

Curriculum vitae

Latest update: March 16, 2012

1. Professional

2011–present *Silicos-it (Schilde, Belgium)*

Founder and managing director

- Chemoinformatics and molecular modelling services: hands-on proof-of-concept work, consultancy, collaborative work and data generation;

2011–present *Apidermix (Antwerpen, Belgium) – Start-up in early proof-of-concept phase*

Scientific inspirator and project leader

- Leading a proof-of-concept project on innovative anti-inflammatory drugs in collaboration with the University of Antwerp (Belgium).

2005–2011 *Silicos NV (Diepenbeek, Belgium)*

Co-founder and chief scientific officer

- Setting up a small company and scientific management thereof;
- Hands-on fee-for-services in the fields of computational chemistry, virtual screening and characterization of compound databases
- Co-developer of the Open Babel C++ API and several open source applications
- Scientific support of the business development activities

2003–2005 *Johnson & Johnson Pharmaceutical Research & Development (Beerse, Belgium)*

Senior manager analytical development

- Project leader of the Aqua-project (optimisation of the method development, validation, and specification documentation processes within Analytical Development, Beerse).

1996–2003 *Johnson & Johnson Pharmaceutical Research & Development (Beerse, Belgium)*

Senior scientist molecular design and chemoinformatics

- Project leader of a number of structure-based drug design and virtual screening projects.
- Project leader of the Computational Chemistry Intrasite project

1995–1996 *Rega-Institute, K. U. Leuven (Leuven, Belgium)*

Post-doctoral scientist molecular modelling (Prof. Piet Herdewijn)

- Computational chemistry studies on modified oligonucleotides as antisense probes;
- Protein structure-based drug design on thymidine kinase.

1993–1995 *Victorian College of Pharmacy (Melbourne, Australia)*

Post-doctoral scientist computational chemistry (Prof. Mark von Itzstein)

- Computational chemistry studies on aldose reductase.

1992–1993 *Obligatory military service (Antwerpen and Gent, Belgium)*

Officer medical service

2. Education

- 1986–1992 *Ph.D. in the Pharmaceutical sciences (K. U. Leuven, Belgium)*
 ‘Modelling of antisense oligonucleotides based upon a crystal structure analysis of some pyranosyl nucleosides’, promotor: Prof. Dr. C. De Ranter
- 1981–1986 *Pharmaceutical sciences (K. U. Leuven, Belgium)*

3. Awards and fellowships

- 2006 *Tech-Art Award 2006*
 First prize for Silicos NV for the most innovative project entitled ‘An integrated in-silico platform for the design of drug-like molecules’
- 1993-1995 *Leuven Research Foundation Fellowship*
- 1993-1994 *NATO Fellowship*

4. Scientific bibliography

Peer-reviewed papers

1. Thijs, G.; Langenaeker, W.; **De Winter, H.** ‘Application of Spectrophores™ to map vendor chemical space using self-organising maps’, *J. Chemoinf.* (2011), **3** (Suppl. 1), 7.
2. Taminiau, J.; Thijs, G.; **De Winter, H.** ‘Pharao: Pharmacophore alignment and optimization’, *J. Mol. Graph. Model.* (2008), **27**, 161-169.
3. Baxter, E.W.; Conway, K.A.; Kennis, L.; Bischoff, F.; Mercken, M.H.; **De Winter, H.L.**; Reynolds, C.H.; Tounge, B.A.; Luo, C.; Scott, M.C.; Huang, Y.; Braeken, M.; Pieters, S.M.A.; Berthelot, D.J.C.; Masure, S.; Bruinzeel, W.D.; Jordan, A.D.; Parker, M.H.; Boyd, R.E.; Qu, J.; Alexander, R.S.; Brenneman, D.E.; Reitz, A.B. ‘2-Amino-3,4-dihydroquinazolines as inhibitors of BACE-1 (β -Site APP Cleaving Enzyme): use of structure based design to convert a micromolar hit into a nanomolar lead’, *J. Med. Chem.* (2007), **50**, 4261–4264.
4. Tinke, A.P.; Vanhoutte, K.; Vanhoutte, F.; De Smet, M.; **De Winter, H.** ‘Laser diffraction and image analysis as a supportive analytical tool in the pharmaceutical development of immediate release direct compression formulations’, *Int. J. Pharm.* (2005), **297**, 80-88.
5. Angibaud, P.; Arts, J.; Van Emelen, K.; Poncelet, V.; Pilatte, I.; Roux, B.; Van Brandt, S.; Verdonck, M.; **De Winter, H.**; Ten Holte, P.; Marien, A.; Floren, W.; Janssens, B.; Van Dun, J.; Aerts, A.; Van Gompel, J.; Gaurrand, S.; Queguiner, L.; Argouillon, J.M.; Van Hijfte, L.; Freyne, E.; Janicot, M. ‘Discovery of pyrimidyl-5-hydroxamic acids as new potent histone deacetylase inhibitors’, *Eur. J. Med. Chem.* (2005), **40**, 597-606.
6. **De Winter, Hans**; Breslin, Henry; Miskowski, Tamara; Kavash, Robert; Somers, Marijke ‘Inhibitor-based validation of a homology model of the active site of tripeptidyl peptidase II’, *J. Mol. Graph. Model.* (2004), **23**, 409-418.
7. Breslin, Henry J.; Miskowski, Tamara A.; Kukla, Michael J.; **De Winter, Hans L.**; Somers, Maria V.F.; Roevens, Peter W.M.; Kavash, Robert W. ‘Tripeptidyl peptidase II (TPP II) inhibitory activity of (S)-2,3-dihydro-2-(1H-imidazol-2-yl)-1H-indoles, a systematic SAR evaluation. Part 2’, *Bioorganic Med. Chem. Lett.* (2003), **13**, 4467-4471.
8. **De Winter, Hans**; Langenaeker, Wilfried. ‘In silico molecular properties at the desk of the bench researcher: the “Computational Chemistry Intrasilico”’, *Chimie Nouvelle* (2003), **21**, 78-81.
9. Breslin, Henry J.; Miskowski, Tamara A.; Kukla, Michael J.; Leister, William H.; **De Winter, Hans L.**; Gauthier, Diane A.; Somers, Maria V.F.; Peeters, Danielle C.G.; Roevens, Peter W.M. ‘Design, synthesis, and tripeptidyl peptidase II inhibitory activity of a novel series of (S)-2,3-dihydro-2-(4-alkyl-1H-imidazol-2-yl)-1H-indoles’, *J. Med. Chem.* (2002), **45**, 5303-5310.

