'Support to Indian Institutes for imparting training' to the Faculty of Medical Colleges/ Research Institutes under Human Resource Development Scheme of Department of Health Research

1. Area of Training: **Drug Chemistry**
(computer aided drug design, synthesis, analysis and pharmacological evaluation)

2. Name of the Institution and contact details:

JSS College of Pharmacy
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3. (a) Name of the Principal Investigator and contact details:

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(b) Name of the Co- Investigators and contact details

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4. Training Module (Programme -Duration of the training- Minimum 4 weeks/1 month)

I. Introduction

Drug chemistry gives us an opportunity to use the knowledge of chemistry, biology and physics in the drug discovery and development process. As part of the development of new chemical entities, advancement in the area of drug design, chemical synthesis and analysis of the synthesized compounds have played a vital role. Specially, computer aided drug design techniques, advances in synthetic chemistry, green chemistry, spectral analysis of new molecules, analytical and bio-analytical method developments have played significant role in discovering new chemical entities for diverse therapeutic applications. Furthermore, pharmacological assays to screen molecules will also play an important role in drug research.

II. Aim of the program

This training program provides an opportunity to learn various computer aided drug design techniques such as QSAR, molecular docking, pharmacophore modeling, virtual screening protocols etc. also synthetic chemistry, microwave assisted organic synthesis, IR, NMR and Mass spectral interpretation and analytical/bio-analytical method development using HPLC. The program includes pharmacological screening protocols to screen molecules. There will be both theory and practical sessions with question and answer sessions after each talk that will encourage cross fertilization of ideas. Thus this training program on Drug Chemistry will expose all the participants to the some of the key aspects of drug research with hands on training.

III. Existing faculty members, their details, positions, available with the institution for imparting training programme.

Department of Pharmaceutical Chemistry				
S. No	**Name of the faculty**	**Qualification**	**Designation**	**Research interest**
1	Dr. G. V. Pujar	M.Pharm., Ph.D.	Professor and Head	Design, synthesis, analysis and evaluation of some novel molecules for tuberculosis targets
2	Dr. B.M. Gurupadayya	M.Pharm., Ph.D.	Professor	Analytical and bioanalytical method developments and validation
3	Dr. Madhusudhan Purohit	M.Pharm., Ph.D.	Professor	Design, synthesis, analysis and evaluation of some novel molecules for cancer targets
4	Dr. R. S. Chandan	M.Pharm.,	Asst. Professor	Analytical method

		Ph.D.		development for drug using HPLC
5	Dr. B.R. Prashantha Kumar	M.Pharm., PGDB, Ph.D.	Asst. Professor	Computer aided design, synthesis, analysis and evaluation of some novel glitazones as possible insulin sensitizers
6	Dr. J. C. Thejaswini	M.Pharm., Ph.D.	Asst. Professor	Analytical method development for different combination of drugs using HPLC
7	Dr. Anand Kumar Tengli	M.Pharm., Ph.D.	Asst. Professor	Impurity profiling and analytical method development for drugs
8	Mr. M.S. Venkatesh	M.Sc.	Asst. Professor	Analysis of drugs for their physic chemical properties
9	Dr. B. Vishwanathan	M.Pharm., Ph.D.	Lecturer	Design, synthesis, analysis and evaluation of some novel ligands for their anticoagulant properties

Department of Pharmacology				
S. No	**Name of the faculty**	**Qualification**	**Designation**	**Area of interest**
1	Dr. S. N. Manjula	M.Pharm., Ph.D.	HOD	*In vitro* and *in vivo* pharmacological evaluation of newer molecules for cancer, diabetes and cognitive diseases.
2	Dr. Krishna K. L.	M.Pharm., Ph.D.	Asst. Professor	Pharmacological evaluation of herbal drugs using newer protocols
3	Dr. Muthuraman	M.Pharm., Ph.D.	Asst. Professor	Pharmacological evaluation of newer drugs using newer protocols
4	Mrs. A. M. Mahalakshmi	M.Pharm.	Lecturer	Pharmacological evaluation of novel ligands
5	Ms. Seema Mehdi	M.Pharm.	Lecturer	Pharmacological evaluation

Tentative list of speakers/trainers from other institutions or industry

1. Dr. Anil Kumar Saxena, CDRI, Lucknow. 2. Dr. M. Elizabeth Sobhia, NIPER, Mohali. 3. Dr. Mugesh, IISc, Bengaluru 4. Dr. R. Raghu, Schrodinger 5. Dr. Pritesh Bhat, Schrodinger 6. Dr. Vinod, Schrodinger 7. Dr. Sunil Kumar M, Certara 8. Dr. Valliappan Kannappan, Annamalai University	9. Dr. MNA Rao, Divis Laboratory, Hyderabad 10. Dr. R. Nageshwar Rao, IICT, Hyderabad 11. Dr. Ravi, Karpagam University, Coimbatore 12. Dr. Laxmi Adhikary, Biocon, Bengaluru 13. Dr. Saikath Banerji, Waters India Ltd., Bengaluru 14. Dr. Raghuram Rao, Kakatiya University, Warangal

