

# **Synthesis, Characterisation and Carbon Dioxide Capture Capacities of Hierarchically Porous Starbons<sup>®</sup>**

## **Supporting Information**

Han Li, Cheng Li, Vitaliy L. Budarin, James H. Clark,\* Michael North,\* Jinxiu Wang and Xiao Wu

The original data used to generate the results reported in this manuscript and supporting information are freely available at  
DOI: 10.15124/f3451289-dcf9-45b2-802e-7175aa073538

## Contents

|                                                                                                          |     |
|----------------------------------------------------------------------------------------------------------|-----|
| Procedures for the synthesis of activated Starbons <sup>®</sup>                                          | 3   |
| Methodology for the characterisation of Starbons <sup>®</sup>                                            | 5   |
| CO <sub>2</sub> adsorption studies                                                                       | 6   |
| TGA-FTIR plots                                                                                           | 7   |
| Nitrogen adsorption isotherms and pore distribution plots                                                | 12  |
| BET-surface areas and pore volumes for S900C15 prepared using different<br>flow rates of CO <sub>2</sub> | 68  |
| Comparison of various isotherm models                                                                    | 71  |
| SEM images                                                                                               | 77  |
| TEM images                                                                                               | 118 |
| ICP-OES data                                                                                             | 123 |
| Tabulation of surface compositions determined by XPS                                                     | 126 |
| XPS plots                                                                                                | 127 |
| Mass and heat flow changes during CO <sub>2</sub> adsorption at 35 °C and 1 bar pressure                 | 131 |
| CO <sub>2</sub> adsorption capacities and heats of CO <sub>2</sub> adsorption at 35 °C                   | 157 |
| Influence of water on CO <sub>2</sub> adsorption at 1 bar pressure                                       | 159 |
| Kinetics of CO <sub>2</sub> adsorption at 1 bar and 35 °C                                                | 161 |
| CO <sub>2</sub> adsorption isotherms (0.1-10 bar)                                                        | 174 |
| Fitting of isotherm models to the experimental CO <sub>2</sub> adsorption data                           | 177 |
| Van't Hoff plots                                                                                         | 181 |
| N <sub>2</sub> adsorption isotherms (0.1-10 bar)                                                         | 182 |
| Fitting of isotherm models to the experimental N <sub>2</sub> adsorption data                            | 184 |
| Selectivities of CO <sub>2</sub> versus N <sub>2</sub> adsorption                                        | 187 |
| Tabulation of material physical properties and CO <sub>2</sub> uptake parameters                         | 189 |
| Plots of textural properties with CO <sub>2</sub> uptake parameters                                      | 197 |
| Mass changes during CO <sub>2</sub> adsorption at 35 °C and various CO <sub>2</sub> partial pressures    | 221 |
| Tabulation of CO <sub>2</sub> adsorption capacities at various CO <sub>2</sub> partial pressures         | 225 |
| Fitting of the Freundlich isotherm to the pressure varied CO <sub>2</sub> adsorption data                | 225 |
| Tabulation of Freundlich parameters for the CO <sub>2</sub> adsorption isotherm                          | 225 |

## Procedures for the synthesis of activated Starbons®

Unactivated Starbons® (X300 and X800) were prepared by the freeze drying method as previously reported (A. Borisova, M. De Bruyn, V. L. Budarin, P. S. Shuttleworth, J. R. Dodson, M. L. Segatto and J. H. Clark, *Macromol. Rapid Commun.* 2015, **36**, 774–779).

### KOH activated Starbons®

Starbon® X300 (1 g) was impregnated with KOH (KOH:X300, 1:1 to 5:1, w:w) using a solution of KOH (100 mL) in EtOH:H<sub>2</sub>O (95:5, v:v) and stirred overnight at room temperature. The solvent was then evaporated at 60 °C under vacuum using a rotary evaporator and the resulting mixture was dried in a vacuum oven at 80 °C for 24 hours. Activation was then carried out by heating the resulting powder in a ceramic crucible placed in a HORIBA Scientific tube furnace under a flow of pure N<sub>2</sub> (100 cm<sup>3</sup> min<sup>-1</sup>) with a heating rate of 2 °C min<sup>-1</sup> to the final temperature of 600, 800 or 1000 °C. The temperature was held at the final temperature for 1 hour, then allowed to cool to room temperature. The residue was then washed first with 2M HCl and then with distilled water until the pH of the filtrate was approximately 7.0, to remove excess KOH and other potassium salts. Residual solvent was removed by centrifugation followed by drying at 80 °C for 24 hours to leave the KOH activated Starbons as black powders.

| Sample  | Yield (g) | Sample  | Yield (g) | Sample | Yield (g) |
|---------|-----------|---------|-----------|--------|-----------|
| S800K1  | 0.265     | A800K1  | 0.270     | P800K2 | 0.344     |
| S800K2  | 0.432     | A800K2  | 0.372     | P800K3 | 0.227     |
| S800K3  | 0.498     | A800K3  | 0.325     | P800K5 | 0.119     |
| S800K4  | 0.284     | A800K4  | 0.262     |        |           |
| S800K5  | 0.252     | A800K5  | 0.144     |        |           |
| S600K4  | 0.390     | A600K2  | 0.379     |        |           |
| S1000K4 | 0.171     | A1000K2 | 0.319     |        |           |

### CO<sub>2</sub> activated Starbons®

CO<sub>2</sub> activation was carried out in a NETZSCH STA409 coupled to a Bruker Equinox 55 FTIR. Starbon® X800 were used as the starting materials. The burn-off wt% of the X800 was monitored by the thermogravimetric instrument and the composition of the gases from the reaction of carbon with CO<sub>2</sub> were analysed in real time using FTIR during the activation process.

X800 (100 mg) was placed in a ceramic cup and heated from room temperature to the required temperature (700 to 1000 °C) with a heating rate of 10 °C min<sup>-1</sup> under a flow of pure CO<sub>2</sub> (flow rate 50 cm<sup>3</sup> min<sup>-1</sup>). The maximum temperature was maintained for the specified period of time (0 to 2 hours). At the end of the activation period, the sample was cooled under a flow of pure N<sub>2</sub> (flow rate 50 cm<sup>3</sup> min<sup>-1</sup>) to give the CO<sub>2</sub> activated Starbons® as black powders.

| Sample   | Yield (mg) | Sample   | Yield (mg) | Sample  | Yield (mg) |
|----------|------------|----------|------------|---------|------------|
| S800C15  | 85.3       | S900C90  | 55.8       | A750C45 | 73.8       |
| S850C15  | 83.4       | S900C120 | 48.5       | A750C60 | 70.0       |
| S900C15  | 77.5       | S950C30  | 53.1       | A750C90 | 61.8       |
| S950C15  | 67.6       | S950C60  | 36.0       | A900C0  | 63.8       |
| S1000C15 | 34.1       | S950C90  | 29.4       | A900C10 | 31.7       |
| S900C30  | 74.0       | S950C120 | 17.5       | P700C50 | 64.5       |
| S900C60  | 63.0       |          |            | P900C0  | 27.1       |

### O<sub>2</sub> activated Starbons<sup>®</sup>

O<sub>2</sub> activation was carried out in a NETZSCH STA409 coupled to a Bruker Equinox 55 FTIR. Starbon<sup>®</sup> X800 were used as the starting materials. The burn-off wt% of the X800 was monitored by the thermogravimetric instrument and the composition of the gases from the reaction of carbon with O<sub>2</sub> was analysed in real time using FTIR during the activation process.

X800 (100 mg) was placed in a ceramic cup, subjected to a flow of 200 cm<sup>3</sup> min<sup>-1</sup> N<sub>2</sub> and 20 cm<sup>3</sup> min<sup>-1</sup> air (overall O<sub>2</sub>=2%) and heated from room temperature to the required temperature (400 to 800 °C) with a heating rate of 10 °C min<sup>-1</sup>. The maximum temperature was maintained for the specified period of time (0 to 1 hour). At the end of the activation period, the sample was cooled under a flow of pure N<sub>2</sub> (flow rate 50 cm<sup>3</sup> min<sup>-1</sup>) to give the O<sub>2</sub> activated Starbons<sup>®</sup> as black powders.

| Sample  | Yield (mg) |  | Sample  | Yield (mg) |  | Sample  | Yield (mg) |
|---------|------------|--|---------|------------|--|---------|------------|
| S700O0  | 81.6       |  | A500O30 | 83.1       |  | P400O50 | 74.5       |
| S750O0  | 74.5       |  | A500O60 | 66.9       |  | P500O30 | 74.3       |
| S800O0  | 70.6       |  | A750O0  | 77.9       |  | P750O0  | 71.7       |
| S750O40 | 49.9       |  |         |            |  |         |            |
| S750O56 | 39.9       |  |         |            |  |         |            |



## Methodology for the characterisation of Starbons<sup>®</sup>

### Porosimetry

The textural properties of all samples were investigated by measuring nitrogen adsorption-desorption isotherms on a Micromeritics ASAP 2020 volumetric adsorption analyser at 77 K. Before the analyses, the powdered samples (~0.1g) were degassed at 200 °C for 8 hours to remove moisture and other contaminants. The BET model was applied for the determination of surface area and the BET surface area was calculated from the nitrogen adsorption data at a relative pressure range of 0.01-0.2; the total pore volume ( $V_{\text{total}}$ ) was estimated at a relative pressure of 0.99; the Barrett-Joyner-Halenda (BJH) method was used for determination of mesopore volume and mesopore size distribution. The HK method for carbon materials with slit-shaped pores was applied for the determination of micropore volume ( $V_{\text{micro}}$ ), ultramicropore volume ( $V_{\text{ultramicro}}$ ) and micropore size distribution. The DFT method assuming a slit pore model and a non-local DFT method (NLDF) assuming a non-homogeneous fluid at a solid interface in a slit pore model were also applied for the characterisation of the pore volumes in the activated Starbons<sup>®</sup>.

### ICP-OES analysis

ICP-OES analysis of the elemental composition of Starbon<sup>®</sup> samples was carried out by the Biorenewables Development Centre using an Agilent 7700 series inductively coupled plasma-optical emission spectrometry (ICP-OES). Samples (~50 mg) were digested by a solution of nitric acid and hydrogen peroxide (10 mL, 4:1, v:v). The mixture was microwave heated to 200 °C over 30 minutes, and the temperature was held at 200 °C for 15 minutes. After cooling down, the mixtures transferred into 100 mL conical flasks and diluted to up to the mark with distilled water and then analysed. The results for each element were fitted onto a calibration curve. The results recorded were then multiplied by the dilution factor, to produce the concentration for each element in the samples.

### CHN analysis

The quantity of carbon, hydrogen and nitrogen in Starbon<sup>®</sup> samples were determined by the CHN analysis service of the University of York using an Exeter Analytical Inc. CE-440 analyser and a high temperature combustion method.

### XPS analysis

Surface characterization by XPS analysis was performed by the UK national XPS service at the University of Cardiff using a Thermo K-Alpha+ XPS fitted with a monochromated Al  $K\alpha$  X-ray source. Data were collected at a pass energy of 2150 eV for survey spectra and 40 eV for high-resolution scans. The spectra were collected at a pressure below  $10^{-7}$  Torr and a temperature of 294 K. Peaks were fit with a Shirley background prior to component analysis. Data was analysed using CasaXPS (v2.3.34) after subtraction of the background and using modified sensitivity factors as supplied.

### SEM imaging

The morphology of samples was studied using a scanning electron microscope (SEM, JEOL 7800F) at an accelerating voltage of 5 kV and a working distance of 10 mm with a LED detector. Energy dispersive X-ray spectrometry (EDS) analysis was performed by setting the accelerating voltage to 15 kV. The sample was mounted on an aluminium plate and coated with carbon to increase the conductivity prior to analysis.

### TEM imaging

The morphology of samples was also observed using transmission electron microscopy (JEOL 2011 TEM) at an accelerating voltage of 100 kV. Samples were prepared by sonicating the material in ethanol and depositing it on a holey carbon support film on a 300 mesh copper grid.

## **CO<sub>2</sub> adsorption studies**

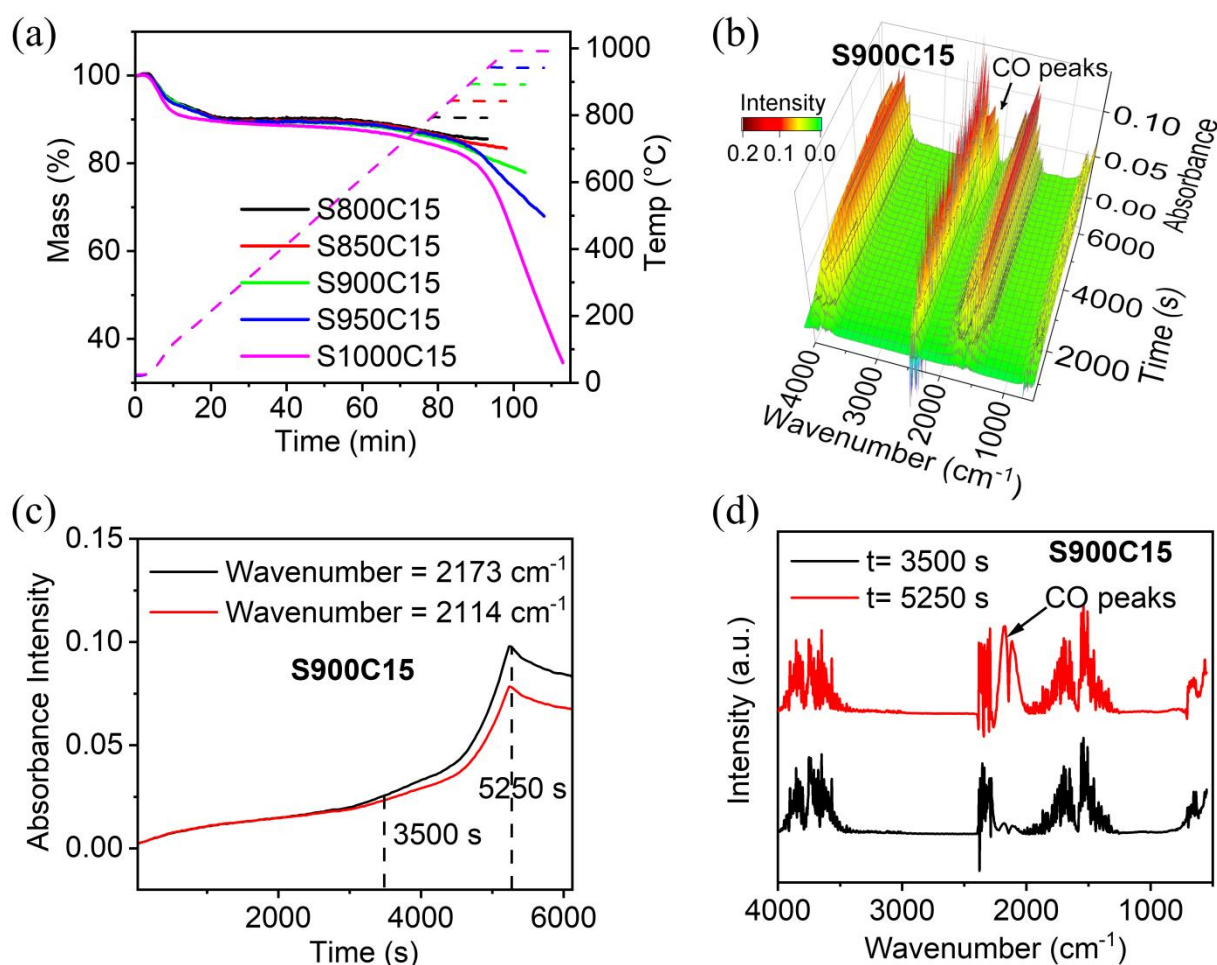
### CO<sub>2</sub>/N<sub>2</sub> composition swing

The CO<sub>2</sub> adsorption of samples was investigated using a STA 625 thermal analyser with a gas composition swing method. Before each measurement, the sample (~10.0 mg) was heated at 373 K for 1 hour under a flow of N<sub>2</sub> (60 ml min<sup>-1</sup>) to ensure the removal of residual water and impurities. After cooling to room temperature under N<sub>2</sub>, the sample was heated to 308 K at 1 °C min<sup>-1</sup> under a flow of N<sub>2</sub> (60 ml min<sup>-1</sup>) and then the temperature was kept at 308 K during remainder of the analysis. A three-way valve was employed to switch the gas flow between pure CO<sub>2</sub> (60 ml min<sup>-1</sup>) and pure N<sub>2</sub> (60 ml min<sup>-1</sup>) for CO<sub>2</sub> adsorption and desorption, respectively. For experiments carried out using CO<sub>2</sub> partial pressures of 0.15-0.83 bar instead of pure CO<sub>2</sub>, the three-way valve was set to give the appropriate CO<sub>2</sub> and N<sub>2</sub> flow rates whilst keeping the total gas flow rate constant at 60 ml min<sup>-1</sup>. The changes in mass and heat flow were recorded by the TGA and DSC capabilities of the STA 625 respectively. Multiple adsorption and desorption cycles were run to determine the reproducibility of the data and the regenerability of the samples. Calculations of adsorption capacities and enthalpies of adsorption were carried out on the basis that the observed changes in mass and heat flow were entirely due to adsorption or desorption of carbon dioxide as other experiments (nitrogen porosimetry at 35 °C, volumetric N<sub>2</sub> adsorption, and the high CO<sub>2</sub> to N<sub>2</sub> selectivities determined volumetrically) showed that at 35 °C, adsorption of N<sub>2</sub> onto these materials was negligible relative to the amount of CO<sub>2</sub> adsorbed.

### CO<sub>2</sub> and N<sub>2</sub> adsorption isotherm studies

The adsorption isotherms of pure CO<sub>2</sub> and N<sub>2</sub> for selected Starbon<sup>®</sup> samples were measured volumetrically at Fudan University, using a Quantachrome Isorb HP2 instrument. Before measurement, all samples were degassed under vacuum at 473 K for 8 hours. The CO<sub>2</sub> and N<sub>2</sub> adsorptions were performed under the same conditions in the range of 0 to 10 bar at 273, 298 and 323 K. For measurements at 273 and 298K, the stainless-steel sample holder was connected to an external circulating cooling device filled with an aqueous solution of ethylene glycol (1:3,v/v) to keep the temperature constant (within a variation of  $\pm 0.02$  °C). For measurements at 323K, the temperature control system was switched to an external heating package.

## TGA-FTIR plots for starch derived CO<sub>2</sub> activated Starbons®



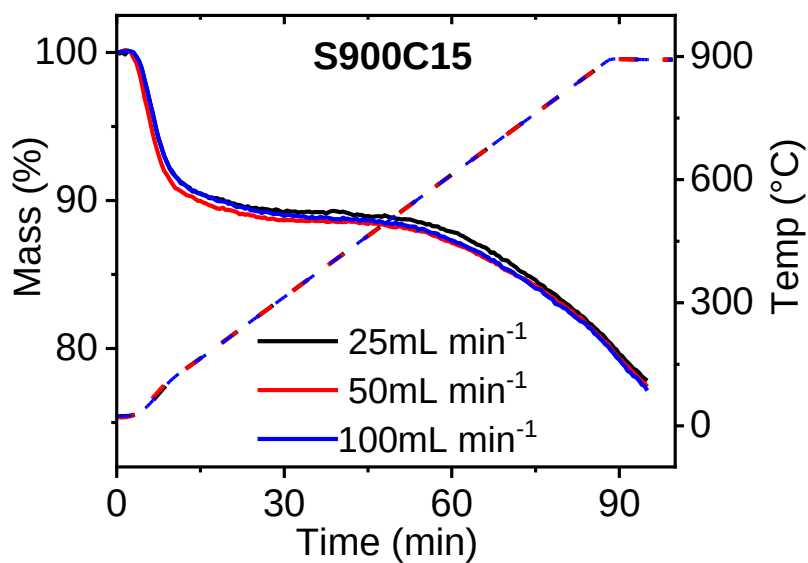
(a) TGA curves of activation time versus temperature and burn-off wt% for CO<sub>2</sub> activation of S800 as the temperature increases from 20 °C. The ca 10% mass loss in the first 10 minutes (up to 100 °C) corresponds to desorption of water and CO<sub>2</sub> from the S800.

(b) Real-time FTIR spectra of the off-gases from the preparation of S900C15 showing that formation of CO becomes pronounced at about 5250 seconds which corresponds to 900 °C.

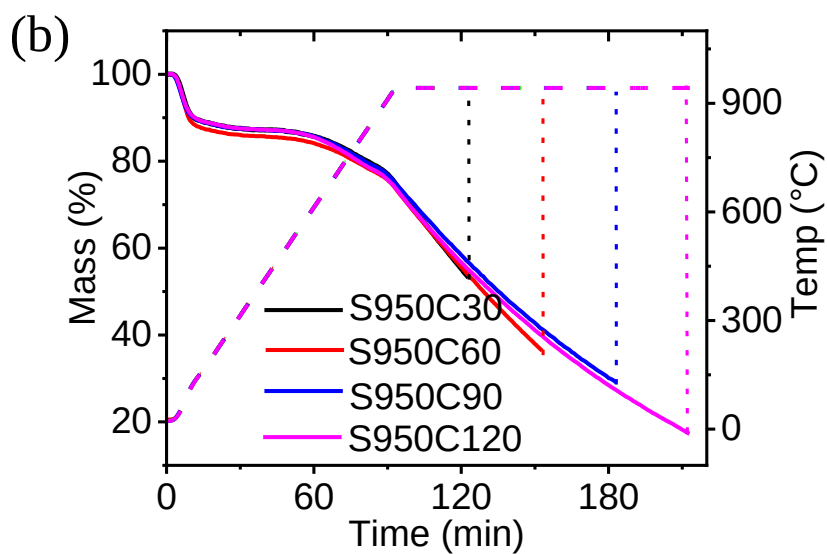
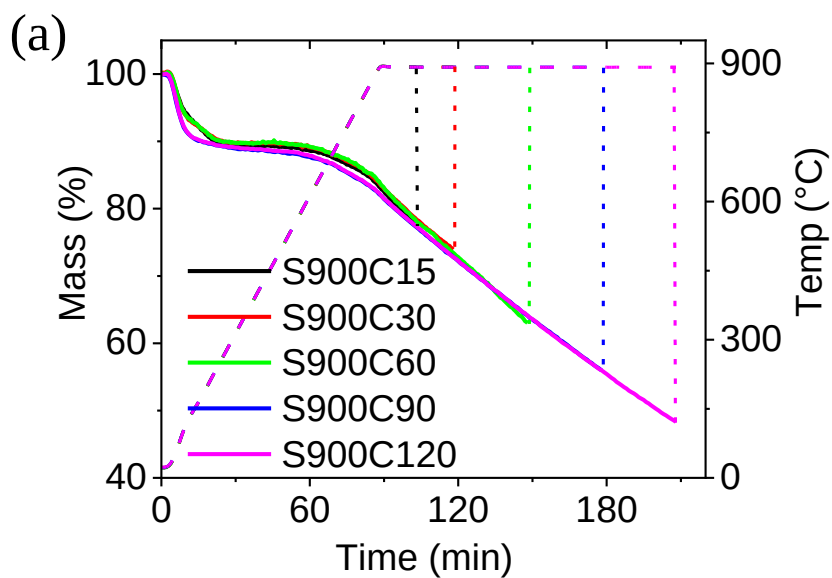
(c) Change of absorbance with time of the FTIR spectral peaks of CO from the preparation of S900C15 showing that CO formation starts at about 3500 seconds (corresponding to 600 °C) and becomes more pronounced at about 5250 seconds (corresponding to 900 °C).

(d) FTIR spectra at 3500 (black) and 5250 seconds (red) from the preparation of S900C15 showing the change in intensity of the CO peaks.

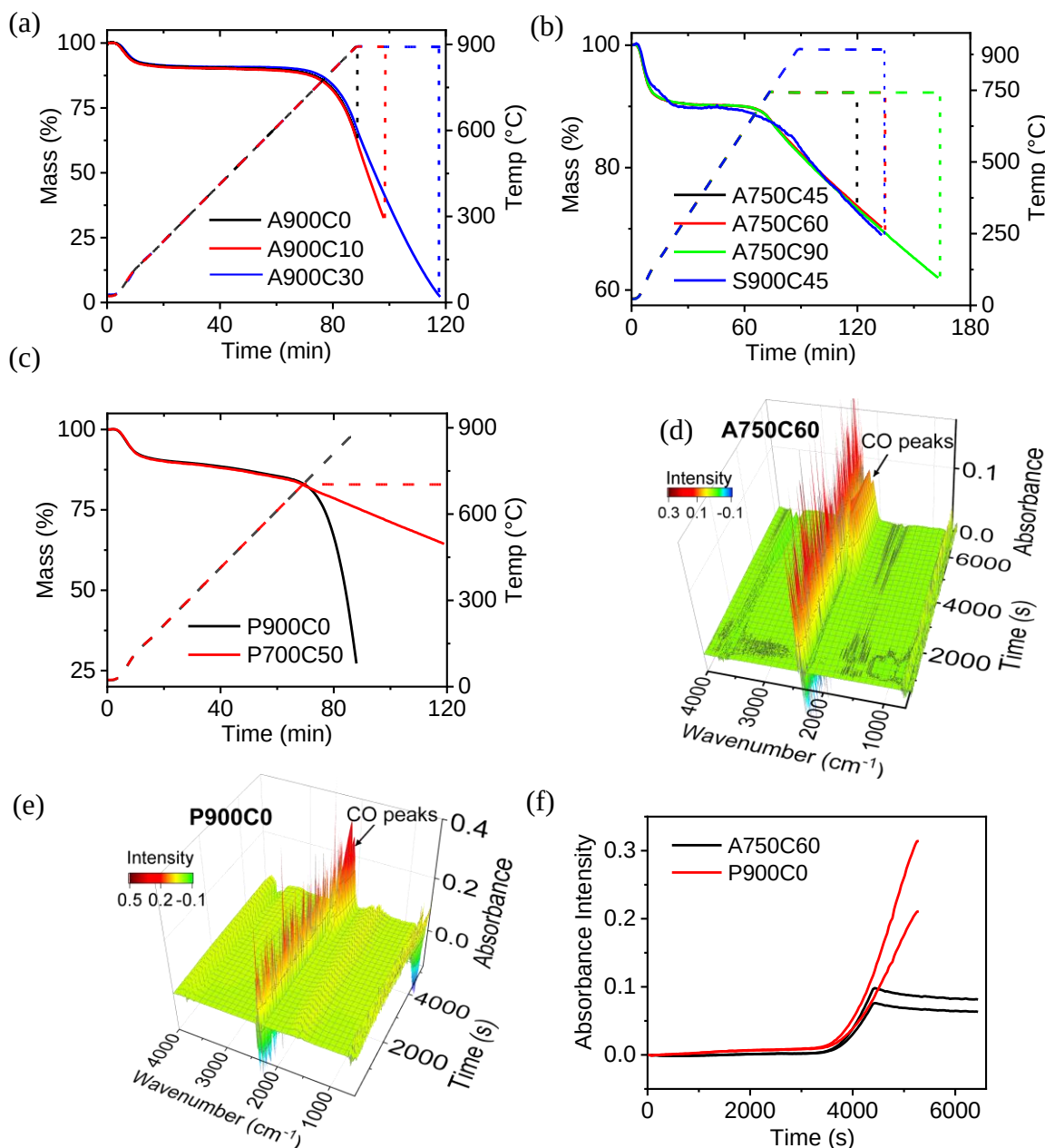
TGA-plots for the synthesis of S900C15 with different flow rates of CO<sub>2</sub>



TGA-plots for the synthesis of S900C15–120 and S950C30–120



## TGA-FTIR plots for alginic acid and pectin derived CO<sub>2</sub> activated Starbons®



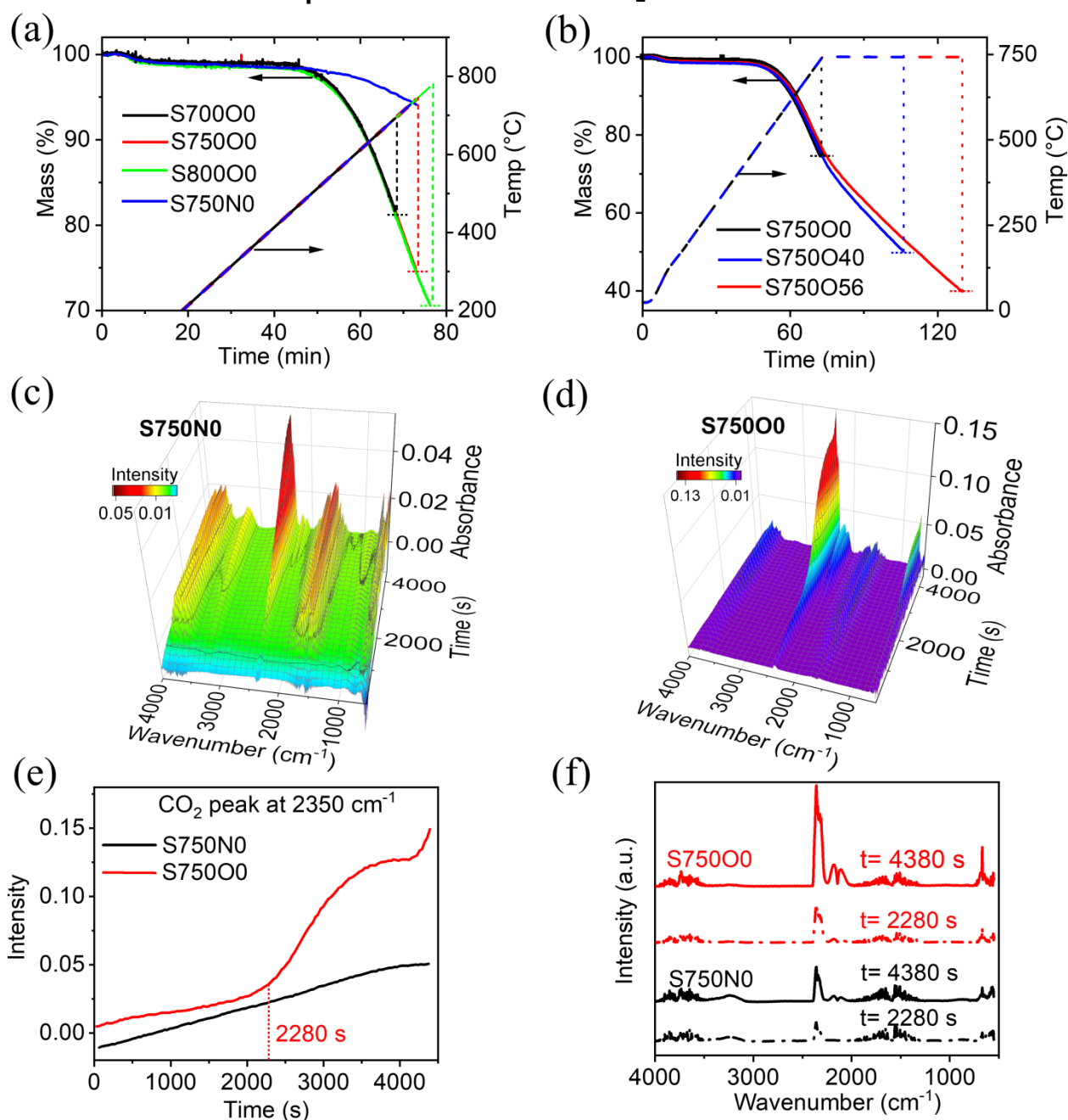
(a,b) TGA curves of activation time versus temperature and burn-off wt% for CO<sub>2</sub> activation of A800 as the temperature increases from 20 °C to 900 °C (a) or 750 °C (b). Plot (b) also shows data for S900C45 to illustrate that alginic acid derived Starbons® are more readily activated with CO<sub>2</sub> than starch derived Starbons®. The ca 10% mass loss in the first 10 minutes (up to 100 °C) corresponds to desorption of water and CO<sub>2</sub> from the A800.

(c) TGA curves of activation time versus temperature and burn-off wt% for CO<sub>2</sub> activation of P800 as the temperature increases from 20 °C. The ca 10% mass loss in the first 10 minutes (up to 100 °C) corresponds to desorption of water and CO<sub>2</sub> from the P800. Comparison of the P900C0 curve in plot (c) with the A900C0 curve in plot (a) shows that pectin derived Starbons® are more readily activated with CO<sub>2</sub> than alginic acid derived Starbons®.

(d,e) Real-time FTIR spectra of the off-gases from the preparation of A750C60 and P900C0 showing that formation of CO becomes pronounced at about 4400 seconds which corresponds to 750 °C.

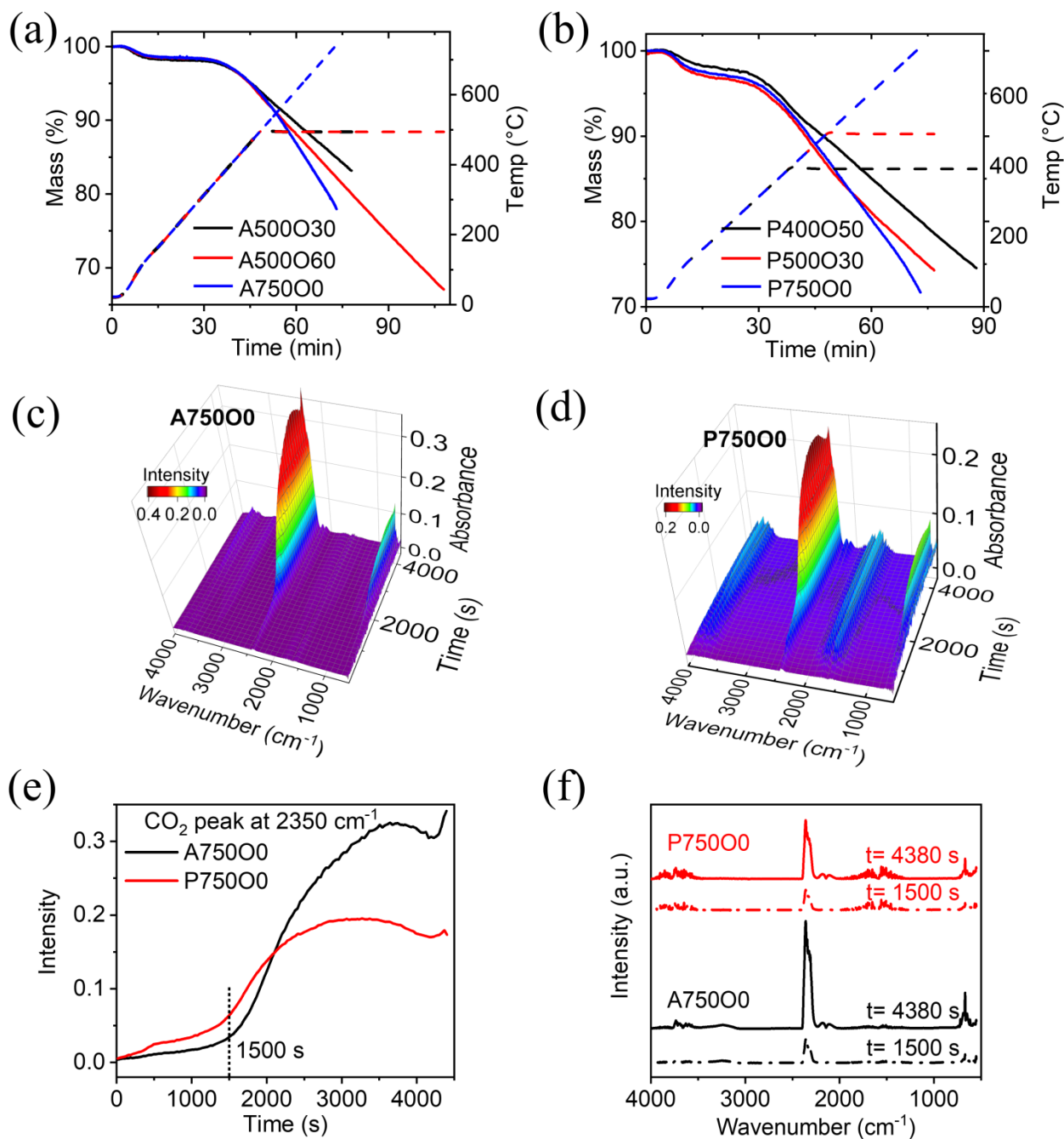
(f) Change of absorbance with time of the FTIR spectral peaks of CO during the synthesis of A700C60 and P900C0 showing that CO formation starts at about 3500 seconds (corresponding to 600 °C).

# TGA-FTIR plots for starch derived O<sub>2</sub> activated Starbons®





## TGA-FTIR plots for alginic acid and pectin derived O<sub>2</sub> activated Starbons<sup>®</sup>



(a,b) TGA curves of activation time versus temperature and burn-off wt% for O<sub>2</sub> activation of A800 (a) or P800 (b) as the temperature increases from 20 °C to 750 °C.

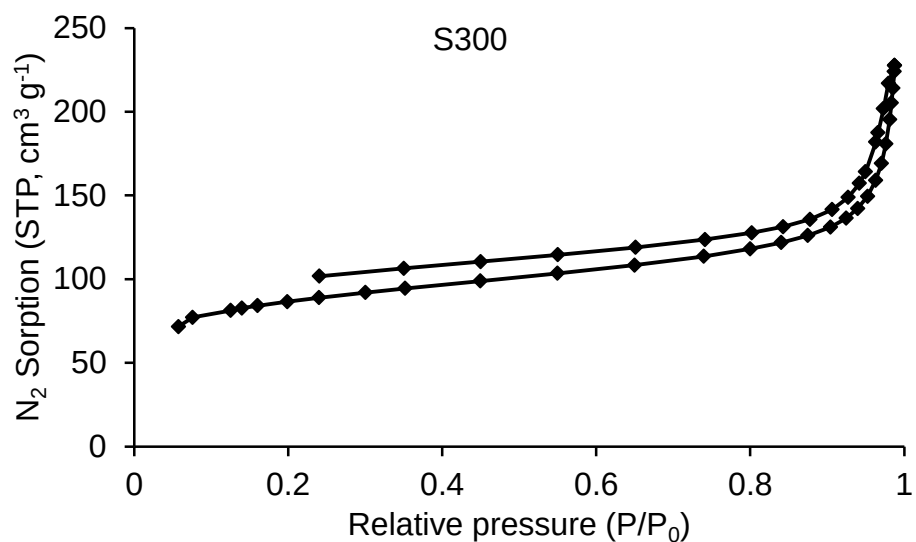
(c,d) Real-time FTIR spectra of the off-gases from the preparation of A750O0 and P750O0 showing that formation of CO<sub>2</sub> becomes pronounced at about 1500 seconds which corresponds to 270 °C.

(e) The change of absorbance at 2350 cm<sup>-1</sup> (CO<sub>2</sub> stretch) with time of the FTIR spectra of the off-gases obtained when A800 and P800 were heated to 750 °C under oxygen. CO<sub>2</sub> evolution increases markedly at 1500 seconds which corresponds to 270 °C.

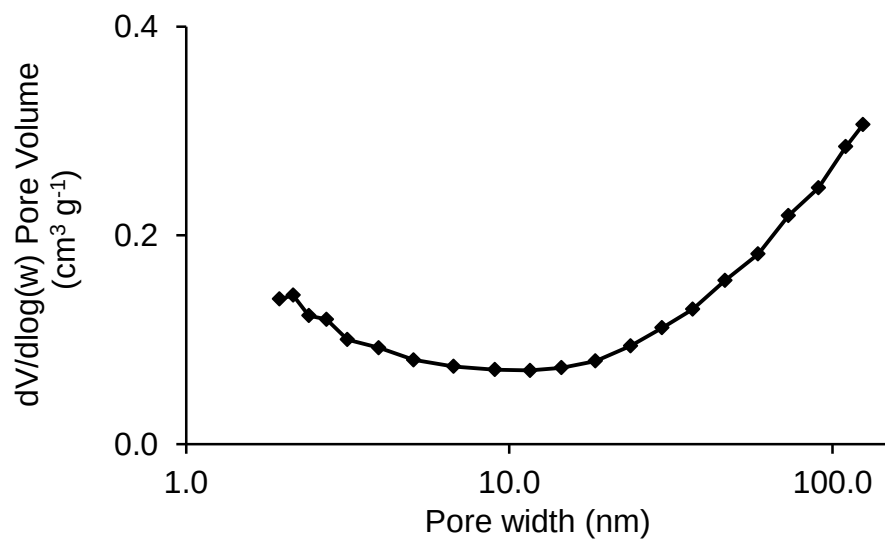
(f) FTIR spectra recorded of the off-gases obtained at 1500 s and 4380 s when A800 and P800 were heated to 750 °C under oxygen.

## Nitrogen adsorption isotherm and pore distribution plots for S300

Nitrogen adsorption isotherm (77K)



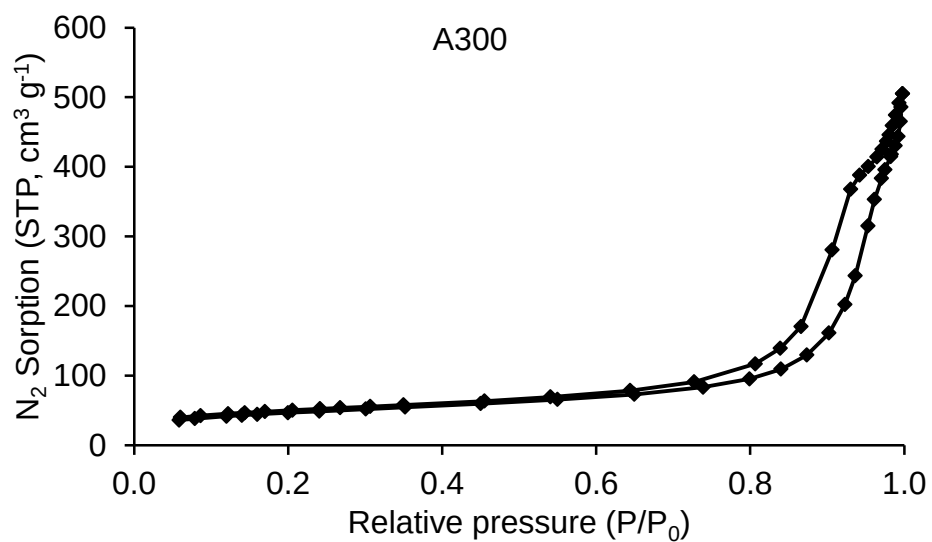
Pore distribution in the mesopore region (BJH method)



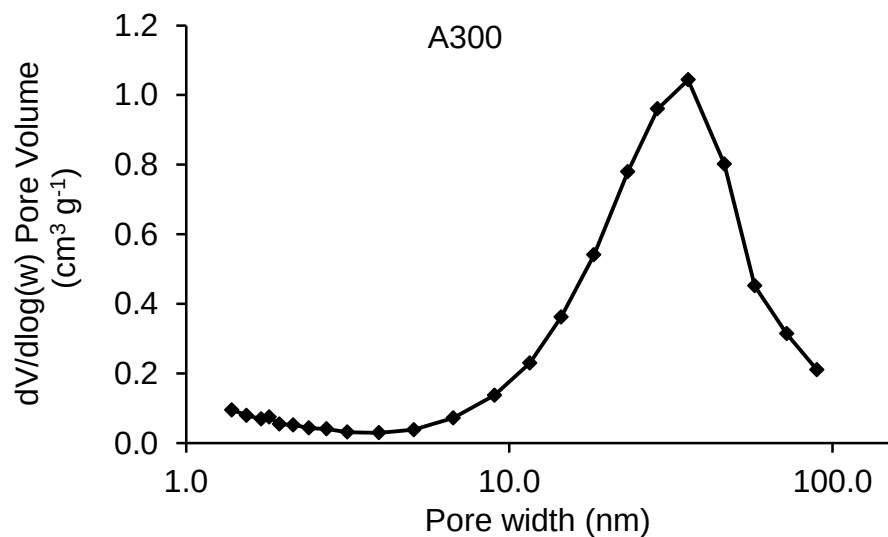


## Nitrogen adsorption isotherm and pore distribution plots for A300

Nitrogen adsorption isotherm (77K)

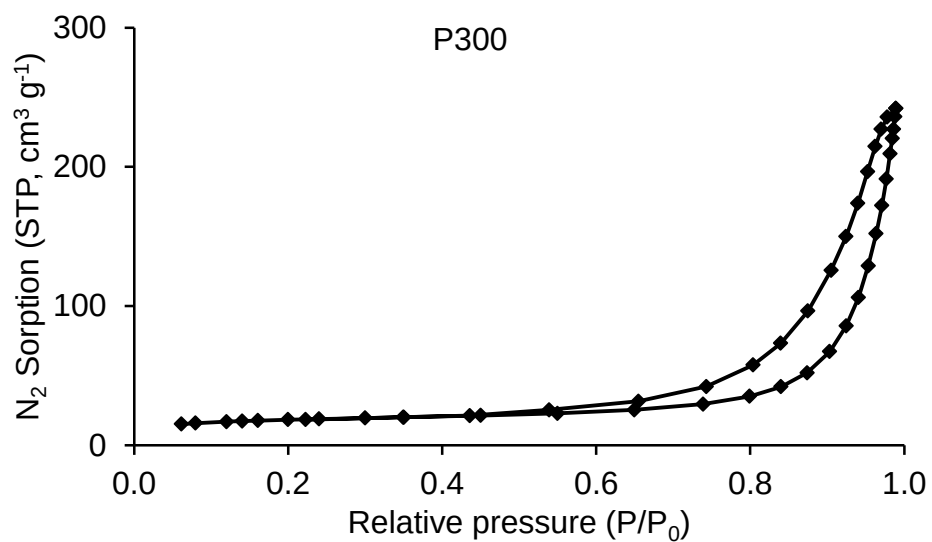


Pore distribution in the mesopore region (BJH method)

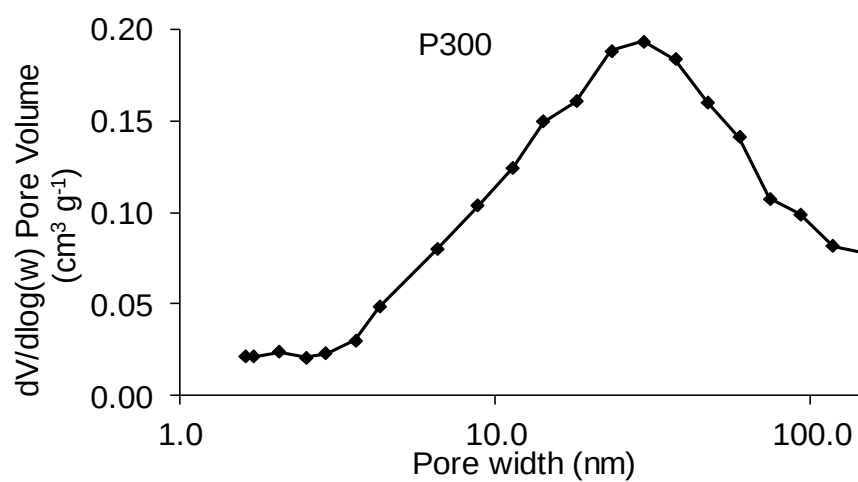


## Nitrogen adsorption isotherm and pore distribution plots for P300

Nitrogen adsorption isotherm (77K)

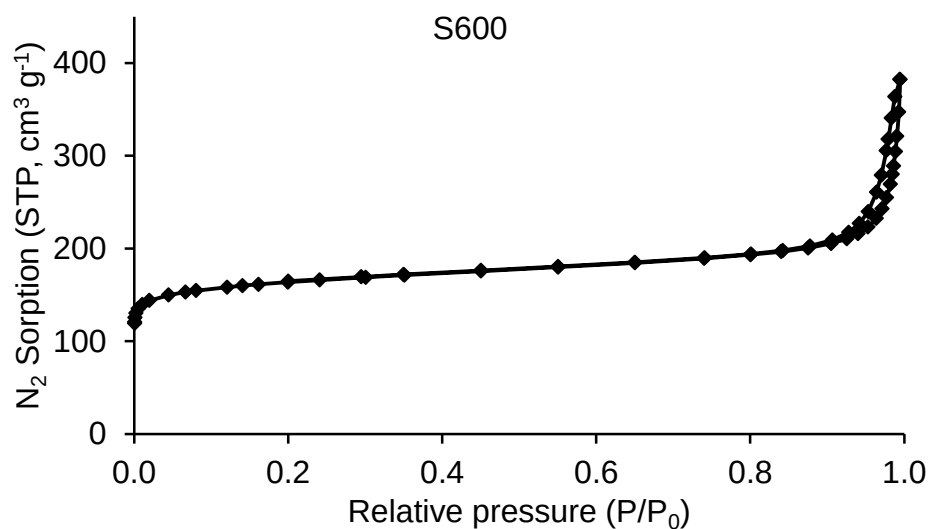


Pore distribution in the mesopore region (BJH method)

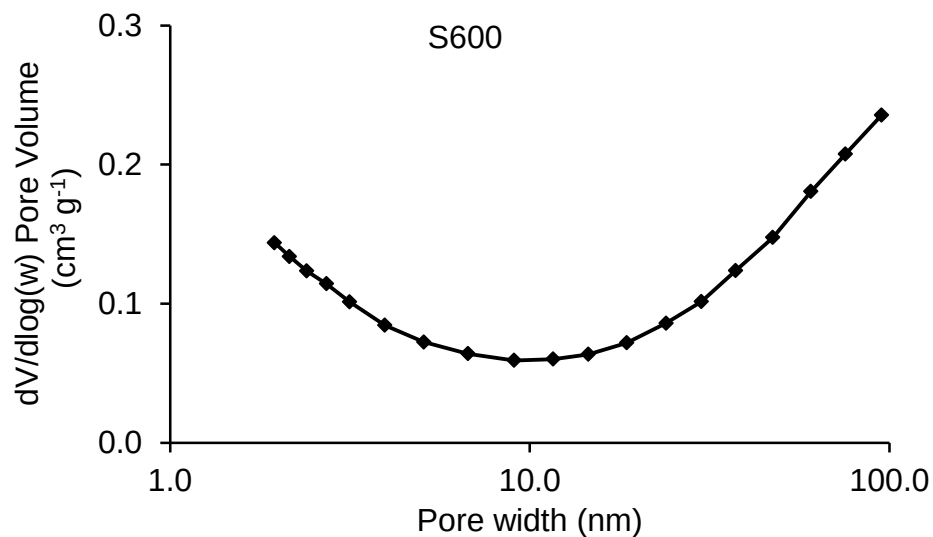


## Nitrogen adsorption isotherm and pore distribution plots for S600

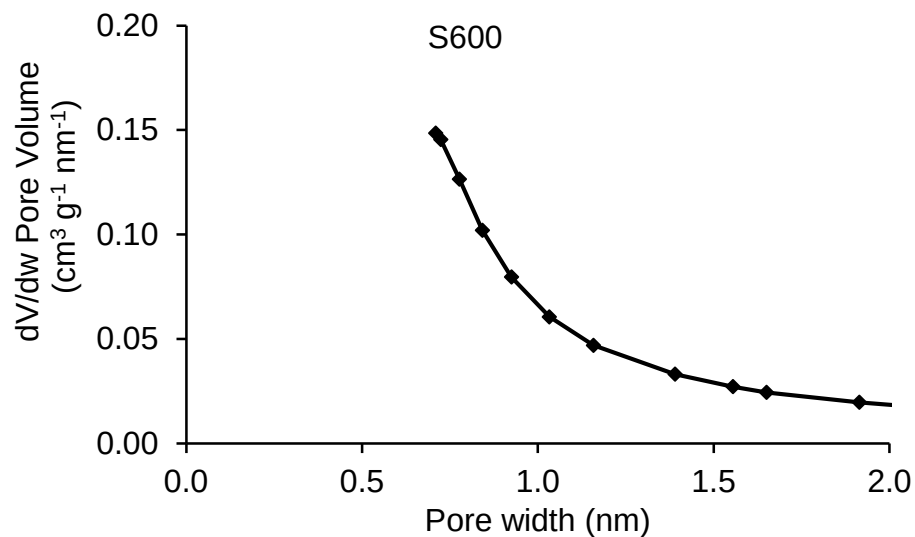
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

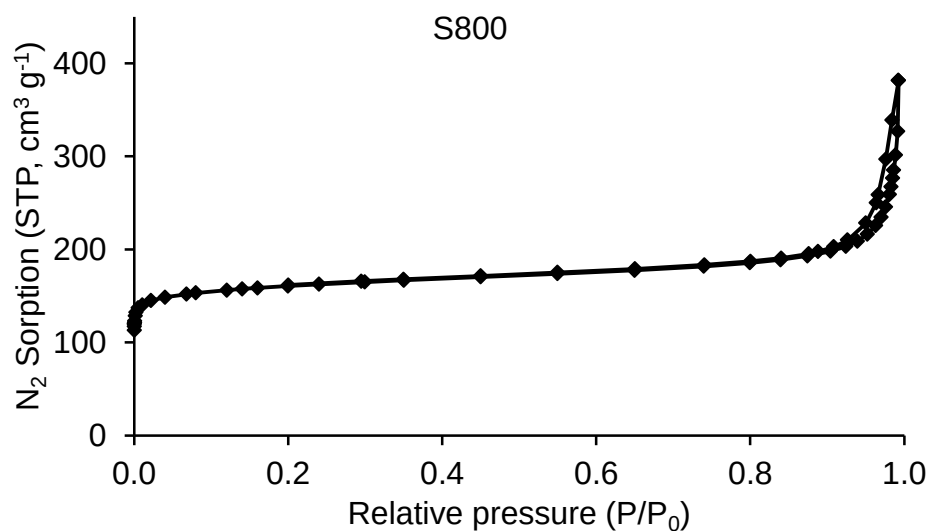


### Pore distribution in the micropore region (HK method)

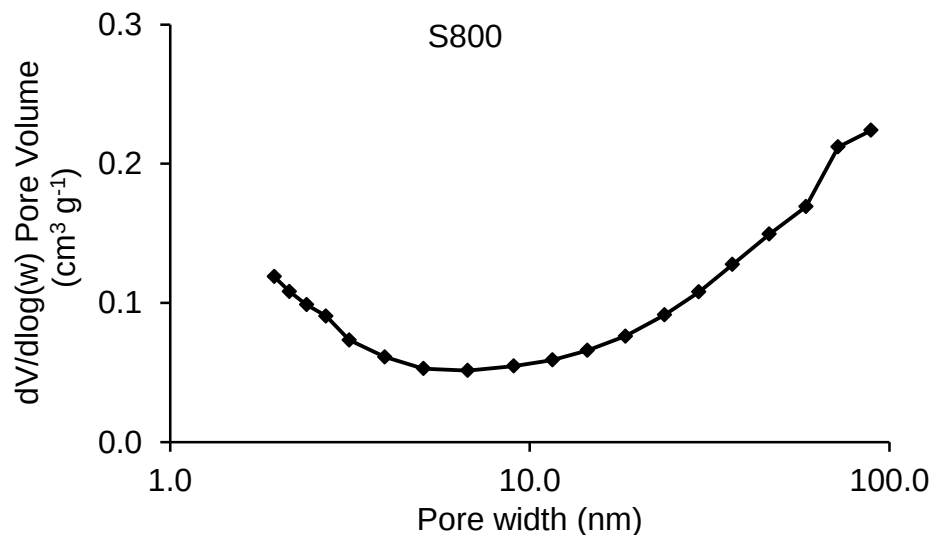


## Nitrogen adsorption isotherm and pore distribution plots for S800

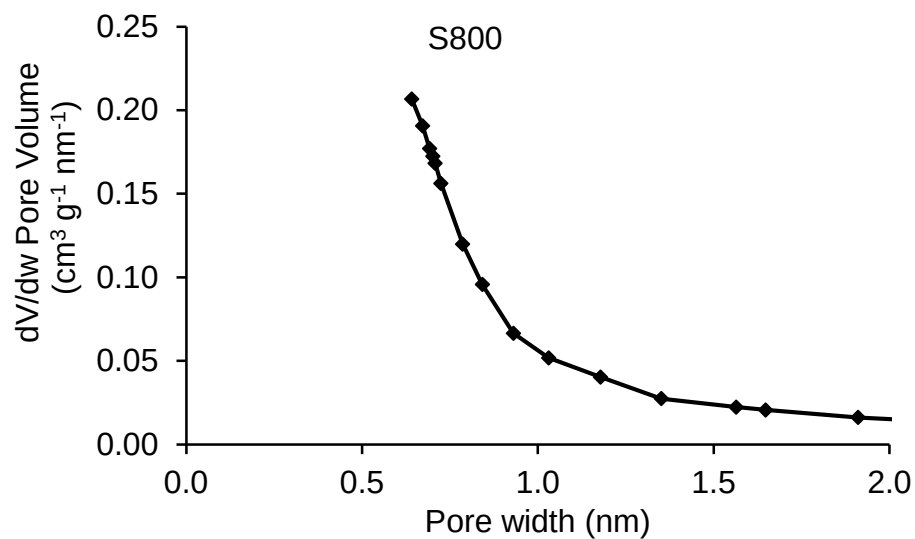
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

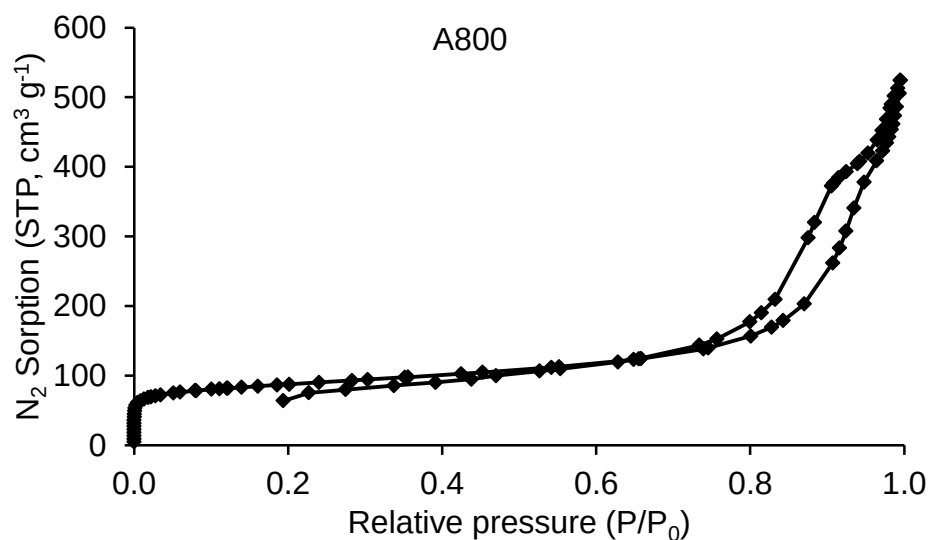


### Pore distribution in the micropore region (HK method)

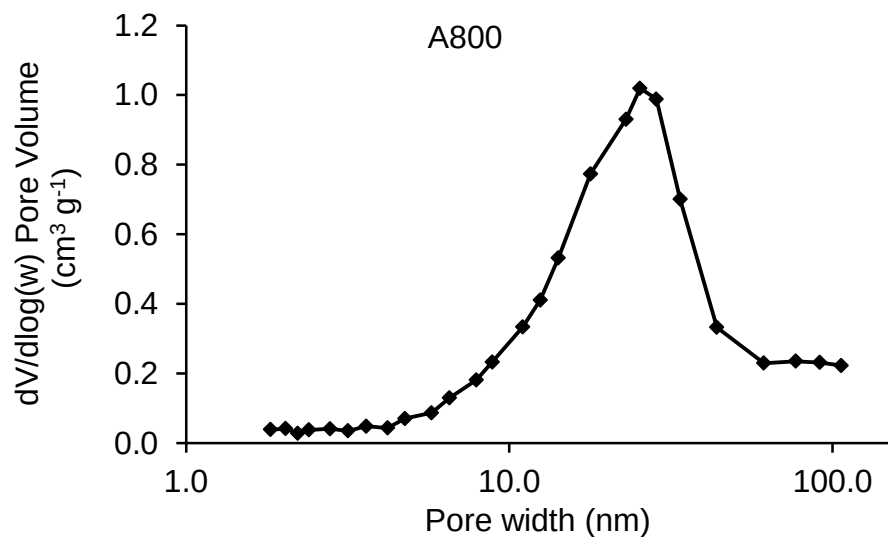


## Nitrogen adsorption isotherm and pore distribution plots for A800

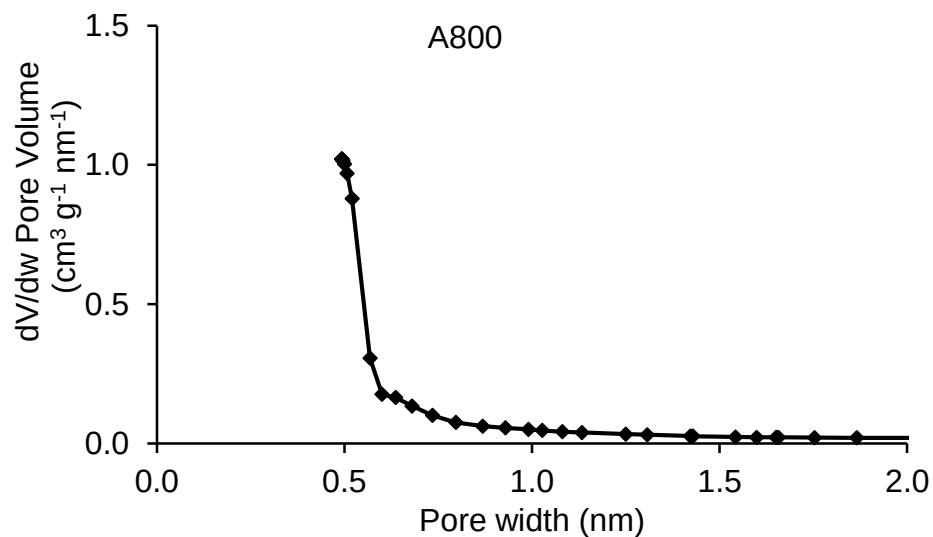
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

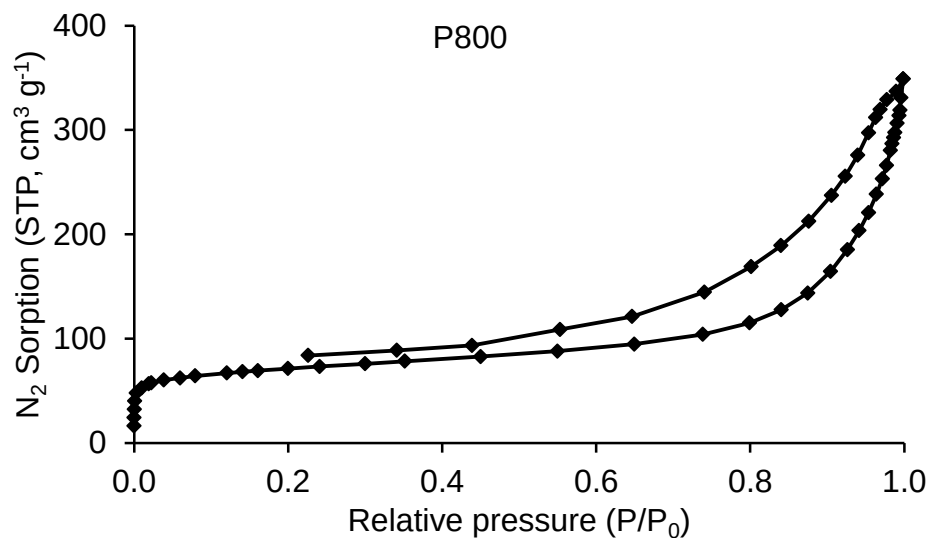


Pore distribution in the micropore region (HK method)

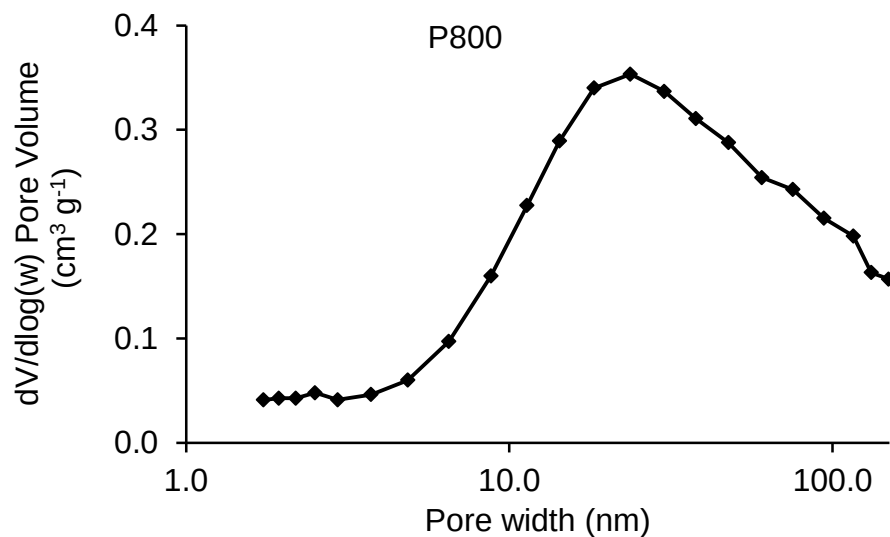


## Nitrogen adsorption isotherm and pore distribution plots for P800

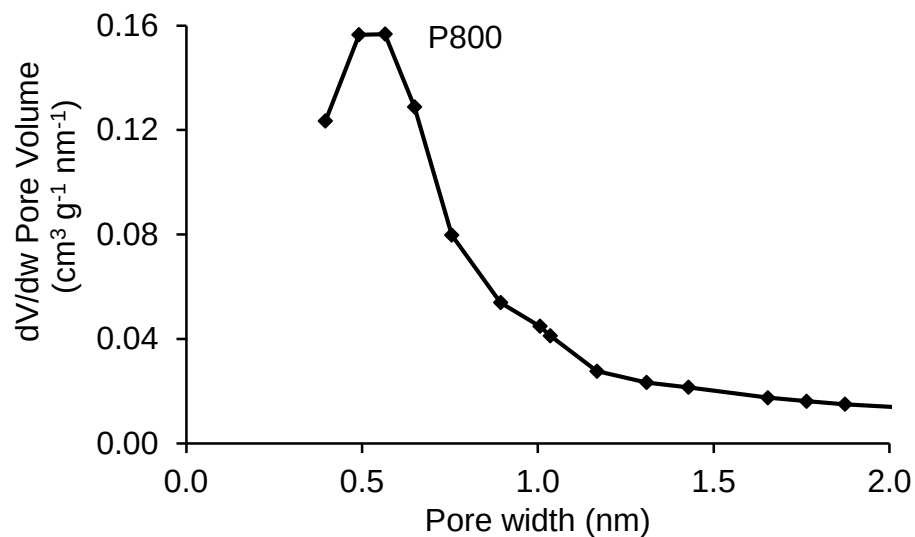
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

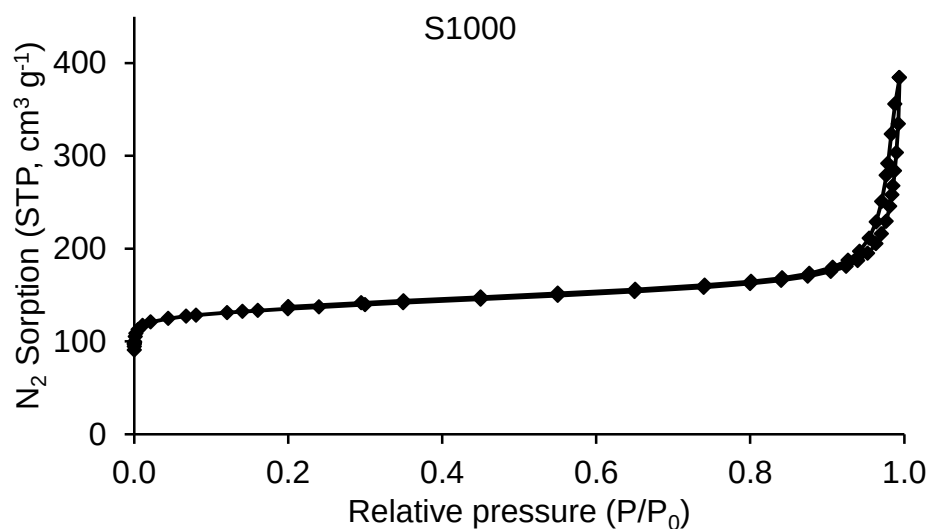


Pore distribution in the micropore region (HK method)

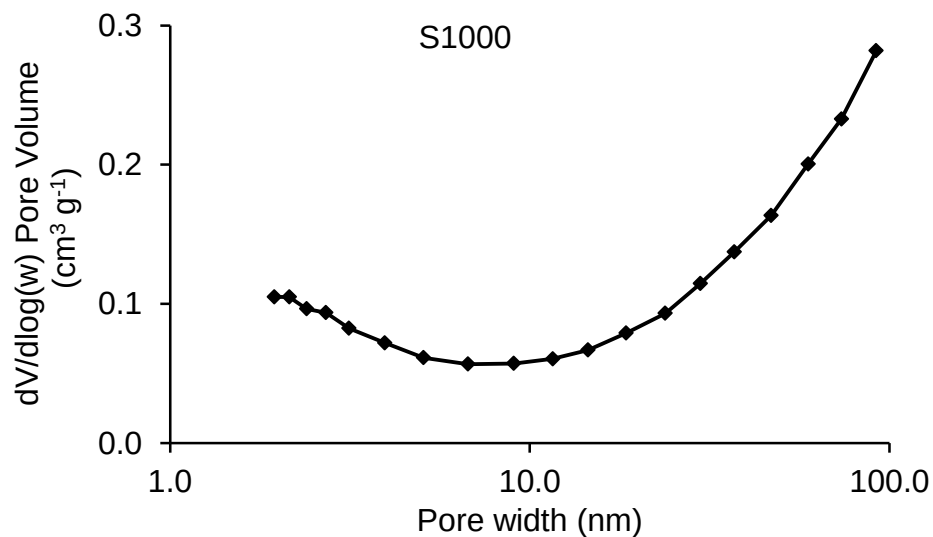


## Nitrogen adsorption isotherm and pore distribution plots for S1000

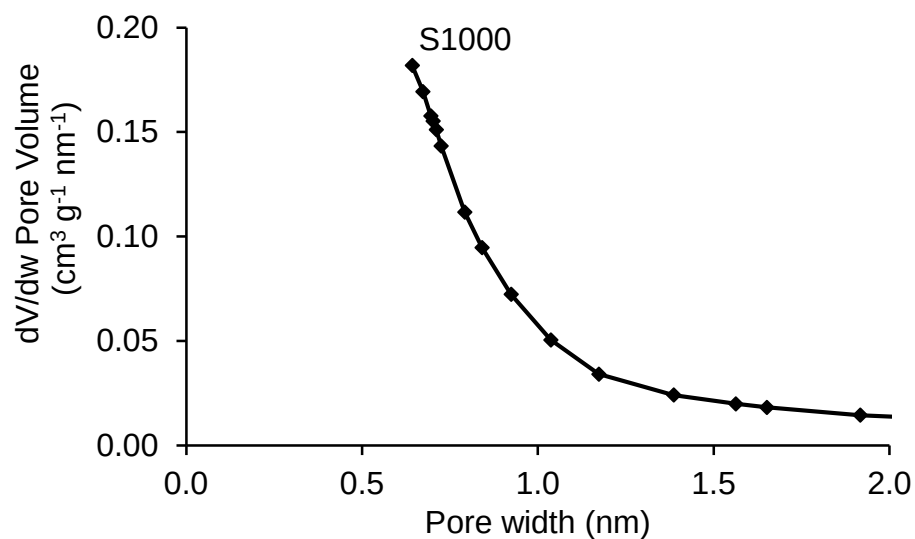
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

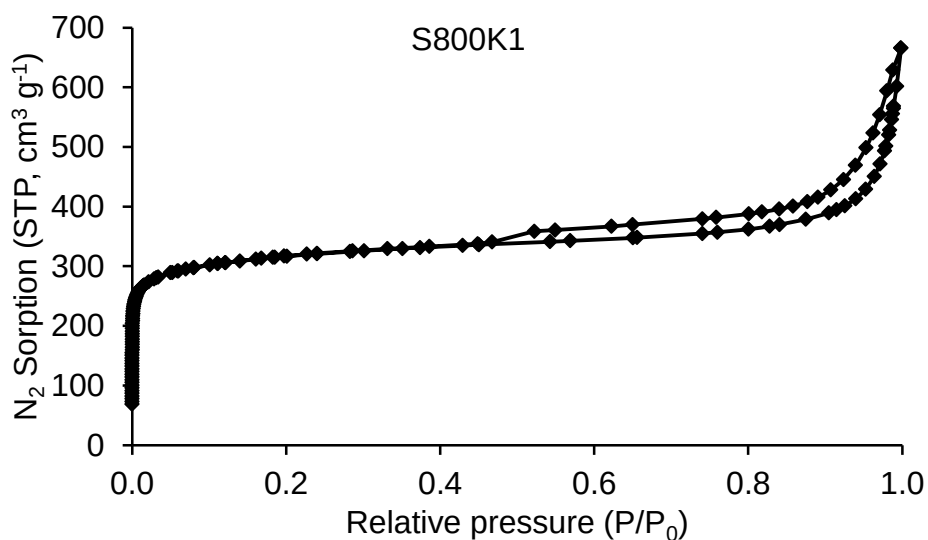


### Pore distribution in the micropore region (HK method)

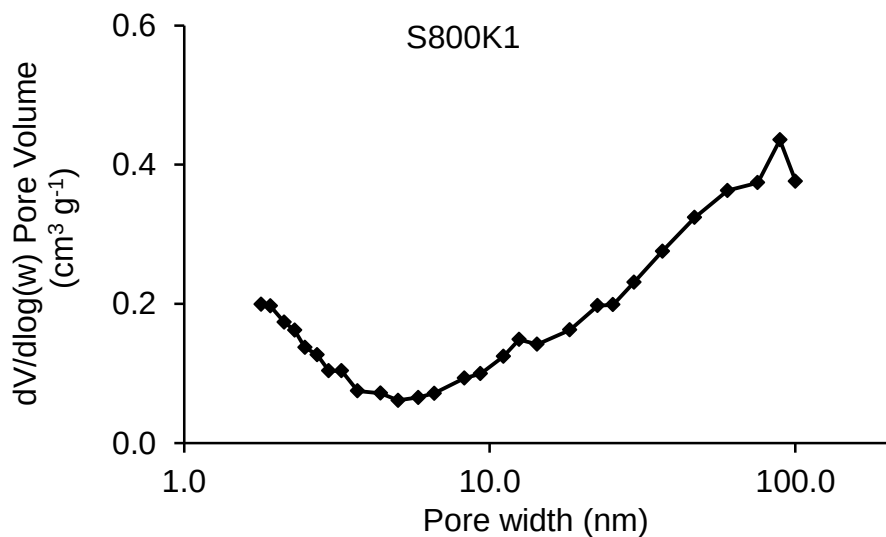


## Nitrogen adsorption isotherm and pore distribution plots for S800K1

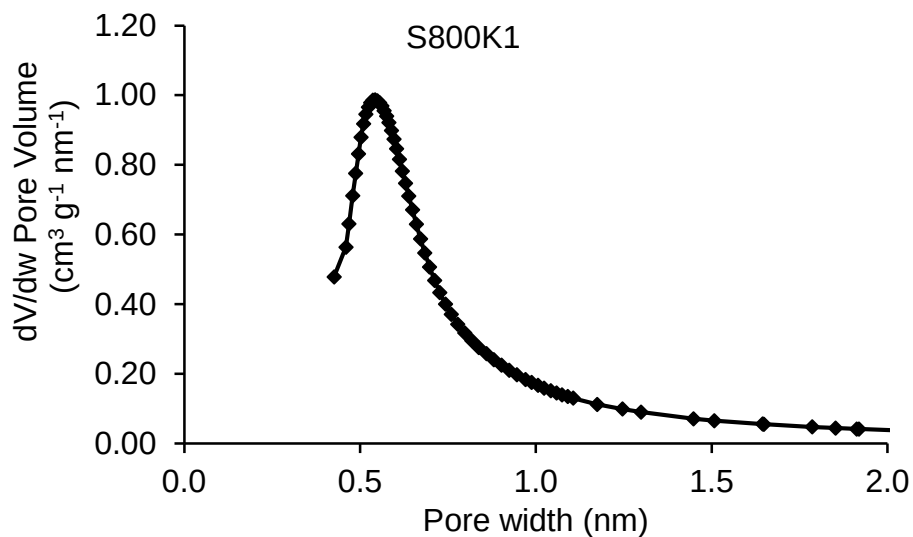
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



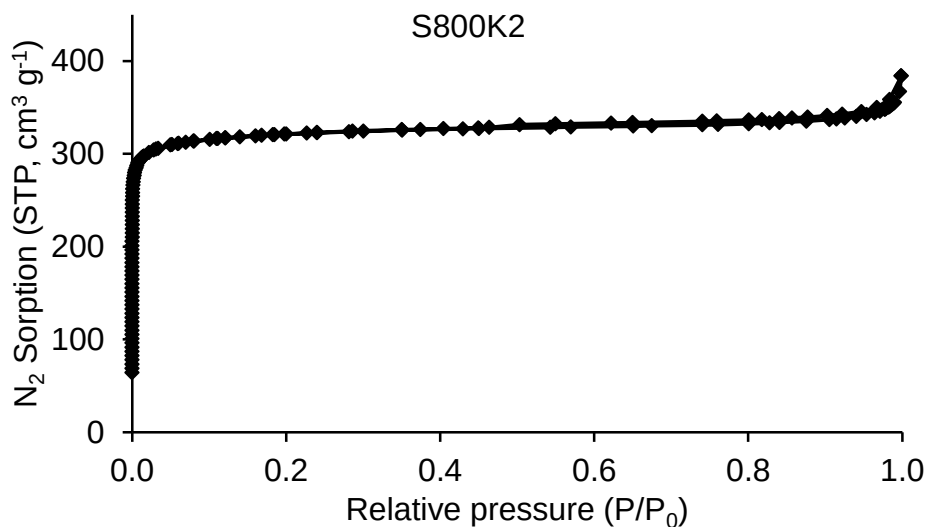
Pore distribution in the micropore region (HK method)



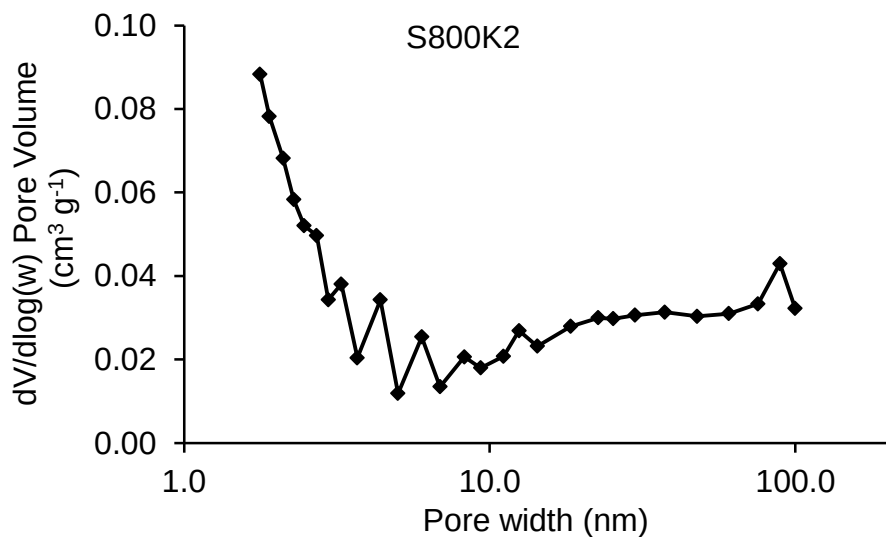


## Nitrogen adsorption isotherm and pore distribution plots for S800K2

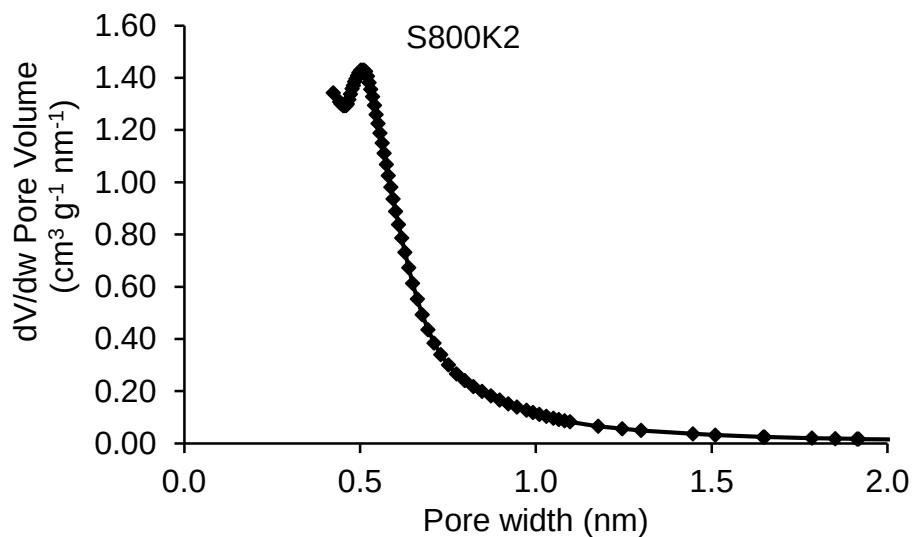
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

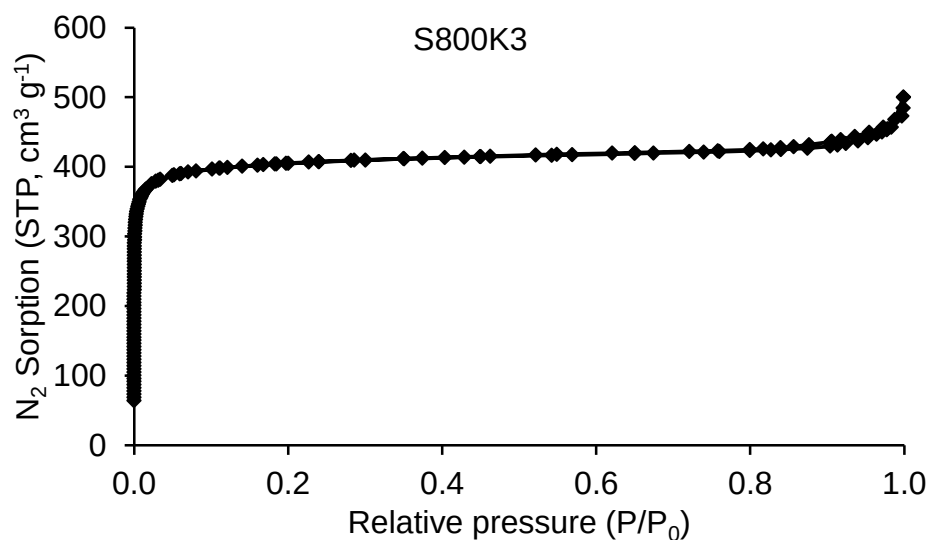


Pore distribution in the micropore region (HK method)

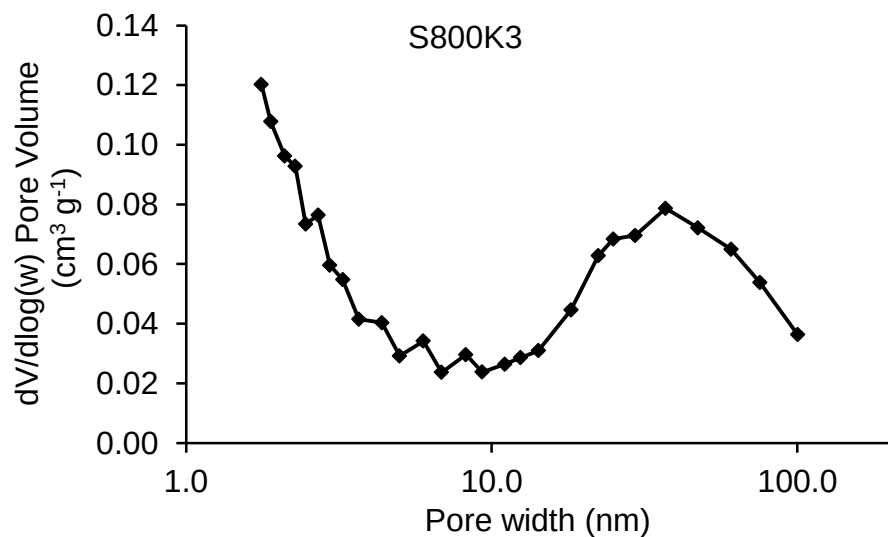


## Nitrogen adsorption isotherm and pore distribution plots for S800K3

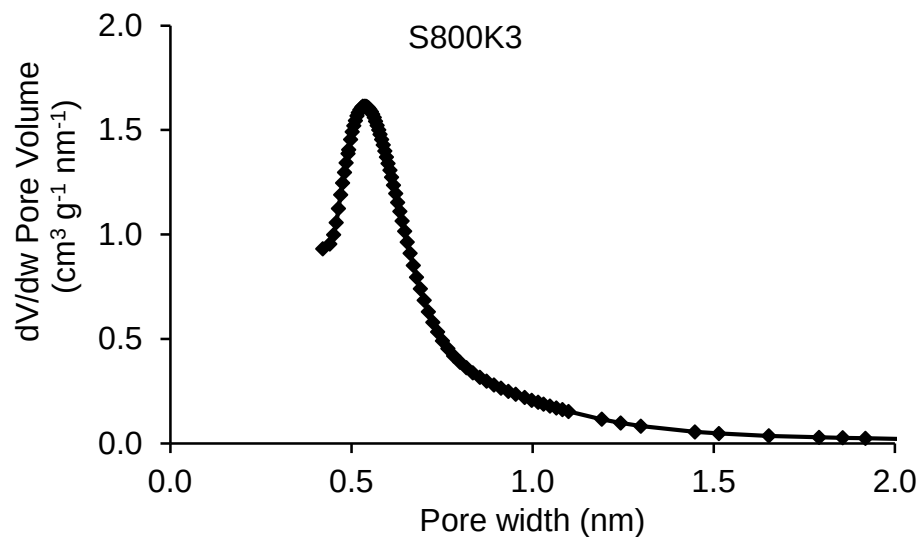
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

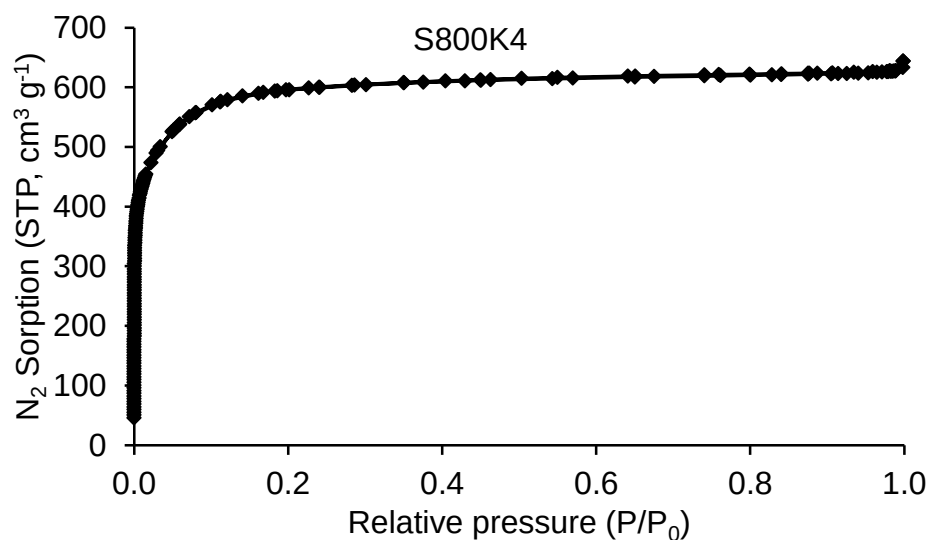


Pore distribution in the micropore region (HK method)

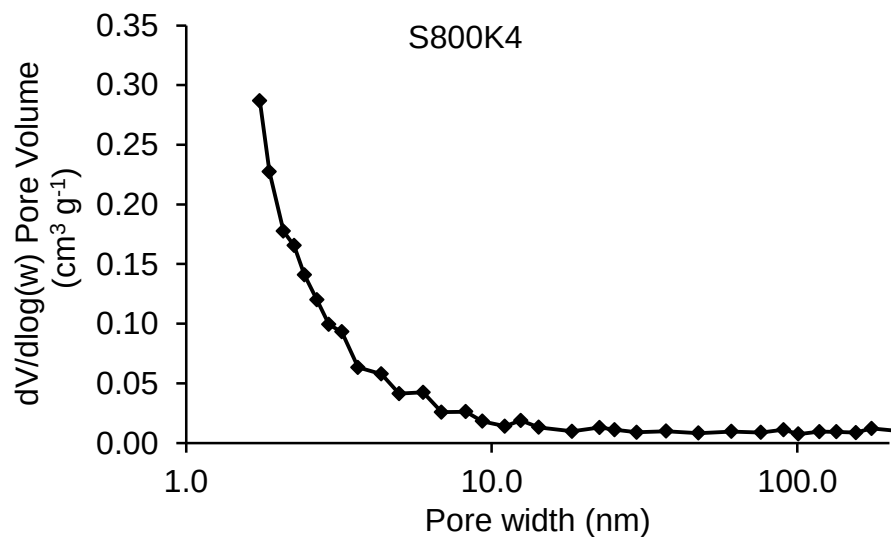


## Nitrogen adsorption isotherm and pore distribution plots for S800K4

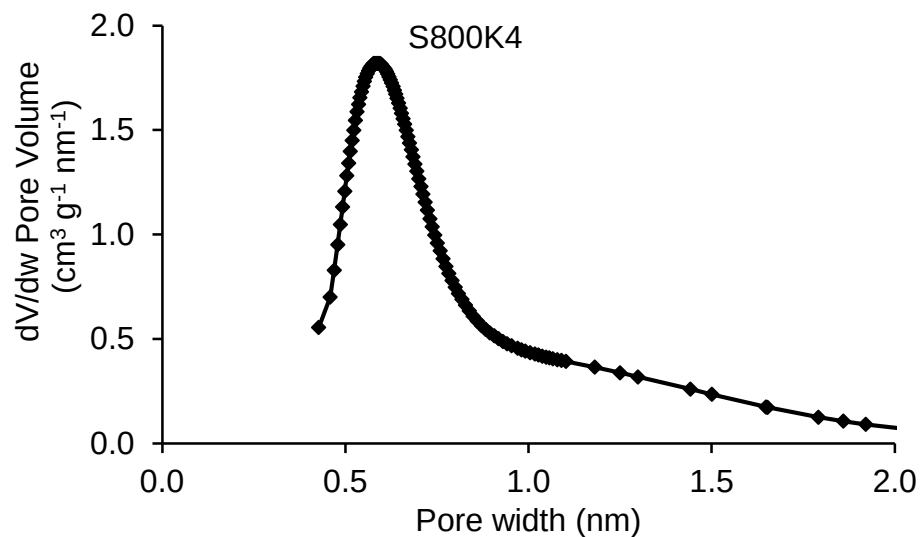
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

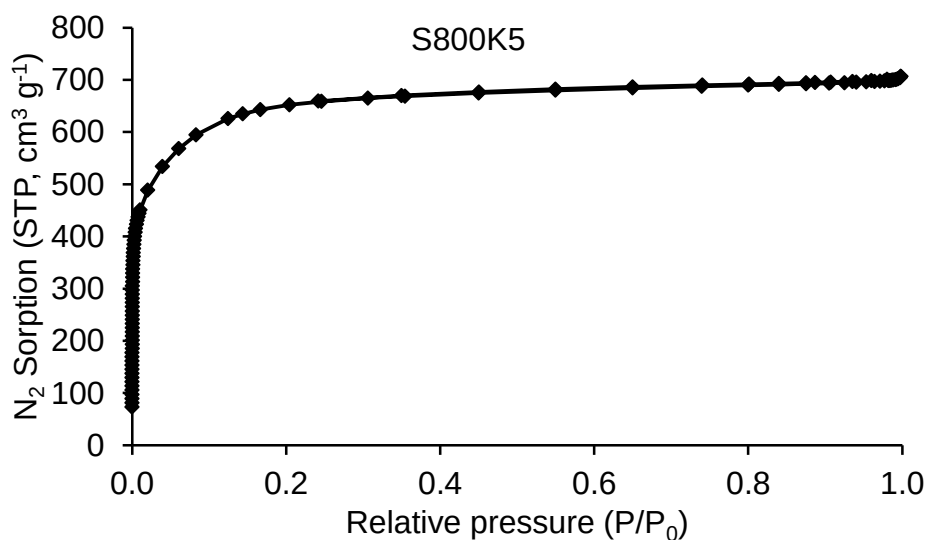


Pore distribution in the micropore region (HK method)

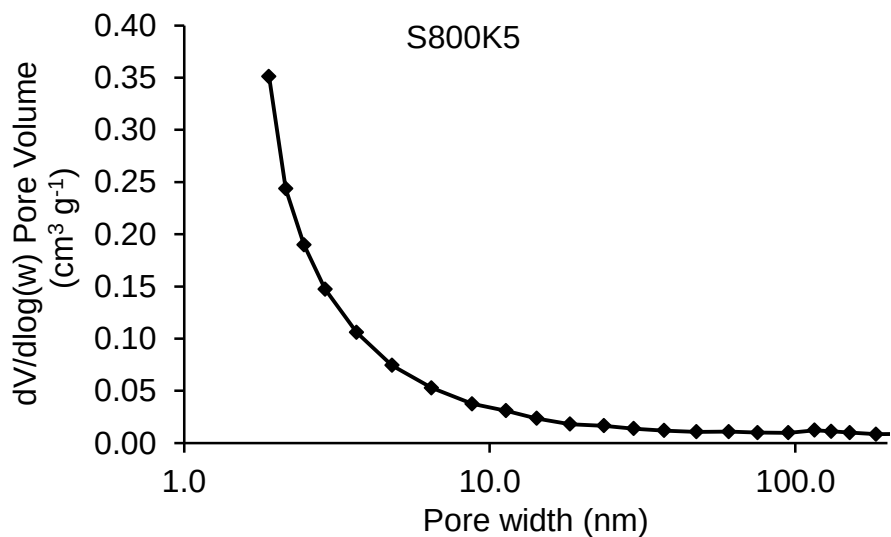


## Nitrogen adsorption isotherm and pore distribution plots for S800K5

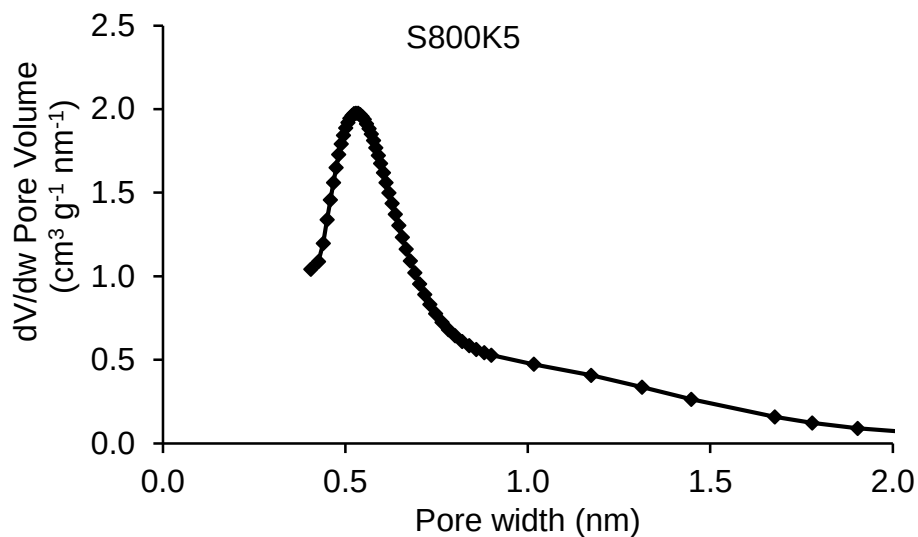
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

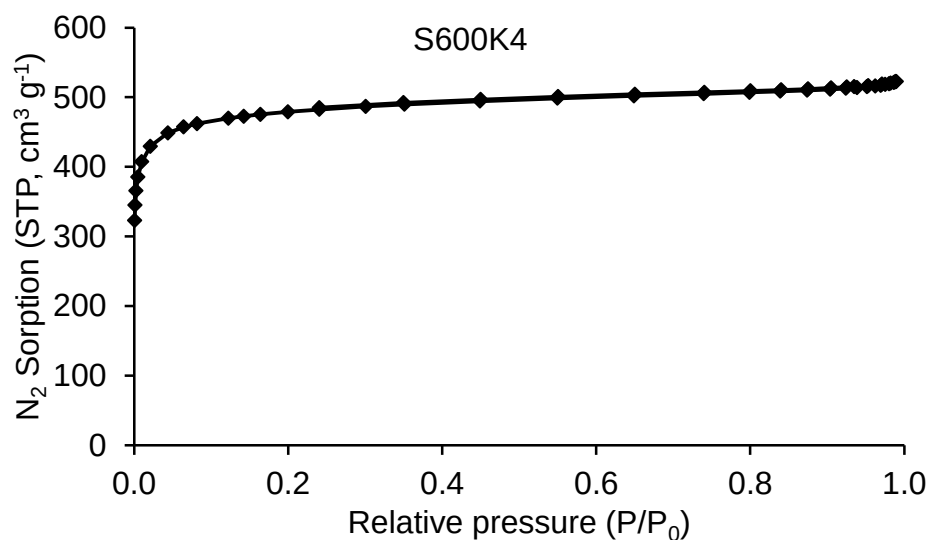


Pore distribution in the micropore region (HK method)

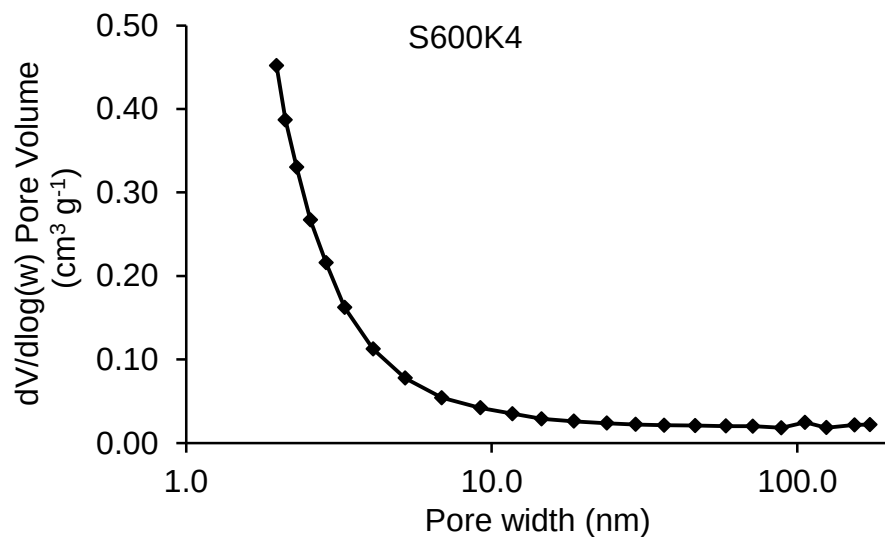


## Nitrogen adsorption isotherm and pore distribution plots for S600K4

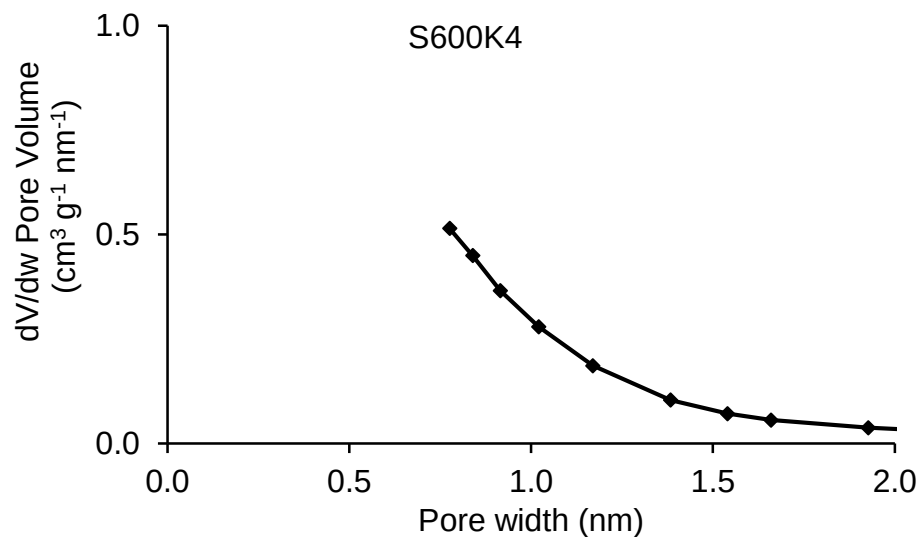
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

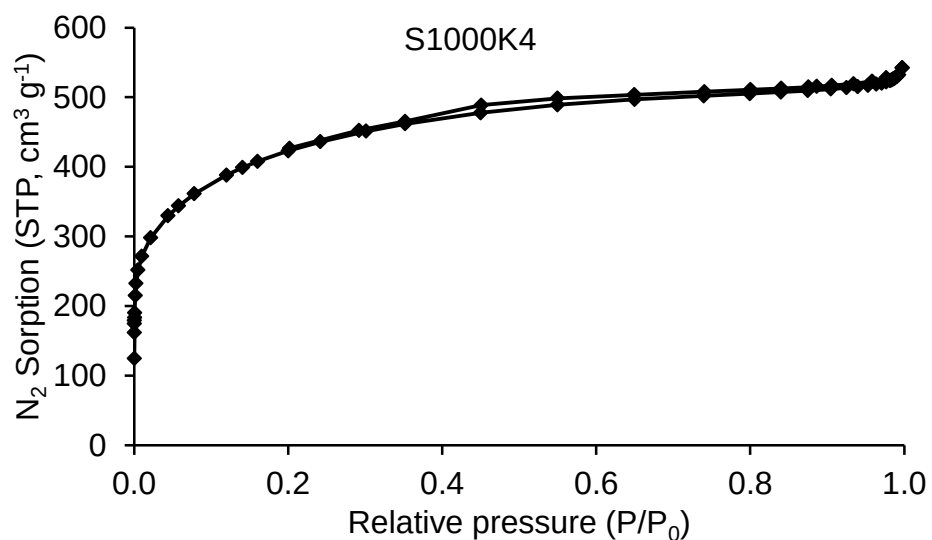


Pore distribution in the micropore region (HK method)

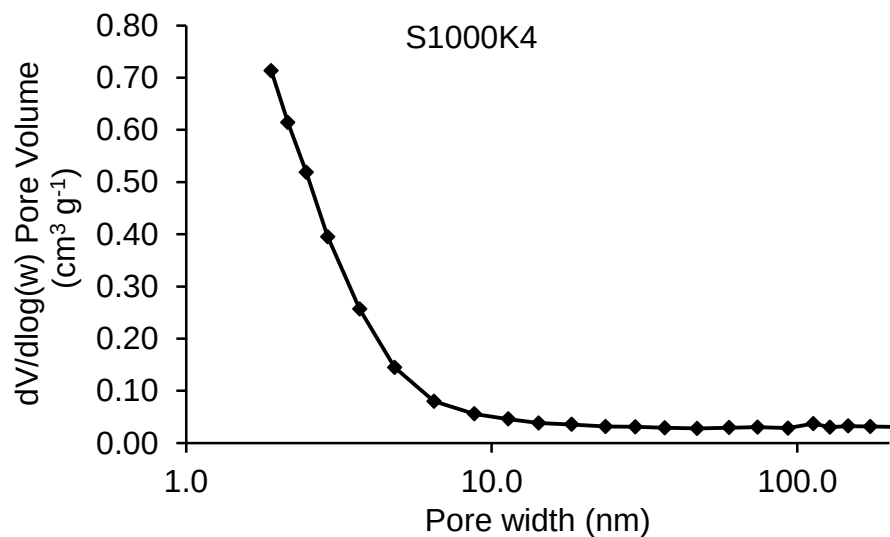


## Nitrogen adsorption isotherm and pore distribution plots for S1000K4

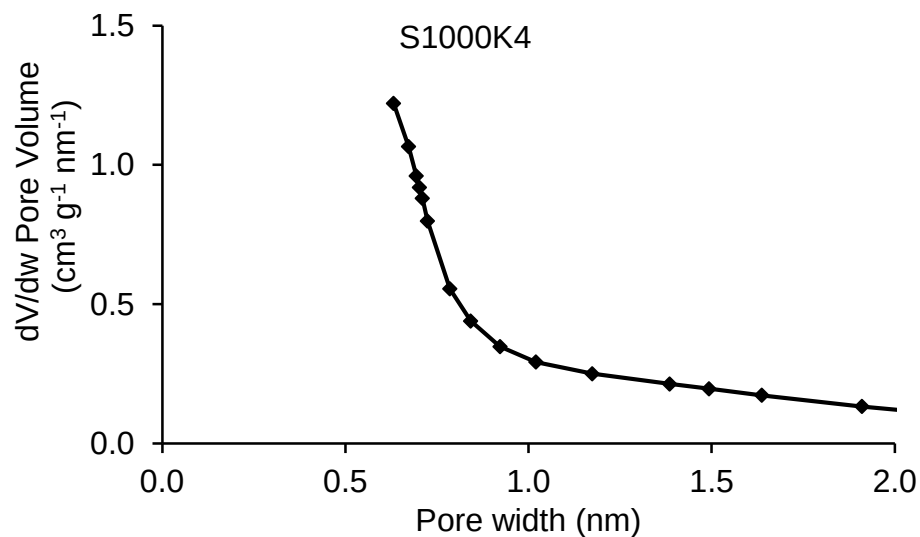
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

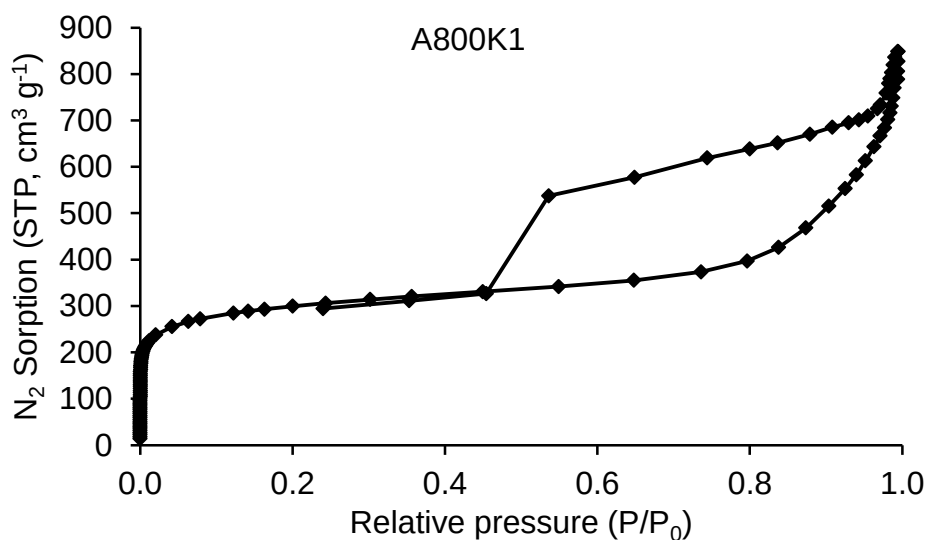


Pore distribution in the micropore region (HK method)

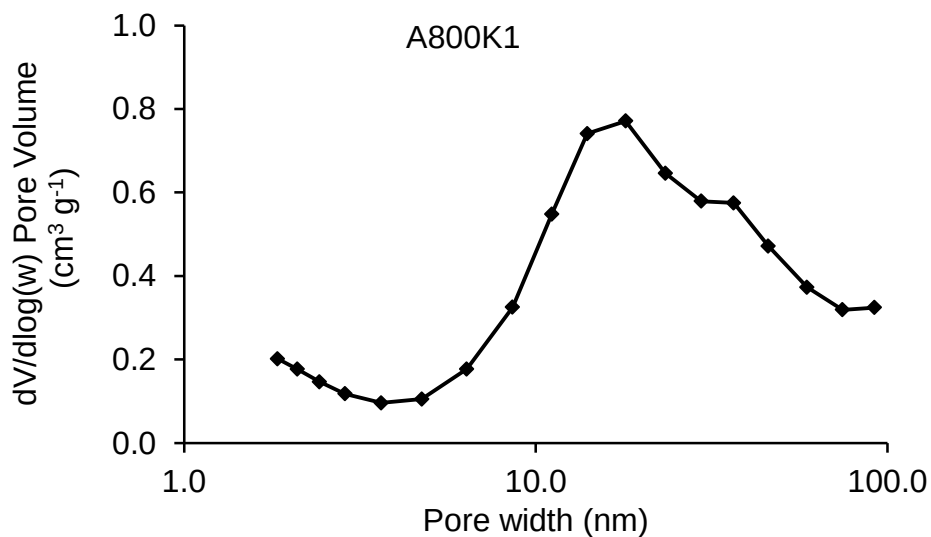


## Nitrogen adsorption isotherm and pore distribution plots for A800K1

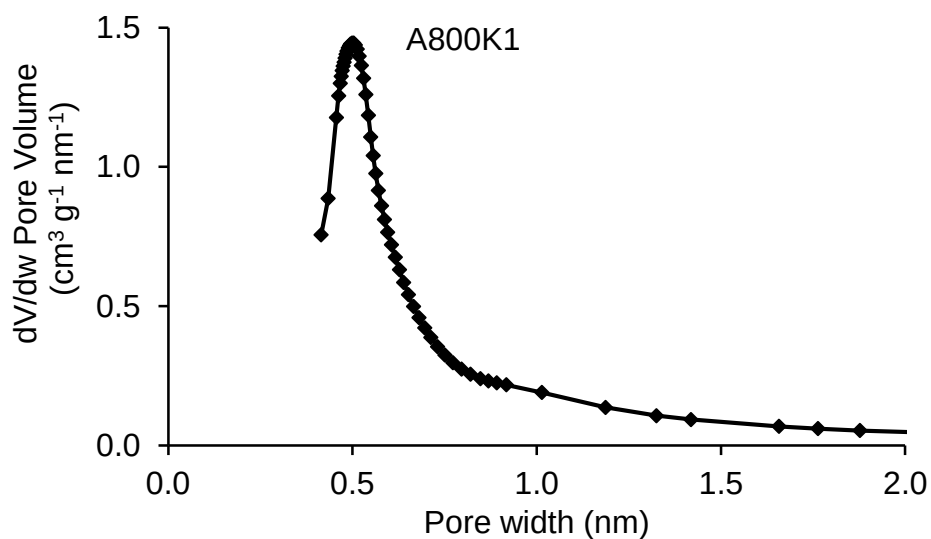
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

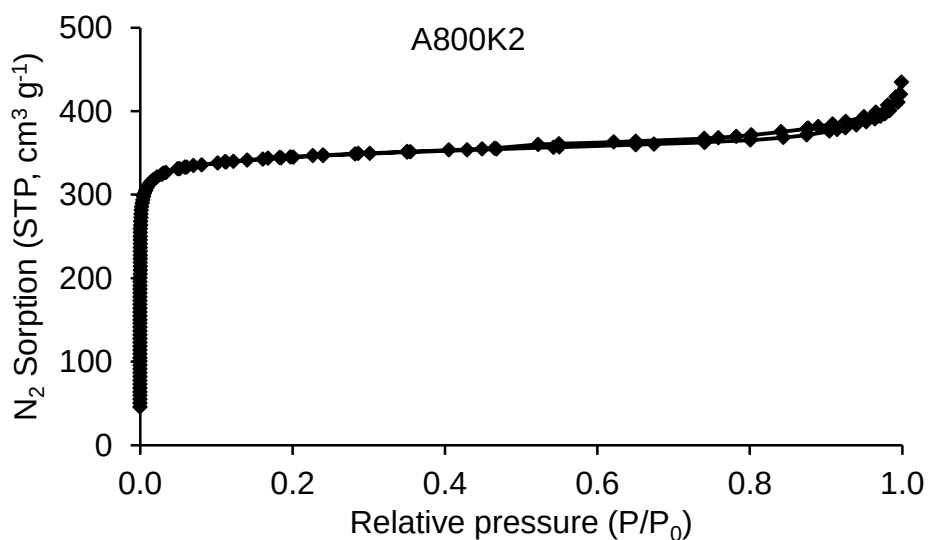


Pore distribution in the micropore region (HK method)

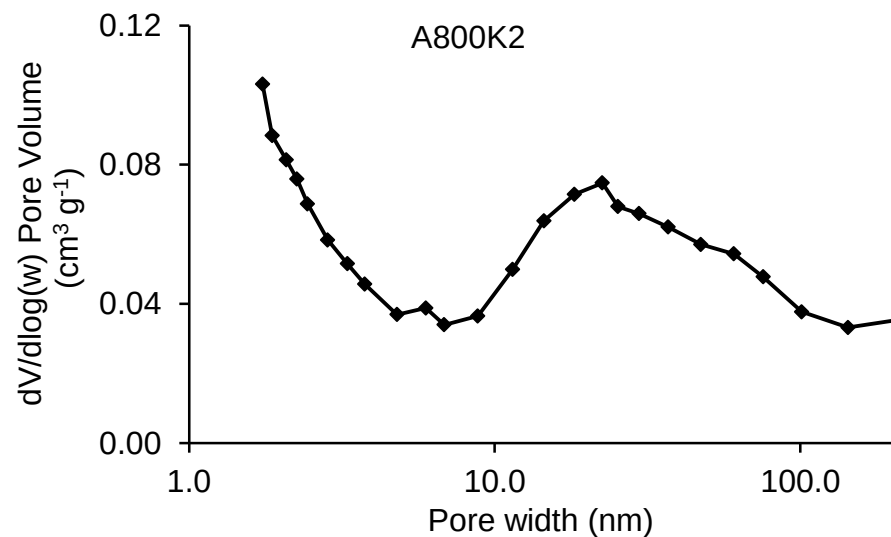


## Nitrogen adsorption isotherm and pore distribution plots for A800K2

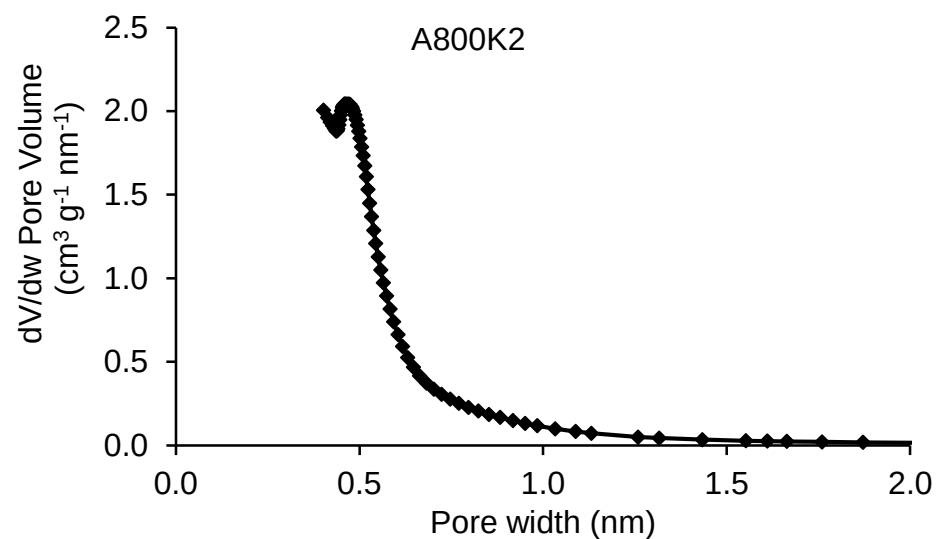
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



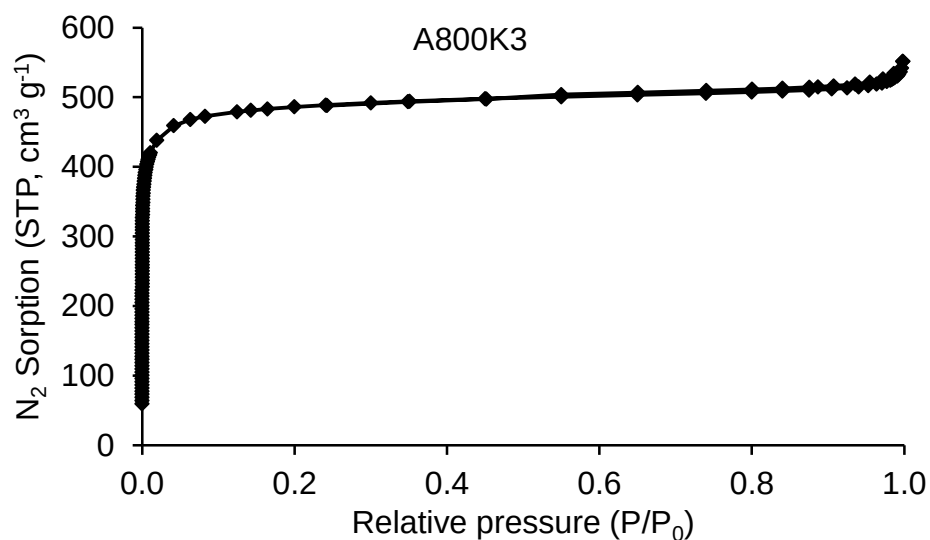
Pore distribution in the micropore region (HK method)



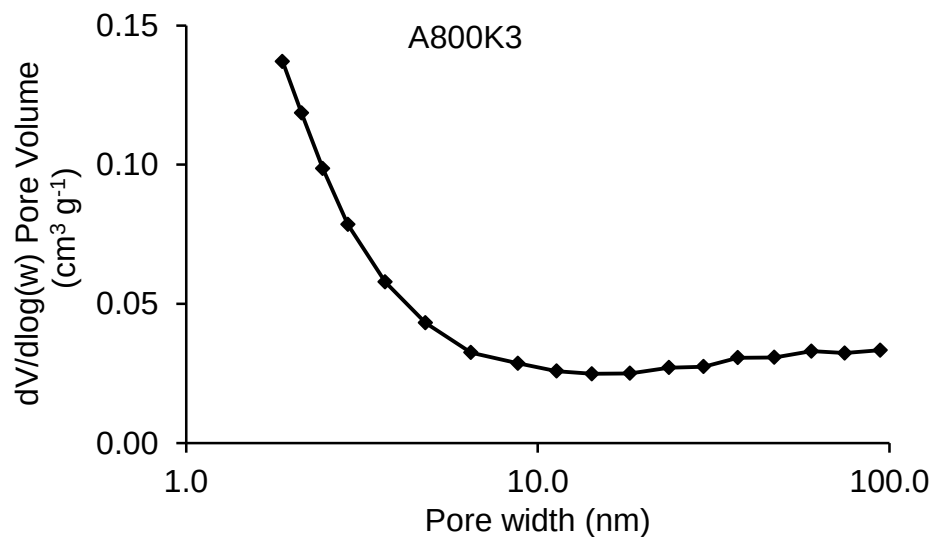


## Nitrogen adsorption isotherm and pore distribution plots for A800K3

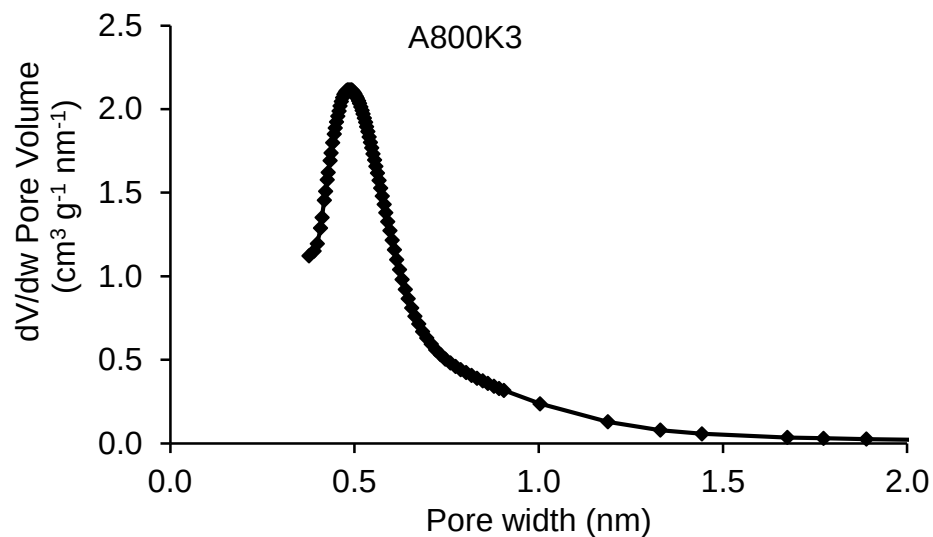
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

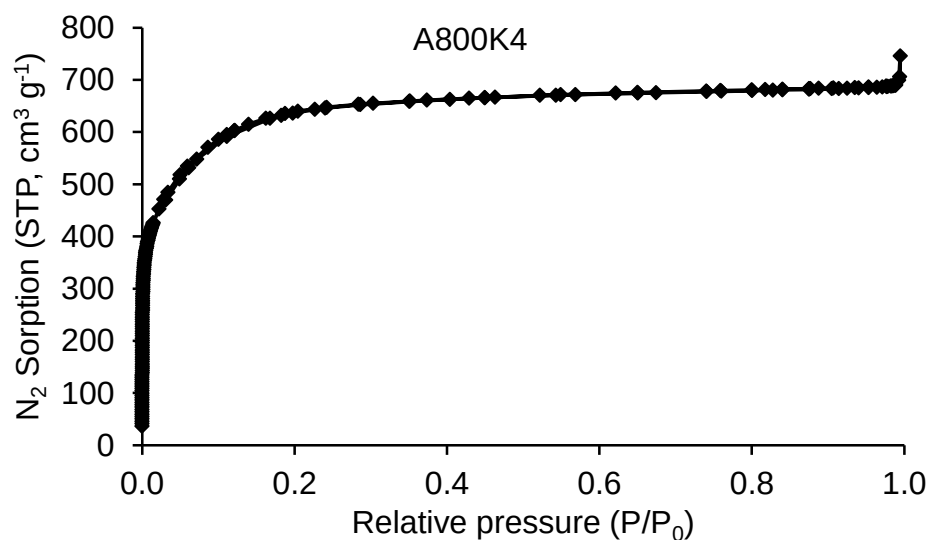


Pore distribution in the micropore region (HK method)

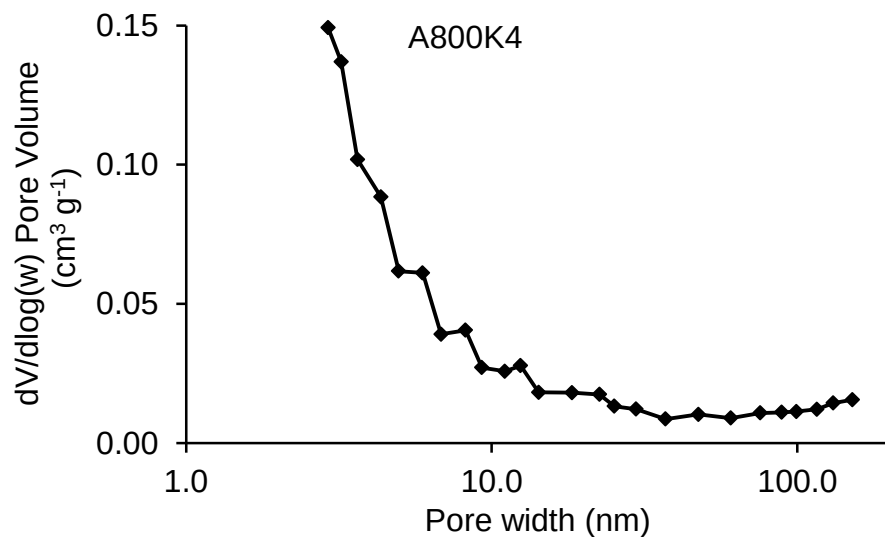


## Nitrogen adsorption isotherm and pore distribution plots for A800K4

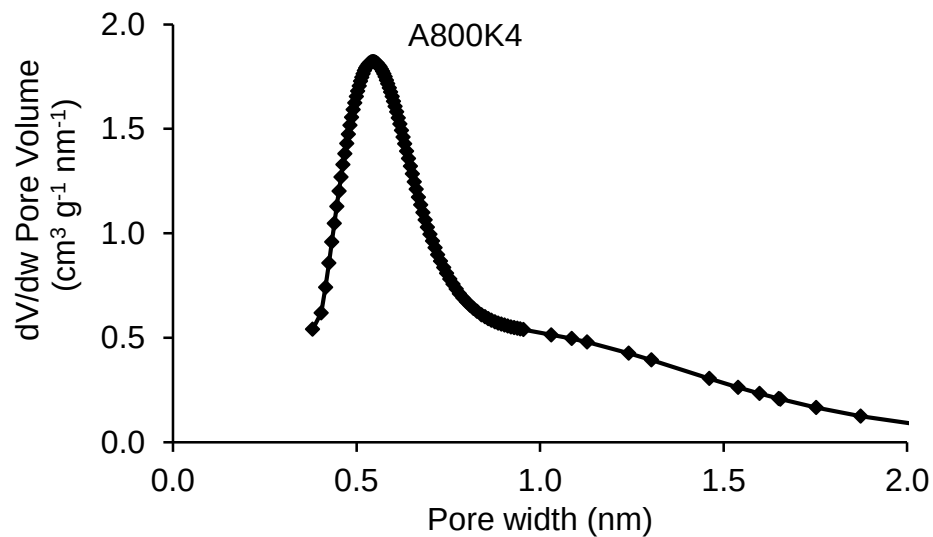
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

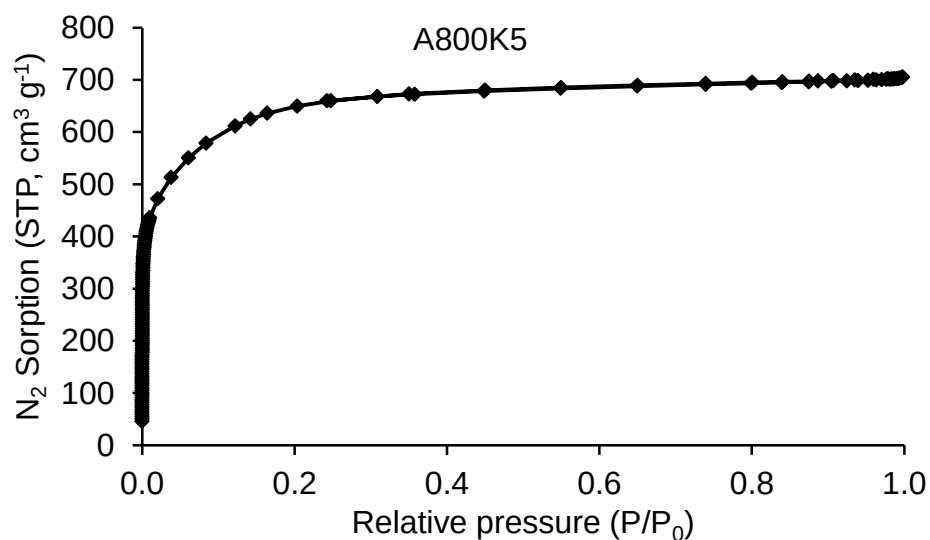


Pore distribution in the micropore region (HK method)

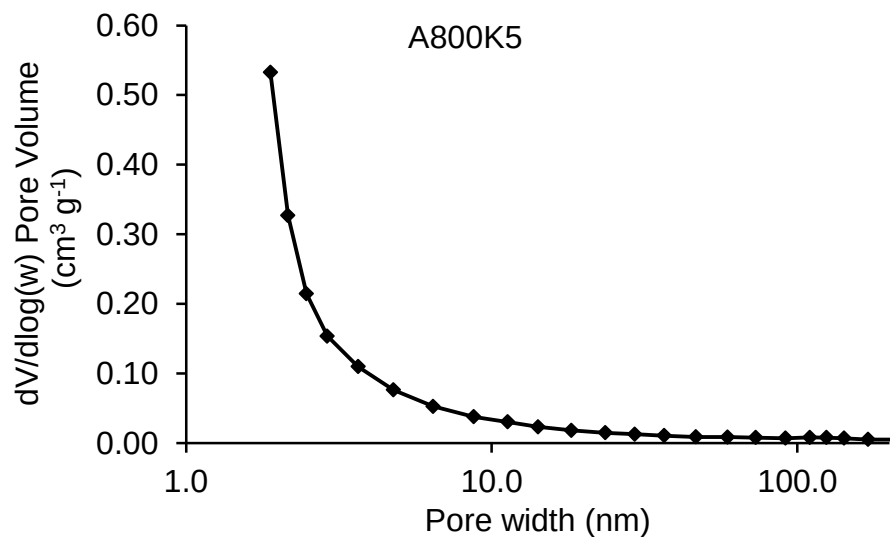


## Nitrogen adsorption isotherm and pore distribution plots for A800K5

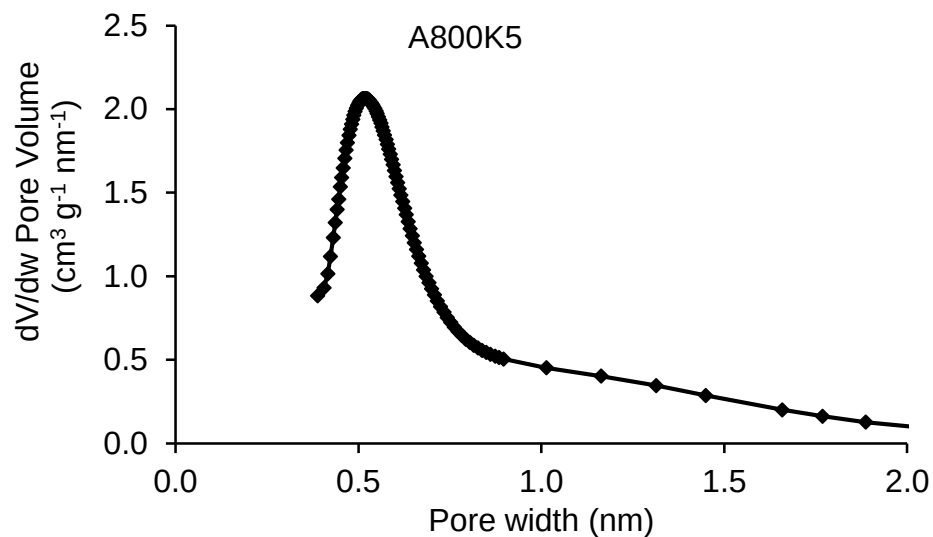
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

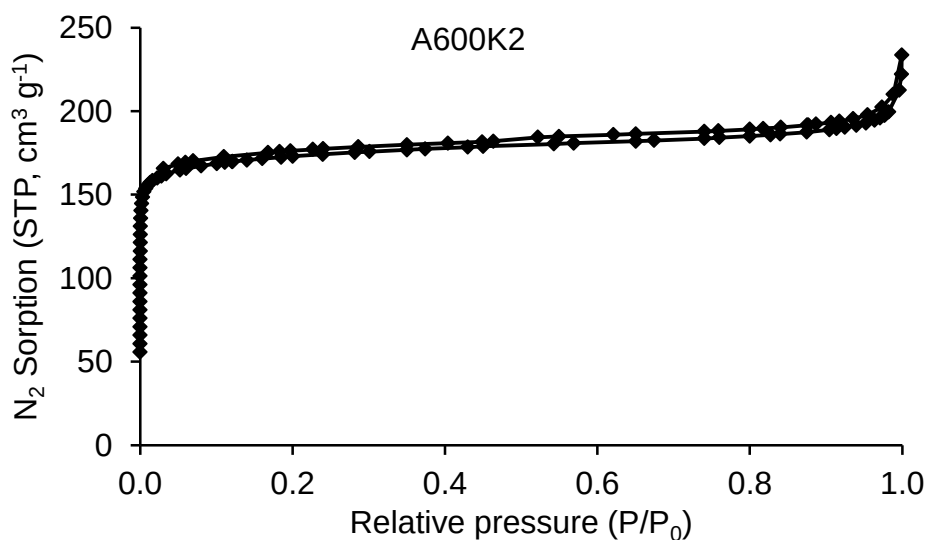


Pore distribution in the micropore region (HK method)

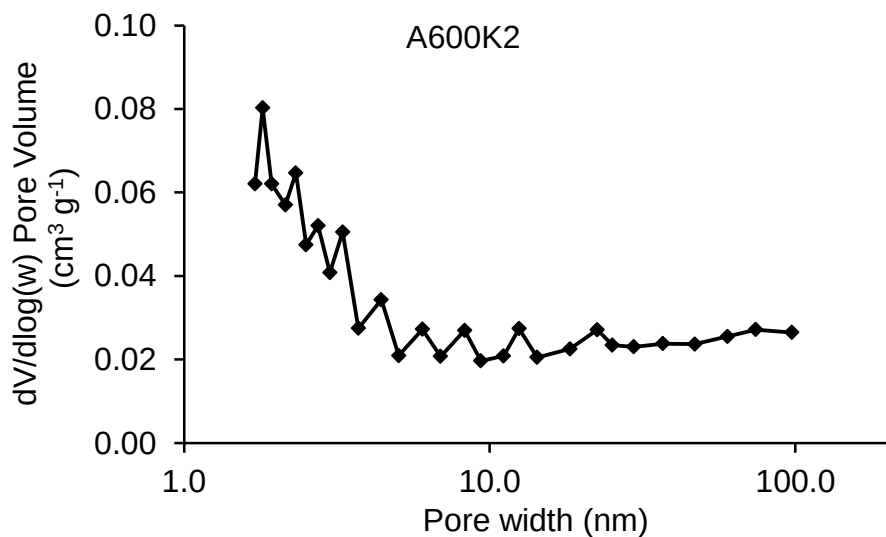


## Nitrogen adsorption isotherm and pore distribution plots for A600K2

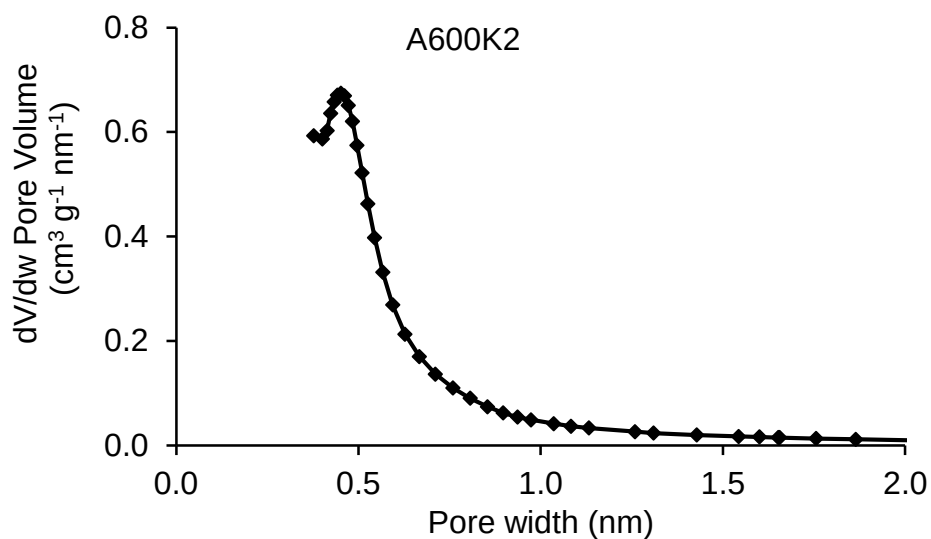
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

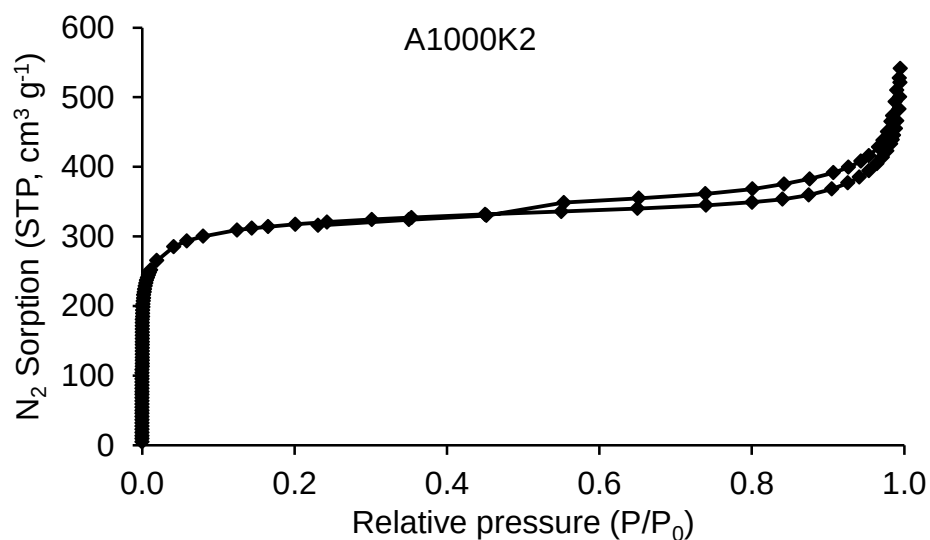


Pore distribution in the micropore region (HK method)

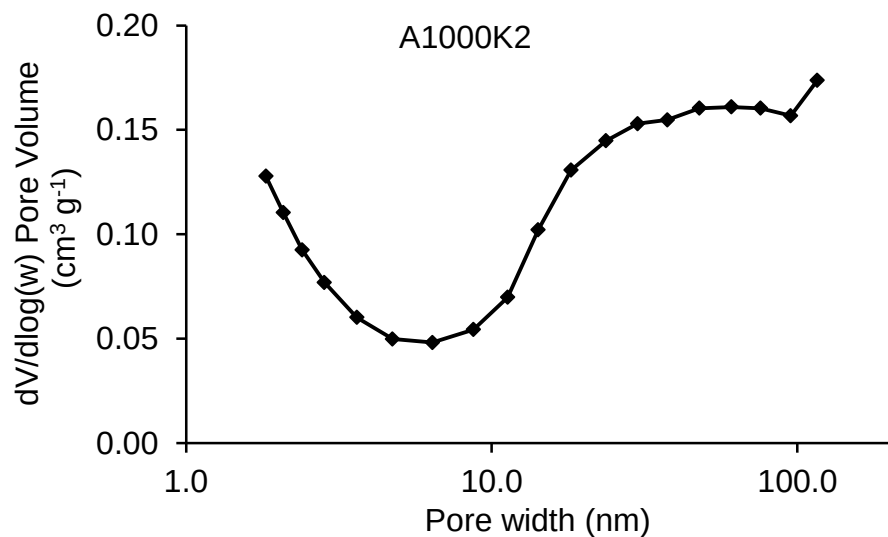


## Nitrogen adsorption isotherm and pore distribution plots for A1000K2

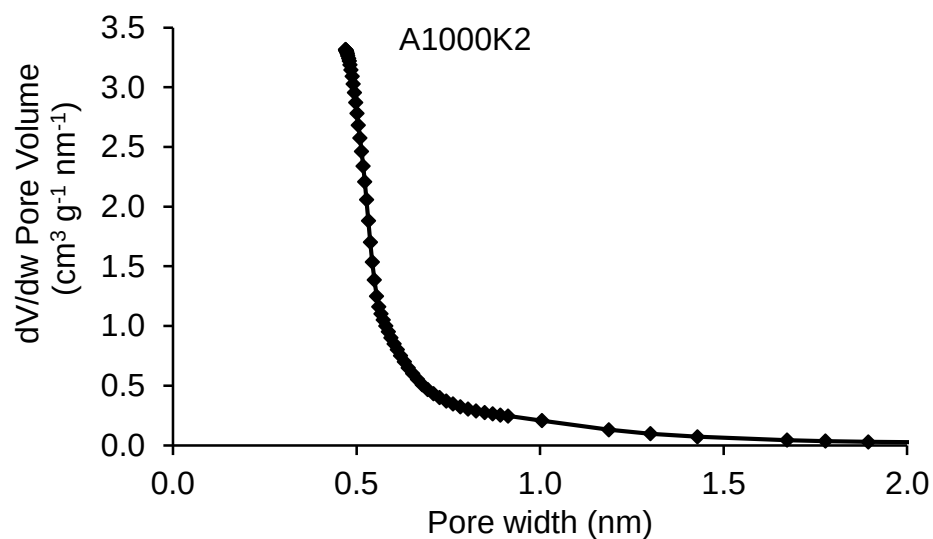
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

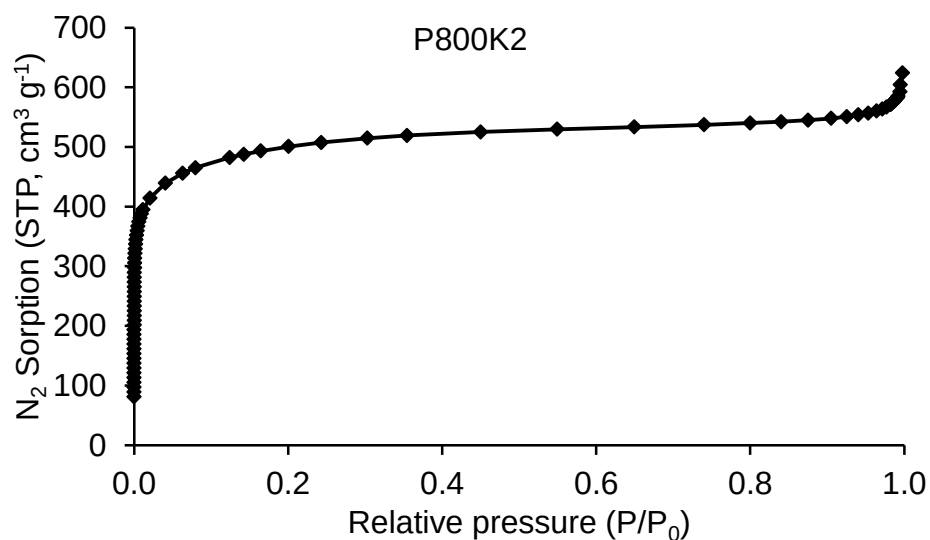


Pore distribution in the micropore region (HK method)

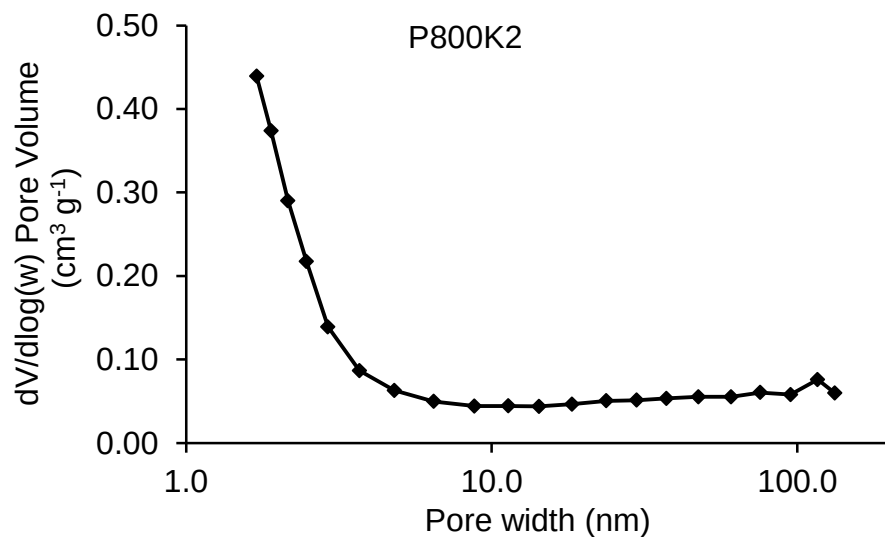


## Nitrogen adsorption isotherm and pore distribution plots for P800K2

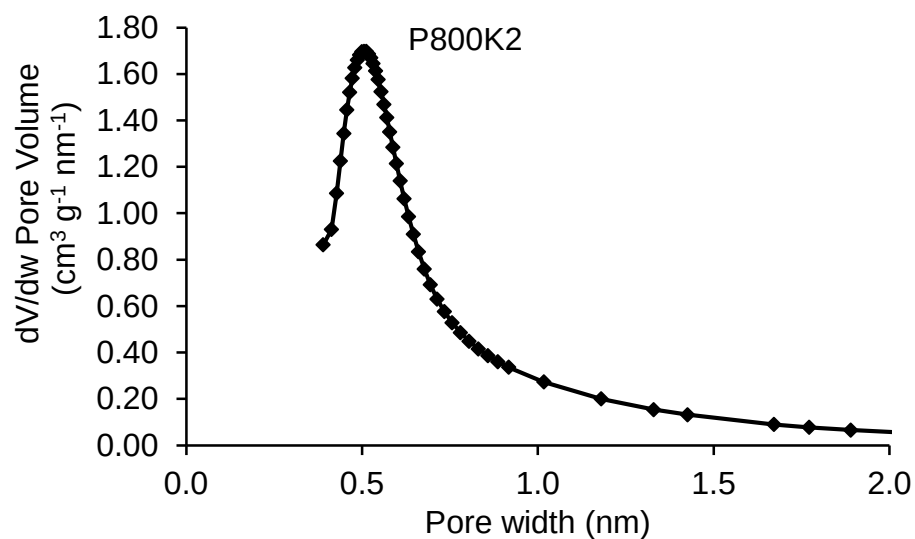
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

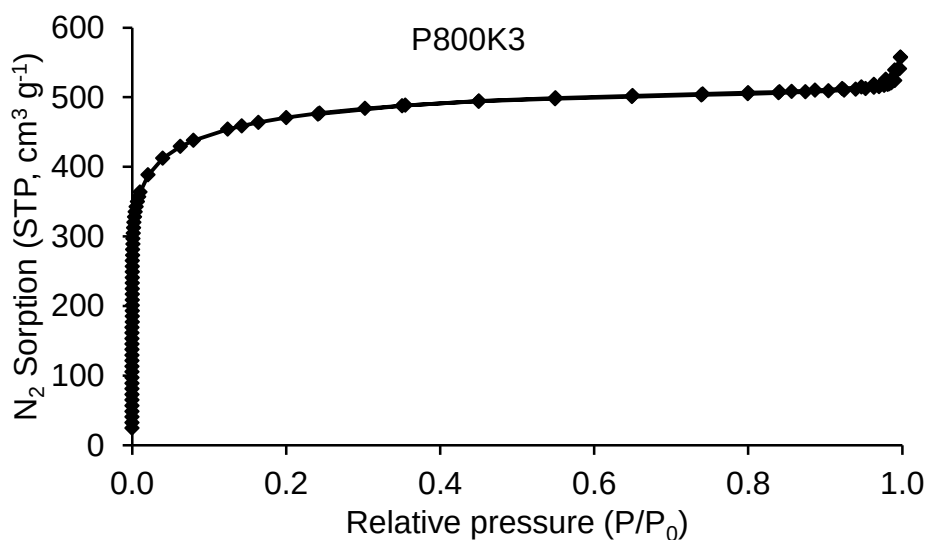


Pore distribution in the micropore region (HK method)

