

## InFarmatik GPCR Fragment library fact sheet

1.) Name: InFarmatik GPCR fragment library.

2.) Library design in brief:

- The objective was to develop a fragment generation tool and a basic set of fragments which could be used in the estimation of GPCR-likeness to targets with known structures. This tool as combined by docking and scoring could be later further completed with new crystal structures of GPCRs and other membrane proteins.
- The in silico work was performed by „mcule.com” with the company’s software suite.
- The concept was validated for 9 selected fragments. All of them showed significant inhibition in D3 binding assays (*in vitro*) at 100 uM concentration, thus experimental validation of our GPCR fragment design approach yielded 100 % hit rate.

3.) GPCR fragment library contains 457 fragments.

4.) Guaranteed purity is 90 % for screening quantities determined by LCMS at 220 nm wavelength. In case of ordering more than 100 mg the delivered purity is at least 95 % determined by proton NMR and by LCMS at 220 nm wavelength.

5.) Cherry picking is allowed. Be aware that price depends on the ordered quantity (number of compounds and weight).

6.) Some representative structures:

