Impact of the Digital Revolution on the Future of Pharmaceutical Science

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"Time to Market" for registering a new medication usually takes 10-12 years. During discovery of a new drug computer assisted drug design plays an important role for optimizing its biological performance, and for reducing side effects. However, during the early development of a drug delivery vehicle such as a tablet or a capsule formulation, **F**ormulation **C**omputer **Ai**ded **D**esign (**F-CAD**) is not yet part of the standard workflow in the pharmaceutical industry This is surprising since computer aided design of vehicles of the automotive and aircraft industry is a standard procedure. Shionogi of Japan was the first company to successfully introduce F-CAD of CINCAP by Go Kimura after completing his PhD thesis[1] at the University of Basel. The core module of F-CAD is the calculation of the Drug Dissolution profile of the Solid Dosage Form. This software uses as first principle the Cellular Automata approach, which is part of the Conway's[2] "Game of Life". For calibration purposes of the type of the in-vitro dissolution method, it is necessary to manufacture at least one F-CAD formulation in the real world. Thus, F-CAD can be used for virtual manufacturing, and for the virtual exploration of the formulation design space[3,4] by using design of experiments (DOE). This workflow leads to important cost savings during the development and scaling up phase being based on quality by design. The presentation also includes a schematic description of the "Holy Grail" coined by Sally Greb (slide adapted) of Pfizer, being described as combination of the virtual laboratory for the design and for manufacturing solid dosage forms, that is most important for implementing the virtual patient[5] project. Indeed, the optimal "Holy Grail" concept covers pharmacometrics and computational disease modeling including software such as DDD plus, Gastro plus, Simcyp, PK-SIM etc. In conclusion, today it is possible to virtually manufacture a tablet of a defined amount of drug substance for large scale industrial production leading to the most challenging goal of the VIRTUAL PATIENT project and question: In future, will it be possible to administer a virtual tablet to a virtual patient saving time and money for expensive clinical trials?

[1]http://edoc.unibas.ch/diss/DissB_9886

[2]https://en.wikipedia.org/wiki/Conway%27s_Game_of_Life

[3]D. Maneerojpakdee, A. Mitrevej (†), N. Sinchaipanid, J. Nowak, H. Leuenberger, An attempt to adopt the workflow of the automotive and aircraft industry for the design of drug delivery vehicles, Pharm Tech Japan, 33, 11, (2017),145（2381) - 156（2392).

[4]H. Leuenberger and M. Leuenberger, Impact of the Digital Revolution on the Future of Formulation Science", European Journal of Pharmaceutical Sciences, 87, (2016) 100-111, invited paper.

[5]Virtual patient and in silico design of solid dosage forms, 12th PBP World Meeting, May 11-14, 2021, invited presentation.