ROYAL SOCIETY OF CHEMISTRY

Data and Data Science at the Royal Society of Chemistry

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How the RSC deals with crystallographic data during peer review

Validation

Deposition

The reviewer can access the crystallographic structure in the CCDC database.

Peer Review

Paper submission

Paper accepted

After the paper is accepted, the CIF can also be made available in ChemSpider.
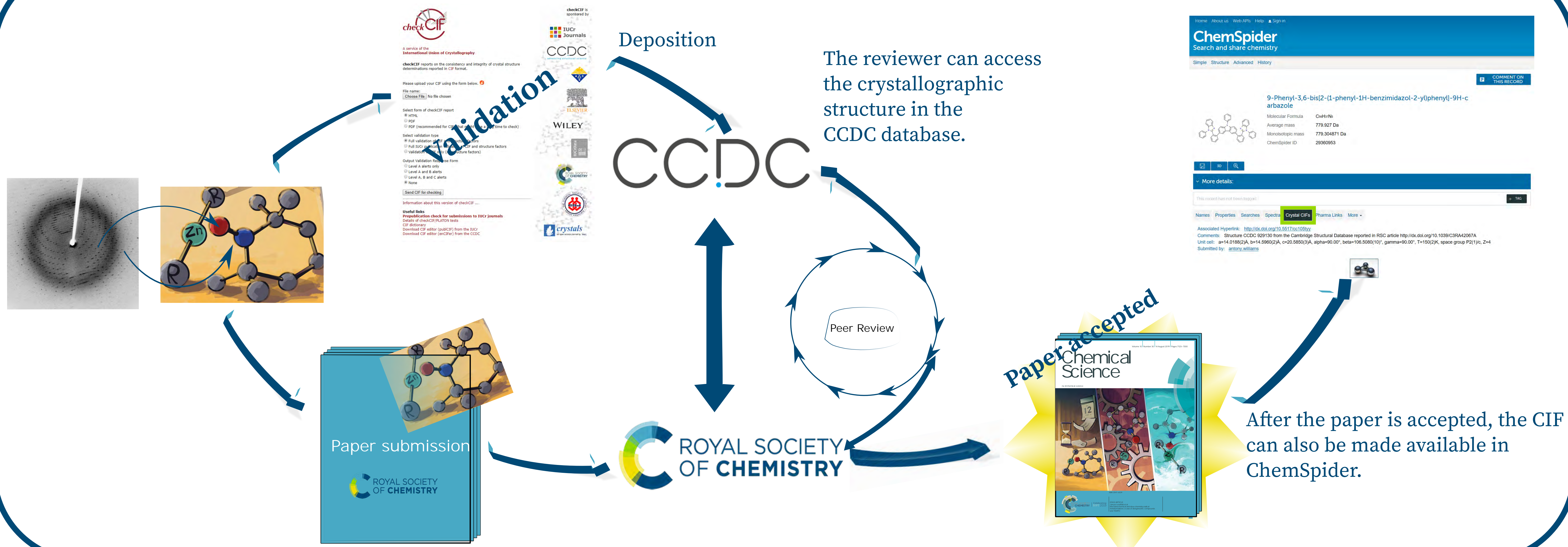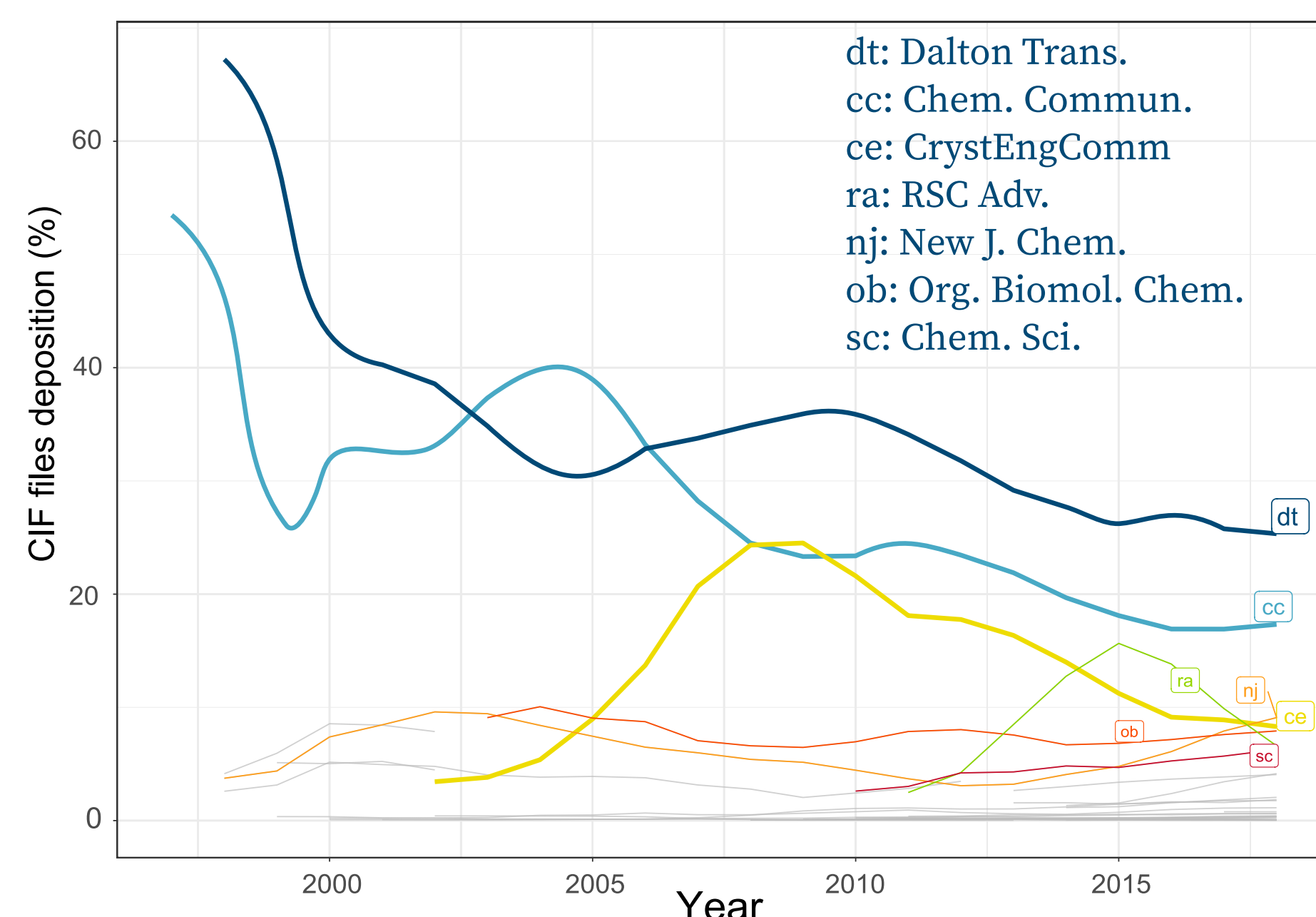
RSC journals and crystallography

