C12_Sample_1 , Compound: X40H77NO8P

Fitted X Abundance: (1.074 +/− 0.007) %

Experimental pattern   •   Theoretical pattern

Normalised intensity

Target mass

C12_Sample_2 , Compound: X40H77NO8P

Fitted X Abundance: (1.081 +/− 0.004) %

Experimental pattern   •   Theoretical pattern

Normalised intensity

Target mass

C12_Sample_3 , Compound: X40H77NO8P

Fitted X Abundance: (1.081 +/− 0.004) %

Experimental pattern   •   Theoretical pattern

Normalised intensity

Target mass
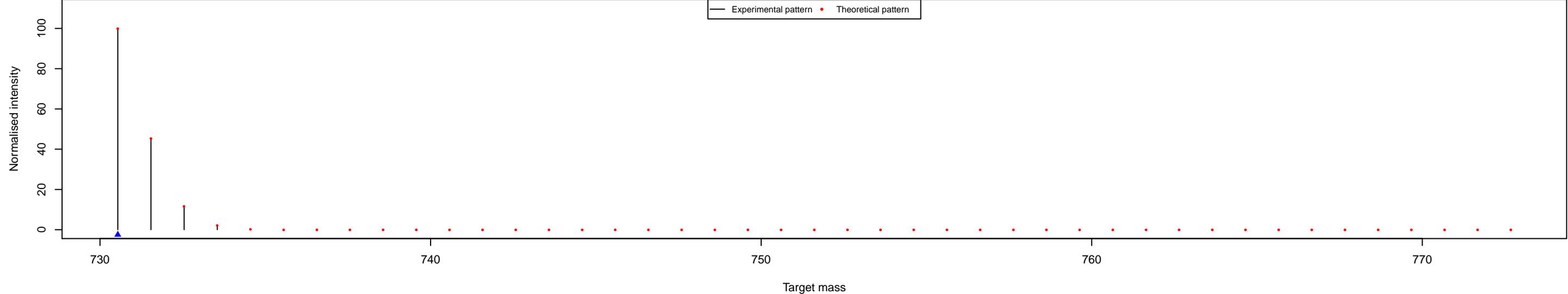
C12_Sample_4 , Compound: X40H77NO8P
Fitted X Abundance: (1.080 +/− 0.005) %
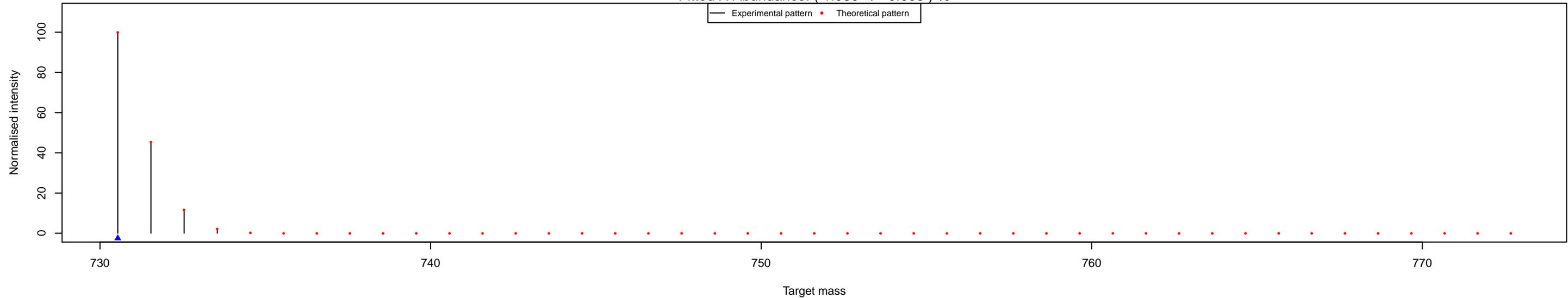
C13_Sample_1 , Compound: X40H77NO8P
### Fitted X Abundance: (98.942 +/− 0.009) %
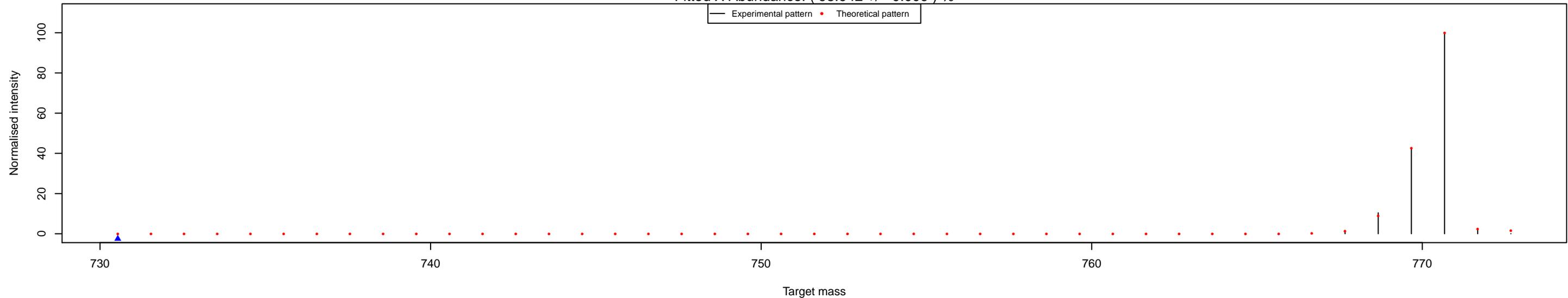

C13_Sample_2 , Compound: X40H77NO8P
### Fitted X Abundance: (98.947 +/− 0.008) %

C13_Sample_3 , Compound: X40H77NO8P

Fitted X Abundance: (98.936 +/− 0.006) %

— Experimental pattern · Theoretical pattern

Target mass

C13_Sample_4 , Compound: X40H77NO8P

Fitted X Abundance: (98.945 +/− 0.008) %

— Experimental pattern · Theoretical pattern

Target mass
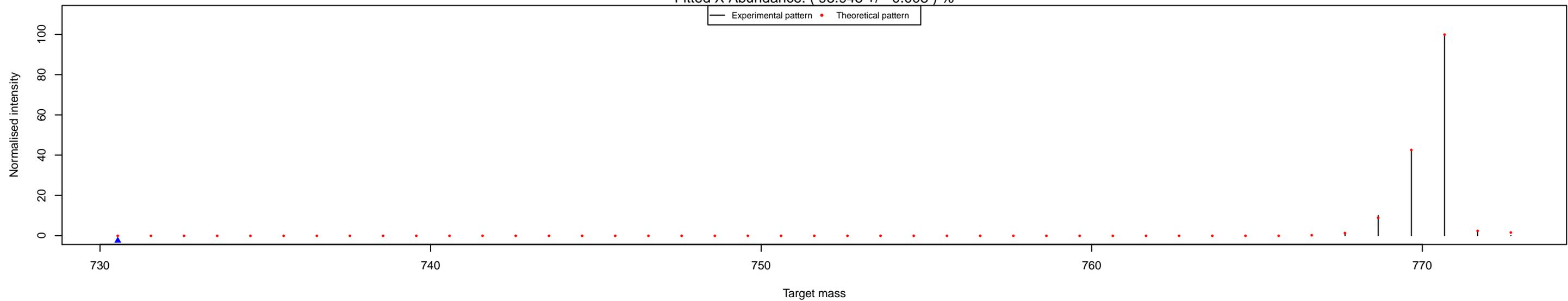
C12_Sample_1 , Compound: X40H79NO8P

Fitted X Abundance: (1.081 +/− 0.007) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
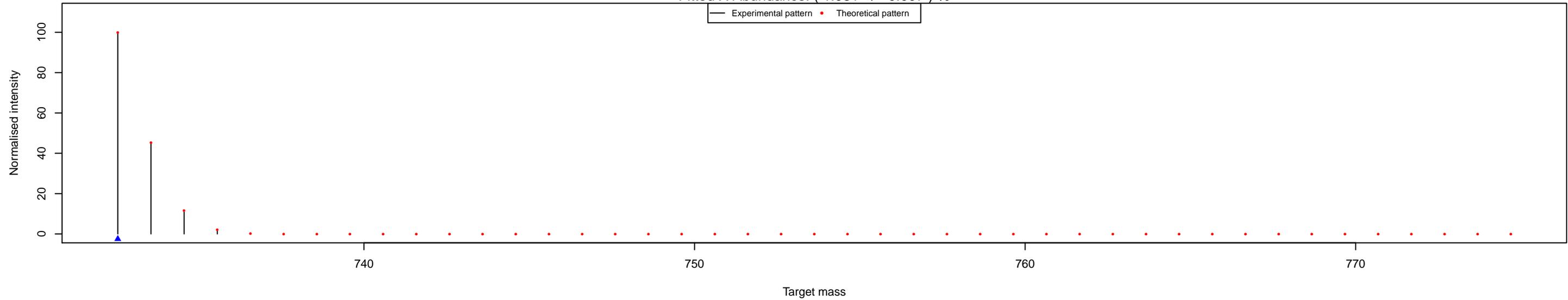
C12_Sample_2 , Compound: X40H79NO8P

Fitted X Abundance: (1.070 +/− 0.007) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
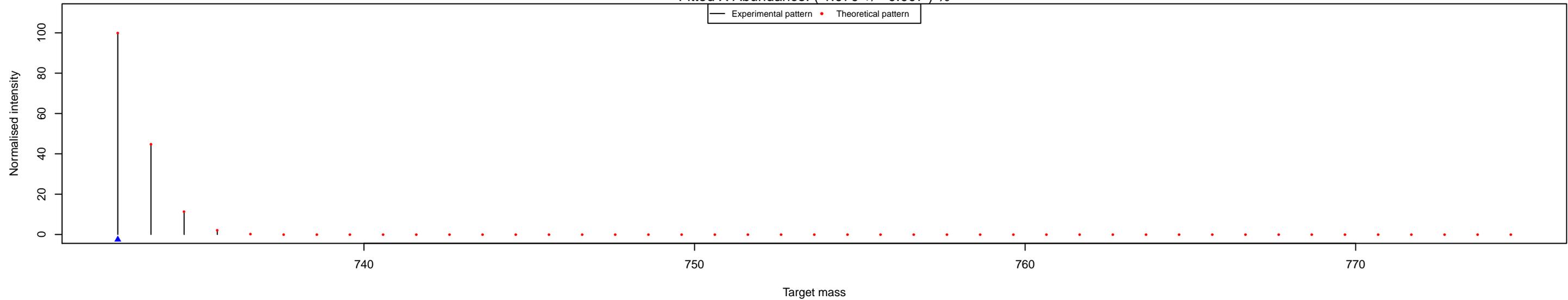
C12_Sample_3 , Compound: X40H79NO8P

Fitted X Abundance: (1.056 +/− 0.007) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
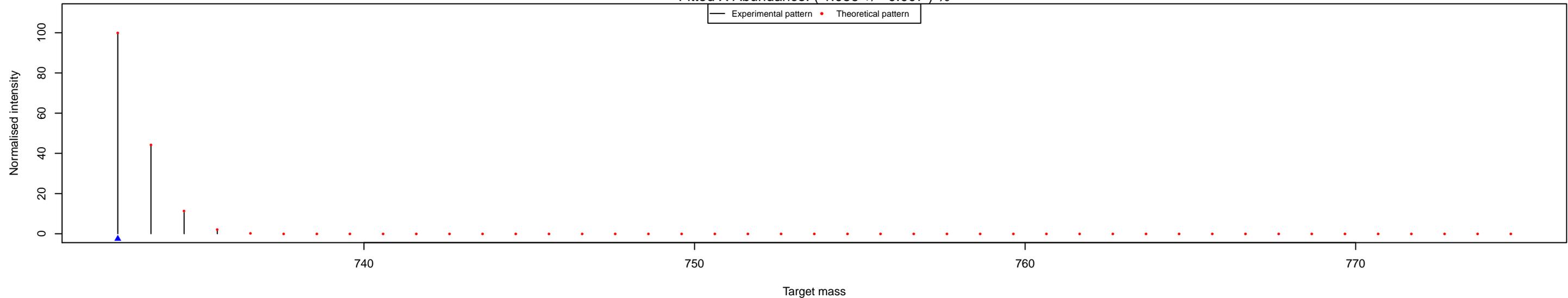
C12_Sample_4 , Compound: X40H79NO8P

