Supporting Information for

Positional Effects of Phosphoserine on β-Hairpin Stability

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Page S1-S10: NMR chemical shift assignments for all peptides

Page S10-S12: Cross-strand NOEs for ***WTTS****,* ***WTTpS****,* ***SWLW, pSWLW, WSWL, WpSWL, WSWS*** *and* ***WSWpS***

Table S1. NMR assignments for **WTTS** in pD 7 buffer at 298.15K.

WTTS	α	β	γ	δ	ε
R	4.17	1.51	1.38	3.05	
W	4.91	3.14	H2 7.20, H4 7.56, H5 7.15, H6 7.22, H7 7.48		
V	4.29	1.98	0.87		
T	4.65	4.08	1.12		
V	4.16	2.02	0.93		
N	4.61	2.93,2.75			
G	4.01,3.80				
K	4.53	1.8	1.42	1.75	2.99
T	4.55	4.1	1.15		
I	4.35	1.89	1.18	0.9	
S	4.43	3.7			
Q	4.32	1.92	2.3		

Table S2. NMR assignments for **WTTpS** in pD 7 buffer at 298.15K.

WTTpS	α	β	γ	δ	ε
R	4.13	1.53	1.32	3.01	
W	4.92	3.19		H2 7.18, H4 7.61, H5 7.14, H6 7.22, H7 7.47	
V	4.23	1.99	0.87		
T	4.54	4.13	1.16		
V	4.13	2.06	0.94		
N	4.65	2.85,2.77			
G	3.97, 3.82				
K	4.52	1.78	1.42	1.68	2.99
T	4.52	4.23	1.16		
I	4.21	1.87	1.46	0.92	
S-PO3	4.46	4.02			
Q	4.27	1.96	2.37		

Table S3. NMR assignments for **Cyclic WTTS** in pD 7 buffer at 298.15K.

Cyclic WTTS	α	β	γ	δ	ε
C	4.5	3.02,2.78			
R	4.59	1.81	1.59	3.18	
W	5.22	3.06	H5 7.06,H2/H6 7.24,H7 7.38,H4 7.46		
V	4.62	2.05	0.88		
T	5.16	3.92	1.02		
V	4.24	1.91	0.91		
N	4.41	3.08,2.77			
G	4.13,3.56				
K	4.73	1.85	1.43	1.71	3.04
T	4.97	3.96	1.16		
I	4.75	1.9	1.16	0.91	
S	4.3	3.25,2.89			
Q	4.53	1.84	2.07,2.22		
C	4.73	3.23,2.89			

Table S4. NMR assignments for **RWVTVNG** in pD 7 buffer at 298.15K.

RWVTVNG	α	β	γ	δ	ε
R	4.13	1.55	1.37	3.05	
W	4.76	3.34,3.22	H2 7.21, H4 7.62, H5 7.08, H6 7.22, H7 7.44		
V	4.12	2	0.87		
T	4.34	4.16	1.19		
V	4.13	2.1	0.93		
N	4.69	2.86,2.75			
G	3.88				

Table S5. NMR assignments for **NGKTIpSQ** in pD 7 buffer at 298.15K.

NGKTIpSQ	α	β	γ	δ	ε
N	4.69	2.82			
G	3.94				
K	4.45	1.86	1.43	1.75	3
T	4.39	4.31	1.21		
I	4.14	1.91	1.51,1.24	0.94	
S-PO3	4.55	4.14			
Q	4.31	1.99	2.39		

Table S6. NMR assignments for **NGKTISQ** in pD 7 buffer at 298.15K.

NGKTISQ	α	β	γ	δ	ε
N	4.68	2.82			
G	3.95				
K	4.38	1.82	1.42	1.78	
T	4.35	4.18	1.2		
I	4.21	1.88	1.47	0.92	
S	4.46	3.86			
Q	4.34	1.99	2.38		

Table S7. NMR assignments for **SWLW** in pD 7 buffer at 298.15K.

