

## ACQUITY UPLC PDA Analysis of Biocides (Part 2) Pass or Fail Custom Calculation

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### Abstract

This application note describes the benefits of using a simple custom calculation created to determine if the biocide concentration in a sample passes or fails user set criteria. This type of custom calculation eliminates the need for manual calculation and prevents potential human errors.

### Benefits

- Increases laboratory productivity by enabling the high resolution, high sensitivity separations of biocides in three minutes.
  - Helps improve decision-making, and ensure product quality by rapidly extracting and delivering critical QC data based on user criteria.
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### Introduction

Making more informed decisions in less time is essential in today's Cosmetics, Personal Care, and Food analytical laboratories. Whether you work in method development, quality assurance, new product development, or testing for biocides, you seek a productivity edge. Waters ACQUITY UPLC System provides

that edge, enabling high resolution, high sensitivity biocide separations in three minutes.<sup>1</sup> Better quality information on product biocide levels can now be generated far more rapidly than with traditional HPLC methods. UPLC combined with Empower 3 Software can effectively run separations, analyze data, and report results automatically. With the custom calculation function of Empower 3, raw data can be converted into the required format and the critical results can be used quickly by decision-makers to further enhance productivity. This application note describes the benefits of using a simple custom calculation created to determine if the biocide concentration in a sample passes or fails user set criteria. This type of custom calculation eliminates the need for manual calculation and prevents potential human errors. The ability to deliver critical information with speed and accuracy can help manufacturers reduce failed products, avoid product recalls and liability litigations. An example detailing the creation of a custom calculation shown in the note is provided in the Experimental section.

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## Experimental

### QC Criteria Example for Biocide

Kathon amount < 4.85 ppm: Fail

Kathon amount > 5.15 ppm: Fail

Kathon amount from 4.85 ppm to 5.15 ppm: Pass

### Create a Custom Field Calculation Method with Empower 3

1. Click Configure System to open the Configuration Manager window, click Projects in the tree.
2. Select and highlight the working project, then right click the highlighted project.
3. Select Properties to open Project Properties window.
4. Click the Custom Fields tab, then click New to open New Custom Field Wizard: Data and Type Selection window.
5. Select the Field Type: Peak, and Data Type: Enum, then click Next to open Source Selection window.
6. Select Data Source: Calculated, Sample Type: Unknown, Peak Type: Group Only, then click Next to open Formula Entry window (Figure 1).

7. In the Operations list, double-click ENUM( and LT(.
8. In the Fields list, double-click Amount, in the formula workspace, enter ,4.85),
9. In the Operations list, double-click LTE(.
10. In the Fields list, double-click Amount, in the formula workspace, enter ,5.15).
11. In the Operations list, double-click GT(.
12. In the Fields list, double-click Amount, in the formula workspace, enter ,5.15)).
13. Click Next to open Translation Definition Table.
14. Enter Fail next to 0, Pass next to 1, Fail next to 2, click Next to open Name Entry window. (Note: you can enter Pass/Fail in another language).
15. Enter a name for the custom field in the Field Name text box: Pass or Fail, click Finish.



Figure 1. Formula Entry window.

### Create Named Groups in the Processing Method

1. From Processing Method window, select the Named Groups tab.
2. Enter Kathon in the Name text box
3. Select the option of Sum Peaks, Curve or Sum Peaks for Quantitation.
4. Drag 1a and 1b from Single Peak Components into the tree of Kathon as shown in Figure 2.

