Dr Vijai Kumar Rai

Assistant Professor
Department of Chemistry
Guru Ghasidas Vishwavidyalaya
(A Central University)
Bilaspur, C.G. – 495 009
INDIA

Email: vijaikrai@hotmail.com

Academic Experience

- **Assistant Professor** (Aug 2011 – Present) – GGV Bilaspur, C.G., India.
- **Assistant Professor** (Aug 2009 – Aug 2011) – SMVD University, Jammu, J&K, India.

Academic Qualification

- **Ph. D.** (Synthetic Organic Chemistry) from **University of Allahabad**, Allahabad, U.P. INDIA.
- **UGC-CSIR-NET** (Chemical Sciences) Exam qualified.
- **UGC-UP SLET** (Chemical Sciences) Exam qualified.
- **M.Sc.** (Organic Chemistry) from DDU Gorakhpur University, Gorakhpur, U.P. INDIA.

Fellowship Received

Junior Research Fellow	Worked as Junior Research Fellow (JRF) in the project entitled *"Microwave Enhanced Synthesis of New Nucleoside Antibiotics"* during research work.
Research Associate	I had been awarded Research Associateship by the *Council of Scientific & Industrial Research (CSIR), New Delhi, Govt. of India* in 2006 (Ref. No. 09/001/(0291)/ 2007/EMR-I).
Postdoctoral Fellow	I had been awarded Postdoctoral Fellowship from the Department of Chemistry, *University of Calgary, Canada* in 2009.

Awards Received

1.	Fast Track Young Scientist Award	4th March, 2011	DST, Government of India, New Delhi, INDIA
2.	Young Scientist Award	10th Feb., 2010	In Chemistry of 5th J K SCIENCE CONGRESS, INDIA
3.	Golden Jubilee Award	21st Nov., 2008	In Physical Sciences, *by* NATIONAL ACADEMY OF SCIENCES, INDIA
4.	Young Scientist Travel Fellowship Award	17th Sep., 2008	DST, Government of India, (ITS Scheme) New Delhi, INDIA
5.	D. R. Bhakuni Award	26th Dec., 2007	In Organic Chemistry, *by* INDIAN CHEMICAL SOCIETY, INDIA
6.	Young Scientist Award	5th Feb., 2007	In Chemical Science *by* INTERNATIONAL ACADEMY OF PHYSICAL SCIENCES, INDIA

Research Grants Received

I have been received ***Three Major Research Projects*** and their details are given as following:

1. Funding Agency: **University Grants Commission (UGC), New Delhi, India**
Ref No.: F. No. 39-764/2010 (SR)
Status: Ongoing/Started w.e.f. 1st Feb. 2011
Amount (approx): Rs. 6 Lacks
Title: *Access to potentially antiviral novel nucleosides using microwave methodology*

2. Funding Agency: **Council of Scientific & Industrial Research (CSIR), New Delhi, India**
Ref No.: No. 01 (2442)/10/(EMR-II)
Status: Ongoing/Started w.e.f. 31st March 2011
Amount (approx): Rs. 20 Lacks
Title: *Access to novel imino-/thiosugar scaffolds from renewable bioresources*

3. Funding Agency: **Department of Science & Technology (DST), New Delhi, India**
Ref No.: No. SR/FT/CS-99/2010
Status: Ongoing/Started w.e.f. 1st October, 2012
Amount (approx): Rs. 26 Lacks
Title: *NHC-/enamine-iminium catalysis in stereocontrolled construction of bioactive scaffolds*

