

Supporting Information

Table 1. Diverse FMN binding folds in the SCOP database^a

Names of folds	General characteristics of the fold
TIM beta/alpha-barrel [51350] ^b	Parallel β -sheet barrel, closed; n=8, S=8; strand order 12345678
Nqo1 FMN-binding domain-like [142018] ^b	3 layers, $\alpha/\beta/\alpha$; parallel β -sheet of 4 strands, order 3214
Cryptochrome/photolyase, N-terminal domain [52424] ^b	3 layers, $\alpha/\beta/\alpha$; parallel β -sheet of 5 strands, order 32145; Rossmann-like
Reductase/isomerase/elongation factor common domain [50412] ^b	Barrel, closed; n=6, S=10; greek-key motif
Split barrel-like [50474] ^b	Barrel; n=6, S=10; greek-key motif
NAD(P)-binding Rossmann-fold domains [51734] ^b	3 layers, $\alpha/\beta/\alpha$; parallel β -sheet of 6 strands, order 321456
Flavodoxin-like [52171] ^b	3 layers, $\alpha/\beta/\alpha$; parallel β -sheet of 5 strands, order 21345
Homo-oligomeric flavin-containing Cys decarboxylases, HFCD [52506] ^b	3 layers, $\alpha/\beta/\alpha$; parallel β -sheet of 6 strands, order 321456
Pyruvate kinase C-terminal domain-like [52934] ^b	3 layers, $\alpha/\beta/\alpha$; mixed β -sheet of 5 strands, order 32145, strand 5 is antiparallel to the rest
Dodecin subunit-like [88797] ^b	2 layers, α/β ; β - α - β (2); antiparallel β -sheet, strand order 132
Ferredoxin-like [54861] ^b	α + β sandwich with antiparallel β -sheet; (β - α - β)x2
FMN-dependent nitroreductase-like [55468] ^b	3 layers, $\alpha/\beta/\alpha$; core (α - β - α - β)x2; antiparallel β -sheet, strand order 1243

Profilin-like [55769] ^b	3 layers, $\alpha/\beta/\alpha$; core 2 α -helices; antiparallel β -sheet of 5 strands, order 21543;
Chorismate synthase, AroC [103262] ^b	3 layers, $\beta/\alpha/\beta$; duplication, consists of two DCoH-like $\beta(2)-\alpha-\beta(2)-\alpha$ structural repeats

^aThis SCOP (Structural Classification of Protein) database is a comprehensive ordering of all proteins with known structures according to their evolutionary, functional and structural relationships. This released version is 1.75.

^bThe numbers in parentheses refer to SCOP ID codes.