Supporting Information

Machine Learning Enables Highly Accurate Predictions of Photophysical Properties of Organic Fluorescent Materials: Emission Wavelengths and Quantum Yields

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1. Methods

ML Algorithms. Several supervised ML algorithms are used in this work, including Support Vector Machine (SVM), Kernel Ridge Regression (KRR), Multi-Layer Perceptron (MLP), k-Nearest Neighbors (kNN), Random Forest (RF), Light Gradient Boosting Machine (LightGBM), and Gradient Boost Regression Tree (GBRT). All except LightGBM can be found in Scikit-learn[S1].

Database/Selection of Training and Test Sets. The database consists of 4371 λ_{em} data, 4237 λ_{abs} data and 3079 PLQY data of organic fluorescent dyes solvated in different solvents gathered from published works, open directories of Dyomics[S2], and fluorophore[S3] database. If multiple peaks were found, the peak with the longest wavelength/largest intensity was collected for absorption/emission data, respectively. Detailed information about the database can be accessed on our website. For individual tests in the presenting work, the database is randomly partitioned into training set (90%) and test set (10%). The standard deviation in the 10-fold cross-validation is performed for the results of ten folds. Error bars in this work are drawn with standard error.

Fingerprints. Various molecular fingerprints were investigated in this research. Most of them were obtained by PaDEL-Descriptor[S4], including MACCS (166 bits), PubChem (881 bits), Substructure (presence and count of SMARTS patterns for Laggner functional group, 614 bits), Estate (E-State fragments, 79 bits), CDK (Chemistry Development Kit Fingerprints, 1024 bits), and CDKex (Chemistry Development Kit fingerprints and extended fingerprints, 2048 bits). Morgan circular fingerprints were generated with size 2048 bits and radius 2 by Rdkit[S5].

Functionalized Structure Descriptors (FSD). E-CDKex_sub (FSD_CDK) was generated directly by PaDEL, combining CDK fingerprints and extended fingerprints with E-States fingerprints and substructure fingerprints (both presence and count).

CDK (1024 bits)	CDK_Extended (1024 bits)	E-States (79 bits)	Functional group presence (307 bits)	Functional group Count (307 nums)

E-MACCS_sub was the combination of MACCS, E-States fingerprints, and substructure fingerprints (both presence and count).

MACCS (166 bits)	E-States (79 bits)	Functional group presence (307 bits)	Functional group Count (307 nums)

E-Morgan_sub (FSD_Morgan) was the combination of Morgan fingerprints, E-States fingerprints, and substructure fingerprints (both presence and count).

Morgan (2048 bits)	E-States (79 bits)	Functional group presence (307 bits)	Functional group Count (307 nums)

Comprehensive General Solvent Descriptor (CGSD). Combine E_t30 [S6], SP, SdP, SA, SB [S7] together. Detailed number of various solvents can be found in the reference. These 5 numbers have been used as the first 5 numbers of the input.

Et(30) (1 num)	SP (1 num)	SdP (1 num)	SA (1 num)	SB (1 num)

Website/Package for Photophysical Properties Prediction. We have deployed a website where users can predict photophysical properties using our ML models (http://www.chemfluor.top). ML models with optimal accuracies (GBRT for λ_{em} and λ_{abs}, LightGBM for Φ_{PL}) are employed as back-end ML models of our online platform. Users can make predictions by inputting SMILES and solvent information. The outputs include maximum emission wavelength, maximum absorption wavelength, and photoluminescence quantum yield. Although the ML models per se are fast, the translation from SMILES to fingerprints by PaDEL costs more time. As a result, Morgan and CGSD have been selected in combination with ensemble model to support rapid prediction. We also provide support for an (offline) python package where new compounds can be added into the training dataset for re-training, making the model learning on-the-fly. We have prepared a small patch for OLED (emission), used as a tutorial to teach users how to introduce their own data. The python package and the patch can be found in supporting data[S8] or downloaded from our website.

Author contributions

C.J. conceived the project, collected the data, optimized the ML-models, analyzed the data, conducted (TD-)DFT calculation and wrote the manuscript. H.B. conceived the project, constructed and optimized the ML-models, and analyzed the data. B.L. analyzed the data, conducted (TD-)DFT calculation and wrote the manuscript. R.L. constructed and optimized the ML-models, analyzed the data, and prepared the web tool. All authors discussed the results and commented on the manuscript.

2. Model optimization

2.1. Detailed information about the screening of the fingerprints and algorithms.

Table S1. Testing results of absorption wavelength and emission wavelength on test set of different ML models with different descriptors as inputs.

Algorithms	Fingerprints	Emission (λ_{em})			Absorption (λ_{abs})		
		MAE/nm	R^2	RMSE/nm	MAE/nm	R^2	RMSE/nm
MLP	E-CDKex_sub	21.986 ± 1.467	0.889 ± 0.017	32.003 ± 2.068	14.064 ± 0.697	0.946 ± 0.009	23.638 ± 2.157
	E-Morgan_sub	22.467 ± 1.883	0.882 ± 0.016	33.849 ± 2.692	15.427 ± 0.580	0.938 ± 0.006	26.104 ± 1.395
	E-Mac_sub	25.610 ± 1.856	0.864 ± 0.015	35.931 ± 1.983	18.878 ± 1.446	0.922 ± 0.022	29.176 ± 3.907
	Morgan	22.143 ± 1.244	0.875 ± 0.019	34.148 ± 2.364	14.879 ± 0.608	0.939 ± 0.007	25.713 ± 1.985
	CDKextended	22.811 ± 1.717	0.874 ± 0.021	34.081 ± 2.871	16.905 ± 1.330	0.924 ± 0.015	28.885 ± 3.484
	CDK	24.431 ± 1.479	0.862 ± 0.022	36.129 ± 2.530	18.550 ± 1.705	0.914 ± 0.015	31.105 ± 3.771
	PubChem	27.030 ± 1.501	0.845 ± 0.011	38.126 ± 1.906	20.537 ± 1.013	0.909 ± 0.011	31.671 ± 2.905
	MACCS	29.834 ± 1.508	0.813 ± 0.017	42.232 ± 2.119	23.790 ± 1.979	0.883 ± 0.022	35.416 ± 2.937
kNN	E-CDKex_sub	19.392 ± 1.080	0.895 ± 0.015	32.991 ± 1.797	13.500 ± 1.260	0.937 ± 0.017	26.252 ± 3.713
	E-Morgan_sub	20.710 ± 1.216	0.869 ± 0.018	35.631 ± 2.456	16.0461 ± 1.191	0.912 ± 0.017	30.936 ± 3.189
	E-Mac_sub	21.248 ± 1.456	0.864 ± 0.017	36.183 ± 3.299	16.669 ± 1.177	0.913 ± 0.014	31.339 ± 2.783
	Morgan	21.091 ± 1.204	0.859 ± 0.023	36.088 ± 2.812	16.336 ± 1.259	0.915 ± 0.017	30.305 ± 3.277
	CDKextended	20.059 ± 1.616	0.882 ± 0.018	34.140 ± 3.177	13.922 ± 0.975	0.935 ± 0.018	26.584 ± 3.041
	CDK	19.835 ± 0.878	0.875 ± 0.014	33.830 ± 2.113	15.089 ± 1.467	0.929 ± 0.017	28.054 ± 4.138
	PubChem	23.168 ± 1.164	0.839 ± 0.019	39.399 ± 1.979	18.128 ± 1.391	0.903 ± 0.015	32.096 ± 3.273
	MACCS	24.364 ± 1.861	0.830 ± 0.029	39.709 ± 3.819	19.225 ± 1.480	0.891 ± 0.021	34.346 ± 3.723
KRR	E-CDKex_sub	19.378 ± 0.858	0.913 ± 0.014	29.516 ± 2.044	13.893 ± 1.055	0.953 ± 0.011	23.503 ± 3.004
	E-Morgan_sub	23.128 ± 1.085	0.886 ± 0.012	32.354 ± 1.287	16.915 ± 0.769	0.938 ± 0.008	26.187 ± 2.020
	E-Mac_sub	29.038 ± 1.117	0.830 ± 0.020	39.999 ± 2.067	23.161 ± 1.562	0.897 ± 0.013	33.616 ± 3.214
	Morgan	26.649 ± 1.156	0.856 ± 0.013	37.323 ± 1.619	20.485 ± 0.723	0.912 ± 0.012	30.527 ± 1.700
	CDKextended	21.502 ± 0.631	0.893 ± 0.009	32.240 ± 1.199	15.127 ± 0.994	0.943 ± 0.015	24.538 ± 2.937
	CDK	25.445 ± 1.258	0.864 ± 0.016	36.221 ± 2.312	20.323 ± 1.031	0.905 ± 0.017	32.155 ± 2.919
	PubChem	33.466 ± 1.482	0.779 ± 0.022	45.863 ± 2.902	27.901 ± 1.489	0.844 ± 0.024	42.043 ± 4.205
	MACCS	38.851 ± 1.415	0.710 ± 0.023	52.681 ± 2.520	33.732 ± 0.892	0.797 ± 0.016	46.779 ± 1.402
SVM	E-CDKex_sub	14.708 ± 0.862	0.933 ± 0.010	25.192 ± 2.054	11.464 ± 0.943	0.956 ± 0.012	22.610 ± 3.269
	E-Morgan_sub	14.726 ± 1.481	0.927 ± 0.017	26.625 ± 3.504	11.644 ± 1.197	0.953 ± 0.015	23.247 ± 3.407
	E-Mac_sub	16.488 ± 0.922	0.907 ± 0.018	29.290 ± 2.351	12.567 ± 0.848	0.941 ± 0.014	24.967 ± 2.609
	Morgan	17.339 ± 0.863	0.910 ± 0.015	28.685 ± 1.977	12.452 ± 0.942	0.946 ± 0.012	24.028 ± 2.893
	CDKextended	15.281 ± 0.675	0.919 ± 0.010	27.404 ± 1.435	11.622 ± 0.608	0.953 ± 0.008	22.541 ± 1.619
	CDK	17.129 ± 0.987	0.908 ± 0.014	29.580 ± 2.307	13.492 ± 0.821	0.936 ± 0.017	26.453 ± 3.729
	PubChem	20.436 ± 1.079	0.874 ± 0.024	33.710 ± 2.756	15.298 ± 1.346	0.923 ± 0.021	28.649 ± 4.621
	MACCS	28.293 ± 1.887	0.791 ± 0.025	45.028 ± 3.280	22.089 ± 1.074	0.865 ± 0.011	38.221 ± 2.193
RF	E-CDKex_sub	17.110 ± 1.204	0.916 ± 0.016	28.029 ± 2.469	11.881 ± 0.924	0.943 ± 0.016	24.369 ± 3.406
	E-Morgan_sub	17.285 ± 1.009	0.908 ± 0.015	29.577 ± 2.398	11.920 ± 1.102	0.941 ± 0.014	25.178 ± 3.450

