

Supplementary material

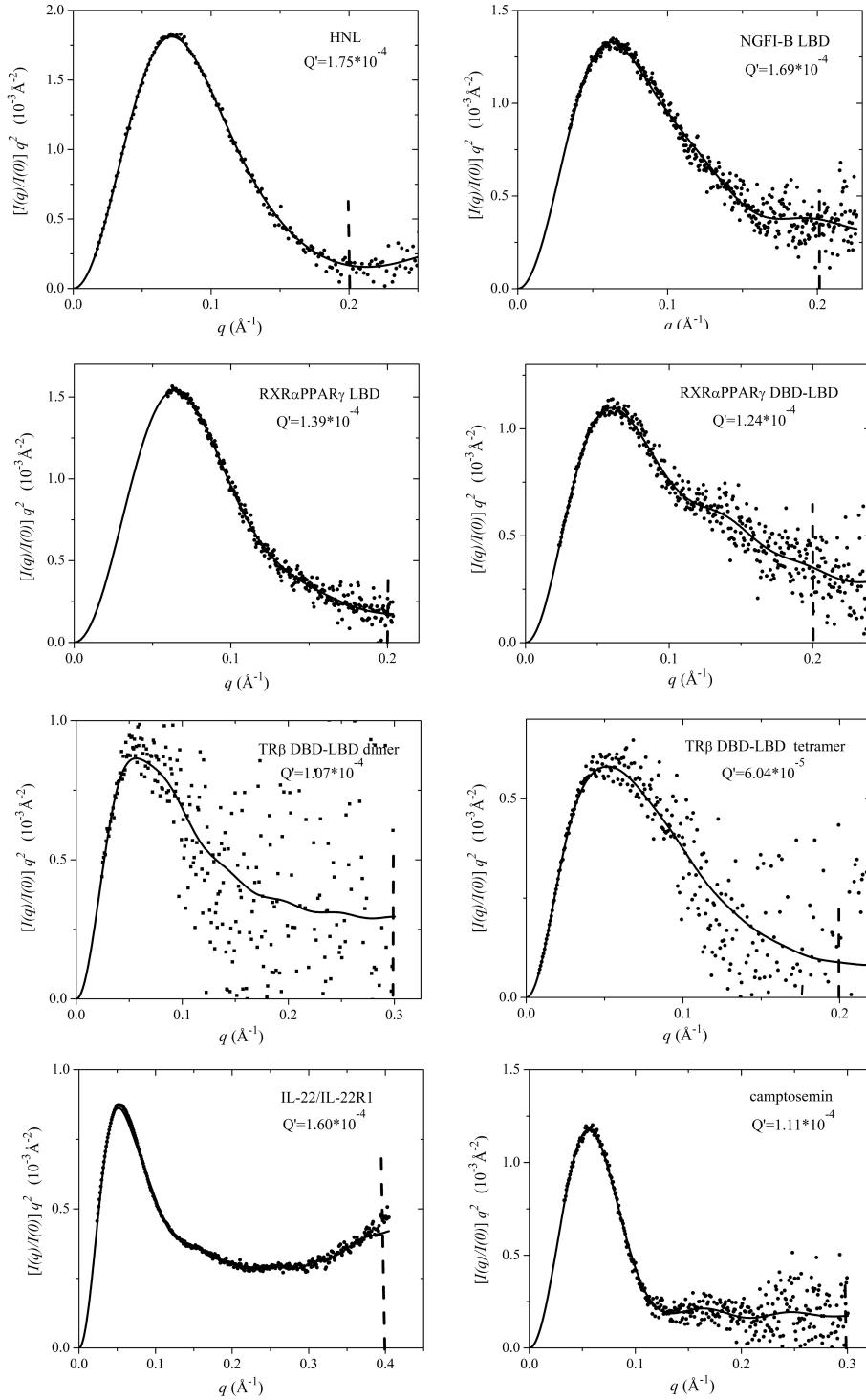


Figure SM1 Kratky plot calculated for several proteins of the Table SM1. The truncated invariant Q'

is reported. Dash line indicates the q_{\max} used to integration $Q' = \int_0^{q_{\max}} I(q)q^2 dq$ (6).

