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Correction: Mechanism of RGD-conjugated nanodevice binding to its target protein integrin $\alpha_v\beta_3$ by atomistic molecular dynamics and machine learning

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Correction for 'Mechanism of RGD-conjugated nanodevice binding to its target protein integrin $\alpha_v\beta_3$ by atomistic molecular dynamics and machine learning' by Giulia Frigerio *et al.*, *Nanoscale*, 2024, **16**, 4063–4081, <https://doi.org/10.1039/D3NR05123D>.

The authors regret some minor errors in the schematic representations given in Fig. 1. The amended figure, with dashed contouring as described in the caption and the correct protonation states of the aspartate and arginine residues, is shown below.

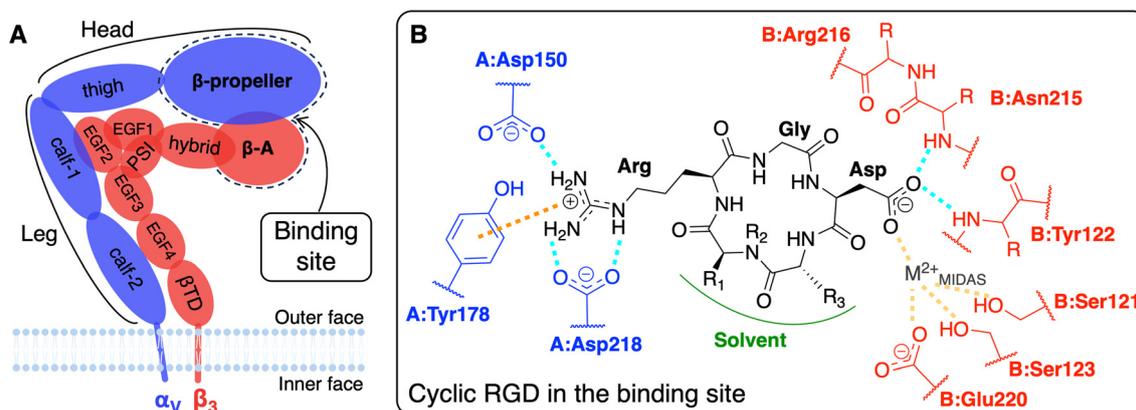


Fig. 1 (A) Integrin $\alpha_v\beta_3$ extracellular segment schematic representation. A dashed line contours the domains of the two subunits which form the binding site. (B) Schematic representation of a generic cyclic pentapeptide ligand and its interactions with the integrin $\alpha_v\beta_3$ binding site, as reported in the literature. In cilengitide R_1 stands for Val side chain, R_2 for CH_3 , and R_3 for D-Phe side chain. In c(RGDyK), the ligand used in this work, R_1 stands for Lys side chain, R_2 for H, and R_3 for D-Tyr side chain. Interactions color code: H-bonds are drawn in cyan, ion- π interactions in orange, and ion coordinating bonds in yellow. The α_v and β_3 subunits and residues are shown in blue and red, respectively. The protein residues are preceded by the letter A and B when they belong to α and β subunits, respectively.

The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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