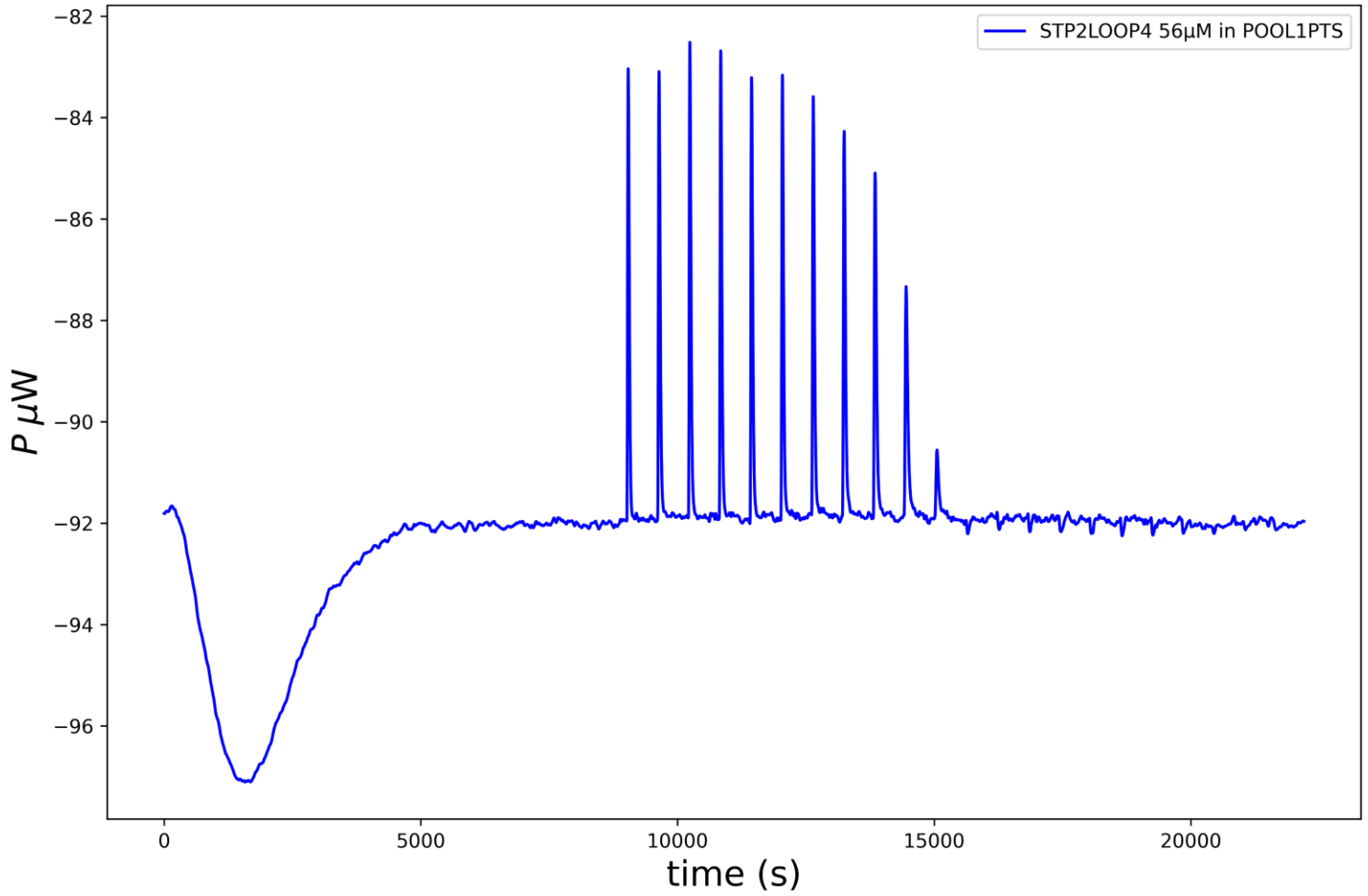
Analysis of ITC data: exemple on 2022-11-14-L4at56uM-in-POOL1PTS-25deg-250rpm.txt

Plot raw data in order to have an global visualisation

Identify:

- time of start : ts = 9000
- Duration of each injection ti = 600
- Number of injection (here 23, usually 25)



