SUPPLEMENTARY MATERIALS

Kaluzhskiy, L. A., Ershov, P. V., Yablokov, E. O., Mezentsev, Y. V., Gnedenko, O. V., Shkel, T. V., Gilep, A. A., Usanov, S. A., Ivanov, A. S. (2021). Screening of potential non-azole inhibitors of lanosterol14-alpha demethylase (CYP51) of Candida fungi. *Biomeditsinskaya khimiya*, 67(1), 42-50. DOI: 10.18097/PBMC20216701042

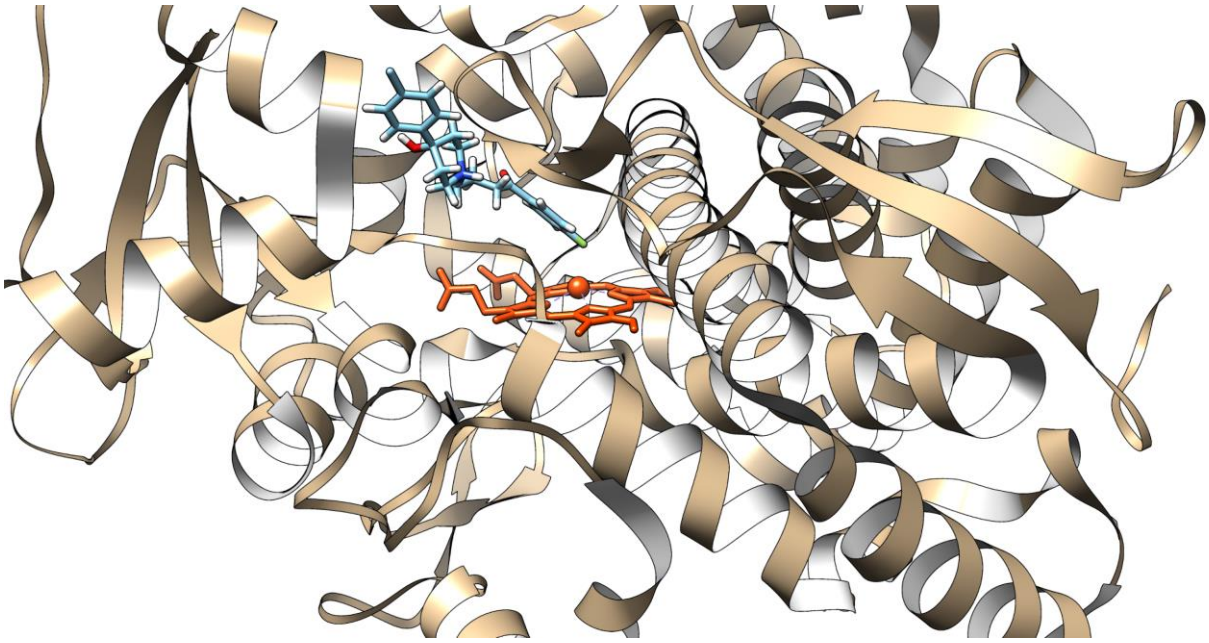


Figure S1. Possible orientation of haloperidol in the active site of CYP51 *Candida albicans* according to molecular docking data.

