

# Supplementary Materials: Heat-Stable Hazelnut Profilin: Molecular Dynamics Simulations and Immunoinformatics Analysis

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**Table S1.** Epitopes prediction of the Cor a 2 at 300 K

| Start             | End | Peptide                         | Number of residues | score |
|-------------------|-----|---------------------------------|--------------------|-------|
| <b>t = 180 ns</b> |     |                                 |                    |       |
| 124               | 130 | DYLIDQG                         | 7                  | 0.731 |
| 107               | 114 | DEPMTPGQ                        | 8                  | 0.679 |
| 87                | 90  | KGPG                            | 4                  | 0.638 |
| 76                | 81  | QGEPGA                          | 6                  | 0.629 |
| 1                 | 11  | MSWQAYGDEHL                     | 11                 | 0.619 |
| 13                | 20  | CEIEGNRL                        | 8                  | 0.602 |
| 51                | 73  | MNDFNEPGSLAPTGLYLGGTKYM         | 23                 | 0.599 |
| 27                | 33  | GHDGSVW                         | 7                  | 0.552 |
| <b>t = 185 ns</b> |     |                                 |                    |       |
| 124               | 130 | DYLIDQG                         | 7                  | 0.763 |
| 107               | 114 | DEPMTPGQ                        | 8                  | 0.651 |
| 1                 | 11  | MSWQAYGDEHL                     | 11                 | 0.643 |
| 55                | 73  | NEPGSLAPTGLYLGGTKYM             | 19                 | 0.639 |
| 76                | 81  | QGEPGA                          | 6                  | 0.624 |
| 40                | 46  | PQLKPEE                         | 7                  | 0.62  |
| 87                | 90  | KGPG                            | 4                  | 0.617 |
| 13                | 20  | CEIEGNRL                        | 8                  | 0.606 |
| <b>t = 190 ns</b> |     |                                 |                    |       |
| 123               | 130 | GDYLIDQG                        | 8                  | 0.688 |
| 107               | 114 | DEPMTPGQ                        | 8                  | 0.665 |
| 1                 | 10  | MSWQAYGDEH                      | 10                 | 0.649 |
| 87                | 90  | KGPG                            | 4                  | 0.633 |
| 52                | 73  | NDFNEPGSLAPTGLYLGGTKYM          | 22                 | 0.625 |
| 76                | 81  | QGEPGA                          | 6                  | 0.596 |
| 13                | 20  | CEIEGNRL                        | 8                  | 0.592 |
| 40                | 46  | PQLKPEE                         | 7                  | 0.591 |
| 27                | 34  | GHDGSVWA                        | 8                  | 0.556 |
| <b>t = 195 ns</b> |     |                                 |                    |       |
| 124               | 130 | DYLIDQG                         | 7                  | 0.742 |
| 40                | 46  | PQLKPEE                         | 7                  | 0.678 |
| 87                | 90  | KGPG                            | 4                  | 0.637 |
| 107               | 115 | DEPMTPGQC                       | 9                  | 0.624 |
| 1                 | 11  | MSWQAYGDEHL                     | 11                 | 0.61  |
| 13                | 20  | CEIEGNRL                        | 8                  | 0.6   |
| 51                | 73  | MNDFNEPGSLAPTGLYLGGTKYM         | 23                 | 0.598 |
| 76                | 81  | QGEPGA                          | 6                  | 0.59  |
| <b>t = 200 ns</b> |     |                                 |                    |       |
| 124               | 130 | DYLIDQG                         | 7                  | 0.72  |
| 40                | 46  | PQLKPEE                         | 7                  | 0.676 |
| 1                 | 10  | MSWQAYGDEH                      | 10                 | 0.66  |
| 87                | 90  | KGPG                            | 4                  | 0.633 |
| 107               | 115 | DEPMTPGQC                       | 9                  | 0.626 |
| 51                | 81  | MNDFNEPGSLAPTGLYLGGTKYMVIQGEPGA | 31                 | 0.6   |
| 13                | 20  | CEIEGNRL                        | 8                  | 0.563 |

