**Figures A1-A8: C&RT analysis for all solubility models (Table 10.2) and permeability models (Table 10.3) presented in Chapter 10**

**Solubility Models (Table 10.2)**



**Figure A1**: Solubility model 1, equal misclassification costs applied



**Figure A2**: Solubility model 2, higher misclassification costs applied to reduce false positives

**Permeability Models (Table 10.3)**

**Figure A3**: Permeability model 1, equal misclassification costs applied



**Figure A4**: Permeability model 2, using predicted solubility from solubility model 1 with equal misclassification costs applied



**Figure A5**: Permeability model 3, using predicted solubility from solubility model 2 with equal misclassification costs applied



**Figure A6**: Permeability model 4, with higher misclassification costs applied to reduce false positives



**Figure A7**: Permeability model 5, using predicted solubility from solubility model 1 with higher misclassification costs applied to reduce false positives



**Figure A8**: Permeability model 6, using predicted solubility from solubility model 2 with higher misclassification costs applied to reduce false positives