Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

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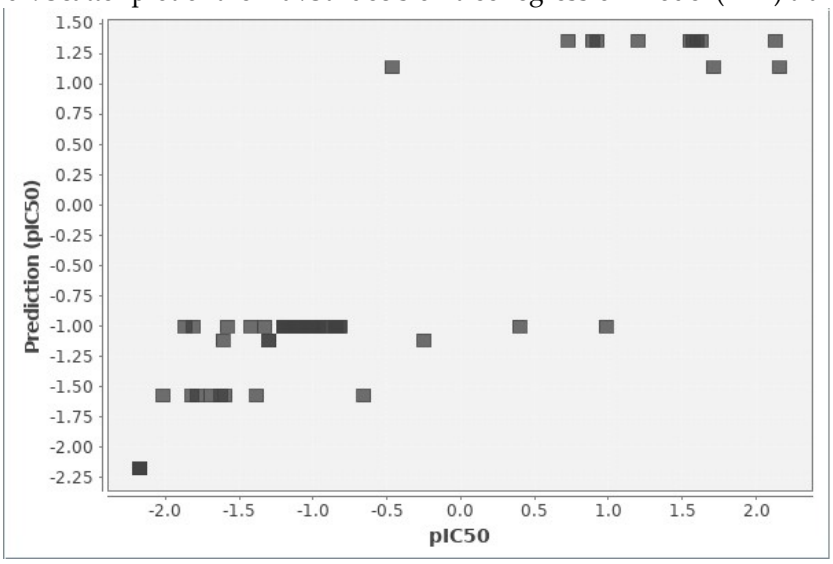
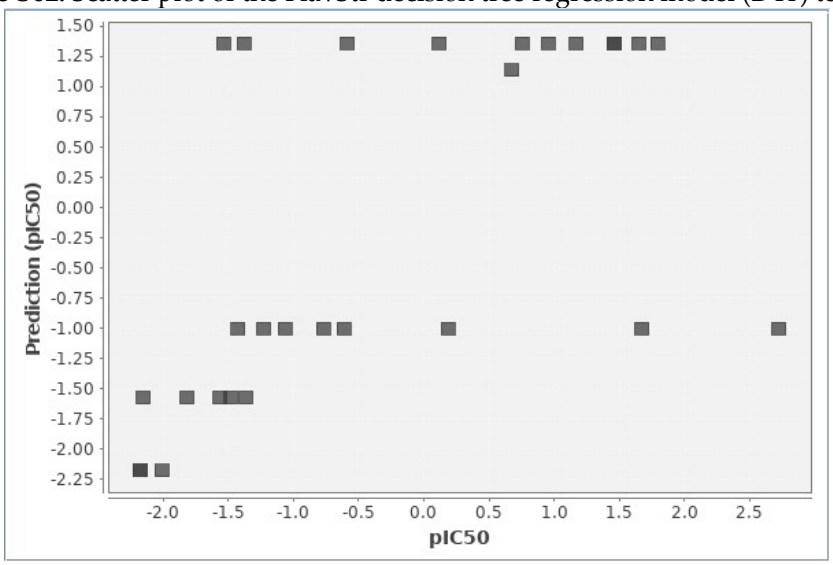
Figure S61. Scatter plot of the FlavStr decision tree regression model (DTr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

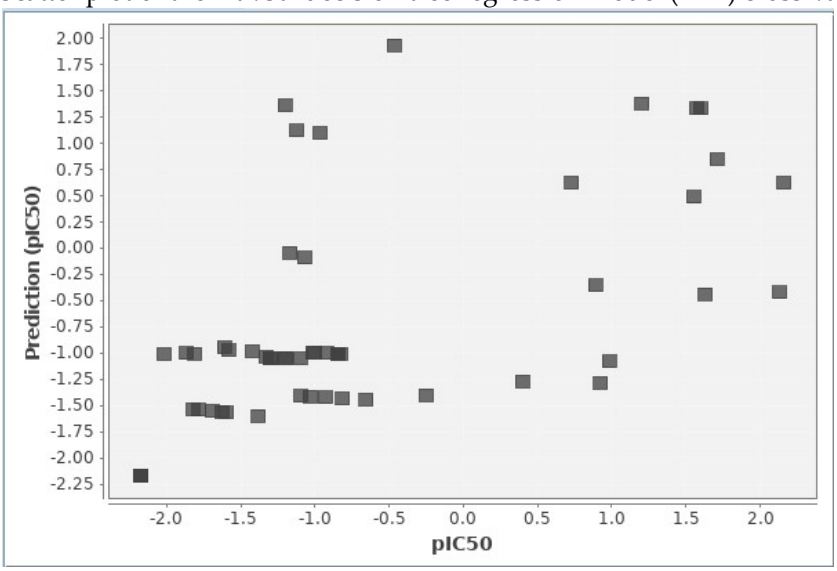
Figure S62. Scatter plot of the FlavStr decision tree regression model (DTr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

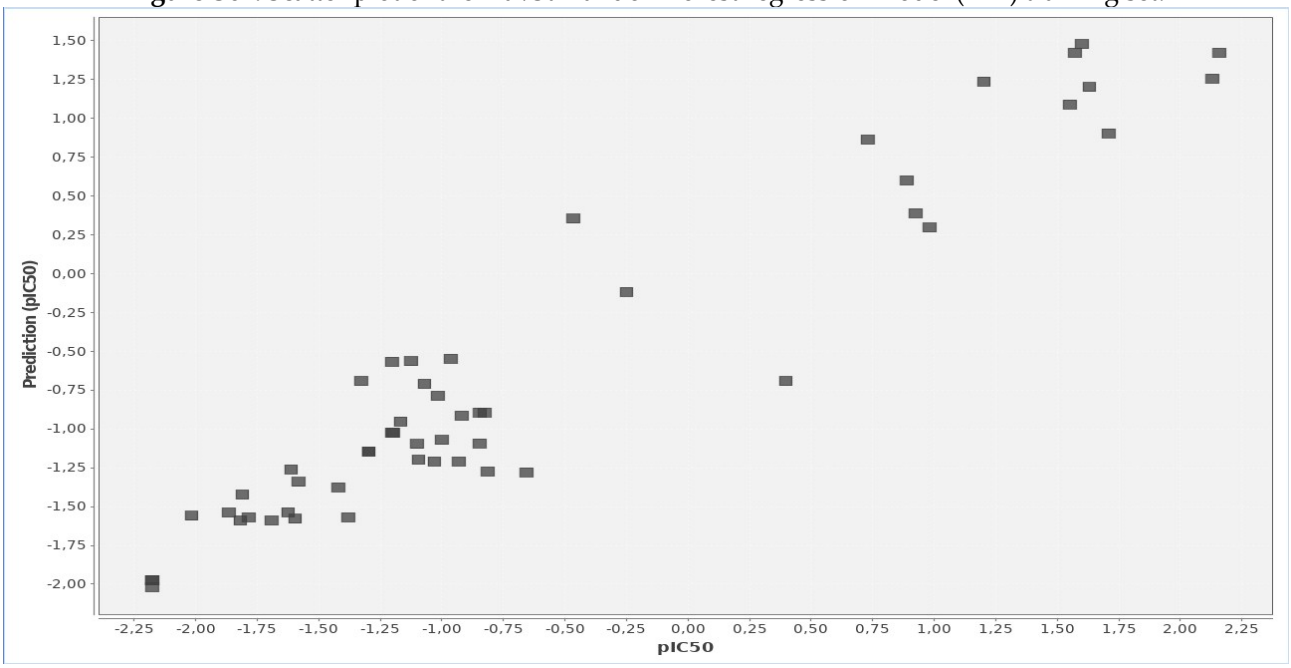
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S63. Scatter plot of the FlavStr decision tree regression model (DTr) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

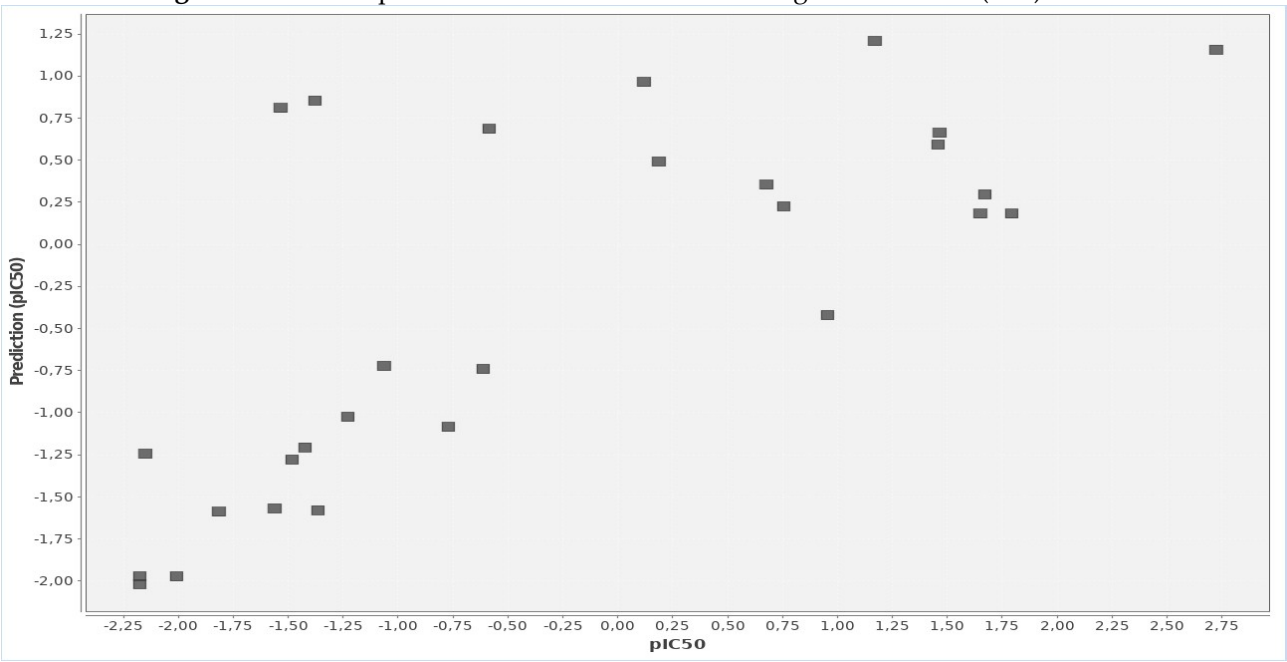
Figure S64. Scatter plot of the FlavStr random forest regression model (RFr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

