

Chemistry Add-In for Word

<http://research.microsoft.com/chem4word/> <http://chem4word.codeplex.com>

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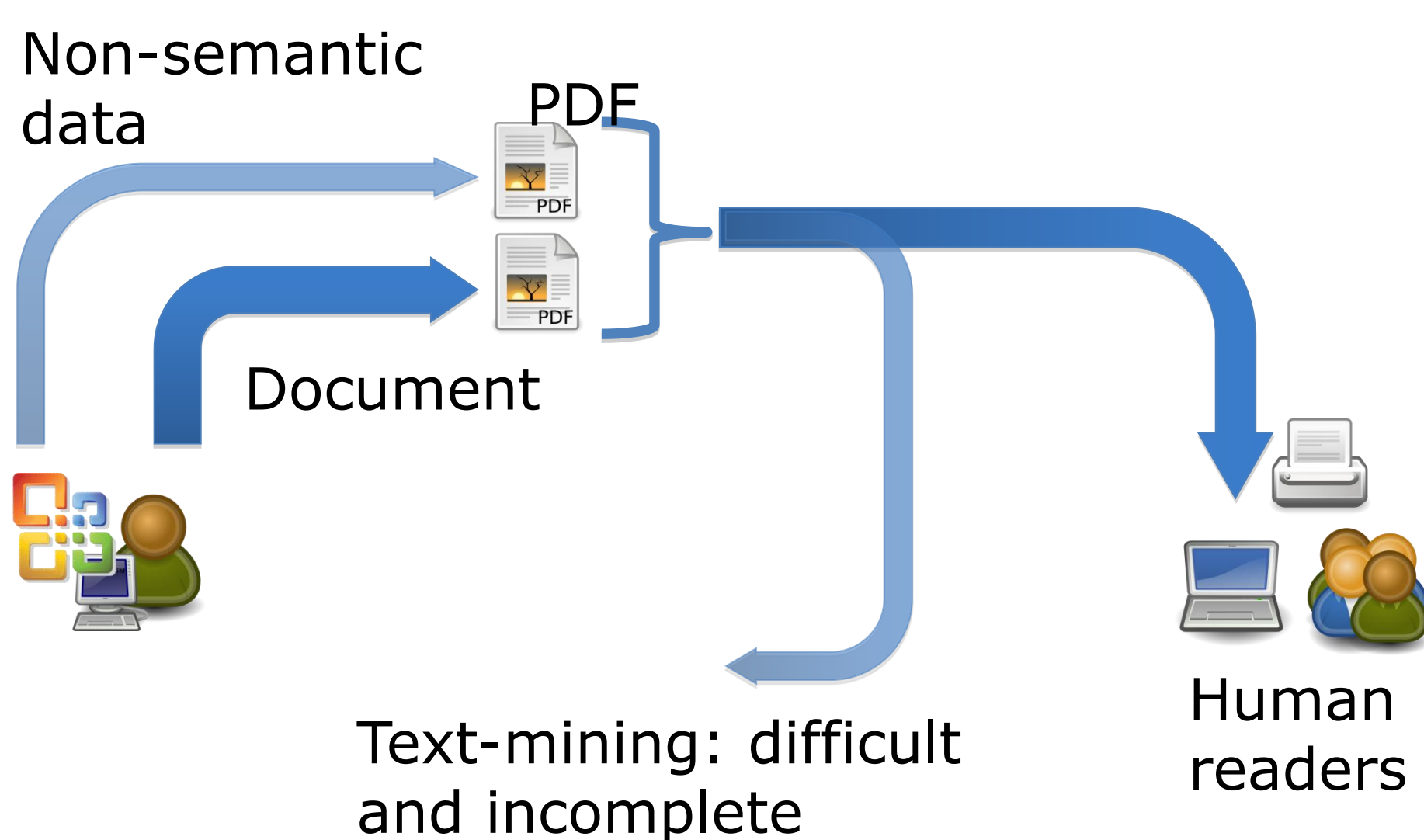
Semantically Editing Chemistry in Word

People (UoC) Peter Murray-Rust, Joe Townsend, Jim Downing. (Microsoft) Lee Dirks, Alex Wade, Oscar Naim, Mike Galos, Tim Haughton.

The Chemistry Add-In for Word, is an open source program that allows chemists to create, edit and manipulate chemistry (labels and 2D structures) in the Word environment. The on screen representation is backed by semantic data in Chemical Markup Language (CML). Combined with domain aware libraries we enable novel functionality in data checking during the authoring process, chemistry-centric article reading support and data-mining applications.

