Supporting Information

Competitive inhibition of the classical complement pathway using exogenous single-chain C1q recognition proteins

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Supplementary figures

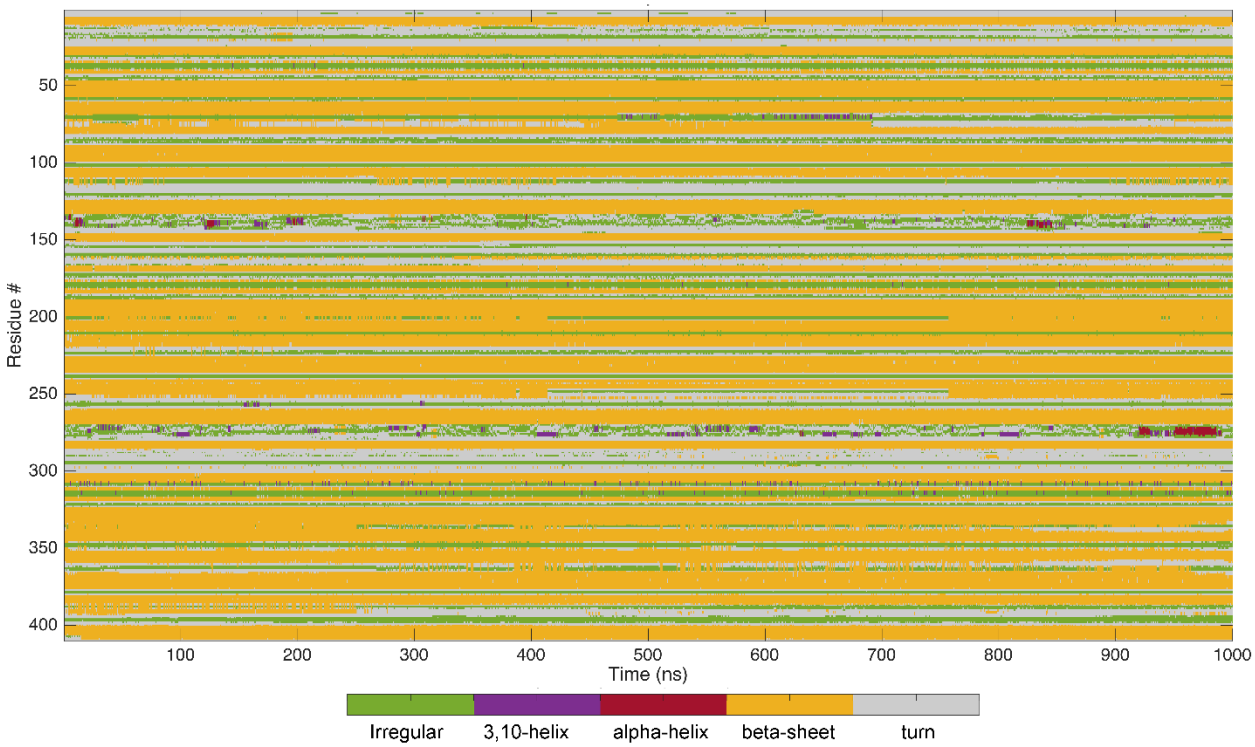


Figure S1. Changes of the secondary structure of sc-gC1q upon 1 µs MD simulation at 300 K. The structure of the protein is fairly stable with moderate fluctuations in the loop regions.

