1   **Supplementary Information**

2   Table S1. Parameters used for the prediction of the three-dimensional structure of *W*XynB1

3   in the YASARA software

Parameter	Descrition
Modeling speed	Slow
PSI-BLAST iterations in template search	10
Maximum allowed (PSI-)BLAST E-value to consider template (EValue Max)	0.5
Maximum number of templates to be used	10
Maximum number of templates with same sequence	1
Maximum oligomerization state	1 and 4
Maximum number of alignment variations per template	5
Maximum number of conformations tried per loop	50
Maximum number of residues added to the termini	10

4

5

6   Table S2. *W*XynB1 model ranking for the 4 best models generated from a total of 25 for the

7   protomer and 45 for the tetramer. In both cases the hybrid models reached the highest hits

	Protomeric model			Tetrameric model		
Rank	Z-score	Template	Residues	Z-score	Template	Residues
1	-1.067	Hybrid model	9-571	-1.394	Hybrid model	10-570
2	-1.194	3C2U	19-561	-1.469	1YRZ	20-559
3	-1.227	3C2U	20-561	-1.470	1YRZ	20-559
4	-1.231	2EXI	20-560	-1.521	2EXJ	20-560

8

9

10   Table S3. *W*XynB1 hybrid models composition. The fragments listed below were combined

11   from other models

Protomeric hybrid model					Tetrameric hybrid model				
First residue	Last residue	Length	From model	Score	First residue	Last residue	Length	From model	Score
10	570	561	2EXK_D01*	-1.553	10	570	561	2EXK_02*	-1.472
9	22	14	3C2U_C04	-1.518	10	570	561	2EXK_02**	-1.462
316	336	21	3C2U_C05	-1.507	456	469	14	2EXJ_01	-1.427
557	571	15	3C2U_C02	-1.472	369	376	8	1YIF_02	-1.418
43	58	16	2EXI_B03	-1.462	332	335	4	1YI7_02	-1.415
					490	493	4	1YRZ_A05	-1.412
					490	493	4	1YRZ_A05	-1.407
					279	282	4	1YRZ_A05	-1.405

12   * Model considered most suitable for hybridization
13   ** Model oligomerizated
14

15

1

16   Table S4. Gel filtration results for *W*XynB1 and the truncated catalytic domain

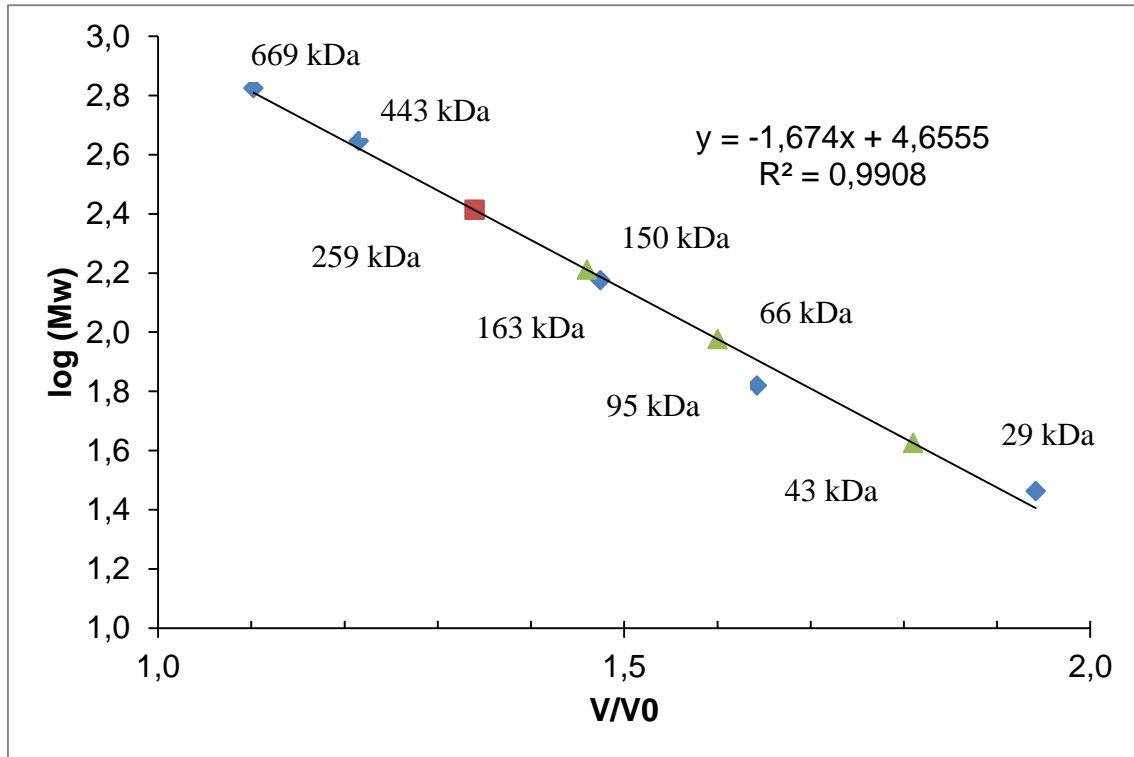|	Peak 1	2	3
*W*XynB1			
V/V0	1.34		
Mw (kDa)	259		
Estimated number of subunits	4		
Truncated catalytic domain			
V/V0	1.81	1.60	1.46
Mw (kDa)	43	95	163
Estimated number of subunits	1	2-3	4
Distribution (%)	35	32	33

