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Magnetic Field Effect on Coenzyme B_{12} and B_6 -Codependent Lysine 5,6-Aminomutase: Switching of J-Resonance Through a Kinetically Competent Radical-Pair Intermediate

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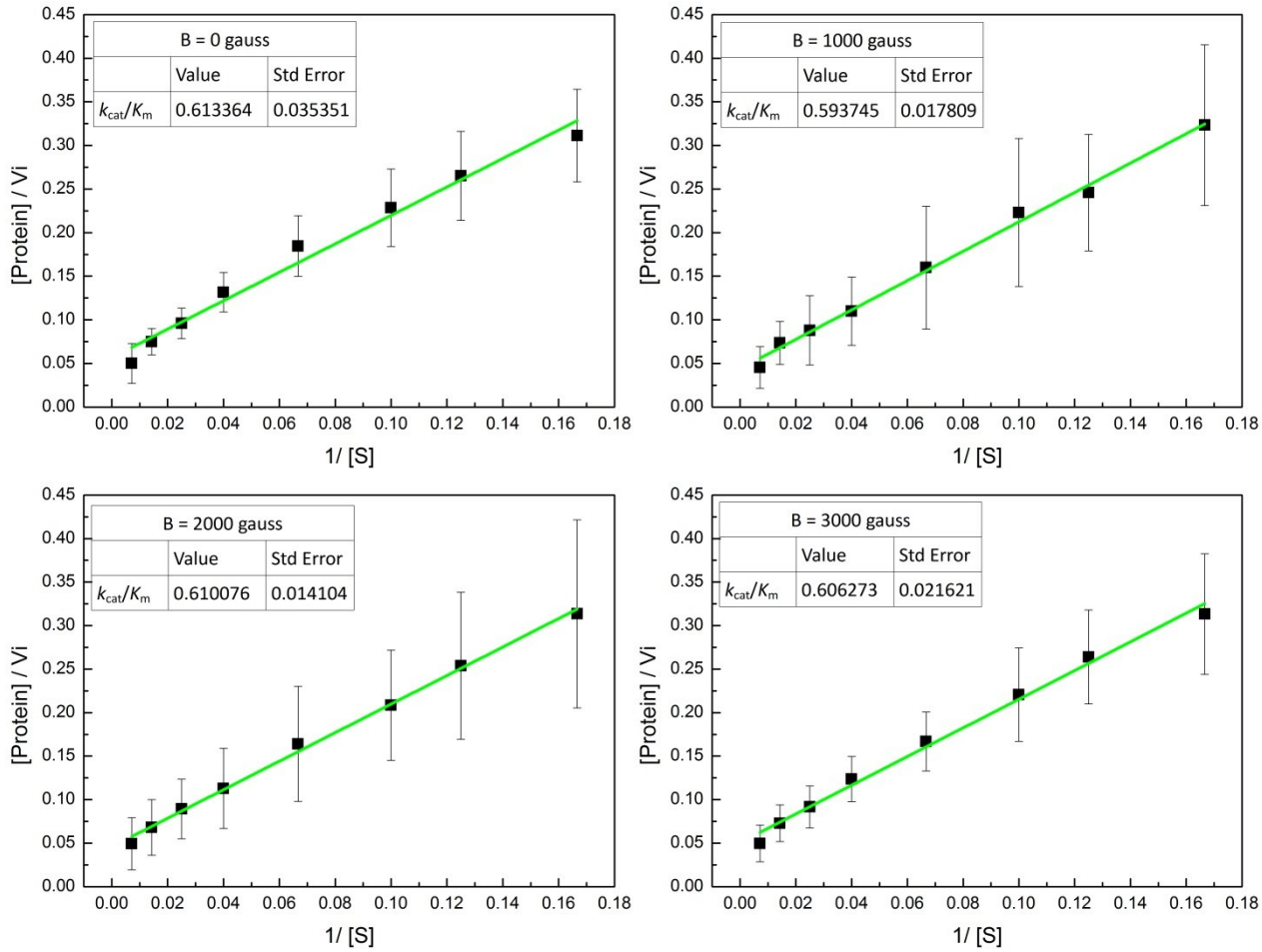
To accompany Figure 2A:

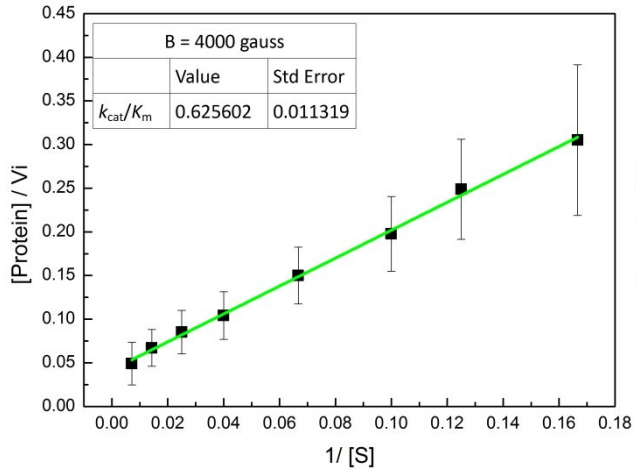
Lineweaver-Burk double reciprocal plot for D-lysine as a substrate:

▩: Each data point represents an average of five data points.

