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Delaunay Tetrahedral Decomposition Structural Alignment. Jeffrey Roach, Shantanu Sharma, Charles W. Carter Jr., Dept. of Biochemistry, Univ. of North Carolina, Chapel Hill NC 27599.

Pairwise and multiple sequence alignments have become fundamental methods in bioinformatic analysis. Although these techniques provide evidence of evolutionary development, protein structure expresses more explicitly evolutionary relationships between individual proteins and protein families. To this end, a novel structural comparison and alignment solution has been developed.

The Delaunay tetrahedralization has shown to be a fairly robust representation of the geometric information inherent in the protein structure. Encoding the tetrahedralization in a one-dimensional representation that preserves much of the secondary structure, the problem of structural alignment is reduced to a problem of sequence alignment (*mutates mutandis*).

The program, Tetrahedral Decomposition Alignment (TetraDA), implementing this technique has been applied to pairwise analysis of the Class I and Class II aminoacyl-tRNA synthetase families. Extensions constraining RMSD and developing multiple structural alignment are discussed.