Supporting information:

Synthesis and ion transport activity of oligoesters containing an environment-sensitive fluorophore

*Joanne M. Moszynski and Thomas M. Fyles**

Department of Chemistry, University of Victoria. Victoria, BC. Canada. V8W 3P6

tmf@uvic.ca

This file contains summary information on the bilayer-clamp conductance experiments conducted with the compound HO_2C-***Trip-G(E3)***-OH. The compound is abbreviated [tGE3] throughout this file.

The information consists of:

- Experimental details and comments on the structure and format of the summary files
- Five summaries of experiments conducted.

Bookmarks are inserted for the five experimental summaries.

Filename	electrolyte
JMM-3	1M CsCl
JMM-4	1M CsCl
JMM-1	1M KCl
JMM-2	1M NMe_4Cl
JMM-5	1M NMe_4Cl

Bilayer clamp experimental details.

The methodology was derived from that previously described (*1*). A model BC-525A bilayer clamp (Warner Instrument Corp.) was used for all planar bilayer experiments, ClampEx 8 and ClampFit 10 (Axon Instruments) were the software used for acquisition and analysis, respectively. Cups used were made of polystyrene and had 250µm diameter apertures. The lipid used in all cases was diphytanoyl phosphatidylcholine (diPhyPC) (Avanti Polar lipids). A stock solution of 25mg/mL lipid in $CHCl_3$ was dried under N_2 and then re-suspended in 200µL decane. For compounds that had to be pre-loaded into the lipid, 0.1 – 1mol% compound in $CHCl_3$ was added to the lipid mix and then dried down. The electrolytes used were 1M KCl, NaCl, CsCl, or NMe_4Cl in 10mM HEPES, 10mM TRIS, pH 7, (unadjusted).

The aperture was primed with 0.5-1µL of decane/lipid, excess solvent was removed by blowing N_2 over the aperture. The cup was then placed into the electrolyte-filled holding cell, consisting of 5mL and 3mL chambers, and salt bridges (KNO_3/Agar) and electrodes (Ag/AgCl) were attached. Bilayers were formed by brushing on 1- 1.5µL of the decane/lipid mix over the aperture, and were monitored for stability, capacitance and resistance for at least 20 minutes before test compound was added. Test compounds were added by injection from an organic solution (typically no more than 1-10µL of solution) or by breaking the lipid-only bilayer and brushing on the compound-preloaded in a lipid mix. All data were hardware filtered (8- pole Bessel filter, 1 kHz) and data was collected in a survey mode using the Gap-free protocol. Bilayers were tested repeatedly for capacitance and resistance. Once formed, 'activity' from pristine bilayers was never observed.

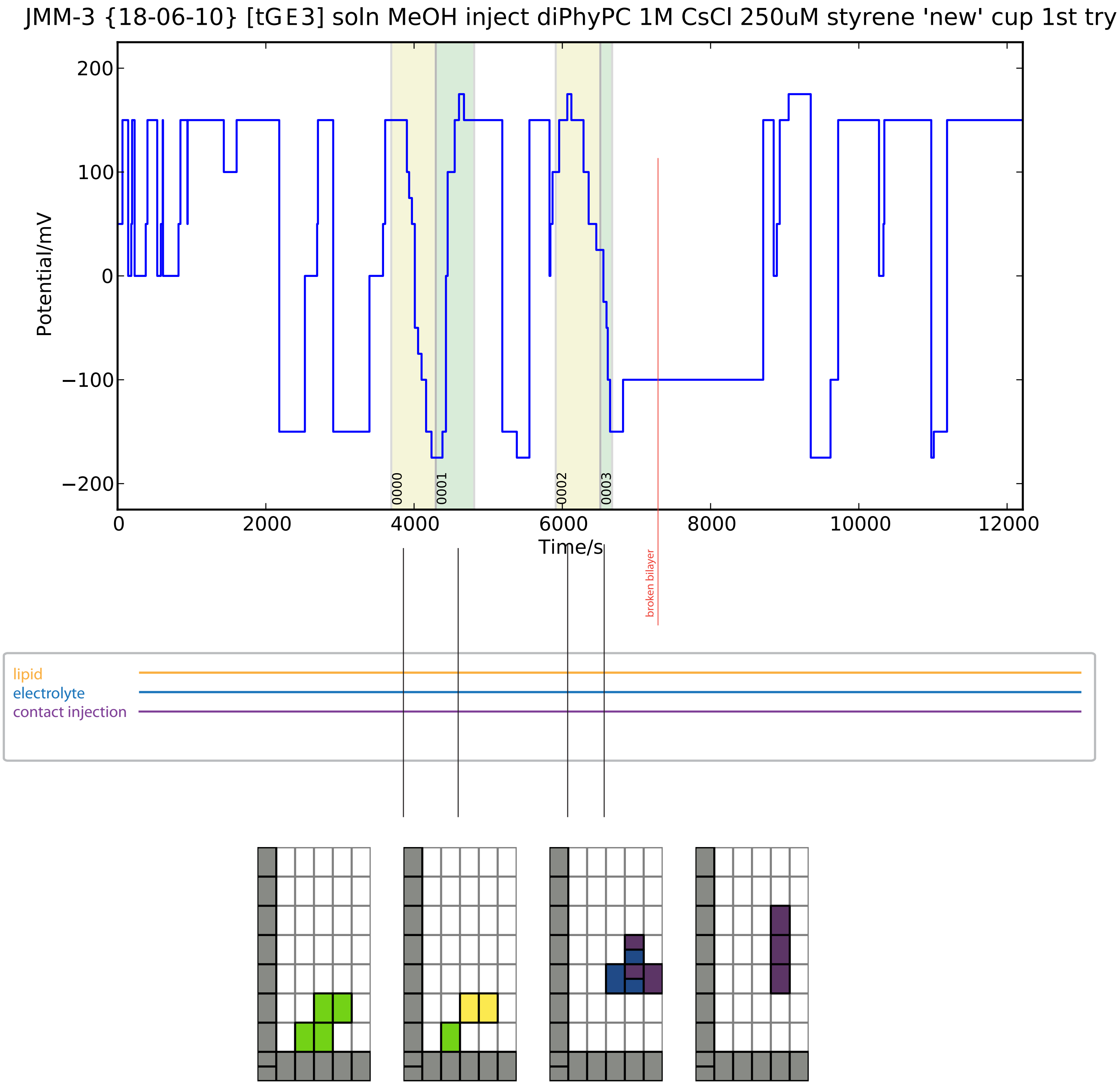
Conductance data summary format.

Each experiment conducted is summarized in a separate file within this portfolio. The structure of each summary is similar consisting of:

- A title of the form: file identifier {date} [compound] details of the experiment
- A plot of the applied potential as a function of the overall experiment time. Color overlays on this plot show the durations of the recorded traces, numbered sequentially 0000 – 00mn. The plot also shows when bilayer breakage occurred (if it did).
- A bar graphic showing the composition of the experiment as it proceeded. The lines establish that the indicated component was continuously present.
- Activity grid summaries for the individual traces recorded. These grids use the notation presented in ref (*2*). The horizontal position gives event duration in log (duration) from 1 to 10^5 millieconds. The vertical position gives conductance in log (conductance) from 1 to 3000 pS in 0.5 log unit steps (1,3,10,30 etc pS). The colour codes are : green = regular "square-top behaviour; yellow = "flicker" behaviour; blue = "multiple open states" behaviour; red = "spike" behaviour; purple = "erratic" behaviour; grey indicates the region cannot be observed due to the instrument and data processing settings of the experiment .
- For each trace recorded there are one or more pages showing the overall trace and selected sections expanded to highlight the various conductance behaviours noted on the activity grid for the experiment.

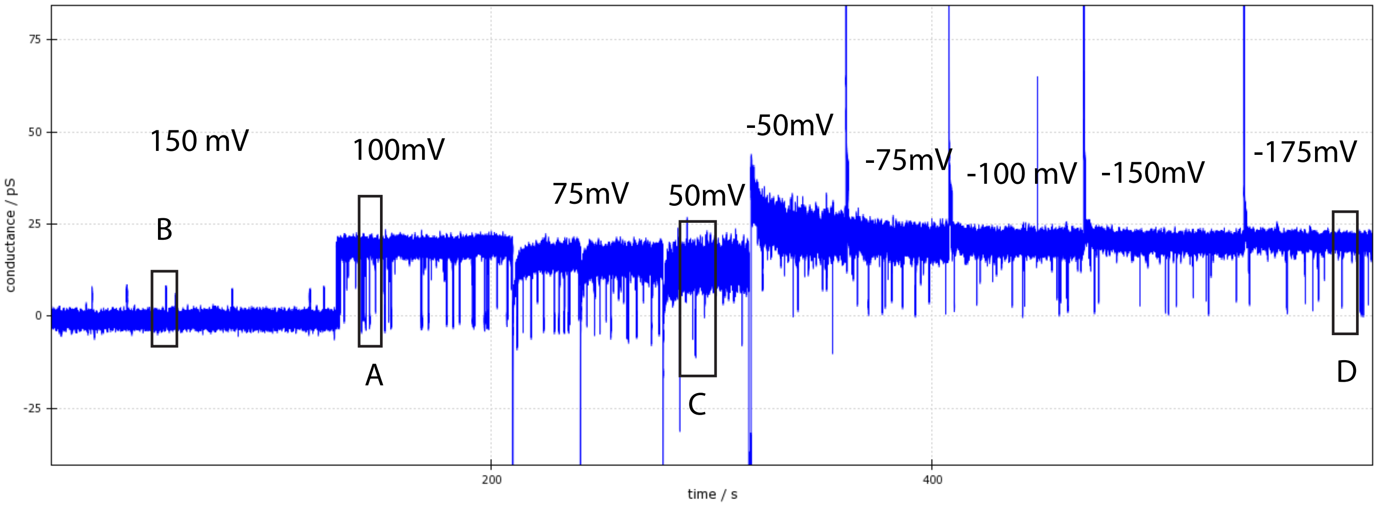
(1) Eggers, P.K.; Fyles, T.M.; Mitchell, K.D.D.; Sutherland, T., *J. Org. Chem.* **2003,** *68*, 1050-1058.

(2) Chui, J.K.W.; Fyles, T.M., *Chem. Soc. Rev.* **2011** DOI: 10.1039/c1cs15099e.

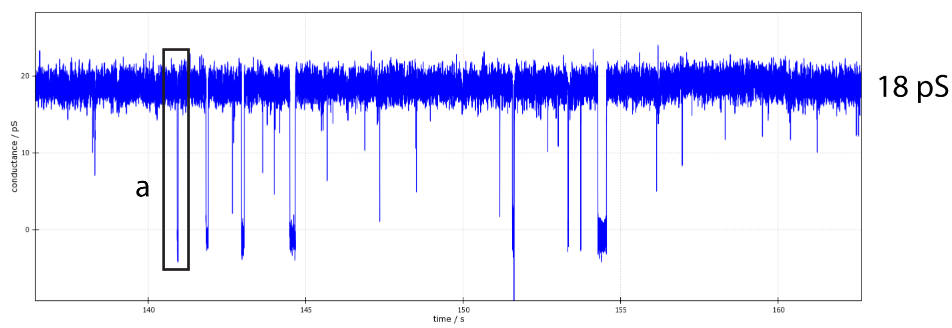

JMM-3 {18-06-10} [tGE3] soln MeOH inject diPhyPC 1M CsCl 250uM styrene 'new' cup 1st try
Potential/mV
200
100
0
−100
−200
0
2000
4000
6000
8000
10000
12000
Time/s
0000
0001
0002
0003
broken bilayer
lipid
electrolyte
contact injection

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

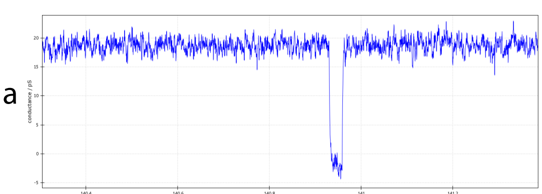
0000



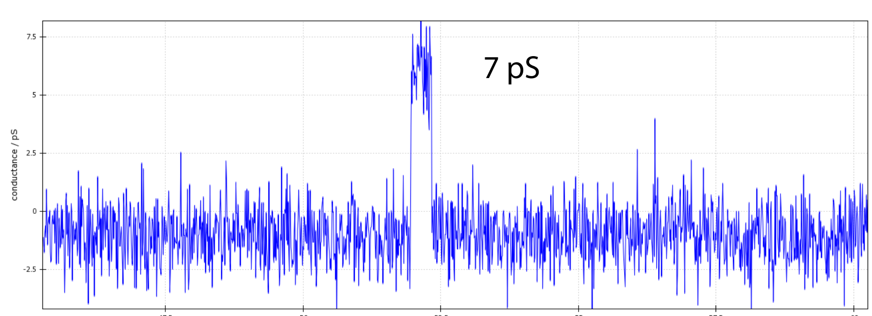
A



a

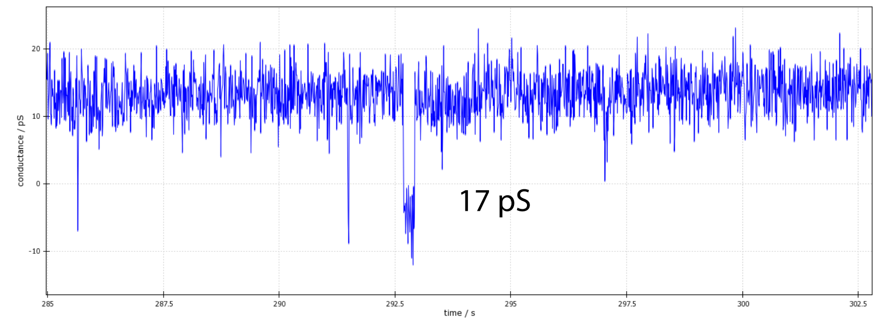


B

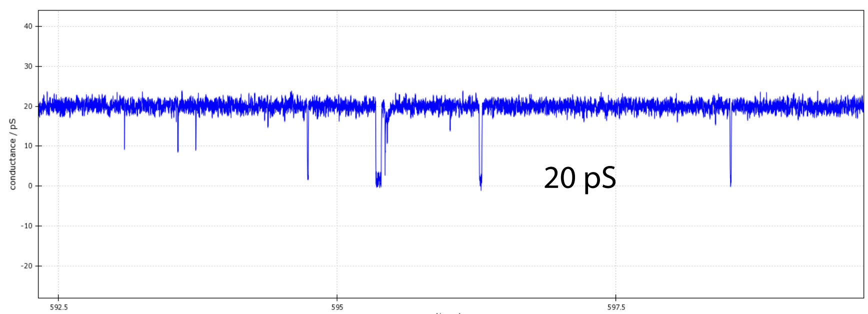


0000 continues...

C

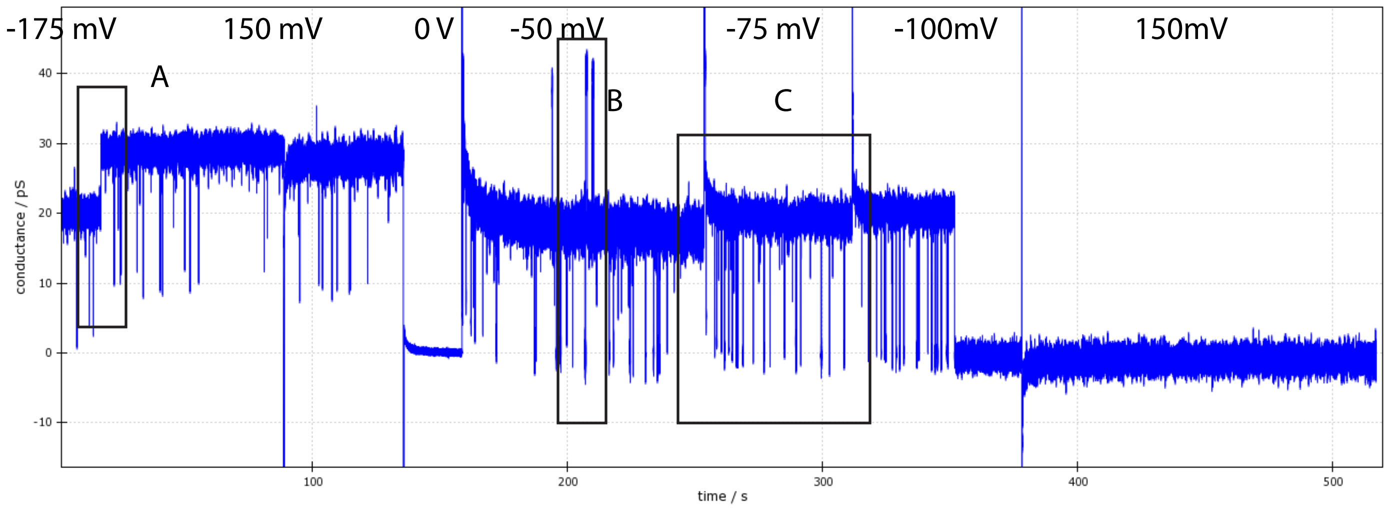


D

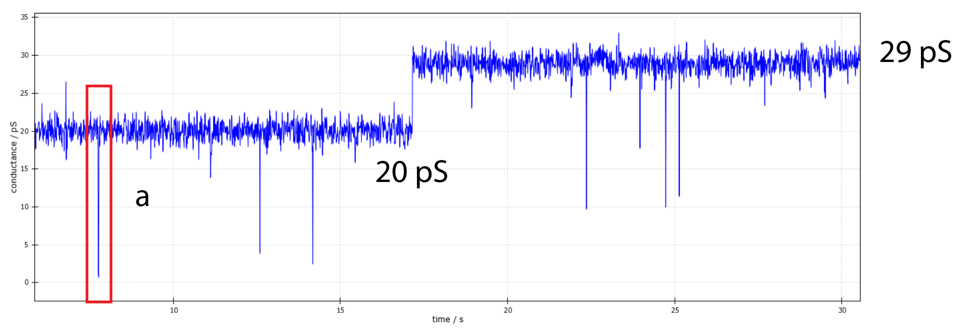


Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

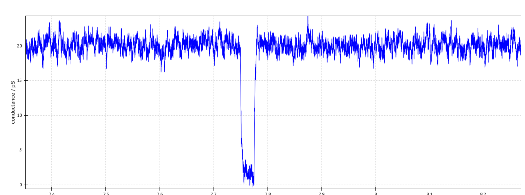
0001



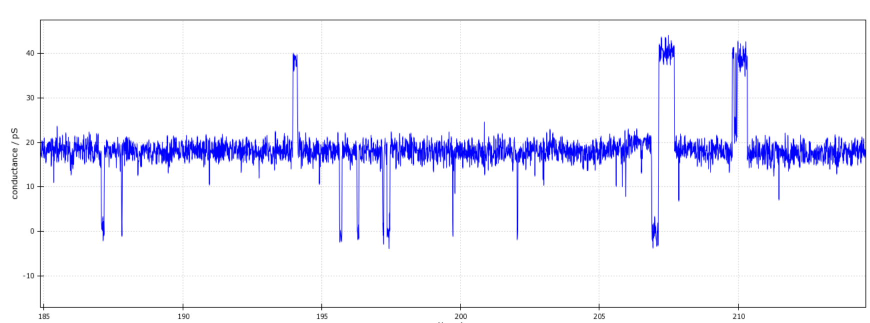
A



a

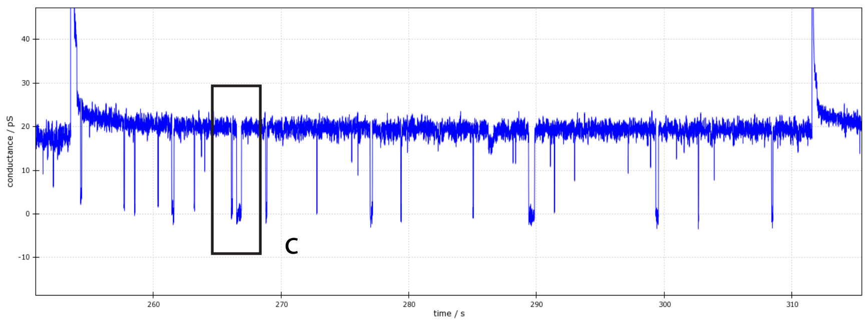


B

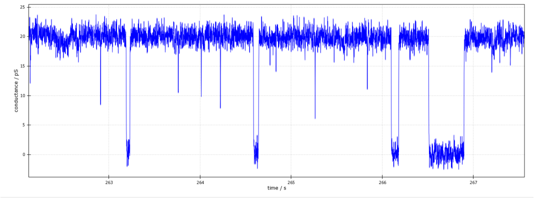


0001 continues...

