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I. Lifson Roig Calculations

1.. Justification for Defining the Length of the Amino Acid Sequence for Peptides 1K. 2K, 3K as 22 The GGG end sequences of 1K, 2K, & 3K prevent helices from extending into the end regions, effectively decoupling the helical core peptide region from the capping residues, which are expected to contribute minimally to the CD minimum at 222 nm. For this reason we have defined an effective peptide length of 22 residues in calculating mean residue ellipticities of Figure 7 of the text and in calculating the mean residue ellipticities of Figures 5 & 6 from experimental molar ellipticities. A quantitative justification is available through a L-R fh calculation. Using either the Doig et al.1995 wg value of 0.05 or our value of 0.3 we calculate equivalent fh values for the full peptide sequence $YKG_2A_4KA_4KA_4KA_3G_3.K\text{-}NH_2$ of 3K and for the truncated sequence $G_2A_4KA_4KA_4KA_3G_2$ as fh = 0.596 and 0.595, respectively. This result also shows that the Doig coefficients for the Y and terminal K make an insignificant contribution to fh.

2. .**Calibration of the L-R Helicity Calculation** As shown in Table I we checked our L-R algorithm by calculating fractional helicities for four peptides for which fh values were reported by Doig and Baldwin 1995 as calculated from experimental mean residue ellipticities. (Literature calculated values of fh were not available for comparison.).

Table I Calibration of the Doig L-R algorithm used in the Text

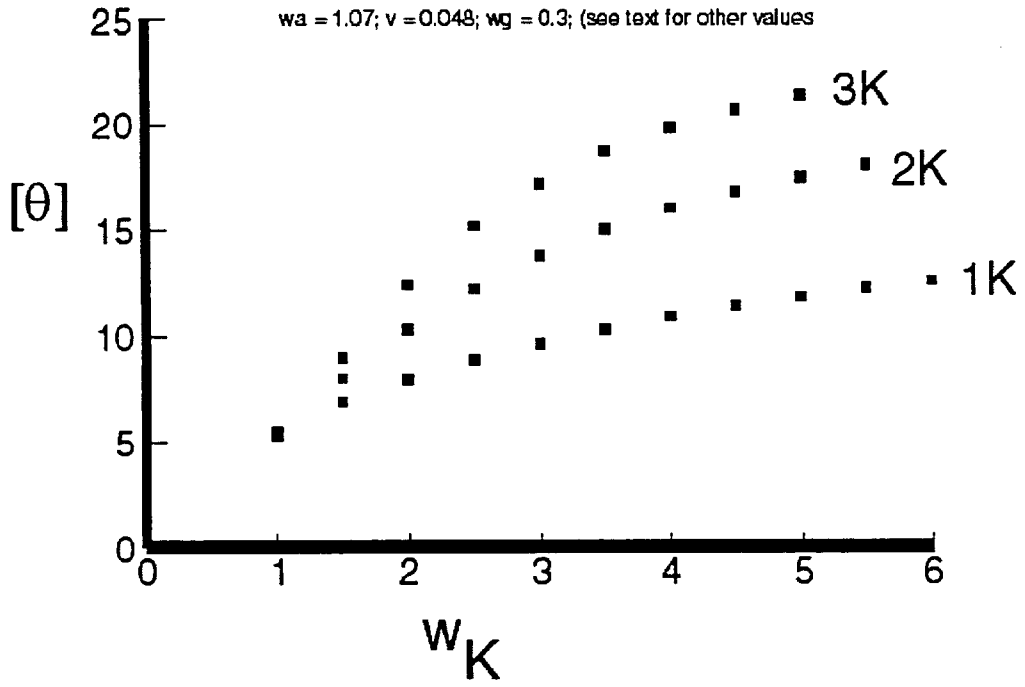
Peptide Sequence	Reptd Fract Hel	Calc Fract Hel
$Ac\text{-}YG_2KA_4KA_4KA_4K\text{-}NH_2$	0.68	0.64
$Ac\text{-}YG_2KA_4KA_4KA_2GAK\text{-}NH_2$	0.465	0.45
$Ac\text{-}YG_2KA_4KA_2GAKA_4K\text{-}NH_2$	0.27	0.23
$Ac\text{-}YG_2KA_2GAKA_4KA_4K\text{-}NH_2$	0.37	0.33

A linear regression of reported and calculated values gives an intercept of 0.037 and a slope of 0.99, showing satisfactory agreement.

