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Supporting Information

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for

A fluorogenic peptide related to the processing site of human SARS corona virus S-protein: Kinetic evaluation and NMR structure elucidation

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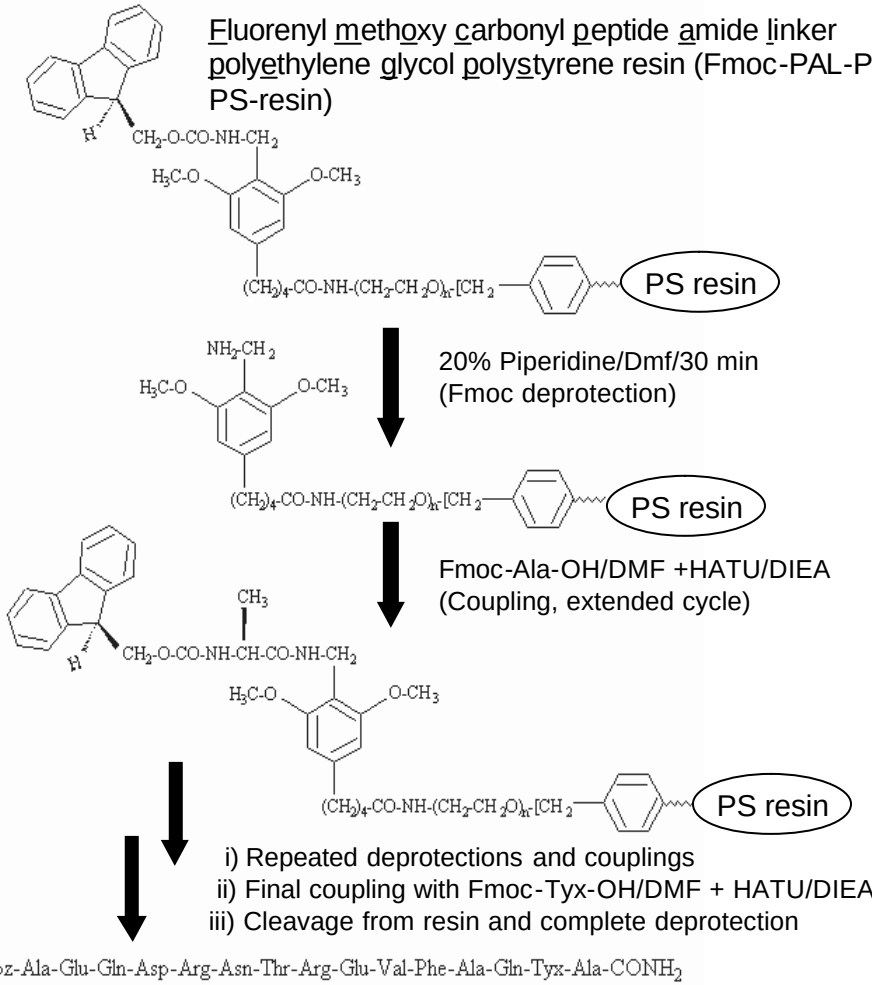
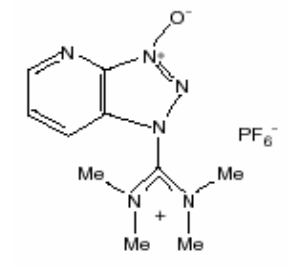
Figure S1. A) Scheme for synthesis of QSARS-4$^{754\text{-}766\ peptide}$ B) Cartoon presentation of fluorescence quenching; C) Chemical structures.