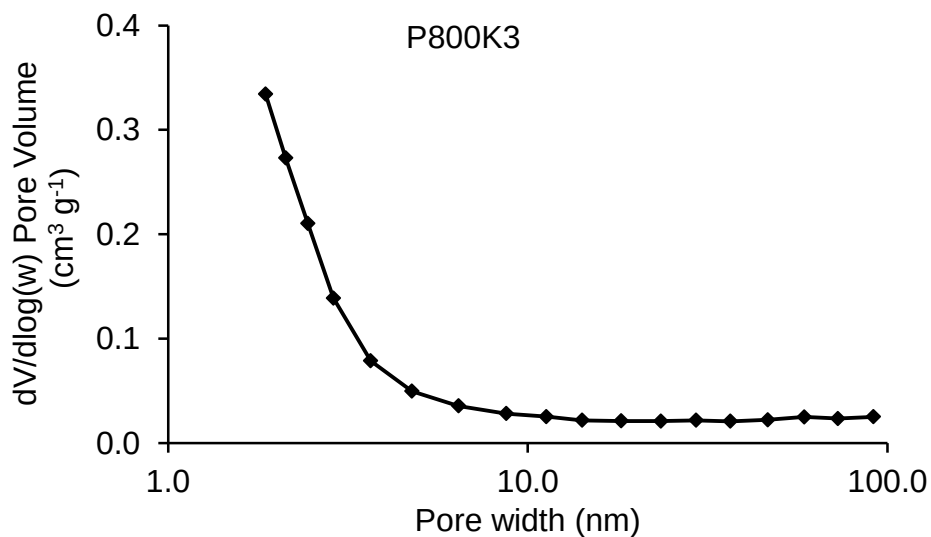


## Nitrogen adsorption isotherm and pore distribution plots for P800K3

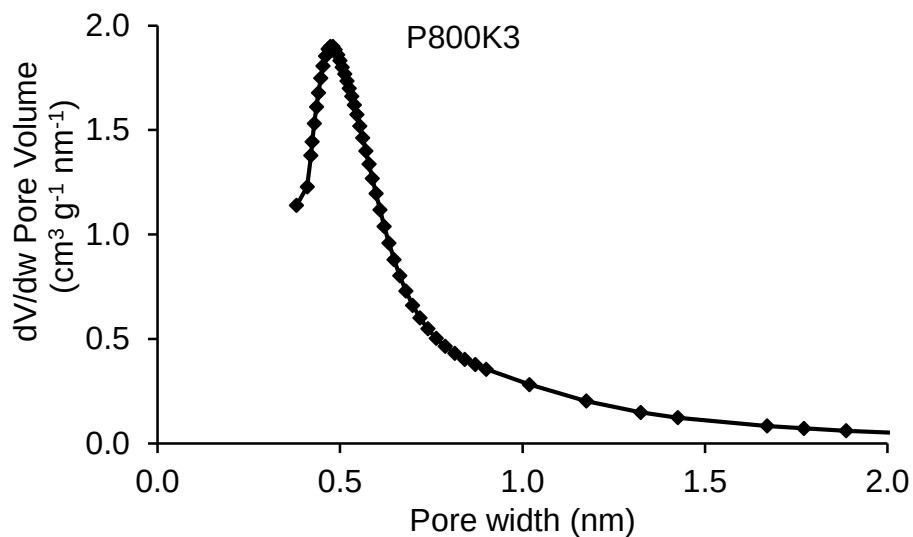
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

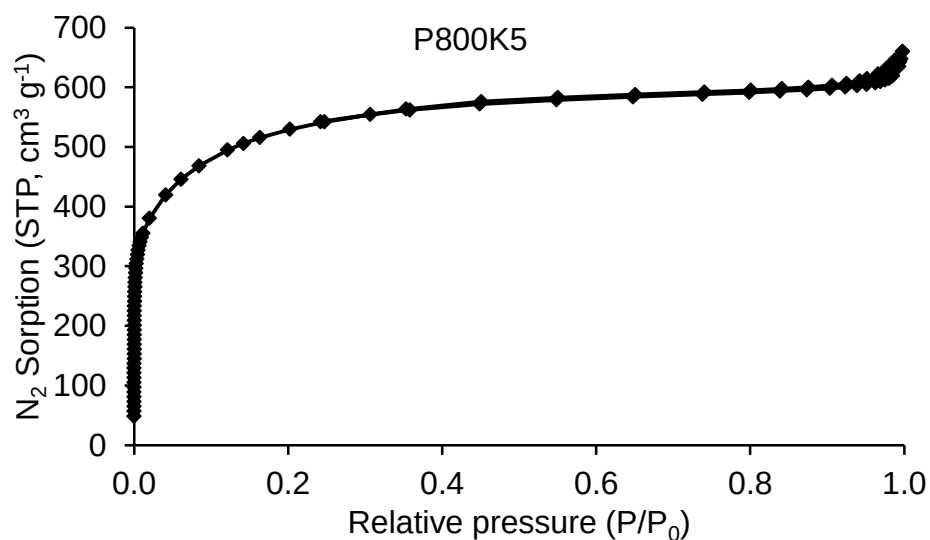


Pore distribution in the micropore region (HK method)

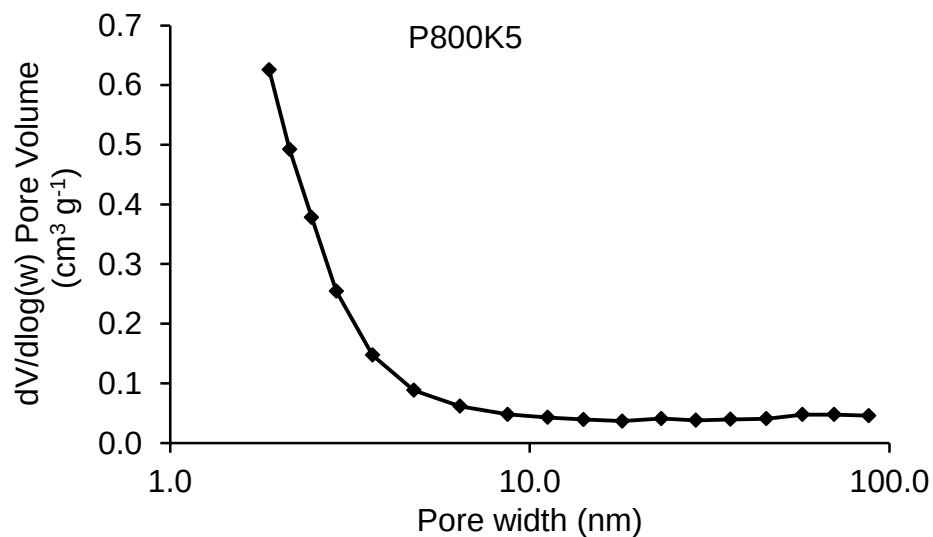


## Nitrogen adsorption isotherm and pore distribution plots for P800K5

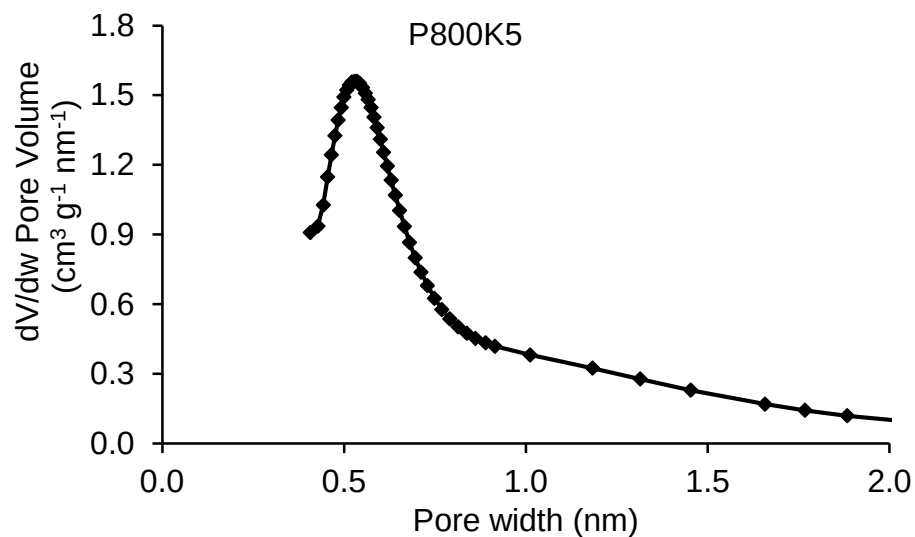
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



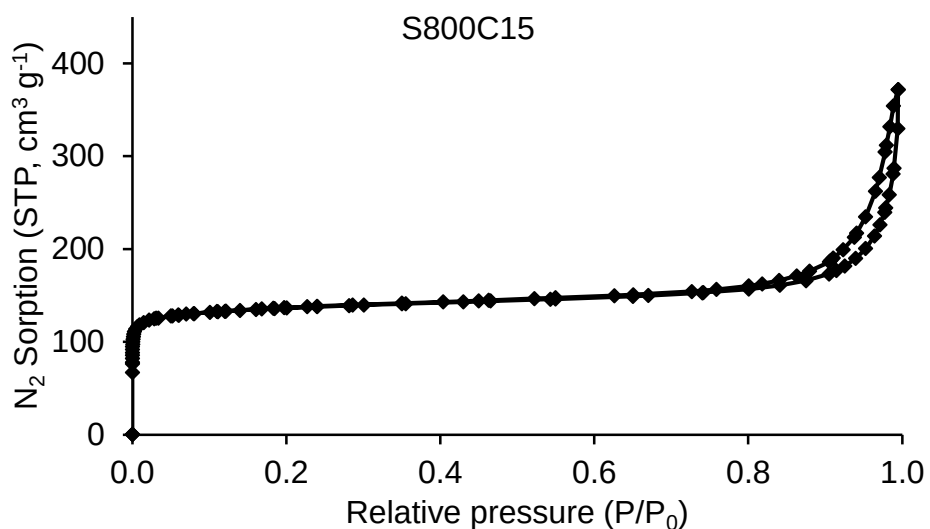
Pore distribution in the micropore region (HK method)



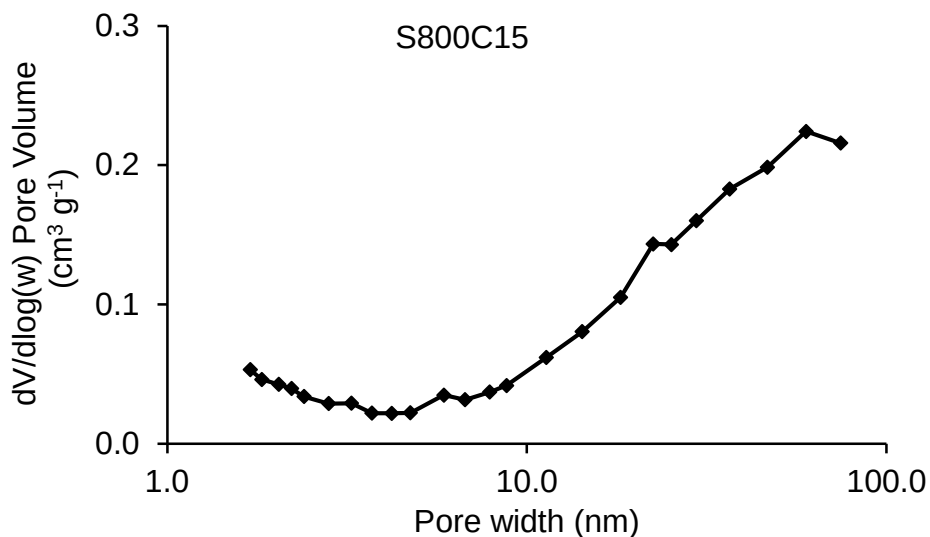


## Nitrogen adsorption isotherm and pore distribution plots for S800C15

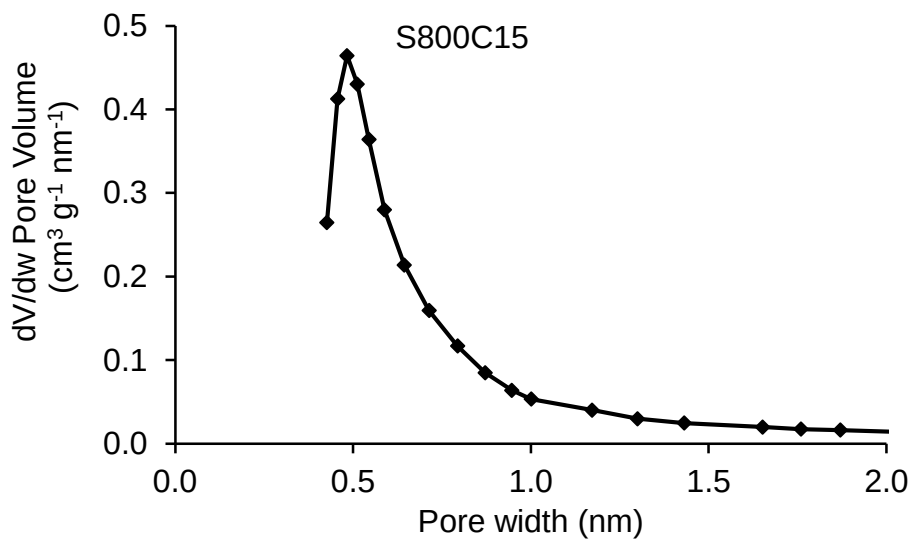
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

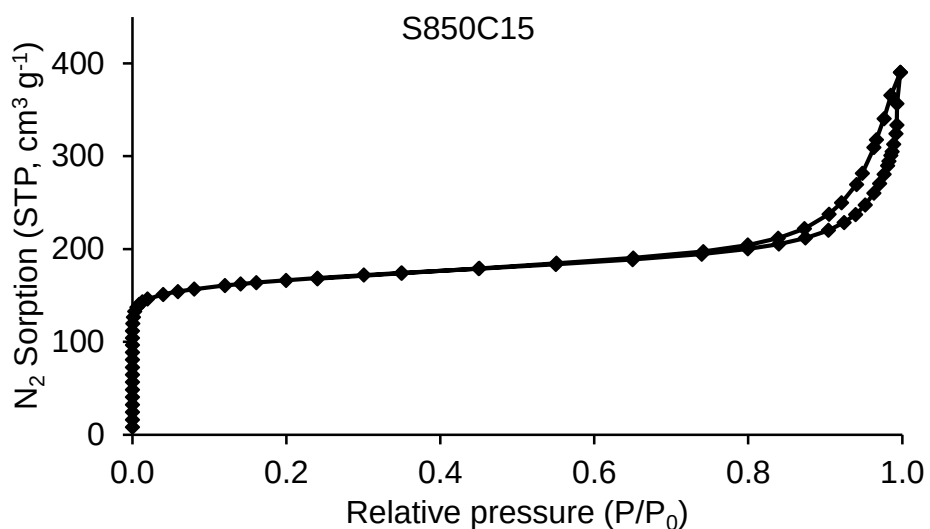


### Pore distribution in the micropore region (HK method)

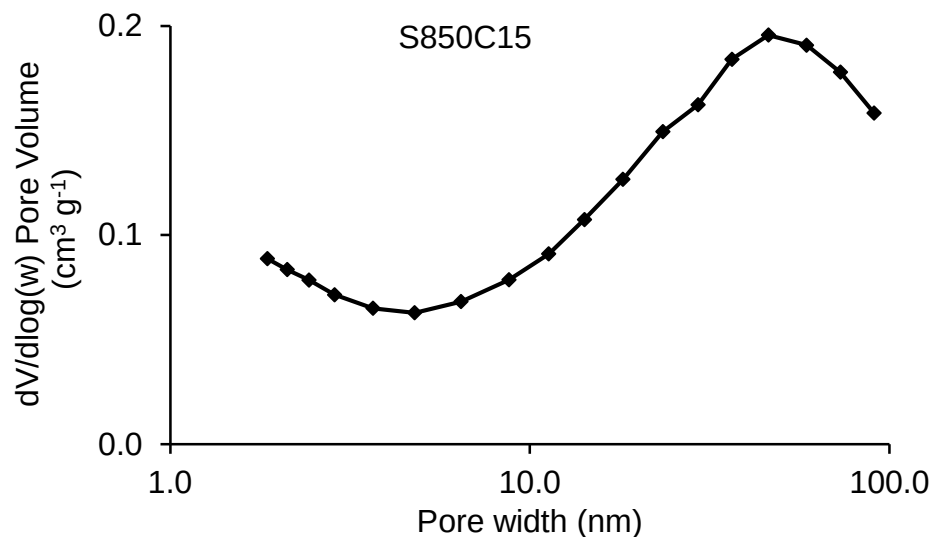


## Nitrogen adsorption isotherm and pore distribution plots for S850C15

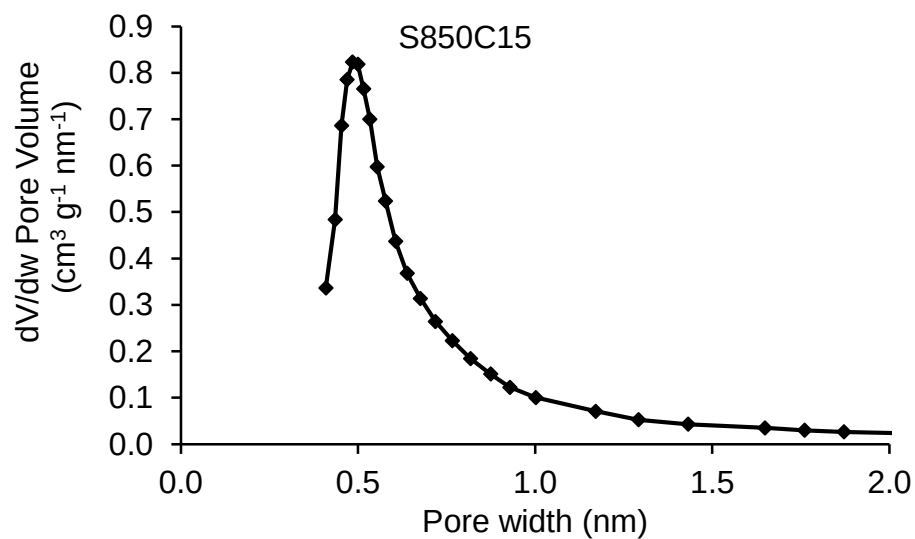
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

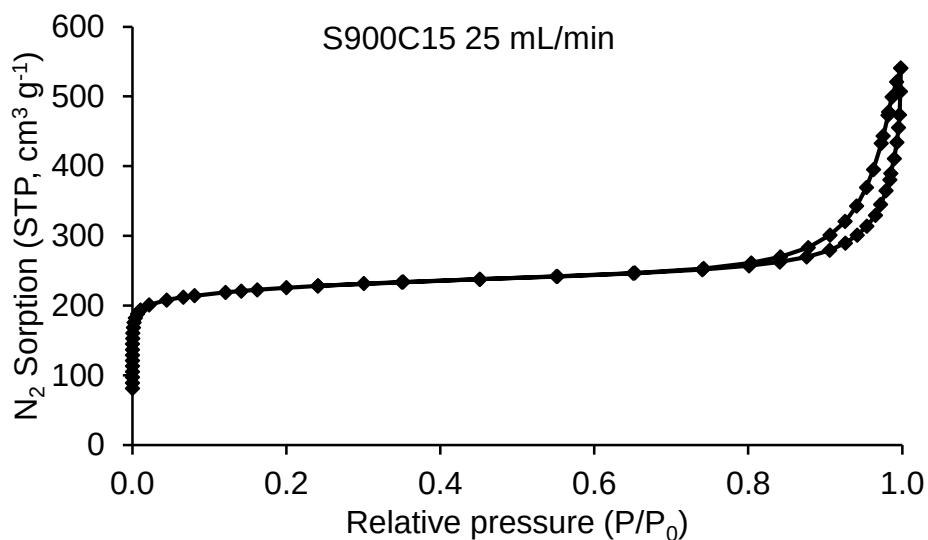


### Pore distribution in the micropore region (HK method)

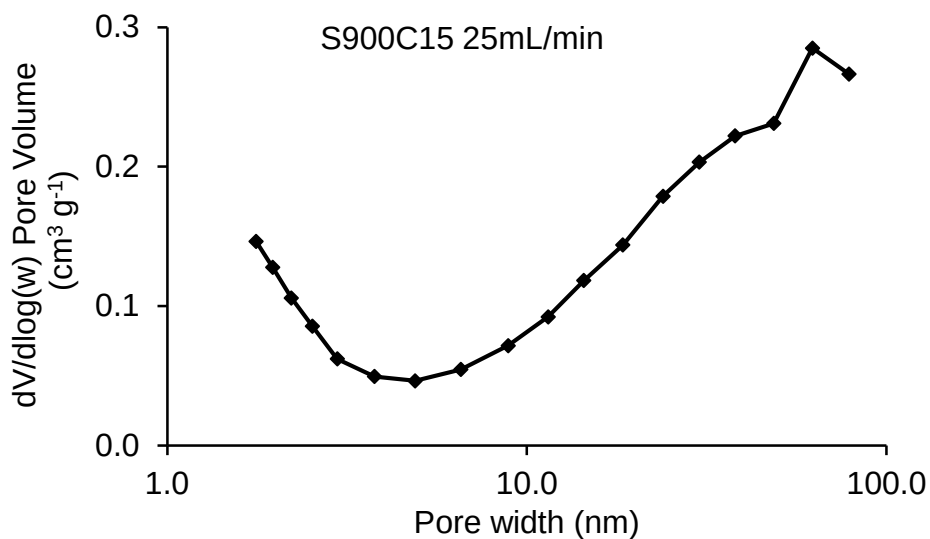


**Nitrogen adsorption isotherm and pore distribution plots for S900C15 with a CO<sub>2</sub> flow rate of 25 mL min<sup>-1</sup>**

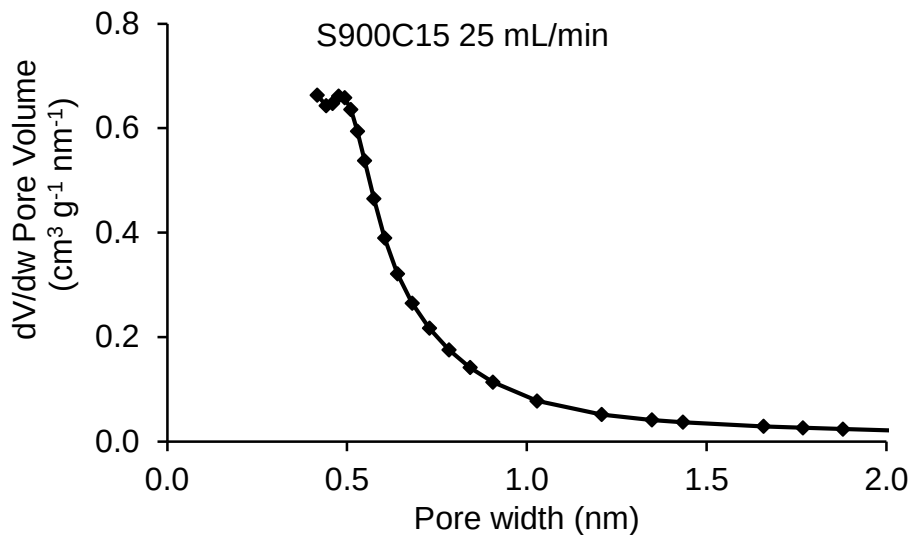
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

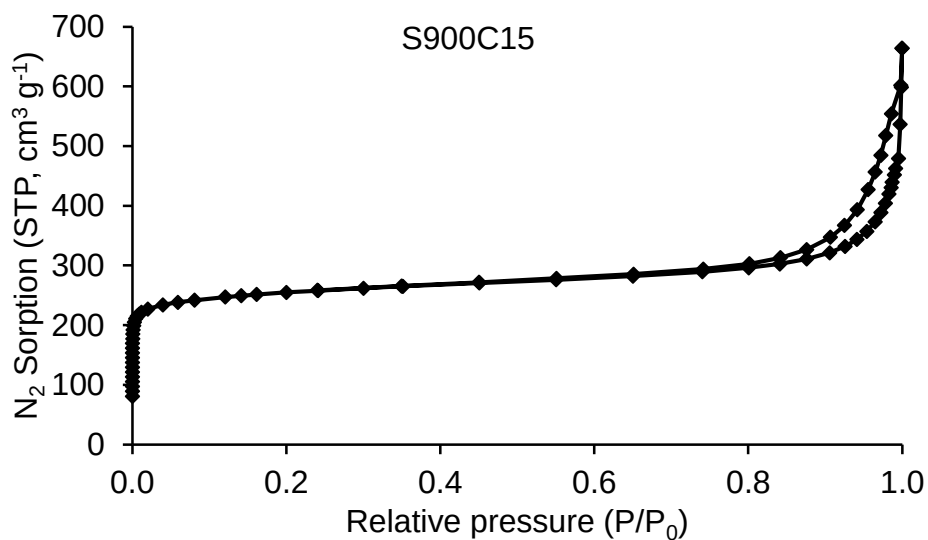


Pore distribution in the micropore region (HK method)

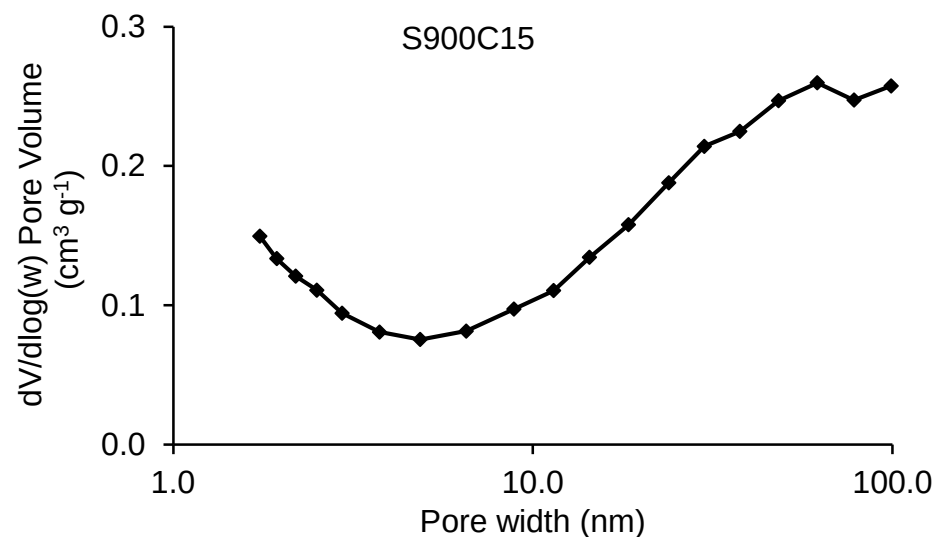


**Nitrogen adsorption isotherm and pore distribution plots for S900C15 with a CO<sub>2</sub> flow rate of 50 mL min<sup>-1</sup> (standard flow rate)**

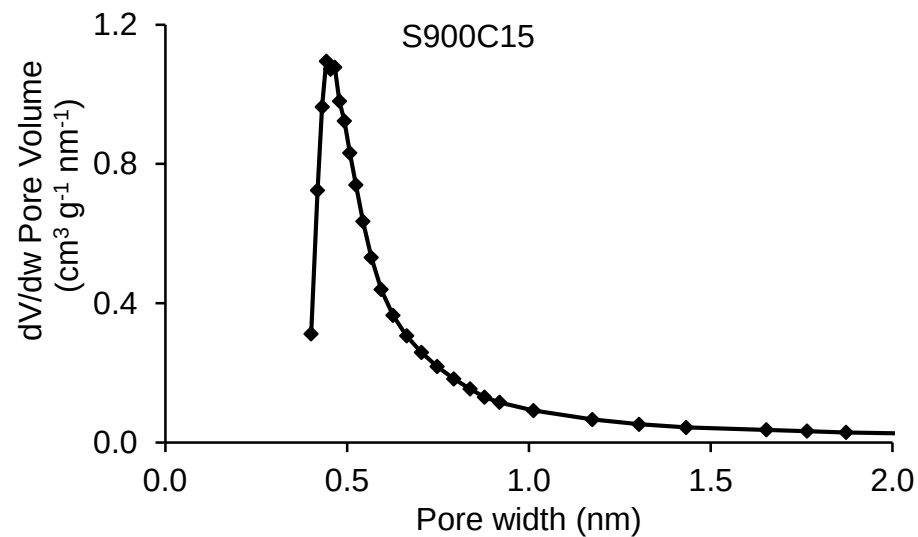
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

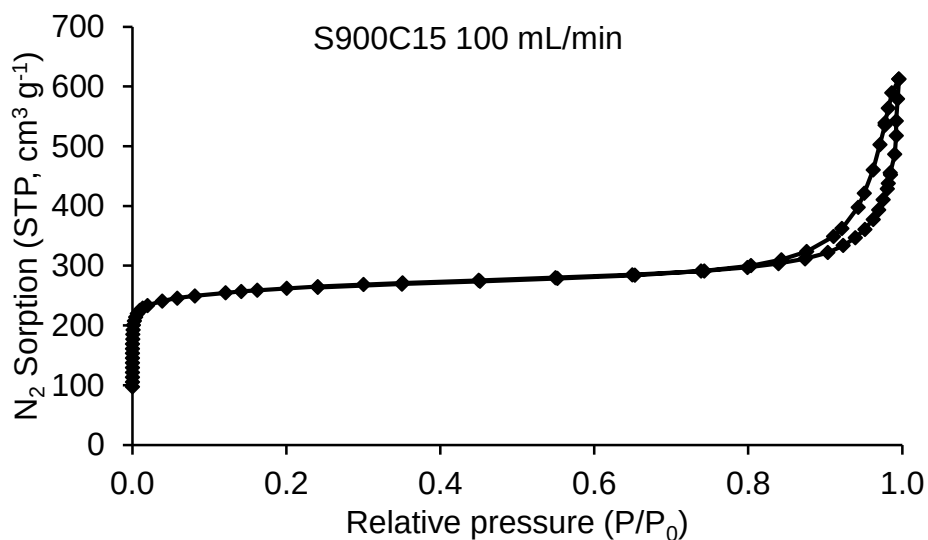


Pore distribution in the micropore region (HK method)

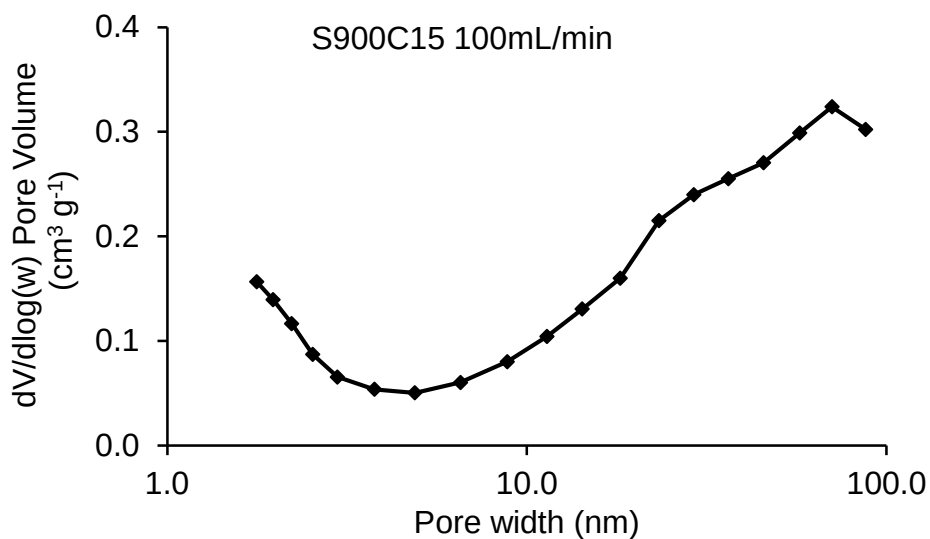


**Nitrogen adsorption isotherm and pore distribution plots for S900C15 with a CO<sub>2</sub> flow rate of 100 mL min<sup>-1</sup>**

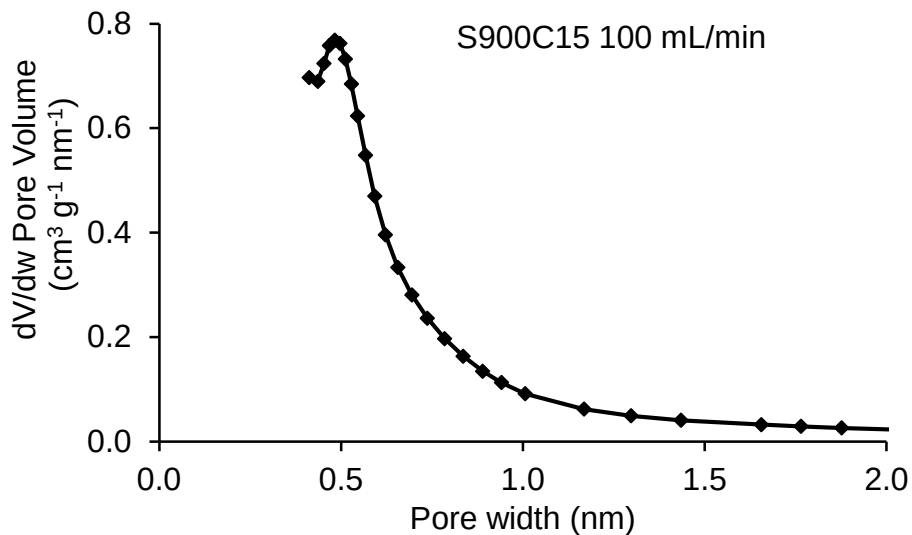
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

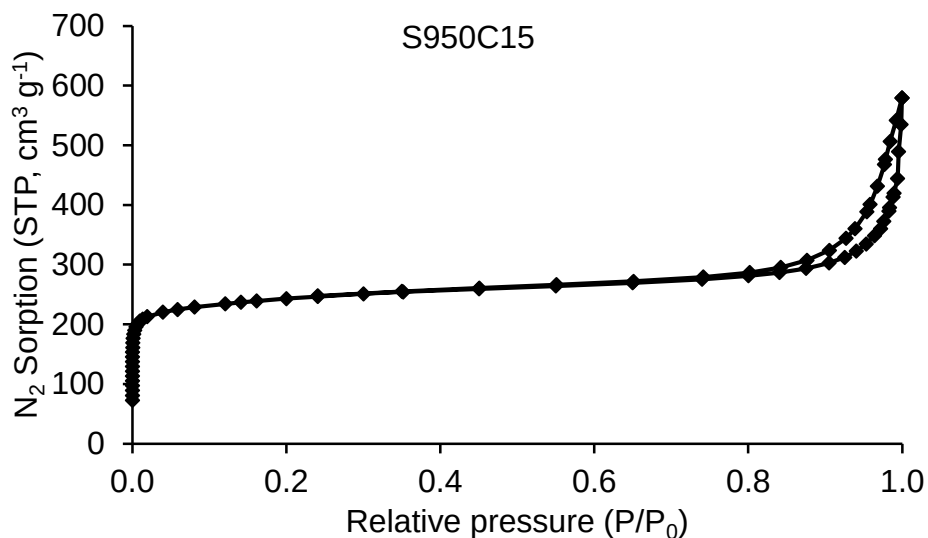


Pore distribution in the micropore region (HK method)

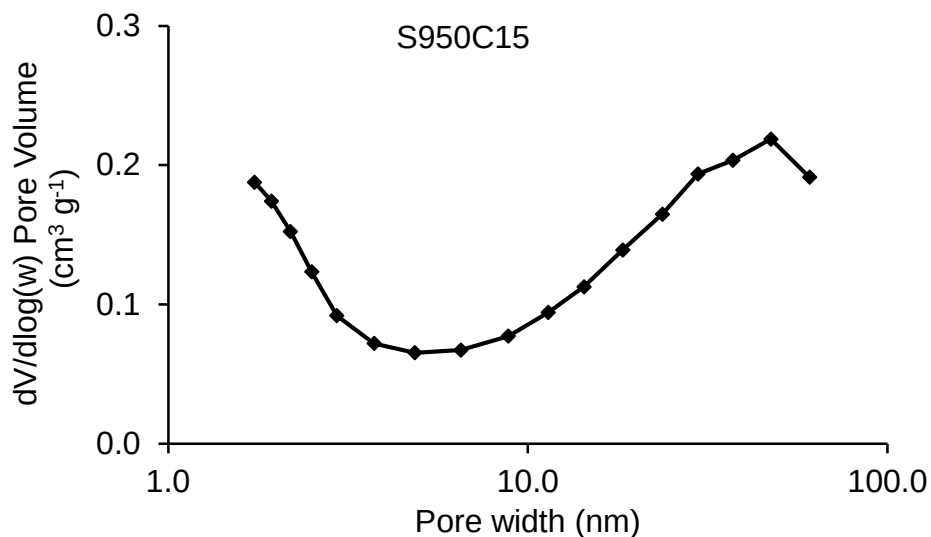


## Nitrogen adsorption isotherm and pore distribution plots for S950C15

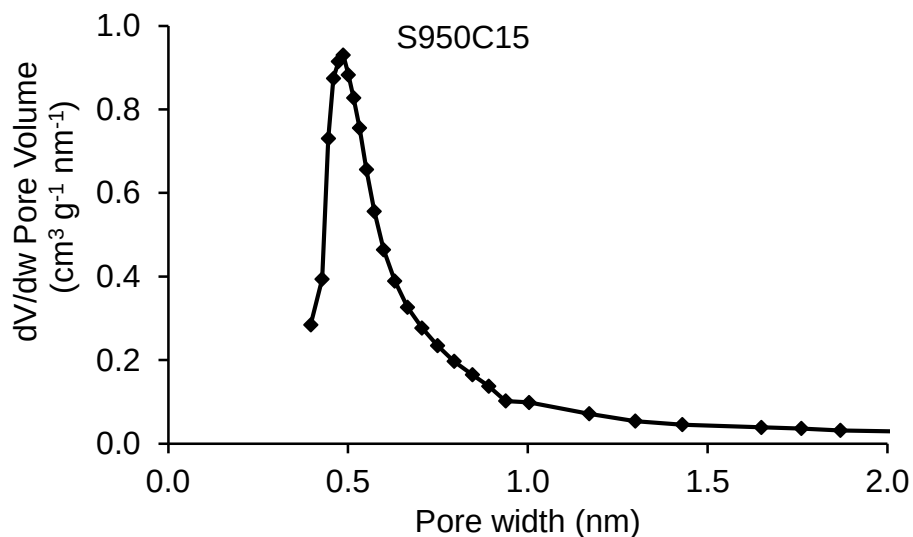
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

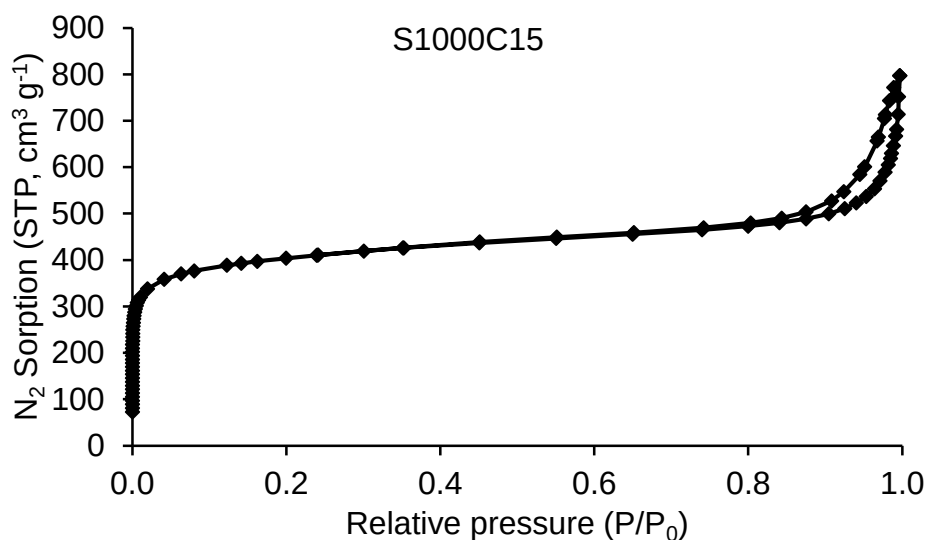


Pore distribution in the micropore region (HK method)

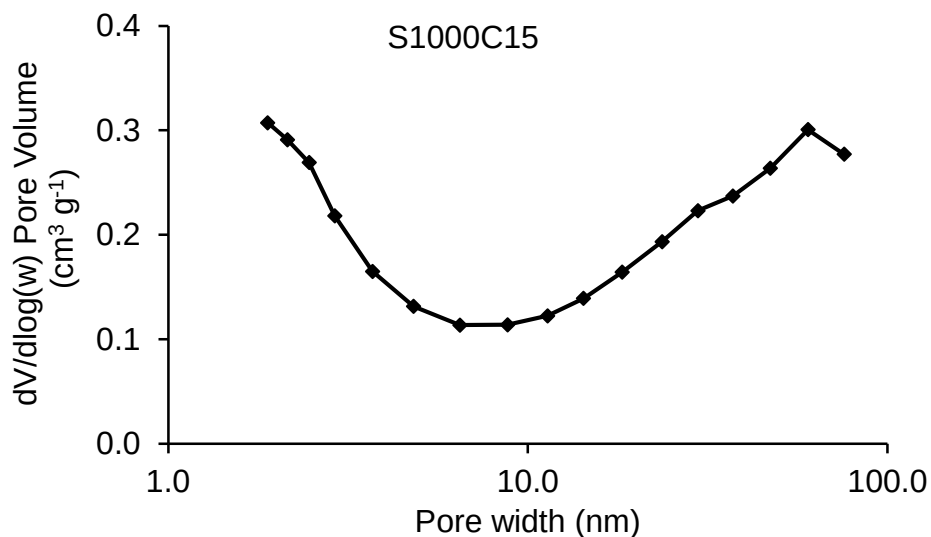


## Nitrogen adsorption isotherm and pore distribution plots for S1000C15

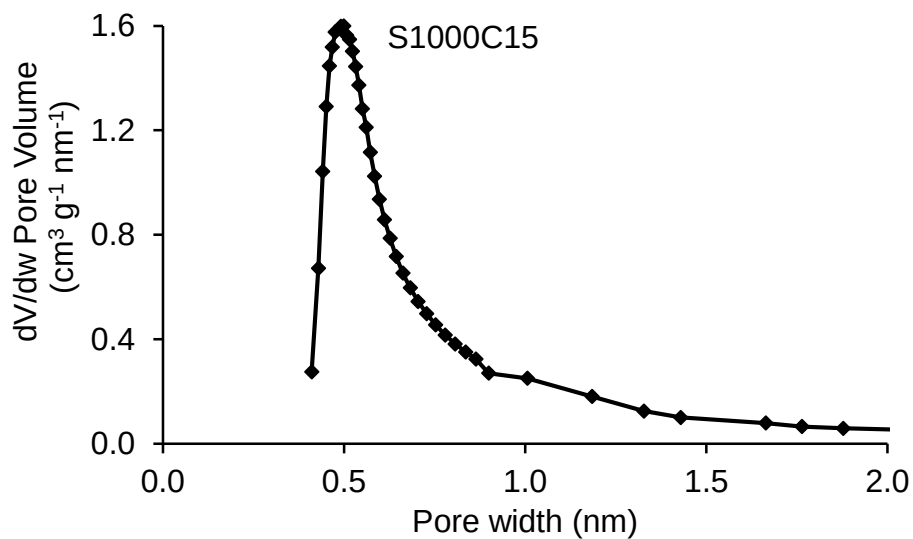
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

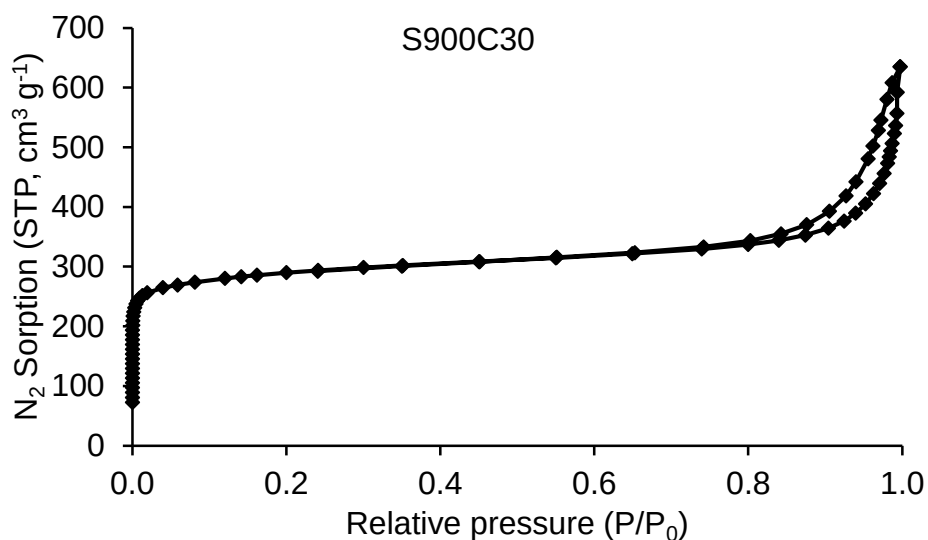


Pore distribution in the micropore region (HK method)

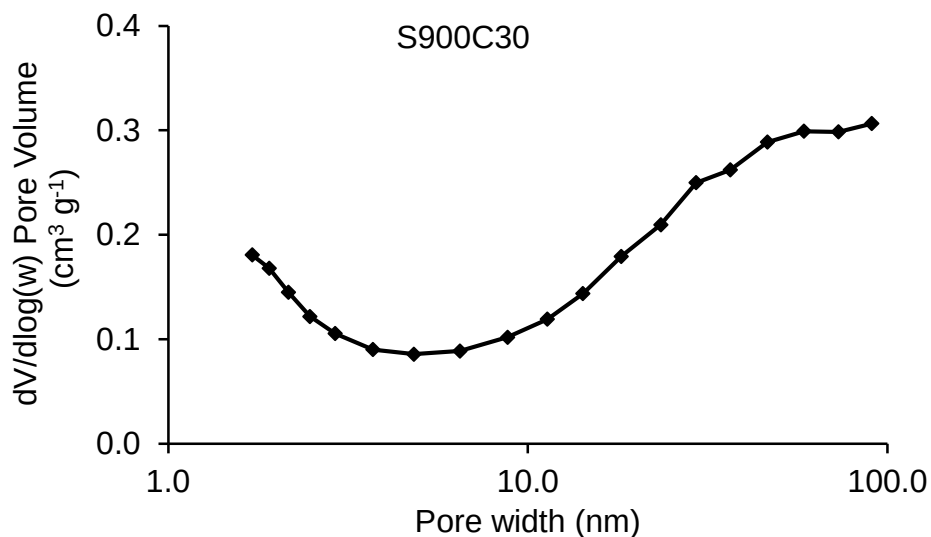


## Nitrogen adsorption isotherm and pore distribution plots for S900C30

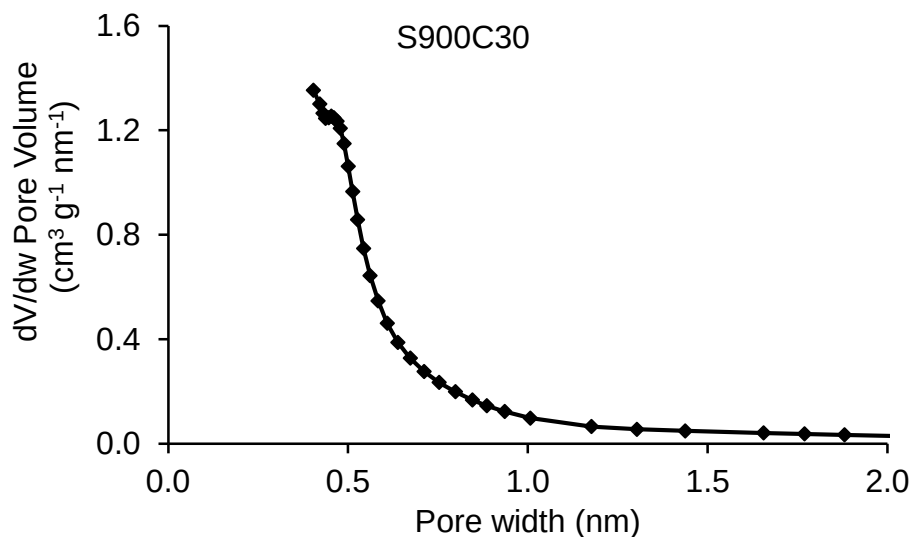
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



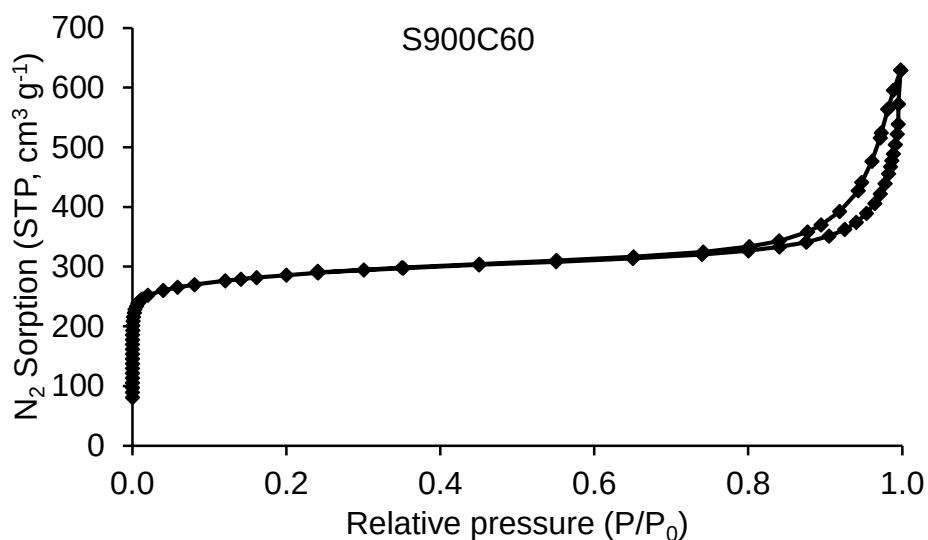
Pore distribution in the micropore region (HK method)



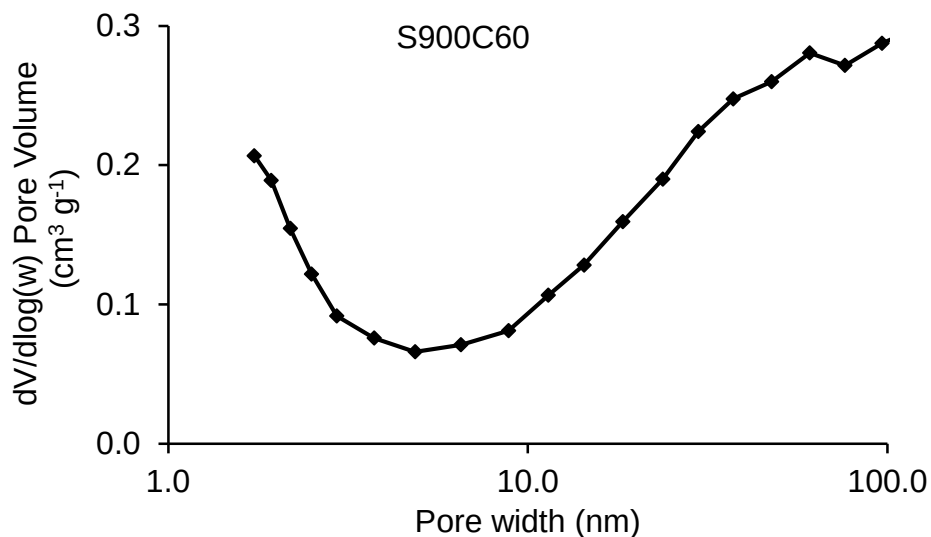


## Nitrogen adsorption isotherm and pore distribution plots for S900C60

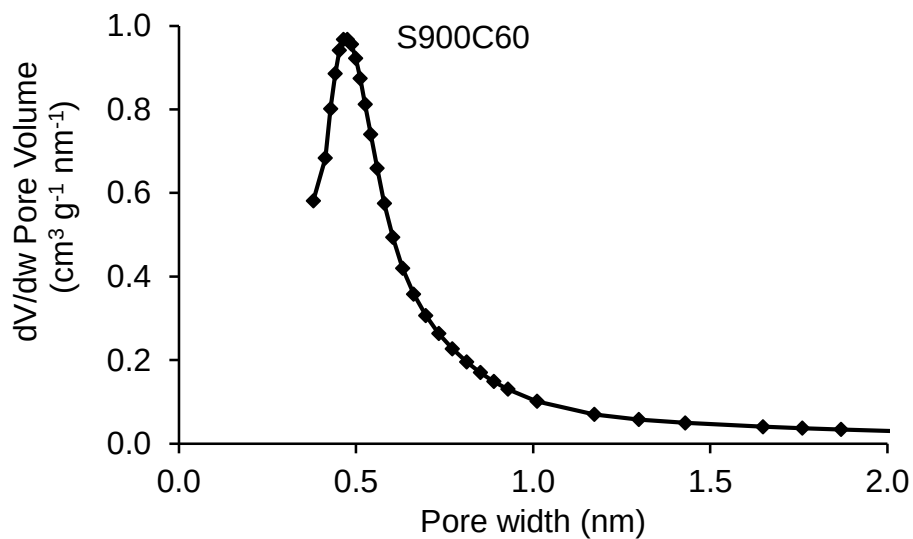
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

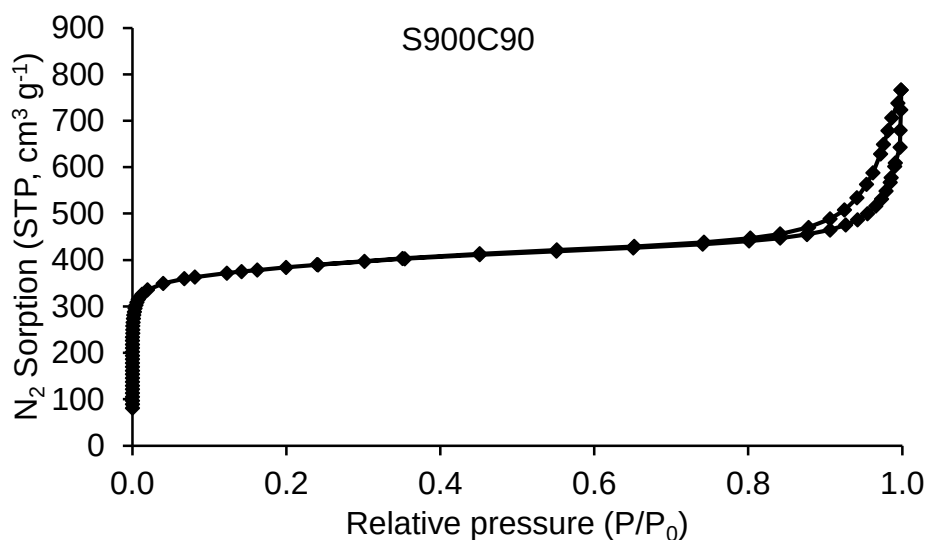


Pore distribution in the micropore region (HK method)

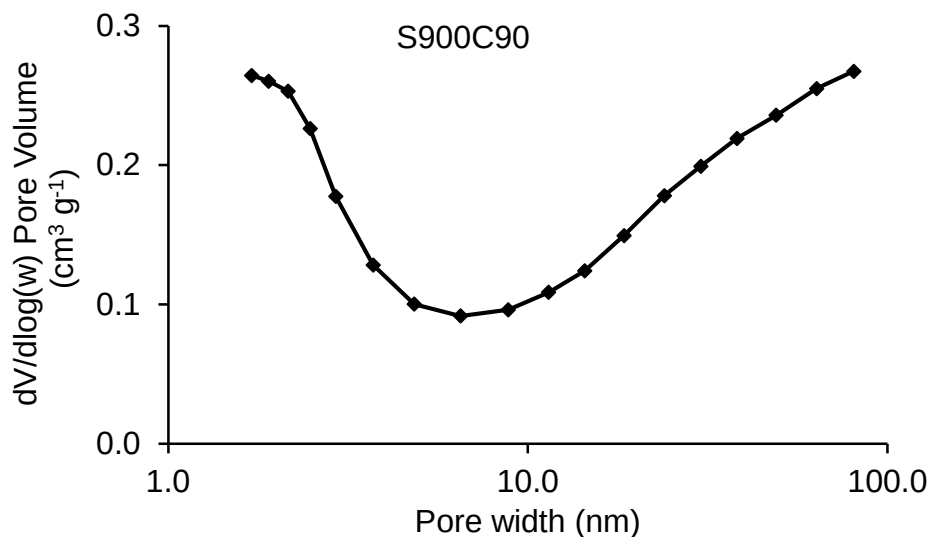


## Nitrogen adsorption isotherm and pore distribution plots for S900C90

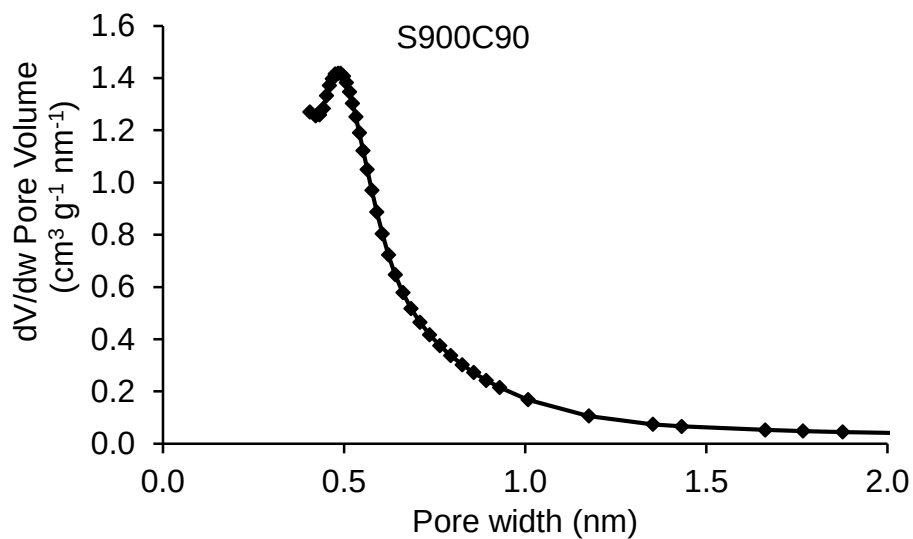
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

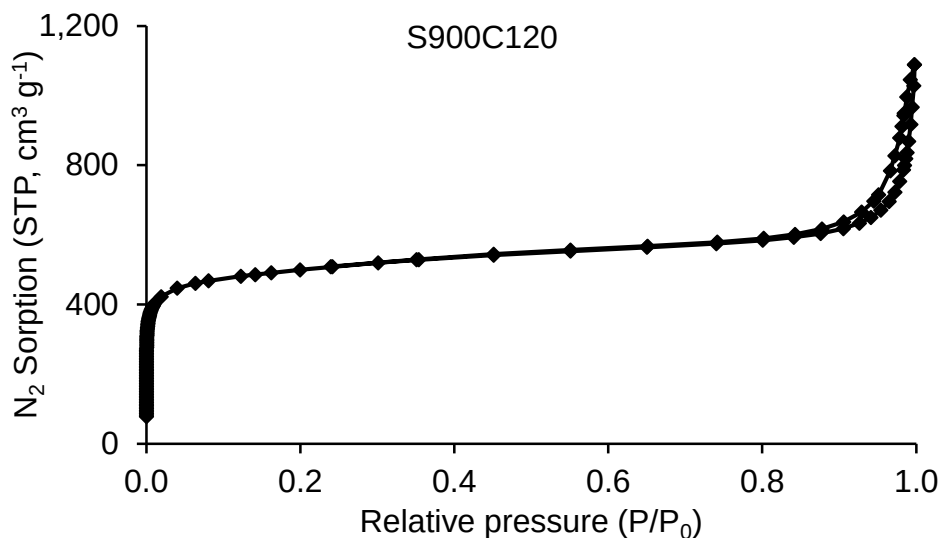


Pore distribution in the micropore region (HK method)

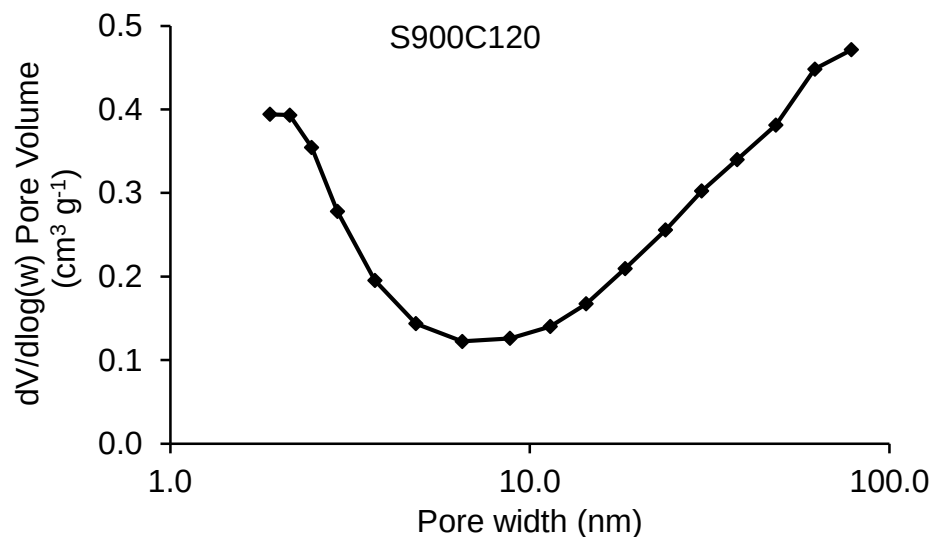


## Nitrogen adsorption isotherm and pore distribution plots for S900C120

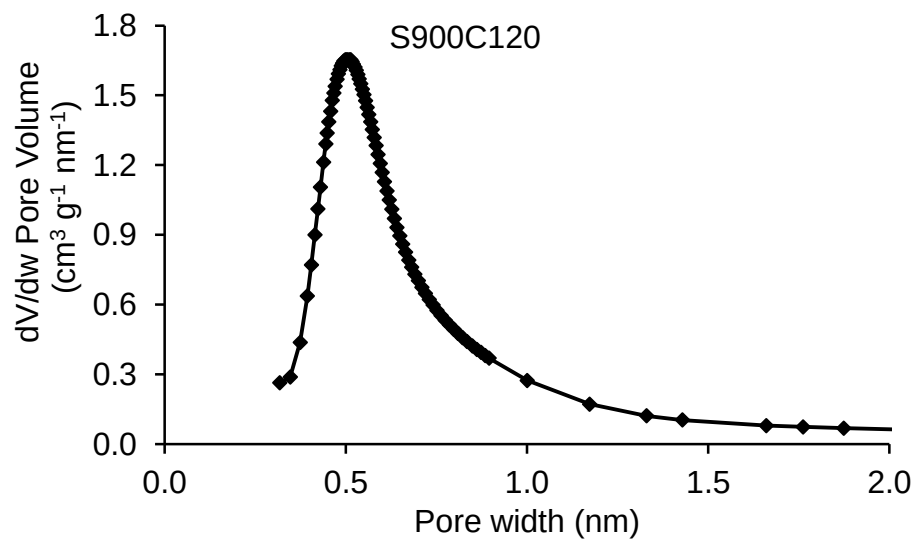
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

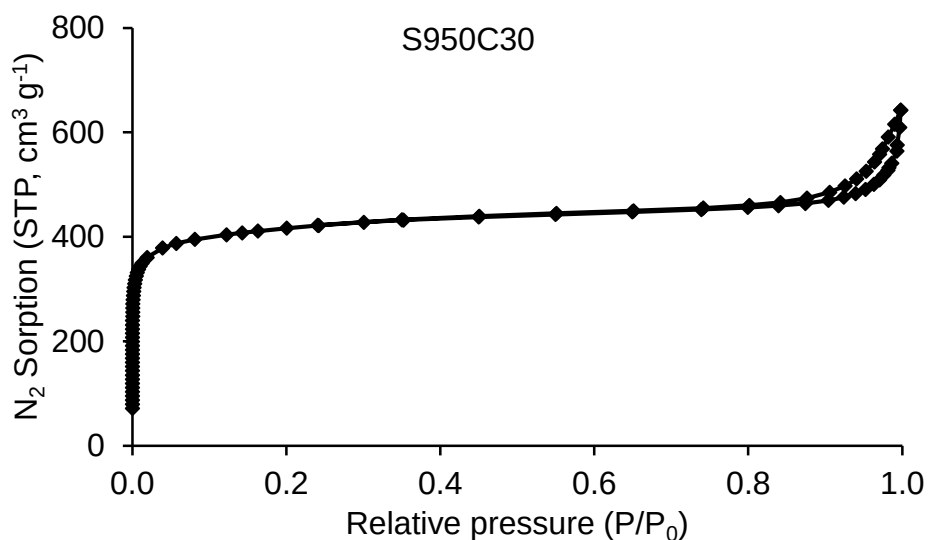


Pore distribution in the micropore region (HK method)

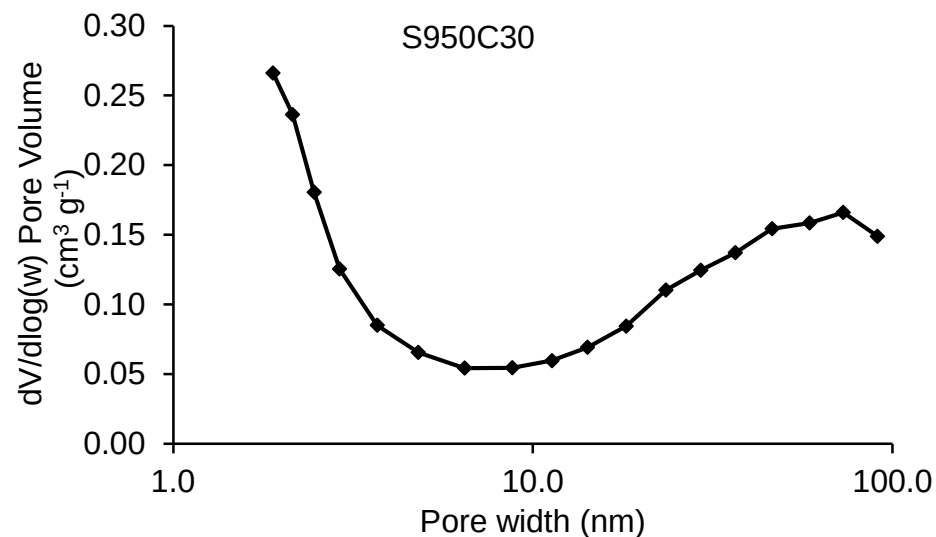


## Nitrogen adsorption isotherm and pore distribution plots for S950C30

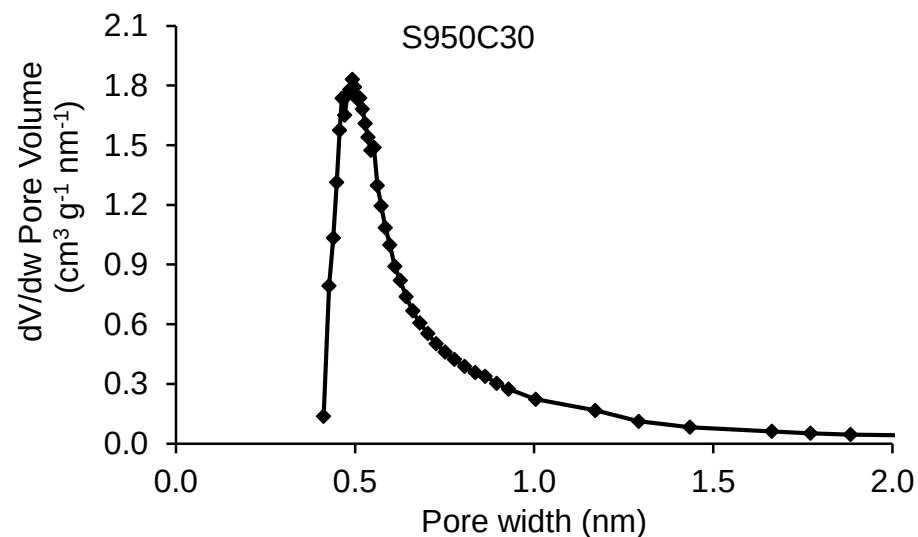
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

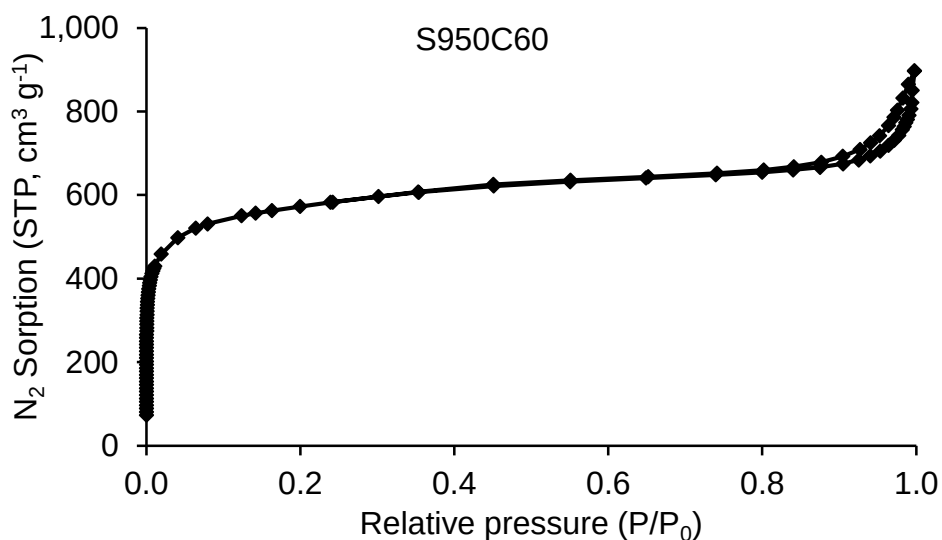


Pore distribution in the micropore region (HK method)

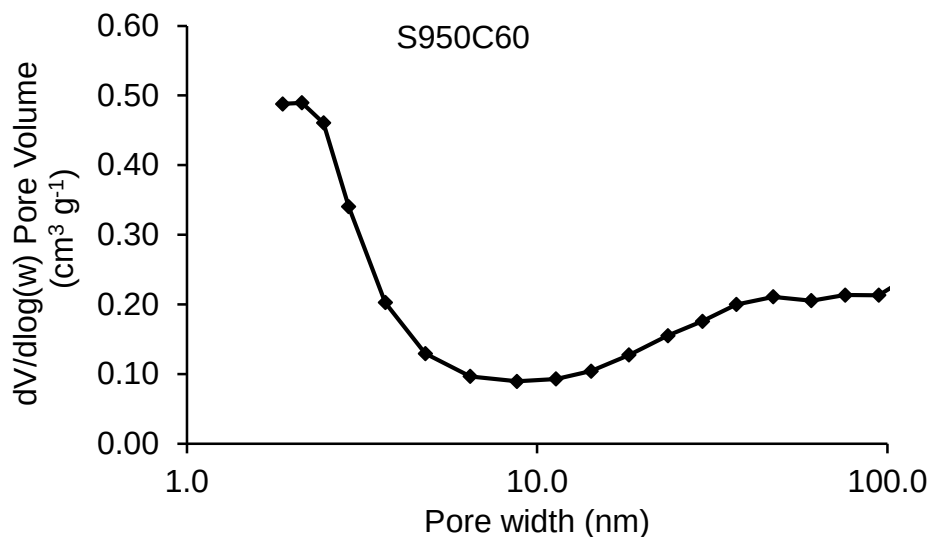


## Nitrogen adsorption isotherm and pore distribution plots for S950C60

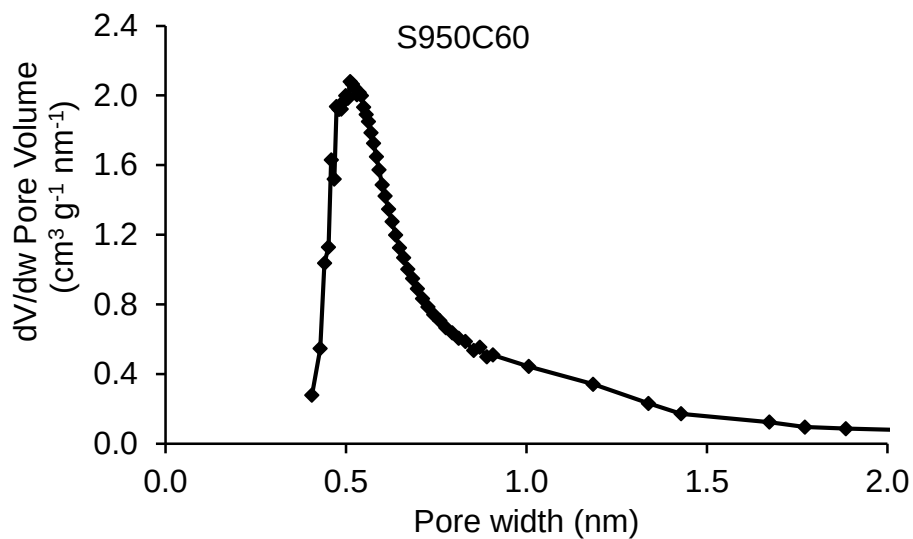
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

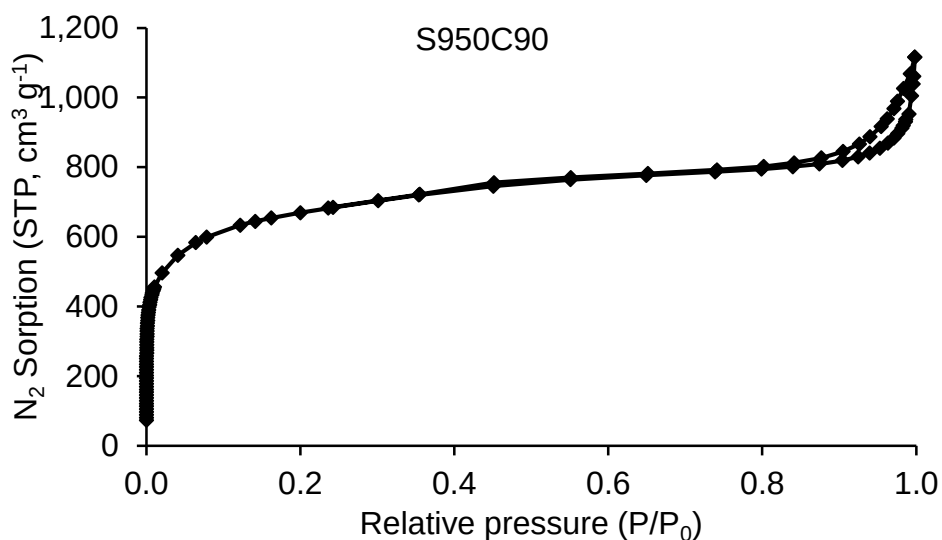


Pore distribution in the micropore region (HK method)

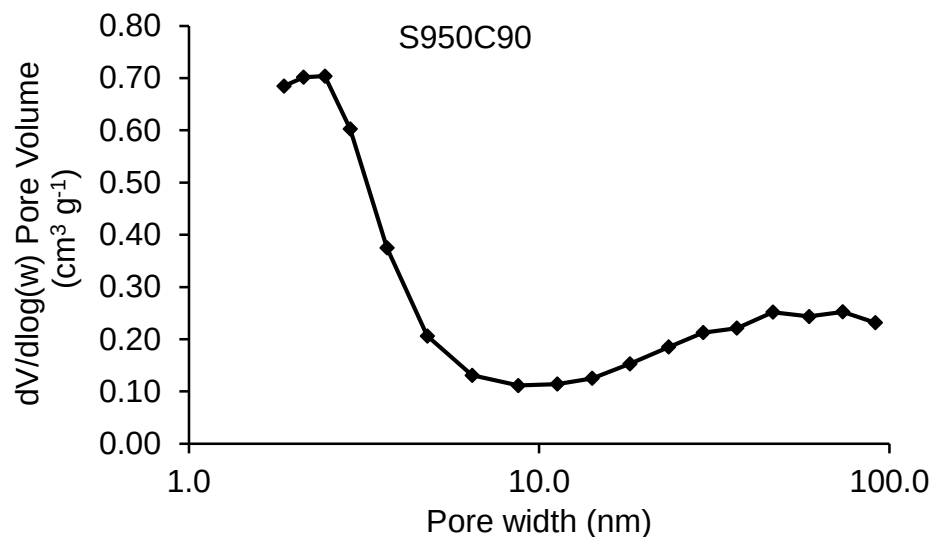


## Nitrogen adsorption isotherm and pore distribution plots for S950C90

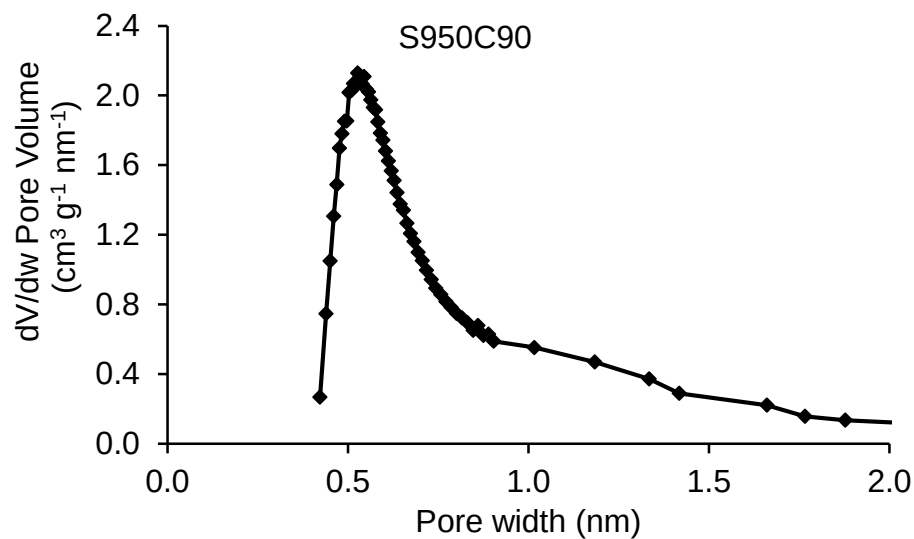
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

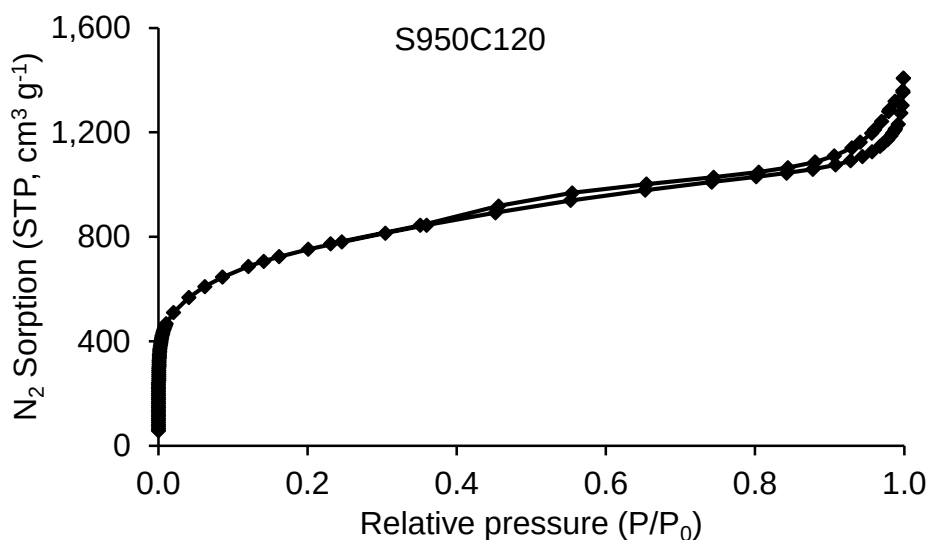


Pore distribution in the micropore region (HK method)

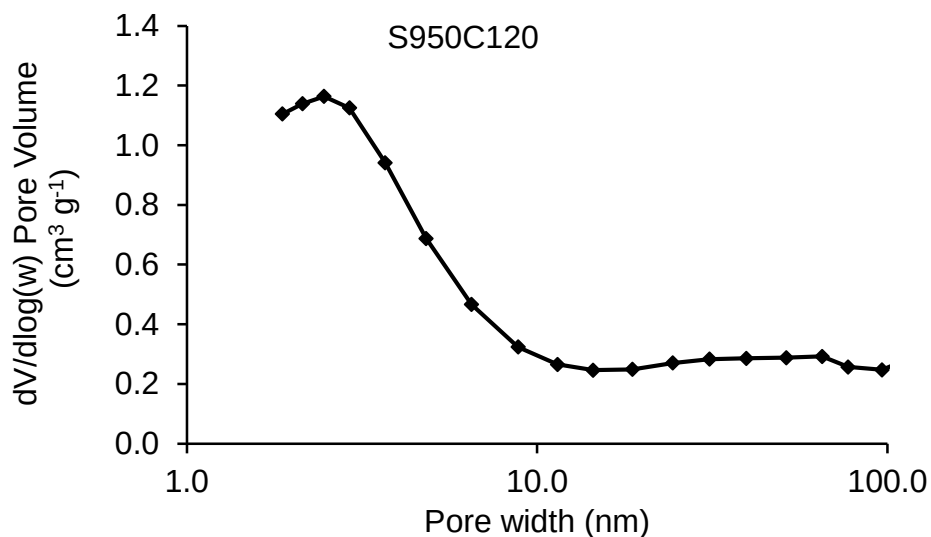


## Nitrogen adsorption isotherm and pore distribution plots for S950C120

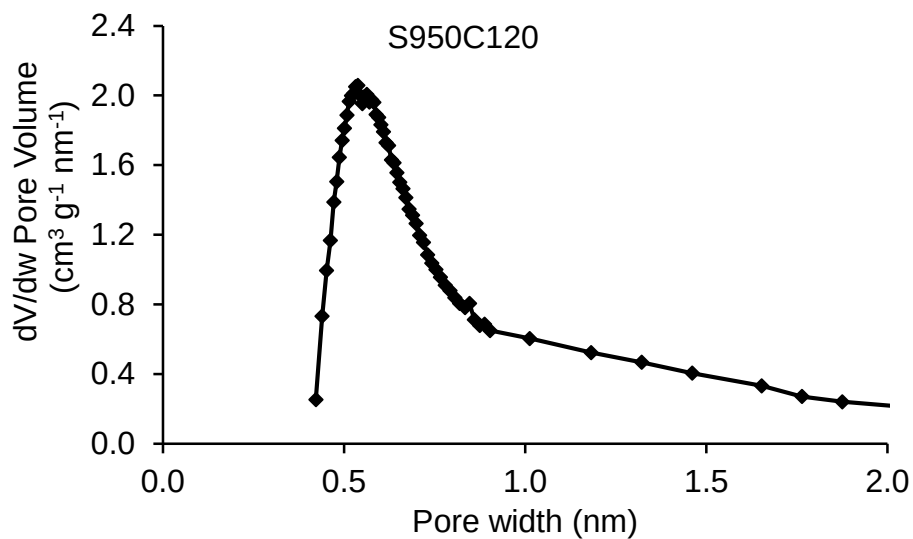
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

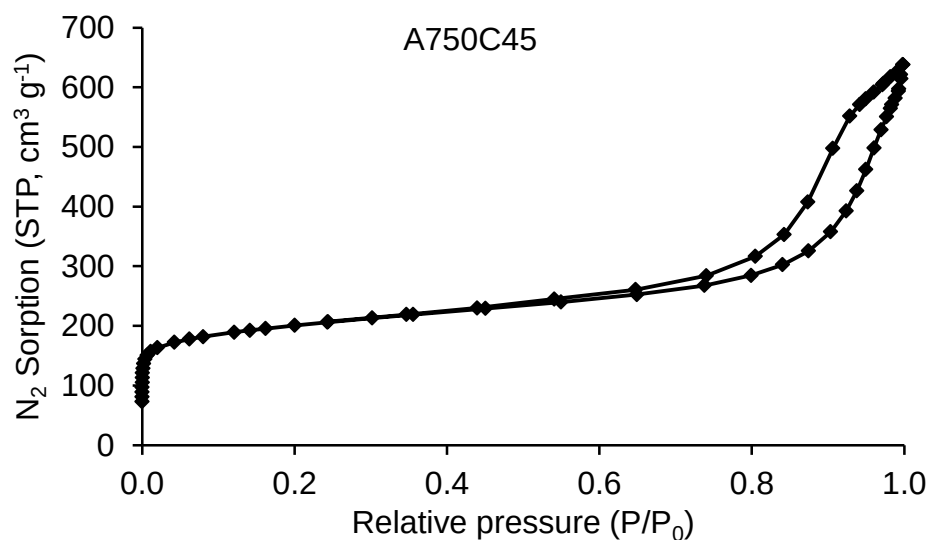


Pore distribution in the micropore region (HK method)

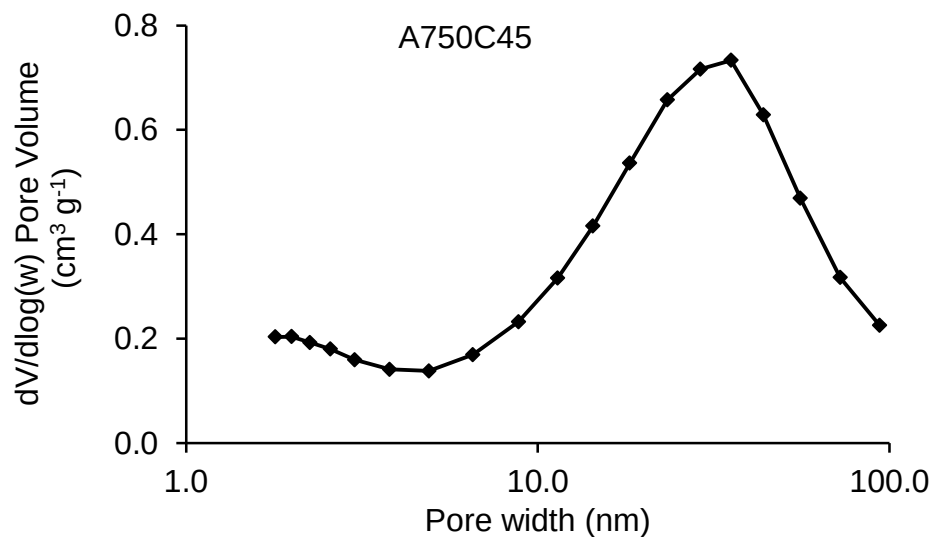


## Nitrogen adsorption isotherm and pore distribution plots for A750C45

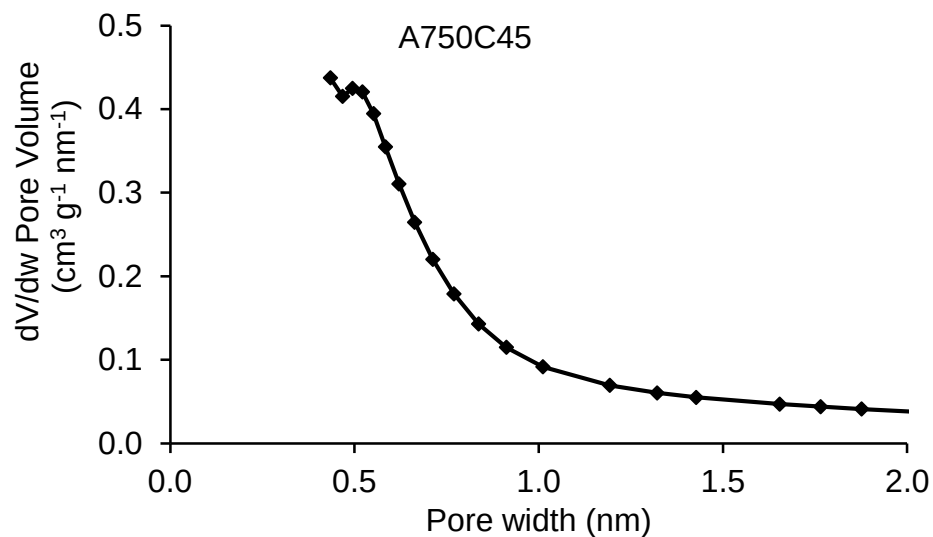
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)



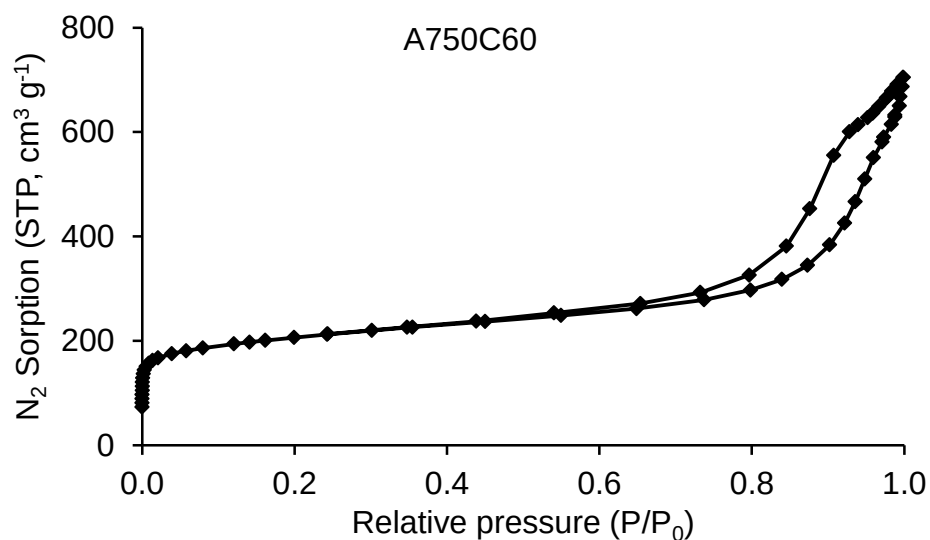
### Pore distribution in the micropore region (HK method)



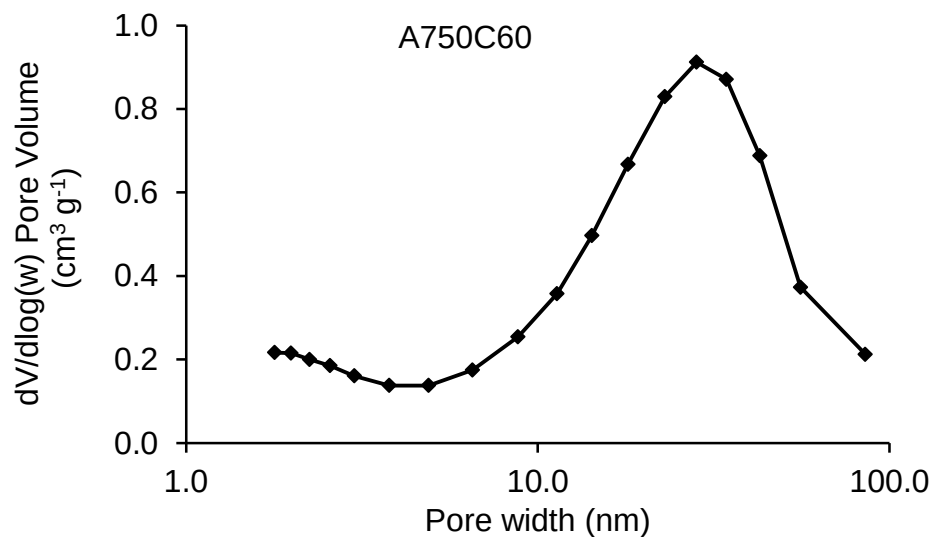


## Nitrogen adsorption isotherm and pore distribution plots for A750C60

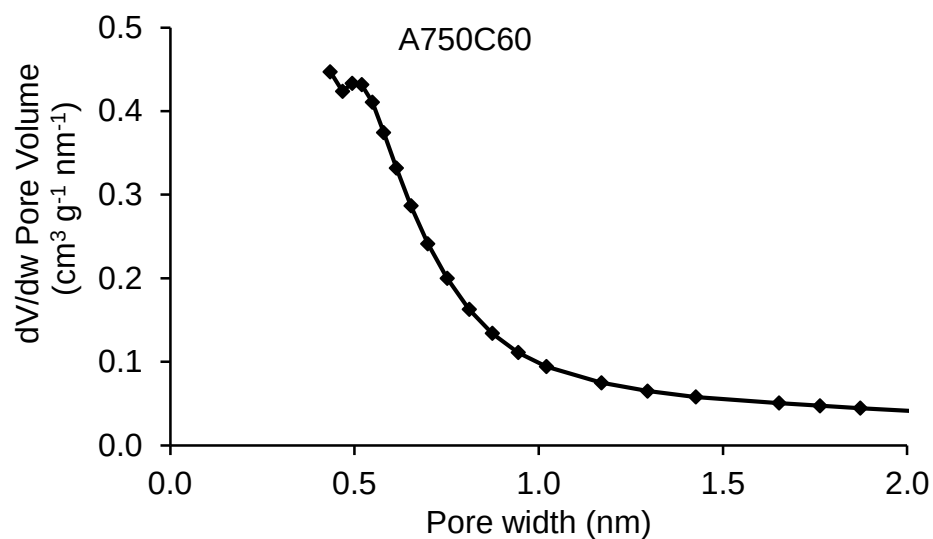
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

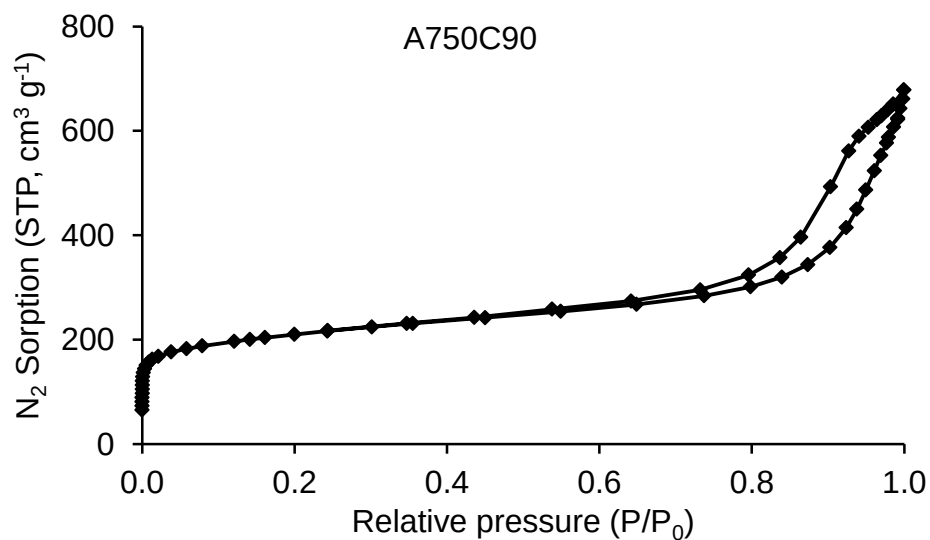


### Pore distribution in the micropore region (HK method)

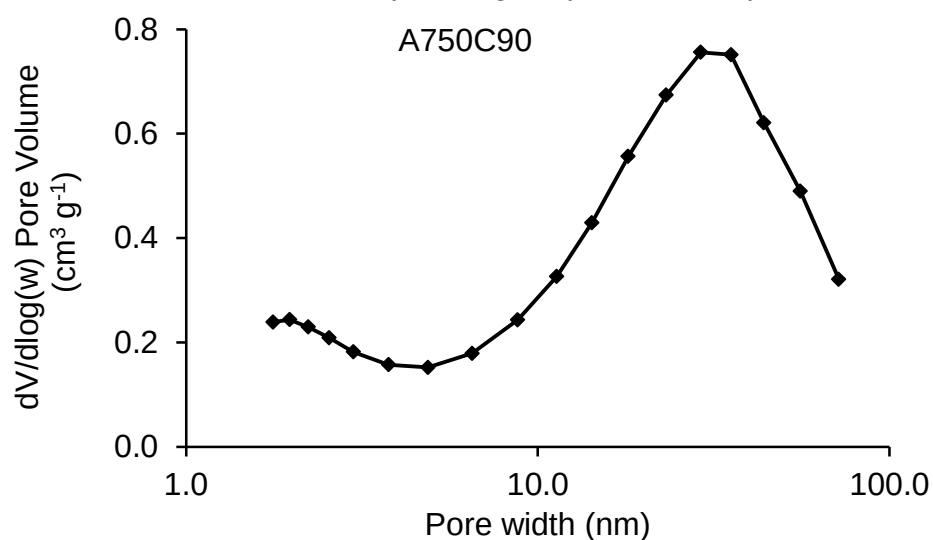


## Nitrogen adsorption isotherm and pore distribution plots for A750C90

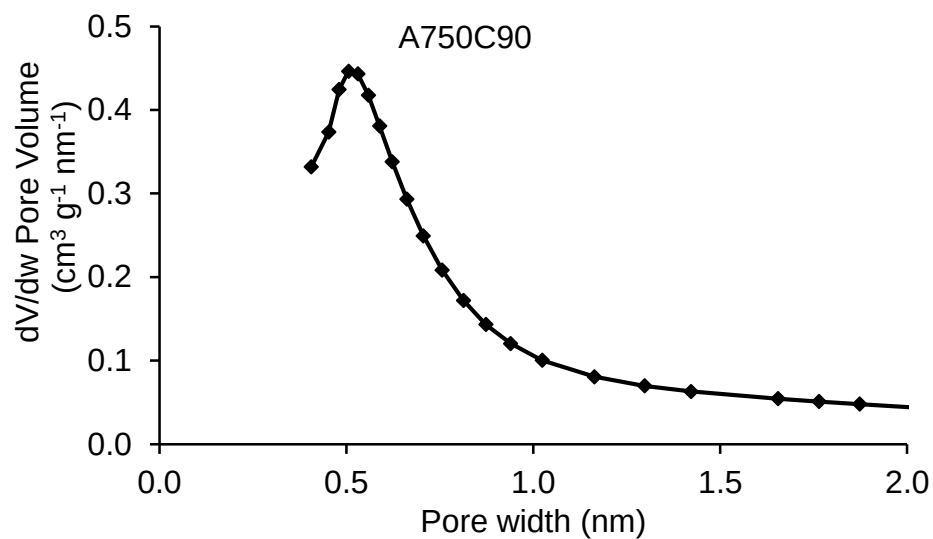
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

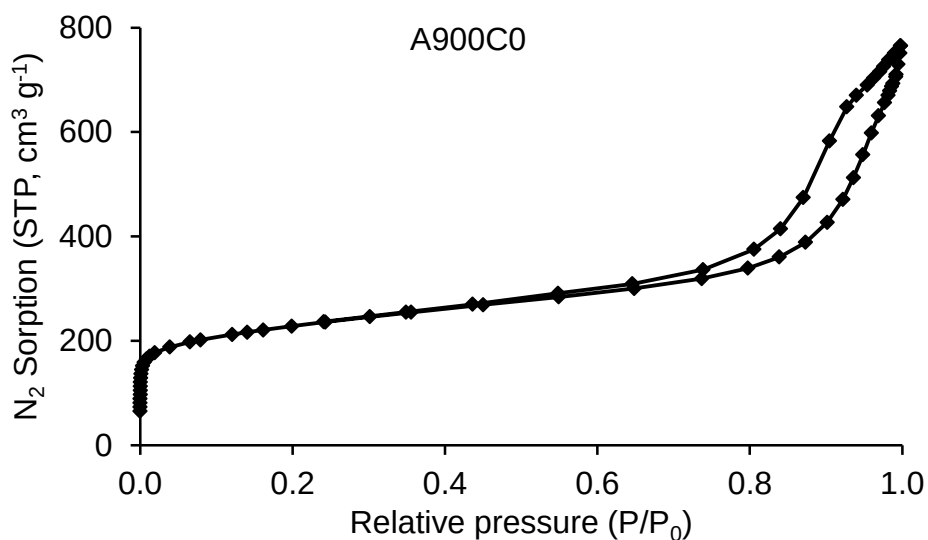


Pore distribution in the micropore region (HK method)

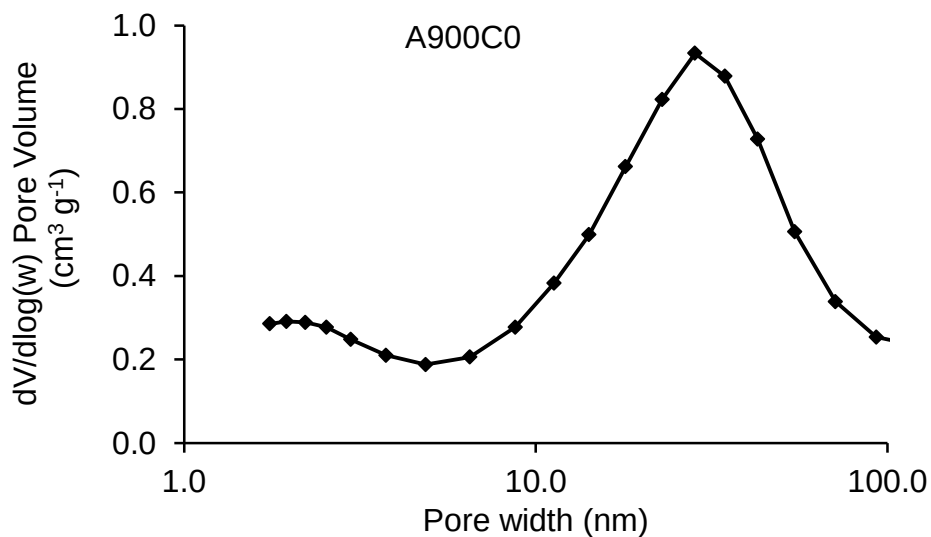


## Nitrogen adsorption isotherm and pore distribution plots for A900C0

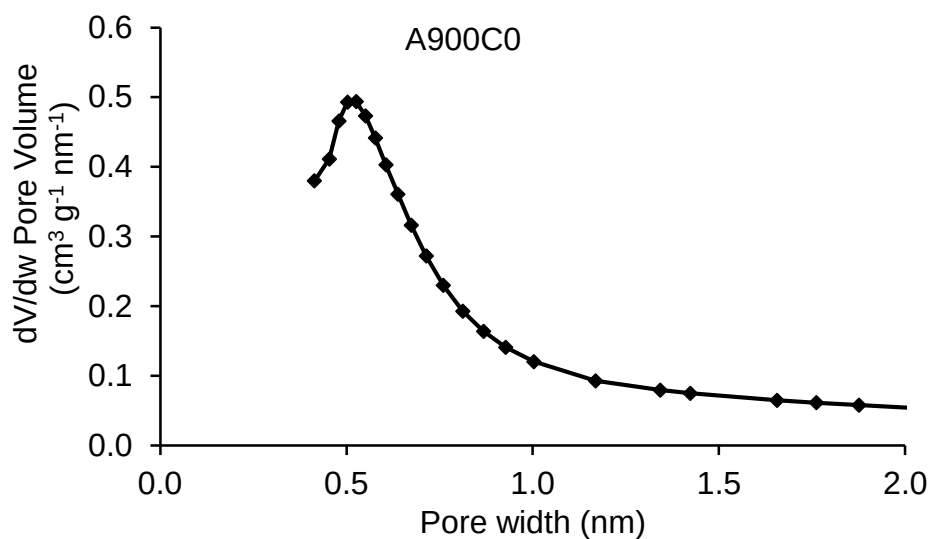
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

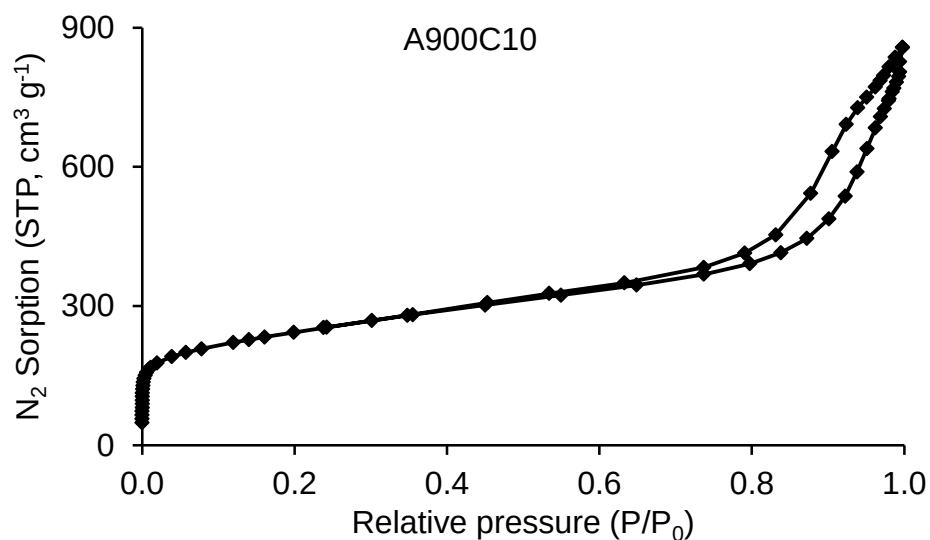


Pore distribution in the micropore region (HK method)

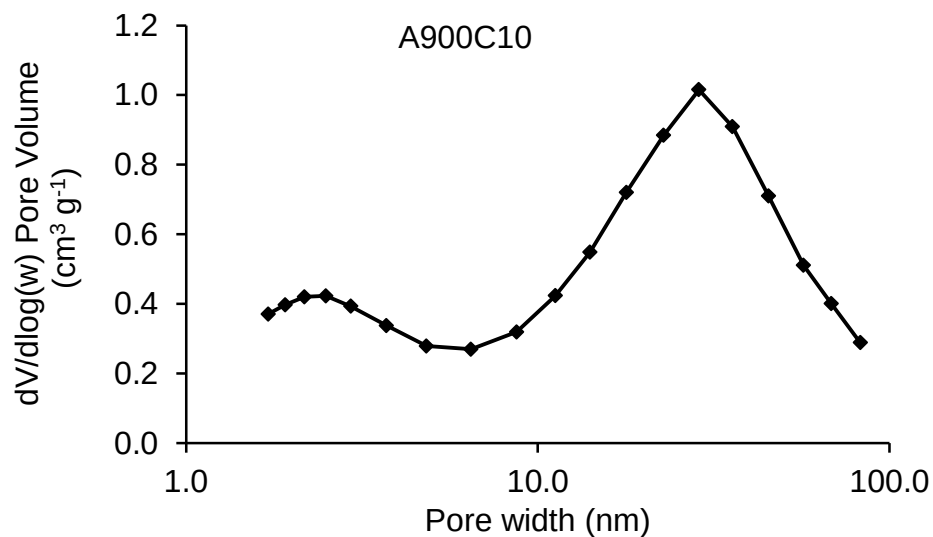


## Nitrogen adsorption isotherm and pore distribution plots for A900C10

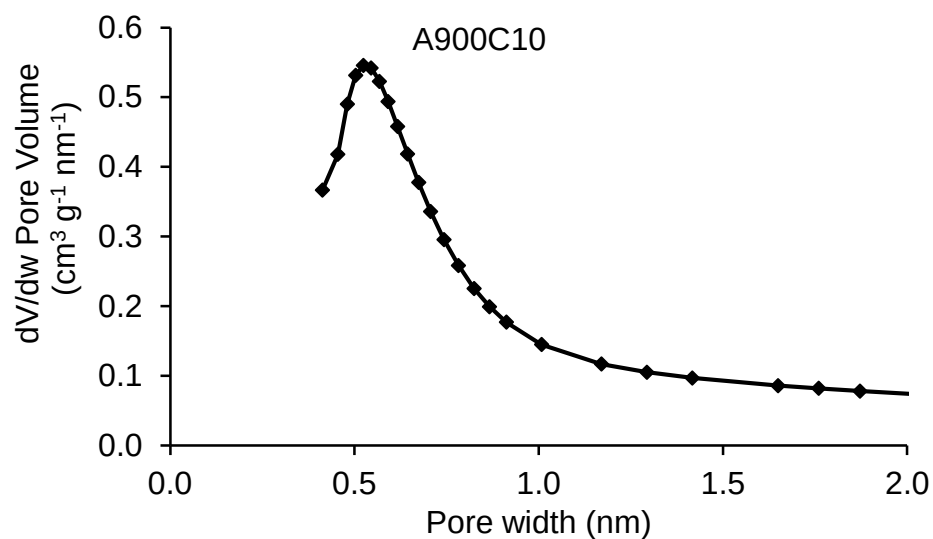
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

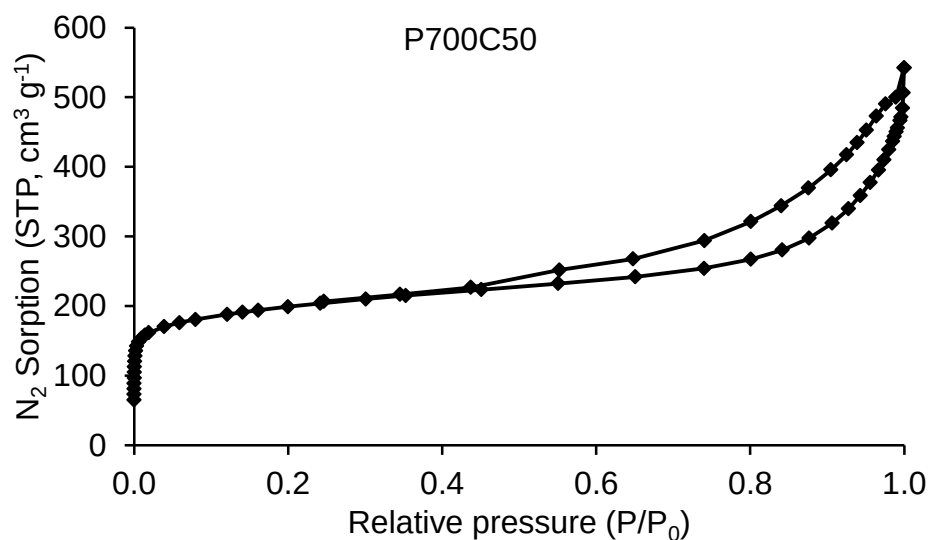


Pore distribution in the micropore region (HK method)

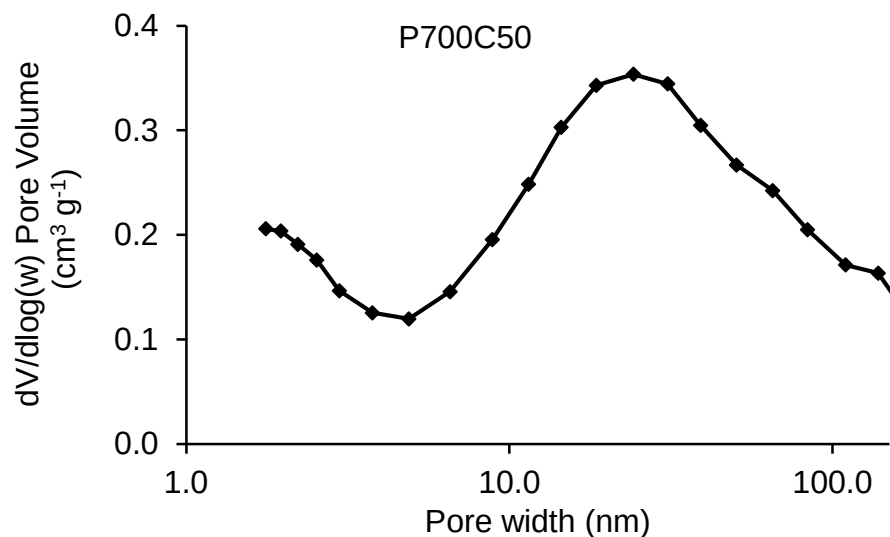


## Nitrogen adsorption isotherm and pore distribution plots for P700C50

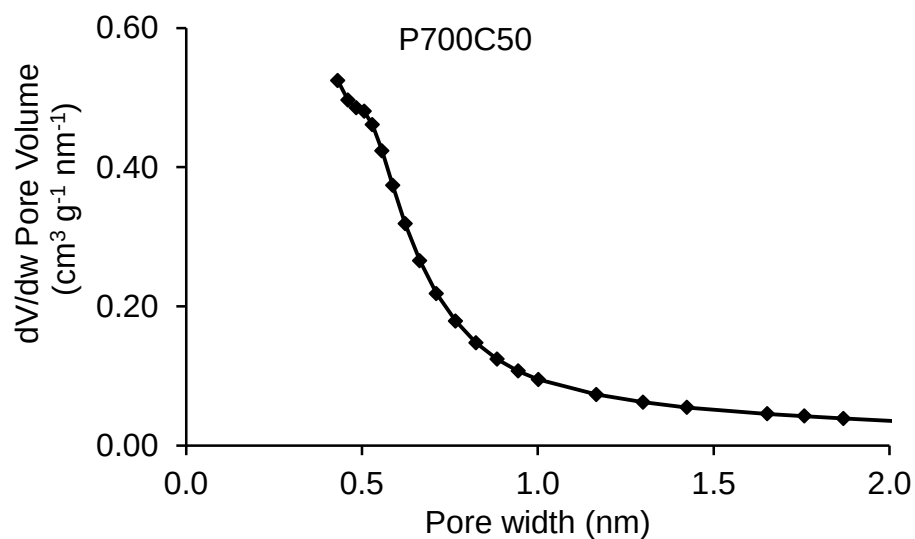
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

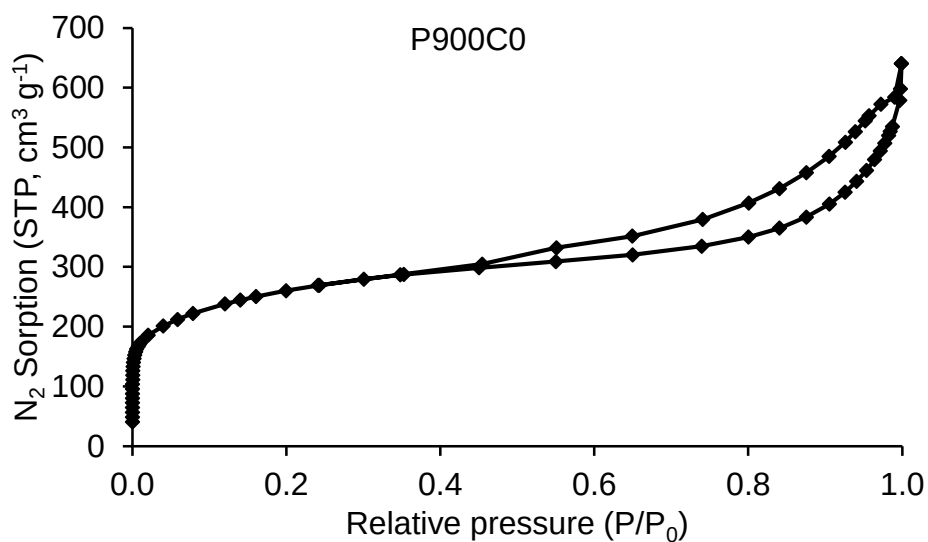


Pore distribution in the micropore region (HK method)

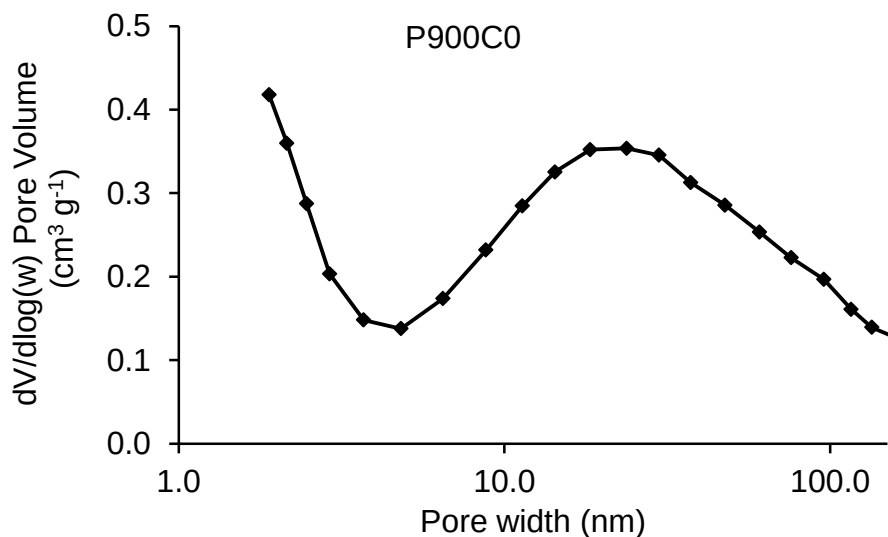


## Nitrogen adsorption isotherm and pore distribution plots for P900C0

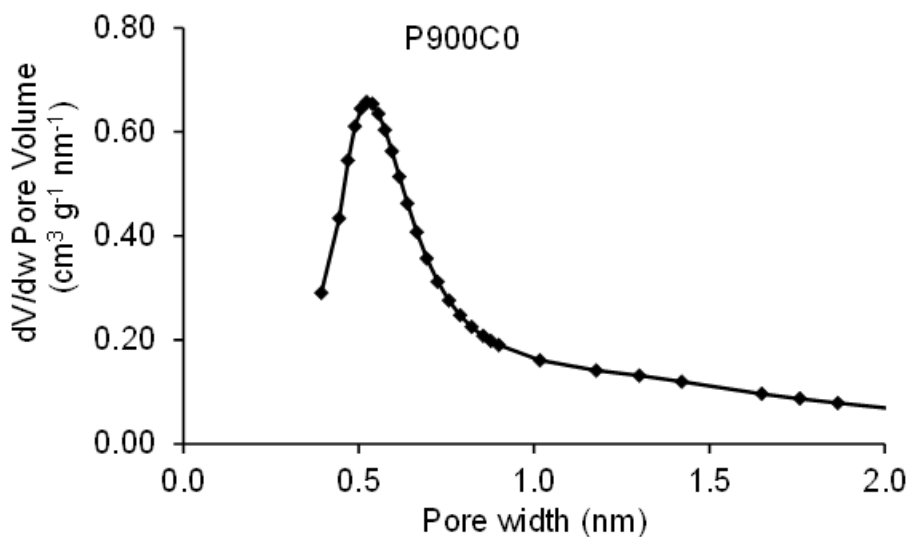
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

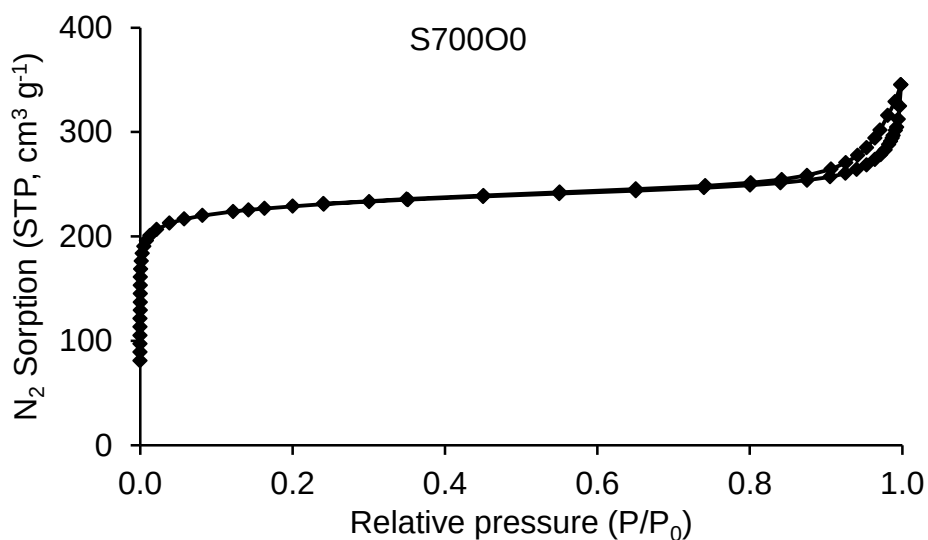


Pore distribution in the micropore region (HK method)

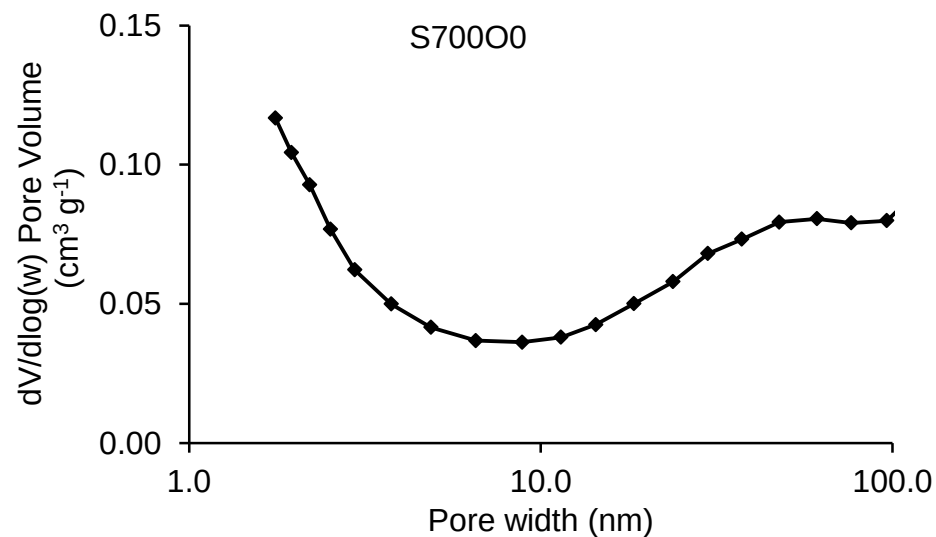


## Nitrogen adsorption isotherm and pore distribution plots for S70000

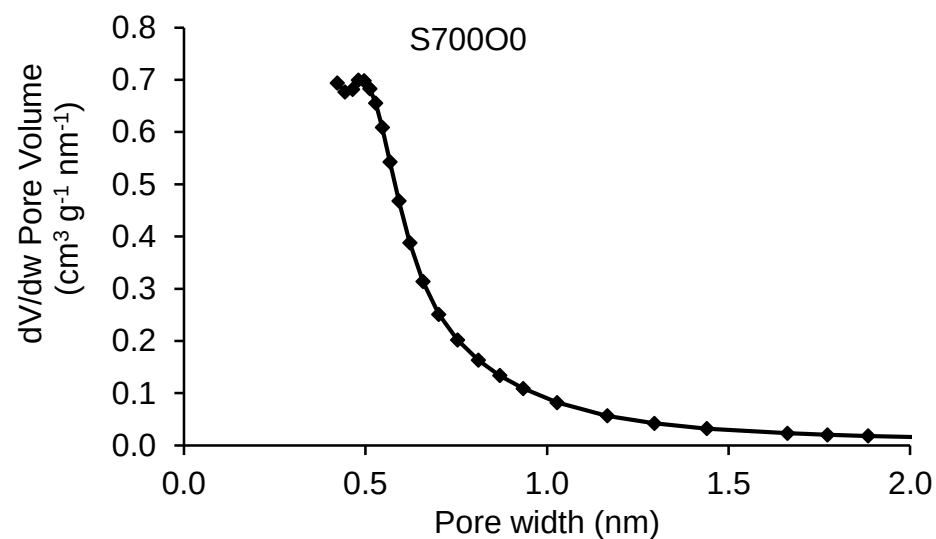
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

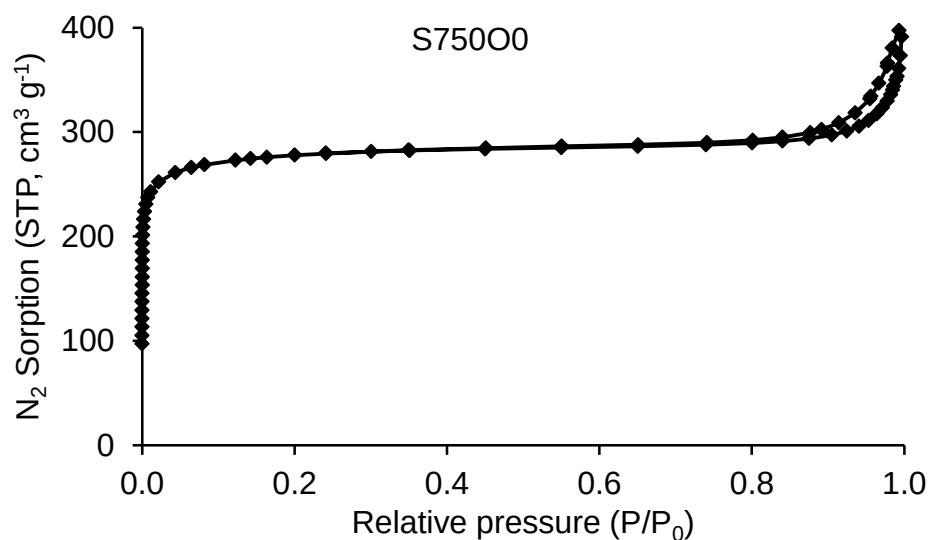


Pore distribution in the micropore region (HK method)

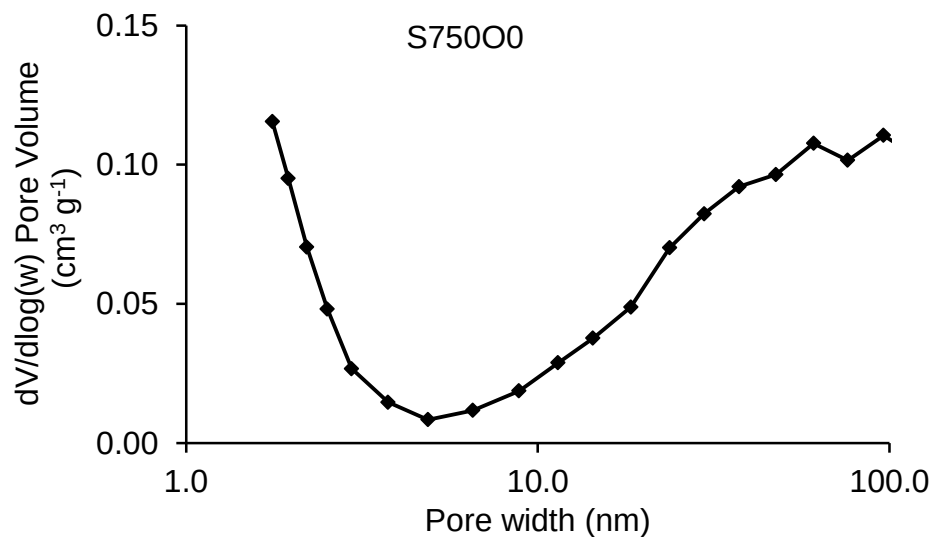


## Nitrogen adsorption isotherm and pore distribution plots for S75000

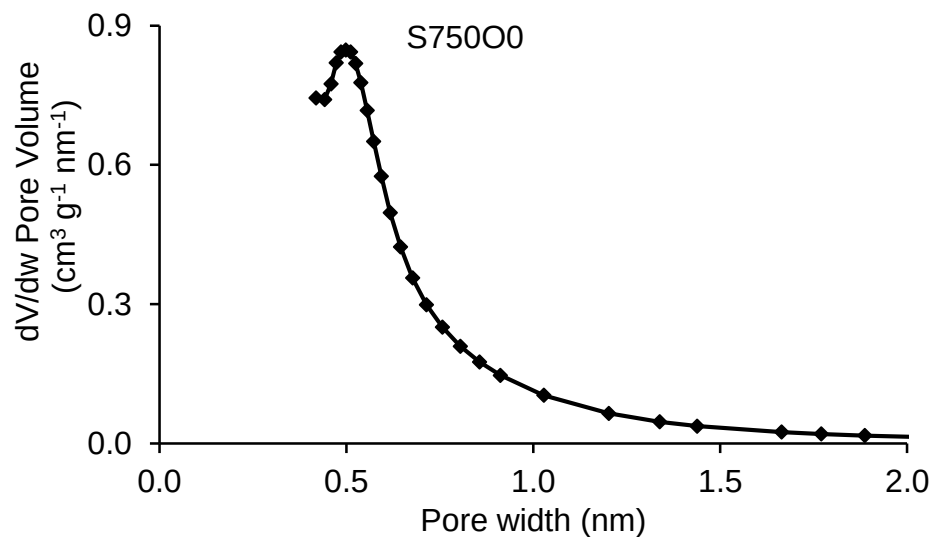
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



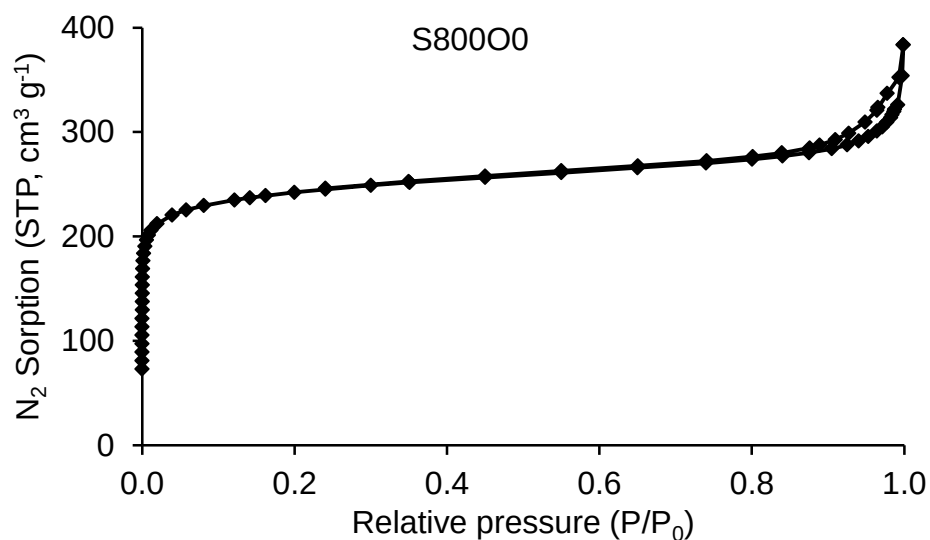
Pore distribution in the micropore region (HK method)



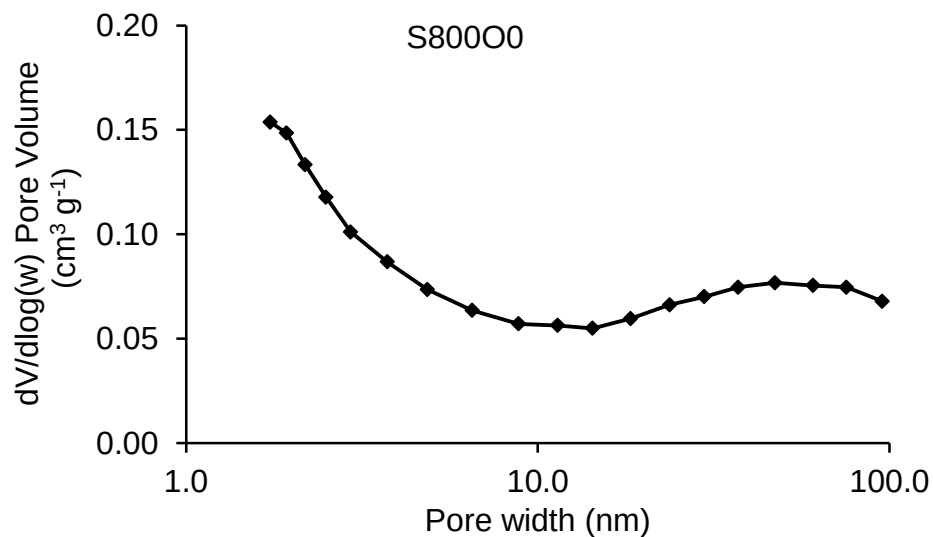


## Nitrogen adsorption isotherm and pore distribution plots for S80000

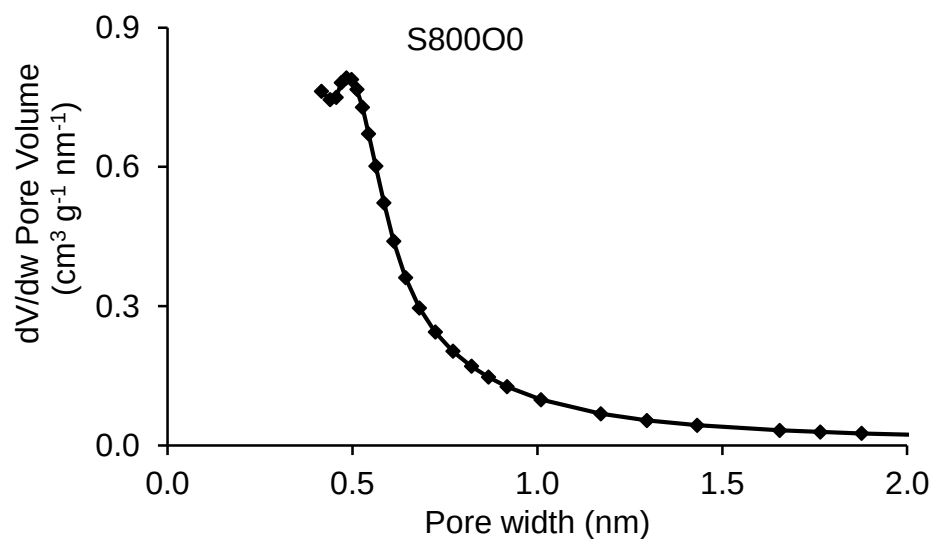
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

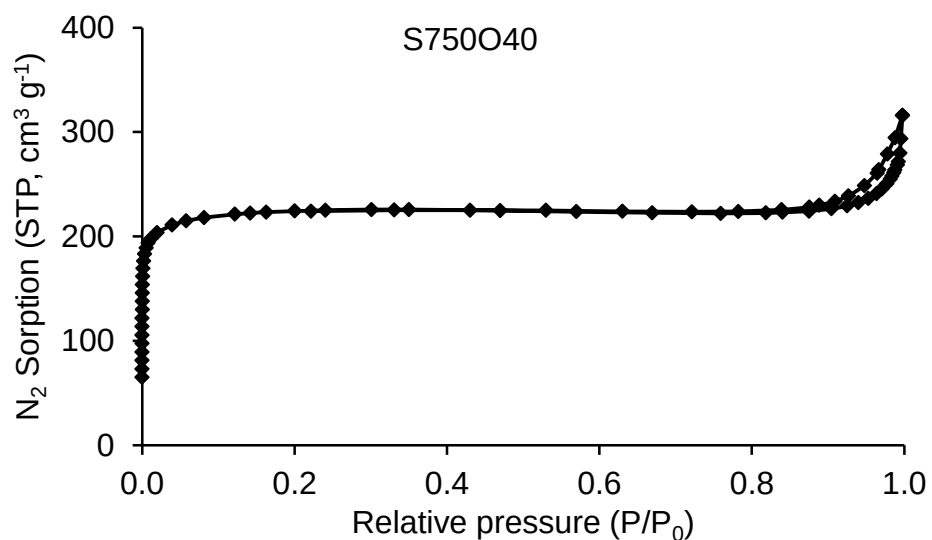


Pore distribution in the micropore region (HK method)

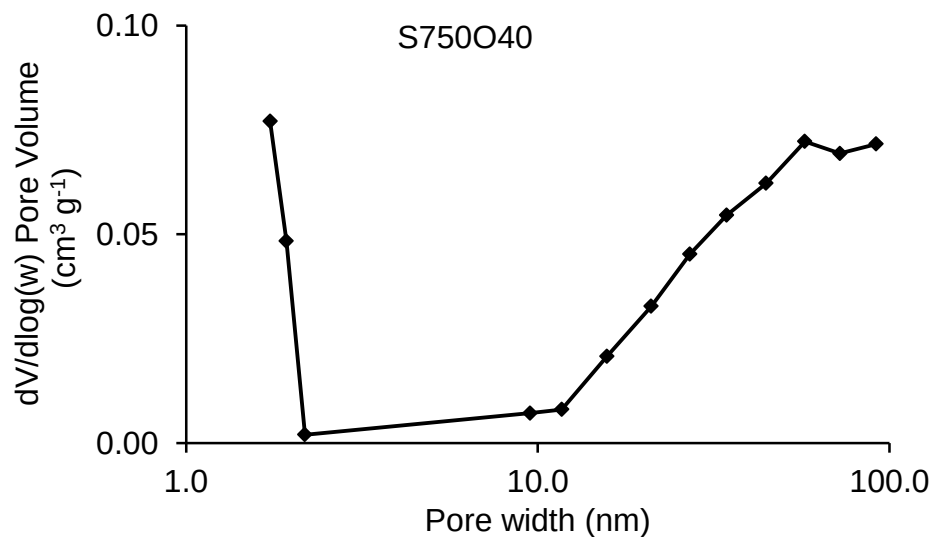


## Nitrogen adsorption isotherm and pore distribution plots for S750O40

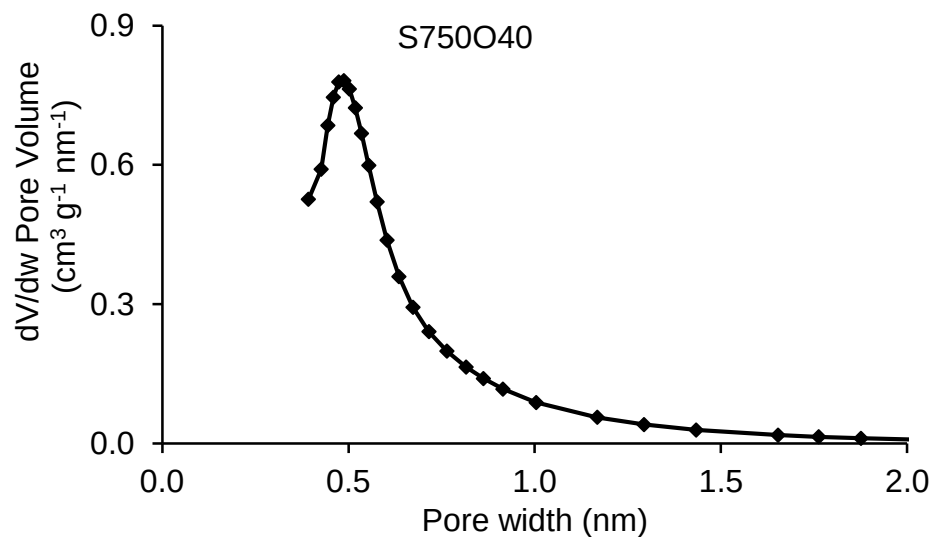
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

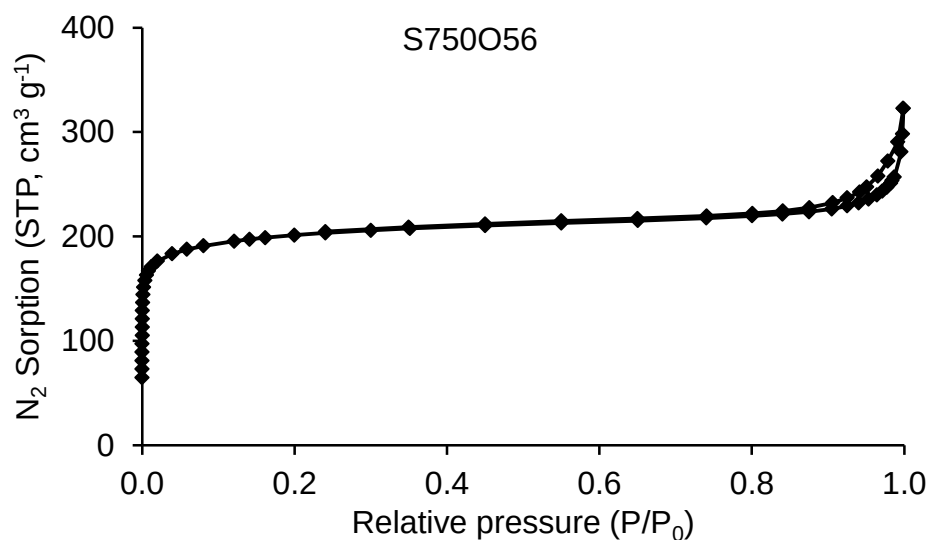


Pore distribution in the micropore region (HK method)

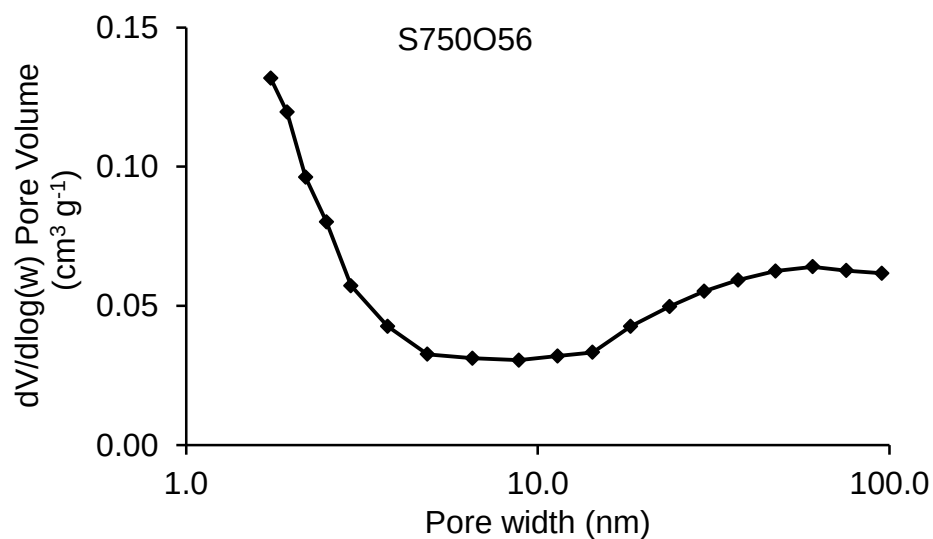


## Nitrogen adsorption isotherm and pore distribution plots for S750O56

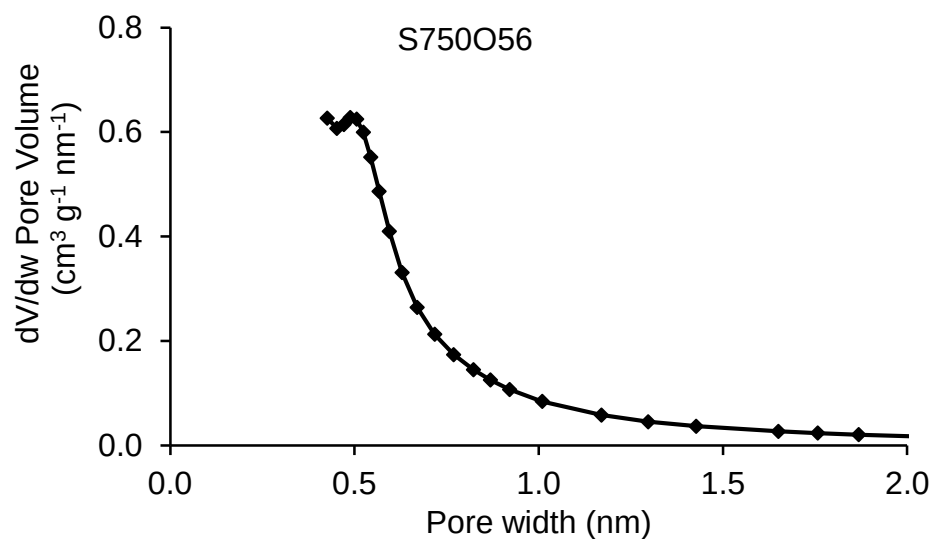
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

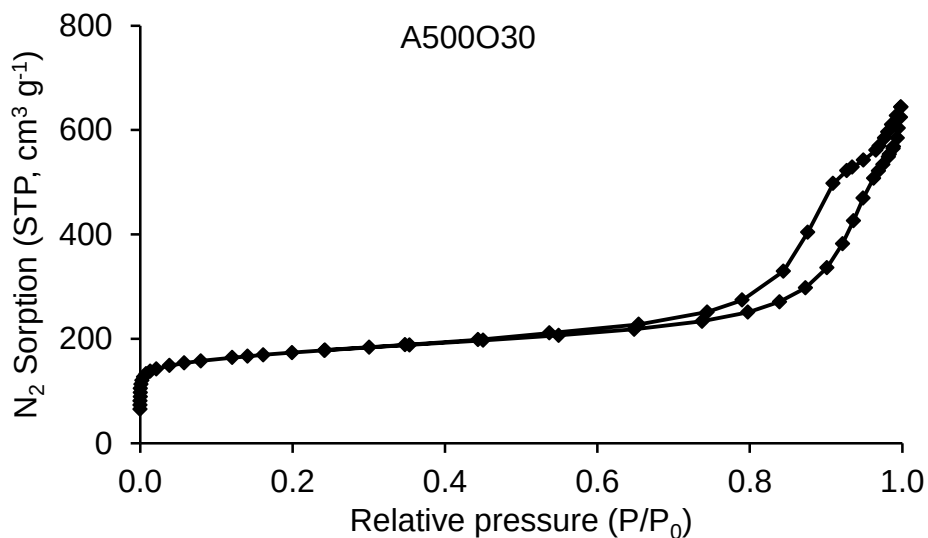


Pore distribution in the micropore region (HK method)

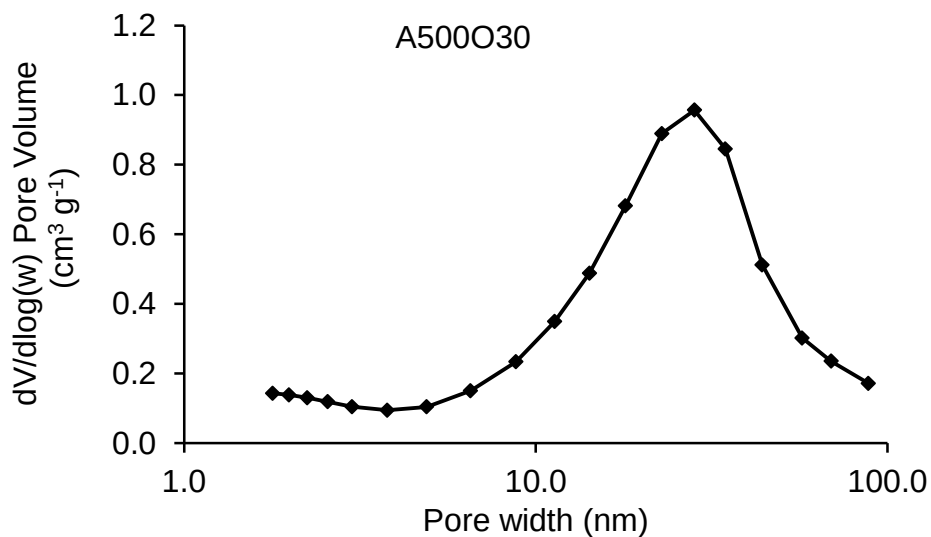


## Nitrogen adsorption isotherm and pore distribution plots for A500O30

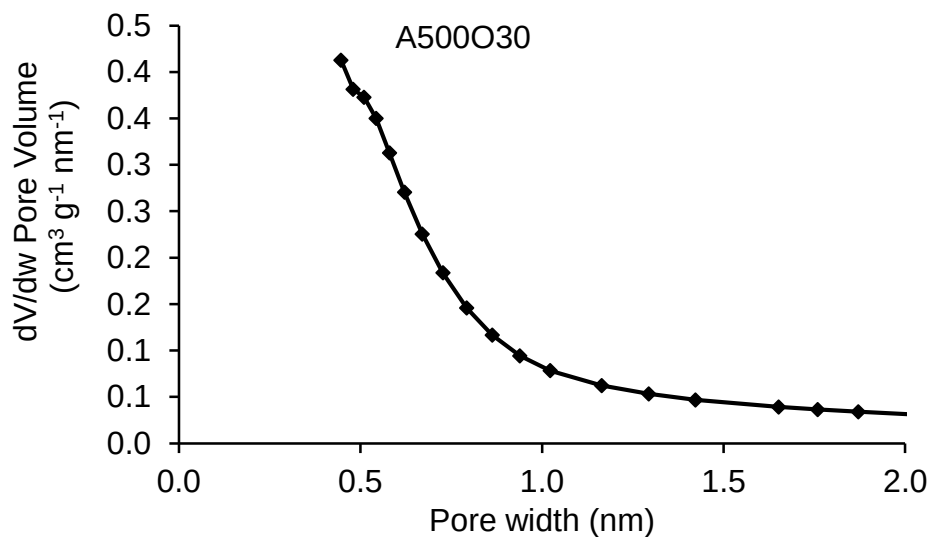
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

