Covalent addition of oxygen, sulphur, nitrogen and phosphorus bases to the activated aromatics and hetero aromatics has been investigated by a number of workers and their work has been thoroughly reviewed.\(^{10,11,16,17}\) However carbon-bonded sigma complexes derived from the carbanions of carbonyl derivatives,\(^{27}\) cyanide ions,\(^{26}\) imidazolide ions,\(^{136}\) amidines,\(^{137}\) enamines\(^{138}\) and a number of organometallic\(^{139-141}\) compounds have been proved efficient because of their amazing stability. Many of such carbanionic sigma complexes and bicyclic adducts prepared in our laboratories have been screened for various biological activities such as antimicrobial activity, anticonvulsant activity and antiseptic activity and proved inactive. The thirst in preparing the biologically active carbanionic sigma complexes, bicyclic adducts and donor-acceptor adducts of nitro aromatics prompted the present investigation to synthesize some new biologically active molecules of good potency and efficacy. As pyrimidine-2,4,6(1H,3H,5H)-trione (barbituric acid) has an active methylene group like \(\beta\)-diketones and \(\beta\)-ketoesters, it is expected to form sigma complexes with electron-deficient nitro aromatics.

Barbituric acid derivatives (barbiturates) are drugs that act as sedative-hypnotic agents. The short acting barbiturates such as thiopental are used as intravenous anaesthetics. The long acting barbiturates such as phenobarbital are anticonvulsant agents. They are used for the suppression of anxiety, induction of sleep and control of seizures.\(^{142-148}\) Epilepsy is a life threatening disorder. About 20-40 million people of the world population are affected by epilepsy. It is more common in children than adults. About 8 per 1000 children under the age of seven years are prone to this dreadful disorder. Prolonged fever in childhood often leads to seizure. Head injuries, stroke and other disease of blood vessels, brain tumor, brain infection, sudden external shock and electrical shock are the important causes of seizure. In the neonatal period, most of the women are likely to get seizure. It is also genetic in origin in some cases. Next to stroke, epilepsy is the second most common
neurological disorder.\(^{149}\) The generalized tonic-clonic epilepticus requires immediate cardiovascular, respiratory, and metabolic management along with antiepileptic drugs. Intravenous phenobarbital (20 mg/kg in adults) is effective in this treatment. Phenobarbital was introduced in 1912. Significant progress was made both in the development of experimental models and in methods for screening and testing of new antiepileptic drugs in the period 1935 to 1960. Thirteen new antiepileptic drugs were developed during this period, but in the last fifty years relatively a few new antiepileptic drugs have been developed. Only a limited number of conventional drugs such as carbamazepine, phenobarbital, phenytoin, primidone and valproate are mainly available for tonic-clonic seizure (grand mal type)\(^{149-151}\). Many of the marketed anticonvulsant drugs have profound side effects.\(^{152-156}\) Hence it is necessary to search for safer and more effective new antiepileptic drugs. This necessitates the present work to synthesize new barbiturates which have anticonvulsant/hypnotic activity (Chapter IV).

The study of substances with high antimicrobial activities is an important area of research in recent years. The major problem associated with the chemical substances as antimicrobial agents is their toxicity not only to the microbial cells but also to the host cells. Certain bacteria and fungi develop drug-resistance on prolonged application of the drug ineffective, so, it becomes essential for the scientists to be in constant search for new antimicrobial agents. This necessitates us to screen the new molecules of the present study towards bacterial and fungal pathogens (Chapter V, VI & VII).

In recent years, nitro compounds have attracted researchers because of their utility in pharmaceutical, agrochemical and fine chemical industries. In the present work, several interesting phenomena have been observed upon mixing 1-chloro-2,4-dinitrobenzene, alkyl 3-oxobutanoates (alkyl group: ethyl, methyl and tert-butyl) and triethylamine, which led to the formation of potent compounds with four nitro groups through carbanionic sigma complex intermediates. Many nitro aromatic molecules are high energy materials to be used as explosives.\(^{157}\) The interest in developing better insensitive high energy density materials (IHEDMS) to be used in explosives,
propellants and pyrotechnics is growing steadily. \textsuperscript{158-165} At present there is a strong requirement for explosives having good thermal stability, impact insensitivity and explosive performance. Emphasis has also been made on cost-effectiveness and eco-friendliness during the synthesis of explosives. \textsuperscript{166-168} As the molecules obtained have four nitro groups and high density (~1.5 g/cm\textsuperscript{3}) their thermal properties have also been examined in the present work (Chapter V).

As phenols and their derivatives are expected to be good antiseptic agents, in the present investigation, the donor-acceptor adducts of 2,4,6-trinitro-1,3-benzenediol (styphnic acid) are examined for their wound healing behaviour. Picric acid always form 1:1 donor-acceptor adducts with amines, as it has only one OH group. In picric acid-aromatic amine adducts, the main stabilizing factor is the proton transfer from OH of nitro compound to the nitrogen atom of the amine. \textsuperscript{114} Unlike picric acid, styphnic acid contains two phenolic OH groups and hence the type of adduct formation with amines and the mode of interaction are to be envisaged. This necessitates us to synthesize and characterize some new adducts of styphnic acid and amines (Chapter VII).

To ascertain the structure deduced from the spectral data, single crystal X-ray analysis has been undertaken on the isolated molecules. X-ray diffraction study throws light on bond angles, bond length and specific/non-specific interactions. Specific and non-specific interactions are responsible for majority of the drug-target interactions which occur in living systems. \textsuperscript{148} These data serve as basis to design drug against diseases. X-ray studies also enlighten the conformation of ring structures. Conformational isomerism, present in almost all commercially available pharmaceuticals as well as compounds under clinical and pre-clinical evaluation, plays a key role in the activity of drug molecules. \textsuperscript{142, 169, 170} As an understanding of the concepts such as preferred conformations, active conformation, advantages and disadvantages of conformational restriction and strategies to develop conformationally restricted analogs is crucial to the chemical design of new compounds, conformation of the two rings present in the biologically active bicyclic adducts has been examined through X-ray diffraction analysis (Chapter VI).