

fragment based strategies for discovery of novel hiv-1 ... - hiv-1, reverse transcriptase and integrase. while any fbdd-generated hiv-1 drugs have yet to enter the clinic, while any fbdd-generated hiv-1 drugs have yet to enter the clinic, recent fbdd initiatives against these two well-characterised hiv-1 targets have reinvestigated antiretroviral drug

discovery of a novel hiv-1 integrase inhibitor from ... - discovery of a novel hiv-1 integrase inhibitor from natural compounds through structure based virtual screening and cell imaging wan-gang gua,c, xuan zhangb, denis tsz-ming ipa, liu-meng yangb, yong-tang zhengb,

computational and synthetic approaches for the discovery ... - pharmacophore modeling and discovery of hiv-1 integrase inhibitors our first aim was to build a simple 3d pharmacophore model representing the distinguishing chemical features of integrase strand transfer inhibitors (insti) and to obtain a useful tool for

development of an alphascreen-based hiv-1 integrase ... - in recent years, hiv-1 integrase (in) has become an established target in the field of antiretroviral drug discovery. however, however, its sole clinically approved inhibitor, the integrase strand transfer inhibitor (insti) raltegravir, has a surprisingly low genetic

molecular modelling and qsar in the discovery of hiv-1 ... - discovery of hiv-1 integrase inhibitors current computer-aided drug design, 2007, vol. 3, no. 3 215 conformations in those structures in which it is ordered.

fueling hiv-1 integrase drug design with structural insights - residue numbers are depicted in black and gray for pfv and hiv-1, respectively. dtg (shown in sticks) can be seen to dtg (shown in sticks) can be seen to coordinate

a historical sketch of the discovery and development of ... - a historical sketch of the discovery and development of hiv-1 integrase inhibitors 1508 expert opin. investig. drugs (2006) 15(12) the crystal structures of the three integrase domains have

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recent advances in the discovery of small-molecule ... - review choi,mallareddy,lu&kolluru n n o o oh raltegravir (1) elvitegravir (2) dolutegravir (3) och 3 o h n f f h f h n o n n ho o h n o o n n oh f o cl o o oh figure 1. clinically used hiv integrase inhibitors.

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alessia petrocchi, fabio bonelli, benedetta crescenzi, monica donghi, marco ferrara,

towards an understanding of the molecular dynamic causes ... - university college london towards an understanding of the molecular dynamic causes of resistance in the hiv-1 integrase by milo a. bem a thesis submitted in partial fulfillment for the

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