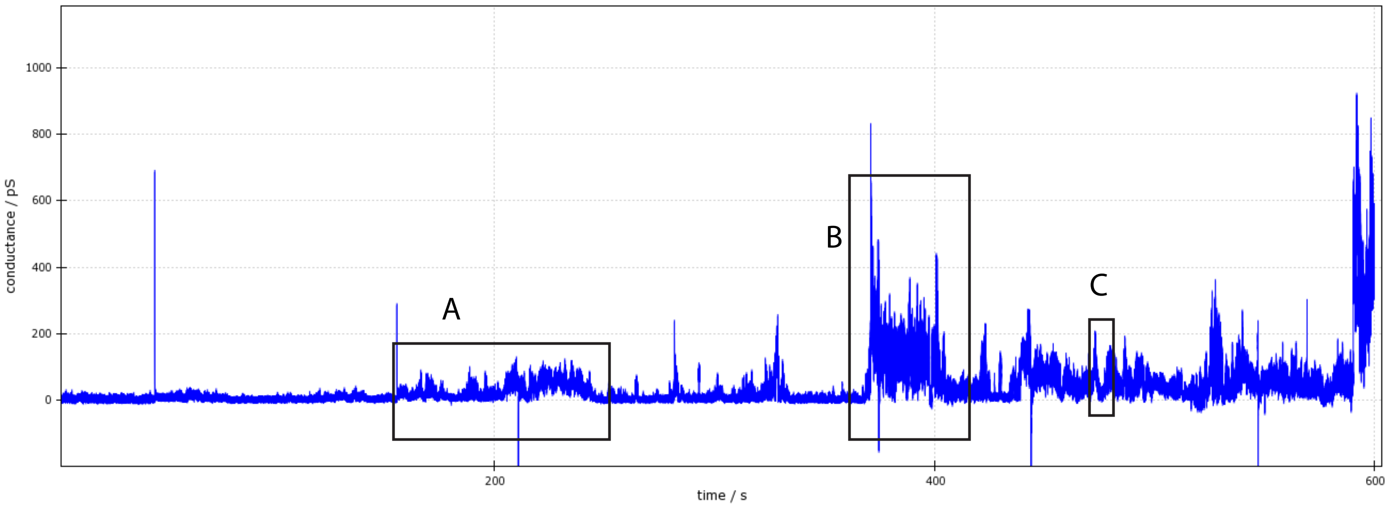
C



c

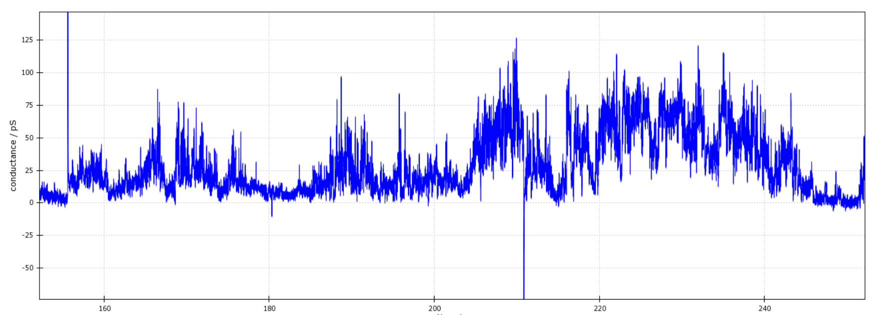


0002



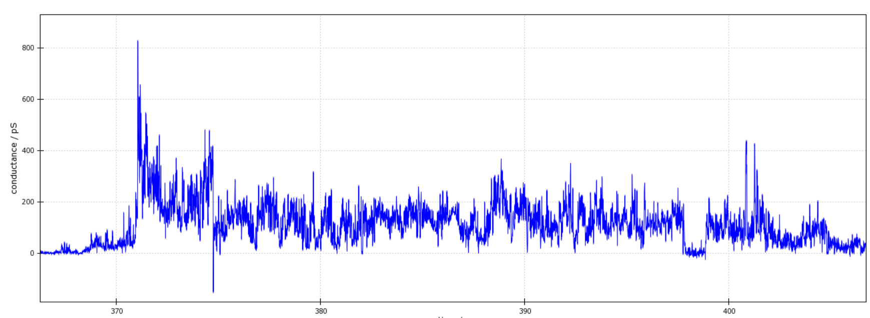
conductance / pS
time / s
1000
800
600
400
200
0
200
400
600
A
B
C

A



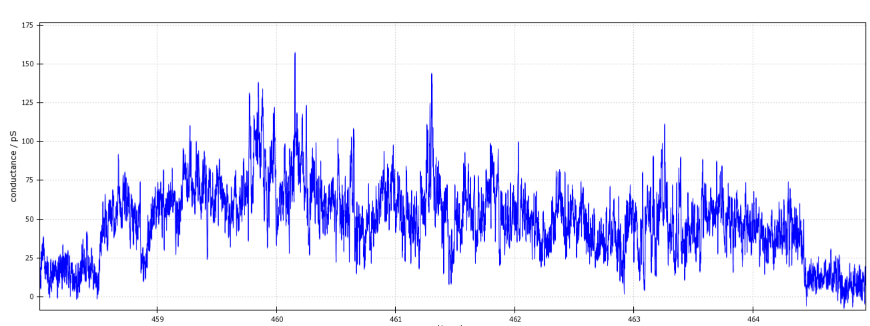
conductance / pS
time / s
125
100
75
50
25
0
-25
-50
160
180
200
220
240

B



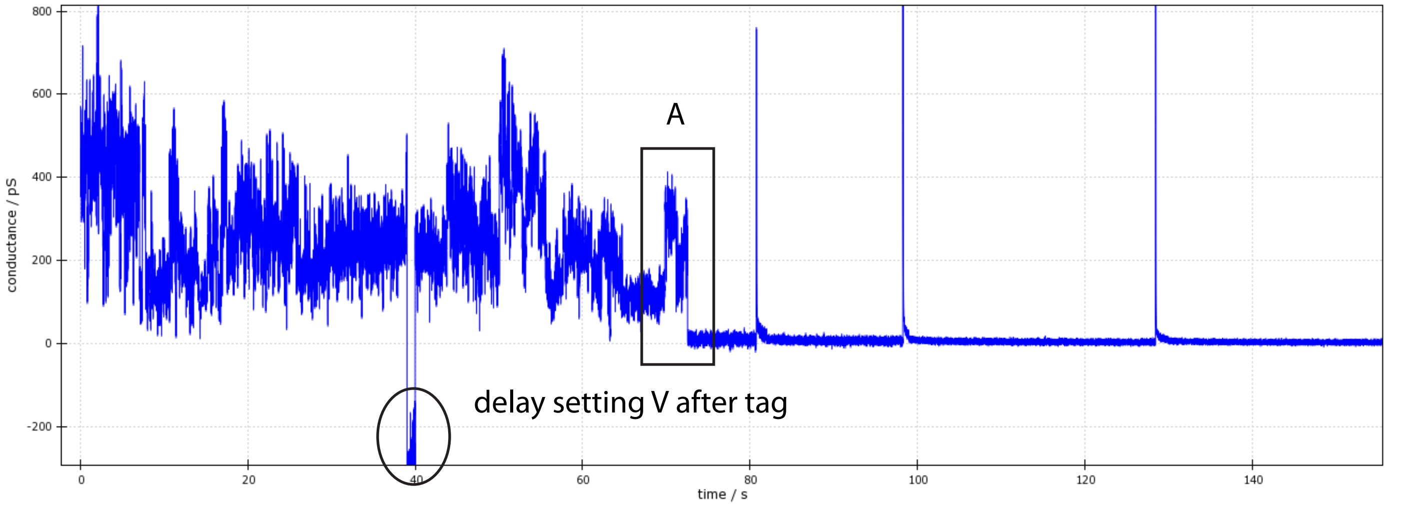
conductance / pS
time / s
800
600
400
200
0
370
380
390
400

C

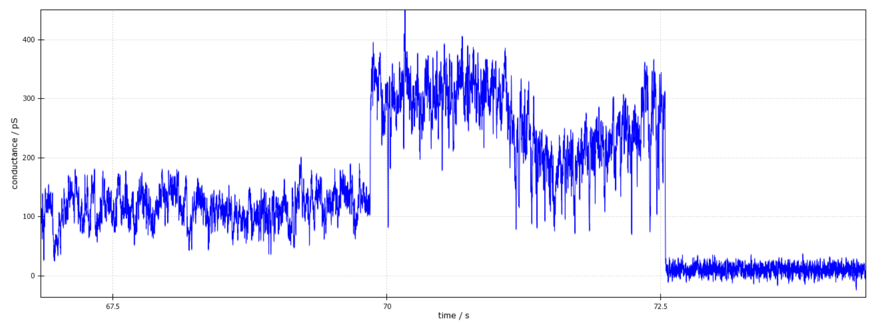


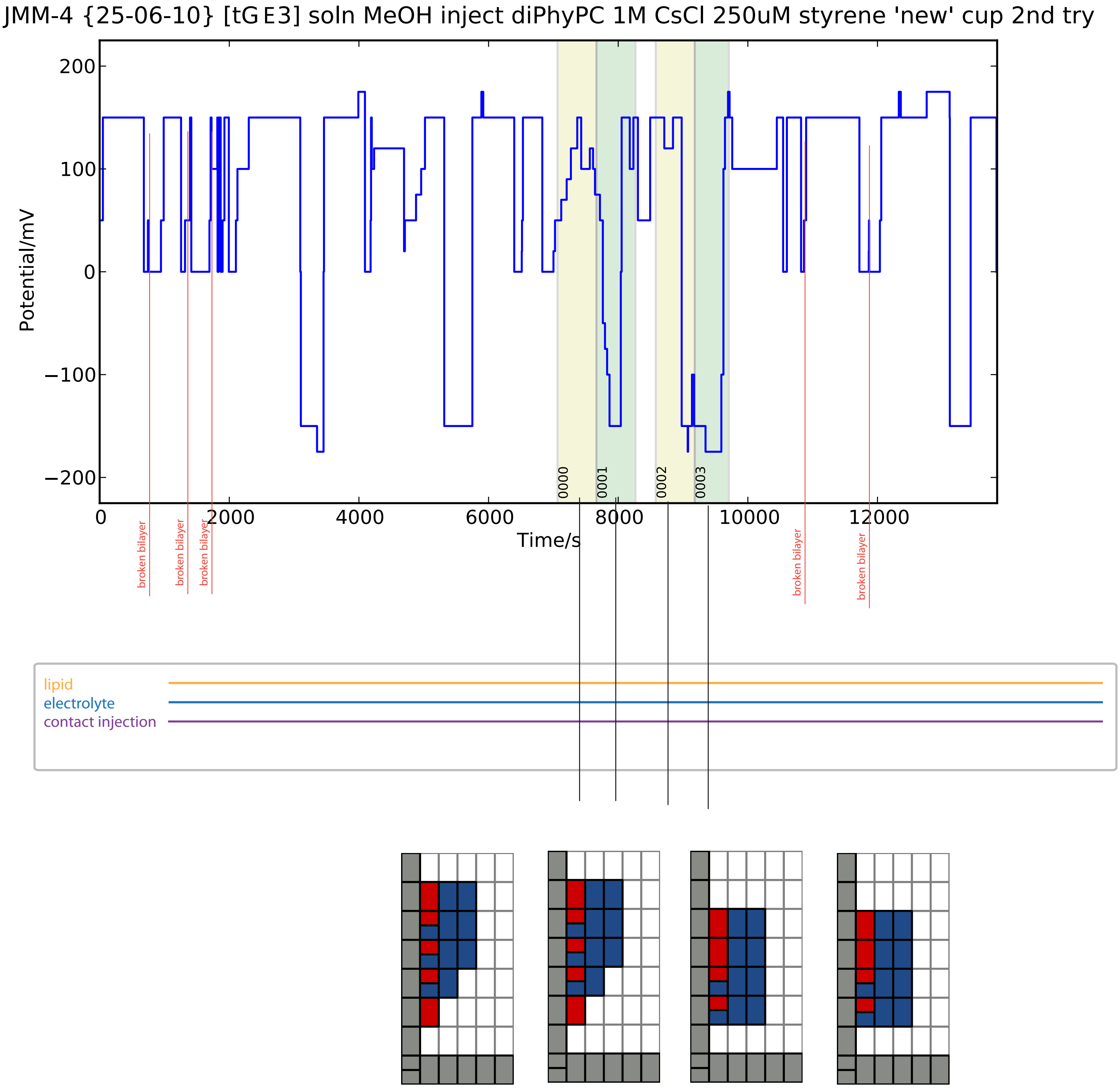
conductance / pS
time / s
175
150
125
100
75
50
25
0
459
460
461
462
463
464

0003

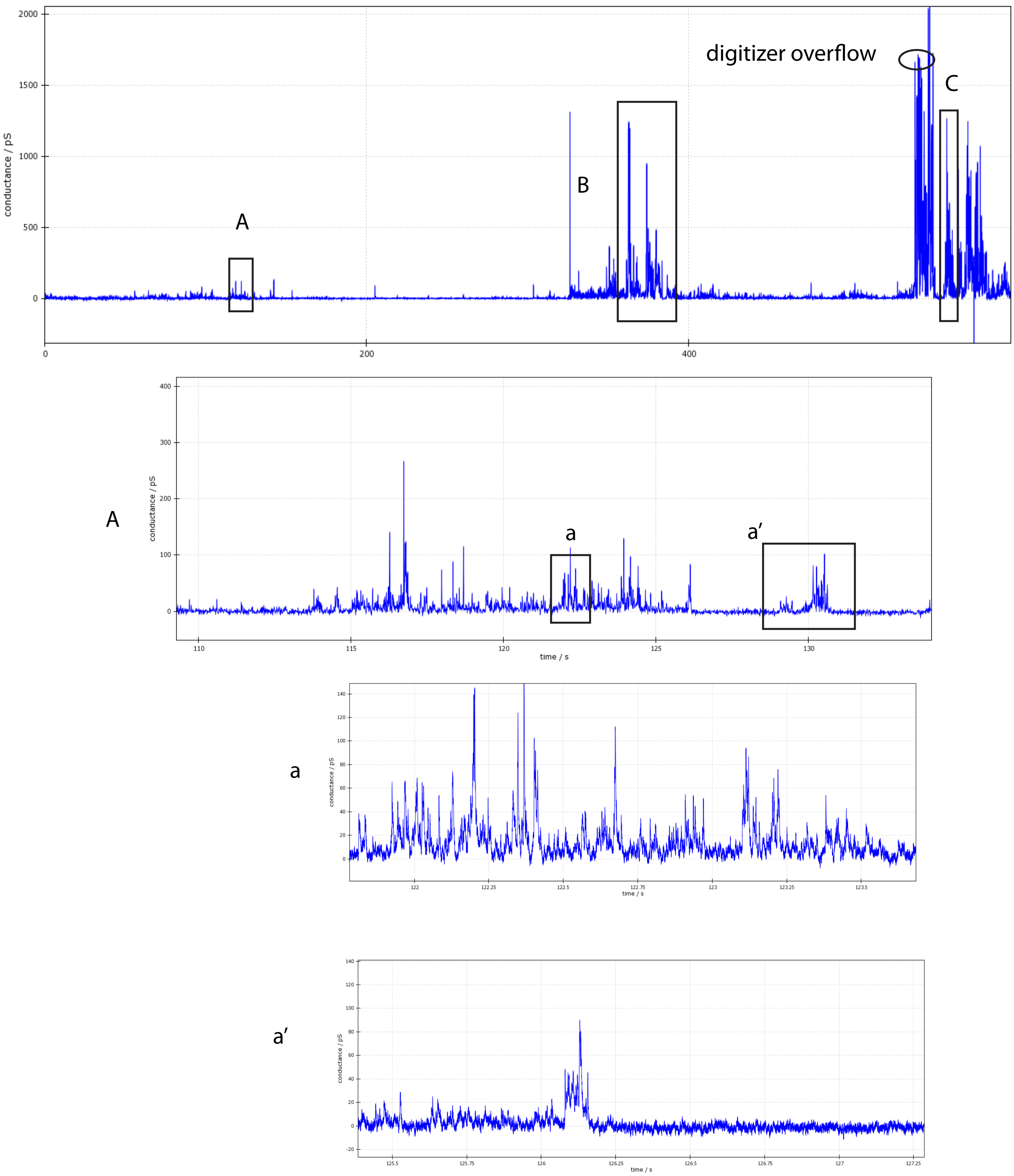

A
delay setting V after tag
conductance / pS
time / s

A


conductance / pS
time / s

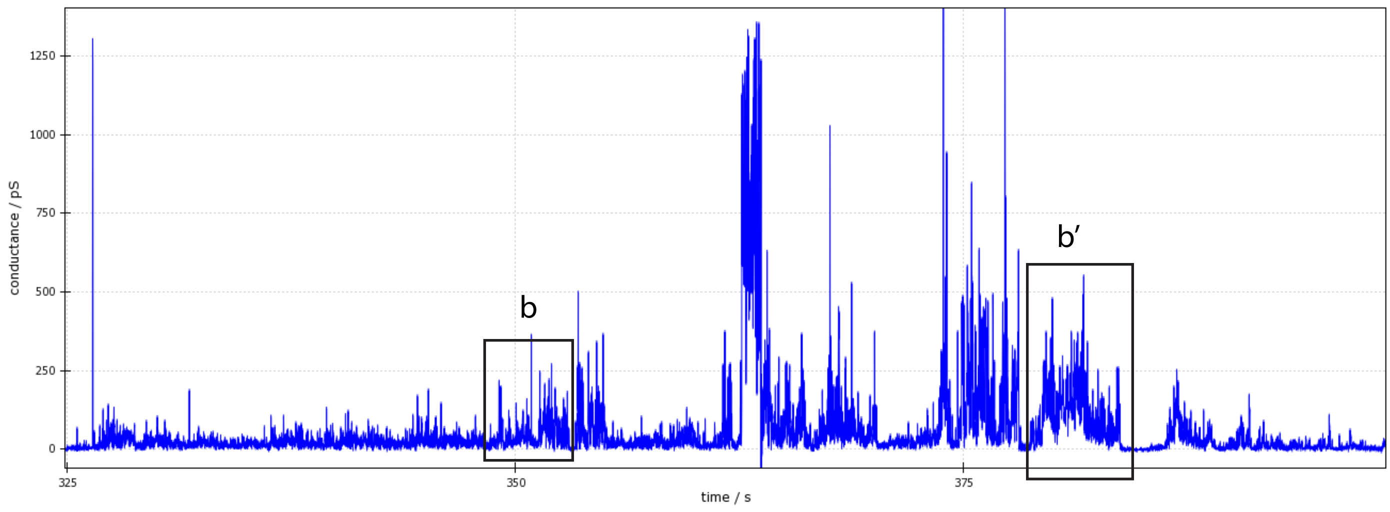

JMM-4 {25-06-10} [tG E3] soln MeOH inject diPhyPC 1M CsCl 250uM styrene 'new' cup 2nd try
Potential/mV
200
100
0
−100
−200
0
2000
4000
6000
8000
10000
12000
Time/s
0000
0001
0002
0003
broken bilayer
broken bilayer
broken bilayer
broken bilayer
broken bilayer
lipid
electrolyte
contact injection

0000

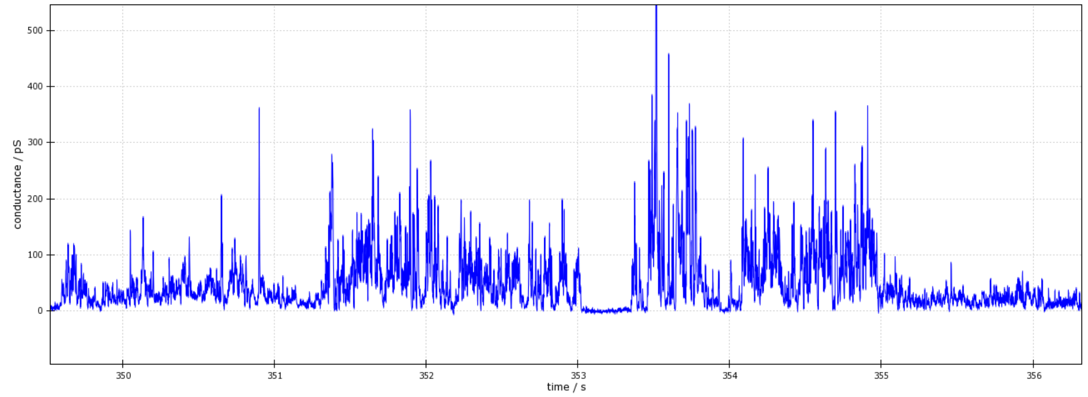


0000 continues..

