARM)

As a PhD student

- Representative "Assistant Academic Staff" (AAP) in the faculty council of the Faculty of Sciences of the VUB 2001-2003
- Representative "Assistant Academic Staff" (AAP) in the department council of the Department of Chemistry of the VUB 2001-2003
- Responsible for the data processing of an alumni survey, conducted in the context of a six-yearly national audit of the education at the Department of Chemistry of the VUB 2001-2002

Publications [total citations (Web of Science): 11 309; H-index: 26]

1. F. Ameli, R. Van de Velde, Y. Vander Heyden, D. Mangelings, K. Vanommeslaeghe, **Solvent-Dependent Conformational Diversity Of Polysaccharide-Based Chiral Selectors**, *J. Chem. Inf. Model.* 2026, DOI: 10.1021/acs.jcim.5c03049.
2. F. Ameli, K. Vanommeslaeghe, Y. Vander Heyden, D. Mangelings, **15 - Supercritical fluid chromatography of stereoisomers**, in *Supercritical Fluid Chromatography and Extraction, Second Edition*, C. West, C. F. Poole, Eds., Elsevier 2026, 353-392.
3. P. De Gauquier, J. Peeters, F. Ameli, E. Lipka, K. Vanommeslaeghe, Y. Vander Heyden, D. Mangelings, **Predicting enantioseparations on polysaccharide-based stationary phases using achiral and chiral molecular descriptors**, *J. Chromatogr. Open* 2025, **8**, 100279.
4. J. Peeters, P. De Gauquier, F. Ameli, Y. Vander Heyden, D. Mangelings, K. Vanommeslaeghe, **Development of Ensemble Steric and Electrostatic Chirality (ESEC) descriptors for modelling chromatographic enantioseparations**, *PLoS One* 2025, **20**(10): e0333635. [Times cited: **2**]
5. J. Peeters, D. De Bundel, K. Vanommeslaeghe, **Molecular dynamics study of differential effects of serotonin-2A-receptor (5-HT2AR) modulators**, *PLoS Comput. Biol.* 2025, **21**(9): e1013000.
6. K. Vanommeslaeghe, **Collagen as a stress test and a tool for improvement of glycine and proline conformations in biomolecular force fields**, *Biophys. J.* 2025, **124**, 2566-2568.
7. J. Peeters, K. Vanommeslaeghe, **A simple model for the Pauli Repulsion with possible utility in QM, MM and Chemical Education**, *J. Chem. Theory Comput.* 2024, **20**, 6728-6737.
8. P. De Gauquier, J. Peeters, K. Vanommeslaeghe, Y. Vander Heyden, D. Mangelings, **Modelling the enantio-recognition of structurally diverse pharmaceuticals on O-substituted polysaccharide-based stationary phases**, *Talanta* 2023, **259**, 124497. [Times cited: **5**]
9. T. D. Hang, H. M. Hung, P. Beckers, N. Desmet, M. Lamrani, A. Massie, E. Hermans, K. Vanommeslaeghe, **Structural investigation of human cystine/glutamate antiporter System xc⁻ (Sxc⁻) using homology modeling and molecular dynamics**, *Front. Mol. Biosci.* 2022, **126**:1064199. [Times cited: **2**]
10. C. Jeong, R. Franklin, K. J. Edler, K. Vanommeslaeghe, S. Krueger, J. E. Curtis, **Styrene-Maleic Acid Copolymer Nanodiscs to Determine the Shape of Membrane Proteins**, *J. Phys. Chem. B* 2022, **126**, 1034-1044. [Times cited: **4**]
11. P. De Gauquier, K. Vanommeslaeghe, Y. Vander Heyden, D. Mangelings, **Modelling approaches for chiral chromatography on polysaccharide-based and macrocyclic antibiotic chiral selectors: A review**, *Anal. Chim. Acta* 2022, **1198**, 338861. [Times cited: **45**]
12. L. A. Burns, J. C. Faver, Z. Zheng, M. S. Marshall, D. G. A. Smith, K. Vanommeslaeghe, A. D. MacKerell Jr., K. M. Merz, and C. D. Sherrill, **The BioFragment Database (BFDdb): An open-data platform for computational chemistry analysis of noncovalent interactions**, *J. Chem. Phys.* 2017, **147**, 161727. [Times cited: **104**]
13. I. S. Gutiérrez, F.-Y. Lin, K. Vanommeslaeghe, J. A. Lemkul, K. A. Armacost, C. L. Brooks III, A. D. MacKerell Jr., **Parametrization of halogen bonds in the CHARMM general force field: Improved treatment of ligand-protein interactions**, *Bioorg. Med. Chem.* 2016, **24**, 4812-4825. [Times cited: **222**]
14. M. G. Cardenas, W. Yu, W. Beguelin, M. R. Teater, H. Geng, R. L. Goldstein, E. Oswald, K. Hatzi, S.-N. Yang, J. Cohen, R. Shaknovich, K. Vanommeslaeghe, H. Cheng, D. Liang, H. J. Cho, J. Abbott, W. Tam, W. Du, J. P. Leonard, O. Elemento, L. Cerchietti, T. Cierpicki, F. Xue, A. D. MacKerell Jr., A. M. Melnick, **Rationally designed BCL6 inhibitors target activated B cell diffuse large B cell lymphoma**, *J. Clin. Invest.* 2016, **126**, 3351-3362. [Times cited: **145**]
15. Y. Xu, K. Vanommeslaeghe, A. Aleksandrov, A. D. MacKerell, Jr., L. Nilsson, **Additive CHARMM Force Field for Naturally Occurring Modified Ribonucleotides**, *J. Comput. Chem.* 2016, **37**, 896-912. [Times cited: **71**]

