

SUPPLEMENTARY INFORMATION

Title:

Synthesis, antidepressant evaluation and docking studies of long-chain alkylnitroquipazines, inhibitors of the serotonin transporter

Authors:

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Figure legends of supplementary material

Figure S1. DPFPG NOE results of **9** x HCl in DMSO-*d*₆ solution. Upper spectrum shows nOe effects and bottom spectrum shows a trace of ¹H NMR in studied solvent. Irradiation of NH signal results in NOE enhancements at marked positions. See assignment in Fig. 2.

Table S1. 5-HT_{1A} receptor binding affinities (K_i , nM) and docking scores (kcal/mol) of **1-12**. The docking scores are based on three parallel docking runs.

<i>Compound</i>	<i>5-HT_{1A} receptor</i>	<i>Docking score</i>
6-NQ	50800 ± 1900	-3.68
1	13700 ± 2400	-2.75
2	18200 ± 300	-2.90
3	842.3 ± 12.6	-4.56
4	2900 ± 800	-1.94
5	2100 ± 400	2.12
6	4900 ± 600	-0.10
7	1700 ± 100	-3.37
8	5200 ± 300	-0.26
9	10600 ± 1800	0.55
10	6700 ± 500	1.46
11	15900 ± 1200	1.48
12	50800 ± 1900	0.98

Table S2: SERT scores (kcal/mol) and localisation of the nitroquinolone moiety.

<i>Ligand</i>	<i>Score</i>	<i>Nitroquinolone</i>
6-NQ	-7.44	Extracellular region
1	-0.17	Central region
2	-6.50	Extracellular region
3	-10.04	Extracellular region
4	-12.82	Central region
5	-16.95	Central region
6	-7.15	Extracellular region
7	-11.88	Extracellular region
8	-8.55	Extracellular region
9	-2.55	Extracellular region
10	-11.94	Central region
11	-0.43	Extracellular region
12	-12.68	Central region