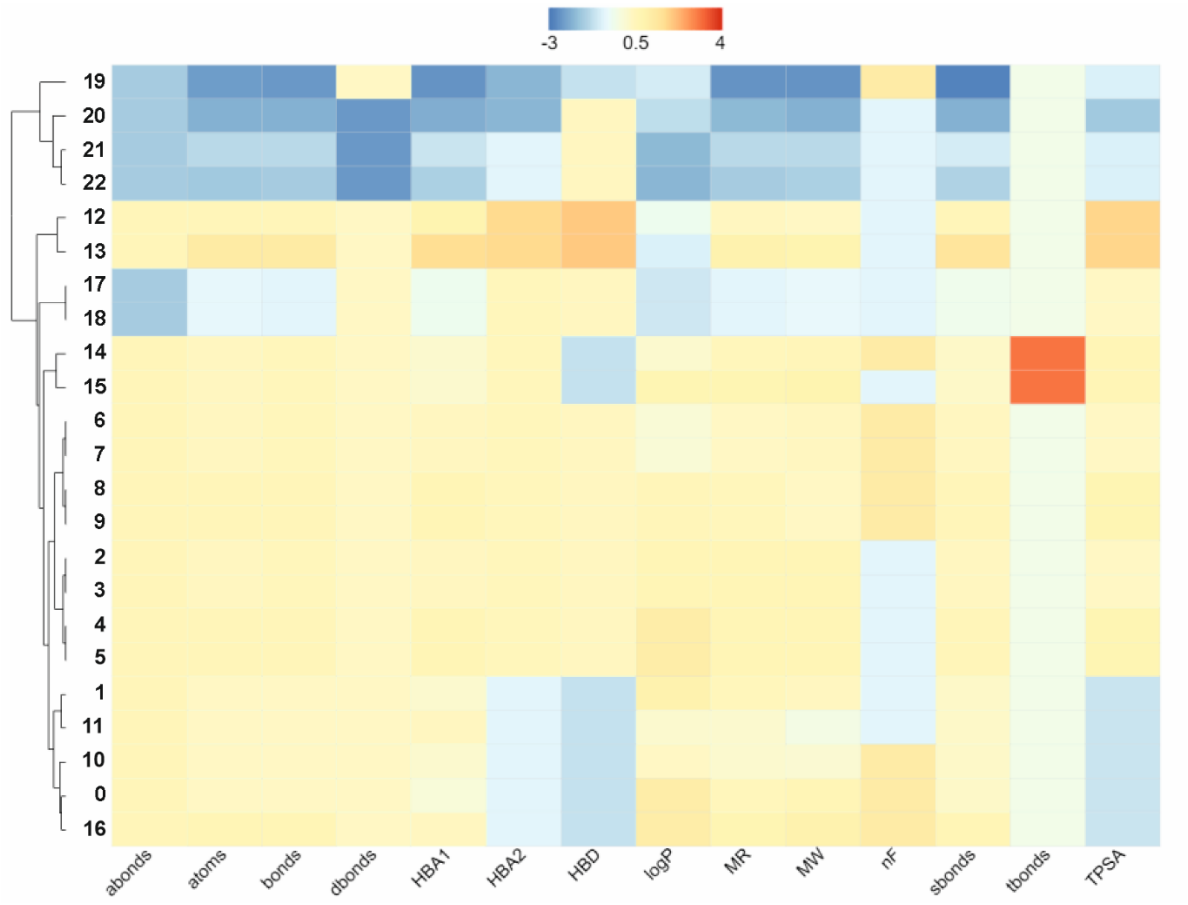


Figure S2. Diagram of physicochemical properties of haloperidol derivatives. Abbreviations: abonds – number of aromatic bonds; atoms – the number of atoms; dbonds – number of double bonds; HBA – number of hydrogen bond acceptors; HBD – number of hydrogen bond donors; logP – octanol / water partition coefficient; MR – molar refraction; MW – molecular weight; nF – number of fluorine atoms; sbonds – number of single links; tbonds – number of triple bonds; TPSA – Topological Polar Surface Area.

