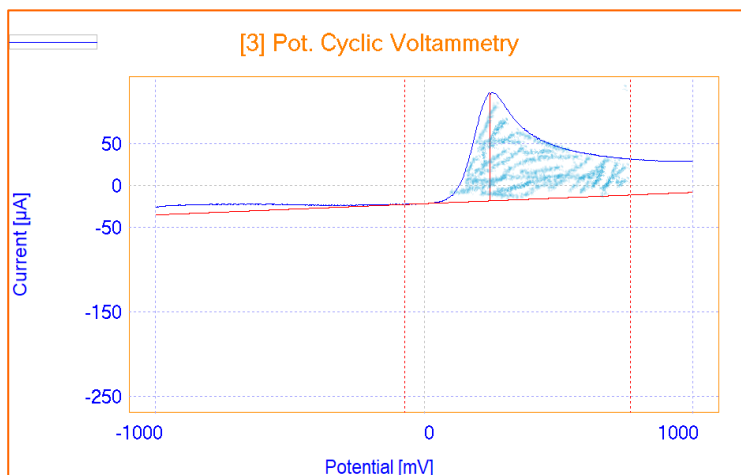




General Electrochemistry AP-GE15

Integration of voltammetric curves



After performing voltammetric methods like CV, LSV, DPV, analyzing the voltammetric peaks gives users valuable information around the electrochemical behavior of their samples both qualitative and quantitative.

Calculating peak surface through integration is one of the curve analysis providing information around sample and electrochemical reaction of interest.



INTRODUCTION

To integrate a peak: locate and display it, determine the base line then click the Draw button in the Peak analysis dialogue box.

The "Peak analysis" dialogue box is accessible by clicking the Peak analysis command in the Processing group of the Curve Ribbon (figure 1).

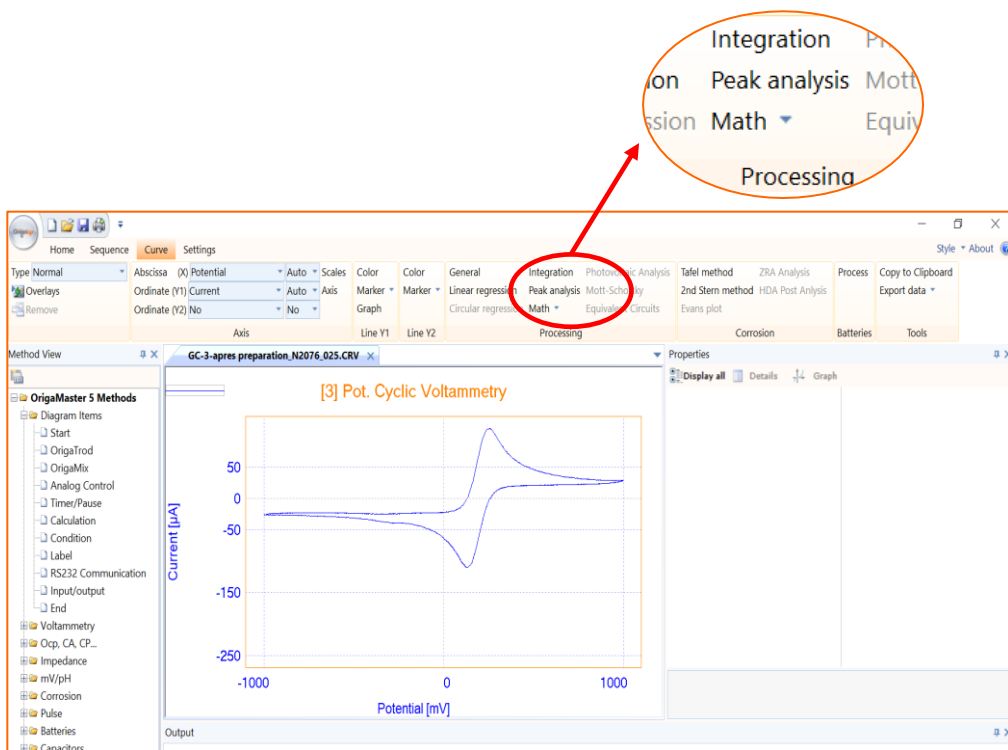


Figure 1: « Peak Analysis » button is found in « Curve » ribbon

Note: If there is no curve loaded, this option is not active in the « curve » ribbon! So first, it is needed to load the curve.



How to select segment of interest

1/3

For example, if the curve is a Cyclic Voltammogram as what is shown in figure 2, it is needed to choose the segment concluding peak by right clicking on the curve and opening « trajet ».