IV. Available infrastructure facilities

Sl. No.	Name of the Equipment	Cost in Rupees	Make and Model
1.	HPLC-Shimadzu-LC-10	12,93,480	Shimadzu, Japan
2.	HPLC-Shimadzu-LC-2010	14,50,000	Shimadzu, Japan
3.	FTIR-8400S	8,15,625	Shimadzu, Japan
4.	GC – 2014 AF	6,52,000	Shimadzu, Japan
5.	DSC-60	12,00000	Shimadzu
6.	UV-VIS Spectrophotometer-1601	2,63,547	Shimadzu, Japan
7.	UV-VIS Spectrophotometer-1700	3,67,200	Shimadzu, Japan
8.	UV-VIS Spectrophotometer – 1800	4.50000	Shimadzu, Japan
9.	UV-VIS Spectrophotometer-1800	4.50000	Shimadzu, Japan
10.	Rotary Evaporator- HS 2005V-N	1.75000	HahnShin, South Koriea
11.	Viscometer DV-II+ with software	4,50,000	Brookefield , USA
12.	Vibra Cell Sonicator	3,76,494	Sonics,USA
13.	Deep Freezer	1,00,000	Remi
14.	Rotary Tablet Machine 10 station	1,30,082	Rimek
15.	Lab spray dryer LSD-48	5,25,000	JISL, Mumbai
16.	Stability chambers (3 No.)	5,73,245	Thermo lab
17.	Kalweka all purpose equipments	7,52,694	Karnavati Engineering Ltd.
18.	Dissolution Apparatus TDT-08L auto sampler	4,50,000	Electrolab
19.	Dissolution Apparatus TDT-08L - 03 Nos.	5,10,000	Electrolab
20.	Dissolution Apparatus TDT-06P - 02 Nos.	2,24,405	Electrolab
21.	Tablet Hardness Tester	1,15,000	Erweka
22.	Orbital Shaking Water Bath	1,27,000	Remi
23.	Electronic balance (1 mg sensitivity) – 06 Nos	1,60,000	Shimadzu BL-220H
24.	Sybyl X Molecular Modeling Software	10,50,000	Tripos, USA
25.	Gold Molecular Modeling Software	1,00000	Cambridge Crystallographic Data Centre (CCDC)
26.	Computer aided drug design laboratory	20,00000	Ten computer workstations in the drug design laboratory loaded with molecular modelling software's
27.	Seminar hall for conducting workshop with audiovisual facilities	-	Capacity of up to 60 people

V. Training schedule with elaborate details day wise or week wise along with the topic.

Sl. No.	Topic	Duration	Details
1.	Computer aided drug design (CADD)	One week	The fellows will be trained on various computer aided drug design techniques such as 2D QSAR, 3D QSAR, Pharmacophore modelling, database searching, modelling proteins and preparation of proteins for docking, docking, ADME properties and molecular dynamics simulations. This module will enables the fellows to understand different virtual screening protocols in drug design. It also helps them to predict biological properties for the newer molecules before their synthesis. The training involves both theory and hands on sessions.
2.	Syntheisis and purification	One week	The fellows will be trained on various techniques of synthetic organic chemistry. Topics related to, disconnection approaches and retrosynthetic analysis will be dealt in detail to understand synthetic strategies to synthesize the designed ligands. There will be practical experiments on organic synthesis for both conventional and microwave assisted synthesis. Purification of synthesised compounds by column chromatography will be demonstrated.
3.	Pharmaceutical Analysis	One week	The fellows will be trained on various aspects of pharmaceutical analysis. Which includes analytical and bioanalytical method development using HPLC and GC for drugs. Validation of developed HPLC method for different drugs. Which includes preparation of sample solutions, mobile phase, extraction of drugs from biological samples etc. Experiment related to DSC.
4.	Pharmacological screening	One week	Pharmacological assays to screen drugs from synthetic source and natural sources. The assays include both in vitro and in vivo using different models. Some advanced pharmacological methods will also be demonstrated to train the fellows.
Total duration		**4 weeks**	

VI. Relevance in public health

Drug chemistry is an important branch of science. It focuses on the interaction between chemicals and organisms. Many drug chemists in this field work on discovering new drugs and sometimes specialize in a specific area of research, such as creating newer molecules or determining how drugs react to the body. Drug chemists have extensive knowledge of the relationship of chemical reactions, analysis and biology and work on developing effective drugs for the people. The drug chemists possess writing skills, critical-thinking abilities and employ strategies to solve new and complex problems with medications thereby offer a valuable contribution to the public health system.

5. Eligibility Conditions for a Fellow

A Permanent faculty member working in a DSIR recognized pharmacy college, medical college, university and drug research or health research institute.