

# How the Crick send samples

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# or how to abuse common lab supplies

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# Automating NMR software installation

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# Homebrew

- The missing package manager for OSX and (linux)
- but now linux == windows
  - windows sub system for linux / WSL2 a full linux VM inside windows with interoperability
- currently I am concentrating on OSX but changes should be minor for the OSs

Homebrew  
Package  
management  
software



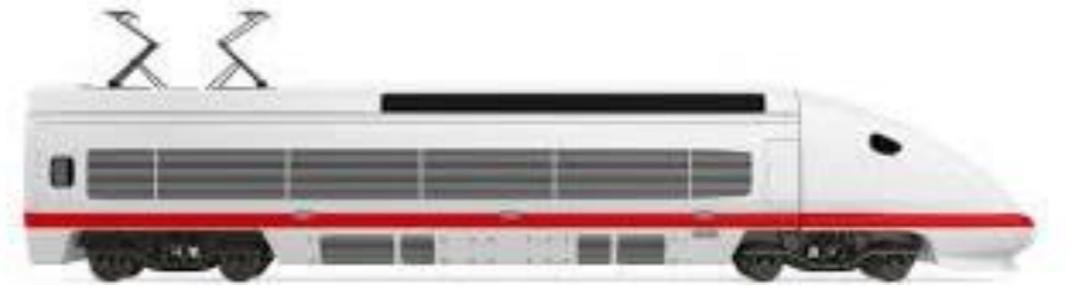
```
caloewen@DESKTOP-2FA6G40: ~  
caloewen@DESKTOP-2FA6G40:~$ sudo /etc/init.d/docker start  
[sudo] password for caloewen:  
* Starting Docker: docker  
caloewen@DESKTOP-2FA6G40:~$ sudo docker run -it alpine ash  
/# ls  
bin  etc  lib  mnt  proc  run  srv  tmp  var  
dev  home  media  opt  root  sbin  sys  usr  
/# cat /etc/alpine-release  
3.9.3  
/# caloewen@DESKTOP-2FA6G40:~$  
caloewen@DESKTOP-2FA6G40:~$
```

Alarms & Clock  
00:00:18.45

Type here to search

# KMS - Kent Module System

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- or

1. Kan't Manage Software

2. Kommon Modules for Spectroscopy

3. Kouldn't Make Software

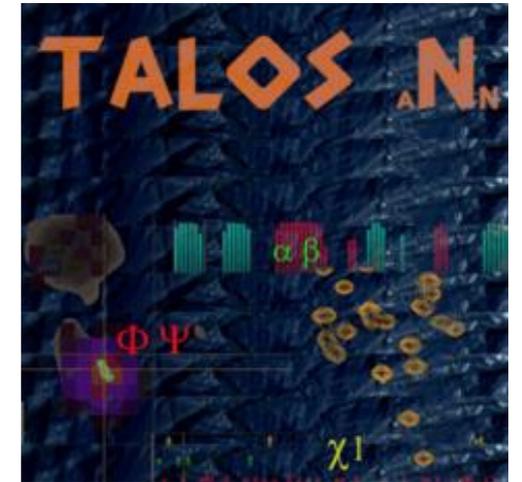
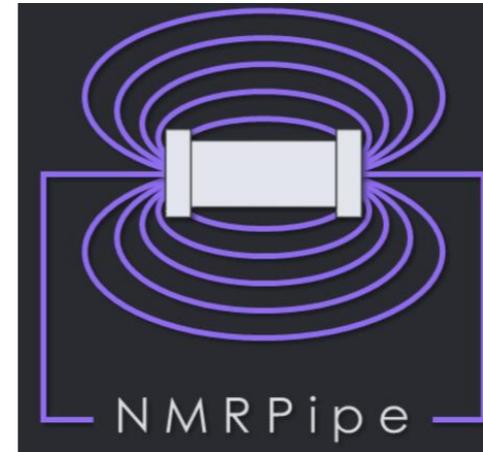
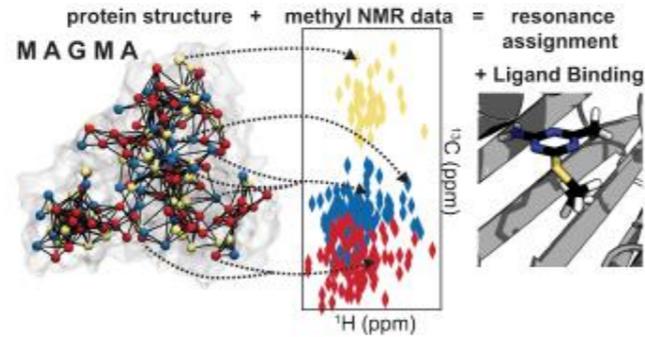
4. Kent Midland and Suburban Railway