3. Calculation of fh and [θ] using wa, wg, and wk Values of Renold, et al. 1996 The term values given in a. were used, except that wa, = 1.07, wg = 0.3 (the mean of the value ranges reported in Kemp, D.S.; Boyd, J.G.; Muendel, C.C., *Nature*, 1991, *352*, 451-454 and in Kemp, D.S. and Tsang, K.Y., unpublished.), and wk = 3.7-4.2 for 3K and 4.2-5.0 for 1K & 2K. The latter

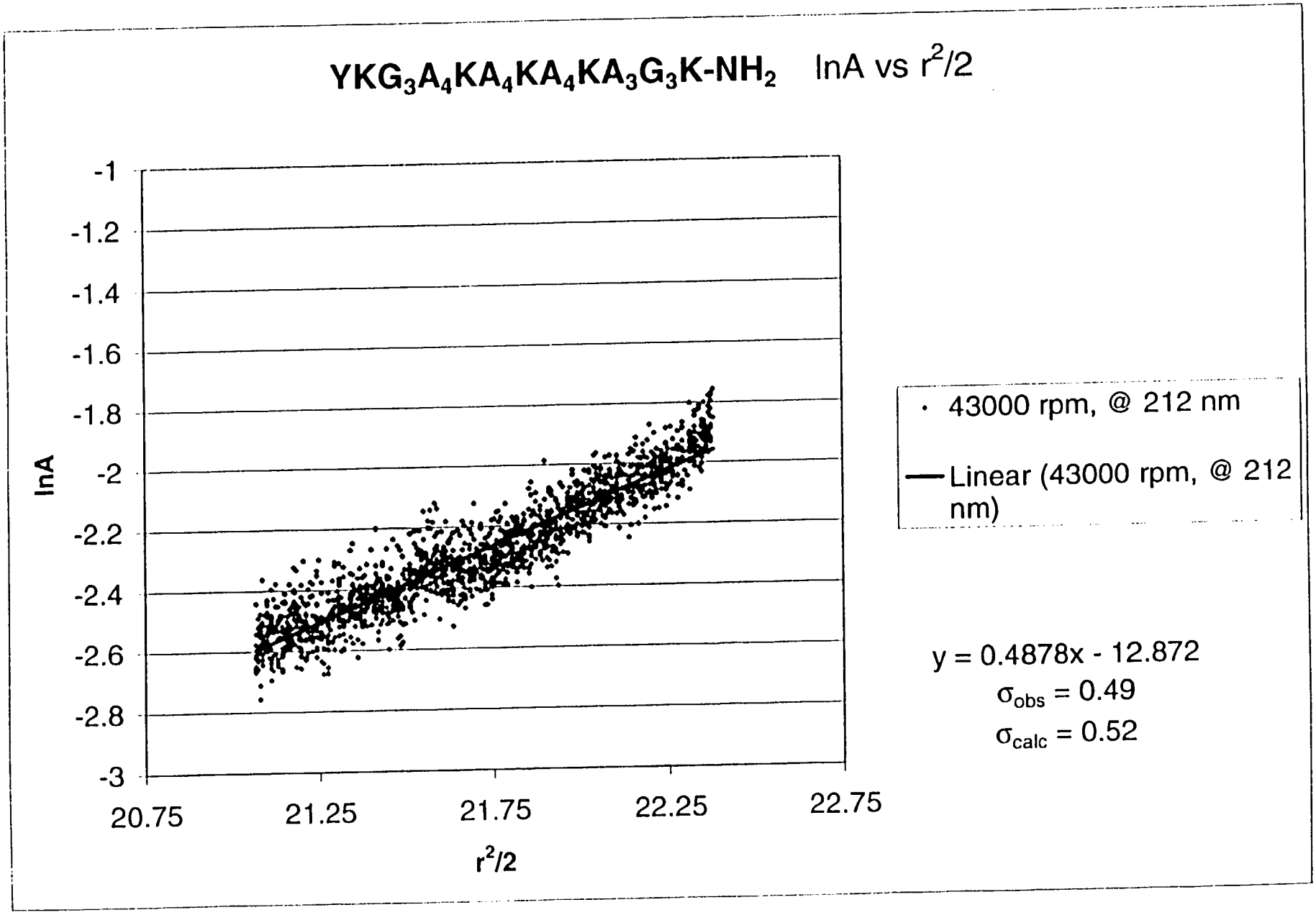
were obtained from the 2° C data of Renold, P., Tsang, K.Y., Shimizu, L.S., Kemp, D. S. J. Am.Chem.Soc., 1996, 118 12234-12235) and reflect the precision of the assignments as well as corrections for the N-templating effect. As seen in Figure 1 which graphs L-R-derived $[\theta]_{222}$ calc. as a function of wk for 3K, 2K, & 1K, in this region of w-space the cited variations in wk do not result in large changes in $[\theta]_{222}$.calc. It can also be shown that as expected, $[\theta]_{222}$ calc. is nearly independent of the n, c, & w values assigned to Y and G, provided they are varied within plausible limits. If the varying wk used in these calculations are replaced by an average <wk> = 3.9, values for assigned $[\theta]_{222}$ for 3K, 2K, 1K are respectively –19.7, –15.8, -10.8×10^3 deg-cm^2-dmol^{-1}, which may be compared with the experimental values of 2°C of –19.9, - 18.1, -9.1. The averaged <wk> value thus result in poorer agreement with experiment for the 2K case than is seen in figure 3B for length-dependent wk, consistent with our previous data (Renold et al. 1996) that demonstrates that two Lys show a measurable destabilizing interaction, even when separated by four Ala residues.

