

**Sacred Heart College (Autonomous)**

**Department of Chemistry**

**MSc Applied Chemistry - Pharmaceutical**

**Course Plan**

**Academic Year 2015 – 16**

**Semester 3**

Semester: Semester 3 Course: **P3CPHT09– Drug Design and Pharmacology**

**Objectives**

To enable the students

- To learn in detail drug design and pharmacology
- To have a thorough idea on application of drugs and their mechanism of action
- To understand the functions of enzymes, receptors , proteins and nucleic acids as drug targets
- To study the biotransformation of drugs

| Session   | Topic/Module   | Hour   | Teacher/invited persons etc. | Method of teaching * | COs |
|-----------|--|--------|------------------------------|----------------------|-----|
| Session 1 | General Principles of Drug Therapy.<br>Relationship between chemical structure,                | 18 Hrs | Dr. Grace Thomas             | Lecture              |     |
| Session 2 | lipid solubility and biological activity of drugs.<br>Stereochemistry and biological activity. |        |                              |                      |     |
| Session 3 | Drug action-receptor theories.   |        |                              |                      |     |
| Session 4 | Drug metabolism–different pathways.  |        |                              |                      |     |

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| Session 5  | Drug design: various factors of drug design, rational drug design. |  |  |  |  |
| Session 6  | Methods of lead discovery: optimisation of the lead,               |  |  |  |  |
| Session 7  | natural and synthetic sources of lead compounds.                   |  |  |  |  |
| Session 8  | Bioisosterism.   |  |  |  |  |
| Session 9  | Prodrug and soft drug concept. Drug synthesis.                     |  |  |  |  |
| Session 10 | Combinatorial synthesis (basic concepts).                          |  |  |  |  |
| Session 11 | Retrosynthetic analysis of benzocaine,                             |  |  |  |  |
| Session 12 | saccharin, salbutamol and benzodiazepines.                         |  |  |  |  |
| Session 13 | Basic concepts of CADD,  |  |  |  |  |
| Session 14 |  |  |  |  |  |

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|------------|--|-------|-----------------|---------|--|
| Session 15 | molecular modeling,  |       |                 |         |  |
| Session 16 | molecular docking.   |       |                 |         |  |
| Session 17 | QSAR physicochemical parameters,   |       |                 |         |  |
|            | introduction to 2D   |       |                 |         |  |
| Session 18 | 3D   |       |                 |         |  |
|            | Introduction to 2D   |       |                 |         |  |
|            | 3D   |       |                 |         |  |
|            | <b>Pharmacology</b>  |       |                 |         |  |
| Session 19 | General principles of pharmacology:  | 6 Hrs | Dr Grace Thomas | Lecture |  |
| Session 20 | biological response to drugs,<br>passage of drugs across membranes.  |       |                 |         |  |
| Session 21 | Pharmacokinetic principles: absorption,  |       |                 |         |  |
| Session 22 | distribution, metabolism and excretion of<br>drugs.  |       |                 |         |  |
| Session 23 | Dose of drugs and routes of administration.  |       |                 |         |  |
| Session 24 | Pharmacodynamic principles: dose response<br>relationships, mechanism of drug action,<br>unusual and adverse responses of drugs, |       |                 |         |  |
| Session 25 | structurally specific and nonspecific drugs.<br>Ferguson's principle   |       |                 |         |  |
| Session 26 | Drug interactions-synergism, antagonism,<br>drug addiction and drug dependence, drug<br>tolerance, drug hypersensitivity.        |       |                 |         |  |

|            | <b>Metallic compounds used in pharmaceutical chemistry</b>    |       |                  | Lecture |  |
|------------|---|-------|------------------|---------|--|
| Session 27 | Calcium lactate, calcium gluconate,                           | 9 Hrs | Dr. Rmakrishna n |         |  |
| Session 28 | iron gluconate, iron fumerate, ferric ammonium citrate,       |       |                  |         |  |
| Session 29 | ferrous sulphate, aluminium hydroxide gel,                    |       |                  |         |  |
| Session 30 | calamin, zinc oxide, zinc stearate,                           |       |                  |         |  |
| Session 31 | magnesium stearate, talc,                                     |       |                  |         |  |
| Session 32 | yellow mercuric oxide, trivalent and pentavalent antomonials, |       |                  |         |  |
| Session 33 | selenium sulfide, lithium salts, gold,                        |       |                  |         |  |
| Session 34 | platinum and bismuth compounds.                               |       |                  |         |  |
| Session 35 | Metal toxicity - cadmium, lead, copper and mercury            |       |                  |         |  |

