Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i  | Class Fold | \( N_i \) | TPR VAST | TPR SHEBA | Fold Name | Fold Description |
|----|-------------|-----------|----------|-----------|-----------|-----------------|
| 1  | a.137       | 3         | 0.000    | 0.167     | Non-globular all-alpha subunits of globular proteins |
| 2  | a.138       | 17        | 0.077    | 0.257     | Multiheme cytochromes | variable number of helices and little beta structure; not a true fold |
| 3  | a.100       | 10        | 0.078    | 0.400     | 6-phosphoglucuronate dehydrogenase C-terminal domain-like | multihelical; common core is formed around two long antiparallel helices related by (pseudo) twofold symmetry |
| 4  | a.43        | 2         | 0.000    | 0.500     | Met repressor-like | core: 4 helices; array of 2 hairpins, opened |
| 5  | a.116       | 5         | 0.400    | 0.650     | GTPase activation domain, GAP | multihelical |
| 6  | a.118       | 51        | 0.082    | 0.467     | alpha-alpha superhelix | multihelical; 2 (curved) layers: alpha-alpha; right-handed superhelix |
| 7  | a.93        | 7         | 0.714    | 0.762     | Heme-dependent peroxidases | multihelical; consists of two all-alpha domains |
| 8  | a.127       | 6         | 0.667    | 0.800     | L-aspartase-like | multihelical, consists of three all-alpha domains |
| 9  | a.133       | 5         | 0.300    | 0.600     | Phospholipase A2, PLA2 | common core: 2 helices, disulphide-linked, and a calcium-binding loop |
| 10 | a.102       | 25        | 0.528    | 0.960     | alpha-alpha toroid | multihelical; up to seven alpha-hairpins are arranged in closed circular array |
| 11 | a.126       | 6         | 0.667    | 0.800     | Serum albumin-like | multihelical; one domain consists of two similar disulphide-linked subdomains |
| 12 | a.3         | 32        | 0.158    | 0.877     | Cytochrome c | core: 3 helices; folded leaf, opened |
| 13 | a.115       | 2         | 0.000    | 1.000     | A virus capsid protein alpha-helical domain | multihelical; three-helical bundle in the core is surrounded by non-conserved helices |
| 14 | a.104       | 12        | 1.000    | 1.000     | Cytochrome P450 | multihelical |
| 15 | a.89        | 2         | 1.000    | 1.000     | Methyl-coenzyme M reductase alpha and beta chain C-terminal domain | multihelical bundle; contains buried central helix |
| 16 | a.96        | 6         | 0.800    | 1.000     | DNA-glycosylase | multihelical; consists of two all-alpha domains |
| 17 | a.128       | 7         | 0.500    | 0.952     | Terpenoid synthases | multihelical; core: 8 helices (C-J) are arranged in 2 parallel layers |
| 18 | a.99        | 3         | 1.000    | 1.000     | Cryptochrome/photolyase FAD-binding domain | multihelical; consists of two all-alpha subdomains |
| 19 | a.153       | 2         | 0.000    | 0.000     | Nuclear receptor coactivator interlocking domain | 3 helices, non-globular array; forms interlocked heterodimers with its targets |
| 20 | a.110       | 2         | 1.000    | 1.000     | Aldehyde ferredoxin oxidoreductase, C-terminal domains | multihelical; consists of two all-alpha domains |
| 21 | a.113       | 2         | 1.000    | 1.000     | DNA repair protein MutS, domain III | multihelical; consists of 2 all-alpha subdomains |
| 22 | a.123       | 11        | 1.000    | 1.000     | Nuclear receptor ligand-binding domain | multihelical; 3 layers or orthogonally packed helices |
| 23 | a.1         | 31        | 0.562    | 0.840     | Globin-like | core: 6 helices; folded leaf, partly opened |
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| $i$ | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name | Fold Description |
|-----|------------|-------|----------|-----------|-----------|------------------|
| 24  | a.86       | 4     | 0.333    | 1.000     | Di-copper centre-containing domain | multihelical |
| 25  | a.111      | 4     | 0.167    | 1.000     | Acid phosphatase/Vanadium-dependent haloperoxidase | multihelical; core: 5-helical bundle; binds cofactor at the beginning of third helix |
| 26  | a.119      | 2     | 1.000    | 1.000     | Lipoxigenase | multihelical |
| 27  | a.103      | 4     | 1.000    | 1.000     | Citrate synthase | multihelical; consists of two all-alpha domains |
| 28  | a.129      | 2     | 1.000    | 1.000     | GroEL equatorial domain-like chaperone equatorial domain | multihelical; 8 helices arranged in 2 parallel layers |
| 29  | a.124      | 3     | 0.667    | 1.000     | Phospholipase C/P1 nuclease | multihelical |
| 30  | a.28       | 9     | 0.139    | 0.694     | Acyl carrier protein-like | 4 helices, bundle; helix 3 is shorter than others; up-and-down |
| 31  | a.39       | 41    | 0.163    | 0.548     | EF Hand-like | core: 4 helices; array of 2 hairpins, opened |
| 32  | a.6        | 7     | 0.286    | 0.595     | Putative DNA-binding domain | core: 3 helices; architecture is similar to that of the "winged helix" fold but topology is different |
| 33  | a.19       | 2     | 1.000    | 1.000     | Fertilization protein | core: 3 helices; bundle, closed, right-handed twist; up-and-down |
| 34  | a.69       | 5     | 0.000    | 0.350     | Left-handed superhelix | core: 4-5 helices; bundle; left-handed superhelix |
| 35  | a.174      | 2     | 1.000    | 1.000     | Double Clp-N motif | multihelical; array |
| 36  | a.97       | 2     | 0.000    | 1.000     | An anticodon-binding domain of class I aminoacyl-tRNA synthetases | multihelical; consists of two all-alpha domains |
| 37  | a.41       | 2     | 1.000    | 1.000     | Domain of poly(ADP-ribose) polymerase | core: 4 helices: bundle; unusual topology |
| 38  | a.146      | 2     | 1.000    | 1.000     | Telomeric repeat binding factor (TRF) dimerisation domain | multihelical; can be divided into an alpha-alpha superhelix domain and a long alpha-haipin dimerisation domain |
| 39  | a.91       | 5     | 0.700    | 1.000     | Regulator of G-protein signalling, RGS | multihelical; consists of two all-alpha subdomains |
| 40  | a.121      | 2     | 0.000    | 1.000     | Tetracyclin repressor-like, C-terminal domain | multihelical; interlocked (homo)dimer |
| 41  | a.130      | 2     | 0.000    | 1.000     | Chorismate mutase II | multihelical; core: 6 helices, bundle |
| 42  | a.21       | 7     | 0.143    | 1.000     | HMG-box | 3 helices; irregular array |
| 43  | a.22       | 14    | 0.242    | 1.000     | Histone-fold | core: 3 helices; long middle helix is flanked at each end with shorter ones |
| 44  | a.55       | 5     | 0.600    | 0.750     | IHF-like DNA-binding proteins | core: 4 helices; bundle, partly opened, capped with a beta-sheet |
| 45  | a.38       | 2     | 0.000    | 1.000     | Helix-loop-helix DNA-binding domain | 4-helices; bundle, closed, left-handed twist; 2 crossover connections |
| 46  | a.105      | 2     | 1.000    | 1.000     | FIS-like | multihelical; intertwined dimer of identical 4-helical subunits |
| 47  | a.112      | 5     | 0.050    | 0.450     | RNA polymerase sigma subunit | multihelical; consists of several all-alpha subdomains |
| 48  | a.4        | 117   | 0.219    | 0.560     | DNA/RNA-binding 3-helical bundle | core: 3-helices; bundle, closed or partly opened, right-handed twist; up-and-down |
| 49  | a.60       | 29    | 0.074    | 0.422     | SAM domain-like | 4-5 helices; bundle of two orthogonally packed alpha-hairpins; involved in the interactions with DNA and proteins |
| i   | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name                                      | Fold Description                                                                 |
|-----|------------|-------|----------|-----------|-----------------------------------------------|--------------------------------------------------------------------------------|
| 50  | a.61       | 6     | 0.200    | 0.600     | Retroviral matrix proteins                     | 4-5 helices; right-handed superhelix                                           |
| 51  | a.74       | 17    | 0.787    | 0.938     | Cyclin-like                                    | core: 5 helices; one helix is surrounded by the others                        |
| 52  | a.79       | 2     | 1.000    | 1.000     | Antitermination factor NusB                    | 6 helices: bundle; one central helix is surrounded by 5 others                |
| 53  | a.11       | 5     | 0.900    | 1.000     | Acryl-CoA binding protein-like                 | core: 3 helices; bundle, closed, left-handed twist; up-and-down               |
| 54  | a.83       | 2     | 1.000    | 1.000     | Guanido kinase N-terminal domain               | irregular array of 6 short helices                                            |
| 55  | a.35       | 11    | 0.245    | 0.836     | lambda repressor-like DNA-binding domains      | core: 4 helices; folded leaf, closed                                           |
| 56  | a.77       | 12    | 0.962    | 0.992     | DEATH domain                                  | 6 helices: closed bundle; greek-key; internal pseudo twofold symmetry         |
| 57  | a.140      | 3     | 0.333    | 1.000     | LEM/SAP HeH motif                              | helix-extended loop-helix; parallel helices                                   |
| 58  | a.156      | 5     | 0.500    | 1.000     | S13-like H2TH domain                           | core: 3-4 helices                                                            |
| 59  | a.20       | 3     | 0.333    | 1.000     | PGBD-like                                     | core: 3 helices; bundle, closed, left-handed twist; parallel                  |
| 60  | a.40       | 6     | 0.667    | 0.967     | CH domain-like                                 | core: 4 helices; bundle                                                      |
| 61  | a.142      | 2     | 1.000    | 1.000     | PTS-regulatory domain, PRD                     | core: 4 helices; bundle, closed, right-handed twist; 1 crossover connection   |
| 62  | a.149      | 2     | 1.000    | 1.000     | RNase III endonuclease catalytic domain        | core: 5 helices; one helix is surrounded by the others                        |
| 63  | a.75       | 2     | 1.000    | 1.000     | Ribosomal protein S7                           | core: 5 helices; contains one more helix and a beta-hairpin outside the core  |
| 64  | a.144      | 4     | 0.167    | 0.750     | PABP domain-like                              | 4 helices; an orthogonal array                                               |
| 65  | a.5        | 10    | 0.167    | 0.756     | RuvA C-terminal domain-like                    | 3 helices; bundle, right-handed twist                                         |
| 66  | a.10       | 2     | 1.000    | 1.000     | Protozoan pheromone proteins                   | 3 helices; bundle, closed, left-handed twist, up-and-down                     |
| 67  | a.158      | 2     | 0.000    | 1.000     | F-box domain                                  | multihelical; interlocked heterodimer with the Skp1 dimerisation domain       |
| 68  | a.37       | 2     | 0.000    | 1.000     | A DNA-binding domain in eukaryotic transcription factors | 4 helices; the long C-terminal helix protrudes from the domain and binds to DNA |
| 69  | a.159      | 2     | 0.000    | 1.000     | Another 3-helical bundle                       | topologically similar to the DNA/RNA-binding bundles; distinct packing        |
| 70  | a.36       | 2     | 1.000    | 1.000     | Signal peptide-binding domain                 | 4 helices; orthogonal array                                                   |
| 71  | a.56       | 3     | 1.000    | 1.000     | CO dehydrogenase ISP C-domain like             | core: 4 helices, bundle                                                      |
| 72  | a.132      | 2     | 1.000    | 1.000     | Heme oxygenase                                | multihelical; bundle                                                          |
