Annexure – IX

UNIVERSITY GRANTS COMMISSION
BAHADUR SHAH ZAFAR MARG
NEW DELHI – 110 002

PROFORMA FOR SUBMISSION OF INFORMATION AT THE TIME OF SENDING THE FINAL REPORT OF THE WORK DONE ON THE PROJECT

1. **Title of the Project:**

   STUDIES OF NOVEL ORGANOSILICON COMPLEXES

2. **NAME AND ADDRESS OF THE PRINCIPAL INVESTIGATOR:**

   Name: Dr. Gurjaspreet Singh
   Office: Department of Chemistry
   Panjab University
   Chandigarh
   Residential: E_1 / 102
   Sector 14, Panjab University
   Chandigarh

3. **NAME AND ADDRESS OF THE INSTITUTION:**

   Department of Chemistry
   Panjab University
   Chandigarh

4. **UGC APPROVAL LETTER NO. AND DATE:**

   UGC Ref. No.F.. 43-213/2014(SR)

   8 September 2015

5. **DATE OF IMPLEMENTATION:**

   1 July, 2015

6. **TENURE OF THE PROJECT:**

   Three years (01/07/2015 to 30/06/2018)

7. **TOTAL GRANT ALLOCATED:**

Rs 888600/-

8. TOTAL GRANT RECEIVED:

Rs 660170/-

9. FINAL EXPENDITURE:

Rs 652260/-

10. TITLE OF THE PROJECT:

Studies of novel organosilicon complexes

11. OBJECTIVES OF THE PROJECT:

(i) To prepare new organosilanes.

(ii) To synthesize a series of new silatranes/ higher coordinated organosilicon compounds.

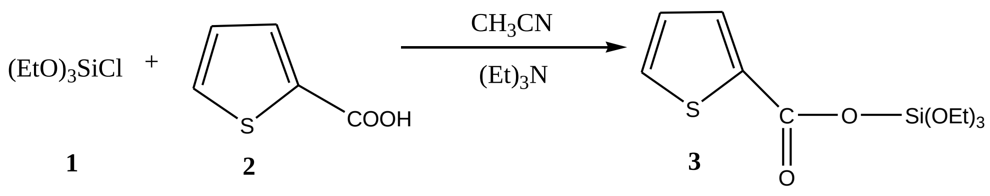
(iii) To characterize the synthesized new higher coordinated organosilicon complexes/silatranes by various spectroscopic techniques.

12. WHETHER OBJECTIVES WERE ACHIEVED

The project has been completed with all the objectives being successfully achieved. The main aim of this project was to obtain various organosilanes and silatranes/ higher coordinated organosilicon complexes. This was done using the methodology outlined in the following schemes.

