

CHEMBIOCHEM

Supporting Information

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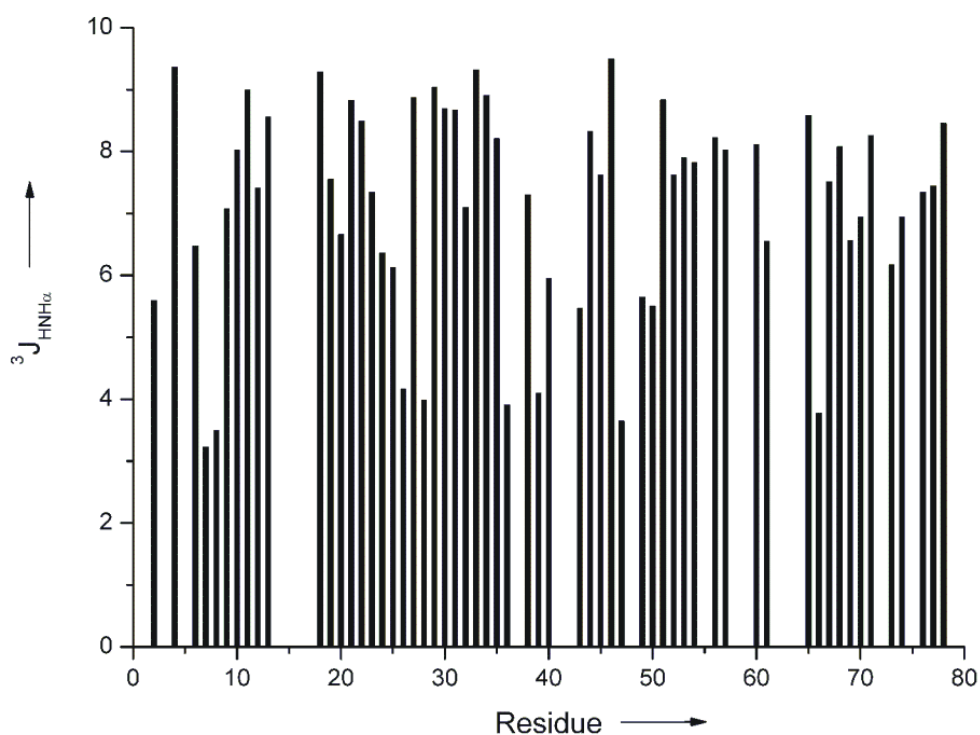
Supporting Information

for

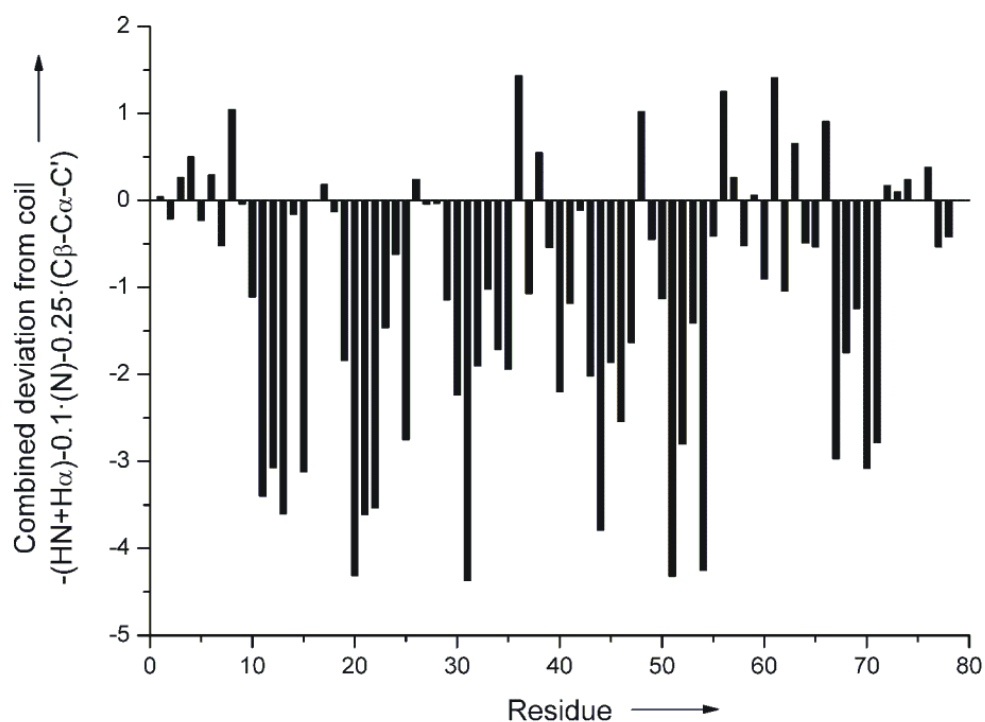
The High Resolution NMR Structure of Parvulostat (Z-2685) from *Streptomyces parvulus* FH-1641: Comparison with Tendamistat from *Streptomyces tendae* 4158

