Journal of Medicinal Chemistry

pubs.acs.org/jmc

Perspective

How Diverse Is Medicinal Chemistry? Insights into Race, Ethnicity, Origin, Gender, and Geography

Richard J. D. Hatley, Steve P. McLachlan, Kathleen Baster, Lucy C. Gelder, and Simon J. F. Macdonald*

Cite This: https://doi.org/10.1021/acs.jmedchem.1c01632

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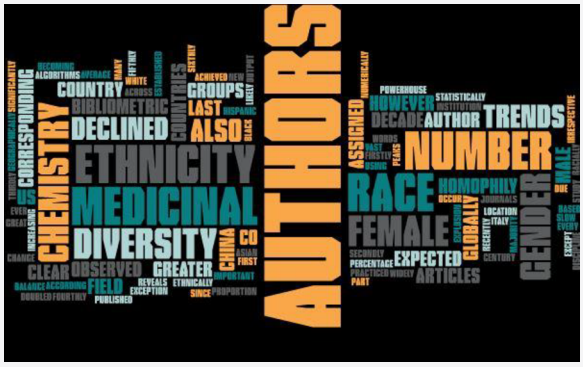
ABSTRACT: A bibliometric study of authors across medicinal chemistry journals over 20 years reveals important trends. Most United States (US) based authors are assigned as racially/ethnically Asian or White; few are Black or Hispanic. More US coauthors have the same race/ethnicity as the corresponding author than expected. The percentage of female authors increased globally, but only slowly. Since 2010, the number of female and male authors declined by 9% and 30%, respectively. Geographically, most authors are male except in Italy where there is gender balance. Gender homophily is observed globally. Geographically, the discipline is now more widely practiced. Article output doubled from 2000 to 2010 with a large increase in articles from China. China excepted, output has since declined. The average number of authors per article rose by a third since 2000. The value of high diversity groups in education, research, and industry cannot be overstated. We recommend diversity is addressed by every medicinal chemist.



■ INTRODUCTION

Chemistry Is Not Diverse. Nobel prizes are some of the most prestigious accolades in science. In chemistry, only 7 women have won a Nobel prize compared to 179 men, a significant difference, even accounting for fewer women in science (*vide infra*).[1,2] There have been no Black Nobel prize winners in any science subject despite widespread and significant contributions.[3] These imbalances permeate science, and action is required.[4]

The Aims of This Perspective. This perspective explores race/ethnicity/origin, gender, and geography of authors of medicinal chemistry articles through bibliometric analyses of published journal information. The aims are to gain a greater understanding of diversity in the field over the last 20 years, to highlight the current status, and to raise awareness of recent trends. The findings should be of value to scientists, managers, and policy makers in medicinal chemistry and may have application in related subjects.

Why Explore Medicinal Chemistry and Not Chemistry in General? Medicinal chemistry was selected for several reasons. First, it is the background of some of the authors (R.J.D.H., S.P.M., and S.J.F.M.); second, it is carried out in academia, industry, and nonprofit institutions; and third it is carried out globally. Fourth, analysis of chemistry articles as a whole provides averaged data from across the subcategories of chemistry, many of which have quite different metrics.[5] For example, the gender balance in organic chemistry is quite different from that of medicinal chemistry which is different again compared to computational chemistry (for further background and references, see the later section titled "Previous Studies in Medicinal Chemistry and Related Fields"). Thus, data from *this* specific field allows clear trends and potential actions to be identified for *this* specific field. Fifthly, this perspective may also provide useful benchmarking data in the field of medicinal chemistry which could then inform diversity policies in the institutions.[6] Finally, the findings may also be valuable to publishers as they seek to address a long-standing issue of how to increase diversity and inclusion in the articles they publish.[7,8]

Diversity—Equal Opportunities and Treatment for All. Why is diversity so important? We highlight two reasons. Primarily, and most importantly, diversity means providing equal opportunities and treatment to all. Second, diversity catalyzes innovation.

Science—and medicinal chemistry here—has in large part been practiced by White males. A recent *Nature* editorial[9] entitled "*Systemic racism: science must listen, learn and change*" states:

Received: September 16, 2021

We recognize that Nature is one of the white institutions that is responsible for bias in research and scholarship. The enterprise of science has been—and remains—complicit in systemic racism...

There is also considerable evidence that scientists are treated differently and have different opportunities according to their gender, race/ethnicity/origin, and/or sexual orientation.[10−12] In science, discrimination is evident in the workplace[13,14] and in educational institutions,[15,16] where, for the latter, student uptake and progression for minority groups at universities is low;[17] the "doctoral dearth" is widespread in the United States (US).[18] Some students have even lacked a sense of belonging.[19] There is evidence of racial and gender discrimination in the hiring of women and minority groups in STEM subjects,[20] a lack of advancement to leadership positions,[21] and lower publication rates for research academics[22] leading to a gender-productivity gap.[23] The devaluation of women's work in science creates cumulative disadvantages in scientific careers.[24] Innovative ideas from minority groups are also frequently devalued and discounted.[25] Gender bias has even been seen in factors affecting sex-related reporting in biomedical journals.[26] Drugs have been marketed with insufficient trials in females, resulting in sex-specific toxicity effects being observed.[27−29] Even a therapeutic, BiDil, was marketed for heart failure for patients who self-report as Black, but this received negative press.[30]

As a result of such widespread discrimination, there are now many initiatives both to raise awareness of these issues and to provide much greater access to science to all[31,32] consistent with Mertonian's norms.[33] The importance of diversity and representation in the sciences is clearly of paramount importance for ethical reasons, so all scientists have the opportunity to meet personal goals and for scientific advancement.

Diversity—Enhancing Innovation. Innovation is particularly relevant to medicinal chemistry. New medicines continue to transform human health and improve the quality of life but drug discovery - of which medicinal chemistry plays a key part - remains enormously challenging and expensive. It is a field with very high social and economic significance where innovation is at a premium and this can be enhanced with a diverse workforce.

High diversity groups provide a number of advantages to solving problems including richer and alternative approaches and access to a wider talent pool. There is substantial evidence that a diverse workforce catalyzes innovation particularly those requiring team efforts,[34] where cognitive,[35] gender[36,37] and race/ethnicity diversity[38] can be invaluable in identifying the best solutions[39] and can lead to greater long-term economic growth.[40]

Historically, a common approach in recruiting—particularly in the pharmaceutical industry—has been "to hire the best" from a subset of the top universities. However, hiring the brightest minds with similar qualifications and experiences from the same universities runs the risk of cognitive and demographic homogeneity which may be suboptimal, in tackling tough problems.[41]

Previous Studies in Medicinal Chemistry and Related Fields. What is already known about diversity in medicinal chemistry? To our knowledge, there have been few studies on the race, ethnicity, or origin[42] of authors or geography, that is, where medicinal chemistry is practiced. In contrast, previous studies have focused on gender balance in science, patents,[43] and chemistry as a whole;[5] the granularity for medicinal chemistry is not reported. The experiences of female chemists and gender balances in some of the subdisciplines in chemistry have been described including computational chemistry,[44] medicinal chemistry,[45−47] organic chemistry,[48] supramolecular chemistry,[49] and process research.[50] Excellent recommendations and calls to action have been made.[51,52] Additionally, preliminary bibliometric studies of chemistry articles focusing on gender by the Royal Society of Chemistry in the United Kingdom (UK)[5] and by Cotton and Seiple[53] have been reported, but we are unaware of detailed data for medicinal chemistry articles as presented here. Other bibliometric studies of medicinal chemistry articles include exploring the geographic origins of articles published from Latin America, India, and China,[54] the contributions of Brazilian[55] and Russian[56] scientists to the field, and a detailed analysis of articles in the *Journal of Medicinal Chemistry*.[57] Previously, we have published data on the number of articles in medicinal chemistry journals over the last two decades noting that while there has been an increase in articles overall particularly from academia and nonindustrial institutions, there has been a decline in those from pharma.[58] The analyses here are an extension of that work.

Summary of the Methodology. Our analyses here focus on bibliographic data from medicinal chemistry articles with the data extracted from Pubmed and Scopus. The algorithms used for race/ethnicity/origin and gender are widely used. These, and some of their limitations, are discussed later. The data set obtained is large enough to provide statistically significant trends (over 640,000 authors in 87,000 articles over 20 years).

Overview of Results. This bibliometric analysis reveals the relative homogeneity of the scientific workforce in two main ways. First, most medicinal chemists are male. In nearly every country, women form a distinct minority of the medicinal chemistry workforce and while this is slowly changing, in some countries at the current rate it will take many decades to reach gender balance. Second, the vast majority of medicinal chemists are (as assigned by an algorithm—see later) either racially or ethnically White or Asian. Based on our analyses, few medicinal chemists are assigned as Black or Hispanic. The proportion of medicinal chemists from these groups are significantly lower compared to the proportions in the general population of some countries even where huge amounts of capital are spent on research, with the US being the prime example. Unlike gender balance, there is no indication that these proportions have changed for either group in the last 20 years. Third, the discipline, which historically[59] was mainly (but certainly not exclusively) carried out in the US, Europe and Japan, has recently widened significantly, particularly in China. Fourthly, the number of authors per publication have risen substantially particularly in the highest impact journal studied.

In the first section of this Perspective, a description of the methodology is provided. Then, in three distinct sections, we present analyses of (i) the race/ethnicity,[60] (ii) gender, and (iii) geographic location of authors in medicinal chemistry. The last section also includes the changes in the average number of authors per article. Some final remarks are then made in the conclusion. Statistical details are provided in the Supporting Information (SI).

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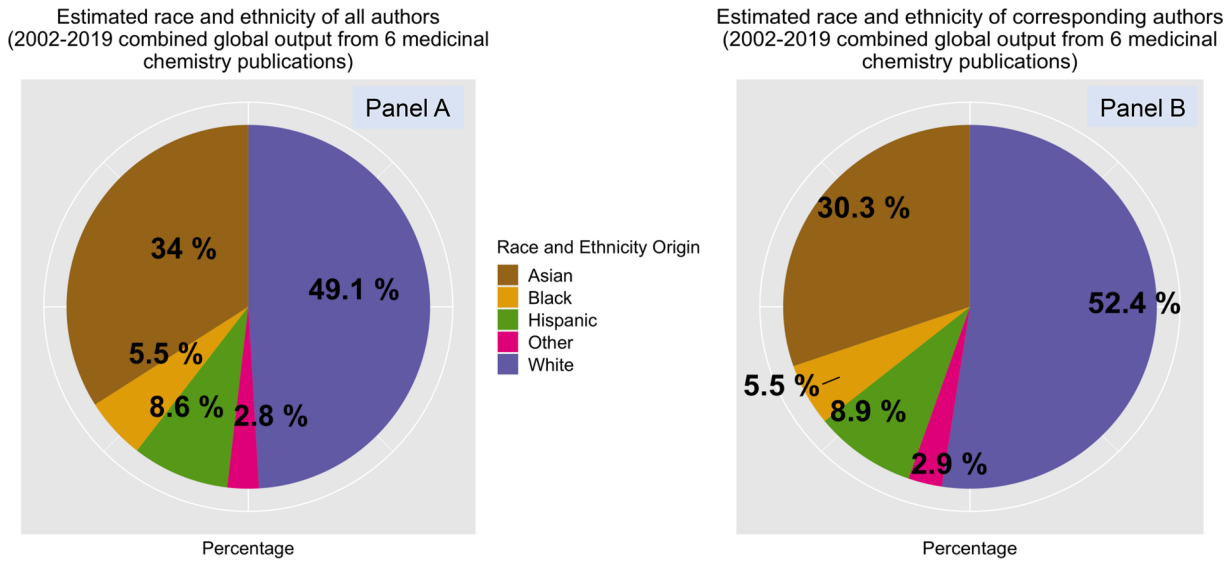

Figure 1. Estimated percentage race/ethnicity/origin of corresponding authors and all authors from all institutions globally based on articles published in the six medicinal chemistry journals from 2002 to 2019. For authors who wrote more than one article, each article is counted separately (*i.e.*, each article is included in the data set). The definition of "Other" is any other race/ethnicity/origin than that listed; see Table S2 for details.