| SI No      | Topic/Module  | Hour/<br>session | Teacher/inv<br>ited persons<br>etc. | Method<br>of<br>teaching<br>* | Remarks:<br>Books,<br>reference etc |
|------------|---|------------------|-------------------------------------|-------------------------------|-------------------------------------|
|            | <b>Drugs acting on CNS</b>  |                  |                                     |                               |                                     |
| Session 36 | General anaesthetics. Inhalation anaesthetics<br>- ether,   | 12Hrs            | Dr. IGA                             | Lecture                       |                                     |
| Session 37 | enflurane, halothane, nitrous oxide,<br>cyclopropane. Intravenous anaesthetics -<br>thiopentone sodium, ketamine.                       |                  |                                     |                               |                                     |
| Session 38 | Hypnotics, sedatives and anxiolytic agents.   |                  |                                     |                               |                                     |
| Session 39 | Anxiolytic agents-benzodiazepines, buspirone<br>and meprobamate.  |                  |                                     |                               |                                     |
| Session 40 | Anticonvulsants: convulsions, types of<br>epilepsy, barbiturates-hydantoins,<br>oxazolidinediones, succinimides and<br>benzodiazepines. |                  |                                     |                               |                                     |
| Session 41 | Analeptics: xanthines, amphetamines,<br>nikethamide and ethamivan.  |                  |                                     |                               |                                     |

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| Session 42 | Centrally acting muscle relaxants: glyceryl ethers-mephenesin, alkane diol derivatives-meprobamate, benzodiazepines-librium, diazepam and baclofen.  |  |  |  |  |
| Session 43 | Antiparkinson's agents: dopamine agonists, dopamine releasing agents and synthetic anticholinergics.   |  |  |  |  |
| Session 44 | Drugs for Alzheimer's disease: cholinergic agonists and acetylcholine esterase inhibitors.   |  |  |  |  |
| Session 45 | Synthesis of the following drugs - Enflurane, Ketamine, Etomidate, Phenobarbital, Diazepam, Chlordiazepoxide, Meprobamate, Buspirone, Ethinamide, Nikethamide, Ethamivan, Trimethadione, Ethosuximide, Denzimol, Topiramate, Mephenesin, Levodopa, Besiperidine and Tacrine. |  |  |  |  |

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|            |  |       |                |         |  |
|            | <b>Analgesics</b>  |       |                |         |  |
| Session 46 | Narcotic analgesics - morphine and its analogues, phenyl(ethyl) piperidines,   | 9 Hrs | Midhun Dominic | Lecture |  |
| Session 47 | diphenyl heptanones and benzocaine derivatives.  |       |                |         |  |
| Session 48 | Antipyretics and NSAIDs: Basic idea of COX I & I inhibitors, salicylates aspirin, p-aminophenol derivatives-paracetamol, phenacetin,       |       |                |         |  |
| Session 49 | pyrazolidinediones phenyl butazone, oxyphenbutazone, anthranilic acid derivatives-   |       |                |         |  |
| Session 50 | mefanamic acid, flufenamic acid, indoleacetic acid derivatives-indomethacin, arylacetic/propionic acid derivatives (ibuprofen, ketoprofen, |       |                |         |  |
| Session 51 | flubiprofen and diclofenac), oxicams (piroxicam and tenoxicam).  |       |                |         |  |
| Session 52 | 5.3 Drugs used for gout - allopurinol, selective COX II inhibitors   |       |                |         |  |
| Session 53 | Synthesis of the following drugs-levorphanol, pethidine, methadone,  |       |                |         |  |
| Session 54 |  |       |                |         |  |

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|--|---|--|--|--|--|
|  | phenyl butazone, flufenamic acid, diclofenac, piroxicam, allopurinol and celicoxib. |  |  |  |  |
|  |   |  |  |  |  |

## References

01. G. Patrick, Medicinal Chemistry, BIOS. 2001.
02. T. Nogrady, D.F. Weaver, Medicinal Chemistry, Oxford University Press, 2005.
03. W.O. Foye, T.L. Lemke, D.A. Williams, Principles of Medicinal Chemistry, 4<sup>th</sup>Edn., Williams & Wilkins, 1995.
04. J.P. Remington, Remington's Pharmaceutical Sciences, Vol.13, , 19th Edn., Mack,1990.
05. D. Sriram , P. Yogeswari, Medicinal Chemistry, Pearson Education India, 2010.
06. K. D. Tripathi, Essentials of Medical Pharmacology, 6th Edn.,Jaypee, 2008
07. L.S. Goodman, A. Gillman, The Pharmacological Basis of Therapeutics, 10<sup>th</sup>Edn., McGraw Hill, 2001.
08. S.S. Kadam, Principles of Medicinal Chemistry, Vol.I& II, Pragati Books, 2008.
09. A. Kar, Medicinal Chemistry, New Age International, 2007.

