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Kenno Vanommeslaeghe, Ph.D.

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Professional and research experience

Tenure-Track Assistant Professor — 2015-present
Vrije Universiteit Brussel, Faculty of Medicine and Pharmacy

Research Specialist, Department of Pharmaceutical Sciences, — 2011-2015
University of Maryland, Baltimore (Baltimore, MD, USA)
- Mentor: Alexander D. MacKerell Jr.
- Research topics:
  - 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
- Mentor: Alexander D. MacKerell Jr.
- Research topics:
  - 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
- Mentor: Paul Geerlings
- Research topics:
  - 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
- Advisors: Dirk Tourwé, Paul Geerlings
- Dissertation: Theoretical study of the catalytic mechanism and inhibition of Histone Deacetylase

Education

Master's in Chemistry, Vrije Universiteit Brussel (Brussels, Belgium), magna cum laude — 1998-2000
- 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

Extra courses taken

- Principles of Molecular Recognition, Université Catholique de Louvain" (UCL, Catholic University of Louvain, Belgium), by Prof. François Diederich (ETH Zürich) — 2003
- Computational Medicinal Chemistry, Institute for Continuing Education in Science (ICES), University of Ghent (Ghent, Belgium) — 2002

Fellowship & Grants

Aspirant FWO (Research Foundation Flanders Ph.D. Scholarship) — 2000
Renewal Aspirant FWO (Research Foundation Flanders Ph.D. Scholarship) — 2002
Contributed to the writing of US NIH R01 grant 2R01GM070855 extension — 2014

Teaching and mentoring activities

- Course titular for Chemistry courses (anorganic / organic / laboratory practice) of 1st Bachelor Biomedical Sciences and Pharmacy — 2015-present
- Invited speaker at workshops and continuing education events; see below — 2009-present
- 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
- Exercises "Organic Chemistry II" for Master in Bioengineering - option Chemistry — 2003-2006

Significant public releases of scientific tools and software

- The CHARMM General Force Field (CGenFF): downloaded more than 18 000 times — 2009
- The CGenFF program: processed more than 100 000 molecules submitted by more than 4 700 users/scientists; licensed for commercial distribution to SilcsBio LLC — 2010

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

Administrative Services

- Representative "Assistant Academic Staff" in the faculty council of the Faculty of Sciences of the VUB — 2001-2003
- Representative "Assistant Academic Staff" 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): 2479; H-index: 18]

1. 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 (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions**, *J. Chem. Phys.* 2017, **147**, 161727.
2. 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: **6**]
3. 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: **14**]
4. 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: **8**]
5. 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.
6. 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: **5**]
7. 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: **19**]
8. 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: **15**]
9. 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: **4**]
10. 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: **8**]
11. 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: **37**]
12. P. Kumar, S. A. Bojarowski, K. N. Jarzembska, 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: **5**]

13. K. Vanommeslaeghe, O. Guvench, A. D. MacKerell Jr., **Molecular Mechanics**, *Curr. Pharm. Des.* 2014, **20**, 3281-3292. [Times cited: **5**]
14. 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: **25**]
15. 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: **40**]
16. 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: **282**]
17. 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: **282**]
18. 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: **117**]
19. 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: **16**]
20. 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: **43**]
21. 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: **12**]
22. 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: **141**]
23. 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: **14**]
24. 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: **1146**]
25. 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: **39**]
26. 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: **24**]
27. 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: **23**]
28. 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: **20**]
29. 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: **47**]
30. 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: **36**]
31. 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: **26**]
32. K. Vanommeslaeghe, G. Elaut, V. Brecx, 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: **20**]

Invited talks at workshops and continuing education events

1. 2012 NIH CHARMM Advanced Tutorial: "Advances in Biomolecular Modelling and Simulations using CHARMM" (Bethasda, MD, USA, 7th-10th of May 2012): K. Vanommeslaeghe, A. D. MacKerell Jr., **The CHARMM Force Field**
2. 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 Cyberenvironment for parametrization (ParamChem)**
3. Mahidol University Department of Pharmaceutical Chemistry Special Lecture (Bankok, 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**