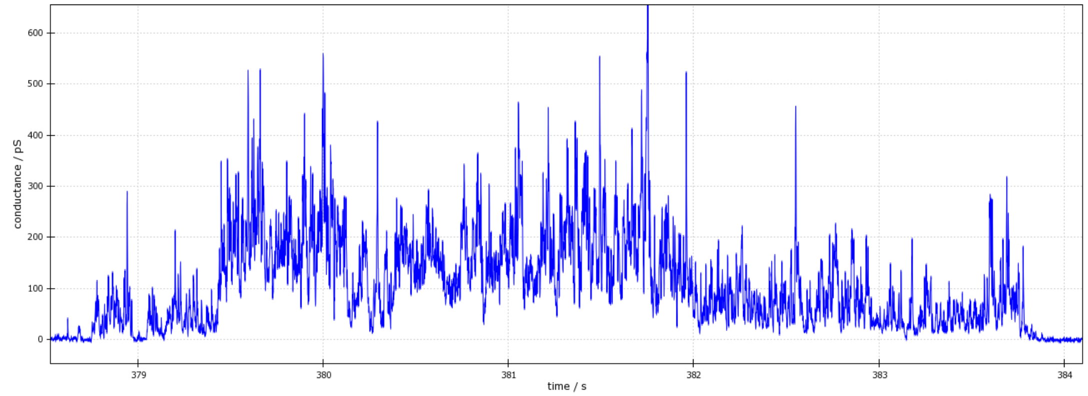
B



b

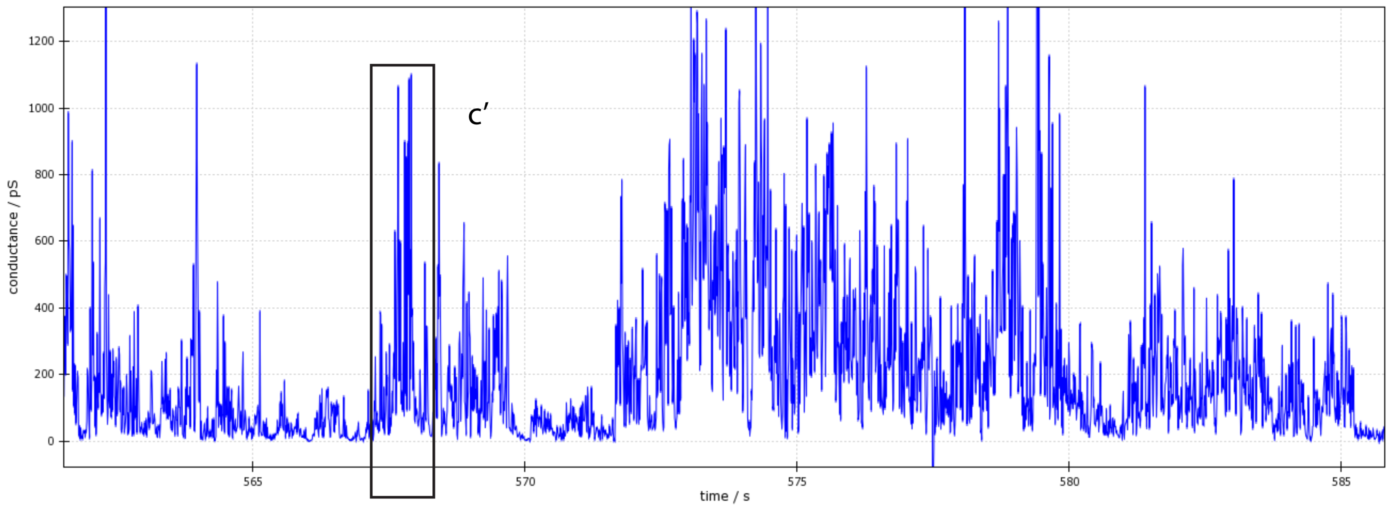


b′

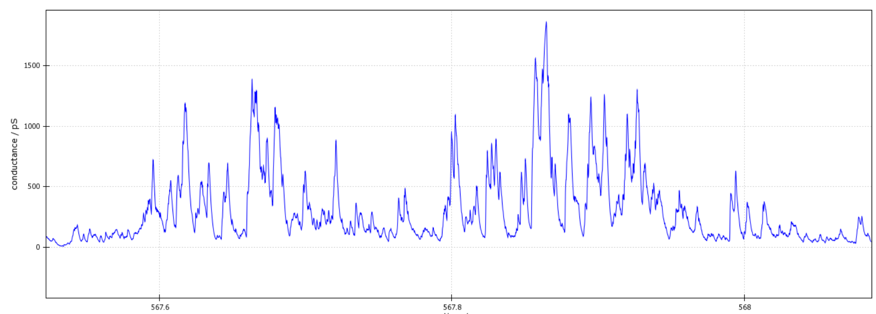


0000 continues..

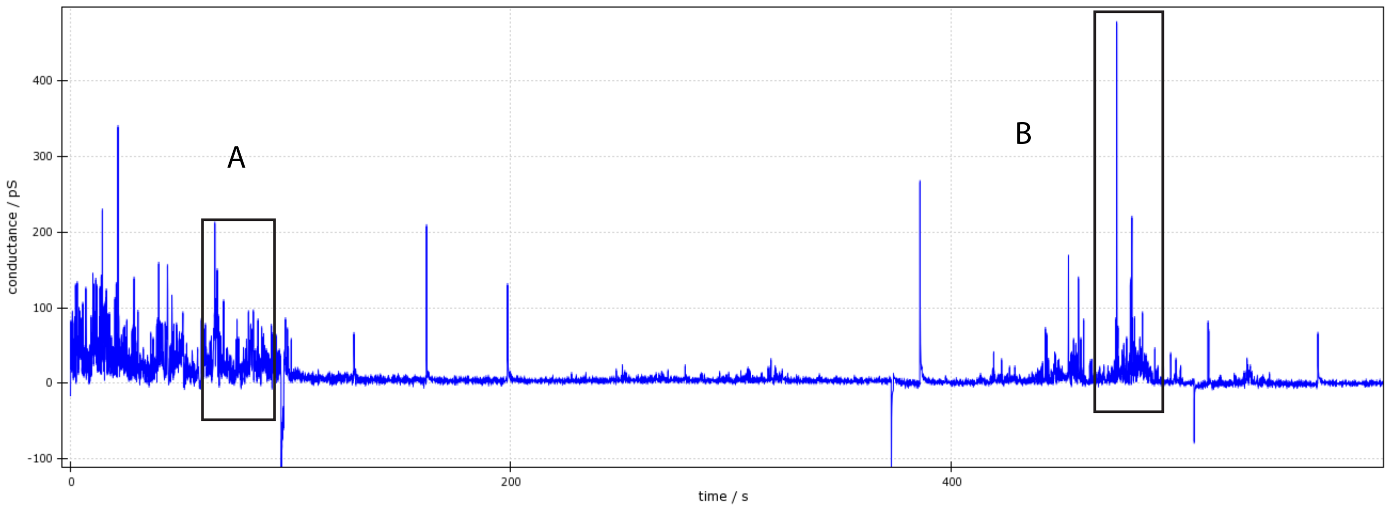
C



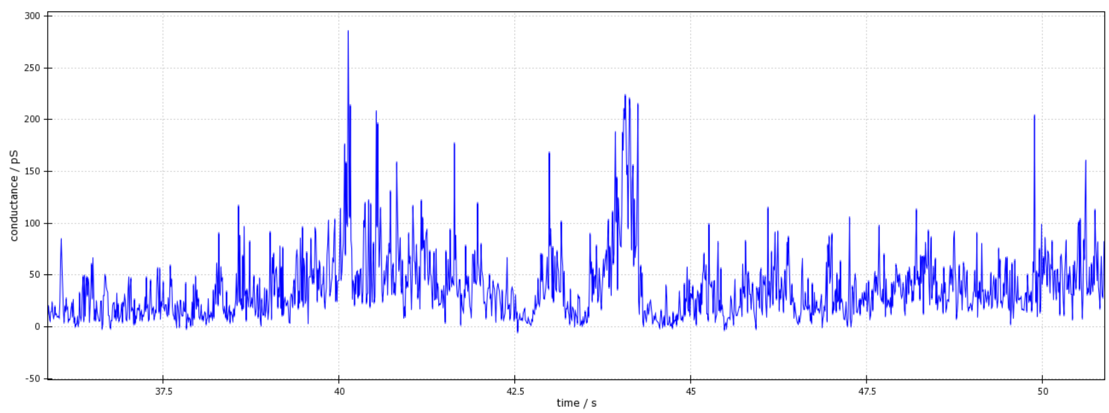
c′



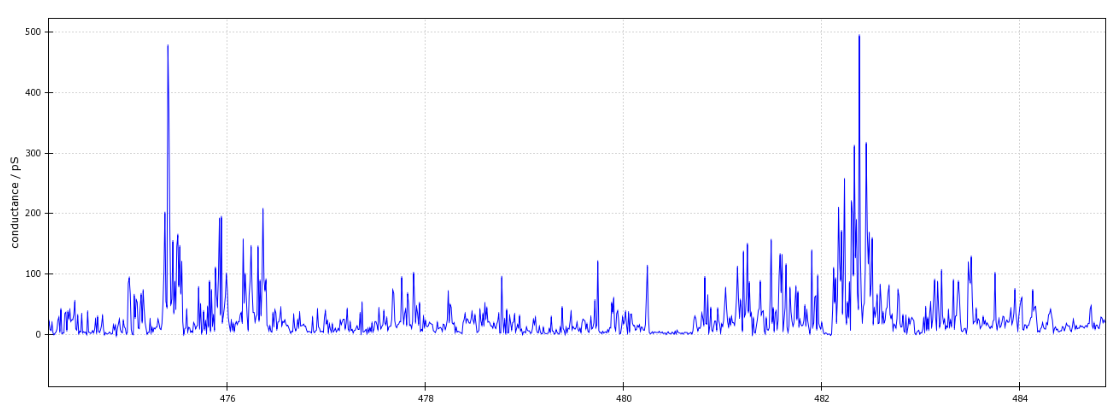
0001


A
B
conductance / pS
400
300
200
100
0
-100
0
200
400
time / s

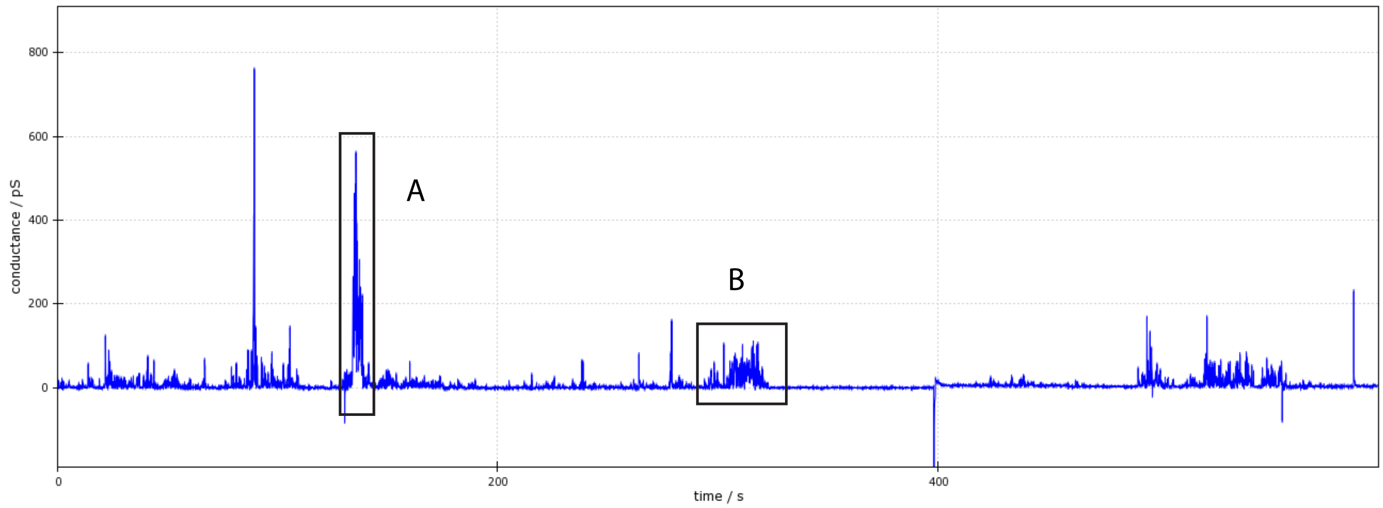
A


conductance / pS
300
250
200
150
100
50
0
-50
37.5
40
42.5
45
47.5
50
time / s

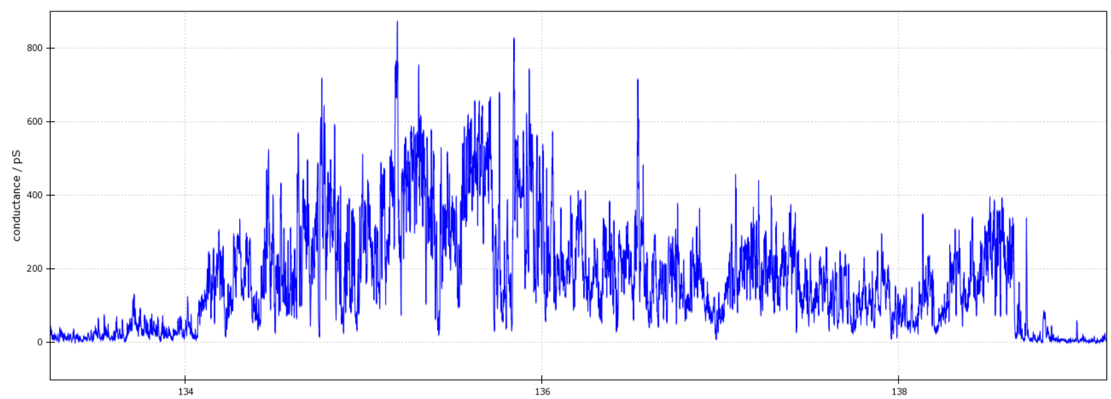
B


conductance / pS
500
400
300
200
100
0
476
478
480
482
484
time / s

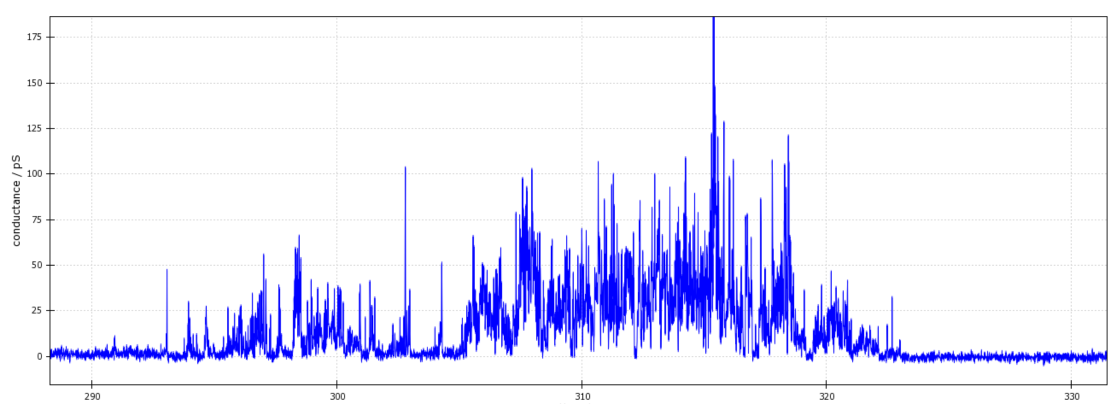
0002


800
600
400
200
0
conductance / pS
A
B
0
200
400
time / s

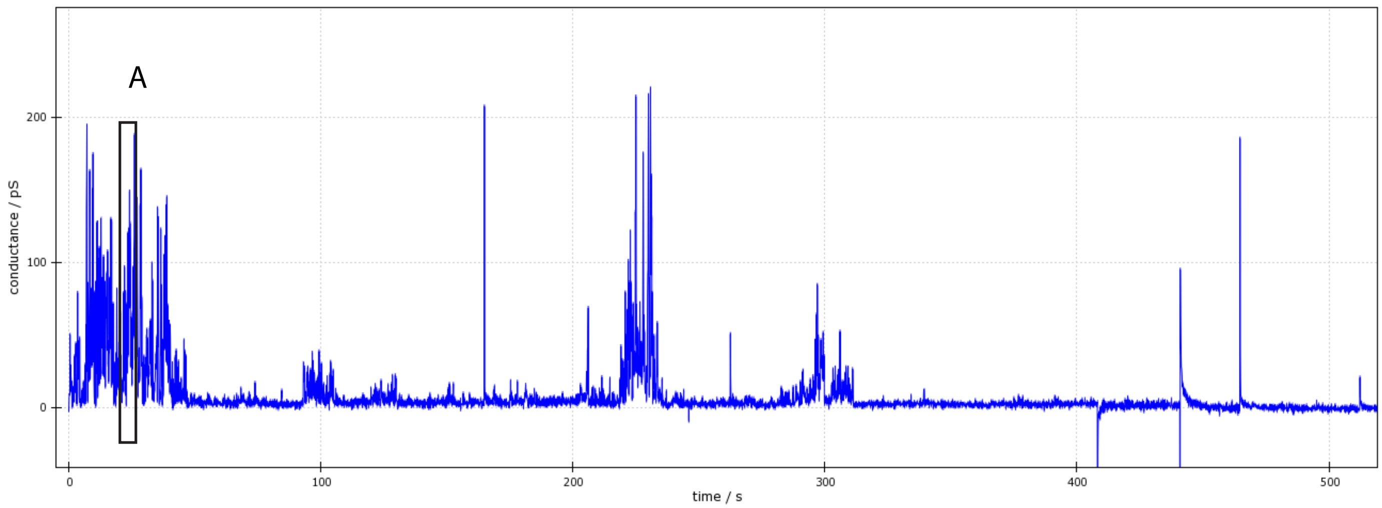
A


800
600
400
200
0
conductance / pS
134
136
138
time / s

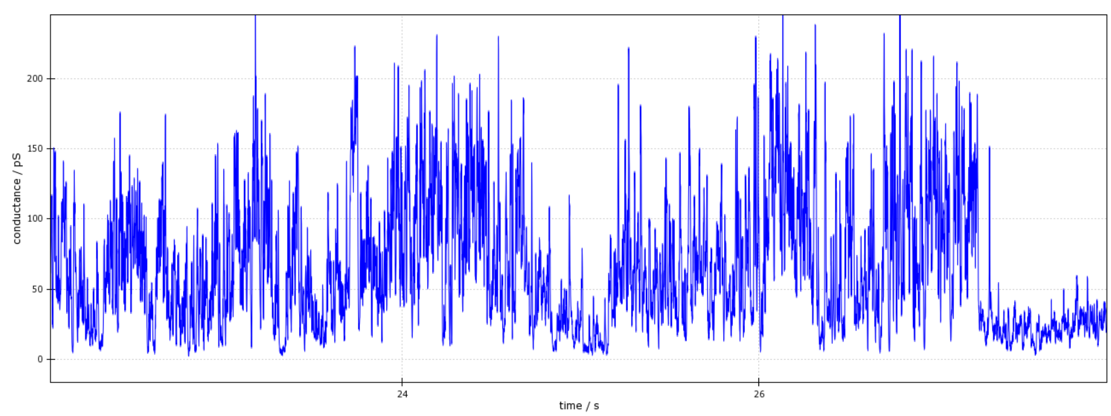
B


175
150
125
100
75
50
25
0
conductance / pS
290
300
310
320
330
time / s

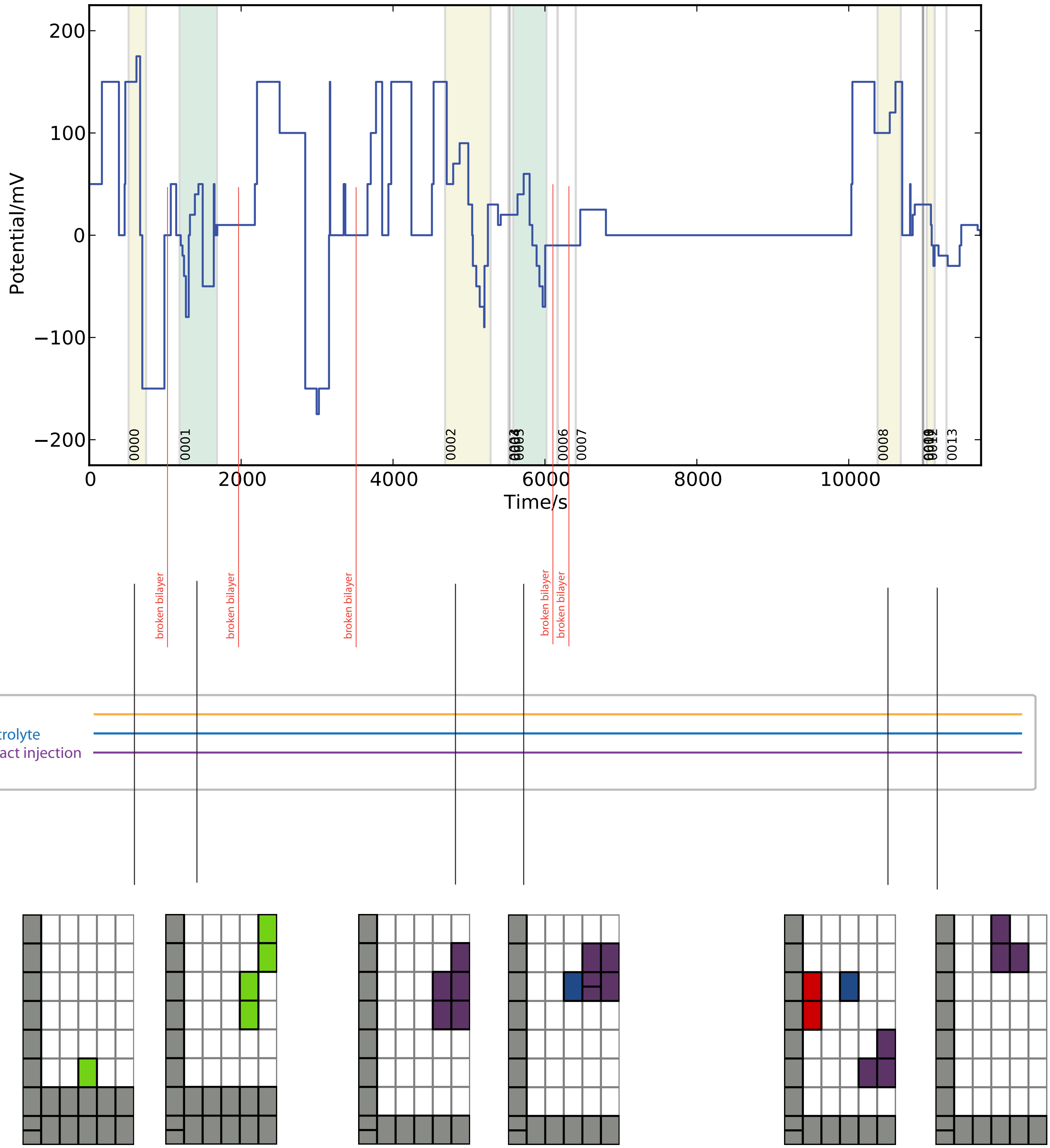
0003


A
200
100
0
conductance / pS
0
100
200
300
400
500
time / s

A

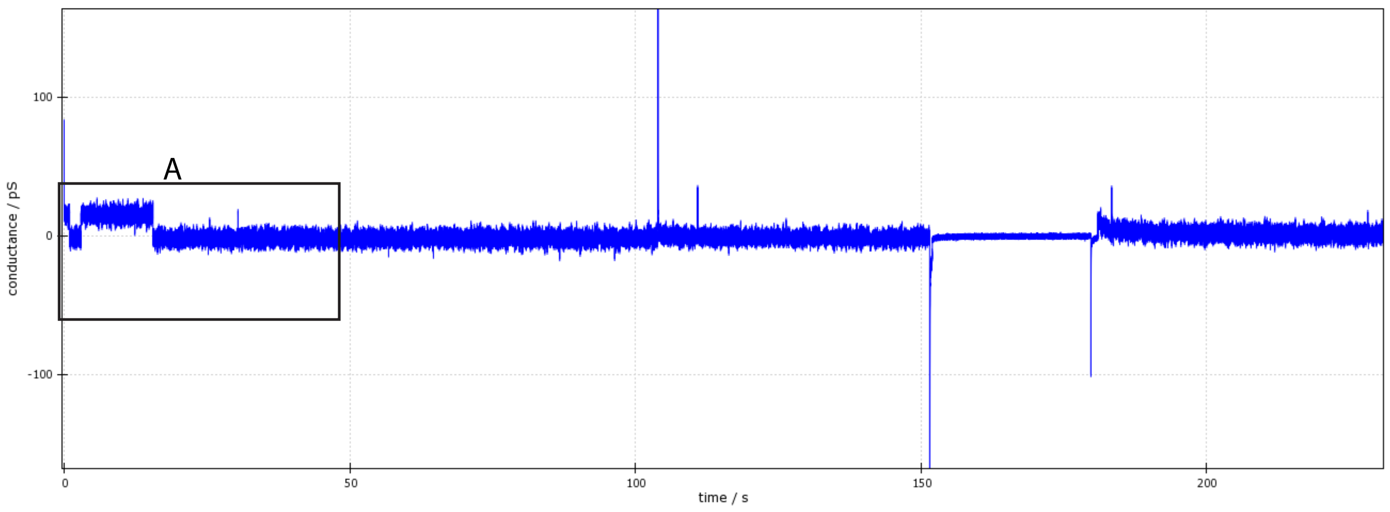

200
150
100
50
0
conductance / pS
24
26
time / s

JMM-01 {06-07-10} [tGE3] soln MeOH inject diPhyPC 1M KCl 250uM styrene 'new' cup 2nd try

