Table S2: List of average 13C chemical shifts (CS; in ppm), corresponding standard deviations (SD; in ppm), and corresponding number of assignments of every nucleus (no.) for samples after spontaneous conversion of ovrecPrP(25-233).

|  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
|  | C | | | Cα | | | Cβ | | | Cγ/Cγ1 | | | Cγ2 | | | Cδ/Cδ1/Cδ2 | | | Cε/Cε1/Cε2 | | | Cζ | | |
|  | CS | SD | no. | CS | SD | no. | CS | SD | no. | CS | SD | no. | CS | SD | no. | CS | SD | no. | CS | SD | no. | CS | SD | no. |
| A1 | 178.7 | 0.11 | 5 | 55.0 | 0.14 | 12 | 18.2 | 0.14 | 13 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A2 | x | x | x | 51.1 | 0.00 | 2 | 22.4 | 0.00 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A3 | 179.6 | 0.23 | 5 | 55.0 | 0.02 | 6 | 17.3 | 0.19 | 7 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A4 | x | x | x | 50.9 | 0.14 | 6 | 23.7 | 0.03 | 6 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A5 | 179.0 | 0.26 | 5 | 54.8 | 0.17 | 12 | 18.6 | 0.13 | 13 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A6 | 178.1 | 0.19 | 5 | 54.9 | 0.12 | 9 | 19.2 | 0.14 | 10 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| A7 | x | x | x | 53.1 | 0.00 | 1 | 20.6 | 0.13 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| D1 | x | x | x | 55.5 | 0.07 | 11 | 41.1 | 0.07 | 13 | 179.7 | 0.10 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |
| D2 | x | x | x | 55.6 | 0.04 | 9 | 41.9 | 0.18 | 12 | 178.0 | 0.03 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |
| E1 | 178.7 | 0.09 | 10 | 54.7 | 0.13 | 24 | 33.3 | 0.10 | 28 | 36.3 | 0.17 | 33 |  |  |  | 183.0 | 0.20 | 7 |  |  |  |  |  |  |
| E2 | 178.3 | 0.16 | 8 | 54.3 | 0.13 | 24 | 32.1 | 0.19 | 25 | 36.4 | 0.17 | 28 |  |  |  | 182.6 | 0.23 | 5 |  |  |  |  |  |  |
| E3 | 178.3 | 0.15 | 4 | 54.4 | 0.19 | 22 | 31.9 | 0.13 | 21 | 37.9 | 0.21 | 19 |  |  |  | 183.3 | 0.08 | 4 |  |  |  |  |  |  |
| F1 | x | x | x | 56.8 | 0.20 | 5 | x | x | x | 138.1 | 0.19 | 5 |  |  |  | x | x | x | x | x | x | x | x | x |
| G1 | 174.0 | 0.00 | 2 | 44.3 | 0.00 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G2 | 172.3 | 0.12 | 3 | 44.9 | 0.03 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G3 | 171.4 | 0.00 | 1 | 44.6 | 0.00 | 1 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G4 | 172.7 | 0.00 | 2 | 45.5 | 0.00 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G5 | 173.3 | 0.00 | 2 | 45.3 | 0.00 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G6 | 173.7 | 0.00 | 2 | 46.3 | 0.00 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G7 | 173.9 | 0.00 | 3 | 46.8 | 0.00 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G8 | 174.6 | 0.03 | 3 | 47.5 | 0.16 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G9 | 176.1 | 0.00 | 2 | 48.0 | 0.00 | 2 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G10 | 175.4 | 0.20 | 3 | 46.9 | 0.07 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G11 | 174.6 | 0.16 | 3 | 