

Supplemental Material

3,17 β -Bis-sulfamoyloxy-2-methoxyestra-1,3,5(10)-triene (STX140) and Non-Steroidal Sulfamate Derivatives Inhibit Carbonic Anhydrase IX: Structure-Activity Optimization for Isoform Selectivity

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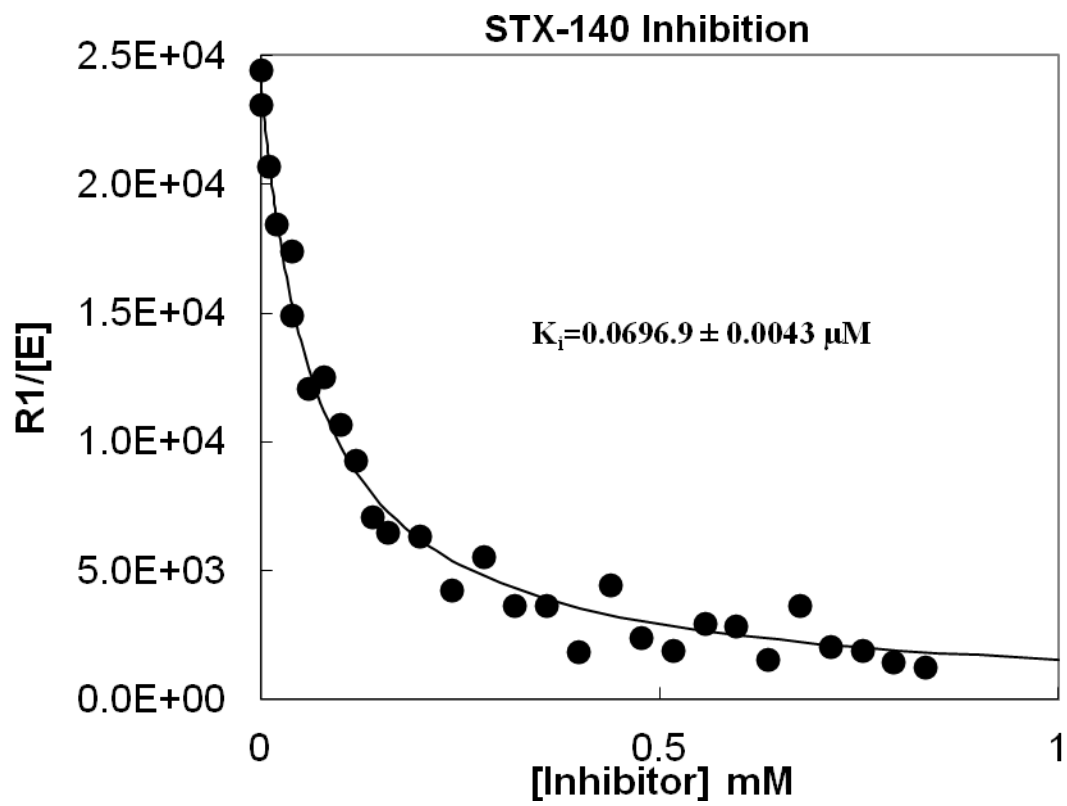
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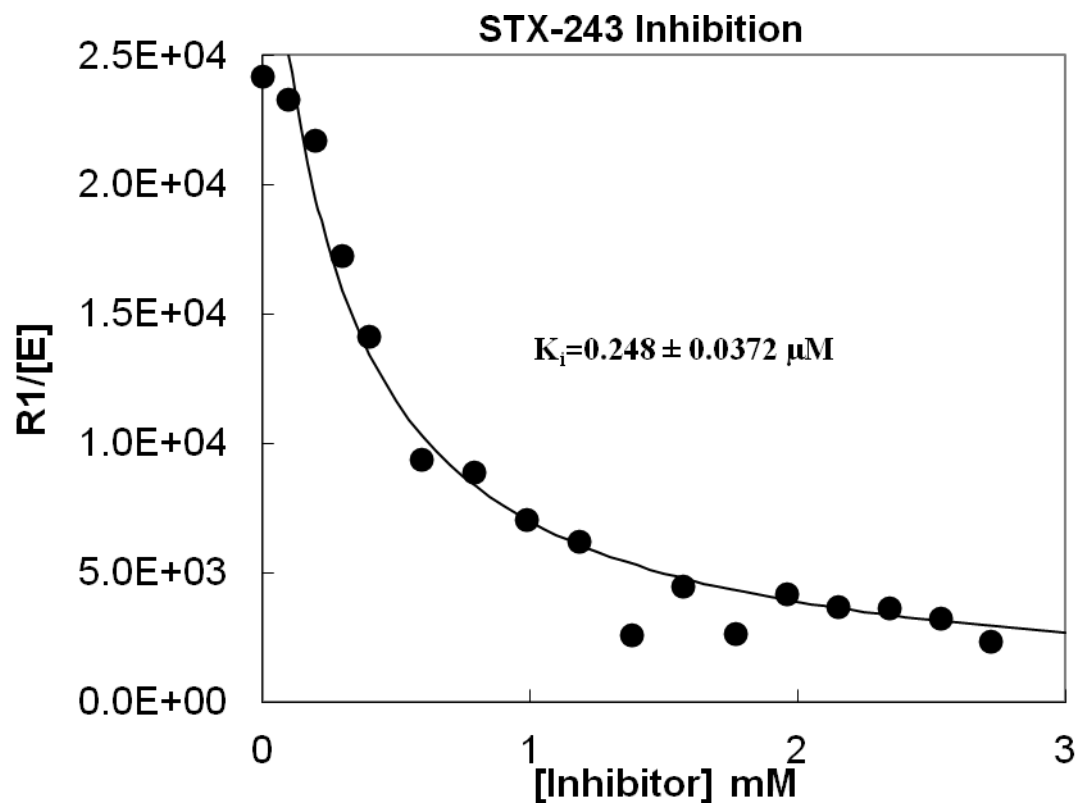
- 1. STX Series CA Inhibition Data**
- 2. Electron Density for STX49, STX140, STX2484, and STX2845 bound in CA IX**

