

2.2.1.

MSc. Chemistry @ Telangana University Lecture By

**Dr. Nagaraj**

Associate Professor, Department of Chemistry, Telangana University

[https://youtu.be/ZyTEtDB0P6A?si=dXdR1HmL9yo\\_L9sv](https://youtu.be/ZyTEtDB0P6A?si=dXdR1HmL9yo_L9sv)

This lecture includes, the M.Sc. Chemistry (Organic Chemistry/Pharmaceutical Chemistry) course structure and Evaluation.

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PRINCIPAL  
UNIVERSITY COLLEGE  
TELANGANA UNIVERSITY  
DICHPALLY-503 322, NIZAMABAD

## <sup>1</sup>H NMR SPECTROSCOPY – VIDEO LECTURES BY

**Dr. NAGA RAJ**

Associate Professor, Department of Chemistry, Telangana University

Syllabus (Topic)	LECTURE	LINK ADDRESS
Magnetic properties of nuclei and principles of NMR	1	<a href="https://youtu.be/bwkGzXO6ADE?si=Eo8PrP58rT7egJtl">https://youtu.be/bwkGzXO6ADE?si=Eo8PrP58rT7egJtl</a>
Presentation, signal integration, equivalent, non equivalent protons, enantiotopic and diastereotopic protons, chemical shifts	2	<a href="https://youtu.be/x1JsJVfINR0?si=IU96ivWKUKHrum0W">https://youtu.be/x1JsJVfINR0?si=IU96ivWKUKHrum0W</a>
Factors affecting the chemical shifts, electro negativity and anisotropy, shielding and deshielding effects	3	<a href="https://youtu.be/t5JDSx9TcjQ?si=aIv6rICOESjB3XCZ">https://youtu.be/t5JDSx9TcjQ?si=aIv6rICOESjB3XCZ</a>
Anisotropic effect, spin-spin coupling, theory of spin-spin coupling	4	<a href="https://youtu.be/3IA4kP3sa5U?si=kDoRvVM_90zFqz0g">https://youtu.be/3IA4kP3sa5U?si=kDoRvVM_90zFqz0g</a>
Mechanism of spin-spin coupling, vicinal, germinal and long range, coupling constants	5	<a href="https://youtu.be/lxKRV7hR-OY?si=uRDvcms_UHP19H8p">https://youtu.be/lxKRV7hR-OY?si=uRDvcms_UHP19H8p</a>
Factors affecting coupling constants, <sup>1</sup> H NMR of organic molecules and metal complexes: ethyl acetate, 2-butanone, mesitylene, para-cetamol, aspirin, ethyl benzoate, benzyl acetate, 2-chloro propionic acid, [HNi(OPEt <sub>3</sub> ) <sub>4</sub> ] <sup>+</sup> , [HRh(CN) <sub>5</sub> ], [Pt(acac) <sub>2</sub> ].	6	<a href="https://youtu.be/QZNMMPibFPQ?si=xt_fFcXKvAnCOLXi">https://youtu.be/QZNMMPibFPQ?si=xt_fFcXKvAnCOLXi</a>
Applications of <sup>1</sup> H NMR spectroscopy: reaction mechanisms (cyclic bromonium ion, electrophilic and nucleophilic substitutions, carbocations and carbanions), E,Z isomers	7	<a href="https://youtu.be/bTACCAfgv5U?si=hNMVkeSn4ZOqQVx7">https://youtu.be/bTACCAfgv5U?si=hNMVkeSn4ZOqQVx7</a>
Conformation of cyclohexane and decalins, hydrogen bonding, C-N rotation, proton exchange processes ( alcohols, amines and carboxylic acids), keto-enol tautomerism	8	<a href="https://youtu.be/se3B_RNihz8?si=r_tVXgd7P7msUsCI">https://youtu.be/se3B_RNihz8?si=r_tVXgd7P7msUsCI</a>
Instrumentation, CW and pulsed FT instrumentation	9	<a href="https://youtu.be/egKpByU_Kow?si=neLkanrcNAqSEPwM">https://youtu.be/egKpByU_Kow?si=neLkanrcNAqSEPwM</a>