Stephan Rehm, Sigeng Han, Ismail Hassani, Alma Sokocevic, Hendrik R.A. Jonker,
Joachim W. Engels, and Harald Schwalbe*

A)



B)



C)

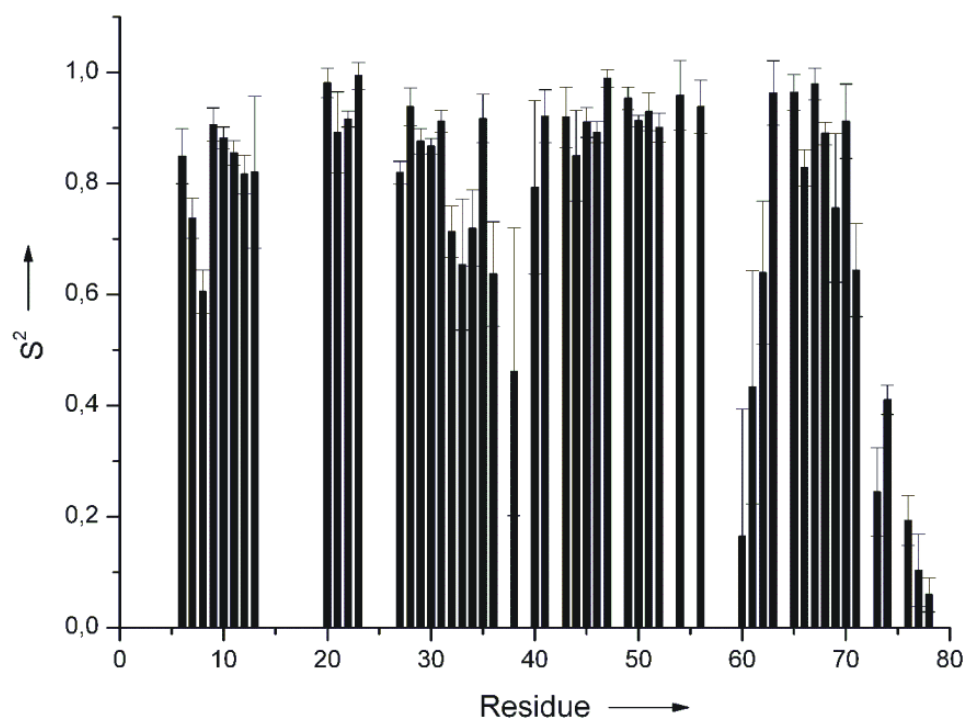


Figure S1. A) $^3J_{HNH\alpha}$ couplings of parvulostat: 51 couplings could be determined. B) Combined chemical shift deviations from random coil values (PSSI^[18]): $H\alpha$, $C\alpha$, $C\beta$, C' , HN , N . C) Order parameter S^2 , as derived from model-free.^[24, 25]