Journals with most structures in the CSD.

Inorg. Chem. (ACS)
Organometallics (ACS)
Dalton Trans. (RSC)
J. Am. Chem. Soc. (ACS)
Acta Cryst. Section E (IUCr)
Polyhedron (Elsevier)
J. Organomet. Chem. (Elsevier)
Inorg. Chim. Acta (Elsevier)
Chem. Eur. J. (Wiley)
Chem. Commun. (RSC)
Angew. Chem. Int. Ed. (Wiley)
Acta Cryst. Section C (IUCr)
Z. Anorg. Allg. Chem. (Wiley)
Tetrahedron (Elsevier)
J. Org. Chem. (ACS)
Eur. J. Inorg. Chem. (Wiley)
CSD Communications (CCDC)
CrystEngComm (RSC)
Cryst. Growth Des. (ACS)
Acta Cryst. Section B (IUCr)

% CSD   Data source: (2016). Acta Cryst. B72, 171-179.
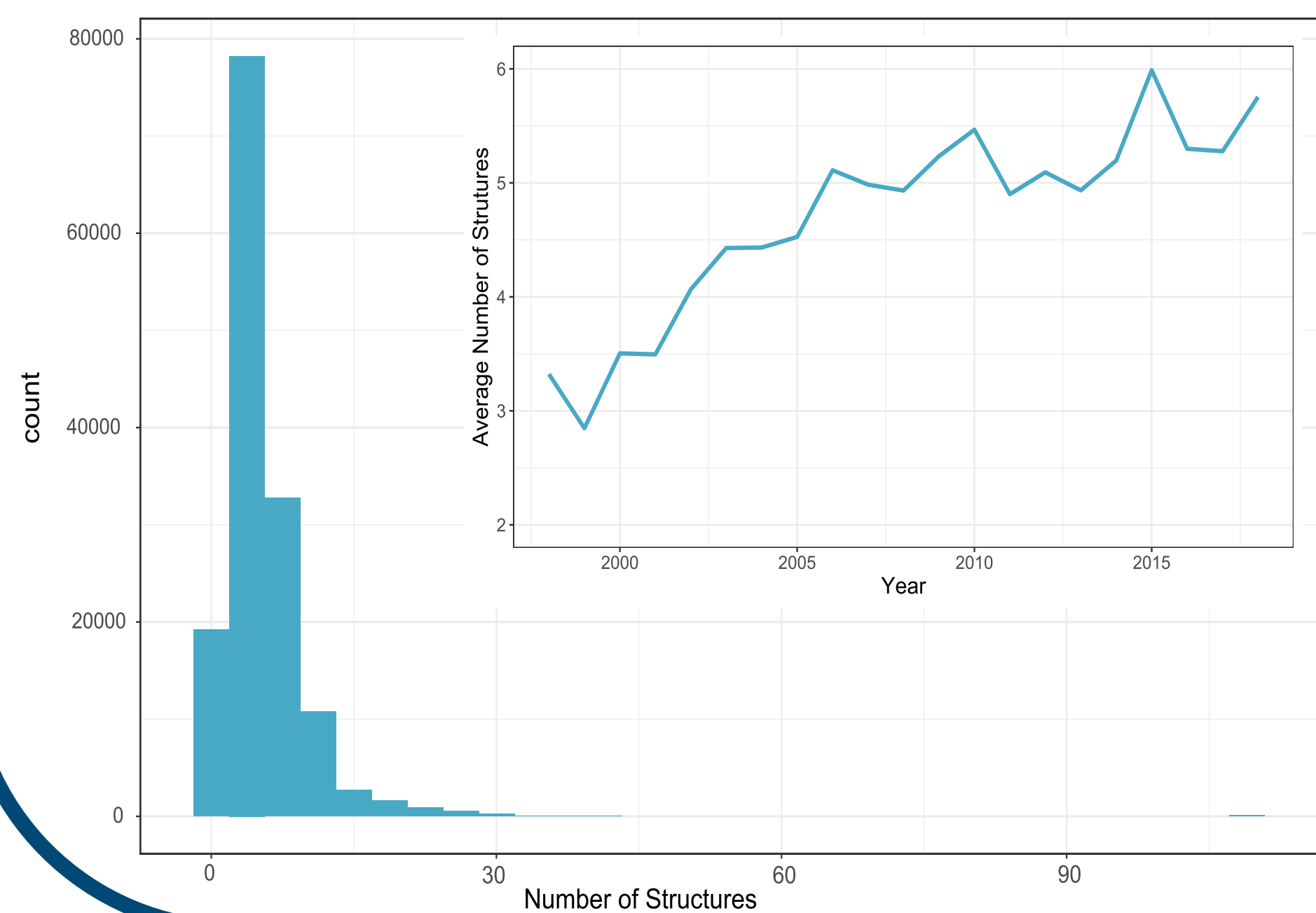
CIF files per journal. This value is normalised to the total number of CIF files that the RSC receives each year.

dt: Dalton Trans.
cc: Chem. Commun.
ce: CrystEngComm
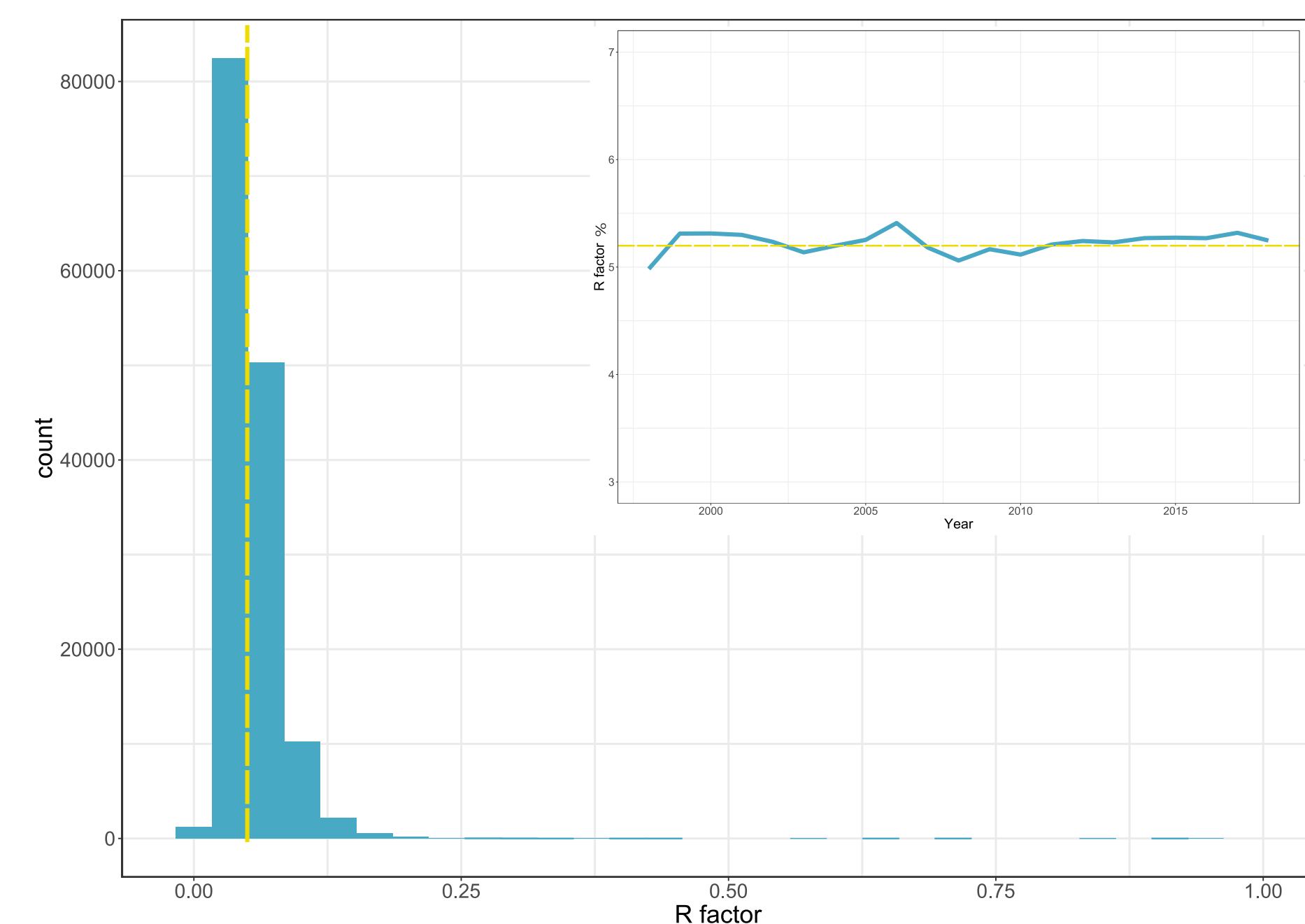ra: RSC Adv.
nj: New J. Chem.
ob: Org. Biomol. Chem.
sc: Chem. Sci.

The mean number of structures per article is about 5.2. The average number of structures per article has increased in the last 20 years.

The most downloaded CIF files from 2015 to the present.