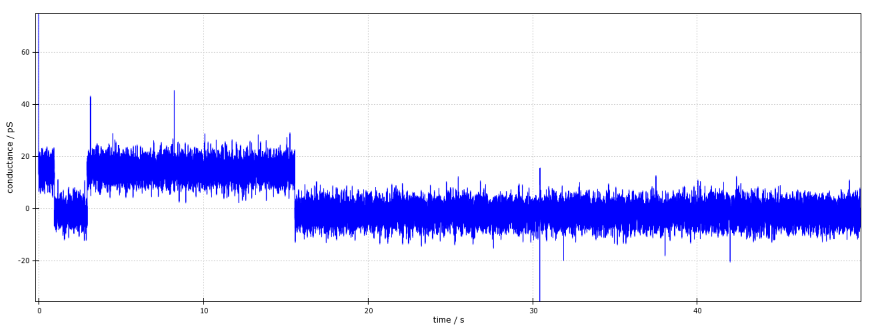


Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

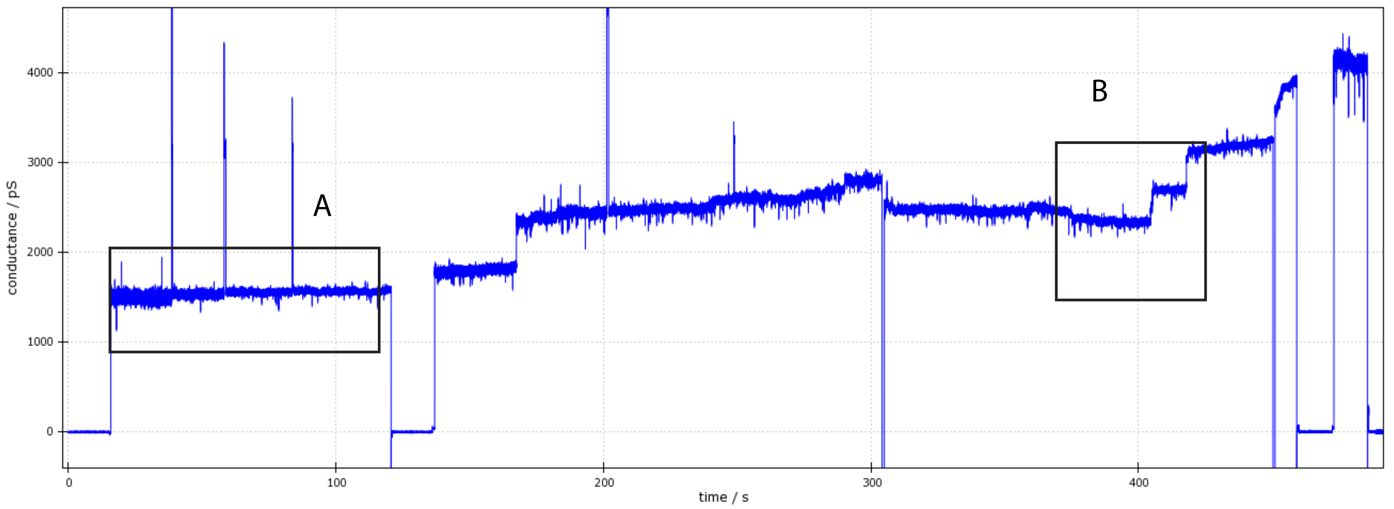
0000



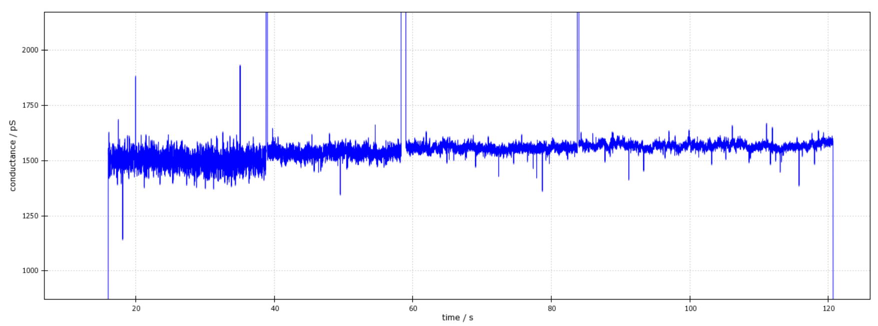
A



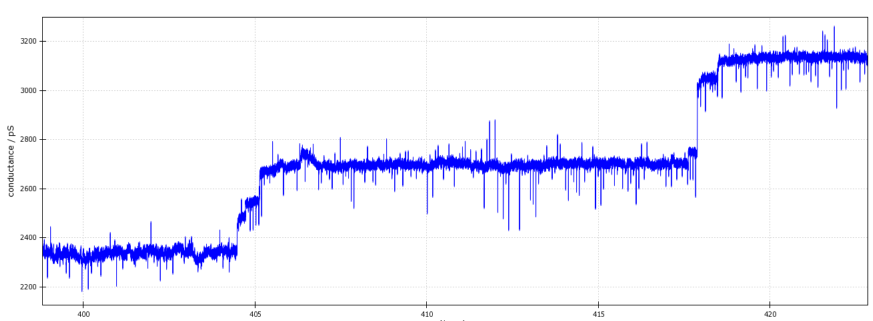
0001


conductance / pS
time / s
A
B

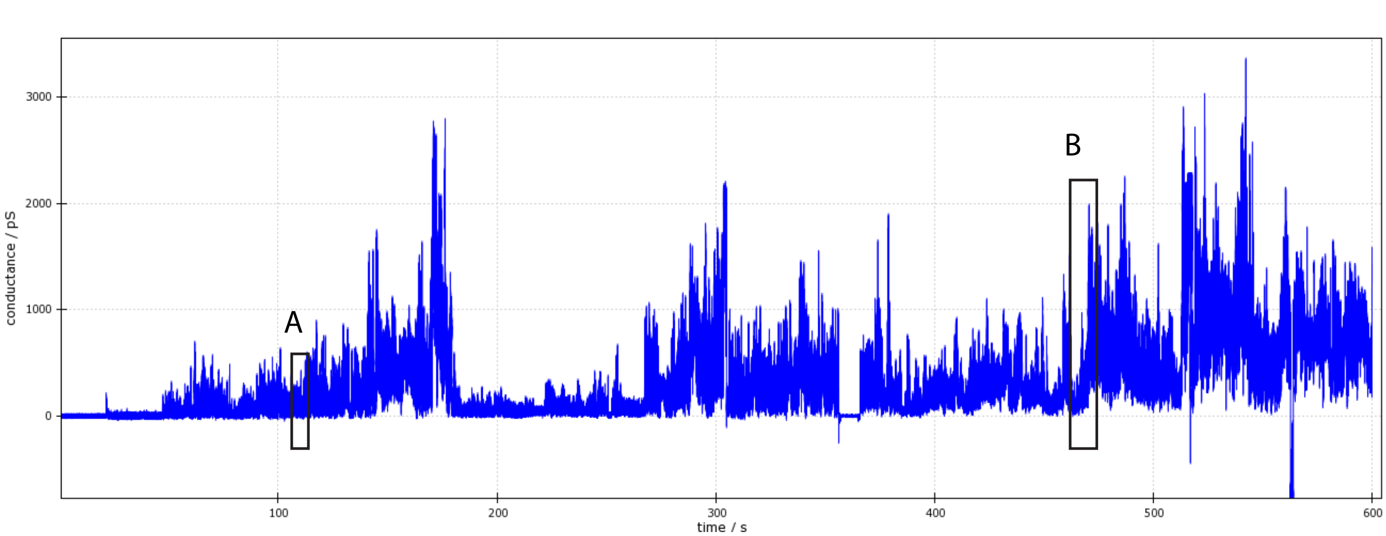
A


conductance / pS
time / s

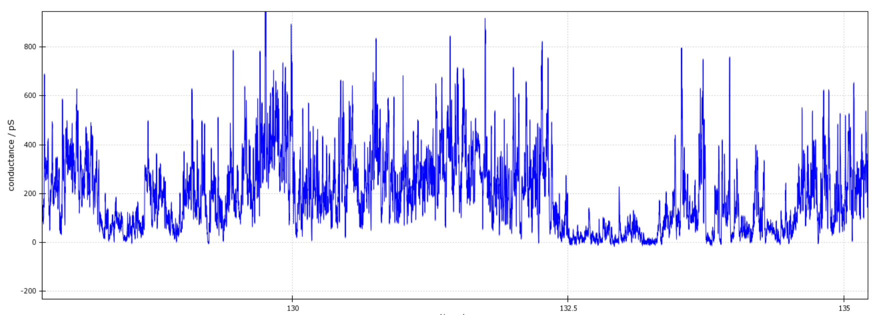
B


conductance / pS
time / s

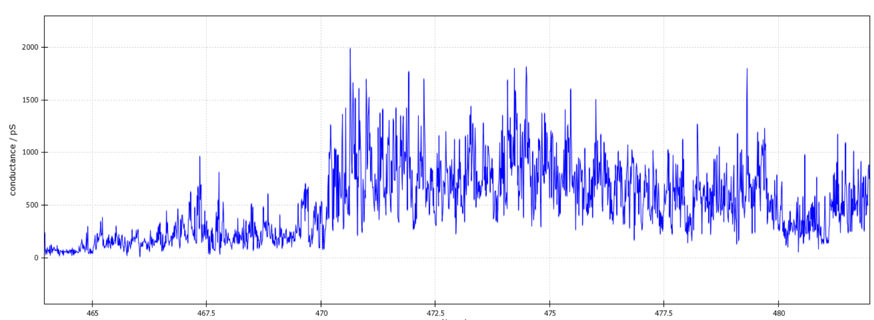
0002


conductance / pS
3000
2000
1000
0
A
B
100
200
300
400
500
600
time / s

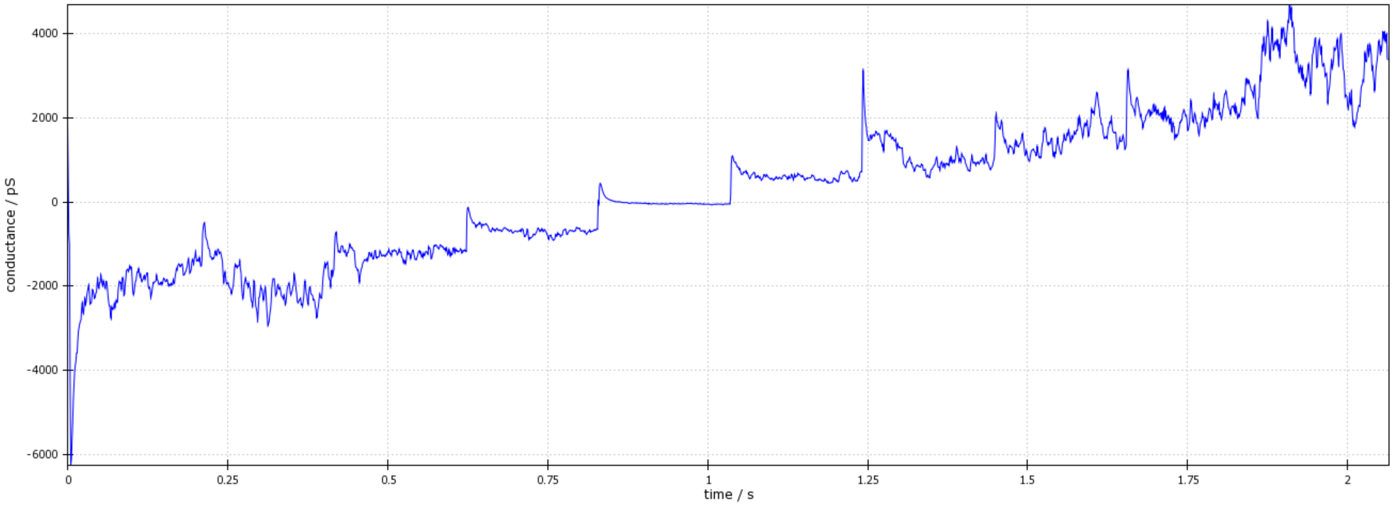
A


conductance / pS
800
600
400
200
0
-200
130
132.5
135
time / s

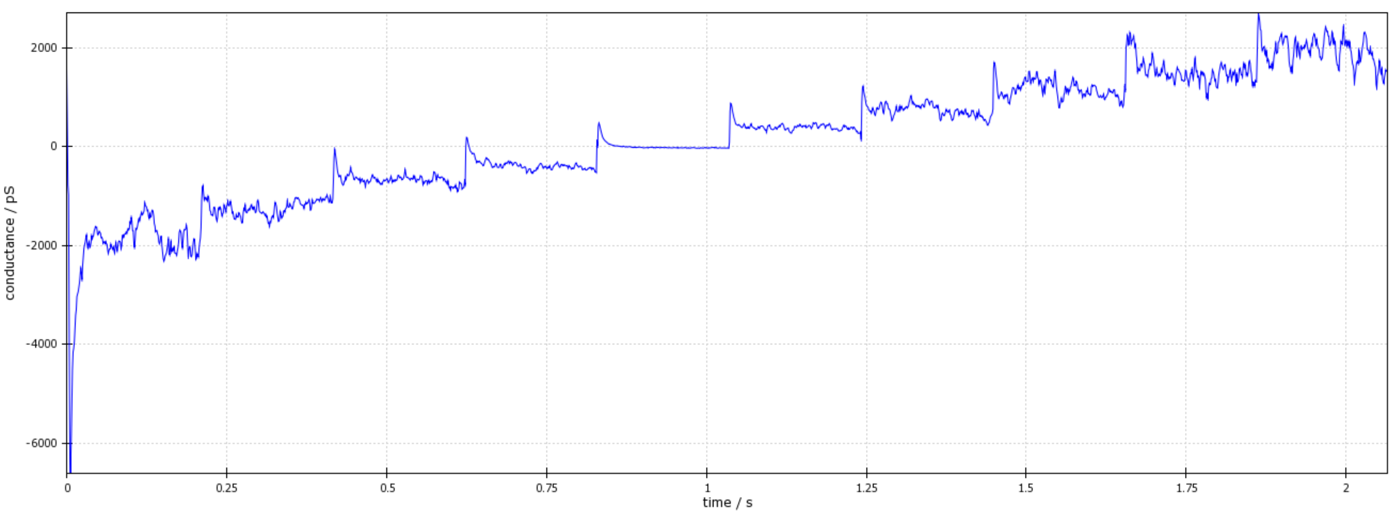
B


conductance / pS
2000
1500
1000
500
0
465
467.5
470
472.5
475
477.5
480
time / s

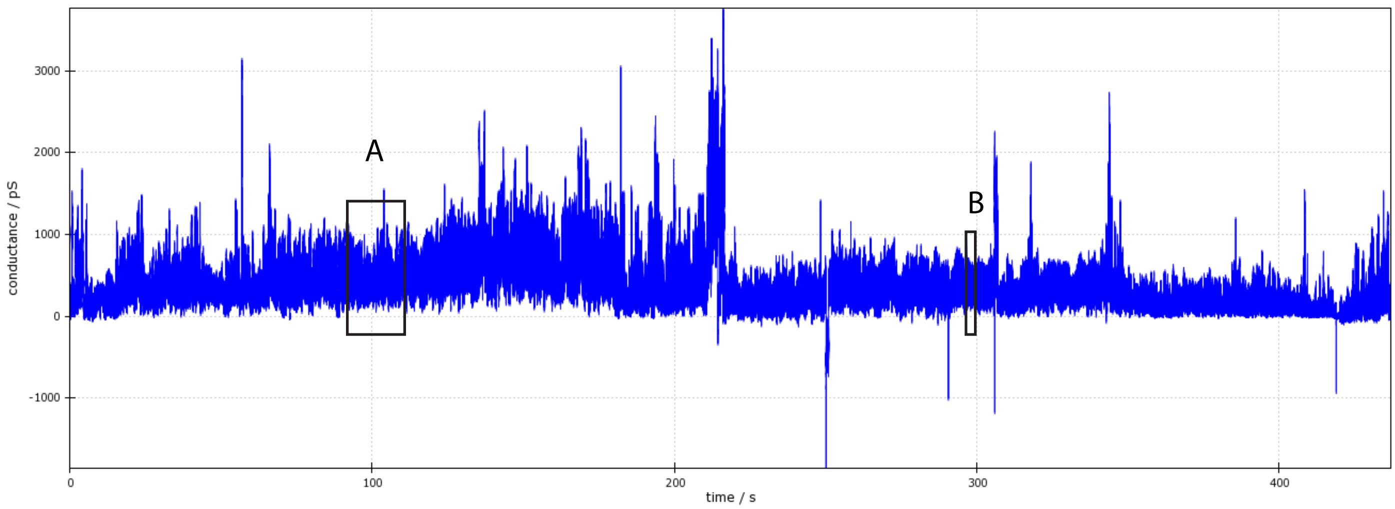
0003


4000
2000
0
-2000
-4000
-6000
conductance / pS
0
0.25
0.5
0.75
1
1.25
1.5
1.75
2
time / s

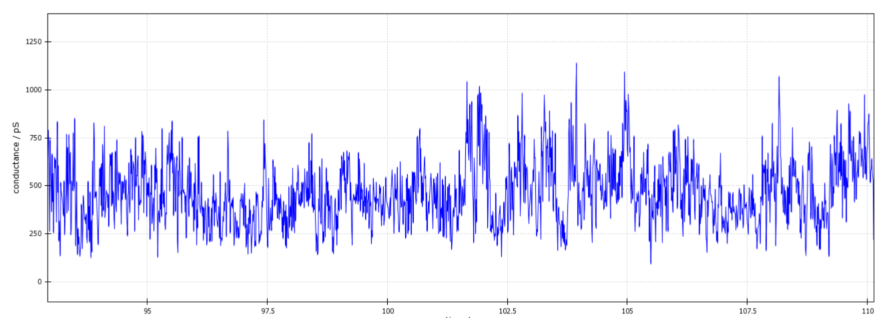
0004


2000
0
-2000
-4000
-6000
conductance / pS
0
0.25
0.5
0.75
1
1.25
1.5
1.75
2
time / s