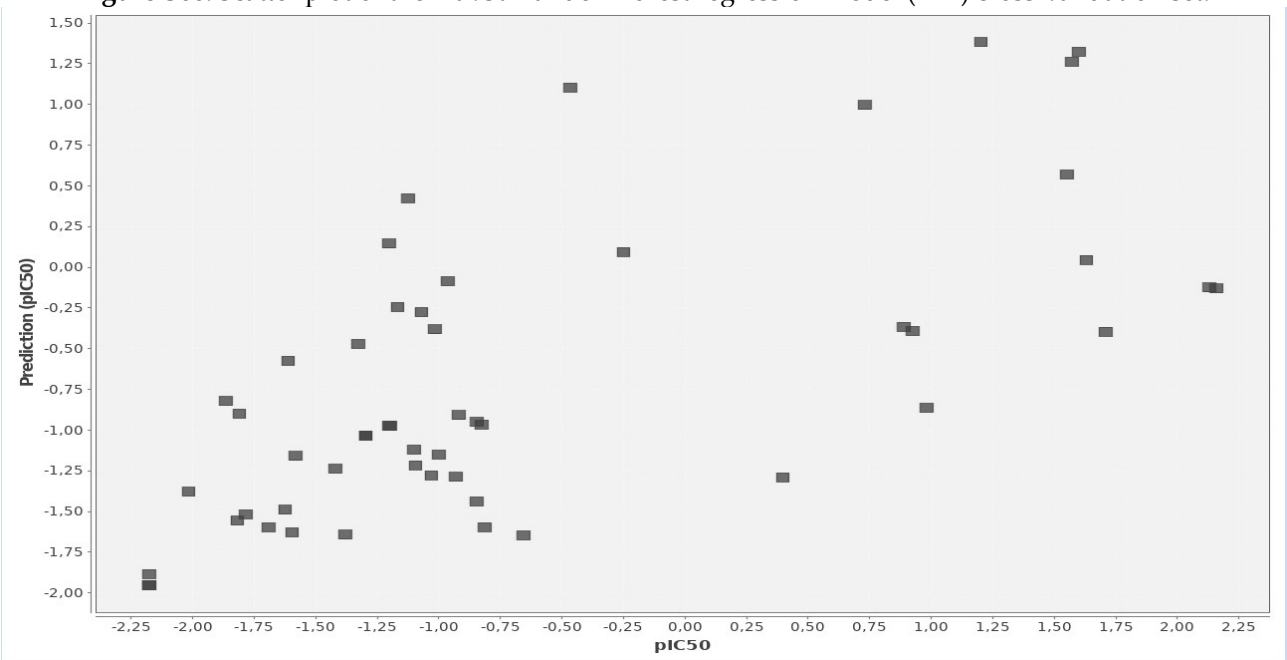
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S65. Scatter plot of the FlavStr random forest regression model (RFr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

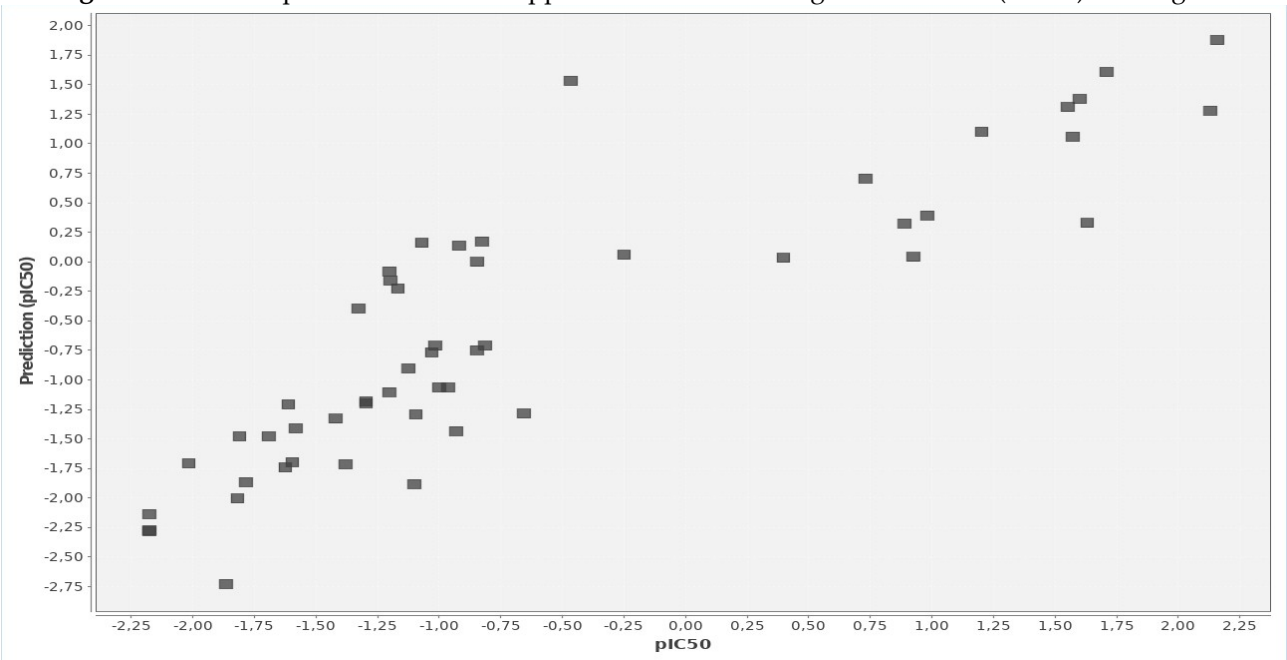
Figure S66. Scatter plot of the FlavStr random forest regression model (RFr) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

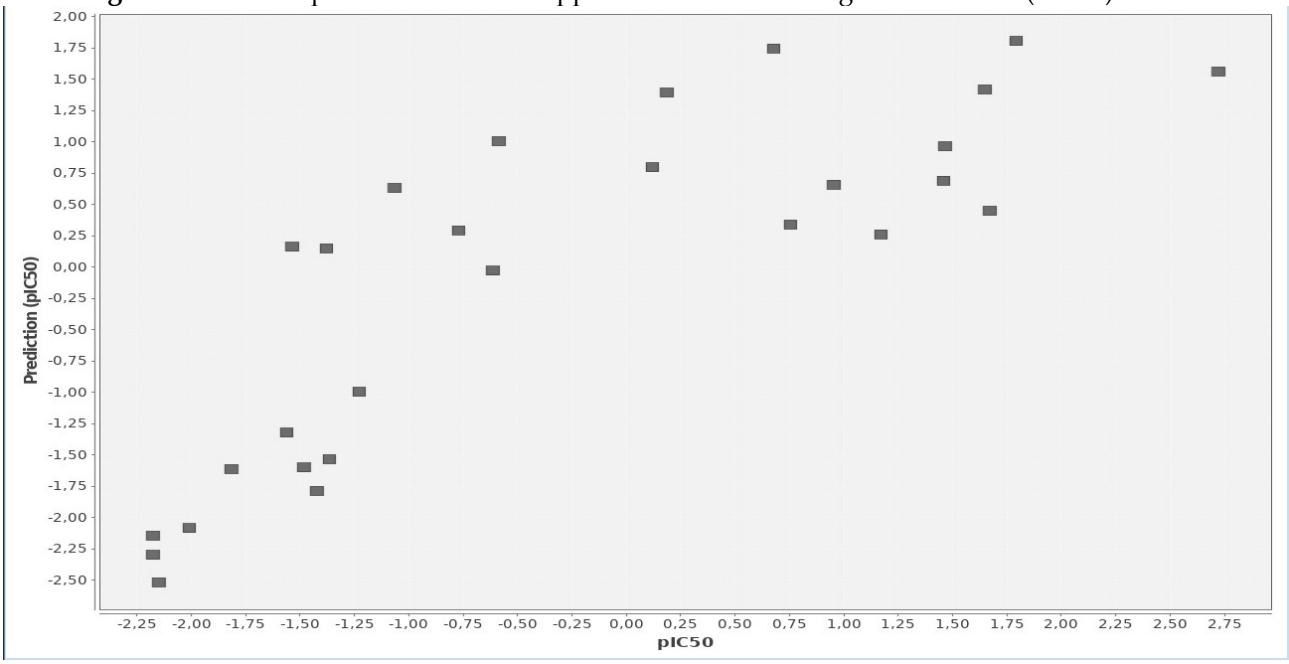
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S67. Scatter plot of the FlavStr support vector machine regression model (SVMr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

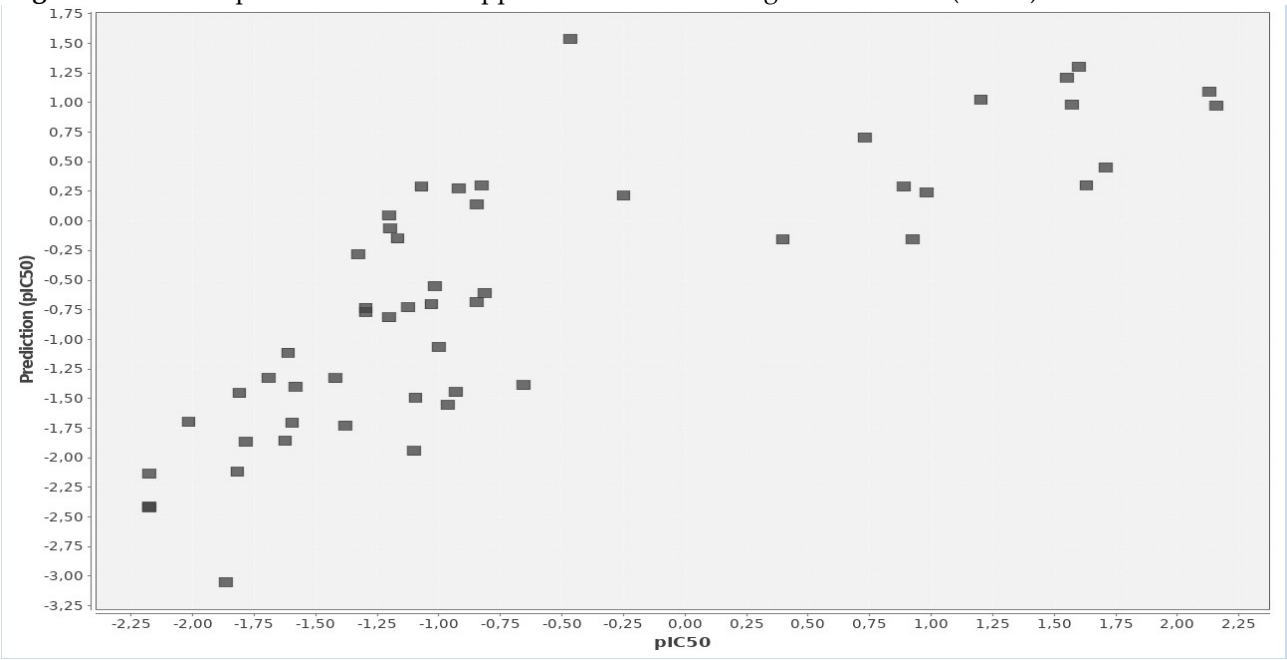
Figure S68. Scatter plot of the FlavStr support vector machine regression model (SVMr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

