

Wim Vranken
Academic
Department of Bio-engineering Sciences
Informatics and Applied Informatics
Chemistry
Basic (bio-) Medical Sciences
Postal address:
Pleinlaan 2
1050
Brussels
Belgium



Email: Wim.Vranken@vub.be
Phone: +32-2-6291996 (VUB), +32-2-6505943 (IB2)

Expertise

Structural Bioinformatics and computational biology

Prediction of biophysical characteristics of proteins from their sequence

Effect of amino acid variants on proteins and organisms

Computational aspects of Nuclear Magnetic Resonance (NMR)

Statistical analysis of NMR data in relation to protein structure

Structure determination of proteins from experimental NMR data

Qualifications

Chemistry, Ph.D., Ghent University

1 Dec 1992 → 19 Dec 1996

Award Date: 19 Dec 1996

Employment

Artificial Intelligence

Vrije Universiteit Brussel

Brussels, Belgium

2 Sep 2022 → present

Structural Biology Brussels

Vrije Universiteit Brussel

Brussels, Belgium

2 Sep 2022 → present

Basic (bio-) Medical Sciences

Vrije Universiteit Brussel

Brussels, Belgium

1 Oct 2021 → 30 Sep 2036

Chemistry

Vrije Universiteit Brussel

Brussels, Belgium

1 Oct 2021 → 30 Sep 2036

Department of Bio-engineering Sciences

Vrije Universiteit Brussel

Brussels, Belgium

1 Oct 2021 → 30 Sep 2036

Informatics and Applied Informatics

Vrije Universiteit Brussel
Brussels, Belgium
1 Oct 2021 → 30 Sep 2036

Academic

Basic (bio-) Medical Sciences
Vrije Universiteit Brussel
Brussels, Belgium
1 Oct 2016 → 30 Sep 2036

Academic

Chemistry
Vrije Universiteit Brussel
Brussels, Belgium
1 Oct 2016 → 30 Sep 2036

Academic

Informatics and Applied Informatics
Vrije Universiteit Brussel
Brussels, Belgium
1 Oct 2016 → 30 Sep 2036

Academic

Department of Bio-engineering Sciences
Vrije Universiteit Brussel
Brussels, Belgium
1 Feb 2012 → 30 Sep 2036

VUB director

Interuniversity Institute of Bioinformatics in Brussels
Brussels, Belgium
1 Apr 2014 → present

Maitre d'enseignement

Université libre de Bruxelles
Brussels, Belgium
1 Jan 2011 → present

Scientific officer (NMR)

European Bioinformatics Institute
Cambridge, United Kingdom
1 Oct 2001 → 30 Sep 2010

Research Fellow

Biotechnology Research Institute, National Research Council, Montreal
Canada
1 Jan 2000 → 31 Aug 2001

Postdoctoral researcher

Université libre de Bruxelles
Brussels, Belgium
1 Jan 1999 → 31 Dec 1999

Postdoctoral researcher

Biotechnology Research Institute, National Research Council, Montreal
Canada
1 Jan 1997 → 31 Dec 1998

Research output

Deciphering the RRM-RNA recognition code: A computational analysis

Roca Martinez, J., Dhondge, H. B., Sattler, M. & Vranken, W., 23 Jan 2023, In: PLoS Computational Biology. 19, 1, 24 p., e1010859.

Deep mutational scanning of essential bacterial proteins can guide antibiotic development

Dewachter, L., Brooks, A. N., Noon, K., Cialek, C., Clark-ElSayed, A., Schalck, T., Krishnamurthy, N., Versées, W., Vranken, W. & Michiels, J., 16 Jan 2023, In: Nature Communications. 14, 1, 16 p., 241.

Evolution of CRISPR-associated endonucleases as inferred from resurrected proteins

Alonso-Lerma, B., Jabalera, Y., Samperio, S., Morin, M., Fernandez, A., Hille, L. T., Silverstein, R. A., Quesada-Ganuza, A., Reifs, A., Fernández-Peñalver, S., Benitez, Y., Soletto, L., Gavira, J. A., Diaz, A., Vranken, W., Sanchez-Mejias, A., Güell, M., Mojica, F. J. M., Kleinstiver, B. P., Moreno-Pelayo, M. A. & 2 others, Montoliu, L. & Perez-Jimenez, R., Jan 2023, In: Nature Microbiology. 8, 1, p. 77-90 14 p.

