



1. **Name of Faculty Member** : Dr. Kamal Nain Singh
2. **Designation** : Professor
3. **Contact details :**

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4. **Area of specialization :** Synthetic and Mechanistic Organic Chemistry

5. **Awards / Honours / Fellowships:**

- Awarded J.R.F. by C.S.I.R. from 1988 -90.
- Awarded S.R.F. from 1991-93.

6. **List of best publications:**

1. Experimental and computational study of stereoselectivity and reactivity in Lewis acid promoted Lithiation of tertiary amines Kessar, S.V.; Singh, P.; **Singh, K.N.**; Venugopalan, P.; Kaur, A.; Bharatam, , P.V.; Sharma, A.K. *J. Amer. Chem. Soc.* **2007**, *129*, 4506-4507. (Impact factor 9.9)
2. A study of BF₃ promoted lithiation of aniline and DFT calculations on the role of lithium fluorine interaction. Kessar, S.V.; Singh, P.; **Singh, K.N.**; Venugopalan, P.; Kaur, A.; Bharatam, , P.V.; Sharma, A.K.; Lata S. *Angew. Chem. Int. Ed.* **2008**, *47*, 4703. (Impact factor 13.45).
3. Evaluation of antidepressant activity of 1-(7-methoxy-2- methyl)-1,2,3,4-tetrahydroisoquinoline 4-yl)-cyclohexanol, a β -substituted phenethyl amine in mice. Ashish Dhir,; Malik, S.; **Singh, K. N.**; Kessar, S. V. Kulkarni, S. K.

European Neuropsychopharmacology. **2010**, *21*, 705-714.

(Impact Factor 3.4).

4. C-1 Alkynylation of N-methyltetrahydroisoquinoline through CDC: A direct access to phenethylisoquinoline alkaloids. **Singh, K. N.**; Singh, P.; Singh, Paramjit.; Kaur, A. *SYNLETT* **2012**, *23*, 760-64 (Impact Factor 2.5).

5. Nucleophilic addition of β -amino carbanion to arynes: One pot synthesis of 4-aryl-N-methyl-1,2,3,4-tetrahydroisoquinolines. **Singh, K. N.**; Singh, P.; Singh, Paramjit.; Deol, Y.S. *Organic Letters* **2012**, *14*(9), 2202-2205. (Impact Factor 5.8).

6. Pyrrolidine based organocatalyst for efficient asymmetric Micheal addition of cyclic ketones to β - nitrostyrenes. **Singh, K. N.**; Singh, P.; Singh, Paramjit.; Sharma , S. *Bioorganic & Medicinal Chemistry Letters* **2012**, *22*, 4225. (Impact Factor 2.4).

7. (2*S*)-2-(Phenylsulfinylmethyl)pyrrolidine catalyzed efficient stereoselective Michael addition of cyclohexanone and cyclopentanone to nitroolefins, **Singh, K. N** ,* Paramjit Singh, Amarjit Kaur, Pushpinder Singh, Sandeep Kumar Sharma, Sadhika Khullar, Sanjay K. Mandal *Synthesis*, **2013**, *45*, 1406. (**Impact Factor 2.50**)

8. Cross dehydrogenative coupling of dithiolanes with ketones and indoles under metal free conditions, **Singh, K. N**, Paramjit Singh, Pushpinder Singh, Yogita Maheshwary, Satinder V. Kessar and Aanchal Batra *Synlett*, 2013, 1963 (**Impact Factor 2.71**)

9. Metal free oxidative C-Se coupling of formamides and diselenides using aqueous *tert*-butyl hydroperoxide Pushpinder Singh, Aanchal Batra, Paramjit Singh, Amarjit Kaur, and **Kamal Nain Singh** *Eur. J. Org. Chem* 2013, 7688, (**Impact Factor 2.5**)

7. Highlights of research work:

Many methods for α -elaboration of primary and secondary amines are reported in literature but for tertiary amines no procedure had been developed. In this context Lewis acid complexation of tertiary amines for α -activation was investigated and after considerable experimental work, Lewis acids activation methodology has been developed as a general and efficient procedure for α -elaboration of activated and non activated tertiary amines.

The Lewis acid promoted deprotonation of tertiary amines has been extended to cyclic and acyclic tertiary amines and also to the synthesis of large numbers of alkaloids including compounds of pharmacological interest like metazocine and dextrorphan. This methodology works well even in tertiary amines having a secondary alkyl group like N-ethyl piperidine. Rearrangements of Lewis acid complexes of N-allyl and N-benzyl tertiary amines have been used to provide a facile method for conversion of tertiary amines to secondary amines. Reaction of 3-alkoxy phthalide with α -azaanion provides a one pot synthesis of spirobenzylisoquinoline alkaloids and 1, 3-oxygenated cyclopentane unit present in a variety of natural products. Lewis acid promoted methodology provides a facile synthesis of quinuclidine carbinols known to possess antiviral and antiarrhythmic activity.

One pot procedure for synthesis 1-aryl and 4-aryl via coupling of α and γ -amino carbanion derived from N-methyl-1,2,3,4-tetrahydroisoquinoline and in situ generated benzyne has been developed.

Any other information:

Research projects) ongoing and completed

S. No.	Title of Project	Funding Agency	Period	Status
1.	Generation and synthetic applications of azacarbonions and azaallylic carbonions.	C.S.I.R. (5.2 Lacs)	1997-2000	Completed
2.	Synthesis of catalysts, medicinal agents and surfactants derived from azapolycyclo frame work.	C.S.I.R. (9.5 Lacs)	2003-2006	Completed
3.	Experimental and theoretical study of some heteroatom effects on generation and reactivity of carbonions and radical intermediates.	D.S.T. (18.6 Lacs)	2003-2006	Completed
4.	Development of stereoselective processes from Lewis acid complexes of tertiary amines	C.S.I.R. (13 Lacs)	2007-2010	Completed
5	Metallation of C-H bonds activated by heteroatom Lewis acid complexation	D.S.T. (20Lacs)	2008-2012	Completed
6	Nucleophilic addition of amino carbonions to in-situ generated benzyne; development of a one pot arylation procedure under metal free conditions for synthesis of isoquinoline alkaloids and related compounds. On going , CSIR (19 lacs)			

Supervision of Ph.D. dissertation:

S. No.	Name of scholar	Degree	Title of Dissertation	Present status
1	J. Singh	Ph.D	Design synthesis and haracterization of 2-picoly and methyl substituted 2-pyridyl chalcogen (Se, Te) compounds and their derivatives.	Awarded Ph.D. Degree in 2003
2	Rajiv Kapoor	Ph.D	Study of some heteroatom effects on generation and reactivity of carbanionic and radical intermeadiates.	Awarded Ph.D. Degree in 2006
3	Arvind Kumar	Ph.D	Study of selectivity in lithation reactions and its application in syntesis	Awarded Ph.D. Degree in 2008
4	Sneh Lata	Ph.D	Studies towards the synthesis of isoquinoline alkaloids through-α aza-carbanios	Awarded Ph.D. Degree in 2009
5	Pushpinder Singh	Ph.D	Selectivity in some new methodologies for synthetic elaboration at α-C-H centers of tertiary amines	Awarded Ph.D. Degree in 2013
6	Five students are working for their Ph.D degree			