



# The Molecular Graphics and Modelling Society

## 37<sup>th</sup> Annual General Meeting

*Wednesday, 29th August, 2018, at 5:15 pm*

*Murray Edwards College, University of Cambridge, Cambridge, UK.*

<https://discretebiology.com>

### *Minutes*

1. Minutes of the 36<sup>th</sup> AGM held at the Manchester Institute of Biotechnology Lecture Theatre, The University of Manchester, 131 Princess Street, Manchester, M1 7DN, UK.

- The minutes were approved.

2. Matters arising

- There were no matters arising.

3. Chairman's Annual Report

- PB presented the Chair's report:

“The Molecular Graphics and Modelling Society was founded in 1981 as a charitable organization with the key goal of promoting education and research into scientific endeavors that develop or utilize molecular modelling and computer graphics techniques. Historically and still very much to this day, the main mechanism for achieving that goal is through the delivering and support of scientific meetings and workshops such as this current “Discrete Biology” meeting held here in Murray Edwards College, Cambridge. At this point in time, I'd like to extend my thanks to Dr Ben Hall for his organization of this meeting, which looks like it will be a great success.

This past year has been another very successful one for the MGMS with several well-attended meetings. The first was a one-day meeting held at the School of Oriental

and African Studies (SOAS) titled “MD in Pharma” on the 11th April 2017 and brought together many leading exponents of molecular dynamics in both the pharmaceutical industry and academia. I would like to extend my thanks in particular to Ben Cossins and the three sponsors (UCB, Boehringer Ingelheim and Schrödinger) for making that meeting so successful.

The second meeting was a three-day meeting focused on “QM/MM Methods and Applications” held on the 4-6th September, 2017, at the University of Manchester. This was another very successful and timely meeting and highlighted the strength and depth of this subject within the UK and Europe in general. My thanks to Richard Bryce, Sam De Visser and Sam Hay for putting together an excellent program and a smooth-running event.

The final event of 2017 was the Young Modellers Forum held for the third time at the University of Greenwich on the 24th November, 2017. The standard of presentations at this event continues to be excellent and serves as a fantastic showcase of the young talent that is coming through in this field not only from the UK but also from the rest of Europe. It continues to be well attended and supported by the industrial sector and provides an excellent opportunity for rich interactions to develop between industrial and academic researchers.

There was strong competition for the coveted 12 poster and 12 oral presentation places. The winners of the talk prizes were Adam Baskerville (University of Sussex), Hannah Bruce Macdonald (University of Southampton) and Nick Fowler (University of Manchester). The winners of the poster prizes were Marc Daemgen (University of Oxford) and Ricardo Parra- Cruz (University of Nottingham). My particular thanks are extended this year to Jiayun Pang, who was once again ably supported by Louise Birch, Steve Maginn and Mike Mazanetz. □

The 2018 YMF will be the next conference after this AGM and will once again be held at the University of Greenwich on the 30th November 2018. My thanks in advance once again go to Jiayun Pang and this year also to Mike Mazanetz, Louise Birch and Steve Maginn.

On the 11th and 12th of April 2018, the MGMS partnered with the UK-QSAR and cheminformatics group to host a joint meeting entitled “Structure-Activity Relationships” at the University of Cardiff. This was a very well attended meeting and thoroughly enjoyed by all concerned. My thanks to Steve Maginn, Jamie Platts and Brendan Howlin and colleagues at UKQSAR for such a splendid and smooth-running conference.

Shortly after this meeting we were all deeply saddened to learn of the passing of Dr Frank Blaney on the 14th April 2018. Frank was a founding member of the MGMS and remained intimately connected to it ever since. He served as Chair of the MGMS and was

also responsible for the organisation of many successful conferences throughout his life. He was a long-standing member of the computational chemistry community and had a particularly strong interest in membrane proteins including GPCRs, ion channels and transporters. He also had an interest in using QM methods to understand cytochrome P450s. Following a long career at GSK, his interest and substantial expertise in GPCRs led to his becoming a consultant, working closely with Heptares Therapeutics. He was a fount of knowledge for computational chemistry and we will all miss him very much indeed.

The sponsorship of prizes is another important way in which the Society seeks to promote computational chemistry. The prestigious MGMS Silver Jubilee Prize (in its 10th year) was awarded to Dr David Glowacki for his excellent work on interactive visualization. My congratulations to him. Given the interactive nature of his work (using virtual reality headsets etc), the MGMS is pleased that Dr Glowacki will give a mini lecture tour so please go along if you get the opportunity to see and interact with molecules!