Error bar: Standard deviation from the mean of five data points

Green line: Linear regression with function $\frac{[protein]}{Vi} = (\frac{k_{cat}}{K_m})^{-1}\frac{1}{[S]} + \frac{1}{k_{cat}}$

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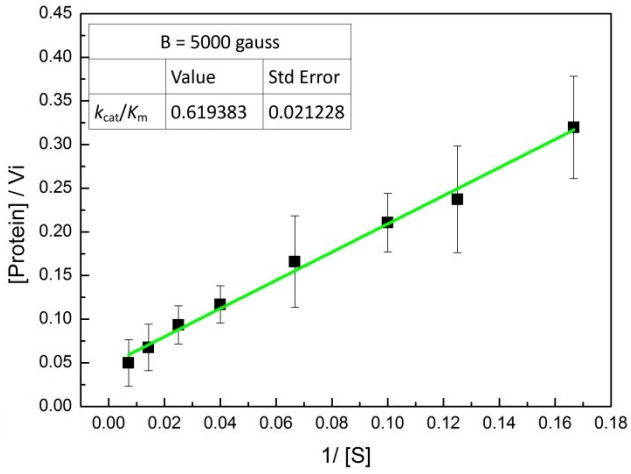
[Protein] / Vi
1/ [S]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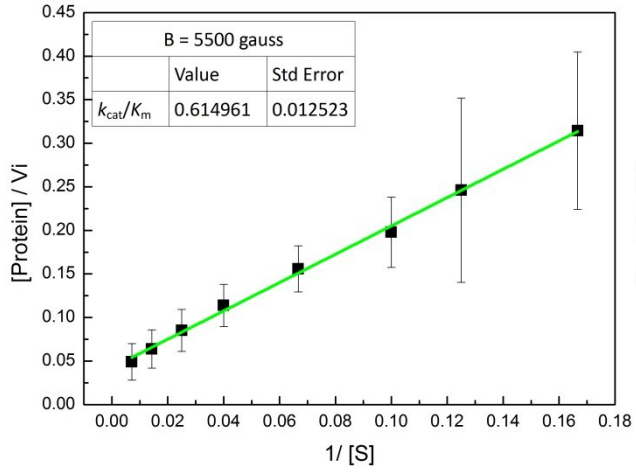
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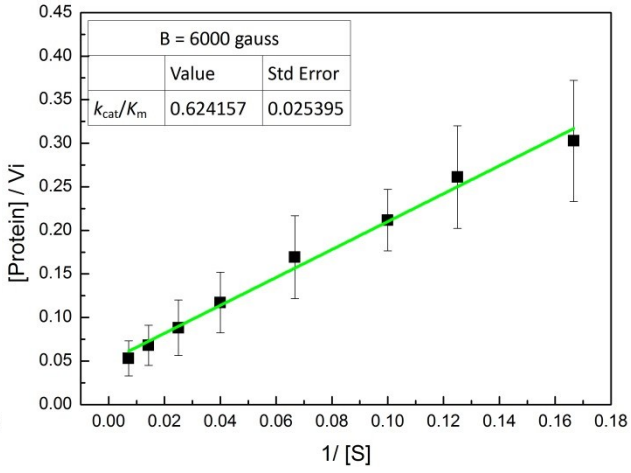
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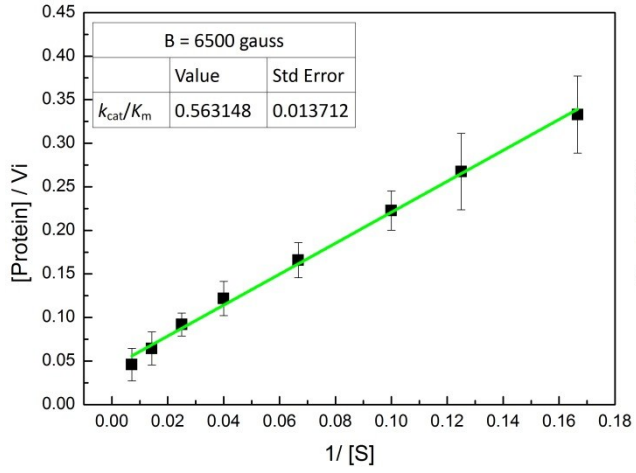
