# RESUME

| | | |
|---|---|---|
| Name | : | Dr. M. Vijjulatha |
| Educational Qualification | : | M. Sc., Ph. D. |
| Profession | : | Professor,<br>Department of Chemistry, University College of Science, Osmania University,<br>Hyderabad – 500 007 |
| Date of birth | : | 15th September, 1970 |
| Nationality | : | Indian |
| Gender | : | Female |
| Residential address | : | Dr. M. Vijjulatha<br>H.No. 5-9-9/14, Naubath Pahad,<br>Hyderabad-500 004, Telangana.<br>Telephone: 040 – 23232142<br>Mobile: 9866845408 |

**Educational background**

- B.Sc., -Botany, Zoology, Chemistry. Osmania University, 1987-90.
- M.Sc., - Chemistry: University of Hyderabad, Hyderabad.
  1990 – 1992.
- M. Sc., Project work was done in Organic Chemistry (Carbohydrates/ Sugars), under the supervision of Prof. M. Nagarajan, Dean School of Chemistry, University of Hyderabad, Hyderabad.
- Qualified "CSIR-UGC National Entrance Test" conducted by Council of Scientific and Industrial Research (CSIR), held in the year 1992.

- Worked for Ph.D. in Chemistry on the project entitled "Synthesis, Structure and Reactivity of some Cyclic Phosphorus Compounds" under the Supervision of Dr. K. C. Kumaraswamy, Reader, School of Chemistry, University of Hyderabad. Submitted thesis in the month of December 1998.

## Awards

- Awarded Junior Research Fellowship (JRF, 1993-95) and Senior Research Fellowship (SRF, 1995-98) Council of Scientific and Industrial Research (CSIR), Government of India.
- Best poster Award for "Inhibitors of Dihydrofolate Reductase (Pneumocystis Carnii): A computational design". K. Meena Kumari, S. Sree Kanth, L.Yamini and ***M. Vijjulatha.*** **National Symposium on Chemistry and Technology A Synergetic Approach**.30$^{th}$ September – 2$^{nd}$ October 2007, Nizam College, Hyderabad.
- Best poster Award for A combination of Homology modeling and 3D QSAR studies of Quinozoline analogues on Mammalian Dihydrofolate Reductase enzyme. L. Yamini, K. Abhishek and **M. Vijjulatha**. Fourth Indo – US lecture series on discrete mathematical chemistry, 6$^{th}$ – 9$^{th}$ January, 2009. Nizam college Hyderabad.
- Best poster Award for "3D QSAR studies on Quinazolinone derivatives as $5HT_7$ inhibitors. Fatima Sabiha, Aparna Chitta, Mohan Babu Jatavath, and **M. Vijjulatha.** Current Trends in Pharmaceutical Sciences, 12$^{th}$ November 2011. Birla Institute of Technology and Science, BITS, Pilani, Hyderabad campus.
- Best poster Award for "Molecular modeling studies on Pyridazinone and pyridinone as HCV-1 NS5B Polymerase Inhibitors". V. Radhika, S. Sree Kanth and **M.Vijjulatha.** Current Trends in Pharmaceutical Sciences-2012, 17$^{th}$ November 2012. Birla Institute of Technology and Science Pilani, Hyderabad campus
- Best poster Award for "Evaluation of Protein Ligand Affinities of HIV – 1 Protease Inhibitors based on Monte Carlo Simulations" S. Sree Kanth and **M. Vijjulatha** Chemistry with Computers – 2014 18$^{th}$ and 19$^{th}$ January. Indian Institute of Chemical Technology (IICT) and International Institute of Information Technology (IIIT), Hyderabad.
- Best Paper award for "A Computational study of PARP-1 inhibitors using 3D QSAR (CoMFA & CoMSIA) as a tool" V. Radhika and **M. Vijjulatha**. International conference on Science Technology Engineering & Mathematics (STEM) Education & Faculty Development – November 6$^{th}$ – 11$^{th}$ 2017, organized by Faculty of Science St Francis College for Women Hyderabad.
- Best Teacher award by Vasavi Seva Kendram, Vasavi Club, Hyd on 10$^{th}$ Sept 2017.
- Elected as **Fellow of Telangana Academy of Sciences** on 28$^{th}$ April 2018.
- **State award for meritorious Teachers**-2019 by Government of Telangana. on 5$^{th}$ Sept 2019.
- Sectional President for Organic Chemistry section of Indian Council of Chemists - 2021

## Professional / Employment Record

- Worked as Assistant Professor in Department of Chemistry, Nizam collage since December 1999 till December 2008.
- Worked as Associate Professor in Department of Chemistry, Nizam collage since December 2008 till December 2013.
- Worked as Associate Professor in Department of Chemistry, University college of Science, Osmania University till December 2013.
- Working as Professor in Department of Chemistry, University college of Science, Osmania University Since December 2013 till date.
- Dean Development and UGC Affairs Osmania University, from October 2020 to 5th July 2021.
- Director Central facilities for research and Development (CFRD), from May 2021 to 21st July 2021.
- Principal, University College for Women, Osmania University, since 5th July 2021 till date.

### Ph. D Awards

1. Dr. S. Sree Kanth was awarded Ph. D for his thesis entitled "**Design and synthesis of highly potent molecules for inhibition of AIDS**". Under the supervision of Dr. M. Vijjualatha, Assoc. Prof., Dept. of Chemistry, Nizam College, Osmania University (October, 2012)
2. Dr. L. Yamini was awarded Ph. D for her thesis entitled "**Computer Aided Drug Design and Synthesis of DHFR Inhibitors**". Under the supervision of Dr. M. Vijjualatha, Assoc. Prof., Dept. of Chemistry, Nizam College, Osmania University (July, 2013)

3. Dr. K. Meena Kumari was awarded Ph. D for her thesis entitled "**Computational Design, Synthesis and Activity studies of DNA Synthesis and Unzipping Inhibitors"** Under the supervision of Dr. M. Vijjualatha, Assoc. Prof., Dept. of Chemistry, University College of Science, Osmania University (December, 2014)

4. Dr. **B.Saikrishna** was awarded Ph. D for her thesis entitled "In Silico Drug Design and Synthesis of Potential Novel Antimalarial Agents" Under the supervision of Dr. M. Vijjualatha, Assoc. Prof., Dept. of Chemistry, University College of Science, Osmania University (November 2016)

5. **Dr. Mohan babu jatavath** was awarded Ph. D for her thesis entitled "Design of inhibitors for cognitive disorder using computational studies" Under the supervision of Dr. M. Vijjualatha, Assoc. Prof., Dept. of Chemistry, University College of Science, Osmania University (November 2016)

6. **Dr. Sabiha Fathima** was awarded Ph. D for her thesis entitled "**Computational**

**Design and Synthesis of Poly (ADP-Ribose) polymerase-1 (PARP-1) Inhibitors"** Under the supervision of Dr. M. Vijjualatha, Assoc. Prof., Dept. of Chemistry, University College of Science, Osmania University (December, 2016)

7. **Dr. V. Radhika** was awarded Ph.D for her thesis entitled "**Identification and Synthesis of Antiviral Drugs, using Drug Design Techniques**" Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University (November, 2017)

8. **Dr. Raju Bathini** was awarded Ph D for his thesis entitled "**Design and Synthesis of Metastasis, Angiogenesis and Vasculogenesis Inhibitors**" Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University (October, 2018)

9. **Dr. Ramesh Iteboina** was awarded Ph D for his thesis entitled **"Computational Design, Synthesis and Biological Evaluation of Novel Anticancer Agents Targeting JAKSTAT Signaling Pathway"** Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University (December, 2018)

10. **Dr.SaiKiran Reddy** was awarded Ph D for his thesis entitled **"In Silico Design and Analysis of 1,3,4-Oxadiazole based cyclic peptides"** Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University ( February 2019)

11. **Dr. Srilata Ballu** was awarded Ph D for his thesis entitled "**Computer Aided Drug Design, Synthesis and Biological Evaluation of Antibacterial Agents against Wild and Resistant Strains of Staphylococcus Aureus**" Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University (April 2019)

12. **Dr. Rama Krishna Munnaluri** was awarded Ph D for his thesis entitled **"Insilico strategies in developing new inhibitors against molecular targets in HIV and Mycobacterium tuberculosis"** Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University (February 2020)

13. **Dr. Janaiah Chevula as awarded Ph.D for his thesis entitled "Computational design, synthesis and biological evaluation of new chloroquinoline and 2,4,5-triaryl imidazole derivatives"** Under the supervision of Prof. M. Vijjualatha, Dept. of Chemistry, University College of Science, Osmania University (January 2021)

## List of Publications

Citations – 856
H- Index – 16
I10-index - 31

1. Ring opening reactions of cyclic chlorophosphites and synthesis of (amino) chlorophosphonium salts via silylamines. KCK Swamy, MA Said, ***M. Vijjulatha Journal of Chemical Sciences*** **1994,** 106 (3), 796. (Impact factor 1.495)

2. Rings and cages containing phosphorus, arsenic and antimony-new chemistry. MA Said, ***M. Vijjulatha***, KCK Swamy. ***Journal of Chemical Sciences*** **1996**, 108 (3), 299. (Impact factor 1.495)

3. The 1:1 Antimony Trichloride Adduct of Chloro Bis (2, 6-Dimethyl piperidin-1-yl) Phosphine Oxide. ***M. Vijjulatha***, K. C. Kumara Swamy, V. Huch and M. Veith, ***Acta Crystallogr***., **1997**, C53, 1789. (cited: 3)(Impact factor 2.892)

4. The reaction of Chlorophosphates with Strong Bases: Synthesis and Characterization of the Phosphonate salts. ***M. Vijjulatha***, K. Praveen Kumar, K. C. Kumara Swamy and J. J. Vittal, ***Tetrahedron lett.,*** **1998**, 39, 1819. (Cited: 9) (impact factor 2.39) (Cited: 11)

5. Synthesis, Reactivity and Structure of Spirocyclic Products Derived from Octachlorotetraphosphazenes. Comparison to Spirocyclic Cyclotriphosphazenes and Linear Phospazanes. ***M. Vijjulatha***, Sudha KumaraSwamy C. Muthiah, K. C. Kumara Swamy and U. Engelhardt, ***J. Chem. Soc. Dalton Trans.,*** **1999**, 891. (impact factor 3.806) (Cited: 23)

6. Synthesis and Structure of New Symmetrically and Unsymmetrically Substituted Cyclodiphosphazanes. ***M. Vijjulatha,*** K. C. Kumara Swamy, J. J. Vittal and L. L. Koh, ***Polyhedron***, **1999**, 18, 2249. (impact factor 1.946) (Cited: 20)

7. Synthesis and Structure of New bicyclic 1, 3, Di-*t*-butyl-1, 3, 2-$\lambda^3$**,** 4-$\lambda^3$- diaza-diphosphetidines containing ten and eleven – membered rings. ***M. Vijjulatha***, Sudha KumaraSwamy and U. Engelhardt, ***Polyhedron***, **1999**, 18, 2557. (impact factor 1.946) (Cited : 28)

8. Oxidative Addition Reaction on Bicyclic Cyclodiphosphazanes. K. C. Kumara Swamy, K. Praveen Kumar, ***M. Vijjulatha,*** K. Praveen ***Phosph. Sulf. Silicon,*** **2001**, 168, 355 (Cited: 4)

9. Structure Aided Drug Designing – an Overview, ***M. Vijjulatha***. ***J. T. R. Chem.,*** **2003** 10(2), 21-25

10. Docking of Cyclic Urea on HIV – 1 Aspartic Protease. ***M. Vijjulatha,*** K. Meena Kumari and B. Smitha. ***J. T. R. Chem.,*** **2003** 10(2), 17-20.

