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Supplemental Information

Protein Composition Determines the Effect of Crowding on the Properties of Disordered Proteins

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Supplementary Information for ” Protein composition determines effect of crowding on the properties of disordered proteins”

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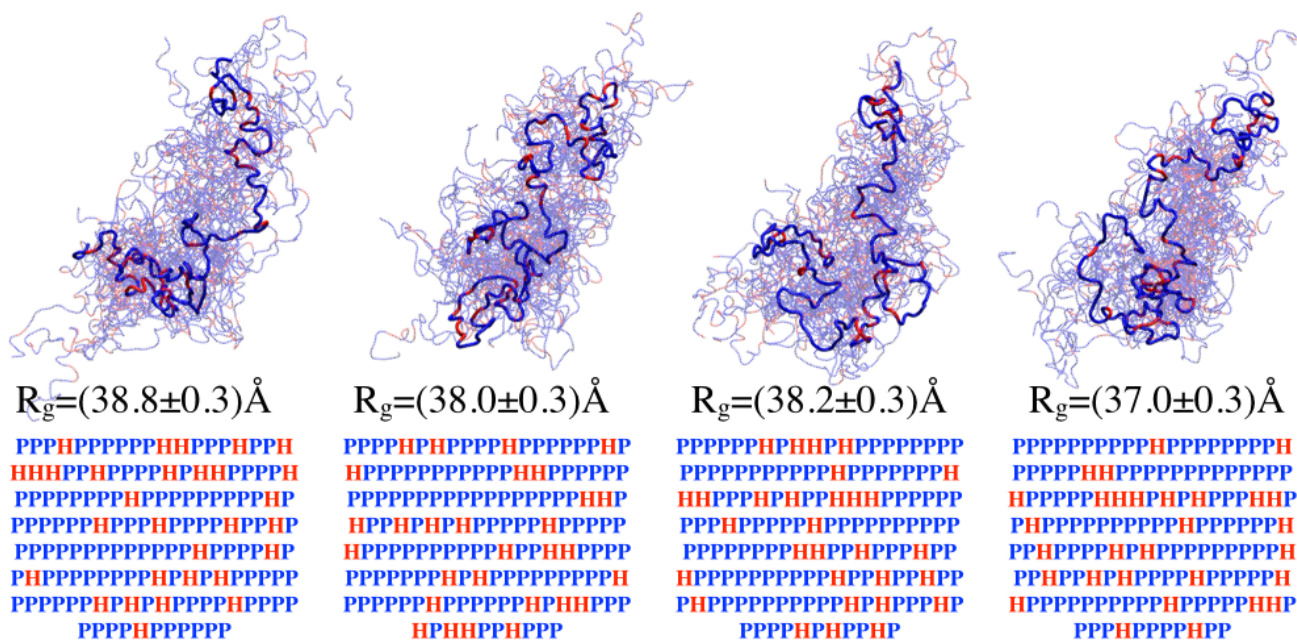


Figure 1: The four random sequences generated for $\langle h \rangle = 0.2$ and $N=150$. Images show a representative snapshot of each sequence in bulk, as well as a representative ensemble of 15 conformations (transparent). In addition to the average R_g of each sequence's total ensemble, the letter sequence is shown, where H and P represent hydrophobic and hydrophilic (polar) residues, respectively.

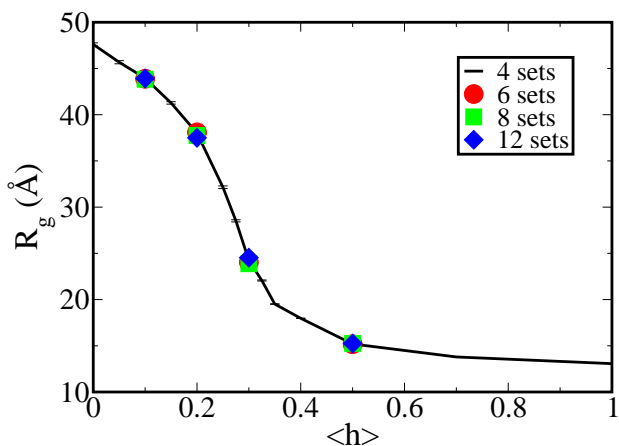


Figure 2: R_g vs. $\langle h \rangle$ for the 150-mer IDP in bulk, comparing the results from varying numbers of sequences for $\langle h \rangle = 0.1, 0.2, 0.3,$ and 0.5 . Each sequence is simulated for $5E8$ steps.

