DISCIPLINE SPECIFIC ELECTIVE COURSE – (BIOMED-DSE-) GREEN CHEMISTRY METHODS IN PHARMACEUTICAL AND INDUSTRIAL APPLICATIONS

CREDIT DISTRIBUTION, ELIGIBILITY AND PRE-REQUISITES OF THE COURSE

Course title & Code	Credits	Credit distribution of the course			Eligibility criteria	Pre-requisite of the course	Department offering the course
		Lecture	Tutorial	Practical /Practice			
Green Chemistry Methods in Pharmaceutical and Industrial Applications	**4**	**3**	**-**	**1**	**XII Pass with Physics, Chemistry & biology**	**Basic knowledge of organic reactions**	**Biomedical Science**

Learning objectives

The objective of this course is to make students aware of

- The toxicity, hazard and risk of chemical substances as well as to be aware of the importance of green chemistry in today's world.
- To familiarize students with environment-friendly alternatives for the synthesis of various chemicals.
- ·Course will help to understand the usage of various green approaches in synthetic chemistry and their applications for sustainable development.

Learning outcomes

After studying this course students should be able to:

- Understand the twelve principles of green chemistry and gain an in-depth understanding of chemical toxicity, hazard, and associated risk.
- Learn to create non-toxic chemicals, products, and processes than current alternatives.
- Comprehend the importance of inherently safer design for accident prevention
- ·Understand the advantages of using catalysts and biocatalysts, use of renewable feedstocks and green solvents for environmental protection.
- Appreciate the role of green chemistry in innovatively solving environmental issues.
- Green chemistry is a mean to maximize revenues, productivity, and sustainability while producing zero waste. They are also motivated to practice green chemistry by success stories and real-life examples.

SYLLABUS

Unit I: Introduction to Green Chemistry (10 hrs)

Importance of Green Chemistry: Green Chemistry in nature (for example nitrogen fixation, photosynthesis, glucogenesis/ glycolysis), Twelve principles of green Chemistry:Prevention of waste, Atom economy, Designing less hazardous chemical synthesis, Designing safer products, Safer solvents and auxiliaries, Design for energy efficiency, Renewable resources, Reduce derivative, Use of selective catalyst, Design for degradation, You cannot control what you cannot measure, Inherently safer chemistry for accident prevention, Important environmental laws, the Pollution Prevention Act of 1990, Limitations and Obstacles in the Pursuit of the Goals of Green Chemistry.

Unit II: Conventional Chemistry vs Green Chemistry (10 hrs)

General concept of mixing of orbitals (Hybridization), Role of various electronic effects in the modulation of reactions; Homolytic and Heterolytic cleavage. Substitution reactions (hydrolysis of alkyl halides and Hydrolysis of esters), Addition reactions (Hydrogenation of alkenes), Elimination reactions (Hoffman elimination, Decarboxylation), Rearrangement (Diels-Alder reactions), Cis-trans isomerisation of alkenes, Condensation reactions: Aldol (replacement of ethanol with solvent free reaction) and Benzoin (replacement of KCN, TPP, Thiamine HCl). Prevention of waste/by-product pollution, calculation of atom economy with reference to above reactions.

Unit III: Green Solvents (10 hrs)

- Conventional solvents (Ethanol, Acetone, chloroform, DCM) and Green Solvents (water/buffer, supercritical fluids, ethyl lactate, Ionic liquids). Buffers (Phosphate, Acetate) and buffer action (concept of pKa), Relative acids/basic strength of organic acids and bases (aliphatic and aromatic).
- Advantages of green solvents in chemical synthesis: Supercritical CO_2 in the separation of coffee from coffee beans and perfume industry, water as a green solvent in reactions (Benzoin condensation, Hofmann Elimination, methyl benzoate to benzoic acid and Decarboxylation reaction).
- Ionic liquids: physicochemical properties, Advantages and Disadvantages (purification of complex mixtures and cost), Reactions of Ionic liquids: Imidazolium based ionic liquid for the synthesis of antiviral drug trifluridine, hydrogenation of alkenes, Diels-Alder reaction with copper (II) bisoxazolium complex having imidazolium tag.