Keywords: Carbonic Anhydrase IX, Inhibitors, Cancer, Sulfamates

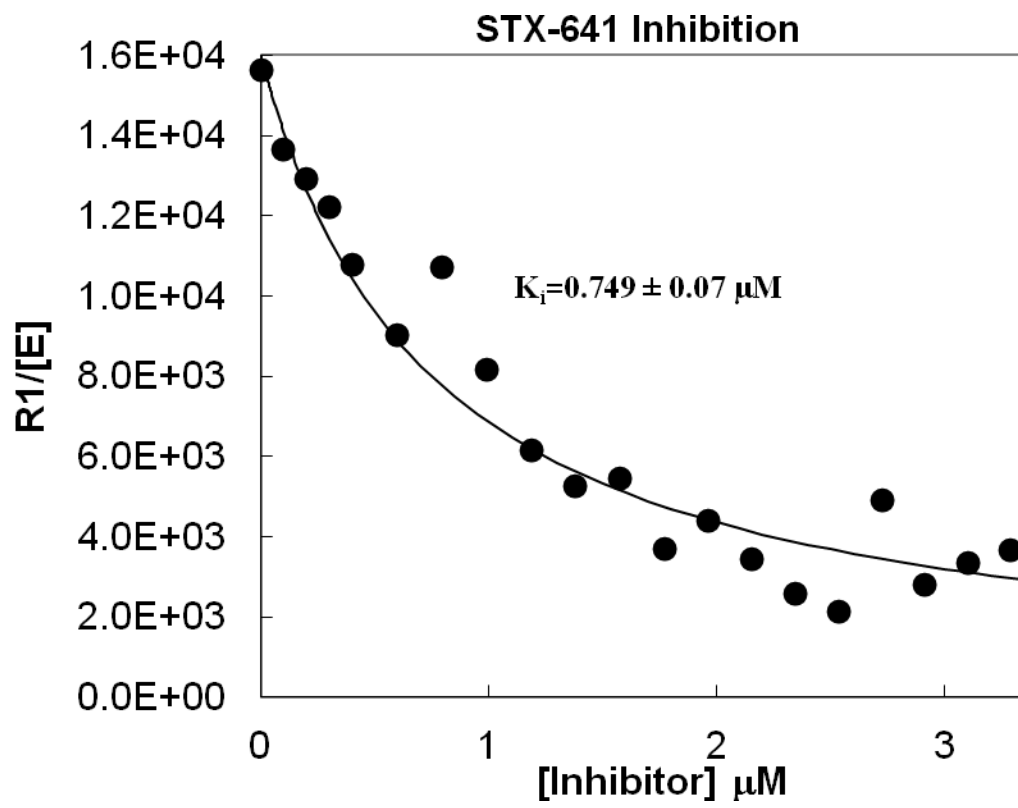
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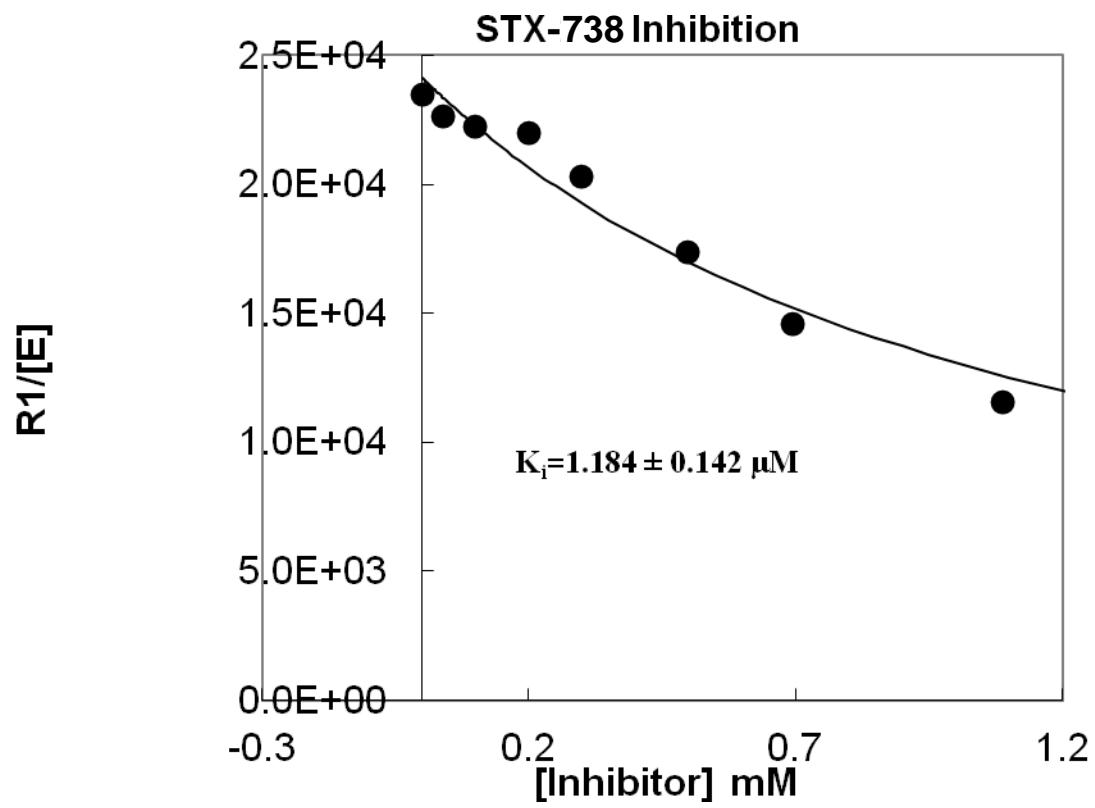
