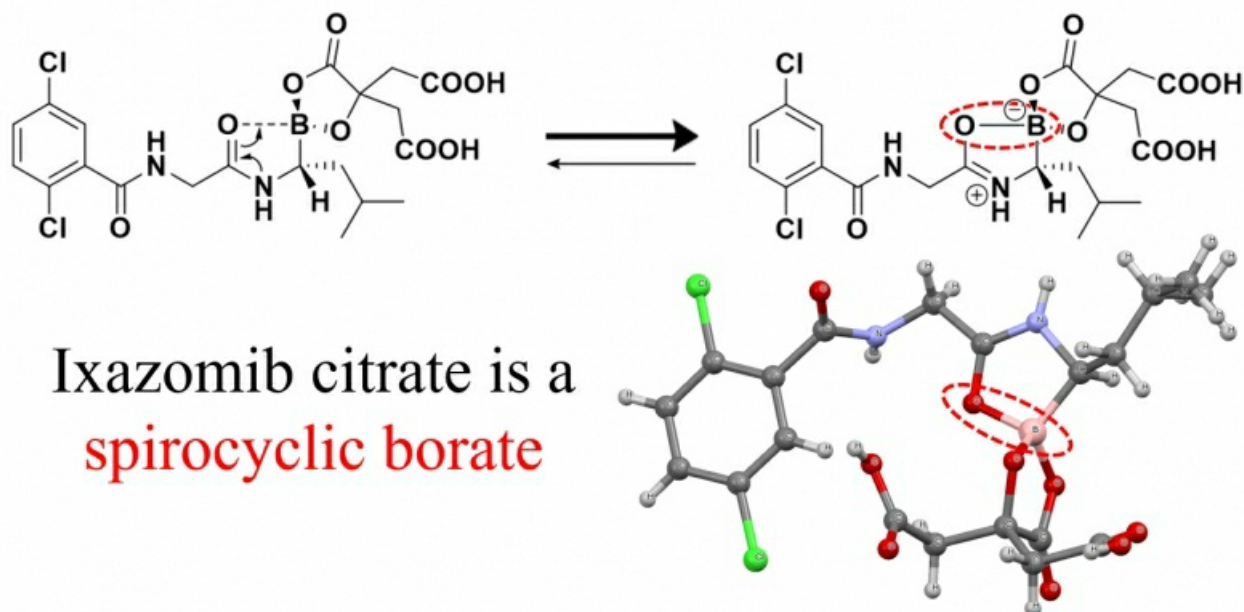


*True molecular structure of ixazomib citrate*Eliska Skorepova<sup>1</sup>, Igor Cerna<sup>2</sup>, Ruzena Vlasakova<sup>2</sup>, Vit Zvonicek<sup>1</sup><sup>1</sup>University Of Chemistry And Technology Prague, Prague 6, Czech Republic, <sup>2</sup>Zentiva k.s., Prague, Czech Republic  
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Ixazomib citrate is a very recently approved anti-cancer drug. In all currently available literature, the molecule is characterized as containing a borate cycle formed when ixazomib is reacted with citric acid to form a stabilized ixazomib citrate that can be administered orally. However, in this work, we will show that none of the up-to-date presented structural formulas of ixazomib citrate are fully accurate. Through the combination of single-crystal and powder X-ray diffraction, solid-state NMR and DFT quantum mechanical calculations we show that, in addition to the citrate ring, another 5-membered ring is formed. These two rings are connected by the boron atom, making this compound a spirocyclic borate.

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