| 73  | a.25       | 14    | 0.346    | 0.670     | Ferritin-like                                  | core: 4 helices; bundle, closed, left-handed twist; 1 crossover connection    |
| 74  | a.87       | 6     | 0.633    | 1.000     | DBL homology domain (DH-domain)                | multihelical; core: 5-helical bundle                                          |
| 75  | a.29       | 12    | 0.197    | 0.576     | Bromodomain-like                               | 4 helices; bundle; minor mirror variant of up-and-down topology              |
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| i  | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name                                                                 | Fold Description                                                                                           |
|----|------------|-------|----------|-----------|---------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------|
| 76 | a.26       | 26    | 0.385    | 0.878     | 4-helical cytokines                                                       | core: 4 helices; bundle, closed; left-handed twist; 2 crossover connections                                |
| 77 | a.66       | 2     | 1.000    | 1.000     | Transducin (alpha subunit), insertion domain                              | 5 helices; folded leaf                                                                                   |
| 78 | a.48       | 3     | 0.000    | 0.333     | N-cbl like                                                                | 4 helices; bundle, left-handed twist; left-handed superhelix                                              |
| 79 | a.24       | 31    | 0.253    | 0.703     | Four-helical up-and-down bundle                                           | core: 4 helices; bundle, closed or partly opened, left-handed twist; up-and-down                           |
| 80 | a.73       | 3     | 1.000    | 1.000     | Retrovirus capsid protein, N-terminal core domain                         | core: 5 helices; bundle                                                                                   |
| 81 | a.80       | 4     | 1.000    | 1.000     | DNA polymerase III clamp loader subunits, C-terminal domain               | core: 5 helices: bundle                                                                                   |
| 82 | a.63       | 2     | 1.000    | 1.000     | Apolipoporhin-III                                                         | 5 helices; bundle, closed, left-handed twist                                                              |
| 83 | a.23       | 5     | 0.000    | 0.050     | Open three-helical up-and-down bundle                                     | core: 3 helices; bundle, open                                                                              |
| 84 | a.27       | 9     | 0.583    | 0.889     | Anticodon-binding domain of a subclass of class I aminoacyl-tRNA synthetases | core: 4 helices; bundle; one loop crosses over one side of the bundle                                       |
| 85 | a.45       | 20    | 0.779    | 1.000     | Glutathione S-transferase (GST), C-terminal domain                        | core: 4 helices; bundle, closed, left-handed twist; right-handed superhelix                               |
| 86 | a.46       | 4     | 0.500    | 1.000     | Methionine synthase domain-like                                           | 4 helices; bundle, left-handed twist; right-handed superhelix                                             |
| 87 | a.52       | 5     | 0.250    | 0.950     | Bifunctional inhibitor/lipid-transfer protein/seed storage 2S albumin      | 4 helices; folded leaf; right-handed superhelix                                                           |
| 88 | a.65       | 3     | 1.000    | 0.667     | Annexin                                                                   | 5 helices; folded leaf; closed                                                                            |
| 89 | a.85       | 2     | 1.000    | 1.000     | Hemocyanin, N-terminal domain                                              | 6 helices; bundle; one central helix is surrounded by 5 others                                           |
| 90 | a.64       | 5     | 0.300    | 0.750     | Saposin-like                                                              | 5 helices; folded leaf, closed                                                                            |
| 91 | a.71       | 3     | 1.000    | 1.000     | ERP29 C domain-like                                                       | 5 helices; bundle                                                                                         |
| 92 | a.16       | 2     | 0.000    | 1.000     | S15/N11 RNA-binding domain                                                | 3 helices; irregular array                                                                               |
| 93 | a.2        | 17    | 0.033    | 0.632     | Long alpha-hairpin                                                        | 2 helices; antiparallel hairpin, left-handed twist                                                        |
| 94 | a.47       | 5     | 0.200    | 1.000     | STAT-like                                                                 | 4 long helices; bundle, left-handed twist (coiled colil); right-handed superhelix                         |
| 95 | a.7        | 19    | 0.202    | 0.854     | Spectrin repeat-like                                                      | 3 helices; bundle, closed, left-handed twist; up-and-down                                               |
| 96 | a.44       | 2     | 1.000    | 1.000     | Disulphide-bond formation facilitator (DSBA), insertion domain            | 4 helices; bundle, partly opened, left-handed twist; up-and-down                                         |
| 97 | a.8        | 3     | 0.667    | 1.000     | immunoglobulin/albumin-binding domain-like                                | 3 helices; bundle, closed, left-handed twist; up-and-down; mirror topology to the spectrin-like fold     |
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| i   | Class Fold | N_i | TPR VAST | TPR SHEBA | Fold Name                                      | Fold Description                                                                 |
|-----|------------|-----|-----------|------------|------------------------------------------------|----------------------------------------------------------------------------------|
| 98  | b.68       | 14  | 0.912     | 0.978      | 6-bladed beta-propeller                          | consists of six 4-stranded beta-sheet motifs; meander                            |
| 99  | b.69       | 19  | 0.772     | 0.988      | 7-bladed beta-propeller                          | consists of seven 4-stranded beta-sheet motifs; meander                          |
| 100 | b.66       | 5   | 1.000     | 1.000      | 4-bladed beta-propeller                          | consists of four 4-stranded beta-sheet motifs; meander                           |
| 101 | b.67       | 2   | 1.000     | 1.000      | 5-bladed beta-propeller                          | consists of five 4-stranded beta-sheet motifs; meander                           |
| 102 | b.70       | 5   | 0.600     | 0.900      | 8-bladed beta-propeller                          | consists of eight 4-bladed beta-propeller; meander                               |
| 103 | b.1        | 241 | 0.701     | 0.680      | Immunoglobulin-like beta-sandwich                | sandwich; 7 strands in 2 sheets; greek-key                                       |
|     | b.2        | 27  | 0.368     | 0.425      | Common fold of diphtheria toxin/transcription    | sandwich; 9 strands in 2 sheet; greek-key; subclass of immunoglobin-like fold    |
|     |            |     |           |            | factors/cytchrome f                              |                                                                                  |
| 105 | b.3        | 11  | 0.673     | 0.582      | Prealbumin-like                                 | sandwich; 7 strands in 2 sheets, greek-key                                       |
| 106 | b.7        | 14  | 0.725     | 0.758      | C2 domain-like                                  | sandwich; 8 strands in 2 sheets; greek-key                                       |
| 107 | b.12       | 4   | 1.000     | 1.000      | Lipase/lipoxygenase domain                       | sandwich; 8 strands in 2 sheets; complex topology                               |
|     |            |     |           |            | (PLAT/LH2 domain)                                |                                                                                  |
| 108 | b.24       | 3   | 1.000     | 1.000      | Hyaluronate lyase-like, C-terminal domain        | sandwich, 10 strands in 2 sheets; "folded meander"                              |
| 109 | b.71       | 21  | 0.924     | 0.964      | alpha-Amylase, C-terminal beta-sheet domain      | folded sheet; greek-key                                                        |
| 110 | b.106      | 3   | 0.000     | 0.000      | Phage tail proteins                              | core: barrel; n=6, S=10; greek-key; topologically similar to the FWN-binding split barrel |
| 111 | b.85       | 13  | 0.192     | 0.250      | beta-clip                                       | double-stranded ribbon sharply bent in two places; the ribbon ends form          |
|     |            |     |           |            |                                                   | incomplete barrel; jelly-roll                                                  |
| 112 | b.82       | 31  | 0.277     | 0.359      | Double-stranded beta-helix                      | one turn of helix is made by two pairs of antiparallel strands linked with       |
|     |            |     |           |            |                                                   | short turns                                                                     |
| 113 | b.30       | 11  | 0.400     | 0.555      | Supersandwich                                   | sandwich; 18 strands in 2 sheets                                                |
| 114 | b.21       | 3   | 0.333     | 0.333      | Virus attachment protein                        | sandwich, 10 strands in 2 sheets; greek-key                                      |
| 115 | b.83       | 2   | 0.000     | 0.000      | Triple beta-spiral                              | trimer formed by the interlocking beta-hairpin repeat units                     |
| 116 | b.37       | 2   | 0.000     | 0.500      | N-terminal domains of the minor coat protein g3p | core: barrel, in some members open; n*=4, S*=8; meander                          |
| 117 | b.53       | 3   | 0.333     | 0.500      | Ribosomal protein L25-like                      | barrel, closed; n=6, S=10; complex topology                                     |
| 118 | b.29       | 33  | 0.455     | 0.729      | Concanavalin A-like lectins/glucanases          | sandwich; 12-14 strands in 2 sheets; complex topology                           |
| 119 | b.92       | 8   | 0.411     | 0.786      | Composite domain of metallo-                    | pseudobarrel; mixed sheet of 7 strand folded upon itself and "buckled" by two bet turns |
|     |            |     |           |            | dependent hydrolases                            |                                                                                  |
| 120 | b.45       | 4   | 0.833     | 0.750      | FMN-binding split barrel                        | barrel; n=6, S=10; greek-key                                                     |
| 121 | b.35       | 9   | 0.514     | 0.708      | GroES-like                                      | contains barrel, partly opened; n*=4, S*=8; meander                             |
