Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Conformational properties of 1,4- and 1,5-substituted 1,2,3-triazole amino acids – building units for peptidic foldamers

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Table S1. Conformers of 4Tzl as obtained at the RHF/3-21G level of theory.

Conf.	φ	θ	ζ	ρ	ψ	μ	*ΔE(kcal/mol)*
1	-73.9	69.7	-179.7	-178.8	101.5	35.5	0.0
2	-74.0	68.1	179.4	178.9	-102.7	-36.3	0.0
3	-57.7	103.6	-167.7	168.3	-62.2	1.8	2.4
4	179.2	-178.0	179.7	178.2	-97.2	-37.9	3.0
5	-76.4	63.4	-179.6	-179.1	-53.2	-166.9	3.5
6	-74.2	75.9	-179.7	178.0	49.5	164.4	3.6
7	175.8	-175.6	-179.1	-175.9	-41.5	-160.3	4.6
8	-122.8	135.6	179.2	175.8	43.2	161.2	4.8
9	-58.2	-28.5	170.2	-163.9	65.1	5.3	4.8
10	-120.8	32.4	179.9	-177.2	-45.5	-162.6	4.9
11	-124.7	34.5	178.4	175.5	38.2	157.7	5.6
12	74.5	-65.9	179.5	178.3	33.4	-79.5	6.7

Table S2. Conformers of 5Tzl as obtained at the RHF/3-21G level of theory.

Conf.	*Sec. struct.*	φ	θ	ζ	ρ	ψ	ΔE(kcal/mol)
1	H14	-111.9	55.3	-4.8	-94.5	-48.3	0.00
2	C8	93.8	62.4	-3.5	-84.6	-61.4	1.31
3	Turn	-101.3	68.7	-3.3	-93.1	-146.3	2.87
4	2-Helix	-88.9	93.1	3.5	71.1	151.1	3.27
5	H8	164.3	-48.6	4.3	95.1	122.6	3.28
6	H8b	102.4	30.0	-5.8	68.7	65.1	3.78
7	Spiral	-91.0	93.2	4.8	92.1	43.2	3.88
8	H10	-100.6	84.3	2.3	69.6	-111.3	3.98
9		85.8	98.6	3.5	-69.6	-151.9	4.03
10	H10/Turn2	-70.7	147.3	4.3	-75.4	9.5	4.50
11		-133.9	39.4	-11.4	58.2	33.3	4.70
12	Turn	-69.6	107.0	3.8	-137.2	62.9	6.04
13		77.7	100.6	1.99	72.1	60.7	6.26
14	S	111.1	169.9	-2.8	-90.9	-44.6	6.38
15		-77.6	148.6	-3.0	-64.5	-56.0	6.75
16		111.4	168.6	2.5	92.3	37.0	6.77
17	H20	-154.6	62.7	2.5	98.5	33.9	6.93
18		-116.0	-83.3	-4.5	81.7	20.0	7.33
19	Ext	-105.9	-176.7	-0.7	71.0	155.7	7.35
20		124.1	156.1	0.5	63.6	158.8	9.02
21		180.0	180.0	0.0	180.0	0.0	13.45
22		180.0	0.0	0.0	180.0	0.0	19.16
23		180.0	180.0	0.0	0.0	180.0	19.81
24		0.0	180.0	0.0	180.0	0.0	21.49
25		180.0	180.0	0.0	180.0	180.0	24.61
26		180.0	180.0	0.0	0.0	0.0	30.76
27		0.0	0.0	0.0	180.0	0.0	36.88

Figure S1. 2D NOESY of BOC-4Tzl (**1**)

