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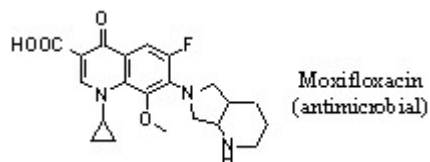
## Exploring Chemical Space for the Need of Medicinal Chemistry – Theory and Practice

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Comprehensive enumeration and generation of structure library of all the theoretically possible compounds, the so-called "chemical universe" or "chemical space" [1] attracted interest of scientists long ago. The interest was driven by the possibility of finding in the chemical space the molecules possessing optimal properties for a particular application before undertaking their synthesis. In this work, a "bottom-up" principle of comprehensive chemical library generation will be illustrated on a particular class of chemical compounds - Conformationally Restricted bicyclic secondary Diamines (CRD). Many compounds possessing fragments of CRD became marketed drugs; one of the most successful examples is shown below. This fact proves advantages of the CRD in drug design. The generation of the CRD library and analysis showed its great potential in medicinal chemistry. Practical aspects will be also discussed.



[1] C.M.Dobson, *Nature*, **432**, (2004), p. 824.