

Virtual Humans in Medical Education and Training

Andrea Townsend-Nicholson

Meeting the unmet need – CompBioMed1 (2016-2019)



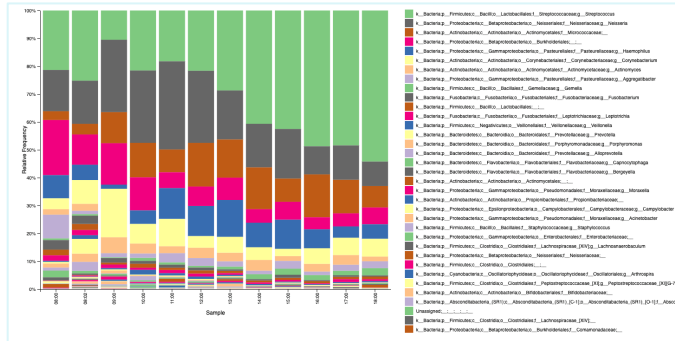
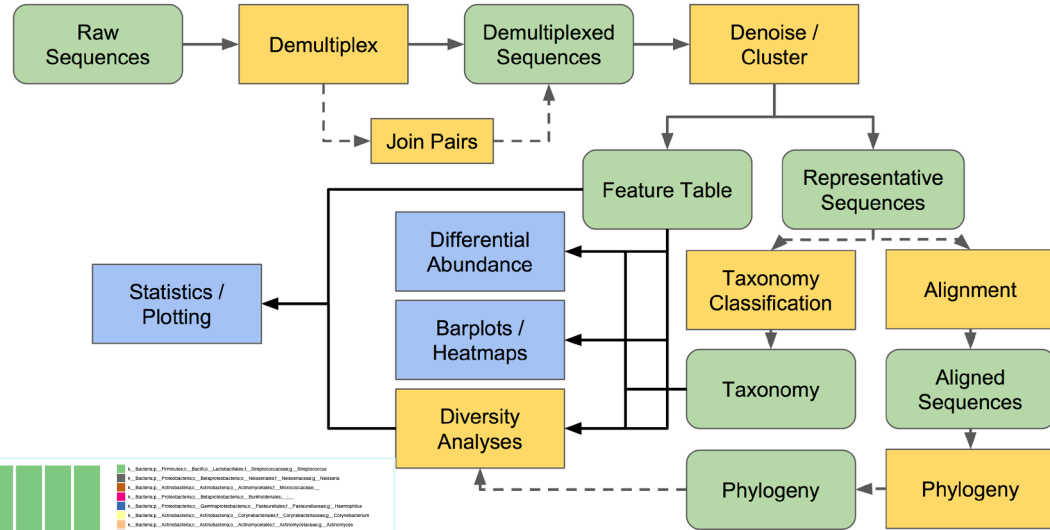
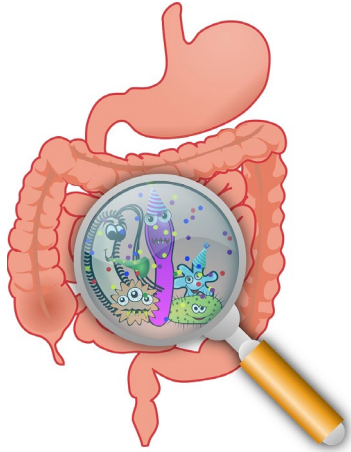
Domain access to supercomputers in 2016

Field	HE Postgraduate Degree (%)	Archer Use (%)	HPC Access to Field (%)
Medical	24	0.2	0.8
Biological	22	9.8	44.5
Physical	25	60.7	243
Mathematical	4	9.5	238
Engineering	20	18.6	0.93
Other	4	1.2	30
Total	100	100	

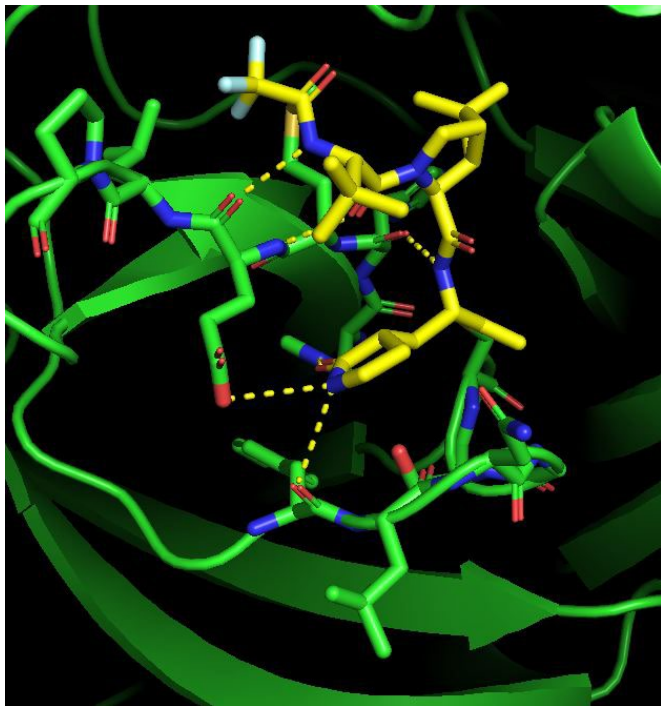
Embedding training in the university curriculum

