

H2020 EINFRA-5-2015



[www.bioexcel.eu](http://www.bioexcel.eu)

Project Number 675728

## D4.4 – Dissemination Report and Updated Plan

*WP4: Training and Dissemination*



Copyright© 2015-2018 The partners of the BioExcel Consortium



This work is licensed under a [Creative Commons Attribution 4.0 International License](https://creativecommons.org/licenses/by/4.0/).

## Document Information

<b>Deliverable Number</b>	D4.4
<b>Deliverable Name</b>	Dissemination Report and Updated Plan
<b>Due Date</b>	2017-04-31 (PM18)
<b>Deliverable Lead</b>	KTH
<b>Authors</b>	Rossen Apostolov (KTH), Vera Matser (EBI), Mirren White (EPCC), Ian Harrow (ICH)
<b>Keywords</b>	Project Management
<b>WP</b>	WP4
<b>Nature</b>	Report
<b>Dissemination Level</b>	Public
<b>Final Version Date</b>	2017-04-27
<b>Reviewed by</b>	PMB
<b>MGT Board Approval</b>	2017-04-28

## Document History

<b>Partner</b>	<b>Date</b>	<b>Comments</b>	<b>Version</b>
KTH	2017-04-17	First draft	0.1
KTH	2017-04-25	Social media analysis	0.2
KTH	2017-04-27	Updates	0.3
KTH	2017-04-28	Final version	0.4

## **Executive Summary**

This document reports on the dissemination activities of BioExcel for the period until 30 April 2017. Together with D4.5 – Training Report and Updated Plan (PM18), this deliverable gives a complete overview of the work completed under work package 4. The current D4.4 presents information about the project website, social media channels, dissemination events and publications, while D4.5 focusses on the BioExcel Training Programme. Where content overlaps, we specify if a subset of information is presented and refer to the deliverable with the most detailed overview.

The project website is one of the main channels for connecting with the wider communities. Its content has substantially increased over the time of the project and it attracts a healthy regular traffic. Social media activities have been successful for promotion. Mailinglists and newsletters have been established for communication with specific interest groups. Webinars have been particularly popular not only for promotion but for providing a long-lasting expertise to researchers. Through extensive participation in 41 dissemination events in addition to 28 training ones we have been able to outreach to a large proportion of user base. 23 articles have been published in scientific journals and conference publications. A promotional video that showcases the mission and vision of the center has been produced for further distribution. Several important collaborations have been established with partnering organizations – ELIXIR, OpenPHACTS and MolSSI, and others are in ongoing discussions.

## **Contents**

<b><u>1</u></b>	<b><u>WEBSITE</u></b>	<b><u>6</u></b>
1.1	BLOGS BY TRAVEL GRANTEES	6
1.2	FUTURE PLANS	7
<b><u>2</u></b>	<b><u>MAILING LISTS AND NEWSLETTERS</u></b>	<b><u>8</u></b>
<b><u>3</u></b>	<b><u>SOCIAL MEDIA</u></b>	<b><u>9</u></b>
3.1	TWITTER	9
3.2	LINKEDIN	13
3.3	FUTURE STRATEGY	15
<b><u>4</u></b>	<b><u>PROMOTIONAL VIDEO</u></b>	<b><u>16</u></b>
<b><u>5</u></b>	<b><u>PUBLICATIONS</u></b>	<b><u>16</u></b>
<b><u>6</u></b>	<b><u>OUTREACH AND DISSEMINATION EVENTS</u></b>	<b><u>18</u></b>
<b><u>7</u></b>	<b><u>BIOEXCEL DISSEMINATION AND EVENT GUIDELINES</u></b>	<b><u>21</u></b>
7.1	BIOEXCEL DISSEMINATION CHANNELS	21
7.2	IMAGES	23
7.3	WEBINAR DISSEMINATION	23
7.4	EVENT GUIDELINES	23
7.4.1	INTEREST GROUP EVENTS	23
7.4.2	TRAINING EVENTS	24
<b><u>8</u></b>	<b><u>WEBINARS</u></b>	<b><u>25</u></b>
<b><u>9</u></b>	<b><u>INTERFACING WITH INDUSTRY</u></b>	<b><u>26</u></b>
<b><u>10</u></b>	<b><u>COLLABORATIONS</u></b>	<b><u>27</u></b>
<b><u>11</u></b>	<b><u>CONCLUSIONS</u></b>	<b><u>27</u></b>
<b><u>12</u></b>	<b><u>ANNEX</u></b>	<b><u>28</u></b>
12.1	PROPOSAL FOR A STRATEGIC PARTNERSHIP (TEMPLATE)	28
12.2	MOU FOR STRATEGIC PARTNERSHIP (TEMPLATE)	29
12.3	MOU FOR COLLABORATIVE PARTNERSHIP (TEMPLATE)	31

## 1 Website

The website is the one of the main mediums for sharing and promoting information about the activities in the center. It has grown significantly in terms of content and visits during the past year. In Table 1 we present several statistics about the portal usage.

*Table 1. Website Stats (April 1 2016 – April 1 2017)*

Pageviews	27991
Sessions	14053
Unique visitors	8996
New users (%)	63.6
Returning Users (%)	36.4
Average session duration (mins)	1:48
Bounce rate (%)	58.7
Most users per month	1120 (March 2017)
Least users per month	522 (December 2016)
Average users per month	750
Top 5 User Locations (% of sessions)	UK (17.3), USA (13.2), Spain (10.7), Germany (6.3), India (6.0)

In Table 2 are listed the 10 most popular pages. Some of them are related to quite popular events. For the rest we plan to improve them and make them more prominent.

*Table 2. Most popular pages on [www.bioexcel.eu](http://www.bioexcel.eu).*

<b>10 Most popular pages</b>	<b>% of total pageviews</b>
Home page	26.1
Webinar category	3.4
Workflow training event	2.9
Partners page	2.6
BioExcel SIG	2.2
Events category	2.2
Interest Groups Landing Page	2.2
2017 Spring School Event	2.2
Contact page	2.2
GROMACS software page	2.0

### 1.1 Blogs by travel grantees

BioExcel offers a limited number of fixed amount travel grants for each of the BioExcel Training events. The beneficiaries of the grants are asked to write a blog post for us, either about their experiences at the course, their research interests (in layman's terms) or a relevant scientific topic (e.g. <http://bioexcel.eu/hear-from-our-travel-grant-beneficiaries/>). The grants are described in more detail in D4.5-Training Report and Updated Plan.

## 1.2 Future plans

The webportal has already grown substantially since its first inception at the start of the project. The quantity and types of content has increased, and this requires that we update the presentation layout correspondingly. The future plans for development include:

- Substantial redesign of the landing page

The landing page of every project needs to present in a balanced way information both for newcomers (what is the project about, who are the people, what they do, etc.), as well as for repeated users (what are the upcoming events/webinars..., what new content is available, who to talk to about a potential collaboration, etc...). Given the amount of available material and ongoing activities, it becomes more challenging to find the appropriate balance. For that, starting in PM20 will start working with a professional designer to restructure the landing page. In Figure 1 we show an initial mockup of the new front page redesign.

