**Revised Syllabus to be implemented during 2015-16**

**M.Sc. II: Organic Chemistry**

**Semester III**

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<td>Organic Reaction Mechanism</td>
<td>48</td>
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<td>CHO-351</td>
<td>Spectroscopic Methods in Structure Determination</td>
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<td>CHO-352</td>
<td>Organic Stereochemistry</td>
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<td>Pericyclic Reactions, Photochemistry and Heterocyclic Chemistry</td>
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**Semester IV**

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<td>Designing Organic Synthesis and Asymmetric Synthesis</td>
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**M.Sc. II: Organic Chemistry Practical**

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<td>CHO-448</td>
<td>Project/Industrial training/ Green Chemistry and Chemical Biology Experiments</td>
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Each practical course should be of 6 h/week/batch. Practical batch for each course should comprise of 8 students only.
# Equivalence of previous Syllabus

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<td>CH-353 Free Radicals, Photochemistry, Pericyclic Reactions and their Applications</td>
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<td>CHO-450</td>
<td>Chemistry of Natural Products</td>
<td>CH-450 Chemistry of Natural Products</td>
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M.Sc. Organic Chemistry PART-II
REVISED SYLLABUS-2014

CHO-350: Organic Reaction Mechanism [4 credits, 48 Lectures]

1. Carbanions-Formation, stability and related name reactions [14L]
   Ref. 1, 2, 3 Vol.A and 7
2. Enamines –formation and applications, Ref. 3 [4L]
3. NGP : Neighbouring group participation , Ref. 1 [6L]
4. Reactions of carbenes and nitrenes Ref.3 Vol B [4L]
5. Free radicals: [14L]
   Generation of radicals, Stable free radicals, Nucleophilic and electrophilic radicals,
   Characteristics reactions, -Free radical substitution, addition to multiple bonds,
   Radicals in synthesis: Inter and intra molecular C-C bond formation via mercuric
   hydride, tin hydride, thiol dionors, cleavage of C-X, C-Sn, C-Co, C-S, O-O bonds.
   Oxidative coupling. C-C bond formation in aromatics, SNAr reactions
   Ref. 1, 3 Vol A, 6
6. Mechanisms in Biological Chemistry (Ref. 5) [6L]

References:
1. Mechanism and structure in Organic Chemistry – E. S. Gould (Holt, Rinehart and
   Winston)
2. Advanced organic chemistry by J. March, 6th Ed.
   University Press (2001)

CHO-351: Spectroscopic Methods in Structure Determination [4 credits, 48 Lectures]

1H NMR Spectroscopy (14 L)

Chemical shift, factors influencing chemical shift, deshielding, chemical shift values and
 correlation for protons bonded to carbons (aliphatic, olefinic, aldehydic, aromatic) and
 other nuclei (alcohols, phenols, enols, acids, amides and mercaptans), chemical exchange,
 effect of deuteration, spin-spin coupling, (n+1) rule, complex spin-spin interaction between
two, three, four and five nuclei (first order spectra), factors effecting coupling constant “J”,
classification of spin system like AB, AX, AX2, ABX, AMX, ABC, A2B2. Spin decoupling,
Factors affecting coupling constant, simplification of complex spectra, nuclear magnetic double resonance, spin decoupling, contact shift reagents, solvent effects, nuclear overhauser effect (NOE), resonance of other nuclei like $^{31}\text{P}$, $^{19}\text{F}$

**$^{13}\text{C}$ NMR spectroscopy**  
(8 L)

FT NMR, Types of $^{13}\text{C}$ NMR Spectra: un-decoupled, Proton decoupled, Off resonance, APT, INEPT, DEPT, chemical shift, calculations of chemical shifts of aliphatic, olefinic, alkyne, aromatic, hetero aromatic and carbonyl carbons, factors affecting chemical shifts, Homo nuclear ($^{13}\text{C}-^{13}\text{C}$) and Hetero nuclear ($^{13}\text{C}-^{1}\text{H}$)coupling constants.

**2D NMR Techniques**  
(6 L)

General idea about two dimensional NMR spectroscopy, Correlation spectroscopy (COSY)- Homo COSY ($^{1}\text{H}-^{1}\text{H}$), TOCSY, Hetero COSY (HMQC, HMBC), Homo and Hetero nuclear 2D resolved spectroscopy, NOESY and 2D-INADEQUATE experiments and their applications.

