

Practical realities of computer-aided drug design

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Computational chemistry can provide valuable tools for use at various stages of drug discovery. It is nevertheless important to continually assess the capabilities of such tools in a way that takes account of the wider environment. The practical application of various computational methods at GSK will be described covering a diverse spectrum of applications. Particular emphasis will be placed on the impact and opportunities provided by new technologies and methodologies and on some of the key challenges that we face.