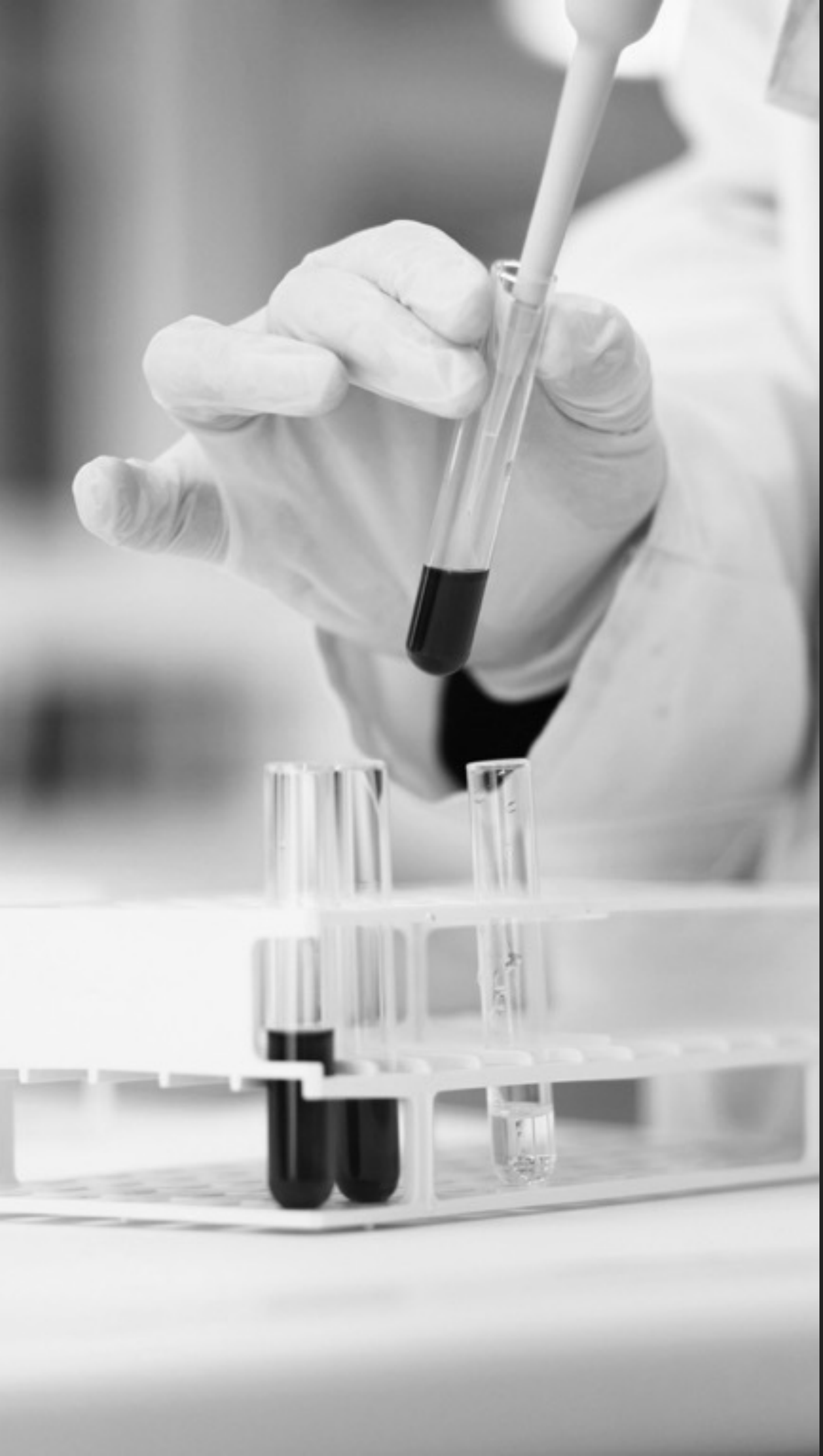


NMR 統計分析工具

BATMAN

模型

- BATMAN 使用貝氏統計模型來分析。

$$\mathbf{y} = \mathbf{y}^{c} + \mathbf{y}^{u} + \varepsilon, \quad \varepsilon \sim N(0, \mathbf{I}/\lambda)$$

