ROYAL SOCIETY OF **CHEMISTRY** | CHEMICAL INFORMATION AND COMPUTER APPLICATIONS GROUP
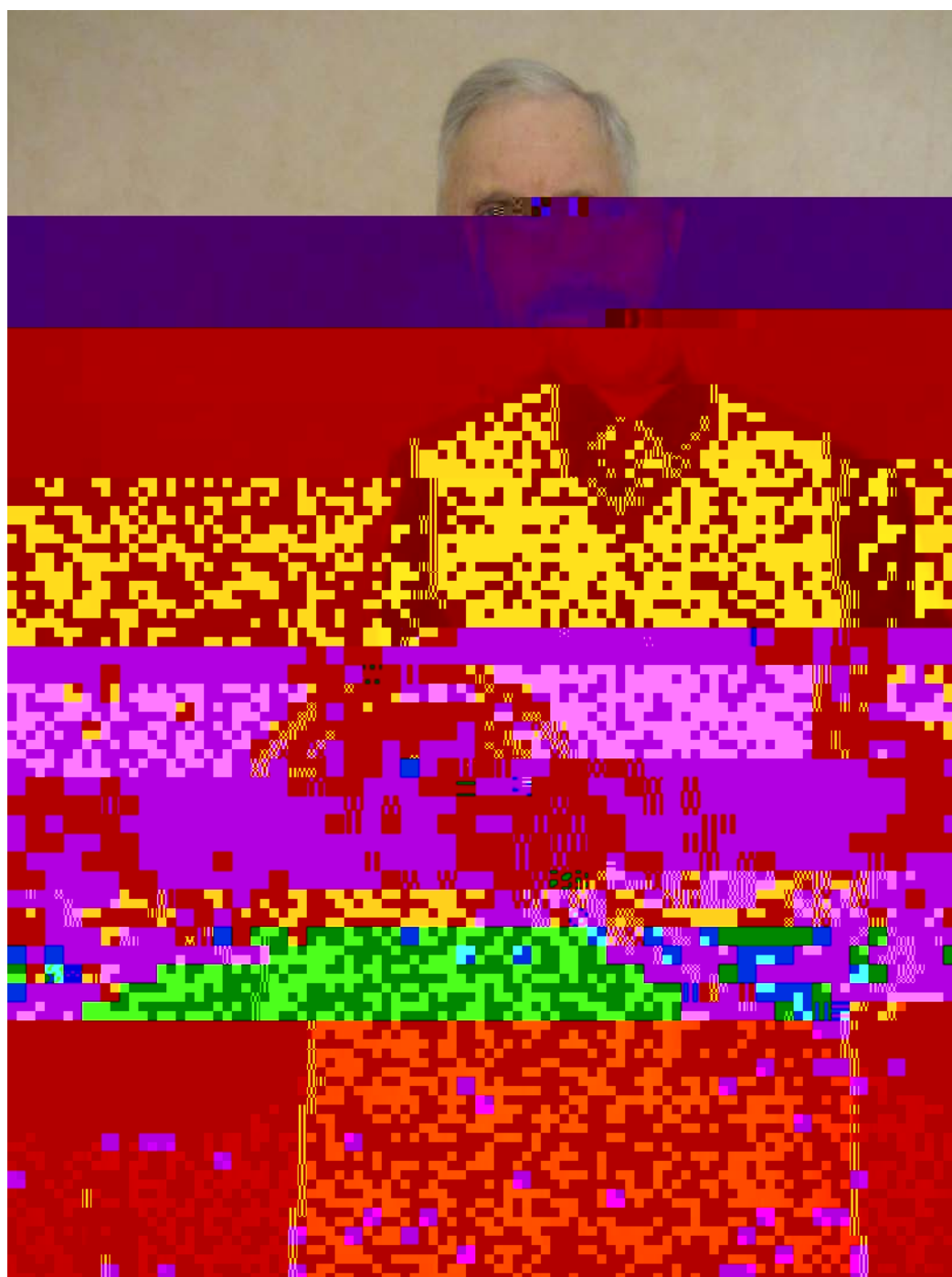
NEWSLETTER Winter 2015

Recognition for Doug Veal's long service

Proposed CICAG Meetings for 2016

x   **Mobile chemistry: content, compute, collaborate**

x   **Chemical structure representation: what would Dalton do now?**

x   **"Chemoinformatics for Drug Design"**

Meeting Report: Measurement, Information and Innovation Digital Disruption in the Chemical Laboratory

Contributed by RSC CICAG Chair Dr Helen Cooke

x
x
x

- x The purpose, praticalities, pitfalls and policies of managing and sharing data in the UK.

- x Allotrope Foundation, how a data standard and taxonomy for analytical data will support data integration and knowledge generation.

- x Why we should embrace learnings from other industries.
- x HELM (Hierarchical Editing Language for Macromolecules): A Pistoia Alliance project providing a standard for the storage and exchange of macromolecule structural information in the information ecosystem

- x Ensuring the machine learner gets the right tuition and AI gets its nose; standardisation and benchmarking in diagnostic marker discovery in exhaled breath.

- x Building the utopian dream – toward the integrated, paperless drug discovery lab.

- x Using machine learning and cloud technologies for point of care in vitro diagnostics.

- x Enabling creative scientists to focus on science: automation, workflows, dashboards, insight, aha!!!

- x Building the links

Tony Kent Strix Award

The UK e-Information Group, Geological Society, Burlington House, 6th. November 2015

Speakers at the 2015 Tony Kent Strix Annual Lecture
Susan D5(e)-4/P <</Md databSpe Tm Kent Ste Q BT /P <<(t)u1veJ BT196k.W.003 y <<(t

was the result successful? Were people happy with the results?

http://research.microsoft.com/~sdumais

Other Awards –Calls for nominations

CSA Trust Grants

2017 Herman Skolnik Award: Call for Nominations

Closing date: 1st June 2016

2016 Lucille M. Wert Scholarship: Call for Applications

Closing date: 1st February 2016

2016 CINF Scholarship for Scientific Excellence: Call for Applications.

Other Awards –Recent Recipients

2016 Herman Skolnik Award   **Stephen Bryant**   **Evan Bolton**

Dr Stephen Heller Receives the 2015 Patterson-Crane Award

Jason Farradane Award   **Sheila Webber**

Student Bursaries

Chemical Information / Cheminformatics and related Books

1. [In Silico Medicinal Chemistry: Computational Methods to Support Drug Design](link), Nathan Brown, RSC Nov 2015

The third section considers statistical learning methods, an integral aspect of computational drug discovery, and some of the best methods we have to investigate different properties. An introduction to

National Chemical Database Service News

British Patent Information Professionals Presentations: "A Day in the Life of an Independent Patent Searcher"

X

PatentPak Key Features

X
X

X

X

Trials for PatentPak on STN are now available.

Derwent Markush Resource (file name DWPIM) on STN® - The unified solution for generic chemical structure searching comes true

CAS Training in the UK 2016

CAS Training in the UK 2016

Other Meetings/Conferences in 2016

Other News Items

Understanding Impact Factors

Dept. for Business, Innovation and Skills, metrics and non-selective QR allocation

Many InChIs and quite some feat

Digital Instructional Materials Gaining Ground in Science/STEM Education

DCL Announces Technology Breakthrough at USPTO: Over 1 Million Pages Each Month Automatically Transformed Into Searchable, Minable Content

Elsevier Solutions Address the Challenges of Lead Optimization in Early Drug Discovery

Chemical Information and Computation 2015, Number One. 249th ACS National Meeting and Exposition