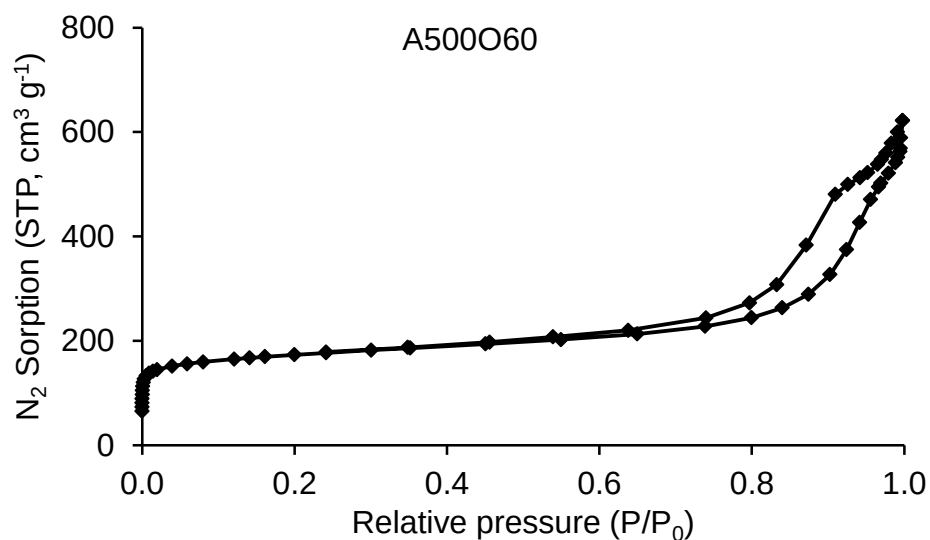


### Pore distribution in the micropore region (HK method)

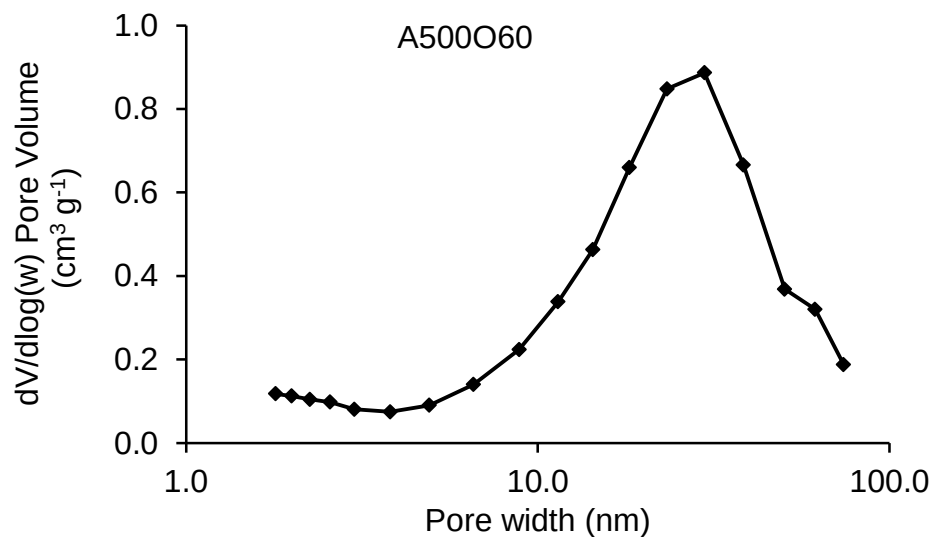


## Nitrogen adsorption isotherm and pore distribution plots for A500O60

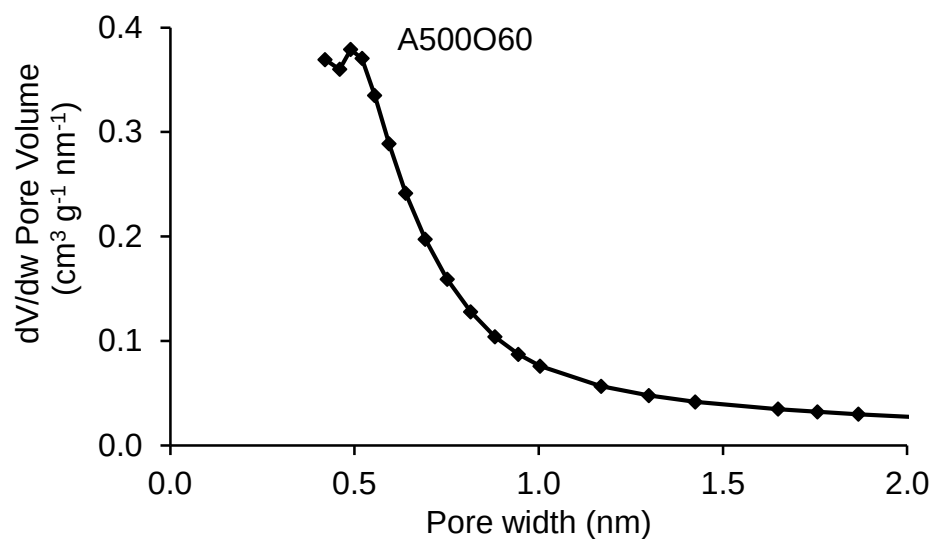
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

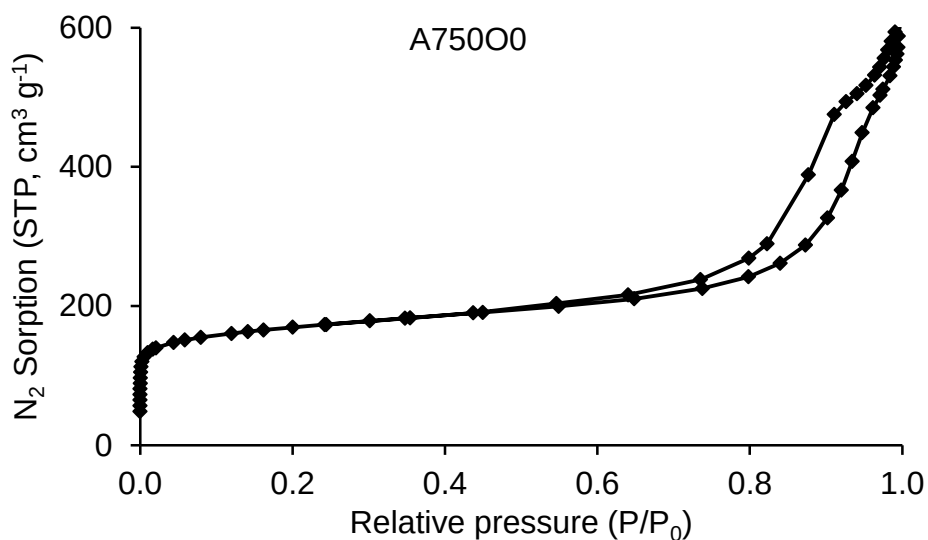


### Pore distribution in the micropore region (HK method)

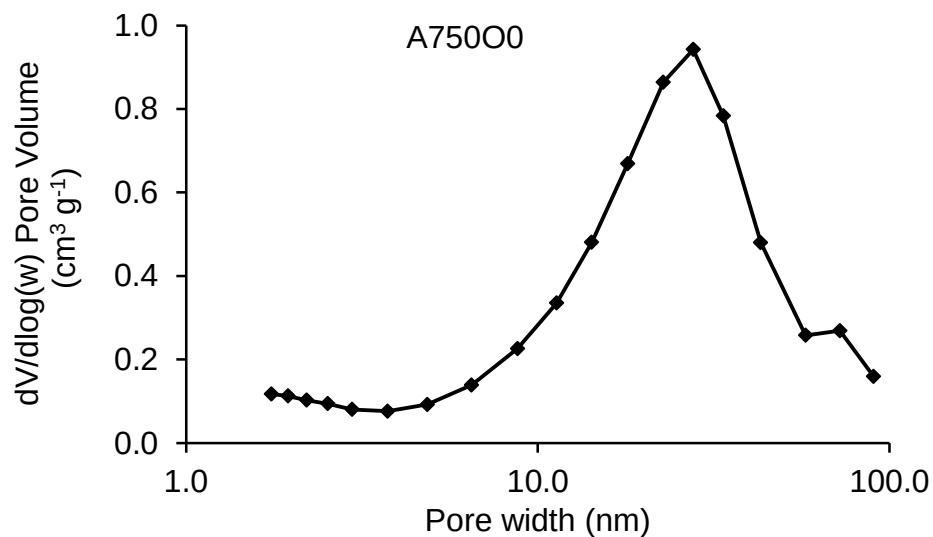


## Nitrogen adsorption isotherm and pore distribution plots for A750O0

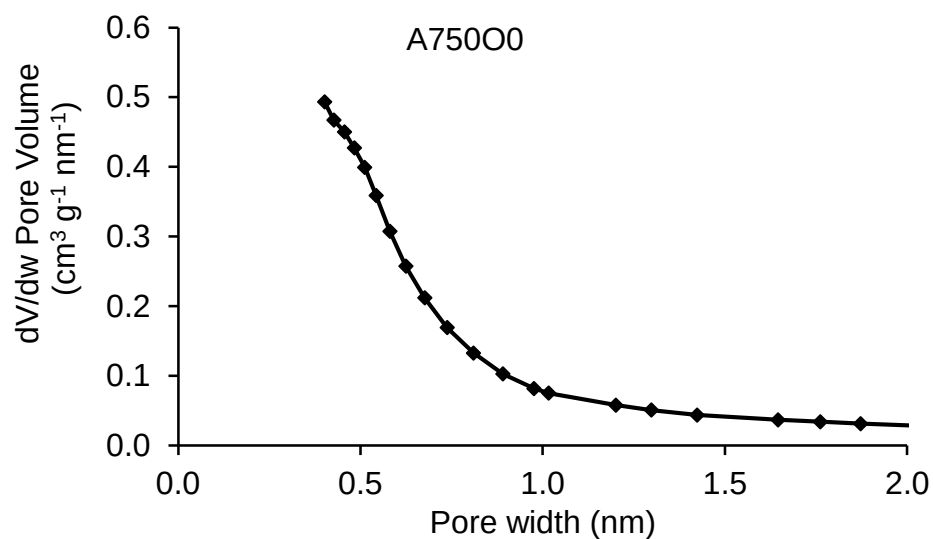
### Nitrogen adsorption isotherm (77K)



### Pore distribution in the mesopore region (BJH method)

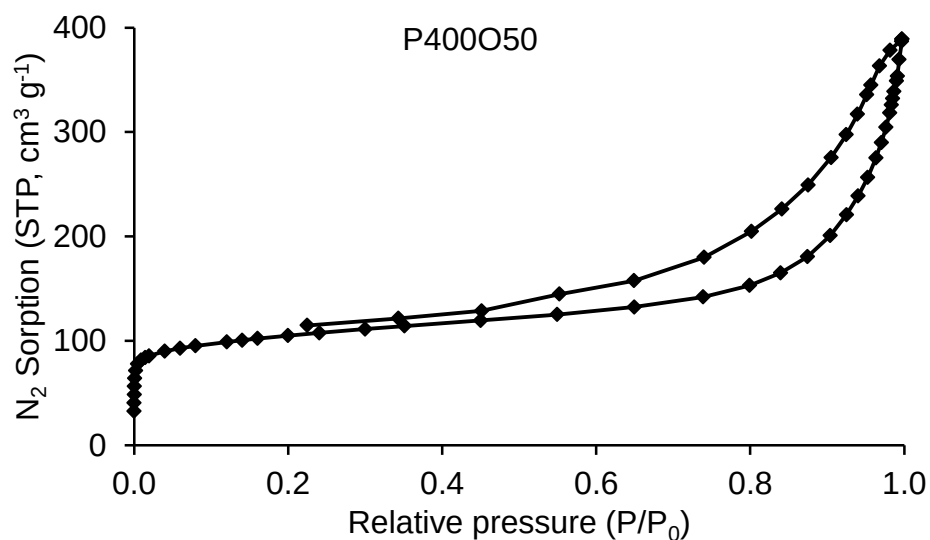


### Pore distribution in the micropore region (HK method)

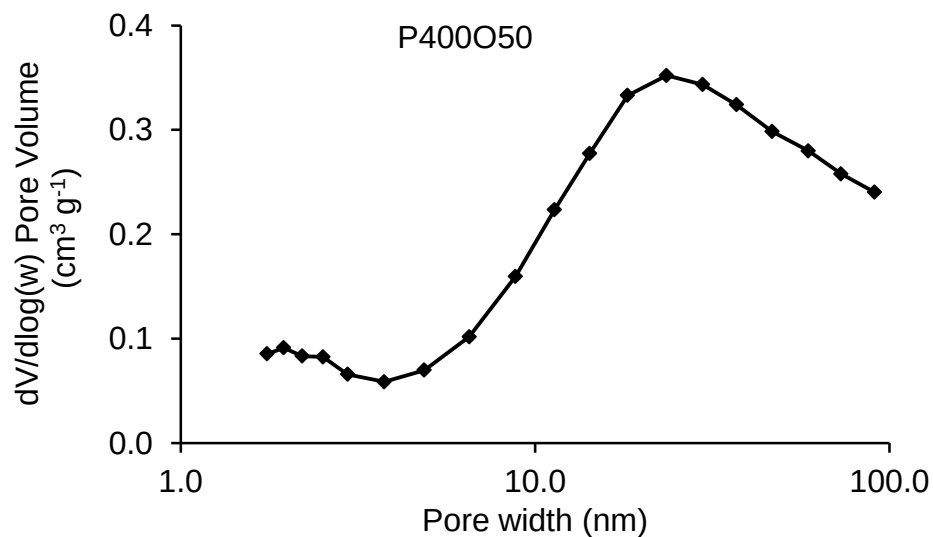


## Nitrogen adsorption isotherm and pore distribution plots for P400O50

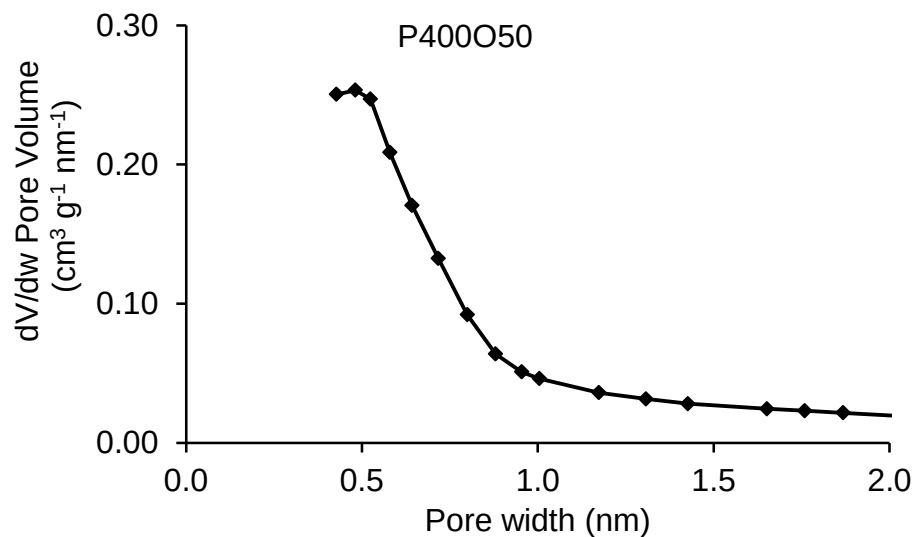
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)

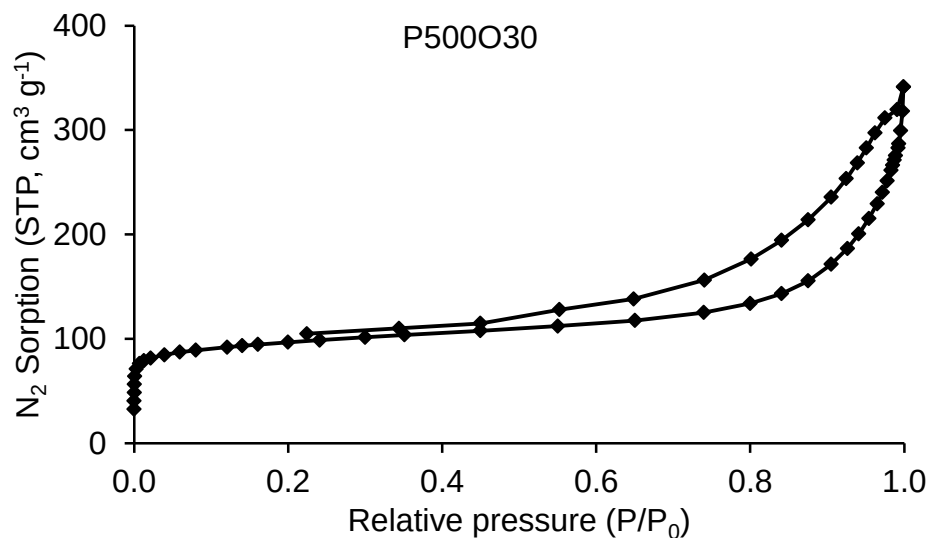


Pore distribution in the micropore region (HK method)

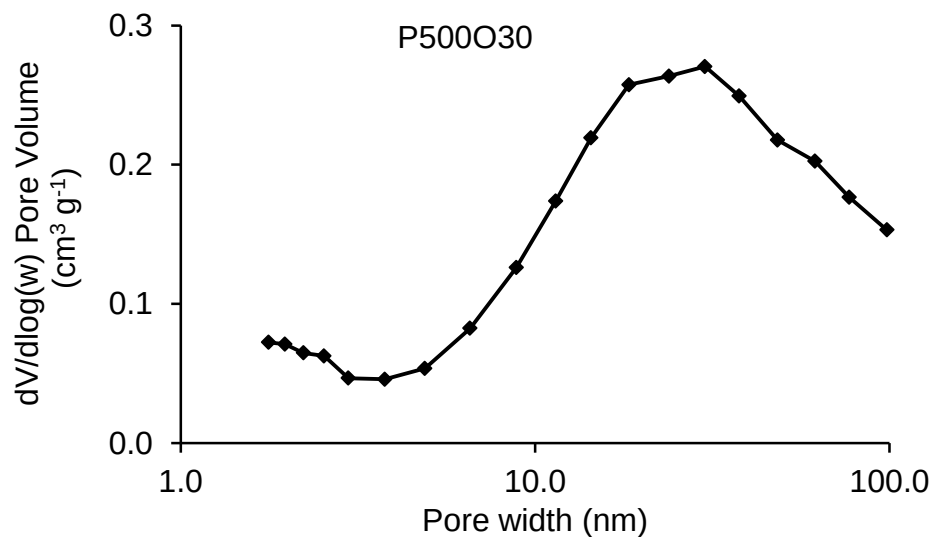


## Nitrogen adsorption isotherm and pore distribution plots for P500O30

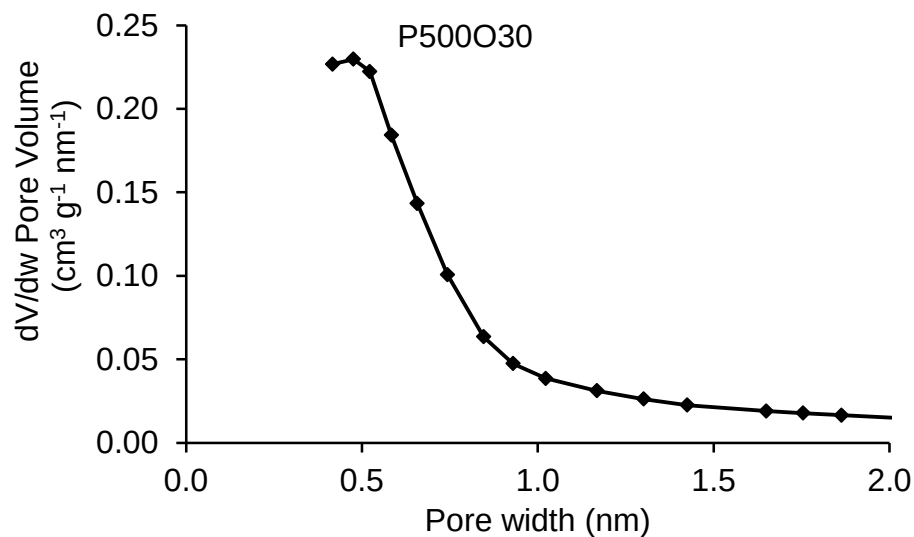
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



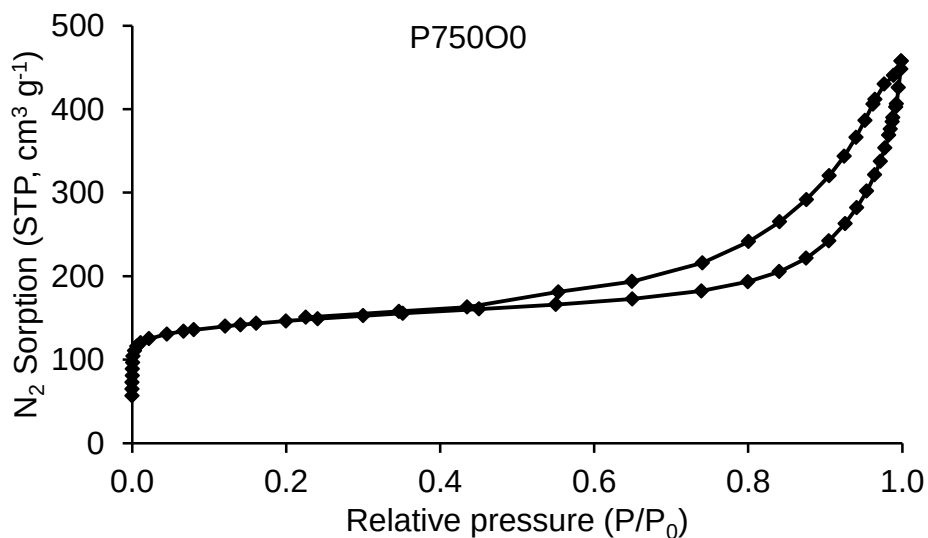
Pore distribution in the micropore region (HK method)



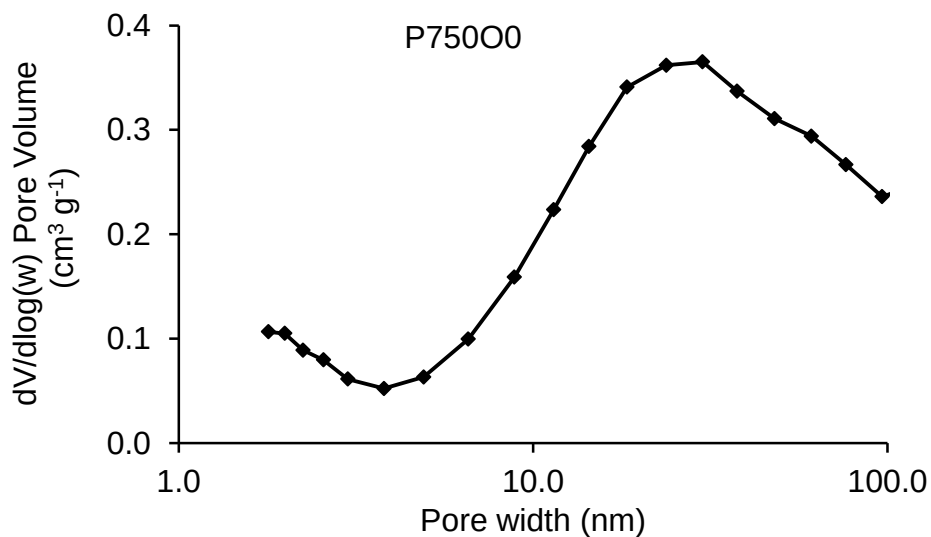


## Nitrogen adsorption isotherm and pore distribution plots for P750O0

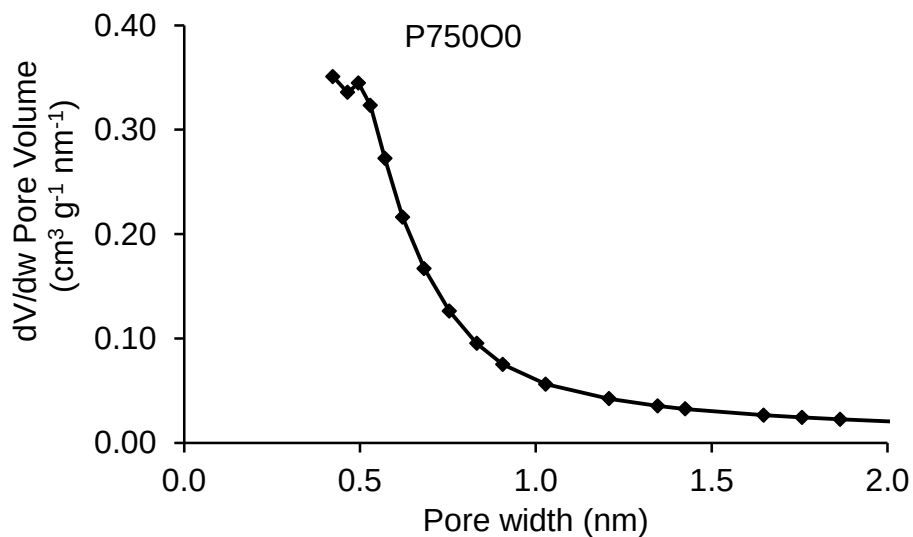
Nitrogen adsorption isotherm (77K)



Pore distribution in the mesopore region (BJH method)



Pore distribution in the micropore region (HK method)



**BET-surface areas and pore volumes for S900C15 prepared using different flow rates of CO<sub>2</sub>**

| <b>CO<sub>2</sub> flow rate (cm<sup>3</sup> min<sup>-1</sup>)</b> | <b>S<sub>BET</sub><br/>(m<sup>2</sup> g<sup>-1</sup>)</b> | <b>V<sub>micro</sub><br/>(cm<sup>3</sup> g<sup>-1</sup>)<sup>a,b</sup></b> | <b>V<sub>ultramicro</sub><br/>(cm<sup>3</sup> g<sup>-1</sup>)<sup>a</sup></b> | <b>V<sub>meso</sub><br/>(cm<sup>3</sup> g<sup>-1</sup>)<sup>c</sup></b> | <b>V<sub>total</sub><br/>(cm<sup>3</sup> g<sup>-1</sup>)<sup>d</sup></b> | <b>micropore<br/>(%)<sup>e</sup></b> | <b>ultramicropore<br/>(%)</b> |
|-------------------------------------------------------------------|-----------------------------------------------------------|----------------------------------------------------------------------------|-------------------------------------------------------------------------------|-------------------------------------------------------------------------|--------------------------------------------------------------------------|--------------------------------------|-------------------------------|
| 25                                                                | 873                                                       | 0.35                                                                       | 0.27                                                                          | 0.35                                                                    | 0.70                                                                     | 50.0                                 | 38.6                          |
| 50                                                                | 983                                                       | 0.39                                                                       | 0.31                                                                          | 0.38                                                                    | 0.77                                                                     | 50.6                                 | 40.3                          |
| 100                                                               | 1,020                                                     | 0.41                                                                       | 0.31                                                                          | 0.52                                                                    | 0.94                                                                     | 43.6                                 | 33.0                          |

a) Calculated based on the HK model.

b) Includes the ultramicropore volume.

c) Calculated based on the BJH model.

d) Determined from nitrogen adsorbed at P/P<sub>0</sub>=0.99.

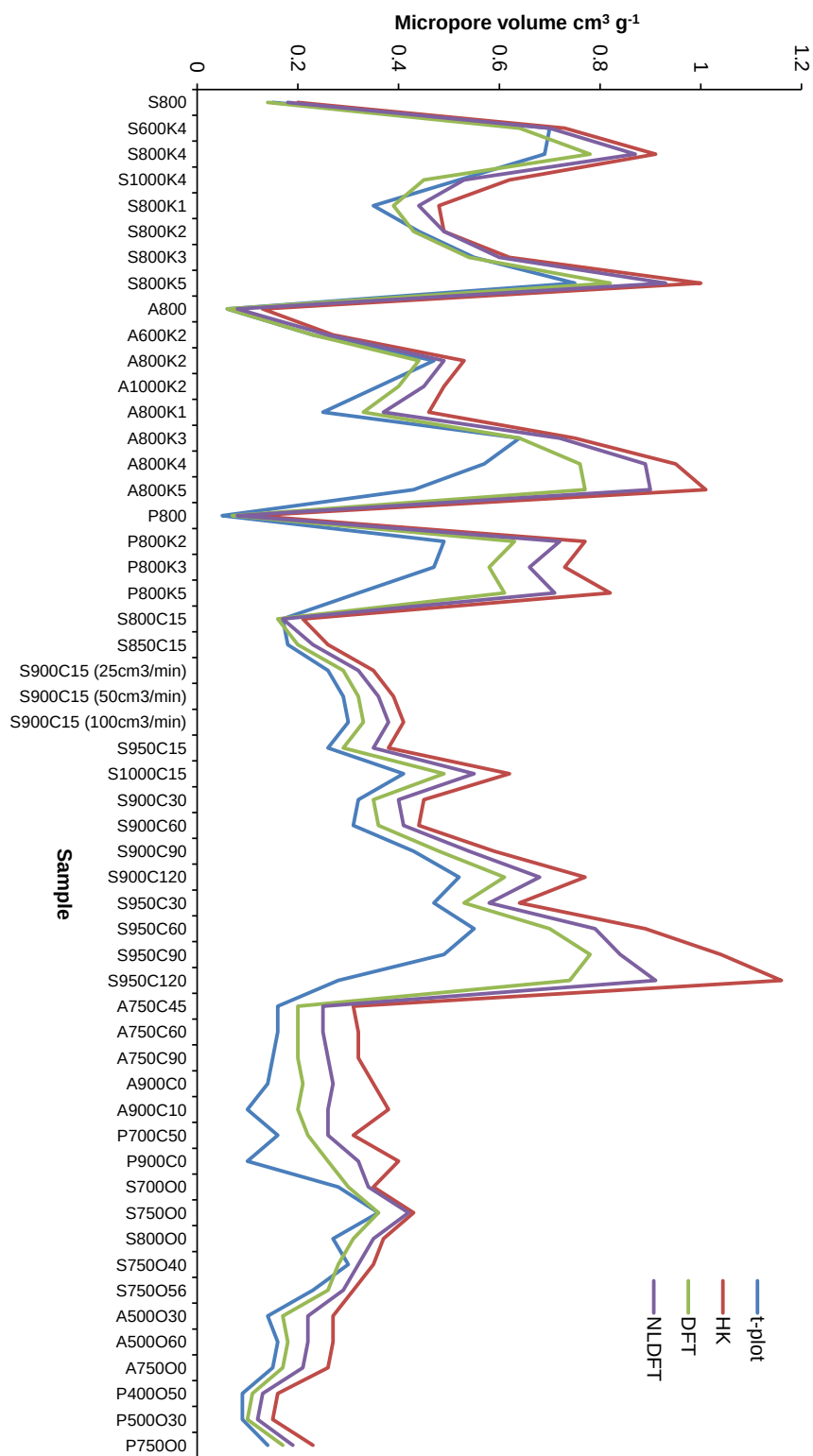
e) Includes the ultramicropore %.

## Comparison of various isotherm models

Determination of  $V_{\text{micro}}$  ( $\text{cm}^3 \text{g}^{-1}$ )

| Material                          | t-plot | HK   | DFT  | NLDFT |
|-----------------------------------|--------|------|------|-------|
| S800                              | 0.15   | 0.20 | 0.14 | 0.18  |
| S600K4                            | 0.70   | 0.73 | 0.64 | 0.70  |
| S800K4                            | 0.69   | 0.91 | 0.78 | 0.87  |
| S1000K4                           | 0.52   | 0.62 | 0.45 | 0.53  |
| S800K1                            | 0.35   | 0.48 | 0.39 | 0.44  |
| S800K2                            | 0.44   | 0.49 | 0.43 | 0.49  |
| S800K3                            | 0.55   | 0.62 | 0.54 | 0.60  |
| S800K5                            | 0.75   | 1.00 | 0.82 | 0.93  |
| A800                              | 0.06   | 0.13 | 0.06 | 0.08  |
| A600K2                            | 0.23   | 0.27 | 0.23 | 0.26  |
| A800K2                            | 0.47   | 0.53 | 0.44 | 0.49  |
| A1000K2                           | 0.36   | 0.49 | 0.40 | 0.45  |
| A800K1                            | 0.25   | 0.46 | 0.33 | 0.37  |
| A800K3                            | 0.64   | 0.75 | 0.64 | 0.72  |
| A800K4                            | 0.57   | 0.95 | 0.76 | 0.89  |
| A800K5                            | 0.43   | 1.01 | 0.77 | 0.90  |
| P800                              | 0.05   | 0.11 | 0.07 | 0.08  |
| P800K2                            | 0.49   | 0.77 | 0.63 | 0.72  |
| P800K3                            | 0.47   | 0.73 | 0.58 | 0.66  |
| P800K5                            | 0.32   | 0.82 | 0.61 | 0.71  |
| S800C15                           | 0.17   | 0.21 | 0.16 | 0.17  |
| S850C15                           | 0.18   | 0.26 | 0.20 | 0.23  |
| S900C15 (25cm <sup>3</sup> /min)  | 0.26   | 0.35 | 0.29 | 0.32  |
| S900C15 (50cm <sup>3</sup> /min)  | 0.29   | 0.39 | 0.32 | 0.36  |
| S900C15 (100cm <sup>3</sup> /min) | 0.30   | 0.41 | 0.33 | 0.38  |
| S950C15                           | 0.26   | 0.38 | 0.29 | 0.35  |
| S1000C15                          | 0.41   | 0.62 | 0.49 | 0.55  |
| S900C30                           | 0.32   | 0.45 | 0.35 | 0.40  |
| S900C60                           | 0.31   | 0.44 | 0.36 | 0.41  |
| S900C90                           | 0.43   | 0.59 | 0.48 | 0.54  |
| S900C120                          | 0.52   | 0.77 | 0.61 | 0.68  |
| S950C30                           | 0.47   | 0.64 | 0.53 | 0.58  |
| S950C60                           | 0.55   | 0.89 | 0.70 | 0.79  |
| S950C90                           | 0.49   | 1.04 | 0.78 | 0.84  |
| S950C120                          | 0.28   | 1.16 | 0.74 | 0.91  |
| A750C45                           | 0.16   | 0.31 | 0.20 | 0.25  |
| A750C60                           | 0.16   | 0.32 | 0.20 | 0.25  |
| A750C90                           | 0.15   | 0.32 | 0.20 | 0.26  |
| A900C0                            | 0.14   | 0.35 | 0.21 | 0.27  |
| A900C10                           | 0.10   | 0.38 | 0.20 | 0.26  |
| P700C50                           | 0.16   | 0.31 | 0.22 | 0.26  |
| P900C0                            | 0.10   | 0.40 | 0.26 | 0.32  |
| S700O0                            | 0.28   | 0.35 | 0.30 | 0.34  |
| S750O0                            | 0.36   | 0.43 | 0.36 | 0.42  |
| S800O0                            | 0.27   | 0.37 | 0.31 | 0.35  |

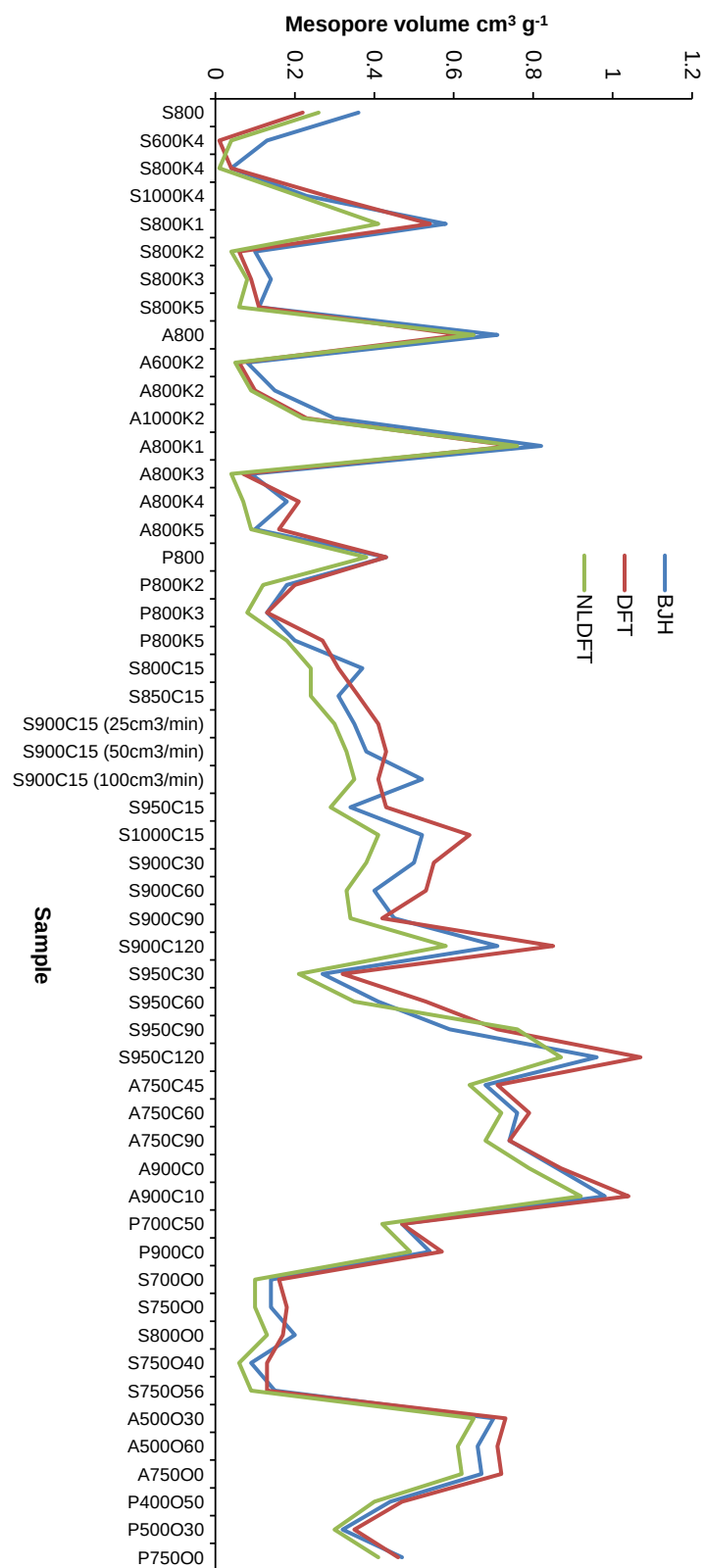
| Material | t-plot | HK   | DFT  | NLDFT |
|----------|--------|------|------|-------|
| S750O40  | 0.30   | 0.35 | 0.28 | 0.32  |
| S750O56  | 0.23   | 0.31 | 0.26 | 0.29  |
| A500O30  | 0.14   | 0.27 | 0.17 | 0.22  |
| A500O60  | 0.16   | 0.27 | 0.18 | 0.22  |
| A750O0   | 0.15   | 0.26 | 0.17 | 0.21  |
| P400O50  | 0.09   | 0.16 | 0.11 | 0.13  |
| P500O30  | 0.09   | 0.15 | 0.10 | 0.12  |
| P750O0   | 0.14   | 0.23 | 0.17 | 0.19  |



Determination of  $V_{\text{meso}}$  ( $\text{cm}^3 \text{g}^{-1}$ )

| Material                          | BJH  | DFT  | NLDFT |
|-----------------------------------|------|------|-------|
| S800                              | 0.36 | 0.22 | 0.26  |
| S600K4                            | 0.13 | 0.01 | 0.04  |
| S800K4                            | 0.04 | 0.04 | 0.01  |
| S1000K4                           | 0.23 | 0.28 | 0.21  |
| S800K1                            | 0.58 | 0.54 | 0.41  |
| S800K2                            | 0.10 | 0.06 | 0.04  |
| S800K3                            | 0.14 | 0.09 | 0.08  |
| S800K5                            | 0.11 | 0.11 | 0.06  |
| A800                              | 0.71 | 0.62 | 0.65  |
| A600K2                            | 0.08 | 0.06 | 0.05  |
| A800K2                            | 0.15 | 0.10 | 0.09  |
| A1000K2                           | 0.30 | 0.23 | 0.22  |
| A800K1                            | 0.82 | 0.75 | 0.76  |
| A800K3                            | 0.09 | 0.07 | 0.04  |
| A800K4                            | 0.18 | 0.21 | 0.07  |
| A800K5                            | 0.10 | 0.16 | 0.09  |
| P800                              | 0.43 | 0.43 | 0.38  |
| P800K2                            | 0.18 | 0.20 | 0.12  |
| P800K3                            | 0.13 | 0.13 | 0.08  |
| P800K5                            | 0.20 | 0.27 | 0.18  |
| S800C15                           | 0.37 | 0.31 | 0.24  |
| S850C15                           | 0.31 | 0.36 | 0.24  |
| S900C15 (25cm <sup>3</sup> /min)  | 0.35 | 0.41 | 0.30  |
| S900C15 (50cm <sup>3</sup> /min)  | 0.38 | 0.43 | 0.33  |
| S900C15 (100cm <sup>3</sup> /min) | 0.52 | 0.41 | 0.35  |
| S950C15                           | 0.34 | 0.43 | 0.29  |
| S1000C15                          | 0.52 | 0.64 | 0.41  |
| S900C30                           | 0.50 | 0.55 | 0.38  |
| S900C60                           | 0.40 | 0.53 | 0.33  |
| S900C90                           | 0.45 | 0.42 | 0.34  |
| S900C120                          | 0.71 | 0.85 | 0.58  |
| S950C30                           | 0.27 | 0.32 | 0.21  |
| S950C60                           | 0.41 | 0.53 | 0.35  |
| S950C90                           | 0.59 | 0.71 | 0.76  |
| S950C120                          | 0.96 | 1.07 | 0.87  |
| A750C45                           | 0.68 | 0.71 | 0.64  |
| A750C60                           | 0.76 | 0.79 | 0.72  |
| A750C90                           | 0.74 | 0.74 | 0.68  |
| A900C0                            | 0.86 | 0.87 | 0.79  |
| A900C10                           | 0.98 | 1.04 | 0.92  |
| P700C50                           | 0.47 | 0.47 | 0.42  |
| P900C0                            | 0.54 | 0.57 | 0.49  |
| S700O0                            | 0.14 | 0.16 | 0.10  |
| S750O0                            | 0.14 | 0.18 | 0.10  |
| S800O0                            | 0.20 | 0.17 | 0.13  |
| S750O40                           | 0.09 | 0.13 | 0.06  |
| S750O56                           | 0.15 | 0.13 | 0.09  |

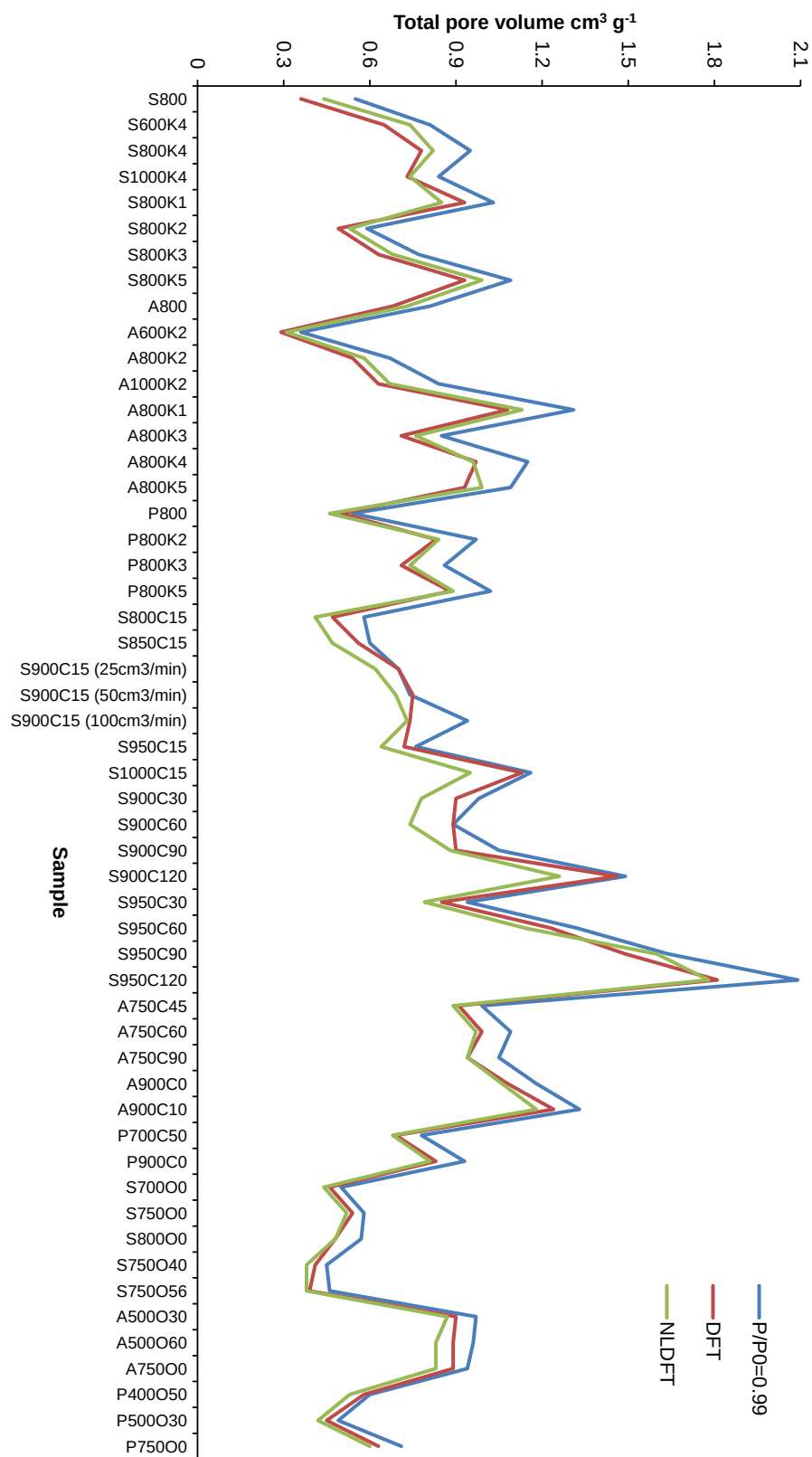
| Material | BJH  | DFT  | NLDFT |
|----------|------|------|-------|
| A500O30  | 0.70 | 0.73 | 0.65  |
| A500O60  | 0.66 | 0.71 | 0.61  |
| A750O0   | 0.67 | 0.72 | 0.62  |
| P400O50  | 0.44 | 0.47 | 0.40  |
| P500O30  | 0.32 | 0.35 | 0.30  |
| P750O0   | 0.47 | 0.46 | 0.41  |



Determination of  $V_{\text{total}}$  ( $\text{cm}^3 \text{g}^{-1}$ )

| Material                          | P/P <sub>0</sub> =0.99 | DFT  | NLDFT |
|-----------------------------------|------------------------|------|-------|
| S800                              | 0.55                   | 0.36 | 0.44  |
| S600K4                            | 0.81                   | 0.65 | 0.74  |
| S800K4                            | 0.95                   | 0.78 | 0.82  |
| S1000K4                           | 0.84                   | 0.73 | 0.74  |
| S800K1                            | 1.03                   | 0.93 | 0.85  |
| S800K2                            | 0.59                   | 0.49 | 0.53  |
| S800K3                            | 0.77                   | 0.63 | 0.68  |
| S800K5                            | 1.09                   | 0.93 | 0.99  |
| A800                              | 0.81                   | 0.68 | 0.73  |
| A600K2                            | 0.36                   | 0.29 | 0.31  |
| A800K2                            | 0.67                   | 0.54 | 0.58  |
| A1000K2                           | 0.84                   | 0.63 | 0.67  |
| A800K1                            | 1.31                   | 1.08 | 1.13  |
| A800K3                            | 0.85                   | 0.71 | 0.76  |
| A800K4                            | 1.15                   | 0.97 | 0.96  |
| A800K5                            | 1.09                   | 0.93 | 0.99  |
| P800                              | 0.54                   | 0.50 | 0.46  |
| P800K2                            | 0.97                   | 0.83 | 0.84  |
| P800K3                            | 0.86                   | 0.71 | 0.74  |
| P800K5                            | 1.02                   | 0.88 | 0.89  |
| S800C15                           | 0.58                   | 0.47 | 0.41  |
| S850C15                           | 0.60                   | 0.56 | 0.47  |
| S900C15 (25cm <sup>3</sup> /min)  | 0.70                   | 0.70 | 0.62  |
| S900C15 (50cm <sup>3</sup> /min)  | 0.74                   | 0.75 | 0.69  |
| S900C15 (100cm <sup>3</sup> /min) | 0.94                   | 0.74 | 0.73  |
| S950C15                           | 0.76                   | 0.72 | 0.64  |
| S1000C15                          | 1.16                   | 1.13 | 0.95  |
| S900C30                           | 0.98                   | 0.90 | 0.78  |
| S900C60                           | 0.89                   | 0.89 | 0.74  |
| S900C90                           | 1.05                   | 0.90 | 0.88  |
| S900C120                          | 1.49                   | 1.46 | 1.26  |
| S950C30                           | 0.94                   | 0.85 | 0.79  |
| S950C60                           | 1.32                   | 1.23 | 1.14  |
| S950C90                           | 1.64                   | 1.49 | 1.60  |
| S950C120                          | 2.09                   | 1.81 | 1.78  |
| A750C45                           | 0.99                   | 0.91 | 0.89  |
| A750C60                           | 1.09                   | 0.99 | 0.97  |
| A750C90                           | 1.05                   | 0.94 | 0.94  |
| A900C0                            | 1.18                   | 1.08 | 1.06  |
| A900C10                           | 1.33                   | 1.24 | 1.18  |
| P700C50                           | 0.78                   | 0.69 | 0.68  |
| P900C0                            | 0.93                   | 0.83 | 0.81  |
| S700O0                            | 0.50                   | 0.46 | 0.44  |
| S750O0                            | 0.58                   | 0.54 | 0.52  |
| S800O0                            | 0.57                   | 0.48 | 0.48  |
| S750O40                           | 0.45                   | 0.41 | 0.38  |
| S750O56                           | 0.46                   | 0.39 | 0.38  |

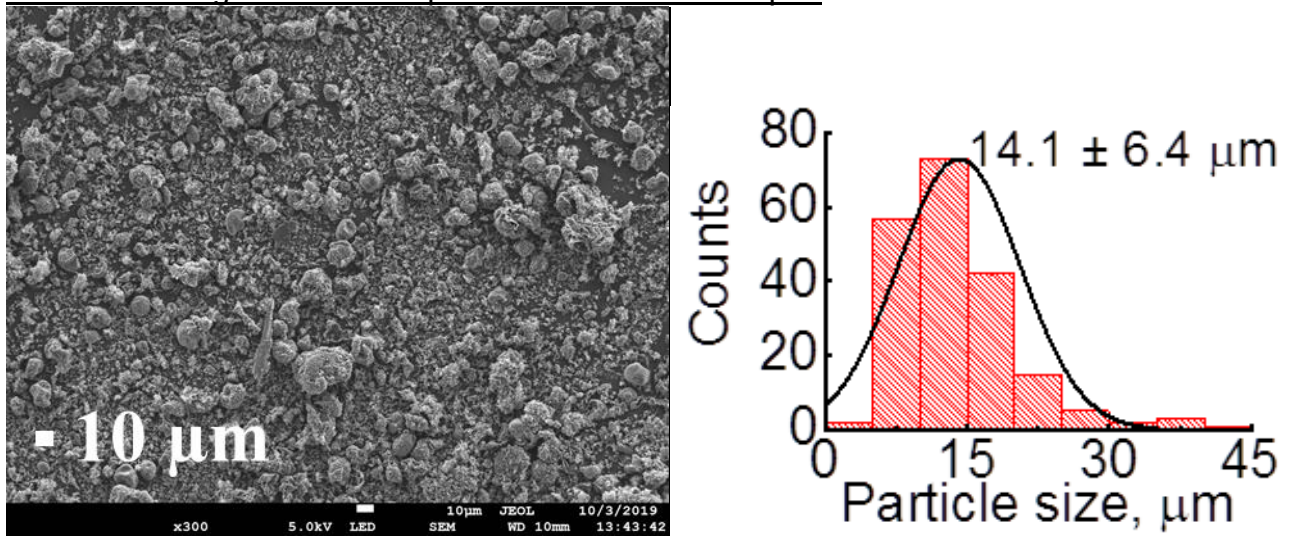
| Material | $P/P_0=0.99$ | DFT  | NLDFT |
|----------|--------------|------|-------|
| A500O30  | 0.97         | 0.90 | 0.87  |
| A500O60  | 0.96         | 0.89 | 0.83  |
| A750O0   | 0.94         | 0.89 | 0.83  |
| P400O50  | 0.60         | 0.58 | 0.53  |
| P500O30  | 0.49         | 0.45 | 0.42  |
| P750O0   | 0.71         | 0.63 | 0.60  |



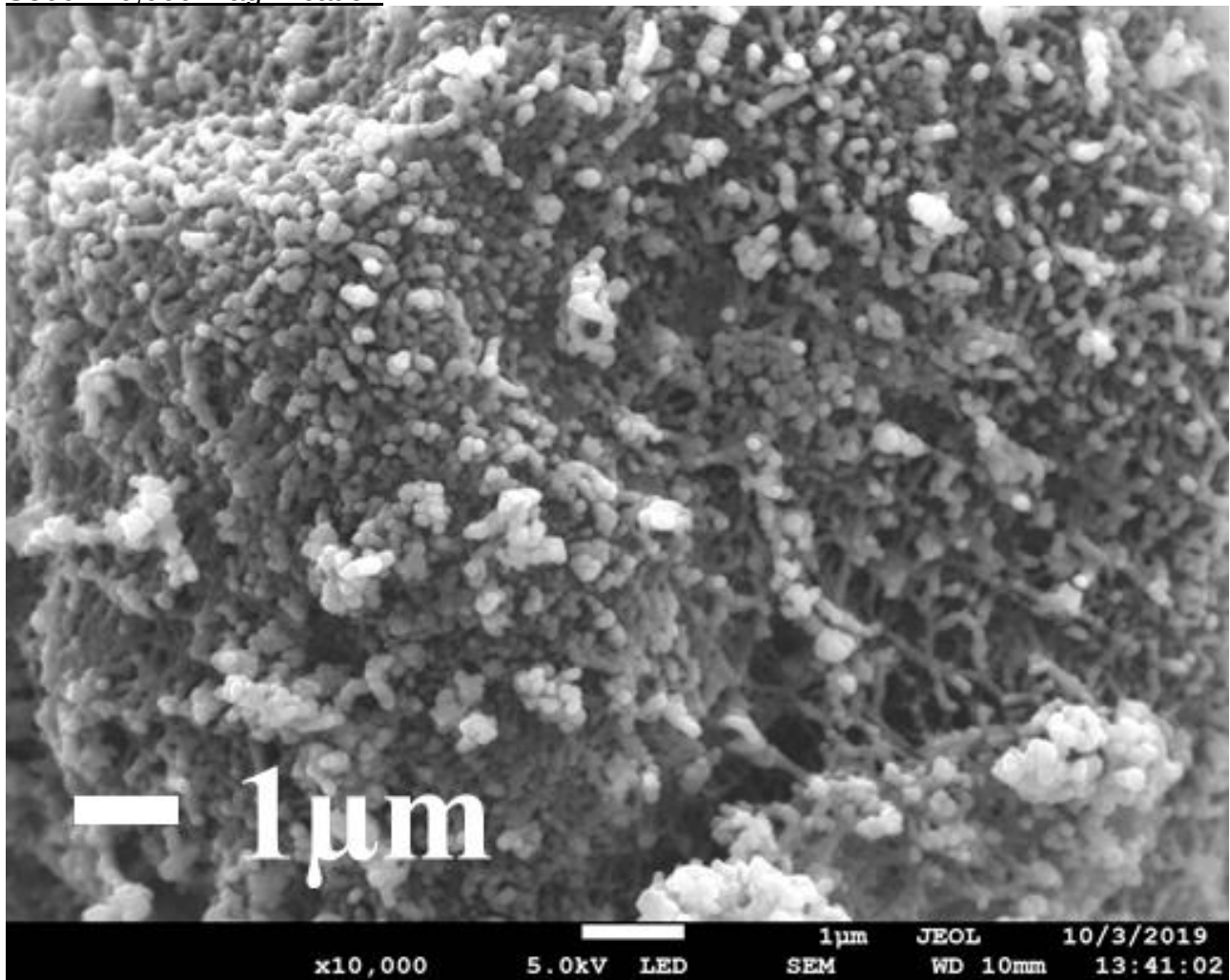


## SEM Images for S800

S800 x300 magnification and particle size distribution plot

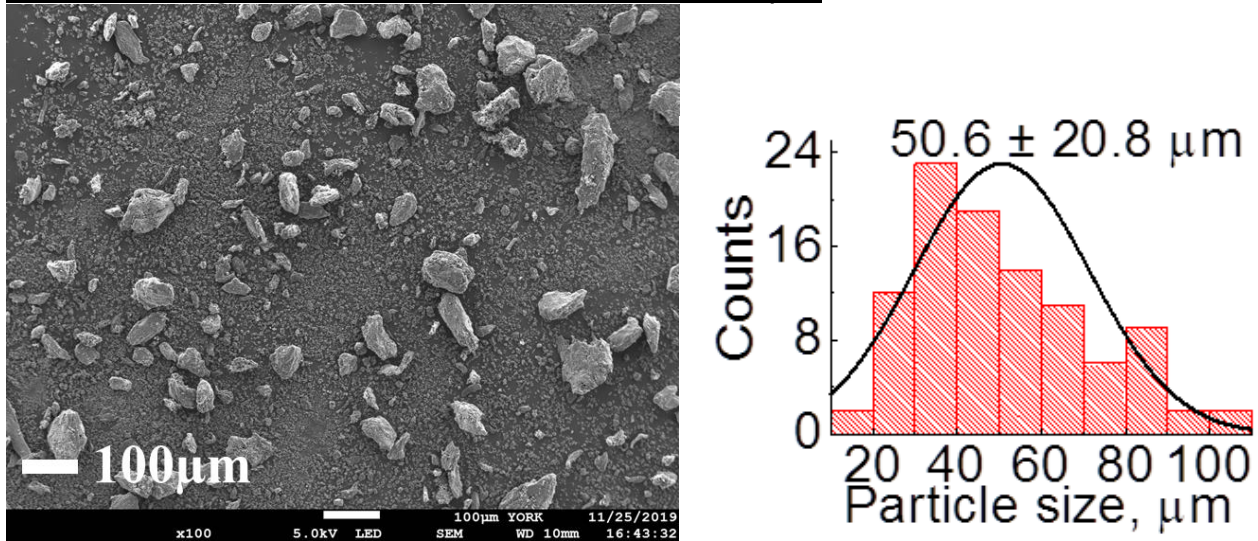


S800 x10,000 magnification

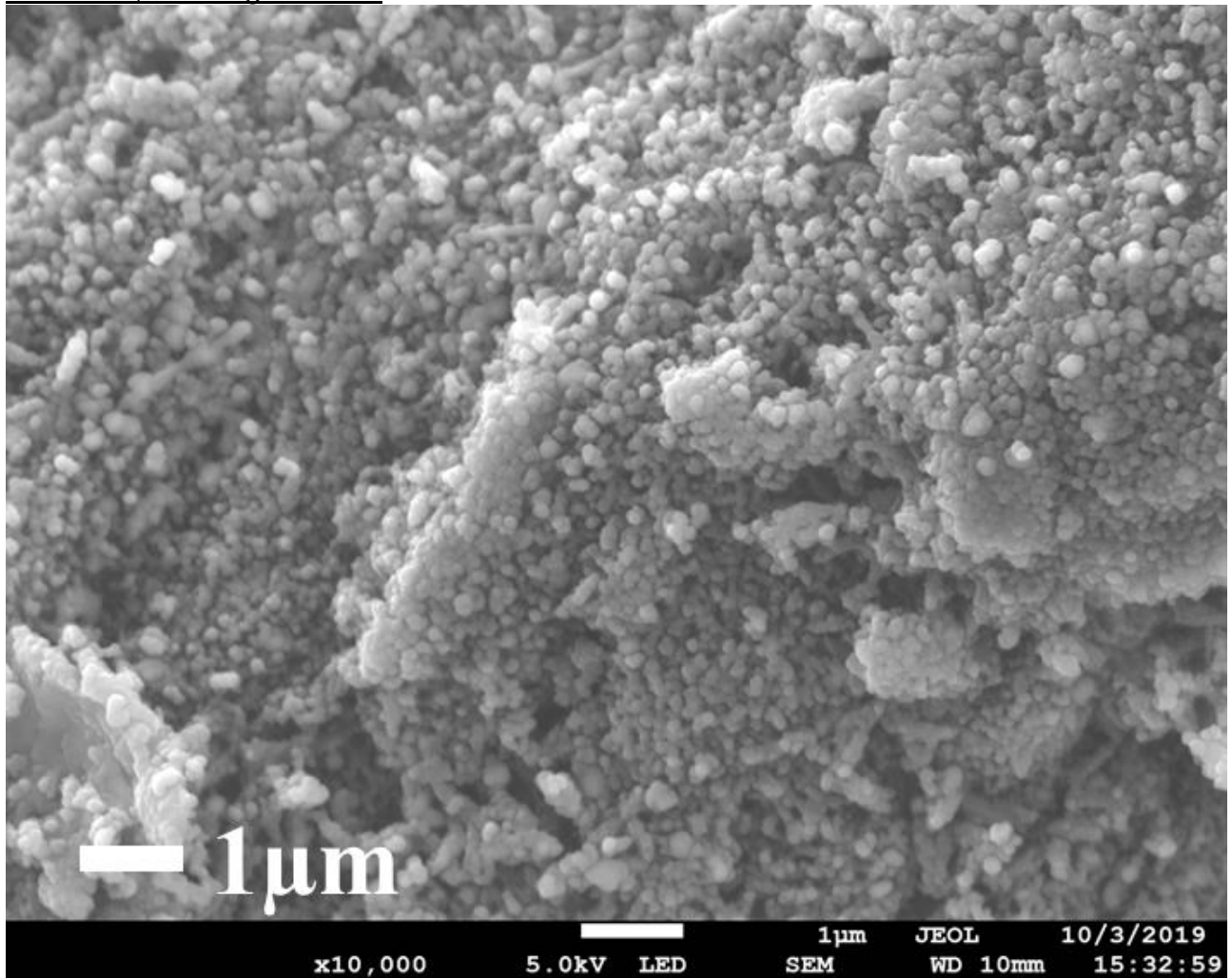


## SEM Images for A800

A800 x100 magnification and particle size distribution plot



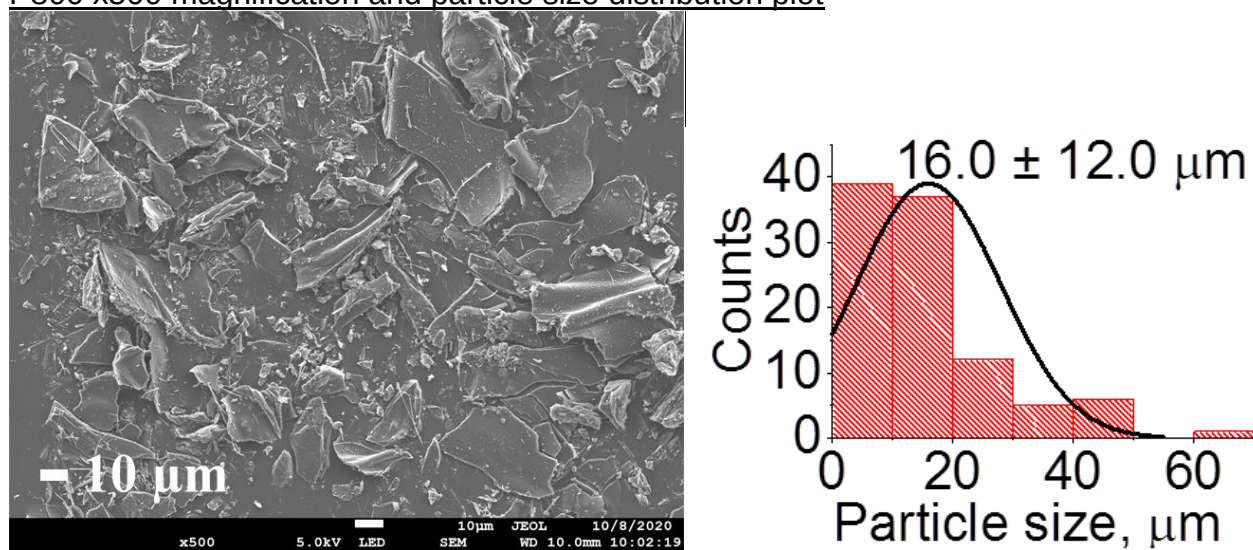
A800 x10,000 magnification



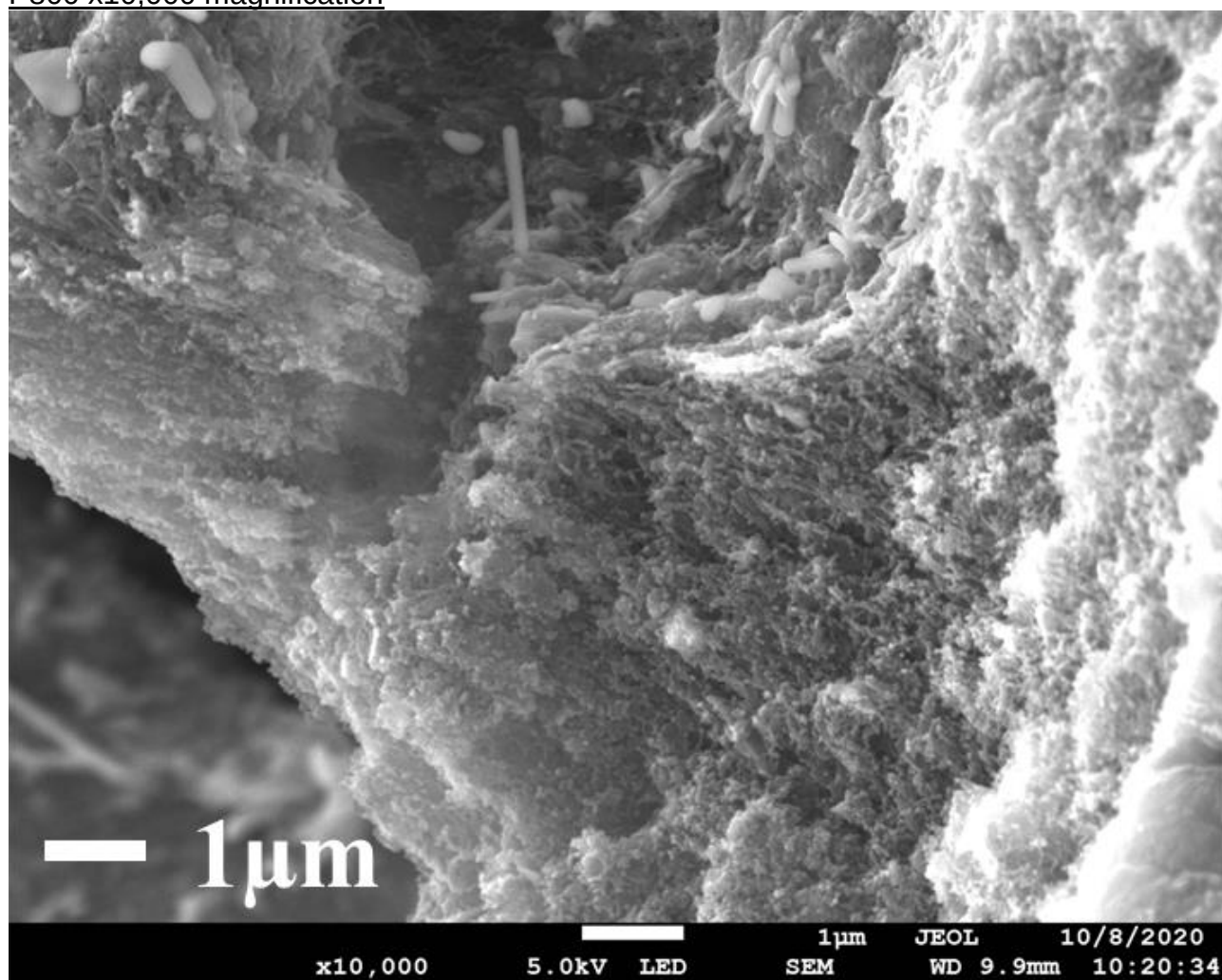


## SEM Images for P800

P800 x500 magnification and particle size distribution plot

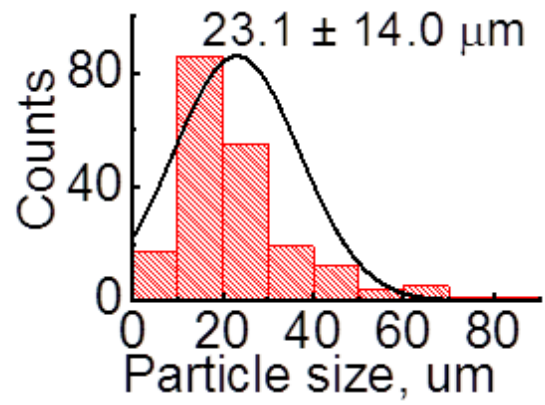
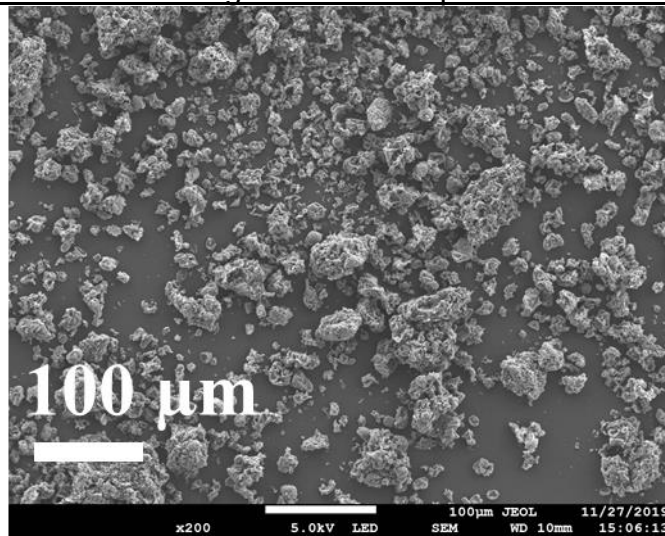


P800 x10,000 magnification

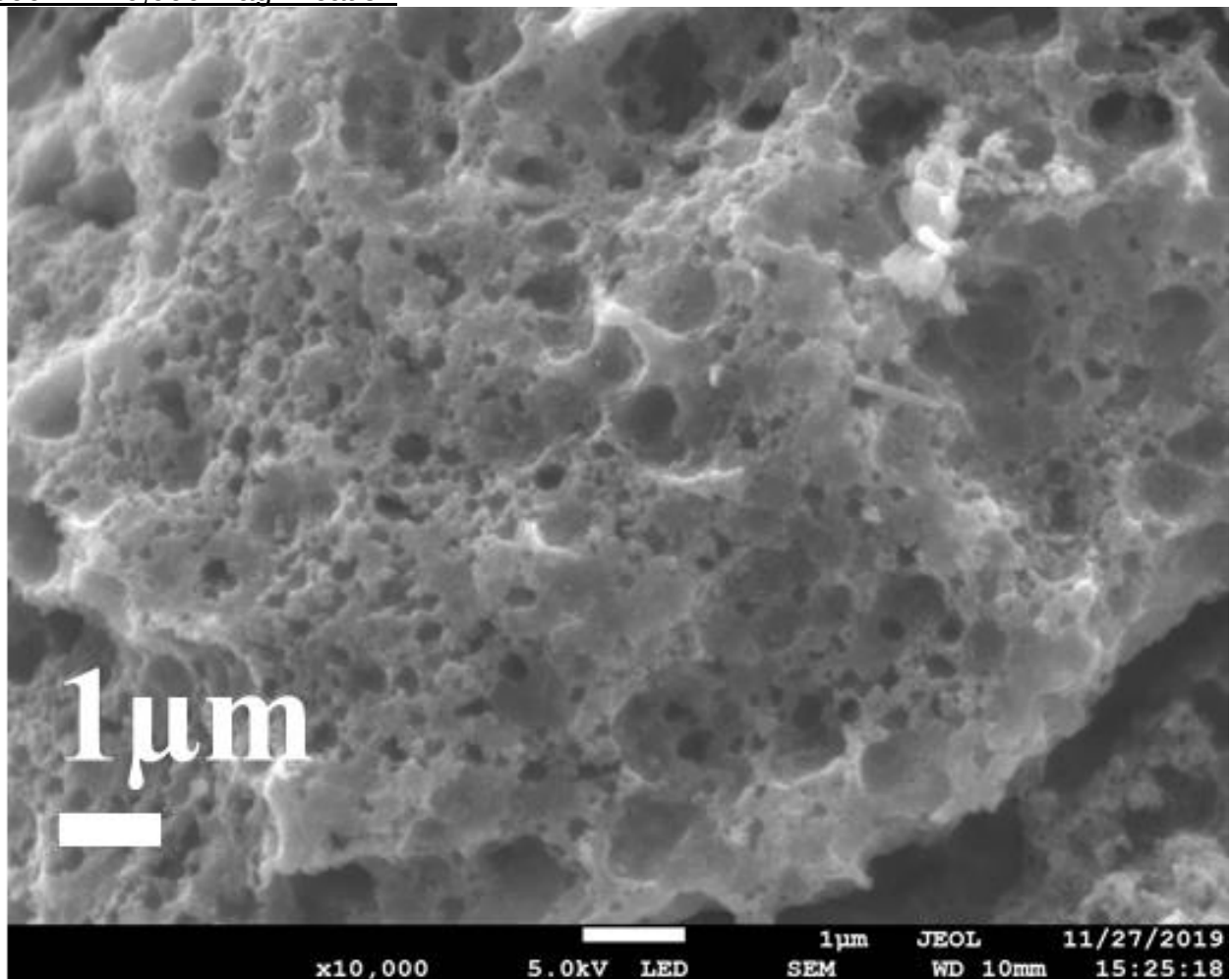


## SEM Images for S800K1

S800K1 x200 magnification and particle size distribution plot



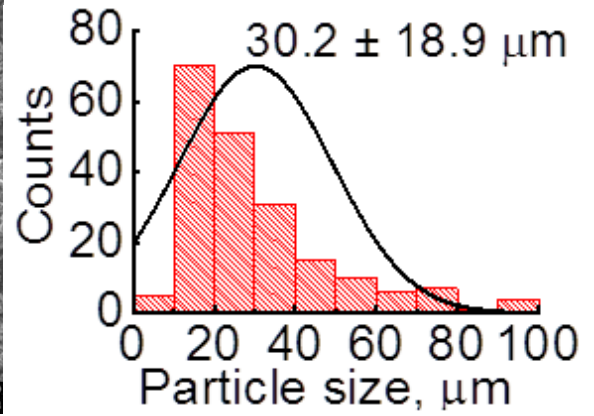
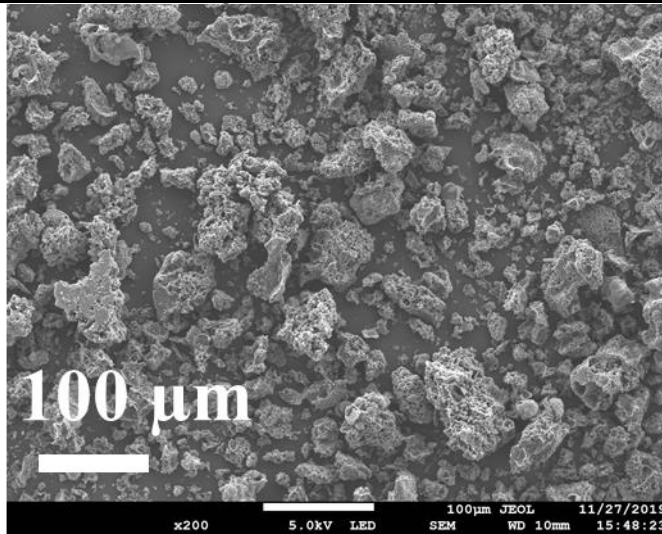
S800K1 x10,000 magnification



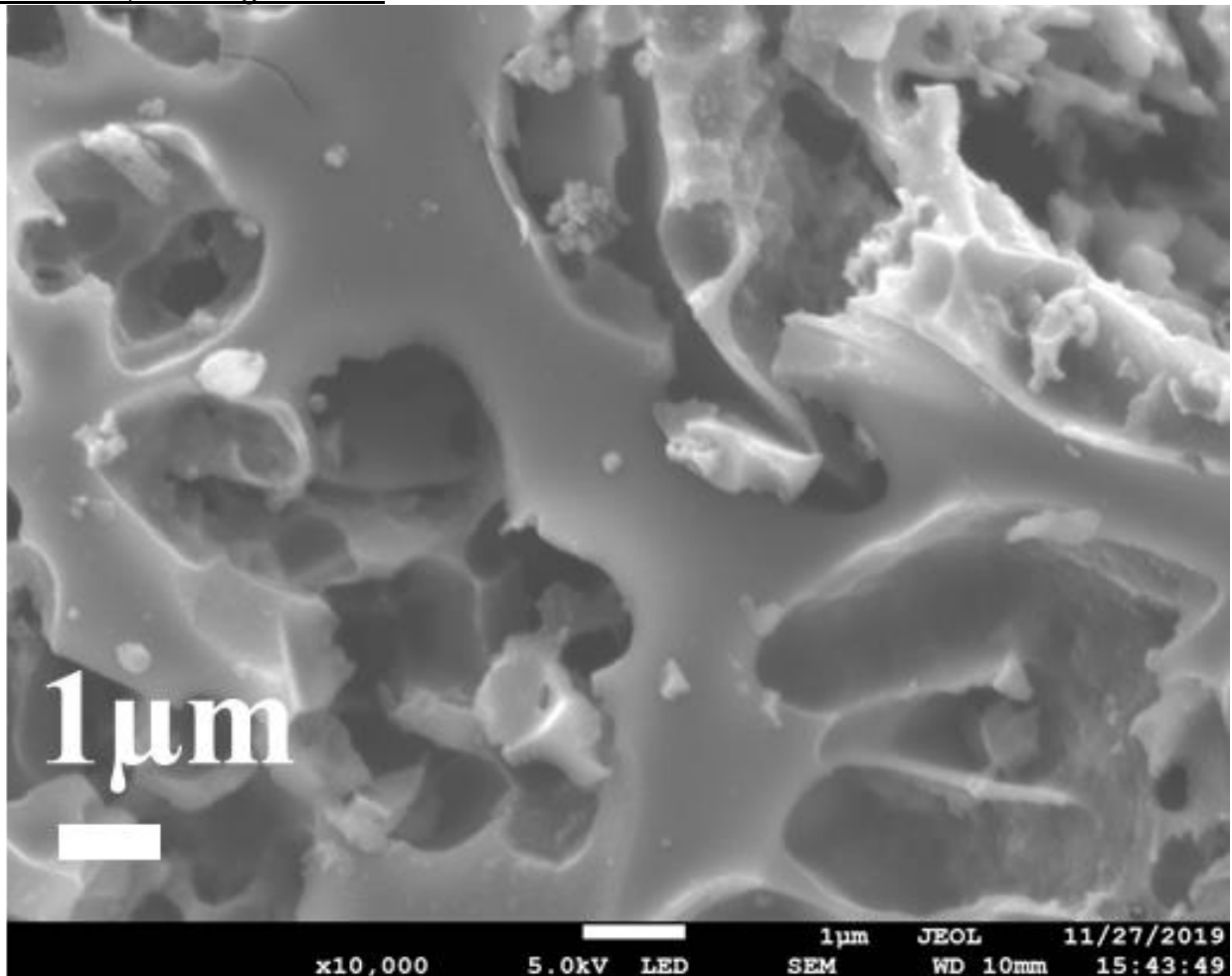


## SEM Images for S800K2

S800K2 x200 magnification and particle size distribution plot

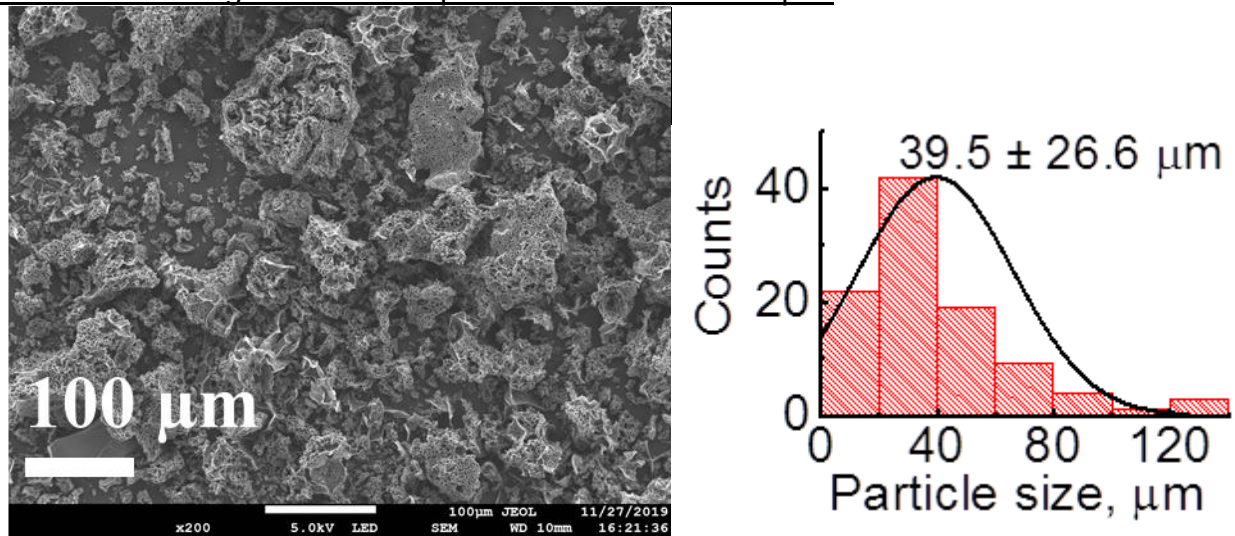


S800K2 x10,000 magnification

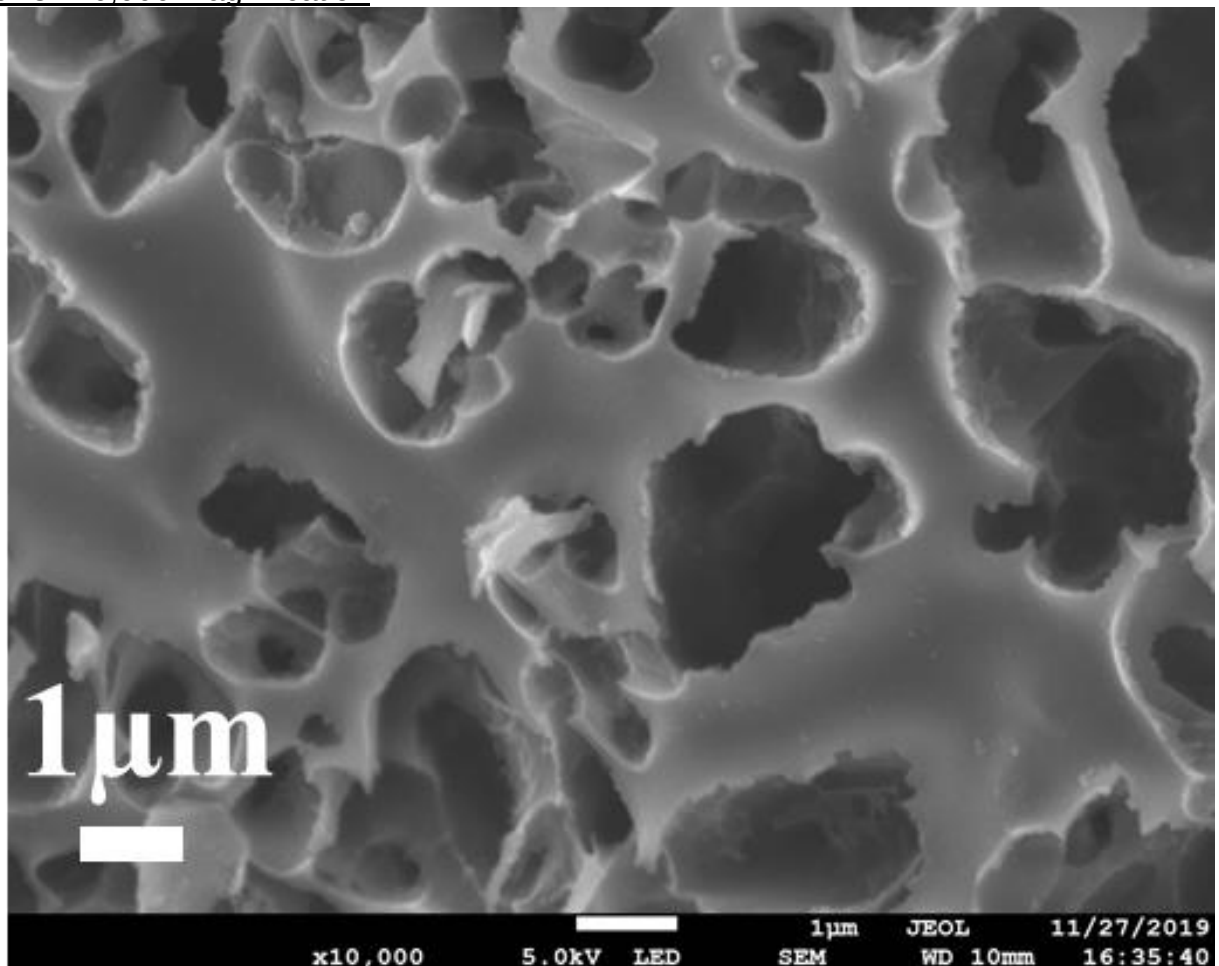


## SEM Images for S800K3

S800K3 x200 magnification and particle size distribution plot

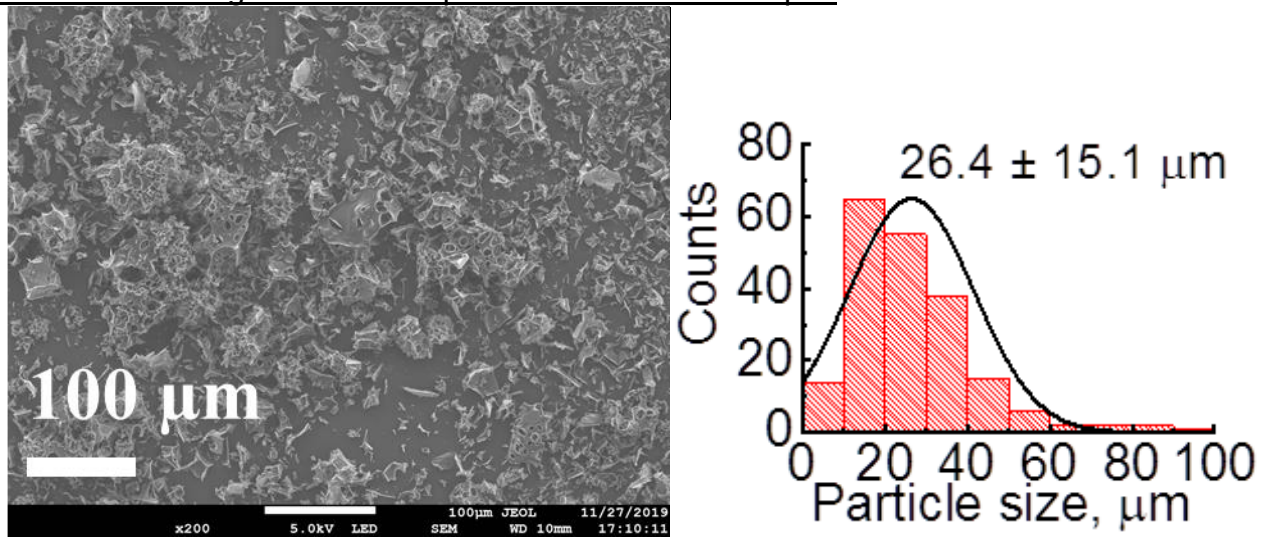


S800K3 x10,000 magnification

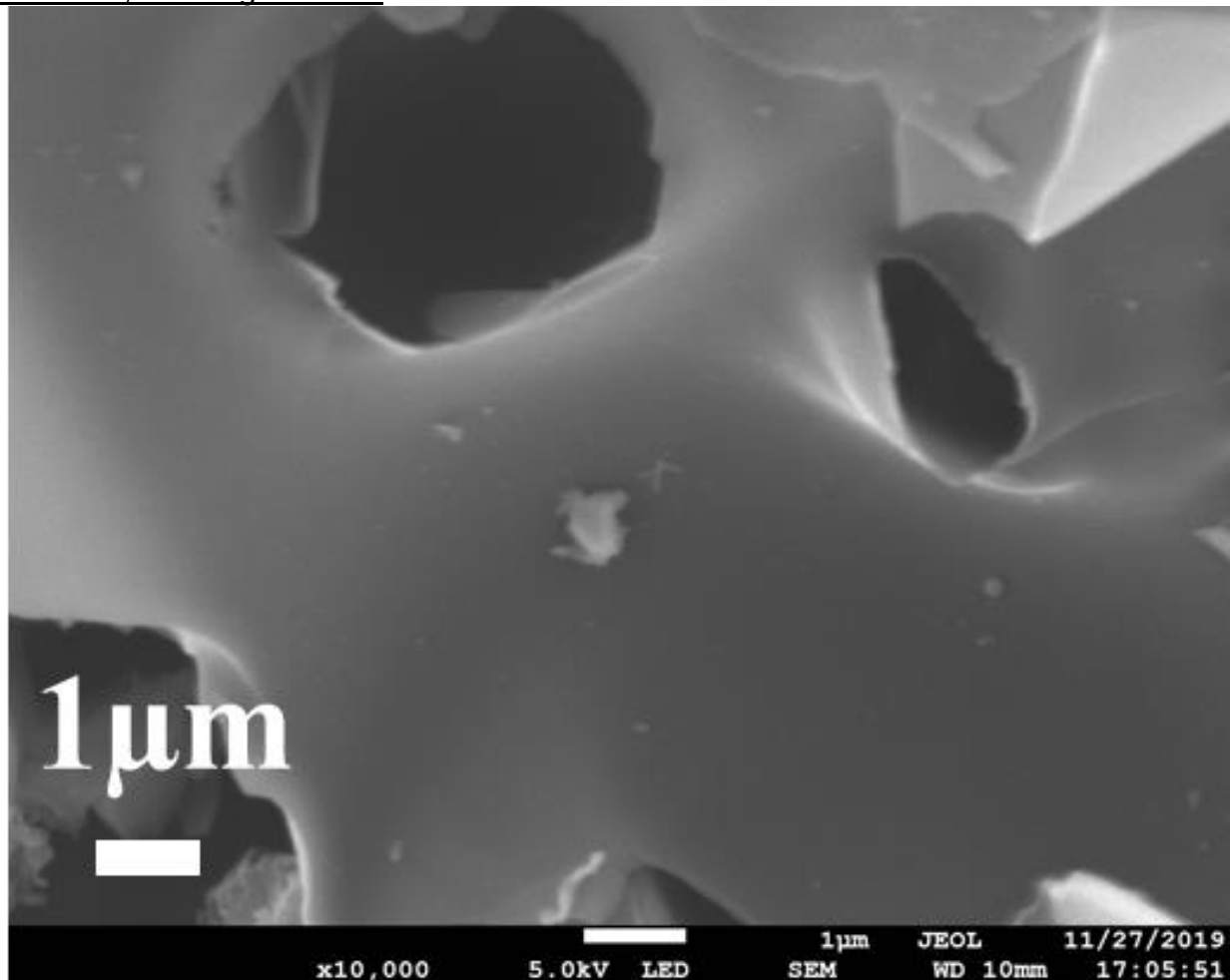


## SEM Images for S800K4

S800K4 x200 magnification and particle size distribution plot



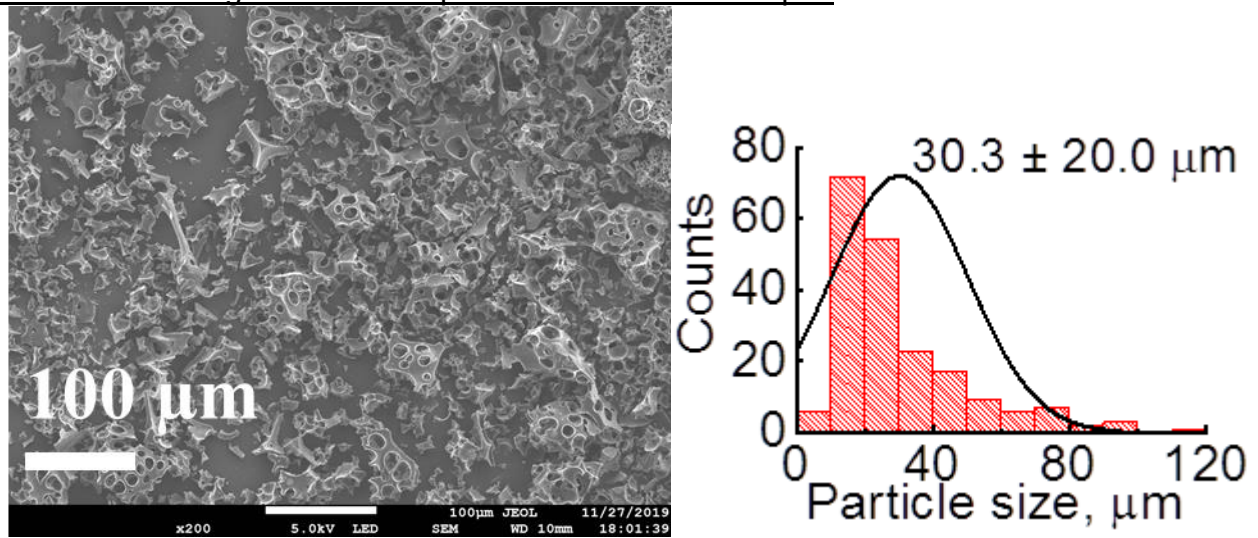
S800K4 x10,000 magnification



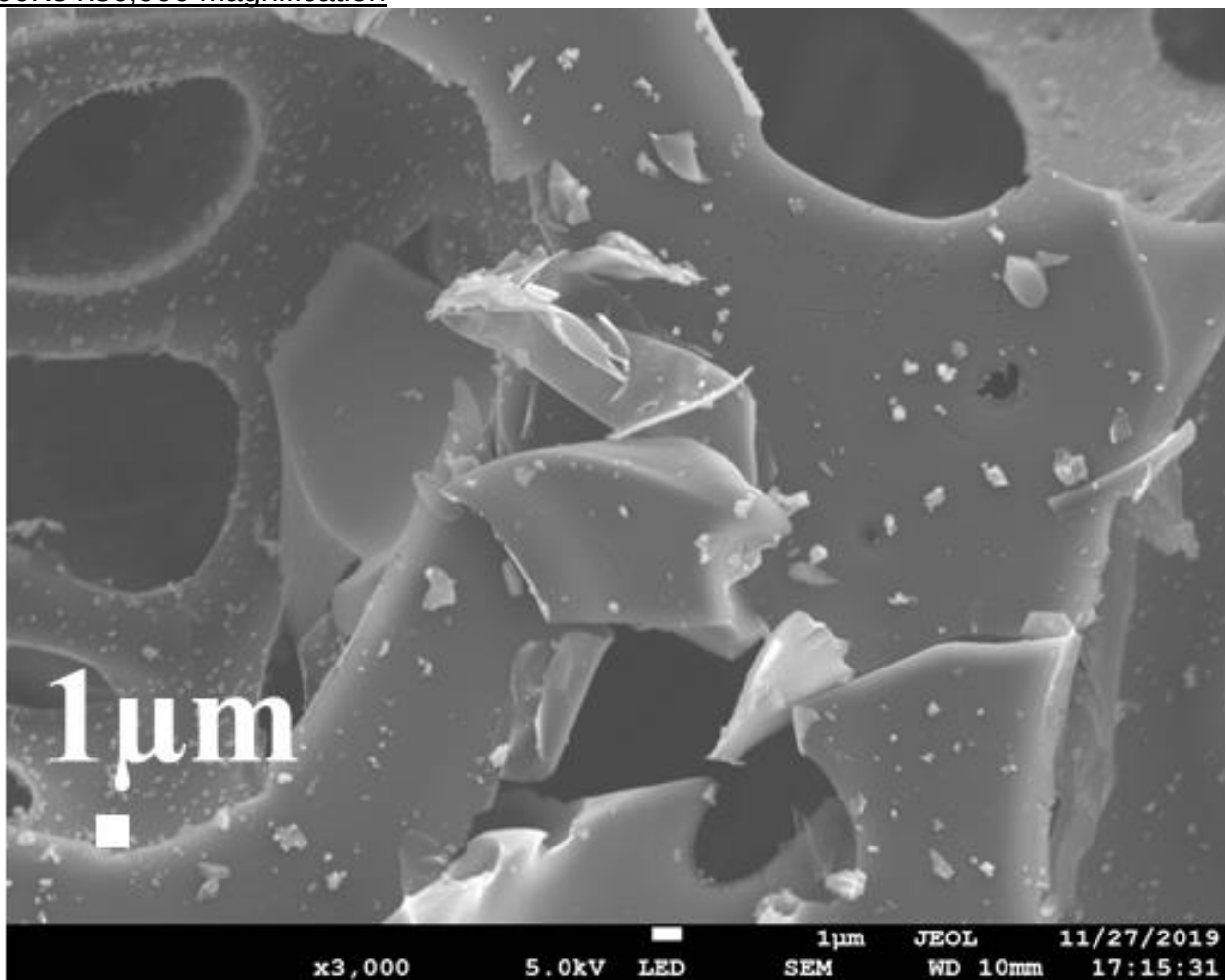


## SEM Images for S800K5

S800K5 x200 magnification and particle size distribution plot



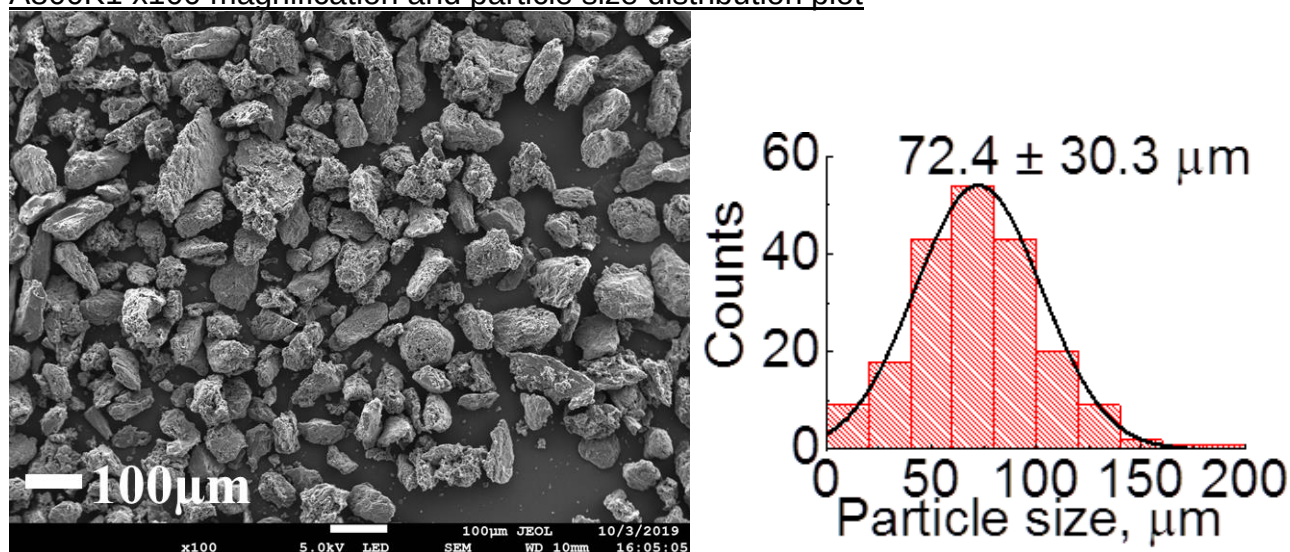
S800K5 x30,000 magnification



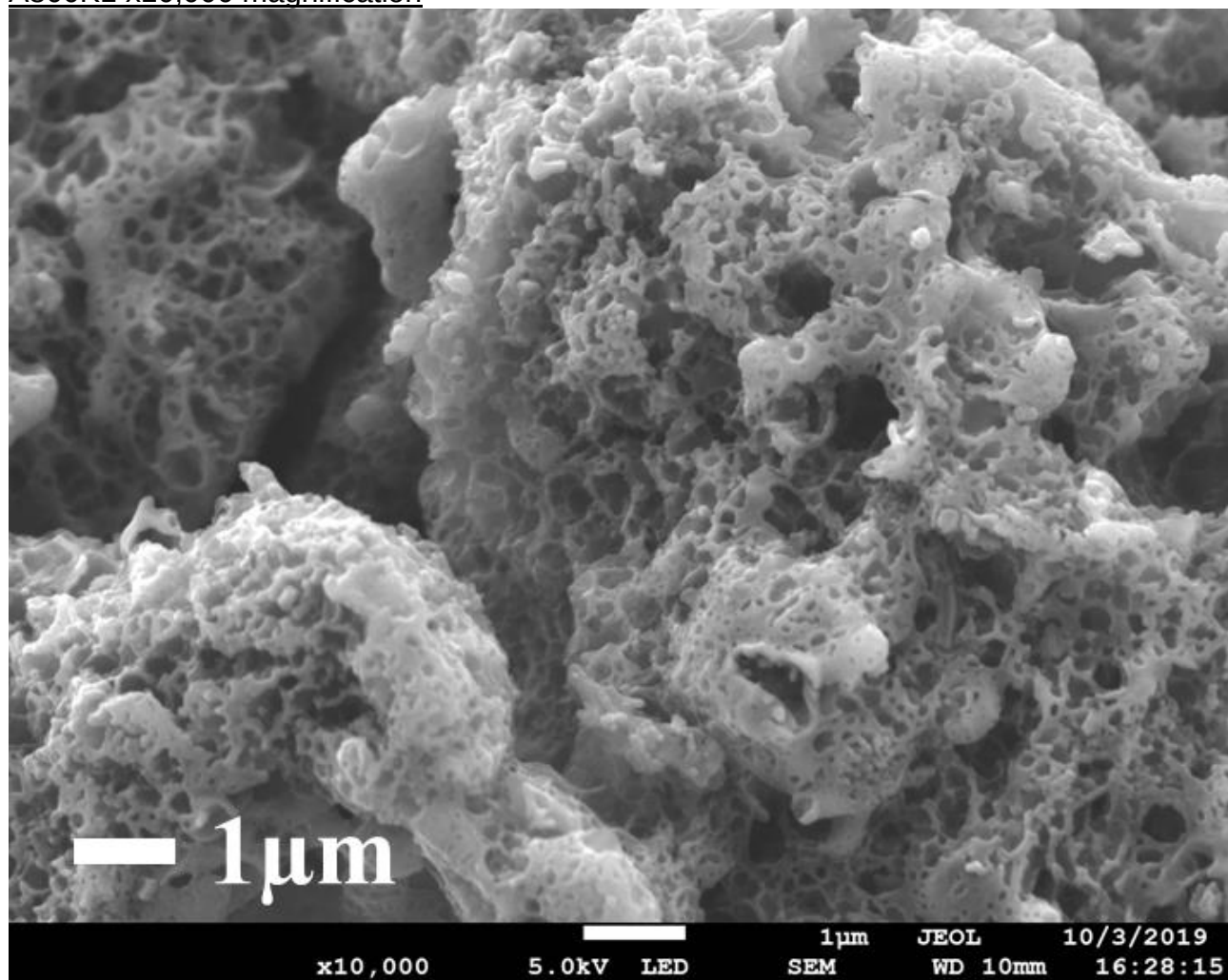


## SEM Images for A800K1

A800K1 x100 magnification and particle size distribution plot

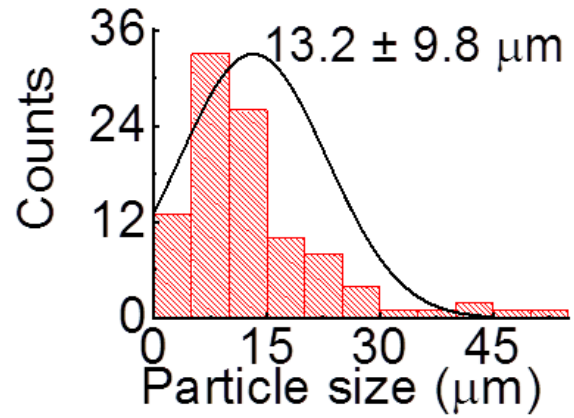
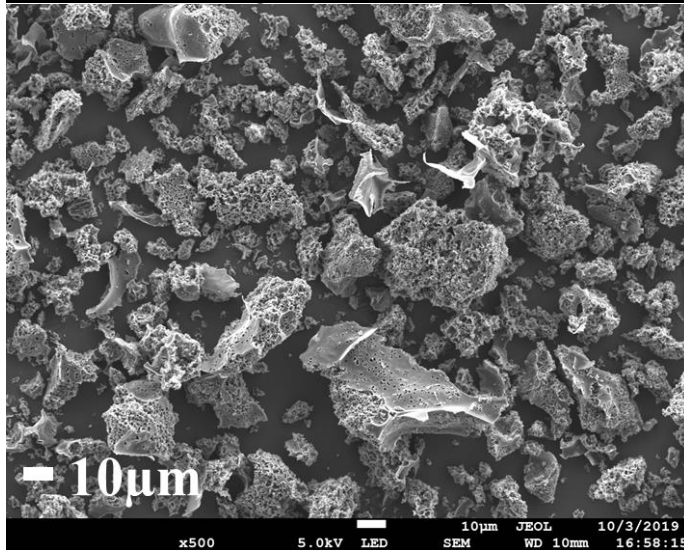


A800K1 x10,000 magnification

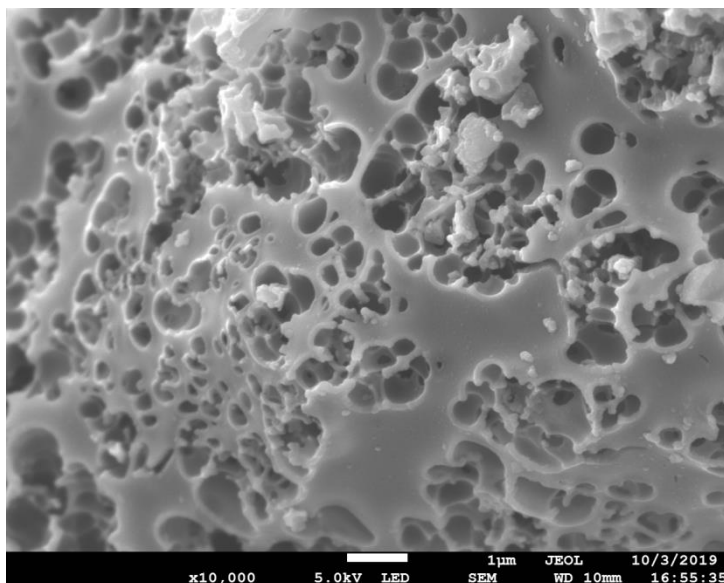
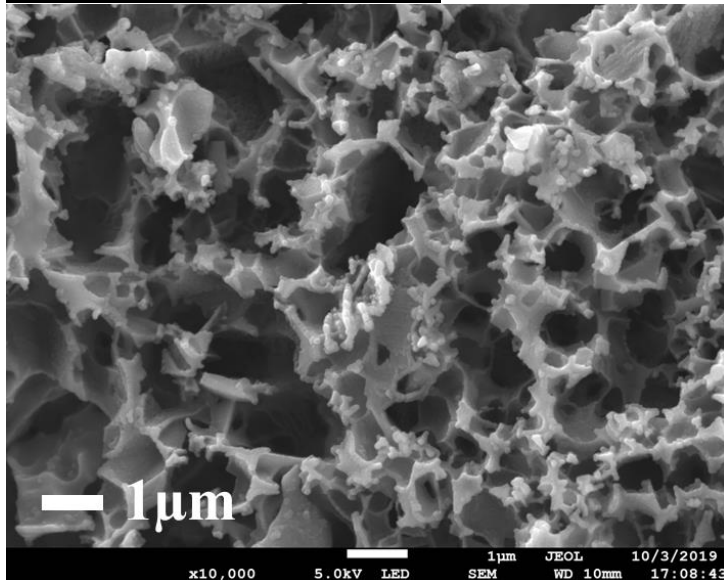


## SEM Images for A800K2

A800K2 x500 magnification and particle size distribution plot



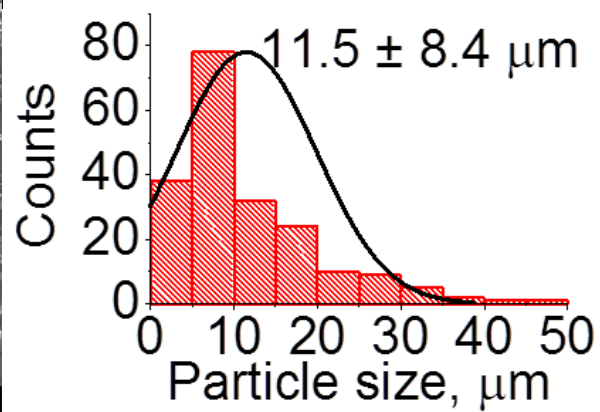
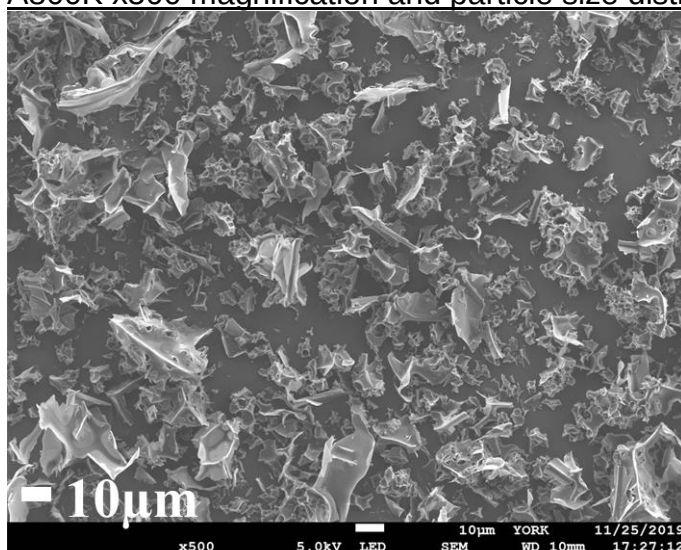
A800K2 x10,000 magnification



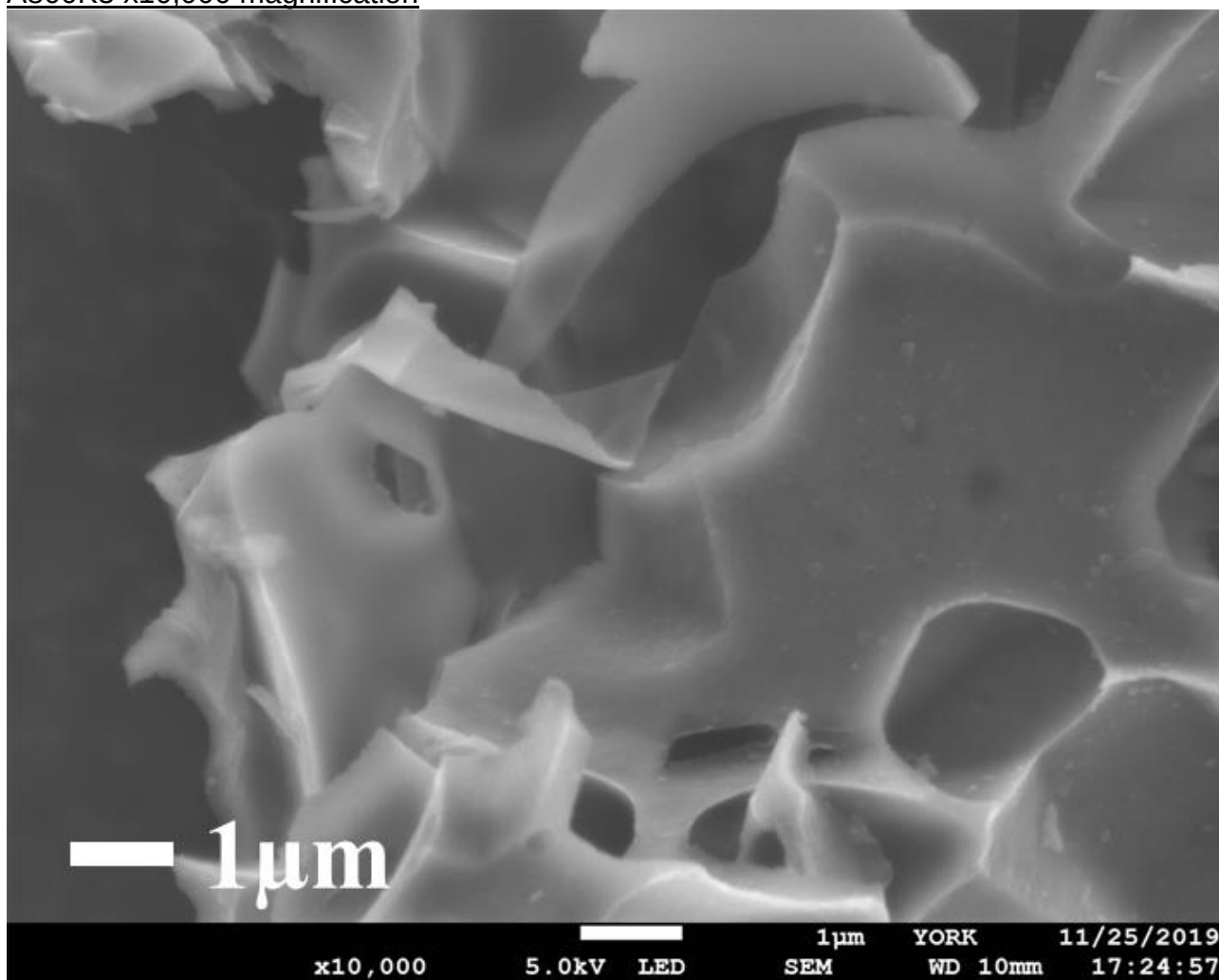


## SEM Images for A800K3

A800K x500 magnification and particle size distribution plot

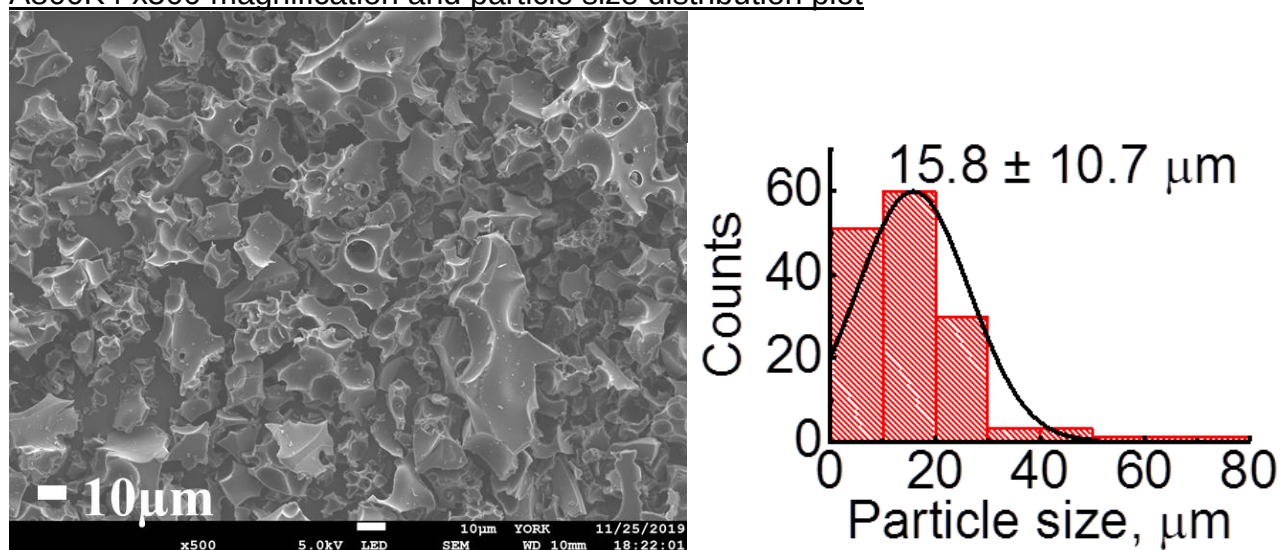


A800K3 x10,000 magnification

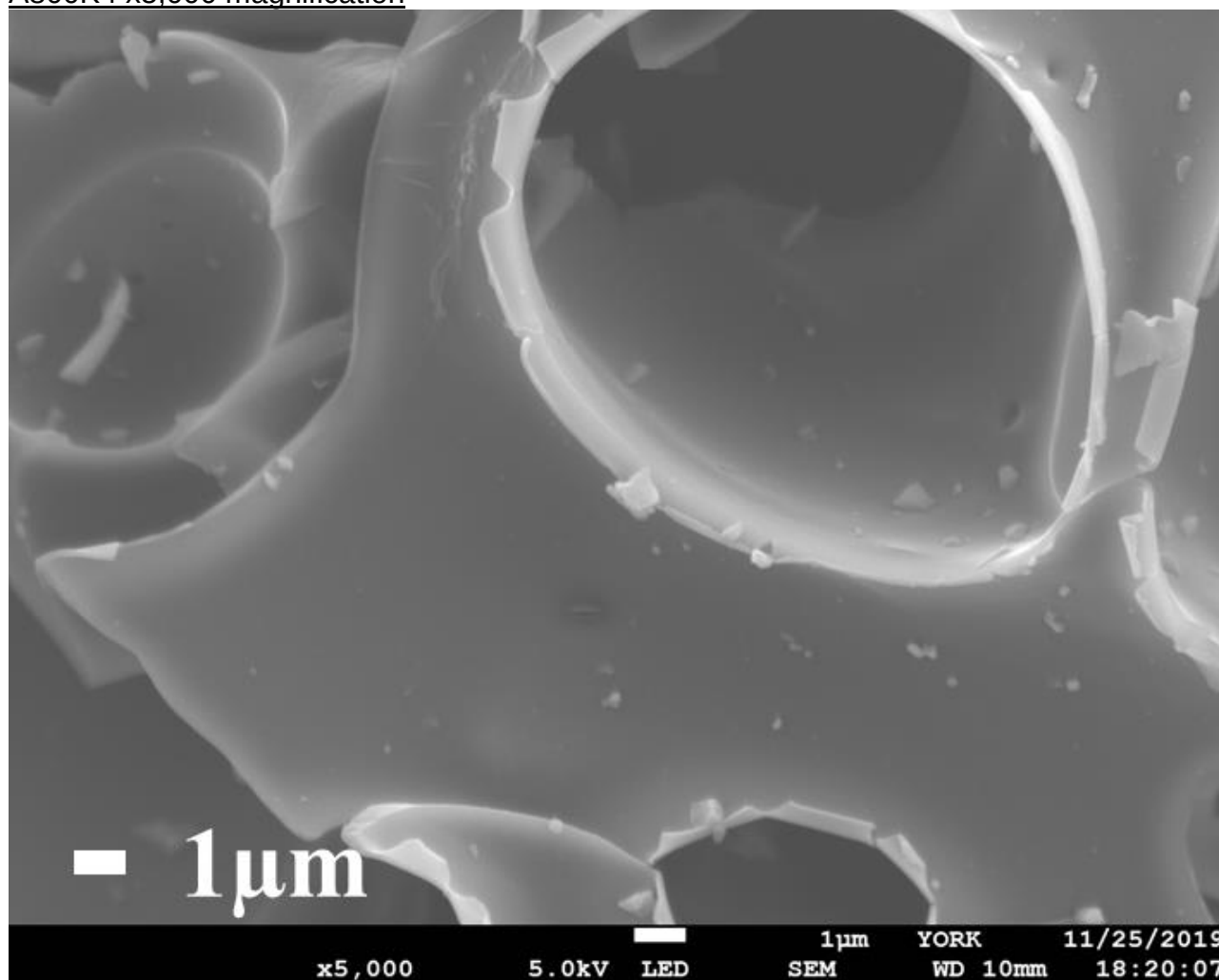


## SEM Images for A800K4

A800K4 x500 magnification and particle size distribution plot

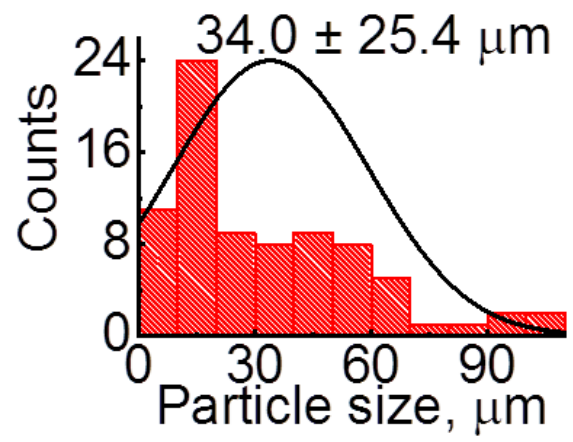
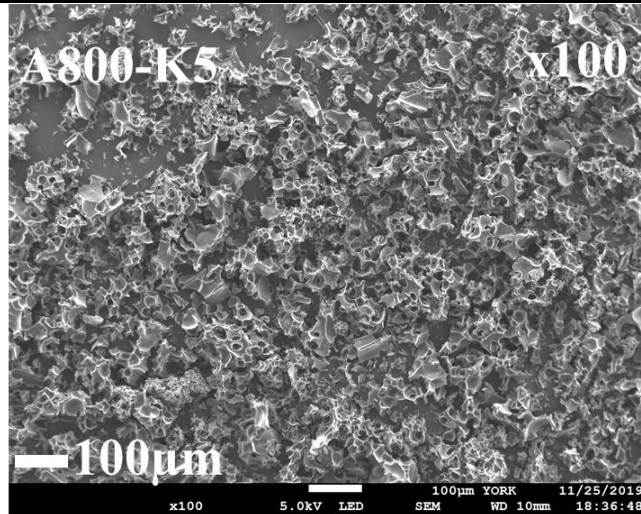


A800K4 x5,000 magnification

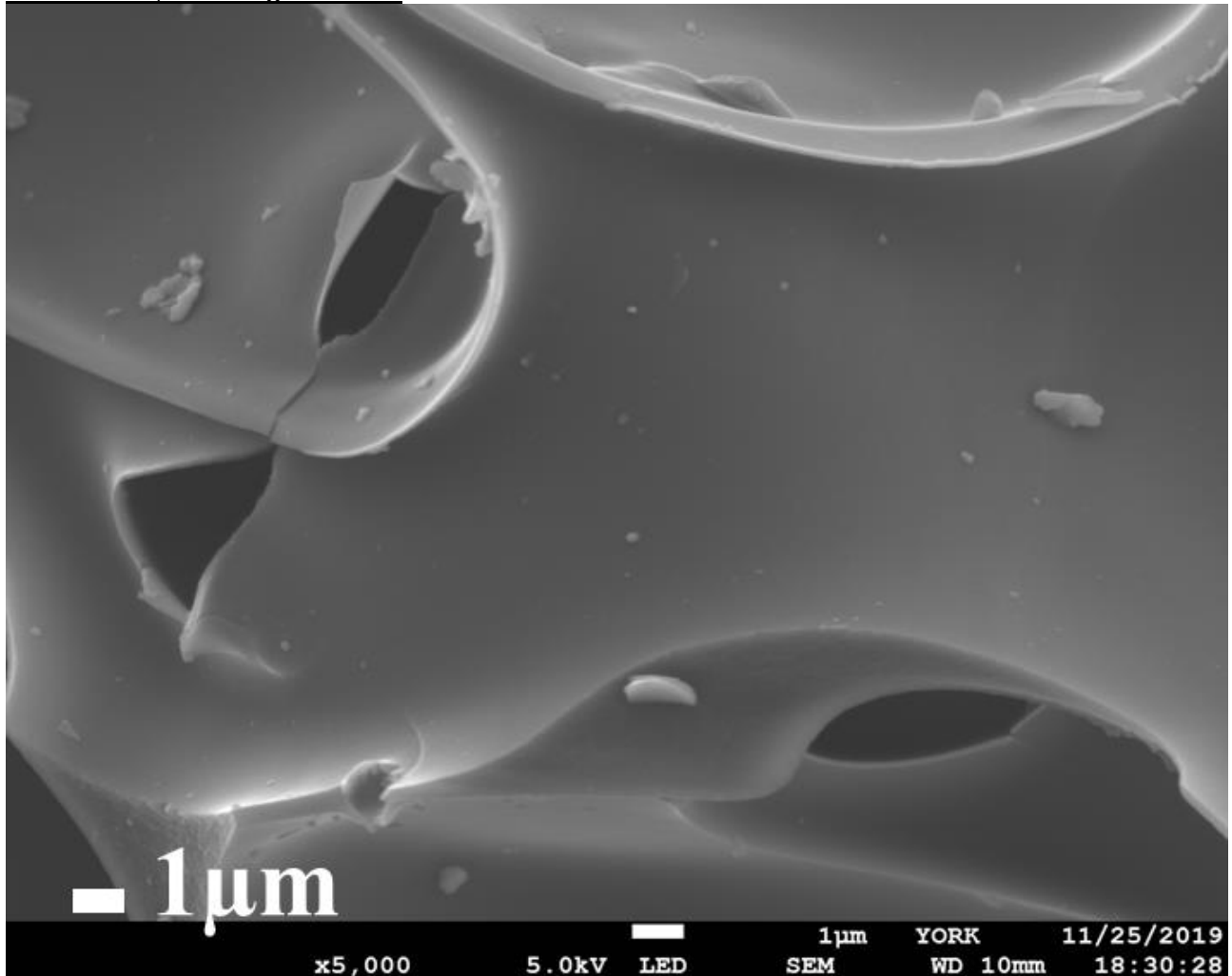


## SEM Images for A800K5

A800K5 x100 magnification and particle size distribution plot



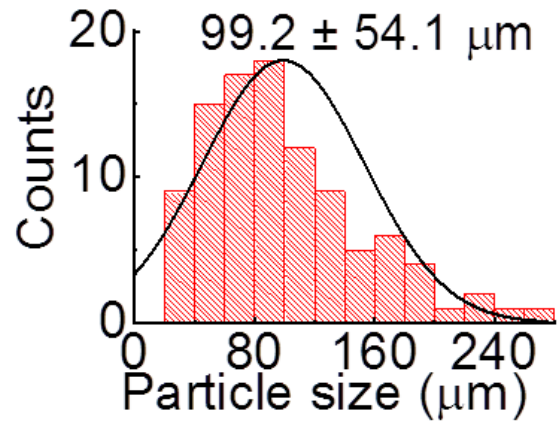
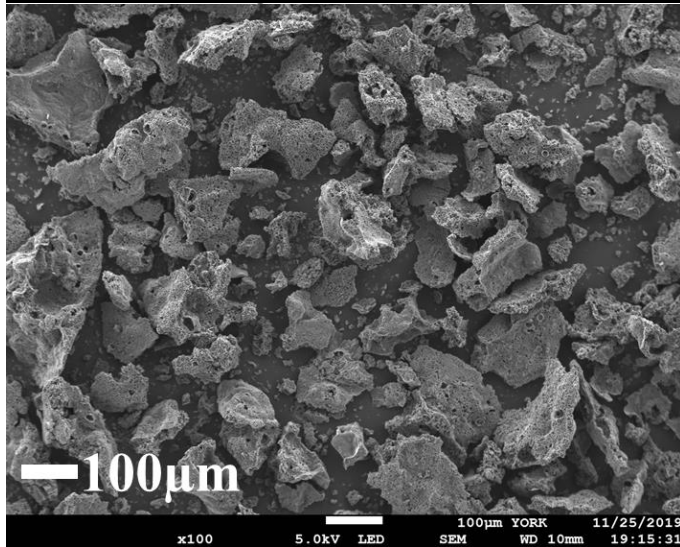
A800K5 x5,000 magnification



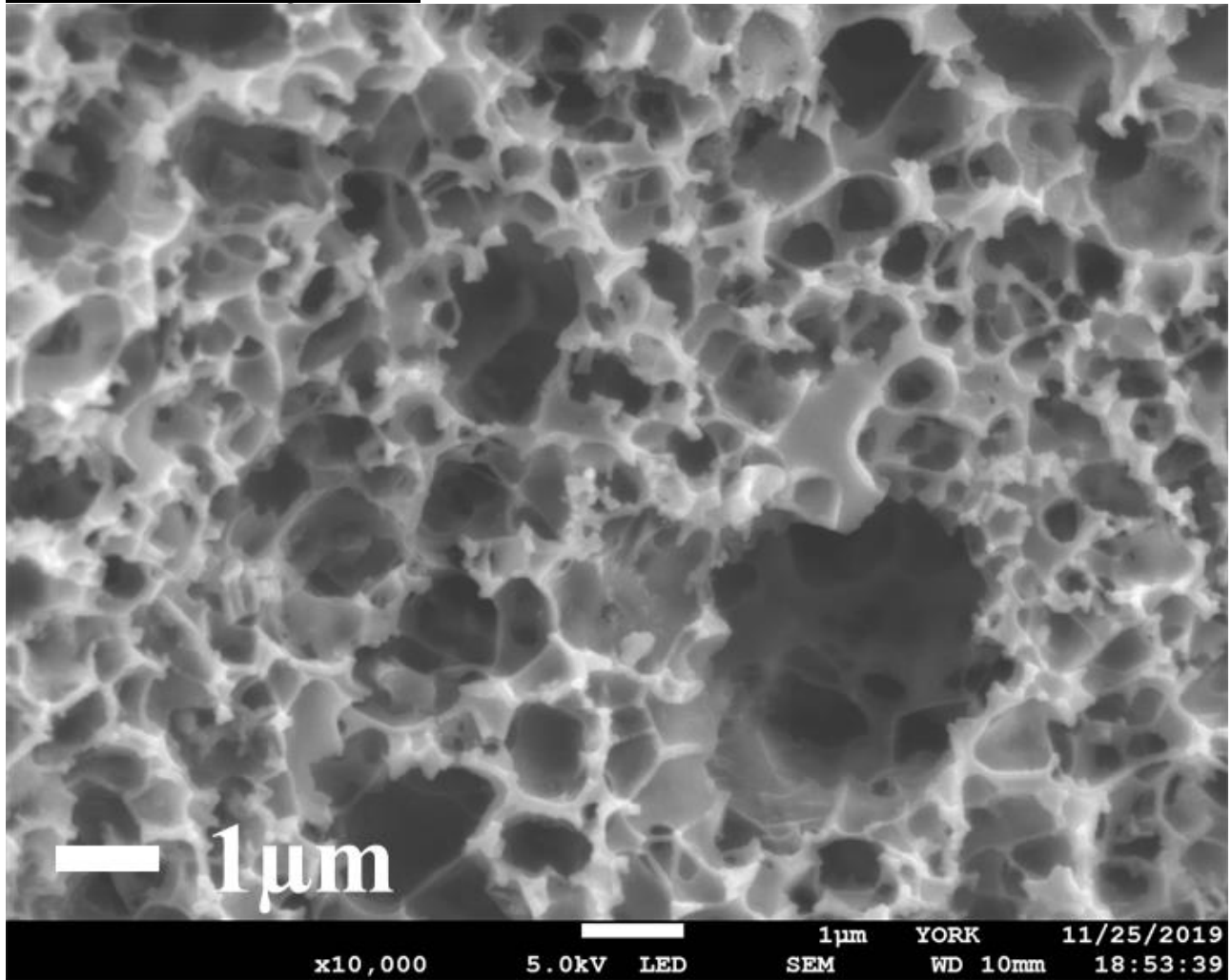


## SEM Images for A600K2

A600K2 x100 magnification and particle size distribution plot

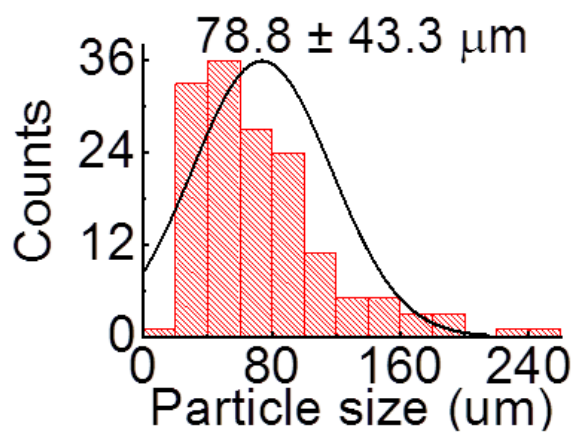
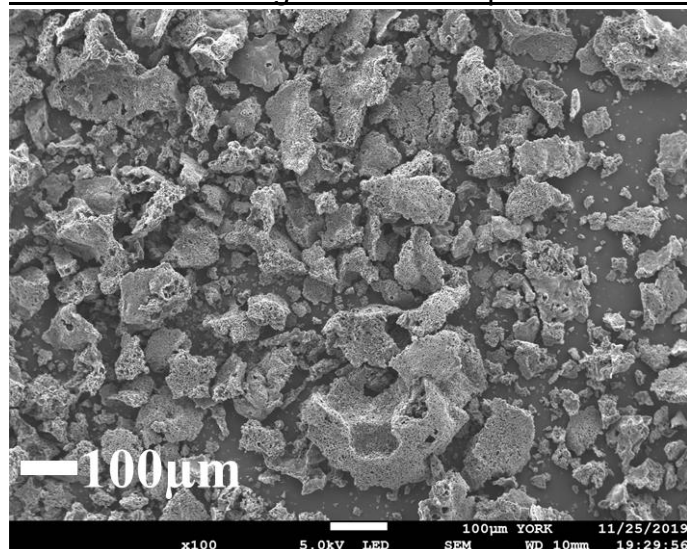


A600K2 x10,000 magnification

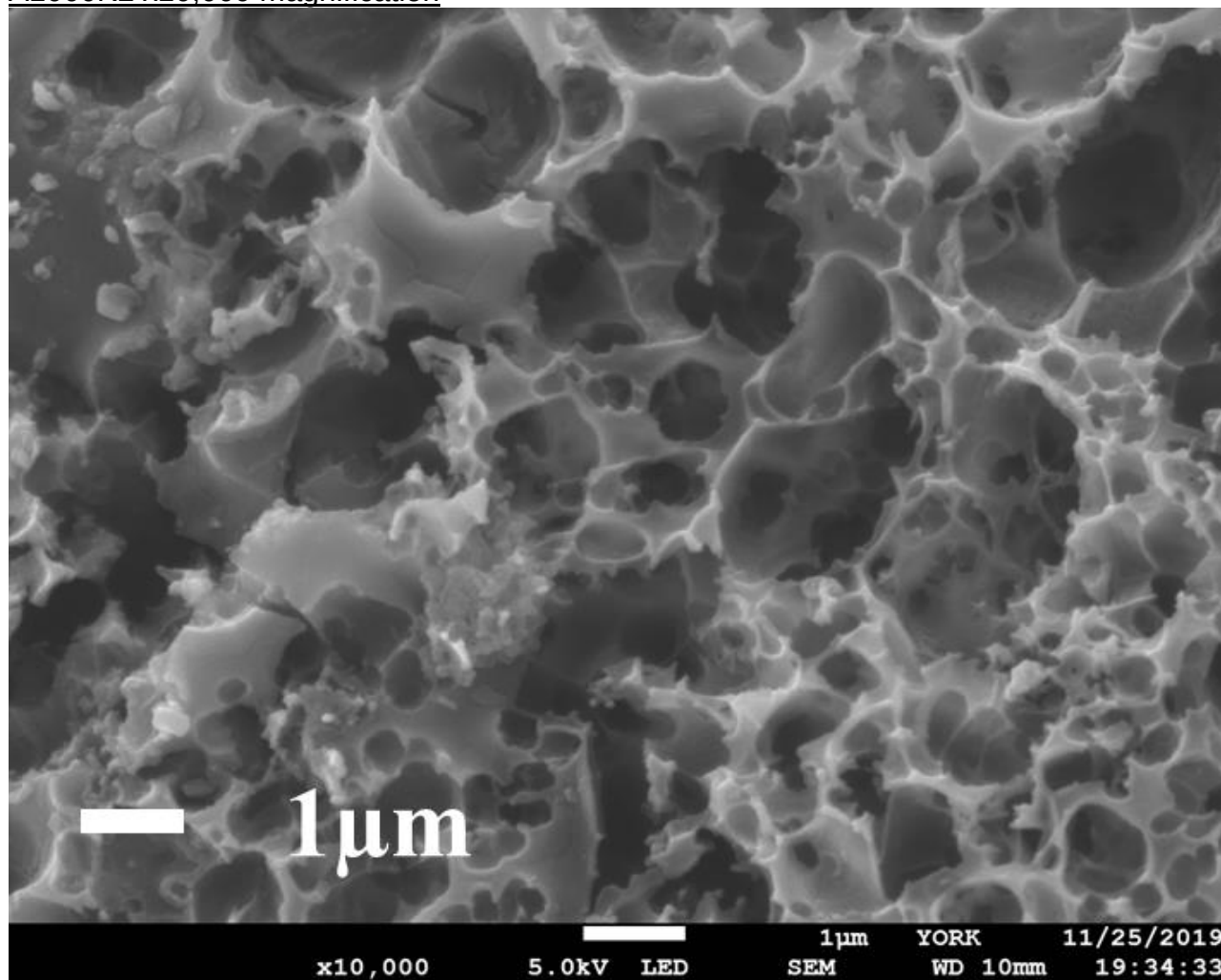


## SEM Images for A1000K2

A1000K2 x100 magnification and particle size distribution plot



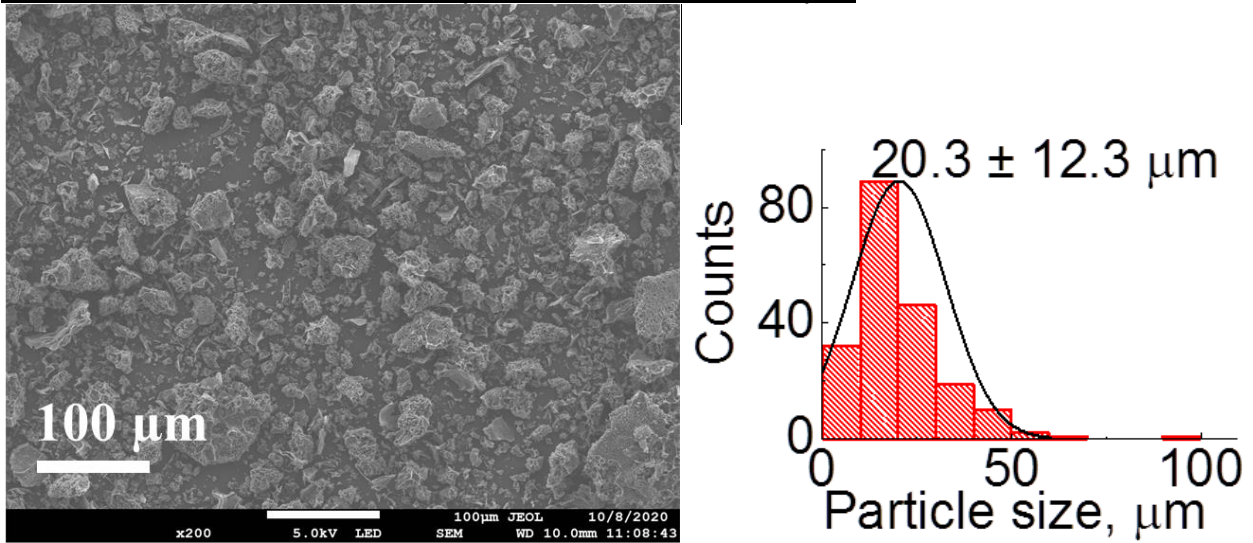
A1000K2 x10,000 magnification



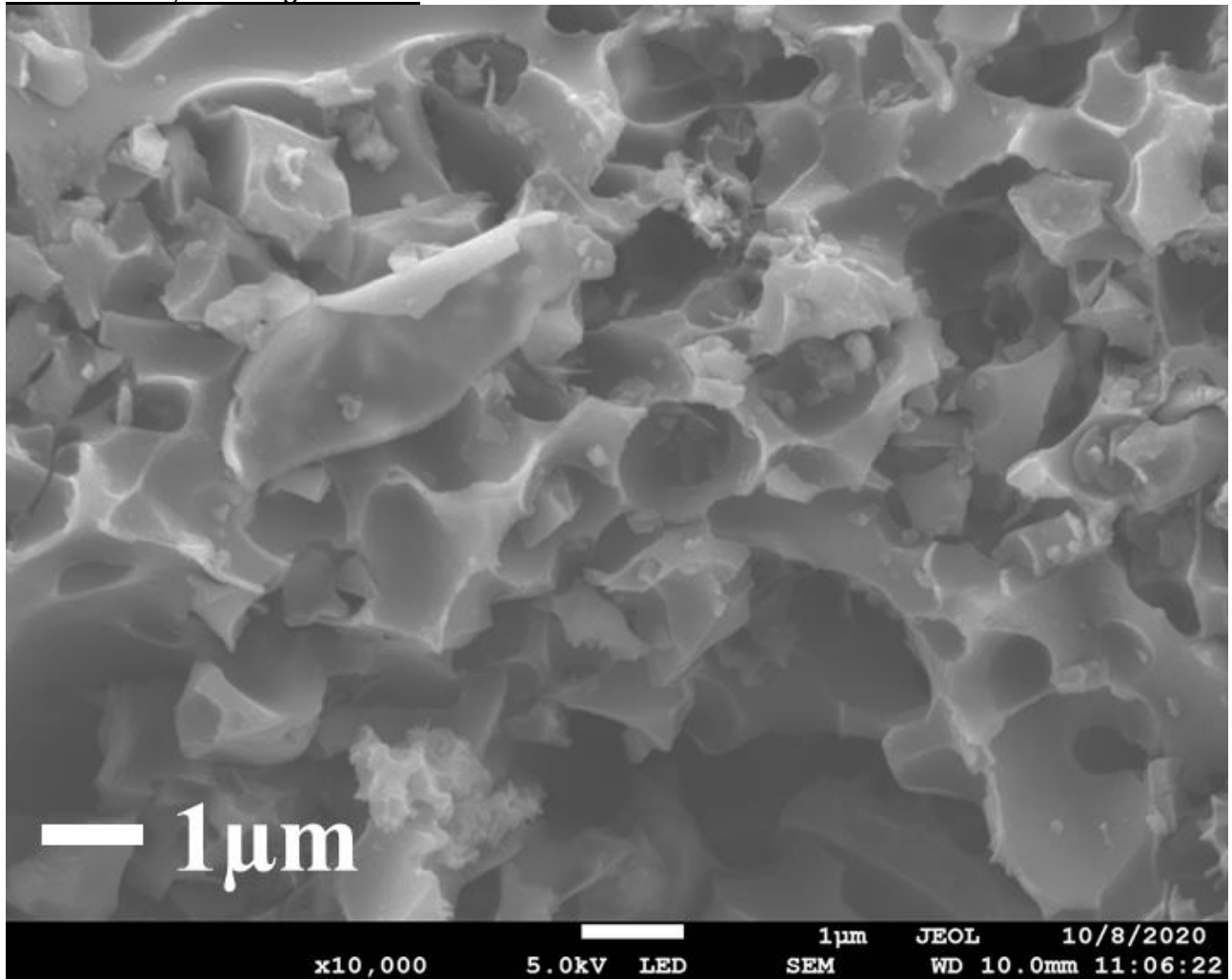


## SEM Images for P800K2

P800K2 x200 magnification and particle size distribution plot



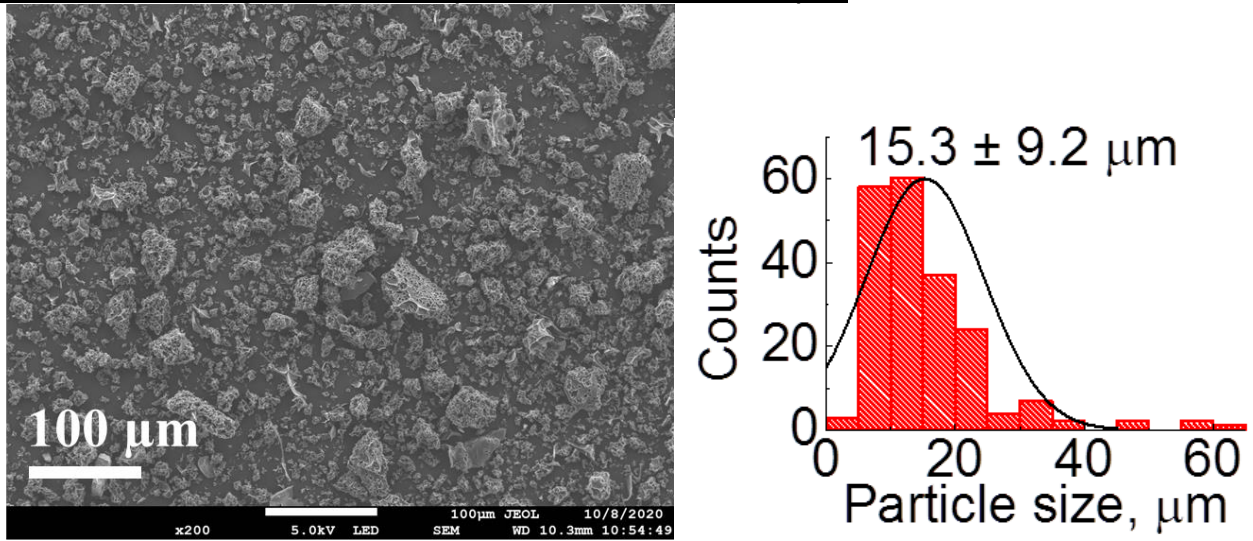
P800K2 x10,000 magnification



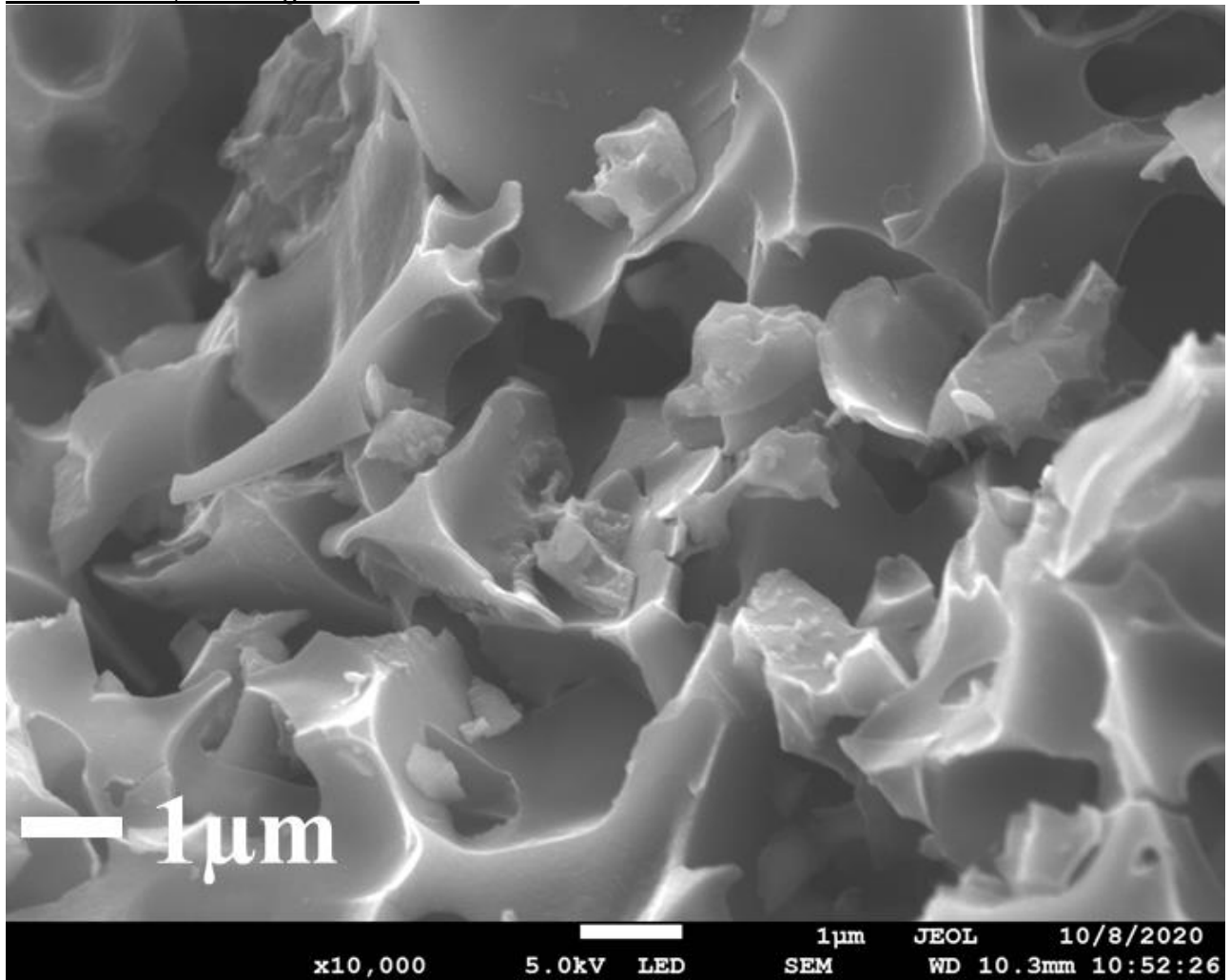


## SEM Images for P800K3

P800K3 x200 magnification and particle size distribution plot

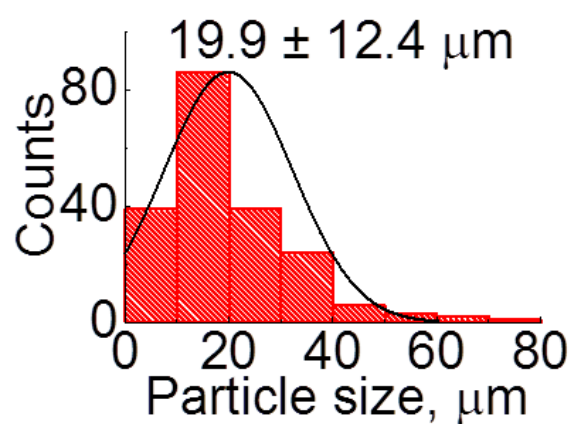
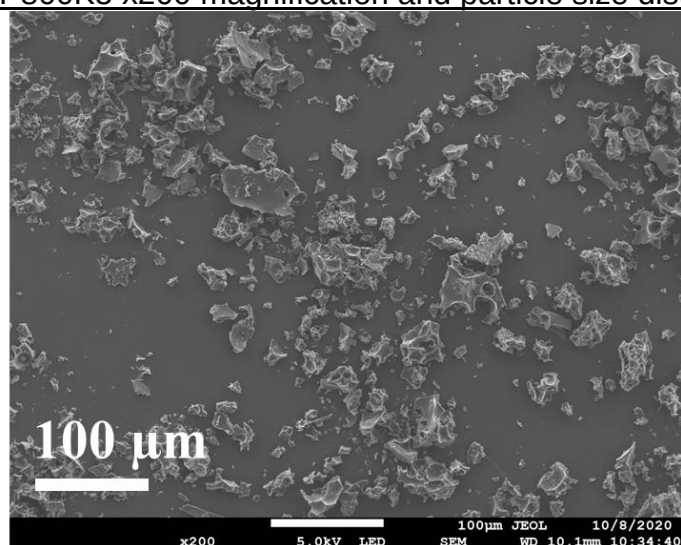