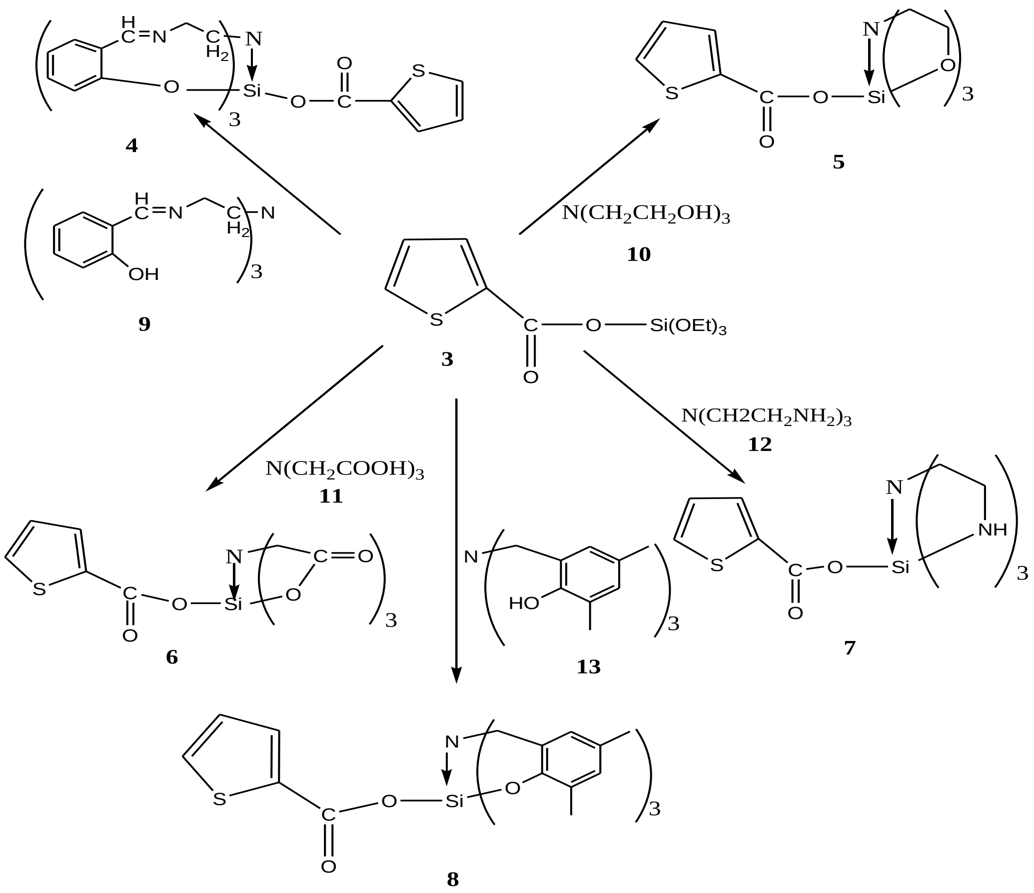
Scheme I.

The synthesis of organosilane (3) was done by refluxing thiophene carboxylic acid (2) with silane (1) using triethylamine as base.



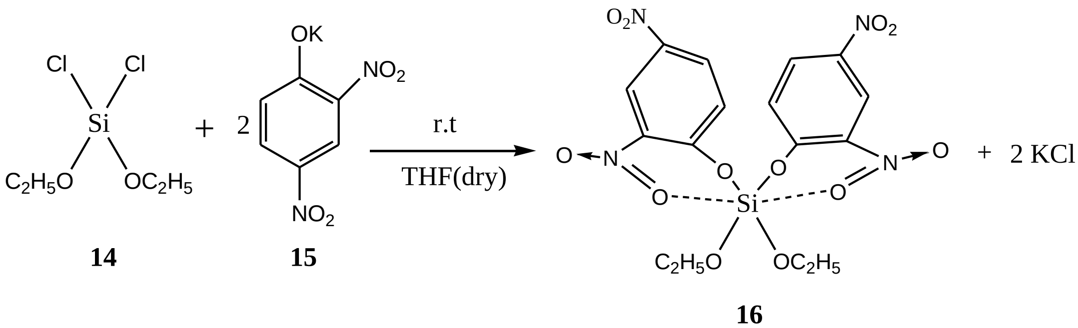
Scheme II.

In order to study the reactivity of silane **(3)**, different tripodal ligands were employed to synthesize hypervalent complexes **(4-8)**.