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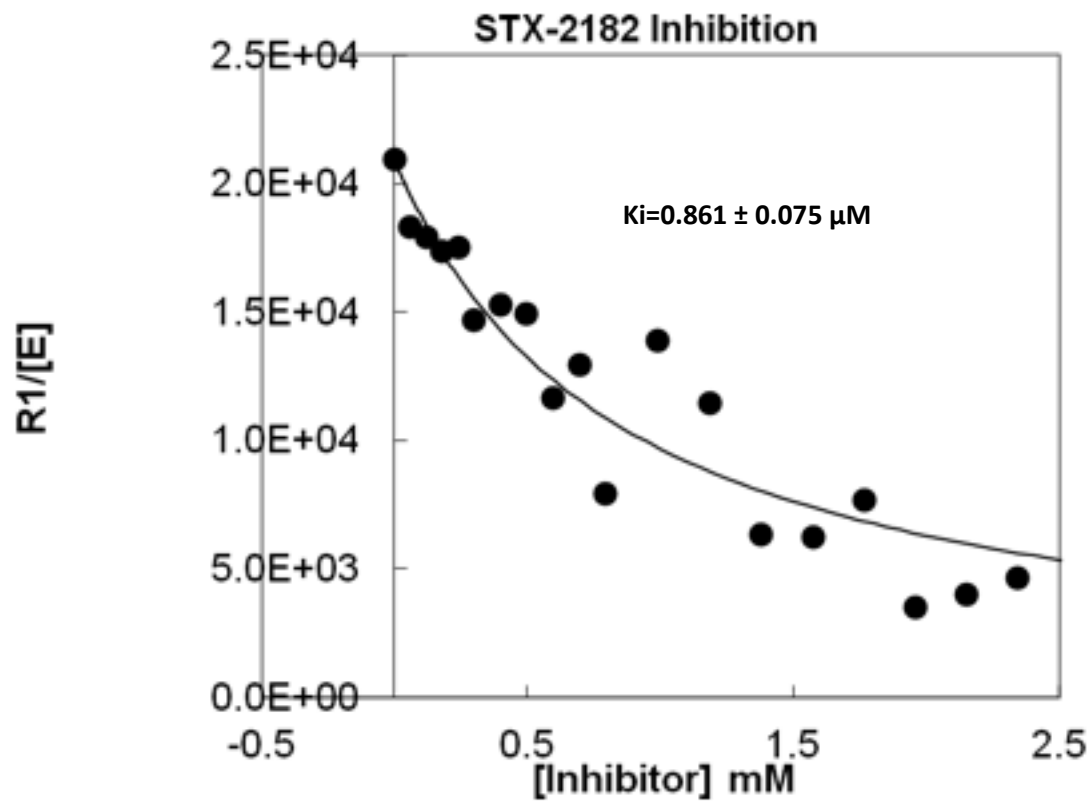
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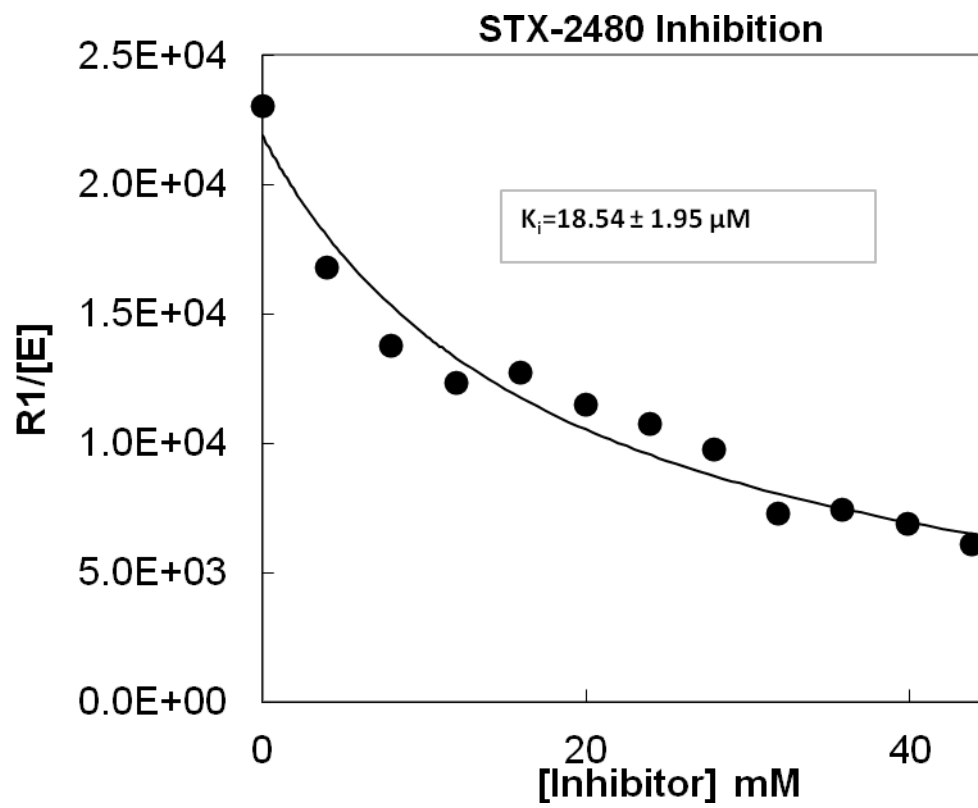
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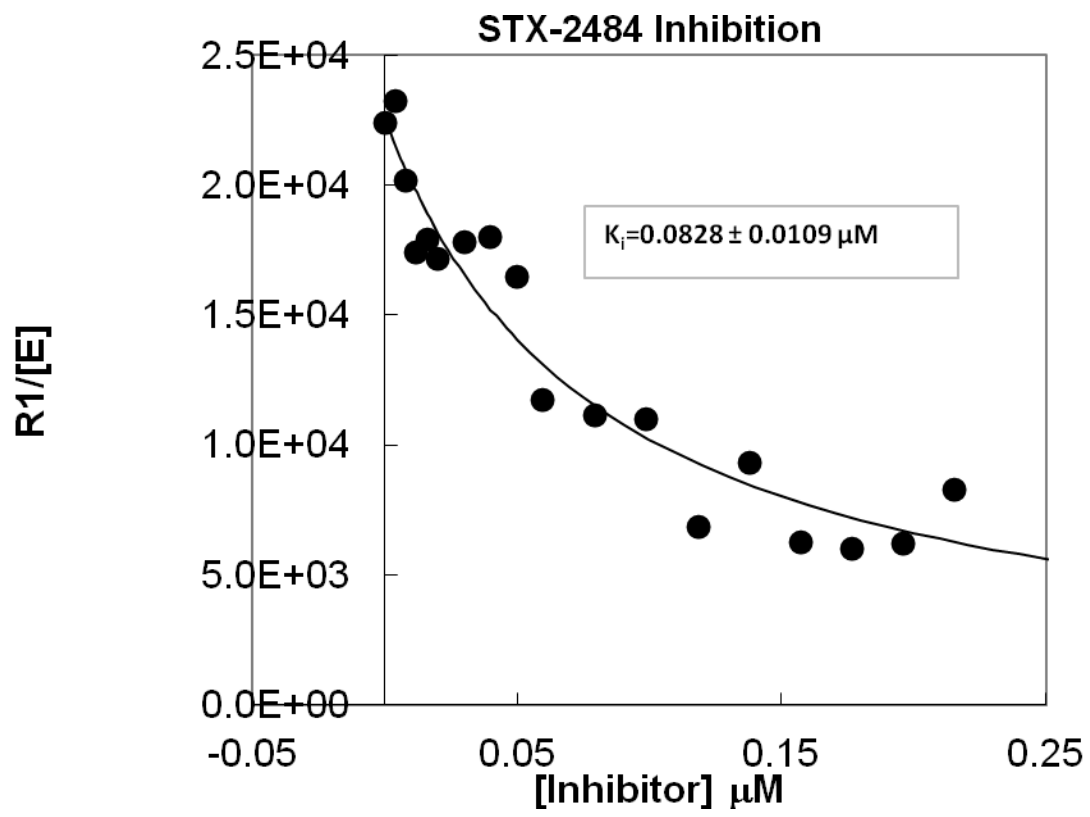
