SUPPLEMENTARY MATERIAL TO THE ARTICLE «Assessment of structural changes in proteins and surrounding water molecules in solution according to SAXS and MD data»

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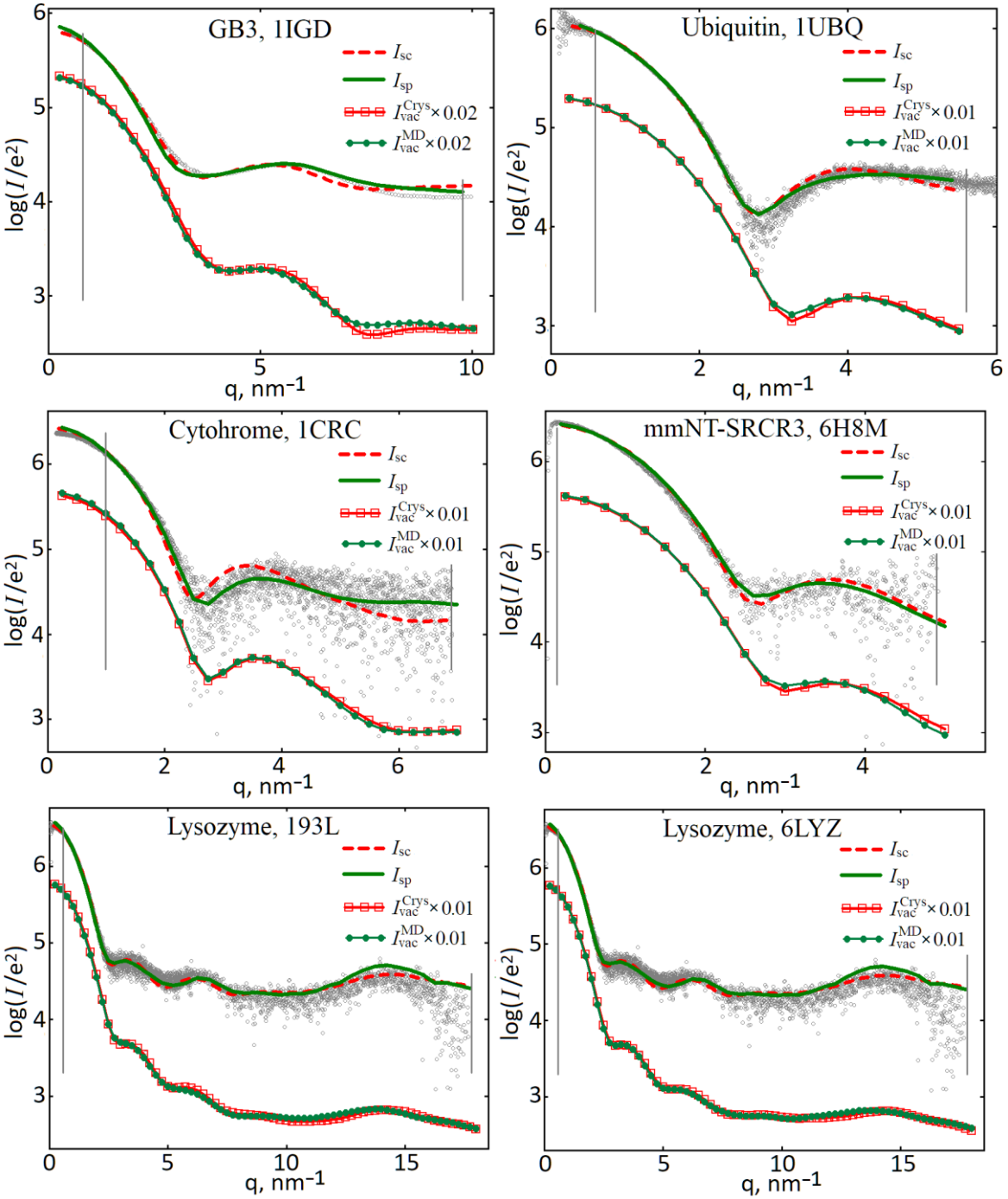
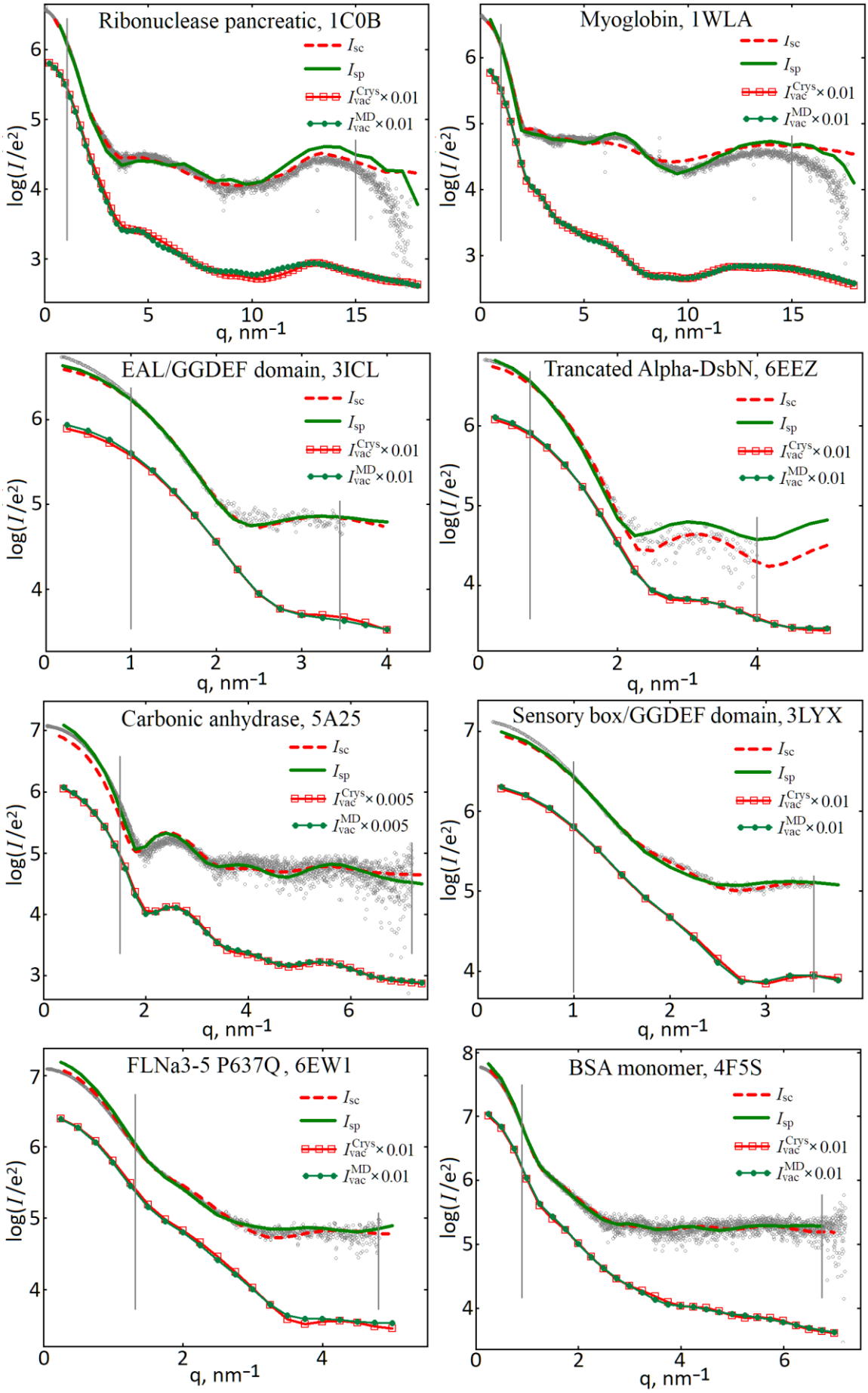
Curves for all considered proteins are presented in Fig. 1s.