METHODOLOGY

Extensive details of the methodology and limitations are provided in the SI. Key points are described here.

Journal Selection. Analyzed here are articles from a set of medicinal chemistry journals over an 18−20 year period. The journals selected are those that predominantly publish original research and are based on the "Journal Citation Report" category for "medicinal chemistry" from Clarivate (see the SI). The four journals studied that predominantly published full articles were *Bioorganic Medicinal Chemistry* (BMC), *ChemMedChem* (CMC), the *European Journal of Medicinal Chemistry* (EJMC), and the *Journal of Medicinal Chemistry* (JMC). The three journals that mainly published communications or letters were *ACS Medicinal Chemistry Letters* (ACS MCL), *Bioorganic Medicinal Chemistry Letters* (BMCL) and *MedChemComm* (MCC) (which was renamed *RSC Medicinal Chemistry* in 2020). The *Journal of Organic Chemistry* (JOC) is used as a comparator high quality journal from a single subdiscipline of chemistry (organic chemistry). The resultant journal set therefore are the more well-known and prestigious in the field (based on impact factor). These are also the journals that, from over 60 years in the field, the authors recognized as primary sources for medicinal chemistry research (see the SI).[58,61]

Race/Ethnicity/Origin Algorithms. All author names were assigned race, ethnicity or origin using established algorithms based on US[62] and UK[63] voting or census data where *race/ethnicity/origin is self-reported*. Comments on the weaknesses and bias of both algorithms are described in the original papers.[62,63]

To address the ambiguity in the assignment of names using the US algorithm, statistical simulations were carried out 10 000 times to improve the assignments of race/ethnicity and reduce the possibility of racial/ethnic profiling. Additional details of statistical methods are provided in the SI.

It is appreciated that there are concerns regarding the assignment of race/ethnicity/origin in the context of a growing number of people with a multiracial and multiethnic background. The terms "race and ethnicity" used here are those used in reported data from the US and UK censuses. The difference in the meanings of "race" and "ethnicity" are complex.[60] For example, the literature that describes the algorithms used here, uses the word "ethnicity" but the US census uses the word "race".

Gender Algorithms. Authors were assigned gender in a binary fashion (that is, as male or female) using established algorithms, and statistical simulations were also carried out for gender assignments (provided in the SI).

A limitation to this gender assignment methodology is that it only assigns sex and does not take account of nonbinary individuals or individuals who identify as gender neutral or other gender categories. Data on this important area is lacking to the best of our knowledge, which means we have been unable to take account of nonbinary members of the medicinal chemistry community. Recent studies of transgender individuals in the US by Meerwijk and Sevelius estimated prevalence at around 390 people out of 100 000 and, quoting directly from their study, "may be more indicative for younger adults" than the entire population although a referee pointed out that there may be an age-correlated social stigma on transgenderism.[64] In another study from the US, the transgender or gender nonconforming populations is estimated at between 0.1 to 2% of the general population depending on inclusion criteria and location.[65] Based on these studies, it is therefore unlikely that the number of transgender or gender neutral authors would change the conclusions.

Intersectionality and Major Limitations. Details of these are provided in the SI.

RACE AND ETHNICITY

In an ideal world, the ethnic makeup of employees of a large institution might be expected to reflect the population demographic of the country concerned, but in reality this is rare.[66] For many complex reasons beyond the scope of this Perspective, representation of minority ethnic/racial groups in certain workplaces and fields is significantly unbalanced

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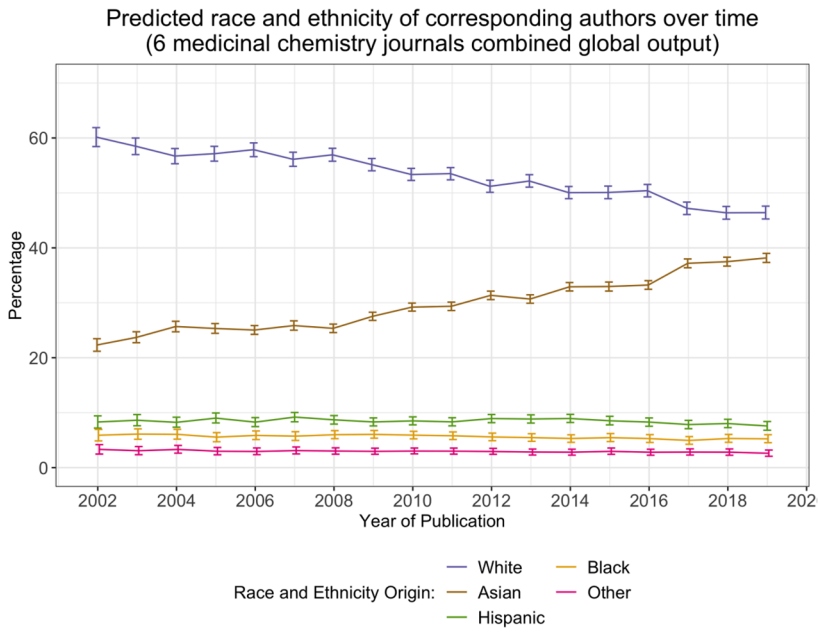

Figure 2. Ethnicity/race/origin of corresponding authors globally from six medicinal chemistry journals combined from 2002 to 2019 based on the US ethnicity algorithm.

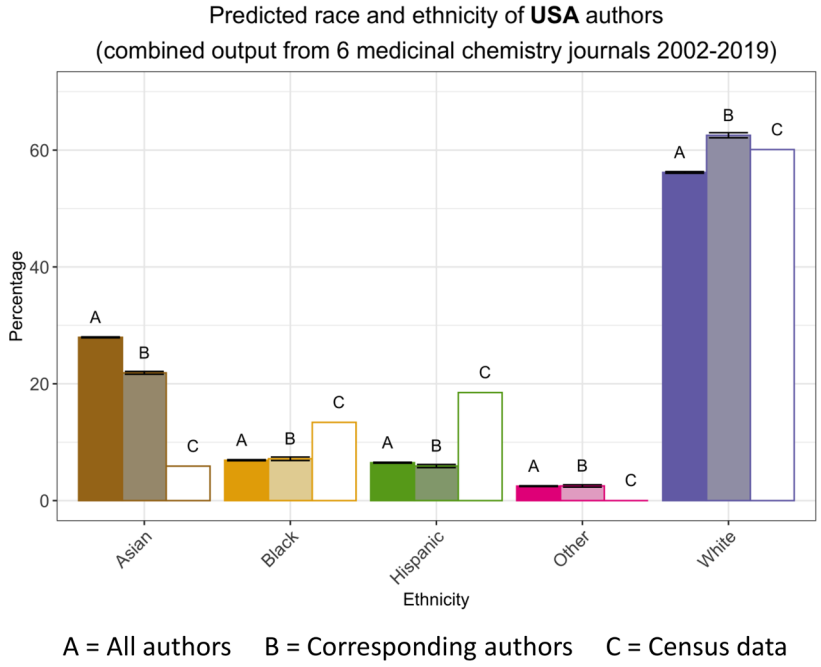

Figure 3. Ethnicity/race/origin of authors for US based institutions in six medicinal chemistry journals from 2002 to 2019 compared to US population estimates in July 2019.[71] The first, second and third bars in each cluster marked "A", "B", and "C" represent all authors, corresponding authors, and census percentages, respectively. (Error bars are included but are very small; see the SI for further data.)

including in the field of medicinal chemistry as described in this bibliometric analysis. In this section, we predict the race/ethnicity/origin for authors of medicinal chemistry papers by applying commonly used algorithms based on recent US[62] and UK[63] census data.

The Application of the US Algorithm to All Authors and Corresponding Authors Globally. For all institutions globally from 2002 to 2019, the vast majority of authors are assigned as Asian (34%) or White (49%) (Figure 1). There are markedly fewer Hispanic authors (9%) (most of whom are likely to be authors of papers originating from Spain—see later) and even fewer Black authors (5.5%). Compared to global demographics, authors from Black racial or ethnic groups are significantly under-represented (5.5% vs 12.5% of the world population) which contrasts with the geographic chemistry-publishing population (see later).[60] The race/ethnicity/origin of global *corresponding* authors and global *all* authors are very similar (Figure 1), although these data mask individual country differences (see later).

The Percentage of Corresponding Authors Assigned as Asian Has Nearly Doubled in 18 Years. A different picture from that in Figure 1 is seen however for the race/

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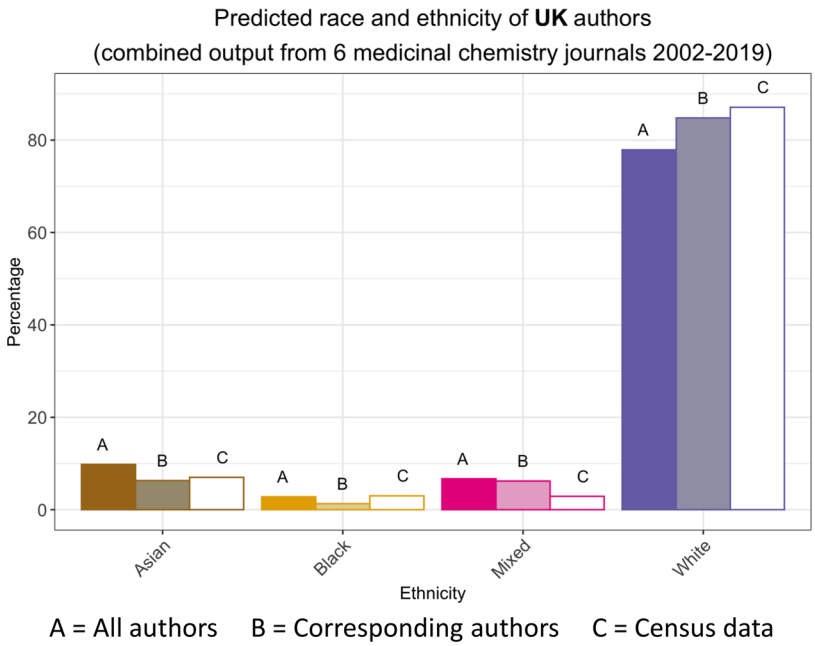

Figure 4. Race or ethnicity of UK based authors in six medicinal chemistry journals between 2002 and 2019 based on unique author names. Corresponding authors n = 1069; all authors n = 8500.

ethnicity/origin of corresponding authors over time (Figure 2). The recent rapid growth of publications from China (see later) meant that, by 2019, the ratio of Asian to White authors moved from around 1:3 to 1:1.2. If the underlying factors for trends continue, then within the next 5−10 years the majority of corresponding authors will be assigned as Asian.