Abstracts and Presentations

Contributions to proceedings of international conferences

1. K. Vanommeslaeghe, F. De Proft, S. Loverix, C. Van Alsenoy, D. Tourwé, P. Geerlings, **Quantum Chemical Study of the Catalytic Mechanism of a Histone Deacetylase Analogue**, *QSAR and Molecular Modelling in Rational Design of Bioactive Molecules: Proceedings of the 15th European Symposium on QSAR and Molecular Modelling*, E. Akı-Şener and I. Yalçin (Editors), CADD&D Society in Turkey (Ankara, Turkey) 2005, 462–463
2. S. Ballet, C. Tömböly, K. Van Rompaey, R. De Wachter, K. Vanommeslaeghe, M. Biesemans, R. Willem, J. Van Betsbrugge, D. Tourwé, **The 2-Benzazepin-3-one Structure as a β-turn Mimic: Synthesis and Conformational Analysis**, *Peptides 2004: Proceedings of the 3rd International and 28th European Peptide Symposium*, M. Flegel, M. Fridkin, C. Gilon and J. Slaninova (Editors), Kenes International (Genève, Zwitserland) 2005, 698–699
3. D. Tourwé, S. Van Cauwenberghe, K. Vanommeslaeghe, E. Mannekens, P. Geerlings, G. Tóth, A. Péter, J. Czombos, **Modifications of the Tic Residue in TIPP-Peptides**, *Peptides: The Wave of the Future*, M. Lebl and R. A. Houghten (Editors), American Peptide Society 2001, 683–684

Invited oral presentations at international and national (USA) conferences

4. 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 oral presentations at international and national (USA) conferences

5. 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**
6. 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)**
7. 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)**
8. 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**
9. 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**

Contributed oral presentations at local conferences

10. 43nd Middle Atlantic Regional Meeting of the American Chemical Society (Baltimore, MD, USA, 31st of May – 2nd of June 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., **Initial guess generation and dihedral parameter optimization in the ParamChem force field parametrization engine**
11. "7de Vlaams Jongerencongres van de Chemie" (7th Flemish youth symposium on Chemistry, Ghent, Belgium, 16th of April 2004): K. Vanommeslaeghe, **Theoretical study of the catalytic mechanism and the inhibition of a Histone Deacetylase analogue**

Poster presentations at international and national (USA) conferences (listed only when presenting author)

12. Biophysical Society 59th Annual Meeting (Baltimore, MD, USA, 7th-11th of March 2015): K. Vanommeslaeghe, A. D. MacKerell Jr., **A CHARMM-compatible force field for peptoids and α-methylated peptides with (φ,ψ) energy correction grid**
13. Biophysical Society 55th Annual Meeting (Baltimore, MD, USA, 5th-9th of March 2011): K. Vanommeslaeghe, J. Gosh, N. K. Polani, M. Sheetz, S. V. Pamidighantam, J. W. D. Connolly, A. D. MacKerell Jr., **Automation of the CHARMM General Force Field for Drug-Like Molecules**
14. XXIth International Symposium on Medicinal Chemistry (Brussels, Belgium, 5th-9th of September 2010): K. Vanommeslaeghe, N. Singh, N. K. Polani, S. V. Pamidighantam, M. Sheetz, J. W. D. Connolly, A. E. Roitberg, A. D. MacKerell Jr., **Automation of the CHARMM General Force Field for Computer-Aided Drug Design**
15. XXth International Symposium on Medicinal Chemistry (Vienna, Austria, 31st of August - 4th of September 2008): K. Vanommeslaeghe, E. Hatcher, C. Acharya, S. Kundu, S. Zhong, J. Shim, E. Darian, O. Guvench, P. Lopes, I. Vorobyov, A. D. MacKerell Jr., **Development of parameters for the CHARMM General Force Field (CGenFF)**
16. XXth International Symposium on Medicinal Chemistry (Vienna, Austria, 31st of August - 4th of September 2008): K. Vanommeslaeghe, G. F. Da Silva, A. F. Gethu, X. Zhu, S. Zhong, L. Cerchietti, M. Matthews, J. M. Polo, A. Coop, G. G. Privé, A. Melnick, A. D. MacKerell Jr., **Idetification of binding sites for BCL-6 inhibitors and virtual screening**
17. 1st European Chemistry Congress (Budapest, Hungary, 27th-31st of August 2006): K. Vanommeslaeghe, P. Mignon, S. Loverix, D. Tourwé, P. Geerlings, **Influence of stacking on the hydrogen bond donating capacity of nucleic bases**
18. Chemical Reactivity (Brussels, Belgium, 5th-7th of April 2006): K. Vanommeslaeghe, P. Mignon, S. Loverix, D. Tourwé, P. Geerlings, **Influence of stacking on the hydrogen bond donating capacity of nucleic bases**
19. 4th J&JPRD Symposium on Drug Discovery (Antwerp, Belgium, 7th-8th of April 2005): K. Vanommeslaeghe, S. Loverix, F. De Proft, C. Van Alsenoy, P. Geerlings, D. Tourwé, **Theoretical Study of the Catalytic Mechanism and Inhibition of a Histone Deacetylase Analogue.** (**nominated for Best Poster Award**)
20. The 15th European symposium on Quantitative Structure-Activity Relationships & Molecular Modelling (Istanbul, Turkey, 5th-10th of September 2004): K. Vanommeslaeghe, F. De Proft, S. Loverix, C. Van Alsenoy, D. Tourwé, P. Geerlings, **Theoretical Study of the Catalytic Mechanism and Inhibition of a Histone Deacetylase Analogue**
21. 10th International Conference on the Applications of Density Functional Theory (Brussels, Belgium 7th-12th of September 2003): K. Vanommeslaeghe, P. Geerlings, F. De Proft, C. Van Alsenoy, J. C. Martins, D. Tourwé, **Study of the catalytic mechanism and inhibition of a Histone Deacetylase analogue**
22. Second Swiss - French Meeting On Medicinal Chemistry (Beaune, France, 1st-4th of July 2003): K. Vanommeslaeghe, P. Geerlings, F. De Proft, C. Van Alsenoy, J. C. Martins, D. Tourwé, **Ab Initio study of the catalytic mechanism of a Histone Deacetylase analogue**
23. XVIIth International Symposium on Medicinal Chemistry (Barcelona, Spain, 1st-5th of September 2002): K. Vanommeslaeghe, P. Geerlings, F. De Proft, C. Van Alsenoy, J. C. Martins, D. Tourwé, **Ab Initio study of the binding of Trichostatin A (TSA) in the active site of Histone Deacetylase Like Protein (HDLP)**