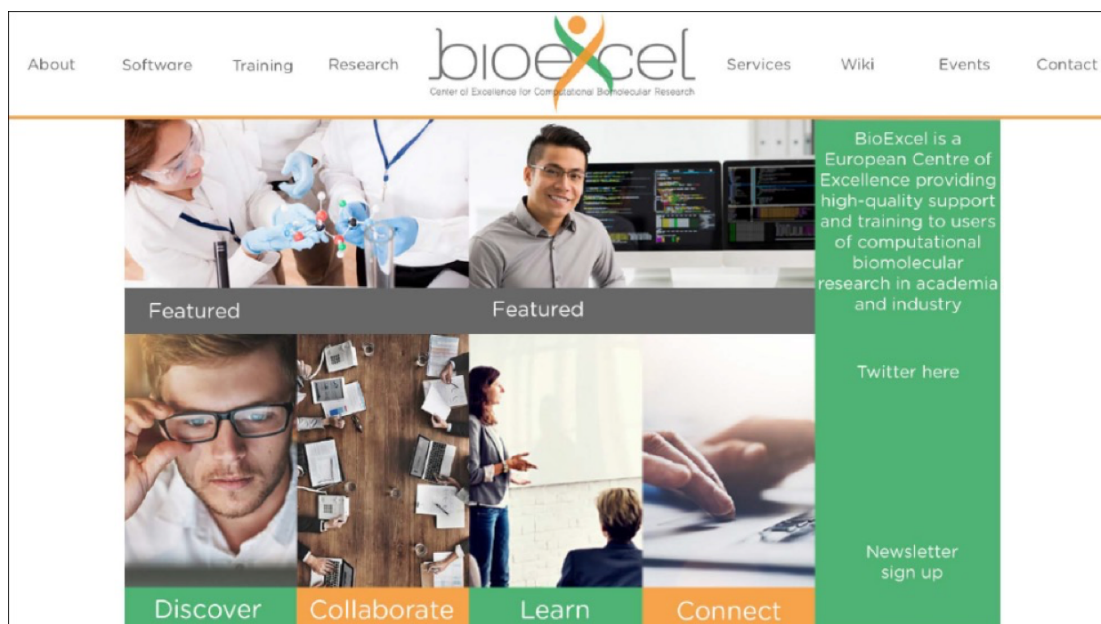


Figure 1. Mockup of a new front page design

- Restructuring the menus

Since the launch of the portal, the most important sub-pages were organized around several main items in a single top-level menu – “About”, “Research”, “Software”, “Services” and “Events”. However, currently they seem to be insufficient to expose the depth of content, which has been produced over the last year and a half. Thus, along with redesign of the front page we will work on improving the menu structure as well for improved usability.

- Embedding external services

In addition to the above redesign work, we consider linking to webservice, which are provided by BioExcel partners on external websites and are relevant to the activities in the center. Those include several webportals which are managed by UU, IRB, BSC, EBI and UMAN.

## 2 Mailing lists and newsletters

Mailing lists and newsletters are some of the channels that we use for communication with the wider audience. Visitors to the center website are encouraged to subscribe to the general BioExcel mailing list. This mailing list is used to keep users informed about upcoming events, webinars, relevant new material, success stories etc. via mostly monthly newsletters. Attendees to the BioExcel educational webinar series are also added to this mailing list. Archives of the newsletters are available at <http://bioexcel.eu/about/newsletters>.

In addition to the general mailing list, we have separate lists of people who have expressed interest in joining the different Interest Groups (IGs). Currently we have the following lists and number of subscribers:

- BioExcel General Mailinglist – **435** (includes those who have subscribed directly and those who have attended the webinars)
- Entry Level Users IG - **24**
- Free Energy IG - **31**
- Hybrid Methods IG - **25**
- Industry IG - **26**
- Integrative Modelling IG - **33**
- Integrative Modelling webinar series - **70**
- Training IG – **20**

One drawback of the current usage is that the mailing lists are for announcements only and do not provide for an easy feedback to the rest of the group. Instead, members are encouraged to use the forums at <http://ask.bioexcel.eu>, but so far we have not been successful at stimulating activity.

In order to address the current state, we are planning on the following alternative actions:

- Increased “seeding” by IG leaders (or their delegates) to ask questions, or make comments.
- Increased inter-linking (e.g. with YouTube webinar pages)
- Survey IG members on what they want from a forum and what would make them use it more
- Scheduled real-time discussion on the forum of a particular topic
- Visit related discussion places (e.g. other forums) and link back to an answer or question on our forum
- Replace IG-related forums in some or all cases with real-time chat using our community channel on gitter.com.



### 3 Social media

BioExcel actively engages with a number of social media channels with the aim of increasing the visibility of the Centre of Excellence and to advertise the opportunities we offer. Below we will briefly introduce the social media basics, what we can measure through channel analytics and what benchmarks we use for success.

Two key concepts in terms of social media are your **reach**, this is the number of people that see your content, and **impressions**, which are the number of times your content is displayed on people's feed/timeline/page. There is a distinction between free content (organic) versus paid reach and impressions. All our content, regardless of the channel, is free and therefore is capture under organic audience.

An important distinction to make is the number of followers versus organic audience. A follower, for example on twitter, is another Twitter account that has followed you to receive your Tweets in their Home timeline. The organic audience is everyone who has your content displayed in their feed/timeline/page. Similar metrics exist for the other social media channels though the name may be slightly different.

Followers can engage with your content, on twitter this would be a mention, retweet, hashtag or direct message while the LinkedIn equivalent is a like, comment or share.

The engagement rate is the best way to measure the success of your content; defined by the number of engagements divided by the number of impressions. This approximates to, out of the people that saw your content, what percentage did something about it.

Industry benchmarks for successful engagement rates

Twitter	1.5 %
Facebook	1%
LinkedIn	0.54%

As could be expected, a smaller, more specific audience is easier to engage. We therefore expect engagement rates to drop when the number of followers increase. Or phrased differently, we expect to need to work harder to maintain current engagement rates when followers increase.

#### 3.1 Twitter

Using Twitter Analytics (<https://analytics.twitter.com>) we are able to analyse a number of aspects of our twitter account. The BioExcel twitter account (@BioExcelCoE) currently has 225 followers (updated 18/04/2017); we have tweeted 263 times and are following 179 other twitter accounts.

After hitting a plateau of 105 followers, we have taken a more active approach to our social media channels and we expect to have double the number of followers by the end of March 2017 (Figure 2). We have increased the number of tweets

going out from the @BioExcelCoE account and are currently averaging around one tweet every other day (working days only) (Figure 3). We would like to further increase this to an average of one every working day. In order to do this we need to generate additional and new types of twitter content, as well as engage in conversations.

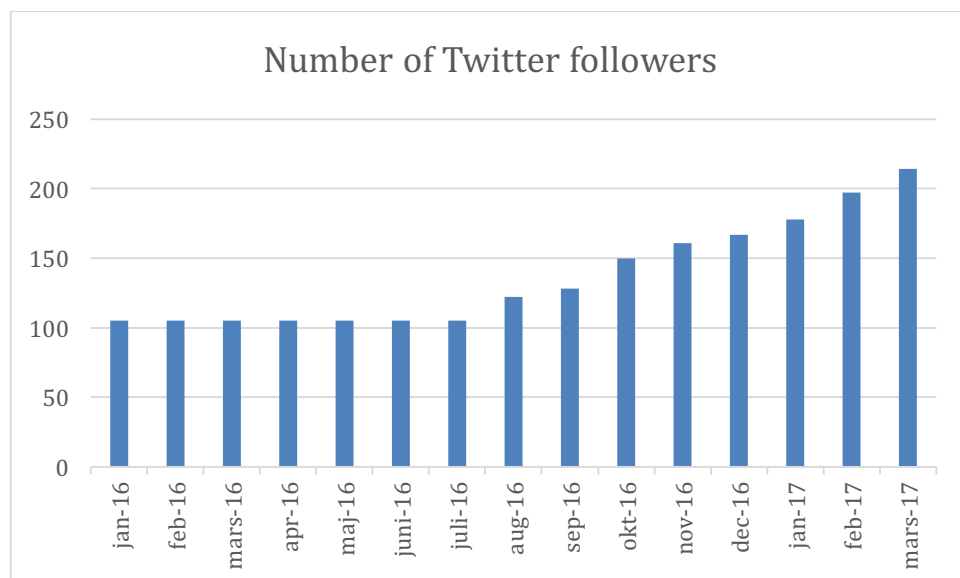


Figure 2. Number of @BioExcelCoE twitter followers.