The data suggest that, over the same time period, there was little change in the number of corresponding authors assigned as Black or Hispanic (Figure 2). One factor in these trends at a global level is that the number of students transitioning to higher education and studying science in different countries varies widely.[67] Another factor is likely to be reflected in the gross domestic spending on R&D by different countries. A country's budget for science funding is likely to ultimately influence medicinal chemistry publication output, and clearly large countries with large and increasing budgets for science will produce more articles than small countries with small budgets for science. For example, US science funding grew 4.3% annually between 2000 and 2017, while in China it grew at 17% annually and the Chinese budget for science is now similar, if not higher, than the US budget.[68] In contrast, many other countries whose populations are not predominantly White or Asian have far smaller budgets for R&D.[69]

Even in Countries Like the US *with* High Research Spending *and* a Significant Black or Hispanic Population, Black and Hispanic Authors Are Significantly Under-represented. It is mainly European countries and the US who have diverse populations as defined by the algorithms used here *and* who publish large numbers of medicinal chemistry articles. (The racial and ethnic diversities of China and Japan lie outside the race or ethnic groups categorized by the algorithms being used).[70] It might be expected that there would be a greater number of authors assigned as Black or Hispanic in countries such as the US (or the UK; see the next section) as they have large R&D budgets and sizable minorities in their populations. However, this is not the case with authors assigned as Black or Hispanic. Using the algorithm based on the US census and only using articles with a US correspondence address, corresponding authors of Black (7%) and Hispanic origins (6%) are about *2 and 3 times under-represented*, respectively, compared to the makeup of the general US population of 13% and 19%, respectively (Figure 3).[71] In contrast, corresponding authors assigned as Asian are around *3.5 times* over-represented (22% vs 6%) and those assigned as White are slightly over-represented compared with the census data for the general population at around 60% (Figure 3). All these values are statistically significant (see the SI). These findings align with those generally observed in STEM subjects in the US.[72,73]

In the US, this Black under-representation echoes other evidence that there are few Black medicinal chemists. For example, between 2012 and 2017, 5−7% of bachelor degrees awarded in chemistry in the US were received by Black African Americans, that is, between 1170 and 1337 degrees awarded annually.[74,75] In 2020, of 1696 chemistry doctorates awarded to US citizens or permanent residents, 45 were Black African Americans (2.6%).[76] In the same year, out of 47 doctorates awarded in medicinal chemistry, the comparative number is 3 (6.4%)[76] and "among the 49 large [PhD] programs, only two nontenured faculty members [were] African American."[77,78] And the data presented here suggest very few medicinal chemistry authors are racially or ethnically Black. With increasing levels of education and seniority, from graduate to PhD to academic or industrial medicinal chemistry positions, decreasing numbers of Black chemists continue sufficiently far in the field to become an author or corresponding author of a medicinal chemistry article. The contrast with the over-representation of authors assigned as Asian is stark. A recent explanation for the socioeconomic success of Asian Americans historically has been that "Asian students [exert] greater academic effort"[79,80] and a greater percentage of Asian Americans do enroll in college compared to other racial or ethnic groups.[81] Recent research also suggests that another

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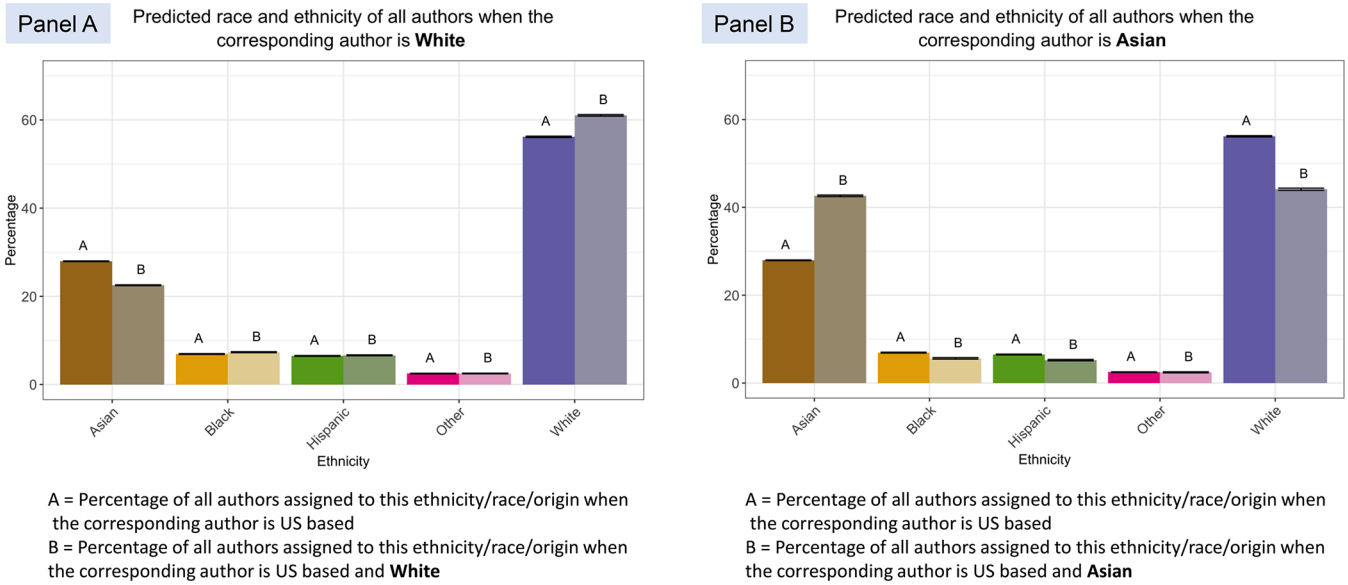

Figure 5. Percentage of race or ethnicity of all authors from US based institutions in six medicinal chemistry journals from 2002 to 2019 when the corresponding author is assigned as White (panel A) or Asian (panel B).

major factor is simply that, postworld War II, discrimination declined.[79]

The under-representation of Black authors in the US has been ascribed to the lack of black role models,[82−84] socio-economic status,[85] that the final cost of education loans is twice as large as for other racial or ethnic groups[86] and discrimination.

Even leaving aside the ethical obligation of providing equal opportunity for all, the research which says ethnic diversity leads to better science is compelling.[39]

The corresponding author of an article is usually an academic, project or team leader with coauthors usually being students, postdoctoral assistants, or team members. Given the large data set, it might be expected that the proportion of race/ethnicity/origin of corresponding authors in the US and coauthors might be similar. While this is the case for authors assigned as Black or Hispanic, it is not the case for White or Asian authors. There are about 6% *more* White corresponding authors than White coauthors and about 6% *fewer* Asian corresponding authors than Asian coauthors (Figure 3). Put another way, while corresponding authors are *ca.* 3:1 White:Asian, most coauthors are *ca.* 2:1 White:Asian. This suggests that most academic (and probably pharma) groups or teams are composed of mainly White and Asian scientists but are more often than not run by leaders who are assigned as White.

This might reflect that there is a strong prevalence for these races/ethnicities to pursue careers in medicinal chemistry. In addition, it may reflect that numerous US research groups have large contingents of international students many of whom come from, and subsequently return to, Asia, Europe, and Australasia. However, there still remains a noticeable absence of coauthors of US based articles who are Black or Hispanic. For visiting international scientists, this presumably reflects, in part at least, the relative lack of chemists of this race/ethnicity/origin.[74]

The Racial or Ethnicity Proportions of UK Authors Appear More Aligned to That of the General UK Population. For UK institutions, the race/ethnicity of authors was assigned using the UK-derived Ethnicity Estimator.[63] However, statistical analysis of the race/ethnicity of authors based in the UK has not been possible due to the output from the algorithm[87] and it is more difficult to distinguish between White, Black and Mixed race or ethnicity in the UK based on names alone. With those caveats, however, the distribution of authors is closer to the natural makeup of the general population (2011 census data) (Figure 4).[88] The vast majority of authors are of White race or ethnicity (∼78%) which is a slight under-representation compared to the makeup of the UK population. The percentage of racially or ethnically Black authors publishing (2.8%) is similar to the percentage of this racial or ethnic group in the population (3.0%). As seen in the US but to a much lesser degree, more authors are assigned as Asian, compared to the UK population as a whole (9.8% vs. 7.0%). This is also the case with authors whose race or ethnicity is assigned as Mixed.

These data contrast with race and ethnicity data from UK higher education statistics.[89,90] An RSC report from 2006,[91] details that 90% of UK domiciled PhD students were White and only 0.7% were Black (African or Caribbean) and by 2017/8 these percentages were 83.5% and 1.3%, respectively.[42] As in the US, with increasing seniority through career progression, the percentage of Black chemists falls.[42] This is attributed to people not having conversations around race for STEM subjects, a sense of isolation, and lack of role models for Black chemists (as in the US) and a lack of a safe environment to raise issues of racism.[42] In an article published in 2020, Robert Mokaya, a Black chemistry professor at the University of Nottingham, is quoted as saying that, in 2008, he was the first Black chemistry professor appointed in the UK[42] and knows of no further appointments since then.

Racial/Ethnic Homophily between the Corresponding Author and Coauthors in the US. We next compared the race/ethnicity/origin of US corresponding authors with that of their coauthors. When the corresponding author is assigned as Asian or White, a higher than expected proportion of coauthors have the same race/ethnicity/origin. For example, if the corresponding author is assigned as White, about 5%

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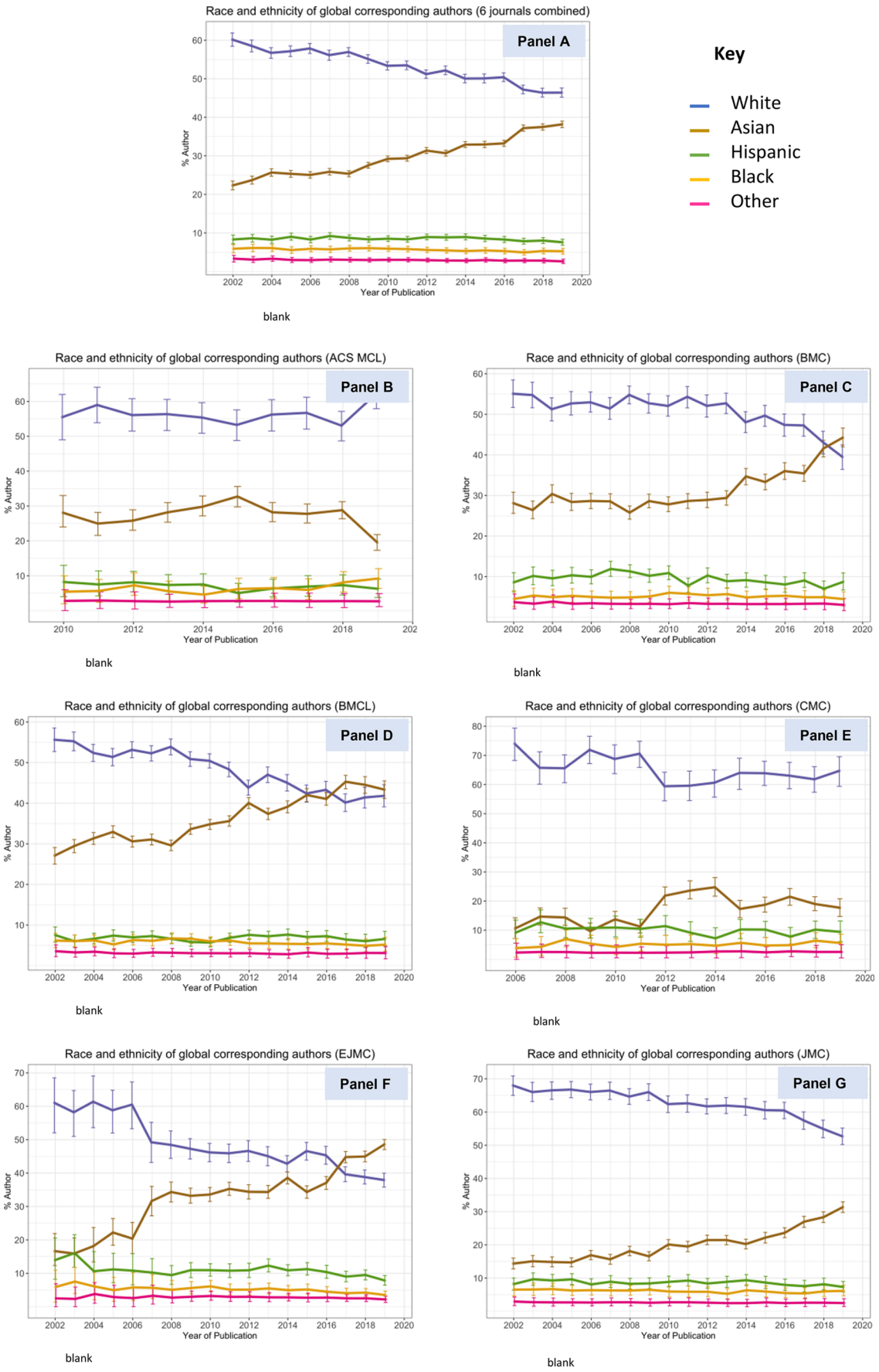

Figure 6. Ethnicity of all global corresponding authors for each journal over time as assigned by the US algorithm.

