

Supplementary Information

Figure S1. ^1H -700 MHz spectrum of the AD-specific peptide vaccine Ag85B₂₄₁₋₂₅₅-GPSL-Tau₂₂₉₋₂₃₇[pThr231/pSer235].

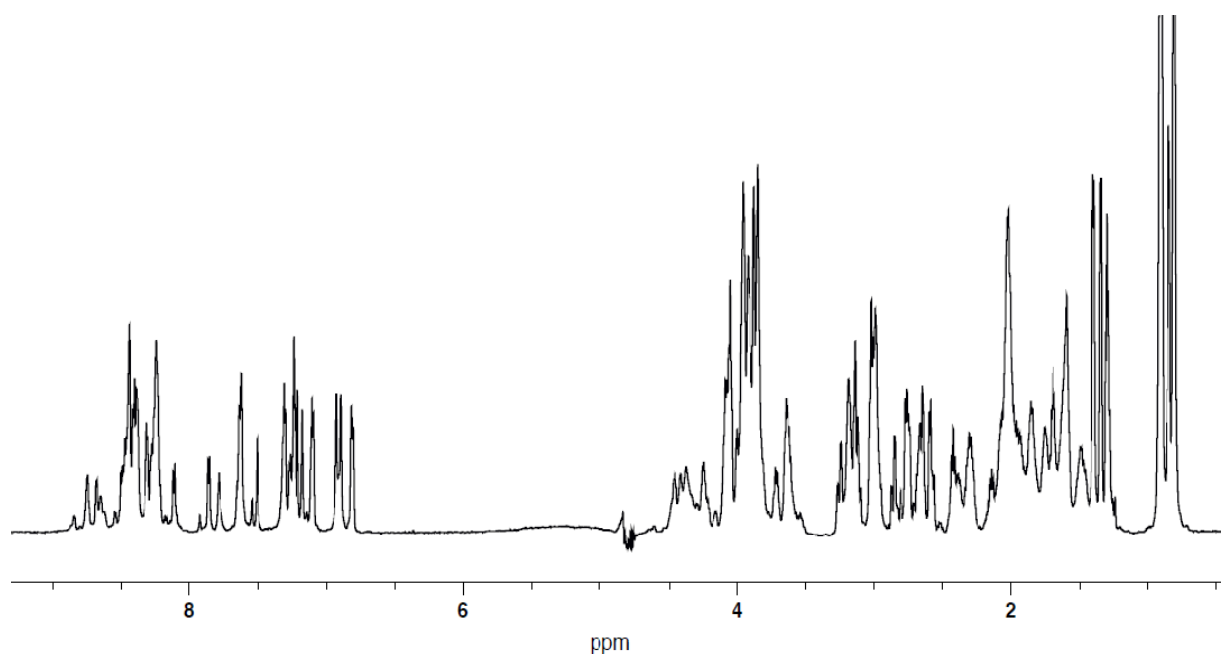


Figure S2. TObal Correlation SpectroscOpY (TOCSY) spectrum of the AD-specific peptide vaccine Ag85B₂₄₁₋₂₅₅-GPSL-Tau₂₂₉₋₂₃₇[pThr231/pSer235].