	E-Mac_sub	17.700 ± 1.048	0.910 ± 0.015	29.061 ± 2.417	13.095 ± 0.882	0.938 ± 0.016	26.196 ± 3.725
	Morgan	19.370 ± 1.210	0.885 ± 0.017	32.664 ± 2.503	12.775 ± 1.291	0.940 ± 0.014	25.685 ± 2.659
	CDKextended	18.710 ± 1.215	0.896 ± 0.016	31.402 ± 2.612	12.831 ± 0.783	0.937 ± 0.012	25.803 ± 2.632
	CDK	18.776 ± 1.058	0.894 ± 0.013	31.414 ± 2.162	13.749 ± 1.116	0.928 ± 0.018	27.869 ± 3.388
	PubChem	19.864 ± 1.177	0.886 ± 0.017	32.921 ± 2.328	14.261 ± 0.847	0.926 ± 0.013	28.643 ± 2.692
	MACCS	21.421 ± 1.398	0.870 ± 0.020	35.060 ± 2.899	15.104 ± 1.269	0.922 ± 0.013	29.147 ± 3.149
LightGBM	E-CDKex_sub	15.907 ± 0.889	0.923 ± 0.011	27.086 ± 1.932	11.609 ± 0.868	0.952 ± 0.010	23.079 ± 2.598
	E-Morgan_sub	16.099 ± 1.003	0.926 ± 0.012	26.323 ± 2.104	11.837 ± 0.921	0.954 ± 0.011	22.430 ± 2.868
	E-Mac_sub	16.754 ± 1.063	0.918 ± 0.014	27.851 ± 2.424	12.726 ± 1.231	0.946 ± 0.015	24.315 ± 3.803
	Morgan	18.726 ± 1.029	0.905 ± 0.013	30.092 ± 2.144	13.538 ± 0.979	0.944 ± 0.012	24.830 ± 2.898
	CDKextended	17.059 ± 1.011	0.913 ± 0.011	28.995 ± 1.955	11.785 ± 0.765	0.948 ± 0.013	23.645 ± 2.765
	CDK	17.590 ± 1.087	0.907 ± 0.015	29.595 ± 2.347	13.301 ± 1.226	0.938 ± 0.015	26.093 ± 3.062
	PubChem	19.293 ± 1.191	0.896 ± 0.016	31.358 ± 2.459	15.237 ± 0.891	0.931 ± 0.018	27.429 ± 3.324
	MACCS	20.477 ± 1.191	0.885 ± 0.018	32.718 ± 2.282	16.347 ± 0.852	0.917 ± 0.012	30.459 ± 1.889
GBRT	E-CDKex_sub	14.608 ± 1.022	0.932 ± 0.012	25.583 ± 2.495	11.054 ± 1.038	0.952 ± 0.013	23.432 ± 2.976
	E-Morgan_sub	15.431 ± 1.100	0.928 ± 0.016	25.971 ± 2.623	11.475 ± 1.117	0.953 ± 0.013	22.584 ± 3.700
	E-Mac_sub	15.764 ± 0.926	0.924 ± 0.016	26.863 ± 2.440	11.910 ± 0.664	0.949 ± 0.008	23.800 ± 2.375
	Morgan	17.753 ± 0.990	0.911 ± 0.009	29.105 ± 2.064	12.968 ± 0.988	0.948 ± 0.014	23.580 ± 3.661
	CDKextended	15.179 ± 0.906	0.925 ± 0.011	26.350 ± 2.026	11.588 ± 0.474	0.952 ± 0.006	23.420 ± 1.325
	CDK	15.670 ± 0.806	0.920 ± 0.020	27.187 ± 2.362	12.031 ± 1.255	0.945 ± 0.014	24.595 ± 3.946
	PubChem	17.343 ± 1.095	0.905 ± 0.011	29.748 ± 2.417	13.152 ± 1.066	0.945 ± 0.010	24.198 ± 2.061
	MACCS	19.602 ± 1.478	0.889 ± 0.021	32.803 ± 2.798	14.358 ± 1.137	0.931 ± 0.016	27.842 ± 3.066

2.2. In-depth analysis and comparison of algorithms.

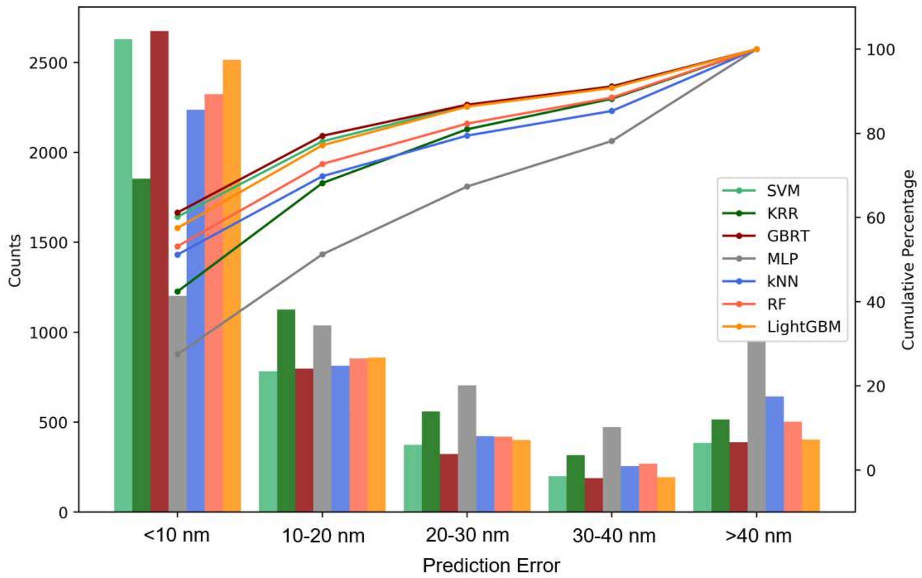


Figure S1. Error distribution of prediction results under different algorithms with FSD_CDK.

