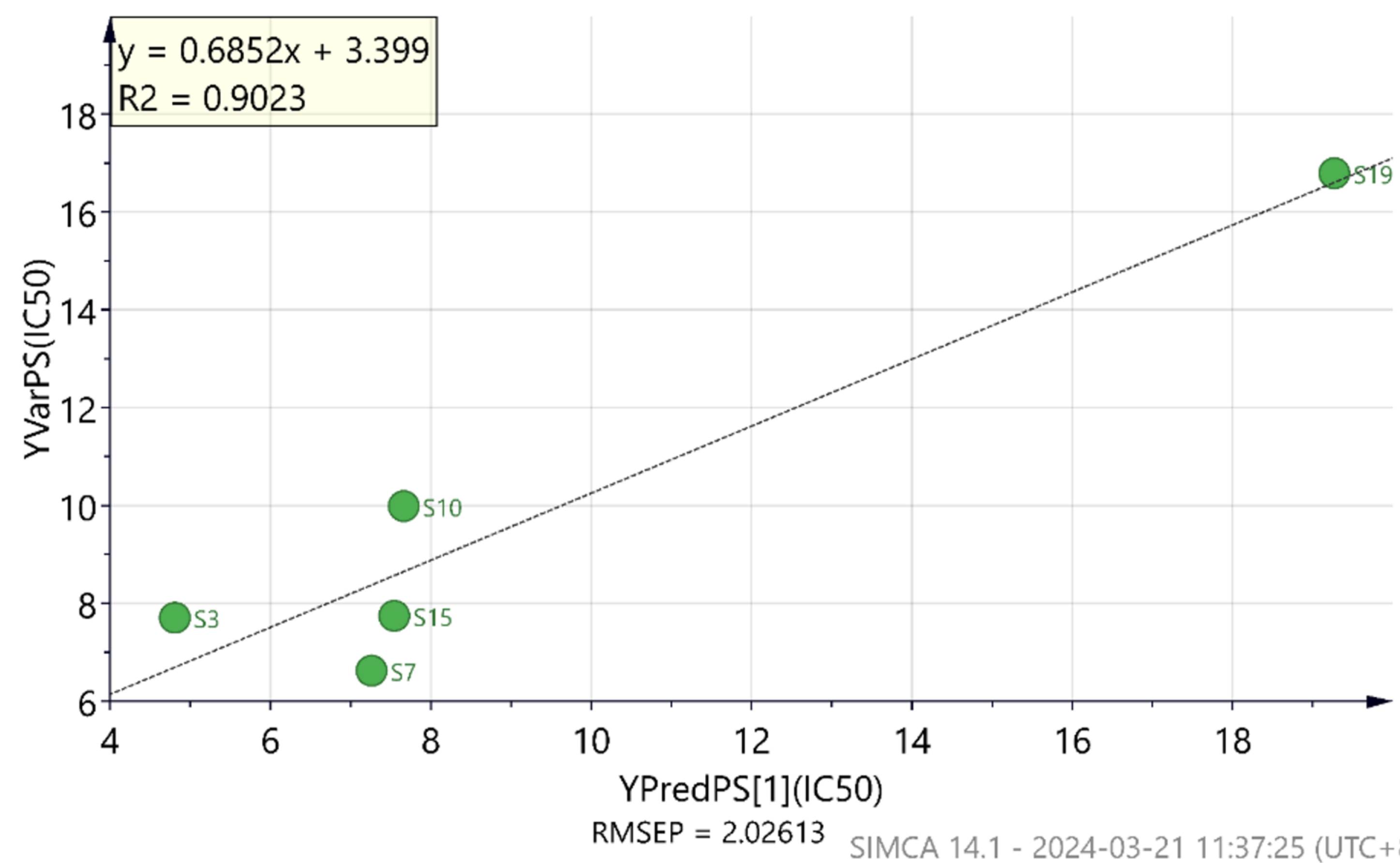
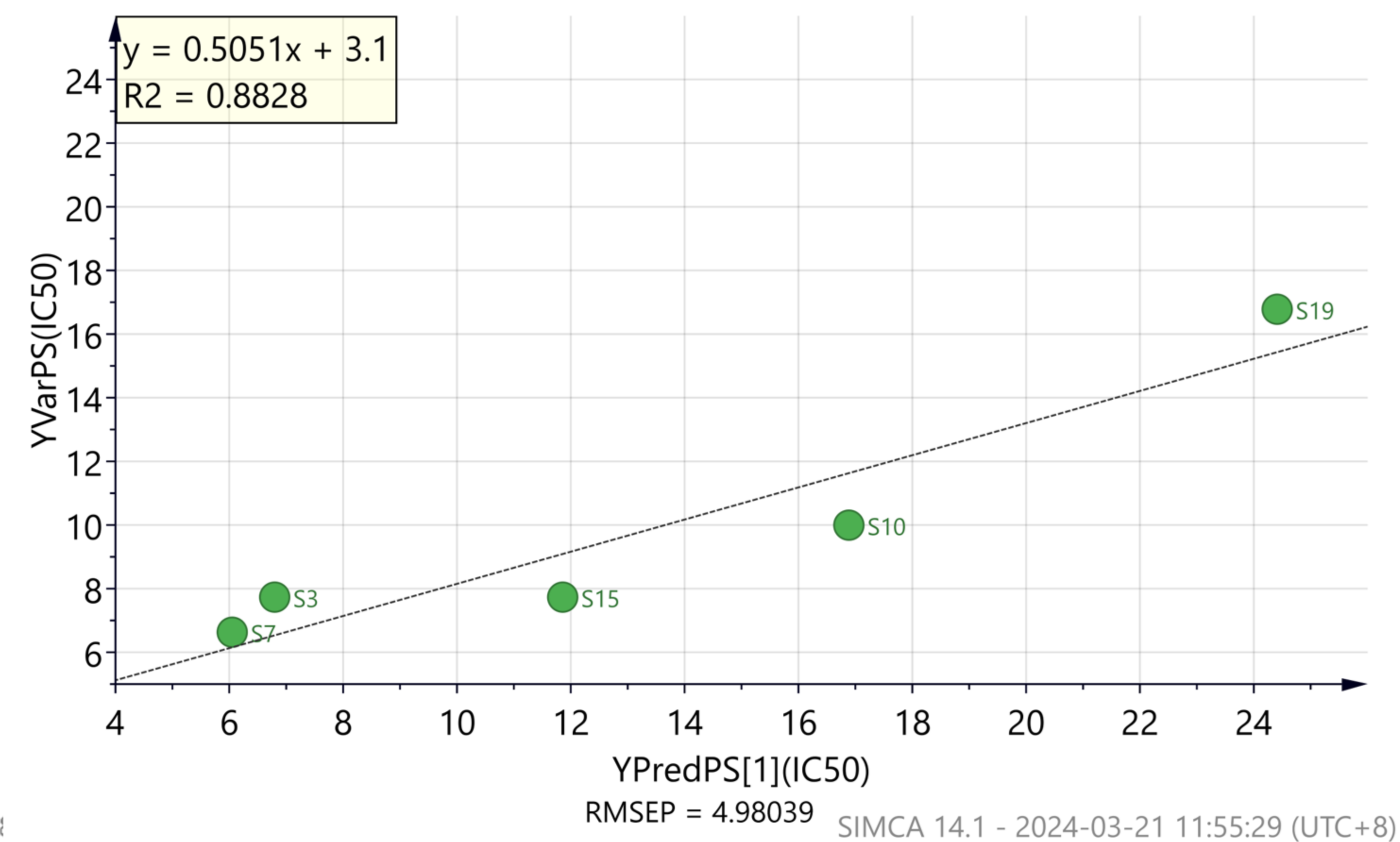