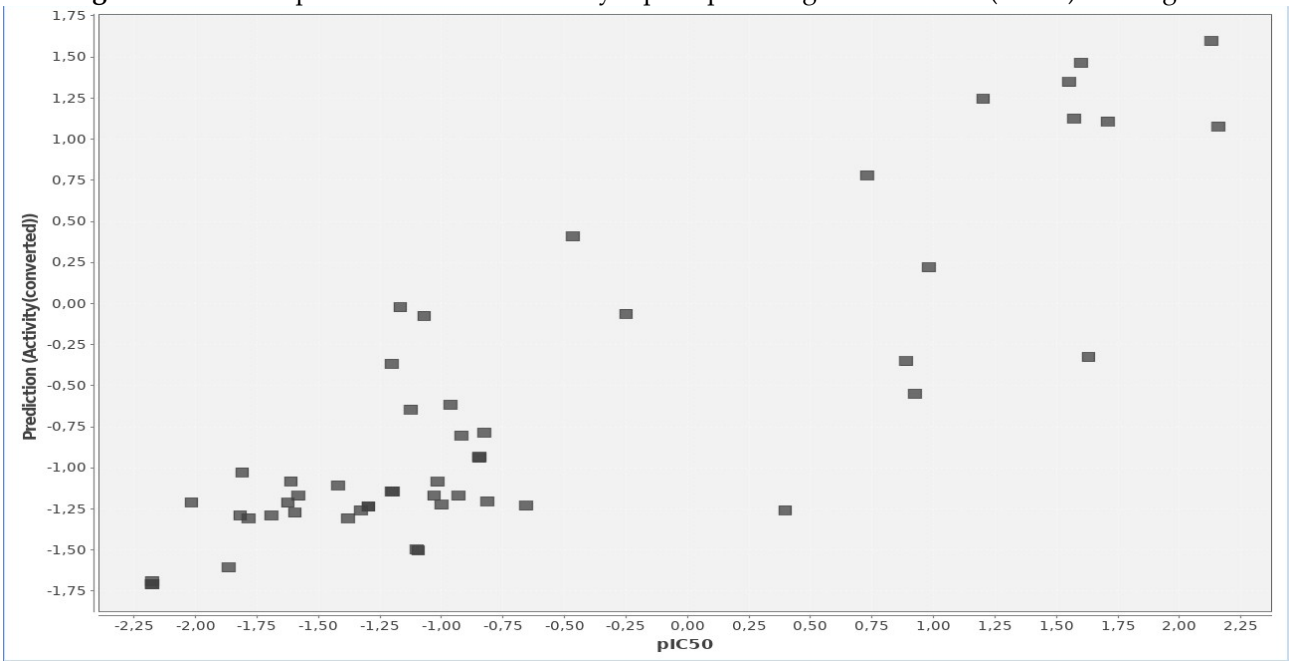
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S69. Scatter plot of the FlavStr support vector machine regression model (SVMr) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

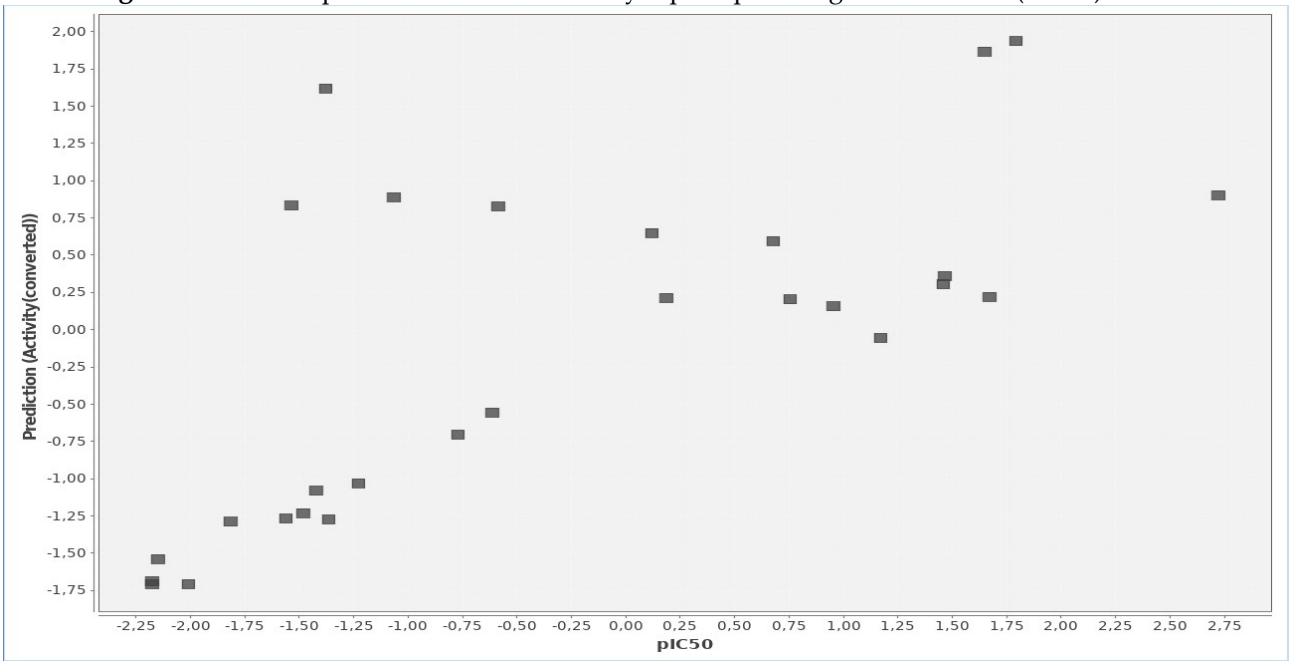
Figure S70. Scatter plot of the FlavStr multilayer perceptron regression model (MLPr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

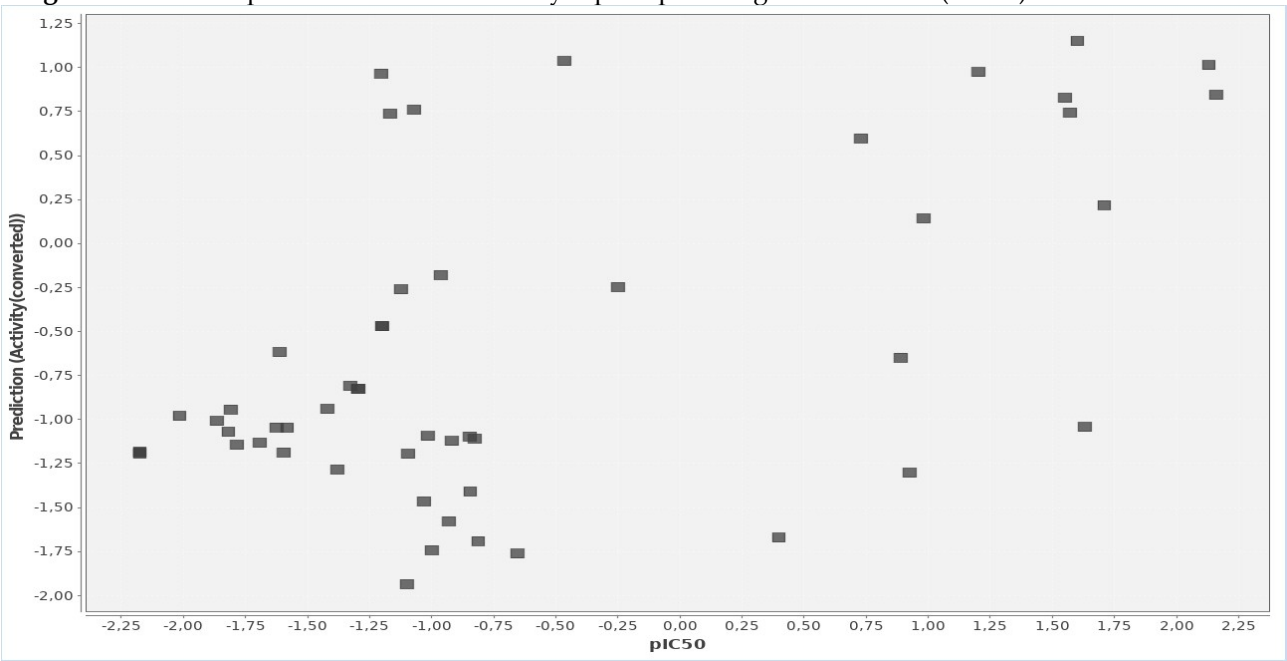
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S71. Scatter plot of the FlavStr multilayer perceptron regression model (MLPr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

