

New Journal of Chemistry Supporting Information

Design, Synthesis, Biological Evaluation and Molecular Modelling of Substituted pyrrolo[2,1-a]isoquinolinone derivatives: Discovery of Potent Inhibitors of AChE and BChE

Oscar Parravicini¹, Emilio Angelina², Roque Spinelli³, Francisco Garibotto¹, Alvaro S. Siano³, Laura Vila⁴, Nuria Cabedo^{4,5}, Diego Cortes⁵ and Ricardo D. Enriz^{1*}

¹Facultad de Química, Bioquímica y Farmacia, Universidad Nacional de San Luis; Instituto Multidisciplinario de Investigaciones Biológicas (IMIBIO-SL). Ejército de los Andes 950, 5700 San Luis, Argentina.

²Laboratorio de Estructura Molecular y Propiedades, IQUIBA-NEA, Universidad Nacional del Nordeste, CONICET, FaCENA. Av. Libertad 5470, Corrientes 3400, Argentina.

³Laboratorio de Péptidos Bioactivos, Departamento de Química Orgánica, Facultad de Bioquímica y Ciencias Biológicas, Universidad Nacional del Litoral, Santa Fe, Argentina.

⁴Instituto de Investigación Sanitaria INCLIVA. 46010 Valencia, Spain.

⁵Departamento de Farmacología, Facultad de Farmacia, Universidad de Valencia. 46100 Burjassot, Valencia, Spain.

* Corresponding author. E-mail address: denriz@unsl.edu.ar (R. D. Enriz).

Figure S1. AChE inhibitory activity. % of AChE activity as a function of the concentration of compounds **1-15**.

Figure S2. BChE inhibitory activity. % of BChE activity as a function of the concentration of compounds **1-15**.

Figure S3. AChE and BChE inhibitory activity. % of enzymatic activity as a function of the concentration of compounds of rivastigmine.

Figure S4. Spatial view of AChE-**12** and AChE-**13** complexes overimposed.