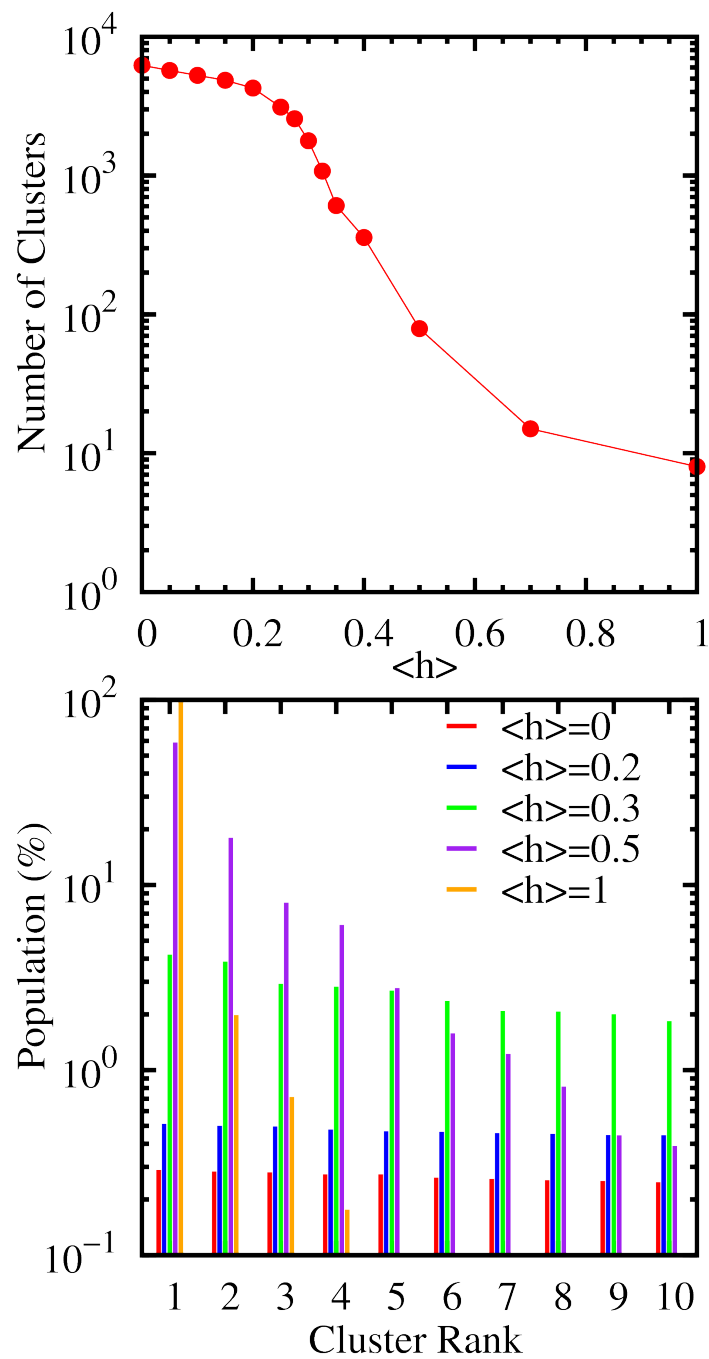


Figure 3: Number of clusters vs. $\langle h \rangle$ for the 150-mer IDP in bulk (above). Population of top ten clusters for selected $\langle h \rangle$ values (below).

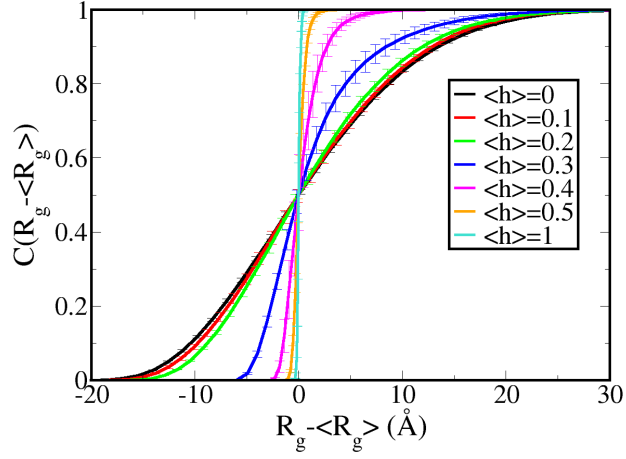


Figure 4: Cumulative R_g distributions shifted by the the median value for IDPs of varying $\langle h \rangle$ in bulk.