10. C.O. Wilson, J.M. Beale, J.H. Block, Textbook of Organic Medicinal and Pharmaceutical Chemistry, 12th Edn., Lippincott Williams and Wilkins, 2010

| <b>COURSE PLAN</b>           |   |  |                      |   |                 |
|------------------------------|---|--|----------------------|---|-----------------|
| <b>ACADEMIC YEAR 2015-16</b> |   |  |                      |   |                 |
| <b>PROGRAMME</b>             | : | <i>M.Sc. Applied Chemistry - Pharmaceutical</i>  | <b>LECTURE HOURS</b> | : | 72              |
| <b>SEMESTER</b>              | : | 3  | <b>CREDITS</b>       | : | 4               |
| <b>SUBJECT TITLE</b>         | : | <i>Organic Syntheses</i>   | <b>SUBJECT CODE</b>  | : | <i>P3CPHT10</i> |
| <b>COURSE TEACHERS</b>       | : | <i>Dr. V.S. Sebastian (VSS) ; Dr. Franklin J (FJ) ; Dr. Grace Thomas (GT) ;<br/>Dr. Ignatious Abraham (IGA); Dr. June Cyriac (JUC)</i> |                      |   |                 |
| <b>Instructional Hours</b>   | : |  |                      |   |                 |

| GT  | No. of Session | Session Topic and Discussion Theme   | Value additions   |  |  |
|---|----------------|--|---|--|--|
| <i>UNIT 1 : Organic Synthesis via Oxidation and Reduction</i><br>(18 hours) | 1              | Survey of organic reagents and reactions in organic chemistry with special reference to oxidation and reduction. |   |  |  |
|   | 2              | Metal based and non-metal based oxidations of alcohols to carbonyls (Chromium, Manganese)                        |   |  |  |
|   | 3              | Metal based and non-metal based oxidations of alcohols to carbonyls (aluminium and DMSO based reagents)          | ICT   |  |  |
|   | 4              | alkenes to epoxides (peroxides/per acids based)-   |   |  |  |
|   | 5              | Sharpless asymmetric epoxidation,  |   |  |  |
|   | 6              | Jacobsen epoxidation, Shi epoxidation  |   |  |  |
|   | 7              | alkenes to diols   | Assignment No:2   |  |  |
|   | 8              | (Manganese and Osmium based)-Prevost reaction  |   |  |  |
|   | 9              | Woodward modification  |   |  |  |
|   |                | <b>FIRST INTERNAL EXAMINATION</b>  |   |  |  |
|   |                | <i>Text Books</i>  | <ul style="list-style-type: none"> <li>❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.</li> <li>❖ F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.</li> <li>❖ W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.</li> <li>❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001. L. Finar, <i>Organic Chemistry</i> - Volume I &amp; II - Pearson Education.</li> </ul> |  |  |
|   | 10             | alkenes to carbonyls with bond cleavage (Manganese and lead based, ozonolysis)                                   |   |  |  |
|   | 11             | alkenes to alcohols/carbonyls without bond cleavage  |   |  |  |
|   | 12             | - hydroboration-oxidation, Wacker oxidation, selenium/chromium based allylic oxidation                           |   |  |  |

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|------------------------------------|---|---|--|--|
|                                    | 13  | ketones to ester/lactones- Baeyer-Villiger oxidation  |  |  |
|                                    | 14  | . Catalytic hydrogenation (Heterogeneous: Palladium/Platinum/Rhodium and Nickel. Homogeneous: Wilkinson). |  |  |
|                                    | 15  | Metal based reductions- Birch reduction, pinacol formation, acyloin formation                             |  |  |
|                                    | 16  | Hydride transfer reagents from Group III and Group IV in reductions - LiAlH <sub>4</sub> ,.               |  |  |
|                                    | 17  | DIBAL-H, Red-Al, NaBH <sub>4</sub> and NaCNBH <sub>3</sub> , selectrides                                  |  |  |
|                                    | 18  | trialkylsilanes and trialkylstannane. Meerwein-Ponndorf-Verley reduction. Baker's yeast                   |  |  |
| <b>SECOND INTERNAL EXAMINATION</b> |   |   |  |  |
| <b>Text Books</b>                  | <ul style="list-style-type: none"> <li>❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.</li> <li>❖ F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.</li> <li>❖ W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.</li> <li>❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001. L. Finar, <i>Organic Chemistry</i> - Volume I &amp; II - Pearson Education.</li> </ul> |   |  |  |

**FJ**

| <i>Unit II</i>  | <b>No. of Sessions</b>                     | <b>Session Topic and Discussion Theme</b>                | <b>Value additions</b>   |  |  |
|---|--|--|--------------------------|--|--|
| <i>Modern Synthetic Methods and Reagents<br/>(18 Hours)</i> | 1  | Baylis-Hillman reaction,                                 |                          |  |  |
|   | 2  | Henry reaction, Nef reaction,                            |                          |  |  |
|   | 3  | Kulinkovich reaction, Ritter reaction,                   |                          |  |  |
|   | 4  | Sakurai reaction, Tishchenko reaction, Ugi reaction,     |                          |  |  |
|   | 5  | Noyori reaction. Brook rearrangement.                    |                          |  |  |
|   | 7  | Tebbe olefination.                                       |                          |  |  |
|   | 8  | Metal mediated C-C and C-X coupling reactions: Heck,     |                          |  |  |
|   | 9  | Stille,  |                          |  |  |
|   | 10   | Suzuki,  |                          |  |  |
|   | <b>1<sup>st</sup> Internal Examination</b> |  |                          |  |  |
|   | 11   | Suzuki-Miyaura,  |                          |  |  |
|   | 12   | Negishi-Sonogashira, Nozaki-Hiyama,                      | Power Point Presentation |  |  |
|   | 13   | Buchwald-Hartwig, Ullmann and Glaser coupling reactions. |                          |  |  |
|   | 14   | Wohl-Ziegler reaction. Reagents such as NBS              |                          |  |  |
|   | 15   | DDQ and DCC  |                          |  |  |
|   | 16   | Gilman reagent.  |                          |  |  |
|   | <b>2<sup>nd</sup> Internal Examination</b> |  |                          |  |  |
|   | 17   | Introduction to multicomponent reactions                 |                          |  |  |
| 18  | Click reaction                             |  |                          |  |  |
| <b>End Semester Examination</b>                             |  |  |                          |  |  |