| 122 | b.40       | 87  | 0.414     | 0.571      | OB-fold                                        | barrel, closed or partly opened n=5, S=10 or S=8; greek-key                      |
| 123 | b.84       | 14  | 0.275     | 0.522      | Barrel-sandwich hybrid                          | sandwich of half-barrel shaped beta-sheets                                      |
| 124 | b.42       | 24  | 0.998     | 0.835      | beta-Trefoil                                    | barrel, closed; n=6, S=12; and a hairpin triplet; meander                      |
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| i    | Class Fold | N_i | TPR VAST | TPR SHEBA | Fold Name                       | Fold Description                                                                 |
|------|------------|-----|----------|-----------|---------------------------------|----------------------------------------------------------------------------------|
| 125  | b.88       | 3   | 0.333    | 0.833     | Mss4-like                       | complex fold made of several coiled beta-sheets                                   |
| 126  | b.80       | 11  | 0.455    | 0.827     | Single-stranded right-handed    | superhelix with each turn made by 3 strands with short links                      |
|      |            |     |          |           | beta-helix                      |                                                                                   |
| 127  | b.81       | 9   | 1.000    | 0.972     | Single-stranded left-handed     | superhelix with each turn made by 3 strands with short links                      |
|      |            |     |          |           | beta-helix                      |                                                                                   |
| 128  | b.57       | 3   | 1.000    | 1.000     | Herpes virus serine proteinase,  | core: barrel, closed; n=7, S=8; complex topology                                 |
|      |            |     |          |           | assemblin                       |                                                                                   |
| 129  | b.47       | 31  | 0.920    | 0.994     | Trypsin-like serine proteases   | barrel, closed; n=6, S=8; greek-key                                               |
| 130  | b.77       | 5   | 0.900    | 1.000     | beta-Prism I                    | consists of 3 4-stranded sheets; strands are parallel to the 3-fold axis          |
| 131  | b.26       | 5   | 0.750    | 1.000     | SMAD/FHA domain                 | sandwich; 11 strands in 2 sheets; greek-key                                       |
| 132  | b.41       | 2   | 1.000    | 1.000     | Photosynthetic reaction centre, | core: barrel, partly opened; n*=5, S*=8; meander                                 |
|      |            |     |          |           | H-chain, cytoplasmic domain     |                                                                                   |
| 133  | b.87       | 4   | 0.667    | 1.000     | LexA/Signal peptidase           | complex fold made of several coiled beta-sheets; contains an SH3-like barrel      |
| 134  | b.62       | 2   | 1.000    | 1.000     | Cyclophilin (peptidylprolyl     | barrel, closed; n=8, S=10; complex topology                                       |
|      |            |     |          |           | isomerase)                      |                                                                                   |
| 135  | b.36       | 15  | 0.790    | 1.000     | PDZ domain-like                 | contains barrel, partly opened; n*=4, S*=8; meander; capped by alpha-helix       |
| 136  | b.118      | 2   | 1.000    | 1.000     | FAS1 domain                     | core: barrel, closed; n=7, S=12; meander                                          |
| 137  | b.113      | 4   | 1.000    | 1.000     | N-terminal domain of MutM-like  | pseudobarrel; capped on both ends by alpha-helices                                |
|      |            |     |          |           | DNA repair proteins             |                                                                                   |
| 138  | b.39       | 2   | 1.000    | 1.000     | Ribosomal protein L14           | barrel, closed; n=5, S=8, meander                                                |
| 139  | b.17       | 3   | 1.000    | 1.000     | PEBP-like                       | sandwich; 8 strands in 2 sheets; greek-key: partial topological similarity to immunoglobulin-like folds |
| 140  | b.6        | 38  | 0.908    | 0.922     | Cupredoxin-like                 | sandwich; 7 strands in 2 sheets, greek-key                                        |
| 141  | b.55       | 28  | 0.927    | 0.975     | PH domain-like                  | barrel, partly opened; n*=6, S*=12; meander; capped by an alpha-helix            |
| 142  | b.64       | 2   | 1.000    | 1.000     | Mannose 6-phosphate receptor    | barrel, partly open; n*=8, S*=10; one psi loop                                    |
|      |            |     |          |           | domain                          |                                                                                   |
| 143  | b.74       | 4   | 1.000    | 1.000     | Carbonic anhydrase              | single sheet; 10 strands                                                          |
| 144  | b.65       | 2   | 1.000    | 1.000     | triple barrel                   | dimer of two non-identical subunits; forms two similar barrels, n=8, S=10 each, that are fused together with the formation of third barrel, n=6, S=8 |
| 145  | b.46       | 2   | 1.000    | 1.000     | FMT C-terminal domain-like      | barrel, open; n*=6, S*=10; greek-key                                              |
| 146  | b.86       | 4   | 1.000    | 1.000     | Hedgehog/intein (Hint) domain   | complex fold made of five beta-hairpin units and a b-ribbon arc                   |
| 147  | b.50       | 12  | 0.697    | 0.682     | Acid proteases                  | barrel, closed; n=6, S=10, complex topology                                       |
| 148  | b.52       | 12  | 0.712    | 0.886     | Double psi beta-barrel          | barrel, closed; n=6, S=10; complex topology with crossover (psi) loops           |
| 149  | b.51       | 4   | 0.667    | 1.000     | ValRS/IleRS/LeuRS editing       | core: barrel, closed; n=6, S=8; topology is similar to that of the acid proteases barrel |
|      |            |     |          |           | domain                          |                                                                                   |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i   | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name | Fold Description |
|-----|------------|-------|----------|-----------|-----------|------------------|
| 150 | b.76       | 2     | 0.000    | 1.000     | open-sided beta-meander | single sheet formed by beta-hairpin repeats; exposed on both sides in the middle |
| 151 | b.91       | 2     | 1.000    | 1.000     | E2 regulatory, transactivation domain | complex fold made of bifurcated and coiled beta-sheets |
| 152 | b.11       | 11    | 0.909    | 0.955     | gamma-Crystallin-like | sandwich; 8 strands in 2 sheets; greek-key |
| 153 | b.93       | 2     | 1.000    | 1.000     | Epsilon subunit of F1F0-ATP synthase N-terminal domain | pseudobarrel: sandwich of two sheets packed at a positive interstrand angle and interconnected with many short turns |
| 154 | b.15       | 3     | 1.000    | 1.000     | HSP20-like chaperones | sandwich; 8 strands in 2 sheets; greek-key |
| 155 | b.63       | 2     | 1.000    | 1.000     | Oncogene products | barrel, closed; n=8, S=10; one overside connection |
| 156 | b.33       | 6     | 1.000    | 1.000     | ISP domain | consists of two all-beta subdomains: conserved small domain has a rubredoxin-like fold; larger domain consists of 6 beta-stands packed in either sandwich of two 3-stranded sheets or closed barrel (n=6; S=8) |
| 157 | b.8        | 3     | 1.000    | 1.000     | TRAF domain-like | sandwich; 8 strands in 2 sheets; greek-key |
| 158 | b.60       | 21    | 0.717    | 0.895     | Lipocalins | barrel, closed or opened; n=8, S=12; meander |
| 159 | b.61       | 9     | 0.917    | 0.903     | Streptavidin-like | barrel, closed; n=8, S=10; meander |
| 160 | b.43       | 27    | 0.769    | 0.724     | Reductase/isomerase/elongation factor common domain | barrel, closed; n=6, S=10; greek-key |
| 161 | b.49       | 4     | 0.500    | 0.500     | Domain of alpha and beta subunits of F1 ATP synthase-like | barrel, closed; n=6, S=8; greek-key |
| 162 | b.58       | 5     | 0.700    | 0.600     | PK beta-barrel domain-like | barrel, closed; n=7, S=10; complex topology |
| 163 | b.44       | 3     | 0.667    | 1.000     | EF-Tu/eEF-1alpha/eIF2-gamma C-terminal domain | barrel, closed; n=6, S=10; greek-key |
| 164 | b.107      | 2     | 1.000    | 1.000     | Urease metallochaperone UreE, N-terminal domain | barrel, closed; n=6, S=8; a crossover loop topology |
| 165 | b.4        | 2     | 1.000    | 1.000     | HSP40/DnaJ peptide-binding domain | sandwich; 6 strands in 2 sheets |
| 166 | b.34       | 52    | 0.407    | 0.604     | SH3-like barrel | barrel, partly opened; n*=4, S*=8; meander |
| 167 | b.38       | 10    | 0.911    | 1.000     | Sm-like fold | core: barrel, open; n*=4, S*=8; meander; SH3-like topology |
| 168 | b.56       | 2     | 1.000    | 1.000     | Transcription factor IIA (TFIIA), N-terminal domain | barrel, closed; n=6, S=12; mixed beta-sheet |
| 169 | b.72       | 10    | 0.322    | 0.600     | WW domain-like | core: 3-stranded meander beta-sheet |
| 170 | b.10       | 41    | 0.463    | 0.712     | Viral coat and capsid proteins | sandwich; 8 strands in 2 sheets; jelly-roll |
| 171 | b.19       | 6     | 0.367    | 0.500     | Viral protein domain | sandwich; 9 strands in 2 sheets; jelly-roll; form trimers |
| 172 | b.13       | 11    | 0.436    | 0.691     | Nucleoasmin/PINase F-like | sandwich; 8 strands in 2 sheets; jelly-rol |
| 173 | b.18       | 24    | 0.601    | 0.832     | Galactose-binding domain-like | sandwich; 9 strands in 2 sheets; jelly-roll |
| 174 | b.22       | 7     | 1.000    | 1.000     | TNF-like | sandwich, 10 strands in 2 sheets; jelly-rol |
| 175 | b.23       | 2     | 1.000    | 1.000     | Spermadhesin, CUB domain | sandwich, 10 strands in 2 sheets; jelly-rol |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i   | Class Fold | N_i | TPR  | TPR  | Fold Name                      | Fold Description                                                                 |
|-----|------------|-----|------|------|--------------------------------|-----------------------------------------------------------------------------------|
| 176 | c.1        | 182 | 0.863| 0.746| TIM beta/alpha-barrel         | contains parallel beta-sheet barrel; closed; n=8, S=8; strand order 12345678        |
| 177 | c.6        | 3   | 1.000| 1.000| Cellulases                    | variant of beta/alpha barrel; parallel beta-sheet barrel, closed, n=7, S=8; strand order 1234567 |
| 178 | c.10       | 18  | 0.546| 0.892| Leucine-rich repeat, LRR      | 2 curved layers, a/b; parallel beta-sheet; order 1234...N                           |
| 179 | c.14       | 11  | 0.827| 0.682| ClpP/crotonase                | core: 4 turns of (beta-beta-alpha)n superhelix                                     |
| 180 | c.12       | 2   | 1.000| 0.500| Ribosomal proteins L15p and L18e | core: three turns of irregular (beta-beta-alpha)n superhelix                       |
| 181 | c.7        | 4   | 0.833| 1.000| PFL-like glycyl radical enzymes | contains: barrel, closed; n=10, S=10; accommodates a hairpin loop inside the barrel |
| 182 | c.117      | 3   | 1.000| 1.000| Amidase signature (AS) enzymes | possible duplication: the topologies of N- and C-terminal halves are similar; 3 layers: a/b/a; single mixed beta-sheet of 10 strands, order 213549A867 (A=10); strands from 5 to 9 are antiparallel to the rest |