16. C. Domene, C. Jorgensen, [K. Vanommeslaeghe](#), C. J. Schofield, A. D. MacKerell Jr., **Quantifying the Binding Interaction between the Hypoxia-Inducible Transcription Factor and the von Hippel–Lindau Suppressor**, *J. Chem. Theory Comput.* 2015, **11**, 3946-3954. [Times cited: **2**]
17. C. Jorgensen, L. Darre, [K. Vanommeslaeghe](#), K. Omoto, D. Pryde, C. Domene, **In-silico identification of PAP-1 binding sites in the Kv1.2 potassium channel**, *Mol. Pharmaceutics* 2015, **12**, 1299-1307. [Times cited: **16**]
18. [K. Vanommeslaeghe](#), M. Yang, A. D. MacKerell Jr., **Robustness in the fitting of Molecular Mechanics parameters**, *J. Comput. Chem.* 2015, **36**, 1083-1101. [Times cited: **62**]
19. S. Jo, X. Cheng, S. M. Islam, L. Huang, H. Rui, A. Zhu, H. S. Lee, Y. Qi, W. Han, [K. Vanommeslaeghe](#), A. D. MacKerell Jr., Benoît Roux, W. Im, **CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues**, *Adv. Protein Chem. Struct. Biol.* 2014, **96**, 235-265. [Times cited: **295**]
20. N. R. Kern, H. S. Lee, E. L. Wu, S. Park, [K. Vanommeslaeghe](#), A. D. MacKerell Jr., J. B. Klauda, S. Jo, W. Im, **Lipid-Linked Oligosaccharides in Membranes Sample Conformations that Facilitate Binding to Oligosaccharyltransferase**, *Biophys. J.* 2014, **107**, 1885-1895. [Times cited: **21**]
21. S. S. Mallajosyula, [K. Vanommeslaeghe](#), A. D. MacKerell Jr., **Perturbation of Long-Range Water Dynamics as the Mechanism for the Antifreeze Activity of Antifreeze Glycoprotein**, *J. Phys. Chem. B* 2014, **118**, 11696-11706. [Times cited: **37**]
22. [K. Vanommeslaeghe](#), A. D. MacKerell Jr., **CHARMM additive and polarizable force fields for biophysics and computer-aided drug design**, *Biochim. Biophys. Acta* 2014, **1850**, 861-871. [Times cited: **211**]
23. P. Kumar, S. A. Bojarowski, K. N. Jarzemska, S. Domagała, [K. Vanommeslaeghe](#), A. D. MacKerell Jr., P. M. Dominiak, **A Comparative Study of Transferable Aspherical Pseudoatom Databank and Classical Force Fields for Predicting Electrostatic Interactions in Molecular Dimers**, *J. Chem. Theory Comput.* 2014, **10**, 1652-1664. [Times cited: **28**]
24. [K. Vanommeslaeghe](#), O. Guvench, A. D. MacKerell Jr., **Molecular Mechanics**, *Curr. Pharm. Des.* 2014, **20**, 3281-3292. [Times cited: **93**]
25. K.-Y. Jung, [K. Vanommeslaeghe](#), M. E. Lanning, J. L. Yap, C. Gordon, P. T. Wilder, A. D. MacKerell Jr., S. Fletcher, **Amphipathic α -helix mimetics based on a 1,2-diphenylacetylene scaffold**, *Org. Lett.* 2013, **15**, 3234-3237. [Times cited: **39**]
26. X. Cao, J. L. Yap, M. K. Newell-Rogers, C. Peddaboina, W. Jiang, H. T. Papaconstantinou, D. Jupitor, A. Rai, K.-Y. Jung, R. P. Tubin, W. Yu, [K. Vanommeslaeghe](#), P. T. Wilder, A. D. MacKerell Jr., S. Fletcher, R. W. Smythe, **The novel BH3 alpha-helix mimetic JY-1-106 induces apoptosis in a subset of cancer cells (lung cancer, colon cancer and mesothelioma) by disrupting Bcl-x_L and Mcl-1 protein-protein interactions with Bak**, *Mol. Cancer* 2013, **12**:42. [Times cited: **74**]
27. [K. Vanommeslaeghe](#), E. P. Raman, A. D. MacKerell Jr., **Automation of the CHARMM General Force Field (CGenFF) II: Assignment of bonded parameters and partial atomic charges**, *J. Chem. Inf. Model.* 2012, **52**, 3155-3168 [Times cited: **1412**]
28. [K. Vanommeslaeghe](#), A. D. MacKerell Jr., **Automation of the CHARMM General Force Field (CGenFF) I: bond perception and atom typing**, *J. Chem. Inf. Model.* 2012, **52**, 3144-3154 [Times cited: **1677**]
29. W. Yu, X. He, [K. Vanommeslaeghe](#), A. D. MacKerell Jr., **Extension of the CHARMM General Force Field to Sulfonyl-Containing Compounds and Its Utility in Biomolecular Simulations**, *J. Comput. Chem.* 2012, **33**, 2451-2468 [Times cited: **769**]
30. E. P. Raman, [K. Vanommeslaeghe](#), A. D. MacKerell Jr., **Site-Specific Fragment Identification Guided by Single-Step Free Energy Perturbation Calculations**, *J. Chem. Theory Comput.* 2012, **8**, 3513-3525 [Times cited: **29**]
31. J. L. Yap, X. B. Cao, [K. Vanommeslaeghe](#), K. Y. Jung, C. Peddaboina, P. T. Wilder, A. Nan, A. D. MacKerell Jr., W. R. Smythe, S. Fletcher, **Relaxation of the rigid backbone of an oligoamide-foldamer-based α -helix mimetic: identification of potent Bcl-x_L inhibitors**, *Org. Biomol. Chem.* 2012, **10**, 2928-2933 [Times cited: **61**]
32. A. Krishtal, D. Geldof, [K. Vanommeslaeghe](#), C. Van Alsenoy, P. Geerlings, **Evaluating London Dispersion Interactions in DFT: A Nonlocal Anisotropic Buckingham – Hirshfeld Model**, *J. Chem. Theory Comput.* 2012, **8**, 125-134 [Times cited: **17**]
33. O. Guvench, S. S. Mallajosyula, E. P. Raman, E. Hatcher, [K. Vanommeslaeghe](#), T. J. Foster, F. W. Jamison, A. D. MacKerell Jr., **CHARMM Additive All-Atom Force Field for Carbohydrate Derivatives and Its Utility in Polysaccharide and Carbohydrate-Protein Modeling**, *J. Chem. Theory Comput.* 2011, **7**, 3162-3180 [Times cited: **566**]
34. A. Krishtal, [K. Vanommeslaeghe](#), D. Geldof, C. Van Alsenoy, P. Geerlings, **Importance of anisotropy in the evaluation of dispersion interactions**, *Phys. Rev. A* 2011, **83**, 024501 [Times cited: **16**]
35. [K. Vanommeslaeghe](#), E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov, A. D. MacKerell Jr., **CHARMM General Force Field (CGenFF): A force field for drug-like molecules compatible with the CHARMM all-atom additive biological force fields**, *J. Comput. Chem.* 2010, **31** (4), 671-690 [Times cited: **5006**]
36. A. Krishtal, [K. Vanommeslaeghe](#), A. Olasz, T. Veszprémi, C. Van Alsenoy, P. Geerlings, **Accurate interaction energies at DFT level by means of an efficient dispersion correction**, *J. Chem. Phys.* 2009, **130**, 174101 [Times cited: **46**]

