Synthetic Peptides as Structural Maquettes of Angiotensin-I Converting Enzyme Catalytic Sites

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SUPPORTING INFORMATION

Table S1: φ and ψ dihedral angles of the Zn^{2+}-$ACE_C(37)$ peptide at 298K (H_2O/TFE-*d2* 34%/66% v/v. pH=4.9).

Table S2: φ and ψ dihedral angles of the the Zn^{2+}-$ACE_N(37)$ peptide at 298K (H_2O/TFE-*d2* 34%/66% v/v. pH=4.9).

Figure S1: Fingerprint regions of 600- MHz NOESY of $ACE_N(37)$ peptide recorded at T= 298 K. Characteristic long-range NOE connectivities between Tyr 368 with His 388, as well as with Phe 387 present only in the ACEN_37 peptide.

Figure S2: **Left:** Superimposition of Zn^{2+}-$ACE_C(37)$ DYANA 20 best models calculated with NMR data in blue and the crystal structure of ACE_C in complex with lisinopril in yellow (pdb code:***1O86***). The calculated RMSD value is 0.775 for the backbone atoms. **Right:** Ribbon representation of the crystal structure of ACE_C in complex with lisinopril and the mean NMR calculated structure of Zn^{2+}-$ACE_C(37)$. The calculated RMSD value is 3.595 for the backbone atoms.

Figure S3: Left: Superimposition of Zn^{2+}-$ACE_N(37)$ DYANA 20 best models calculated with NMR data in blue and the crystal structure of ACE_C in complex with lisinopril in yellow (pdb code:***2C6N***). The calculated RMSD value is 1.42 for the backbone atoms. **Right:** Ribbon representation of the crystal structure of ACE_N in complex with lisinopril and the mean NMR calculated structure of Zn^{2+}-$ACE_N(37)$. The calculated RMSD value is 3.802 for the backbone atoms.

Table S1: φ and ψ dihedral angles (in degrees) of the Zn^{2+}-$ACE_C(37)$ peptide at 298K (H_2O/TFE-*d2* 34%/66% v/v. pH=4.9).

Residue		φ	ψ
1	**His**	**---**	**-60.2**+/-77.2
2	**His**	**-28.7**+/-71.6	**133.7**+/-81.4
3	**Glu**	**-117.3**+/-94.6	**-20.5**+/-10.0
4	**Met**	**-123.9**+/-20.0	**28.5**+/-13.6
5	**Gly**	**-130.3**+/-25.8	**-79.5**+/-16.0
6	**His**	**-50.9**+/-6.6	**-34.2**+/-4.7
7	**Ile**	**-65.0**+/-1.3	**-37.4**+/-2.6
8	**Gln**	**-50.1**+/-2.6	**-40.6**+/-1.8
9	**Tyr**	**-69.7**+/-2.3	**-45.9**+/-1.0
10	**Phe**	**-62.8**+/-1.0	**-30.3**+/-2.1
11	**Met**	**-84.3**+/-2.9	**-26.3**+/-2.2
12	**Gln**	**-68.8**+/-2.2	**-30.0**+/-1.4
13	**Tyr**	**-50.6**+/-1.1	**-36.2**+/-3.0
14	**Lys**	**-74.6**+/-1.0	**-25.8**+/-0.8
15	**Asp**	**-87.2**+/-2.3	**54.5**+/-1.4
16	**Leu**	**-64.6**+/-1.1	**-42.8**+/-0.3
17	**Pro**	**---**	**-1.8**+/-1.2
18	**Val**	**-126.4**+/-1.4	**1.4**+/-0.7
19	**Ala**	**-60.1**+/-1.4	**-15.5**+/-0.9
20	**Leu**	**-85.6**+/-0.9	**5.8**+/-1.7
21	**Arg**	**-135.4**+/-2.7	**-43.5**+/-0.4
22	**Glu**	**-83.5**+/-5.5	**-41.3**+/-2.2
23	**Gly**	**-79.3**+/-1.7	**-10.3**+/-5.3
24	**Ala**	**-102.0**+/-10.2	**14.8**+/-4.0
25	**Asn**	**-122.2**+/-5.8	**75.1**+/-7.8
26	**Pro**	**---**	**-10.6**+/-2.7
27	**Gly**	**-112.9**+/-9.2	**20.0**+/-3.9
28	**Phe**	**-138.0**+/-2.8	**-44.8**+/-3.3
29	**His**	**-65.9**+/-4.4	**-23.1**+/-1.8
30	**Glu**	**-112.8**+/-1.3	**-15.9**+/-1.7
31	**Ala**	**-77.0**+/-3.3	**-54.7**+/-1.3
32	**Ile**	**-59.6**+/-1.1	**-18.2**+/-1.4
33	**Gly**	**-104.3**+/-1.8	**-17.3**+/-1.2
34	**Asp**	**-86.4**+/-3.9	**-31.9**+/-3.3
35	**Val**	**-63.3**+/-3.9	**-49.4**+/-1.9
36	**Leu**	**-64.6**+/-8.7	**-11.0**+/-6.4
37	**Ala**	**-149.3**+/-14.5	**-60.3**+/-53.3