**Mass Spectrometry**  
(10 L)

Instrumentation, various methods of ionization (field ionization, field desorption, SIMS, FAB, MALDI, Californium plasma), different detectors (magnetic analyzer, ion cyclotron analyzer, Quadrupole mass filter, time of flight (TOF). Rules of fragmentation of different functional groups, factors controlling fragmentation

**Problems based on joint application of UV, IR, PMR, CMR, and Mass.**  
(10 L) 
(Including reaction sequences)

**References:**
4. Absorption spectroscopy of organic molecules – V. M. Parikh
10. Spectroscopic identification of organic compound- R M Silverstein, G C Bassler and T C Morril, John Wiley
11. Introduction to NMR spectroscopy-R J Abrahm, J Fisher and P loftus Wiley
12. Organic spectroscopy-William kemp, E L B with McMillan
15. Practical NMR spectroscopy-ML Martin, J J Delpench, and D J Martyin
17. Spectroscopy in organic chemistry- C N R Rao and J R Ferraro
18. NMR –Basic principle and application-H Guntur
19. Interpretation of NMR spectra-Roy H Bible
20. Mass spectrometry organic chemical applications, J H Banyon

**CHO-352: Organic Stereochemistry**

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<th>Reference</th>
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<td>2. Stereochemistry of rings other than six membered</td>
<td>Ref. 1, 4, 5, 6</td>
<td>(8L)</td>
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<td>3. Fused Bridged and caged rings</td>
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<td>4. Resolution of racemic modification</td>
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<td>5. Geometrical Isomerism and Stereochemistry of olefins Ref.1, 2</td>
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<td>6. Determination of stereochemistry organic compounds using NMR.</td>
<td></td>
<td>(4L)</td>
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</table>

**CHO-352: Organic Stereochemistry**

**References:**

1. Stereochemistry of carbon compounds - E. L. Eliel
2. Stereochemistry of carbon compounds - E. L. Eliel and S. H. Wilen
4. Stereochemistry of organic compounds –Nasipuri
5. Stereochemistry of organic compounds-Kalsi
6. Organic stereochemistry – Jagdamba Singh
CHO-353: Photochemistry, Pericyclic Reactions and Heterocyclic Chemistry

[4 credits, 48 Lectures]

1. **Photochemistry** [12L]
   General basic principles, photochemistry of carbonyl compounds, alkenes, dienes, polyenes and aromatic compounds, photorearrangements, Barton reaction
   Ref. 1,2,3,4
   Application of photochemical reactions in synthesis – Isocomene
   Ref. 8, 9

2. **Pericyclic reactions** [12L]
   Electroyclic, cycloaddition, sigmatropic and ene reactions. 1,3-dipolar additions, Analysis by correlation diagrams, FMO approach and ATS concept. Application of pericyclic reactions.
   Ref. 1, 3, 5, 6, 7, 13

3. **Heterocyclic Chemistry** (24 L)
   a) Five and six membered heterocycles with one and two hetero atoms:
      Synthesis, reactivity, aromatic character and importance of following heterocyclic rings: Furan, Pyrrole, Thiophene, Pyrazole, Imidazole, Pyridine
   b) Condensed five and six membered heterocycles:
      Benzofuran, Indole, Quinoline
   c) Condensed five membered heterocycles:
      Benzoazole, Benzthiazole, Benzimidazole
   d) Five and six membered heterocycles with more than two hetero atoms:
      Synthesis, reactivity, aromatic character and importance of following heterocycles:
      1,2,3-triazole, 1,2,4-oxadiazole, 1,2,5-oxadiazole, tetrazole,
      Ref. 14-20

**References:**

2. Excited states in Organic Chemistry- J.A. Barltrop and J.D. Coyle, John Wiley & sons
11. Pericyclic reactions- Gill and Willis
12. Frontier orbitals and organic chemical reactions-Ian Fleming, John Wiley & sons
CHO–450 Chemistry of Natural Products [4 credits, 48 Lectures]

1. Structure and stereochemistry of Hardwickiic acid, Camptothecin and podophyllotoxin
   Ref. 1 to 4 and 11
2. Synthesis of
   i) Taxol Ref. 6
   ii) Estrone and Mifepristone Ref. 6, 7
   iii) Juvabione (K.Mori and Matsui, Pawson and Cheung Synthesis) Ref.12
   iv) Fredericamycin A Ref. 5
3. Biogenesis – The building blocks and construction mechanism of
   1. Terpenoids – Mono, Sesqui, Di and Triterpenoids and cholesterol
   2. Alkaloids derived from ornithine, lysine, nicotinic acid, tyrosine and tryptophan.
   3. The shikimate pathway – cinnamic acids, lignans and lignin, coumarins, flavonoids and stilbens, isoflavonoids and terpenoid quinones.
   Ref. 8, 9, 10

References:
3. (i) Tetrahedron Letters, 3751 (1964),
4. Chemistry of Natural products- Kalsi
8. Medicinal Natural Products - A Biosynthetic approach by Paul M. Dewick 2nd Ed.(Wiley)
CHO-451: Advanced Synthetic Organic Chemistry  [4 credits, 48 Lectures]