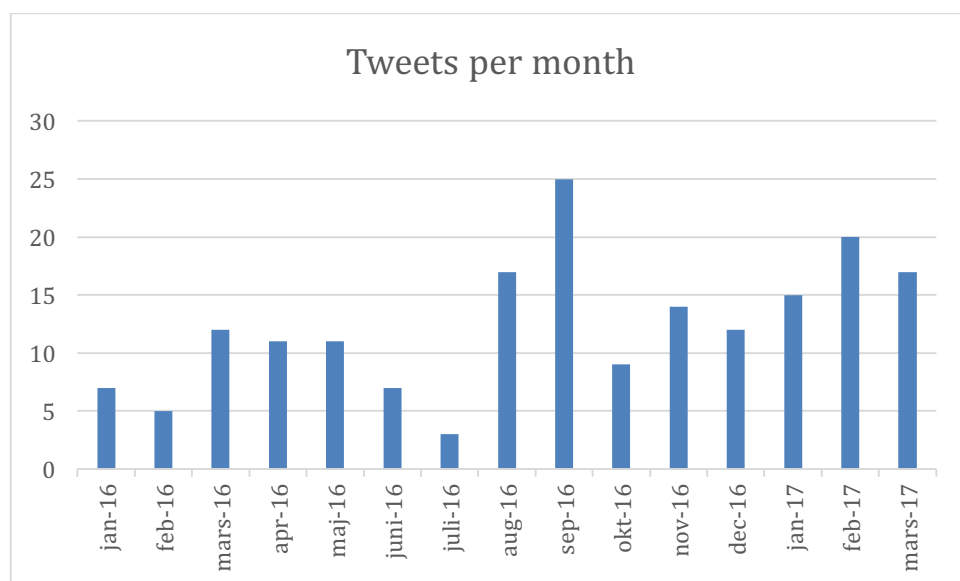


Figure 3. Number of tweets sent by @BioExcelCoE, this number does not include retweets made by the account.

We have described the concept of engagement rate above, the average of the @BioExcel engagement rate across the lifetime of the account is 0.75%. When we look at the period of 1<sup>st</sup> February to 18<sup>th</sup> April the average engagement rate is 1.1% with the highest three tweets having rates of 10.32%, 9.61% and 6.02%. Figure 4 shows the engagement rate of the tweets in the selected period, over half the tweets (21-43) meet the industry standard of a good engagement rate (1.5%). Some tweets are very recent and may increase their engagement rate over time.

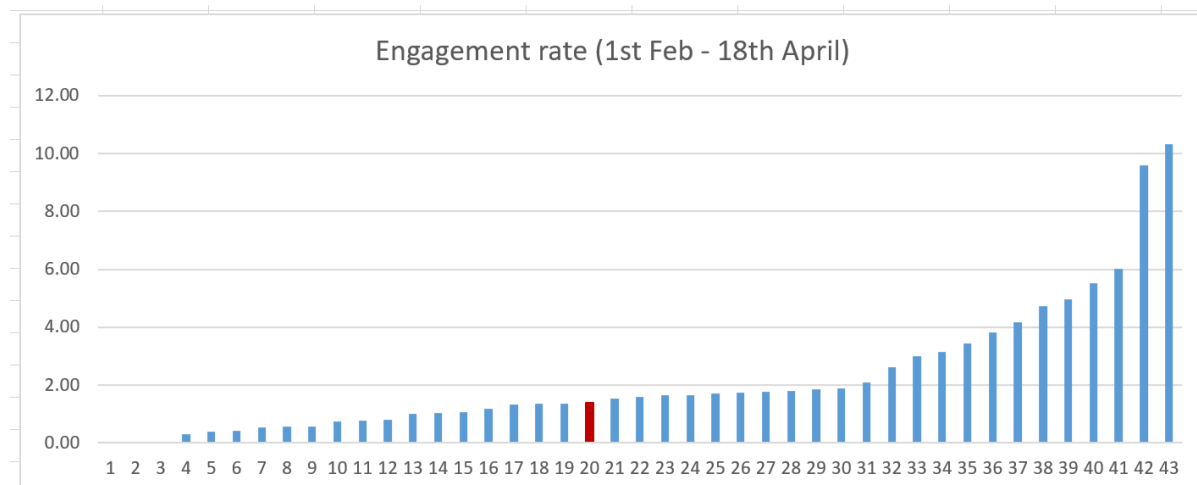


Figure 4. Engagement rate of the @BioExcel tweets in the period of 1st February and 18th April. Tweets 21 – 43 have an engagement rate above the industry standard 1.5%.

Some charts in twitter analytics require a minimum number of users, for example, with our current number of followers (225 – 18/04/2017) the demographics option is not visible for our followers but we can access this information for our organic audience.

Figure 5 shows the gender split for BioExcel followers and our organic audience. Though heavily male biased, this split is actually quite good considering the gender split in HPC and science in general.

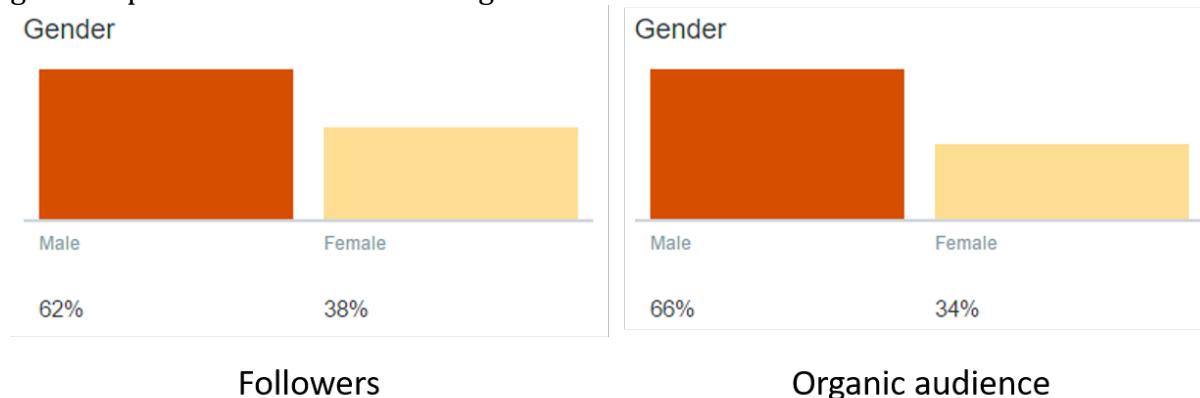


Figure 5. Gender split across @BioExcelCoE followers and organic audience.

Almost half of our organic audience is in the 25-34 age category (Figure 6). Considering the fact that twitter analytics suggests that 40% of all twitter users (based on United States) are in the 18-24 age category we can conclude we have not sufficiently engaged this group of users.

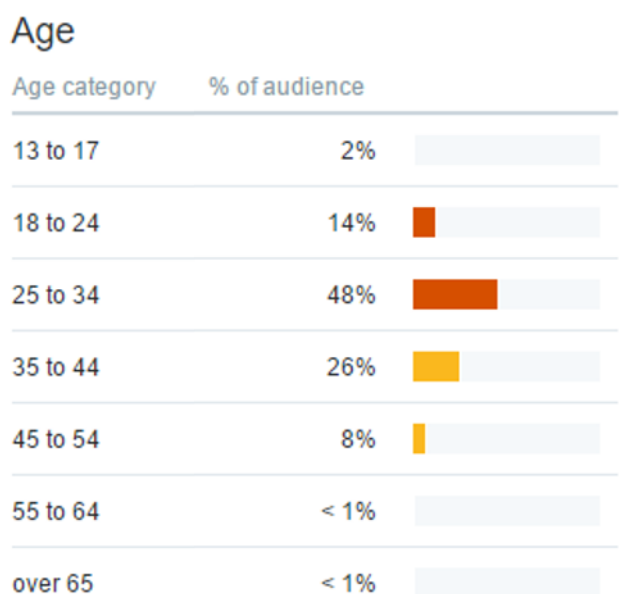


Figure 6. Age of Organic audience, this information is currently not available for our followers.

We are able to analyse country for our followers as well as organic audience (Figure 7). Almost 37% of our followers are from the United Kingdom and Spain; this is probably in part a reflection of the fact that the BioExcel partners in the UK and Spain are active on twitter. Additional factors will be the proportion and total population that is on twitter for each country.