Research Papers Published

Year	S. No.	Published Papers	Impact Factor
2013	1.	*Tetrahedron Lett.*, **2013**, *54*, 1071.	2.660
	2.	*Synlett* **2013**, *24*, 97.	2.838
	3.	*Nucleosides, Nucleotides & Nucleic acids*, **2013**, *32*, 247.	0.723
	4.	*Tetrahedron Lett.*, **2013**, *54*, 6479.	2.660
2012	5.	*Synthetic Commun.*, **2012**, *42*, 1489.	1.200
2011	6.	*Green Chem.* **2011**, *13*, 1217.	**6.820**
	7.	*Eur. J. Org Chem.*, **2011**, 4302.	3.192
	8.	*Tetrahedron Lett.*, **2011**, *52*, 125.	2.660
2010	9.	*Synthesis*, **2010** 4051.	2.572
	10.	*Synlett* **2010,** 2649.	2.838
	11.	*Synthesis* **2010**, 2957.	2.572
	12.	*Tetrahedron Lett.* **2010**, *51*, 1657.	2.660
	13.	*Synlett* **2010**, 240.	2.838
2009	14.	*J. Chem. Res.* **2009**, 520.	0.444
	15.	*Green Chem.* **2009**, *11*, 878	**6.820**
	16.	*Synlett*, **2009**, 1423.	2.838
	17.	*Tetrahedron Lett.*, **2009**, *50*, 2414.	2.660
	18.	*Tetrahedron Lett.*, **2009**, *50*, 2208.	2.660
	19.	*Tetrahedron*, **2009**, *65*, 1305.	3.269
2008	20.	*Nucleosides, Nucleotides & Nucleic acids*, **2008**, *27*, 1227.	0.723
	21.	*Tetrahedron Lett.*, **2008**, *49*, 5553.	2.660
	22.	*Synlett*, **2008**, 2257.	2.838
	23.	*J. Heterocyclic Chem.*, **2008**, *45*, 1315.	0.813
	24.	*Tetrahedron*, **2008,** *64*, 4246.	3.269
	25.	*Tetrahedron Lett.*, **2008**, *49*, 2377.	2.660

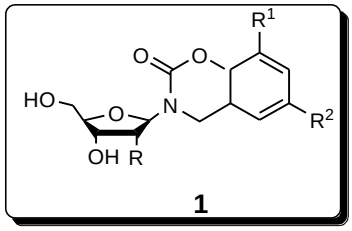
Year	S. No.	Published Papers	Impact Factor
	26.	*Tetrahedron*, **2008,** *64*, 1420.	3.269
	27.	*Synlett*, **2008**, 0529.	2.838
	28.	*Tetrahedron Lett.*, **2008**, *49*, 687.	2.660
2007	29.	*Synthesis*, **2007**, 3831.	2.572
	30.	*Synlett*, **2007**, 1905.	2.838
	31.	*Tetrahedron Lett.*, **2007**, *48*, 8037.	2.660
	32.	*Tetrahedron Lett.*, **2007**, *48*, 7793.	2.660
	33.	*Tetrahedron*, **2007,** *63*, 6924.	3.269
	34.	*Tetrahedron Lett.*, **2007**, *48*, 4899.	2.660
	35.	*Lett. Org. Chem.*, **2007,** *4*, 47.	1.200
	36.	*Synlett*, **2007**, 1227.	2.838
2006	37.	*Tetrahedron Lett.*, **2006**, *47*, 395.	2.660
	38.	*Synthesis*, **2006**, 1868.	2.572
	39.	*Green Chem.*, **2006**, *8*, 455.	**6.820**
	40.	*Tetrahedron*, **2006**, *62*, 5464.	3.269
	41.	*Tetrahedron*, **2006**, *62*, 8029.	3.269
2005	42.	*Tetrahedron*, **2005,** *61*, 10013.	3.269
2004	43.	*Tetrahedron Lett.*, **2004**, *45*, 5351.	2.660
		Aggregate Impact Factor	**121.87**
		Average Impact Factor	**2.83**
		h-index	**12**
		i10-index	**19**

