

Structural studies of genomes and proteomes are essentially limited to a small number of dimensions. The primary structure of a polynucleotide or a polypeptide is a one-dimensional entity, whereas folded structures can be traced in three-dimensions, and their temporal changes can be described by adding time as a fourth dimension. In contrast, functional properties can be expressed in numerous dimensions defined by the parameters investigated.

In addition to the eventual goal of evolving enzymes with tailor-made activities, we wanted to explore the distribution of members of a mutant library in functional substrate-activity space. This information could provide a basis for choosing the optimal variants from a suitable 'quasi-species' of a mutant library (Eigen *et al.*, 1988) to be parents for a subsequent generation of mutants. The optimal parentage for a new generation is not limited to the mutants that have evolved the furthest in a desired direction, since their genetic background may be too narrow (Ness *et al.*, 1999). Therefore, the identification of an entire group of near-optimal mutants is an important task.

The gene superfamily of glutathione transferases (GSTs) illustrates how similar structures can display widely different properties. GSTs were originally discovered as a group of detoxication enzymes catalyzing the conjugation of a wide variety of electrophilic substances with the sulfhydryl group of the tripeptide glutathione (GSH) (Josephy and Mannervik, 2006). The three-dimensional structure is highly conserved