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Claus Rosenkrantz Hansen, CBS

Rasmus Rindom Riise, UCPH Library



Agenda:

- **Basics of copyright**
- **Creative Commons licenses**
- **Q&A**

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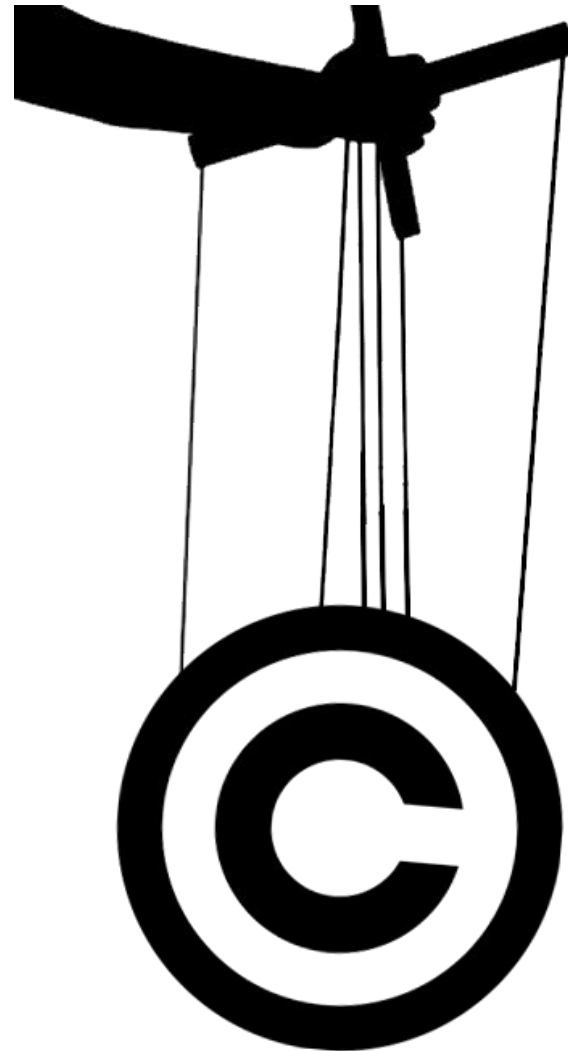
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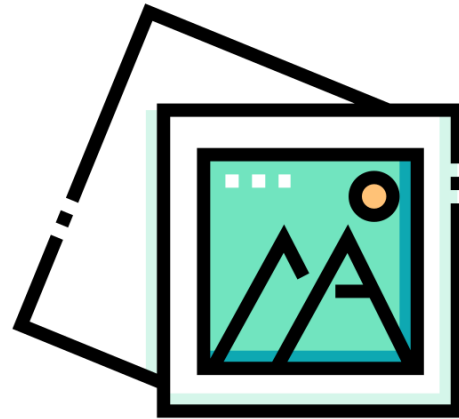
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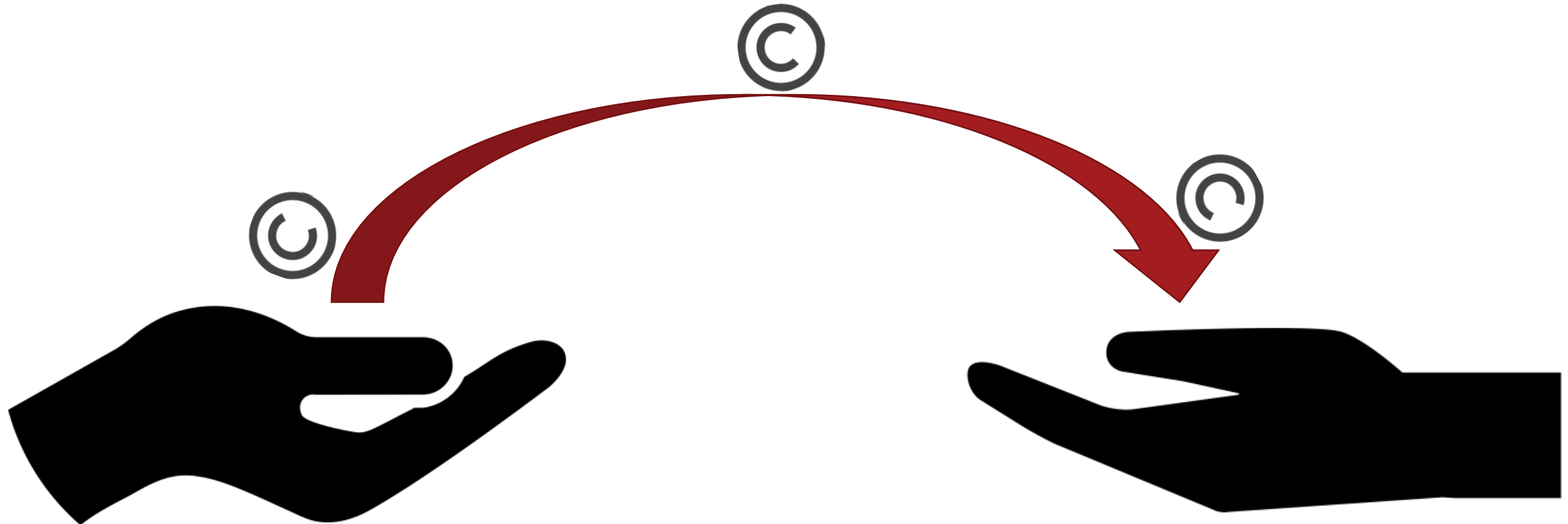
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- Ideas
- Opinions
- Facts
- Natural phenomena
- And a lot more...