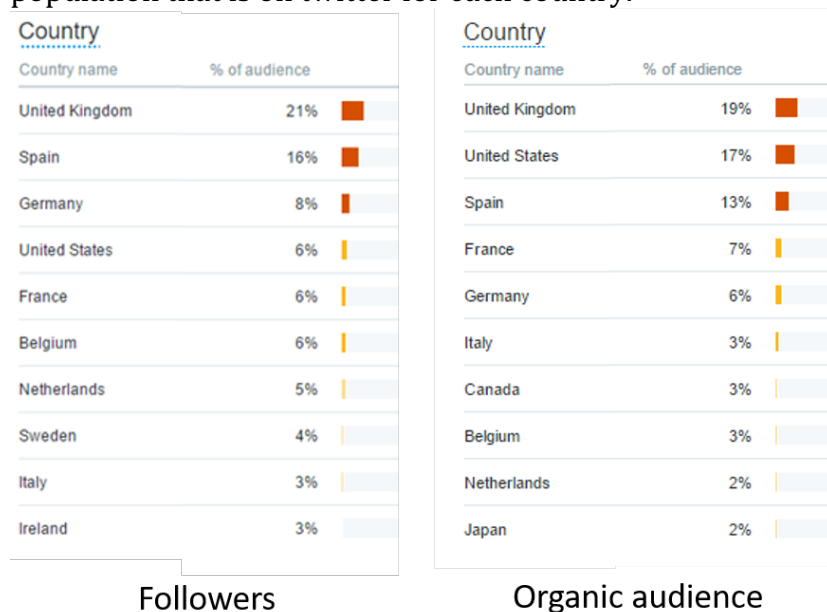


Figure 7. Country of followers and organic audience

It is sometimes tempting to draw conclusions about the success of a twitter account purely based on the number of followers. Comparison can provide a useful indicator if suitable reference points are available. However, comparing the BioExcel account to, for instance the EMBL-EBI (@emlebi) twitter account is not realistic. EMBL-EBI has been on twitter since March 2010, tweeted 5,563 times and has 22.5K followers (updated 09/03/2017). For this reason, we will use the other Centres of Excellence as a benchmark; based on this comparison we can

conclude that we are one of the more active CoEs on twitter and are performing well. Note that we cannot see the engagement rates for other twitter accounts, which would be a better indicator.

Table 3. Comparison of @BioExcelCoE to similar initiatives (updated 18/04/2017)

Account	Followers	Tweets
@BioExcelCoE	225	264
@CompBioMed	93	40
@POP_HPC	167	117
@MaX CoE	97	131
@esiwace	135	309
@ECAM2020	30	8
@NoMaDCoE	116	152
@CoeGSS	278	405

### 3.2 LinkedIn

WP4 actively encourages the BioExcel members to register themselves as BioExcel employees and to follow the BioExcel company page. To date BioExcel has 69 followers and 17 registered employees (updated 09/03/2017, Figure 8).

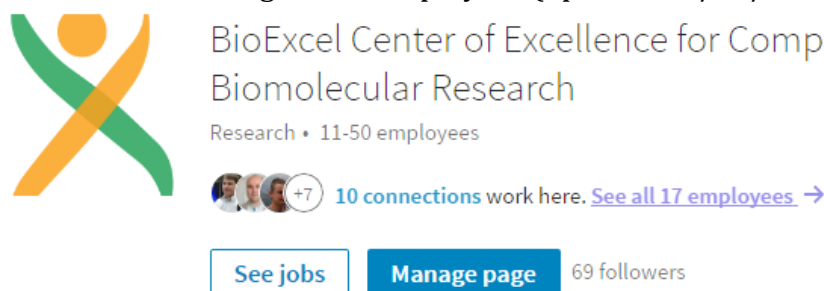


Figure 8. LinkedIn overview of BioExcel company page.

We have only recently started regular updates on our BioExcel company page. Due to our currently low number of followers, our engagement rate is very high; we will likely see this rate drop as we gain more followers. LinkedIn provides useful summary statistics to the administrators of a company page highlighting the number of impressions, clicks, engagement rate and social interactions (shares & likes).

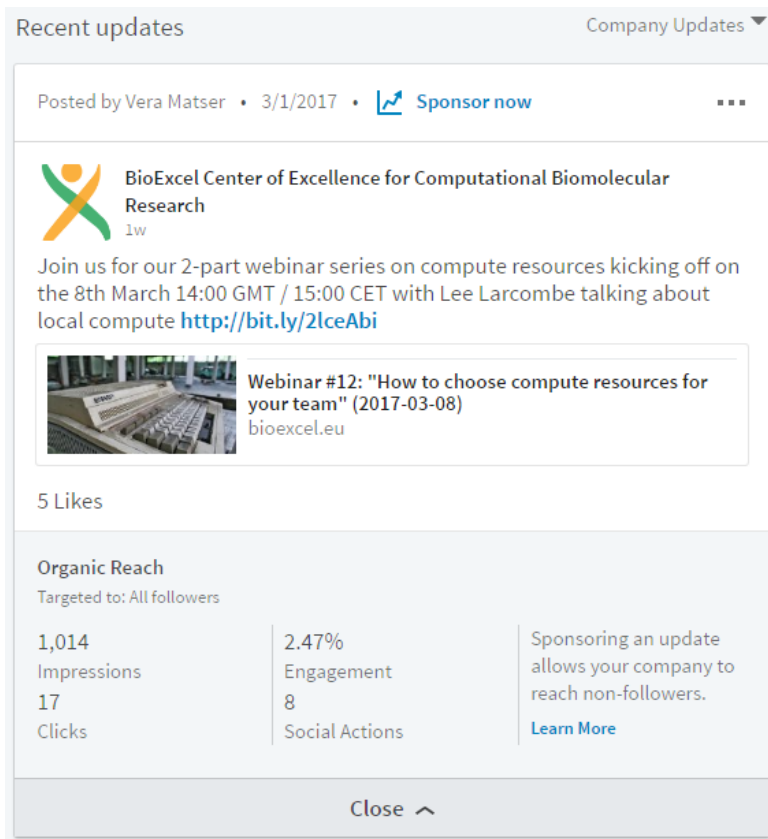


Figure 9. Summary analytics for recent updates on LinkedIn company page

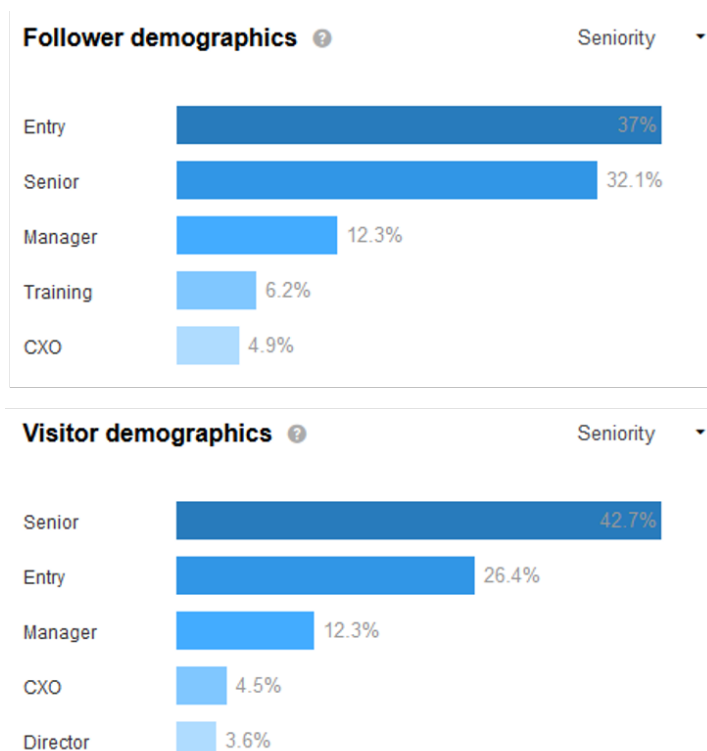


Figure 10. LinkedIn analytics of seniority across followers and visitors.

In contrary to what we would expect, our followers on LinkedIn are entry level (37%), though our visitor seniority does show a 42.7% senior category. In general,

LinkedIn as a platform is best placed to reach predominantly senior and higher level professionals.

We will continue to track our LinkedIn statistics while trying to increase our number of followers.

Separate to the BioExcel company page, individuals can provide updates to relevant groups from their personal account. As the work package leader of Training and dissemination, I post updates on behalf of BioExcel to the following groups:

- High Performance Computing (HPC) - 16,617 members
- Women in HPC - 370 members
- HPC Knowledge - 232 members

### 3.3 Future strategy

A number of conclusions can be drawn from our social media analysis:

- We are currently not reaching the age group 18 – 24 effectively. This is problematic as some of our events are targeted at early stage researchers (e.g. PhD). This may be part responsible for our low numbers of registrants.
- We need to find influencers to increase our reach in different countries as well as within the different research communities.