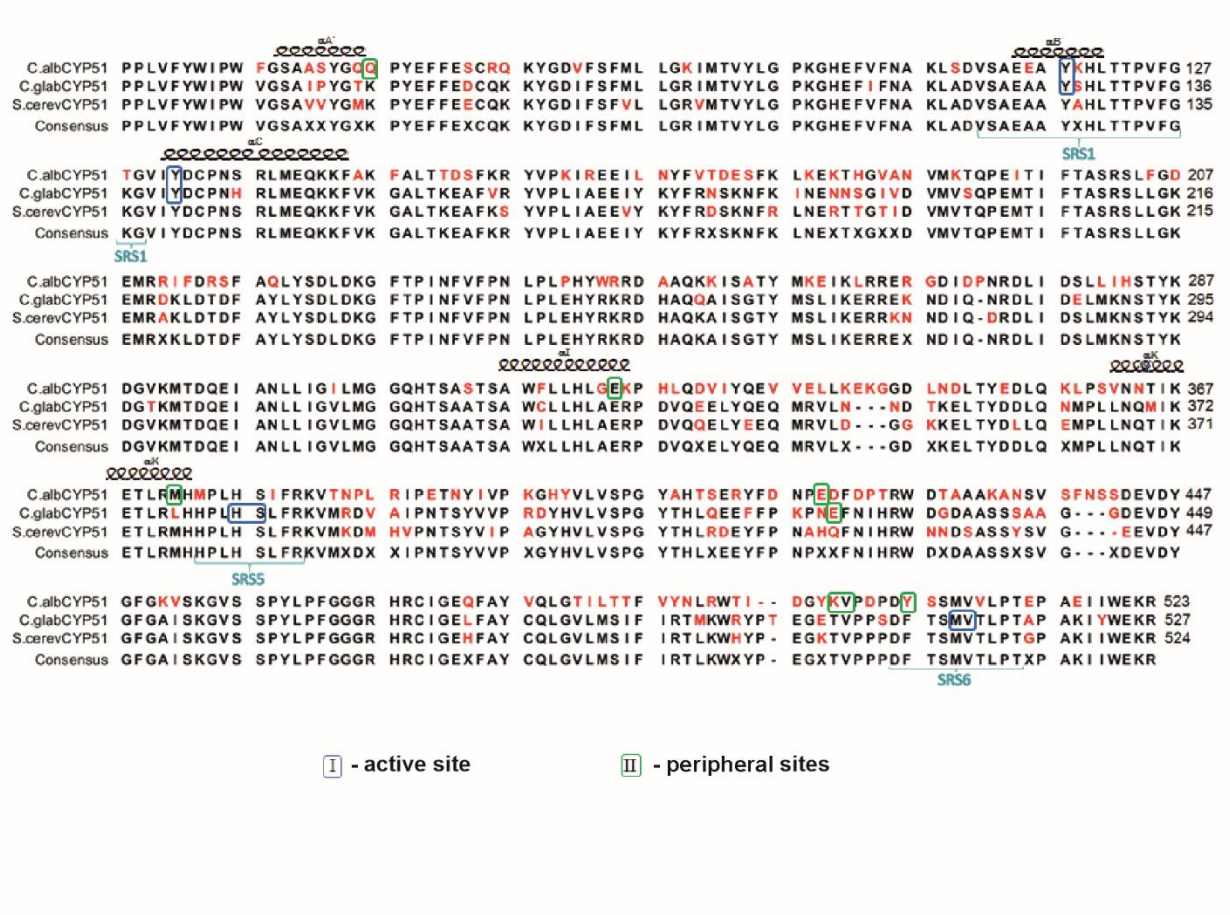
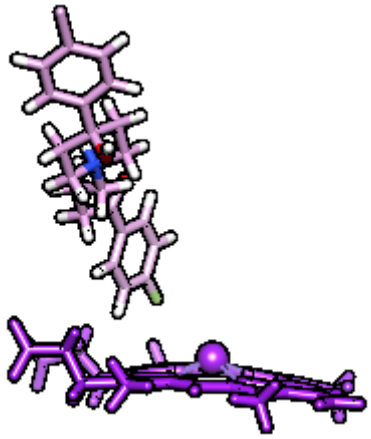
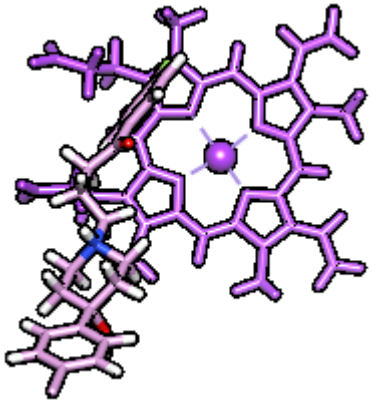
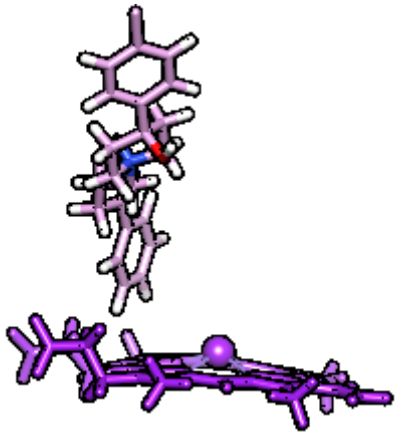
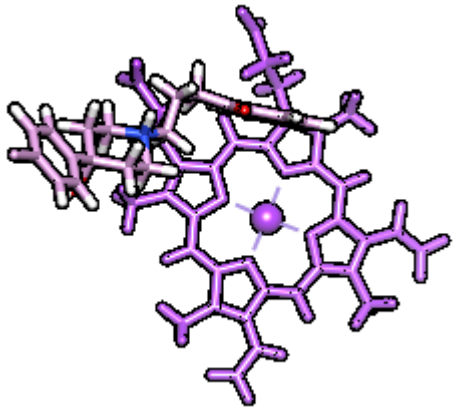
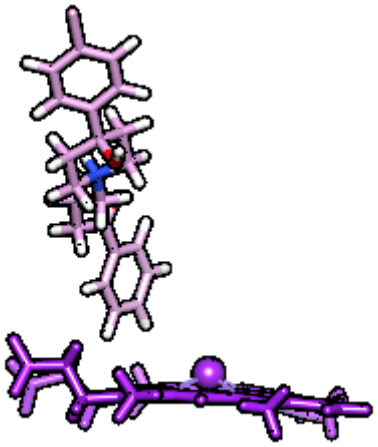
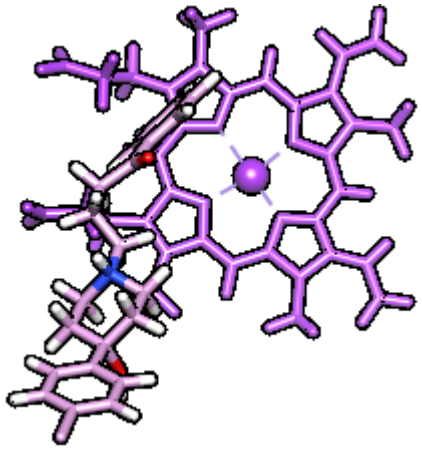
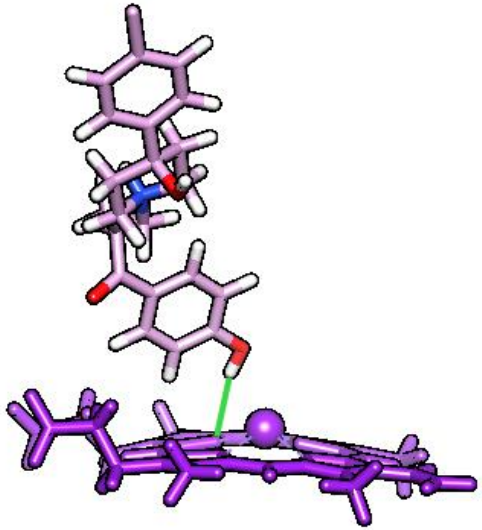
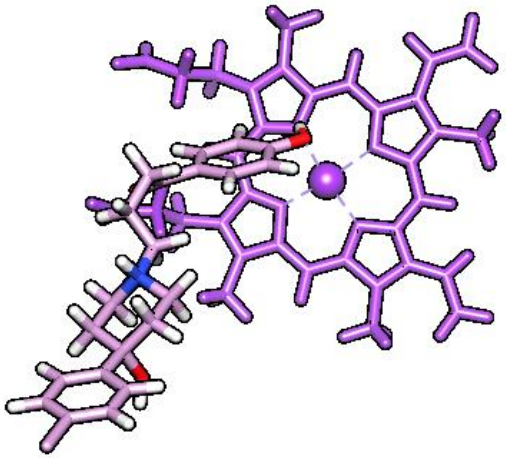
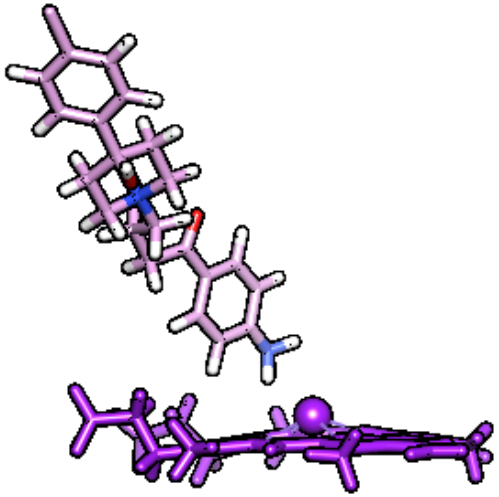
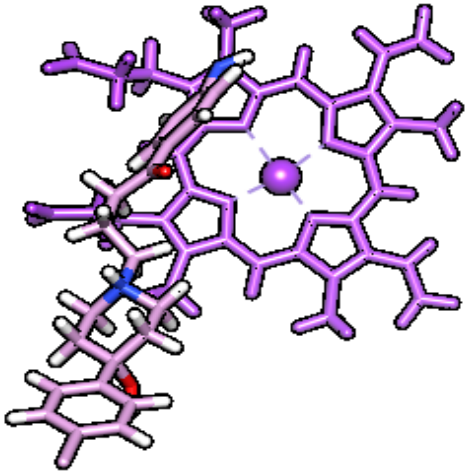
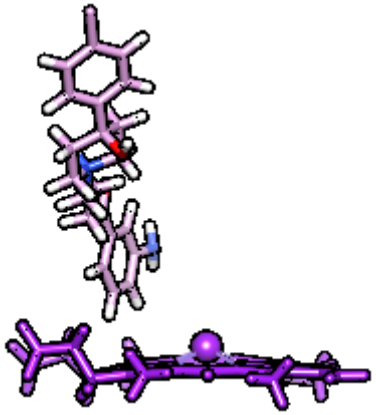
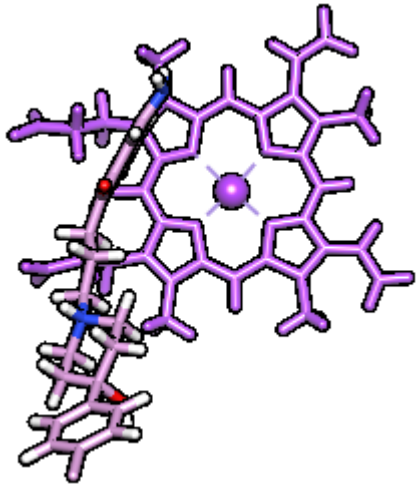