**Table S2.** Epitopes prediction of the Cor a 2 at 350 K

| Start             | End | Peptide              | Number of residues | score |
|-------------------|-----|----------------------|--------------------|-------|
| <b>t = 180 ns</b> |     |                      |                    |       |
| 68                | 81  | GGTKYMVIQGEPGA       | 14                 | 0.514 |
| 27                | 32  | GHDGSV               | 6                  | 0.551 |
| 13                | 19  | CEIEGNR              | 7                  | 0.579 |
| 87                | 90  | KGPG                 | 4                  | 0.621 |
| 51                | 65  | MNDFNEPGSLAPTGL      | 15                 | 0.629 |
| 40                | 49  | PQLKPEEITG           | 10                 | 0.664 |
| 1                 | 10  | MSWQAYGDEH           | 10                 | 0.669 |
| 107               | 117 | DEPMTPGQCNM          | 11                 | 0.701 |
| 125               | 130 | YLIDQG               | 6                  | 0.737 |
| <b>t = 185 ns</b> |     |                      |                    |       |
| 126               | 130 | LIDQG                | 5                  | 0.757 |
| 108               | 117 | EPMTPGQCNM           | 10                 | 0.728 |
| 75                | 81  | IQGEPGA              | 7                  | 0.699 |
| 1                 | 10  | MSWQAYGDEH           | 10                 | 0.676 |
| 50                | 60  | VMNDFNEPGSL          | 11                 | 0.674 |
| 40                | 47  | PQLKPEEI             | 8                  | 0.643 |
| 13                | 18  | CEIEGN               | 6                  | 0.599 |
| 66                | 73  | YLGGTKYM             | 8                  | 0.547 |
| 27                | 31  | GHDGS                | 5                  | 0.529 |
| <b>t = 190 ns</b> |     |                      |                    |       |
| 126               | 130 | LIDQG                | 5                  | 0.786 |
| 108               | 117 | EPMTPGQCNM           | 10                 | 0.716 |
| 51                | 60  | MNDFNEPGSL           | 10                 | 0.678 |
| 40                | 47  | PQLKPEEI             | 8                  | 0.664 |
| 1                 | 11  | MSWQAYGDEHL          | 11                 | 0.648 |
| 13                | 19  | CEIEGNR              | 7                  | 0.579 |
| 62                | 81  | PTGLYLGGTKYMVIQGEPGA | 20                 | 0.541 |
| <b>t = 195 ns</b> |     |                      |                    |       |
| 54                | 59  | FNEPGS               | 6                  | 0.758 |
| 76                | 81  | QGEPGA               | 6                  | 0.738 |
| 108               | 117 | EPMTPGQCNM           | 10                 | 0.721 |
| 1                 | 9   | MSWQAYGDE            | 9                  | 0.706 |
| 40                | 47  | PQLKPEEI             | 8                  | 0.684 |
| 123               | 130 | GDYLIDQG             | 8                  | 0.616 |
| 13                | 18  | CEIEGN               | 6                  | 0.59  |
| 27                | 31  | GHDGS                | 5                  | 0.537 |
| 62                | 73  | PTGLYLGGTKYM         | 12                 | 0.517 |
| <b>t = 200 ns</b> |     |                      |                    |       |
| 40                | 47  | PQLKPEEI             | 8                  | 0.738 |
| 52                | 64  | NDFNEPGSLAPTGL       | 13                 | 0.669 |
| 1                 | 10  | MSWQAYGDEH           | 10                 | 0.667 |
| 107               | 117 | DEPMTPGQCNM          | 11                 | 0.666 |
| 86                | 89  | KKGP                 | 4                  | 0.644 |
| 123               | 130 | GDYLIDQG             | 8                  | 0.6   |
| 68                | 81  | GGTKYMVIQGEPGA       | 14                 | 0.557 |
| 13                | 20  | CEIEGNRL             | 8                  | 0.554 |

|    |    |       |   |       |
|----|----|-------|---|-------|
| 27 | 31 | GHDGS | 5 | 0.534 |
|----|----|-------|---|-------|

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**Table S3.** Epitopes prediction of the Cor a 2 at 400 K