Copyright basics

- The Threshold of Originality
- Copyright lasts for 70 years after the death of the originator
- What if a work has two or more originators?

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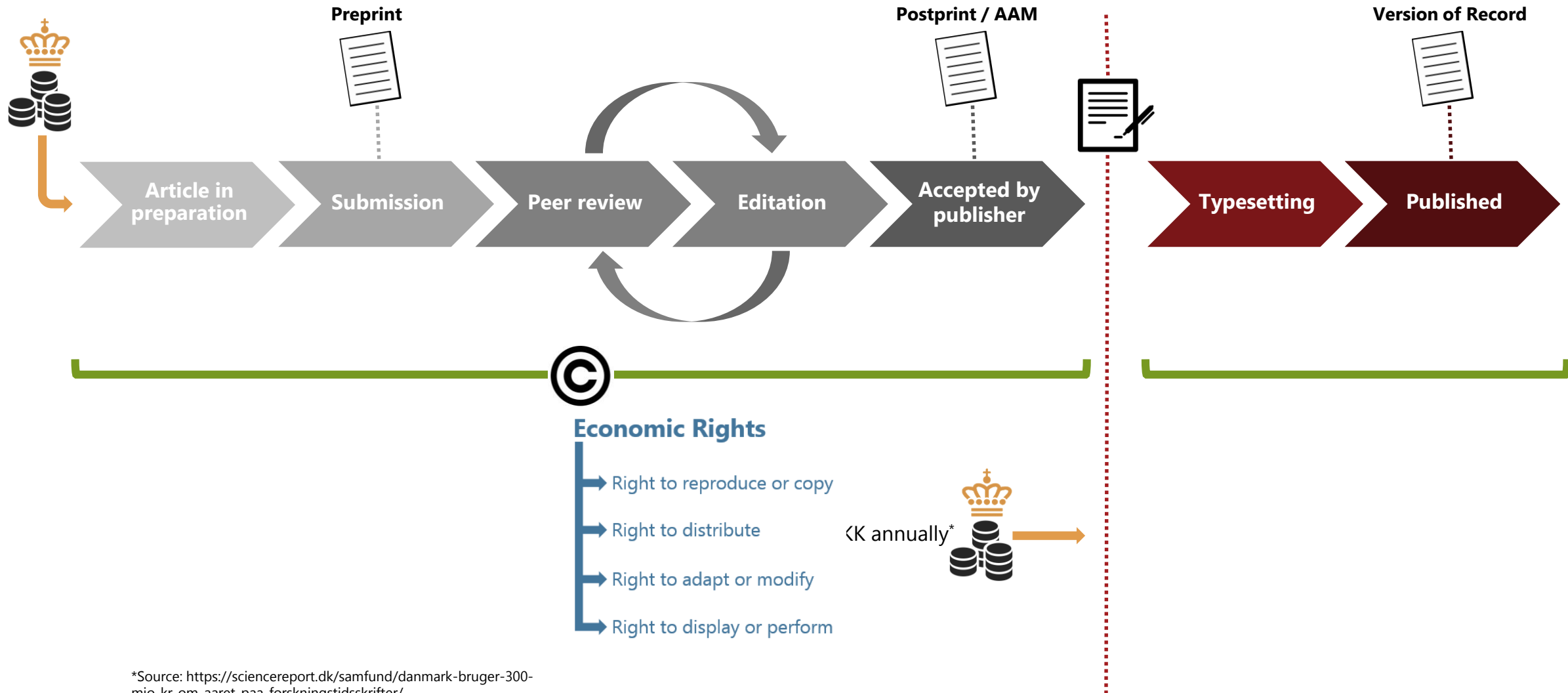


