

SUPPORTING INFORMATION

Light-Induced Subunit Dissociation by a LOV domain Photoreceptor from
Rhodobacter sphaeroides

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Table S1. Structural and refinement statistics for RsLOV crystallographic data of the dark and light state structures and L32V and A138Y dark state variant structures.

	Dark ₁	Dark ₂	Light	L32V variant	A138Y Variant
Data Collection					
Space group	P 2 ₁ 2 ₁ 2 ₁	P 6 ₅	P 6 ₅	P 2 ₁ 2 ₁ 2 ₁	P 6 ₅
a, b, c (Å)	65.8, 70.5, 74.4	108.1, 108.1, 84.6	109.4, 109.4, 85.5	54.4, 73.2, 95.3	105.9, 105.9, 84.1
Unique reflections	9886	28665	21851	28265	15712
Resolution (Å)	2.70	2.20	2.34	1.95	2.64
Last shell (Å)	2.70 – 2.75	2.20 – 2.24	2.34 – 2.38	1.95 – 1.98	2.64 – 2.69
Redundancy (overall/last shell)	3.7/3.1	11.3/10.5	3.6/3.4	13.8/9.7	10.7/9.6
Completeness (%/last shell)	99.8/99.2	100.0/100.0	88.7/93.1	99.6/90.9	99.8/100.0
I/σ (overall/last shell)	31.1/4.5	52.7/4.0	21.7/3.1	30.5/4.6	46.0/5.3
Linear R-fac (R _{merge}) (overall/last shell)	0.107/0.36 6	0.079/0.58 5	0.115/0.50 7	0.092/0.395	0.075/0.51 1
Refinement					
R _{work} (%)	0.193	0.207	0.204	0.173	0.191
R _{free} (%)	0.251	0.226	0.244	0.201	0.240
No. atoms	2791	2870	2885	3150	2872
No. water molecules	2	63	80	332	41
Mean B value	57.4	59.1	37.2	22.6	38.8
B value (waters)	49.4	59.0	29.0	28.5	28.9
B value (ligands/ions)	49.2	51.9	28.35	20.3	22.1
RMSD from ideal bond lengths (Å)	0.008	0.008	0.008	0.007	0.008
RMSD from ideal bond angles (°)	1.2	1.2	1.3	1.1	1.4
Ramachandran statistics (%)					
Most favored	88.0	91.7	90.1	94.7	89.4
Additionally Allowed	11.7	7.6	9.6	4.6	9.3
Generously Allowed	0.3	0.7	0.3	0.7	1.3
Disallowed	0.0	0.0	0.0	0.0	0.0
PDB entry	4HJ4	4HJ6	4HNB	4HIA	4HJ3