| 183 | c.83       | 2   | 1.000| 1.000| Aconitase iron-sulfur domain  | consists of three similar domains with 3 layers (a/b/a) each; duplication          |
| 184 | c.43       | 7   | 0.714| 0.833| CoA-dependent acyltransferases | core: 2 layers, a/b; mixed beta-sheet of 6 strands, order 324561; strands 3 & 6 are antiparallel to the rest |
| 185 | c.74       | 3   | 1.000| 1.000| AraD-like aldolase/epimerase  | 3 layers: a/b/a; mixed (mostly antiparallel) beta-sheet of 9 strands, order 432159876; left-handed crossover between strands 4 and 5 |
| 186 | c.107      | 2   | 0.000| 1.000| DHH phosphoesterases         | consists of two non-similar domains                                              |
| 187 | c.37       | 122 | 0.281| 0.283| P-loop containing nucleotide triphosphate hydrolases | 3 layers: a/b/a, parallel or mixed beta-sheets of variable sizes                  |
| 188 | c.92       | 11  | 0.455| 0.664| Chelatase-like                | duplication: tandem repeat of two domains; 3 layers (a/b/a); parallel beta-sheet of 4 strands, order 2134 |
| 189 | c.52       | 23  | 0.202| 0.294| Restriction endonuclease-like | core: 3 layers, a/b/a; mixed beta-sheet of 5 strands, order 12345; strands 2 & 5 are antiparallel to the rest |
| 190 | c.55       | 53  | 0.279| 0.379| Ribonuclease H-like motif     | 3 layers: a/b/a; mixed beta-sheet of 5 strands, order 32145; strand 2 is antiparallel to the rest |
| 191 | c.9        | 2   | 0.000| 0.000| Barstar-like                 | 2 layers, a/b; parallel beta-sheet of 3 strands, order 123                        |
| 192 | c.94       | 25  | 0.443| 0.790| Periplasmic binding protein-like II | consists of two similar intertwined domain with 3 layers (a/b/a) each: duplication |
| 193 | c.76       | 6   | 0.600| 1.000| Alkaline phosphatase-like     | core:3 layers: a/b/a; mixed beta-sheet of 8 strands, order 43516728, strand 7 is antiparallel to the rest |
| 194 | c.97       | 4   | 0.833| 0.750| Cytidine deaminase-like      | core: alpha-beta(2)-(alpha-beta)2; 3 layers (a/b/a); mixed beta-sheet of 4 strands, order 2134; strand 2 is antiparallel to the rest |
| 195 | c.47       | 51  | 0.908| 0.864| Thioredoxin fold             | core: 3 layers, a/b/a; mixed beta-sheet of 4 strands, order 4312; strand 3 is antiparallel to the rest |
| i  | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name                                                                 | Fold Description                                                                                                                                                                                                 |
|----|------------|------|----------|-----------|--------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 196| c.67       | 35   | 0.966    | 1.000     | PLP-dependent transferases                                                | main domain: 3 layers: a/b/a, mixed beta-sheet of 7 strands, order 3245671; strand 7 is antiparallel to the rest                                                                                     |
| 197| c.81       | 5    | 1.000    | 1.000     | Formate dehydrogenase/DMSO reductase, domains 1-3                        | contains two similar intertwined domains related by pseudodyad; duplication                                                                                                                                   |
| 198| c.22       | 2    | 1.000    | 1.000     | Ribosomal protein L4                                                      | 3 layers, a/b/a; core: parallel beta-sheet of 4 strands, order 1423                                                                                                                                      |
| 199| c.82       | 7    | 1.000    | 1.000     | ALDH-like                                                                | consists of two similar domains with 3 layers (a/b/a) each; duplication                                                                                                                                       |
| 200| c.77       | 4    | 1.000    | 1.000     | Isocitrate/Isopropylmalate dehydrogenases                                 | consists of two intertwined (sub)domains related by pseudodyad; duplication                                                                                                                                   |
| 201| c.109      | 4    | 1.000    | 1.000     | PEP carboxykinase N-terminal domain                                       | contains mixed beta-sheets; topology is partly similar to that of the catalytic C-terminal domain                                                                                                           |
| 202| c.91       | 4    | 0.917    | 1.000     | PEP carboxykinase-like                                                   | contains a P-loop NTP-binding motif; mixed beta-sheet folds into a barrel-like structure with helices packed on one side                                                                               |
| 203| c.68       | 15   | 0.948    | 0.981     | Nucleotide-diphospho-sugar transferases                                  | 3 layers: a/b/a; mixed beta-sheet of 7 strands, order 3214657; strand 6 is antiparallel to the rest                                                                                                 |
| 204| c.79       | 6    | 1.000    | 1.000     | Tryptophan synthase beta subunit-like PLP-dependent enzymes              | consists of two similar domains related by pseudodyad; duplication                                                                                                                                    |
| 205| c.8        | 10   | 0.422    | 0.644     | The "swivelling" beta/beta/alpha domain                                 | 3 layers: b/b/a; the central sheet is parallel, and the other one is antiparallel; there are some variations in topology                                                                          |
| 206| c.98       | 4    | 0.833    | 1.000     | MurF and HprK N-domain-like                                             | core: 3 layers, a/b/a; parallel beta-sheet of 4 strands, order 1234; structural similarity of the MurF and HprK extends beyond the core.                                                           |
| 207| c.86       | 2    | 1.000    | 1.000     | Phosphoglycerate kinase                                                 | consists of two non-similar domains, 3 layers (a/b/a) each                                                                                                                                            |
| 208| c.45       | 12   | 1.000    | 1.000     | (Phosphotyrosine protein) phosphatases II                                | core: 3 layers, a/b/a; parallel beta-sheet of 4 strands, order 1432                                                                                                                                        |
| 209| c.60       | 7    | 0.762    | 0.976     | Phosphoglycerate mutase-like                                            | core: 3 layers, a/b/a; mixed beta-sheet of 6 strands, order 324156; strand 5 is antiparallel to the rest                                                                                          |
| 210| c.71       | 8    | 1.000    | 1.000     | Dihydrofolate reductases                                                | 3 layers: a/b/a; mixed beta-sheet of 8 strands, order 34251687; strand 8 is antiparallel to the rest                                                                                              |
| 211| c.84       | 6    | 1.000    | 0.767     | Phosphoglucomutase, first 3 domains                                      | consists of three similar domains with 3 layers (a/b/a) each; duplication                                                                                                                                |
| 212| c.95       | 13   | 0.885    | 0.981     | Thiolase-like                                                            | consists of two similar domains related by pseudodyad; duplication                                                                                                                                     |
| 213| c.101      | 13   | 1.000    | 1.000     | Undecaprenyl diphosphate synthase                                       | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 342156                                                                                                                                      |
| 214| c.73       | 2    | 1.000    | 1.000     | Carbamate kinase-like                                                   | 3 layers: a/b/a; mixed (mainly parallel) beta-sheet of 8 strands, order 34215786; strand 8 is antiparallel to the rest                                                                 |
| 215| c.27       | 3    | 1.000    | 1.000     | Nucleoside phosphorylase/phosphoribosyltransferase catalytic domain     | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32145; Rossmann-like                                                                                                                        |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i  | Class | Fold | N_i | TPR  | TPR  | Fold Name | Fold Description |
|----|-------|------|-----|------|------|-----------|------------------|
| 216 | c.66  | 35   | 0.707 | 0.731 | S-adenosyl-L-methionine-dependent methyltransferases | core: 3 layers, a/b/a; mixed beta-sheet of 7 strands; strand 7 is antiparallel to the rest |
| 217 | c.72  | 15   | 0.771 | 0.714 | Ribokinase-like | core: 3 layers: a/b/a; mixed beta-sheet of 8 strands; order 21345678; strand 7 is antiparallel to the rest |
| 218 | c.87  | 6    | 0.533 | 0.933 | UDP-Glycosyltransferase/glycogen phosphorylase | consists of two non-similar domains with 3 layers (a/b/a) each |
| 219 | c.70  | 2    | 1.000 | 1.000 | Nucleoside hydrolase | core: 3 layers, a/b/a; mixed beta-sheet of 8 strands; order 31245687; strand 7 is antiparallel to the rest |
| 220 | c.35  | 3    | 1.000 | 0.667 | Phosphosugar hydrolase | core: 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 312456 |
| 221 | c.63  | 5    | 0.600 | 0.950 | CoA transferase | core: 3 layers: a/b/a; beta-sheet of 7 strands, order 4321567; part of sheet is folded upon itself and forms a barrel-like structure |
| 222 | c.106 | 2    | 1.000 | 1.000 | SurE-like | 3 layers: a/b/a; mixed beta-sheet of 9 strands, order 342156789; strands 3, 8 and 9 are antiparallel to the rest; left-handed crossover connection between strands 6 and 7 |
| 223 | c.18  | 2    | 1.000 | 1.000 | DNA glycosylase | 3 layers, a/b/a; core: parallel beta-sheet of 4 strands, order 2134 |
| 224 | c.51  | 13   | 0.718 | 0.718 | Anticodon-binding domain-like | 3 layers: a/b/a; core: parallel beta-sheet of 4 strands, order 2134 |
| 225 | c.39  | 2    | 1.000 | 1.000 | Nicotinate mononucleotide:5,6-dimethylbenzimidazole phosphoribosyltransferase (CobT) | 3 layers: a/b/a, parallel beta-sheet of 7 strands, order 3124567 |
| 226 | c.13  | 3    | 1.000 | 0.667 | SpoIIa-like | core: 4 turns of a (beta-alpha)n superhelix |
| 227 | c.36  | 19   | 0.982 | 0.933 | Thiamin diphosphate-binding fold (THDP-binding) | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 213465 |
| 228 | c.41  | 4    | 1.000 | 1.000 | Subtilisin-like | 3 layers: a/b/a, parallel beta-sheet of 7 strands, order 2314567; left-handed crossover connection between strands 2 & 3 |
| 229 | c.17  | 3    | 0.667 | 0.833 | Caspase-like | 3 layers: a/b/a; core: parallel beta-sheet of 4 strands, order 2134 |
| 230 | c.93  | 13   | 0.718 | 1.000 | Periplasmic binding protein-like 1 | consists of two similar intertwined domain with 3 layers (a/b/a) each: duplication |
| 231 | c.89  | 2    | 1.000 | 1.000 | Phosphofructokinase | consists of two non-similar domains, 3 layers (a/b/a) each |
| 232 | c.42  | 3    | 1.000 | 1.000 | Arginine/deacetylase | 3 layers: a/b/a, parallel beta-sheet of 8 strands, order 21387456 |