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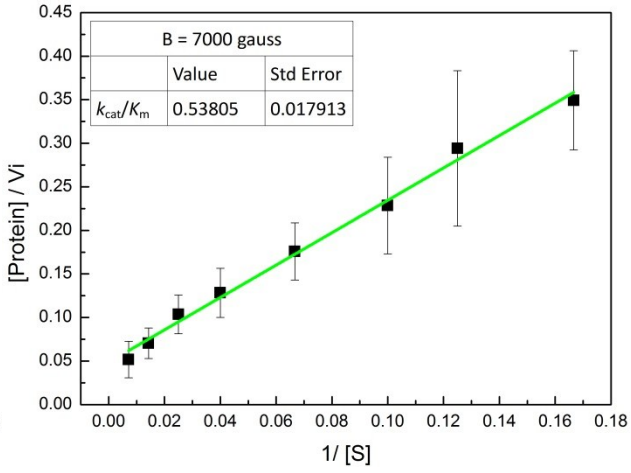
1/ [S]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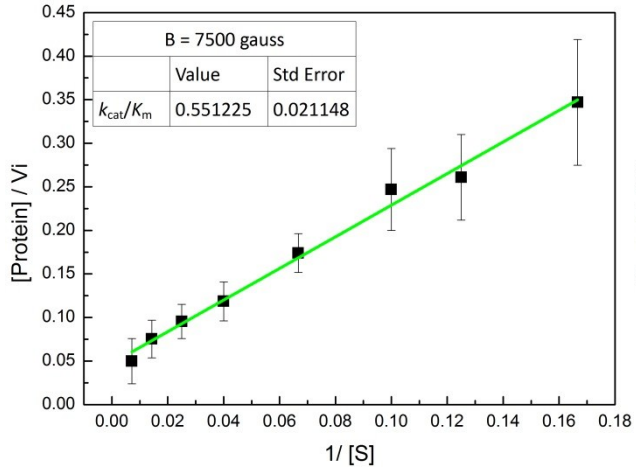
[Protein] / Vi
1/ [S]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Std Error
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0.551225
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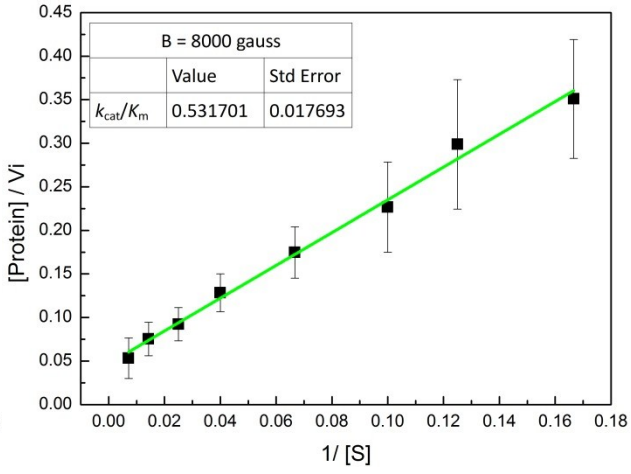
1/ [S]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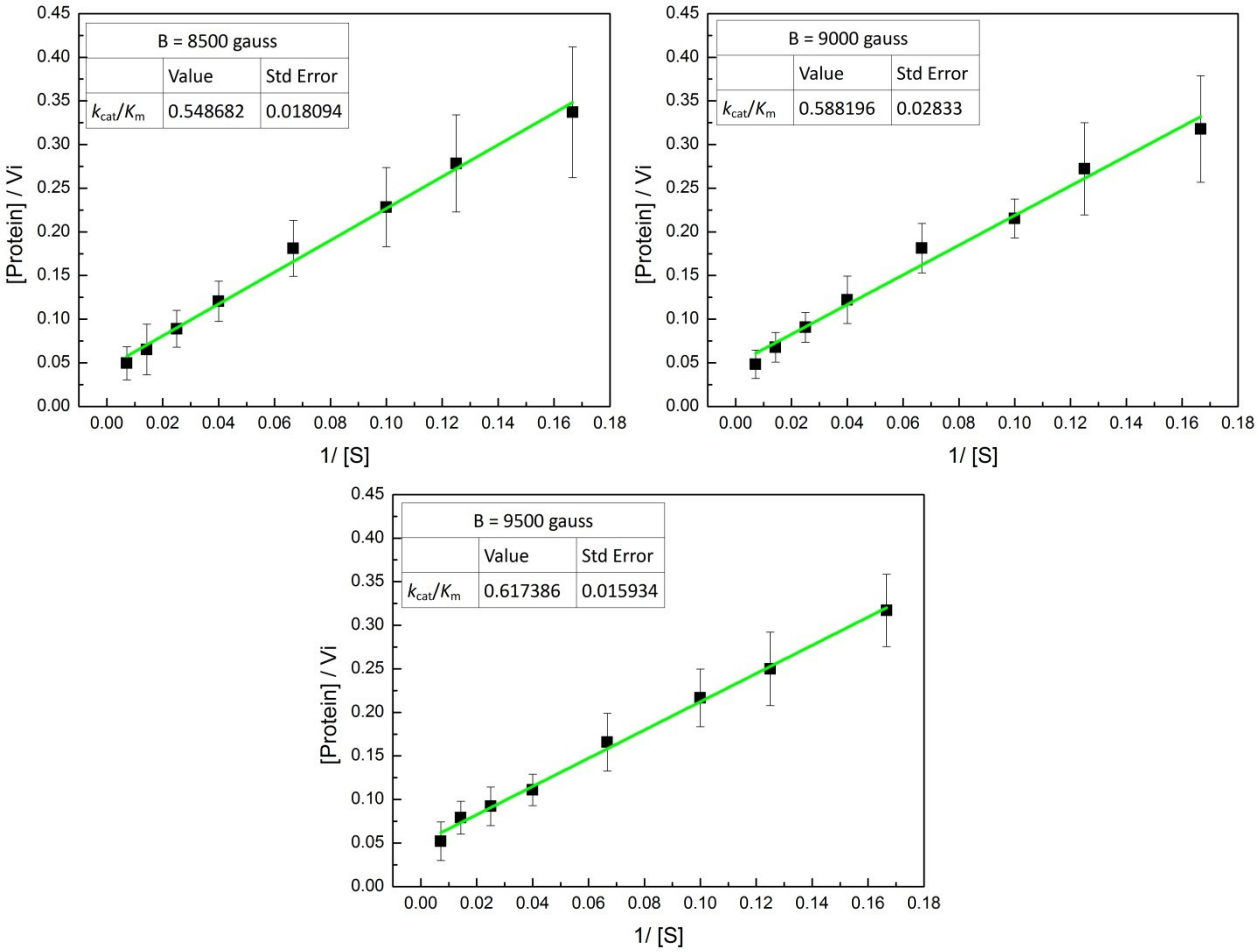
[Protein] / Vi
1/ [S]



