Supporting Information

The 1,2,3-Triazole Ring as a Disulfide Bond Mimetic in Chimeric AGRP-Melanocortin Peptide: Design, Synthesis, and Functional Characterization

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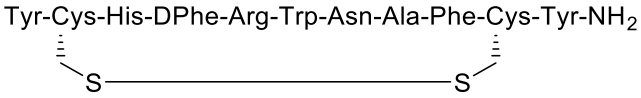
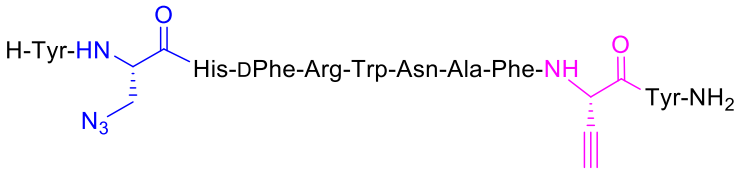
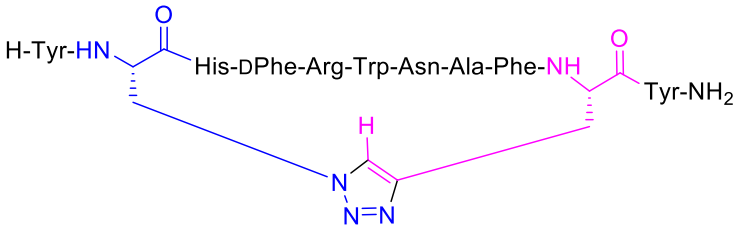
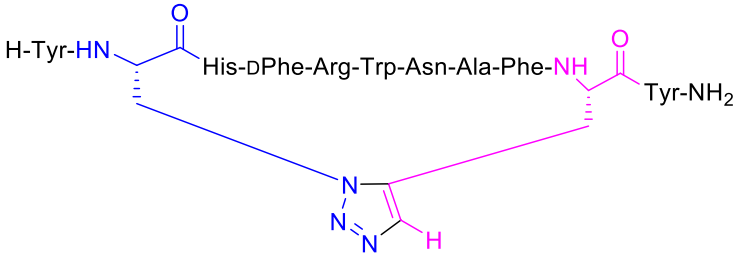
