Figures S1-S18. Figures showing the C&RT analysis for all models presented in Tables 7.2 and Tables 7.3 in Chapter 7

**Figure S1**. C&RT model selecting all molecular descriptors using TS1 training set with equal misclassification costs applied (Model 1)

**Figure S2.** C&RT model using TS1 with equal misclassification costs applied using descriptor set 1 (Model 2)

**Figure S3.** C&RT model using TS1 with equal misclassification costs applied using descriptor set 2 (Model 3)

**Figure S4.** C&RT model using TS1 with equal misclassification costs applied using descriptor set 4 (Model 4)

**Figure S5**. C&RT model selecting all molecular descriptors using TS1 training set with higher misclassification costs applied to reduce false positives (Model 5)

**Figure S6.** C&RT model using TS1 with higher misclassification costs applied to reduce false positives using descriptor set 1 (Model 6)

**Figure S7.** C&RT model using TS1 with higher misclassification costs applied to reduce false positives using descriptor set 2 (Model 7)

**Figure S8.** C&RT model using TS1 with higher misclassification costs applied to reduce false positives using descriptor set 4 (Model 8)

**Figure S9**. C&RT model selecting all molecular descriptors using TS1 training set with higher misclassification costs applied to reduce false negatives (Model 9)

**Figure S10.** C&RT model using TS1 with higher misclassification costs applied to reduce false negatives using descriptor set 1 (Model 10)

**Figure S11.** C&RT model using TS1 with higher misclassification costs applied to reduce false negatives using descriptor set 2 (Model 11)



**Figure S12.** C&RT model using TS1 with higher misclassification costs applied to reduce false negatives using descriptor set 4 (Model 12)

****

**Figure S13**. C&RT model selecting all molecular descriptors using TS2 training set with equal misclassification costs applied (Model 13)



**Figure S14.** C&RT model using TS2 with equal misclassification costs applied using descriptor set 3 (Model 13)

**Figure S15.** C&RT model using TS2 with equal misclassification costs applied using descriptor set 4 (Model 15)



**Figure S16**. C&RT model selecting all molecular descriptors using TS2 training set with higher misclassification costs applied to reduce false positives (Model 16)



**Figure S17.** C&RT model using TS2 with higher misclassification costs applied to reduce false positives using descriptor set 3 (Model 17)



**Figure S18.** C&RT model using TS2 with higher misclassification costs applied to reduce false positives using descriptor set 4 (Model 18)