Course Code: BSC202

Course Name: Chemistry-I (Concepts in chemistry for engineering)

(Organic reactions and synthesis of a drug molecule)

(Lecture-Part 1)

For

B.Tech. CSE

Semester: II

By

Dr. Abhijeet Kumar

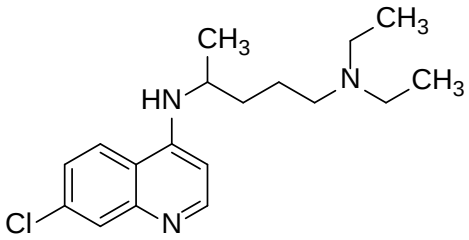
Department of Chemistry

Mahatma Gandhi Central University

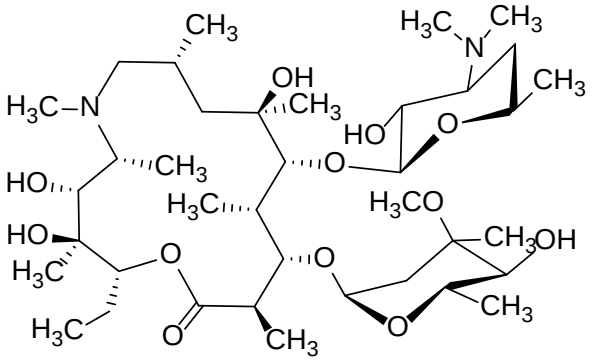
Role of Organic Chemist for Human Welfare

- ***Drug Discovery***
- ***Agrochemicals***
- ***Food Industry***
- ***Dye and Paint Industry***

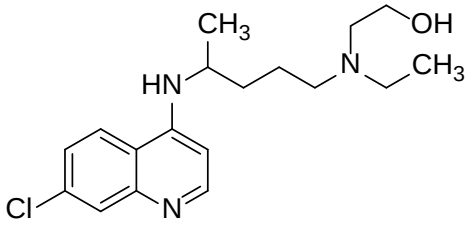
Drugs Which Have Attracted Attention in Last Few Months In Relation to COVID-19.



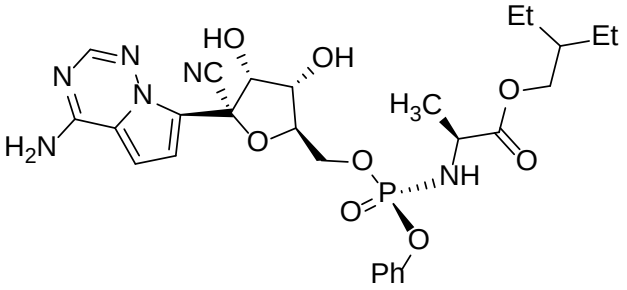
Chloroquine



Azithromycin



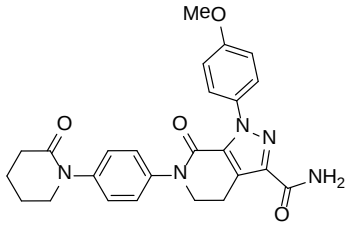
Hydroxychloroquine



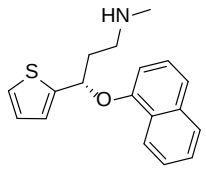
Remdesivir

Cell Research , volume 30, pages 269–271(2020); Int J Antimicrob Agents. (2020) *(in press)*

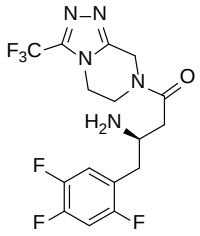
Some of The Best Selling Drugs



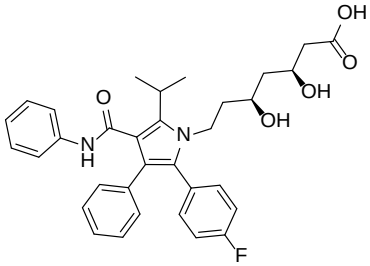
Eloquis (Apixaban)/
Cardiovascular disease