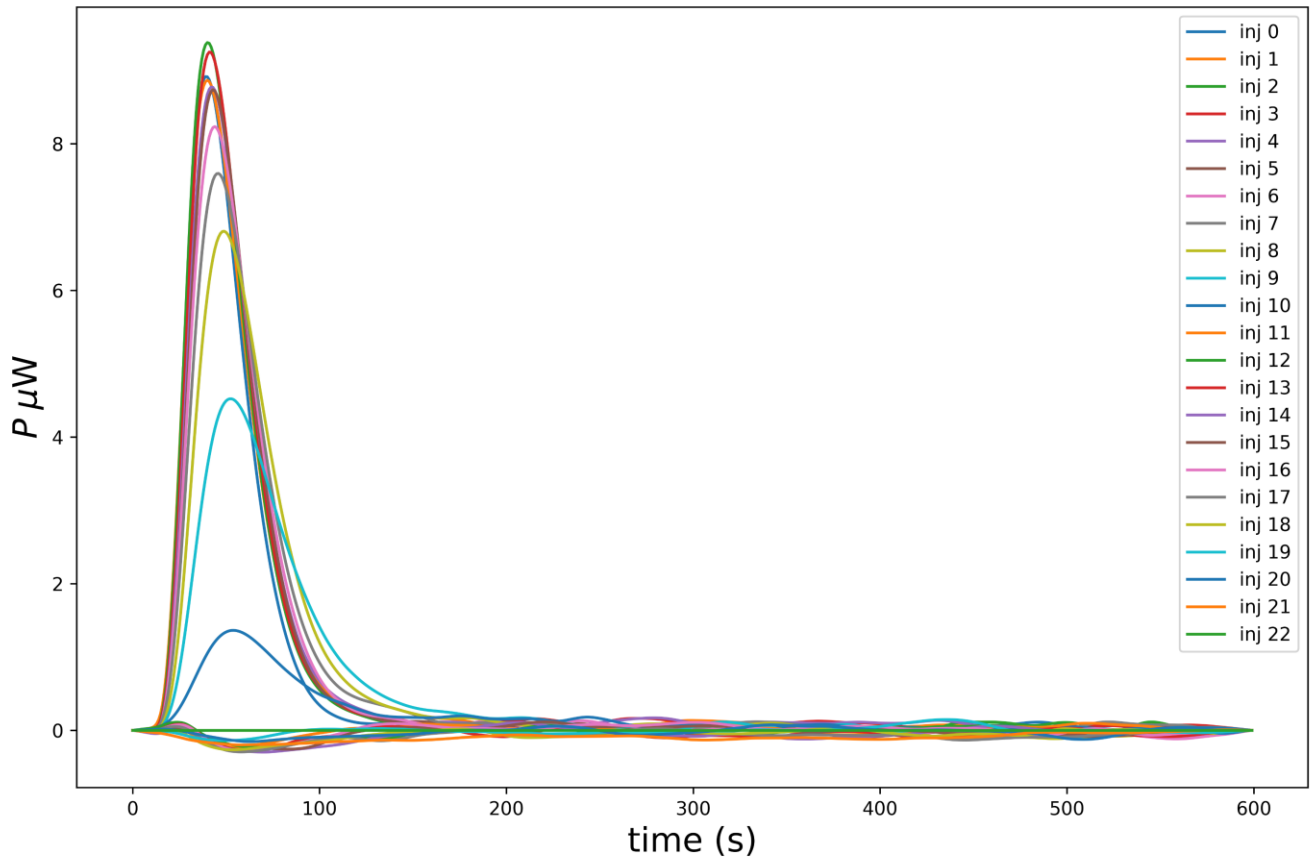
Each injection is separated and flattened to remove drift in the background

```
P1split = split_injection(P1, t1s,t1i,N1)
```