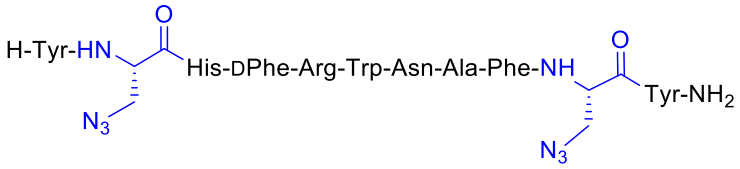
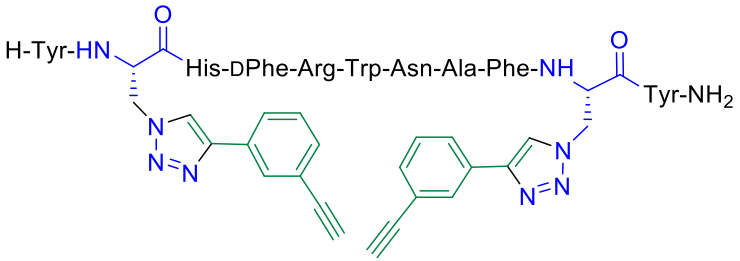
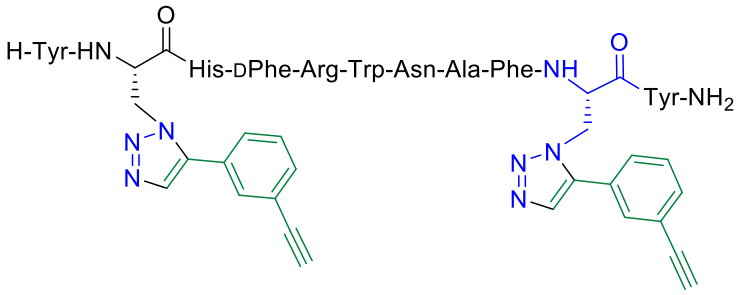
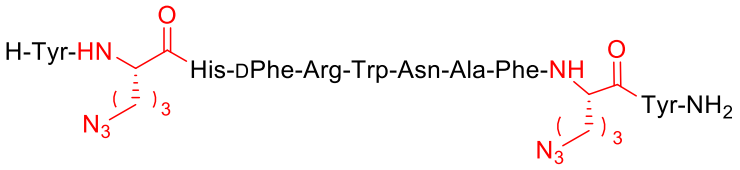
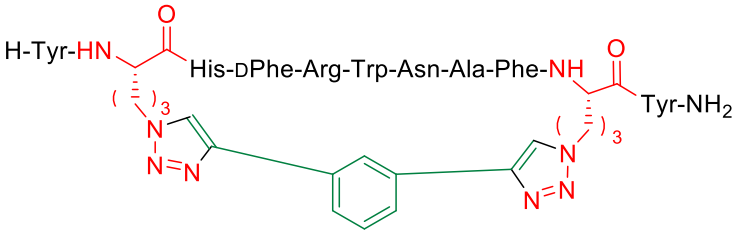
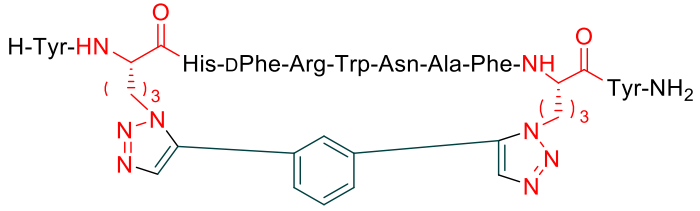
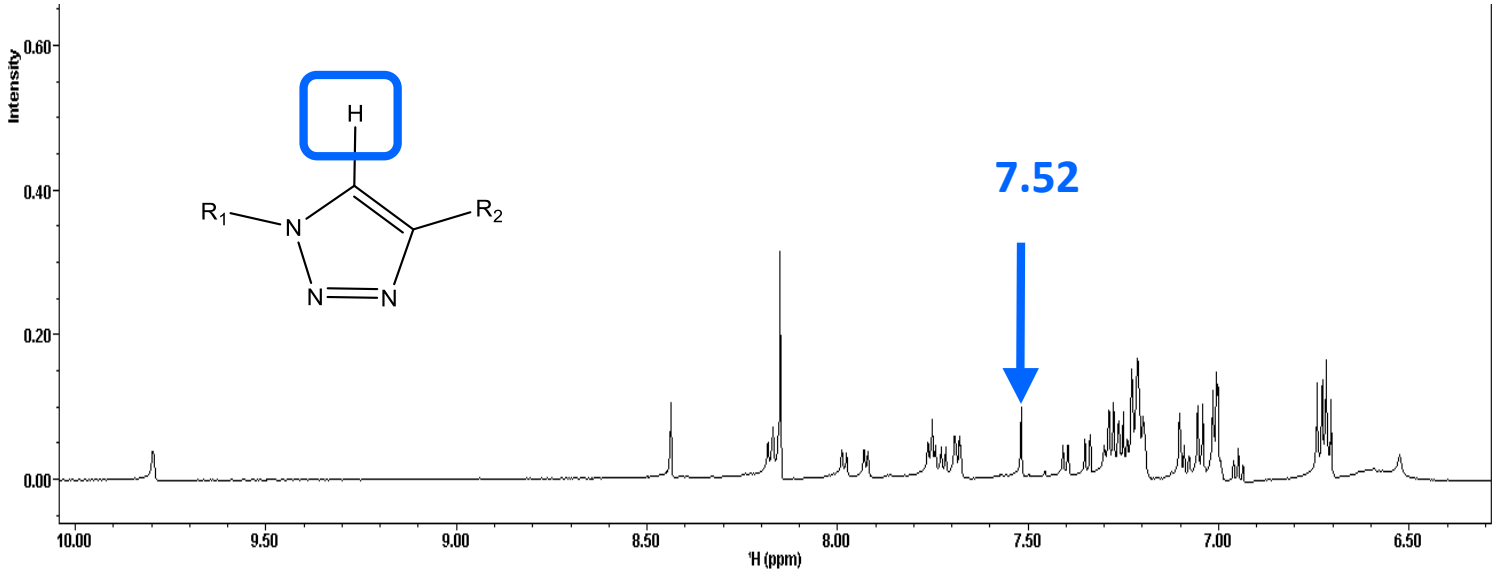
Table S1: Analytical Data for the Peptides Synthesized in This Study [a]