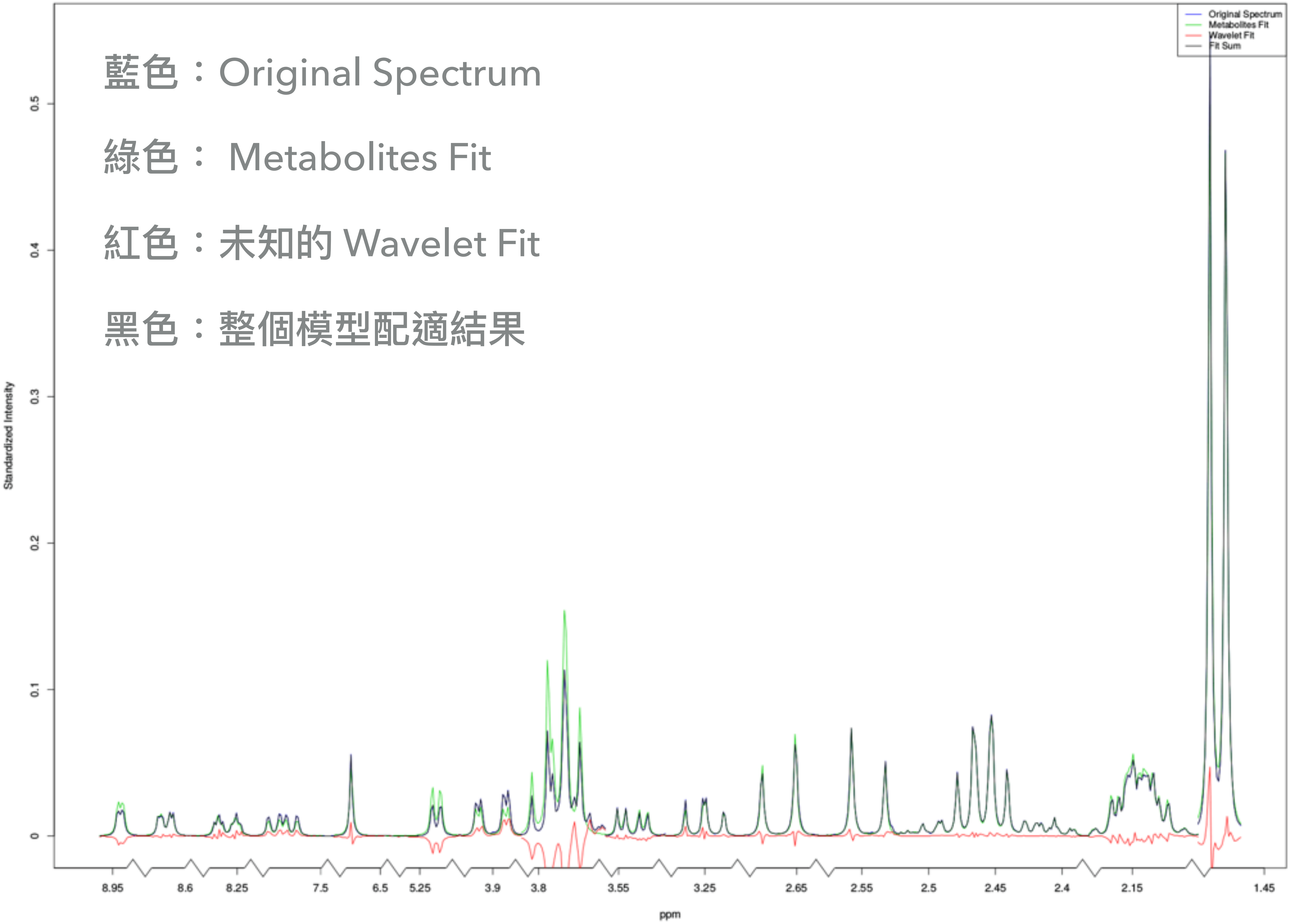
$\mathbf{y}^{c}$: catalogued metabolites

