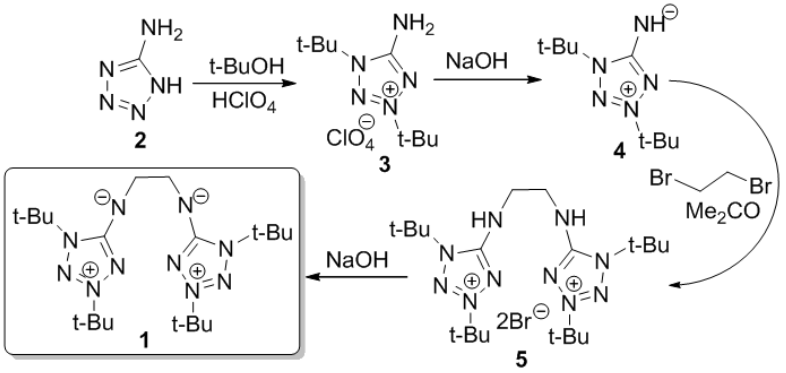

Structures of obtained compounds were characterized by NMR, IR and MS.

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Novel cholesterol-like steroids with artificial side chains: design as molecular probes or potential drugs precursors: docking studies against selected human and mycobacterial steroid-operating proteins

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Various 3-beta-hydroxysteroids with artificial side-chains (substituents at C17) have been developed that are analogues to fluorescent cholesterol, such as 22-NBD-cholesterol, BODIPY-cholesterol. These compounds with azide, alkyne or nitrile groups in side-chains have found popularity due to their properties as small bioorthogonal tags enabling detection *via* both click-chemistry based conjugation and Raman microscopy. Previously we described

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.

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

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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