Evolutionary adaptation of the protein folding pathway for secretability

Smets, D., Tsirigotaki, A., Smit, J. H., Krishnamurthy, S., Portaliou, A. G., Vorobieva, A., Vranken, W., Karamanou, S. & Economou, A., 1 Dec 2022, In: EMBO Journal. 41, 23, p. e111344

Panoramic Perspective on Human Phosphosites

Ramasamy, P., Vandermarliere, E., Vranken, W. F. & Martens, L., 5 Aug 2022, In: Journal of Proteome Research. 21, 8, p. 1894-1915 22 p.

Challenges in describing the conformation and dynamics of proteins with ambiguous behavior

Roca Martinez, J., Lazar, T., Gavalda Garcia, J., Bickel, D., Pancsa, R., Dixit, B., Tzavella, K., Ramasamy, P., Sanchez Fornaris, M., Grau, I. & Vranken, W., 3 Aug 2022, In: Frontiers in Molecular Biosciences. 9, 17 p., 959956.

Prediction of Disordered Regions in Proteins with Recurrent Neural Networks and Protein Dynamics

Orlando, G., Raimondi, D., Codicè, F., Tabaro, F. & Vranken, W., 30 Jun 2022, In: Journal of Molecular Biology. 434, 12, p. 167579 167579.

Evolutionary adaptation of the folding pathway for secretability

Smets, D., Tsirigotaki, A., Smit, J. H., Krishnamurthy, S., Portaliou, A. G., Vorobieva, A., Vranken, W., Karamanou, S. & Economou, A., 3 Apr 2022, In: BIORXIV. 2022, 51 p.

A roadmap to scientific software deployment: bio2Byte Tools as a use case

Gavalda Garcia, J., Díaz, A. & Vranken, W., 11 Mar 2022.

PDBe-KB: collaboratively defining the biological context of structural data

PDBe-KB consortium, 7 Jan 2022, In: Nucleic Acids Research. 50, D1, p. D534-D542 9 p.

MutaFrame - an interpretative visualization framework for deleteriousness prediction of missense variants in the human exome

Ancien, F., Pucci, F., Vranken, W. & Rooman, M., 1 Jan 2022, In: Bioinformatics. 38, 1, p. 265-266 2 p.

Massively parallel interrogation of protein fragment secretability using SECRiFY reveals features influencing secretory system transit

Boone, M., Ramasamy, P., Zuallaert, J., Bouwmeester, R., Van Moer, B., Maddelein, D., Turan, D., Hulstaert, N., Eeckhaut, H., Vandermarliere, E., Martens, L., Degroeve, S., De Neve, W., Vranken, W. & Callewaert, N., 5 Nov 2021, In: Nature Communications. 12, 1, 16 p., 6414.

Computational resources for identifying and describing proteins driving liquid-liquid phase separation

Panca, R., Vranken, W. & Mészáros, B., 2 Sep 2021, In: Briefings in Bioinformatics. 22, 5, bbaa408.

Interpreting a black box predictor to gain insights into early folding mechanisms

Grau, I., Nowé, A. & Vranken, W., Aug 2021, In: Computational and Structural Biotechnology Journal. 19, p. 4919-4930 12 p.

b2bTools: Online predictions for protein biophysical features and their conservation

Kagami, L. P., Gavalda Garcia, J., Roca Martinez, J. & Vranken, W., 15 Jun 2021.

b2bTools: online predictions for protein biophysical features and their conservation

Kagami, L. P., Orlando, G., Raimondi, D., Ancien, F., Dixit, B., Gavalda-García, J., Ramasamy, P., Roca-Martínez, J., Tzavella, K. & Vranken, W., 31 May 2021, In: Nucleic Acids Research. 49, W1, p. W52-W59 8 p.

Critical assessment of protein intrinsic disorder prediction

CAID Predictors & DisProt Curators, May 2021, In: Nature Methods. 18, 5, p. 472-481 10 p.

