Exploiting The Promise of Combinatorial Chemistry
Successful Strategies & Proof of Concept Case Studies

FRIDAY 25TH JUNE 1999 - THE MERCHANT CENTRE, LONDON

Industry has embraced Combinatorial Chemistry totally but has it contributed to the number of NCE's entering the clinic as promised?

"Combinatorial chemistry - a technology for creating molecules en masse and testing them rapidly for desirable properties - continues to branch out rapidly. Compared with conventional one-molecule-at-a-time discovery strategies, many researchers see combinatorial chemistry as a better way to discover new drugs..."
Chemical & Engineering News, April 1998

This unique strategic forum will look at the potential of Combinatorial Chemistry, in terms of lead identification and lead optimisation, and will allow participants to debate actual successes and failures of Combinatorial Chemistry and its true worth in the drug discovery process.

08.30 Coffee & Registration

09.00 New Dimensions of Combinatorial Chemistry & It's Value to the Drug Discovery Process
Dr Lutz Weber, Chief Scientific Officer
Morphochem AG, Germany
- High diversity combinatorial chemistry: varying both backbones and substituents within one library
- Evolutionary chemistry – optimisation of compound properties by biological feedback driven synthesis
- Functional diversity, structure-reactivity and structure-property correlation of high diversity combinatorial libraries
- Measures for success: gradients of evolutionary learning and bit-wise regularity coefficients
- Integrating chemistry, biology and artificial learning methods into one drug discovery process

09.45 Drug Research: From Serendipity to Rational Design
Professor Dr Hugo Kubinyi, Combinatorial Chemistry & Molecular Modelling
BASF AG, Germany
In traditional drug research, natural products and serendipitous discoveries played a significant role. Nowadays, structure-based and computer-aided drug design, using e.g., the programmes LUDI for de *novo* design and FlexX for ligand docking, are becoming more and more important. These techniques will be further extended by a combinatorial design of ligands in their binding site.

10.30 Refreshment Break & Opportunity to Visit Exhibition

11.00 The Value of Combinatorial Chemistry to Boost Diversity for Lead Discovery
Dr Matthias Schwarz, Scientist, Department of Chemistry
Serono Pharmaceutical Research Institute, Switzerland

11.45 Cost Effectiveness Versus Traditional Compound Generation
(TBC) Dr Robin W Spencer, Assistant Director, New Leads Chemistry & Biology
Pfizer Central Research, USA
The economic valuation of combinatorial and parallel methods depends on the tasks to which they are applied, our observed successes and failures to date, and a cost/benefit analysis of alternatives. This presentation will provide examples from our lead discovery experience in an overall cost/benefit context.

12.30 Lunch & Opportunity to Visit Exhibition

Proof of Concept Case Studies: Successful Identification of Lead Compounds Through Combinatorial Approaches

13.30 Strucure-Based Computational Screening of Virtual Combinatorial Libraries & its Application to the Discovery of Novel Serine Protease Inhibitors.
Dr Stephen C Young, Head of Synthetic Chemistry
Proteus Molecular Design Ltd, UK
Case Study
Combinatorial Chemistry and Structure-Based Drug Design have shown themselves to be effective methods for finding lead compounds but each has limitations. A new approach, which combines benefits of both methodologies without some of the deficiencies, is now coming to the fore. This comprises building a virtual combinatorial library which is screened for complementar against a receptor structure. The resulting focussed sub-library, in theory, has a higher hit per compound ratio than a random and diverse library of related chemistry. Here we describe how our PRO_SELECT methodology has been used to create small librari targeted against the therapeutically important serine proteases thrombin, trypsin and factor Xa. A high proportion of 'hits' were obtained. For factor Xa the process was used iteratively starting from a small template molecule. This ultimately led to a series of potent and selective molecules with strong clinical potential. Whi we have exemplified this approach in cases with well defined structure using very small but diverse libraries, the same approacl could be used in designing slightly larger combinatorial libraries focussed on targets with less clearly defined structures.