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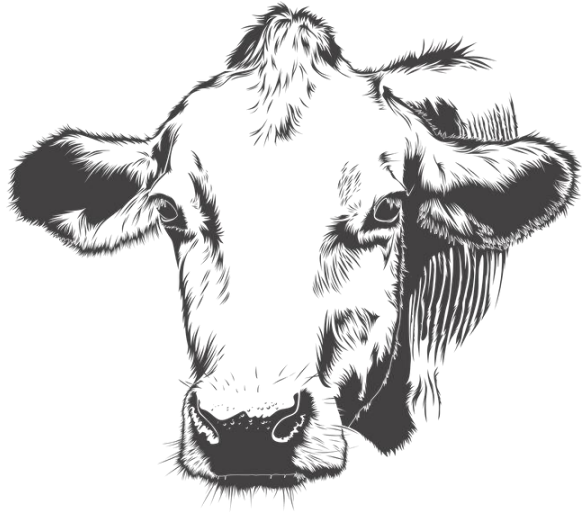
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Both Reactivity and Accessibility Are Important in Cytochrome P450 Metabolism: A Combined DFT and MD Study of Fenamic Acids in BM3 Mutants

Rasmus Leth, Bogac Ercig, Lars Olsen and Flemming Steen Jørgensen*

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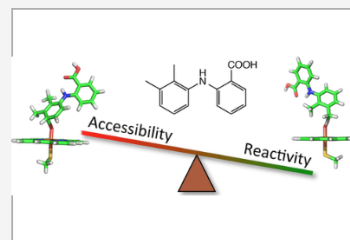
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Supporting Info (1)

SUBJECTS:

Abstract

Cytochrome P450 102A1 from *Bacillus megaterium* (BM3) is a fatty acid hydroxylase that has one of the highest turnover rates of any mono-oxygenase. Recent studies have shown how mutants of BM3 can produce metabolites of known drug compounds similar to those observed in humans. Single-point mutations in the binding pocket change the regioselective metabolism of fenamic acids from aromatic hydroxylation to aliphatic hydroxylation. This study is concerned with the individual contribution from accessibility and reactivity for drug metabolism with a future goal to develop fast methods for prediction. For a BM3 M11 mutant as well as the M11 V87F and M11 V87I mutants, we studied the metabolism of the nonsteroidal anti-inflammatory drugs (NSAIDs) mefenamic acid, meclofenamic acid, tolfenamic acid, and diclofenac. Density functional theory (DFT; B3LYP and B3LYP-D3) calculations for all possible reactions were performed using a porphyrin model reacting with the four substrates. Molecular dynamics (MD) simulations were used to determine the potential sites of metabolism that are accessible. Finally, we combine reactivity and accessibility for each potential site to interpret the experimentally determined metabolism. Generally, the 3 and 5 positions (on the ring containing the acidic substituent) and the 2', 3', and 4' positions are most reactive, whereas 4, 5, 3', and 4' are most accessible. Combining reactivity and accessibility show that the 5, 3', and 4' positions are predicted to be most prone to be metabolized, in agreement with experimentally observed data. Reactivity seems to be the dominant factor in the CYP-mediated metabolism of these NSAIDs, which is consistent with previously published methods based solely on reactivity.