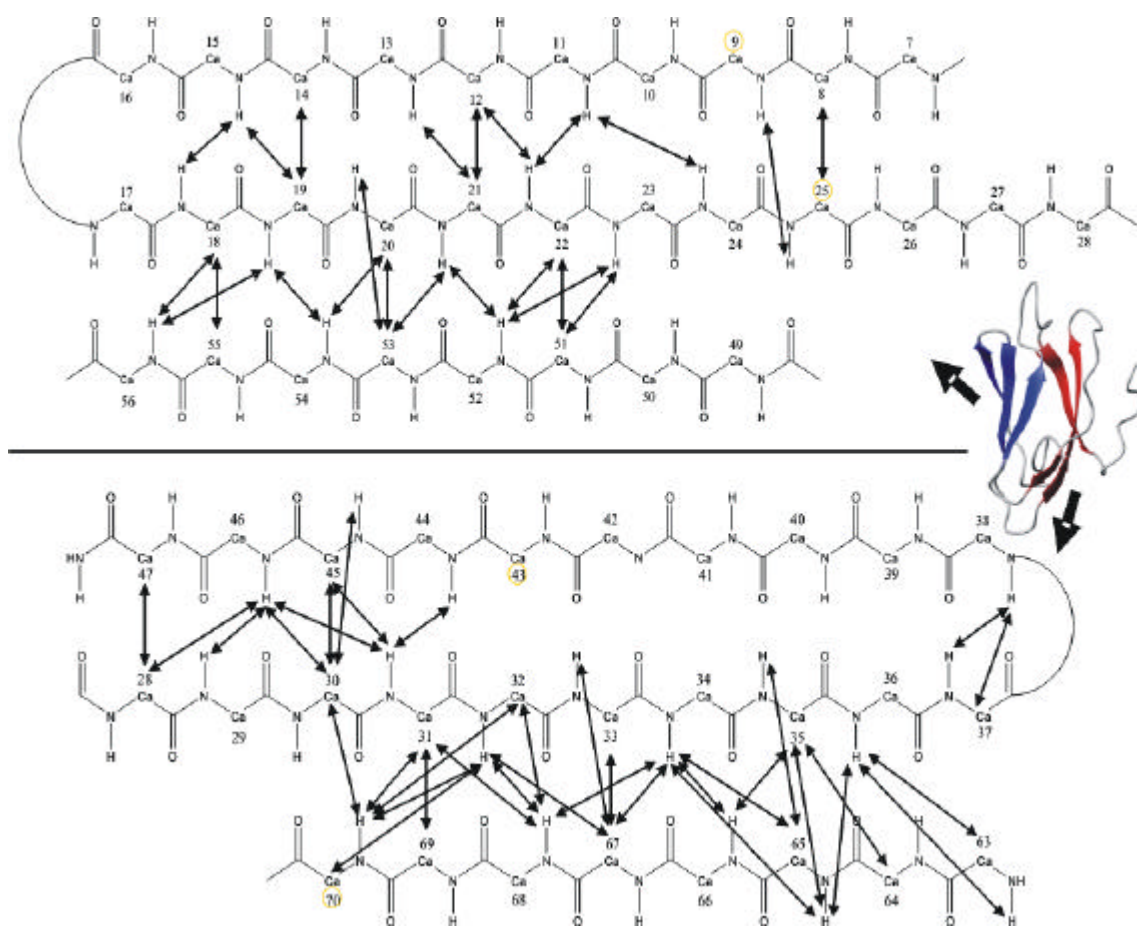
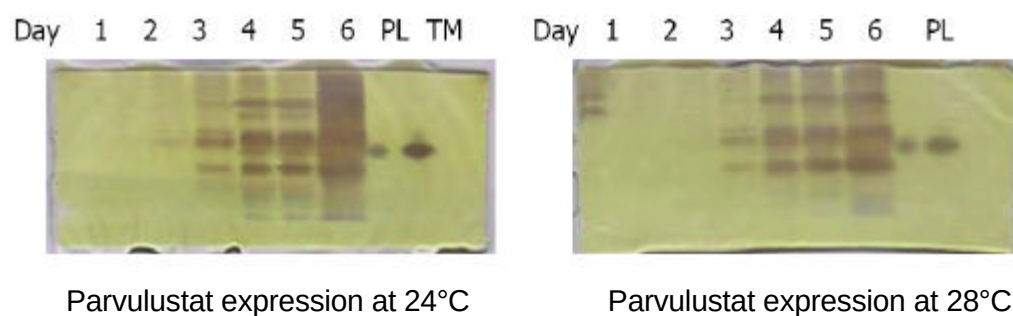