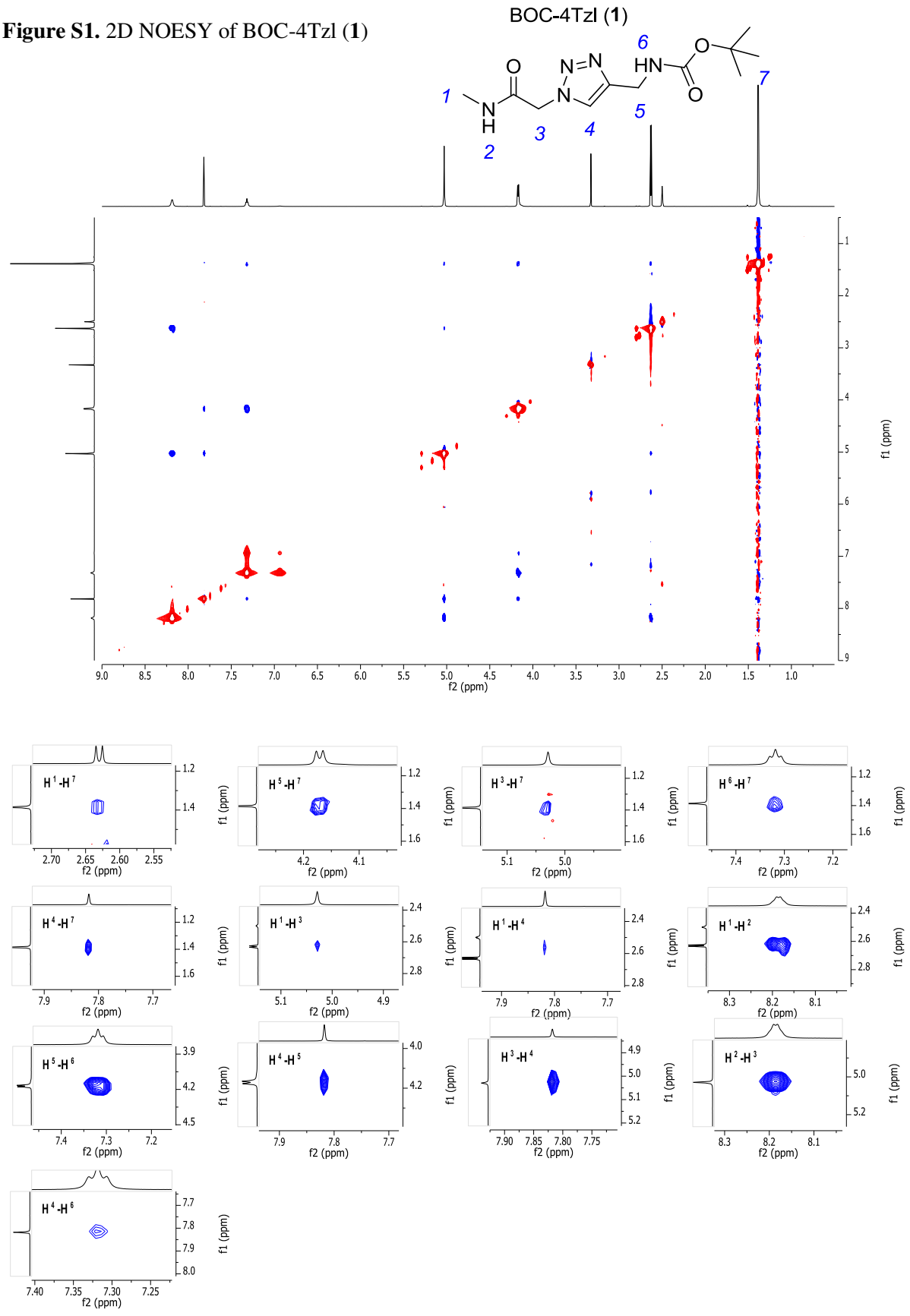


Figure S2. 2D NOESY of BOC-5Tzl (**2**)