Supporting Information

The Supporting Information is available free of charge on the ACS Publications website at DOI: 10.1021/acs.jcim.8b00750.

- Transition state structures for the *N*-hydroxylation (amine), aromatic hydroxylation (3, 4, 5, 6, 4', and 5'), and aliphatic hydroxylation (Me-3') reactions of meclofenamic acid; transition state structures for the *N*-hydroxylation (amine), aromatic hydroxylation (3, 4, 5, 6, 4', 5', and 6'), and aliphatic hydroxylation (Me-2) reactions of tolfenamic acid; transition state structures for the *N*-hydroxylation (amine) and aromatic hydroxylation (3, 4, 5, 6, 3', 4', and 5') reactions of diclofenac; docking poses of meclofenamic acid, diclofenac, and tolfenamic acid in BM3 M11 representing aliphatic hydroxylation (only for meclofenamic acid) and aromatic hydroxylation on both aromatic ring; snapshots from the MD simulations of meclofenamic acid in the three different binding modes for the three BM3 mutants; snapshots from the MD simulations of tolfenamic acid in the two different binding modes for the three BM3 mutants; snapshots from the

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THE POETICS OF PENAL TRANSPORTATION:
ROBERT SOUTHEY'S *BOTANY-BAY*
ECLOGUES

Robert W. Rix is Associate Professor at the University of Copenhagen. He has published widely on several aspects of the eighteenth century and romanticism, including religious movements, politics, and print culture.

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by exiled convicts who have been transported to Australia to work in the British penal colony popularly known as Botany Bay (located close to present-day Sydney). As Dorice Williams Elliott has shown in a recent monograph, the transported criminal was very much a "literary figure," appearing in several prominent novels.² However, her wide-ranging discussion does not include the writings of Southey or the other poets I will examine in this article. Southey invents his fictional speakers to highlight the plight of the convicts, and the poems clearly belong with the corpus of his early political writing, such as the first draft of *Joan of Arc*, *The Fall of Robespierre* (acts II and III), and *Wat Tyler* (all written 1793–1794). Following these radical works, Southey wrote a number of humanitarian poems on the slave trade and poverty (1795–1797). Romantic political poetry of the 1790s has been widely examined, including Southey's work, but the *Botany-Bay Eclogues* tend to be "exiled" from these discussions, at least no focused critical study has emerged.³ This article hopes to fill the critical gap.

Because of Southey's radicalism and his sentimental gesturing in the poems, it is easy to assume that they would contain an outright condemnation of transportation. Yet the argument I propose is that Southey looks at banishment

Robert W. Rix is Associate Professor at the University of Copenhagen. He has published widely on several aspects of the eighteenth century and romanticism, including religious movements, politics, and print culture.

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Original Article



COVID-19 pandemic and derogation to
human rights

Audrey Lebet

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KEYWORDS: COVID-19, public health, human rights, derogation, European Court of Human Rights

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- 1 Coronavirus COVID-19 Global Cases by the Center for Systems Science and Engineering (CSSE) at John Hopkins, <https://gisanddata.maps.arcgis.com/apps/opsdashboard/index.html#/bda7594740fd40299423467b48e9ecf6>.
- 2 <https://audiovisual.ec.europa.eu/en/topnews/M-004631> (accessed Apr. 7, 2020).

