
Exploring ethnobotanical uses of the African flora for the search of target base anti-cancer agents using mechanism base assays

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Despite continuing scientific and commercial interests in cancer research around drug discovery, both developing and developed countries are still trapped in the grip of this deadly and dreadful disease.¹ Naturally occurring compounds represent about half of the chemotherapeutic agents which have so far been put on the market for cancer treatment. In this study we have developed a new data base (AfroCancer) comprising of ~ 400 compounds from African medicinal plants, which have shown *in vitro* and/or *in vivo* anti-cancer, cytotoxic and antiproliferative activities.² Diversity analysis of the AfroCancer data base has been carried out in comparison with known anti-cancer agents comprising ~ 1,500 published naturally occurring plant-based compounds from around the world, to show that the two data sets do not occupy the same chemical space.^{2,3} To demonstrate the potential utility of the database for *in silico* screening, the interactions between the compounds from the AfroCancer data base and selected anticancer drug targets have been analyzed by *in silico* modelling. Additionally, an *in silico* assessment of toxicity of the AfroCancer database was carried out with the use of eighty-eight (88) toxicity endpoints predicted by Lhasa's expert knowledge-based system (Derek),⁴ showing that only an insignificant proportion of the promising anti-cancer agents could show high toxicity profiles.

Key words

Cancer, Africa, Natural products, Chemotaxonomy, Cheminformatics

References

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