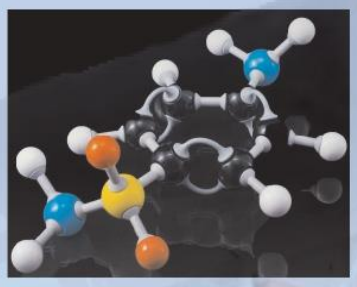
DDDR-2021

International Symposium On Drug Design and Development Research (December 17-18,2021)

To Commemorate

70th

Birthday of Prof. (Dr.) Anil Kumar Saxena



Hosted by:

Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur-244713, India

Website: www.giper.edu.in

Schedule of DDDR2021

Day 1 (December 17, 2021)	
Time	Event
0930 to 1045	Registration
1100 to 1300	Inauguration and Felicitation a) Welcome note + Lamp lightening followed by Saraswati Vandana (1100 to 1110) b) Organizing Secretary speech (1110 to 1115) c) Director Sir speech (1115 to 1120) d) Chief Guest speech (1120 to 1125) e) Guest of Honor speech (1125 to 1130) f) E-book of abstract opening (1130 to 1135) g) Videos and notes sent by scientists and students (1135 to 1305) i) Cake cutting (1305 to 1315) j) Chairman Sir speech (1315 to 1325) k) Vote of thanks (1325 to 1330)
1330 to 1400	Lunch
SCIENTIFIC SESSION I Chairperson: Prof. (Dr.) V. P. Kamboj	
1430 to 1500	L1: Prof. Vladimir Poroikov
1500 to 1530	L2: Prof. Esin Aki
1530 to 1600	L3: Prof. Athina Geronikaki
1600 to 1630	Tea
1630 to 1830	E poster session (Chairperson: Prof. Shradha Sinha and Prof. Kapil Kumar)
Day 2 (December 18, 2021)	
SCIENTIFIC SESSION II Chairperson: Prof. (Dr.) Ashok Hajare	
9.30 to 10.00	L4 Dr. Subhash C. Basak
1000 to 1030	L5 Prof. P. V. Bharatam
1030 to 1100	L6 Prof. A K Saxena
1100 to 1130	L7 Prof. Indira Ghosh
1130 to 1200	Tea
	SCIENTIFIC SESSION III Chairperson: Prof. Mridula Saxena
1200 to 1230	L8 Prof. Ashesh Nandy
1230 to 1250	L9 Dr. Sisir Nandi
1250to 1310	L10 Dr. Chandra Sourabh Azad
1310 to 1330	L11 Dr. Zeeshan Fatima
1330 to 1430	Lunch and Offline Poster Session
	SCIENTIFIC SESSION IV Chairperson: Prof. A. K. Saxena
1430 to 1500	L12 Dr. Marjan Vracko
1500 to 1530	L13 Prof. Kunal Roy
1530 to 1600	Valedictory Session
1600 to 1615	Vote of thanks
1615	High Tea

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EX- Director ICAR-IVRI, JD CADRAD,
Director IBT, National Fellow, Advisor WHO.
Member, Animal Welfare Board of India
Member, CPCSEA (Govt. of India)

To
Chairman
GIPER, Jaspur Road
Kashipur-244713 US Nagar
Uttarakhand

Dated: 17-12-2021

Message

I am happy to learn that GIPER is organizing an International Symposium on ***Drug Design and Development Research (DDDR-2021)*** on December17-18, 2021 to commemorate the 70th birthday of Prof (Dr) Anil Kumar Saxena Chairman and founder of the institute. It is very pertinent and timely to organize symposium on this important topic among the scientists, students, teachers and young professionals of interdisciplinary fields of pharmaceutical and medical sciences. Needless to mention that allopathic medicines are now showing various kinds of serious side effects and people around the world are switching on to the herbal or natural formulations for the management of their health issues. India is pioneer in this having thousands year old natural health management system of Ayurveda, which can play an important role in the improvement and management of human, animal and environmental health. I believe the young professionals getting training in your institute are taking care of the rich reservoir of medicinal and wellness products from plants, soil and animals. I wish a great success of this symposium in enriching the knowledge of the people on new drug design and developing methods and their humane testing on animals for the welfare of the society.

(RS Chauhan)
Professor and Head, Veterinary Pathology

VEER MADHO SINGH BHANDARI
UTTARAKHAND TECHNICAL UNIVERSITY
वीर माधो सिंह भण्डारी
उत्तराखण्ड प्रौद्योगिकी विश्वविद्यालय

Dr. P.P. Dhyani
Vice Chancellor
डॉ० पी० पी० ध्यानी
कुलपति

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Ref. No. 537/VC/UTU/21

Date. 13/12/21

Message

It is my great pleasure to note that **Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur** is organizing an international symposium entitled **Drug Design and Development Research (DDDR-2021)** from 17-18 December 2021. It makes a very good sense for excellent in the eve of 2021 because this both offline and online symposia will be a brain storming for the leading scientists, young researchers, academicians and students globally to update their knowledge on latest drug design and development on medicines, health protection, pharmaceuticals, molecular and drug discovery research. I complement you for the efforts.

With warm wishes for the success of this symposia.

(Dr. P.P. Dhyani)
Vice-Chancellor,
Veer Madho Singh Bhandari
Uttarakhand Technical
University
Dehradun

From the Chairman's Desk

Message

I am delighted to note that Global Institute of Pharmaceutical education and research (GIPER), Kashipur, is organizing an International symposium on "**Drug Design and Development Research** (**DDDR-2021**)" in online and offline mode. I am grateful to GIPER for organizing it to commemorate my 70th birthday. The subject of the conference is closest to my heart and mind, to which I have dedicated more than 50 years of my career at CSIR-Central Drug Research Institute, Lucknow. I am pleased to note that many of my friends, colleagues, students including the staff of GIPER are participating in it. Drug design and development is of key importance in the process of drug discovery and development. It is very essential for any country and for the health care of the people. It has been well realized in the past two years with Covid-19 pandemic. It is of immense pleasure that outstanding speakers from abroad and India who have been very close to me for more than 20 years have kindly agreed to deliver lectures in this symposium and good number of young participants are presenting their works on posters. It will be useful to the participant particularly the young innovative minds to interact on the common platform with the experts. The exposure of the students from GIPER and other institutions will be helpful to them in improvising their knowledge.

I am very thankful to the dignitaries who have kindly consented for gracing it through their messages and presence. I gratefully acknowledge the efforts of the organizers including staff and students of the GIPER and wish it a great success.

Anil Kumar Saxena

From the desk of Chairman (DDDR-2021) and Organizing Secretary (DDDR-2021)

Greetings, wish you all a good scene for an excellent end of 2021 with this International symposium (online and off-line mode) on **Drug Design and Development Research** (**DDDR-2021**) hosted by **Global Institute of Pharmaceutical Education and Research (GIPER), Kashipur-244713, Uttarakhand, India** from **December 17-18, 2021** to commemorate the 70th Birthday of Prof. (Dr.) Anil Kumar Saxena, Chairman GIPER and patron of this conference who contributed much to enrich drug research in India and created much human resources for it in the country would welcome your good wishes. It is our privileged to honor Dr. A. K. Saxena who is a father figure of Indian Drug Discovery Research.

We welcome you all to share your knowledge and views with the global audience at **symposium**. We appreciate your work and are sure that your presence will be a critical addition to our conference. The symposium will provide a forum for bringing together leading scientists, students and young innovative minds from different parts of the globe to share a single platform to discuss latest developments in the emerging and interdisciplinary field of pharmaceutical and medical sciences. We hope to offer you a memorable experience in exploring new ideas and opportunities. We thank all participants, speakers, honorable national and international advisory board members. Thanks to all staff members of the GIPER to make a grand success of this symposium.

Dr. Sisir Nandi
Organizing Secreatary
DDDR-2021

Dr. Deepak Teotia
Chairman
DDDR-2021

Dr. Nitya Anand
Ex-Director
Central Drug Research Institute
Lucknow (India)

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It is indeed a great pleasure to know that Global Institute of Pharmaceutical Education & Research (GIPER) is organizing an international symposium on Drug Design and Development Research (DDDR-2021) to commemorate the 70th Birthday of Prof. (Dr.) Anil Kumar Saxena who is also the Chairman of the institute. The symposium is well fitting as Dr. Saxena's professional career of over 52 years has been devoted to medicinal chemistry and New Drug Discovery Research. He is today one of the leading medicinal chemists and perhaps the only one who has not only developed a working interface between classical medicinal chemistry based on practical determination of structure-activity relationship and Computer Aided Drug Design (CADD) techniques for developing and refining the concept of "freezing" the most favored conformation of known active compounds and /or incorporating the active substructures in new prototypes (medicinal chemical hybridization), and optimization of the biological activities. Dr. Saxena has designed and synthesized compounds belonging to a variety of heterocyclic systems. Quite early in his career, using the above concept of drug design, he synthesized octahydropyrazinopyridoindoles, a new class of CNS depressants, which resulted in the discovery of a novel neuroleptic drug, Centbutindole which was approved for marketing.

He has established models using 2D, 3D QSARs and structure-based drug design. He has successfully utilized the models through virtual screening in prioritizing the molecules for synthesis from the designed focused libraries. This has resulted in the discovery of different new chemical entities (NCE's) which are at different stages of drug development as anti-hypertensive, antithrombotic, anti-Alzheimer's, anti-tuberculosis, PTP-1B inhibitors and BMP stimulators. He has also given attention to process development, so that the products which are developed can be made available at prices affordable in India. He is really a multifaceted medicinal chemist, and has set a good example of how a productive medicinal chemist should function. Some of the products discovered by his group are licensed to industries. Dr. Saxena is today one of the leading medicinal chemists with 72 national/international patents, 231 original research papers published in reputed journals and 24 invited chapters and review articles published in classic medicinal books and leading world periodicals. Dr. Saxena is still very active and has published several book articles and also edited two volumes in Topics in Medicinal Chemistry published by Springer Verlag including the latest one titled "Biophysical and computational tools in drug discovery".

I can say with a sense of pride that Anil has been my research student and I could see his exemplary features right from the time he joined me as the youngest JRF at the age of 18, and by 22 he had his PhD degree during which he synthesized the first set of classic pyrazinopyridoindoles and pyrazinoisoquinolines as CNS agents. He decided to stay on at CDRI and I cherished his decision. His trajectory has gone up and up since then. Nothing satisfies a teacher more than when his student excels him and this is what has happened with Anil, who started as a Junior Research Fellow and became the Chief Scientist and Head of Medicinal and Process Chemistry Division in CDRI before his superannuation. Apart from his scientific achievements Anil has established GIPER in the memory of his father and grandfather. I feel happy to wish him good health with many more active years and also the symposium a great success.

Nitya Anand.

BIRTHDAY WISHES

It is a great honour to be invited to participate in the celebration of Dr. Saxena on his 70th birthday. I first met with Dr. Saxena during a long-standing scientific collaboration at the beginning of the century between the highly esteemed research institute, CDRI, in Lucknow, U.P., and my company at the time, Novo Nordisk in Denmark. Dr. Saxena was instrumental in accomplishing a hugely successful interaction between the two institutes. This was based on his scientific insights, his diligent attention to logistics, and his open-minded approach towards the collaborators, which created a most important atmosphere of trust between the parties. Later, I attended the successful GIPER Conference in Kashipur 2019, and was truly impressed by Dr. Saxena's ability to create a great, comprehensive scientific programme, to initiate excellent discussions with speakers and audience and, again, creating an atmosphere of trust, friendship, and confidence. The huge effort in Dr. Saxena's emphasis on education and guidance of the students manifested itself during the conference, not only at the Medical School, but also by a most appreciated visit to his impressive school in Kashipur, which he founded and is heading up. I send my sincere appreciation and gratitude to Dr. Saxena at this moment in his life and career.

Dr. Ian Ahnfelt-Rønne
Copenhagen, Denmark

Dr Saxena is known to me for the last 43 years. It started in M Sc in 1978 at Chemistry Department, Lucknow University when he delivered "Husain Zaheer Memorial Oration". The topic was very extremely novel amazing for a student, that is, quantification of biological activity. He explained about Quantitative Structure Activity Relationship, something beyond the thought process of an inquisitive mind. I never knew that someday I shall meet him face to face and discuss. Luckily, after my Ph D I got a research fellowship in Medicinal Chemistry Division of CDRI. Since then to today I am in touch with him as a wonderful human being. I wish him very healthy and happy years in future.

Dr. V. L. Sharma
Ex-Senior Principal Scientist
Medicinal & Process Chemistry Division
CSIR-Central Drug Research Institute

Dr. Saxena's immense contribution to drug discovery programs at CDRI are remembered and cherished. The flagship CDRI Conference, CTDDR, which initiated by him continues to attract leading researchers. I wish him a very happy 70th birthday, and many productive years as a researcher, mentor, and teacher.

Dr. Saman Habib
Chief Scientist, CSIR-CDRI

Please convey my heartiest greetings to Dr Saxena. May God bless him with long and healthy life.

Dr. Ashok Sharma

I, Arimardan Singh Kushwaha joined Dr. Anil Kumar Saxena research team in 1987 as graduate trainee at the age of mere 24. He is an extremely distinguished personality, a great philosopher and human being, world renowned Enthusiast Scientist in his research field of Medicinal Chemistry

and CADD & CAMM. I was directly associated with him till his retirement in CSIR-CDRI for almost 3 decades. Dr. Saxena not only groomed me in our professional areas but also taught me how to be a socially responsible being in society. I, on his 70th Birthday, salute him on his achievements and wishing him a long life along with good health. Happy Birthday Sir!

Mr. Arimardan Singh Kushwaha
Senior Technical Officer,
CSIR-CDRI, Lucknow

My journey as a dedicated researcher started dated back in Feb 2019, when I got the chance to meet Dr. Anil K Saxena. I don't know what he has seen in me to take me as his Ph.D. student, but I still remember his words, "Azad, I made a scientist in you, and I think I am done with my job." Still, I am a big fan of his energy and enthusiasm towards science and doing something meaningful for society, and GIPER is an excellent example of his efforts in this regard. I want to thank Dr. Saxena for mentoring me not only for my research but also for mentoring me in my life. I wish him good health and hope to see him soon.

Dr. C S Azad

My Best Wishes to Dr. Saxena and your endeavors and every success for forthcoming international symposium DDDR-2021.

Dr. D. Amla
CSIR-NBRI

On the occasion of the 70th Birthday of Dr AK Saxena, I feel pride in recapitulating his contribution to science and society for over 45 years. Great medicinal chemist, wonderful supervisor and most importantly friend of friends. We shared several meetings, each time we learned from each other and enjoyed our scientific discussion. I wish him 30 more years of active life.

Dr. Y. K. Gupta

"Wishing Prof Saxena a fabulous birthday. Sir, your unparalleled wisdom has made me who I am today. You have made a great impact in my life and I will always appreciate you. Your inspirational words have been a great motivation for me in life. I'm so blessed to have had the opportunity to be called your student. You're such a wonderful and inspiring teacher and leader. As you celebrate your birthday today, may you live many more years in wisdom and knowledge" .

Dr. Gyanendra Pandey

Dr. Saxena turning 70 is still so energetic and active in research. I wish you very happy birthday sir. You are my role model because I have been trained by the true scientist like you. I convey my deep regards to you. I want to share that I met first Dr. Saxena in the year of 2006 in INDO-US conference in Bangalore. That time I was a doctoral student. I was really impressed by his

incredible lecture delivered on antimalarial drug design based on pharmacophore modelling which had been printed in my brain. From that time I was thinking a lot to work with Dr. Saxena such a dynamic and eminent devotee in science and technology. My dreams came true at the time of my post doctoral study at NIC, Slovenia when again I had an interaction with him at CMTPI-2011 conference at Maribour in Slovenia. Without any more thinking, I accepted his offer and joined in GIPER since last December 2012. I have realized the integrity, courage, fortitude, honesty and good behaviors that enrich my morality to maintain very good relationships with all fellow citizens throughout the life. I have been learning a lot till today so I am blessed with him and it is my privilege to become an obedient student of Dr. Saxena. This is my achievement in life. I wish you many happy returns of the day. I pray to God for your good health, safety and happiness. Thank you very much Sir for introducing me in the thirst area of drug design and discovery research.

Dr. Sisir Nandi,
GIPER, Kashipur

It is an honor and pleasure for me to write a few words about this wonderful person, an eminent scientist, a dedicated researcher and a passionate academician Dr. A. K. Saxena, the Father of QSAR in India, on his 70th Birthday. I was fortunate enough to meet this legend at CTPMS 2020 at Uttarakhand and was etched with his deliberations and the perseverance with which he enthralled the audience in awe- A true scientist in the area of drug discovery. I was blessed once again when I happen to be a part of his collaborative team. I have learnt great lessons from him which motivated me over and over again and helped me to broaden my outlook towards science. I am delighted that GIPER has arranged such a wonderful session where eminent scientists and young researchers shall exchange their academic thoughts and novel ideas which to me is the best way to celebrate the birthday of such an extra ordinary person. Wishing you Happy Birthday Sir and praying to Almighty for your good health so that you keep on inspiring us to do science in a better way. I wish a grand success of this event.

Dr. AsmitaSamadder,
University of Kalyani, WB, India

Summer of 2019 changed my life literally. I was a pre-final year student who did not know anything about the drug discovery and role of QSAR in it, but fortunately I got selected for INSA fellowship under the guidance of Dr A K Saxena at CDRI. His passion towards drug discovery research and teaching and training new students is highly infectious. On my first day, he introduced me to QSAR and in that one hour lecture, he taught me all the basic knowledge of it which build my foundation in this fascinating field. I would really like to thank him for always answering my naive questions during our interactions and always supporting me whenever I needed his help. I will pray to the almighty that you would live longer and would keep to inspire and train more students like me who want to pursue a career in drug discovery and development.