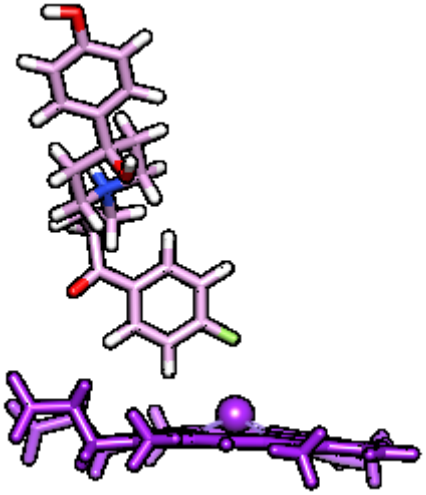
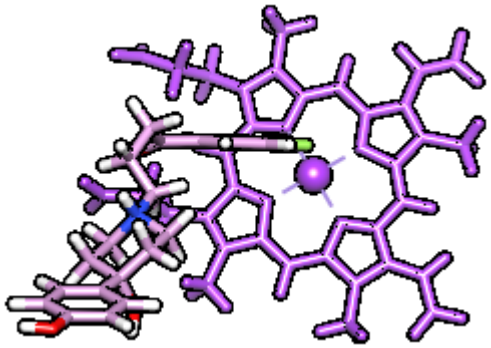
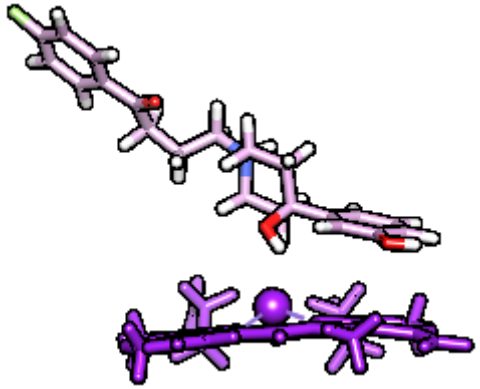
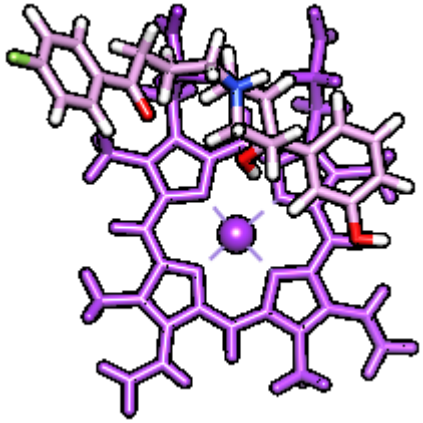
Figure S3. Alignment of CYP51 amino acid sequences of *Candida albicans* (**C. alb**) and *Candida glabrata* (**C. glab**) as well as yeast from the class *Saccharomyces*. The figure shows the amino acid residues that, according to the results of molecular docking, can participate in the binding with acetylsalicylic acid, ibuprofen, haloperidol and chloropromazine (see Table 2). Abbreviations: SRS – Substrate Recognition Site; αB, αC, αK – alpha-helices; Amino acid residues that differ from the CYP51 consensus sequence of different organisms are highlighted in red.