P800K3 x10,000 magnification

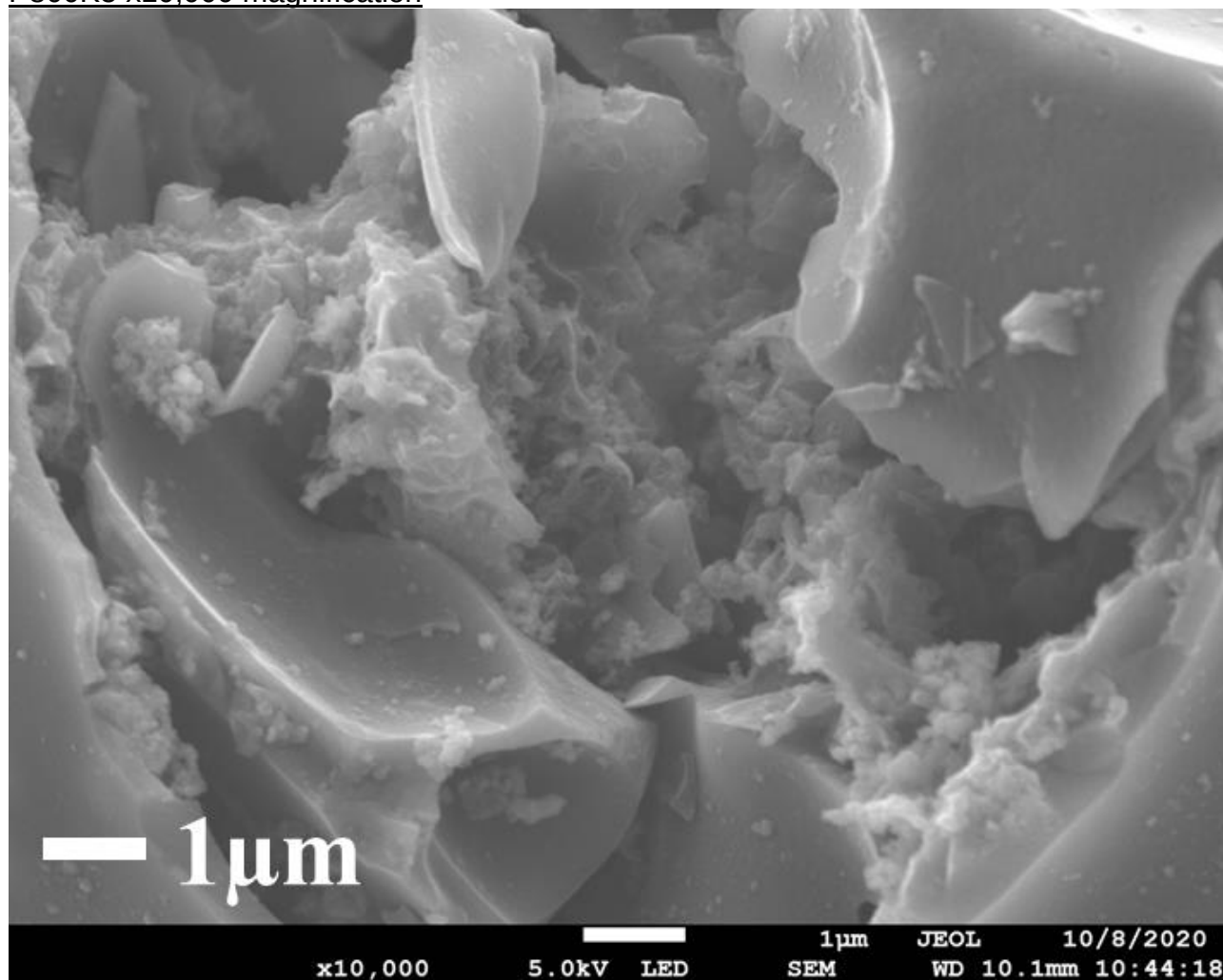


## SEM Images for P800K5

P800K5 x200 magnification and particle size distribution plot

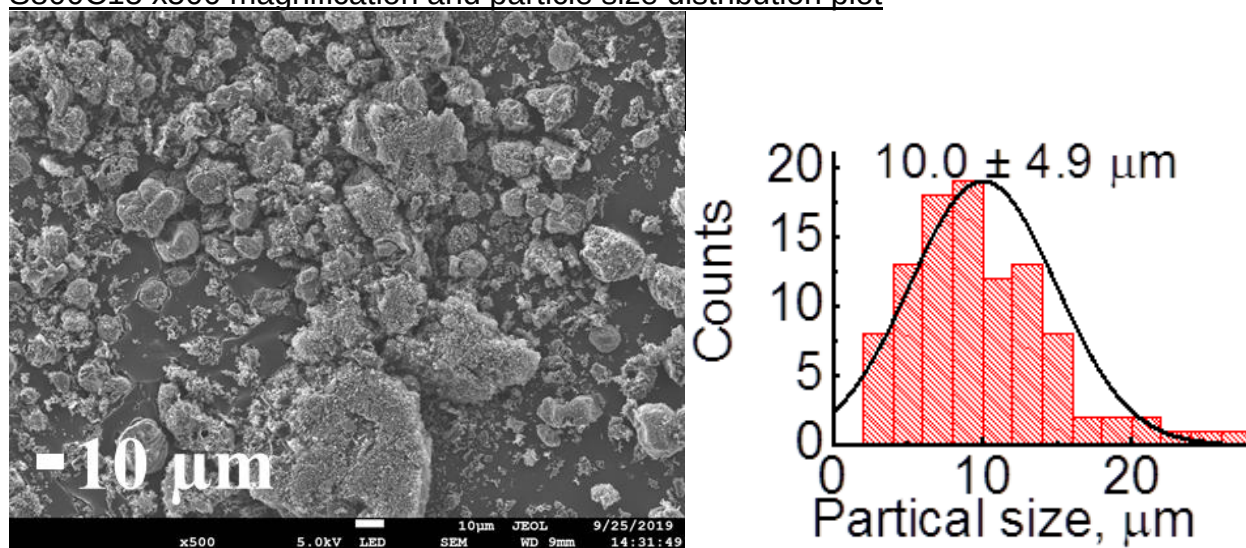


P800K5 x10,000 magnification

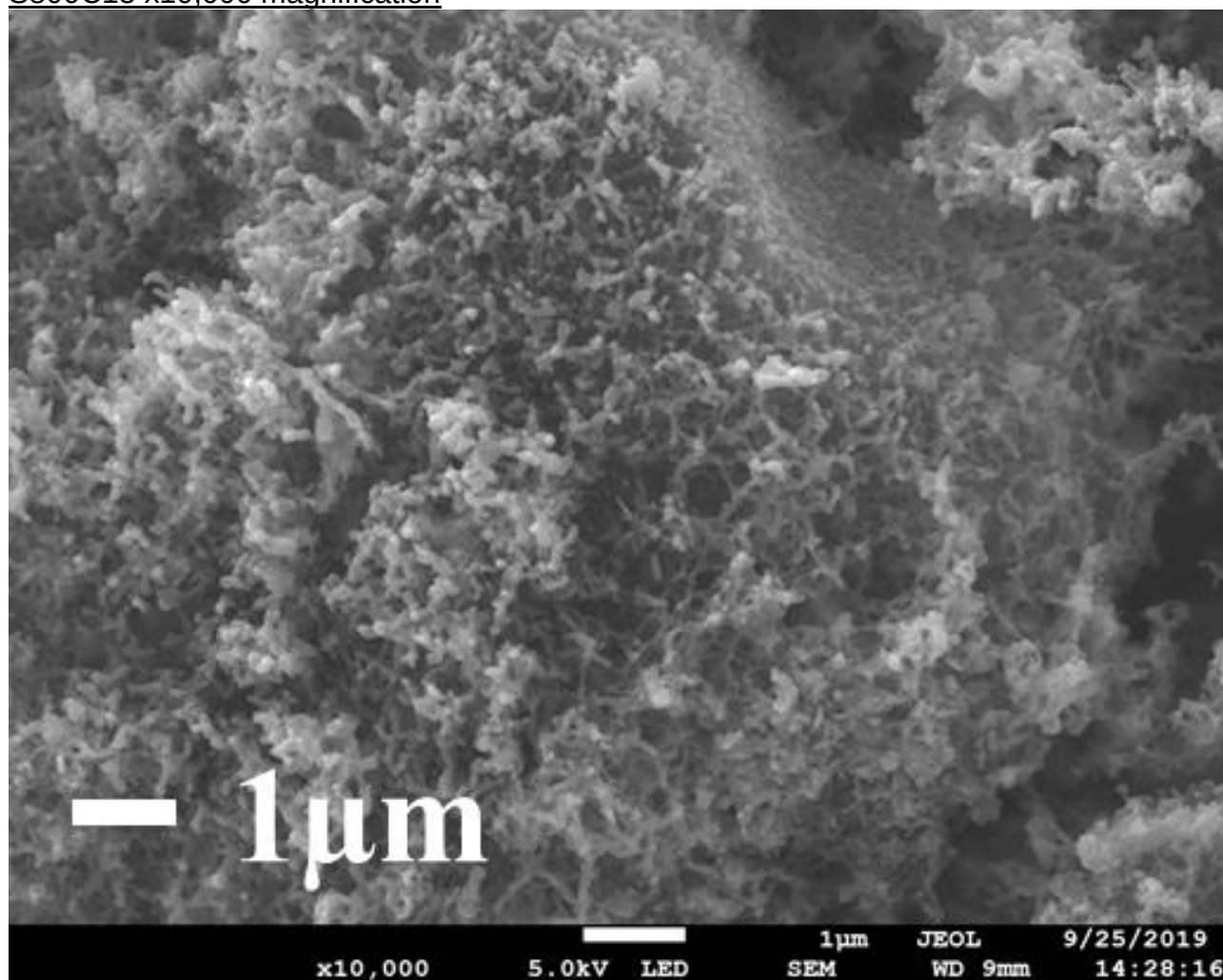


## SEM Images for S800C15

S800C15 x500 magnification and particle size distribution plot



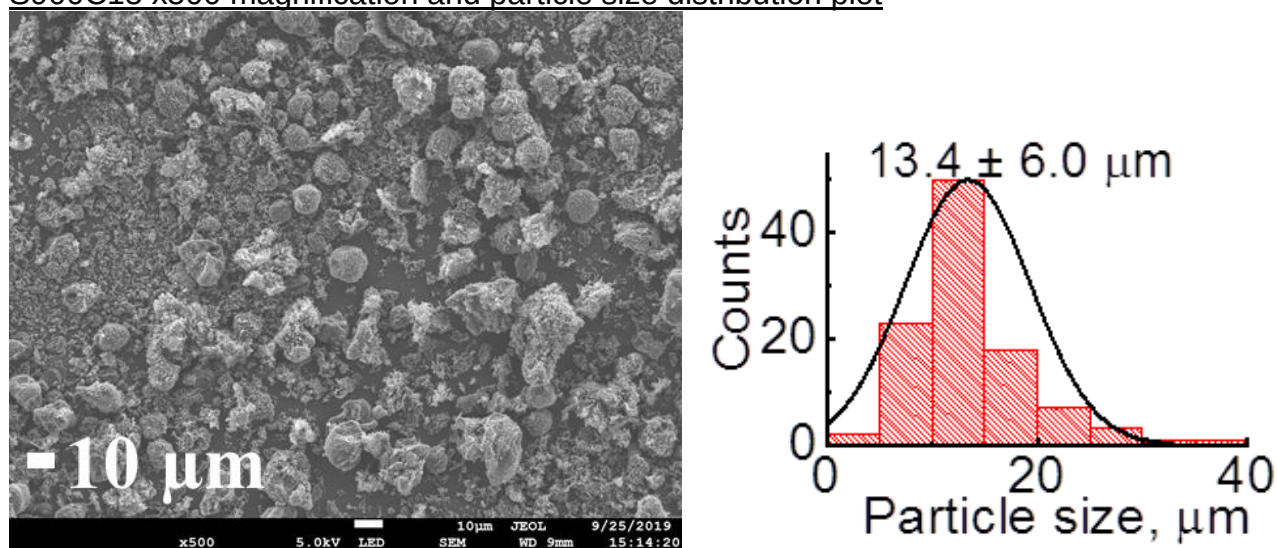
S800C15 x10,000 magnification



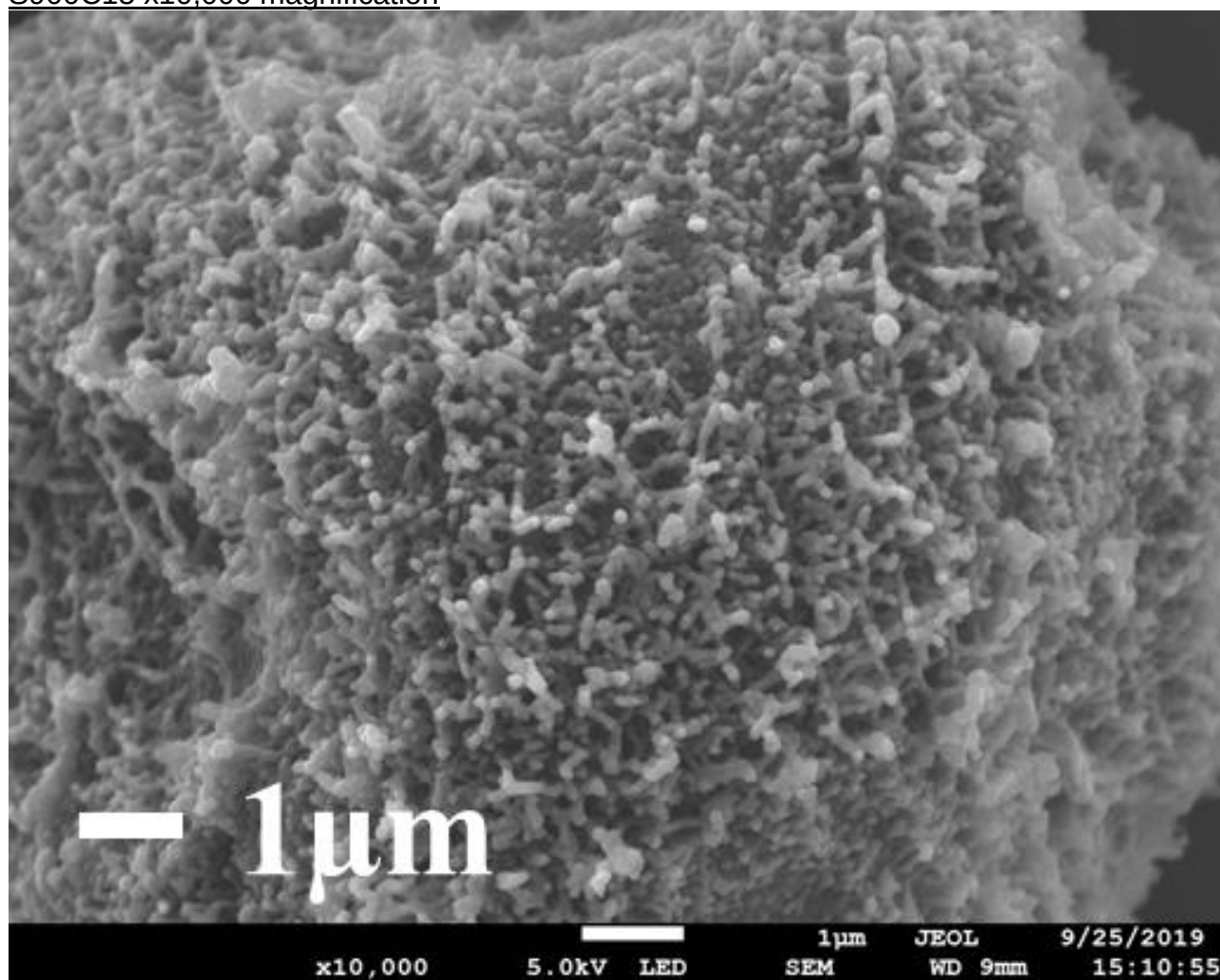


## SEM Images for S900C15

S900C15 x500 magnification and particle size distribution plot

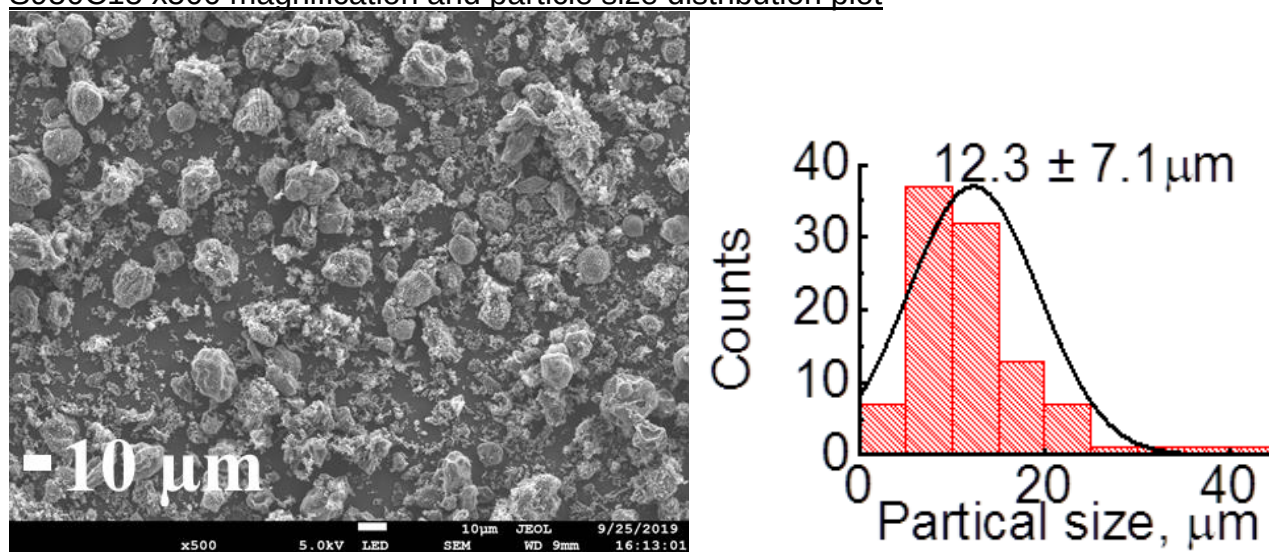


S900C15 x10,000 magnification

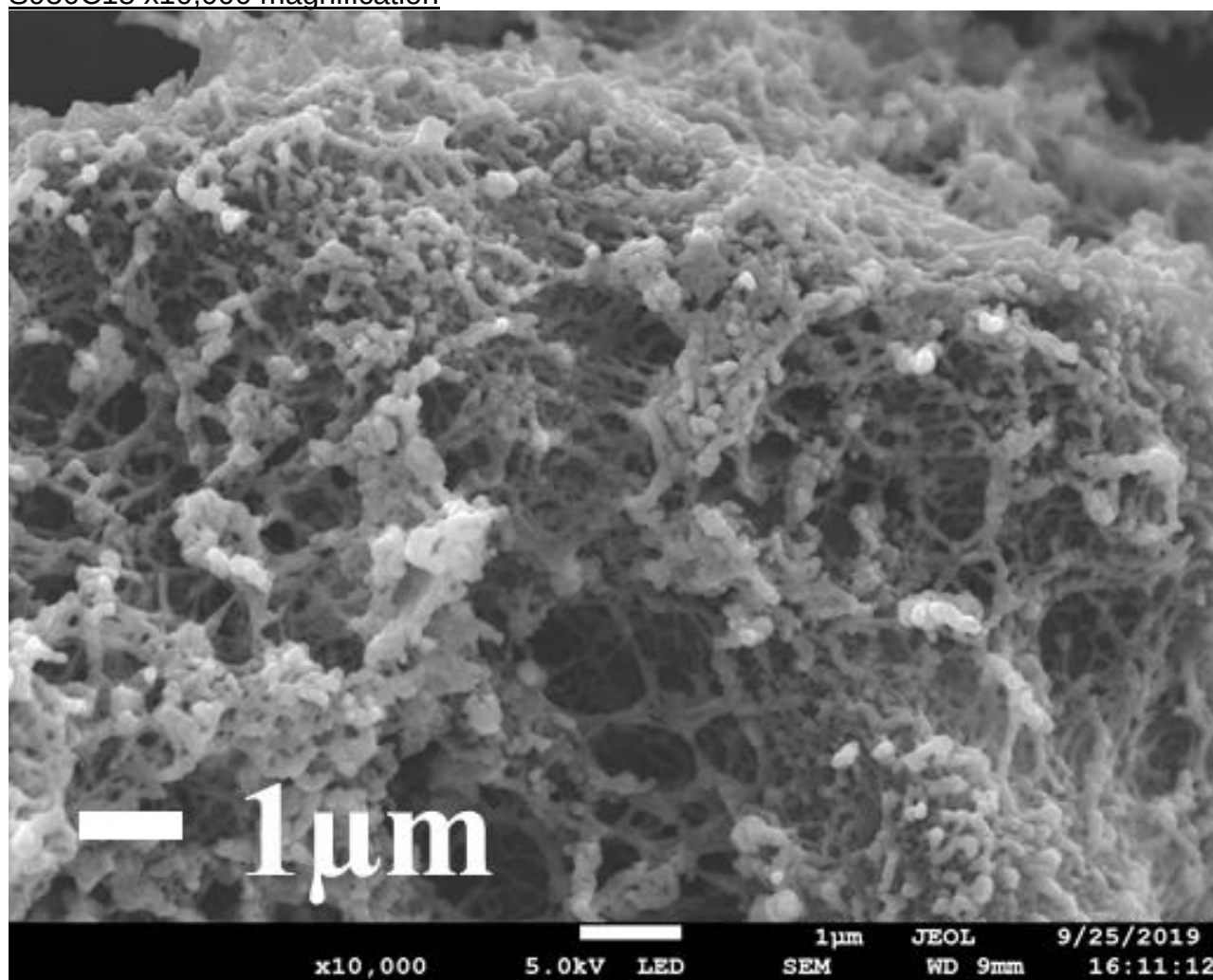


## SEM Images for S950C15

S950C15 x500 magnification and particle size distribution plot



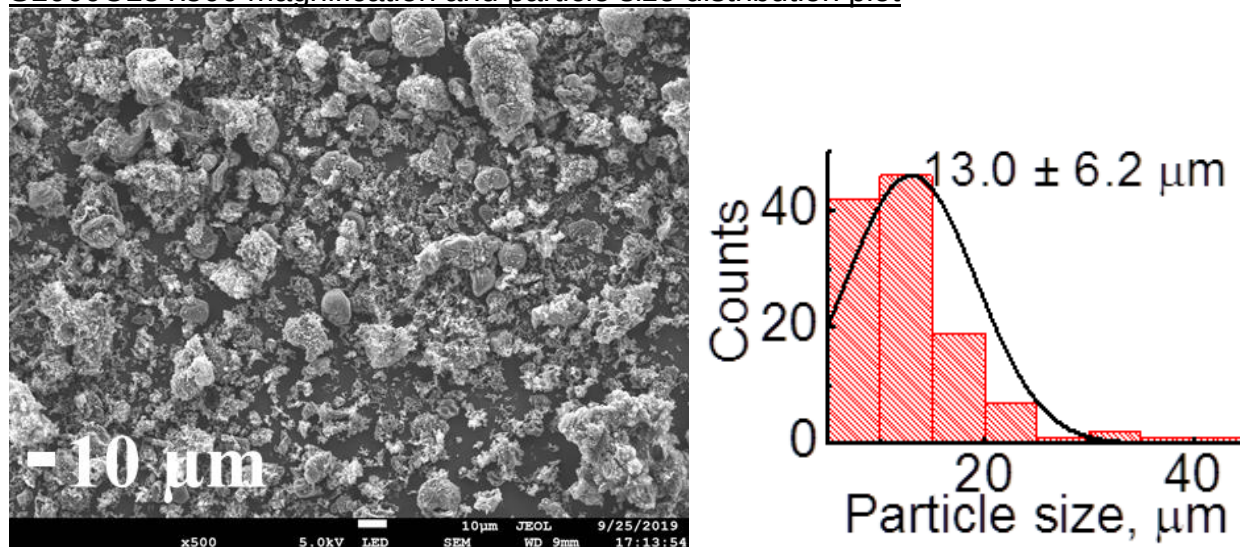
S950C15 x10,000 magnification



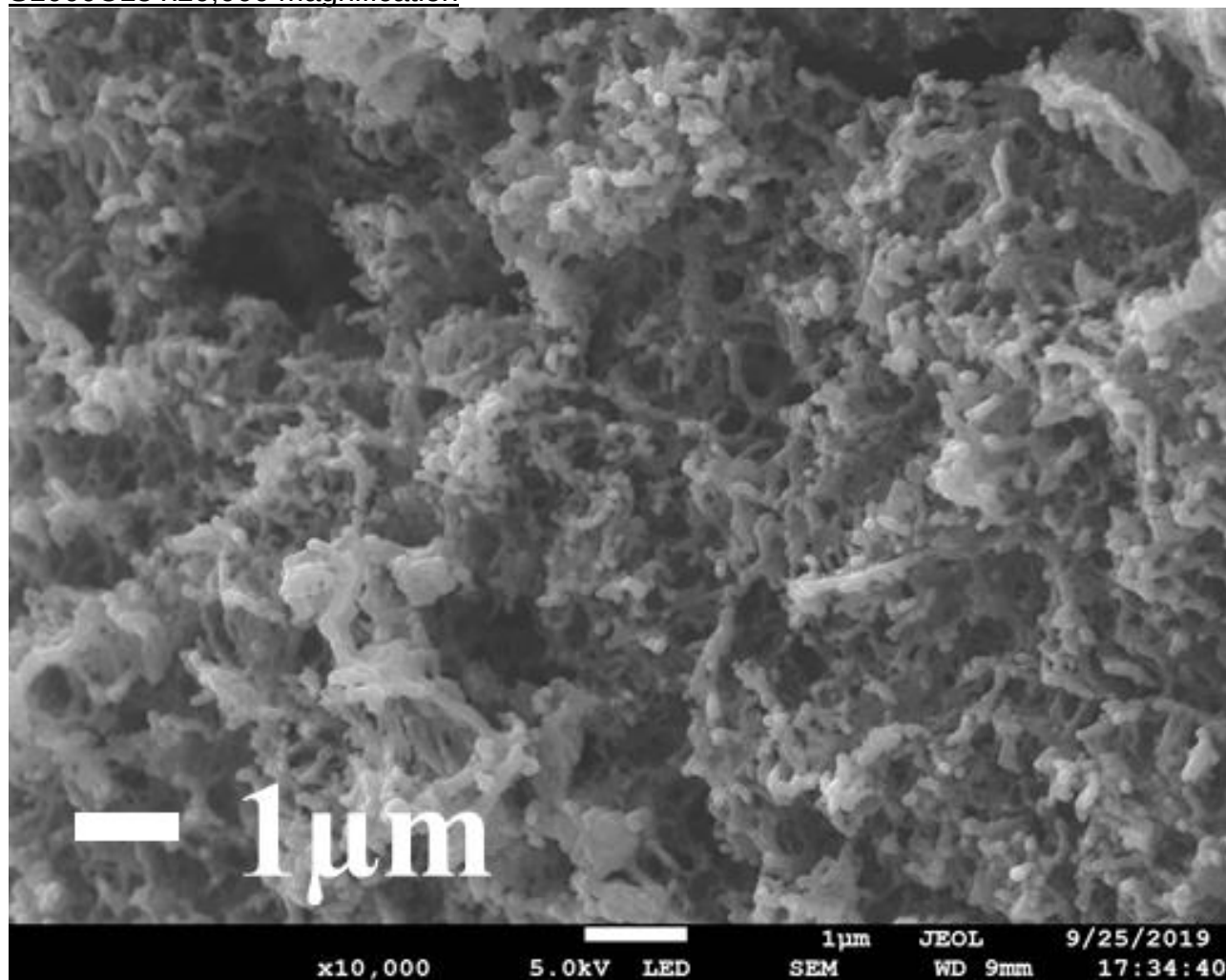


## SEM Images for S1000C15

S1000C15 x500 magnification and particle size distribution plot

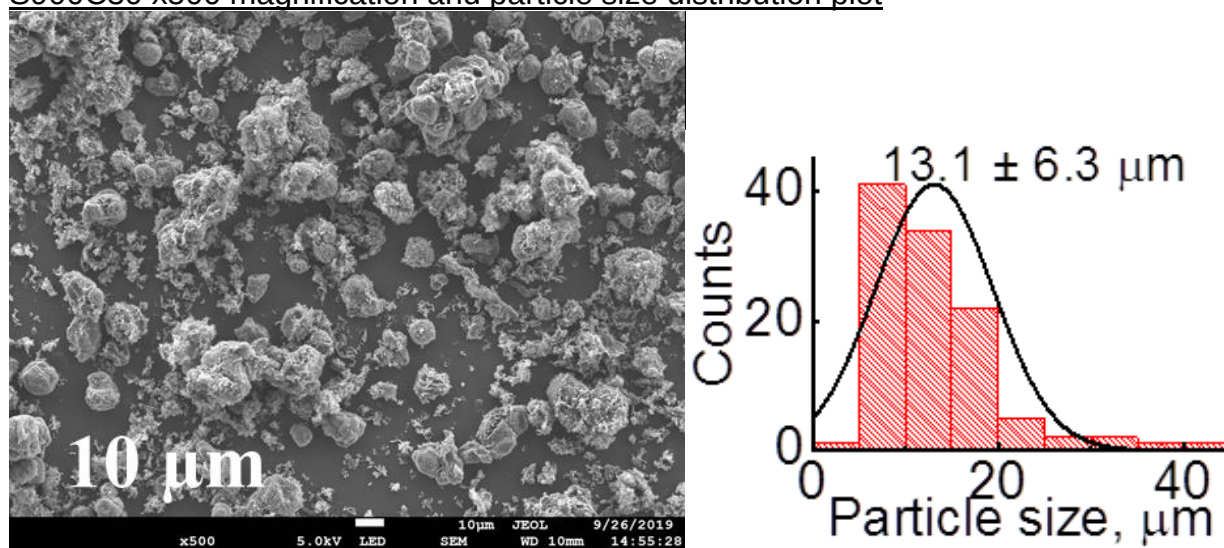


S1000C15 x10,000 magnification

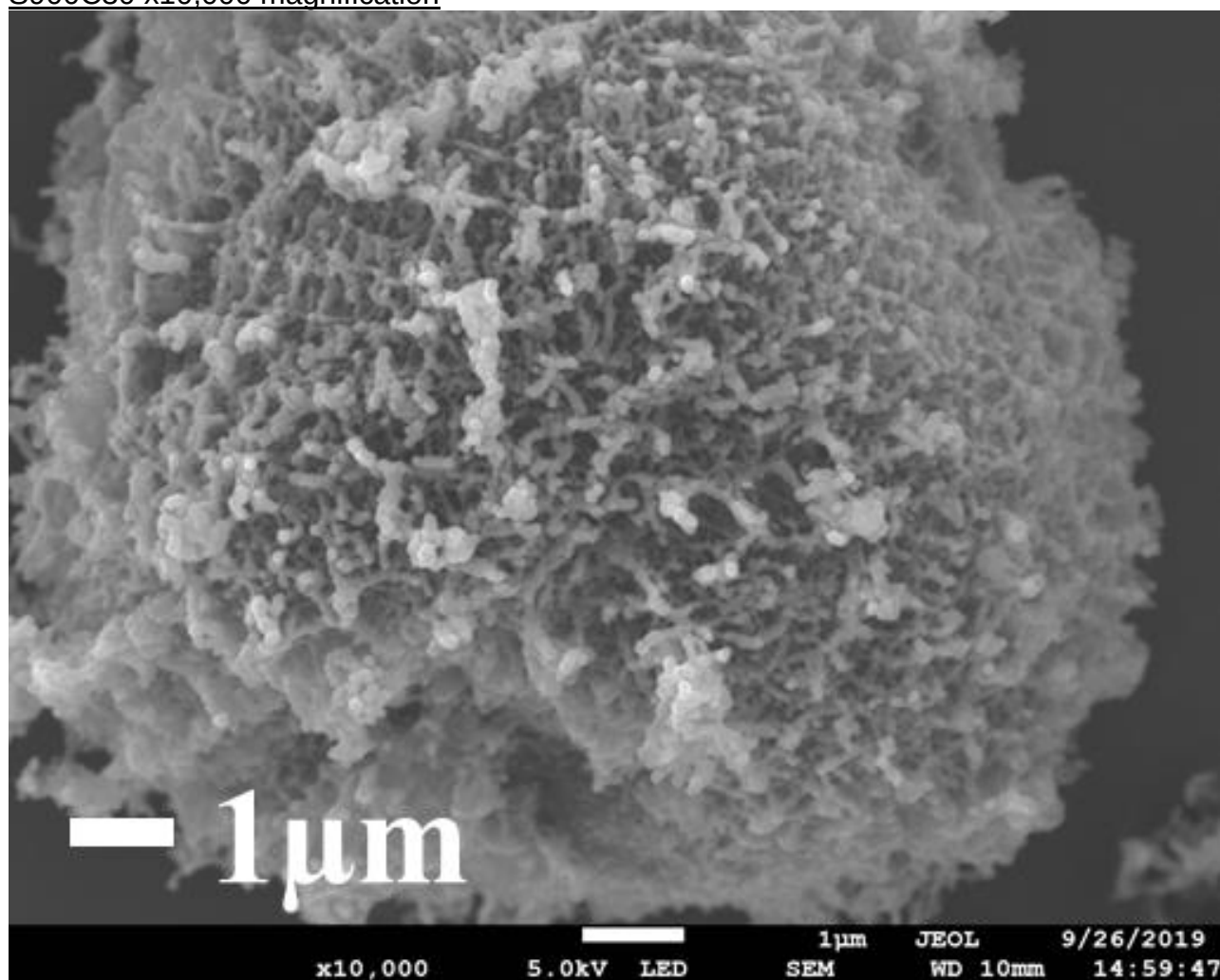


## SEM Images for S900C30

S900C30 x500 magnification and particle size distribution plot



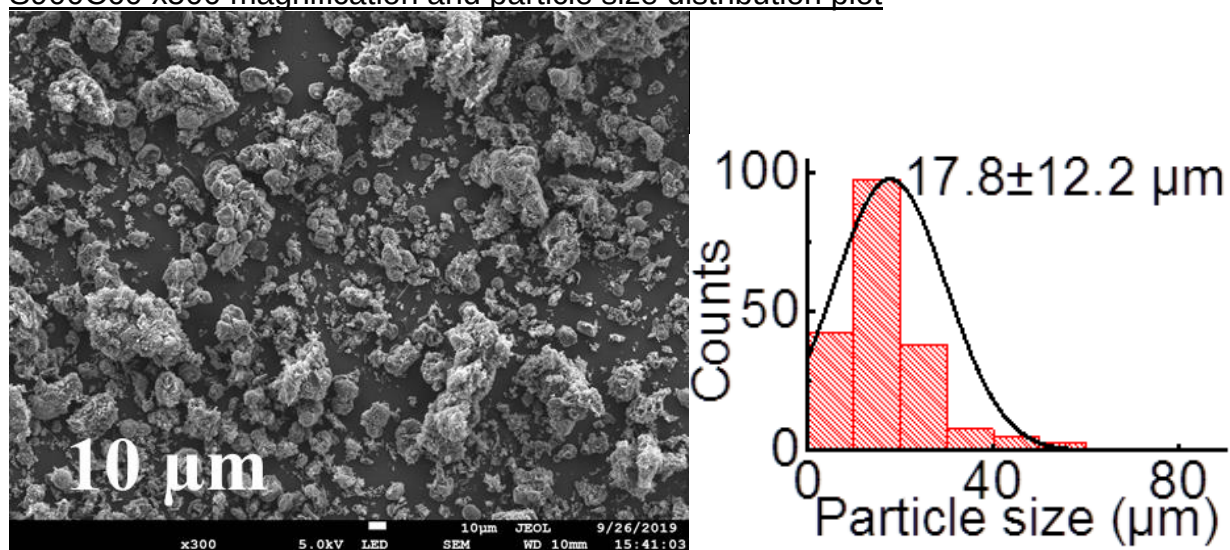
S900C30 x10,000 magnification



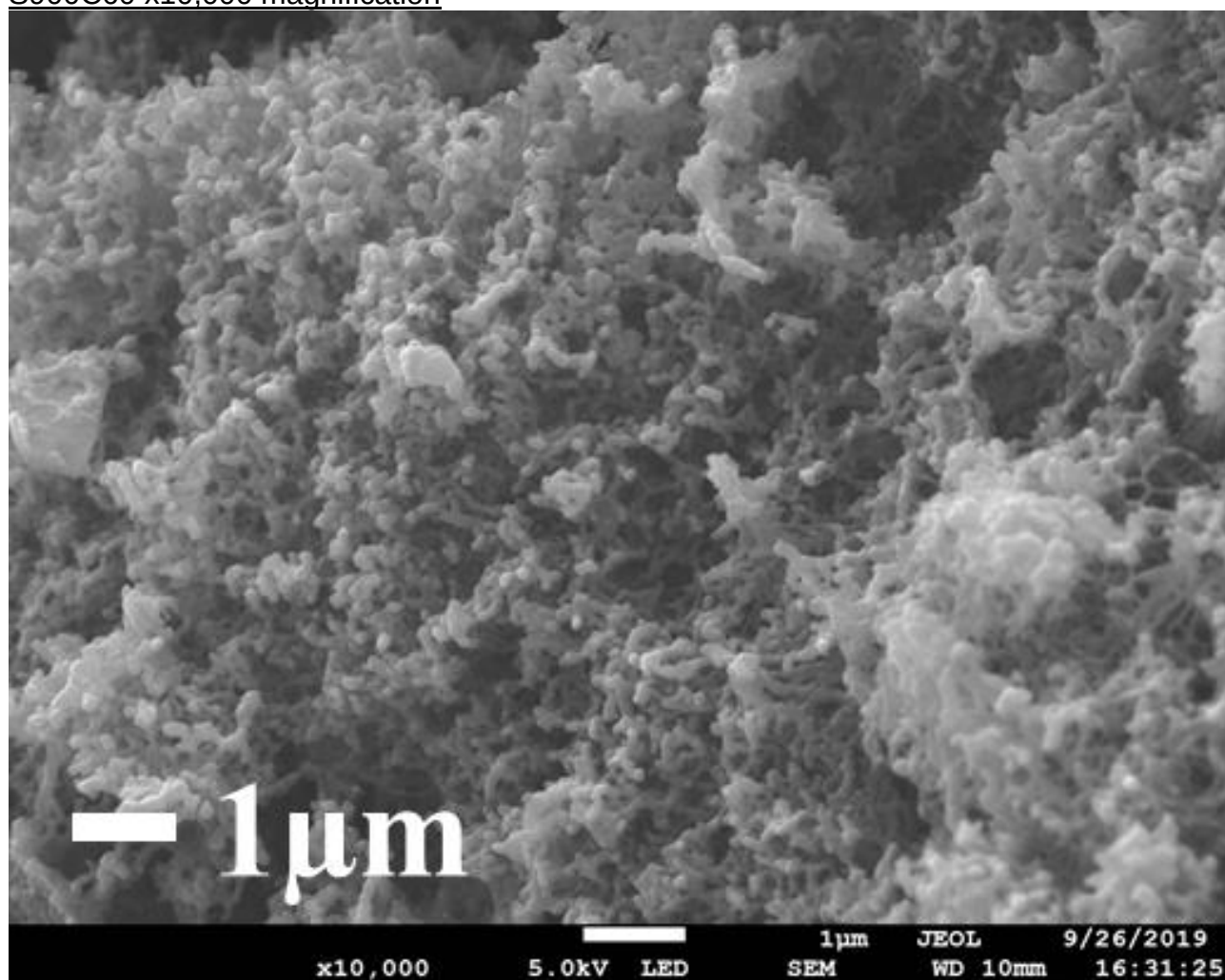


## SEM Images for S900C60

S900C60 x500 magnification and particle size distribution plot



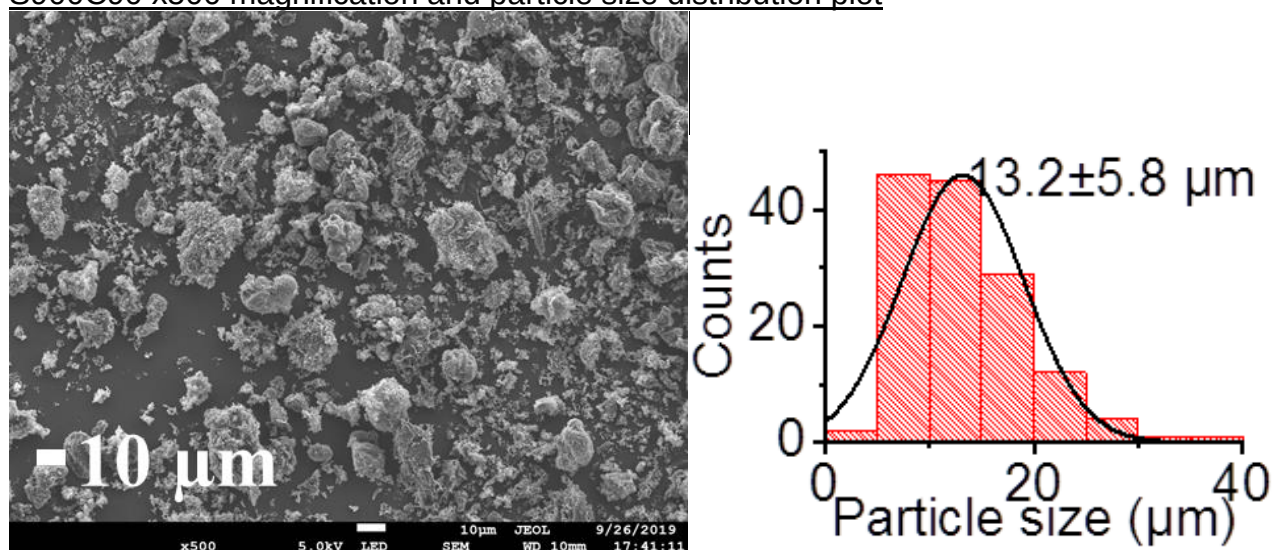
S900C60 x10,000 magnification



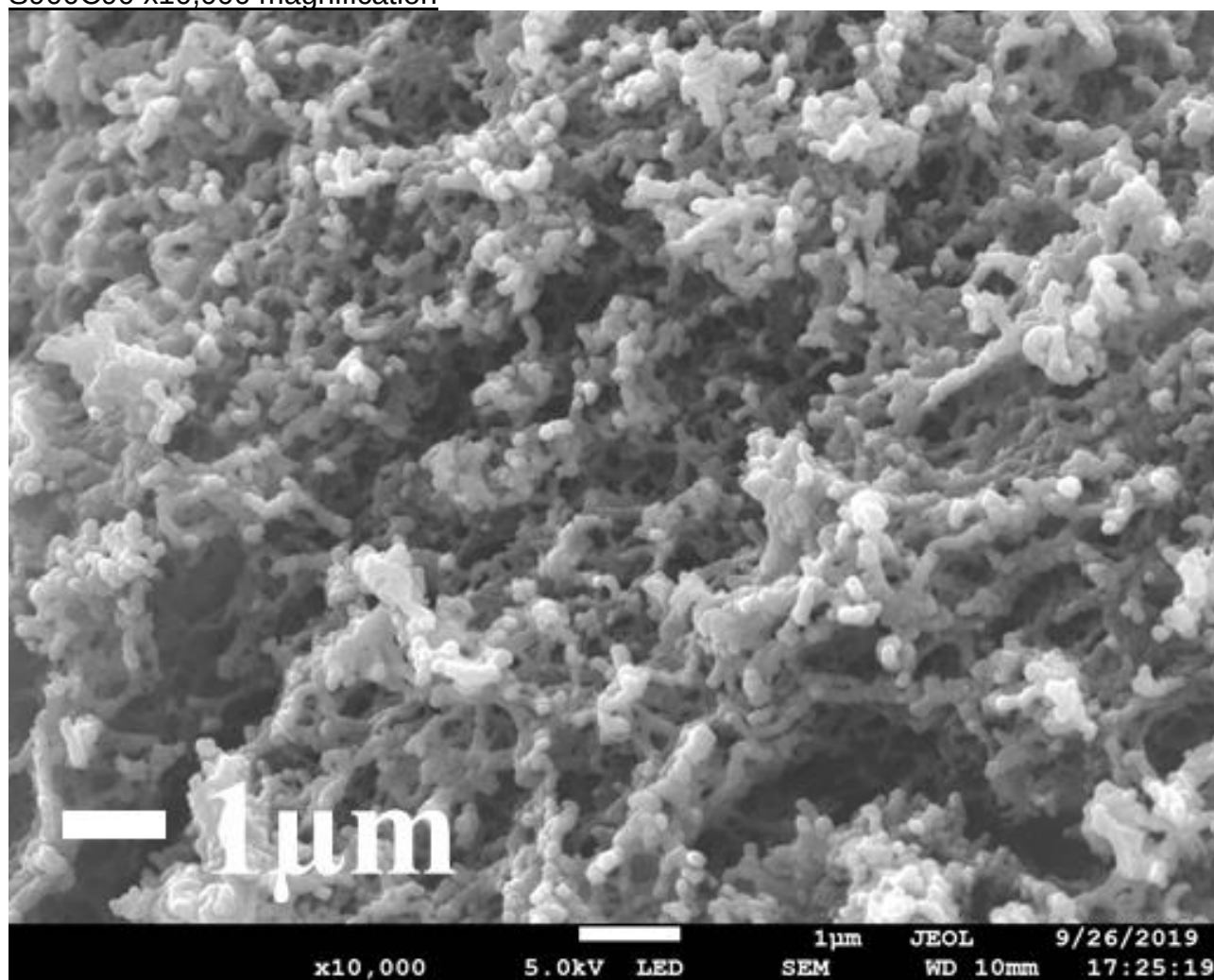


## SEM Images for S900C90

S900C90 x500 magnification and particle size distribution plot

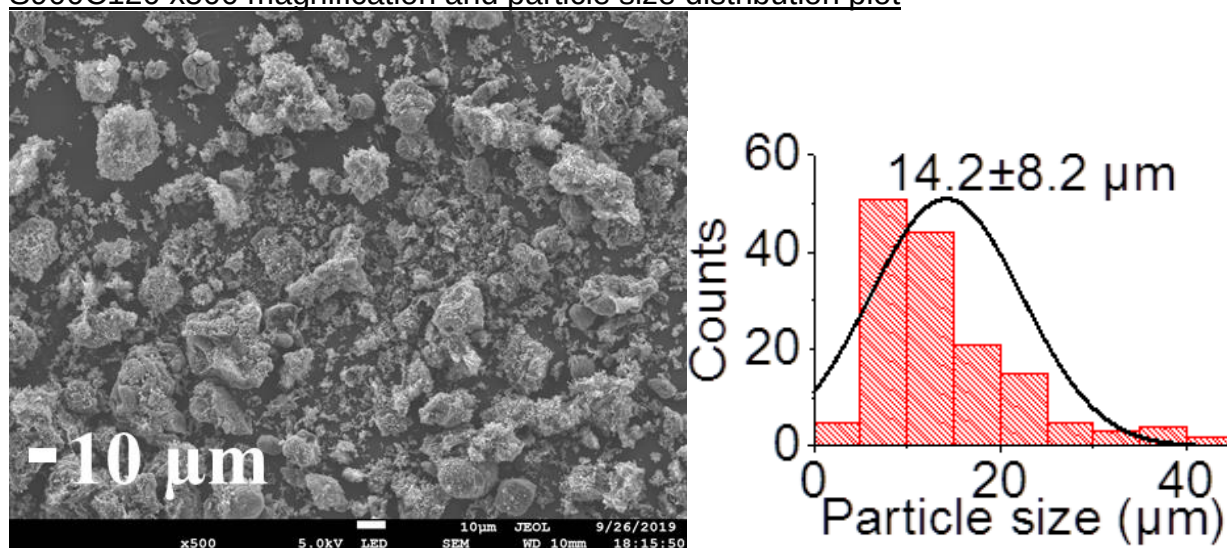


S900C90 x10,000 magnification

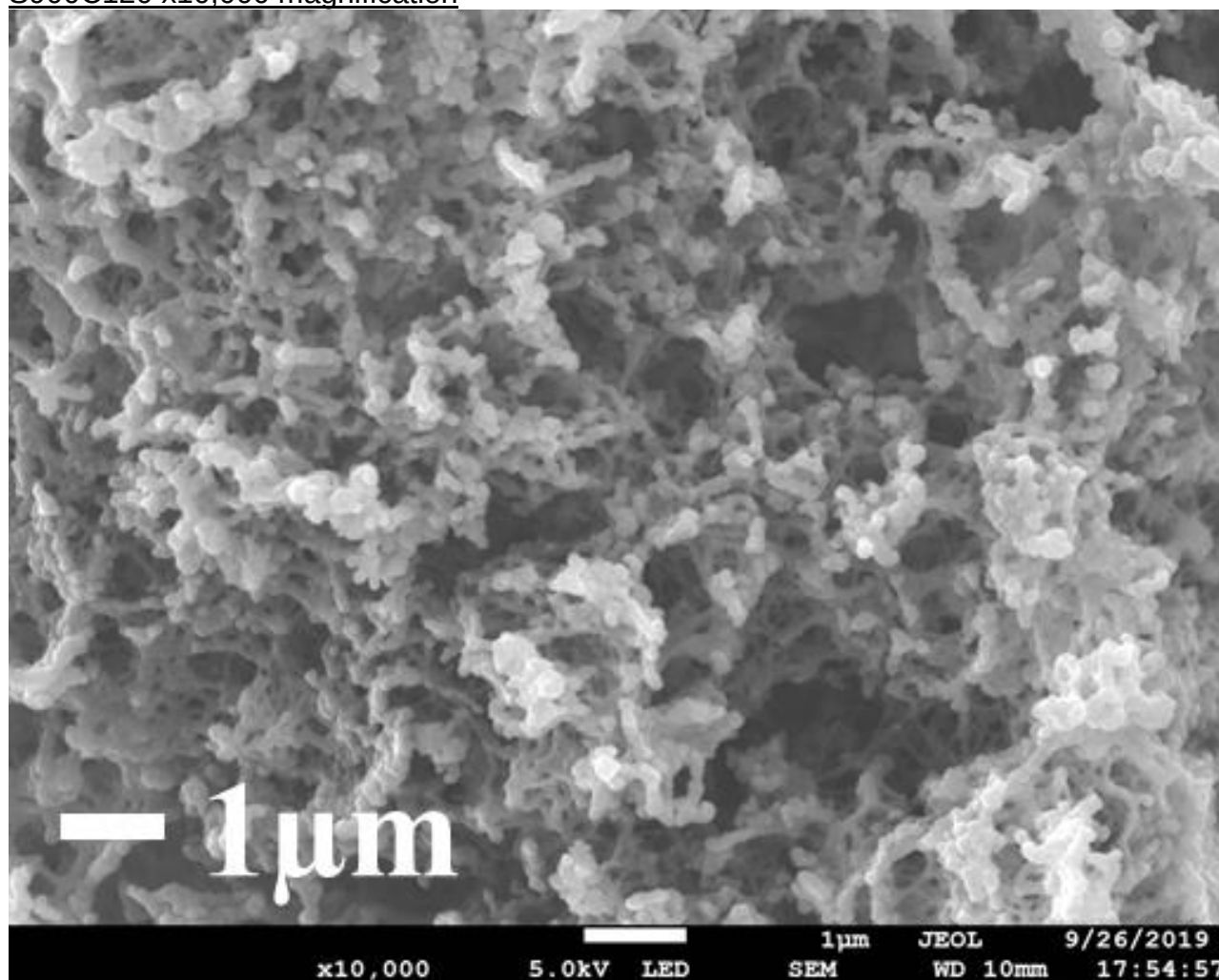


## SEM Images for S900C120

S900C120 x500 magnification and particle size distribution plot



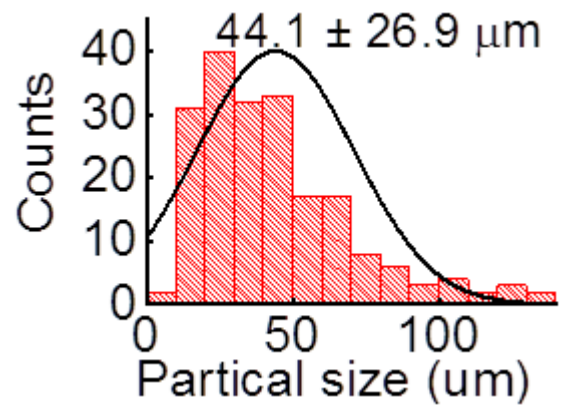
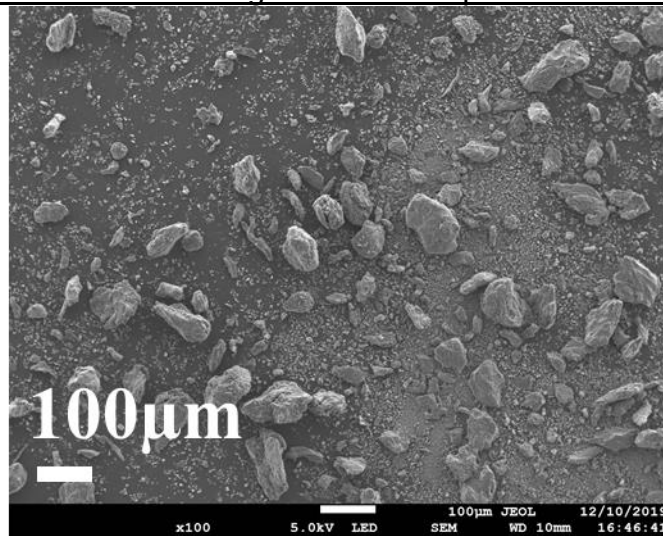
S900C120 x10,000 magnification



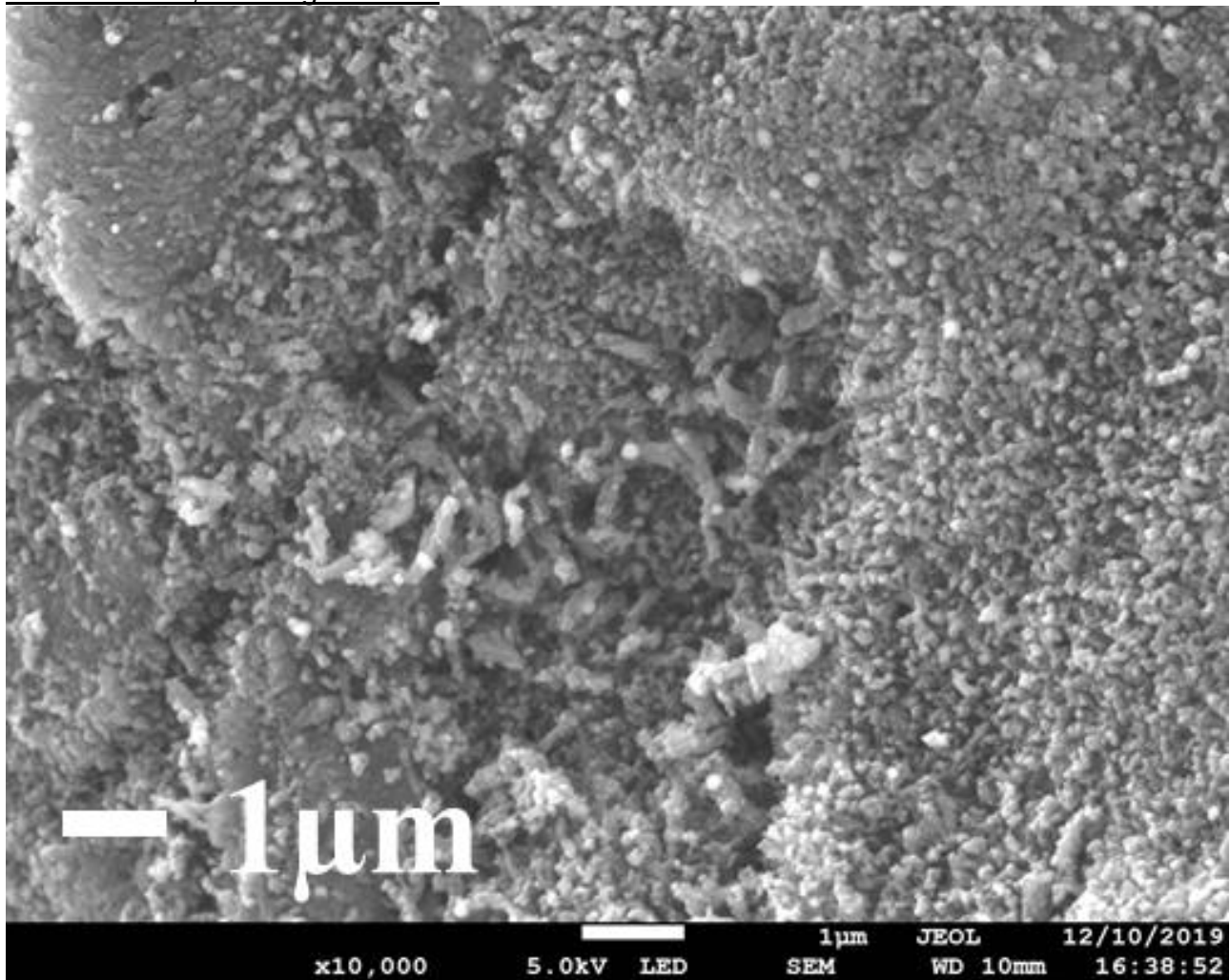


## SEM Images for A750C45

A750C45 x100 magnification and particle size distribution plot

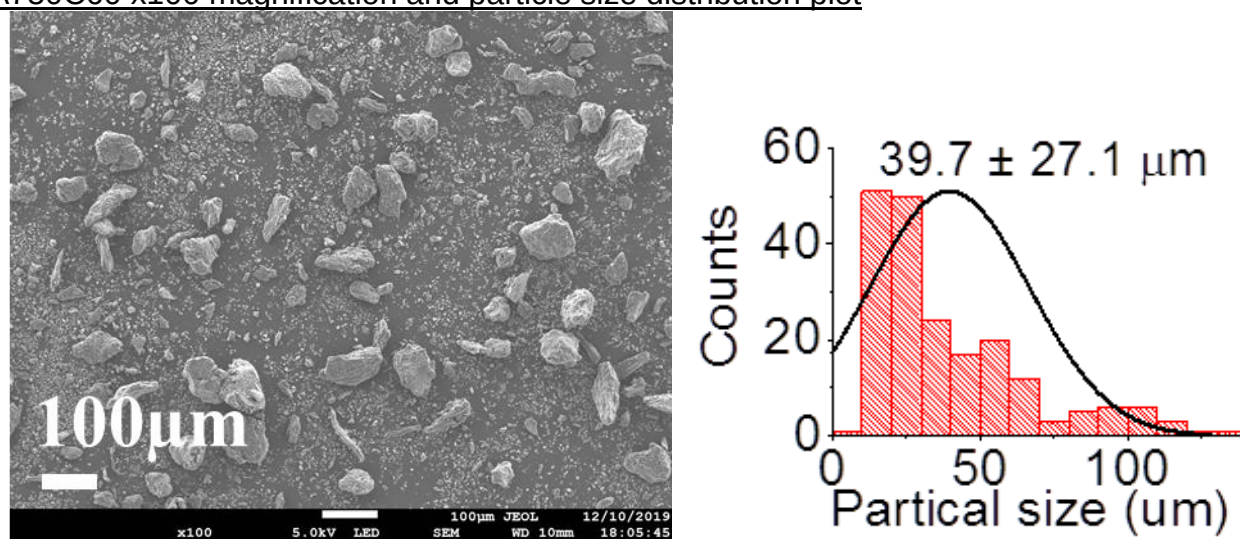


A750C45 x10,000 magnification

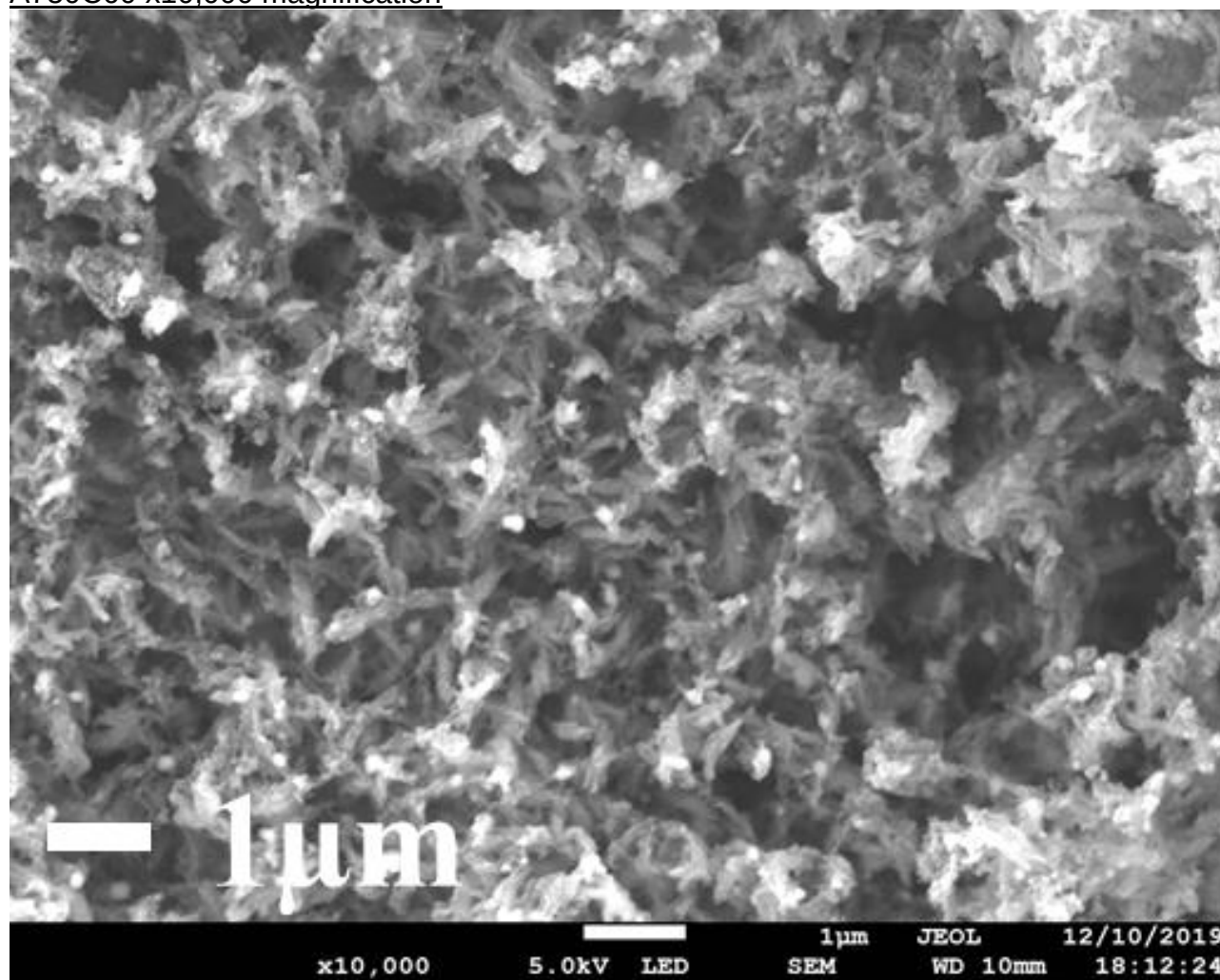


## SEM Images for A750C60

A750C60 x100 magnification and particle size distribution plot



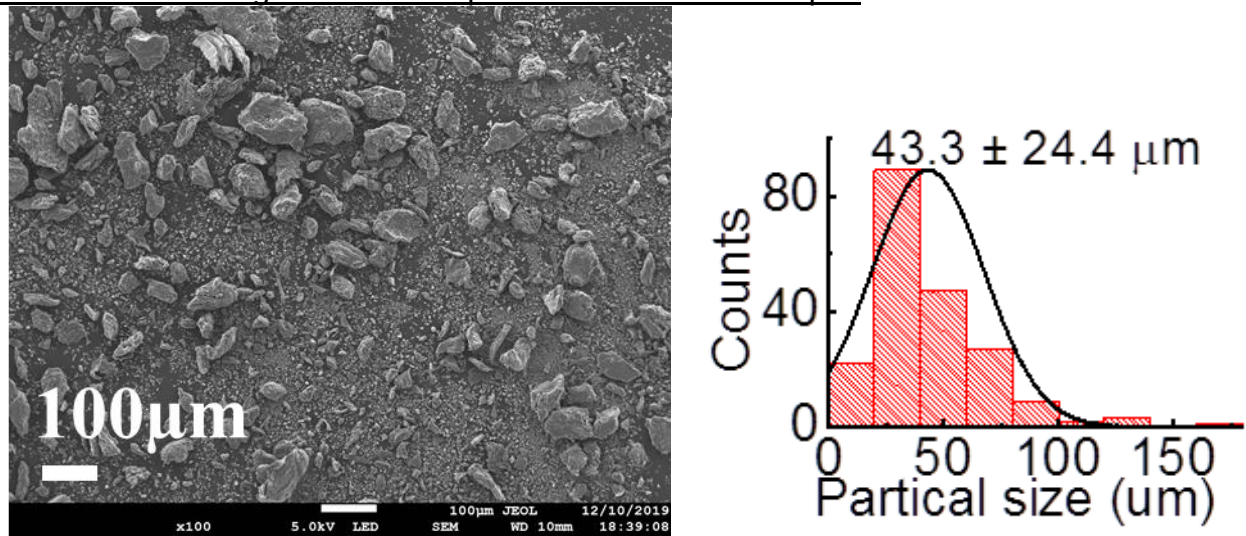
A750C60 x10,000 magnification



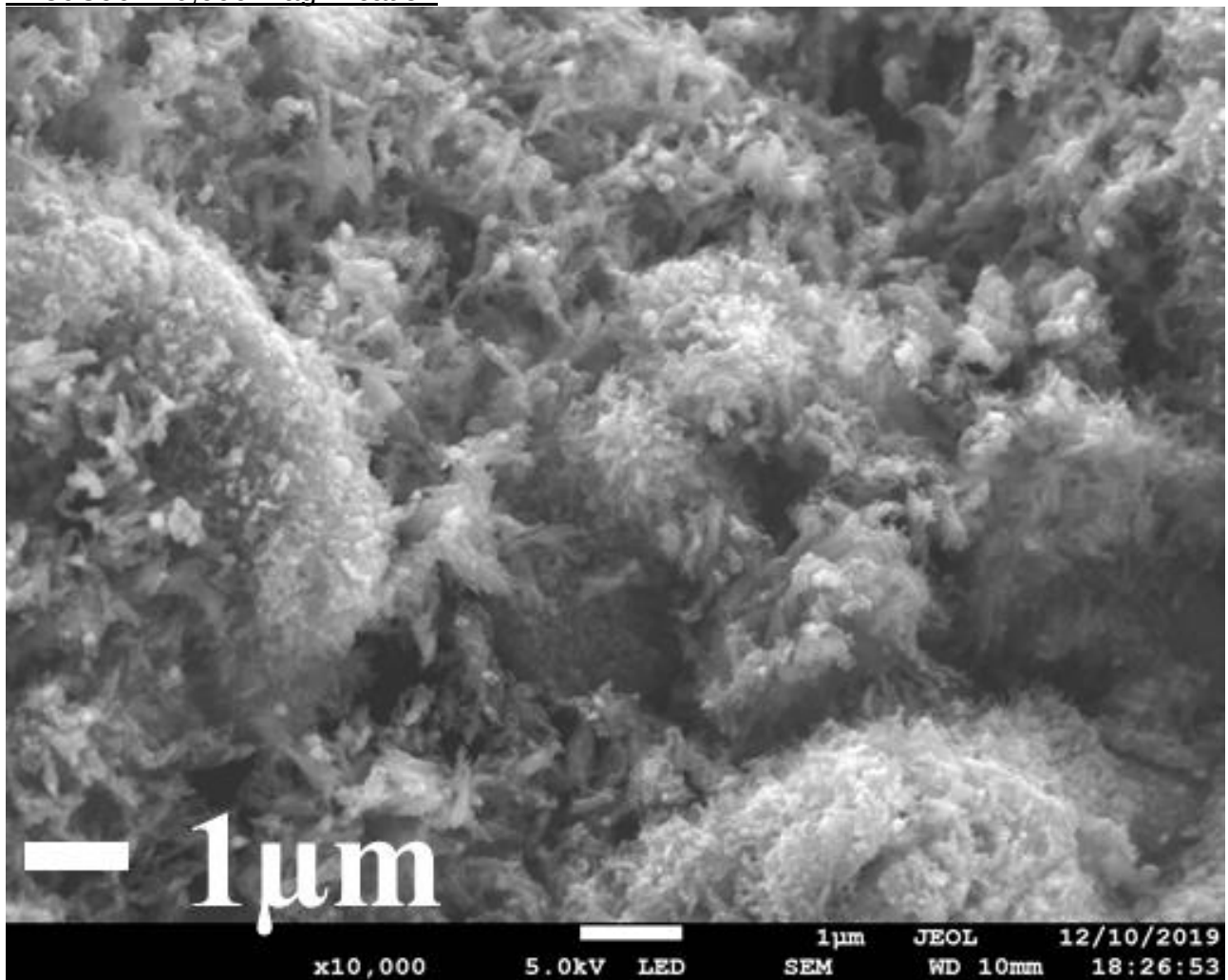


## SEM Images for A750C90

A750C90 x100 magnification and particle size distribution plot

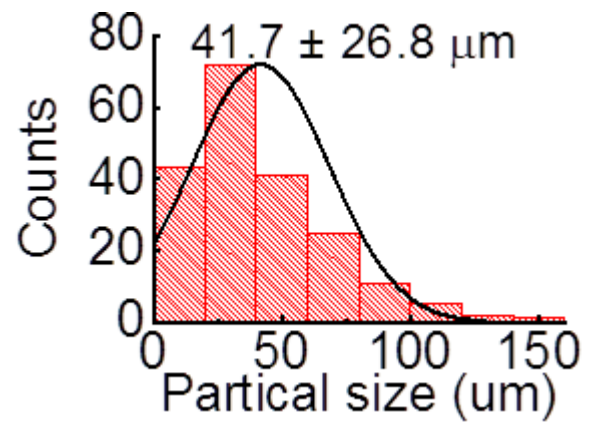
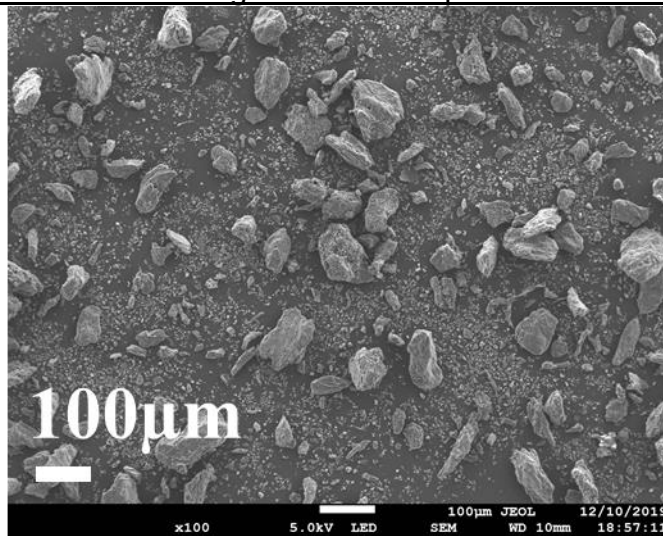


A750C90 x10,000 magnification

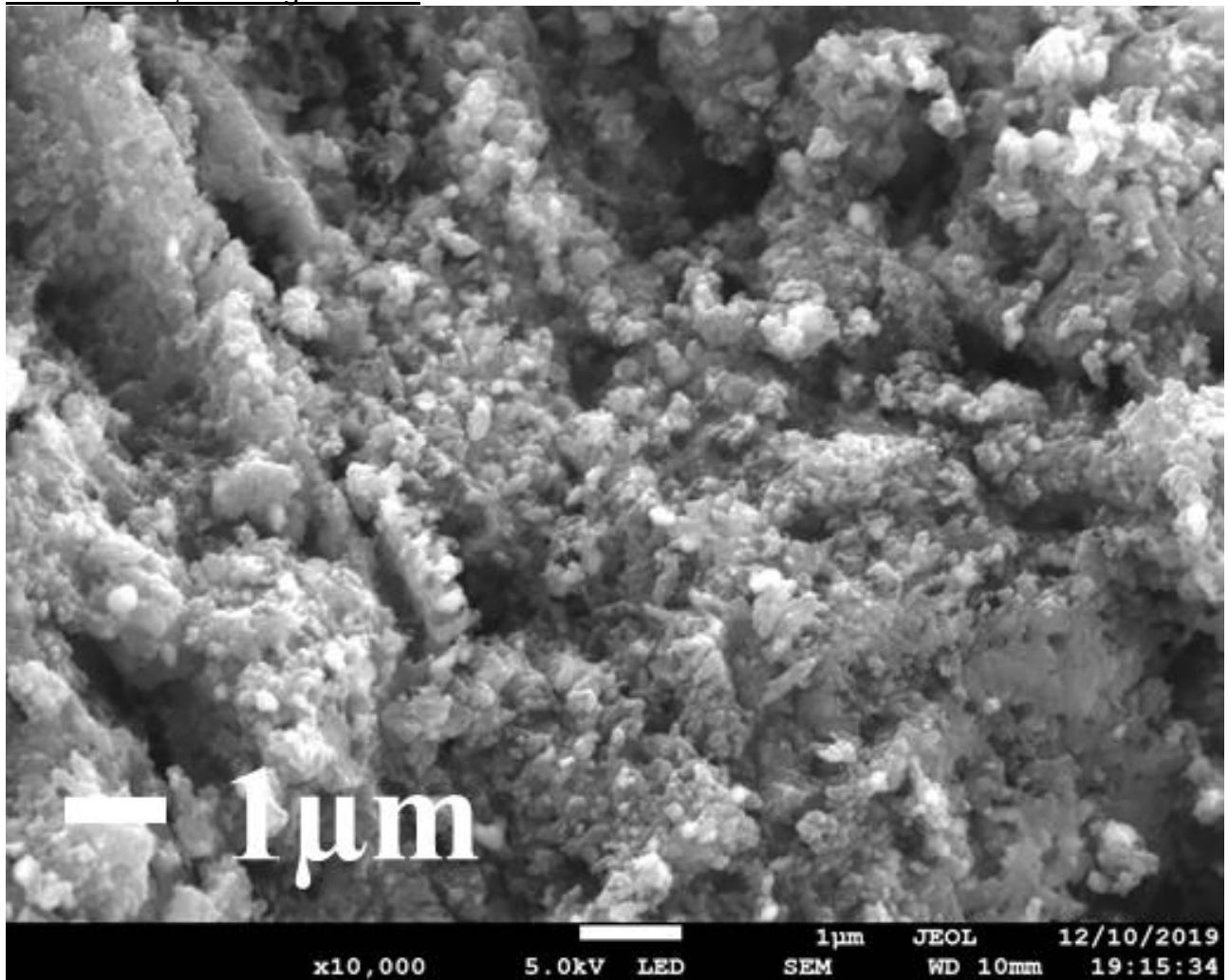


## SEM Images for A900C0

A900C0 x100 magnification and particle size distribution plot



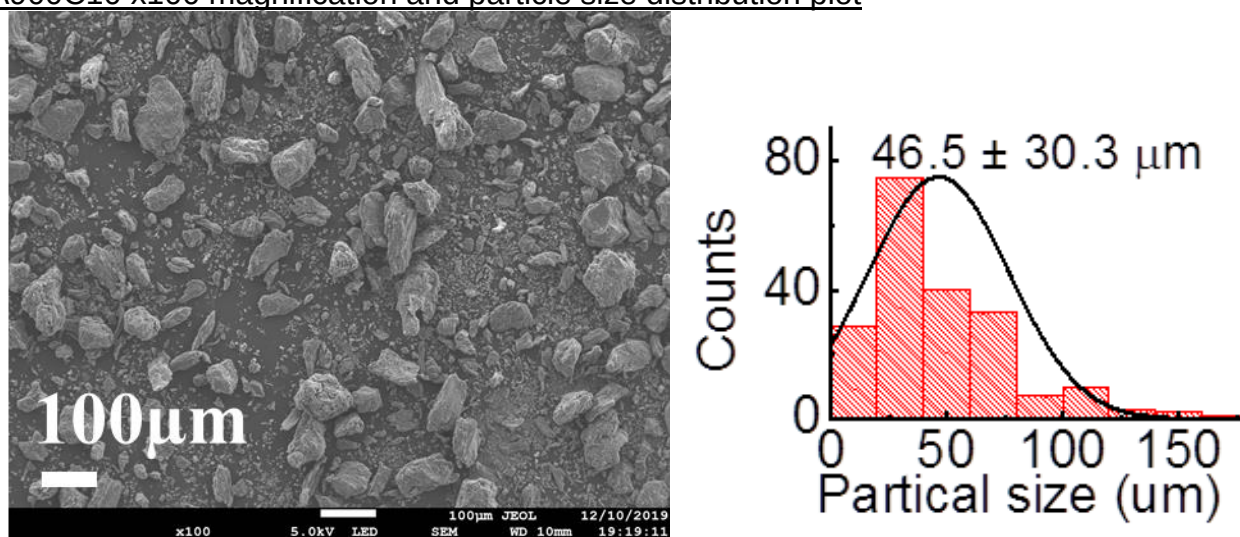
A900C0 x10,000 magnification



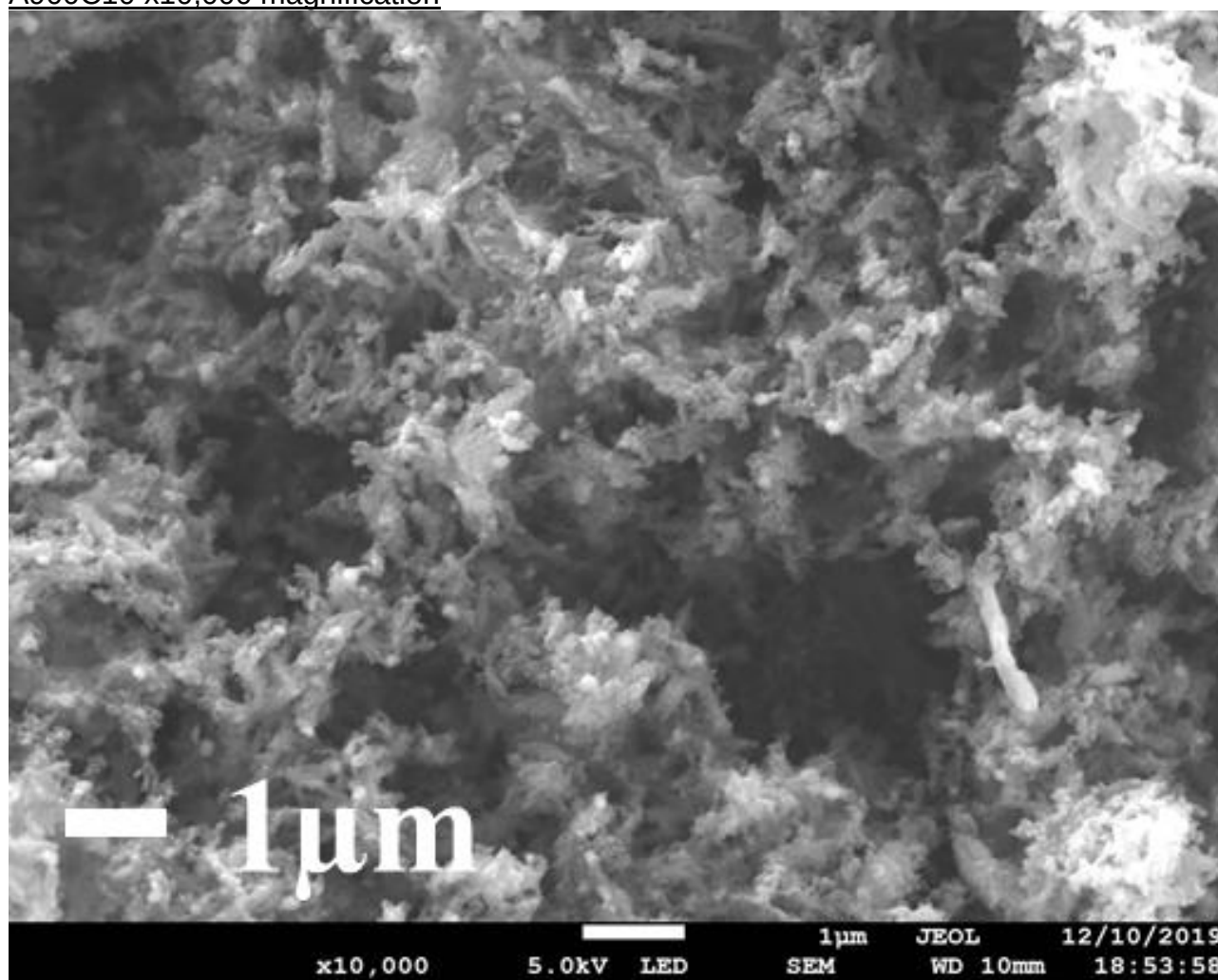


## SEM Images for A900C10

A900C10 x100 magnification and particle size distribution plot

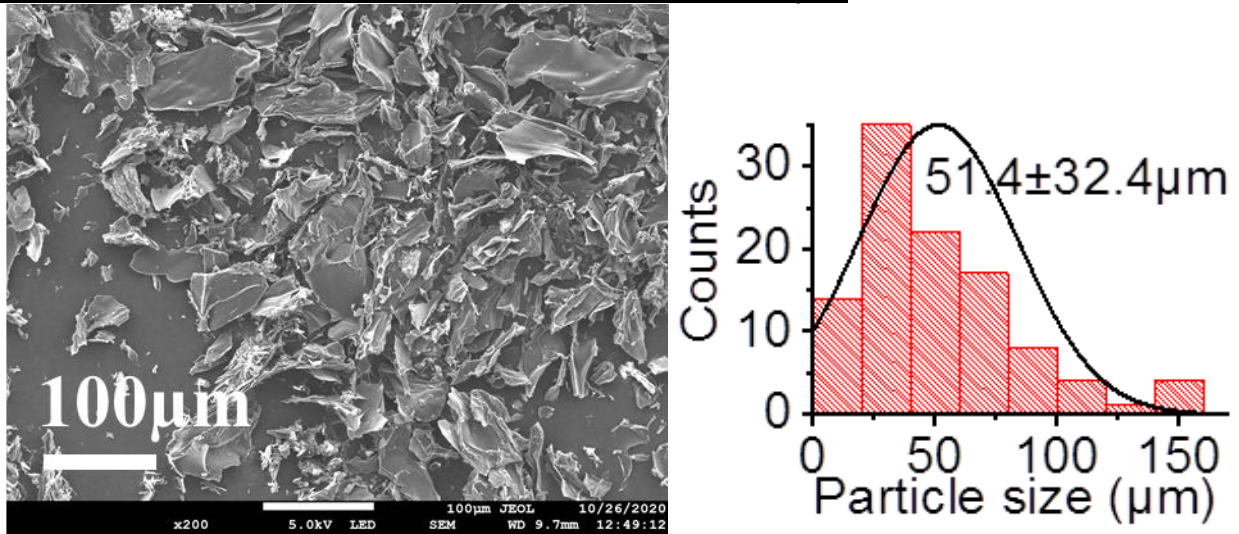


A900C10 x10,000 magnification

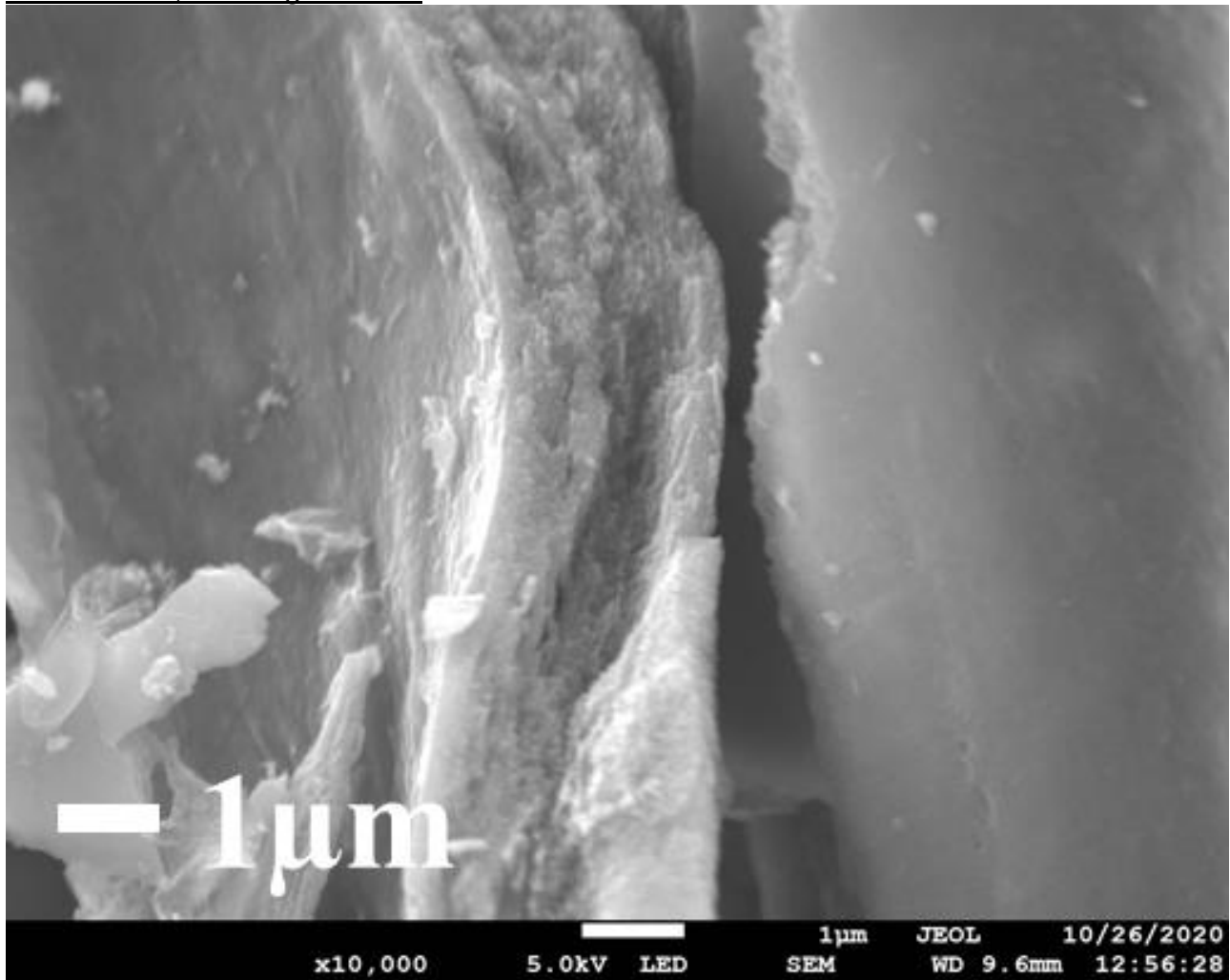


## SEM Images for P900C0

P900C0 x200 magnification and particle size distribution plot



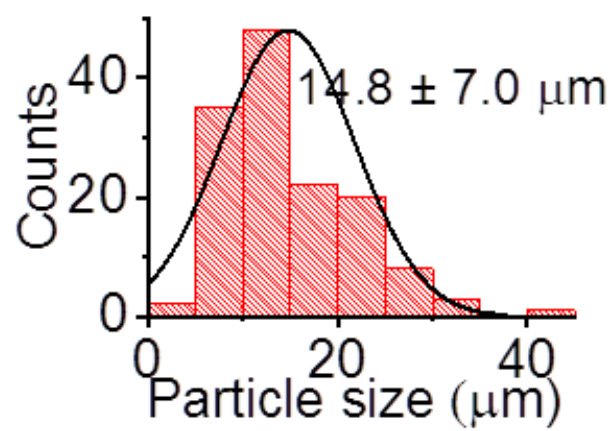
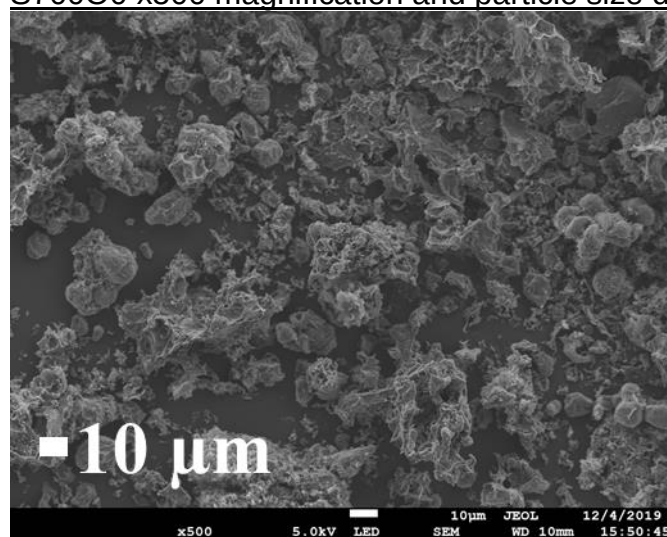
P900C0 x10,000 magnification



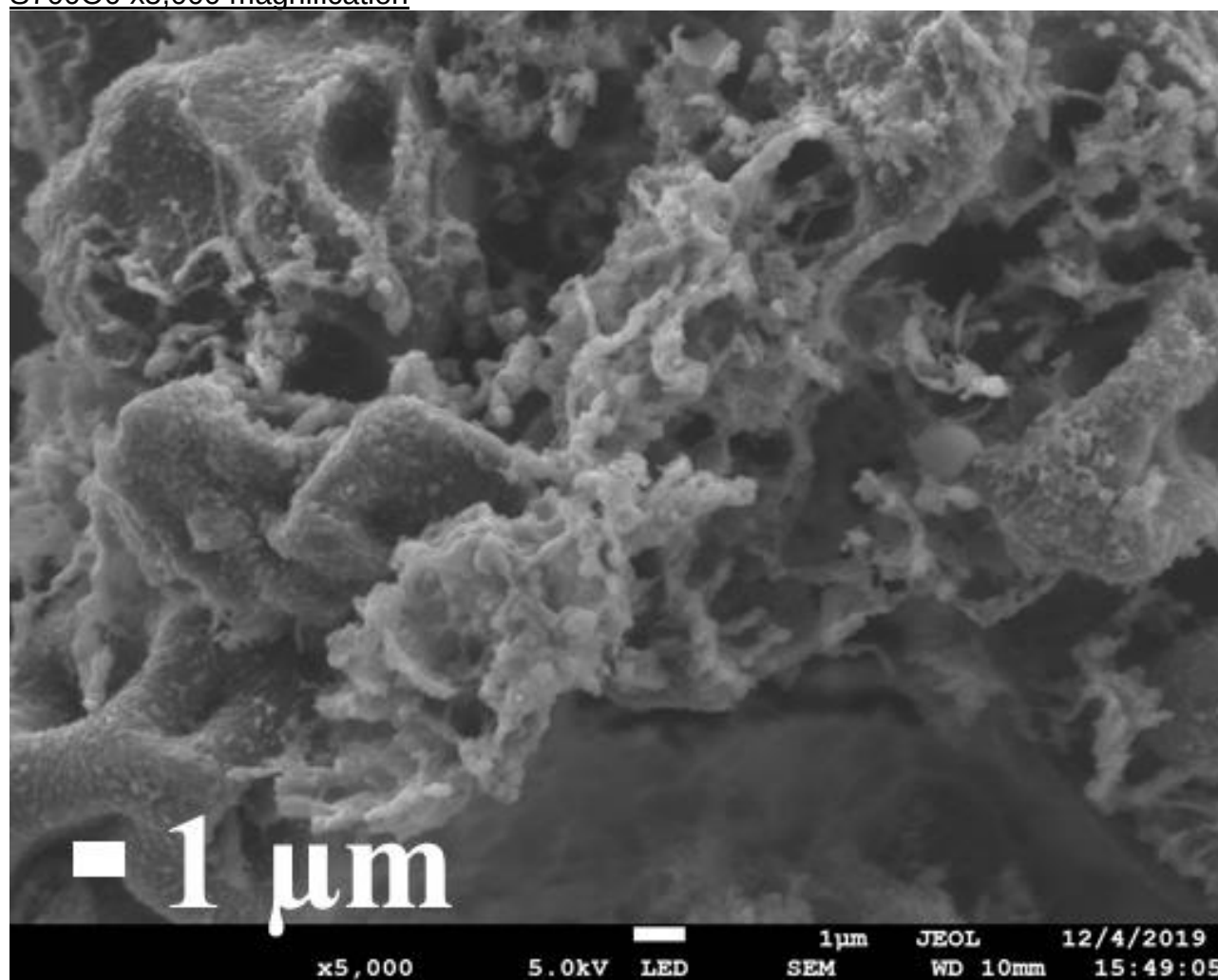


## SEM Images for S700O0

S700O0 x500 magnification and particle size distribution plot

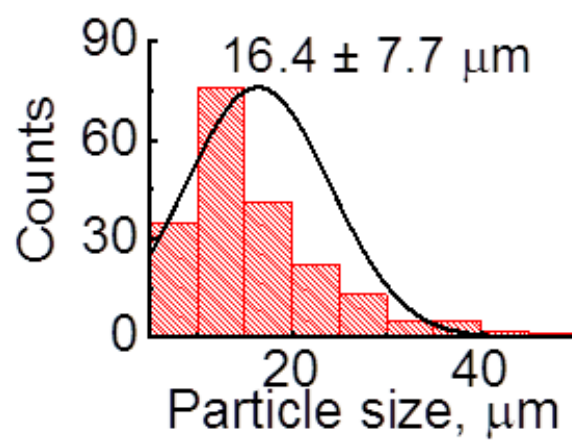
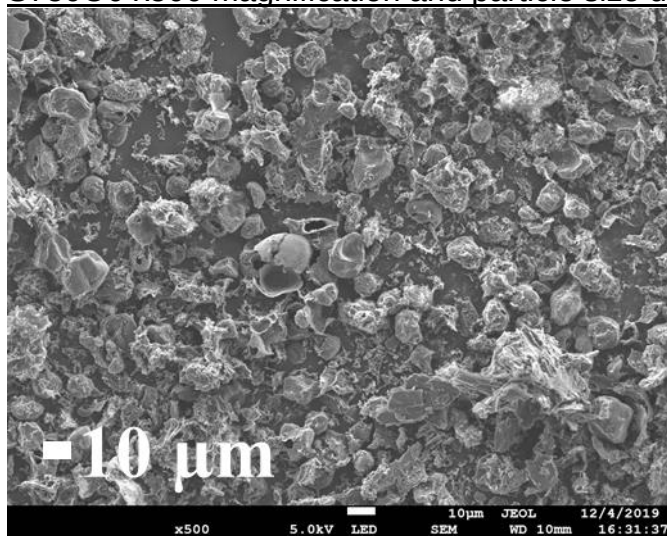


S700O0 x5,000 magnification

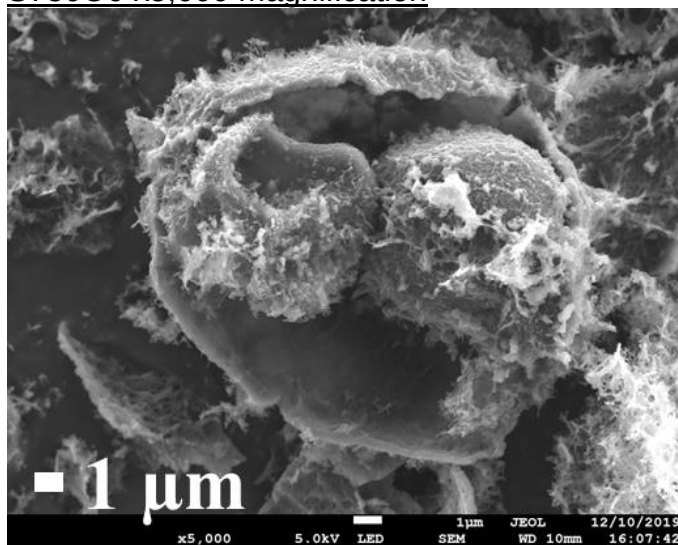


## SEM Images for S750O0

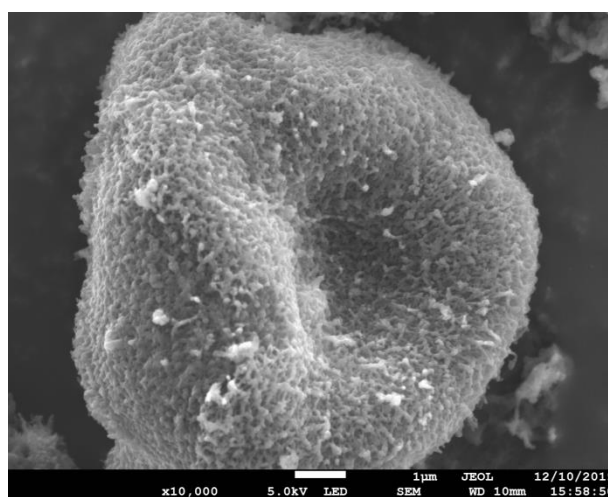
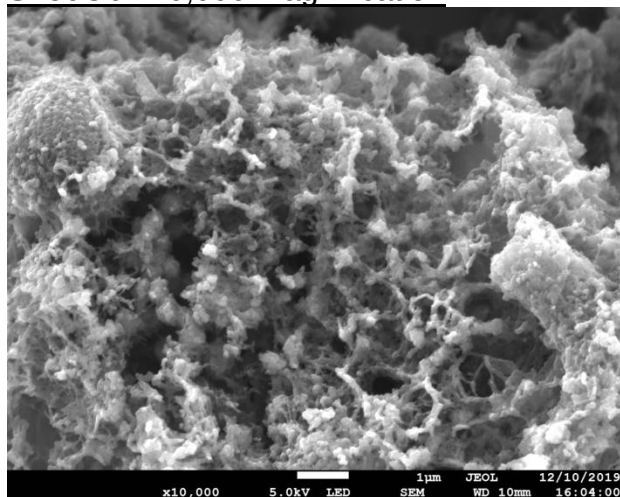
S750O0 x500 magnification and particle size distribution plot



S750O0 x5,000 magnification



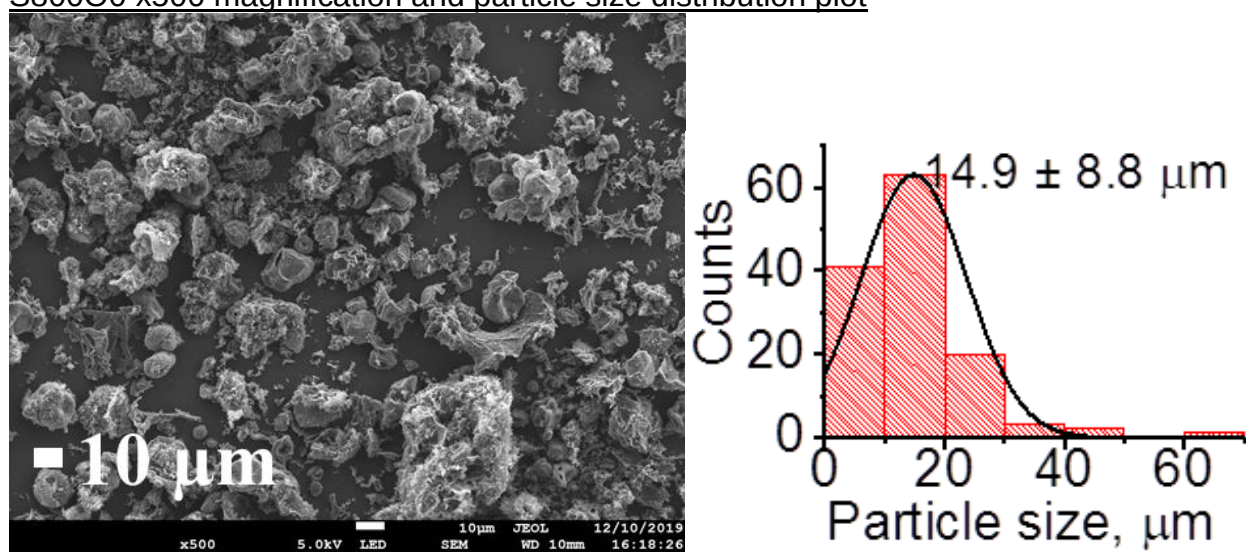
S750O0 x10,000 magnification



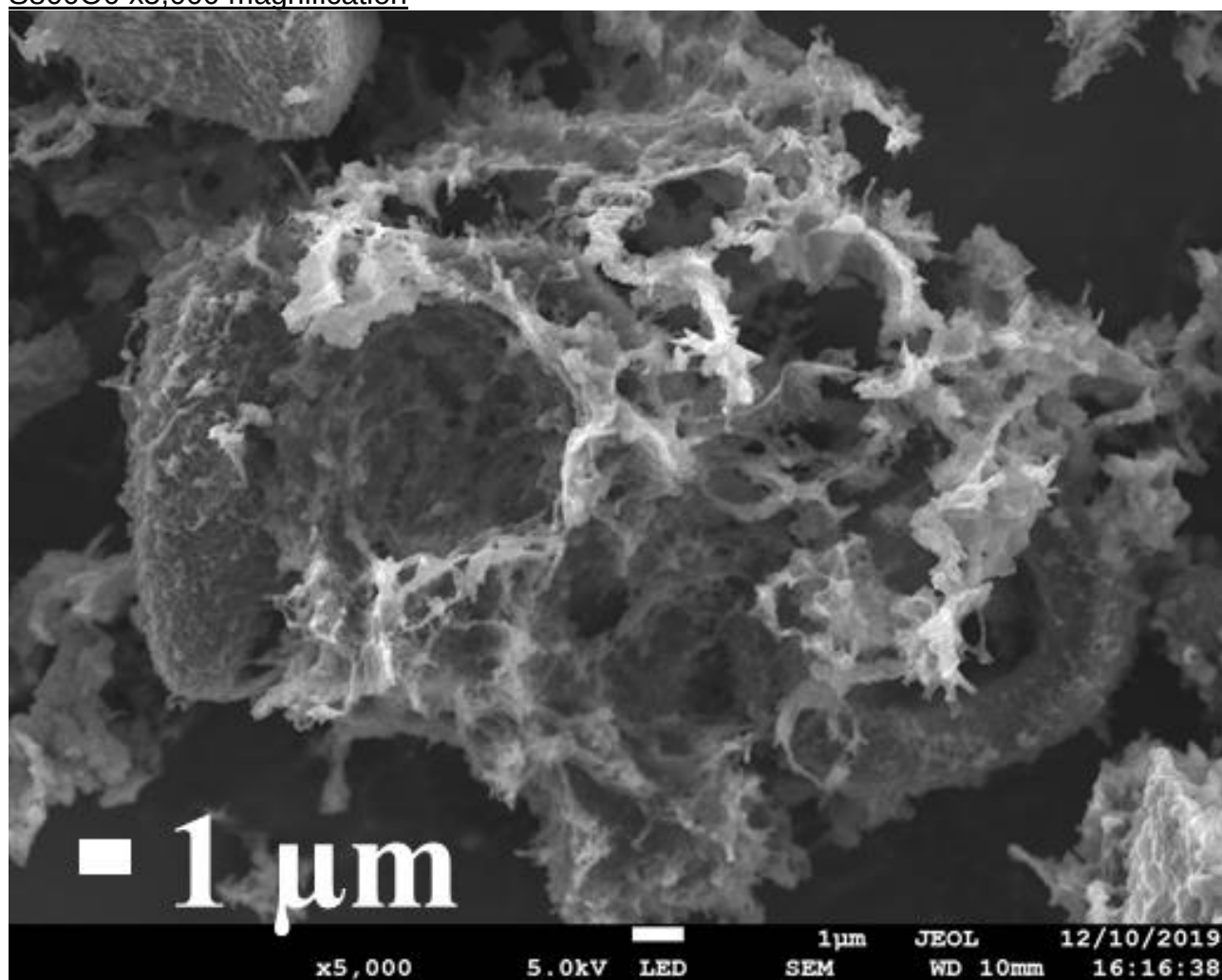


## SEM Images for S800O0

S800O0 x500 magnification and particle size distribution plot

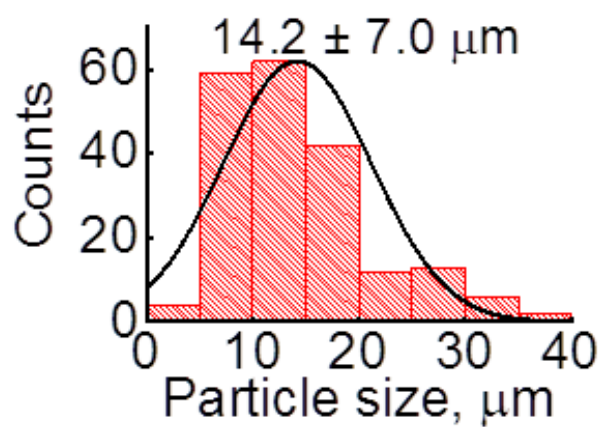
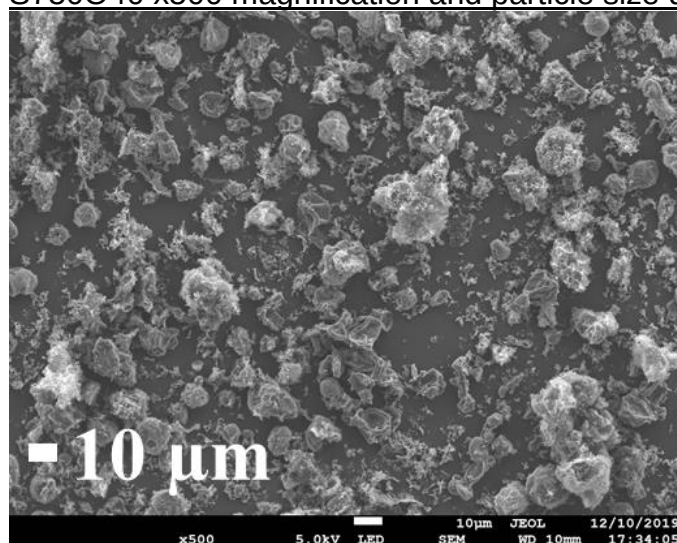


S800O0 x5,000 magnification

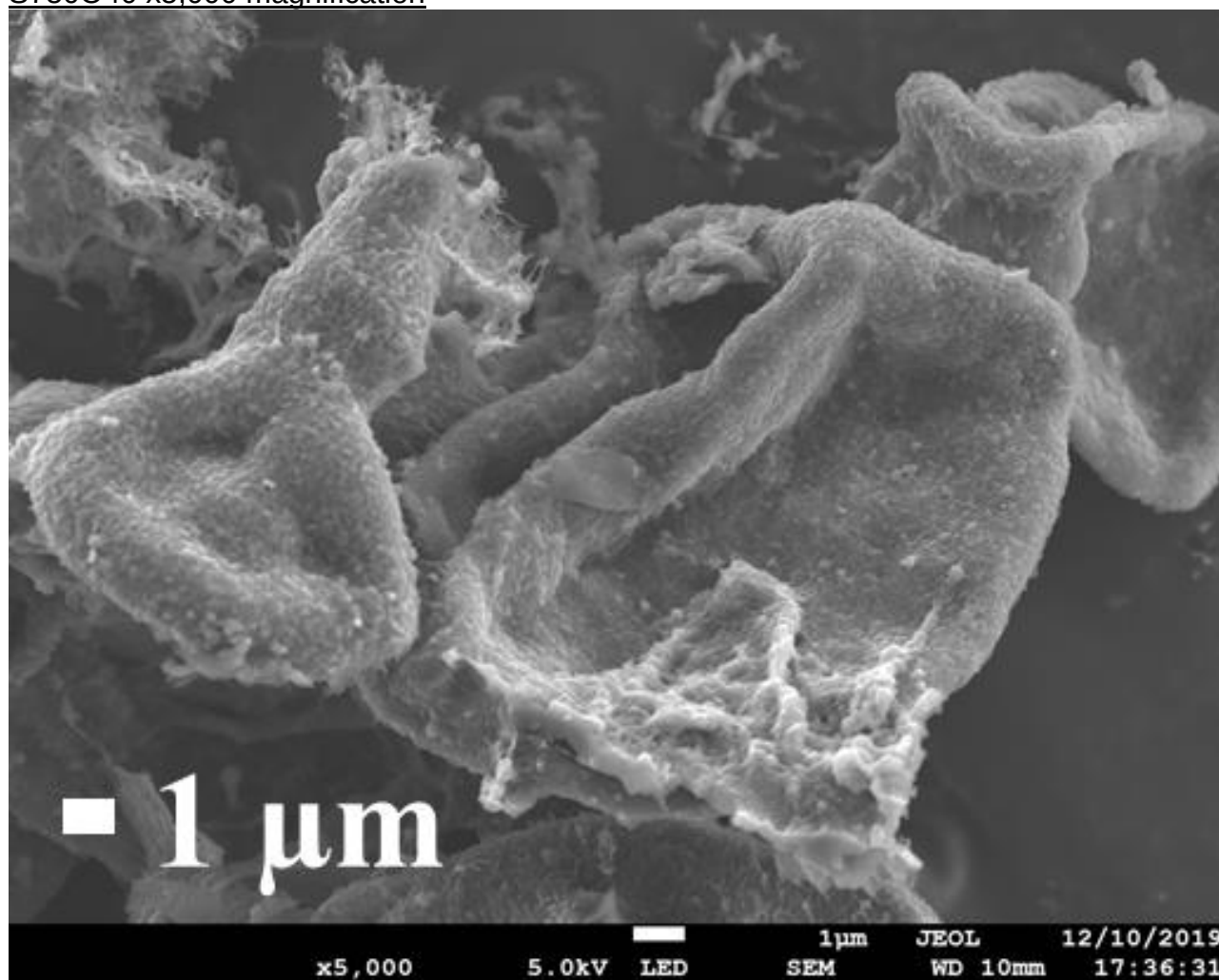


## SEM Images for S750O40

S750O40 x500 magnification and particle size distribution plot



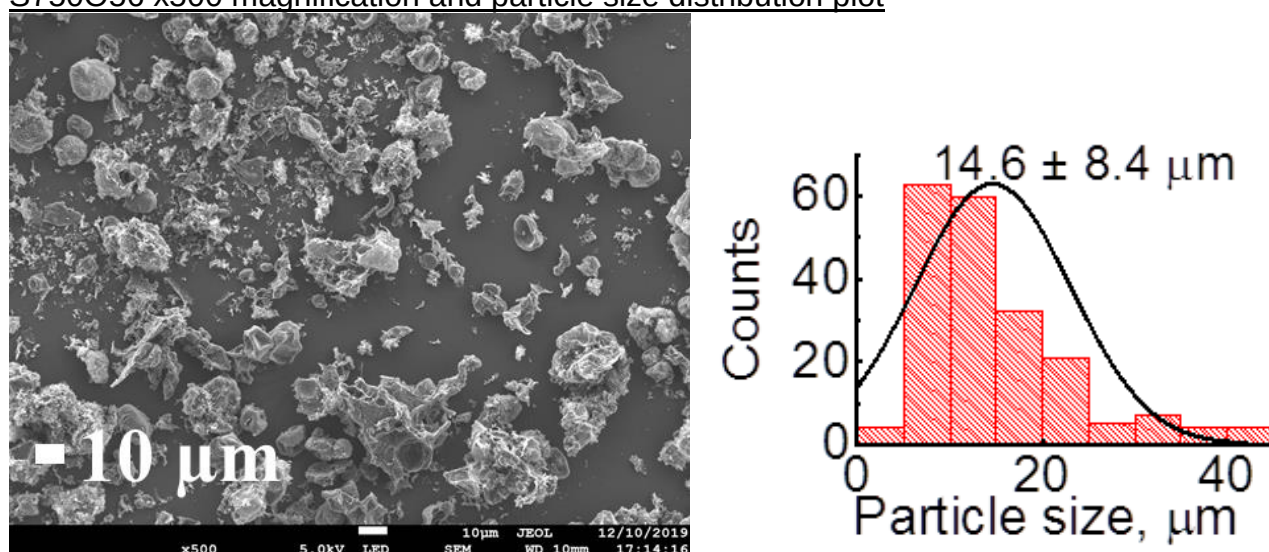
S750O40 x5,000 magnification



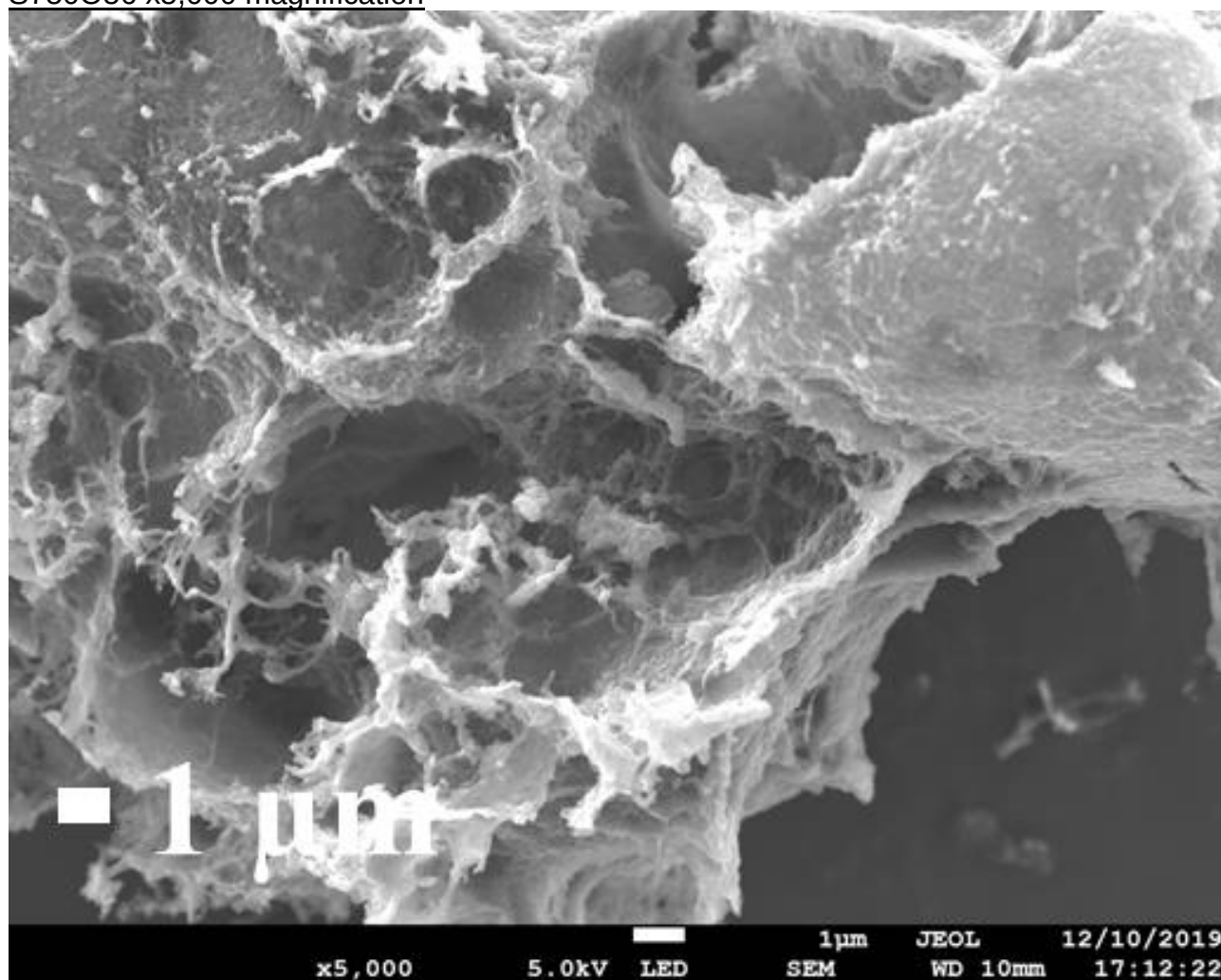


## SEM Images for S750O56

S750O56 x500 magnification and particle size distribution plot

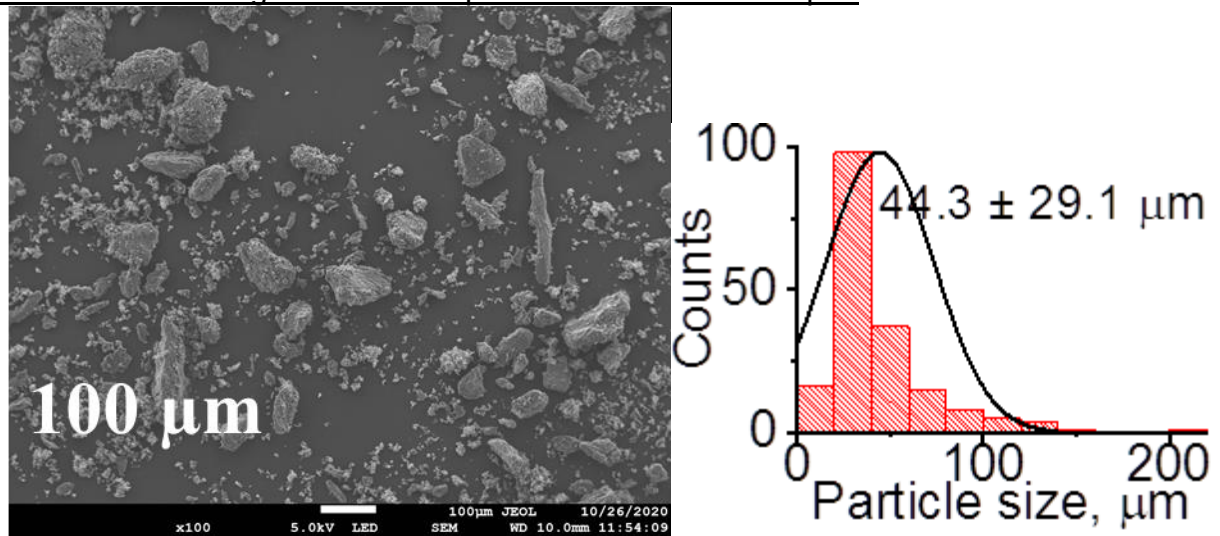


S750O56 x5,000 magnification

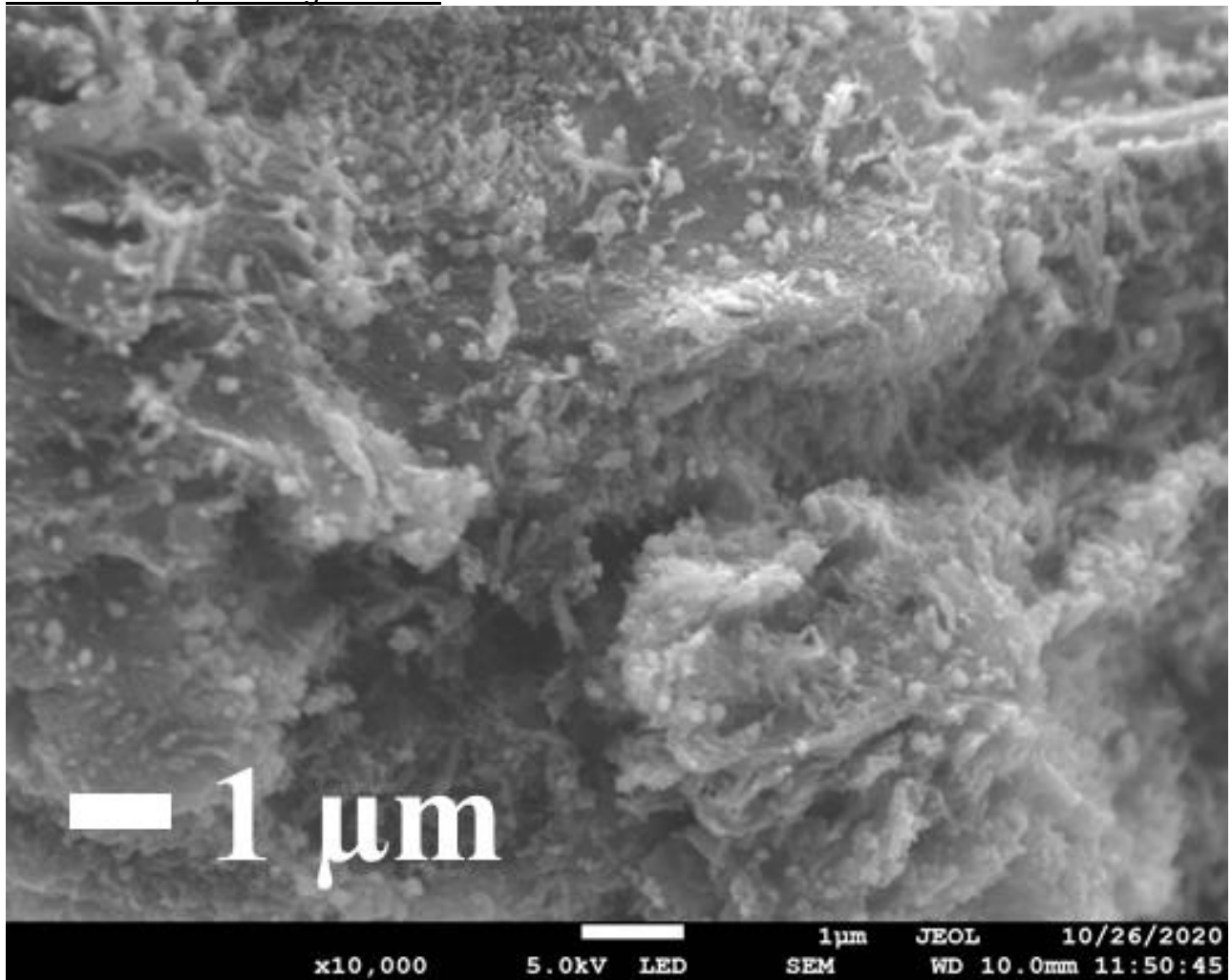


## SEM Images for A500O30

A500O30 x100 magnification and particle size distribution plot

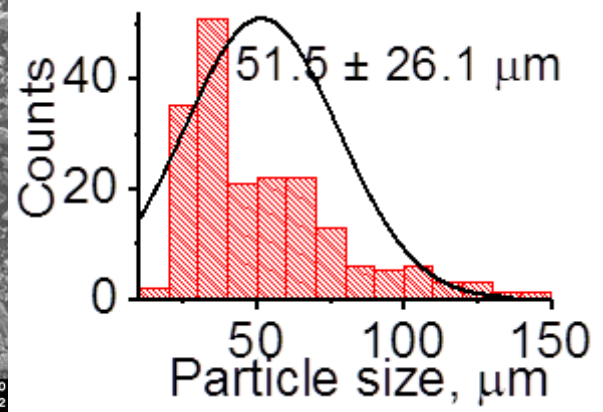
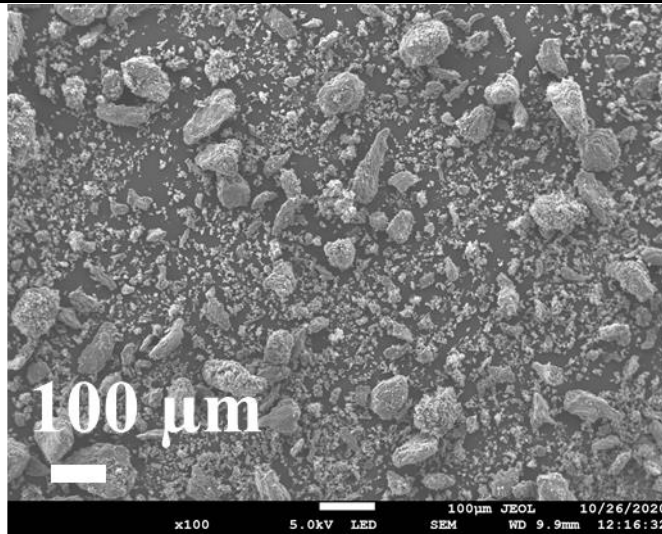


A500O30 x10,000 magnification

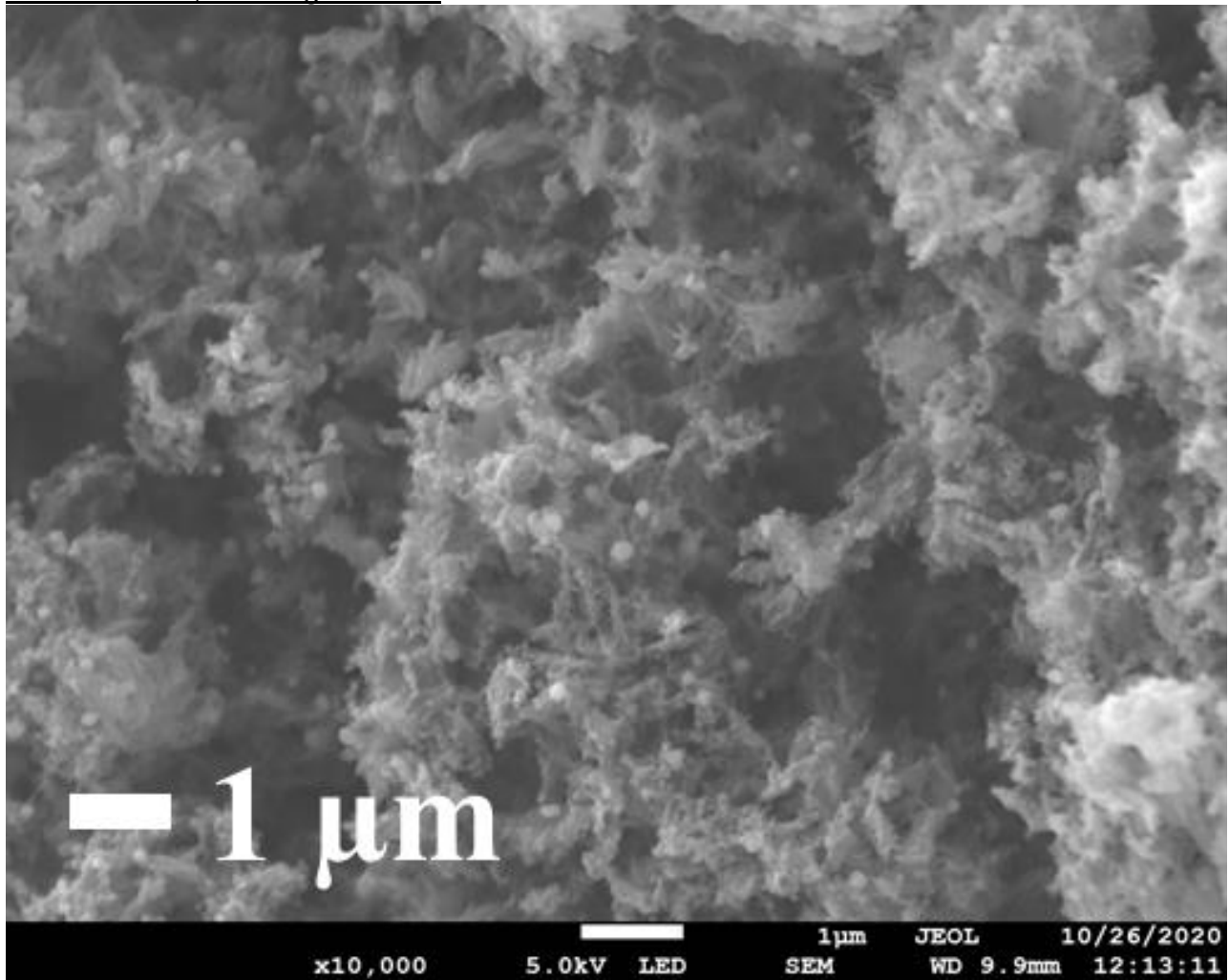


## SEM Images for A500O60

A500O60 x100 magnification and particle size distribution plot



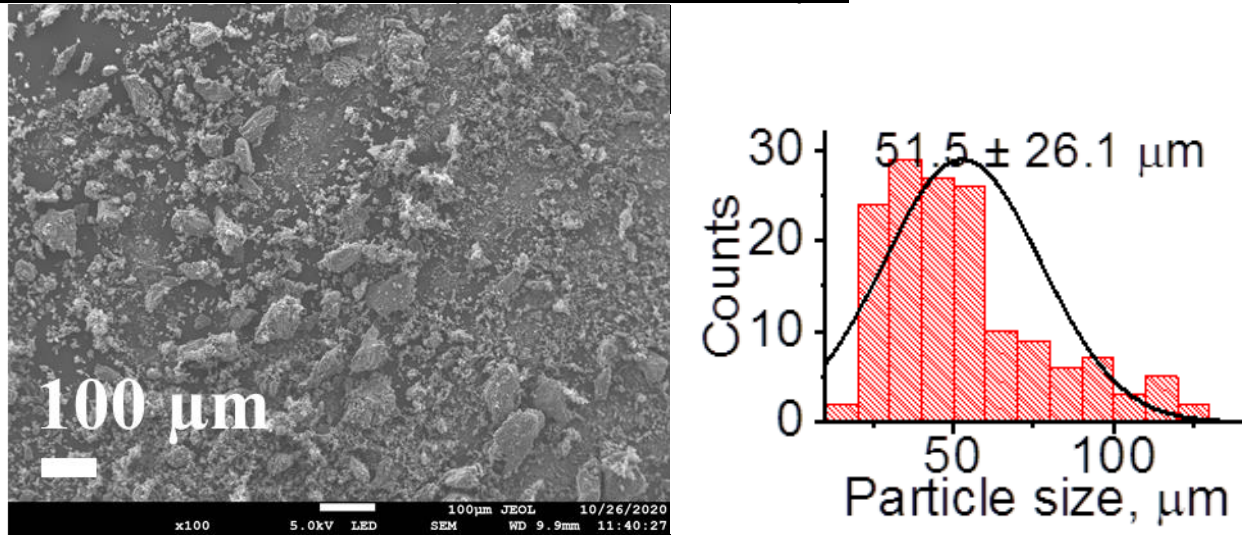
A500O60 x10,000 magnification



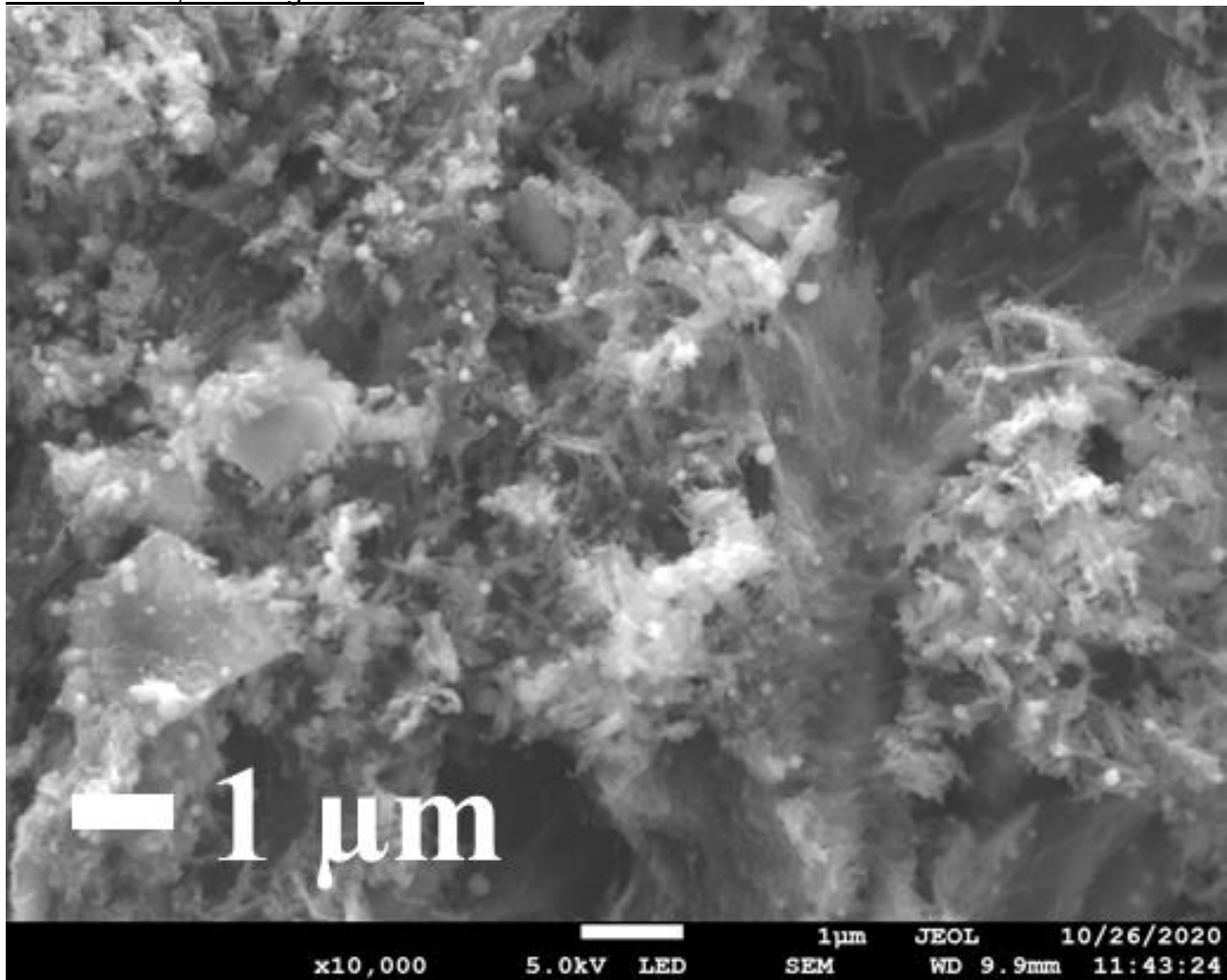


## SEM Images for A750O0

A750O0 x100 magnification and particle size distribution plot

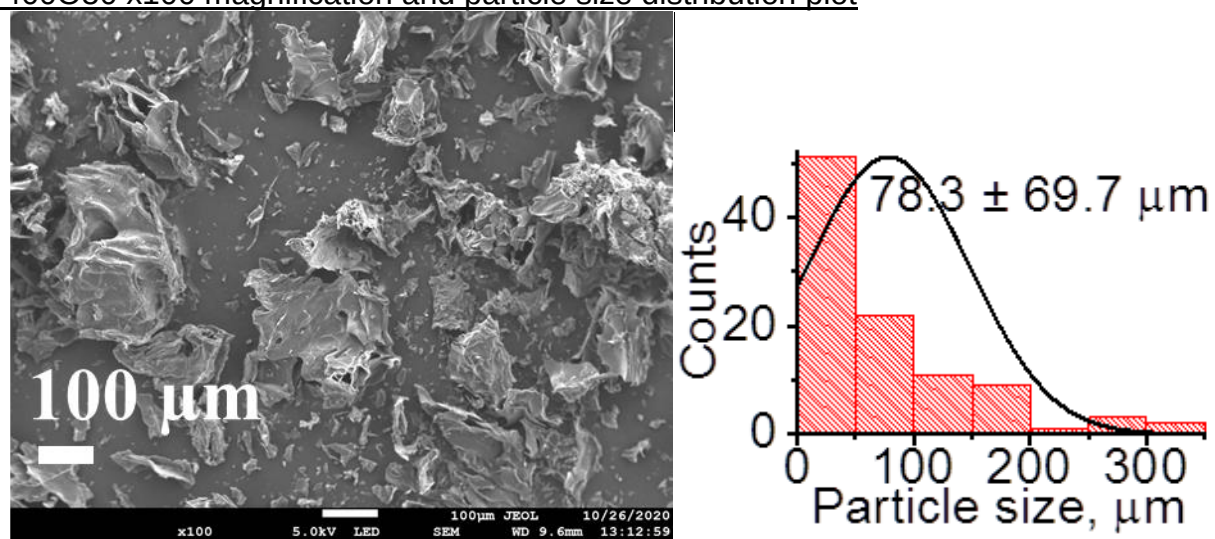


A750O0 x10,000 magnification

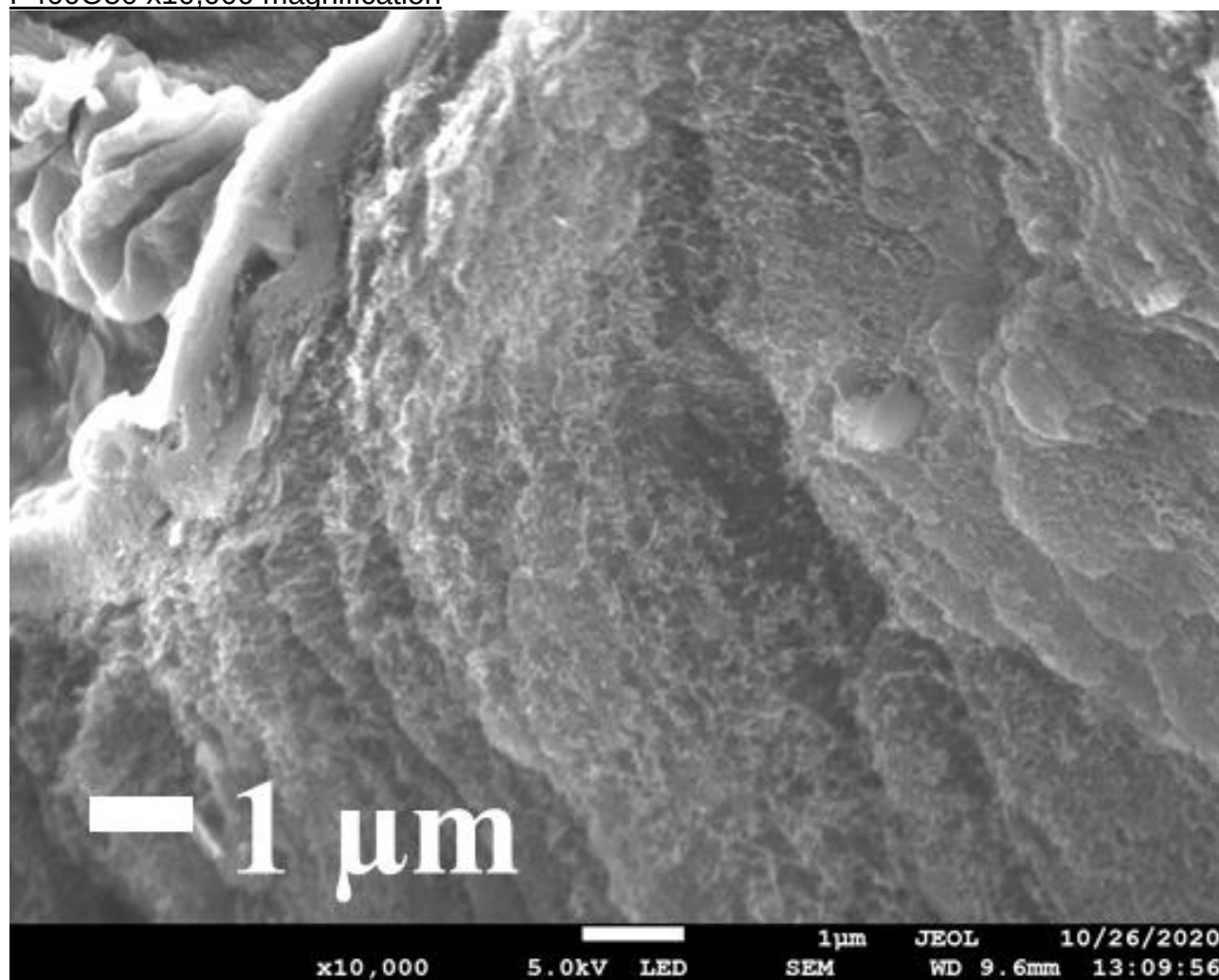


## SEM Images for P400O50

P400O50 x100 magnification and particle size distribution plot

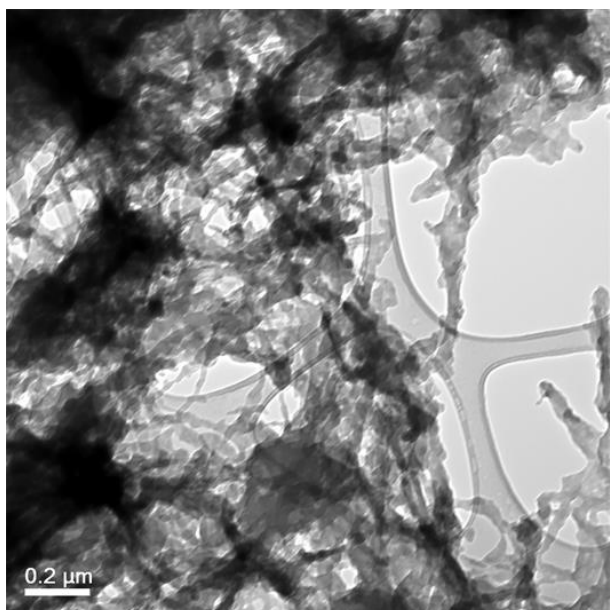


P400O50 x10,000 magnification

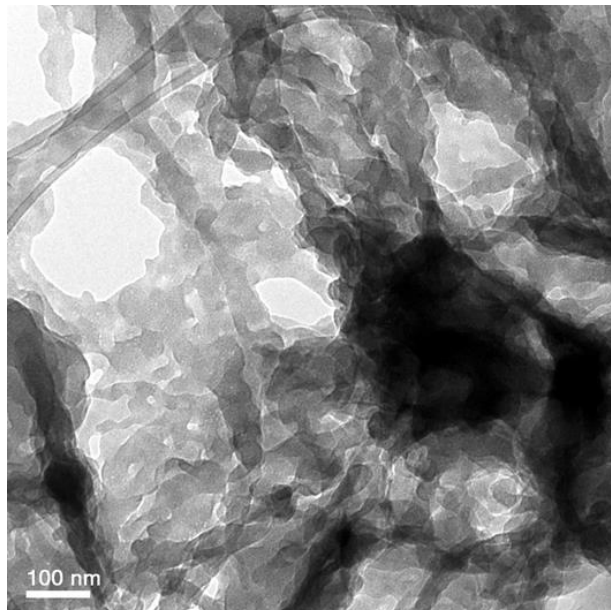


## TEM Images

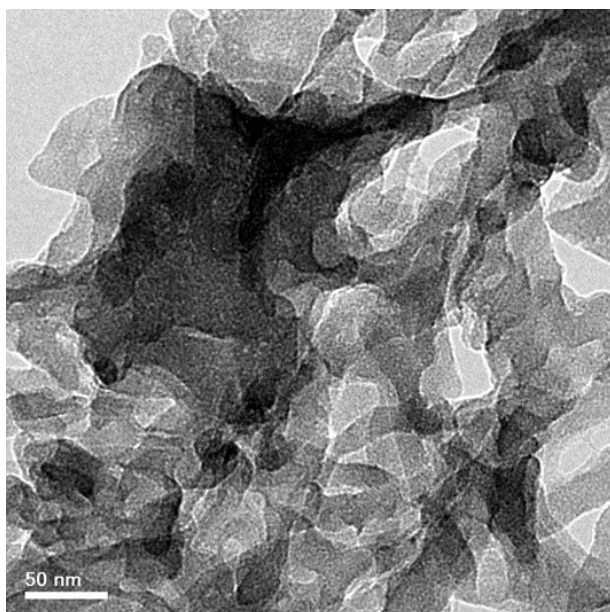
S800



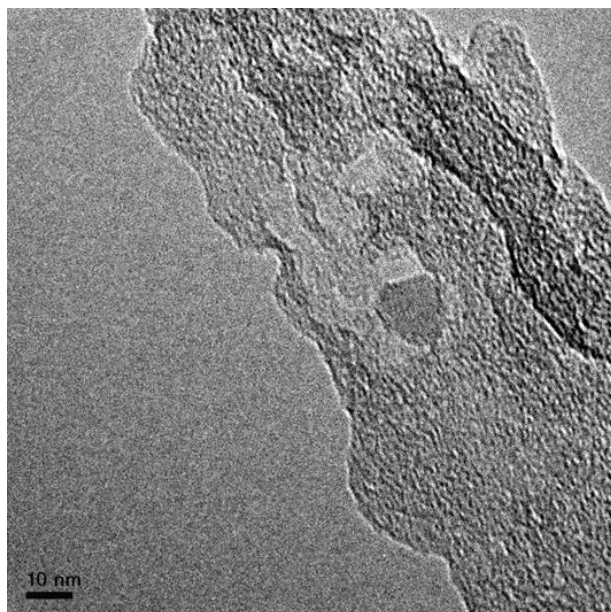
The grey curved lines visible to the right and centre of this image are the carbon film on copper grid that the sample is supported on.



The grey curved lines visible to the top left of this image are the carbon film on copper grid that the sample is supported on.