Table S2. Testing results of absorption/emission wavelength with 10-fold cross validation of different ML models with FSD_CDK as inputs.

Algorithms	*r*	R^2	MAE/nm	RMSE/nm	MAE/eV	RMSE/eV	<20 nm	>40 nm
				Emission				
MLP	0.947 ± 0.009	0.893 ± 0.017	18.941 ± 0.999	29.500 ± 2.097	0.088 ± 0.006	0.144 ± 0.014	70.0%	11.9%
kNN	0.932 ± 0.007	0.867 ± 0.014	19.664 ± 0.910	33.049 ± 1.969	0.089 ± 0.005	0.151 ± 0.011	69.3%	14.6%
KRR	0.948 ± 0.009	0.897 ± 0.017	19.315 ± 1.522	28.991 ± 3.078	0.089 ± 0.007	0.137 ± 0.014	67.5%	11.6%
SVM	0.959 ± 0.009	0.918 ± 0.018	14.419 ± 0.683	25.736 ± 2.531	0.067 ± 0.003	0.126 ± 0.012	79.0%	8.9%
RF	0.951 ± 0.006	0.901 ± 0.012	17.247 ± 1.255	28.460 ± 2.381	0.079 ± 0.006	0.133 ± 0.013	72.3%	11.5%
LightGBM	0.957 ± 0.008	0.916 ± 0.016	15.295 ± 0.839	26.192 ± 2.044	0.071 ± 0.005	0.126 ± 0.013	77.0%	9.7%
GBRT	0.962 ± 0.007	0.925 ± 0.014	14.307 ± 1.118	24.768 ± 2.238	0.066 ± 0.005	0.119 ± 0.012	79.2%	8.7%
				Absorption				
MLP	0.971 ± 0.005	0.940 ± 0.009	14.530 ± 1.069	24.517 ± 2.357	0.096 ± 0.007	0.168 ± 0.016	79.4%	7.1%
kNN	0.963 ± 0.010	0.928 ± 0.019	13.850 ± 1.283	26.856 ± 3.690	0.090 ± 0.009	0.174 ± 0.025	80.7%	8.5%
KRR	0.972 ± 0.007	0.945 ± 0.013	13.814 ± 0.931	23.372 ± 2.863	0.093 ± 0.009	0.161 ± 0.021	81.0%	7.0%
SVM	0.975 ± 0.005	0.951 ± 0.010	11.187 ± 0.984	22.217 ± 2.625	0.076 ± 0.006	0.157 ± 0.015	84.8%	6.1%
RF	0.969 ± 0.007	0.938 ± 0.013	12.478 ± 0.942	24.872 ± 2.677	0.082 ± 0.005	0.164 ± 0.019	83.1%	7.7%
LightGBM	0.973 ± 0.005	0.946 ± 0.009	11.614 ± 0.548	23.177 ± 1.845	0.077 ± 0.005	0.156 ± 0.019	84.3%	7.1%
GBRT	0.977 ± 0.005	0.954 ± 0.010	10.471 ± 1.023	21.459 ± 2.565	0.070 ± 0.006	0.146 ± 0.019	86.7%	5.7%

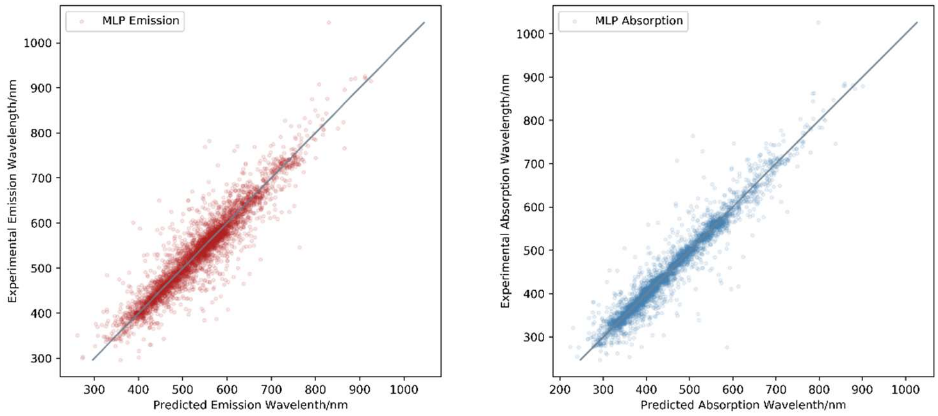


Figure S2. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **MLP**/FSD_CDK.

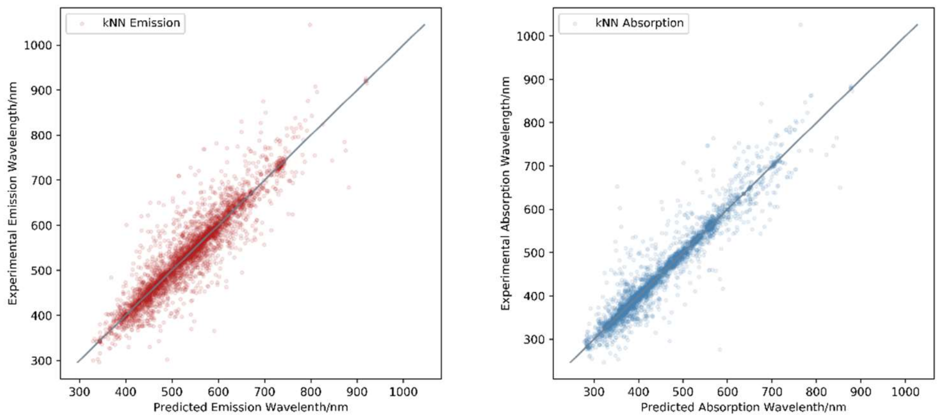


Figure S3. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **kNN**/FSD_CDK.

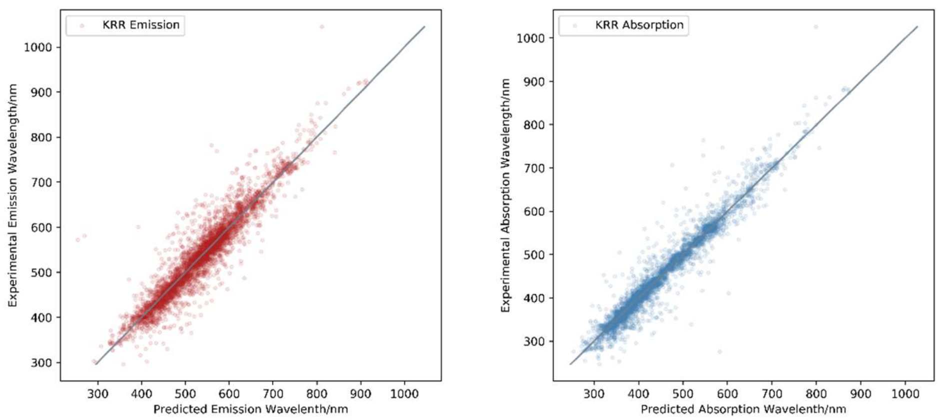


Figure S4. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **KRR**/FSD_CDK.

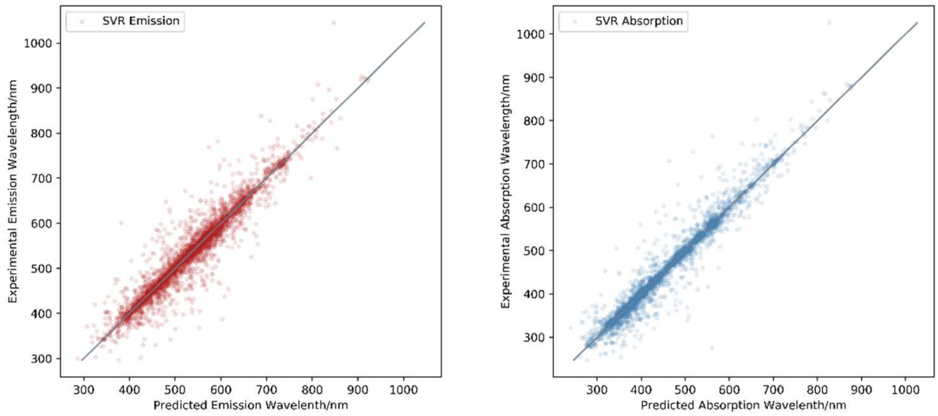


Figure S5. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **SVM**/FSD_CDK.