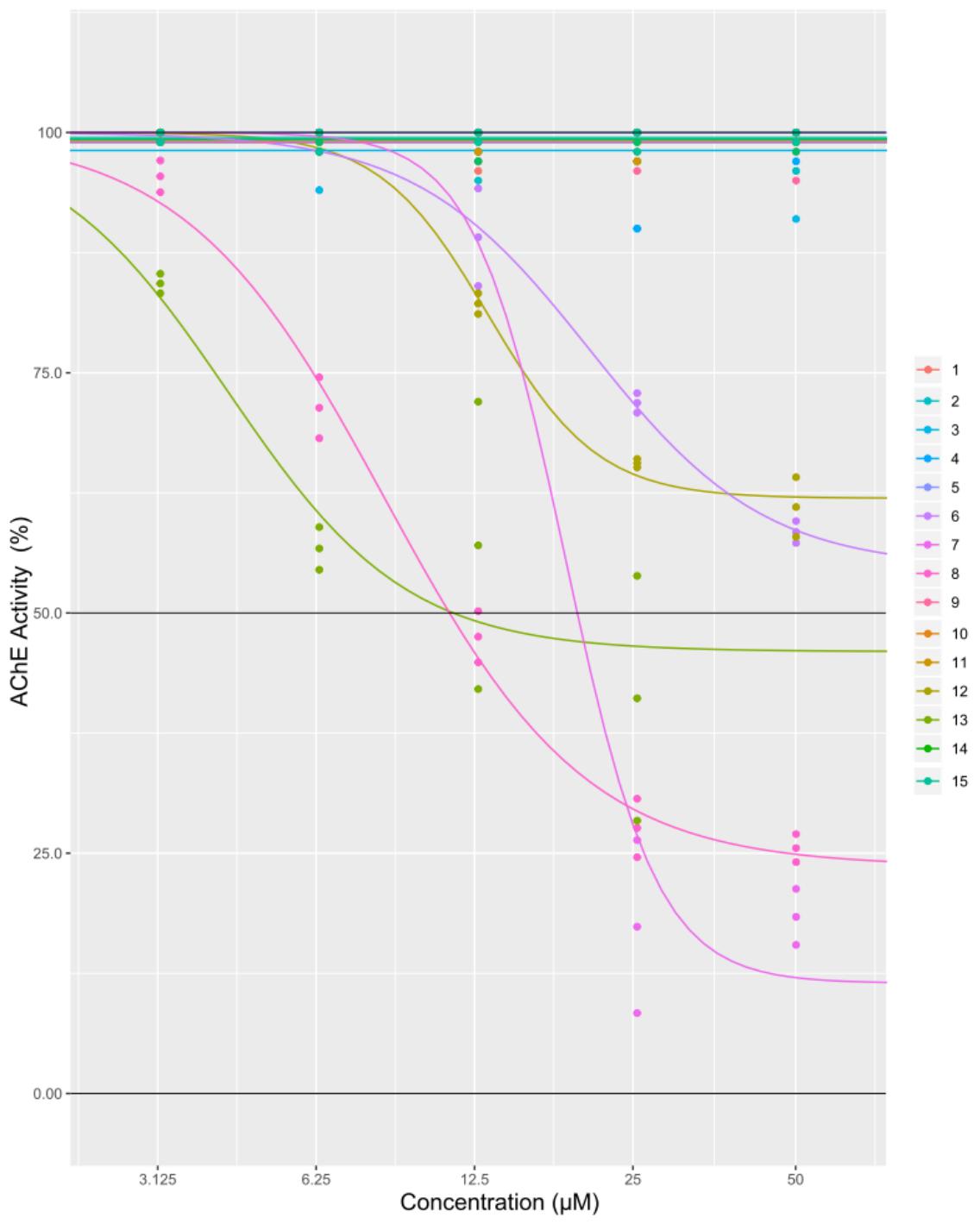


Figure S1. AChE inhibitory activity. % of AChE activity as a function of the concentration of compounds **1-15**.