The following actions will be taken to improve our reach through the BioExcel social media channels:

- Create a Facebook channel with the aim of reaching the 18-24 age group more effectively. If we are reaching additional users in this age bracket we can consider expanding to [Instagram](#) as well.
- Provide regular updates on the LinkedIn company page
- We need to find influencers in the BioExcel research domain and use influencers to reach countries where we currently have limited reach.
- Set aside time to start conversations of twitter to increase engagement rate and tweet frequency.
- Increase the number of tweets to an average of one every working day.
- Increase the involvement of all BioExcel partners on social media and dissemination by reaching out to their personal and institutional channels
- Start tracking registrants for new events and webinars to track how effective our different dissemination channels are.
- Trail new content types
  - o E.g. short interviews with BioExcel staff for the BioExcel Facebook page (also suitable for twitter).
  - o Track local/international news items, events, birthdays of scientists etc.

## 4 Promotional Video

We have produced a video about the structure, activities and goals of BioExcel as an additional vehicle for promoting the center. The video features interviews with several members of the management board who give a brief overview of the different expertise in the center, the service offerings, community engagement and support and long-term plans. The video is in the final stages of production at the time of writing of this deliverable and will be available at our YouTube channel: <https://goo.gl/5dBzmw>

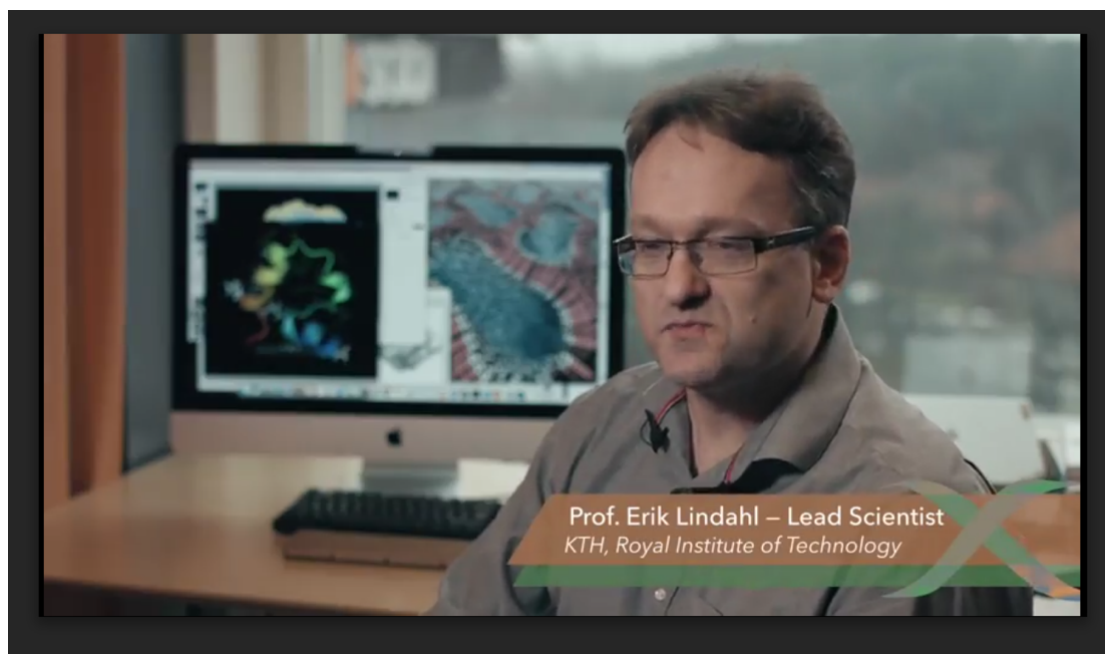


Figure 11. Screenshot of the BioExcel promotional video.

## 5 Publications

Since the beginning of the project and up to April 2017, the consortium has published 24 publications listed in Table 4.

Table 4. Publications of research work that has been supported by BioExcel.

Publication Type	Authors	Year	Title	Journal/Event Name	DOI
Journal article	Adam Hospital et. al	2015	BIGNASim: a NoSQL database structure and analysis portal for nucleic acids simulation data	Nucleic Acids Research	10.1093/nar/gkv1301
Journal article	Ivan Ivani et al.	2015	Parmbsc1: a refined force field for DNA simulations	Nature Methods	10.1038/nmeth.3658
Journal article	João P.G.L.M. Rodrigues et al.	2016	Molecular dynamics characterization of the conformational landscape of small peptides: A series of hands-on collaborative practical sessions for undergraduate students	Biochemistry and Molecular Biology Education	10.1002/bmb.20941



Journal article	G.C.P. van Zundert et al	2016	The HADDOCK2.2 Web Server: User-Friendly Integrative Modeling of Biomolecular Complexes	Journal of Molecular Biology	doi:10.1016/j.jmb.2015.09.014
Journal article	Vytautas Gapsys et al	2016	Accurate and Rigorous Prediction of the Changes in Protein Free Energies in a Large-Scale Mutation Scan	Angewandte Chemie International Edition	DOI:10.1002/anie.201510054
Journal article	Dans PD et al	2016	Multiscale simulation of DNA	Current opinions in Structural Biology	doi: 10.1016/j.sbi.2015.11.011
Journal article	Dans PD et al	2016	Long-time scale dynamics of the Drew Dickerson Dodecamer	Nucleic Acids Research	doi: 10.1093/nar/gkw264
Journal article	Shkurti S. et al	2016	pyPcazip: A PCA-based toolkit for compression and analysis of molecular simulation data.	Software X.	<a href="http://dx.doi.org/10.1016/j.softx.2016.04.002">http://dx.doi.org/10.1016/j.softx.2016.04.002</a>
Journal article	Candotti M and Orozco M	2016	The Differential Response of Proteins to Macromolecular Crowding.	PLOS Computational Biology	<a href="http://dx.doi.org/10.1371/journal.pcbi.1005040">http://dx.doi.org/10.1371/journal.pcbi.1005040</a>
Journal article	Martin Kotev et al	2016	Challenges of docking in large, flexible and promiscuous binding sites	Bioorganic & Medicinal Chemistry	<a href="http://dx.doi.org/10.1016/j.bmc.2016.08.010">http://dx.doi.org/10.1016/j.bmc.2016.08.010</a>
Journal article	Orellana L. et al	2016	Prediction and validation of protein intermediate states from structurally rich ensembles and coarse-grained simulations.	Nature Communications	DOI: 10.1038/ncomms12575
Journal article	A.D. Spiliotopoulos et al	2016	dMM-PBSA: a new HADDOCK scoring function for protein-peptide docking.	Frontiers in Molecular Biosciences	doi:10.3389/fmolb.2016.00046
Journal article	C. Geng et al	2016	Exploring the interplay between experimental methods and the performance of predictors of binding affinity change upon mutations in protein complexes.	Protein Engineering, Design, and Selection	<a href="http://dx.doi.org/10.1093/protein/gzw020">http://dx.doi.org/10.1093/protein/gzw020</a>
Journal article	Rhys Grinter et al	2016	Structure of the bacterial plant-ferredoxin receptor Fusa	Nature Communications	doi:10.1038/ncomms13308
Journal article	A. Villar-Piquéa et al	2016	Environmental and genetic factors support the dissociation between $\alpha$ -synuclein aggregation and toxicity	Proceedings of the National Academy of Sciences of the United States of America	10.1073/pnas.1606791113
Journal article	Eva S. Cunha et al	2016	Mechanism of Structural Tuning of the Hepatitis C Virus Human Cellular	Structure (Cell Press)	<a href="http://dx.doi.org/10.1016/j.str.2016.11.003">http://dx.doi.org/10.1016/j.str.2016.11.003</a>