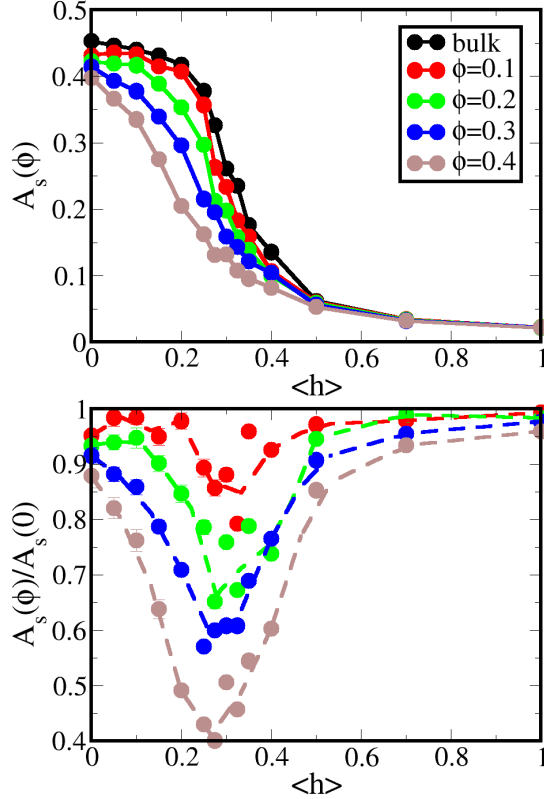


Figure 5: Average asphericity, A_s , of the IDPs as a function of $\langle h \rangle$ shows the same trend as R_g in crowders. Above, A_s in bulk ranges from 0.45 at $\langle h \rangle = 0$ to 0.022 at $\langle h \rangle = 1$, while crowding reduces the asphericity, particularly for $\langle h \rangle \approx 0.25$. Scaling A_s by that in bulk (below) shows a non-monotonic collapse, similar to that seen in the R_g (see main text Figure 2). Data shown is for $r_c = 13 \text{ \AA}$.