Peptide	Sequence	HPLC k' (System 1)	HPLC k' (System 2)	*m/z* Calcd.	*m/z* Found	Selected IR values (cm^{-1})
1		4.5	8.0	1505.6	1506.6	ND
2		4.4	9.0	1508.6	1509.0	1665.8, 2110.8, 3284.0
3		5.4	9.6	1508.6	1509.6	1676.6, 3385.9
6		5.4	8.8	1508.6	1509.6	1678.0, 3373.7

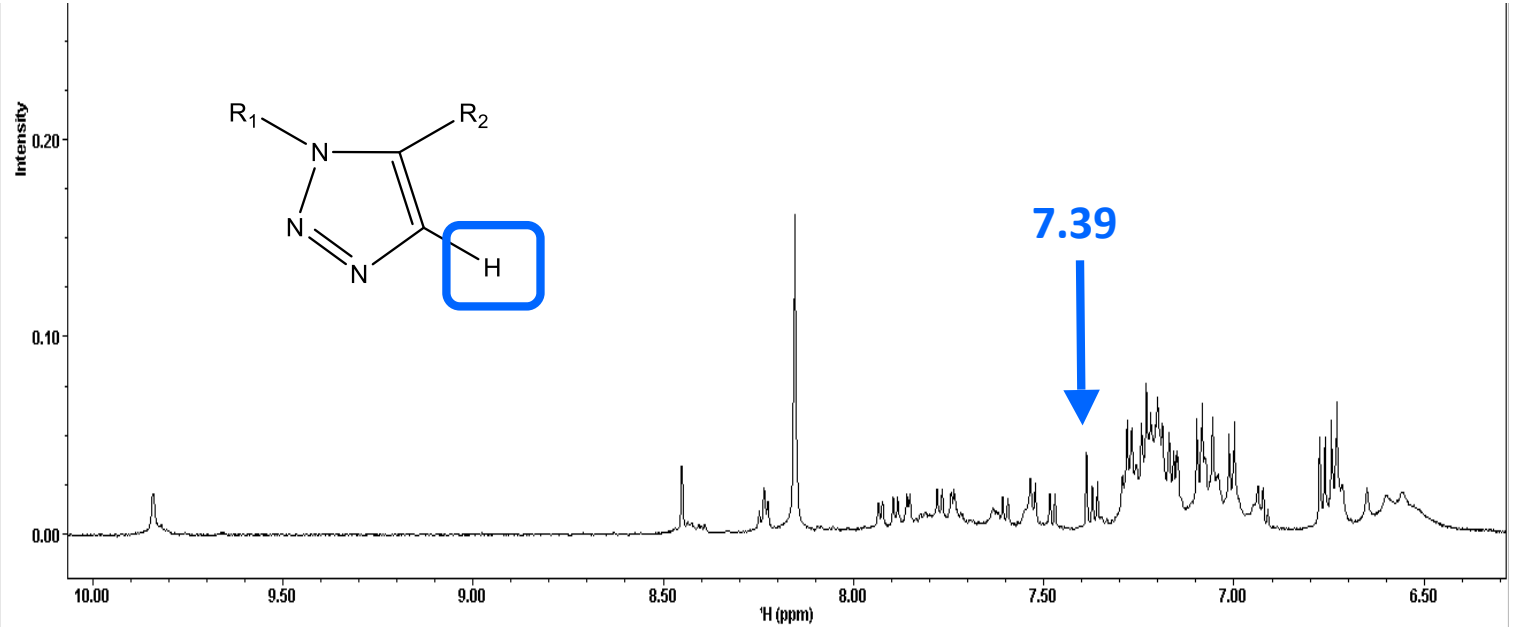
7		5.4	10.1	1525.6	1525.6	1673.2, 2111.2, 3284.8
8		7.6	13.1	1777.8	1778.8	2341.9, 2359.8, 3583.3
12		7.4	11.5	1777.8	1777.8	1676.5, 3301.0
13		6.2	10.1	1581.7	1581.7	1672.3, 2103.6, 3682.6

