Supplementary Material (ESI) for Organic & Biomolecular Chemistry

SUPPORTING INFORMATION

Substituted Pyrazolo[3,4-b]Pyridines as Human A1 Adenosine Antagonists: Developments in the Understanding the Receptor Stereoselectivity

Tiziano Tuccinardi, Alessandra Tania Zizzari, Chiara Brullo, Simona Daniele, Francesca Musumeci, Silvia Schenone*, Maria Letizia Trincavelli, Claudia Martini, Adriano Martinelli, Gianluca Giorgi, Maurizio Botta

Supplementary Figures 1-3

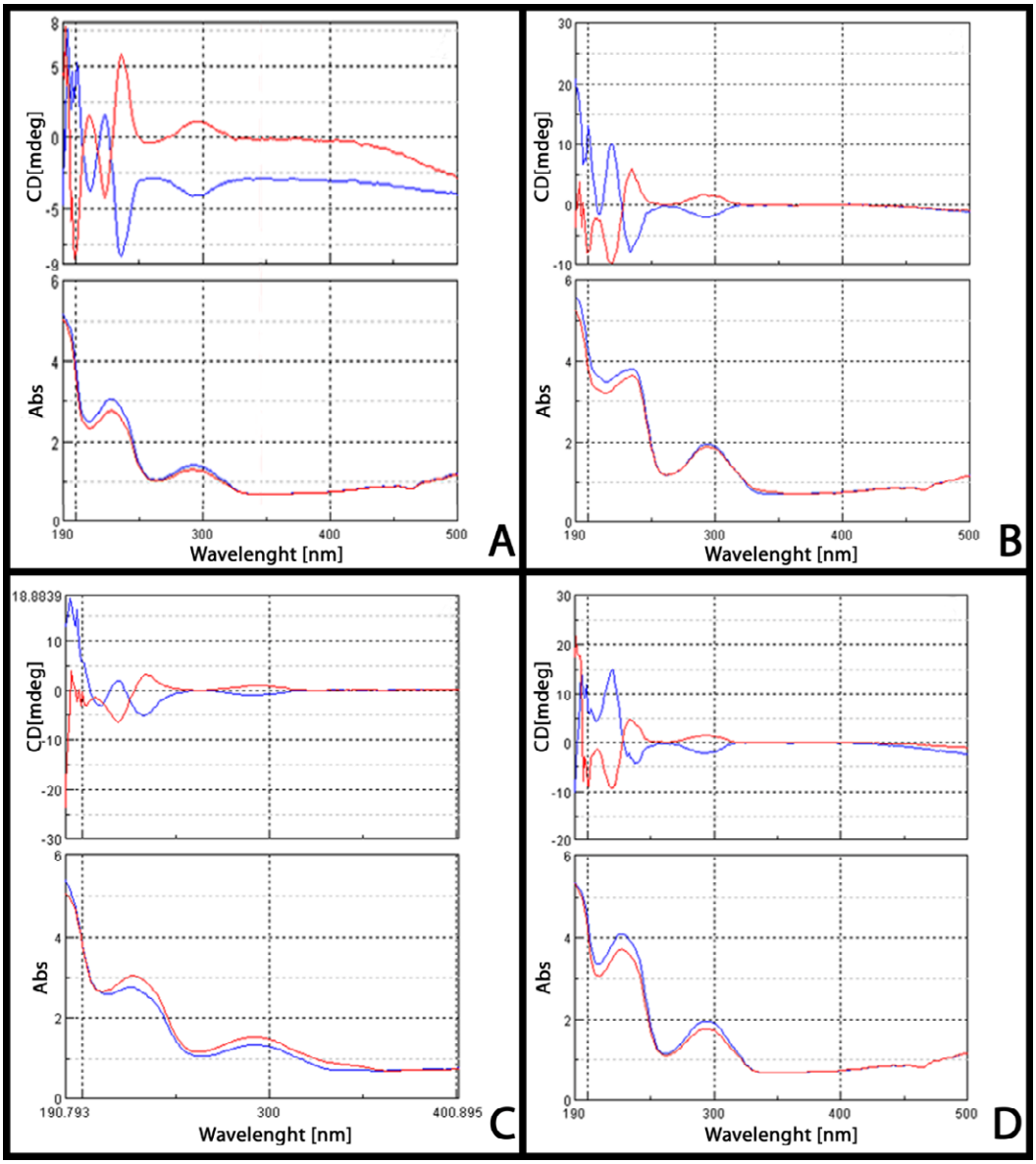

Figure 1. CD spectra (ethanol, room temperature) of the enantiomers of compounds **2** (A), **3** (B), **4** (C), **5** (D) obtained from the racemic mixture separations. The first eluate is blu and the second one is red.

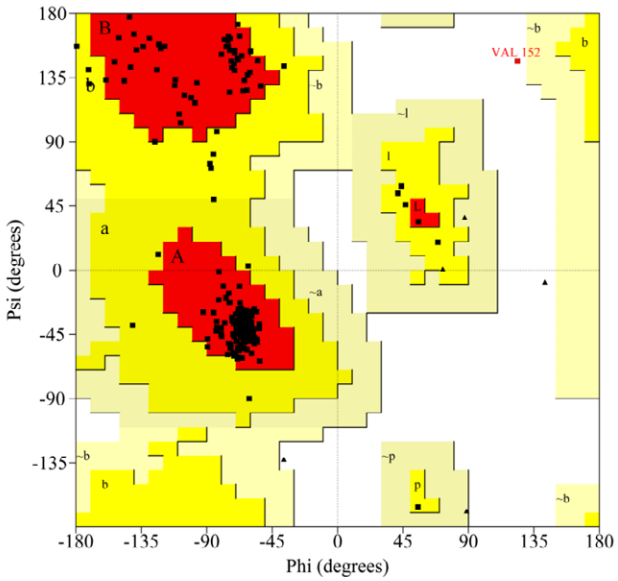

Figure 2. Ramachandran plot of the human A_1AR model. The most favoured regions are coloured red, allowed, generously allowed and disallowed regions are indicated as yellow, light yellow and white regions, respectively. The residues in the disallowed region are marked in red.

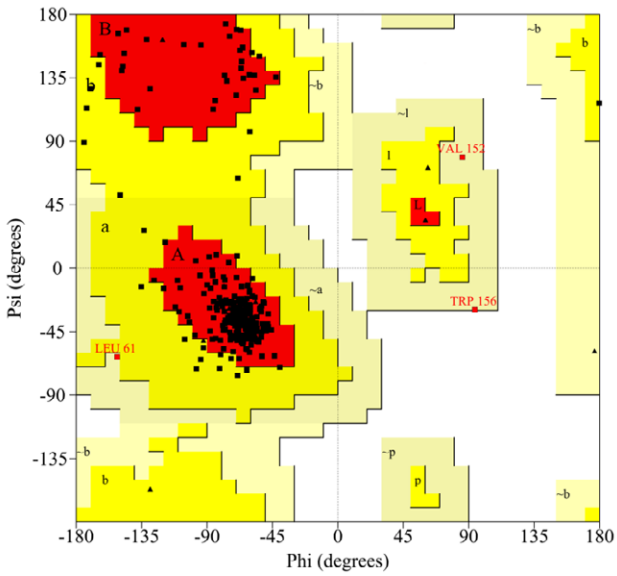

Figure 3. Ramachandran plot of the minimized average structure of the last 4.4 ns of MD of the human A1AR model. The most favoured regions are coloured red, allowed, generously allowed and disallowed regions are indicated as yellow, light yellow and white regions, respectively. The residues in the disallowed region are marked in red.