

Designed glucopeptides mimetics of myelin protein epitopes as synthetic probes for the detection of autoantibodies, biomarkers of multiple sclerosis

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Supplementary Information

Table 1. ¹H chemical shift of CSF114(Glc) in DPC/SDS (90/10 M/M) micelle solution.

NH exchange rate (f, fast; m, moderately slow; s, slow).

CSF114(Glc)in DPC/SDS								Hδ exchange rate
Residue	HN	C ^α H	C ^β H	C ^γ H	C ^δ H	C ^ε H	Others	
Thr1								
Pro2		4.452	1.922 2.276	1.780	3.750 3.569			f
Arg3	8.511	4.276	1.711 1.580	1.531	3.103	7.267		f
Val4	8.113	4.103	1.968	0.829			Hζ 7.040	f
Glu5	8.377	4.447	1.953 1.827	2.224			Qζ7.791	m
Arg6	8.481	4.287	1.744 1.635	1.513	3.084	7.334	Hζ7.140	f
Asn(Glc)7	8.658	4.593	2.858 2.750		HD21 8.861		*	f
Gly8	8.464	3.850 3.716						f
His9	8.239	4.733	3.217/3.103		7.203		Qβ 3.166	f
Ser10	8.492	4.445	3.856 3.717					f
Val11	8.306	4.047	1.962	0.736				f
Phe12	8.085	4.467	3.063 2.923			7.171		s
Leu13	7.697	4.295	1.572	1.520	QD1 0.810 QD2 0.757			f
Ala14	7.882	4.256	1.288					s
Pro15		4.058	1.960 1.756	1.693	3.471 3.383			
Tyr16	7.569	4.253	2.962 2.650		6.940	6.717		s
Gly17	8.088	3.878 3.699						s
Trp18	7.585	4.483	3.293 3.181		6.990	10.429 7.392	Hζ27.260 Hζ36.716	s
Met19	7.721	4.106	1.834	2.048				s
Val20	7.544	4.095	2.035	0.779				
Lys21	7.798	4.135	1.767 1.692	1.354	1.595	2.888	Qζ 7.541	s
H1		H2	H3		H4		H5	
4.838		3.767	3.415		3.295		3.631	

Table 2. ^1H chemical shift of SP077 in DPC/SDS (90/10, M/M) micelle solution.

NH exchange rate (f, fast; m, moderately slow; s, slow).

SP077 in DPC/SDS								H δ exchange rate
Residue	HN	C $^{\alpha}$ H	C $^{\beta}$ H	C $^{\gamma}$ H	C $^{\delta}$ H	C $^{\epsilon}$ H	Others	
Thr1		4.109	3.917	1.222				
Phe2	8.979	4.654	3.152/3.055			7.291		
Arg3	8.271	4.246	1.809/1.731	1.552	3.152	7.316		
Val4	8.001	3.979	2.104	0.924				
Leu5	8.000	4.355	1.747/1.646	1.561	0.918/0.841			
Arg6	7.998	4.171	1.833/1.755	1.603	3.151	7.315		
Asn(Glc)7	8.491	4.731	2.931/2.818		8.923		*	
Gly8	8.322	4.039/3.917						m
Thr9	8.025	4.371	4.266	1.221				m
Ser10	8.269	4.394	3.929/3.828					m
Val11	7.986	3.956	1.982	0.770/0.709				m
Phe12	7.852	4.539	3.160/2.953		7.137	7.639	H ζ 7.238	m
Leu13	7.643	4.298	1.548	1.439	0.884/0.839			m
His14	8.079	4.927	3.158/3.088		8.550/7.290			m
Pro15		3.799	1.906/1.859	3.543	1.734			
Asn16	8.500	4.546	2.814/2.743		7.678/6.782			
Lys17	8.106	4.226	1.709	1.188	1.533	2.819	Q ζ 7.543	
Trp18	8.038	4.712	3.264		7.144	10.346/7.536	HH2 7.0442 H ζ 7.438/6.984	
Thr19	7.947	4.395	5.460	1.162				
Val20	7.999	4.145	2.109	0.927				
Lys21	8.061	4.210	1.834/1.739	1.391	1.635	2.943	Q ζ 7.577	
H1		H2		H3		H4		H5
5.552		3.816		3.461		3.361		3.680