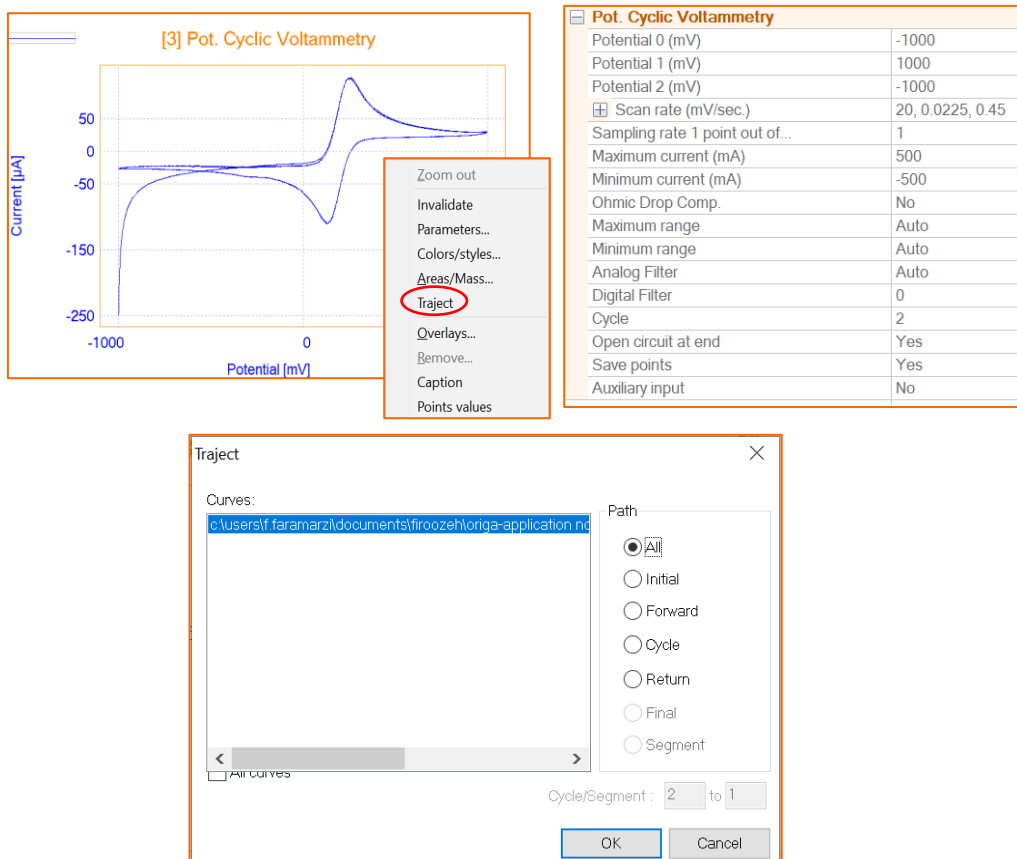


Figure 2: Cyclic voltammogram, parameters of the test and Trajet window



How to select segment of interest

2 / 3

There are 3 important options in « traject » window for choosing the segment:

- **Initial** which will show the initial sweeping from P0 to P1 (figure 3).

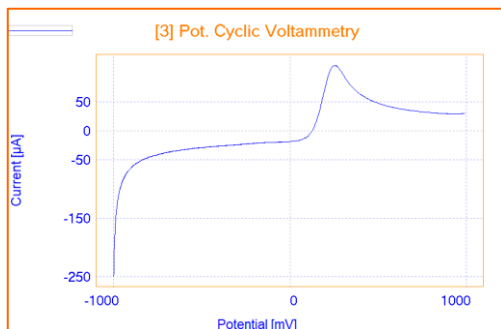
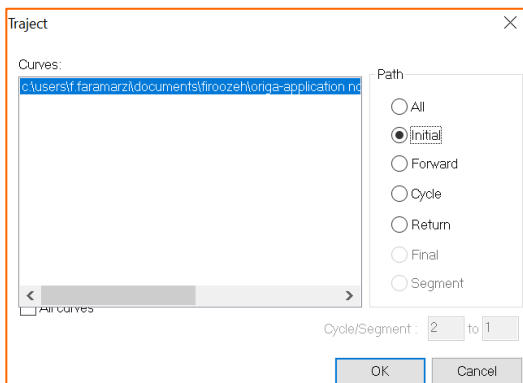


Figure 3: Initial object in « traject » window

- **Forward** which corresponds to sweeping from P1 to P2 (figure 4).