45.9 | 0.08 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G12 | 174.2 | 0.07 | 3 | 45.7 | 0.13 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G13 | 175.4 | 0.01 | 3 | 45.2 | 0.09 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G14 | 174.5 | 0.00 | 3 | 45.0 | 0.00 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G15 | 174.9 | 0.09 | 3 | 44.6 | 0.01 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| G16 | 173.7 | 0.06 | 3 | 44.8 | 0.08 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| H1 | x | x | x | 57.1 | 0.18 | 21 | 30.2 | 0.18 | 15 | 129.2 | 0.18 | 13 |  |  |  | 120.7 | 0.15 | 6 | 138.6 | 0.19 | 9 |  |  |  |
| H2 | x | x | x | 57.5 | 0.11 | 13 | 29.6 | 0.09 | 12 | 129.5 | 0.19 | 12 |  |  |  | 124.0 | 0.00 | 1 | 139.1 | 0.15 | 10 |  |  |  |
| I1 | x | x | x | 59.7 | 0.19 | 27 | 41.2 | 0.20 | 32 | 27.5 | 0.09 | 40 | 16.8 | 0.06 | 21 | 15.0 | 0.14 | 20 |  |  |  |  |  |  |
| I2 | x | x | x | 57.8 | 0.12 | 24 | 43.4 | 0.06 | 36 | 26.6 | 0.08 | 39 | 16.9 | 0.02 | 18 | 15.3 | 0.06 | 15 |  |  |  |  |  |  |
| I3 | x | x | x | 59.7 | 0.24 | 9 | 39.3 | 0.22 | 8 | 27.1 | 0.22 | 8 | 19.0 | 0.13 | 3 | 13.9 | 0.10 | 4 |  |  |  |  |  |  |
| K1 | x | x | x | 54.5 | 0.15 | 16 | 39.5 | 0.13 | 15 | 27.8 | 0.09 | 33 |  |  |  | 31.8 | 0.03 | 18 | 43.0 | 0.07 | 18 |  |  |  |
| K2 | x | x | x | 53.9 | 0.20 | 16 | 38.2 | 0.10 | 22 | 28.4 | 0.07 | 31 |  |  |  | 32.2 | 0.10 | 23 | 42.6 | 0.15 | 14 |  |  |  |
| K3 | x | x | x | 55.0 | 0.18 | 21 | 36.0 | 0.19 | 26 | 25.6 | 0.19 | 28 |  |  |  | 33.0 | 0.15 | 26 | 42.2 | 0.14 | 17 |  |  |  |
| L1 | x | x | x | 56.7 | 0.19 | 19 | 42.2 | 0.13 | 31 | 27.2 | 0.20 | 28 |  |  |  | 25.1 | 0.08 | 16 |  |  |  |  |  |  |
| L2 | x | x | x | 57.8 | 0.10 | 21 | 43.4 | 0.09 | 24 | 26.7 | 0.17 | 27 |  |  |  | 23.3 | 0.19 | 6 |  |  |  |  |  |  |
| L3 | x | x | x | 55.7 | 0.17 | 18 | 41.2 | 0.16 | 23 | 27.4 | 0.23 | 20 |  |  |  | 22.5 | 0.00 | 1 |  |  |  |  |  |  |
| M1 | x | x | x | x | x | x | x | x | x | 31.6 | 0.22 | 3 |  |  |  |  |  |  | 21.3 | 0.04 | 3 |  |  |  |
| M2 | x | x | x | x | x | x | x | x | x | 31.7 | 0.14 | 2 |  |  |  |  |  |  | 22.1 | 0.06 | 2 |  |  |  |
| M3 | x | x | x | x | x | x | x | x | x | 31.5 | 0.16 | 3 |  |  |  |  |  |  | 22.9 | 0.10 | 3 |  |  |  |
| M4 | x | x | x | x | x | x | x | x | x | 29.9 | 0.05 | 3 |  |  |  |  |  |  | 24.4 | 0.12 | 3 |  |  |  |
| M5 | x | x | x | x | x | x | x | x | x | 31.3 | 0.08 | 2 |  |  |  |  |  |  | 23.7 | 0.07 | 2 |  |  |  |
| N1 | x | x | x | 52.3 | 0.05 | 12 | 42.7 | 0.07 | 12 | x | x | x |  |  |  |  |  |  |  |  |  |  |  |  |
| N2 | x | x | x | 53.0 | 0.11 | 12 | 43.1 | 0.08 | 12 | x | x | x |  |  |  |  |  |  |  |  |  |  |  |  |
| N3 | x | x | x | 52.4 | 0.15 | 12 | 41.4 | 0.11 | 12 | x | x | x |  |  |  |  |  |  |  |  |  |  |  |  |
| P1 | x | x | x | 63.3 | 0.22 | 24 | 31.6 | 0.18 | 30 | 27.6 | 0.15 | 31 |  |  |  | 50.3 | 0.13 | 27 |  |  |  |  |  |  |