J. Mater. Chem. A, 2013, **1**, 5628-5641
Chem. Commun. 2007, 2820-2822
Chem. Commun., 2012, **48**, 9831-9833
Chem. Commun., 2006, 284-286
Chem. Commun., 2008, 4732-4734
Chem. Commun., 2006, 959-961
Chem. Commun., 2010, **46**, 767-769
CrystEngComm, 2013, **15**, 654-657
Chem. Commun., 2011, **47**, 8037-8039
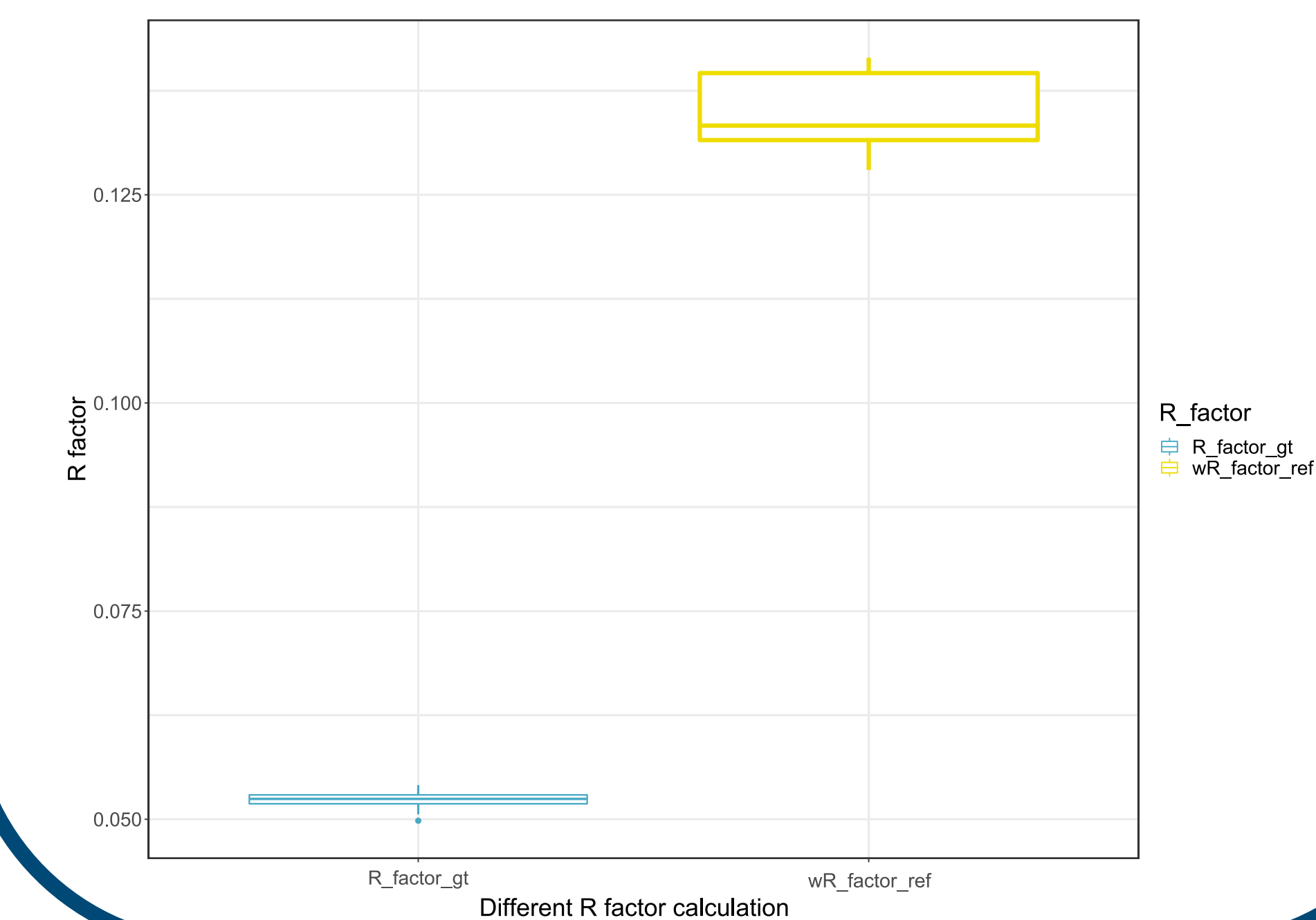Chem. Commun., 2006, 1488-1490

