MCR 2009
Proceedings of the 4th International Conference on Multi-Component Reactions and Related Chemistry, Ekaterinburg, Russia
ADVANCES IN EXPERIMENTAL MEDICINE AND BIOLOGY

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Introduction to the Proceedings of the Fourth International Conference on Multi-Component Reactions and Related Chemistry

Maxim A. Mironov

The Fourth International Conference on Multi-Component Reactions and Related Chemistry was held in Ekaterinburg, Russia, from May 24 to 28, 2009. The conference evolved from a great tradition that was started by Prof. Ivar Ugi, who can be considered the father of the concept of Multi-Component Reactions (MCRs) and the grandfather of combinatorial chemistry. This meeting was a continuation of three highly successful conferences on the same topic that were held in Munich in 2000, in Genova in 2003, and in Amsterdam in 2006. All of the conferences had about 250 participants, about half of them coming from private companies. The quality and variety of the presented lectures greatly contributed to this outcome. Due to its unique geographical position on the border of Europe and Asia, Ekaterinburg assumes the role of an important center of cooperation between the East and the West. This place was ideal for the Fourth International Conference on Multi-Component Reactions and Related Chemistry, chaired by Prof. Oleg Chupakhin and Dr. Maxim Mironov, where 134 scientists from 17 countries covering Europe, North America, South Asia, and the Pacific regions discussed recent progress and further developments in the field. A total of 43 oral presentations and 52 posters were delivered. Our event was supported by two leader companies in pharma research: ChemDiv Inc. and Abbott Laboratories, and also by the Russian Academy of Science and Springer Science+Business Media. Materials of the conference were published in a special issue of Molecular Diversity (Springer). The conference was accompanied by an exhibition and training courses, which featured participation from the pharma industry, analytical equipment providers, and publishers.

The scientific program of the conference focused on MCRs, which are a rapidly expanding research area in medicinal chemistry and materials science. The classical MCR chemistry is well-known to those who have studied organic chemistry at the university level. Many of these classical reactions are named reactions, such as the Mannich reaction and its intramolecular variant, the Pictet–Spengler reaction, the Strecker synthesis, the Ugi four-component condensation, and many others. Nowadays, the number of research groups active in the MCR field is growing.

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rapidly and novel MCRs are being discovered or developed on a weekly basis. The
number of publications in the MCR area has increased dramatically, reaching sev-
eral hundred articles per year. More and more companies continue to adopt this
chemistry in their synthetic repertoire. There are several advantages of synthesis
using MCRs. First, they are fully amenable to automated synthesis because there is
no need to isolate any intermediates and the experiments are carried out in a single
reaction vessel. Second, MCRs are more convergent than synthesis pathways based
on a sequence of uni- and bimolecular reactions. In addition, MCRs are a particular
case of reaction networks, which can be considered a model of natural processes
and prebiotic evolution. Although the main focus of the conference was on MCRs,
its scope embraced organic synthesis via tandem or cascade reactions, combinator-
rrial approaches to new materials, catalysts, and supramolecular structures. The
conference was organized in six sections: (1) Catalysis and Multi-Component
Reactions; (2) Multi-Component Reactions in Heterocyclic Chemistry; (3) Multi-
Component Reactions in Drug Discovery; (4) Novel Reagents for Multi-Component
Reactions; (5) Design of Multi-Component Reactions; and (6) Multi-Component
Reactions in Supramolecular Chemistry and Material Science.
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Session 1
Catalysis and Multi-Component Reactions
Recent Progress in Asymmetric Two-Center Catalysis

Masakatsu Shibasaki

We have been studying the development of new asymmetric two-center catalysis using rare earth alkoxides and bifunctional sugar and related ligands. In The Fourth International Conference on Multi-Component Reactions and Related Chemistry (MCR 2009), new catalytic asymmetric reactions using catalysts 1 and 2 and catalytic asymmetric syntheses of ranirestat 3 and tamiflu 4 will be presented.

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Reference

Efficiency in Chemistry: From Hydrogen Autotransfer to Multi-component Catalysts

Miguel Yus

One important task concerning any chemical process has to do with the so-called atomic efficiency (AE), which can considerably modify the concept of yield corresponding to a chemical reaction: Even working with a high chemical yield a reaction can be inefficient when the main part of the reactant’s structure is not included in the final product. Two interesting processes will be the subject of this presentation: (a) the hydrogen autotransfer reaction, in which an alcohol is used as the electrophilic component in the alkylation of a carbonyl compound; water is the only byproduct in the process, which is, therefore, of great value from an atom-efficiency point of view (1); and (b) the magnetite-catalyzed multi-component aza-Sakurai reaction, of considerable interest from a synthetic efficiency point of view (2).

\[ \text{R}_1\text{O} + \text{R}_2\text{OH} \xrightarrow{\text{cat.}} \text{R}_1\text{O}\text{R}_2 \] (Eq. 1)

\[ \text{R}_1\text{R}_2\text{O} + \text{ClR}_3 + \text{R}_4^3\text{SiNu} + (\text{Me}_3\text{Si})_2\text{NH} \xrightarrow{\text{cat.}} \text{HN}\text{R}_1\text{R}_2\text{Nu} \] (Eq. 2)

References


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