In recognition of Frank Blaney's work with the MGMS, the committee was unanimous in their approval that the Silver Jubilee Prize be renamed "The Frank Blaney Prize". If you know someone who might be eligible for the prize next time, then please do encourage them to apply. Note that it is also possible to self-nominate, but you must find someone to write a letter of support. We will begin the process this autumn. Full details will appear on the website shortly.

The MGMS also regularly holds lecture tours. Dr Andrew Leach of the EMBL EBI has commenced his lecture tour and has already visited Manchester. The lectures at Southampton and Dundee are still to take place so keep your eyes out for those events. The success of these activities, which play a vital role in promoting computational chemistry and the cohesiveness of our community, are underpinned by the generous sponsorship of companies and organisations but also the tireless involvement of local meeting organisers and MGMS committee members. The work of the Society depends on the hard work of these volunteers. I would like to thank all of them for their commitment, enthusiasm and support over the past year. My particular thanks go to Garrett Morris and Brendan Howlin for their hard work as Secretary and Treasurer respectively. My thanks also to Jamie Platts for all his hard work as Editor of the Journal of Molecular Graphics and Modelling. It would be great to see more members publish their work in this journal. I also thank Steve Maginn for his hard work as Membership secretary and for ensuring people are aware of conferences and workshops. I also thank Stuart Firth-Clarke for all his efforts in keeping the website up to date and for Shozeb Haider for offering to take this on this year.

As the Society enters its 38th year, I can confidently report to this meeting that the MGMS continues to make a significant impact in developing and promoting computational chemistry, through its meetings, lecture tours, prize and other activities.

The Society exists for the computational chemistry community and depends on your support. There are many ways to become more connected to the MGMS, by visiting our website ([www.mgms.org](http://www.mgms.org)), joining our LinkedIn group (“Molecular Graphics and Modelling Society”) and primarily through becoming a member. If you would like to find out more about the Society or make suggestions for meetings that you would like to see and get involved with, then please do contact myself or other committee members.

#### 4. Secretary’s Annual Report

- GMM presented the MGMS Secretary’s Report:

“In addition to the current meeting, Discrete Models and Formal Verification in Biology, at Murray Edwards College, University of Cambridge, UK (29-31 August, 2018), the MGMS has been involved in the organisation and support of the following events since the last AGM:

- **MD in Pharma**
  - School of Oriental and African Studies (SOAS), London, UK. 11 April, 2017.
- **QM/MM Methods and Applications**
  - University of Manchester, Manchester, UK. 4-6 September, 2017.
- **Young Modellers’ Forum, 2017**
  - University of Greenwich, London, UK. 24 November, 2017.
- **Structure-Activity Relationships (Joint MGMS & UK-QSAR meeting)**
  - University of Cardiff, Cardiff, UK. 11-12 April, 2018.

We would like to thank everyone who helped run these events, the sponsors, and all of you who attended. Please keep an eye on our website and LinkedIn page for details and get in touch if you would like any further information.

#### **Composition of the MGMS Executive Committee**

The composition of the current committee/trustees is given below (dates of election are given in parentheses). Many thanks to all of the committee for their hard work over the year.

<b>Chairman</b>	Phil Biggin (2016)
<b>Secretary</b>	Garrett M. Morris (2014)
<b>Treasurer</b>	Brendan Howlin (2015)
<b>Membership Secretary</b>	Steve Maginn (2016)
<b>Meetings Secretary</b>	—
<b>Journal Editor</b>	Jamie Platts (2016)
<b>Ordinary Members (7)</b>	Richard Bryce (2014)
	Stuart Firth-Clark (2014)

	Shozeb Haider (2014)
	Val Gillett (2015)
	Jiayun Pang (2015)
	Irina Tikhonova (2015)
	Adrian Mulholland (2016)

Co-opted members for the current year were: Louise Birch, Ewa Chudyk, Tim Clark, Ben Cossins, Xiao Lewell, Mike Mazanetz, Michelle A. Sahai, and Dave Winkler.”

## 5. Treasurer’s Annual Report

Brendan Howlin, MGMS Treasurer, submitted detailed report which is available by contacting the Secretary, and presented this report, including the following highlights:

“(1) The Meeting on QM/MM Methods and Applications which was held on 4-6 Sept 2017 at the University of Manchester, generated an MGMS portion of the profits of £5457;

(2) The joint meeting with the UK-QSAR Society in Cardiff on Structure-Activity Relationships, April 11-12, 2018 did not generate any profit as UK-QSAR does not handle money.