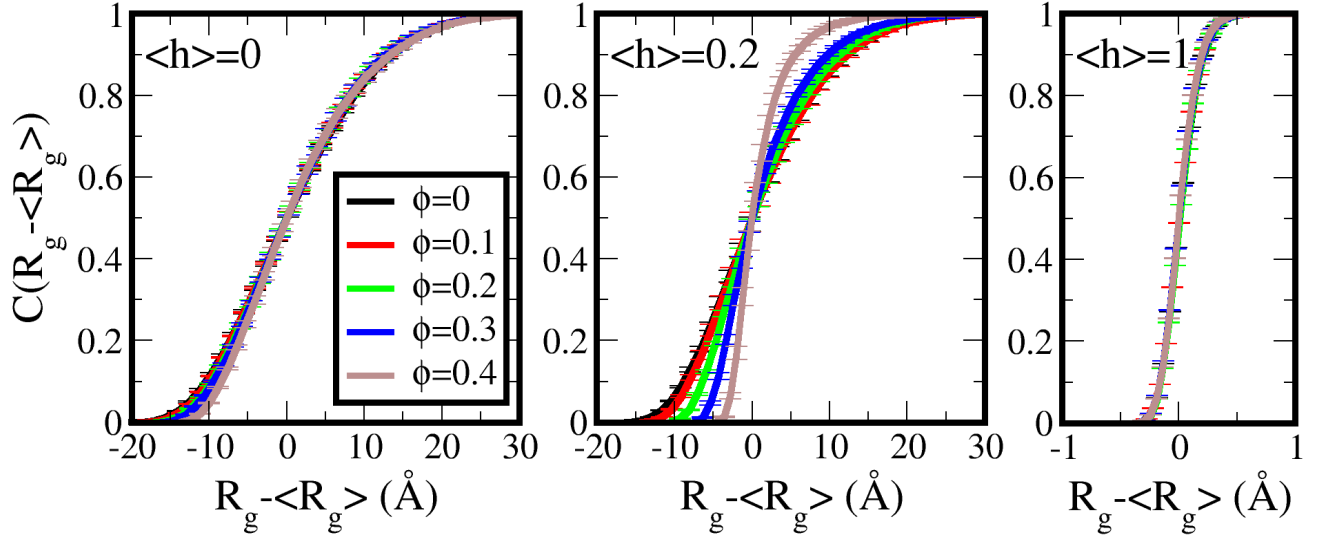


Figure 6: Cumulative R_g distributions shifted by the the median value for $\langle h \rangle = 0, 0.2,$ and 1 in bulk (black) and in crowders of radius $r_c = 13$ Å.

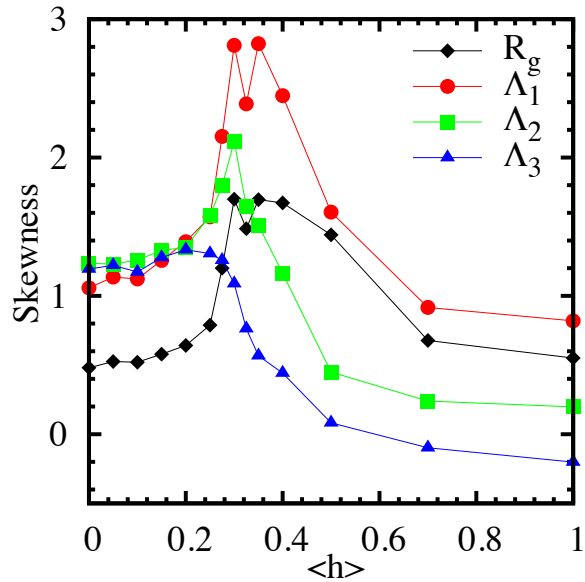


Figure 7: Skewness of the R_g distribution (black diamonds) as well as the three eigenvalues of the gyration tensor ($\Lambda_1, \Lambda_2, \Lambda_3$) vs. $\langle h \rangle$, showing a maximum at intermediate $\langle h \rangle$ values.

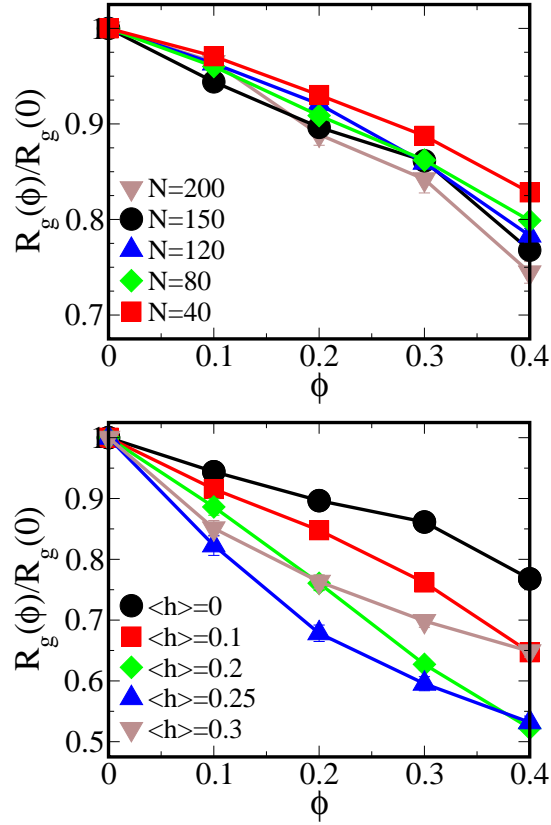


Figure 8: $R_g(\phi)$ of the IDP chain within crowders scaled by that in bulk for varying for N and $\langle h \rangle$, while the size of the polymer relative to the crowders ($R_g(0)/r_c$) is maintained at 3.66. Above, the IDP length (N) is varied for the fully hydrophilic ($\langle h \rangle = 0$) chain, and r_c is manipulated to maintain the same polymer-to-crowder size ratio. Below, the r_c is again manipulated while N is held constant at 150 and changes in bulk R_g are effected by varying $\langle h \rangle$.

