



Review of Organic and Chemical Synthesis

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Abstract : After the discovery of penicillin by Alexander Fleming, antibiotics were regarded as wonder drugs for curing virtually all infections. However, the careless use and overconsumption of antibiotics in both human and veterinary medicine have led to the emergence of antibiotic-resistant bacterial strains. Of major concern is the development of antibiotic resistance in *Staphylococcus aureus*, primarily because *S. aureus* is frequently associated with hospital and community-acquired infections. Infections with multi-drug resistant *S. aureus* have become responsible for huge healthcare costs and are projected to be responsible for more deaths this year in the United States than HIV/AIDS. Despite this increasing problem of antibiotic resistance, the number of different antibiotics available is dwindling and there are only a handful of new antibiotics in the drug development pipeline. Therefore, there is an urgent need for new antibacterial drugs preferably with new modes of action to potentially avoid cross-resistance.

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Introduction : The antimicrobial potential of simple organic acids is well established in the literature viz. sorbic acid, cinnamic acid, anacardic acid, veratric acid, myristic acid, caprylic acid, anthranilic acid and dodecanoic acid. The literature reports reveal that the gallic acid and its derivatives possess wide spectrum of biological activities like antimicrobial, anticancer, antiviral, anti-inflammatory, analgesic and anti-HIV activities.

QSAR models are highly effective in describing the structural basis of biological activity. The success of QSAR approach can be explained by the insight offered into the structural determination of chemical properties and the possibility to estimate the properties of new chemical compounds without the need to synthesize and test them.

In light of abovementioned facts and in continuation of our research efforts in the field of synthesis, antimicrobial evaluation and QSAR studies, we hereby report the synthesis, antimicrobial evaluation and QSAR studies of gallic acid derivatives.

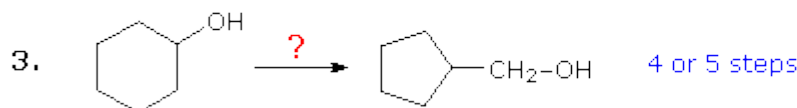
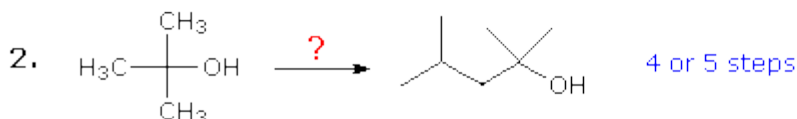
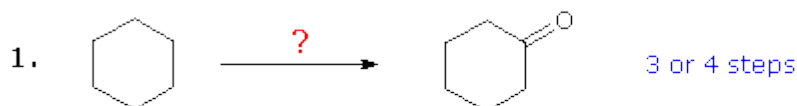
Organic Synthesis:

The study of organic chemistry exposes a student to a wide range of interrelated reactions. Alkenes, for example, may be converted to structurally similar alkanes, alcohols, alkyl halides, epoxides, glycols and boranes; cleaved to smaller aldehydes, ketones and carboxylic acids; and enlarged by carbocation and radical additions as well as cycloadditions. All of these products may be transformed subsequently to a host of new compounds incorporating a wide variety of functional groups, and thereby open to even further elaboration. Consequently, the logical conception of a multistep synthesis for the construction of a designated compound from a specified starting material becomes one of the most challenging problems that may be posed.



A one or two step sequence of simple reactions is not that difficult to deduce. If, for example, one is asked to prepare meso-3,4-hexanediol from 3-hexyne, most students realize it will be necessary to reduce the alkyne to cis or trans-3-hexene before undertaking glycol formation. Permanganate or osmium tetroxide hydroxylation of cis-3-hexene would form the desired meso isomer. From trans-3-hexene it would be necessary to first epoxidize the alkene with a peracid, followed by ring opening with hydroxide ion. This example illustrates a common feature in synthesis: often there is more than one effective procedure that leads to the desired product.

The three examples shown below are illustrative. The first is a simple functional group conversion problem, that may initially seem difficult. It is often helpful to work such problems backwards, starting from the product. In this case it should be apparent that cyclohexanol may be substituted for cyclohexanone, since the latter could then be made by a simple oxidation. Also, since cyclohexane (and alkanes in general) is relatively unreactive, bromination (or chlorination) would seem to be an obvious first step. At this point one is tempted to convert bromocyclohexane to cyclohexanol by an S_N2 reaction with hydroxide ion. This reaction would undoubtedly be accompanied by $E2$ elimination, so it would be cleaner, although one step longer, to first make cyclohexene and then hydrate it by any of several methods (e.g. oxymercuration and hydroboration) including the one shown by clicking on the diagram.