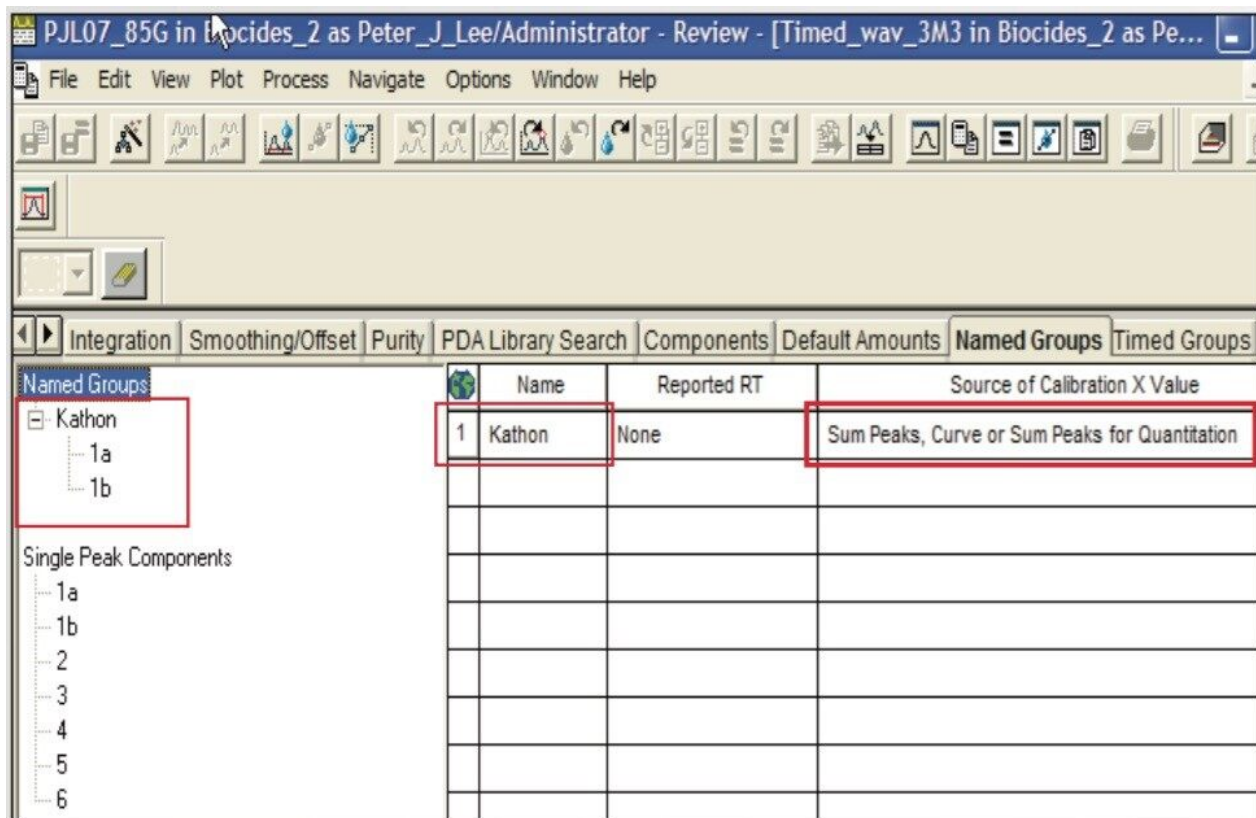


Figure 2. Processing method window.

## Sample preparation and UPLC Methods

The methods used are the same as described previously<sup>1</sup> Analytes are Kathon CG/ICP [containing 0.4% 2-methyl-4-isothiazolin-3-one (1a), 1.2% 5-chloro-2-methyl-4-isothiazolin-3-one (1b)], Carbendazim (2), Benzisothiazol-3(2H)-one (3), 2-phenoxyethanol (4), Benzoic Acid (5), and Methylparaben (6).