SWLW	α	β	γ	δ	ε
R	4.33	1.72	1.51	3.11	
S	4.86	3.26,4.34			
V	4.21	1.9	0.87		
W	4.94	3	H2/H6 7.20, H4 7.62, H5 7.05, H7 7.41		
V	4.34	1.92	0.79		
N	4.39	3.05/2.72			
G	4.14,3.69				
K	4.61	1.73	1.37	1.71	3
L	3.95	1.19	0.76	0.35,0.12	
I	4.36	1.87	1.18	0.81	
W	4.75	3.11	H2 7.20, H4 7.51, H5 7.15, H6 7.25, H7 7.51		
Q	4.28	1.73/1.93	2.12		

Table S8. NMR assignments for **pSWLW** in pD 7 buffer at 298.15K.

pSWLW	α	β	γ	δ	ε
R	4.35	1.83	1.69	3.2	
S-PO3	4.5	4.12,3.97			
V	4.26	1.98	0.9		
W	5	3.01	H2 7.19, H4 7.43, H5 7.05, H6 7.19, H7 7.56		
V	4.11	2.09	0.83		
N	4.46	3.03,2.73			
G	4.12/3.78				
K	4.58	1.75	1.37	1.71	2.96
L	4.05	1.21	n/a	0.73	
I	4.19	1.84	n/a	0.78	
W	4.66	3.24	H2 7.25, H4 7.48, H5 7.13, H6 7.19, H7 7.61		
Q	4.12	1.76	2.03		

Table S9. NMR assignments for **WSWL** in pD 7 buffer at 298.15K.

WSWL	α	β	γ	δ	ε
R	4.45	1.65	1.52	3.15	
W	5.09	2.96	H2 7.14, H4 7.40, H5 7.00, H6 7.18, H7 7.36		
V	4.11	1.86	0.82		
S	4.44	3.16,2.12			
V	4.57	1.96	0.84		
N	4.3	2.68,3.01			
G	3.99,3.36				
K	4.54	1.75	1.38	1.69	2.99
W	5.1	3.01	H2 7.14, H4 7.59, H5 7.00, H6 7.18, H7 7.40		
I	4.67	1.83		0.83	
L	3.89	1.18	0.31	0.19,-0.0029	
Q	4.31	1.85	2.21,2.00		

Table S10. NMR assignments for **WpSWL** in pD 7 buffer at 298.15K.

WpSWL	α	β	γ	δ	ε
R	4.38	1.67	1.51	3.12	
W	5.05	3.07,3.19	H2 7.13, H4 7.44, H5 7.06, H6 7.31, H7 7.41		
V	4.38	1.97	0.83		
S-PO3	4.56	3.66,3.38			
V	4.07	1.97	0.87		
N	4.47	2.93,2.71			
G	3.94, 3.73				
K	4.44	1.73	1.34	1.69	2.94
W	4.9	3.01	H2 7.21, H4 7.63, H5 7.16, H6 7.21, H7 7.50		
I	4.46	1.71	N/A	0.85	
L	3.99	1.32	0.71	0.55,0.35	
Q	4.28	1.88,2.04	2.27		

Table S11. NMR assignments for **RSVWVNG** in pD 7 buffer at 298.15K.

RSVWVNG	α	β	γ	δ	ε
R	4.27	1.69	1.56	3.13	
S	4.52	3.75			
V	4.08	1.97	0.79		
W	4.68	3.17	H2 7.20, H4 7.63, H5 7.15, H6 7.23, H7 7.47		
V	3.99	1.93	0.82		
N	4.51	2.66			
G	3.87				

Table S12. NMR assignments for **RSpVWVNG** in pD 7 buffer at 298.15K.

RSpVWVNG	α	β	γ	δ	ε
R	4.21	1.72	1.61	3.09	
S-PO3	4.42	4.05			
V	4.04	1.98	0.78		
W	4.61	3.18	H2 7.21, H4 7.64, H5 7.17, H6 7.21, H7 7.49		
V	3.92	1.87	0.77		
N	4.44	2.67			
G	3.82				

Table S13. NMR assignments for **NGKLIWQ** in pD 7 buffer at 298.15K.

NGKLIWQ	α	β	γ	δ	ε
N	4.52	2.76,2.8			
G	3.9				
K	4.26		1.36	1.67	2.92
L	4.3	1.54	1.45	0.86	
I	4.09	1.78	1.37,1.12	0.8	
W	4.64	3.28	H2/H6 7.23, H4 7.61, H5 7.15, H7 7.47		
Q	4.12	1.76	2.02		

Table S14. NMR assignments for **RWVSVNG** in pD 7 buffer at 298.15K.

RWVSVNG	α	β	γ	δ	ε
R	4.11	1.53	1.36	3.02	
W	4.68	3.18	H5 7.13, H2/H6 7.19, H7 7.45, H4 7.58		
V	4	1.92	0.81		
S	4.33	3.78			
V	4.1	2.07	0.88		
N	4.64	2.71			
G	3.83				

Table S15. NMR assignments for **RWVSpVNG** in pD 7 buffer at 298.15K.

