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Design and synthesis of novel pyrimidone analogues as HIV-1 integrase inhibitors

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A series of novel pyrimidone analogues have been designed and synthesized as HIV-1 integrase (IN) inhibitors. This study demonstrated that introducing a substituent in the N1-position of the pyrimidone scaffold does not significantly influence IN inhibitory activity. Molecular docking studies showed these compounds could occupy the IN active site and form pi-pi interactions with viral DNA nucleotides DC16 and DA17 to displace reactive viral DNA 3'OH and block intasome activity.

Keywords: HIV-1, Integrase inhibitors, Pyrimidone analogues.

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