$\mathbf{y}^{u}$: uncatalogued metabolites

使用 BATMAN

```
# 安裝 BATMAN 套件

install.packages("doSNOW")

install.packages(“plotrix")

install.packages(“batman", repos=“http://R-Forge.R-project.org”)

# 載入 BATMAN 套件

library(batman)

# 使用 BATMAN 套件

bm <- batman()
```

NMR Spectrum 2: X2



藍色：Original Spectrum

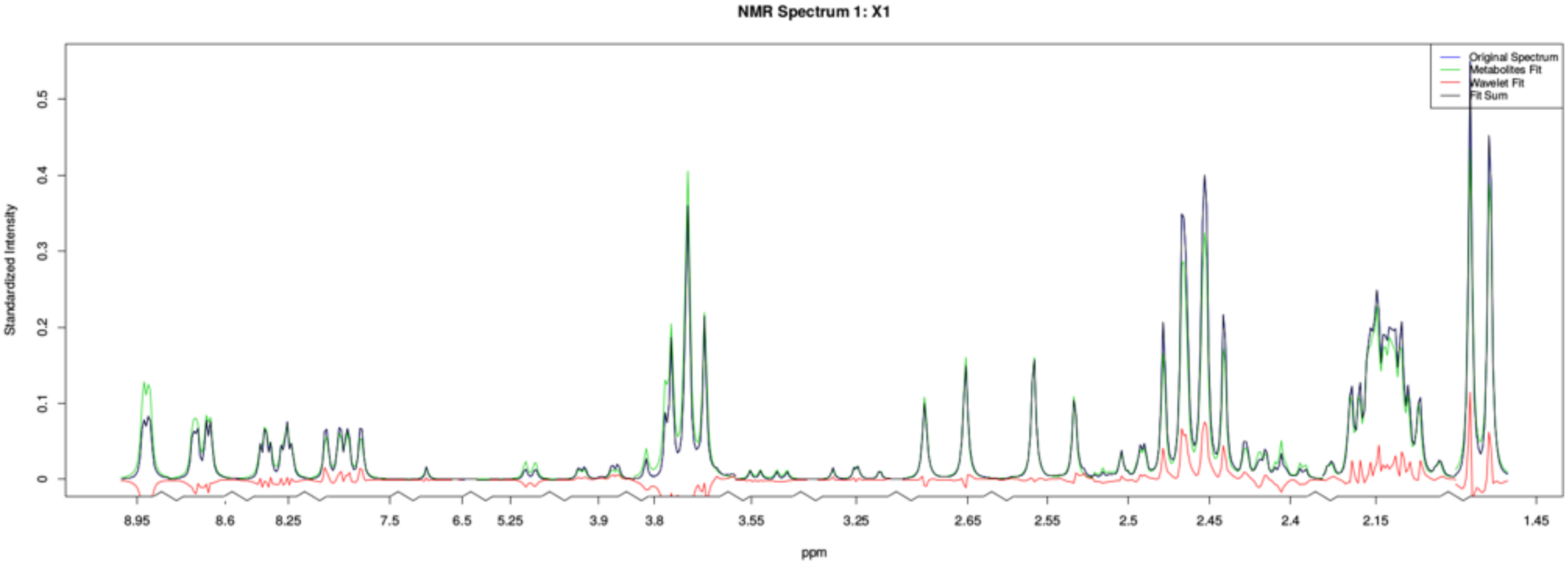
綠色： Metabolites Fit

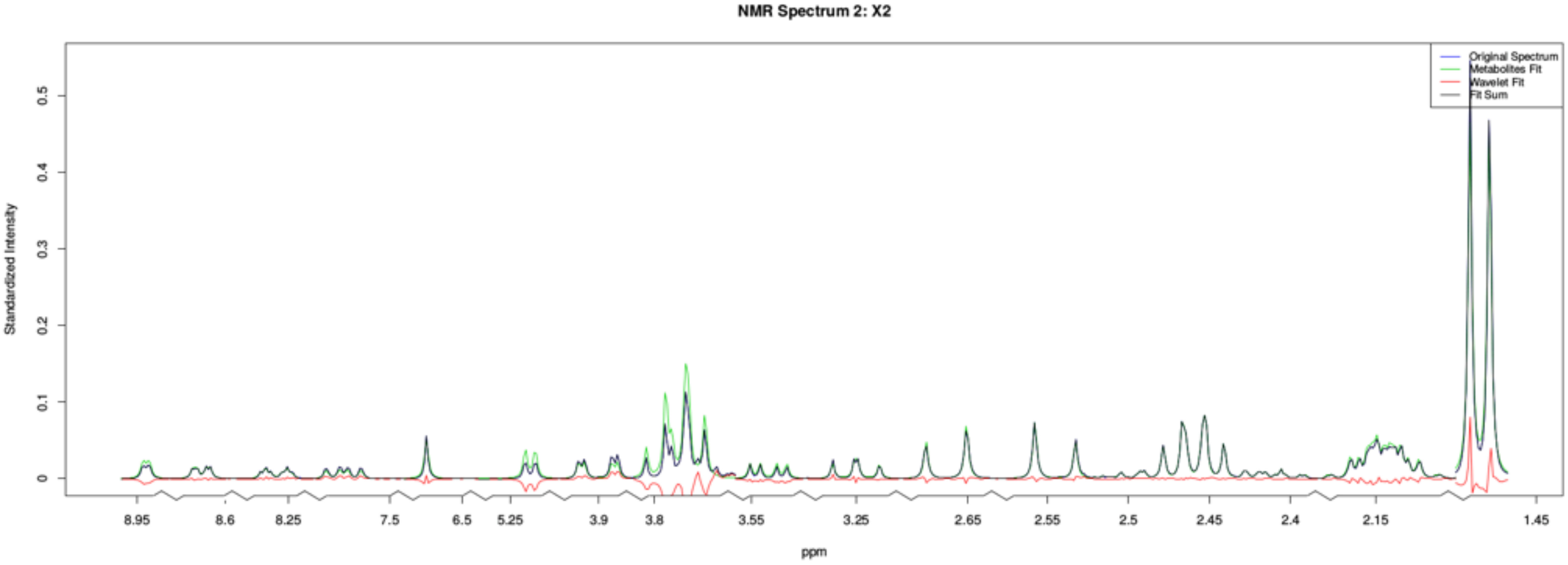
紅色：未知的 Wavelet Fit