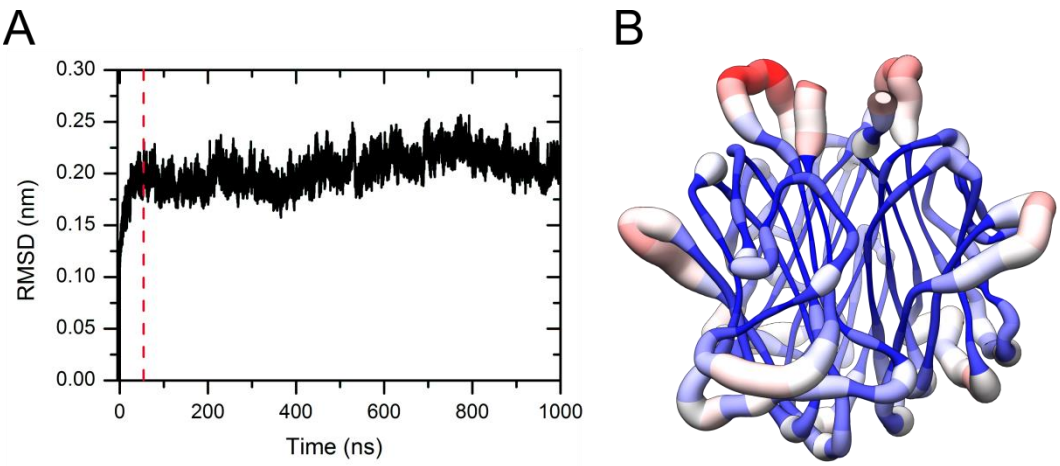


Figure S2. Stability of sc-gC1q and flexible regions as revealed by MD. (A) RMSD from the initial homology model during MD simulation of 1 μs. Within 50 ns, sc-gC1q chain finds its optimal conformation which is kept stable during MD simulation. **(B)** "β-factor" plot of sc-gC1q calculated from the MD trajectory. The thickness and colour of the tube reflect the flexibility of the backbone along the polypeptide chain. Thin tube with dark blue colour shows the most rigid parts in the β-sheet structure, while the flexible loop regions are shown with red thick tube.

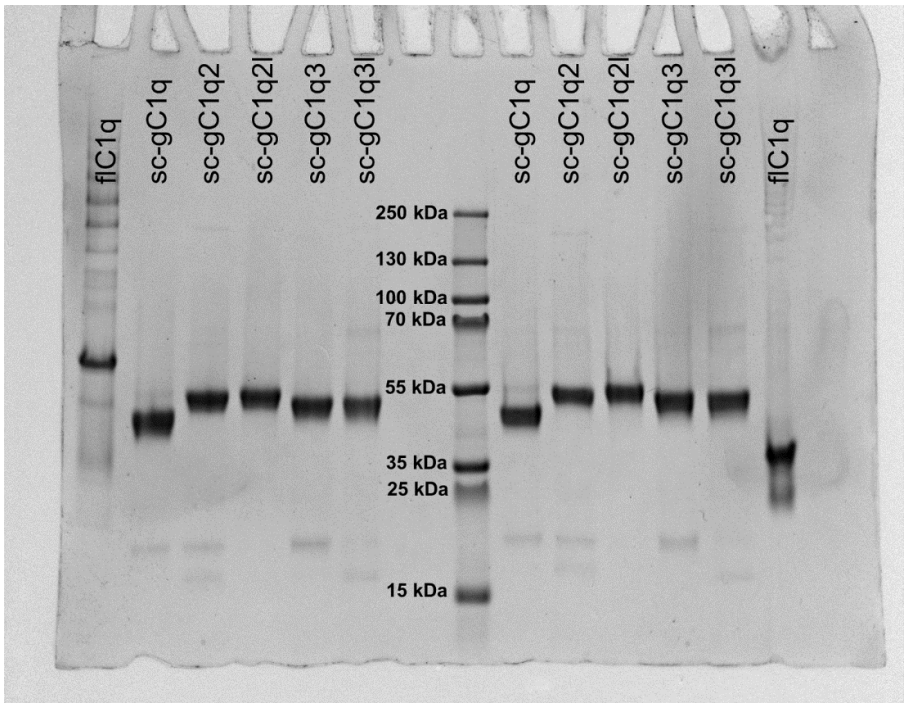


Figure S3. SDS-PAGE of C1q and sc-C1q proteins. Reducing (left) and non-reducing (right) SDS-PAGE shows the purity of the proteins applied. From left to right: C1q, sc-gC1q, sc-gC1q2, sc-gC1q2l, sc-gC1q3, sc-gC1q3l, protein marker (PageRuler Plus Prestained Protein ladder, Thermo Scientific).