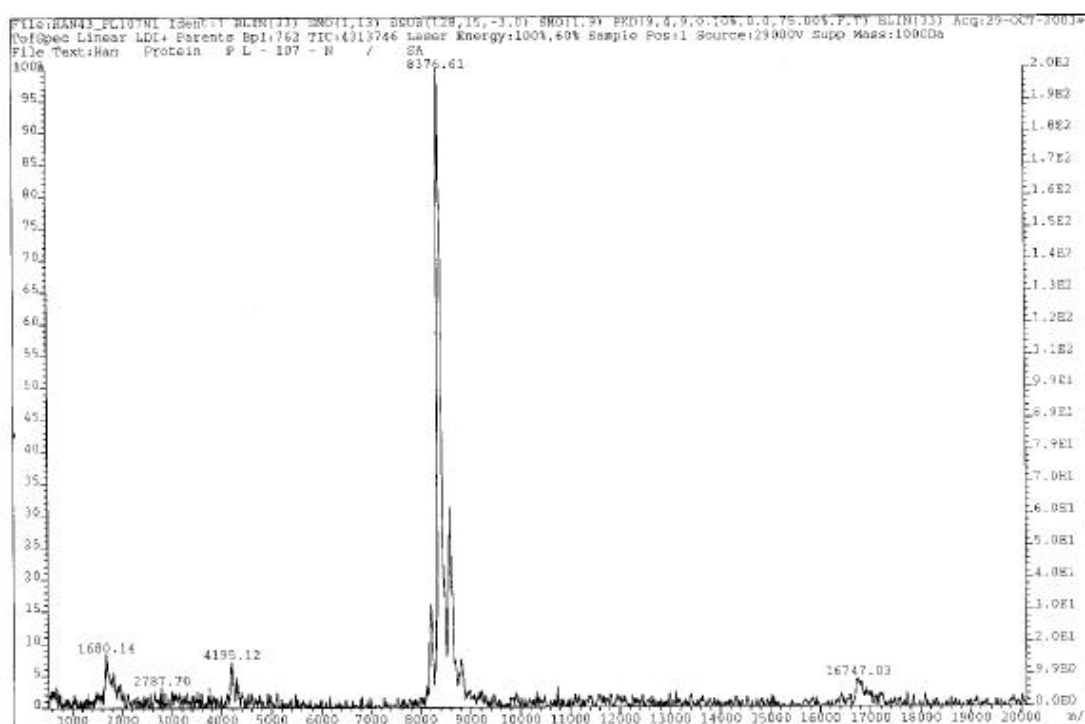