RWVSpVNG	α	β	γ	δ	ε
R	4.21	1.63	1,45	3.1	
W	4.69	3.25	H5 7.18,H2/6 7.24, H4/7 7.6		
V	4.04	1.93	0.85		
S-PO3	4.42	4.12			
V	4.1	2.09	0.94		
N	4.71	2.88.2.78			
G	3.88				

Table S16. NMR assignments for **SWLV** in pD 4 buffer at 298.15K.

SWLV	α	β	γ	δ	ε
R	4.38	1.65	1.77	3.19	
S	4.85	3.65			
V	4.35	1.96			
W	5	3.06	H2 7.14 H4 7.45 H5 7.03 H6 7.16 H7 7.45		
V	4.16	0.83	1.86		
N	4.44	2.74,3.08			
G	4.09, 3.66				
K	4.63	1.77	1.42	1.74	3.03
L	3.87	1.19	0.37	0.12	
I	4.23	1.81		0.83	
V	4.16	0.83	1.86		
Q	4.38	1.96	2.31		

Table S17. NMR assignments for **pSWLV** in pD 4 buffer at 298.15K.

pSWLV	α	β	γ	δ	ε
R	4.36	1.8	1.69	3.21	
S-PO3	4.7	4.02			
V	4.29	1.97	0.87		
W	4.99	3.06	H2 7.13 H4 7.46 H5 7.05 H6 7.18 H7 7.47		
V	4.14	1.99	0.87		
N	4.45	3.65,2.73			
G	4.13, 3.77				
K	4.59	1.77	1.39	1.72	2.99
L	3.81	1.25	0.96	0.52,0.31	
I	4.21	1.86	1.28	0.83	
V	4.21	1.88	0.89		
Q	4.29	1.97	2.32		

Table S18. NMR assignments for **NGKWILQ** in pD 7 buffer at 298.15K.

NGKWILQ	α	β	γ	δ	ε
N	4.64				
G	3.83				
K	4.21		1.2	1.69	2.87
W	4.7	3.24	H5 7.18,H2/H6 7.22,H4 7.69,H7 7.49		
I	4.06	1.73		0.8	
L	4.25	1.58	0.93	0.9	
Q	4.26	1.96	2.34		

Table S19. NMR assignments for **Cyclic SWLW** in pD 7 buffer at 298.15K.

Cyclic SWLW	α	β	γ	δ	ε
C	4.88	3.21,2.87			
R	4.56	1.79	1.51	3.13	
S	4.7				
V	4.22	1.88	0.86		
W	4.94	3.02		H2 7.16, H4 7.44, H5 6.99, H6 7.16, H7 7.40	
V	4.35	1.9	0.78		
N	4.36	3.06,2.07			
G	4.15,3.66				
K	4.61	1.7	1.36		2.99
L	3.92	1.13	0.61	0.32,0.19	
I	4.43	1.86	1.14	0.81	
W	4.8			H2 7.16, H4 7.44, H5 6.99, H6 7.09, H7 7.31	
Q	4.53	1.84	2.13		
C	5.09	2.96,2.18			

Table S20. NMR assignments for **Cyclic WSWL** in pD 7 buffer at 298.15K.

Cyclic WSWL	α	β	γ	δ	ε
C	4.75	n/a			
R	4.68	1.85	1.66	3.18	
W	5.16	n/a	H2 7.23, H4 7.50, H6 7.17, H5 6.99 , H7 7.47		
V	4.12	1.9	0.85		
S	4.46	3.06,1.99			
V	4.65	1.96	0.86		
N	4.31	3.01,2.71			
G	4.03,3.35				
K	4.59	1.72	1.41		3.02
W	5.16	n/a	H2 7.23, H4 7.43, H5 7.03, H6 7.21, H7 7.38		
I	4.71	1.89		0.88	
L	3.88	1.27	0.37	-0.27,0.89	
Q	4.55	1.86	2.17		
C	4.76	n/a			

Table S21. NMR assignments for **WSWS** in pD 7 buffer at 298.15K.

WSWS	α	β	γ	δ	ε
R	4.31	1.65	1.47	3.11	
W	4.96	3.06	H2 7.19, H4 7.45, H5 7.05, H6 7.19, H7 7.40		
V	4.44	1.97	0.86		
S	4.51	3.35,2.79			
V	4.14	1.95	0.89		
N	4.46	2.96,2.73			
G	3.98,3.46				
K	4.48	1.69	1.36		2.98
W	5.04	3.04,3.19	H2 7.14, H4 7.40, H5 7.05, H6 7.19, H7 7.36		
I	4.51	1.86	1.18	0.89	
S	4.24	3.42,3.22			
Q	4.31	1.87	2.26,2.09		

Table S22. NMR assignments for **WpSWS** in pD 7 buffer at 298.15K.

