

Keeping up the momentum: Brief report from the InChI San Diego workshop

Ray Boucher
Richard Kidd

Three strategic pillars

Global adoption and use

Increasing engagement with the chemistry community for the benefit of science and business



Maintenance & extension of the InChI and applications

To facilitate rapid and effective research discovery and business innovation



Governance

To provide an organizational framework that ensures the sustainability of the standard



Rolling workshops

Mar 2017 – EBI Hinxton

Aug 2017 – NIH Bethesda

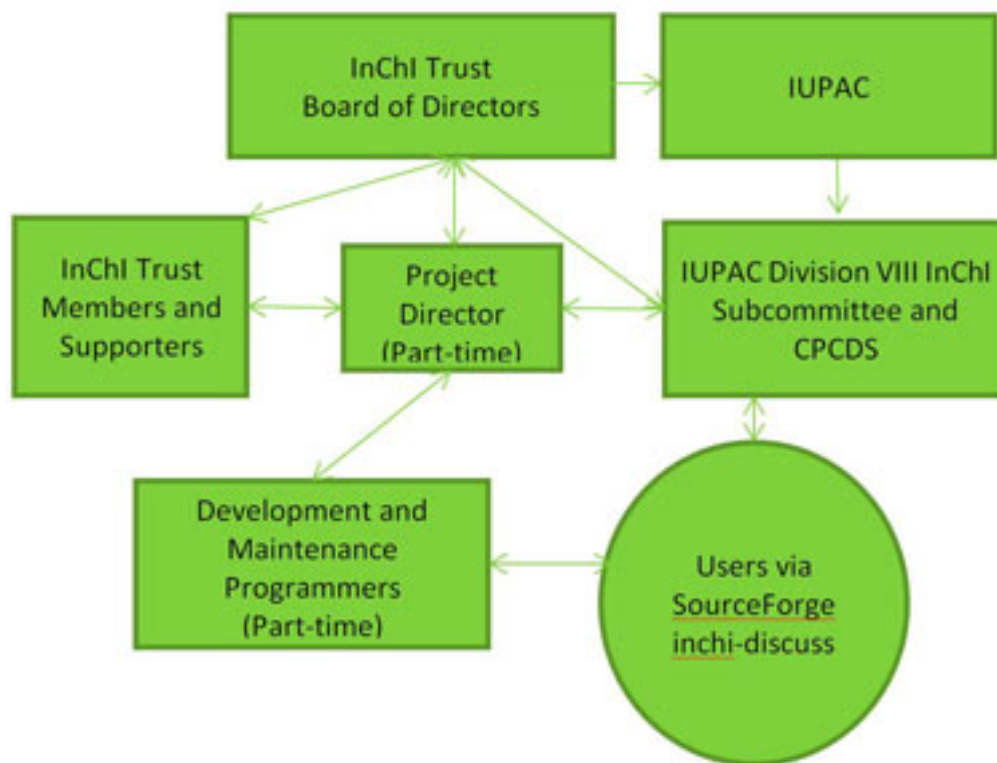
Aug 2018 – Boston MA

Feb 2019 – Cambridge UK

Jun 2019 – IUPAC InChI Subcommittee meeting, Paris

Aug 2019 – San Diego CA

Governance



San Diego 23-24th

Community perspectives

Steve Boyer	Patents
Steffen Pauly	Deposit from publications to public databases
Lutz Weber	Ontologies
Tina Qin	Teaching InChI to chemistry students
Peter Linstrom	WebBook
Bob Belford	Education - InChI OER
Hunter Moseley	Isotopologues
Richard Kidd	Open Source development for InChI
Roger Sayle	SMILES and IUPAC
Yulia Borodina	FDA - recent developments, current challenges
Markus Bussen	ChemChain

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Project and working group updates

Ian Bruno	Organometallics
Alex Clark	Mixtures, MInChI
Richard Hartshorn	QR Codes
Gerd Blanke	Reaction InChI, RInChI
Andrey Yerin	Polymers
Marc Nicklaus	Tautomers
David Deng	HELM Update
Vin Scalfani	IUPAC SMILES+

