Supporting Information

Bimolecular Nucleophilic Substitution Reactions: Predictive Models for Rate Constants and Molecular Reaction Pairs Analysis

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Supporting information

1. Description of 10 best individual models selected for consensus calculations

Model N	Fragmentation type	Kernel type	RMSE, ($\log k$)	Q^2
1	Sequences of atoms and bonds; length min=1, max=6, explicit charges	Gaussian	0.38± 0.008	0.89± 0.004
2	Atom centered fragments based on sequences of bonds; length min=1, max=3; explicit charges	Gaussian	0.4± 0.011	0.88± 0.007
3	Sequences of atoms and bonds; length min=2, max=6, explicit charges	Gaussian	0.39± 0.006	0.88± 0.006
4	Augmented atoms; sphere radius min=1, max=6; explicit charges	Gaussian	0.42± 0.014	0.87± 0.009
5	Sequences of atoms and bonds; length min=2, max=6;	Gaussian	0.4± 0.007	0.88± 0.005
6	Augmented atoms; sphere radius min=1, max=7;	Polynomial	0.4± 0.016	0.89± 0.009
7	Sequences of atoms and bonds, min=3, max=4;	Polynomial	0.41± 0.014	0.87± 0.008
8	Sequences of atoms and bonds; length min=2, max=6, explicit charges; all possible	Gaussian	0.42± 0.008	0.87± 0.005

	sequences;			
9	Sequences of atoms and bonds; length min=1, max=7, explicit charges	Gaussian	0.41± 0.009	0.87± 0.005
10	Sequences of atoms and bonds; length min=1, max=6, explicit charges	Polynomial	0.42± 0.008	0.87± 0.005

2. Description of Web interface for models' application.

For model publication, in-house client-server application has been developed. A client side description is described below.

The model's application to a query reaction proceeds in 3 steps: structure preparation, setting the condition (solvent, temperature and pressure) and analysis of the results. The first page of predictor contains User manual and tools for interactive building and uploading of chemical structures (the **Add** task, Figure S1).

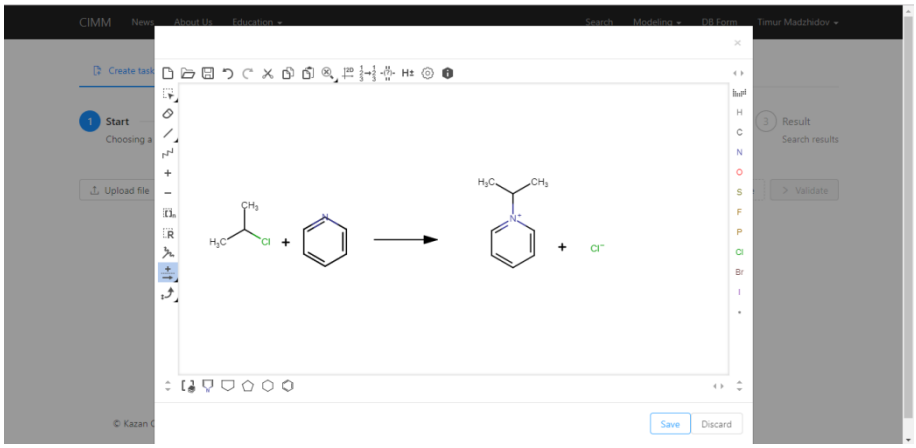

Figure S1. Interactive preparation of query reaction with *Marvin Web*.

Then, the one should click the button "**Validate**" (Figure S2) which launches procedures of structure verification, structure standardization and atom-to-atom mapping.

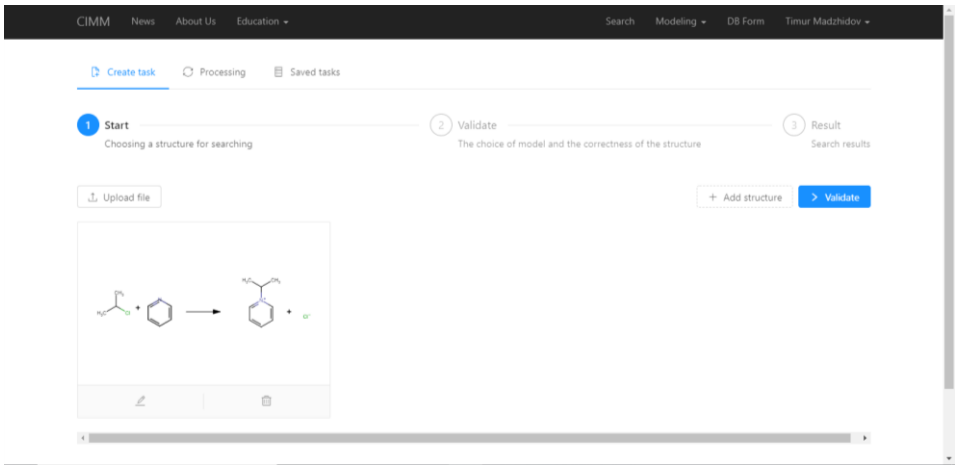

Figure S2. Structure validation step.