17

18

Table S5. Prediction of inter-molecular hydrogen bonds based on the model of the tetramer of *W*Xyn43.

Residues with distances relevant for hydrogen bond formation are shown.

Donor Atom	Chain	Acceptor Atom	Chain	Donor-Acceptor Distance (Å)	Donor-H-Acceptor Distance (Å)
Dimer-forming hydrogen bonds					
Arg 120 $N^{\eta 1}$	A	Asp 529 $O^{\delta 1}$	D	3.0	2.2
Arg 120 $N^{\eta 1}$	A	Asp 529 $O^{\delta 2}$	D	3.3	2.4
Arg 120 $N^{\eta 2}$	A	Asp 529 $O^{\delta 1}$	D	3.0	2.2
Arg 120 $N^{\eta 2}$	A	Asp 529 $O^{\delta 2}$	D	3.0	2.1
Gly 123 N	A	Ser 526 O	D	2.9	1.9
Arg 148 $N^{\eta 1}$	A	Asp 428 $O^{\delta 2}$	D	2.9	2.0
Arg 148 $N^{\eta 2}$	A	Lys 426 O	D	3.1	2.3
Arg 148 $N^{\eta 2}$	A	Asp 428 $O^{\delta 2}$	D	3.1	2.2
Tyr 150 O^{η}	A	Glu 435 $O^{\varepsilon 2}$	D	2.7	1.7
Thr 173 $O^{\gamma 1}$	A	Tyr 528 O^{η}	D	2.8	1.9
Ser 372 N	A	Asp 100 $O^{\delta 2}$	D	2.8	1.8
Ser 372 O^{γ}	A	Asp 100 $O^{\delta 1}$	D	2.7	1.8
Asn 375 $N^{\delta 2}$	A	Asp 100 $O^{\delta 2}$	D	3.0	2.0
Tyr 404 O^{η}	A	Trp 145 O	D	2.8	1.8
Gln 405 $N^{\varepsilon 2}$	A	Val 124 O	D	2.8	1.9
Gln 405 $N^{\varepsilon 2}$	A	Trp 145 O	D	3.2	2.3
Arg 444 N^{ε}	A	Ser 508 O	D	2.9	1.9
Arg 444 $N^{\eta 1}$	A	Gln 507 O	D	3.1	2.4
Gly 446 N	A	Asp 95 O	D	2.9	1.9
Ser 450 N	A	Glu 149 $O^{\varepsilon 1}$	D	2.9	1.9
Lys 453 N^{ζ}	A	Glu 149 $O^{\varepsilon 1}$	D	3.0	2.1
Tyr 525 O^{η}	A	Lys 99 O	D	2.8	1.8
Tyr 525 O^{η}	A	Thr 173 $O^{\gamma 1}$	D	2.9	1.9
Tetramer-forming hydrogen bonds					
His 152 $N^{\delta 1}$	C	Glu 276 $O^{\varepsilon 1}$	A	2.9	1.9
Tyr 242 O^{η}	C	Asp 182 $O^{\delta 2}$	A	2.7	1.8
Ser 277 O^{γ}	C	Val 183 O	A	2.7	1.7
Ser 278 N	C	Asp 182 O	A	3.0	2.1
Ser 278 O^{γ}	C	Asp 182 $O^{\delta 2}$	A	2.7	1.7
His 152 $N^{\delta 1}$	C	Glu 276 $O^{\varepsilon 1}$	A	2.9	1.9

19

20 Figure S1. Molecular weight determination of *W*XynB1 by gel filtration. Red data point

21 indicates the position of *W*XynB1on the standard curve (blue data points) and green points

22 represents the data for the truncated catalytic domain.

The equation shown on the chart:

$$y = -1{,}674x + 4{,}6555$$
$$R^2 = 0{,}9908$$

23

24

25