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Organic & Biomolecular Chemistry

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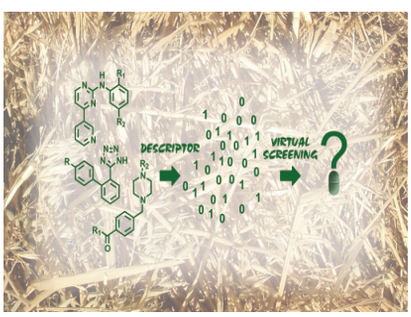
Incorporating Acta Chemica Scandinavica



Cover
See Jérôme Hert, Peter Willett, David J. Wilton, Pierre Acklin, Kamal Azzaoui, Edgar Jacoby and Ansgar Schuffenhauer, pp. 3256–3266.
Comparison of topological descriptors: which representation is the most effective at finding the needle in the chemical haystack?

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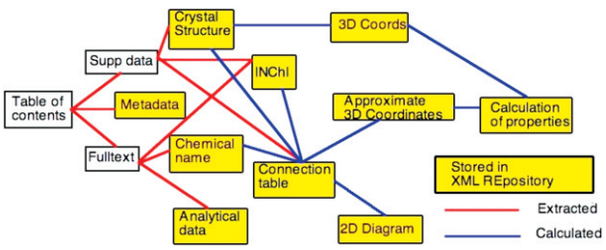
contents

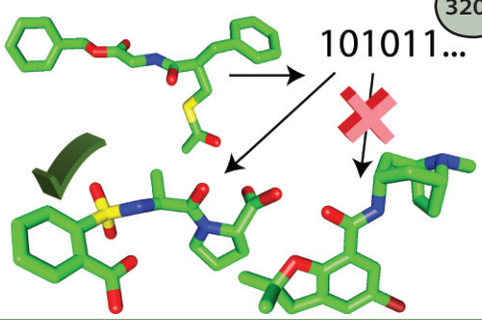
PERSPECTIVES



Representation and use of chemistry in the global electronic age

Peter Murray-Rust, Henry S. Rzepa, Simon. M. Tyrrell and Yong Zhang

We present an overview of the current state of public semantic chemistry and propose new approaches at a strategic and a detailed level.

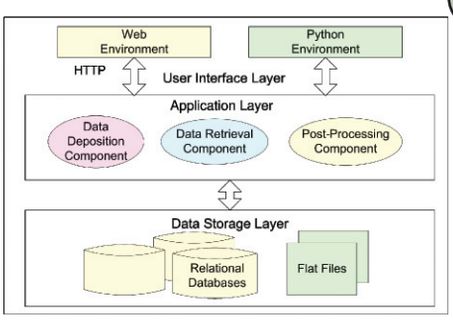


Molecular similarity: a key technique in molecular informatics

Andreas Bender and Robert C. Glen

The concept of similarity has been applied to a wide range of molecular informatics problems. We review, contrast and criticize the underlying assumptions and applications.

COMMUNICATION

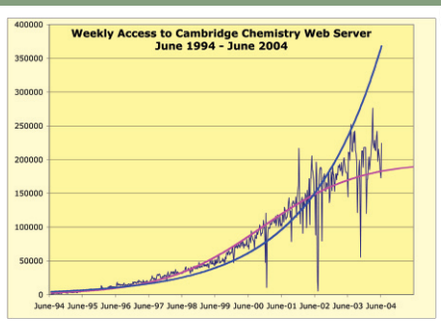


BioSimGrid: towards a worldwide repository for biomolecular simulations

Kaihsu Tai, Stuart Murdock, Bing Wu, Muan Hong Ng, Steven Johnston, Hans Fangohr, Simon J. Cox, Paul Jeffreys, Jonathan W. Essex and Mark S. P. Sansom

BioSimGrid is a database for biomolecular simulations, or, a 'Protein Data Bank extended in time' for molecular dynamics trajectories.

