

Supporting Information

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Digital filters for molecular interaction field descriptors

## **Support Information**

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**Figure S1**. Dendograms derived from the Hierarchical Cluster Analysis used to determine the training and test sets. The samples assign in red were chosen to compose the test set.



**Figure S2**. Grid points left, for dataset (1), after using correlation cutoffs on the LJ (A) and Coulomb (B) fields.



**Figure S3**. Grid points left, for dataset (2), after using correlation cutoffs on the LJ (A) and Coulomb (B) fields.



Figure S4. Grid points left, for dataset (2), after using CDDA cutoffs on the LJ (A) and Coulomb (B) fields.



**Figure S5**. The best PLS model for data set (2). Negatively correlated descriptors are depicted in red, and positive ones in blue. Red and dark blue are Coulomb descriptors and light blue sphere denote a single LJ descriptor.



Figure S6. Validation graphs for the final model for dataset (2).



**Figure S7**. Grid points left, for dataset (3), after using correlation cutoffs on the LJ (A) and Coulomb (B) fields.



Figure S8. Grid points left, for dataset (3), after using CDDA cutoffs on the LJ (A) and Coulomb (B) fields.



**Figure S9**. The best PLS model for data set (3). Negatively correlated descriptors are depicted in red, and blue ones denote positively correlated descriptors. Red and dark blue are Coulomb descriptors. The light blue spheres denote LJ descriptors.



Figure S10. Validation graphs for the final model for dataset (3).

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