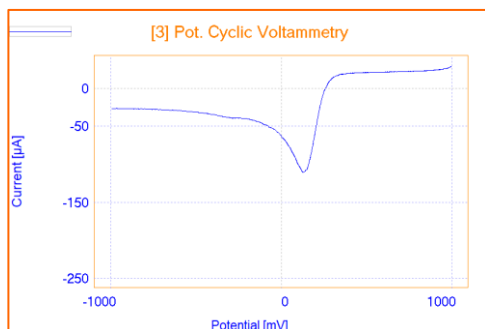
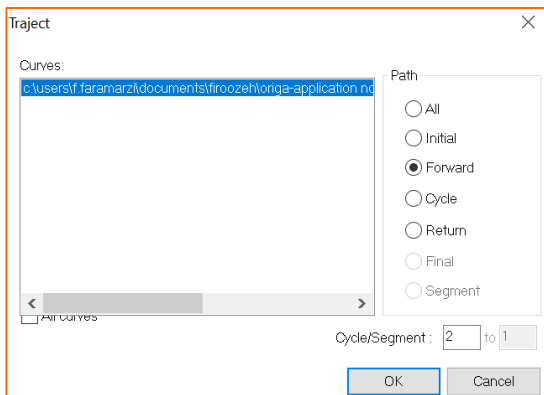


Figure 4: Forward object in « traject » window



How to select segment of interest

3/3

- **Return** which is related to sweeping from P2 to P1 (figure 5).

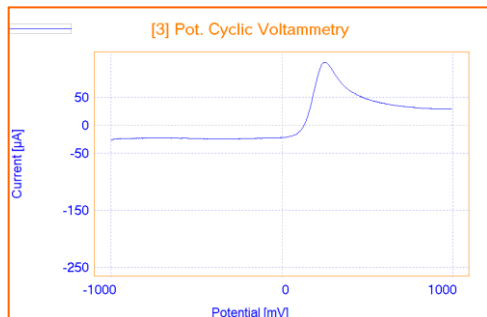
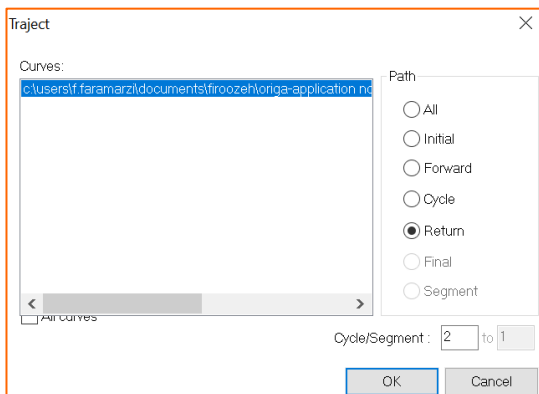


Figure 5: Return object in « traject » window

In case of having more than 1 cycle, in the « Cycle/Segment » box, the cycle of interest could be chosen.

Note: The « Segment » was designed to fit Staircase method.



How to select integration area

1/2

After choosing the segment, now it is time to open « Peak Analysis » in curve ribbon and follow the steps below to integrate the peak:

A



In « Peak analysis » window there are 4 options to define the peak baseline:

- No
- Regression
- Manual
- Polynomial

B

Peak analysis - GC-3-apres preparation_N2076_025.CRV

Base line Mode

☒ No
☐ Regression
☐ Manual
☐ Polynomial

		mV	µA
Point 1	13297	999.428	29.713
Point 2	22167	998.001	29.663

Results

From: 13297 To: 22167 mV

Integration Total

Positive

Negative

Peak Position

Height

Width

☐ Zoom Draw Refresh Save Close

Figure 6: 4 mode of baseline definition for peak



How to select integration area

2/2

In Results part, it is possible to define the integration area. By default, the software always considers the whole curve. But if a special zone of curve is considered, then in “**From**” and “**To**” boxes, integration area could be defined. Then by clicking on “**Draw**” button, the results will be shown.

C

Peak analysis - GC-3-apres preparation_N2076_025.CRV

Base line
Mode

☒ No
☐ Regression
☐ Manual
☐ Polynomial

		mV	μA
Point 1	8862	-999.427	-26.69
Point 2	13296	999.534	29.715

Results

From: 8862 To: 13296 -999.427 999.534 mV

Integration	Peak
Total	Position
Positive	Height
Negative	Width

D

☐ Zoom **Draw** Refresh Save Close

Figure 7: Boxes related to choosing integration area



Definition of integration area

1/2

You can select the first and last points of the integration area (figure 8) and recalculate the integration data (by clicking again on the **Draw** button). The integration area is displayed in C/cm² and W/cm² for current/potential/time files and in C/cm² for current/time files.