11. Formation of phosphonates and pyrophosphates in the reaction of Chlorophosphate esters with strong organic bases. K. V. Pavan Kumar, K. Praveen Kumar, ***M. Vijjulatha*** and K.C.Kumara Swamy ***J. Chem. Sci.,*** 116(6) **2004**, 311-317. (impact factor 1.298) (cited: 3)

12. Analysis of $C_{3v}$ Point Group. ***M. Vijjulatha*** & S. Sree Kanth. ***J. T. R. Chem.,*** **2005** 12(2), 70-82.

13. Analysis of Octahedral Point group ***.M. Vijjulatha*** & S. Sree Kanth. ***J. T. R. Chem.,*** **2005** 12(2), 61-69.

14. Computational design of novel cyclic urea as HIV-1 protease inhibitor. ***M. Vijjulatha*** & S. Sree Kanth. **Cent. Eur. J. Chem., 5(4), 2007,** 1064-1072. (Impact Factor: 1.06) (Cited : 6)

15. Docking of Cephalotaxus Species on Dihydrofolate Reductace (DHFR) Homosepians. ***M. Vijjulatha,*** R. U. Shilpa, J. Madhavi. ***J. T. R. Chem., 14(1), 2007,*** 38-43.

16. Novel High Affinity Human Dihydrofolate Reductase Inhibitors (DHFR): A Computational Design and docking Studies using Glide. ***M.Vijjulatha***, S. Sree Kanth, & L.Yamini. ***J. T. R. Chem., 14(1), 2007***, 30-37.

17. Tetrahydroxy Cyclic Urea – Potent Inhibitor for HIV – 1 Protease wild type and mutant type, A computational Design. ***M.Vijjulatha,*** S. Sree Kanth. ***Jour. of Chem., 5(3), 584-592, 2008.*** (Impact Factor: 0.716) (Cited : 5) (Impact factor 3.069)

18. Inhibitors of Human Dihydrofolate Reductase: A computational design and docking studies using Glide. Lingala Yamini and ***M. Vijjulatha***. ***Jour. of Chem., 5(2), 263-270, 2008.*** (Impact Factor: 0.716) (Cited : 8) (Impact factor 3.069)

19. Docking and QSAR Studies for Inhibitors of Thymidylate Synthase, Kotni Meena Kumari, Sivan Sree Kanth, and **Manga Vijjulatha***, ***Internet Electron. J. Mol. Des, 7(6), 131-141, 2008.*** (Cited : 1)

20. Comparative Molecular Field Analysis (CoMFA) for Thiotetrazole alkynylacetanilides, non-nucleoside inhibitors of HIV-1 Double Mutant K103N/Y181C Reverse Transcriptase. S. Sree Kanth, K.S. Abhishake and **M. Vijjulatha***, ***E-Jour. of Chem., 2009, 6 (3),*** *651-658.* (Impact Factor: 1.63)

21. CoMFA and CoMSIA studies on inhibitors of HIV-1 Integrase – Bicyclic Pyrimidinones. V. Radhika, S. Sree kanth and **M. Vijjulatha***, ***Jour. of Chem.,*** 7(S1)**, 2010,** S75 – S84**.** (Impact Factor: 0.716) (Cited: 4)

22. Molecular Docking and 3D-Qsar Studies on Triazolinone And Pyridazinone, A Non-Nucleoside Inhibitor of HIV-1 Reverse Transcriptase. S. Sree kanth and **M. Vijjulatha***, ***J. Mol. Model.*** 16(6)**, 2010,** 1169 -1178**.** (Impact Factor: 1.88) (Cited : 31)

23. Docking and 3D – QSAR studies on p38α MAP kinase inhibitors. J. Mohan Babu S. Sree kanth, Lingala Yamini and ***M. Vijjulatha*, Jour. of Chem.,*** 8(4), **2011,** 1596 – 1605**.** (Impact Factor: 0.716) (cited: 3) (Impact factor 3.069)

24. Molecular Docking, 3D QSAR and Designing of New Quinazolinone Analogues as DHFR Inhibitors. L.Yamini, K.Meena Kumari and ***M. Vijjulatha*, Bull. Kor. Chem. Soc. 32(7) 2011,*** 2433 -2442. (Impact Factor: 0.96) (cited: 2)

25. Multiple Receptor Conformation Docking and dock pose clustering as a tool for CoMFA and CoMSIA analysis – A case study on HIV – 1 Protease Inhibitor. S. Sree kanth and **M. Vijjulatha***, ***J. Mol. Model.*** 18, **2012**, 569 – 582. (Impact Factor: 1.88) (Cited: 9)

26. Design, synthesis, Molecular docking and biological evaluation of new dithiocarbamates substituted benzimidazole and chalcones as possible chemotherapeutic agents. Keerthana. B, Swathi Reddy J., Saritha Jyostna T, Sree Kanth S, **Vijjulatha M*.** ***Biorg. Med. Chem Lett.***, **2012**, 22, 3274-3277. (Impact Factor: 2.66) (Cited : 35)

27. Molecular Docking and 3D-QSAR studies on inhibition of DNA damage signaling enzyme Human poly (ADP-Ribose) polymerase – 1 (PARP – 1). Sabiha Fatima, S. Sree kanth, and **Vijjulatha Manga* J**. ***Recep. And Signal Transd.*** **2012, 32(4)**, 214-224. (Impact Factor: 2.277) (Cited: 14)

28. Pharmacophore Modelling, 3D QSAR and docking studies on Quinazoline antifolates Thymidylate Synthase Inhibitors. Kotni Meena Kumari, and **Vijjulatha Manga*** ***J. Pharm. Res***., **2012, 5(12)**.

29. Combining Docking and 3D QSAR Protocols in Identification and Design of New Cycloguanil Derivatives as Plasmodium falciparum DHFR Inhibitors. **Manga Vijjulatha*,** Balabadra SaiKrishna, Lingala Yamini and Bonepalli Rama Rao ***J. Pharm. Res***., **2012, 5** ***(6), 3285-3289***.

30. Design of Novel Quinazolinone Derivatives as Inhibitors for $5HT_7$ GPCR Receptor. Aparna Chitta, Mohan Babu Jatavath, Fatima Sabiha, and **Vijjulatha Manga* J**. ***Recep. and Signal Transd.*** **2012, 32(1)**, **3-16**. (Impact Factor: 2.277) (Cited: 1)

31. 3D-QSAR of Pyrrolo Pyrimidine and Thieno Pyrimidine Compounds as Human Thymidylate Synthase Inhibitors using CoMFA and CoMSIA. Kotni Meena Kumari, Lingala Yamini and ***M. Vijjulatha****. ***Journal of Chem.,*** **2012, 9(4), 1699-1710**. (Impact Factor: 0.716) (cited:1) (impact factor 3.069)

32. Molecular modeling studies on Pyridazinone and pyridinone as HCV-1 NS5B Polymerase Inhibitors**.** V. Radhika, S. Sree Kanth and **M. Vijjulatha***., ***Int. J. Pharm. Bio. Sci., 2013, 4(2), 152 - 167***

33. Molecular docking guided structure based design of Symmetrical N, N' - disubstituted urea/thiourea as HIV-1 gp120 - CD4 binding inhibitors. Sree Kanth Sivan, Radhika

Vangala and **Vijjulatha Manga***., ***Bioorg. Med. Chem.*****, 2013**, 21 (15), 4591-4599 (Impact factor: 2.903) (Cited: 15)

34. Design, Synthesis and Antimicrobial Evaluation of Novel 1,3-Oxazolidin-2-One Derivatives". Nisha Chandna, Jitander K. Kapoor, Varsha Goyal, Neeraj K.Aggarwal, Kotni Meena Kumari and **Manga Vijjulatha**, **Current Topics in Medicinal Chemistry**, **2013**, *14,* 2062-2075. (Impact factor: 4.20) (cited:1)

35. Molecular Docking and 3D-QSAR studies on Substituted Imidazoles as Inhibitors of P38α MAP kinase. Mohan Babu Jatavath, Sabiha Fatima, Sree Kanth Sivan, **Vijjulatha Manga***., ***Chem. Sci. Trans.* 2014 *3(1),*** 268 - 280**.**

36. 3D QSAR based design of novel substituted urea molecules as heparanase inhibitors**,** Raju Bathini, Sabiha Fatima, Sree Kanth Sivan, and **Vijjulatha Manga***, ***J. of Pharm. Res.* 2013,** *7*, 754 - 761.

37. Molecular Docking and 3D-QSAR Based Design of Novel Imidazopyridinone Derivatives as *Pseudomonas Aeruginosa* Thymidylate Kinase Inhibitors. S. Vikram Kumar Goud, P. Sai Kiran Reddy,S. Sree Kanth, and **M. Vijjulatha***, ***Chem. Sci. Trans.* 2014,** 3 (2), 498 - 509. (Impact factor: 0.606) (cited: 1)

38. 3D QSAR based design of novel oxindole derivative as $5HT_7$ inhibitors. Aparna Chitta, Sree Kanth Sivan and **Vijjulatha Manga* J**. ***Recep. and Signal Transd.* 2014**, 34, 185 – 194. (Impact factor: 2.277) ISSN No. 1079-9893.

39. Synthesis, docking and evaluation of antioxidant and antimicrobial activities of novel 1,2,4-triazolo[3,4-b][1,3,4]thiadiazol-6-yl)selenopheno[2,3-*d*]pyrimidines. Y. Kotaiah, K. Nagaraju, N. Harikrishna, C. Venkata Rao, L. Yamini, **M. Vijjulatha *European Journal of Medicinal Chemistry* 2014**, *75*, 195 – 202. (Impact factor 3.499) ISSN No.0223-5234. (Cited: 33)

40. Multi – Receptor Based Docking and 3D QSAR studies on Human Poly (ADP – ribose) Polymerase – 1 (PARP – 1) inhibitors Sabiha Fatima, Mohan Babu Jatavath, Bathini Raju, Sivan Sree Kanth and **Vijjulatha Manga* J.** ***Recep. and Signal Transd.* 2014**, 34(5), 417 – 430. (Impact factor: 2.277) (cited: 1)

41. Induced Fit Docking, Pharmacophore Modeling and Molecular Dynamic Simulations on Thiazolidinedione derivatives to explore key interactions with Tyr48 in Polyol pathway Ravi Raja Tejasvi Merugu, Lingala Yamini and **Vijjulatha Manga**J. Mol. Model.*** 20(7), **2014,** 2347- 2360. (Impact factor: 2.277) ISSN No. 1610-2940. (cited: 1)

42. Molecular docking and MM/GBSA integrated protocol for designing small molecule inhibitors against HIV-1 gp41. Ramakrishna Munnaluri, Sree Kanth Sivan and **Vijjulatha Manga*** ***Med Chem Res*, 2015**, 24, 829 - 841. (Impact factor: 1.436) ISSN No. 1054-2523. (cited: 2)

43. Molecular docking, 3D QSAR studies of Indole hydrazone as staphylococcus aureus pyruvate kinase inhibitor, Srilata Ballu, Ramesh Itteboina, Sree Kanth Sivan, **Vijjulatha Manga*** ***World J Pharm Sci*** 2014; 2(10) : 1206-1217. ISSN No. 2278-4357

44. Microwave Assisted Synthesis, Molecular Docking and HIV-1 gp120 – CD4 Binding Inhibition Studies of Symmetrical N, N' -disubstituted Urea/Thiourea, Sree Kanth Sivan, Radhika Vangala, **Vijjulatha Manga***, ***Chem Sci Trans.,*** 2014, 3(4), 1418-1426 (Impact factor: 0.606) ISSN No. 2278-3458 (Cited: 2)

45. Synthesis, antimicrobial activity and molecular docking of novel tetracyclic scaffolds incorporating a flavonoid framework with medium sized oxygen heterocycles Dongamanti Ashok, Aamate Vikas Kumar, Devulapally Mohan Gandhi, Gundu Srinivas, Kotni Meena Kumari, **Manga Vijjulatha**, Sridhar Balasubramanian, Prasad Ernala ***Bioorganic & Med.Chem.Lett.***2015, 30; 25(4):898-903. (Impact factor: 2.420) ISSN No. 0960-894X (Cited: 4)

