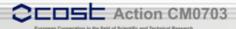




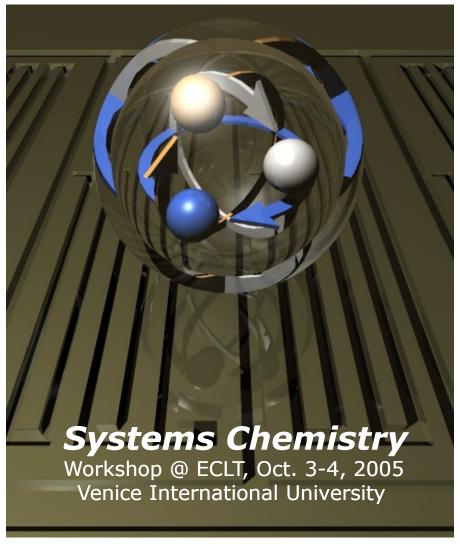
Systems CHEMISTRY Action Overview

Günter von Kiedrowski, Ruhr University Bochum









Accidentally in the same week:

Systems Chemistry: Kinetic and Computational Analysis of a Nearly Exponential Organic Replicator:

M. Kindermann et al., ANIE 2005, 44, 6750-6755.



ESF-COST High-Level Research Conference Hotel Villa del Mare Maratea, Italy October 3-7, 2008



EUROPEAN ECIENCE COUNDATION

Speakers:

Gonen Ashkenasy, Beer Sheva Vladik A. Avetisov, Moscow Carlos F. Barbas III. La Jolla Steven A. Benner, Gainesville/FL Donna Blackmond, London James Cleaves, Washington George Cody, Washington Ben Feringa, Groningen M. Reza Ghadiri, La Jolla Piet Herdewijn, Leuven Ludovic Jullien, Paris Stuart Kauffman, Calgary Christoph Kuhn, Zurich Meir Lahav, Rehovot John S. McCaskill, Bochum Pierre A. Monnard, Odense Peter Nielsen, Copenhagen Douglas Philp, St. Andrews Addy Pross, Beer Sheva Peter Schuster, Vienna Kenso Soai, Tokyo Pasquale Stano, Rome Eörs Szathmáry, Budapest Svetlana B. Tsogoeva, Erlangen Günter von Kiedrowski, Bochum Arthur C. Weber, Mountain View/CA

Organizers:

Chair: Günter von Kiedrowski, Bochum Vice chair: Dieter Schinzer, Magdeburg Contact: Antje Teegler, ESF, Brussels Peter Strazewski, Lyon Zbigniew Zagorski, Warsaw Josep M. Ribo, Barcelona John S. McCaskill, Bochum Eörs Szathmary, Budapest

Chembiogenesis 2008







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Journal of Systems Chemistry is a new peer-reviewed open access journal from <u>Chemistry Central</u> covering all aspects of systems chemistry including (but not limited to):

- o experimental and theoretical studies of complex molecular networks
- o catalytic and autocatalytic systems
- o self-replicating and self-reproducing chemical systems
- o dynamic combinatorial chemistry
- o emergent phenomena in molecular networks
- information processing by chemical reactions
- o bifurcation and chiral symmetry breaking
- o bottom up approaches to synthetic biology and chemical evolution
- research on chemical self-organization inspired by the problems of the origin and synthesis of life
- research from the conjunction of supramolecular, prebiotic and biomimetic chemistry, theoretical biology, complex systems physics, and earth, planetary and space sciences with a center in chemistry









- •"genetic"
- •"metabolic"
- •"confined"
- •"asymmetric"





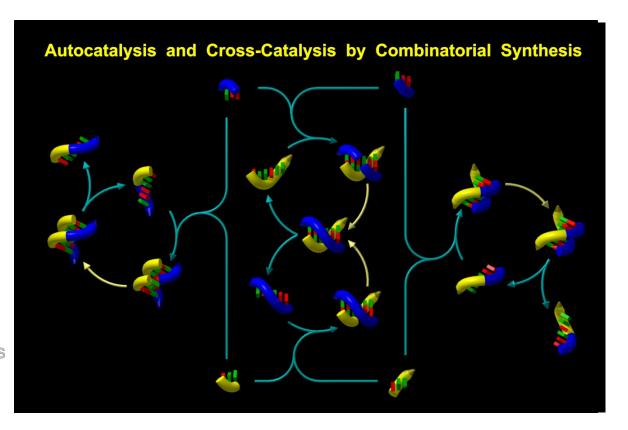


- •"genetic"
- "metabolic"
- •"confined"
- ·"asymmetric"

in terms of dynamics:

...from
autocatalytic replicators
...via
cross-catalytic replicators
...to

replicator networks







- •"genetic"
- •,,metabolic
- •"confined"
- •,,asymmetric"



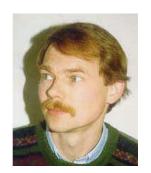
Marie-Christine Maurel, Paris, FR



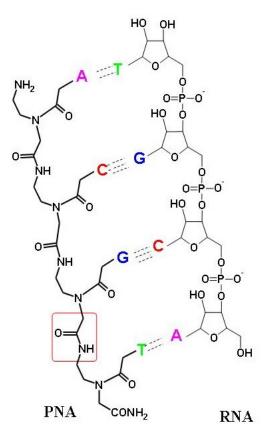
Clemens Richert, Karlsruhe, DE



Piet Herdewijn, Leuven, BE



Peter E. Nielsen, Copenhagen, DK



in terms of structure:

...from nucleic acids & mimics

...via peptide replicators

small organic replicators





- ·•"genetic"
- •"metabolic"
- •"confined"
- ·"asymmetric"



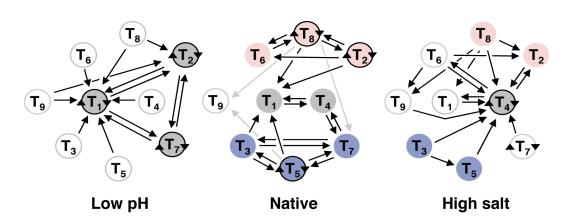
Gonen Ashkenasy, Ben Gurion Univ., IL

in terms of structure:

...from nucleic acids & mimics

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small organic replicators



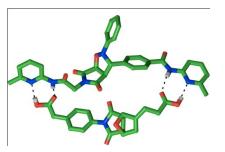




- •"genetic"
- •,,metabolic
- •"confined"
- "asymmetric"



Douglas Philp, St. Andrews, UK





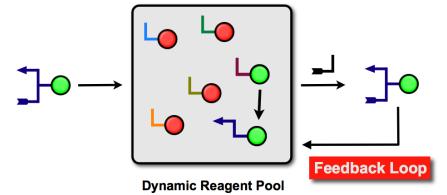
Sijbren Otto Cambridge, UK

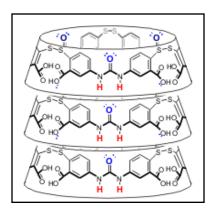
in terms of structure:

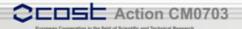
...from nucleic acids & mimics

...via peptide replicators

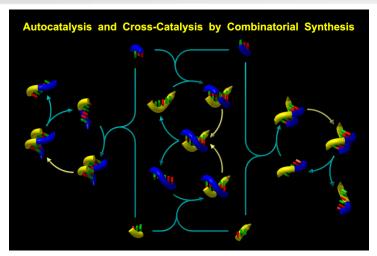
...to small organic replicators





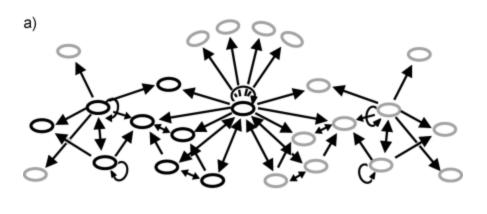


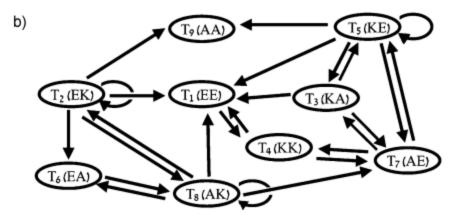




Cross-catalytic replication: Combine more than four precursors...

http://www.nature.com/chemistry/looking_back/index.html



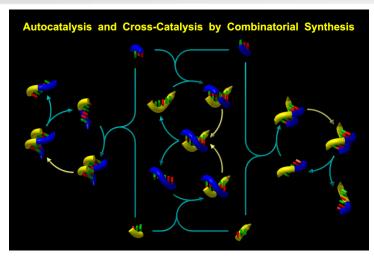


...and arrive at Molecular Networks

The Road to Nonenzymatic Molecular Networks Z. Dadon, N. Wagner, G. Ashkenasy, *ANIE* **2008**, *47*, 6128-6136