Online biophysical predictions for SARS-CoV-2 proteins

Kagami, L., Roca-Martínez, J., Gavalda-García, J., Ramasamy, P., Feenstra, K. A. & Vranken, W. F., 23 Apr 2021, In: BMC Cell Biology. 22, 1, 7 p., 23.

MobiDB: intrinsically disordered proteins in 2021

Piovesan, D., Necci, M., Escobedo, N., Monzon, A. M., Hatos, A., Micetic, I., Quaglia, F., Paladin, L., Ramasamy, P., Dosztanyi, Z., Vranken, W. F., Davey, N. E., Parisi, G., Fuxreiter, M. & Tosatto, S. C. E., 8 Jan 2021, In: Nucleic Acids Research. 49, D1, p. D361-D367 7 p.

Megabodies expand the nanobody toolkit for protein structure determination by single-particle cryo-EM

Uchański, T., Masiulis, S., Fischer, B., Kalichuk, V., López-Sánchez, U., Zarkadas, E., Weckener, M., Sente, A., Ward, P., Wohlkönig, A., Zögg, T., Remaut, H., Naismith, J. H., Nury, H., Vranken, W., Aricescu, A. R., Pardon, E. & Steyaert, J., Jan 2021, In: Nature Methods. 18, 1, p. 60-68 9 p.

Encore Abstract: Interpreting a Black-Box Predictor to Gain Insights into Early Folding Mechanisms

Grau, I., Nowé, A. & Vranken, W., 2021, p. 674-676. 3 p.

Fusion protein with a toxin and scaffold protein

Steyaert, J., Pardon, E. & Vranken, W., 2021, Patent No. EP3898658

Fusion proteins comprising a cytokine and scaffold protein

Steyaert, J., Pardon, E., Wohlkönig, A., Kalichuk, V., Vranken, W., Uchanski, T., Chevigné, A. & Szpakowska, M., 2021, Patent No. EP3898664

DynaMine v2, an updated version of the sequence-to-dynamics predictor

Gavalda Garcia, J., Roca Martinez, J. & Vranken, W., 27 Oct 2020.

Scop3P: A Comprehensive Resource of Human Phosphosites within Their Full Context

Ramasamy, P., Turan, D., Tichshenko, N., Hulstaert, N., Vandermarliere, E., Vranken, W. & Martens, L., 7 Aug 2020, In: Journal of Proteome Research. 19, 8, p. 3478-3486 9 p.

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Orlando, G., Silva, A., Macedo-Ribeiro, S., Raimondi, D. & Vranken, W., 1 Apr 2020, In: Bioinformatics. 36, 7, p. 2076-2081 6 p.

Distance-based metrics to compare disordered protein ensembles

Lazar, T., Guharoy, M., Vranken, W., Rauscher, S., Wodak, S. & Tompa, P., 13 Feb 2020.

DisProt: intrinsic protein disorder annotation in 2020

Hatos, A., Hajdu-Soltesz, B., Monzon, A. M., Palopoli, N., Alvarez, L., Aykac-Fas, B., Bassot, C., Benitez, G. I., Bevilacqua, M., Chasapi, A., Chemes, L., Davey, N., Davidovic, R., Dunker, A. K., Elofsson, A., Gobeill, J., Sudha, G., Guharoy, M., Horvath, T., Iglesias, V. & 43 others, Kajava, A. V., Kovacs, O. P., Lamb, J., Lambrugh, M., Lazar, T., Leclercq, J., Leonardi, E., Macedo-Ribeiro, S., Macossay Castillo, M., Maiani, E., Manso, J. A., Marino-Buslje, C., Martinez-Perez, E., Mészáros, B., Micetic, I., Minervini, G., Murvai, N., Necci, M., Ouzounis, C., Pajkos, M., Paladin, L., Pancsa, R. A., Papaleo, E., Parisi, G. D., Pasche, E., Pereira, P. J. B., Promponas, V. J., Pujols, J., Quaglia, F., Ruch, P., Salvatore, M., Schad, E., Szabo, B., Szaniszló, T., Tamana, S., Tantos, A., Veljković, N., Ventura, S., Vranken, W., Dosztányi, Z., Tompa, P., Tosatto, S. C. E. & Piovesan, D., 8 Jan 2020, In: Nucleic Acids Research. 48, D1, p. D269-D276 gkz975.