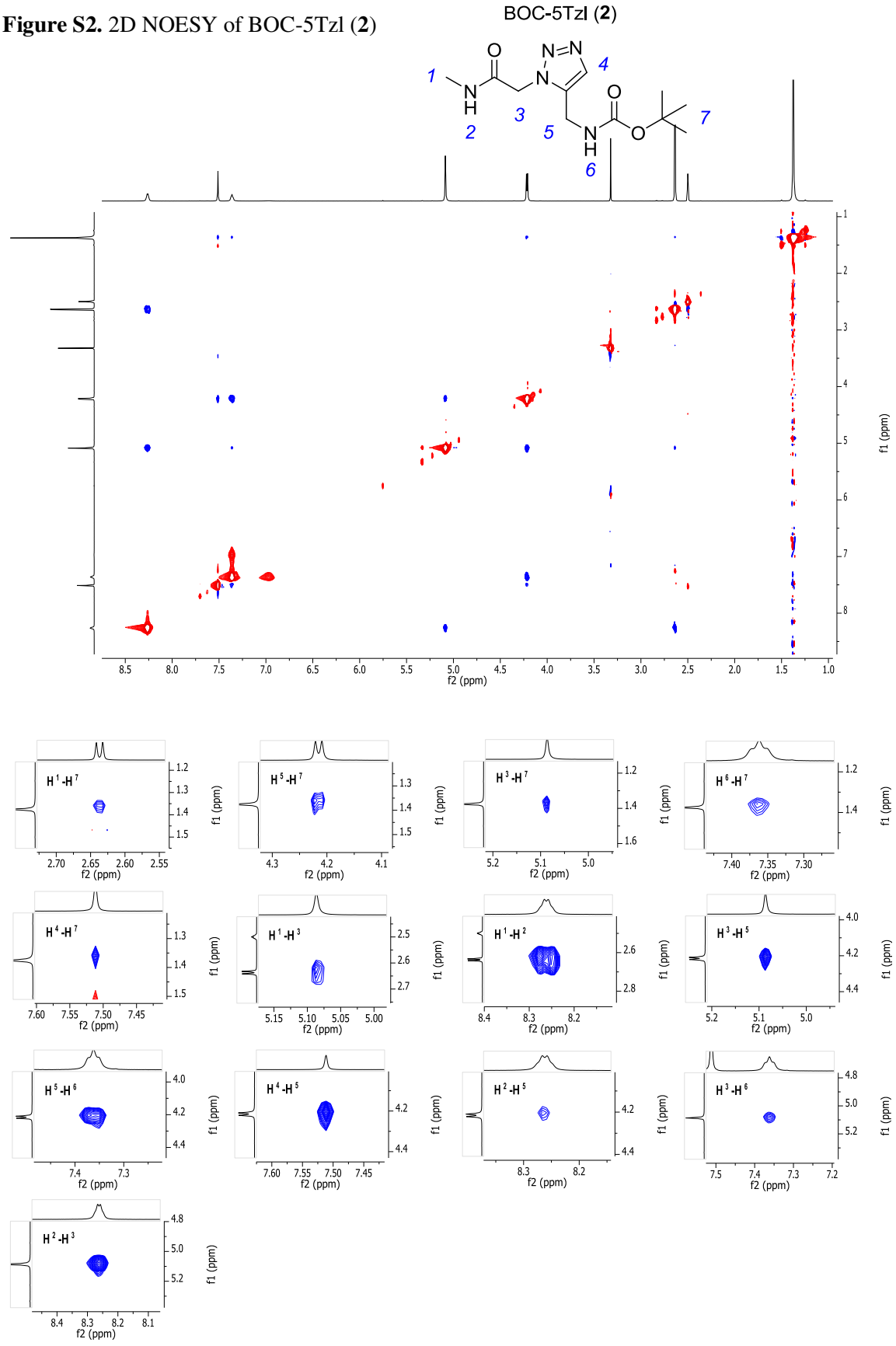


Table S3. Analysis of the BOC-5Tzl conformers in view of the 2D NMR NOESY crosspeaks. Presence or absence of each obtained crosspeak is marked for each conformer obtained for BOC-5Tzl by calculations. For more details see Table 5 and main text.

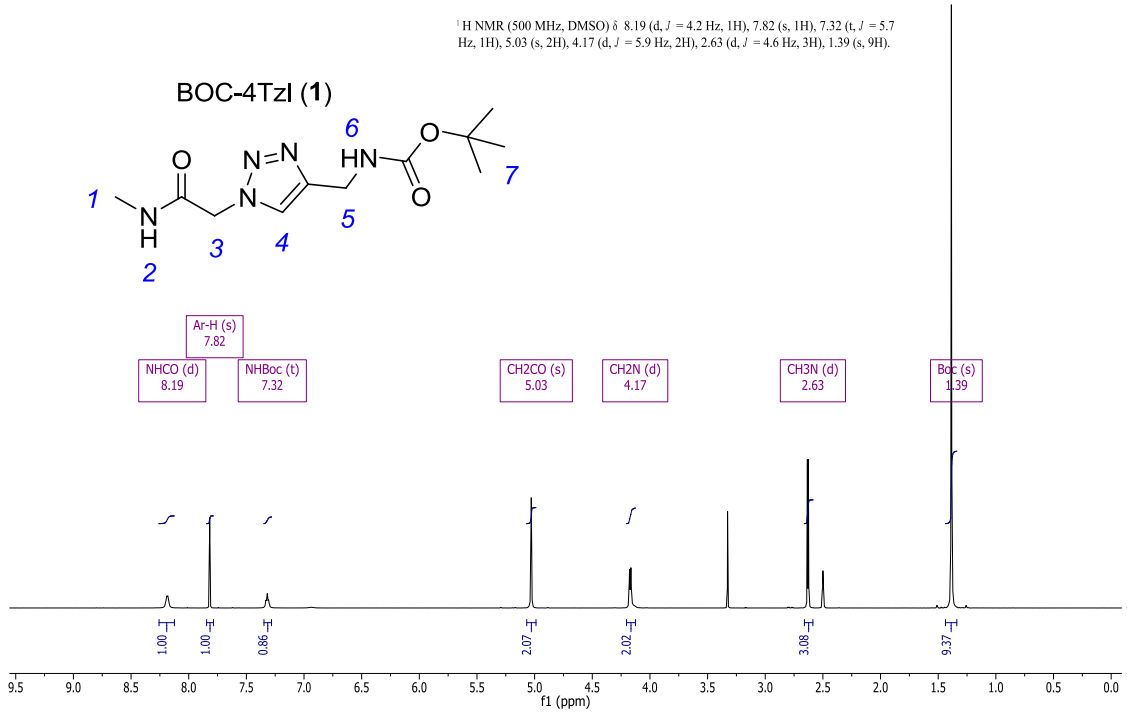
Conf.	NOE H-H Crosspeaks[b]							Comments	Rel. En.[c]
	H^1-H^{7a}	H^2-H^5	H^3-H^6	H^3-H^7	H^4-H^6	H^4-H^7	H^5-H^7		
BOC-5Tzl-1	X	X	X	X	X	-	-	2-6: 2.9Å (missing from NOEs)	LOW
BOC-5Tzl-2	X	-	X	X	-	-	-		LOW
BOC-5Tzl-3	X	X	X	X	X	-	X	2-7: 2.7Å (missing from NOEs)	LOW
BOC-5Tzl-4	-	-	X	X	X	-	-		MODERATE
BOC-5Tzl-6	-	X	X	X	-	-	-	1-5: 3.2Å (missing from NOEs), H-bond fixes the distance	HIGH
BOC-5Tzl-7	-	X	X	X	X	-	-		MODERATE
BOC-5Tzl-8	-	X	X	X	X	-	-	2-7: 3.4Å (missing from NOEs), H-bond fixes the distance	LOW
BOC-5Tzl-10	X	X	-	-	X	X	-		LOW
BOC-5Tzl-14	-	X	-	-	X	X	-		HIGH

