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Lahsasni, S.[e] , Ben Hadda, T.[a] , Masand, V.[b] , Pathan, N.B.[c] , Parvez, A.[d] , Warad, I.[i] , Shaheen, U.[f] , Bader, A.[f] , Aljofan, M.[g h]

POM analyses of Raltegravir derivatives: A new reflection enlightening the mechanism of HIV-integrase inhibition
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[a] Laboratoire Chimie Matériaux, Faculté Sciences, Université Med Premier, Oujda, Morocco
[b] Department of Chemistry, Vidya Bharati College, Camp, Amravati, Maharashtra, India
[c] Department of Chemistry, Institute of Science, Civil Lines, Nagpur, MS 440001, India
[d] Prince Sultan Military Medical City, Riyadh, 11159, Saudi Arabia
[e] Department of Chemistry, Science College, King Saud University, Riyadh, Saudi Arabia
[f] Department of Pharmacognosy, Faculty of Pharmacy, Umm Al-Qura University, Makkah, 21955, Saudi Arabia
[g] Department of Microbiology, School of Medicine, Nursing and Health Sciences, Monash University, Clayton, VIC, Australia
[h] Pharmacy College, Qassim University, Buraidah, Saudi Arabia
[i] Department of Chemistry, AN-Najah National University, P.O. Box 7, Nablus, Palestine

Abstract
Petra/Osiris/Molinspiration analysis (POM) is a promising new bioinformatical approach to establish structure and activity correlations. In the present study, we have reported the POM analyses of Raltegravir analogues that have aimed to figure out the structural features of HIV-integrase inhibitory activity. The resulting model exhibited two controllable bidentate O, O-pockets taken into consideration contributions from the steric and electrostatic fields. The POM analysis has provided interesting insights into the understanding the steric and electronic structural requirements for HIV-IN inhibitory activity. Furthermore, all the molecules were subjected to the toxicity assessment using Molinspiration and Osiris calculations. Among the various HIV-IN inhibitors, compound 27 (Raltegravir) displayed optimum drug-like characteristic activity with low toxicity. The mechanism of HIV-integrase inhibition by different Raltegravir derivatives is also discussed. This study also concluded that the bioactivity of DKA analogues should be discussed on the basis of catalytic activity of bimetallic complexes, not just on the basis of DKA or Raltegravir/HIV-integrase interaction. © 2014 Springer Science+Business Media.

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Bimetallic system; Diketo acid; HIV-integrase inhibitors; POM (Petra/Osiris/Molinspiration) analysis; Raltegravir

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