Dave MacMillan was born in Bellshill, Scotland and received his undergraduate degree in chemistry at the University of Glasgow, where he worked with Dr. Ernie Colvin. In 1990, he began his doctoral studies under the direction of Professor Larry Overman at the University of California, Irvine, before undertaking a postdoctoral position with Professor Dave Evans at Harvard University (1996). He began his independent career at University of California, Berkeley in July of 1998 before moving to Caltech in June of 2000 (Earle C. Anthony Chair of Organic Chemistry). In 2006, Dave moved to the east coast of the US to take up the position of James S. McDonnell Distinguished University Professor at Princeton University and he became Department Chair in 2010.

Dave has received several awards including the ACS Award for Creativity in Organic Synthesis (2011), the Mitsui Catalysis Award (2011), ACS Cope Scholar Award (2007), ACS EJ Corey Award (2005), the Corday-Morgan Medal (2005).

In 2012 Dave became a Fellow of the Royal Society (FRS), and a Fellow of the American Academy of Arts and Sciences.

Dave is currently editor-in-chief of the new RSC journal "Chemical Sciences"

Dave is a member of the scientific advisory boards of Lexicon pharmaceuticals and Firmenich, and a permanent member of the RSRC board at Merck. He is also a scientific consultant with Merck (worldwide), Amgen (worldwide), Abbott Research Laboratories, Johnson & Johnson Pharmaceuticals, UCB-Celtech, Constellation Pharmaceuticals and Gilead Research Laboratories.

Along with Dr. Paul Reider, Dave is a co-founder of Chiromics LLC, a growing biotech that seeks to devise new strategies and screening techniques for the identification of drug-like molecules.