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In silico pharmacokinetics prediction and druggability assessment of phytochemicals from *Curcuma Caesia roxb*

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A total of 103x3=309 compounds were taken for the study. They were sieved, and the functional lead was obtained through various filters. Compound (No 3), the most efficient molecule selected from black turmeric. This compound showed by metabolic prediction and simplified pharmacophore analysis, a good cancer inhibition potential. In future, it will be worthwhile to check the pharmaceutical and pharmacokinetic behavior of the compound *in vitro* and *in vivo*. In silico assessment showed that the binding site of the analyzed candidates is very much identical to the expected site of Peptidyl-prolyl cis-trans isomerase (PIN). The knowledge of the binding modes with the PIN is likely to help and develop a more potent multi-point inhibitor for cancer. Thus the present study "will allow the preclinical development studies to be designed and conducted in a timely, cost-effective manner and most likely allow the candidates to have an early entry" from bench-side to bedside.