

## David W Ritchie (1959 – 2019) OBITUARY



David Ritchie was born in 1959 in Glasgow, Scotland. He obtained his PhD at the University of Aberdeen in 1998, under the supervision of Graham Kemp and John Forthergill, on the subject "Parametric Protein Shape Recognition". His thesis brought the foundation of his famous docking program Hex, using spherical polar Fourier correlations<sup>1</sup>, which made him a major figure in the worldwide docking community.

A few years later in 2008, as he was lecturer at the Department of Computing Science of the University of Aberdeen, Bernard Maigret, a french CNRS scientist who was also working with spherical harmonics for 3D shape comparison of chemical molecules, attracted him at the LORIA (Nancy) for a 3-year "Chaire Inria" for invited scientists. In 2009, he co-founded with Bernard Maigret, Marie-Dominique Devignes and Michel Souchet the Harmonic Pharma startup for applying his fast algorithms of 3D shape recognition to drug repositionning.

He was then recruited as an INRIA research director in 2011 and he founded the CAPSID team ("Computational Algorithms for Protein Structures and Interactions") in 2015. His major and most famous scientific contributions include the KPAX engine for flexible alignment of protein structures (post-doc of V. Venkatraman), the SAM program for docking symmetrical protein complexes (collaboration with S. Grudinin), the KBDOCK 3D database of protein domain interactions and binding sites for template-based docking (thesis of A. Ghoorah), and the gEM-tools for docking by fitting into cryo-EM maps (Post-Doc of T. Van Hoang).

Most recently, he supervised the development of EC- and GO-DomainMiner for automatic discovery of new protein domain annotations (Thesis Z. Alborzi), GrAPFI for the automatic functional annotation of protein sequences (thesis B. Sarker), and EROS-DOCK for protein docking by rotational search (Thesis M.-E. Ruiz Echarte).

People who worked with him mostly remember a brilliant, creative, rigorous and curious scientist, a constructive and always positive collaborator, as well as a modest, caring and humorous person. Dave was very fond of the scientific environment and working conditions of Inria/LORIA in Nancy. The nearby Vosges mountains and nature also allowed him to escape for long sporting hikes that he loved to share with his colleagues. A few months ago, he told his sister that his ten years in France were the happiest of his life.

We will miss him sorely.

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<sup>1</sup> *Accelerating and Focusing Protein-Protein Docking Correlations Using Multi-Dimensional Rotational FFT Generating Functions*. D.W. Ritchie, D. Kozakov, and S. Vajda (2008). [Bioinformatics](#), **24** 1865-1873.