| Start             | End | Peptide                | Number of residues | score |
|-------------------|-----|------------------------|--------------------|-------|
| <b>t = 180 ns</b> |     |                        |                    |       |
| 123               | 130 | GDYLIDQG               | 8                  | 0.785 |
| 1                 | 11  | MSWQAYGDEHL            | 11                 | 0.685 |
| 36                | 52  | SSTFPQLKPEEITGVMN      | 17                 | 0.657 |
| 55                | 63  | NEPGSLAPT              | 9                  | 0.656 |
| 28                | 33  | HDGSVW                 | 6                  | 0.608 |
| 108               | 115 | EPMTPGQC               | 8                  | 0.563 |
| 96                | 99  | KTSQ                   | 4                  | 0.544 |
| 13                | 20  | CEIEGNRL               | 8                  | 0.523 |
| <b>t = 185 ns</b> |     |                        |                    |       |
| 40                | 52  | PQLKPEEITGVMN          | 13                 | 0.767 |
| 120               | 130 | ERLGDYLIDQG            | 11                 | 0.684 |
| 54                | 63  | FNEPGSLAPT             | 10                 | 0.67  |
| 1                 | 10  | MSWQAYGDEH             | 10                 | 0.667 |
| 86                | 89  | KKGP                   | 4                  | 0.623 |
| 108               | 114 | EPMTPGQ                | 7                  | 0.604 |
| 75                | 81  | IQGEPGA                | 7                  | 0.59  |
| 13                | 18  | CEIEGN                 | 6                  | 0.587 |
| <b>t = 190 ns</b> |     |                        |                    |       |
| 123               | 130 | GDYLIDQG               | 8                  | 0.778 |
| 44                | 64  | PEEITGVMNDFNEPGSLAPTG  | 21                 | 0.722 |
| 1                 | 11  | MSWQAYGDEHL            | 11                 | 0.647 |
| 107               | 114 | DEPMTPGQ               | 8                  | 0.626 |
| 76                | 81  | QGEPGA                 | 6                  | 0.571 |
| 13                | 19  | CEIEGNR                | 7                  | 0.543 |
| <b>t = 195 ns</b> |     |                        |                    |       |
| 123               | 130 | GDYLIDQG               | 8                  | 0.805 |
| 1                 | 10  | MSWQAYGDEH             | 10                 | 0.671 |
| 44                | 65  | PEEITGVMNDFNEPGSLAPTGL | 22                 | 0.667 |
| 27                | 33  | GHDGSVW                | 7                  | 0.602 |
| 97                | 100 | TSQA                   | 4                  | 0.594 |
| 108               | 115 | EPMTPGQC               | 8                  | 0.588 |
| 13                | 18  | CEIEGN                 | 6                  | 0.577 |
| <b>t = 200 ns</b> |     |                        |                    |       |
| 123               | 130 | GDYLIDQG               | 8                  | 0.792 |
| 108               | 114 | EPMTPGQ                | 7                  | 0.662 |
| 44                | 64  | PEEITGVMNDFNEPGSLAPTG  | 21                 | 0.649 |
| 76                | 81  | QGEPGA                 | 6                  | 0.64  |
| 1                 | 19  | MSWQAYGDEHLMCEIEGNR    | 19                 | 0.613 |
| 28                | 33  | HDGSVW                 | 6                  | 0.556 |
| 69                | 73  | GTKYM                  | 5                  | 0.526 |