			Receptor CD81 Large Extracellular Loop		
Conference article	Kyle Chard et al	2016	I'll Take That to Go: Big Data Bags and Minimal Identifiers for Exchange of Large, Complex Datasets.	IEEE International Conference on Big Data 2016	
Conference article	Antonis Troumpoukis et al	2016	Developing a Benchmark Suite for Semantic Web Data from Existing Workflows	BLINK 2016 Workshop on Benchmarking Linked Data	
Journal article	Iman Pouya et al.	2016	Copernicus, a hybrid dataflow and peer-to-peer scientific computing platform for efficient large-scale ensemble sampling	Future Generation Computer Systems	<a href="http://doi.org/10.1016/j.future.2016.11.004">http://doi.org/10.1016/j.future.2016.11.004</a>
Journal article	Dari Kimanius et al	2016	Accelerated cryo-EM structure determination with parallelisation using GPUs in RELION-2	eLife Sciences	<a href="http://dx.doi.org/10.7554/eLife.18722">http://dx.doi.org/10.7554/eLife.18722</a>
Journal article	Adam Hospital et al	2017	The Multiple Roles of Waters in Protein Solvation	The Journal of Physical Chemistry B	DOI: 10.1021/acs.jpcc.6b09676
Journal article	Li J. et al	2017	Proton Dynamics in Protein Mass Spectrometry.	Journal of Physical Chemistry Letters	doi: 10.1021/acs.jpclett.7b00127
Journal article	Vytautas Gapsys and Bert L. de Groot	2017	pmx Webserver: A User Friendly Interface for Alchemy	Journal of Chemical Information and Modelling	10.1021/acs.jcim.6b00498
Journal article	van Zundert et al	2017	The DisVis and PowerFit web servers: Explorative and Integrative Modeling of Biomolecular Complexes.	Journal of Molecular Biology	10.1016/j.jmb.2016.11.032

## 6 Outreach and dissemination events

Since the start of the project, we have participated in 41 events at which BioExcel has been featured (Table 5). Training events are not part of the table, they are reported in deliverable D4.5 “Training report and updated plan”.

Table 5. Outreach and dissemination events.

Date	Event Name	Location	Participants
9th November 2015	11th Concertation Meeting for H2020 e-Infra Projects	Brussels, Belgium	50
18–19 February 2016	Open PHACTS 2-day conference on Linking Life Science Data: Design to Implementation, and Beyond	Vienna, Austria	30

22 February 2016	Symposium on computation applied to Life Sciences (BSC/IRB)	Barcelona, Spain	40
7-8 March 2016	EMBL-EBI SME Forum	Hinxton, UK	52
17-18 March 2016	VIB Conference: Applied Bioinformatics in Life Sciences	Leuven, Belgium	100
26-29 April 2016	EASC2016	Stockholm, Sweden	60
9-13 May 2016	HPC Summit, organized by EXDCI	Prague, Czech Republic	100
10-12 May 2016	PRACEdays16/ETP4HPC Workshop	Prague, Czech Republic	200
18-20 May 2016	Tools registry hackathon	Paris, France	46
23-25 May 2016	CECAM Workshop: Structural and Functional Annotation of Bioinorganic Systems: Perspectives and Challenges from Theory and Experiments	Pisa, Italy	44
15-17 June 2016	BITS 2016: 13th Annual Meeting of the Bioinformatics Italian Society	Salerno, Italy	25
19-23rd June 2016	ISC-HPC/EsD workshop	Frankfurt, Germany	40
19-26 June, 2016	EMBO Global Exchange Lecture Course on Structural and Biophysical Methods for Biological Macromolecules in Solution	Suwon, South Korea	40
27 June 2016	Summer Workshop of the Biochemistry Division of Korean Chemical Society	KAIST, Daejeon, South Korea	300
27-29 June 2016	6th International Conference on the Development of Biomedical Engineering in Vietnam	Ho Chi Minh City, Vietnam	50
30 June - 1 July 2016	Workshop: Simulating molecular dynamics for drug design	Hanoi, Vietnam	30
4-7 July 2016	CECAM Workshop: Interactions and Transport of Charged Species in Bulk and at Interfaces	Vienna, Austria	30
5-7 July 2016	EMBL conference: Lifelong Learning in Biomedical Sciences	Heidelberg, Germany	100
24-29 July 2016	Gordon Research Conference: Theory and Simulation Across Scales in Molecular Science	Girona, Spain	100

1-3 August, 2016	Hybrid approaches to describe molecular machines: Introduction to molecular modelling for experimentalists	Vienna, Austria	20
20-21 September 2016	EXDCI Technical meeting	Barcelona, Spain	30
25-28 September	The Annual Meeting of the German Biophysical Society 2016	Erlangen, Germany	20
28-30 September 2016	Digital Infrastructures for Research 2016	Krakow, Poland	30
19-21 October 2016	VI-SEEM Life Sciences regional training	Belgrade, Serbia	40
27-29 October, 2016	Modelling of protein interaction	Lawrence KS, USA	100
16 November 2016	Netherlands Society on Biomolecular Modelling Autumn Meeting	Utrecht, Netherlands	70
13-18 November 2016	SC 16	Salt Lake City, Utah, USA	100
20-23 November, 2016	EMBO conference on Molecular Machines: Integrative Structural and Molecular Biology	Heidelberg, Germany	200
5-6 December 2016	IAS-Symposium 2016	Jülich, Germany	50
19-20 January 2017	WesLife All-Hands meeting	Florence, Italy	50
5-10 March 2017	IGSC 2017	Taipei, Taiwan	40
24-25 March 2017	Hunfeld Workshop 2017	Hunfeld, Germany	40
26-31 March 2017	ENC 2017	Asilomar, California, USA	900
3-4 April 2017	Workshop on Hybrid Methods in Molecular Simulation (HPC-LEAP with BioExcel)	Cagliari, Italy	30

3-5 April 2017	Ion transport from physics to physiology: the missing rungs in the ladder	Lausanne, Switzerland	30
10-12 April 2017	First International Conference on "Multiscale simulation in complex biomolecular systems: linking computation to experimental validation"	Hanoi, Vietnam	20
10-13 April 2017	Computational approaches to the study of protein interactions and rational drug design	Padova, Italy	30
11-12 April 2017	CompBioMed All-hands meeting	Barcelona, Spain	50
14 April 2017	Satellite Meeting on "Recent Advances in computational and experimental molecular biophysics"	Ho Chi Minh City	25
24-26 April, 2017	Understanding protein-protein interactions: From molecules to organisms	Lyon, France	30
24-26 April, 2017	CCPEM spring symposium	Oxfordshire, UK	30

## 7 BioExcel dissemination and event guidelines

Here we outline the BioExcel dissemination and event guidelines. It is a “living document” curated by WP3/WP4 and suggestions are being added by anyone in the CoE. The document provides useful information about the available communication channels, standard working practice and tips & tricks. As of PM18 the content is added to the D4.4 and D4.5 deliverables but the document will evolve beyond that timeframe. It is related to the identified WP4 risk “R16: Low numbers of delegates at training events or workshops”.

The guidelines in this section cover usage of the BioExcel dissemination channels, images, webinar dissemination, and Interest Group events. The guidelines which specifically relate to training events are presented in section 3.6.1 of deliverable D4.5-Training report and updated plan. The full document (at PM18) can be viewed <https://goo.gl/9zdtDN>.

### 7.1 BioExcel Dissemination channels

Below is a list of the BioExcel dissemination channels and which consortium member you can contact to add content to the channel.

**Trello card:** <https://trello.com/c/knFE907B/130-bioexcel-dissemination-channels>

We have basic analytics for most of these channels and we give you feedback on how well everyone’s content is doing

- **Twitter** - <https://twitter.com/bioexcelcoe>
  - Contact Vera or Mirren
    - You can forward what you want to advertise or request a retweet if you tweeted from your own account.
  - Limit of 140 characters
  - Use image or gif
  - Recommendation: use no more than 2-3 # and no more than 1 link
  - Use @ to link people to your message

- Googlesheet has an overview of who within BioExcel uses which social media platforms and how to find them:  
[https://docs.google.com/spreadsheets/d/1oeb1O664CAsMj1IcumetDT5GeHGc\\_jsBj097h130aJQ/edit?usp=sharing](https://docs.google.com/spreadsheets/d/1oeb1O664CAsMj1IcumetDT5GeHGc_jsBj097h130aJQ/edit?usp=sharing)

### **LinkedIn**

- Contact Vera to add content
  - Updates on events, webinar, blog posts etc
    - Short text with link
  - Add yourself as an BioExcel Employee by adding a new position in your profile (Experience section), search for BioExcel under company. You will automatically be added as employee on the BioExcel company page.
  - New website content is **not** automatically added to LinkedIn, this has been disabled as it does not work properly at this stage.
- **Website**
    - Contact Mirren if you need help to add content, alternatively add the content yourself. Mirren/Vera/Rossen can talk you through the interface.
    - Consider writing a blog post about your work/new release
      - Let Mirren & Vera know so we can publicize the blog post
    - **Note:** Publishing a page will automatically send a tweet and google + message.
      - By default the tweet will be the title of the post and the link - **you shouldn't leave it this way!**
      - Use the 'Edit details' option in the 'Publish' panel - this will allow you to customise the tweet with your own text, #tags etc.
      - Alternatively you can untick the boxes if you do not want a tweet/update to be sent.
      - Speak to Mirren if any issues.

