ChemPager and how to make 37 kg of RG7834

Georg Wuitschik

F.Hoffmann-La Roche Ltd., Grenzacherstrasse, 4070 Basel Georg.wuitschik@roche.com

For any given compound there are a myriad ways of synthesis. What constitutes a GOOD route however is difficult to pin down and changes significantly from discovery chemistry to development. This talk seeks to elucidate the journey of RG7834 from initial tox batches to its demise as a potential treatment against Hepatitis B:

In this talk, the different routes to prepare this compound will be discussed as well as the problems encountered along the way, and an attempt will be made to compare them using data analysis. For this, we developed and published ChemPager. ^[1] This tool can convert a broad variety of input data into actionable metrics and can be used to perform scenario calculations and predictions ^[2].

- [1] D. Kaiser, J. Yang, G. Wuitschik, Org. Process Res. Dev, 2018, 22, 1222-1235.
- [2] H. Loureiro, M. Prem, G. Wuitschik, *Chimia*, **2019**, *73*, 724-729.