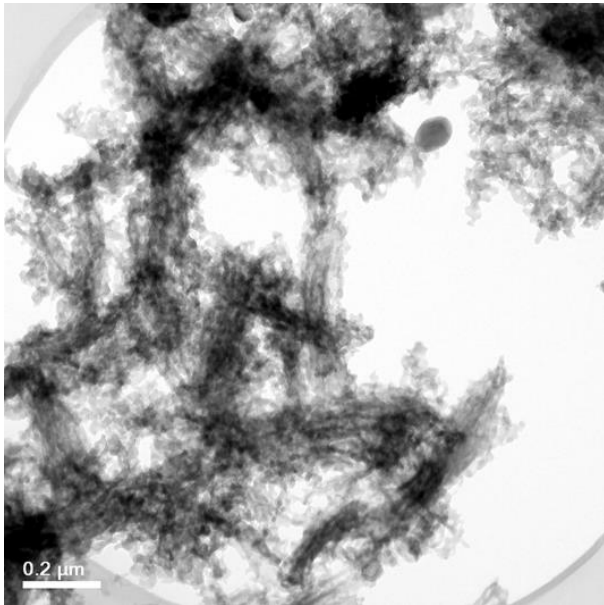
Mesopores are visible as pale grey areas and micropores as white dots in this image.



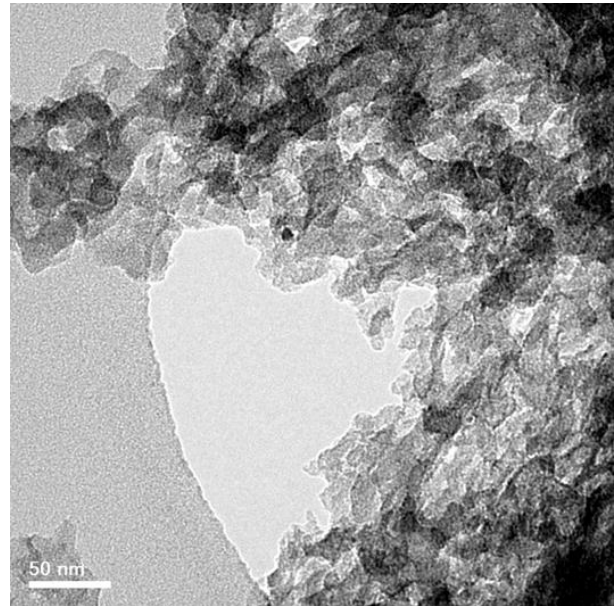
The smooth grey areas to the left and top right of this image are areas where there is no sample. Mesopores are visible as pale grey areas and micropores are visible as white dots in the sample.



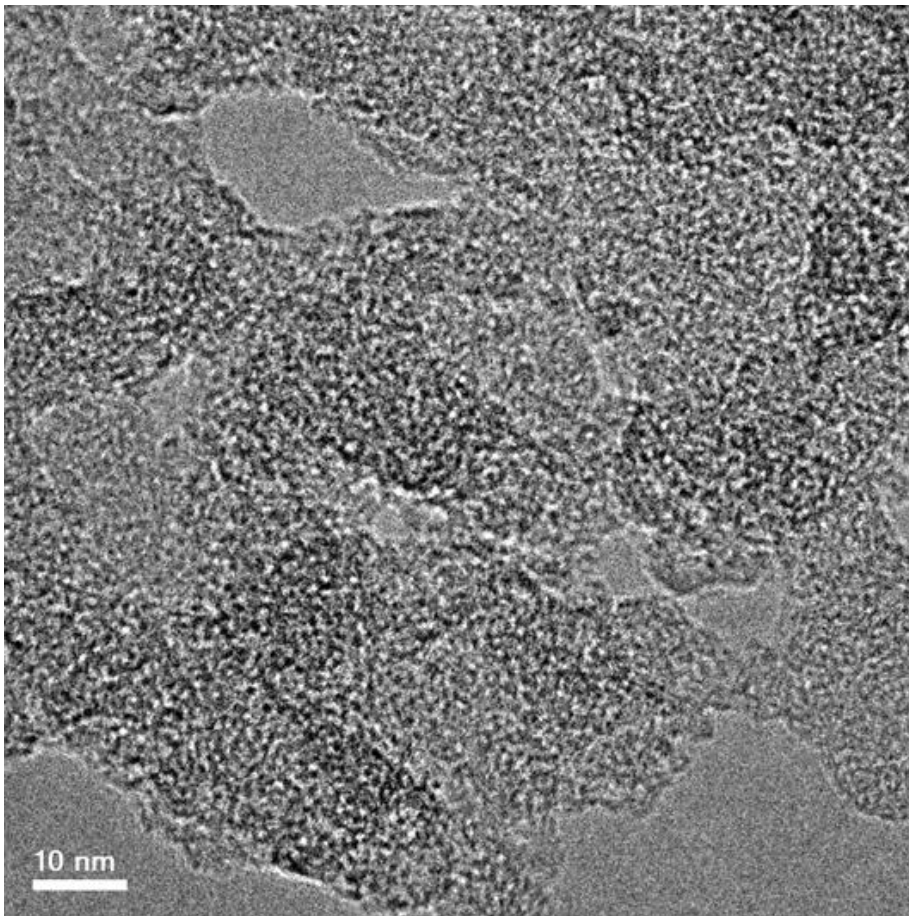
A800



The smooth grey areas in the corners of this image are the carbon film that the sample is supported on.

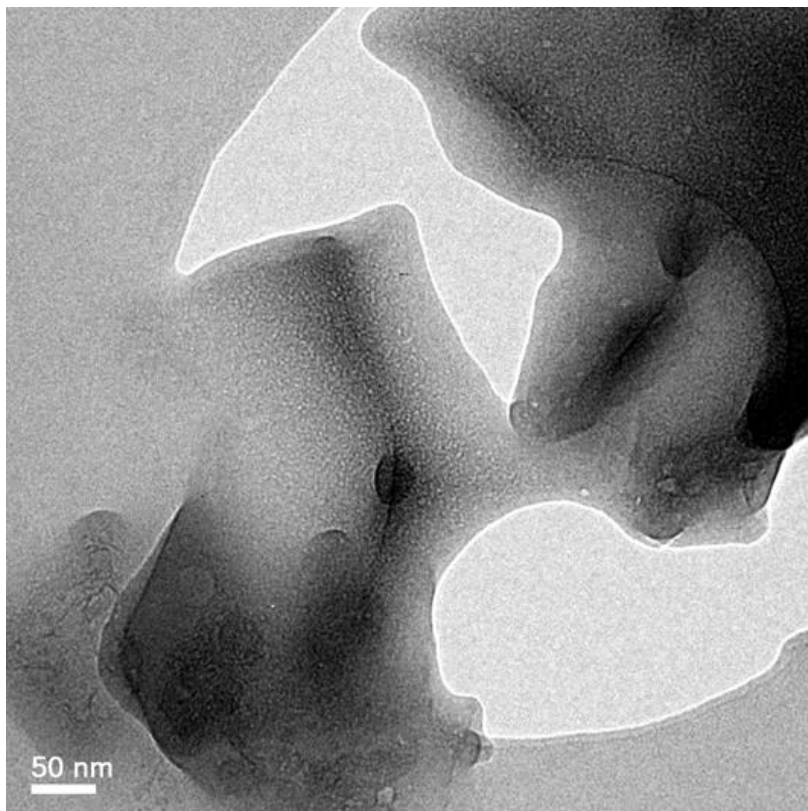


The smooth grey area to the left of this image is the carbon film that the sample is supported on. Mesopores are visible as pale areas within the sample.

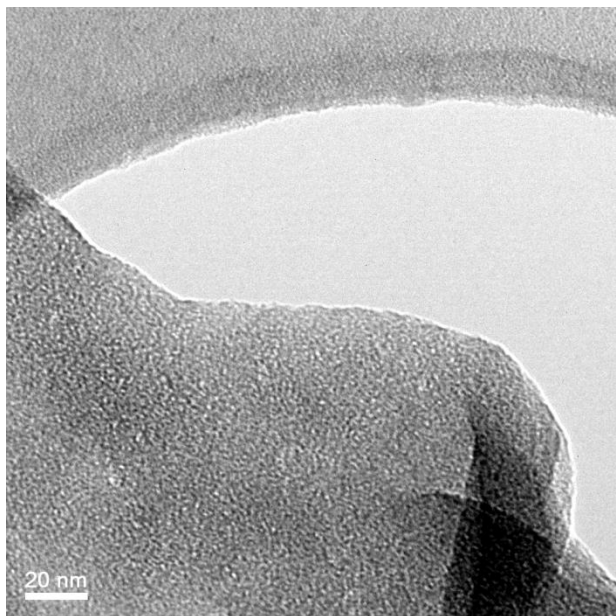


The smooth grey areas in this image are areas where there is no sample. Those at the bottom are beyond the edge of the particle, those surrounded by sample are mesopores. Micropores are visible as white dots in the sample.

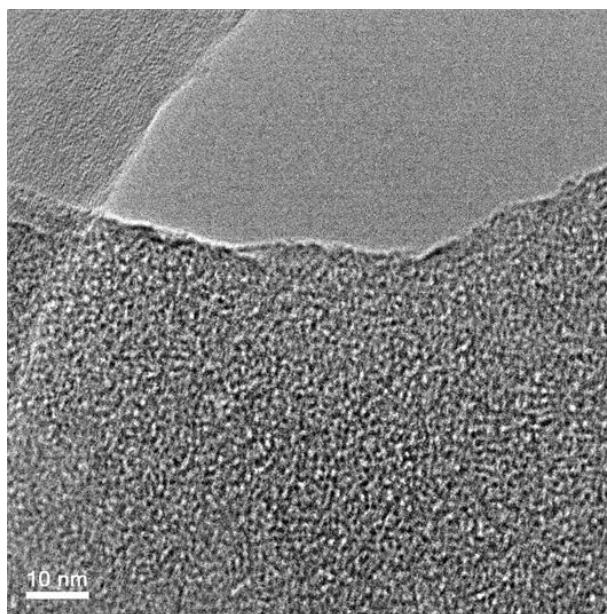
S800K2



The palest areas in this image are two macropores and mesopores are also visible within the sample.

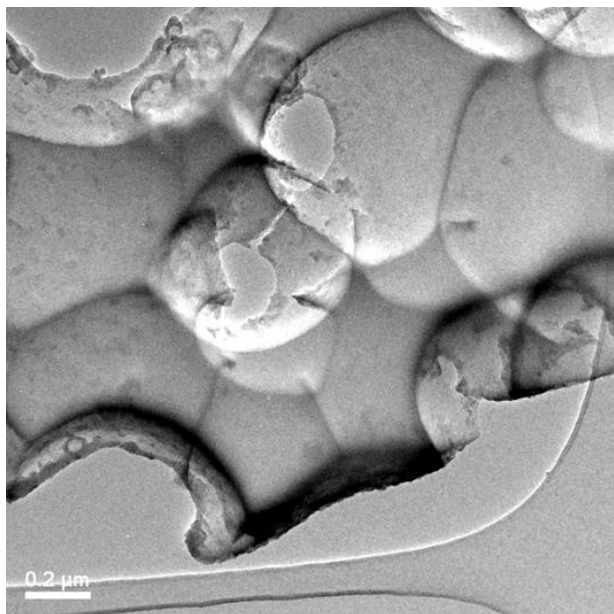


The slightly rough grey area at the top of this image is the carbon film supported on a copper grid. The smoother grey area below it is an area where there is no sample. Micropores are visible as white dots in the sample.

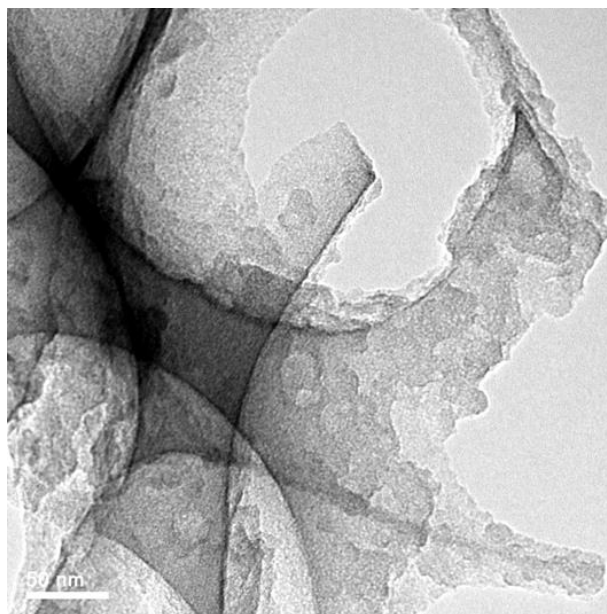


The slightly rough grey area at the top left of this image is the carbon film supported on a copper grid. The smoother grey area in the top right is an area where there is no sample. Micropores are visible as white dots in the sample.

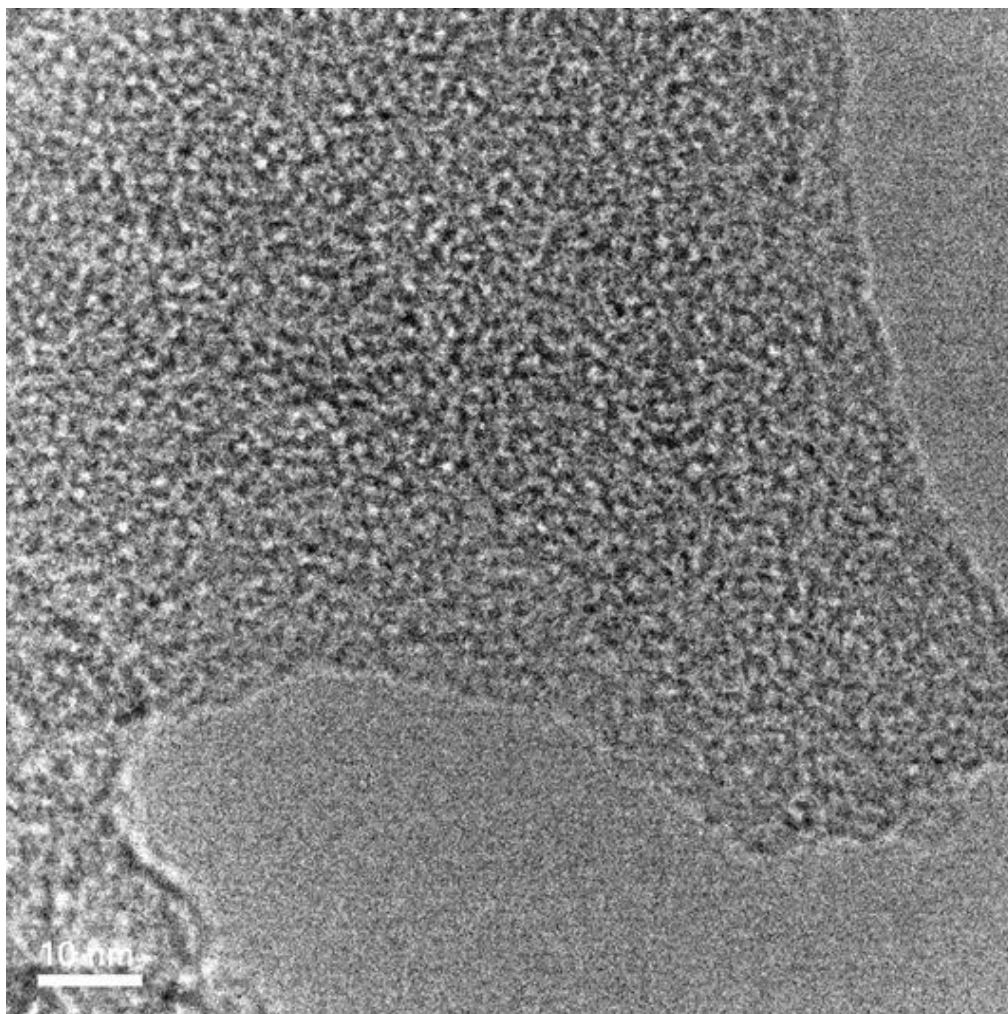
A800K2



The smooth grey curve at the bottom and lower right of this image is the carbon film that the sample is supported on.



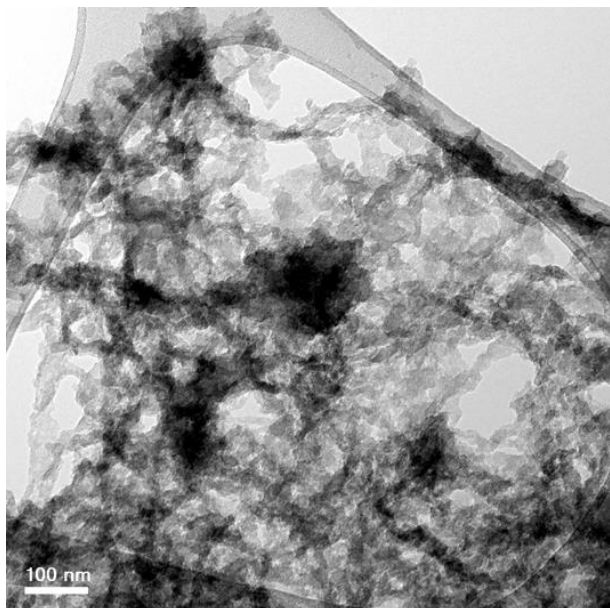
This image shows mesopores within the sample.



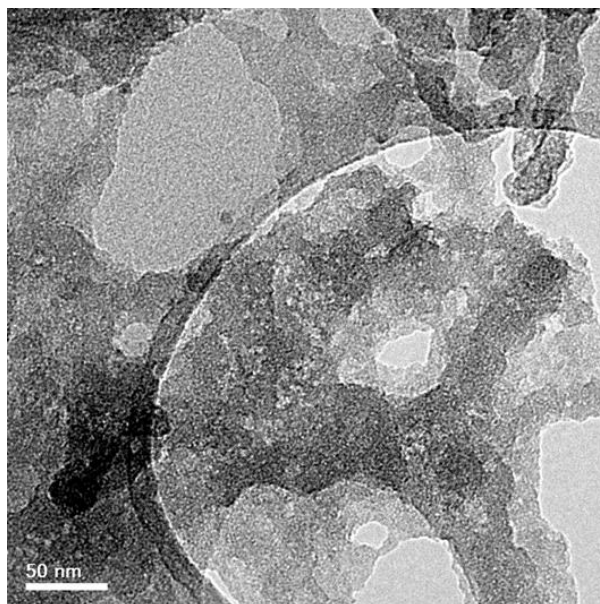
The smooth grey area at the bottom of this image is an area with no sample. Micropores are visible as white dots in the sample.



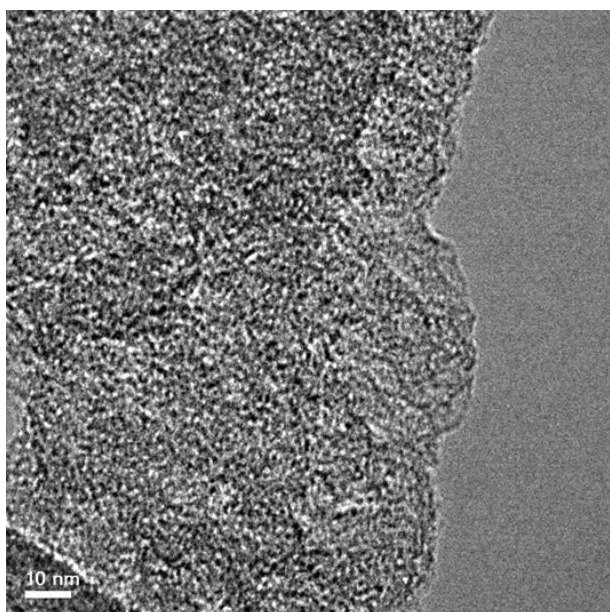
## S950C90



The grey curve at the top of this image is the carbon film that the sample is supported on.



The left and top of this image is sample sitting on top of the carbon film. The right side is sample not on the film. Various sizes of mesopores are visible.



The smooth grey area at the right of this image is an area with no sample. Micropores are visible as white dots in the sample.

# ICP-OES data for unactivated and KOH activated starch derived Starbons®

| Element        | S800 (ppm)  | S800K1 (ppm) | S800K2 (ppm) | S800K3 (ppm) | S800K4 (ppm) | S800K5 (ppm) | S600K4 (ppm) | S1000K4 (ppm) |
|----------------|-------------|--------------|--------------|--------------|--------------|--------------|--------------|---------------|
| Ag             | 0.92        | <LOQ         | <LOQ         | 0.04         | 0.29         | <LOQ         | 0.55         | 1.95          |
| Al             | 46.11       | 7.03         | 13.30        | 5.20         | 77.60        | 33.68        | 73.63        | 128.95        |
| As             | 53.96       | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | 14.10        | 3.36          |
| Au             | 0.99        | 4.33         | <LOQ         | 5.33         | 0.26         | <LOQ         | 1.50         | 1.42          |
| B              | 3.96        | 23.23        | 15.98        | 17.24        | 16.49        | 26.71        | 18.26        | 50.29         |
| Ba             | 5.71        | 3.82         | 4.26         | 3.39         | 13.60        | 4.48         | 9.21         | 19.61         |
| Be             | <LOQ        | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ          |
| Bi             | 22.85       | 18.53        | 7.94         | 8.92         | < 1.15       | 9.41         | 8.48         | 1.00          |
| Ca             | 1986.22     | 937.41       | 976.67       | 1110.57      | 2190.61      | 1128.38      | 2727.20      | 4656.83       |
| Cd             | 0.13        | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ          |
| Co             | 1.82        | <LOQ         | <LOQ         | <LOQ         | <LOQ         | 0.55         | <LOQ         | <LOQ          |
| Cr             | 1.63        | 2.39         | 7.30         | 5.11         | 7.13         | 129.92       | 11.20        | 36.89         |
| Cu             | 16.56       | 10.72        | 13.39        | 8.85         | 21.72        | 28.47        | 51.05        | 74.94         |
| Fe             | 133.75      | 95.82        | 274.51       | 65.91        | 191.20       | 1351.97      | 249.35       | 336.82        |
| Hg             | 12.10       | 1.60         | 1.83         | 1.28         | 0.49         | <LOQ         | 6.68         | 1.12          |
| K              | 66.01       | 218.91       | 202.17       | 231.48       | 366.96       | 427.90       | 116.75       | 305.46        |
| La             | 3.27        | 0.44         | <LOQ         | 0.39         | 1.24         | 0.33         | 5.55         | 5.89          |
| Li             | <LOQ        | 0.05         | 0.19         | 0.10         | 0.46         | 0.33         | <LOQ         | <LOQ          |
| Mg             | 174.32      | 90.32        | 91.30        | 112.36       | 181.20       | 107.37       | 215.25       | 324.13        |
| Mn             | 2.87        | 2.77         | 2.69         | 1.76         | 28.38        | 54.85        | 4.02         | 11.98         |
| Mo             | 3.85        | 1.05         | 2.71         | 0.83         | <LOQ         | 24.71        | 2.68         | 3.10          |
| Na             | 695.18      | 195.28       | 191.93       | 255.39       | 327.93       | 257.90       | 424.03       | 692.25        |
| Ni             | 9.06        | <LOQ         | 2.22         | 2.14         | 6.52         | 19.97        | 4.79         | 15.35         |
| P              | 330.37      | 13.28        | 29.29        | <LOQ         | 0.28         | 31.73        | 79.87        | 25.07         |
| Pb             | 13.89       | <LOQ         | <LOQ         | 0.07         | <LOQ         | <LOQ         | <LOQ         | <LOQ          |
| Pd             | 0.66        | 3.14         | 3.68         | 2.67         | 0.19         | 1.18         | 3.69         | <LOQ          |
| Pt             | <LOQ        | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ          |
| Rb             | <LOQ        | 26.98        | 24.97        | 24.66        | <LOQ         | 29.32        | <LOQ         | <LOQ          |
| S              | 2968.00     | 405.00       | 844.00       | 1109.00      | 1400.00      | 958.00       | 3785.00      | 8674.00       |
| Sb             | 7.56        | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | 6.76         | 9.79          |
| Sc             | 0.25        | 0.26         | 0.36         | 0.13         | 0.27         | 0.39         | 0.36         | 0.61          |
| Se             | 48.73       | <LOQ         | <LOQ         | 4.85         | <LOQ         | <LOQ         | <LOQ         | <LOQ          |
| Si             | 189.51      | 209.35       | 155.78       | 95.48        | 771.94       | 164.22       | 570.15       | 1403.61       |
| Sn             | 23.80       | <LOQ         | <LOQ         | <LOQ         | <LOQ         | 8.98         | <LOQ         | <LOQ          |
| Sr             | 34.81       | 15.35        | 15.82        | 19.80        | 29.96        | 18.55        | 46.20        | 69.21         |
| Te             | <LOQ        | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ         | <LOQ          |
| Ti             | 43.33       | 30.69        | 50.42        | 9.04         | 14.71        | 29.13        | 190.01       | 131.54        |
| Tl             | 26.26       | <LOQ         | <LOQ         | <LOQ         | <LOQ         | 5.74         | <LOQ         | <LOQ          |
| V              | 2.18        | 0.46         | 1.05         | 1.38         | 2.58         | 24.71        | 3.59         | 4.80          |
| W              | 14.25       | <LOQ         | <LOQ         | <LOQ         | <LOQ         | 2.28         | 13.33        | 0.55          |
| Zn             | 9.42        | 3.02         | 2.81         | 2.19         | 6.58         | 13.56        | 216.57       | 109.78        |
| Zr             | 7.40        | 2.07         | 1.08         | 3.34         | 3.95         | 3.06         | 13.92        | 28.43         |
| <b>Total %</b> | <b>0.70</b> | <b>0.23</b>  | <b>0.29</b>  | <b>0.31</b>  | <b>0.57</b>  | <b>0.49</b>  | <b>0.89</b>  | <b>1.71</b>   |

LOQ is the limit of quantification which is three times the limit of detection. These elements were assumed to have a concentration of 0 in calculating the total.

# ICP-OES data for CO<sub>2</sub> and O<sub>2</sub> activated starch derived Starbons®

| Element        | S950C90 (ppm) | S75000 (ppm) |
|----------------|---------------|--------------|
| Ag             | <LOQ          | 69632.89     |
| Al             | 972.84        | 284.52       |
| As             | 1.15          | <LOQ         |
| Au             | 1.11          | 0.58         |
| B              | 81.43         | 197.51       |
| Ba             | 15.17         | 4.29         |
| Be             | <LOQ          | <LOQ         |
| Bi             | 5.86          | 22.95        |
| Ca             | 2076.32       | 849.48       |
| Cd             | 1.97          | 9.42         |
| Co             | 1.09          | 1.33         |
| Cr             | 27.78         | 1.08         |
| Cu             | 29.64         | 7.36         |
| Fe             | 7654.31       | 752.16       |
| Hg             | <LOQ          | 0.56         |
| K              | 1217.87       | 534.68       |
| La             | 0.73          | 0.18         |
| Li             | <LOQ          | <LOQ         |
| Mg             | 407.60        | 308.21       |
| Mn             | 17.71         | 5.49         |
| Mo             | 41.90         | <LOQ         |
| Na             | 1738.85       | 1567.46      |
| Ni             | 33.29         | 16.53        |
| P              | 9292.77       | <LOQ         |
| Pb             | 40.35         | 117.86       |
| Pd             | 1.88          | <LOQ         |
| Pt             | 0.19          | 3.04         |
| Rb             | 1.83          | <LOQ         |
| S              | 17338.36      | 17338.36     |
| Sb             | 0.27          | 0.76         |
| Sc             | <LOQ          | <LOQ         |
| Se             | <LOQ          | <LOQ         |
| Si             | <LOQ          | <LOQ         |
| Sn             | <LOQ          | <LOQ         |
| Sr             | 6.06          | 2.45         |
| Te             | <LOQ          | <LOQ         |
| Ti             | 34.33         | <LOQ         |
| Tl             | <LOQ          | <LOQ         |
| V              | 1.06          | 0.91         |
| W              | 1.56          | 1.14         |
| Zn             | 115.52        | 97.89        |
| Zr             | <LOQ          | 83.84        |
| <b>Total %</b> | <b>4.12</b>   | <b>9.18</b>  |

LOQ is the limit of quantification which is three times the limit of detection. These elements were assumed to have a concentration of 0 in calculating the total.

**ICP-OES data for alginic acid and pectin derived Starbons<sup>®</sup>**

| Element        | A800 (ppm)  | A800K2 (ppm) | A750C60 (ppm) | A750O0 (ppm) | P800 (ppm)  | P800K2 (ppm) | P700C50 (ppm) | P400O50 (ppm) |
|----------------|-------------|--------------|---------------|--------------|-------------|--------------|---------------|---------------|
| Ag             | 0.29        | 0.06         | <LOQ          | <LOQ         | <LOQ        | 8.14         | <LOQ          | <LOQ          |
| Al             | 775.51      | 14.11        | 530.75        | 441.71       | 183.76      | 1315.95      | 809.18        | 128.98        |
| As             | 4.41        | 0.59         | 0.87          | 0.68         | <LOQ        | 1.32         | 1.10          | <LOQ          |
| Au             | 15.71       | 7.44         | 0.03          | 0.41         | 3.02        | 3.05         | 21.64         | 3.84          |
| B              | <LOQ        | 15.54        | 22.10         | 23.15        | 6.31        | 14.95        | 85.95         | 100.90        |
| Ba             | 513.28      | 2.17         | 386.17        | 309.68       | 10.68       | 14.65        | 18.45         | 6.48          |
| Be             | <LOQ        | <LOQ         | <LOQ          | <LOQ         | <LOQ        | <LOQ         | <LOQ          | <LOQ          |
| Bi             | 16.51       | 18.68        | 0.98          | 0.61         | 13.32       | 115.96       | <LOQ          | 1.09          |
| Ca             | 53668.26    | 336.60       | 33755.13      | 27424.69     | 2838.49     | 254.88       | 5526.43       | 2037.26       |
| Cd             | 0.43        | 0.51         | <LOQ          | 0.04         | <LOQ        | 0.74         | 4.55          | <LOQ          |
| Co             | 0.62        | 0.53         | 0.27          | 0.27         | 0.27        | 2.65         | 1.86          | 0.19          |
| Cr             | 15.18       | 14.80        | 9.92          | 8.38         | 24.60       | 40.76        | 63.98         | 18.81         |
| Cu             | 10.55       | 15.54        | 3.19          | 3.84         | 22.98       | 8.36         | 54.19         | 18.00         |
| Fe             | 1108.85     | 1201.33      | 749.32        | 613.34       | 450.60      | 245.53       | 561.60        | 130.62        |
| Hg             | <LOQ        | <LOQ         | <LOQ          | <LOQ         | <LOQ        | <LOQ         | <LOQ          | <LOQ          |
| K              | 861.13      | 392.60       | 1895.14       | 815.18       | 431.08      | 380.12       | 15862.25      | 8087.16       |
| La             | 1.53        | <LOQ         | 1.03          | 0.68         | 0.09        | 0.31         | 1.23          | 0.18          |
| Li             | <LOQ        | <LOQ         | 7.66          | <LOQ         | <LOQ        | <LOQ         | <LOQ          | <LOQ          |
| Mg             | 1398.24     | 10.93        | 879.41        | 722.32       | 796.12      | 35.63        | 1558.88       | 602.36        |
| Mn             | 19.25       | 4.35         | 12.93         | 10.32        | 14.60       | 1.37         | 25.94         | 9.66          |
| Mo             | 3.03        | 135.92       | <LOQ          | 9.76         | <LOQ        | <LOQ         | <LOQ          | <LOQ          |
| Na             | 5669.44     | 173.56       | 3662.93       | 3244.67      | 50109.90    | 239.63       | 92553.72      | 38083.53      |
| Ni             | 37.82       | 407.38       | 3.56          | 5.77         | 15.39       | 12.41        | 37.91         | 10.21         |
| P              | 1858.65     | <LOQ         | 1521.39       | 1383.82      | 1030.84     | 106.47       | 2802.42       | <LOQ          |
| Pb             | 9.40        | 2.90         | <LOQ          | 0.67         | 2.80        | 4.47         | 34.61         | <LOQ          |
| Pd             | 0.86        | 0.67         | 0.09          | <LOQ         | 0.47        | 0.47         | <LOQ          | 2.04          |
| Pt             | 0.00        | <LOQ         | 0.10          | 0.16         | <LOQ        | <LOQ         | 0.61          | 0.84          |
| Rb             | 0.93        | 3.34         | 1.16          | 0.39         | 5.31        | 0.80         | 10.63         | 6.24          |
| S              | 5892.63     | 5516.81      | <LOQ          | 5915.10      | 4483.56     | 6779.44      | <LOQ          | <LOQ          |
| Sb             | 0.46        | 1.41         | <LOQ          | 0.06         | 0.80        | 2.40         | 0.78          | <LOQ          |
| Sc             | 15.23       | 14.56        | <LOQ          | <LOQ         | 11.66       | 16.49        | <LOQ          | <LOQ          |
| Se             | <LOQ        | <LOQ         | <LOQ          | <LOQ         | <LOQ        | 5.55         | <LOQ          | <LOQ          |
| Si             | 8119.84     | 8796.03      | <LOQ          | <LOQ         | 6741.60     | 7950.26      | <LOQ          | <LOQ          |
| Sn             | 2.48        | 1.95         | <LOQ          | <LOQ         | 1.72        | 11.35        | <LOQ          | <LOQ          |
| Sr             | 898.51      | 1.87         | 875.60        | 721.56       | 14.60       | 0.69         | 33.43         | 15.87         |
| Te             | <LOQ        | <LOQ         | <LOQ          | <LOQ         | <LOQ        | <LOQ         | <LOQ          | <LOQ          |
| Ti             | 25.65       | 26.70        | 31.06         | 24.40        | 5.62        | 25.70        | <LOQ          | <LOQ          |
| Tl             | 7.15        | 2.27         | <LOQ          | <LOQ         | 1.12        | 1.01         | <LOQ          | <LOQ          |
| V              | 1.72        | 1.33         | 0.96          | 0.90         | <LOQ        | <LOQ         | 1.47          | 0.04          |
| W              | 1.35        | 1.46         | 0.76          | 0.53         | 0.26        | 4.53         | 0.17          | <LOQ          |
| Zn             | 30.15       | 21.36        | <LOQ          | 25.94        | 5.13        | 18.02        | 117.50        | <LOQ          |
| Zr             | 1.48        | 10.80        | <LOQ          | <LOQ         | 1.12        | 9.09         | <LOQ          | <LOQ          |
| <b>Total %</b> | <b>8.10</b> | <b>1.72</b>  | <b>4.44</b>   | <b>4.17</b>  | <b>6.72</b> | <b>1.76</b>  | <b>12.02</b>  | <b>4.93</b>   |

LOQ is the limit of quantification which is three times the limit of detection. These elements were assumed to have a concentration of 0 in calculating the total.

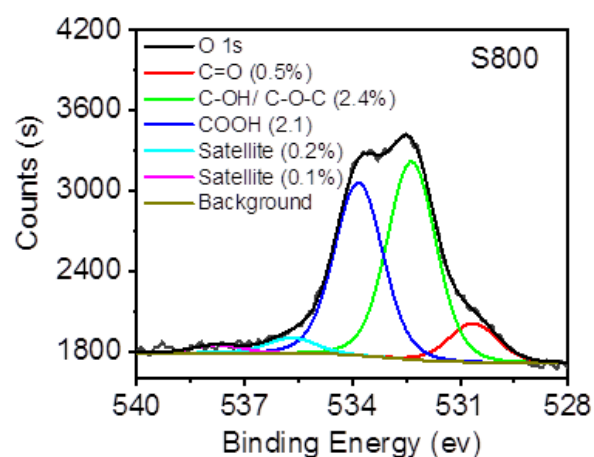
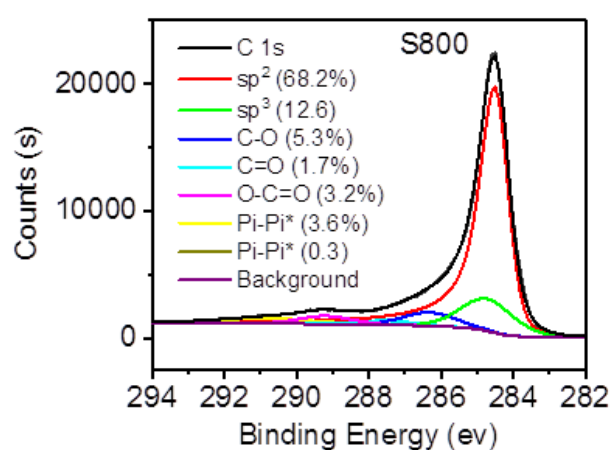
### Surface compositions determined by XPS

| Sample  | C%          | O%   | Ca% | K%  | N%  | Na% | Si% | S%  |
|---------|-------------|------|-----|-----|-----|-----|-----|-----|
| S800    | 94.8 (91.6) | 5.2  |     |     |     |     |     |     |
| A800    | 87.4 (80.9) | 9.3  | 2.0 |     | 0.4 | 0.6 |     | 0.4 |
| P800    | 76.2 (72.1) | 14.4 | 0.2 | 0.6 | 0.7 | 7.7 |     | 0.2 |
| S800K2  | 86.3 (83.8) | 13.5 |     |     |     | 0.2 |     |     |
| A800K2  | 84.8 (70)   | 14.4 |     |     | 0.4 | 0.2 |     | 0.1 |
| P800K2  | 91.0 (68.6) | 8.8  |     |     |     | 0.2 |     |     |
| S950C90 | 98.5 (88.7) | 1.3  |     |     |     |     |     | 0.1 |
| A750C60 | 90.9 (74.7) | 6.8  | 1.5 |     | 0.2 | 0.4 |     | 0.2 |
| P700C50 | 77.2 (62.7) | 13.8 | 0.1 | 0.4 | 0.9 | 7.5 |     | 0.1 |
| S750O0  | 98.2 (84.6) | 1.5  |     |     |     | 0.1 | 0.2 | 0.1 |
| A750O0  | 90.4 (78.3) | 7.1  | 1.4 |     | 0.4 | 0.4 |     | 0.2 |
| P400O50 | 72.1 (66.8) | 17.2 | 0.2 | 0.4 | 1.0 | 9.2 |     |     |

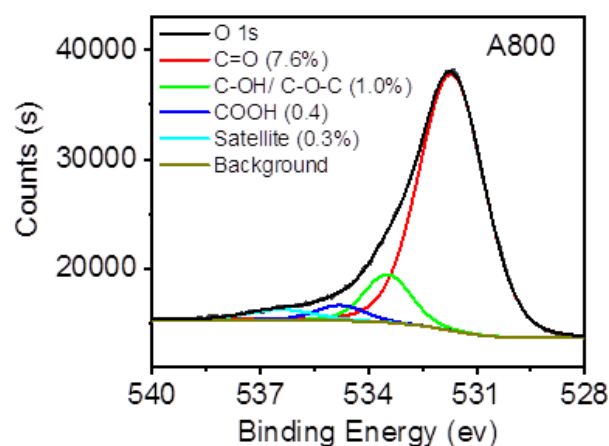
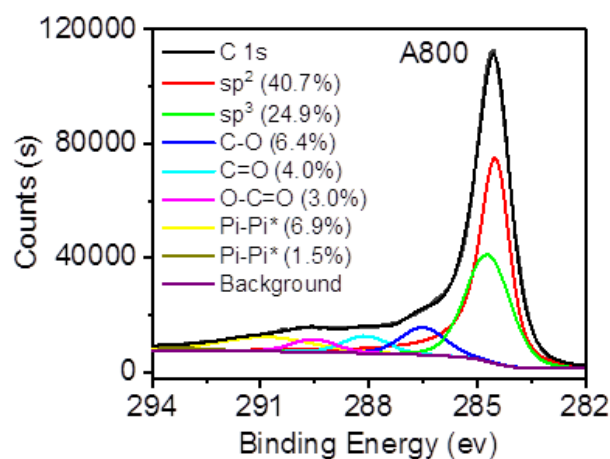
The figure in brackets is the % carbon in the bulk material determined by combustion analysis.

## XPS plots

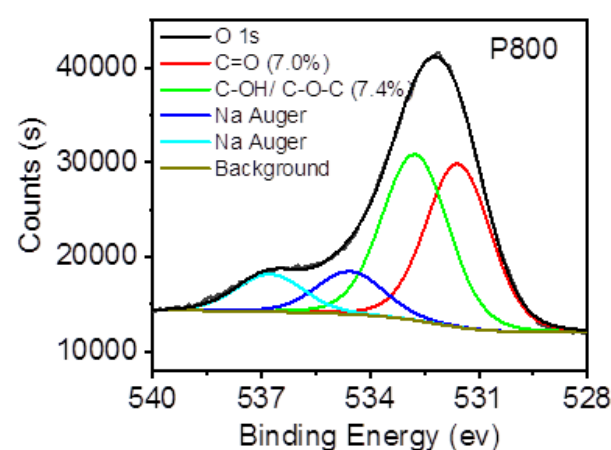
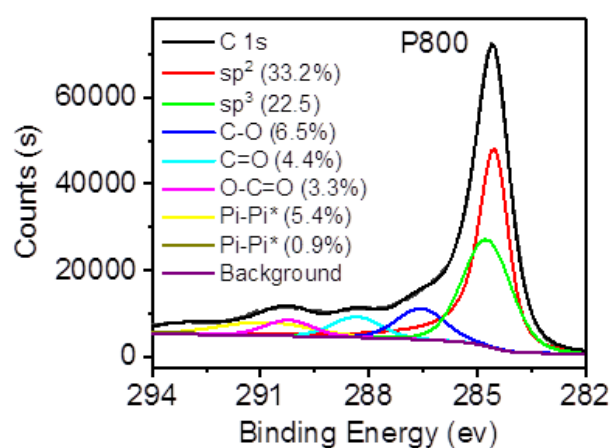
### S800



### A800

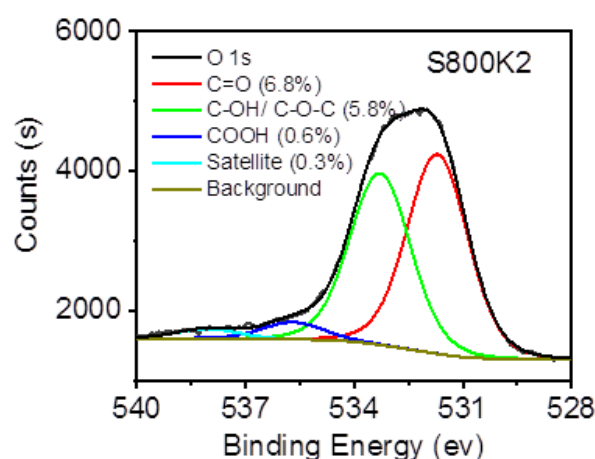
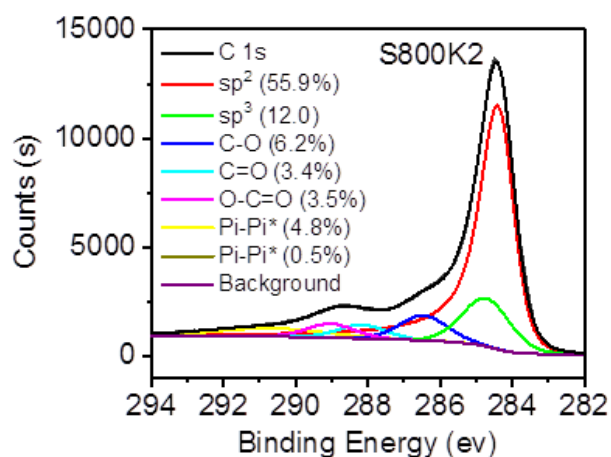


### P800

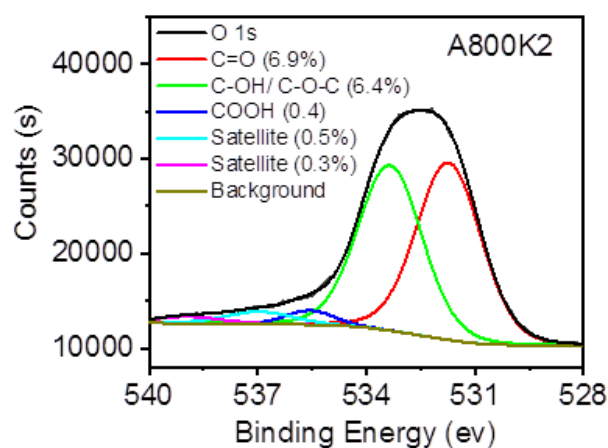
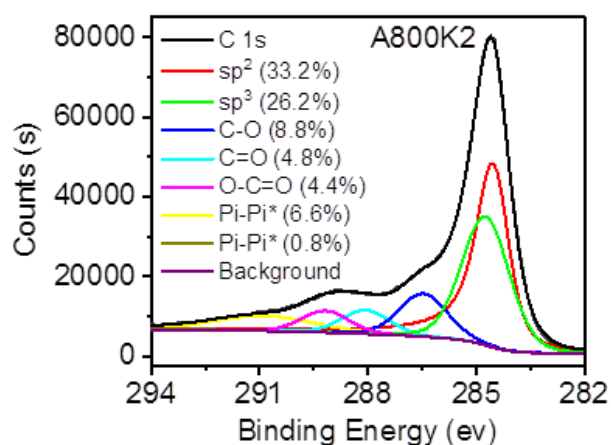




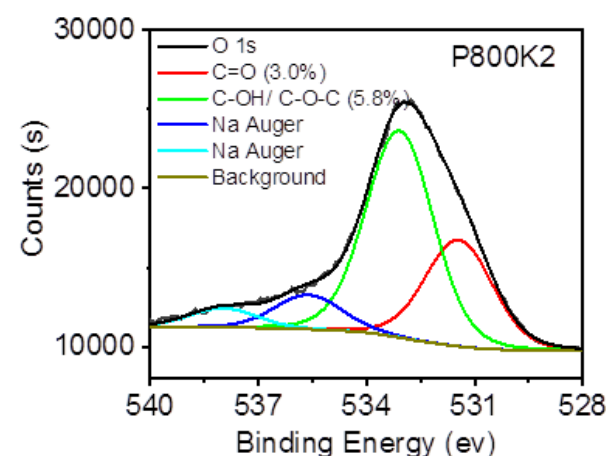
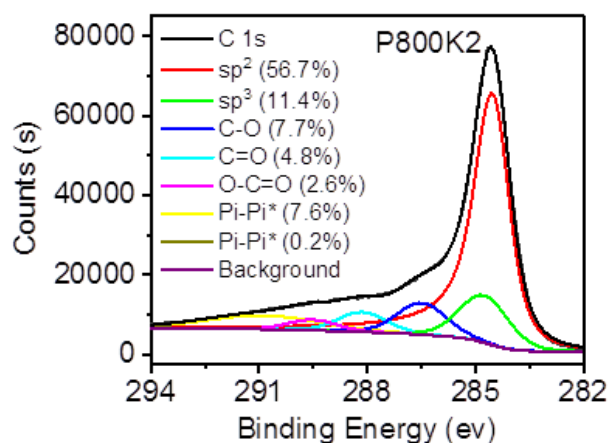
### S800K2



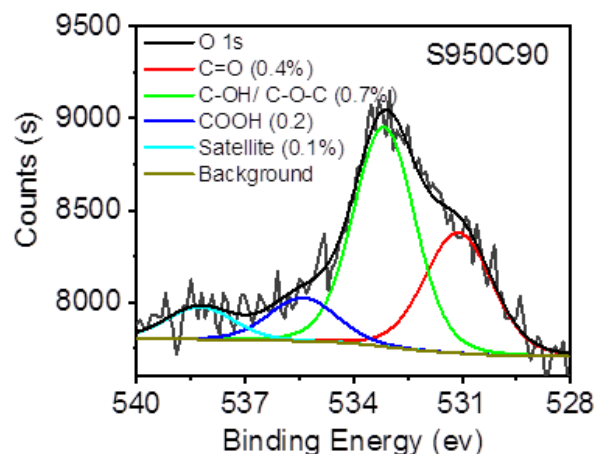
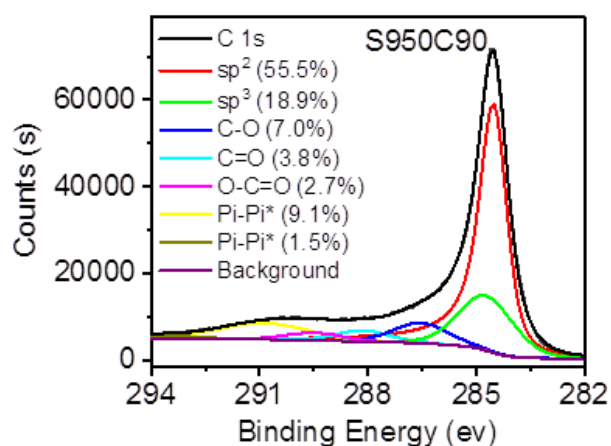
### A800K2



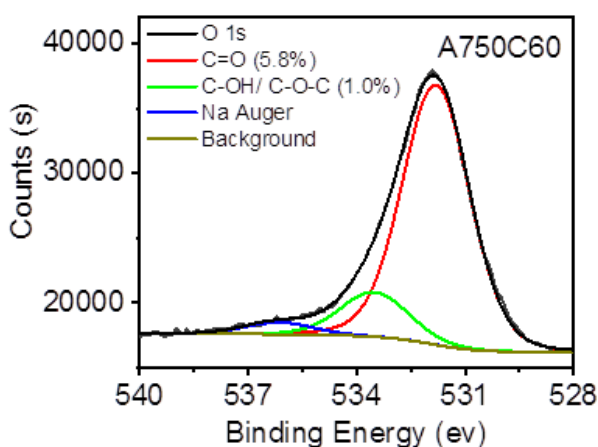
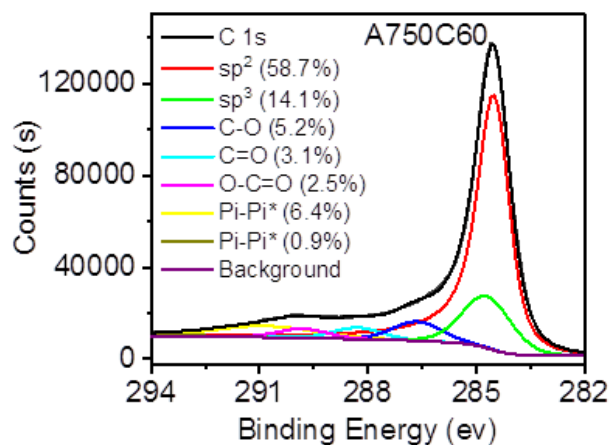
### P800K2



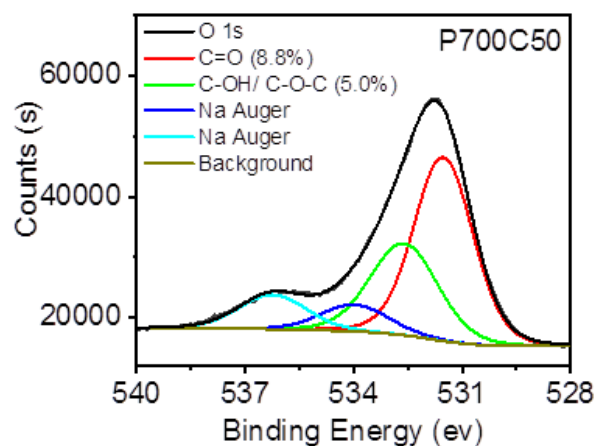
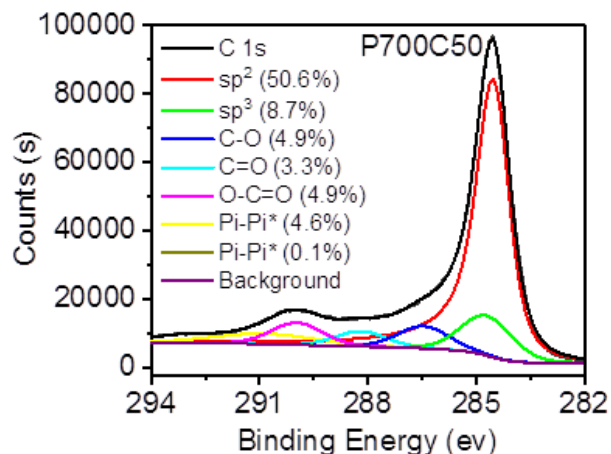
### S950C90



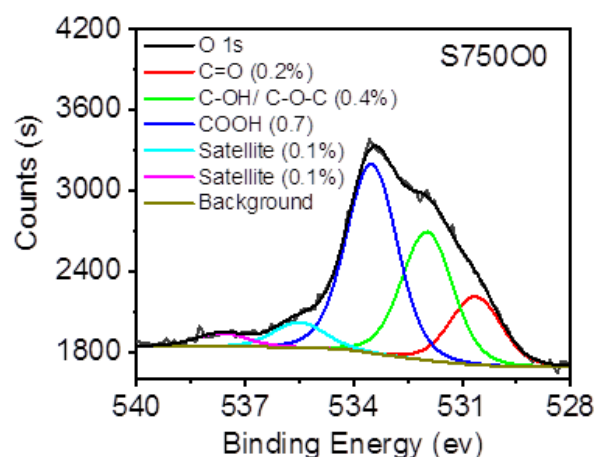
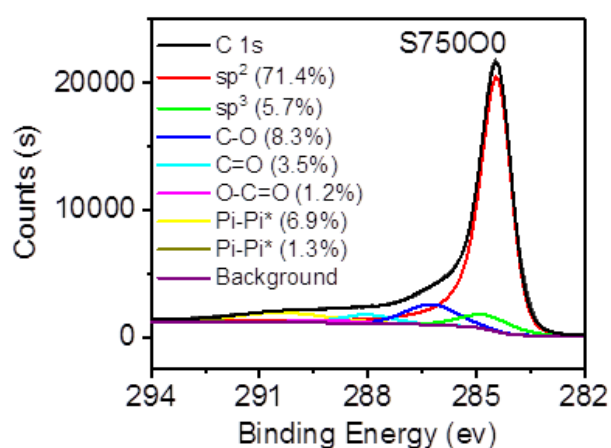
### A750C60



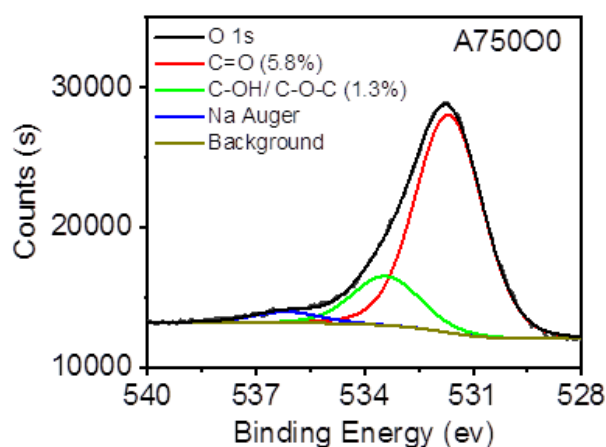
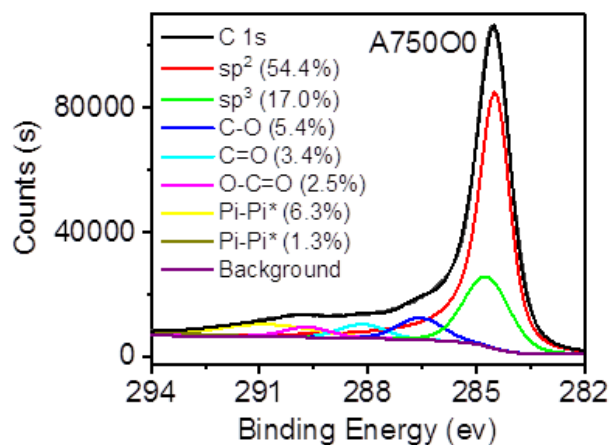
### P700C50



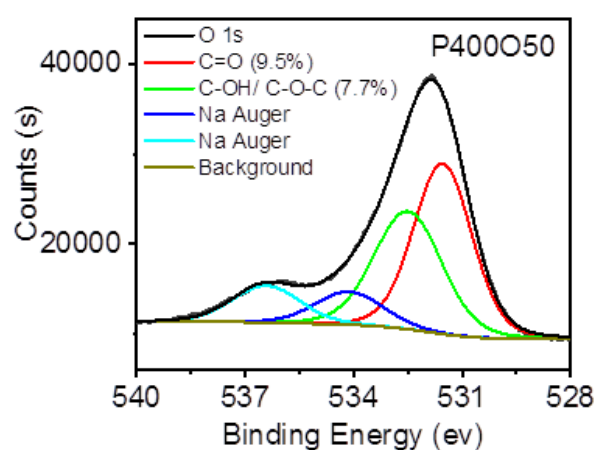
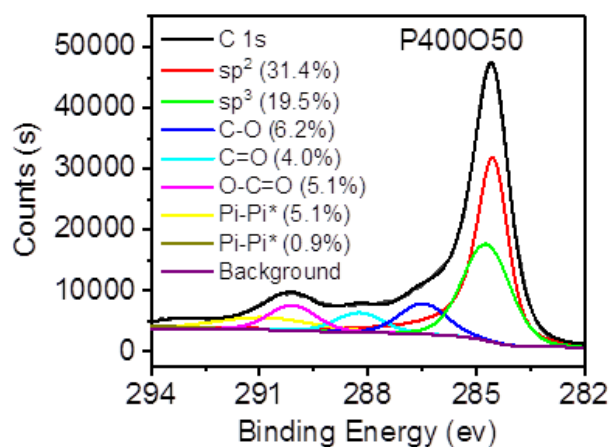
### S750O0