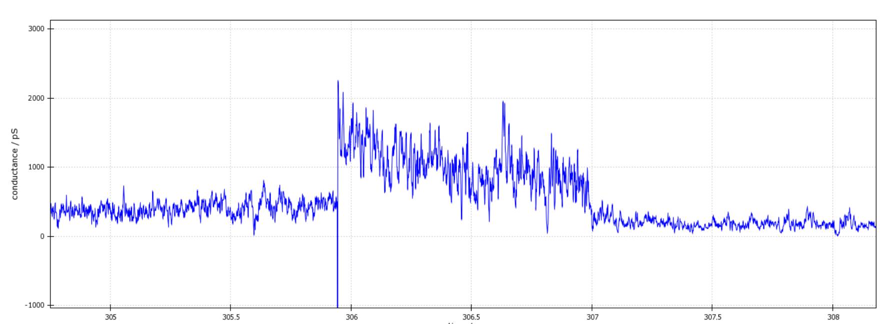
0005


A
B
conductance / pS
3000
2000
1000
0
-1000
0
100
200
300
400
time / s

A

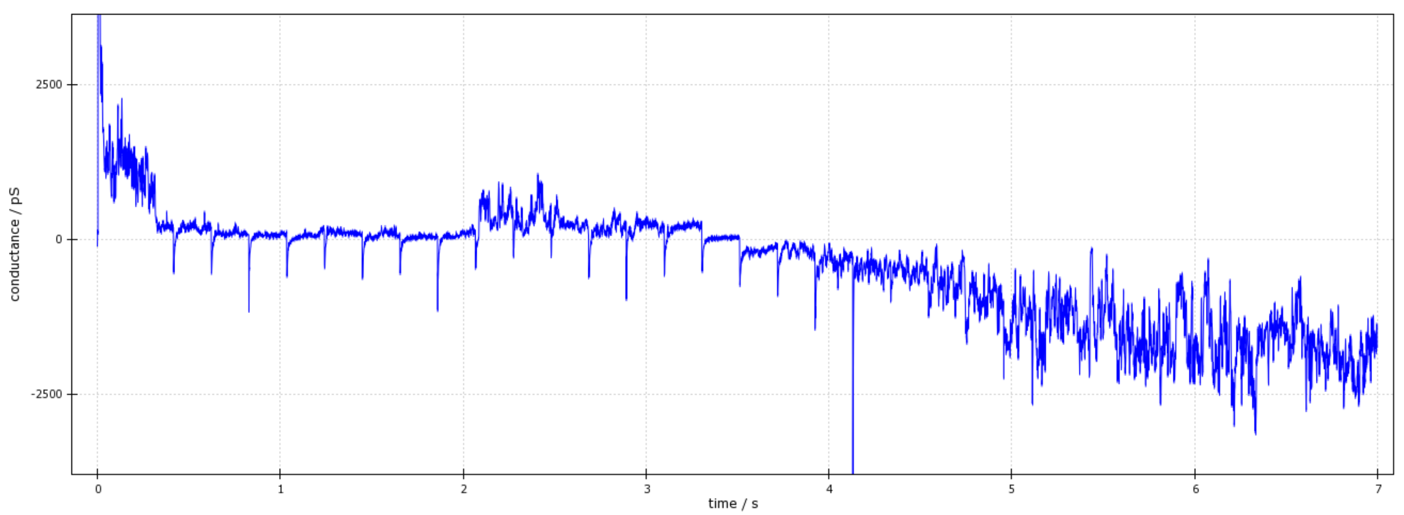

conductance / pS
1250
1000
750
500
250
0
95
97.5
100
102.5
105
107.5
110
time / s

B

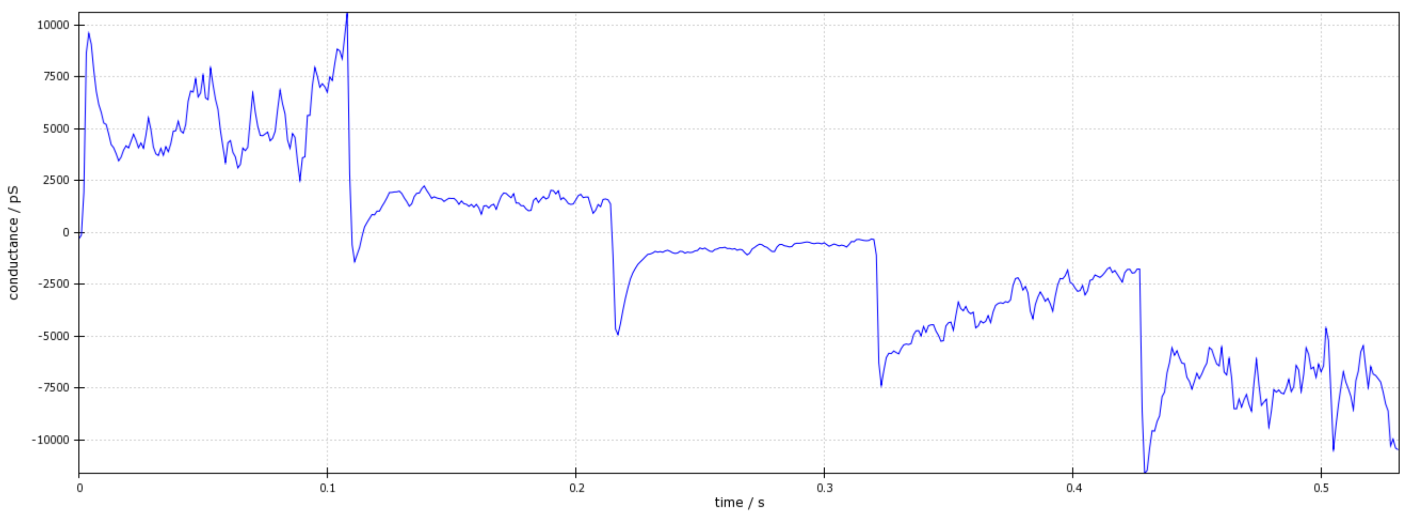

conductance / pS
3000
2000
1000
0
-1000
305
305.5
306
306.5
307
307.5
308
time / s