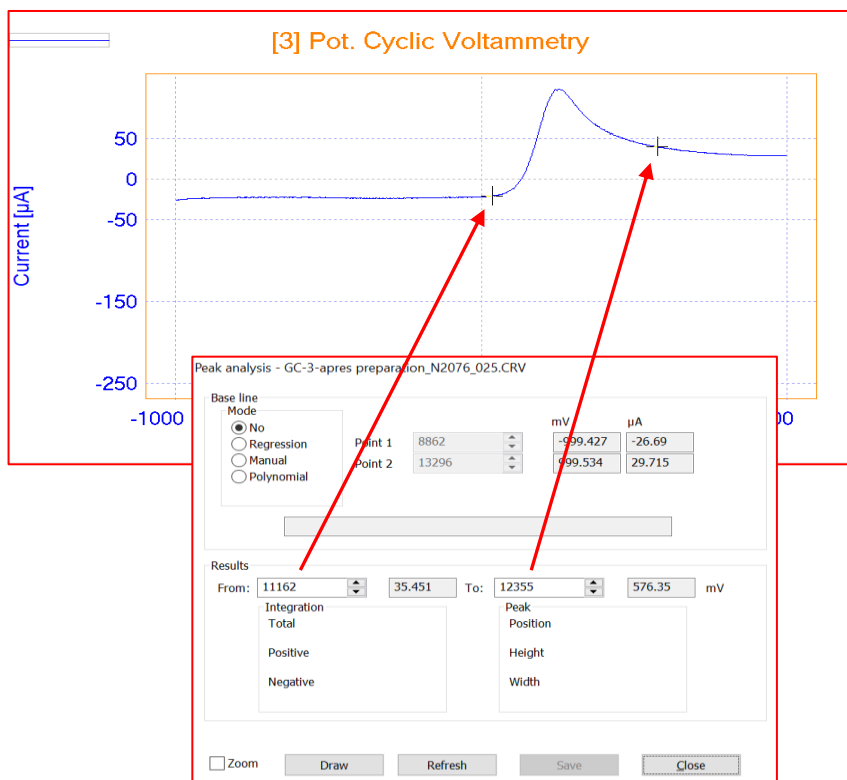


Figure 8: Selection of integration area.

First click on "**From**" button the click on the curve and select from which point the integration zone start, and then click on "**To**" button, then click on the curve to select in which zone the integration last.



Definition of integration area

2/2

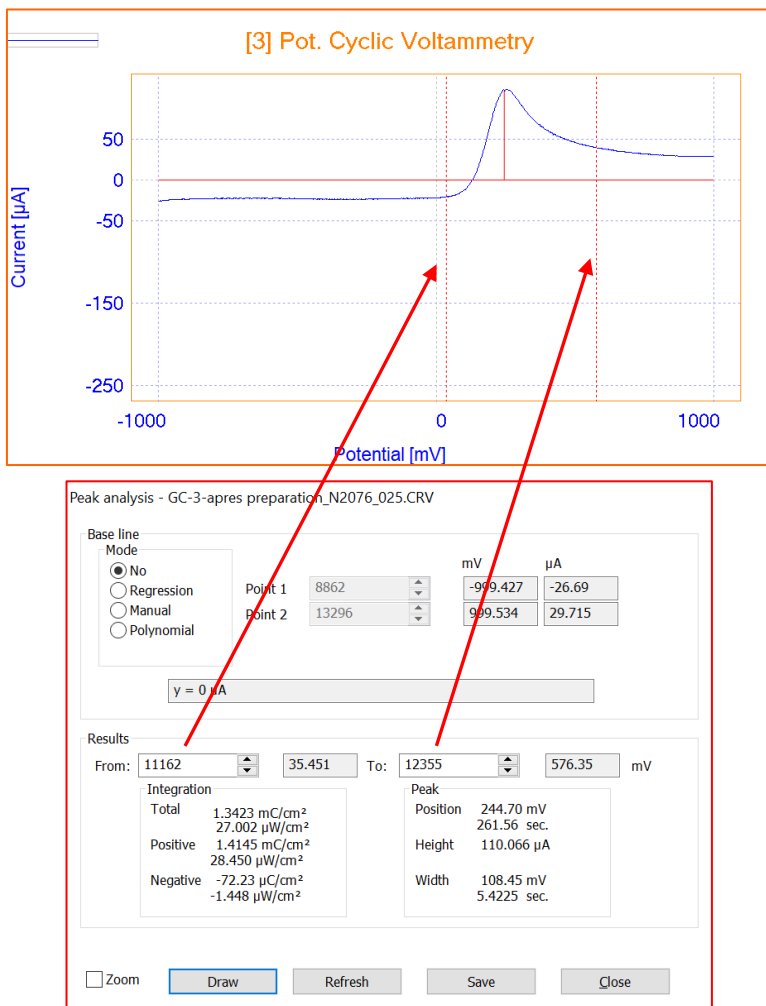


Figure 9: Results and data showing after clicking on « Draw » Button; Integration area is shown by red vertical lines.