Current publishing practice

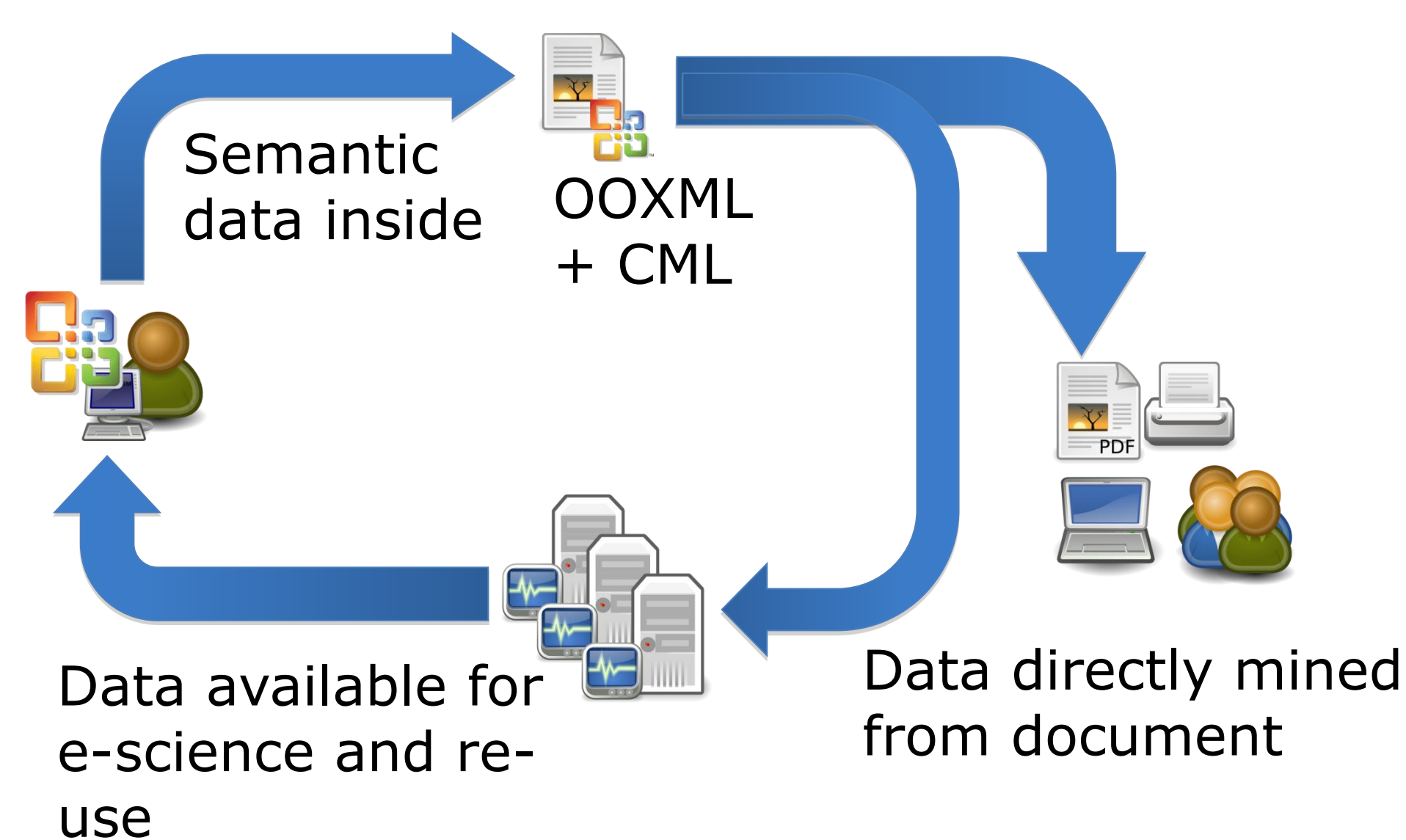
... is broken for data-rich science



- Data publication difficult and unsupported
- Insufficient data to fully support research

With Chemistry Add-In for Word

... the cycle is closed



- Data preparation integrated into user workflow
- Open Standards promote Open Semantic Science

The Add-In (.NET) links a semantic chemistry engine (.NUMBO) through a command interface (CID) to a chemistry zone. Chemistry zones are textual or graphic renderings within a Word document (DOCX). All content and relationships are bound to CML in the DOCX package.

Preparation of 4-(tert-butyl-dimethyl-silyloxy)butyne

To a solution of butynol alcohol **154** in DCM (250 ml) at 0°C was added TBDMS-Cl (1.02 eq, 0.24 mol, 36.18 g) and DMA (MW=122.17, 200 mg, 1.6 mmol). Et₃N (MW=101.19, bp=89°C, 0.25 mol, 25.29 g = 34.8 ml) was subsequently added via syringe and the reaction mixture stirred at 0°C for 2 h, after which it was warmed to rt and stirred for a further 6 h, until completion as judged by tlc. The mixture was poured onto saturated NH₄Cl solution (800 ml) and extracted with Et₂O (3 x 300 ml). The combined organic extracts were washed with brine (500 ml) and dried (MgSO₄), filtered, and concentrated *in vacuo*, yielding an oil which was purified by filtration through a pad of SiO₂ (eluent PE:Et₂O 10:1) giving compound **170** (36.10 g, 19.6 mmol, 83%) as colourless oil.

The navigator gives an overall view of the chemistry in the document and allows users to insert linked or copied data.

Domain aware software and semantic data allows intelligent context menus to help users.

Different representations of the same data – all linked to the same backing CML.

A complete record of the changes to the data is retained in the customXML.

```
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