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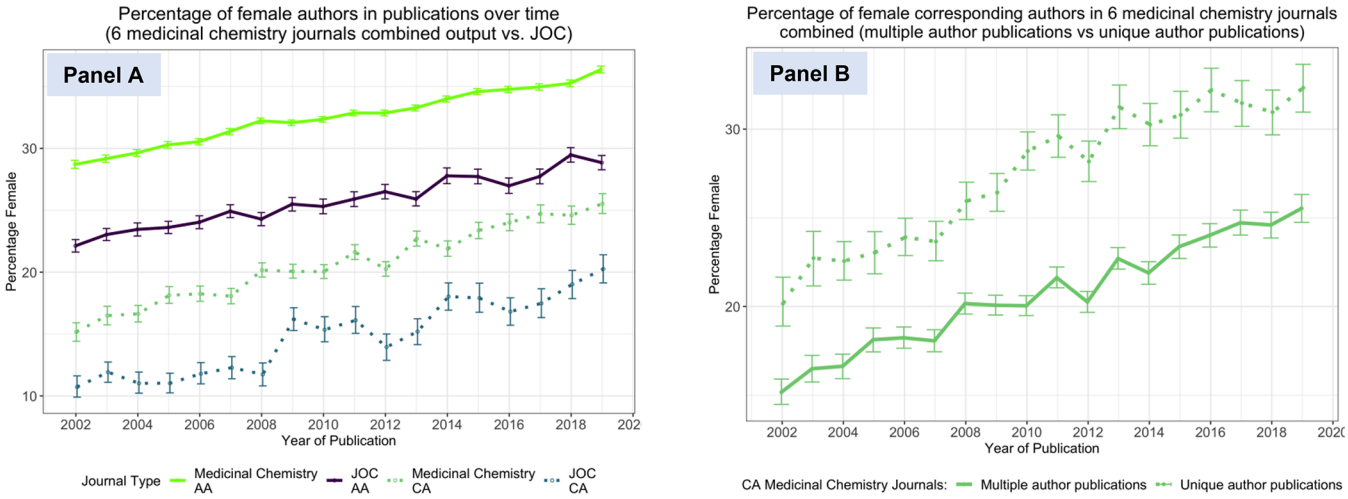

Figure 7. Panel A: Graph showing the percentage of *all* female authors and *corresponding* female authors of medicinal chemistry articles and similarly for authors of articles in JOC. Panel B: Percentage of all female authors (as in panel A) including multiple articles from the same author alongside unique authors (*i.e.,* where authors publishing multiple articles are just counted once). AA means All Authors, and CA means Corresponding Authors.

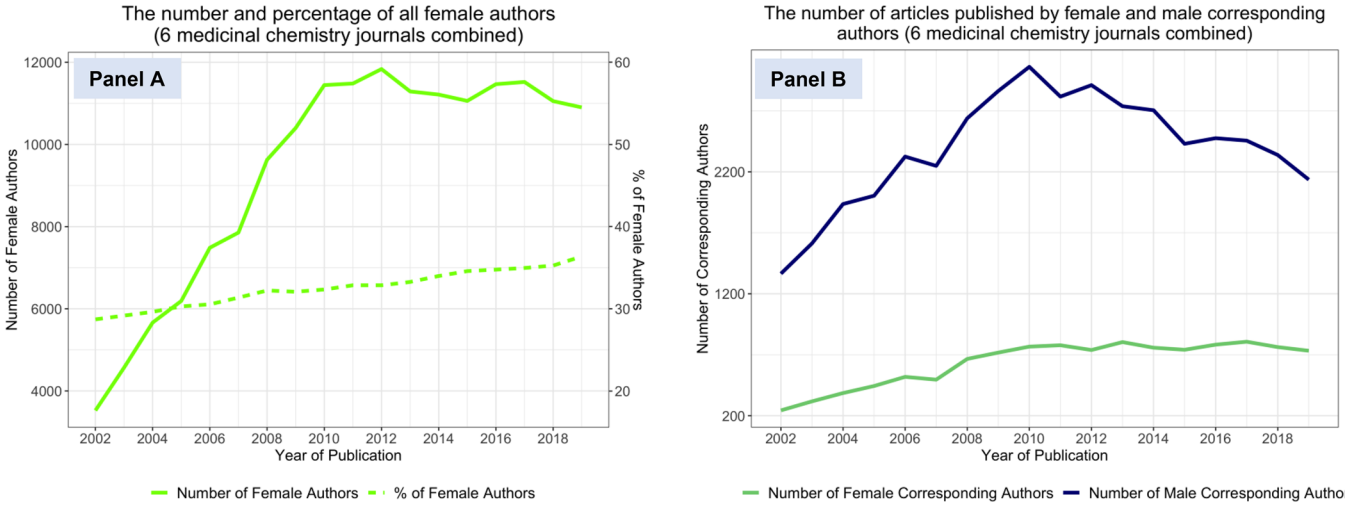

Figure 8. Panel A: Number and percentage of all female authors from 2002 to 2019. Panel B: Number of female or male corresponding authors from 2002 to 2019.

higher than the expected number (based on all authors) of their coauthors are also White and about 5% fewer than expected are Asian (Figure 5 panel A). The effect is more pronounced with Asian corresponding authors. Asian corresponding authors have, on average, about 27% more Asian coauthors than expected and 12% fewer than expected coauthors who are White (Figure 5 panel B). Significant homophily effects are also seen with authors assigned as Black and Hispanic authors although to a much lesser degree. This race/ethnicity/origin homophily may reflect a natural confirmation bias,[92] the natural tendency for humans to associate more with individuals who look like themselves[93] and/or that individuals are more likely to collaborate with those who are geographically closer. Homophily is also observed with gender (see later).[94]

The Race/Ethnicity/Origin of Corresponding Authors in the Medicinal Chemistry Journals Shows a Consistent Rise of Authors Assigned as Asian. We next looked at whether there was a preference for certain races/ethnicities/origins to publish in particular journals and interestingly there is. Globally, authors assigned as Asian show a preference for publishing in BMCL, BMC, and EJMC and much less for CMC or JMC whereas those assigned as White publish more in ACS MCL, CMC, and JMC and much less in EJMC (see also Figure S2). The geographical location of the author and the journal impact factor probably play a role here (see later).

As seen earlier (Figure 2), looking at the same data over time shows a steady rise in articles from authors assigned as Asian (Figure 6). At the start of the time periods for each journal, most corresponding authors were assigned as White. But by 2019, this is only true of ACS MCL, CMC, and JMC. For BMC and BMCL, there are now equal numbers of White and Asian authors, and for EJMC there are now more Asian than White authors. Only ACS MCL and CMC show little change in the race or ethnicity of corresponding authors over time.

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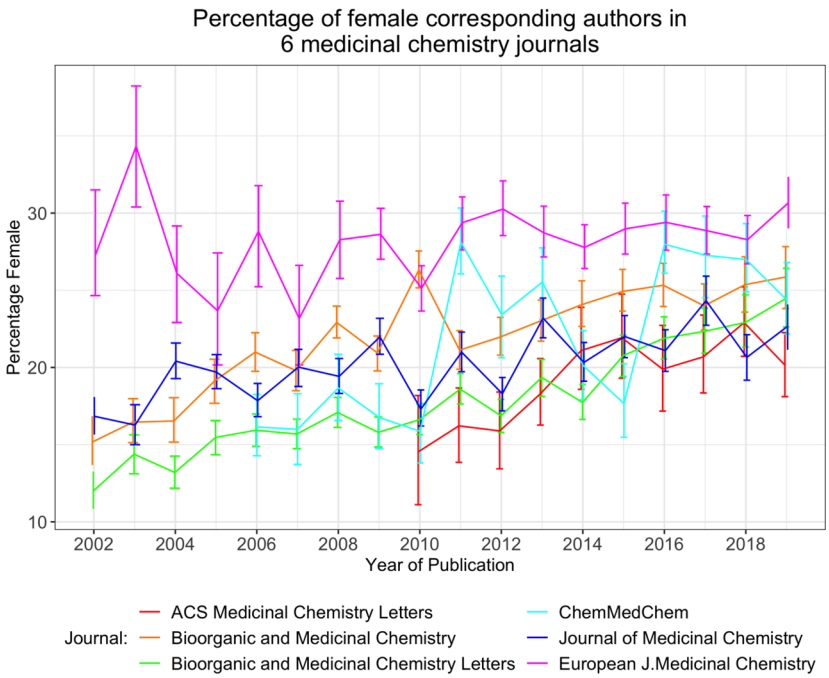

Figure 9. Graph showing the percentage of female *corresponding* authors in the journals between 2002 and 2019.

■ GENDER

In this section, we examine the gender balance of both corresponding and coauthors for the medicinal chemistry journals between 2002 and 2019. We explore the gender balance trends for the journals and for authors based in different countries and highlight pronounced gender homophily between corresponding authors and coauthors. In general, there is substantial gender imbalance although one of the major publishing countries has achieved gender balance in the discipline.

The Percentage of Female Authors Has Increased Slowly over the Last Two Decades. The percentage of female *corresponding* authors of medicinal chemistry articles in these journals has increased significantly in 18 years from about 15% to 25% (Figure 7 panel A). This compares to current estimates of 28.4% women in research and development worldwide.[95] At the present rate, it will take around 40 years to reach gender parity. Just over a third of *all* authors are now female, having risen around 7% over the time period. These percentages are low but not as low as those for synthetic chemistry where, over the time period, female *corresponding* authors have risen from about 11% to 20% as judged by the data for JOC.[96]

Male Corresponding Authors Are, on Average, More Prolific than Female Corresponding Authors. We also looked at the unique number of female corresponding authors, that is, where the female author publishing multiple articles in the time period is just counted once (dotted green line, Figure 7 panel B).[97] Over the time period, the number of female authors increased by around 50%, and if a similar rate of growth continues, then gender parity will be reached in less than 20 years. Of course, this is the *percentage* of female corresponding authors not their total output (solid green line, Figure 8 panel B) which is lower. Put another way, female corresponding authors on average publish less than male corresponding authors and, according to Barabasi *et al.*,[98] over the entire careers of STEM scientists this is true mainly because men stay in a discipline longer than women. However, on an annual basis, they have very similar outputs. They ascribe this paradox to differences between the genders in their career lengths and dropout rates alongside many other factors.[98] Barabasi's hypothesis is controversial with numerous other studies suggesting that men publish substantially more than women, the so-called "productivity puzzle",[99] with explanations ranging from differences in family responsibilities[100] to differences in academic rank[101] *inter alia*.