Fitted X Abundance: (1.069 +/− 0.007) %

Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
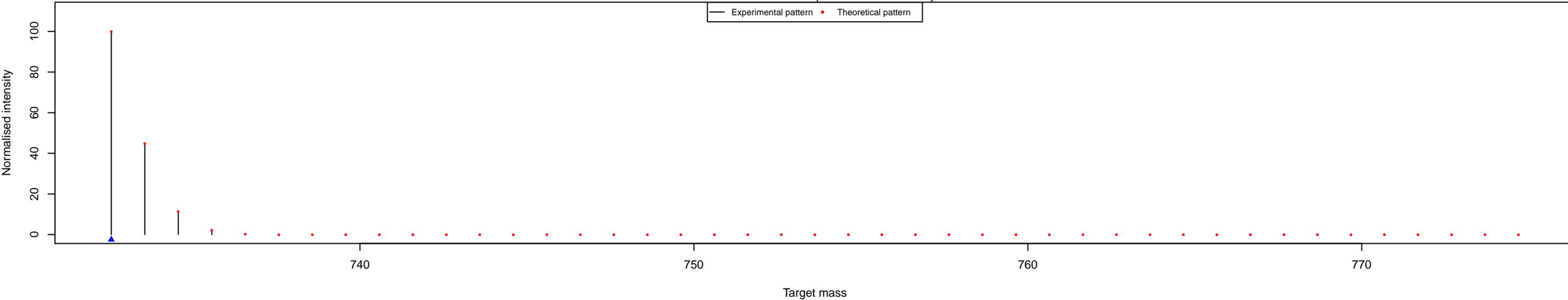
C13_Sample_1 , Compound: X40H79NO8P

Fitted X Abundance: (98.963 +/− 0.007) %

Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
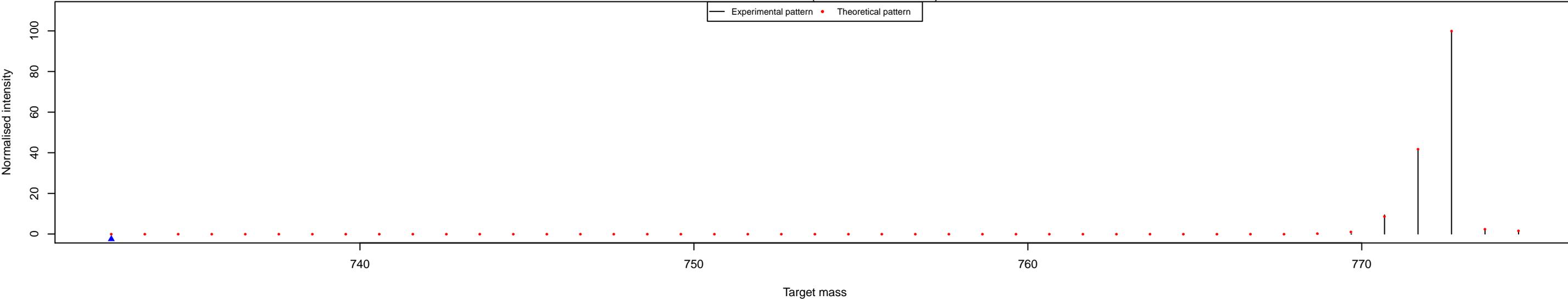
C13_Sample_2 , Compound: X40H79NO8P

Fitted X Abundance: (98.954 +/− 0.006) %

Experimental pattern • Theoretical pattern
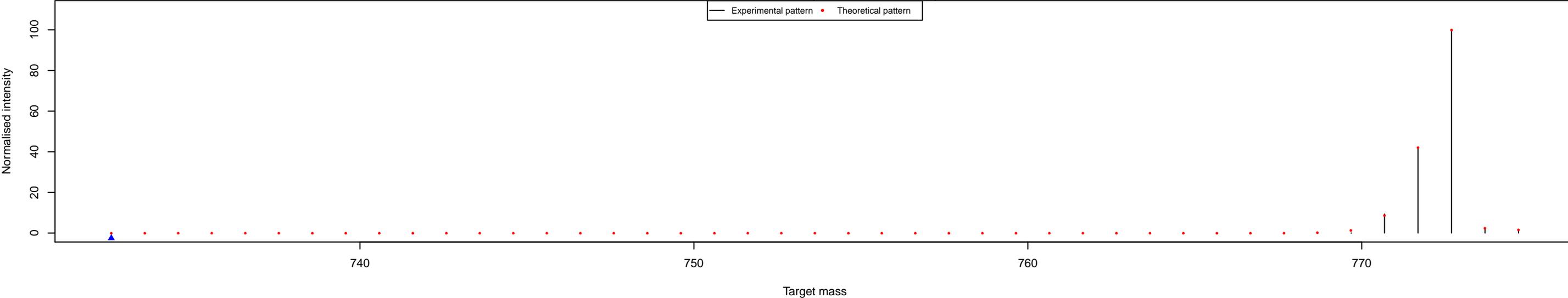
Normalised intensity

Target mass

C13_Sample_3 , Compound: X40H79NO8P

Fitted X Abundance: (98.971 +/− 0.005) %

— Experimental pattern • Theoretical pattern

C13_Sample_4 , Compound: X40H79NO8P
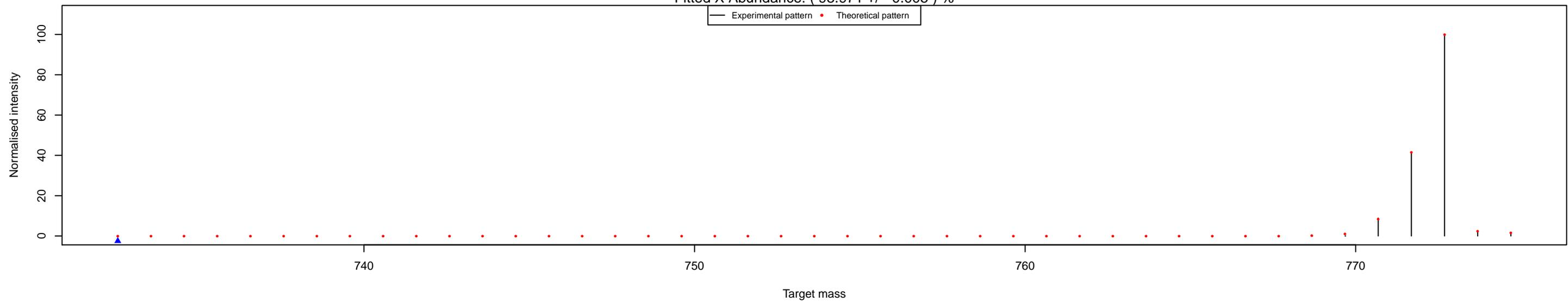
Fitted X Abundance: (98.965 +/− 0.005) %

— Experimental pattern • Theoretical pattern
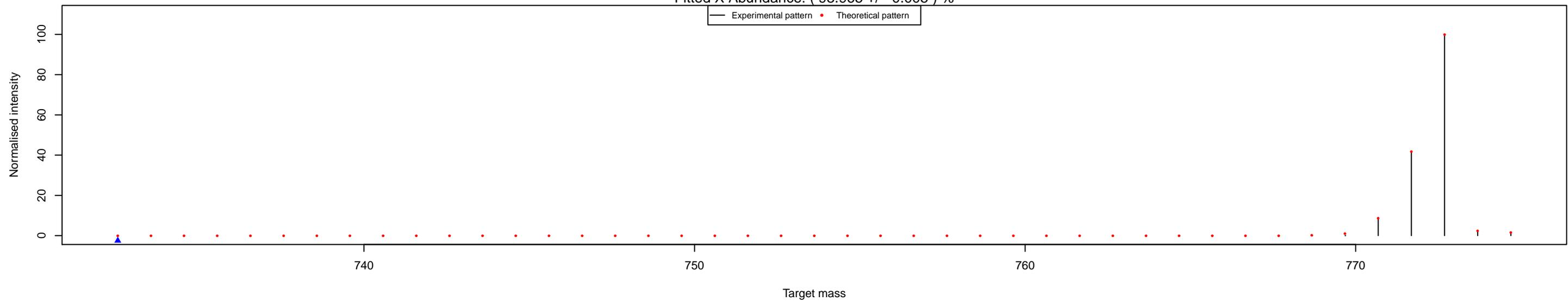
C12_Sample_1 , Compound: X42H81NO8P

Fitted X Abundance: (1.079 +/− 0.007) %

Experimental pattern • Theoretical pattern
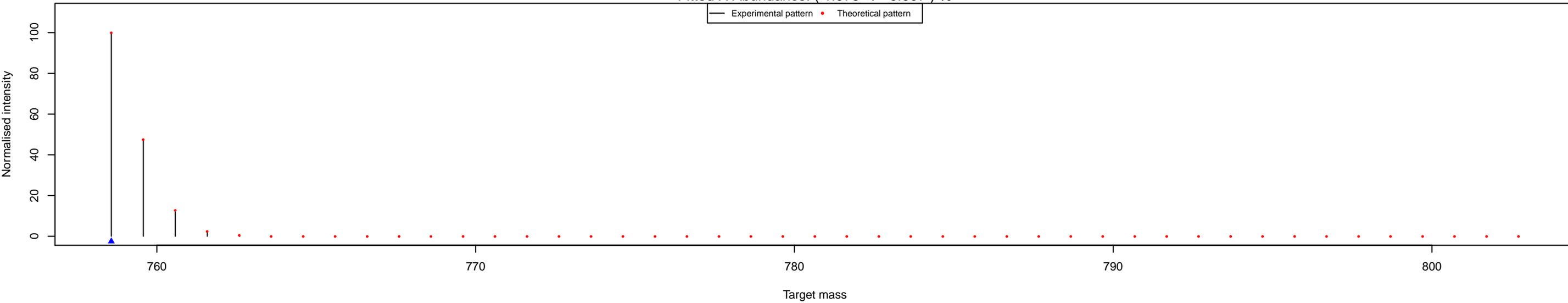
C12_Sample_2 , Compound: X42H81NO8P

Fitted X Abundance: (1.081 +/− 0.006) %

Experimental pattern • Theoretical pattern
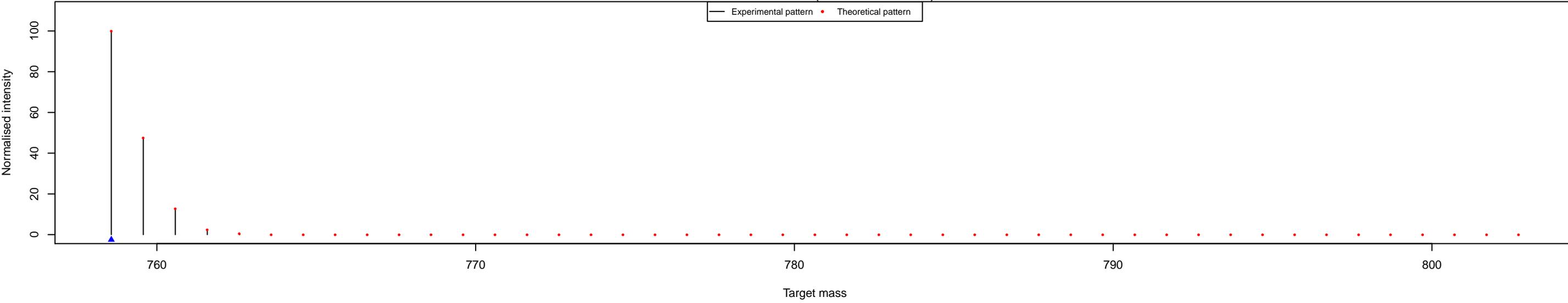
C12_Sample_3 , Compound: X42H81NO8P

Fitted X Abundance: (1.082 +/− 0.004) %

Experimental pattern • Theoretical pattern
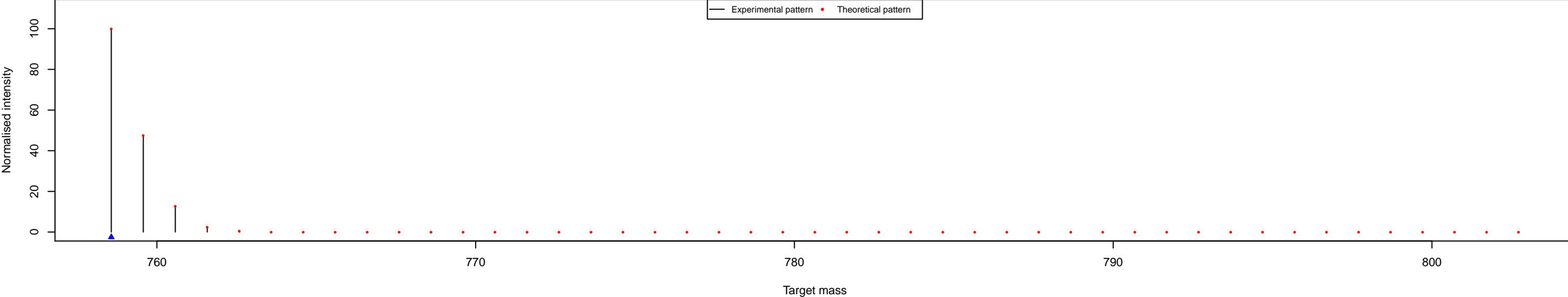
C12_Sample_4 , Compound: X42H81NO8P

