Benzimidazole-based derivatives as privileged scaffold developed for the treatment of the RSV infection: a computational study exploring the potency and cytotoxicity profiles

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SUPPLEMENTAL DATA

S1. $^1$H-NMR and $^{13}$C-NMR spectra. 2-[(1H-1,2,3-Benzotriazol-1-yl)methyl]-1-[2-(N,N-dimethylamino)ethyl]-5-methylbenzimidazole (157)
S2 $^1$H-NMR and $^{13}$C-NMR spectra. 2-[(1H-1,2,3-Benzotriazol-1-yl)methyl]-1-[(1S,9aR)-(octahydro-2H-quinolin-1-yl)ethyl]-5- methylbenzimidazole (158)
S3. Distribution of the predicted pEC$_{50}$ values of the training set compounds (a) and a representation of the experimental (blue dots and line) and predicted potency (dark orange dots and line) trend observed within the test set compounds (b), according to model A CoMFA analysis.
S4. Distribution of the predicted pEC₅₀ values of the training set compounds (a) and a representation of the experimental (blue dots and line) and predicted potency (dark orange dots and line) trend observed within the test set compounds (b), according to model A CoMSIA analysis.
S5. Distribution of the predicted pCC$_{50}$ values of the training set compounds (a) and a representation of the experimental (blue dots and line) and predicted potency (dark orange dots and line) trend observed within the test set compounds (b), according to model B CoMFA analysis.
S6. Distribution of the predicted pCC$_{50}$ values of the training set compounds (a) and a representation of the experimental (blue dots and line) and predicted potency (dark orange dots and line) trend observed within the test set compounds (b), according to model B CoMSIA analysis.
S7. Model A CoMSIA hydrophobic favoured (yellow area) and disfavoured (white area) regions are shown around the anti-RSV agents 44 (a) and 11 (b). The compounds are displayed in ball and stick mode (C atom: white).
S8. Model A CoMSIA H-bond acceptor favoured (magenta area) and disfavoured (red area) contour maps are displayed around benzimidazoles 44 (a) and 11 (b). The compounds are displayed in ball and stick mode (C atom: white).
S9. Model A CoMSIA H-bond donor favoured (cyan area) and disfavoured (purple area) contour maps are shown around the anti-RSV agents 44 (a) and 11 (b). The compounds are displayed in ball and stick mode (C atom: white).