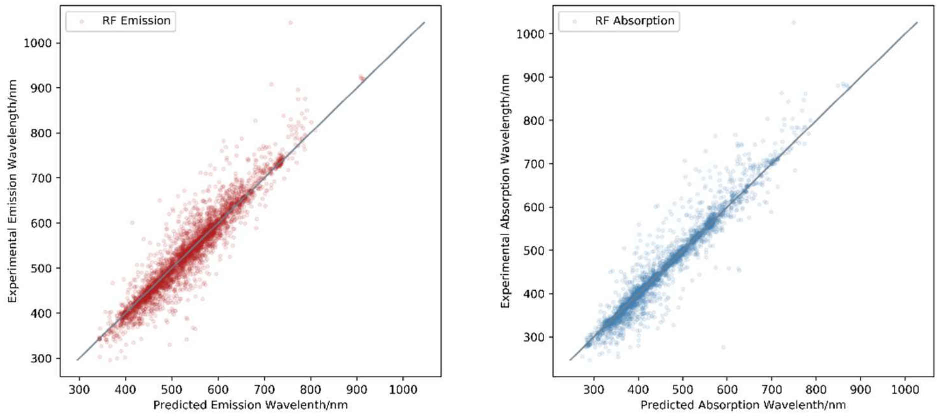


Figure S6. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **RF**/FSD_CDK.

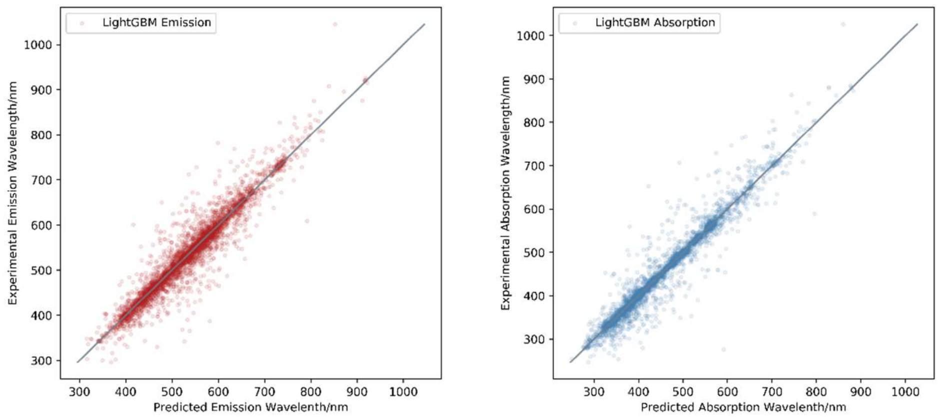


Figure S7. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **LightGBM**/FSD_CDK.

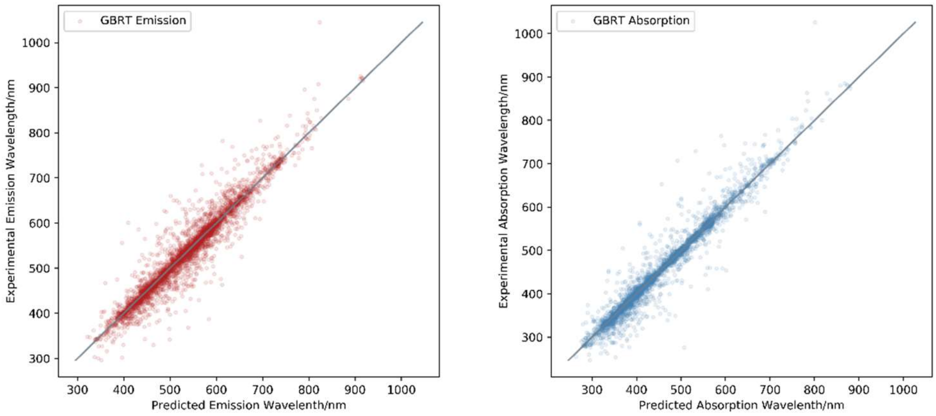


Figure S8. Scatter plots of prediction results of maximum emission(left)/absorption(right) wavelength with **GBRT**/FSD_CDK.

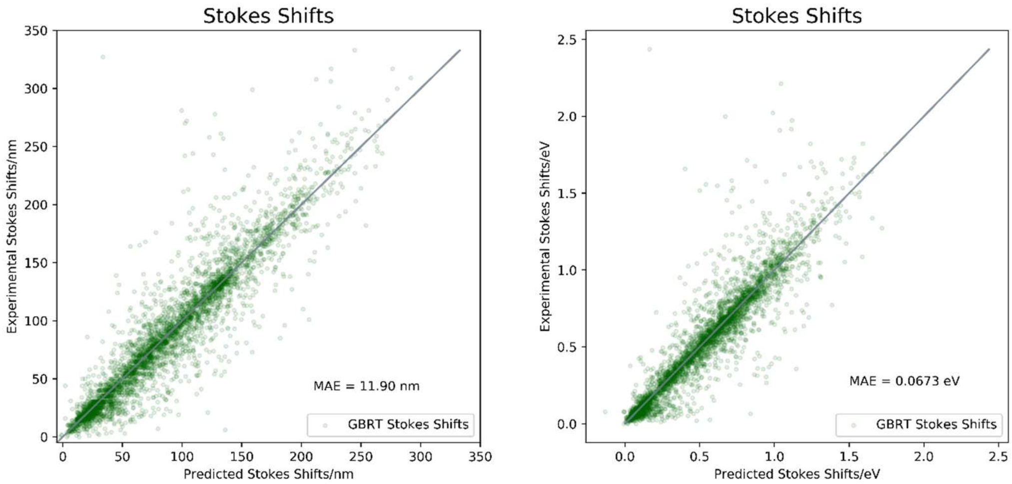


Figure S9. Scatter plots of prediction results of stokes shift in the case of wavelength/nm (left) and energy/eV (right) as scale (left) with **GBRT**/FSD_CDK.

2.3. Molecular-based partition for the prediction of emission wavelength.

Pseudocode of the Ensemble model.

Algorithm Stacking

Input: Train set, Cross Validation Value k

Output: ensemble learner

Step 1: split the train set into k parts

```
shuffle the dataset
split the train set into k parts
```

Step 2: do k-fold validation for each base learner to get the input data of the meta learner

```
for i from 1 to fold time:
    take the i-th part of train set as the test set of cross validation
    take the rest train set as the train set of cross validation

    for each base learner:
        fit each weak learner with the train set of cross validation
        predict the test set of cross validation
    end for
end for
merge each predict result
```

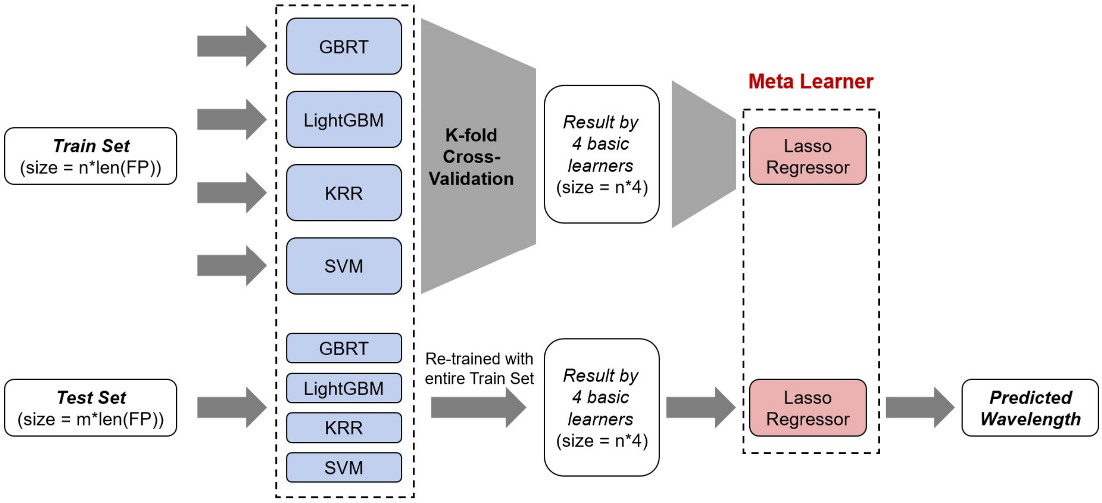
Thus far, we obtain a matrix having the same number of rows with train set and the number of columns is the number of base learner. Each row represents the same molecular as the train set. We can directly use this matrix as input feature and the label of train set to train the meta learner.