14		7.4	12.0	1707.8	1708.6	1699.7, 3648.6
16		6.9	11.0	1707.8	1708.7	1679.9, 3405.7

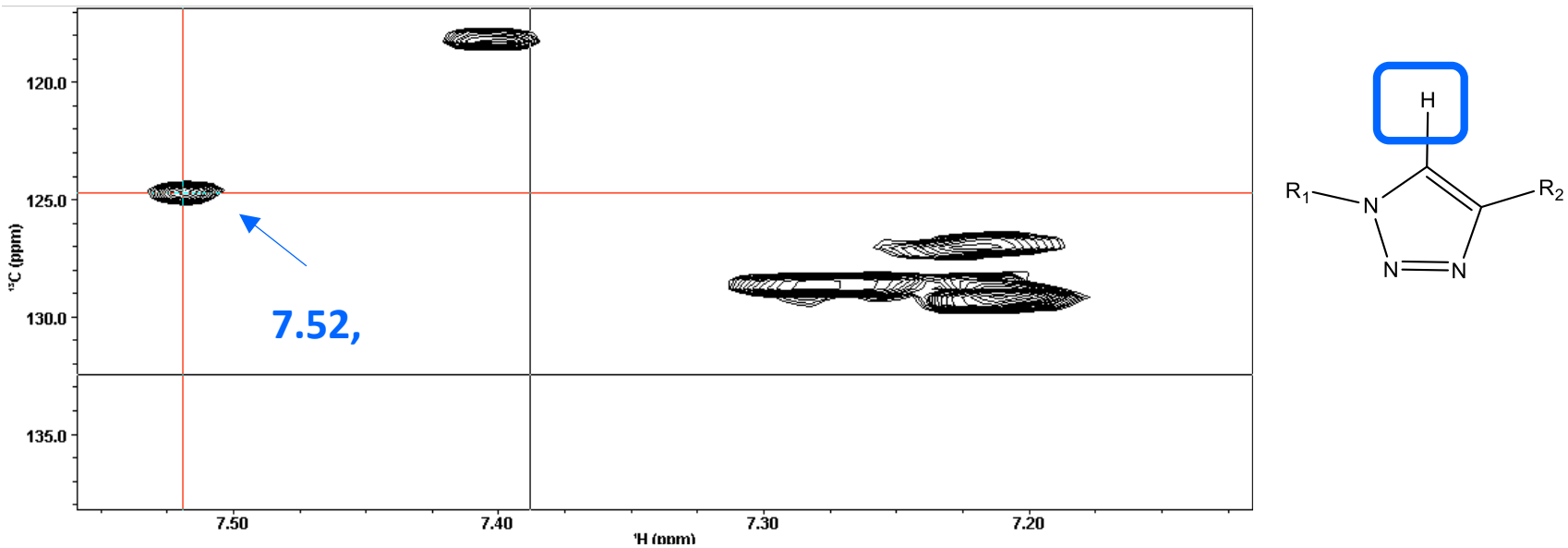
[a]The HPLC k' value equals [(peptide retention time – solvent retention time)/ solvent retention time]. Two different solvent systems were used. Solvent system 1 is 10% acetonitrile (ACN) in 0.1% trifluoroacetic acid/H_2O with a gradient to 90% acetonitrile over 35 min. Solvent system 2 is 10% methanol (MeOH) in 0.1% trifluoroacetic acid/ H_2O with a gradient to 90% methanol over 35 min. An analytical Vydac C18 column (Vydac 218TP104) with a flow rate of 1.5 mL/min was used for analytical characterization. The compound purity was determined by RP-HPLC in both solvent systems at a wavelength of 214 nm. All compounds were found to be ≥95% pure. ND: not determined. Mass was determined by ESI-MS on a ABI 3200Q Trap.