Fitted X Abundance: (1.076 +/− 0.008) %

Experimental pattern • Theoretical pattern
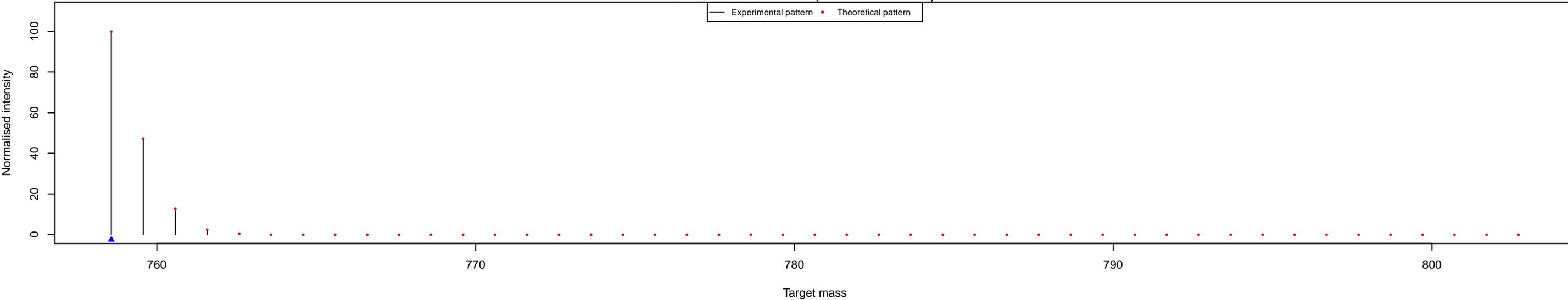
C13_Sample_1 , Compound: X42H81NO8P

Fitted X Abundance: (98.941 +/− 0.008) %

Experimental pattern • Theoretical pattern
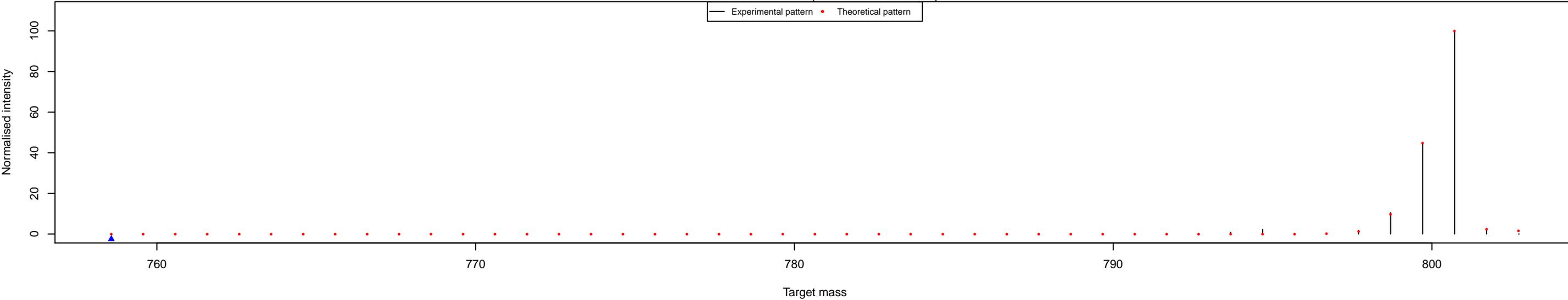
C13_Sample_2 , Compound: X42H81NO8P

Fitted X Abundance: (98.939 +/− 0.010) %

Experimental pattern • Theoretical pattern
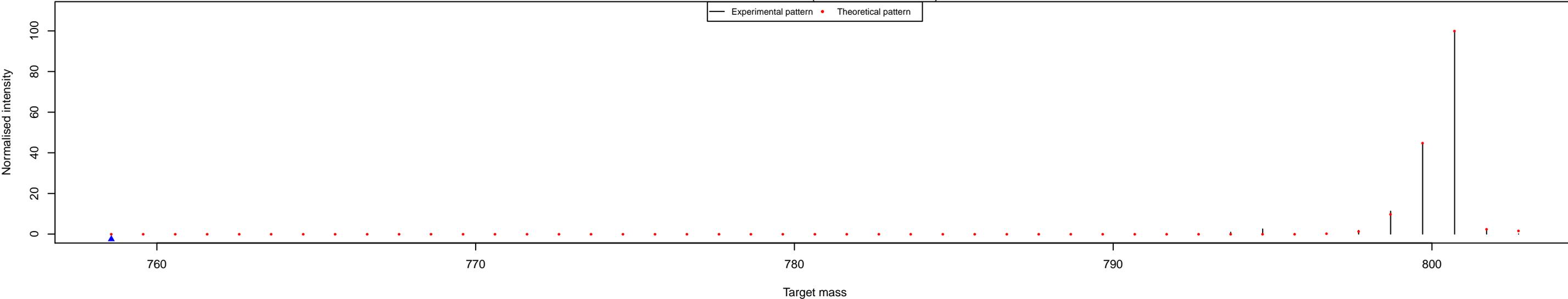
C13_Sample_3 , Compound: X42H81NO8P

Fitted X Abundance: (98.945 +/− 0.009) %
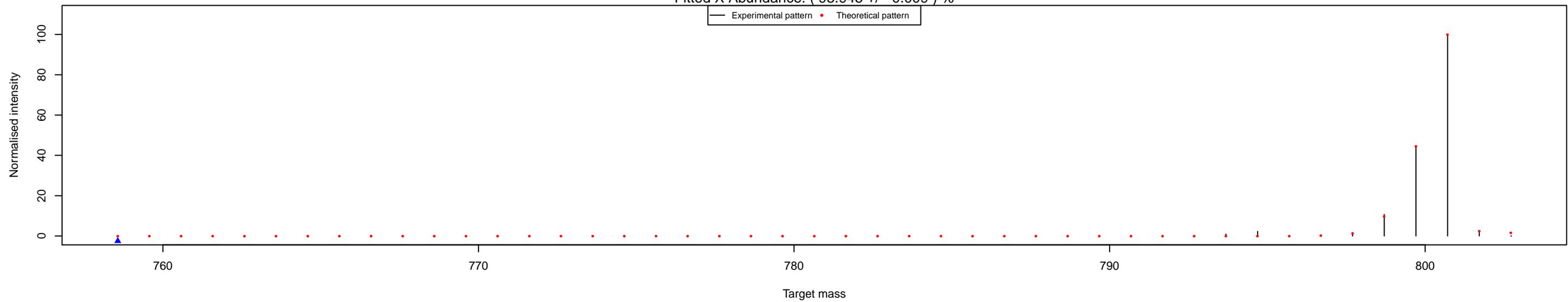
Experimental pattern • Theoretical pattern

C13_Sample_4 , Compound: X42H81NO8P

Fitted X Abundance: (98.936 +/− 0.009) %

Experimental pattern • Theoretical pattern
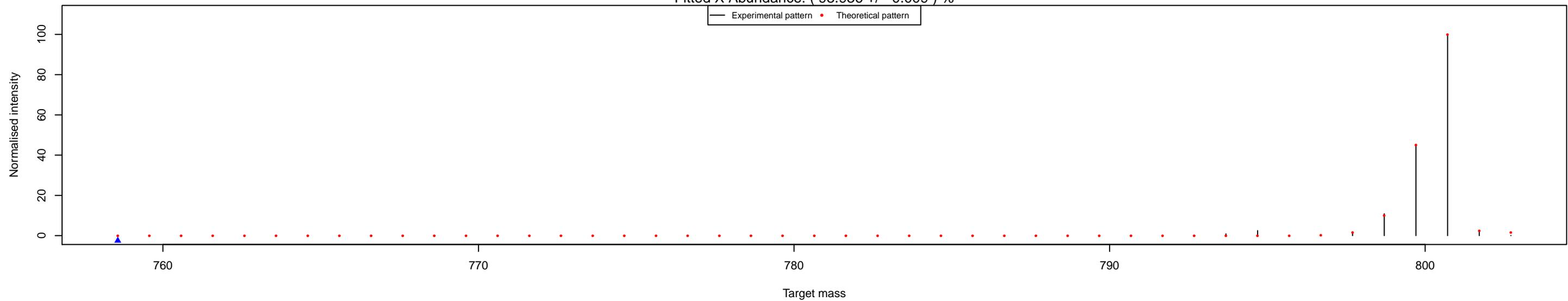
C12_Sample_1 , Compound: X42H83NO8P

Fitted X Abundance: (1.086 +/− 0.009) %

Experimental pattern • Theoretical pattern
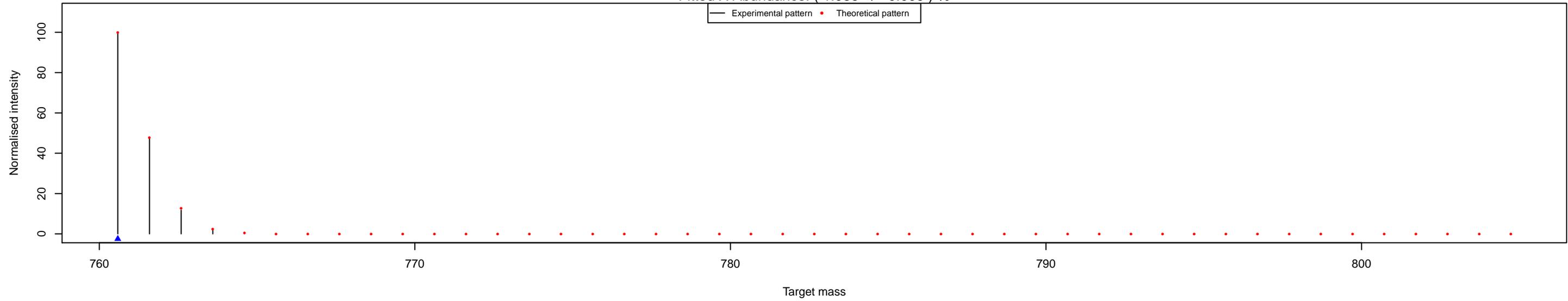
C12_Sample_2 , Compound: X42H83NO8P

Fitted X Abundance: (1.063 +/− 0.010) %

Experimental pattern • Theoretical pattern
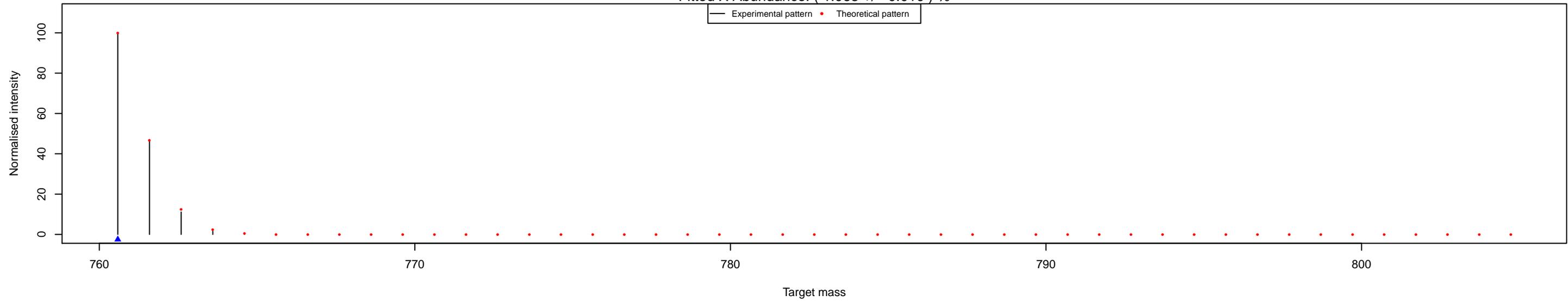
C12_Sample_3 , Compound: X42H83NO8P