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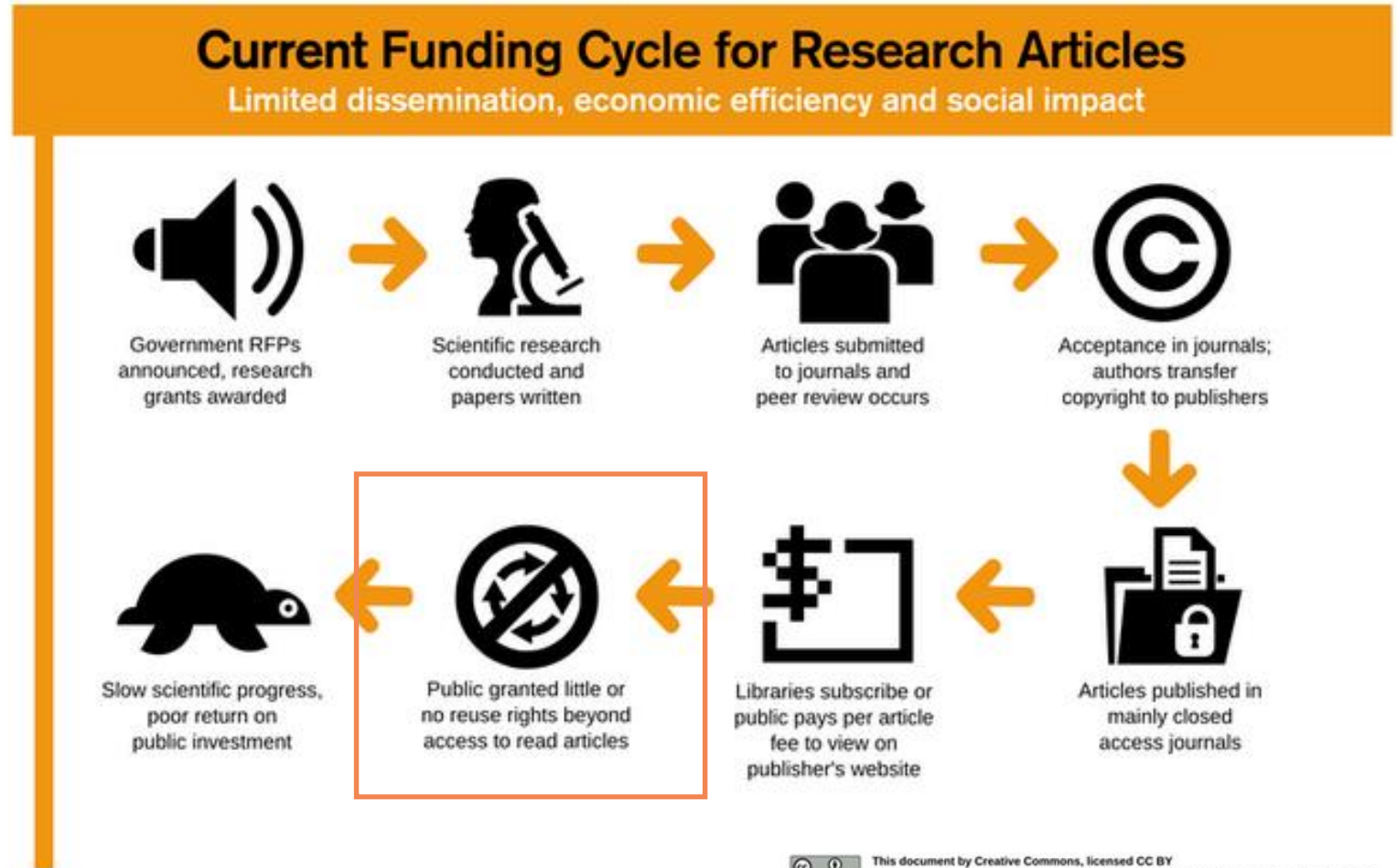