| 233 | c.50  | 2    | 1.000 | 1.000 | Leucine aminopeptidase (Aminopeptidase A), N-terminal domain | 3 layers: a/b/a; mixed beta-sheet of 5 strands, order 23145; strand 2 is antiparallel to the rest |
| 234 | c.56  | 24   | 0.757 | 0.761 | Phosphorylase/hydrolase-like | core: 3 layers, a/b/a; mixed beta-sheet of 5 strands: order 21354; strand 4 is antiparallel to the rest; contains crossover loops |
| 235 | c.69  | 51   | 0.847 | 0.892 | alpha/beta-Hydrolases | core: 3 layers, a/b/a; mixed beta-sheet of 8 strands, order 12435678; strand 2 is antiparallel to the rest |
| 236 | c.15  | 7    | 0.571 | 0.810 | BRCT domain | 3 layers, a/b/a; core: parallel beta-sheet of 4 strands, order 2134 |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i   | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name                                      | Fold Description                                                                 |
|-----|------------|------|----------|-----------|-----------------------------------------------|----------------------------------------------------------------------------------|
| 237 | c.80       | 6    | 0.867    | 0.833     | SIS domain                                    | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 21345                   |
| 238 | c.61       | 17   | 0.790    | 0.960     | PRTase-like                                   | core: 3 layers, a/b/a; mixed beta-sheet of 6 strands, order 321456; strand 3 is antiparallel to the rest |
| 239 | c.19       | 3    | 0.667    | 0.500     | FabD/lysophospholipase-like                   | core: 3 layers, a/b/a; mixed beta-sheet of 6 strands, order 432156; strand 4 is antiparallel to the rest |
| 240 | c.46       | 7    | 0.738    | 0.976     | Rhodanese/Cell cycle control phosphatase      | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32451                   |
| 241 | c.26       | 42   | 0.563    | 0.595     | Adenine nucleotid alpha hydrolase-like        | core: 3 layers, a/b/a; parallel beta-sheet of 5 strands, order 32145             |
| 242 | c.53       | 9    | 0.750    | 0.444     | Resolvase-like                                | Core: 3 layers: a/b/a; mixed beta-sheet of 5 strands, order 21345; strand 5 is antiparallel to the rest |
| 243 | c.58       | 11   | 0.491    | 0.555     | Aminoacid dehydrogenase-like, N-terminal domain | core: 3 layers: a/b/a; parallel beta-sheet of 4 strands; 2134                    |
| 244 | c.100      | 2    | 1.000    | 1.000     | Thiamin pyrophosphokinase, catalytic domain   | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 432156                 |
| 245 | c.28       | 4    | 1.000    | 1.000     | Cryptochrome/photolyase, N-terminal domain     | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32145; Rossmann-like     |
| 246 | c.25       | 12   | 1.000    | 1.000     | Ferredoxin reductase-like, C-terminal NADP-linked domain | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32145                   |
| 247 | c.24       | 3    | 1.000    | 1.000     | Methylglyoxal synthase-like                   | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32145                   |
| 248 | c.30       | 11   | 0.873    | 0.991     | PreATP-grasp domain                           | 3 layers: a/b/a; parallel or mixed beta-sheet of 4 to 6 strands                 |
| 249 | c.78       | 12   | 0.871    | 0.515     | ATC-like                                      | consists of two similar domains related by pseudodyad; duplication              |
| 250 | c.108      | 1    | 0.982    | 0.836     | HAD-like                                      | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 321456                 |
| 251 | c.116      | 5    | 1.000    | 1.000     | alpha/beta knot                               | core: 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 21435; contains a deep trefoil knot |
| 252 | c.31       | 10   | 0.978    | 0.822     | DHS-like NAD/FAD-binding domain               | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 321456; Rossmann-like |
| 253 | c.114      | 2    | 1.000    | 1.000     | YchN-like                                     | 3 layers: a/b/a, core: parallel beta-sheet of 5 strands, order 43215            |
| 254 | c.3        | 46   | 0.969    | 0.801     | FAD/NAD(P)-binding domain                    | core: 3 layers, b/b/a; central parallel beta-sheet of 5 strands, order 32145; top antiparallel beta-sheet of 3 strands, meander |
| 255 | c.4        | 7    | 1.000    | 0.952     | Nucleotide-binding domain                     | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32145; Rossmann-like  |
| 256 | c.49       | 6    | 0.867    | 0.633     | Pyruvate kinase C-terminal domain-like        | 3 layers: a/b/a; mixed beta-sheet of 5 strands, order 32145, strand 5 is antiparallel to the rest |
| 257 | c.59       | 5    | 1.000    | 1.000     | MurD-like peptide ligases, peptide-binding domain | 3 layers: a/b/a; mixed beta-sheet of 6 strands, order 126345; strand 1 is antiparallel to the rest |
| 258 | c.16       | 3    | 1.000    | 1.000     | Lumazine synthase                             | 3 layers, a/b/a; core: parallel beta-sheet of 4 strands, order 2134             |
| 259 | c.57       | 3    | 1.000    | 1.000     | Molybdenum cofactor biosynthesis proteins     | 3 layers: a/b/a; mixed beta-sheet of 5 strands; order 21354, strand 5 is antiparallel to the rest; permutation of the Phosphorylase/hydrolase-like fold |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i  | Class Fold | Ni | TPR VAST | TPR SHEBA | Fold Name                                                                 | Fold Description                                                                 |
|----|------------|----|----------|-----------|--------------------------------------------------------------------------|----------------------------------------------------------------------------------|
| 260| c.44       | 3  | 1.000    | 1.000     | Phosphotyrosine protein phosphatases I-like                              | 3 layers: a/b/a; parallel beta-sheet of 4 strands, order 2134                     |
| 261| c.48       | 5  | 1.000    | 1.000     | TK C-terminal domain-like                                               | 3 layers: a/b/a; mixed beta-sheet of 5 strands, order 13245, strand 1 is antiparallel to the rest |
| 262| c.2        | 99 | 0.885    | 0.741     | NAD(P)-binding Rossmann-fold domains                                     | core: 3 layers, a/b/a; parallel beta-sheet of 6 strands, order 321456           |
| 263| c.33       | 3  | 1.000    | 1.000     | Cysteine hydrolase                                                       | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 321456                 |
| 264| c.32       | 2  | 1.000    | 1.000     | Tubulin, GTPase domain                                                   | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 321456                 |
| 265| c.34       | 2  | 1.000    | 1.000     | DFP DNA/pantothenate metabolism flavoprotein                            | 3 layers: a/b/a; parallel beta-sheet of 6 strands, order 321456                 |
| 266| c.23       | 65 | 0.830    | 0.677     | Flavodoxin-like                                                          | 3 layers, a/b/a; parallel beta-sheet of 5 strand, order 21345                  |
| 267| c.62       | 8  | 1.000    | 0.982     | vWA-like                                                                 | core: 3 layers, a/b/a; mixed beta-sheet of 6 strands, order 32146; strand 3 is antiparallel to the rest |
| 268| c.65       | 3  | 1.000    | 1.000     | Formyltransferase                                                        | 3 layers: a/b/a; mixed beta-sheet of 7 strands, order 3214567; strand 6 is antiparallel to the rest |
| 269| c.5        | 2  | 1.000    | 1.000     | MurCD N-terminal domain                                                  | 3 layers: a/b/a; parallel beta-sheet of 5 strands, order 32145; incomplete Rossmann-like fold; binds UDP group |
| 270| d.142      | 20 | 0.482    | 0.516     | ATP-grasp                                                               | Consists of two subdomains with different alpha+beta folds                     |
| 271| d.143      | 3  | 0.333    | 0.333     | SAICAR synthase-like                                                     | consists of two alpha+beta subdomains                                          |
| 272| d.144      | 26 | 0.751    | 0.886     | Protein kinase-like (PK-like)                                            | consists of two alpha+beta domains, C-terminal domain is mostly alpha helical  |
| 273| d.104      | 15 | 0.810    | 0.900     | Class II aaRS and biotin synthetases                                     | contains large mixed beta-sheet                                               |
| 274| d.122      | 11 | 0.709    | 0.845     | ATPase domain of HSP90 chaperone/DNA topoisomerase II/histidine kinase    | 8 stranded mixed beta-sheet; 2 layers: alpha/beta                              |
| 275| d.14       | 16 | 0.633    | 0.738     | Ribosomal protein S5 domain 2-like                                       | core: beta(3)-alpha-alpha-alpha; 2 layers: alpha/beta; left-handed crossover  |
| 276| d.87       | 13 | 0.615    | 0.583     | CO dehydrogenase flavoprotein C-domain-like                             | core: beta(3,4)-alpha(3); alpha+beta sandwich                                  |
| 277| d.153      | 25 | 0.687    | 0.788     | Ntn hydrolase-like                                                       | 4 layers: alpha/beta/beta/alpha; has an unusual sheet-to-sheet packing        |
| 278| d.166      | 10 | 0.400    | 0.422     | ADP-ribosylation                                                         | unusual fold                                                                  |
| 279| d.184      | 2  | 0.000    | 0.000     | Non-globular alpha+beta subunits of globular proteins                   | (                                                                              |
| 280| d.4        | 4  | 0.000    | 0.250     | His-Me finger endonucleases                                              | core: (alpha)-beta-omega_loop-beta-alpha; embedded in larger different structures |
| 281| d.3        | 20 | 0.179    | 0.368     | Cysteine proteinases                                                     | consists of one alpha-helix and 4 strands of antiparallel beta-sheet and contains the catalytic triad Cys-His-Asn |
| 282| d.92       | 24 | 0.259    | 0.359     | Zincin-like                                                             | contains mixed beta sheet with connection over free side of the sheet          |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| Fold | TPR | TPR | Fold Name | Fold Description |
|------|-----|-----|-----------|------------------|
| 283  | 0.000 | 0.500 | SRCR-like unusual fold; disulphide-rich; core: beta-x-alpha-beta-loop-beta |
| 284  | 0.333 | 0.438 | FKBP-like core: beta(2)-alpha-beta(2); antiparallel beta-sheet |
| 285  | 0.000 | 0.000 | RPB5-like RNA polymerase subunit core: beta-alpha-beta-alpha-beta(2); 2 layers, alpha/beta |
| 286  | 0.152 | 0.614 | Lysozyme-like common alpha+beta motif for the active site region |
| 287  | 0.624 | 0.552 | Bacillus chorismate mutase-like core: beta-alpha-beta-alpha-beta(2); mixed beta-sheet: order 1423, strand 4 is antiparallel to the rest |
| 288  | 0.267 | 0.490 | Glyceraldehyde-3-phosphate dehydrogenase-like, C-terminal domain core: alpha-beta-alpha-beta(3); mixed sheet: 2134, strand 2 is parallel to strand 1 |
| 289  | 0.730 | 0.797 | C-type lectin-like unusual fold |
| 290  | 0.473 | 0.907 | Glyoxalase/Bleomycin resistance protein/Dihydroxybiphenyl dioxygenase beta-alpha-beta(3); 2 layers: alpha/beta |
| 291  | 0.611 | 0.637 | Profilin-like core: 2 alpha-helices and 5-stranded antiparallel sheet: order 21543; 3 layers: alpha/beta/alpha |