Fitted X Abundance: (1.085 +/− 0.009) %

Experimental pattern • Theoretical pattern
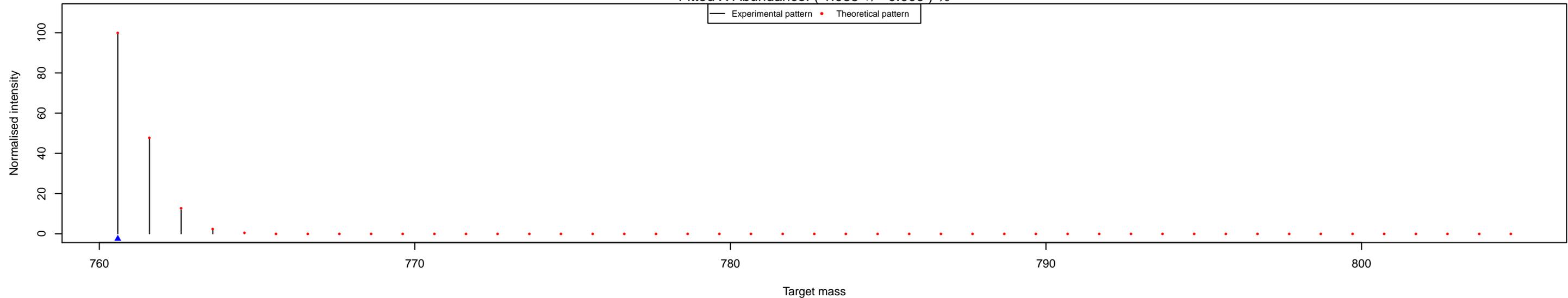
C12_Sample_4 , Compound: X42H83NO8P

Fitted X Abundance: (1.066 +/− 0.012) %

| Experimental pattern | • Theoretical pattern |
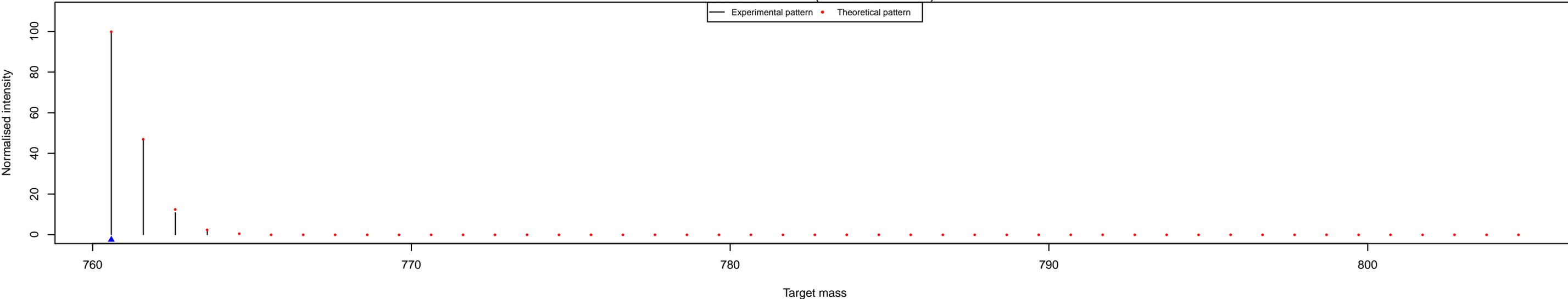
Target mass

C13_Sample_1 , Compound: X42H83NO8P

Fitted X Abundance: (98.971 +/− 0.004) %

| Experimental pattern | • Theoretical pattern |

Target mass
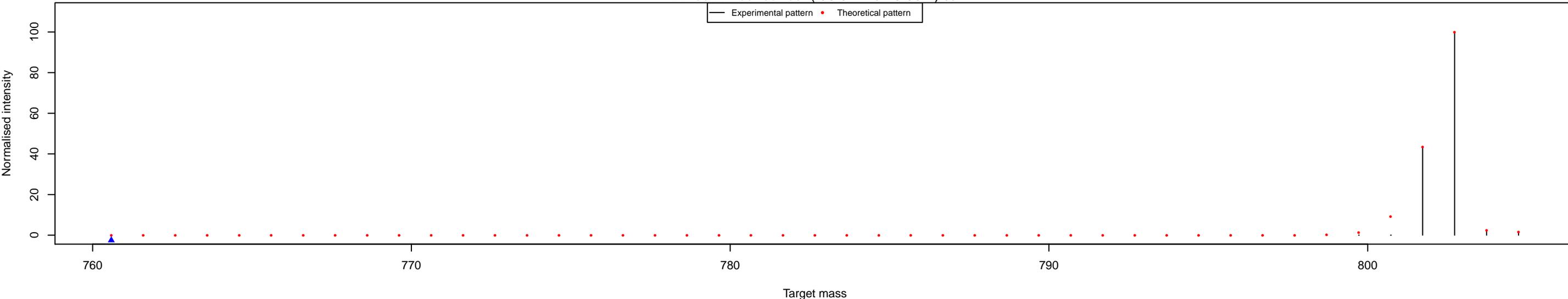
C13_Sample_2 , Compound: X42H83NO8P

Fitted X Abundance: (99.003 +/− 0.023) %

| Experimental pattern | • Theoretical pattern |

Target mass
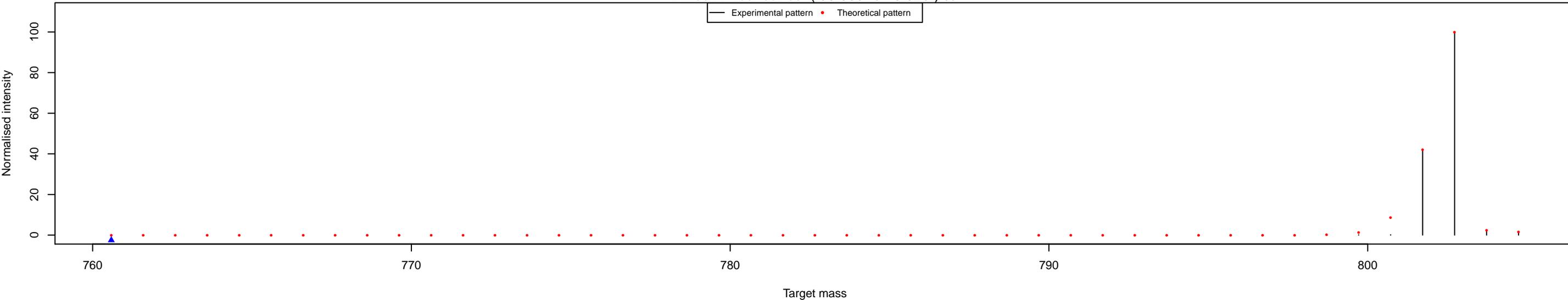
C13_Sample_3 , Compound: X42H83NO8P

Fitted X Abundance: (98.988 +/− 0.004) %
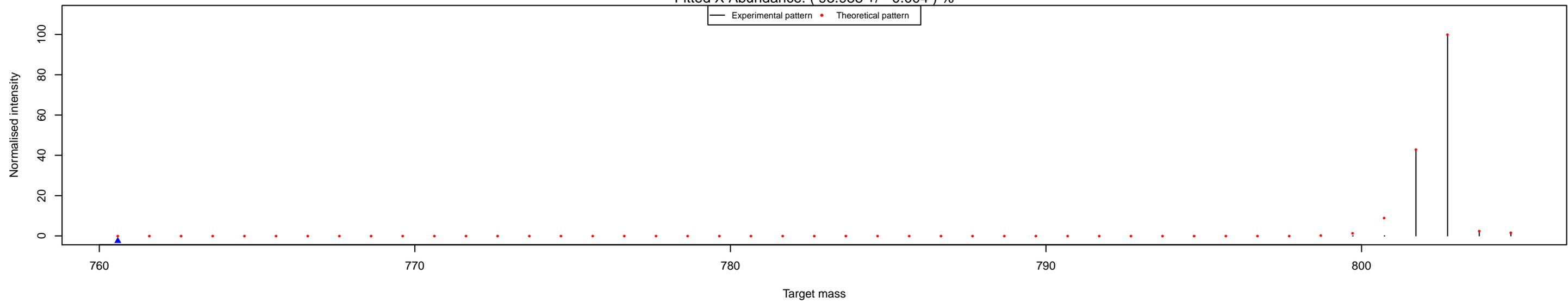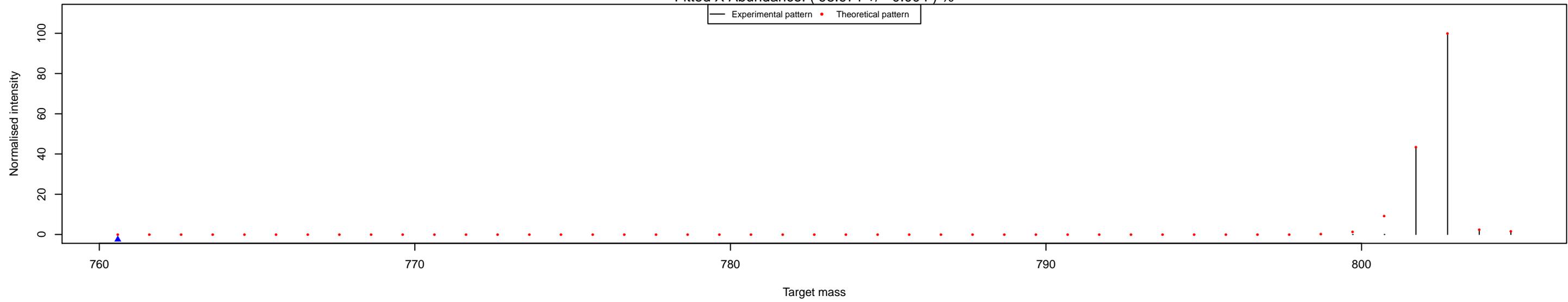
— Experimental pattern   • Theoretical pattern

Normalised intensity

Target mass

C13_Sample_4 , Compound: X42H83NO8P

Fitted X Abundance: (98.971 +/− 0.004) %

— Experimental pattern   • Theoretical pattern

Normalised intensity

Target mass

C12_Sample_1 , Compound: X51H96NO6
### Fitted X Abundance: (1.089 +/− 0.033) %
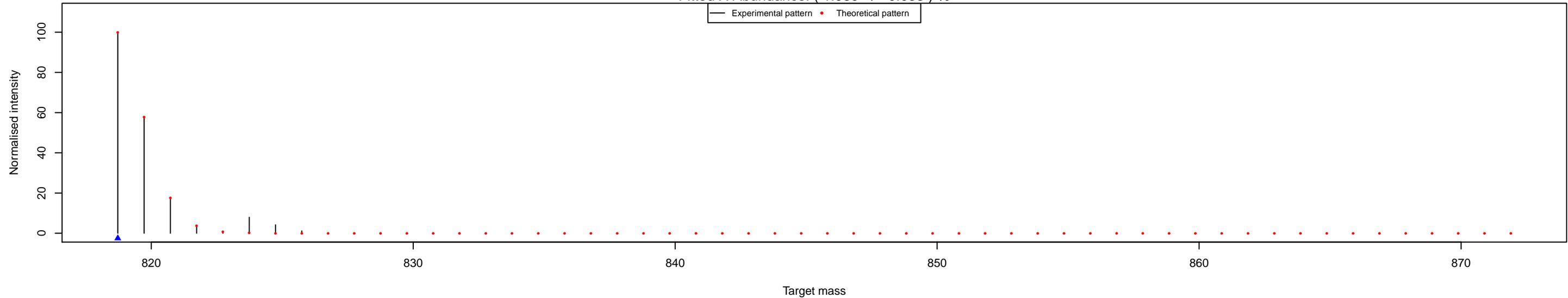
C12_Sample_2 , Compound: X51H96NO6
Fitted X Abundance: (1.084 +/− 0.041) %
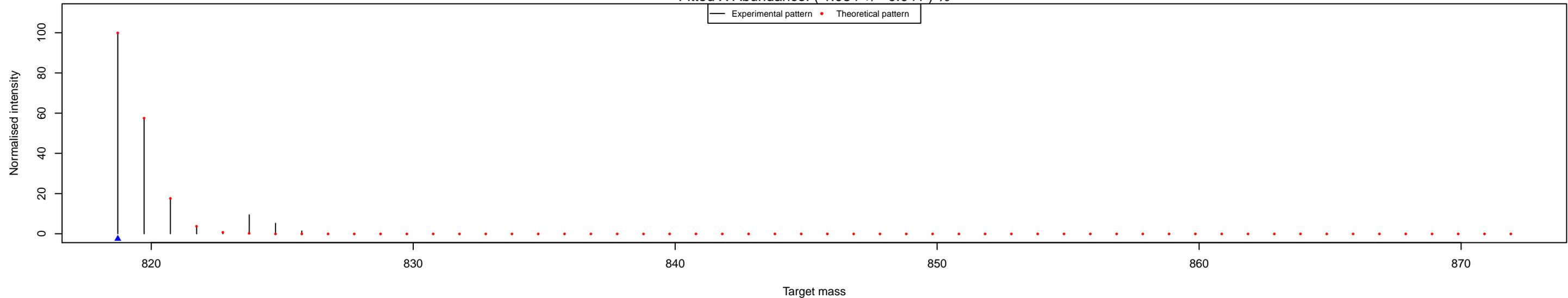
C12_Sample_3 , Compound: X51H96NO6
Fitted X Abundance: (1.090 +/− 0.039) %
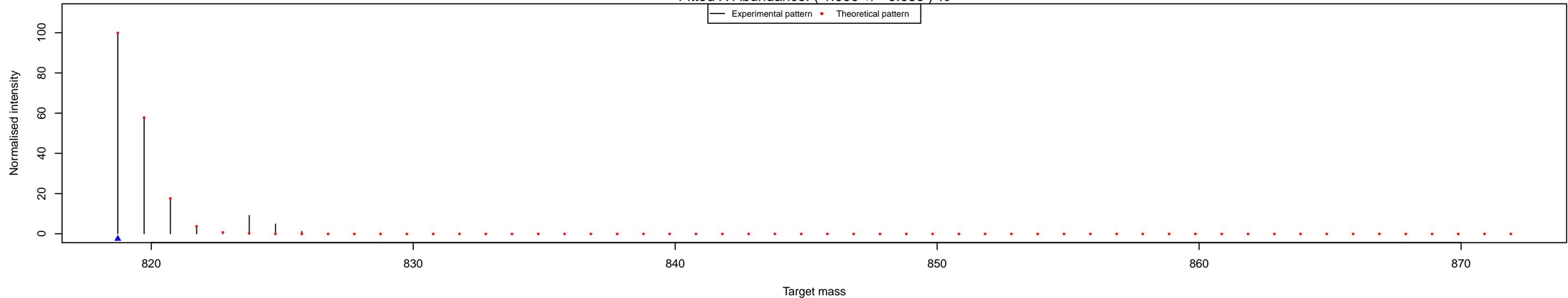
C12_Sample_4 , Compound: X51H96NO6