黑色：整個模型配適結果

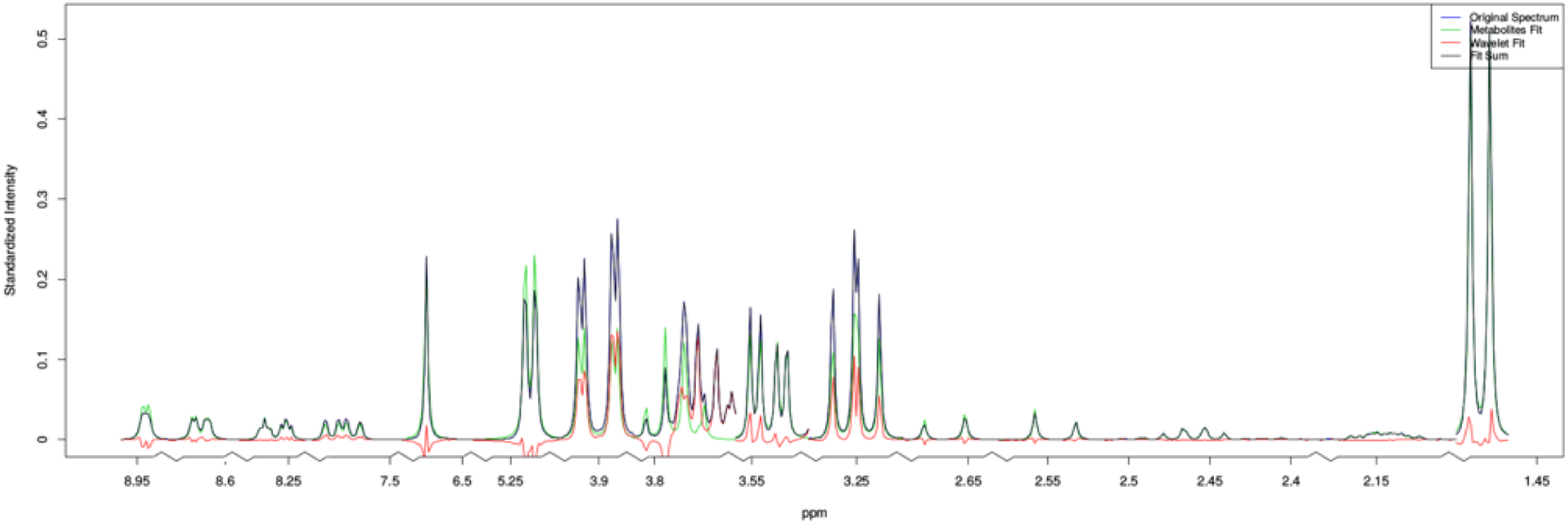
多頻譜（平行計算）

```
% runBATMAN/BatmanInput/batmanOptions.txt 設定檔

specNo - Ranges of spectra number to be included (e.g. 1,3-4 etc.): 1-4

paraProc - No of parallel processes (multicores) (only 1 core will be used for single spectrum): 4

nItBurnin - Number of burn-in iterations: 7000

nItPostBurnin - Number of post-burn-in iterations: 1000

# 重新執行 R 指令

bm <- batman()
```