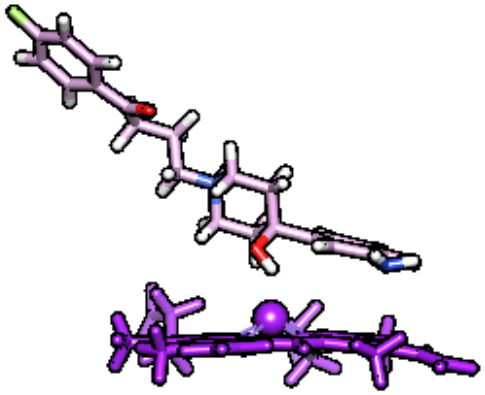
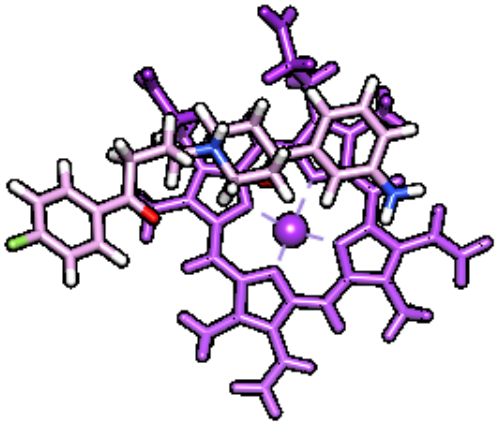
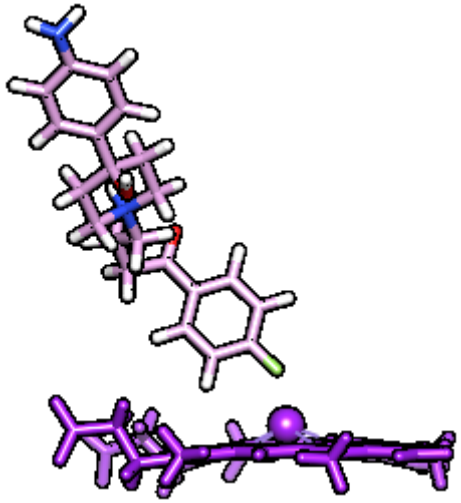
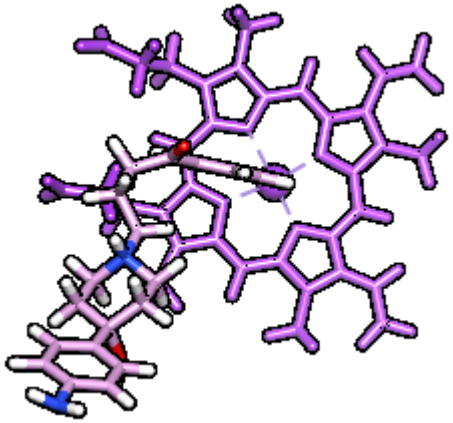
Table S1. Prediction of the orientation of haloperidol structural derivatives (see main text, table 4) relative to the heme cofactor in the CYP51 active site of *Candida albicans* (based on molecular docking data obtained from the SwissDock Web server)

