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The aim of my work is to use a structure-based design approach in combination with parallel synthesis to generate libraries of potential blockers of AQP channels. The rational design of AQP blockers is made on existing inhibitors such as tetraethylammonium, in silico data-base methods, and molecular dynamics simulation.

My studies focused on the development of epoxyde ring opening (click) chemistry to access a variety of glycerol analogues, and to provide the basis for rational library design. Routes towards β-amino alcohols libraries are being developed using a wide range of commercially available amines, home-made epoxydes with microwave-assisted chemistry. This panel of new compounds will help us to optimise potential leads, achieve higher affinity and better selectivity towards AQP, and study their structure activity relationship.