14.15 Discovery of New Medicinally Useful Agents: Novel Anti-infectiv Versus Resistant Gram-Positive Bacteria
Dr James R Hauske, Senior Vice President, Discovery
Sepracor Inc., USA
Case Study
We have synthesized a series of novel molecules via combinatoria methods, which demonstrate very interesting *in vitro* and *in vivo* activity versus resistant gram-positive infections. In this study, combinatorial methods provided both lead-seeking and lead optimisation libraries, which were linked to a variety *of in vitro* ADME, toxicological and physico-chemical property screens affording compounds with more useful, drug-like properties. This presentation will describe:
(1)Solid and solution phase combinatorial approaches to a novel structure class of small molecules.
(2)Lead generation and lead optimisation.
(3)*In vitro* assessment of antibacterial activity versus resistant gram-positive organisms.
(4)*In vitro* ADME assessment and optimisation of lead structures
(5) *In vivo* assessment of the optimised lead structures.

15.00 ROUND TABLE DISCUSSION
Is Combinatorial Chemistry Living Up to Its Claims of Accelerati and Increasing Productivity in Drug Discovery? How Does Your Company Measure the Success of Combinatorial Chemistry Efforts? What are the Defining Factors of Success? When and/or will the industry see the benefits in terms of successful clinical candidates? What is the future of Combinatorial Chemistry in Lea Optimisation?

16.00 End of Conference

COMBINATORIAL CHEMISTRY - IT1129
23rd - 24th June 1999, The Merchant Centre, London

EXPLOITING THE PROMISE OF COMBINATORIAL CHEMISTRY - DY1134
25th June 1999, The Merchant Centre, London

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Combinatorial Chemistry 99

Novel Strategies, Chemistry, Purification & Chemoinformatics

Wednesday 23rd – Thursday 24th June 1999, The Merchant Centre, London

- Hear What Strategies and Library Designs are being Adopted by Your Competitors
- Learn about Novel Chemistries that Researchers are Developing
- Familiarise yourself with the Latest Purification and Characterisation Techniques an Applications in Development
- Update yourself on how Combinatorial Chemistry is being Used in Lead Optimisation and other Industrial Applications
- Listen to Overviews of Architecture, Software Tools and Strategy being Used and Designed to Manage and Analyse Chemical Data

PLUS

Exploiting The Promise of Combinatorial Chemistry

Successful Strategies & Proof of Concept Case Studies

Friday 25th June 1999

- Is Combinatorial Chemistry Living Up to Its Claims of Accelerating and increasing Productivity in Drug Discovery?
- How Does Your Company Measure the Success of Combinatorial Chemistry Efforts?
- What are the Defining Factors of Success?
- Hear Case Studies of Some Success Stories of Compounds in Clinic

"The motivating theme for combinatorial chemistry might be to be able to make a million variants of any structural template and screen them. Cheaper and faster are better. When we can accomplish this within a week, then perhaps the intellectual challenges will be gone. However, I can assure you that we are far, far from that vision today" – Dr Anthony W Czarnik, Vice President for Chemistry, IRORI **Chemical & Engineering News, April 6, 1998**

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COMBINAT
NOVEL STRATEGIES, CHEMISTRY

WEDNESDAY 23RD – THURSDAY 24TH JUNE 1999 ● THE MERCHANT CENTRE, LONDOI

Evolution of Combinatorial Chemistry

Within the last 10 years, combinatorial chemistry has been largely adopted by the pharmaceutical and biotechnology industries. From the first technological developments to the current widespread integration into discovery and other applications, there are questions being raised as to the ultimate quality and diversity of the leads it has generated for drug discovery.

