

Jonathan S. Mason PhD CChem FRSC



Jon is a Senior Research Fellow at Heptares Therapeutics in the UK leading Computer-Assisted Drug Design (CADD) approaches for GPCR structure-based drug design, scientifically responsible for the computational chemistry team and part of the scientific leadership team of Fiona Marshall (CSO). A 'high end' GPCR design approach combining structure, water energetics, lipophilic hotspots and biophysical data is being developed.

Jon has 34 years of global pharmaceutical drug discovery experience and is an experienced leader and scientific expert for drug design technologies (computational medicinal chemistry / CADD, structural biology, *in silico* ADME/tox etc). He previously led teams involving computational and lead discovery chemistry at Lundbeck in Copenhagen (Divisional Director), computational chemistry, structural biology, medicinal informatics and knowledge discovery at Pfizer in the UK (Executive Director MISD) and Bristol-Myers Squibb in the US (Director SB&M). Prior to these Jon was at Rhône-Poulenc Rorer (now Sanofi) in the UK, France and US, building and leading CADD teams.

Jon started his career as a synthetic medicinal chemist (PhD, Queen Mary, University of London), 5 years later becoming an early pioneer of the use of computational approaches in discovery research, particularly the development and use of 3D pharmacophore fingerprint methods for both protein structure-based drug design (SBDD) and ligand-based similarity/diversity approaches, together with *de novo* design & target class approaches. He later instigated the use of biological fingerprints to tackle attrition-related problems including lead selection / differentiation. Current focus includes fragment-based design and bringing full binding site water networks and their energetics into routine drug design as an essential component to enable more effective ligand design for GPCR and enzyme targets and new perspectives for druggability.