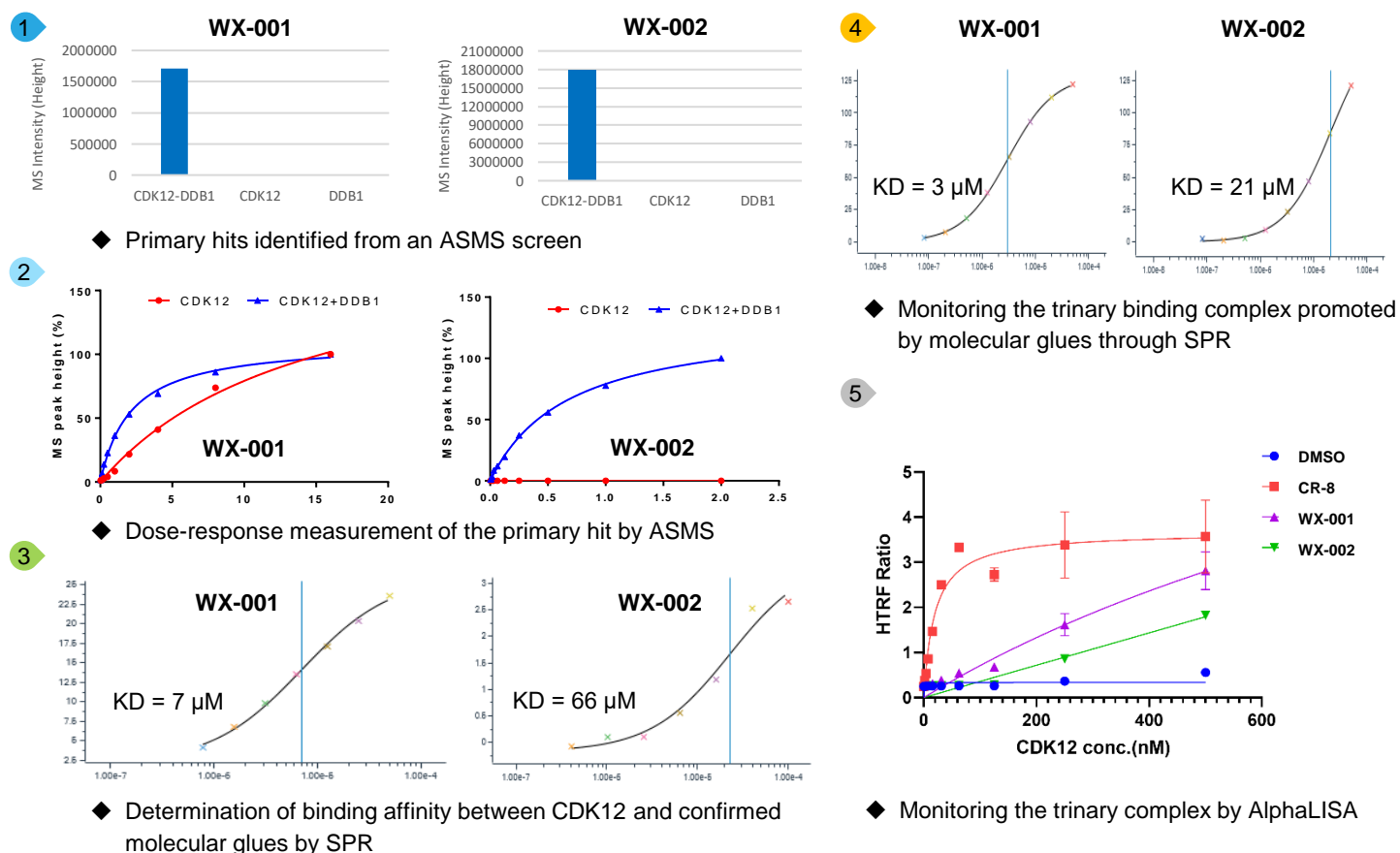


Affinity Selection Mass Spectrometry (ASMS)

Abstract: Molecular glues possess the remarkable ability to induce protein-protein interactions. In the pursuit of targeting the CDK12/CCNK/DDB1 complex, an ASMS screening strategy had been employed, resulting in the successful identification of two active molecular glues from a subset of 2000 small molecules within the WuXi AppTec compound library. Validation efforts have revealed compelling findings: the two small molecules exhibit affinities of 7 μM and 66 μM with CDK12, respectively. Furthermore, outcomes from SPR (trinary binding affinity of 3 μM and 22 μM , respectively) and AlphaLISA assays have unequivocally demonstrated that both small molecules significantly facilitate the formation of the CDK12/CCNK/DDB1 complex.

Application of ASMS for Molecular Glue Discovery Targeting the CDK12/CCNK/DDB1 Complex



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