COMMENT

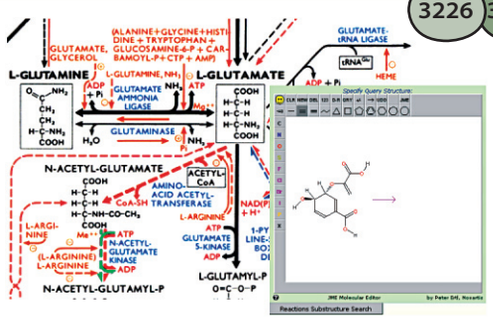


Chemistry on the world-wide-web: a ten year experiment

Jonathan M. Goodman

The impact of the world wide web on chemistry has been dramatic, but there are signs that its use is approaching a plateau.

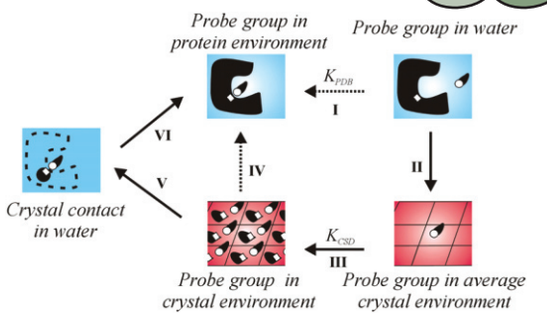
ARTICLES



Enabling the exploration of biochemical pathways

Martin Reitz, Oliver Sacher, Aleksey Tarkhov, Dietrich Trümbach and Johann Gasteiger

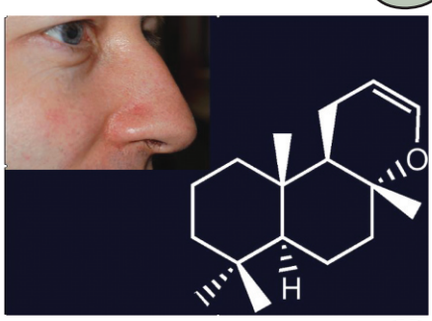
A database of metabolic reactions has been created enabling the application of chemoinformatic methods for understanding biochemical reactions.



Combined use of physicochemical data and small-molecule crystallographic contact propensities to predict interactions in protein binding sites

J. Willem M. Nissink and Robin Taylor

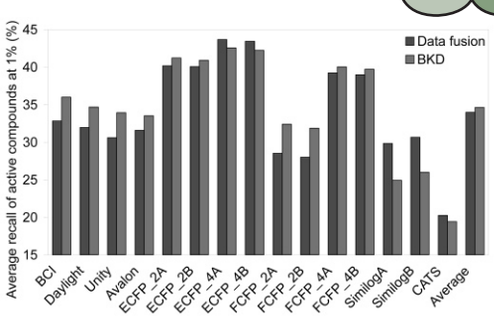
Combination of crystallographic knowledge on non-bonded interactions and hydrophobicity data allows prediction of protein–ligand interactions.



A structure–odour relationship study using EVA descriptors and hierarchical clustering

Shin-ya Takane and John B. O. Mitchell

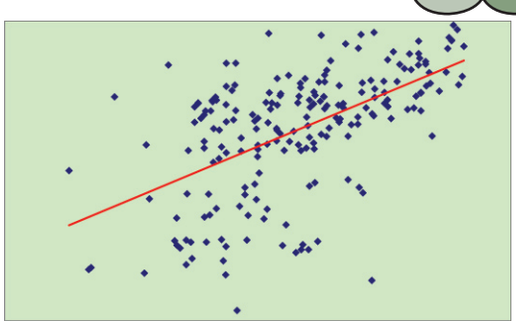
Structure–odour relationship analyses using hierarchical clustering were carried out on a diverse dataset of 47 molecules from seven odour categories. The alignment-independent descriptor EVA (EigenVAlue) and the UNITY 2D fingerprint were used. The dendrograms produced by EVA consistently outperformed those from UNITY 2D in reproducing the experimental odour classifications.