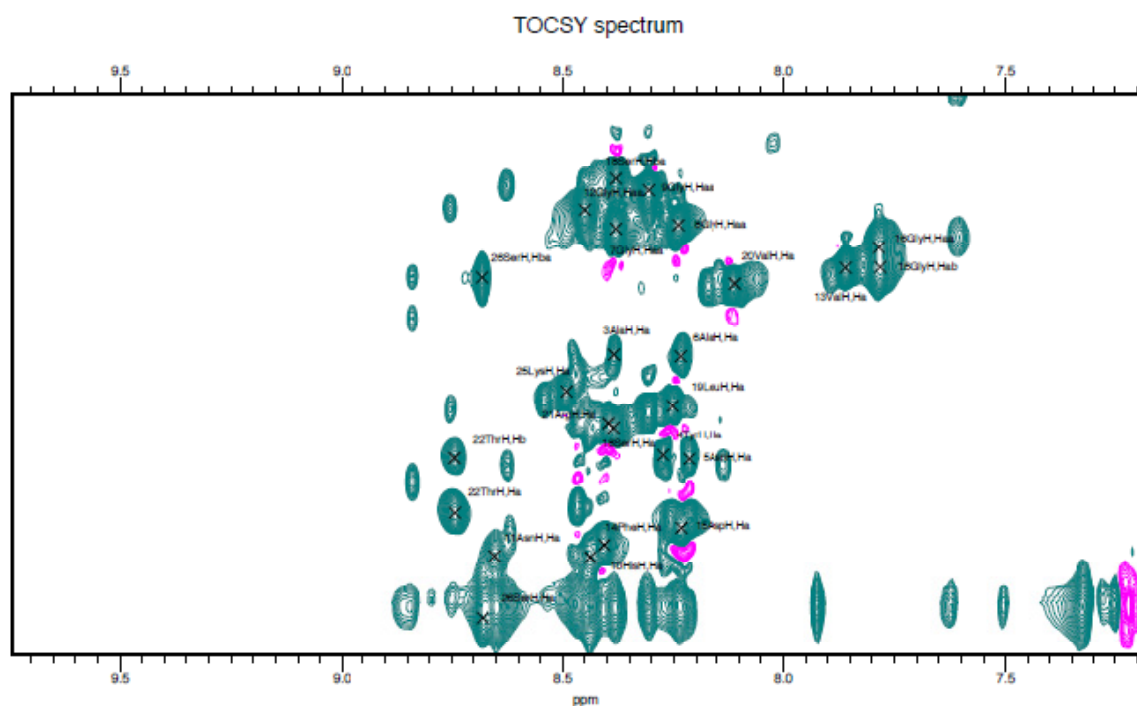


Table S1. Chemical shift assignment of the AD-specific peptide vaccine Ag85B₂₄₁₋₂₅₅-GPSL-Tau₂₂₉₋₂₃₇[pThr231/pSer235].

Amino acid	Atom name	Atom type	Value
3Ala	CO	13C	178.613
3Ala	Cβ	13C	19.793
3Ala	H	1H	8.384
3Ala	Hα	1H	4.244
3Ala	Hβ*	1H	1.285
3Ala	N	15N	124.155
4Tyr	CO	13C	176.250
4Tyr	Cα	13C	58.820
4Tyr	Cβ	13C	39.167
4Tyr	Cδ	13C	133.706
4Tyr	Cε	13C	118.808
4Tyr	Cγ	13C	131.280
4Tyr	H	1H	8.274
4Tyr	Hα	1H	4.475
4Tyr	Hβa	1H	2.989
4Tyr	Hδ*	1H	7.101
4Tyr	Hε*	1H	6.810
4Tyr	N	15N	119.694
5Asn	CO	13C	176.004
5Asn	H	1H	8.216
5Asn	Hα	1H	4.480
5Asn	Hβa	1H	2.650
5Asn	Hβb	1H	2.758
5Asn	Hδ2a	1H	6.891
5Asn	Hδ2b	1H	7.644
5Asn	N	15N	119.398
5Asn	Nδ2	15N	112.956
6Ala	CO	13C	178.522
6Ala	Cα	13C	53.427
6Ala	Cβ	13C	19.668
6Ala	H	1H	8.234
6Ala	Hα	1H	4.246
6Ala	Hβ*	1H	1.396
6Ala	N	15N	124.996
7Gly	Cα	13C	46.057
7Gly	H	1H	8.380
7Gly	Hαa	1H	3.963
7Gly	N	15N	107.905
8Gly	Cα	13C	45.873
8Gly	H	1H	8.239
8Gly	Hαa	1H	3.953
8Gly	N	15N	108.691
9Gly	Cα	13C	45.816
9Gly	H	1H	8.307
9Gly	Hαa	1H	3.876

Table S1. Cont.

