



4TH NATIONAL RETROSYNTHESIS COMPETITION 2016



COMPETITION DETAILS

Please find below, the further details of the 4th National Retrosynthesis Competition 2017:

Timescale:

- First round structure will be available from Monday 31st October 2016 onwards
- Final first round entries to be submitted no later than 17:00 (GMT) on Friday 16th December 2016

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
- Second round structures will be sent to the selected teams on Monday 16th January 2017
- Second round teams will present at the final on Friday, 10th March 2017

Venue

The final will be held at the Society of Chemical Industry, Belgrave Square on Friday 10th March 2017, 10:30 – 17:00 (GMT).

Registration to attend the final will begin in January 2017 and will be limited to a first come-first served basis. Limited priority will be given to supporters from team's presenting at the final.

The event will be free but travel and/or accommodation will not be provided.

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

Based on feedback from previous events and to open the event to a wider audience, there will be no age limit to enter the 2017 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. Therefore the team should aim to maximise the participation of these individuals and it is suggested that more experienced team members use their knowledge to facilitate discussion and contribute to proposals.

Institutions/Companies/Universities

Teams should originate from one company or department. Smaller industrial or academic departments who will be allowed to submit joint entries but these must be approved by the Organising Committee in advance of submission. Multiple teams from the same Institutions/Companies/Universities are encouraged although team members are restricted to contributing to one entry.

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.

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.

Specific criteria for each round

1st round

The attached template **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 both retro- **and** forward synthesis (4+4, 3+5, etc)
- The final page should contain references. Where possible, please include doi links.

Formatting

- Structures must be drawn using one of the following programmes and styles:
 - ChemDraw - ACS 1996
 - ISIS – JACS or JOC settings
 - Symyx draw - ACS Document

Chemistry Schemes

All forward synthesis must contain proposed:

- Reagents
- Solvents
- Yields (based on sound literature references where possible)
- **NB** yields less than 20% should be justified
- Enantiomeric Excess (based on sound literature references where possible)
- Bullet points should be used to describe key points

2nd round - final

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.

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;
- 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 Robert Wybrow (robert.wybrow@syngenta.com)

Twitter: Follow @UKRetroComp; LinkedIn: Join the "UK Retrosynthesis Competition" group