Comparison of topological descriptors for similarity-based virtual screening using multiple bioactive reference structures

Jérôme Hert, Peter Willett, David J. Wilton, Pierre Acklin, Kamal Azzaoui, Edgar Jacoby and Ansgar Schuffenhauer

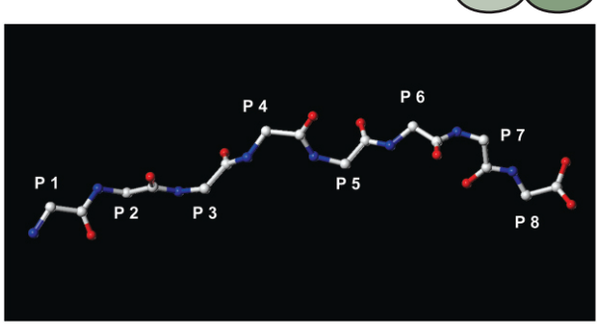
Demonstrates the general effectiveness of 2D fingerprints based on circular fragment substructures when used for similarity-based virtual screening.



Predicting protein–ligand binding affinities: a low scoring game?

Philip M. Marsden, Dushyanthan Puvanendrampillai, John B. O. Mitchell and Robert C. Glen

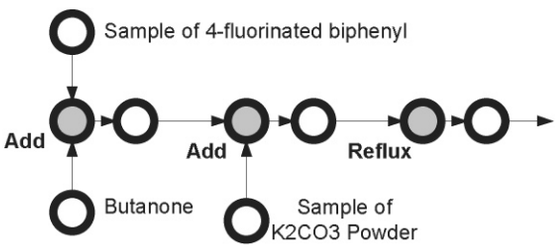
Accurate prediction of the binding energies for diverse sets of protein–ligand complexes is extremely difficult. On a given dataset, investigations show that two algorithms for producing consensus scoring functions generally perform slightly better than the best of five individual scoring functions.



New horizons in mouse immunoinformatics: reliable *in silico* prediction of mouse class I histocompatibility major complex peptide binding affinity

Channa K. Hattotuwagama, Pingping Guan, Irini A. Doytchinova and Darren R. Flower

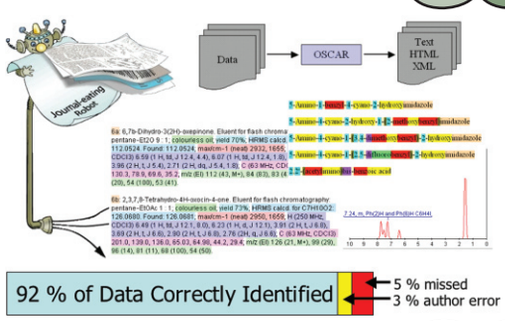
The QSAR-additive method is an established immunoinformatics technique used for the quantitative prediction of peptide-major histocompatibility complex (MHC) binding affinity.



The semantic smart laboratory: a system for supporting the chemical *e*Scientist

Gareth Hughes, Hugo Mills, David De Roure, Jeremy G. Frey, Luc Moreau, m. c. schraefel, Graham Smith and Ed Zaluska

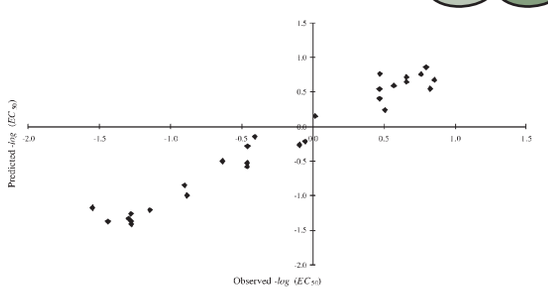
The Comb*e*chem project has used Semantic Web technologies in a system which supports and captures a chemistry experiment from plan to execution.