Amino acid	Atom name	Atom type	Value
9Gly	N	15N	108.495
10His	C α	13C	56.004
10His	C β	13C	29.800
10His	C δ 2	13C	120.563
10His	C ϵ 1	13C	137.120
10His	C γ	13C	132.426
10His	H	1H	8.438
10His	H α	1H	4.702
10His	H β a	1H	3.117
10His	H β b	1H	3.248
10His	H δ 2	1H	7.211
10His	H ϵ 1	1H	8.426
10His	N	15N	118.373
11Asn	C α	13C	53.992
11Asn	C β	13C	39.498
11Asn	H	1H	8.651
11Asn	H α	1H	4.703
11Asn	H β a	1H	2.754
11Asn	H β b	1H	2.861
11Asn	H δ 2a	1H	6.922
11Asn	H δ 2b	1H	7.619
11Asn	N	15N	120.193
11Asn	N δ 2	15N	113.019
12Gly	C α	13C	45.988
12Gly	H	1H	8.450
12Gly	H α a	1H	3.918
12Gly	N	15N	109.375
13Val	C α	13C	62.965
13Val	C β	13C	33.271
13Val	C γ a	13C	21.356
13Val	H	1H	7.858
13Val	H α	1H	4.049
13Val	H β	1H	1.963
13Val	H γ a*	1H	0.807
13Val	N	15N	119.458
14Phe	C α	13C	58.112
14Phe	C β	13C	40.304
14Phe	C δ *	13C	132.464
14Phe	C ϵ *	13C	131.936
14Phe	C γ	13C	139.659
14Phe	C ξ	13C	130.393
14Phe	H	1H	8.406
14Phe	H α	1H	4.679
14Phe	H β a	1H	2.966
14Phe	H β b	1H	3.155
14Phe	H δ *	1H	7.236

Table S1. Cont.

Amino acid	Atom name	Atom type	Value
14Phe	H ϵ^*	1H	7.304
14Phe	H ξ	1H	7.265
14Phe	N	15N	123.887
15Asp	CO	13C	176.355
15Asp	C α	13C	54.609
15Asp	H	1H	8.233
15Asp	H α	1H	4.644
15Asp	H β a	1H	2.650
15Asp	H β b	1H	2.745
15Asp	N	15N	122.855
16Gly	H	1H	7.784
16Gly	H α a	1H	4.025
16Gly	CO	13C	176.434
16Gly	C α	13C	45.536
16Gly	N	15N	108.966
17Pro	H α	1H	4.454
17Pro	H β a	1H	1.927
17Pro	H β b	1H	2.295
17Pro	H δ a	1H	3.629
17Pro	H δ b	1H	3.642
17Pro	H γ a	1H	2.024
17Pro	H γ b	1H	2.298
17Pro	C α	13C	64.187
17Pro	C β	13C	32.836
17Pro	C δ	13C	50.547
17Pro	C γ	13C	28.038
18Ser	H	1H	8.381
18Ser	H α	1H	4.412
18Ser	H β	1H	3.849
18Ser	CO	13C	177.637
18Ser	C α	13C	59.021
18Ser	C β	13C	64.260
18Ser	N	15N	115.746
19Leu	H	1H	8.252
19Leu	H α	1H	4.360
19Leu	H β	1H	1.592
19Leu	H δ a*	1H	0.848
19Leu	H δ b*	1H	0.900
19Leu	H γ	1H	1.605
19Leu	CO	13C	177.656
19Leu	C α	13C	56.261
19Leu	C β	13C	42.934
19Leu	C δ a	13C	24.186
19Leu	C δ b	13C	25.475
19Leu	C γ	13C	27.646
19Leu	N	15N	124.652
20Val	CO	13C	176.294

Table S1. Cont.

