

Supplementary data for the article:

Penjišević, J. Z.; Šukalović, V. V.; Andrić, D. B.; Roglić, G. M.; Šoškić, V.; Kostić-Rajačić, S. V. Synthesis, Biological, and Computational Evaluation of Substituted 1-(2-Methoxyphenyl)-4-(1-Phenethylpiperidin-4-Yl)Piperazines and 1-(2-Methoxyphenyl)-4-[(1-Phenethylpiperidin-4-Yl)Methyl]Piperazines as Dopaminergic Ligands. *Archiv der Pharmazie* **2016**, 614–626. <https://doi.org/10.1002/ardp.201600081>

Supplemental Material: Novel Compounds and Biological Screening Results
Synthesis, Biological and Computational Evaluation of Substituted
(2-Methoxyphenyl)piperazine Dopaminergic Ligands

Jelena Z. Penjišević¹, Vladimir V. Šukalović¹, Deana B. Andrić², Goran M. Roglić², Vukić V. Šoškić³ and Slađana V. Kostić-Rajačić¹

¹ICTM – Center of Chemistry, University of Belgrade, Njegoseva 12, Belgrade, Serbia

²Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, Serbia

³ORGENTEC Diagnostica GmbH, Carl-Zeiss-Street 49-51, Mainz, Germany, Tel. 0049613192580, Fax: 00496131925858, Email: vukic.soskic@orgentec.com.

Compound No.	InChI	Biological Activity (D ₂ K _i) ^a
11	BPKYZOGOXYSDOF-UHFFFAOYSA-N	3278 nM
12	JUXZYKYLTDLWBX-UHFFFAOYSA-N	2538 nM
13	ZIYZTTOPGMGSNC-UHFFFAOYSA-N	708 nM
14	ODAZIJVHBVTDMQ-UHFFFAOYSA-N	1589 nM
15	URXMOGPROZHKBT-UHFFFAOYSA-N	1593 nM
16	MGBUABONVLEBPY-UHFFFAOYSA-N	450 nM
17	HLRHAQCZZBFXHJ-UHFFFAOYSA-N	146 nM
18	XOCICHKBLXOODM-UHFFFAOYSA-N	1465 nM
19	LGTPFUCUWWNSRA-UHFFFAOYSA-N	930 nM
20	KFYGVGLBKGEMBA-UHFFFAOYSA-N	500 nM
21	ZLSJKFSRJNPCIL-UHFFFAOYSA-N	229 nM
22	RMUFFHSONGNQJB-UHFFFAOYSA-N	360 nM
23	ZOTZUMHVOTXUDP-UHFFFAOYSA-N	1779 nM
24	RYRWSCFPXHLLDE-UHFFFAOYSA-N	319 nM

25	LZPRTFLNGLFFHL-UHFFFAOYSA-N	54 nM
26	ZGXDZDPAQYXKHG-UHFFFAOYSA-N	1530 nM

^a All the newly synthesized ligands were evaluated for their affinity to D₂DAR *in vitro* competitive displacement assay of the [³H]-spiperone according to:

Tomic, M. Kundakovic, B. Butorovic, V. Vasilev, D. Dragovic, G. Roglic, D. Ignjatovic, V. Soskic, S. Kostic-Rajacic, *Pharmazie* **2003**, 58, 677-678.