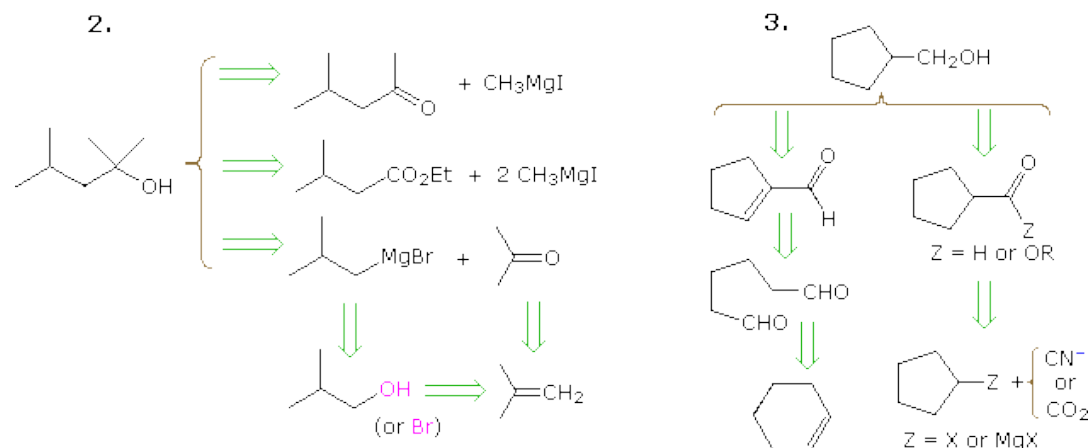
Plausible solutions for the second and third problem will also appear above at this point. In problem 2 the desired product has seven carbon atoms and the starting material has four. Clearly, two intermediates derived from the starting compound must be joined together, and one carbon must be lost, either before or after this bonding takes place. The 3° -alcohol function in the product suggests formation by a Grignard addition to a ketone, and isobutene appears to be a good precursor to each of these reactants, as shown. The reactant and product compounds in the third problem are isomers, but some kind of bond-breaking and bond-making sequence is clearly necessary for this structural change to occur. One possible procedure is shown above. Acid-catalyzed rearrangement of cyclohexene oxide, followed by reduction might also serve.

The useful approach of working out syntheses starting from the target molecule and working backward toward simpler starting materials has been formalized by Prof. E. J. Corey (Harvard) and termed



retrosynthetic analysis. In this procedure the target molecule is transformed progressively into simpler structures by disconnecting selected carbon-carbon bonds. These disconnections rest on transforms, which are the reverse of plausible synthetic constructions. Each simpler structure, so generated, becomes the starting point for further disconnections, leading to a branched set of interrelated intermediates. A retrosynthetic transform is depicted by the \Rightarrow symbol, as shown below for previous examples 2 & 3. Once a complete analysis has been conducted, the desired synthesis may be carried out by application of the reactions underlying the transforms.

Examples of Retrosynthetic Analysis

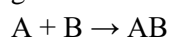


The above diagram does not provide a complete set of transforms for these target compounds. When a starting material is specified, as in the above problems, the proposed pathways must reflect that constraint. Thus the 4-methyl-2-pentanone and 3-methylbutyrate ester options in example 2, while entirely reasonable, do not fit well with a tert-butanol start. Likewise, a cyclopentyl intermediate might provide an excellent route to the product in example 3, but does not meet the specified conditions of the problem.

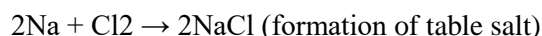
Organic synthesis is a special branch of chemical synthesis dealing with the synthesis of organic compounds. In the total synthesis of a complex product it may take multiple steps to synthesize the product of interest, and inordinate amounts of time. Skill in organic synthesis is prized among chemists and the synthesis of exceptionally valuable or difficult compounds has won chemists such as Robert Burns Woodward the Nobel Prize for Chemistry. If a chemical synthesis starts from basic laboratory compounds and yields something new, it is a purely synthetic process. If it starts from a product isolated from plants or animals and then proceeds to new compounds, the synthesis is described as a semi synthetic process.

Narrow definition

The other meaning of chemical synthesis is narrow and restricted to a specific kind of chemical reaction, a direct combination reaction, in which two or more reactants combine to form a single product. The general form of a direct combination reaction is:



where A and B are elements or compounds, and AB is a compound consisting of A and B. Examples of combination reactions include:





$S + O_2 \rightarrow SO_2$ (formation of sulfur dioxide)

$4Fe + 3O_2 \rightarrow 2Fe_2O_3$ (iron rusting)

$CO_2 + H_2O \rightarrow H_2CO_3$ (carbon dioxide dissolving and reacting with water to form carbonic acid)

4 special synthesis rules:

metal-oxide + $H_2O \rightarrow$ metal(OH)

non-metal-oxide + $H_2O \rightarrow$ oxo-acid

metal-chloride + $O_2 \rightarrow$ metal-chlorate

metal-oxide + $CO_2 \rightarrow$ metal carbonate (CO_3)

Chemical synthesis:

Chemical synthesis is a purposeful execution of chemical reactions to obtain a product, or several products.^[1] This happens by physical and chemical manipulations usually involving one or more reactions. In modern laboratory usage, this tends to imply that the process is reproducible, reliable, and established to work in multiple laboratories.

A chemical synthesis begins by selection of compounds that are known as reagents or reactants. Various reaction types can be applied to these to synthesize the product, or an intermediate product. This requires mixing the compounds in a reaction vessel such as a chemical reactor or a simple round-bottom flask. Many reactions require some form of work-up procedure before the final product is isolated.

The amount of product in a chemical synthesis is the reaction yield. Typically, chemical yields are expressed as a weight in grams (in a laboratory setting) or as a percentage of the total theoretical quantity of product that could be produced. A side reaction is an unwanted chemical reaction taking place that diminishes the yield of the desired product.

In science, when working with chemicals we call this process chemical synthesis. Chemical synthesis involves the combination of two or more atoms (or molecules) to make a product. Given the number of different ways to combine these atoms (or molecules), there are an endless variety of chemical compounds that can be synthesized.

Chemical synthesis is a very useful technique. For example, a scientist studying biology can make a compound that targets nasty cancer cells. Or a chemical scientist may create a compound to understand how it behaves in nature or under certain conditions.

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