Step 3: train the meta learner

```
fit the meta learner, using the matrix above.
```

Step 4: retrain every base learner (in previous steps base learners were trained with k-1 part of k-validation)

```
for each weak learner in every weak learner:
    fit each weak learner with the train set
end for
return base learners and meta learner
```



Scheme S1. Illustration of the ensemble model.

Table S3. Prediction result of molecule-based partition with different algorithms[1].

Algorithms	***r***	**R^2**	**MAE/nm**	**RMSE/nm**	**MAE/eV**	**RMSE/eV**
KRR	0.916(0.844)	0.837(0.697)	22.48(26.47)	36.14(43.67)	0.105(0.126)	0.206(0.284)
SVM	0.944(0.911)	0.891(0.827)	18.75(21.77)	29.61(32.97)	0.088(0.098)	0.143(0.151)
GBRT	0.952(0.915)	0.906(0.836)	17.36(20.83)	27.43(32.10)	0.080(0.093)	0.129(0.144)
LightGBM	0.936(0.882)	0.875(0.775)	20.65(26.42)	31.61(37.64)	0.093(0.115)	0.146(0.163)
Ensemble	0.953(0.922)	0.907(0.849)	17.20(19.79)	27.30(30.83)	0.080(0.089)	0.129(0.139)

[1] The data are the overall prediction results, and the data in parentheses are the results of *part2* (molecules appeared more than once).

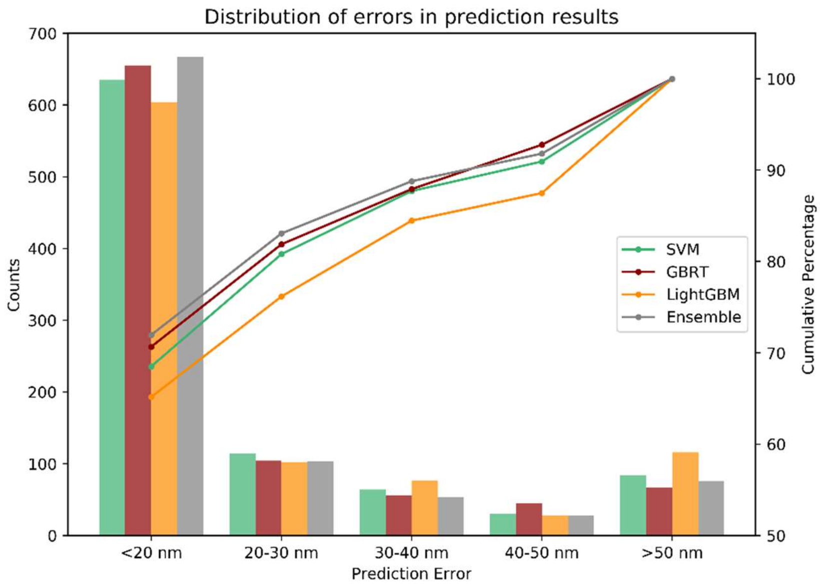


Figure S10. Error distribution for SVM, GBRT, LightGBM and Ensemble model. The FSD_CDK fingerprint is employed in all these assessments.

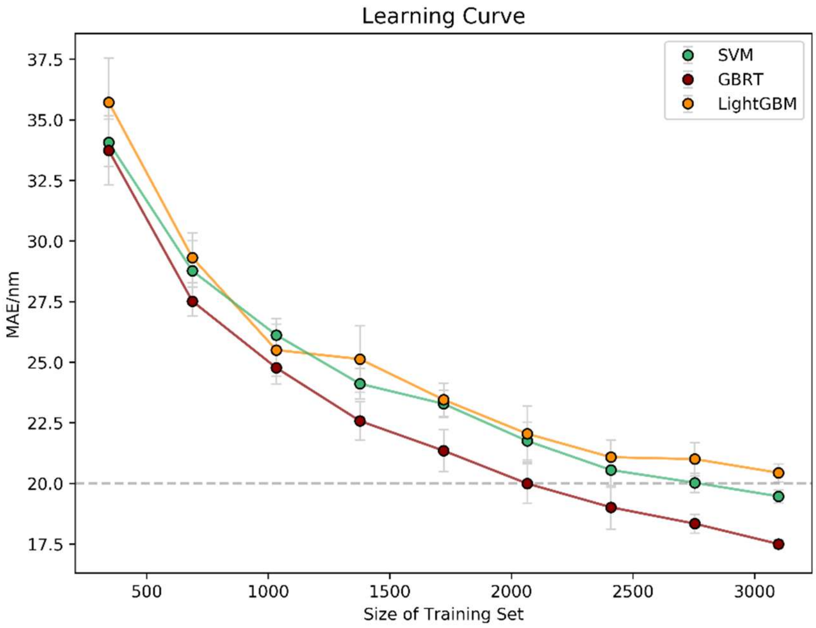


Figure S11. Learning curve (nm) of LightGBM, GBRT and SVM under molecule-based partition.

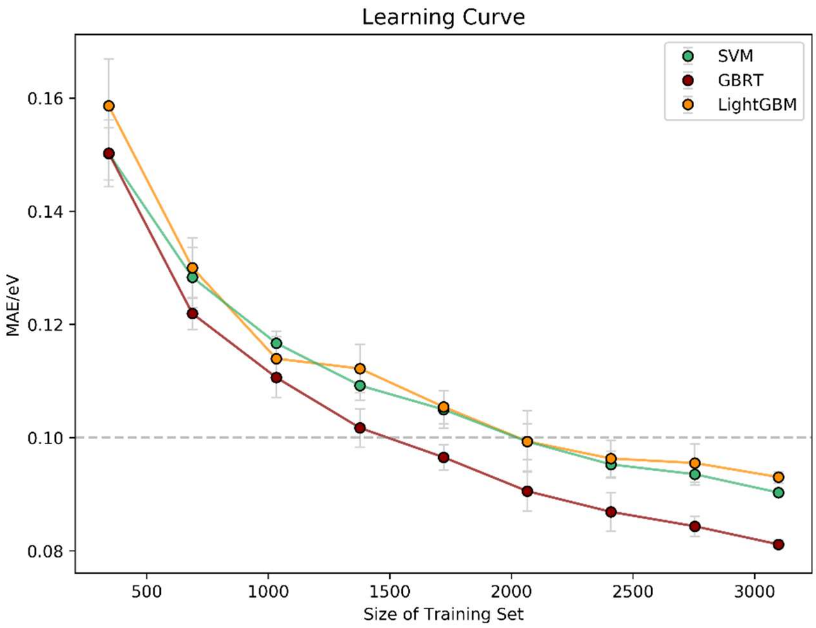


Figure S12. Learning curve (eV) of LightGBM, GBRT and SVM under molecule-based partition.