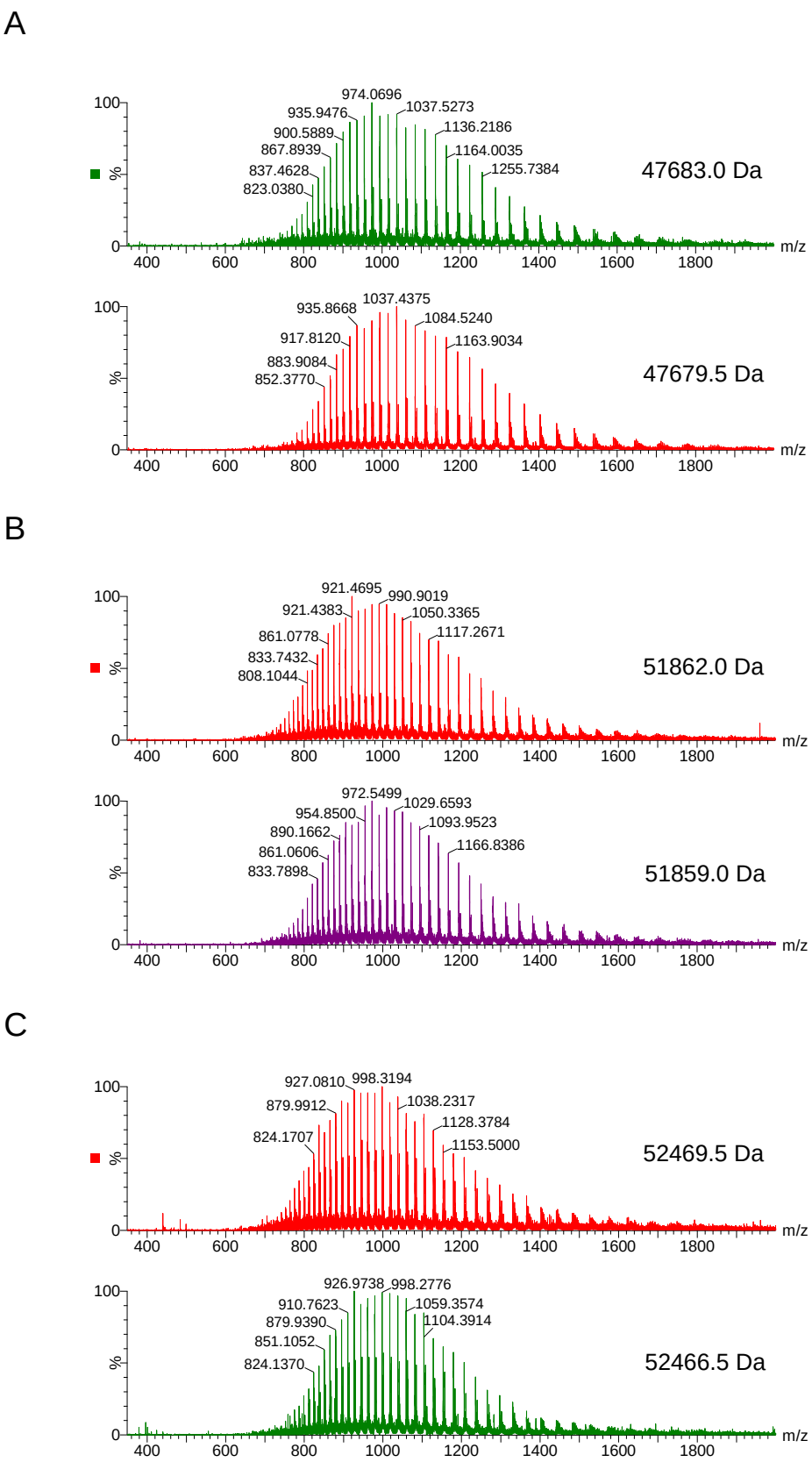
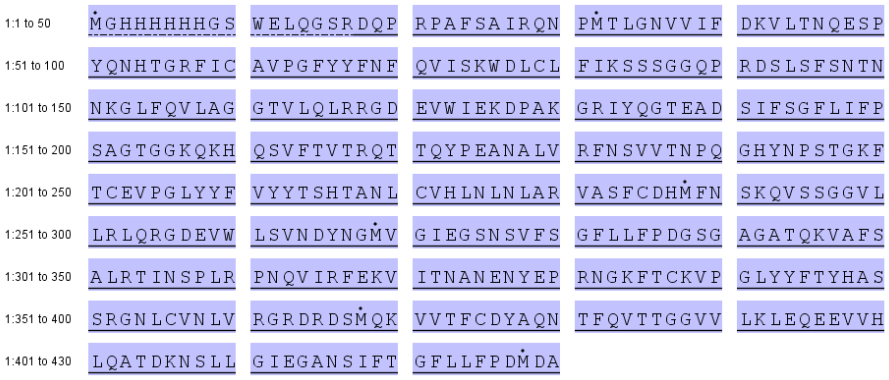
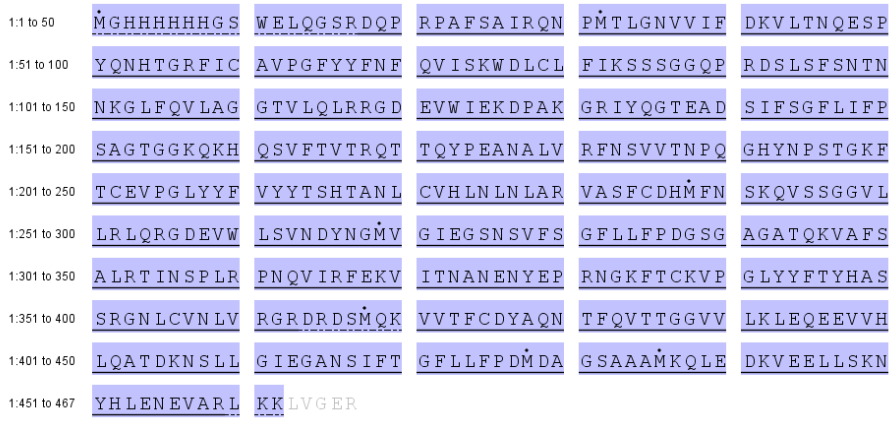