46. QM/MM Docking Strategy and Prime/MM-GBSA Calculation of Celecoxib Analogues as N-myristoyltransferase Inhibitors Nisha Chandna, Kotni Meena Kumari, Chetan Sharma, **Manga Vijjulatha**, Jitander K. Kapoor and Pawan K. Sharma, **Virology & Mycology** 2015, 4(1), 141-149. http://dx.doi.org/10.4172/2161-0517.1000141. ISSN No. 2161-0517

47. 3D pharmacophore modeling and docking studies of 1-amino-5H-pyrido [4, 3-b] indol-4-carboxamide inhibitors of Janus Kinase 2 (JAK2) Ramesh Itteboina, Srilata Ballu, Sree Kanth Sivan, Sailu Pathkala, **Vijjulatha Manga*** ***World J Pharm Sci*** 2015; 3(5): 890-902. (Impact factor: 2.819)

48. Pharmacophore modelling and docking studies of pyrrolidinyl pyridine and pyrazinone analogues as prolyl oligopeptidase(POP) inhibitors Mohan Babu Jatavath, Lingala Yamini, Sree Kanth Sivan and **Vijjulatha Manga* Journal of Chemical and Pharmaceutical Research,** 7(10), 2015. (Impact factor: 0.35)

49. An integrated molecular modeling approach for *In silico* design of new Tetracyclic derivatives as ALK inhibitors Sai kiran Reddy Peddi, Sree Kanth Sivan, **Vijjulatha Manga* J.** ***Recep. and Signal Transd.*** 36 (5), (**2016**) 488-504. (Impact factor: 2.277) (cited: 6)

50. Bioisosteres Of Brassinin: Synthesis, Molecular Docking And Chemotherapeutic Activity O. Navneetha, S. Anuradha Bai, M. S. N. Sandhya, Sree Kanth Sivan, **Vijjulatha Manga,** Saritha Jyostna Tangeda **Indo American Journal of Pharmaceutical Research,**7 **2016**, 4070- 4079. (Impact factor: 0.437) (cited: 2)

51. 3D-QSAR studies on substituted Purines as HIV-1 TAR inhibitors, A Non-trivial target of HIV-1, Saikiran Reddy Peddi, Janaiah Chevula, Sree Kanth Sivan, and **Vijjulatha**

**Manga* Research Journal of Pharmaceutical, Biological and Chemical Sciences 7(4) 2016** 1102 -1111(Impact factor: 2.092)

52. Molecular docking, 3D QSAR and dynamics simulation studies of imidazopyrrolopyridines as janus kinase 1 (JAK 1) inhibitors, Ramesh Itteboina, Srilata Ballu, Sree Kanth Sivan, **Vijjulatha Manga Computational Biology and Chemistry** 64, **2016** 33-46. (Impact factor: 1.793) (Cited: 9)

53. Quinazolinones–Phenylquinoxaline hybrids with unsaturation/saturation linkers as novel anti-proliferative agents Jyothsna Devi Palem, Gopi Reddy Alugubelli , Rajashaker Bantu, Lingaiah Nagarapu,Sowjanya Polepalli, S. Nishanth Jain, Raju Bathini, **Vijjulatha Manga** ***Bioorganic & Med.Chem.Lett.*** 26 **2016** 3014–3018. (Impact factor: 2.420) (cited: 1)

54. Microwave-assisted synthesis, molecular docking and antimicrobial activity of novel 2-(3-aryl,1-phenyl-1H-pyrazol-4-yl)-8H-pyrano[2,3-f]chromen-4-ones Dongamanti Ashok Kavitha Rangu Velagapuri Hanumantha Rao Srinivas Gundu Ballu Srilata **Manga Vijjulatha**, **Med Chem Res 2016** 25:501–514 (Impact factor: 1.436) (Cited: 9)
55. Molecular docking, MM/GBSA and 3D-QSAR studies on EGFR inhibitors, Raju bathini, Sree Kanth sivan, Sabiha Fatima and **Vijjulatha Manga*** **J. Chem. Sci. 2016** 128 (7), 1163-1173. (Impact factor: 1.085) (cited: 8)

56. Microwave assisted synthesis, biological evaluation, and molecular docking of novel chroman scaffolds incorporating spirochromanone framework, Dongamanti Ashok, Devulapally Mohan Gandhi, Aamate Vikas Kumar, Gundu Srinivas, Malladi Srinivas Reddy, Sivan Sree Kanth, **Manga Vijjulatha Med Chem Res 2016** 25 (12), 2882-2894. doi:10.1007/s00044-016-1699-3 (Impact factor: 1.436) (cited: 4)

57. Design, synthesis and docking studies of novel 1,2-dihydro-4-hydroxy-2-oxoquinoline-3-carboxamide derivatives as a potential anti-proliferative agents, Saleha Banu, Rajitha Bollu, Rajashaker Bantu, Lingaiah Nagarapu, Sowjanya, Polepalli, Nishant Jain, Radhika Vangala, **Vijjulatha Manga** ***European Journal of Medicinal Chemistry*** 125, **2017** 400-410. 10.1016/j.ejmech.2016.09.062 (Impact factor 3.499) (cited: 9)

58. Synthesis and evaluation of naphthyl bearing 1,2,3-triazole analogs as antiplasmodial agents, cytotoxicity and docking studies Saikrishna Balabadra, MeenaKumari Kotni, **Vijjulatha Manga*** Aparna Devi Allanki, Rajesh Prasad, Puran Singh Sijwali **Bioorganic & Medicinal Chemistry** 25 **2017** 221–232. (Impact factor 2.930)

59. Design, synthesis, molecular docking and antimycobacterial evaluation of some novel 1,2,3-triazolyl xanthenones, G Linga Goud, S Ramesh, Ashok Dongamanti, V Prabhakar Reddy, Sriram Dharmarajan, Perumal Yogeeswari, Saikrishna Balabadra and **Vijjulatha Manga**, ***Med. Chem. Commun.***, 8, **2017**, 559 – 570. (Impact factor 2.495)

60. A novel piperazine linked ß-amino alcohols bearing a benzosuberone scaffolds as anti-proliferative agents Sowmya Vanguru, Lavanya Jilla, Yasodakrishna Sajja, Rajashaker

Bantu, Lingaiah Nagarapu, Jagadeesh Babu Nanubolu, Bala Bhaskar, Nishant Jain, Sreekanth Sivan, **Vijjulatha Manga**, ***Bioorganic & Med.Chem.Lett.*** **2017** 27 (4), 792-796. (Impact factor 2.42)

61. Synthesis, Spectral Characterization, DNA/ Protein Binding, DNA Cleavage, Cytotoxicity, Antioxidative and Molecular Docking Studies of Cu(II)Complexes Containing Schiff Base-bpy/Phen Ligands, Berelli Anupam, Airva Aruna, **Vijjulatha Manga**, Sreekanth Sivan, Madamsetty Vijay Sagar, Ravula Chandrashekar **J Fluoresc 2017** 27 (3), 953-965. (Impact factor 4.010)

62. Integrating Multiple Receptor Conformation Docking and Multi Dimensional QSAR for Enhancing Accuracy of Binding Affinity Prediction, Vangala Radhika, Hassan A. Jaraf, Sivan S. Kanth and **Manga Vijjulatha*, Current Computer-Aided Drug Design**, **2017**, 13 (2), 127-142.(Impact factor 1.2)

63. Synthesis of tert-butyl (substituted benzamido)phenylcarbamate derivatives: anti-inflammatory activity and docking studies, Shankar Bhookya, Jalapathi Pochampally, Anil Valeru1, Vianala Sunitha, Saikrishna Balabadra, **Vijjulatha Manga**, Karunakar rao Kudle, **J Chem. Biol 2017**, 1-11 DOI 10.1007/s12154-017-0168-x (Impact factor 4.106)

64. Computational analysis of ABL kinase mutations allows predicting drug sensitivity against selective kinase inhibitors, Swapna Kamasani, Sravani Akula, Sree Kanth Sivan, **Vijjulatha Manga**, Justus Duyster, Dashavantha Reddy Vudem and Rama Krishna Kancha, **Tumor Biology 2017** 39 (5), 1010428317701643, 1-7. (Impact factor 3.650)

65. Synthesis, biological evaluation and molecular docking of spirofurochromanone derivatives as anti-inflammatory and antioxidant agents, D Ashok, EVL Madhuri, M Sarasija, SS Kanth, **M Vijjulatha**, MD Alaparthi, **RSC Advances 2017** 7, (41), 25710-25724. (Cited: 1) (Impact factor 3.108)

66. Molecular modeling-driven approach for identification of Janus kinase 1 inhibitors through 3D-QSAR, docking and molecular dynamics simulations, Ramesh Itteboina, Srilata Ballu, Sree Kanth Sivan & **Vijjulatha Manga 2017 Journal of Receptors and Signal Transduction**, http://dx.doi.org/10.1080/10799893.2017.1328442 1532-4281 (Online) (Impact factor: 2.277)

67. Synthesis, antibacterial activity and docking studies of 1,2,3-triazole tagged thieno[2,3-d]pyrimidinone derivatives, Aruna Kumari Maddineni, Settypalli Triloknadh, Nallapaneni Harikrishna, **Vijjulatha Manga**, Venkatata Rao Chunduri **2017 J. Heterocyclic Chem**.,54, 3672 (Impact factor: 0.893)

68. Bis-spirochromanones as potent inhibitors of *Mycobacterium tuberculosis*: synthesis and biological evaluation Ashok Dongamanti Vikas Kumar Aamate, Mohan Gandhi Devulapally, Srinivas Gundu, Saikrishna Balabadra, **Vijjulatha Manga**, Perumal

Yogeeswari, Dharmarajan Sriram, Sridhar Balasubramanian **2017 Mol Divers DOI 10.1007/s11030-017-9779-y** ( Impact factor 2.229)

69. In Silico Design: Those Accentuate Assembly of HIV-1 Capsid Tamalapakula Vani, Balabadra Sai Krishna, Munnaluri Rama Krishna, **Manga Vijjulatha 2017 Nov Appro Drug Des Dev. 2(5) : 555600.**

70. Computational analysis of epidermal growth factor receptor mutations predicts differential drug sensitivity profiles towards kinase inhibitors **2018** Sravani Akula, Swapn Kaamasani, SreeKanth Sivan, **Vijjulatha Manga**, Dashavantha Reddy Vudem, Rama Krishna Kancha **J Thorac Oncol.** 2018 May; 13(5):721-726. DOI: https://doi.org/10.1016/j.jtho.2018.01.003 ( Impact factor 12.460)

71. Rational Design of Methicillin Resistance Staphylococcus aureus inhibitors through 3D-QSAR, molecular Docking and molecular dynamics simulation Srilata Ballu, Ramesh itteboina, Sree Kanth Sivan, **Vijjulatha Manga*. 2018 Computational Biology and Chemistry** 73, 95 -104 ( Impact factor 1.412)

72. Multiple receptor conformation docking, dock pose clustering and 3D QSAR driven approach exploring new HIV-1 RT inhibitors Saikiran Reddy Peddi, Nihaya Abdulsattear Mohammed, Ammar Adil Hussein, Sree Kanth Sivan, **Vijjulatha Manga* 2018 Structural Chemistry https://doi.org/10.1007/s11224-018-1082-8** (Impact factor 2.019)

73. In silico Quest Guided by Physico-chemical Descriptors of Bedaquiline for New Scaffolds with Potential Inhibitory Capacity Against Homology Model of Mycobacterium F1F0 ATP Synthase, Rama Krishna Munnaluri and **Vijjulatha Manga* 2018 Asian J Chem.** 30(4), 21145- 53 (Impact factor 3.698)