Ribonuclease pancreatic, 1C0B
Myoglobin, 1WLA
EAL/GGDEF domain, 3ICL
Trancated Alpha-DsbN, 6EEZ
Carbonic anhydrase, 5A25
Sensory box/GGDEF domain, 3LYX
FLNa3-5 P637Q, 6EW1
BSA monomer, 4F5S
I_{sc}
I_{sp}
$I_{vac}^{Crys}\times 0.01$
$I_{vac}^{MD}\times 0.01$
$I_{vac}^{Crys}\times 0.005$
$I_{vac}^{MD}\times 0.005$
log(I/e²)
q, nm⁻¹

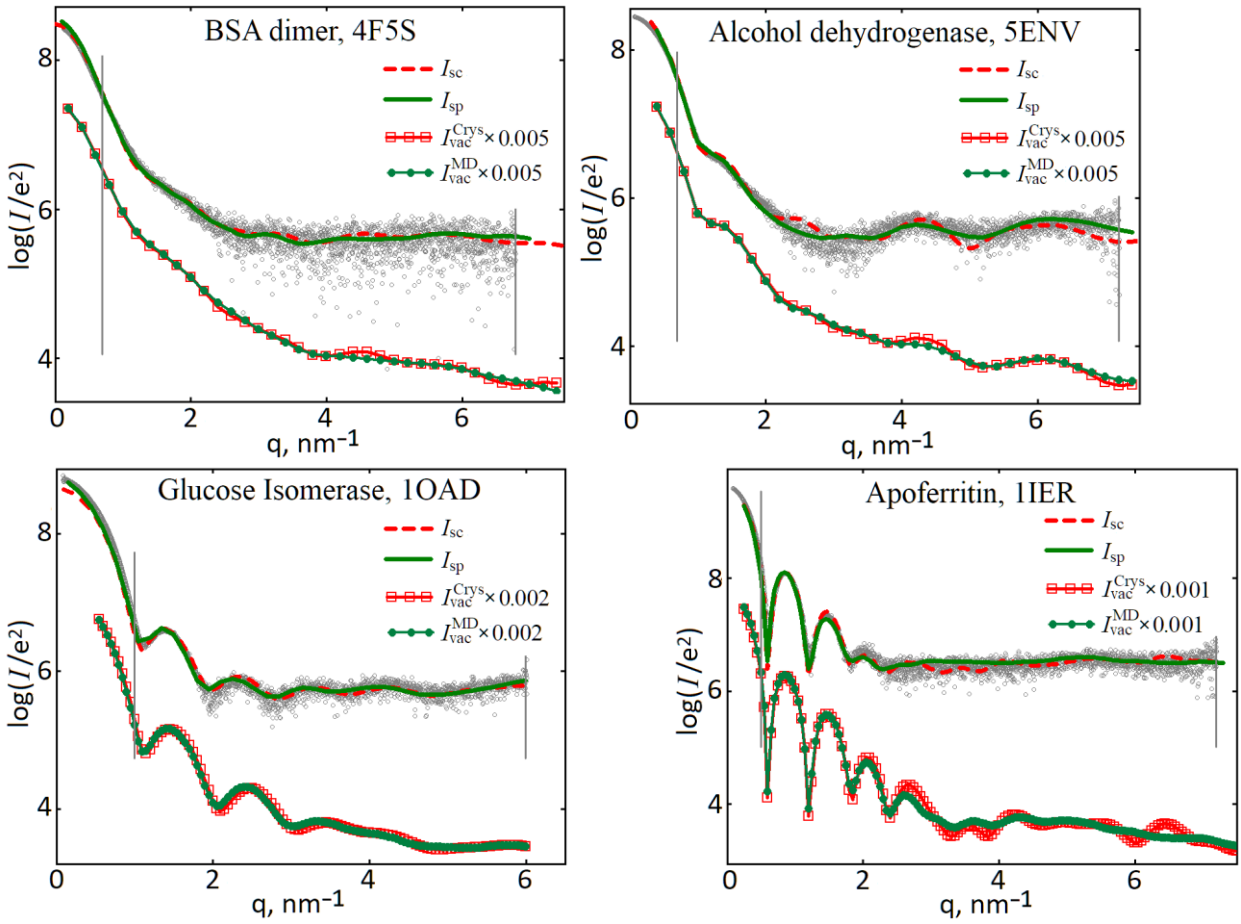


Fig. 1s. Experimental and calculated scattering curves for 18 considered proteins. Experimental curves: $I_{exp}(q)$ (circles); calculated curves: $I_{sp}(q)$ are the SASPAR curves; $I_{sc}(q)$ are the SASCUBE curves; $I_{vac}^{MD}(q)$ are the «vacuum curves» averaged for all MD simulation frames; $I_{vac}^{Crys}(q)$ are the «vacuum curves» for proteins in crystalline form. Hereinafter, the experimental curves were shifted in a logarithmic scale, using a scale factor, to align them with the calculated curves. For each protein, its name and its PDB code are given. The vertical lines mark the boundaries of the region where the calculated and experimental curves are compared.