Chemical documents: machine understanding and automated information extraction

Joe A. Townsend, Sam E. Adams, Christopher A. Waudby, Vanessa K. de Souza, Jonathan M. Goodman and Peter Murray-Rust

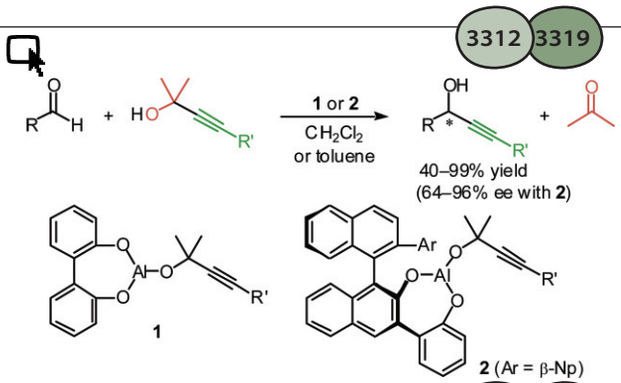
Processes for the automated extraction of useful information from unstructured chemical documents are described.



Optimising the EVA descriptor for prediction of biological activity

Martyn Ford, Laurie Phillips and Adrian Stevens

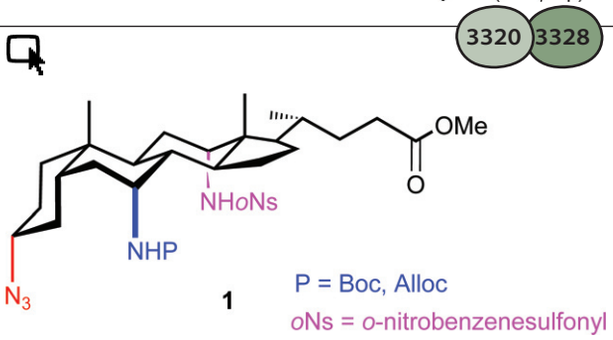
This paper investigates the inotropic potential of calcium channel agonists using a novel QSAR descriptor, EVA, constructed from their vibrational modes.



Meerwein–Ponndorf–Verley alkynylation of aldehydes: Essential modification of aluminium alkoxides for rate acceleration and asymmetric synthesis

Takashi Ooi, Tomoya Miura, Kohsuke Ohmatsu, Akira Saito and Keiji Maruoka

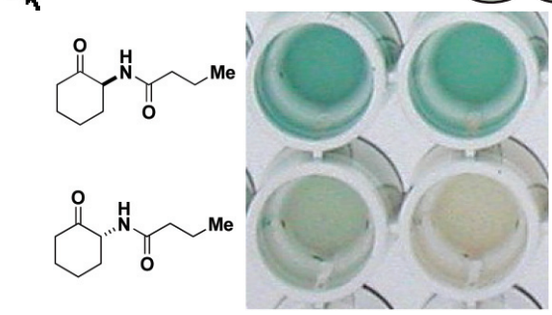
The Meerwein–Ponndorf–Verley alkynyl transfer from tertiary propargylic alcohol to aldehyde carbonyl with **1**, and chiral **2** enables the asymmetric version.



Differentially-protected steroidal triamines; scaffolds with potential for medicinal, supramolecular, and combinatorial chemistry

Vicente del Amo, Laura Siracusa, Theodoros Markidis, Beatriz Baragaña, Khadga M. Bhattarai, Marta Galobardes, Gregorio Naredo, M. Nieves Pérez-Payán and Anthony P. Davis

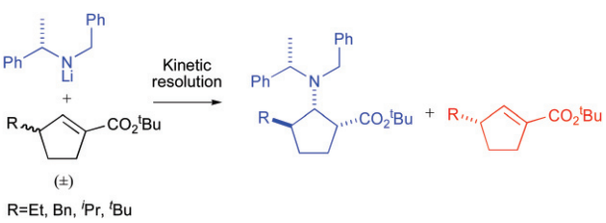
Steroids **1** may be deprotected sequentially to reveal three co-directed amino groups. These scaffolds have been prepared in *ca.* 40% overall yield from inexpensive cholic acid.