# Current Modules

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- Open source based on GIT written in Ruby!
- Takes care to respect licenses
- 4 components
  - update manager (currently gary but to be replace by a robot)
  - licensing scripts (when required)
  - installation scripts including tests
  - continuous integrations test (next step)

currently have 10 packages



Rosetta



# Simple to use

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```
> setup_kms.sh
```

```
> brew tap kms/kms file:///<path to git repository>
```

```
> brew install xplor --with-config=xplor_garyt.yml
```

```
file xplor_garyt.yml
```

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```
xplor_nih:
```

```
  user_name : . # your username here
```

```
  password  : . # your password here
```

# Important things

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- packages cryptographically checked using SHA256

```
class Magma < Formula

  include Language::Python::Virtualenv

  option name 'with-config=', description 'the file describing the configuration for the install'

  desc 'MAGMA a program for assigning methyl resonances using through space NMR data'
  homepage 'http://magma.chem.ox.ac.uk/'
  url val 'uri://ox.ac.uk/848723e03a871c1bb3279807f2ce89f2/MAGMA_1.2.3.tar.gz',
      specs using: MagmaDownloadStrategy
  # not the true download link this must be entered into the config file to be matched against the hash
  sha256 'd06157ab3a55b2b806b3a9140d21d4bbe9d2a52411d7b9758074bc38b82711c5'
  version '1.2.3'

  resource name 'numpy' do
    url val 'https://files.pythonhosted.org/packages/2b/26/07472b0de91851b6656cbc86e2f0d5d3a3128e7580f23295ef58b6862d6c/numpy-1.'
    sha256 '31d3fe5b673e99d33d70cfee2ea8fe8dccc60f265c3ed990873a88647e3dd288'
  end
end
```

- packages installed in /usr/local/bin which is on PATH
- no need for root privileges all packages are standalone
- alternative install locations possible

$^{13}\text{C}$  incredibly insensitive but so resolved & sensitive

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# Sensitivity

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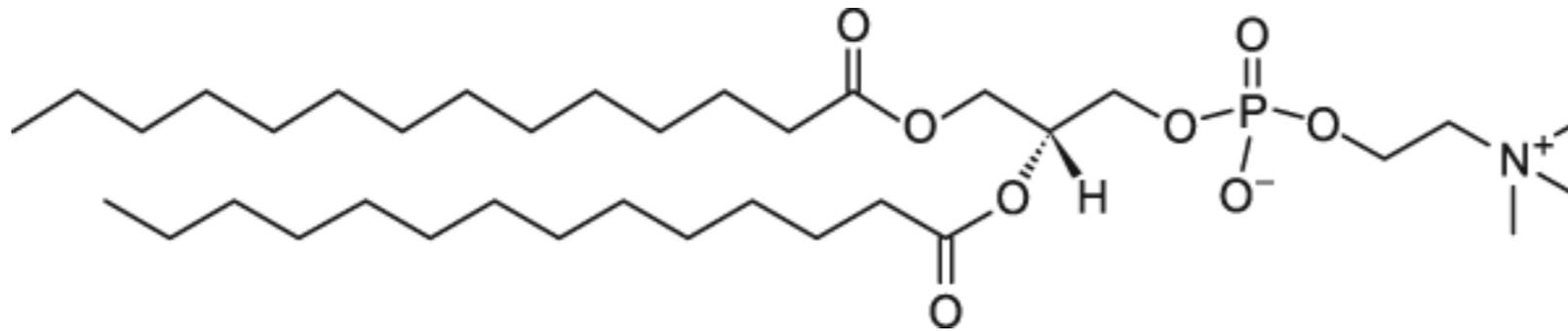
- s/n ~3% of  $^1\text{H}$

$$S/N \propto n \gamma_e \sqrt{\gamma_d^3 B_o^3 t}$$

- But cryoprobes and even 1.7mm ones
- 5mM quite good enough ... lipids / lipidomics in  $\text{CDCl}_3$
- For a typical human **cell lipids** account for about 40% of mass