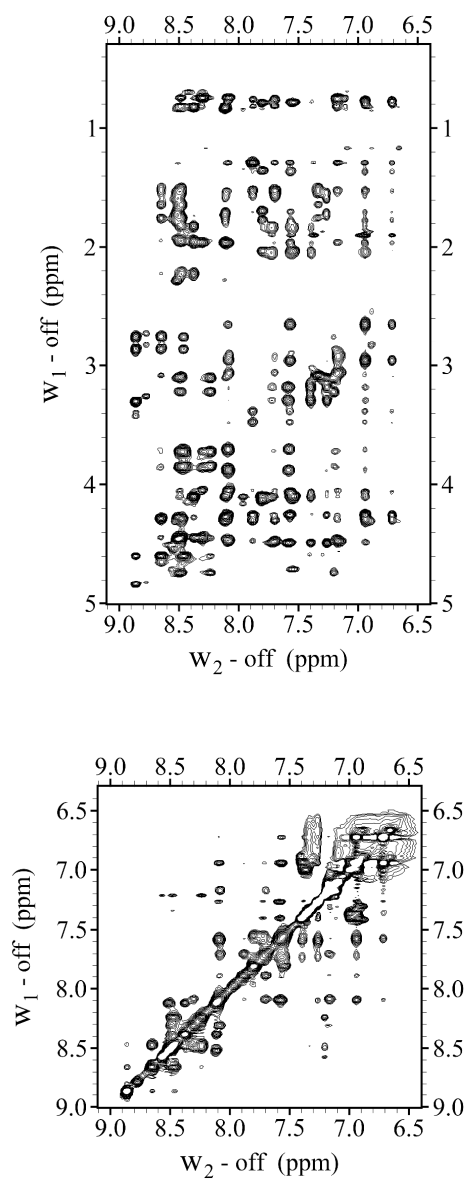


Figure 1. Finger region (top) and amide region (bottom) of the NOESY spectra of CSF114 in DPC/SDS (90/10 M/M) micelle solution.

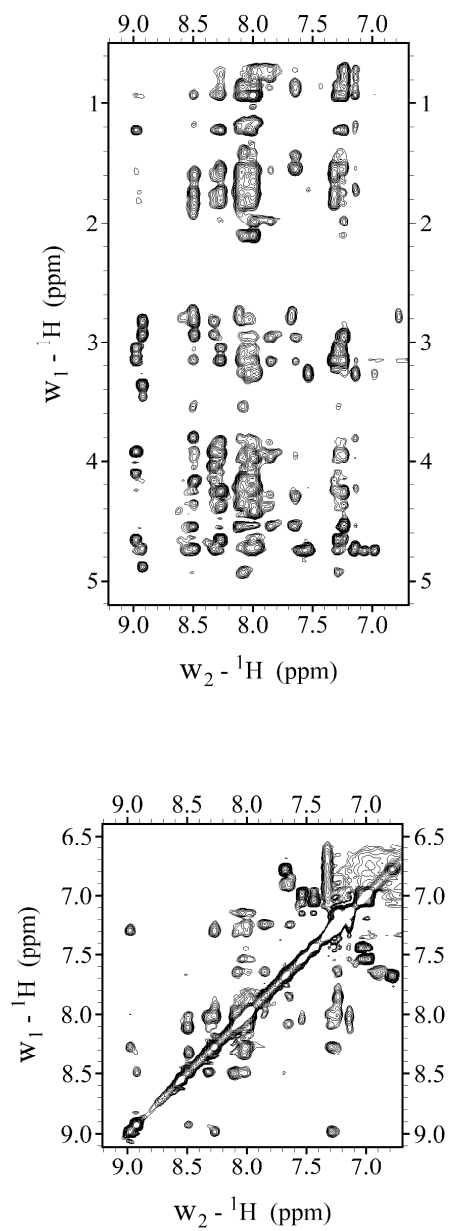


Figure 2. Finger region (top) and amide region (bottom) of the NOESY spectra of SP077 in DPC/SDS (90/10 M/M) micelle solution.