Synthesis and stability of small molecule probes for *Pseudomonas aeruginosa* quorum sensing modulation

Freija G. Glansdorp, Gemma L. Thomas, Jungjoon K. Lee, Jenny M. Dutton, George P. C. Salmond, Martin Welch and David R. Spring

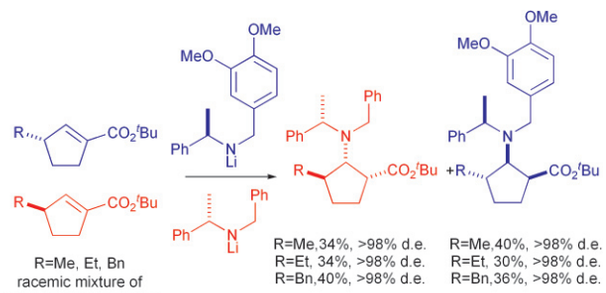
The non-racemic syntheses of *P. aeruginosa* quorum sensing modulators and their respective stabilities under conditions similar to assay media are described. The (*S*)-enantiomers appear to be the active isomers.



Kinetic resolution of *tert*-butyl (*RS*)-3-alkylcyclopentene-1-carboxylates for the synthesis of homochiral 3-alkyl-cispentacin and 3-alkyl-transpentacin derivatives

Mark E. Bunnage, Stephen G. Davies, Richard M. Parkin, Paul M. Roberts, Andrew D. Smith and Jonathan M. Withey

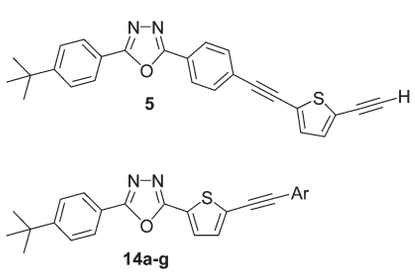
Kinetic resolution of a range of (*RS*)-3-alkylcyclopentene-1-carboxylates with lithium (*S*)-*N*-benzyl-*N*-α-methylbenzylamide proceeds efficiently (*E* > 80) to give, after deprotection, a range of 1,2-*syn*-2,3-*anti*-3-alkylcispentacins and 1,2-*anti*-2,3-*anti*-3-alkyltranspentacin hydrochlorides in >98% de.



Parallel kinetic resolution of *tert*-butyl (*RS*)-3-alkyl–cyclopentene-1-carboxylates for the asymmetric synthesis of 3-alkyl–cispentacin derivatives

Stephen G. Davies, A. Christopher Garner, Marcus J. C. Long, Andrew D. Smith, Miles J. Sweet and Jonathan M. Withey

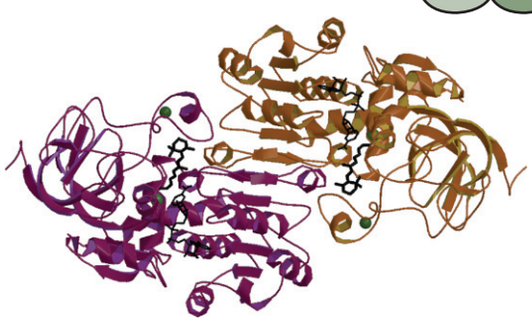
The efficient parallel kinetic resolution of a range of *tert*-butyl (*RS*)-3-alkyl–cyclopentene-1-carboxylates with a pseudoenantiomeric mixture of homochiral lithium (*S*)-*N*-benzyl-*N*-α-methylbenzylamide and lithium (*R*)-*N*-3,4-dimethoxybenzyl-*N*-α-methylbenzylamide has been achieved.



Ethynyl π-extended 2,5-diphenyl-1,3,4-oxadiazoles and 2-phenyl 5-(2-thienyl)-1,3,4-oxadiazoles: synthesis, X-ray crystal structures and optical properties

Gregory Hughes, David Kreher, Changsheng Wang, Andrei S. Batsanov and Martin R. Bryce

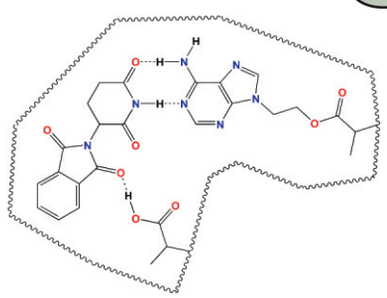
A range of 2,5-diaryl-1,3,4-oxadiazole chromophores with extended ethynyl π-conjugation have been synthesised. Their optical and structural properties are reported.