- **BioExcel Mailing list**

- Contact Rossen, Adam C or Vera
- We need to be careful with using this mailing list. Ideally an update should be part of the BioExcel newsletter

- **Facebook**

- To be designed
- Contact Vera or Mirren

- **Forums at ask.BioExcel.eu**
  - Here we plan to make a completely different category for announcement of events.

## 7.2 Images

Using images with your social media updates is a very effective way to increase the engagement rate (applicable to all platforms).

Please be mindful that you need to check if the license of an image allows you to share the image on social media/websites. Below are links to different image resources that are either free to use or are our own stock images. If in doubt please check with Mirren & Vera.

- Some images on bscw (also generic BioExcel introduction slides)
    - <http://kth-bscw.epcc.ed.ac.uk/sec/bscw.cgi/8131>
- Google images can be filter by license (Settings < Advanced search < Then narrow your results by... < usage rights)
- Free stock images
- <https://pixabay.com/>
  - <https://www.pexels.com/>

## 7.3 Webinar dissemination

See Trello: <https://trello.com/c/zmeBCyPS/212-advertising-campaign-for-webinars-checklist>

### Checklist for Webinar Advertising Campaign

1. Current webinar includes last slide to advertise the next webinar
2. Three weeks prior to webinar date send email to invite registration
3. Two weeks prior to webinar disseminate publicity via email to network
4. One week prior to webinar date send reminder to registrants
5. One week prior to webinar send email to invite registration
6. One day prior to webinar date send reminder to registrants

## 7.4 Event guidelines

Not all of the guidelines below will be applicable for your event. The list below is meant to give you ideas and point you to helpful resources. It also points out where we have BioExcel templates that we would like you to use (and why).

### 7.4.1 Interest Group Events

WP3 has a budget for Interest Group meetings or workshops. This could be:-

- a group of people you'd like to bring together to discuss or work on something BioExcel-related

- a purpose for such a workshop, which we could then follow up and look for interested people?
- considering the option of having an “open call” for ideas from the wider community

WP3 effort can be used to help organise these events.

WP3 will consider providing contributions to an event if we can get something tangible in return to help with our CoE, e.g.

- An hour with some of the speakers and lecturers to discuss what they’d like from a CoE.
- Video interviews with speakers/lecturers mentioning BioExcel and why they think it’s good
- An hour with some of the speakers/lecturers to identify important challenges in their field over the next 5 years. This can influence the BioExcel roadmap over that period.

Visible recognition to incentivise through a “Supported by BioExcel” badge online and at the event.

#### **7.4.2 Training events**

This sub-section is specifically reported in D4.5-Training Report and Updated Plan. We have included it here for completeness.

##### **Pre-course preparation**

- Define learning outcomes for the course
- Define objectives for the course
- Clearly defined audience for the workshop, including any prerequisites
- As a guideline try and open the registration event up to 6 months before the date (programme can be in draft with fixed beginning and end times); register interest list can be implemented at an earlier stage.

##### **Programme**

- Address course expectations at the beginning of the course. Ideally with time allocated to introductions. This could be in group if you have lots of people attending.
  - Gamestorming has useful activities that can be used to capture participants expectations and icebreakers <http://gamestorming.com/category/icebreakers/>

Reserve time to fill in the feedback form and a wrap-up/conclusion session at the end

If possible try and mix hands on and lecture rather than big blocks (not always possible)

- People’s attention span is short

Add sufficient time for breaks to the programme, besides allowing the participants to network it also gives you a time buffer if a session overruns.

If budget allows add a socialising event e.g. dinner, excursion, reception etc



Consider using a [Slack channel](#), Gitter, or twitter hashtag to encourage community building

Consider gender balance when putting your speaker list together

### Post-event

- Post course survey - should be filled in during the course
  - Contact Vera Matser for the surveymonkey template, please use the template as WP4 KPIs are dependent on the questions.

De-brief with trainers and organisers to discuss participant feedback and their own impressions of the course

Define improvements for the next iteration if applicable

Post 6 months survey to ascertain long-term feedback

- Done by WP4 as part of quality assessment & impact

### Tips & Tricks

- Make trainers/facilitators life easier by giving participants 2 coloured post-it notes during hands-on session, to be place on the top of the monitor (sticking up). Green = done with task, Pink = I need help or You've lost me. Gives a quick overview of the status of the room and lowers the barrier for shy participants to ask for help.
- Worried that people are going to leave early on the last day? Add a highly regarded keynote speaker at the end.

## 8 Webinars

Webinars are one of the main services provided by the center and are organized by WP3. Since they are also one of the important dissemination channels with cumulatively over 1000 views so far, we are reporting the statistics in the current deliverable. Their progress will be followed in upcoming deliverables.

At the time of writing of this document, we have organized 13 webinars (<http://bioexcel.eu/webinars>). The topics, which were presented, aimed to cover the different expertise available in the center (Table 6), while three of the webinars are specifically aiming at providing users with the necessary background knowledge needed to take advantage of the BioExcel services; we have named these webinars the educational webinar series. They are highlighted in D4.5.

*Table 6. BioExcel webinar series - statistics*

Date	Webinar	# Registrants	# Views of recording
2016-04-29	"Integrative modelling of biomolecular complexes with HADDOCK"	30	338
2016-05-11	"Performance Tuning and Optimization of GROMACS"	113	688
2016-05-25	"Atomistic Molecular Dynamics Setup with MDWeb"	92	227

2016-06-10	“Mutation free energy calculations with pmx”	55	262
2016-06-30	“QM/MM approaches in CPMD”	22	185
2016-09-07	“Best bang for your buck: Optimizing cluster and simulation setup for GROMACS”	16	180
2016-10-12	“PRODIGY, a web server to predict of binding affinities in protein-protein complexes”	39	227
2016-11-16	“Large-scale analytical workflows on the cloud using Galaxy and Globus”	45	21
2016-11-23	“Defining training requirements for biomolecular researchers with high computational needs”	18	45
2017-02-08	“Assessing structure quality in the PDB archive”	24	50
2017-02-15	“Robust solutions for cryoEM fitting and visualisation of interaction space”	35	47
2017-03-08	“How to choose compute resources for your team”	21	26
2017-03-15	“Accessing Cloud & HTC Resources in BioExcel”	13	

Slides from the webinars are shared via the SlideShare platform (<https://www.slideshare.net/BioExcel>). We are planning to offer them as well via Zenodo (<https://zenodo.org/communities/bioexcel>), which we already use for providing project deliverables and other publications.

## 9 Interfacing with Industry

One of the center’s main channels for outreach and dissemination of project outcomes directly to industrial users is through the “Practical applications for industry IG”. Over 30 individuals have signed up to the group who represent 23 different companies in the pharmaceutical, agrichemical and food supply sectors of life science research and development. One member of the interest group, Zara Sands from UCB ([www.ucb.com](http://www.ucb.com)) joined our Scientific Advisory Board.

The Industry IG meets regularly through teleconferences to focus on practical interests that are relevant to industry. These include 1) Published use case applications e.g. virtual screening, antibody engineering and mutations; 2) BioExcel pilot use cases and workflows e.g. mutations, virtual screening, biomolecular complexes and molecular recognition.

Best practices for success are being shared by the Industry IG. This is being done through working together to understand and fix pain points and challenges for exploiting the full potential of Molecular Modelling and Simulations. The Industry IG benefits from strong relationships with the developers of the core BioExcel applications and workflows. The resources generated by the Industry IG activities will be accessed through the BioExcel Web portal. The Industry IG will provide opportunities for the provision of professional consultancy services.