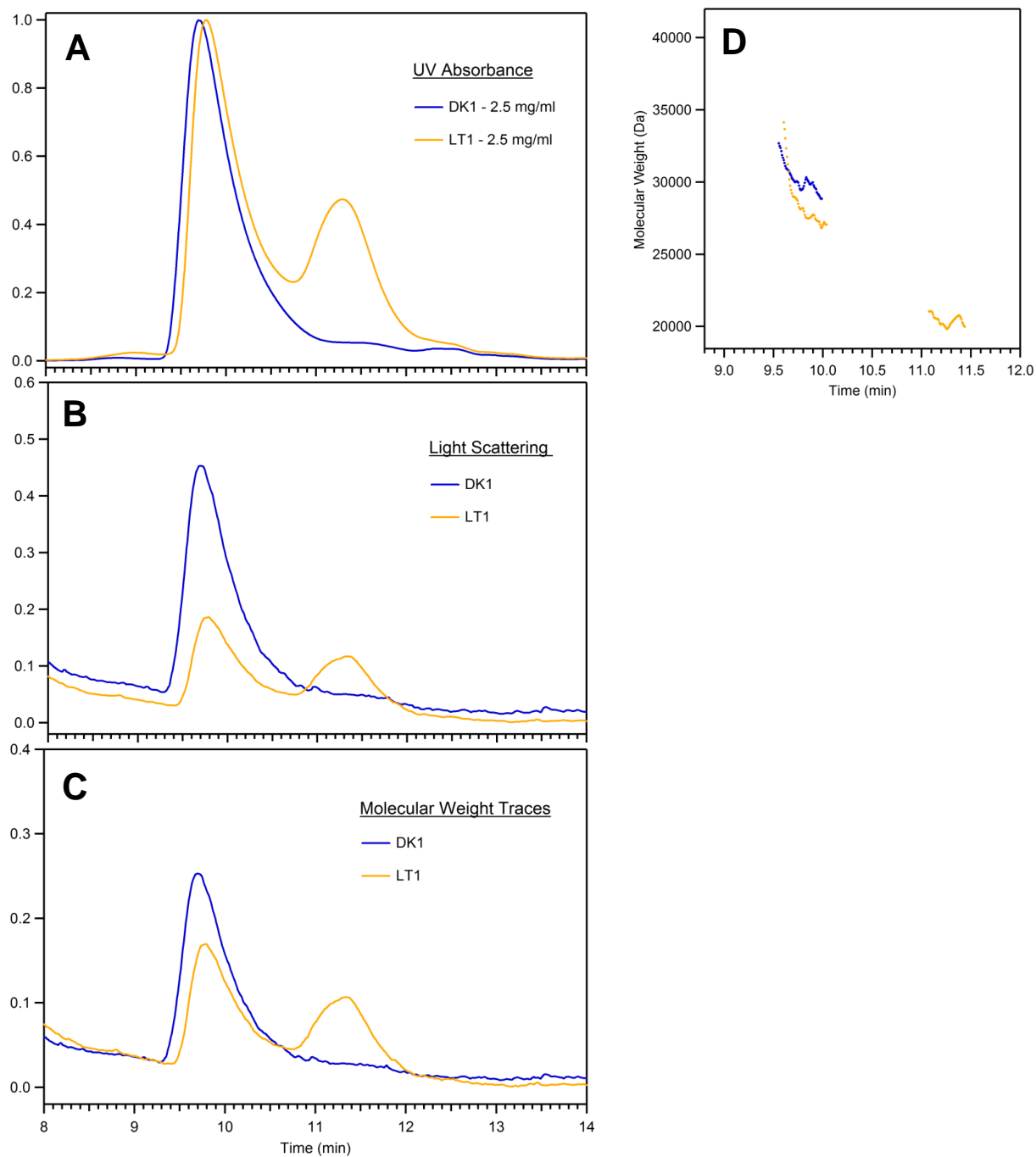


Figure S1. Data obtained by SEC-MALS, dark state samples in blue, light state samples in red/orange (A) UV Absorbance (B) Light Scattering (C) Molecular weight traces (D) Molecular weight timepoints. Samples were run in the following order: LT then DK.

Table S2. Molecular weight data obtained by SEC-MALS.

Sample	Concentration (mg/mL)	Time (min)	Peak 1: MW (kDa)	Peak 2: MW (kDa)
Light 2.5 mg/mL	2.5	20	28.2	20.4
Dark 2.5 mg/mL	2.5	110	30.2	---