This year's conference highlights:

- Recent developments in strategy and library design
- Cutting-edge chemistries
- Novel techniques for purification and characterisation
- Different applications of Combinatorial Chemistry
- The use of IT, software and chemoinformatic tools in design and analysis
- Exploiting the promise of Combinatorial Chemistry and successful strategies
- Highlights of Proof of Concept studies on leads generated by Combinatorial Chemistry

What some of our delegates said about our previous Combinatorial Chemistry conferences?

"This event was a powerful learning tool and a mixing pot of personal experiences" – Mrs Ana Reis-Machado, Labor Qualitas

"Consistently high standard covering topics of current interest" – Dr David Brown, Associate Research Director, Glaxo Wellcome R&D

"Good overview of the field. Unique place to share ideas/opinions" – Dr Gilbert Marciniak, Synthelabo Biomoleculaire

Who Should Attend This Years Conference?

Vice President/Director/Heads of Medicinal Chemistry and Le Discovery * Group Leaders and Laboratory Heads * Resear Scientists * Senior Management and Corporate Strategists * Softwa and Chemoinformatic Specialists *

Wednesday 23rd June 1999

09.00 Coffee & Registration

Recent Developments in Combinatorial Chemistry Strategy & Library Design

09.30 The Trend Towards Design in Focussed Libraries

Dr Mike Hann, Computational Chemistry Group Leader
Glaxo Wellcome R&D, UK

The technologies of library synthesis and HTS allow us to make huge numbers of molecules and screen them. However, the futility of doing this in the absence of some strategy as to what to make as appropriate molecules for lead generation and optimisation into drug like molecules has become apparent. For instance, there will always be more potential molecules that could be made than can be screened, so choices must be made. The *in silico* world of virtual libraries is where this choice is increasingly being done. The background of and the potential for success with these methods will be discussed and illustrated with a range of techniques that are in use at Glaxo Wellcome.

10.15 Pitfalls That May Arise In the Design of a Combinatorial Library: Similarity & Dissimilarity

Professor Dr Hugo Kubinyi, Combinatorial Chemistry & Molecular Modelling
BASF AG, Germany

Chemically related compounds most often have similar biological activities. This fundamental relationship has led to the discovery and stepwise optimisation of many valuable drugs. However, several examples will be discussed where presumably closely related compounds show very different modes of action and/or biological potencies.

11.00 Refreshment Break & Opportunity to Visit Exhibition

11.30 Application of Polymer-bound Chalcogenes as Novel Traceless Linkers in Solid Phase Synthesis

Dr Thomas Ruhland, Research Chemist, Department of Combinatorial Chemistry
H Lundbeck A/S, Denmark

The development of a novel traceless linking strategy for the solid-phase synthesis of small non-peptide compounds by the use of resin-bound selenium is described. Compounds were attached by direct loading without the requirement of an auxiliary spacer. We demonstrate the synthesis of a small sized library of single alkyl aryl ethers with two points of diversity by the Mitsunobu reaction. The selenium-alkyl bond that attaches the alkyl aryl ethers to the resin was smoothly cleaved under radial conditions by homolysis with tributylstannano and catalytic amount of AIBN to generate an aliphatic C-H bond in the liberated ethers. The selenium atom remains immobilised during the entire synthesis, and in the cleavage step, tributylstannyl phenyl selenide is scavenged on the resin. Reaction monitoring was facilitated by the use of gradient high-resolution magic angle spinning 2D-NMR. This new linking method can be applied to solid-phase synthesis of many classes of organic compounds under a brand variation of reaction conditions.

12.15 RECAP-Retrosynthetic Combinatorial Analysis Procedure: A Powerful New Technique for Identifying Privileged Molecular Fragments With UsefulApplications in Targeted Libraries

Dr Duncan B Judd, Group Leader Lead Design, Discovery Technology
Glaxo Wellcome R&D, UK

RECAP is a powerful tool for identifying biologically privileged fragments for use in the synthesis of targeted libraries. The RECA technique involves the use of databases of compounds with know biological activity which are 'cleaved' electronically at bonds amenable to combinatorial chemistry. The fragments and motifs can be readily used as building blocks to prepare combinatorial libraries rich in biologically privileged substructural motifs. Thes libraries may be used in lead generation or lead optimisation. Th paper will discuss the principles of the technique and illustrate w specific examples.