Mr. Karanpreet

Sir, you have been a very friendly supervisor and mentor since the onset of my doctoral research journey in 2008 to till date. Working under your supervision has been very gratifying and I have learned and grown a lot. My sincere and heartfelt gratitude and appreciation to you for giving me

with the constant guidance and counsel I needed to succeed in the PhD program and in my development as a Researcher-cum-Academician. My success is your blessing. Thank you again. Have a very wonderful time

Dr. Kuldeep K. Roy

Dr. Anil Kumar Saxena is one the precious gems among CDRI alumni. He has a versatile, energetic and an inspiring personality. He infused motivation in many junior and senior scholars, colleagues, and employees. The aura of his magnetic personality is such that among others, his past critics are also his fan in present. His social and scientific network is extended globally, and has become stronger with time. His mentoring helped many to thrive in different scientific arenas all over the globe. The contribution of Dr. Saxena in Indian Drug Discovery research, especially in CADD, is profound. I am honored and fortunate to mention about Dr. Saxena on the occasion of DDDR 2021 and his 70th Birthday. Happy 70th Birthday Dr. Saxena! I cordially thank you, and appreciate all your encouragement and support.

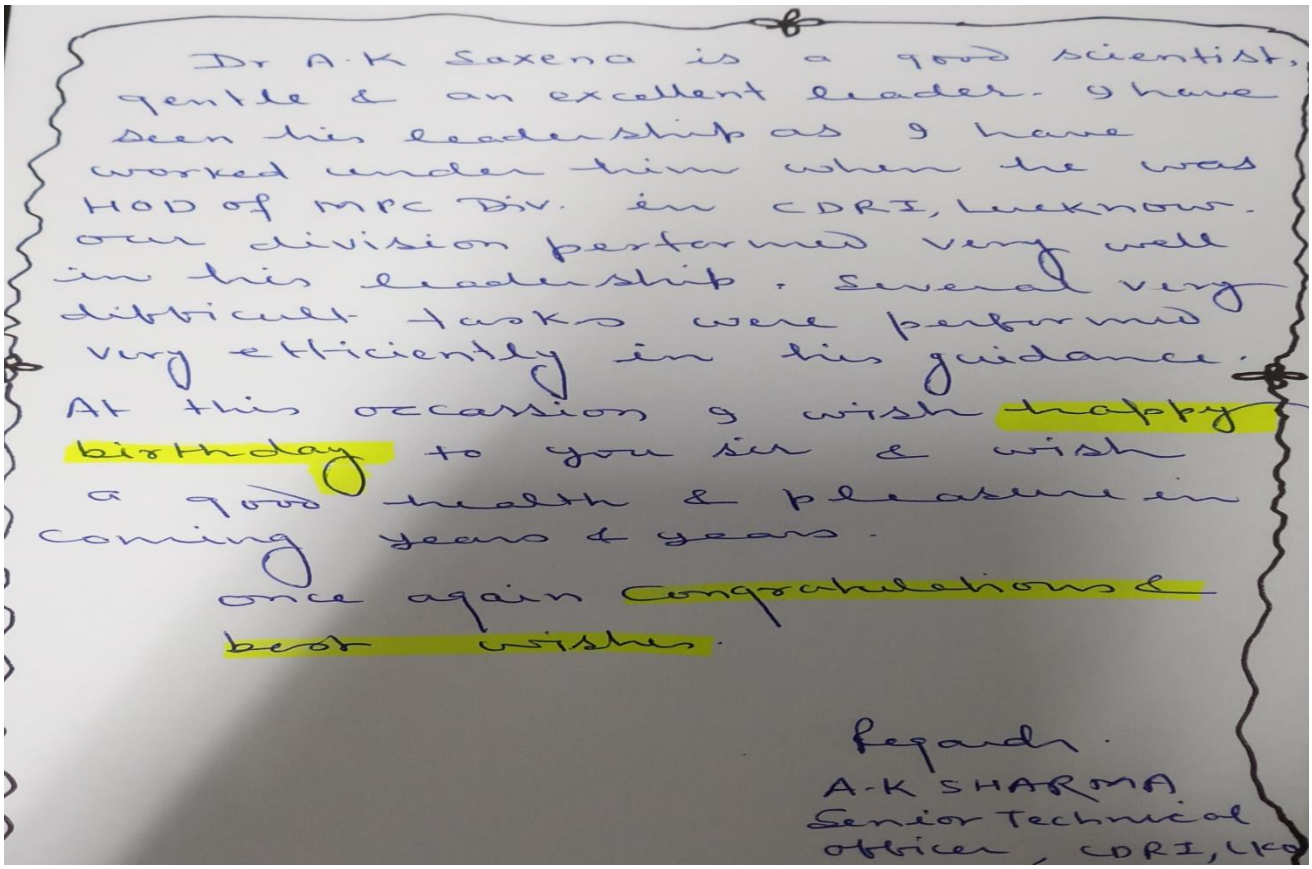
Dr. Neeraj Shakya,
Toronto, Canada

I wish a happy birthday to Dr. Anil Saxena, my esteemed collaborator who turned 70 today. I have a fond memory of collaborating with him to discover an orally active secretagogue of bone morphogenetic protein-2 that promotes fracture healing in preclinical studies. The study was published in the Journal of Medicinal Chemistry one of the flagship journals of the American Chemical Society. I wish him a long healthy and scientifically active life ahead, and he being a prolific researcher, I am sure he is headed that way.

Dr. Naibedya Chattopadhyay,
Chief Scientist, CSIR-CDRI, Lucknow

The dense foggy morning of Lucknow winter didn't deter the enthusiasm of the entire CDRI family to welcome the newly arrived Director of the institute on 19th December 2008, the day I met Dr. AK Saxena for the first time in person. It was a very hectic day with taking over the duty, video conference with DGCSIR along with the senior scientists, meeting all employees over steaming cup of coffee in the sprawling lawn behind the legendary banyan tree of Chattar Manzil, addressing them and many more. This was topped with a pleasant evening with Dr. Saxena and Mridula-ji who took us, me and my wife Susmita, to Royal Cafe in Hazratganj for a splendid dinner. The first meeting laid the foundation for a long-lasting friendship between our two families. During my five years of stay at CDRI, I was always very ably guided in all matters by an experienced elder like Dr. Saxena with his vast experience in drug discovery research and also in administration. The complex exercise of drug design and drug discovery seemed so effortless, easy, and natural in him. It was a great learning experience for me. His love for medicinal chemistry, and drug discovery research that he inherited from a legendary guru like Dr. Nityanand is truly inspiring to his associates, subordinates, and students. My wife joins me to wish Dr. Saxena a very Happy Birthday and many happy returns of the day. Pray for his long, healthy, and very active life. With the best,

Dr. Tushar & Susmita



Wish Dr. Saxena very happy 70th birthday. Also best wishes for International Symposium.

Dr. R C Gupta

I feel good to get an opportunity to write about respected Dr. Saxena Sir who was my Ph.D. mentor at the Central Drug Research Institute, Lucknow. He is globally renowned for his exceptional knowledge of medicinal chemistry and drug design and I feel privileged for being his student. His dedication and enthusiasm for research are truly inspiring and always motivated me during my Ph.D. tenure. I'll always remember him with the deepest respect and affection for his scientific guidance and moral support. I wish him good health and happiness on his birthday.

Dr. Shome S. Bhunia

Congratulation for
Dr. Anil Kumar Saxena
on the occasion of his 70th birthday

It is with great pleasure that I wish Dr. Anil Saxena all the best for his 70th birthday. I regret that I cannot participate in person at DDDR-2021 at GIPER.

It is fair to say that Dr. Saxena is a pioneer in Computer-Aided Drug Design introducing it in India and training many students and co-workers in this field. Of particular importance is the International Symposium on Current Trends in Drug Discovery Research (CTDDR) that he initiated and arranged several times. These symposia have put CDRI on the international scientific map and have greatly contributed to the scientific reputation of CDRI.

In 2010 I had the pleasure of visiting GIPER and thus see personally Dr. Saxena`s achievements in supporting GIPER and experience the scientific enthusiasm of the students of GIPER.

Anil I wish you all the best, particularly health, and many more years in research and teaching.

Prof. Dr. Johann Gasteiger
University Erlangen-Nuremberg
Computer-Chemie-Centrum

Prof. Dr. Johann Gasteiger
University Erlangen-Nuremberg,
Computer-Chemie-Centrum

"On this occasion of DDR-17-18 December 2021, I would like to take some time to reflect about wonderful moments we've shared together at CDRI. I wish you would always remain busy in promoting scientific temperament in future generations.You're such a wonderful legendary innovator to establish computer aided drug discovery research and inspiring mentor with vast knowledge you imparted is beyond priceless. May God forever bless you today and always. Wishing you my dear friend a fabulous 70th birthday.

Dr. V.K. Bajpai

First of all, I thank you Dr. Sisir Nandi for organizing such a wonderful event and proving me an opportunity to connect with you all here.I wish you Dr. Saxena a very happy birthday and pray for his good health and happy life ahead! Hereby, I would like share few glimpses of my experiences with Dr. Saxena. I joined Dr. Saxena's lab in CDRI in Nov 2014 and worked with his team for about two and a half years as a Sr. Research Associate. Dr. Saxena provided me enormous support and freedom in establish a new lab in my style, inspired me to take independent decisions in leading the project and managing the team in my way. He developed me as a leader. His valuable guidance is helping me not only in professional life but also in personal life. I thank you Dr. Saxena for being my mentor and shaping me as a better person. At the last, I wish you all a great success in your projects and a happy new year you all! Thank you for your patience!

Dr. Ratni

About GIPER

Global Institute of Pharmaceutical Education and Research (GIPER) is one of the premier pharmacy academic and innovative research institutes of India. It is situated at the city of Kashipur, Udham Singh Nagar, Uttarakhand. It is run by Prof. (Dr.) A. K. Saxena, legendary figure in India and pioneer of drug discovery research who also heads Krishna Memorial Trust (KMT) with the aim to be an academic excellence of pharmaceutical education and research, to develop keen interest in creation, preservation and dissertation of knowledge thus leading to the flowering of world-wide student's intellectual and creative competence. The institute is striving hard since inception towards academic excellence as it is a dream project of world renowned scientists. GIPER offers D. Pharm. approved by UBTER, All India Council for Technical Education (AICTE) and Pharmacy Council of India (PCI), B.Pharm. and M. Pharm. with two specializations such as Pharmaceutics and Pharmaceutical Chemistry approved by All India Council for Technical Education (AICTE) and Pharmacy Council of India (PCI), Govt. of India, New Delhi and affiliated to Uttarakhand Technical University, Dehradun. We are going to impart our student's high quality education and research, develop their skills, broaden their mental horizon and nurture them into competent and talented professionals to meet the challenges of new millennium. GIPER inculcates students for human values and professional ethics which promote creation of knowledge and innovation. GIPRER has highly educated and experienced faculties from India and abroad. We have well established libraries with a number of textbooks and references and different national and international journals with Wi-Fi internet access. The institute has excellent equipped and sophisticated laboratories with latest state of drug discovery research. It is putting emphasis on leading research, on projects having applied potential and is looking forward to a successful

Industry-Institute liaison towards closed partnership. Research projects based on anti tubercular drug design and its synthesis are being carried out under CSIR-OSDD scheme. The institute carried out research project entitled "Study of ground water quality of Kashipur industrial area**"** granted by Indian Institute of Technology, Roorkee. The institute signs a Memorandum of Understanding (MoU) with International Medical University (IMU), Malaysia, InterBioScreen Ltd., Chernogolovka (Moscow, Russia), Aristotle University of Thessaloniki, Greece and Institute of Biomedical Chemistry of Rus. Acad. Med. Sci., Moscow. GIPER is the first pharmacy institution of India which had organized an **International Seminar on Pharmaceutical Education and Research** in its first year of establishment in 2010. These were attended by eminent scientists and researchers from USA, Germany, Italy, Russia, France, Greece, Hongkong, Canada etc. In 2012 a national seminar based on **Computer-Aided Drug Design (CADD)** supported by Schrodinger Inc., USA had been organised in this campus. Thus it is an opportunity to expand our young aspirants boundaries, platforms for research collaboration and learning, and recognitions for those who strive to travel. A national seminar entitled "**Current Perspective on Drug Discovery and Pharmacoinformatics**" had been organized by GIPER on last 26 - 27 April 2014 attended by the eminent scientists, academicians, students, researchers, professionals and technocrats engaged in the multi disciplinary fields of Pharmaceutical sciences and industries. GIPER organized an international seminar entitled "Global trends in health and environment**"** on 3rd Feb 2016 at GIPER campus attended by leading scientists and researchers from different parts of the world. On 27-30 October 2017 GIPER has organised"9th International Symposium on Computational Methods in Toxicology and Pharmacology Integrating Internet Resources (CMTPI)" in Goa, India which was attended by more than 170 researchers from different corners of the world. GIPER organized CTPMS-2020 achieved tremendous success with the participation of 16 countries scientists and young researchers. GIPER stands within fifth rank in Uttarakhand where faculty have been generating incredible research articles more than 90 published in high impact factor journals. Drug design research to combat Cancer, Malaria, Tuberculosis, Alzheimer disease, Diabetes and physicochemical treatment of drinking water testing are being carried out the our Institution. Our students have been selected through campus in various multinational pharma industries such as FDC, Macleod's, Ranbaxy, Dr. Reddy's Lab, THEMIS Medicare, AKUMS etc. Now students rush to GIPER to take up pharma as a career which will in turn help to construct the global healthcare. Although GIPER has started M. Pharm. with two specializations, it will be developing as Centre of Excellence with multi-disciplinary collaborative research activities by the generation of highly qualified students with a high degree of creditability and creative potency to meet global competence to fulfill its name.

BIO SKETCHES

OF

RESOURCE PERSONS

Dr. Anil Kumar Saxena

Dr. A.K. Saxena, Emeritus Scientist, Ex- Chief Scientist and Head of the Medicinal & Process Chemistry Division, Central Drug Research Institute, Lucknow, India is actively involved in the domain of Medicinal Chemistry & Computer Aided Drug Design (CADD), and drug development research. During his 50 years of research experience he has published about 215 research papers, 24 reviews/articles in books and/monographs, and has 70 patents to his credit. He has delivered >189 invited lectures, chaired >52 session and has made >57 visits abroad. He has supervised more than 200 post graduates for their research projects and 45 students for their PhD degrees. He is the recipient of several awards, including Alexander von Humboldt Fellowship, INSA Young Scientist Medal , Themis Chemicals UDCT Diamond Jubilee Distinguished Fellowship, Ranbaxy Research Award in Pharmaceutical Sciences, an Honorary Medal for outstanding contributions to Medicinal Chemistry and International Scientific collaboration (Scientific partnership Foundation, Moscow, Russia, 2004) and the Prof. P.K. Bose Memorial Award (Indian Chemical Society,2009). He is Fellow of Royal Society of Chemistry, UK, and is also series editor for book series "Topics in Medicinal Chemistry" published by Springer Verlag. He is the Editorial Board Member of different prominent journals like, Medicinal Chemistry Research, SAR and QSAR in Environmental Research, online International journal ARKIVOC, and Patent Evaluator: Current Drugs, U.K. He is also member of several committees including American Chemical Society.

Dr. Ashesh Nandy

Dr Ashesh Nandy did his PhD in theoretical Physics and later switched to molecular biology. He was one of the pioneers in the new field of graphical representations of biomolecular sequences and study of sequence characteristics, sequence analysis, sequence homologies, molecular phylogeny, etc. His group also developed mathematical frameworks for quantitative assessment of the

graphical plots and indexes of DNA/RNA/protein sequences for quantitative sequence comparison. He has edited books and journals and published widely in national and international journals, most recently on peptide vaccine design.

Prof. Athina Geronikaki

Athina Geronikaki graduated from Tashkent State University in 1971 and gained the specialty of organic chemist. In 1977 she defended her PhD thesis and received the Ph.D grade in Chemistry (Ph.D, Doctor of Philosophy in Chemistry). In 1984 she graduated from School of Pharmacy of Aristotelian University of Thessaloniki. From 2006-2016 she is the Head of the Department of Pharm. Chemistry. Since 2010 she is Full Professor of Medicinal Chemistry of School of Pharmacy of Aristotle University of Thessaloniki. During 2009-2011 she was Vice President of School of Pharmacy of Aristotle University of Thessaloniki. In July 2013 Prof. Geronikaki was elected as a Full member of Mediterranean Academy of Science and Arts and in 2015 Member of European Academy of Science and Arts. Her scientific interest is: Chemistry of natural products isolation, determination of structure; Chemistry of biologically active compounds and evaluation of their activity, using different computational methods. She organized three International conferences: Computational Methods in Toxicology and Pharmacology, Integrating Internet Resources (CMTPI) (2003) Thessaloniki; 4th Eurasian Meeting on heterocyclic Chemistry , 2006 , Thessaloniki, 8th CMTPI -2015 and 23^{d} Hellenic Symposium in Medicinal Chemistry, 2017. Published more than 179 papers and 4 chapters in a book. Wrote 4 books for student. Has 23 Erasmus agreements and is University coordinator of Paul Ehrlich PhD Network in Medicinal Chemistry. Scientific interest: Heterocyclic chemistry of biologically active compounds (thiazoles, benzothiazoles, triazoles, thiazolidinones), medicinal chemistry (anti-inflammatory activity, COX/LOX inhibitors, PTP1B inhibitors, HIV inhibitors, antimicrobials.)

Dr. Chandra Sourabh Azad

Dr. Chandra Sourabh Azad was born and raised in Uttar Pradesh, India. Following his graduation from Hindu College Moradabad, which is associated with Mahatma Jyotiba Phule Rohilkhand

(MJP) University, he earned a gold medal for his master's degree in organic chemistry from the MJP Rohilkhand University campus. He completed his Ph.D. at the Council of Scientific and Industrial Research (CSIR) Central Drug Research Institute in Lucknow, India, under the guidance of Dr. Anil K Saxena. He joined Professor Mark Olson's research group as a postdoctoral fellow at Tianjin University, China, after completing his first postdoctoral fellowship at Guru Gobind Singh Indraprastha University in New Delhi. In September 2021, he joined Professor Fraser Stoddart's (Noble laureate 2016 Chemistry) research group, focusing on the synthesis and fluorescence characteristics of supramolecular self-assemblies and molecular machines.