R-factor

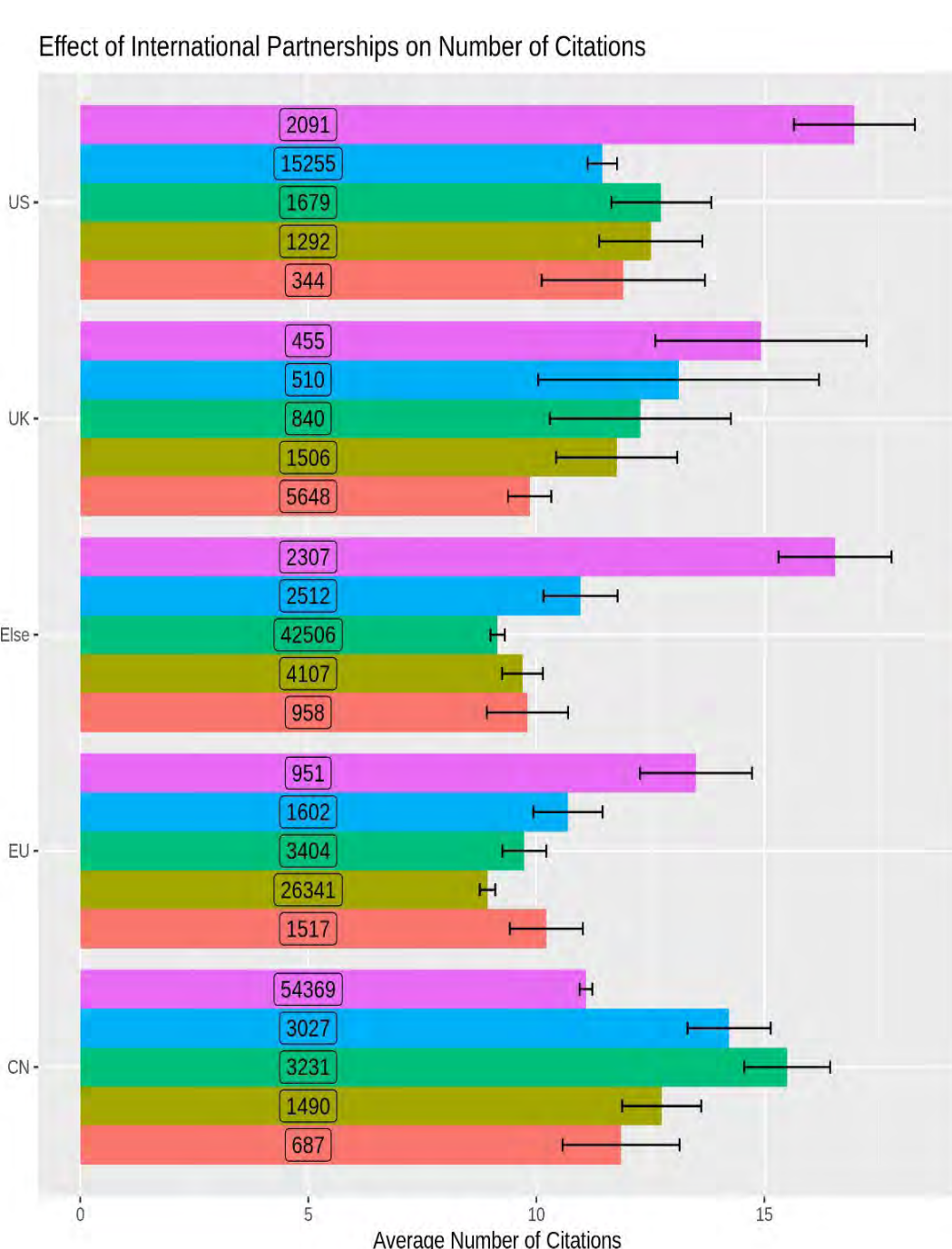The majority of structures in RSC journals have an R-factor of about 1%.