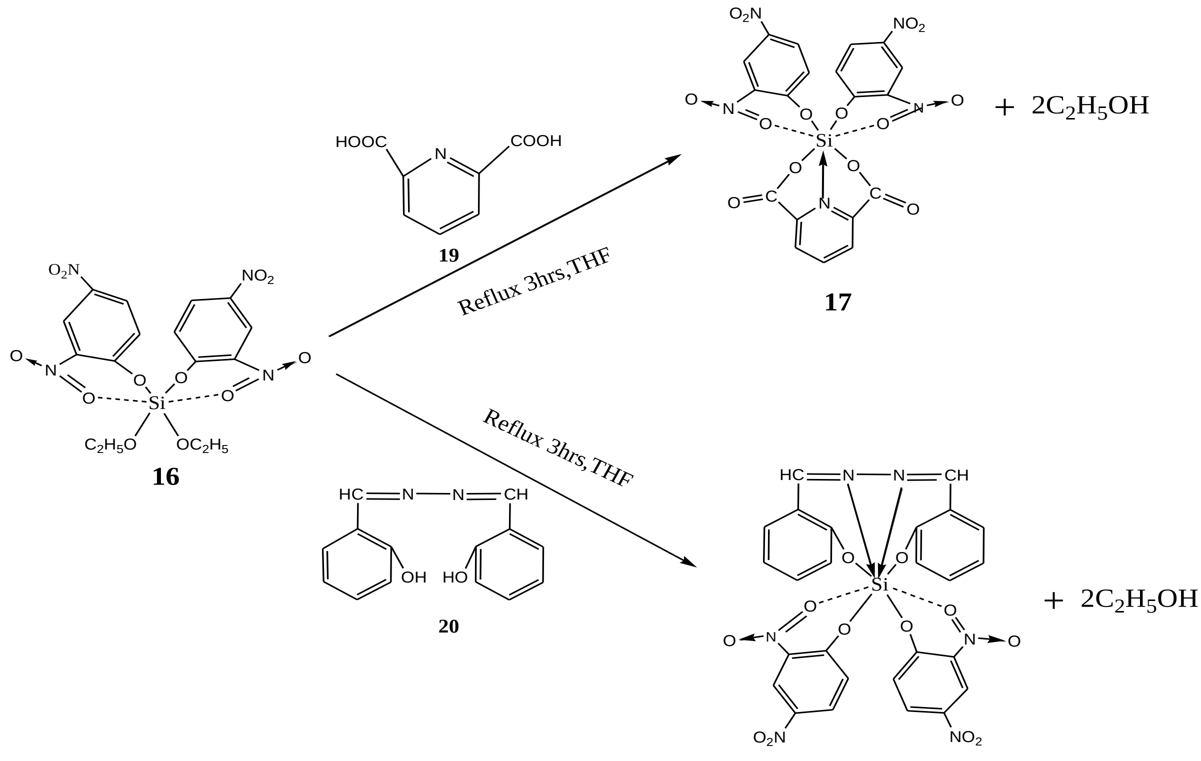
Scheme III.

The hypervalent complex of silicon **16** was synthesized by the reaction of diethoxydichlorosilane with 2, 4-dinitrophenol as depicted below.



Scheme IV

The reactivity of **16** was studied with dipicolinic acid and schiff's base of hydrazine and salicylaldehyde to form compounds **17** and **18** as shown below:



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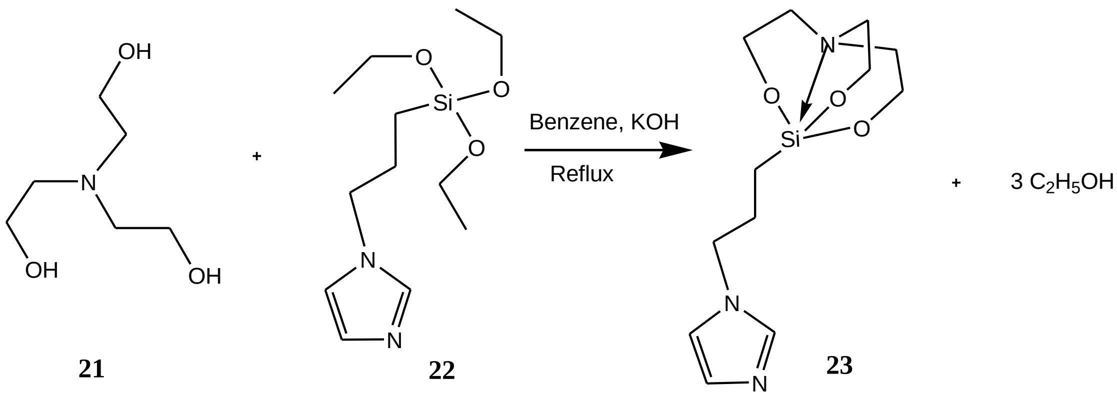
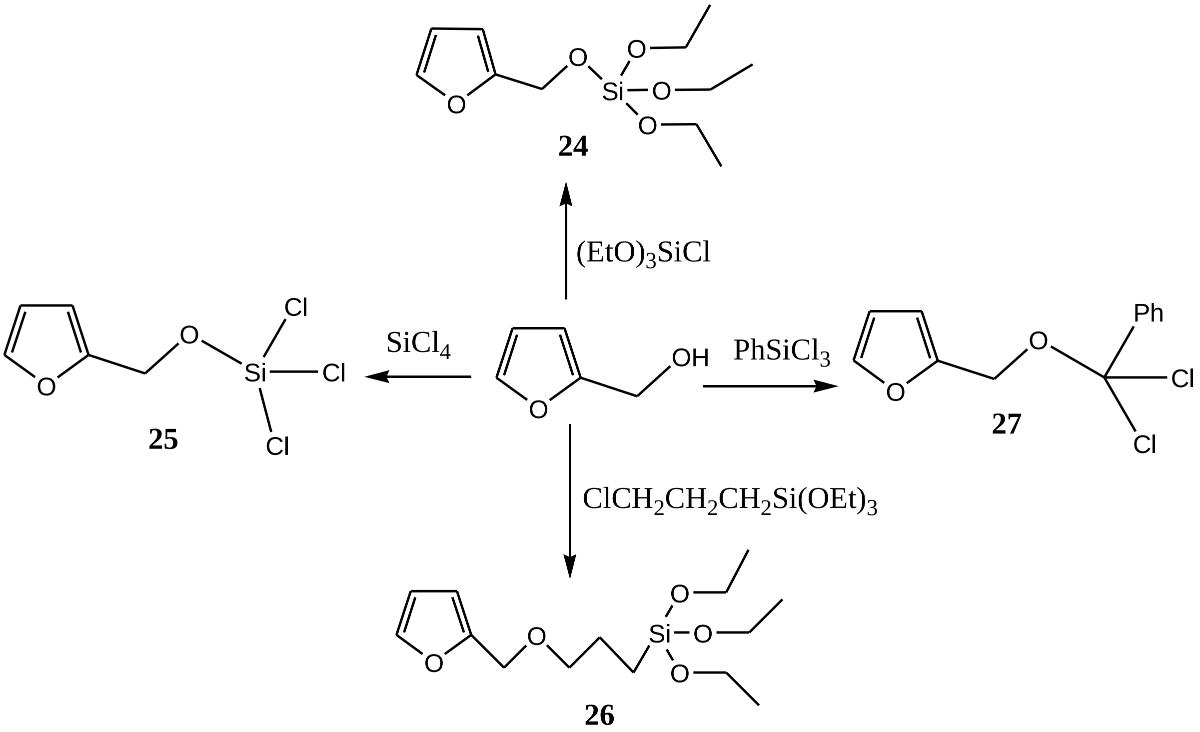
Scheme V

The formation of silatrane **23** was achieved by following the reaction pathway as below:



