7TH NATIONAL RETROSYNTHESIS COMPETITION 2020

COMPETITION DETAILS

Please find below, the further details of the 7th National Retrosynthesis Competition 2020:

IMPORTANT: Only a retrosynthesis is to be submitted for the first round molecule (NOT a forward synthesis)

Timescale

- First round structure will be available from Monday 30th September 2019 onwards on various platforms, including the SCI/RSC event websites, Twitter, LinkedIn and OrgNet
- Final first round entries to be submitted to Jaspria Roda (Jaspria.Roda@soci.org) no later than 17:00 (GMT) on Friday 13th December 2019
  NB Entries submitted after this time will not be judged
- The judging panel will select a **maximum** of 10 entries to progress to the second round
- Teams selected to participate in the second round will be notified by Monday 13th January 2020
- Second round teams will present at the final on Friday, 13th March 2020.

Venue

The final will be held at the Royal Society of Chemistry (Burlington House, Piccadilly, Mayfair, London W1J 0BA), on Friday 13 March 2020, 10:30 – 17:00 (GMT).
Registration to attend the final will open in January 2020 and will be on a first come-first served basis. Limited priority will be given to supporters of the team's presenting at the final.
The event will be free to attend but travel and/or accommodation expenses will not be provided, apart from team members presenting at the final.

Team Information

Size
It is recommended that each team consists of no more than 8 people; however a **maximum of 4** people will be allowed to present at the final.

Age / Team Composition
Based on feedback from previous events and to open the event to a wider audience, there will be no age limit to enter the 2020 competition. However, the Organising Committee would like to stress that the spirit of the competition is to showcase the skills of early career chemists within the UK. The teams should aim to maximise the

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participation of these individuals and use more experienced team members' knowledge to facilitate discussion and contribute to proposals. The Organising Committee also promotes and values diversity within the teams.

Institutions / Companies / Universities
Teams can originate from a single company / institution / university with cross departmental teams encouraged. However, team members are restricted to contributing to only one entry. Joint entries are also encouraged although this must be made clear to the Organising Committee and judges at the time of submission.

Competition Details
Judging Criteria
The presentations/entries will be judged on the following factors which are applicable independent of the molecule:

- Elegance of disconnections and synthesis, in particular the application of existing chemistry to new problems
- Feasibility of route, to include literature precedence for non-trivial steps – a high degree of probability of success is essential
- Conciseness of synthesis from readily available inexpensive (ideally <£10/g) precursors
- Presentation to be concise, clear and logical

Where demonstrating a high probability of success for new transformations and new chemistry might appear challenging, teams are encouraged to address this by, for instance in critical and/or higher risk steps, (a) showing that competing pathways have been identified and why the desired pathway is deemed most likely, and/or (b) showing how their design is flexible enough to accommodate contingency routes.

The first round entries will be judged by one academic and one industrial judge to ensure impartiality. In the event that two judges cannot make a selection, then the other two judges will be asked for their opinion and a decision made.

FEEDBACK WILL NOT BE PROVIDED AT ANY STAGE OF THE PROCESS

Research Discovery Applications/Chemistry Information Tools/Search Engines
All proposed chemical routes must be substantiated by sound chemical reasoning and literature references. No hypothetical chemistry transformations should be included.
Use of applications such as SciFinder and Reaxys are encouraged.

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Specific criteria for each round

1st round – IMPORTANT: Only a retrosynthesis is to be submitted for the first round (NOT a forward synthesis)

The template provided on the website **must** be used for all competition submissions for the first round and adhere to the key points below:

Length

- The presentation must be a **maximum** of 10 pages.
- The title page must contain:
  - team name
  - names of team members
  - company or institution(s) represented
- A maximum of 8 pages for the retrosynthesis of the molecule
- The final page should contain references. Where possible, please include doi links.

Formatting

- Please save your submission file as "**Company/University Name – Team Name**"
- Structures should be drawn using one of the following programmes and styles:
  - ChemDraw - ACS 1996
  - ISIS – JACS or JOC settings
  - Symyx draw - ACS Document

Computational Modelling

Use of computational modelling is encouraged to support ideas/theories/proof of concept but it will be considered a part of a chemist's retrosynthetic toolkit, and extra points will not be awarded for using it. If computational modelling is used, as with any other tool, teams must be prepared to respond in-depth questioning.

2nd round – final IMPORTANT: A forward synthesis should be presented in the second round (a short retrosynthesis may be part of your presentation)

There are no restrictions to the format or content for the final but all presentations will be strictly limited to 15 minutes. The judging panel will take presentation style and content into account, so it is recommended that the chemical formatting mentioned above or similar is maintained. Key steps of the retrosynthesis may be presented, but the focus of the presentation should be on the forward synthesis.

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Chemistry Schemes
All forward synthesis must contain proposed:

- Reagents
- Solvents
- Yields (based on sound literature references where possible)
- Enantiomeric Excess (based on sound literature references where possible)
- Bullet points should be used to describe key points

Judging Criteria
All of the criteria for round one with the addition of verbal presentation/communication skills both during the presentation itself and answering the questions, as well as demonstrating a depth of chemistry when answering questions from the audience.

Copyright

- The submitted reaction schemes will not be kept confidential, and in entering the competition and accepting the T&C, the group submitting the scheme agrees and consent to the same.
- Any IP rights that subsist in the submitted materials must not infringe the rights of any third parties.
- Both SCI and RSC own a worldwide, non-exclusive right to:
    - Publish any reaction schemes submitted to SCI in any medium whatsoever;
    - Modify and publish any reaction schemes submitted to SCI in any medium whatsoever.
    - Publish any presentations submitted to SCI in any medium whatsoever, including live streaming the event.
- Any other specific items or documents submitted to SCI for the purpose of the competition may also be published, these items should be treated in the same way
- Unless formally agreed with the SCI or the Competition Organising Committee, the details of the authors and their affiliations (as the authors) shall be published

Further Information
For further information or questions, please contact Jason Camp (j.camp@bath.ac.uk) or the SCI's Conference Team: conferences@soci.org or Jaspria.Roda@soci.org
Twitter: Follow @UKRetroComp
LinkedIn: Join the "UK Retrosynthesis Competition" group