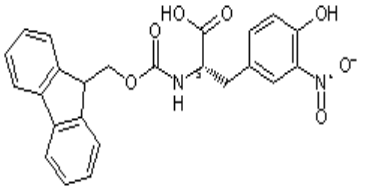
A)



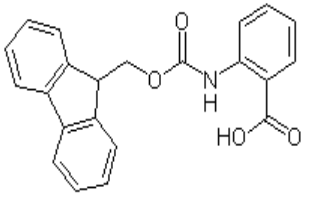
C)



HATU



Fmoc 3-nitrotyrosine (Fmoc-Tyx)



Fmoc 2-amino benzoic acid (Fmoc-Abz)

B)

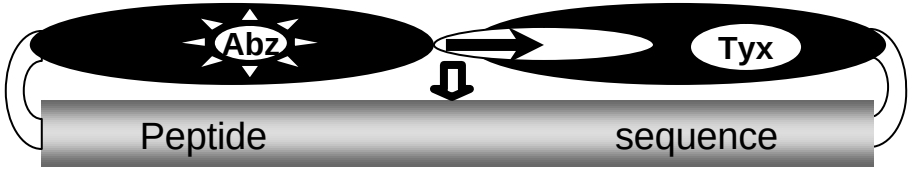
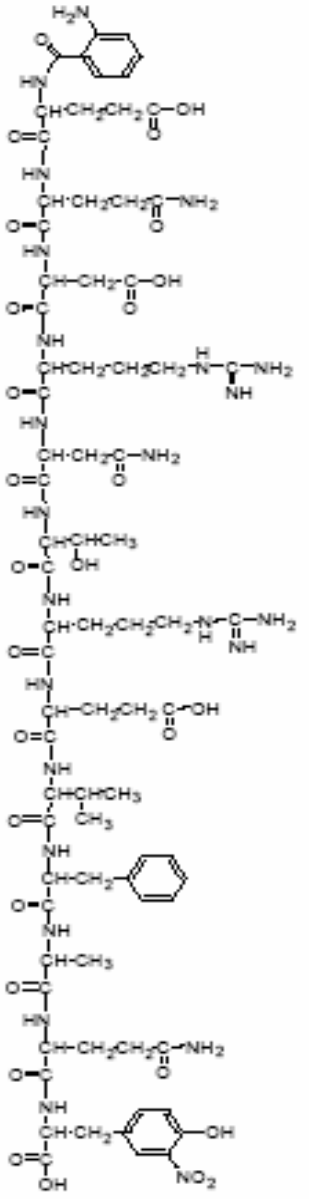


Figure S2. 1D proton NMR data of QSARS-4 peptide



AA	N-H	*N–H ROESY correlation*	α-H	*α-H ROESY correlation*	β1, β2-H	γ, δ and/or aromatic H's
Abz						(7.39, 7.18, 6.73, 6.68, aromatics)
E1	8.565	*7.38 (Abz Ar-H)*	4.24	*8.50 (E8-NH)*	1.90, 2.05	2.20
Q2	8.195	*4.14 (R7-αH) 2.99 F10-βH*	4.06	*7.92 (V9-NH)*	1.75	2.00, 2.05
D3	8.287	*4.16 (E8-αH)*	4.44		2.52, 2.58	
R4	8.141	*4.44 (D3-αH)*	4.107		1.46	1.65, 1.68
N5	8.405	*4.107 (R4-αH)*	4.57		2.65, 2.70	
T6	7.905	*4.57 (N5-αH)*	4.125	*8.10 (R7-NH)*	4.125	1.05
R7	8.105	*4.125 (T6-αH)*	4.14	*8.20 (Q2-NH)*	*1.46*	1.65, 1.68
E8	8.490	*4.24 (E1-αH)*	4.16	*8.28 (D3-NH)*	1.82, 1.92	2.22
V9	7.925	4.16 *(E8-αH)*	3.84	*8.095 (F10-NH)*	1.81	0.65, 0.70
F10	8.090	*3.84 (V9-αH)*	4.45		2.84, 2.99	7.08-7.20 aromatics
A11	8.019	*4.45 (F10-αH)*	4.045		1.115	
Q12	8.055	*4.05 (A11-αH)*	3.99	*8.095 (NY13-NH)*	1.73	1.99, 2.04
NY13	8.095	*3.99 (Q12-αH)*	4.445		2.78, 3.02	(7.73, 7.28, 6.83, aromatics)

Figure S3. ROESY spectrum of QSARS-4 peptide showing various correlations.

