Article

Cinnamic Derivatives as Antitubercular Agents: Characterization by Quantitative Structure-Activity Relationship Studies

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**Table S1.** Range of variability of descriptors for the training and test sets.

|  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- |
| **Sets** | **Max or min values for descriptors**  **in set** | **pMIC** | ***a3*** | ***a1*** | ***Polar Surface area*** | ***Hanse Polarity parameter*** |
| **Training** | max | 6.5849 | 121.721 | 120.818 | 86.64 | 7.7686 |
| min | 2.8067 | 109.802 | 112.361 | 40.46 | 2.9472 |
| **Test** | max | 6.5229 | 121.721 | 120.760 | 91.18 | 8.1976 |
| min | 3.0223 | 107.325 | 112.127 | 54.38 | 3.0740 |

**Table S2.** Results of the Y-randomization (30 shuffles) and the QUIK rule for the best model.

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| Y-randomization | 0.909 | 0.139 | 0.837 |
| QUIK rule | Kxy = 35.17 > Kx = 30.26 | | |

**Table S3.** Intercorrelation matrix between any two descriptors and between one descriptor and a linear combination of all other descriptors. The outliers were not considered to compute these matrix values.

|  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- |
| Descriptors | a3 | a1 | PSA | HansPol | Linear combination with all other 3 descriptors |
| a3 |  | 0.350 | 0.035 | 0.363 | 0.363 |
| a1 |  |  | 0.022 | 0.004 | 0.353 |
| PSA |  |  |  | 0.065 | 0.109 |
| HansPol |  |  |  |  | 0.080 |