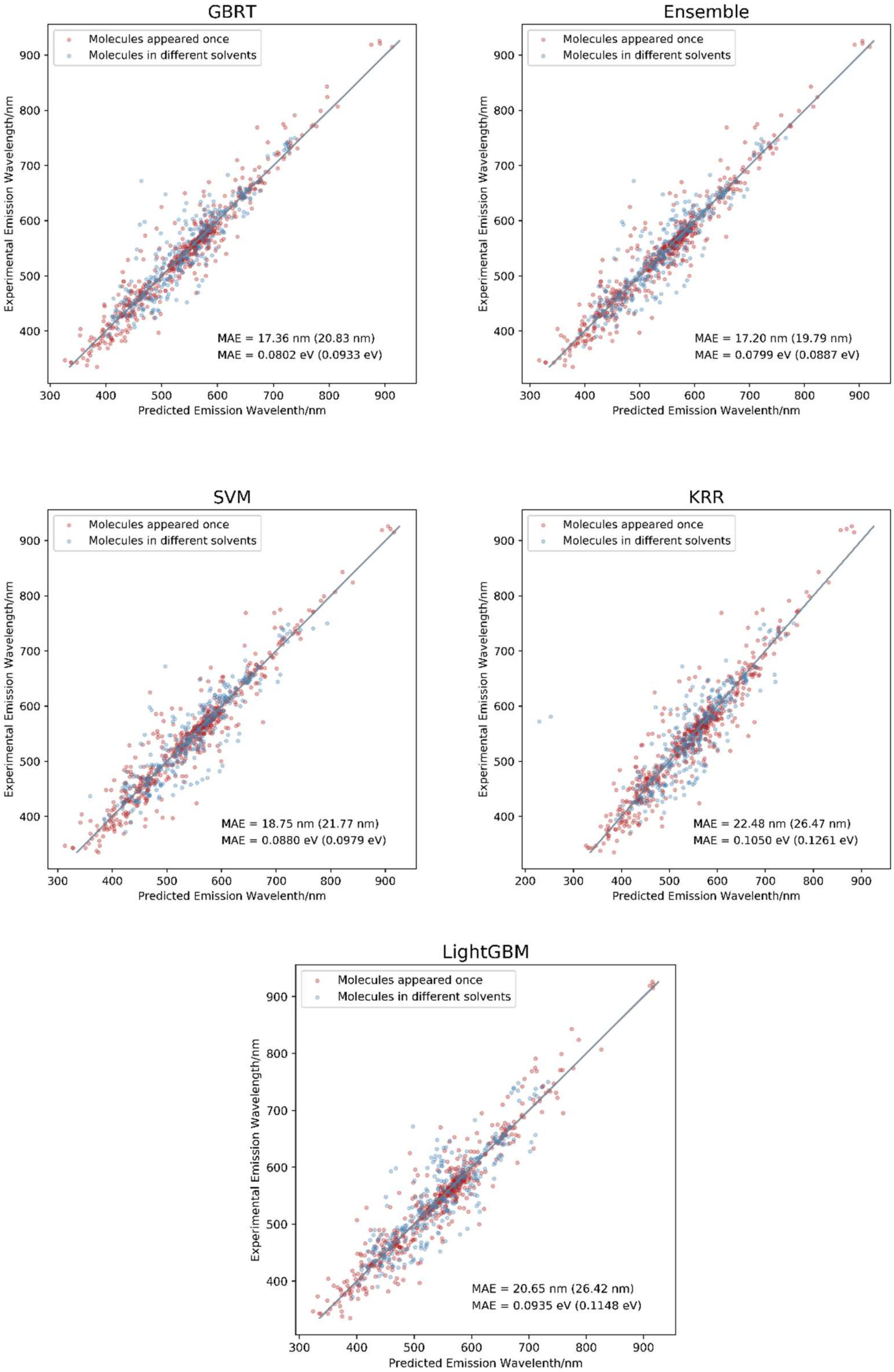


Figure S13. Scatter plots of prediction results of maximum emission wavelength based on molecule-based partition with different algorithms, the red points represent *part2* (molecules appeared more than once) and the blue points represent *part1* (molecules appeared only once)

3. PLQY prediction model

3.1. Regressor model.

3.1.1. Model optimization.

Table S4. Performance of various fingerprints in predicting PLQY with LightGBM regressor models.

Fingerprints	**PLQY**		
	r	MAE	RMSE
E-CDKex_sub	**0.843 ± 0.028**	**0.110 ± 0.009**	**0.164 ± 0.014**
E-Morgan_sub	0.832 ± 0.015	0.116 ± 0.005	0.171 ± 0.008
E-Mac_sub	0.829 ± 0.024	0.118 ± 0.007	0.172 ± 0.010
Morgan	0.833 ± 0.014	0.117 ± 0.005	0.169 ± 0.008
CDKextended	0.828 ± 0.023	0.117 ± 0.007	0.175 ± 0.009
CDK	0.830 ± 0.029	0.114 ± 0.006	0.170 ± 0.011
PubChem	0.816 ± 0.019	0.120 ± 0.007	0.174 ± 0.009
MACCS	0.802 ± 0.017	0.124 ± 0.007	0.181 ± 0.010

Table S5. Performance of various algorithms in predicting PLQY with FSD_CDK.

Algorithms	PLQY			
	r	MAE	RMSE	R^2
SVR	0.806 ± 0.027	0.132 ± 0.047	0.182 ± 0.013	0.646 ± 0.047
KRR	0.814 ± 0.018	0.125 ± 0.030	0.179 ± 0.008	0.660 ± 0.030
GBRT	0.846 ± 0.024	0.112 ± 0.041	0.167 ± 0.010	0.713 ± 0.041
MLP	0.776 ± 0.022	0.145 ± 0.043	0.203 ± 0.013	0.562 ± 0.043
kNN	0.787 ± 0.039	0.129 ± 0.065	0.190 ± 0.014	0.613 ± 0.065
RF	0.836 ± 0.022	0.121 ± 0.034	0.170 ± 0.007	0.691 ± 0.034
LightGBM	**0.848 ± 0.015**	**0.111 ± 0.009**	**0.163 ± 0.008**	**0.716 ± 0.027**

3.1.2. Further analysis.

Table S6. Performance of predicting PLQY with overall dataset and only QY>0.1 with 10-fold cross-validation (FSD_CDK/LightGBM).

Entry	Dataset	*r*	MAE	RMSE
1	All datapoints	0.843	0.111	0.163
2	Samples with QY>0.1	0.790	0.116	0.167

Table S7. Performance of predicting PLQY with different size of test set. (FSD_CDK/LightGBM)

Size of Test Set	PLQY		
	r	MAE	RMSE
0.1	0.843 ± 0.028	0.110 ± 0.009	0.164 ± 0.014
0.2	0.821 ± 0.015	0.120 ± 0.004	0.175 ± 0.006
0.3	0.820 ± 0.015	0.122 ± 0.004	0.177 ± 0.007
0.4	0.811 ± 0.015	0.126 ± 0.005	0.180 ± 0.007
0.5	0.789 ± 0.012	0.132 ±0.002	0.190 ± 0.004
0.6	0.762 ± 0.007	0.141 ± 0.002	0.201 ± 0.003
0.7	0.726 ± 0.018	0.152 ± 0.004	0.214 ± 0.006
0.8	0.675 ± 0.013	0.167 ± 0.003	0.230 ± 0.004
0.9	0.576 ± 0.023	0.194 ± 0.004	0.257 ± 0.006

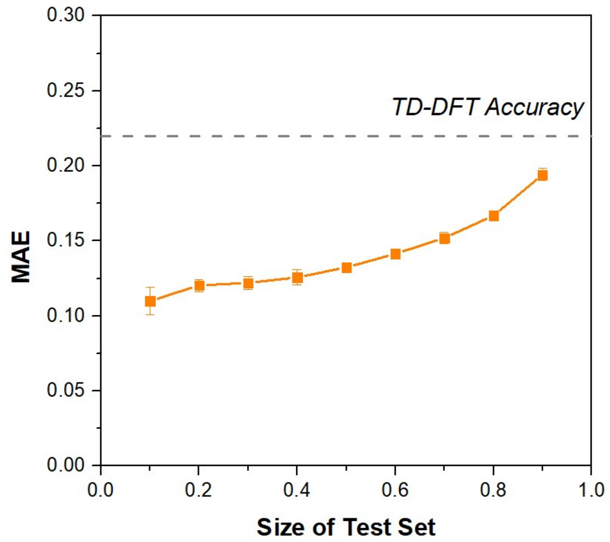


Figure S14. Change of MAE of PLQY prediction with the variation of proportions of the test set. (TD-DFT accuracy = 0.22 [S9])

3.1.3. Oversampling in regressor model.

Using only the high-quality **integration sphere** data (the quality of the data is only determined by the measured method), the ML predictions show higher r and R^2 in cross validation (Table S8), suggesting improvement in accuracy. As the considerably lower experimental error by the integration sphere method helps ML better recognize the structural-property relationship. Such result is very exciting, because at most time the decrease of the database will decrease accuracy. The increase of MAE can be ascribed to the high deviation of the high-quality data, as suggested by the violin plot shown in Figure S16. We can find that the subset obtained with the old-style method (or low-quality dataset) are more concentrated in the low QY region. In contrast, the relative distribution of the absolutely determined QY is more evenly distributed, which will cause a lower MAE at the same level of error. Due to the higher Pearson correlation coefficient as well as the smaller dataset, we can assume that the performance is better after trimming dataset.