74. Structural insights of Staphylococcus aureus FtsZ inhibitors through molecular docking, 3D-SAR and molecular Simulations Srilatha Ballu, Ramesh Itteboina, Sree Kanth Sivan & **Vijjulatha Manga 2018 Journal of receptor and signal Transduction,** 38(1), 61-70. (Impact factor: 2.277)

75. Synthesis, ant-microbial activity of some novel substituted (5-(3-(1*H*-benzo[d]imidazole-2-yl)-4-hydroxybenzyl)benzofuran-2-yl)(phenyl)mentanone analogs Bhookya Shankar, Pochampally Jalapati, Balabadra SaiKrishna, Shyam Perugu **vijjulatha Manga 2018,** Chemistry Central Journal 12:1 http://doi.org/10.1186/s13065-017-0364-3 (Impact Factor 2.442)

76. Dimers of coumarin-1,2,3-triazole hybrids bearing alkyl spacer: Design, microwave-assisted synthesis, molecular docking and evaluation as antimycobacterial and antimicrobial agents Dongamanti Ashok, Srinivas Gundu, Vikas Kumar Aamate, Mohan Gandhi Devulapally, Raju Bathini, **Vijjulatha Manga 2018 Journal of Molecular structure** 1157, 312-321. (Impact Factor 2.011)

77. Design, synthesis, biological evaluation and in silico molecular docking studies of novel benzochromeno[2,3-d]thiazolopyrimidine derivatives Sonyanaik Banoth, Sakram Boda, Shyam Perugu, SaiKrishna Balabadra, **Vijjulatha Manga**, **2018 Res Chem Intermed.** https://doi.org/10.1007/s 11164-017-32011-3. (Impact factor 1.674)

78. Pharmacophore modeling, 3D-QSAR, docking and molecular dynamic simulations on topoisomerase IV inhibitors of wild type *Staphylococcus aureus* Srilatha Ballu, Ramesh Itteboina, Sree Kanth Sivan, **Vijjulatha Manga* 2018 Struct Chem http://doi.org/10.1007/s11224-017-1056-2** (Impact factor 2.019)

79. One-pot synthesis, biological evaluation and molecular docking studies of fused thiazolo[2,3-b]pyrimidinone-pyrazolylcoumarin hybrids Ramesh Gondru Saikiran Reddy Peddi **Vijjulatha Manga** Manjulatha Khanapur Rajitha Gali Narsimha Sirassu Rajitha Bavantula **2018 Molecular Diversity,** 22, 943-956. https://doi.org/10.1007/s11030-018-9845-0 ( Impact Factor 2.229)

80. Discovery and design of new PI3K inhibitors through pharmacophore-based virtual screening, molecular docking, and binding free energy analysis Saikiran Reddy Peddi & Sree Kanth Sivan & Vijjulatha Manga* **Struct Chem 2018** 29(6), 1753-66. https://doi.org/10.1007/s11224-018-1154-9 (Impact factor 2.019)

81. Synthesis, anticancer activity and docking studies of N-phenyl-2-(2-((4-phenyl piperazin-1-yl) methyl)-1H-benzo [d] imidazol-1-yl)acetamides, Lingaiah Boddu, Ashok Kumar Pagudala, Durgaiah Gandamalla, Saikrishna Balabadra, **Vijjulatha Manga**, Narsimha Reddy Yellu , Subhashini N.J.P, **Journal of Molecular Structure** 1166 (2018) 362-368. (Impact factor: 2.011)

82. Molecular dynamics and MM/GBSA-integrated protocol probing the correlation between biological activities and binding free energies of HIV-1 TAR RNA inhibitors Saikiran Reddy Peddi, Sree Kanth Sivan & **Vijjulatha Manga* Journal of Biomolecular Structure and Dynamics, 2018** 36(2), 486-503. (impact factor 4.986) (Cited by 10)

83. A Quest for New Antimalarial Agents with Improved Specificity Guided by Molecular Docking, 3D QSAR and Molecular Dynamics Simulation Studies Janaiah Chevula, Saikrishna Balabadra, Sree Kanth Sivan and **Vijjulatha Manga*** **Asian J Chem**; Vol. 30, No. 9 (2018), 1944-1952. DOI: 10.14233/ajchem.2018.21332 (Impact factor: 3.698)

84. Computational studies on N-phenyl pyrrole derivatives as MmpL3 inhibitors in Mycobacterium tuberculosis RamaKrishna Munnaluri[a], Saikiran Reddy Peddi[a], Sree Kanth Sivan, **Vijjulatha Manga*** **Computational Biology and Chemistry** 78 (2019) 81–94. (Impact factor: 1.331)
85. Novel benzosuberone conjugates as potential anti-proliferative agents: Design, synthesis and molecular docking studies Suresh Kasaboina a, Rajitha Bollu a, Venkatesh Ramineni , P. Mary Gomedhika, Kavitha Korra, Sai Roopika Basaboina, Uma Devi

Holagunda , Lingaiah Nagarapu, Naresh Dumala , Paramjit Grover, Raju Bathini, **M. Vijjulatha. Journal of Molecular Structure** 1180 (2019) 355e362 (Impact factor: 2.011)

86. 3-(2-(5-Amino-3-aryl-1H-pyrazol-1-yl)thiazol-4-yl)-2H-chromen-2-ones as Potential Anticancer Agents: Synthesis, Anticancer Activity Evaluation and Molecular Docking Studies Krishnaiah Vaarla, Santosh Karnewar, Devayani Panuganti, Saikiran Reddy Peddi, Rajeswar Rao Vedula, **Vijjulatha Manga**, and Srigiridhar Kotamraju. **ChemistrySelect** 2019, 4, 4324 –4330. (Impact factor: 1.716)

87. Ramesh Itteboina, Srilata Ballu, Sree Kanth Sivan & **Vijjulatha Manga** (2019) Molecular docking, 3D-QSAR, molecular dynamics, synthesis and anticancer activity of tyrosine kinase 2 (TYK 2) inhibitors, **Journal of Receptors and Signal Transduction**, 38:5-6, 462-474, DOI: 10.1080/10799893.2019.1585453 (Impact factor 2.2)

88. CH B Praveena Devi, K Vijay, B Hari Babu, Syed Farooq Adil, M Mujahid Alam, **M Vijjulatha**, Mohd Bismillah Ansari CuSO4/sodium ascorbate catalysed synthesis of benzosuberone and 1,2,3-triazole conjugates: Design, synthesis and in vitro anti-proliferative activity **Journal of Saudi Chemical Society** 2019 https://doi.org/10.1016/j.jscs.2019.05.002 (Impact factor 2.759)

89. D. Ashoka, E. V. L. Madhuria, , M. Sarasija, S. Sree Kanth, **M. Vijjulatha**, Akkiraju Anjini Gayatri, Someswar Rao Sagurthi, N. Sai Krishna Synthesis of Biaryl Derivatives of Spirofurochromanone in Water and Their Anticancer Activity **Russian Journal of General Chemistry**, 2019, Vol. 89, No. 10, pp. 2129–2135. (Impact factor 0.643)
90. V. Radhika · S. Sree Kanth P. Saikiran Reddy · **M. Vijjulatha** Computational design, synthesis and evaluation of new sulphonamide derivatives targeting HIV‑1 gp120, **Journal of Computer-Aided Molecular Design 34,** 39-54 (https ://doi.org/10.1007/s1082 2-019-00258 -0) 2020 (Impact factor 3.220)
91. Sudhir Reddy Peddi, Saikiran Reddy Peddi, Sreekanth Sivan, Radhika Veerati and Vijjulatha Manga Integrated molecular docking, 3D QSAR and molecular dynamics simulation studies on indole derivatives for designing new Pim-1 inhibitors, **Journal of Receptors and Signal Transduction, https://doi.org/10.1080/10799893.2020.1713809** 2020 (Impact factor 1.629)
92. Prashanth Kumar Kolluri, Nirmala Gurrapu, N.J.P. Subhashini, Shravani Putta, Surya Sathyanarayana Singh, Tamalapakula Vani, **Vijjulatha Manga**. Design, synthesis of novel (Z)-2-(3-(4-((3-benzyl-2,4-dioxothiazolidin-5-ylidene) methyl)-1-phenyl-1H-pyrazol-3-yl)phenoxy)-N-arylacetamide derivatives: Evaluation of cytotoxic activity and molecular docking studies, **Journal of Molecular Structure, 2020,** Vol 1202, https://doi.org/10.1016/j.molstruc.2019.127300 (Impact factor 2.120)
93. In-Silico Screening and Design of Low Molecular Weight Cyclophilin-A Inhibitors That Assist HIV-1 Capsid Assembly, T Vani, **Vijjulatha Manga** SSRN 3528023, **2020**
94. Design and synthesis of novel (Z)-5-((1,3-diphenyl-1H-pyrazol-4-yl)methylene)-3-((1-substituted phenyl-1H-1,2,3-triazol-4-yl)methyl)thiazolidine-2,4-diones: a potential cytotoxic scaffolds and their molecular modeling studies N. J. P. Subhashini · Kolluri

Prashanth Kumar · Edigi Praveen Kumar · Putta Shravani Surya Sathyanarayana Singh Tamalapakula Vani · **Manga Vijjulatha Molecular Diversity, https://doi.org/10.1007/s11030-020-10093-3 2020** (Impact factor 2.229)

95. Microwave-assisted synthesis, biological evaluation and molecular docking studies of new coumarin based 1,2,3-triazoles, Ravinder Dharavath, Nalaparaju Nagaraju, M. Ram Reddy, D. Ashok, M. Sarasija, **M. Vijjulatha**, Vani T, K. Jyothi and G. Prashanthi, **RSC Adv**., **2020**, 10, 11615 (Impact factor 3.049)
96. Design and synthesis of new thiazoles by microwave-assisted method: Evaluation as an anti-breast cancer agents and molecular docking studies, S Mamidala, VS Mudigunda, SR Peddi, KK Bokara, **V Manga**, RR Vedula, **Synthetic Communications**, 1-14, 2020. (Impact factor 1.796)
97. Microwave irradiated one pot, three component synthesis of a new series of hybrid coumarin based thiazoles: Antibacterial evaluation and molecular docking studies, Srikanth Mamidala, Sudhir Reddy Peddi, R Kowshik Aravilli, Parameshwara Chary Jilloju, **Vijjulatha Manga**, Rajeswar Rao Vedula, **Journal of Molecular Structure** 1225 (2021) 129114 (Impact factor 2.011)
98. Synthesis, biological evaluation, and molecular docking studies of novel pyrazole, pyrazoline-clubbed pyridine as potential antimicrobial agents. Nisheeth C. Desai Darshita V. Vaja Jahnvi D. Monapara **Vijjulatha Manga** Tamalapakula Vani **J Heterocyclic Chem**. 2021; 1–14., DOI: 10.1002/jhet.4208. (Impact factor 1.484)
99. Interaction of vanadium metal complexes with protein tyrosine phosphatase-1B enzyme along with identification of active site of enzyme by molecular modeling Ayub Shaik, Vani Kondaparthy, Rambabu Aveli, **M. Vijjulatha**, S. Sree Kanth, Deva Das Manwal Inorganic Chemistry Communications 126 (2021) 108499 https://doi.org/10.1016/j.inoche.2021.108499 (Impact factor 1.943)
100. Design Synthesis and Biological Evaluation of Dithiocarbamate Substituted 2-Aminobenzothiazole Derivatives as Proviral Integration Site of Moloney Murine Leukaemia Virus 1 Kinase Inhibitors P. Sai Harshita, CH.Supriya, Selina Sravanthi, V. Jyothi, S. R. Peddi, **Vijjulatha Manga**, V. Saddanapu T. Saritha Jyostna, Indian J Pharm Sci 2020;82(6):1015-1024 (Impact factor 0.721)
101. A facile one-pot, three component syntheses of a new series of 1,3,4-thiadiazines: Anticancer evaluation and molecular docking studies, Srikanth Mamidala, Venugopal Vangala, Saikiran Reddy Peddi, Raju Chedupakaa, Vijjulatha Manga, Rajeswar Rao Vedula, **Journal of Molecular Structure** 1233 (2021) 130111 (Impact factor 2.011)
102. Synthesis, antitubercular, antimicrobial activities and molecular docking study of quinoline bearing dihydropyrimidines. Nisheeth C. Desai, Ghanshyam M. Kotadiya, Krunalsinh A. Jadeja, Keyur N. Shah, Alimamad H. Malani, **Vijjulatha Manga**, Tamalapakula Vani, Bioorganic Chemistry, Volume 115, October 2021, 105173 (Impact Factor 5.275)
103. Integrated computational approach for in silico design of new purinyl pyridine derivatives as B-Raf kinase inhibitors, Vinutha Kuchana, Vaeshnavi Kashetti, Sai Kiran Reddy Peddi, Sreekanth Sivan & Vijjulatha Manga* (2021) DOI: 10.1080/10799893.2021.1999472