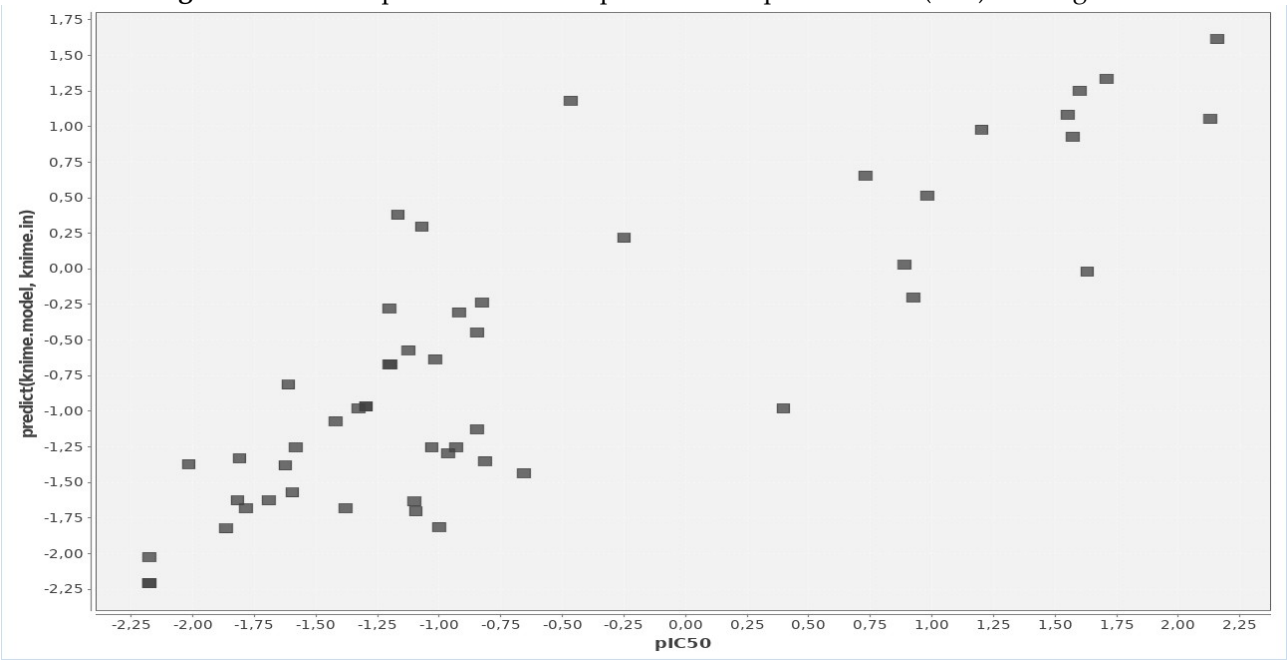
Figure S72. Scatter plot of the FlavStr multilayer perceptron regression model (MLPr) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

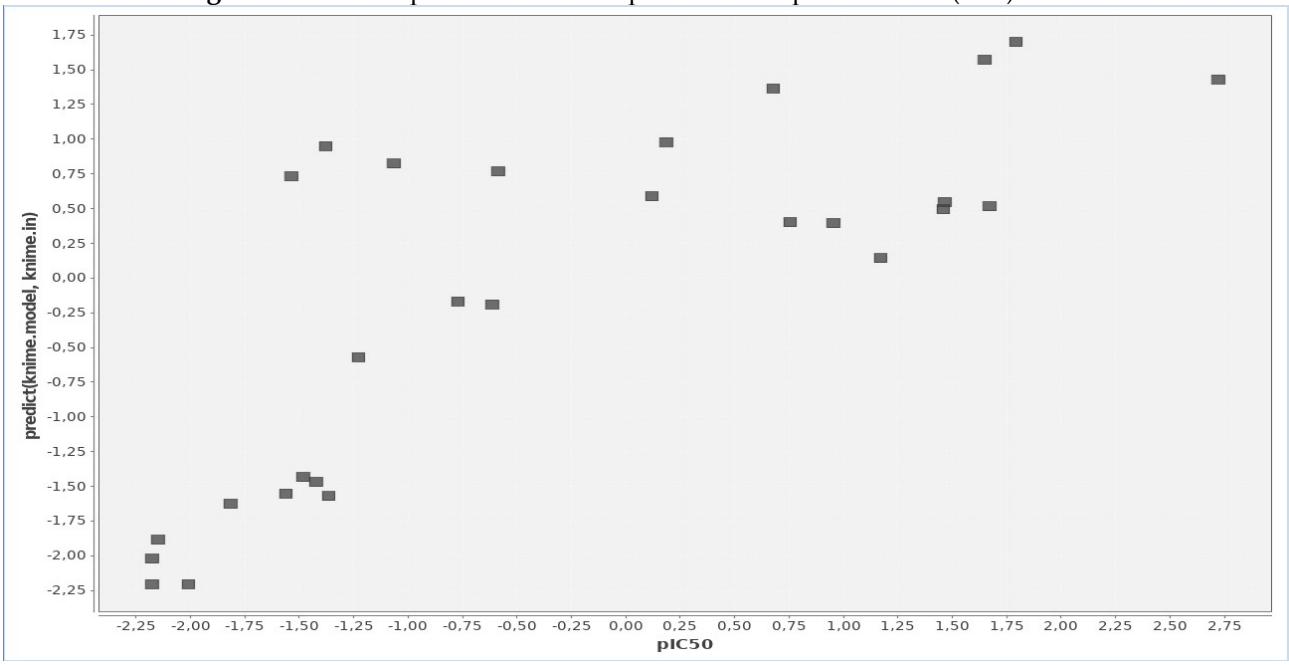
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S73. Scatter plot of the FlavStr partial least squares model (PLS) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

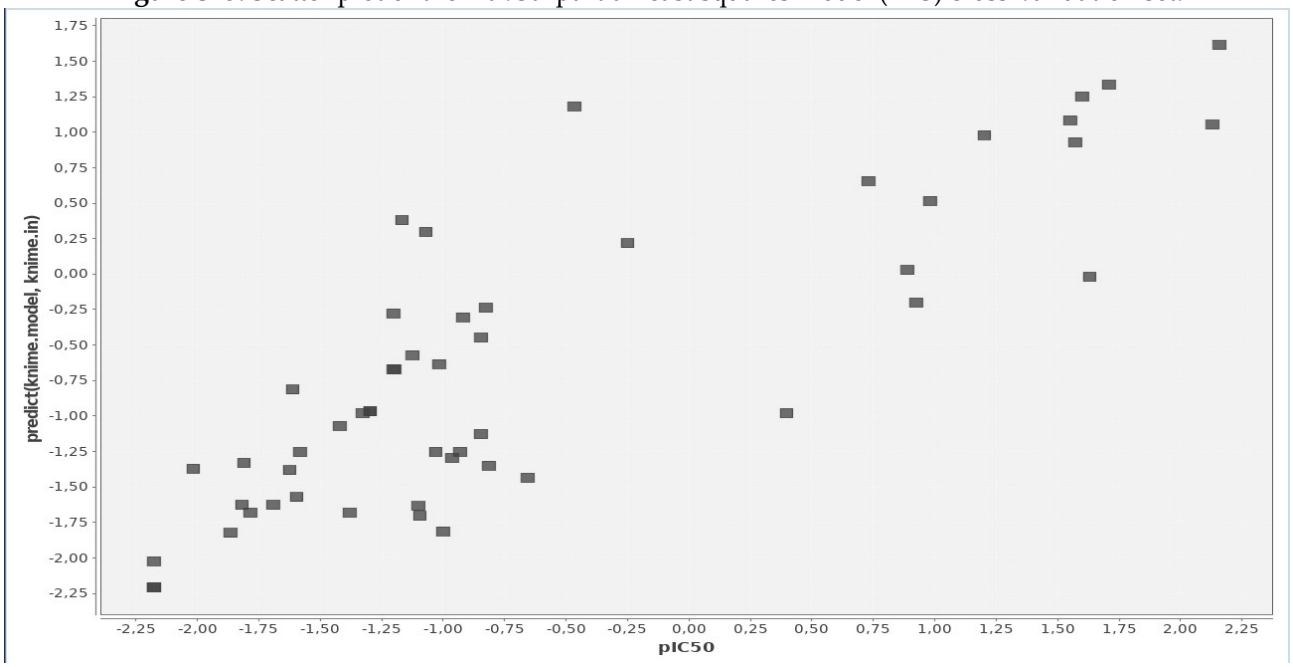
Figure S74. Scatter plot of the FlavStr partial least squares model (PLS) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

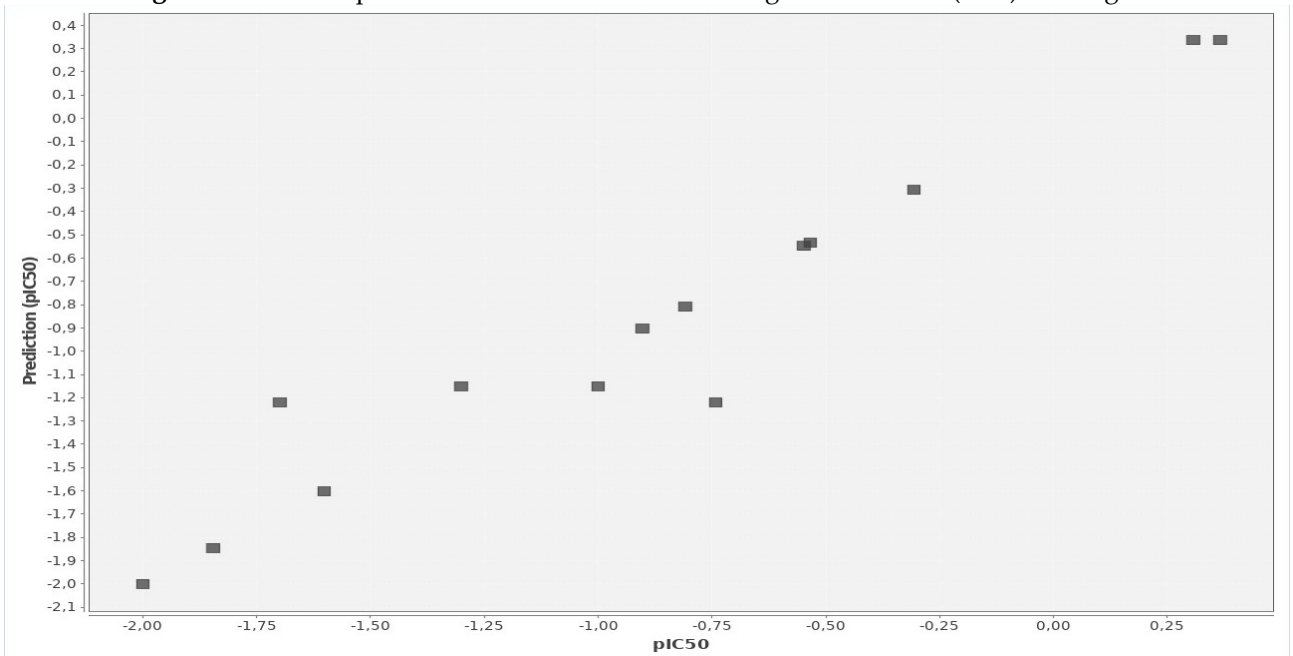
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S75. Scatter plot of the FlavStr partial least squares model (PLS) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