Table S8. Test result of the different (sub)dataset with 10-fold cross validation.

	r	**R^2**	**MAE**	**RMSE**
Full Dataset	0.848 ± 0.015	0.716 ± 0.027	0.111 ± 0.009	0.163 ± 0.008
Trimmed High-Quality Subset	0.859 ± 0.036	0.733 ± 0.064	0.119 ± 0.011	0.172 ± 0.018

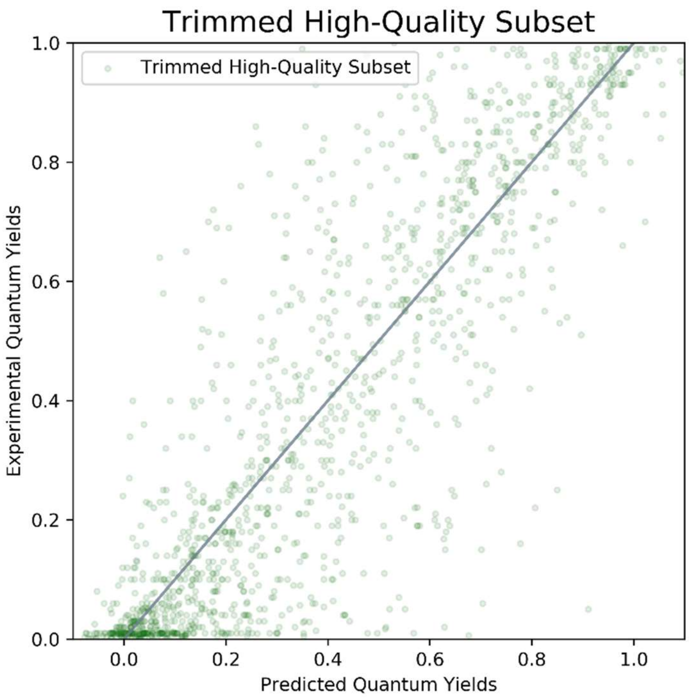


Figure S15. Scatter plots of prediction results of quantum yields in high-quality subset with **GBRT**/FSD_CDK.(10-fold cross-validation)

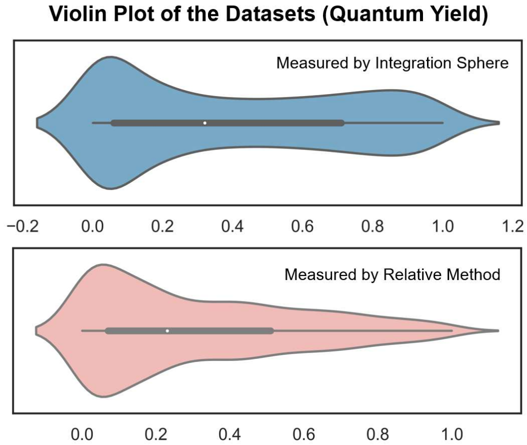


Figure S16. Violin plot of two sub-datasets, measured by absolute method(top) and relative method(down), respectively.

Despite the improvement in accuracy, the shrinking of dataset is likely to undermine generalizability. Note that the relative method subset is densely distributed where QY < 0.2, an interval in which the error of the relative method is not completely unacceptable. Making use of this fact, we have employed an oversampling strategy where the relative method subset is also partly involved to balance accuracy and generalizability. We take 10-fold cross-validation to the high-quality sub-dataset and compare three situations: 1) training set is only nine folds in the high-quality subset; 2) training set is nine folds in high-quality sub-dataset and all the data in the low-quality subset; 3) training set is the same as the second one, but we oversample of the data with high-quality. The same test set is used to allow comparison between the three situations. According to the results in Table S9, we can find that the accuracy decreases with the introduction of low-quality data (Entry 1 vs Entry 2), but a nearly identical accuracy is obtained with the oversample dataset (Entry 1 vs Entry 3). These results recommend oversampling model as a better choice owing to the high accuracy and generalizability.

Table S9. Test result of the three situations.

Entry	Dataset	*r*	R^2	MAE	RMSE
1	Only High Quality Sub-dataset	0.859 ± 0.036	0.733 ± 0.064	0.119 ± 0.011	0.172 ± 0.018
2	Normal Sampling Method	0.855 ± 0.030	0.727 ± 0.053	0.122 ± 0.010	0.175 ± 0.019
3	Oversample[1]	0.859 ± 0.036	0.734 ± 0.067	0.118 ± 0.011	0.172 ± 0.019

[1] The high-quality sub-dataset was sampled for three times, while the low-quality sub-dataset was sampled only once.

3.1.4. Solvent Effect and molecule-based partition.

Table S10. Feature importance of the solvent descriptors in different ML models[1]

Solvent Descriptor	Abs_GBRT[2]	Em_GBRT[3]	QY_LightGBM_Clf[4]	QY_LightGBM_Reg[5]	QY_GBRT_Reg[6]
Et(30)	0.28%	2.00%	4.03%	3.80%	3.21%
Dipolarity	0.09%	0.41%	3.38%	3.76%	1.45%
Polarizability	0.07%	1.77%	2.63%	2.38%	3.03%
Acidity	0.16%	0.97%	1.49%	1.51%	2.33%
Basicity	0.09%	0.70%	3.15%	3.24%	1.82%
overall	0.69%	5.84%	14.68%	14.68%	11.84%

[1] The absorption prediction model based on GBRT/FSD_CDK.

Table S11. Prediction result with different sampling method.

Entry	Training/Test Partition	*r*	MAE
1	Datapoint-based[1]	0.821	0.120
2	Molecule-based	0.793 (0.771)	0.131 (0.151)

[1] Result in Table S7.

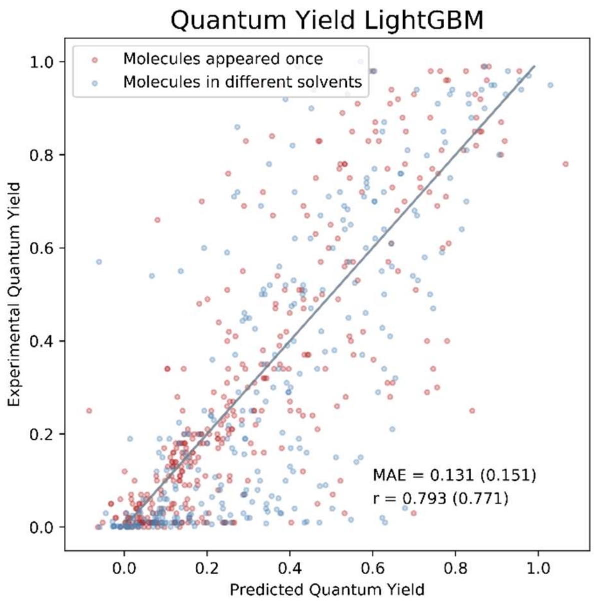
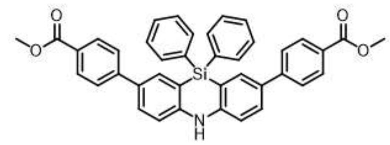


Figure S17. Scatter plots of prediction results of PLQY based on molecule-based partition with LightGBM/FSD_CDK, the red points represent *part2* (molecules appeared more than once) and the blue points represent *part1* (molecules appeared only once)



Predicted QY	Experimental QY	Solvent
0.474	0.67	CH_2Cl_2
0.531	0.69	Toluene
0.521	0.72	THF
0.411	0.62	DMF
0.374	0.56	MeCN
0.409	0.53	1-Butanol
0.339	0.50	EtOH
0.193	0.25	MeOH

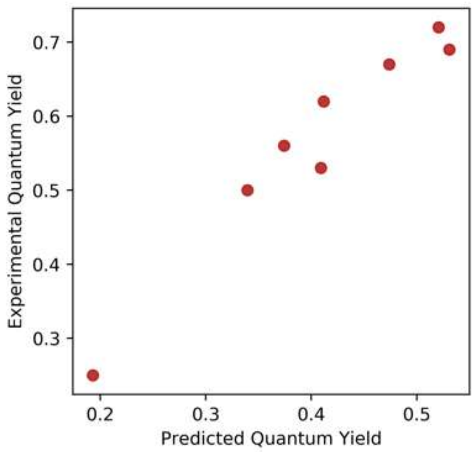
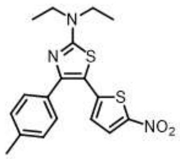


Figure S18. Selected examples in sub-dataset *part 2* and prediction result in compare with experimental result.