Table S2: φ and ψ dihedral angles (in degrees) of the the Zn^{2+}-ACE_N(37) peptide at 298K (H_2O/TFE-*d2* 34%/66% v/v. pH=4.9).

Residue		φ	ψ
1	**His**	---	**80.1**+/-79.0
2	**His**	**-116.1**+/-80.7	**98.4**+/-82.1
3	**Glu**	**-75.2**+/-77.2	**35.5**+/-17.3
4	**Met**	**-59.3**+/-81.1	**25.7**+/-61.3
5	**Gly**	**128.3**+/-38.9	**7.0**+/-31.6
6	**His**	**-89.1**+/-19.8	**-43.9**+/-12.3
7	**Ile**	**-61.4**+/-5.6	**-45.2**+/-7.6
8	**Gln**	**-63.2**+/-6.1	**-28.0**+/-4.0
9	**Tyr**	**-73.0**+/-3.9	**-17.1**+/-4.3
10	**Tyr**	**-112.1**+/-3.0	**-42.4**+/-4.5
11	**Leu**	**-52.9**+/-6.1	**-45.2**+/-1.6
12	**Gln**	**-78.0**+/-1.8	**-22.0**+/-2.5
13	**Tyr**	**-84.0**+/-4.5	**-1.0**+/-4.3
14	**Lys**	**-41.7**+/-8.6	**-39.6**+/-9.2
15	**Asp**	**-165.3**+/-10.2	**86.1**+/-30.4
16	**Leu**	**-107.2**+/-15.4	**160.5**+/-1.0
17	**Pro**	**---**	**-6.2**+/-2.2
18	**Val**	**37.9**+/-1.9	**87.2**+/-2.9
19	**Ser**	**-129.1**+/-8.2	**-44.1**+/-3.4
20	**Leu**	**-96.4**+/-4.3	**6.6**+/-6.8
21	**Arg**	**-124.2**+/-7.8	**-44.2**+/-4.1
22	**Arg**	**-42.5**+/-8.5	**-27.4**+/-6.7
23	**Gly**	**-140.4**+/-19.3	**-13.7**+/-37.6
24	**Ala**	**-103.6**+/-35.2	**-87.4**+/-6.6
25	**Asn**	**43.2**+/-31.9	**67.1**+/-11.8
26	**Pro**	**---**	**-9.5**+/-4.9
27	**Gly**	**142.1**+/-9.4	**101.4**+/-8.6
28	**Phe**	**-128.7**+/-14.7	**-44.2**+/-5.6
29	**His**	**-47.1**+/-9.4	**-57.0**+/-10.3
30	**Glu**	**-83.6**+/-2.2	**-24.0**+/-1.4
31	**Ala**	**-58.0**+/-6.9	**-52.5**+/-3.4
32	**Ile**	**-58.3**+/-2.9	**-42.4**+/-0.4
33	**Gly**	**-65.9**+/-2.3	**-33.0**+/-1.1
34	**Asp**	**-72.9**+/-3.0	**-9.8**+/-2.2
35	**Val**	**-96.8**+/-4.6	**-26.9**+/-4.1
36	**Leu**	**-104.1**+/-25.4	**6.3**+/-53.4
37	**Ala**	**-126.7**+/-59.8	**-93.9**+/-77.1