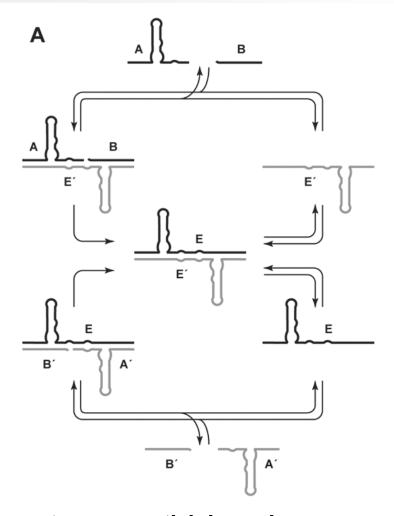






Cross-catalytic replication: From parabolic...

http://www.nature.com/chemistry/looking_back/index.html



...to exponential dynamics

Self-sustained replication of an RNA enzyme T.A. Lincoln & G.F. Joyce, *Science* **2009**, *323*, 1229





Systems Chemistry on Ribozyme Self-Construction: Evidence for Anabolic Autocatalysis in a Recombination Network

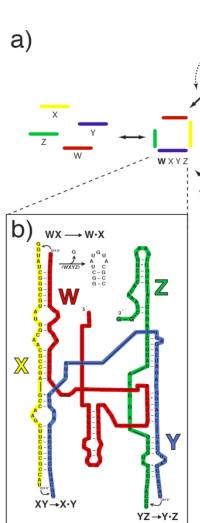
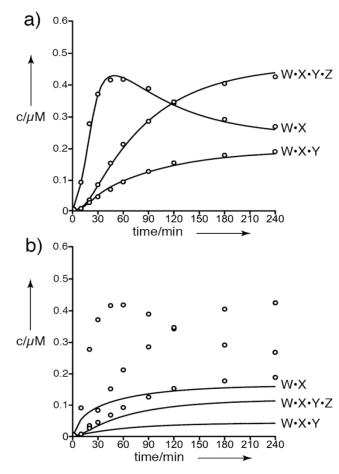


Figure 2. Kinetic modeling of the system. a) Concentrations of observables W·X, W·X·Y and W·X·Y·Z as a function of time. Open circles represent experimental data obtained from denaturing PAGE and autoradiography.^[27] Curves are a best fit of the model to the kinetic data using the program SimFit. c) Result of removing the autocatalytic rate constants from the model after fitting.



Scheme 1. The anabolic autocatalytic reaction network formed from the four fragments of the Azoarcus ribozyme. a) A scheme of covalent bond (*) forming reactions from the four fragments, through a series of non-covalent intermediates, to the fully covalent ribozyme W*X*Y*Z. Double-sided arrows indicate reversible phosphodiester bond formation, which is catalyzed initially by the non-covalent complex. Curved arrows indicate feedback by W*X*Y*Z to catalyze its own production in a single step (solid), or by catalyzing the production of an intermediate (dashed). Intermediates can also catalyze their own production as indicated by the grey curved arrow. b) Proposed secondary structure of non-covalent intermediates, and the tRNA-like splicing mechanism.

E.J. Hayden, G. von Kiedrowski, N. Lehman, *ANIE* **2008**, *47*, 8424-8428 News and views: B. Seelig, *Nature Chem. Biol.* **2008**, *4*, 654-655





- "genetic"
 "metabolic"
 "confined"
 asymmetric
- The Formose Reaction CH₂(OH)₂ $CH_{S}O \mid -OH_{S}$ $CH_2O + Ca(OAc)_2$ pH 12 CH₂OH CH_2O CHO glycol aldehyde, СНОН glycerine aldehyde, СНОН CHO mixture of isomeric CH₂OH СНОН aldo- and keto-GC after derivatisation as CH₂OH tetroses, pentoses, n-butoxim-trifluoracetates hexoses etc. CH₂OH CH₂OH C = 0CH₂O CHOH C = 0Butlerow (1861), Decker (1982) CH₂OH CH₂OH





- "genetic" "metabolic" ...confined"



John Sutherland, Manchester, UK

$$\begin{array}{c} O \\ H \\ NH_2 \end{array} \longrightarrow \begin{array}{c} NC \\ N \\ H_2N \end{array} \longrightarrow \begin{array}{c} H_2O \\ H_2N \\ H \end{array} \longrightarrow \begin{array}{c} O \\ H_2N \\ H \end{array}$$

$$AICN \qquad AICA$$



Raffaele Saladino, Tuscia Univ., IT

Süßes Leben: Pentose-Aminooxazoline – Intermediate in einer möglichen präbiotischen Nucleosidsynthese - können in Wasser unter Umgehung des entsprechenden Zuckers hergestellt werden. 2-Aminooxazol, ein Kondensationsprodukt aus Glycolaldehyd und Cyanamid, reagiert mit Glyceraldehyd unter milden Bedingungen in einem bemerkenswerten und nahezu quantitativen Prozess, der hochstereoselektiv für Ribose- und Arabinose-Aminooxazoline ist.