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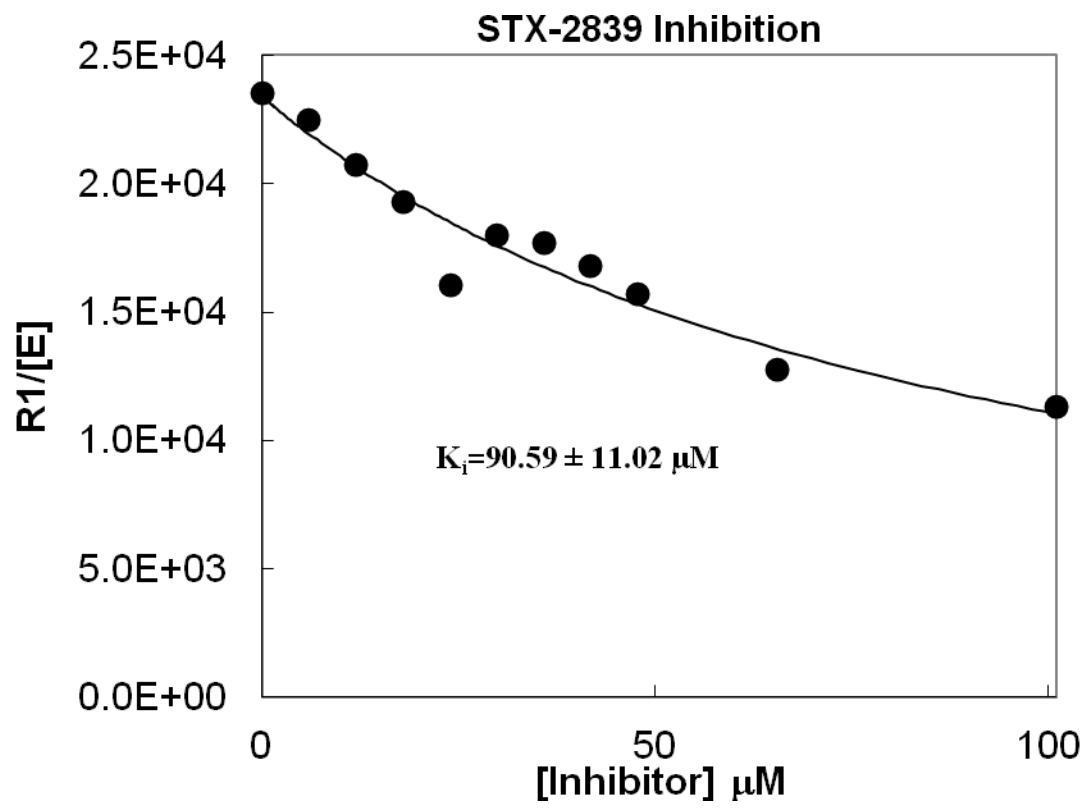
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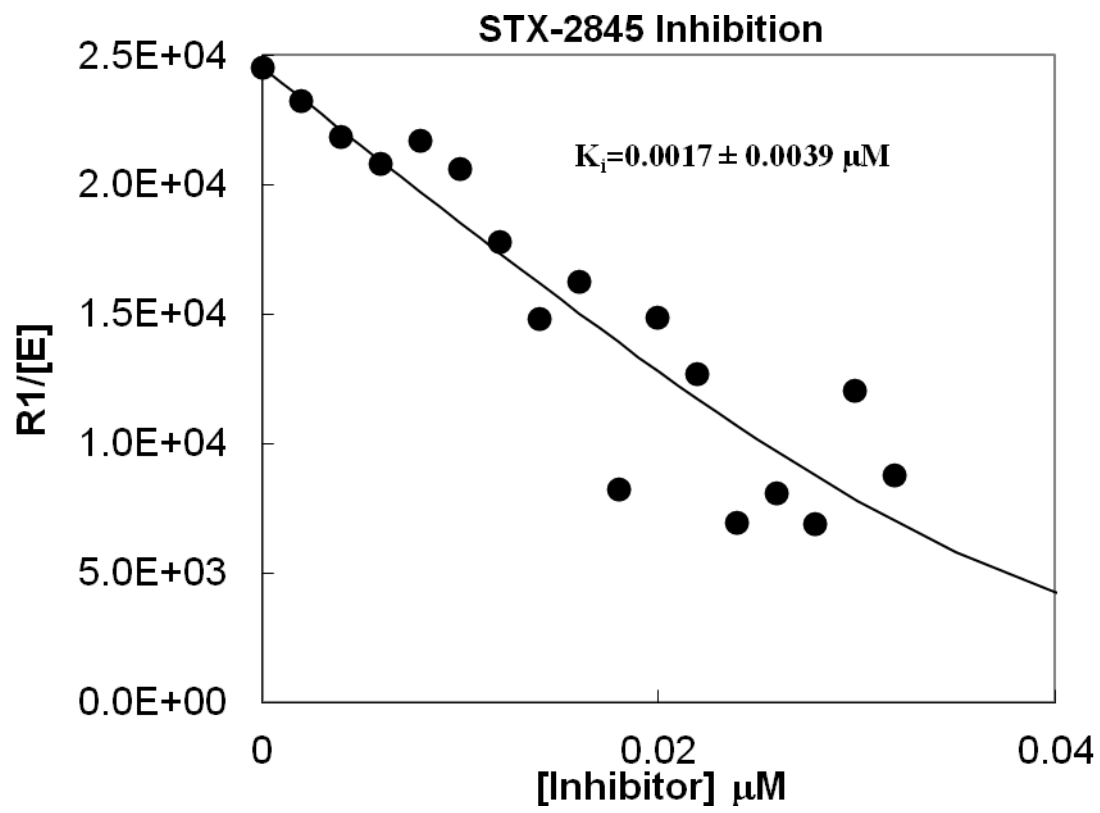
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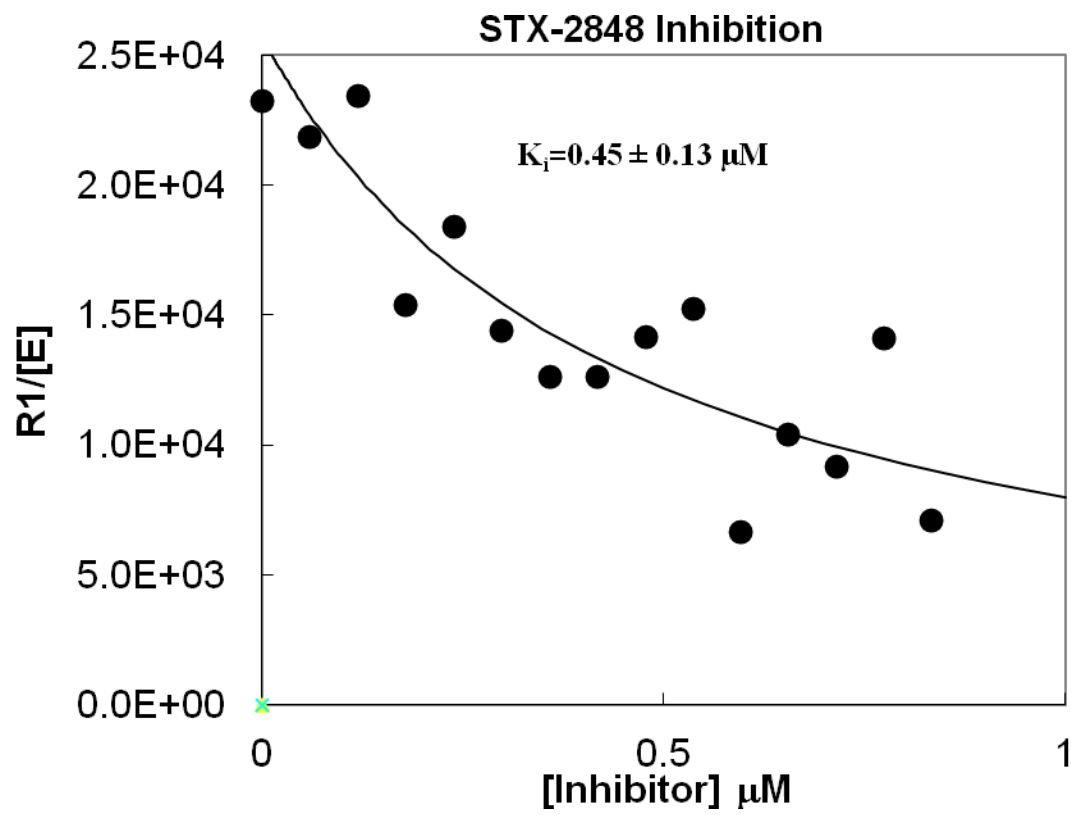