It makes sense to compare the scattering curves obtained with the SASPAR program with the curves calculated using only the programs where: first, the solvent is taken into account explicitly based on MD, and, second, no additional parameters are introduced into the structural model of the scattering system. Therefore, when calculating scattering curves, the closest analogue to SASPAR is the program used on the WAXSIS server. Fig.2s shows the experimental scattering curve of the BSA monomer and the curves calculated with SASPAR and WAXSIS programs. As can be seen, the scattering curves are fairly close to each other and describe the experimental scattering curve equally well.

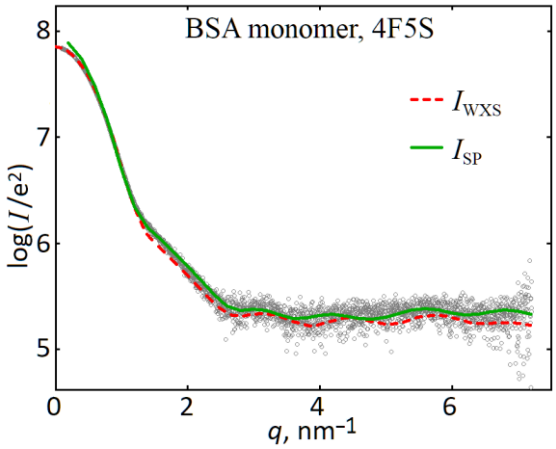


Fig. 2s. The experimental scattering curve (circles) of the BSA monomer and curves I_{SP}, I_{WXS} calculated with SASPAR and WAXSIS programs, respectively.

The scattering curves calculations for all single-domain proteins were made with the MD program Desmond, and for multi-domain proteins, the MD software package Gromacs 2019-3 was used. It is interesting to reveal how the choice of an MD program affects the scattering curves of proteins. The SASPAR curves for the proteins 6LYZ and 1UBQ calculated with both programs are shown in Fig. 3s. As seen in the figures, the SASPAR curves are rather similar for each protein, and the small discrepancies in the wide-angle range are within the limits of an experimental error. Values χ_{log} obtained by the formula similar to formula (6) are: χ_{log} = 2.3% (6LYZ), χ_{log} = 2.0% (1UBQ), and the entire region of the scattering curves shown in the graph was used to obtain these values.

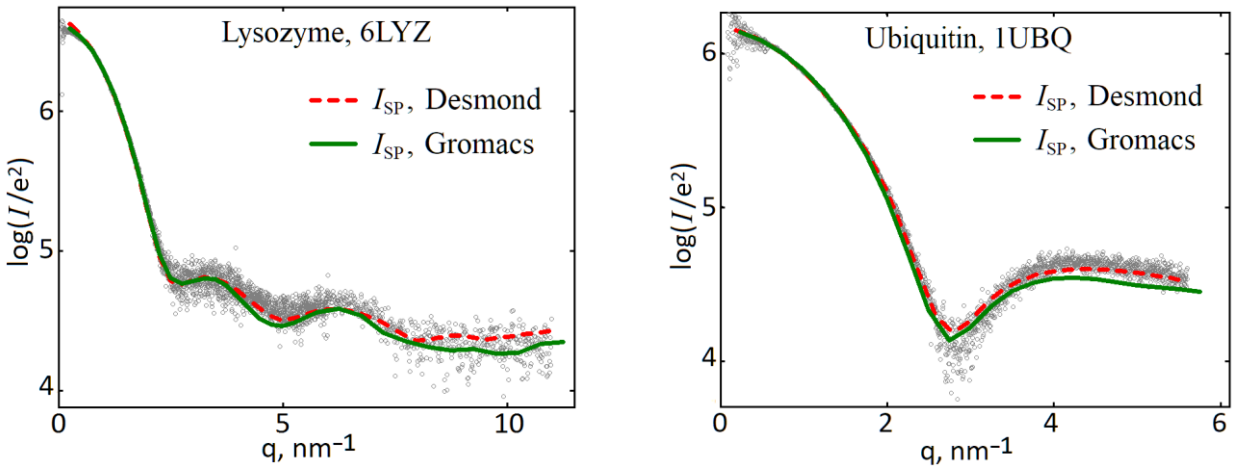


Fig. 3s. Comparison of the MD-based SASPAR curves $I_{sp}(q)$ obtained with Desmond and Gromacs programs for two proteins.