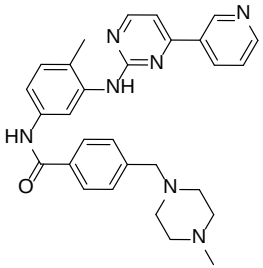
Cymbalta (Duloxetine)/
Neurological Disorder



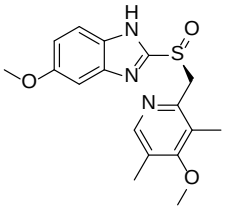
Januvia (Sitagliptin)/
Diabetes



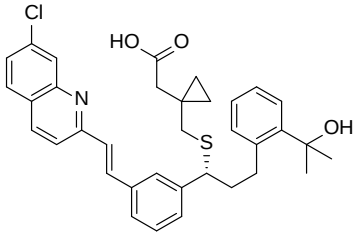
Lipitor (Atorvastatin)/
Cardiovascular disease



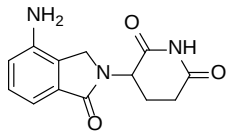
Gleevac (Imatinib)/
Cancer



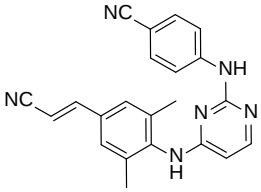
Nexium (Esomeprazole)/
Gastrointestinal disorder



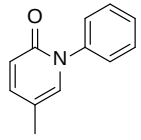
Singulair (Montelukast)/
Respiratory disorders



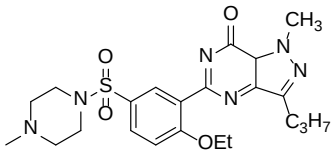
Revlimid (Lenalidomide)/
Oncology



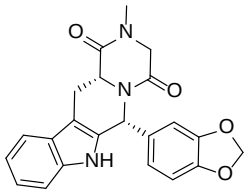
Edurant (Rilpivirine)/
Infectious Disease



Esbriet (Pirfenidone)
(Autoimmune disorder)



Viagra (Sildenafil)/
Sexual Health



Cialis (Tadaafil)/
Sexual Health

Role of Chemist in Drug Discovery

- *Identification of lead compounds*
- *Design and Synthesis of Novel Drug Molecules*
- *Isolation and Purification of Therapeutically important compounds from natural sources such as Plants.*
- *Characterization of compounds*
- *Development of efficient synthetic methodology*

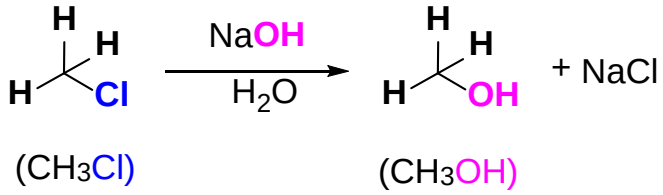
- ***But without the knowledge of different types of organic reactions, design of a synthetic pathway for achieving the synthesis of any organic compound is tough to imagine!***

Introduction to Different Types of Organic Reactions

➢ ***Substitution Reaction:*** *As the term 'Substitution' indicates that in this type of reactions, one group substitutes/replace another existing group.*

➢ *Characteristic reactions of saturated compounds such as alkanes and alkyl halides and of aromatic compounds (even though they are unsaturated).*

➢ *For example, chloromethane reacts with sodium hydroxide to produce methyl alcohol and sodium chloride (Scheme 1)*



Scheme 1: Example of Substitution Reaction

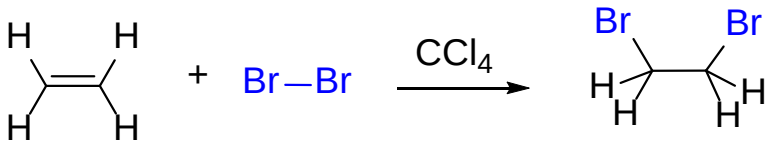
➢***Addition Reaction****:*

➢ *As the term 'Addition' indicates that in this type of reactions, reacting species adds together to become one.*