## Patent Publication

1. **HIV-1 gp120 Inhibitors,** Vijjulatha Manga, Sree Kanth Sivan and Rupalatha Maddala. Application No. **2522/CHE/2012,** Published October 5th 2012.
2. **Bicyclic Nitrogen Containing Heterocycles as DNA Intercalators,** Vijjulatha Manga and K. Meena Kumari (Applied)

**Papers presented in Symposium**

1. Rings and Cages containing Phosphorus, Arsenic and Antimony – New Chemistry. Musa. A. Said, ***M. Vijjulatha*** and K. C. Kumara Swamy Modern Trends in Inorganic Chemistry (MTIC) Aug 17–19, 1995, University of Hyderabad, Hyderabad.
2. New Cyclic Phosphoranes and Phosphonate: - Synthesis, Structure and Reactivity. Sudha Kumaraswamy, K. Praveen Kumar, ***M. Vijjulatha,*** Arunamani and K. C. Kumara Swamy National Symposium in Chemistry, Jan 27-30, 1999, Indian Institute of Science (IISC), Bangalore.
3. Novel High Affinity Human Dihydrofolate Reductase Inhibitors (DHFR): A Computational Design and docking Studies using Glide. ***M.Vijjulatha***, S. Sree Kanth, L.Yamini. National Conference on Current Research trends and Developments in Heterocyclic Chemistry. Mar 17-18, 2006. Osmania University, Hyderabad.
4. A Computational Design of Novel Symmetrical Cyclic Urease as HIV Protease Inhibitors. S. Sree Kanth and ***M. Vijjulatha***. International Conference on Heterocyclic Chemistry. December 16 – 19, 2006 University of Rajasthan, Jaipur.
5. Novel High Affinity Human Dihydrofolate Reductase Inhibitors (DHFR): A computational design and docking studies using Glide. L.Yamini and ***M. Vijjulatha***. International Conference on Heterocyclic Chemistry. December 16 – 19, 2006 University of Rajasthan, Jaipur.
6. Novel High Affinity Human Thimidylate Synthase inhibitors. K. Meena Kumari and **M. Vijjulatha**. National conference on Frontiers in Chemistry. February 23-24, 2007. Kakathiya University, Warangal.
7. Docking and QSAR studies of New computationally Designed Thimidylate synthase Inhibitors. K. Meena Kumari, S. Sree Kanth, L.Yamini and ***M. Vijjulatha.*** Indo-German conference on Modeling Chemical and Biological (Re) activity. 26-29th, September 2007. IICT, Hyderabad.
8. Inhibitors of Dihydrofolate Reductase (Pneumocystis Carnii): A computational design. K. Meena Kumari, S. Sree Kanth, L.Yamini and ***M. Vijjulatha*** **.**National Symposium on Chemistry and Technology A Synergetic Approach.30th September – 2nd October 2007, Nizam College, Hyderabad. **(Best poster award)**
9. Targeting HIV-1 through Molecular Modeling studies of CCR5 using Modeller, M. Prasanna Sheela, S. Sreekanth and **M. Vijjulatha**. National Conference on Recent Advances in Chemistry, 3-5th Oct 2008. Dungar College, Bikaner.
10. Comparative Molecular Field Analysis (CoMFA) for Thiotetrazole alkynylacetanilides a non-nucleoside inhibitor of HIV-1 double mutant K103N/Y181C reverse transcriptase. S. Sreekanth and **M. Vijjulatha**. National Conference on Recent Advances in Chemistry, 3-5th Oct 2008. Dungar College, Bikaner.
11. CoMFA studies on inhibitors of HIV- 1 integrase - bicyclic pyrimidinones. V. Radhika, S. Sreekanth and **M. Vijjulatha** National Conference on Recent Advances in Chemistry, 3-5th Oct 2008. Dungar College, Bikaner.

12. A combination of Homology modeling and 3D QSAR studies of Quinozoline analogues on Mammalian Dihydrofolate Reductase enzyme. L. Yamini, K. Abhishek and **M. Vijjulatha**. Fourth Indo – US lecture series on discrete mathematical chemistry, $6^{th}$ – $9^{th}$ January, 2009. Nizam College, Hyderabad. **(Best poster award)**
13. CoMFA and CoMSIA Studies on Inhibitors of HIV – 1 Integrase – Bicyclic Pyrimidinones V. Radhika, S. Sreekanth and **M. Vijjulatha** Fourth Indo – US lecture series on discrete mathematical chemistry, $6^{th}$ – $9^{th}$ January, 2009. Nizam College, Hyderabad.
14. Docking and 2D QSAR on Quinazoline analogues as E.*Coli* Thymidyalte Synthase inhibitors. K. Meena Kumar, S. Sreekanth and **M. Vijjulatha,** Fourth Indo – US lecture series on discrete mathematical chemistry, $6^{th}$ – $9^{th}$ January, 2009. Nizam College, Hyderabad.
15. Atom Based and Receptor Based (CoMFA & CoMSIA) studies on Triazalinone and Pyridazinone a non – nucleoside inhibitor of HIV -1 Reverse Trascriptase. S. Sree Kanth and ***M. Vijjulatha****, National Conference on Recent Advances in Chemistry, $6^{th}$ – $7^{th}$ February 2009, Department of Chemistry, Osmania University, Hyderabad.
16. Comparitive Molecular Field Analysis (CoMFA) for R – 2 – (sec – butyl amino) – N – (2 - methyl – 5 – α (Methyl carbamoyl) Phenyl) thiazol – 5 – carboxamide inhibitors of P38 α MAP Kinase. J. Mohan Babu and ***M. Vijjulatha****, National Conference on Recent Advances in Chemistry, $6^{th}$ – $7^{th}$ February 2009, Department of Chemistry, Osmania University, Hyderabad.
17. Molecular Modeling of Rat liver DHFR, Activesite Similarity with Mouse DHFR and Receptor based 3D –QSAR Study on Structurally Diverse Antifolates. L. Yamini (Oral Presentation) and ***M. Vijjulatha****, *International Conference on Open Source Computer Aided Drug Design (OSCADD).* $22^{nd}$ – $26^{th}$ March, 2009, Institute of Microbial Technology, Chandigarh.
18. Molecular Docking and 3D – QSAR studies on Triazolinone and Pyridazinone, A Non Nucleoside Inhibitors of HIV – 1 Reverse Trascriptase. S. Sree Kanth and ***M. Vijjulatha****, International Conference on Open Source Computer Aided Drug Design (OSCADD).* $22^{nd}$ – $26^{th}$ March, 2009, Institute of Microbial Technology, Chandigarh.
19. Homology modeling, 2D – QSAR and docking studies of HIV – 1 inhibitors targeting Human CCR5 protein. M. Ravi Raja Tejasvi, S. Sree Kanth and ***M. Vijjulatha****, DNA – The Decisive Evidence. $17^{th}$ – $19^{th}$ August, 2009, Andhra Pradesh Police Academy (APPA), Himayath Sagar, Hyderabad.
20. New Strategic Approach for Bifunctional Protein Modeling and Docking studies on Pyrimidine based Derivatives as Antifolates on Toxoplasma gondii (Tg) Lingala Yamini & **Vijjulatha Manga* 14th ISCB International Conference (ISCBC-2010)** $15^{th}$ – $18^{th}$ January 2010 Central Drug Research Institute, Lucknow.
21. 3D QSAR and Molecular Docking Studies of Thiazolone Based Sulfonamides as Inhibitors of HCV NS5B Polymerase. V. Radhika and **M. Vijjulatha*.** NDCS, January 30th, 2010. P.G. College of Science, Saifabad, Osmania University, Hyderabad.
22. Multiple receptor docking and dock pose clustering as tool for CoMFA and CoMSIA studies. **Manga Vijjulatha*** ***International conference on Analytical and Bioanalytical Techniques 2010.*** $1^{st}$ to $3^{rd}$ Nov. 2010, Hyderabad.

23. Diversity Oriented privileged structures as drug molecules. **Manga Vijjulatha*** ***International conference on Analytical and Bioanalytical Techniques 2010.*** 1st to 3rd Nov. 2010, Hyderabad
24. Combining Docking and 3D QSAR protocols in identification and design of new Cycloguanil derivatives as Plasmodium falciparum DHFR inhibitors. Balabadra Sai Krishna, Lingala Yamini & ***M. Vijjulatha*.*** National Conference on Biological Chemistry, 29-30th November, 2010, Gitam University, Visakhapatnam.
25. Multiple Receptor conformation Docking and Dock pose Clustering as a New Method for Receptor dependent 3D QSAR Technique in Designing of Human DHFR Inhibitors. Lingala Yamini, Sree Kanth Sivan and ***M. Vijjulatha* UK-India Medchem 2011*** from Feb 25-26th 2011. NIPER-IICT, Hyderabad.
26. Combining Ligand - based Pharmacophore Modeling and Receptor guided QSAR Analysis for the Discovery of New potent Thymidylate Synthase Inhibitors. Kotni Meena Kumari and ***M. Vijjulatha*, UK-India Medchem 2011*** from Feb 25-26th 2011. NIPER-IICT, Hyderabad.
27. Free Energy binding calculations from MM/GBSA approach and its applications in finding the mode of binding for JAK3 inhibitors Lingala Yamini and ***M. Vijjulatha*,*** International Conference on Applied Theory On Molecular System (ATOMS 2011)from Nov 2nd - 5th 2011.IICT Hyderabad.
28. Design of Human Poly(ADP-Ribose) Polymerase – 1 (PARP – 1) inhibitors as anticancer agents using Docking and 3D QSAR studies. Sabiha Fatima, S. Sree kanth and ***M. Vijjultha****, National seminar on Recent advances in Heterocyclic Chemistry (NSRAHC – 2011) from Nov 4 - 5th 2011. JNTU Hyderabad.
29. 3D QSAR based design of novel human Heparanase inhibitors. Raju Bathini, S. Sree kanth and ***M. Vijjultha****, National seminar on Recent advances in Heterocyclic Chemistry (NSRAHC – 2011) from Nov 4 - 5th 2011. JNTU Hyderabad.
30. 3D QSAR studies on Quinazolinone derivatives as $5HT_7$ inhibitors. Fatima Sabiha, Aparna Chitta, Mohan Babu Jatavath & ***M. Vijjulatha*.*** Current Trends in Pharmaceutical Sciences, 12th November 2011. Birla Institute of Technology and Science, Pilani, Hyderabad campus. **(Best poster award)**
31. Virtual High Throughput Screening of Human Thymidylate Synthase Inhibitors. K.Meena Kumari, B. Sai Krishna, V. Radhika & ***M. Vijjulatha****. Chemical Constellation Cheminar 2012, 10-12th September, 2012, Department of Chemistry, Dr B R Ambedkar National Institute of Technology, Jalandhar.
32. Multi-receptor based docking and 3D QSAR Studies on Human Poly(ADP-ribose) polymerase-1(PARP-1) Inhibitors. Sabiha Fatima, J. Mohan Babu, B. Raju and ***M.Vijjulatha****. Chemical Constellation Cheminar 2012, 10-12th September, 2012, Department of Chemistry, Dr B R Ambedkar National Institute of Technology, Jalandhar.
33. 3D QSAR studies on benzothiazol and benzoxazol-2-amino derivatives as antibacterial agents. P. Kiranmayee. K. Sowmya, S. Sree Kanth & **M. Vijjulatha*** *SusCon-2012,* 10-11th Oct 2012, Institute of Science, GITAM University, Vishakapatanam.
34. Molecular Modeling Studies of Tetracyclic Benzofuran Derivatives as Anaplastic Lymphoma Kinase Inhibitors**.** P. Sai Kiran Reddy, S. Vikram Kumar Goud, S. Sree Kanth & **M. Vijjulatha*** *SusCon-2012,* 10-11th Oct 2012, Institute of Science, GITAM University, Vishakapatanam.