Prof. (Dr.) Esin Aki Yalcin

Prof. Esin Aki-Yalcin is a full professor at the Department of Pharmaceutical Chemistry, Faculty of Pharmacy, Ankara University since 1993. She has been organized 3 International Meetings and 2 workshops as the Chair in "Medicinal Chemistry" and "Rational Drug Design" areas in Turkey since 2004. She has been some of the administrative jobs in Ankara University such as; Chair of Pharmaceutical Chemistry Department (1999-2002), Chair of Pharmaceutical Sciences Division (2003-2006), Acting Dean of Faculty of Pharmacy (2008-2009), Advisor to the Rector (2009-2014) She published around 100 articles and a book. She has an European patent as a anticancer drug candidate. She is the owner of the Medal "Badge of Honor" and Honorable Diploma of International Scientific Partnership Foundation, 2007. She worked as the Executive Committee member of QSAR and Chemoinformatic Society (2004-2014) and honored as the "Fellowship" of Asian Federation of Medicinal Chemistry in 2013. She is the elected President of "Asian Federation of Medicinal Chemistry" 2018-2020.

Prof. Indira Ghosh

Prof. Indira Ghosh is working in JNU since 2008 as Dean & Professor to steer the School of computational & integrative sciences, which deals with computational approach to Biology, Chemistry, and Economics etc. She has nourished the school as Center of Excellence under Department of Biotechnology (DBT), Govt. of India (GoI) in Computational Biology and spearheaded to initiate a new stream supported by UGC, called complex systems, harvesting few faculties from Physics and Econophysics. She has been one amongst the earlier scientists to realize

the importance of Bioinformatics and initiated M.Sc courses in Pune University (SPPU) when she joined as Professor in Institute of Bioinformatics & Biotechnology in Pune in 2003, leaving her corporate job from AstraZeneca in Bangalore. After completion of M.Sc. in Physics from Calcutta University she received in 1982 her PhD at IIISc, Bangalore under the guidance of Prof. V.S.R.Rao in Molecular Biophysics, a group lead by G.N.Ramachandran. She joined University of Houston, USA as Fulbright Scholar during 1983-1986 with Prof. J. Andrew McCammon and contributed to novel method in computational Biology. She published one of the first Docking algorithms in early eighties as a part of her thesis and developed difference of Free Energy calculation method in Biomolecules during her post-doc. Her major contributions are to develop and contribute in the field of Bio & Chemoinformatic, using Systems Biology approach to find pathway & target enzymes and developing novel tools for molecular simulations and pharmacophore design using known protein structure. She has guided 12 Ph.D, 5 M. Tech & 20 M.Sc students, mentored 7 Research Associates since last 15 years (academic) to direct them towards the evolving field of Computational Biology. During 2003-2017 She has completed 12 projects supported by IBM, DBT, IUTSSF & DeITY, some of them have potential to collaborate with industry and has published 65 papers as communicating author.

Prof. (Dr.) Kunal Roy

Dr. Kunal Roy is Professor & Ex-Head of the Department of Pharmaceutical Technology, Jadavpur University, Kolkata, India (https://sites.google.com/site/kunalroyindia). He has been a recipient of the Commonwealth Academic Staff Fellowship (University of Manchester, 2007) and Marie Curie International Incoming Fellowship (University of Manchester, 2013) and was a former visiting scientist of Istituto di Ricerche Farmacologiche "Mario Negri" IRCCS, Milano. Italy. The field of his research interest is Quantitative Structure-Activity Relationship (QSAR) and Molecular Modeling with application in Drug Design, Property Modeling, and Predictive Ecotoxicology. Dr. Roy has published more than 300 research articles (ORCID: http://orcid.org/0000-0003-4486-8074) in refereed journals (current SCOPUS *h* index 45; total citations till date 10557). He has also coauthored two QSAR related books (with Academic Press and Springer Nature), edited six QSAR books (Springer Nature, Academic Press, and IGI Global), and published more than ten book chapters. Dr. Roy is the Co-Editor-in-Chief of *Molecular Diversity* (Springer Nature) and Editor-in-Chief of *International Journal of Quantitative Structure-Property Relationships* (IGI Global). Dr. Roy serves on the Editorial Boards of several international journals Prof. Roy has been recipient of several awards including the AICTE Career Award (2003-04), DST Fast Track Scheme for Young Scientists (2005), Bioorganic and Medicinal Chemistry Most Cited Paper 2003-2006, 2004-2007, and 2006-2009 Awards from Elsevier, The Netherlands, Bioorganic and Medicinal Chemistry Letters Most Cited Paper 2006-2009 Award from Elsevier, The Netherlands, etc.

Dr. Marjan Vračko

Dr. Marjan Vračko is senior researcher at Kemijski Inštitut/National Institute of Chemistry in Ljubljana, Slovenia. Since 1994 hisresearch is focused to QSAR(quantitativestructure-activityrelationship) modelling ofbiological/toxical properties of compounds, to quantum chemistry, to chemometrics (numerical analysis of proteomic and genomic data) and to modeling of interaction between receptors and molecules. He obtained his PhD (1990) under supervision of Prof. Janos Ladik from University of Erlangen, FR Germany in the fieldof quantum chemistry.Later on hewas post doc atthe Columbia Universityof New York and at the University of Namur, BE (Faculté Universitaire Notre Dame de la Paix, Namur). In 1994 he joined theNational Institute of Chemistry in Ljubljana. In 2005 he was senior visiting researcher at the Joint Research Centre of EuropeanCommission, Ispra where he worked on applications of (Q) SAR methods for regulatory purposes. He is author of 90 scientific papers and several chapters (Hirsch index h = 31). From 2000 to 2021 he supervised three doctoral candidates and six post doctoral researches, who proceed their careers in Academia and in multinational companies (Nestle, KNÖLL GmbH, SPM AG Liechtenstein).

Prof. Prasad V. Bharatam

Prof. Bharatam is currently a Professor in Department of Medicinal Chemistry in National Institute of Pharmaceutical Education and Research (NIPER), Mohali. His field of specialization includes Medicinal Chemistry, Theoretical Organic Chemistry, Organic Synthesis, Molecular Modeling and Pharmacoinformatics. Prof. Bharatam completed his Ph.D. in 1990 from Univ. of Hyderabad, India in Applied Theoretical Chemistry. He has a total of37years research experience which includes 4 years in USA and Germany and 27 years of teaching experience. Apart from his current position he had held various positions such as Assoc. Dean (Academics) during 2015-2016 and Dean, NIPER, SAS Nagar during 2016-2018. He is the recipient of various awards such as OPPI Scientist Award in Medicinal Chemistry in 2009, Ranbaxy Research Award in Pharmaceutical Sciences in 2008, Chem. Research Society of India – Medal in 2008, Fellowship of Royal Society of Chemistry, London in 2007, IBM Faculty Award in 2007 and Fellowship of Alexander von Humboldt Stiftung, Bonn in 2002 etc. Till now he has supervised 36 Ph. D. students, 173 M.S. Pharm. students, 16 M. Sc. Chem. Students and 12 Fellows. He has received 15 Govt. funded projects, 6 Institutional grants and 2 Industrial grants. Prof. Bharatam has 258 Original Scientific articles (non-

Indian journals), 19 Original Scientific articles (Indian Journals), 23 Reviews (peer reviewed) and Book Chapters (peer reviewed) and 15 Science Education articles to his name.

Prof. Vladimir Poroikov

Vladimir Poroikov is currently the Principal Researcher and Head of Department for Bioinformatics & Laboratory for Structure-Function Based Drug Design at the Institute of Biomedical Chemistry, Moscow, Russia. In 1996-2015, he was the Professor of Medical-Biological Faculty at the N.I. Pirogov Russian National Research Medical University. Graduated as M.Sc. Physicist (1974) and earned his Ph.D. degree in Biophysics at the M.V. Lomonosov Moscow State University, Moscow (1981), and Dr.Sci. degree in Pharmacology at the National Research Center for Biologically Active Compounds, Staraya Kupavna, Moscow Region (1995). He has been awarded by the High Attestation Commission of Russian Federation as Professor in Biochemistry (2000) and Professor in Mathematical Biology & Bioinformatics (2013). Vladimir Poroikov has been elected as the Correspondent Member of Russian Academy of Sciences (2019). Member of the Council for Grants of the President of the Russian Federation, the Expert Board of the Skolkovo Foundation and the Expert Council of the Sirius University of Science and Technology; Expert of the Russian Academy of Sciences, the Ministry of Education and Science, the Russian Science Foundation and the Russian Foundation of Basic Research. Member of the American Chemical Society, Russian Biochemical Society; Society of Russian Pharmacologists. Editorial Board Member: Biology Direct, SAR and QSAR in Environmental Research, International Journal of Quantitative Structure-Property Relationships, Biomedical Chemistry, Pharmaceutical Chemistry Journal. Reviewer: Scientific Reports, ACS Pharmacology & Translational Sciences, ACS Omega, Journal of Chemical Information and Modeling, Chemical Research in Toxicology, Frontiers in Pharmacology, Briefings in Bioinformatics, Expert Opinion on Drug Discovery, etc. Co-author of 320 publications in the peer-reviewed journals and book chapters with over 4,600 citations (Publons' h-index is 36). Scientific Advisory Board Member and/or Keynote/Invited/Oral Speaker of more than 12 International conferences and symposia in the past three years.

Prof. (Dr.) Sisir Nandi

Dr. Sisir Nandi completed Ph.D. from Indian Institute of Chemical Biology (CSIR), Kolkata as a CSIR -GATE fellow and had been awarded Ph. D. in Pharmacy degree (2011) by the Jadavpur University, India. He did his Post-Doctoral research as the European Union Marie Curie fellowship in Laboratory of Chemometrics, National Institute of Chemistry, Ljubljana, Slovenia, Europe. His specialization is Pharmaceutical Chemistry and research is based on the area of drug design which includes QSAR & drug design, biological activity prediction of lead compounds, ligand-receptor interactions, virtual screening, combinatorial library design and lead-hopping. He published more than 90 original research articles and reviews in reputed international journals having high impact factor. He published 5 book chapters Springer Nature and Bentham book. He presented his research work in many international conferences around the world. He is Guest Editors of Current Signal Transduction Therapy and Current Pharmaceutical Design and Editorial advisory board of The Cancer Immunology Journal, Journal of Bioanalysis and Biomedicine, J Dev Drugs, Advanced Techniques in Clinical Microbiology, Journal of Computational Methods in Molecular Design; and many others. He has organized international conferences like CPDDP-2014, CMTPI 2017 and CTPMS 2020 as Organising Secretary. Dr. Nandi as PI completed the project entitled "Study of ground water quality of Kashipur industrial area" granted by Water for Welfare: An Uttarakhand Initiative" (WFW-UI), IIT Roorkee in the academic year of 2018-19. He is having more than 15 years of research experience. He has been guiding many masters and doctoral students.

Dr. Subhash C. Basak

Dr. Subhash C. Basak is a Senior Scientist at the Natural Resources Research Institute and an Adjunct Professor at the Department of Chemistry and Biochemistry, University of Minnesota Duluth, USA. Dr. Basak received his PhD degree in biochemistry from the University of Calcutta. During the past four decades he has pioneered research in the development of novel mathematical chemo descriptors and bio descriptors principally via applications of discrete mathematics on chemical and biological systems. He also published extensively on the use of such descriptors along with proper statistical methods in drug design, predictive toxicology, characterization of emerging pathogens as well as nano toxicology. Some specific areas of his research include: a) Formulation of new topological indices, b) Study of intercorrelation of molecular descriptors, c)

(HiQSAR)and (QMSA) studies using topological, geometrical, and quantum chemical descriptors, combinatorial libraries, f) characterization of DNA/ RNA sequences, g)proteomics maps, characterization of molecular chirality, Differential QSAR (Diff QSAR), Mathematical nanotoxicoproteomics, Computer-Assisted Approaches to Rational Design of Peptide Vaccines, and q) Explore the philosophical basis of mathematical chemistry. He has collaborated with over fifty research scientists around the world. Such collaborations resulted in the publication of more than 230 peer reviewed journal articles, book chapters, and reviews. Dr. Basak and coworkers developed three software, viz. POLLY, APProbe, and Triplet, for the calculation of molecular chemo descriptors of chemicals. He edited two books, one on network analysis published by Wiley and the other is a two volume comprehensive treatise on mathematical chemistry and its applications published by Bentham Science Publishers and Elsevier. Dr. Basak has been Chairperson from USA of two continuing international workshop series on mathematical chemistry and since 1998 organized thirteen international workshops on mathematical chemistry. During the past three decades Dr. Basak received more than 6 million US dollars in research grants and contracts from various private and public funding agencies.

Dr. Zeeshan Fatima

Dr. Zeeshan Fatima is working as a Associate Professor in Amity University Lucknow. She completed her Ph.D from CSIR-CDRI in 2007. She published more than 20 research and review articles, 02 International patents, and filed 02 filed national patents in her credit. She has been guiding many Ph D and masters scholars. She obtained the b**est oral presentation award for paper entitled** Docking Studies of Anti Alzheimers Compounds" in National Symposium on Integration of Natural Healthcare Systems and Modern science: Potential merits and future roadmap , held on 2-3 November ,2019, organized at Bhimrao Ambedkar University (BBAU), Lucknow by TBRS . And also achieved the Second prize to paper presentation entitled "Data base management" in ICMR & CSIR sponsored National Seminar On "Biostatistics and Research Methodology with an overview on clinical Research" held on 12-13 Feb 2011, at PSIT Campus, organized by organized by Institute of Pharmacy, Pranveer Singh Institute of Technology, Kanpur**.**

ABSTRACTS

OF

RESOURCE PERSONS

Classical to modern drug design: a perspective

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Drug design being the most crucial step in the drug discovery and development process has always been very challenging. In the present scenario of the global recession it is more demanding due to generic competition, patent expirations and decreasing innovations. Among the most feasible techniques, the classical approach of identification of drug candidates from natural resources or random screening program has been costly, labor intensive and slow. The combinatorial chemistry coupled with high throughput screening (HTS), the expected solution in nineties was also unsuccessful. The advancements in, molecular biology including human genome revelation, synthetic organic chemistry, computational technologies and robotics have led to a paradigm shift in the drug discovery process. The application of computer aided drug design (CADD) techniques has a great potential in augmenting the lead identification and optimization process by using new genomics and proteomics derived targets and chemical libraries through virtual high throughput screening on structure based and ligand based models as exemplified in our own work in the identification of novel molecules as potent, neuroleptic, anti-hypertensive, anti-histamines (H1), anti-Alzheimer, anti-tubercular agents. Since Indian pharma industry has expertise in generics, the repositioning of existing drugs i.e. developing new uses of existing drugs is getting more rewarding as exemplified in case of SARS-CoV-2.

A preliminary analysis and prediction method of mutations in different viruses using mathematical q_R characterization and pattern recognition

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Studying mutations can help us in understanding the patterns in changes in the genome sequence of a virus. This can lead us to develop drugs and vaccines to inhibit the growth of an epidemic. Through our set of novel algorithms, we have established a methodology to analyse mutational changes in a pathogen to determine the conserved regions and a protocol to find vaccine targets against such viruses. For this purpose, we have employed 2D Polar plot and q_R characterization to cluster different protein sequences, temporal, demographic and hotspot analyses, followed by a two-stepped mathematical model for identifying the vaccine candidates. These algorithms have previously been used to study new mutations in SARS-CoV-2 providing a relatively early detection of variant D614G, L84S and grouped mutations in nsp2. Analysis of latest mutated species of COVID-19 helps us to understand the potentiality of their pathogenicity and the possible impact of predicted vaccines.

4-(Indol-3-yl) thiazole-2-amines and 4-ιndol-3-yl)thiazole acylamines as Novel antimicrobial agents. Synthesis, in silico and in vitro evaluation.

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Herein we report the design, synthesis, computational and experimental evaluation of the antimicrobial activity of twenty nine 4-(indol-3-yl) thiazole-2-amines and 4-ιndol-3-yl) thiazole acylamines. All synthesized compounds exhibited antibacterial activity against six Gram-positive and Gram-negative bacteria in different extent. Thus, MIC for indole derivatives was in range of 0.06-1.88 mg/ml, while in group of methyl indole derivatives only six out of fourteen compounds have MIC at 0.47-1.88 mg/ml. The most sensitive bacterium was *S. typhimurium*, whereas *S. aureus* was the most resistant. The best antibacterial activity was observed for compound **5x** (MIC0.06-0.12mg/ml). Three most active compounds **5d, 5m** and **5x** being evaluated against three resistant strains, MRSA, *P. aeruginosa* and *E. coli*, were more potent against MRSA than ampicillin. Among three most active compounds **5m** and **5x**) showed stronger inhibition of biofilm formation than both reference compounds in concentration of MIC. Furthermore, **5d, 5m** and **5x** were determined for the interactions with antibiotic streptomycin using checkboard assay. All of the examined compounds were additive with streptomycin Antifungal activity of some compounds exceeded or were equipotent with those of the reference antifungal agents bifonazole and ketoconazole. The best activity was expressed by compound **5g**. All compounds exhibited moderate to good Drug-likeness scores ranged from -0.63 to 0.29. The docking studies indicated a probable involvement of *E.coli* Mur B inhibition in the antibacterial action, while CYP51 inhibition is likely responsible for antifungal activity of the tested compounds. Finally, the assessment of cellular cytotoxicity of the compounds in normal human MRC-5 cells revealed that compounds are not toxic.

Synthesis of highly fluorescent thiazolo-thiazole based self templated surfactants as a sensor of Tryptophane and Melatonin

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Tryptophan (Trp) is a necessary component of proteins for creating and sustaining a positive nitrogen balance in the human body. Due to its scarcity in plants, it is commonly included as a supplementary amino acid to diets, food goods, and medicinal formulae. A high dose of Trp, on the other hand, may cause sleepiness, nausea, dizziness, and a lack of appetite, among other things. As a result, detecting Trp in a simple, sensitive, and timely manner is critical for public health. To encounter this challenge, our group developed a new self-templated self-assembled bipyridinium-(Thiazolo-Thiazole) TTz surfactants. The CMCs of three bipyridinium-TTz amphiphiles can be modulated, causing self-assembly to occur at significantly lower surfactant concentrations by employing the principles of preorganization and self template-directed self-assembly in water. The templating phenomenon was further investigated in the presence of biologically essential molecules, e.g., L-tryptophane and Melatonin. The fluorescence emission intensity of the synthesized surfactants was found to be significantly quenched with the L-tryptophan and melatonin. As a result, synthesized surfactants were well explored as sensors for tryptamine derivatives like L-tryptophan and Melatonin.