Präbiotische Chemie

C. Anastasi, M. A. Crowe, M. W. Powner, J. D. Sutherland* ______ 6322 - 6325

Direct Assembly of Nucleoside Precursors from Two- and Three-Carbon Units



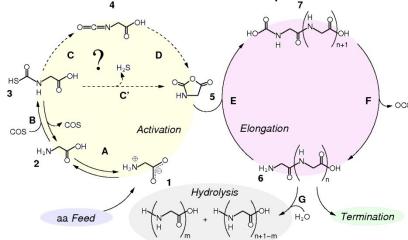


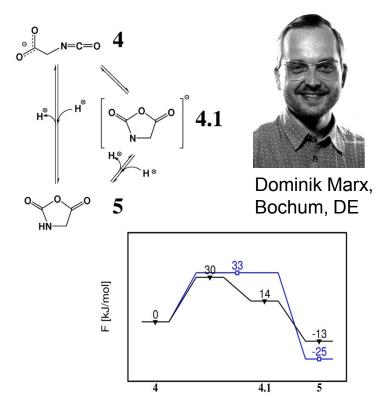


- •"metabolic"
- •"confined"
- "asymmetric



Robert Pascal, Montpellier, FR





Detailed ab initio simululation of various aspects of prebiotic peptide synthesis

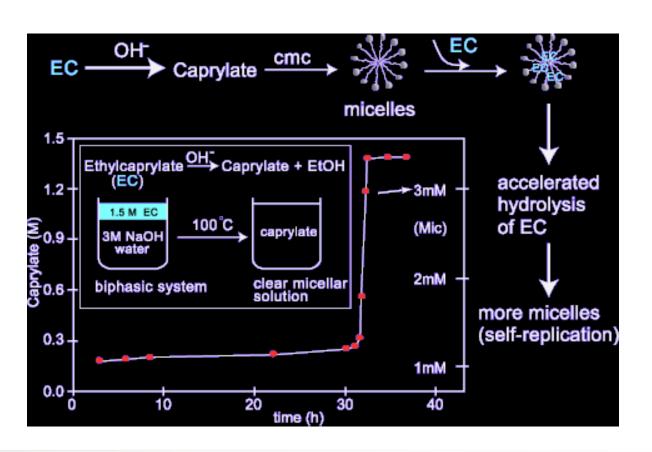




- •"genetic"
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Pier-Luigi Luisi, Rome, IT



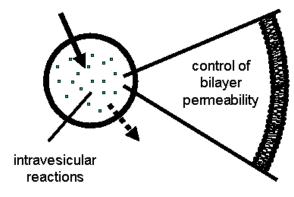




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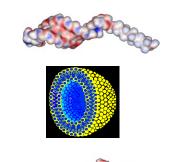


Peter Walde, ETH Zurich, CH





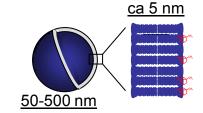
Peter Strazewski, Lyon, FR







Jan Bart Ravoo, Munster, DE



Molecular recognition at vesicle surfaces (PNAS 2007, 104, 8986)





- •"genetic"
- •"metabolic"
- •"confined"
- "asymmetric



John McCaskill, Bochum, DE



Enzo Gallori, Florence, IT

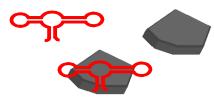
Ribozymes @ minerals

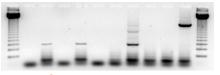


Jay Siegel, Zurich U, SW

chemical replicators
@ µ-fluidic electronic cells







Test for activity changes

pericyclic reactions/ organic replicators @ cubic lipid phases/ µ-fluidics/ anti-clays





- •"genetic"
- •"metabolic"
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- •,,asymmetric"







- •"genetic"
- ·"metabolic"
- •"confined"

Product

Educt

"asymmetric"