### A750O0

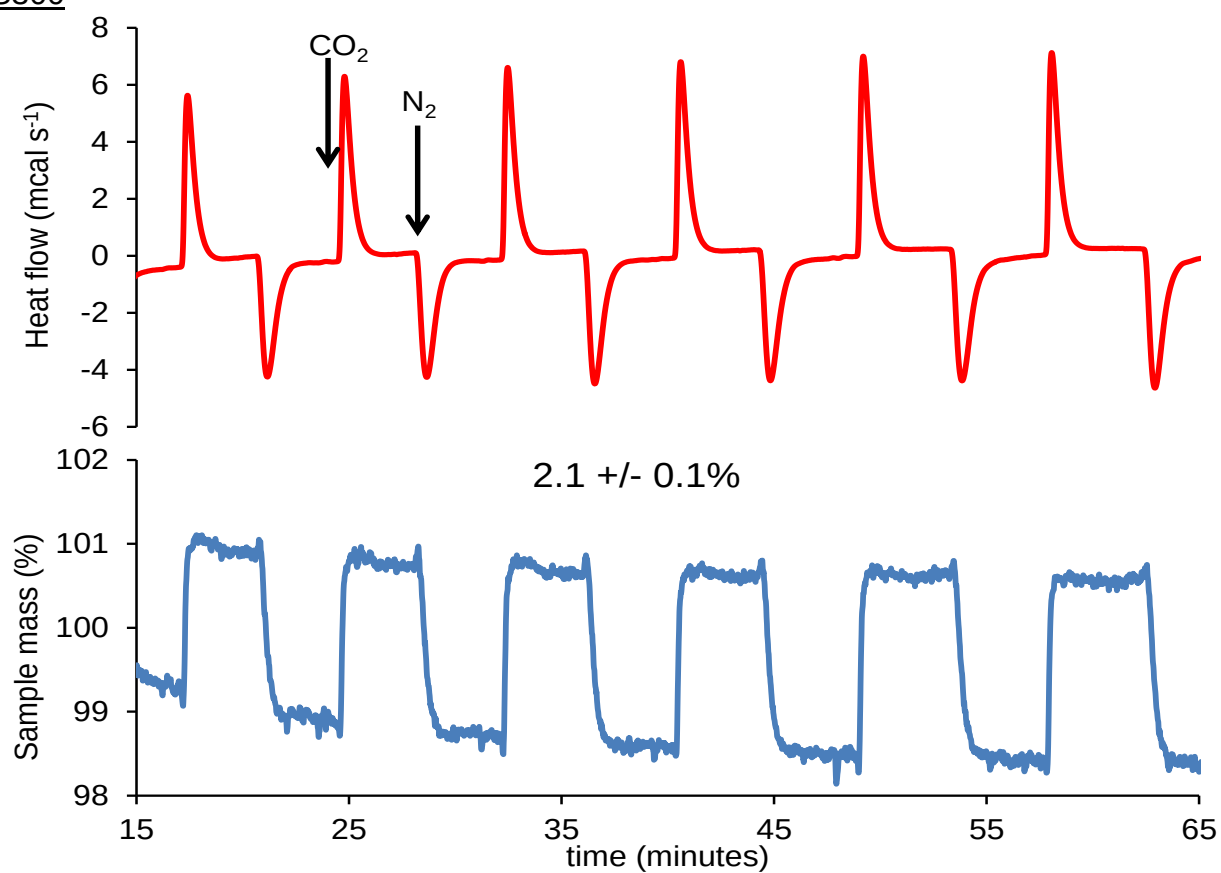


### P400O50

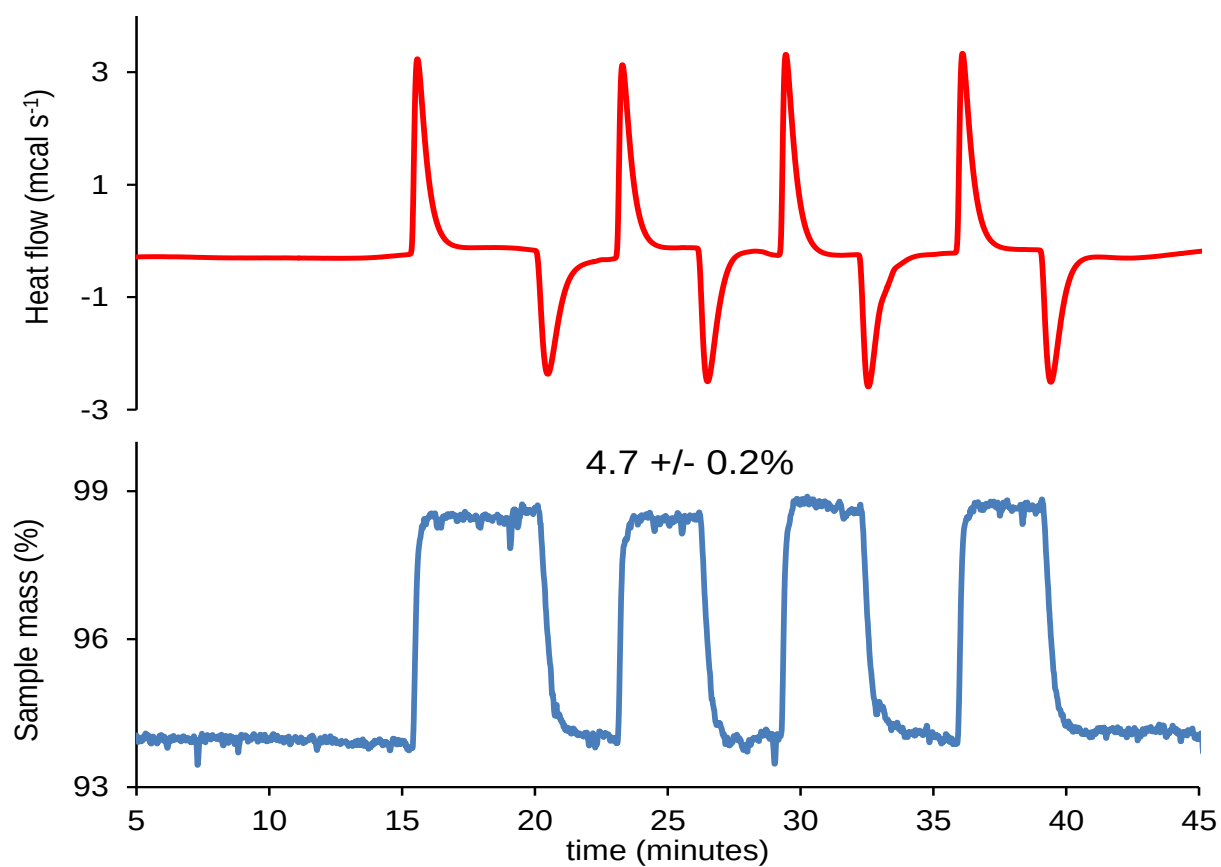


# Mass and heat flow changes during CO<sub>2</sub> adsorption at 35 °C and 1 bar pressure

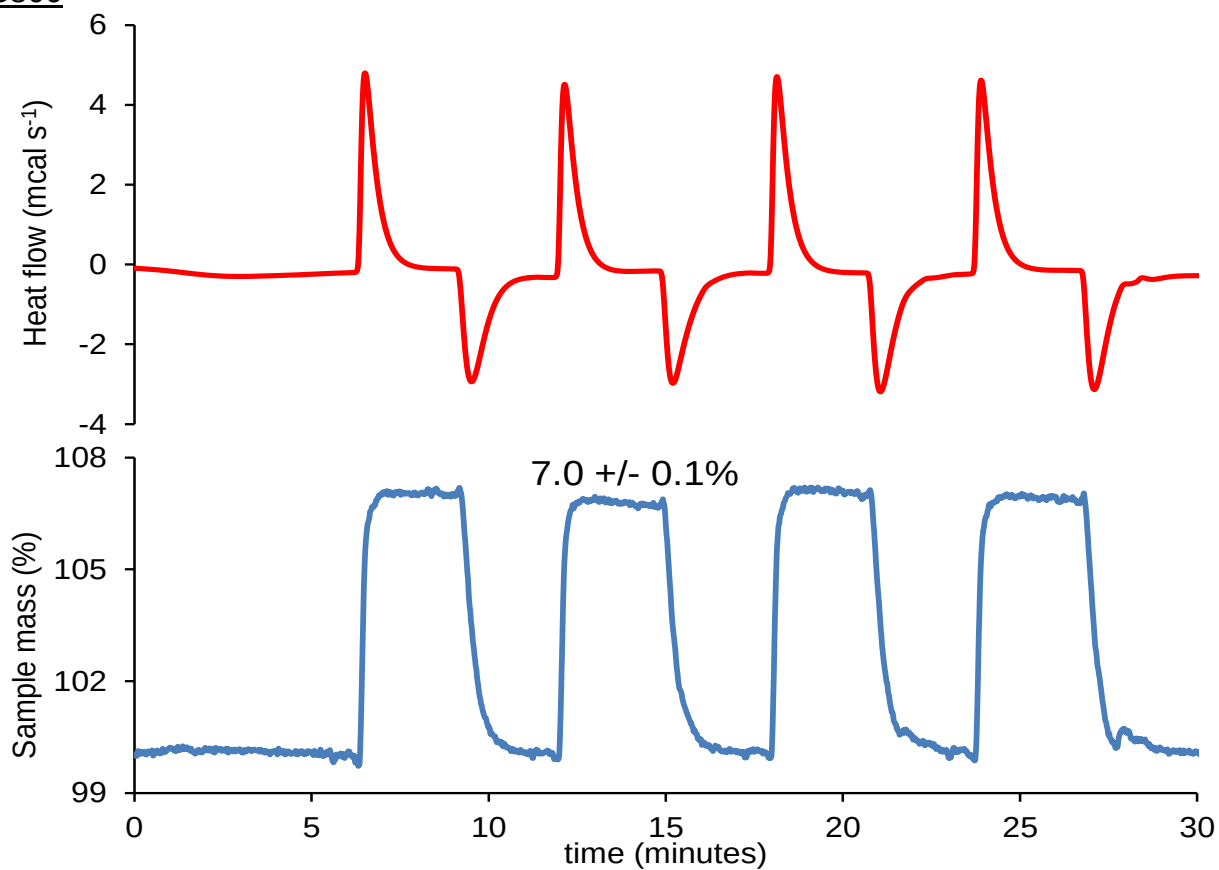
S300



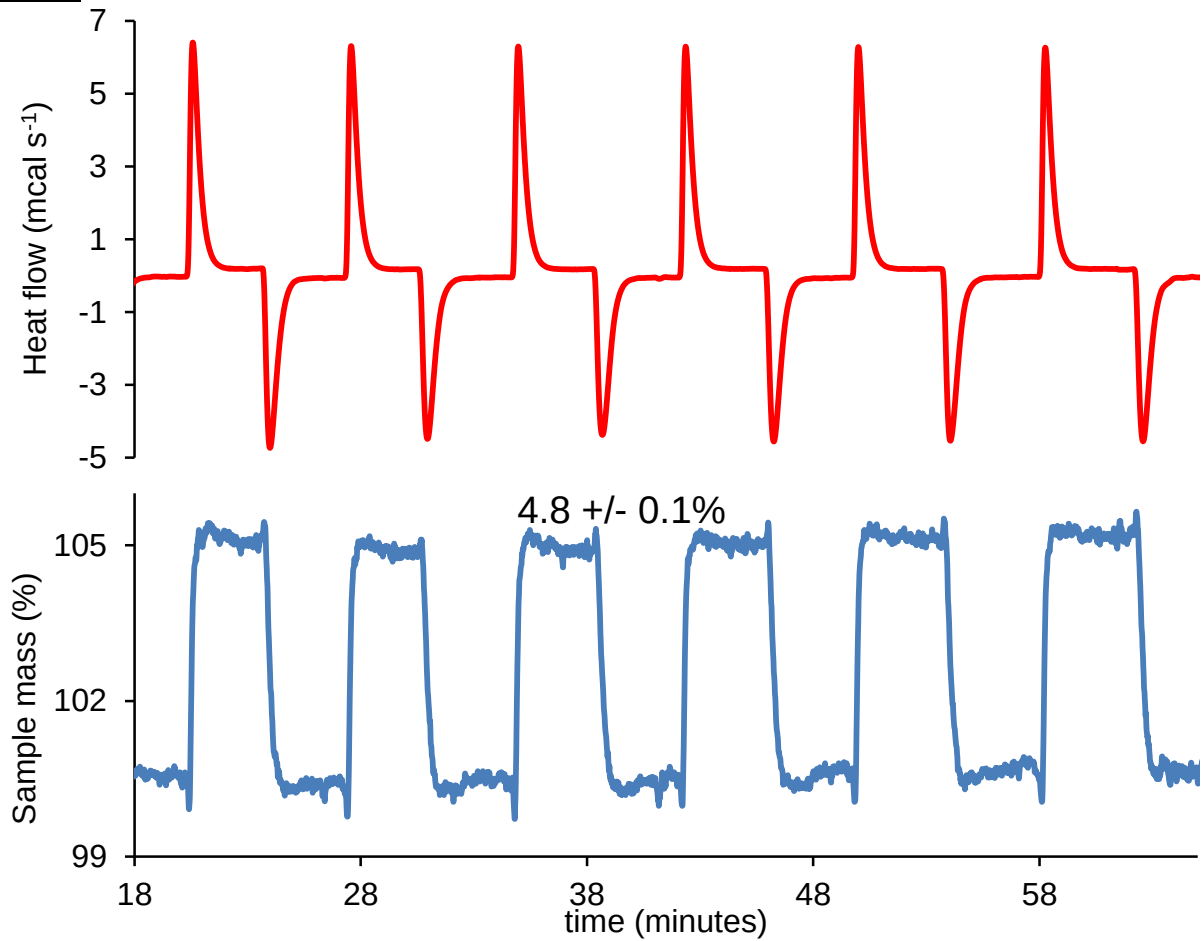
S600



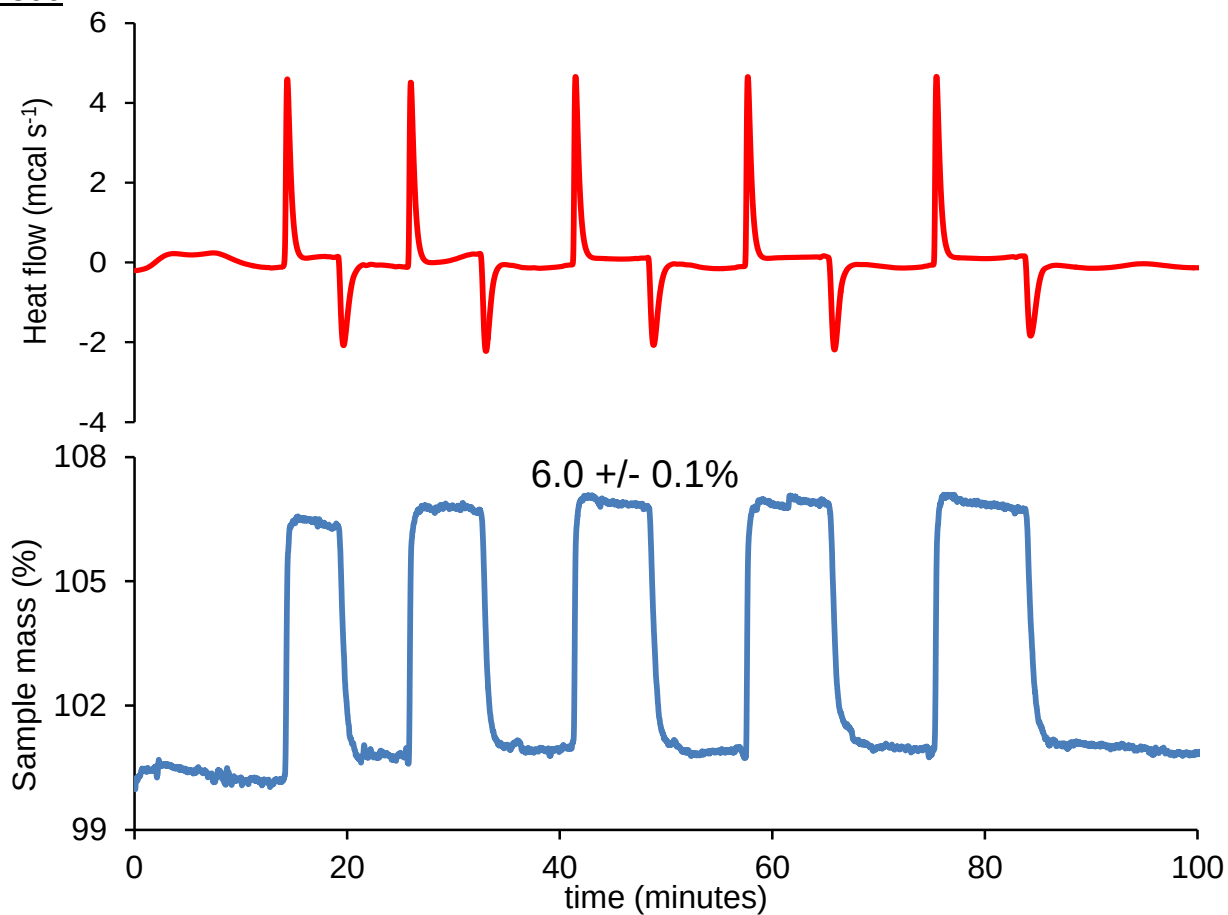
S800



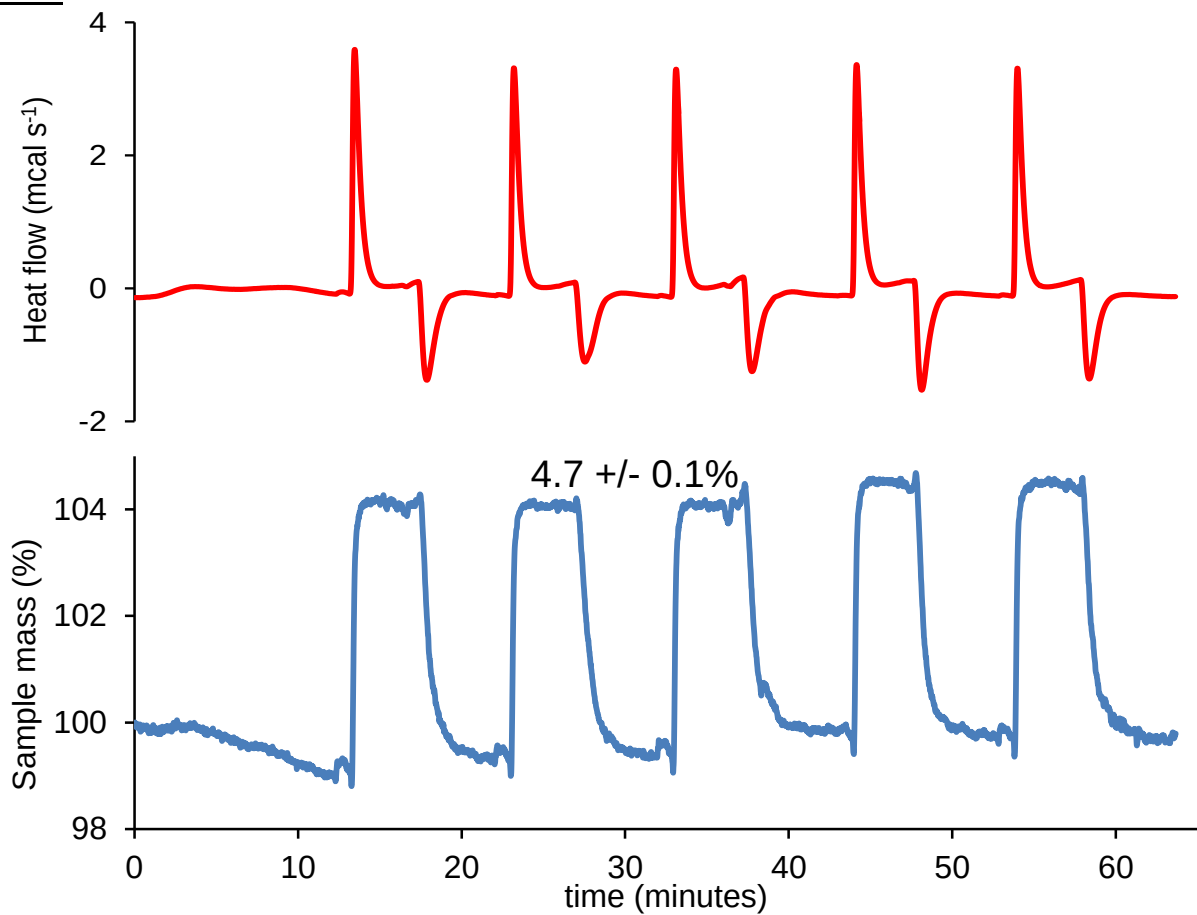
S1000



A800

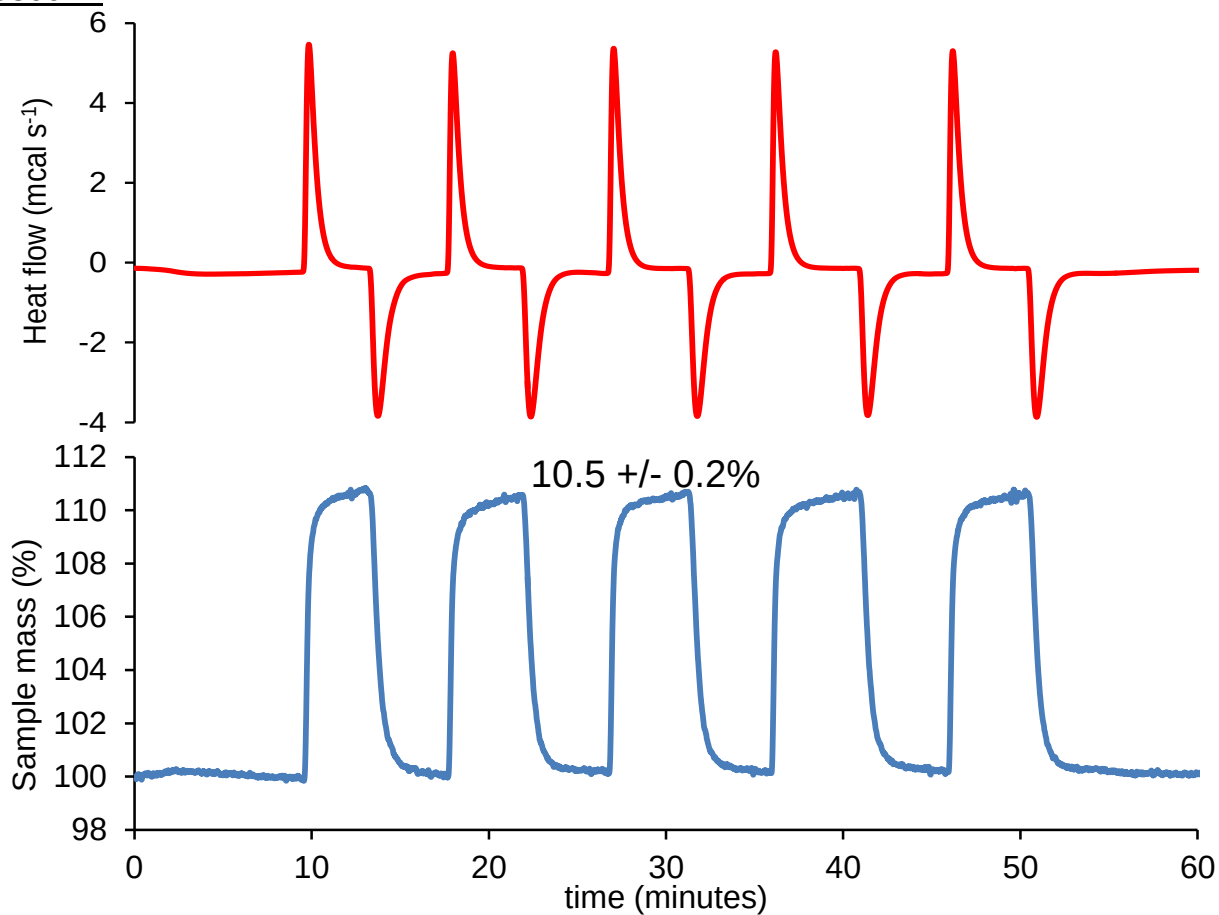


P800

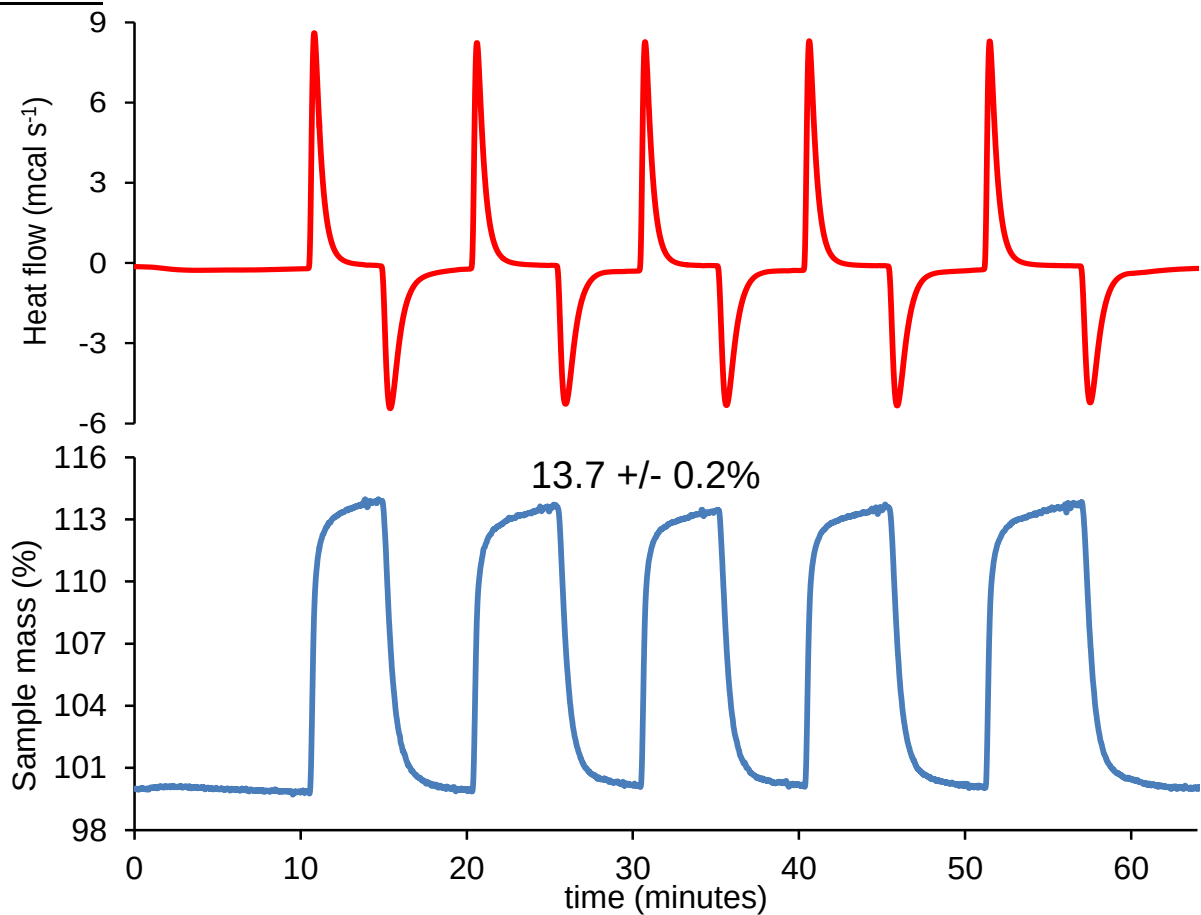




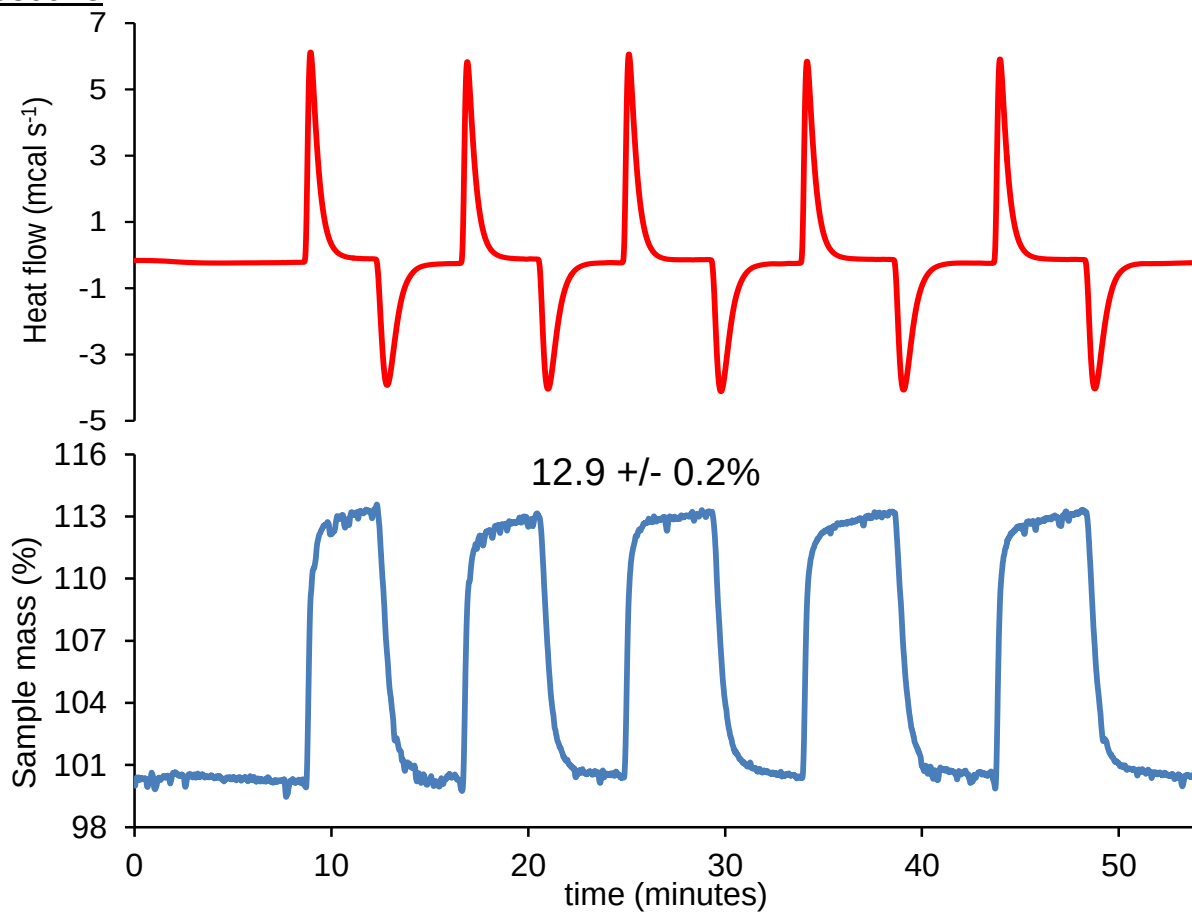
S800K1



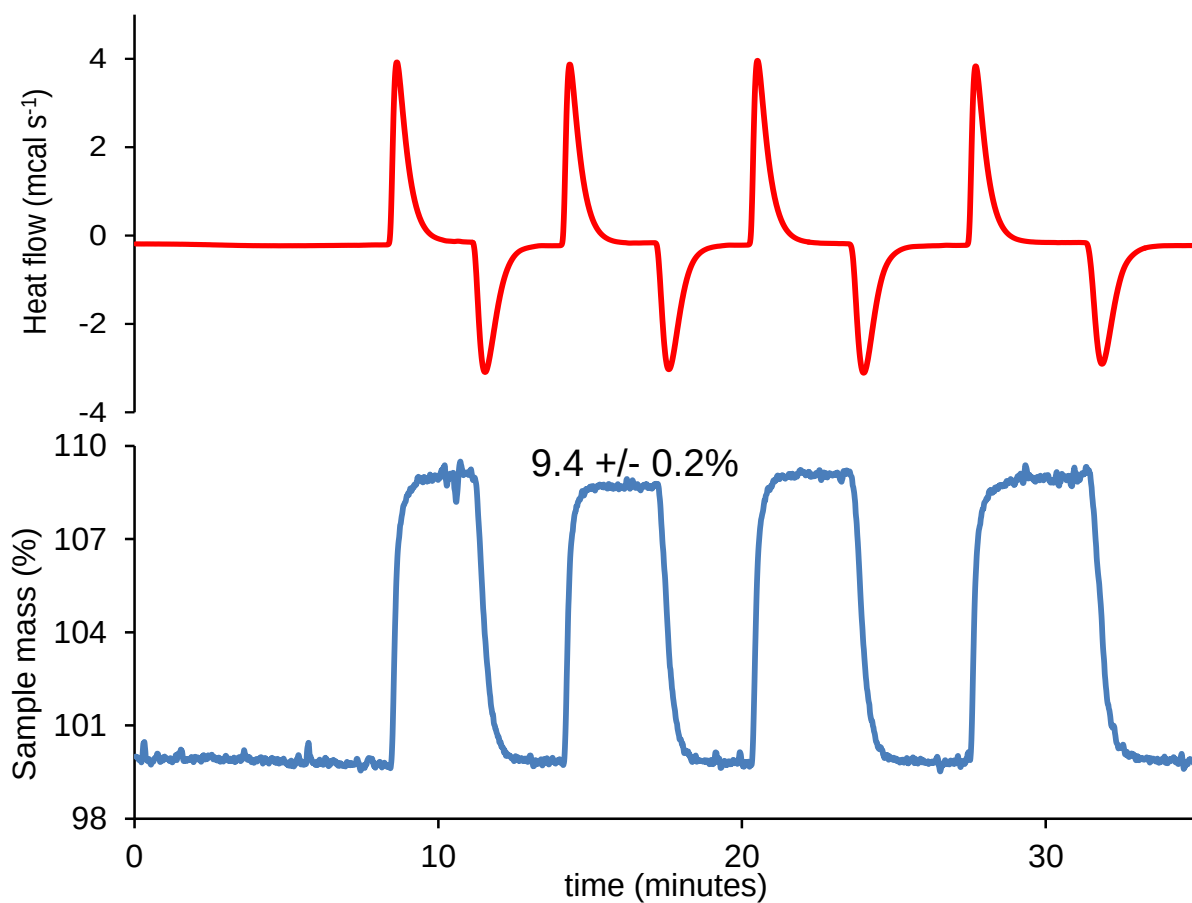
S800K2



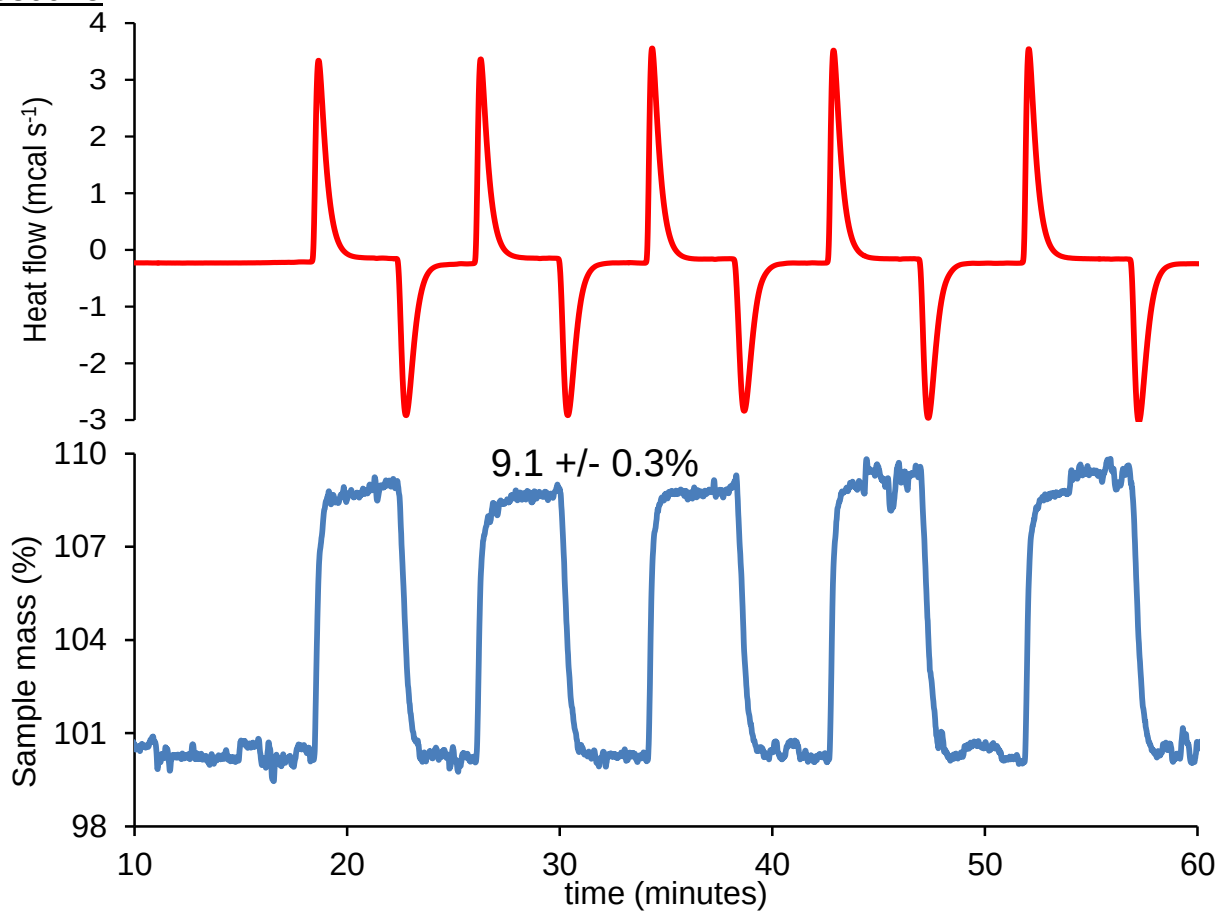
S800K3



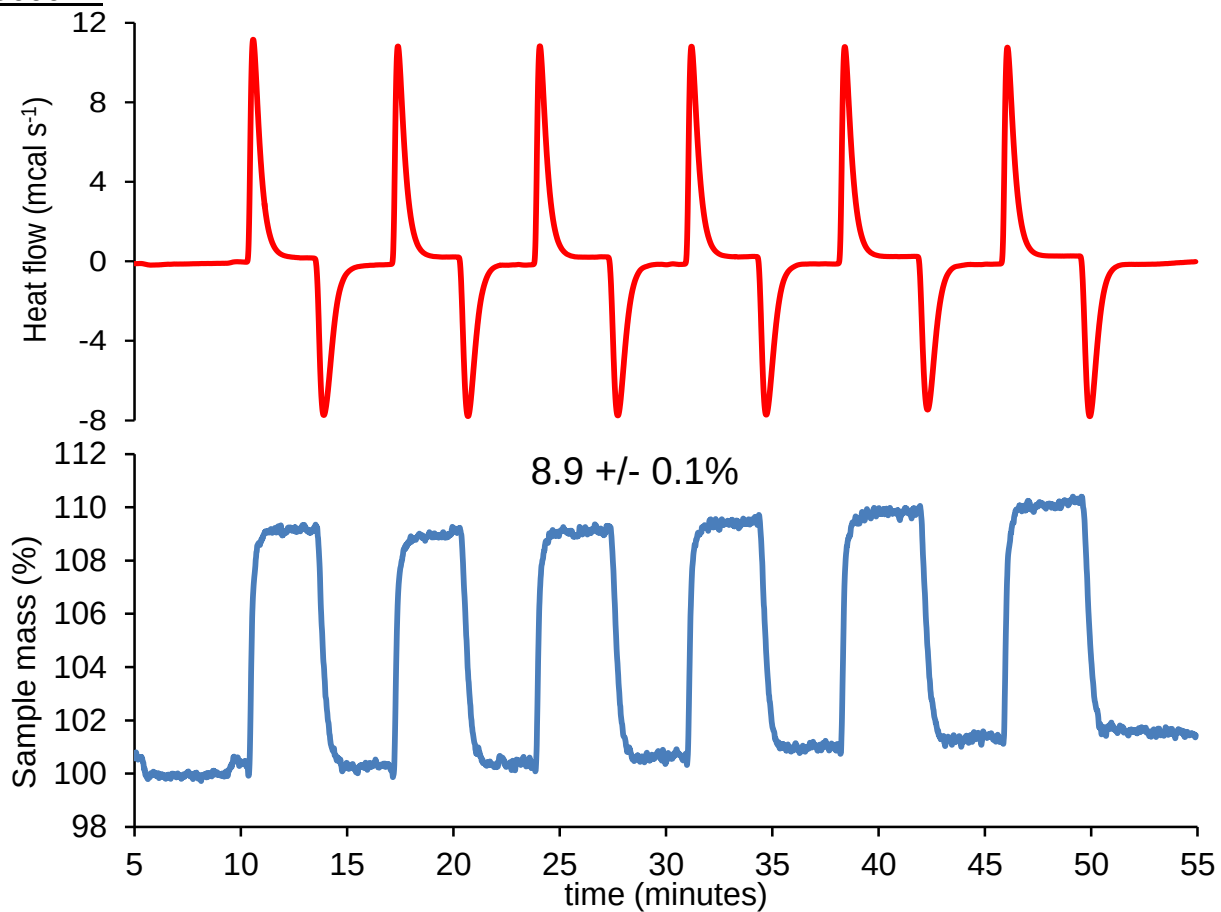
S800K4



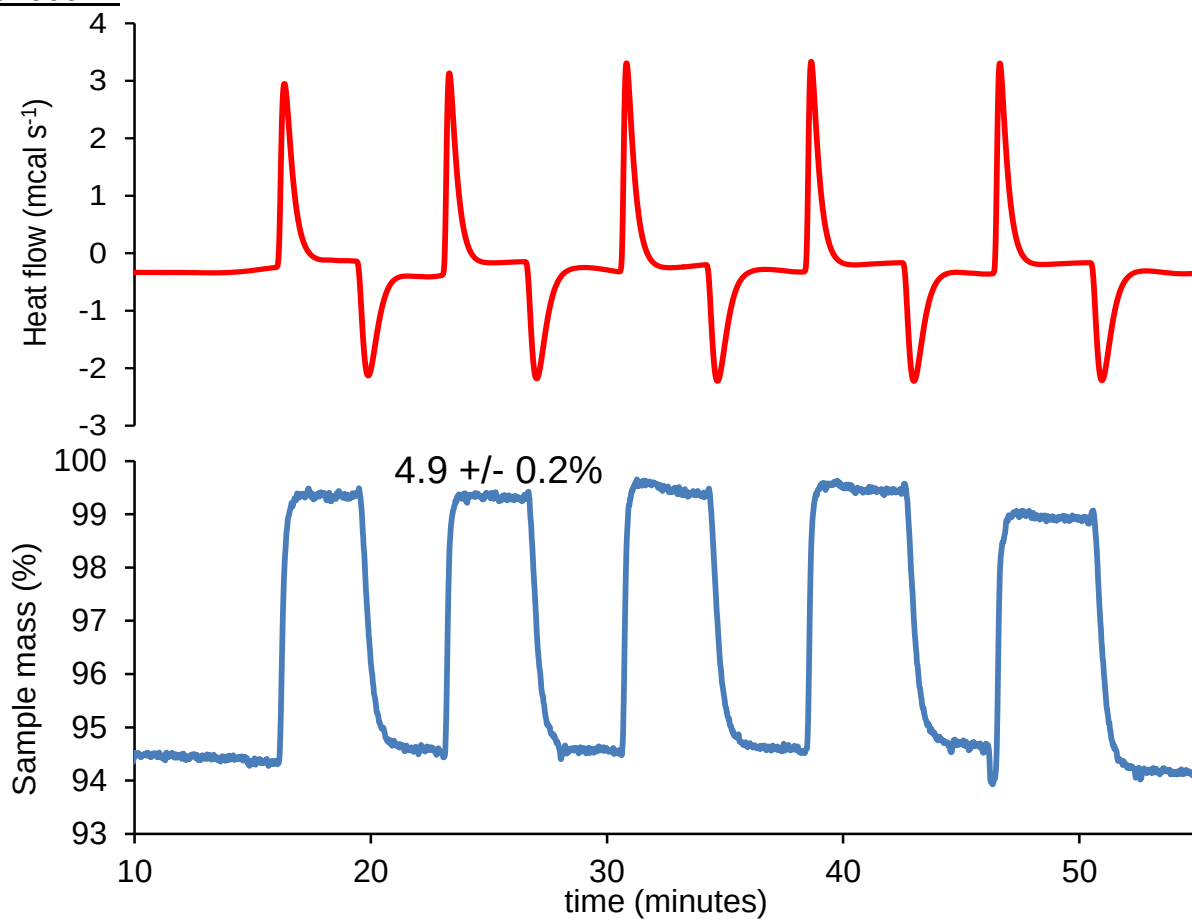
S800K5



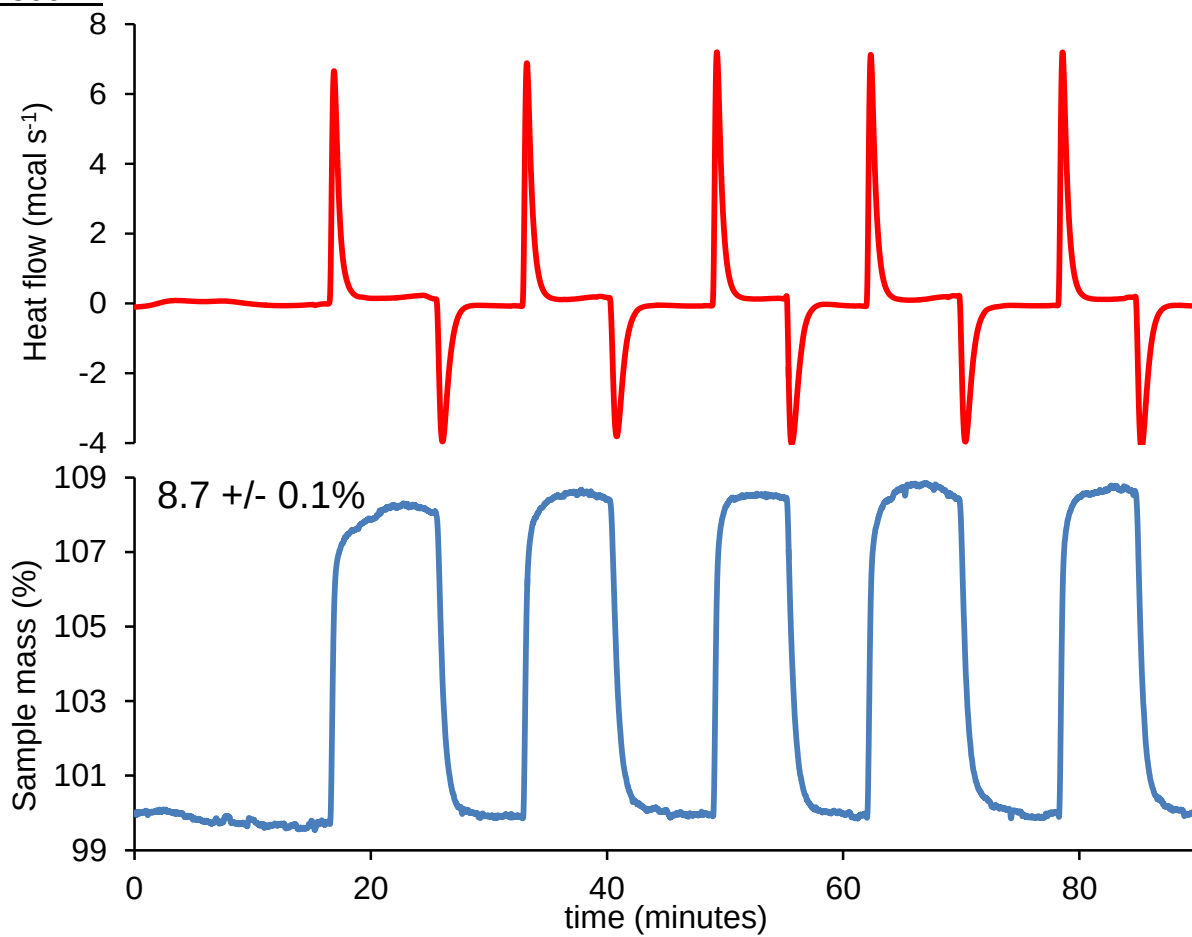
S600K4



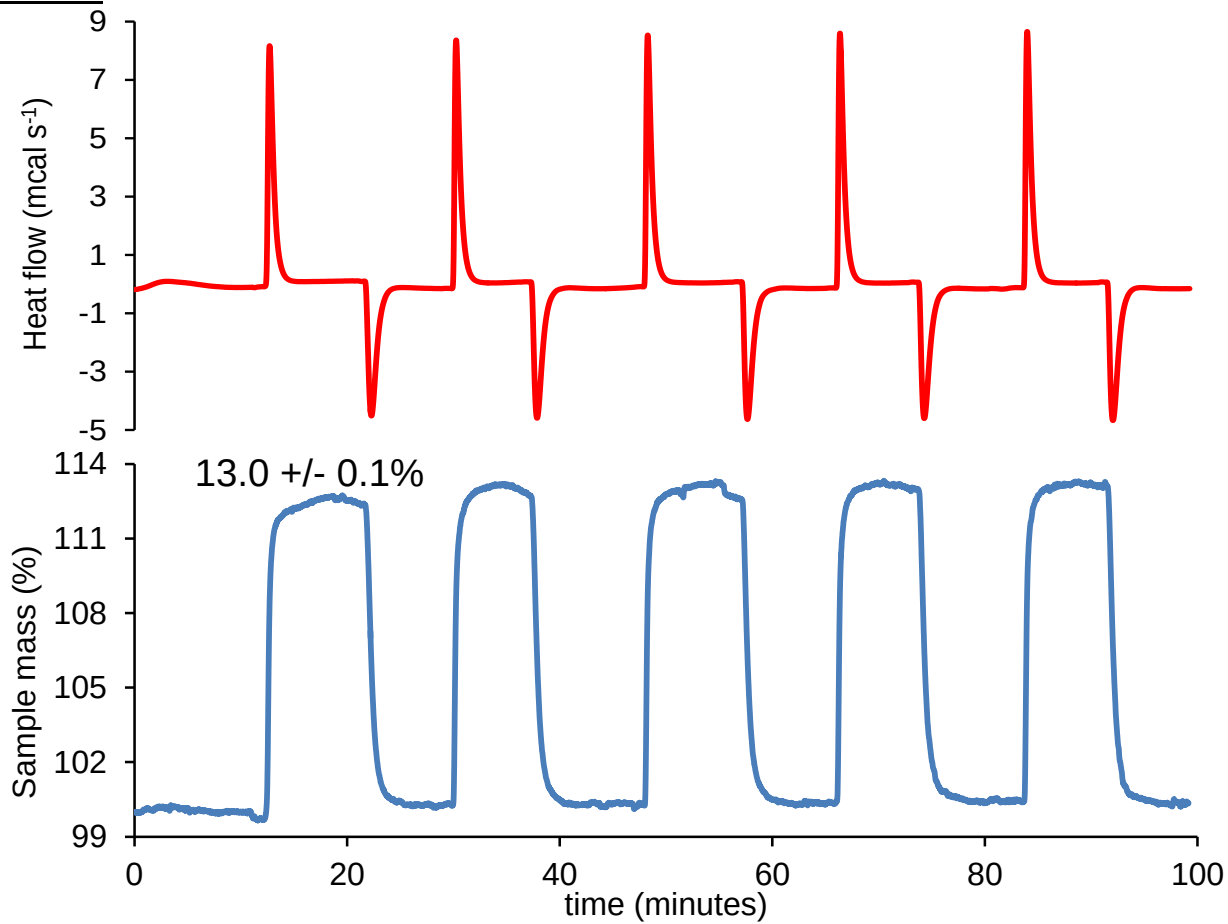
S1000K4



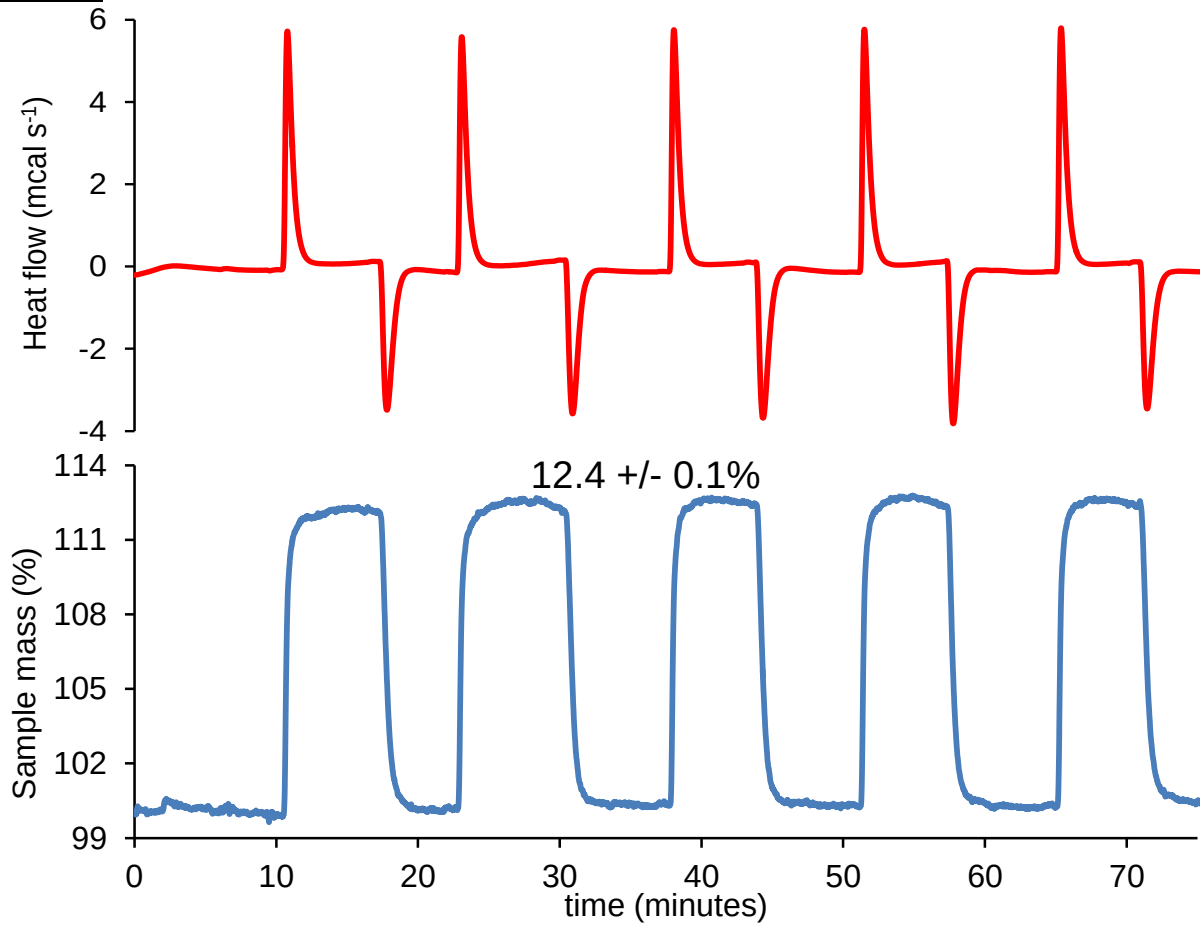
A800K1



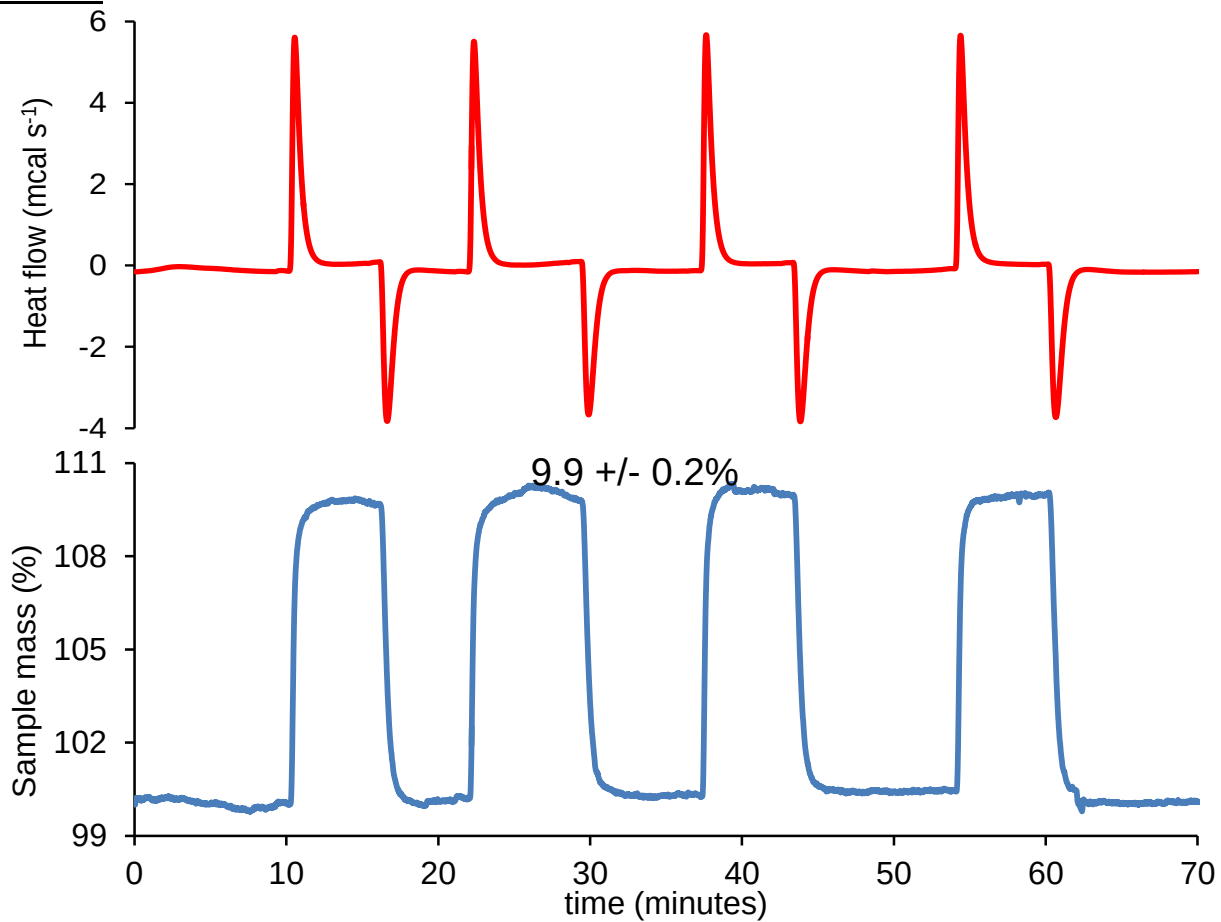
A800K2



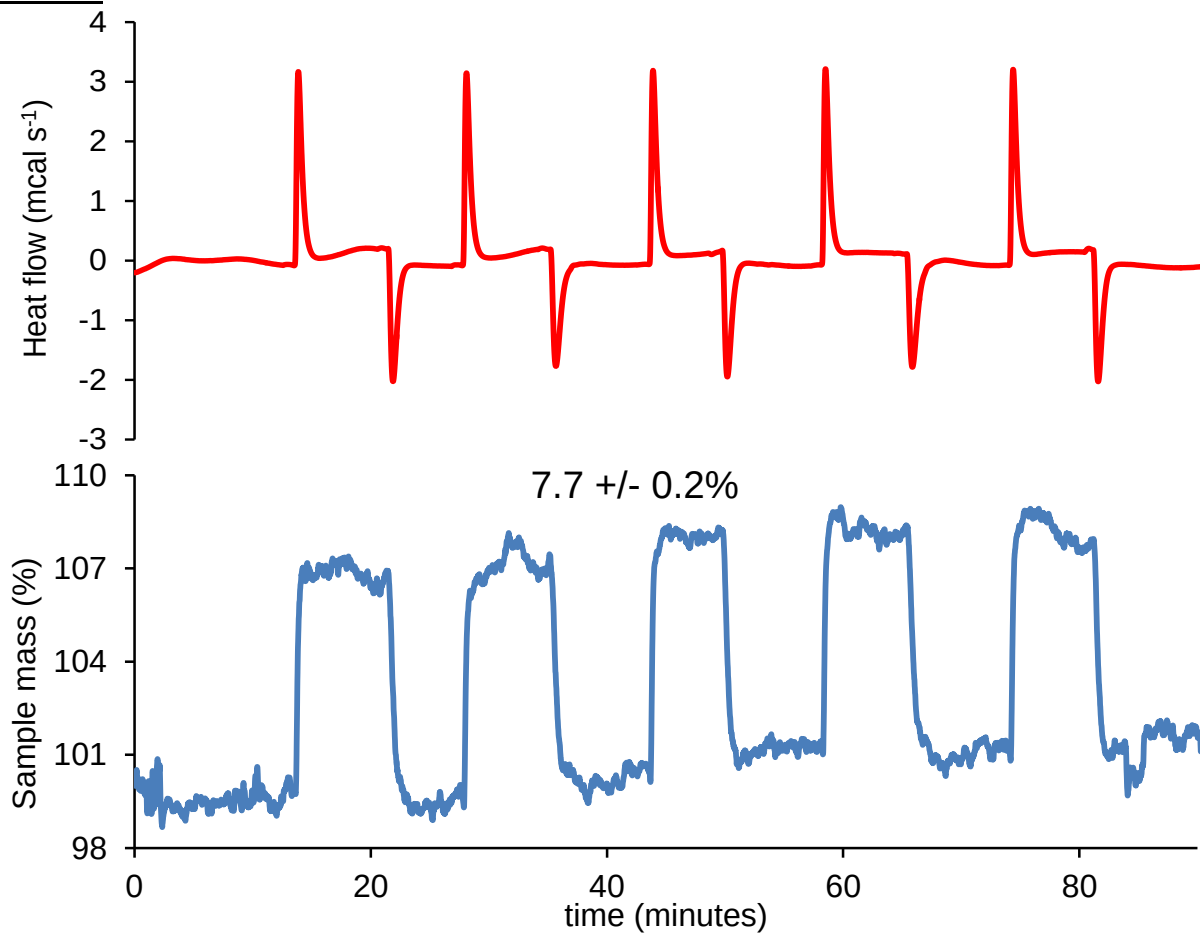
A800K3



A800K4

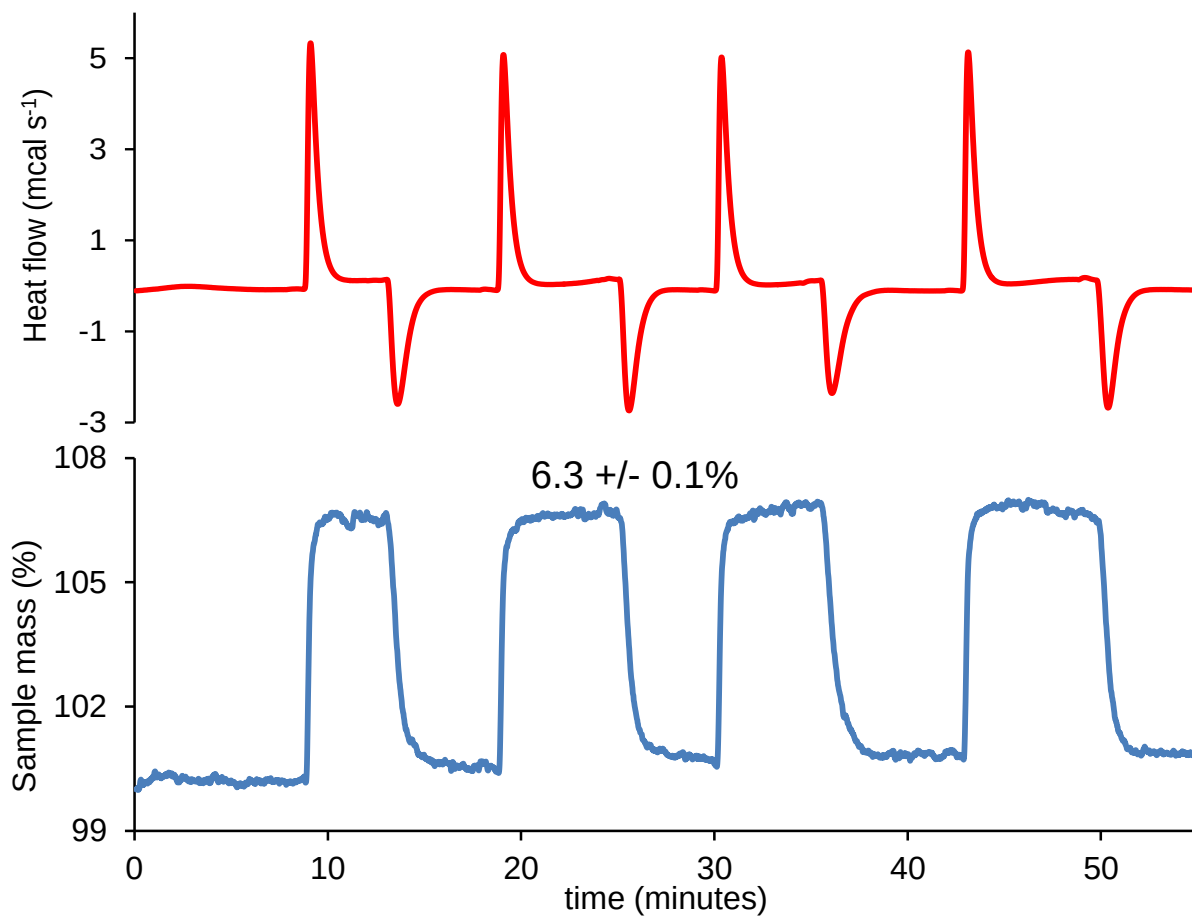


A800K5

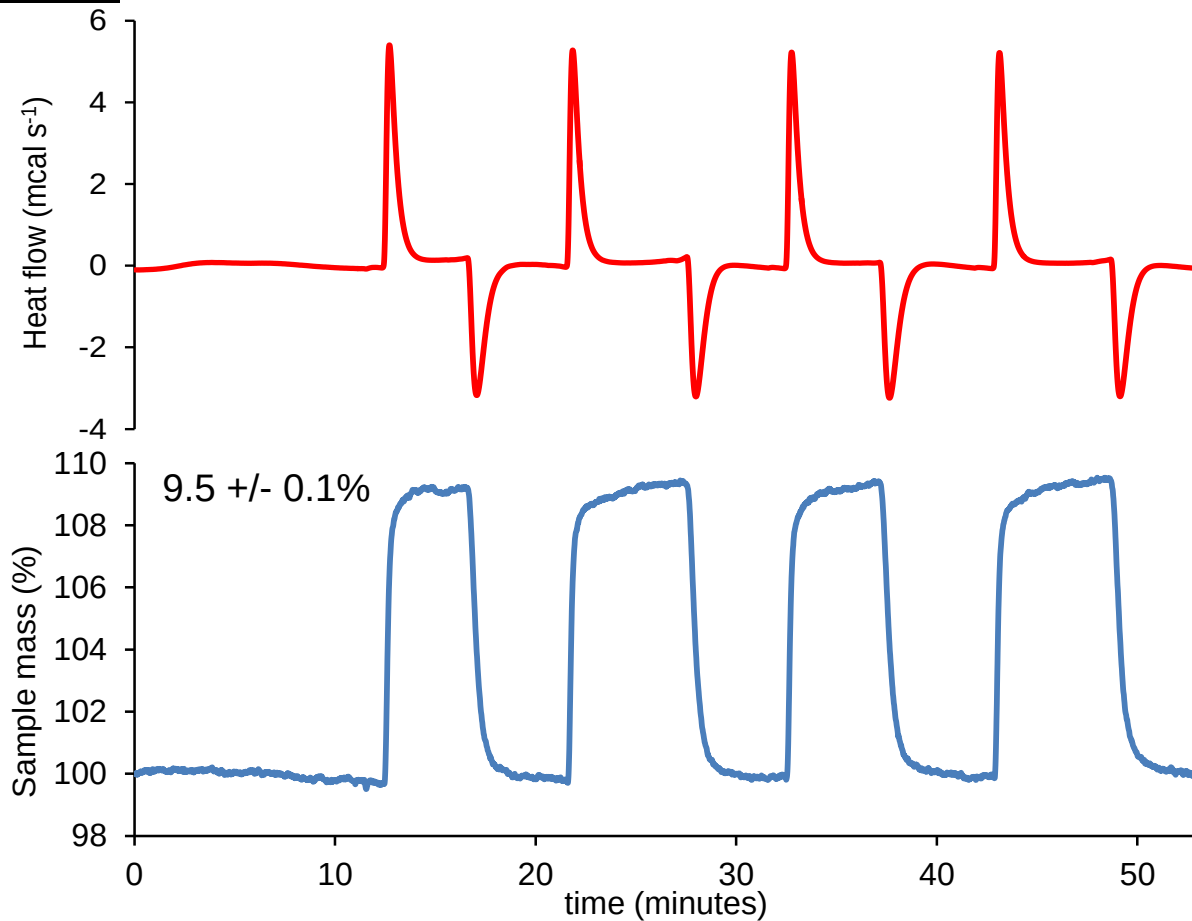




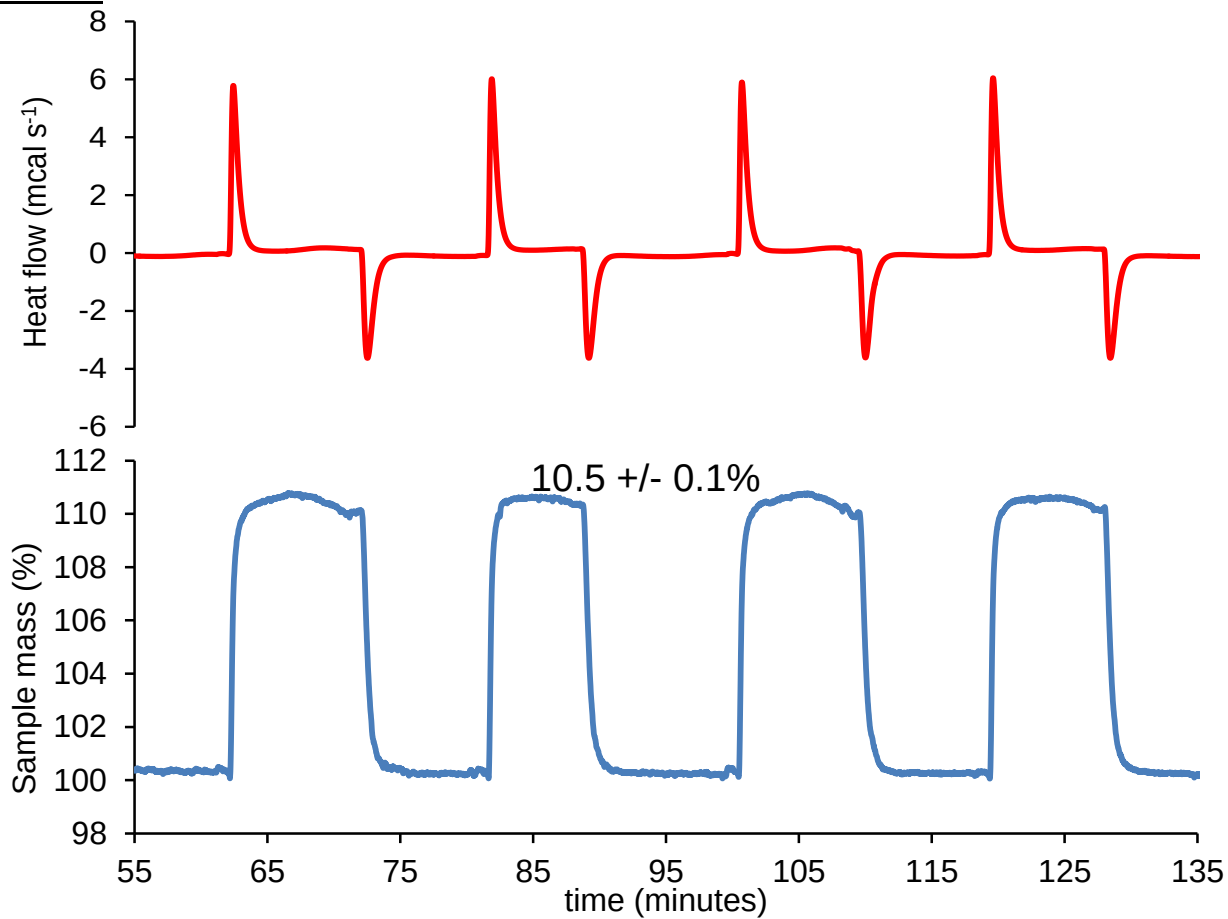
A600K2



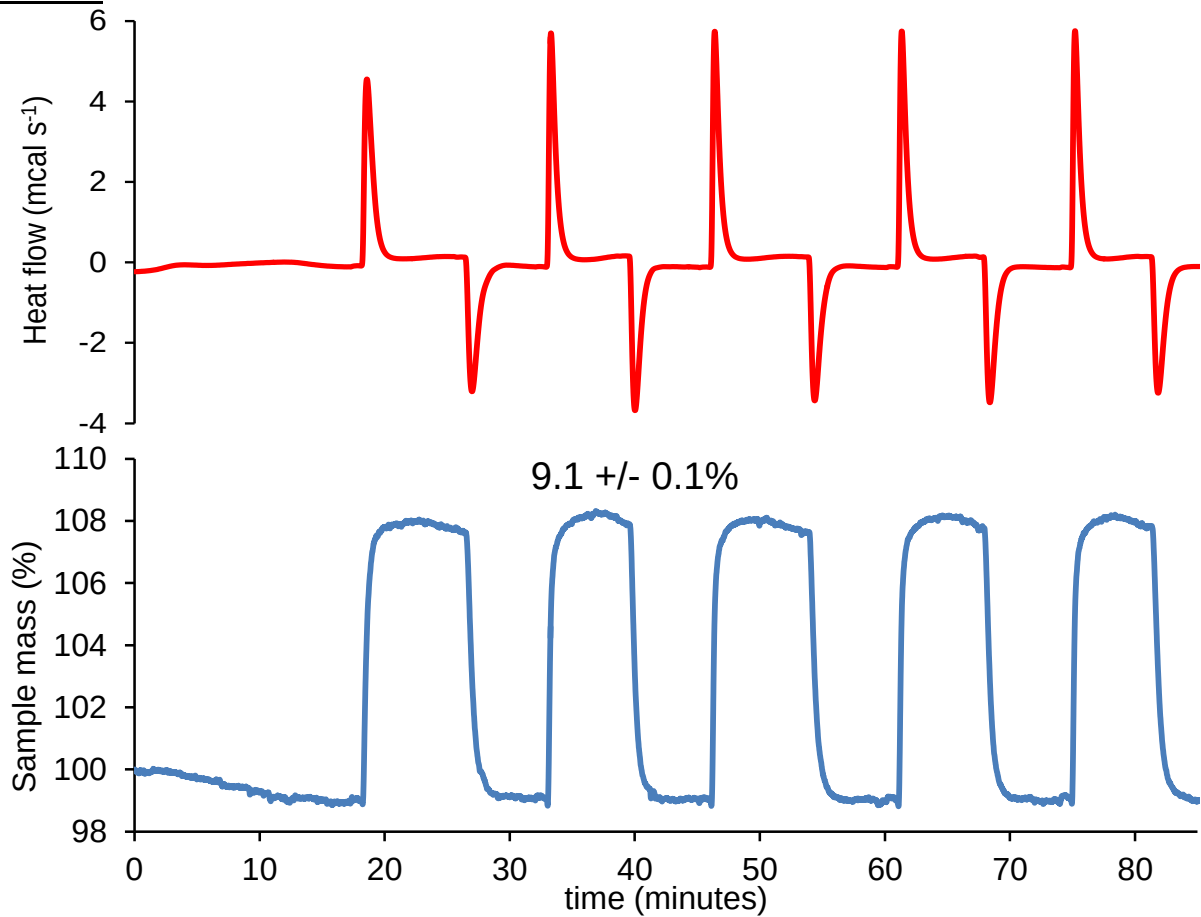
A1000K2



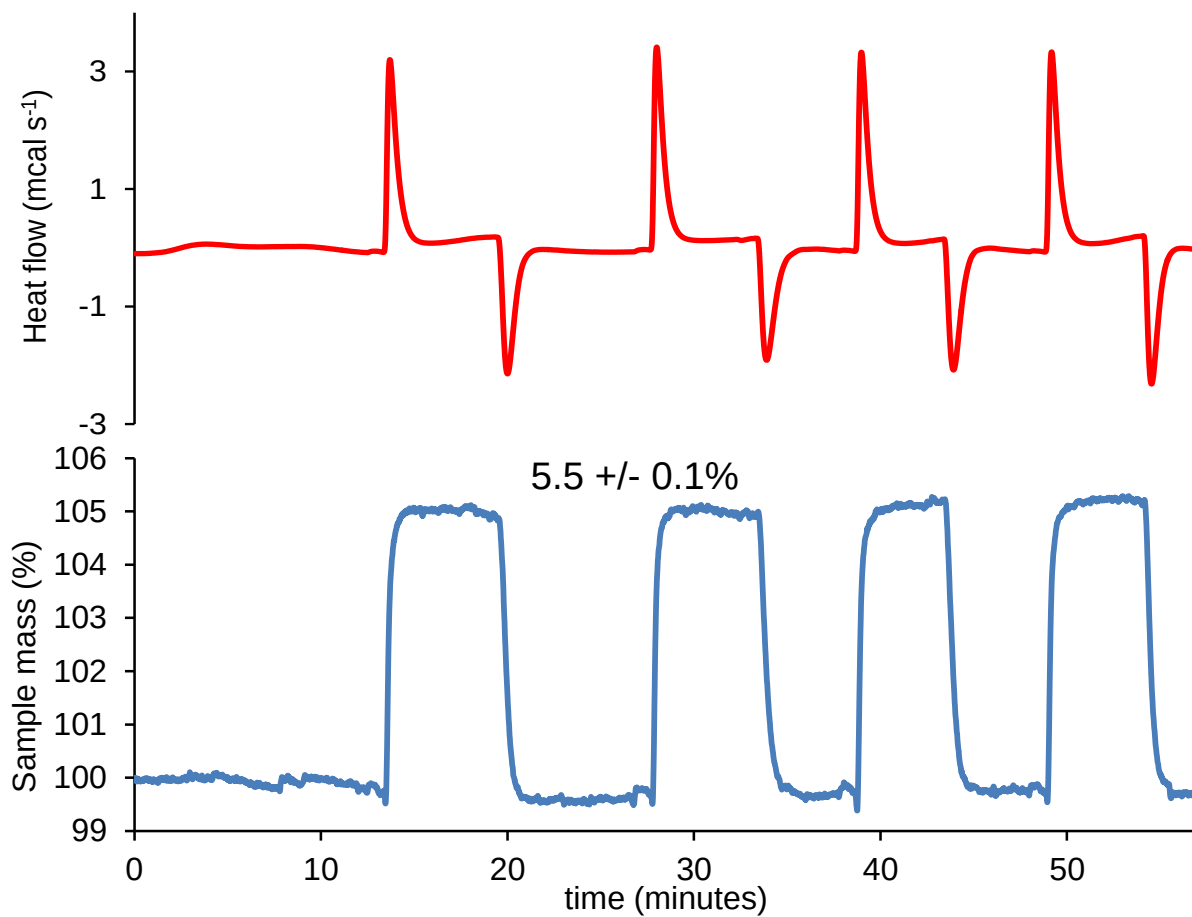
P800K2



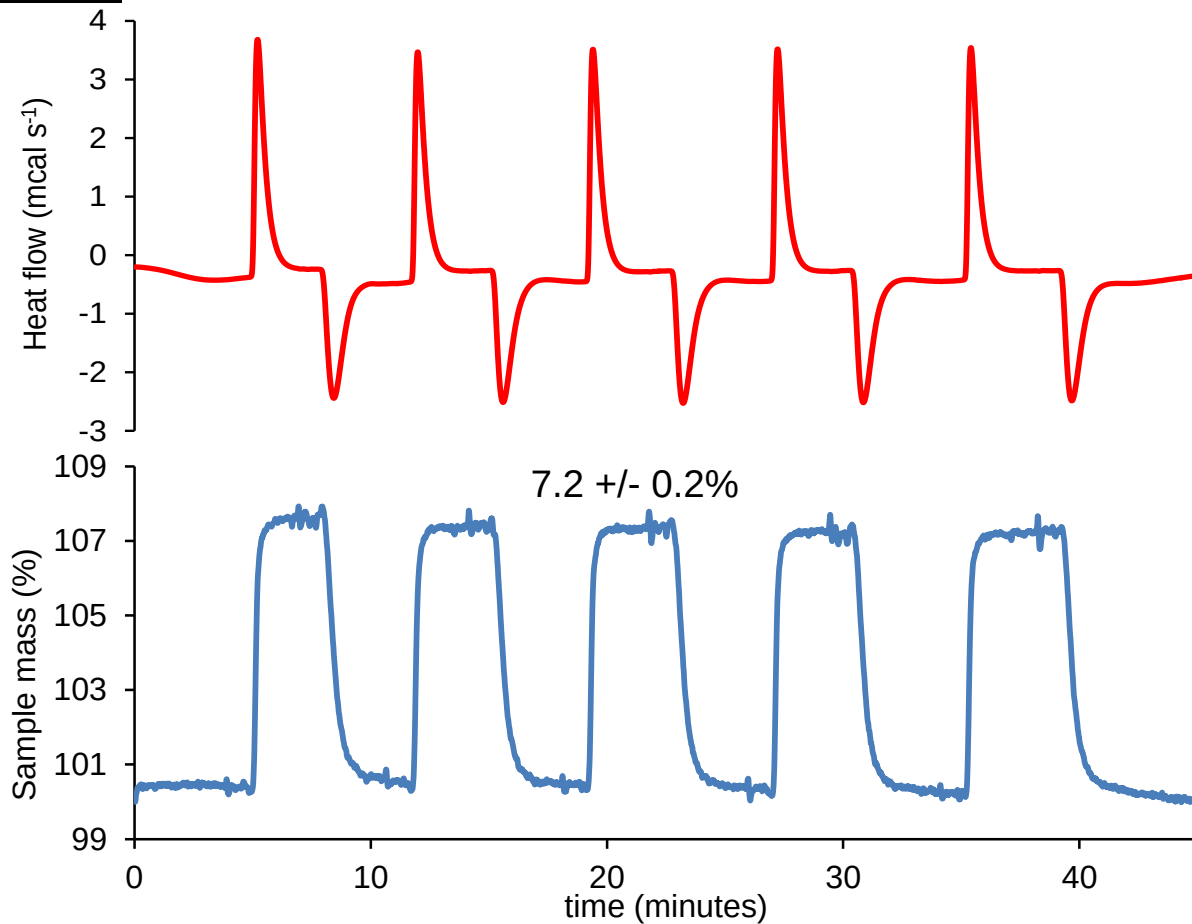
P800K3



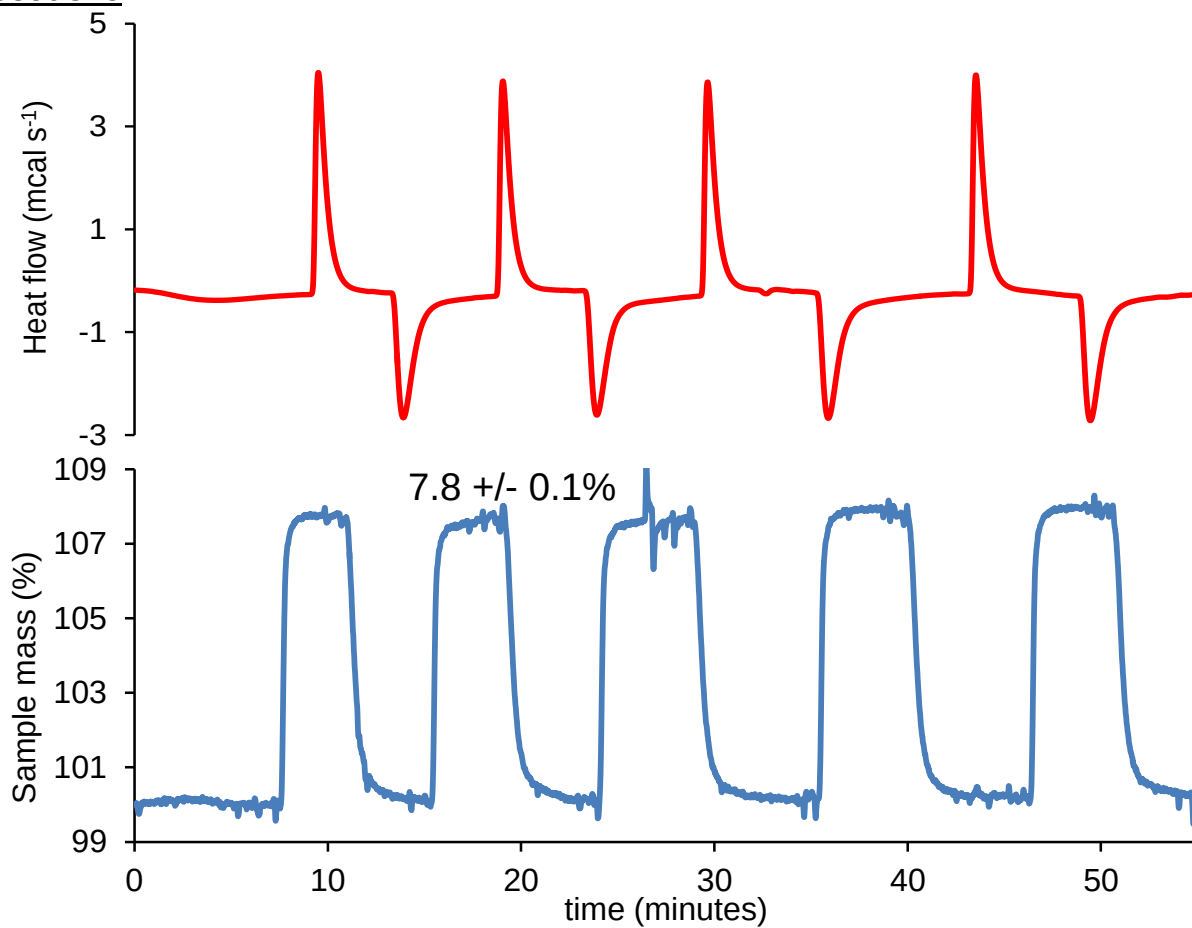
P800K5



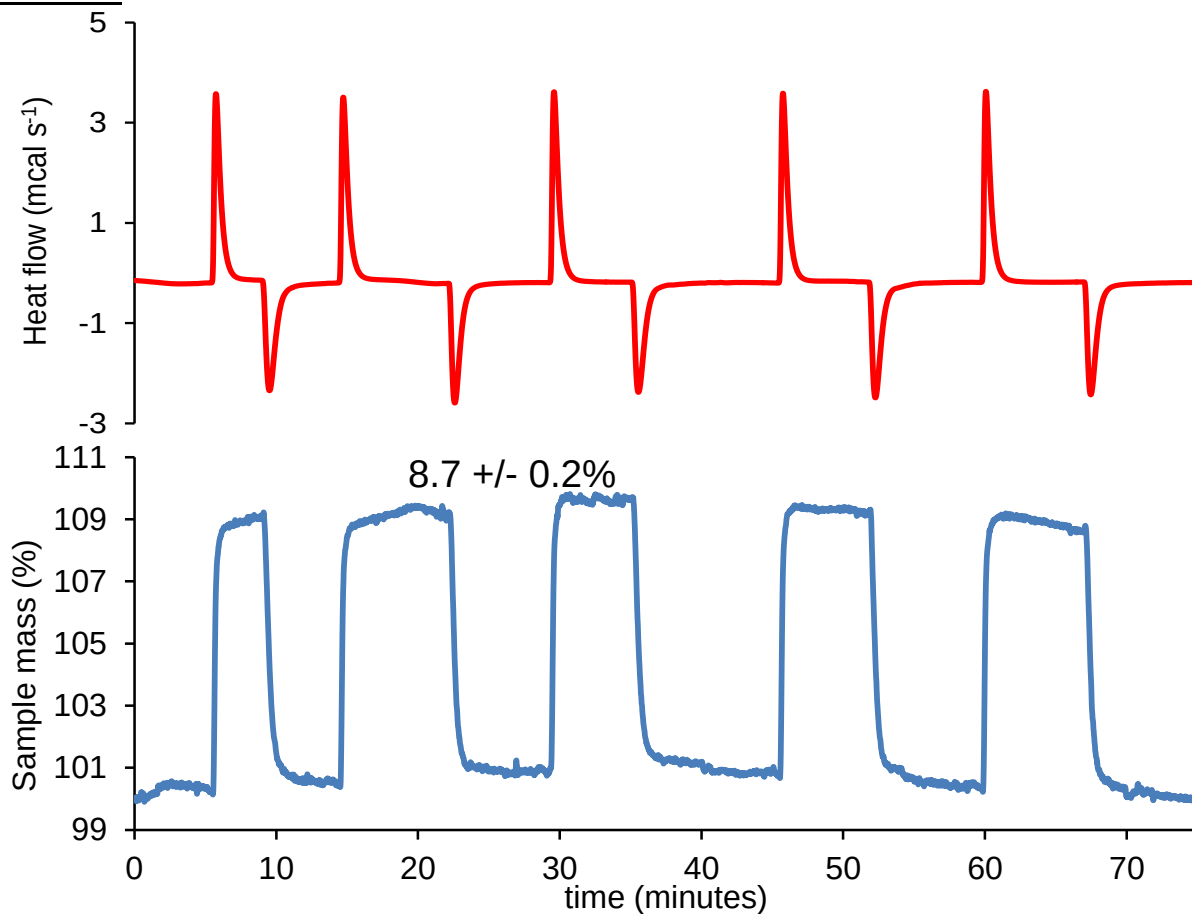
S800C15



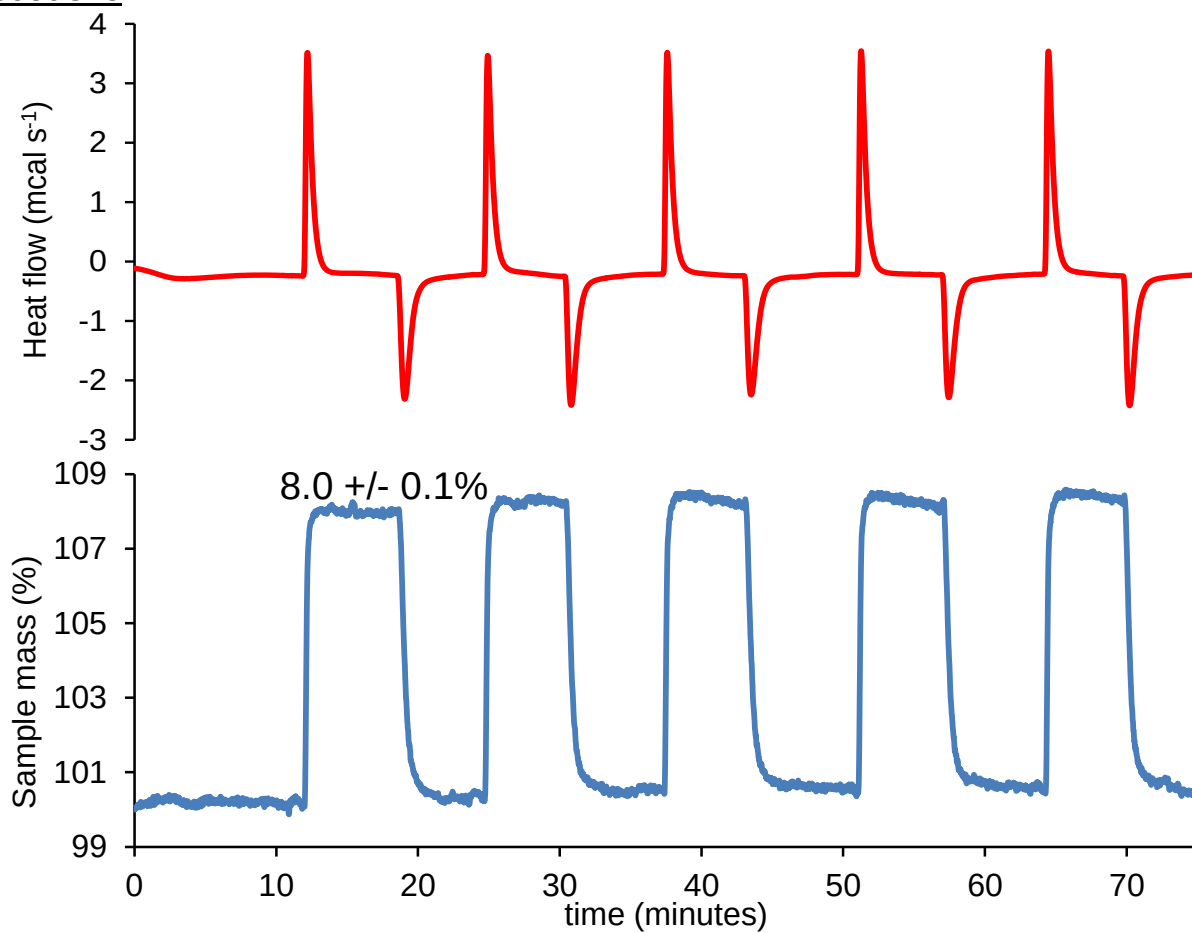
S850C15



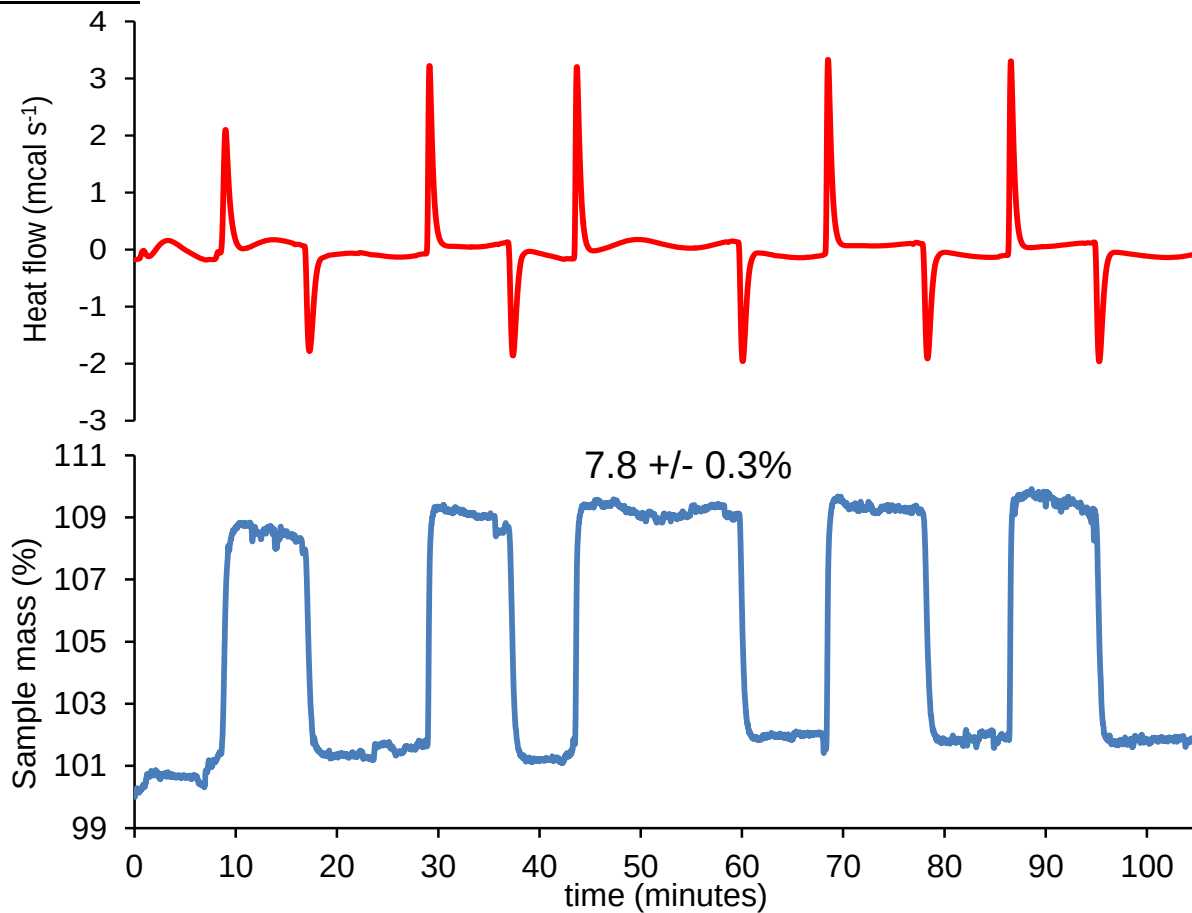
S900C15



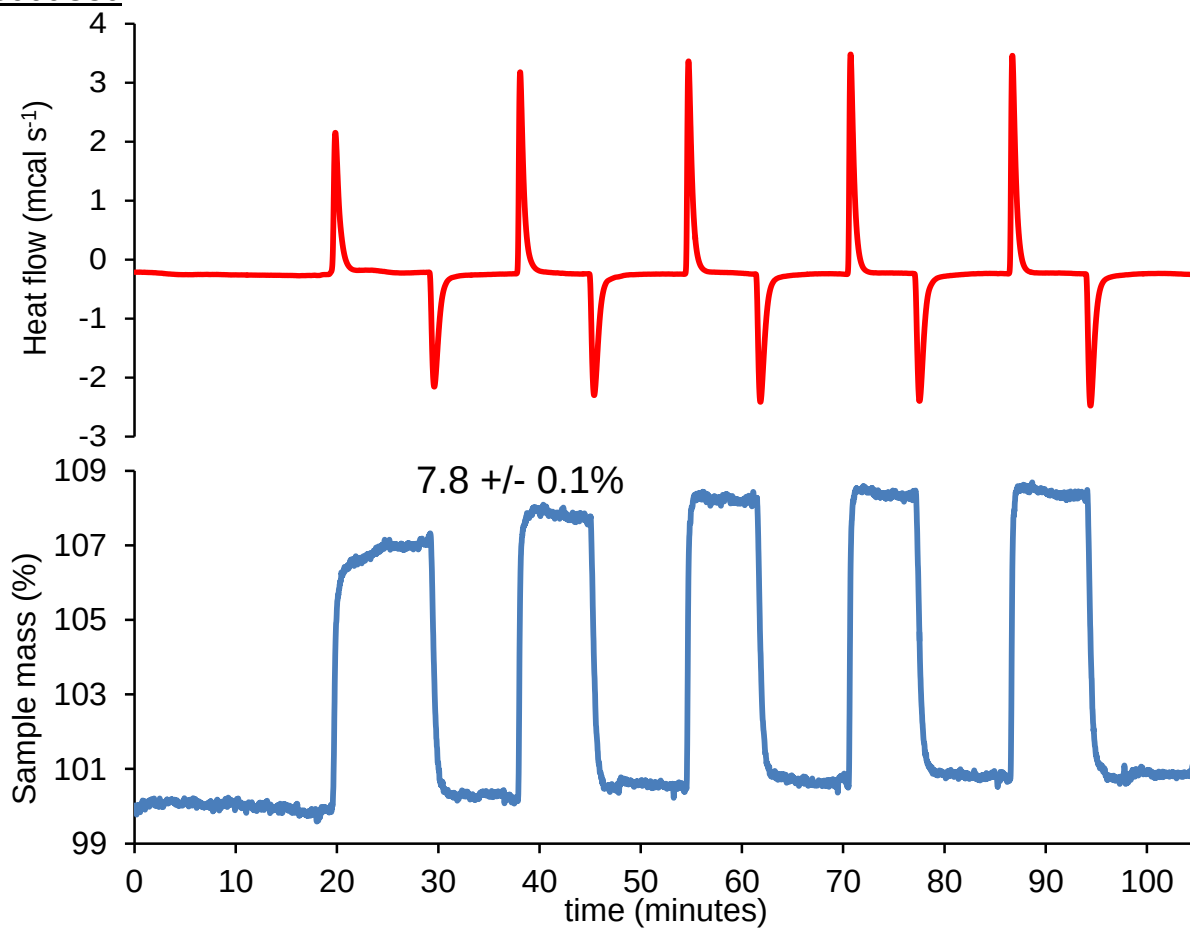
S950C15



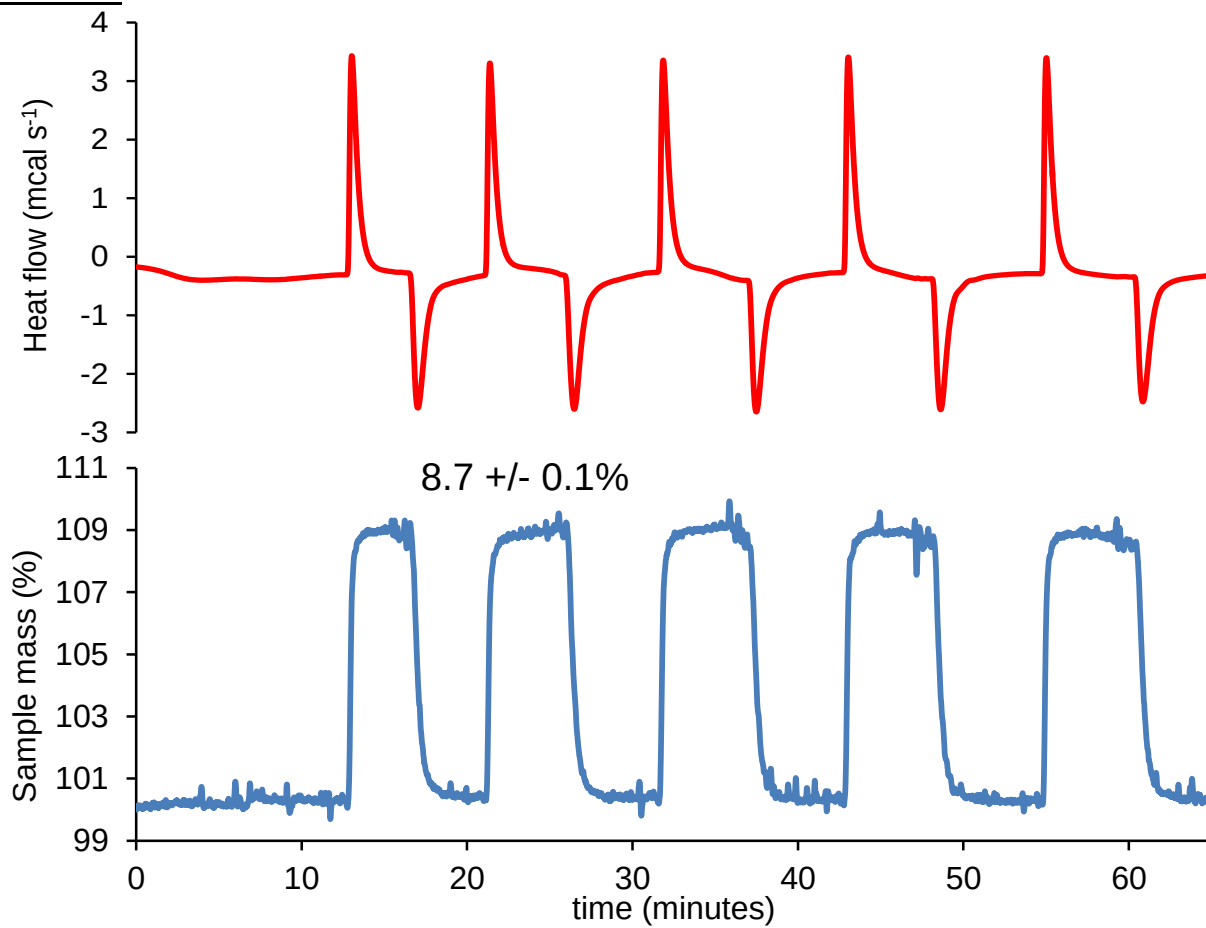
S1000C15



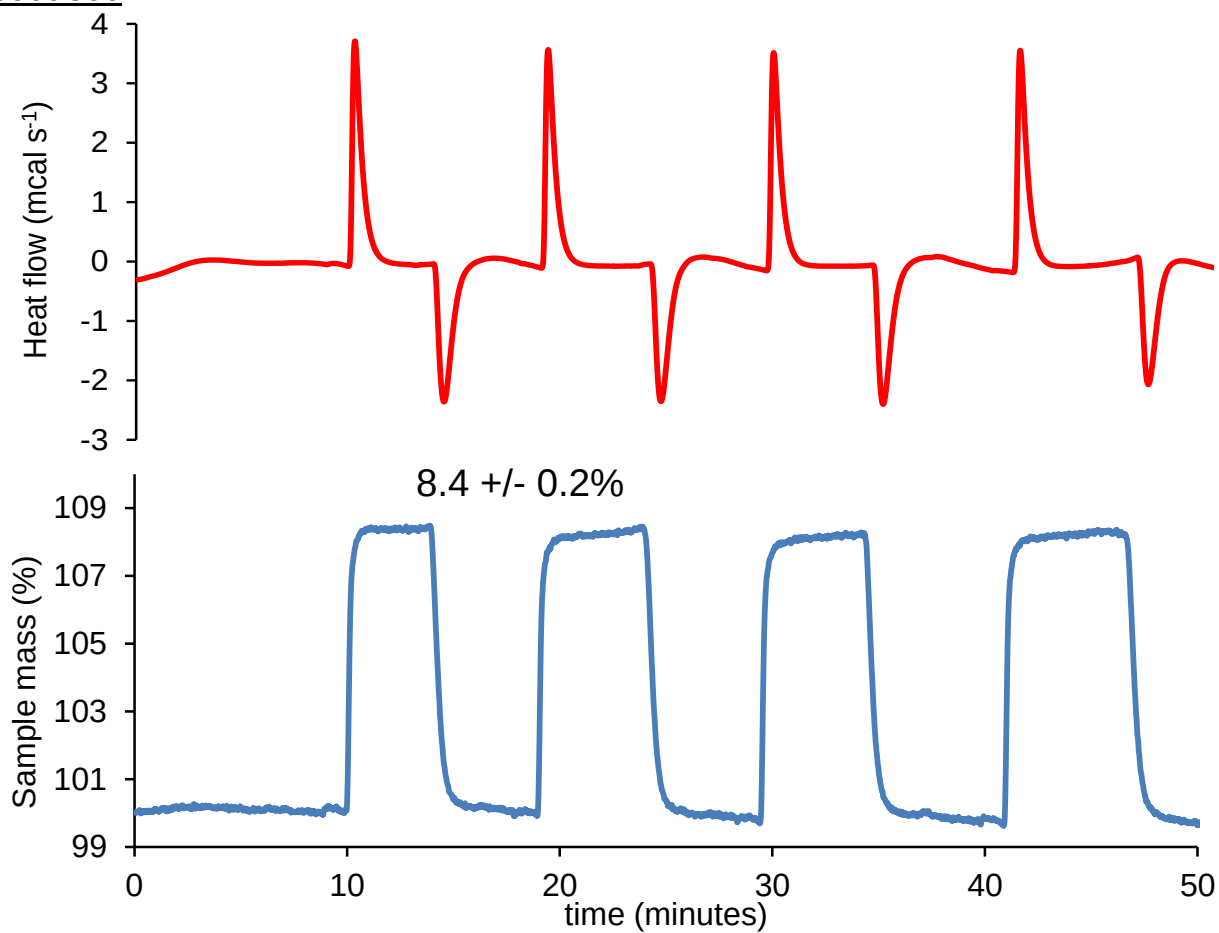
S900C30



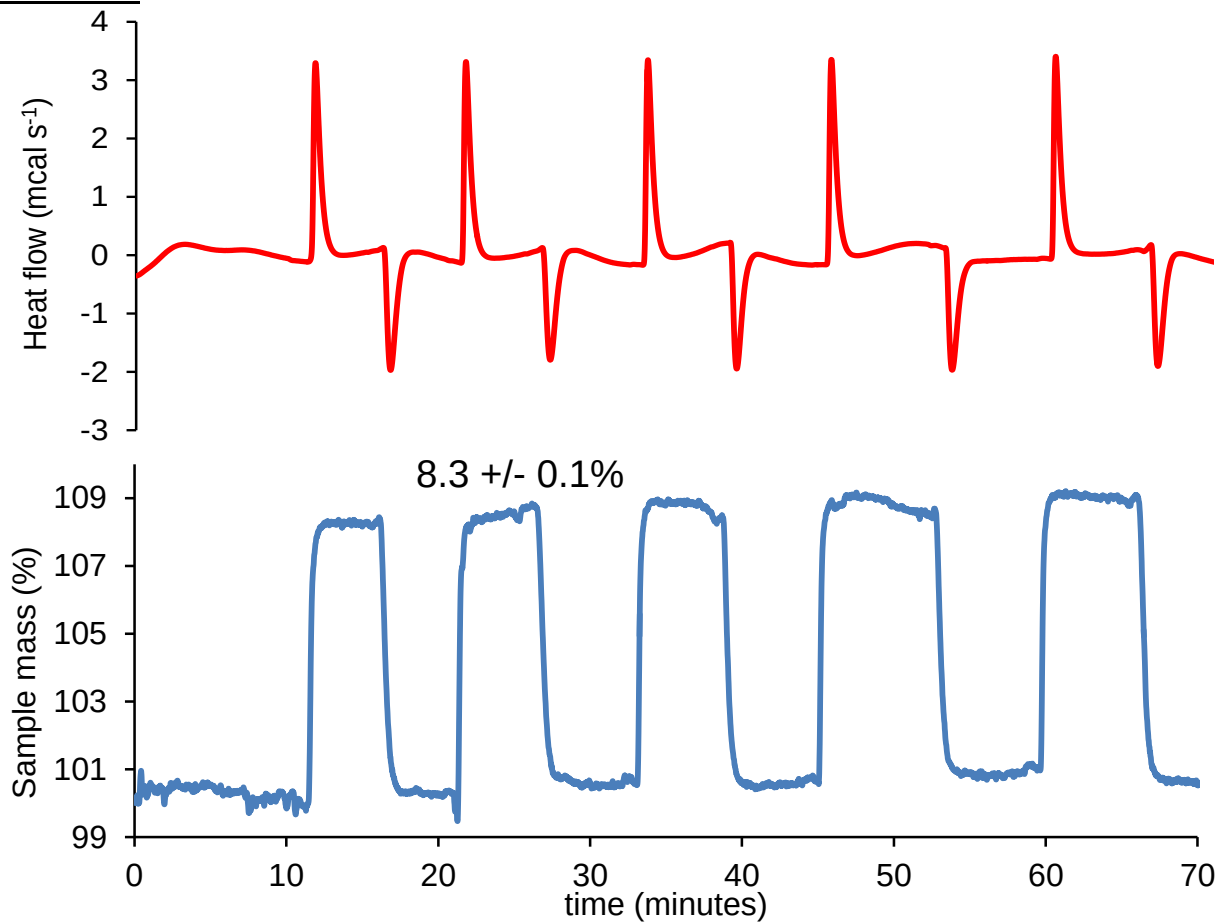
S900C60



S900C90

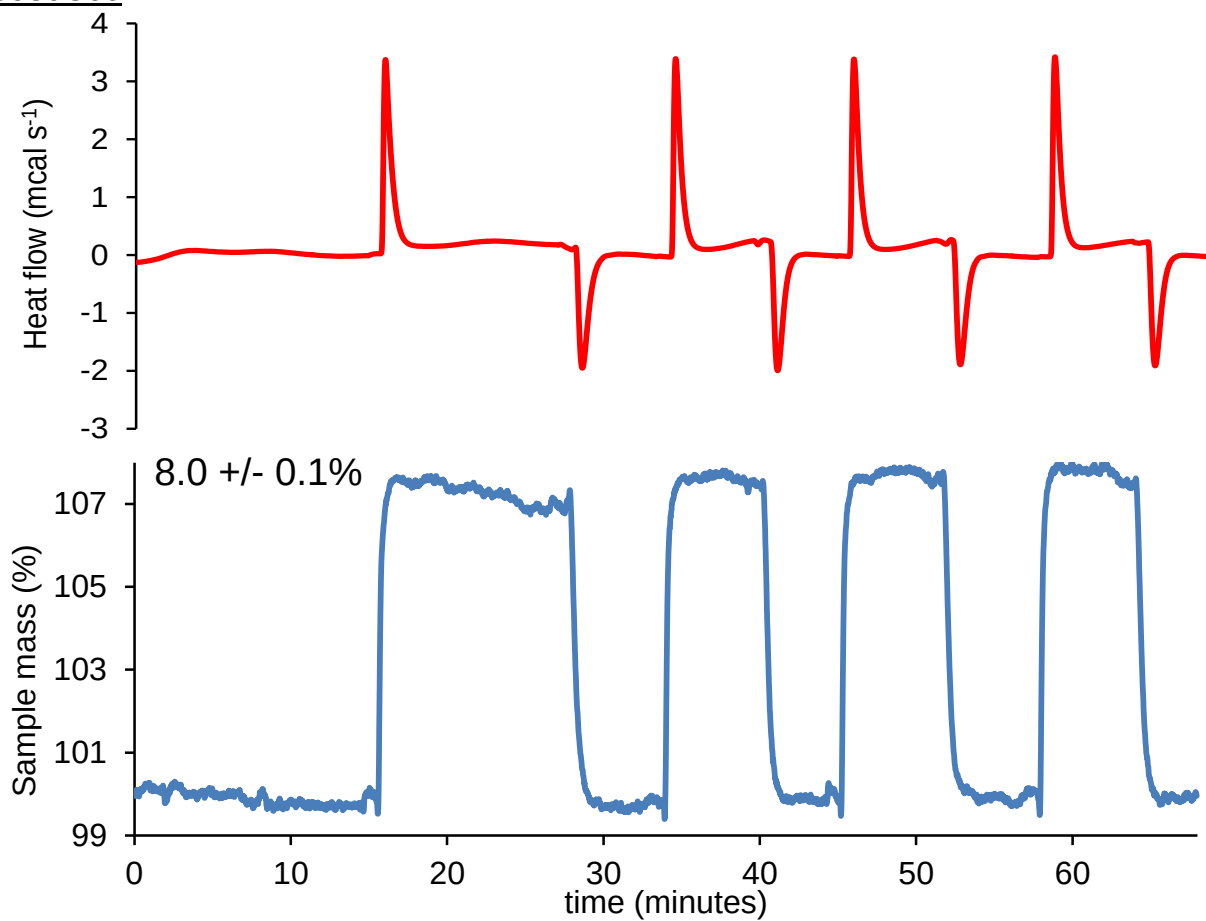


S900C120

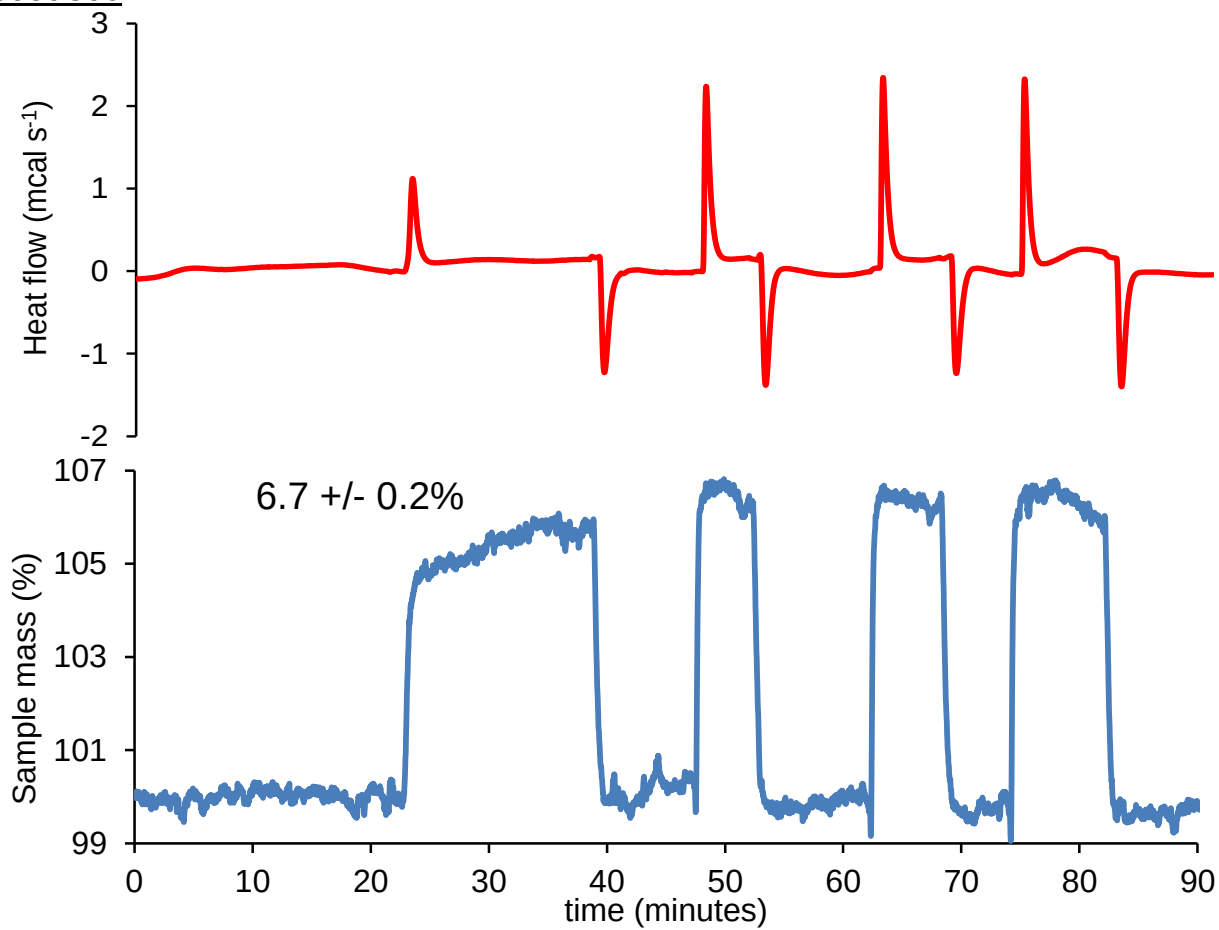




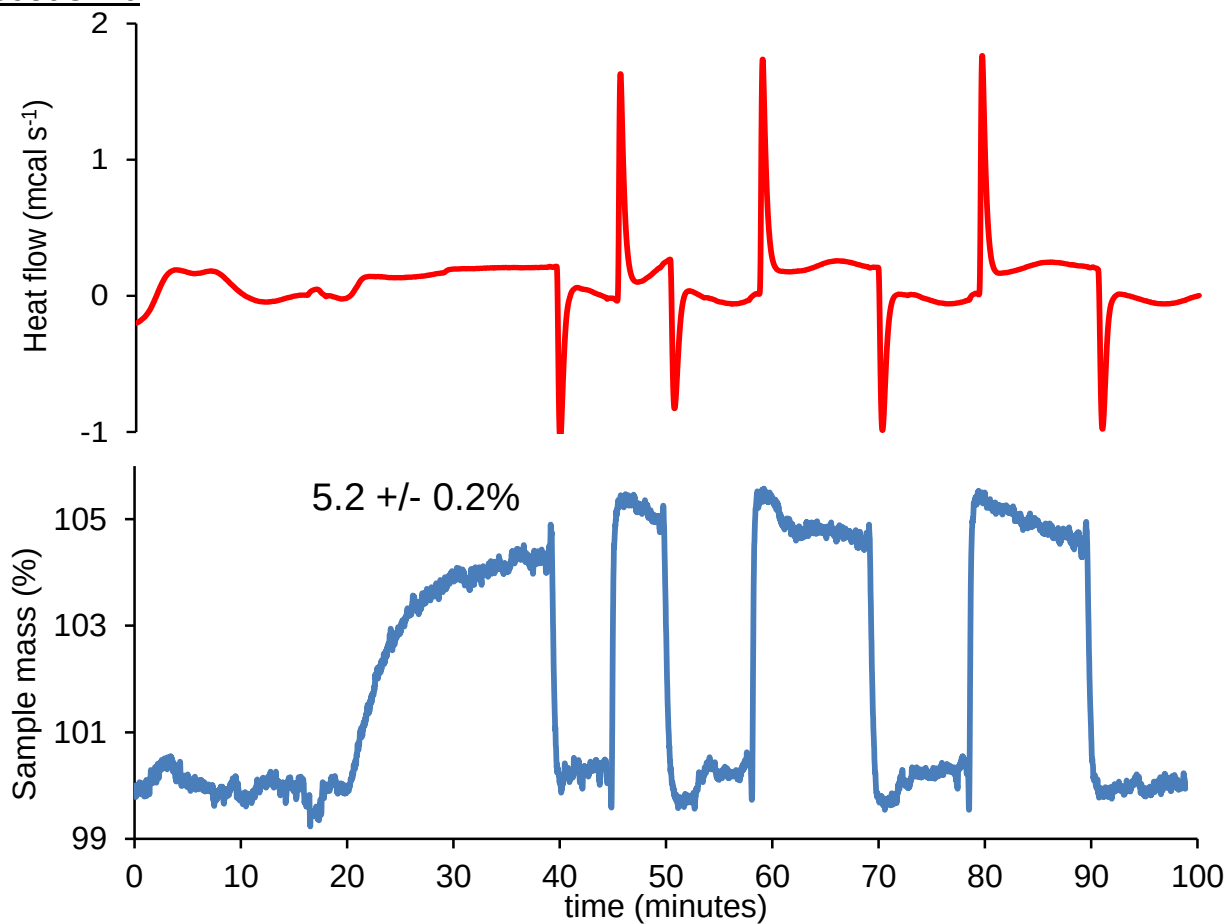
S950C60



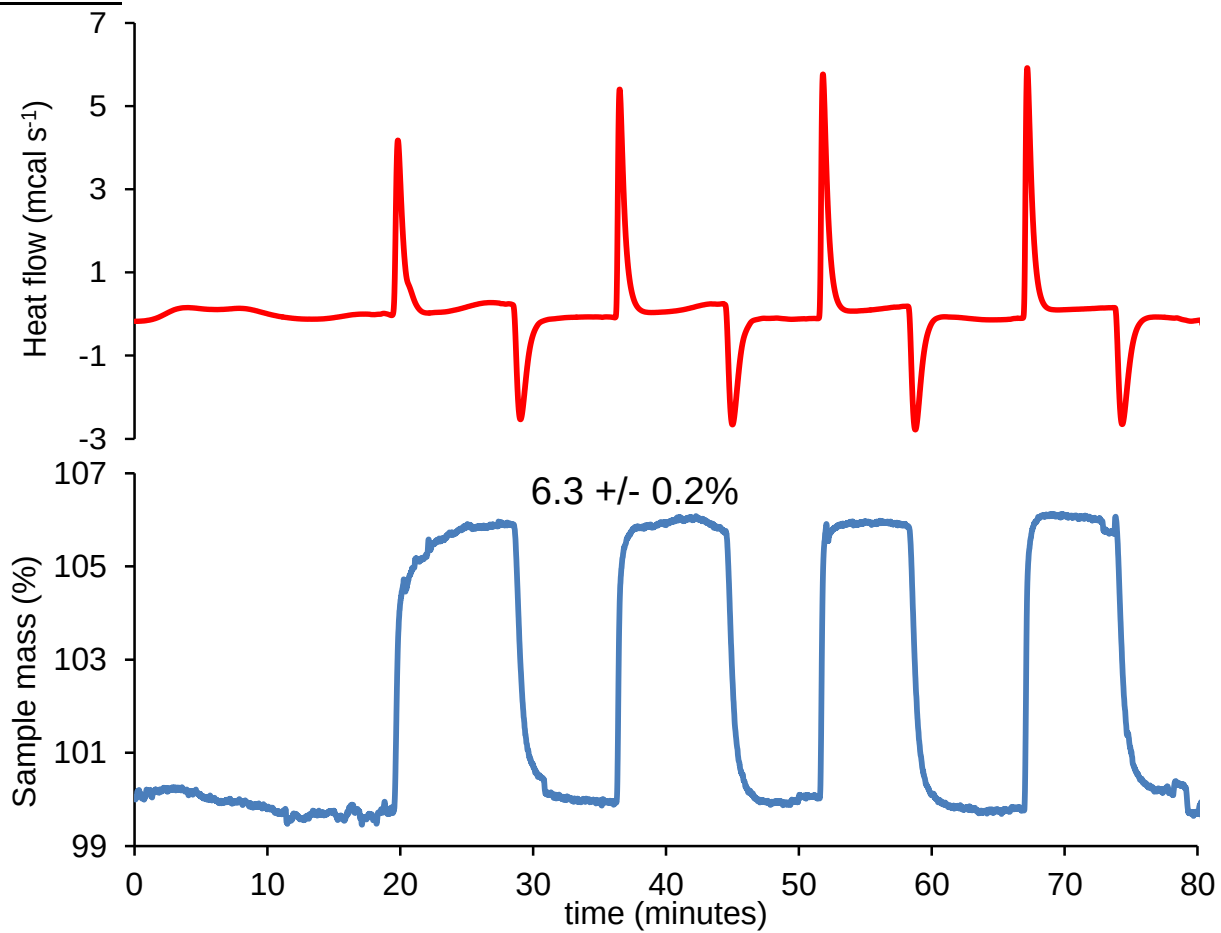
S950C90



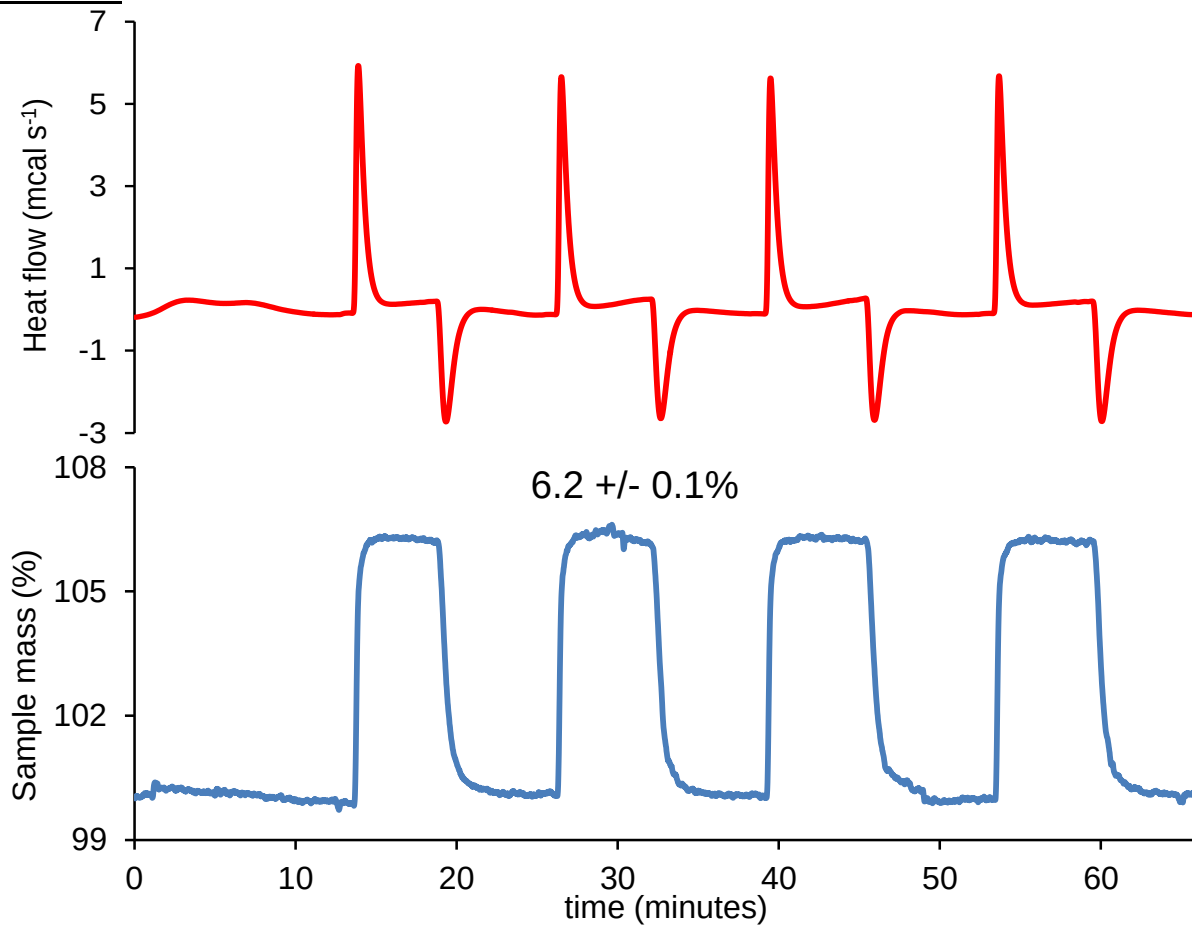
S950C120



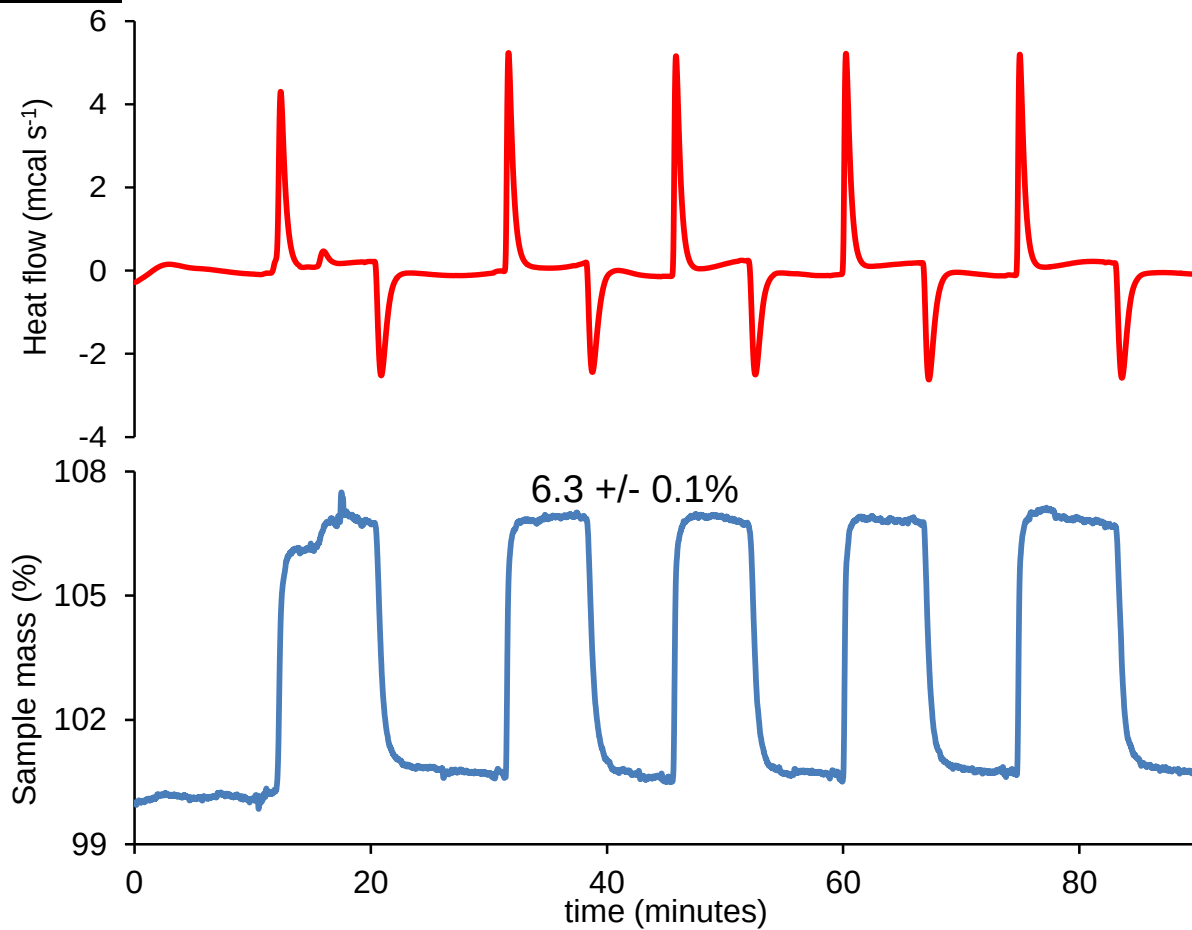
A750C45



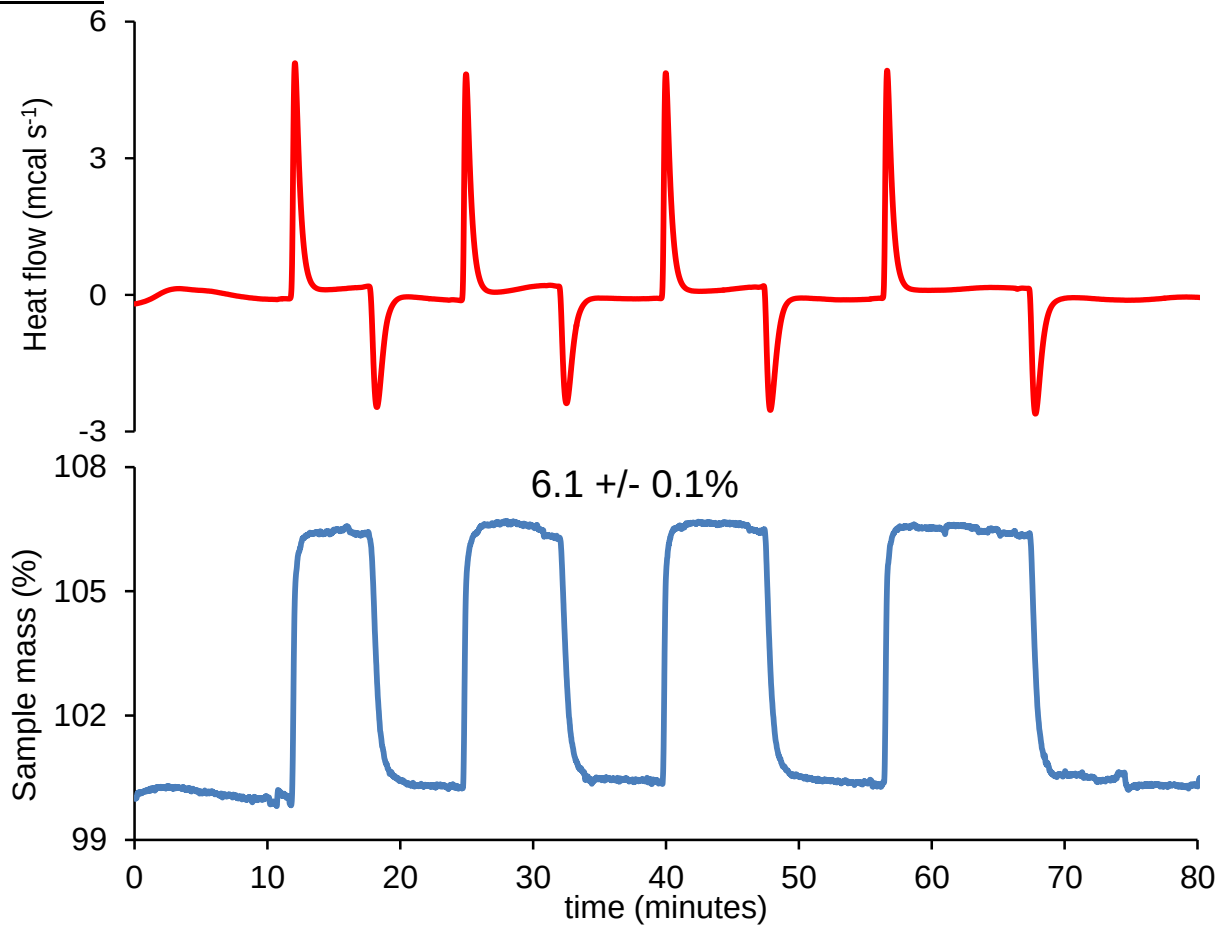
A750C60



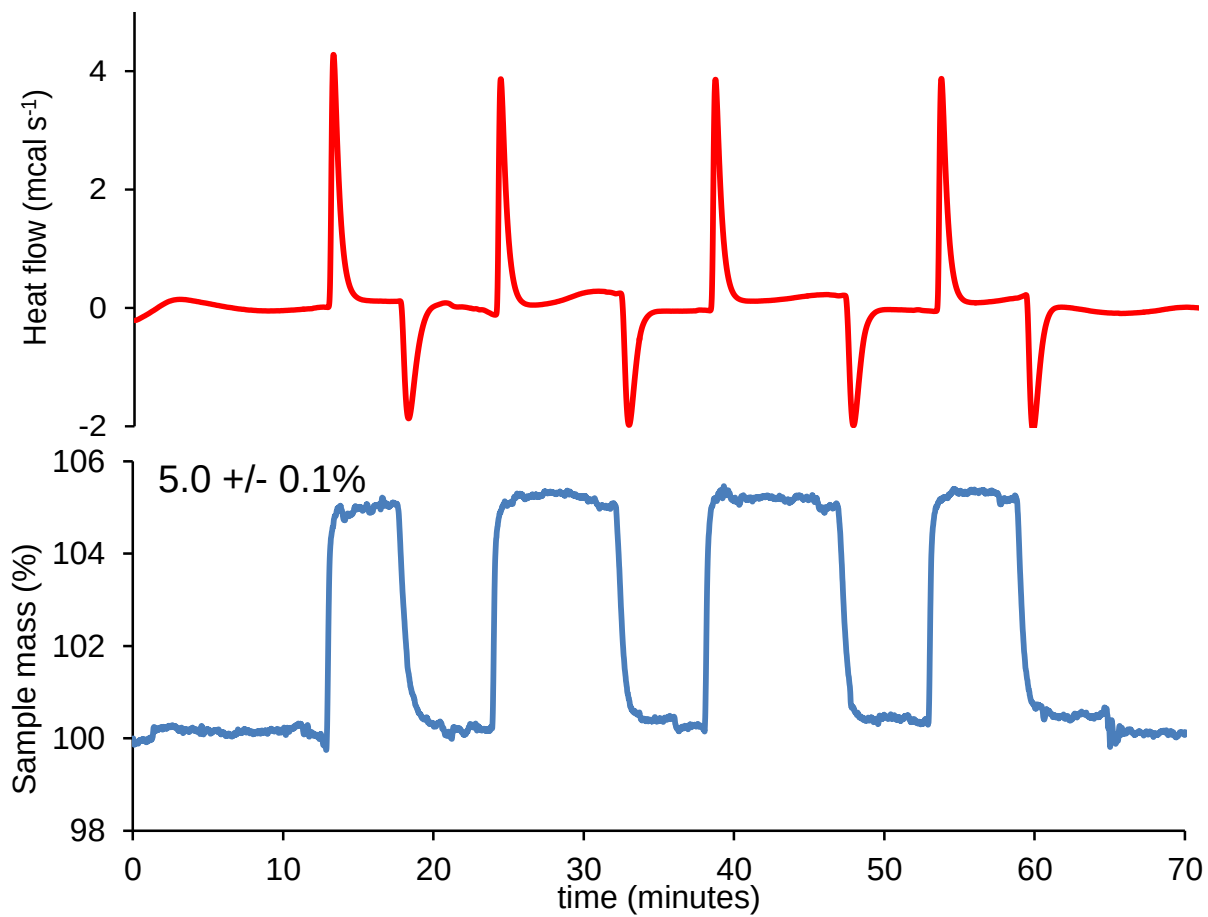
A750C90



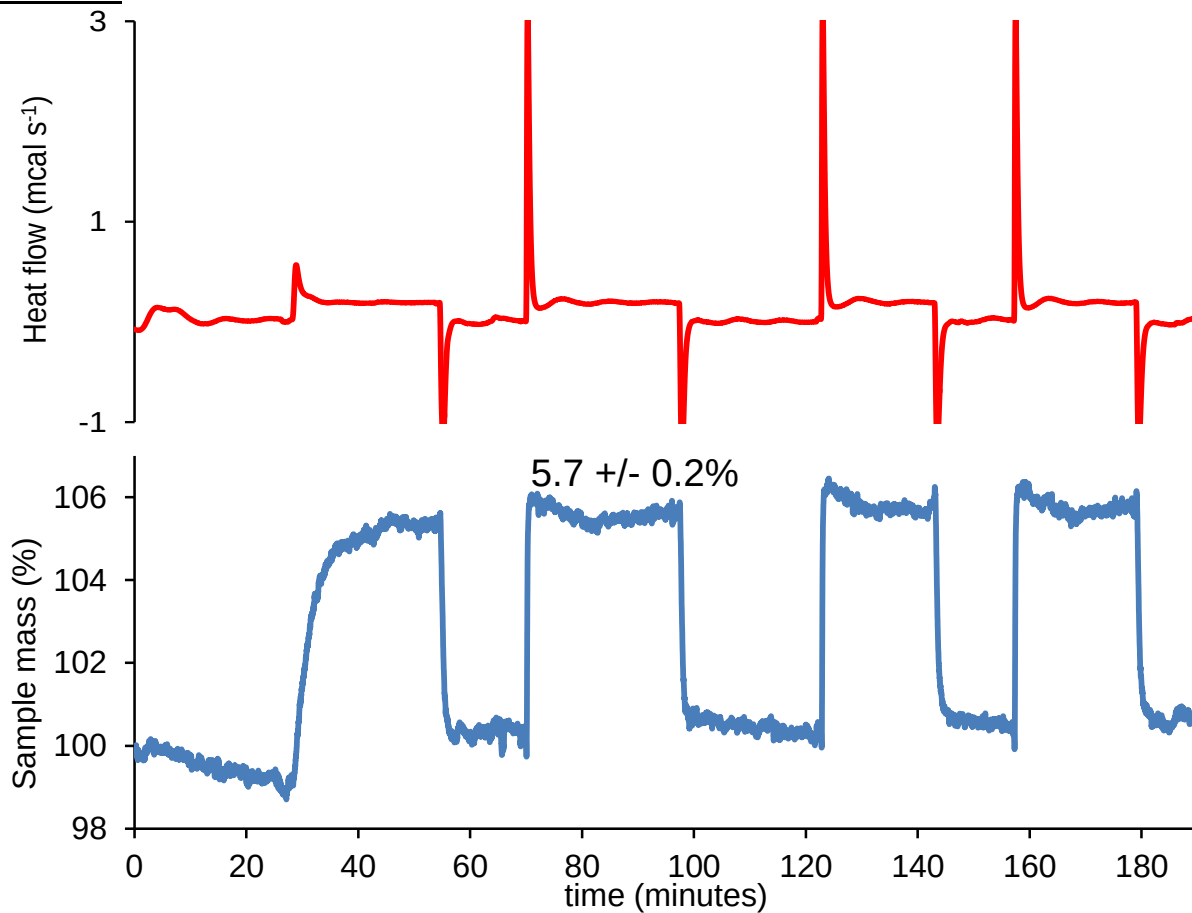
A900C0



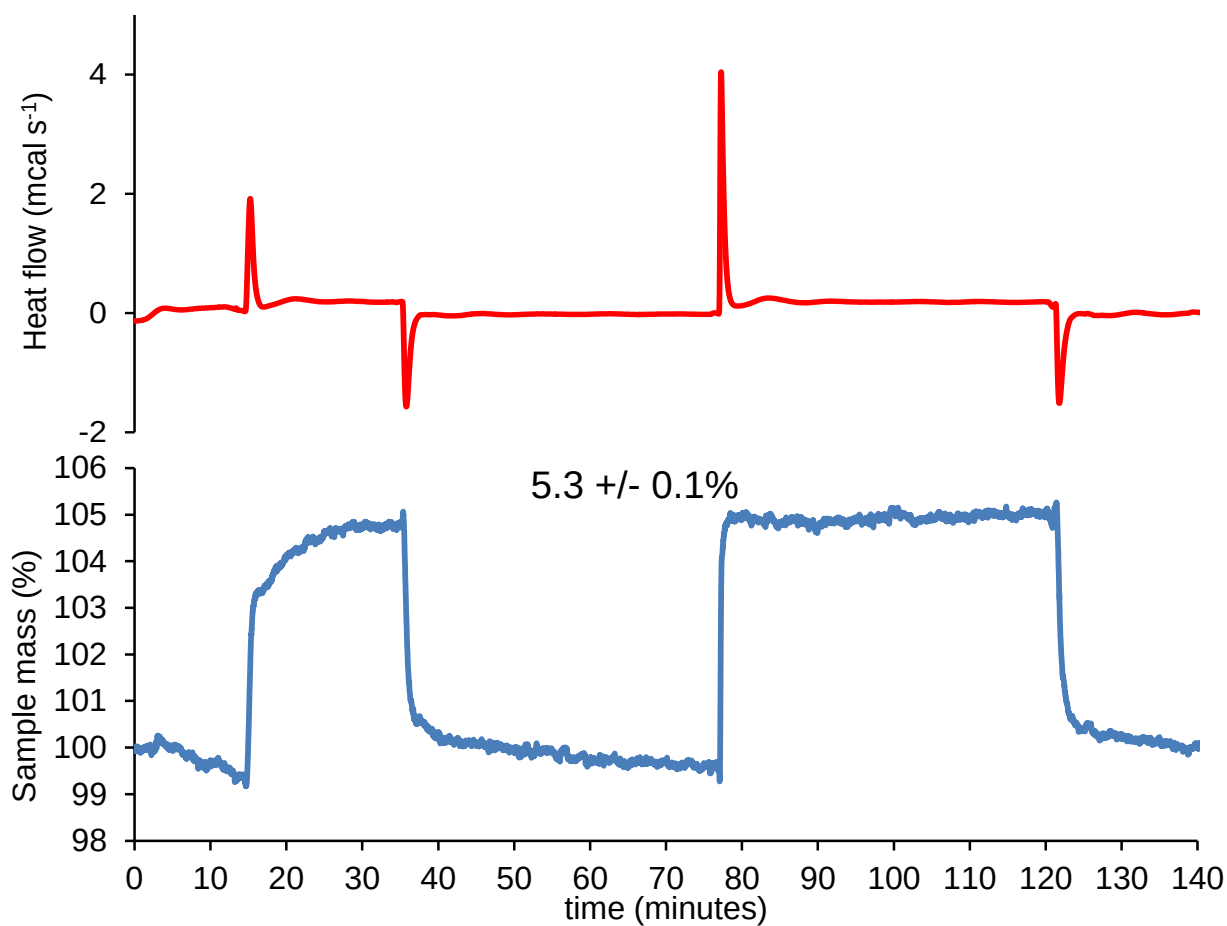
A900C10



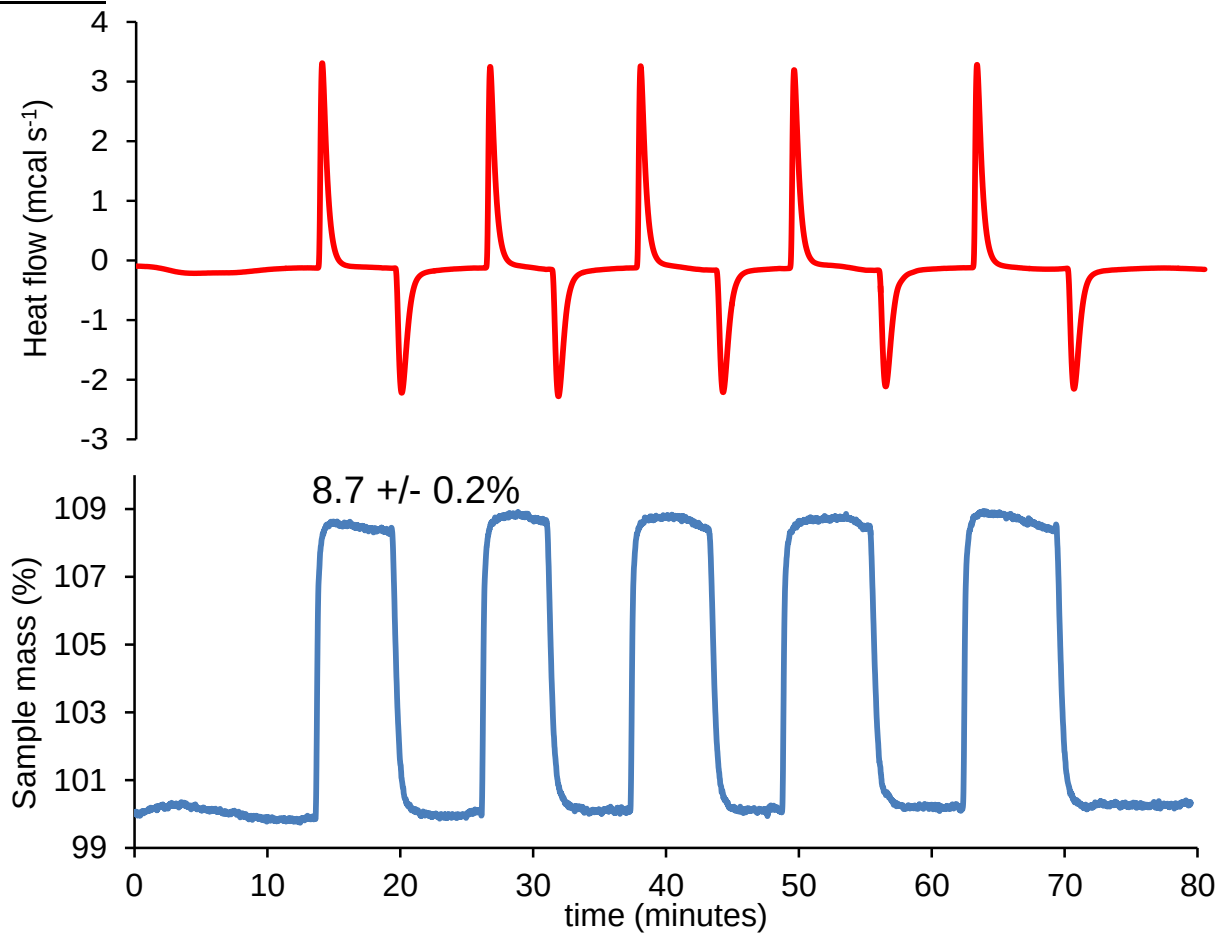
P700C50



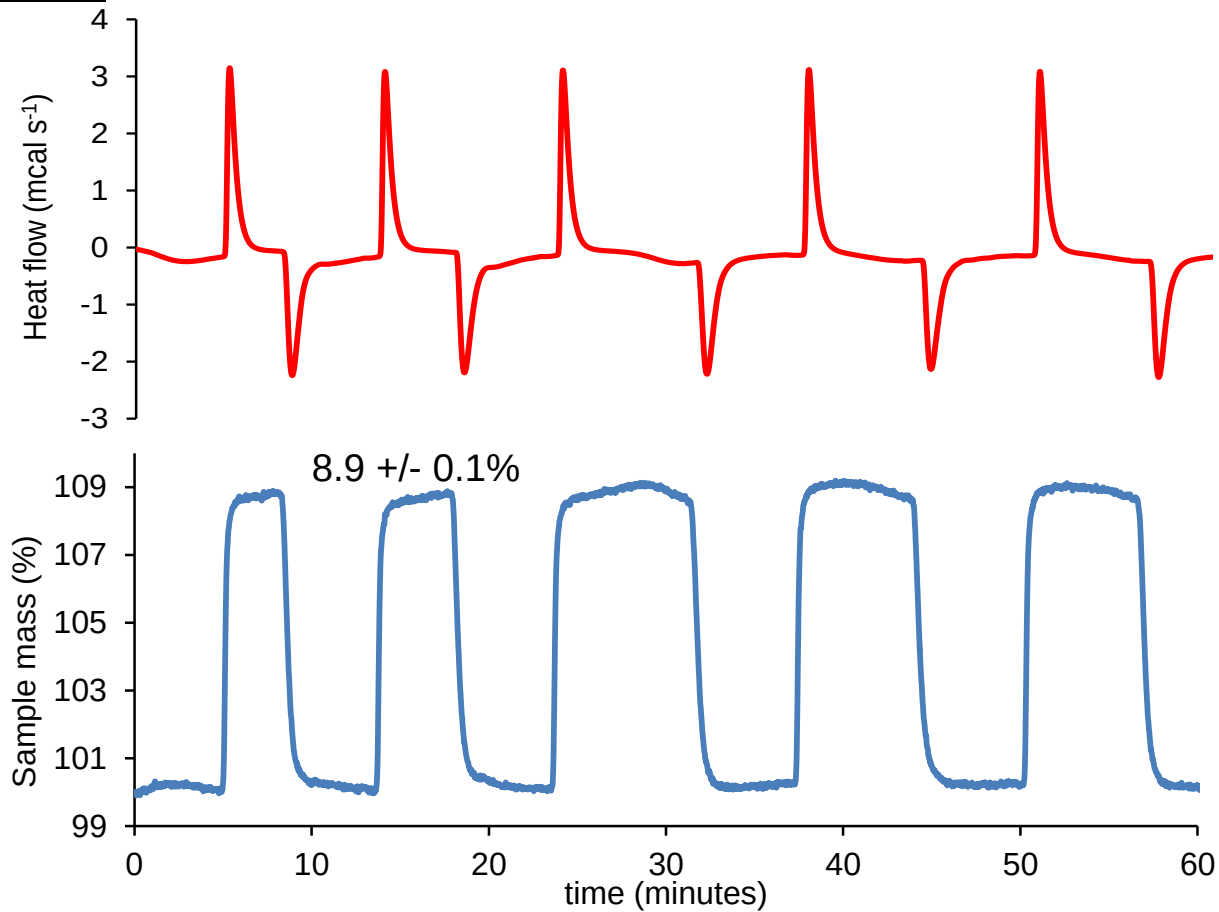
P900C0



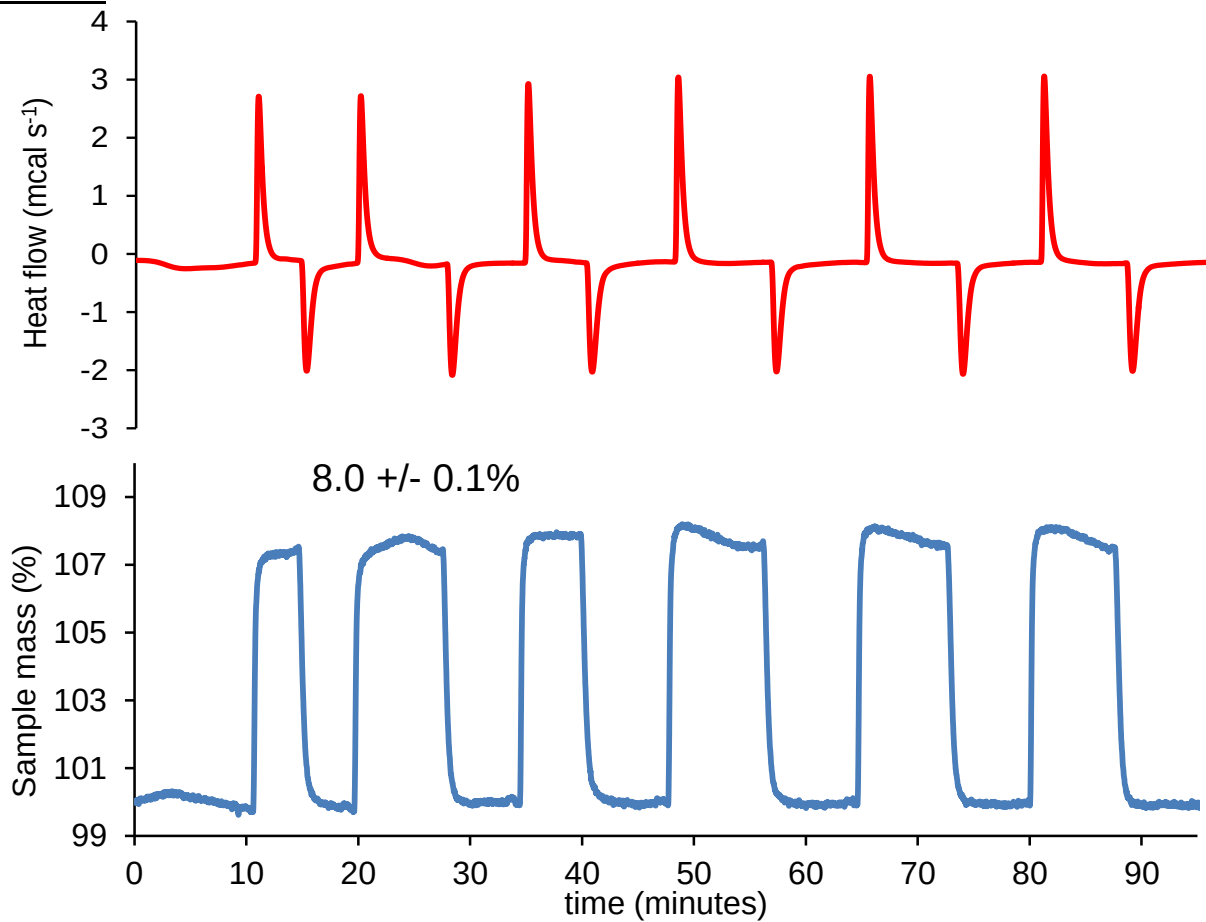
S70000



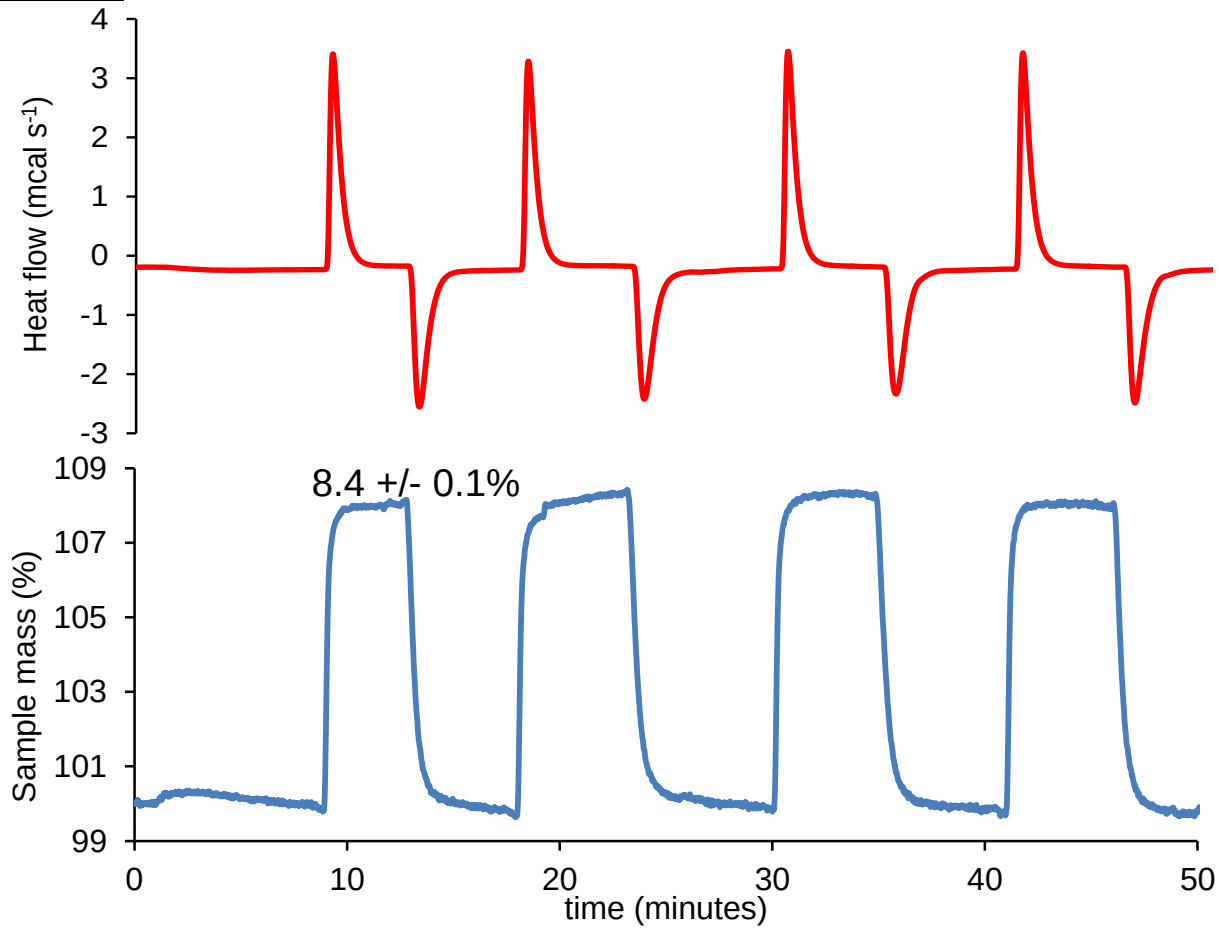
S75000



S80000

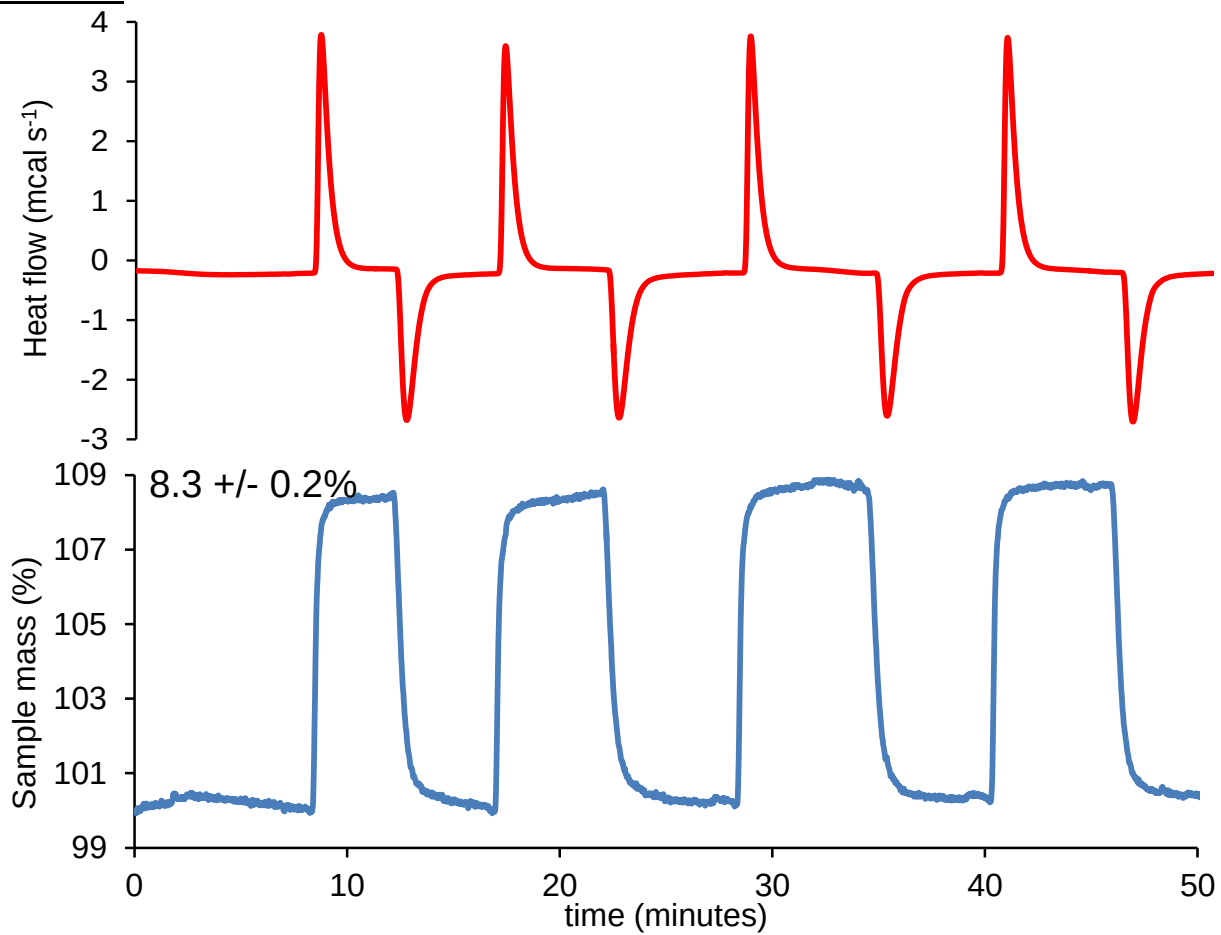


S750040

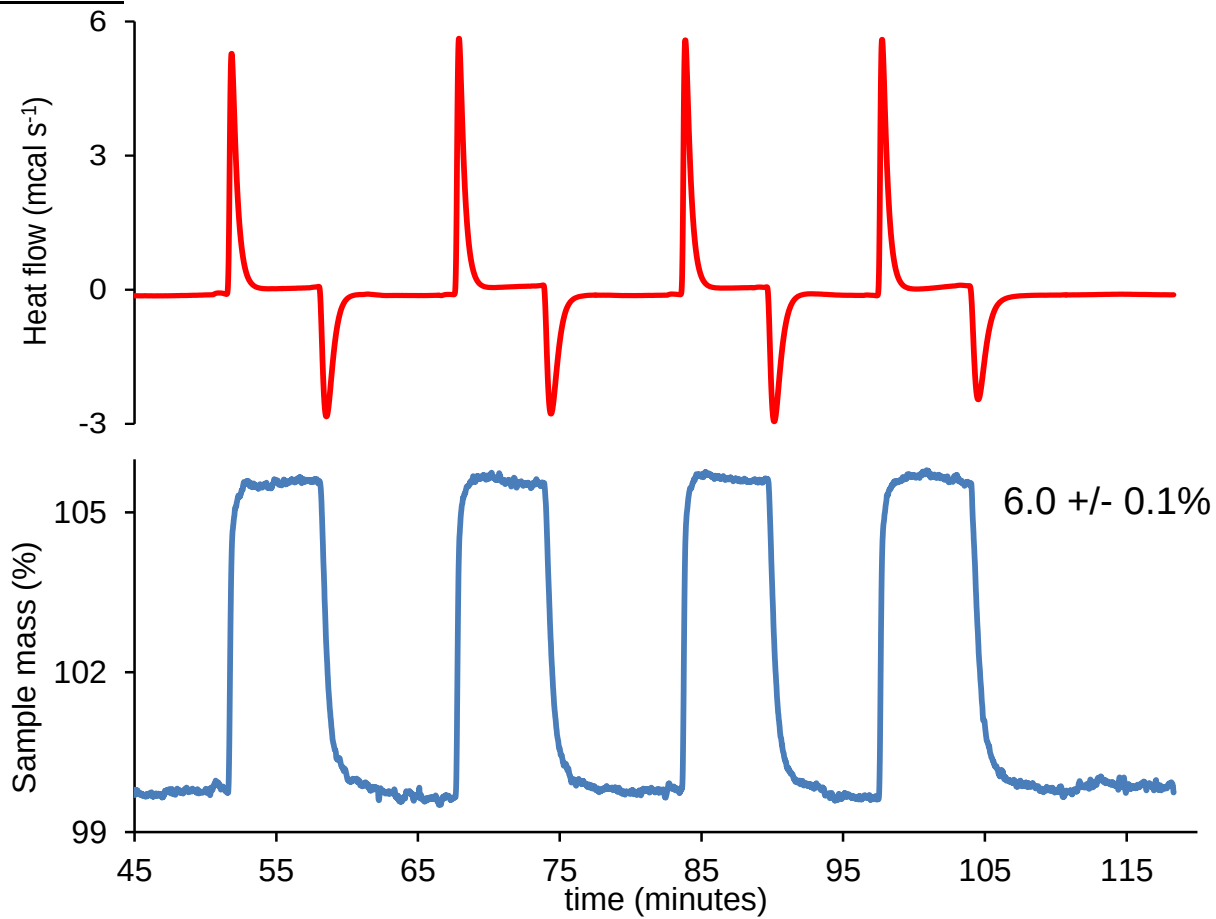




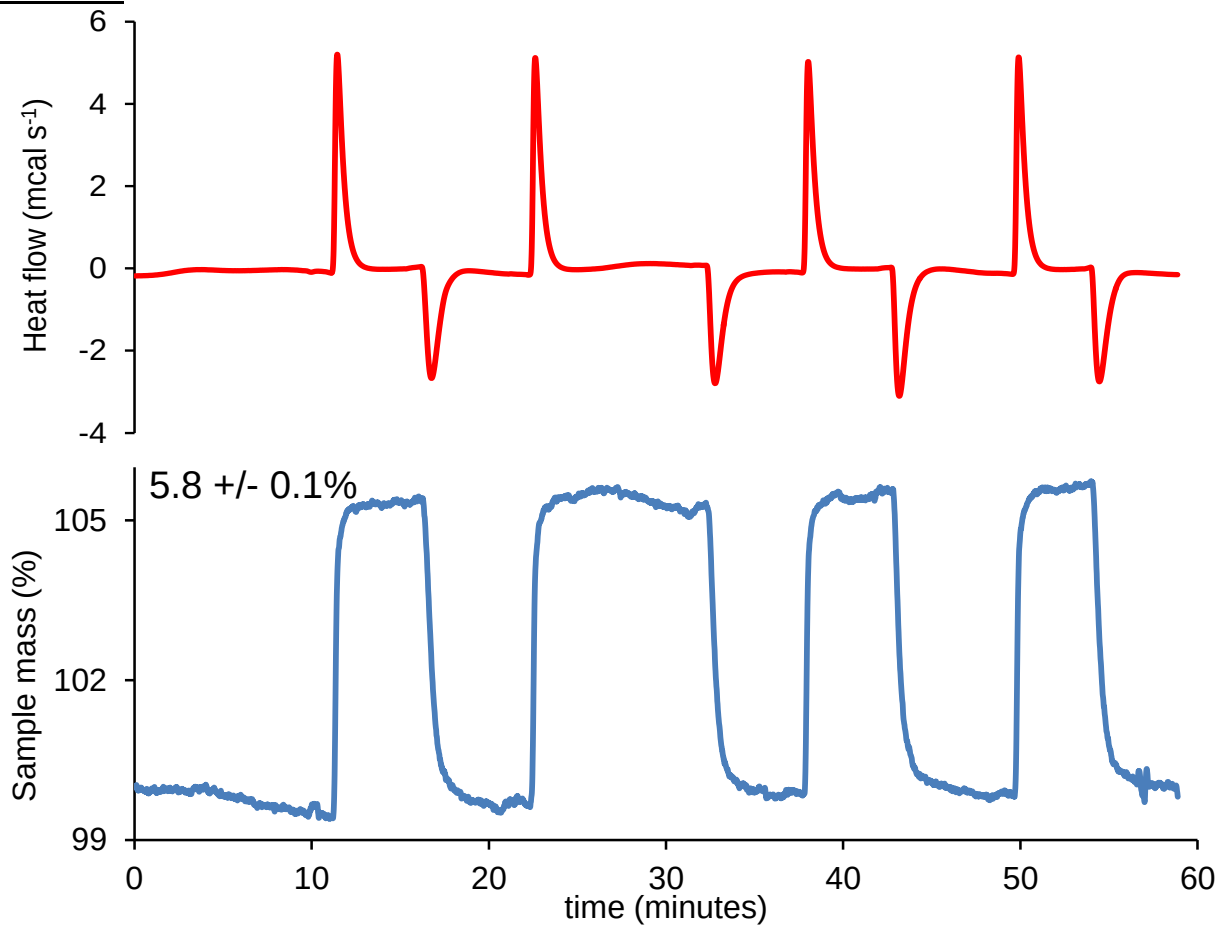
S750O56



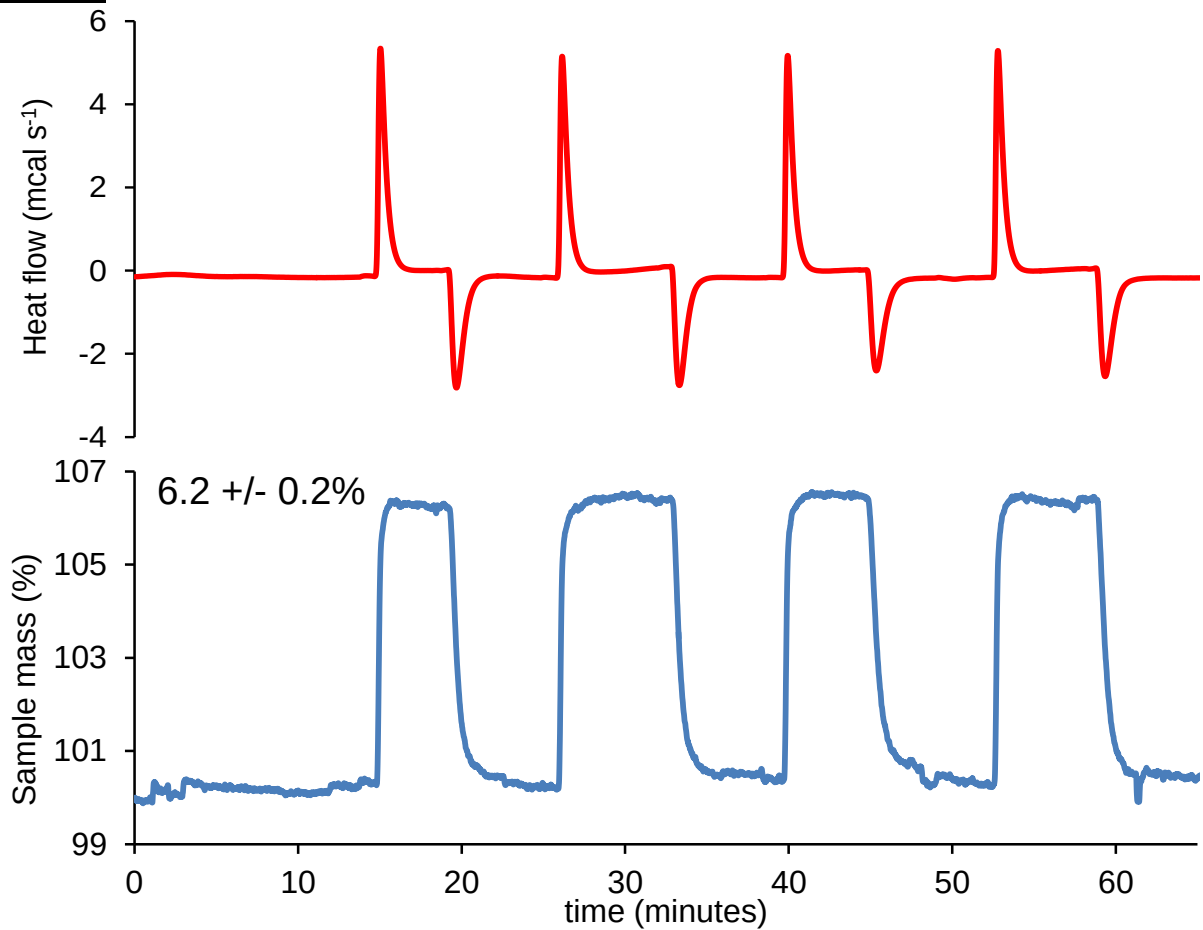
A500O30



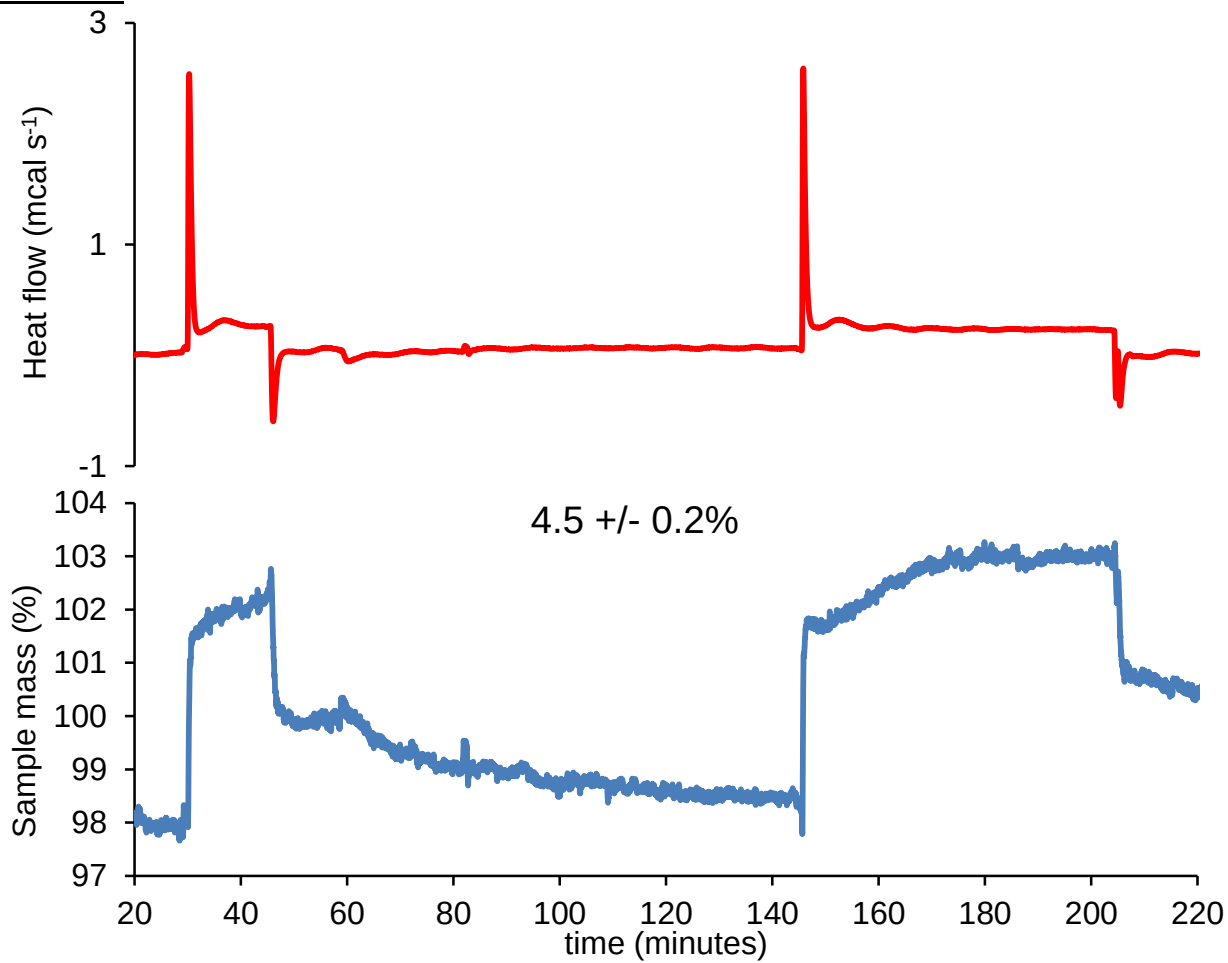
A500O60



A750O0



P400O50



**CO<sub>2</sub> adsorption capacities and heats of CO<sub>2</sub> adsorption at 35 °C**

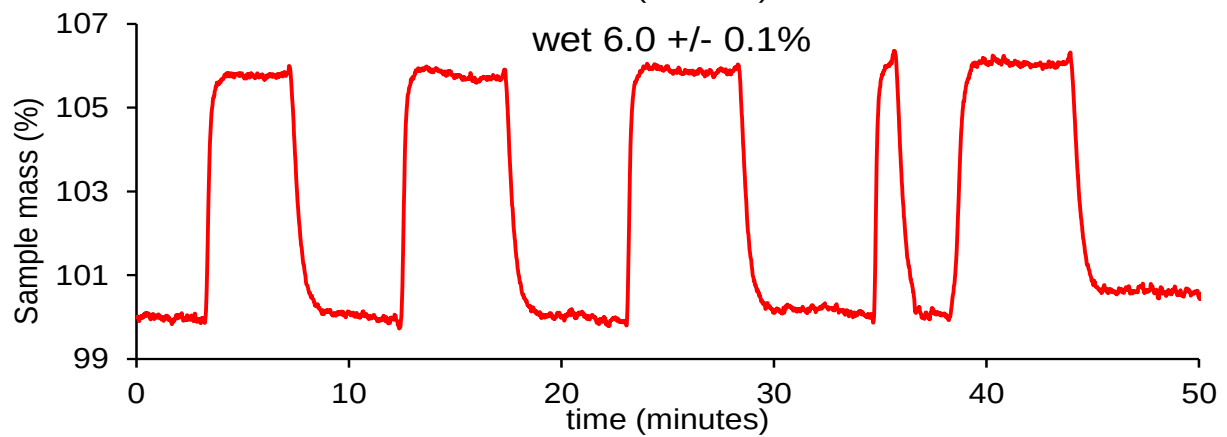
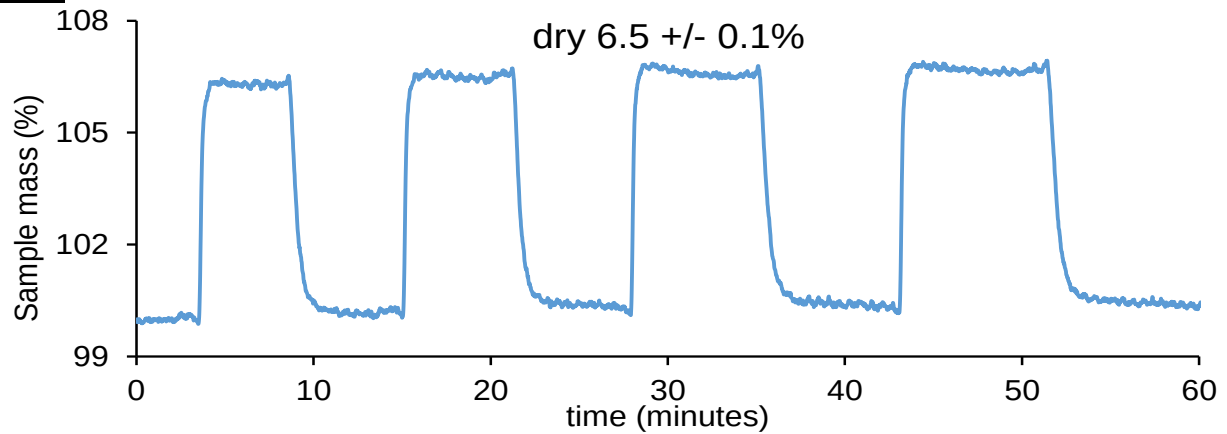
| Entry | Material            | CO <sub>2</sub> uptake (%) <sup>a</sup> | CO <sub>2</sub> uptake (mmol g <sup>-1</sup> ) <sup>a</sup> | ΔH <sub>ads</sub> (KJ mol <sup>-1</sup> ) <sup>a</sup> |
|-------|---------------------|-----------------------------------------|-------------------------------------------------------------|--------------------------------------------------------|
| 1     | AC <sup>b,c</sup>   | 1.8 ± 0.4                               | 0.41 ± 0.09                                                 | -27.3 ± 0.5                                            |
| 2     | S800SE <sup>c</sup> | 4.4 ± 0.3                               | 1.00 ± 0.07                                                 | -22.7 ± 0.7                                            |
| 3     | A800SE <sup>c</sup> | 3.4 ± 0.3                               | 0.77 ± 0.07                                                 | -27.2 ± 2.4                                            |
| 4     | S300                | 2.1 ± 0.1                               | 0.48 ± 0.02                                                 | -40.2 ± 4.8                                            |
| 5     | S600                | 4.7 ± 0.2                               | 1.07 ± 0.05                                                 | -42.4 ± 1.3                                            |
| 6     | S800                | 7.0 ± 0.1                               | 1.59 ± 0.02                                                 | -35.3 ± 1.9                                            |
| 7     | S1000               | 4.8 ± 0.1                               | 1.09 ± 0.02                                                 | -38.3 ± 1.7                                            |
| 8     | A800                | 6.0 ± 0.1                               | 1.36 ± 0.02                                                 | -48.6 ± 2.8                                            |
| 9     | P800                | 4.7 ± 0.1                               | 1.07 ± 0.02                                                 | -52.9 ± 1.3                                            |
| 10    | S800K1              | 10.5 ± 0.2                              | 2.39 ± 0.05                                                 | -31.7 ± 0.7                                            |
| 11    | S800K2              | 13.7 ± 0.2                              | 3.11 ± 0.05                                                 | -33.6 ± 0.8                                            |
| 12    | S800K3              | 12.9 ± 0.2                              | 2.93 ± 0.05                                                 | -32.7 ± 0.5                                            |
| 13    | S800K4              | 9.4 ± 0.2                               | 2.14 ± 0.05                                                 | -30.9 ± 0.4                                            |
| 14    | S800K5              | 9.1 ± 0.3                               | 2.07 ± 0.07                                                 | -26.7 ± 1.0                                            |
| 15    | S600K4              | 8.9 ± 0.1                               | 2.02 ± 0.02                                                 | -29.1 ± 0.3                                            |
| 16    | S1000K4             | 4.9 ± 0.2                               | 1.11 ± 0.05                                                 | -34.5 ± 0.8                                            |
| 17    | A800K1              | 8.7 ± 0.1                               | 1.98 ± 0.02                                                 | -38.0 ± 1.1                                            |
| 18    | A800K2              | 13.0 ± 0.1                              | 2.95 ± 0.02                                                 | -38.6 ± 0.9                                            |
| 19    | A800K3              | 12.4 ± 0.1                              | 2.82 ± 0.02                                                 | -36.1 ± 0.9                                            |
| 20    | A800K4              | 9.9 ± 0.2                               | 2.25 ± 0.05                                                 | -33.3 ± 1.5                                            |
| 21    | A800K5              | 7.7 ± 0.2                               | 1.75 ± 0.05                                                 | -38.2 ± 2.4                                            |
| 22    | A600K2              | 6.3 ± 0.1                               | 1.64 ± 0.02                                                 | -46.0 ± 2.5                                            |
| 23    | A1000K2             | 9.5 ± 0.1                               | 2.16 ± 0.02                                                 | -38.5 ± 1.1                                            |
| 24    | P800K2              | 10.5 ± 0.1                              | 2.39 ± 0.02                                                 | -36.9 ± 0.4                                            |
| 25    | P800K3              | 9.1 ± 0.1                               | 2.07 ± 0.02                                                 | -35.1 ± 0.3                                            |
| 26    | P800K5              | 5.5 ± 0.1                               | 1.25 ± 0.02                                                 | -37.6 ± 1.4                                            |
| 27    | S800C15             | 7.2 ± 0.2                               | 1.64 ± 0.05                                                 | -25.0 ± 5.1                                            |
| 28    | S850C15             | 7.8 ± 0.1                               | 1.77 ± 0.02                                                 | -36.3 ± 2.0                                            |
| 29    | S900C15             | 8.7 ± 0.2                               | 1.98 ± 0.05                                                 | -35.8 ± 0.4                                            |
| 30    | S950C15             | 8.0 ± 0.1                               | 1.82 ± 0.02                                                 | -34.9 ± 0.4                                            |
| 31    | S1000C15            | 7.8 ± 0.3                               | 1.77 ± 0.07                                                 | -40.2 ± 2.7                                            |
| 32    | S900C30             | 7.8 ± 0.1                               | 1.77 ± 0.02                                                 | -31.9 ± 1.0                                            |
| 33    | S900C60             | 8.7 ± 0.1                               | 1.98 ± 0.02                                                 | -36.4 ± 3.5                                            |
| 34    | S900C90             | 8.4 ± 0.2                               | 1.91 ± 0.05                                                 | -37.4 ± 2.7                                            |
| 35    | S900C120            | 8.3 ± 0.1                               | 1.89 ± 0.02                                                 | -35.9 ± 3.2                                            |
| 36    | S950C60             | 8.0 ± 0.1                               | 1.82 ± 0.02                                                 | -42.7 ± 2.9                                            |
| 37    | S950C90             | 6.7 ± 0.2                               | 1.52 ± 0.05                                                 | -46.7 ± 4.4                                            |
| 38    | S950C120            | 5.2 ± 0.2                               | 1.18 ± 0.05                                                 | -53.7 ± 4.7                                            |

| Entry | Material | CO <sub>2</sub> uptake (%) | CO <sub>2</sub> uptake (mmol g <sup>-1</sup> ) | ΔH <sub>ads</sub> (KJ mol <sup>-1</sup> ) |
|-------|----------|----------------------------|------------------------------------------------|-------------------------------------------|
| 39    | A750C45  | 6.3 ± 0.2                  | 1.43 ± 0.05                                    | -45.7 ± 2.0                               |
| 40    | A750C60  | 6.2 ± 0.1                  | 1.41 ± 0.02                                    | -47.5 ± 1.4                               |
| 41    | A750C90  | 6.3 ± 0.1                  | 1.43 ± 0.02                                    | -43.7 ± 1.8                               |
| 42    | A900C0   | 6.1 ± 0.1                  | 1.39 ± 0.02                                    | -46.4 ± 2.0                               |
| 43    | A900C10  | 5.0 ± 0.1                  | 1.14 ± 0.02                                    | -48.2 ± 4.5                               |
| 44    | P700C50  | 5.7 ± 0.1                  | 1.30 ± 0.02                                    | -68.5 ± 2.2                               |
| 45    | P900C0   | 5.3 ± 0.1                  | 1.20 ± 0.02                                    | -69.0 ± 7.1                               |
| 46    | S700O0   | 8.7 ± 0.2                  | 1.98 ± 0.05                                    | -32.2 ± 0.1                               |
| 47    | S750O0   | 8.9 ± 0.1                  | 2.02 ± 0.02                                    | -34.6 ± 0.9                               |
| 48    | S800O0   | 8.0 ± 0.1                  | 1.82 ± 0.02                                    | -30.0 ± 1.1                               |
| 49    | S750O40  | 8.4 ± 0.1                  | 1.91 ± 0.02                                    | -30.8 ± 0.5                               |
| 50    | S750O56  | 8.3 ± 0.2                  | 1.89 ± 0.05                                    | -36.7 ± 0.9                               |
| 51    | A500O30  | 6.0 ± 0.1                  | 1.36 ± 0.02                                    | -47.0 ± 1.4                               |
| 52    | A500O60  | 5.8 ± 0.1                  | 1.32 ± 0.02                                    | -46.3 ± 1.2                               |
| 53    | A750O0   | 6.2 ± 0.2                  | 1.41 ± 0.05                                    | -30.6 ± 1.4                               |
| 54    | P400O50  | 4.5 ± 0.2                  | 1.02 ± 0.05                                    | -73.5 ± 1.0                               |

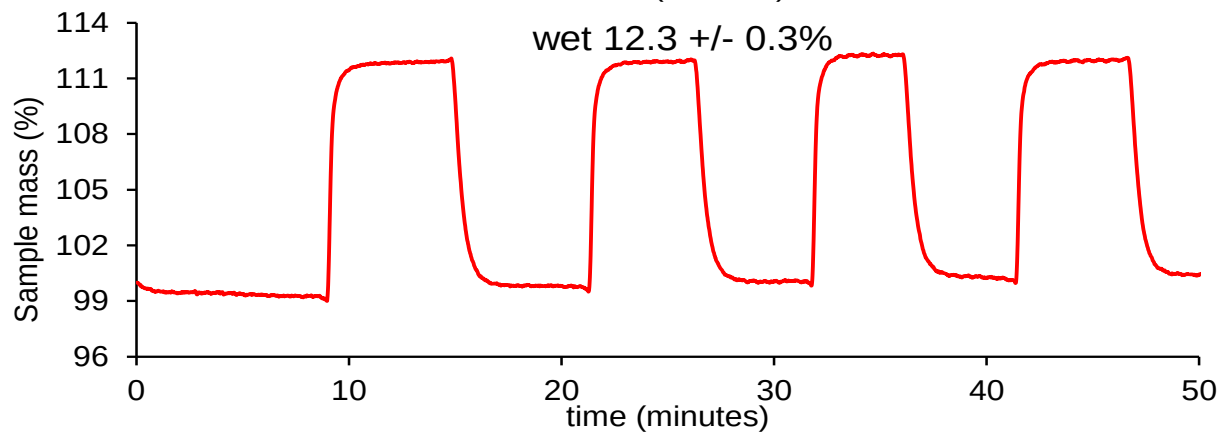
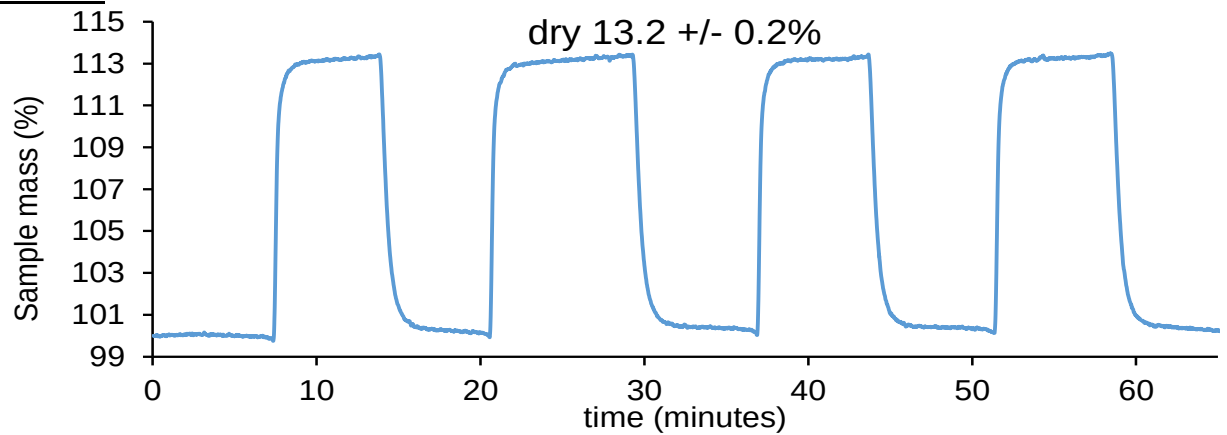
a) Measured at 1 bar pressure during gas composition swing between pure nitrogen and pure carbon dioxide. Each value is the mean ± one standard deviation. b) AC = Norit activated carbon. c) Materials prepared by the older solvent exchange method and data taken from: G. Dura, V. L. Budarin, J. A. Castro-Osma, P. S. Shuttleworth, S. C. Z. Quek, J. H. Clark and M. North, *Angew. Chem. Int. Ed.* 2016, **55**, 9173–9177.

## Influence of water on CO<sub>2</sub> adsorption at 1 bar pressure

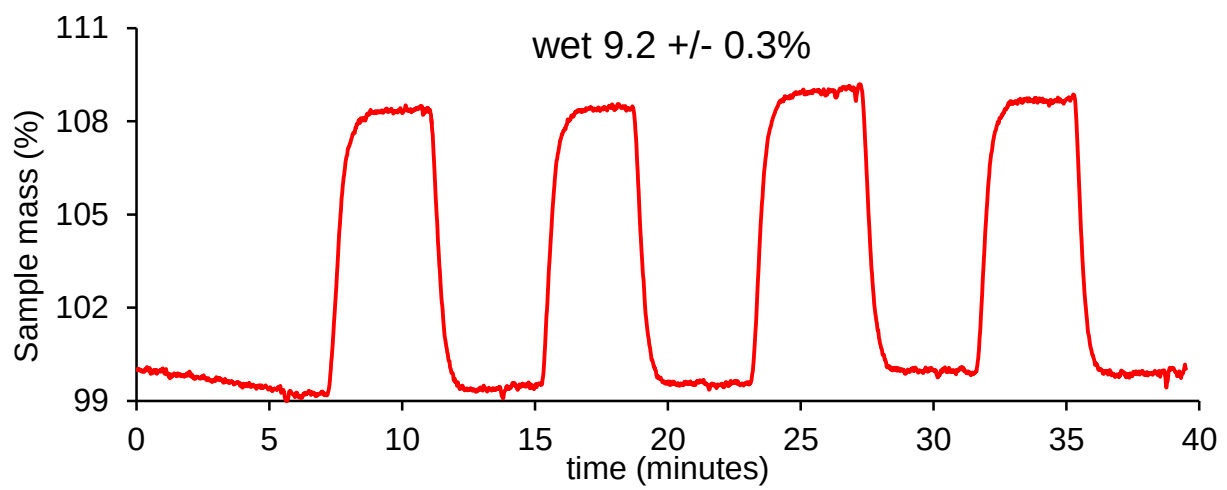
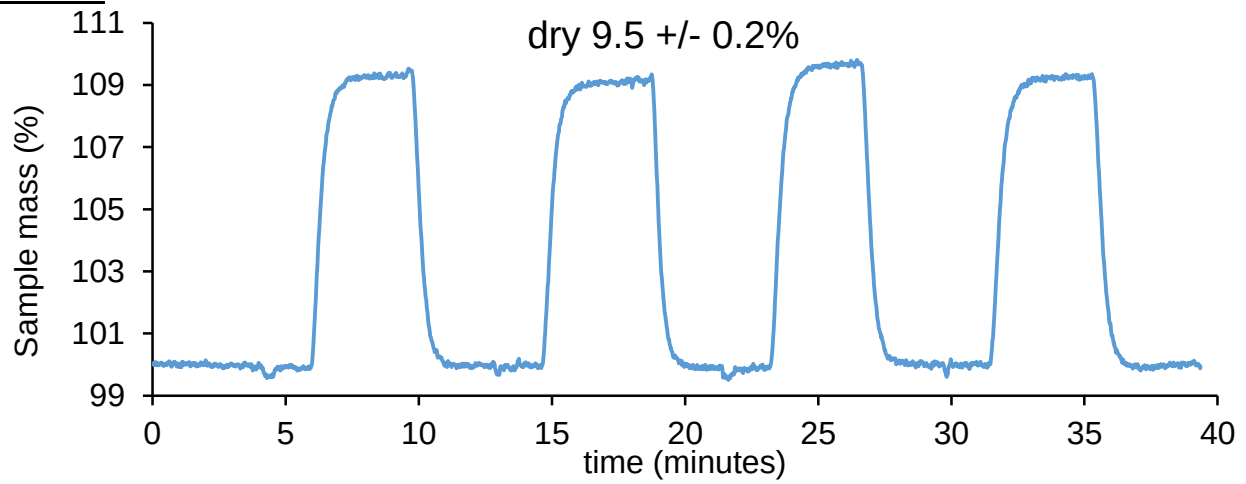
S800



S800K2



S800K5





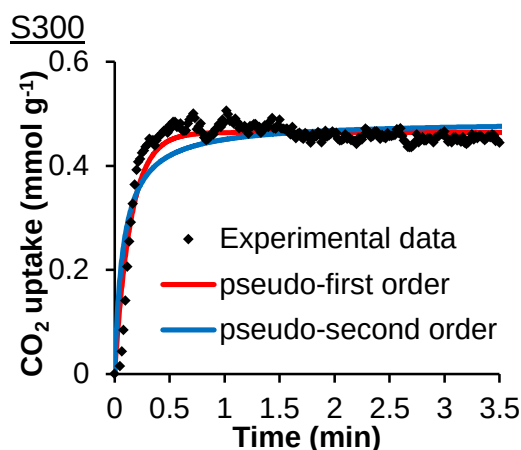
## Kinetics of CO<sub>2</sub> adsorption at 1 bar and 35 °C

The pseudo-first order plot is obtained by plotting  $q_t = q_e(1 - e^{-K_1 t})$ .

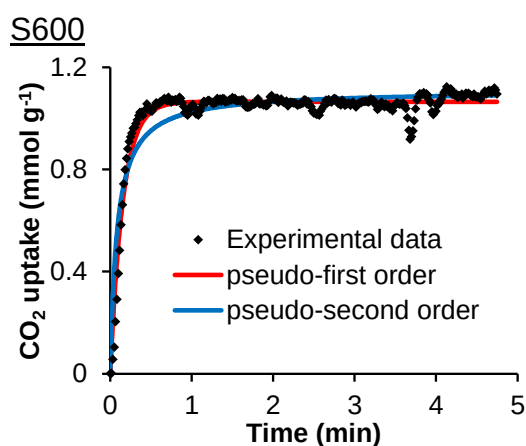
The pseudo-second order plot is obtained by plotting  $q_t = K_2 q_e^2 t / (1 + K_2 q_e t)$

The Sum of Squared Errors (SSE) is calculated as  $\sum [(q_{t,exp} - q_{t,cal})]^2$

where  $q_t$  is the amount of CO<sub>2</sub> adsorbed at time  $t$ ;  $q_e$  is the amount of CO<sub>2</sub> adsorbed at equilibrium; and  $K_1$  (min<sup>-1</sup>) and  $K_2$  (g mmol<sup>-1</sup> min<sup>-1</sup>) are the first and second order rate constants.  $q_{t,exp}$  and  $q_{t,cal}$  are the experimental and calculated adsorption capacity. The experimental and modelled plots and the best fit parameters are below. A higher value of linear regression correlation coefficient ( $R^2$ ) and a lower value of SSE represent a goodness of fit.

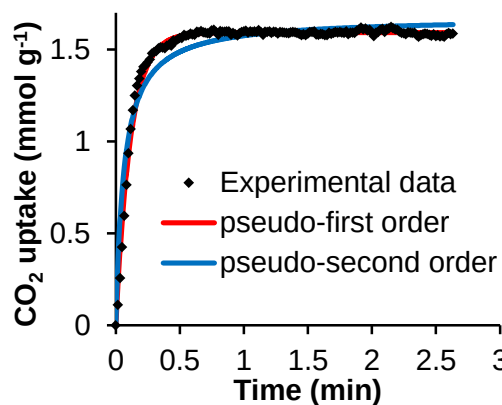


| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 0.44                                         | 6.81                                            | 0.46                                          | 0.91  | 0.13 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 0.44                                         | 25.75                                           | 0.49                                          | 0.78  | 0.31 |



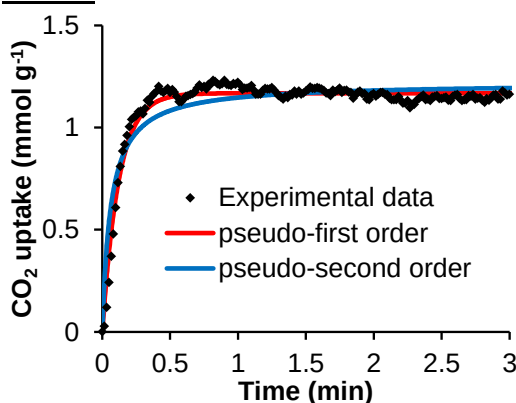
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.07                                         | 6.55                                            | 1.07                                          | 0.94  | 0.40 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.07                                         | 10.90                                           | 1.11                                          | 0.86  | 0.99 |

S800



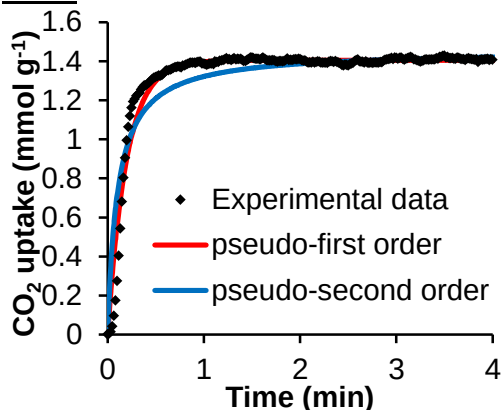
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.62                                         | 8.85                                            | 1.59                                          | 0.99  | 1.99 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.62                                         | 9.50                                            | 1.67                                          | 0.93  | 8.67 |

S1000



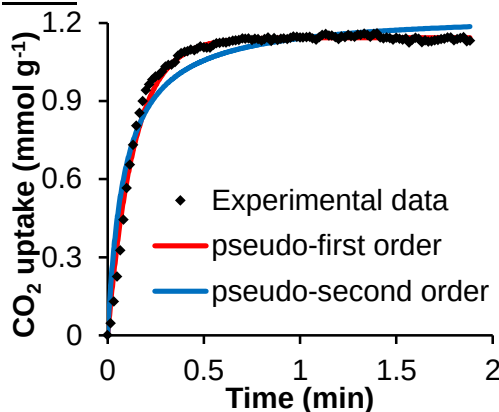
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.09                                         | 8.32                                            | 1.17                                          | 0.96  | 0.26 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.09                                         | 13.13                                           | 1.21                                          | 0.86  | 0.91 |

A800



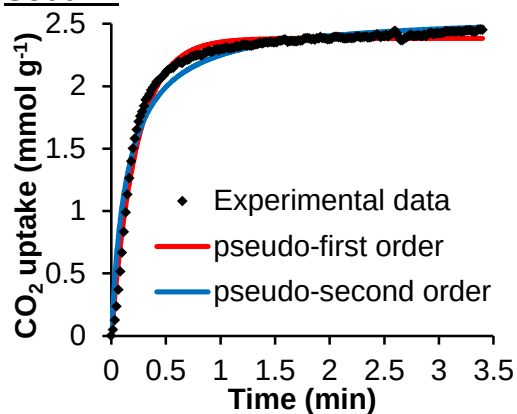
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.36                                         | 5.16                                            | 1.41                                          | 0.95  | 0.70 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.36                                         | 6.66                                            | 1.46                                          | 0.86  | 2.08 |

P800



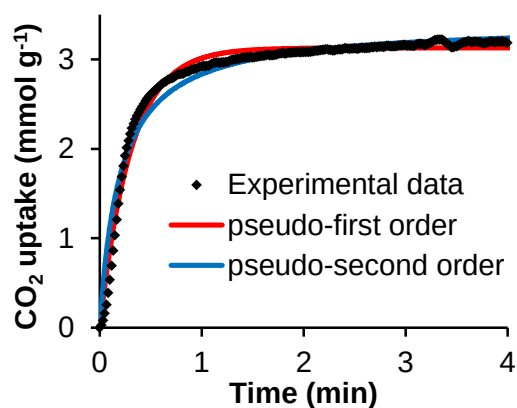
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.07                                         | 7.33                                            | 1.14                                          | 0.99  | 0.08 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.07                                         | 9.21                                            | 1.24                                          | 0.94  | 0.37 |

S800K1



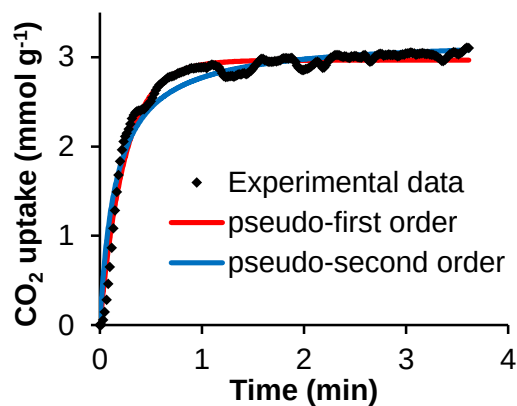
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.4                                          | 4.36                                            | 2.38                                          | 0.98  | 0.66 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.4                                          | 2.63                                            | 2.58                                          | 0.96  | 1.60 |

S800K2



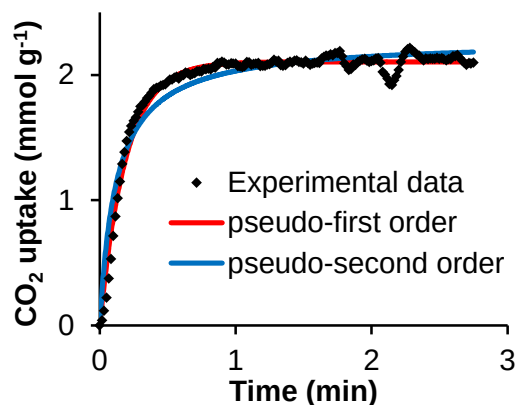
| Pseudo-first order model                     |                                                 |                                               |       |       |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|-------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE   |
| 3.22                                         | 3.30                                            | 3.13                                          | 0.98  | 3.24  |
| Pseudo-second order model                    |                                                 |                                               |       |       |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE   |
| 3.22                                         | 1.48                                            | 3.40                                          | 0.96  | 12.11 |

S800K3



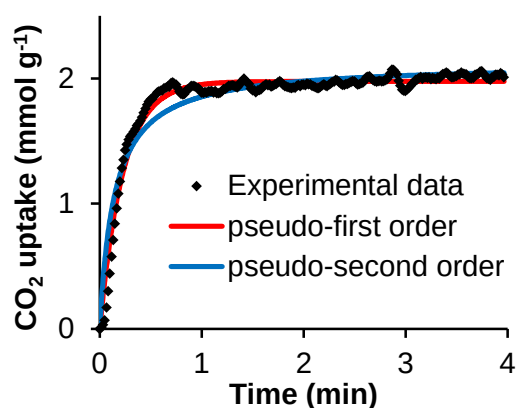
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.93                                         | 4.05                                            | 2.97                                          | 0.97  | 2.11 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.93                                         | 1.93                                            | 3.22                                          | 0.94  | 3.86 |

S800K4



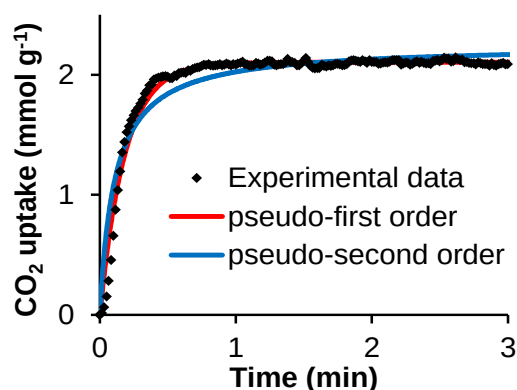
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.14                                         | 5.25                                            | 2.10                                          | 0.98  | 0.64 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.14                                         | 3.60                                            | 2.28                                          | 0.93  | 1.82 |

### S800K5



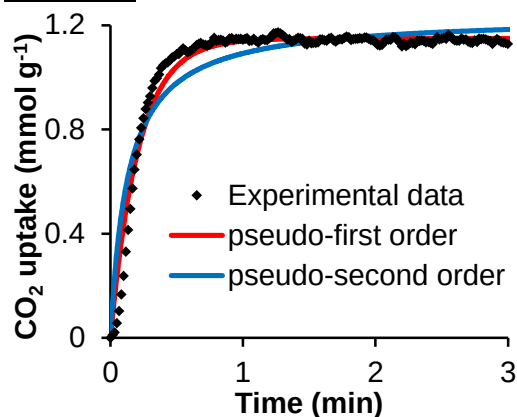
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.06                                         | 4.38                                            | 1.98                                          | 0.97  | 1.04 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.06                                         | 3.29                                            | 2.12                                          | 0.92  | 2.57 |

### S600K4



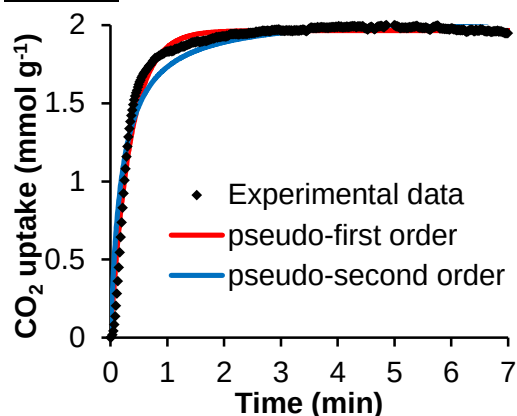
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.02                                         | 5.51                                            | 2.10                                          | 0.97  | 0.71 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.02                                         | 4.03                                            | 2.25                                          | 0.91  | 2.44 |

### S1000K4



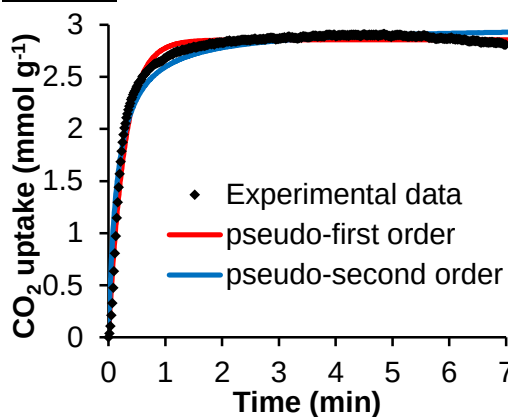
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.11                                         | 4.74                                            | 1.15                                          | 0.97  | 0.33 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.11                                         | 6.16                                            | 1.24                                          | 0.89  | 1.10 |

### A800K1



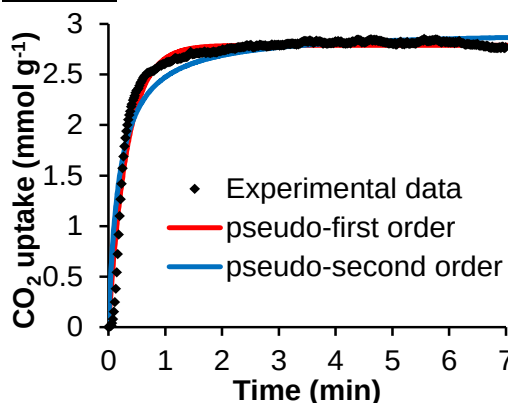
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 2.92                                            | 1.96                                          | 0.97  | 1.15 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 2.39                                            | 2.08                                          | 0.93  | 3.26 |

A800K2



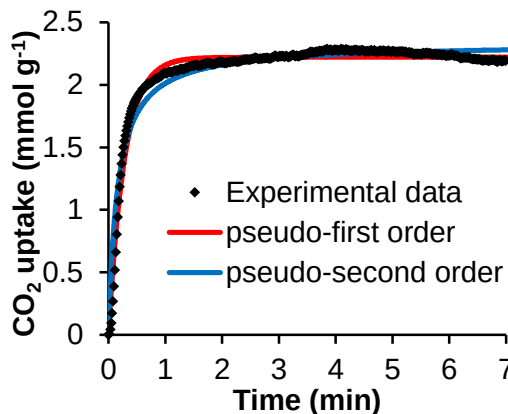
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.90                                         | 3.60                                            | 2.85                                          | 0.98  | 1.42 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.90                                         | 2.18                                            | 2.99                                          | 0.95  | 3.80 |

A800K3



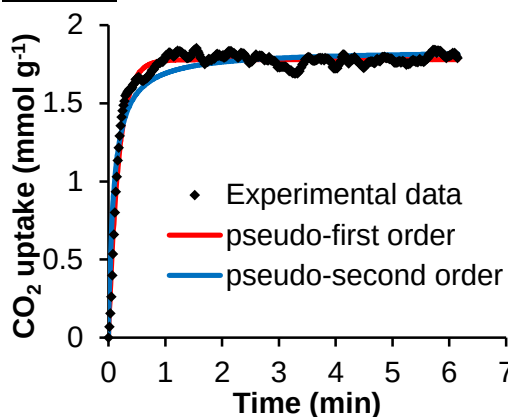
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.82                                         | 3.06                                            | 2.79                                          | 0.96  | 3.49 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.82                                         | 1.79                                            | 2.94                                          | 0.91  | 8.54 |

A800K4



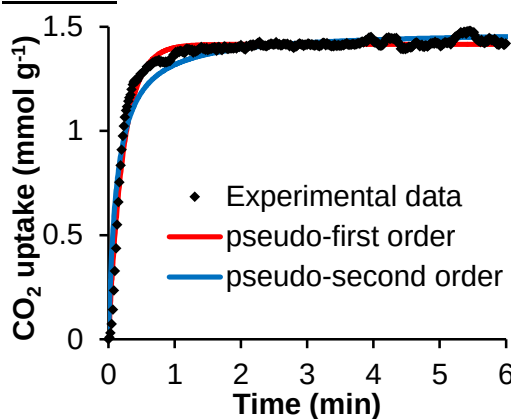
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.25                                         | 3.55                                            | 2.22                                          | 0.97  | 1.39 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.25                                         | 2.70                                            | 2.33                                          | 0.93  | 3.02 |

A800K5



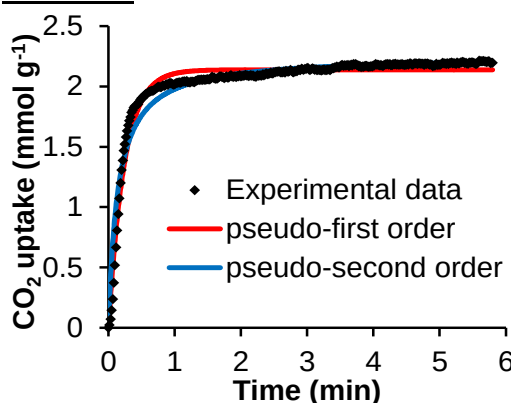
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.75                                         | 5.68                                            | 1.78                                          | 0.97  | 0.61 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.75                                         | 6.06                                            | 1.84                                          | 0.90  | 1.93 |

A600K2



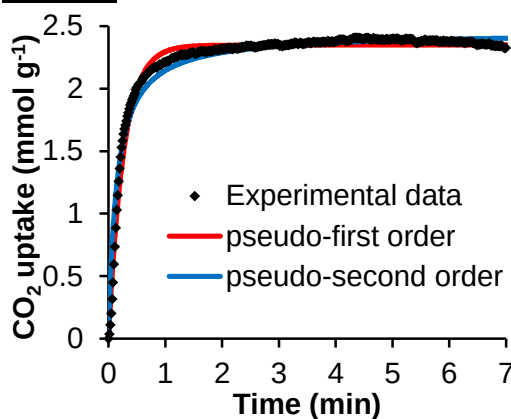
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.48                                         | 4.52                                            | 1.42                                          | 0.97  | 0.50 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.48                                         | 5.39                                            | 1.48                                          | 0.92  | 1.22 |

A1000K2



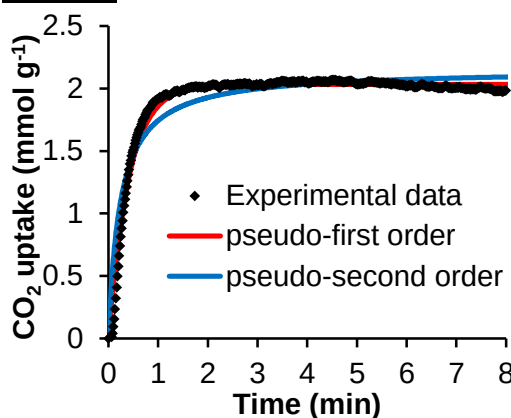
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.16                                         | 4.22                                            | 2.14                                          | 0.96  | 1.39 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.16                                         | 3.12                                            | 2.26                                          | 0.95  | 2.00 |

P800K2



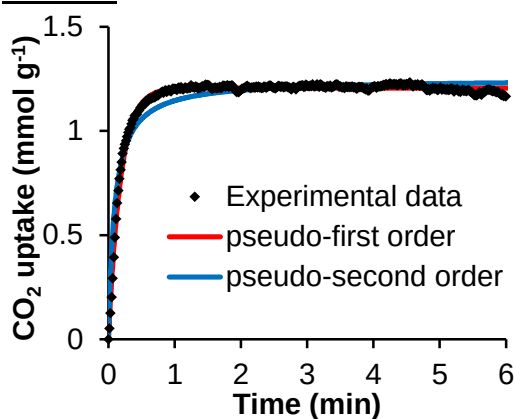
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.39                                         | 3.79                                            | 2.35                                          | 0.98  | 1.01 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.39                                         | 2.84                                            | 2.45                                          | 0.95  | 2.22 |

P800K3



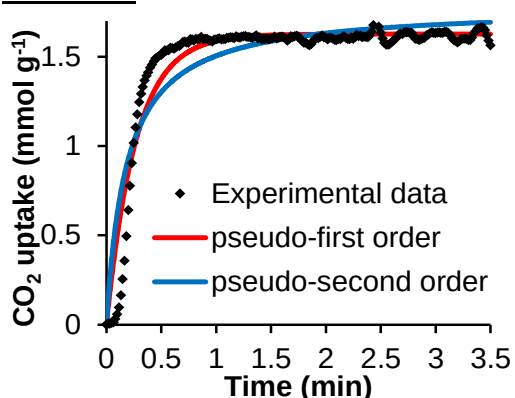
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.06                                         | 2.46                                            | 2.03                                          | 0.97  | 1.46 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.06                                         | 1.98                                            | 2.15                                          | 0.89  | 6.06 |

#### P800K5



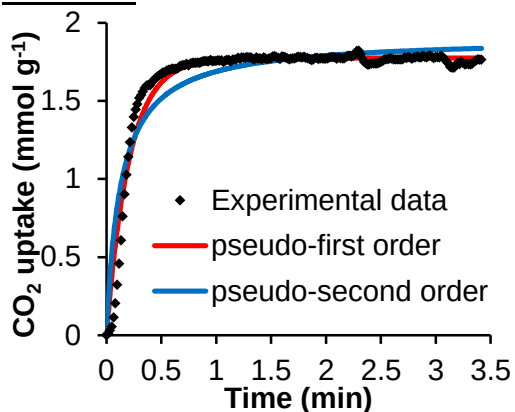
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.22                                         | 5.57                                            | 1.21                                          | 0.99  | 0.09 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.22                                         | 8.80                                            | 1.25                                          | 0.93  | 0.62 |

#### S800C15



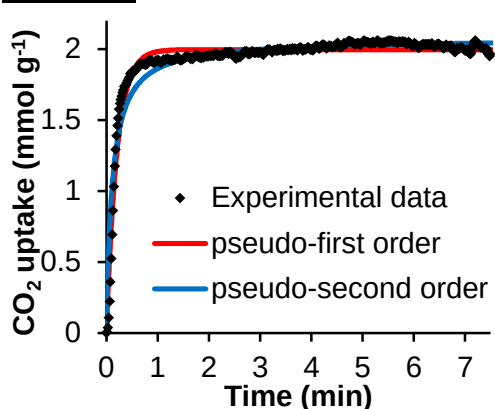
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.64                                         | 3.74                                            | 1.63                                          | 0.92  | 2.19 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.64                                         | 3.04                                            | 1.78                                          | 0.84  | 4.27 |

#### S850C15



| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.77                                         | 4.85                                            | 1.78                                          | 0.95  | 1.08 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.77                                         | 4.07                                            | 1.91                                          | 0.88  | 2.91 |

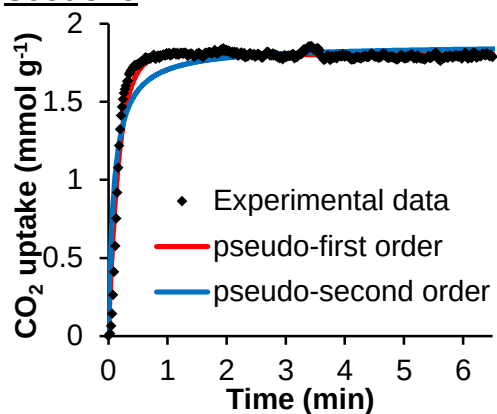
#### S900C15



| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 4.93                                            | 2.00                                          | 0.95  | 1.40 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 4.27                                            | 2.07                                          | 0.92  | 2.49 |

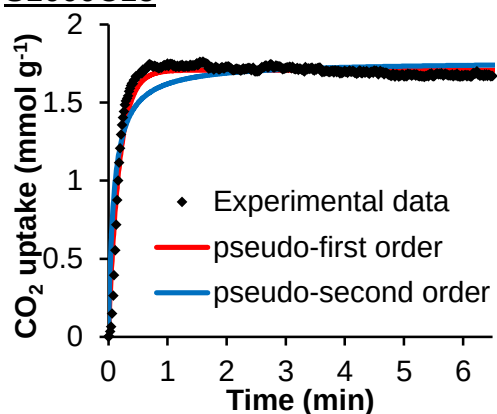


S950C15



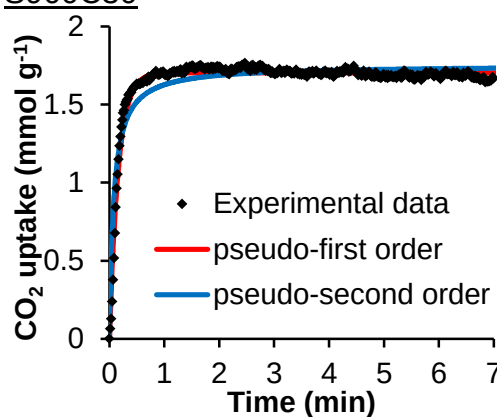
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.82                                         | 5.59                                            | 1.80                                          | 0.95  | 1.23 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.82                                         | 5.77                                            | 1.86                                          | 0.84  | 3.81 |

S1000C15



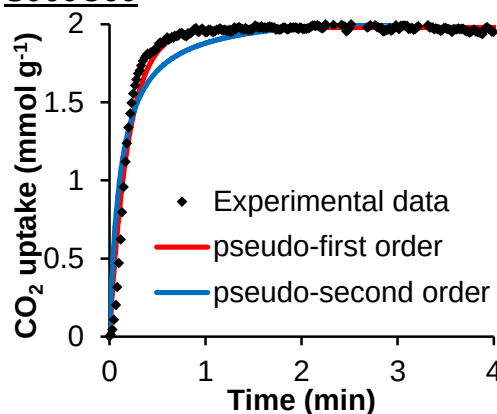
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.74                                         | 5.58                                            | 1.71                                          | 0.94  | 1.21 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.74                                         | 6.36                                            | 1.76                                          | 0.81  | 4.03 |

S900C30



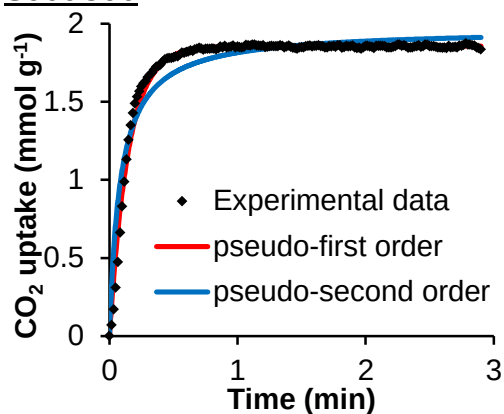
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.74                                         | 6.29                                            | 1.70                                          | 0.97  | 0.48 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.74                                         | 7.41                                            | 1.75                                          | 0.88  | 2.11 |

S900C60



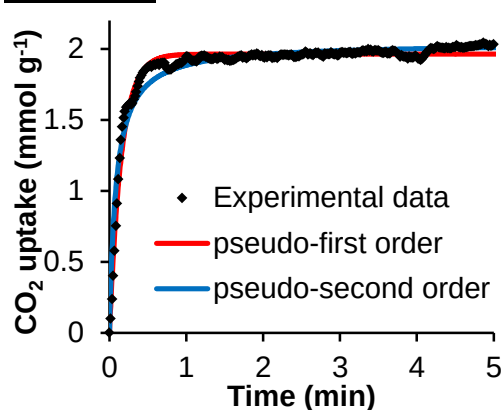
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 5.08                                            | 1.98                                          | 0.97  | 0.95 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 4.15                                            | 2.10                                          | 0.89  | 3.09 |

S900C90



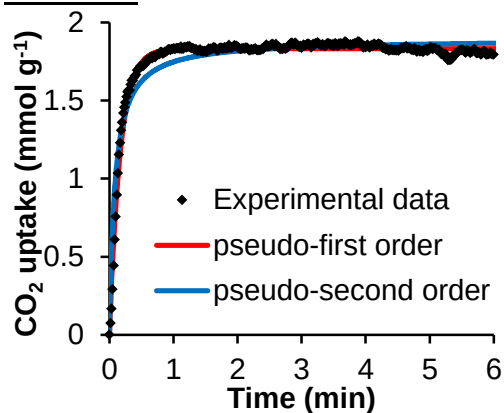
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.86                                         | 6.90                                            | 1.86                                          | 0.99  | 0.25 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.86                                         | 6.03                                            | 1.97                                          | 0.92  | 1.31 |

S900C120



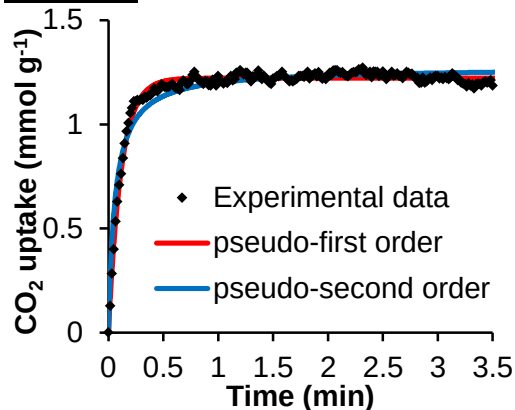
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.89                                         | 6.50                                            | 1.96                                          | 0.97  | 0.57 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.89                                         | 5.85                                            | 2.04                                          | 0.95  | 1.02 |

S950C60



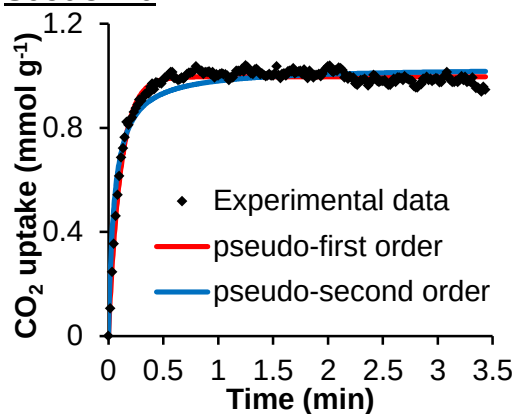
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.82                                         | 6.04                                            | 1.83                                          | 0.98  | 0.34 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.82                                         | 6.36                                            | 1.89                                          | 0.91  | 1.68 |

S950C90



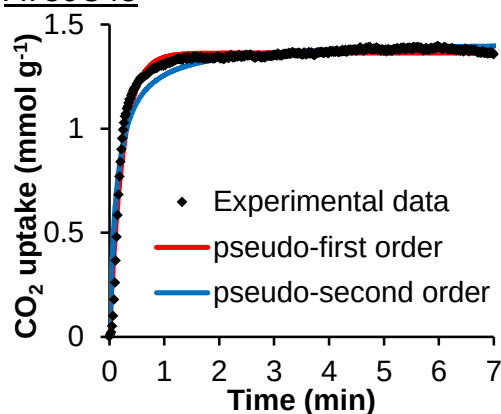
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.52                                         | 8.71                                            | 1.22                                          | 0.98  | 0.11 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.52                                         | 13.06                                           | 1.27                                          | 0.94  | 0.33 |

S950C120



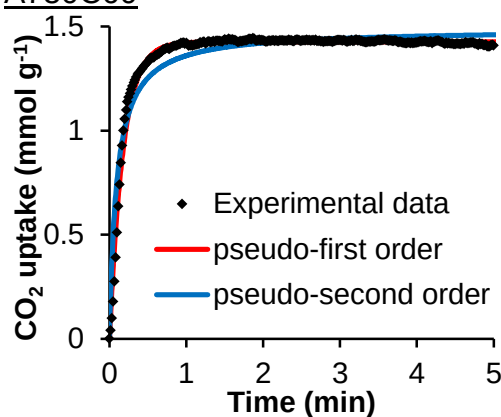
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.04                                         | 9.10                                            | 1.00                                          | 0.98  | 0.09 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.04                                         | 17.91                                           | 1.03                                          | 0.91  | 0.31 |

A750C45



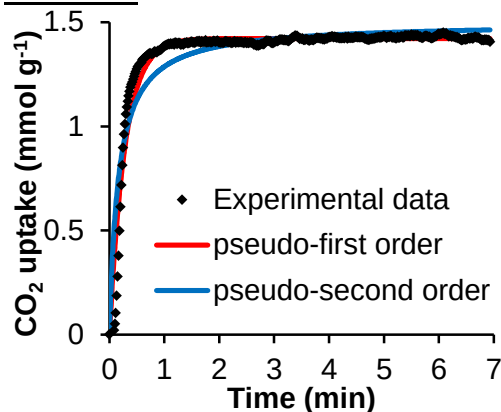
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.39                                         | 4.23                                            | 1.36                                          | 0.97  | 0.50 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.39                                         | 5.32                                            | 1.42                                          | 0.92  | 1.21 |

A750C60



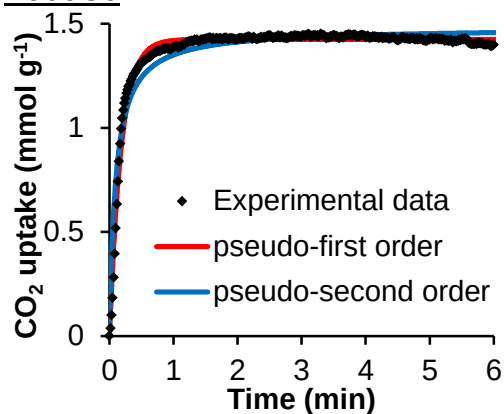
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.41                                         | 5.71                                            | 1.43                                          | 0.98  | 0.20 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.41                                         | 7.18                                            | 1.49                                          | 0.92  | 1.03 |

A750C90



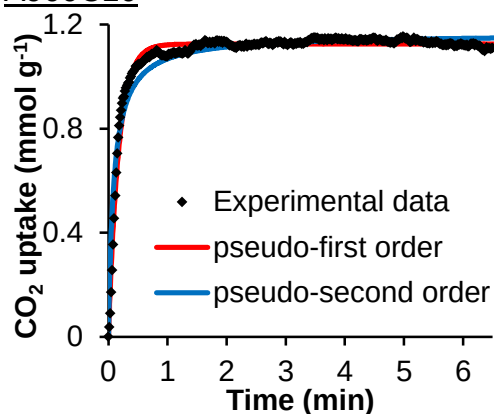
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.43                                         | 3.57                                            | 1.42                                          | 0.94  | 1.23 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.43                                         | 4.07                                            | 1.50                                          | 0.87  | 2.94 |

A900C0



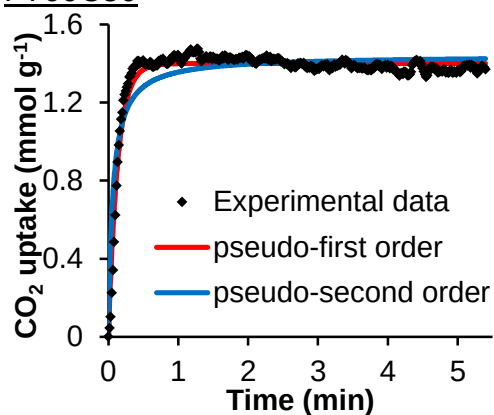
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.39                                         | 5.49                                            | 1.43                                          | 0.98  | 0.26 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.39                                         | 7.03                                            | 1.48                                          | 0.93  | 0.93 |

A900C10



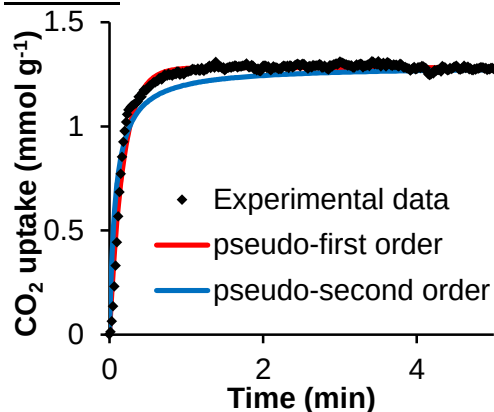
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.14                                         | 5.85                                            | 1.13                                          | 0.98  | 0.19 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.14                                         | 9.61                                            | 1.16                                          | 0.93  | 0.50 |

P700C50



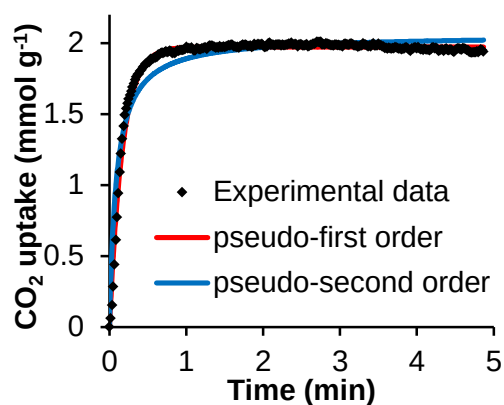
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.30                                         | 6.60                                            | 1.40                                          | 0.95  | 0.53 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.30                                         | 11.08                                           | 1.44                                          | 0.82  | 1.85 |

P900C0



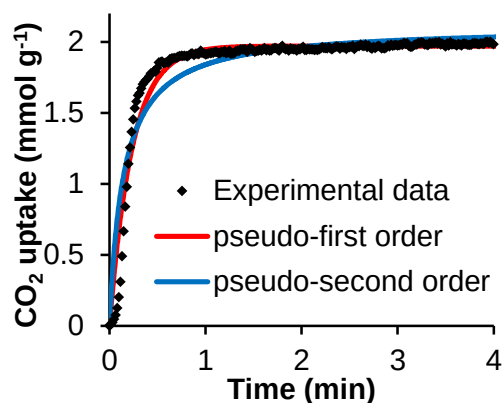
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.20                                         | 5.71                                            | 1.28                                          | 0.90  | 1.18 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.20                                         | 10.07                                           | 1.29                                          | 0.83  | 2.05 |

S70000



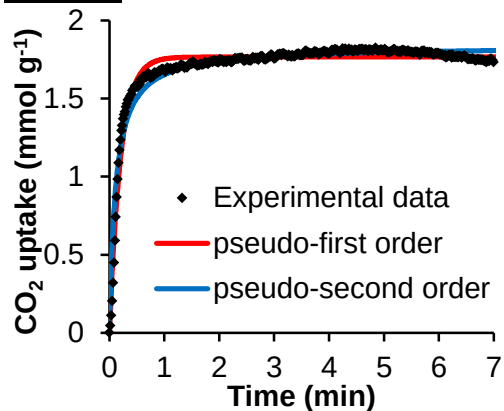
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 6.00                                            | 1.97                                          | 0.98  | 0.34 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.98                                         | 5.48                                            | 2.06                                          | 0.92  | 1.87 |

S75000



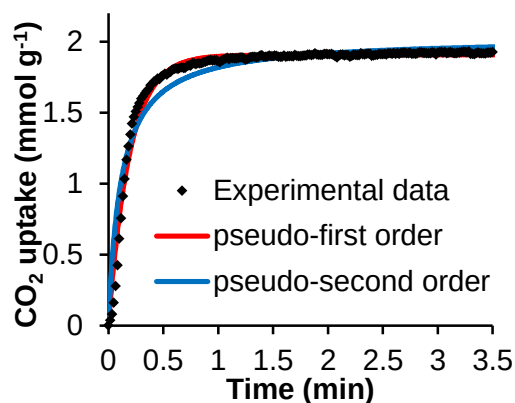
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.01                                         | 4.29                                            | 1.97                                          | 0.95  | 1.75 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 2.01                                         | 3.25                                            | 2.11                                          | 0.88  | 3.96 |

S80000



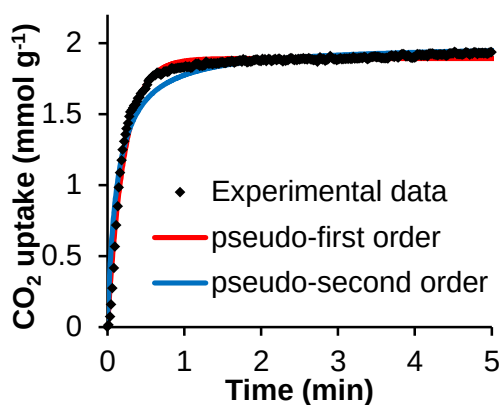
| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.82                                         | 4.98                                            | 1.77                                          | 0.96  | 0.81 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.82                                         | 4.95                                            | 1.84                                          | 0.95  | 1.16 |

S750040



| Pseudo-first order model                     |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> )                      | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.91                                         | 5.22                                            | 1.91                                          | 0.98  | 0.50 |
| Pseudo-second order model                    |                                                 |                                               |       |      |
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.91                                         | 4.30                                            | 2.03                                          | 0.93  | 1.66 |

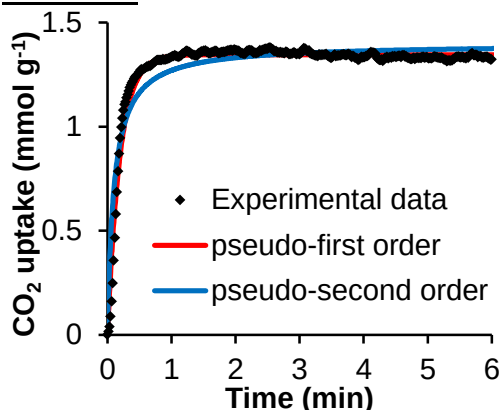
S750O56



| Pseudo-first order model                     |                            |                                               |       |      |
|----------------------------------------------|----------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.89                                         | 4.65                       | 1.89                                          | 0.98  | 0.51 |

| Pseudo-second order model                    |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.89                                         | 4.04                                            | 2.00                                          | 0.95  | 1.40 |

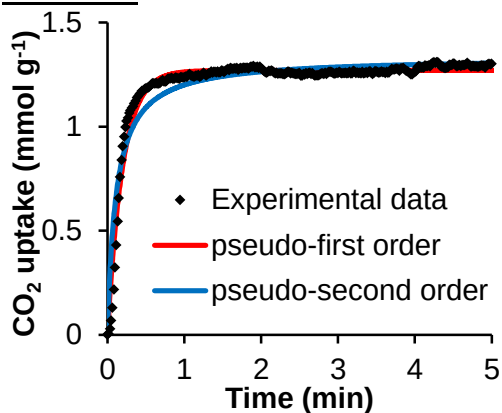
A500O30



| Pseudo-first order model                     |                            |                                               |       |      |
|----------------------------------------------|----------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.34                                         | 5.20                       | 1.35                                          | 0.97  | 0.41 |

| Pseudo-second order model                    |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.34                                         | 7.11                                            | 1.40                                          | 0.88  | 1.59 |

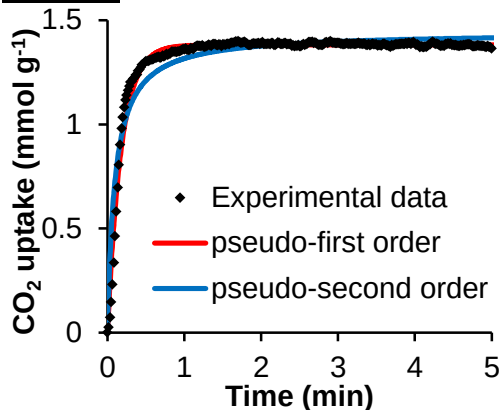
A500O60



| Pseudo-first order model                     |                            |                                               |       |      |
|----------------------------------------------|----------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.32                                         | 5.14                       | 1.27                                          | 0.96  | 0.43 |

| Pseudo-second order model                    |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.32                                         | 6.73                                            | 1.33                                          | 0.90  | 1.14 |

A750O0

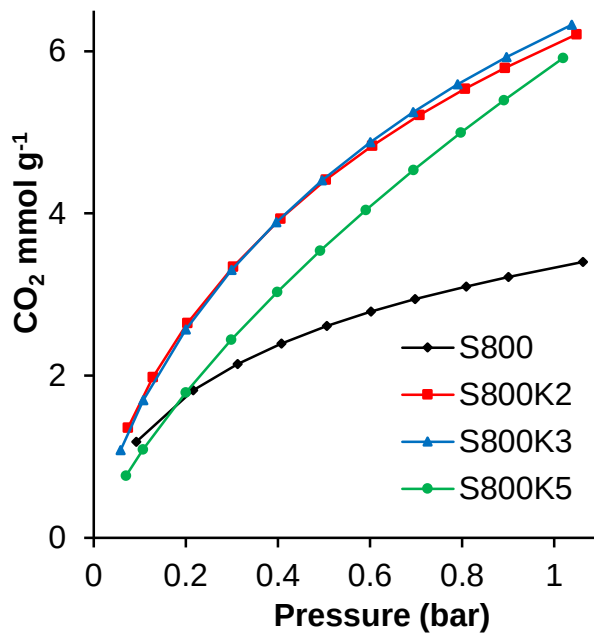
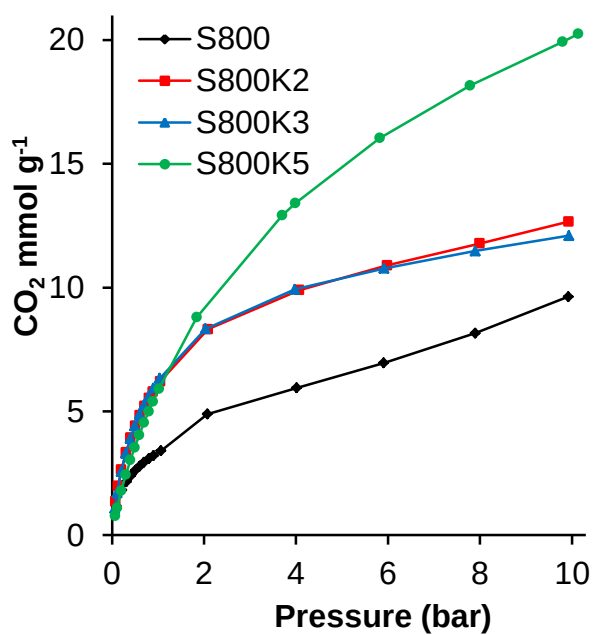


| Pseudo-first order model                     |                            |                                               |       |      |
|----------------------------------------------|----------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_1$ (min <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.39                                         | 5.69                       | 1.38                                          | 0.98  | 0.29 |

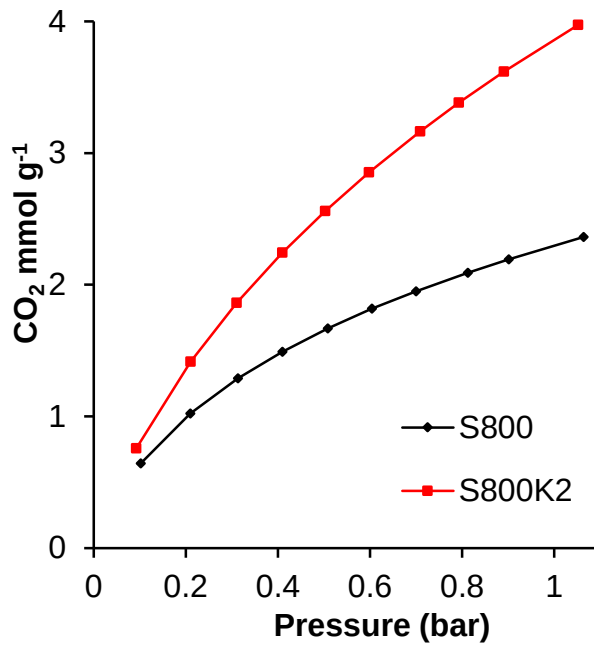
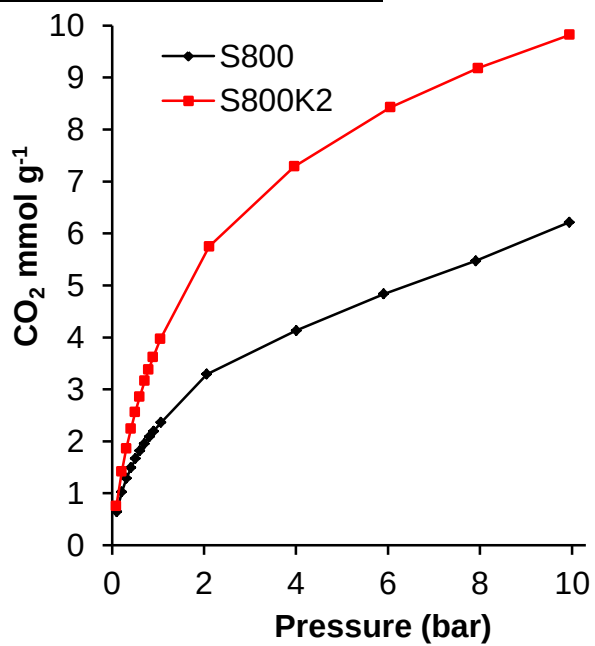
| Pseudo-second order model                    |                                                 |                                               |       |      |
|----------------------------------------------|-------------------------------------------------|-----------------------------------------------|-------|------|
| $q_e(\text{exp})$<br>(mmol g <sup>-1</sup> ) | $K_2$ (g min <sup>-1</sup> mmol <sup>-1</sup> ) | $q_e(\text{calc})$<br>(mmol g <sup>-1</sup> ) | $R^2$ | SSE  |
| 1.39                                         | 7.22                                            | 1.44                                          | 0.91  | 1.08 |

## CO<sub>2</sub> adsorption isotherms (0.1-10 bar)

S800, S800K2, S800K3 and S800K5 at 0 °C

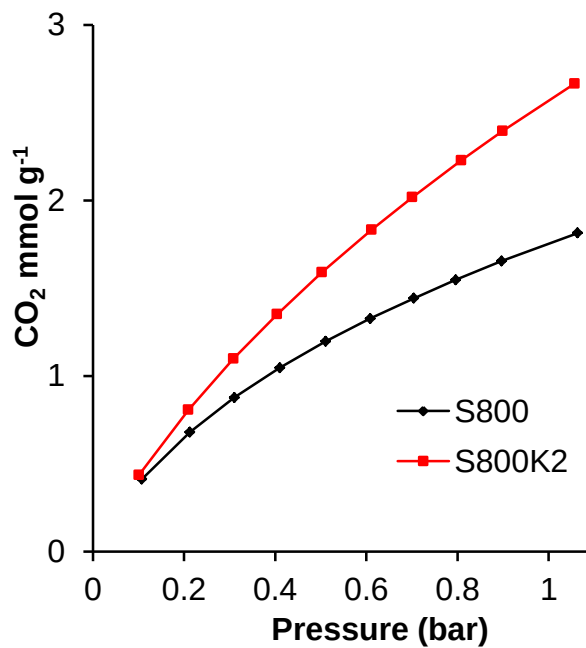
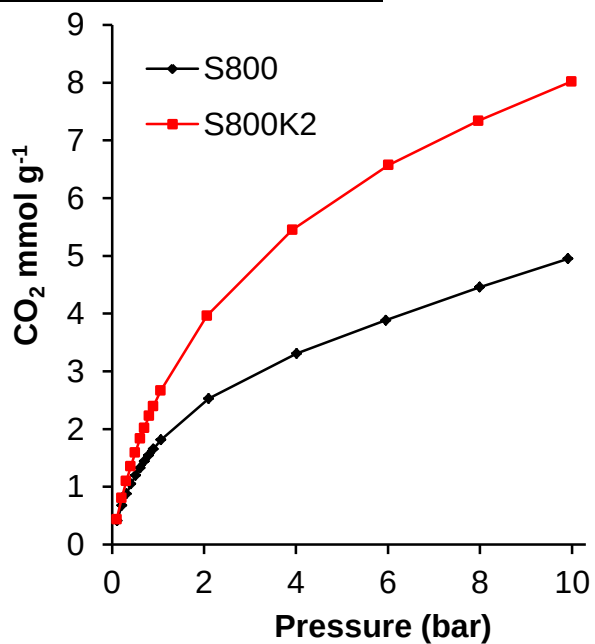


S800 and S800K2 at 25 °C

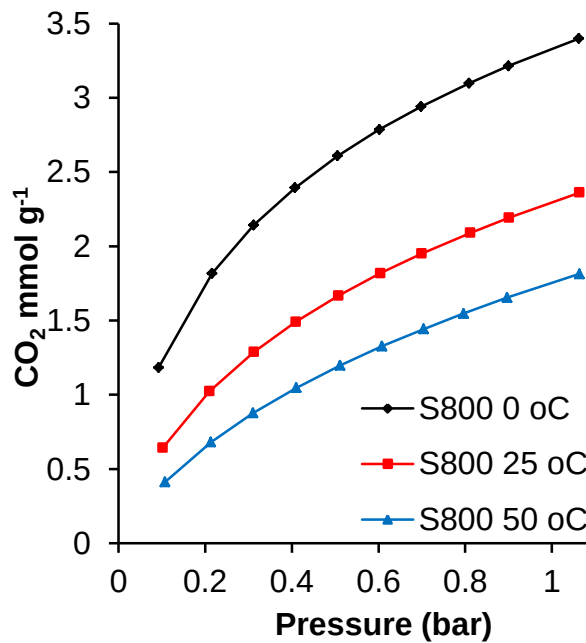
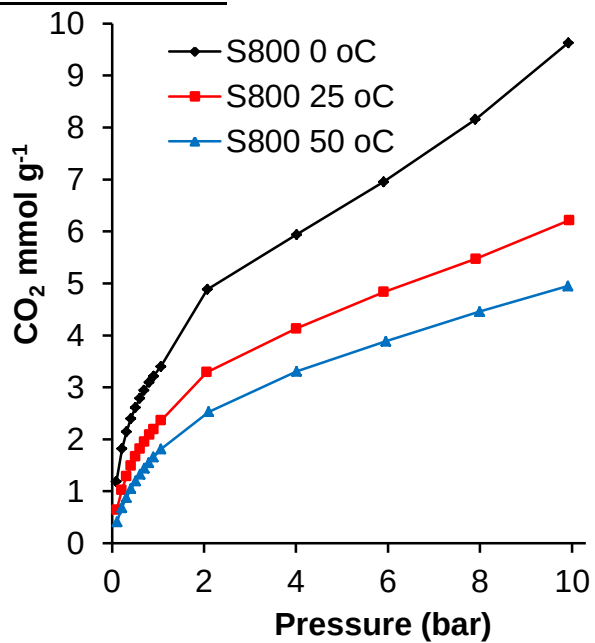




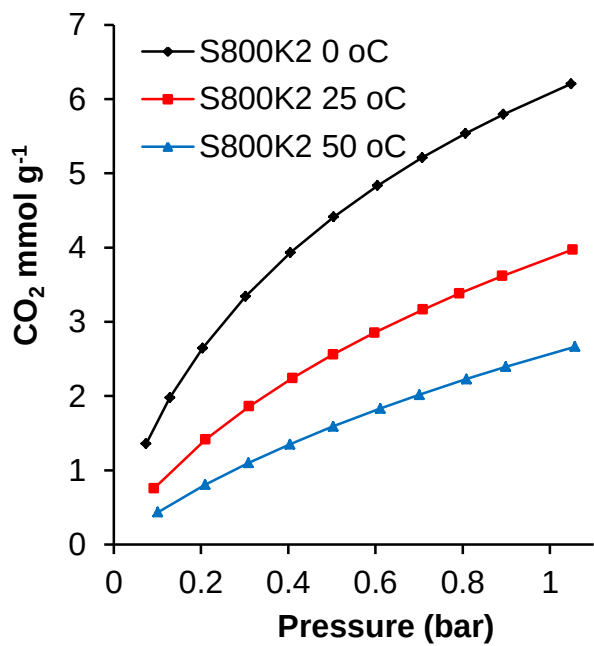
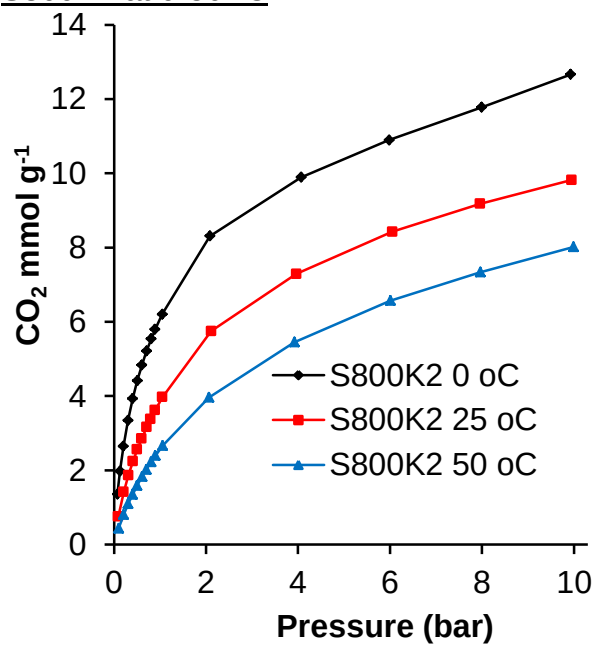
S800 and S800K2 at 50 °C



S800 at 0-50 °C



S800K2 at 0-50 °C



## Fitting of isotherm models to the experimental data

Three isotherm models (Langmuir, Freundlich and Temkin) were used to analyse the equilibrium adsorption of CO<sub>2</sub> and N<sub>2</sub> on S800, S00K2, S800K3 and S800K5. The models are represented by the following equations:

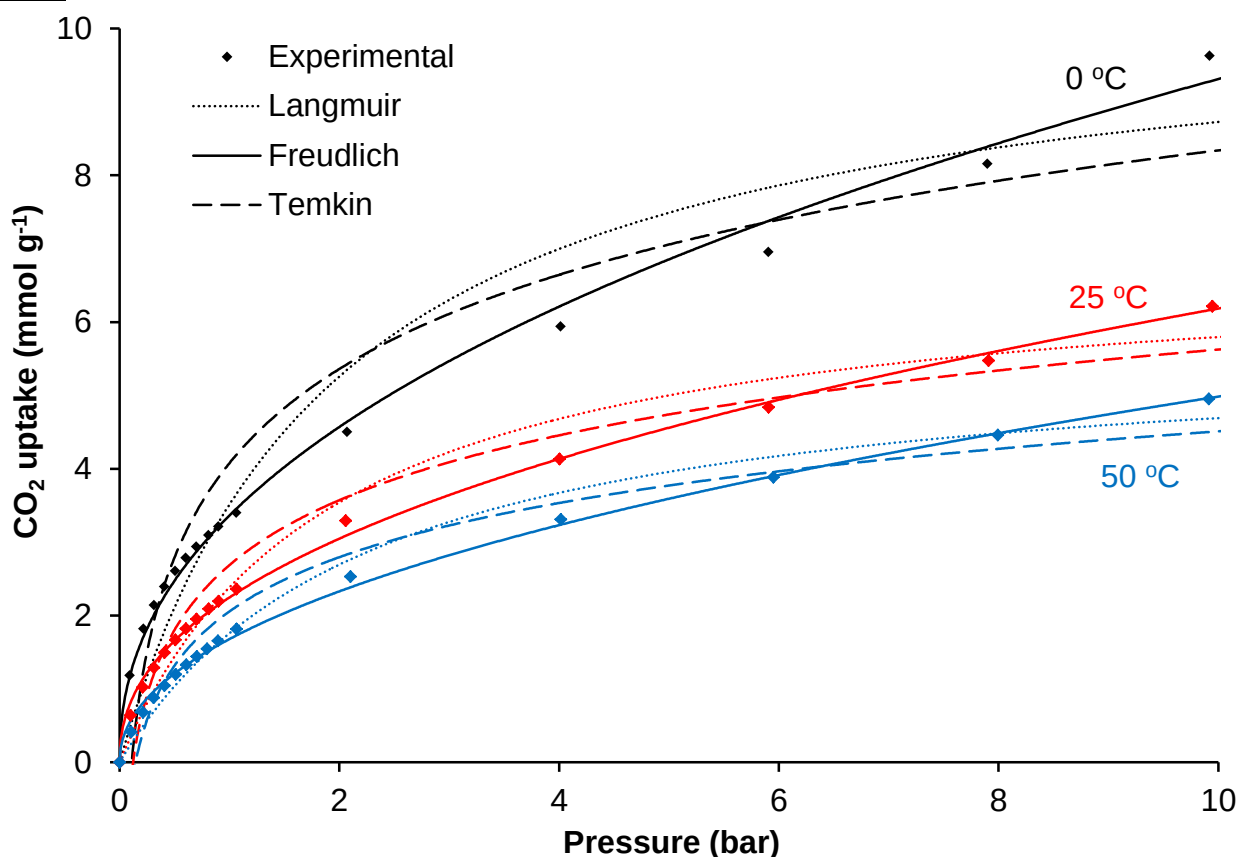
Langmuir:  $q_e = q_m K_L P / (1 + K_L P)$

Freundlich:  $q_e = K_F P^{1/n}$

Temkin:  $q_e = B \ln(K_T P)$

$q_m$  (mmol g<sup>-1</sup>) is the maximum adsorption capacity,  $q_e$  (mmol g<sup>-1</sup>) is the amount adsorbed at equilibrium,  $P$  (atm) is the pressure at equilibrium,  $K_L$  (atm<sup>-1</sup>) is the Langmuir constant,  $K_F$  (mmol g<sup>-1</sup> atm<sup>-1/n</sup>) and  $n$  are Freundlich constants indicating the adsorption intensity, and  $K_T$  (atm<sup>-1</sup>) is the Temkin constant.