**Table S4.** Epitopes prediction of the Cor a 2 at 450 K

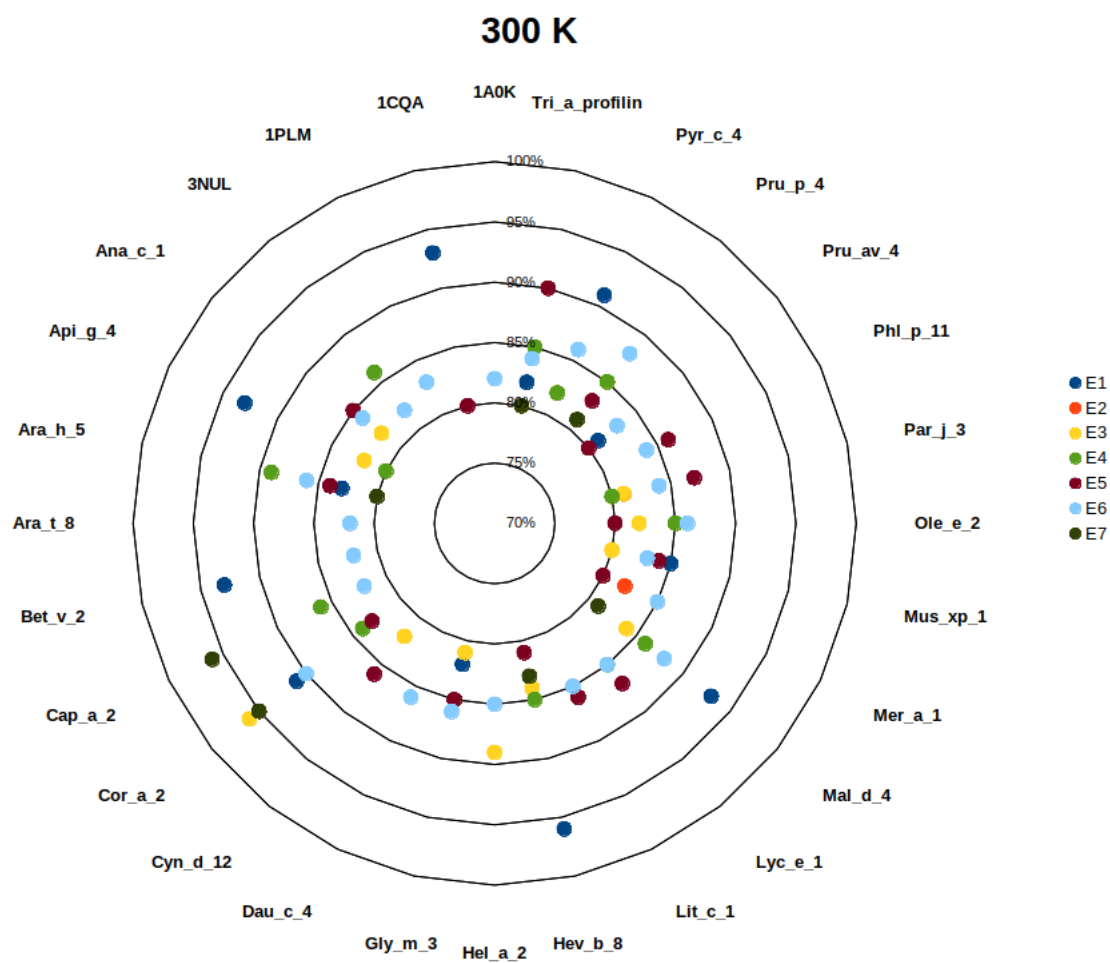
| Start             | End | Peptide               | Number of residues | score |
|-------------------|-----|-----------------------|--------------------|-------|
| <b>t = 180 ns</b> |     |                       |                    |       |
| 65                | 72  | LYLGGTKY              | 8                  | 0.827 |
| 4                 | 19  | QAYGDEHLMCEIEGNR      | 16                 | 0.682 |
| 119               | 130 | VERLGDYLIDQG          | 12                 | 0.672 |
| 96                | 100 | KTSQA                 | 5                  | 0.671 |
| 27                | 33  | GHDGSVW               | 7                  | 0.611 |
| 52                | 59  | NDFNEPGS              | 8                  | 0.604 |
| 42                | 49  | LKPEEITG              | 8                  | 0.6   |
| <b>t = 185 ns</b> |     |                       |                    |       |
| 65                | 72  | LYLGGTKY              | 8                  | 0.755 |
| 27                | 30  | GHDG                  | 4                  | 0.688 |
| 51                | 58  | MNDFNEPG              | 8                  | 0.675 |
| 1                 | 19  | MSWQAYGDEHLMCEIEGNR   | 19                 | 0.655 |
| 107               | 115 | DEPMTPGQC             | 9                  | 0.62  |
| 44                | 49  | PEEITG                | 6                  | 0.613 |
| 117               | 127 | MIVERLGDYLI           | 11                 | 0.599 |
| <b>t = 190 ns</b> |     |                       |                    |       |
| 119               | 130 | VERLGDYLIDQG          | 12                 | 0.772 |
| 95                | 100 | KKTSQA                | 6                  | 0.74  |
| 27                | 30  | GHDG                  | 4                  | 0.692 |
| 1                 | 15  | MSWQAYGDEHLMCEI       | 15                 | 0.636 |
| 38                | 58  | TFPQLKPEEITGVMNDFNEPG | 21                 | 0.616 |
| 107               | 115 | DEPMTPGQC             | 9                  | 0.596 |
| <b>t = 195 ns</b> |     |                       |                    |       |
| 125               | 130 | YLIDQG                | 6                  | 0.745 |
| 1                 | 17  | MSWQAYGDEHLMCEIEG     | 17                 | 0.738 |
| 68                | 72  | GGTKY                 | 5                  | 0.689 |
| 106               | 116 | YDEPMTPGQCN           | 11                 | 0.667 |
| 44                | 61  | PEEITGVMNDFNEPGSLA    | 18                 | 0.665 |
| <b>t = 200 ns</b> |     |                       |                    |       |
| 125               | 130 | YLIDQG                | 6                  | 0.837 |
| 68                | 72  | GGTKY                 | 5                  | 0.717 |
| 1                 | 17  | MSWQAYGDEHLMCEIEG     | 17                 | 0.7   |
| 41                | 60  | QLKPEEITGVMNDFNEPGSL  | 20                 | 0.657 |
| 107               | 117 | DEPMTPGQCNM           | 11                 | 0.612 |
| 27                | 30  | GHDG                  | 4                  | 0.575 |
| 78                | 89  | EPGAVIRGKKGP          | 12                 | 0.524 |

