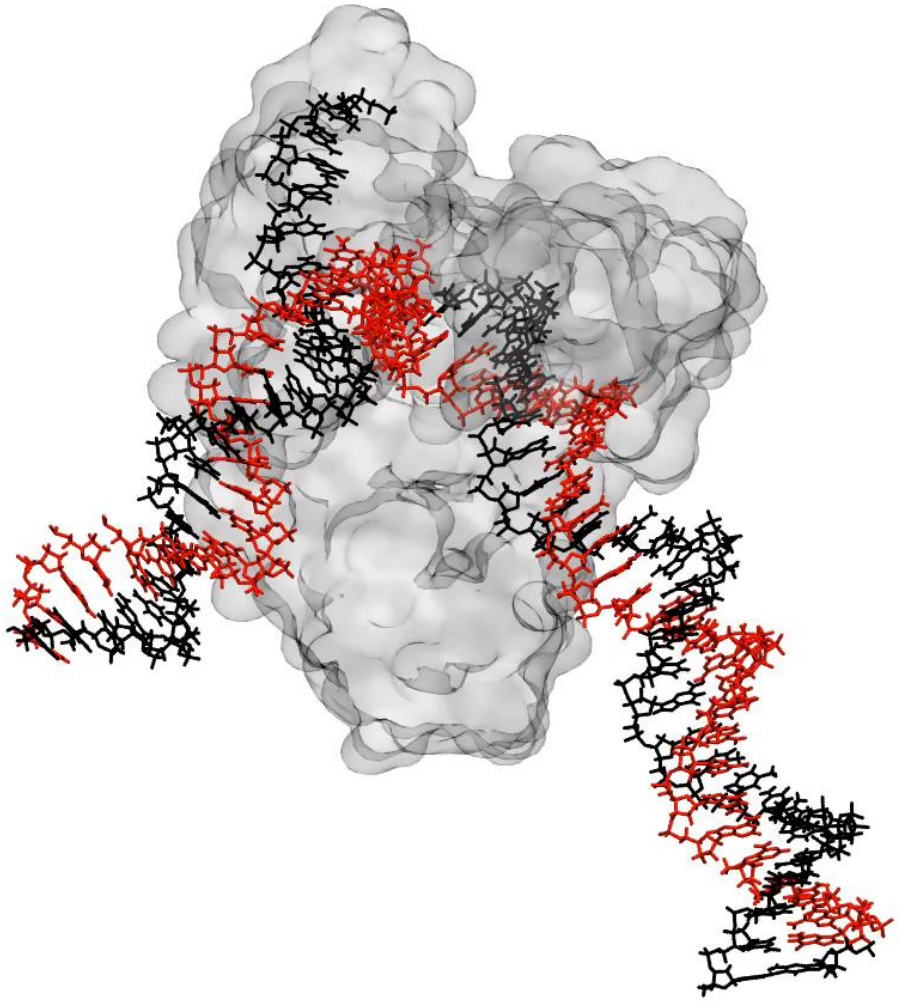
Democratising Single-molecule FRET: What is Open Science?



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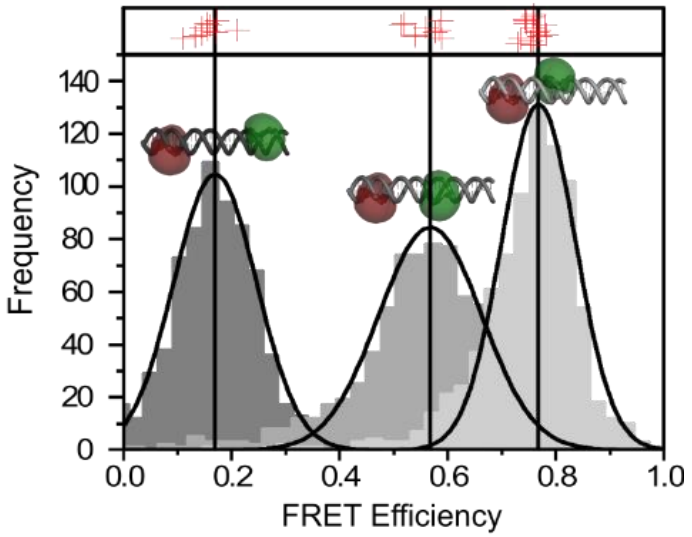
@Craggs_Lab