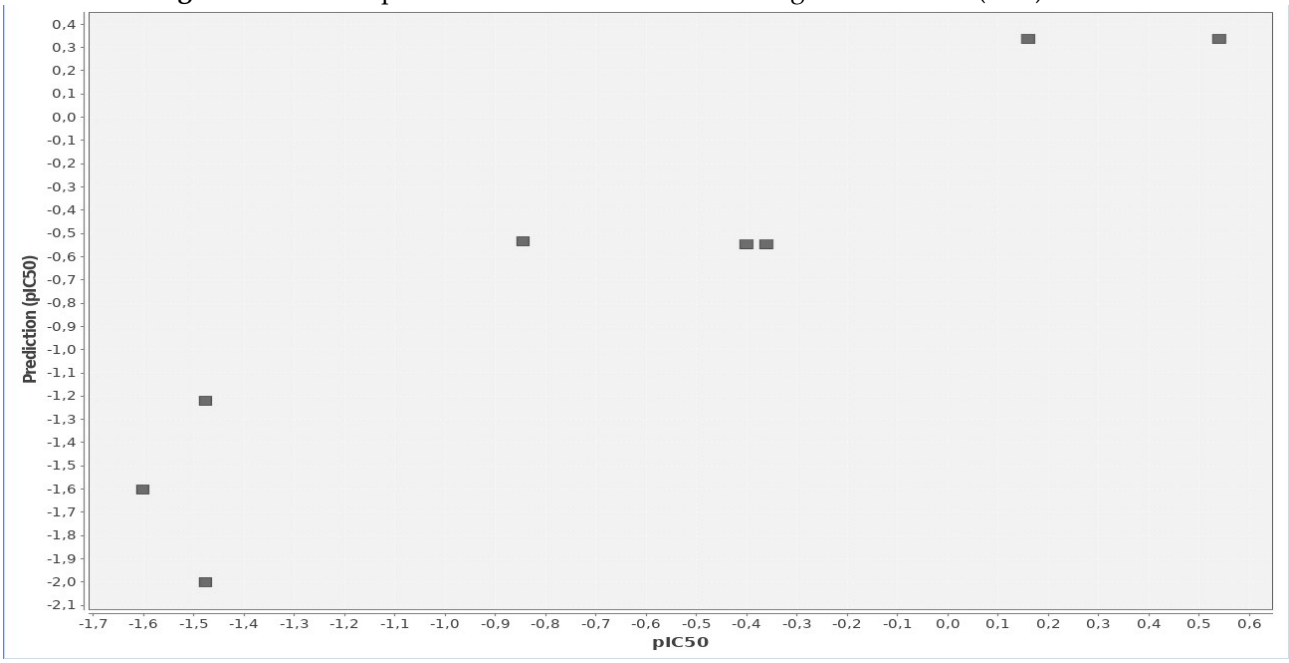
Figure S76. Scatter plot of the FlavEnz decision tree regression model (DTr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

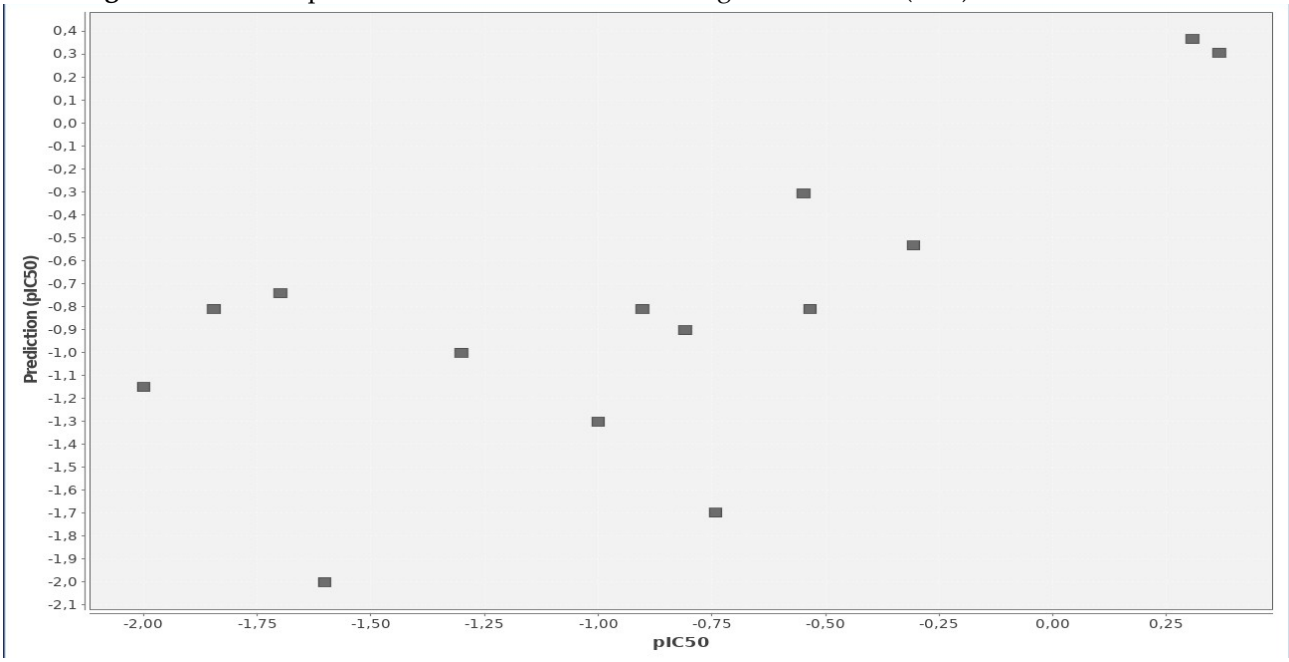
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S77. Scatter plot of the FlavEnz decision tree regression model (DTr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

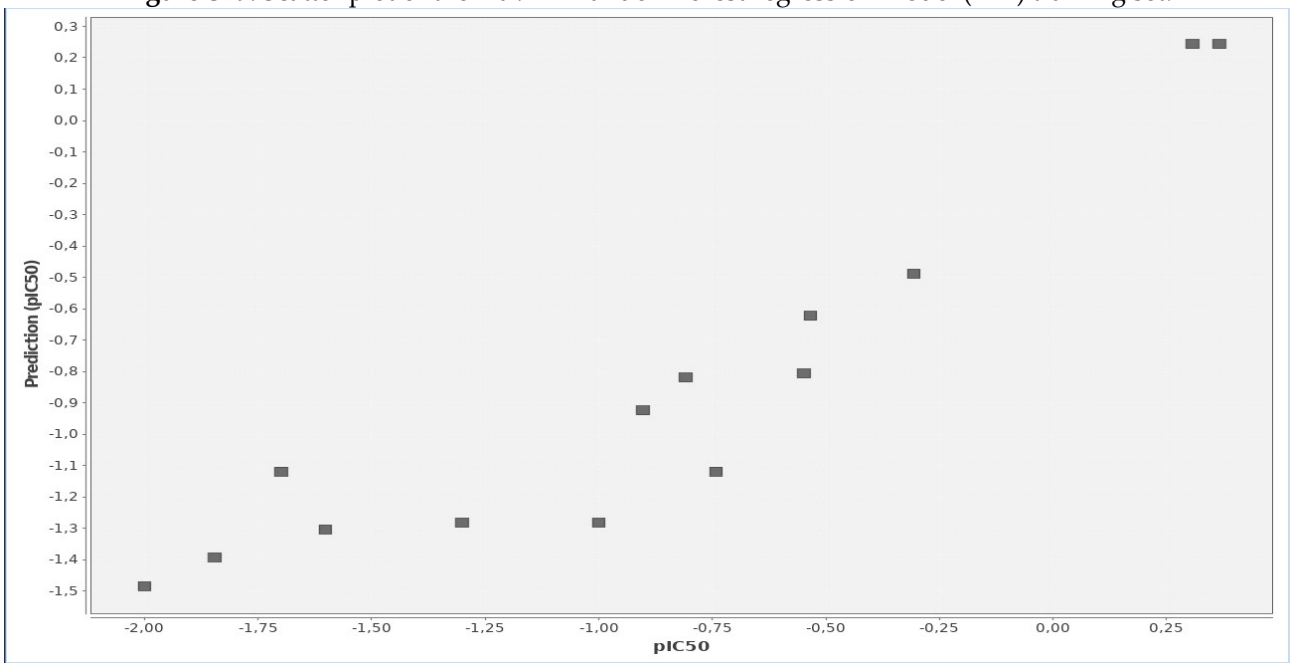
Figure S78. Scatter plot of the FlavEnz decision tree regression model (DTr) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