Figures 8 and 9 show how to choose integration area by clicking on the desired zones of the curve and extracting data afterward.



Baseline mode = No

1/6

1 Peak analysis - base line = No (Y1 axis)

For **Mode** select **Base line = No**. The Base line will be considered as $Y1=0$ (Point 1 and Point 2 are set to the first and last point of the curve and it cannot be changed). Here it is not possible to define point 1 and point 2.

In other modes, **Point 1** and **Point 2** will be involved in the **Base line** determination process. It means the baseline will be passed from these two points.

After clicking on "Draw" button, in the results part, integration data will be shown (Figure 10).

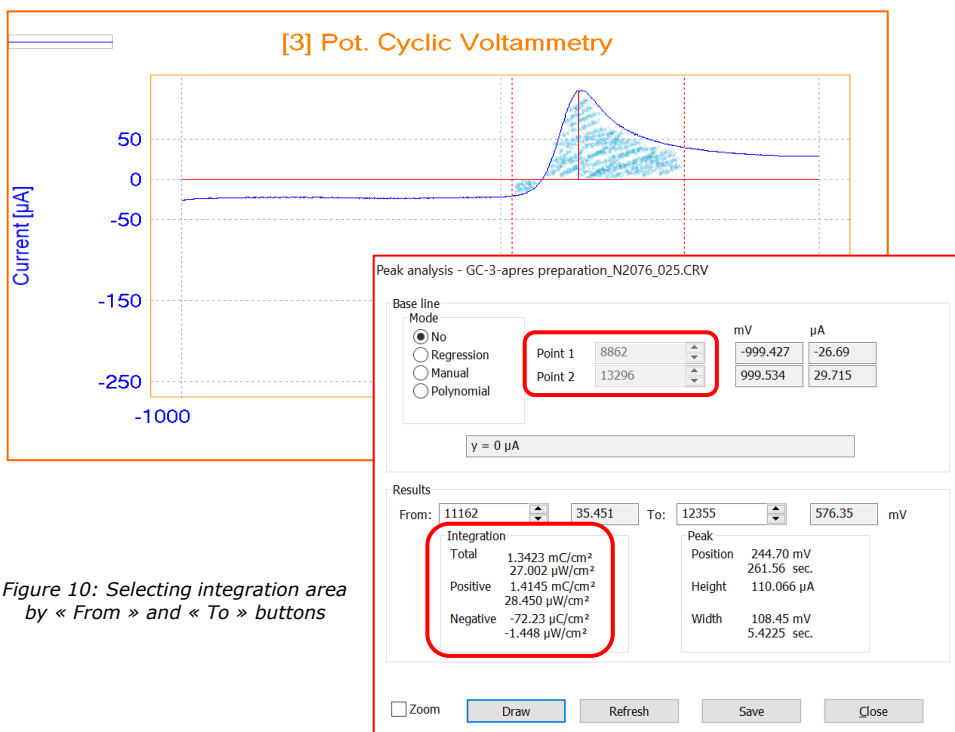


Figure 10: Selecting integration area by « From » and « To » buttons

Baseline mode = Regression

2/6

2

Peak analysis - base line = linear regression

For **Mode** select **Base line = Regression**, a linear regression is performed between 2 selected points of the curve. The curve must show a linear region before and/or after the peak and the line found must fit the base of the peak. As it is shown in figure 11, in the first step two points must be selected to define the regression line by clicking on the "**point 1**" box and then click on the curve to choose the first point, then by clicking on the "**point 2**" box and click on the curve to select the second point.