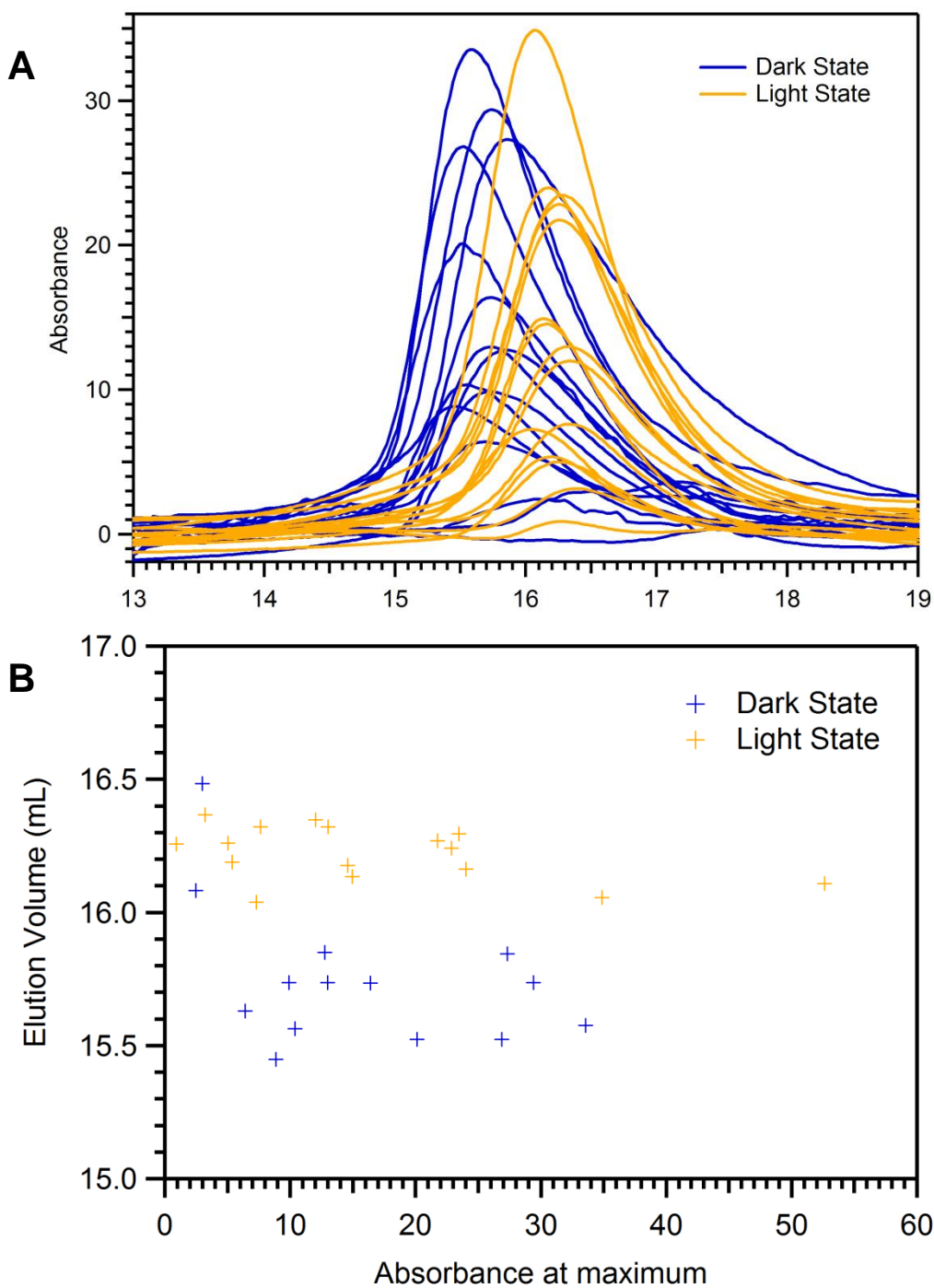


Figure S2. Data obtained by analytical SEC: dark state samples in blue, light state samples in orange (A) UV Absorbance (B) Elution volume at maximum absorbance at 280 nm for 30 samples.

Table S3. SAXS data generated from GNOM and shape reconstruction statistics using ATSAS suite.

State, concentration (mg/mL)	Reciprocal space: R _g	Real space: R _g	s _{min}	sR _g limits	I(0)	D _{max}	NSD DAMAVER (var) 10 models	MW (kDa)	Total estimate
LT, 2.5	20.87	20.91 ± 0.13	0.0098	0.55 – 1.38	48.59 ± 0.25	65.36	0.548 ± 0.021	27.8	0.889
LT, 5	21.84	21.86 ± 0.06	0.0098	0.38 – 1.03	90.51 ± 0.24	67.99	0.537 ± 0.016	30.8	0.827
LT, 10	23.47	23.54 ± 0.21	0.0098	0.42 – 1.28	150.70 ± 0.67	93.88	0.586 ± 0.027	34.2	0.685
DK, 2.5	21.94	21.99 ± 0.16	0.0098	0.52 – 1.30	57.10 ± 0.34	74.40	0.563 ± 0.030	31.4	0.844
DK, 5	23.24	23.27 ± 0.10	0.0098	0.45 – 1.17	105.21 ± 0.21	76.02	0.583 ± 0.053	40.3	0.869
DK, 10	24.39	24.41 ± 0.04	0.0098	0.45 – 1.26	172.64 ± 0.28	75.69	0.558 ± 0.019	42.9	0.715