**Table S5.** Epitopes prediction of the Cor a 2 at 500 K

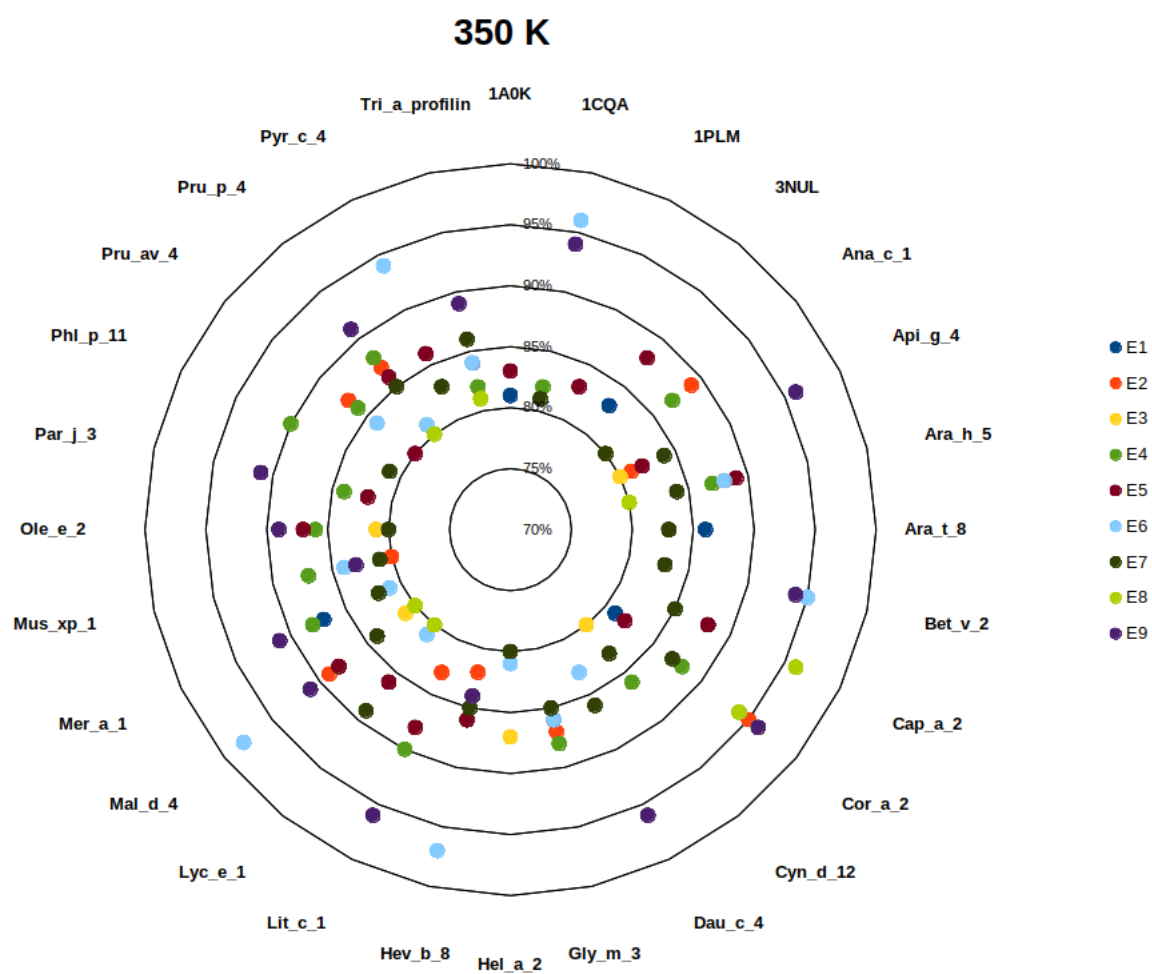
| Start             | End | Peptide                      | Number of residues | score |
|-------------------|-----|------------------------------|--------------------|-------|
| <b>t = 180 ns</b> |     |                              |                    |       |
| 110               | 128 | MTPGQCNMIVERLGDYLID          | 19                 | 0.745 |
| 1                 | 10  | MSWQAYGDEH                   | 10                 | 0.704 |
| 58                | 80  | GSLAPTGLYLGGTKYMVIQGEPC      | 23                 | 0.678 |
| 29                | 34  | DGSVWA                       | 6                  | 0.591 |
| 42                | 55  | LKPEEITGVMNDFN               | 14                 | 0.591 |
| 87                | 90  | KGPG                         | 4                  | 0.563 |
| <b>t = 185 ns</b> |     |                              |                    |       |
| 62                | 69  | PTGLYLGG                     | 8                  | 0.729 |
| 41                | 58  | QLKPEEITGVMNDFNEPG           | 18                 | 0.691 |
| 1                 | 21  | MSWQAYGDEHLMCEIEGNRLA        | 21                 | 0.667 |
| 85                | 92  | GKKGPGGV                     | 8                  | 0.652 |
| 104               | 127 | GIYDEPMTPGQCNMIVERLGDYLI     | 24                 | 0.589 |
| <b>t = 190 ns</b> |     |                              |                    |       |
| 40                | 60  | PQLKPEEITGVMNDFNEPGSL        | 21                 | 0.701 |
| 1                 | 21  | MSWQAYGDEHLMCEIEGNRLA        | 21                 | 0.691 |
| 84                | 92  | RGKKGPGGV                    | 9                  | 0.597 |
| 65                | 72  | LYLGGTKY                     | 8                  | 0.57  |
| 104               | 127 | GIYDEPMTPGQCNMIVERLGDYLI     | 24                 | 0.55  |
| <b>t = 195 ns</b> |     |                              |                    |       |
| 11                | 20  | LMCEIEGNRL                   | 10                 | 0.724 |
| 38                | 65  | TFPQLKPEEITGVMNDFNEPGSLAPTGL | 28                 | 0.697 |
| 106               | 127 | YDEPMTPGQCNMIVERLGDYLI       | 22                 | 0.684 |
| 4                 | 8   | QAYGD                        | 5                  | 0.602 |
| 85                | 91  | GKKGPGG                      | 7                  | 0.588 |
| <b>t = 200 ns</b> |     |                              |                    |       |
| 1                 | 7   | MSWQAYG                      | 7                  | 0.808 |
| 47                | 66  | ITGVMNDFNEPGSLAPTGLY         | 20                 | 0.754 |
| 107               | 126 | DEPMTPGQCNMIVERLGDYL         | 20                 | 0.728 |
| 29                | 40  | DGSVWAQSSTFP                 | 12                 | 0.624 |
| 76                | 80  | QGEPC                        | 5                  | 0.522 |