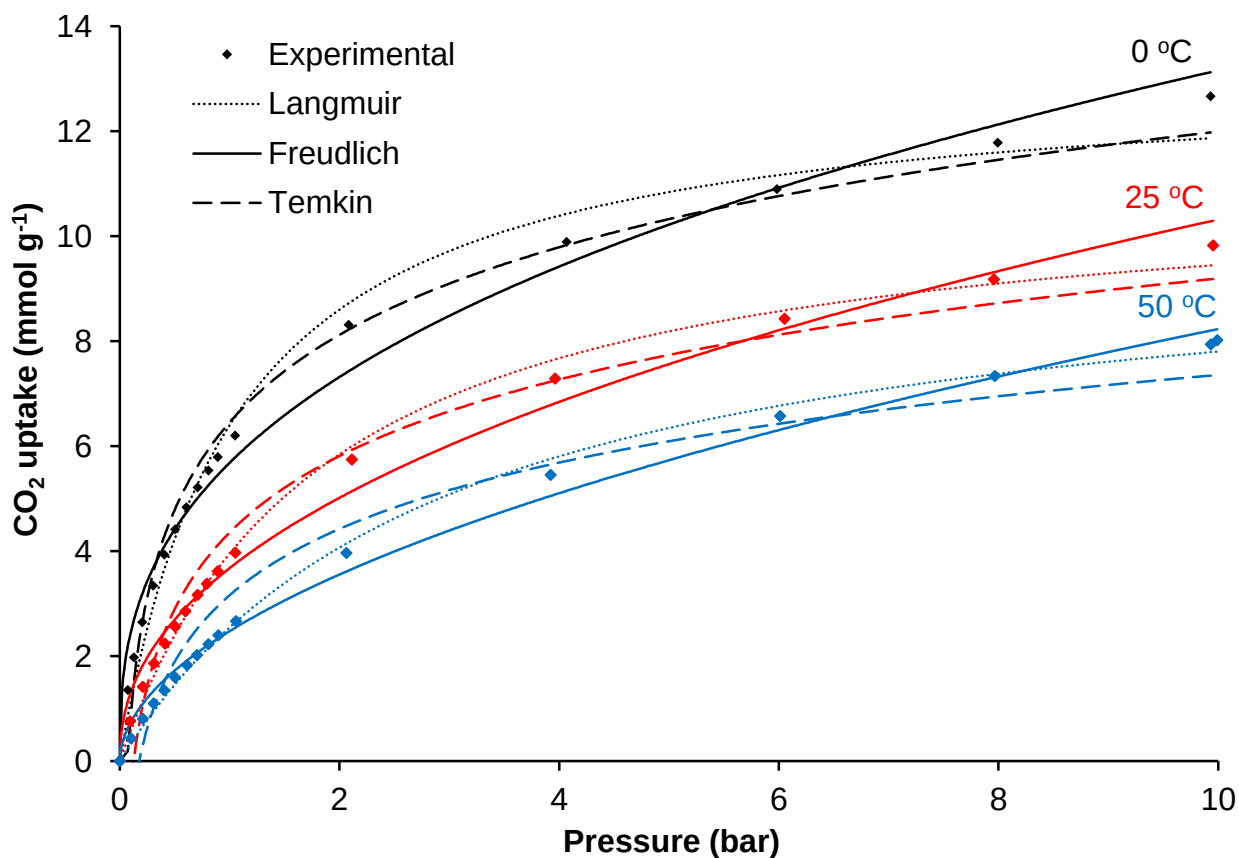
### S800



### Optimised parameters for isotherm fitting

| Model      | Parameters                                        | Temperature (°C) |       |       |
|------------|---------------------------------------------------|------------------|-------|-------|
|            |                                                   | 0                | 25    | 50    |
| Langmuir   | $q_m$ (mmol g <sup>-1</sup> )                     | 10.4             | 6.9   | 5.8   |
|            | $K_L$ (atm <sup>-1</sup> )                        | 0.51             | 0.53  | 0.44  |
|            | $R^2$                                             | 0.950            | 0.978 | 0.986 |
| Freundlich | $K_F$ (mmol g <sup>-1</sup> atm <sup>-1/n</sup> ) | 3.36             | 2.25  | 1.68  |
|            | $1/n$                                             | 0.44             | 0.44  | 0.47  |
|            | $R^2$                                             | 0.995            | 0.998 | 0.998 |
| Temkin     | $B$ (KJ mol <sup>-1</sup> )                       | 1.85             | 1.28  | 1.07  |
|            | $K_T$ (atm <sup>-1</sup> )                        | 9.06             | 8.24  | 6.90  |
|            | $R^2$                                             | 0.930            | 0.961 | 0.962 |

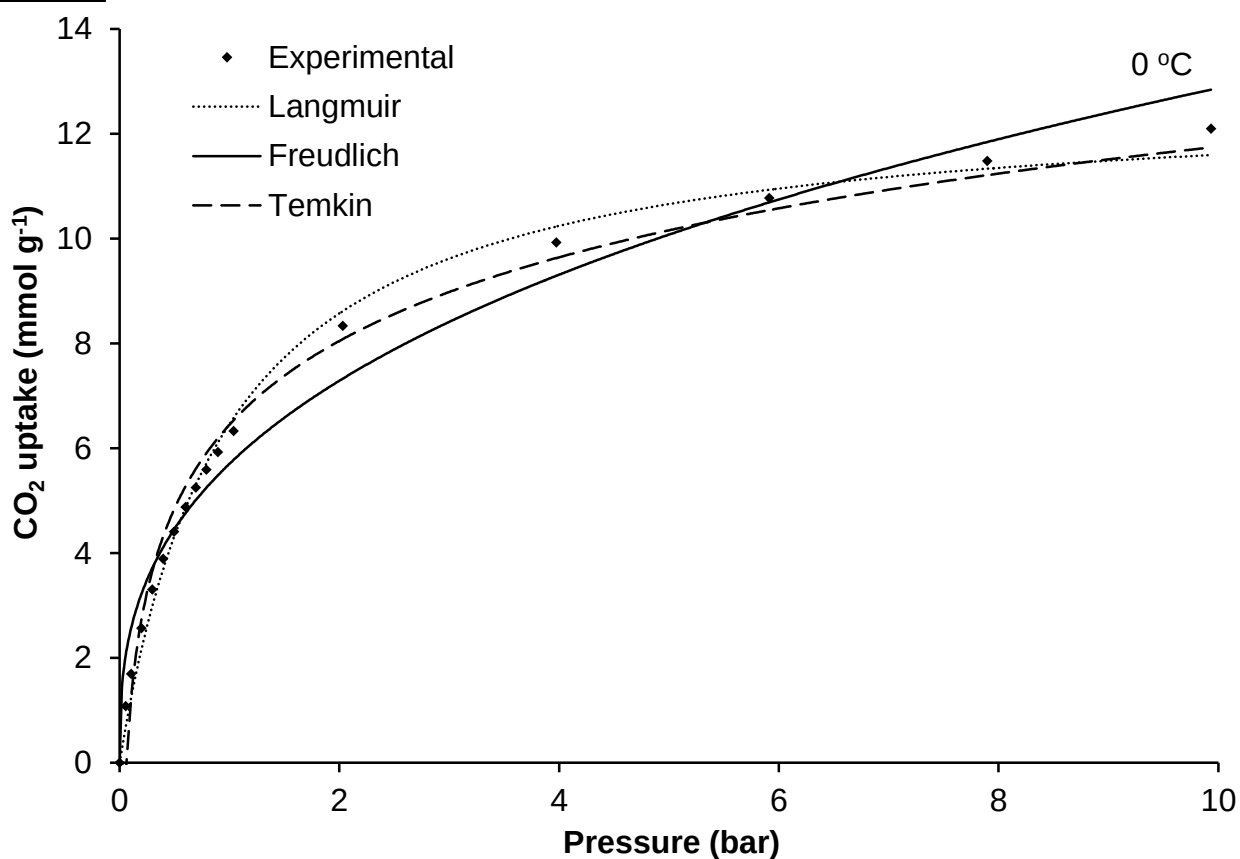
S800K2



Optimised parameters for isotherm fitting

| Model      | Parameters                                        | Temperature (°C) |       |       |
|------------|---------------------------------------------------|------------------|-------|-------|
|            |                                                   | 0                | 25    | 50    |
| Langmuir   | $q_m$ (mmol g <sup>-1</sup> )                     | 13.1             | 11.2  | 10.1  |
|            | $K_L$ (atm <sup>-1</sup> )                        | 0.95             | 0.55  | 0.34  |
|            | $R^2$                                             | 0.989            | 0.996 | 0.997 |
| Freundlich | $K_F$ (mmol g <sup>-1</sup> atm <sup>-1/n</sup> ) | 5.68             | 3.68  | 2.45  |
|            | $1/n$                                             | 0.36             | 0.45  | 0.52  |
|            | $R^2$                                             | 0.985            | 0.989 | 0.993 |
| Temkin     | $B$ (KJ mol <sup>-1</sup> )                       | 2.41             | 2.10  | 1.82  |
|            | $K_T$ (atm <sup>-1</sup> )                        | 14.64            | 7.94  | 5.66  |
|            | $R^2$                                             | 0.985            | 0.968 | 0.956 |

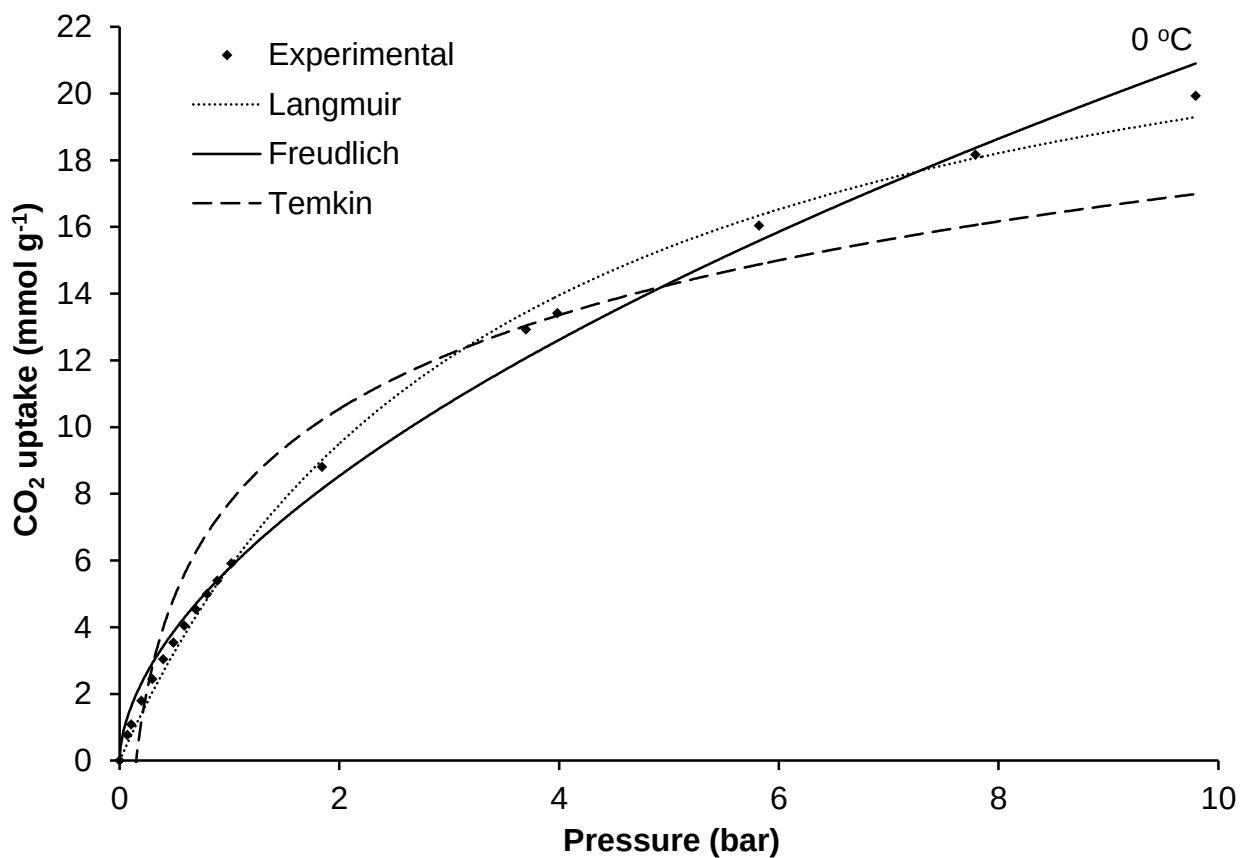
S800K3



Optimised parameters for isotherm fitting

| Model      | Parameters                                        | Temperature (0 °C) |
|------------|---------------------------------------------------|--------------------|
| Langmuir   | $q_m$ (mmol g <sup>-1</sup> )                     | 12.7               |
|            | $K_L$ (atm <sup>-1</sup> )                        | 1.03               |
|            | $R^2$                                             | 0.995              |
| Freundlich | $K_F$ (mmol g <sup>-1</sup> atm <sup>-1/n</sup> ) | 5.71               |
|            | $1/n$                                             | 0.35               |
|            | $R^2$                                             | 0.988              |
| Temkin     | $B$ (KJ mol <sup>-1</sup> )                       | 2.30               |
|            | $K_T$ (atm <sup>-1</sup> )                        | 16.45              |
|            | $R^2$                                             | 0.986              |

## S800K5



### Optimised parameters for isotherm fitting

| Model      | Parameters                                        | Temperature (0 °C) |
|------------|---------------------------------------------------|--------------------|
| Langmuir   | $q_m$ (mmol g <sup>-1</sup> )                     | 26.2               |
|            | $K_L$ (atm <sup>-1</sup> )                        | 0.284              |
|            | $R^2$                                             | 0.997              |
| Freundlich | $K_F$ (mmol g <sup>-1</sup> atm <sup>-1/n</sup> ) | 5.78               |
|            | $1/n$                                             | 0.564              |
|            | $R^2$                                             | 0.993              |
| Temkin     | $B$ (KJ mol <sup>-1</sup> )                       | 4.06               |
|            | $K_T$ (atm <sup>-1</sup> )                        | 6.74               |
|            | $R^2$                                             | 0.917              |

## Van't Hoff plots

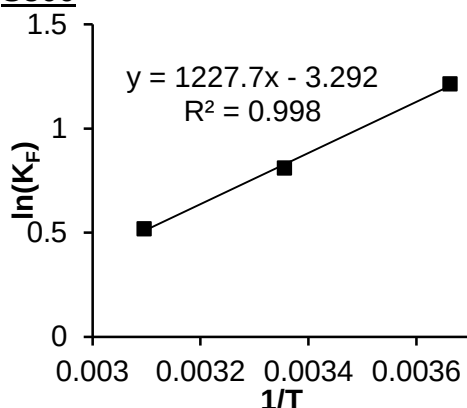
The change in Gibbs free energy  $\Delta G^0$  (KJ mol<sup>-1</sup>), standard molar adsorption enthalpy  $\Delta H^0$  (KJ mol<sup>-1</sup>) and entropy  $\Delta S^0$  (J mol<sup>-1</sup> K<sup>-1</sup>) were calculated using the equations:

$$\Delta G^0 = -RT \ln K_F$$

$$\ln K_F = \Delta S^0 / R - \Delta H^0 / RT$$

where,  $K_F$  is the Freundlich equilibrium constant and  $\Delta H^0$  and  $\Delta S^0$  can be obtained from the slope and intercept of van't Hoff plot.

S800



| T (K) | 1/T      | $K_F$   | $\ln(K_F)$ |
|-------|----------|---------|------------|
| 273   | 0.003663 | 3.36428 | 1.213214   |
| 298   | 0.003356 | 2.2477  | 0.809907   |
| 323   | 0.003096 | 1.67964 | 0.518579   |

$$R = 8.314$$

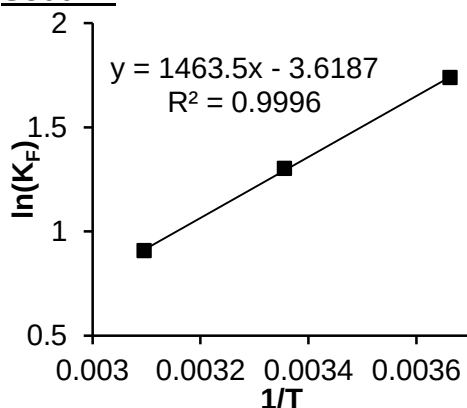
$$\text{Slope} (= -\Delta H^0/R) = 1227.7$$

$$\Delta H^0 \text{ (KJ mol}^{-1}\text{)} = -10.21$$

$$\text{Intercept} (= \Delta S^0/R) = -3.292$$

$$\Delta S^0 \text{ (J mol}^{-1} \text{ K}^{-1}\text{)} = -27.37$$

S800K2



| T (K) | 1/T      | $K_F$   | $\ln(K_F)$ |
|-------|----------|---------|------------|
| 273   | 0.003663 | 5.68403 | 1.73766    |
| 298   | 0.003356 | 3.67787 | 1.302334   |
| 323   | 0.003096 | 2.47682 | 0.906975   |

$$R = 8.314$$

$$\text{Slope} (= -\Delta H^0/R) = 1463.5$$

$$\Delta H^0 \text{ (KJ mol}^{-1}\text{)} = -12.17$$

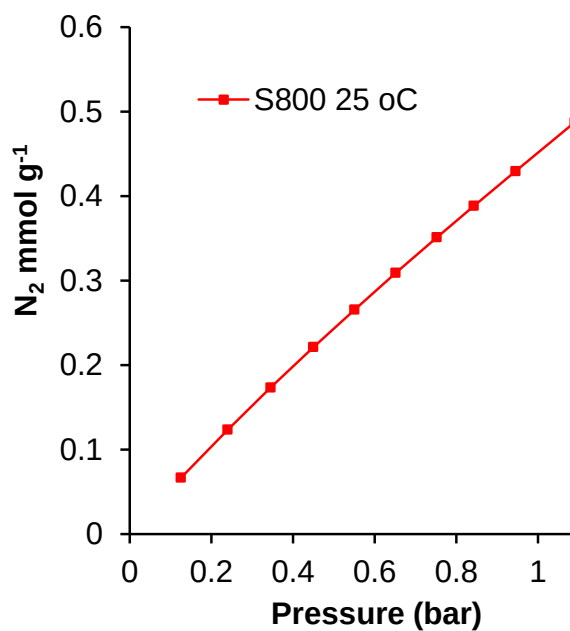
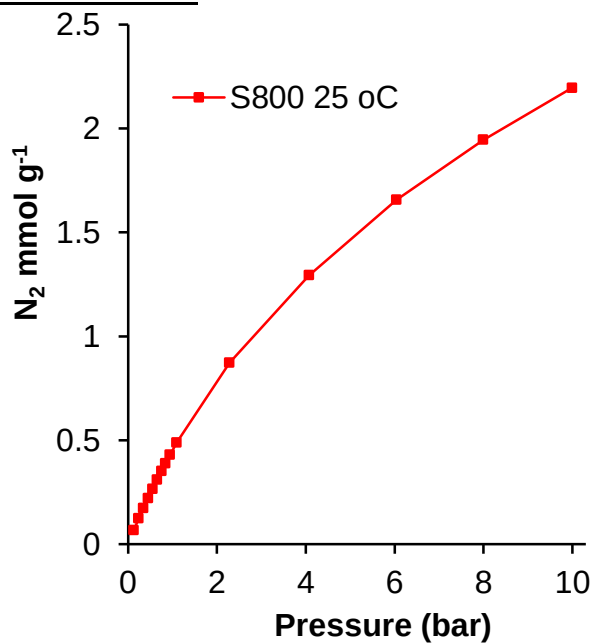
$$\text{Intercept} (= \Delta S^0/R) = -3.6187$$

$$\Delta S^0 \text{ (J mol}^{-1} \text{ K}^{-1}\text{)} = -30.09$$

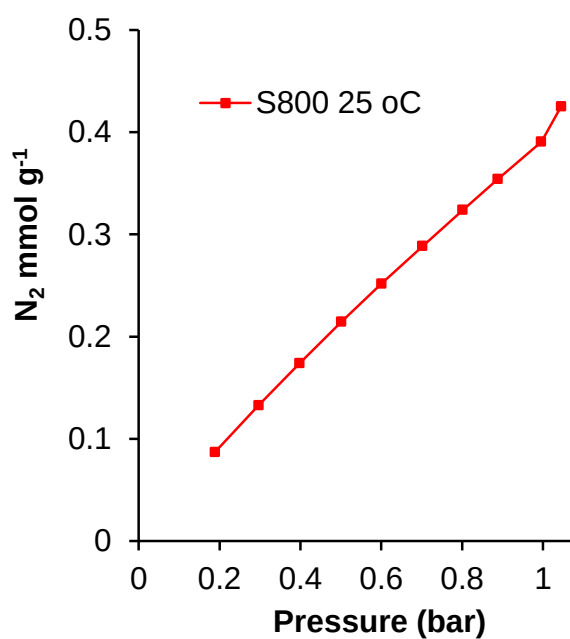
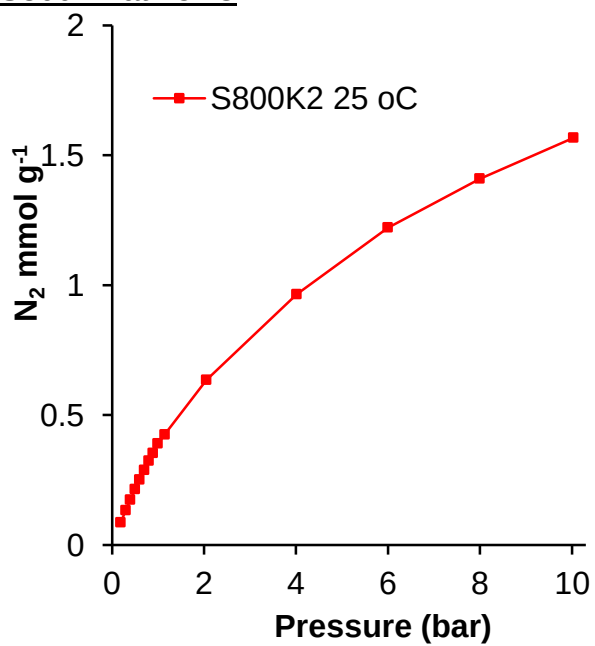


## N<sub>2</sub> adsorption isotherms (0.1-10 bar)

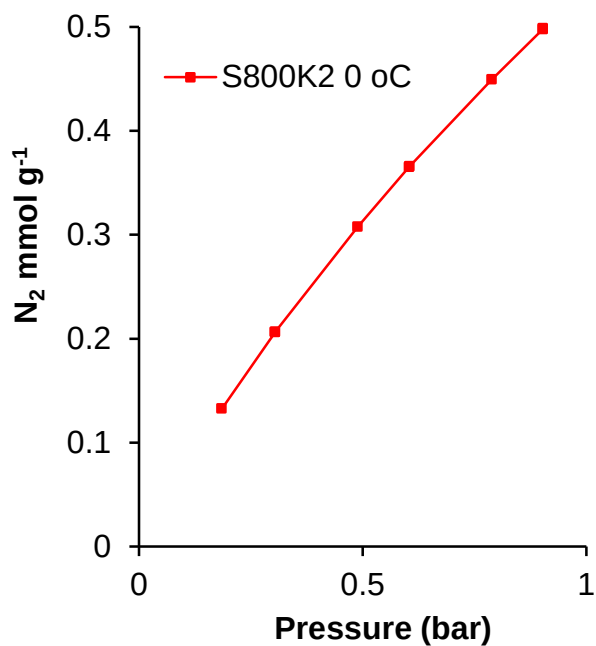
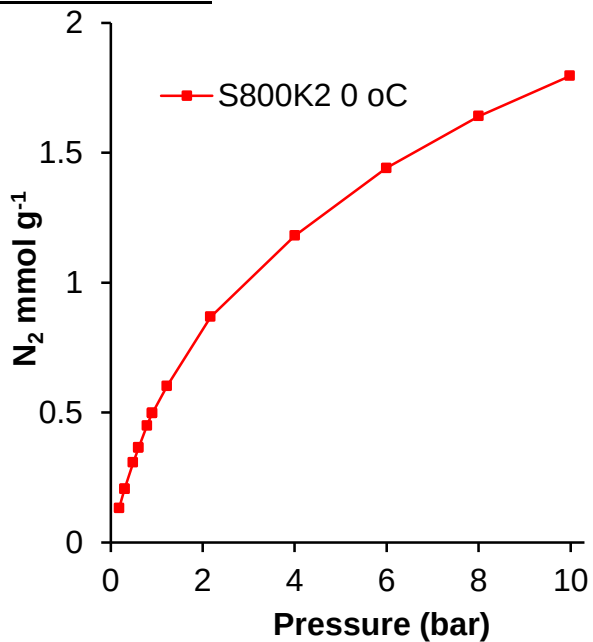
S800 at 25 °C



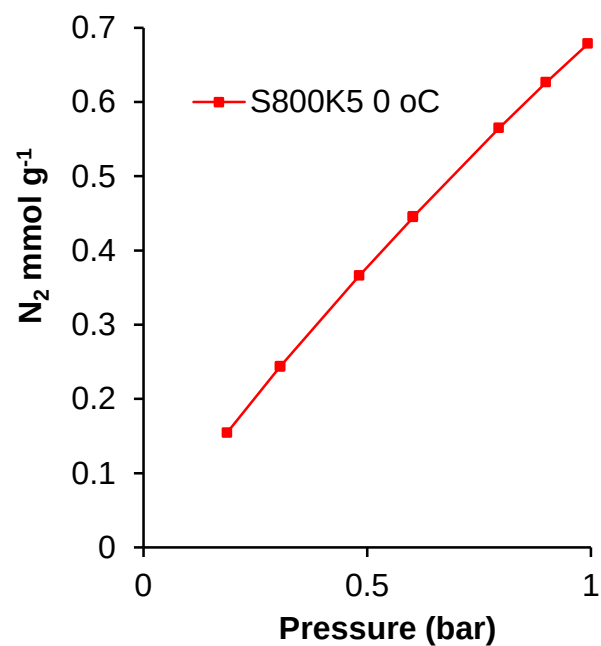
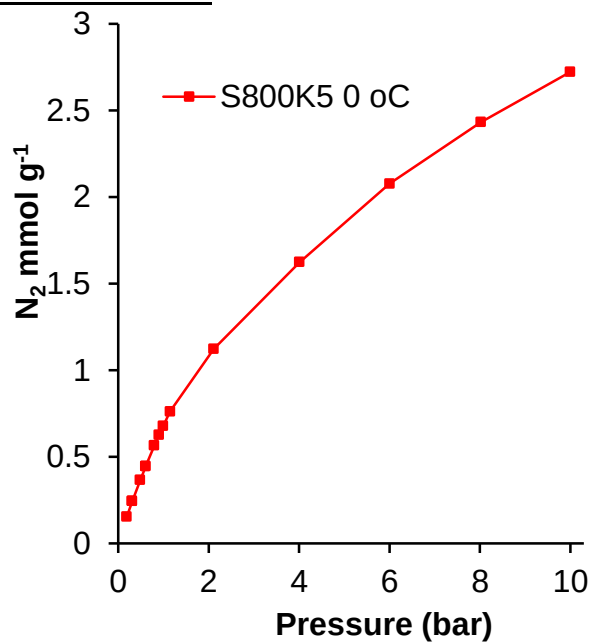
S800K2 at 25 °C



S800K2 at 0 °C

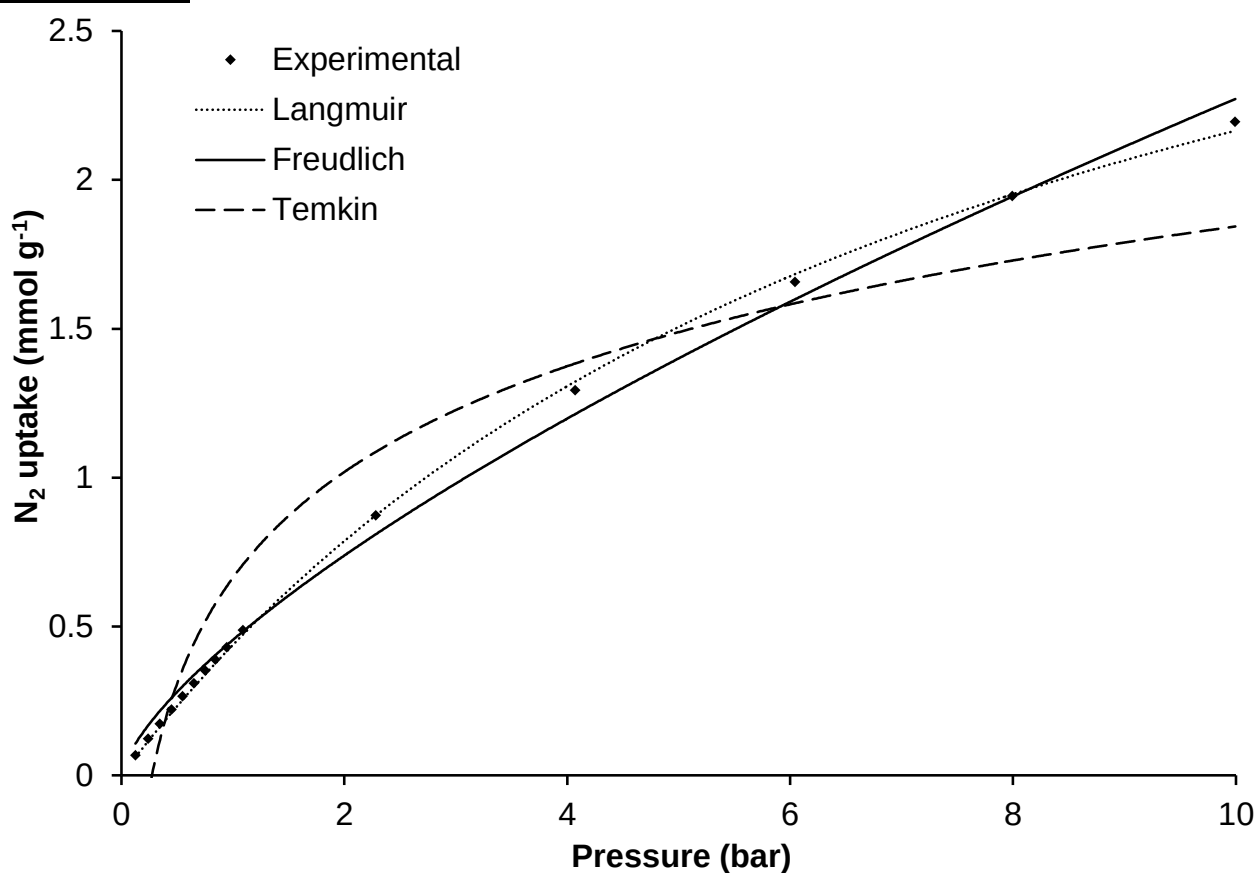


S800K5 at 0 °C



## Fitting of isotherm models to the experimental N<sub>2</sub> adsorption data

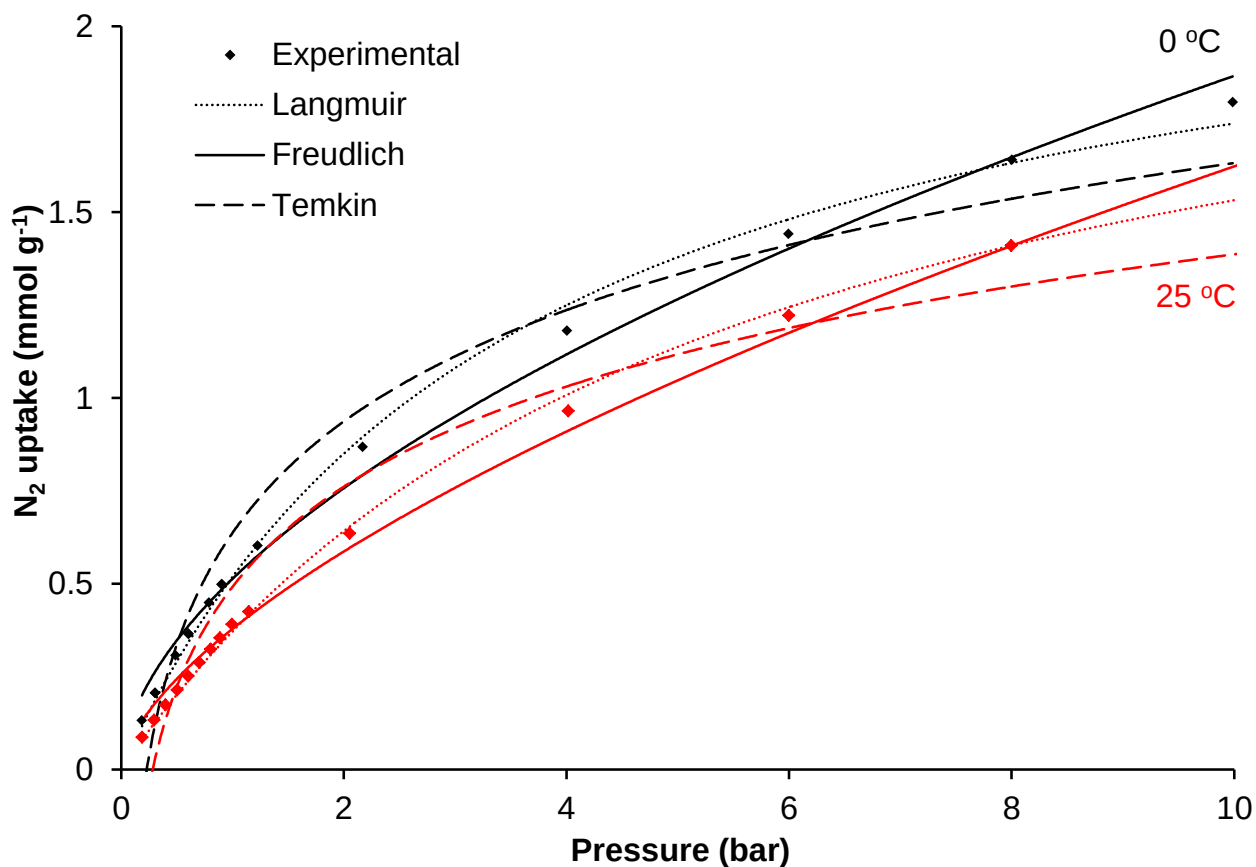
S800 at 25 °C



### Optimised parameters for isotherm fitting

| Model      | Parameters                                        | Value |
|------------|---------------------------------------------------|-------|
| Langmuir   | $q_m$ (mmol g <sup>-1</sup> )                     | 3.9   |
|            | $K_L$ (atm <sup>-1</sup> )                        | 0.13  |
|            | $R^2$                                             | 0.999 |
| Freundlich | $K_F$ (mmol g <sup>-1</sup> atm <sup>-1/n</sup> ) | 0.46  |
|            | $1/n$                                             | 0.70  |
|            | $R^2$                                             | 0.996 |
| Temkin     | $B$ (KJ mol <sup>-1</sup> )                       | 0.51  |
|            | $K_T$ (atm <sup>-1</sup> )                        | 3.67  |
|            | $R^2$                                             | 0.905 |

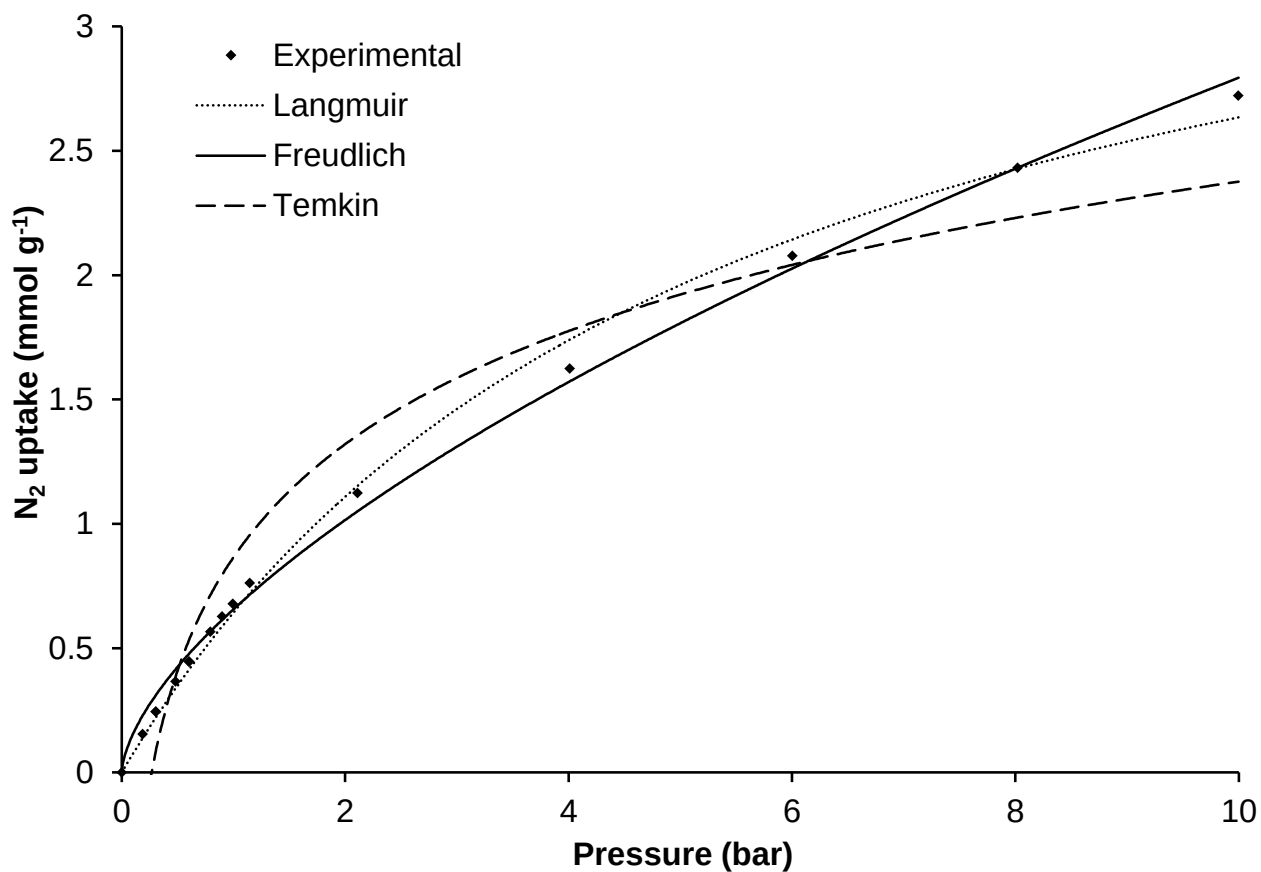
### S800K2 at 0 and 25 °C



### Optimised parameters for isotherm fitting

| Model      | Parameters                                       | Temperature (°C) |       |
|------------|--------------------------------------------------|------------------|-------|
|            |                                                  | 0                | 25    |
| Langmuir   | $q_m$ ( $\text{mmol g}^{-1}$ )                   | 2.4              | 2.4   |
|            | $K_L$ ( $\text{atm}^{-1}$ )                      | 0.28             | 0.19  |
|            | $R^2$                                            | 0.997            | 0.998 |
| Freundlich | $K_F$ ( $\text{mmol g}^{-1} \text{atm}^{-1/n}$ ) | 0.51             | 0.38  |
|            | $1/n$                                            | 0.56             | 0.63  |
|            | $R^2$                                            | 0.993            | 0.995 |
| Temkin     | $B$ ( $\text{KJ mol}^{-1}$ )                     | 0.40             | 0.39  |
|            | $K_T$ ( $\text{atm}^{-1}$ )                      | 4.37             | 3.55  |
|            | $R^2$                                            | 0.961            | 0.944 |

### S800K5 at 0 °C



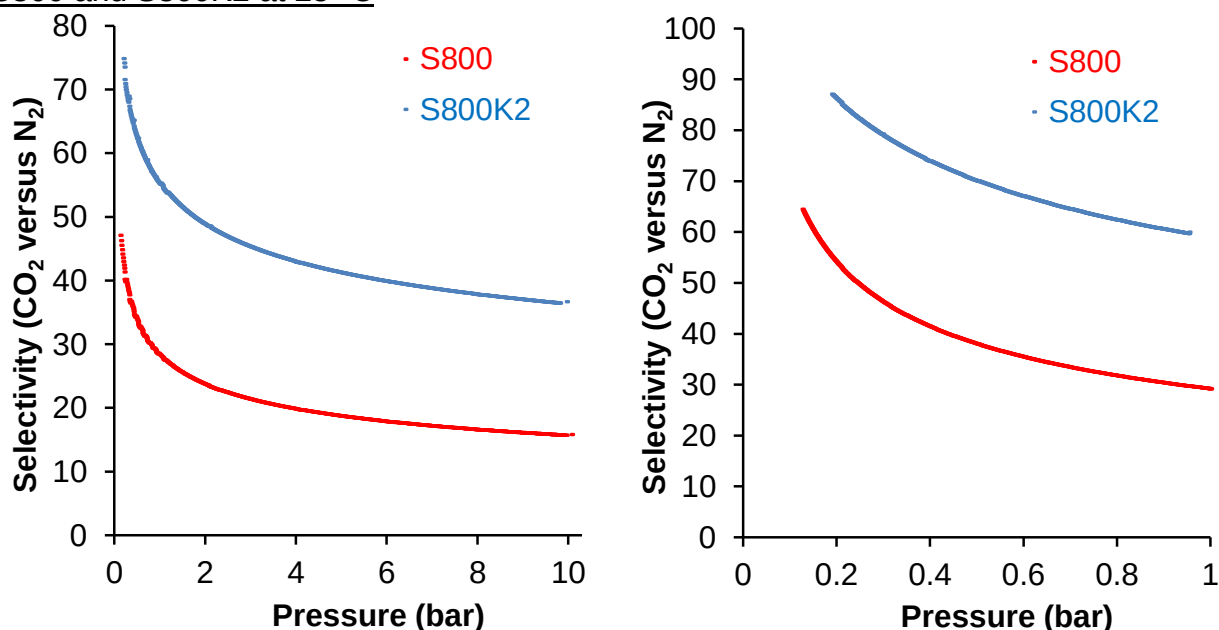
### Optimised parameters for isotherm fitting

| Model      | Parameters                                        | Value |
|------------|---------------------------------------------------|-------|
| Langmuir   | $q_m$ (mmol g <sup>-1</sup> )                     | 4.0   |
|            | $K_L$ (atm <sup>-1</sup> )                        | 0.19  |
|            | $R^2$                                             | 0.997 |
| Freundlich | $K_F$ (mmol g <sup>-1</sup> atm <sup>-1/n</sup> ) | 0.66  |
|            | $1/n$                                             | 0.63  |
|            | $R^2$                                             | 0.997 |
| Temkin     | $B$ (KJ mol <sup>-1</sup> )                       | 0.60  |
|            | $K_T$ (atm <sup>-1</sup> )                        | 3.74  |
|            | $R^2$                                             | 0.947 |

## Selectivities of CO<sub>2</sub> versus N<sub>2</sub> adsorption

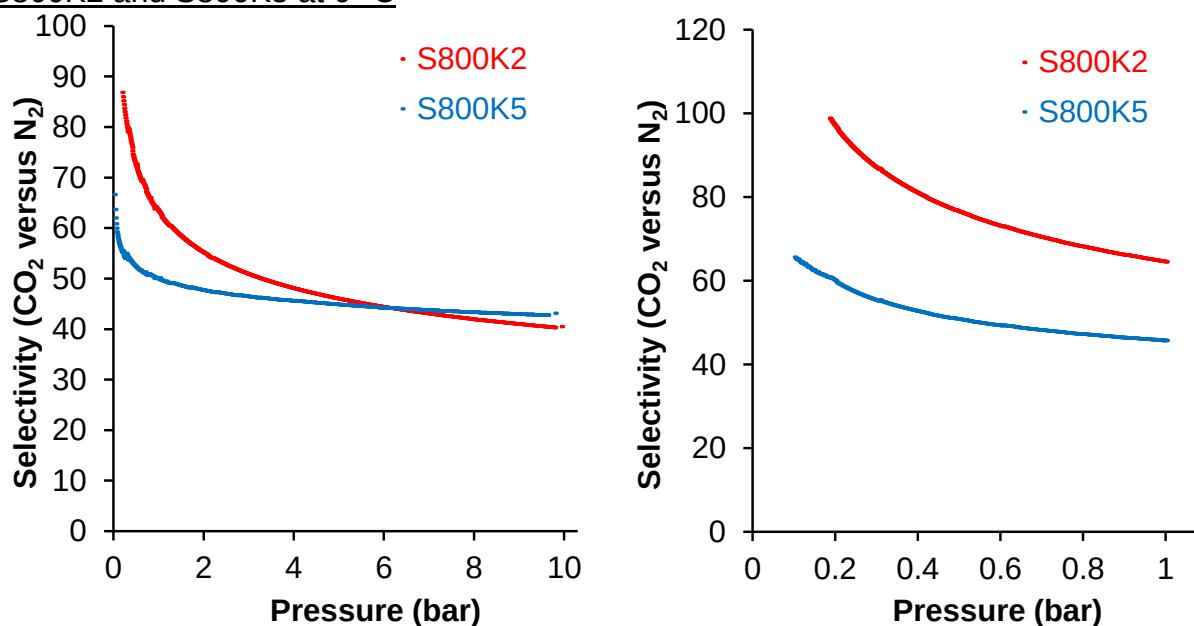
The selectivity of CO<sub>2</sub> versus N<sub>2</sub> adsorption was calculated based on the single component adsorption isotherms by applying Ideal Adsorbed Solutions Theory (IAST):  $S=(q_1p_2)/(q_2p_1)$  where  $q_1$  (mmol g<sup>-1</sup>) and  $q_2$  (mmol g<sup>-1</sup>) are the amount of CO<sub>2</sub> adsorbed at the equilibrium partial pressures of  $p_1$  (bar) and  $p_2$  (bar), respectively. The typical composition of post-combustion flue gas is 15% CO<sub>2</sub> and 85% N<sub>2</sub> by volume. Therefore, the equilibrium partial pressures of N<sub>2</sub> and CO<sub>2</sub> in the bulk phase were deemed to be 0.85 bar and 0.15 bar.

### S800 and S800K2 at 25 °C



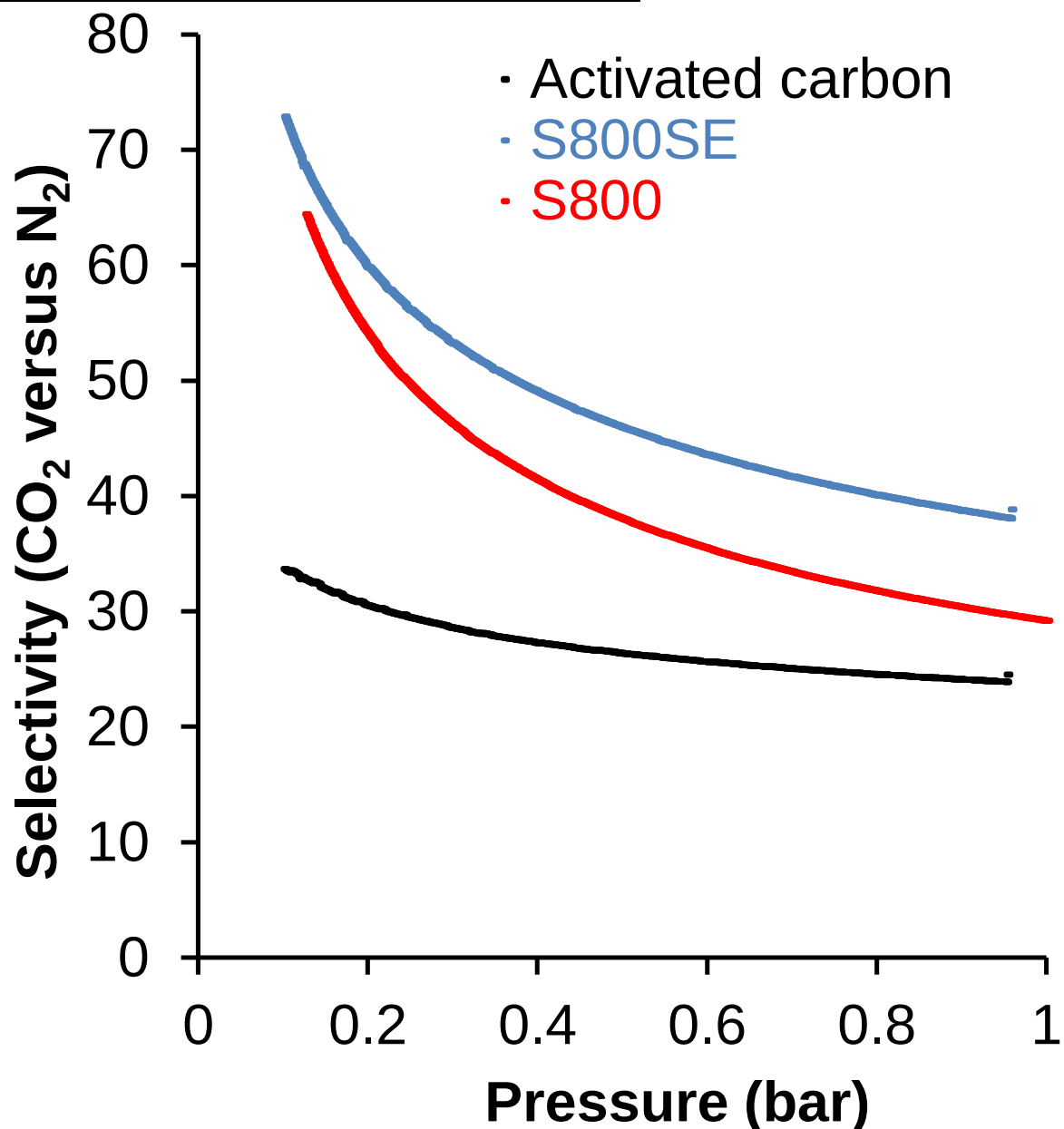
The 0-1 bar graph is plotted using data calculated using only the 0-1 bar adsorption isotherms. This will give low pressure selectivities (0-1 bar) that are more accurate than those calculated using the whole 0-10 bar adsorption isotherms.

### S800K2 and S800K5 at 0 °C



The 0.1-1 bar graph is plotted using data calculated using only the 0.1-1 bar adsorption isotherms. This will give low pressure selectivities (0.1-1 bar) that are more accurate than those calculated using the whole 0.1-10 bar adsorption isotherms.

Norit activated carbon, S800SE and S800 at 25 °C



CO<sub>2</sub> and N<sub>2</sub> adsorption isotherm data for Norit activated carbon and S800SE (prepared by the solvent exchange method) are taken from (*Angew. Chem. Int. Ed.* **2016**, 55, 9173–9177) and compared with the data obtained in this work for S800. As the Norit activated carbon and S800SE data was measured by porosimetry, only 0.1-1 bar data is available.

Tabulation of selectivities

| SAMPLE                 | Selectivity at 1 bar | Selectivity at 10 bar |
|------------------------|----------------------|-----------------------|
| Activated Carbon 25 °C | 24.5                 |                       |
| S800SE                 | 38.7                 |                       |
| S800 25 °C             | 29.1                 | 15.7                  |
| S800K2 25 °C           | 59.9                 | 36.6                  |
| S800K2 0 °C            | 64.5                 | 40.5                  |
| S800K5 0 °C            | 45.6                 | 43.1                  |



Tabulation of material physical properties and CO<sub>2</sub> uptake parameters

| Material | Ultramicropore surface area (m <sup>2</sup> g <sup>-1</sup> ) | Micropore surface area (m <sup>2</sup> g <sup>-1</sup> ) | External surface area (m <sup>2</sup> g <sup>-1</sup> ) | BET surface area (m <sup>2</sup> g <sup>-1</sup> ) | Ultramicropore volume <sub>&lt;0.7 nm</sub> (cm <sup>3</sup> g <sup>-1</sup> ) | CO <sub>2</sub> uptake (mmol g <sup>-1</sup> ) | CO <sub>2</sub> adsorption enthalpy (-KJ mol <sup>-1</sup> ) | K <sub>1</sub> for CO <sub>2</sub> adsorption (min <sup>-1</sup> ) |
|----------|---------------------------------------------------------------|----------------------------------------------------------|---------------------------------------------------------|----------------------------------------------------|--------------------------------------------------------------------------------|------------------------------------------------|--------------------------------------------------------------|--------------------------------------------------------------------|
| S300     |                                                               | 154                                                      | 151                                                     | 305                                                |                                                                                | 0.48                                           | 40.2                                                         | 6.81                                                               |
| S600     |                                                               | 533                                                      | 94                                                      | 627                                                | 0.18                                                                           | 1.07                                           | 42.4                                                         | 6.55                                                               |
| S800     | 253                                                           | 543                                                      | 76                                                      | 619                                                | 0.19                                                                           | 1.59                                           | 35.3                                                         | 8.85                                                               |
| S1000    | 210                                                           | 437                                                      | 83                                                      | 520                                                | 0.15                                                                           | 1.09                                           | 38.3                                                         | 8.32                                                               |
| A800     | 161                                                           | 160                                                      | 163                                                     | 322                                                | 0.08                                                                           | 1.36                                           | 48.6                                                         | 5.16                                                               |
| P800     | 142                                                           | 135                                                      | 127                                                     | 262                                                | 0.07                                                                           | 1.07                                           | 52.9                                                         | 7.33                                                               |
| S600K4   | 467                                                           | 1784                                                     | 106                                                     | 1890                                               | 0.5                                                                            | 2.02                                           | 29.1                                                         | 5.51                                                               |
| S1000K4  | 316                                                           | 1151                                                     | 353                                                     | 1503                                               | 0.28                                                                           | 1.11                                           | 34.5                                                         | 4.74                                                               |
| S800K1   | 868                                                           | 908                                                      | 306                                                     | 1214                                               | 0.32                                                                           | 2.39                                           | 31.7                                                         | 4.36                                                               |
| S800K2   | 1225                                                          | 1177                                                     | 117                                                     | 1294                                               | 0.39                                                                           | 3.11                                           | 33.6                                                         | 3.3                                                                |
| S800K3   | 1105                                                          | 1468                                                     | 165                                                     | 1633                                               | 0.45                                                                           | 2.93                                           | 32.7                                                         | 4.05                                                               |
| S800K4   | 727                                                           | 1781                                                     | 518                                                     | 2299                                               | 0.46                                                                           | 2.14                                           | 30.9                                                         | 5.25                                                               |
| S800K5   | 804                                                           | 1404                                                     | 1048                                                    | 2452                                               | 0.57                                                                           | 2.07                                           | 26.7                                                         | 4.38                                                               |
| A600K2   | 718                                                           | 598                                                      | 89                                                      | 687                                                | 0.22                                                                           | 1.64                                           | 46                                                           | 4.52                                                               |
| A800K2   | 837                                                           | 1249                                                     | 143                                                     | 1392                                               | 0.43                                                                           | 2.95                                           | 38.5                                                         | 3.6                                                                |
| A1000K2  | 230                                                           | 923                                                      | 311                                                     | 1233                                               | 0.33                                                                           | 2.16                                           | 38                                                           | 4.22                                                               |
| A800K1   | 271                                                           | 626                                                      | 491                                                     | 1117                                               | 0.29                                                                           | 1.98                                           | 38.6                                                         | 2.92                                                               |
| A800K3   | 1017                                                          | 1699                                                     | 253                                                     | 1952                                               | 0.57                                                                           | 2.82                                           | 36.1                                                         | 3.06                                                               |
| A800K4   | 529                                                           | 1482                                                     | 937                                                     | 2419                                               | 0.39                                                                           | 2.25                                           | 33.3                                                         | 3.55                                                               |
| A800K5   | 669                                                           | 1102                                                     | 1311                                                    | 2414                                               | 0.55                                                                           | 1.75                                           | 38.2                                                         | 5.68                                                               |
| P800K2   | 960                                                           | 1251                                                     | 644                                                     | 1895                                               | 0.52                                                                           | 2.39                                           | 36.9                                                         | 3.79                                                               |
| P800K3   | 705                                                           | 1152                                                     | 594                                                     | 1747                                               | 0.47                                                                           | 2.07                                           | 35.1                                                         | 2.46                                                               |
| P800K5   | 572                                                           | 812                                                      | 1142                                                    | 1954                                               | 0.43                                                                           | 1.25                                           | 37.6                                                         | 5.57                                                               |
| S800C15  | 103                                                           | 430                                                      | 99                                                      | 529                                                | 0.17                                                                           | 1.64                                           | 25                                                           | 3.74                                                               |
| S850C15  | 600                                                           | 462                                                      | 175                                                     | 637                                                | 0.2                                                                            | 1.77                                           | 36.3                                                         | 4.85                                                               |
| S900C15  | 931                                                           | 745                                                      | 238                                                     | 983                                                | 0.31                                                                           | 1.98                                           | 35.8                                                         | 4.93                                                               |

|                 |      |      |      |      |      |      |      |      |
|-----------------|------|------|------|------|------|------|------|------|
| <b>S950C15</b>  | 738  | 668  | 261  | 930  | 0.28 | 1.82 | 34.9 | 5.59 |
| <b>S1000C15</b> | 803  | 1033 | 502  | 1535 | 0.42 | 1.77 | 40.2 | 5.58 |
| <b>S900C30</b>  | 940  | 827  | 292  | 1119 | 0.34 | 1.77 | 31.9 | 6.29 |
| <b>S900C60</b>  | 934  | 805  | 292  | 1097 | 0.33 | 1.98 | 36.4 | 5.08 |
| <b>S900C90</b>  | 935  | 1089 | 386  | 1475 | 0.43 | 1.91 | 37.4 | 6.9  |
| <b>S900C120</b> | 1022 | 1331 | 583  | 1914 | 0.52 | 1.89 | 35.9 | 6.5  |
| <b>S950C60</b>  | 802  | 1418 | 761  | 2180 | 0.53 | 1.82 | 42.7 | 6.04 |
| <b>S950C90</b>  | 731  | 1193 | 1264 | 2457 | 0.56 | 1.52 | 46.7 | 8.71 |
| <b>S950C120</b> | 609  | 703  | 2030 | 2733 | 0.56 | 1.18 | 53.7 | 9.1  |
| <b>A750C45</b>  | 13   | 393  | 344  | 738  | 0.21 | 1.43 | 45.7 | 4.23 |
| <b>A750C60</b>  | 13   | 385  | 371  | 756  | 0.21 | 1.41 | 47.5 | 5.71 |
| <b>A750C90</b>  | 544  | 363  | 399  | 762  | 0.21 | 1.43 | 43.7 | 3.57 |
| <b>A900C0</b>   | 30   | 343  | 479  | 822  | 0.22 | 1.39 | 46.4 | 5.49 |
| <b>A900C10</b>  | 29   | 237  | 631  | 868  | 0.21 | 1.14 | 48.2 | 5.85 |
| <b>P700C50</b>  | 586  | 404  | 330  | 734  | 0.21 | 1.30 | 68.5 | 6.6  |
| <b>P900C0</b>   | 401  | 260  | 686  | 946  | 0.22 | 1.20 | 69   | 5.71 |
| <b>S700O0</b>   | 770  | 732  | 165  | 897  | 0.27 | 1.98 | 32.2 | 6    |
| <b>S750O0</b>   | 369  | 933  | 168  | 1100 | 0.33 | 2.02 | 34.6 | 4.29 |
| <b>S800O0</b>   | 724  | 704  | 230  | 935  | 0.28 | 1.82 | 30   | 4.98 |
| <b>S750O40</b>  | 632  | 772  | 118  | 889  | 0.27 | 1.91 | 30.8 | 5.22 |
| <b>S750O56</b>  | 604  | 590  | 188  | 777  | 0.23 | 1.89 | 36.7 | 4.65 |
| <b>A500O30</b>  | 23   | 354  | 286  | 640  | 0.18 | 1.36 | 47   | 5.2  |
| <b>A500O60</b>  | 123  | 396  | 251  | 647  | 0.19 | 1.32 | 46.3 | 5.14 |
| <b>A750O0</b>   | 505  | 364  | 265  | 629  | 0.17 | 1.41 | 30.6 | 5.69 |
| <b>P400O50</b>  | 293  | 209  | 177  | 385  | 0.11 | 1.02 | 73.5 |      |

BET surface area = External surface area + micropore surface area

Micropore volume = Ultramicropore volume + supramicropore volume

Ultramicropore surface area is determined by the DFT model

| Material | Supramicropore<br>volume <sub>0.7-2 nm</sub><br>(cm <sup>3</sup> g <sup>-1</sup> ) | Micropore<br>volume <sub>&lt;2 nm</sub><br>(cm <sup>3</sup> g <sup>-1</sup> ) | Mesopore<br>volume<br>(cm <sup>3</sup> g <sup>-1</sup> ) | Total pore<br>volume<br>P/P <sub>0</sub> =0.99<br>(cm <sup>3</sup> g <sup>-1</sup> ) | Ultramicropore<br>volume / total<br>pore volume | CO <sub>2</sub><br>uptake<br>(mmol g <sup>-1</sup> ) | CO <sub>2</sub><br>adsorption<br>enthalpy<br>(-KJ mol <sup>-1</sup> ) | K <sub>1</sub> for CO <sub>2</sub><br>adsorption<br>(min <sup>-1</sup> ) |
|----------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------|----------------------------------------------------------|--------------------------------------------------------------------------------------|-------------------------------------------------|------------------------------------------------------|-----------------------------------------------------------------------|--------------------------------------------------------------------------|
| S300     | 0.13                                                                               | 0.13                                                                          | 0.22                                                     | 0.35                                                                                 |                                                 | 0.48                                                 | 40.2                                                                  | 6.81                                                                     |
| S600     | 0.07                                                                               | 0.25                                                                          | 0.34                                                     | 0.59                                                                                 | 0.31                                            | 1.07                                                 | 42.4                                                                  | 6.55                                                                     |
| S800     | 0.05                                                                               | 0.24                                                                          | 0.35                                                     | 0.59                                                                                 | 0.32                                            | 1.59                                                 | 35.3                                                                  | 8.85                                                                     |
| S1000    | 0.05                                                                               | 0.2                                                                           | 0.39                                                     | 0.59                                                                                 | 0.25                                            | 1.09                                                 | 38.3                                                                  | 8.32                                                                     |
| A800     | 0.05                                                                               | 0.13                                                                          | 0.71                                                     | 0.81                                                                                 | 0.1                                             | 1.36                                                 | 48.6                                                                  | 5.16                                                                     |
| P800     | 0.04                                                                               | 0.11                                                                          | 0.43                                                     | 0.54                                                                                 | 0.13                                            | 1.07                                                 | 52.9                                                                  | 7.33                                                                     |
| S600K4   | 0.23                                                                               | 0.73                                                                          | 0.13                                                     | 0.84                                                                                 | 0.6                                             | 2.02                                                 | 29.1                                                                  | 5.51                                                                     |
| S1000K4  | 0.34                                                                               | 0.62                                                                          | 0.23                                                     | 0.84                                                                                 | 0.33                                            | 1.11                                                 | 34.5                                                                  | 4.74                                                                     |
| S800K1   | 0.16                                                                               | 0.48                                                                          | 0.58                                                     | 1.06                                                                                 | 0.3                                             | 2.39                                                 | 31.7                                                                  | 4.36                                                                     |
| S800K2   | 0.1                                                                                | 0.49                                                                          | 0.1                                                      | 0.59                                                                                 | 0.66                                            | 3.11                                                 | 33.6                                                                  | 3.3                                                                      |
| S800K3   | 0.17                                                                               | 0.62                                                                          | 0.14                                                     | 0.77                                                                                 | 0.58                                            | 2.93                                                 | 32.7                                                                  | 4.05                                                                     |
| S800K4   | 0.45                                                                               | 0.91                                                                          | 0.07                                                     | 0.98                                                                                 | 0.47                                            | 2.14                                                 | 30.9                                                                  | 5.25                                                                     |
| S800K5   | 0.43                                                                               | 1                                                                             | 0.09                                                     | 1.09                                                                                 | 0.52                                            | 2.07                                                 | 26.7                                                                  | 4.38                                                                     |
| A600K2   | 0.05                                                                               | 0.27                                                                          | 0.08                                                     | 0.36                                                                                 | 0.61                                            | 1.64                                                 | 46                                                                    | 4.52                                                                     |
| A800K2   | 0.1                                                                                | 0.53                                                                          | 0.15                                                     | 0.67                                                                                 | 0.64                                            | 2.95                                                 | 38.5                                                                  | 3.6                                                                      |
| A1000K2  | 0.16                                                                               | 0.49                                                                          | 0.3                                                      | 0.8                                                                                  | 0.41                                            | 2.16                                                 | 38                                                                    | 4.22                                                                     |
| A800K1   | 0.17                                                                               | 0.46                                                                          | 0.82                                                     | 1.31                                                                                 | 0.22                                            | 1.98                                                 | 38.6                                                                  | 2.92                                                                     |
| A800K3   | 0.18                                                                               | 0.75                                                                          | 0.09                                                     | 0.85                                                                                 | 0.67                                            | 2.82                                                 | 36.1                                                                  | 3.06                                                                     |
| A800K4   | 0.56                                                                               | 0.95                                                                          | 0.18                                                     | 1.15                                                                                 | 0.34                                            | 2.25                                                 | 33.3                                                                  | 3.55                                                                     |
| A800K5   | 0.46                                                                               | 1.01                                                                          | 0.1                                                      | 1.09                                                                                 | 0.51                                            | 1.75                                                 | 38.2                                                                  | 5.68                                                                     |
| P800K2   | 0.25                                                                               | 0.77                                                                          | 0.18                                                     | 0.97                                                                                 | 0.54                                            | 2.39                                                 | 36.9                                                                  | 3.79                                                                     |
| P800K3   | 0.26                                                                               | 0.73                                                                          | 0.13                                                     | 0.86                                                                                 | 0.55                                            | 2.07                                                 | 35.1                                                                  | 2.46                                                                     |
| P800K5   | 0.39                                                                               | 0.82                                                                          | 0.2                                                      | 1.02                                                                                 | 0.42                                            | 1.25                                                 | 37.6                                                                  | 5.57                                                                     |
| S800C15  | 0.04                                                                               | 0.21                                                                          | 0.37                                                     | 0.58                                                                                 | 0.29                                            | 1.64                                                 | 25                                                                    | 3.74                                                                     |
| S850C15  | 0.06                                                                               | 0.26                                                                          | 0.31                                                     | 0.6                                                                                  | 0.33                                            | 1.77                                                 | 36.3                                                                  | 4.85                                                                     |
| S900C15  | 0.08                                                                               | 0.39                                                                          | 0.38                                                     | 0.77                                                                                 | 0.4                                             | 1.98                                                 | 35.8                                                                  | 4.93                                                                     |
| S950C15  | 0.1                                                                                | 0.38                                                                          | 0.35                                                     | 0.73                                                                                 | 0.38                                            | 1.82                                                 | 34.9                                                                  | 5.59                                                                     |

|                 |      |      |      |      |      |      |      |      |
|-----------------|------|------|------|------|------|------|------|------|
| <b>S1000C15</b> | 0.2  | 0.62 | 0.52 | 1.16 | 0.36 | 1.77 | 40.2 | 5.58 |
| <b>S900C30</b>  | 0.11 | 0.45 | 0.5  | 0.98 | 0.35 | 1.77 | 31.9 | 6.29 |
| <b>S900C60</b>  | 0.11 | 0.44 | 0.4  | 0.89 | 0.37 | 1.98 | 36.4 | 5.08 |
| <b>S900C90</b>  | 0.16 | 0.59 | 0.45 | 1.05 | 0.41 | 1.91 | 37.4 | 6.9  |
| <b>S900C120</b> | 0.25 | 0.77 | 0.71 | 1.49 | 0.35 | 1.89 | 35.9 | 6.5  |
| <b>S950C60</b>  | 0.36 | 0.89 | 0.41 | 1.32 | 0.4  | 1.82 | 42.7 | 6.04 |
| <b>S950C90</b>  | 0.48 | 1.04 | 0.59 | 1.64 | 0.34 | 1.52 | 46.7 | 8.71 |
| <b>S950C120</b> | 0.6  | 1.16 | 0.96 | 2.09 | 0.27 | 1.18 | 53.7 | 9.1  |
| <b>A750C45</b>  | 0.1  | 0.31 | 0.68 | 0.99 | 0.21 | 1.43 | 45.7 | 4.23 |
| <b>A750C60</b>  | 0.11 | 0.32 | 0.76 | 1.09 | 0.19 | 1.41 | 47.5 | 5.71 |
| <b>A750C90</b>  | 0.11 | 0.32 | 0.74 | 1.05 | 0.2  | 1.43 | 43.7 | 3.57 |
| <b>A900C0</b>   | 0.13 | 0.35 | 0.86 | 1.18 | 0.19 | 1.39 | 46.4 | 5.49 |
| <b>A900C10</b>  | 0.17 | 0.38 | 0.98 | 1.33 | 0.16 | 1.14 | 48.2 | 5.85 |
| <b>P700C50</b>  | 0.1  | 0.31 | 0.47 | 0.78 | 0.27 | 1.30 | 68.5 | 6.6  |
| <b>P900C0</b>   | 0.18 | 0.4  | 0.54 | 0.93 | 0.24 | 1.20 | 69   | 5.71 |
| <b>S700O0</b>   | 0.08 | 0.35 | 0.14 | 0.5  | 0.54 | 1.98 | 32.2 | 6    |
| <b>S750O0</b>   | 0.1  | 0.43 | 0.14 | 0.58 | 0.57 | 2.02 | 34.6 | 4.29 |
| <b>S800O0</b>   | 0.09 | 0.37 | 0.2  | 0.57 | 0.49 | 1.82 | 30   | 4.98 |
| <b>S750O40</b>  | 0.08 | 0.35 | 0.09 | 0.45 | 0.6  | 1.91 | 30.8 | 5.22 |
| <b>S750O56</b>  | 0.08 | 0.31 | 0.15 | 0.46 | 0.5  | 1.89 | 36.7 | 4.65 |
| <b>A500O30</b>  | 0.09 | 0.27 | 0.7  | 0.97 | 0.19 | 1.36 | 47   | 5.2  |
| <b>A500O60</b>  | 0.08 | 0.27 | 0.66 | 0.96 | 0.2  | 1.32 | 46.3 | 5.14 |
| <b>A750O0</b>   | 0.09 | 0.26 | 0.67 | 0.94 | 0.18 | 1.41 | 30.6 | 5.69 |
| <b>P400O50</b>  | 0.05 | 0.16 | 0.44 | 0.6  | 0.18 | 1.02 | 73.5 |      |

BET surface area = External surface area + micropore surface area  
Micropore volume = Ultramicropore volume + supramicropore volume  
Ultramicropore surface area is determined by the DFT model

| Material | Supramicropore<br>volume / total<br>pore volume | Micropore<br>volume / total<br>pore volume | Mesopore<br>volume / total<br>pore volume | Micropore volume<br>/ mesopore volume | CO <sub>2</sub><br>uptake<br>(mmol g <sup>-1</sup> ) | CO <sub>2</sub> adsorption<br>enthalpy<br>(-KJ mol <sup>-1</sup> ) | K <sub>1</sub> for CO <sub>2</sub><br>adsorption<br>(min <sup>-1</sup> ) |
|----------|-------------------------------------------------|--------------------------------------------|-------------------------------------------|---------------------------------------|------------------------------------------------------|--------------------------------------------------------------------|--------------------------------------------------------------------------|
| S300     | 0.37                                            | 0.37                                       | 0.63                                      | 0.59                                  | 0.48                                                 | 40.2                                                               | 6.81                                                                     |
| S600     | 0.12                                            | 0.42                                       | 0.58                                      | 0.74                                  | 1.07                                                 | 42.4                                                               | 6.55                                                                     |
| S800     | 0.08                                            | 0.41                                       | 0.59                                      | 0.69                                  | 1.59                                                 | 35.3                                                               | 8.85                                                                     |
| S1000    | 0.08                                            | 0.34                                       | 0.66                                      | 0.51                                  | 1.09                                                 | 38.3                                                               | 8.32                                                                     |
| A800     | 0.06                                            | 0.16                                       | 0.88                                      | 0.18                                  | 1.36                                                 | 48.6                                                               | 5.16                                                                     |
| P800     | 0.07                                            | 0.2                                        | 0.80                                      | 0.26                                  | 1.07                                                 | 52.9                                                               | 7.33                                                                     |
| S600K4   | 0.27                                            | 0.87                                       | 0.15                                      | 5.62                                  | 2.02                                                 | 29.1                                                               | 5.51                                                                     |
| S1000K4  | 0.40                                            | 0.74                                       | 0.27                                      | 2.70                                  | 1.11                                                 | 34.5                                                               | 4.74                                                                     |
| S800K1   | 0.15                                            | 0.45                                       | 0.55                                      | 0.83                                  | 2.39                                                 | 31.7                                                               | 4.36                                                                     |
| S800K2   | 0.17                                            | 0.83                                       | 0.17                                      | 4.90                                  | 3.11                                                 | 33.6                                                               | 3.3                                                                      |
| S800K3   | 0.22                                            | 0.81                                       | 0.18                                      | 4.43                                  | 2.93                                                 | 32.7                                                               | 4.05                                                                     |
| S800K4   | 0.46                                            | 0.93                                       | 0.07                                      | 13.00                                 | 2.14                                                 | 30.9                                                               | 5.25                                                                     |
| S800K5   | 0.39                                            | 0.92                                       | 0.08                                      | 11.11                                 | 2.07                                                 | 26.7                                                               | 4.38                                                                     |
| A600K2   | 0.14                                            | 0.75                                       | 0.22                                      | 3.38                                  | 1.64                                                 | 46                                                                 | 4.52                                                                     |
| A800K2   | 0.15                                            | 0.79                                       | 0.22                                      | 3.53                                  | 2.95                                                 | 38.5                                                               | 3.6                                                                      |
| A1000K2  | 0.20                                            | 0.61                                       | 0.38                                      | 1.63                                  | 2.16                                                 | 38                                                                 | 4.22                                                                     |
| A800K1   | 0.13                                            | 0.35                                       | 0.63                                      | 0.56                                  | 1.98                                                 | 38.6                                                               | 2.92                                                                     |
| A800K3   | 0.21                                            | 0.88                                       | 0.11                                      | 8.33                                  | 2.82                                                 | 36.1                                                               | 3.06                                                                     |
| A800K4   | 0.49                                            | 0.83                                       | 0.16                                      | 5.28                                  | 2.25                                                 | 33.3                                                               | 3.55                                                                     |
| A800K5   | 0.42                                            | 0.93                                       | 0.09                                      | 10.10                                 | 1.75                                                 | 38.2                                                               | 5.68                                                                     |
| P800K2   | 0.26                                            | 0.79                                       | 0.19                                      | 4.28                                  | 2.39                                                 | 36.9                                                               | 3.79                                                                     |
| P800K3   | 0.30                                            | 0.85                                       | 0.15                                      | 5.62                                  | 2.07                                                 | 35.1                                                               | 2.46                                                                     |
| P800K5   | 0.38                                            | 0.8                                        | 0.20                                      | 4.10                                  | 1.25                                                 | 37.6                                                               | 5.57                                                                     |
| S800C15  | 0.07                                            | 0.36                                       | 0.64                                      | 0.57                                  | 1.64                                                 | 25                                                                 | 3.74                                                                     |
| S850C15  | 0.10                                            | 0.43                                       | 0.52                                      | 0.84                                  | 1.77                                                 | 36.3                                                               | 4.85                                                                     |
| S900C15  | 0.10                                            | 0.51                                       | 0.49                                      | 1.03                                  | 1.98                                                 | 35.8                                                               | 4.93                                                                     |
| S950C15  | 0.14                                            | 0.52                                       | 0.48                                      | 1.09                                  | 1.82                                                 | 34.9                                                               | 5.59                                                                     |
| S1000C15 | 0.17                                            | 0.53                                       | 0.45                                      | 1.19                                  | 1.77                                                 | 40.2                                                               | 5.58                                                                     |

|                 |      |      |      |      |      |      |      |
|-----------------|------|------|------|------|------|------|------|
| <b>S900C30</b>  | 0.11 | 0.46 | 0.51 | 0.90 | 1.77 | 31.9 | 6.29 |
| <b>S900C60</b>  | 0.12 | 0.49 | 0.45 | 1.10 | 1.98 | 36.4 | 5.08 |
| <b>S900C90</b>  | 0.15 | 0.56 | 0.43 | 1.31 | 1.91 | 37.4 | 6.9  |
| <b>S900C120</b> | 0.17 | 0.52 | 0.48 | 1.08 | 1.89 | 35.9 | 6.5  |
| <b>S950C60</b>  | 0.27 | 0.67 | 0.31 | 2.17 | 1.82 | 42.7 | 6.04 |
| <b>S950C90</b>  | 0.29 | 0.63 | 0.36 | 1.76 | 1.52 | 46.7 | 8.71 |
| <b>S950C120</b> | 0.29 | 0.56 | 0.46 | 1.21 | 1.18 | 53.7 | 9.1  |
| <b>A750C45</b>  | 0.10 | 0.31 | 0.69 | 0.46 | 1.43 | 45.7 | 4.23 |
| <b>A750C60</b>  | 0.10 | 0.29 | 0.70 | 0.42 | 1.41 | 47.5 | 5.71 |
| <b>A750C90</b>  | 0.10 | 0.3  | 0.70 | 0.43 | 1.43 | 43.7 | 3.57 |
| <b>A900C0</b>   | 0.11 | 0.3  | 0.73 | 0.41 | 1.39 | 46.4 | 5.49 |
| <b>A900C10</b>  | 0.13 | 0.29 | 0.74 | 0.39 | 1.14 | 48.2 | 5.85 |
| <b>P700C50</b>  | 0.13 | 0.4  | 0.60 | 0.66 | 1.30 | 68.5 | 6.6  |
| <b>P900C0</b>   | 0.19 | 0.43 | 0.58 | 0.74 | 1.20 | 69   | 5.71 |
| <b>S700O0</b>   | 0.16 | 0.7  | 0.28 | 2.50 | 1.98 | 32.2 | 6    |
| <b>S750O0</b>   | 0.17 | 0.74 | 0.24 | 3.07 | 2.02 | 34.6 | 4.29 |
| <b>S800O0</b>   | 0.16 | 0.65 | 0.35 | 1.85 | 1.82 | 30   | 4.98 |
| <b>S750O40</b>  | 0.18 | 0.78 | 0.20 | 3.89 | 1.91 | 30.8 | 5.22 |
| <b>S750O56</b>  | 0.17 | 0.67 | 0.33 | 2.07 | 1.89 | 36.7 | 4.65 |
| <b>A500O30</b>  | 0.09 | 0.28 | 0.72 | 0.39 | 1.36 | 47   | 5.2  |
| <b>A500O60</b>  | 0.08 | 0.28 | 0.69 | 0.41 | 1.32 | 46.3 | 5.14 |
| <b>A750O0</b>   | 0.10 | 0.28 | 0.71 | 0.39 | 1.41 | 30.6 | 5.69 |
| <b>P400O50</b>  | 0.08 | 0.27 | 0.73 | 0.36 | 1.02 | 73.5 |      |

BET surface area = External surface area + micropore surface area

Micropore volume = Ultramicropore volume + supramicropore volume

Ultramicropore surface area is determined by the DFT model

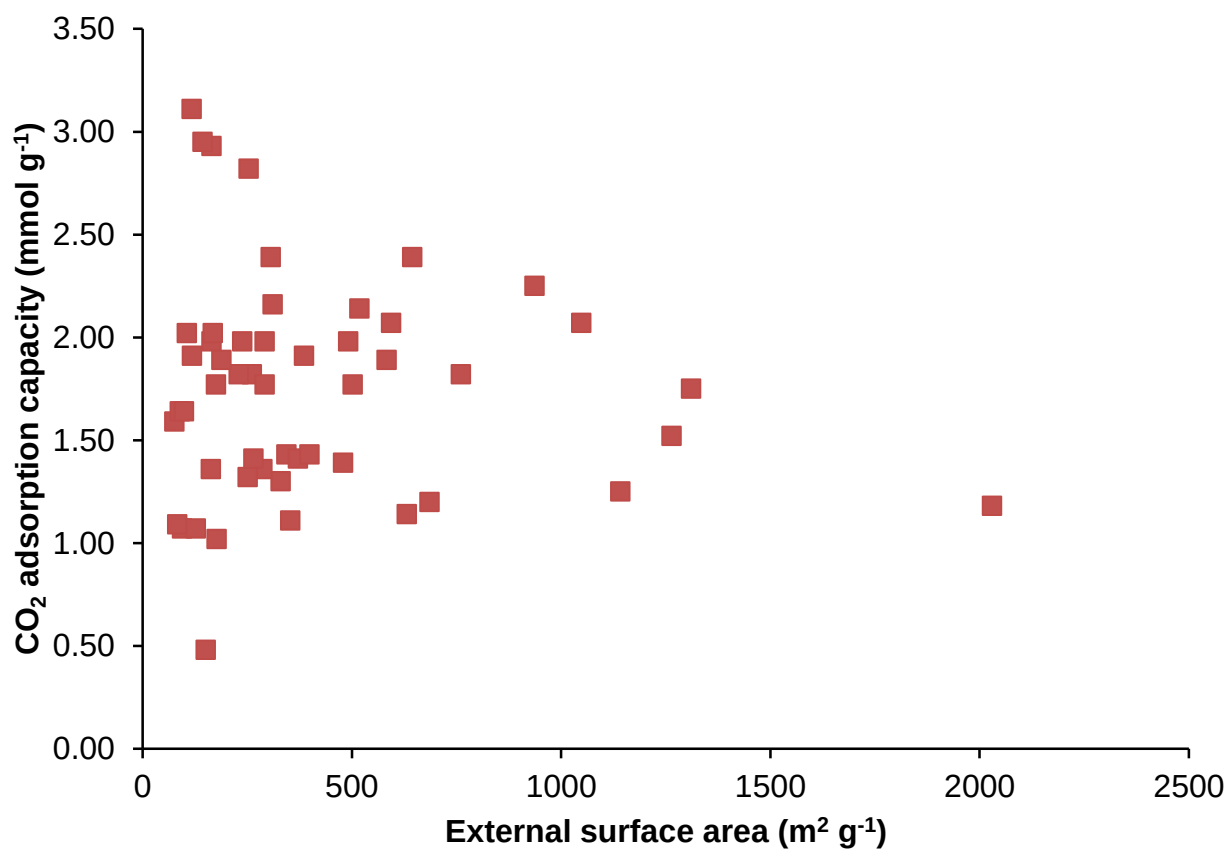
| Material | Ultramicropore<br>Volume <sub>0.4-0.7 nm</sub> (cm <sup>3</sup> g <sup>-1</sup> ) | Ultramicropore (0.4-0.7 nm)<br>volume / total pore volume | CO <sub>2</sub> uptake<br>(mmol g <sup>-1</sup> ) | CO <sub>2</sub> adsorption<br>enthalpy (-KJ mol <sup>-1</sup> ) | K <sub>1</sub> for CO <sub>2</sub><br>adsorption (min <sup>-1</sup> ) |
|----------|-----------------------------------------------------------------------------------|-----------------------------------------------------------|---------------------------------------------------|-----------------------------------------------------------------|-----------------------------------------------------------------------|
| S300     |                                                                                   |                                                           | 0.48                                              | 40.2                                                            | 6.81                                                                  |
| S600     | 0.18                                                                              | 0.31                                                      | 1.07                                              | 42.4                                                            | 6.55                                                                  |
| S800     | 0.18                                                                              | 0.31                                                      | 1.59                                              | 35.3                                                            | 8.85                                                                  |
| S1000    | 0.14                                                                              | 0.24                                                      | 1.09                                              | 38.3                                                            | 8.32                                                                  |
| A800     | 0.07                                                                              | 0.09                                                      | 1.36                                              | 48.6                                                            | 5.16                                                                  |
| P800     | 0.04                                                                              | 0.07                                                      | 1.07                                              | 52.9                                                            | 7.33                                                                  |
| S600K4   | 0.4                                                                               | 0.48                                                      | 2.02                                              | 29.1                                                            | 5.51                                                                  |
| S1000K4  | 0.19                                                                              | 0.23                                                      | 1.11                                              | 34.5                                                            | 4.74                                                                  |
| S800K1   | 0.23                                                                              | 0.22                                                      | 2.39                                              | 31.7                                                            | 4.36                                                                  |
| S800K2   | 0.29                                                                              | 0.49                                                      | 3.11                                              | 33.6                                                            | 3.3                                                                   |
| S800K3   | 0.35                                                                              | 0.45                                                      | 2.93                                              | 32.7                                                            | 4.05                                                                  |
| S800K4   | 0.39                                                                              | 0.40                                                      | 2.14                                              | 30.9                                                            | 5.25                                                                  |
| S800K5   | 0.46                                                                              | 0.42                                                      | 2.07                                              | 26.7                                                            | 4.38                                                                  |
| A600K2   | 0.13                                                                              | 0.36                                                      | 1.64                                              | 46                                                              | 4.52                                                                  |
| A800K2   | 0.36                                                                              | 0.54                                                      | 2.95                                              | 38.5                                                            | 3.6                                                                   |
| A1000K2  | 0.32                                                                              | 0.40                                                      | 2.16                                              | 38                                                              | 4.22                                                                  |
| A800K1   | 0.27                                                                              | 0.21                                                      | 1.98                                              | 38.6                                                            | 2.92                                                                  |
| A800K3   | 0.48                                                                              | 0.56                                                      | 2.82                                              | 36.1                                                            | 3.06                                                                  |
| A800K4   | 0.33                                                                              | 0.29                                                      | 2.25                                              | 33.3                                                            | 3.55                                                                  |
| A800K5   | 0.48                                                                              | 0.44                                                      | 1.75                                              | 38.2                                                            | 5.68                                                                  |
| P800K2   | 0.39                                                                              | 0.40                                                      | 2.39                                              | 36.9                                                            | 3.79                                                                  |
| P800K3   | 0.43                                                                              | 0.50                                                      | 2.07                                              | 35.1                                                            | 2.46                                                                  |
| P800K5   | 0.35                                                                              | 0.34                                                      | 1.25                                              | 37.6                                                            | 5.57                                                                  |
| S800C15  | 0.16                                                                              | 0.28                                                      | 1.64                                              | 25                                                              | 3.74                                                                  |
| S850C15  | 0.19                                                                              | 0.32                                                      | 1.77                                              | 36.3                                                            | 4.85                                                                  |
| S900C15  | 0.18                                                                              | 0.23                                                      | 1.98                                              | 35.8                                                            | 4.93                                                                  |
| S950C15  | 0.17                                                                              | 0.23                                                      | 1.82                                              | 34.9                                                            | 5.59                                                                  |
| S1000C15 | 0.31                                                                              | 0.27                                                      | 1.77                                              | 40.2                                                            | 5.58                                                                  |
| S900C30  | 0.23                                                                              | 0.23                                                      | 1.77                                              | 31.9                                                            | 6.29                                                                  |

|                 |      |      |      |      |      |
|-----------------|------|------|------|------|------|
| <b>S900C60</b>  | 0.2  | 0.22 | 1.98 | 36.4 | 5.08 |
| <b>S900C90</b>  | 0.3  | 0.29 | 1.91 | 37.4 | 6.9  |
| <b>S900C120</b> | 0.4  | 0.27 | 1.89 | 35.9 | 6.5  |
| <b>S950C60</b>  | 0.42 | 0.32 | 1.82 | 42.7 | 6.04 |
| <b>S950C90</b>  | 0.45 | 0.27 | 1.52 | 46.7 | 8.71 |
| <b>S950C120</b> | 0.47 | 0.22 | 1.18 | 53.7 | 9.1  |
| <b>A750C45</b>  | 0.1  | 0.10 | 1.43 | 45.7 | 4.23 |
| <b>A750C60</b>  | 0.1  | 0.09 | 1.41 | 47.5 | 5.71 |
| <b>A750C90</b>  | 0.11 | 0.10 | 1.43 | 43.7 | 3.57 |
| <b>A900C0</b>   | 0.12 | 0.10 | 1.39 | 46.4 | 5.49 |
| <b>A900C10</b>  | 0.13 | 0.10 | 1.14 | 48.2 | 5.85 |
| <b>P700C50</b>  | 0.11 | 0.14 | 1.30 | 68.5 | 6.6  |
| <b>P900C0</b>   | 0.16 | 0.17 | 1.20 | 69   | 5.71 |
| <b>S700O0</b>   | 0.14 | 0.28 | 1.98 | 32.2 | 6    |
| <b>S750O0</b>   | 0.18 | 0.31 | 2.02 | 34.6 | 4.29 |
| <b>S800O0</b>   | 0.17 | 0.30 | 1.82 | 30   | 4.98 |
| <b>S750O40</b>  | 0.17 | 0.38 | 1.91 | 30.8 | 5.22 |
| <b>S750O56</b>  | 0.13 | 0.28 | 1.89 | 36.7 | 4.65 |
| <b>A500O30</b>  | 0.08 | 0.08 | 1.36 | 47   | 5.2  |
| <b>A500O60</b>  | 0.09 | 0.09 | 1.32 | 46.3 | 5.14 |
| <b>A750O0</b>   | 0.09 | 0.10 | 1.41 | 30.6 | 5.69 |
| <b>P400O50</b>  | 0.06 | 0.10 | 1.02 | 73.5 |      |

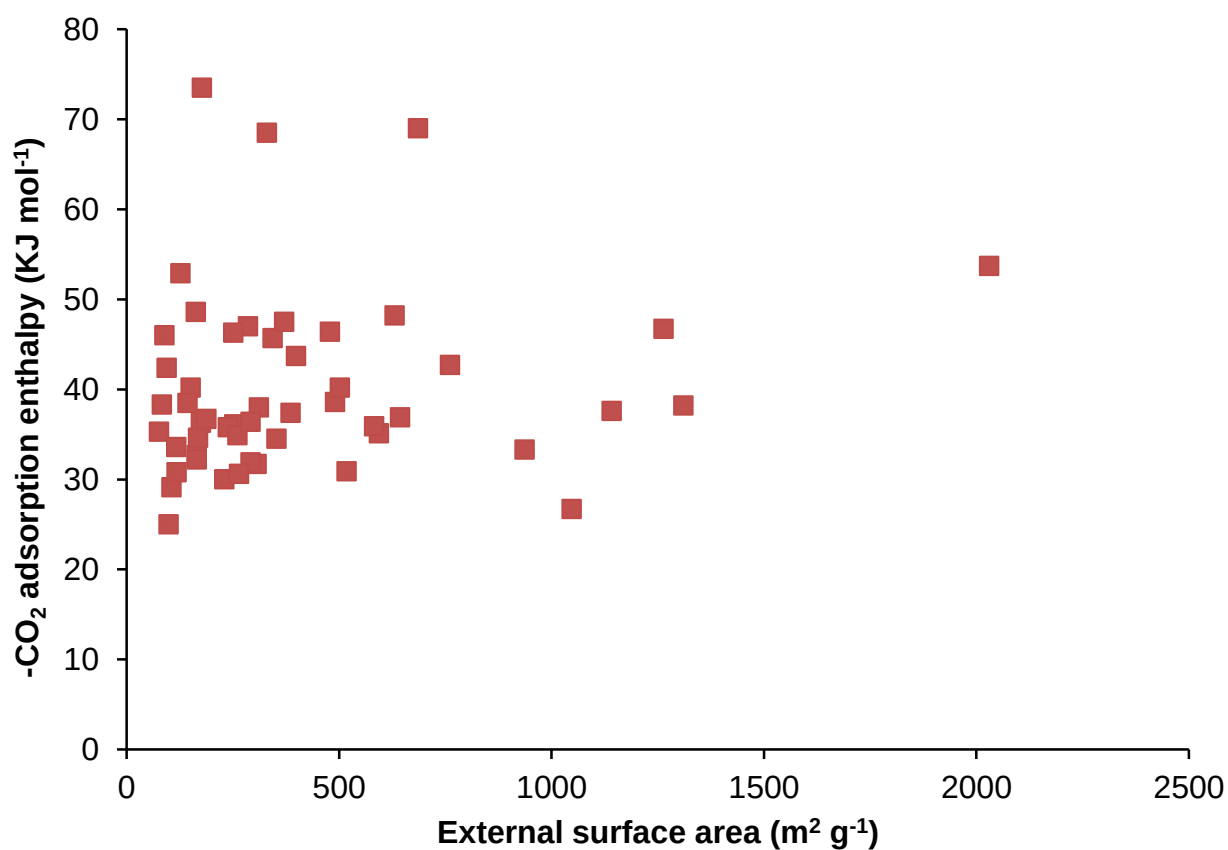


## Plots of textural properties with CO<sub>2</sub> uptake parameters

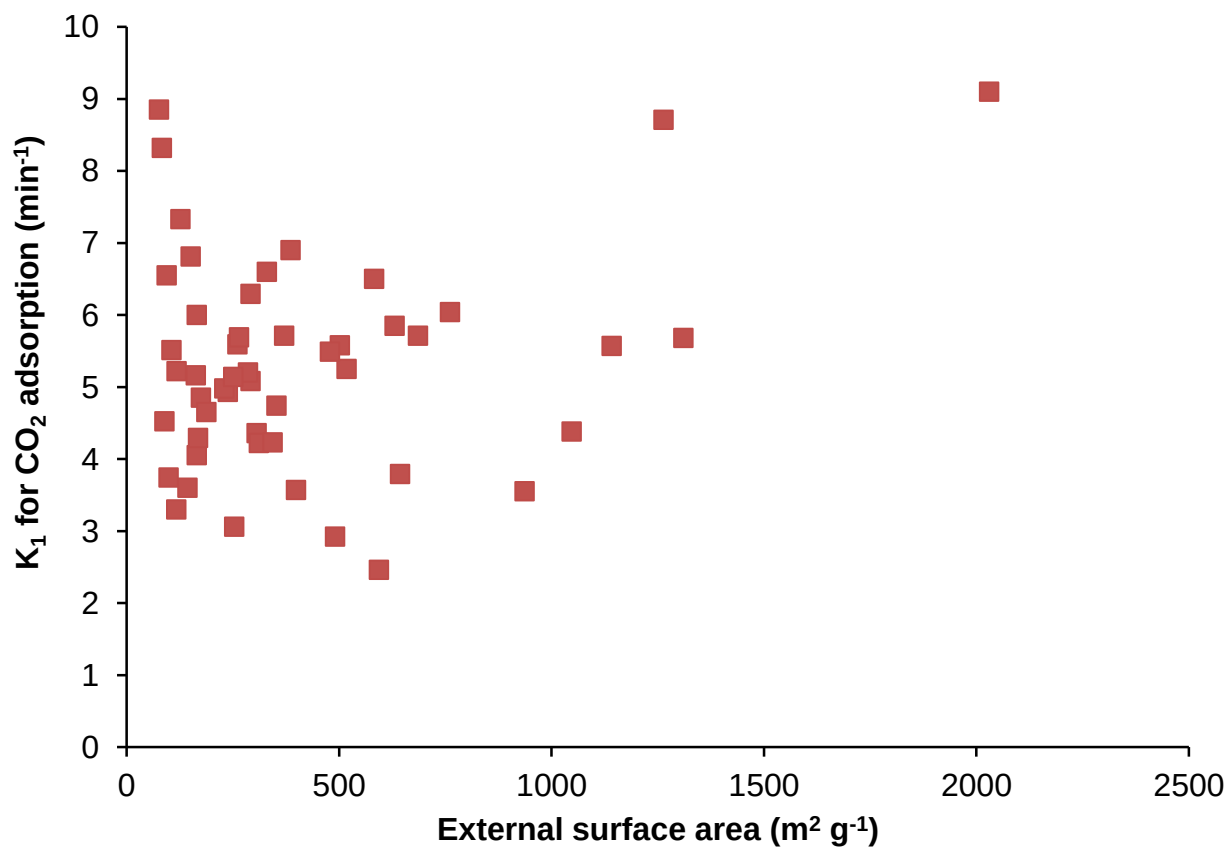
Plot of CO<sub>2</sub> adsorption capacity against external surface area



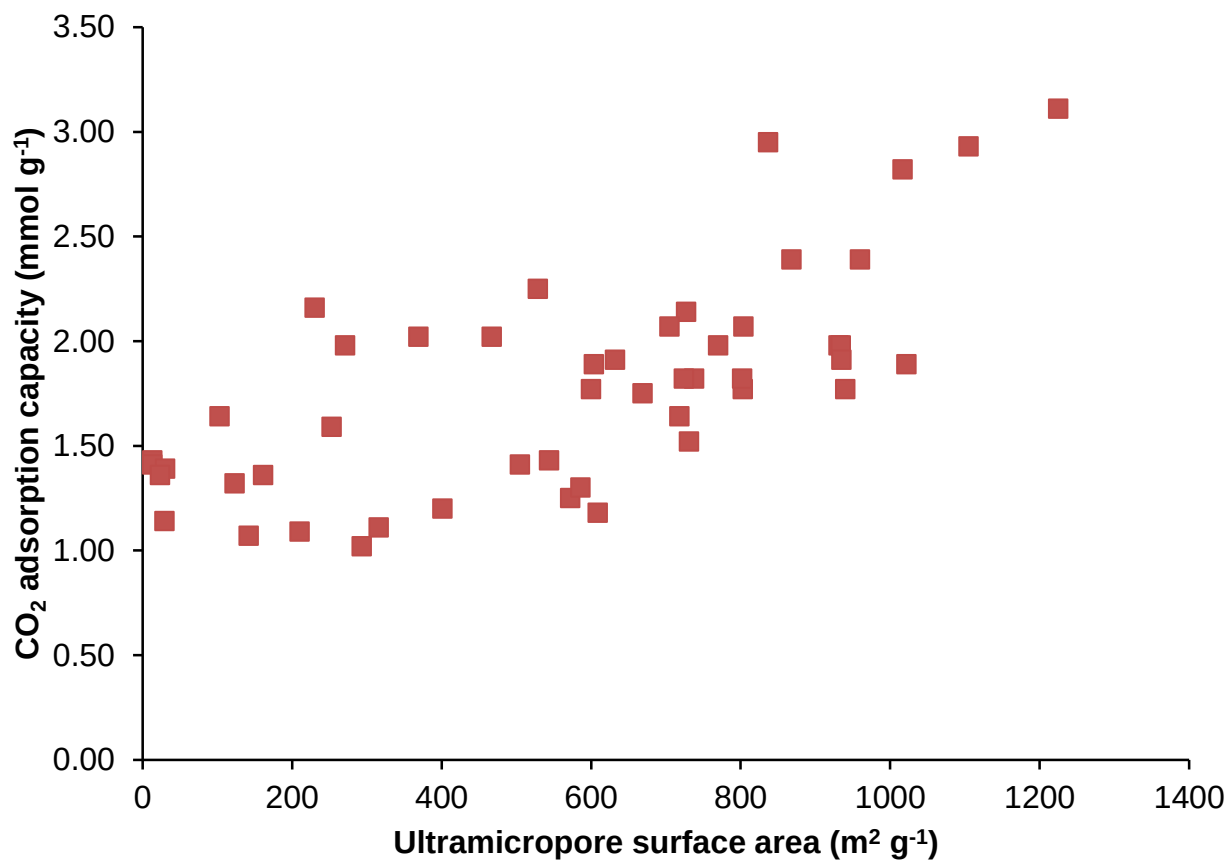
Plot of CO<sub>2</sub> adsorption enthalpy against external surface area



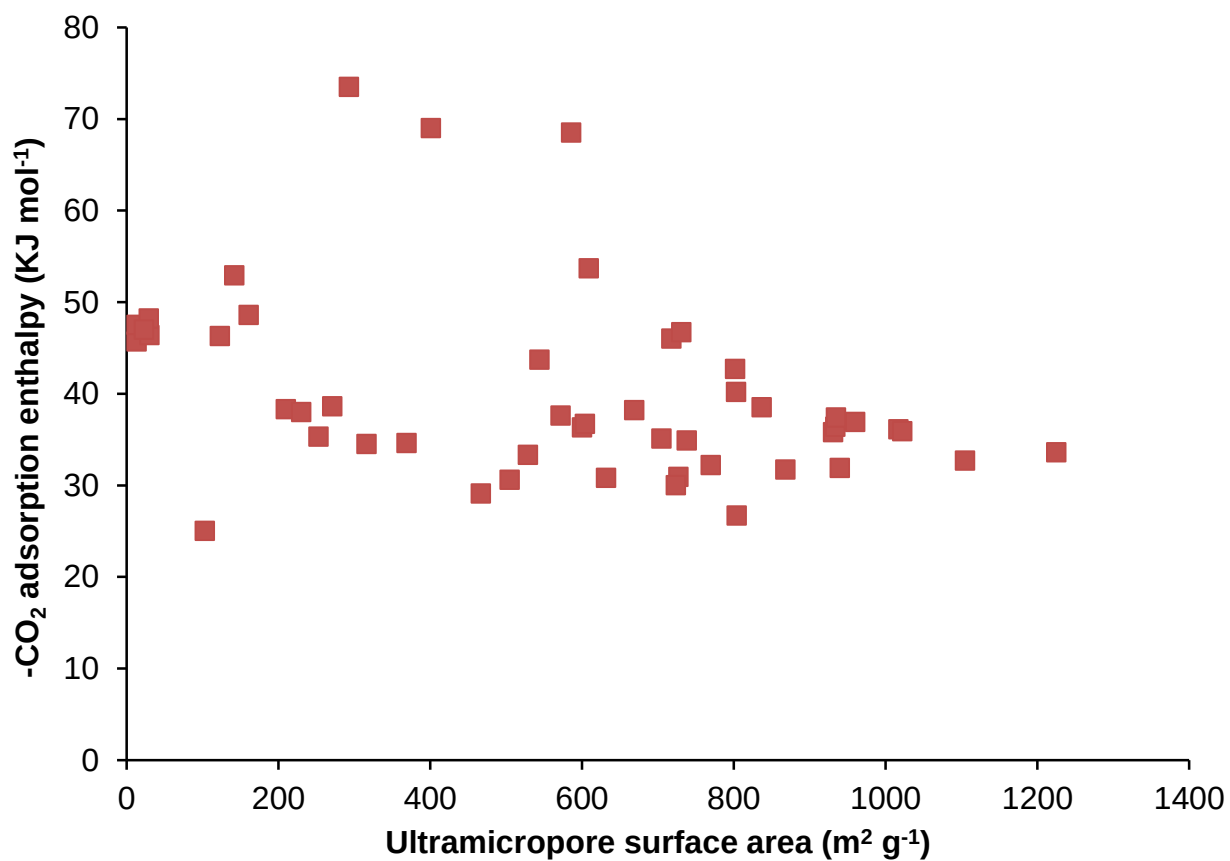
Plot of  $K_1$  for  $\text{CO}_2$  adsorption against external surface area



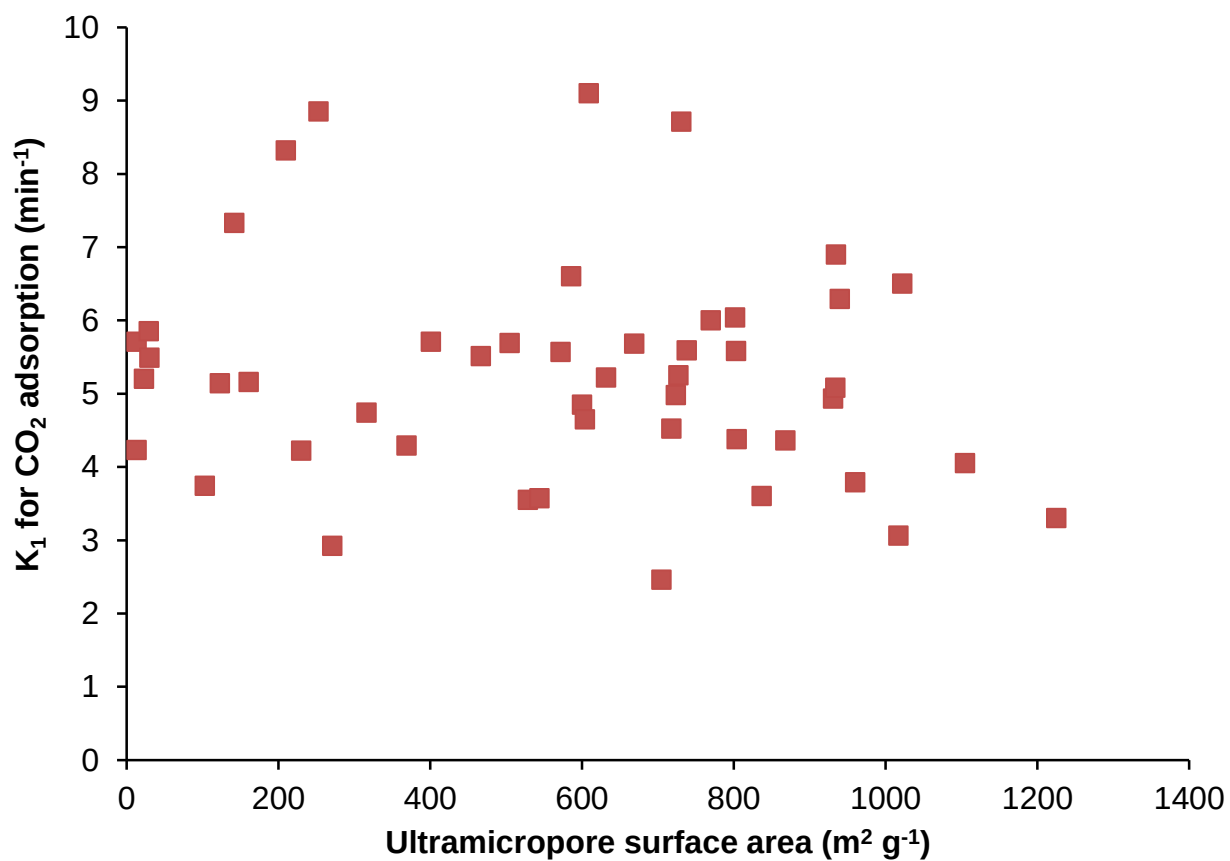
Plot of  $\text{CO}_2$  adsorption capacity against ultramicropore surface area



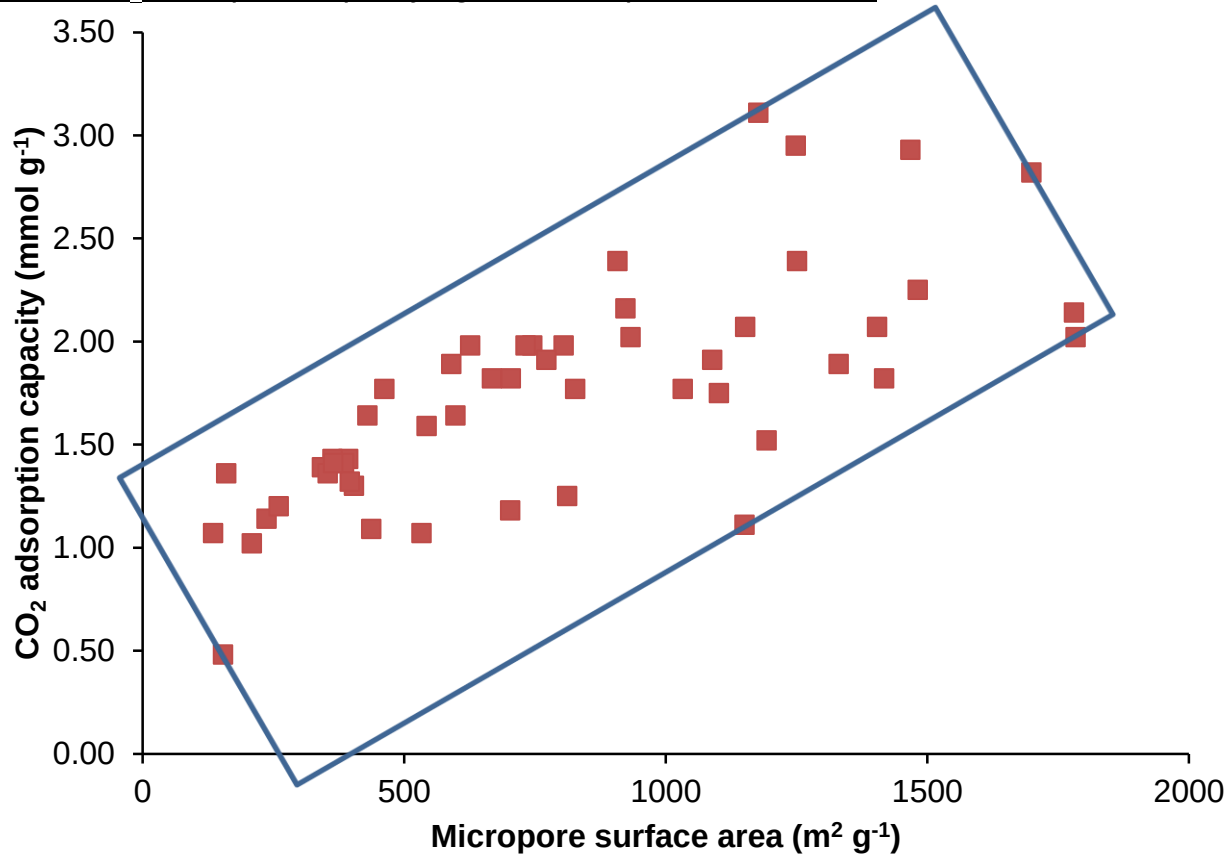
Plot of CO<sub>2</sub> adsorption enthalpy against ultramicropore surface area



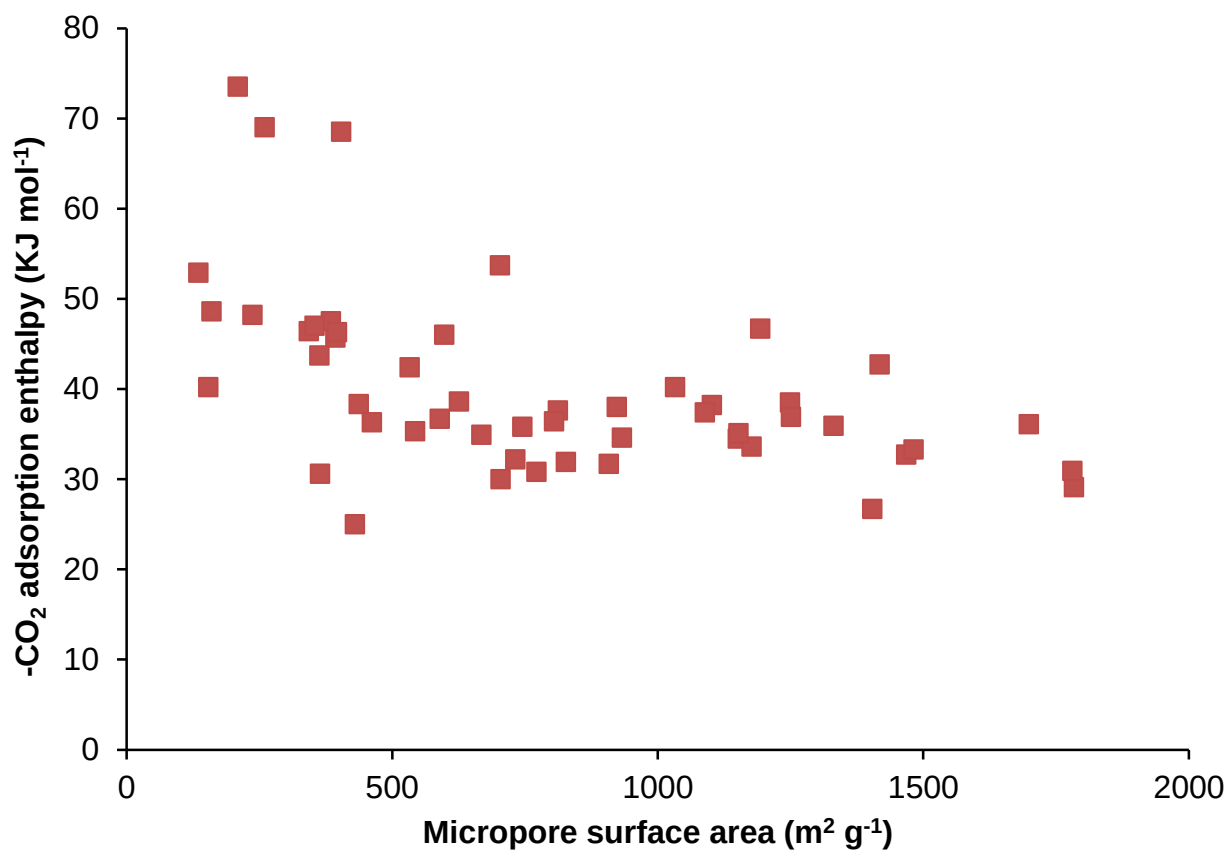
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against ultramicropore surface area



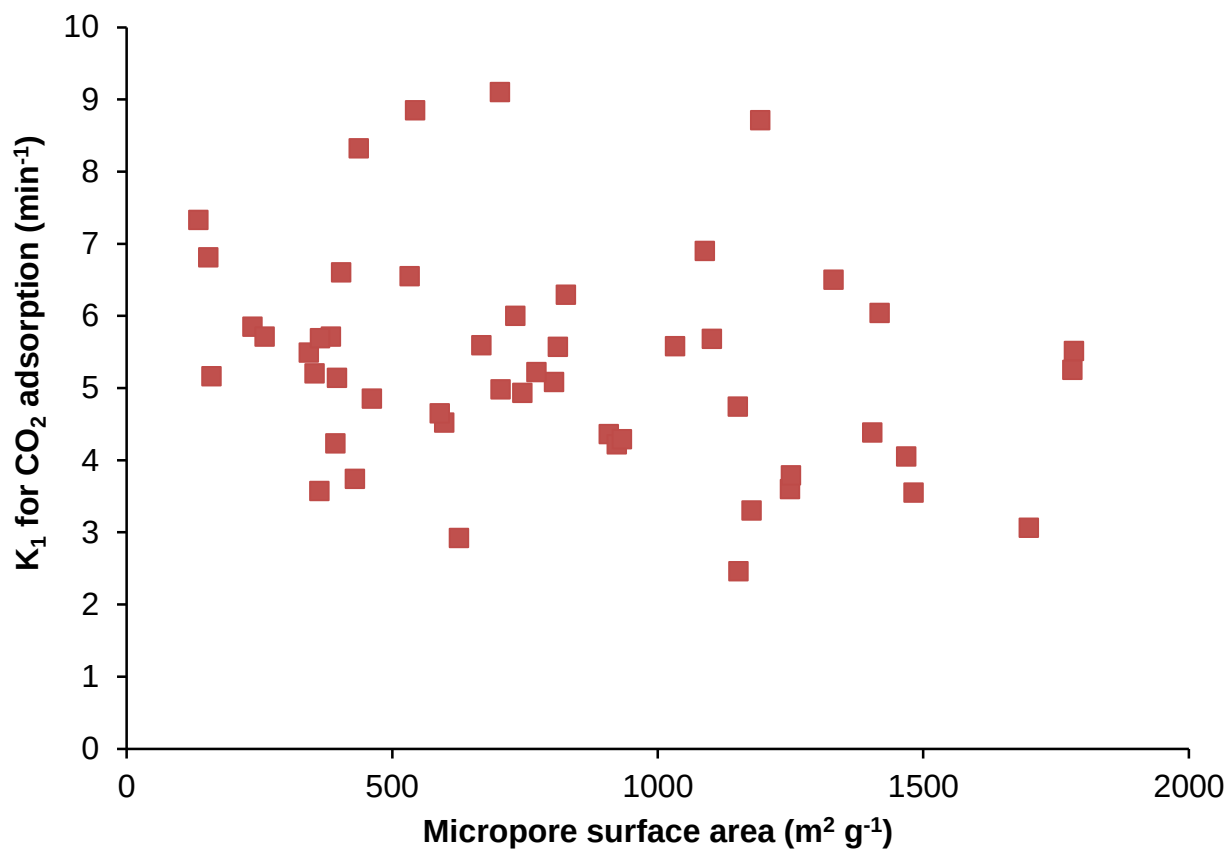
Plot of CO<sub>2</sub> adsorption capacity against micropore surface area



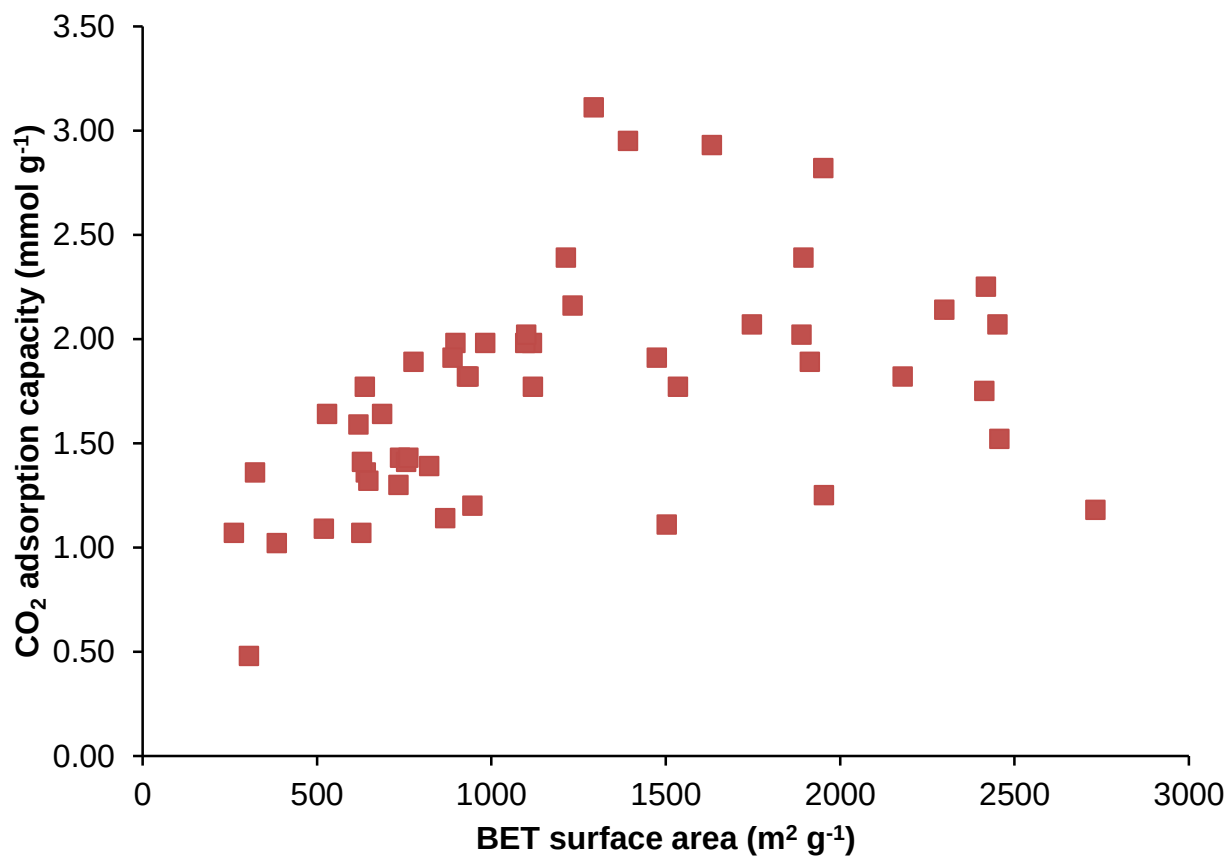
Plot of CO<sub>2</sub> adsorption enthalpy against micropore surface area



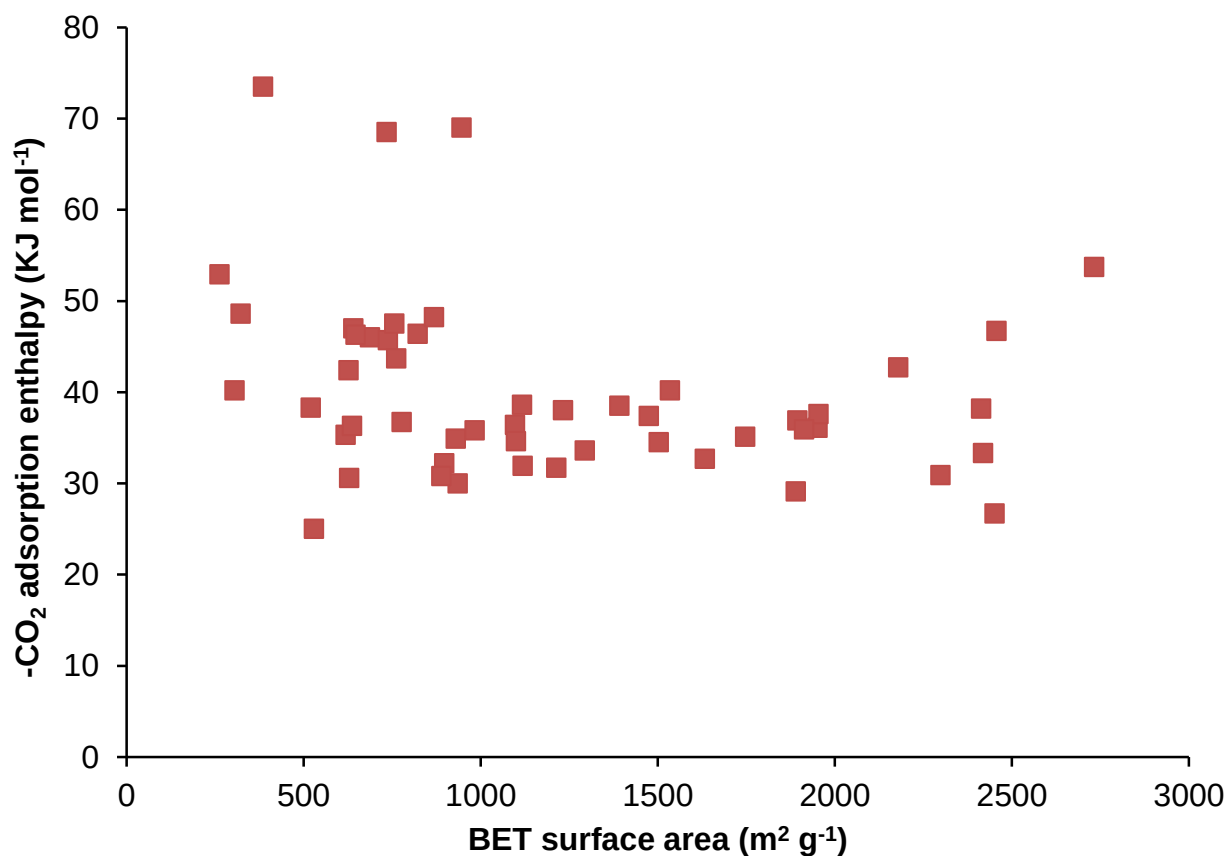
Plot of  $K_1$  for  $\text{CO}_2$  adsorption against micropore surface area



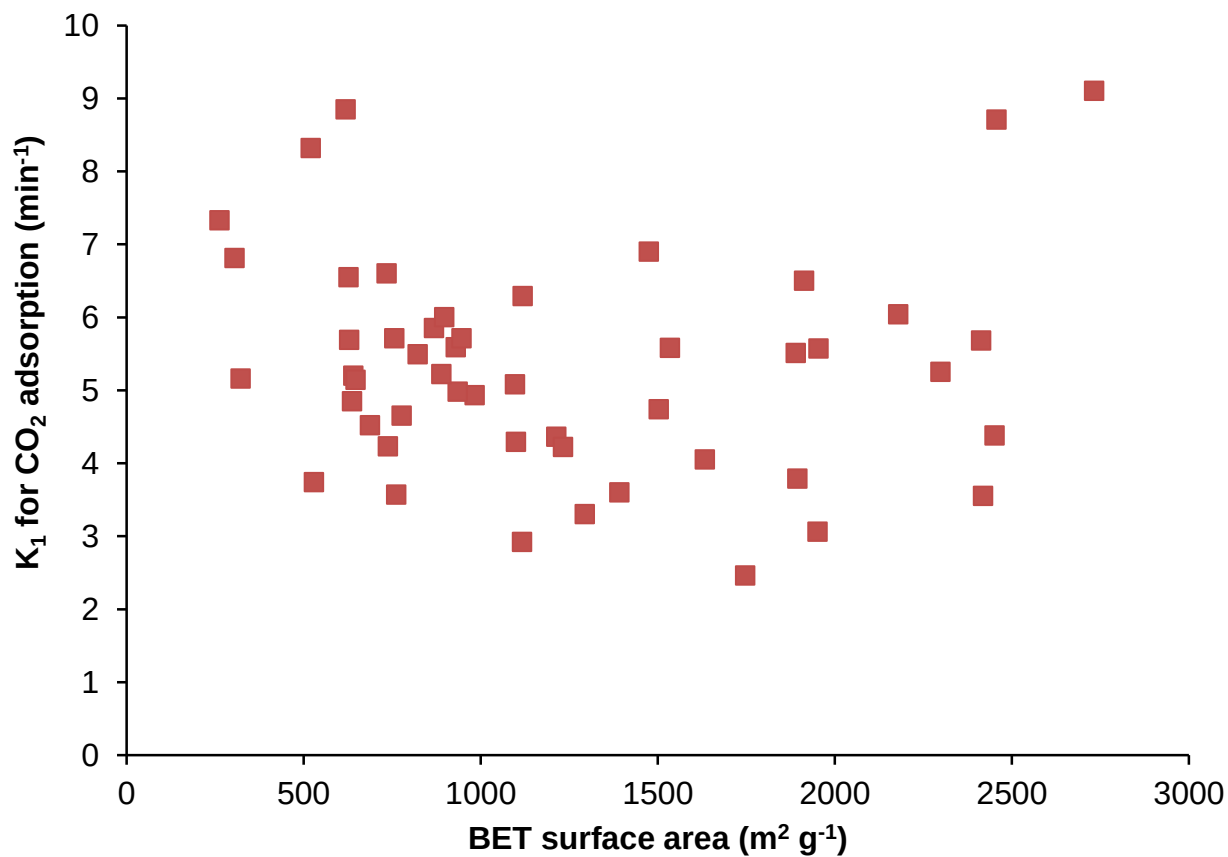
Plot of  $\text{CO}_2$  adsorption capacity against BET surface area