Open Science

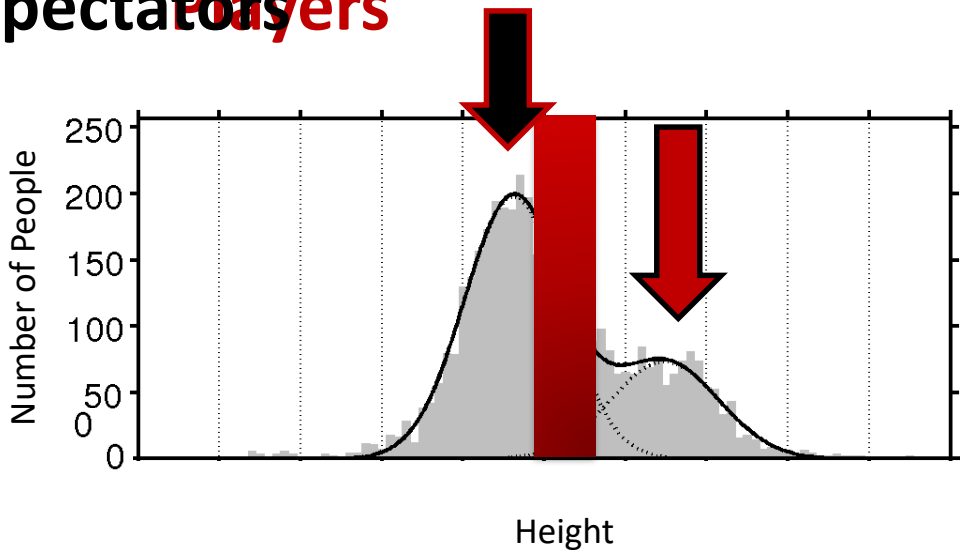
- Open Hardware
- Open Software
- Open File Formats
- Open Data
- Open Analysis
- Open Access



Nature Methods (2018) **15** 669
Nature Communications (2020) **11** 5641

Conformational Ensembles in Biology

Spectators **Players**



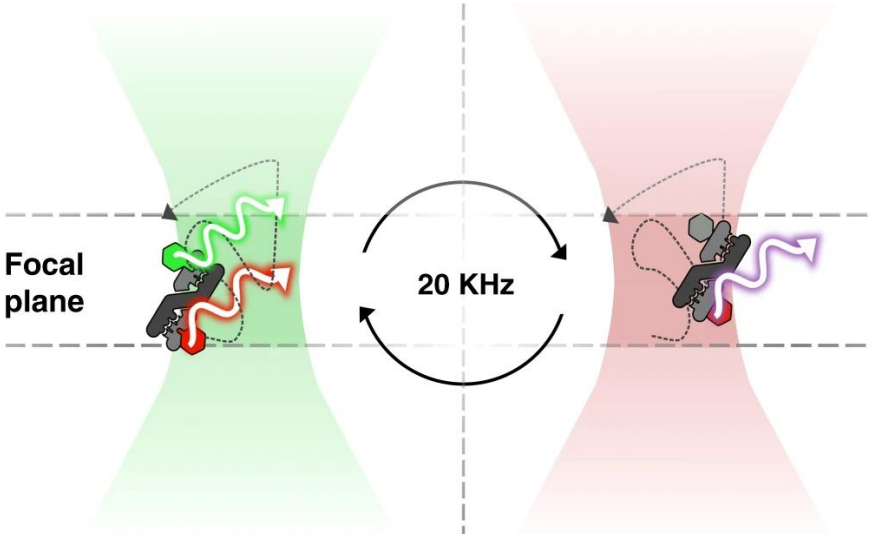
Population averages can be misleading!