$$s = 4\pi\sin(\theta)/\lambda$$

2θ = scattering angle

λ = radiation wavelength

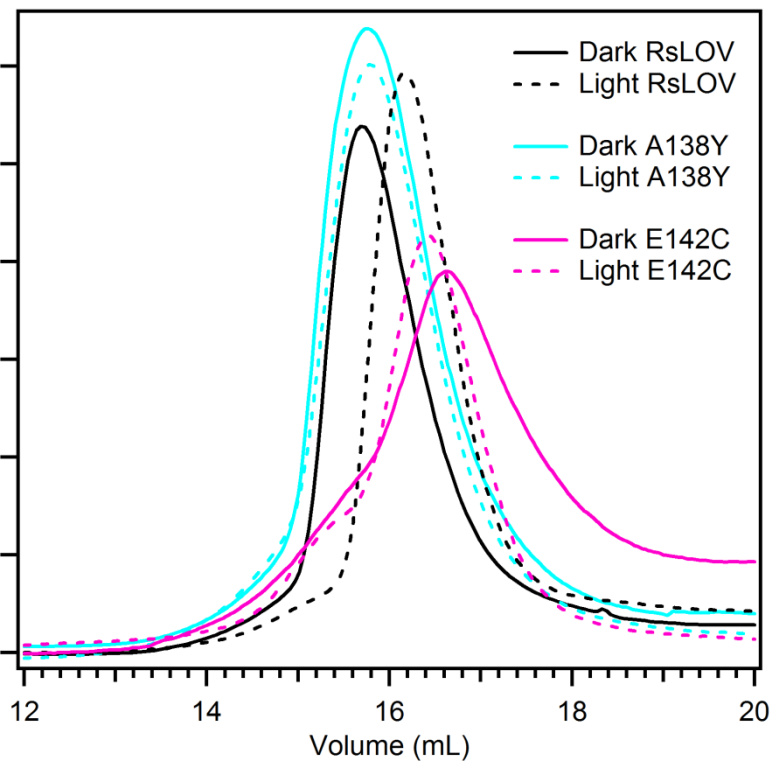
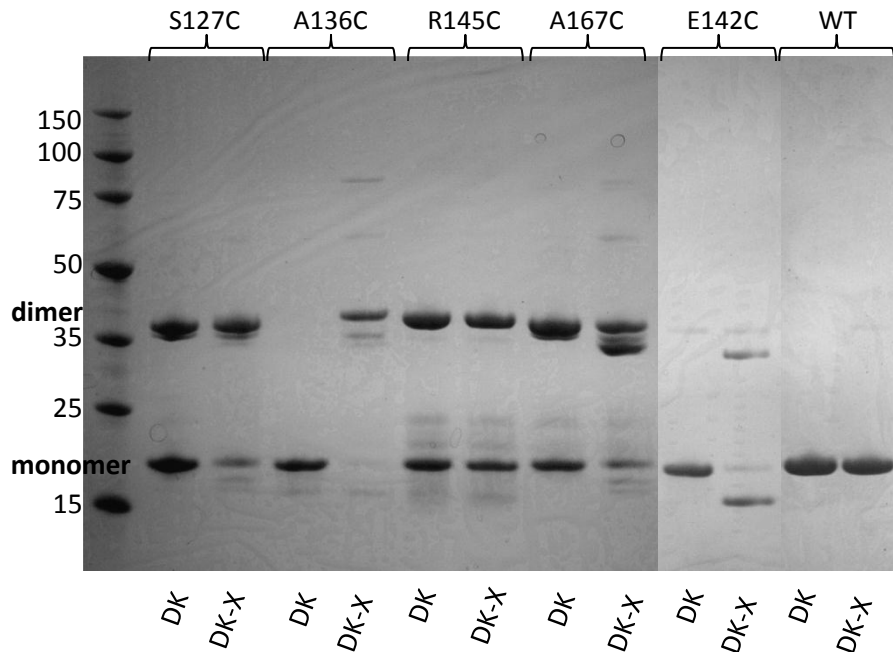


Figure S3. (A) SDS PAGE gel of variants S127C, A136C, R145C, E142C, and WT RsLOV in the dark, DK, and in the dark with addition of Cu(phen)₃ as crosslinking agent, DK-X. (B) Data obtained by analytical SEC: dark state samples in solid line, light state samples dashed: WT RsLOV (black), A138Y (aqua), E142C (pink).

