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(71)**Name of Applicant :**
1)Ms. Arti Sanjay Jadhav
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
2)Dr. Shrinivas Krishna Mohite
3)Mrs. Deepa Shivaji Yadav
4)Ms. Amruta Sharad Pawar
5)Mr. Akshay Ashok Thorat
6)Mr. Rohankumar Jayram Suryavanshi
7)Ms. Snehal Sanjay Patil
8)Ms. Smita Prakash Kamalakar
9)Mr. Aniket Arun Karale
10)Ms. Shubhangi Yashwant Khade
11)Dr. Manojkumar Mukundrao Nitalikar
Name of Applicant : NA
Address of Applicant : NA
(72)**Name of Inventor :**
1)Ms. Arti Sanjay Jadhav
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
2)Dr. Shrinivas Krishna Mohite
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
3)Mrs. Deepa Shivaji Yadav
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
4)Ms. Amruta Sharad Pawar
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
5)Mr. Akshay Ashok Thorat
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
6)Mr. Rohankumar Jayram Suryavanshi
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
7)Ms. Snehal Sanjay Patil
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
8)Ms. Smita Prakash Kamalakar
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
9)Mr. Aniket Arun Karale
Address of Applicant :Department of Pharmaceutical Chemistry, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
10)Ms. Shubhangi Yashwant Khade
Address of Applicant :Department of Pharmaceutics, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------
11)Dr. Manojkumar Mukundrao Nitalikar
Address of Applicant :Department of Pharmaceutics, Rajarambapu College of Pharmacy, Kasegaon, Sangli, Maharashtra, Pin Code: 415404 Kasegaon ---------- ----------

(57) Abstract :
The present invention relates to a series of substituted derivatives of 1,3,4-oxadiazole using both the convention method and microwave radiation assistance method where the compound synthesized by microwave radiation method produces high yield and purity. Synthesized compounds are analyzed by TLC. Compounds have a strong affinity for binding to receptor- potent inhibitors NUDT5, which suppress hormone signaling in breast cancer. The optimal geometry of contact between ligand- receptor complexes with lowest energy were docked using three separate scoring functions i.e., the dock score alone, electrostatics, and the combination of steric and electrostatic forces. 5-flurouracil has a dock score of -53.65.

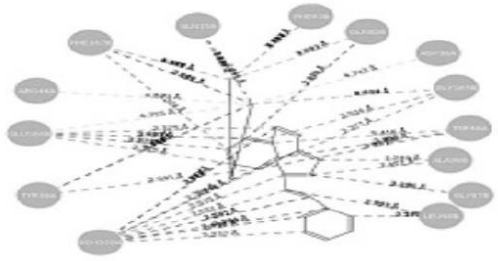

Figure 1

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