Figure S2. NOE contact map of the two β -sheets of parvulostat; upper part: β -strands 1,2 and 5 (including active site), lower part β -strands 3,4 and 6; yellow circles indicate the 4 cysteines.

A)



B)



C)

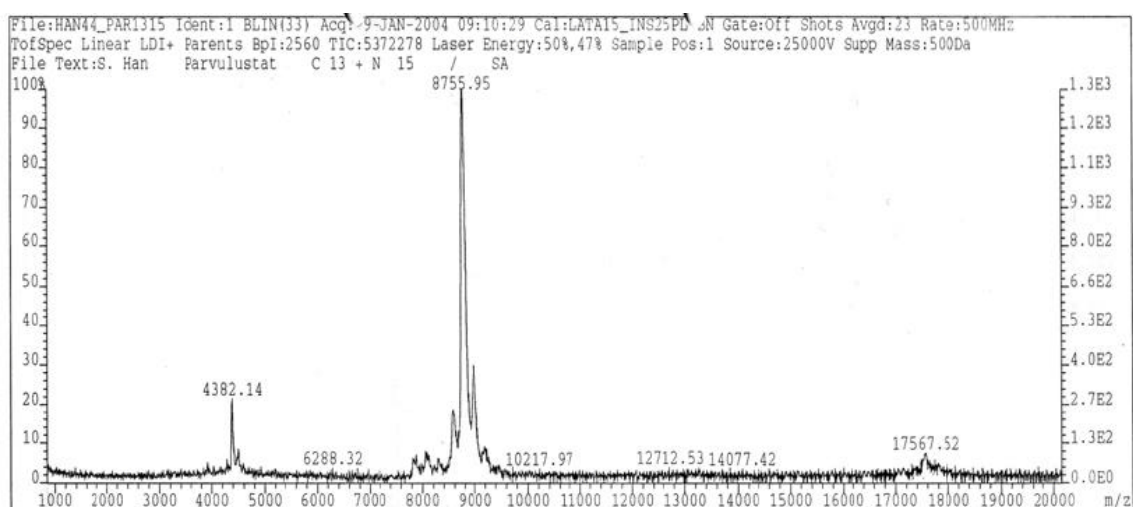
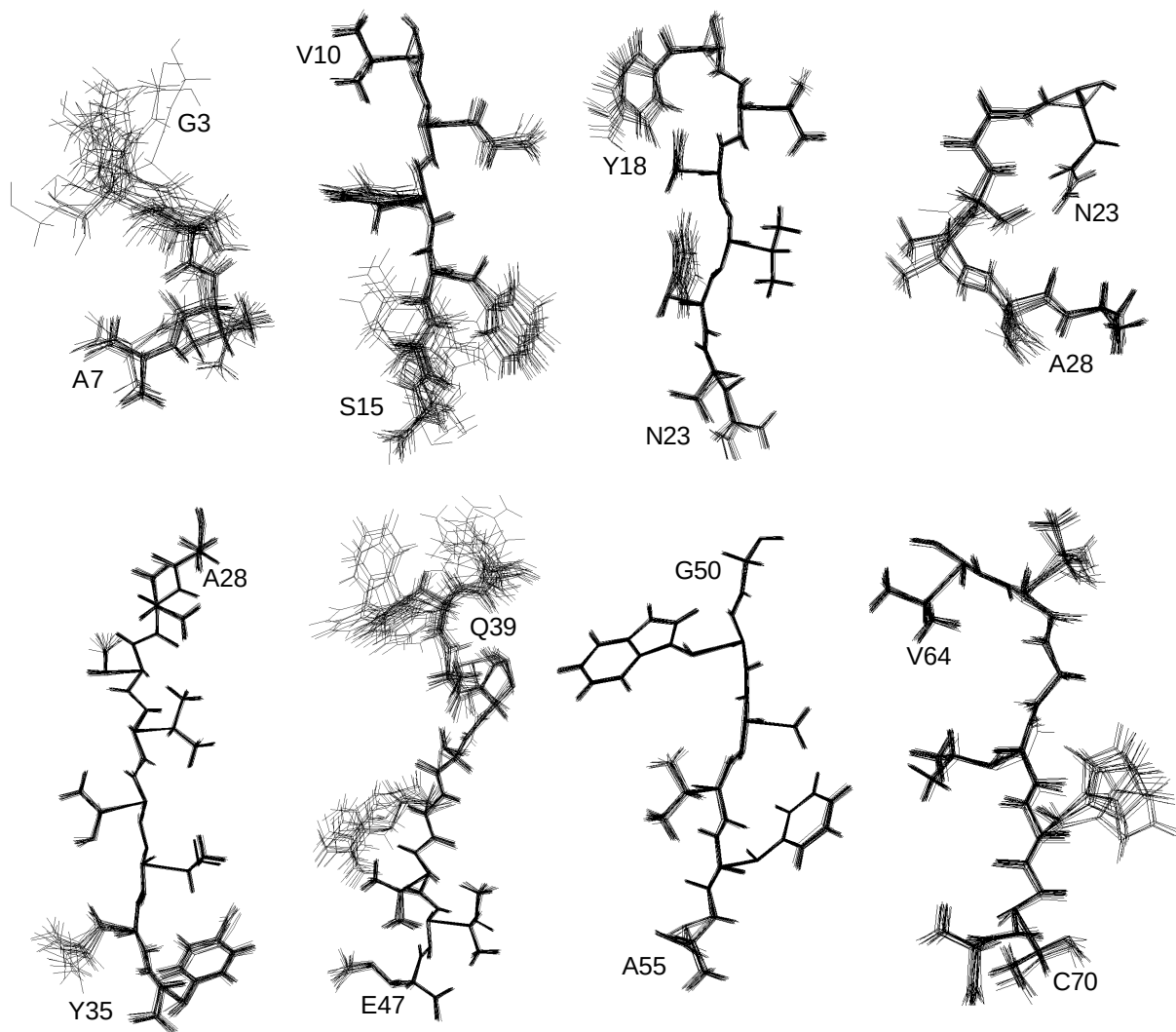


Figure S3. A) SDS-PAGE Gel of parvulustat expression at 24°C and 28°C. B) MALDI MS spectrum of ^{15}N labelled parvulustat. C) MALDI MS spectrum ^{15}N ^{13}C labelled parvulustat.

