📈 Auto Peak Detection & AUC Calculation — Explained Simply

This tool was designed to replicate what researchers already do manually — identify the meaningful part of the PFAS destruction curve (where the signal rises and falls) — and do it automatically and consistently.

Here’s the logic in simple terms:

✅ 1. Finding the Baseline

At the beginning of every experiment, the signal is usually flat — no PFAS breakdown is happening yet. We assume this flat region represents the background noise or baseline.

So, we calculate the average of the first 10 readings to understand what “normal” looks like.

Why?  
This gives us a reference to tell when something *important* starts happening.

✅ 2. Setting a Threshold to Catch the Start of the Signal

Once PFAS starts breaking down, the signal (intensity) goes above normal. But small bumps can happen by chance, so we don’t react to small changes.

We only trigger a “start” when the signal rises by at least 20% above the baseline.

Why 20%?  
It’s a buffer to avoid false triggers due to tiny noise fluctuations.

✅ 3. Finding Where the Peak Begins (Start of Destruction)

The script scans the signal line by line and picks the first point where the signal goes above the 20% threshold.

This is where actual PFAS destruction likely begins.

✅ 4. Finding Where It Ends (Signal Returns to Normal)

After the peak, the signal drops. The script keeps scanning until the signal drops back close to the baseline — within 5% of it.

That’s when we consider the PFAS destruction has ended and the signal is back to its resting level.

✅ 5. Calculating the AUC (Area Under the Curve)

Between the start and end we just found, we compute the area under the curve.

We use the trapezoidal rule to do this. Imagine cutting the curve into thin slices shaped like trapezoids (like squished rectangles). We add up all those trapezoids to estimate the total area.

Why AUC matters?  
This area represents the total amount of CO₂ released during the PFAS breakdown — it gives us a single value that summarizes how much reaction occurred.

Why trapezoids?  
It’s the most reliable and simple way to approximate area when working with curves made from data points.

📊 Visualization

When you use the tool:

* It shows the whole curve (including baseline)
* It highlights the red peak region where PFAS activity was detected
* It shades the area we calculated — which is your AUC

📘 Interpretation: Manual Sum vs. AUC

🔹 Manual Sum of Intensities (~7.000e-10)

The manual calculation involves directly summing the intensity values over the visible peak region.

This gives a rough estimate of total signal strength, but it does not account for how long the signal lasted.

Units are simply in Torr (or arbitrary intensity units), not Torr·seconds, and the result cannot be used in quantitative comparisons or scientific modeling.

👉 Think of this as a quick visual score, not a scientific metric.

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🔹 Automated AUC (1.1282e-06 unit·s)

The AUC calculated using the trapezoidal rule represents the total area under the intensity-time curve.

It correctly considers both the signal magnitude and how long it was sustained, giving a result in Torr·seconds (or signal units × time).

This value provides a quantitative, reproducible measure of total PFAS-related gas release, and is suitable for comparison across experiments and for reporting purposes.

👉 This is the physically meaningful metric that reflects actual PFAS destruction.

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✅ Final Message for Researchers

While the manual sum gives a helpful estimate, the AUC is a scientifically accurate measure of total PFAS decomposition signal.

It enables standardized comparisons across runs and reflects both the magnitude and duration of the signal.