Fitted X Abundance: (1.098 +/− 0.042) %

Experimental pattern · Theoretical pattern

Normalised intensity

Target mass
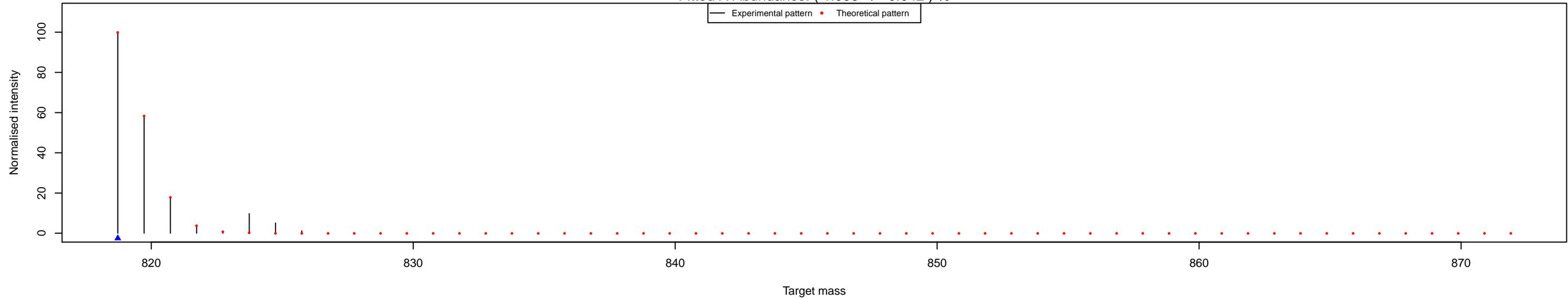
C13_Sample_1 , Compound: X51H96NO6

Fitted X Abundance: (98.965 +/− 0.008) %

Experimental pattern · Theoretical pattern

Normalised intensity

Target mass
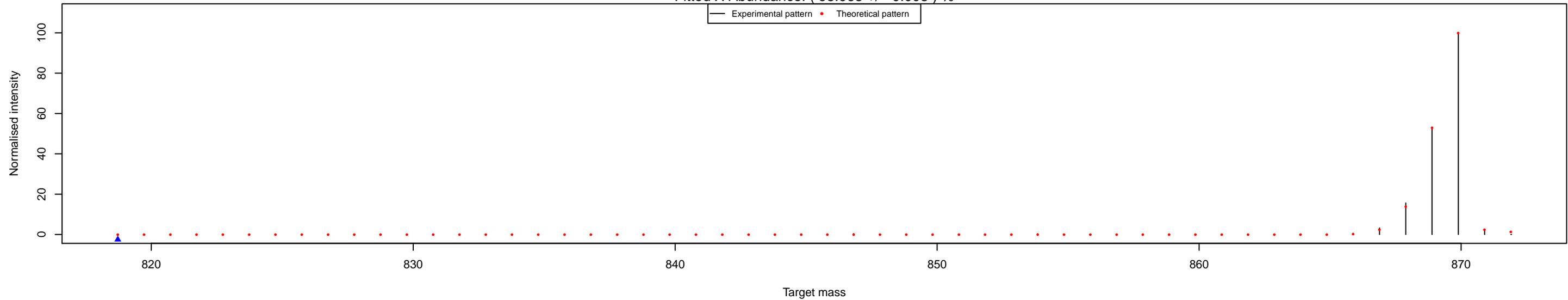
C13_Sample_2 , Compound: X51H96NO6

Fitted X Abundance: (98.964 +/− 0.010) %

Experimental pattern · Theoretical pattern
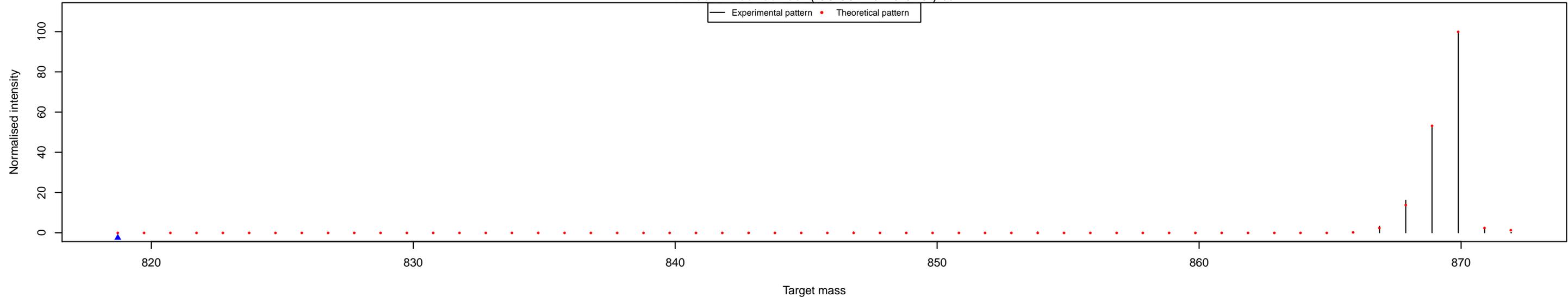
Normalised intensity

Target mass

C13_Sample_3 , Compound: X51H96NO6

Fitted X Abundance: (98.960 +/− 0.007) %
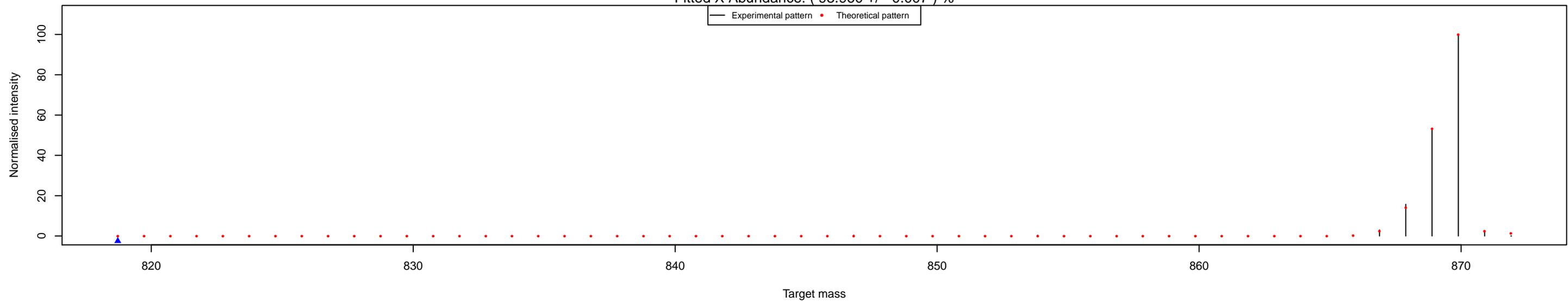
Experimental pattern ● Theoretical pattern

C13_Sample_4 , Compound: X51H96NO6

Fitted X Abundance: (98.968 +/− 0.008) %

Experimental pattern ● Theoretical pattern
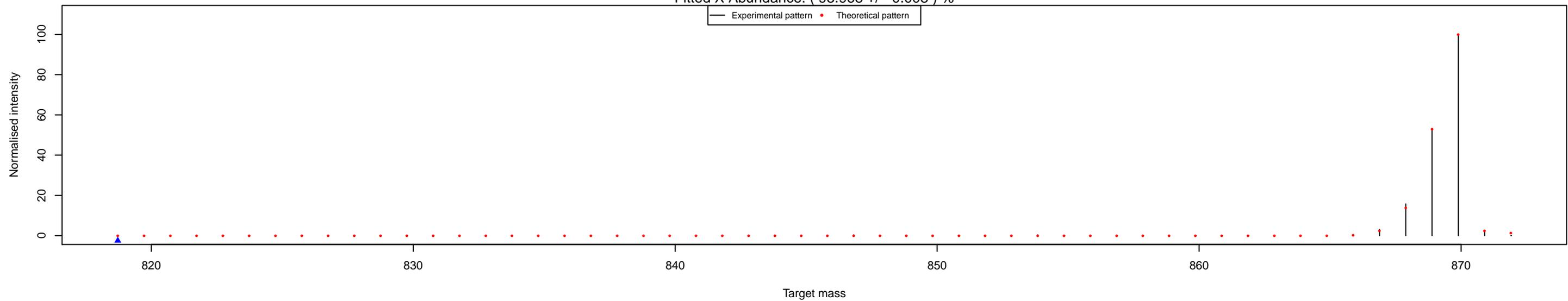
C12_Sample_1 , Compound: X51H98NO6

Fitted X Abundance: (1.084 +/− 0.086) %

— Experimental pattern • Theoretical pattern
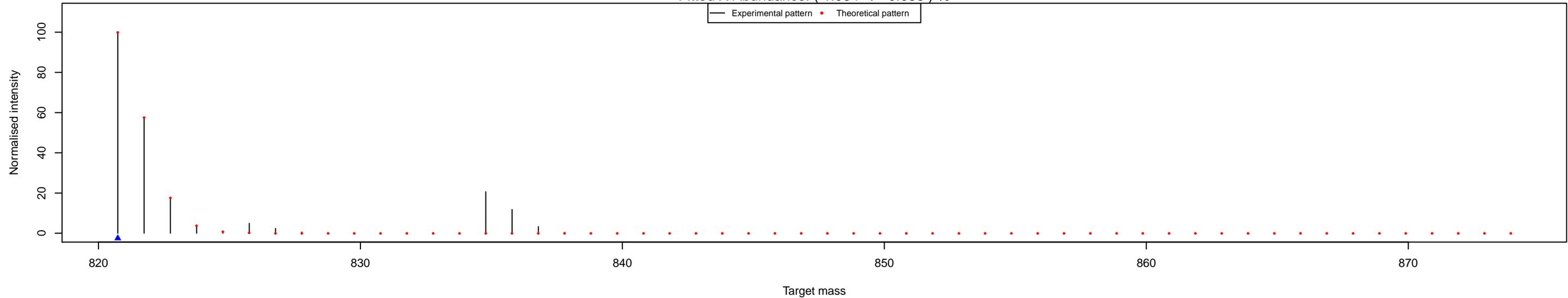
C12_Sample_2 , Compound: X51H98NO6

