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Acalabrutinib as a novel hope for the treatment of breast and lung cancer: an in-silico proof of concept

[Khaparkhantikar, Kedar^a](#); [Maji, Indrani^a](#); [Gupta, Sunil Kumar^b](#); [Mahajan, Srushti^a](#); [Aalhate, Mayur^a](#);[Sriram, Anitha^a](#); [Gupta, Ujala^a](#); [Guru, Santosh Kumar^c](#); [Kulkarni, Prachi^d](#); [Singh, Pankaj Kumar^a](#) [Save all to author list](#)^a Department of Pharmaceutics, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, India^b Department of Bioinformatics, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, India^c Department of Biological Science, National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad, India^d Department of Physiology, Shri B. M. Patil Medical College, Hospital & Research Centre BLDE (Deemed to be University), Karnataka, Vijayapura, India[Full text options](#) [Export](#) [Abstract](#)[Author keywords](#)[Reaxys Chemistry database information](#)[Indexed keywords](#)[Sustainable Development Goals 2023](#)[SciVal Topics](#)[Chemicals and CAS Registry Numbers](#)[Metrics](#)**Abstract**

Drug repurposing is proved to be a groundbreaking concept in the field of cancer research, accelerating the pace of de novo drug discovery by investigating the anti-cancer activity of the already approved drugs. On the other hand, it got highly benefitted from the advancement in the in-silico tools and techniques, which are used to build up the initial “proof of concept” based on the drug-target interaction. Acalabrutinib (ACL) is a well-known drug for the treatment of hematological malignancies.

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But, the therapeutic ability of ACL against solid tumors is still unexplored. Thereby, the activity of ACL on breast cancer and lung cancer was evaluated utilizing different computational methods. A series of proteins such as VEGFR1, ALK, BCL2, CXCR-4, mTOR, AKT, PI3K, HER-2, and Estrogen receptors were selected based on their involvement in the progression of the breast as well as lung cancer. A multi-level computational study starting from protein-ligand docking to molecular dynamic (MD) simulations were performed to detect the binding potential of ACL towards the selected proteins. Results of the study led to the identification of ACL as a ligand that showed a high docking score and binding energy with HER-2, mTOR, and VEGFR-1 successively. Whereas, the MD simulations study has also shown good docked complex stability of ACL with HER2 and VEGFR1. Our findings suggest that interaction with those receptors can lead to preventive action on both breast and lung cancer, thus it can be concluded that ACL could be a potential molecule for the same purpose. Communicated by Ramaswamy H. Sarma. © 2023 Informa UK Limited, trading as Taylor & Francis Group.

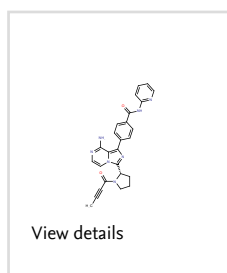
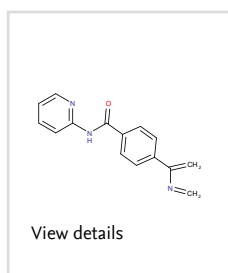
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acalabrutinib; breast cancer; drug repurposing; ligand-protein docking; lung cancer; MD simulations


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