37. A. Olasz, K. Vanommeslaeghe, A. Krishtal, T. Veszprémi, C. Van Alsenoy, P. Geerlings, **The use of atomic intrinsic polarizabilities in the evaluation of the dispersion energy**, *J. Chem. Phys.* 2007, **127**, 224105 [Times cited: **35**]
38. K. Vanommeslaeghe, P. Mignon, S. Loverix, D. Tourwé, P. Geerlings, **Influence of stacking on the hydrogen bond donating capacity of nucleic bases**, *J. Chem. Theory Comput.* 2006, **2** (5), 1444-1452 [Times cited: **29**]
39. K. Van Rompaey, S. Ballet, C. Tömböly, R. De Wachter, K. Vanommeslaeghe, M. Biesemans, R. Willem, D. Tourwé, **Synthesis and evaluation of the β -turn properties of 4-amino-1,2,4,5-tetrahydro-2-benzazepin-3-ones and of their spirocyclic derivative**, *Eur. J. Org. Chem.* 2006, 2899–2911 [Times cited: **24**]
40. K. Vanommeslaeghe, S. Loverix, P. Geerlings, D. Tourwé, **DFT-based Ranking of Zinc-chelating Groups in Histone Deacetylase Inhibitors**, *Bioorg. Med. Chem.* 2005, **13** (21), 6070–6082 [Times cited: **55**]
41. K. Vanommeslaeghe, F. De Proft, S. Loverix, D. Tourwé, P. Geerlings, **Theoretical study revealing the functioning of a novel combination of catalytic motives in Histone Deacetylase**, *Bioorg. Med. Chem.* 2005, **13** (12), 3987–3992 [Times cited: **43**]
42. K. Vanommeslaeghe, C. Van Alsenoy, F. De Proft, J. C. Martins, D. Tourwé, P. Geerlings, **Ab Initio study of the binding of Trichostatin A (TSA) in the active site of Histone Deacetylase Like Protein (HDLP)**, *Org. Biomol. Chem.* 2003, **1** (16), 2951–2957 [Times cited: **29**]
43. K. Vanommeslaeghe, G. Elaut, V. Brex, P. Papeleu, K. Iterbeke, P. Geerlings, D. Tourwé, V. Rogiers, **Amide analogues of TSA: synthesis, binding mode analysis and HDAC inhibition**, *Bioorg. Med. Chem. Lett.* 2003, **13** (11), 1861–1864 [Times cited: **26**]