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|---|--|---|--------------------------|--|--|
| <i>Text Books</i>   | <ul style="list-style-type: none"> <li>❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.</li> <li>❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press.</li> <li>❖ R.O.C. Norman, J.M. Coxon, Principles of Organic Synthesis, 3rd Edn., Chapman and Hall, 1993.</li> <li>❖ V.K. Ahluwalia, L.S. Kumar, S. Kumar, Chemistry of Natural Products, CRS</li> </ul> |   |                          |  |  |
| <b>JUC</b>  |  |   |                          |  |  |
| <i>Unit III</i>   | <b>No. of Sessions</b>   | <b>Session Topic and Discussion Theme</b>   | <b>Value additions</b>   |  |  |
| <b>Construction of Carbocyclic and Heterocyclic Ring Systems</b><br>(9 Hours) | 1  | Different approaches towards the synthesis of three, four, five and six-membered rings.   |                          |  |  |
|   | 2  | Photochemical approaches for the synthesis of four membered rings-oxetanes and cyclobutanes   |                          |  |  |
|   | 3  | ketene cycloaddition (inter and intra molecular), Pauson-Khand reaction,  | Power Point Presentation |  |  |
|   | 4  | Volhardt reaction, Bergman cyclization,   |                          |  |  |
|   | 5  | Nazarov cyclization, Mitsunobu reaction,  |                          |  |  |
|   | 6  | cation-olefin cyclization and radical-olefin cyclization.   |                          |  |  |
|   | <b>1<sup>st</sup> Internal Examination</b>   |   |                          |  |  |
|   | 7  | Inter-conversion of ring systems (contraction and expansion)-Demjenov reaction  |                          |  |  |
|   | 8  | Reformatsky reaction. Construction of macrocyclic rings-ring closing metathesis.  |                          |  |  |
|   | 9  | Formation of heterocyclic rings: 5-membered ring heterocyclic compounds with one or more than one hetero atom like N, S or O - pyrrole, furan, thiophene, imidazole, thiazole and oxazole |                          |  |  |
|   | <b>2<sup>nd</sup> Internal Examination</b>   |   |                          |  |  |

|                   |   |
|-------------------|---|
| <i>Text Books</i> | <ul style="list-style-type: none"> <li>❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.</li> <li>❖ F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.</li> <li>❖ W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.</li> <li>❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.</li> <li>❖ R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley &amp; Sons, 1994.</li> </ul> |
|-------------------|---|

| <b>VSS</b>                                      |                        |  |                          |  |
|---|------------------------|--|--------------------------|--|
| <i>Unit IV</i>                                  | <b>No. of Sessions</b> | <b>Session Topic and Discussion Theme</b>  | <b>Value additions</b>   |  |
| <i>Protecting group Chemistry<br/>(9 Hours)</i> | 1                      | Protection and deprotection of hydroxy, carboxyl,                                  |                          |  |
|   | 2                      | carbonyl, and amino groups. Chemo and regio selective protection and deprotection. |                          |  |
|   | 3                      | Illustration of protection and deprotection in synthesis.                          | Power Point Presentation |  |
|   | 4                      | Protection and deprotection in peptide synthesis.                                  |                          |  |
|   | 5                      | common protecting groups used in peptide synthesis,                                | Group Discussion         |  |
|   | 6                      | protecting groups used in solution phase and                                       |                          |  |

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|  | 7   | solid phase peptide synthesis (SPPS).              |  |  |
|  | 8   | Functional equivalence and reactivity Umpolung.    |  |  |
|  | 9   | Role of trimethyl silyl group in organic synthesis |  |  |
| <b>I<sup>st</sup> Internal Examination</b> |   |  |  |  |
| <i>Text Books</i>                          | <ul style="list-style-type: none"> <li>❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.</li> <li>❖ F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.</li> <li>❖ W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.</li> <li>❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.</li> <li>❖ R. Noyori, Asymmetric Catalysis in Organic Synthesis, John Wiley &amp; Sons, 1994.</li> </ul> |  |  |  |