Insight into Mechanism of Action of Anticancer Heterocyclic Compounds

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Some benzazole derivatives were synthesized and tested for their eukaryotic DNA topoisomerase II inhibitory activity in a cell free system[2,3]. Because one of the mechanisms of cancer therapy is the inhibition of DNA- topoisomerase by blocking the action of topoisomerase II, which controls the changes in DNA structure by catalyzing the breaking and rejoining of the phosphodiester backbone of DNA strands during the normal cell cycle[1]. The DNA binding and cleavage domain is one of the active sites of this enzyme. Introduction of these breaks subsequently leads to apoptosis and cell death. Interaction mechanism of DNA topoisomerase II and the series of heterocyclic compounds has been defined by using molecular modeling techniques such as molecular docking and pharmacophore analysis performed by Discovery Studio[4] and LigandScout[5]. The virtual screening were also done to propose some more active benzazoles as a result of this study.

Designing of Novel Chemicals using Molecular Multi-target Approach on COVID-19 target.

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After Dec2019, the pandemic situation that emerged due to the viral infection (COVID19) has not only halted most of the global and local activities also took toll of 5.2 million deaths and 262.2 million people suffered worldwide. Coronaviruses (CoVs) are enveloped viruses encapsulating the largest RNA genome with the capability to infect many species of animals, including humans. In general, CoVs are responsible for acute and chronic respiratory problems, gastrointestinal, and CNS related problems .Due to the focused research, a considerable amount of multidimensional data has been generated in a very short time to understand the fundamental behaviour of the virus, which is useful for novel therapeutic development to combat this disease, different routes have been considered, one of the fast is repurposing of the known drugs which have identified potential antiviral candidates [1]. Among the existing antivirals, nine protease inhibitors have been found to have low micromolar range inhibition (EC50). Broad-spectrum antiviral agents (BSAA) have been utilized to determine the antiviral potency/activity against SARS-CoV-2 [2] , as another approach. More lengthy process is to find ab initio fragments based approach like large-scale high-throughput fragment building blocks are screened against $3CL^{pro}$ protein. Proteases are always found as promising antiviral target proteins and in the case of SARSCoV-2, cysteine proteases such as 3CLpro (chymotrypsin-like protease)and PL pro (papain-like protease) serve the same. Both cysteine proteases are involved in the cleavage process of polypeptide coming out from the RNA genome of the virus, and this cleavage assists in the replication apparatus complex formation necessary for the viral existence. In the present study, we have used our method Clique Pharm [3], and attempted to generate the multi-target specific ab-initio pharmacophore models to search for the specific novel inhibitors from a database of antiviral chemicals. Apo-structures of both cysteine proteases are used to design the different sizes and types of the pharmacophore models, which are further utilized for screening the local setup chemical database to identify the multi-class specific inhibitors.

A New Similarity-Based Read-across Algorithm for the Prediction of SmallDatasets - Case Studies with Nanotoxicity Data

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Nanotechnology is an important area of science developed in 21st century, and it is being further advanced with time. Various new and modern technologies are utilized to produce different nanomaterials and nanoparticles now-a-days, and these are used in various fields of industries and society. The nanoparticles are very effective due to their small size (1-100 nM), unique physicochemical properties, and large surface area: volume ratio. Due to their random use, the nanomaterials are dumped improperly affecting the environment adversely. They can pass the plasma membrane with ease due to their small particle size and hence can cause toxicity also. The regulatory agencies are working continuously to assess the risk associated with the nanoparticles and nanomaterials. They rely mostly on the computational toxicity prediction to avoid the complexities associated with laboratory experimentation. QSAR and Read-across are mostly used to fill the data gaps and for the risk and hazard assessment. In the present communication, we propose a new similarity based read-across algorithm for the prediction of toxicity (biological activity in general) of untested compounds from structural analogues.Three similarity estimation techniques such as, Euclidean distance based similarity, Gaussian kernel function similarity, and Laplacian kernel function similarity are used in this algorithm. The new algorithm is properly validated against three published nanotoxicity datasets. The quality of predictions depends on the selection of the distance threshold, similarity threshold, and the number of most similar training compounds. In this work, best predictions were obtained after selecting 0.4 – 0.5 as the distance threshold, 0.00 – 0.05 as the similarity threshold, and 2– 5 as the number of most similar training compounds. After toxicity prediction of test set compounds, the external validation metrics such as $Q^2_{ext\_F1}$, $Q^2_{ext\_F2}$, RMSEp were calculated. The computed metric valuesclearly justify the efficiency of the new read-across method and accuracy of the generated data by the proposed algorithm. A java based computer program (available at https://sites.google.com/jadavpuruniversity.in/dtc-lab-software/home) has also been developed based on the proposed algorithm which can effectively predict the toxicity of unknown NPs after providing the structural information of chemical analogues. The new algorithm andthe program can be used for the data gap filling, prioritizing existing and new NPs, and for the risk assessments of NPs.

Chemometrics in the global view of toxicity – from proteomics to organism effect

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In understanding of xenobiotic-organism interaction the computational modeling plays an important role. Here, we are focused on toxicology.In a new toxicology paradigm a toxic effect is considered as the adverse outcome pathway (AOP). Entire AOP represents a cascade of events, which occur after the exposure to a chemical on: molecular- , organelle- , cellular- , tissue- , organ- , organism- , and population- level. Our focus is placed on computational modeling of these events. We present the chemometrical methods, which play central role in analysis of proteomics data, the modelling of xenobiotics-protein (endocrine receptors) interaction and the clustering (grouping) of chemicals. As chemometrical methods we present: the principal component analysis (PCA), self organizing maps (SOM), genetic algorithm (GA) and distance analysis including Mahalanobis distance. In the presentation we show the mathematical basis of mentioned methods. Later on, we present the applications on analysis of proteomic and genomic data [1-3], and the clustering of compounds on basis of similarity among them. Different data sets are analyzed: the set of compounds tested on endocrine disruption activity, PAHs and PCBs [3, 4].

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3D thinking in drug discovery

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One of the important characteristic features of great medicinal chemists is to think in three dimensions (Murcko MA (2018) J Med. Chem. 2018, 61:7419-7424). This aspect is particularly true in the field of Computer Aided Drug Discovery. The QSAR, molecular docking, molecular dynamics, pharmacophore mapping, virtual screening, de novo design, etc. all the technologies apply 3D structures and hence 3D thinking is very essential. The AIDD methods also require 3D information of the drugs. The drug receptor interactions are always in the 3D mode. In this talk, the details of 3D thinking as applied to anti-malarial research will be presented.

Drug repurposing for covid-19 therapy: challenges and opportunities

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Drug repositioning is the identification of new indications for the approved medicines. The availability of information on pharmacological and toxicological characteristics provides conditions for rapid introduction of launched drugs for a new nosology. The need to respond quickly to the COVID-19 pandemic has spurred large-scale research in this direction. To identify new pharmacological effects of known drugs, *in silico* and *in vitro* studies are carried out. Computer estimates are obtained by modeling the interaction of analyzed compounds with molecular targets, identifying analogs based on structural similarity, analyzing structure-activity relationships using machine learning methods, and establishing associations using network pharmacology. Pre-selection of potentially active compounds based on *in silico* evaluations significantly increases the chances of success. Several large-scale experimental studies are devoted to in vitro screening for one or several targets from 1,400 to 12,000 drugs, making it possible to select some "candidates" for repositioning. In many cases, the results obtained for the same drugs in different test systems do not agree with each other. The observed contradictions could be explained by the absence of standardization of the assays developed by various researchers independently of each other and the lack of generally accepted reference drugs. The possibilities and limitations of drug repositioning in the face of the COVID-19 pandemic and ways to mitigate new biogenic threats in the future will be discussed. This study is performed with the support of the Russian Ministry of Science and Higher Education (project No. 121102900156-6) and the Russian Foundation of Basic Research (project No. 20-04-60285).

Structure-based screening and repurposing of chemotherapeutics to combat COVID-19

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SARS-CoV-2, novel strain of coronavirus diseases, has deceased the incredible lives of people around the world since the end of 2019. In such a critical situation, where every life is gasping for breath, under the suffocating veil of SARS CoV-2, there is an exigency to develop an effective remedial measure to mitigate the fatality of coronavirus. There is no specific small molecule chemotherapeutics except few vaccines available to combat COVID-19. Some US-FDA approved drugs have been repurposed to tackle this dreadful virus. Our laboratory screened many chemotherapeutics including antimalarials and antivirals to repurpose against COVID-19 using structure-based docking simulation. This is to specify that the developed docking score based single parametric model has been taken as a barometer to screen many more chemotherapeutics to combat COVID-19 . Preventive natural medicines have also been studied by our group to combat various targets of SARS-CoV-2. Therefore, this expertise and current research have been devoted for the mankind.

Applications of mathematical chemo descriptors and proteomics-based biodescriptors in QSAR: Applications to mutagenicity, blood-brain barrier entry and nanotoxicity assessment

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Since the middle of the twentieth century there has been a growth spurt in research on the development and use of invariants of molecular graphs. Such chemo descriptors have emerged as important tools for quantitative structure-activity/ toxicity relationship (QSAR/ QSTR) studies. In the post-genomic era, omics technologies like proteomics have emerged as useful source of information for the exploration and characterization of bioactivity and toxicity of chemicals. Our team used various strategies for the development of bio descriptors from proteomics data and their use in the characterization of perturbation of the cellular proteome by exposure to drugs and priority pollutants. This presentation will discuss results of our QSAR/ QSTR studies using high-dimensional chemo descriptors space derived using robust statistical and machine learning methods. We will also discuss our integrated chemo bio descriptor approach where a combination of chemo descriptors and bio descriptors were used for model building.

Novel Carbamates as potential Acetylcholinesterase inhibitors for Alzheimer's Disease

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Alzheimer's disease is a neurodegenerative disorder that mainly affects the elderly. The disease progress with age and the patients suffering from it are not able to perform simple daily routine activities. The drugs that provide symptomatic relief includesacetylcholinesterase inhibitors and N-methyl-D-aspartate receptor antagonist. Recently Aducanumab,an amyloid beta-directed antibody has been approved by FDAfor Alzheimer's. The side effect of the therapy includes brain swelling and tiny brain bleeds. So, there is still a need to find safe and efficacious treatment for Alzheimer's. In this study, we report some of the novel carbamates that have been docked and compared with the standard drug Rivastigmine. The binding scores of the docked carbamates are better than Rivastigmine.

Keywords: Carbamate, acetylcholinesterase inhibitors, Alzheimer's Disease

ABSTRACTS

OF

PARTICIPANTS

POLY (METHYLACRYLATE) AS A NOVEL POLYMER MATERIAL FOR DESIGNING ORAL DRUG DELIVERY SYSTEMS WITH CONTROLLED RELEASE PROPERTIES

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The oral route of drug administration in the gastrointestinal tract is by far the most common, and it can be used for both systemic drug delivery and treating local gastrointestinal diseases. Drug delivery to specific regions of the upper or lower gastrointestinal tract can also be improved with the right formulation. Polymers make up a large portion of the materials used in controlled release formulations and drug-targeting systems due to their diverse topology and chemistry. By providing controlled release of therapeutic agents in constant doses over long periods of time, cyclic dosage, and tunable release of both hydrophilic and hydrophobic drugs, they have contributed significantly to the advancement of drug delivery technology. Eudragit is a brand of polymethacrylate-based copolymers with a wide range of applications. Anionic, cationic, and neutral copolymers based on methacrylic acid, methacrylic/acrylic esters, or their derivatives are included. Eudragits are amorphous polymers with glass transition temperatures ranging from 9 to 150 degrees Celsius. Eudragits are inert, non-biodegradable, and non-toxic. Eudragit L, which is anionic and soluble at pH > 6, is used for enteric coating, whereas Eudragit S, which is soluble at pH > 7, is used for colon targeting. The physicochemical properties and applications of various grades of Eudragit in colon-specific/enteric-coated/sustained release drug delivery and taste masking are discussed in this review.

TAPPING THE CHEMICAL SPACE FOR QcrB INHIBITORS USING ARTIFICIAL INTELLIGENCE

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We report our attempts to utilize artificial intelligence to understand the chemical space that is most suitable to develop QcrB inhibitors as anti-tubercular agents. The training and validation sets were curated from the literature and the feature space mainly comprises various chemical fingerprints as descriptors to understand the structural requirements for QcrB inhibitors. We used eight ML algorithms, including random forest (RF), decision trees (DT), support vector machine (SVM), and extreme gradient boosting (XGBoost) to develop classification-based models. The results demonstrated that the SVM outperforms other classification models exemplified by a superior area under the receiver operating characteristic curve (AUC-ROC) of 0.80. This model was applied on different sets to depict its accuracy and reliability. Furthermore, we will make these models openly available through a web application named Q-TB.

SELF-NANOEMULSIFYING DRUG DELIVERY SYSTEM FOR IMPROVEMENT OF POORLY SOLUBLE AND LOW BIOAVAILABLE DRUGS

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Biopharmaceutical Classification System (BCS) present a significant challenge in oral formulations due to their low solubility and permeability, as solubility enhancement approaches alone may not be sufficient to improve oral bioavailability of these drugs. The Self Nanoemulsifying Drug Delivery System (SNEDDS) is a novel drug delivery system designed to improve the water solubility of medications that are ineffectively water soluble. Encapsulating a drug in SNEDDSs can improve solubilization, GI tract stability, and absorption, resulting in increased bioavailability. The use of solid SNEDDS in the form of dry, solid powders would help to overcome the limitations of liquid SNEDDS by improving patient compliance and stability. The use of solid SNEDDS in the form of dry, solid powders would help to overcome the limitations of liquid SNEDDS. Solid dosage forms are more stable and easier to handle than liquid systems, so efforts are being made to convert liquid systems to solid SNEDDS. Solid carriers are being used to convert Liquid SNEDDS to Solid SNEDDS.

DEVELOPMENT AND EVALUATION OF MICRO EMULSION FORMULATIONS OF NEBIVOLOL FOR SOLUBILITY ENHANCEMENT

Alfisha Saifi*, Dr. Kapil Kumar Chauhan

Nebivolol HCl is a newer drug of β1-adrenergic blocker category, basically used as anti-hypertensive. It is a 3rd generation, antagonist, having NO (nitric oxide) enhancing vasodilator properties It has 12% oral bioavailability, because of its pre systemic metabolism by the means of cytochrome P450 2D6 enzymes. Its log P value is 4.03 and 5mg is its daily dose. It is highly lipophilic drug and belongs to class BCS II, with slow dissolution. Bioavailability of any drug can be improved by avoiding its first pass metabolism and promoting solubility. Several researchers have worked on the development of ME formulations on different poor water-soluble drugs, to increase their solubility.The purpose of this study is an attempt to enhance the solubility to improve the bioavailability of nebivolol drug by developing a novel delivery system that is microemulsion (ME) . ME formulations were developed using different oil, surfactant and co-surfactants in different ratio and studied on various parameters. Different preformulation tests done on received sample of Nebivolol. FTIR study was performed in order to find out any interactions between the ingredients. Based on the solubility Capmul Pg-12 was finalized oil, Tween 80 as surfactant, propylene glycol as the cosurfactant based on solubility and emulsification efficiency . Five Nebivolol ME formulations were successfully developed by use of oil, water, SA and Co-SA different ratio. Prepared formulations were studied for different properties- transmittance (%), pH, refractive index, viscosity, drug content, and solubility. It was seen that after 4 hours of diffusion, the drug released from the formulation ME5 is faster and more than that of the other i.e., 90.2□0.06%.It was found that ME5 was more stable and Soluble than other prepared formulations. With the better solubilty the bioavailability of Nebivolol will increased and helps in faster absorption and High diffusion in systemic circulation with lower or no risk of degradation. It somehow also reduced frequent intake of drug.

MODELLING AND CHARACTERIZATION OF PROTEOLYSIS PROCESS FOR DECIPHERING UNDERLYING ENZYMATIC ACTIVITY IN INDUSTRIAL FOOD DIGESTION PROCESS

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Proteases in industrial food processing is an ever-evolving critical element in the design and development of new food products. With the advancement of enzyme technologies and mass spectrometric techniques, the design of food processing has become more tailored than ever before. In Addition to innovation in physical and chemical factors which control proteolysis, a plethora of enzymatic combinations and innovative sources have been discovered to aid these food processing steps. As the proteolysis process in biological systems holds the key to the understanding of end-product bioactivity, a variety of approaches have been attempted for understanding the complex in-vivo process. Digestion mapping, mathematical modeling and in-vitro digestion models are some of the interesting approaches among them.Peptidomics techniques, cleavage predictors and related databases made this area more accessible for investigation. In this presentation author briefly discussed the application of proteases in industrial food processing techniques with a brief walkthrough protease activity mapping techniques.A holistic understanding on the industrial protease activity mapping process with their outcome is the main goal of this presentation.

TAIL-APPROACH BASED SYNTHESIS OF NOVEL BENZENESULFONAMIDES AS HUMAN CARBONIC ANHYDRASE I, II, IV AND IX INHIBITORS

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The α- class of carbonic anhydrase (CA) comprises of sixteen isoforms in mammals, of which fifteen are well established in humans, known as human associated carbonic anhydrases (hCAs).The regulated activity of these isoforms is essential for many important physiological activities in the body, while their overexpression leads to many diseases. So, in quest to discover novel carbonic anhydrase inhibitors (CAIs) and inspired by the scope of sulfonamide based heterocyclic inhibitors of hCAs, we designed and synthesized novel sulfonamide derivatives containing tail moieties of diverse nature and 1,2,3-triazole ring as linker group. Further, after thorough characterization of the synthesized derivatives by rigorous analysis of their spectral data (^{1}H NMR, ^{13}C NMR, IR and HR-MS), these were screened in-vitro against physiologically important hCA I, II, IV and IX isoforms. Inhibition results showed that atleast half of the series derivatives exhibited moderate inhibition profile against ubiquitous hCA I isoform. Some derivatives possessed potent as well as selective inhibition against cytosolic hCA II isoform. All derivatives presented moderate to weak inhibition towards hCA IV, while transmembrane tumor associated isoform hCA IX was effectively inhibited by all the newly synthesized analogues. Thus, these insights can be used to generate more such type of novel CAIs with enhanced potency and selectivity.