35. Molecular modeling studies on Pyridazinone and pyridinone as HCV-1 NS5B Polymerase Inhibitors. V. Radhika, S. Sree Kanth and **M.Vijjulatha*** *Current Trends in Pharmaceutical Sciences-2012*, 17th November 2012. Birla Institute of Technology and Science Pilani, Hyderabad campus**. (Best poster award)**
36. Docking and 3D QSAR studies on Substituted Imidazoles as p38α MAP Kinase inhibitors**.** Mohan babu Jatavath, Sreekanth Sivan, Fathima Sabiha **and Vijjulatha Manga*** *Current Trends in Pharmaceutical Sciences-2012*, 17th November 2012. Birla Institute of Technology and Science Pilani, Hyderabad campus**.**
**37.** Receptor based 6D QSAR studies on cyclic urea as inhibitors of HIV-1 Protease, V.Radhika, S.Sree Kanth, **M.Vijjulatha***, *UK-India Medchem 2013*, 22-23rd March 2013. IICT, Hyderabad
**38.** Pharmacophore Mapping, 3D QSAR and Docking Studies on inhibitors of Prolyl oligopeptidase (POP) Mohan Babu Jatavath, Sree Kanth Sivan and **Vijjulatha Manga*,** *Recent advances in Computer Aided Drug Design*, IISc Bangalore, 16th-17th Sep, 2013.
**39.** Molecular docking guided structure based design of novel HIV-1 entry inhibitors, Ramakrishna Munnaluri, Sree Kanth Sivan, Radhika Vangala and **Vijjulatha Manga*,** *Recent advances in Computer Aided Drug Design*, IISc Bangalore, 16th-17th Sep, 2013.
**40.** Evaluation of Protein Ligand Affinities of HIV – 1 Protease Inhibitors based on Monte Carlo Simulations" S. Sree Kanth and **M. Vijjulatha*** International symposium on Chemistry with Computers –. Indian Institute of Chemical Technology (IICT) and Institute of Information Technology (IIIT), Hyderabad18th and 19th January 2014. **(Best poster award)**
**41.** Receptor based 3D QSAR studies on p38 MAP Kinase inhibitors using Multiple Receptor Conformation Docking and Dock Pose Clustering as tool**.** Mohan Babu Jatavath, Balabadra SaiKrishna, Sabiha Fatima and **Vijjulatha Manga***. International Conference in Chemical Biology - Indian Institute of Chemical Technology (IICT), Hyderabad 6th and 8th February 2014.
**42.** Improving the odds of success on HIV-1 gp120 inhibitors: A computational study using Molecular docking and MM-GBSA Radhika Vangala, Ramesh Itteboina, Sree Kanth Sivan, **Vijjulatha Manga***. International Conference in Chemical Biology - Indian Institute of Chemical Technology (IICT), Hyderabad 6th and 8th February 2014.
**43.** Molecular Docking and MM-GBSA Integrated Protocol for Identifying Novel HIV-1 gp41 Inhibitors Ramakrishna Munnaluri, Mustafa Kamel Joudah, Sree Kanth Sivan, **Vijjulatha Manga*** International Conference in Chemical Biology - Indian Institute of Chemical Technology (IICT), Hyderabad 6th and 8th February 2014.
44. Insilico studies on HIV-1 TAR RNA inhibitors, Janaiah Chevula, Vangala Radhika, Sree Kanth Sivan, **Manga Vijjulatha***, (Oral Presentation) National seminar on Computer Simulations: Chemistry of Bioactive Molecules, SV College, Suryapet, Nalgonda, 6th and 7th August, 2014
45. Docking based design of p38 alpha MAP Kinase inhibitors, N.V.S.S. Kanthi, Mohan Babu Jatavath,Sree Kanth Sivan, **Manga Vijjulatha***, (Oral Presentation) National seminar on Computer Simulations: Chemistry of Bioactive Molecules, SV College, Suryapet, Nalgonda, 6th and 7th August, 2014
**46.** Pharmacophore modeling and 3D-QSAR studies on new 2-Methyl-6-Ureido-4-Quinolinamides as DHFR inhibitors in *Plasmodium falciparum*, Nandini Gundaram, SaiKrishna Balabadra, Sree Kanth Sivan, **Manga Vijjulatha***, (Oral Presentation)

National seminar on Computer Simulations: Chemistry of Bioactive Molecules, SV College, Suryapet, Nalgonda, 6th and 7th August, 2014.

47. Molecular Docking guided 3D QSAR Studies on p38α Map kinase Inhibitors, N.V.S.S. Kanthi, Mohan Babu Jatavath, Sree Kanth Sivan, Vijjulatha Manga*, National conference on bioinformatics drug discovery and microbial technology in PGRRCDE Osmania University, Hyderabad, December 22-31, 2014
48. Homology Modelling of *Pf* N-Myristoyl Transferase and comparative 3D-QSAR studies on NMT inhibitors of *Plasmodium falciparum(Pf) and Plasmodium vivax (Pv),* Nandini Gundaram, B. SaiKrishna, S. Sree Kanth, **Vijjulatha Manga***, National conference on bioinformatics drug discovery and microbial technology in PGRRCDE Osmania University, Hyderabad, December 22-31, 2014
49. Insilco design of novel antimalarial agents applying receptor based QSAR technique, G. Nandini, S. Sree Kanth and **M. Vijjulatha***, Recent Trends in SBCADD-2015", Alagappa Univeristy, Karakudi, 24th – 27nd February, 2015
50. Developing novel inhibitors of HIV-1 entry using Insilico studies, V.Radhika, N.V.S.S. Kanthi and **M. Vijjulatha***, Recent Trends in SBCADD-2015", Alagappa Univeristy, Karakudi, 24th – 27nd February, 2015
51. Pharmacophore based virtual screening and molecular docking of PARP-1 inhibitors, Vangala Radhika, Sabiha Fatima, **Manga Vijjulatha***,(Oral Presentation) National seminar on Frontiers in Chemical Research and Analysis, ***St. Francis College for Women,*** Hyderabad, 24th – 25th July 2015.
52. Rational design of HIV-1Capsid inhibitors based on 3D-QSAR studies, Tamalapakula Vani, Sree Kanth Sivan, **Manga Vijjulatha***, National seminar on Frontiers in Chemical Research and Analysis, ***St. Francis College for Women,*** Hyderabad, 24th – 25th July 2015.
53. Extrapolating pharmacophore requirements for *Pf* HGXPRT using PHASE and Molecular docking studies, Nandini Gundaram, Vangala Radhika, Manga Vijjulatha*, National seminar on Frontiers in Chemical Research and Analysis, ***St. Francis College for Women,*** Hyderabad, 24th – 25th July 2015.
54. Molecular Modeling driven approach for identification of Janus kinase 1 Inhibitors through 3D-QSAR, Docking and Molecular Dynamics Simulations Ramesh itteboina, Srilata Ballu, Sree Kanth Sivan, **Vijjulatha Manga*** International Conference of International Academy of Physical Sciences (CONIAPSXX) on *Recent advances in physical sciences and future challenge**s,*** Department of chemistry Osmania university Hyderabad, 14th – 16th July 2017.
55. Molecular docking, MM/GBSA and 3D-QSAR studies on EGFR inhibitors. Raju Bathini, Sree Kanth Sivan, Sabiha Fatima and **Vijjulatha Manga*** International Conference of International Academy of Physical Sciences (CONIAPSXX) on *Recent advances in physical sciences and future challenge**s,*** Department of chemistry Osmania university Hyderabad, 14th – 16th July 2017.
56. Molecular Dynamics and MM/GBSA-integrated protocol probing the correlation between biological activities and binding free energies of HIV-1 TAR RNA inhibitors Saikiran Reddy Peddi, Sree Kanth Sivan, **Vijjulatha Manga*** International Conference of International Academy of Physical Sciences (CONIAPSXX) on *Recent advances in physical sciences and future challenge**s,*** Department of chemistry Osmania university Hyderabad, 14th – 16th July 2017.

57. Multiple receptor conformation docking, dock pose clustering and 3D QSAR driven approach exploring new HIV-1 RT inhibitors. RadhikaVangala, Saikiran Reddy Peddi, Sree Kanth Sivan, **Vijjulatha Manga*** International Conference of International Academy of Physical Sciences (CONIAPSXX) on *Recent advances in physical sciences and future challenge**s,*** Department of chemistry Osmania university Hyderabad, 14th – 16th July 2017.
58. Synthesis, Characterization & Biological Activity Studies of N-Substituted Pyrazole Derivatives of P38 MAP Kinase inhibitors. Mohan Babu Jatava, Sabiha Fatima and **Vijjulatha Manga*** International Conference of International Academy of Physical Sciences (CONIAPSXX) on *Recent advances in physical sciences and future challenge**s,*** Department of chemistry Osmania university Hyderabad, 14th – 16th July 2017.
59. Receptor Based 3D QSAR Analysis of Toxoplasma Gondii DHFR Inhibitors. Pathkala Sailu, Rama Krishna Munnaluri, Janaiah Chevula and **Vijjulatha Manga*** International Conference of International Academy of Physical Sciences (CONIAPSXX) on *Recent advances in physical sciences and future challenge**s,*** Department of chemistry Osmania university Hyderabad, 14th – 16th July 2017.
60. A Computational study of PARP-1 nhibitors using 3D QSAR (CoMFA & CoMSIA) as a tool. V. Radhika and **M. Vijjulatha***. International conference on Science Technology Engineering & Mathematics (STEM) Education & Faculty Development – November 6th – 11th 2017, (Best Paper award) St Francis college Hyderabad.
61. Computational design synthesis and biological evaluation of human PARP -1 inhibitors as anti-cancer agents. Sabiha Fatima and **M. Vijjulatha*** International conference on Science Technology Engineering & Mathematics (STEM) Education & Faculty Development – November 6th – 11th 2017, (Best Paper award) St Francis college Hyderabad.
62. Combined molecular docking and 3D QSAR studies on indole derivatives as Pim-1 inhibitors, Sudhir Reddy Peddi, Sahithi Reddy Andru, Sree Kanth Sivan, **Vijjulatha Manga*** International Conference on Chemistry for Sustainable future (CFSF 2018) – 7th-9th Aug 2018
63. Discovery of new BMX inhibitors through pharmacophore based virtual screening, Sudhir Reddy Peddi **Manga Vijjulatha***,(Oral Presentation) International Conference on Chemistry for Sustainable future (CFSF 2018) – 7th-9th Aug 2018
64. Indole derivatives as Pim 3 inhibitors: Discovery of new molecules through Pharmacophore modeling and 3D QSAR studies Sudhir Reddy Peddia, Saikiran Reddya, Sree Kanth Sivan, **Vijjulatha Manga*** OPENTOX ASIA 2019 – Workshop CSIR – Indian Institute of Chemical Technology, Hyderaba March 1-3, 2019
65. Molecular modeling studies on aryl derivatives for designing new inhibitors against HIV-1 reverse transcriptase Kishan Chevulaa, Sree Kanth Sivan, Vijjulatha Manga* OPENTOX ASIA 2019 – Workshop CSIR – Indian Institute of Chemical Technology, Hyderaba March 1-3, 2019
66. Insilico analysis of HIV-1 Protease mutational patterns & prediction of drug sensitivity & resistivity profiles towards FDA approved protease inhibitors Laxmi Chaitanya Neeladri, Vaeshnavi Kashetti and Vijjulatha Manga* 8th PhD/MS National Poster Symposium on"Recent Advances in Chemical and Pharmaceutical Sciences" (RACPS-2019) Organized by Royal Society of Chemistry (London-UK)-Local Section Deccan

