

Supplementary Figures

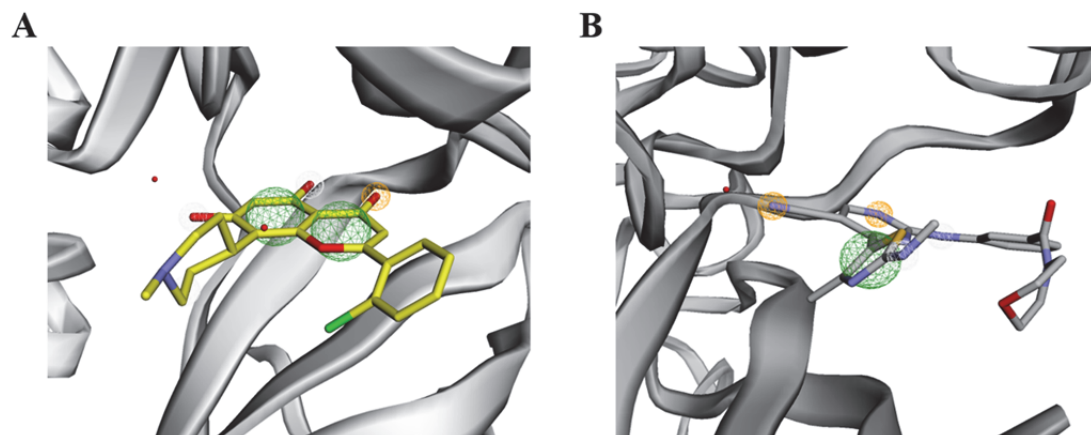
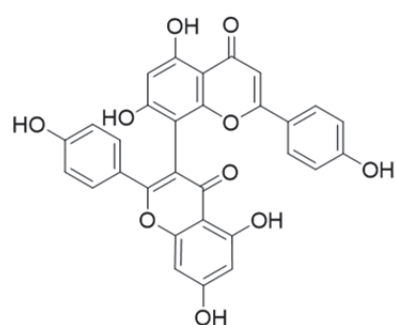
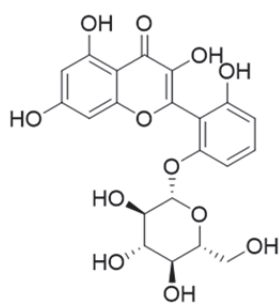


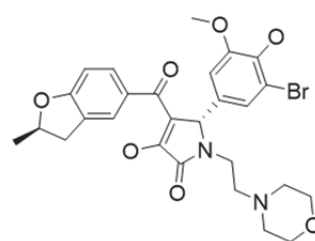
Fig. S1. pharmacophore models of virtual screening. **A** CDK1/Cyclin B1 complex binding with flavopiridol. **B** CDK2/Cyclin A complex binding with a 2-amino-4-heteroaryl- pyrimidine inhibitor.



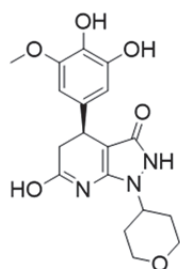
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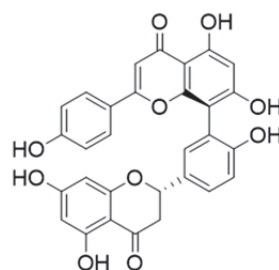
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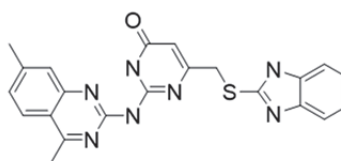
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Fig. S2. the chemical structure of representative compounds.