STANDARDISATION AND ISOLATIONOF BIOACTIVE FRACTION OFRHIZOMES OF *SAUSSUREA COSTUS* (FALC.) LIPSCHITZ TO IDENTIFY BIOACTIVE COMPOUNDS FOR CANCER TREATMENT

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Saussureacostus(Falc.) Lipschitz,commonly known as ‘kuth’is a robust perennial herb of the Western Himalayas. *S. costus*was first listed in Appendix II of CITES (the Convention on International Trade in Endangered Species of Wild Flora and Fauna) on 1.7.1975and later up listed to Appendix I in 1985. Due to immensebiological potential this plant is frequently used in various indigenous systems of medicines such as China, India, Japan and Korea. A methanolic extract of the plant was subjected to fractionation. The different fractions such hexane, chloroform and butanol were subjected to screening against various cancer cell lines where chloroform fractions have shown immense potential and then standardization of the active fraction is carried out to assess the quantity of secondary metabolites. We have isolated 15 secondary metabolites and four of them appeared to be new chemical entities which are characterized by detailed MS, 1D and 2D NMR spectroscopy further isolation of active constituents is still in progress. However, the isolated compounds SC01, SC03 and SC06 have shown good bioactivity against various cancer cell lines.For SAR study semisynthetic modification of these active compounds is in progress so as to developed novel anticancer drugs.

IN SILICO PHYTOTOXICITY MODELING OF DIVERSE PESTICIDES ON ALLIUM CEPA

Anjali Murmu, Purusottam Banjare, Jagadish Singh, Partha Pratim Roy

With the aim of identification of toxic nature of the diverse pesticides on *Allium Cepa*, experimental toxicity value (EC_{25} and NOEL) were collected from OPP database and was subjected to Quantitative Structure Toxicity Relationship (QSTR) analysis in accordance OECD principles of QSAR model validation. The QSTR models development was done by using multiple linear regressions (MLR) using ordinary least squares (OLS) and genetic algorithm (GA) was used for the feature selection. All the developed MLR-OLS models were found to be sturdy enough in terms of statistics with cross validation coefficient value (Q^2_{LOO} = 0.619 - 0.748). The predictive power of the developed models were assured by high values of external validation parameters (Q^2F_n = 0.662 - 0.845, CCC = 0.844 - 0.867). The prediction reliability was extensively analyzed by the application of leverage approach of Applicability Domain (AD). The models indicated that the number of oxygen, SO_2, distance between the secondary nitrogen, and the present of bulky groups influence the toxicity of pesticides. Finally, prediction and prioritization of the pesticides with no experimental phytotoxicity value for two end points (EC_{25} and NOEL) was done. Occurrence of similar prioritized pesticides for both endpoints indicated that the either of the endpoints can be used for ecotoxicological study of the pesticides. The results that obtained from this research work will help the scientific community and society in depicting the environmental impacts of pesticides.

NOVEL DRUG DELIVERY SYSTEM LOADED WITH NATURAL AGENT FOR AUGMENTED ARTHRITIS THERAPY

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Rheumatoid arthritis is chronic, progressive, autoimmune disease characterized by systemic inflammation, the bone, cartilage, tendons, and ligaments of joints are destroyed. All this damage to the joints causes deformities and bone erosion, usually very painful to patients. Many synthetic medications are prescribed as conventional treatment for rheumatoid arthritis, but they have side effects that can adversely affect the therapeutic outcome. *Calotropis procera* is described in Ayurvedic literature for the treatment of inflammation and arthritic disorder. The bark and leaves of *Calotropis procera* are known to show anti-inflammatory and analgesic effects. The leaves contain mainly the chemical constituents α-amyrin, α-amyrin acetate, β-sitosterol, urosolic acid which are responsible for the antiarthritic activity, anti-inflammatory activity, and analgesic effect. Microsponges delivery system is a highly cross-linked, porous, polymeric microsphere, a polymeric system consisting of porous microspheres that can entrap and release drugs into the skin over a long period of time, which could be incorporated into a formulated product such as a gel, cream, liquid or powder. The present work is focused on the development of microsponges of *Calotropis procera* by quasi emulsion solvent diffusion method and loaded them in gel to deliver the drug in form of a novel drug delivery system (NDDS) as a topical formulation for the treatment of arthritis.Accordingly, the current investigation showed that the *Calotropis procera* markedlyreduced the paw inflammation, hence it has great potential in the treatment of RA.

COVID-19 POTENTIAL TARGETS: BIG CHALLENGES TO QUEST SPECIFIC TREATMENT

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The novel strain SARS-COV-2 of coronavirus disease(COVID-19) became pandemic at the end of 2019 with an unprecedented global crisis by infecting around 11 million people in more than 200 countries. The important structural proteins such as nucleocapsid protein (N), membrane protein (M), an envelope protein (E), and spike protein (S) related to COVID-19 are discussed. The topology of these various targets has explored utilizing structure-based design and crystallographic studies. The literature reported that the N-protein processes the viral genome to the host cell during replication. The “N-terminal domain” and “C-terminal domain” contributes towards localization in the endoplasmic region and dimerization respectively. The M protein determines the shape of coronavirus and also assists S protein to integrate with the Golgi-endoplasmic region complex leading to the stabilization of the virion. The viral spike protein (S) attaches cellular receptors. Currently, there is no permanent cure and treatment of COVID-19 hence researchers are repurposing a suitable combination of drugs including antiviral, antimalarial, antiparasitic, and anti-bacterial, hypertensive receptor blockers, immunosuppressant’s, anti-arthritis drugs, including ayurvedic formulations.

HEPATOPROTECTIVE EFFECT OF COMBINED EXTRACTS+ VITAMINS AGAINST ANTITUBERCULAR DRUGS INDUCED HEPATOTOXICITY IN ALBINO RATS

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The present study was aimed to investigate the hepatoprotective activity of the Combined extracts+ Vitamins against antitubercular drugs induced hepatotoxicity in Wistar albino rats. Hepatotoxicity was induced in albino rats by a combination of isoniazid(7.5mg/kg), rifampicin(10mg/kg), and pyrazinamide(35mg/kg) given orally as a suspension in distilled water for 30 days. Combined extracts and Vitamins (500mg/kg Bw) significantly ($P<0.05$-$P<0.001$) reduce the antitubercular drugs induced.hepatic toxicity towards normal. Combined extracts and Vitamins were hepatoprotective against antitubercular drugs induced hepatotoxicity in albino rats.

DESIGN SYNTHESIS AND EVALUATION OF PHTHALIMIDE DERIVATIVES AS TARGETED VEGRF INHIBITORS FOR BREAST CANCER

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Cancer is the second leading cause of death globally and is a matter of concern. Phthalimide scaffold possesses many types of biological activities and has recently been reported substantial antitumor activity. We have designed a library of Phthalimide derivatives by using a structure-based drug design approach by targeting vascular endothelial growth factor receptor (VEGFR). The docking results show the possible mechanism and binding mode of compounds in the active site of protein (PDB ID: 2OH4). The final library also screened for *in silico* ADMET and drug-likeness properties to get safer and drug-like hit molecules. The top 15 hit molecules (B1-B15) were synthesized and characterized with the help of FT-IR, ^{1}H NMR, ^{13}C NMR, Mass Spectroscopy, and C, H, N analysis. All the synthesized Phthalimide derivatives were evaluated for their *in vitro* anticancer activity against breast cancer cell line (MCF7). Most of the compounds showed moderate-to-potent anti-proliferative activity against MCF 7 cells. Amongst all, compound B9 showed the most potent activity in µM range. The docking result shows the specific interactions for the most potent compound in active site.

ISOLATION AND IDENTIFICATION OF ANTI-CANCER MOLECULAR LEADS FROM CLINICALLY EFFECTIVE PLANT PIPER CUBEBA.

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*Piper cubeba*belongs to family piperaceae, (common name cubeb pepper). Traditionally it's used for treatment of various diseases, like gonorrhoea, dysentery, syphilis, abdominal pain and asthma and has also inhibitory effect on Hepatitis-C virus protease.In Moroccan and Chinese traditional medicine as one of the important plants for the treatment of cancer. Several of its medicinal properties have been proven by scientific studies, including anti-inflammatory, analgesic,antimicrobial, antiestrogenic, hepatoprotective, antiparasitic and cytotoxic activities. These biological activities are mainly due to the presence of bioactive lignin's.Present study was undertaken to explore bioassay guided fractionation, isolation of chemical constituents from bioactive fractions so that potential cytotoxicity of fractions and pure isolates against five different human carcinomacell linesColon (HCT, MCF), Pancreas(MIA-PACA), Breast(SH-SYSY) and Lung(A549) using mechanistic in-vitro and in-vivo assays. This study has never been explored for particular bioactivity systematically before. So far we have isolated 14 compounds which include (−)-cubebin, (−)-hinokinin,(−)-yatinisolated compounds were characterized by using spectroscopic techniques NMR (1D and 2D), HRMS further isolation is continuous. Isolated active marker compounds will be used for the standardization of these plants as herbal drugs using HPLC and HPTLC.

GREEN SYNTHESIS OF NANOPARTICLES

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Nanoparticle synthesis using microorganisms and plants by green synthesis technology is biologically safe, cost-effective, and environment-friendly. Plants and microorganisms have established the power to devour and accumulate inorganic metal ions from their neighboring niche. Every biological system varies in its capabilities to supply metallic nanoparticles. However, not all biological organisms can produce nanoparticles due to their enzymatic activities and intrinsic metabolic processes. These biosynthesized metallic nanoparticles have a range of unlimited pharmaceutical applications including delivery of drugs or genes, detection of pathogens or proteins, and tissue engineering. In materials science, “green” synthesis has gained extensive attention as a reliable, sustainable, and eco-friendly protocol for synthesizing a wide range of materials/nanomaterials including metal/metal oxides nanomaterials, hybrid materials, and bioinspired materials .In this review, we summarized the fundamental processes and mechanisms of “green” synthesis approaches, especially for metal and metal oxide [e.g., gold (Au), silver (Ag), copper oxide (CuO), and zinc oxide (ZnO)] nanoparticles using natural extracts. Importantly, we explored the role of biological components, essential phytochemicals (e.g., flavonoids, alkaloids, terpenoids, amides, and aldehydes) as reducing agents and solvent systems. The stability/toxicity of nanoparticles and the associated surface engineering techniques for achieving biocompatibility are also discussed. Finally, we covered applications of such synthesized products to environmental remediation in terms of antimicrobial activity, catalytic activity, removal of pollutants dyes, and heavy metal ion sensing

QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP MODELS UTILIZING THEORETICAL STRUCTURAL DESCRIPTORS CALCULATED FROM THE STRUCTURE OF 6-FLOUOROQUINOLONES COMPOUNDS.

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Most alarming is the emergence of multidrug-resistance tuberculosis (MDR-TB). MDR-TB urgently needs to develop new second line anti-mycobacterial chemotherapeutic including chloroquinolones. In the present thesis, an attempt has been made for the development of quantitative structure activity relationship models utilizing theoretical structural descriptors calculated from the structure of chloroquinolones compounds. A number of QSAR has been generated and validated as per the statistical rules. Then the validated QSAR model has been applied for prediction of anti-mycobacterial activities for new congeneric compound. The study in this direction may focus important structural descriptors modeled in QSAR, which are crucial for the designing of new lead like active congeneric compound. Statistically validated models could be utilized for predicting highly active Chloroquinolones compounds obtained by generating virtual compounds based on combinatorial library generation approach. some of the Chloroquinolones predicted hits could be synthesized and tested for experimental validation .

QUANTITATIVE DETERMINATION OF TOTAL PHENOLIC CONTENT AND ANTIOXIDANT POTENTIAL OF METHANOLIC PLANT EXTRACTS

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Herbs are utilized for their medicinal purpose several thousand years earlier. But the use of modern medicine was very popular inlast century and herbal medicine suffered a setback Herbal medicines have profound availability and fewer side effectsand thus use of herbs are again gaining popularity. Medicinal plants continue to be an important therapeutic aid for various human ailments. The antioxidant activity of medicinal plants are capable of terminating the chain reactions that damage cells by removing free radical intermediates and inhibiting other antioxidation reactions thereby reducing stress responsible for many degenerative disorders.The present study aimed to determine the quantitative phytochemical and *in-vitro*antioxidant activityof Leaf of *Centella asiatica*, *Camellia sinensis,*and Bulb of *Allium sepa.*Quantitative analysis for total phenolic content was carried outby the FolinCiocalteau reagent method and the *in-vitro* antioxidant activity of methanolic extracts was assessed by the DPPH assay method using standard protocols. Total phenolic content was calculated by the standard regression curve of Gallic acid and the results were expressed as Gallic acid equivalent (mg/g).For the DPPH radical scavenging activity ascorbic acid was used as a reference standard while methanol was used as control. The results show High phenolic content adequate antioxidant activity.

PERSONALISED DOSAGE FORM

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Personalized drug delivery systems (PDDS), implying the patient-tailored dose, dosage form, frequency of administration and drug release kinetics, and digital health platforms for diagnosis and treatment monitoring, patient adherence, and traceability of drug products, are emerging scientific area. Personalized medicine is based on the categorization of patients into several groups by means of practices, interventions, or dosage forms which are modified specifically for the patient on their diseased risk and expected response. Other terminology synonymies with personalized medicine are stratified medicine, precision medicine, and P4 medicine. Patient genetic content or any cellular or molecular analyses through diagnostic testing are the basis for individualization of dosage forms. Each human has an exclusive variation of genome. This advanced technology of personalized medicine is relied on testing of patient's fundamental biology, DNA, RNA, or protein which helps in disease/disorder confirmation. The techniques comprise of are genome sequencing, RNA sequencing, etc. A genome-wide association study is conducted to investigate the link of disease with a mutation. This study will focus on the genome sequence study of one disease and then, genome sequence of many patients with that disease will be done. Customized drug delivery systems are the result of this concept. It involves three-dimensional (3D) printing which is connected to freeform fabrication techniques, namely, layer-by-layer technology of depositing materials (digitally controlled) to generate freeform geometries. Despite of enormous potential, still 3D bio printing technique is facing a regulatory challenge to achieve its maximum potential in pharmaceutical industry this review provides an overview of advanced design solutions for new products such as interactive personalized treatment that would interconnect the pharmaceutical and digital worlds. Furthermore, we discuss the recent advancements in the pharmaceutical supply chain (PSC) management and related limitations of the current mass production model

PHYTOCHEMICAL INVESTIGATION OF CHEMICAL CONSITUENT OF *TINOSPORA CORDIFOLIA* TO IDENTIFY NOVEL NCE'S FOR ANTIVIRAL TREATMENT

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Tinospora cordifolia commonly called as Amrita or Guduchi belongs to the family ofMenispermaceae. *T.cordifolia* in India, it grows right from Kumaon Mountains to Kanyakumari. It is also found in tropical and subtropical countries such as China, Africa, Myanmar, Srilanka and Burma. It is considered as an essential herbal plant of Indian system of medicine (ISM)and has been used in the treatment of cold, fever(viral), urinary problem, dysentery, skin diseases, leprosy, diabetes,Alzheimer's, Parkinson's and many more diseases. The extract of this plantpossess antioxidant, antimicrobial, antibacterial, antifungal,anticancer,HIV-potential, antitoxic, antioxidant,antistress, wound healing, immunomodulating activities. In the presentInvestigation we have carried out isolation of the secondary metabolites from *T.cordifolia* to discover novel bioactive compounds for Antiviral activitiesand semisynthetic modifications of these bioactive leads is in progress.We have standardized the bioactive chloroform and butanol fractions with the help of marker compounds using existing analytical techniques (HPLC, and LC-MS).Until nowa total of fourteen compounds have been isolated seven from chloroform extract viz 8-Hydroxytinosporide, Syringin, Tinosporicide and some common steroid compounds like β-sitosterol, β-sitosterol glycoside,and alkaloidslike Berberine, Isocolumbin, Magnoflorine and Tinocordiside from butanol fraction and four of them are new chemical entities.Further isolation is continuingon butanol fraction. The isolated compounds are characterized by using NMR (1D and 2D), HRMS and other spectroscopic techniques.Since alkaloids like Berberine, Isocolumbin, Magnoflorine and Tinocordiside are reported to have high binding affinity against variant of SARS-CoV-2 strains we look for isolation of more potent and novel compounds having antiviral activities.

A COMPUTATIONAL APPROACH FOR THE IDENTIFICATION OF NOVEL INHIBITORS AGAINST PENICILLIN BINDING PROTEIN

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Antimicrobial resistance has been rising in past few years due to the overuse and exploitation of existing antimicrobials. This has motivated the search for novel scaffold that has the capability of rapid antimicrobial action. The hybridized pyrimidines have attracted us due to their widespread biological activities such as antibacterial and antifungal activities. Here in, a series of pyrimidine based antimicrobial agents were selected for the 2D quantitative structure activity relationship analysis (2D QSAR) and docking study. The exploration of the chemical structures in combination with the biological activity in CPMLR led to the detection of six descriptors (Constitutional descriptors, Topological descriptors, Modified Burden Eigenvalues and 2D autocorrelations) for modeling the activity. The resulted QSAR model has been validated using combinatorial protocol in multiple linear regression (CP-MLR) and partial least squares (PLS) analysis. The best QSAR model displays the r^2_tvalue of 0.594, Q^2_{LOO} value of 0.779, Q^2_{L5O} value of 0.767. Further docking study was executed using AutodockVina against Penicillin binding protein (PBP2a).

