Title: MCE-18 - a novel molecular descriptor to reveal current medicinal chemistry trends in Big Pharma.

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Summary:
The paradigm of “drug-like-ness” dramatically altered the behavior of the medicinal chemistry community for a long time. In recent years, scientists have empirically found a significant increase in key properties of drugs that have moved structures closer to the periphery or the outside of the rule-of-five “cage”. Herein, we show that for the past decade, the number of molecules claimed in patent records by major pharmaceutical companies has dramatically decreased, which may lead to a “chemical singularity”. New compounds containing fragments with increased 3D complexity are generally larger, slightly more lipophilic, and more polar. A core difference between this study and recently published papers is that we consider the nature and quality of sp3-rich frameworks rather than sp3 count. We introduce the original descriptor MCE-18, which stands for medicinal chemistry evolution, 2018, and this measure can effectively score molecules by novelty in terms of their cumulative sp3 complexity.
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