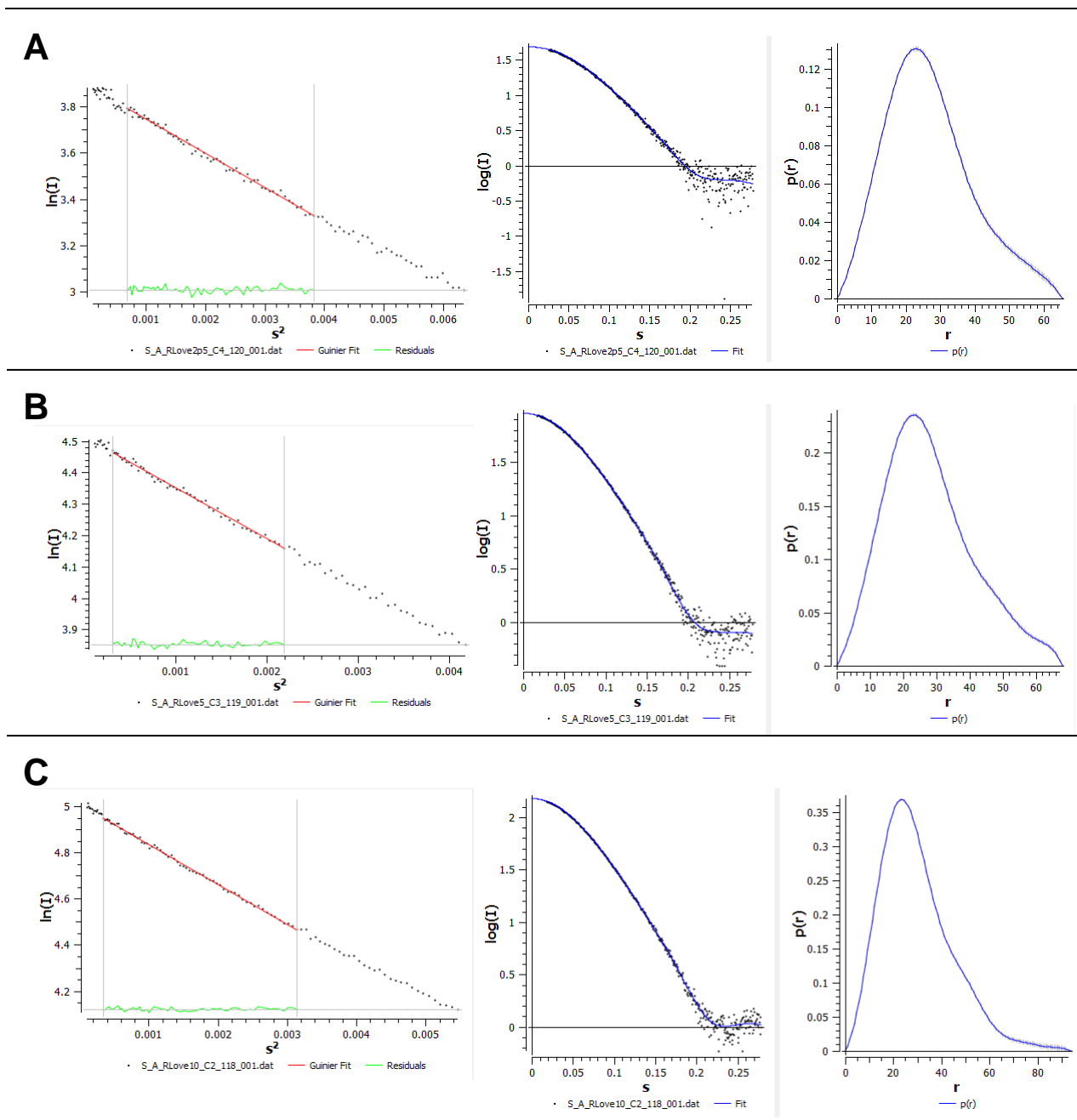


Figure S4. Data obtained by SAXS, light state samples of RsLOV (A) 2.5 mg/mL (B) 5.0 mg/mL (C) 10.0 mg/mL. Plots from left to right: Guinier plot, $\ln(I)$ vs s^2 (left), $\log(I)$ vs s (middle), $P(r)$ vs r (right).