Figure 1 Lifson-Roig Modeling
of mean residue ellipticity as a function of w_K



II. **Ultracentrifugation Analyses**

The accompanying pages show plots of 1) plots of lnA vs $r^2/2$ for raw data (unaveraged over the 10 data sets collected at each radial position), 2) Raw data as collected from the cell, including end effects, presented as plots of A vs radial position r, 3) Plots of residuals for the lnA vs $r^2/2$ correlation. Included as text is the standard error of the linear regressin and the lower and upper 95 % confidence limits for the slopes. It should be noted that these define the precision of the analysis for each of the three peptides.

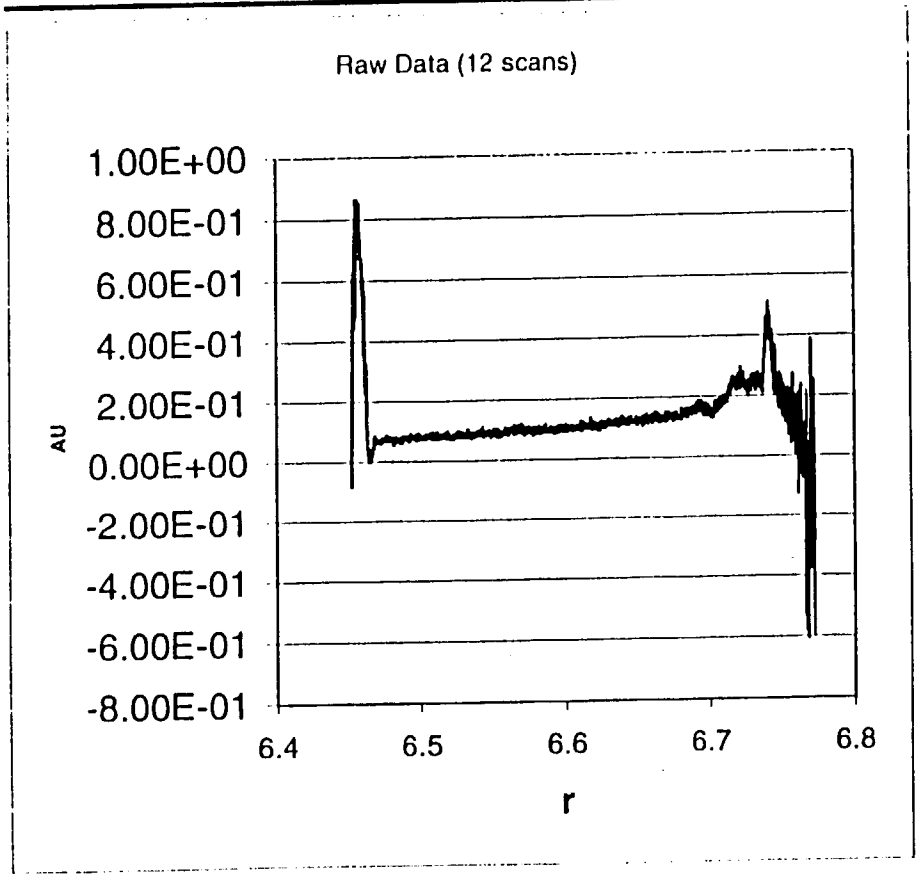


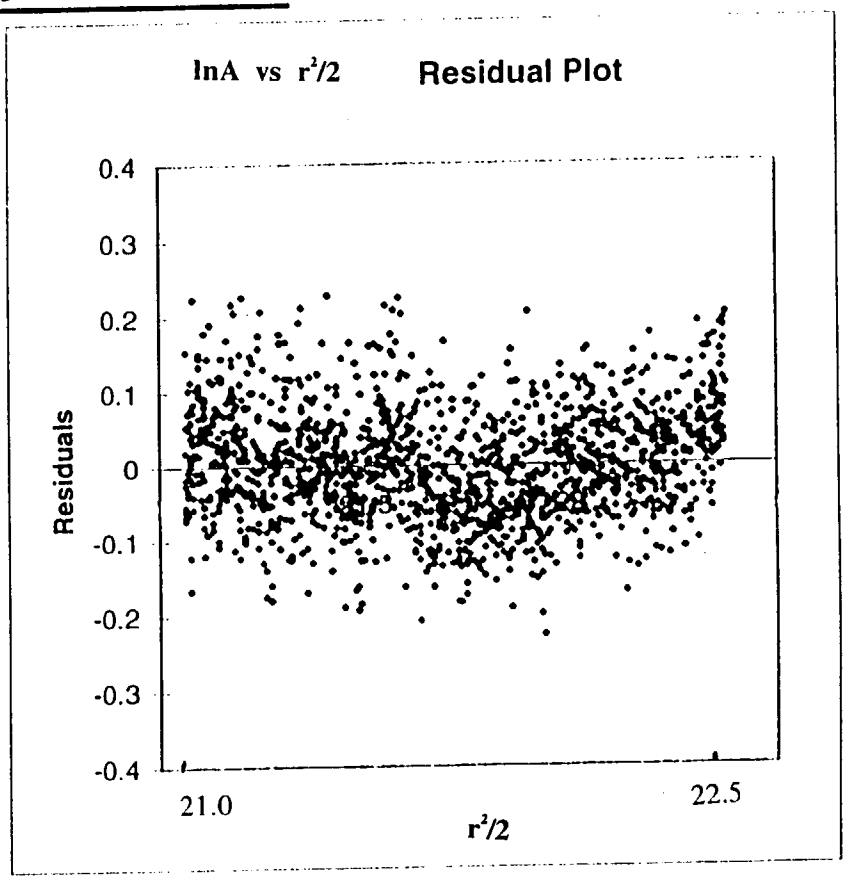
Sedimentation Equilibrium Data Analysis SUMMARY For $YKG_3A_4KA_4KA_4KA_3G_3K\text{-}NH_2$ (lnA vs $r^2/2$)