(RSC-LSD) & National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad on 21st December 2019 at NIPER, Hyderabad

67. Computational Analysis of point and compound mutations on HIV-1 Protease to predict differential drug sensitivity and resistivity profiles towards FDA approved drugs Vaeshnavi Kashetti, Shaik Khajavali and Vijjulatha Manga* 8th PhD/MS National Poster Symposium on"Recent Advances in Chemical and Pharmaceutical Sciences" (RACPS-2019) Organized by Royal Society of Chemistry (London-UK)-Local Section Deccan (RSC-LSD) & National Institute of Pharmaceutical Education and Research (NIPER), Hyderabad on 21st December 2019 at NIPER, Hyderabad
68. Docked Based approach to design new HIV-1 Non-nucleoside Reverse Transcriptase inhibitors (NNRTI's) Kishan Chevula, Nagesh Patnam, Vijjulatha Manga* Indian Council of Chemists, XXXVIII ANNUAL CONFERENCE, 26-28th December, 2019 held at Jaipur National University, Jaipur, Rajasthan.
69. Docking based approach towards design of new Rodanine derivatives in polyol pathway, Nagesh Patnam, Kishan Chavula and Vijjulatha Manga* Indian Council of Chemists, XXXVIII ANNUAL CONFERENCE, 26-28th December, 2019 held at Jaipur National University, Jaipur, Rajasthan.
70. Computational study of Mutational effects on HIV -1 Protease using FDA approved drugs to understand the selectivity and resistivity for Anti-retroviral therapy, Laxmi Chaitanya Neeladri, Vaeshnavi Kashetti and Vijjulatha Manga* Indian Council of Chemists, XXXVIII ANNUAL CONFERENCE, 26-28th December, 2019 held at Jaipur National University, Jaipur, Rajasthan.
71. In silico screening and design of low molecular weight Cyclophilin - A inhibitors that assist HIV-1 Capsid assembly, Vani Tamalpakula, Vijjulatha Manga* International Conference on Drug Discovery, Feb 29-March 2020, Bits pilani, Hyderabad.
72. Pharmacophore based virtual screening and docking of different sulfonamide derivatives of 5HT7 antagonist, Nahid Fatema, Qasim ullah, L. Yamini, **M. Vijjulatha*** Oral presentation in the XXXIX Annual National Conference of the Indian Council of Chemists going to be held at Veer Narmad South Gujarat University, Udhana - Magdalla Road, Surat, Gujarat - 395007 on 10-11 April, 2021.
73. Multitudinal 3D-QSAR pharmacophore mapping, molecular docking, MM/GBSA and molecular dynamics simulation protocols to discover new PDGFRα inhibitors, Saikiran Reddy, Ramalingam Kundenapally, Sree Kanth Sivan, **Vijjulatha Manga*** Poster presentation in the XXXIX Annual National Conference of the Indian Council of Chemists going to be held at Veer Narmad South Gujarat University, Udhana - Magdalla Road, Surat, Gujarat - 395007 on 10-11 April, 2021.
74. MULTI-TARGET-DIRECTED LIGANDS: A CHALLENGING RATIONALISED DRUG DESIGN APPROACH WITH ITS PHARMACOLOGICAL EVALUATION AS HIV-1 INHIBITORS by **Tamalapakula Vani, Dr. Vijjulatha Manga*** Oral presentation (CYSA) in the XXXIX Annual National Conference of the Indian Council of Chemists going to be held at Veer Narmad South Gujarat University, Udhana - Magdalla Road, Surat, Gujarat - 395007 on 10-11 April, 2021

## Lectures

1. Synthesis, Structure and reactivity of some cyclic phosphorus compounds. ***M.Vijjulatha***, Silver Jubilee Symposium on perspectives in contemporary Chemistry, Nov 12th, 1999, University of Hyderabad, India.
2. A.P.R.E.I. Society Hyderabad. Intermediate and EAMCET Orientation in Chemistry - 2005 to Junior Lecturers Working in A. P.R.JR. Colleges, Oct 5th 2005 From 9.30 am to 11.00 am.
3. Resource person for Medicinal Chemistry (M. S. Pharm.) at NIPER, Hyderabad.
4. Resource person for P. G. Diploma in Cheminformatics at Nizam College, Hyderabad.
5. Invited Lecture on **Asymmetric Synthesis** - One day workshop on '**Stereochemistry**' 21st –Sep-2013, St. Ann's P.G College for Women.
6. Invited lecture on **Computer Aided Drug Design and Microwave assisted Synthesis of Novel HIV-1 Inhibitors** at International Conference on Nano-Bio and Materials Sciences during January, 08-10, 2014
7. Invited lecture on **Computer Aided Drug Design** at Refresher course in JNTU-Hyderabad on 31st July 2014.
8. Invited lecture on **Docking based design of HIV-1 Entry Inhibitors targeting gp41 Pocket** at National Seminar on Computer simulations: Chemistry of Bioactive Molecules at Sri Venkateswara College (U.G & P.G) Amaravadi Nagar Suryapet during August 06-07, 2014.
9. Invited lecture on Combating antimalarial drug resistance by developing novel molecules throught Insilico studies at National conference on bioinformatics drug discovery and microbial technology in PGRRCDE Osmania University, Hyderabad during December 22-31, 2014.
10. Invited lecture on **Design of Heterocyclic compounds based on Computer Aided Drug Design methods** at National Seminar on New aspects of Heterocyclic Chemistry in Medchem and Chemical Biology at R.B.V.R.R. Women's College, Hyderabad February 19th and 20th , 2015.
11. Invited lecture on **Design of Various Lead Molecules based on computer aided drug design methods** at Refresher course on "**Recent innovations in NDDS through nanotechnology for various diseases**" in JNTU - Hyderabad on 6th March, 2015.
12. Invited lecture on **Medicinal Chemistry and Molecular Modelling, a synergistic approach for Drug Design** at National seminar on Frontiers in Chemical Research and Analysis, ***St. Francis College for Women,*** Hyderabad, 24th – 25th July 2015.
13. Invited lecture on **Design of Lead molecules based on Computer Aided Drug Design methods** at Refresher course in JNTU-Hyderabad on 3rd September 2015.
14. Extension lecture on **Structure activity relationship, Pharmacodynamic and pharmacokinetic aspects of chiral drugs and Allosteric binding, thermodynamics of drug interactions with the receptor** at NIPER Hyderabad on 26th and 27th October 2016
15. Invited lecture on **Drug Design and Discovery: A computational Perspective** at a three week Refresher Course on **"Knowledge sharing enables and barriers in Pharmaceutical Research & Development"** organized by UGC-Human Resource Development Centre, JNTUH on 3rd December 2016

16. Extension lecture on **Molecular Modeling and Docking** at ***Department of Pharmacy*** Osmania University Hyderabad November 2016
17. Extension lecture on **Homology modeling** at ***Department of Pharmacy*** Osmania University Hyderabad December 2016
18. Extension lecture on **Pericyclic reaction** at UGC sponsored two day workshop for Chemistry teachers at ***R.B.V.R.R. Women's College***, Hyderabad February 14th and 15th, 2017
19. Extension lecture on **Diversity oriented synthesis based on Pericyclic reactions** on 1st March 2017, at ***St. Ann's P.G College for Women***. Hyderabad.
20. Extension lecture on **Symmetry and stereochemistry** on 30th August 2017, at ***Keshav Memorial Institute of Commerce & Science***, Hyderabad
21. Extension lecture on **Asymmetric synthesis** on 18th September 2017, at ***St. Francis College for Women,*** Hyderabad
22. Extension lecture on **Supramolecular Chemistry – An Overview** on 22nd September 2017, at **St. Poius College for women, Hyderabad**
23. Invited lecture on **In Quest of New inhibitors with specificity – A Synergistic approach** at National Meeting of Synthetic and Theoretical Chemists (NMSTC – 2017) held at School of Chemistry, **University of Hyderabad**, Hyderabad on 13th and 14th October 2017
24. Extension lecture on **Pericyclic reaction** on ***31st October*** **2017** at ***R.B.V.R.R. Women's College***, Hyderabad
25. Resource person for **Molecular Modeling and medicinal Chemistry** in refresher course on Recent Trends in Chemical Sciences and Technology held on 15th -6th Mar 2018 at **Department of Chemistry Osmania University**.
26. Lecture on **Computer Aided Drug Design** on 17th march 2018, at **Anwarul uloom college**, Hyderabad
27. Lecture on **Molecular modelling** on 7th April 2018, at **Shatavahana University**, Karimnagar
28. Lecture on **Computer Aided Drug Design** on 17th April 2018, at Sarojini Naidu Vanitha Maha Vidyalaya Hyderabad Telangana
29. Lecture on "**Homology Modeling**" on 27th April 2018 at National Workshop on 'Bioinformatics and Sequence Analysis' held on 26th -28th April, 2018 Department of Zoology, **Kakatiya University**, Warangal TS, India
30. Lecture on "Introduction to Computer Aided Drug Design" on 29th October 2018 at 3-day National Workshop on Molecular Modeling Using Open Source Software, held on 29th -31st October 2018 at Department of Chemistry University College of Science Osmania University, Hyderabad.
31. Extension lecture on **Asymmetric synthesis** on 24th January, 2019 at ***R.B.V.R.R. Women's College***, Hyderabad
32. Lecture on "Structure based drug design" on 29th October 2018 at Workshop on "Molecular Docking Applications in Drug at ***R.B.V.R.R. Women's College***, Hyderabad
33. Lecture on "Computational analysis of mutations allows predicting drug resistance/sensitivity against inhibitors" on 3rd March 2019 OPENTOX ASIA 2019 – Workshop CSIR – **Indian Institute of Chemical Technology, Hyderabad** March 1-3, 2019