## Results and Discussion

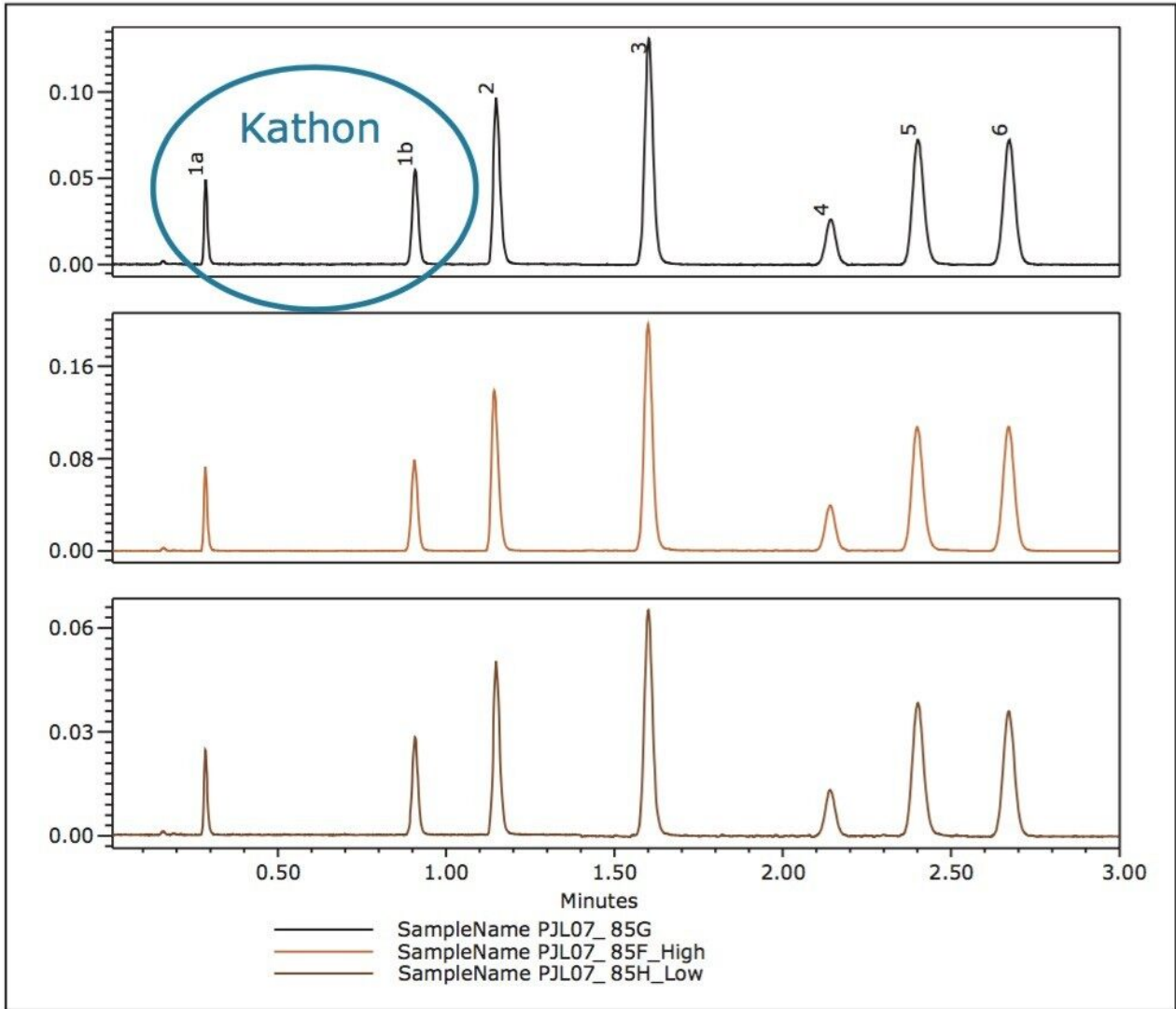


Figure 3. UPLC chromatograms of three biocide samples.

Figure 3 shows chromatograms of three biocide samples. There are seven well-resolved peaks in each sample. 1a and 1b are the two active ingredients of Kathon. The amount of 1a and 1b in each sample can be calculated automatically in Empower 3 Software from calibration curves as described previously.<sup>1</sup>

For this discussion, a passable QC level for the Kathon biocide is the range 4.85 ppm to 5.15 ppm. To determine Pass or Fail biocide status of each sample, the amount of total Kathon must be calculated, that is the sum of 1a and 1b, and the result must be compared with the QC criteria.