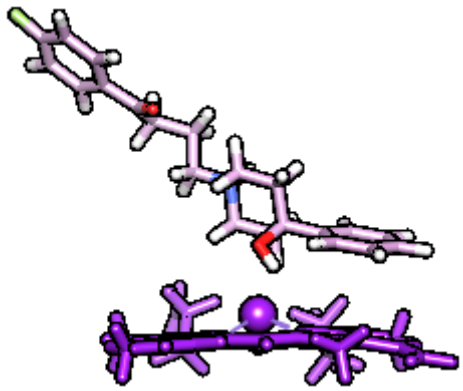
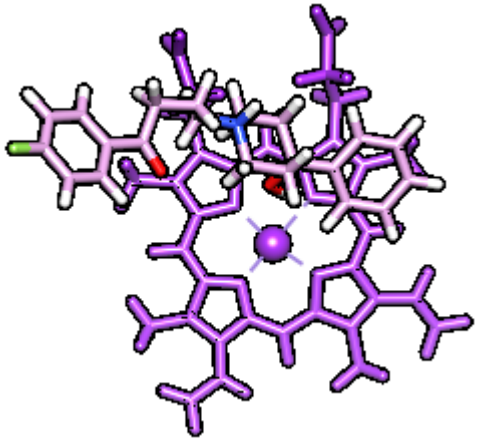
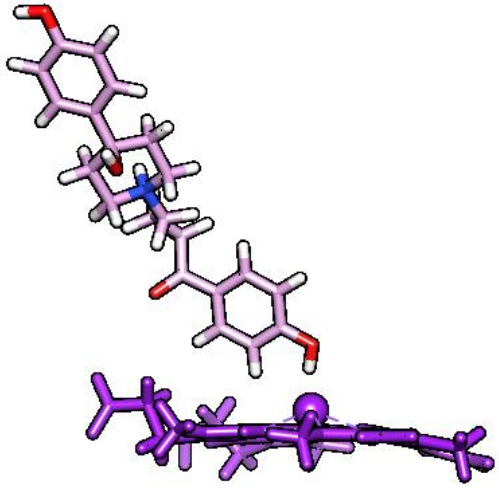
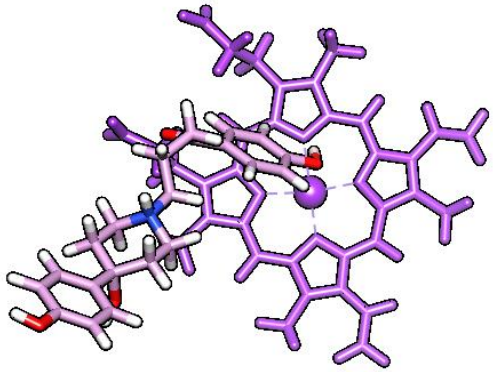
Compound №	**Side view**	**Floor projection**	**Model parameters:** **cluster (rank), *FullFitness (kcal/mol), *SimpleFitness (kcal/mol), **ΔG (kcal/mol)**
0			0(0), -2190, -23.00, -9.3
1			0(0), -2188, -21.85, -9.1

