Finding a way out of the Labyrinth: Degrader induced ternary complex modelling

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With the exponential growth in the development of targeted protein degraders come significant challenges for the structural biology and computational modelling communities. Numerous examples now exist in the literature of the exquisite SAR possible through modifications of these molecules and this has driven a need to generate atomic level ternary complex information to assist degrader design and elucidate mechanism of action. Here we will present our approach combining biophysical and computational methods to generate weighted models to support medicinal chemistry campaigns.