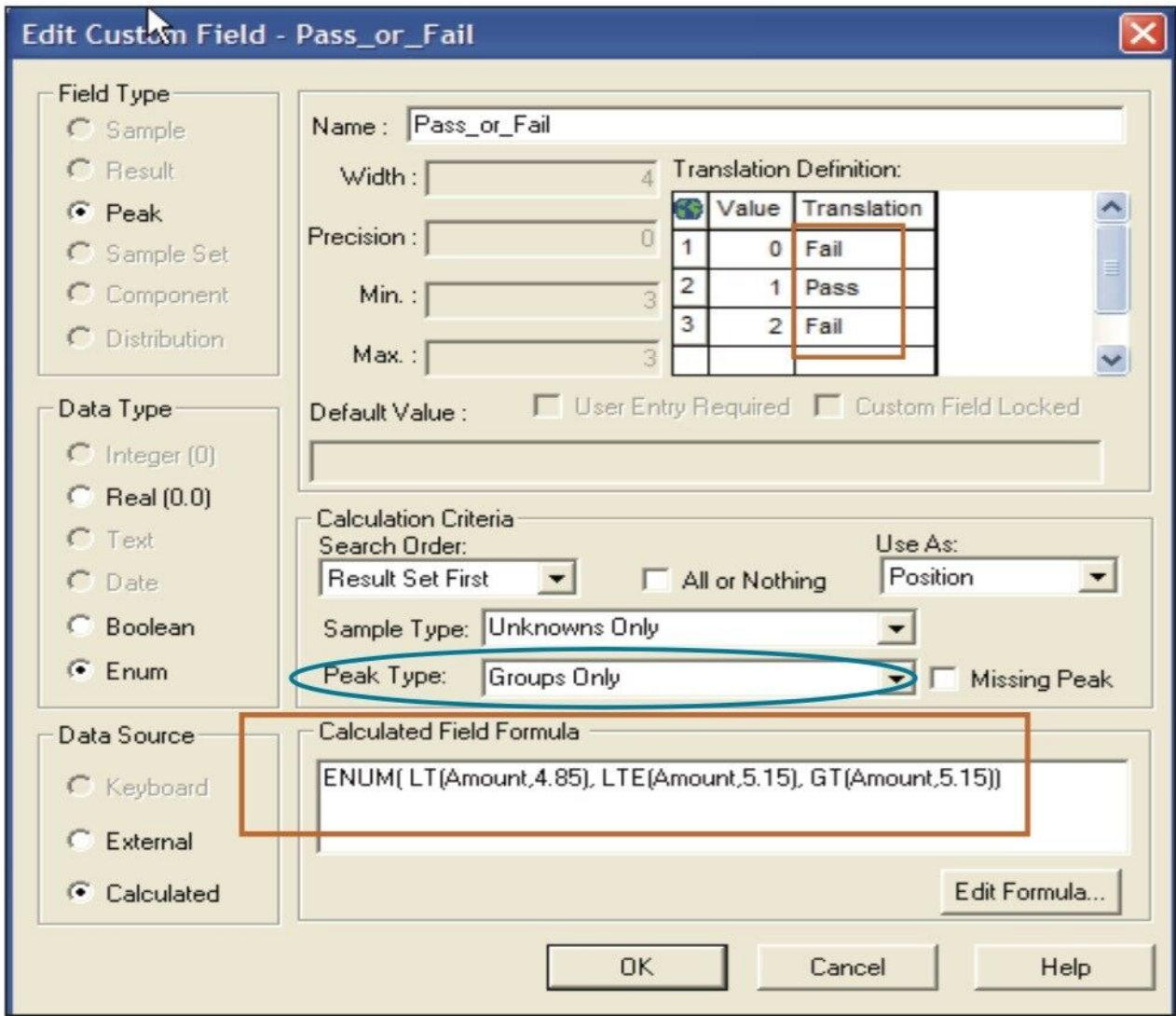


Figure 4. Custom Field formula.

Figure 4 shows the Custom Field Formula described in the Experimental section. The QC Pass or Fail criteria is based on the Kathon biocide content ( $5 \text{ ppm} \pm 3\%$ ).

Using both the Named Groups and Custom Field calculation functions, Empower can be set up to automatically calculate and report the quantity of Kathon in each sample and determine if the sample met the QC criteria (Table 1). In an enterprise environment, the critical Pass or Fail results can be e-mailed to product and plant management. These advanced functions of Empower eliminate the need for manual calculations, which saves time and reduces errors.

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	SampleName	Component	Amount (ppm)	Pass/Fail
1	PJL07_85G	Kathon	5.03	Pass
2	PJL07_85H_Low	Kathon	2.57	Fail
3	PJL07_85F_High	Kathon	7.43	Fail

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Table 1. Biocides Test: Pass or Fail.

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## Conclusion

Hundreds of biocide containing product samples can be automatically analyzed on a daily basis using the Waters ACQUITY UPLC PDA System with Empower 3 Software. Critical product QC information can be accurately extracted and rapidly delivered based on user set criteria. The method represents a significant productivity enhancement relative to the manual verification of QC biocide data. It can be very effective for food, cosmetics and personal care manufacturers, and formulators to have a report with a simple Pass or Fail for the sample displayed.

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## References

1. PJ Lee, AJ Di Gioia, ACQUITY UPLC/PDA Analysis of Biocides (Part 1), Waters application note no. 720001832 2006.

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## Featured Products

[ACQUITY UPLC System <https://www.waters.com/514207>](https://www.waters.com/514207)

[ACQUITY UPLC PDA Detector <https://www.waters.com/514225>](https://www.waters.com/514225)

[Empower 3 Chromatography Data Software <https://www.waters.com/10190669>](https://www.waters.com/10190669)



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