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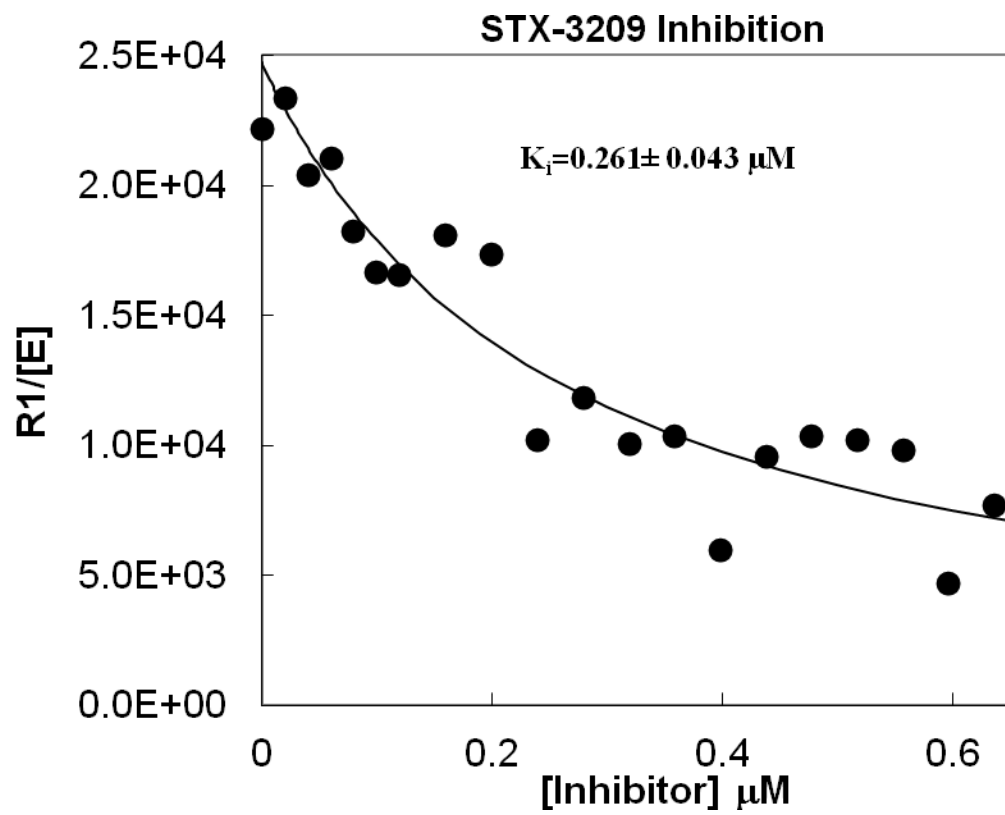
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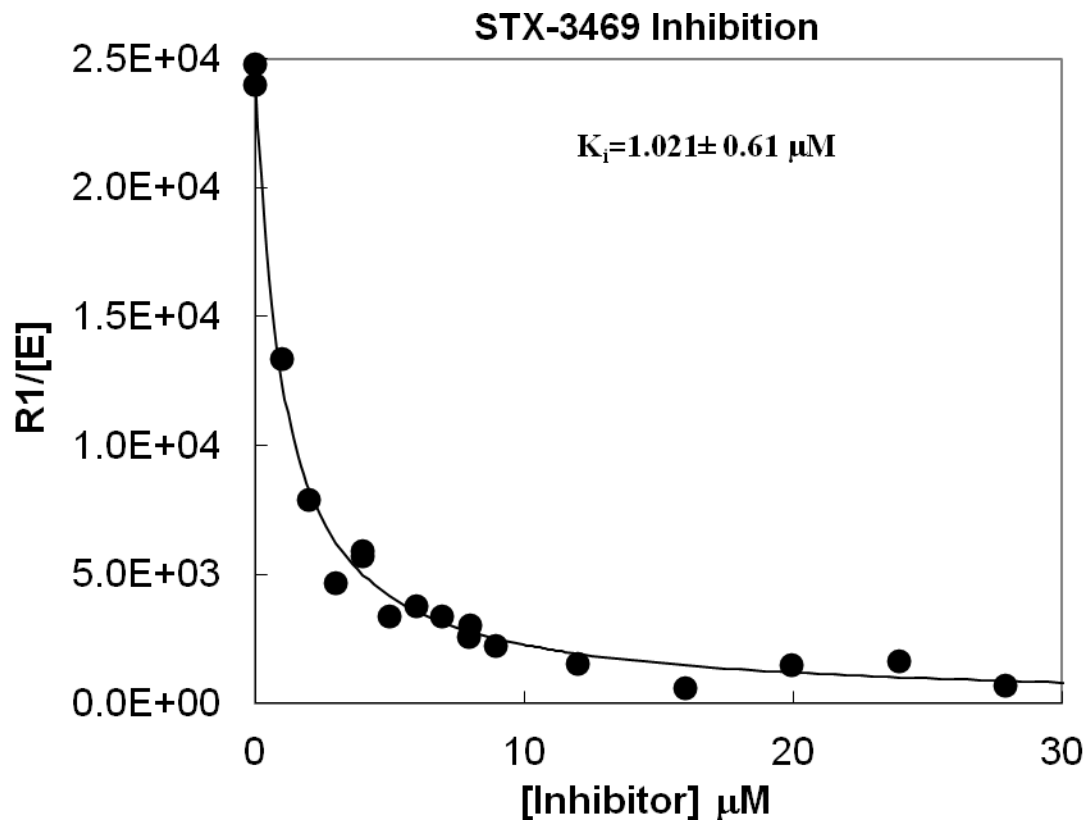
