**Supplementary Information**

**Protein Sequences**

**WT**

SANTYWQYWT DGGGTVNATN GPGGNYSVTW RDTGNFVVGK GWEIGSPNRT

IHYNAGVWEP SGNGYLTLYG WTRNQLIEYY VVDNWGTYRP TGTHRGTVVS

DGGTYDIYTT MRYNAPSIDG TQTFQQFWSV RQSKRPTGNN VSITFSNHVN

AWRNAGMNLG SSWSYQVLAT EGYQSSGRSN VTVW

**D32G**

SANTYWQYWT DGGGTVNATN GPGGNYSVTW R**G**TGNFVVGK GWEIGSPNRT

IHYNAGVWEP SGNGYLTLYG WTRNQLIEYY VVDNWGTYRP TGTHRGTVVS

DGGTYDIYTT MRYNAPSIDG TQTFQQFWSV RQSKRPTGNN VSITFSNHVN

AWRNAGMNLG SSWSYQVLAT EGYQSSGRSN VTVW

**S100C/N147C**

SANTYWQYWT DGGGTVNATN GPGGNYSVTW RDTGNFVVGK GWEIGSPNRT

IHYNAGVWEP SGNGYLTLYG WTRNQLIEYY VVDNWGTYRP TGTHRGTVV**C**

DGGTYDIYTT MRYNAPSIDG TQTFQQFWSV RQSKRPTGNN VSITFS**C**HVN

AWRNAGMNLG SSWSYQVLAT EGYQSSGRSN VTVW

**A155S**

SANTYWQYWT DGGGTVNATN GPGGNYSVTW RDTGNFVVGK GWEIGSPNRT

IHYNAGVWEP SGNGYLTLYG WTRNQLIEYY VVDNWGTYRP TGTHRGTVVS

DGGTYDIYTT MRYNAPSIDG TQTFQQFWSV RQSKRPTGNN VSITFSNHVN

AWRN**S**GMNLG SSWSYQVLAT EGYQSSGRSN VTVW

**Primer Design**



**Table S1:**Oligonucleotide primer sequences designed for each of the four mutated points by using snapgene viewer 2.2.2 software (from GSL Biotech; available at www.snapgene.com)

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| --- | --- | --- | --- | --- | --- | --- | --- | --- | --- |
| |  |  | | --- | --- | |  |  | |  | |   a) wildtype xyn11A | |  |  | | --- | --- | |  |  | |  | |   b) D32G |
| |  |  | | --- | --- | |  |  | |  | |   c) S100C/N147C | |  |  | | --- | --- | |  |  | |  | |   d) A155S |
| **Figure S1:**Quality assessments (Sequence Identity, Sequence Similarity, GMQE, and QMEAN) for the starting structures obtained by homology modelling using SWISSMODEL workspace of a) wildtype xyn11A, b) D32G mutant, c) S100C/N147C mutant, and d) A155S mutant. | |
|  | |

|  |  |  |
| --- | --- | --- |
| a) | b) | c) |
| **Figure S2:**Simulation temperatures measured during 11-ns equilibrations of the MD simulations at a) 300K b) 400K and e) 500K in this study. | | |



**Figure S3:**Hydrogen bonding between residues A151 and S155 from the A155S mutant simulation