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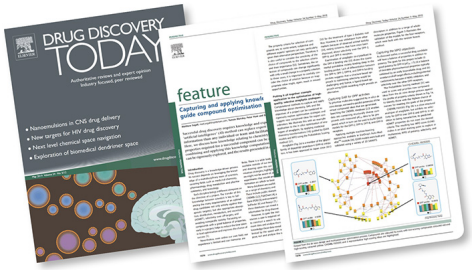
Successful drug discovery requires knowledge and experience across many disciplines, and no current 'artificial intelligence' (AI) method can replace expert scientists. However, computers can recall more information than any individual or team and facilitate the transfer of knowledge across disciplines. Here, we discuss how knowledge relating to chemistry and the biological and physicochemical properties required for a successful compound can be captured. Furthermore, we illustrate how, by combining and applying this knowledge computationally, a broader range of optimisation strategies can be rigorously explored, and the results presented in an intuitive way for consideration by the experts.



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