WpSWS	α	β	γ	δ	ε
R	4.23	1.63	1.44	3.05	
W	4.79	3.15	H2 7.18 H4 7.49 H5 7.13 H6 7.25 H7 7.49		
V	4.12	1.95	0.84		
S-PO3	4.48	3.96			
V	4.04	1.95	0.84		
N	4.64	2.74			
G	3.84				
K	4.28	1.66	1.25	1.64	2.9
W	4.79	3.15	H2 7.18 H4 7.49 H5 7.18 H6 7.25 H7 7.49		
I	4.18	1.74	1.07	0.82	
S	4.28	3.72			
Q	4.33	2.03,2.21	2.4		

Table S23. NMR assignments for **WSWpS** in pD 7 buffer at 298.15K.

WSWpS	α	β	γ	δ	ε
R	4.18	1.5	1.25	2.93	
W	4.87	3.06	H2 7.12 , H4 7.37 ,H5 7.05, H6,7.19 H7 7.42		
V	4.29	1.89	0.81		
S	4.46	3.52, 3.20			
V	4.11	2.03	0.93		
N	4.54	2.94,2.75			
G	3.95, 3.60				
K	4.43	1.74	1.33	1.67	2.96
W	4.87	3.06	H2 7.12 , H4 7.42 ,H5 7.05, H6,7.16 H7 7.42		
I	4.39	1.8	1.15	0.88	
S-PO3	4.43	3.97			
Q	4.28	1.92	2.31		

Table S24. NMR assignments for **WpSWpS** in pD 7 buffer at 298.15K.

WpSWpS	α	β	γ	δ	ε
R	4.2	1.63	1.45	3.09	
W	4.67	3.25	H2 7.15, H4 7.63, H5 7.15, H6 7.22, H7 7.52		
V	4.1	2.1	0.9		
S-PO3	4.45	4.04			
V	4.05	2.06	0.9		
N	4.7	2.78			
G	3.88				
K	4.29	1.66	1.31	1.63	2.91
W	4.7	3.25	H2 7.15, H4 7.63, H5 7.15, H6 7.22, H7 7.52		
I	4.1	1.69	1.08	0.81	
S-PO3	4.33	4.01, 4.07			
Q	4.25	1.94	2.35,2.18		

Table S25. NMR assignments for **NGKWISQ** in pD 7 buffer at 298.15K

NGKWISQ	α	β	γ	δ	ε
N	4.67	2.78			
G	3.83				
K	4.24	1.62	1.24		2.89
W	4.68	3.24	H2/H6 7.22, H4 7.61, H5 7.14, H7 7.48		
I	4.07	1.72	1.07	0.83	
S	4.29	3.82			
Q	4.3	1.98	2.36		

Table S26. NMR assignments for **NGKWIpSQ** in pD 7 buffer at 298.15K.

NGKWIpSQ	α	β	γ	δ	ε
N	4.67	2.78			
G	3.83				
K	4.28	1.64	1.27		2.91
W	4.68	3.27	H2 7.17, H4 7.57, H5 7.12, H6 7.20, H7 7.44		
I	4.08	1.71	1.07	0.83	
S-PO3	4.38	4.1			
Q	4.29	1.97	2.35		

Table S27. NMR assignments for **Cyclic WSWS** in pD 7 buffer at 298.15K.

cyclic WSWS	α	β	γ	δ	ε
C	4.95	2.90,3.08			
R	4.62	1.82	1.59	3.14	
W	5.02	2.89	H2 7.22, H4 7.43, H5 7.03, H6 7.22, H7 7.33		
V	4.62	1.98	0.86		
S	4.65	2.88			
V	4.12	1.81	0.86		
N	4.29	3.07,2.70			
G	4.04,3.36				
K	4.57	1.85	1.4	1.71	3.02
W	5.29	3.09, 2.97	H2 7.15, H4 7.33, H5 7.03, H6 7.22, H7 7.28		
I	4.73	1.9		0.9	
S	4.45	3.10,2.07			
Q	4.53	1.83	2.20,2.05		
C	5.1	3			