The upward trends in female corresponding authors and all authors are remarkably constant given the macroscale changes that occurred in the field over the time period: the huge growth of authors from China, the downscaling of Western based pharma along with the outsourcing of many drug discovery activities to CROs. It suggests more female medicinal chemists are either writing papers and/or remaining in the discipline for longer in more leadership roles.

However, what is less obvious is that while the *percentage* of female authors has increased, the actual *numbers* of authors varied. The number of all female authors almost tripled between 2002 and 2010 but then leveled off and gradually declined by about 8% from 2012 to 2019 (Figure 8 panel A). The decline suggests the publishing global medicinal chemistry community (if not the whole community itself) is shrinking as from their peaks, the number of male corresponding authors has significantly dropped by about 30%, and female corresponding authors leveled off (Figure 8 panel B). This may be a consequence of big pharma downsizing[58] and reduced funding for chemistry in many countries[102] which was not offset by the rise in authors from China (see later).

These plots include articles written by Chinese authors where gender assignment is less robust. So, a reasonable question to ask is whether the trends change when these authors are excluded? The answer is they change very little which is suggestive that the algorithm is reasonably accurate (see Figure S3 in the SI).

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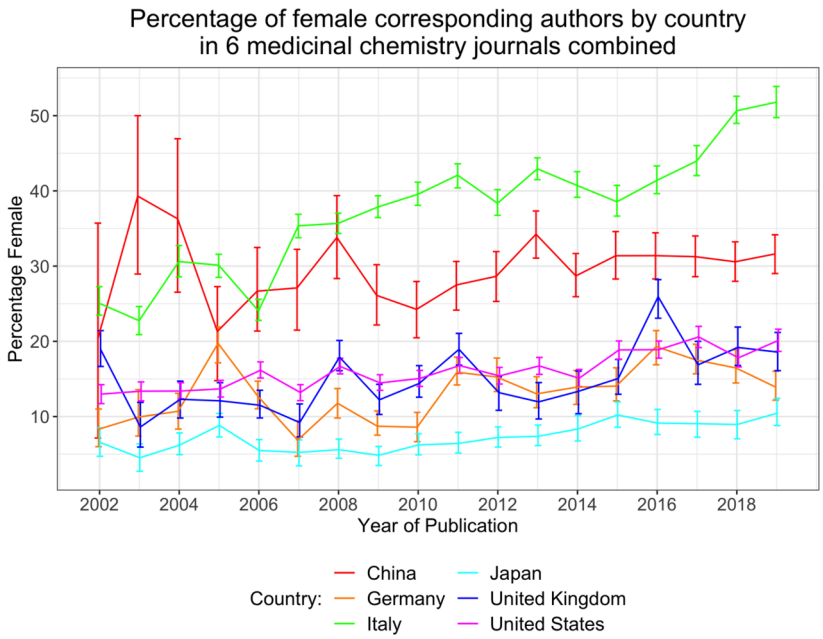

Figure 10. Gender balance of corresponding authors for some of the main countries that publish medicinal chemistry.

The Journal with the Highest Percentage of Female Corresponding Authors for Full Papers is EJMC and for Letters is BMCL—There May Be Good Reasons for This. EJMC consistently has the highest proportion of female *corresponding* authors (except for 2010) ranging from 23% to 34% (Figure 9) of all the journals studied. For letters, there is little difference between the percentage of female corresponding authors for ACS MCL and BMCL of between 12% and 24% (Figure 9). Several comments are worth making. First, while the error bars are large, a significantly higher proportion authors in EJMC are female compared to JMC the highest impact journal in the field. Second, while the data are noisy, of all the journals, BMC and BMCL appear to be consistently publishing increasing percentages of articles from female corresponding authors over time. Third, as will be seen in the next section, countries with a higher proportion of female corresponding authors have a preference for publishing in EJMC in contrast to JMC.

It is worth noting that the highest impact journals publishing full papers (JMC) and letters (ACS MCL) have some of the lowest proportions of female corresponding authors from the journals studied;[103] both journals are taking action to support systemic changes.[45,46,104] This may reflect the gender balance in higher ranking institutions, which tend to be poorer—as authors from these institutions are on balance more likely to publish in higher impact journals.[96] A further underpinning reason is likely to be the "leaky pipeline" for female medicinal chemists.[43,51]

In essence, the leaky pipeline refers to the tendency for the proportion of women in the discipline to decrease with increasing levels of education and seniority.[105] By most measures,[106] an article in JMC has a comparatively higher impact than one in EJMC. So, by the time a corresponding author has sufficient experience and seniority to publish in JMC, and bearing in mind that nearly half of US female scientists leave full-time science after having their first child (about twice the rate of male scientists),[107] there are fewer female than male medicinal chemists. Although there is evidence that there are fewer female corresponding authors in prestigious journals,[108] which also applies in chemistry journals,[5] in this study, we found no difference in journal impact factor between male and female corresponding authors.

Italy Is the Torchbearer for Female Authors. Of all the major countries who publish medicinal chemistry (see the section on geography below), only Italy now has an approximately even gender balance of corresponding authors which was achieved in 2018 (Figure 10). The US, UK, China, Japan, and Germany lag far behind (Figure 10; data for over 70 countries are shown in the SI). Note the gender assignment of authors from China and the resultant trend shown are less certain (note the larger error bars) due to the difficulty in assigning gender to Chinese names (see "Gender algorithms" in the SI). The rise in female authorship in Italy is statistically significant, whereas for the other countries shown the changes mostly are not (see the SI). Italy achieved gender balance for all authors around 2010, and although the gender balance of all authors for the other major publishing countries is better than that for corresponding authors, it is still far from parity (data not shown). This gender balance among corresponding authors in Italy probably derives in large part from the even gender balance of professors and researchers in Italian universities[109,110] and contrasts with other countries such as the UK[111] or US[112] where there are many fewer female researchers and professors than male counterparts.[113]

The trend seen in Italy reflects that women account for 74% of Masters students in the chemistry/pharmaceutical disciplines and, in 2017, female Ph.D. students participating in the European School of Medicinal Chemistry outnumbered male colleagues. However, these numbers change significantly with appointment to professor level. In 2017, of 75 full professor appointments in medicinal chemistry, only 21 (28%) were women, despite near parity in gender balance (45% women) at entry level academic positions.[45]

Whatever the Journal, the Location of the Corresponding Author, or the Type of Institution, There Is Consistent Homophily—That Is, A Higher than Expected Number of Female Coauthors When the Corresponding Author Is Female. Between 2002 and

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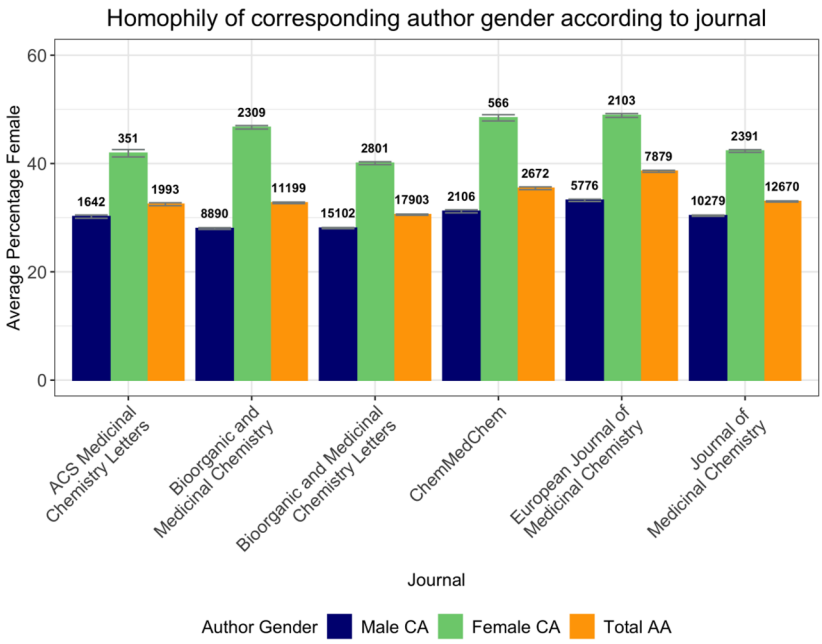

Figure 11. Average number of female authors per article when the corresponding author is female or male. Note the green bars, which are the percentages of authors who are female when the corresponding author is *female*, are consistently higher than the blue bars, which are the percentages of authors who are female when the corresponding author is *male*. The orange bars represent the average percentage of all authors who are female for each journal. The numbers above the bars refer to the corresponding author count.

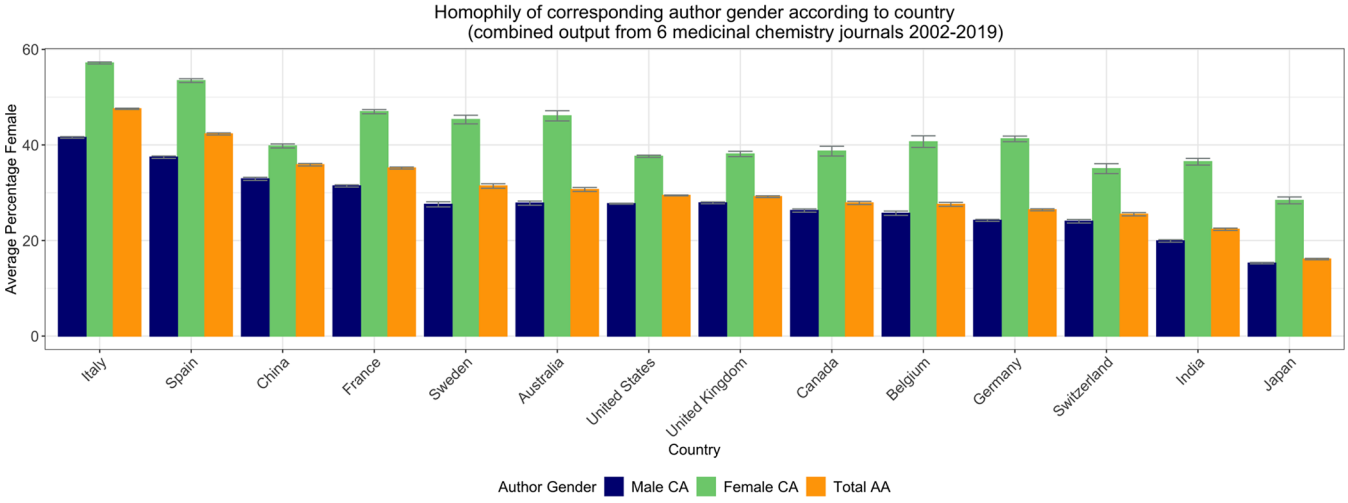

Figure 12. The degree of gender homophily may vary but is consistently seen irrespective of the country in which the corresponding author is based. Note the green bars, which are the percentages of authors who are female when the corresponding author is *female*, are consistently higher than the blue bars, which are the percentages of authors who are female when the corresponding author is *male*. The orange bars represent the average percentage of all authors who are female for each country. Countries are ranked from the highest to lowest percentage of female corresponding authors.