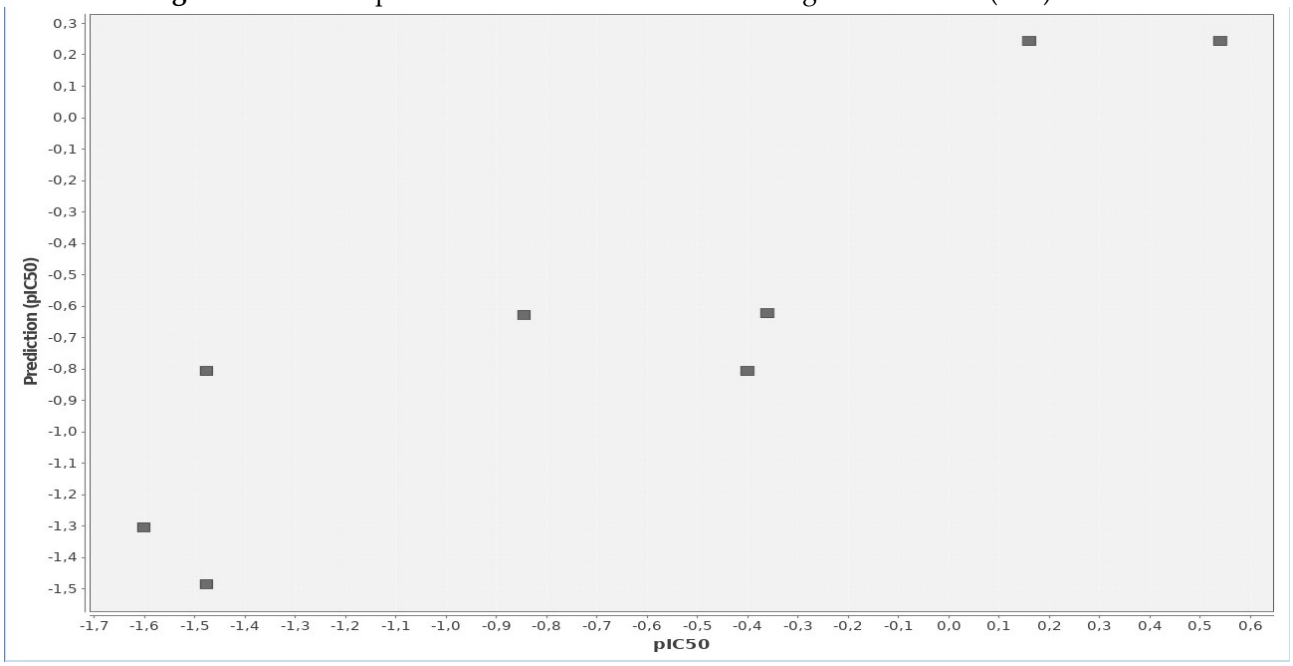
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S79. Scatter plot of the FlavEnz random forest regression model (RFr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

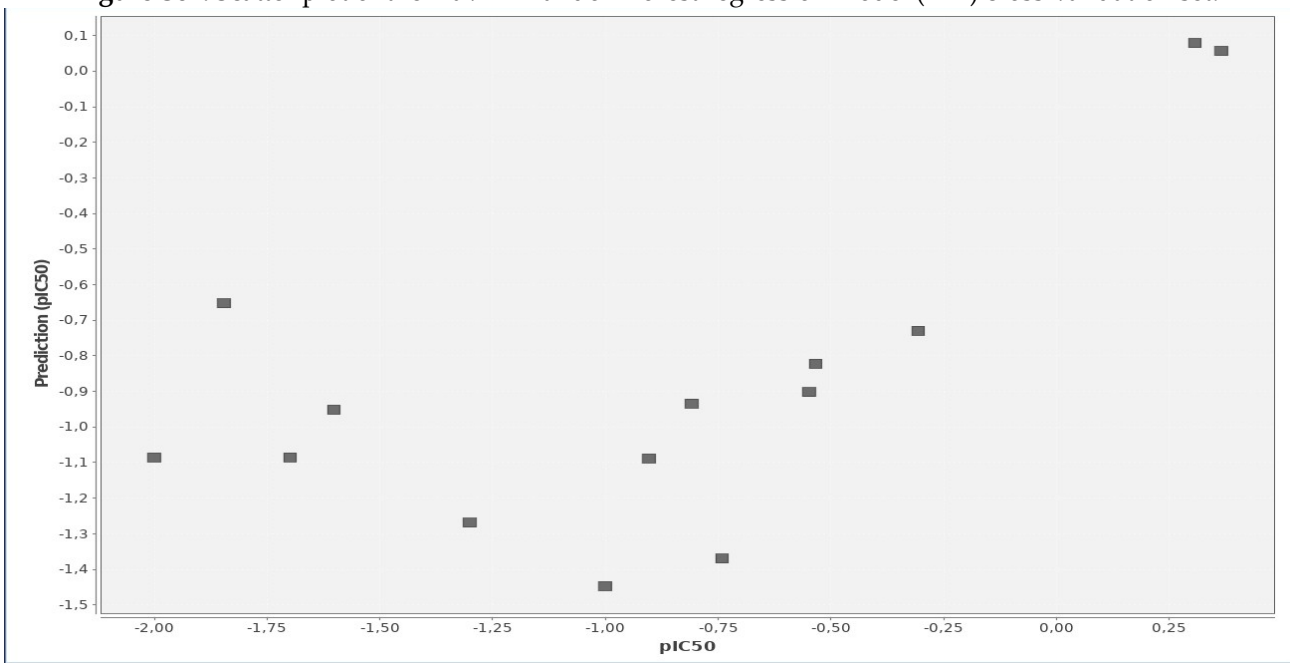
Figure S80. Scatter plot of the FlavEnz random forest regression model (RFr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

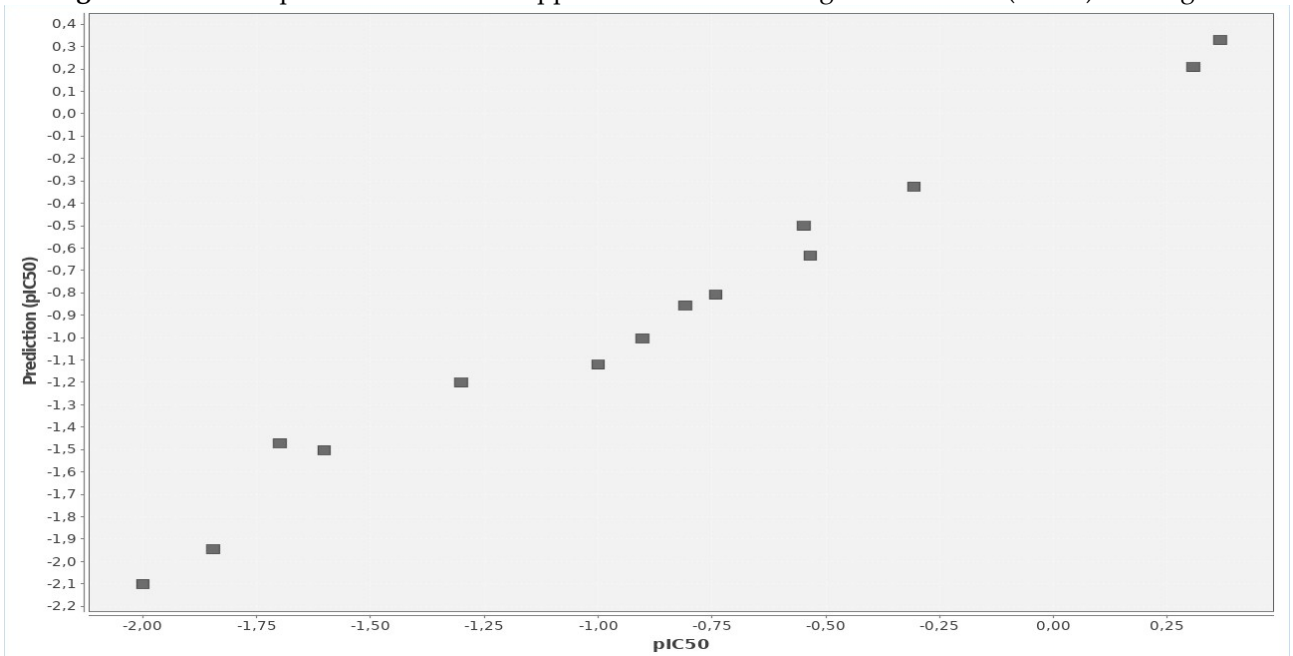
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S81. Scatter plot of the FlavEnz random forest regression model (RFr) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

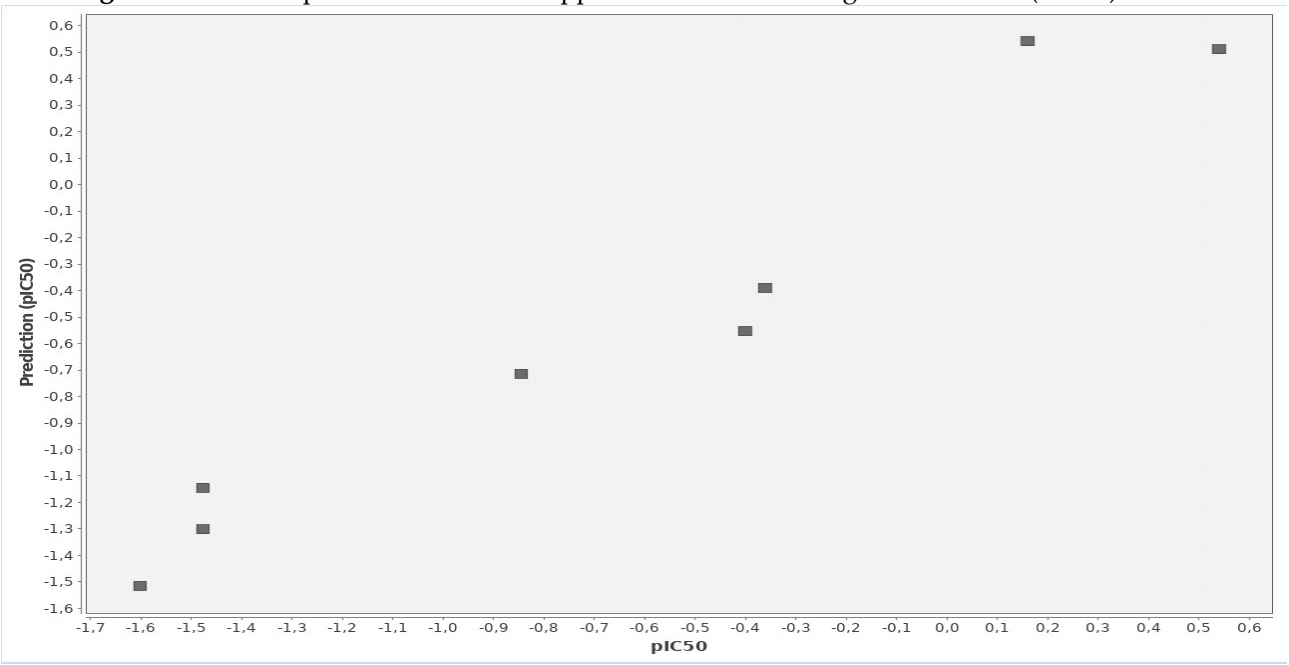
Figure S82. Scatter plot of the FlavEnz support vector machine regression model (SVMr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