Need to interrogate **single molecules**

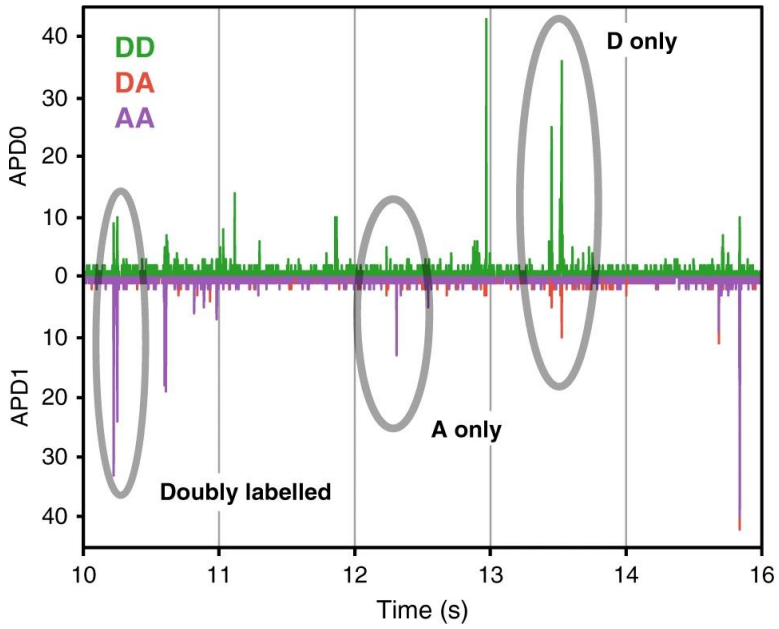
Or obtain experimental conformational ensembles