| P2 | x | x | x | 63.4 | 0.17 | 20 | 32.3 | 0.16 | 31 | 27.4 | 0.12 | 31 |  |  |  | 50.5 | 0.14 | 22 |  |  |  |  |  |  |
| P3 | x | x | x | 62.2 | 0.19 | 18 | 31.0 | 0.18 | 25 | 27.3 | 0.13 | 30 |  |  |  | 50.2 | 0.16 | 27 |  |  |  |  |  |  |
| P4 | x | x | x | 63.0 | 0.20 | 23 | 32.5 | 0.08 | 31 | 27.8 | 0.14 | 30 |  |  |  | 51.3 | 0.18 | 24 |  |  |  |  |  |  |
| Q1 | x | x | x | 53.9 | 0.15 | 18 | 30.0 | 0.20 | 17 | 34.8 | 0.19 | 15 |  |  |  | 181.2 | 0.15 | 6 |  |  |  |  |  |  |
| Q2 | x | x | x | 54.7 | 0.13 | 14 | 28.7 | 0.15 | 15 | 34.0 | 0.16 | 16 |  |  |  | 181.1 | 0.24 | 3 |  |  |  |  |  |  |
| Q3 | x | x | x | 56.1 | 0.13 | 14 | 27.9 | 0.27 | 14 | 33.7 | 0.24 | 16 |  |  |  | 181.2 | 0.07 | 2 |  |  |  |  |  |  |
| R1 | x | x | x | 57.6 | 0.23 | 14 | 28.6 | 0.14 | 29 | 27.4 | 0.23 | 28 |  |  |  | 44.2 | 0.10 | 23 |  |  |  | 159.3 | 0.11 | 10 |
| R2 | x | x | x | 57.5 | 0.11 | 15 | 29.5 | 0.22 | 22 | 28.0 | 0.12 | 22 |  |  |  | 43.6 | 0.17 | 19 |  |  |  | 159.8 | 0.10 | 4 |
| R3 | x | x | x | 57.2 | 0.09 | 17 | 30.2 | 0.20 | 36 | 27.8 | 0.20 | 28 |  |  |  | 42.9 | 0.21 | 25 |  |  |  | 159.0 | 0.15 | 4 |
| S1 | x | x | x | 56.2 | 0.10 | 12 | 64.1 | 0.10 | 12 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| S2 | x | x | x | 58.0 | 0.08 | 7 | 64.2 | 0.14 | 7 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| S3 | x | x | x | 58.7 | 0.19 | 6 | 63.6 | 0.23 | 6 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| S4 | x | x | x | 57.1 | 0.21 | 5 | 64.4 | 0.13 | 5 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| S5 | x | x | x | 61.1 | 0.04 | 3 | 64.2 | 0.14 | 3 |  |  |  |  |  |  |  |  |  |  |  |  |  |  |  |
| T1 | 173.5 | 0.10 | 10 | 61.9 | 0.18 | 22 | 70.9 | 0.16 | 26 |  |  |  | 21.4 | 0.18 | 24 |  |  |  |  |  |  |  |  |  |
| T2 | 175.2 | 0.08 | 13 | 61.6 | 0.08 | 16 | 69.6 | 0.11 | 19 |  |  |  | 21.1 | 0.14 | 28 |  |  |  |  |  |  |  |  |  |
| T3 | 177.1 | 0.12 | 13 | 60.8 | 0.16 | 23 | 69.3 | 0.13 | 29 |  |  |  | 25.1 | 0.09 | 21 |  |  |  |  |  |  |  |  |  |
| V1 | x | x | x | 60.3 | 0.11 | 14 | 35.0 | 0.03 | 16 | 20.6 | 0.16 | 14 |  |  |  |  |  |  |  |  |  |  |  |  |
| V2 | x | x | x | 61.5 | 0.13 | 23 | 34.7 | 0.10 | 23 | 21.0 | 0.16 | 24 |  |  |  |  |  |  |  |  |  |  |  |  |
| V3 | x | x | x | 65.0 | 0.19 | 6 | 31.6 | 0.11 | 6 | x | x | x |  |  |  |  |  |  |  |  |  |  |  |  |
| Y1 | x | x | x | 56.9 | 0.14 | 19 | 39.0 | 0.17 | 21 | 131.4 | 0.20 | 16 |  |  |  | 134.3 | 0.17 | 19 | 118.5 | 0.14 | 18 | 157.1 | 0.15 | 9 |
| Y2 | x | x | x | 56.4 | 0.14 | 9 | 40.4 | 0.16 | 7 | 131.9 | 0.07 | 8 |  |  |  | 133.7 | 0.12 | 13 | 118.2 | 0.15 | 17 | 158.8 | 0.18 | 4 |
| Y3 | x | x | x | 57.3 | 0.15 | 12 | 40.8 | 0.10 | 7 | 131.9 | 0.19 | 10 |  |  |  | 133.7 | 0.14 | 13 | 118.2 | 0.05 | 17 | 158.7 | 0.00 | 3 |
| Y4 | x | x | x | 57.3 | 0.20 | 14 | 38.9 | 0.24 | 15 | 128.7 | 0.13 | 10 |  |  |  | 132.8 | 0.14 | 20 | 118.3 | 0.17 | 15 | 157.9 | 0.23 | 10 |

Spins that could not be identified due to bad dispersion or absence are marked by crosses.