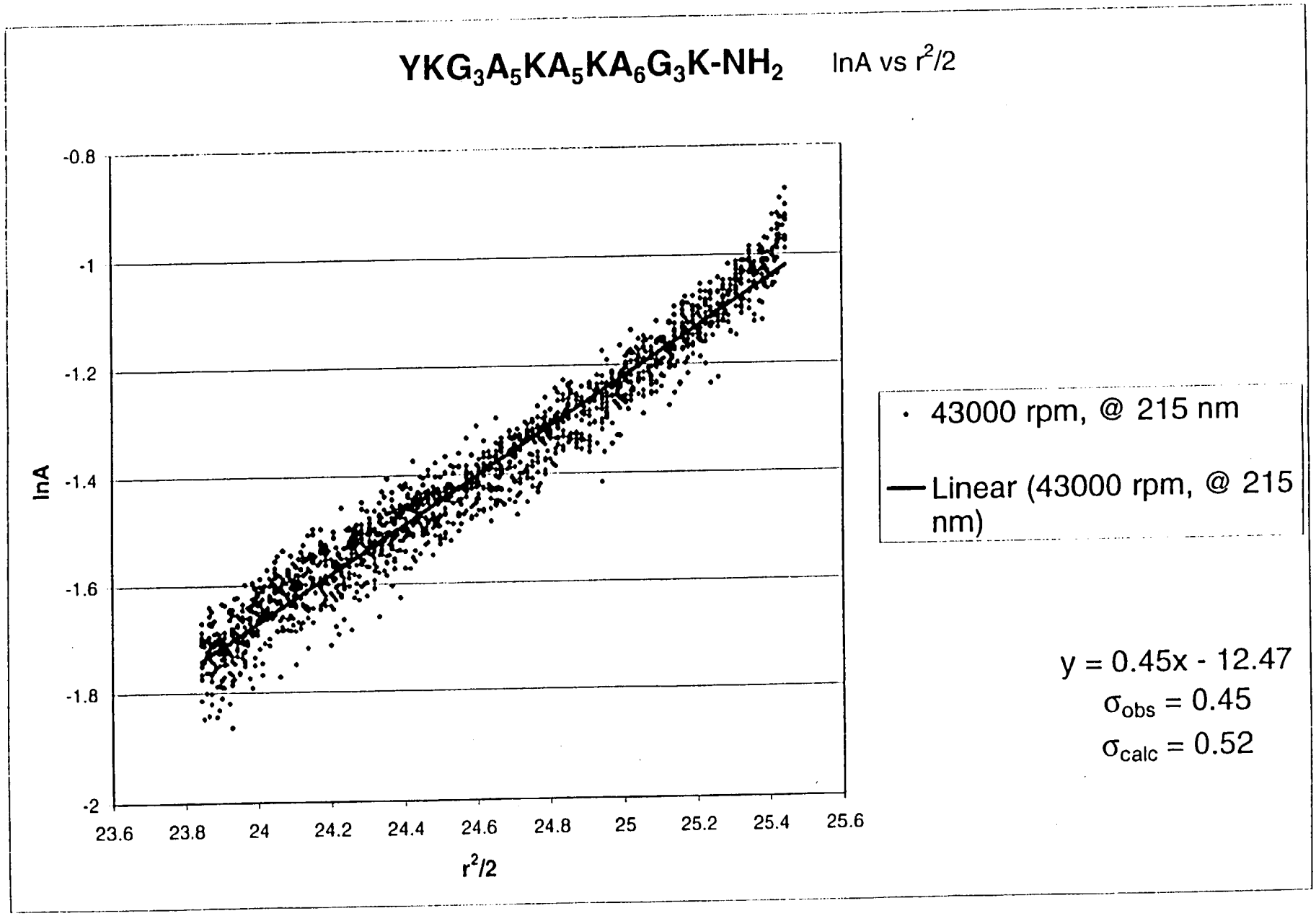
1520 data points, 2.2 μM solution, 43,000 rpm

σ_{obs} = 0.49 $Mw_{obs} = 2.1 \times 10^3$ σ_{calc} = 0.52 $Mw_{calc} = 2.2 \times 10^3$

	Coefficients	*Standard Error*	*Lower 95%*	*Upper 95.0%*
Intercept	-12.87172	0.109898	-13.08728	-12.65615
X Variable	0.487764	0.005062	0.477835	0.497693