Single-molecule FRET on freely diffusing molecules

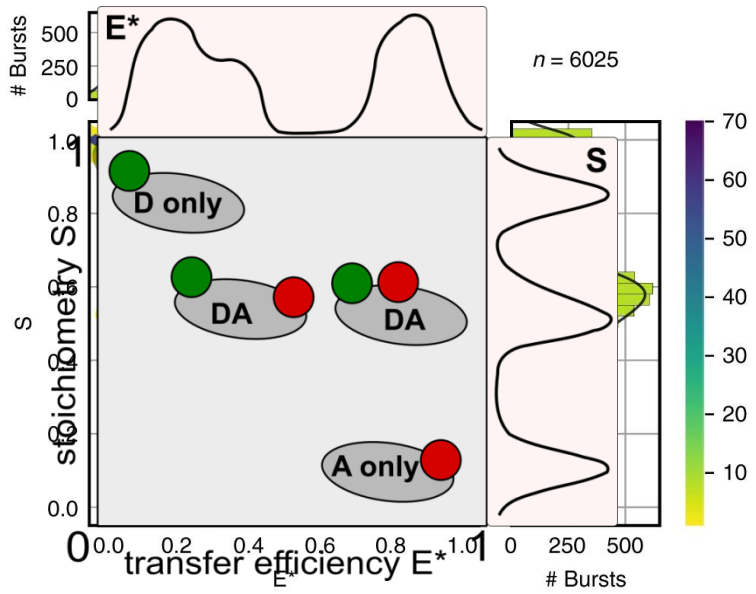
Alternating Laser Excitation



Single molecules => Bursts of Photons



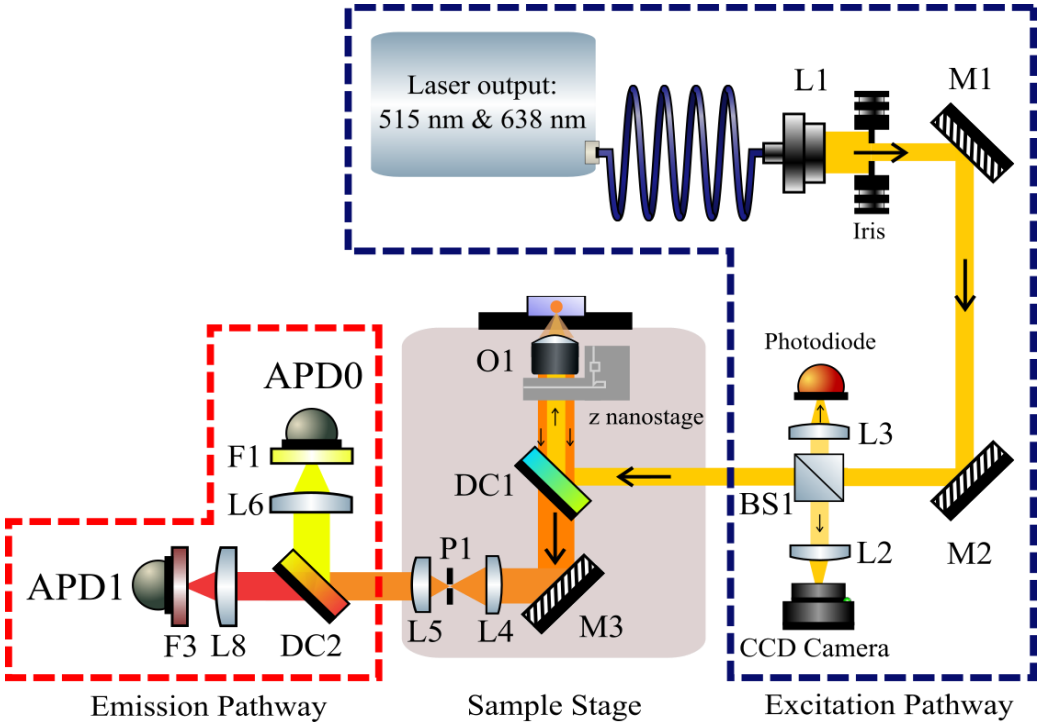
Histogram combined data



£400,000

Confocal smFRET
Buy one?

#smfBox : Open Hardware



- Economic
- Robust
- Compact
- Easy to assemble
- Easy to use
- Open source
- Biologist proof!

The University Of Sheffield.

Department of Chemistry

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National Student Survey 2018

Researchers establish new way to measure molecules

Dr Tim Craggs contributed to a major worldwide study to measure exact distances within molecules down to the scale of one millionth of the width of a human hair. Two of our students built the microscope that helped make it possible.

Full story →

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INFORMATION FOR STAFF AND CURRENT STUDENTS

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News

Researchers establish new way to measure molecules which could help develop new targeted drugs

Students build single molecule FRET microscope for world-class biological imaging lab

Dr Tom Anderson shortlisted for prestigious international fiction prize

More news →

#smfBox : Open Hardware

nature COMMUNICATIONS

ARTICLE

https://doi.org/10.1038/s41467-020-19468-4 OPEN

Check for updates

The smfBox is an open-source platform for single-molecule FRET

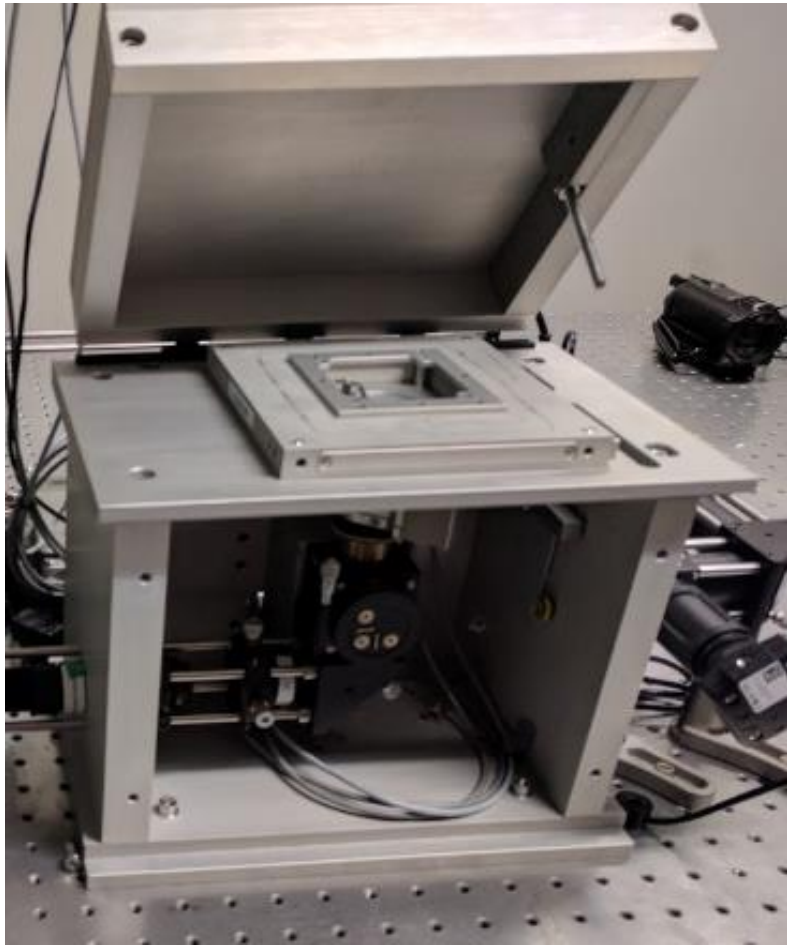
Benjamin Ambrose[1,4], James M. Baxter[1,4], John Cully[1,4], Matthew Willmott[1], Elliot M. Steele[2], Benji C. Bateman[3], Marisa L. Martin-Fernandez[3], Ashley Cadby[2], Jonathan Shewring[1], Marleen Aaldering[1] & Timothy D. Craggs[1✉]

