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Erratum

Erratum to "Molecular modeling of modified peptides, potent inhibitors of the xWNT8 and hWNT8 proteins" [J. Mol. Graph. Model. 26 (7) (2008) 1179–1187]

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The authors regret the misprints, which were made in the paper (mostly in amino acid numbering). The authors are grateful to Dr. Clerc Carron for his important remarks.

In Fig. 2 xWnt8-hWnt8a alignment should be as follows.

Fig. 2. Amino acid sequences alignment for mFzd8-hFzd8 and xWnt8-hWnt8a pairs. The mFzd8 and hFzd8 sequences begin from Glu32 amino acid. mFzd8 sequence is sequence of 1IJY structure.

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Fig. 7 should be as follows.

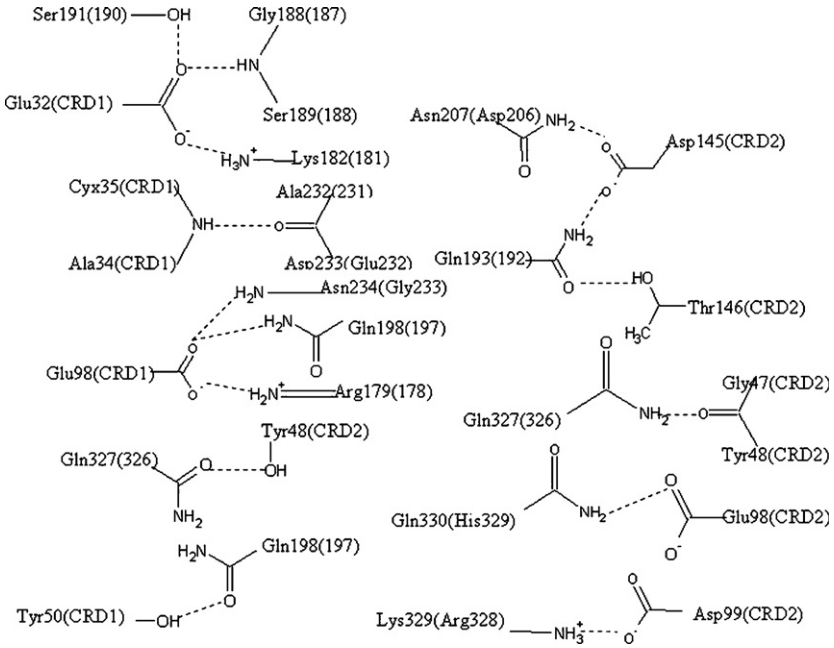

Fig. 7. The interactions mFzd8-xWnt8 and hFzd8-hWnt8a (in parenthesis). CRD1 and CRD2 show corresponding domains of Fzd-receptors. Side chain functional groups are shown for xWnt8 protein. Only functional groups are shown.

Page 1182

The paragraph, which starts with: "The region around the Gln193(192) amino acid is favorable for H-bond formation" was duplicated by the publisher.

Page 1183

Right column, correct text is:

The introduction of hydrophobic 1–4 atomic substituents into ligands is effective for the interactions with the Ile309 amino acid of xWnt8 protein. In the case of the hWnt8-protein the amino acid Val308 corresponds to the Ile309 amino acid of the xWnt8. In the case of hWnt8 protein the hydrophobic region around the Val308 is larger than that of Ile309 and enables one to introduce a hydrophobic substituent with a longer chain. The amino acid residue Glu308(307) can form hydrogen bonds with amino groups and with hydroxyl and amide groups as well. The amino acids Lys306(305), Lys324(323), Lys329(Arg328) (Lys pocket) potentially can bind many negatively charged functional groups, such as carboxyl or phenolate.

Page 1185

Left column, correct text is:

The Gln330 of the xWnt8 protein corresponds to the His329 in the hWnt8 protein, which may be interesting since the Gln330 is not charged, and His329 is charged positively.

Top of the right column, correct text is:

The Asp99 of the CRD2-domain interacts electrostatically with the Lys329(Arg328).

The Asp99 of the CRD1-domain interacts electrostatically with the Arg122(Lys121) and also forms a hydrogen bond with the NH-group of the Ile123(Thr122).

In Fig. 6 correct amino acids numbering is the following: Glu308(307), Lys306(305), Thr307(306), Ile309(Val308), Val331(330). Arg63 and Arg122 side chains should be: $-(CH_2)_3NHC(=NH_2^+)NH_2$.

In Fig. 8 xWnt8-protein surface is shown.

Ref. [18] A. Sali, T.L. Blundell, Comparative protein modelling by satisfaction of spatial restraints. J. Mol. Biol. 234 (1993) 779–815.