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Working group breakouts

Gerd Blanke	Reaction Inchi, RInChI
Andrey Yerin	Stereochemical configuration
Leah Rae McEwen, Evan Bolton	Large Molecules - complementarity w/ HELM, w/ Mixtures
Bob Belford	Education - InChI OER
Andrey Yerin	Stereochemical configuration
Vin Scalfani, Greg Landrum	SMILES+

**And where
are we now?**

**Where are we
going?**

**What
should we
do?**

**What can
we do?**

**How far?
Extension vs
application?**

**Do we widen the
coverage, to new
areas (and areas
well outside
traditional
chemistry)?**

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Panel sessions

Ray Boucher	How to broaden community engagement
Jonathan Goodman	Small molecule variability
Marc Nicklaus	InChI 2.0

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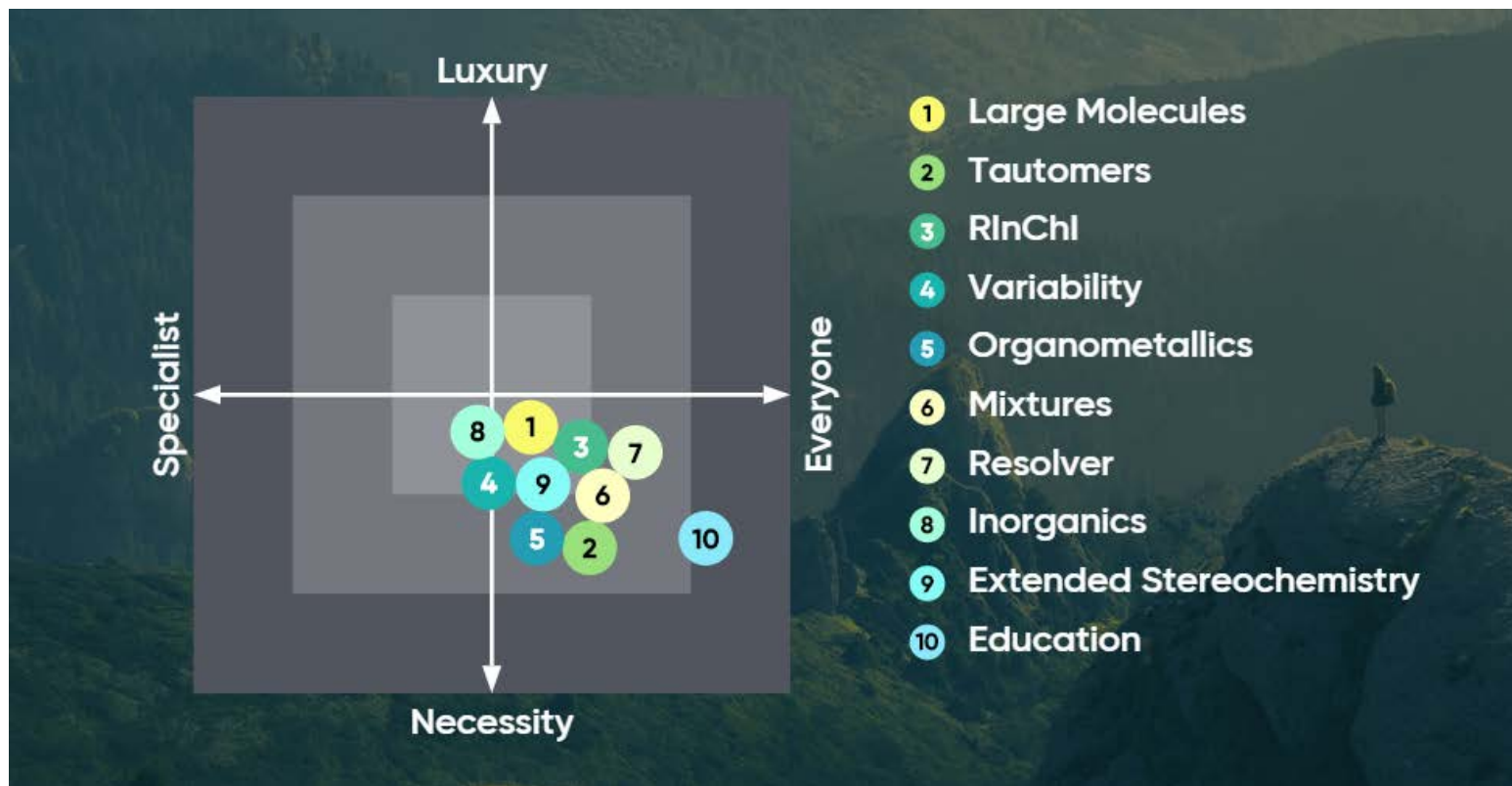
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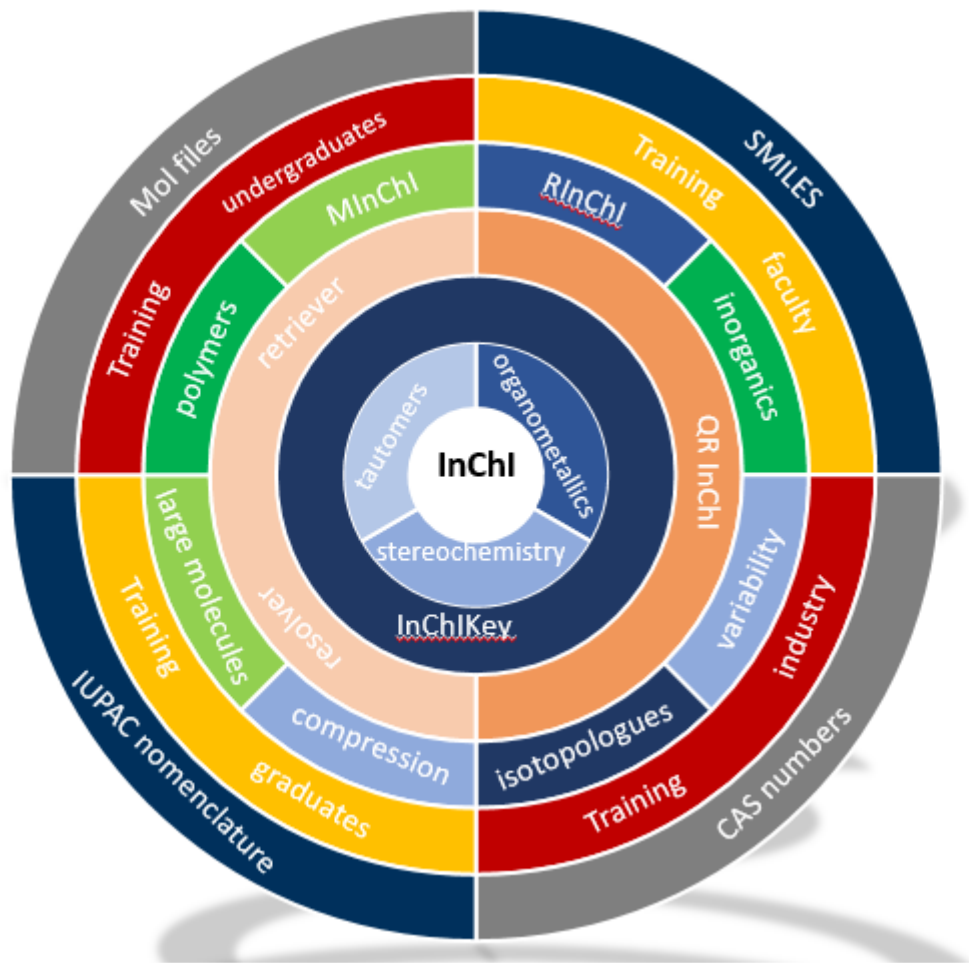
**How far?
Extension vs
application?**

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Most important?



(n = 18) additional votes welcome, [menti.com](https://www.menti.com) then add code 70 93 99



InChI
canonical
representifier
for molecules

Next meetings

Similar symposium/workshops

San Francisco Aug 2020

**Thanks to all involved:
contributors, participants,
organisers**



InChI TRUST

How far we've come...



FAXGPCHRFPCX00-LXTPJMTPSA-N



Include non-patent literature (Google Scholar)

Search and read the full text of patents from around the world.