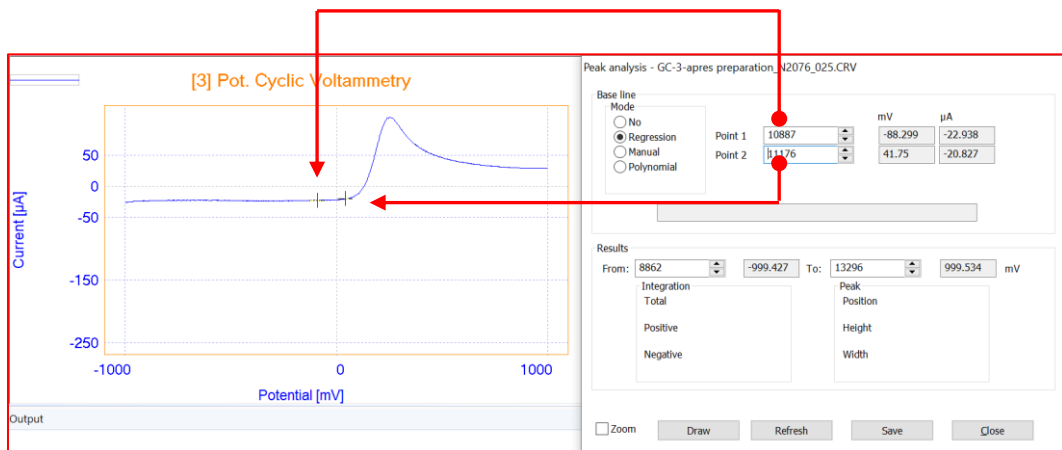


Figure 11: Selecting points for regression line

After that in the "Results" part, the integration area must be selected on the curve as it is explained in page 5.

Figure 7, shows data extracted data through these explanations.



Baseline mode = Regression

3/6

2

Peak analysis - base line = linear regression

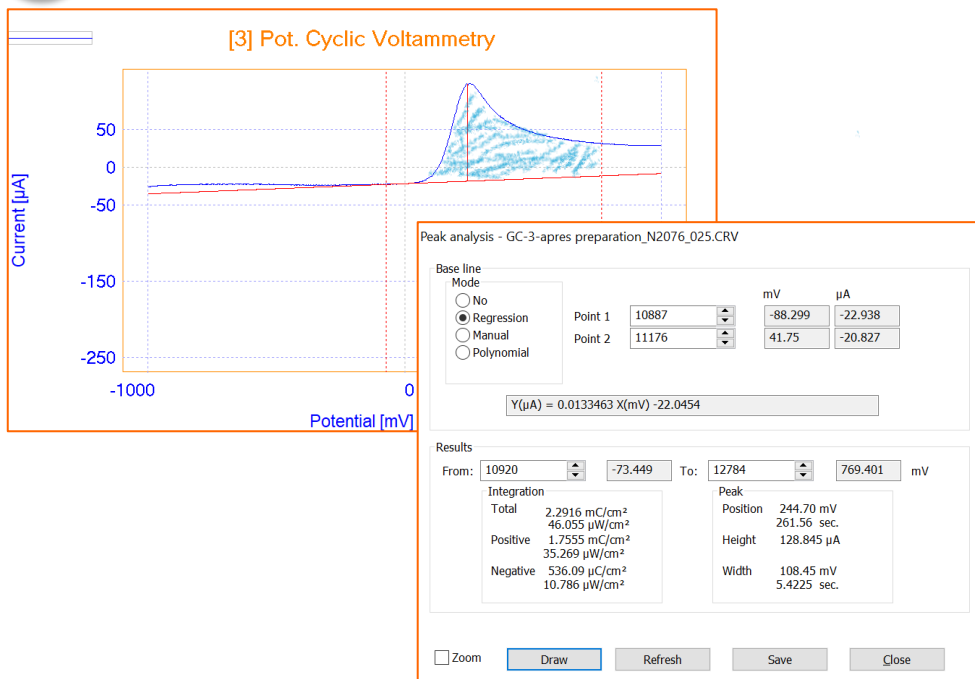


Figure 12: Data about peak analysis and integration could be found in « Results » part of window

Data of the reverse peak can be extracted in the same way as well (Figure 12):

- Selecting 2 points for regression line
- Defining integration area
- Extracting data : Peak (position, height and width) ; Integration data

Note: By clicking on « Refresh » all the process (choosing baseline, defining integration area) could be done from beginning.



Baseline mode = Manual

4/6

3

Peak analysis - base line = Manual

For **Mode** select **Base line = Manual**.

The base line is determined and plotted between 2 selected points of the curve. This mode is adapted to any type of curve peaks.