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|------------------------------|---|---|----------------------|------------|
| <b>COURSE PLAN</b>           |   |   |                      |            |
| <b>ACADEMIC YEAR 2015-16</b> |   |   |                      |            |
| <b>PROGRAMME</b>             | : | <i>M.Sc. Applied Chemistry - Pharmaceutical</i>   | <b>LECTURE HOURS</b> | : 72       |
| <b>SEMESTER</b>              | : | 3   | <b>CREDITS</b>       | : 4        |
| <b>SUBJECT TITLE</b>         | : | <i>Physical Chemistry</i>   | <b>SUBJECT CODE</b>  | : P3CPHT11 |
| <b>COURSE TEACHERS</b>       | : | <i>Dr Jorphin Joseph, Dr Jinu George, Dr Ignatious Abrhaham, Dr Abi T G</i>                                   |                      |            |
| <b>COURSE OBJECTIVES</b>     | : | To understand the basic concepts in Surface Chemistry, Electrochemistry, Photochemistry and Chemical Kinetics |                      |            |

| <b>IGA</b>  |   |   |                        |  |
|---|---|---|------------------------|--|
| <b>Unit V</b>   | <b>No. of Sessions</b>  | <b>Session Topic and Discussion Theme</b>                                     | <b>Value additions</b> |  |
| <b>Retrosynthetic Analysis</b><br>(9 Hours)               | 1   | Basic principles and terminology of retrosynthesis: method.                   |                        |  |
|   | 2   | synthesis of aromatic compounds, one group                                    |                        |  |
|   | 3   | two group C-X disconnections, one group C-C and two group C-C disconnections. |                        |  |
|   | 4   | Amine and alkene synthesis: important strategies of retrosynthesis,           |                        |  |
|   | 5   | functional group transposition, important functional group interconversions.  |                        |  |
|   | 6   | important functional group interconversions,                                  |                        |  |
|   | 7   | Enantioselective synthesis of Corey lactone                                   |                        |  |
|   | 8   | longifolene and luciferin.  |                        |  |
|   | 9   | Umpolung equivalent – Peterson olefination, enolate formation, Ireland        |                        |  |
|   | <b>1<sup>st</sup> Internal Examination</b>  |   |                        |  |
| <b>Unit VI</b>  | <b>No. of Sessions</b>  | <b>Session Topic and Discussion Theme</b>                                     | <b>Value additions</b> |  |
| <b>Biosynthesis and Biomimetic Synthesis</b><br>(9 Hours) | 1   | Basic principles of the biosynthesis of terpenes,                             |                        |  |
|   | 2   | steroids, alkaloids,.   |                        |  |
|   | 3   | carbohydrates,  |                        |  |
|   | 4   | proteins and nucleic acids. e   |                        |  |
|   | 5   | Biosynthesis of cholesterol,  |                        |  |
|   | 6   | $\alpha$ - terpineol, morphine  |                        |  |
|   | 7   | glucose and phenyl alanine.   |                        |  |
|   | 8   | Biogenesis of isoprenoids and alkaloids.                                      |                        |  |
|   | 9   | Biomimetic synthesis of progesterone and spatrein                             |                        |  |
| <b>2<sup>nd</sup> Internal Examination</b>                |   |   |                        |  |
| <b>Text Books</b>   | <ul style="list-style-type: none"> <li>❖ M.B. Smith, Organic Synthesis, 3rd Edn., Wavefunction Inc., 2010.</li> <li>❖ F.A. Carey, R. I. Sundberg, Advanced Organic Chemistry, Part A and B, 5th Edn., Springer, 2007.</li> <li>❖ W. Carruthers, I. Coldham, Modern Methods of Organic Synthesis, 4th Edn., Cambridge University Press, 2004.</li> <li>❖ J. Clayden, N. Greeves, S. Warren, P. Wothers, Organic Chemistry, Oxford University Press, 2001.</li> </ul> |   |                        |  |

❖ R. Noyori, *Asymmetric Catalysis in Organic Synthesis*, John Wiley & Sons, 1994.