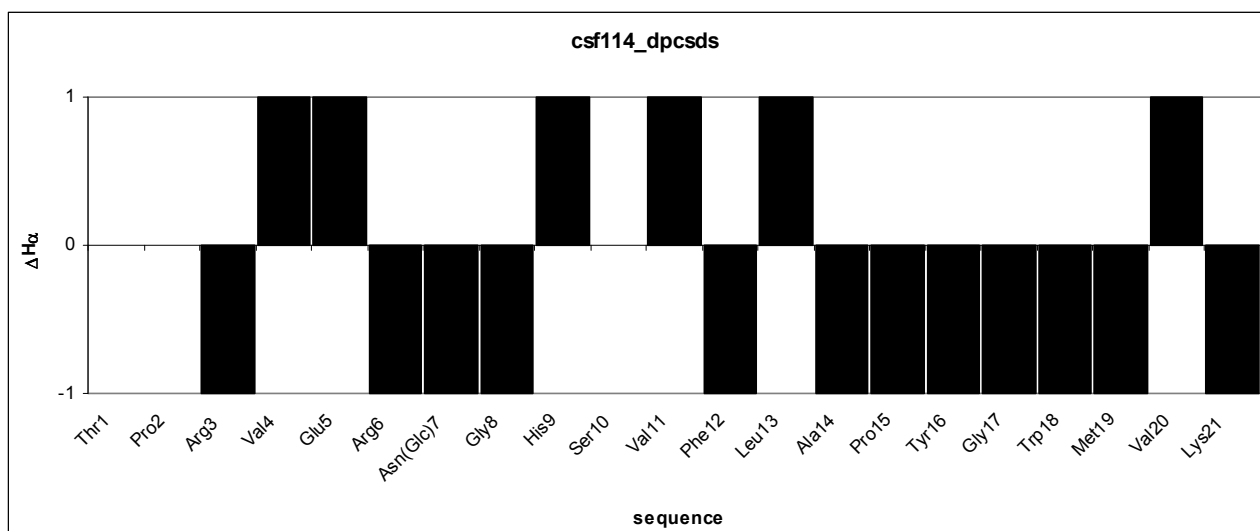


Figure 3. CH α chemical shifts differences of CSF114(Glc) in DPC/SDS micelles.

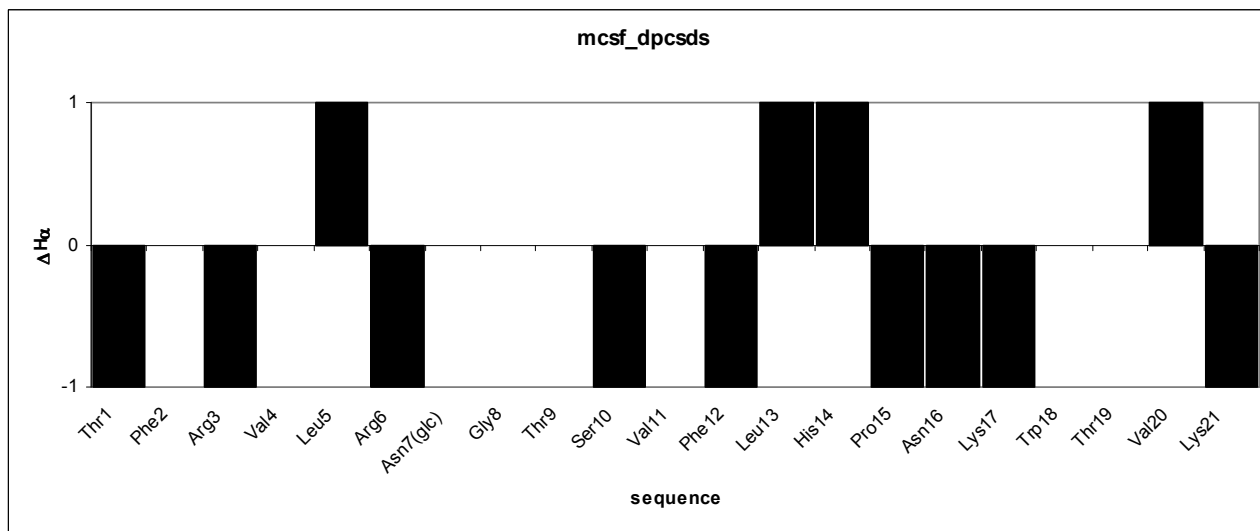


Figure 4. CH α chemical shifts differences of SP077 in DPC/SDS micelles.