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Fusion protein with a toxin and scaffold protein

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Fusion proteins comprising a cytokine and scaffold protein

Steyaert, J., Pardon, E., Wohlkönig, A., Kalichuk, V., Vranken, W., Uchanski, T., Chevigné, A. & Szpakowska, M., 2020, Patent No. WO2020127983

Novel antigen-binding chimeric proteins and methods and uses thereof

Steyaert, J., Pardon, E., Uchanski, T. & Vranken, W., 2020, Patent No. EP3704160

Exploring the limitations of biophysical propensity scales coupled with machine learning for protein sequence analysis

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Computational identification of prion-like RNA-binding proteins that form liquid phase-separated condensates

Orlando, G., Raimondi, D., Tabaro, F., Codicé, F., Moreau, Y. & Vranken, W., 1 Nov 2019, In: Bioinformatics. 35, 22, p. 4617-4623 7 p.

RNAct: Enabling proteins with RNA recognition motifs for synthetic biology and bio-analytics

Gavalda Garcia, J., Roca Martinez, J. & Vranken, W., 25 Oct 2019.

An intrinsically disordered proteins community for ELIXIR

Davey, N. E., Babu, M. M., Blackledge, M., Bridge, A., Capella-Gutierrez, S., Dosztányi, Z., Drysdale, R., Edwards, R. J., Elofsson, A., Felli, I. C., Gibson, T. J., Gutmanas, A., Hancock, J. M., Harrow, J., Higgins, D., Jeffries, C. M., Le Mercier, P., Mészáros, B., Necci, M., Notredame, C. & 24 others, Orchard, S., Ouzounis, C. A., Pancsa, R., Papaleo, E., Pierattelli, R., Piovesan, D., Promponas, V. J., Ruch, P., Rustici, G., Romero, P., Santivijai, S., Saunders, G., Schuler, B., Sharan, M., Shields, D. C., Sussman, J. L., Tedds, J. A., Tompa, P., Turewicz, M., Vondrasek, J., Vranken, W. F., Wallace, B. A., Wichapong, K. & Tosatto, S. C. E., 15 Oct 2019, In: F1000Research. 8, 19 p., 1753.

Author Correction: Exploring the Sequence-based Prediction of Folding Initiation Sites in Proteins

Raimondi, D., Orlando, G., Pancsa, R., Khan, T. & Vranken, W. F., 15 Aug 2019, In: Scientific Reports - Nature. 9, 1, 12140.

Structural Basis of the Subcellular Topology Landscape of Escherichia coli

Loos, M. S., Ramakrishnan, R., Vranken, W., Tsirigotaki, A., Tsare, E-P., Zorzini, V., Geyter, J. D., Yuan, B., Tsamardinos, I., Klappa, M., Schymkowitz, J., Rousseau, F., Karamanou, S. & Economou, A., 24 Jul 2019, In: Frontiers in Microbiology. 10, p. 1-22 22 p., 1670.

Scop3P: the bridge between human phosphosites, protein structure and proteomics data

Ramasamy, P., Turan, D., Vandermarliere, E., Martens, L. & Vranken, W., Jul 2019, In: FEBS Open Bio. 9, p. 258-259 2 p.

Auto-encoding NMR chemical shifts from their native vector space to a residue-level biophysical index

Orlando, G., Raimondi, D. & Vranken, W. F., 7 Jun 2019, In: Nature Communications. 10, 1, 9 p., 2511.

Novel antigen-binding chimeric proteins and methods and uses thereof

Steyaert, J., Pardon, E., Uchanski, T. & Vranken, W., 2019, Patent No. WO2019086548

Large-scale in-silico statistical mutagenesis analysis sheds light on the deleteriousness landscape of the human proteome

Raimondi, D., Orlando, G., Tabaro, F., Lenaerts, T., Rooman, M., Moreau, Y. & Vranken, W. F., 19 Nov 2018, In: Scientific Reports - Nature. 8, 1, p. 16980 11 p., 16980.

Ultra-fast global homology detection with Discrete Cosine Transform and Dynamic Time Warping

Raimondi, D., Orlando, G., Moreau, Y. & Vranken, W. F., 15 Sep 2018, In: Bioinformatics. 34, 18, p. 3118-3125 8 p.