**Instructional Hours**

: *4 HOURS/WEEK*

|   | No. of Session | Session Topic and Discussion Theme  | Value additions |  |
|---|----------------|---|-----------------|--|
| <b>UNIT 1 CHEMICAL KINETICS I</b><br>(14 hours) | 1              | <b>Theories of reaction rates:</b> Collision theory-steric factor, potential energy surfaces.                               |                 |  |
|   | 2              | Conventional transition state theory-Eyring equation,   |                 |  |
|   | 3              | Comparison of the two theories.   | Assignment      |  |
|   | 4              | Thermodynamic formulation of the two theories.  |                 |  |
|   | 5              | Thermodynamic formulation of the reaction rates.  |                 |  |
|   | 6              | Significance of $\Delta G^*$ , $\Delta H^*$ and $\Delta S^*$ . Volume of activation.  |                 |  |
|   | 7              | Effect of pressure and volume on velocity of gas reactions.   |                 |  |
|   | 8              | <b>Introduction</b> to Molecular Reaction Dynamics  |                 |  |
|   | 9              | <b>FIRST INTERNAL EXAMINATION</b>   |                 |  |
| <b>Text Books</b>                               | 1.             | J. Rajaram, J.C. Kuriakose, Kinetics and Mechanisms of Chemical Transformations, Macmillan India, 2000.                     |                 |  |
|   | 2.             | K.J. Laidler, Chemical kinetics, 3 <sup>rd</sup> Edn. Harper & Row, 1987.   |                 |  |
|   | 3.             | C. Kalidas, Chemical Kinetic Methods: Principles of Fast Reaction Techniques and Applications, New Age International, 2005. |                 |  |
|   | 4.             | J.W. Moore, R.G. Pearson, Kinetics and Mechanisms, John Wiley & Sons, 1981.   |                 |  |
|   | 5.             | P.W. Atkins, Physical Chemistry, ELBS, 1994.  |                 |  |
|   |                |   |                 |  |
|   | 10             | <b>Lindemann-Hinshelwood mechanism</b>  | ICT             |  |

|  |                        |  |                         |  |
|--|------------------------|--|-------------------------|--|
|  | 11                     | Qualitative idea of RRKM theory  |                         |  |
|  | <b>No. of Session</b>  | <b>Session Topic and Discussion Theme</b>  | <b>Value additions</b>  |  |
|  | 12                     | Chain reactions, free radical and chain reactions  |                         |  |
|  | 13                     | Steady state treatment, kinetics of H <sub>2</sub> -Cl <sub>2</sub> and H <sub>2</sub> -Br <sub>2</sub> reactions,   | Group Discussion        |  |
|  |                        | <b>SECOND INTERNAL EXAMINATION</b>   |                         |  |
| <b>CHEMICAL KINETICS - II (14 Hrs.)</b>    | 14                     | Rice –Herzfeld mechanism, Branching chains H <sub>2</sub> -O <sub>2</sub>  |                         |  |
|  | 15                     | Semenov-Hinshelwood mechanism of explosive reactions.  |                         |  |
|  | 16                     | <b>Kinetics of polymerization:</b> mechanism of step growth  |                         |  |
|  | 17                     | Ionic and addition polymerization  | PowerPoint presentation |  |
|  | 18                     | Kinetics of anionic and cationic polymerization.   | PowerPoint presentation |  |
| <b>Unit III</b>                            | <b>No. of Sessions</b> | <b>Session Topic and Discussion Theme</b>  | <b>Value additions</b>  |  |
| Unit 4: Nanotechnology and Green Chemistry | 1                      | Basic principles of nanochemistry,.  |                         |  |
|  | 2                      | methods of synthesis of nanomaterials, a brief study of carbon nanotubes, fullerenes, quantum dots and metal nanoparticles. Applications of nanomaterials in medicine: immunogold labelling, |                         |  |
|  | 3                      | applications in medical diagnosis,   |                         |  |
|  | 4                      | nanobased drug delivery,   |                         |  |
|  | 5                      | biomimetic nanotechnology,   |                         |  |
|  | 6                      | DNA nanotechnology and structural biomimicry.  |                         |  |

| <b>1<sup>st</sup> Internal Examination</b>   |  |   |   |  |
|--|--|---|---|--|
|  | 8  | 5.2 Principles of green chemistry                             |   |  |
|  | 9  | basic concepts, atom economy, twelve laws of green chemistry, | Power Point Presentation                                |  |
| <i>Text Books</i>  |  |   |   |  |
| <b>No. of Sessions</b>   | <b>Session Topic and Discussion Theme</b>  |   | <b>Value additions</b>                                  |  |
| 10   | principles of green organic synthesis.   |   |   |  |
| 11   | 5.3 Green alternatives of organic synthesis:   |   | Power Point Presentation                                |  |
| 12   | coenzyme catalysed reactions,  |   | Power Point Presentation                                |  |
| 13   | green alternatives of molecular rearrangements,  |   |   |  |
| 14   | electrophilic aromatic substitution reactions,   |   | Group Discussion  |  |
| <b>2<sup>nd</sup> Internal Examination</b>   |  |   |   |  |
| 15   | oxidation-reduction reactions, clay catalysed synthesis,                                 |   |   |  |
| 16   | condensation reactions. Green photochemical reactions.                                   |   |   |  |
| 17   | Microwave assisted organic synthesis.  |   | Individual Assignment:<br>Various intermolecular forces |  |
| 18   | 5.4 Green chemistry in the pharmaceutical industry: Ibuprofen manufacture, biocatalysis. |   |   |  |
| <p>Reference:</p> <p>Principles of green chemistry, basic concepts, atom economy, twelve laws of green chemistry, principles of green organic synthesis.</p> <p>5.3 Green alternatives of organic synthesis: coenzyme catalysed reactions, green alternatives of molecular rearrangements, electrophilic aromatic substitution reactions, oxidation-reduction reactions, clay catalysed synthesis, condensation reactions. Green photochemical reactions.</p> <p>Microwave assisted organic synthesis.</p> <p>5.4 Green chemistry in the pharmaceutical industry: Ibuprofen manufacture, biocatalysis.</p> |  |   |   |  |
| <i>Unit IV</i>   | <b>No. of Sessions</b>   | <b>Session Topic and Discussion Theme</b>                     | <b>Value additions</b>                                  |  |

