37 'Proteochemometrics Modelling': A Technique for the Design of GPCR Ligands, Kinase Inhibitors and Personalizing HIV Treatment

UNIVERSITY OF CAMBRIDGE

Oscar Méndez-Lucio, Qurrat ul Ain, Gerard JP van Westen, Bart Lenselink, Isidro Cortés-Ciriano, Therese Malliavin and Andreas Bender*

- Proteochemometric modelling (PCM) has recently been developed as a bioactivity modelling method.
- Combines the chemical (drug) and biological (protein target) space in a joint model.
- Relates a series of compounds with a series of targets.
- Usually performs better than QSAR as it integrates more information.