A)



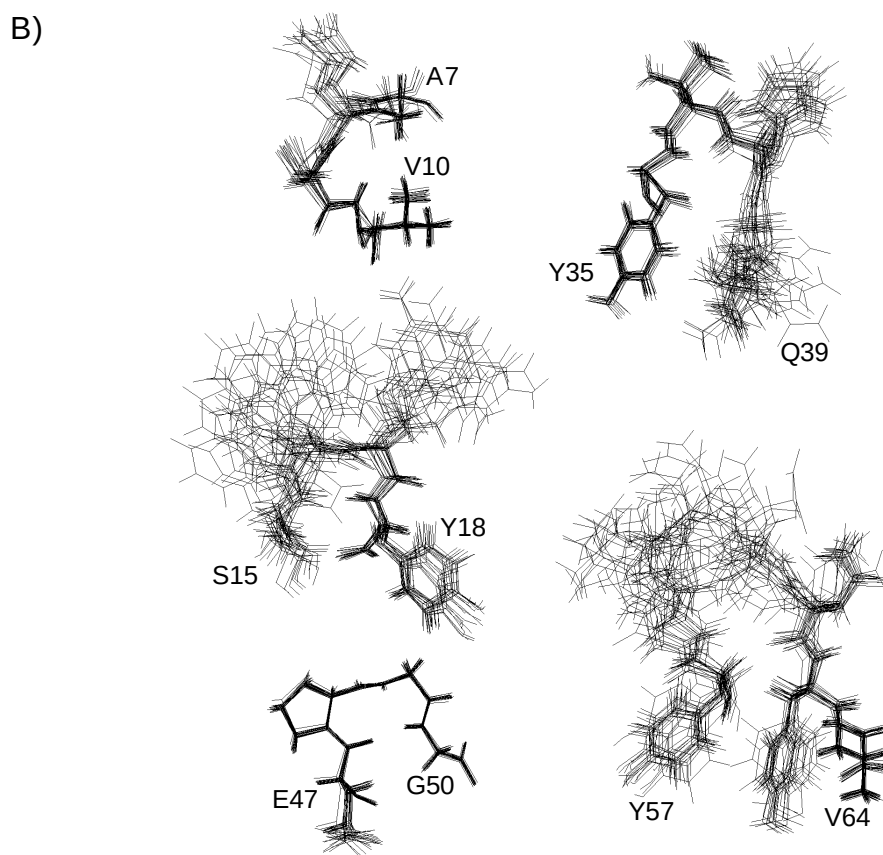


Figure S4. Presentation of the individual segments of the best fit of the superimposed best fit of the 20 parvulostat structures; plotted are all heavy atoms. A) Individual strands of the anti-parallel β -sheets compared to tendamistat (3-7, 10-15, 18-23, 23-28, 28-35, 39-47, 50-55, 64-70). B) Remaining segments like turns or non-regular secondary structures (7-10, 15-18, 35-39, 47-50, 57-64).

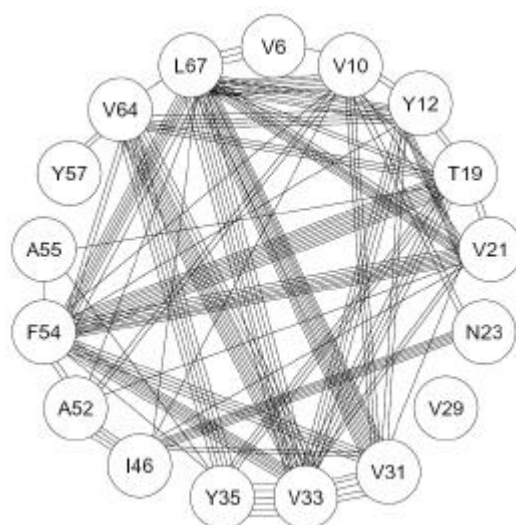


Figure S5. Presentation of sidechain-sidechain-NOE's of the amino acids that point their side chains into the interior of the protein.