Homology modelling-driven study leading to the discovery of the first mouse Trace Amine-

Associated Receptor 5 (TAAR5) antagonists

Elena Cichero^a*, Stefano Espinoza^b, Michele Tonelli^a, Silvia Franchini^c, Andrey S. Gerasimov^d, Claudia Sorbi^c, Raul R. Gainetdinov^{b,d,e}, Livio Brasili^c and Paola Fossa^a

^aDepartment of Pharmacy, University of Genoa, Viale Benedetto XV,3 - 16132 Genoa, Italy

^bDepartment of Neuroscience and Brain Technologies, Istituto Italiano di Tecnologia, Genova, Italy

^cDepartment of Life Sciences, University of Modena and Reggio Emilia, Via Campi 183, 41125

Modena, Italy

^dInstitute of Translational Biomedicine, St. Petersburg State University, 199034, St. Petersburg, Russia

^eSkolkovo Institute of Science and Technology, Skolkovo, 143025, Moscow Region, Russia

SUPPORTING INFORMATION



S1. Ramachandran plot of the mTAAR5 receptor. Favoured and allowed values fall within green and orange lines, while disfavoured parameters fall out of orange areas.



S2. Ramachandran plot of the hTAAR5 receptor. Favoured and allowed values fall within green and

orange lines, while disfavoured parameters fall out of orange areas.



S3. Distribution of the hydrophobic (orange) and hydrophilic (cyan) properties on the mTAAR5 (A) and hTAAR5 (B) model surface is depicted.