https://craggslab.github.io/smfBox/index.html

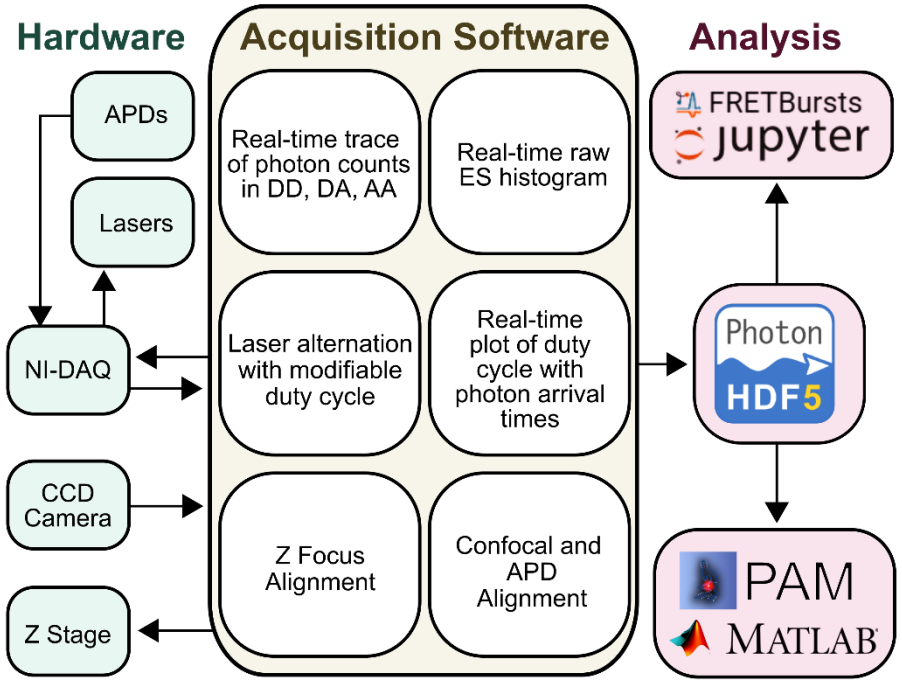
Full parts list and build instructions - GitHub / BioRxiv