Comparison of weighted R-factor for all reflections included in the refinement (wR_factor_ref) and the one calculated on the reflections judged significantly intense (R_factor_gt).
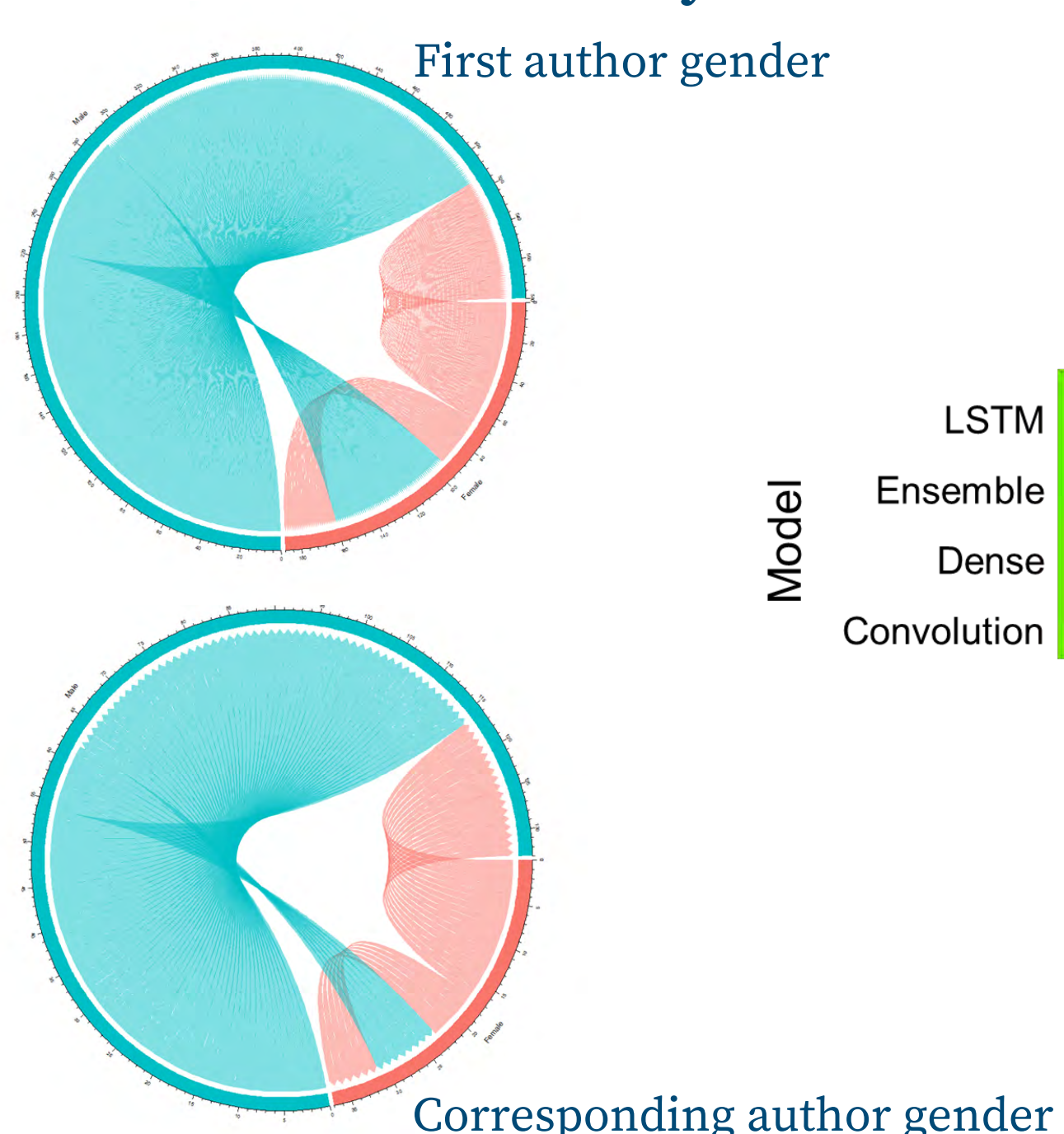

R_factor
  R_factor_gt
  wR_factor_ref

Recent research by the Data Science team, www.rsc.org/data-science

Collaborations in chemistry

Effect of International Partnerships on Number of Citations

Collaboration
  UK
  EU
  Everywhere Else
  US
  CN

Gender bias in chemistry

First author gender

Corresponding author gender

Deep learning for NMR and NLP.

F_1
0.4 0.6 0.8
• = Best result