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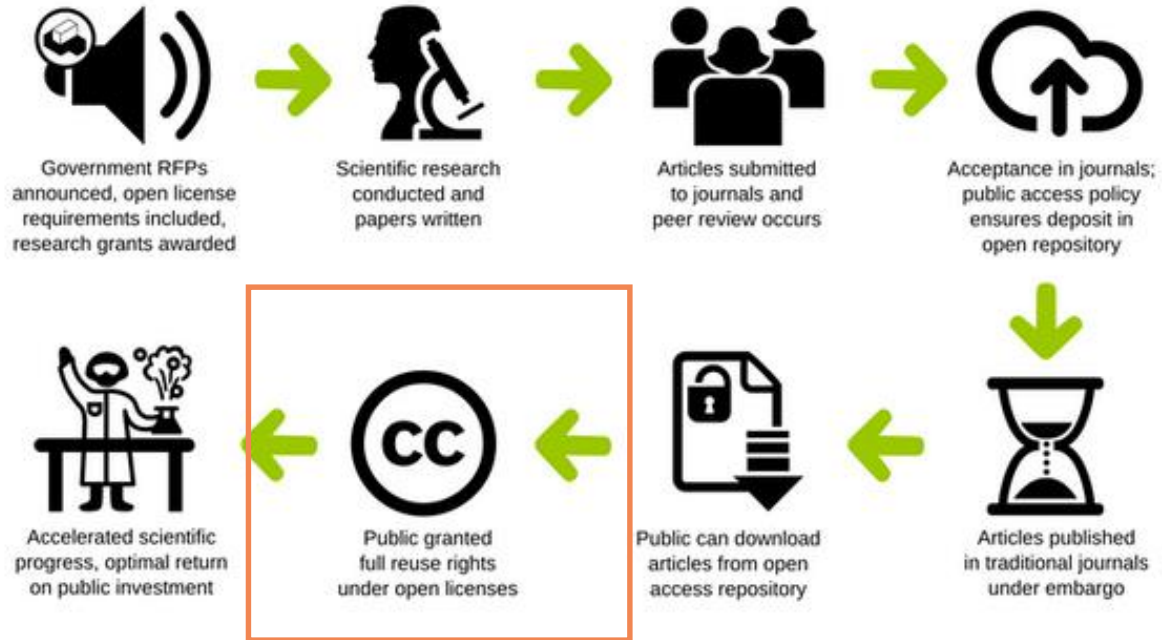
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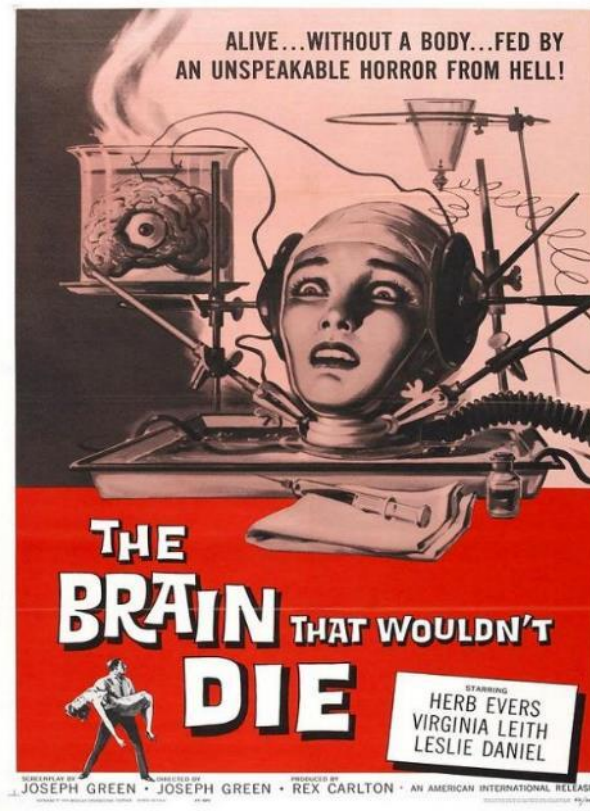
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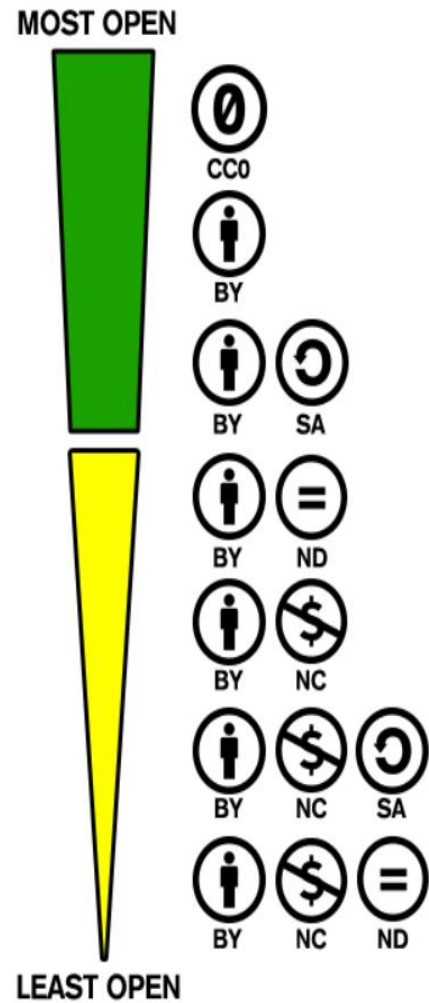
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Rifkin et al. *Microbiome* (2020) 8:62
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Multi-proxy analyses of a mid-15th century Middle Iron Age Bantu-speaker palaeo-faecal specimen elucidates the configuration of the 'ancestral' sub-Saharan African intestinal microbiome