Academic Year	Medicine students	Biosciences students	Extracurricular Course	Total number of students
2017-2018	40	89	40	169
2018-2019	20	104	38	162
2019-2020	20	108	31	159
2020-2021	40	86	35	161
2021-2022	55	370	40	465
2022-2023	84	472	16	572
2023-2024	43	800	>30	910
	339	2029	200	2518

Microbiome analyses (USFD SSC/UCL BIOC0003, BIOC0023)



Molecular Dynamics simulations (USFD SSC/UCL BIOC0003)



SARS-CoV-2 Mpro and nirmatrelvir

- MPro-wild type, MPro-A, MPro-B
- 46 different antiviral ligands
- 120 first year biochemistry students
- Ensemble-based replicas (n=16)

Used GROMACS on ARCHER2 to calculate average ligand movement (RMSD)

Used VMD to visualise ligand movement

“Archer's a lovely machine, but the entrance way is strewn with twitching non-computer scientists”

Embedding training in the university curriculum

Trainees	Training type	Protocol	Total number of trainees
Medical students	Curricular	Microbiome	339
Medical students	Curricular	MD	5
Bioscience students	Curricular	Microbiome	1234
Bioscience students	Curricular	MD	118*
Medical students	Extracurricular	Microbiome	-
Bioscience students	Extracurricular	Microbiome	-
Other	Workshops	Microbiome	205*
Other	External Engagement	Microbiome	-

Bringing a new technology into a classical domain

- Getting code on machines
 - QIIME1, QIIME2
- Getting users on machines
 - “laptop buffering” and pre-prep routine
 - On-prem vs cloud
- Using machines properly (Snellius vs ARCHER2 vs nUCLeus)
 - 5 second year medical students
 - 120 Year 1 Biochemistry undergraduates
- Scaling on machines
- Managing expectations
 - Users
 - Facilities and charging models: ARCHER2 vs Snellius
 - Policymakers

Charging models and new users



- Snellius (SURF)
- Tier 1
- 128 cores/node
- Minimum charge 16 cores
- Metagenomics (16 cores/run)



- ARCHER2 (EPCC)
- Tier 1
- 128 cores/node
- Minimum charge 1 node
- MD (1 ensemble of 50 replicas or 8 ensembles of 16 replicas each)

Successes

- From command line to ARCHER2 in year 1
- From microbiome to Frontier in 2.5 years
- 2 escapees to CS
- 2 medics doing computational PhDs
- The Virtual Human meets 400 medical students a year as part of their SSC



This is to certify that

Andrea Townsend-Nicholson

has been awarded a UCL Medical School

Top Teacher Award 2024-25 for SSC

A handwritten signature in blue ink that reads 'J. Hines'.

Prof John Hines

Academic Lead for Quality Assurance and Enhancement
UCL Medical School

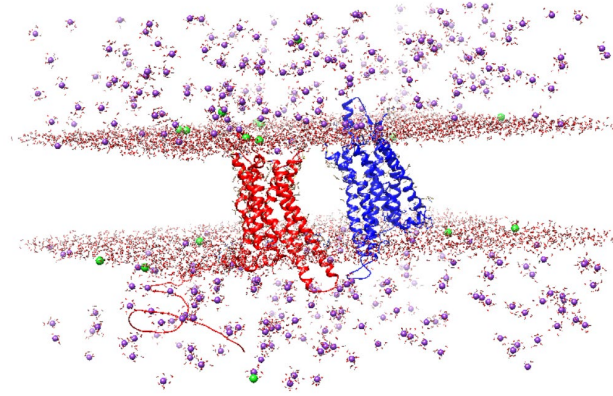
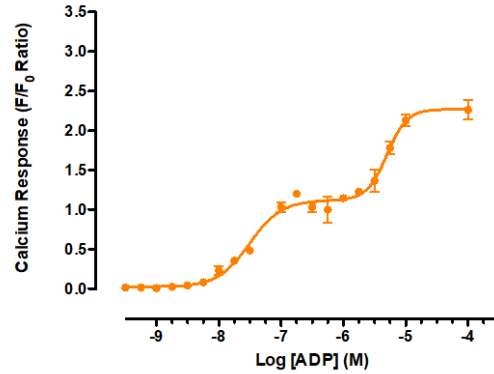