DIPHENYL METHANOL CARBAMATESAS AN ACETYLCHOLINESTERASE INHIBITORS

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Alzheimer's disease is a progressive neurodegenerative disorder which should be tackled with drug targeting acetyl-cholinesterase enzyme. A series of diphenyl methanol derivatives were synthesized, characterized. Further modified Ellman's colorimetric method was used for the quantitative assessment of acetyl-cholinesterase inhibition potential.Rivastigmine was used as positive control. However the derivatives were not as active as the positive control rivastigmine, but a general better activity was shown. The best result was for EK_{13}which showed $IC_{50}$of 27.51µM. These results indicated that di-phenyl methanol carbamate derivatives can function as scaffolds for AD. Further derivatizations should be done to improve their AChE inhibition profile.

OPTIMIZATION AND EVALUATION OF PIPERINE LOADED HERBOSOMES FOR THEIR ANTIOXIDANT AND HEPATOPROTECTIVE POTENTIAL

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Because of its low aqueous solubility, piperine is classed as a class II medicine in the biopharmaceutical classification system. Piperine herbosomes were developed as a result to improve the solubility rate and in-vivo liver-protective effect of piperine, and physicochemical features were employed to demonstrate herbosome formation. For all formulations, the piperine-herbosome formulation displayed spherical particle size. Evaluate all formulations P1-P25, the in-vitro drug release rate and percent entrapment efficiency was calculated. It illustrates the complex's ability to release for an extended period of time. This indicates that it may have a longer retention time inside the body, extending the effect's duration. Using the DPPH scavenging method, the antioxidant capability of pure piperine was measured, with an IC50 value of 107.590.11 g/mL compared to a formulation with an IC50 value of 93.9260.03 g/mL. The hepatoprotective activity of Swiss albino mice of either sex was investigated. Hepatotoxicity was discovered on the eight day. On the ninth day, the parameters were assessed after a single oral dose of CCl4 (0.5 ml) produced hepatotoxicity. Based on drug content and drug entrapment, this formulation is the best. The biochemical markers measured included serum glutamic oxaloacetic transaminase (SGOT), serum glutamic-pyruvic transaminase (SGPT), alkaline phosphatase (ALP), and total bilirubin. In comparison to the normal control (1610.31 IU/L, 52.780.28 IU/L, 121.120.14 IU/L, and 0.633 1.44 IU/L), and the P2 formulation (163.230.49 IU/L, 66.90.05 IU/L, 128.31.115 IU/L, and 0.645 0.67 IU/L, respectively).

CHITOSAN BASED MICROPARTICLE FOR URAPIDIL DELIVERY BY ION-GELATION TECHNIQUE

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The current study deals with drug loaded microparticles incorporating hydrogels and small polyanionic electrolytes. The mechanical strength was ascertained by entrapment efficiency and texture analyzer. Chitosan-based hydrogels and the combination of poloxamer and further microparticles are prepared by ion-induced aggregation technique in polyanionic electrolyte medium. During the preparation, poloxamer is incorporated to improve the mechanical strength, which is ascertained in terms of adhesive strength (tensile strength) by texture analyzer and entrapment efficiency. The prepared microparticles are subjected to micrometric studies, swelling index, surface morphology study, drug-polymer interaction study, and zeta analysis. It was observed that there is an increase in entrapment efficiency with the progressive increase in poloxamer. In addition to that, adhesive strength was also studied by texture analyzer for all microparticles. Sodium citrate-based products exhibited better values compared to sodium sulfate and sodium tripolyphosphate-based. A significant finding was recorded for the swelling properties in relation to pH attributed to polyanions. SEM study revealed prominent porous surfaces for sodium tripolyphosphate microparticles. The study revealed that the addition of poloxamer improved the strength, identified by entrapment efficiency and texture analysis. It confirmed, SCP4 microparticle was found to be the best formulation among all.

REPOSITIONING OF RDRP INHIBITORS AGAINST HCV NS5B POLYMERASE UTILIZING STRUCTURE-BASED MOLECULAR DOCKING

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Hepatitis C Virus (HCV) is very dreadful as it can attack an estimated 71 million people around the world. The World Health Organization (WHO) reported that every year about 399000 people die due to HCV caused by chronic cirrhosis and liver cancer globally. There are many drugs available for the treatment of HCV. But drug resistance and toxicity are major issues. The quest for potential drugs utilizing repositioning would be a very useful and economical method to combat the HCV. ***Methods***: One of the most HCV targets is RNA dependent RNA polymerase (RdRp). The RdRp is common in HCV, Dengue virus (DENV), Zika virus (ZIKV), and Yellow fever virus (YFV) belonging to the same family of Flaviviridae. An attempt has been made in the present study to repositioning different DENV, ZIKV, and YFV RdRp inhibitors against HCV NS5B polymerase utilizing structure-based molecular docking which explores the affinity and mode of binding of these RdRp inhibitors. Several 87 compounds having dengue, yellow fever and zika RdRp inhibitory activities have been taken into consideration for the screening of potential RdRp leads utilizing docking simulation which focuses the affinity and mode of binding of sofosbuvir diphosphate which is a standard HCV, RdRp inhibitor. ***Conclusion***: It was found that the compounds 6 (N-sulfonylanthranilic acid derivative), 17 (R1479), 20 (DMB220), 23 (FD-83-KI26), 40 (CCG-7648), 50 (T-1106), 65 (mycophenolic acid), and 69 (DMB213) can produce docking score with the range of -7.602 to -8.971 Kcal/Mol having almost same mode of interaction as compared to the reference drug molecule. The drugs mentioned above can produce satisfactory affinity to bind the hepatitis C viral RdRp and thus may be used to treat the disease. Therefore, these predicted compounds may be potential leads for further testing of anti HCV activity and can be repurposed to combat HCV. The high throughput shotgun of drug repurposing utilizing structure-based docking simulation freeware would be a cost-effective way to screen the potential anti-HCV leads.

A REVIEW ON THE NOVEL TREATMENT OF MYASTHENIA GRAVIS

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Autoimmune myasthenia gravis is a neuromuscular junction disorder marked clinically by fatigable muscle weakness and serologically by the presence of auto antibodies against acetylcholine receptor, muscle specific kinase or lipoprotein related potein-4.The immunepathogenesis is T-cell driven and there exist a complex interplay between CD4+ T cell and B cell. In AchR MG accounts for about 85% of the population , IgG1 and IgG3 antibodies predominate and cause activation of complement pathways. In muscle specific kinase blocking activation of the argin- LRP4-MuSK complex. The conventional treatment of myasthenia gravis include broad spectrum immunosuppressive treatment with corticosteroid, azathioprine, methotrexate, cyclosporine, tacrolimus. Recently FDA approved novel immunotherapies for MG including Eculizumab, Rituximab, Zilucoplan, Ravulizumab, Nipocalimab, Monarsen, Bortezomib.The mechanism of action of rituximab is bind to CD-20, it lowers levels of B cell and slow down the progression of MG but the serious ADR of rituximab is increased thirst or urination, swelling of hands or feet and eculizumab is the first drug approved for refractory – myasthenia gravis and a long acting humanized monoclonal antibody targeted against complement C5.

THE IMPACT AND INTEGRATIVE APPROACHES OF ALZHEIMER'S DISEASE AND DEMENTIA

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Alzheimer's disease (AD) and dementia are chronic diseases with progressive deterioration of cognition, function and behaviour leading to severe disability and death. The Prevalence of AD and dementia is constantly increasing because of the Progressive aging of the population . Symptoms occur because nerve cells (neurons) in parts of the brain involving in Thinking, Learning and memory have been damaged or destroyed . The accumulation of the protein fragment beta-amyloid into clumps (called beta-amyloid plaques) outside neurons and the accumulation of an abnormal form of the protein tau (called tau tangles) inside neurons are two of several brain changes associated with Alzheimer's. The FDA has approved Aducanumab for mitigation of Alzheimer disease. Aducanumab is an beta amyloid directed monoclonal antibody. Non-Pharmacological interventions seemed to be more effective for reducing aggression and agitation, may play a role in the treatment of AD and dementia. The main Non-Pharmacological treatment types, which were reviewed here, include exercise and motor rehabilitation, cognitive rehabilitation. A meta-analysis found that aerobic exercise and a combination of aerobic and non-aerobic exercise had positive effect on cognitive function in people living with Alzheimer's and dementia. The Alzheimer's disease was found to be one of the multiple cause of death due to effect of COVID-19 pandemic.

IDENTIFYING PROMISING STARTING CANDIDATES AS DUAL AGONISTS FOR MU AND KAPPA OPIOID RECEPTORS BY BIOISOSTERIC LIBRARY GENERATION AND MOLECULAR DOCKING

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Among analgesic drugs, the opioid class of compounds have been found to be invaluable in chronic pain and severe pain of terminal conditions such as cancer and rheumatoid arthritis.In addition, they generate severe side effects such as depression and physical dependence, which emphasize the need for new improved drugs. In a previous study, it has been shown that the dual kappa/mu receptor agonists produce fewer side effects than selective agonists. The objective of present study was to identify promising candidates which can bind to mu and kappa opioid receptors simultaneously using bioisoteric library generation and docking. In this study, we have used bioisosteric replacement techniques to identify dual agonists with activities at mu and kappa opioid receptors. Hits were enriched based on the pharmacophore fitting and interactions with both the receptors. From a starting bioisosteric library of 1,43000 compounds we have identified top 25 compounds using various virtual screening process. These 25 compounds led to identification of top 3 hits based on docking. The top 3 hits could be considered as promising starting compounds for identifying agonist as they found to be stable in molecular simulations with both the receptors.

ASSESSMENT OF TOXICITY OF METAL OXIDE AND HYDROXIDE NANOPARTICLES USING QSAR MODELING APPROACH

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Nanotechnology is a promising area of research. Therefore, a detailed understanding of risk assessment of nanomaterials and their behavior to the biological system is required before working with any metallic oxide (hydroxide) nanoparticles (Me_{Ox}NPs). Due to the limited sources it is impossible to perform empirical testingof all toxicity endpoints of Me_{Ox}NPs. Quantitative structure-activity relationship (QSAR) models are widely accepted to predict the toxicity of untested nanomaterials. In the present study, QSTR models were developed to evaluate cytotoxicity of Me_{Ox}NPs towards RAW 264.7 cells. MLR and PLS models were developed with 25 NPs (nanoparticles) from 6 metal (hydro) oxides families (SiO_2, TiO_2, CeO_2, ALOOH, ZnO, and Ni $(OH)_2$) using the release of lactate dehydrogenase (ldh_R) from the cell as the endpoint. Multiple linear regression (MLR) models were developed using Best Subset Selection methods followed by enhancement of model derived predictions by the application of intelligent Consensus Predictor (ICP) tool. Besides, a partial least squares (PLS) model was also developed using the Small Dataset Modeler software which can handle limited number of data points. Periodic table descriptors and some physicochemical descriptors have been used to characterize the nanostructure of MeOxNPs. All models were validated by employing internal and external validation metrics followed by randomization test and applicability domain (AD) study. The statistical parameters suggested the robustness of the models. The insights from both the models suggested that electronegativity, solubility, formation of a metal cation increases the cytotoxicity whereas non-metal NPs and rise of oxidation degree contribute to low toxicity towards RAW 264.7 cell. A short proposed mechanism has also been explained to determine the cause of cellular toxicity by the MeOx NPs.

PREDICTION OF AQUATIC TOXICITY OF CHEMICAL MIXTURES USING 2D-QSAR AND APPLICATION OF CROSS-VALIDATION STRATEGIES TO AVOID OVERESTIMATION OF MODEL PERFORMANCE

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The rapid industrialization has led to the generation of various organic chemicals and multi-component mixtures which affect the environment adversely. Although organic chemicals are often exposed to the environment as a form of chemical mixtures rather than individual compounds, there is insufficient toxicity data available for the chemical mixtures due to the associated complexities. Most importantly, the nature of toxicity of mixtures is completely different from the individual chemicals, which makes the evaluation more difficult and challenging. In this paper, we have developed a QSAR model for a mixture data set for the prediction of the aquatic toxicity. The mixture descriptors have been calculated by the weighted descriptor generation approach. Partial least squares (PLS) regression has been used to model the response variable (*Log 1/EC*$_{50}$ against *Photobacteriumphosphoreum*) and the structural features of the mixtures of polar and non-polar narcotic toxicants. The model has been developed and validated by the Organization of Economic Co-operation and Development (OECD) norms and also cross-validated by mixtures-out and compounds-out cross-validation to nullify the developmental bias. The predictivity of the model has been judged by Prediction Reliability Indicator (PRI) tool using a newly designed external validation set (Mixture dataset) and proved to be externally predictive. The new model is robust, reproducible, extremely predictive, easily interpretable, and can be used for the prediction of aquatic toxicity of any untested chemical mixtures (under the domain of applicability) without prior preparation.

EUDRAGIT POLYMERS: APPLICABILITY AND APPROACHES IN NOVEL DRUG DELIVERY SYSTEMS

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Polymers are essential to the functionality and importance of medicinal formulations. Eudragit polymers have enabled the development of new drug delivery systems (NDDS) by modifying drug release patterns. The primary goal of continuous medication release is to produce more effective treatments by removing the possibility of underdosing and overdose. Other benefits include maintaining medication concentrations within the target range, requiring fewer administrations, maximizing drug usage, and improving patient compliance. This review paper provides an overview of Eudragit polymer categorization, nomenclature, physiological, and pharmacological characteristics. Eudragit polymers are classified based on their use or the type of formulation produced, which includes time-controlled drug release via sustained release formulations, gastro-resistance and GI via enteric formulations, and moisture protection and odor/taste masking via protective formulations. Eudragit polymers are available in a variety of physical forms with various degrees of solubility, including aqueous dispersion, organic solution, granule, and powder. Results: Eudragit polymers have a variety of drug release mechanisms and uses in a variety of drug delivery methods, including ocular, buccal, sublingual, enteric, oral, colon, vaccination, gene, vaginal, and transdermal drug administration.

AN OVERVIEW OF INDIA NATIONAL AIDS CONTROL PROGRAM AND ROLE OF PHARMACY PROFESSIONAL IN ADDRESSING COUNTRIES PUBLIC HEALTH CHALLENGES

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To combat challenge of HIV/AIDS epidemic in India, National AIDS Control Organization was established in the year 1992 by Ministry of Health, Government of India. National AIDS control Program envisions an India where every person living with HIV has access to quality care and is treated with dignity. Effective prevention, care and support for HIV/AIDS is possible in an environment where human rights are respected and where those infected or affected by HIV/AIDS live a life without stigma and discrimination. Youth of India and young Pharmacy professional can play a major and important role in preventing spread of communicable disease like HIV/AIDS, Hepatitis, Tuberculosis and COVID-19 by contributing n ongoing research with respect to finding cure and advance treatment for these diseases, Supply chain Management, strengthening community and creating awareness among the society to stop and Prevent the spread of deadly communicable diseases and eliminating it as public health threat. In last two years since outbreak of COVID-19 pandemic, Indian public health infrastructure and health services has come up as one of major area which require improvement to prevent the public from dreadful future epidemic and pandemics. Through this presentation an attempt has been by author to create awareness among young pharmacy professional about the role that they can play in improving and combating challenges of countries public health programs.

AN OVERVIEW ON GESTATIONAL DIABETES

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Gestational diabetes is a condition in which a women without diabetes develop increased blood sugar level during pregnancy because of insulin resistance and chronic subclinical inflammatory process. These two states are triggered mainly by secretion of proinflammatory cytokines and by abnormal function of adipose tissue.Risk factor include having Polycystic ovarian syndrome, family history of type 2 diabetes, overweight. A fasting glucose level more than 126mg/dl or a random plasma glucose more than 200mg/dl meets the threshold for the diagnosis of gestational diabetes. Particular level of circulating micro RNAs can be used as biomarkers.Infant of mothers with gestational diabetes are vulnerable to several chemical imbalances such as low serum calcium and low serum magnesium level but in general there are two major problems of gestational diabetes: macrosomia and hypoglycemia.Metformin was given to women used in pregestational diabetic women and women with polycystic ovary syndrome who suffer from infertility.Aspart and Lispro are safe and effective options for rapid acting insulin during pregnancy. The impact of first covid 19 wave on gestational diabetes has been evaluated.

Keywords:-Polycystic ovarian syndrome, gestational diabetes, macrosomia, hypoglycemia.

QUANTITATIVE STRUCTURE ACTIVITY RELATIONSHIP (QSAR) STUDIES ON FLOURO-QUINOLONES(FQS) FOR THERE ANTI T.B ACTIVITY

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Tuberculosis (TB) is the most important global infectisious killer disease responsible for 1.5 million deaths every year due to TB caused by Mycobacterium Tuberculosis. The major problem about the mycobacterium tuberculosis infection is multi- and extended drug resistant tuberculosis (MDR & XDR-TB). Among several antitubercular drugs are being in clinical trials. A series of 25 fluroquinolones (FQs) have been evaluated for their antitubercular activity having (inhibition of DNA gyrase). In order to understand the influence of different physicochemical (hydrophobic, electronic & steric) and structural parameters like Partition Coefficient(PC) , Electronic energy(E.E), Homo energy, Lumo energy, Cannolly Accessible Area(CAA), Cannolly Molecular Area(CMA), Cannolly Solvent-Excluded Volume(CSEV), Total Valence Connectivity (TVC) and Molar Refrectivity (MR) parameters on inhibition of DNA gyrase (IC_{50}) activity, the Quantitative structure activity relationship (QSAR) models have been developed using the computed parameters as independent and activity (-log IC_{50}) as dependent variable. Among these parameters the hydrophobic parameters (PC),steric parameter (MR) and Cannolly Molecular Area(CMA) positively contributes while electronic parameter (E.E) negatively contribute for the activity.

