

Table 2. Summary of Connectivities Observed in 2D NMR Experiments of CPST

Experiment	¹ H Signal	Residue					Set
		α-MurNAc ^a	α-GalA ^b	β-Rha ^c	β-GlcNAc ^d	S	
NOESY	H1	H2,bH3',bH4' ^w	H2,cH4',cH6'	H2,H3,H5,dH4'	H3,H5,bH4'	H3',H _g ' ^w	
	H2	H3		H3	H4' ^w	H _g ' ^w	
	H2'	H3'				H _g ' ^w	
	H3	H5,H2' ^w	H4,H5	H5,bH5' ^w	H5	H _g ' ^w	
	H4	H2' ^w ,H3' ^w	H5,dH5' ^w	H6	H5' ^w	H _g ' ^w	
	H5	H6	cH3' ^w ,cH4' ^w			H _g ' ^w	
HOHAHA	H _α					H _g ' ^w	
	H _β					H _g ' ^w	
	^h H _N	H2,H3,H(Me-NAC),aH1' ⁱ ,dH _N ' ⁱ			H3,H(Me-NAC),aH4'	H _g ' ^w ,H _β ',H _α ' ^w ,bH5' ^w ,cH5' ^w ,dH1' ^w	
	H1	H2,H3,H4,H5	H2,H3,H4	H2	H2,H3,H4,H5,H6	H _β ',H _g ' ^w	
	H2'	H3'				H _α ',H _β ',H _g ' ^w	
	H5	H2,H3,H4,H6	H4			H _α ',H _β ',H _g ' ^w	
HMBC	H _α					H _g ' ^w	
	^h H _N (20ms)	H2				H _g ' ^w	
	^h H _N (50ms)	H2,H3,H4' ^w				H _α ',H _β ',H _g ' ^w	
	H1	a3,a5,b3' ⁱ	b3,b5,c4' ⁱ	c2,d4' ⁱ	b4' ⁱ		
	H2	a3	b3	c3,c4	d1,d3		
	H2'	a3',a3	b2,a1' ⁱ	c4	d2,d4		
H3	a2,a4,a2'						
H3'	a1' ^{i,c} ,a2'						
H4	a3,a6' ^w	b2,b3,d1' ⁱ	c5	d3' ^w ,d5' ^w ,c1' ⁱ			
H4							
H5							
H6		a4' ^w ,a5' ^w	b1,b4,b6' ^c	c5,c4			
SELHMBC ^c	H3'	a1'					
	H5		b6				
	H(Me-NAc)	a(CO-NAC)				d(CO-NAC)	

^tExcept for aH3/aH4 and cH4/cH5, all cross peaks expected for vicinal coupling partners were observed in DQF-COSY; however, bH4/bH5 and cH1/cH2 cross peaks were weak (see text for explanation). In water suppressed DQF-COSY, cross peaks were observed between the three amide protons and their vicinal partners (i.e. aH2, dH2 and sH_g). Also one bond HMQC connectivities were observed for all protons. For simplicity ¹³C resonances are indicated only by the residue symbol and the number of the carbon atom; eg. a3 refers to aC3.

^cConnectivity to a carbonyl carbon; ^hConnectivities from water suppressed experiments;

ⁱInter residual connectivities; ^wWeak intensity.