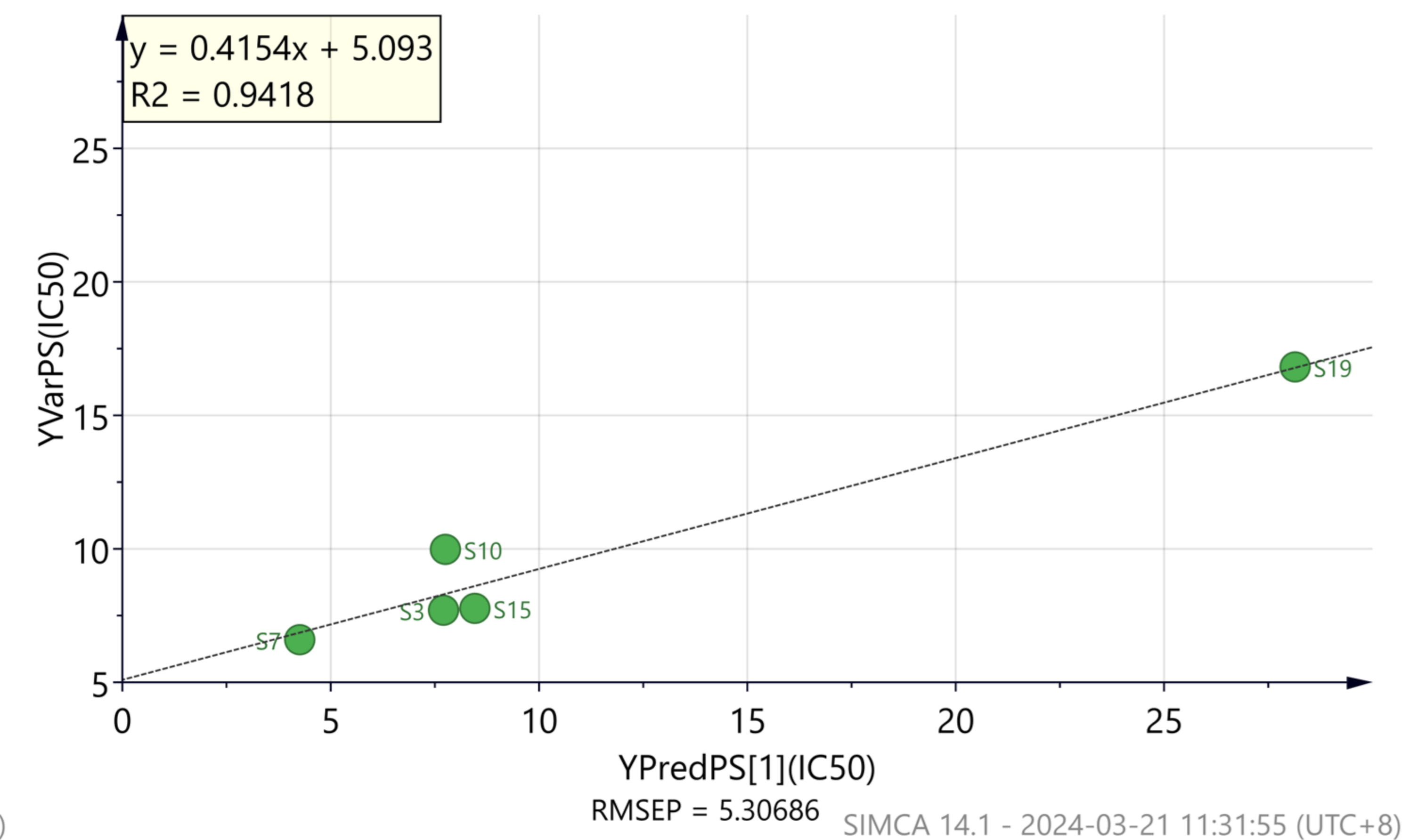
A



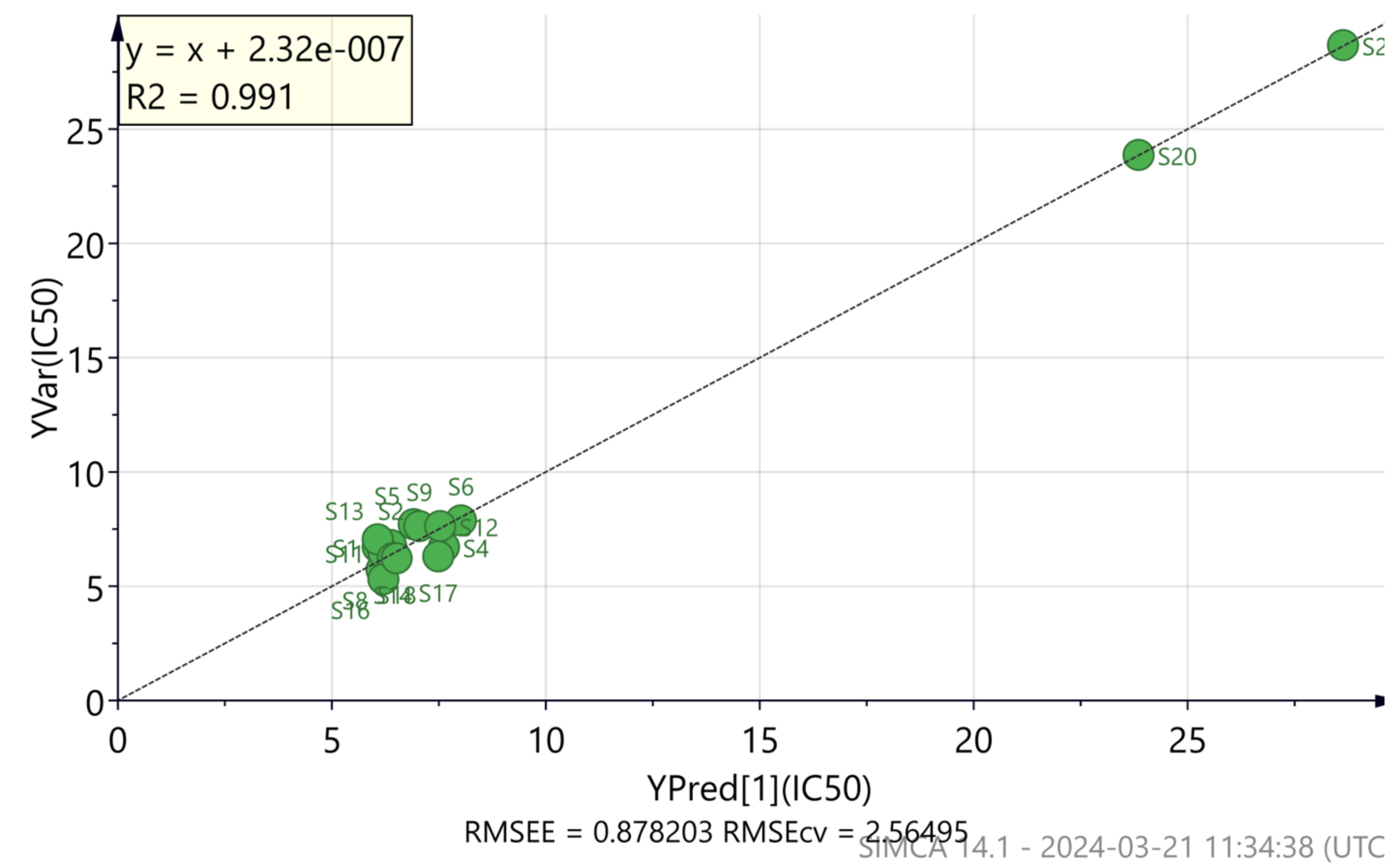