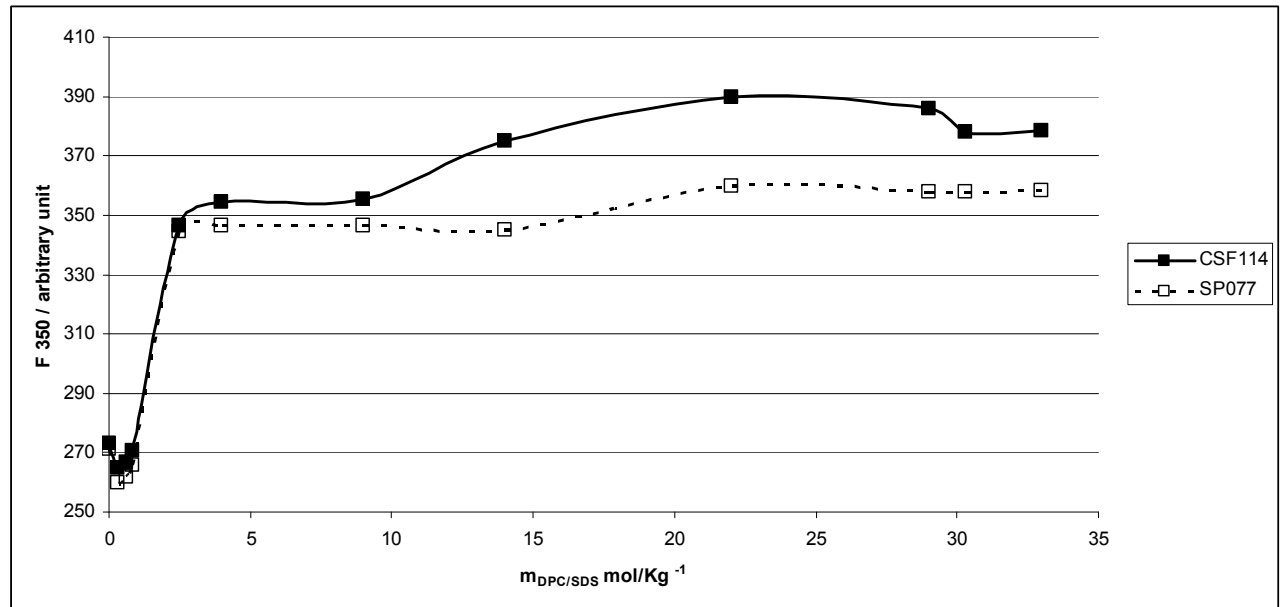


Figure 5. Trps fluorescence variation of CSF114(Glc) (full square) and SP077 (empty square) at $\lambda=350$ nm, with increasing DPC /SDS concentrations.