10. Boon, Greet; Langenaeker, Wilfried; De Proft, Frank; **De Winter, Hans**; Tollenaere, Jan P.; Geerlinks, Paul. 'Systematic study of the quality of various quantum similarity descriptors. Use of the autocorrelation function and principal component analysis', *J. Phys. Chem. A* (2001), **105**, 8805-8814.
11. Froeyen, Mattheus; Wroblowski, Berthold; Esnouf, Robert; **De Winter, Hans**; Allart, Brigitte; Lescrinier, Eveline; Herdewijn, Piet. 'Molecular-dynamics studies of single-stranded hexitol, alritol, mannitol, and ribose nucleic acids (HNA, MNA, ANA, and RNA, resp.) and of the stability of HNA-RNA, ANA-RNA, and MNA-RNA duplexes', *Helv. Chim. Acta* (2000), **83**, 2153-2182.
12. Herdewijn, P.; Allart, B.; De Bouvere, B.; **De Winter, H.**; Hendrix, C.; Hossain, N.; Schepers, G.; Verheggen, I.; Wroblowski, B.; Van Aerschot, A. 'Properties of oligonucleotides with six membered carbohydrate mimics and a 1,4-relationship between the base moiety and the hydroxymethyl group', *Nucleosides Nucleotides* (1999), **18**, 1371-1376.
13. Peeters, Oswald M.; Blaton, Norbert M.; De Ranter, Camiel J.; **De Winter, Hans L.** '(+)-(2*R*-cis)-dimethyl-(10-bromo-2,3,3a,8-tetrahydridibenz[c,f]isoxazolo[2,3-a]azepine-2-yl-methyl)amine', *Acta Cryst.* (1999), **C55**, 794-796.
14. Engels, Michael F.M.; **De Winter, Hans**; Tollenaere, Jan P. 'A decision tree learning approach for the classification and analysis of high-throughput screening data', *Molecular modeling and prediction of bioactivity, Proceedings of the 12th European Symposium on QSAR*. (1998), Edited by Klaus Gundertofte and Flemming Steen Jorgensen, 429-430.
15. **De Winter, H.**; Lescrinier, E.; Van Aerschot, A.; Herdewijn, P. 'Molecular dynamics simulation to investigate differences in minor groove hydration of HNA/RNA hybrids as compared to HNA/DNA complexes', *J. Am. Chem. Soc.* (1998), **120**, 5381-5394.
16. De Bouvere, B.; Kerremans, L.; Hendrix, C.; **De Winter, H.**; Schepers, G.; Van Aerschot, A.; Herdewijn, P. 'Hexitol nucleic acids (HNA): synthesis and properties', *Nucleosides Nucleotides* (1997), **16**, 973-976.
17. Maurinsh, Yuris; Schraml, Jan; **De Winter, Hans**; Blaton, Norbert; Peeters, Oswald; Lescrinier, Eveline; Rozenski, Jef; Van Aerschot, Arthur; De Clercq, Erik; Busson, Roger; Herdewijn, Piet. 'Synthesis and conformational study of 3-hydroxy-4-(hydroxymethyl)-1-cyclo-hexanyl purines and pyrimidines', *J. Org. Chem.* (1997), **62**, 2861-2871.
18. Lescrinier, Theo; Busson, Roger; **De Winter, Hans**; Hendrix, Chris; Janssen, Gerard; Pannecouque, Christophe; Rozenski, Jef; Van Aerschot, Arthur; Herdewijn, Piet. 'α-Amino acids derived from ornithine as building blocks for peptide synthesis', *J. Pept. Res.* (1997), **49**, 183-189.
19. **De Winter, Hans**; Herdewijn, Piet. 'Understanding the binding of 5-substituted 2'-deoxyuridine substrates to thymidine kinase of herpes simplex virus type-1', *J. Med. Chem.* (1996), **39**, 4727-4737.
20. Luyten, Ingrid; **De Winter, Hans**; Busson, Roger; Lescrinier, Theo; Creuven, Isabelle; Durant, Francois; Balzarini, Jan; De Clercq, Erik; Herdewijn, Piet. 'Synthesis of 2'-deoxy-5-(iso-thiazol-5-yl)uridine and its interaction with the HSV-1 thymidine kinase', *Helv. Chim. Acta* (1996), **79**, 1462-1474.
21. **De Winter, Hans L.**; von Itzstein, Mark. 'Molecular modeling calculations on the binding of *D*- and *L*-xylose to wild-type aldose reductase and its H110Q and H110A mutants', *Adv. Exp. Med. Biol.* (1995), **372**, 223-227.
22. Doboszewski, Bogdan; **De Winter, Hans**; Van Aerschot, Arthur; Herdewijn, Piet. 'Synthesis of 3'-deoxy-3'-C-hydroxymethyl-aldopentopyranosyl nucleosides and their incorporation in oligo-nucleotides. Part II', *Tetrahedron* (1995), **51**, 12319-12336.
