

Analysing protein channels: From automatic detection to path exploration

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Channels are a common structural feature of proteins and play a crucial role for protein function. To simplify the analysis of protein channels we developed a program that automatically detects and generates a path through the channel.

Starting with the *Connolly* surface of the protein, we use a grid-based algorithm and *ray tracing* techniques to identify regions that form a channel. By applying heuristic operations it is then possible to define one access point for each channel entry. The determination of a path starting at a specific access point, leading through the channel and terminating at a different access point is achieved with a SSSP-algorithm (Single Source Shortest Path, here *Dijkstra* algorithm). A potential function guarantees the maximum distance between the path and the surface of the channel. Our approach is not restricted to special channel geometries, nor to a two access point channel (e.g. one entry, one exit). Even branched channels with more than two access points can be evaluated, resulting in more than one path.

The path information is utilised to easily navigate through the channel and generate camera flights for visual analysis of the channel environment (as implemented in our MOLCAD II program). In addition, physicochemical properties can be calculated along the path, revealing gradients of the properties between entry and exit of the channel. Exemplary results are presented for a cytochrome P450 enzyme and a 20S proteasome core particle.