2019, around 30% of all authors are female (orange bars in Figure 11). However, when an article is written by a female author, on average there is one and a half times the number of female coauthors (around 45%, green bars Figure 11) than would be expected (30%). This effect is statistically significant for each journal (see the SI) and changes very little over the 18 year time period (data not shown). Articles written by male authors have commensurately fewer female coauthors (blue bars, Figure 11). This homophily effect was noted recently for chemistry journals[5] and also in publishing across the life sciences[114] with suggested explanations being "women seeking to avoid harassment or sexism from men",[114] discrimination or avoidance of women by elite research groups,[101,114] the elevated gender gap among senior researchers, and scientists preferring to collaborate with like-minded people (ie of the same gender).[114] This last reason is one we have encountered most frequently in our own experience.[115] A recent experiment with female engineering students in small work groups suggests that female peers made a big difference to motivation, verbal participation, and career aspiration.[116]

Interestingly, statistically significant gender homophily is seen in every country studied and despite those countries having widely differing cultures and gender issue awareness (Figure 12 and SI). The effect is least pronounced with China

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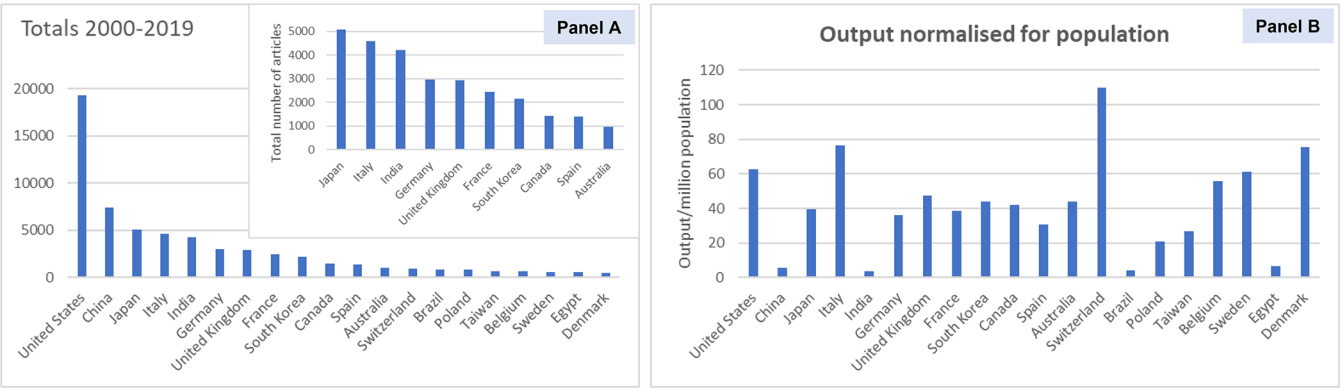

Figure 13. Panel A: Total number of articles published *cumulatively* between 2000 and 2019 according to the country where the corresponding authors were based. The inset graph shows the total articles published for countries other than the US and China on an expanded scale. Panel B: Total number of articles normalized according to country population (based on Organization for Economic Cooperation and Development 2010 population estimates).

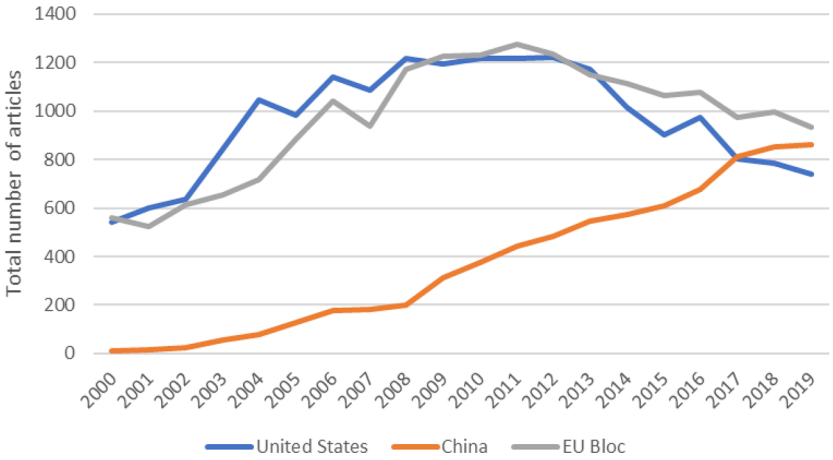

Figure 14. Total number of articles published *annually* between 2000 and 2019 by the US, China, and EU bloc. The EU bloc is defined as the 19 countries in the EU at some point over the 20 year period and are Italy, Germany, UK, France, Spain, Poland, Belgium, Sweden, Denmark, The Netherlands, Greece, Czech Republic, Portugal, Austria, Hungary, Finland, Ireland, Croatia, and Slovenia.

based female corresponding authors (although gender assignment of Chinese names has higher error; see earlier) and then with Italy, which has the best gender balance of all the main publishing countries, and is most pronounced with Australia, Germany, and India based female corresponding authors. As discussed above with race/ethnicity/origin, the choices female students make about the subdisciplines of chemistry in which to study or work are likely to be influenced in part by the number of females already in the discipline and the seniority of the roles they occupy. In other words, strong female role models in a particular subdiscipline of chemistry are likely to attract female students.[117]

■ GEOGRAPHICAL ORIGIN OF CORRESPONDING AUTHORS IN MEDICINAL CHEMISTRY

Over the last 20 years, where have the corresponding authors of medicinal chemistry articles been based? And given that, in the last 20 years, the number of medicinal chemistry articles published has more than doubled,[58] how was this growth distributed globally?[118] This section explores these questions.

Most Articles between 2000 and 2019 Were Written by US Based Authors, but Output from China Based Authors Has Recently Soared. Cumulatively, across the last two decades, US based (corresponding) authors wrote 28.5% (*ca.* 19 337 out of a total of *ca.* 67 746) out of all published articles, far more than any other country (Figure 13 panel A). However, these data mask the rise of China based authors who, since 2017, now publish more papers than the US and nearly as many as the EU bloc. The increase in output is staggering: in 2000, there were 9 publications from China, but by 2019 there were 862 (Figure 14).

Normalizing the data according to population size (Figure 13 panel B) shows Switzerland, Denmark, Italy, and the US as having the highest output per capita and China and India among the lowest.[119]

Which Are the Top Publishing Countries Beside the US and China? Based on the total number of medicinal chemistry articles over the 20 years, the countries that published the most articles beside the US and China were (in descending order) Japan, Italy, India, Germany, UK, France, South Korea, Canada, Spain, and Australia. We call these countries, excluding China and including the US and Switzerland, the "established nations", meaning they have a historical record of being the major publishers of medicinal chemistry in these journals over the two decades. However, these graphs only tell part of the story.

The Years of Higher Medicinal Chemistry Funding and Output for the Established Nations Appear to Be

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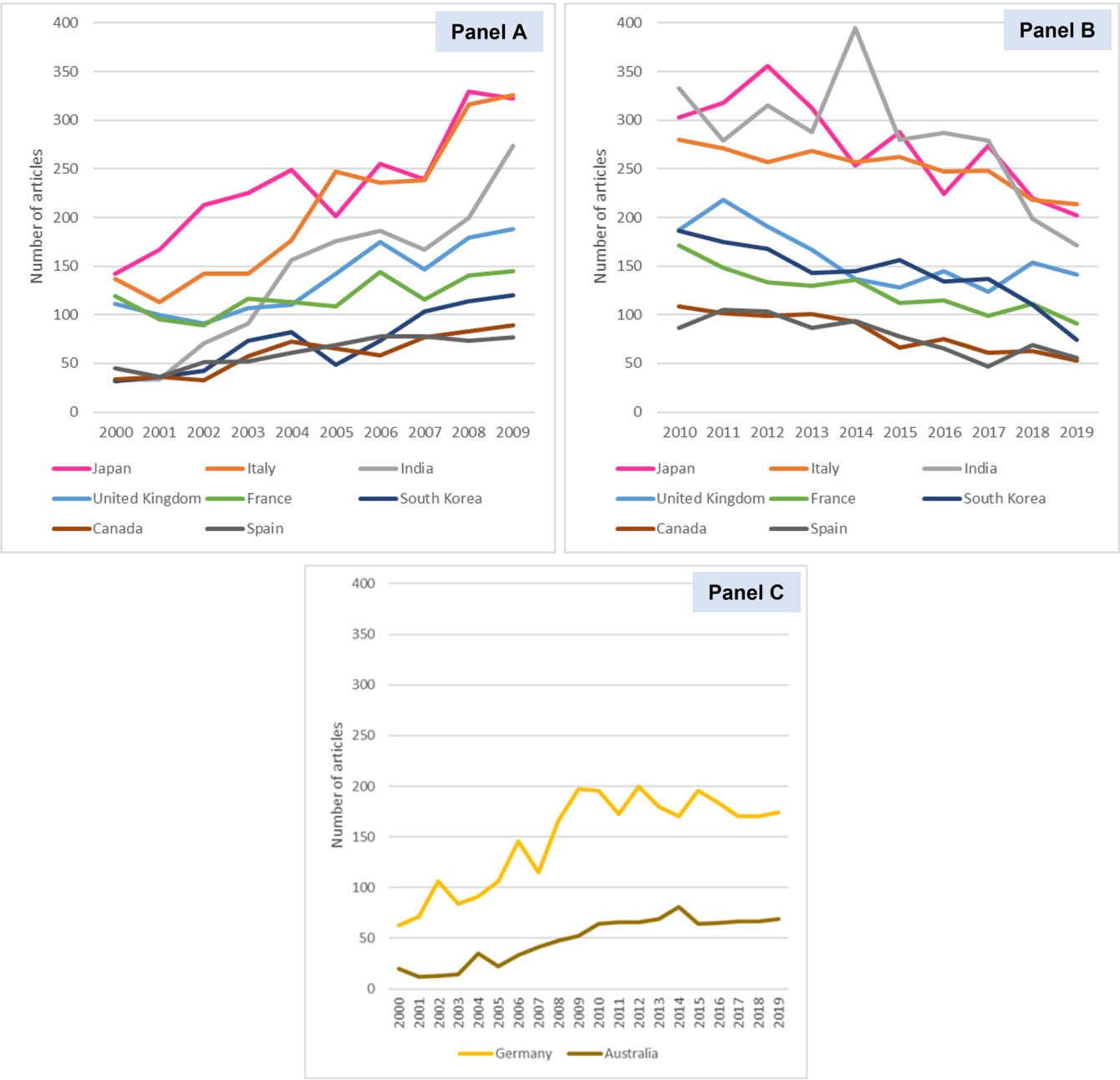

Figure 15. Number of articles (combined data in all the medicinal chemistry journals) for ten of the established nations (excluding the US) who published medicinal chemistry between 2000 and 2019. For clarity, the data are shown for 2000–2009 (panel A), for 2010–2019 (panel B), and for Germany and Australia (panel C) which are the only countries where the number of articles published over the second decade was maintained.

Over. Between 2000 and 2009, publication output from all the established nations approximately doubled (Figures 14; Figure 15 panels A and C) with the exception of articles from France which only rose from 119 in 2000 to 145 in 2009. But the following decade, from 2010 to 2019 (Figure 14; Figure 15 panel B), saw more or less a uniform decline in outputs. Papers from US authors dropped from the peak by 40% and from EU authors by 27% (Figure 14). Most of the established countries still published more in 2019 than in 2000 (the exception being France; see the SI), but the trends year by year were generally downward or plateauing (Figure 15 panels B and C). Over the whole time period, output from India followed a similar bell-shaped curve but Indian authors still published about 5 times as many papers in 2019 compared to 2000. In contrast to the established nations, between 2008 and 2019, articles from China authors rose by *over 3-fold* although this growth leveled out in 2018–2019 (Figure 14).