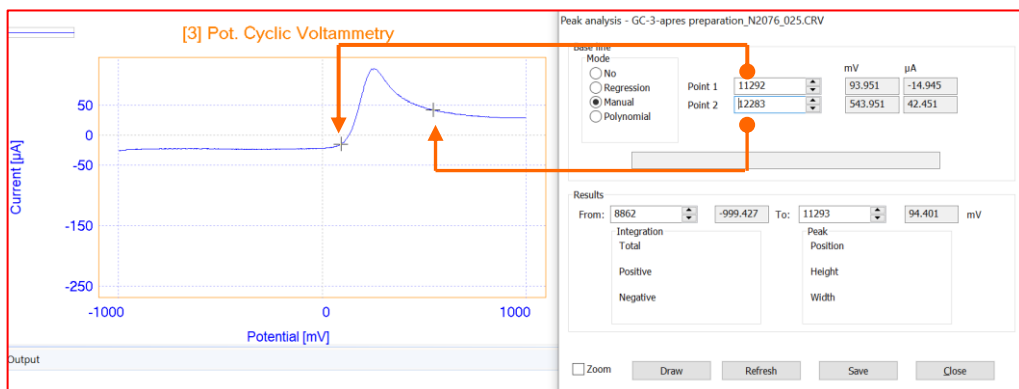


Figure 13: in manual mode, the base line will pass through 2 selected points that is chosen in Point 1 and Point 2 boxes

To select **Point 1**, click in the **Point 1** box in the **Peak analysis** window then click a point on the . The point selected is displayed with a cross.

Select **Point 2** of the curve as the last point of the regression interval like this as well (Figure 13).

The curve points having an abscissa between **Point 1** and **Point 2** will be involved in the **Base line** regression process.

If you want to select another regression interval, click the **Refresh** button then select a new interval.

Again "integration area" could be selected as it is explained on page 5.



Baseline mode = Manual

5/6

3

Peak analysis - base line = Manual

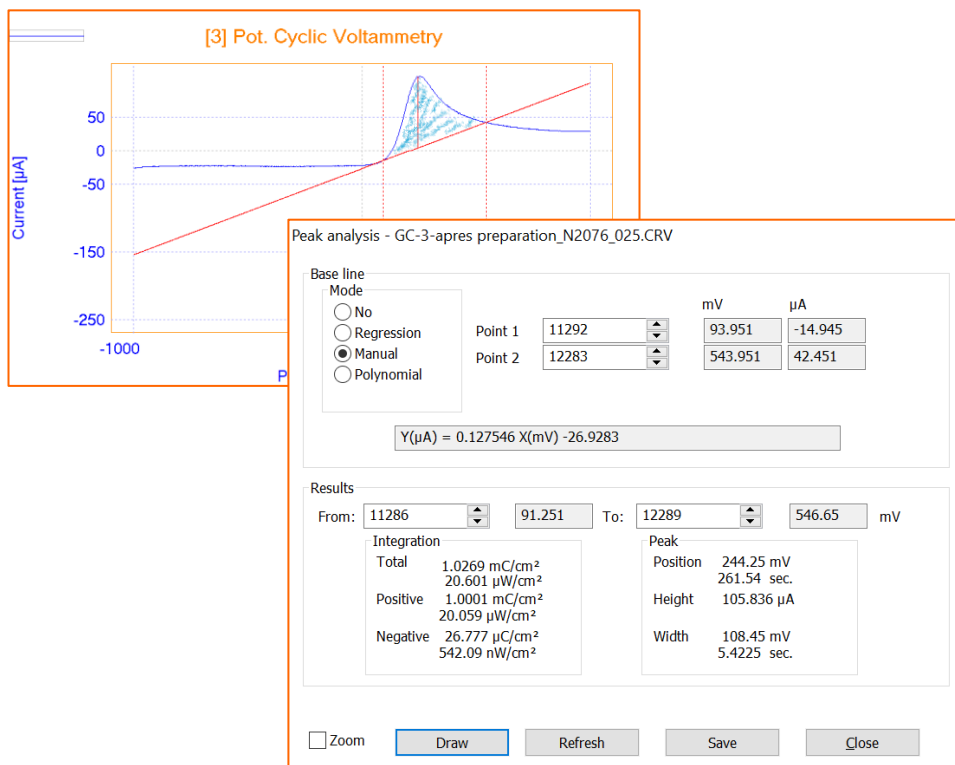


Figure 14: data peak analysis extracted from « manual » regression

Figure 14 shows data extracted from peak analysis window performing « Manuel » regression.



Baseline mode = Polynomial

6/6

4

Peak analysis - base line = Polynomial

For **Mode** select **Base line = Polynomial** a polynomial regression is performed between 2 selected regions of the curve. The curve must show a parabolic region before and after the peak and the parabolic curve found must fit the base of the peak.