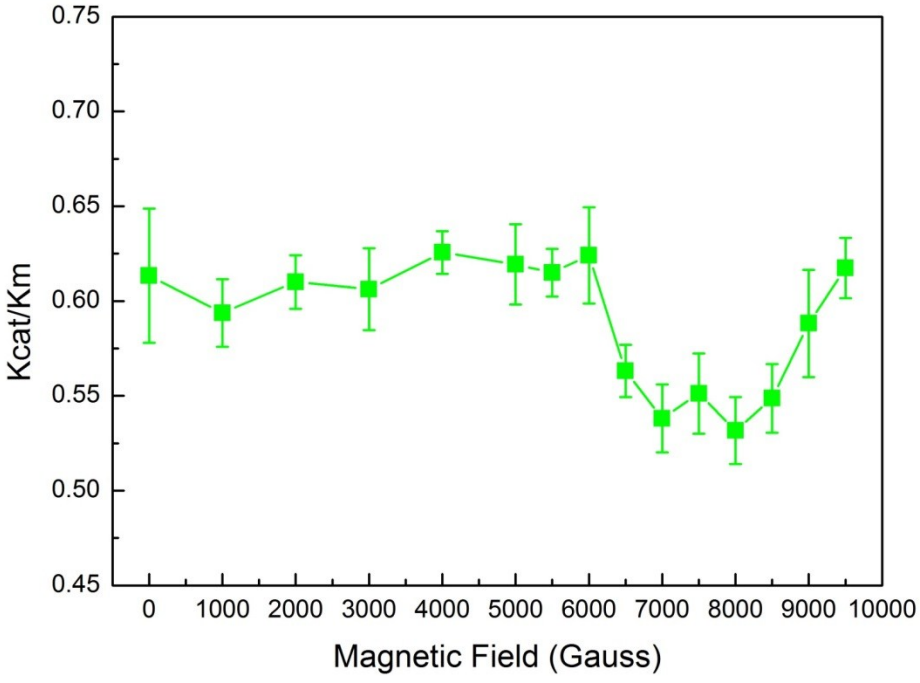


Figure S1: MF dependence of k_{cat}/K_m in reaction of 5,6-LAM from *Clostridium sticklandii* with unlabelled D-lysine. Each data point was obtained by Lineweaver-Burk double reciprocal fitting to the mean of five independent batches of kinetic experiments. Error bar shows the standard error in the Lineweaver-Burk double reciprocal fitting in determining the value of k_{cat}/K_m.