➢ *Characteristic of compounds with multiple bonds such as alkene, alkyne.*

Continued…

➢***Addition Reaction***: In an addition *all parts of the adding reagent appear in the product; two molecules become one:*

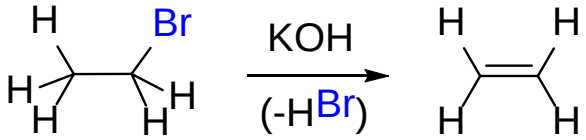


1,2-dibromoethane

Scheme 2: Addition of bromine to ethene (an example of addition reaction)

➢ *For example, Bromine is adding across the double bond of ethene to form 1,2-dibromoethane (Scheme 2).*

➢***Elimination Reaction***: *Eliminations are the opposite of additions. An example is dehydrohalogenation reaction (Scheme 3).*

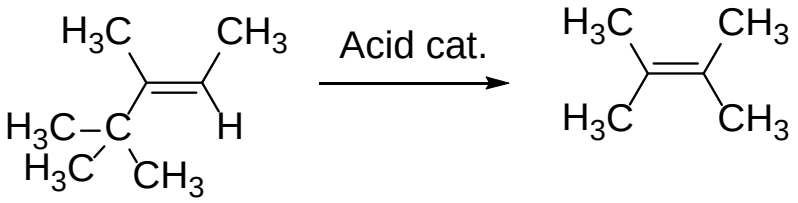


Scheme 3: Elimination reaction towards formation of alkene

➢ *In an elimination one molecule loses the elements of another small molecule.*

Rearrangement Reaction:

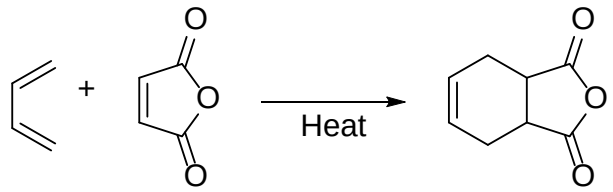
- *In a rearrangement a molecule undergoes* ***a reorganization of its constituent parts****.*
- *For example, heating the following alkene with a strong acid causes the formation of another isomeric alkene (Scheme 4)*



Scheme 4: Rearrangement of alkene to its isomer

Pericyclic Reaction:

- *Reaction in which electrons move round a circle and there are no positive or negative charges on any intermediates—indeed, there are no intermediates at all. This type of reaction is called pericyclic Reaction. Diels–Alder reaction (Scheme 5)* is one of such popular example.



Scheme 5: Example of pericyclic reaction (Diels–Alder reaction)

Substitution Reaction

- ***Substitution Reaction:*** *As the term 'Substitution' indicates that in this type of reactions, one group substitutes/replace another existing group.*

- *Broadly It could further be classified as: (Based on the nature of incoming group)*

(a) ***Nucleophilic Substitution Reaction****:*

- *Incoming* ***nucleophile*** *(meaning nucleus loving; the nucleo- part of the name comes from nucleus, the positive center of an atom) replaces the existing group (leaving group)*
- *A nucleophile is a Lewis base that seeks a positive center replaces the existing group.*

(b) Electrophilic Substitution: *Generally observed in case of aromatic compounds.*

- *Incoming* ***electrophile*** *(meaning electron loving) replaces the existing group (leaving group)*
- *Electrophiles are reagents that seek electrons so as to achieve a stable shell of electrons like that of a noble gas.*

References

- *Student may also consult following study materials and books:*

1. *Organic Chemistry, Publisher: John Wiley & Sons, Inc.; 10th edition; Authors: T. W. G. Solomons and C. B. Fryhle.*

2. *Organic Chemistry'; Publisher: Oxford University Press; 2nd edition; Authors: Jonathan Clayden , Nick Greeves , Stuart Warren.*

Rest of the topics of this unit will be discussed in next part of the lecture.

Stay Happy, Healthy and Safe!