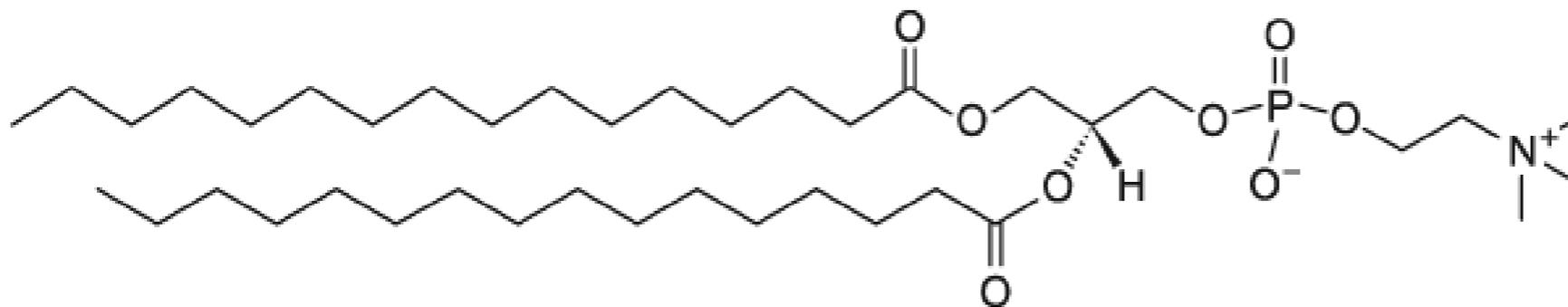
# Helen lipidomics

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14:0 PC (DMPC)

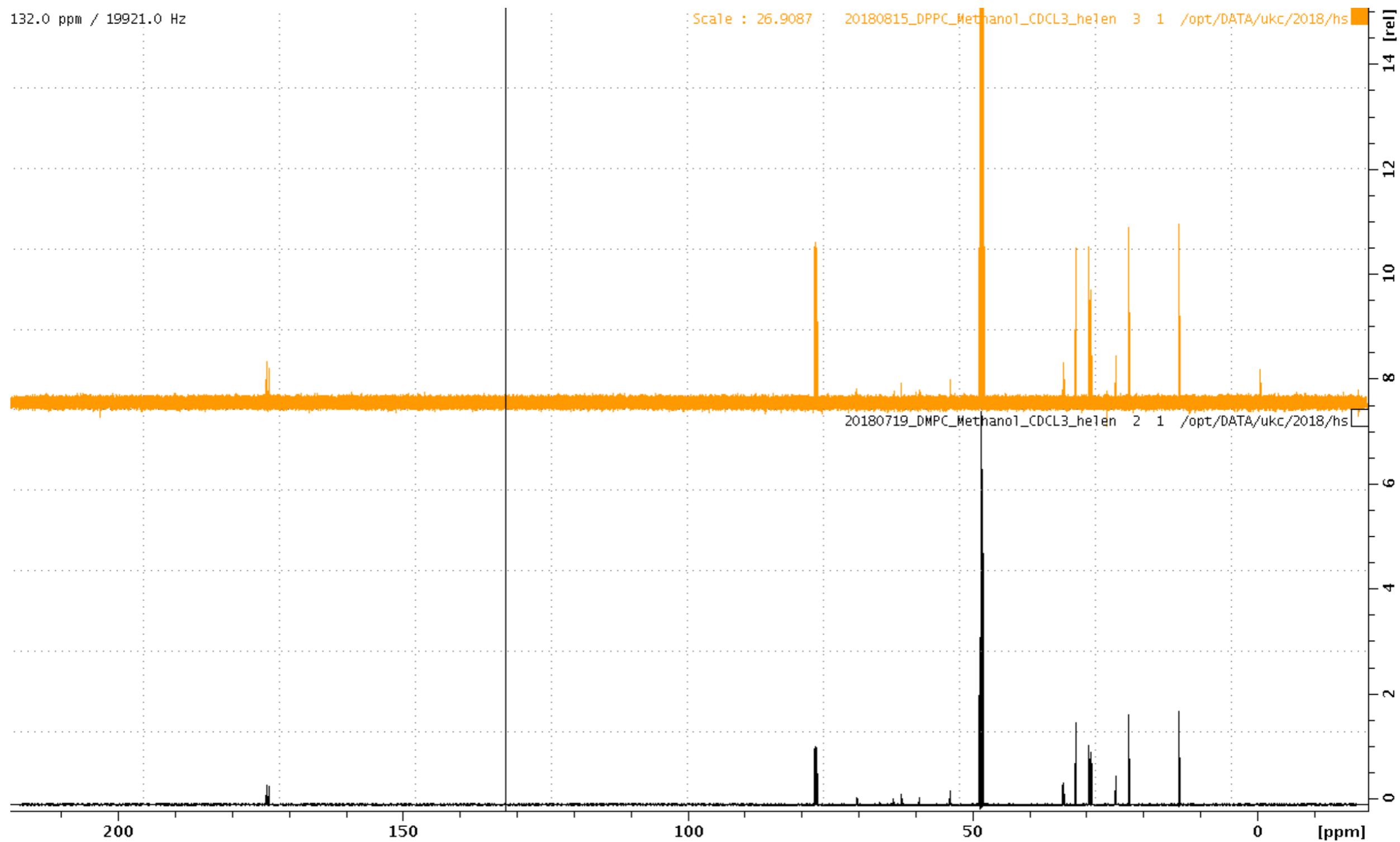
1,2-dimyristoyl-sn-glycero-3-phosphocholine