In the new version of the website, we are planning a dedicated area for the collection of material that is of particular interest to industry.

Finally, we are planning to attend SME focused events such the Eurostars innovation week (<https://www.eurostars-eureka.eu/eurostars-day-2017>) and relevant biomolecular conferences attended by pharma companies in order to establish presence and to seek opportunities for collaboration and consultancy.

## 10 Collaborations

Engaging with external collaborators is a very important aspect of BioExcel. We have established a three-step process for establishing partnership.

The first step in becoming a strategic partner involves the submission of a “**Proposal for a strategic partnership**” (template is in Annex). The proposal is a one page document that describes 1) the contact points in the third party, 2) the BioExcel contact for communication and 3) areas of common interest. The document is submitted to the BioExcel project manager who presents it for approval to the Executive Board.

If the proposal is accepted, then the coordinators of both BioExcel and the partner institution sign the actual “**MoU for Strategic Partnership**” (template is in Annex). The document is a brief description of the two partners and specifies the general guidelines for the partnership.

In cases where the two partners have already identified specific goals to be achieved, then an “**MoU for Collaborative Partnership**” (template is in Annex) is being signed. The most important difference in this MoU is the list of specific milestones and deadlines to be met as part of the partnership.

We are using suggested templates for all documents. However, in some cases the text is modified to reflect specific legal requirements of the partnering organization.

As of the current reporting period, PM18, we have the following partnerships:

- Open PHACTS foundations (<http://openphacts.org/>) – MoU for Strategic Partnership signed
- ELIXIR (<http://elixir-europe.org/>) – MoU for Collaborative Partnership signed
- MolSSI (<http://molssi.org/>) - MoU for Strategic Partnership finalized and pending signing
- INSTRUCT (<https://www.structuralbiology.eu/>) – ongoing discussion

## 11 Conclusions

In this reporting period, we have established BioExcel as a strong brand among the relevant communities. Increased dissemination and training activities during

the reporting period have increased the outreach and popularized the center and the outcome of our work. The website is seeing a healthy traffic, which we expect to gradually increase as more material is being added and the knowledge resource center expanded (as explained in D4.5). Our presence in social media is satisfactory and future plans include targeting additional segments of the user groups. We are building our conference presence with booth exhibitions, starting with one of Europe’s most important events, the ECCB/ISMB conference (<https://www.iscb.org/ismbeccb2017-exhibitors-sponsors/exhibitorlist>), and including events targeting SMEs and practical application of computational techniques for pharmaceutical research.

## 12 ANNEX

### 12.1 Proposal for a strategic partnership (template)

#### Proposal for a Strategic Partnership with BioExcel CoE

Thank you for your interest in becoming a BioExcel Strategic Partner. Please use this form to provide the necessary information for the application process. This form needs to be completed both by the applicant organization and the BioExcel contact in communication.

<b>Name of the Organisation:</b>			
<b>Website:</b>			
<b>Name of main contact in applicant organisation:</b>		<b>Email address:</b>	
<b>Role/job title of contact:</b>			
<b>Name of secondary contact in applicant organisation (Optional)</b>		<b>Email address: (Optional)</b>	
<b>Name of BioExcel contact:</b>		<b>Email address of BioExcel contact:</b>	
<b>Description of the applicant organisation - for inclusion in any publicity message (2-3 sentences)</b>			
<b>Description of why the BioExcel contact thinks that the organisation should be invited to become a Strategic Partner of BioExcel (2-3 sentences).</b>			

<b>Should the organisation be considered for Collaborative Partnership in the future?</b>	Yes/No
<b>Specify the particular area(s) of common interest</b>	1) 2) 3)

Please send this form to Rossen Apostolov (rossen@kth.se).

## 12.2 MoU for Strategic Partnership (template)

### **Memorandum of Understanding Strategic Partnership Agreement**

between <<ORGANIZATION>> and BioExcel Center of Excellence

1. This Memorandum of Understanding (MoU) signifies a statement of intent to collaborate between the BioExcel Center of Excellence (hereafter “BioExcel CoE”) and << Organisation>>, but is **not a legally binding document**. This MoU does not restrict the rights of either party to enter into collaborative agreements, contracts or working relationships with other parties.
2. This MoU recognizes the intention of BioExcel CoE and <<Organisation>> to establish a relationship to co-operate in a range of areas in the scope of BioExcel and to work together for their mutual benefit.
3. The period covered by this MoU is from the date of signing to 31 October 2018 and will be reviewed thereafter. Each party has the right to discontinue the arrangements subject to a period of 3 months’ notice being given. The MoU may also be terminated at any time by mutual consent of both parties. In any cases of discontinuance, the parties will honour agreed commitments either via accepted arrangements or suitable alternatives negotiated at that point.
4. **Separate agreements will be required for any and all collaborative projects that the parties wish to enter into. The parties understand that any financial considerations associated with any form of collaborative project will be dealt with separately via a legal contract. As part of this, the parties agree to cooperate on resolution of contractual and IPR issues.**
5. The parties recognize the importance and value of this MoU in promoting their individual and joint activities. However, each party understands that any activity which includes reference to the other party (such as grant applications) must be sent to and be approved by this party before use. Each party will use reasonable efforts to provide a response within 7 working days.
6. The parties agree to cooperate in establishing the BioExcel CoE, including, but not limited to i) joint projects involving scientists on both sides, ii) sharing of expertise and/or biomolecular software, iii) exchange of students and or teaching material and iv) exchange of expertise, materials, documents or information at the organizational level.

7. The parties agree to encourage collaborative research in the areas of biomolecular research within their respective programmes and with mutual collaborators.
8. The parties agree to encourage the development, publishing and sharing of services that can be used in their mutual support activities, with a view to enabling public access to more of these resources, including within the BioExcel activities.
9. The parties agree, wherever appropriate, to pursue possibilities for bilateral and multilateral collaborations aiming at the development of an interoperable pan-European and global infrastructure for biomolecular research.

---

Date

---

Erwin Laure  
on behalf of BioExcel CoE

---

Date

---

<<partner signature>>  
on behalf of <<organization>>

### 12.3 MoU for Collaborative Partnership (template)

## Memorandum of Understanding Collaborative Partnership Agreement

Between <<ORGANIZATION>> and BioExcel Center of Excellence

#### Background information

**BioExcel CoE** provides the necessary solutions for long-term support of the biomolecular research communities in academia and industry: fast and scalable software, user-friendly automation workflows and a support base of expert core developers. The main services offered by the center include hands-on training, tailored customization of code, personalized consultancy support and community outreach activities.

<<ORGANIZATION>> is ....

#### Purpose

The purpose of this Memorandum of Understanding (MoU) is to define a framework for collaboration between **BioExcel CoE** and <<ORGANIZATION>> and builds on the already established Strategic Partnership MoU. This document outlines the main activities through which the two parties will be collaborating along with timelines, where applicable. **This MoU is not a legally binding document.**

#### Joint Workplan

Below are outlined the main planned activities and timelines, where applicable.

Milestone	BioExcel Activity	Date	<<ORG>> Activity	Date

#### Rights and Responsibilities

This MoU does not prevent either party from cooperating with other projects performing similar activities to those described herein. When considered of mutual benefit, both parties are encouraged to involve third parties in similar activities towards achieving the objectives of this partnership.

#### Commencement date, Duration and Amendments

This MoU becomes effective upon signing by representatives who are authorized to establish agreements on behalf of their organizations. Amendments shall be

valid only if signed by those representatives. This MoU is valid until 31 October 2018 and will be reviewed thereafter.

**Contacts and signatures**

Signed for and on behalf of BioExcel CoE:

Name: Erwin Laure  
Title: BioExcel Coordinator

Tel.: + XX-XX-XXX-XXX  
E-mail: XXXXXXXX

Date: \_\_\_\_\_ Signature: \_\_\_\_\_

Signed for and on behalf of <<**ORGANIZATION**>>:

Name: XXXX XXXXXXXXXXXX  
Title: XXXX XXXXXXXXXXXX

Tel.: +XX-XX-XXX-XXX  
E-mail: XXXXXXXX

Date: \_\_\_\_\_ Signature: \_\_\_\_\_