**Table S6.** Conformational features of beta strands composition of Cor a 2 at different temperatures.

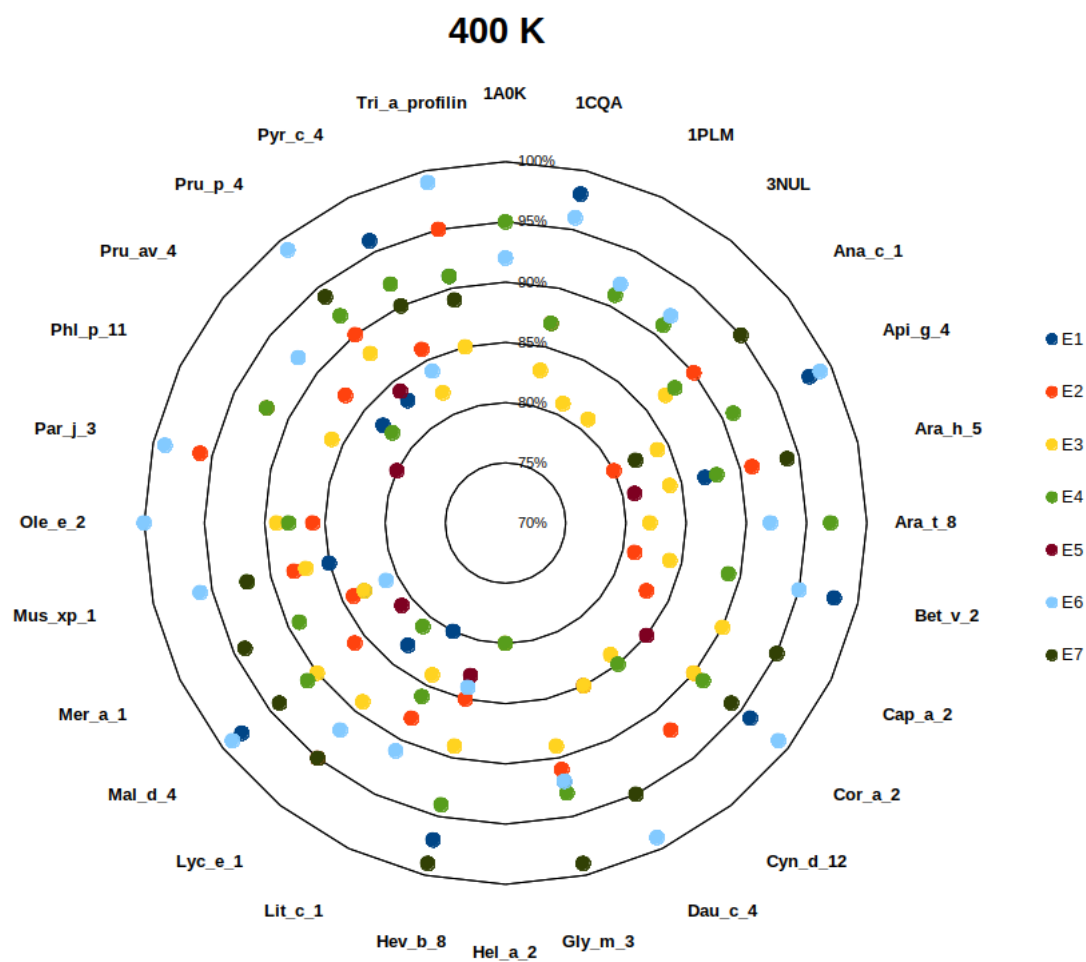
| Temperature | % Strand | No. Beta sheet | No. Strands | Strand Conformation                                                                                     | No. Residues |
|-------------|----------|----------------|-------------|---------------------------------------------------------------------------------------------------------|--------------|
| 300K        | 26.2     | 1              | 7           | Ala22-Ile26<br>Val32-Gln35<br>Leu65-Tyr66<br>Lys71-Val74<br>Val82-Lys86<br>Gly91-Thr97<br>Ala100-Tyr106 | 34           |
| 350K        | 25.4     | 1              | 7           | Ala22-Ile26<br>Ala34-Gln35<br>Leu65-Tyr66<br>Lys71-Ile75<br>Val82-Lys86<br>Gly90-Lys96<br>Leu101-Asp107 | 38           |