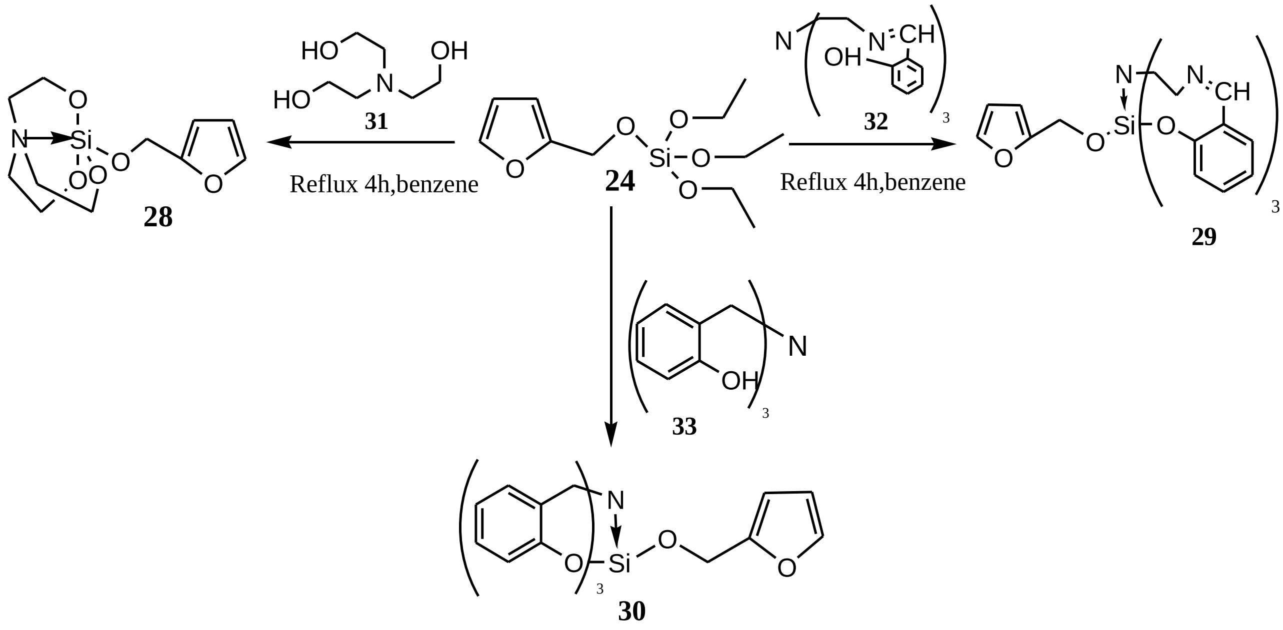
Scheme VI

Furfurylsilanes **24-27** were prepared by the reaction of 2-furancarbinol with silanes respectively as shown below:



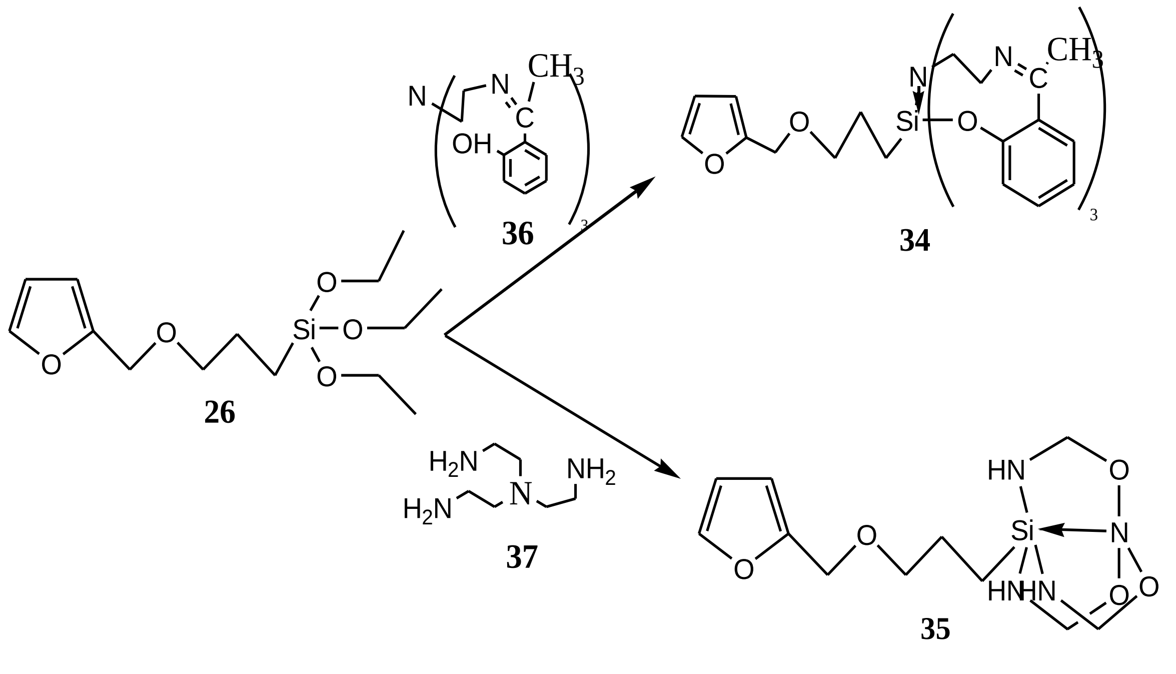
Scheme VII

Silatranes **28-30** were obtained by the transesterifications of silane **24** with tripodal ligands **31-33** respectively as depicted below:



Scheme VIII

Similarly, silane **26** was subjected to reaction with tripodal ligands **36** and **37** to obtain silatranes **34** and **35** as drafted in below.