23. **De Winter, Hans L.**; von Itzstein, Mark. 'Aldose reductase as a target for drug design: molecular modeling calculations on the binding of acyclic sugar substrates to the enzyme', *Biochemistry* (1995), **34**, 8299-8308.
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27. Jottier, W. I.; **De Winter, H. L.**; Peeters, O. M.; Blaton, N. M.; De Ranter, C. J. 'Structure of the antipsychotic drug 3-{2-[4-(6-fluoro-1,2-benzisoxazol-3-yl)-1-piperidinyl]ethyl}-2,9-dimethyl-4H-pyrido[1,2-a]pyrimidin-4-one (Ocaperidone)', *Acta Cryst.* (1992), **C48**, 1827-1830.
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29. **De Winter, H. L.**; De Ranter, C. J.; Blaton, N. M.; Peeters, O. M.; Van Aerschot, A.; Herdewijn, P. 'Structural studies on modified nucleosides. Part XIV. 1-(2,3-Dideoxy-erythro- β -D-hexopyranosyl)cytosine: an example of the conformational and stacking properties of pyranosyl pyrimidine nucleosides: a crystallographic and computational approach', *Acta Crystallogr., Sect. B: Struct. Sci.* (1992), **B48**, 95-103.
30. Herdewijn, P. A. M.; Van Aerschot, A.; Balzarini, J.; De Clercq, E.; Everaert, D. H.; **De Winter, H. L.**; Peeters, O. M.; Blaton, N. M.; De Ranter, C. J. '3'-Fluoro- and 3'-azido-substituted 2',3'-dideoxynucleosides: structure-activity relationship', *Med. Chem. Res.* (1991), **1**, 9-19.
31. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J.; Van Aerschot, A.; Herdewijn, P. 'Structure studied on modified nucleosides. XII. Structure of 1-(2-deoxy-2-fluoro- α -D-arabinopyranosyl)-5-iodouracil', *Acta Cryst.* (1991), **C47**, 2245-2247.
32. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J.; Van Aerschot, A.; Herdewijn, P. 'Structural studies on modified nucleosides. XIII. Structures of two nucleoside analogs: 1-[(2R,6R)-6-hydroxymethyl-1,4-dioxan-2-yl]uracil and 5-bromo-1-[(2R,6R)-6-hydroxymethyl-1,4-dioxan-2-yl]uracil', *Acta Cryst.* (1991), **C47**, 2420-2423.
33. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J.; Van Aerschot, A.; Herdewijn, P. 'Structural studies of modified nucleosides. X. Structures of the 1-(2-deoxy-2-fluoro- β -D-arabinopyranosyl)thymine-water complex and 1-(2-deoxy-2-fluoro- β -D-arabinopyranosyl)-5-ethyluracil', *Acta Cryst.* (1991), **C47**, 1693-1697.
34. Jottier, W. I.; **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J. 'Structure of the antiviral drug ethyl 4-{2-[1-(6-methyl-3-pyridazinyl)-4-piperidinyl]ethoxy}benzoate', *Acta Cryst.* (1991), **C47**, 1517-1520.
35. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J.; Van Aerschot, A.; Herdewijn, P. 'Structural studies on modified nucleosides. VII. Structure of 1-(2-deoxy- β -D-ribosepyranosyl)-5-iodouracil', *Acta Cryst.* (1991), **C47**, 835-837.
36. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J.; Van Aerschot, A.; Herdewijn, P. 'Structural studies of modified nucleosides. VIII. Structures of 1-(2,3-dideoxy-erythro- α -D-hexopyranosyl)thymine and the 1-(2,3-dideoxy-erythro- β -D-hexopyranosyl)thymine.dioxane complex', *Acta Cryst.* (1991), **C47**, 838-842.
37. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J.; Van Aerschot, A.; Herdewijn, P. 'Structure of the modified nucleoside 2',3'-dideoxy-3'-fluorocytidine', *Acta Cryst.* (1991), **C47**, 832-835.
38. **De Winter, H. L.**; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J. 'Structure of the neuroleptic drug N-[(1-allyl-2-pyrrolidinyl)methyl]-6-methoxy-1H-benzotriazole-5-carboxamide hydrochloride (alizapride)', *Acta Cryst.* (1990), **C46**, 667-669.
39. **De Winter, H. L.**; Verlinde, C. L.; Blaton, N. M.; Peeters, O. M.; De Ranter, C. J. 'Structure of the neuroleptic drug 4-amino-N-1-[(1-ethyl-2-pyrrolidinyl)methyl]-5-(ethylsulfonyl)-2-methoxybenzamide (amisulpride)', *Acta Cryst.* (1990), **C46**, 313-317.