Open-source acquisition and analysis software

Ambrose et al. Nature Communications (2020) **11** 5641



£40,000

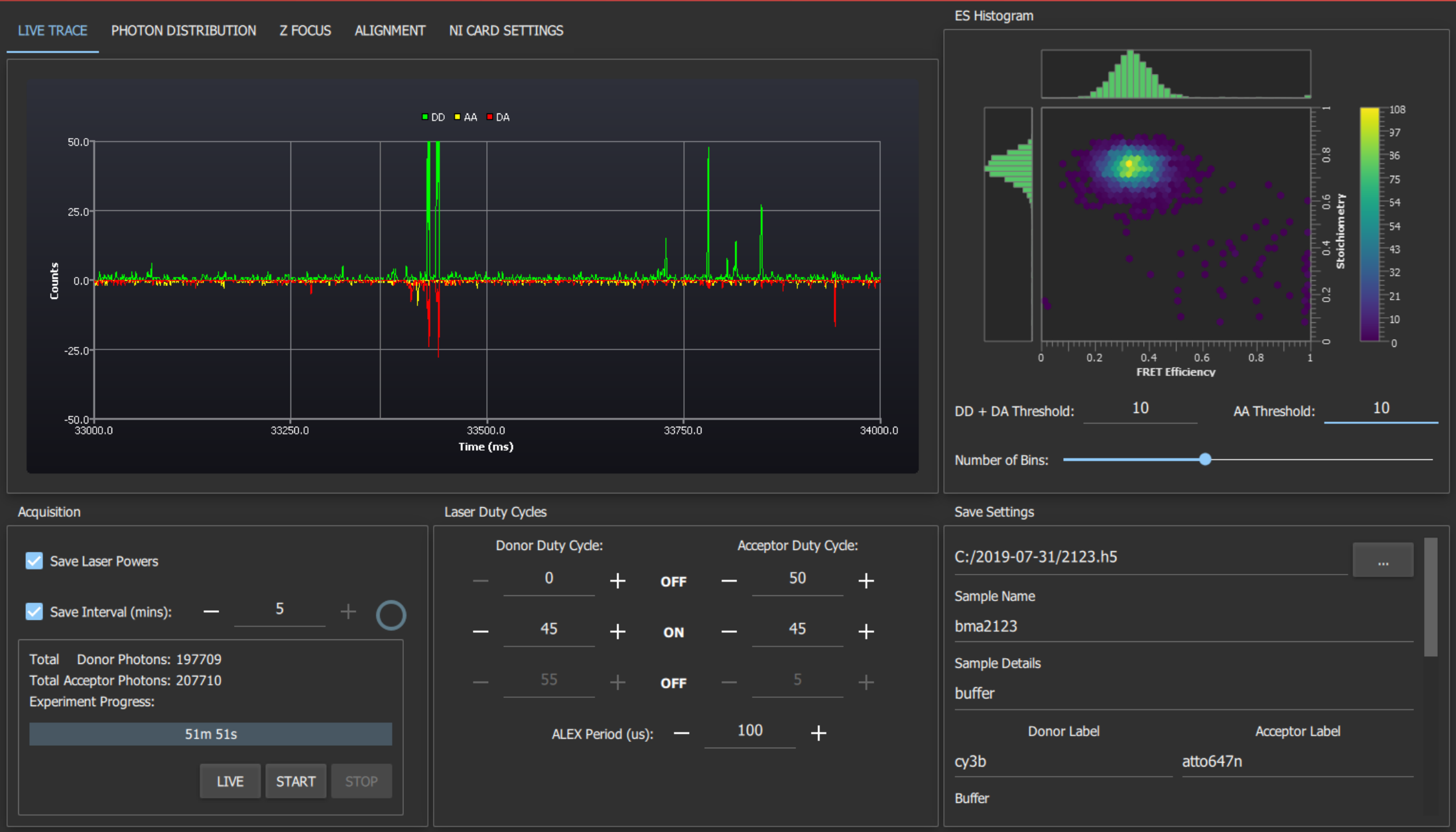


Ben Ambrose

Elliot Steele

Github – all software open source and available

#smfBox: smOtter – Open-source software



Open File Formats

Photon-HDF5

- Meta data and raw data stored together

FAIR data principals

Findable

Accessible

Interoperable

Re-usable

https://photon-hdf5.readthedocs.io

Open Data

Zenodo deposition

- Permanent DOI
- All raw and analysed data

Open Analysis

Photon-HDF5

- Standardised file format
- Readable by many software packages
- Matlab – PAM
- Jupyter Notebooks