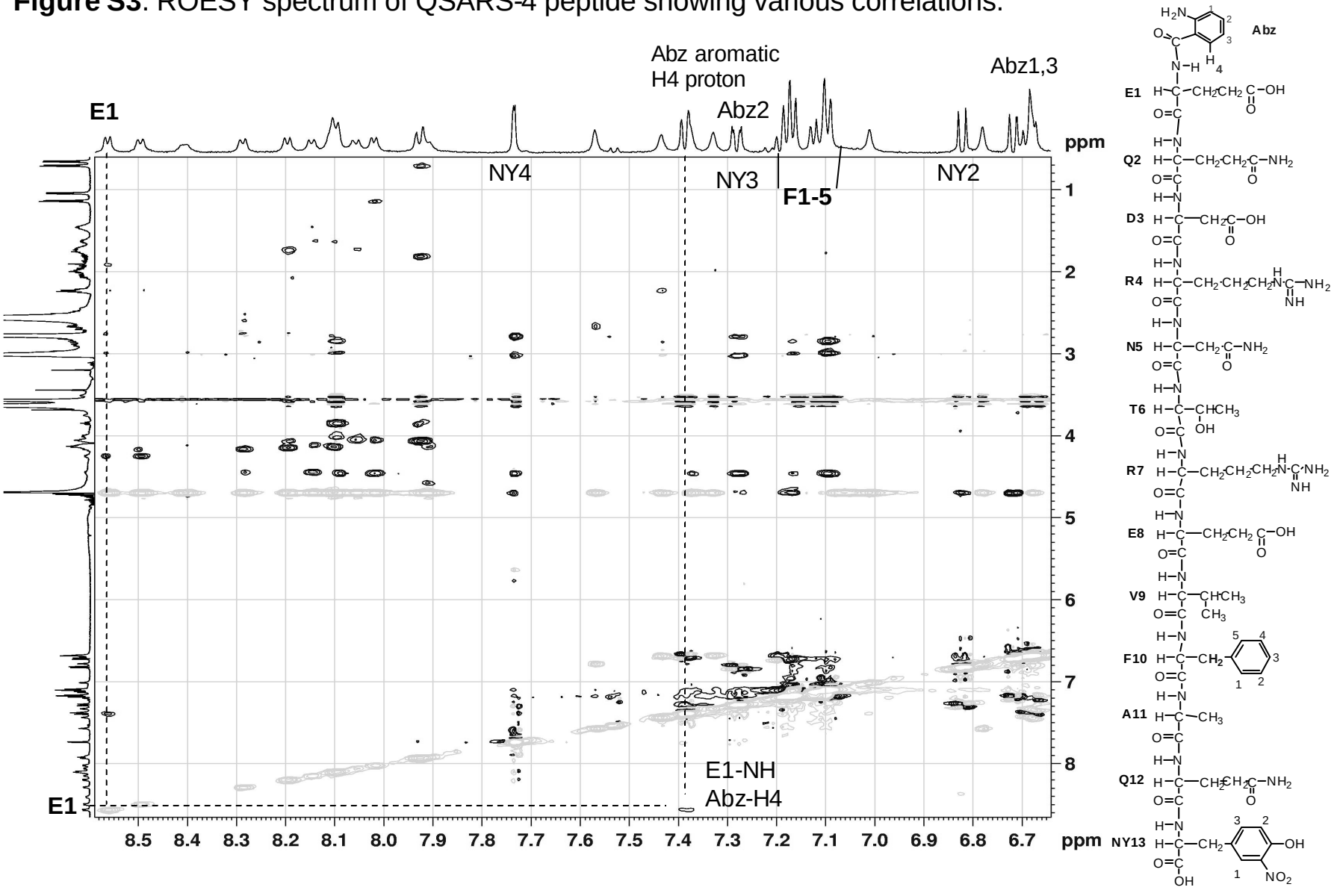


Figure S4. TOCSY spectrum for the fingerprint NH-aliphatic region of the QSARS-4 peptide.