Unit IV: Various Approaches to Green reaction synthesis (10 hrs)

- Enzyme-based reactions: Biocatalyst (concept of stereoselectivity and stereospecificity, and turnover number), Biocatalyst mediated synthesis of Sitagliptin drug and ethanol; Nanocatalysis (oxazole synthesis using nanocatalyst). Photocatalysis: Visible light induced Reactions (syntheses of vitamin D3, cis-trans isomerization of alkenes, waste water treatment with TiO2).
- Microwave-assisted green approach: Principle, merits, demerits and effect of solvent; Microwave-assisted reactions: solvent-free synthesis of aspirin, Renewable starting materials: Synthesis and properties of 5-Aminolevulinic acid (DALA) from levulinic acid. Design of degradable reactions (pesticides), Inherently Safer design in chemical synthesis: Principle and Subdivision eg. Bhopal Gas Tragedy.

Unit V: Pharmaceutical and Industrial Applications for revenue, productivity and sustainability (5 hrs)

Vitamin C used in cosmetics/neutraceuticals industry: Synthesis using enzymes, commercial production of drugs/pharmaceutical product: anti-depressant drug sertraline, Removal of Drug from Waste water: Levofloxacin, an anti-bacterial drug with ZnO nanoparticles, Enzymatic synthesis of Zero Trans-Fats and Oils,

Practical: (30 hrs)

(Wherever wet lab experiments are not possible, the principles and concepts can be demonstrated through any other material or medium including videos/virtual labs etc.) (Any seven)

1. Preparation and characterization of biodiesel from vegetable oil preferably waste cooking oil.
2. Benzoin condensation using thiamine hydrochloride as a catalyst instead of cyanide
3. Mechanochemical solvent-free synthesis of succinic anhydride/phthalic anhydride
4. Hydrolysis of esters/ esterification using green methods.
5. Solvent-free, microwave-assisted one-pot synthesis of phthalocyanine complex of copper (II).
6. Cross aldol condensation reaction using base catalyzed green method.
7. Microwave-assisted synthesis of drug/ drug intermediates (Knoevenagel reaction, Aspirin)
8. Photoreduction of benzophenone to benzopinacol in the presence of sunlight.
9. Acetylation of primary aromatic amine using the green method.
10. Synthesis of nanoparticles using green approach.

Essential Reading:

- Matlack, A.S., Andraos. J, (2022); Introduction to Green Chemistry, 3rd Edition, CRC press (ISBN: 978-1032199429).

- Sharma, R.K.; Bandichhor, R. (2018), Hazardous Reagent Substitution, Royal Society of Chemistry. (ISBN: 978-1-78262-050-1)
- Lancaster, M. (2016), Green Chemistry: An Introductory Text, 3rd Edition, RSC Publishing. (ISBN: 978-1-78262-294-9)
- Wei Zhang, Berkeley W. Cue Jr (2012) "Green Techniques for Organic Synthesis and Medicinal Chemistry" John Wiley & Sons, Ltd (ISBN:9780470711828)
- Sharma, R.K.; Sidhwani, I.T.; Chaudhari, M.K. (2012), Green Chemistry Experiments: A monograph**,** I.K.International Publishing House Pvt Ltd. (ISBN: 978-9381141557)
- Kirchhoff, M.; Ryan, M.A. (2002), Greener approaches to undergraduate chemistry experiment**.** American Chemical Society, Washington DC. (ISBN: 8412-3866-9)
- Anastas, P.T.; Warner, J.C. (2000), Green Chemistry: Theory and Practice, Oxford University Press. (ISBN: 9780-198506980).
- El-Maraghy, C. M., El-Borady, O. M., & El-Naem, O. A. (2020). Effective Removal of Levofloxacin from Pharmaceutical Wastewater Using Synthesized Zinc Oxid, Graphen Oxid Nanoparticles Compared with their Combination. *Scientific Reports*, *10*(1), Article 1. https://doi.org/10.1038/s41598-020-61742-4

Suggestive readings

- Batra. S.K; Gulati, S; Shukla, S, (2020); Practical Green Chemistry: Strategies, Tools & Experiments, Shri Kala Prakashan (ISBN: 978-9385329456)
- Sidhwani, Tucker I; Sharma, R.K, (2020); An Introductory Text on Green Chemistry: For Undergraduate Students, Wiley (ISBN: 978-8126554072)
- Benyus, J.M. (2002); Biomimicry:Innovations Inspired by nature, HarperCollins. (ISBN: 9780060533229)
- Garay,A. L; Pichon, A.; James,S.L. "Solvent-free synthesis of metal complexes" Chem Soc Rev, 2007, 36,846-855.
- James H. Clark, Duncan Macquarrie (2002); Handbook of Green Chemistry and Technology, Wiley (ISBN: 9780632057153)