Polysubstituted pyrimidines: biological and chemical properties

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The pyrimidine ring represents an important pharmacophor and a key structural motif of numerous natural, as well as synthetic biologically active compounds. Various polysubstituted pyrimidines were studied in our team for their interesting and miscellaneous properties, namely antiviral (as non-nucleoside reverse transcriptase inhibitors), anticancer (as inhibitors of cyclin-dependent kinases), and anti-inflammatory (as inhibitors of nitric oxide and/or prostaglandin E2 production).

Some derivatives, e.g. polysubstituted 5-nitrosopyrimidines, were studied for their ability to form strong intramolecular hydrogen bonds. Such compounds were suggested to structurally (and hopefully also biologically) mimic bicyclic heterocycles like purines or pteridines.

Two possible rotamers were often observed depending on other substituents attached to the pyrimidine moiety and in several cases, they could even be isolated as chemical species.

Acknowledgments. The study was supported by IOCB AS CR (RVO61388963), by the Ministry of Interior of the Czech Republic (VG20102015046) and by the Czech Science Foundation (grant no. 15-11223S).