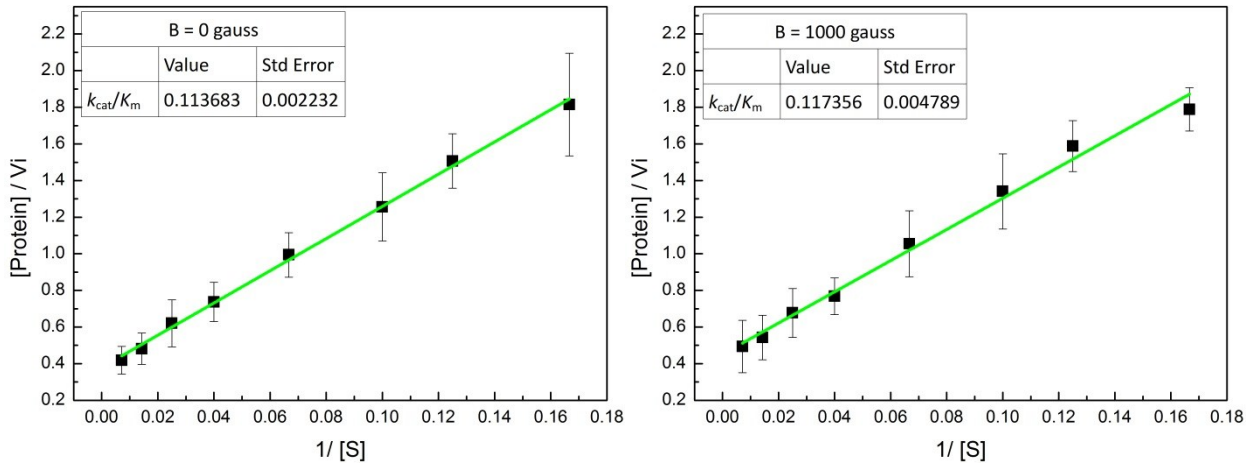
To accompany Figure 2B:

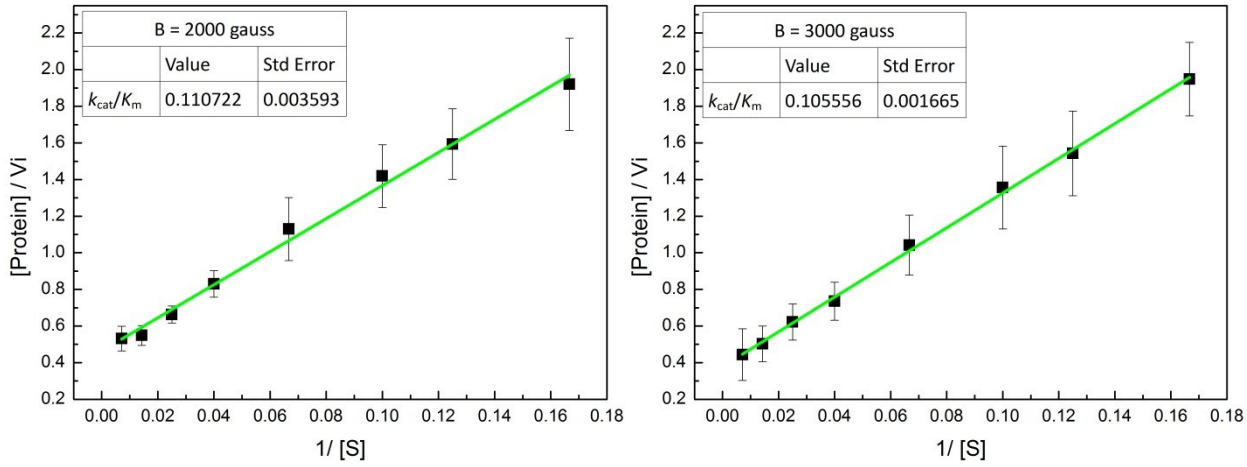
Lineweaver-Burk double reciprocal plot for D-lysine-4,4,5,5,-d_4 as a substrate:

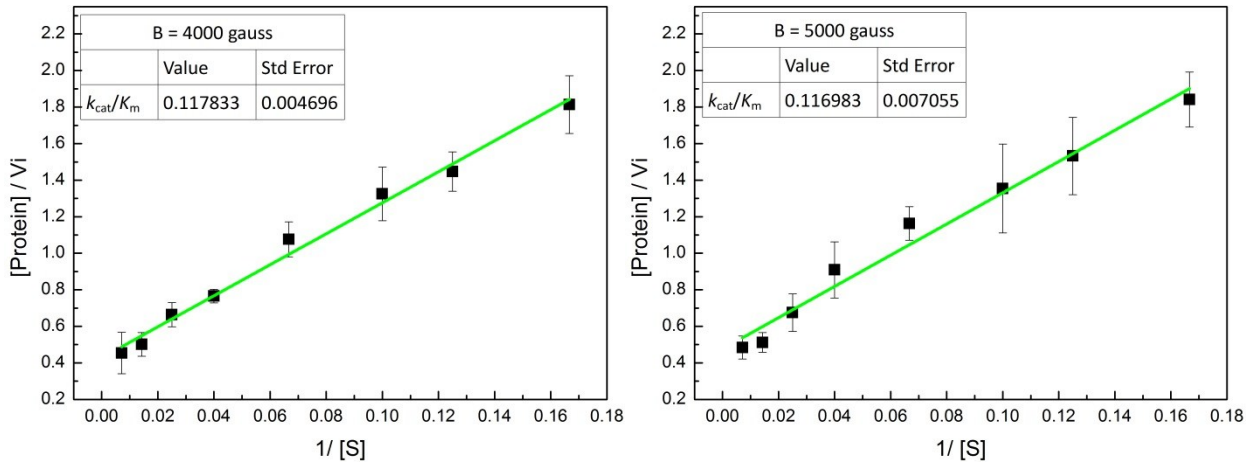
▩: Each data point represents an average of five data points.