13.00 Lunch & Opportunity to Visit Exhibition

Novel Developments in Chemistry, Characterisation, Purification Techniques & Other Applications

14.00 Combinatorial Chemistry: Recent Advances in the Enlistment of Soluble & Insoluble Polymer-Supports

Dr Paul Wentworth, Jr., Assistant Professor, Department of Chemistry
The Scripps Research Institute & Skaggs Institute for Chemical Biology,
USA

Soluble polymers as supports in traditional organic synthesis and combinatorial chemistry are undergoing a rapid re-evaluation. New soluble polymer-supported catalysts, reagents and synthetic targets will be described, with major emphasis focusing on their application as adjuncts to solution-phase library development. In parallel, new resin-supports for solid-phase chemistry have been developed by a novel cross-linking strategy and the physicochemi properties and utility of these beads will be discussed.

14.45 Catch and Release and Resin Capture Strategies for Expedited Workup and Purification

Dr Bernd Renneberg, Applications Chemist
Argonaut Technologies AG, Switzerland

- Basic elements of catch and release and resin capture strategie
- Scavenger resins
- Polymer bound reagents
- Parallel synthesis using the catch and release and resin capture technique

15.30 Refreshment Break & Opportunity to Visit Exhibition

16.00 High Throughput Parallel LC/MS Characterisation & Mass Activated Fraction Collection of Combinatorial Arrays Using oa-TOF & Quadrupole Technology

Dr Ashley B Sage, Project Leader – LC/MS Applications
Micromass UK Limited, UK

With advances in automated parallel synthesis, the construction large combinatorial arrays has become possible but this has resul in a corresponding challenge for the analyst to provide meaningf information on such large sample libraries. In this presentation th

use of LC/MS in combinatorial chemistry type of applications will be discussed with reference to the following topics:

- Automated high throughput characterisation and exact mass determination of synthetic arrays using an orthogonal acceleration time-of-flight (oa-TOF) mass spectrometer
- The design and implementation of a multiplexed electrospray system integrated into a Micromass LCT (oa-TOF) that is capable of rapidly sampling multiple liquid streams in rapid succession, facilitating sample analysis throughput
- Multi-milligram quantity purification of compounds below required purity using both reverse and normal phase HPLC conditions
- Fraction collection by mass activated LC/MS (quadrupole) including automated sample tracking/reporting

16.45 Performance of Parallel, Automated SPE for Purification of Library Products & Bioanalytics
Dr Christoph Fraudeau
Gilson Medical Electronics, France

17.30 *Networking Cocktail Reception*
Delegates and speakers are invited to an informal networking reception in the exhibition after the days presentations

18.30 End of Day One

Thursday 24th June 1999

09.00 Coffee

Novel Developments in Chemistry, Characterisation, Purification Techniques & Other Applications

09.30 Integrating Parallel Purification, Characterisation, Quantitation & Combination/Evaporation
Dr Janice A Ramieri, Product Manager & Patrick Coffey
Biotage, A Division Dyax Corporation, USA
We have defined a specification for High Throughput Organic Chemistry (HTOC) that is designed to transfer crude reaction mixtures to purified compounds of known identity and weight and then to reconstitute them into a format compatible with downstream assay procedures. In order to efficiently and cost-effectively produce libraries of purified synthetic organic compounds; all the processes involved must be integrated to enable rapid material and data transfer.

10.15 Combinatorial Approaches in Catalysis
Dr Thomas Bradshaw, President
The Catalyst Group, USA

- Synthesis of catalysts using combinatorial approaches
- Evaluation of catalysts activity using robotic/combinatorial systems
- Process development for novel reactions including catalysts using combinatorial systems

The presentation will also include an overview of each area with currently active players and the state of development in each area with projected future development directions.

