

Table 1. Proton chemical shift (ppm) values for peptides asFP595-Ia, asFP595-Ib, asFP595-II, asFP595-III, and DsRed-II in H₂O/D₂O at pH 3.2.

Residue ^a in asFP595/DsRed amino acid sequence	Group ^a	asFP595-Ia ^b	asFP595-Ib ^b	asFP595-II ^c	asFP595-III ^c	DsRed-II ^c
Ser-63/Gln-64	C ^α H	4.53	4.40			
	C ^β H ₂	3.92	3.90			
Cys-64/Phe-65	C ^α H	4.64	5.13			
	C ^β H ₂	2.96, 2.99	3.13, 3.27			
Met-65/Gln-66	C ^α H	5.09	5.09	absent	absent	absent
	C ^β H ₂	2.24, 2.30	1.83, 1.98	3.53	3.15	3.09
	C ^γ H ₂	2.64, 2.71	2.51	2.89	3.01	2.78
	C ^ε H ₃ ^d	2.12	2.00	2.16	2.18	
	N ^ε H ₂ ^e					7.08, 7.90
Tyr-66/Tyr-67	C ^β H ^f	7.34	6.88	7.66	7.87	7.83
	C ^δ H	8.14	7.78	8.25	8.22	8.14
	C ^ε H	7.01	6.82	7.02	7.00	6.92
Gly-67/Gly-68	C ^α H ₂	4.63, 4.66	4.37, 4.46	4.74	4.72, 4.77	4.66, 4.79
Ser-68/Ser-69	NH	n/d ^g	n/d ^g	n/d ^g	8.88	8.04
	C ^α H	4.12	4.21	4.46	4.46	4.30
	C ^β H ₂	3.95	3.96, 4.04	3.89	3.90	3.83
Lys-69/Lys-70	NH	n/d ^g		n/d ^g	8.40	
	C ^α H	4.39		4.36	4.38	
	C ^β H ₂	1.79, 1.91		1.76, 1.91	1.77, 1.91	
	C ^γ H ₂	1.47		1.45	1.45	
	C ^δ H ₂	1.70		1.67	1.67	
	C ^ε H ₂	3.01		2.97	2.96	
	N ^η H ₂	n/d ^g		7.54	7.53	
Ala-70 ^h /Val-71	NH	n/d ^g		n/d ^g	8.00	
	C ^α H	4.13		4.12	4.11	
	C ^β H ₃	1.32		1.29	1.30	

^a We use residue and group names of natural (unmodified) amino acids.

^b Measured at 30°C.

^c Measured at 10°C.

^d C^εH₃ of Met-65 in asFP595

^e N^εH₂ of Gln-66 in DsRed

^f Singlet of vinyl proton (of one proton unit) is observed at modified Tyr C^β atom. This signal shows the strong NOE connectivity with the aromatic δ-protons of the phenyl ring.

^g Not determined because the ¹H-NMR spectra for peptides asFP595-Ia, asFP595-Ib, and asFP595-II were not studied in H₂O (10% D₂O).

^h Thr-70 in wild-type asFP595.