B



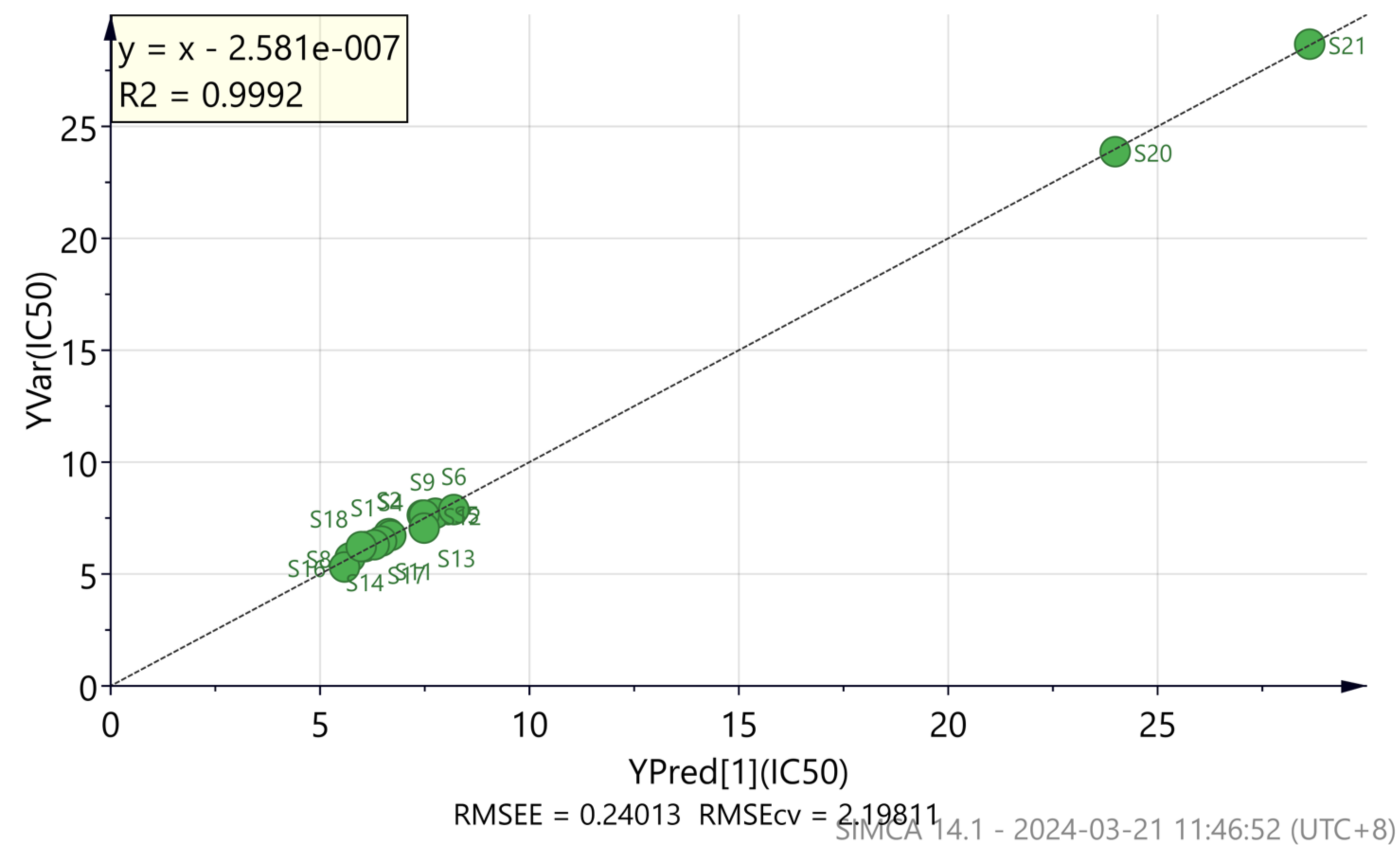
C



D



E



F