| 400K        | 26.2     | 1              | 6           | Leu20-Gly27<br>Val32-Gln35<br>Met73-Ile75<br>Ile83-Lys86<br>Gly90-Lys96<br>Ala100-Asp107                | 34           |
| 450K        | 21.5     | 2              | 4           | Ala23-Ile26<br>Ser31-Ala34<br>Gly91-Thr97<br>Ala100-Tyr106                                              | 22           |
|             |          |                | 2           | Leu65-Leu67<br>Tyr72-Val74                                                                              | 6            |
| 500K        | 15.4     | 1              | 4           | Gly7-His10<br>Val82-Ile83<br>Val92-Thr97<br>Ala100-Asp107                                               | 20           |



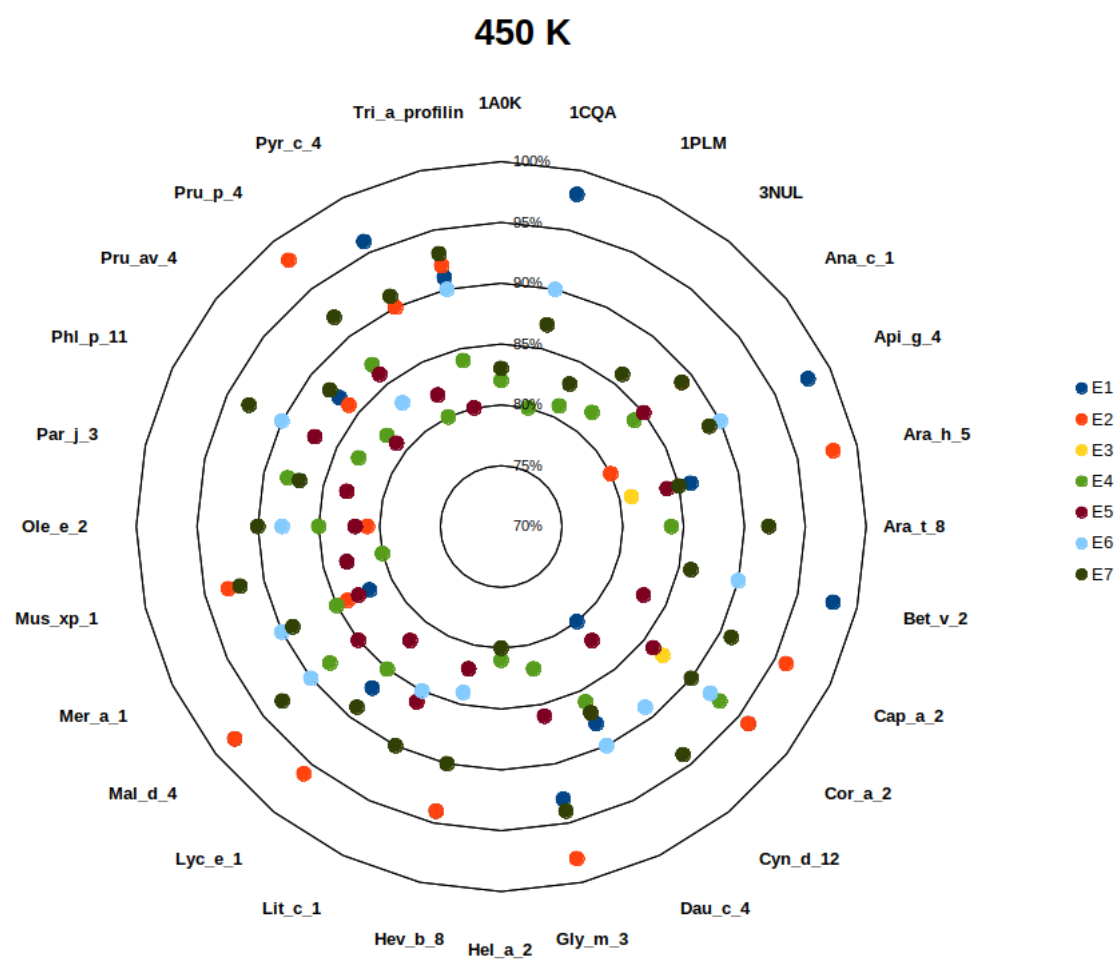
**Figure S1.** Cross-reactivity of profilin at 300K with allergens, the label E1 to E7 correspond for an epitope.