2. C=C formation reactions: Wittig, Horner-Wordworth-Emmons, Shapiro, Bamford-Stevens, McMurry, Julia-Lythgoe and Peterson olefination reactions, Titanium-carbene mediated olefination: Tebbe, Petasis and Nysted reagent [8L]
4. Ring formation reactions: Pausan-Khand, Bergman and Nazarov cyclization [3L]
5. Click chemistry: criterion for click reaction, Sharpless azides cycloadditions [2L]
6. Metathesis: Grubbs 1st and 2nd generation catalyst, Olefin cross coupling (OCM), ring closing (RCM) and ring opening (ROM) metathesis, applications [4L]
7. Use of Boron and Silicon in organic synthesis [8L]
8. Other important reactions: Baylis Hilman, Eschenmoser-Tanabe fragmentation, Mitsunobu reaction [3L]

References:
1. Organic synthesis using transition metals-Roderick Bates (Wiley)
5. Organic synthesis – Michael B. Smith
8. Guidebook to organic synthesis-R K Meckie, D M Smith and R A Atken
9. Organic synthesis- Robert E Ireland
10. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako

CHO-452: Carbohydrate and Chiron approach, Chiral Drugs and Medicinal Chemistry  [4 credits, 48 Lectures]

1. Carbohydrates [4L]
   Introduction of sugars, structures of triose, tetrose, pentose, hexose, stereochemistry and reactions of Glucose, conformation and anomeric effects in hexoses Ref. 1, 2
2. Chiron approach [8L]
   a) Introduction
   b) The concept of chiral templates and chirons wherein the carbon skeleton is the chiral precursor.
   c) Utilisation of the basic concepts for retrosynthetic strategy and synthesis of the following – (S) Propanediol, (R) and (S) – Epichlorohydrin, L (+)-Alanine,
3. Chiral Drugs

a) Introduction of chiral drugs, Eutomer, Distomer and eudesmic ratio,
b) Distomers-a) with no side effects b) with undesirable side effects Synthesis of S-Ibuprofen, S-Metaprolol, Ininvir sulfate, Dextropropoxyphen, (+) Ephedrine, Griseofulvin, R-Indacrinone, hydrochloride, S-S-captopril

References:
2. Organic Chemistry – I. L. Finar, volume II
4. Pharmaceutical Chemistry and drug synthesis – Rot and Kleeman
5. Drug Design – E.J. Arienes

4. Medicinal Chemistry

1. Introduction to drugs, their action and discovery Ref. 1,2,3 [4L]
2. Relation of Drug structure and its chemical and biological properties Ref. 1,2,3 [4L]
3. Structure, activity and quantitative relationship Ref. 1,2,3 [3L]
4. Drug targets like proteins, enzymes, receptors, nucleic acids, lipids and carbohydrates Ref. 2 and 3 [4L]

References:
1. Medicinal Chemistry an Introduction-Gareth Thomas 2nd Ed. Wiley
3. Introduction to Medicinal Chemistry-Alex Gringauz (Wiley)
4. Foye’s Medicinal Chemistry
5. Medicinal Chemistry-A. Burger
6. Medicinal Chemistry-Ashutosh Karr
CHO-453: Designing Organic Synthesis and Asymmetric Synthesis  
[4 credits, 48 Lectures]

1. Designing of organic synthesis: Protection and de-protection of hydroxyl, amino, carboxyl, ketone and aldehyde functions as illustrated in the synthesis of polypeptide and polynucleotide, enamines, Umpolung in organic synthesis, Reterosynthesis. (24L)

2. Principles and applications of asymmetric synthesis: stereoselectivity in cyclic compounds, enantio-selectivity, diastereo-selectivity, enatiomeric and diastereomeric excess, stereoselective aldol reactions. Cram’s rule, Felkin Anh rule, Cram’s chelate model, Asymmetric synthesis, use of chiral auxiliaries, chiral reagents and catalysts, asymmetric hydrogenation, asymmetric epoxidation and asymmetric dihydroxylation. Ref. 3 chapters 33, 34, 35

1. Designing of organic synthesis – S. Warren (Wiley)  
4. Organic synthesis – Michael B. Smith  
6. Guidebook to organic synthesis-R K Meckie, D M Smith and R A Atken  
7. Organic synthesis- Robert E Ireland  
8. Strategic Applications of named reactions in organic synthesis-Laszlo Kurti and Barbara Czako
M.Sc. II: Organic Chemistry Practical

CHO-347: (A) Single stage preparations \[6\text{ Credits}\]

At least fourteen single stage and three Isolation of Natural products should carried out. The preparation should be carried out on micro scale.