Invited talks at workshops and continuing education events

1. Statistical Biophysics Group (SBP), Scuola Internazionale Superiore di Studi Avanzati (SISSA) (Trieste, Italy, 30th of September 2022): K. Vanommeslaeghe, **The CHARMM additive force field: fundamentals and applications**
2. 2012 NIH CHARMM Advanced Tutorial: “Advances in Biomolecular Modelling and Simulations using CHARMM” (Bethesda, MD, USA, 7th-10th of May 2012): K. Vanommeslaeghe, A. D. MacKerell Jr., **The CHARMM Force Field**
3. 2011 NCNR/NSF Summer School on Modeling Neutron Data of Biological Systems (Gaithersburg, MD, USA, 12th-16th of June 2011): K. Vanommeslaeghe, A. D. MacKerell Jr., **CHARMM General Force Field (CGenFF) for medicinal compounds and its implementation in an Extensible Cybereenvironment for parametrization (ParamChem)**
4. Mahidol University Department of Pharmaceutical Chemistry Special Lecture (Bangkok, Thailand, the 18th of May 2011): K. Vanommeslaeghe, A. D. MacKerell Jr., **The CHARMM General Force Field: design, automation and application in Computer-Aided Drug Design**

Oral presentations at international and national (USA) conferences

Invited

1. 2009 Accelrys User Group Meeting (San Diego, CA, USA, 18th-20th of February 2009): K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov, A. D. MacKerell Jr., **CHARMM General Force Field (CGenFF): A force field optimized for drug-like molecules - theory and applications**

Contributed

2. 244th American Chemical Society National Meeting (Philadelphia, PA, USA, 19th-23rd of August 2012): K. Vanommeslaeghe, N. Shen, N. K. Polani, Y. Fan, J. Gosh, C. Herath, S. Marru, M. Pierce, S. Pamidighantam, R. M. Sheetz, A. D. MacKerell Jr., **ParamChem force field parametrization engine: Initial guess generation and dihedral parameter optimization**
3. 238th American Chemical Society National Meeting (Washington, DC, USA, 16th-20st of August 2009): K. Vanommeslaeghe, S. Pamidighantam, R. M. Sheetz, J. W. D. Connolly, A. Roitberg, A. D. MacKerell Jr., **Toward an automatic force field parametrization engine: Assignment of parameters by analogy for the CHARMM General Force Field (CGenFF)**
4. 236th American Chemical Society National Meeting (Philadelphia, PA, USA, 17th-21st of August 2008): K. Vanommeslaeghe, C. Acharya, A. D. MacKerell Jr., **Development of parameters for the CHARMM General Force Field (CGenFF)**
5. 236th American Chemical Society National Meeting (Philadelphia, PA, USA, 17th-21st of August 2008): K. Vanommeslaeghe, A. Olasz, A. Krishtal, T. Veszprémi, C. Van Alsenoy, P. Geerlings, **Post-DFT dispersion correction based on the atomic intrinsic polarizability tensor**
6. Second Joint Italian-Swiss Meeting on Medicinal Chemistry (Modena, Italy, 12th-16th of September 2005): K. Vanommeslaeghe, **Theoretical study of the catalytic mechanism and inhibition of Histone Deacetylase**