Supplementary material:

Table 1: Hit result of BLAST search for similar sequences to GFAP in PDB database

| Sub_ID | %idty | aln_len | q. start | q. end | E-value | bit score |
|--------|-------|---------|----------|--------|---------|-----------|
| 1GK4   | 71.4  | 84      | 294      | 377    | 1.00E-34| 125       |
| 3SSU   | 60.4  | 91      | 65       | 155    | 1.00E-30| 114       |
| 3UF1   | 61    | 105     | 111      | 215    | 1.00E-29| 112       |
| 3S4R   | 59.3  | 91      | 65       | 155    | 3.00E-29| 110       |
| 3KL1   | 62.5  | 72      | 229      | 300    | 3.00E-27| 105       |
| 3SWK   | 62.8  | 86      | 119      | 204    | 5.00E-27| 104       |
| 3T1T   | 58.7  | 75      | 227      | 301    | 6.00E-26| 101       |
| 3TNU   | 42.6  | 129     | 245      | 373    | 6.00E-24| 97.4      |
| 3TNU   | 40    | 130     | 244      | 373    | 3.00E-20| 87.4      |
| 1GK7   | 71.1  | 38      | 67       | 104    | 1.00E-10| 58.2      |
| 1X8Y   | 42.4  | 85      | 293      | 377    | 1.00E-10| 58.9      |
| 1GK6   | 70.7  | 41      | 338      | 378    | 6.00E-10| 56.6      |
| 3V4W   | 47.1  | 70      | 307      | 376    | 3.00E-09| 55.1      |
| 3G1E   | 70.3  | 37      | 68       | 104    | 3.00E-09| 54.3      |
| 3V58   | 47.1  | 70      | 307      | 376    | 4.00E-09| 54.7      |
| 3V4Q   | 47.1  | 70      | 307      | 376    | 5.00E-09| 54.3      |
| 3TYY   | 43.9  | 82      | 299      | 377    | 6.00E-09| 54.7      |
| 2XV5   | 65.7  | 35      | 345      | 379    | 3.00E-07| 48.9      |
| 3OJL   | 23.5  | 200     | 57       | 237    | 2.5     | 30.4      |
| 4F21   | 19.1  | 131     | 67       | 193    | 6.7     | 28.9      |
| 1Y23   | 30    | 70      | 177      | 246    | 9.6     | 28.1      |

Sub_ID = Subject ID, %idty = Percentage of Identity, % +ve = percentage of Positives, aln_len = alignment length, q. start= position of the starting residue of the query, q. end= position of the ending ending residue of the query.

Table 2: Matrix of pairwise equivalences

| PDB ID   | K4 | K6 | K7 | Y  | V5 | E  | LT | S  | S  | SW | TN | TR | TY | Q  | W  | V  |
|----------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
| 4        | SU | K  | U  | T  | Y  | 1  |    |    |    |    |    |    |    |    |    |    |
| R        |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 1G       | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  | A  |
| C        | A  | 27 | 45 | 5  | 32 | 5  | 33 | 31 | 17 | 18 | 12 | 42 | 9  | 42 | 34 | 0  |
| H        | A  | 28 | 20 | 23 | 6  | 12 | 14 | 10 | 6  | 6  | 29 | 17 | 24 | 27 | 0  |    |
| A        | 0  | 19 | 45 | 5  | 32 | 5  | 33 | 31 | 17 | 18 | 12 | 42 | 9  | 42 | 34 | 0  |
| N        | 0  | 28 | 20 | 23 | 6  | 12 | 14 | 10 | 6  | 6  | 29 | 17 | 24 | 27 | 0  |    |
| 1GK6     | A  | 0  | 9  | 28 | 20 | 23 | 6  | 12 | 14 | 10 | 6  | 6  | 29 | 17 | 24 | 27 |
| 1GK7     | A  | 0  | 14 | 28 | 21 | 8  | 24 | 27 | 34 | 37 | 22 | 20 | 14 | 14 | 1  |    |
| 1X8Y     | A  | 0  | 9  | 29 | 7  | 29 | 29 | 12 | 10 | 10 | 39 | 7  | 68 | 66 | 0  |    |
| 2XV5     | A  | 0  | 16 | 9  | 5  | 11 | 4  | 6  | 5  | 9  | 24 | 8  | 6  | 1  |    |    |
| 3G1E     | A  | 0  | 33 | 23 | 37 | 36 | 36 | 22 | 31 | 24 | 30 | 27 | 1  |    |    |    |
| 3KL1     | A  | 0  | 8  | 36 | 8  | 29 | 10 | 5  | 3  | 7  | 9  | 1  |    |    |    |    |
| 3S4R     | A  | 0  | 24 | 9  | 22 | 13 | 22 | 12 | 32 | 30 | 0  |    |    |    |    |    |
| 3SSU     | A  | 0  | 32 | 29 | 25 | 32 | 9  | 32 | 31 | 0  |    |    |    |    |    |    |
| 3SWK     | A  | 0  | 2  | 3  | 17 | 18 | 11 | 10 | 0  |    |    |    |    |    |    |    |
| 3TNU     | A  | 0  | 38 | 14 | 5  | 12 | 13 | 0  |    |    |    |    |    |    |    |    |
| 3TYY     | A  | 0  | 9  | 3  | 10 | 10 | 1  |    |    |    |    |    |    |    |    |    |
| 3UF1     | A  | 0  | 6  | 6  | 1  |    |    |    |    |    |    |    |    |    |    |    |
| 3V4Q     | A  | 0  | 67 | 0  |    |    |    |    |    |    |    |    |    |    |    |    |
Table 3: Detailed information of 5 molecular Surface Cavities

| Cavity Number | Co-ordinates (X,Y,Z) | Volume (Å³) | Radius (Å) | Residues surrounding the cavity |
|---------------|----------------------|-------------|------------|---------------------------------|
| 1             | 59.50, 51.20, 72.90  | 291.84      | 8.11       | A (145), Q (146), A (149), L (155), R (173), H (221), V (226), K (228), P (229), K (356), V (381), T (383), E (401), L (404) |
| 2             | 57.98, 81.35, 35.84  | 115.648     | 7.11       | M (21), G (24), L (31), T (35), L (37), S (53), A (57), K (63), R (66) |
| 3             | 71.65, 60.72, 83.84  | 74.752      | 4.11       | Y (349), I (378), Q (382) |
| 4             | 70.01, 63.56, 46.24  | 58.368      | 4.11       | Q (93), Y (116), Q (129) |
| 5             | 60.72, 52.51, 90.12  | 49.664      | 4.11       | Q (241), I (377), I (379), I (408) |

Å = Angstrom, the one letter codes represent the usual amino acids.