Riaan F. Rifkin^{1,2*}, Surendra Vikram^{1†}, Jean-Baptiste Ramond^{1,2,3}, Alba Rey-Iglesia⁴, Tina B. Brand⁴, Guillaume Porraz^{5,6}, Aurore Val^{6,7}, Grant Hall⁸, Stephan Woodborne^{8,9}, Matthieu Le Bailly¹⁰, Marnie Potgieter¹, Simon J. Underdown^{1,2}, Jessica E. Koopman¹, Don A. Cowan¹, Yves Van de Peer^{1,11,12}, Eske Willerslev^{1,13,14} and Anders J. Hansen^{8*}

Abstract

Background: The archaeological incidence of ancient human faecal material provides a rare opportunity to explore the taxonomic composition and metabolic capacity of the ancestral human intestinal microbiome (IM). Here, we report the results of the shotgun metagenomic analyses of an ancient South African palaeo-faecal specimen.

Methods: Following the recovery of a single desiccated palaeo-faecal specimen from Bushman Rock Shelter in Limpopo Province, South Africa, we applied a multi-proxy analytical protocol to the sample. The extraction of ancient DNA from the specimen and its subsequent shotgun metagenomic sequencing facilitated the taxonomic and metabolic characterisation of this ancient human IM.

Results: Our results indicate that the distal IM of the Neolithic 'Middle Iron Age' (c. AD 1460) Bantu-speaking individual exhibits features indicative of a largely mixed forager-agro-pastoralist diet. Subsequent comparison with the IMs of the Tyrolean Iceman (Otzi) and contemporary Hadza hunter-gatherers, Malawian agro-pastoralists and Italians reveals that this IM precedes recent adaptation to 'Western' diets, including the consumption of coffee, tea, chocolate, citrus and soy, and the use of antibiotics, analgesics and also exposure to various toxic environmental pollutants.

(Continued on next page)

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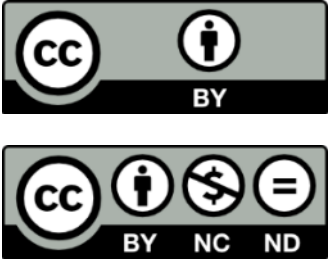
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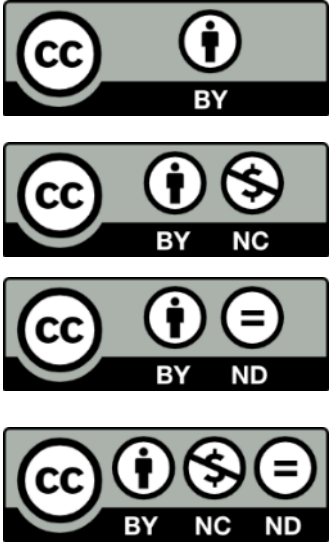