Fitted X Abundance: (1.095 +/− 0.081) %

— Experimental pattern • Theoretical pattern
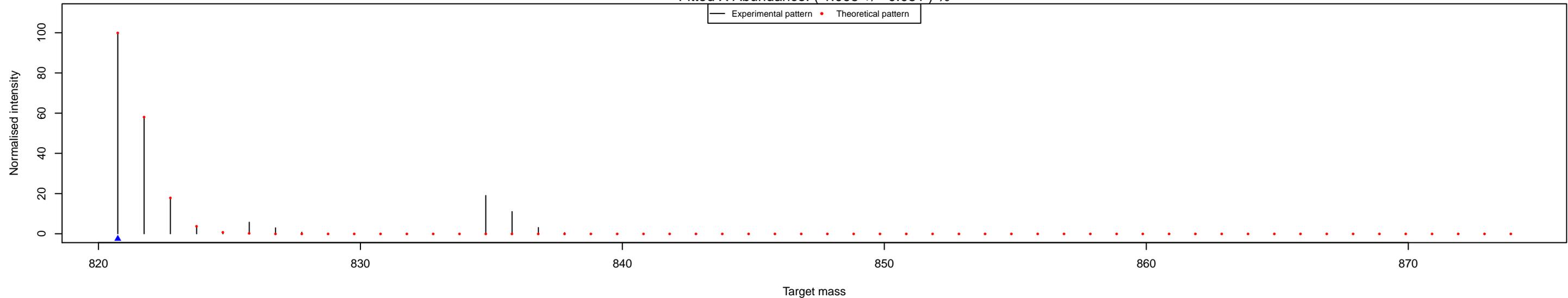
C12_Sample_3 , Compound: X51H98NO6

Fitted X Abundance: (1.089 +/− 0.084) %

— Experimental pattern • Theoretical pattern
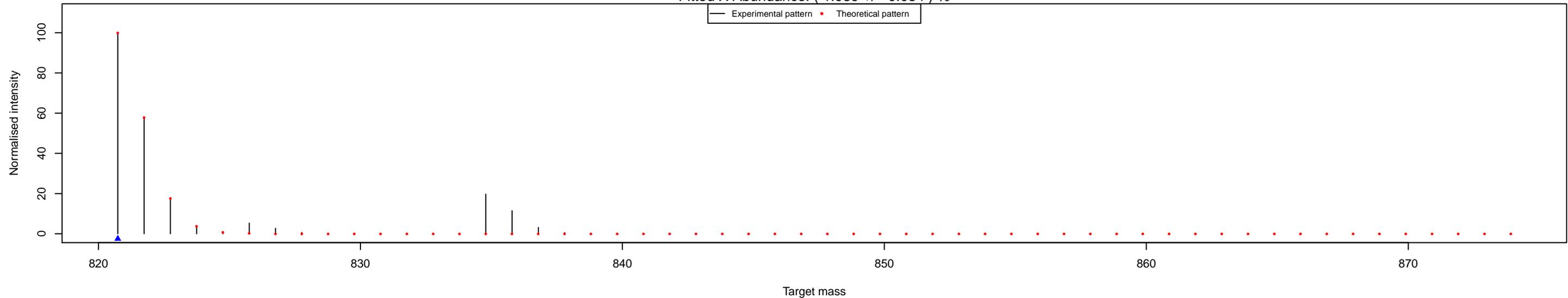
C12_Sample_4 , Compound: X51H98NO6
Fitted X Abundance: (1.098 +/− 0.076) %
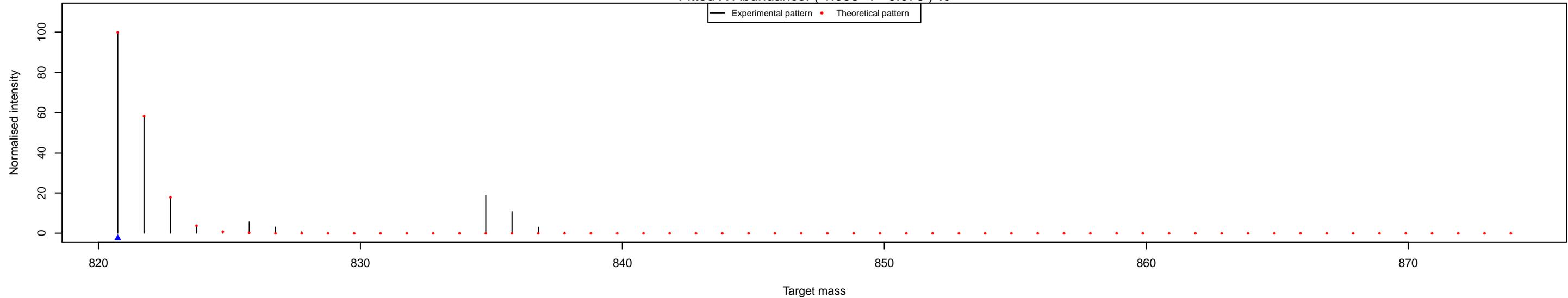
C13_Sample_1 , Compound: X51H98NO6
Fitted X Abundance: (98.959 +/− 0.011) %

C13_Sample_2 , Compound: X51H98NO6
Fitted X Abundance: (98.969 +/− 0.009) %

C13_Sample_3 , Compound: X51H98NO6

Fitted X Abundance: (98.967 +/− 0.007) %

Experimental pattern   Theoretical pattern
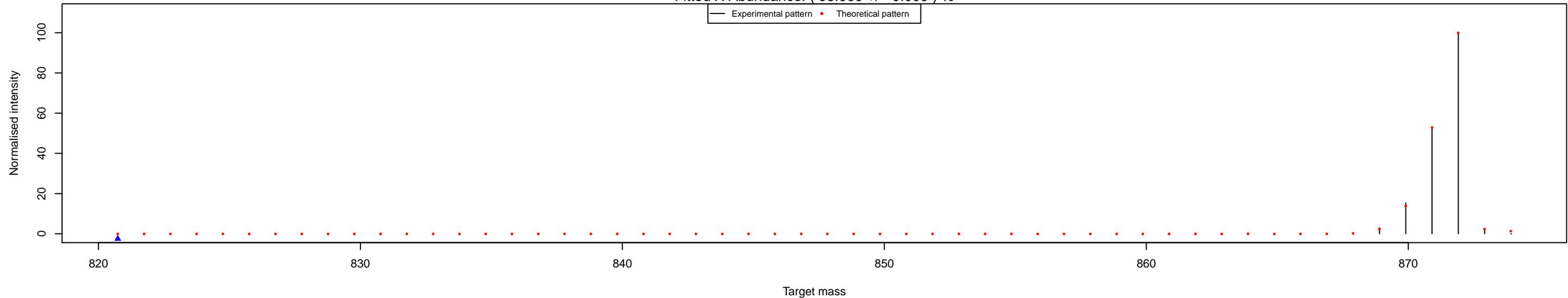
C13_Sample_4 , Compound: X51H98NO6
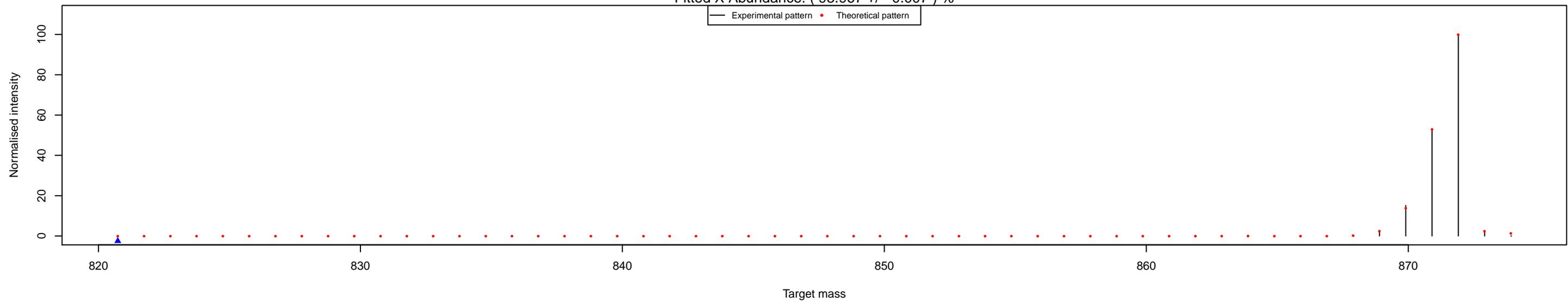
Fitted X Abundance: (98.973 +/− 0.008) %

Experimental pattern   Theoretical pattern
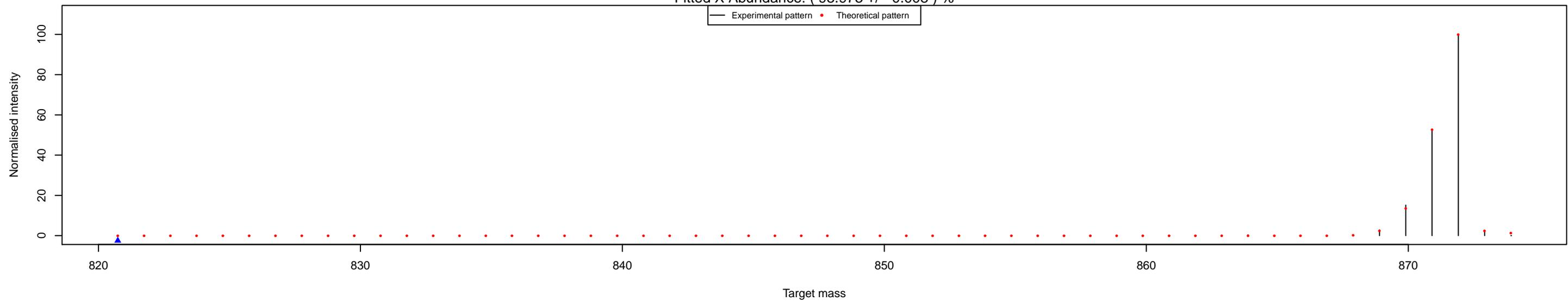
C12_Sample_1 , Compound: X53H100NO6

Fitted X Abundance: (1.092 +/− 0.017) %

Experimental pattern • Theoretical pattern
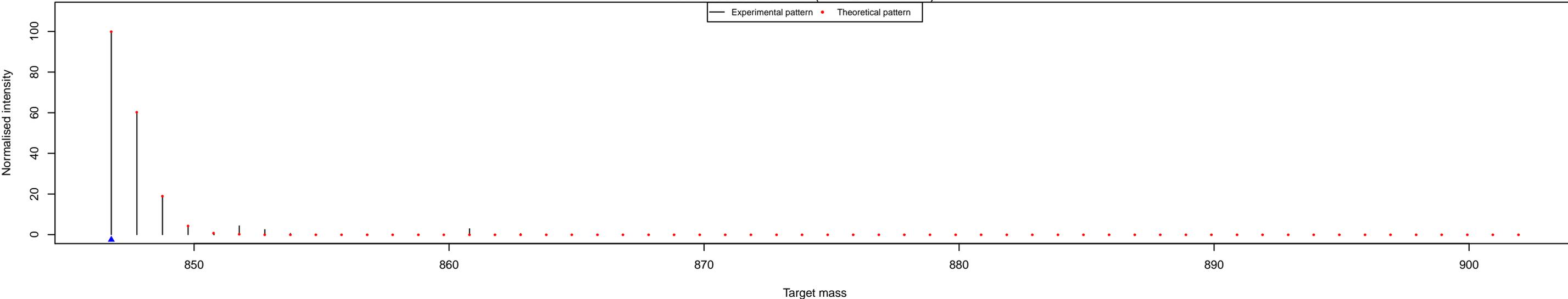
Target mass

C12_Sample_2 , Compound: X53H100NO6

Fitted X Abundance: (1.093 +/− 0.021) %

Experimental pattern • Theoretical pattern

Target mass
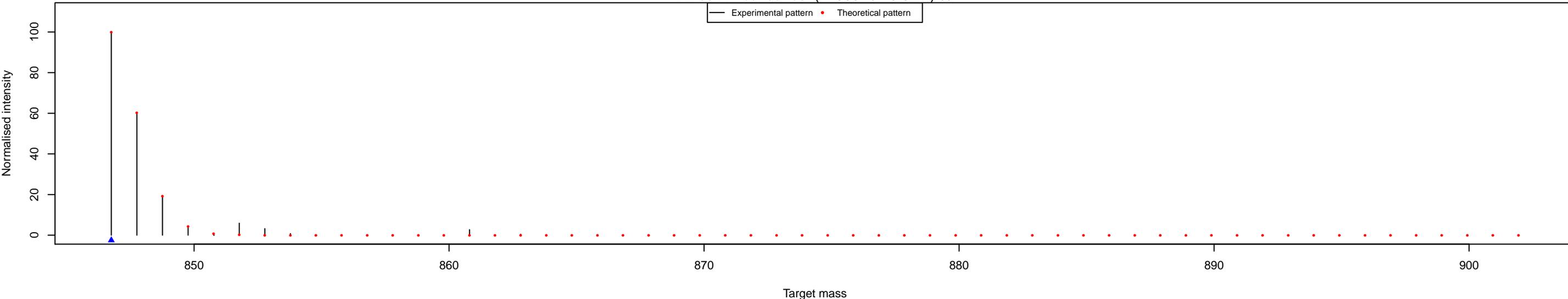
C12_Sample_3 , Compound: X53H100NO6