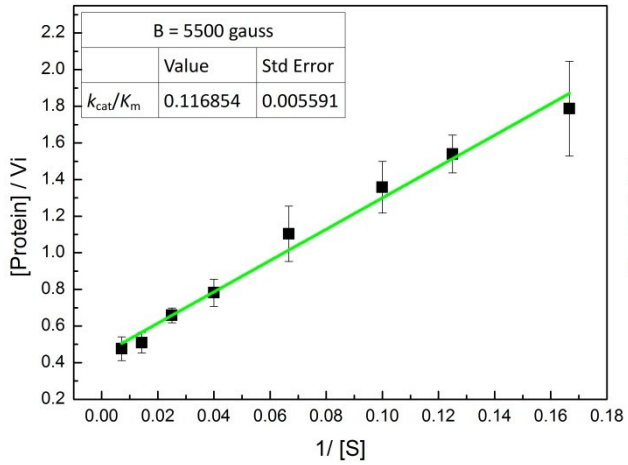
Error bar: Standard deviation from the mean of five data points

Green line: Linear regression with function $\frac{[protein]}{Vi} = (\frac{k_{cat}}{K_m})^{-1}\frac{1}{[S]} + \frac{1}{k_{cat}}$








B = 5500 gauss
Value
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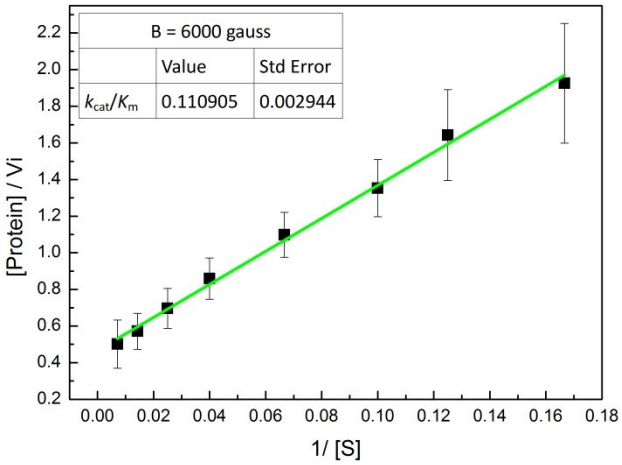
k_{cat}/K_m
0.116854
0.005591
[Protein] / Vi
1/ [S]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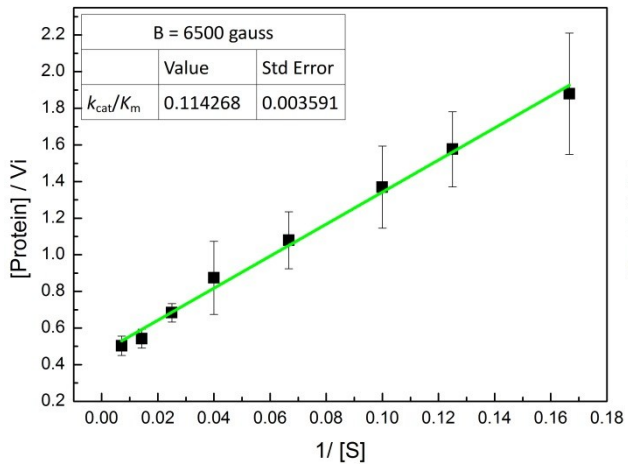
0.002944
[Protein] / Vi
1/ [S]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k_{cat}/K_m