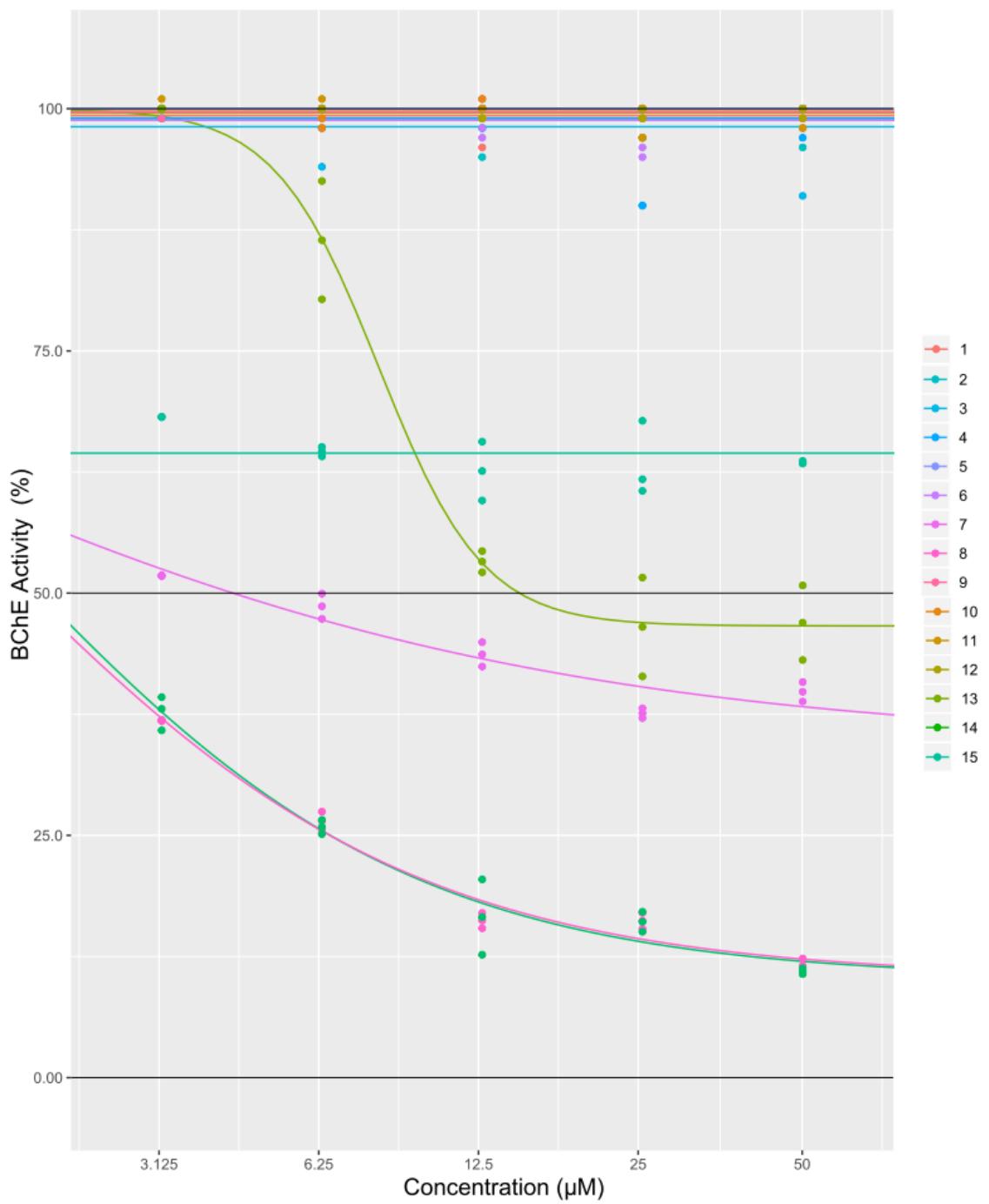


Figure S2. BChE inhibitory activity. % of BChE activity as a function of the concentration of compounds **1-15**.