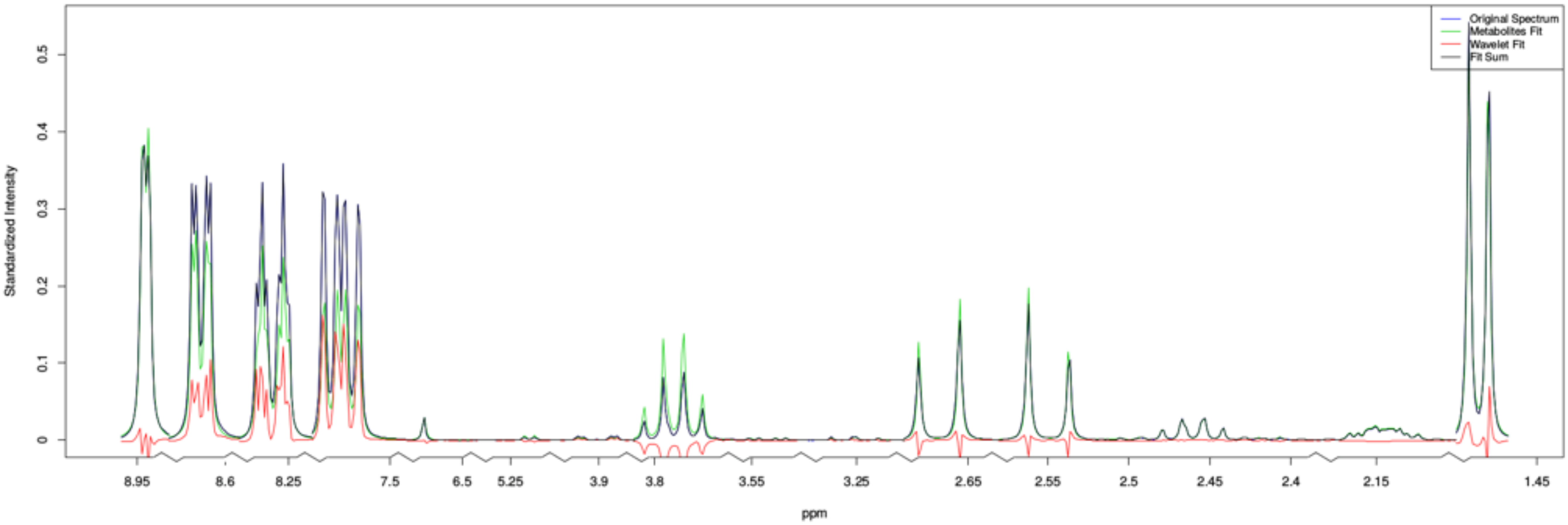

NMR Spectrum 1: X1

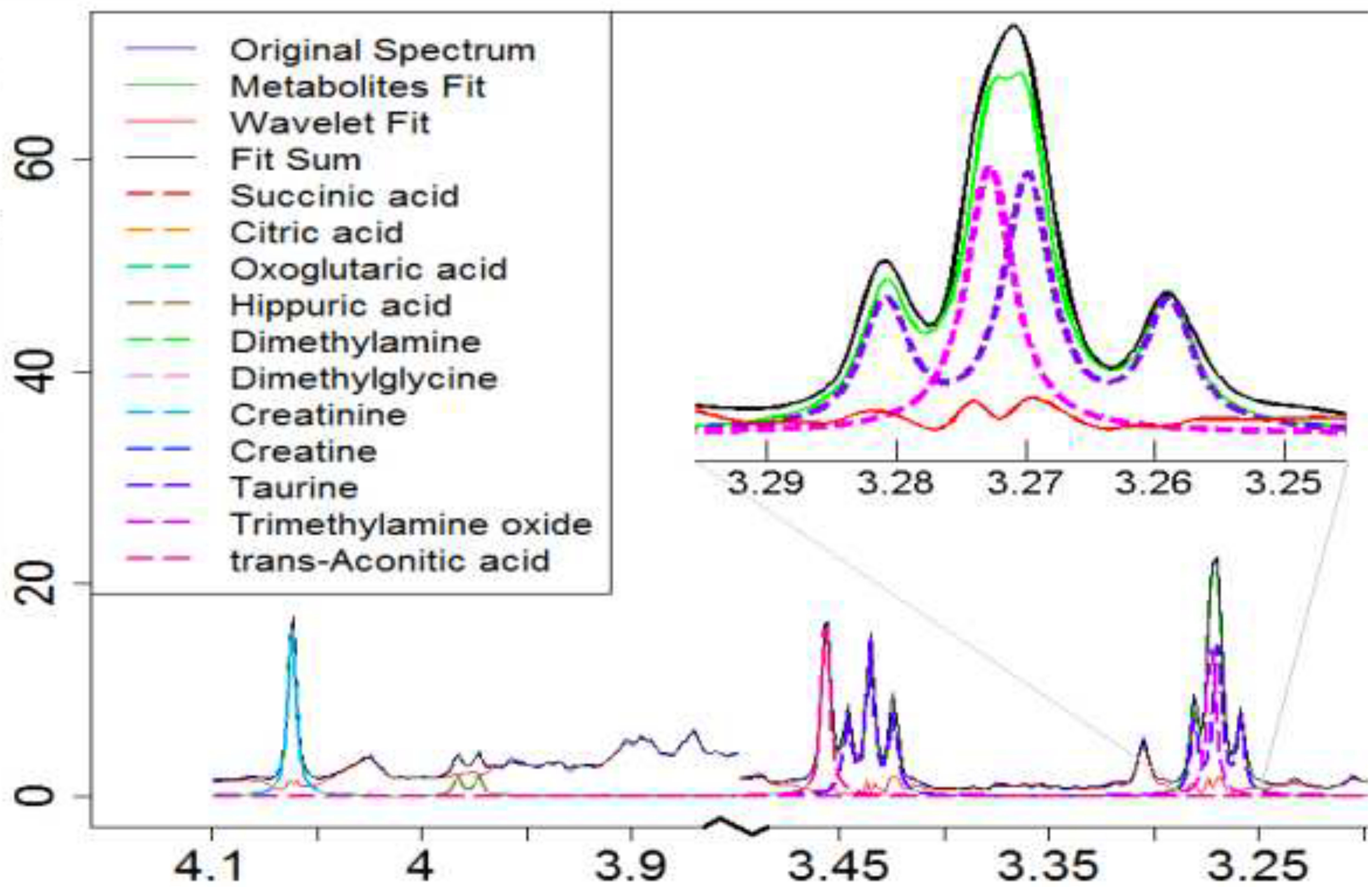

NMR Spectrum 2: X2

NMR Spectrum 3: X3



NMR Spectrum 4: X4




Original Spectrum
Metabolites Fit
Wavelet Fit
Fit Sum
Succinic acid
Citric acid
Oxoglutaric acid
Hippuric acid
Dimethylamine
Dimethylglycine
Creatinine
Creatine
Taurine
Trimethylamine oxide
trans-Aconitic acid
60
40
20
0
4.1
4
3.9
3.45
3.35
3.25
3.29
3.28
3.27
3.26
3.25