Research Highlights

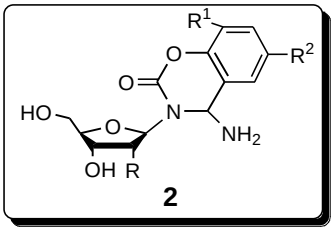
I have been working in the field of Synthetic Organic Chemistry since last over ten years. I have obtained D. Phil. degree from Dept. of Chemistry, University of Allahabad under the supervision of Prof. L. D. S. Yadav. My research work has been devoted to the development of new synthetic routes to various bioactive heterocyclic systems. In these environmentally conscious days, the green chemistry has been of much concern of synthetic chemists which not only provides chemical process with several eco-friendly advantages but also opens up a new horizon in organic synthesis. In my *over ten years of research experience in the Synthetic Organic Chemistry*, I have been working mainly on the development of the following new synthetic routes:

[A]. Synthesis of Benzoxazinone *C*- and *N*-nucleosides:

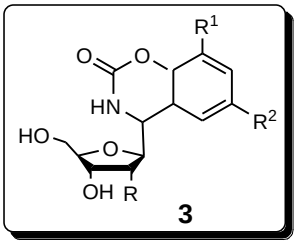
Efavirenz (Sustiva), a benzoxazinone derivative, is a non-nucleoside reverse transcriptase inhibitor that has been approved by the FDA (September 17, 1998) and is presently in clinical use for the treatment of AIDS. In this respect, I have synthesized benzoxazinone *N*-nucleosides **1** (*Tetrahedron Lett.* **2004**, *45*, 5351) and **2** (*Tetrahedron Lett.* **2006**, *47*, 395) and their *C*-nucleosides **3** (*Synlett* **2007**, 1227). Compounds **1** were prepared by K-10 clay catalyzed cycloisomerization of salicylaldehyde 4-(β-D-ribo- or β-D-2'-deoxribofuranosyl) semicarbazones followed by reductive dehydrazination of their 4-hydrazinoderivatives. Compounds **2** were synthesized by K-10 clay supported three- component coupling reactions of substituted salicylaldehydes, ribosyl/deoxyribosylureas and ammonium acetate via cycloisomerisation of a aldimine intermediate. For benzoxazinone *C*-nucleosides **3,** a novel one-pot expeditious synthetic protocol has been developed via dehydrazinative β-glycosylation in aqueous media from the unprotected sugar and a compound containing an activated methylene group (Ref. 3). Recently, we have also reported 1,3-benzoxazine-2-thione C-nucleosides (*Nucleosides, Nucleotides & Nucleic Acids* **2008**, *27*, 1227-1237).



1

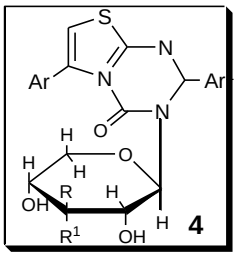


2



3

[B]. Synthesis of Glycon Modified *N*-nucleosides:



4

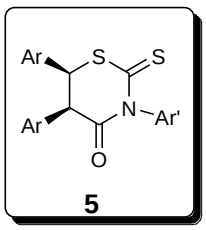
A green protocol involving novel three-component one-pot cyclocondensation reaction of 2-amino-4-aryl-thiazololes, aromatic aldehydes and ammonium thiocyanate under solvent- free MW irradiation conditions expeditiously yields thiazolo-s-triazine nucleobases, which afford the corresponding pyrano N-nucleosides **4** on iodine promoted glycosylation with 1,2,3,4-tetra-O-acetyl-beta-D-ribo-/xylopyranose under MW irradiation followed by deacetylation (Ref. 5).

Ref. 5. ***Lett. Org. Chem.*** **2007**, *4*, 47.