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

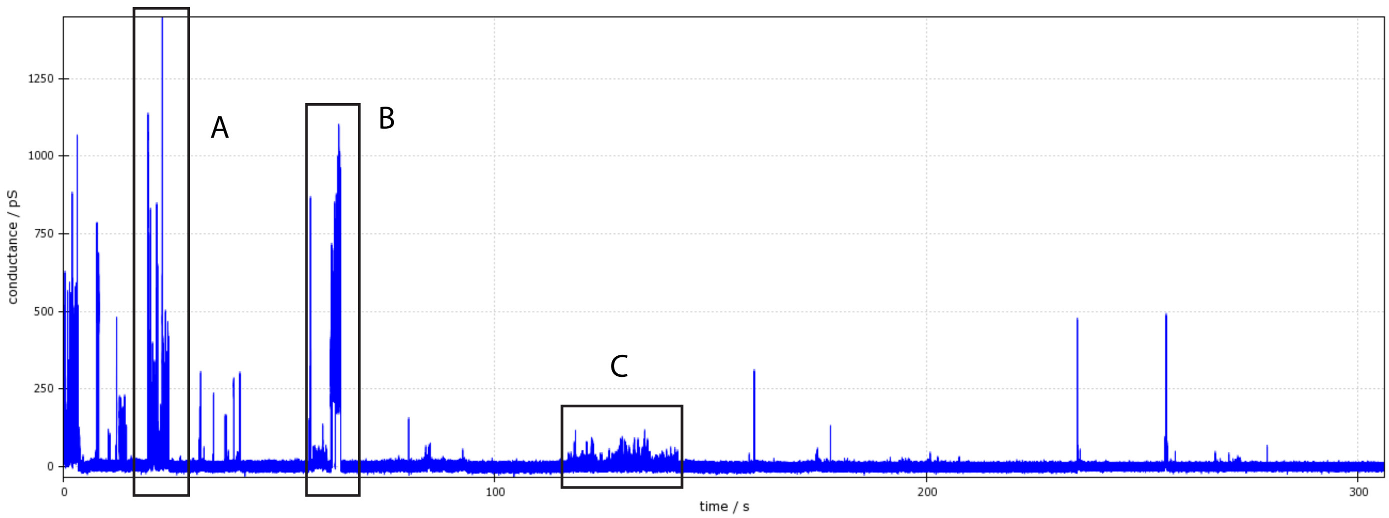
0006



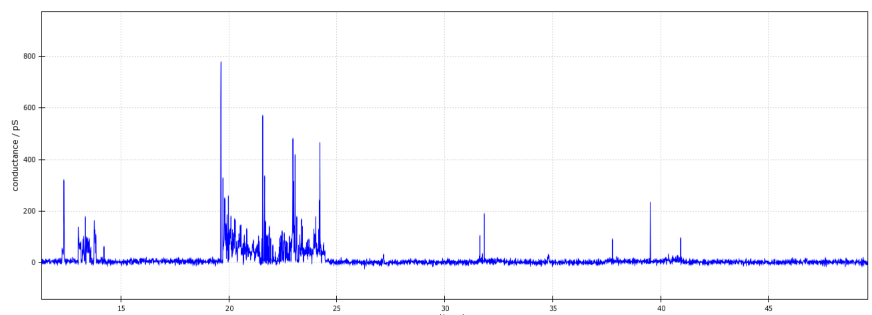
0007



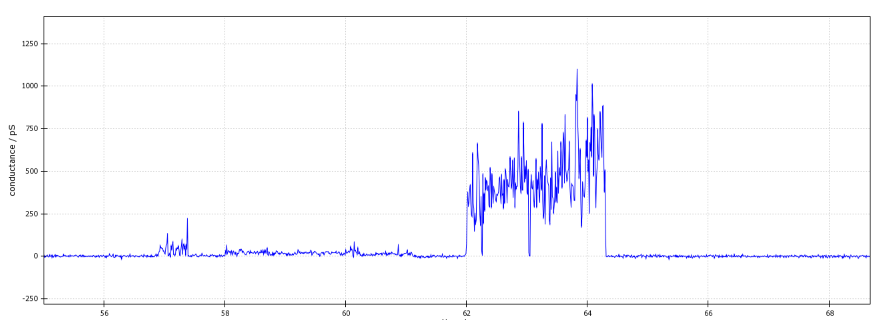
0008


A
B
C
conductance / pS
0
250
500
750
1000
1250
time / s
0
100
200
300

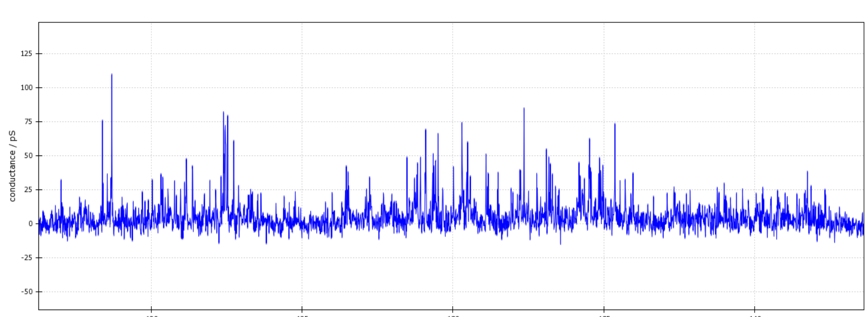
A


conductance / pS
time / s

B

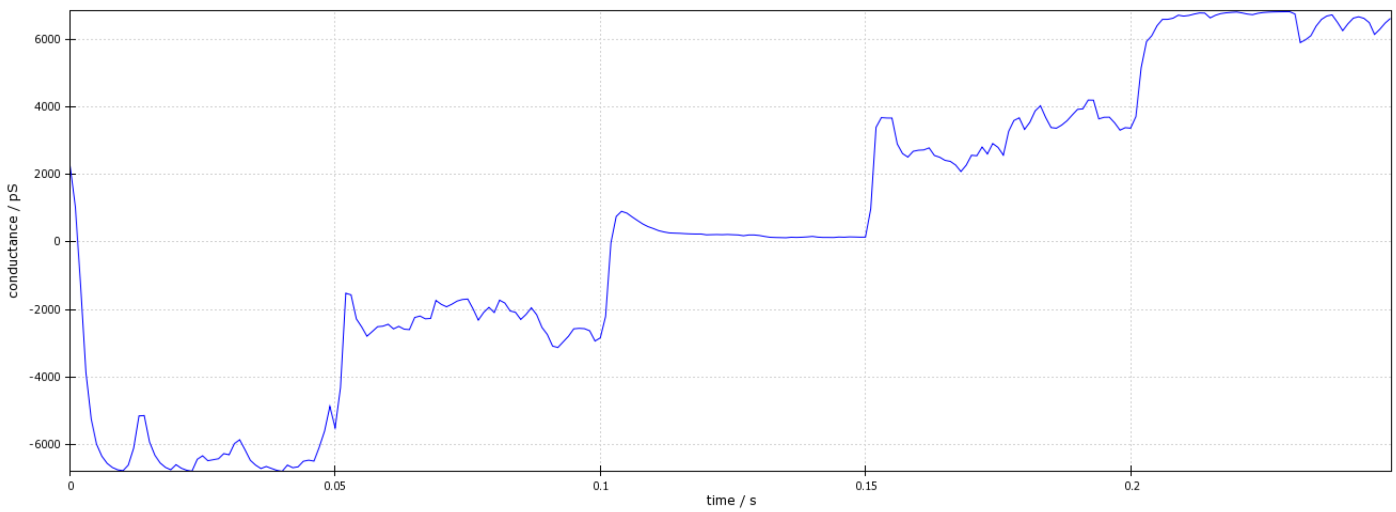

conductance / pS
time / s

C

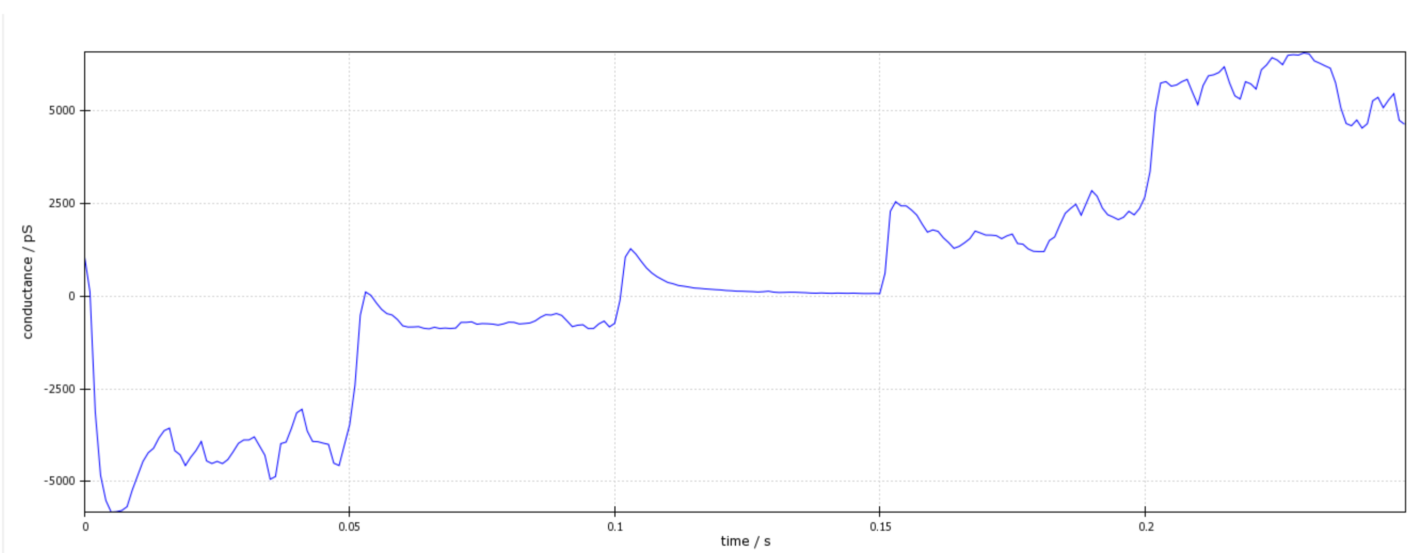

conductance / pS
time / s

0009 blank record; no data

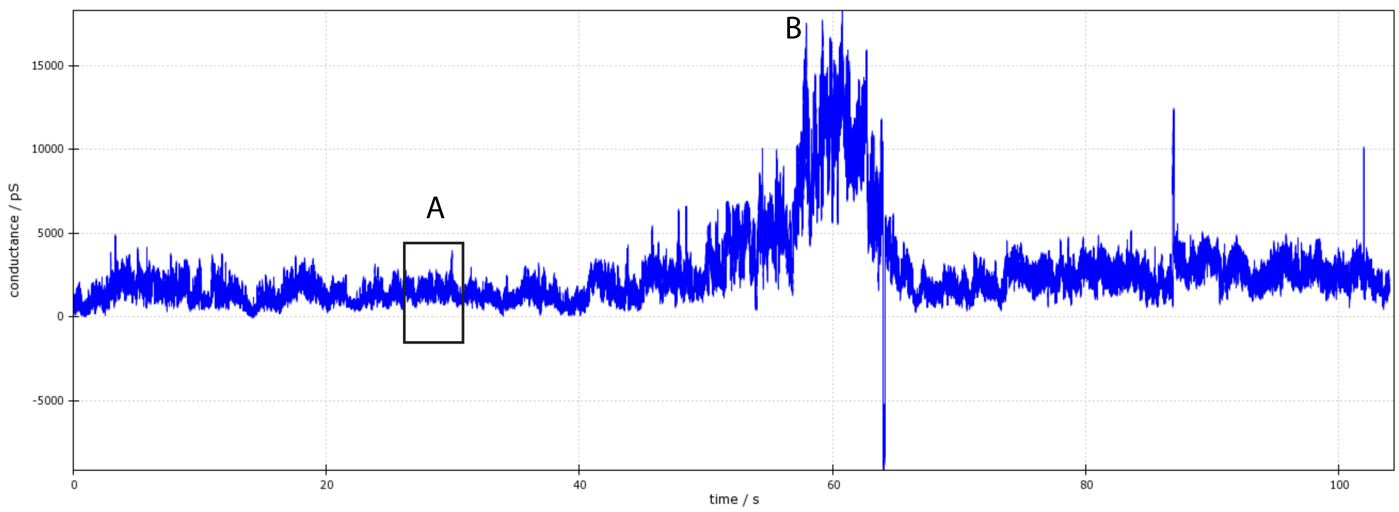
0010



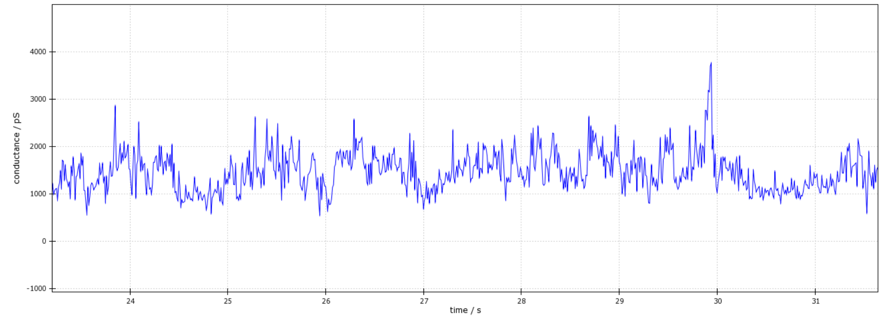
0011



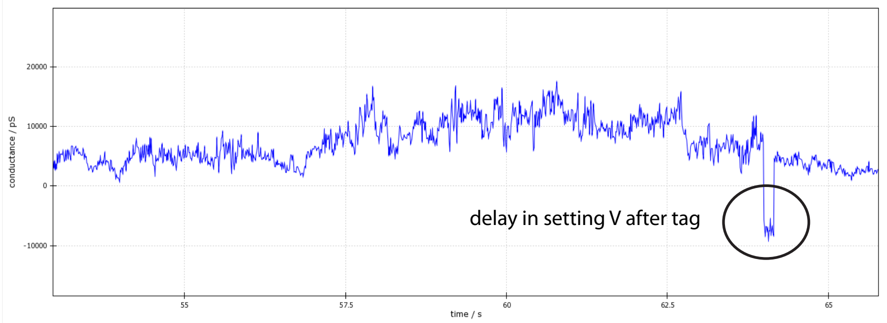
0012


B
A
15000
10000
5000
0
-5000
conductance / pS
0
20
40
60
80
100
time / s

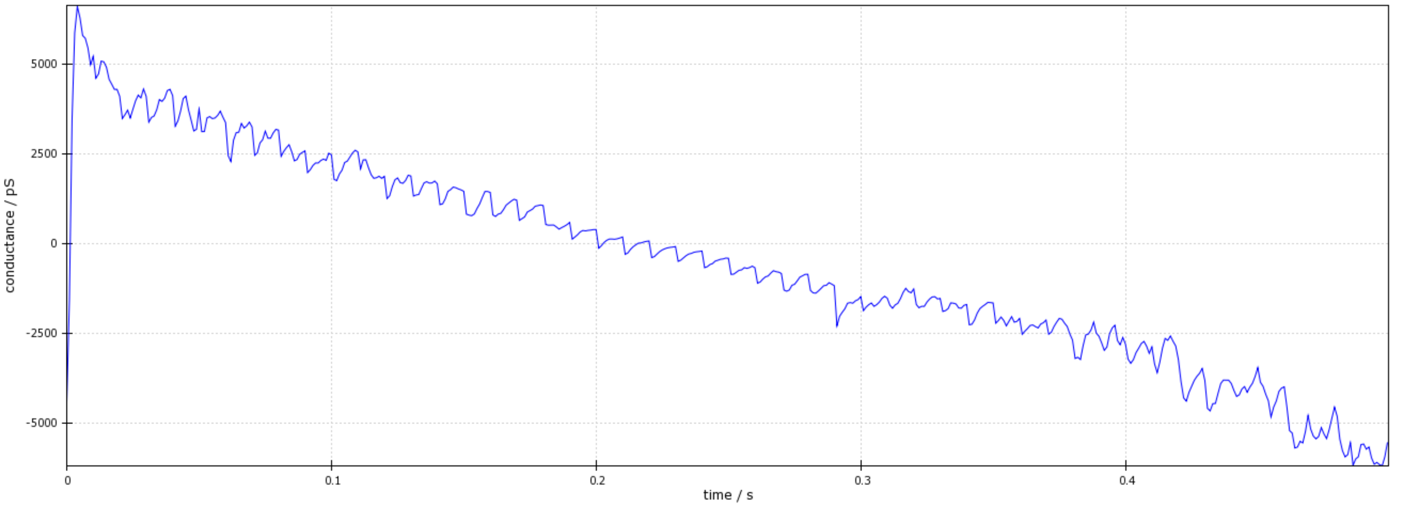
A


4000
3000
2000
1000
0
-1000
conductance / pS
24
25
26
27
28
29
30
31
time / s

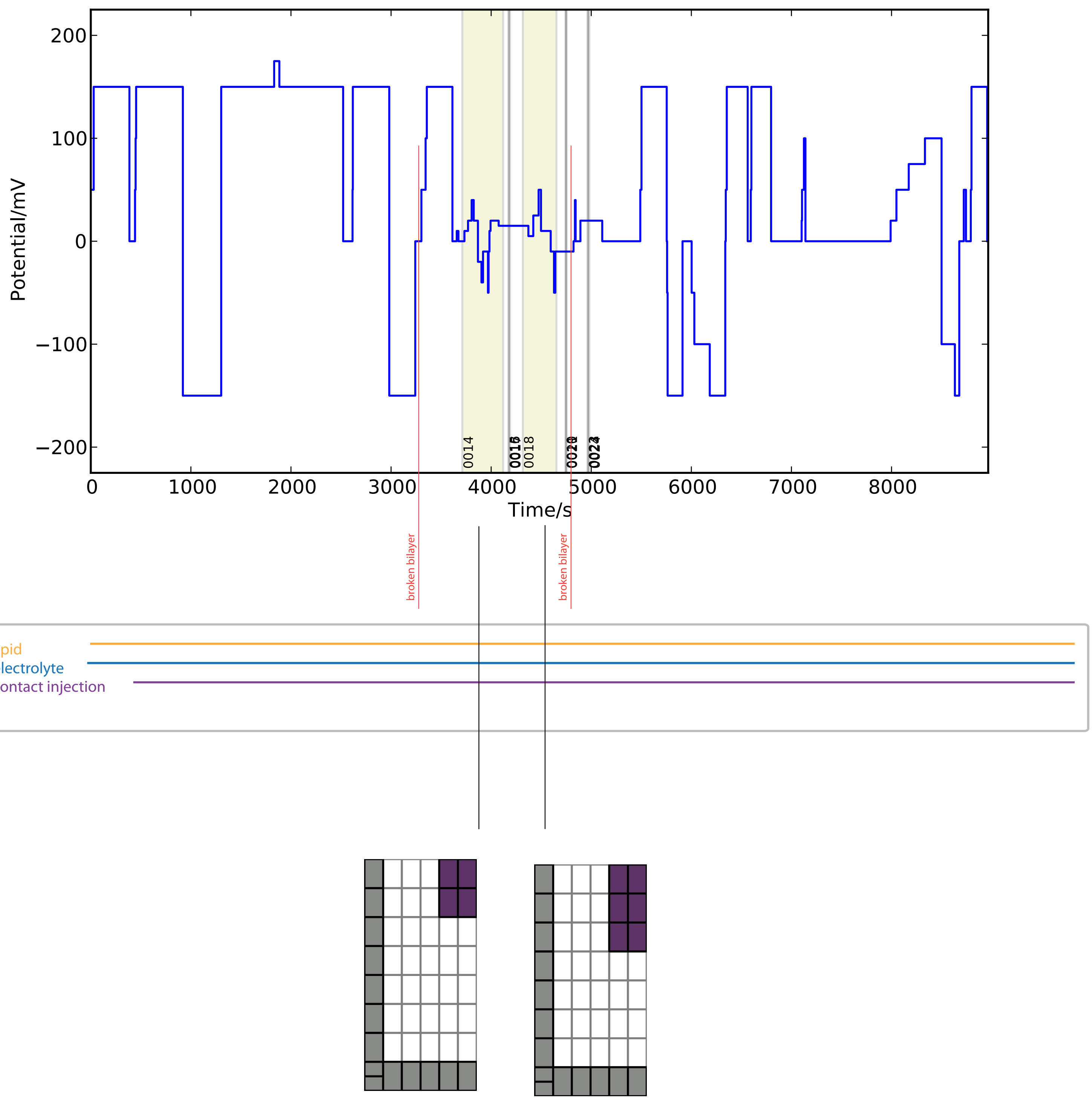
B


20000
10000
0
-10000
conductance / pS
delay in setting V after tag
55
57.5
60
62.5
65
time / s

0013

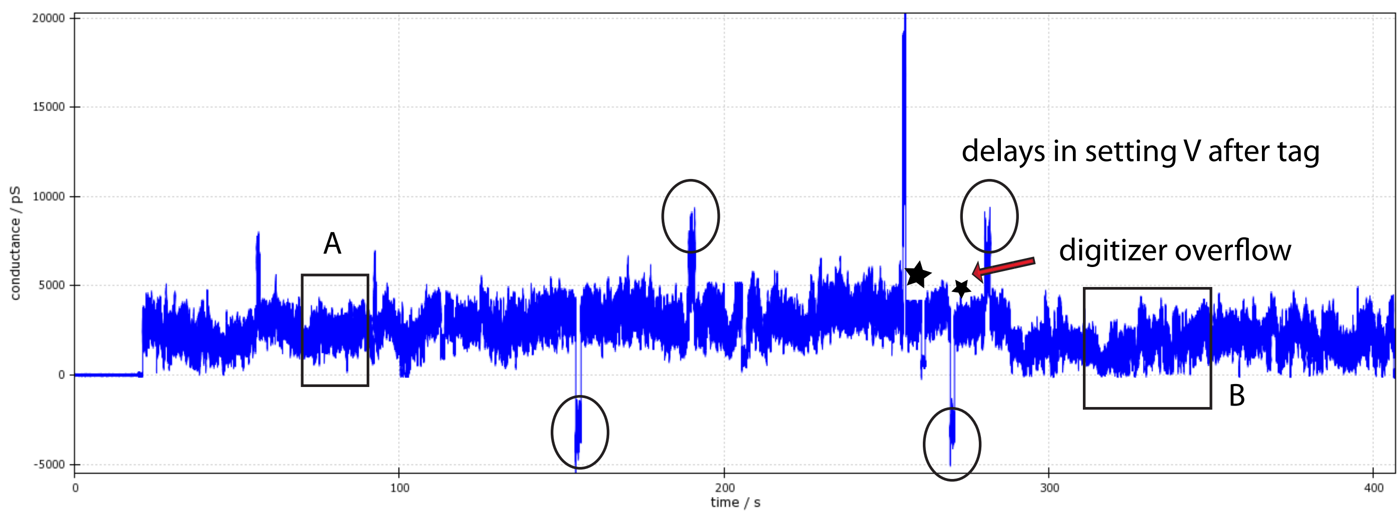


JMM-2 {06-07-10} [tG E3] soln MeOH inject diPhyPC 1M NMe4Cl 250uM styrene 'new' cup 2nd try