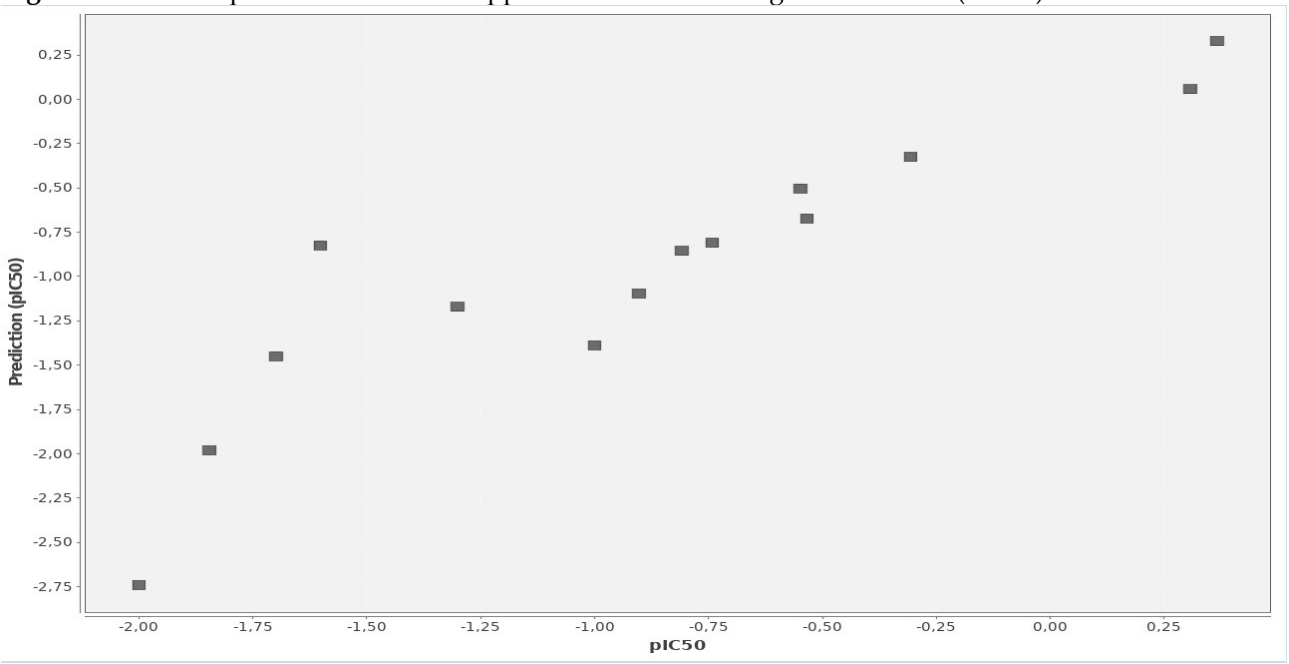
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S83. Scatter plot of the FlavEnz support vector machine regression model (SVMr) test set.



The x axis represents the real pIC_{50} values, while the y axis represents the predicted pIC_{50} values.

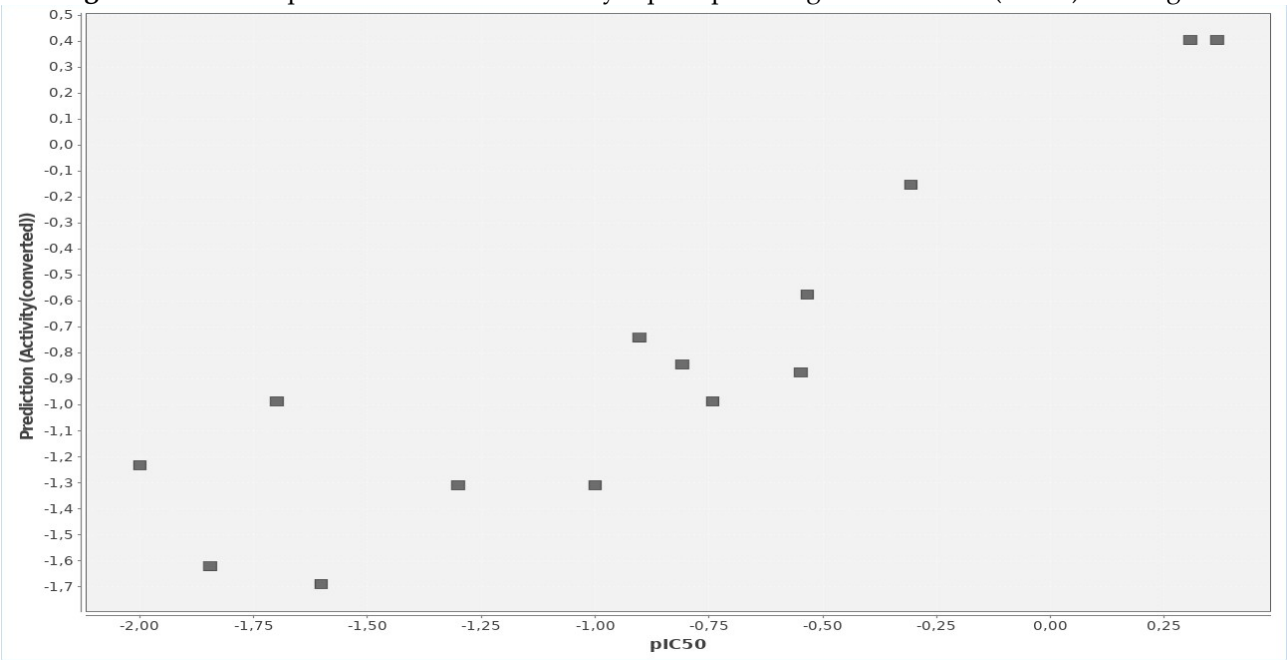
Figure S84. Scatter plot of the FlavEnz support vector machine regression model (SVMr) cross-validation set.



The x axis represents the real pIC_{50} values, while the y axis represents the predicted pIC_{50} values.

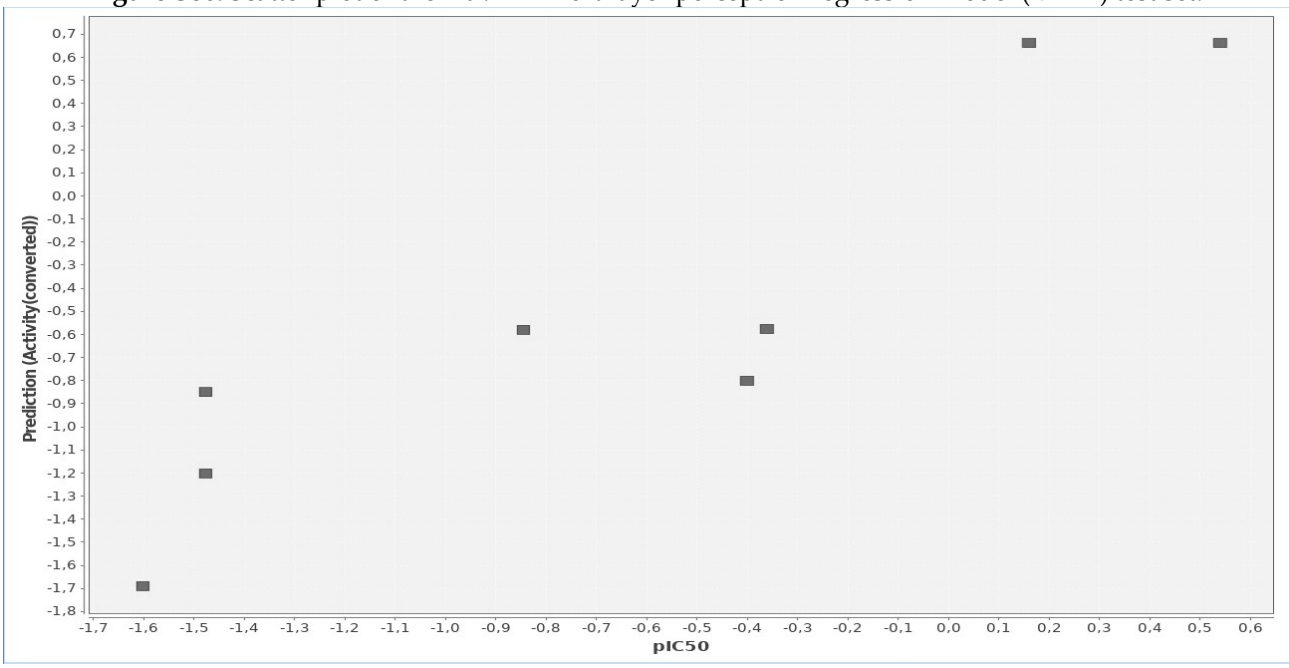
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S85. Scatter plot of the FlavEnz multilayer perceptron regression model (MLPr) training set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

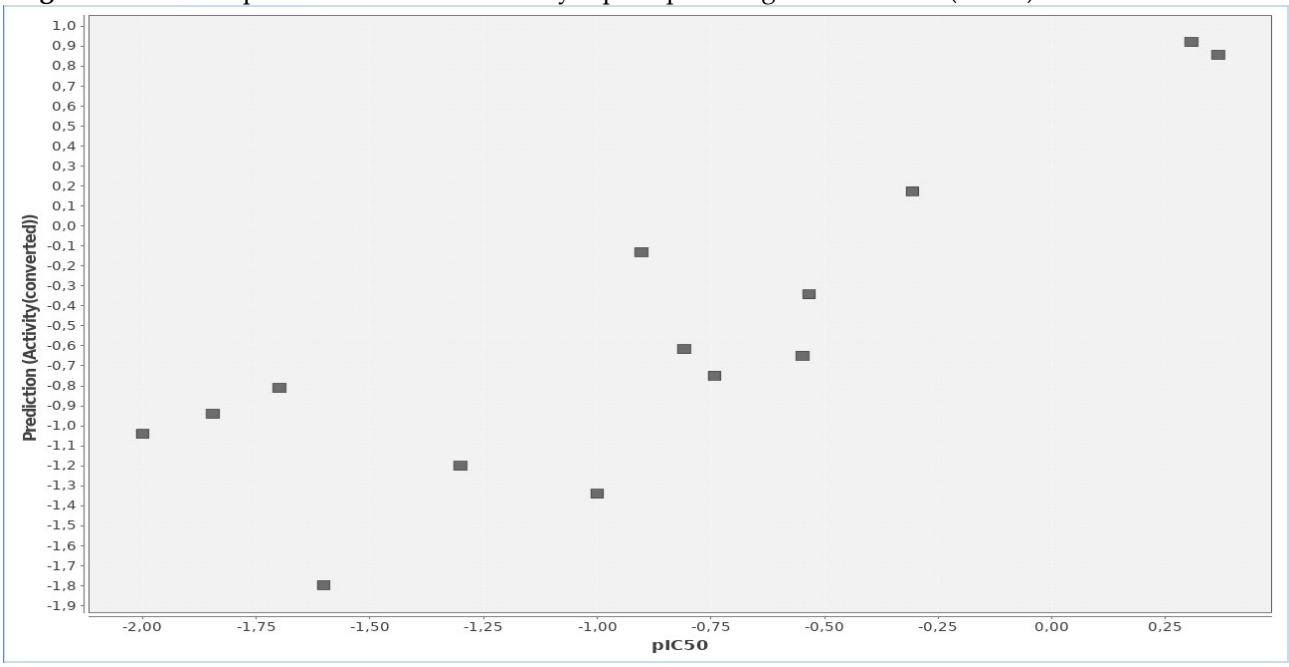
Figure S86. Scatter plot of the FlavEnz multilayer perceptron regression model (MLPr) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