FORMULATIPON DEVELOPMENT OF ORAL DRUG DELIVERY SYSTEM LOADED WITH HERBAL DRUG FOR UROLITHIASIS

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Kidney stones are a frequent occurrence in India and other developing nations. Kidney stones impacted 10-12 % in developed countries. Kidney stones are the most prevalent type of stone found in both men and women .Kidney stones are small, pebble-like substances made from chemicals in your urine. They are formed in the kidneys when high levels of certain substances, such as minerals or salts, get into the urine. Bryophyllum pinnatum leaves showed preventive effect against renal calculi formation and validates its ethnomedicinal use in urinary disorders. It further supports its therapeutic potential for the treatment of urinary calculi. Microsponges are porous, polymeric microspheres that are used mostly for topical use and have recently been used for oral administration. Microsponges are designed to deliver a pharmaceutical active ingredient efficiently at the minimum dose and also to enhance stability, reduce side effects, and modify drug release. To overcome all this problems we move to prepare an extended release formulation with combination of hydrophilic and hydrophobic polymer matrix to maximize the drug loading and prevent drug loss. Polymeric matrix sustained the release with therapeutically effective concentration achieved in the systemic circulation over an extended period of time, thus achieving better compliance of patients.

FORMULATION AND EVALUATION OF POLYHERBAL MATRIX TABLET FOR HEPATOPROTECTIVE ACTIVITY

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The present research explores the hepatoprotective activity of various extracts against experimental hepatotoxicity. When several herbs are combined in a specific ratio, the medicinal effect is increased while toxicity is reduced. Polymers are the building blocks of a pharmaceutical drug delivery system because they control drug release from the device. Polymers are used to protect drugs from the physiological environment and to extend their release time in order to improve their stability. Polyherbal matrix tablet were prepared by the wet granulation method using an aqueous extracts and excipients. This research focuses on matrix tablets, which are one of the most practical methods for developing sustained-release dosage forms, as well as the approaches used in their formulation and evaluation. The therapeutic efficacy of a sustained release matrix tablet with improved efficacy can be increased. It also emphasizes the significance of polyherbalism and matrix Tablet.

PHARMACOPHORE BASED VIRTUAL SCREENING OF DIVERSE COUMARIN DERIVATIES AGAINST BUTYRYLCHOLINESTERASE AS ANTIALZHIMER AGENTS

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Coumarin scaffold is an important class of natural compounds which shows a wide range of biological activities against neurological diseases such as Alzheimer's, Parkinson's disease and etc. In order to envisage the structurally diverse butyrylcholinesterase (BuCh) with better efficacy, ligand-based3D QSAR Pharmacophore model was developed using Discovery Studio Client(DSC 4.1). In order to develop a pharmacophore initially, the dataset was randomly divided into training and test set compounds in the ratio of 50/50. A set of 10 pharmacophore models were generated by training set compounds and validated with test set compounds,Fischer's validation, cost analysis, and ligand profiler heat map analysis. Among the 10 hypothesis, best hypothesis was selected based on different validation parameters(R =0.89, RMS=1.62, cost = 41.74, null cost = 294.727 and fixed cost = 98.3505, Q =0.908,RMSE =0.766).Finally, Virtual screening was performed by applying the selected model to the compounds of MiniMaybridge (n=2000). Among the both database top 100 hit molecules which has best fit value in hypo 1 were selected and subjected to ADMET and drug like properties by using various filters like Lipinski, SMART in DSC 4.1. Finally, 65 hit molecules were obtainedwith drug like and low or non-toxicproperties. These 65 compounds obtained from the screening could be promising choice as butyrylcholinesterase inhibitors or antialzheimer agents.

MICROBEADS AS A DOSAGE FORM FOR ANTIDIABETIC DRUGS

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Diabetes is a chronic disease that is caused when there is impaired secretion of Insulin from the pancreas or when the body is unable to use Insulin. WHO has classified diabetes into 3 types Type 1 diabetes (previously known as non-insulin dependent), Type 2 diabetes (previously known as non-insulin dependent diabetes) and lastly Gestational Diabetes. The complications associated with diabetes include heart attack, kidney failure, leg amputation etc. Microbeads is an upcoming means to administer antidiabetic drugs; the drugs that have shown encouraging results when administered in this form are Metformin microbeads having entrapment efficiency of 90%. Insulin microbeads were administered in rats that decreased the blood glucose level to 88mg/dl. Microbeadsof Glipizide had a drug entrapment of 90%.Development of in vitro 3D TissueFlex Islets model was constructed and used to maintain the functionality of anti-diabetic drug efficacy testing.Insulin loaded alginate calcium microbeads were prepared. Bovine serum albumin entrapped in the form of microbeads by electrostatics in order to entrap Insulin protein effectively. Repaglinide- cholestyramine loaded microbeads showed a drug entrapment of 51-92%. These all drugs have been formulated from their conventional form in to Microbeads for better drug entrapment and release kinetics

SYNTHESIS OF FRAGRANCE MOLECULE AMBROX FROM DIFFERENT NATURAL PRODUCT PRECURSORS

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Ambergris, a waxy substance excreted by the intestinal tract of the sperm whale, has been a highly prized fragrance ingredient for millennia. Because of supply shortage and price inflation, a number of ambergris substitutes have been developed by the fragrance industry. One of the key olfactory components and most appreciated substitutes of ambergris, Ambrox is produced industrially by semi synthesis from sclareol, a diterpene-diol isolated from Clary sage and very high cost of (-) Ambrox probable near $1000 per kilogram so synthesis of Ambrox has been starts in low-priced, like labdanes substrates. Currently synthesis of (-) Ambrox, many industry are using sclareol as a starting material, because its stereo chemical property subsequently correlated and headed for toward ambrox and prepared by good value product. However, natural compounds have potential to be converted ambergris-like odorants and extracted from several different types of plants. Plant terpenoids suitable as starting materials for the semi synthesis of ambrafuran or intermediates, such as ambradiol, that can be used in biocatalytic transformations to yield ambrafuran. In the current study we are investigating low cost method for production of Ambrox from the natural precursors.

DEVELOPMENT AND *IN-VITRO* CHARACTERIZATION OFSELF EMULSIFYING DRUG DELIVERY SYSTEM OF LERCANIDIPINE HCL

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Self-emulsifying drug delivery systemmay be a promising strategy to improve the rate and extent of oral absorptionof lipophilic drugs. Lercanidipine Hydrochloride is a new third generationof anti-hypertensive drug. The oral bio-availability of LCH is approximately 10% when given orally and shows erratic absorption from gastrointestinal tract which is attributed to extensive first pass metabolism and low solubility.An extensive quantitative solubility studies and pseudo-ternary phase diagrams were conducted. Based on the pseudo ternary diagrams four formulations (L1-L_4) of LC-SNEDDS formulated containedrice bran oil: GMO (1:9) as oil phase, tween 80 as surfactant and propionic acid as co-surfactant respectively. The prepared SNEDDS were subjected for evaluation of various parameters like self-emulsification property, FTIR studies, DSC studies, viscosity, globule size determination, cloud point, zeta potential determination, *in-vitro* drug release in biorelevant medium and stability studies.The best formulation L_4has globule size of as low as 8.062 nm and PDI 0.43.Zeta potential was found to be a positive value i.e. 14.3 mV.LC-SNEDDS released more than 80% drug release in all the tested biorelevant media. The results indicated that all the batches showed more than 75% release of LCH in the first five minutes itself and more than 95% at the end of 60 min. In comparison to pure untreated drug which showed only 25% in first 5 min and 37% at the end of 60 min.Thus it can be inferred that formulating LC-SNEDDS of LCH resulted into increase in the rate and extent of dissolution.

NANO PHYTO-PRODUCT SELECTIVELY ACTIVATES CERTAIN PROTEINS TO COMBAT PESTICIDE-INDUCED TOXICITY IN FISH MODEL

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Pesticides get washed off from the agricultural field to nearby water bodies affecting aquatic lifeforms and induce health hazards in human consuming such pesticide intoxicated fishes. Therefore, to combat the issue of bioaccumulation which has now become a global problem we have tried to evaluate role of a PLGA encapsulated phyto-based drug pelargonidin (NPG) and checked its efficacy in protecting pesticide-induced toxicity in Tilapia fish. Cypermethrin (CM) was selected as the pesticide of use based on the reports of its regular use in pest control and in enhancing % crop yield production. PG was chosen for our study for their known geno-protective and cyto-protective efficacy. Results reveal that NPG pre-treatment followed by CM administration showed protective roles against pesticidal toxicity in fish model evaluated through parameters like % cytotoxicity, DNA damage assay, oxidative stress related enzyme profiles, immunofluorescence study, ELISA and histopathology of hepatic tissue. Therefore, our findings reveal that NPG could protect cells and tissues from pesticide-induced toxicity and thus shall be of great help for human welfare in future.

DISCOVERY OF NOVEL GLUCOKINASE ACTIVATORS THROUGH STRUCTURE-BASED PHARMACOPHORE MODELING, VIRTUAL SCREENING AND MOLECULAR DOCKING APPROACHES

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Diabetes mellitus is becoming more prevalent by the day. There are some side effects to the available drug therapies. Glucokinase is a new target for developing new anti-diabetic drugs that work by activating the enzyme. Glucokinase activators convert glucose into glucose-6-phosphate. In this study, structure-based Pharmacophore model was generated; virtual screening was performed using Asinex and Zinc database library compounds. ADMET studies were conducted after molecular docking. ZINC212072098, ZINC212076713, ZINC212080377, ZINC94222677 and ZINC95394375 have shown good binding energies, interactions with ideal amino acid residues and better ADMET results. These compounds will be further used to design novel Glucokinase activators.

A 2D-QSAR APPROACH TO EXPLORE STRUCTURAL FEATURES OF NITROAROMATICS AS HYPOXIC CELL RADIOSENSITIZERS

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Hypoxia is the prime component of tumor microenvironment that plays a pivotal role in cancer progression. Nitroaromatic compounds are known to enhance the sensitivity of hypoxic cells to ionizingradiation. The application of computational tools like Quantitative Structure-Activity Relationship (QSAR) can be used to predict newly developed nitroaromatics or compounds with missing data. In the present work, three datasets consisting of 18 nitrofurans, 11 nitrothiophenes and 84 nitroimidazoles were utilised for two-dimensional QSAR modeling to retrieve their structural features essential to elicit radiosensitivity. The work comprises two parts: (i) local modeling using individual datasets; and (ii) global modeling by clubbing the three datasets. The two-dimensional descriptors were calculated using Dragon (version 7.0) software. The developed models were obtained using various feature selection techniques applied in “Small Dataset Modelling” and “Double Cross Validation” tools available at https://dtclab.webs.com/software-tools. Finally, the models were validated using stringent metrics following the Organisation for Economic Co-operation and Development (OECD) guidelines.The developedmodels are robust, predictive, and are useful tools to predict the radiosensitization of newly developed nitroaromatics. Furthermore, the global model was used to predict 10 external set compounds and the prediction ability was validated using the “prediction reliability indicator” tool.

PREDICTIVE CLASSIFICATION BASED QSTR AND INTERSPECIES CORRELATION FOR THE TOXICITY ASSESSMENT OF DIVERSE PESTICIDES ON MULTIPLE AVIAN SPECIES

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Protection and restoration of different endangered bird species from pesticide exposure is crucial from the point of safety assessment of ecosystem. Toxicity predictions or risk assessment of pesticides by chemometric tools is one of the challenging fields in recent era. In the present study, classification-based QSTR models were developed for a large dataset (n = 516) of diverse pesticides on three avian species (mallard duck, bobwhite quail, and zebra finch) according to the OECD guidelines. The QSTR models were developed by linear discriminant analysis (LDA) method followed by genetic algorithm for feature selection from 2D descriptors calculated from PaDel descriptor software v2.21. All the process from dataset division to models development was done using freely available QSAR-Co software. Different statistical metrics assured the reliability and robustness of the developed models. External compound prediction highlighted predictive nature of the models. The mechanistic interpretation suggested that presence of phosphate, halogens (Cl, Br), ether linkage, and NCOO influence the avian toxicity. Furthermore, model reliability was checked by the application of the standardization approach of the applicability domain (AD). Finally, the developed models provided a priori toxic and non-toxic classification for unknown pesticides (inside AD), with particular emphasis on organophosphate pesticides. The interspecies toxicity correlation and predictions encouraged for their further applicability for the fulfilment of data gaps in vital missing species.

A COMPARATIVE REVIEW BETWEEN SOLID LIPID NANOPARTICLES AND NANOSTRUCTURED LIPID CARRIERS

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During the last few decades, lipid nanoparticles (LNPs) have gained a lot of attention. Lipid-based nanoparticles are divided into two categories: solid lipid nanoparticles (SLNs) and nanostructured lipid carriers (NLCs). SLNs are spherical nanoparticles with a drug-containing solid lipid core stabilised with surfactants and designed to increase drug molecules bioavailability. SLNs have a number of advantages, but they also have a number of disadvantages, including limited drug loading, drug expulsion, and crystallisation during long term storage. The introduction of a new generation of lipid nanoparticles, the NLC, where a solid lipid is combined with liquid lipid, has avoided or decreased these limitations. The ability to control drug release is an extra benefit of NLC formulations. LNPs have a lot of potential for delivering active medicinal components to the target site. LNPs improve treatment effectiveness and reduce negative effects by boosting the active medication concentration in the target organ. This research compares the structure of SLNs and NLCs, as well as their releasecharacteristics, method of preparation and applications.

REPOSITIONING AND HIGH THROUGHPUT SCREENING OF 4-AMINOQUINOLINE COMPOUND AGAINST CANCER

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The 4-amino quinolone background is an idea for new drugs production. Quinolone along with derivatives have different activities including anticancer potential. They have been made and revealed for various exercises. Quinolines are broadly utilized as "parental" mixtures to make atoms with clinical guides, solely with against malarial and hostile to microbial exercises. As per reports of various researchers they have potential to hold of Quinoline and its reporters have newly been read for their methods of capacity in the hold of proteasome, tubulin polymerization, and DNA fix. Therefore, it has been assumed to have the anticancer actions of quinolone compounds. 4-aminoquinolines are well-known for showing very potent antimalarial activities. In the advanced learning a work has been made to screen and repurpose the 4-aminoquinoline antimalarial compounds against malignancy. The screening of compounds has been carried out by in-silico simulation based on their structural properties and computed pharmacophore to minimize the time, labor and money and animal sacrifices.

POTENCY OF CURCUMIN IN THE MANAGEMENT OF RHEUMATOID ARTHRITIS AND PSORIATIC ARTHRITIS

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Rheumatoid arthritis (RA) and Psoriatic arthritis (PsA) are chronic inflammatory illness recognized by joint pain and swelling, along with systemic symptoms. The distinction between RA and PsA may be complicated to make since their clinical presentations and symptoms are so similar. Patients having rheumatoid arthritis and psoriatic arthritis may have lesser comorbidities, a reduced mortality rate, as well as greater standard of living or activities. Rheumatoid arthritis and psoriatic arthritis are treated in a palliative manner since they are not curable disease. To alleviate the symptoms, numerous therapy plans were established utilising diverse medicine systems throughout the world; nevertheless, treatment efficacy has been limited. Allopathic medicines such as nonsteroidal anti-inflammatory medicines (NSAIDs) and disease-modifying anti-rheumatic drugs (DMARDs) is usually the cornerstone of treatment. Allopathic medicines have serious side effects, and long term-consumption degrades one's living standard. Hyperacidity, oedema, stomach ulcers, gastrointestinal bleeding, perforation, and reduced appetite are many of the most common adverse effects. Curcumin, the primary active component within Curcuma longa (turmeric), has been demonstrated to become most helpful in the therapy of rheumatoid arthritis and psoriatic arthritis, with effectiveness attributed towards its mode of activity. Even though several in vitro and in vivo research have demonstrated their safety as well as effectiveness profile, further placebo-controlled prospective studies are required before oral curcumin may become suggested as a viable therapy for rheumatoid arthritis along with psoriatic arthritis.

EXPLORING QSAR ANALYSIS OF AZOLES DERIVATIVES AS A ANTICANCER AGENTS FOR THE TREATMENT OF LIVER CANCER

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Cancer is deathly disease in all over world. Among the cancers, the Liver cancer is one of the important cancers which begin in the cells of the liver. The most common form of liver cancer begins in cells called hepatocytes and is called **hepatocellular carcinoma** (HCC). In the present study, a series of 63 azoles derivatives having anticancer activities were subjected to QSAR analyses using 2D descriptors calculated from PaDEL descriptor software (V2.21). Two different splitting technique namely response based and structure based splitting were used to divide the whole data set into training and test set compounds. Several models were developed by using training set compounds by using multiple linear regressions (MLR) followed by genetic algorithm (GA) for subset selection. Among the several models best model were selected for each splitting and externally validated by applying the models to respective test set compounds. All the selected models were robust and predictive enough with high value of different internal and external validation parameters (internal Q^2_{Loo} = 0.620-0.628, R^2 = 0.694-0.712, R^2_{adj} = 0.665-0.683), external R^2_{pred} = 0.619-0.813, r^2m_{avg} = 0.662-0.627, CCC_{ext} = 0.813-0.757). All the analysis from dataset splitting to model development was done using QSARINS (V2.24) software. The mechanistic interpretation of descriptors indicated that the presence of electron withdrawing groups, bulky groups nitrogenous heterocyclic ring at 2nd and 5th position of azoles influence the anticancer activity of azoles. The developed models will be helpful in designing of newer azole derivatives with anticancer activity for the treatment of liver cancer.

DEVLOPMENT & CHARACTERIZATION OF FIMASARTAN TABLET USING UV SPECTROSCOPY

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Fimasartan is the non-peptide angiotensine II receptor agonist which is used in the hypertension. A simple accurate & cost-effective method is developed for the estimation of Fimasartan tablet using uv spectrophotometer in the API & bulk dosage form. The Fimasartan shows λmax at 261 nm using 10% methanol solution.Fimasartan obeyed Beer-Lambert's law in the concentration range of 10-50μg/ml with correlation coefficient (r^2) of 0.999. The accuracy of the method was confirmed by the recovery studies, by adding a known amount of the pure drug to the formulation and the percentage recovery was found to between 98.5 to 100.08% w/w, indicating that the developed method is accurate which indicates a good accuracy of the method and it shows that the method was free from the interference of excipients used in the formulation. The precision of the method was reported in terms of the relative standard deviation and it should be evaluated by using a minimum of 6 determinations over 100 % concentration which shows % RSD less than2 indicates that the method was precise.The limit of detection and quantification was found to be 3 & 9.11 respectively. The percentage purity of the marketed formulation was found to be 97.18 % w/w. The proposed spectrophotometric method was validated as per the ICH Q1A (R2) guidelines.