Figure S4. Intact mass spectra of sc-gC1q (A), sc-gC1q2 (B), and sc-gC1g2l protein (C). Lower figures: non-reduced protein, upper figures: reduced protein. Molecular masses are indicated in the figure and are in agreement within 20 ppm with the theoretical values. The difference between reduced and non-reduced samples indicate the presence of two disulfide bonds.

A



B



C

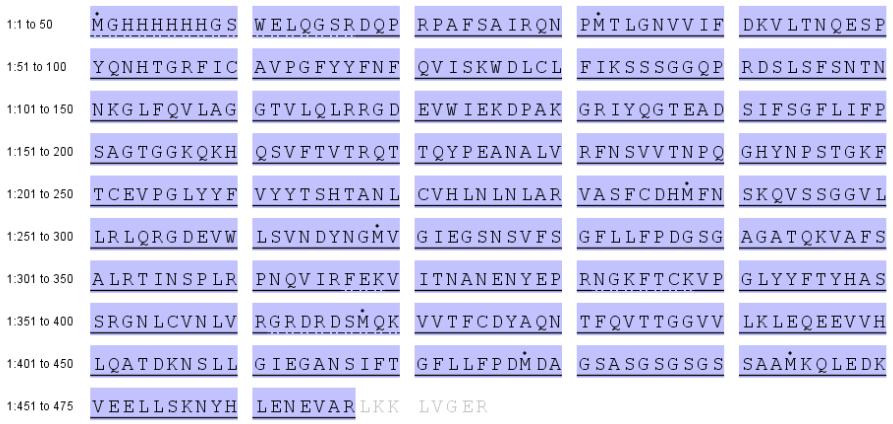


Figure S5. LC-MS/MS-based coverage map of sc-gC1q (A), sc-gC1q2 (B) and sc-gC1q2l protein (C) after tryptic digestion. Methionine oxidation was labelled with a dot and is observable in a low fraction. Solid line: Number of sequential fragment ions is above 4. Dashed line: Number of sequential fragment ions is below 4. Most of the N-terminal metionin residues are cleaved off by the *E. coli*, however, in a low fraction, it is visible.