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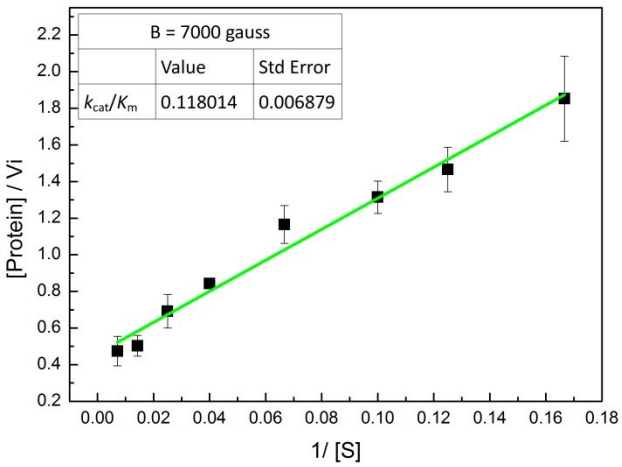
1/ [S]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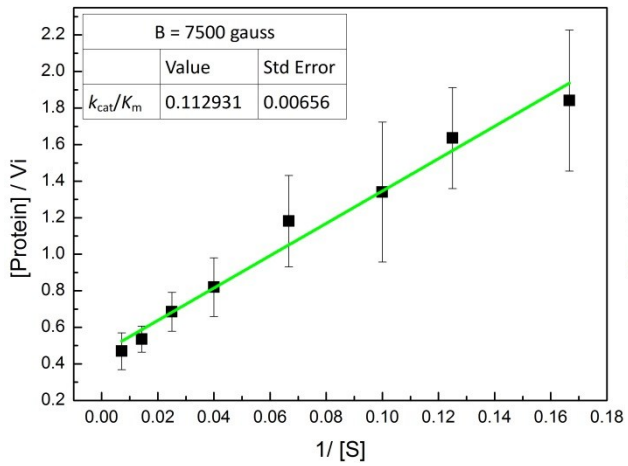
1/ [S]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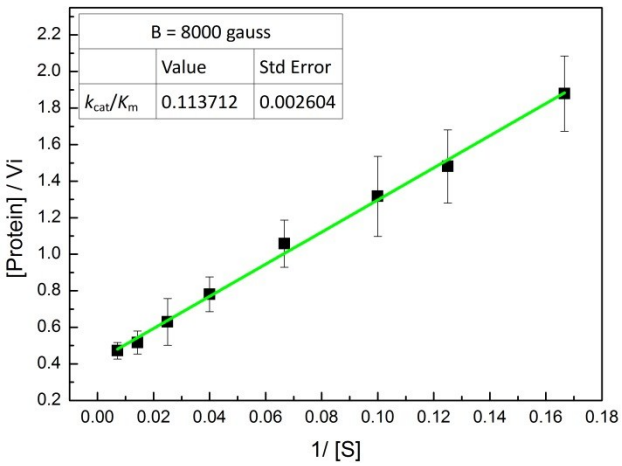
1/ [S]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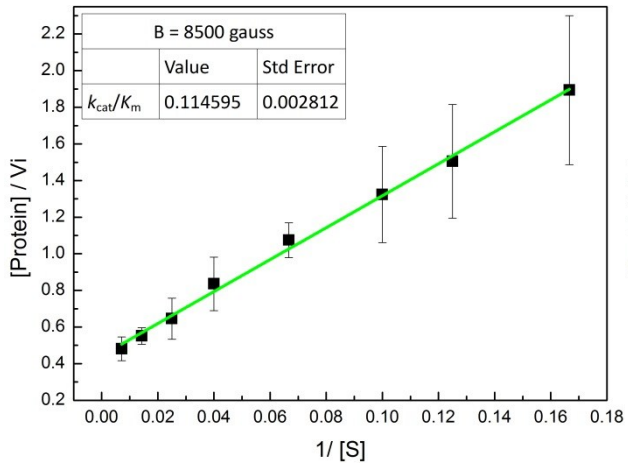
0.002604
[Protein] / Vi
1/ [S]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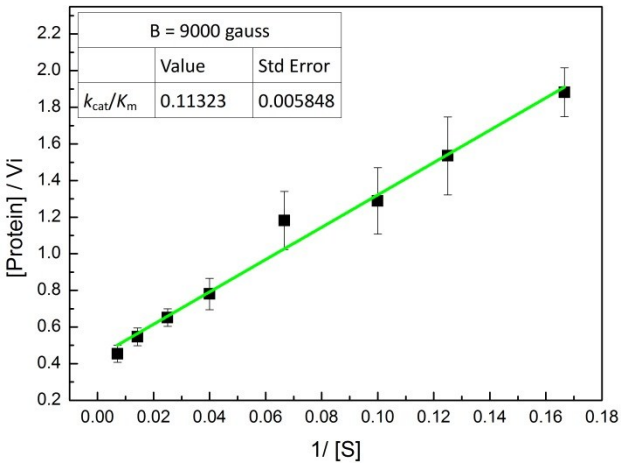
1/ [S]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0.005848
[Protein] / Vi
1/ [S]