|  |  |  |   |  |  |
|--|--|--|---|--|--|
| <b>SURFACE CHEMISTRY AND COLLOIDS</b>      | 1  | 4.2 Spectroscopic techniques for probing solid surfaces  |   |  |  |
|  | 2  | Temperature programmed desorption (TPD)  |   |  |  |
|  | 3  | Reflection absorption infrared spectroscopy (RAIRS)  |   |  |  |
|  | 4  | High resolution electron energy loss spectroscopy (HREELS).  |   |  |  |
|  | 5  | 4.3 Surface films -Introduction film pressure  |   |  |  |
|  | 7  | criteria for spreading of one liquid on another  |   |  |  |
|  | <b>1<sup>st</sup> Internal Examination</b> |  |   |  |  |
|  | 8  | <b>4.4 Adsorption from solutions</b>   |   |  |  |
|  | 9  | Electrostatic adsorption, Gibbs adsorption isotherm (derivation) - verifications.                        | Power Point Presentation                                |  |  |
| <b>Unit IV</b>                             | <b>No. of Sessions</b>                     | <b>Session Topic and Discussion Theme</b>  | <b>Value additions</b>                                  |  |  |
|  | 10   | <b>4.5 Colloids &amp; Micellar systems</b>   |   |  |  |
|  | 11   | Types of colloids, Electrical properties of colloids   | Power Point Presentation                                |  |  |
|  | 12   | Electrical double layer, zeta potential  | Power Point Presentation                                |  |  |
|  | 13   | Miscelles, and miscellisation  |   |  |  |
|  | 14   | Structure of miscelles - ionic miscelles.  | Group Discussion  |  |  |
| <b>2<sup>nd</sup> Internal Examination</b> |  |  |   |  |  |
|  | 15   | ➤ <b>5.1 Laws of Photochemistry:</b>   |   |  |  |
|  | 16   | Grothus –Draper Law, Stark-Einstein’s Law, Laws of light absorption, Quantum yield. Chemical actinometry |   |  |  |
|  |  |  |   |  |  |
|  |  |  |   |  |  |
|  | 17   | ➤ Excimers and exciplexes, photosensitization  | Individual Assignment:<br>Various intermolecular forces |  |  |
|  | 18   | chemiluminescence, bioluminescence, thermo luminescence  |   |  |  |

| <i>Unit V</i>         | <b>No. of Sessions</b>                     | <b>Session Topic and Discussion Theme</b>   | <b>Value additions</b>                                  |  |  |
|-----------------------|--|---|---|--|--|
| <b>PHOTOCHEMISTRY</b> | 1  | pulse radiolysis, hydrated electrons, photo stationary state, dimerization of anthracene.                 |   |  |  |
|                       | 2  | <b>5.2Photo physical processes in electronically excited molecules,</b>                                   |   |  |  |
|                       | 3  | Jablonsky diagram   |   |  |  |
|                       | 4  | Fluorescence and Phosphorescence.   |   |  |  |
|                       | 5  | Quenching of fluorescence and its kinetics  |   |  |  |
|                       | 7  | Stern-Volmer equation, static and dynamic quenching.  |   |  |  |
|                       | <b>1<sup>st</sup> Internal Examination</b> |   |   |  |  |
|                       | 8  | Concentration quenching,  |   |  |  |
|                       | 9  | E-type and P-type. Effect of temperature on emissions,  | Power Point Presentation                                |  |  |
|                       | <b>No. of Sessions</b>                     | <b>Session Topic and Discussion Theme</b>   | <b>Value additions</b>                                  |  |  |
|                       | 10   | Two photon absorption spectroscopy  |   |  |  |
|                       | 11   | Principle of utilization of solar energy  | Power Point Presentation                                |  |  |
|                       | 12   | Solar cells and their working.  | Power Point Presentation                                |  |  |
|                       | 13   | Photochemistry of vision.   |   |  |  |
|                       | 14   | delayed fluorescence,   | Group Discussion  |  |  |
|                       | <b>2<sup>nd</sup> Internal Examination</b> |   |   |  |  |
|                       | 15   | Numericals  |   |  |  |
|                       | 16   | Revision  |   |  |  |
|                       | 17   | Revision  | Individual Assignment:<br>Various intermolecular forces |  |  |
|                       | 18   | Revision  |   |  |  |
| <b>Text Books</b>     | 6.   | D.A. McQuarrie, J.D. Simon, Physical chemistry: A Molecular Approach, University Science Books, 1997      |   |  |  |
|                       | 8.   | K.K. Rohatgi-Mukherjee, Fundamentals of Photochemistry, 2 <sup>nd</sup> Edn. New Age International, 1986. |   |  |  |
|                       | 9.   | G. Aruldas, Molecular structure and Spectroscopy, PHI Learning, 2007.                                     |   |  |  |
|                       | 10.  | M.R Wright, An Introduction to Chemical Kinetics, John Interscience-2007                                  |   |  |  |
|                       | 11.  | A.W & Sons, Adamson, A.P. Gast, Physical chemistry of surfaces, 6 <sup>th</sup> Edn, John Wiley, 1997     |   |  |  |
|                       | 12.  | D.O. Cowan, R.L. Drisko, Elements of Organic Photochemistry, Plenum Press., 1976                          |   |  |  |