(3) The MGMS Bank accounts were successfully transferred to CAF Bank owing to dissatisfaction with HSBC.

(4) The MGMS bank account balances, as of 20/08/18, are: Current: £40,454.31 and Savings: £17,001.63”

## 6. MGMS Membership and Fees

Steve Maginn, MGMS Membership Secretary, presented the following report, including the new Data Usage Statement required by GDPR:

“MGMS membership currently stands at a figure of 182. All members who joined in 2016 and have not renewed have been removed from the list, and those who joined through attendance at the QMMM meeting in Manchester in September 2017 have been added (62 people). Attendees at the joint MGMS / UKQSAR conference in Cardiff in April 2018 did not automatically receive membership of the Society, as registration for that event was free of charge. Conference / meeting attendance remains by far the biggest source of members for the Society.

Regular emailings of items of interest to the membership (relevant job opportunities, relevant non-commercial conference notifications, society news etc.) continue to be sent through a webmail address, membership@mgms.org to members who have consented to

receive them; they can opt out at any time. The MGMS is therefore compliant with the European Union's GDPR rules. These rules also state that members are entitled to know how their data is used – therefore the MGMS has produced a Data Usage Statement as follows;

#### DATA USAGE STATEMENT:

The MGMS keeps information on its members' names, postal addresses (where supplied) and email addresses, solely for the purposes of identifying current membership status when member discounts on conference registrations are claimed, and for contacting members concerning society news and business. Email addresses are also used to send information about relevant conferences and job vacancies, although any member may opt out of this by contacting [membership@mgms.org](mailto:membership@mgms.org) at any time. Members' details are not provided to any other organisation for any purpose."

#### 7. The Journal of Molecular Graphics and Modelling Society

The following report was submitted by the Editor of the JMGM, Jamie Platts:

"Following the death of Dr Jeffrey Madura in March 2017, we are pleased to announce that Emilio Esposito has taken over as US-based editor. Emilio has interests in computational chemistry and machine learning, and their applications in pharmaceuticals and also in chemical education, and is highly active within the ACS COMP division.

Elsevier plan to reinstate the "Best Graphics" prize and name this in honour of Jeff's memory. Emilio and I will select outstanding graphics from 2018 submissions and nominate these for the award.

Impact factor rose slightly for 2017 to 1.885 (from 1.754) from 765 submissions and 270 accepted articles (36% acceptance rate). 2018 figures suggest further increase in submissions is likely.

Submissions from MGMS members are very welcome! We are also keen to recruit new, motivated members of our Editorial Board: please express any interest to me.

Submissions welcome from all aspects of molecular modelling and computational chemistry. Full paper or short communication. Also review articles or commentaries. Fast publication: 3.7 weeks submission to first decision; 7 weeks submission to final decision; 2 weeks acceptance to citable online; and Open Access is available"

#### 8. Election of Trustees/Committee Members and Chair

- Retiring: No-one.

- Re-standing: Brendan Howlin (Treasurer), Val Gillet (Ordinary Member), Jiayun Pang (Ordinary Member), and Irina Tikhonova (Ordinary Member).

As no-one stood against those re-standing, everyone re-standing was re-elected.

Following the AGM elections, the Committee consists of:

<b>Chairman</b>	Phil Biggin (2016)
<b>Secretary</b>	Garrett M. Morris (2017)
<b>Treasurer</b>	Brendan Howlin (2018)
<b>Membership Secretary</b>	Steve Maginn (2016)
<b>Meetings Secretary</b>	—
<b>Journal Editor</b>	Jamie Platts (2016)
<b>Ordinary Members (7)</b>	Richard Bryce (2017)
	Stuart Firth-Clark (2017)
	Shozeb Haider (2017)
	Val Gillett (2018)
	Jiayun Pang (2018)
	Irina Tikhonova (2018)
	Adrian Mulholland (2016)

Co-opted members for 2017-2018 are Louise Birch, Ewa Chudyk, Tim Clark, Ben Cossins, Xiao Lewell, Mike Mazanetz, Michelle Sahai, and Dave Winkler.

9. Any other business

There was no other business.

10. Date and location of next AGM:

The AGM will be held alongside the “Sheffield Cheminformatics 2019” meeting at the University of Sheffield, at approximately 5 pm on Wednesday, June 17th, 2019.