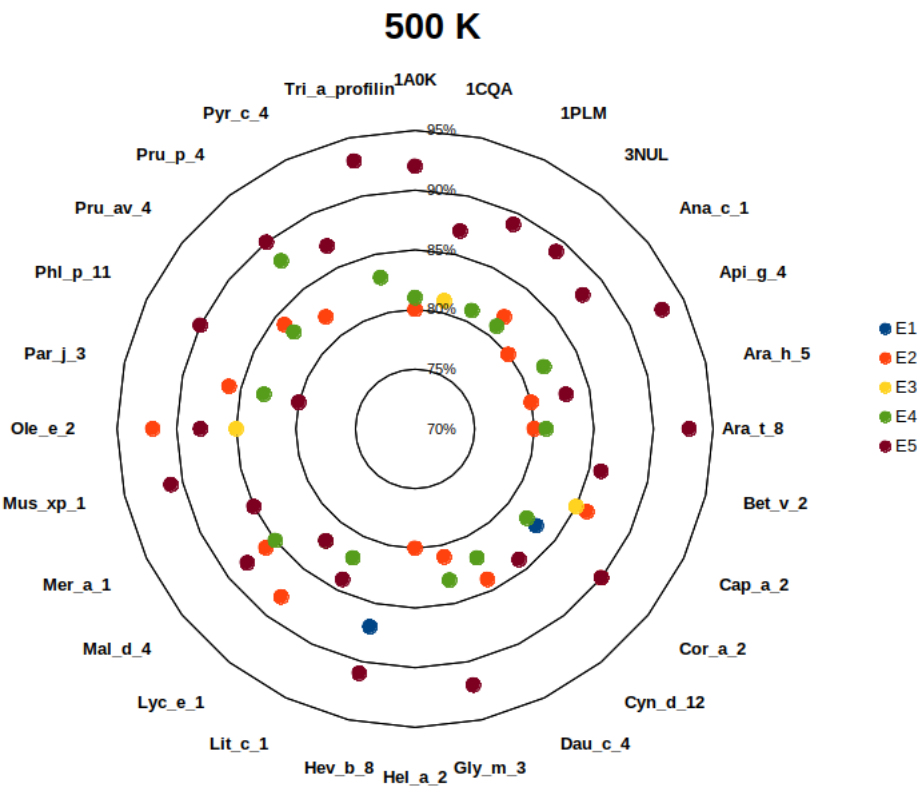
**Figure S2.** Cross-reactivity of profilin at 350K with allergens, the label E1 to E9 correspond for an epitope.



**Figure S3.** Cross-reactivity of profilin at 400K with allergens, the label E1 to E7 correspond for an epitope.



**Figure S4.** Cross-reactivity of profilin at 450K with allergens, the label E1 to E7 correspond for an epitope.



**Figure S5.** Cross-reactivity of profilin at 500K with allergens, the label E1 to E5 correspond for an epitope.