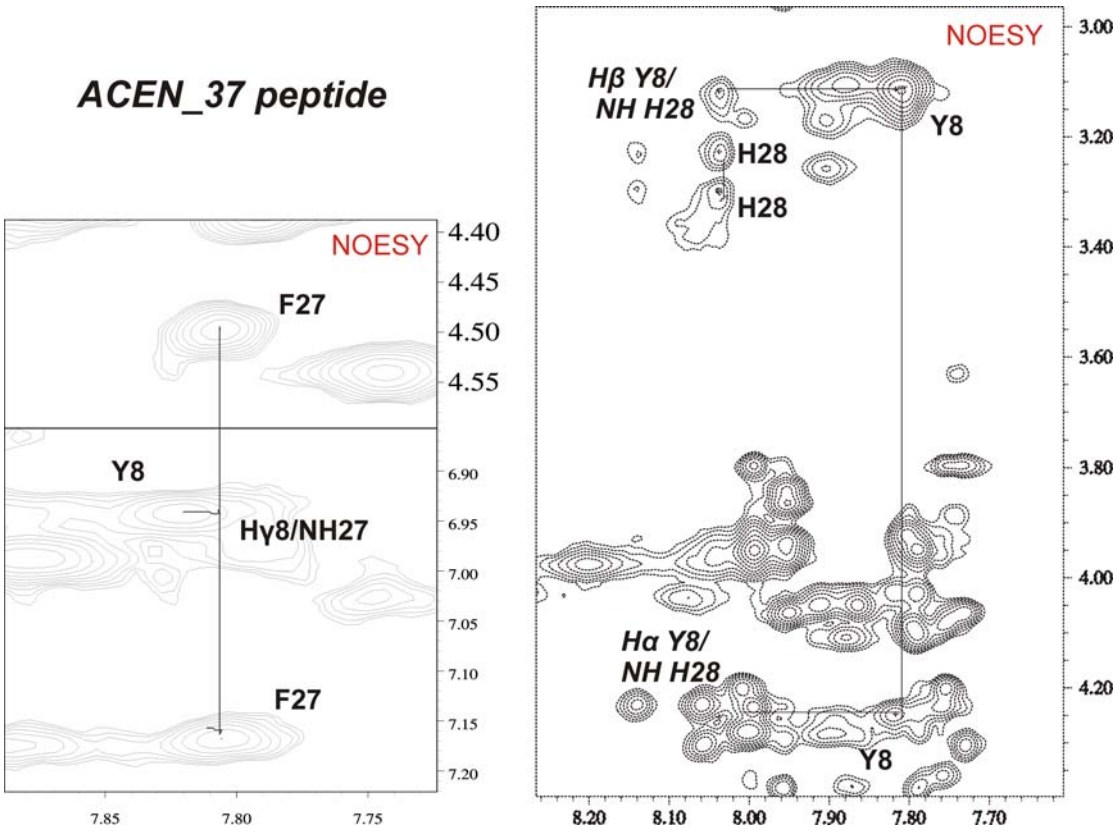
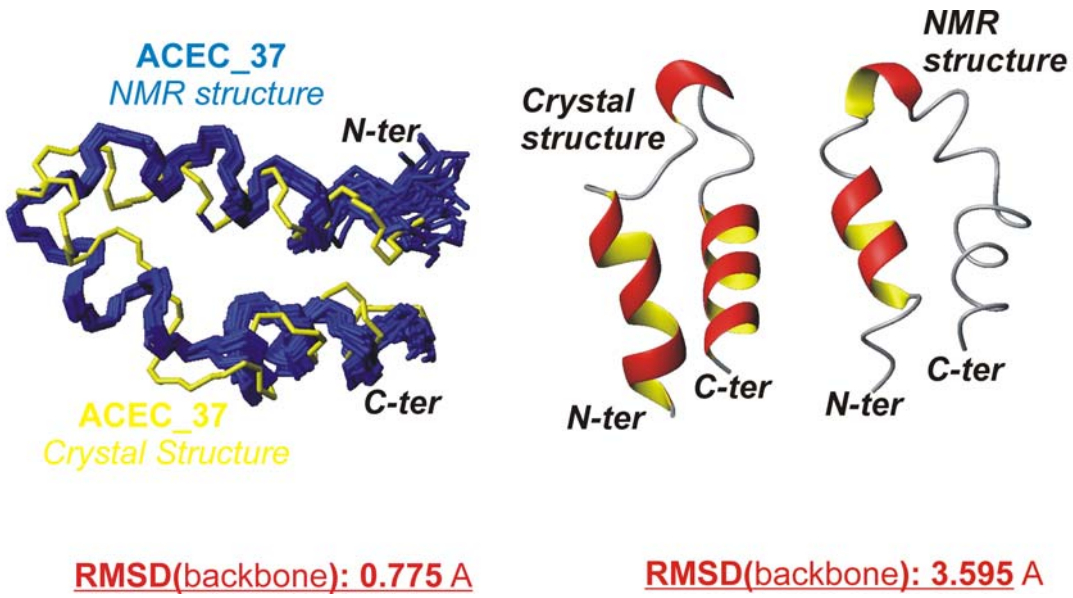


