

A Mechanistic Study on the Inhibition of α -Chymotrypsin by a Macrocyclic Peptidomimetic Aldehyde

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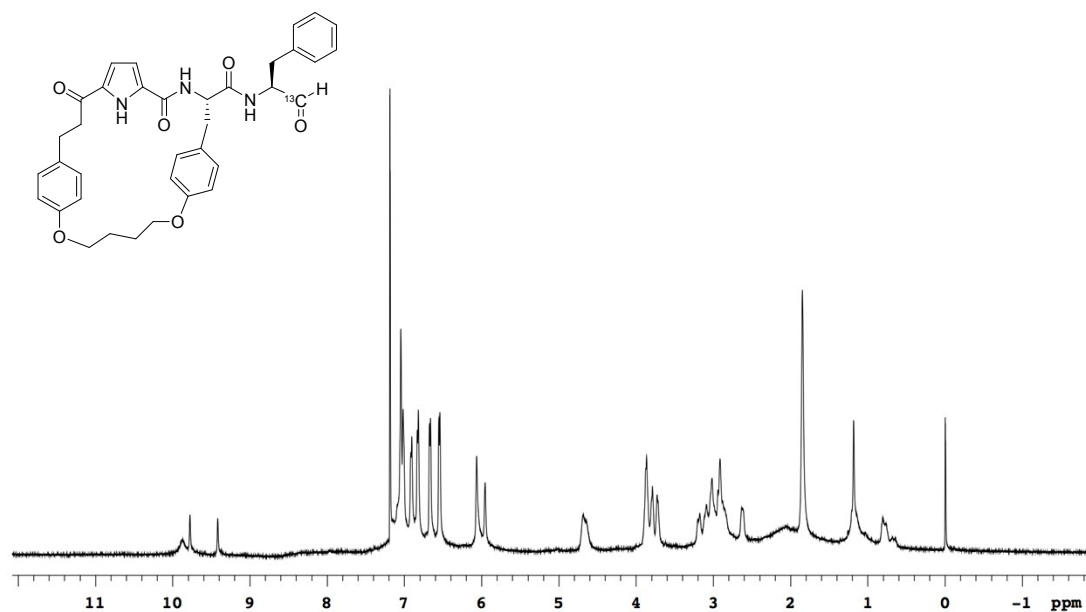
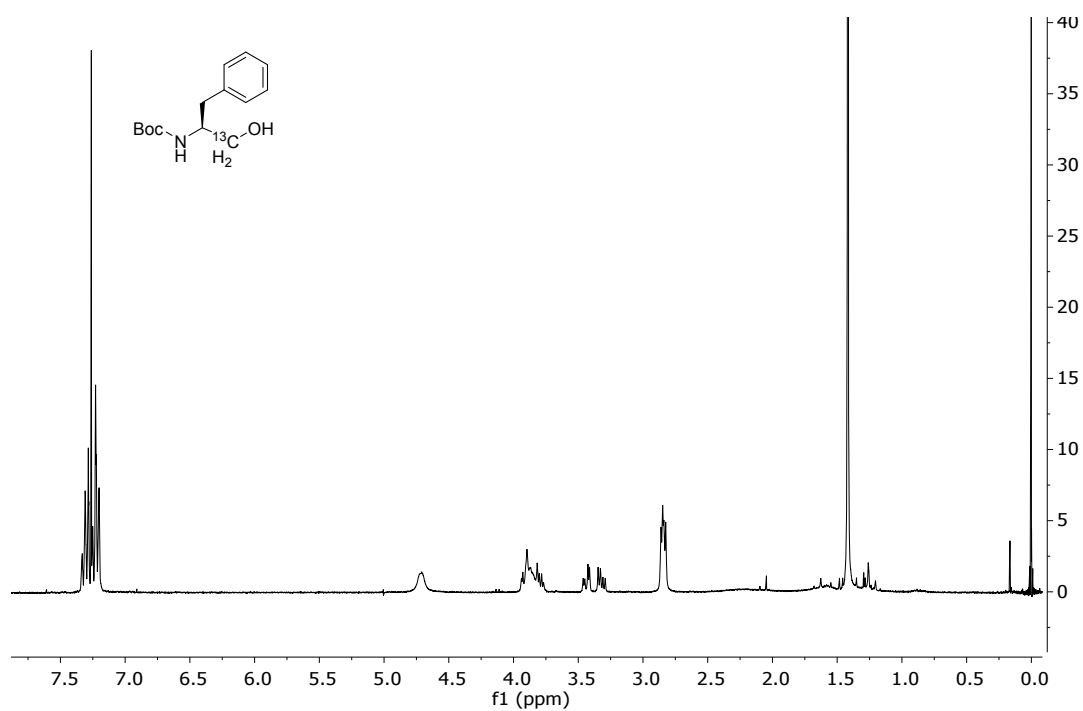
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Wavelength (Å)	1.54
Resolution range (Å)	35 – 2.2
Space Group	P2 ₁
Unique Reflections	43565 (4172)
Multiplicity	4.5 (3.9)
Completeness (%)	98.5 (93.8)
Mean I/ sigma (I)	6.1 (2.9)
Wilson B-factor	21.1
R-merge	8.6 (29.3)
R-pim	4.9 (17.8)
R-factor	20.6 (25.3)
R-free	26.8 (36.3)
Protein Subunits in ASU	4
Total Number of Atoms	7479
Macromolecule Atoms	6794
Ligands Atoms	180
Water Atoms	505
Protein Residues	928
RMS bonds (Å)	0.012
RMS angles (°)	1.38
Ramachandran favoured (%)	96.1
Average B-factor Total	10.0
Macromolecule B-factor	9.9
Solvent B-factor	11.5