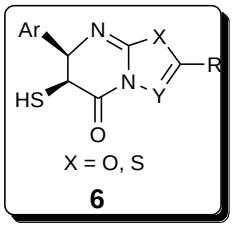
[C]. Stereo/-Chemo/- and Regeoselective Syntheses:

Nowadays, selectivity in organic reactions, *i.e.* stereoselectivity, regioselectivity and chemoselectivity has become a much challenging and demanding area for synthetic chemists. In this respect, we have developed ***diastereoselective synthetic protocols*** for 1,3-thiazines **5** (Ref. 5) and azolopyrimidines **6** (*Tetrahedron* **2006**, *62*, 5464) using 2-methyl-2-phenyl-1,3-oxathiolan-5-one, a novel mercaptoacetyl transfer agent **7** reported from our laboratory (*Tetrahedron* **2005**, *61*, 10013). In addition, we have also developed a ***diastereoselective green protocol*** for annulation of *s*-triazine ring on thiazoles **8** (*Green Chem.* **2006**, *8*, 455) and have devised a ***chemoselective annulation*** of 1,3-dithiin, -thiazine and -oxathiin rings on thiazoles **9**, **10**, and **11** involving tandem Knoevenagel, Michael and ring transformation reactions employing solvent-free MW irradiation conditions in a one-pot procedure (*Tetrahedron* **2006**, *62*, 8029). Very recently, ***regio/-*** *and* ***stereoselective***

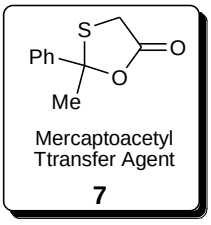
synthetic routes for amino/ mercaptodithiazolopyrimidines **12** from thiourea have been developed by us (*Tetrahedron* **2007**, *63*, 6924, *Synthesis* **2007**, 3831).



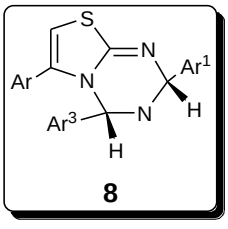
5



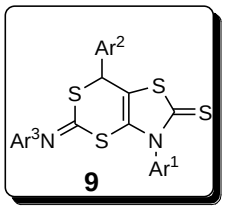
6



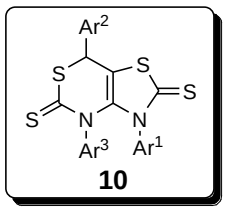
7



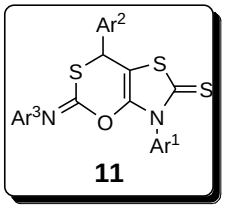
8



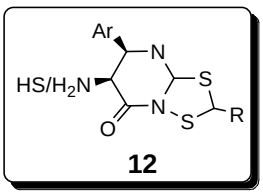
9



10



11



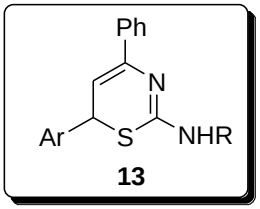
12

[D]. Active-Copper Promoted *N*-Arylations in Aqueous Media:

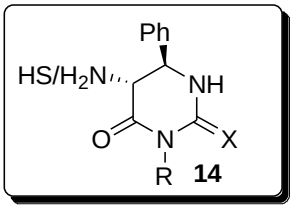
We have reported active-copper-promoted mild and expeditious *N*-arylations of amines, amides, imides, and β-lactams with aryl halides under MW irradiation conditions. These reactions can be performed in aqueous media as well as under solvent-free conditions to give good yields (*Synthesis* **2006**, 1868). Interestingly, no base is used in these reactions and the active copper itself acts as the halogen acceptor. Very recently, we have reported the catalyst-free synthesis of pharmaceutically and chemically important 3-mercaptocoumarins in water (*Green Chem.* **2009**, *11*, 878).