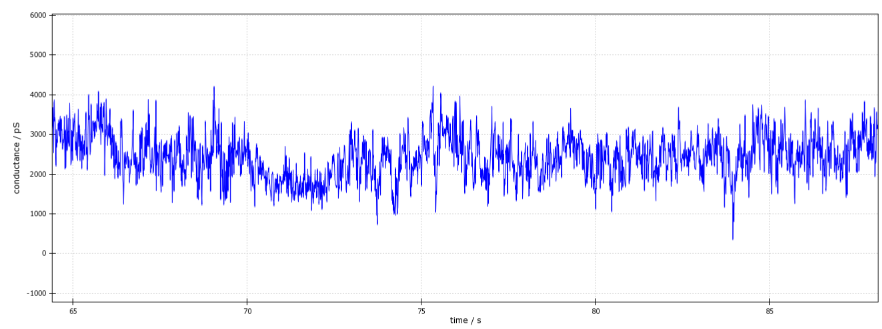


Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

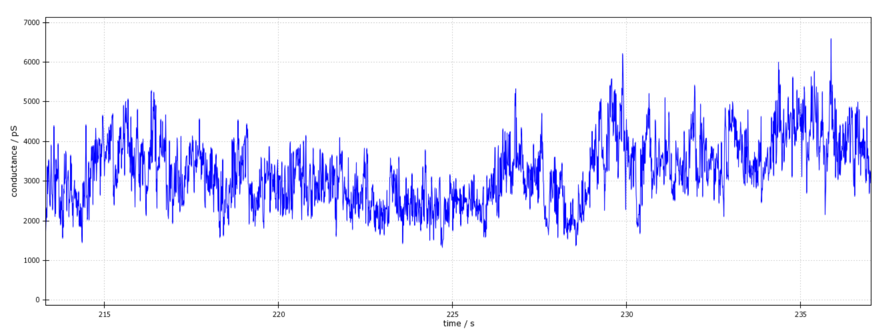
0014



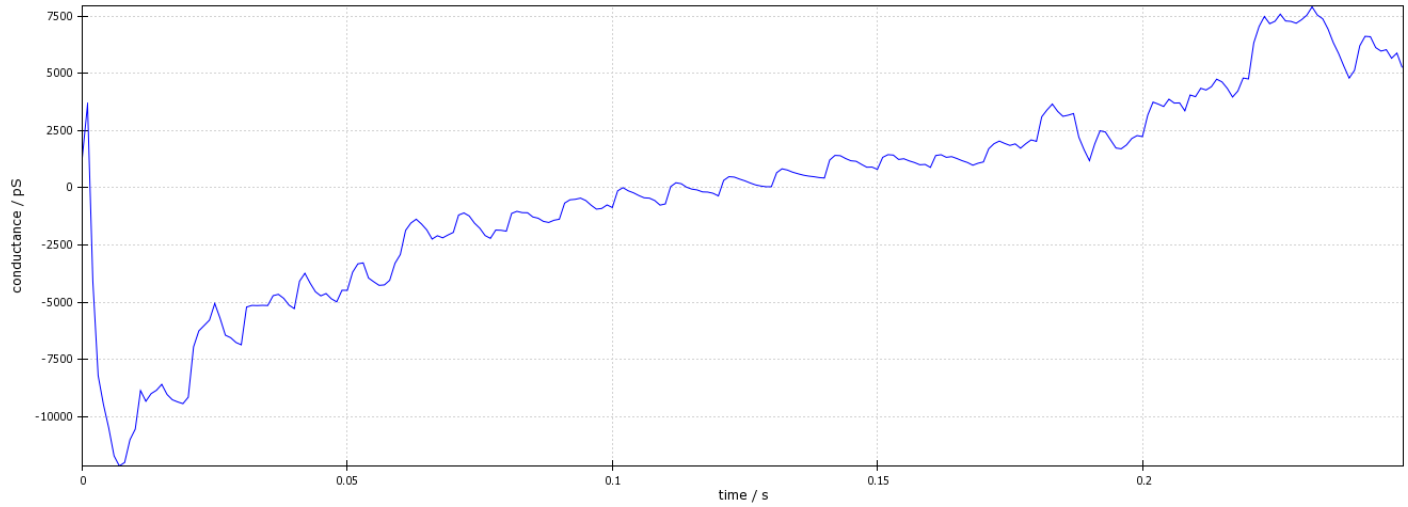
A



B



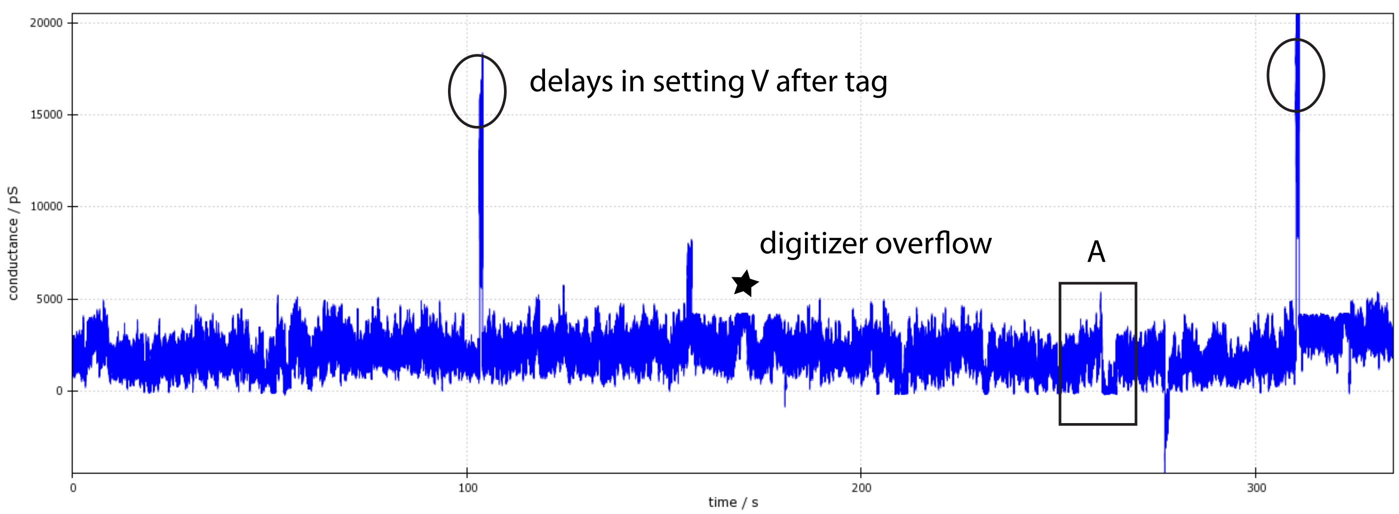
0015



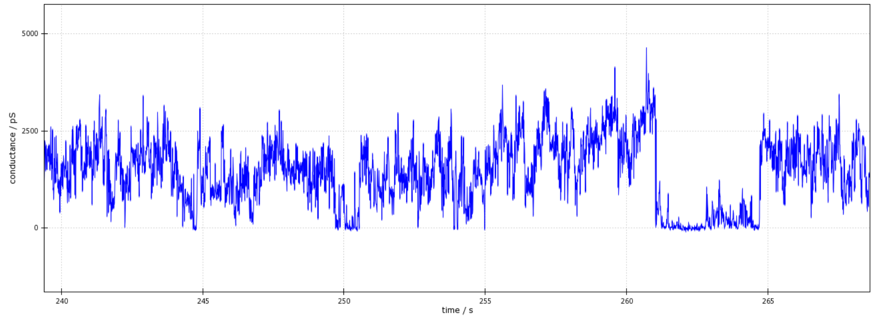
0016 - blank file; no data

0017 - blank file; no data

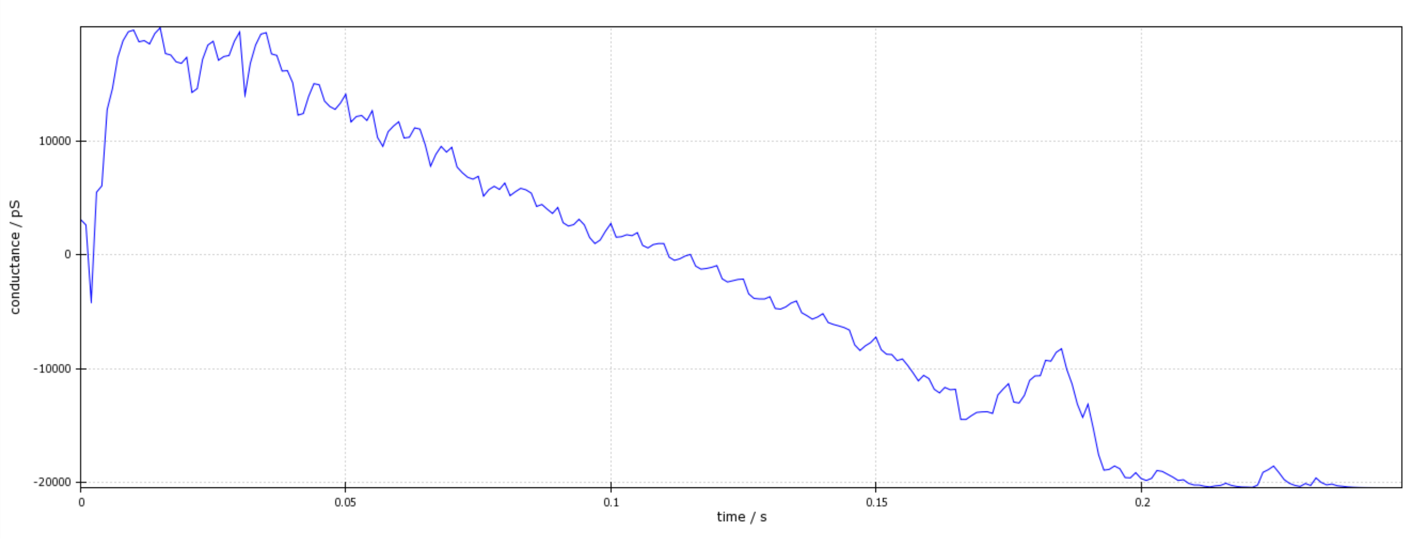
0018



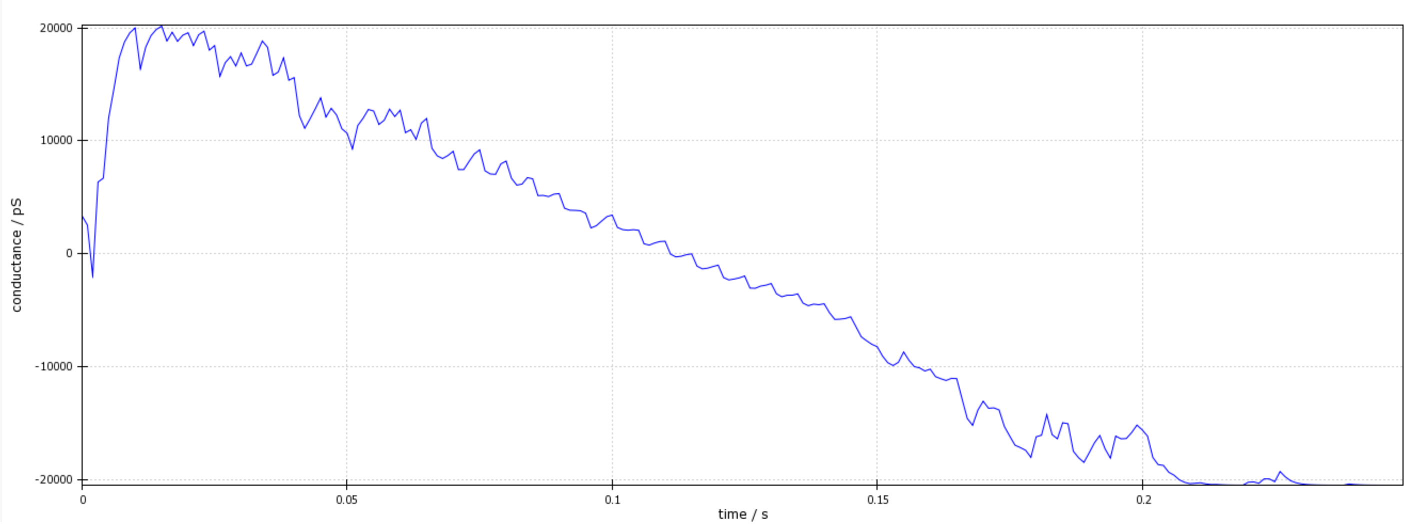
A



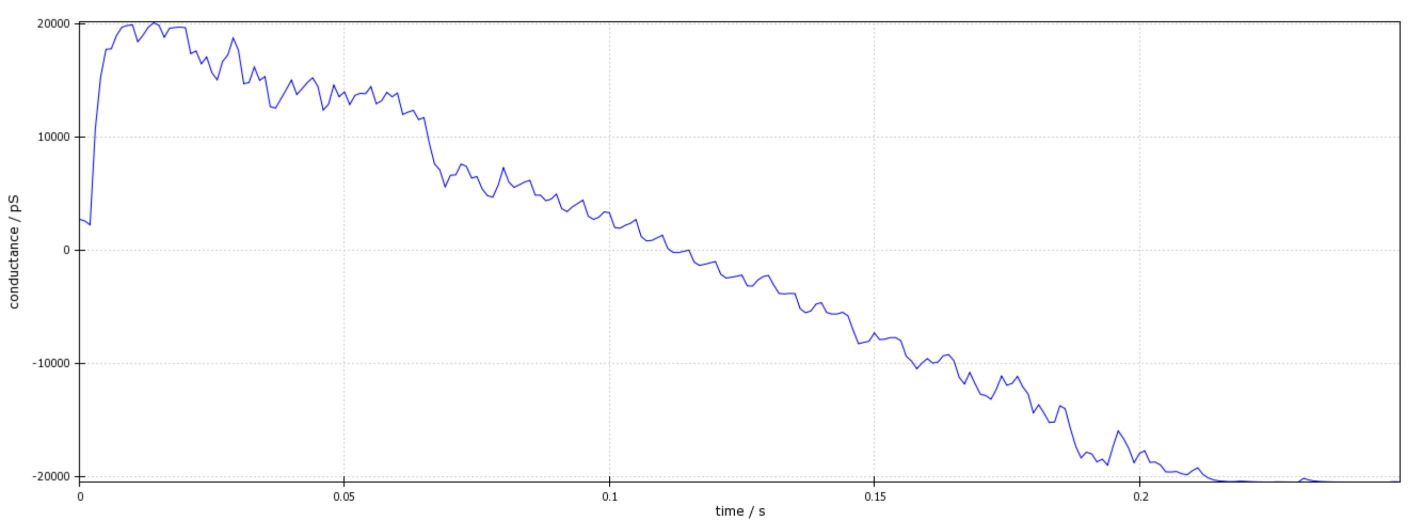
0019



0020

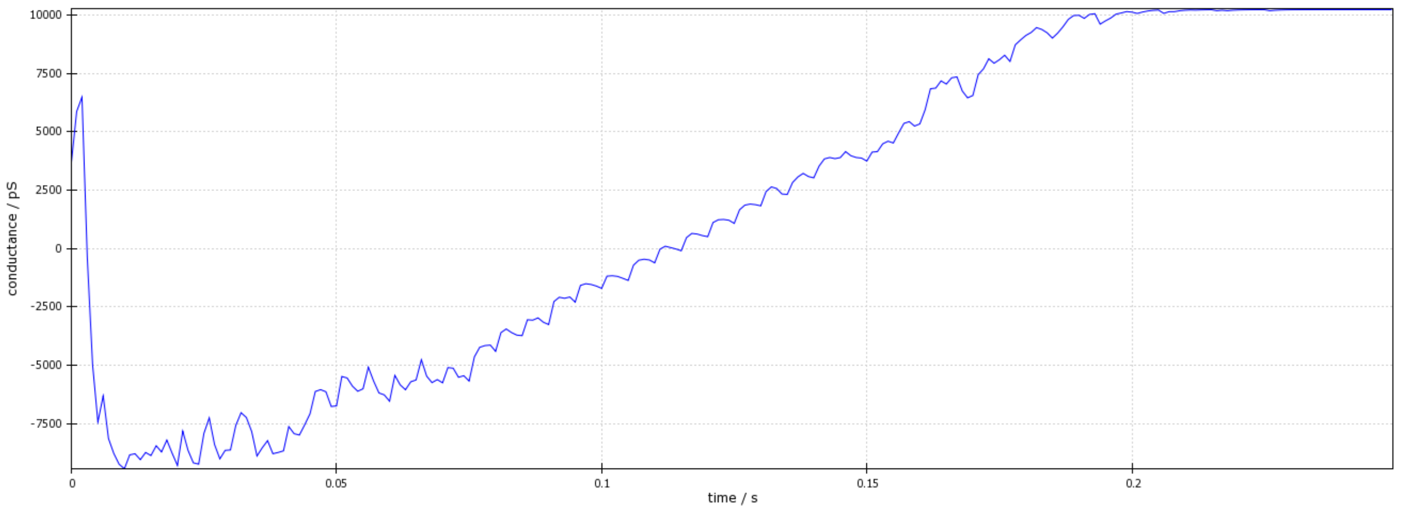


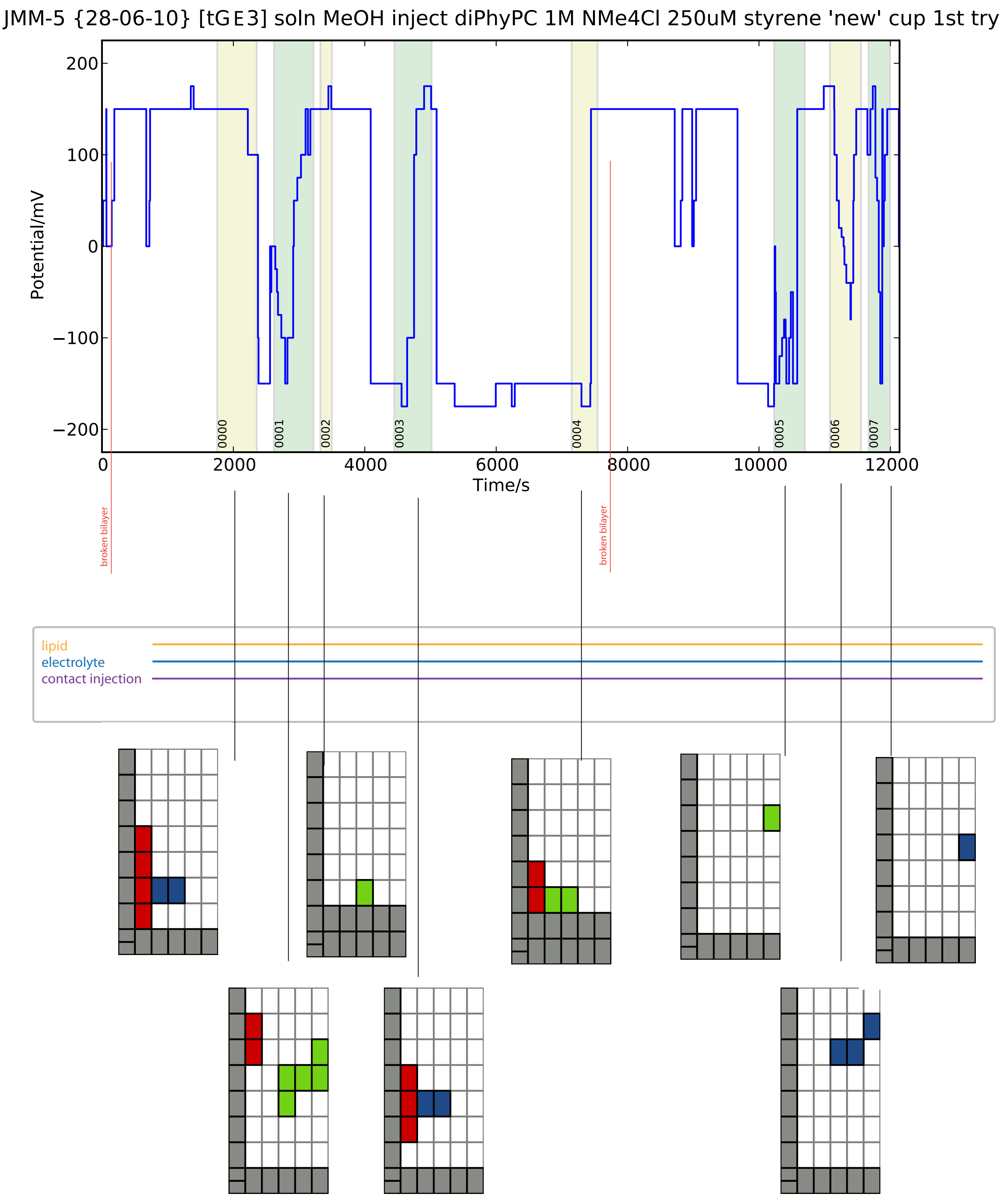
0021



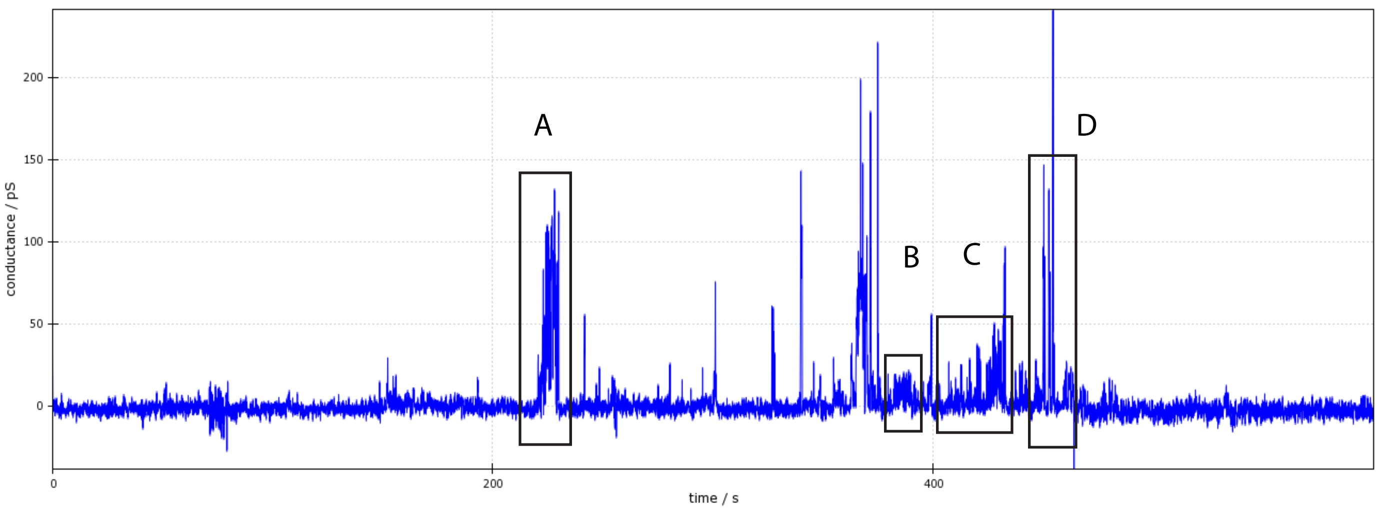
0021 blank file; no data

0022

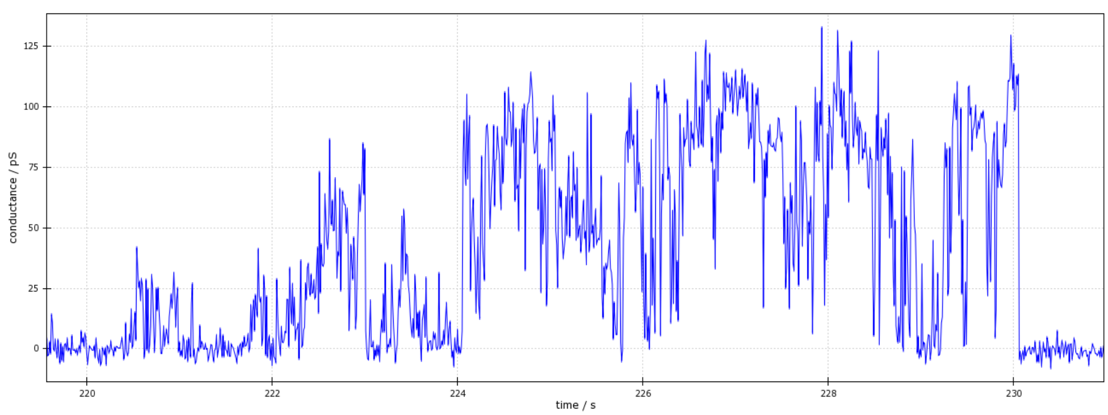



JMM-5 {28-06-10} [tGE3] soln MeOH inject diPhyPC 1M NMe4Cl 250uM styrene 'new' cup 1st try
Potential/mV
Time/s
0000
0001
0002
0003
0004
0005
0006
0007
broken bilayer
broken bilayer
lipid
electrolyte
contact injection

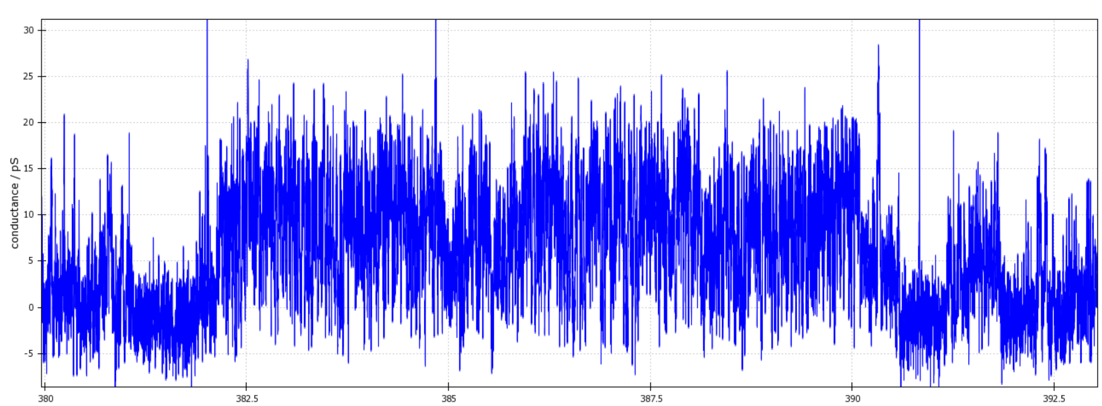
0000


A
B
C
D
conductance / pS
time / s
0
50
100
150
200
0
200
400

A

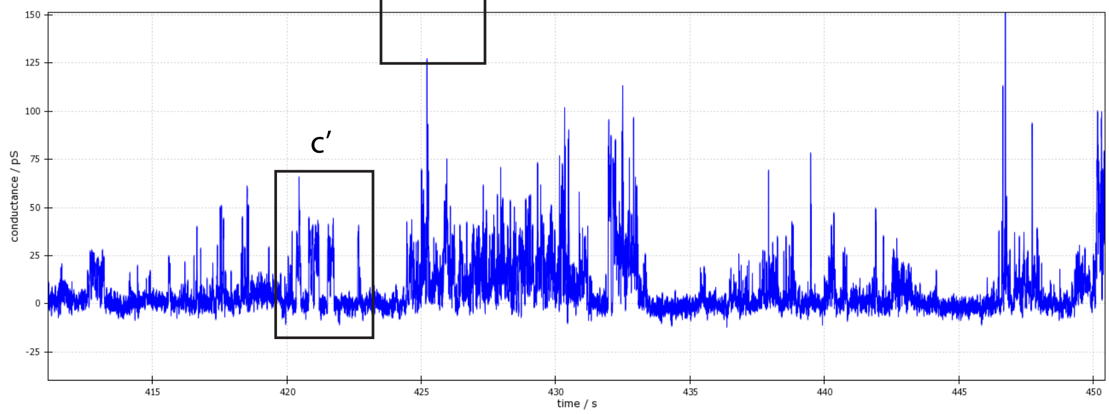

conductance / pS
time / s
0
25
50
75
100
125
220
222
224
226
228
230

B

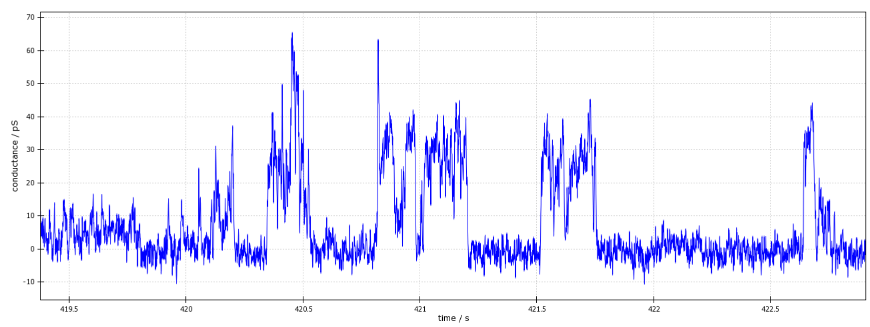

conductance / pS
time / s
-5
0
5
10
15
20
25
30
380
382.5
385
387.5
390
392.5

0000 comtinues..