| 292  | 0.522 | 0.685 | Cystatin-like Core: alpha-beta(4); helix packs against coiled antiparallel beta-sheet |
| 293  | 0.697 | 0.697 | beta-hairpin-alpha-hairpin repeat multiple repeats of beta(2)-alpha(2) motif |
| 294  | 0.571 | 0.976 | DNA breaking-rejoining enzymes core: alpha3-beta3-alpha4; one side of beta-sheet is exposed |
| 295  | 1.000 | 1.000 | Argininosuccinate synthetase, C-terminal domain unusual fold |
| 296  | 1.000 | 1.000 | Molybdenum cofactor-binding domain beta(2)-alpha-beta-alpha-beta; 2 layers: a/b; mixed sheet: order 1243: crossing loops |
| 297  | 0.800 | 1.000 | Nudix beta(2)-alpha-beta(3)-alpha; 3 layers: alpha/beta/alpha; mixed sheet |
| 298  | 1.000 | 1.000 | ADC synthase duplication: contains four repeats of alpha-beta(2)-beta motif arranged in a 4 layer core structure: alpha/beta/beta/alpha; orthogonally packed beta-sheets |
| 299  | 1.000 | 1.000 | FAH unusual fold; contains 3 layers of beta-sheet structure |
| 300  | 1.000 | 1.000 | FAD-binding domain consists of two alpha+beta subdomains |
| 301  | 1.000 | 1.000 | Fibrinogen C-terminal domain-like unusual fold |
| 302  | 1.000 | 1.000 | Peptide deformylase alpha-beta(5)-alpha; 3 layers: a/b/a; meander beta-sheet wraps around the C-terminal alpha-helix |
| 303  | 1.000 | 1.000 | Nitric oxide (NO) synthase oxygenase domain unusual fold |
| 304  | 1.000 | 1.000 | Ribonuclease Rh-like alpha+beta fold |
| i  | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name                                                                 | Fold Description                                                                 |
|----|------------|------|----------|-----------|---------------------------------------------------------------------------|--------------------------------------------------------------------------------|
| 305| d.162      | 11   | 1.000    | 1.000     | Lactate & malate dehydrogenases, C-terminal domain                        | unusual fold, defines family                                                    |
| 306| d.185      | 13   | 0.718    | 0.981     | LuxS/MPP-like metallohydrolase                                            | core: beta-alpha-beta(2)-alpha(2); 2 layers: alpha/beta                        |
| 307| d.115      | 4    | 1.000    | 1.000     | YrdC/RibB                                                                 | core: alpha-beta(2)-alpha-beta-alpha(2)-beta(2)-alpha-beta-alpha-beta; 3 layers; mixed twisted sheet of 7 strands; order 7126354; strands 7 and 1 are parallel to each other |
| 308| d.165      | 7    | 1.000    | 1.000     | Ribosome inactivating proteins (RIP)                                      | contains mixed beta-sheet                                                       |
| 309| d.136      | 5    | 0.800    | 0.950     | Phospholipase D/nuclease                                                  | beta-alpha-beta-alpha-beta-alpha(4)-alpha; mixed sheet: order 1765234          |
| 310| d.157      | 7    | 1.000    | 1.000     | Metallo-hydrolase/oxidoreductase                                           | duplication of beta(4)-alpha-beta-alpha motif; 4 layers a/b/b/a; mixed beta-sheets |
| 311| d.108      | 15   | 0.790    | 0.876     | Acyl-CoA N-acyltransferases (Nat)                                          | 3 layers: a/b/a; contains mixed beta-sheet                                     |
| 312| d.109      | 14   | 0.621    | 0.934     | Gelsolin-like                                                             | 3 layers: a/b/a; contains mixed beta-sheet                                     |
| 313| d.117      | 3    | 1.000    | 1.000     | Thymidylate synthase/dCMP hydroyxymethylase                               | contains large mixed beta-sheet                                                |
| 314| d.168      | 4    | 0.833    | 1.000     | Succinate dehydrogenase/fumarate reductase flavoprotein, catalytic domain | unusual fold                                                                  |
| 315| d.73       | 2    | 1.000    | 1.000     | RuBiSCo, small subunit                                                    | alpha-beta(2)-alpha-beta(2); 2 layers, alpha/beta                            |
| 316| d.131      | 13   | 1.000    | 1.000     | DNA clamp                                                                | contains two helices and two beta sheets                                       |
| 317| d.44       | 3    | 0.667    | 1.000     | Fe,Mn superoxide dismutase (SOD), C-terminal domain                      | alpha-beta(2)-alpha-beta-alpha(2); 3 strands of antiparallel sheet: 213       |
| 318| d.118      | 2    | 0.000    | 1.000     | N-acetylmuramoyl-L-alanine amidase-like                                    | contains mixed beta-sheet                                                      |
| 319| d.126      | 5    | 0.900    | 1.000     | Penttein, beta/alpaha-propeller                                          | duplication: composed of 5 alpha-beta-beta(2)-alpha units arranged around pseudo fivefold axis |
| 320| d.106      | 2    | 1.000    | 1.000     | Sterol carrier protein, SCP                                              | alpha-beta(3)-(crossover)-beta-(alpha)-beta; 3 layers: a/b/a; antiparallel beta-sheet of 5 strands; order 32145 |
| 321| d.137      | 3    | 0.333    | 0.833     | Monoxygenase (hydroxylase) regulatory protein                            | corner-like structure formed by two sheets and filled in with 2-3 helices     |
| 322| d.75       | 3    | 1.000    | 0.667     | MutS N-terminal domain-like                                              | beta(2)-alpha-beta(2)-alpha; 2 layers, alpha/beta                            |
| 323| d.77       | 2    | 1.000    | 1.000     | Ribosomal protein L5                                                      | beta-alpha-beta(2)-alpha-beta(3)-alpha; 2 layers, alpha/beta; antiparallel beta-sheet: order 231654 |
| 324| d.175      | 2    | 0.000    | 1.000     | Penicillin binding protein dimerisation domain                            | unusual fold                                                                  |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i   | Class Fold | Ni | TPR VAST | TPR SHEBA | Fold Name | Fold Description |
|-----|------------|----|----------|-----------|-----------|-----------------|
| 325 | d.225      | 2  | 1.000    | 1.000     | Multidrug efflux transporter | Intertwined pseudo hexamer of an alpha+beta motif |
| 325 | d.225      | 2  | 1.000    | 1.000     | AcrB TolC docking domain; DN and DC subdomains |
| 326 | d.112      | 3  | 1.000    | 1.000     | Phosphotransferase/anion transport protein | beta-alpha(2)-beta(3)-alpha(3); 3 layers, alpha/beta/alpha; mixed sheet: order 1342; loop crossing |
| 327 | d.178      | 2  | 1.000    | 1.000     | Aromatic aminoacid monooxynogenases, catalytic and oligomerization domains | unusual fold |
| 328 | d.15       | 56 | 0.535    | 0.775     | beta-Grasp (ubiquitin-like) | core: beta(2)-alpha-beta(2); mixed beta-sheet 2143 |
| 329 | d.66       | 5  | 0.550    | 0.850     | Alpha-L RNA-binding motif | alpha(2)-beta(2)-loop-beta; 2 layers: alpha/beta |
| 330 | d.120      | 4  | 1.000    | 1.000     | Cytochrome b5 | small, heme-binding fold |
| 331 | d.42       | 6  | 0.867    | 1.000     | POZ domain | core: beta(2)-alpha(2)-beta(2)-alpha(2); 2 layers a/b; mixed sheet: 2143 |
| 332 | d.189      | 3  | 0.333    | 1.000     | PX domain | beta(3)-alpha(4); meander beta-sheet packed against array of helices; contains Pro-rich stretch |
| 333 | d.201      | 3  | 1.000    | 1.000     | SRP19 | beta-alpha-beta(2)-alpha; 2 layers: alpha/beta |
| 334 | d.1        | 5  | 0.400    | 1.000     | Microbial ribonucleases | single helix packs against antiparallel beta-sheet |
| 335 | d.24       | 3  | 0.833    | 1.000     | Pilin | contains very long N-terminal helix, which end is packed against beta-sheet |
| 336 | d.127      | 5  | 1.000    | 1.000     | Creatinase/aminopeptidase | duplication: composed of two very similar alpha+beta folds |
| 337 | d.21       | 2  | 1.000    | 1.000     | Diaminopimelate epimerase | mixed beta-sheet folds into a barrel (n=8, S=14) around the central helix |
| 338 | d.5        | 4  | 1.000    | 1.000     | RNase A-like | contains long curved beta-sheet and 3 helices |
| 339 | d.93       | 15 | 0.738    | 1.000     | SH2-like | 3 layers: a/b/a; antiparallel beta-sheet of 5 strands is flaked by two helices |
| 340 | d.88       | 2  | 0.000    | 1.000     | SRF-like | alpha-beta(2)-alpha; dimer; 3 layers a/b/a; antiparallel beta-sheet |
| 341 | d.18       | 2  | 0.000    | 0.000     | ssDNA-binding transcriptional regulator domain | helix-swapped dimer of beta(4)-alpha motifs |
| 342 | d.85       | 3  | 0.667    | 1.000     | RNA bacteriophage capsid protein | 6-standed beta-sheet followed with 2 helices; meander |
| 343 | d.217      | 2  | 1.000    | 1.000     | SAND domain-like | core: three short helices packed against a barrel-like beta-sheet; some similarity to the SH3-like fold |
| 344 | d.9        | 17 | 0.592    | 0.904     | IL8-like | beta(3)-alpha |
| 345 | d.101      | 2  | 0.000    | 1.000     | Polynucleotide phosphorylase/guanosine pentaphosphate synthase (PNPase/GPSI), domains 2 and 5 | beta(2)-alpha-beta(2)-alpha; 3 layers: alpha/beta/alpha; antiparallel sheet: order 2134 |
| 346 | d.19       | 15 | 0.881    | 0.971     | MHC antigen-recognition domain | dimeric |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i   | Class Fold | Nᵢ | TPR VAST | TPR SHEBA | Fold Name                                                                 | Fold Description                                                                 |
|-----|------------|----|----------|-----------|---------------------------------------------------------------------------|---------------------------------------------------------------------------------|
| 347 | d.83       | 2  | 0.000    | 1.000     | Bactericidal permeability-increasing protein, BPI                          | beta-alpha-beta(5)-alpha-beta2; 2 layers: alpha/beta; antiparallel sheet        |
| 348 | d.128      | 3  | 0.333    | 1.000     | Glutamine synthase/guanido kinase                                          |                                                                                 |
| 349 | d.179      | 2  | 1.000    | 1.000     | Substrate-binding domain of HMG-CoA reductase                              | unusual fold                                                                   |
| 350 | d.198      | 7  | 0.548    | 0.881     | Secretion chaperone-like                                                   | alpha-beta(3)-alpha-beta(2)-alpha; 2 layers: alpha/beta                       |
| 351 | d.100      | 2  | 1.000    | 1.000     | L9 N-domain-like                                                           | beta(2)-alpha-beta-alpha; 3 layers: alpha/beta/alpah                          |
| 352 | d.13       | 5  | 0.800    | 0.900     | HIT-like                                                                   | alpha-beta(3)-alpha-beta(2); 3 layers: alpha/beta/alpah                       |
| 353 | d.173      | 2  | 1.000    | 1.000     | Methionine synthase activation domain-like                                 | unusual fold; core: beta-alpha-beta(2)-beta(2)-alpha-beta-alpha-beta; antiparallel beta-sheet: order 12354 |
| 354 | d.90       | 4  | 1.000    | 1.000     | NADH oxidase/flavin reductase                                              | core: (alpha-beta-alpha-beta)2; 3 layers a/b/a; antiparallel beta-sheet: 1243   |
| 355 | d.6        | 2  | 0.000    | 1.000     | Prion-like                                                                 | beta-alpha-beta-alpha(2); antiparallel beta-ribbon                             |
| 356 | d.202      | 2  | 1.000    | 1.000     | Transcription factor NusA, N-terminal domain                               | alpha-beta(3)-alpha-beta-alpha; bifurcated coiled beta-sheet                    |
