

Abstract Submitted  
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**Fly-casting in a reaction limited binding of pKID-KIX<sup>1</sup>** TALANT RUZMETOV, JOHN PORTMAN, Physics KSU, PORTMAN'S GROUP TEAM — Flexible and robust nature of encounter complex is an advantage for Natively Unstructured Proteins (IDPs) to facilitate fast molecular recognition associated with coupled folding and binding. Several factors involving the weak non-specific interactions between the IDP and its binding partner can lead to enhanced binding rates such as Fly-casting and reduced orientational constraints of flexible binding partners. Here we investigate how overcoming desolvation barriers between the binding partners influences coupled folding and binding kinetics of an IDP (pKID) to its target (KIX). We compare the free energy binding surface and kinetics for models with and without desolvation barriers between pKID and KIX for a range of flexibilities. We find that compared to a more structured unbound protein, the simulated binding rate of flexible binding partners is an order of magnitude faster. This difference in binding rate, which is much larger than the range without desolvation barriers, can be understood by the ability of a flexible binding partner to overcome desolvation barriers sequentially while rigid proteins must overcome them more collectively. In addition, carefully choosing reaction coordinate, we witness Fly-casting in the reaction limited binding regime.

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