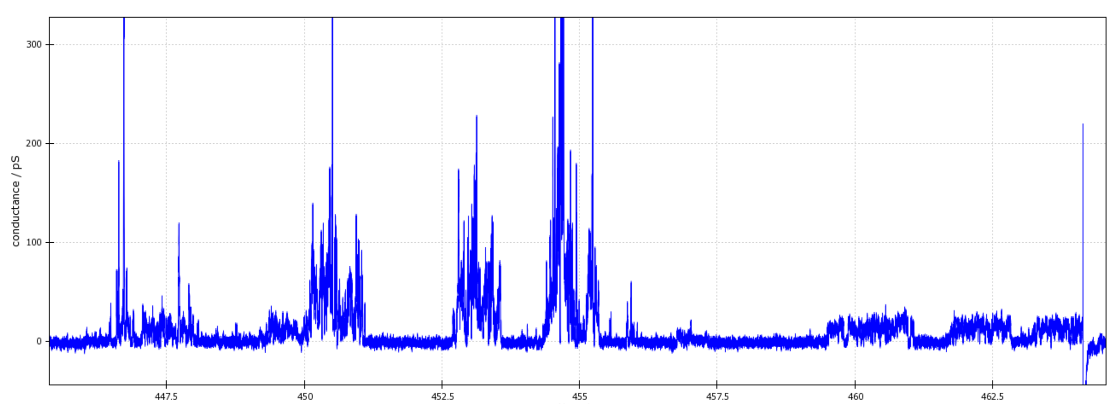
C



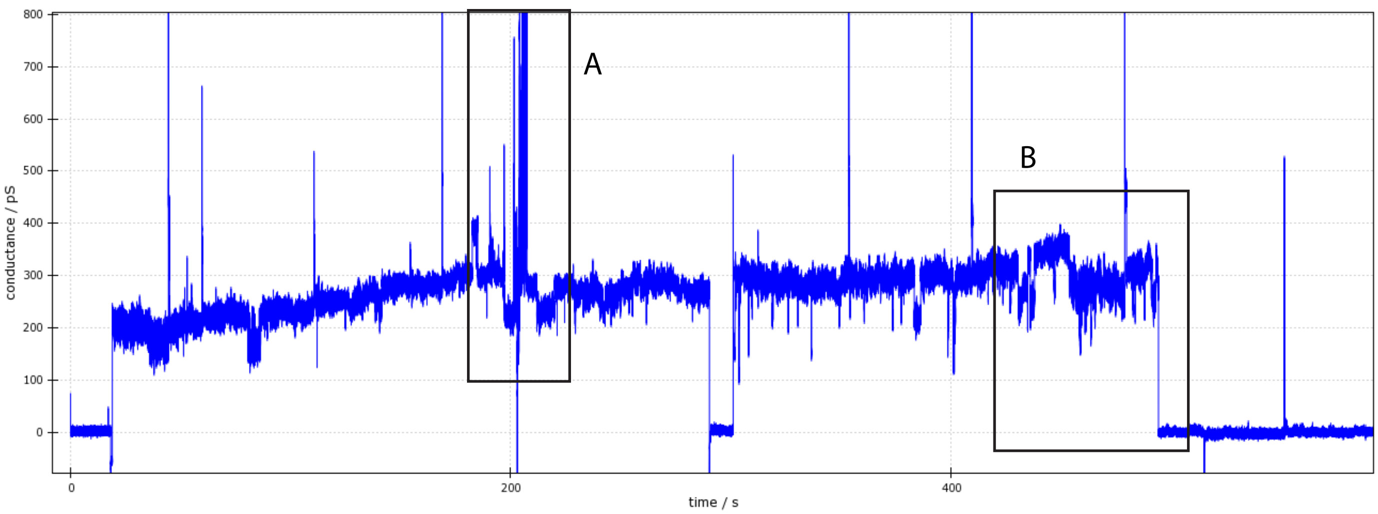
c′



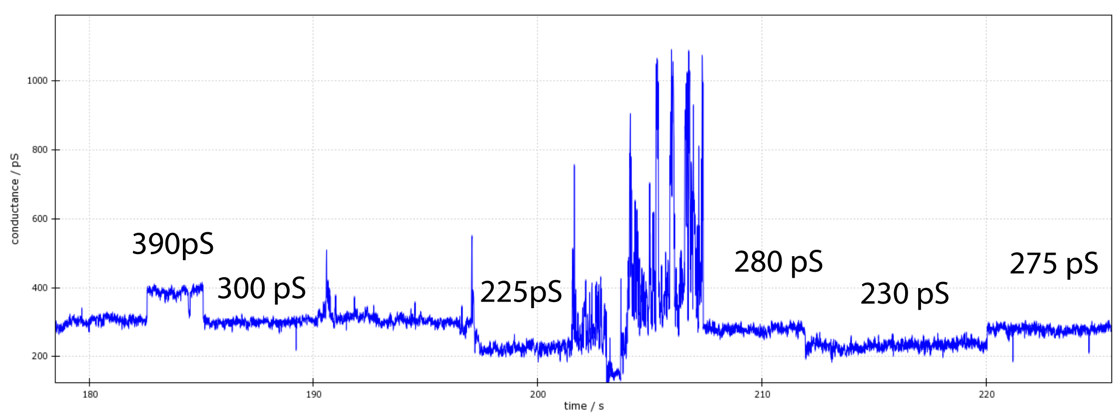
D



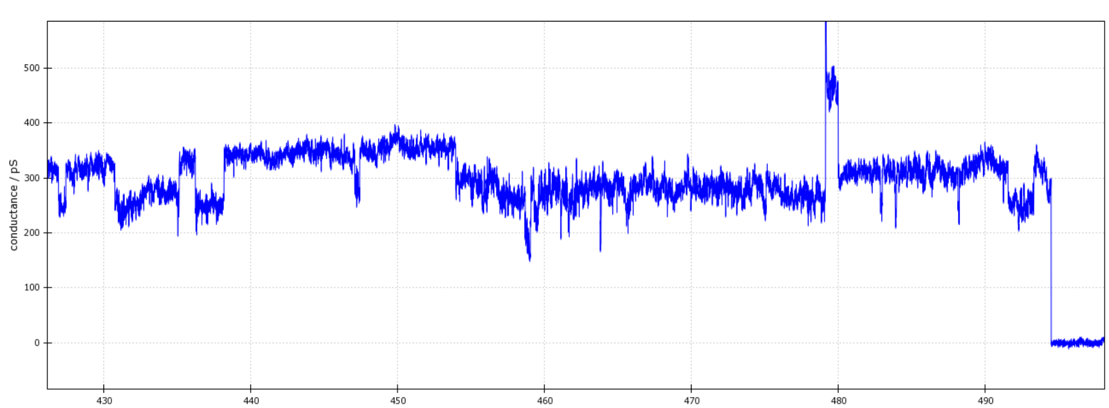
0001


conductance / pS
time / s
A
B

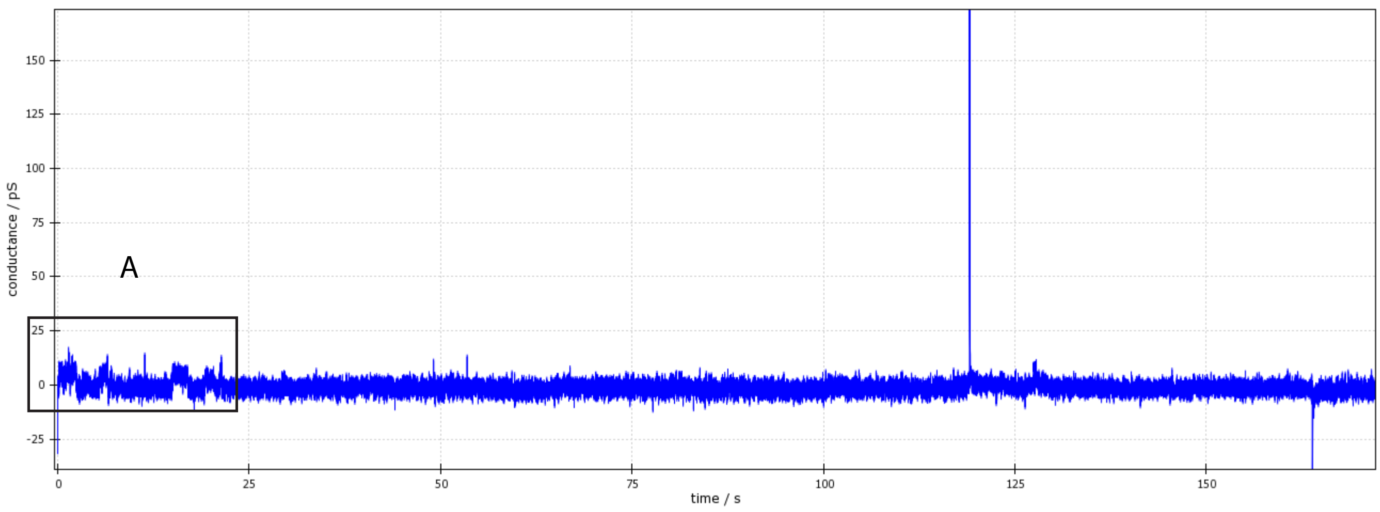
A


conductance / pS
time / s
390pS
300 pS
225pS
280 pS
230 pS
275 pS

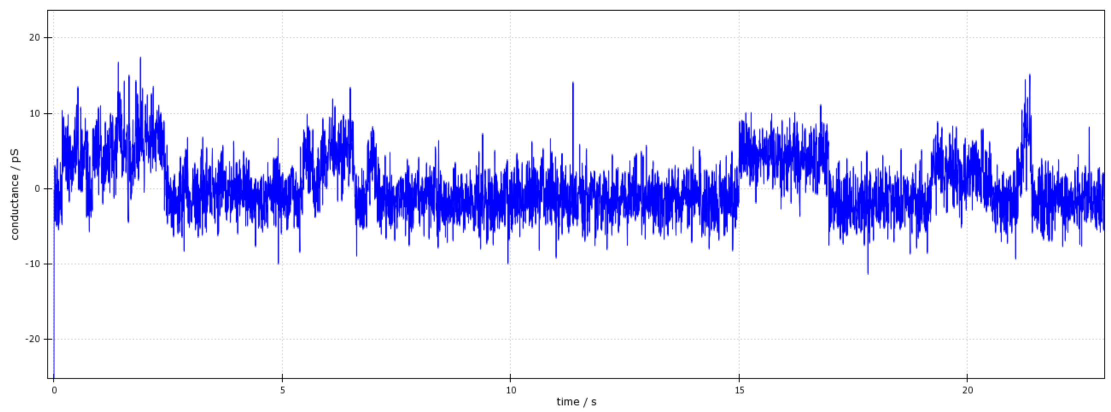
B


conductance / pS
time / s

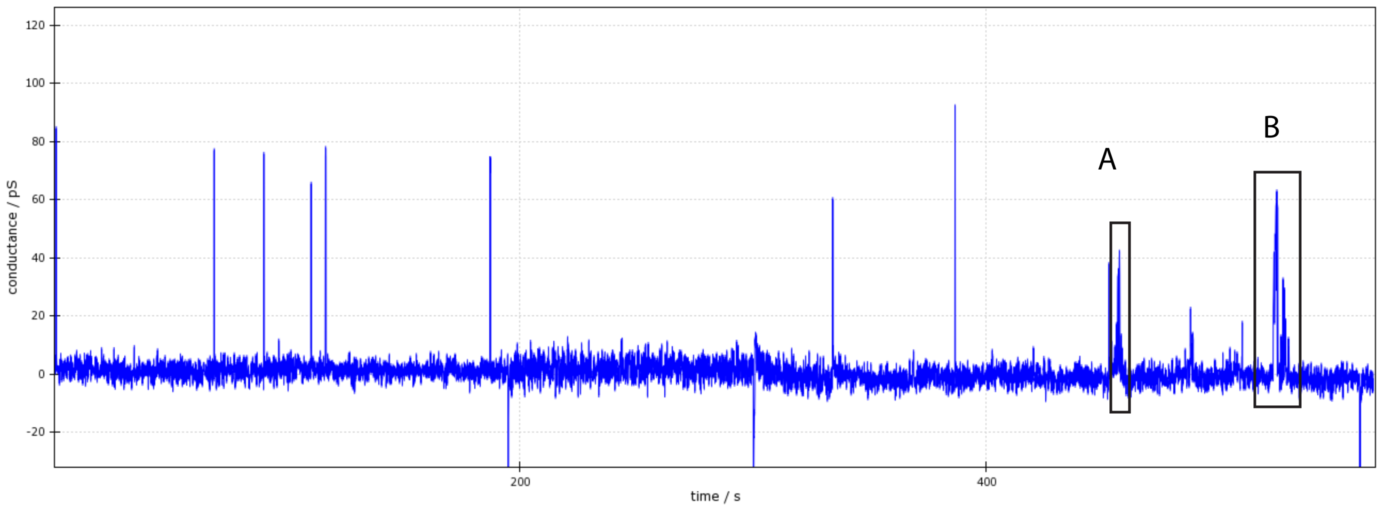
0002



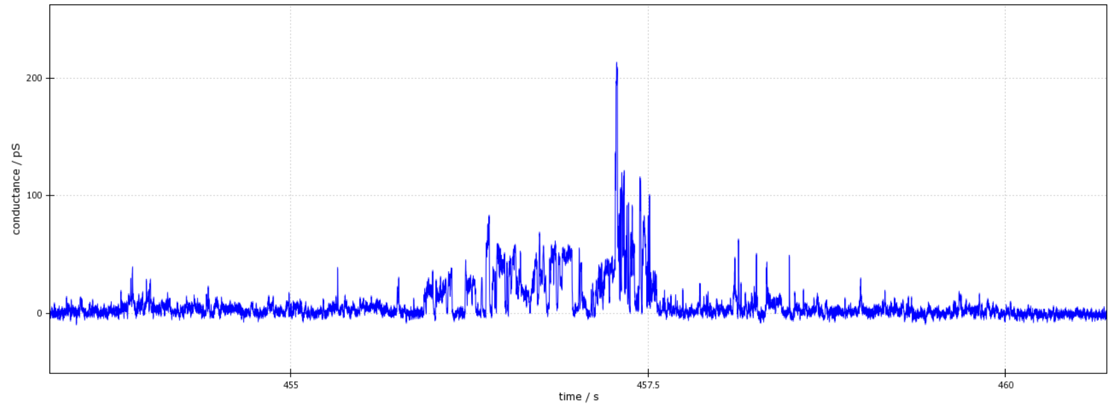
A



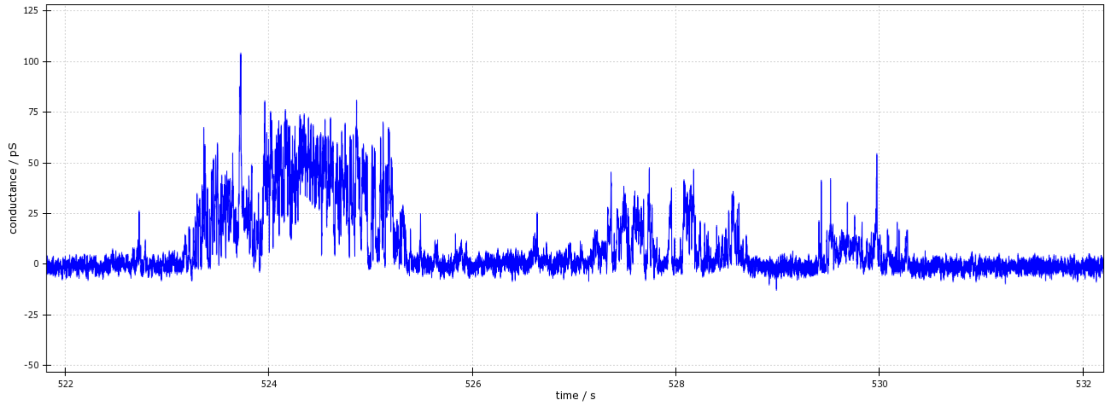
0003


A
B
conductance / pS
time / s

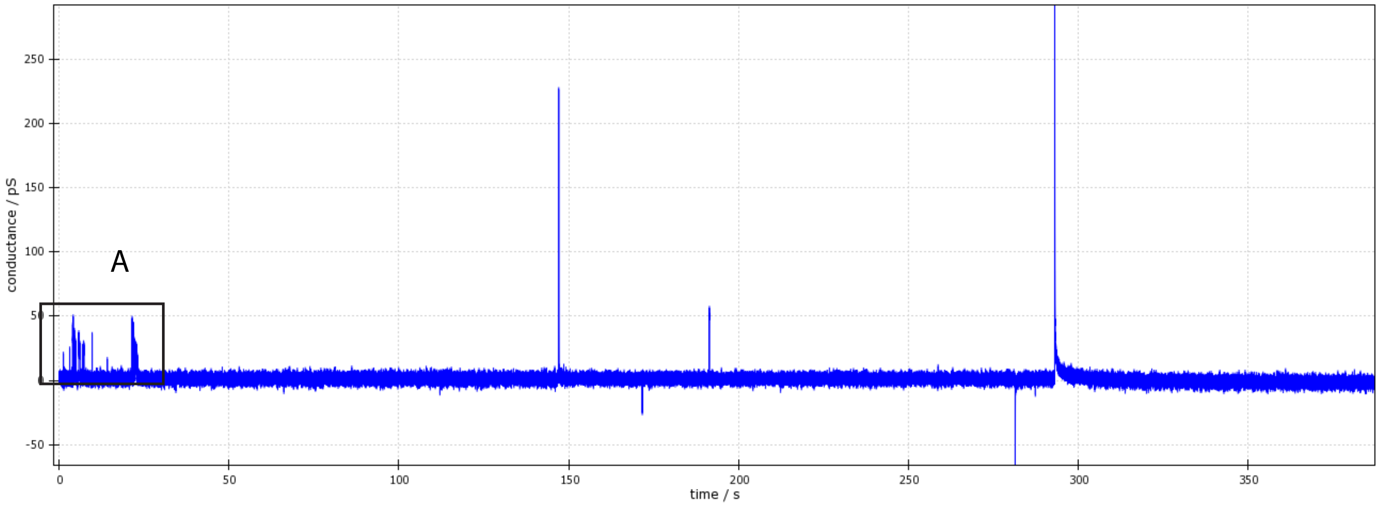
A


conductance / pS
time / s

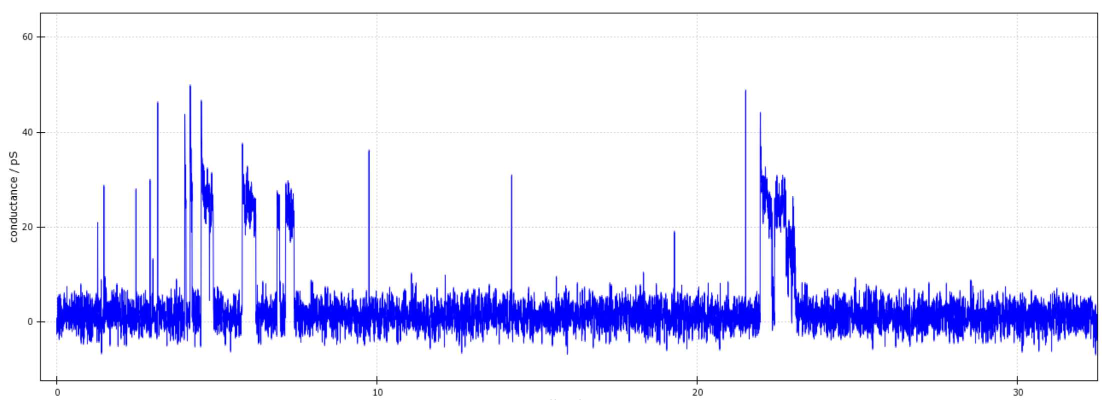
B


conductance / pS
time / s

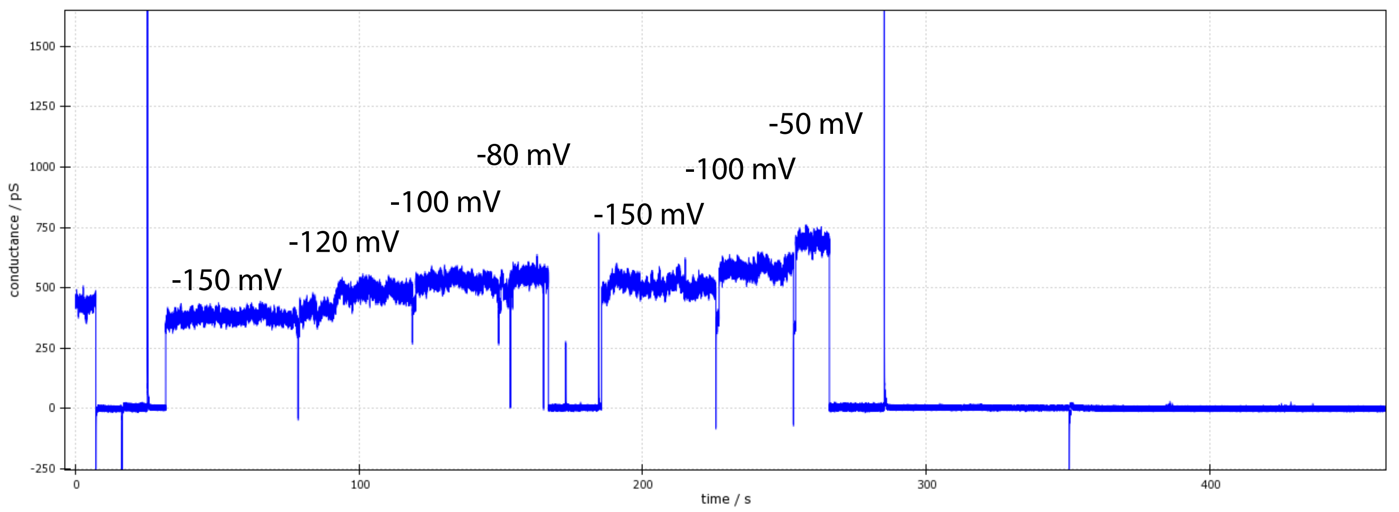
0004


A
conductance / pS
-50
0
50
100
150
200
250
time / s
0
50
100
150
200
250
300
350

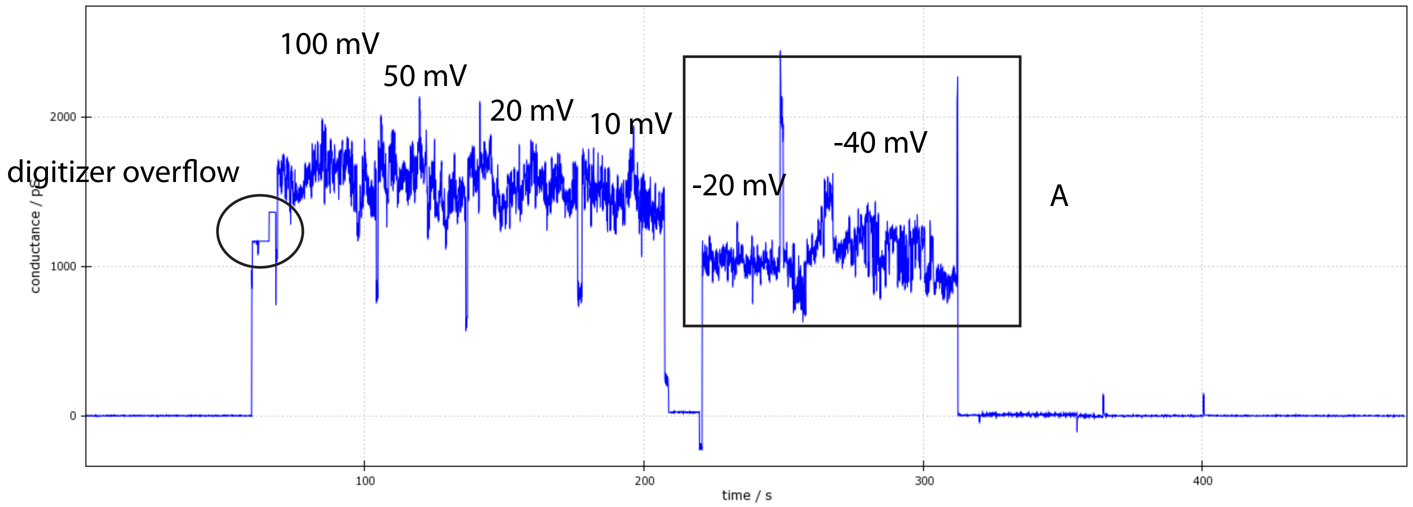
A


conductance / pS
0
20
40
60
time / s
0
10
20
30

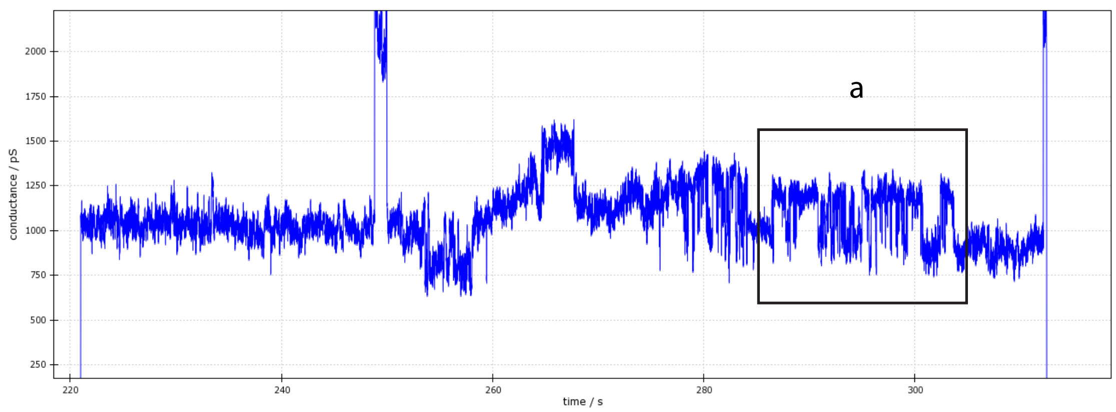
0005


-50 mV
-80 mV
-100 mV
-100 mV
-150 mV
-120 mV
-150 mV
1500
1250
1000
750
500
250
0
-250
conductance / pS
0
100
200
300
400
time / s

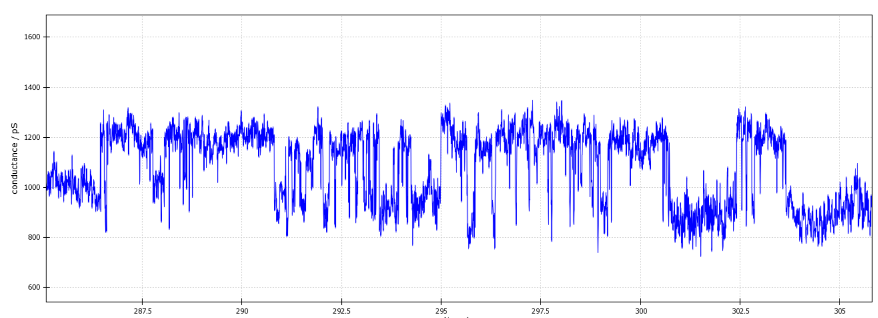
0006


100 mV
50 mV
20 mV
10 mV
-20 mV
-40 mV
digitizer overflow
A
conductance / pS
time / s

A

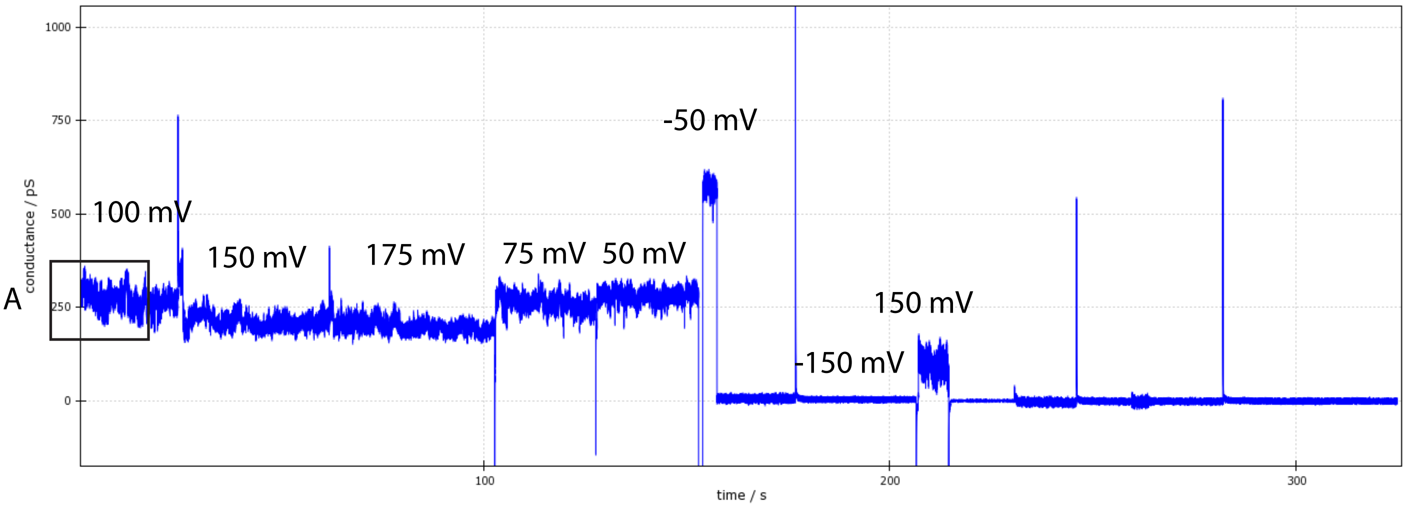

a
conductance / pS
time / s

a


conductance / pS
time / s

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

0007



A