IN SILICO MOLECULAR DOCKING COUPLED *IN VIVO* STUDY TO DETERMINE ACTIVATION OF p53 AND PARP BY PELARGONIDIN TO PREVENT FOOD-ADDITIVE INDUCED DIABETES

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Diabetes is a metabolic malady that arises due to irregular and abnormal functioning of pancreatic β cells resulting in disruption of insulin producing capacity from the islets of Langerhans. Food additive induced diabetes has become a major health concern issue globally. Alloxan, a food additive used by the flour industry, has been reported alarmingly to induce diabetes by destroying insulin-producing β-cells in the pancreas when administered in mice and cause hyperglycemia, genotoxicity and chromosomal aberration. In order to prevent the alloxan-induced diabetes, treatment with pelargonidin having anti-genotoxic effect was performed in vivo which shows a significant reduction in chromosomal anomaly and blood glucose level. In addition, overexpression of two proteins- p53 and PARP was noticed in pelargonidin pre-treated alloxan administered mice when compared to control. Further, in silico molecular docking of the pelargonidin was done to predict the mode of binding in p53 and PARP, identifying important amino acid residues of the targets and to establish a level of a meaningful drug-protein interaction to control the virulence of disease. Therefore, *in vivo* study corroborates with *in-silico* modelling showing its ability for protein-drug interaction which may pave the most effective therapeutic tool in future drug discovery.

EXPLORING THE LANDSCAPE OF NATURAL INHIBITORS OF NSP13 HELICASE: AN IN SILICO INVESTIGATION

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The human race has been grappling with COVID-19 pandemic since early 2020. At the time of writing this communication 173,674,509 confirmed cases of COVID-19, including 3,744,408 deaths, had been reported to WHO. Fast, efficient, and safe interventions are warranted to control this deadly COVID 19 pandemic. Various proteins in the life cycle of SARS-CoV2 are being targeted for the development of antiviral interventions. The non-structural proteins are in fact one of the most opportune drug targets for developing antivirals due to their key biological implications and sequence conservation. Nsp 13 is a helicase necessary for viral replication through the unwinding duplex DNA and RNA from 5'to 3' direction and is being actively pursued as a drug target against COVID-19. Thus, in the present study, we have explored natural inhibitors of Nsp 13 helicase. Biological molecules similar to known inhibitors for SARS-CoV2 helicase have been searched and compiled from the database Indian Medicinal Plants, Phytochemistry And Therapeutics (IMPPAT). These natural molecules were then docked to ADP binding site and nucleic acid binding site (NCB site) on the helicase using the "COVID-19 Docking Server" (http://ncov.schanglab.org.cn) to evaluate their potential binding. Notable findings include ploypodosaponins derived from *Polypodium vulgare*, amongst several other natural molecules. These natural molecules can be investigated as potential antiviral leads and also the source plant preparations can be included in herbal preparations.

METALLIC NANOPARTICLES PRESIDING HEPATOTOXICITY

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Metallic nanoparticles (MNPs) are new engineering materials with broad prospects for biomedical applications; thus, their safety has drawn great concern. The liver is the main detoxification organ of vertebrates. However, many issues concerning the interactions between MNPs and biological systems (cells and tissues) are unclear, particularly the toxic effects of MNPs on hepatocytes and other liver cells. Numerous researchers have shown that some MNPs can induce decreased cell survival rate, production of reactive oxygen species (ROS), mitochondrial damage, DNA strand breaks, and even autophagy, pyroptosis, apoptosis, or other forms of cell death. This mainly focuses on the recent researches on the liver toxicity of MNPs and its mechanisms at cellular and subcellular levels to provide a scientific basis for the subsequent hepatotoxicity studies of MNPs.

A REVIEW ON: DRUG DISCOVERY AND DEVELOPMENT PROCESS

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The idea for a new drug development can come from a variety of sources which include the current necessities of the market, new emerging diseases, academic and clinical research, commercial sector, etc. Our aim is to help scientists whose research may be relevant to drug discovery and/or development to frame their research report in a way that appropriately places their findings within the drug discovery and development process and thereby support effective translation of preclinical research to humans. Drug discovery is a process which aims at identifying a compound therapeutically useful in curing and treating disease. This process involves the identification of candidates, synthesis, characterization, validation, optimization, screening and assays for therapeutic efficacy. Once a compound has shown its significance in these investigations, it will initiate the process of drug development earlier to clinical trials. Studies that contribute to solving any of the many scientific and operational issues involved in the development process can improve the efficiency of the process. New drug development process must continue through several stages in order to make a medicine that is safe, effective, and has approved all regulatory requirements. Once a target for discovery has been chosen, the pharmaceutical industries or the associated academic centers work on the early processes to identify the chemical molecules with suitable characteristics to make the targeted drugs. This article will look into the key concepts of drug discovery, drug development and clinical stages of the drug discovery.

PHYTO-BASED THERAPEUTIC APPROACH IN ATTENUATION OF FOOD-ADDITIVE INDUCED OXIDATIVE STRESS AND HYPERGLYCEMIA IN MICE

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Food additives like Alloxan (ALX) used in the flour industries for white flour bleaching, acts as a potential food contaminant which is reported to cause DNA damage and induce hyperglycemic conditions in living cells. Due to its structural analogy with glucose, ALX gets its access into the β cells of pancreas through the GLUT2 transporters easily and thereby aids in free radical generation, DNA damage and hyperglycemic condition. Therefore, in order to combat the incidence of ALX-induced health hazards in animal models, plant-based therapeutic approach with less cytotoxic effects have been preferred to the new synthetic anti-diabetic drugs. Since there is a lack of scientific validation towards the use of natural products as alternative medicine; Morroniside, a non-toxic, anti-diabetic phyto-based compound has been chosen for studying its ability to interact with the DNA and other cellular targets of possible signaling cascades. In this study, % cell viability, DNA damage, oxidative stress, histopathological alterations in hepatic and pancreatic tissues, quantitative expressions of associated proteins have been assessed to ascertain the protective efficacy of Morroniside against hyperglycemic condition induced by ALX administration in mice model. Results reveal that Morroniside pre-treatment could prevent the ALX-induced oxidative stress, thereby limiting the extent of DNA damage and diminishing the level of % cyto-toxicity of the pancreatic cells by regulating the expression of proteins involved in glucose homeostasis as well as apoptosis. Therefore, the experimental results provide an understanding of the phyto-based compound Morroniside as an advanced therapeutic arsenal for management of diabetics in future.

TRPA1 AS THERAPEUTIC TARGET FOR NEUROPATHIC PAIN

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Pain, an unpleasant sensation, and emotional experience in our daily life, is an alert of tissue injury to prevent further or impending tissue damage.Chronic neuropathic pain is a common significant and debilitating problem that presents a major challenge to healthcare. Neuropathic pain is “pain that comes from direct consequence of a lesion or disease which affect the somatosensory system”. The pain may be categorized as central or peripheral depending on the locale of injury or lesion. Common causes of neuropathic pain include nerve pressure or nerve damage after surgery or trauma, viral infections, cancer, vascular malformations, alcoholism, neurological conditions such as multiple sclerosis and metabolic conditions such as diabetes. NSAIDS becoming inefficient in neuropathic pain utilizing opioids as therapeutic agents but sedation and addiction being side effect affecting majorly. So therapeutic approach targeting TRPA1 receptors leading to beneficiary treatment with less side effects. Many recent investigative research *Insilico* and *Invivo* targeting on TRPA1 as target site.

SELECTED PHARMACOGNOSTIC DRUGS TO TREAT LUNG INJURY OF COVID-19

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The newly emerged SARS-CoV-2 strains from the coronavirus (CoV) family is one of the most significant pandemics, with widespreadmorbidity and mortality globally. Developing antiviral drugs is achallenge for the scientific community and pharmaceutical industryto medicateassorted health issues of COVID-19. During this healthemergency, repurposing of existing antiviral, antiinflammatory or antimalarial drugs arecaptivative for controlling SARS-CoV-2. The phytochemicalsselected based on ethnomedicinal information forin vitroantiviral studies could beof propitious drugs for treating COVID-19. Among the diverse complications of COVID-19, lung injury hasaccomplishedremarkable attention. The selected phytochemicals with prominent anti-inflammatory effects possess significant outcomes to turn down lung injury causedby severe acute respiratory syndrome coronavirus 2 (SARS-CoV-2). This inscriptionbrings insights in the potentialapplication of phytochemicals and their derivativestodevelop safe drugs against SARS-CoV-2.

Prediction of Androgen Receptor Binding Affinity of Endocrine Disruptors by 2D-QSAR Approach

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Endocrine Disruptor Compounds (EDCs) are synthetic or natural molecules in the environment that promote adverse modifications of endogenous hormone regulation in humans and/or in animals.By interfering with the body's endocrine system, these chemicals produce adverse developmental, reproductive, neurological, and immune effects in animals, abnormal growth patterns, and neurodevelopmental delays in children.Among these, certain compounds mimic the role of androgen which is responsible for controlling the development and maintenance of male sexual characteristics. In the present research, we have utilized the application of a two-dimensional quantitative structure-activity relationship (2D-QSAR)modeling technique to analyze the structural features of these chemicals responsible for binding to the androgen receptors (logRBA) in rats. We have collected the androgen receptor binding data from EDKB database (https://www.fda.gov/science-research/endocrine-disruptor-knowledge-base/accessing-edkb-database). We have then employed the **DTC-QSAR** tool, aavailable at https://dtclab.webs.com/software-tools for dataset division, feature selection, and model development. This tool is a complete package providing a user-friendly, easy-to-use GUI to develop regressionor classification-based QSAR models and involves variable selection techniques (genetic algorithm and best subset selection) also. Data division was done by the Euclidean Distance approach method followed by feature selection using Genetic Algorithm technique. The final PLS was evaluated usingvarious stringent validation criteria. The developed model is robust, predictive, and should be a useful tool to predict the binding nature of EDCs to the androgen receptor. From the model we interpreted that hydrophobicity due to features such aspresence of CHRX2 group (X=Cl), number of aliphatic tertiary carbons, aromatic group count, in addition to presence of O & F at the topological distance 8 and minimum atom type electrotopologicalstate for the OH groupcontributes to the receptor affinity and thus increase toxicity,while presence of polar functionality like phenol, enol and carboxy groups decrease the receptor binding affinity and reduce toxicity.

Soil Ecotoxicity Prediction against*Folsomia Candida* using 2D-QSAR Approach

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Soil ecotoxicological test is an essential tool for risk assessment of various xenobiotic chemicals. Such tests can be performed using soil invertebrates by exposing them to specified soil contaminating chemicals. Soil invertebrates provide various ecosystem services (i.e. soil transformations beneficial for mankind). For example, soil invertebrates may influence mineralization of nutrients in soil organic matter (SOM), affecting the ‘’soil fertility’’ – important factor from the agricultural aspect. Hence, soil invertebrates serve as an outstanding biological indicator of terrestrial ecosystem and overall soil quality, considering their high sensitivity when compared to other indicators of soil quality (physical/chemical).Therefore, laboratory tests using invertebrates can be considered as the mainstay of ecotoxicological impact assessment. Quantitative and/ or qualitative results elicited from such tests help several regulatory authorities across the globe, to determine the ecological risk level of substances and safe exposures limits for human and soil biota. Thus, such valuable information enable governmental regulatory authorities to control manufacturing output and sale of pesticides, to decide threshold limit for safe application of residues to agricultural soils, etc. However,laboratory tests (both *in vivo* and *in vitro*) are costly and time-consuming affairs and involve extensive use of animals. Hence, such tests cannot be extended entirely for predicting toxicity of novel compounds. As a result, an alternative *in-silico approach*of quantitative structure–activity relationships (QSARs) is used for environmental risk assessment for novel compounds, free of the exhaustive use of test animals under the REACH regulations in the EU.Inthis background, necessary limited data available from laboratory tests on the soil invertebrate *Folsomia Candida* (C. name:Springtail) are collated from the database of ECOTOX(cfpub.epa.gov/ecotox). Data is collected for the endpoint - pEC50 only. Samples of total 45 chemical compounds were selected against which chemical descriptors were calculated for each compound. Then the whole dataset is split into a test dataset (11 compounds) and a training dataset(34 compounds), based on Euclidean Distance Based approach. Using genetic algorithm, significant descriptors out of all descriptors’pool were selected. Finally, a PLS model is built based on those significant descriptors. Both internal and external validations metrics of this PLS model are well-balanced and within the acceptable range as per the OECD criteria. From the aforementioned parameters, certain conclusion on general contribution can be made: Firstly, with the increase in number of electron donor groups and consequent hydrogen bond interactions, the toxicity (pEC50) increases. The soil toxicity can increase with the increase in aqueous solubility of compounds. Secondly, it was seen from the data that whennumber of rings of order 5 increases, then toxicity (pEC50) increases. Lastly, a negative correlation was observed between number of substitution to aromatic rings and toxicity (pEC50).

TURMERIC AGAINST CANCER

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Cancer is a disease in which some of the body's cells grow uncontrollably and spread to other parts of the body. Cancer can start almost anywhere in the human body, which is made up of trillions of cells. Normally, human cells grow and multiply (through a process called cell division) to form new cells as the body needs them. When cells grow old or become damaged, they die, and new cells take their place. Sometimes this orderly process breaks down, and abnormal or damaged cells grow and multiply when they shouldn't. These cells may form tumors, which are lumps of tissue. Tumors can be cancerous or not cancerous.

Cancer means no answer of abnormal cell division. Major toxicity of anticancer synthetic chemotherapy is that it can kill cancer cells along with normal cells. Therefore, natural resources such as turmeric may be effective treatment without having any toxicity. We must take antioxidant fruit and vegetables containing vitamin C that can detoxify the reactive oxidative species [**ROS]** and toxics responsible for mutagenecity and cancer.

EVALUATING THE THERAPEUTICS EFFECTS OF PEPTIDE IN NEUTRALIZING THE SNAKE VENOM ACTIVITY

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Snakebite is amongst the foremost neglected topical disease (NTD) plaguing the world today. The World Health Organization (WHO) estimates over 2.7 million annual cases of clinical illness following snake envenomation, with over 500,000 of those resulting in death or permanent disabilities. The present study was aimed to evaluate the therapeutic effect of peptide for checking the snake venom activity of viper venom or common krait venom. Firstly the haemolytic activity of viper venom or krait venom was checked by taking the human blood sample. After that we used anti-snake venom peptides (ASV-10, ASV-15) for inhibiting effect of viper and common krait venom.So when we treated common krait and Russelli viper venom with RBCs they showed (67.2% in krait venom and 59.6% with viper venom) haemolysis. Thereafter we used 3 different peptides were used for inhibiting the activity of peptides. It can be concluded that this *in-vitro* studies provide a new finding of antisnake venom peptide for preventing the lysis of the RBCs cells in the blood. It can be concluded that out of these peptide that is ASV-10 or ASV-15 shows promising effect against snake bite. In this study we also used another peptide different peptide for understanding the specificity of main peptide.

Keywords: Snakevenom; Antisnake venom; Hemolysis; Common krait; and Russelli viper.

Identification of DHFRinhibitors through Computer Aided Drug Design (CADD)techniques as Anti-Toxoplasmosis agents

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Toxoplasmosis is an infectious disease caused by *Toxoplasmosis Gondii* parasite. It is most common in cat family but human and other animals also get infected. In case of infected pregnant woman, the disease may pass to their unborn foetus and lead to congenital Toxoplasmosis. In United States, it is estimated that 11% of the population above 6 years and older have been infected. In disease is prevalent in Uttarakhand due to the presence of forest areas in which the hosts survive. Toxoplasmosis may be transmitted through blood transfusion or organtransplant. The disease is significant because it has zoonotic potential for parasite transmission. Easeof transmission and dangerous consequences of the disease warrants discovery of new drugs. For this purpose, compounds inhibiting *Toxoplasma gondii* dihydrofolate reductase (DHFR) such as derivatives of 6,7-disubstituted 2,4-Diaminopteridines etc were taken to perform docking studies. The ligand-based drug design (LBDD) was also performed with a good r^2 value of 0.7982 and q^2value of 0.6035. The docking results also corroborated with the LBDD. The virtual screening of the preferred model may be useful in virtual screening of chemical libraries to identify the molecules as potential dihydrofolate reductase inhibitors.

Natural Sourced Immunostimulators to Combat COVID-19

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Coronavirus disease was first found in 1930 in chicken. Outbreak of SARS-CoV strain occurred in 2003 (China) followed by the outbreak of MERS-CoV strain in 2012 (Saudi Arabia). A new coronavirus strain (SARS-CoV-2) of SARS-CoV was identified in humans by the end of 2019 in Wuhan, China. It created COVID-19 viral diseases which engulf many lives and breakdown the security and economy of more than 170 countries around world. Indians have a lot of natural resources which stabilize the passive immunity. The present attempt has discussed on mother natural gifts of foods and medicines to combat the COVID-19.

Phytochemicals to combat SARS-CoV-2 mediated lung injury

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Corona virus are a large family of viruses that are known to cause illness ranging from the common cold to more severe diseases such as Severe Acute Respiratory Syndrome (SARS). First corona virus was discovered in chickens in 1930. SARS- CoV strain erupted in china in the year 2003 followed by MERS- CoV strain erupted in 2009 in Saudi Arabia. Again a novel strain of corona virus which is called as SARS-CoV-2 erupted in wuhan ,china at the end of the year 2019. The SARS-CoV-2 is very contageous . Rapidly it has engulfed many many lakhs lives ,caused breakdown of economy and life security for more than 170 countries around the world. The present study is an attempt to cure the COVID-19 associated lung injury utilizing phytoactive components.

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