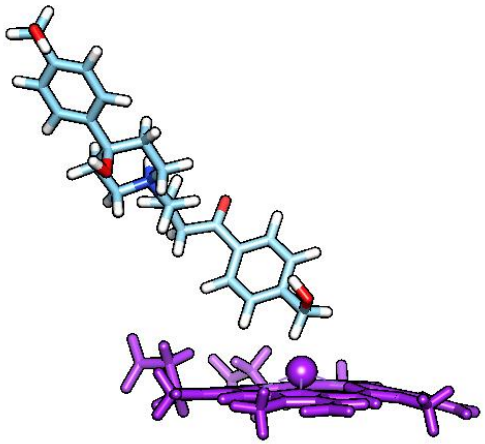
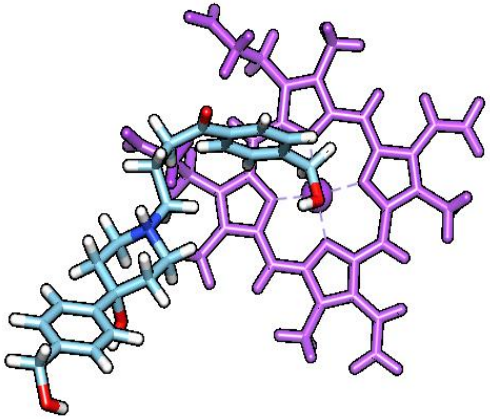
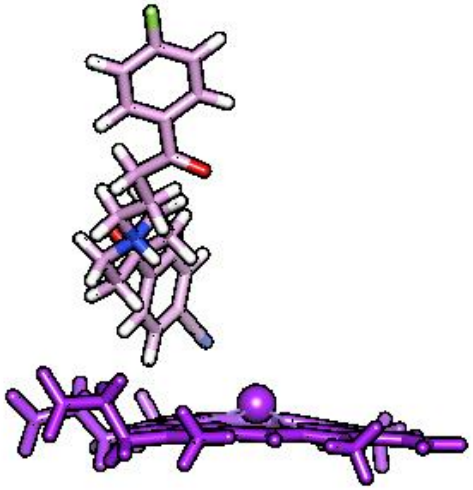
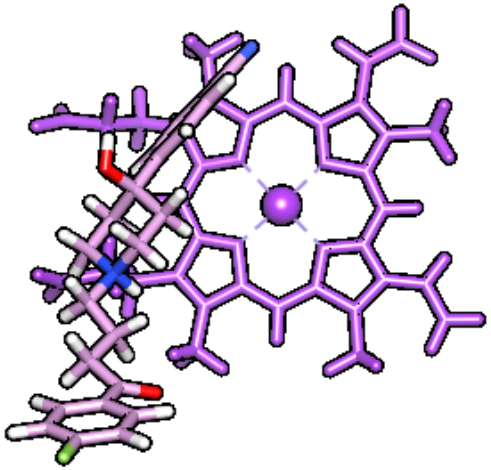
2			0(0), -2188, -21.9, -9.1
3			1(0), -2190, -20.8, -8.6, H+-bond

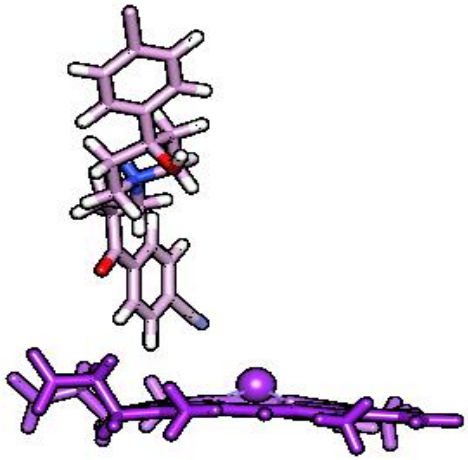
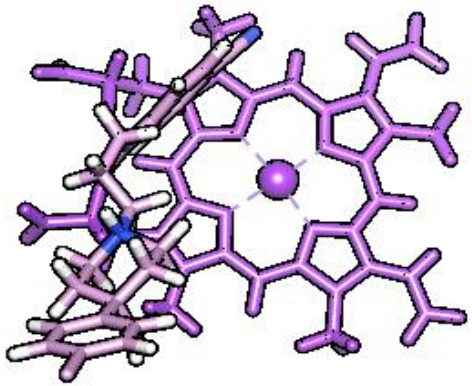
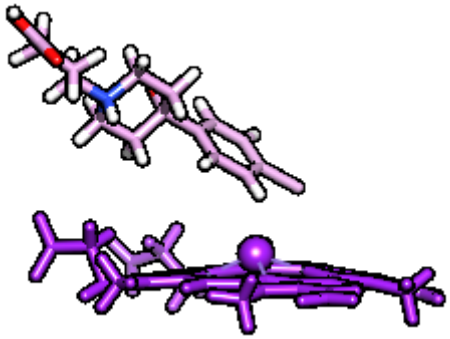
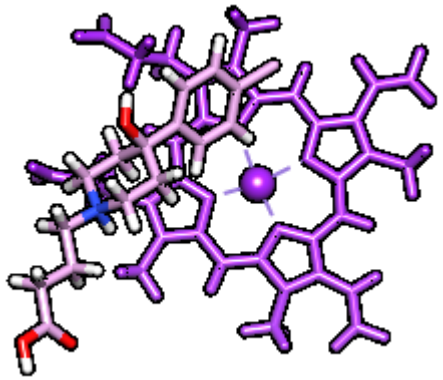
4			0(0), -2196, -17.0, -9.2
5			0(0), -2196, -15.5, -9.1