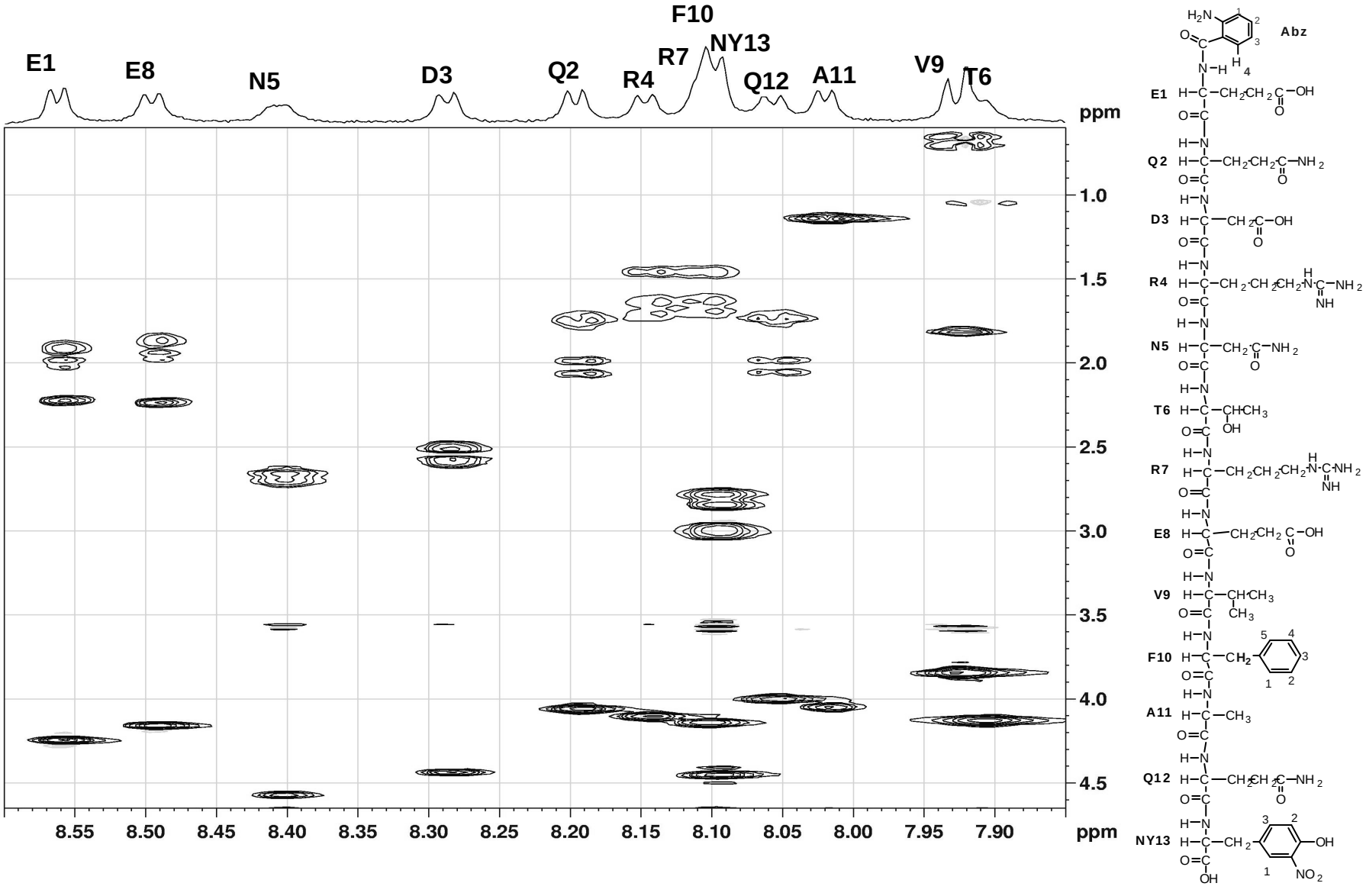


Figure S5. ROESY spectrum of QSARS-4.