13. ACHIEVEMENTS FROM THE PROJECT:

The project resulted in 25 international publications in high-impact refereed journals with impact factor up to 5.667. Besides this, five PhD students have been successfully awarded degrees for the work carried out in this project. In particular, the presence of hydrogen bond acceptor groups like nitrogen and oxygen can have utmost importance in supramolecular chemistry.

14. SUMMARY OF THE FINDINGS:

In this project, some novel organosilicon complexes have been synthesized. Organosilicon complexes attract interest from both the structural and reactivity point of view. Studies on organosilicon derivatives made a valuable contribution in diverse range of biological activities, this includes pilotropic, antiviral, anti-inflammatory, antienzymatic, antitumour, antibacterial, antifungal activities, and burns healing effects. In recent years a number of authors evinced interest in organosilicon derivatives of the nitrogen-heterocycles which came into use as synthons in organic chemistry for the properties of biological active compounds. The introduction of an organosilicon substituent's containing hypervalent silicon atom into nitrogen heterocycles molecule changes considerably their electronic structure and reactivity. The modifications of heterocyclic compounds give rise to new classes of biological active products promising for medicine and agriculture.

Nitrogen heterocycles in organosilicon complexes have a long history and remain a front-runner for bioactive applications. The imidazole ring is ubiquitous in nature and plays a critical role in many structures within the human body, notably as histamine and histidine. The presence of a donor pyridine-like nitrogen atom within the ring, capable of selective binding cationic species also converts the imidazole derivatives into excellent metal ion sensors. The polar imidazole ring suggests a plethora of emerging material science and biophysical applications. The organosilicon complexes containing imidazole moiety are scarce and so synthesis of organosilicon complexes possessing this moiety have been done.

Thiophene moiety is found in cephalothin antibiotics. It is also used as an important solvent and chemical intermediate. The sulphur atom in thiophene is unreactive but the adjacent carbon atoms are susceptible to attack by electrophiles. It is more reactive then benzene towards electrophilic substitution reactions. One of the thiophene derivatives, that is thiophene-2-carboxylic acid, is reported as potent inhibitor of HCV NSSB polymerase and is used for HCV subgenomic RNA replication. Particularly interesting in this aspect of thiophene derivatives is the synthesis of thiophene-containing metalated species, considering that thiophene-based materials are a very important class of organic materials because of their biological, electronic, magnetic and optical properties. The combination of thiophene moieties with metal units could lead to a promising family of complexes with potential in all of the aforementioned areas of chemistry and material science (solar cells, anticancer activity, electron shuttles, etc.). These derivatives are also being used in manufacturing dyes, aroma compounds and pharmaceuticals. They are also used as monomers to make condensation polymers. For these reasons, we have studied organosilicon complexes of thiophene-based compounds.

15. CONTRIBUTION TO THE SOCIETY:

The outcome of this project is quite relevant to our society. The project was about synthesis of some novel organosilicon complexes which can be used in the numerous fields of supramolecular chemistry such as sensing, drug delivery, etc.

16. WHETHER ANY PH.D. ENROLLED/PRODUCED OUT OF THE PROJECT: 5

17. NO. OF PUBLICATIONS OUT OF THE PROJECT: 25 Published and 2 communicated. Following is the list of published and communicated papers:

1. **Gurjaspreet Singh**, Aanchal Arora, Sunita Rani, Indresh Kumar Maurya, Darpandeep Aulakh, Mario Wriedt.; Heteroarylchalcone allied triazole conjugated organosilatranes: synthesis, spectral analysis,antimicrobial screening, photophysical and theoretical investigations **RSC Adv., 2016, 6, 82057–82081.**
2. **Gurjaspeet Singh,** Sunita Rani, Amandeep Saroa, Aanchal Arora.; Organo-functionalizedtrimethoxysilanes featuring thioesterlinkage:Synthetic and UV-Vis spectral investigations **J. Organomet.Chem.,2016 ,808 , 1-11**.
3. **Gurjaspreet Singh ,** Amandeep Saroa, Sunita Rani, Promila, Sheenam Girdhar, Subash C Sahoo, D. Choquesillo-Lazarte.; Substituted phenyl urea and thioureasilatranes: Synthesis,characterization and anion recognition properties by photophysicaland theoretical studies., **Polyhedron., 2016,112 ,51–60**
4. **Gurjaspreet Singh**, Sunita Rani.; Organosilatranes with Acylthiourea Derivatives – Metal-Ion Binding, Substituent-Dependent Sensitivity, and Prospects forthe Fabrication of Magnetic Hybrids., **Eur. J. Inorg. Chem. 2016, 3000–3011 DOI: 10.1002/ejic.201600204**
5. **Gurjaspreet Singh**, Sunita Rani, Aanchal Arora, Darpandeep Aulakh, Mario Wriedt., Thioester-appended organosilatranes: synthetic investigations and application in the modification of magnetic silica surfaces., ***New J. Chem.*, 2016, 40, 6200—6213**
6. **Gurjaspreet Singh,** Akshpreet Singh, Jasbhinder Singh, Darpandeep Aulakh, Mario Wriedt, Cristo´bal Espinosa, M. Angeles Esteban, Rakesh Sehgal, Kapil Goyal and Shweta Sinha, First synthesis of pyrene-functionalized silatranes for mechanistic insights into their potential anti-parasitic and anti-oxidation activities. ***New J. Chem.*, 2017, 41, 15165- 15172.**
7. **Gurjaspreet Singh,** Aanchal Arora, Sunita Rani, Pooja Kalra, Darpandeep Aulakh and Mario Wriedt, A family of silatrane-armed triazole-encapped salicylaldehyde-derived Schiff bases: Synthesis, spectral analysis, and antimicrobial and quantum chemical evaluation**; Applied Organometallic Chemistry 2017**, **31, 3728.**
8. **Gurjaspreet Singh,** Satinderpal singh, Hemant Sharma, Jandeep Singh and Narinder Singh: Design and Synthesis of Novel Fluorescent Phthalimide Based Silatranes: Ratiometric Estimation of Mg2+ Ion**. Asian journal of Chemistry, 2017, 29,2074-2078.**
9. **Gurjaspreet Singh**, Aanchal Arora, Sunita Rani, Pooja kalra and Manoj kumar: A

Click generated triethoxysilane tethered ferrocene-chalcone-triazole triad for selective and colorimetric detection of Cu2+ ions. **Chemistry Select 2017, 2, 3637 -3647.**

10. **Gurjaspreet Singh**, Sunita Rani, Aanchal Arora, Sanchita, D. Mehta. Organic-inorganic nano-hybrid decorated by copper (II) incarceration: A versatile catalytic assembly for the swift reduction of aromatic nitro and dye compounds. **Molecular Catalysis. 2017, 431, 15-26**.
11. **Gurjaspreet Singh ,** Amandeep Saroa, Rupinder Tewari, Parvinder Kaur ; Aza-Michael Addition of γ -Aminopropylsilatranes to Substituted N-Phenylmaleimides: Design and Synthesis of a Heterocyclic Amine Receptor and Their Preliminary Antimicrobial Studies : **Silicon 2017, 9, 495–501.**
12. **Gurjaspreet Singh, Sunita Rani**; A proficient magnetic nano-platform with covalently assembled methyl red indicator for the dual recognition of pH and Hg2+, **Sensors and Actuators B: Chemical. 2017, 244, 861-875.**
13. **Gurjaspreet Singh,** Amandeep Saroa, Sunita Rani, Promila, Subash Sahoo and Duane Choquesillo-Lazarte : Unsymmetrical urea silatranes: Synthesis, characterization and a selective on-off fluorescence response to acetate anion" has been accepted for publication in **Arabian Journal of Chemistry, 2017, 10,523-531**
14. **Gurjaspreet Singh**, Amandeep Saroa, Sheenam Girdhar, Promila: Synthesis and thermal decomposition studies of silicon (IV)compounds with N,N'bis salicylidene) Ethylenediimine **Silicon, 2017, 9, 159-163.**
15. **Gurjaspreet Singh,** Jasbhinder Singh, Akshpreet Singh, Jandeep Singh, Manoj Kumar, Kshitiz Gupta and Sanjay Chhibber. Synthesis, characterization and antibacterial studies of schiff based 1,2,3-triazole bridged silatranes. **Journal of Organometallic Chemistry 2018, 871, 21-27**.
16. **Gurjaspreet Singh,** Akshpreet Singh, Pinky Satija and Kavita Chowdhary. The first report of the synthesis of organo-functionalized triethoxysilanes via a Knoevenagel condensation approach. **New J. Chem. 2018, 42, 12467**.
17. **Gurjaspreet Singh,** Jasbhinder Singh, Jandeep Singh, Akshpreet Singh, Kshitiz Gupta, Sanjay Chhibber and Vikas Verma. Schiff Based Silatranyl Compounds Exhibiting 'Fe3+ and Mn2+ Fluorescence Dual Ion Sensing and Antibacterial Activity'. **Silicon, 2018, doi.org/10.1007/s12633-018-9822-3.**
18. **Gurjaspreet Singh,** Geetika Sharma, Pooja Kalra, Sanchita, Vikas Verma, V. Ferretti, Synthesis and Structural Characterization of first Adenine containing Organosilicon Nucleobase for the recognition of Cu2+ ion. **Inorganica Chimica**