b. Copies of NMR spectra

Figure S1. ^1H NMR of compound **8**.Figure S2. ^1H NMR of compound **17**.

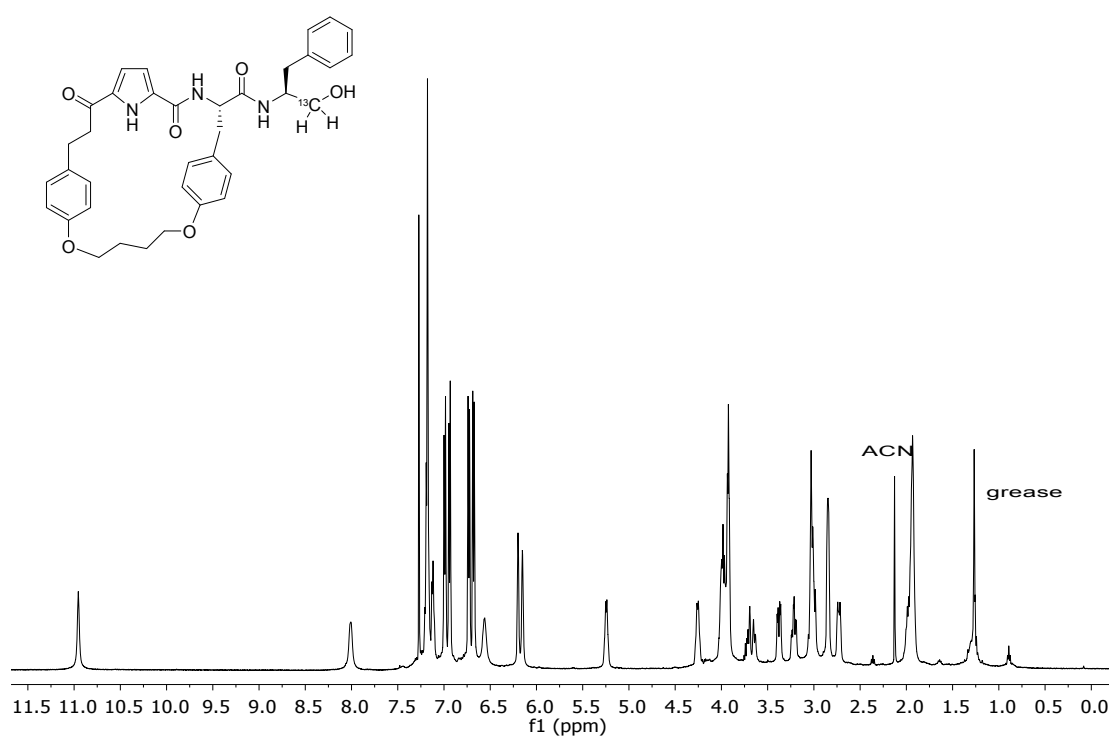


Figure S3. ^1H NMR of compound **19**.

c. Copies of analytical HPLC traces

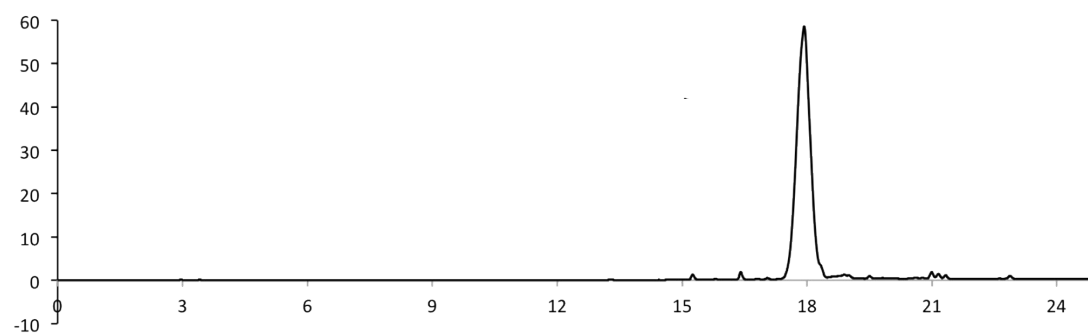


Figure S4. Analytical HPLC trace for compound **8**.