Biophysical validation of fully disordered proteins

Lazar, T., Váradi, M., Vranken, W., Guha Roy, M., Wodak, S. & Tompa, P., 3 Jul 2018.

Biophysical validation of fully disordered proteins

Lazar, T., Varadi, M., Vranken, W., Guha Roy, M., Wodak, S. J. & Tompa, P., 8 Feb 2018.

Lexicon visualization library and javascript for scientific data visualization

Tanyalcin, I., Assaf, C. A., Ferte, J., Ancien, F., Khan, T., Smits, G., Rooman, M. & Vranken, W., 1 Feb 2018, In: Computing in Science and Engineering. 20, 1, p. 50-65 16 p.

RINspect: a Cytoscape app for centrality analyses and DynaMine flexibility prediction

Brysbart, G., Lorgouilloux, K., Vranken, W. & Lensink, M. F., 15 Jan 2018, In: Bioinformatics. 34, 2, p. 294-296 3 p.

MobiDB 3.0: more annotations for intrinsic disorder, conformational diversity and interactions in proteins

Piovesan, D., Tabaro, F., Paladin, L., Necci, M., Micetic, I., Camilloni, C., Davey, N., Dosztányi, Z., Mészáros, B., Monzon, A. M., Parisi, G., Schad, E., Sormanni, P., Tompa, P., Vendruscolo, M., Vranken, W. F. & Tosatto, S. C. E., 4 Jan 2018, In: Nucleic Acids Research. 46, D1, p. D471-D476 6 p.

SVM-dependent pairwise HMM: an application to Protein pairwise alignments

Orlando, G., Raimondi, D., Khan, T., Lenaerts, T. & Vranken, W., 15 Dec 2017, In: Bioinformatics. 33, 24, p. 3902-3908 7 p.

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Varadi, M., De Baets, G., Vranken, W. F., Tompa, P. & Pancsa, R., 13 Oct 2017, In: Nucleic Acids Research. 46, D1, p. D387-D392 6 p.

Exploring the Sequence-based Prediction of Folding Initiation Sites in Proteins

Raimondi, D., Orlando, G., Pancsa, R., Khan, T. & Vranken, W. F., 18 Aug 2017, In: Scientific Reports - Nature. 7, 1, p. 8826 11 p., 8826.

DEOGEN2: prediction and interactive visualization of single amino acid variant deleteriousness in human proteins
Raimondi, D., Tanyalcin, I., Ferte, J., Gazzo, A., Orlando, G., Lenaerts, T., Rooman, M. & Vranken, W., 3 Jul 2017, In: Nucleic Acids Research. 45, W1, p. W201-W206

Seeing the Trees through the Forest: Sequence-based Homo- and Heteromeric Protein-protein Interaction sites prediction using Random Forest

Hou, Q., De Geest, P., Vranken, W. F., Heringa, J. & Feenstra, K. A., 15 May 2017, In: Bioinformatics. 33, 10, p. 1479-1487 9 p.

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Multilevel biological characterization of exomic variants at the protein level significantly improves the identification of their deleterious effects

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Early Folding Events, Local Interactions, and Conservation of Protein Backbone Rigidity

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Analysis of the structural quality of the CASD-NMR 2013 entries

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NMR Exchange Format: a unified and open standard for representation of NMR restraint data

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Computational approaches for inferring the functions of intrinsically disordered proteins

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Study of the structural and dynamic effects in the FimH adhesin upon α -D-heptyl mannose binding

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Small-Angle X-Ray Scattering- and Nuclear Magnetic Resonance-Derived Conformational Ensemble of the Highly Flexible Antitoxin PaaA2.

Sterckx, Y., Volkov, O., Vranken, W., Kragelj, J., Ringkjøbing Jensen, M., Buts, L., Garcia Pino, A., Jove, T., Van Melderen, L., Blackledge, M., Van Nuland, N. & Loris, R., 2014, In: *Structure*. 22, 6, p. 854-865 12 p.

The DynaMine webserver: predicting protein dynamics from sequence

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From protein sequence to dynamics and disorder with DynaMine

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