[E]. Ionic Liquid Mediated Organic Synthesis:

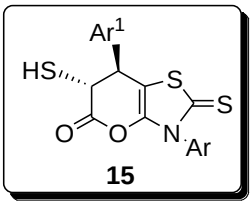
We have disclosed an efficient conjugate hydrothiocyanation of chalcones with a *task-specific ionic liquid* ([Bmim]SCN), The application of this protocol in heterocyclic chemistry is demonstrated by a one-pot synthesis of 1,3-thiazines **13** (*Tetrahedron Lett.* **2007**, *48*, 7793). A chiral ionic liquid-catalyzed, efficient and unprecedented version of the Biginelli reaction using novel variants of its active methylene component, viz. 2-phenyl-1,3-oxazol-5-one/2-methyl-2-phenyl-1,3-oxathiolan-5-one, with benzaldehyde and urea/thiourea enantio- and diastereoselectively, yields 5-amino-/mercaptoperhydropyrimidines **14** (*Tetrahedron* **2008**, *64*, 1420). Recently, a stereocontrolled route to mercaptopyranothiazole **15** has been developed using one-pot multi-component protocol in chiral ionic liquid (*J. Heterocyclic Chem.* **2008**, *45*, 1315). Furthermore, we have also developed a one-pot protocol for 2-amino-5-mercapto or 2,5-diamino-1,3-thiazines using ionic-liquid ([Bmim]Br) (*Tetrahedron* **2009**, *65*, 1306). Very recently, we have reported the one-pot [Bmim]OH-mediated synthesis of 3-benzamidocoumarins **16** (*Tetrahedron Lett.* **2009**, *50*, 2208).



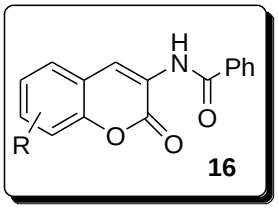
13



14



15

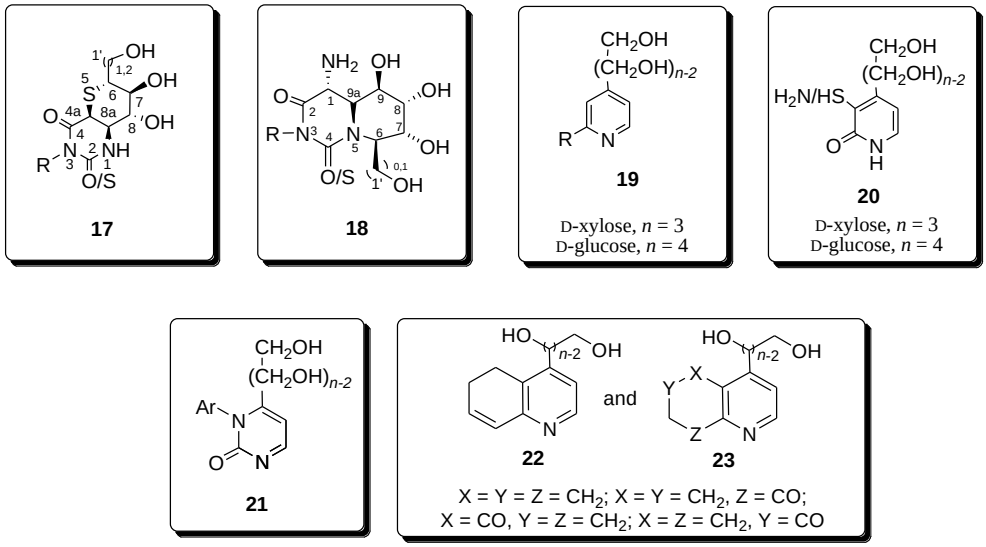


16

[E]. Biorenewable Resources in Organic Synthesis:

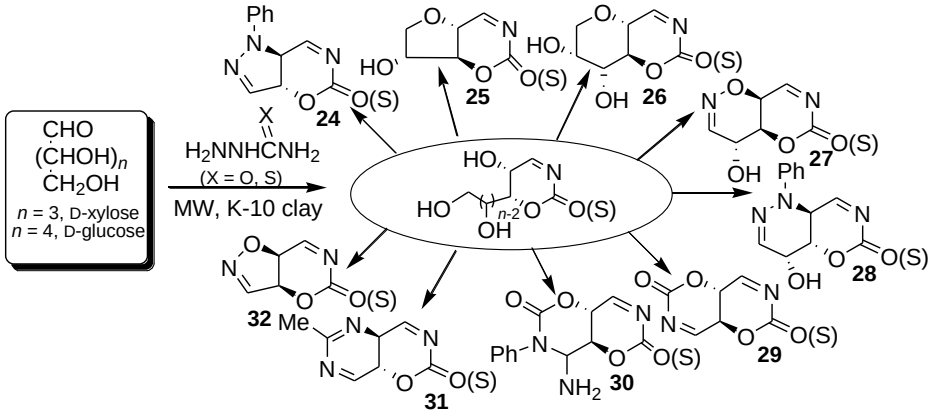
"*A raw material as feedstock should be renewable rather than depleting wherever technically and economically practicable.*" This quotation is one of the 12 principles of green chemistry and thus, "renewable resources" is a new and rapidly developing concept in the environmental and chemical sciences that concerns the wide use of biorenewable materials for industry. In this context, we have utilized carbohydrate feedstocks as raw material in "***Biginelli Reaction***" and we have developed an efficient Ce(III)-catalyzed diastereoselective synthesis of iminosugar annulated-(**17,** *Synlett* **2007**, 1905) and montmorillonite K-10 clay-catalyzed annulated **(18**, *Tetrahedron Lett.* **2007**, *48*, 4899**)** polyfunctionalized pyrimidine scaffolds of pharmacological potential under solvent-free MW irradiation conditions in a one-pot procedure. Recently, we have developed an original method for polyhydroxyalkylpyridines **(19)** and their 3-amino/mercapto-2-

pyridinone analogues **(20)** using unprotected aldoses as biorenewable resources via enol-driven Michael-type addition of lactones/ketones to aldose-derived 1,3-oxazin-2-ones followed by decarboxylative ring transformation (*Synlett* **2008**, 529). Very recently, we envisaged a K-10 clay-catalyzed amine-driven dehydrative ring transformation approach to pyrimidines (**21**, *Tetrahedron Lett.* **2008**, *49*, 2377) and enol-driven ring transformation approach to dihydro- (**22**, *Synlett* **2008**, 2257) and tetrahydroquinolines (**23**, *Synlett* **2008**, 2257) from carbohydrates as biorenewable resources.



[F]. Diversity Oriented Synthesis:

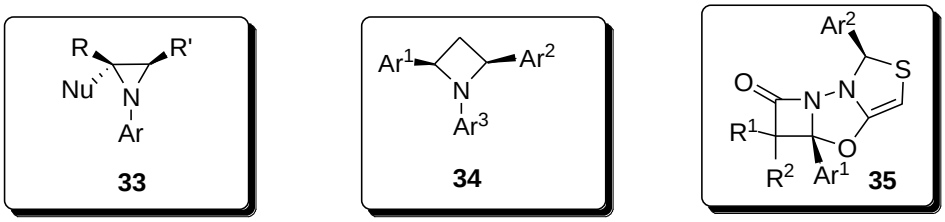
We have developed a general, straightforward diversity oriented synthetic approach for the synthesis of various 1,3-oxazin-2-one(thione)-fused *N*- and *O*-heterocyclic systems (**24**-**32**) using D-glucose and D-xylose as biorenewable resources under solvent-free microwave irradiation conditions (*Tetrahedron* **2008**, *64*, 4246) and also by employing $Cu(OTf)_2$ as catalyst (*J. Chem. Res.* **2009**, 522) where, $Cu(OTf)_2$ acts as dehydrazinating and N-arylating reagent.