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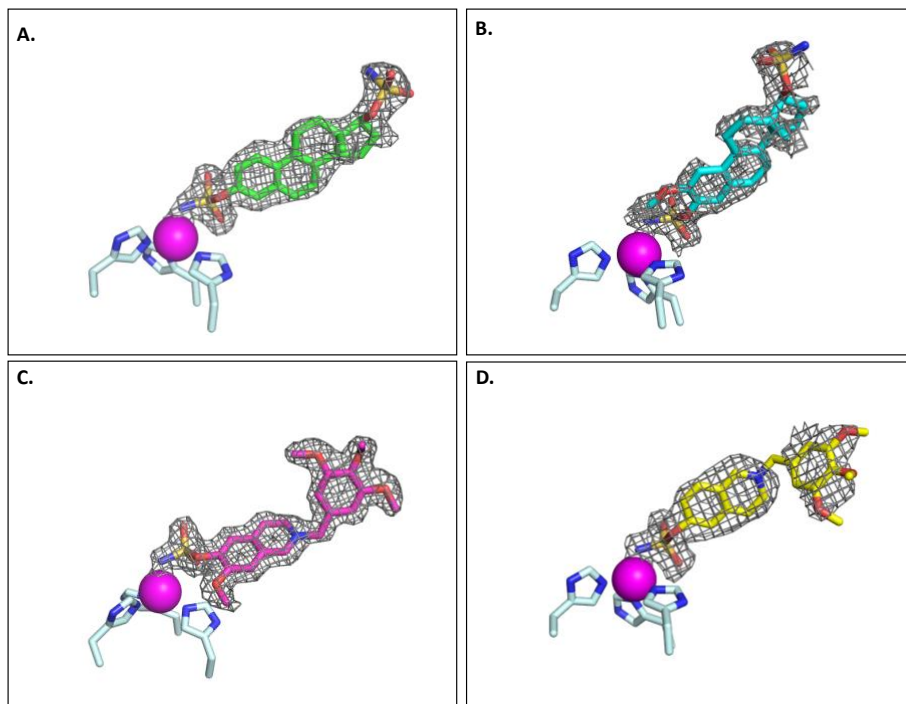
K.



L.



Supplemental Figure 1: Kinetic Data for STX Series of Inhibitors **A)** STX140 **B)** STX243 **C)** STX641 **D)** STX738 **E)** STX2182 **F)** STX2480 **G)** STX2484 **H)** STX2839 **I)** STX2845 **J)** STX2848 **K)** STX3209 **L)** STX3469



Supplemental Figure 2: Electron Density Maps for STX Inhibitors **A)** STX49 density at 0.7 σ **B)** STX140 density at 0.7 σ **C)** STX2484 density at 1.0 σ **D)** STX2845 density at 1.0 σ