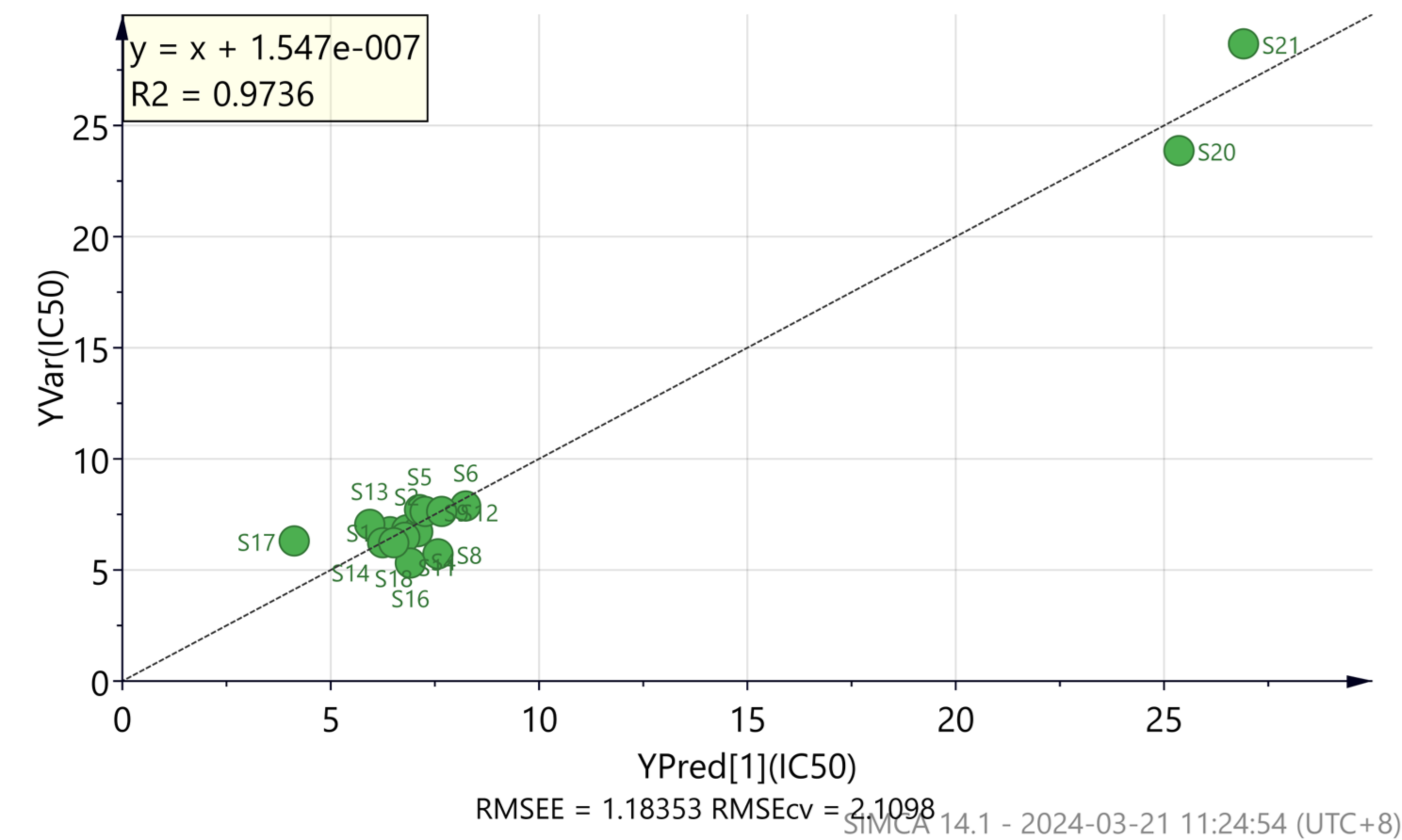


Fig. S3. The validation set of peak areas and IC₅₀ value correlations for FT-IR (A), UV (B) and HPLC (C). The training set of peak areas and IC₅₀ value correlations for FT-IR (D), UV (E) and HPLC (F).