## ELECTRONIC (UV) SPECTROSCOPY – VIDEO LECTURES BY

**Dr. NAGA RAJ**

**Associate Professor, Department of Chemistry, Telangana University**

Syllabus (Topic)	LECTURE	LINK ADDRESS
Principle of UV spectroscopy, elementary energy levels of molecules, types of electronic transitions in molecules, chromophores:	1	<a href="https://youtu.be/Wg_Syvi_76I?si=INOiG0QI1YdPHGr4">https://youtu.be/Wg_Syvi_76I?si=INOiG0QI1YdPHGr4</a>
Solvent and structural influences on absorption maxima, stereochemical factors: cis-trans isomers, and cross conjugation.	2	<a href="https://youtu.be/9Q9sHX3Uh1o?si=XU31-bPCucLZdEJT">https://youtu.be/9Q9sHX3Uh1o?si=XU31-bPCucLZdEJT</a>
Woodward-Fieser rules for conjugated dienes and trienes	3	<a href="https://youtu.be/jAzEvCKMtjQ?si=qmFepHsIycc0sB31">https://youtu.be/jAzEvCKMtjQ?si=qmFepHsIycc0sB31</a>
Woodward-Fieser rules for unsaturated carbonyl compounds	4	<a href="https://youtu.be/6j1PxbVhIpk?si=K7hjYXqRdkN8BTra">https://youtu.be/6j1PxbVhIpk?si=K7hjYXqRdkN8BTra</a>
Woodward-Fieser rules for benzene and its derivatives	5	<a href="https://youtu.be/XwQVAgBMKus?si=XKJ9_vkw5ZrflkXWK">https://youtu.be/XwQVAgBMKus?si=XKJ9_vkw5ZrflkXWK</a>
Woodward-fieser rules for polynuclear aromatic hydrocarbons and diketones Woodward-Kuhn rules for polyenes	6	<a href="https://youtu.be/u4UOQH5IUkY?si=QlpdWem8tq7Otvaw">https://youtu.be/u4UOQH5IUkY?si=QlpdWem8tq7Otvaw</a>
Beer's law application to mixture analysis and dissociation constant of a weak acid	7	<a href="https://youtu.be/KjPclZu8z3c?si=D4ynufsb0O2DPCZE">https://youtu.be/KjPclZu8z3c?si=D4ynufsb0O2DPCZE</a>

## NMR SPECTROSCOPY-II – VIDEO LECTURES BY

**Dr. NAGA RAJ**

**Associate Professor, Department of Chemistry, Telangana University**

Syllabus (Topic)	LECTURE	LINK ADDRESS
<sup>1</sup> H NMR spectroscopy: Introduction Designation of Nuclei (Nomenclature) First order NMR Spectra	1	<a href="https://youtu.be/c-OuZQ0MNUU">https://youtu.be/c-OuZQ0MNUU</a>
Non First Order Spectra (II order) <sup>1</sup> H NMR Spectrum of AX, AX <sub>2</sub> , AX <sub>3</sub> , A <sub>2</sub> X <sub>3</sub> , AMX and AB, ABC Systems	2	<a href="https://youtu.be/5oG7virO9sg">https://youtu.be/5oG7virO9sg</a>
Simplification of Complex Spectra by use of Lanthanide shift reagents Double Resonance Techniques	3	<a href="https://youtu.be/gIOesVwTYfU">https://youtu.be/gIOesVwTYfU</a>
Nuclear Overhauser Enhancement (NOE) Increased Field Strength Deuterium Exchange Techniques.	4	<a href="https://youtu.be/d6CGvbMNuzo">https://youtu.be/d6CGvbMNuzo</a>
Discrimination of enantiomers by Chiral NMR Solvents (CSAs) Chiral Lanthanide Shift Reagents Mosher's Acid Fluxional Molecules Study of Fluxional Molecules: Bullvalene	5	<a href="https://youtu.be/gxu03kZnNvg">https://youtu.be/gxu03kZnNvg</a>
[ $\eta^5$ -C <sub>5</sub> H <sub>5</sub> M] [ $\eta^5$ -(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> Ti $\eta^1$ -(C <sub>5</sub> H <sub>5</sub> ) <sub>2</sub> ] [ $\eta^4$ C <sub>8</sub> H <sub>8</sub> Ru(CO) <sub>3</sub> ] <sup>19</sup> F NMR spectroscopy <sup>19</sup> F Chemical Shifts Coupling Constants <sup>19</sup> F NMR Spectrum of: 1,2-dichloro-1,1-difluoroethane, BrF <sub>5</sub> , SF <sub>4</sub> , PF <sub>5</sub> , ClF <sub>3</sub> , IF <sub>5</sub> , [HF <sub>2</sub> ] <sup>-</sup>	6	<a href="https://youtu.be/5cMB4AU_kl0">https://youtu.be/5cMB4AU_kl0</a>
<sup>31</sup> P NMR Spectroscopy <sup>31</sup> P Chemical Shifts Coupling Constants <sup>31</sup> P NMR Spectrum of: ATP, Ph <sub>3</sub> PSe, P <sub>4</sub> S <sub>3</sub> , P(OCH <sub>3</sub> ) <sub>3</sub> , H <sub>3</sub> PO <sub>4</sub> , H <sub>3</sub> PO <sub>3</sub> , H <sub>3</sub> PO <sub>2</sub> , HPF <sub>2</sub> , PF <sub>6</sub> <sup>-</sup> , PH <sub>3</sub> , [Rh(PPh <sub>3</sub> )Cl <sub>3</sub> ]	7	<a href="https://youtu.be/NAkyP7zIPFo">https://youtu.be/NAkyP7zIPFo</a>
Solid state NMR Magic Angle Spinning (MAS) Applications	8	<a href="https://youtu.be/Ct7PemSgM3o">https://youtu.be/Ct7PemSgM3o</a>