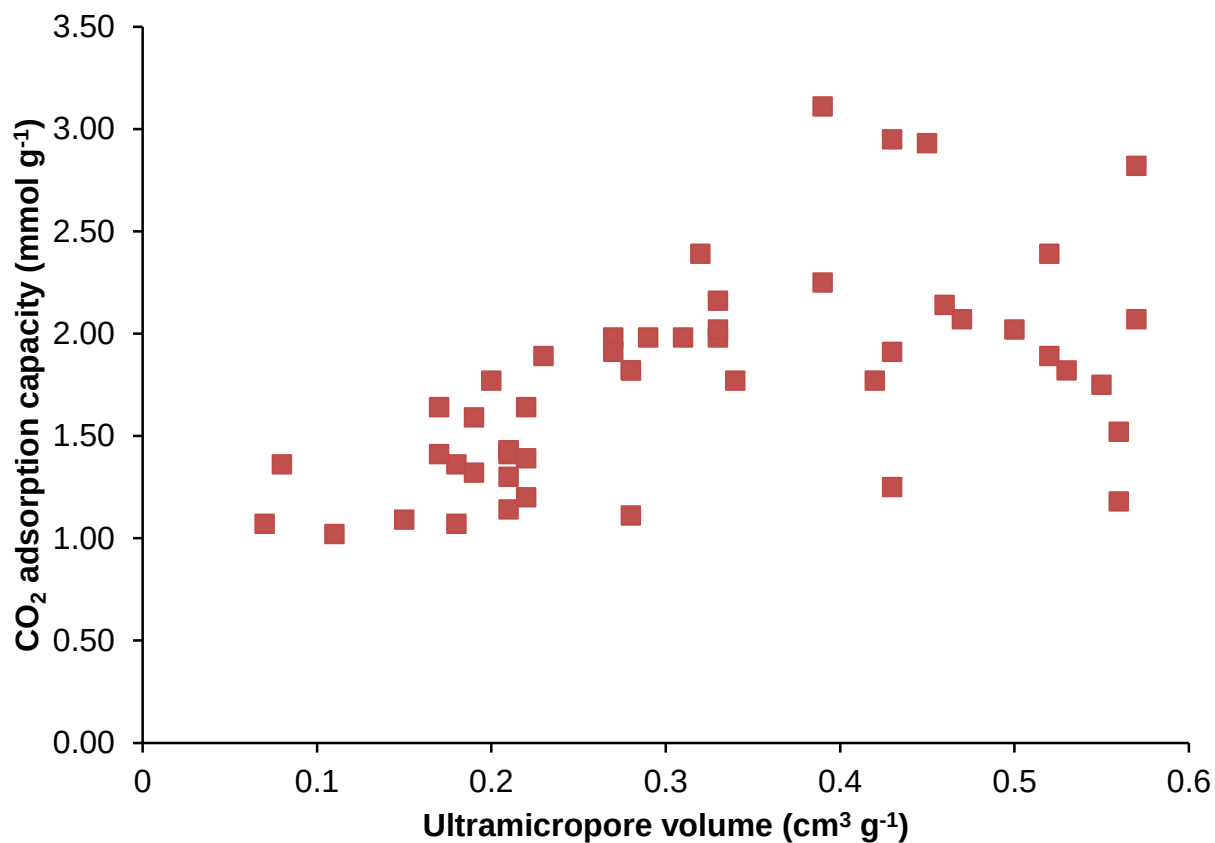
Plot of CO<sub>2</sub> adsorption enthalpy against BET surface area



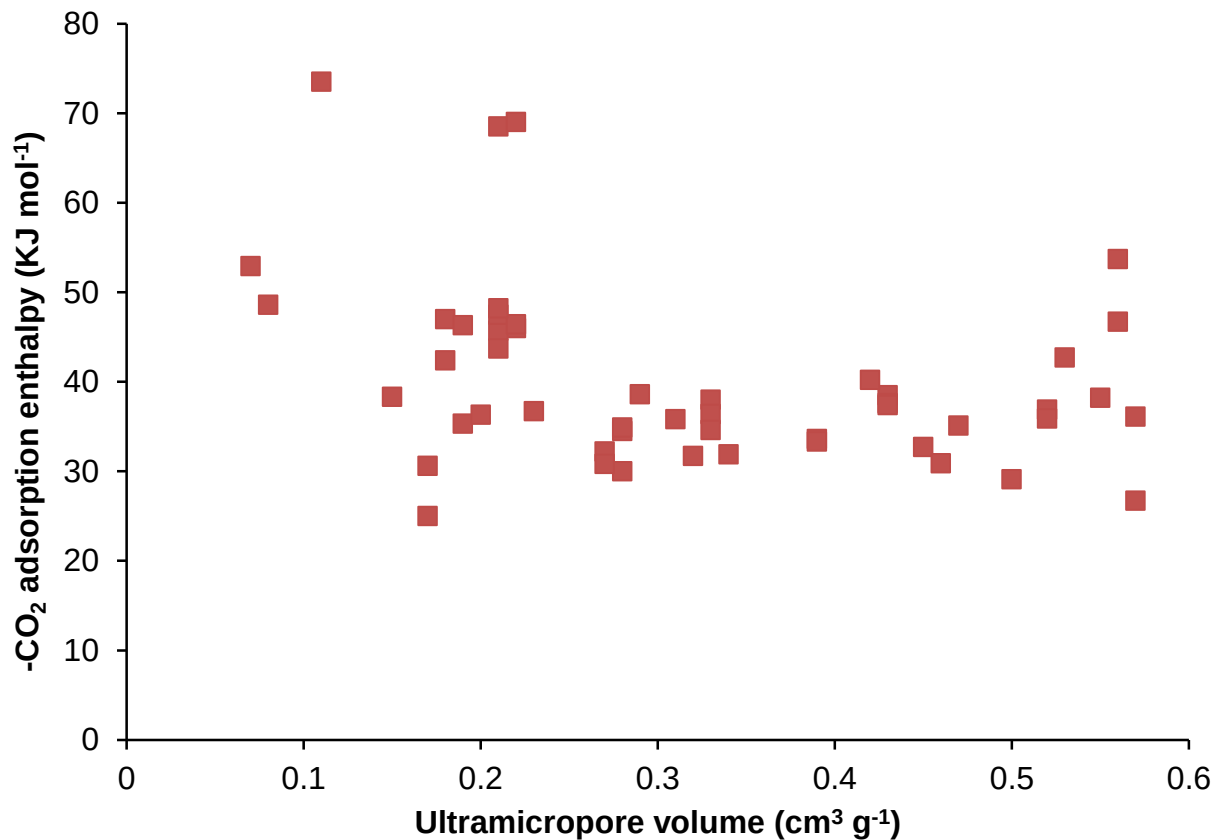
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against BET surface area



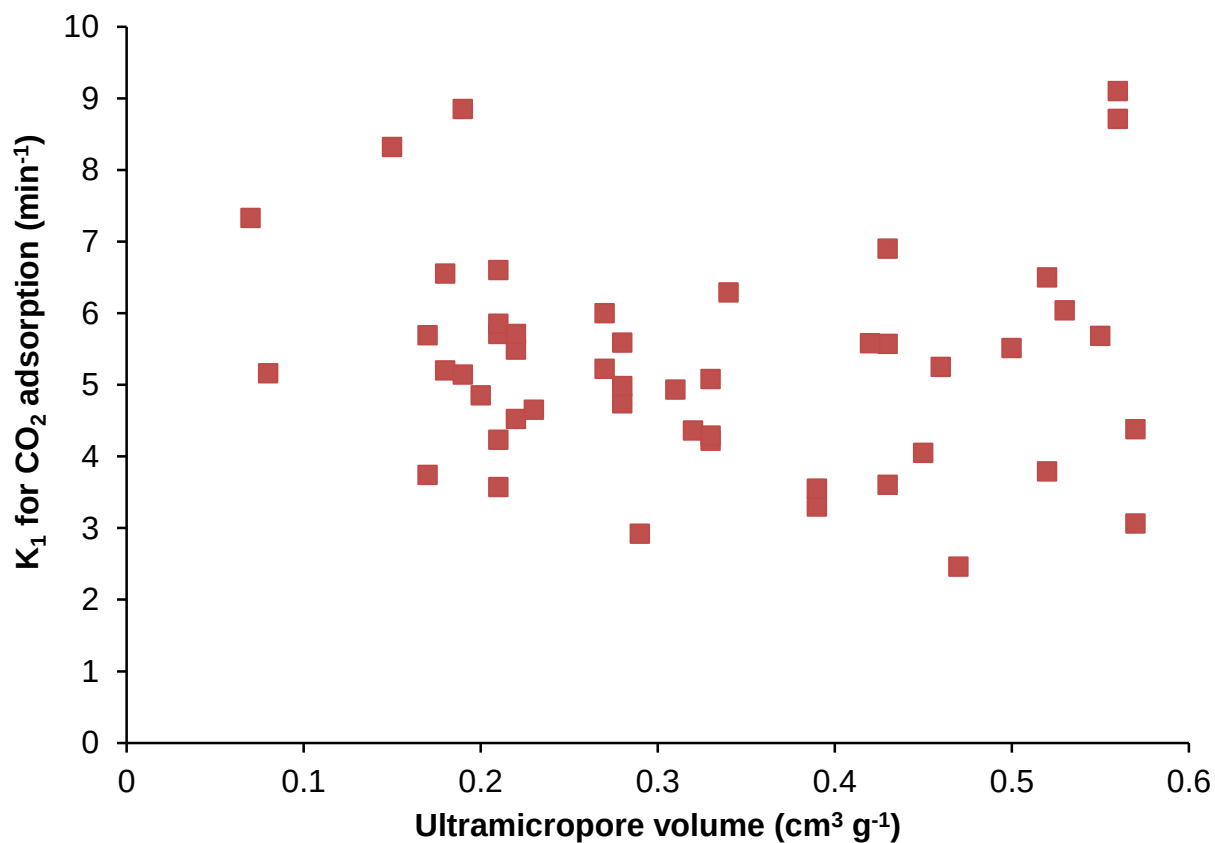
Plot of CO<sub>2</sub> adsorption capacity against ultramicropore volume



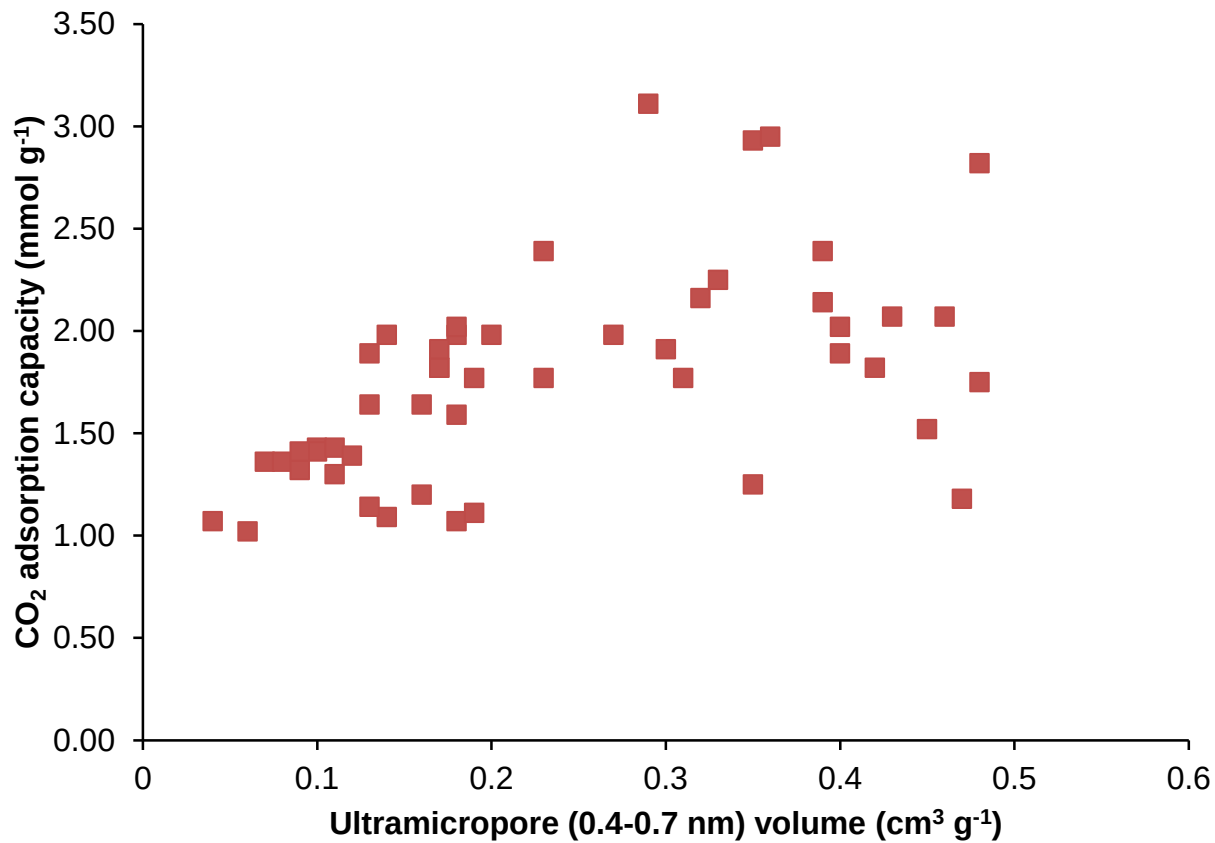
Plot of CO<sub>2</sub> adsorption enthalpy against ultramicropore volume



Plot of  $K_1$  for  $\text{CO}_2$  adsorption against ultramicropore volume

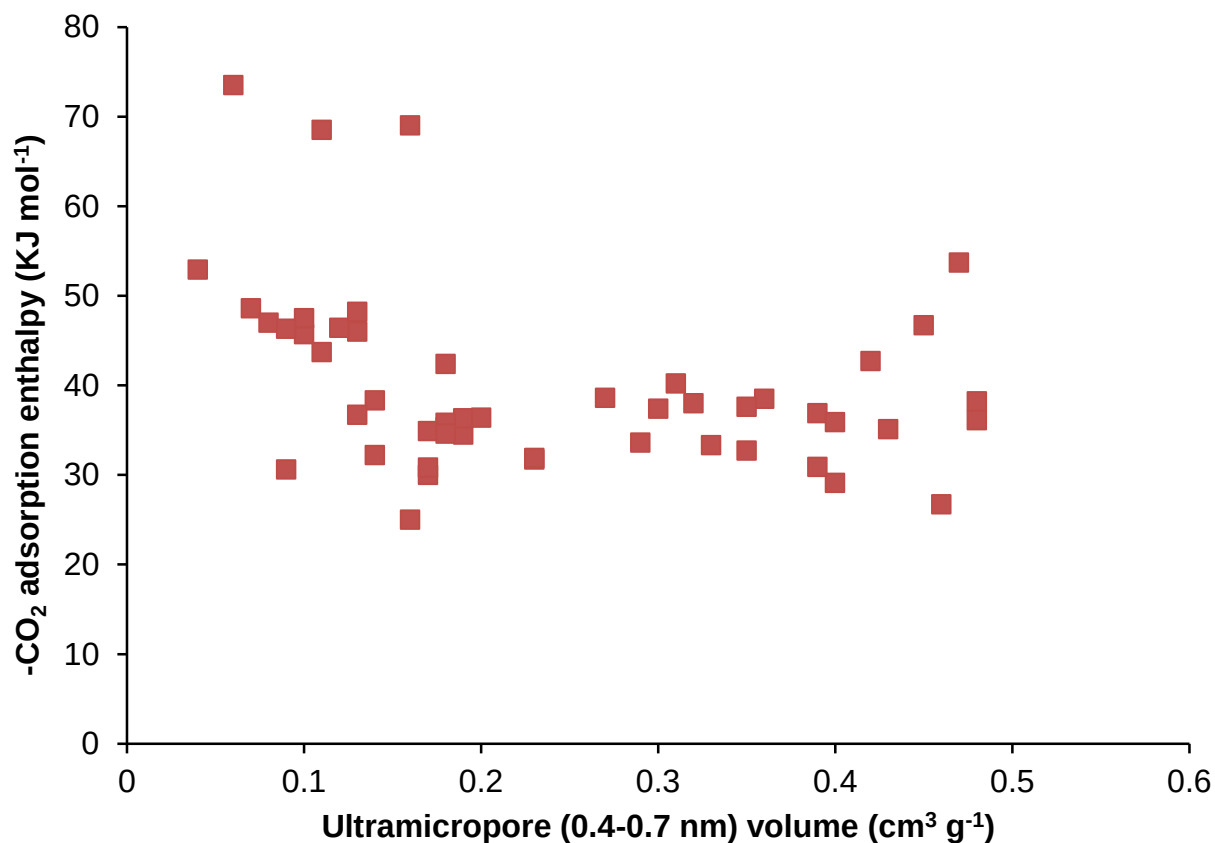


Plot of  $\text{CO}_2$  adsorption capacity against ultramicropore (0.4-0.7 nm) volume

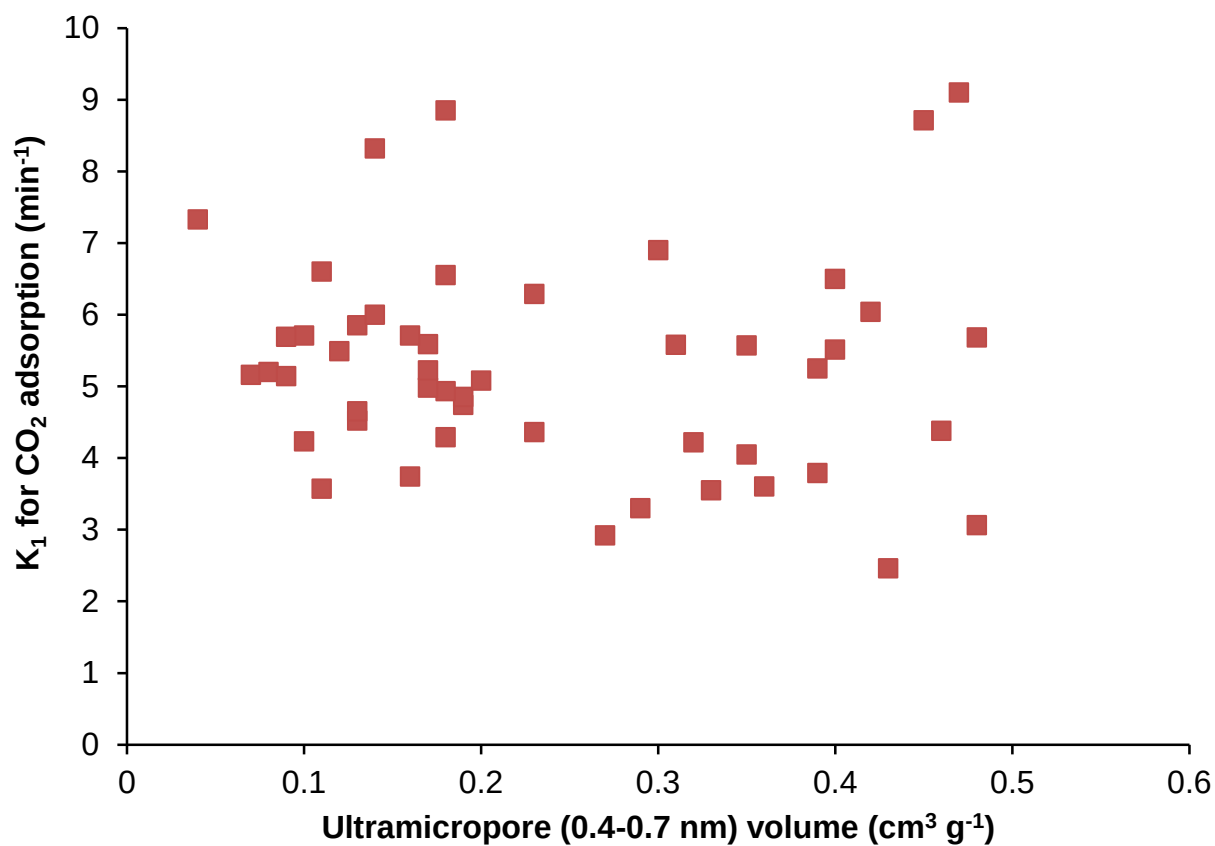




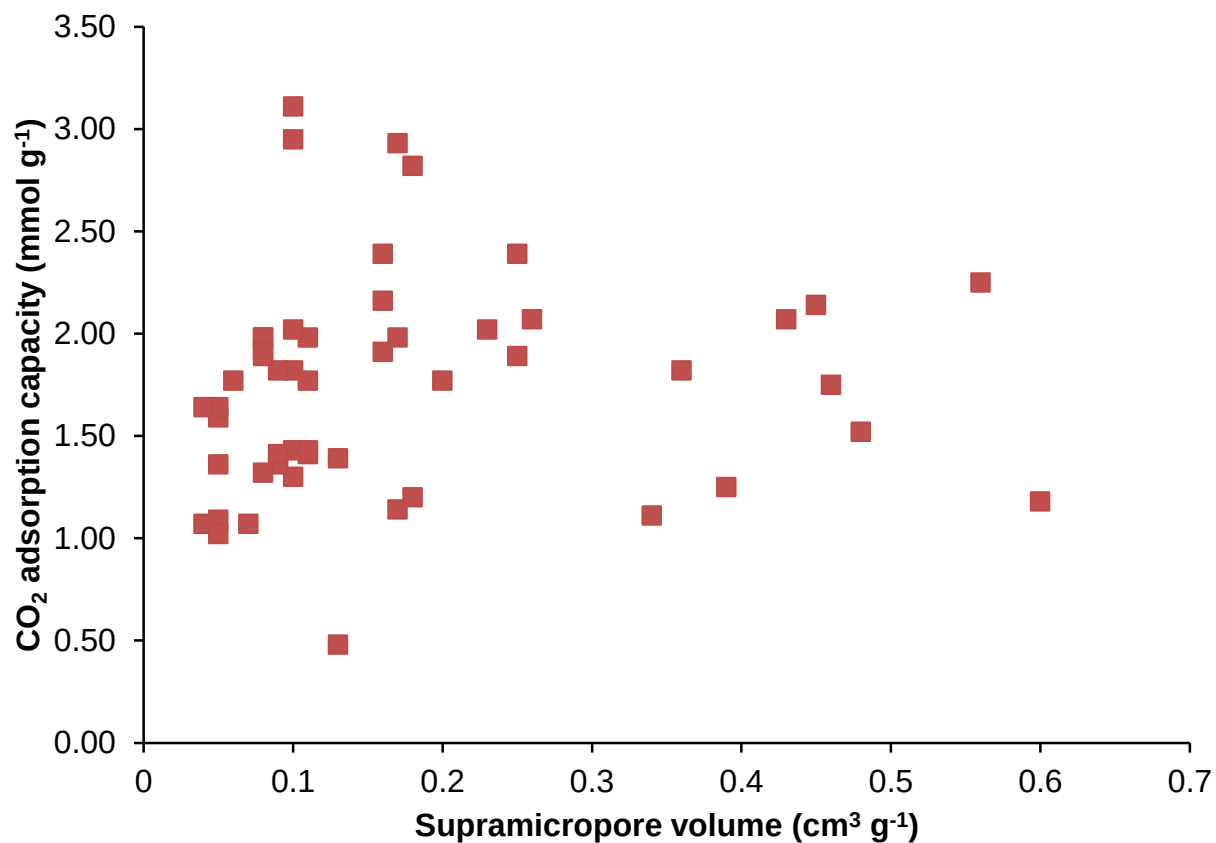
Plot of CO<sub>2</sub> adsorption enthalpy against ultramicropore (0.4-0.7 nm) volume



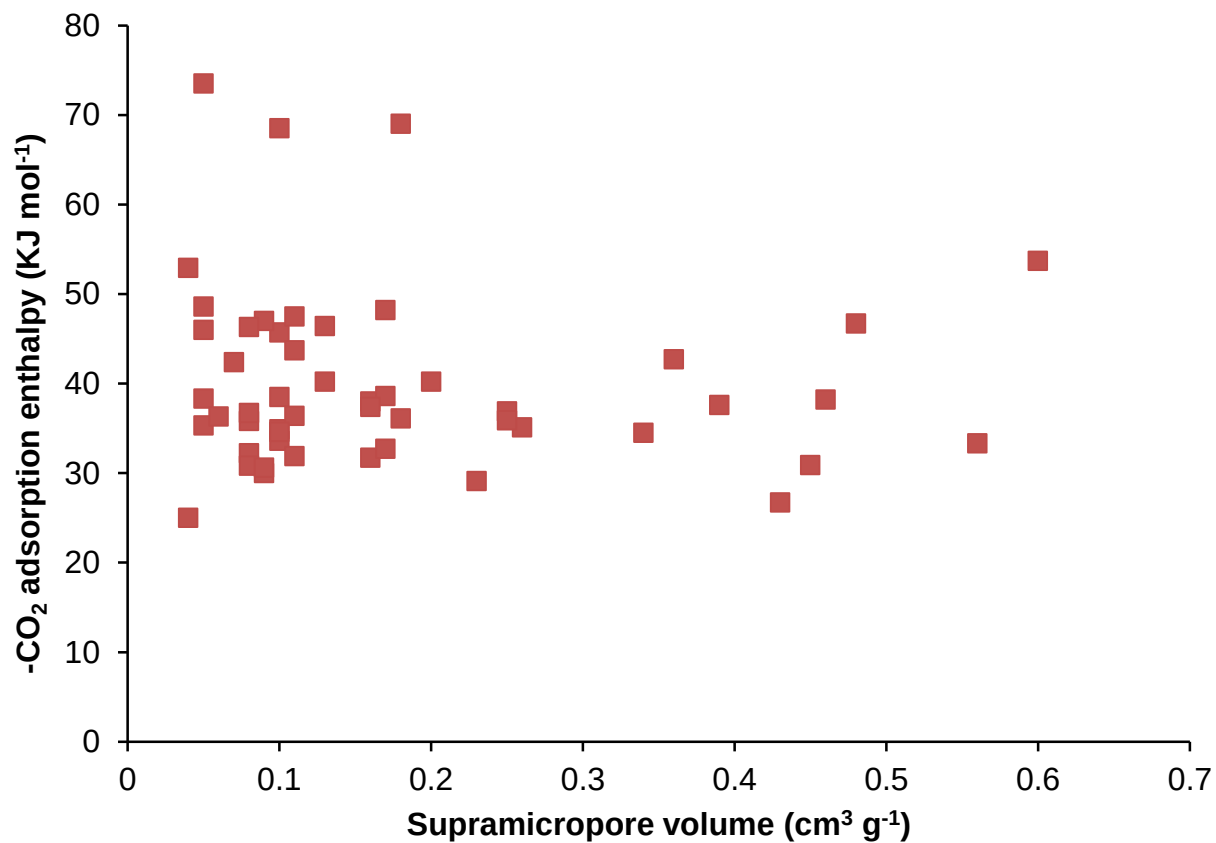
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against ultramicropore (0.4-0.7 nm) volume



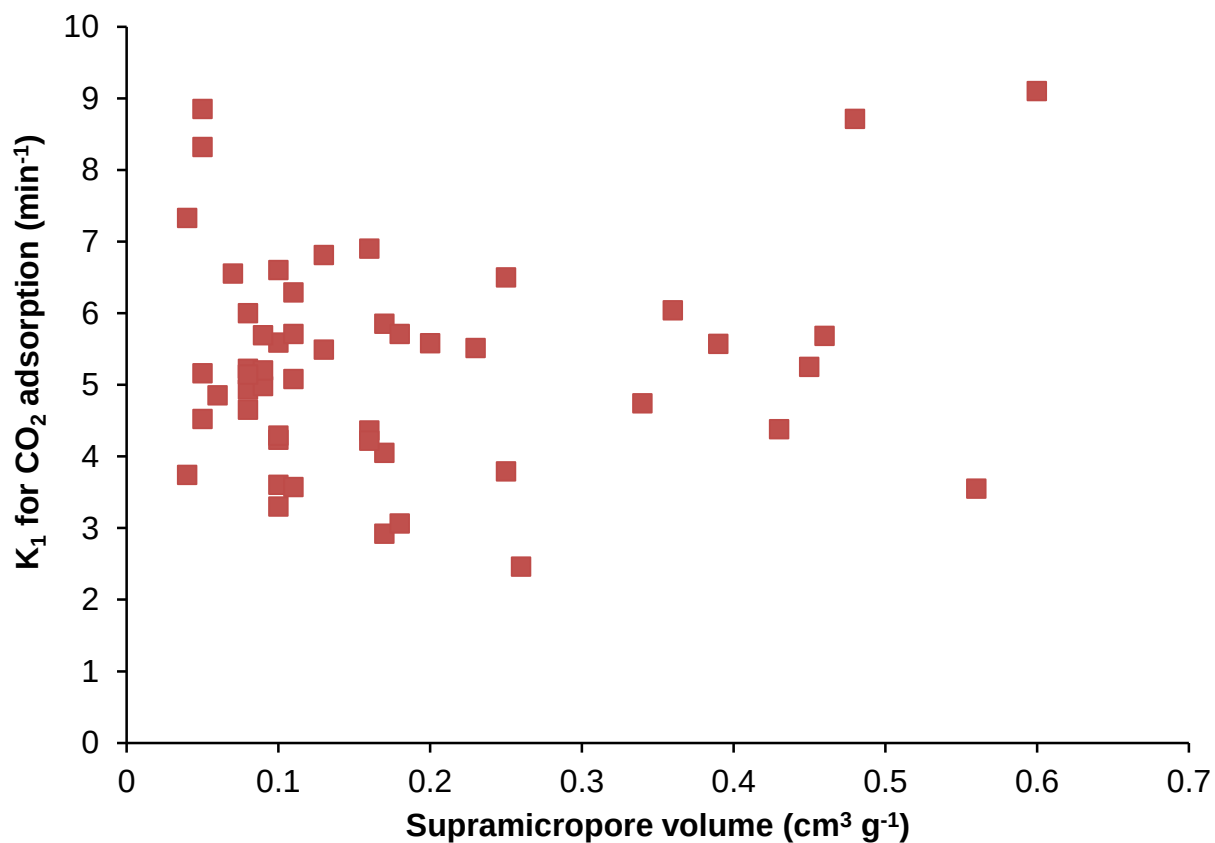
Plot of CO<sub>2</sub> adsorption capacity against supramicropore volume



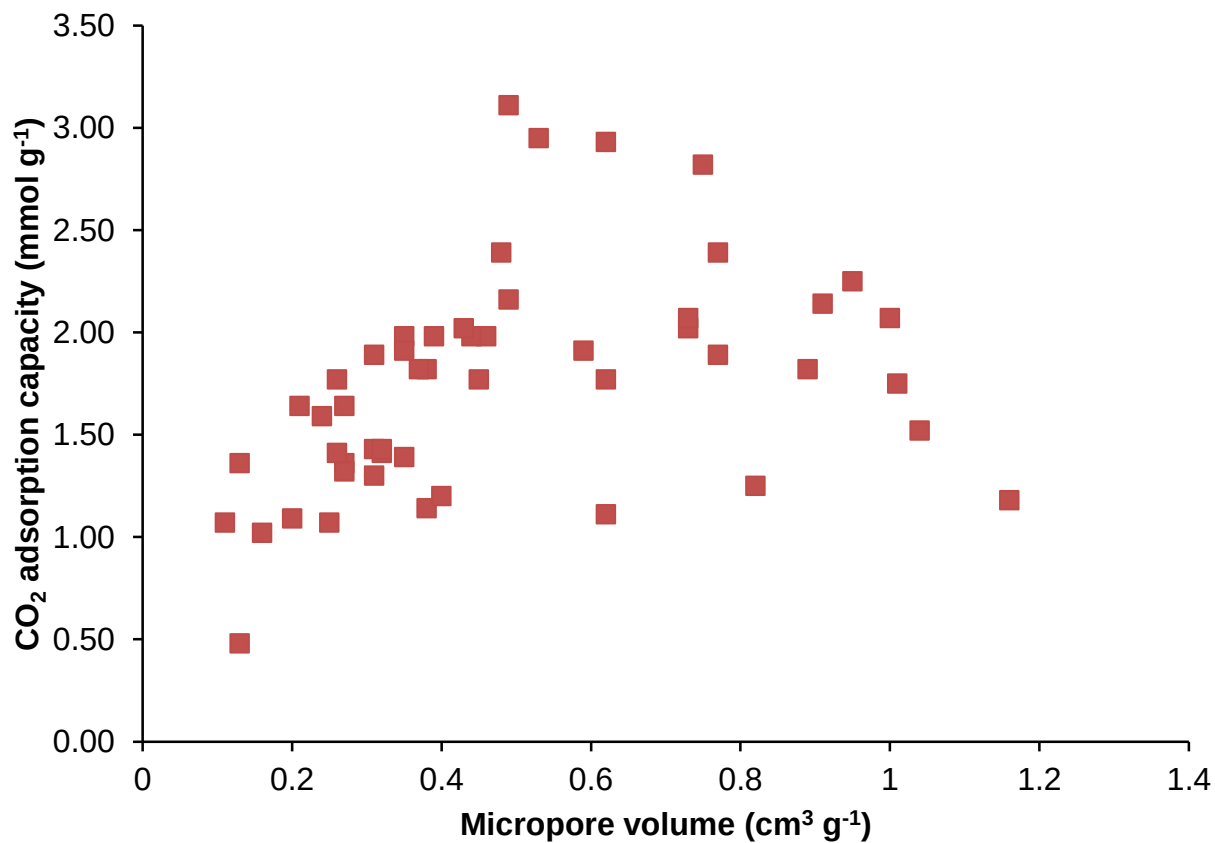
Plot of CO<sub>2</sub> adsorption enthalpy against supramicropore volume



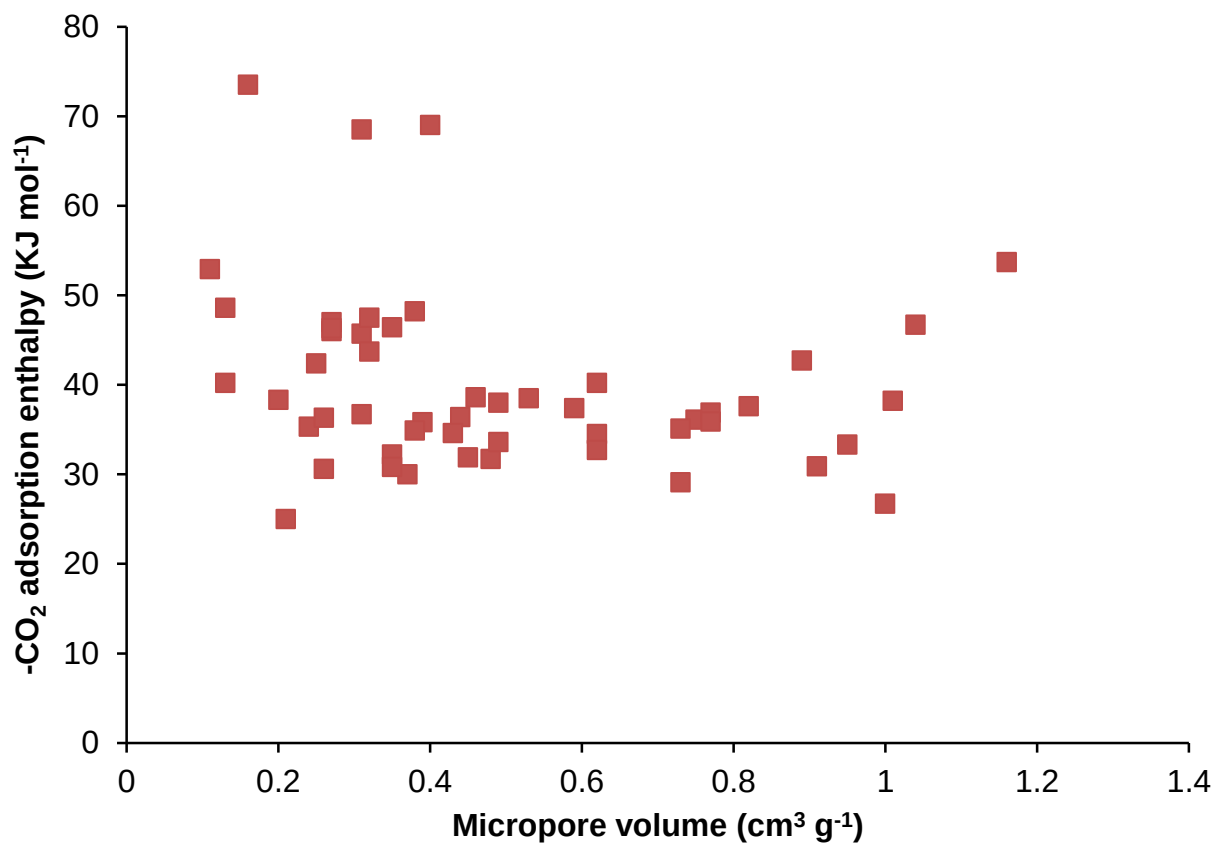
Plot of  $K_1$  for  $\text{CO}_2$  adsorption against supramicropore volume



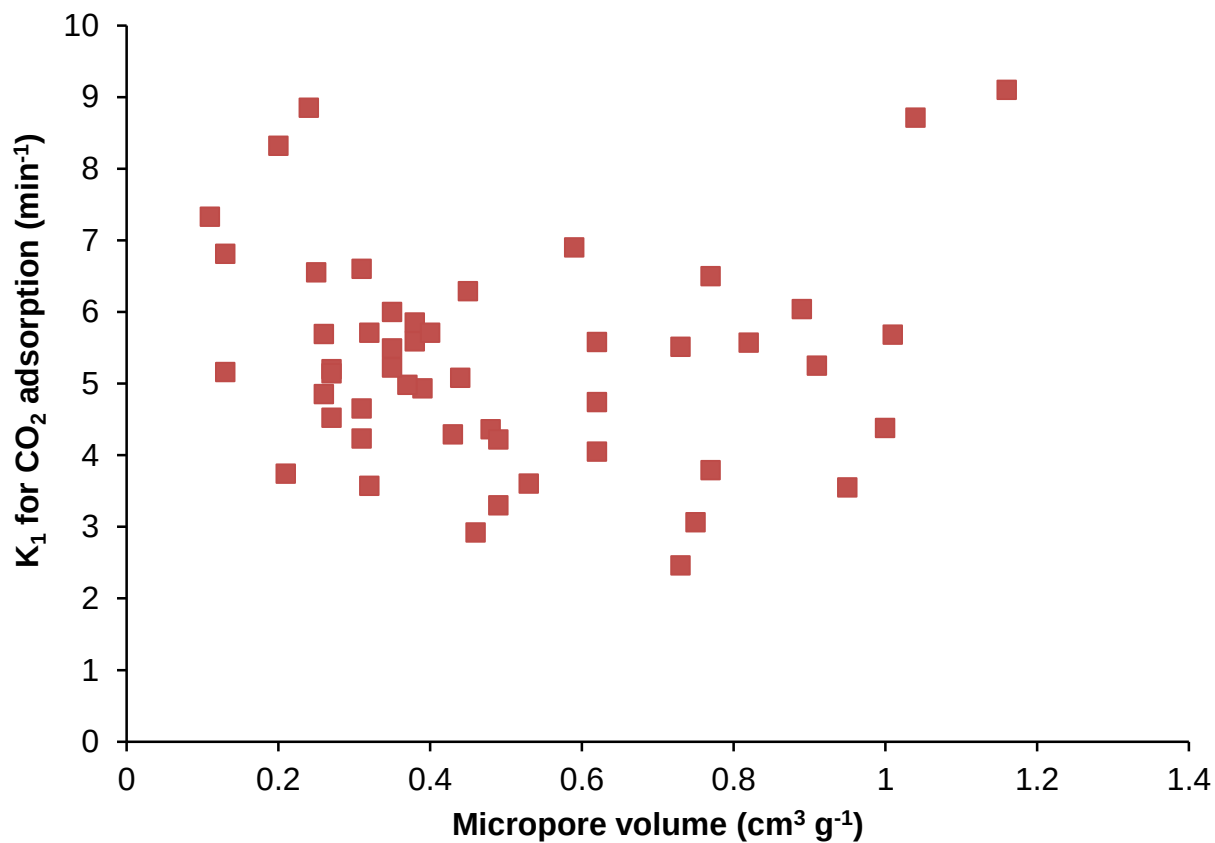
Plot of  $\text{CO}_2$  adsorption capacity against micropore volume



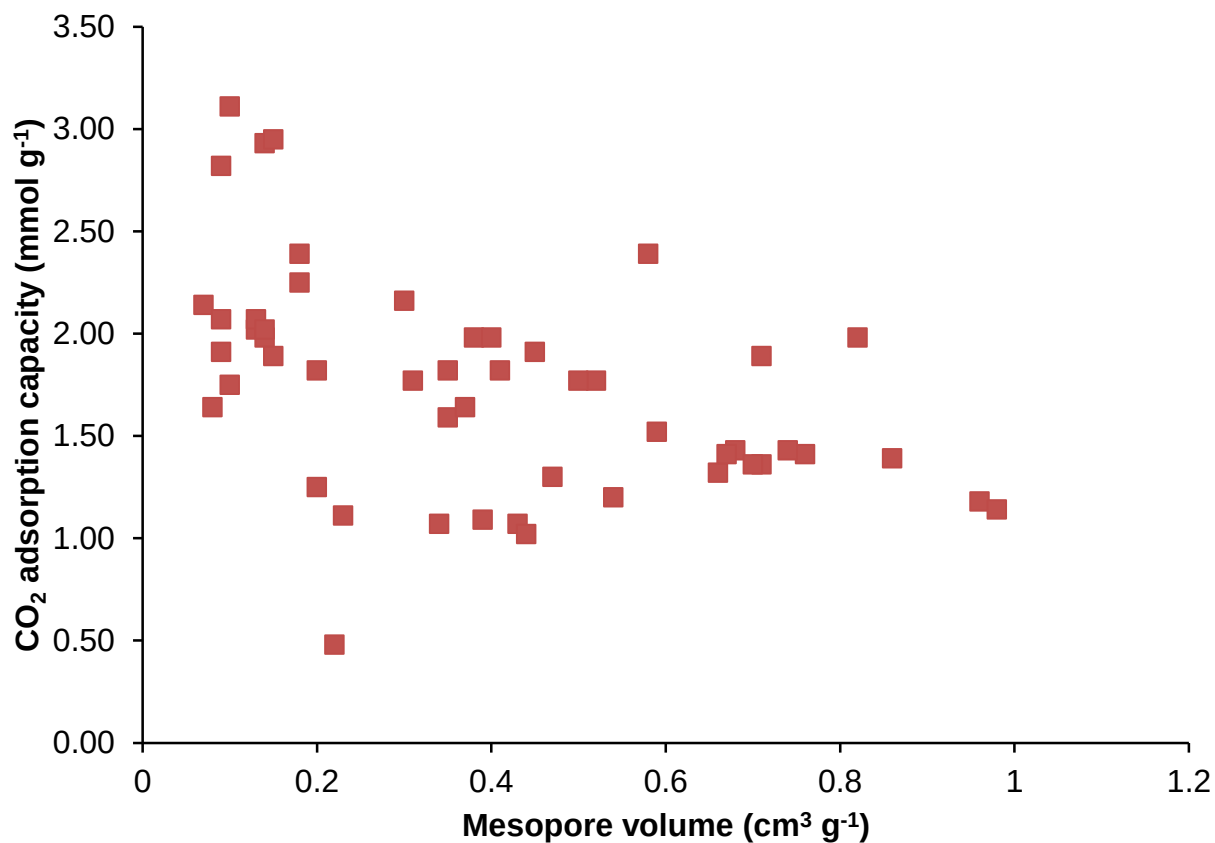
Plot of CO<sub>2</sub> adsorption enthalpy against micropore volume



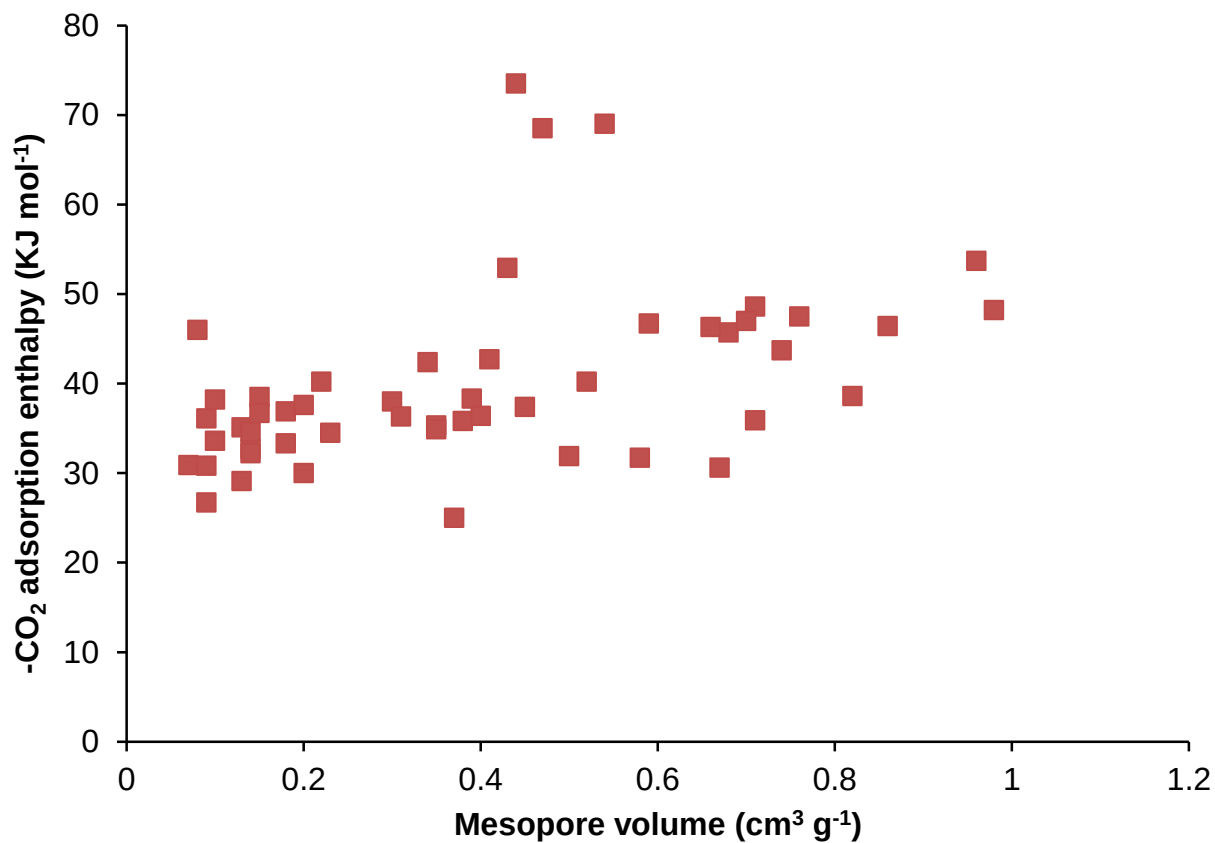
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against micropore volume



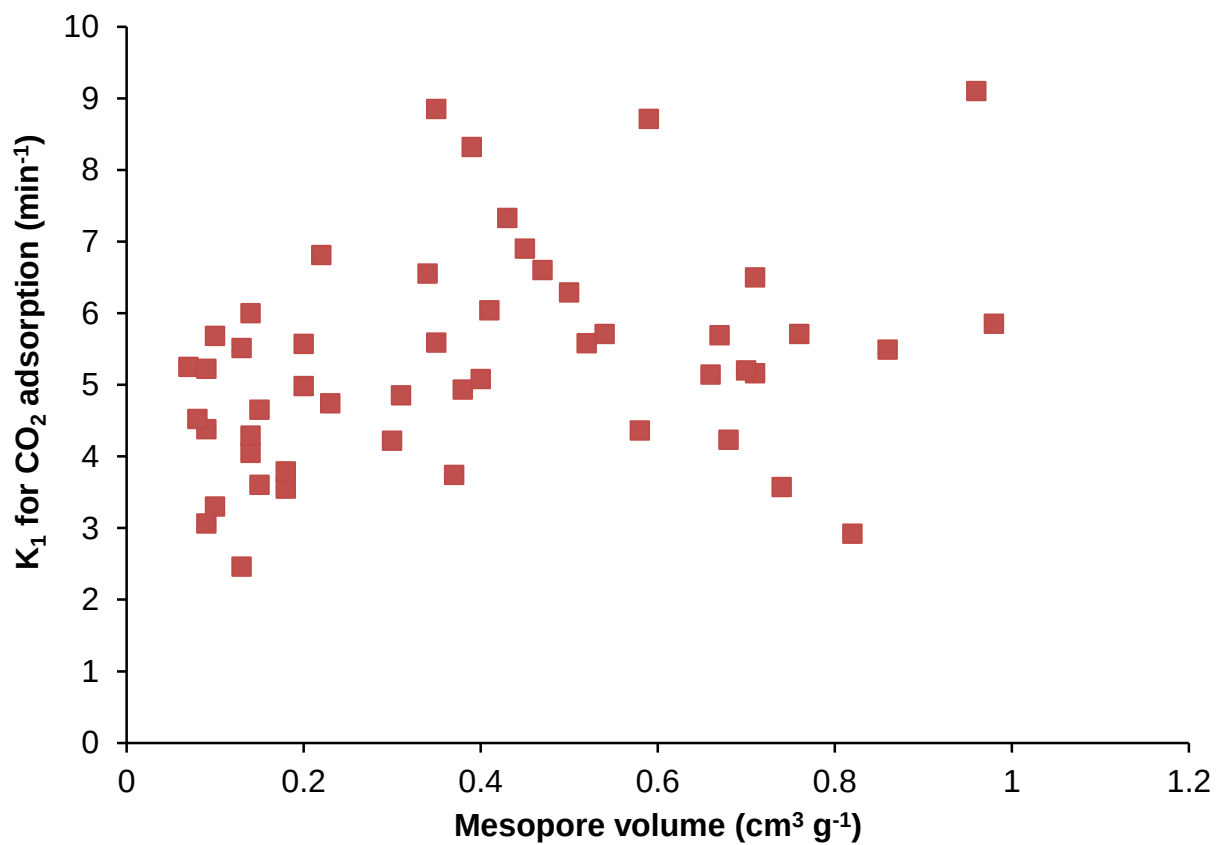
Plot of CO<sub>2</sub> adsorption capacity against mesopore volume



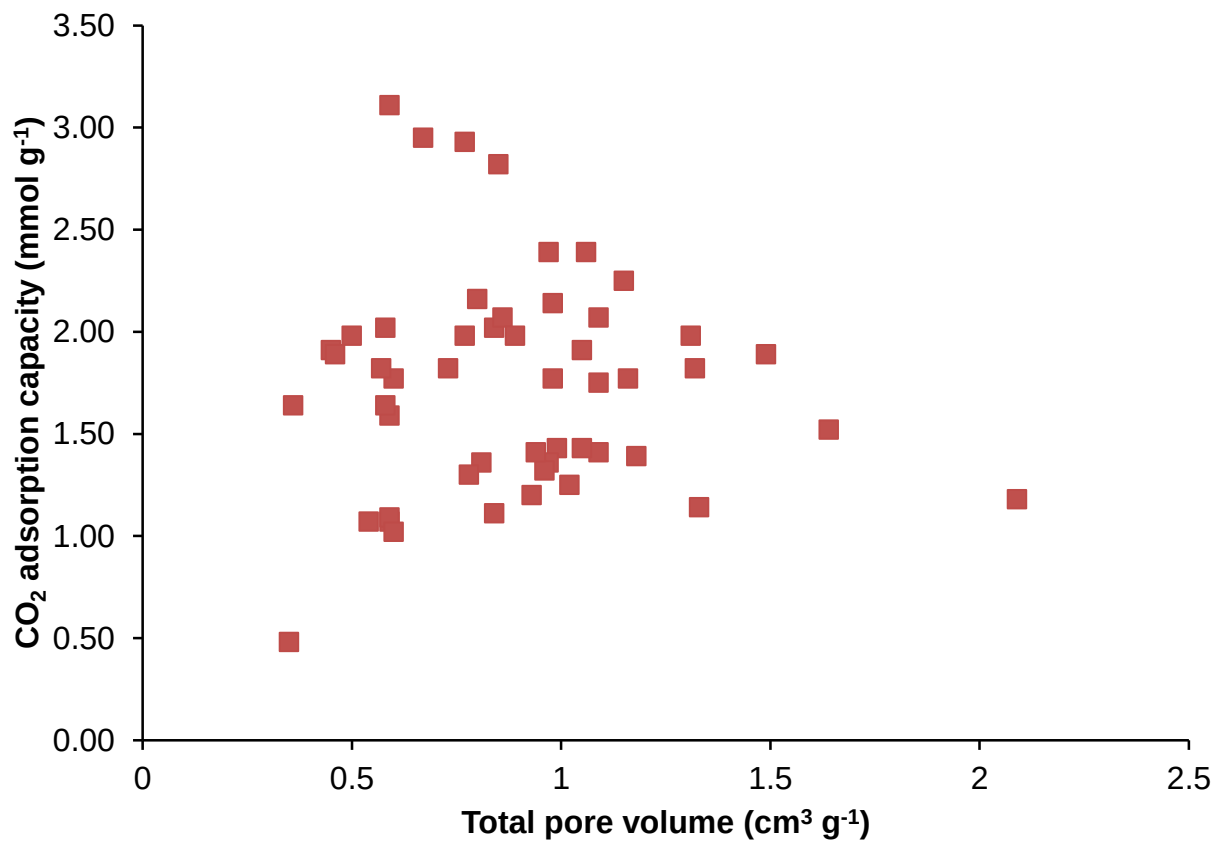
Plot of CO<sub>2</sub> adsorption enthalpy against mesopore volume



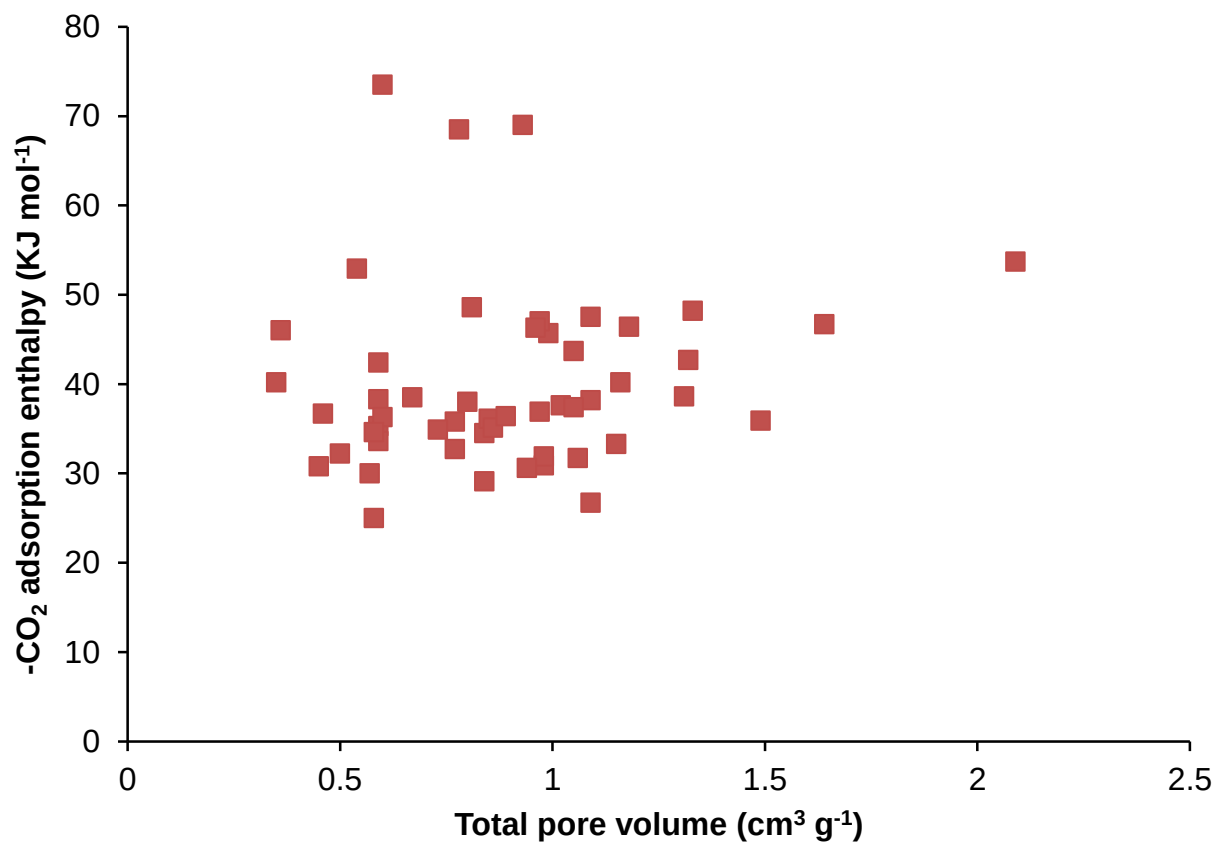
Plot of  $K_1$  for CO<sub>2</sub> adsorption against mesopore volume



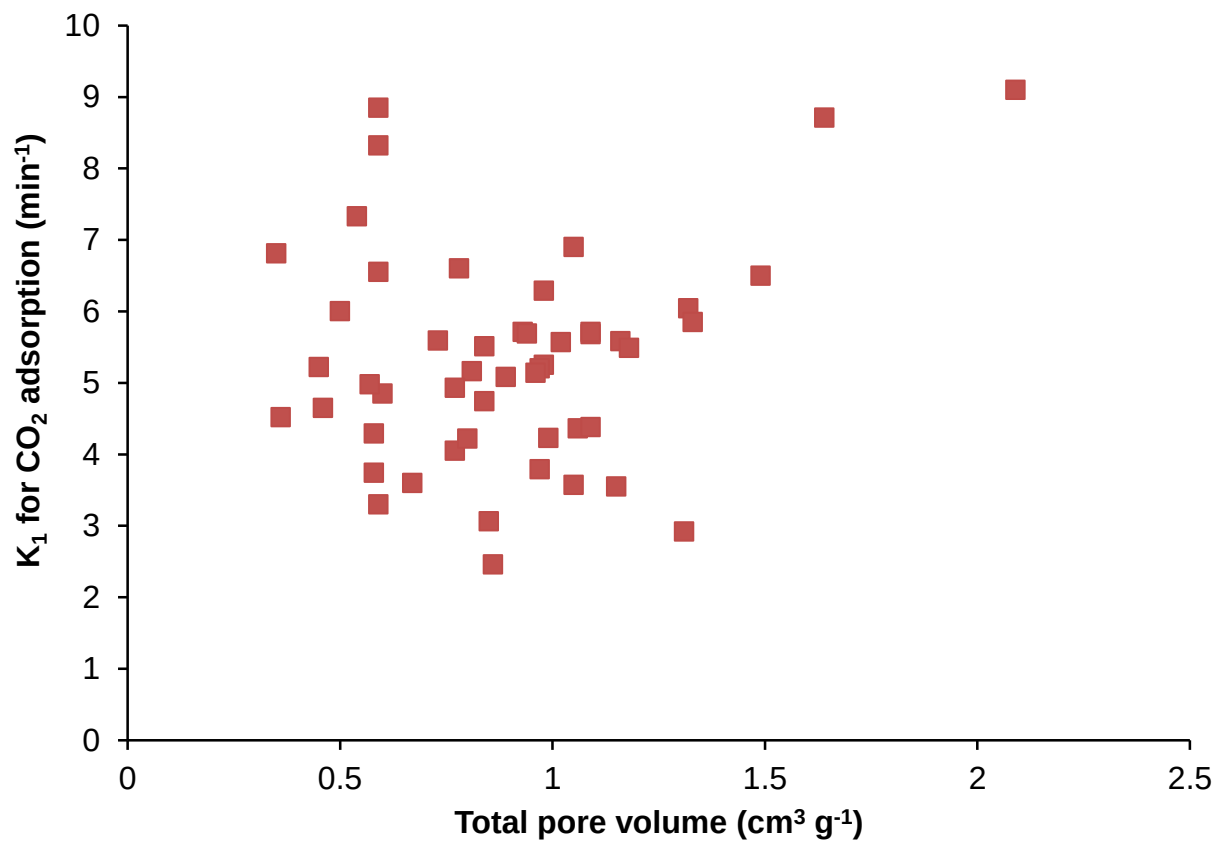
Plot of CO<sub>2</sub> adsorption capacity against total pore volume



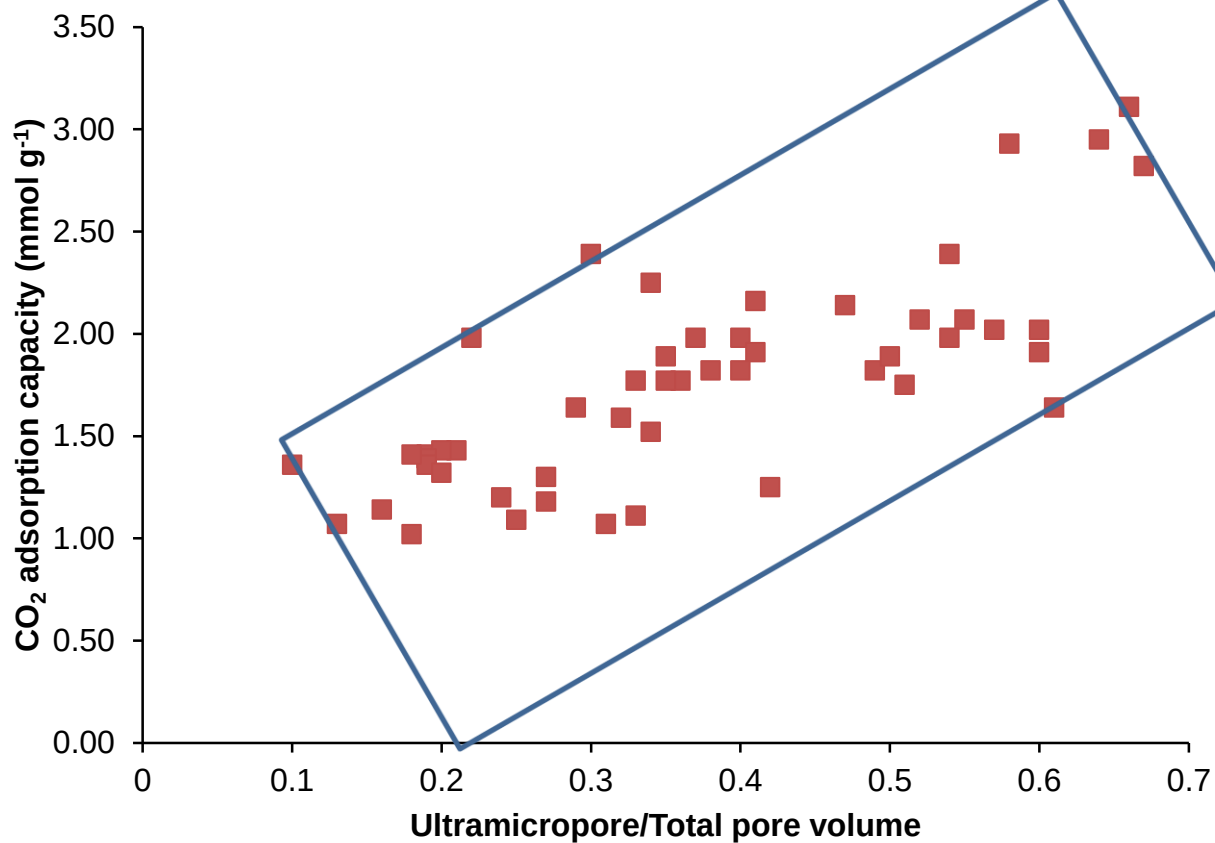
Plot of CO<sub>2</sub> adsorption enthalpy against total pore volume



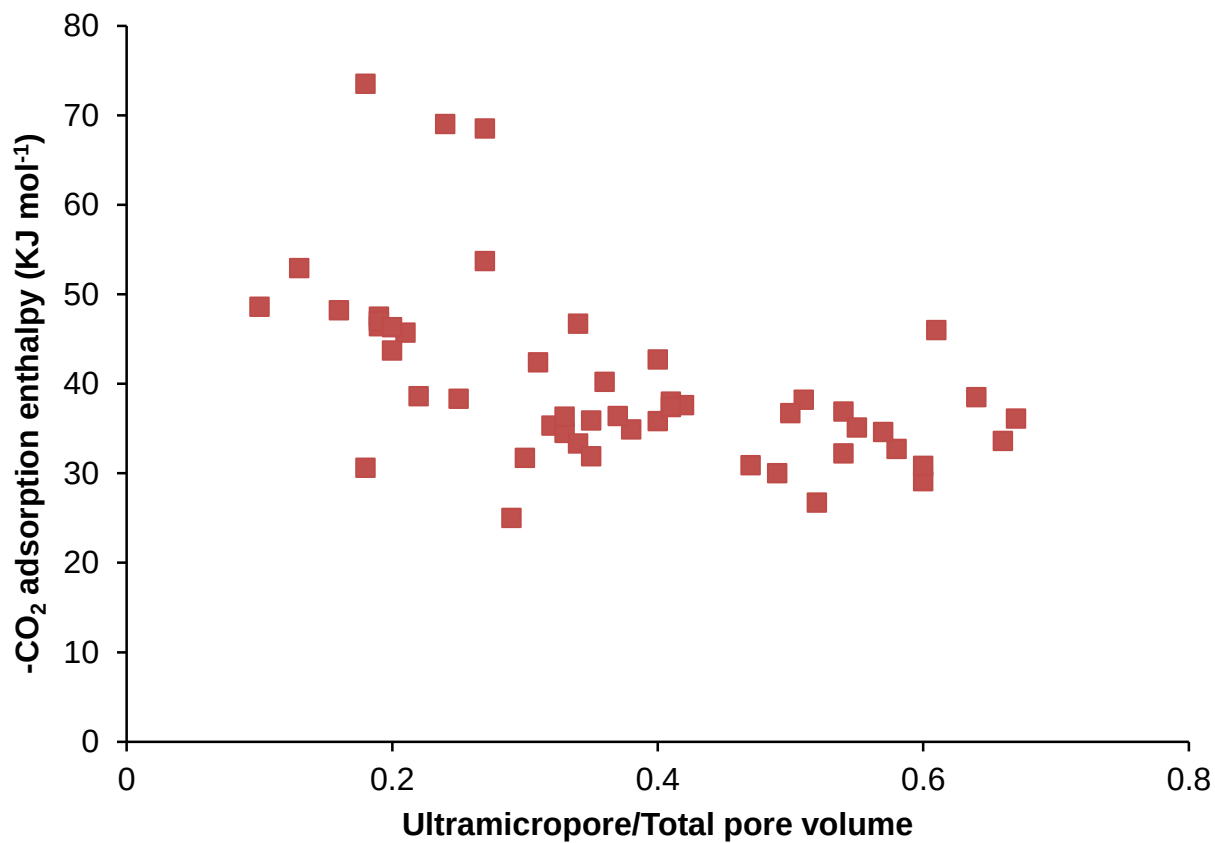
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against total pore volume



Plot of CO<sub>2</sub> adsorption capacity against ultramicropore volume/total pore volume

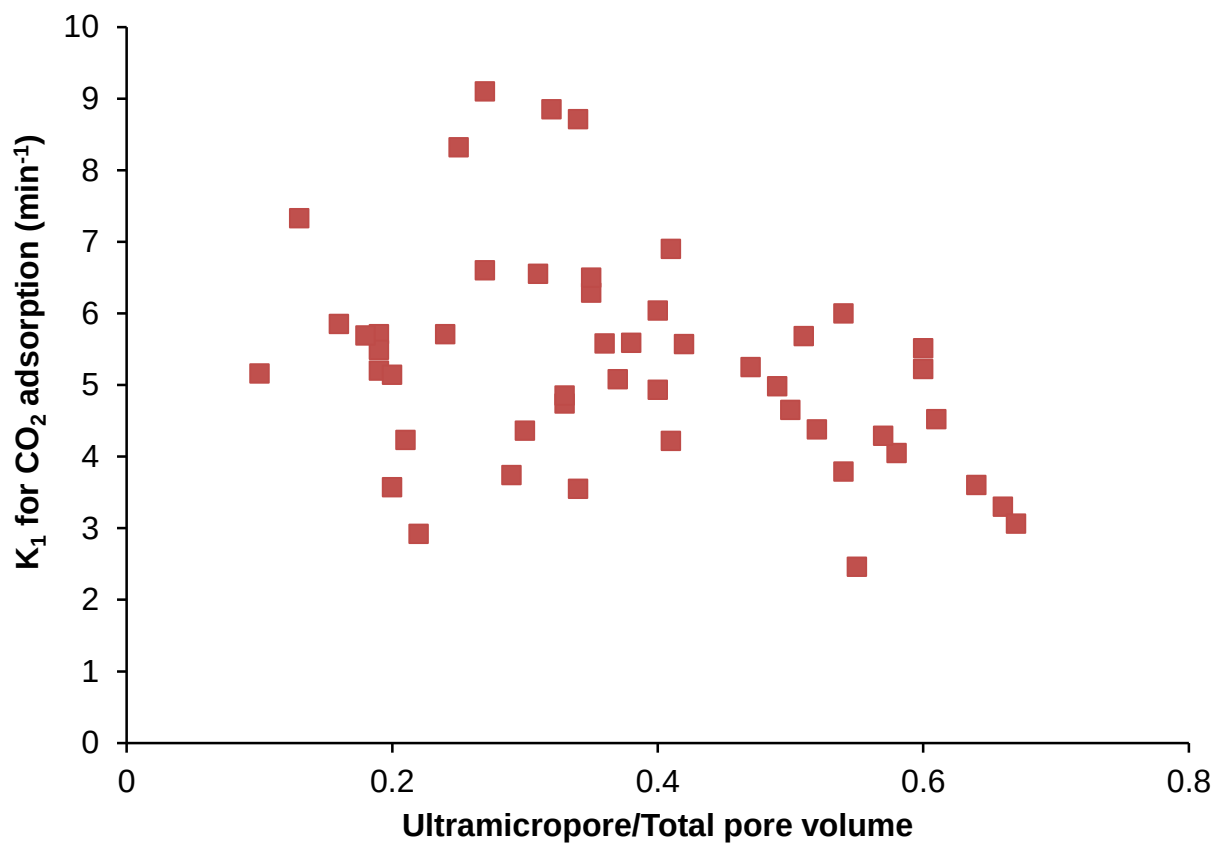


Plot of CO<sub>2</sub> adsorption enthalpy against ultramicropore volume/total pore volume

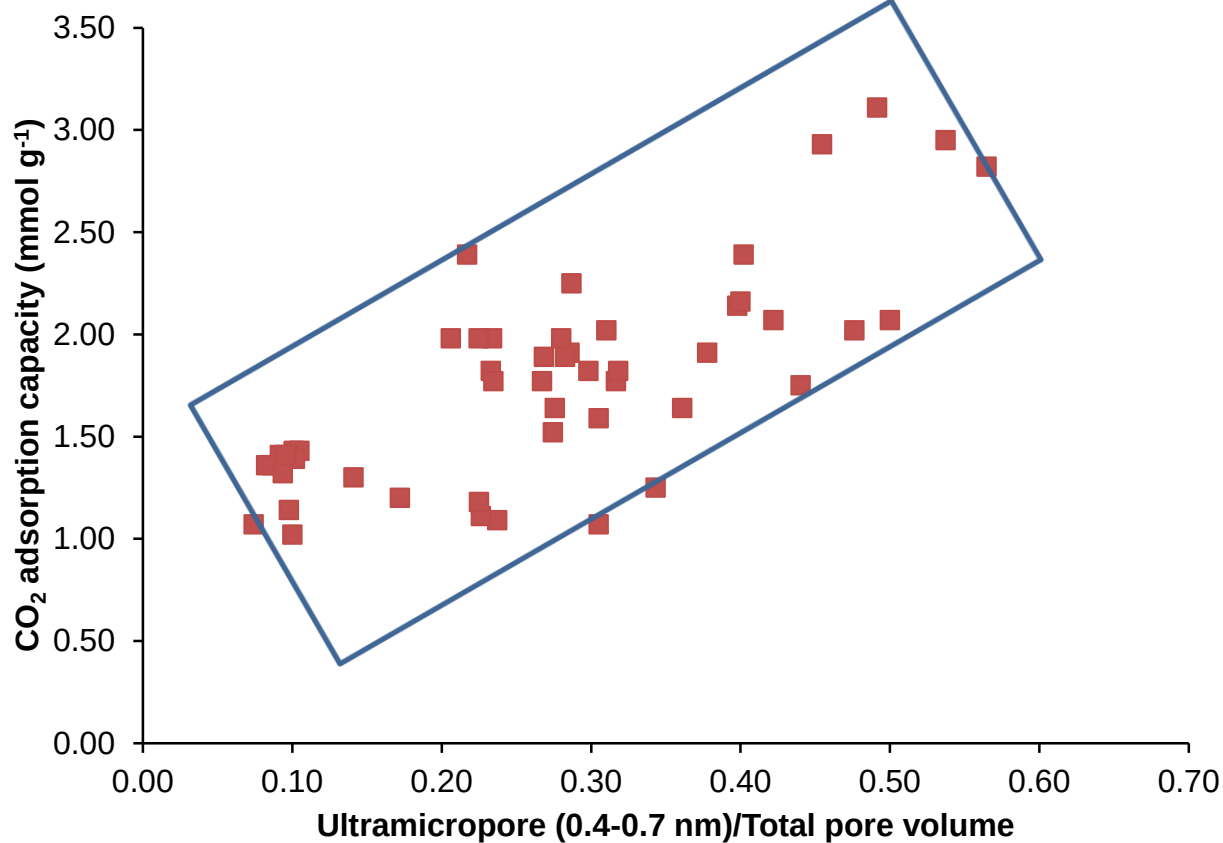




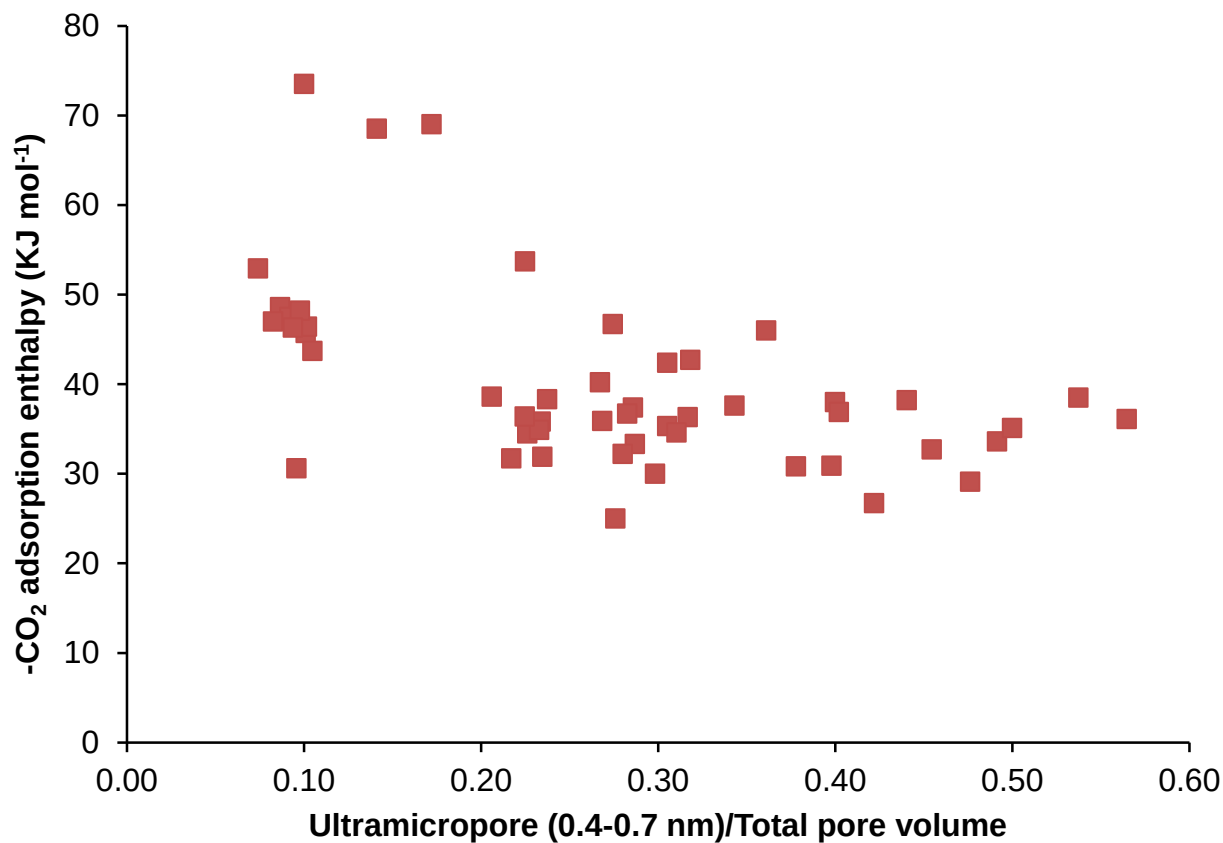
Plot of  $K_1$  for  $\text{CO}_2$  adsorption against ultramicropore volume/total pore volume



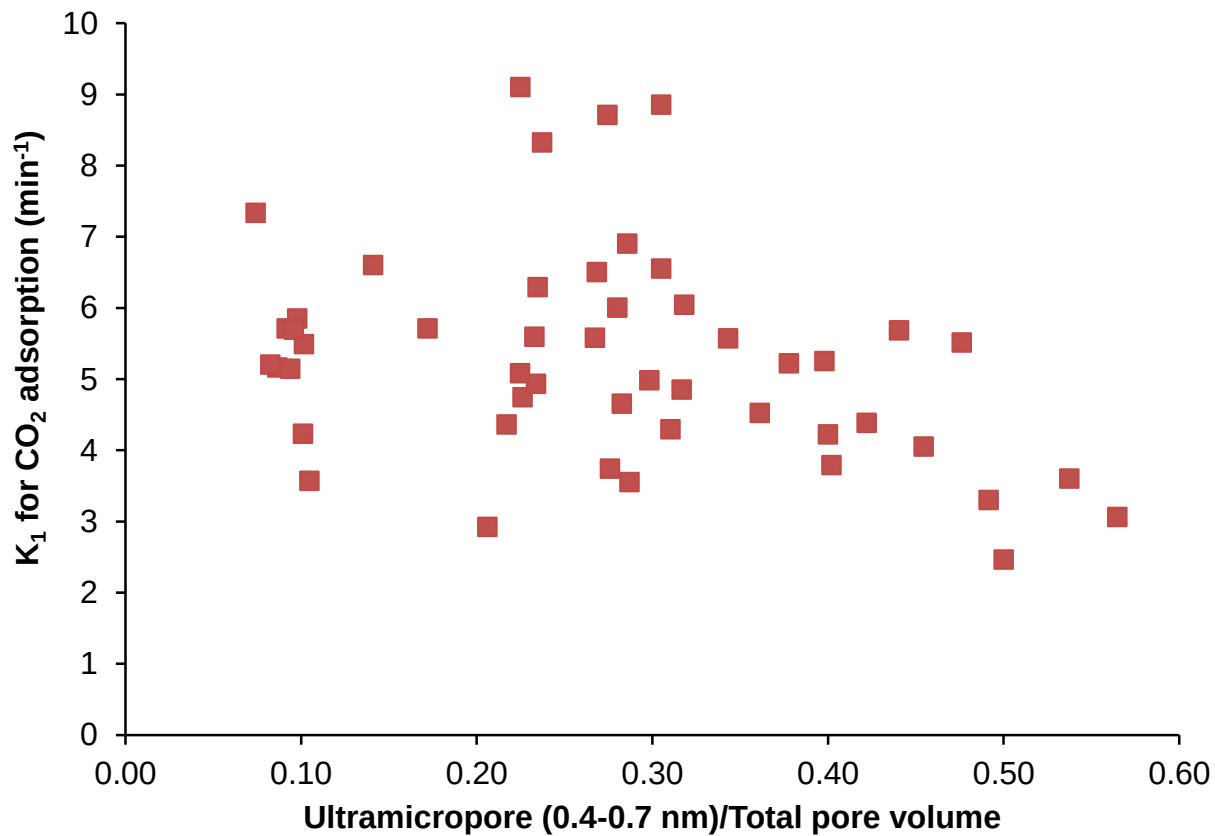
Plot of  $\text{CO}_2$  adsorption capacity against ultramicropore (0.4-0.7 nm) volume/total pore volume



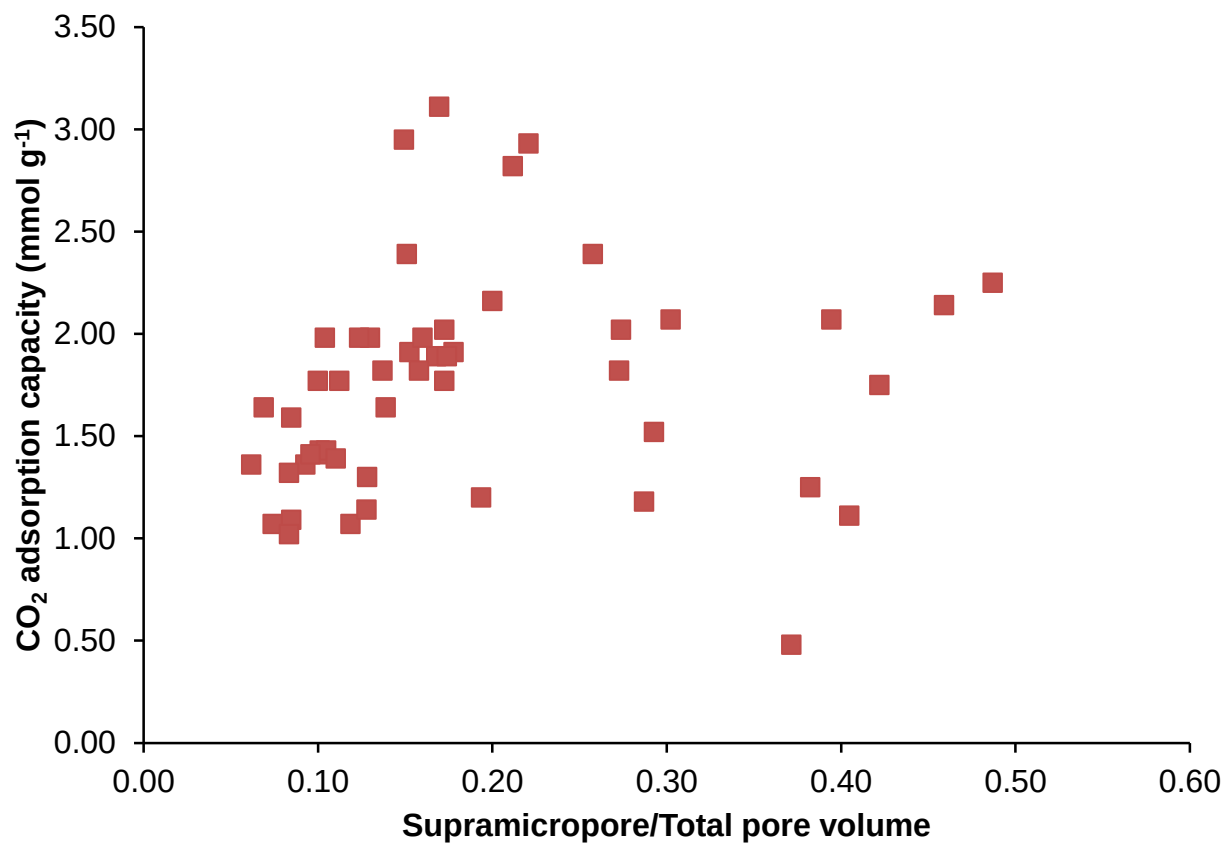
Plot of CO<sub>2</sub> adsorption enthalpy against ultramicropore (0.4-0.7 nm) volume/total pore volume



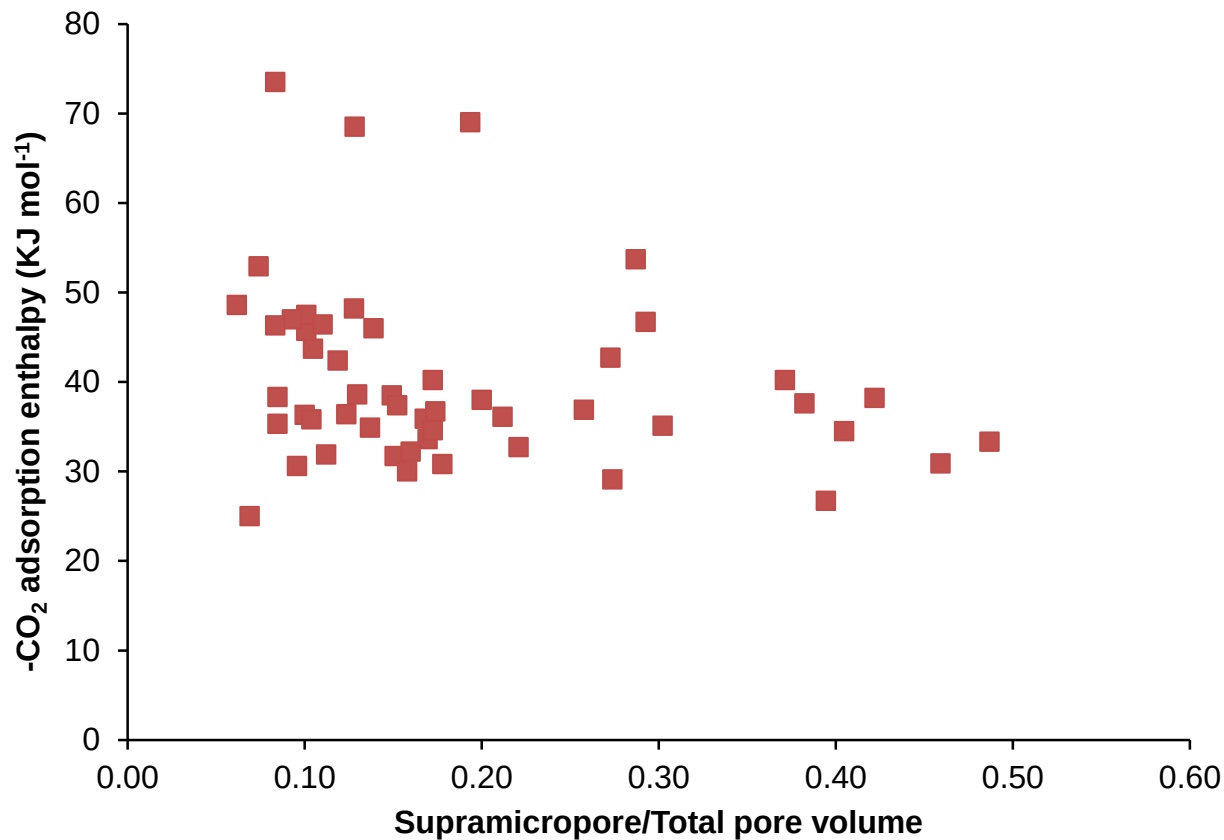
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against ultramicropore (0.4-0.7 nm) volume/total pore volume



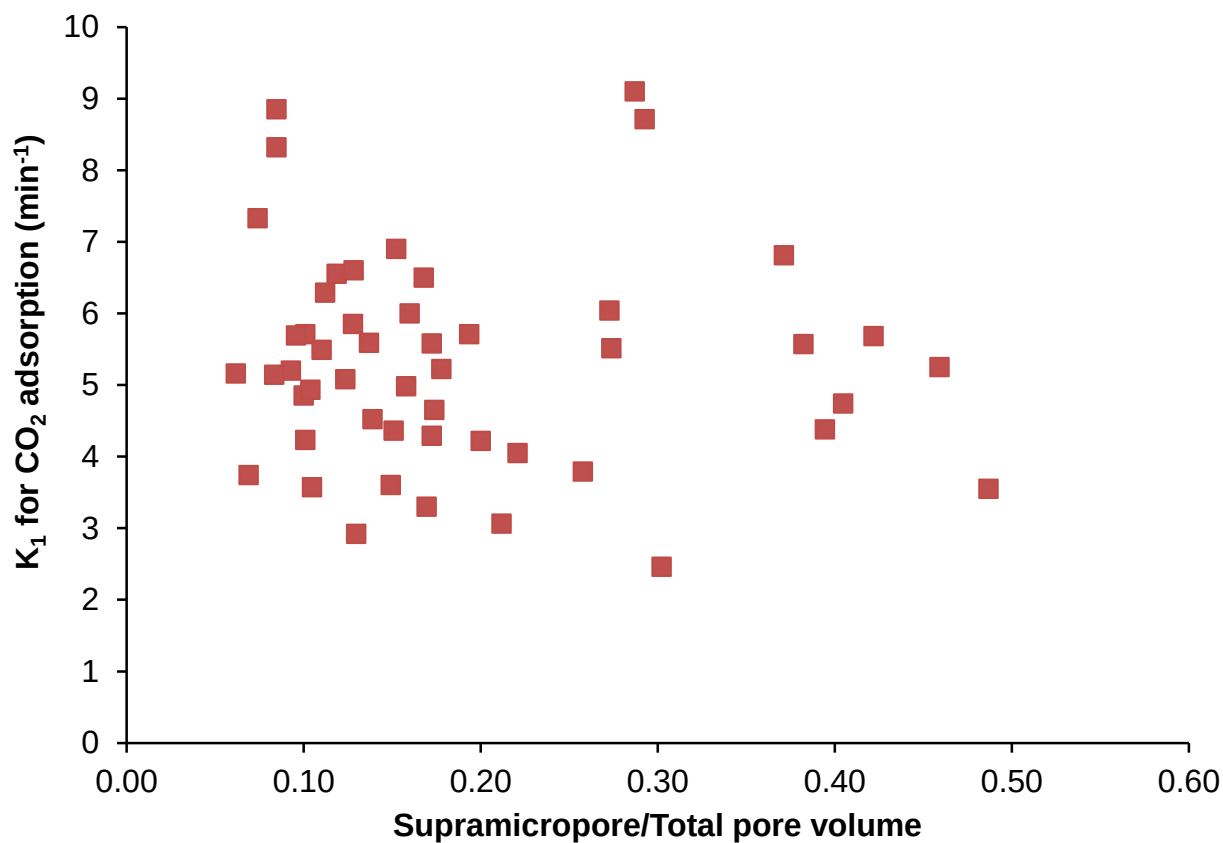
Plot of CO<sub>2</sub> adsorption capacity against supramicropore volume/total pore volume



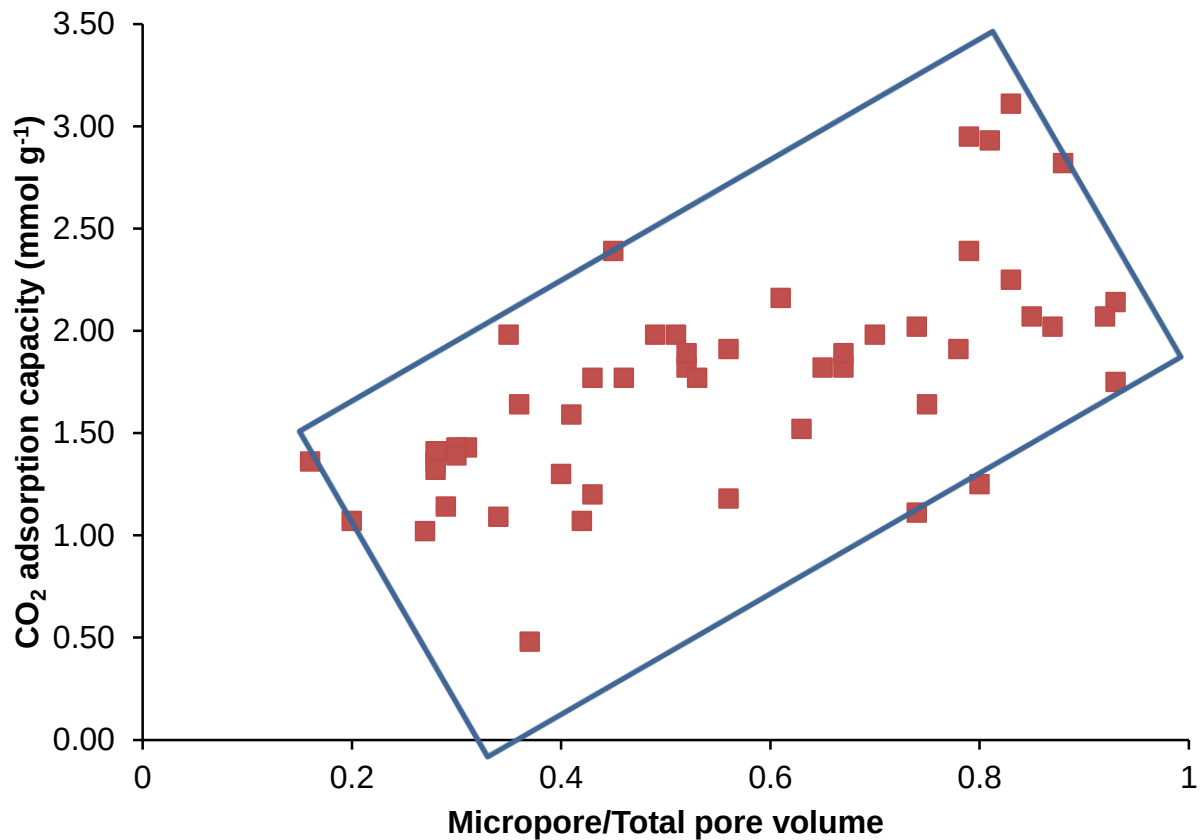
Plot of CO<sub>2</sub> adsorption enthalpy against supramicropore volume/total pore volume



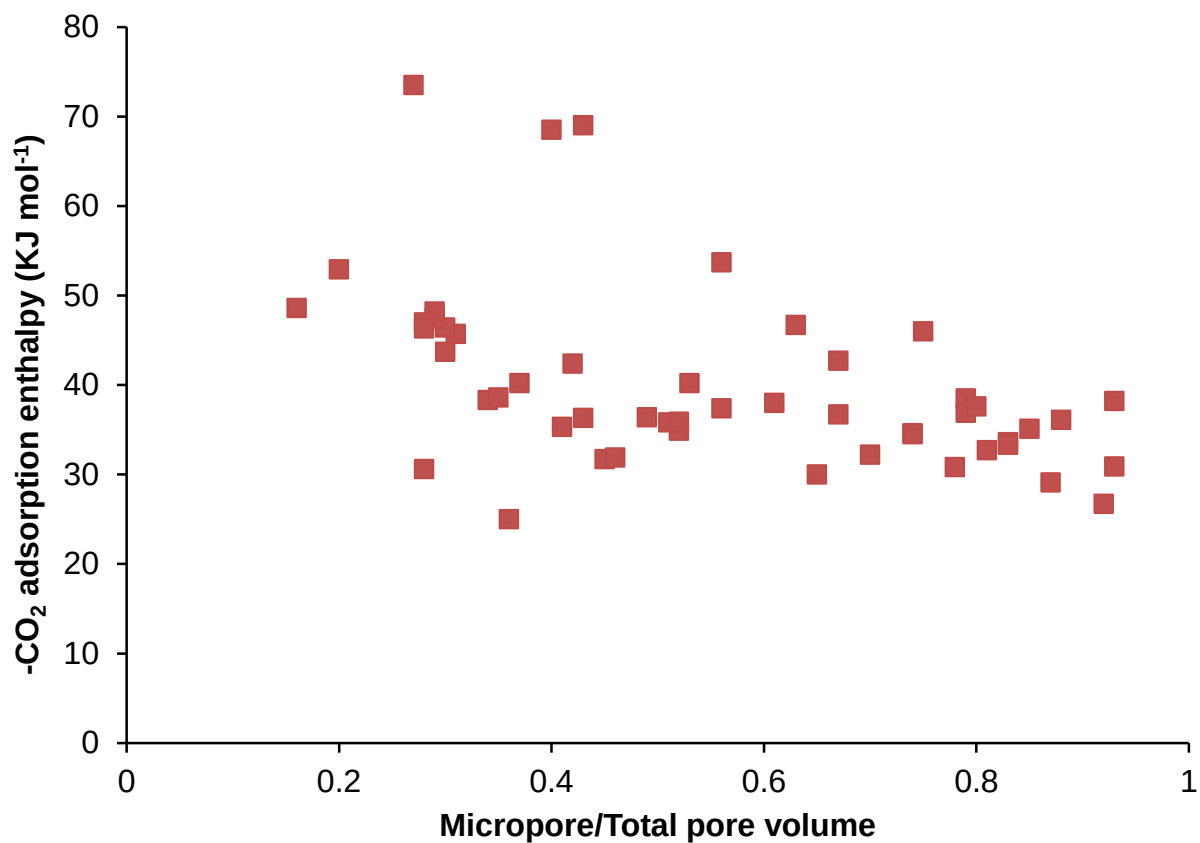
Plot of  $K_1$  for  $\text{CO}_2$  adsorption against supramicropore volume/total pore volume



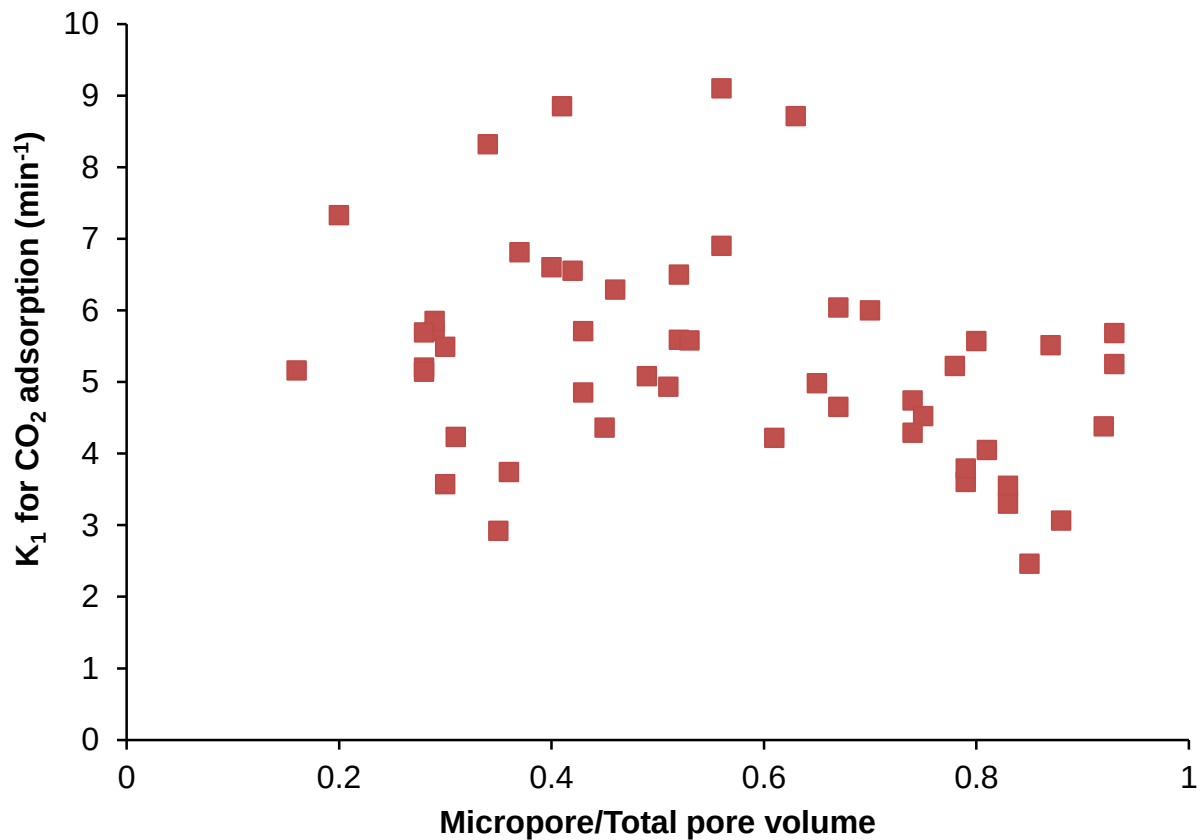
Plot of  $\text{CO}_2$  adsorption capacity against micropore volume/total pore volume



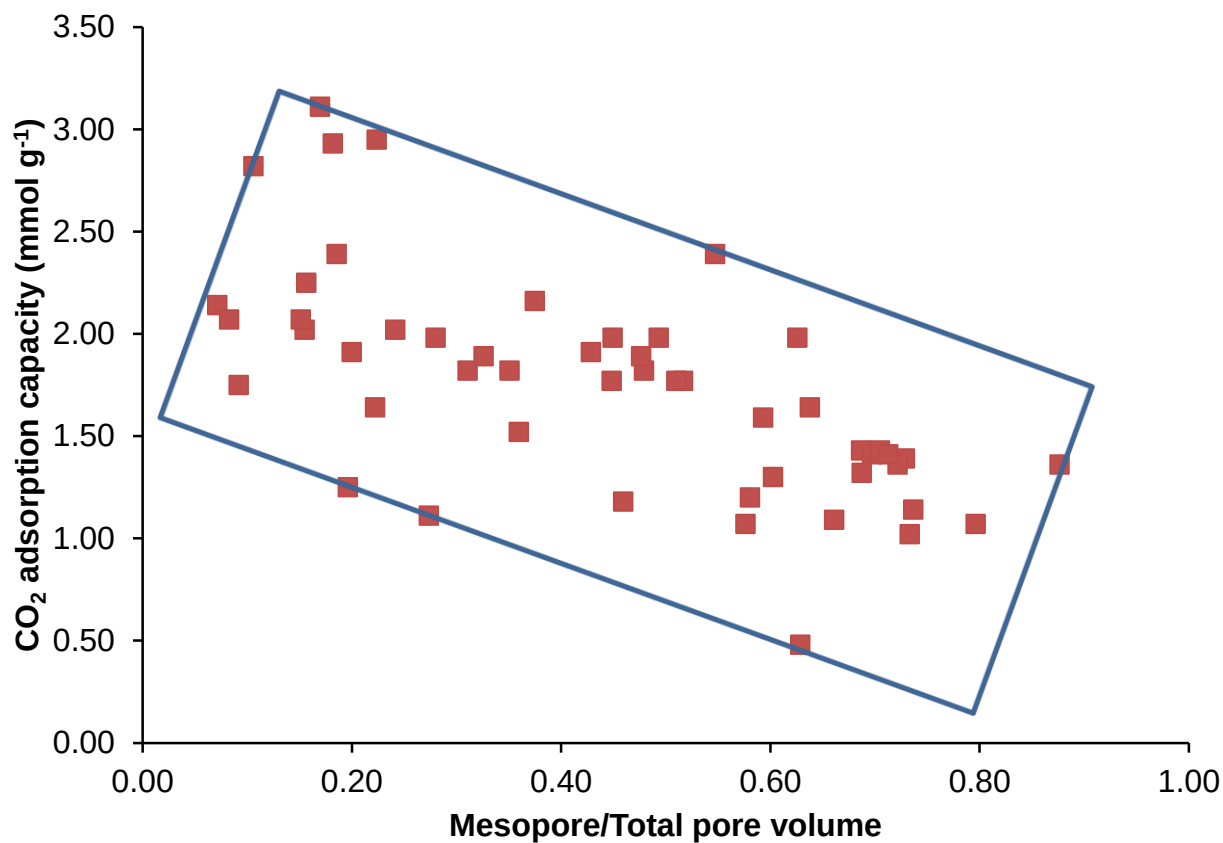
Plot of CO<sub>2</sub> adsorption enthalpy against micropore volume/total pore volume



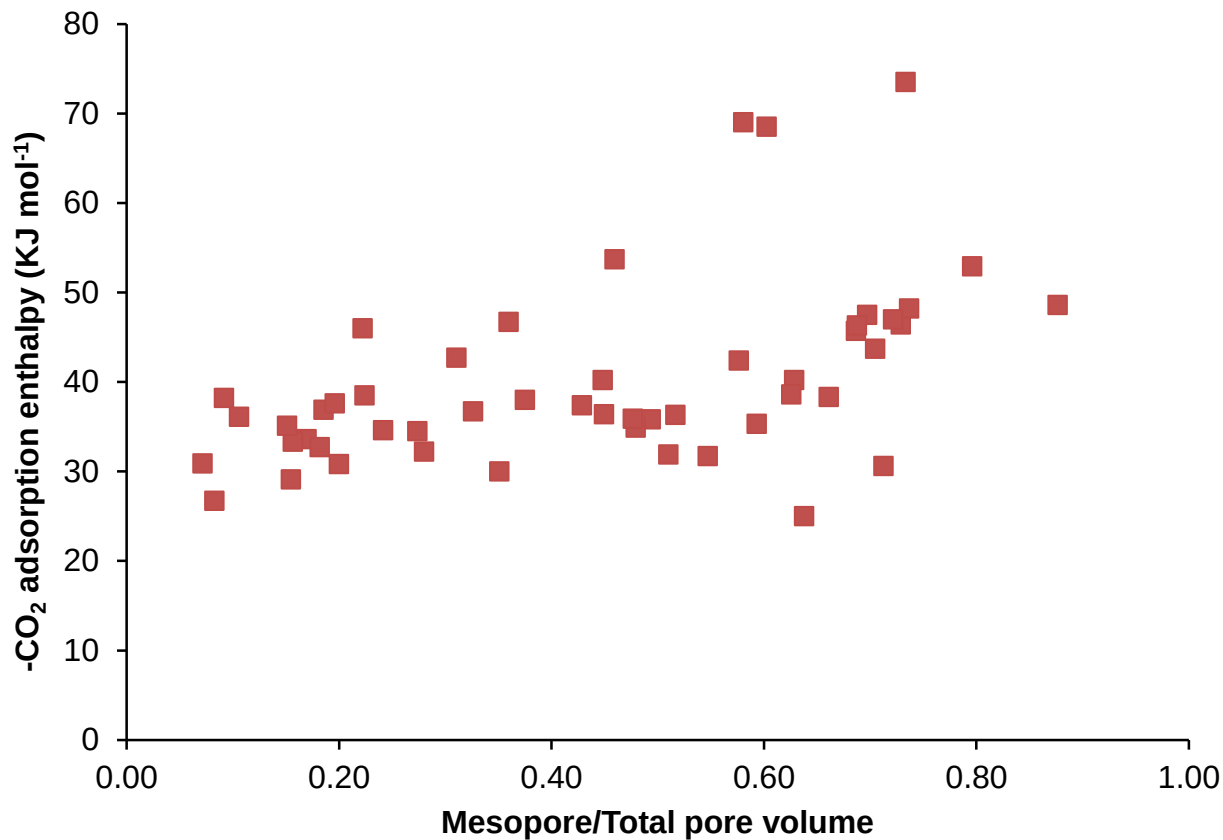
Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against micropore volume/total pore volume



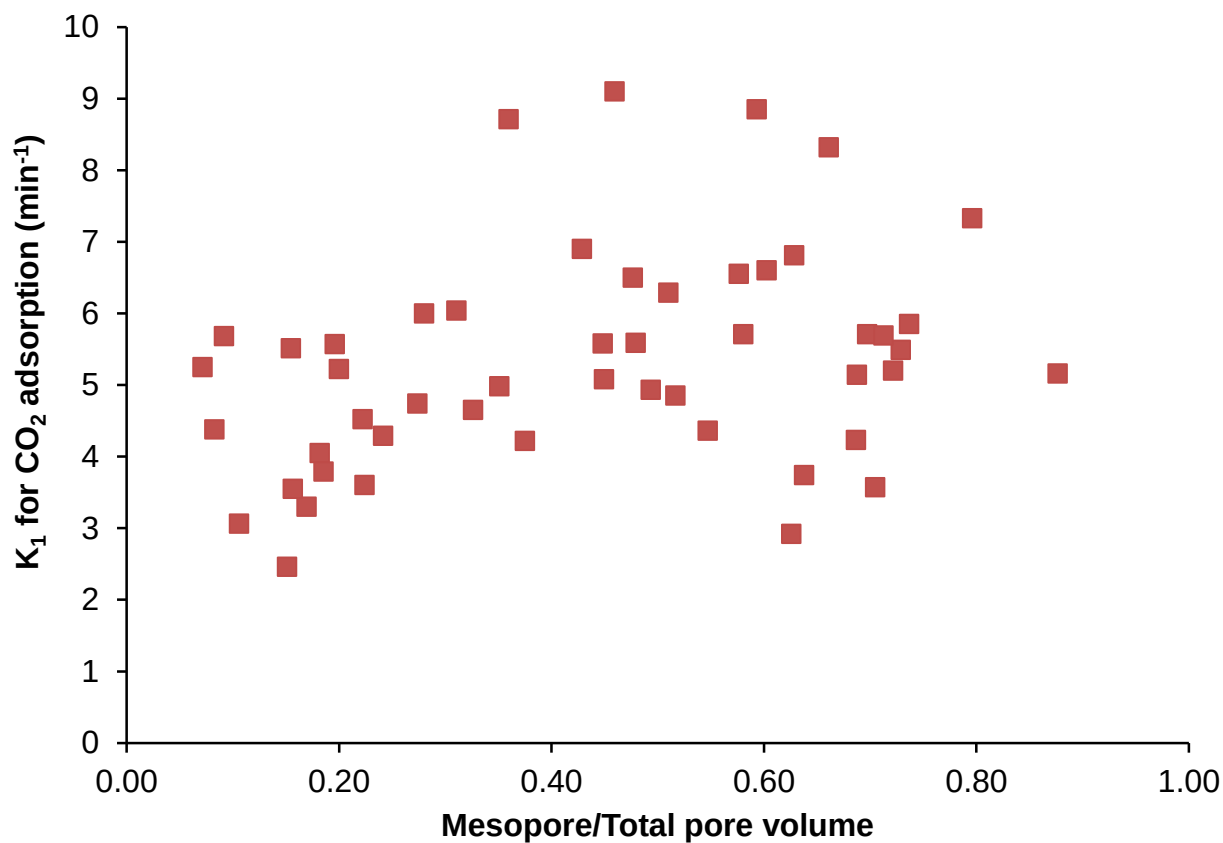
Plot of CO<sub>2</sub> adsorption capacity against mesopore volume/total pore volume



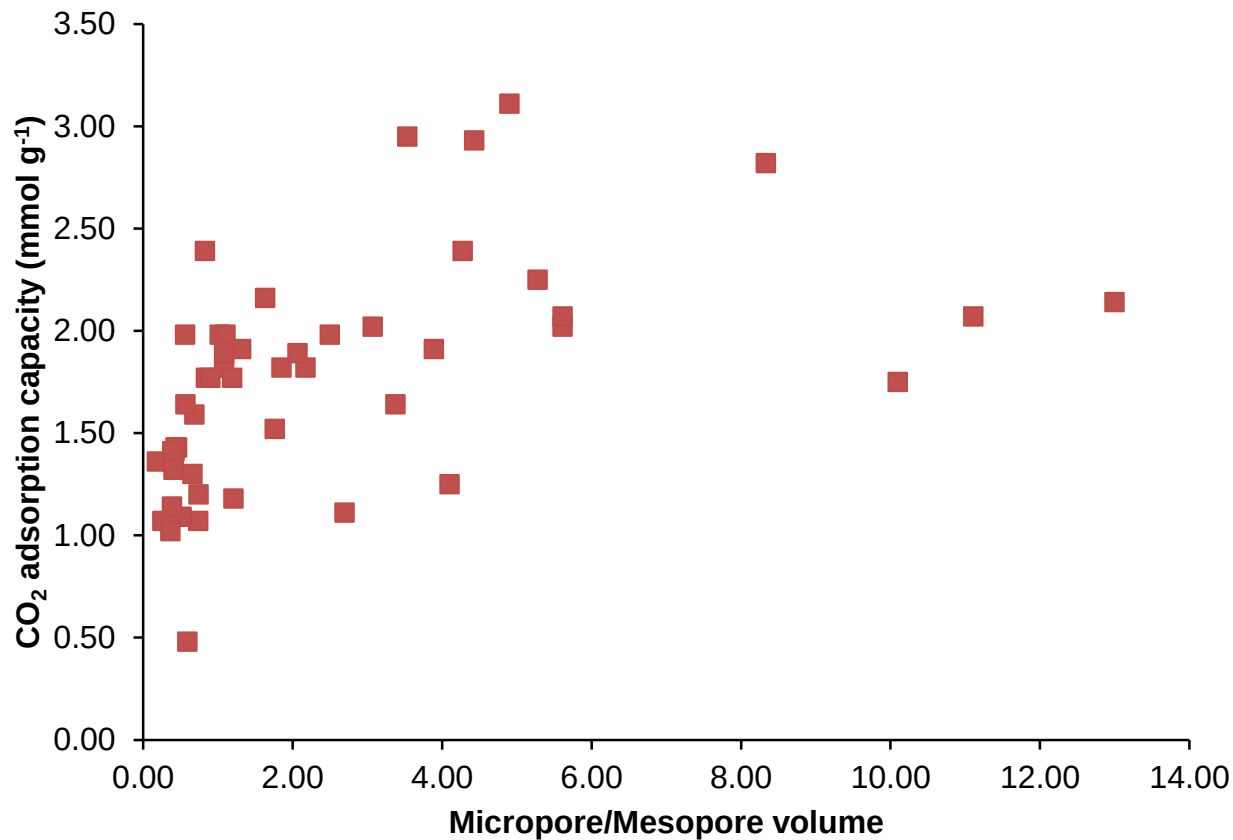
Plot of CO<sub>2</sub> adsorption enthalpy against mesopore volume/total pore volume



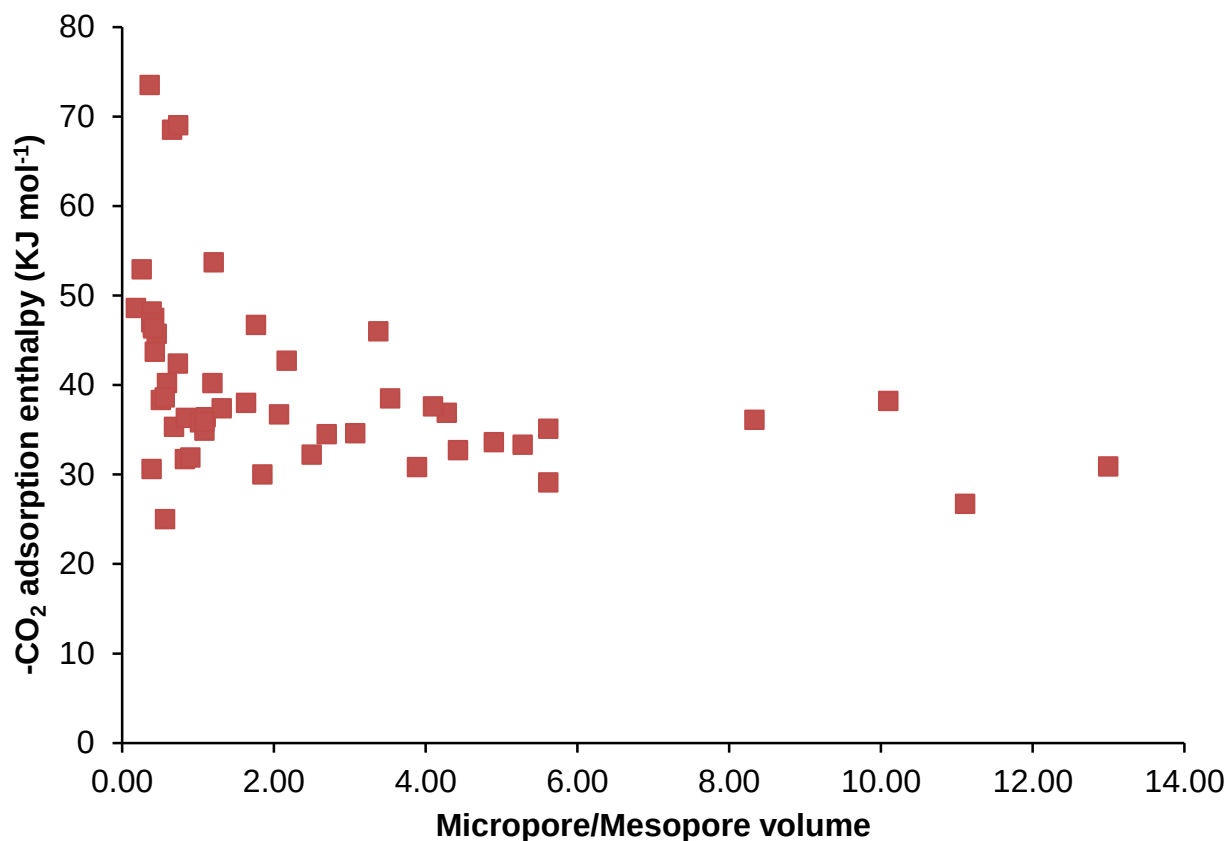
Plot of  $K_1$  for CO<sub>2</sub> adsorption against mesopore volume/total pore volume



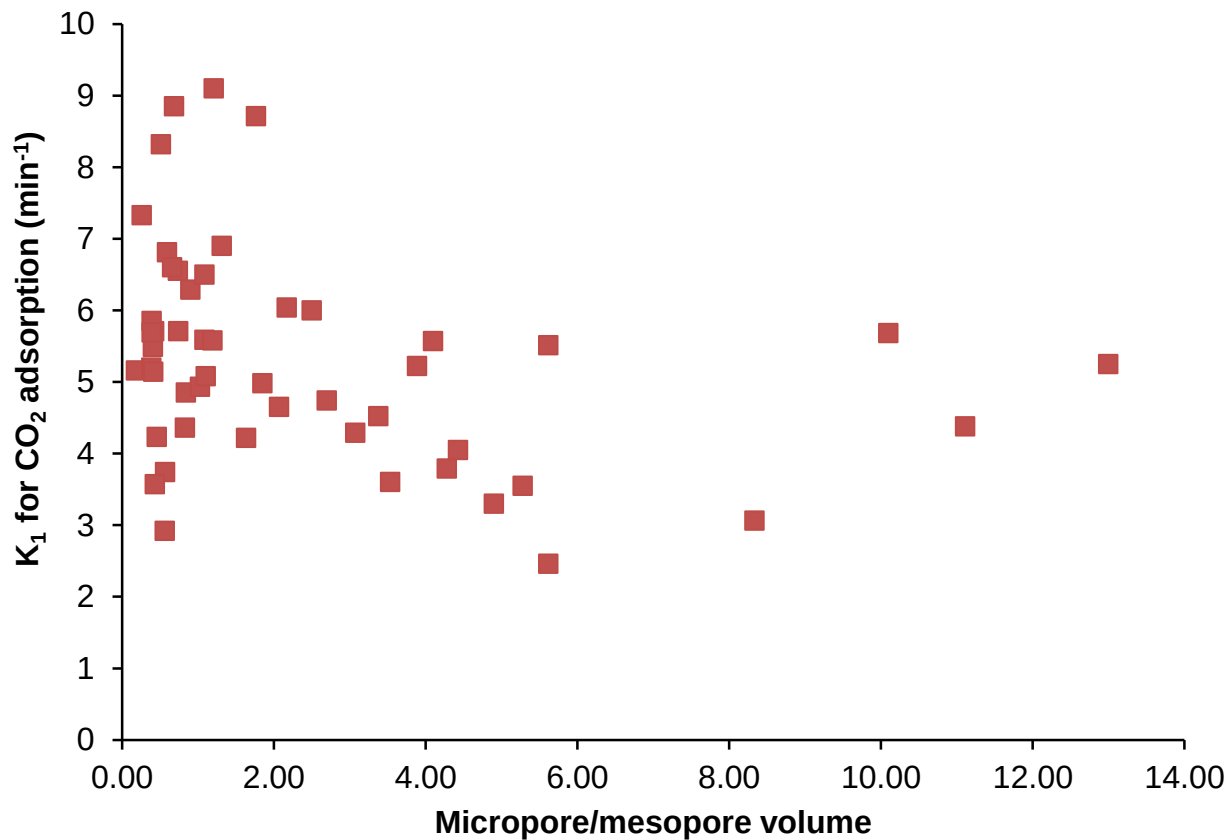
Plot of CO<sub>2</sub> adsorption capacity against micropore volume/mesopore volume



Plot of CO<sub>2</sub> adsorption enthalpy against micropore volume/mesopore volume



Plot of K<sub>1</sub> for CO<sub>2</sub> adsorption against micropore volume/mesopore volume

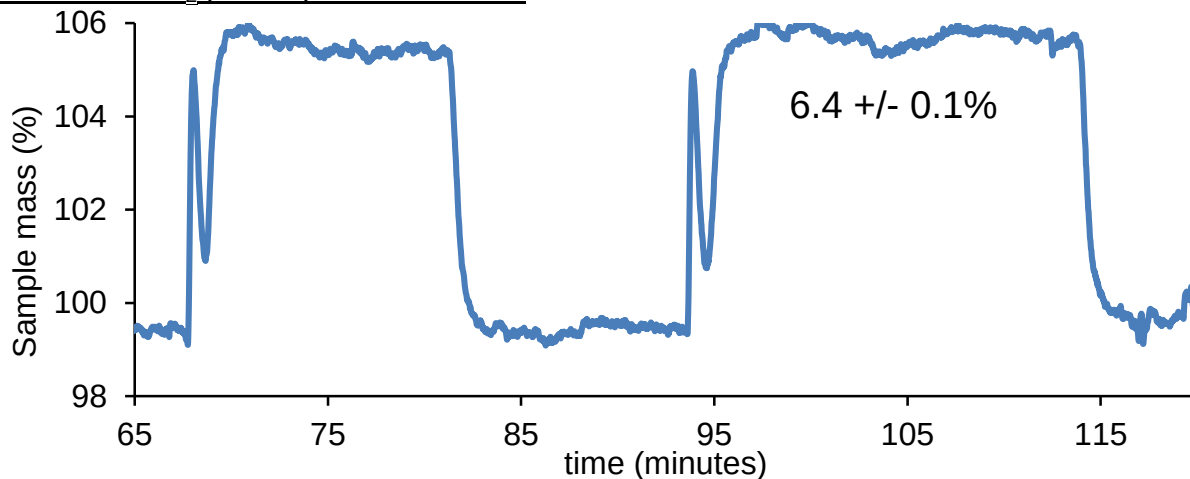




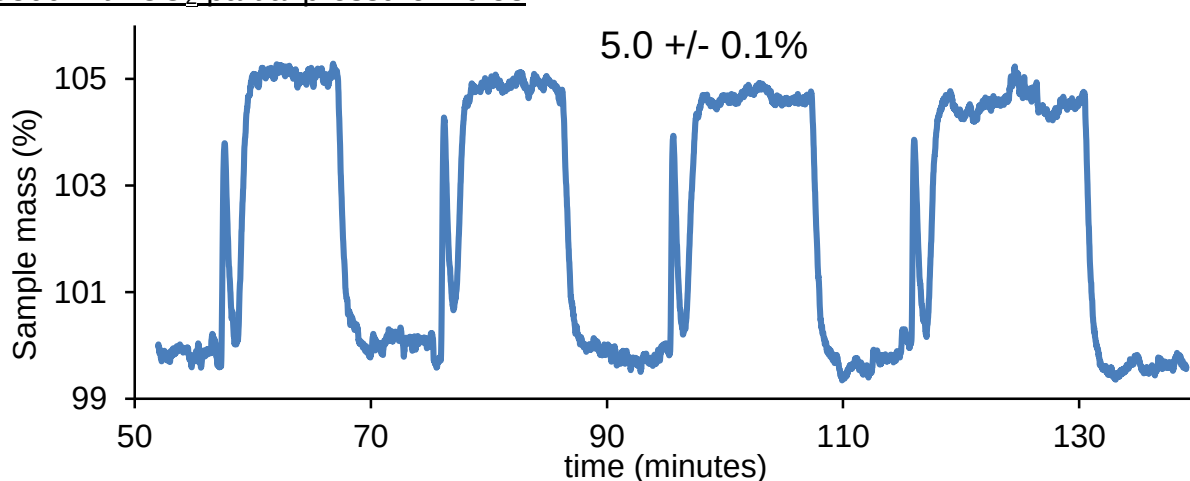
## Mass changes during CO<sub>2</sub> adsorption at 35 °C and various CO<sub>2</sub> partial pressures

The spikes visible before each CO<sub>2</sub> adsorption are artifacts caused by pressure and flow rate fluctuations as the CO<sub>2</sub> gas supply was opened and the supply of CO<sub>2</sub> and N<sub>2</sub> was rebalanced.

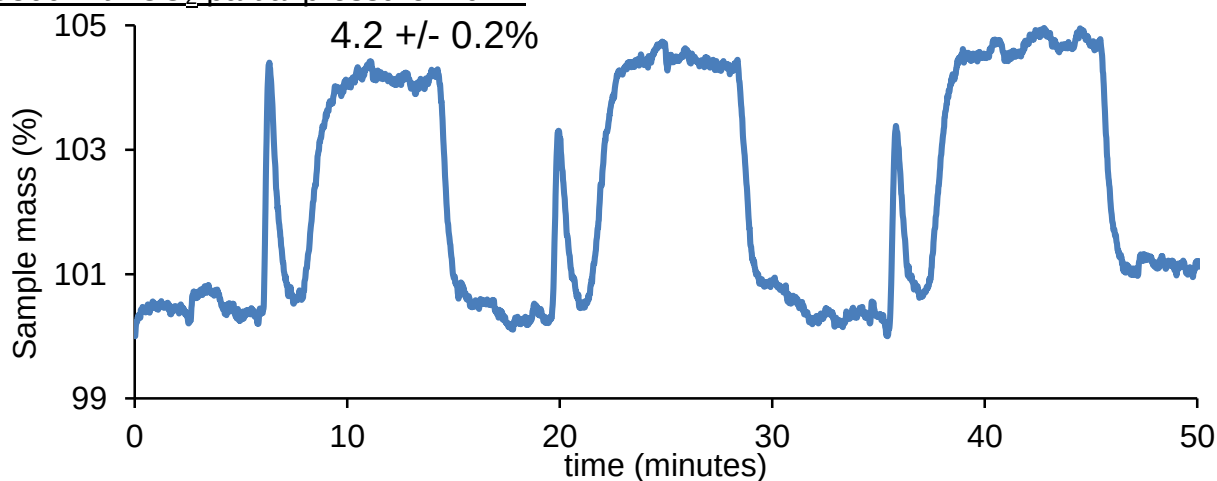
S800 with CO<sub>2</sub> partial pressure = 0.83



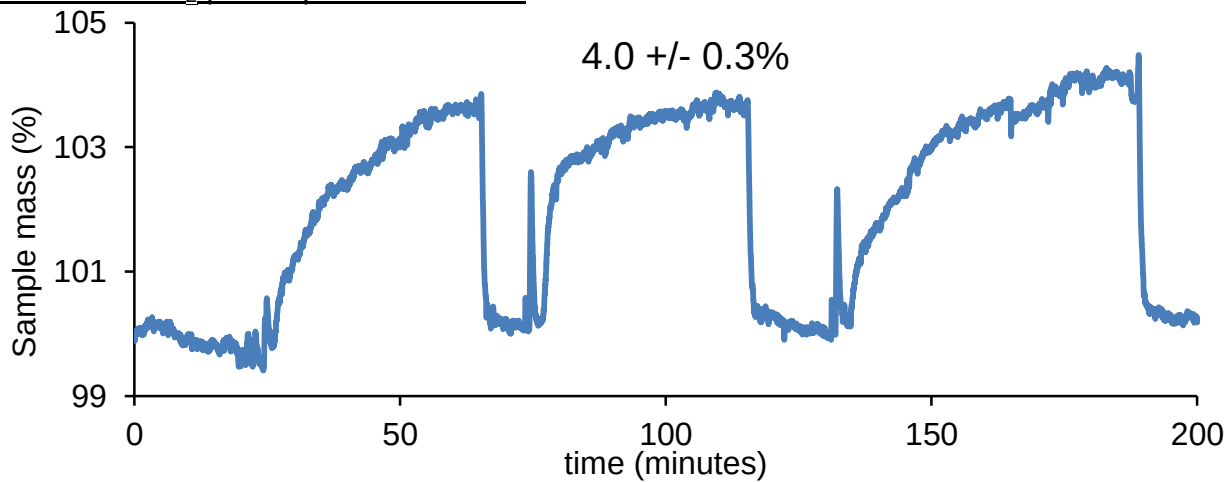
S800 with CO<sub>2</sub> partial pressure = 0.58



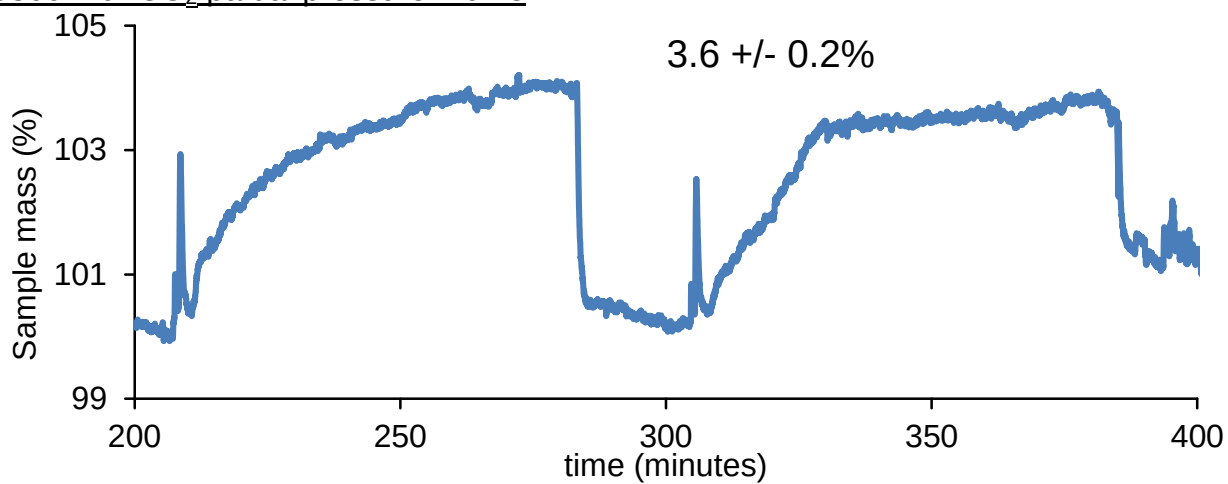
S800 with CO<sub>2</sub> partial pressure = 0.42



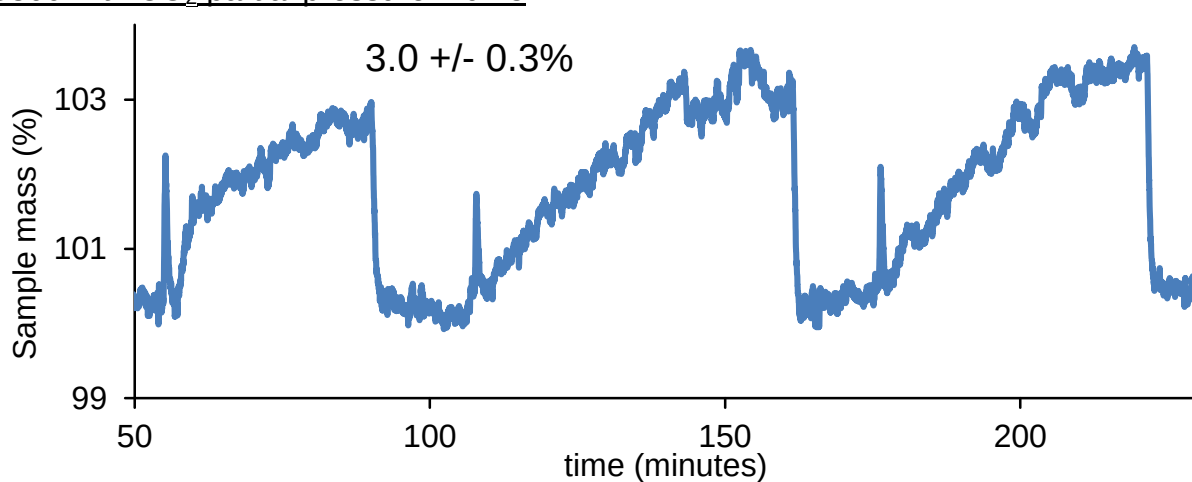
S800 with CO<sub>2</sub> partial pressure = 0.33



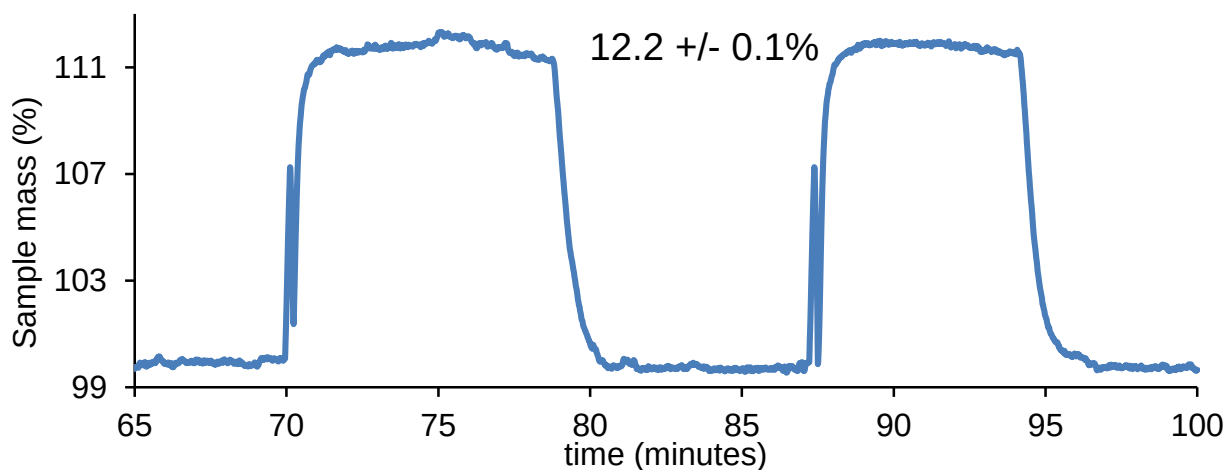
S800 with CO<sub>2</sub> partial pressure = 0.25



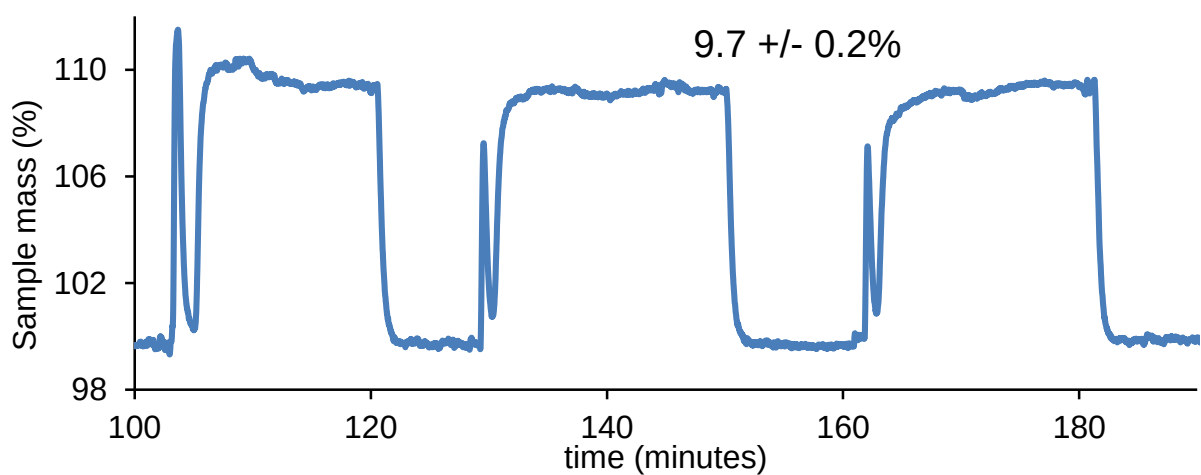
S800 with CO<sub>2</sub> partial pressure = 0.15



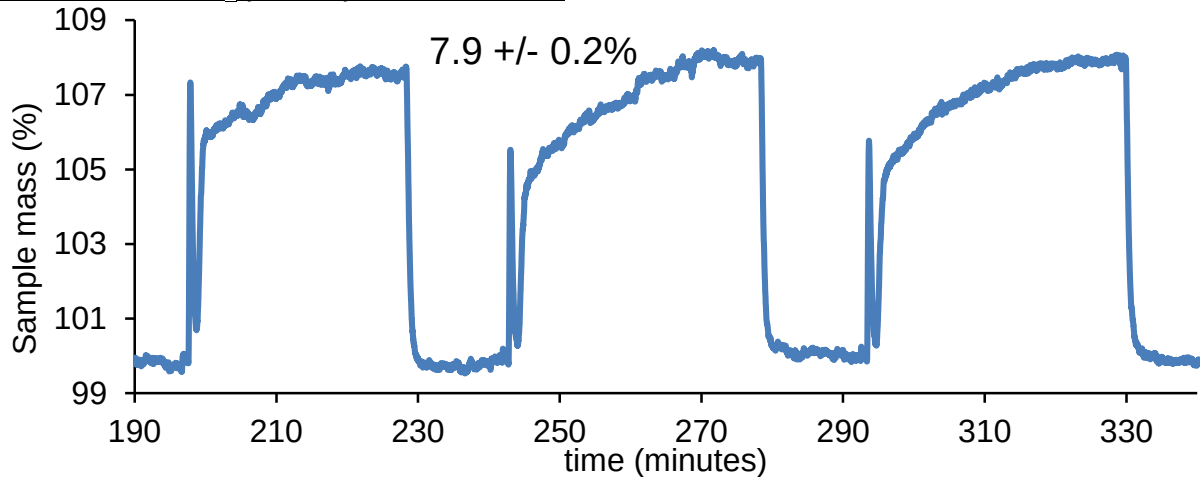
S800K2 with CO<sub>2</sub> partial pressure = 0.83



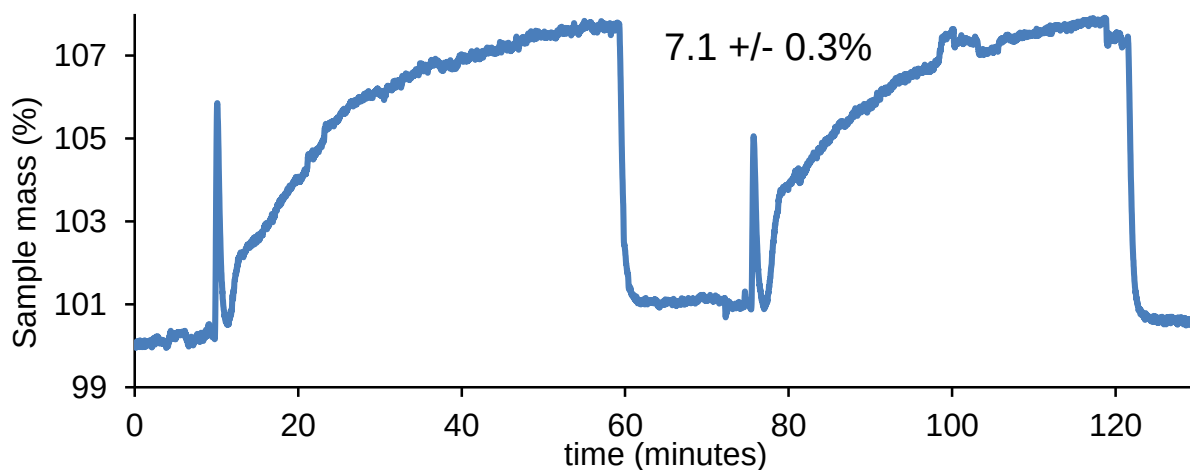
S800K2 with CO<sub>2</sub> partial pressure = 0.58



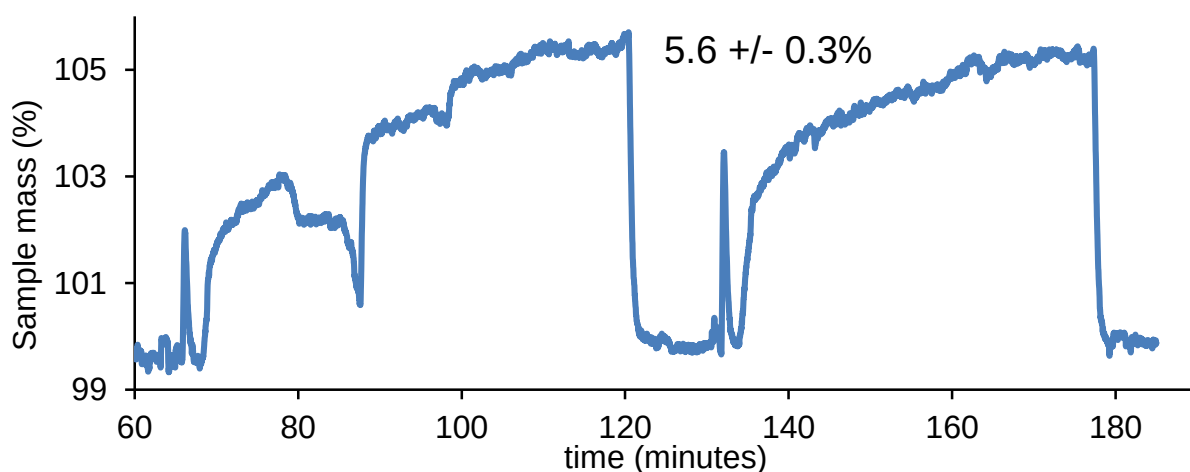
S800K2 with CO<sub>2</sub> partial pressure = 0.42



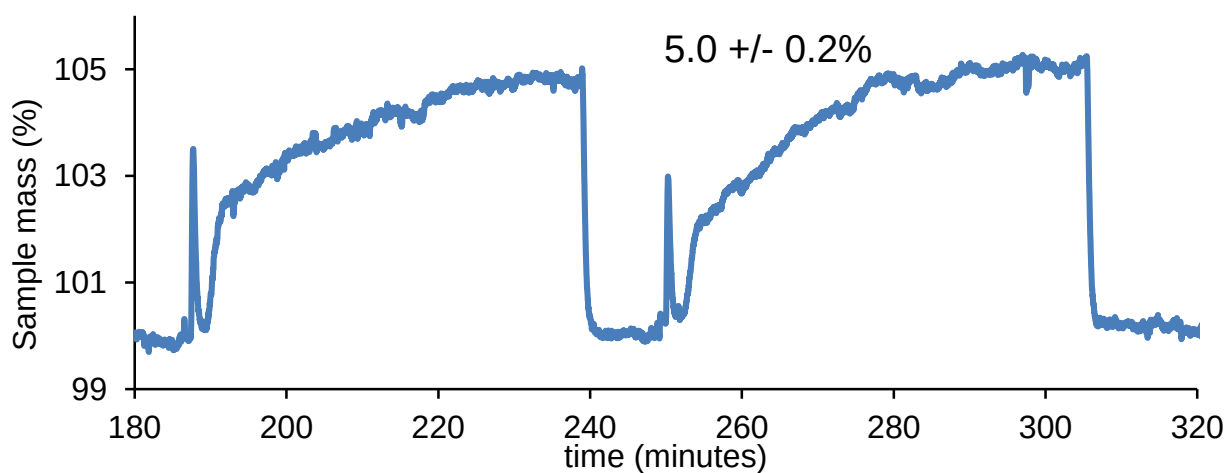
S800K2 with CO<sub>2</sub> partial pressure = 0.33



S800K2 with CO<sub>2</sub> partial pressure = 0.25



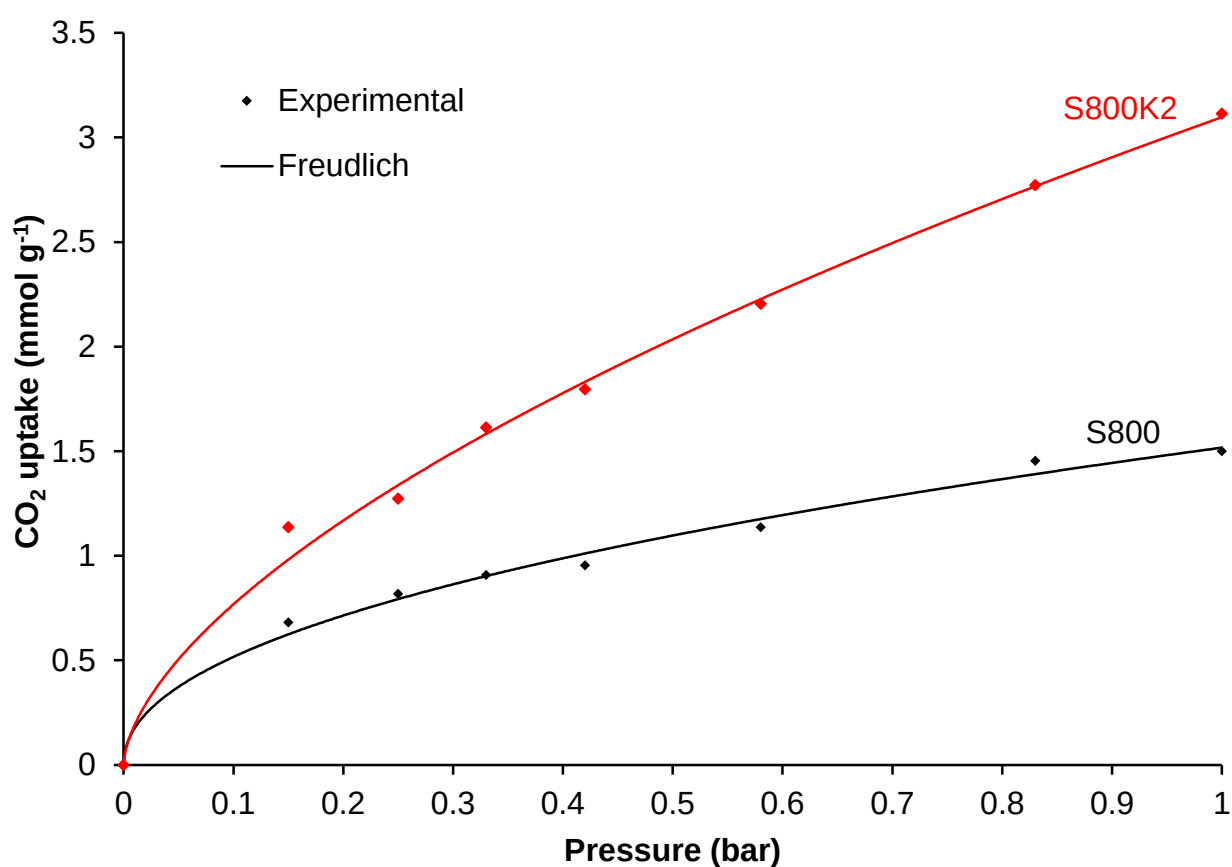
S800K2 with CO<sub>2</sub> partial pressure = 0.15



Tabulation of CO<sub>2</sub> adsorption capacities at various CO<sub>2</sub> partial pressures

| CO <sub>2</sub> content (%) | CO <sub>2</sub> partial pressure (bar) | CO <sub>2</sub> uptake |                      |          |                      |
|-----------------------------|----------------------------------------|------------------------|----------------------|----------|----------------------|
|                             |                                        | S800                   |                      | S800K2   |                      |
|                             |                                        | %                      | mmol g <sup>-1</sup> | %        | mmol g <sup>-1</sup> |
| 100                         | 1                                      | 6.7±0.1                | 1.50±0.02            | 13.7±0.2 | 3.11±0.05            |
| 83                          | 0.83                                   | 6.4±0.1                | 1.45±0.02            | 12.2±0.1 | 2.77±0.02            |
| 58                          | 0.58                                   | 5.0±0.1                | 1.14±0.02            | 9.7±0.2  | 2.20±0.05            |
| 42                          | 0.42                                   | 4.2±0.2                | 0.95±0.05            | 7.9±0.2  | 1.80±0.05            |
| 33                          | 0.33                                   | 4.0±0.3                | 0.91±0.07            | 7.1±0.3  | 1.61±0.07            |
| 25                          | 0.25                                   | 3.6±0.2                | 0.82±0.05            | 5.6±0.3  | 1.27±0.07            |
| 15                          | 0.15                                   | 3.0±0.3                | 0.68±0.07            | 5.0±0.2  | 1.14±0.05            |

Fitting of the Freundlich isotherm to the pressure varied CO<sub>2</sub> adsorption data



Tabulation of Freundlich parameters for the CO<sub>2</sub> adsorption isotherm

| Model      | Parameters                                        | S800  | S800K2 |
|------------|---------------------------------------------------|-------|--------|
| Freundlich | $K_F$ (mmol g <sup>-1</sup> bar <sup>-1/n</sup> ) | 1.757 | 3.097  |
|            | 1/n                                               | 0.468 | 0.606  |
|            | R <sup>2</sup>                                    | 0.994 | 0.998  |

Gibbs free energies (-1.4 KJ mol<sup>-1</sup> for S800 and -2.9 KJ mol<sup>-1</sup> for S800K2) calculated based on the adsorption constant  $K_F$  at 308 K ( $\Delta G^0 = -RT \ln K_F$ ) are consistent with the values obtained using pure carbon dioxide at 298 K and 323K (-2.1 and -1.4 KJ mol<sup>-1</sup> for S800; and -3.2 and -2.5 KJ mol<sup>-1</sup> for S800K2) given in Table 4 of the manuscript.