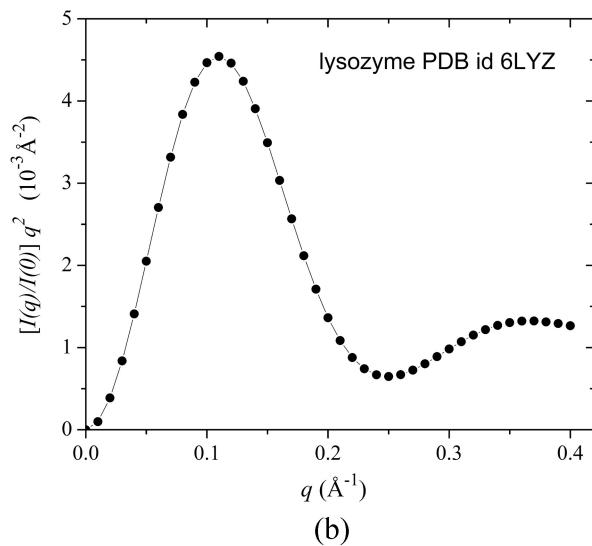
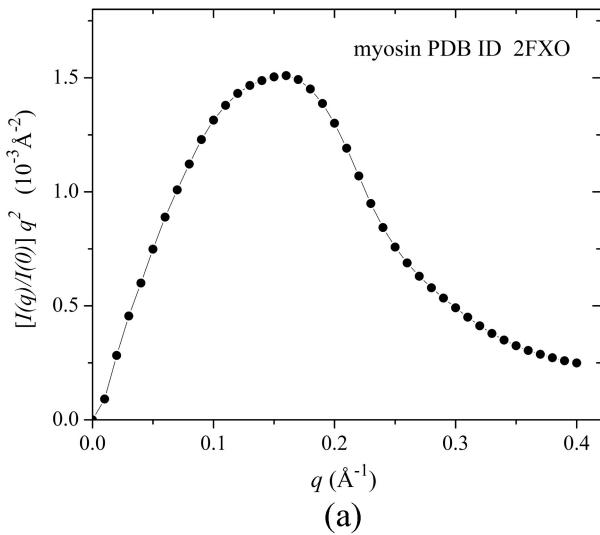


Figure SM2 Technical limitations of the proposed method were analyzed using two extreme cases: (a) an extremely anisotropic and elongated protein, myosin (PDB id 2FXO), with a nominal molecular weight of 29.76 kDa and (b) a small globular protein, lysozyme (PDB id 6LYZ), with a nominal molecular weight of 14.60 kDa. The Kratky plots were obtained from simulated SAXS curves calculated by CRYSTAL (Svergun *et al.*, 1995) and plotted in the range of $0 \text{ Å}^{-1} < q < 0.4 \text{ Å}^{-1}$.

Table SM1 Molecular weights calculated from data of a single SAXS curve for a number of different proteins. n=1, 2, ... refer to monomer, dimer, etc. The last column reports the modulus of the relative discrepancy between the molecular weights derived from SAXS results (oligomer MWSAXS) and the expected molecular weights (Oligomer MW).

Protein [#]	Reference	Monomer MW (kDa)	n	Oligomer MW (kDa)	q_{max} (A ⁻¹)	Oligomer MW _{SAXS} (kDa)	Discr. (%)
lysozyme	unpublished results	14.60	1	14.60	0.2	13.8	5.5
IL-22 dimer	Oliveira Neto <i>et al.</i> , 2008	16.84	2	33.68	0.3	32.1	4.7
LepFNR	Nascimento <i>et al.</i> , 2007	34.40	1	34.40	0.3	35.2	2.3
PPAR γ DBD-LBD	unpublished results	42.02	1	42.02	0.2	45.0	7.1
α Gal	Golubev <i>et al.</i> , 2004	48.76	1	48.76	0.2	52.5	7.7
NGFI-B LBD	Calgaro <i>et al.</i> , 2007	24.50	2	49.00	0.2	52.7	7.6
HNL	Unpublished results	27.10	2	54.20	0.3	51.7	4.6
RXR α /PPAR γ LBD	Unpublished results	30.18/32.08	2	62.26	0.2	66.3	6.5
DM43	Neves-Ferreira <i>et al.</i> , 2002	32.39	2	64.78	0.3	63.9	1.4
BSA	unpublished results	66.00	1	66.00	0.3	61.6	6.7
IL-22 tetramer	Oliveira Neto <i>et al.</i> , 2008	16.84	4	67.36	0.3	64.3	4.5
PSK-2	Cabrera <i>et al.</i> , 2007	34.00	2	68.00	0.2	74.5	9.9
RXR α /PPAR γ DBD-LBD	unpublished results	37.45/42.02	2	79.47	0.2	74.5	6.3
IL-22/IL-22R1	Oliveira Neto <i>et al.</i> , 2008	39.95	2	79.90	0.4	73.9	7.5
TR β DBD-LBD dimer	Figueira <i>et al.</i> , 2007	41.20	2	82.40	0.3	74.9	9.1
camposemin	unpublished results	25.97	4	103.88	0.3	96.4	7.2
PEPCK	Trapani <i>et al.</i> , 2001	58.00	2	116.00	0.2	114.9	0.9
PFK-2 with ATP	Cabrera <i>et al.</i> , 2007	34.00	4	136.00	0.4	129.3	4.9
deacetylase	Ferreira <i>et al.</i> , 2006	41.00	4	164.00	0.4	167.1	1.9
TR β DBD-LBD tetramer	Figueira <i>et al.</i> , 2007	41.20	4	164.80	0.2	160.7	2.5
THI1	Godoi <i>et al.</i> , 2006	26.70	8	213.60	0.3	218.2	2.2