Fitted X Abundance: (1.093 +/− 0.020) %

Experimental pattern • Theoretical pattern

Target mass
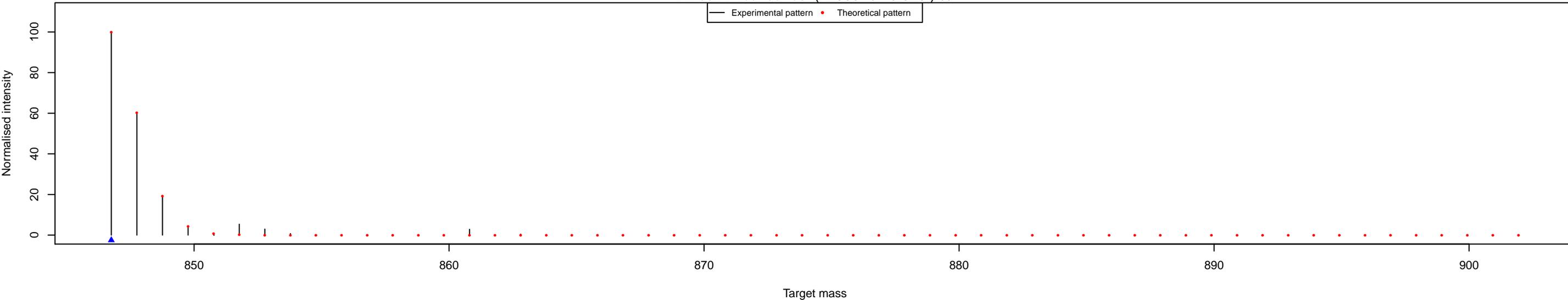
C12_Sample_4 , Compound: X53H100NO6

Fitted X Abundance: (1.091 +/− 0.021) %

— Experimental pattern   • Theoretical pattern
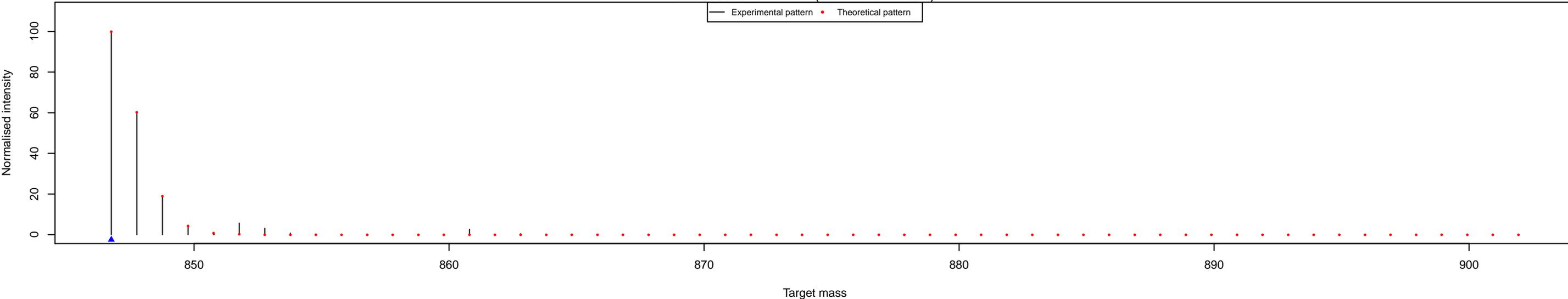
C13_Sample_1 , Compound: X53H100NO6

Fitted X Abundance: (98.961 +/− 0.012) %

— Experimental pattern   • Theoretical pattern

C13_Sample_2 , Compound: X53H100NO6

Fitted X Abundance: (98.969 +/− 0.010) %

— Experimental pattern   • Theoretical pattern

C13_Sample_3 , Compound: X53H100NO6

Fitted X Abundance: (98.969 +/− 0.010) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
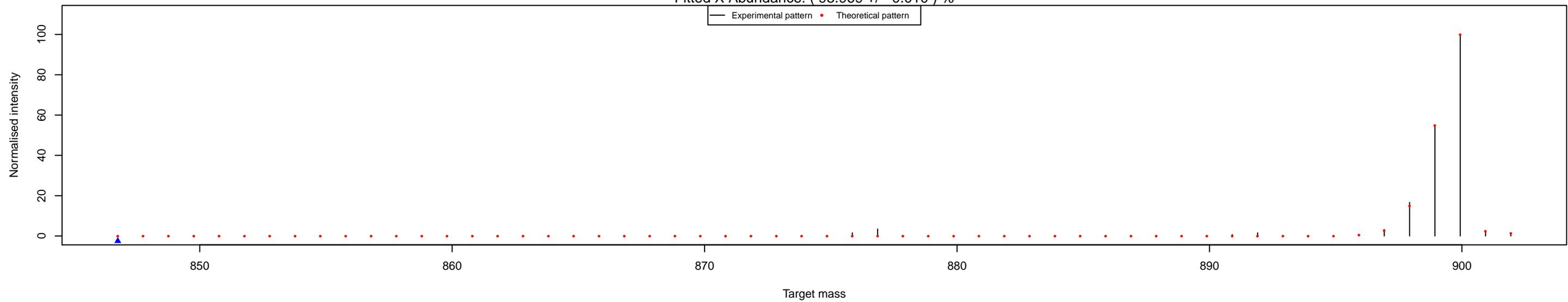
C13_Sample_4 , Compound: X53H100NO6

Fitted X Abundance: (98.968 +/− 0.009) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass

C12_Sample_1 , Compound: X53H102NO6
Fitted X Abundance: (1.095 +/− 0.017) %
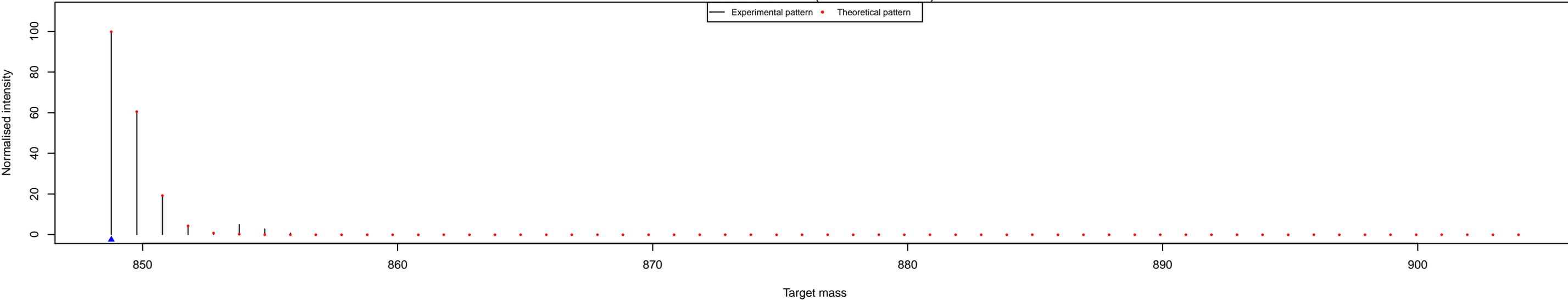
C12_Sample_2 , Compound: X53H102NO6
Fitted X Abundance: (1.103 +/− 0.023) %
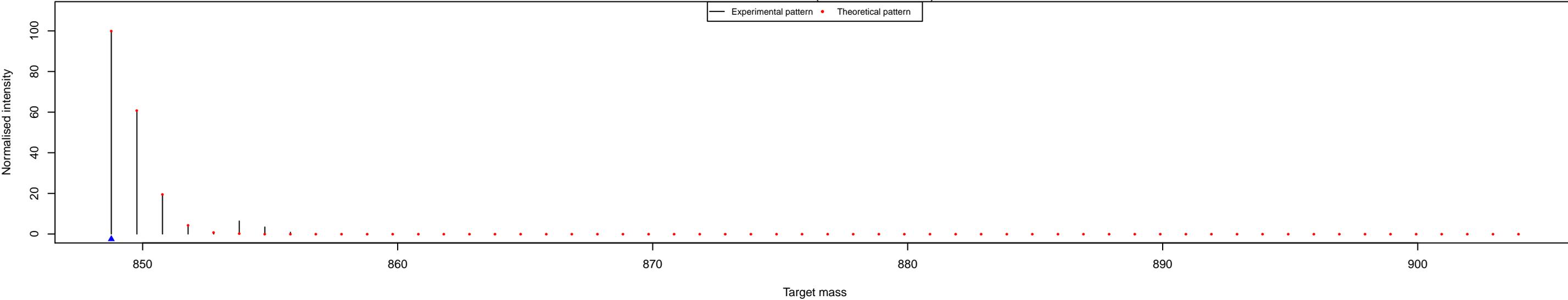
C12_Sample_3 , Compound: X53H102NO6
Fitted X Abundance: (1.097 +/− 0.020) %

**C12_Sample_4 , Compound: X53H102NO6**

Fitted X Abundance: (1.093 +/− 0.021) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass

C13_Sample_1 , Compound: X53H102NO6

Fitted X Abundance: (98.959 +/− 0.010) %

— Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
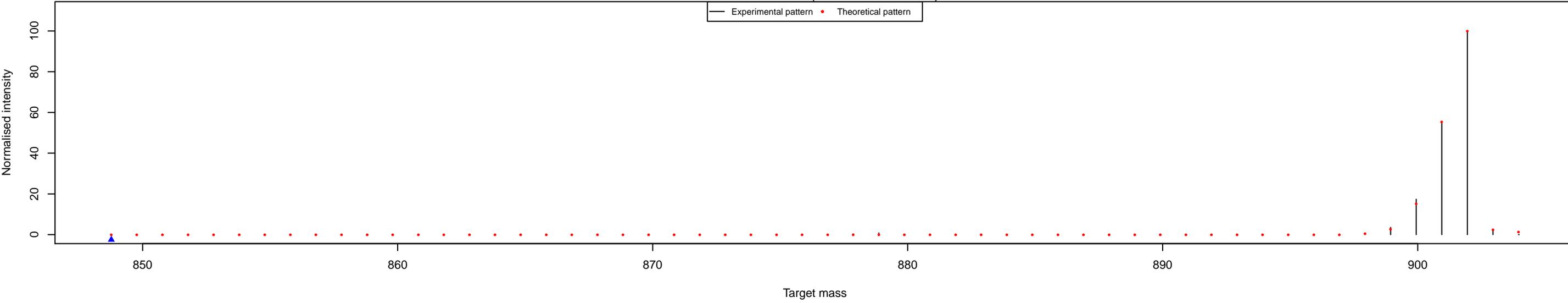
C13_Sample_2 , Compound: X53H102NO6

Fitted X Abundance: (98.978 +/− 0.011) %

— Experimental pattern • Theoretical pattern
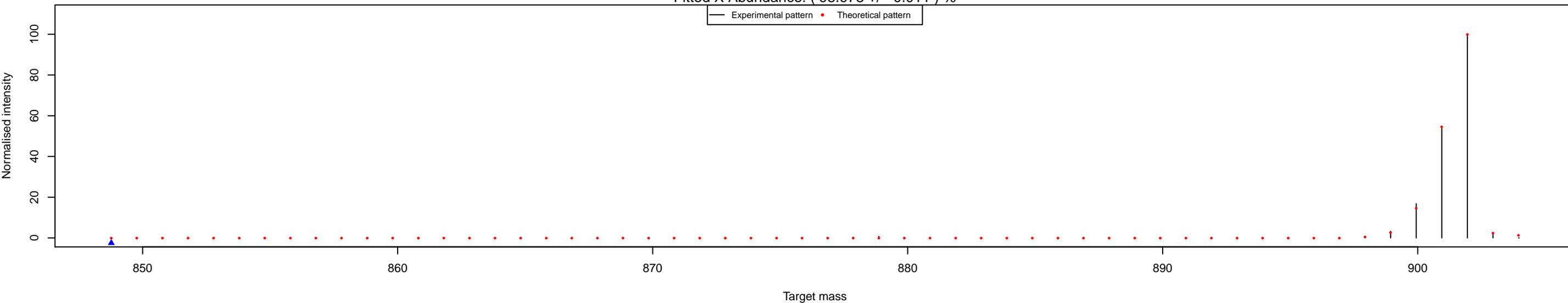
Normalised intensity