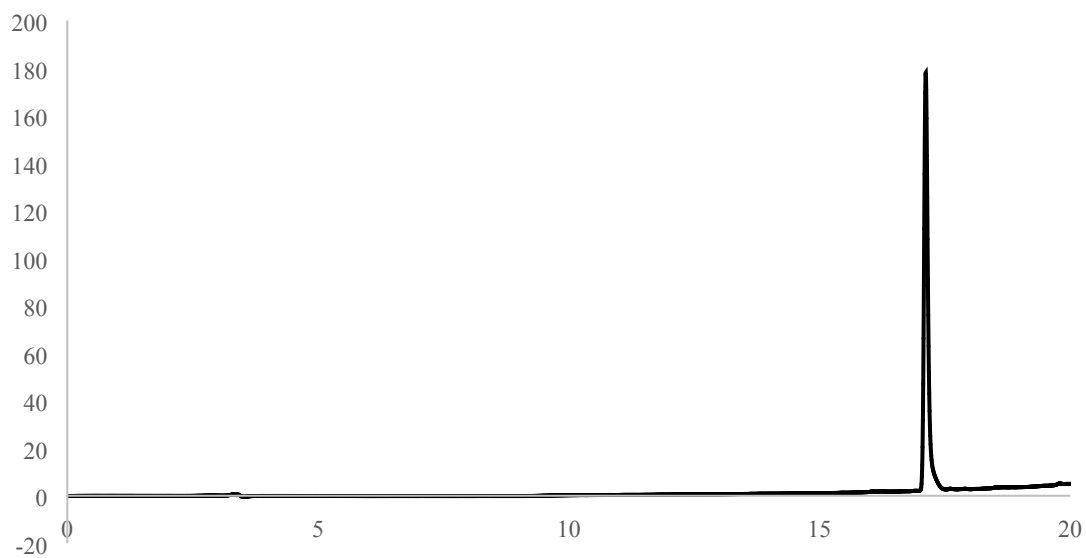


Figure S5. Analytical HPLC trace for compound **17**

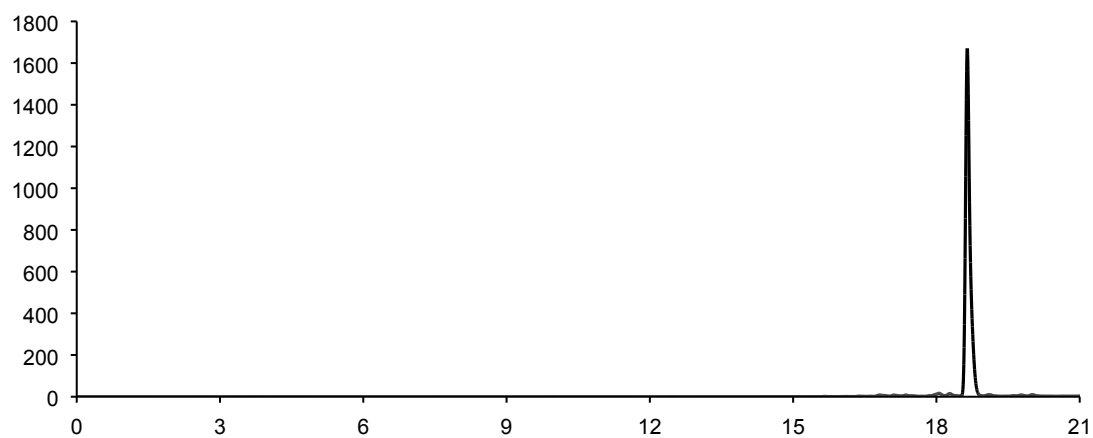


Figure S6. Analytical HPLC trace for compound **19**.

d. Reference

(1) Chua, K. C. H.; Pietsch, M.; Zhang, X.; Hautmann, S.; Chan, H. Y.; Bruning, J. B.; Gütschow, M.; Abell, A. D. *Angew. Chem. Int. Ed.* **2014**, *53*, 7828.