Figure S1: Fingerprint regions of 600- MHz NOESY of Zn^{2+}-$ACE_N(37)$ peptide recorded at T= 298 K. Characteristic long-range NOE connectivities between Tyr^8 with His^{28}, as well as with Phe^{27} present only in the Zn^{2+}-$ACE_N(37)$ peptide.



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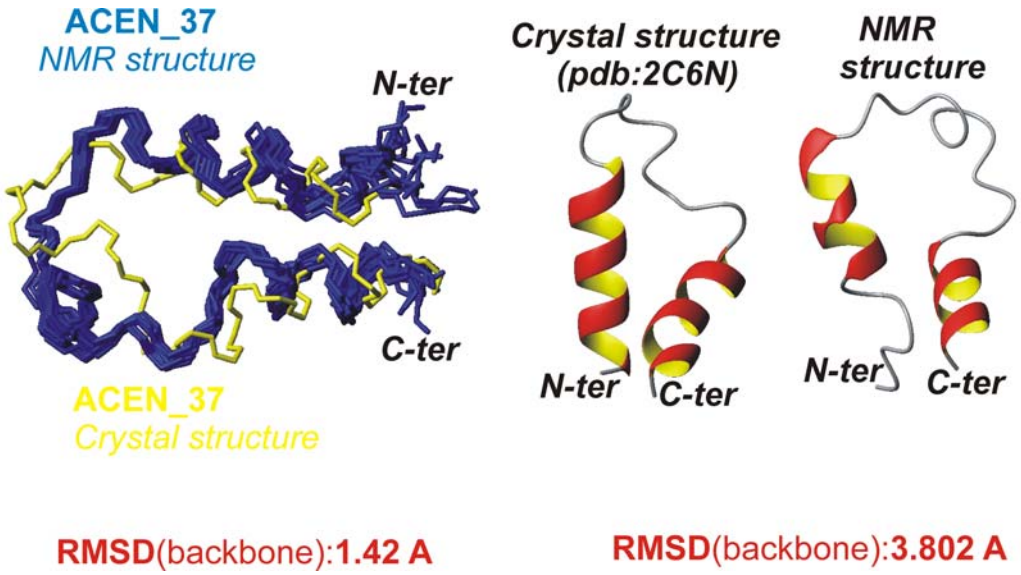

Figure S3: **Left:** Superimposition of Zn^{2+}-ACE_N(37) DYANA 20 best models calculated with NMR data in blue and the crystal structure of ACE_C in complex with lisinopril in yellow (pdb code:***2C6N***). The calculated RMSD value is 1.42 Å for the backbone atoms. **Right:** Ribbon representation of the crystal structure of ACE_N in complex with lisinopril and the mean NMR calculated structure of Zn^{2+}-ACE_N(37). The calculated RMSD value is 3.802 Å for the backbone atoms.