34. Lecture on **Computer Aided Drug Design** 19th March 2019 at 3-day workshop on teaching pedagogy for PG teachers in Chemistry **Osmania University**.
35. Lecture on **QSAR** on 20th March 2019 at 3-day workshop on teaching pedagogy for PG teachers in Chemistry, Osmania University.
36. Extension lecture on **Supramolecular Chemistry – An Overview** on 20th August 2019, at **St. Francis College for women, Hyderabad**
37. Lecture on **Bioinformatics Tools for Drug Discovery** at **National workshop on Recent Trends in Bioinformatics for Exploratory Analysis and Visualization of Biological data** held on Jan 16th, **2020** at ***St. Francis College for Women,*** Hyderabad
38. Lecture on **Computer Aided Drug Design** at **One Day workshop on "molecular modelling using open source softwares Sponsored by DST-SERB under Scientific and Social Responsibility** held on 15 Feb, 2020 at Department of Chemistry, Osmania University, Hyderabad.
39. Lecture on **Molecular modeling** at **One Day workshop on Molecular Modeling and Vibrational Spectroscopy GENOS'20 held on 9th April 2020 at** Department of Chemical Engineering, JNTUH-CEH
40. Lecture on QSAR and Molecular Modeling on 13th March 2020 at Shatavahana University
41. Online lecture at University PG college Mahabubnagar, Palamuru University, E-lecture series on **"Basic concepts of chemistry"** on **24th July 2020.**
42. Webinar on Online FDP on Research Methodology and Software Tools in Research, organized by St. Poius X Degree and PG College for Women held on 29th July 2020.
43. webinar on "In silico design, Synthesis and Evaluation of 2-amino-4-anilino-6, 7-dimethoxy quinazoline derivatives targeting VEGFR-2 as potential angiogenic and cancer inhibitors" at Two-day virtual international conference on CURRENT RESEARCH TRENDS IN CHEMICAL SCIENCES (CRTCS-2020) organized by University college for Women, Hyderabad held on 10th and 11th September 2020.
44. Webinar on Online FDP on "Research Methodology and Software Tools in Research", at two weeks **online** Faculty Development Program (FDP) on '**Research Methodologies and Statistical Data Analysis**" from 16 Nov to 28 Nov 2020. Organized by Chaitanya Bharathi Institute of Technology.
45. Webinar on "UGC Guidelines & it's Implications" at Kasturba Gandhi Degree & PG college for Women on 12th December 2020
46. Webinar on "Improving Academic writing and research abilities" at ***R.B.V.R.R. Women's College***, Hyderabad on 5th January 2021
47. Webinar on one week FDP for chemistry Teachers o "Traditional Classroom to Virtual labs: improvisation of teaching & learning Chemistry" from 27th Jan 2021 to 2nd Feb 2021 organized by Anwar Uloom College on 27th Jan 2021 at 12.00 am
48. Webinar at National e-Workshop on "An Insight of Molecular Modelling" organized by Little Flower Degree College, Uppal Hyderabad on 22nd Feb 2021 at 3.00pm
49. Webinar at UGC Sponsored Two-week Online Refresher Course on "Novel Therapeutic approaches in Drug Discovery & Development against Pandemic Diseases" (01-03-2021 to 16-03-2021) Organized by UGC – Human Resource Development Centre, Jawaharlal Nehru Technological University Hyderabad Kukatpally, Hyderabad, T.S. on

"Molecular Modeling Approaches in Computer Aided Drug Design (CADD) – A Hands on Session" on 15th March 2021 at 3.00 pm.

50. Webinar at UGC Sponsored Two-week Online Refresher Course on "Novel Therapeutic approaches in Drug Discovery & Development against Pandemic Diseases" (01-03-2021 to 16-03-2021) Organized by UGC – Human Resource Development Centre, Jawaharlal Nehru Technological University Hyderabad Kukatpally, Hyderabad, T.S. on "Drug Design & Development against Pandemic Diseases Based on CADD" on 15th March 2021 at 4.30 pm.
51. Webinar at **XXXIX Annual National Conference of the Indian Council of Chemists** on 11th April 2021 "Computational analysis of HIV-1 protease & SARS-CoV-2 main Protease (SARS-CoV-2Mpro) mutations predicts differential drug sensitivity & resistivity profiles towards protease inhibitors.
52. Key Note Speaker on "Role of Cheminformatics in Drug Design and Discovery" for the 5-day Faculty development program at ***R.B.V.R.R. Women's College***, Hyderabad on 6th September 2021
53. Guest of Honour & Speaker on Webinar on 25th October 2021 "Research Methodology & Article writing" lecture on "Academic writing and Research abilities". at Mahatma Gandhi University, Nalgonda TS
54. Webinar a Three days international conference on Green and Sustainable Development in Chemical Sciences (25-10-21 to 27-10-21), *invited speaker at Webinar on* "Insilico strategies for Design of Novel molecules" at K.R.T. Arts, B.H. Commerce on 27th October 2021.
55. Guest lecture at two-day Induction programme at university college of Technology, Osmania University on 8th December 2021 from 9.30 AM to 11.30Am on "**Roll of Chemistry for Engineers**"

## Courses, Symposia and Workshops attended.

- Refresher course in Bioinformatics sponsored by UGC in Academic staff college, University of Hyderabad, from Oct 29th – Nov 18th 2002 and obtained "A" grade (>75%).

- Refresher course in Chemistry sponsored by UGC in Academic staff college, Osmania University, Hyderabad, from Oct 4th – Oct 27th 2004 and obtained "A" grade (>75%).

- Grammar of Proteins by Prof. Balaram IISC at IICT August 2004

- Schrödinger Software Solutions (Glide) by Dr. Shashidhar Rao De Shaw at Fortune Katriya Hotel 2004.

- 3 – Day workshop on Bioinformatics and Molecular Modeling at Nizam college Hyderabad, from 18th to 20th Oct 2001.

- Third national conference of Chemistry teachers – 2003 at Osmania University, on 15th Nov 2003

- 5 – Day National workshop on Molecular Modeling and Drug Designing using Tripos (Sybyl Software) organized by department of Genetics and Prof. G. Ram Reddy Centre for Distance education, Osmania University, Hyderabad, from 9th to 13th Feb 2005.

- 10- Day National workshop on Developing Multimedia Content and Learning Objects. Organized by Nizam college, Hyderabad with partial support from Commonwealth of Learning and Commonwealth Educational Media Centre for Asia, New Delhi, 11th-21st July, 2007

- 2 – Day National workshop on Molecular Modeling and Drug Designing using Glide organized by department of Chemistry, P.G College of Science, Osmania University, Hyderabad, from 26th to 27th Feb 2010.

- 2 – Day International workshop on Molecular Modeling and Drug Design – Tripos workshop on drug design tools, organized by Indian Institute of Science (IISc) Bangalore from 10th to 11th may 2010.

- 5-Day workshop on Introduction to Gaussian 16: Theory and Practice Hyderabad, India from 20th to 24th January 2020.

## Granted Projects:

- UGC Major Research Project entitled: Computational Design, Synthesis and Activity Studies of Novel High Affinity Human Dihydrofolate Reductase (DHFR) Inhibitors. Ref. No. F – 33 – 281/ 2007, Duration 3 years, 2008-2011. (3,58,500) (Completed)

- DST "**Young Scientist Scheme**" (Chemical Science): Computational Design and Synthesis of Novel Cyclic Urea as HIV – 1 Protease Inhibitors. Ref. No. SR/FT/CS-040/2009, Duration 3 years, 2010-2013. (Rs 7,68,000) (Completed)

- CSIR Research Scheme entitled: Computational Design, Docking, QSAR, Synthetic and Activity Studies on Thymidylate Synthase (Human and E.coli). Ref.No. 01/(2436)/10/EMR-II, 2011-2014. (Rs 20,95,800). (Completed)

- DST-SERB Empowerment and Equity Opportunities for Excellence in Science: "Computational design and synthesis of small molecule inhibitors targeting non-trivial proteins of HIV-1". Ref. No. SB/EMEQ-004/2013, 2013-2017. (Rs 46,00,000)

- DST Women Scientist Scheme A (***Ms. Sabiha Fatima)*** Computational Design and Synthesis of PARP – 1 inhibitors, 2013-2016. (Rs 17,80,000) (Completed)

- UGC Major Research Project entitled: Combining Multiple receptor conformation docking and 3D QSAR protocols for identification and design of Novel *Cycloguanil* derivatives as *Plasmodium falciparum* DHFR inhibitors. Ref. No. 42-233/2013-2017. (Rs 13,97,800) (Completed)

- UGC-UPE Focused area of research "Diversity oriented privileged structures as Anti-cancer and Anti-malarial drug molecules." Ref No. 23/UGC/UPE/FAR/OU/2014 (Completed)

- UGC-UPE Focused area of research "Design, synthesis and activity studies of novel kinase inhibitors targeting signalling cascade in cell proliferation." Ref No.60/UGC/UPE/FAR/ OU/ 2017. (Completed)

- UGC-UPE Focused area of research "In Silico Designing of Aldose Reductase Inhibitors for the Treatment of Diabetic Retinopathy" Ref No.60/UGC/UPE/FAR/ OU/ 2019. (Completed)

- DST-PURSE Programme "Signaling and Metabolism based Development of Therapeutic Targets for Age Related Pathologies with Focus on Cancer" 2017- 2021 (4,00,000)

- DST SERB Empowerment and Equity Opportunities for Excellence in Science: "Computational Analysis of Mutational Effects on HIV-1 Antiretroviral Therapy and Target Oriented Synthesis of Potential Lead molecules", Sanction No: EEQ/2018/000117 2019-2023 (42,00,000)

- CSIR Research Scheme entitled "Development of molecular based novel inhibitors on signaling with focus on PI3K-AKT-mTOR pathway" Sanction No: 02(02480)/19. 2019-2023. (21,80,400)

- DBT-BIRAC COVID-19 Research Consortium "Synthesis and anti-viral evaluation of newly designed nucleoside analogs beyond repurposing through revamping against emerging corona virus 2019 nCoV/SARS-CoV-2 by computational protocols" 2019-2021 (45,00,000)

## Organization of Conference/ Seminar/Events:

- Organized a one day seminar on "Drug Designing" An Insight – Scope and Challenges. On 20$^{th}$ July, 2007. With the support of Indian Institute of Chemical Technology. Hyderabad, at Department of Chemistry, Nizam College Hyderabad.

- Organized a 2 - day workshop on "Computational Drug Design for Research Aspirants." On 30th and 31st October 2009, at Department of Chemistry, Nizam College Hyderabad.

- Organized a 2 - day workshop on "Computational Drug Design" On 3rd and 4th April, 2014, at Department of Chemistry, University College of Science, Osmania University, Hyderabad.

- Organized a 3-day National Workshop on "Molecular Modeling Using Open Source Software", held on 29th - 31st October 2018 at Department of Chemistry University College of Science Osmania University, Hyderabad

- Organized a one day Molecular Modeling Workshop using Open source software's on 15th February 2020 at department of Chemistry department of Chemistry, Osmania University

- Organized a Two day National webinar on Online teaching tools for the faculty on 5th and 6th August 2020 at department of Chemistry department of Chemistry, Osmania University
-

## Books

Molecular Modeling Using Open Source Software's – Manual (For Beginners)
Prof. M. Vijjulatha, Dr. S. Sree Kanth and Dr. S. Gururaj.

## Coordination

- Course Coordinator for Cheminformatics (Add on course) sponsored by UGC under Career Oriented Program at Nizam College till July 2013.

- DST-FIST level-0 coordinator at Nizam College Hyderabad till December 2013.

- DST-FIST Level – 1 coordinator at Department of Chemistry, Osmania University.

## Administrative Experience

- **Dean, Development & UGC Affairs (23rd October 2020 to 4th July 2021)**
- **Principal, University College for Women, Koti (5th July 2021 till date)**

## Flagship contributions

- New methodology developed for synthesis of N, N'-symmetrical disubstituted urea/thiourea – an eco-friendly, VOC free microwave assisted synthesis as HIV-1 gp120 CD4 binding inhibitors.
- Novel Cyclic peptide with arginine moiety were developed that can act as potent HIV-1 TAR RNA inhibitors.
- HIV-1 CA inhibitors were designed and synthesized, these act as multi-target inhibitors as they can inhibit HIV-1 protease, Integrase and Reverse transcriptase.
- Amalgamation of MRCD protocol to 6D QSAR studies was used for determining accurate binding affinity values.
- New series of naphthyl bearing 1,2,3-triazoles were synthesized that showed potent anti plasmodial activity compared to Pyrimethamine against resistant strain.

## Panel Member and Evaluator

- Selection committee member for appointment of teaching faculty in Central University of Karnataka on 31st December 2019
- Poster Evaluator in International Conference on Drug Discovery, Feb 29-March 2020, Bits Palani, Hyderabad.
- Selection Committee member of Indian Institute of Chemical Technology (IICT), Hyderabad.

Dr. M. Vijjulatha.