Product-Substrate Complex

Product-Dimer

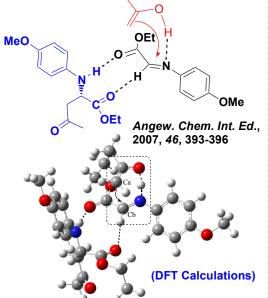


Donna Blackmond. London, UK



 Mechanism of the Soai reaction

 Chirality amplification by eutectic freezing of scalemic AA mixtures





Svetlana Tsogoeva, Erlangen, DE





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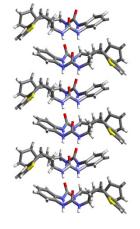
Ben L. Feringa, Groningen, NL

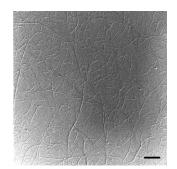


Josep M. Ribó, Barcelona, SP



Meir Lahav, Rehovot, IL



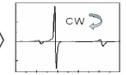


Chiral symmetry breaking by nucleation-growth processes in supramolecular systems: From gels to crystals









h

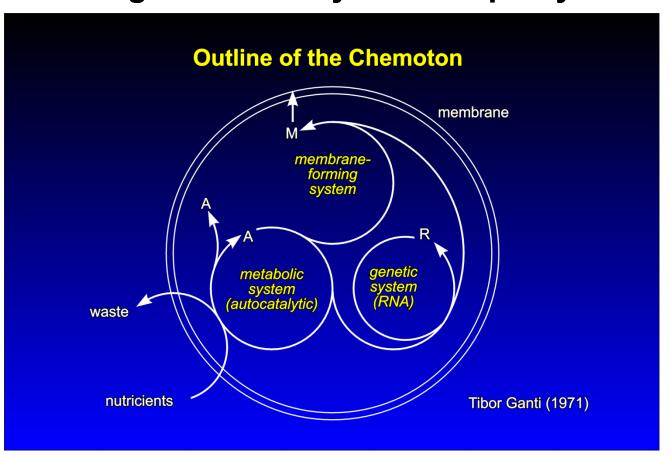








Budapest, HU

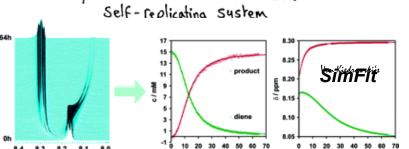








Prof. Kiedrowski achieves phenomonal success with a new Self-codication suctem

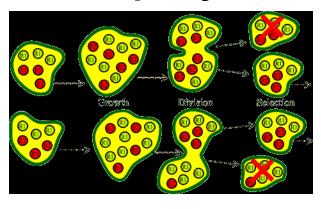




Günter von Kiedrowski, Bochum, DE



Eörs Szathmáry, Budapest, HU



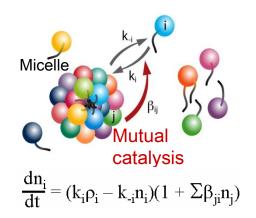
The pragmatic approach toward supersystem construction: Try pairwise integration before daring triple integration!

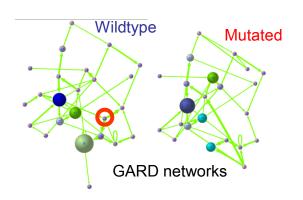
Genetic (G) GM
Metabolic (M) GC GMC (Chemoton)
Confined (C) MC

GC: The Chromatographized Replicator Model









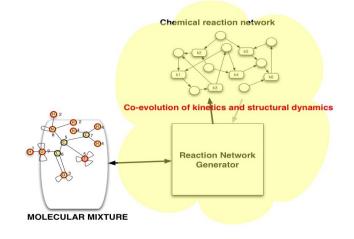


Doron Lancet, Rehovot, IL

The Graded
Autocatalysis
Replication
Domain (GARD)
model: mutually
catalytic
networks in a
Lipid World



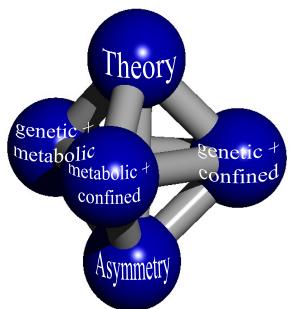
Hugues Bersini, Brussels, BE







Action Structure, Organization & Timetable



- •MC elected Steering Group with chair, vice, WG heads, STSM manager, dissemination manager, ESR speaker
- •STSMs as dedicated instruments for ESR-based knowledge transfer
- •Gender issue balance at the level of ESR exchange

Timetable of the proposed COST Action on Systems Chemistry

