Supporting information

Exploring the effectiveness of novel benzimidazoles as CB2 ligands: synthesis, biological evaluation, molecular docking studies and ADMET prediction

Michele Tonelli,*[,a] Elena Cichero,[a] Alì Mokhtar,[b] Alessandro Rabbito,[b] Bruno Tasso,[a] Paola Fossa[a] and Alessia Ligresti[b]

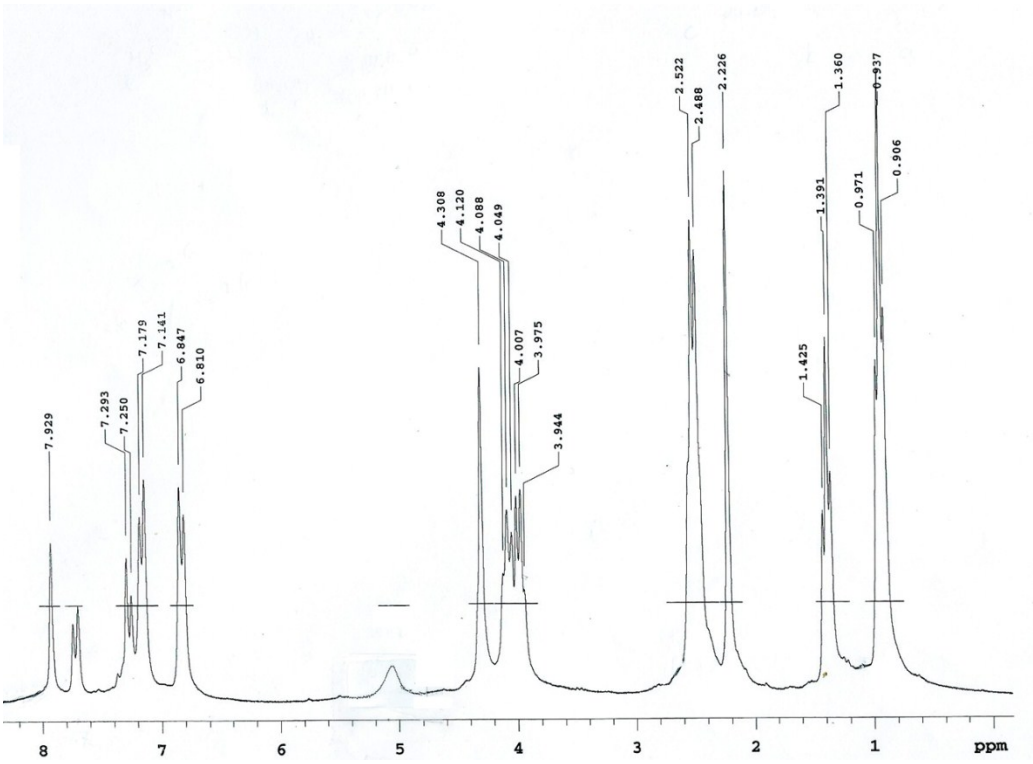
[a]Dipartimento di Farmacia, Università degli Studi di Genova, Viale Benedetto XV, 3, 16132 Genova -Italy.

[b]National Research Council of Italy, Institute of Biomolecular Chemistry, Endocannabinoid Research Group, Via Campi Flegrei 34, 80078 Pozzuoli (Na) - Italy.

Table 1S. Binding affinity values estimated by molecular docking studies of the reference compounds **2b**, **3b** and **5b** (Figure 3) as well as of the compounds **1**-**4**, **8**, **11** and **12** within the hCB2 receptor.

Receptor-Ligand Complex (LeadIT)	Binding Affinity Energy ΔG (kJ/mol)
hCB2-**1**	-15.0
hCB2-**2**	-18.0
hCB2-**3**	-25.0
hCB2-**4**	-21.0
hCB2-**8**	-23.0
hCB2-**11**	-28.0
hCB2-**12**	-8.0
hCB2-**2b**	-37.0
hCB2-**3b**	-46.9
hCB2-**5b**	-43.8

^{1}H NMR spectra of compound **14**.



^{13}C NMR spectra of compound **14**.