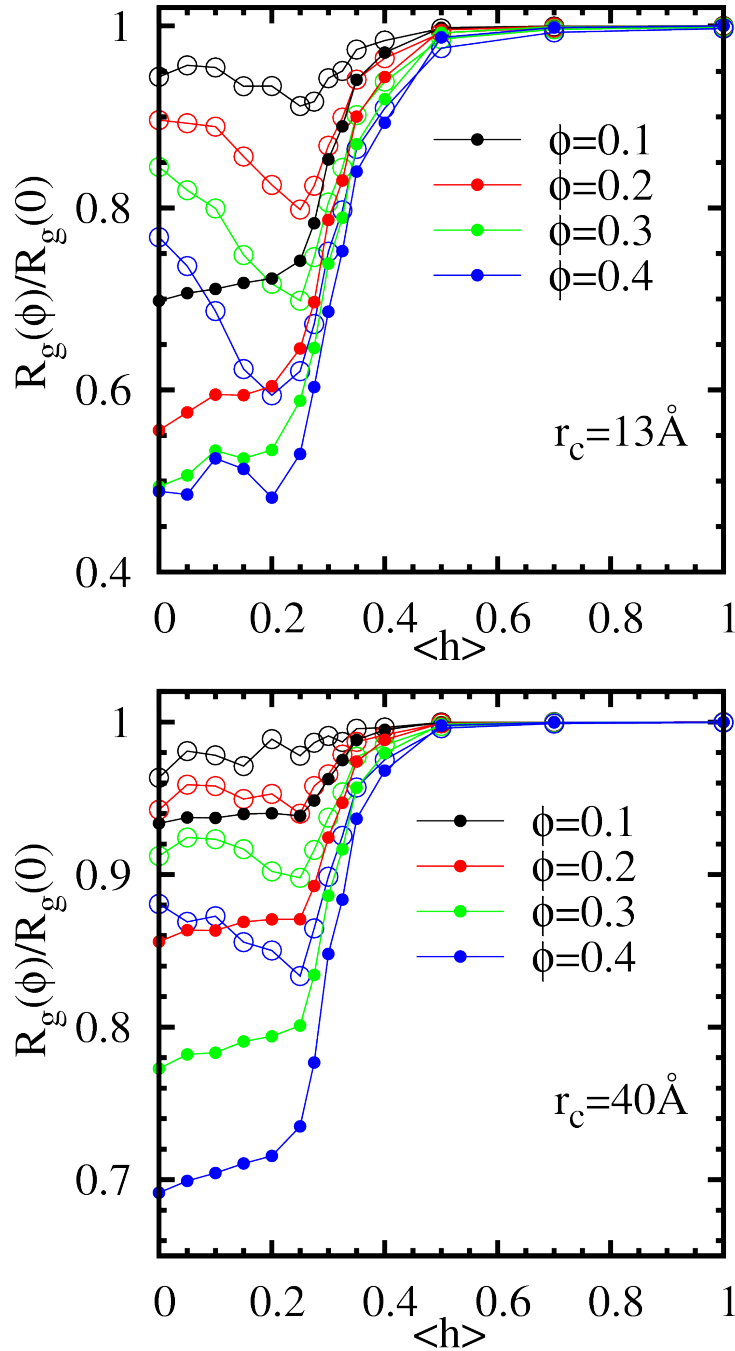


Figure 9: $R_g(\phi)/R_g(0)$ for our 150-mer IDP polymers (open symbols) and the corresponding predictions by the ellipsoid model with free-volume theory (solid symbols) with a scaling factor $s = 1$. The simulation results are compared with theoretical predictions for $r_c = 13 \text{ \AA}$ (above) and 40 \AA (below), at crowding volume fractions $\phi = 0.1 - 0.4$.