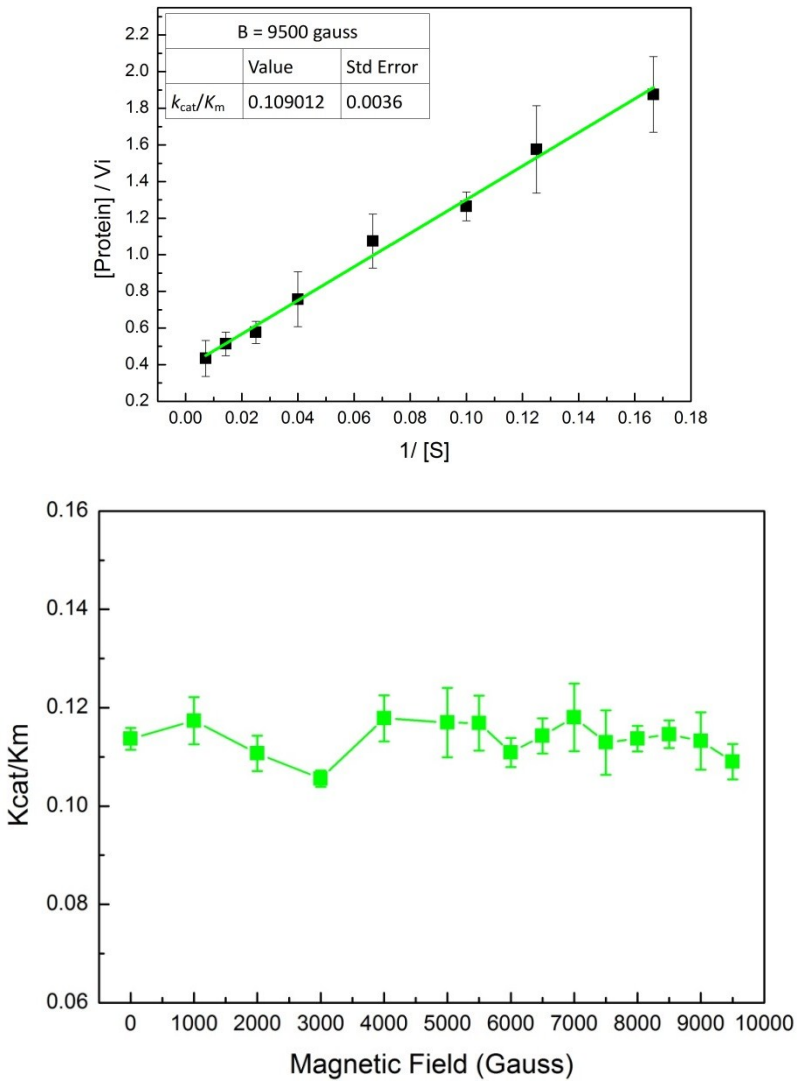

Figure S2. MF dependence of k_{cat}/K_m in reaction of 5,6-LAM from *Clostridium sticklandii* with D-lysine-4,4,5,5,-d_4. Each data point was obtained by Lineweaver-Burk double reciprocal fitting to the mean of five independent batches of kinetic experiments. Error bar shows the standard error in the Lineweaver-Burk double reciprocal fitting in determining the value of k_{cat}/K_m.

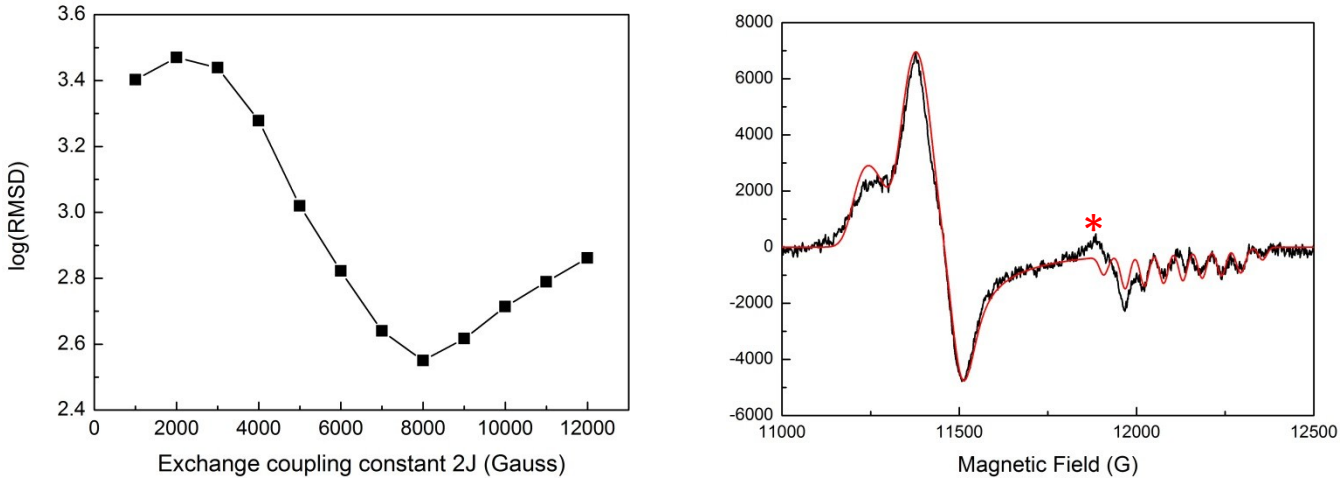

Figure S3. (Left) Quantitative goodness of fit showing the best fit occurs at |2J| = 8000 gauss. RMSD is defined as square root of [mean (experiment – simulation)^2]. (Right) Overlay of experimental spectrum with simulated spectrum at |2J| = 8000 gauss. Other simulation parameters are as indicated in Figure 4. The additional signal (starred feature) indicates the onset of tautomerization of the transient radical into a persistent radical.