Acta, 2018, 479, 74-82.

19. **Gurjaspreet Singh,** Geetika Sharma, Sanchita, Pooja Kalra, Daizy Rani Batish and Vikas Verma. Role of Alkyl Silatranes as Plant Growth Regulators: Comparative Substitution effect on Root and Shoot Development of Wheat and Maize. **Journal of the Science of Food and Agriculture, 2018, doi: 10.1002/jsfa.9052**
20. **Gurjaspreet Singh,** Shally Girdhar, Akshpreet Singh, Amandeep Saroa, Jaspreet Singh Lakhi, Sadhika Khullar, and Sanjay K. Mandal, Selective mercury ion recognition using methyl red (MR) based silatrane sensor. **New Journal of Chemistry, 2018, 42, 6315-6321.**
21. **Gurjaspreet Singh,** Sanchita, Sunita Rani, Geetika Sharma, Pooja Kalra, Coumarin–derived Organosilatranes: Functionalization at magnetic silica surface and selective recognition of Hg2+ ion, **Sensors and Actuators B. 2018, 266, 861-872**
22. **Gurjaspreet Singh**, Kavita Chowdhary, Pinky Satija, Akshpreet Singh, Baljinder Singh, Kashmir Singh, Cristo´bal Espinosa, M. Angeles Esteban, Rakesh Sehgal, Vikas Verma, Synthesis and Immobilization of Benzothiazole-Appended Triazole-Silane: Biological Evaluation and Molecular Docking Approach. **Chemistry Select, 2018, 3, 1609– 1614.**
23. **Gurjaspreet Singh,** Pooja Kalra , Aanchal Arora , Sanchita , Geetika Sharma , Akshpreet Singh , Vikas Verma, Design and synthesis of indole triazole pendant siloxy framework as a chemo sensor for sensing of Cu2+ and Ni2+: A comparison between traditional and microwave method, **Inorganica Chimica Acta , 2018, 473 , 186–193**
24. **Gurjaspreet Singh,** Aanchal Arora, Akshpreet Singh, Pooja Kalra, Sunita Rani, Kashmir Singh, Indresh K. Maurya, and Rahul S. Mandal**.** Molecular Design, Synthesis,Computational Screening, Antimicrobial Evaluation and Molecular Docking Study of Acetylinic Isatin Hybrids, **Chemistry Select 2018, 3, 1942– 1952.**
25. **Gurjaspreet Singh,** Pooja Kalra, Aanchal Arora, Akshpreet Singh, Geetika Sharma, Sanchita, Indresh Kumar Maurya, Sanjay Dutta, Parthapratim Munshi, Vikas Verma, Acetylenic Indole-Encapsulated Schiff Bases: Synthesis, In Silico Studies as Potent Antimicrobial Agents, Cytotoxic Evaluation and Synergistic Effects, **Chemistry Select 2018, 3, 2366– 2375.**

(PRINCIPAL INVESTIGATOR) **(REGISTRAR/PRINCIPAL)**