Amino acid	Atom name	Atom type	Value
20Val	C α	13C	62.763
20Val	C β	13C	33.209
20Val	C γ a	13C	21.650
20Val	H	1H	8.112
20Val	H α	1H	4.088
20Val	H β	1H	2.030
20Val	H γ a*	1H	0.912
20Val	N	15N	121.738
21Arg	CO	13C	175.057
21Arg	C α	13C	56.388
21Arg	C β	13C	31.716
21Arg	C γ	13C	27.512
21Arg	H	1H	8.396
21Arg	H α	1H	4.401
21Arg	H β a	1H	1.751
21Arg	H β b	1H	1.854
21Arg	H δ a	1H	3.187
21Arg	H ϵ	1H	7.325
21Arg	H γ a	1H	1.622
21Arg	H ξ *	1H	1.293
21Arg	N	15N	125.856
21Arg	Ne	15N	84.990
22Thr	C α	13C	60.572
22Thr	C β	13C	73.766
22Thr	C γ 2	13C	21.244
22Thr	H	1H	8.743
22Thr	H α	1H	4.605
22Thr	H β	1H	4.476
22Thr	H γ 2*	1H	1.340
22Thr	N	15N	119.675
23Pro	C α	13C	62.347
23Pro	C β	13C	31.583
23Pro	C δ	13C	31.796
23Pro	C γ	13C	28.197
23Pro	H α	1H	4.658
23Pro	H β a	1H	1.861
23Pro	H β b	1H	2.378
23Pro	H δ a	1H	3.715
23Pro	H δ b	1H	3.945
23Pro	H γ a	1H	1.997
23Pro	H γ b	1H	2.083
24Pro	C α	13C	63.616
24Pro	C β	13C	33.050
24Pro	C δ	13C	51.030
24Pro	C γ	13C	28.087
24Pro	H α	1H	4.449
24Pro	H β a	1H	1.907

Table S1. Cont.

Amino acid	Atom name	Atom type	Value
24Pro	H β b	1H	2.298
24Pro	H δ a	1H	3.637
24Pro	H δ b	1H	3.810
24Pro	H γ a	1H	2.023
25Lys	CO	13C	177.060
25Lys	C α	13C	56.646
25Lys	C β	13C	33.851
25Lys	C δ	13C	29.606
25Lys	C ϵ	13C	42.772
25Lys	C γ	13C	25.117
25Lys	H	1H	8.491
25Lys	H α	1H	4.326
25Lys	H β a	1H	1.758
25Lys	H β b	1H	1.831
25Lys	H δ a	1H	1.699
25Lys	H ϵ a	1H	3.020
25Lys	H γ a	1H	1.487
25Lys	N	15N	122.431
26Ser	CO	13C	173.601
26Ser	C β	13C	66.117
26Ser	H	1H	8.679
26Ser	H α	1H	4.834
26Ser	H β a	1H	4.070
26Ser	N	15N	118.769

Table S2. $^3J_{\text{HN-H}\alpha}$ analysis from experimental data (Exp) and Flexible Meccano (FM) ensemble.

Amino acid	$^3J_{\text{HN-H}\alpha}$ Exp (Hz) ^a	$^3J_{\text{HN-H}\alpha}$ FM (Hz)	$\Delta J = J_{\text{Exp}} - J_{\text{FM}}$
1Gln		7.1	
2Asp			
3Ala		6.3	
4Tyr	7.0	7.6	-0.6
5Asn		7.5	
6Ala	6.0	6.3	-0.4
7Gly	5.9	6.2	-0.3
8Gly	6.1	6.2	-0.1
9Gly	6.0	6.2	-0.2
10His		7.4	
11Asn		7.5	
12Gly	7.1	6.2	0.9
13Val	7.8	7.8	0.0
14Phe	7.5	7.5	-0.1
15Asp	7.7	7.2	0.5
16Gly	5.7	5.7	0.1
17Pro			
18Ser	7.0	6.9	0.1

Table S2. *Cont.*

Amino acid	$^3J_{\text{HN-H}\alpha}$ Exp (Hz) ^a	$^3J_{\text{HN-H}\alpha}$ FM (Hz)	$\Delta J = J_{\text{Exp}} - J_{\text{FM}}$
19Leu		7.3	
20Val	8.0	7.8	0.1
21Arg	7.1	7.2	-0.1
22Thr		7.8	
23Pro			
24Pro			
25Lys	7.0	7.2	-0.1
26Ser		7.8	
27Pro			
28Ser			

a. The digital resolution of DQF-COSY spectrum was 1.8 Hz/point.