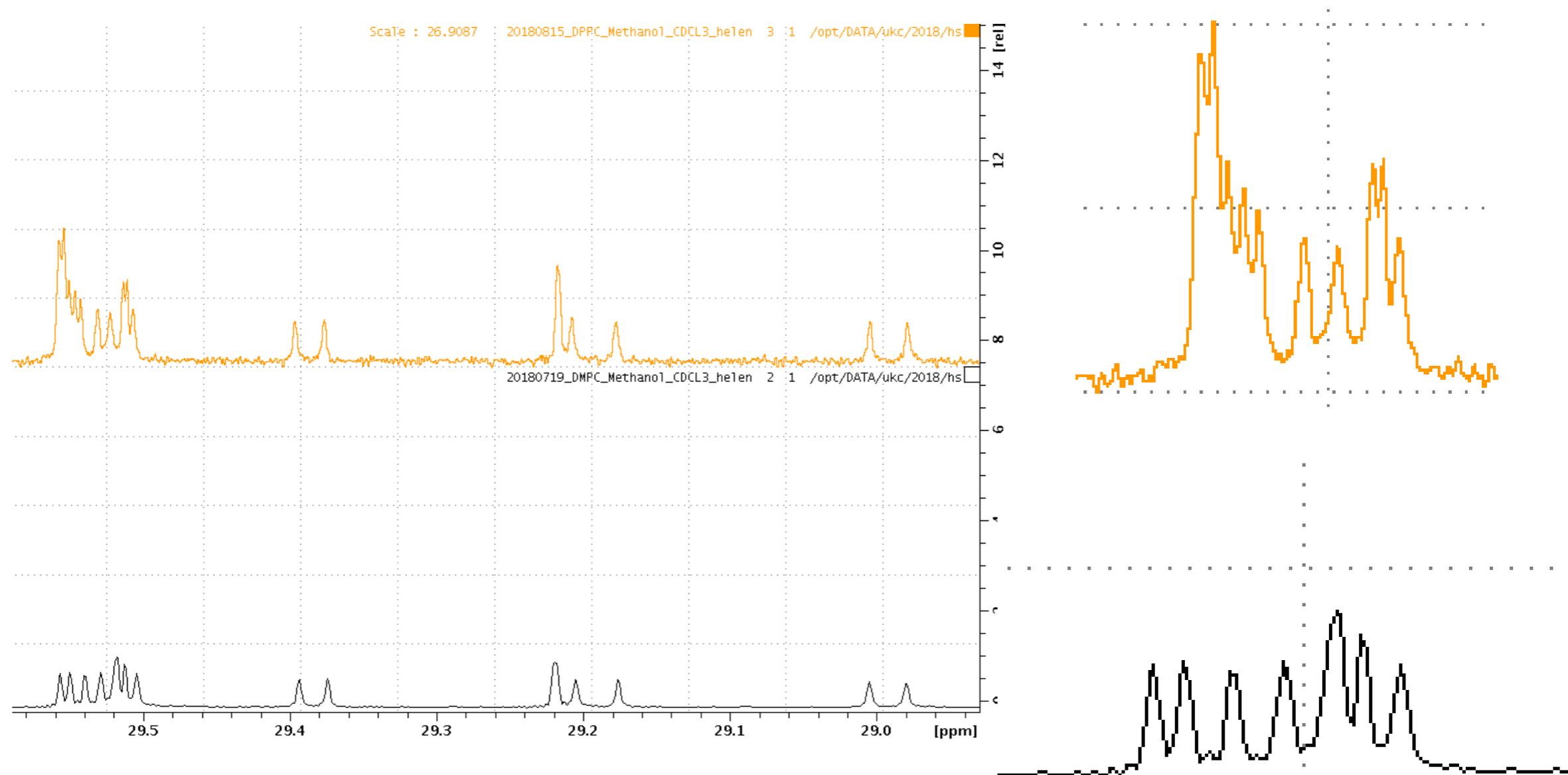
16:0 PC (DPPC)

1,2-dipalmitoyl-sn-glycero-3-phosphocholine

# $^{13}\text{C}$ DMPC vs DPPC



# $^{13}\text{C}$ DMPC vs DPPC at scale



# Advert: we have a research masters available

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