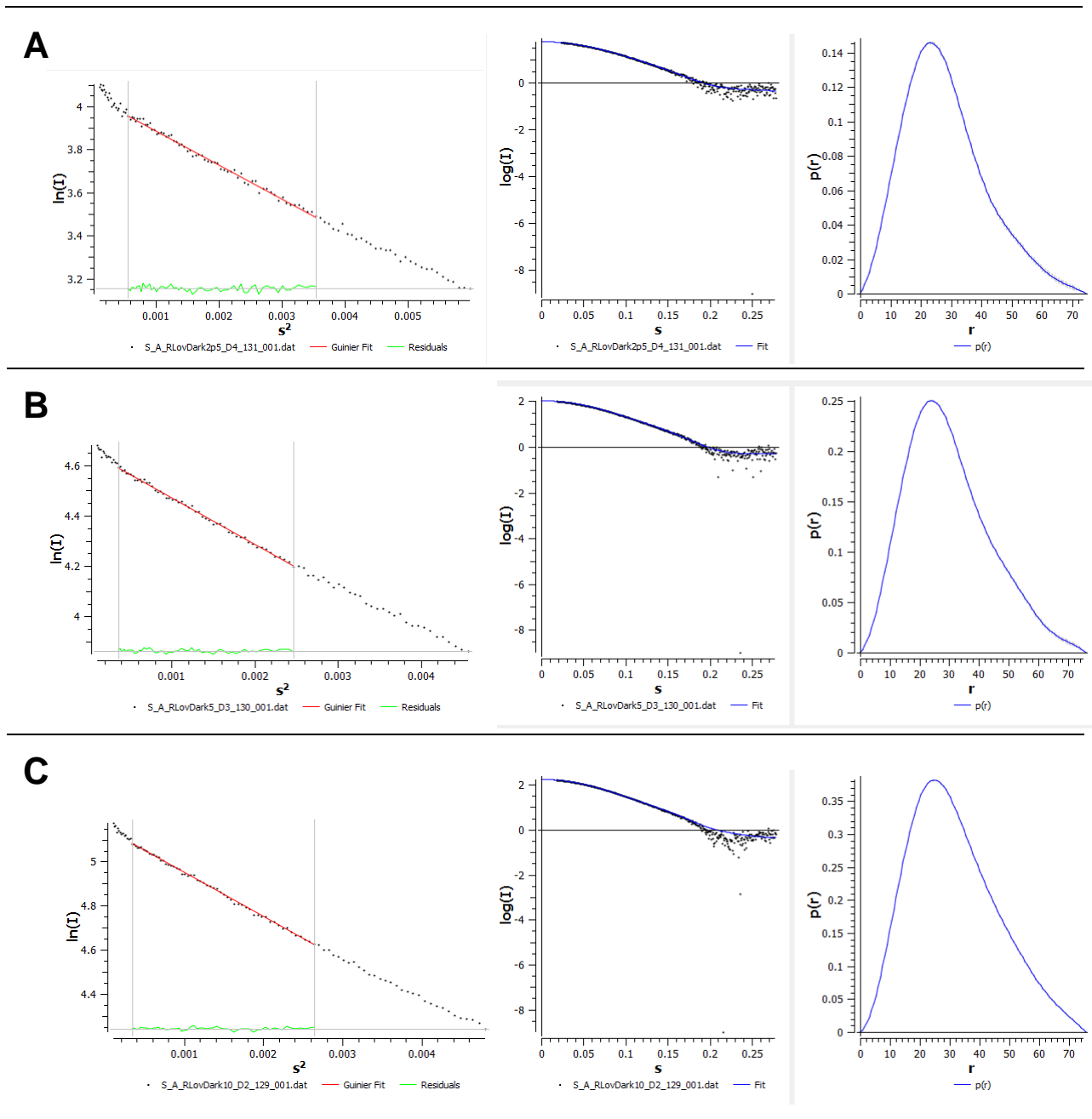


Figure S5. Data obtained by SAXS, dark state samples of RsLOV (A) 2.5 mg/mL (B) 5.0 mg/mL (C) 10.0 mg/mL. Plots from left to right: Guinier plot, $\ln(I)$ vs s^2 (left), $\log(I)$ vs s (middle), $P(r)$ vs r (right).