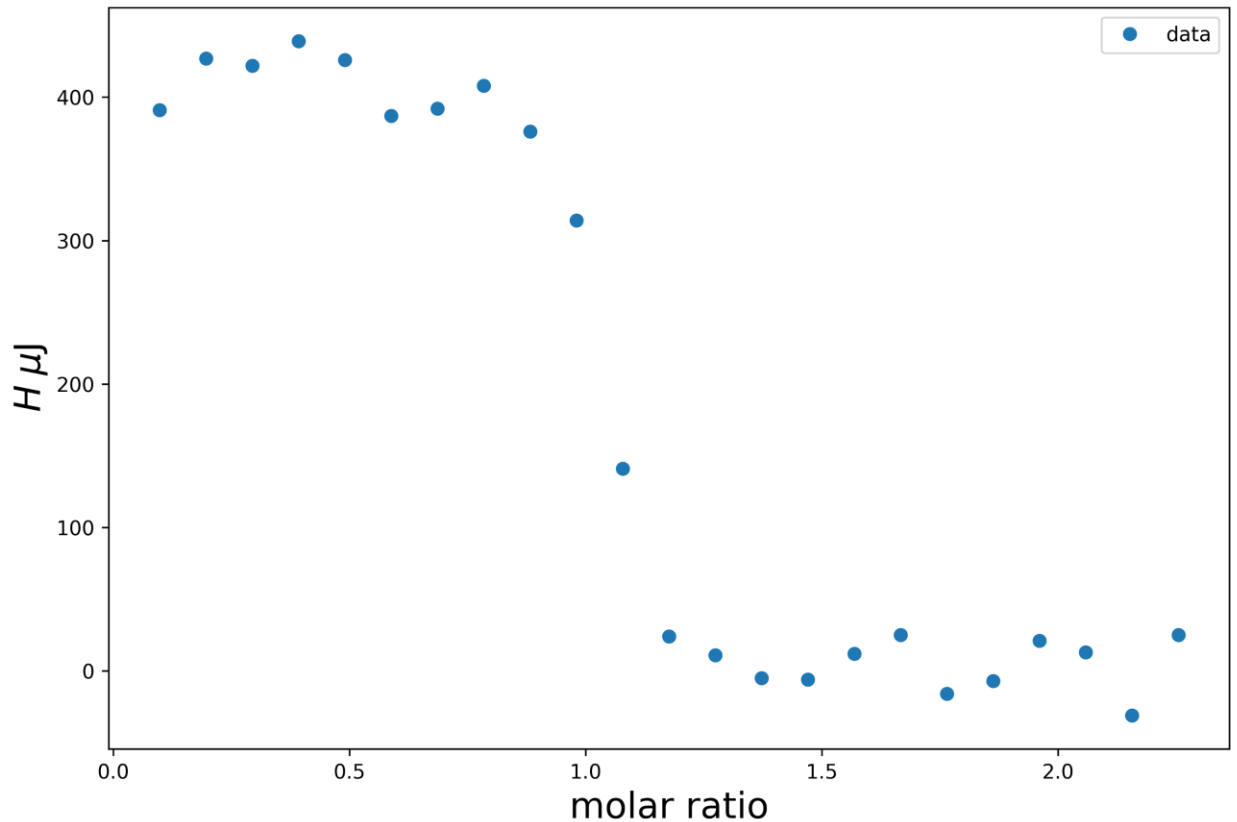
Return an numpy array of dimension (N1 lines) x (t1i columns) so each line is the data for an injection

```
P1flat = P1split
time1s = np.arange(t1i)
for index, Pin in enumerate(P1split):
    P1flat[index] = flat_injection(time1s,Pin)
```

Withdraw from each injection a linear background so the the first and last element of the line are 0



Each peak is then integrated and the average of the last values is substracted so that heat is zero at the end. We assume that the reaction is complete, it seems coherent with the sharp drop around the molar ration x=1 wich is also adjusted approximately here. (In fact in this curve the injection number would be more relevant)



modelling

we will assume a chemical reaction of the form

$$A + B \rightarrow AB$$

with the following parameters

1. ΔH
2. $K_{eq} = \exp(-\frac{\Delta G}{RT})$
3. x_0 the ratio of the concentrations in the syringe and the sample cell

We assume that the concentration in the syringe is correctly measured (because it has a larger value ?)

We assume that the volume of the calorimeter is fixed $V_0 = 1 \times 10^{-3}$ L and the injection volume is $V_{inj} = 10 \times 10^{-6}$ L. We assume that the initial concentration of species A is $C_{B,0} \times x_0$ and species B in the syringe is $C_{B,0}$. We define severals quantities as a function of the injection number i. The volume is :

$$V(i) = V_0 + i \times V_{inj}$$

the mole number of species AB after i injections is :

$$n_{AB,i} = [AB]_i V(i)$$

the mole number and concentration of free A after i injections is :

$$n_{A,i} = n_{A,0} - n_{AB,i}$$
$$[A]_i = \frac{n_{A,0}}{V(i)} - [AB]_i$$

the mole number and concentration of free B after i injections is :