The process of selecting point 1 and point 2 for baseline is like Manuel part, just in this case the baseline is not a straight line, it is polynomial regression.

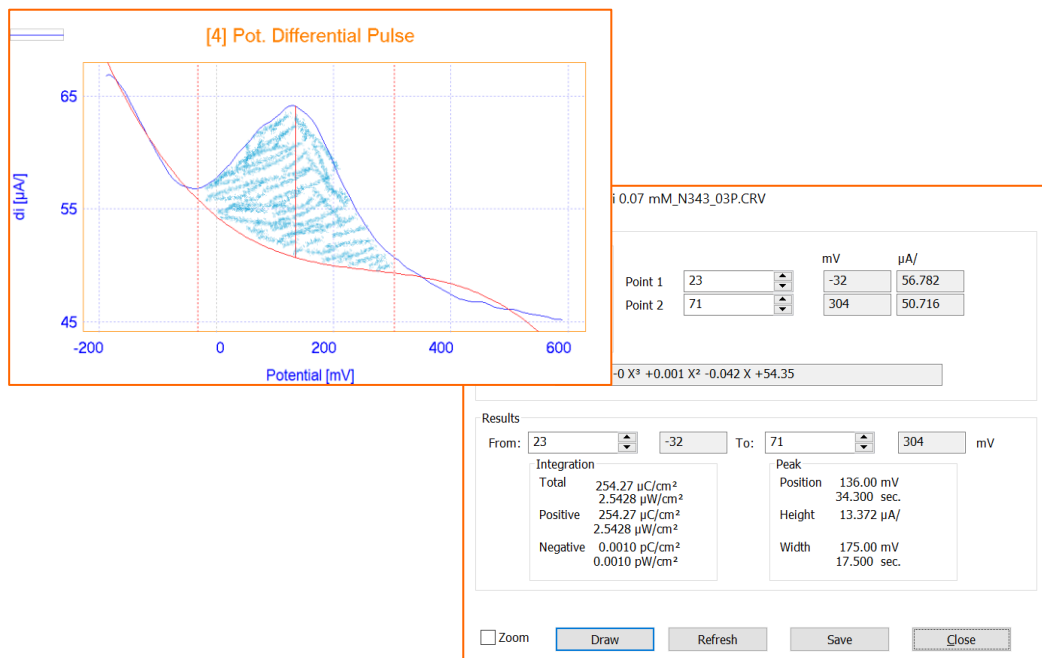


Figure 15: data peak analysis extracted from « Polynomial » regression

Figure 15 shows results extracting from polynomial regression. "Integration area" is selected as like page 5.



About « Results » part

Peak analysis - GC-3-apres preparation_N2076_025.CRV

Base line Mode

☐ No
☐ Regression
☐ Manual
☒ Polynomial

		mV	μA
Point 1	19989	14.751	-22.227
Point 2	21277	597.501	38.78

$Y(\mu A) = -0 X^3 + 0.001 X^2 + 0.089 X - 17.147$

Results

From: 20024 To: 21309 611.9 mV

A

Integration

Total	1.0992 mC/cm ² 22.067 μW/cm ²
Positive	1.1203 mC/cm ² 22.489 μW/cm ²
Negative	-21.08 μC/cm ² -421.6 nW/cm ²

B

Peak

Position	243.80 mV 461.20 sec.
Height	105.95 μA
Width	118.80 mV 5.9390 sec.

☐ Zoom

Figure 16: Peak analysis window after selecting the « Draw » button

The most important part of "Peak analysis" window is "Results". In this part after defining the baseline and the integration area, by clicking on "Draw" button, information about voltammetric peak will be shown:

A) Integration

In this part total area is correspond to all area of the curve. Positive and Negative are related to area above and under the baseline in the integration area.

B) Peak

In this part, Position, Height and Width of the curve will be shown.

INSTRUMENT AND ELECTRODES



Figure 17: OrigaStat OGS100

Electrode setup

Reference Electrode (REF)	Calomel Type: OGR003
Counter Electrode (AUX)	Platinum wire Ø1mm Type: OGV005
Working Electrode (WRK)	Pt tip Ø2mm EMOGTPD2CIAL
Electrolyte	KCl 10 gr/L
Sample	Ferri/Ferro Cyanide 0.01 M
Instrument	OrigaStat OGS100
Software	OrigaMaster 2.4.0.9

REF

Calomel



AUX

Platinum wire Ø1 mm



WRK

Platinum Ø2 mm



OrigaLys ElectroChem SAS

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