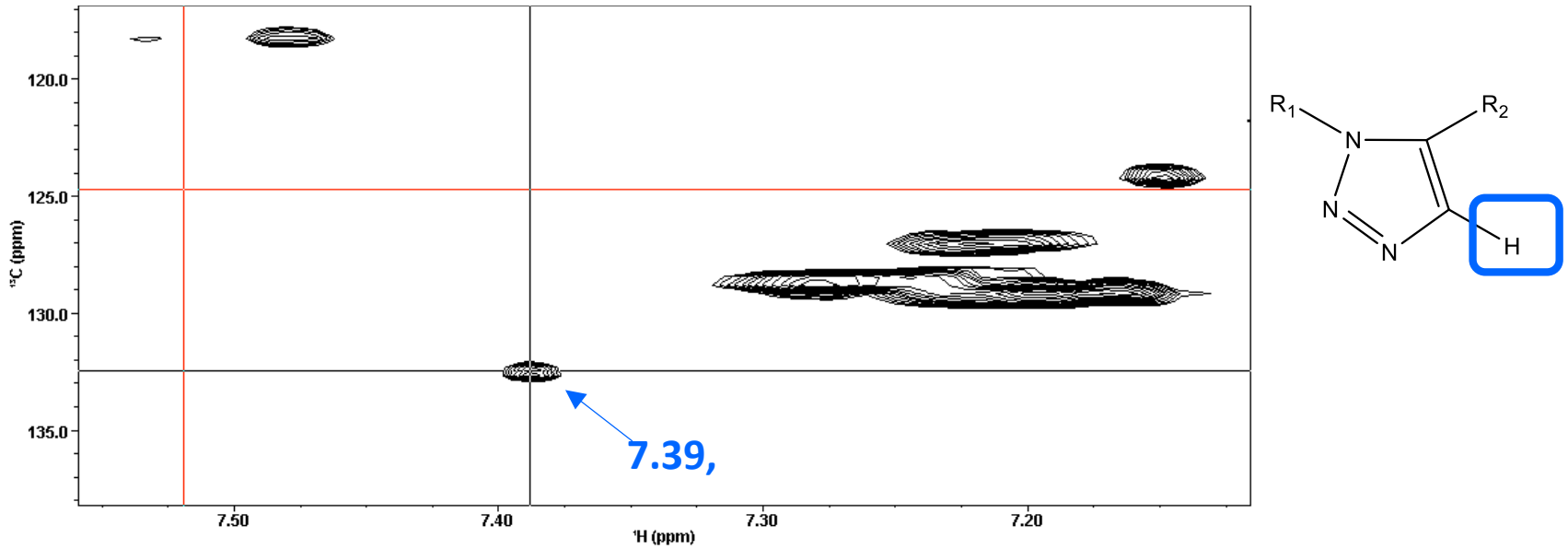
Supplemental Figure 1: ^{1}H-NMR spectrum of compound **3.**



Supplemental Figure 2: ^{1}H-NMR spectrum of compound **6.**



Supplemental Figure 3: HSQC (^{1}H-^{13}C) spectrum of compound **3** containing the 1,4-Disubstituted triazole**.**



Supplemental Figure 4: HSQC (^{1}H-^{13}C) spectrum of compound **6** containing the 1,5-disubstituted triazole.