The reasons for these changes in output are discussed elsewhere,[58] but the financial crisis of 2008, the downsizing of Western big pharma, and the huge growth in funding of science in China are likely factors (see earlier). They are striking too because, in general, scientific articles increase at the rate of 4–9% per year.[118] The number of articles published might also be influenced by the research cultures of different countries and, as mentioned elsewhere, the type of institution. Many industrial institutions, for example, only publish a small fraction of their research.[58] Publishing also depends on funding systems; the research culture in some countries has changed

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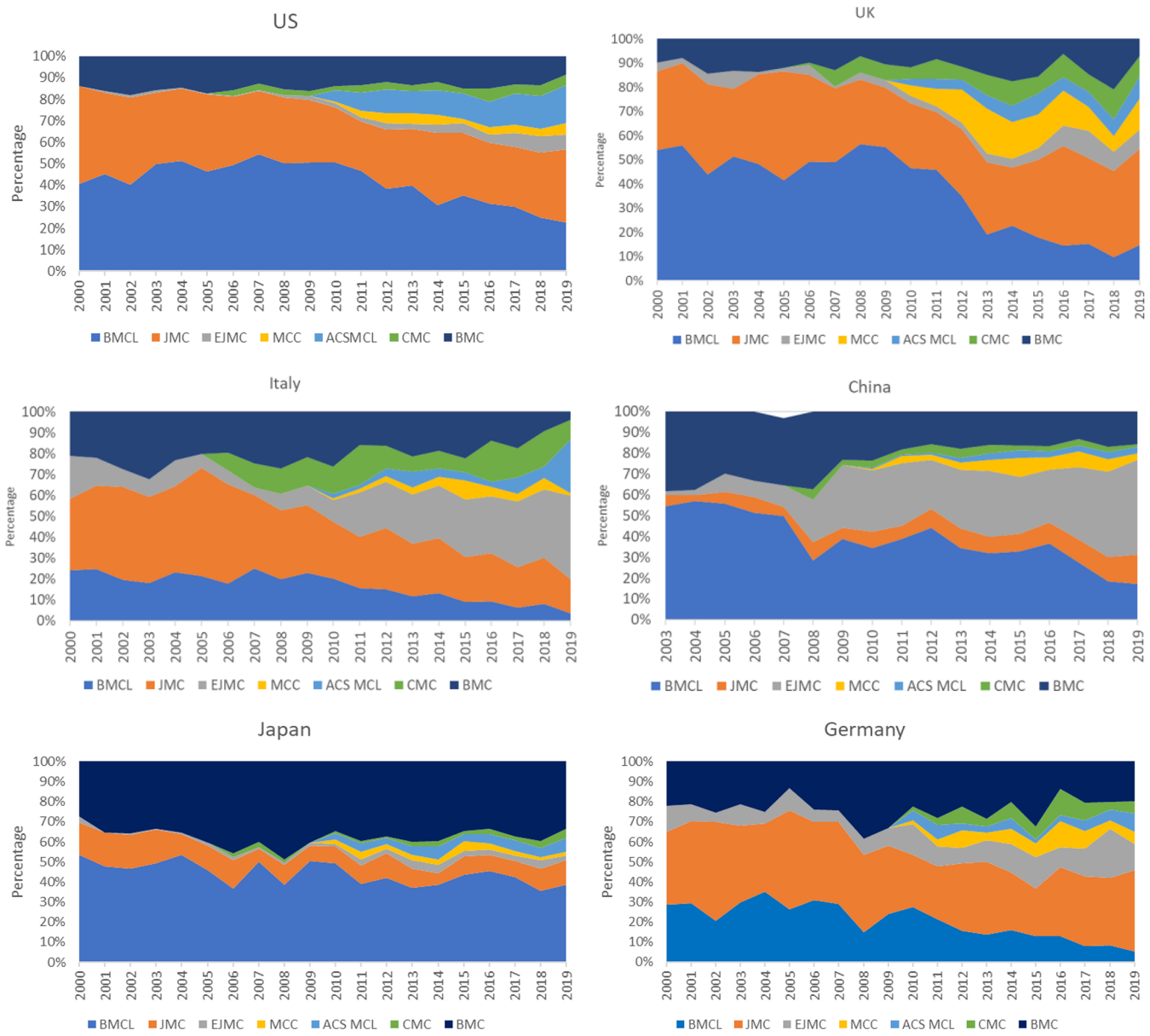

Figure 16. Journals in which corresponding authors based in different countries publish as a percentage from 2000 to 2019.

from "publish or perish" toward fewer but "higher quality" publications in higher impact journals.[120] In China, however, there is a strong culture that linked rewards at the individual and institutional levels to journal impact factors.[121]

As a Discipline, Medicinal Chemistry Is Now Practiced in Many More Countries. Around 67 countries published medicinal chemistry articles in 2019 compared with 46 countries in 2000, an increase of around 50%.[122] To provide a snapshot of those involved and the change in output, the top 20 locations of corresponding authors in terms of articles published for 2000 were compared with 2019 (see SI Table S14).

The 2000 ranking is dominated by the established nations with China in 17th place with only 9 publications. An output of only 7 publications from Belgian corresponding authors was sufficient to be ranked twentieth. In contrast, by 2019, the outputs have generally increased significantly for almost every country and with Brazil, Russia, and Egypt entering the top 20 ranking.

It is interesting that, among the US and EU nations, only Germany has moved up the rankings with many of the other countries moving down; the US, Japan, France,[123] Spain,[102] Switzerland, and the UK have all dropped down the rankings. This probably reflects budget changes for chemistry in some of these countries[124] (with Spain[102] and Italy[125] experiencing significant budget declines) alongside the impact of globalization.[58]

The Location of a Corresponding Author Has a Large Bearing on the Journal in Which They Publish. In general, and probably for a variety of cultural reasons, corresponding authors from the same country tend to publish in the same journals albeit with changes over time (Figure 16). US authors generally prefer JMC, BMCL, and increasingly for letters ACS MCL. UK authors prefer JMC as do Italian authors, although the latter have gradually switched to EJMC. Japanese authors in contrast consistently prefer BMCL and BMC, and Chinese authors prefer BMCL and BMC and increasingly EJMC.

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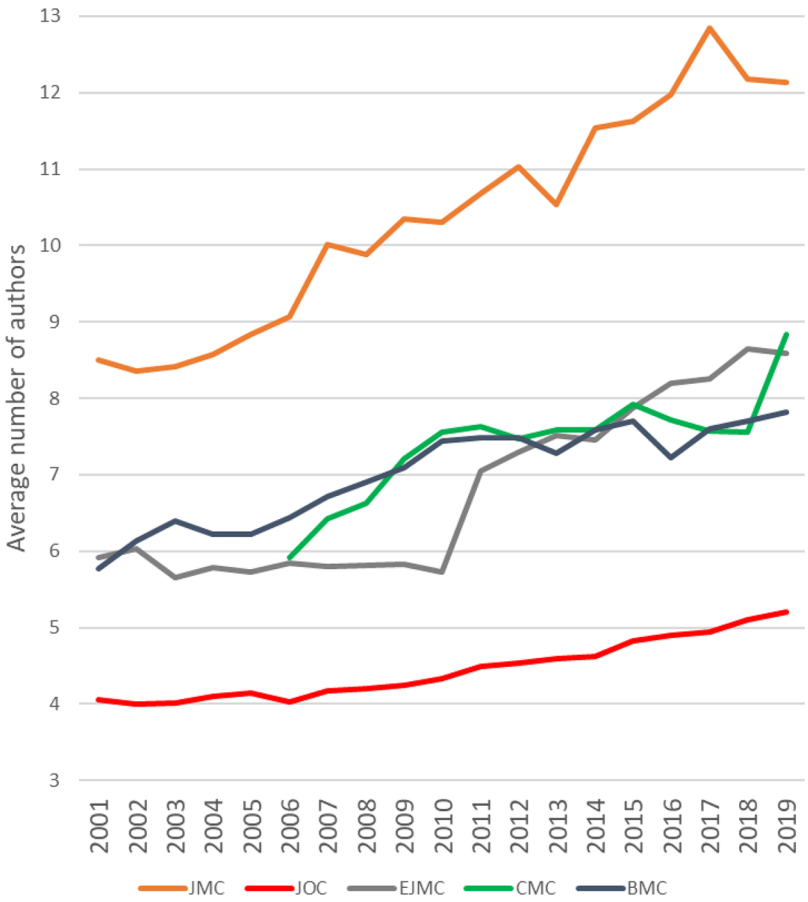

Figure 17. Average number of authors per full article in JMC, EJMC, CMC, BMC, and JOC.

Authors consider many factors in deciding in which journal to publish. In US and European cultures, there is an emphasis in publishing in the journal with the highest impact as these carry weight in career progression.[126] Authors can also favor journals published by their local chemical societies and may indeed feel some obligation to do so. Well-known and well-respected academics are sometimes appointed as editors, and they can be highly influential in encouraging and sourcing articles from the country where they are based and can have a mandate to maintain or raise the quality of what is accepted for publication.

Most Articles in JMC Are Written by US Corresponding Authors, but as a Percentage of Total Output the US Output Is No Different from That of Other Established Nations. As the premier journal in the field based on multiple measures,[106] a few comments are worth making about JMC articles. In terms of absolute numbers of articles, JMC has been and is primarily a journal for US based corresponding authors; they wrote 40% of the articles over the 20 year period (see SI). Between 2003 and 2014, articles from Italian based authors were the next most common, although between 2005 and 2019 the article count dropped almost 4-fold. Articles from corresponding authors in China have risen steeply since 2014 and replaced Italy in second place since 2016.

The absolute numbers of articles in JMC from different countries vary considerably, but so do the countries' total outputs. We therefore also explored what proportion of a country's output is published in JMC. What is notable is that all the established nations (with the exception of Japan presumably for historic, cultural, and linguistic reasons) have a similar percentage of their entire output appearing in JMC (see the SI). While US based corresponding authors contribute the most articles *numerically* by far, as a *percentage* they are no different to the other established nations.

Also, of note is that, as a percentage of their total output, articles in JMC from several of the established nations, namely Italy, France, and Spain, have declined (see the SI). While the reasons for these trends are undoubtedly multifactorial, it is concerning that some of these countries are publishing less science in the highest impact journal in the field.