$$n_{B,i} = n_{B,i} - n_{AB,i}$$
$$[B]_i = \frac{n_{B,i}}{V(i)} - [AB]_i$$

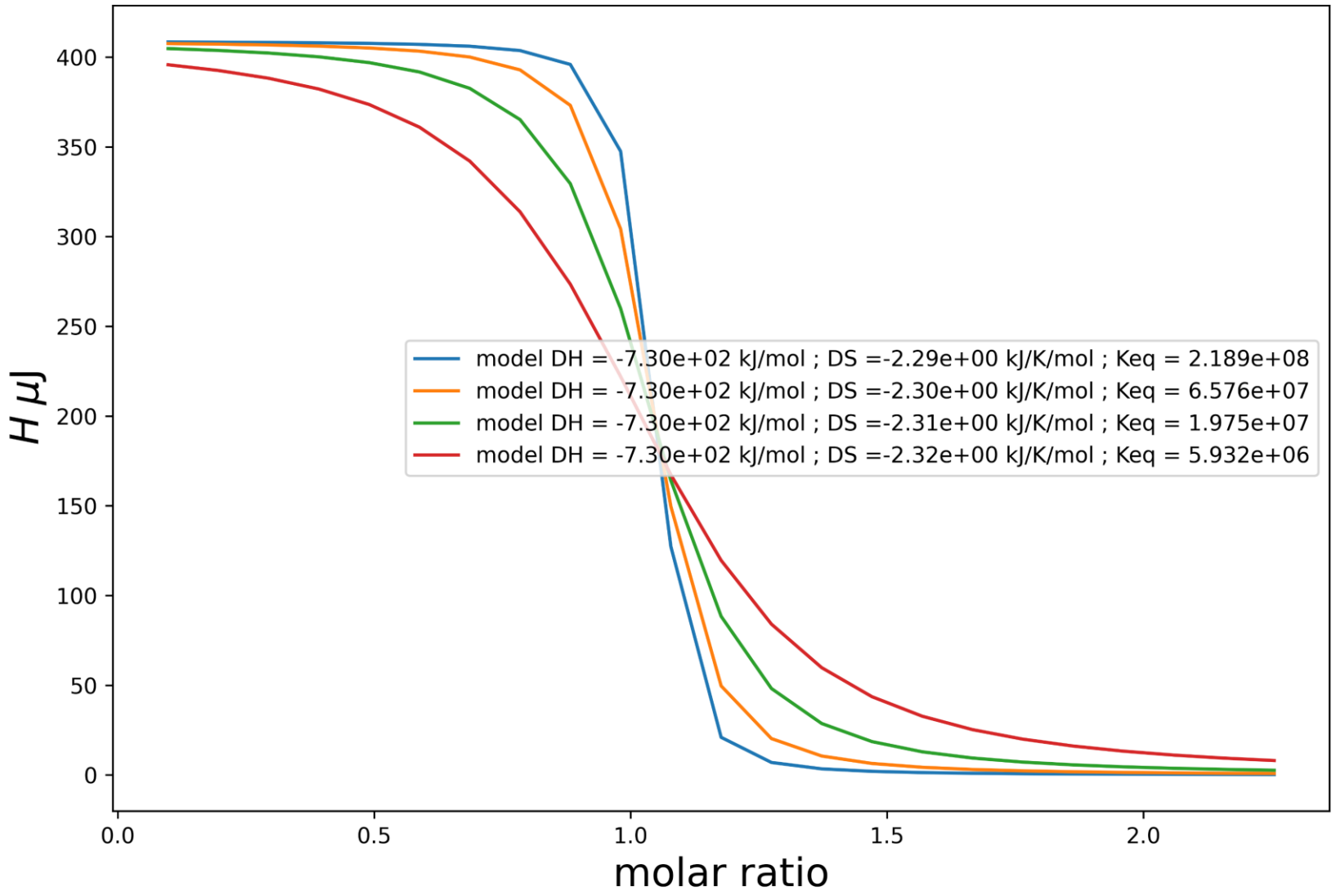
These quantities are related through the equilibrium constant:

$$K_{eq} = \frac{[AB]_i}{[A]_i [B]_i}$$
$$[AB]_i = K_{eq} \left(\frac{n_{A,0}}{V(i)} - [AB]_i \right) \left(\frac{n_{B,i}}{V(i)} - [AB]_i \right)$$

As a consequence it is possible to find the evolution of the concentration of free AB as a function of the injection number by soliving the following second order polynomial:

$$[AB]_i^2 - \left(\frac{n_{A,0}}{V(i)} + \frac{n_{B,i}}{V(i)} + \frac{1}{K_{eq}} \right) [AB]_i + \frac{n_{A,0}}{V(i)} \frac{n_{B,i}}{V(i)} = 0$$

Result of the modelisation



Qualitative best agreement