1. 'Computational Medicinal Chemistry and Drug Discovery', Patrick Bultinck, **Hans De Winter**, Jan P. Tollenaere, and Wilfried Langenaeker, editors. USA 2004, 794 pp. Publisher Marcel Dekker Inc., New York, N.Y.

Patents

1. **De Winter, Hans L. J.**; Langenaeker, Wilfried (2008, 2009) 'Method for evolving molecules and computer program for implementing the same', WO 2008/025571, EP1895436, EP2062184, HK 1130922 – transferred in 2011 to Virtual Proteins BV, The Netherlands.
2. **De Winter, Hans L. J.**; Langenaeker, Wilfried (2007, 2010) 'Descriptors of three-dimensional objects, uses thereof and a method to generate the same', WO 2009/146735, EP1862927, HK 1115654 – transferred in 2011 to Virtual Proteins BV, The Netherlands.
3. Van Emelen, Kristof; Arts, Janine; Backx, Leo J. J.; **De Winter, Hans L. J.**; Van Brandt, Sven F. A.; Verdonck, Marc G. C.; Meerpoel, Lieven; Pilatte, Isabelle N. Poncelet, Virginie S.; Dyatkin, Alexey B.; Van heusden, Jimmy A. V. (2004, 2007, 2011). 'Sulfonyl-derivatives as novel inhibitors of histone deacetylase', EP1485365, CA 2476586, KR 1020047011013, SG 2004054938.
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5. Van Emelen, Kristof; Arts, Janine; Backx, Leo J. J.; De Winter, Hans L. J.; Van Brandt, Sven F. A. (2004) 'Sulfonyl-derivatives as novel inhibitors of histone deacetylase', TW 092105283.
6. Van Emelen, Kristof; Arts, Janine; Backx, Leo J. J.; **De Winter, Hans L. J.**; Van Brandt, Sven F. A.; Verdonck, Marc G. C.; Meerpoel, Lieven; Pilatte, Isabelle N. C.; Poncelet, Virginie S.; Dyatkin, Alexey B. (2003) 'Sulfonyl-derivatives as novel inhibitors of histone deacetylase', WO 2003/076422, HK 1078311.
7. Van Emelen, Kristof; Backx, Leo J. J.; Van Brandt, Sven F. A.; Angibaud, Patrick R.; Pilatte, Isabelle N. C.; Verdonck, Marc G. C.; De Winter, Hans L. J.; Van Heusden, Jimmy A. V. (2004, 2007, 2011) 'Sulfonylamino-derivatives as novel inhibitors of histone deacetylase', CA 2476186, SG 2004054946, KR 1020047011020, TW 092105280.
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10. Baxter, Ellen; Boyd, Robert; Coats, Steve; Jordan, Alfonzo; Reitz, Allen; Reynolds, Charles H.; Scott, Malcolm; Schulz, Mark; **De Winter, Hans L. J.** (2006, 2007) 'Novel 2-amino-quinazoline derivatives useful as inhibitors of beta-secretase (bace)', WO 2006/017844, EP1776350, CN 200580034011.
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