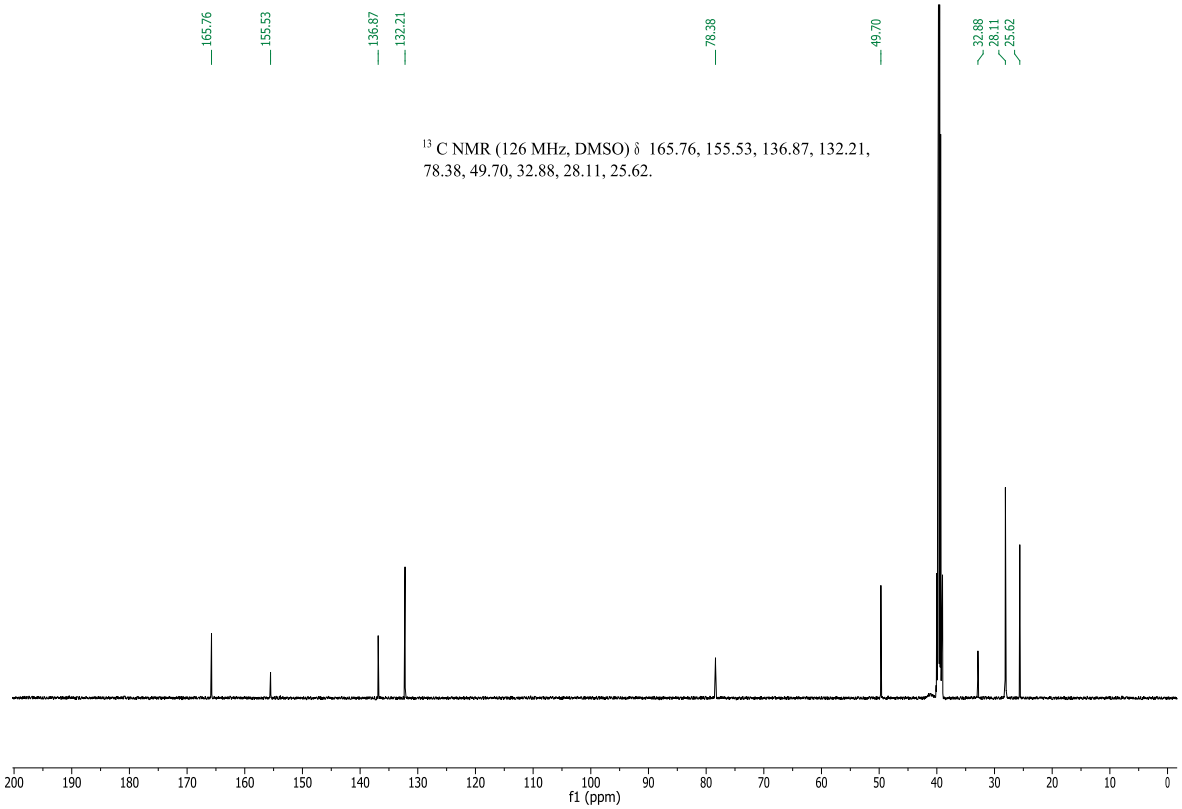
[a] For numbering of protons in BOC-5Tzl see Figure S2.

[b] Only those crosspeaks were considered which, based on the structural analysis of conformers, should not appear for every conformer obtained by calculations.

[c] Relative energy range based on values obtained for BOC-5Tzl (Table 5 in main text).

^{1}H and ^{13}C spectra of BOC-4Tzl (1)





^{1}H and ^{13}C spectra of BOC-5Tzl (2)