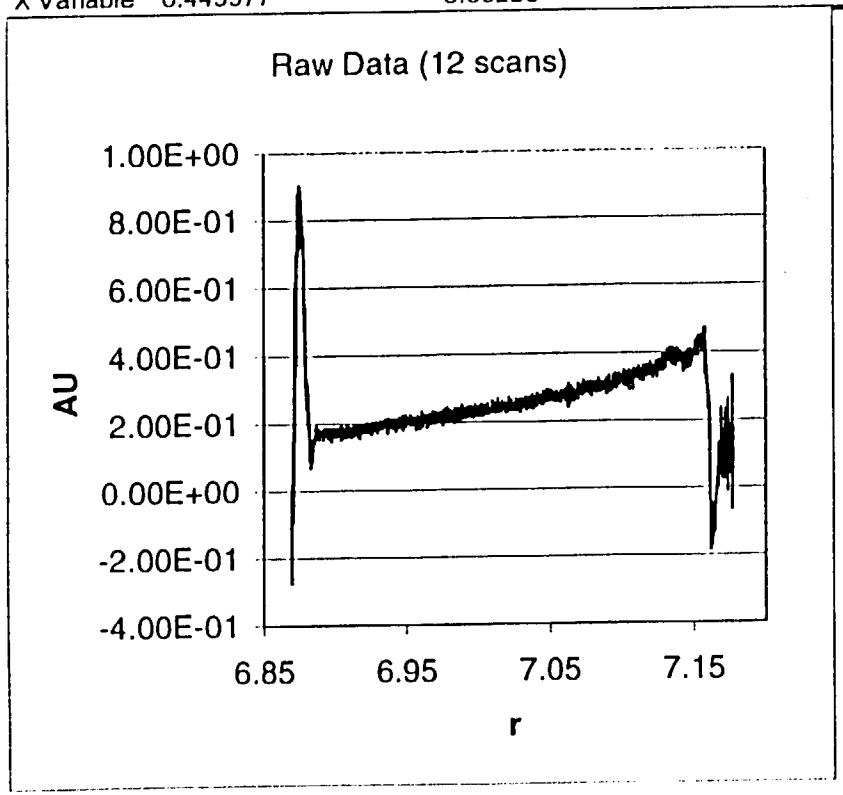


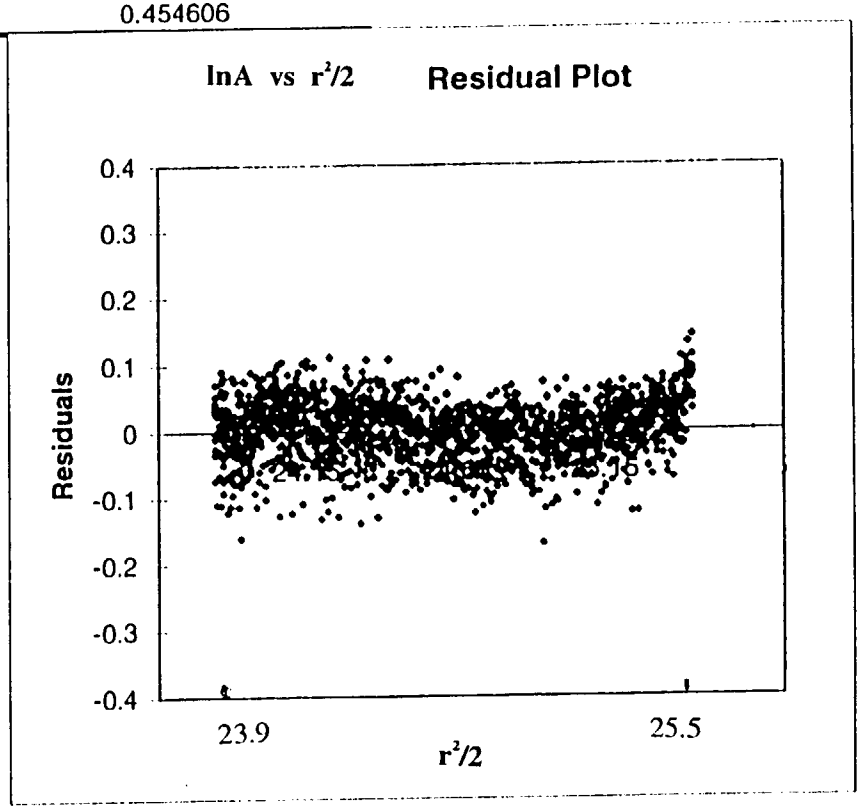
Sedimentation Equilibrium Data Anaylsis SUMMARY For $YKG_3A_5KA_5KA_6G_3K\text{-}NH_2$ (lnA vs $r^2/2$)