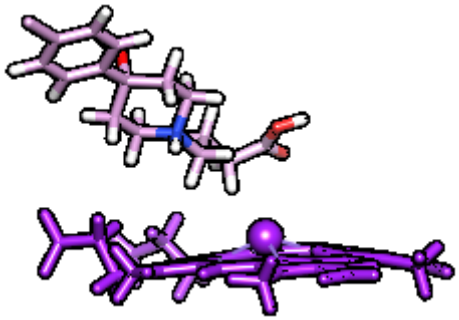
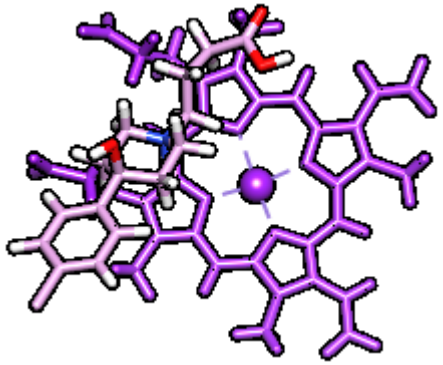
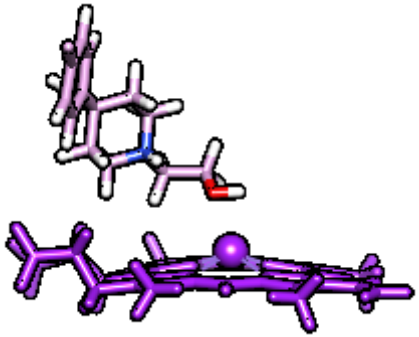
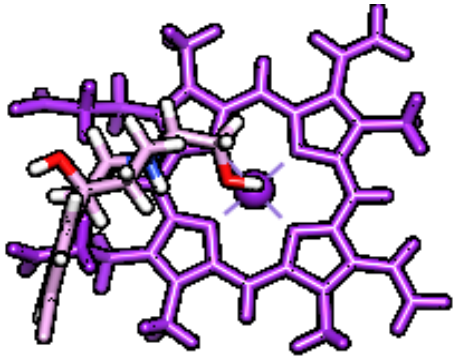
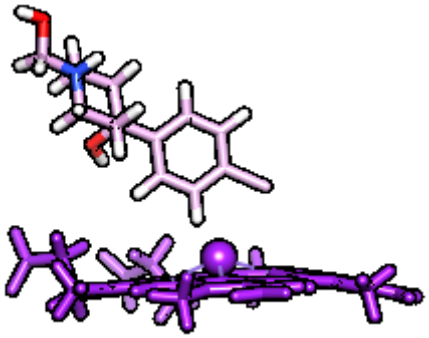
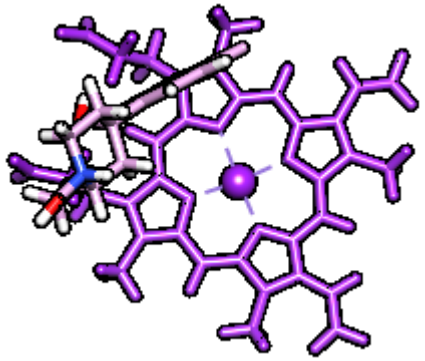
6			0(2), -2188, -18.8, -8.3
7			0(0), -2191, -17.9, -8.6

8			1(0), -2189, -10.2, -8.6
9			0(0), -2192, -14.5, -9.0

10			1(0), -2184, -16.3, -8.7
12			0(2), -2196, -20.3, -8.3

13			0(3), -2182, -16.1, -9.1
14			1(0), -2172, -15.0, -8.4

15			0(1), -2178, -22.3, -8.9
17			1(0), -2219, -30.8, -8.2

18			0(0), -220, -29.0, -8.2
21			0(2), -2168, -13.9, -7.3
22			1(3), -2232, -21.3, -6.9

*Swiss Dock scoring function parameters (for further details see [1,2])

**ΔG — binding energy

REFERENCES

1. *Grosdidier A., Zoete V., Michielin O.* (2011) Nucleic Acids Res, **39**, W270-277. DOI:10.1093/nar/gkr366
2. *Grosdidier A., Zoete V., Michielin O.* (2011) J Comput Chem, **32**, 2149–59. DOI:10.1002/jcc.21797