Target mass

C13_Sample_3 , Compound: X53H102NO6

Fitted X Abundance: (98.973 +/− 0.008) %

Experimental pattern • Theoretical pattern

Normalised intensity

Target mass

C13_Sample_4 , Compound: X53H102NO6

Fitted X Abundance: (98.969 +/− 0.007) %

Experimental pattern • Theoretical pattern

Normalised intensity

Target mass
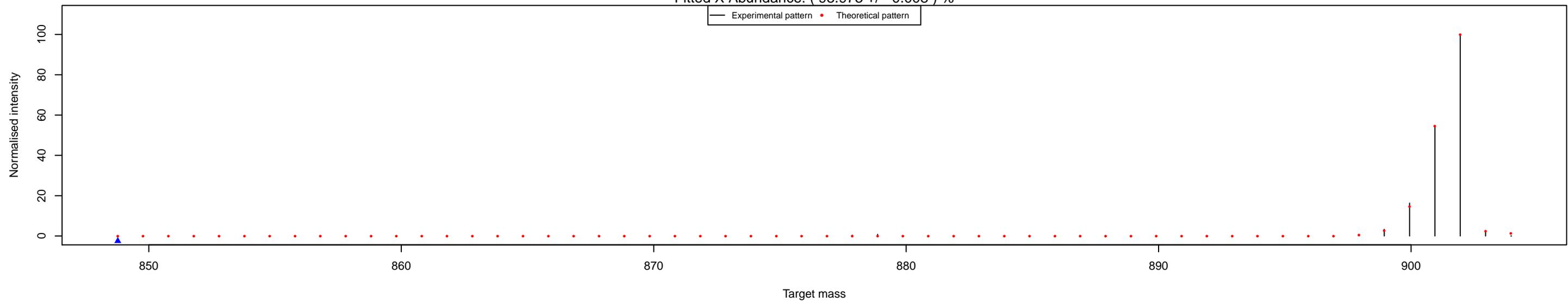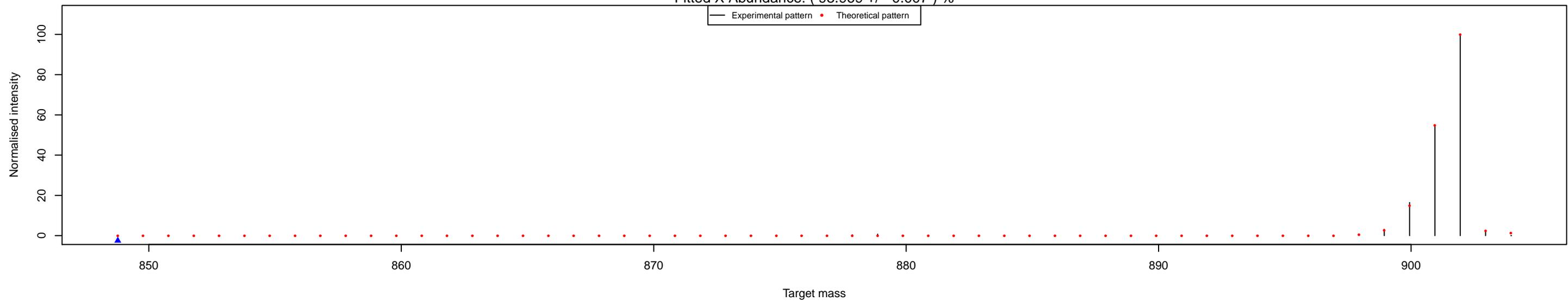
C12_Sample_1 , Compound: X55H106NO6

Fitted X Abundance: (1.099 +/− 0.019) %

Experimental pattern   Theoretical pattern
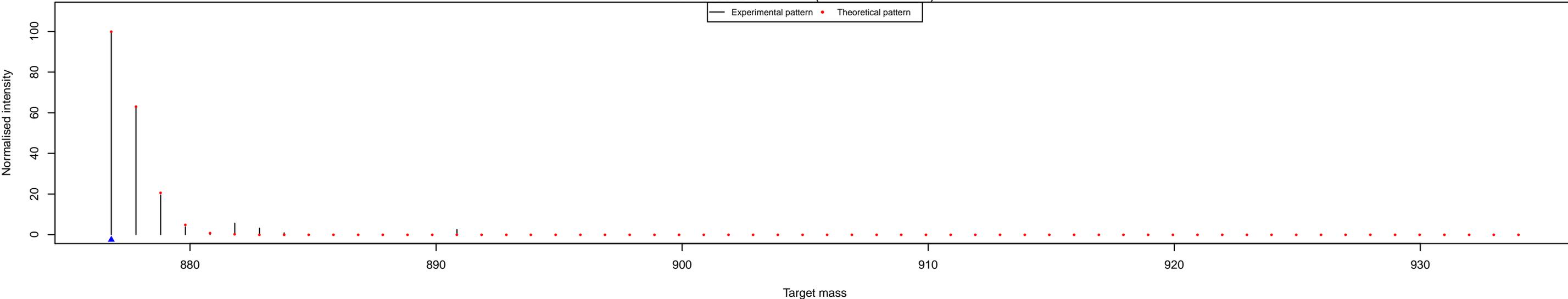
C12_Sample_2 , Compound: X55H106NO6

Fitted X Abundance: (1.102 +/− 0.021) %

Experimental pattern   Theoretical pattern
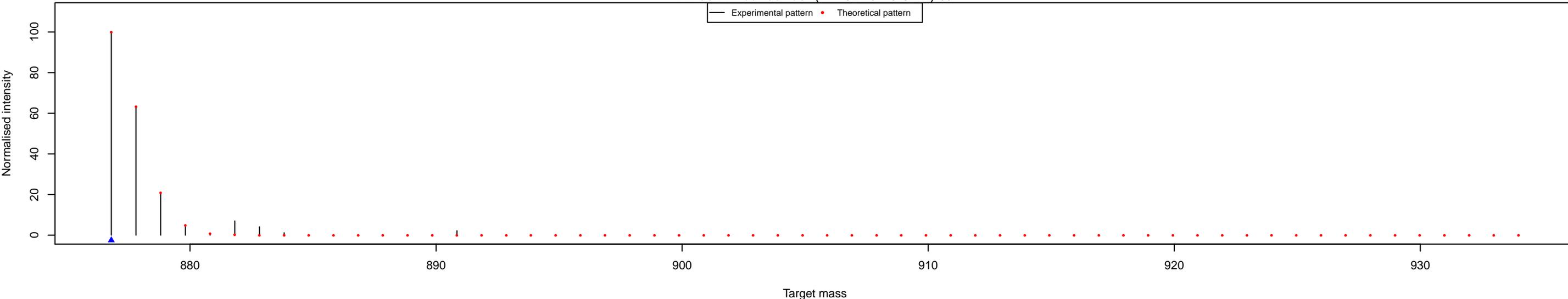
C12_Sample_3 , Compound: X55H106NO6

Fitted X Abundance: (1.104 +/− 0.023) %

Experimental pattern   Theoretical pattern
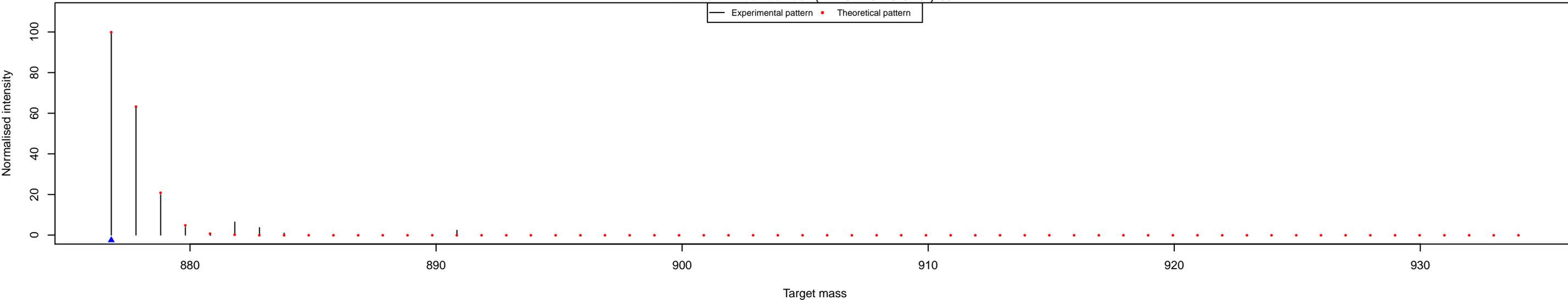
C12_Sample_4 , Compound: X55H106NO6

Fitted X Abundance: (1.097 +/− 0.022) %
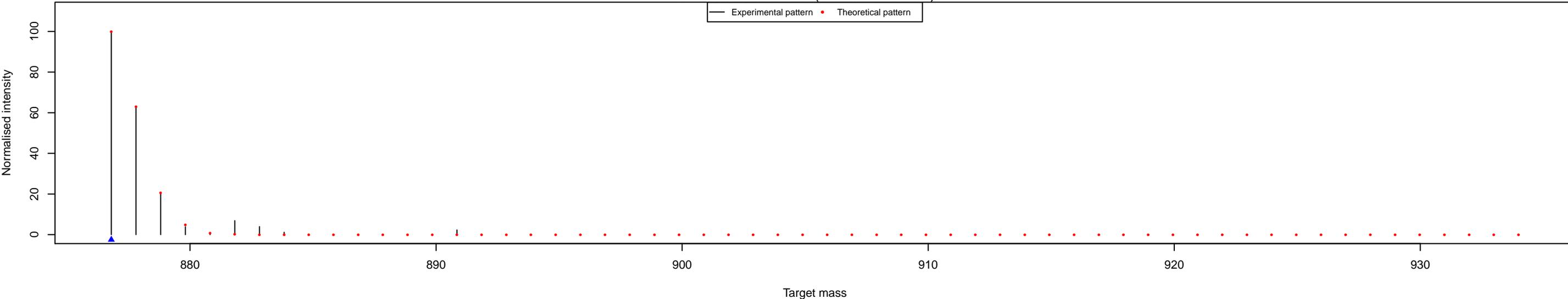
C13_Sample_1 , Compound: X55H106NO6

Fitted X Abundance: (98.963 +/− 0.013) %
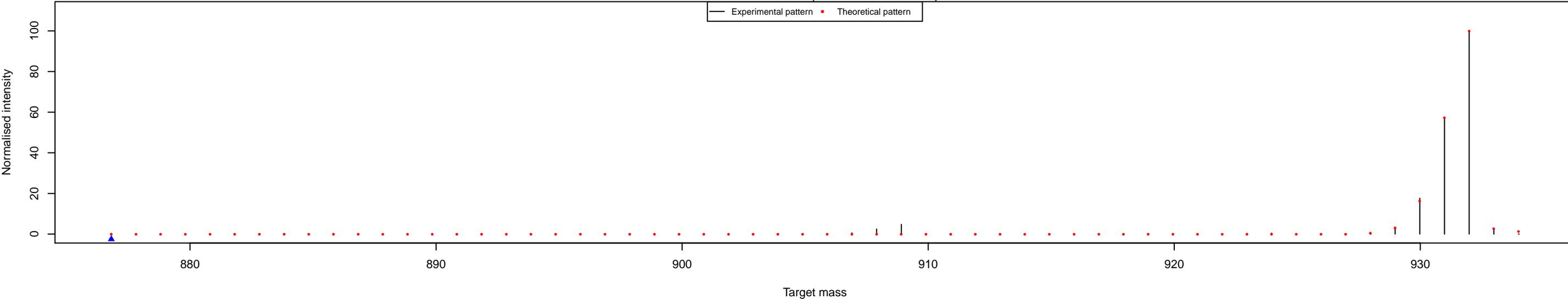
C13_Sample_2 , Compound: X55H106NO6

Fitted X Abundance: (98.971 +/− 0.012) %

C13_Sample_3 , Compound: X55H106NO6

Fitted X Abundance: (98.976 +/− 0.015) %

Experimental pattern ・ Theoretical pattern

C13_Sample_4 , Compound: X55H106NO6

Fitted X Abundance: (98.972 +/− 0.012) %

Experimental pattern ・ Theoretical pattern