Figure S1. NOES of WTTS

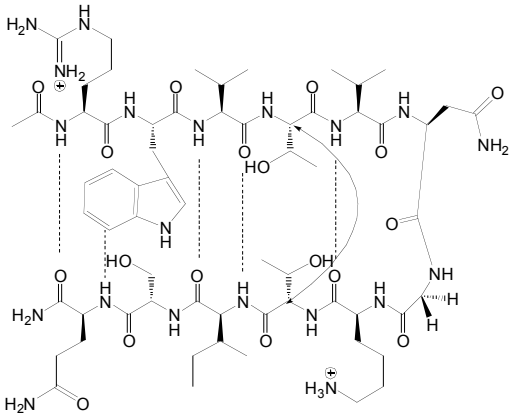

Figure S2 NOES of SWLW

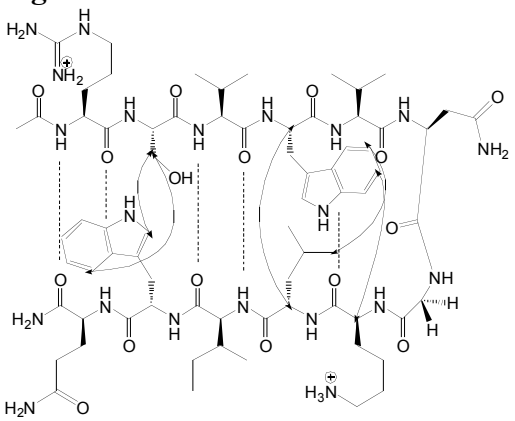

Figure S3 NOES of pSWLW

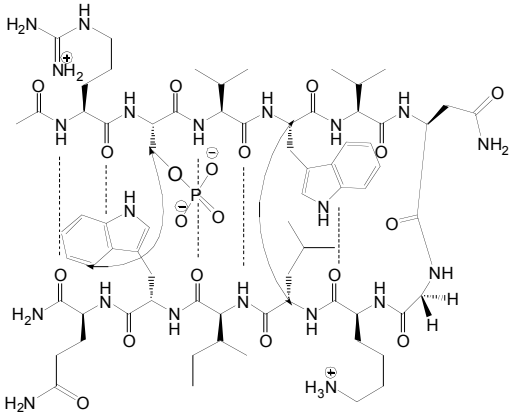

Figure S4 NOES of WSWL

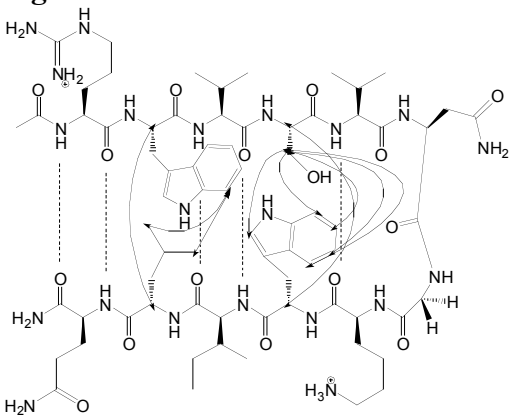

Figure S5 NOES of WpSWL

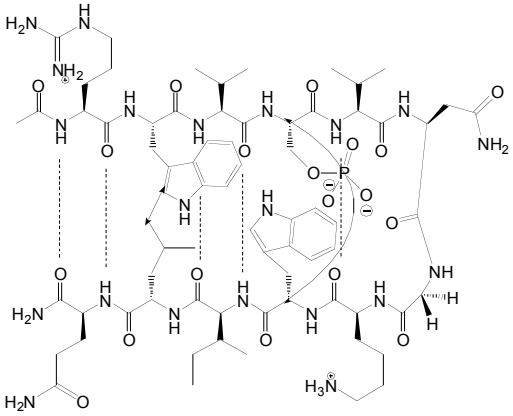

Figure S6. NOES of WSWS

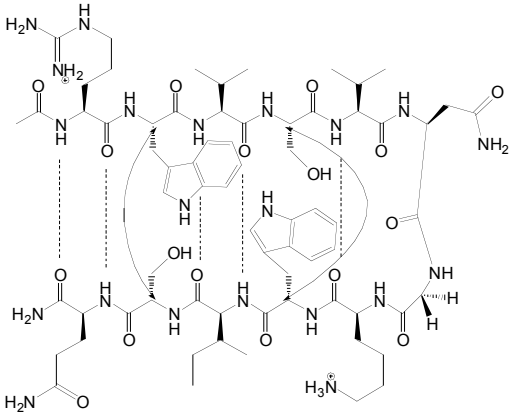

Figure S7. NOES of WSWpS