Time in the Field Is Needed to Deliver the Most Impactful Science. A greater proportion of articles from the established nations appear in JMC compared to newer nations (see the SI). So, while numerically the number of articles from corresponding authors in China in JMC is the second highest (after US authors), as a proportion of their total output this is still quite low. This may indicate the amount of time it takes to build sufficient experience, collaborations, depth of research, and infrastructure to publish a higher percentage of articles in JMC. Of course, JMC articles are written in English and this represents an additional challenge for authors for whom English is not their native language or script. There is also potential for bias from journal editors and reviewers regarding manuscripts from reputable research institution and nations more positively compared to lesser-known institutions and/or countries in the field.[127]

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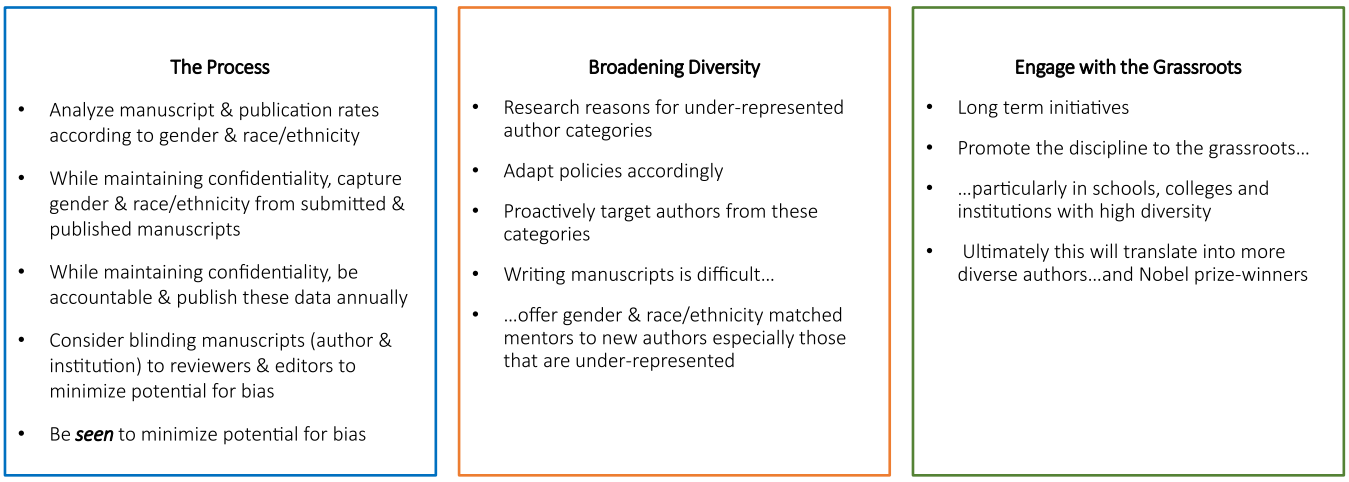

Figure 18. Ideas for publishing houses to consider to encourage greater diversity among authors.[131]

THE NUMBER OF AUTHORS PER ARTICLE

In this section, the number of authors per article or letter are explored according to journal and institution category.

Over 20 years, the Number of Authors per Full Articles Has Increased by 33−50%. Articles in JMC, the Highest Impact Journal, Have a Third More Authors per Article than Other Full Article Journals. Full research articles published in journals have, on average, about 33−50% more authors now than they did 20 years ago (Figure 17). Articles in JMC also, on average, have about a third more authors than those in other full article journals (Figure 17). These trends presumably reflect the greater interdisciplinarity of the field, larger drug discovery teams, and more collaborative (and potentially fewer) projects. They also align with the general trend in science of increasing team size.[34]

The contrast for the average author numbers for a medicinal chemistry or drug discovery project with synthetic chemistry (JOC) is striking and probably echoes the factors above, particularly the interdisciplinarity, without which progress would be slow. Skilled scientists from varied disciplines (outside of chemistry) are required to progress a medicinal chemistry project. These results support the literature in that they describe the increasing importance of teams and collaboration in generating the best knowledge and that an increase in the number of authors leads to an increase in journal impact.[128]

The number of authors for letters, that is, in ACS MCL, BMCL, and MCC, have remained approximately similar to an average of about 11, 8, and 7 authors per letter, respectively, and may reflect the relative impact factors of the journals.

CONCLUSION

The trends from this bibliometric analysis of medicinal chemistry publications are clear and thought provoking.

- The vast majority of medicinal chemists are assigned as either White or Asian.
- Even in the US which has a significant Black and Hispanic populations *and* that has high levels of funding for chemistry, there is a noticeable absence of chemists assigned as Black or Hispanic.
- While progress has been made, and with the notable exception of Italy, the majority of medicinal chemists who published articles in this time period worldwide were male. Progress has been slow particularly in countries that publish large numbers of medicinal chemistry articles. Despite these countries having progressive cultures and goals for greater female representation, the gender balance of authors is still heavily skewed toward male authors and male corresponding authors in particular.[129]
- Medicinal chemists on average tend to publish with medicinal chemists of the same gender whatever the location or culture.
- As a discipline, medicinal chemistry is much more widely practiced now than previously with a huge rise in output from China. In the last two decades, most medicinal chemistry was carried out in the US, but if current trends continue, the main locus for the discipline will soon become China.
- The geographic location of the corresponding author (alongside the quality of the work being published) correlates with which journal is selected for publishing their medicinal chemistry. It is clear that the impact factor of the chosen journal is more important in some regions than others. Anecdotally, the influence of certain journal editors is probably also a factor.
- The average number of authors per article has increased significantly. This reflects the increasing complexity and interdisciplinarity of medicinal chemistry over the time period.

These trends derived from bibliometric data largely reflect our own experience of working within medicinal chemistry in industry. While we stress this may be unrepresentative, it does provide an example of the practical expression of diversity in a big pharma in the UK for 20−30 years. We recall only a handful chemists who were Black. Gender balanced teams were rare simply because of the lower numbers of female chemists. There was a much lower percentage of senior chemists who were female compared to the percentage of junior chemists who were female; visible evidence of the "leaky pipeline" at first hand.

What is striking is most, if not all, of these institutions had and have diversity policies. And a common challenge is to allow the diverse *minority* to focus as much on the science as the *majority* rather than spending considerable time on other, important but nonscientific, initiatives where their diversity was desired or required. There were many examples where we

https://doi.org/10.1021/acs.jmedchem.1c01632
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formed a distinct impression that addressing diversity was regarded as an upstream or downstream problem to the medicinal chemistry or chemistry department. Diversity was and probably still is often regarded as someone else's or some other institution's responsibility. Genuine ownership of the issues by some parts of the chemistry community can sometimes be difficult to discern and, while inexcusable, may be understandable given the pressure many chemists work under to deliver projects, write high impact papers, secure funding, and so on. Setting diversity objectives, provision of resources to the average chemist, and, most importantly, allocating some time to address diversity would undoubtedly make a difference.

In addition, the editorial houses themselves should take proactive action (see Figure 18 for ideas). These include minimizing the potential for bias in the review process, ensuring diversity among the authors of articles they publish, ensuring diversity among the editors and reviewers who make decisions on the submitted manuscripts, and holding themselves to account by regularly disclosing their diversity metrics in each of these areas.[130]

An analysis of the trends described here between academia and industry is in preparation.

■ ASSOCIATED CONTENT

Supporting Information

The Supporting Information is available free of charge at https://pubs.acs.org/doi/10.1021/acs.jmedchem.1c01632.

(1) Methodology and limitations, (2) statistical methods and statistic tables, (3) additional plots and figures, and (4) further notes on geography (PDF)

■ AUTHOR INFORMATION

Corresponding Author

Simon J. F. Macdonald − *RGDscience Ltd, Hitchin, Herts SG4 9SP, United Kingdom;* orcid.org/0000-0002-4859-8246; Email: simonmacdonald@rgdscience.com

Authors

Richard J. D. Hatley − *RGDscience Ltd, Hitchin, Herts SG4 9SP, United Kingdom;* orcid.org/0000-0002-3172-2511

Steve P. McLachlan − *Data & Computational Science, GlaxoSmithKline Medicines Research Centre, Stevenage, Herts SG1 2NY, United Kingdom*

Kathleen Baster − *Statistical Services Unit, University of Sheffield, Sheffield S3 7RH, United Kingdom*

Lucy C. Gelder − *Statistical Services Unit, University of Sheffield, Sheffield S3 7RH, United Kingdom*

Complete contact information is available at: https://pubs.acs.org/10.1021/acs.jmedchem.1c01632

Notes

The authors declare no competing financial interest.

Biographies

Richard J. D. Hatley received his DPhil degree from the University of Oxford and has worked as a medicinal chemist on many drug discovery programs since joining GlaxoSmithKline in 2000, contributing to the discovery of several small molecules that have entered clinical trials. Additionally, he has organized several RSC medicinal chemistry conferences on Fibrosis in 2015 & 2017 and on Integrins in 2019. He is an honorary lecturer in medicinal chemistry at the University of East Anglia and from 2019, he has been a director at RGDscience Ltd, a medicinal chemistry and drug discovery consulting company.

Steven P. McLachlan received his Ph.D. in organic chemistry from the University of Liverpool in 2000. He joined GlaxoSmithKline in 2016 as an information scientist, and his work is focused on search and information consultancy as part of the external data strategy at GSK.

Kathleen Baster has a BSc (Hons) in Mathematics and Statistics and an MSc in Statistics. She has 22 years of experience of statistical consultancy at several companies in Ireland and England. She has worked at the Statistical Services Unit (SSU), University of Sheffield, for 16 of those years, most recently as a Principal Consultant. The SSU offers bespoke services of statistical advice and support for a wide variety of projects and clinical trials, for clients in both the academic and private sectors. Support is available for the whole project timeline from planning and sample size calculations through to reports and publications. Kathleen is an experienced consultant, programmer and project manager for a team with a reputation for high quality delivery.

Lucy C. Gelder has a BSc (Hons) in Mathematics and an MSc and PhD in Statistics. She has 10 years of experience in healthcare analysis for cancer intelligence (Trent Cancer Registry, Sheffield UK) and spent 5 years providing statistical support for nursing and midwifery projects (Edith Cowan University, Perth WA). Since 2017 she has worked as a Senior Consultant for the Statistical Services Unit (SSU) at the University of Sheffield. Lucy is an experienced statistical programmer and mainly uses R and SAS to carry out analyses and create publication ready tables, figures and reports.

Simon J. F. Macdonald received his Ph.D. degree from the University of Manchester, carried out postdoctoral studies at the University of Alabama and then joined Glaxo Group Research (now GlaxoSmithKline) in the UK in 1988. He has worked in many therapeutic areas during his career and respiratory in particular and was most recently involved in an integrin inhibitor project for fibrotic diseases. He was also involved with designing and teaching undergraduate medicinal chemistry modules at the University of Nottingham where he is a visiting professor. Since 2019, he has been a director at RGDscience Ltd.

■ ACKNOWLEDGMENTS

The authors acknowledge the use of the Ethnicity Estimator software produced by UCL's Consumer Data Research Centre in partnership with the Office for National Statistics and funded by the Economic and Social Research Council.[63] They thank the Royal Society of Chemistry Inclusion and Diversity Fund for part funding of this work. They also thank Helen Gosling and Fiona Macdonald Box for valuable discussions and for alerting us to the ethnicity assigning algorithms.

■ ABBREVIATIONS USED

AA, all authors; ACS MCL, ACS Medicinal Chemistry Letters; BMC, Bioorganic Medicinal Chemistry; BMCL, Bioorganic Medicinal Chemistry Letters; CA, corresponding authors; CMC, ChemMedChem, EJMC, European Journal of Medicinal Chemistry; JMC, Journal of Medicinal Chemistry; JOC, Journal of Organic Chemistry; MCC, MedChemComm; UK, United Kingdom; US, United States

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(129) These trends may reflect the gender demographic in the field, although it is possible (although in our view unlikely given the extensive literature on the gender of scientists) that there are large numbers of female medicinal chemists who do not publish, publish less, or are not included as authors on articles compared to their male counterparts.
(130) The Royal Society of Chemistry have published data on the gender diversity of editors and reviewers in their journals. See ref 5.
(131) A referee suggested that asking authors of a manuscript for their gender and race/ethnicity/origin might lead to bias in the review of their manuscript. That is why we propose that, while maintaining confidentiality, the data is published so any bias becomes easier to identify. In addition, clear self-reported data allows trends to be identified more accurately and appropriate interventions designed.

https://doi.org/10.1021/acs.jmedchem.1c01632
J. Med. Chem. XXXX, XXX, XXX−XXX