Additions and Corrections

2004, Volume 47

Alfonso Carotenuto, Paolo Grieco, Pietro Campiglia, Ettore Novellino, and Paolo Rovero*: Unraveling the Active Conformation of Urotensin II.

Page 1658. The following sentences should be after the third paragraph of the Discussion.

Kinney and co-workers (Kinney, W. A.; Almond, H. R., Jr.; Qi, J.; Smith, C. E.; Santulli, R. J.; de Garavilla, L.; Andrade-Gordon, P.; Cho, D. S.; Everson, A. M.; Feinstein, M. A.; Leung, P. A.; Maryanoff, B. E. Structure-Function Analysis of Urotensin II and Its Use in the Construction of a Ligand-Receptor Working Model. Angew. Chem., Int. Ed. 2002, 41, 2940-2944) reported a structure-function study of U-II that established its minimal active size and key structural features. They used this information, in conjunction with molecular modeling of the GPCR, to derive a three-dimensional structure of the U-II-receptor complex. From visual inspection, the receptor-bound conformation found by these authors shows the WKY pharmacophoric region to be less geometrically compact compared to our model. Since the pharmacophoric distances in our structure nicely agree with those measured in a semirigid nonpeptide agonist, we believe that the "active" U-II conformation is more consistent with our NMR-derived conformation than with the fully theoretical receptorbond conformation found by Kinney and co-workers.

JM040837V

10.1021/jm040837v Published on Web 07/01/2004