## MASS SPECTROMETRY – VIDEO LECTURES BY

**Dr. NAGA RAJ**

**Associate Professor, Department of Chemistry, Telangana University**

Syllabus (Topic)	LECTURE	LINK ADDRESS
Origin of Mass Spectrum Principles of EI Mass Spectrometer Presentation of Mass Spectrum Isotopic Peaks Calculation of Isotopic Peak Intensities	I	<a href="https://youtu.be/VY7-3ZFXaLI">https://youtu.be/VY7-3ZFXaLI</a>
Nitrogen Rule Types of fragments: Odd Electron and Even Electron Neutral and Charged Species (Even Electron Rule) Principle of: Electron Ionization (EI) Chemical Ionization (CI) Fast Atom Bombardment (FAB)	2	<a href="https://youtu.be/bEuC3zBYmzg">https://youtu.be/bEuC3zBYmzg</a>
Secondary Ion Mass Spectrometry (SIMS) Electro spray Ionization (ESI) Matrix Assisted Laser Desorption Ionization Determination of Molecular Formula	3	<a href="https://youtu.be/P9uhCVHZBqU">https://youtu.be/P9uhCVHZBqU</a>
Determination of Molecular Formula for different examples	4	<a href="https://youtu.be/vmzQl9aPCDg">https://youtu.be/vmzQl9aPCDg</a>
Determination of Molecular Formula Classification of Fragmentation Processes Heterolytic Cleavage, Homolytic Cleavage $\alpha$ -Cleavage, $\beta$ -Cleavage, Allylic Cleavage, Benzylic Cleavage Retro Diels Alder Fragmentation (RDA)	5	<a href="https://youtu.be/J1E4W4rSJAc">https://youtu.be/J1E4W4rSJAc</a>
Scrambling Reaction McLaferty Rearrangement Elimination & Rearrangement Ortho Effect	6	<a href="https://youtu.be/XRtj2O3vSY">https://youtu.be/XRtj2O3vSY</a>
Salient Features of Fragmentation Pattern of Organic Compounds Meta Stable Ions (M*) Peaks Introduction to principle and applications of GC-MS & LC-MS	7	<a href="https://youtu.be/E3oBq04re_U">https://youtu.be/E3oBq04re_U</a>

## **$^{13}\text{C}$ NMR SPECTROSCOPY– VIDEO LECTURES BY**

**Dr. NAGA RAJ**

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Syllabus (Topic)	LECTURE	LINK ADDRESS
Introduction to $^{13}\text{C}$ NMR Information from $^{13}\text{C}$ NMR	<b>1</b>	<a href="https://youtu.be/XGjCvJwonM8">https://youtu.be/XGjCvJwonM8</a>
Comparison of CMR & PMR	<b>2</b>	<a href="https://youtu.be/M6rtai V6nE">https://youtu.be/M6rtai V6nE</a>
Spin Decoupling Experiment Types of $^{13}\text{C}$ NMR Spectrums Undecoupled $^{13}\text{C}$ NMR Spectra Proton Decoupled $^{13}\text{C}$ NMR Spetra OFF resonance Decoupled $^{13}\text{C}$ NMR Spectra	<b>3</b>	<a href="https://youtu.be/NCF4c05usak">https://youtu.be/NCF4c05usak</a>