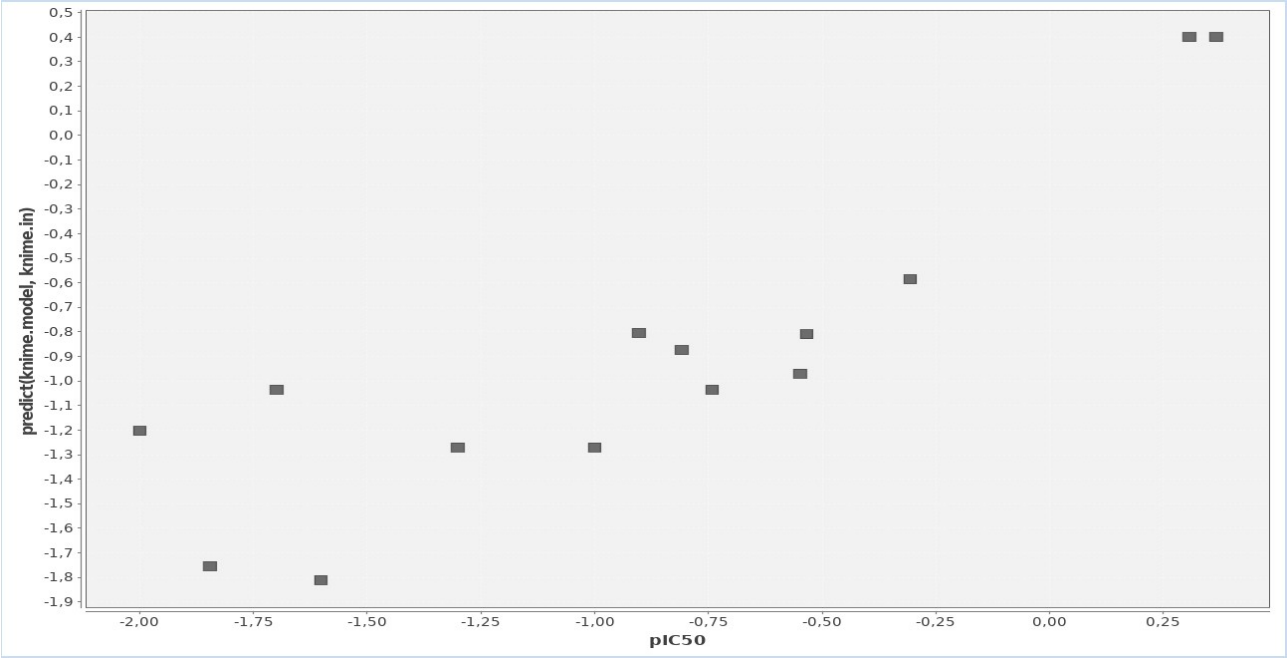
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S87. Scatter plot of the FlavEnz multilayer perceptron regression model (MLPr) cross-validation set.



The x axis represents the real pIC_{50} values, while the y axis represents the predicted pIC_{50} values.

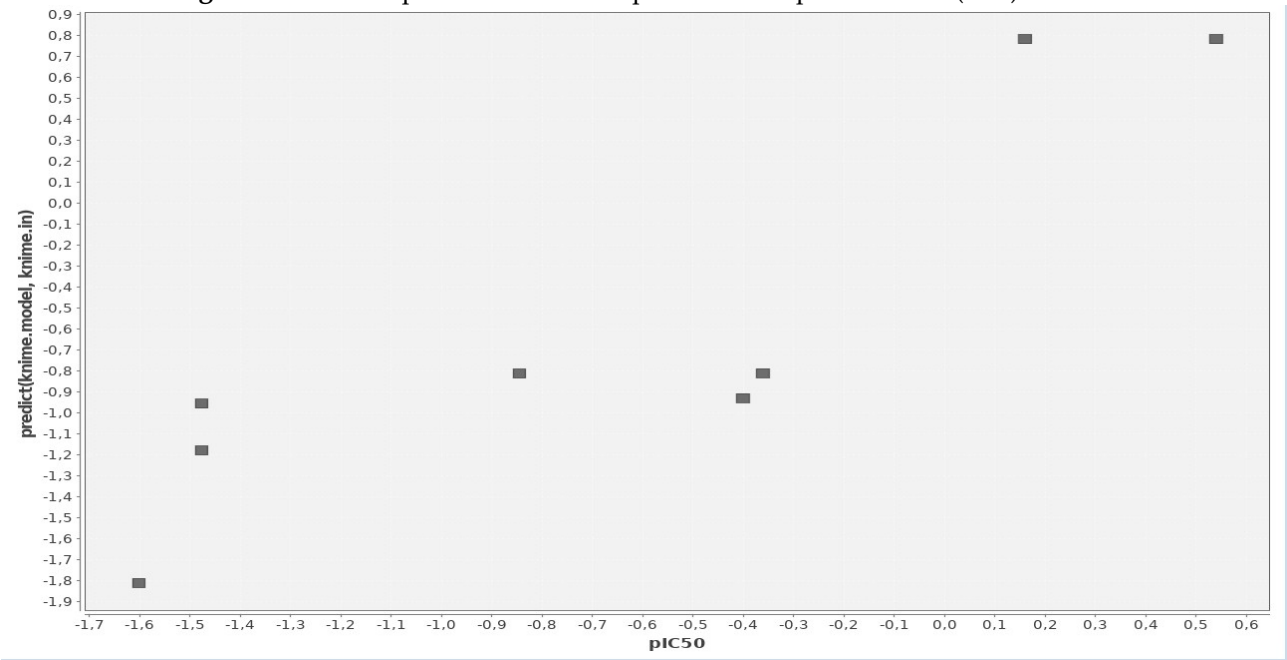
Figure S88. Scatter plot of the FlavEnz partial least squares model (PLS) training set.



The x axis represents the real pIC_{50} values, while the y axis represents the predicted pIC_{50} values.

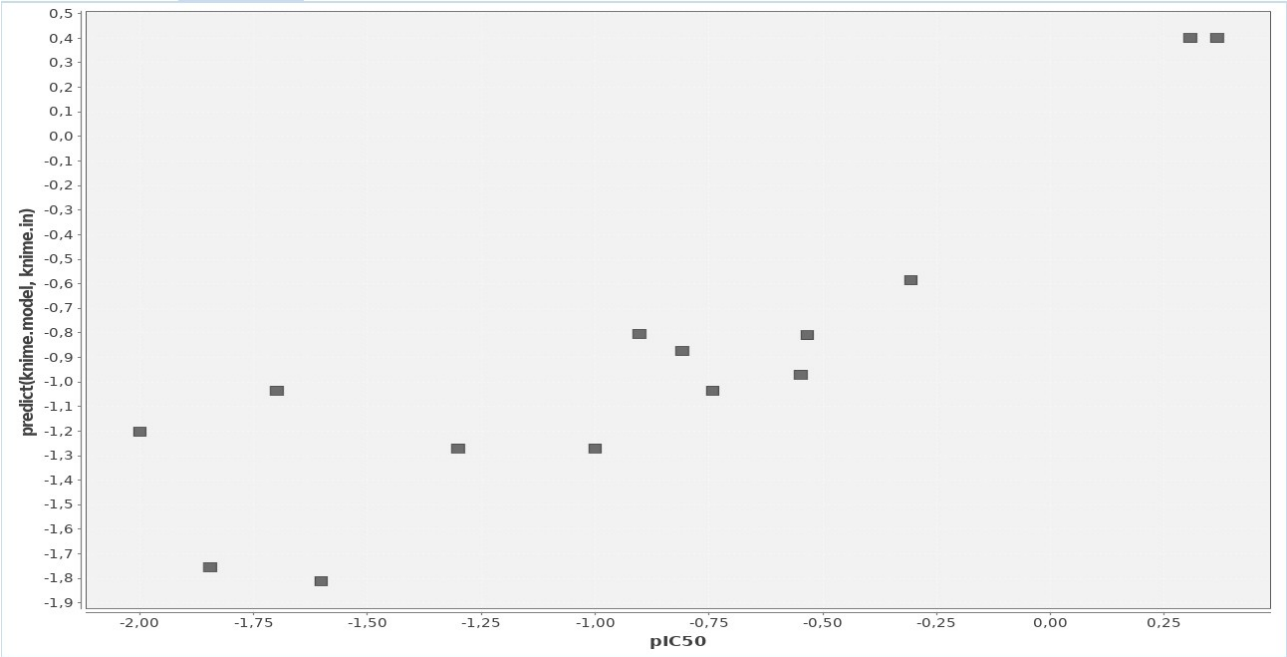
Identification of Pharmacophore Groups with Antimalarial Potential in Flavonoids by QSAR-Based Virtual Screening - Scatter plots

Figure S89. Scatter plot of the FlavEnz partial least squares model (PLS) test set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.

Figure S90. Scatter plot of the FlavEnz partial least squares model (PLS) cross-validation set.



The *x* axis represents the real pIC_{50} values, while the *y* axis represents the predicted pIC_{50} values.