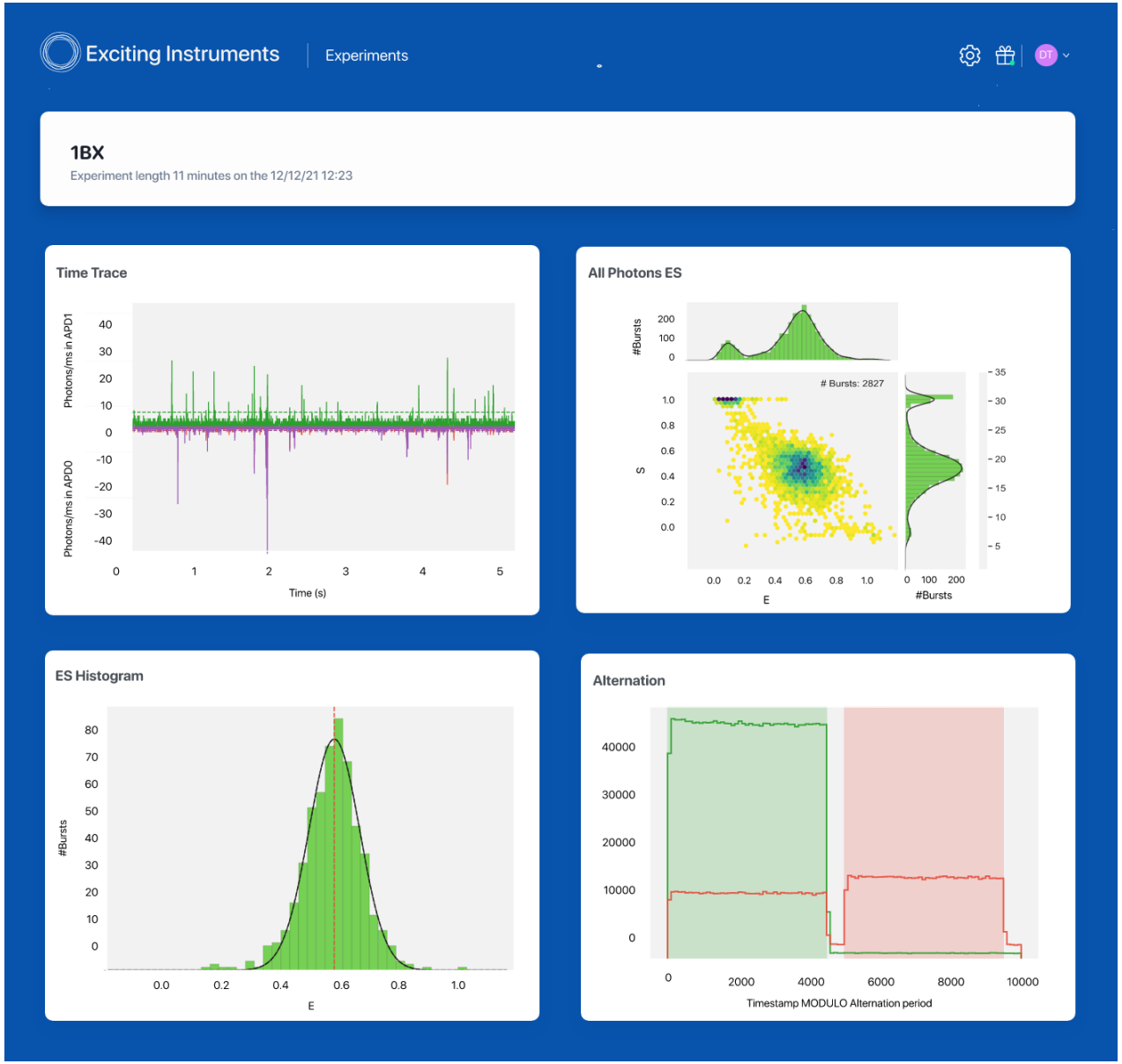
Jupyter Notebooks

- Raw data and analysis available to all
- Run in browser
- Deposit data and analysis together
- Others can re-analyse our data

