[MS45-P11] Modification of pharmaceutical substances for structure analysis Václav Eigner,[a] Jan Čejka[a]

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Pharmaceutical substances are one of the most important compounds produced nowadays. Since the borderline between poison and efficient drug is really thin, they are thoroughly studied before introduction to the market. Not only full chemical composition must be known, but also the absolute structure. The X-ray structural analysis is one of a few analytical methods that can provide the configuration on stereogenic centers. Even though the availability of this method makes it the first choice for absolute structure studies, the demand on sample quality is really high. The single crystals, with no or a few crystallographic defects, are needed for the analysis. The preparation of such material is a challenging task and sometimes it simply cannot be achieved. This is a case of the most successful drug of our time atorvastatin calcium, which is known by the trade name
Lipitor® on the market. This pharmaceutical substance is described by powder diffraction only and not even cell parameters were clearly specified [1, 2]. Even though the structure cannot be directly determined, we can still determine structure of modified pharmaceutical substance. Though raw data will change, partial information will be usable for description of the original structure. For example the absolute structure will either remain the same or becomes inverted in a defined way. The structure of timoprazole [3] will be presented. So far no crystals structures of this particular member of prazole family were published. Several structural modifications of 2-[(pyridin-2-ylmethyl) sulfanyl]1*H*-benzimidazole will be presented as well. The system of present noncovalent bonds will be described, and the conclusions about the structural similarities of modified structures analogous to timoprazole will be made. Also the advancements in atorvastatin calcium modification will be presented.

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