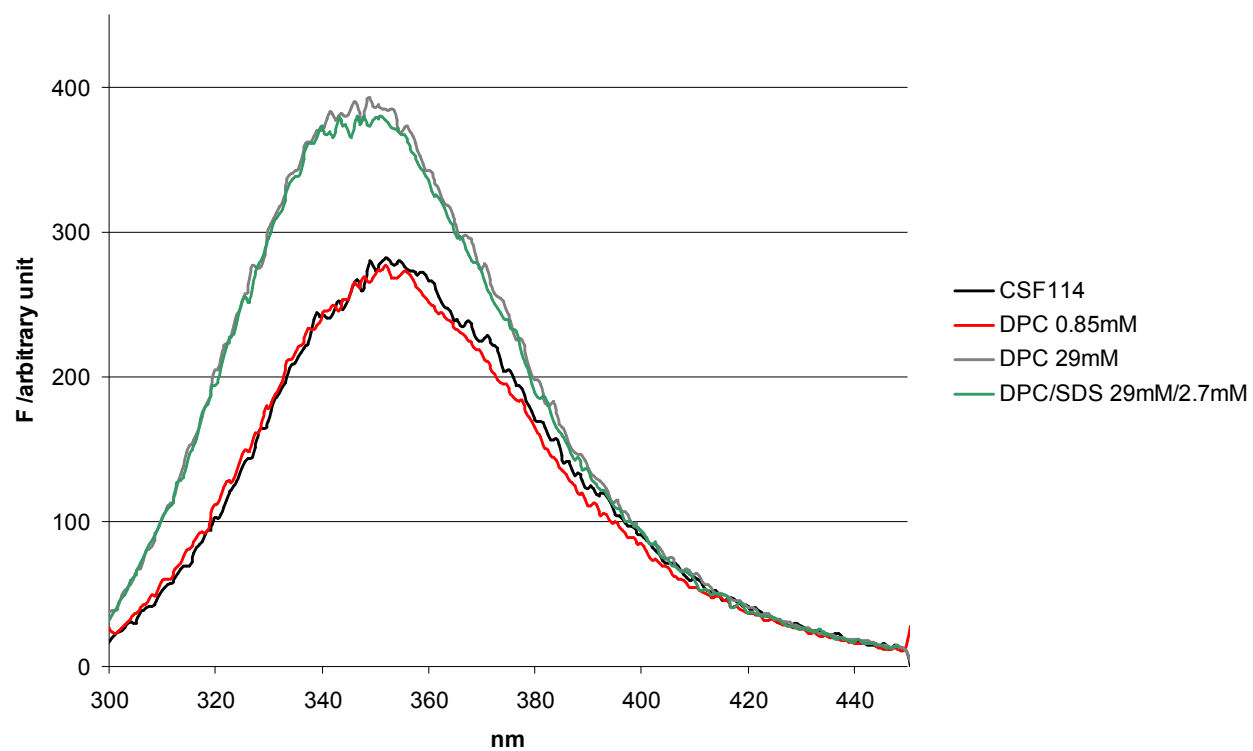


Figure 6. Tryptophan emission spectra (range 300–450 nm) of CSF114(Glc).

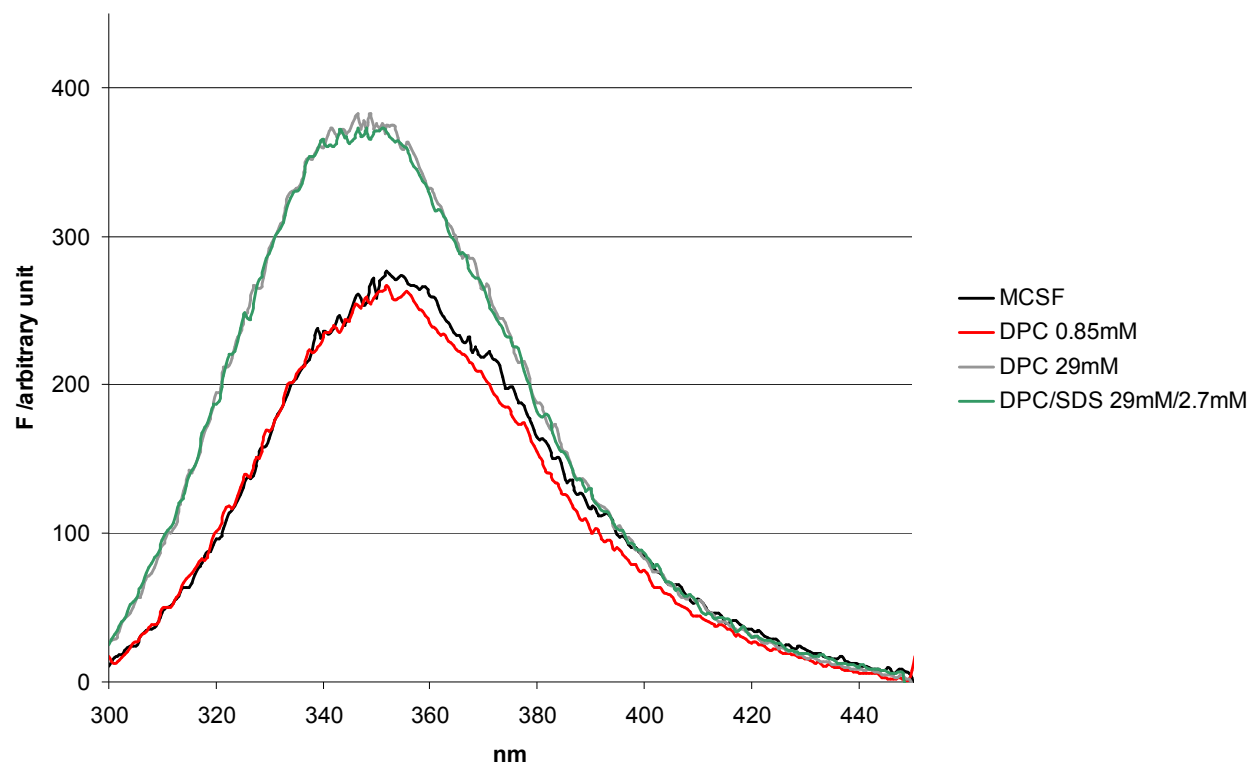


Figure 7. Tryptophan emission spectra (range 300–450 nm) of SP077.