interactions of some fluorescent cholesterol-like compounds with cholesterol-converting oxidoreductases [1–3].

Here we report about design, synthesis and *in silico* docking evaluation of novel original cholesterol-like steroids bearing fluorescent (NBD, BODIPY or indole) or Raman-active (alkyne, nitrile or pyridine) groups, synthesized in our lab, with respect to their interaction with some pharmacologically-relevant cholesterol-operating proteins of human, namely human cytochromes P450 CYP11A1 and 17A1, transport protein STARD1 and receptor RORγt as well as mycobacterial CYP125 (pdb IDs 3mzs, 3ruk, 3p0l, 3kyt, 2x5w, respectively). The first free proteins realize initial steps of steroidogenesis [2], RORγt controls status of immune T helper 17 cells [4], CYP125 initiates cholesterol degradation in mycobacteria [5].

Our computer-aided simulations have demonstrated previously unknown abilities of the steroidal compounds to realize affine interactions with all the proteins mentioned. This allowed us to speculate about perspectives of the usage of the novel probes for studies of the structural and functional properties of the proteins, giving new information about new potential drugs regulating steroidogenesis and steroidal axis of host-pathogen interaction during tuberculosis.

This work was supported by grants from BRFFI (X16P-065) and Belarusian State Program of Scientific Investigations (№ 20161380).

References

1. Y. V. Faletrov [et. al.]. FEBS J. (2013) 280 : 3109.
2. N. N. Sluchanko [et. al.]. Protein Expr. Purif. (2016) 119 : 27.
3. Y. V. Faletrov [et. al.]. Steroids (2017) 117 : 29.
4. L. Jin [et. al.]. Mol. Endocrinol. (2010) 24 : 923.
5. Ortiz de Montellano P. R. J. Inorg. Biochem. (2018) 180 : 235.

Theoretical study on binding steroid analogues bearing BODIPY fluorophores with cytochrome P450 enzymes and STARD1 transport protein

M. S. Horetski, Y. V. Faletrov, N. S. Frolova, E.V. Rudaya V. M. Shkumatov
Research Institute for Physical Chemical Problems, Belarusian State University, Minsk, Belarus, *e-mail: matvey.horetski@gmail.com*

Cytochromes P450 are the most abundant oxidases identified in all kingdoms of life. These enzymes are steroidogenesis responsible and are necessary for vital activity [1]. STARD1 transport protein allows cholesterol transfer within the mitochondrial membrane, followed by cholesterol–P450 scc

interaction [2]. Thus non-covalent bonded conjugates of fluorescent steroid analogues and non-steroidal BODIPY dyes with P450 family and STARD1 protein are suitable for use in live-cell fluorescent microscopy, flow cytometry and etc. [3, 4]. Today only a few compounds with fluorescent scaffold perform properties similar to nature steroid [4]. We decided to propose some new steroid structuresA-D (Fig. 1) with BODIPY moiety able to interact with cytochromes P450 and STARD1 protein.