At the next stage, the user is invited to entry the parameters needed to perform the calculations for a query reaction: a particular model (in our case, this is the model for the rate constant of SN2 reaction), temperature, pressure and solvent (see Figure S3)

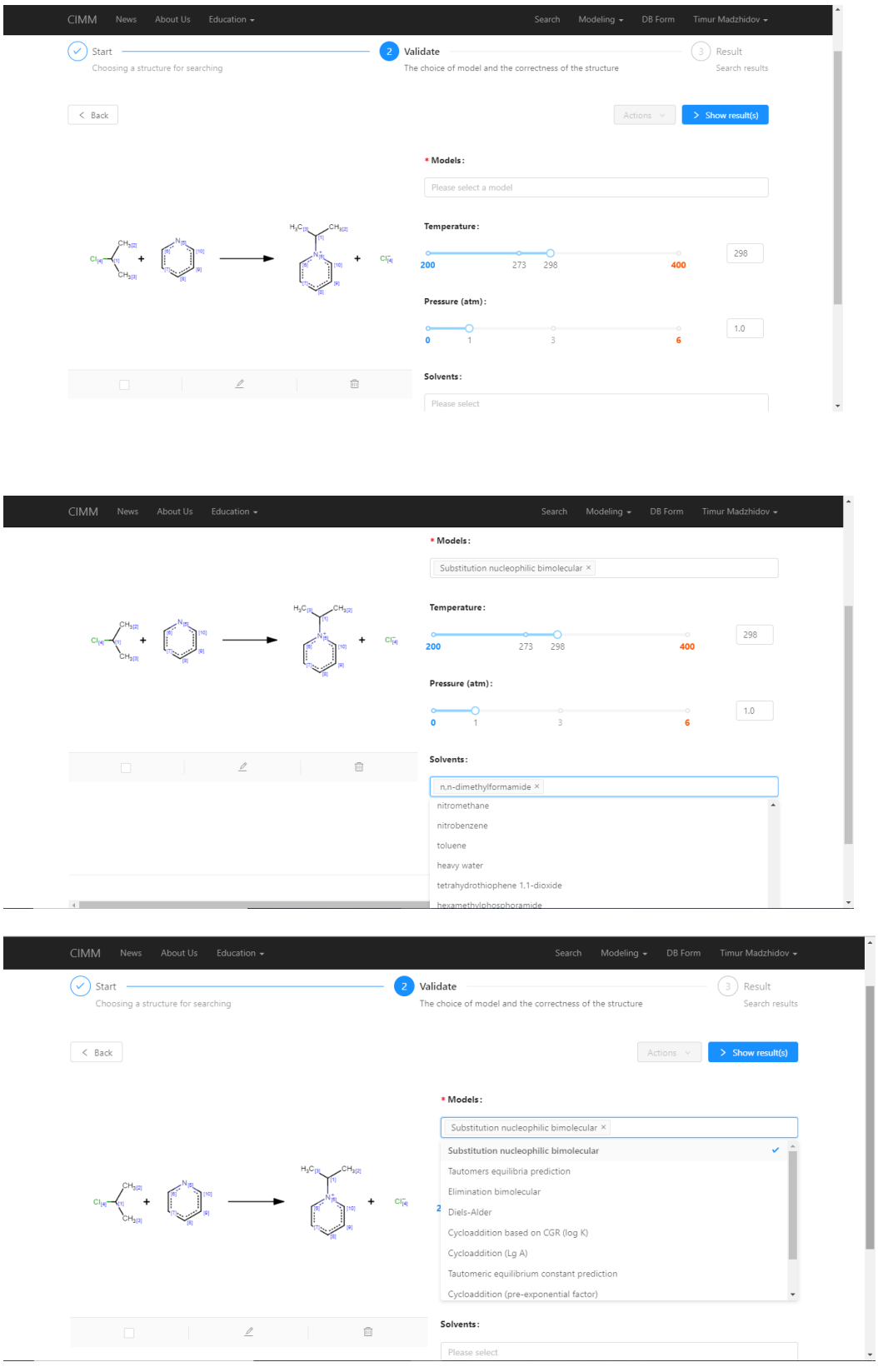

Figure S3. Setting modeling parameters for a query reaction: temperature and pressure (*top)*, solvent (*middle*) and a particular model (*bottom*)

Clicking the "**Show results**" button launches the calculations. This results in displaying the predicted log*k* value and the trustworthy parameter ("optimal", good", "poor") in a separate window (see Figure S4).

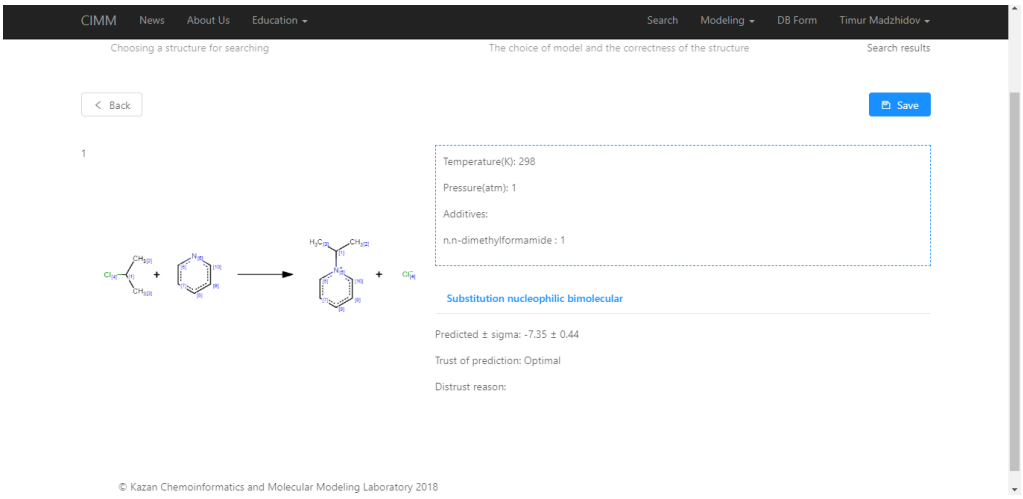

Figure S4. Results of calculations.