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(71)**Name of Applicant :**
1)DR. ABHISHEK TIWARI
Address of Applicant :PHARMACY ACADEMY, IFTM UNIVERSITY, LODHIPUR-RAJPUT, MORADABAD, U.P. 244102, INDIA ---------- ----------
2)DR. VARSHA TIWARI
3)DR. MANISH KUMAR
4)DR. CHANDRA SHEKHAR SHARMA
5)DR. NAVNEET VERMA
6)DR. DEEPAK BHAGWAT
7)DR. RENU
8)DR. AJAY SHARMA
Name of Applicant : NA
Address of Applicant : NA
(72)**Name of Inventor :**
1)DR. ABHISHEK TIWARI
Address of Applicant :PHARMACY ACADEMY, IFTM UNIVERSITY, LODHIPUR-RAJPUT, MORADABAD, U.P. 244102, INDIA ---------- ----------
2)DR. VARSHA TIWARI
Address of Applicant :PHARMACY ACADEMY, IFTM UNIVERSITY, LODHIPUR-RAJPUT, MORADABAD, U.P. 244102, INDIA ---------- ----------
3)DR. MANISH KUMAR
Address of Applicant :M M COLLEGE OF PHARMACY, MAHARISHI MARKANDESHWAR, MULLANA, AMBALA-133207, HARYANA, INDIA ---------- ----------
4)DR. CHANDRA SHEKHAR SHARMA
Address of Applicant :DEPARTMENT OF PHARMACEUTICAL CHEMISTRY, BN COLLEGE OF PHARMACY, UDAIPUR, PIN-CODE: 313001, INDIA ---------- ----------
5)DR. NAVNEET VERMA
Address of Applicant :PHARMACY ACADEMY, IFTM UNIVERSITY, LODHIPUR-RAJPUT, MORADABAD, U.P. 244102, INDIA ---------- ----------
6)DR. DEEPAK BHAGWAT
Address of Applicant :DEPARTMENT OF PHARMACY, PANIPAT INSTITUTE OF ENGINEERING AND TECHNOLOGY, SAMALKHA, DISTRICT PANIPAT- 132102, HARYANA, INDIA ---------- ----------
7)DR. RENU
Address of Applicant :DEPARTMENT OF PHARMACY, GOVT. POLYTECHNIC COLLEGE, UTTAWAR (PALWAL), DEPARTMENT OF TECHNICAL EDUCATION, GOVT. OF HARYANA, HARYANA, INDIA ---------- ----------
8)DR. AJAY SHARMA
Address of Applicant :GOVT. OF NCT OF DELHI, DELHI PHARMACEUTICAL SCIENCES AND RESEARCH UNIVERSITY, PUSHP VIHAR, NEW DELHI 110017 ---------- ----------

(57) Abstract :
Uterine fibroids have increased by a factor of two over the past two decades as women have shifted their priorities from raising a family to advancing their careers. This has led to later marriages and later pregnancy, in addition to increased stress from work and other aspects of modern life. 40 to 50 percent of women with uterine fibroids don't even know they have it. It is estimated that between 25 and 35 percent of women wait until the symptoms have worsened before seeing a gynaecologist for help with things like extended heavy menstrual bleeding and severe pelvic pain. These fibroids can be reduced in size through a number of methods, including as medical or surgical intervention. Progesterone is a crucial hormone that restores the endometrium and controls uterine function. A targeted drug can be developed by blocking the human progesterone receptor. In the current investigation, 25 plant-based molecules are selected and docked onto the 1E3K and 2OVH progesterone receptors. Thansinone, Equol, Fisetin, Genistein, Myrecetin, and Apigenin do well in docking interactions with the 1E3K protein. Among the several compounds tested for docking interactions with the 2OVH protein, (-)-Epicatechin 3-gallate, (-)-Epigallocatechin 3-gallate, Eriodictyol, Genistein, Myricetol, Quercentin, and Tanshinone performed the best. The synthetic progesterone inhibitor Norethindrone Acetate is used to evaluate the docking outcomes. The best compound, thansinone, was analysed using molecular modelling and DFT. The RMSD for the 1E3K protein-ligand complex ranged from 0.10 to 0.42 angstroms, with an average of 0.21 angstroms and a standard deviation of 0.06, while the RMSD for the 2OVH protein-ligand complex ranged from 0.08 to 0.42 angstroms, with an average of 0.20 angstroms and a standard deviation of 0.06. The DFT calculation reveals a sizable energy gap (E), proving the substance's stability.

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