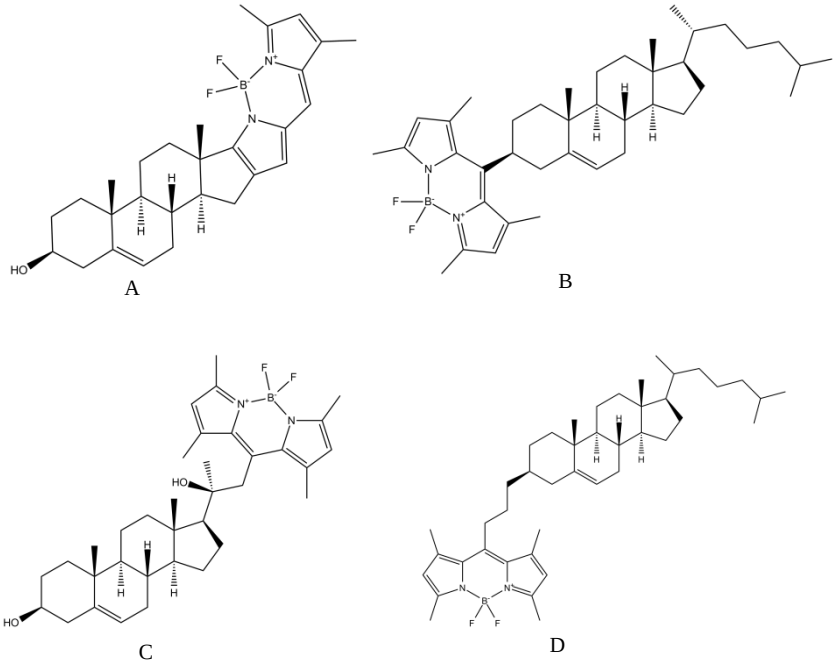

Fig. 1. Proposed BODIPY-labeled steroid structures

For *in silico* work protein structures were taken from the on-line service RCSB Protein Data Bank. Ligand structures for molecular docking were made using Chem Office (CambrigeSoft, USA) with subsequent molecular mechanics (UFF) ground state geometry optimization in Avogadro software (Cambrige, USA). Simulation of ligand-protein interaction was performed in Autodock Vina and Auto Dock Tools (Graphics Laboratory, Scripps Research Institute, USA) software. Calculated free Gibbs energy (kcal/mol) of BODIPY–labeled steroid–protein interactions comparing with native ligands are presented in the Table.

Table. Calculated interaction energies (kcal/mol) of ligands under investigation. PDB proteins codes 3dax, 3v8d and 3sn5 for CYP7A1, 3mzs for CYP11A1, 3p0l for STARD1, 3ruk for CYP17A1, and 5jkw for CYP19A1

	3dax	3v8d	3sn5	3ruk	3mzs	5jkw	3p0l
A	–9.8	–9.8	–10.9	–9.9	–14.0	–10.1	–8.7
B	–10.6	–9.6	–8.8	–9.6	–11.9	–10.4	–8.8
C	–10.5	–9.4	–9.2	–10.6	–9.0	–10.4	–7.5
D	–10.0	–9.6	–10.2	–9.88	–8.7	–9.7	–9.6
Cholesterol	–7.9	–12.2	–12.2	–	–11.9	–	–9.8
Pregnenolone	–	–	–	–11.4	–	–	–
Estrone	–	–	–	–	–	–11.8	–

Theoretical results represent similar affinity of labeled steroids and nature ligands to studied proteins. In case of CYP11A1 affinity to A is better than to native cholesterol. For verification calculation results *in vitro* experiment is required.

Authors are grateful for grant support from the Belarussian State Program of Scientific Investigations (№ 20161380).

References

1. D. C. Lamb [et al.]. JVI. (2009) 83 : 16.
2. C. B. Kallen [et al.]. J. Biol. Chem. (1998) 273 : 41.
3. M. S. Horetski [et al.]. J. Belarus. State. Univ. Chem. (2018) 1, in press.
4. Z. Liu [et al.]. Chembiochem. (2014) 15 : 14.

Methyl methacrylate based resins for road marking systems

M. A. Lasminskaya, I. A. Klimovtsova, E. V. Grinyuk,
G. V. Butovskaya, L. P. Krul
Research Institute for Physical Chemical Problems, Belarusian State University,
Minsk, Belarus, *e-mail: krul@bsu.by*

Copolymers of methyl methacrylate (MMA) with alkyl (meth) acrylates are increasingly being used as the basis for road marking systems [1, 2]. To obtain these systems the copolymers are dissolved in a mixture of MMA with components of redox initiation mixtures for radical polymerization of MMA at ordinary temperatures. However, detailed information concerning the chemical composition of the industrial resins based on MMA, as well as the technological peculiarities of their synthesis is absent.

We determined that the resins of DEGAROUTE®661 (Germany) and INDOPOL HP (Russia), intended for road marking, included copolymers of MMA with n-butyl acrylate (BA), the mole fraction of the latter in the