Synthesis of ring-oxidized retinoids as substrates of mouse class I alcohol dehydrogenase (ADH1)

Marta Domínguez, Rosana Alvarez, Sílvia Martras, Jaume Farrés, Xavier Parés and Angel R. de Lera

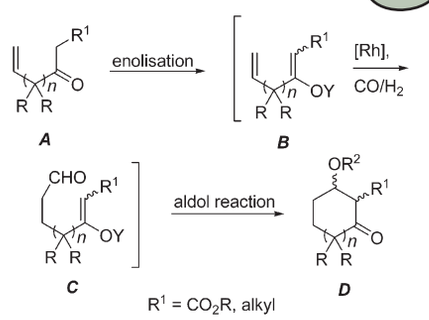
Kinetic constants of mouse class I alcohol dehydrogenase (ADH1) with stereoselectively synthesized ring-oxidized (3,4-didehydro-, 4-hydroxy- and 4-oxo-) retinoids have been determined.



Enantioselective synthetic thalidomide receptors based upon DNA binding motifs

Jenny P. Rosengren, Jesper G. Karlsson and Ian A. Nicholls

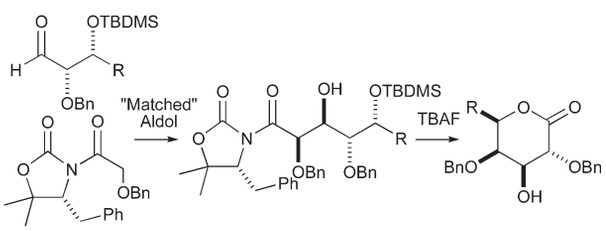
Molecularly imprinted polymer (MIP) synthetic receptors selective for thalidomide have been developed based upon DNA-like binding motifs.



Sequential hydroformylation/aldol reactions: versatile and controllable access to functionalised carbocycles from unsaturated carbonyl compounds

Mark D. Keränen, Kinga Kot, Christoph Hollmann and Peter Eilbracht

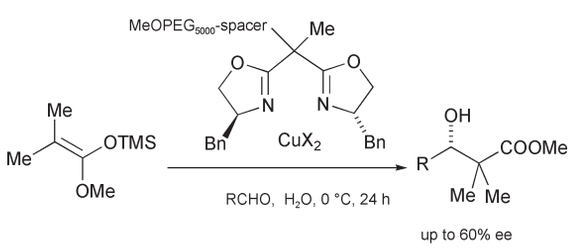
Three different modes of hydroformylation/aldol reaction sequences involving varying aldol additions can be applied to unsaturated ketones and ketoesters to afford the corresponding carbocyclic aldol adducts in good yields.



Double diastereoselective SuperQuat glycolate aldol reactions: Application to the asymmetric synthesis of polyfunctionalised lactones

Stephen G. Davies, Rebecca L. Nicholson and Andrew D. Smith

A range of polyfunctionalised lactones with up to five contiguous stereocentres may be prepared with high stereocontrol by a double diastereoselective aldol protocol with protected homochiral α,β-dihydroxy- or α,β-γ-trihydroxyaldehydes and a chiral glycolate oxazolidinone.



Enantioselective catalysis in water: Mukaiyama-aldol condensation promoted by copper complexes of bisoxazolines supported on poly(ethylene glycol)

Maurizio Benaglia, Mauro Cinquini, Franco Cozzi and Giuseppe Celentano

Cu(II) complexes of poly(ethylene glycol)-supported bisoxazolines are readily recyclable catalysts for the enantioselective Mukaiyama-aldol condensation in water.