UNIVERSITY GRANTS COMMISSION
WESTERN REGIONAL OFFICE
GANESHKHIND, PUNE – 411 007.

PROFORMA FOR SUBMISSION OF INFORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT

1	Name and Address of the Principal Investigator	Dr. Yusufi Mujahid F. No. 1, Kuldeep Housing Society, Vikasnagar, Wanowari, Pune-40
2	Name and Address of the Institution	Abeda Inamdar Senior College of Arts, Science and Commerce, Pune-01
3	UGC Approval No. and Date	F. 47-1133/14 (General/91/WRO) dated 24/03/2017
4	Date of Implementation	24-03-2017
5	Tenure of the Project	31-03-2019
6	Total Grant Allocated	350000/-
7	Total Grant Received	242500/-
8	Final Expenditure	237588/-
9	Title of the Project	Synthesis and Evaluation of Anti-proliferative Potential of Conjugates of Nutraceuticals From Indian Spices
10	Objectives of the Project	To design conjugates of nutraceuticals from Indian Spices To identify the target of the designed conjugates To evaluate the drug likeness of designed conjugates To assess anticancer activity
11	Whether Objectives Were Achieved (Give Details)	The objective of designing new compounds from nutraceuticals from Indian Spices was reached and Nine compounds including eight new derivatives were identified as promising molecules which can be taken up for further investigations.
12	Achievements From the Project	Three nutraceuticals from three Indian spices, which are also the principal constituent of these spices were identified. These biologically active constituents are curcumin from Turmeric (*Curcuma longa*), thymol from Black Cumin (*Nigella sativa*) and eugenol from Clove (*Syzygium aromaticum*). Fragment based drug discovery concept was applied to design eighteen molecules, partially inspired from imatinib. The computational tools were used for the identification of the target proteins implicated in cancer progression and generation of drug resistance to chemotherapeutic treatment. The pharmacokinetic parameters like Physicochemical Properties, Lipophilicity, Water Solubility, Drug Likeness based on Rule of Five and other standards. The GI50 projections showed nine compounds including curcumin and eight new molecules

		derived from curcumin, thymol and eugenol to be active against the cancer cell lines.
13	Summary of the Findings (In 500 Words)	Conjugates of Curcumin, Thymol and Eugenol were designed and biologically active pharmacophores were utilized in the said design. Majority of these conjugates were found to be active against various kinases during the screening for molecular target identification. Some of these kinases are known to have active involvement in oncogenesis, progression and development of resistance against chemotherapeutic treatment. The *in silico* investigations predicted commendable binding interactions with one of the important protein targets Tyrosine kinase AS - a common ancestor of Src and Abl and B.E. were found to be in the range of -6.4 to -11.1 kcal and many molecules show very good binding interactions with the target protein with the residues reported for the standard anticancer drug imatinib. These interactions and binding energies underline the probable mode of action through targeting the tyrosine kinase AS. The Physicochemical Properties, Lipophilicity, Water Solubility, Drug Likeness and bioavailability scores for majority of the designed structures were in the recommended range. The antiproliferative activity projections in terms of GI50 against Breast Cancer Cell lines, Skin cancer cell lines, Leukemia, Colon, Non-Small Cell Lung Cancer and Small Cell Lung Cancer Cell lines, Ovarian, Prostate and Renal and Neuroblastoma cell lines indicate around eight molecules with remarkable anti-proliferative potential against cancerous cell lines.
14	Contribution to the Society (Give Details)	These investigations and projections on pharmaceutical properties of the designed structures may not directly benefit the society at this stage. However, further investigations and improvisations may lead to the synthesis of some drug like molecules with higher safety profile and better target selectivity.
15	Whether Any Ph.D. Enrolled/Produced out of the Project	No
16	No. of Publications out of the Project (Please Attach Re-Prints)	No

(PRINCIPAL INVESTIGATOR)

ABEDA INAMDAR SR. COLLEGE CAMP PUNE-1

(REGISTRAR/PRINCIPAL SIGNATURE & SEAL)

PRINCIPAL
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