[G]. Synthesis of Small Ring *N*-Heterocycles:

Owing to the inherent strain in small ring heterocycles, they are useful as feedstocks in organic synthesis to provide functionalized carbon chain. A general method for a convenient synthesis of 1,2,4-trisubstituted azetidines **34** by reductive cyclization of readily available aza-Michael adducts of chalcones and diethyl *N*-arylphosphoramidates in a one-pot procedure is reported (*Tetrahedron Lett.* **2007**, *48*, 8037), which may find application in organic synthesis. Furthermore, we have developed a novel and efficient aziridination of α-halo ketones (*Tetrahedron Lett.* **2008**, *49*, 687). The reaction of α-halo ketones with diethyl *N*-arylphosphoramidates affords diethyl *N*-aryl-*N*-(2-oxoalkyl)phosphoramidates which undergo reductive (H^--induced) cyclization with sodium borohydride followed by sodium hydride to give 1,2-disubstituted and 1,2,3-trisubstituted aziridines. The cyclization induced by NCS^- or PhS^- affords substituted aziridines functionalized at position 2. The reactions give excellent yields and are highly diastereoselective in favour of *cis* aziridines **33**.

Recently, tricyclic β-lactam antibiotics, generally referred as "*trinems*", have been the subject of considerable study owing to their broad spectrum of antibacterial activity. Besides, the ever-growing new applications of 2-azetidinones in fields ranging from enzyme inhibition to the use of these products as starting materials to develop new synthetic methodologies has triggered a renewed interest in the building of new polycyclic β-lactam systems in an attempt to move away from the classical β-lactam antibiotic structures. In this regard, we envisaged the straightforward synthesis of trinem class of antibiotics, viz highly derivatized azetidino[2,1-*b*]-thiazolo[3,4-*d*]-3*H*-1,3,4-oxadiazol-6-ones **35** (*Tetrahedron Lett.* **2008**, *49*, 5553).



[I]. Morita-Baylis-Hillman (MBH) Chemistry:

Morita-Baylis-Hillman (MBH) adducts bearing allylic hydroxyl and Michael acceptor units and their derivatives have been illustrated as valuable synthons and starting materials for the generation of diverse molecular skeletons employing simple alternatives.[1] Especially, regioselective introduction of nucleophiles at either α- or γ- position of the MBH acetates enables the construction of a variety of bioactive molecules and has become a powerful tool in synthetic organic chemistry. Thus, we have performed the first regio- and diastereoselective direct introduction of α-mercaptoacetic acid/amide units into MBH acetates **36** (*Tetrahedron Lett.* **2009**, *50*, 2414). Furthermore, we have also reported a novel one-pot stereoselective synthesis of *N*-protected α-Amino acids from MBH Acetates **37** (*Synlett* **2009**, 1423).

[J]. N-Heterocyclic Carbenes (NHCs)-catalyzed organic synthesis:

Over the last decade, there has been a continuously growing number of successful and novel applications of *N*-heterocyclic carbenes (NHCs) as organocatalysts and reagents for an expanding set of reactions. This is not only because of the great versatility of these organocatalytic transformations, but also due to the possibilities that arise from the NHC's characteristic causing inversion of the classical reactivity, that is, umpolung. We have disclosed an NHC-catalyzed efficient synthesis of aldol products β-hydroxy-α,β-unsaturated ketones **38** via carbonyl umpolung reaction of enals with terminal epoxides. Furthermore, we also demonstrated its synthetic application and developed a straightforward, convenient, and one-pot process for the synthesis of tetrahydropyran-4-ones **39** in excellent yields (87-90%) via oxy-Michael intramolecular reaction of **38** (*Synlett* **2010**, 240-246). Recently, we have reported an unprecedented synthesis of β'-amino-α,β-unsaturated ketones **40** via regioselective aziridine ring opening. The protocol involves carbonyl umpolung reactivity of enals in which the carbonyl carbon attacks nucleophilically on electrophilic terminal aziridines regiselectively (*Tetrahedron Lett.* **2010**, 51, 1657).