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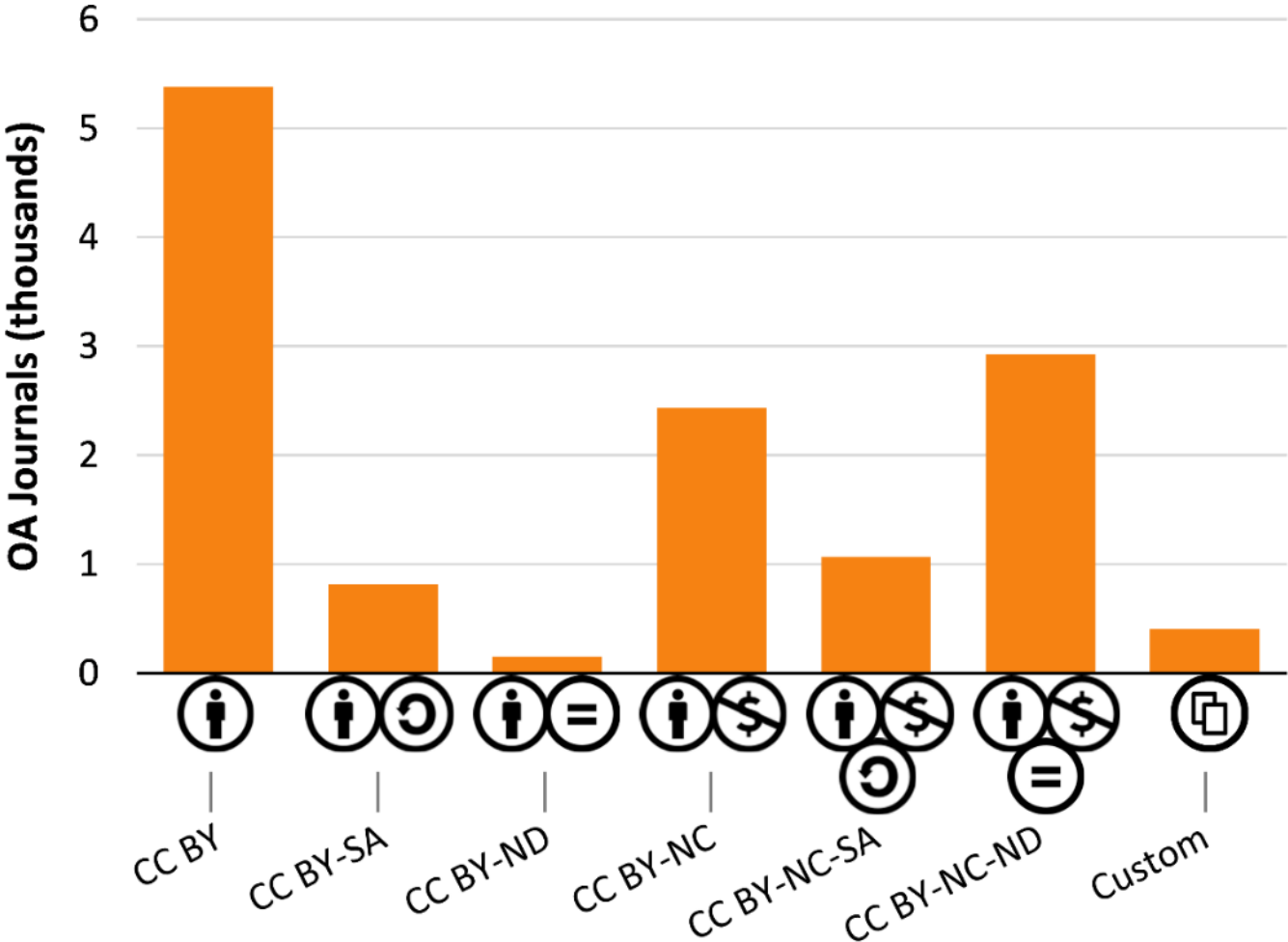
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