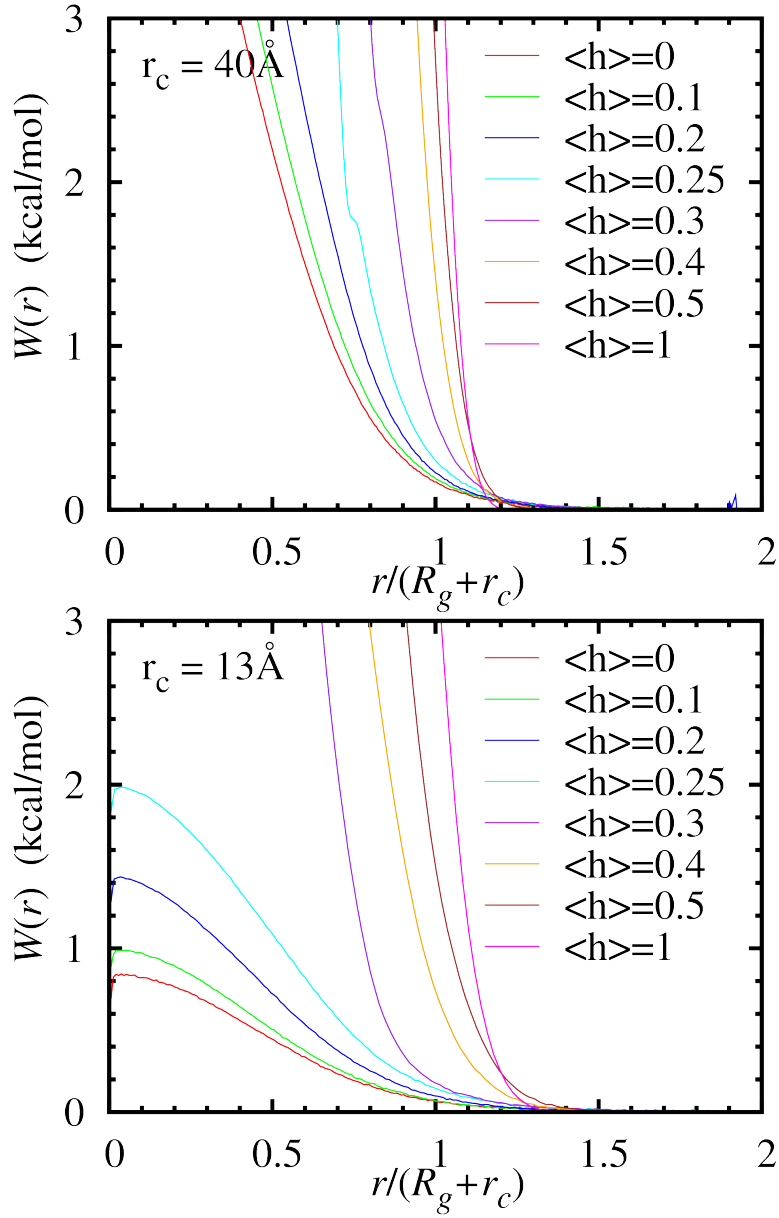


Figure 10: Potential of mean force between a protein chain and a spherical crowder of radius 13 \AA (above) and 40 \AA (below) for different $\langle h \rangle$ values.

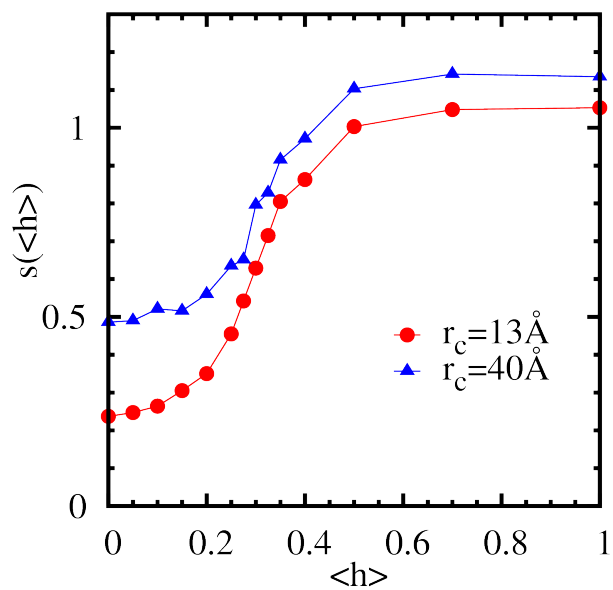


Figure 11: Scaling factor for the principal radii of ellipsoids vs. $\langle h \rangle$ at $r_c = 13$ and 40 \AA .