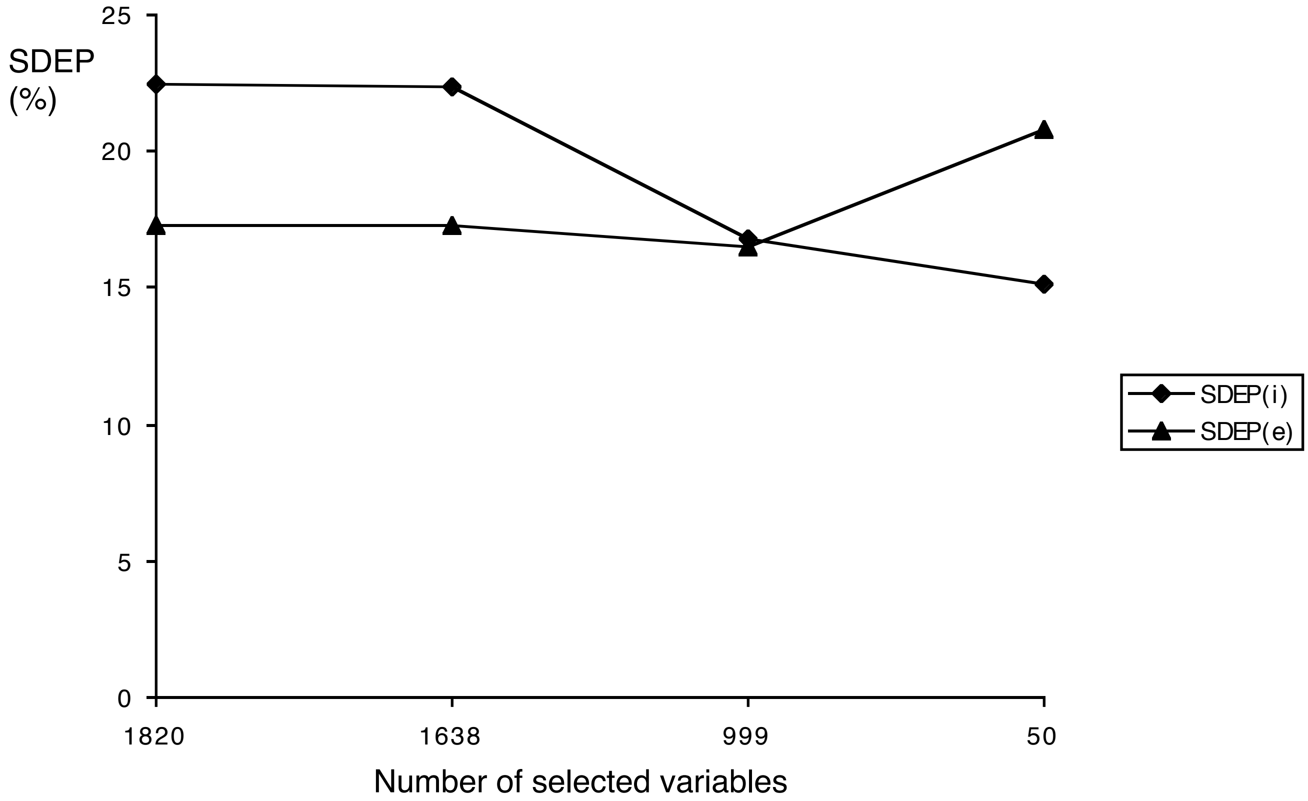

Figure 4**.** Comparison of internal (SDEP$_{(i)}$) and external (SDEP$_{(e)}$) standard deviations of errors in prediction as a function of the number of selected variables in the model. Results for three steps in variable selection are shown: 1) D-optimal selection (1820 -> 1638); 2) FFD selection without elimination of uncertain variables (1638 -> 999); 3) FFD selection with elimination of uncertain variables (999 -> 50). The B-G-C matrix and test set 1 (6 compounds) were used.