11.00 Refreshment Break & Opportunity to Visit Exhibition

Chemoinformatics & Analytical Tools

11.30 Information Management for CombiChem: Integrating Synthetic, Structural, and Analytical Data
Dr David Chapman, President
Afferent Systems, USA
High throughput chemistry produces a deluge of data, including synthetic protocols, compound structures, sample information such as vessel locations and synthetic history and analytical information (spectra and chromatograms). This presentation will describe a chemistry knowledge base architecture that goes beyond traditional chemoinformatics systems to integrate, organise and make sense of these divergent data types.

12.15 Novel Ways to Code Chemical Structures for Correlating Biologi Activity & Determining Chemical Diversity
Professor Dr Johann Gasteiger, Computer Chemie Centrum, Institute of Organic Chemistry
University of Erlangen Nuremberg, Germany

- Hierarchy of structure representation of molecules for: constitution; 3D structure & molecular surfaces
- Rapid, broadly applicable generation of 3D structures
- Handling conformational flexibility
- Neural networks for similarity perception and quantitative modelling of biological activity
- Comparison of libraries of compounds by neural networks
- Definition of similarity and diversity of combinatorial librarie
- Quantitative structure-activity analysis

13.00 Lunch & Opportunity to Visit Exhibition

14.00 Structure Elucidation Software
Dr Herbert Thiele, Manager Software Development
Bruker Daltonik GmbH, Germany
This presentation will provide a summary of software tools for automatic structure elucidation based on different spectroscopic methods:

- Spectroscopic database plus management system for archiving and interpretation of NMR spectra
- Structure generator
- NMR-Spectrum simulation-iteration

14.45 Does 'More Diverse' Mean 'More Informative'?
Dr Nick Perry, R&D
Knoll Pharmaceuticals, UK
Much effort has been expended in devising methods to select structurally diverse subsets from compound libraries with the implicit assumption that 'more diverse' is better. This paper presents a validation study in which the relationship between chemical and biological diversity is explored

15.30 Refreshment Break & Opportunity to Visit Exhibition

16.00 Enhancing the Hit-to-Lead Properties of Diverse Libraries
Dr David E Clark, Research Fellow Computer-Assisted Drug Design
Rhone-Poulenc Rorer, UK

- Challenges posed by HTS and combinatorial chemistry to computational chemistry
- Application of heuristic optimisation strategies to combinatori library design
- Product-based reagent selection using multi-pharmacophore descriptors
- Designing in "drug-like" properties

16.45 Implementation of ChemSpace in the Production of Designed Libraries of Chemical Compounds
Dr Tony Cooper
Tripos Receptor Research, UK
Techniques for the high throughput synthesis of large chemical libraries have developed rapidly over the last few years. For libraries of single compounds with defined structure and purity, tl current challenge lies in high throughput analysis and purificatio technology. An outline of our work in the above areas will be given. Our implementation of ChemSpace for the generation of focused or diverse libraries, within this process, will be described

17.30 End of Conference

Combinatorial Chemistry '99

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By attending this conference our delegates have demonstrated their interest in the field of combinatorial chemisty. You can target this highly focussed audience by raising your company profile through sponsorship of the event, or simply through exhibiting in the networking forum.

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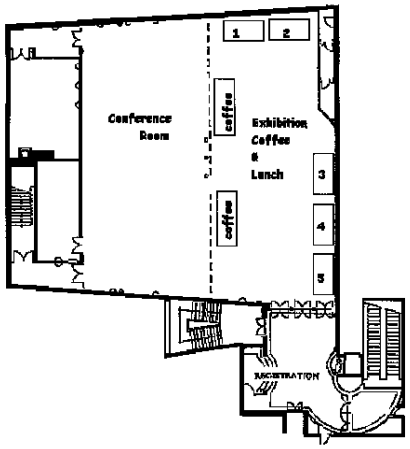

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