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**Programme: M Sc Applied Chemistry - Pharmaceutical**

Semester: III

Course: **P3CPHT12** Spectroscopic Methods In Chemistry

| Term – I (Before I Internal tests) – 30 % of the syllabus |  |              |                              |                      |   |
|---|--|--------------|------------------------------|----------------------|---|
| Sl No   | Topic/Module   | Hour/session | Teacher/invited persons etc. | Method of teaching * | Remarks: Books, reference etc                                     |
| 1   | <b>Unit 1: Drugs acting on ANS<br/>1.1, 1.2, 1.3</b>         | 6 hrs        | Dr Jorphin Joseph            | Lecture ICT enabled  | D.L. Pavia, G.M. Lampman, G.S. Kriz, Introduction to Spectroscopy |
| 2   | <b>Unit 2: Drugs acting on CVS</b>                           | 6 hrs        | Dr. Grace Thomas             | Lecture ICT enabled  |   |
| 3   | <b>Unit 3: Chemotherapy<br/>3.1, 3.2</b>                     | 6 hrs        | Midhun Dominic C D           | Lecture ICT enabled  |   |
| 4   | <b>Unit 4: Antineoplastic Drugs</b>                          | 6 hrs        | Senju Devassykutty           | Lecture              |   |
| 5   | <b>Unit 6: Miscellaneous class of compounds<br/>6.1, 6.2</b> | 6 hrs        | June Cyriac                  | Lecture ICT enabled  |   |

\*ICT enabled, Lecture method (conventional)

| Term – II – 40 % of the syllabus ( before the second Internal tests) |  |              |                              |                      |  |
|--|--|--------------|------------------------------|----------------------|--|
| Sl No  | Topic/Module   | Hour/session | Teacher/invited persons etc. | Method of teaching * | Remarks: Books, reference etc                      |
| 1  | <b>Unit 1: Drugs acting on ANS<br/>1.4, 1.5, 1.6</b> | 6 hrs        | Dr Jorphin Joseph            | Lecture ICT enabled  | W. Kemp, Organic Spectroscopy, 2 <sup>nd</sup> Edn |
| 2  |  | 6 hrs        | Dr. Grace Thomas             | Lecture ICT enabled  |  |

|   |   |       |                       |                        |  |
|---|---|-------|-----------------------|------------------------|--|
| 3 | <b>Unit 3: Chemotherapy<br/>3.3, 3.4</b>                              | 6 hrs | Midhun<br>Dominic C D | Lecture ICT<br>enabled |  |
| 4 |   | 6 hrs | Senju<br>Devassykutty | Lecture                |  |
| 5 | <b>Unit 6: Miscellaneous class of<br/>compounds<br/>6-3, 6.4, 6.5</b> | 6 hrs | June Cyriac           | Lecture ICT<br>enabled |  |

| Term – III – 30 % of the syllabus (before the model examination) |  |                  |                                 |                         |  |
|--|--|------------------|---------------------------------|-------------------------|--|
| Sl<br>No   | Topic/Module   | Hour/<br>session | Teacher/invited<br>persons etc. | Method of<br>teaching * | Remarks: Books,<br>reference etc   |
| 1  | <b>Unit 1: Drugs acting on ANS</b>                               | 6 hrs            | Dr Jorphin<br>Joseph            | Lecture ICT<br>enabled  | R.M. Silverstein,<br>G.C. Bassler, T.C.<br>Morril, Spectroscopic<br>Identification of<br>Organic Compounds,<br>5 <sup>th</sup> Edn., |
| 2  |  | 6 hrs            | Dr. Grace<br>Thomas             | Lecture ICT<br>enabled  |  |
| 3  | <b>Unit 3: Chemotherapy<br/>3.5</b>                              | 6 hrs            | Midhun<br>Dominic C D           | Lecture ICT<br>enabled  |  |
| 4  |  | 6 hrs            | Senju<br>Devassykutty           | Lecture                 |  |
| 5  | <b>Unit 6: Miscellaneous class of<br/>compounds<br/>6.6, 6.7</b> | 6 hrs            | June Cyriac                     | Lecture ICT<br>enabled  |  |