1. 2-Phenyl indole (Fischer indole synthesis),
2. 7-Hydroxy -3-methyl flavone (Baker-Venkatraman reaction),
3. Benzyl alcohol and benzoic acid from benzenaldehyde (Cannizzaro reaction)
4. 4-Chlorotoluene from p-toluidine (Sndmeyer reaction)
5. Benzilic acid from benzoin (Benzilic acid rearrangement)
6. Benzopinacol (Photochemical reaction),
7. 7-Hydroxy-4-methyl coumarin (Pechmann Reaction)
8. 4-Methyl benzophenone (Friedal Craft reaction)
9. Benzanilide (Beckmann rearrangement)
10. Vanillyl alcohol from vanillin (NaBH\textsubscript{4} reduction)
11. 2- and 4-nitrophenols (nitration and separation by steam distillation)
12. Stilbene from benzyl chloride (Wittig reaction)
13. Ethyl cinnamate from benzaldehyde (Wittig reaction)
14. Triphenyl or diphenyl methyl carbinol (Grignard reaction)
15. Benzotriazole
16. 1-Phenyl-3-methyl pyrazol-5-one
17. Glucose pentaacetate
18. 2,4-diethoxycarbonyl-3,4-dimethyl pyrrole from ethyl acetoacetate
19. Quinoline from aniline Skraup synthesis)
20. Benzimidazole from benzyl
21. Cyclohexanol from cyclohexanone (LAH reduction)

B) Isolation of Natural products (Any three)

1. Caffeine from tea leaves (Soxhlet extraction)
2. Piperine from pepper (Soxhlet extraction)
3. Eucalyptus oil from leaves (Steam distillation)
4. Lycopene from tomatoes
5. Trumyristin from nutmeg
6. Cinnamaldehyde from cinnamom
7. Eugenol from clove

References:
1. Practical organic chemistry by Mann & Saunders
CHO-447: Two stage preparations (any Ten) [6 Credits]

1. Benzaldehyde → Benzalacetophenone → Epoxide
2. 4-Nitro toluene → 4-Nitro benzoic acid → 4-Amino benzoic acid
3. Resorcinol → 4-methyl-7-hydroxy coumarin → 4-Methyl-7-acetoxy coumarin
4. Cyclohexanone → Phenyl hydrazone → 1,2,3,4-Tetrahydrocarbazole
5. Hydroquinone → Hydroquinone diacetate → 1,2,4-Triacetoxy benzene
6. Acetanilide → p-Acetamidobenzene sulphonyl chloride → P. Acetamidobenzene sulphonamide
7. p-Amino phenol → p-Acetyl amino phenol → p-Ethoxy acetonilide
8. Hippuric acid → Azalactone → 4-Benzylidene 2-phenyl oxazol-5-one
9. p-Cresol → p-Cresyl benzoate → 2-Hydroxy-5-methyl benzophenone
10. Phthalimide → N-Benzylphthalimide → Benzylamine
11. o-Nitroaniline → o-Phenylenedi amine → Benzimidazole
12. Phthalic acid → Phthalimide → Anthranilic acid
13. Benzyl cyanide → p-Nitrobenzyl cyanide → p-Nitro phenyl acetic acid
14. Hydroquinone → Hydroquinone diacetate → 2,5-Dihydroxy acetopheneone
15. Cyclohexanone → Enamine → 2-Acetyl cyclohexanone
16. α-Pinene → Disiamyl borane → Pinanol

CHO-448: Project/Industrial training/Green Chemistry and Chemical biology experiments (any Twelve) [6 Credits]

1. Preparation of acetonilide from aniline and acetic acid using Zn dust
2. Base catalyzed aldol condensation using LiOH.H₂O as a Catalyst.
3. Bromination of trans-stilbene using sodium bromide and sodium bromate
4. [4+2] cycloaddition reaction in aqueous medium at room temperature
5. Benzil Benzilic acid rearrangement under solvent free condition
6. Thiamine hydrochloride catalyzed synthesis of benzoin from benzaldehyde
7. Clay catalyzed solid state synthesis of 7-hydroxy-4-methylcoumarin
8. Ecofriendly nitration of phenols and its derivatives using Calcium nitrate
9. Bromination of acetonilide using ceric ammonium nitrate in aqueous medium
10. Green approach for preparation of benzopinacolone from bezopinacol using iodine catalyst
11. Preparation of 1, 1-bis-2-naphthol under grinding at room temperature.
12. Solvent free aldol condensation between 3,4-dimethoxybenzaldehyde and 1-indanone
13. Solvent free quantitative solid phase synthesis of azomethines from substituted anilines and substituted benzaldehydes.
14. Sucrose to ethyl alcohol (Baker’s yeast)
15. Asymmetric reduction of EAA by using Baker’s yeast

Note: i) Project/Industrial training students have to perform 6 practical from the above experiments.
ii) 20% students should be given project or industrial training.

Reference:

1. Comprehensive Practical Organic Chemistry by V.K. Ahluwalia and Renu Aggarwal
2. Monograph on Green Chemistry Laboratory Experiments by Green Chemistry Task Force Committee, DST