#Abbreviations : lysozyme – chicken egg white lysozyme; IL-22 – human interleukin-22; LepFNR – ferredoxin reductase from *Leptospira interrogans*; PPAR γ DBD-LBD – DNA and ligand binding domains of human peroxisome proliferator-activated receptor isoform γ ; α Gal – α -galactosidase from *Trichoderma reesei*; NGFI-B LBD – ligand binding domain of human nerve growth factor isotype B; HNL – hydroxynitrile-lyase from *Xylella fastidiosa*; RXR α /PPAR γ LBD – ligand binding domain of complex human retinoid X receptor isoform α with human peroxisome proliferator-activated receptor isoform γ ; DM43 – snake venom metalloproteinase inhibitor from *Didelphis marsupialis* serum; BSA – bovine serum albumin;

PFK-2 - *Escherichia coli* phosphofructokinase-2; RXR α /PPAR γ DBD-LBD – DNA and ligand binding domains of complex human retinoid X receptor isoform α with human peroxisome proliferator-activated receptor isoform γ ; IL-22/IL-22R1 – complex of human interleukin-22 and interleukin-22 receptor; TR β DBD-LBD dimer – human thyroid receptor isoform β construct containing DNA binding domain and ligand binding domain; camptosemin – camptosemin from mature *Cynanchum ellipticum*; PEPCK – phosphoenolpyruvate carboxykinase from *Trypanosoma cruzi*; PFK-2 with ATP – phosphofructokinase-2 from *Escherichia coli* with adenosine triphosphate; Deacetylase – N-acetylglucosamine-6-phosphate deacetylase apoenzyme from *Escherichia coli*; TR β DBD-LBD tetramer – a tetramer of human thyroid receptor isoform β construct containing both DNA binding and ligand binding domains; THI1 – thiazole biosynthetic enzyme from *Arabidopsis thaliana*.

Table SM2 Structural parameters Q' , V' , V and MW and relative discrepancy from myosin (PDB id 2FXO) obtained from simulated SAXS curve to different q_{\max} by CRYSTAL (Svergun *et al.*, 1995), relative discrepancy is taken in comparison with its known molecular weight (29.76 kDa).

myosin	0.1 (\AA^{-1})	0.2 (\AA^{-1})	0.3 (\AA^{-1})	0.4 (\AA^{-1})
Q' (\AA^{-3})	7.08x10 ⁻⁵	2.15x10 ⁻⁴	2.96x10 ⁻⁴	3.30x10 ⁻⁴
V' (\AA^3)	279000	91800	66600	59700
V (\AA^3)	162429	48412	39328	42210
MW_{SAXS} (kDa)	134.9	40.2	32.7	35.0
($\rho_m = 1.37 \text{ g/cm}^3$)				
Relative discrepancy(%)	353.3	35.1	9.9	17.6

Table SM3 Structural parameters Q' , V' , V and MW and relative discrepancy for lysozyme (PDB id 6LYZ) obtained from simulated SAXS curve by CRYSTAL (Svergun *et al.*, 1995), relative discrepancy is taken in comparison with its known molecular weight (14.60 kDa).

lysozyme	0.1 (\AA^{-1})	0.2 (\AA^{-1})	0.3 (\AA^{-1})	0.4 (\AA^{-1})
Q' (\AA^{-3})	2.11x10 ⁻⁴	5.41x10 ⁻⁴	6.24x10 ⁻⁴	7.48x10 ⁻⁴
V' (\AA^3)	93500	36500	31600	26400
V (\AA^3)	49456	14664	15554	16545
MW_{SAXS} (kDa)	41.1	12.2	12.9	13.7
($\rho_m = 1.37 \text{ g/cm}^3$)				
Relative discrepancy(%)	187.0	14.8	9.9	4.3