

SUPPLEMENTARY MATERIAL

MULTIVARIATE ANALYSIS FOR RAPID SCREENING AND PREDICTION OF SOLID-STATE COMPATIBILITY IN PHARMACEUTICAL PREFORMULATION STUDIES—PAVING THE ROAD FOR MACHINE LEARNING¹

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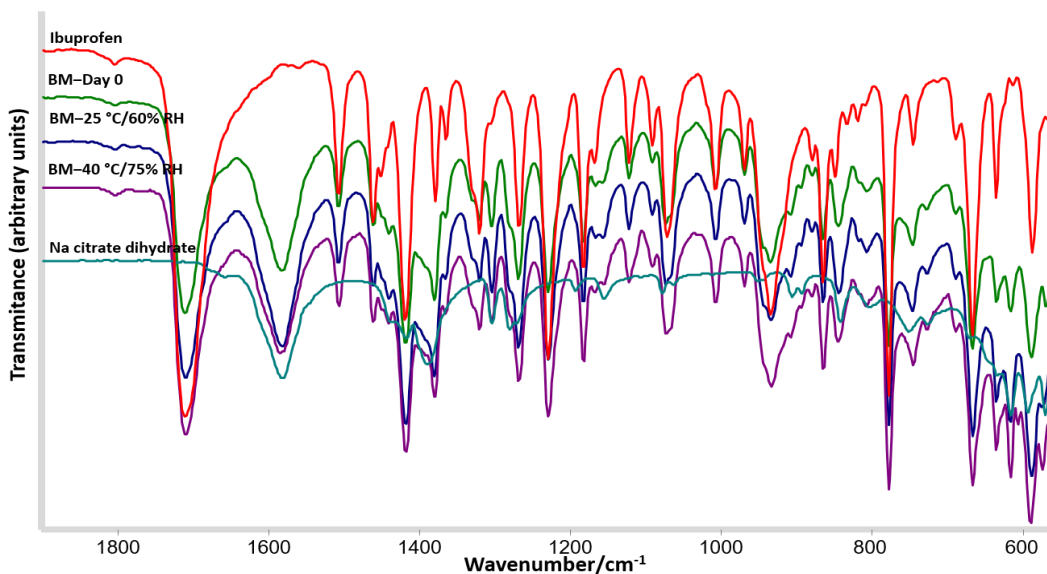


Fig. 1. FTIR spectra in the *fingerprint* region of the unstressed (Day 0) and stressed (Day 30) binary mixture of ibuprofen and sodium citrate dihydrate

¹ Dedicated on the occasion of the Golden Jubilee of the *Macedonian Journal of Chemistry and Chemical Engineering*

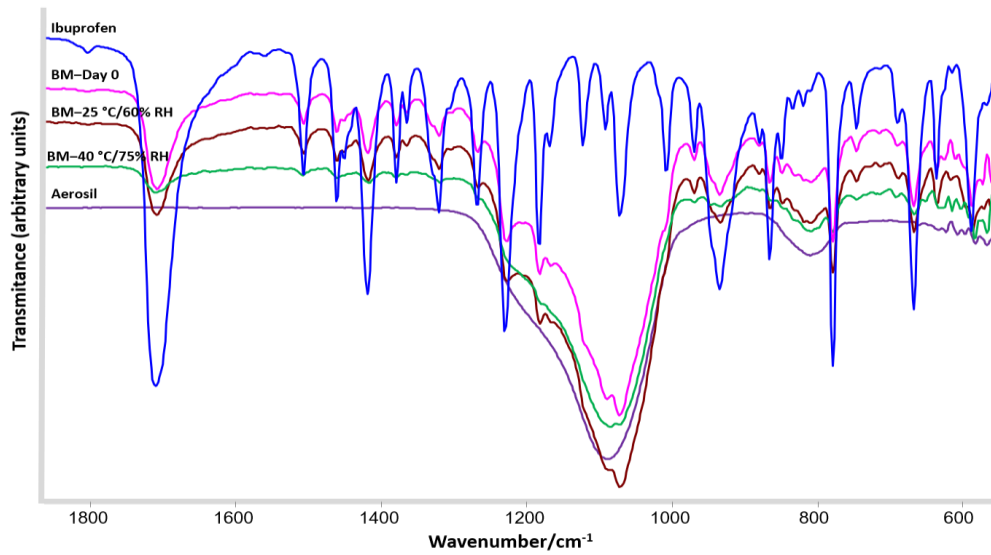


Fig. 2. FTIR spectra in the *fingerprint* region of the unstressed (Day 0) and stressed (Day 30) binary mixture of ibuprofen and Aerosil

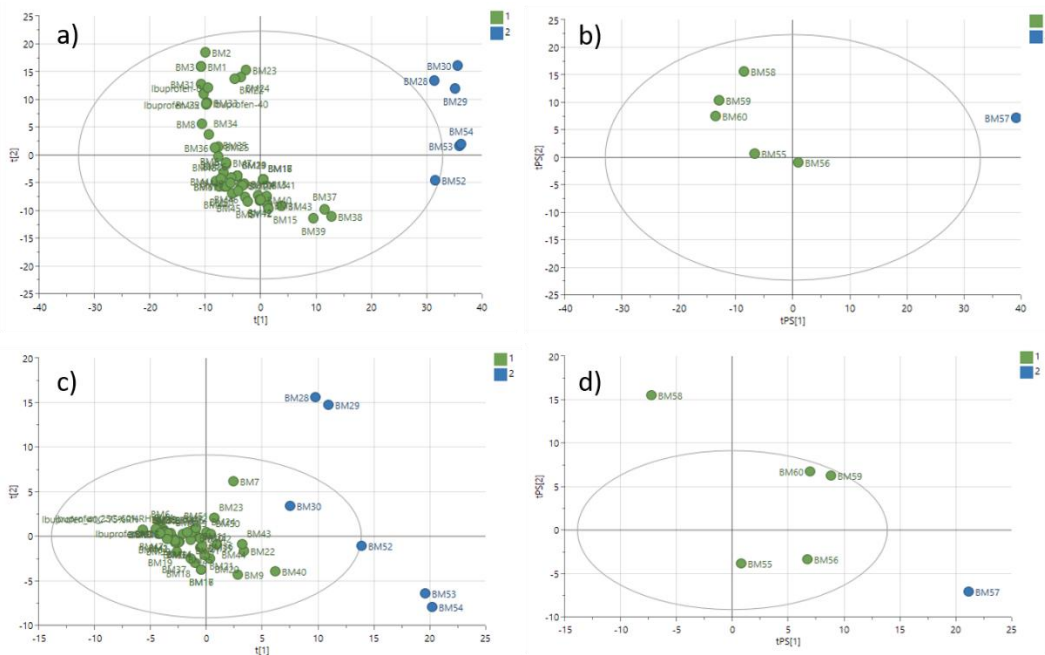


Fig. 3. Comparison between the score scatter plot and predicted plot for the prediction set of the a) and b) FTIR spectra model and c) and d) DSC curves model (green – BMs in which no interaction was detected; blue – BMs in which an interaction was detected)