| 357 | d.218      | 6  | 0.733    | 1.000     | Nucleotidyltransferase                                                     | core: alpha-beta-turn-beta-X-beta-(alpha); mixed beta-sheet, order 123         |
| 358 | d.89       | 4  | 1.000    | 0.917     | Origin of replication-binding domain, RBD-like                             | alpha-beta-alpha-beta(2)-alpha-beta-alpha-beta; 3 layers: alpha/beta/a; antiparallel sheet 41325 |
| 359 | d.65       | 2  | 1.000    | 1.000     | Hedgehog/DD-pepidase                                                       | alpha-beta(2)-alpha-beta(2); 3 layers: alpha/beta                            |
| 360 | d.67       | 5  | 0.500    | 0.250     | RRF/tRNA synthetase additional domain-like                                 | core:alpha-beta(2)-alpha-beta(2); 2 layers: alpha/beta                        |
| 361 | d.181      | 2  | 1.000    | 1.000     | Insert subdomain of RNA polymerase alpha subunit                           | unusual fold; contains a left-handed beta-alpha-beta unit                       |
| 362 | d.212      | 3  | 0.333    | 0.333     | TolA/TonB C-terminal domain                                                | beta(2)-alpha-beta; 2 layers, alpha/beta; left-handed beta-alpha-beta unit in unswapped monomer |
| 363 | d.31       | 4  | 0.333    | 1.000     | Cdc48 domain 2-like                                                       | beta-alpha-beta(3); 2 layers: alpha/beta                                     |
| 364 | d.43       | 3  | 1.000    | 0.667     | Elongation factor Ts (EF-Ts), dimerisation domain                          | beta(2)-alpha(n)-beta; 2 layers a/b; antiparallel sheet: 123                 |
| 365 | d.96       | 7  | 1.000    | 1.000     | T-fold                                                                    | beta(2)-alpha(2)-beta(2); 2 layers: alpha/beta; antiparallel sheet 1234      |
| 366 | d.59       | 2  | 1.000    | 1.000     | Ribosomal protein L30p/L7e                                                 | core: beta-alpha-beta-alpha-beta; antiparallel beta-sheet: order 312; some similarity with the ferredoxin-like fold |
| 367 | d.10       | 5  | 0.600    | 0.450     | DNA-binding domain                                                         | beta(3)-alpha; 2 layers: alpha/beta                                         |
| 368 | d.50       | 9  | 0.611    | 0.778     | dsRBD-like                                                                | alpha-beta(3)-alpha; 2 layers: alpha/beta                                    |
| 369 | d.134      | 2  | 1.000    | 1.000     | Sulfite reductase hemoprotein (SiRHP), domains 2 and 4                     | beta-alpha-beta-alpha-beta(3)-alpha(2,3); mixed sheet: order 12345; left-handed crossover connection between strands 2 and 3 |
| 370 | d.20       | 8  | 0.857    | 1.000     | UBC-like                                                                  | alpha-beta(4)-alpha(3); core: meander beta-sheet plus one helix 2            |
| 371 | d.82       | 3  | 0.667    | 0.333     | N domain of copper amine oxidase-like                                      | alpha-beta(5)-alpha; 2 layers: alpha/beta; meander antiparallel sheet         |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i  | Class Fold | $N_i$ | TPR VAST | TPR SHEBA | Fold Name                                                                 | Fold Description                                                                                                                                 |
|----|------------|-------|-----------|-----------|---------------------------------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 372| d.111      | 2     | 1.000     | 1.000     | PR-1-like                                                                 | alpha-beta-alpha-beta-alpha-beta-alpha; 3 layers, alpha/beta/alpha; mixed sheet: order 1342                                                |
| 373| d.208      | 2     | 1.000     | 1.000     | MTH1598-like                                                               | beta(2)-alpha-beta-alpha-beta-alpha-beta(4); 3 layers: beta/alpha/beta; some similarity to the Hsp33 fold                                |
| 374| d.60       | 3     | 1.000     | 1.000     | Probable bacterial effector-binding domain                                | duplication of beta-alpha-beta(2) motif: antiparallel beta sheet forms barrel (n=6, S=12)                                              |
| 375| d.140      | 2     | 1.000     | 1.000     | Ribosomal protein S8                                                       | consists of 2 different alpha+beta subdomains arranged in a 4-layer structure: b/a/b/a                                                 |
| 376| d.68       | 10    | 0.422     | 0.611     | IF3-like                                                                   | beta-alpha-beta-alpha-beta(2); 2 layers; mixed sheet 1243, strand 4 is antiparallel to the rest                                      |
| 377| d.150      | 3     | 1.000     | 1.000     | 4'-phosphopantetheinyl transferase                                         | bet-alpha(3)-beta(2) motif                                                                                                                |
| 378| d.22       | 3     | 1.000     | 1.000     | GFP-like                                                                   | beta-sheet folds into a barrel (n=11, S=14) around the central helix                                                                     |
| 379| d.38       | 5     | 0.600     | 1.000     | Thioesterase/thiol ester dehydrase-isomerase                               | core: beta-alpha-beta(4); 2 layers: alpha/beta                                                                                         |
| 380| d.129      | 14    | 0.560     | 0.588     | TBP-like                                                                   | beta-alpha-beta(4)-alpha                                                                                                               |
| 381| d.16       | 14    | 0.418     | 0.753     | FAD-linked reductases, C-terminal domain                                   | alpha+beta sandwich                                                                                                                      |
| 382| d.41       | 10    | 0.711     | 0.800     | alpha/beta-Hammerhead                                                     | core: beta-BETA-alpha-beta-beta-beta-beta; contains a beta-hammerhead motif similar to that in barrel-sandwich hybrids             |
| 383| d.146      | 2     | 1.000     | 1.000     | Uridine diphospho-N-Acetylenolpyruvylglucosamine reductase, MurB, C-terminal domain | consists of two alpha+beta subdomains                                                                                                   |
| 384| d.86       | 2     | 1.000     | 1.000     | Translation initiation factor eIF4e                                        | beta(2)-alpha-beta-beta-beta-beta-beta-beta-beta; 2 layers: alpha/beta; antiparallel sheet: 21356478                            |
| 385| d.151      | 4     | 1.000     | 1.000     | DNase I-like                                                               | contains beta-sandwich; duplication of alpha+beta motif                                                                               |
| 386| d.160      | 3     | 1.000     | 1.000     | Nitrilase/N-carbamoyl-D-aminoacid amidohydrolase                           | 4 layers: alpha/beta/beta/alpha; mixed beta sheets; contains duplication                                                             |
| 387| d.159      | 8     | 0.643     | 0.982     | Metallo-dependent phosphatases                                             | 4 layers: alpha/beta/beta/alpha; mixed beta sheets; contains duplication                                                             |
| 388| d.12       | 2     | 0.000     | 0.500     | Ribosomal proteins L23 and L15e                                           | beta-(alpha)-beta-alpha-beta(2); 3 layers: alpha/beta/alpha; antiparallel beta-sheet: order 1243                                    |
| 389| d.95       | 8     | 0.679     | 0.946     | Homing endonuclease-like                                                  | alpha-beta(2)-alpha-beta(2)-alpha-beta(2)-alpha-beta-beta-beta; 2 layers: a/b; antiparallel sheet 1243                             |
| 390| d.206      | 2     | 1.000     | 1.000     | YggU-like                                                                  | beta(2)-loop-alpha-beta-alpha-beta-alpha-beta-alpha-beta; 2 layers: a/b; antiparallel sheet 1243; some similarity to the Homing endonuclease-like fold |
| 391| d.64       | 2     | 1.000     | 1.000     | eIF1-like                                                                  | beta(2)-alpha-beta(2)-alpha-beta; 2 layers: alpha/beta; mixed beta-sheet: order 51243                                               |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i  | Class Fold | \( N_i \) | TPR VAST | TPR SHEBA | Fold Name | Fold Description |
|----|------------|---------|----------|----------|-----------|------------------|
| 392 | d.54       | 8       | 0.964    | 1.000    | Enolase N-terminal domain-like | beta(3)-alpha(3); meander and up-and-down bundle |
| 393 | d.55       | 2       | 1.000    | 1.000    | Ribosomal protein L22 | beta-alpha(3)-beta(2); 2 layers: alpha/beta; related to the enolase/MLE N-domain fold by a circular permutation |
| 394 | d.11       | 2       | 1.000    | 1.000    | Penicillin-binding protein 2x (pbp-2x), c-terminal domain | alpha1-beta3; 2 layers: alpha/beta; order 132 |
| 395 | d.40       | 3       | 1.000    | 1.000    | CI-2 family of serine protease inhibitors | alpha+beta sandwich; loop across free side of beta-sheet |
| 396 | d.37       | 3       | 0.667    | 1.000    | CBS-domain | core: beta-alpha-beta(4); 2 layers: alpha/beta |
| 397 | d.130      | 3       | 0.667    | 1.000    | S-adenosylmethionine synthetase | duplication: consists of 3 similar intertwined domains |
| 398 | d.80       | 6       | 0.600    | 0.967    | Tautomerase/MIF | (beta-alpha-beta(2); 2 layers: alpha/beta; mixed beta-sheet |
| 399 | d.52       | 10      | 0.622    | 0.833    | Alpha-lytic protease prodomain-like | core: alpha-beta(2)-(alpha)-beta; 2 layers: alpha/beta |
| 400 | d.49       | 2       | 1.000    | 1.000    | Signal recognition particle alu RNA binding heterodimer, SRP9/14 | (beta)-alpha-beta(3)-alpha; 2 layers, alpha/beta |
| 401 | d.56       | 2       | 1.000    | 1.000    | GroEL-intermediate domain like | 3-helical bundle packed against 3-stranded mixed beta-sheet |
| 402 | d.105      | 2       | 1.000    | 1.000    | Clathrin adaptor appendage domain | beta-alpha-beta-alpha-beta(4)-alpha; 3 layers: a/b/a; bifurcated antiparallel beta-sheet |
| 403 | d.141      | 4       | 1.000    | 1.000    | Ribosomal protein L6 | consists of two beta-sheets and one alpha-helix packed around single core |
| 404 | d.94       | 4       | 1.000    | 1.000    | HPr-like | beta-alpha-beta(2)-alpha-beta(2)-alpha; 2 layers: a/b; antiparallel sheet 1423 |
| 405 | d.51       | 7       | 1.000    | 1.000    | Eukaryotic type KH-domain (eKH-domain) | beta-alpha(2)-beta(2)-alpha; 2 layers: alpha/beta |
| 406 | d.58       | 133     | 0.530    | 0.512    | Ferredoxin-like | alpha+beta sandwich with antiparallel beta-sheet; (beta-alpha-beta)2x2 |
| 407 | d.74       | 8       | 0.679    | 0.750    | DCoH-like | beta(2)-alpha-beta(2)-alpha; 2 layers, alpha/beta |
| 408 | d.45       | 2       | 1.000    | 1.000    | ClpS-like | beta-alpha(2)-beta-alpha-beta; 2 layers, alpha/beta |
| 409 | e.26       | 3       | 0.333    | 0.333    | Prismane protein-like | 3 domains: (1) spectrin repeat-like 3-helical bundle; (2 and 3) alpha/beta: Rossmann-fold topology |
| 410 | e.8        | 14      | 0.077    | 0.297    | DNA/RNA polymerases | ( |
