

# 5th National Retrosynthesis Competition 2018

## Terms and Conditions

Please find below full details of the 5th National Retrosynthesis Competition 2018, we ask you to read this information carefully before proceeding with your competition entry.

### 1. Timescale

**Monday 2 October 2017:** First round molecule released

**Friday 15 December 2017:** First round entry closes at 5pm. Entries submitted after this time will not be judged.

**Monday 15 January 2018:** Finalists announced. The judging panel will select a maximum of 10 entries to progress to the second round

**Monday 15 January 2018:** Second round molecule released to selected teams

**Friday 16 March 2018:** Competition final. Selected teams present and judges select a winning team.

### 2. Venue

The final will be held at the Royal Society of Chemistry, Burlington House, London on Friday 16th March 2018, 10:30 – 17:00.

Registration to attend the final will open in January 2018 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.

### 3. 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 2018 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 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.

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### 4. 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.

### Specific criteria for the 1st round

The PowerPoint 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
  - name of each team member
  - name of 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



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#### 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 teams have used modelling in their entry, as with any other tool, teams must be prepared to respond in-depth questioning.

#### Specific criteria for the 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.

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@tennantsfinechemicals.com](mailto:robert.wybrow@tennantsfinechemicals.com) or SCI's Conference Team: [conferences@soci.org](mailto:conferences@soci.org) / [daisy.goddard@soci.org](mailto:daisy.goddard@soci.org)

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