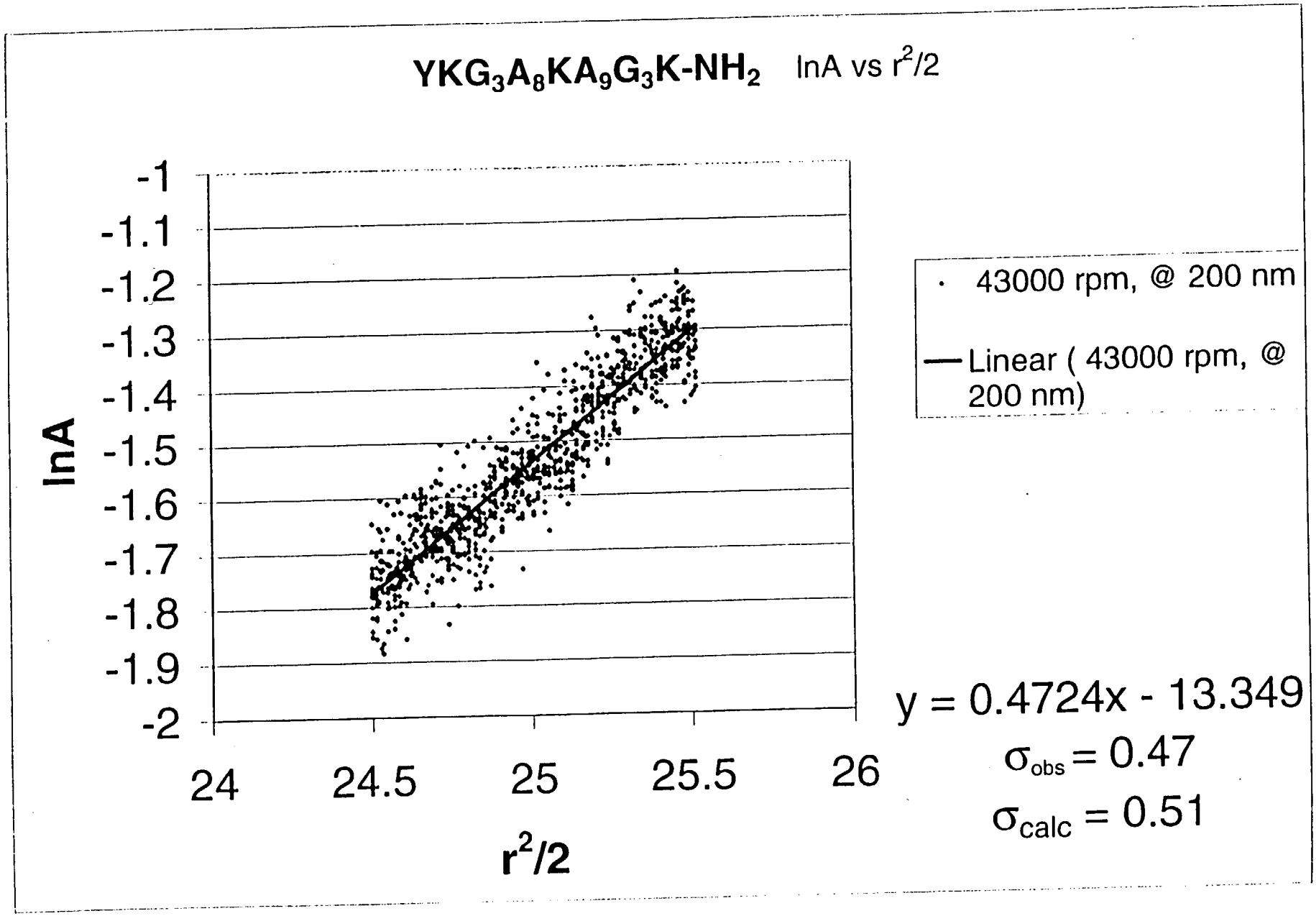
1590 data points, 8.7 μM solution, 43,000 rpm

$\sigma_{obs} = 0.45$ $Mw_{obs} = 1.9 \times 10^3$ $\sigma_{calc} = 0.52$ $Mw_{calc} = 2.2 \times 10^3$

	Coefficients	*Standard Error*	*Lower 95%*	*Upper 95.0%*
Intercept	-12.4704	0.058066	-12.58429	-12.35651
X Variable	0.449977	0.00236	0.445348	0.454606







Sedimentation Equilibrium Data Analysis SUMMARY For $YKG_3A_8KA_9G_3K\text{-}NH_2$ (lnA vs $r^2/2$)

908 data points, 1 μM solution, 43,000 rpm

σ_{obs} = 0.47 $Mw_{obs} = 2.0 \times 10^3$ σ_{calc} = 0.51 $Mw_{calc} = 2.1 \times 10^3$

	Coefficients	*Standard Error*	*Lower 95%*	*Upper 95%*
Intercept	-13.34921	0.158641	-13.66055	-13.03786
X Variable	0.47245	0.006344	0.459999	0.4849