| 411 | e.23       | 3       | 1.000    | 1.000    | Firefly luciferase-like | 4 domains: (1&2) duplication: share the same alpha/beta fold; (3) beta-barrel; (4) alpha+beta |
| 412 | e.5        | 3       | 1.000    | 1.000    | Heme-linked catalases | contains an (8,10) beta-barrel and an all-alpha domain |
| 413 | e.11       | 2       | 1.000    | 1.000    | Type II DNA topoisomerase | 4 domains: (1) toprim alpha/beta; (2) "winged helix"-like; (3) alpha+beta; (4) all-alpha |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i | Class Fold | N_i | TPR VAST | TPR SHEBA | Fold Name | Fold Description |
|---|------------|-----|----------|-----------|-----------|------------------|
| 414 | e.25 | 2 | 1.000 | 1.000 | Sec1/munc18-like (SM) proteins | 3 domains: (1 and 2) alpha+beta; (3) mostly alpha, inserted in domain 2 |
| 415 | e.3 | 14 | 1.000 | 1.000 | beta-Lactamase/D-ala carboxypeptidase | contains a cluster of helices and an alpha+beta sandwich |
| 416 | e.10 | 3 | 1.000 | 1.000 | Prokaryotic type II DNA topoisomerase | 4 domains: (1) Toprim alpha/beta; (2&4) "winged helix"-like; (3) barrel: n=6, S=8 |
| 417 | e.1 | 6 | 1.000 | 1.000 | Serpins | contains a cluster of helices and a beta-sandwich |
| 418 | e.6 | 5 | 1.000 | 1.000 | Acyl-CoA dehydrogenase NM domain-like | 2 domains: (1) all-alpha: 5 helices; (2) contains an open beta-sheet barrel: n*=5, S*=8; complex topology |
| 419 | e.18 | 2 | 1.000 | 1.000 | Nickel-iron hydrogenase, large subunit | 3 domains: (1) all-alpha; (2&3) alpha+beta |
| 420 | e.4 | 2 | 1.000 | 1.000 | ADP ribosyl cyclase-like | contains a cluster of helices and an alpha/beta domain |
| 421 | e.24 | 3 | 0.667 | 1.000 | Ribosomal protein L1 | 2 domains: (1) alpha+beta; (2) alpha/beta (interrupts domain 1) |
| 422 | e.17 | 4 | 1.000 | 1.000 | D-aminoacid aminotransferase-like PLP-dependent enzymes | 2 domains: (1) alpha+beta: beta3-alpha2-beta2; (2) alpha/beta, a part of its mixed sheet forms barrel: n=6, S=8 |
| 423 | e.39 | 2 | 1.000 | 1.000 | YebC-like | 3 domains: (1) 3-helical bundle; (2 and 3 ) alpha+beta of different folds: domain 3 has a ferredoxin-like fold and is inserted in domain 2 |
| 424 | e.7 | 7 | 1.000 | 1.000 | Sugar phosphatases | N-terminal domain is an alpha+beta, C-terminal domain is an alpha/beta with mixed beta-sheet |
| 425 | e.31 | 2 | 1.000 | 1.000 | Ku heterodimer subunits | 3 domains: (1) integrin A-like alpha/beta; (2) beta-barrel (n=7, s=10); (3) helical arm with an HTH motif |
| 426 | e.22 | 3 | 1.000 | 1.000 | Dehydroquinate synthase-like | 2 domains: (1) alpha/beta of a Rossmann-fold topology, binds NAD (2) multihelical array |
| 427 | f.4 | 14 | 0.192 | 0.654 | Transmembrane beta-barrels | not a true fold, gathers together transmembrane barrels of different (n,S) |
| 428 | f.7 | 3 | 0.000 | 0.167 | Lipovitellin-phosvitin complex; beta-sheet shell regions | multi-helical domains of various folds which is thought to unfold in the membrane |
| 429 | f.1 | 11 | 0.145 | 0.182 | Toxins' membrane translocation domains | not a true fold |
| 430 | f.23 | 5 | 0.000 | 0.500 | Single transmembrane helix | multi-helical domains of various folds which is thought to unfold in the membrane |
| 431 | f.21 | 7 | 0.143 | 0.619 | Heme-binding four-helical bundle | core: four transmembrane helices, up-and-down bundle, binds one or two heme groups in between the helices |
| 432 | f.26 | 2 | 1.000 | 1.000 | Bacterial photosystem II reaction centre, L and M subunits | five transmembrane helices forming a sheet-like structure |
| 433 | f.19 | 2 | 1.000 | 1.000 | Aquaporin-like | core: 8 helices, 2 short helices are surrounded by 6 long transmembrane helices |
| 434 | f.10 | 2 | 0.000 | 1.000 | Viral glycoprotein, central and dimerisation domains | 2 intertwined domains; all-beta and alpha+beta |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| i   | Class | Fold | \(N_i\) | TPR\_VAST | TPR\_SHEBA | Fold Name                                           | Fold Description                                                                                                                                 |
|-----|-------|------|---------|-----------|------------|----------------------------------------------------|---------------------------------------------------------------------------------------------------------------------------------------------------|
| 435 | f.6   | 2    | 1.000   | 1.000     |            | Leukocidin (pore-forming toxin)                     | subunit fold contains beta-sandwich of Ig-like (greek-key) topology                                                                               |
| 436 | f.35  | 2    | 1.000   | 1.000     |            | Multidrug efflux transporter AcrB transmembrane domain | 12 transmembrane helices; duplication: the N- and C-terminal halves of the whole proteins are structurally similar                                  |
| 437 | f.17  | 2    | 0.000   | 1.000     |            | Transmembrane helix hairpin                         | two antiparallel transmembrane helices                                                                                                           |
| 438 | f.27  | 2    | 1.000   | 1.000     |            | 14 kDa protein of cytochrome bc1 complex (Ubiquinol-cytochrome c reductase)                     | membrane-associated alpha-helical protein; no transmembrane helices                                                                               |
| 439 | f.13  | 4    | 0.500   | 1.000     |            | Family A G protein-coupled receptor-like             | core: up-and-down bundle of seven transmembrane helices tilted 20 degrees with respect to the plane of the membrane                         |
| 440 | f.24  | 3    | 1.000   | 1.000     |            | Cytochrome c oxidase subunit I-like                 | 12 transmembrane helices in an approximate threefold rotational symmetric arrangement                                                             |
| 441 | f.25  | 2    | 1.000   | 1.000     |            | Cytochrome c oxidase subunit III-like               | core: 7 transmembrane helices organised into two bundles, one formed by the first two helices and the other by the rest                             |
| 442 | f.14  | 2    | 0.000   | 1.000     |            | Voltage-gated potassium channels                    | oligomeric transmembrane alpha-helical proteins                                                                                                   |
| 443 | f.28  | 2    | 1.000   | 1.000     |            | Nonheme 11 kDa protein of cytochrome bc1 complex (Ubiquinol-cytochrome c reductase)               | membrane-associated alpha-helical protein; no transmembrane helices                                                                               |
| 444 | g.39  | 12   | 0.152   | 0.636     |            | Glucocorticoid receptor-like (DNA-binding domain) | alpha-beta metal(zinc)-bound fold                                                                                                                   |
| 445 | g.50  | 3    | 0.000   | 1.000     |            | FYVE/PHD zinc finger                                 | dimetal(zinc)-bound alpha-beta fold                                                                                                               |
| 446 | g.49  | 3    | 0.000   | 1.000     |            | Cysteine-rich domain                                | dimetal(zinc)-bound alpha-beta fold                                                                                                               |
| 447 | g.44  | 7    | 0.429   | 1.000     |            | RING finger domain, C3HC4                            | dimetal(zinc)-bound alpha-beta motif; structurally diverse                                                                                         |
| 448 | g.37  | 5    | 0.400   | 1.000     |            | C2H2 and C2HC zinc fingers                          | alpha-beta metal(zinc)-bound fold: beta-hairpin + alpha-helix                                                                                     |
| 449 | g.10  | 3    | 1.000   | 1.000     |            | Hairpin loop containing domain-like                 | alpha-beta fold with two crossing loops                                                                                                           |
| 450 | g.7   | 10   | 0.722   | 1.000     |            | Snake toxin-like                                    | disulphide-rich fold: nearly all-beta                                                                                                              |
| 451 | g.8   | 9    | 0.944   | 1.000     |            | BPTI-like                                           | disulphide-rich alpha-beta fold                                                                                                                  |
| 452 | g.14  | 5    | 0.100   | 1.000     |            | Kringle-like                                        | disulphide-rich fold; nearly all-beta                                                                                                             |
| 453 | g.15  | 10   | 0.633   | 0.767     |            | Ovomucoid/PCI-1 like inhibitors                     | disulphide-rich small alpha-beta fold                                                                                                             |
| 454 | g.41  | 21   | 0.117   | 0.350     |            | Rubredoxin-like                                     | metal(zinc or iron)-bound fold; sequence contains two CX(n)C motifs, in most cases n = 2                                                        |
| 455 | g.38  | 2    | 0.000   | 1.000     |            | Zn2/Cys6 DNA-binding domain                        | all-alpha dimetal(zinc)-bound fold                                                                                                                |
| 456 | g.17  | 12   | 0.129   | 0.902     |            | Cystine-knot cytokines                              | disulphide-rich fold; common core is all-beta                                                                                                     |
| 457 | g.35  | 4    | 0.500   | 1.000     |            | HIPPIP (high potential iron protein)                | folds around 4Fe-4S cluster                                                                                                                     |
Table 3. True Positive Rates at 1% False Positive Rate, for VAST and SHEBA, for 468 SCOP Folds in the order of the Heat Map.

| $i$ | Class Fold | $N_i$ | TPR | TPR | Fold Name | Fold Description |
|-----|------------|-------|-----|-----|-----------|------------------|
| 458 | g.51       | 2     | 1.000 | 1.000 | Zn-binding domains of ADDBP | metal(zinc)-bound alpha+beta fold |
| 459 | g.52       | 4     | 1.000 | 1.000 | Inhibitor of apoptosis (IAP) repeat | metal(zinc)-bound alpha+beta fold |
| 460 | g.53       | 2     | 0.000 | 1.000 | TAZ domain all-alpha fold; Zn-binding sites are in the loops connecting helices |
| 461 | g.22       | 3     | 0.000 | 1.000 | Serine protease inhibitors disulphide-rich; nearly all-beta |
| 462 | g.24       | 5     | 0.000 | 0.900 | TNF receptor-like duplication: consists of three similar disulphide-rich domains |
| 463 | g.9        | 9     | 0.361 | 0.889 | Defensin-like Disulphide-rich fold, nearly all-beta |
| 464 | g.3        | 38    | 0.238 | 0.472 | Knottins (small inhibitors, toxins, lectins) disulphide-bound fold; contains beta-hairpin with two adjacent disulphides |
| 465 | g.18       | 16    | 0.563 | 0.992 | Complement control module/SCR domain disulphide-rich all-beta fold |
| 466 | g.27       | 5     | 0.900 | 1.000 | Fibronectin type I module disulphide-rich, all-beta |
| 467 | g.4        | 2     | 1.000 | 1.000 | PMP inhibitors disulphide-rich fold; all-beta: 3 antiparallel strands |
| 468 | g.59       | 2     | 0.000 | 0.500 | Zinc-binding domain of translation initiation factor 2 beta zinc-bound beta-ribbon motif |