My 50 Years of Chemoinformatics Research

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My lecture will show my journey from organic chemistry and theoretical chemistry to chemoinformatics. I hope that the audience will benefit in their own research from the presentation of the decisions that were made to develop this new field of research and to adjust my research to funding possibilities. Applications of chemoinformatics to synthesis design and structure elucidation as well as to diverse aspects of drug design will be presented. Chemistry has gained most of its knowledge from data. Therefore, much work was put into the building of databases on chemical information. And, quite early on, chemistry became a field of application for artificial intelligence methods, most notably of artificial neural networks.[1]

More details on my history in chemoinformatics can be obtained in the Summer 2023 Newsletter of the Royal Chemical Society Interest Group Chemical Information and Computer Application Group on pages 5-11:
https://www.rsc.org/globalassets/03-membership-community/connect-with-others/through-interests/interest-groups/cicag/cicag-newsletter-summer-2023.pdf

[1] *Chemistry in Times of Artificial Intelligence*, J. Gasteiger, *ChemPhysChem,* **2020**, *21*, 2233-2242.