https://fretbursts.readthedocs.io

https://photon-hdf5.readthedocs.io

https://pam.readthedocs.io



Open Access

Pre-print publishing

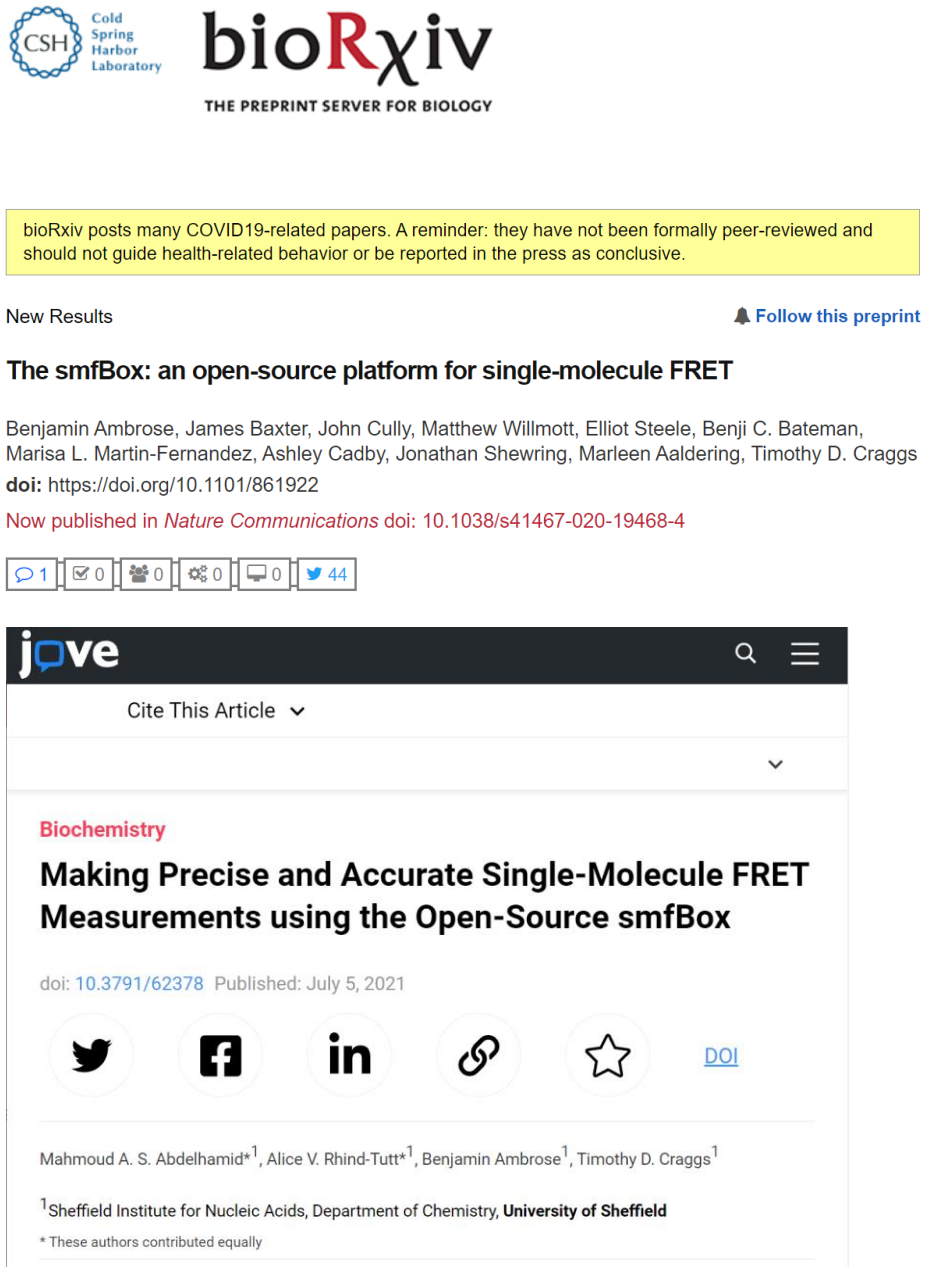
- Get your work out there fast
- Many different pre-print servers

Open Access Publishing

- Nature communications (Open Access)
- Journal of Visual Experiments (Paid open Access)

Making the research accessible:
More than making the publication accessible

What about those who can't build it?



Open Access – Spin out a company:

Exciting Instruments

- Ease-of-use
- smFRET
- FCS
- Cloud connected Software
- Significant innovations mean low ££
- Bench-top operation
- Small footprint

https://excitinginstruments.com/

Thanks

CRAGGS LAB
SINGLE MOLECULE BIOPHYSICS

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Tristan Johnston-Wood
Jon Shewring
James Baxter
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Alice Rhind-Tutt
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Zoe Waller (UCL)	iMotif
Mark Dillingham (Bristol)	SMC-ParABS
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Mark Leake (York)	Aggresomes
Agnes Noy (York)	**Atomistic MD**
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Ashley Cadby (Sheffield)	**Physics**
Grant Hill (Sheffield)	**MD and DFT**
Jane Grasby (Sheffield)	FEN1
Daniel Bose (Sheffield)	eRNA structure
Alison Twelvetrees (Sheffield)	Neuronal Transport
Benji Bateman (RAL)	**smFRET**

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EPSRC Engineering and Physical Sciences Research Council

MRC Medical Research Council

GCRF Global Challenges Research Fund

THE END

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