

Editorial

Guillermo A. Morales

Published online: 10 January 2009
© Springer Science+Business Media B.V. 2009

In this issue of *Molecular Diversity*, we included seven articles: 1 article in the area of computational chemistry and six articles in the area of organic synthesis. Here are the highlights

Computational chemistry

Amić and colleagues studied computationally the radical scavenging activity of flavonoids via calculation of bond dissociation enthalpies (BDE) using the semiempirical PM3 method. The authors generated 83 radical species (RO•) from a set of 29 flavonoids and determined a significant correlation between BDE values and radical scavenging activities.

Organic synthesis

Dotsenko and co-workers present a review-research article on the Biginelli synthesis of 3,4-dihydropyrimidin-2(1H)-ones/-thiones focusing on the nature of catalysts used. The review section includes a comprehensive survey of the catalysts used for this widely used multicomponent reaction. For the research section, the Dotsenko group chose a controversial approach to demonstrate that the Biginelli reaction does not require a complex catalyst at all, simply using NaCl as a catalyst is sufficient. The results and opinion of the authors on the use, or rather “misuse”, of catalysts for the Biginelli reaction are included in the second part of this review-research article.

G. A. Morales (✉)
Semafore Pharmaceuticals Inc., 8496 Georgetown Road,
Indianapolis, IN 46268, USA
e-mail: Editor@Molecular-Diversity.com

Borrel and colleagues report the microwave-assisted synthesis of *N*-substituted 4-amino-2-hydropyrido[2,3-*d*]pyrimidin-7(8*H*)-ones via the selective formation of 4-chloropyridopyrimidine intermediates derived from the reaction of 4-oxopyridopyrimidines with POCl₃. This work offers a robust methodology for the synthesis of compounds with potential kinase inhibitor profiles.

Malgesini and co-workers report an improved and scalable synthesis of ϵ -Boc- ϵ -(3,5-bis-trifluoromethylbenzyl)- α -Fmoc-*L*-lysine. This hexafluorinated orthogonally protected amino acid serves as an excellent tool as its incorporation in peptides allows the study of enzymatic reactions and peptide screening via ¹⁹F NMR spectroscopy.

Zhang and co-workers studied the influence of the ionic liquid 1-butyl-3-methyl imidazolium tetrafluoroborate ([bmim]BF₄) when used as solvent in the one-pot multicomponent synthesis of 4*H*-thiopyran and pyrimidine nucleoside-thiopyran derivatives. Their findings reveal that this reaction proceeds with both aromatic and aliphatic aldehydes without the need to use a catalyst.

Shaabani and colleagues used a 3-component/2-component (3-CR/2-CR) reaction sequence to produce highly substituted imidazo[1,5-*a*]pyrazine derivatives. In this research 2,3-diaminomaleonitrile, ketones and isocyanides afforded 1,6-dihydropyrazine-2,3-dicarbonitriles which in the presence of a iso/thiocyanate further cyclized to afford the final imidazo[1,5-*a*]pyrazines.

Elinson and co-workers present an efficient electrocatalytic approach for the multicomponent reaction of isatins, 3-methyl-2-pyrazolin-5-ones and malononitrile for the synthesis of spirocyclic indole-3,4/8 -pyrano[2,3-*c*]pyrazoles in high yields.

Guillermo A. Morales
Editor in Chief