Poster presentations at local conferences (listed only when presenting author)

24. 2nd Annual Mid-Atlantic Frontiers at the Chemistry-Biology Interface Symposium (Baltimore, MD, USA, 2nd of May 2009): K. Vanommeslaeghe, G. F. Da Silva, A. F. Gethu, X. Zhu, S. Zhong, L. Cerchietti, M. Matthews, J. M. Polo, A. Coop, G. G. Privé, A. Melnick, A. D. MacKerell Jr., **Idetification of binding sites for BCL-6 inhibitors and virtual screening**
25. Quantum Chemistry in Belgium: 7th edition (Mons, Belgium, 27th of January 2006): K. Vanommeslaeghe, S. Loverix, F. De Proft, C. Van Alsenoy, P. Geerlings, D. Tourwé, **Theoretical study of the catalytic mechanism and inhibition of a Histone Deacetylase analogue**
26. 7de Vlaams Jongerencongres van de Chemie (7th Flemish youth symposium on Chemistry, Ghent, Belgium, 16th of April 2004): K. Vanommeslaeghe, F. De Proft, S. Loverix, C. Van Alsenoy, D. Tourwé, P. Geerlings, **Theoretical Study of the catalytic mechanism and inhibition of a Histone Deacetylase analogue**
27. Quantum Chemistry in Belgium: VIth meeting (Ghent, Belgium, 21st of November 2003): K. Vanommeslaeghe, P. Geerlings, F. De Proft, C. Van Alsenoy, J. C. Martins, D. Tourwé, **Study of the catalytic mechanism and inhibition of a Histone Deacetylase analogue**

Contributions to the organization of international conferences

Assisted PI in the organization of international conferences

1. Chemical Reactivity (Brussels, Belgium, 5th-7th of April 2006)
2. 10th International Conference on the Applications of Density Functional Theory (Brussels, Belgium 7th-12th of September 2003)

Scientific community service

- Reviewer for *ACS Chemical Biology, Australian Journal of Chemistry, Current Medicinal Chemistry*, *European Journal of Medicinal Chemistry, Journal of Molecular Graphics and Modelling, Journal of Molecular Modeling, Journal of Physical Chemistry, PLOS ONE, Spectrochimica Acta A, Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation.*
- Assisted PI in reviewing manuscripts for *BMC Bioinformatics*, *Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation, Journal of Computational Chemistry*.
- Presided over "Drug Discovery: Methodology" session at the 244th American Chemical Society National Meeting (August 2012).

Society memberships

- American Chemical Society (2008-present)
- Biophysical Society (2007-present)

Professional skills

Languages:

- Native Dutch
- Equivalent-to-native English
- Moderate French
- Notions of German

Usage of scientific software

- Expert-level skills in the CHARMM molecular simulation program and the CHARMM force fields (lead developer of the CHARMM General Force Field and part of the community of developers of the CHARMM program)
- Proficiency in Sybyl, VMD, Dock, Gaussian, GaussView
- Working knowledge of MOE, Macromodel/Maestro, NAMD, 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 bonded 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 and HTML

Miscellaneous

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