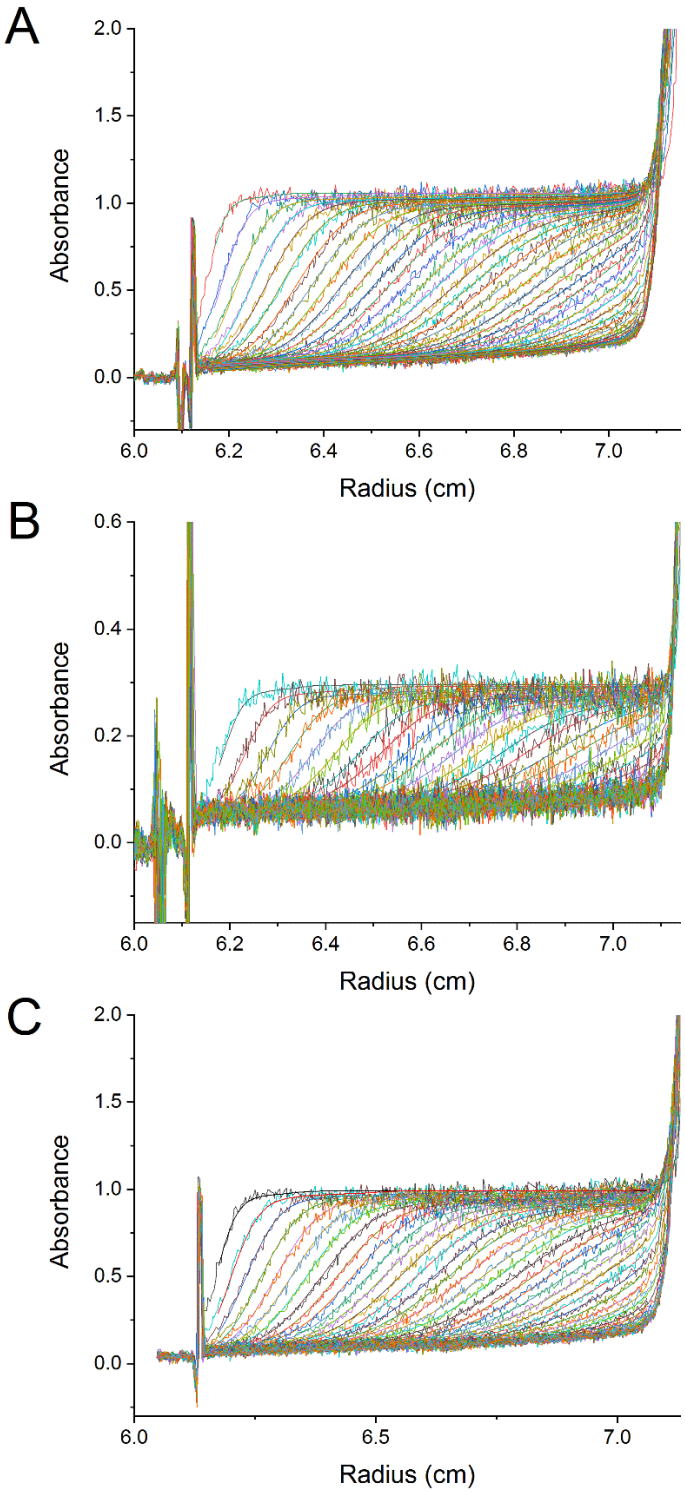


Figure S6. Analytical ultracentrifugation sedimentation velocity experiments of sc-gC1q variants. Absorbance scans along the cells every 10 min and fittings by the Sedfit software are shown for sc-gC1q (**A**), sc-gC1q2 (**B**) and sc-gC1q3 (**C**). Details of the experiments are presented in the *Experimental Procedures.* The distributions of the sedimentation coefficients are shown in **Figure 2B** of the main manuscript.