CompBioMed



Training the trainers (2013-2025)

ADP Effect on G14T-13 (0.25 Log Concentration)



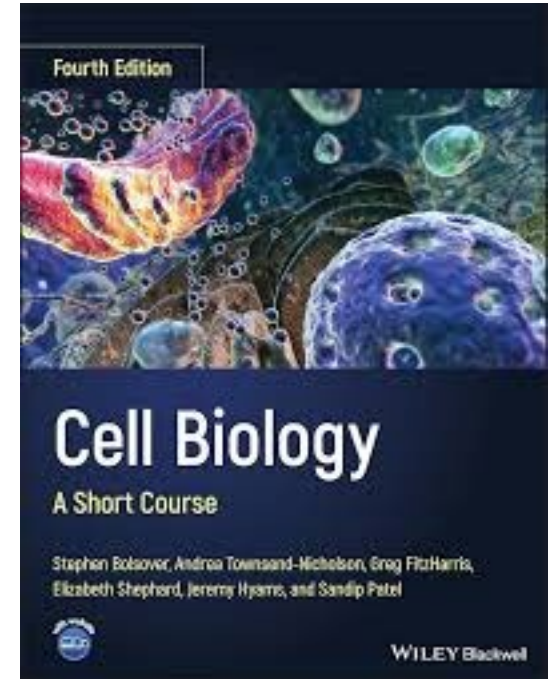
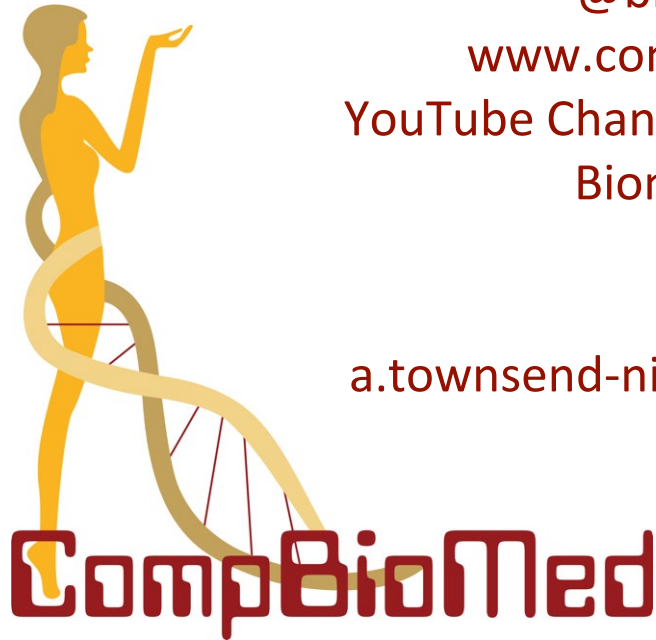
Thank You

@bio_comp

www.combiomed.eu

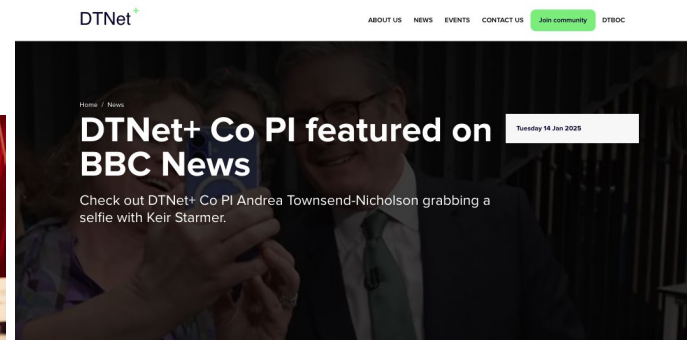
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Knowledge Exchange & Dissemination



If you were watching BBC News at 6 o'clock yesterday (13/01/2025) you might have caught one of our network researchers grabbing a selfie with UK PM Keir Starmer. **Andrea Townsend-Nicholson**, Professor of Biochemistry and Molecular Biology at the University of College London, is a key Co PI within our network and the field of Digital Twins. She was attending the event to explore the future of AI and Digital Twins with engaging conversations.

Missed this moment? Check out the story at [BBC News](#)