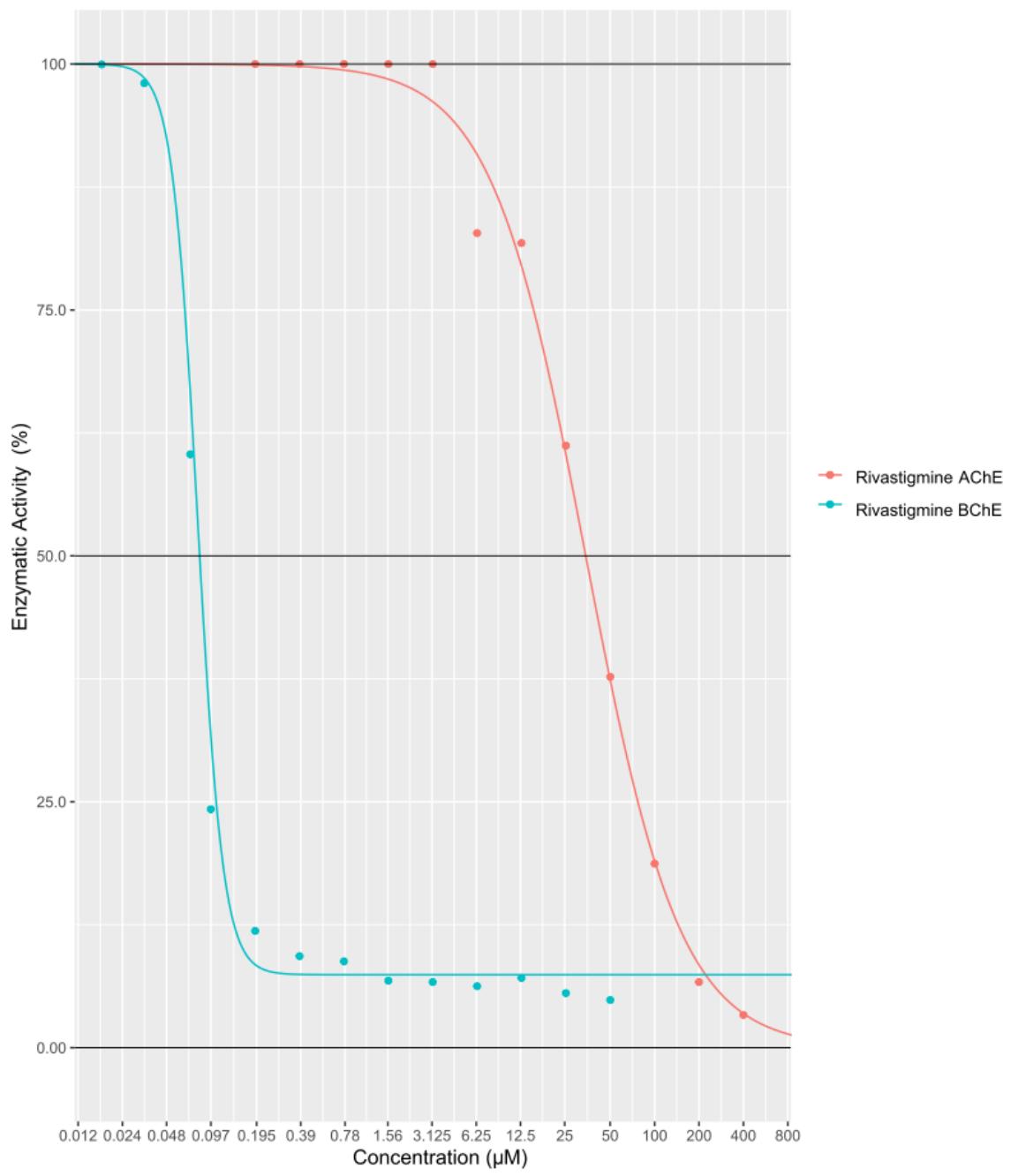


Figure S3. AChE and BChE inhibitory activity. % of enzymatic activity as a function of the concentration of rivastigmine.

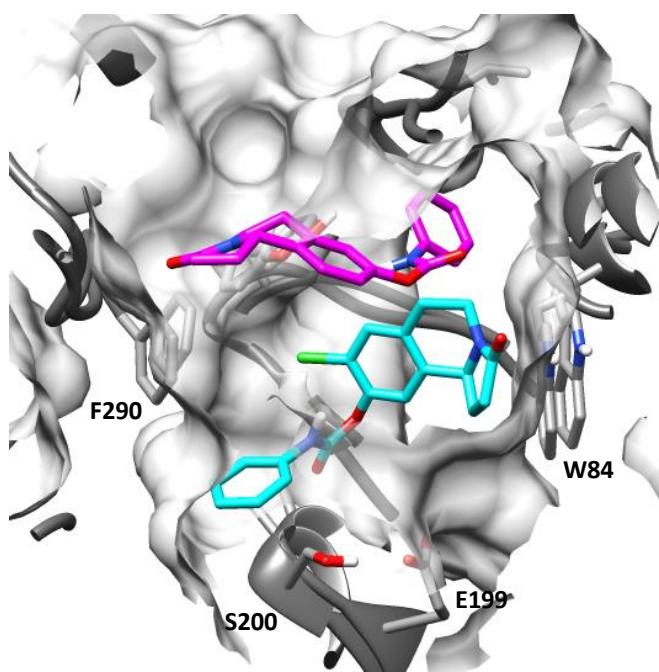


Figure S4. Spatial view of AChE-**12** (magenta) and AChE-**13** (cyan) complexes overimposed for comparison.