## DRUG DESIGN & DRUG DISCOVERY - VIDEO LECTURES BY

**Dr. Nagaraj**

Associate Professor, Department of Chemistry, Telangana University

Syllabus (Topic)	LECTURE	LINK ADDRESS
1) Introduction to Drug Discovery a) Causes of Disease b) Cell Functions c) Drug Definition and Its Properties d) Types of Drugs e) Drug Action 2) Pharmacokinetic Action	1	<a href="https://youtu.be/g_m-Vq-qRIA">https://youtu.be/g_m-Vq-qRIA</a>
a) Drug Administration/Absorption b) Drug Distribution c) Drug Metabolism d) Drug Excretion	2	<a href="https://youtu.be/0aD-wx91RgY">https://youtu.be/0aD-wx91RgY</a>
3) Pharmacodynamic Action 4) Stages Involved in Drug Discovery 5) Disease, Drug Targets, Bio Assay	3	<a href="https://youtu.be/Wb7iKxzxKPO">https://youtu.be/Wb7iKxzxKPO</a>
6) Drug Targets a) Receptors b) Ion Channels c) Enzymes d) Carrier Molecules	4	<a href="https://youtu.be/WWwouy83MZI">https://youtu.be/WWwouy83MZI</a>
7) Nature of Drug – Receptor Interactions a) Ionic Interactions b) Hydrogen Bonding Interactions c) Vander Walls's Interactions d) Dipolar-Dipolar Interactions e) Ion-Dipolar Interactions 8) Theories of Drug Receptor Interactions a) Occupancy Theory b) Induced-Fit Theory c) Macromolecular Perturbation Theory d) Two-State Model of Receptor	5	<a href="https://youtu.be/wSYzeBITue8">https://youtu.be/wSYzeBITue8</a>
9) Drug Discovery Without Lead (Serendipity) a) Penicillin b) Librium	6	<a href="https://youtu.be/CG3A-zryDqo">https://youtu.be/CG3A-zryDqo</a>
10) Discovery of Lead a) Screening of Natural Products b) Synthetic Compound Libraries c) Natural Hormones and Neurotransmitters d) Folklore Drugs e) Natural Products as Lead Structures f) Existing Drugs as Leads (me too drugs)	7	<a href="https://youtu.be/noFkgMtjTjE">https://youtu.be/noFkgMtjTjE</a>
11) Pharmacophore 12) Structure Pruning Technique for Morphine 13) Principles of Design of: a) Agonistic Drug Salbutamol b) Antagonistic Drug Cimitidine c) Enzyme Inhibitor Drug Captopril	8	<a href="https://youtu.be/Q1--z7bP9T8">https://youtu.be/Q1--z7bP9T8</a>
14) Principles of Pro-drug Design	9	<a href="https://youtu.be/d_NFrpovPCo">https://youtu.be/d_NFrpovPCo</a>
15) Introduction to: a) Clinical Trials b) Drug Patents	10	<a href="https://youtu.be/QB3Y_IR64ZY">https://youtu.be/QB3Y_IR64ZY</a>

## LEAD MODIFICATION & SAR STUDIES – VIDEO LECTURES BY

**Dr. Nagaraj**

Associate Professor, Department of Chemistry, Telangana University

Syllabus (Topic)	LECTURE	LINK ADDRESS
I) Lead modification strategies: a) Bioisosterism b) Variation of alkyl substituent, c) Chain homologation d) Chain branching e) Variation of aromatic substituents	1	<a href="https://youtu.be/hY1aSq2EJg">https://youtu.be/hY1aSq2EJg</a>
f) Extension of structure g) Ring expansion and ring contraction h) Ring variation and position of hetero atoms i) Ring fusion j) Simplification of the lead	2	<a href="https://youtu.be/krsHYf4OdA">https://youtu.be/krsHYf4OdA</a>
k) Rigidification of lead II) Discovery of: a) Oxaminquine b) Salbutamol c) Cimitidine d) Captopril III) Structure Activity Relationship Studies SAR a) Sulfa drugs	3	<a href="https://youtu.be/jrVRXWPJvIE">https://youtu.be/jrVRXWPJvIE</a>
b) Benzodiazepines c) Taxol analogs.	4	<a href="https://youtu.be/CXj-Bzm1aBE">https://youtu.be/CXj-Bzm1aBE</a>