Predicted QY	Experimental QY	Solvent
-0.028	0.001	CH_2Cl_2
0.084	0.16	Hexane
0.475	0.421	Toluene
0.037	0.036	THF
-0.0096	0.0001	MeCN
-0.015	0.002	DMSO

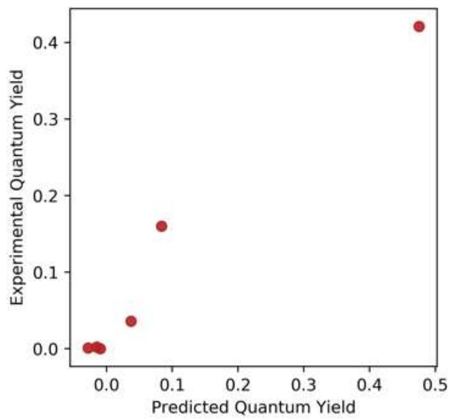
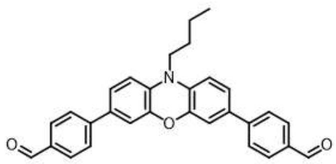


Figure S19. Selected examples in sub-dataset *part 2* and prediction result in compare with experimental result.



Predicted QY	Experimental QY	Solvent
0.161	0.028	hexane
0.336	0.511	Toluene
0.210	0.239	THF
0.156	0.026	Acetone
0.157	0.014	MeCN
0.128	0.01	DMSO

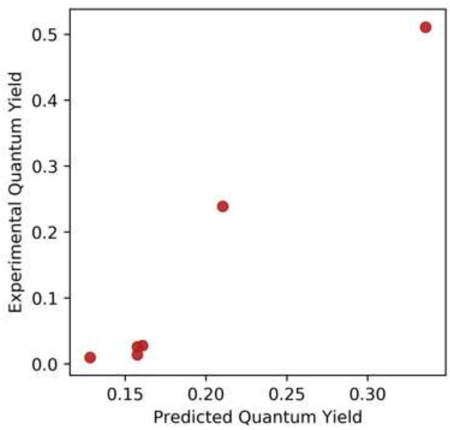


Figure S20. Selected examples in sub-dataset *part 2* and prediction result in compare with experimental result.

3.2. Classifier model.

Table S12. Test result and group ranking of PLQY used for LightGBM model versus the number of fractions (n)

n	Threshold	Accuracy/%
2	0.25	86.41 ± 0.72
3	0.15, 0.60	73.73 ± 0.41
4	0.05, 0.25, 0.60	63.97 ± 1.48
5	0.04, 0.16, 0.40, 0.70	58.24 ± 1.02
6	0.03, 0.10, 0.25, 0.5, 0.75	57.89 ± 0.50

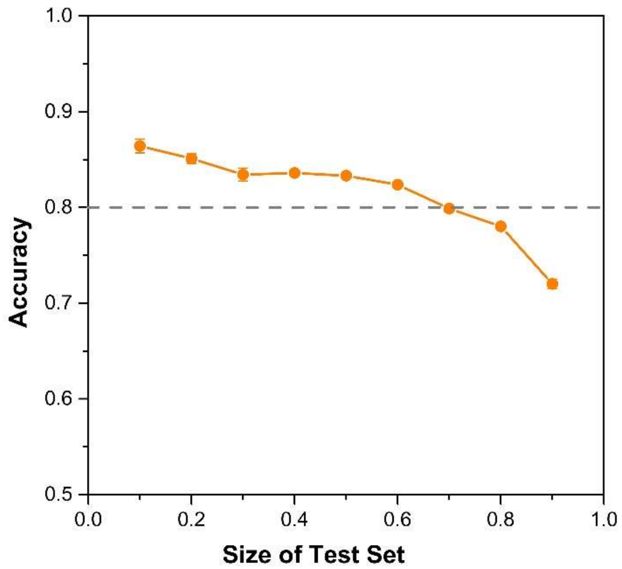


Figure S21. Change of accuracy of PLQY prediction with the variation of proportions of the test set. (threshold = 0.25)

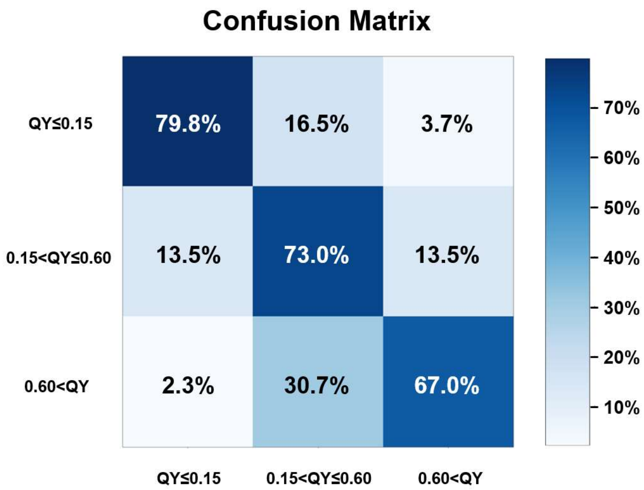


Figure S22. Testing results of test set (10%) with LightGBM classification model and n=3. (PLQY-prediction)

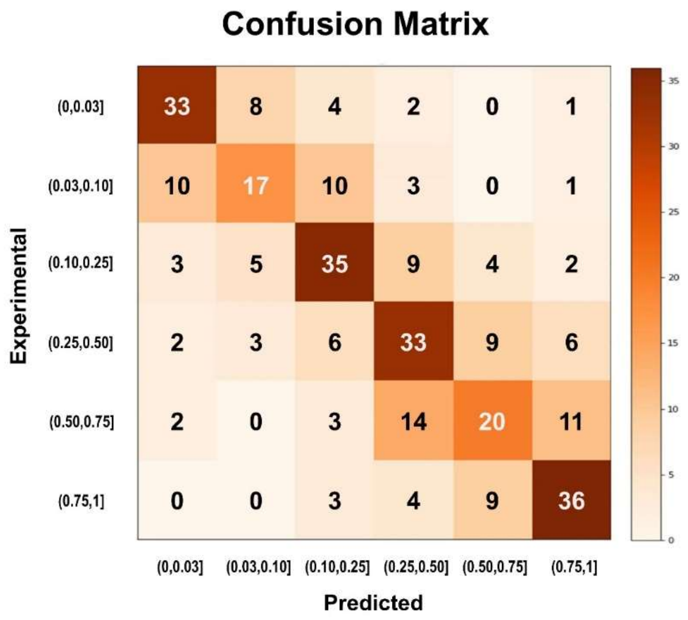


Figure S23. Testing results of test set with LightGBM classification model (n=6). (PLQY-prediction)

Table S13. Detail of 22 selected molecules for prediction of PLQY used as practical problems

Experimental PLQY	Predicted (0.25)	Solvent	Reference (DOI)
0.03	1	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.38	1	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.06	0	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.16	1	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.06	0	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.21	1	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.15	1	$CHCl_3$	10.1016/j.dyepig.2020.108396
0.85	1	Acetone	10.1016/j.dyepig.2020.108339
0.39	0	DMSO	10.1016/j.dyepig.2020.108339
0.55	1	Acetone	10.1016/j.dyepig.2020.108339
0.27	0	DMSO	10.1016/j.dyepig.2020.108339
0.31	1	Acetone	10.1016/j.dyepig.2020.108339
0.09	0	DMSO	10.1016/j.dyepig.2020.108339
0.81	1	CH_2Cl_2	10.1016/j.dyepig.2020.108339
0.68	1	CH_2Cl_2	10.1016/j.dyepig.2020.108339
0.53	1	CH_2Cl_2	10.1016/j.dyepig.2020.108339
0.75	1	MeCN	10.1021/acs.orglett.0c01086
0.72	1	MeCN	10.1021/acs.orglett.0c01086
0.69	1	MeCN	10.1021/acs.orglett.0c01086
0.59	1	MeCN	10.1021/acs.orglett.0c01086
0.68	1	MeCN	10.1021/acs.orglett.0c01086
0.67	1	MeCN	10.1021/acs.orglett.0c01086

The SMILES of tested molecules could be found in file stored for test molecules.

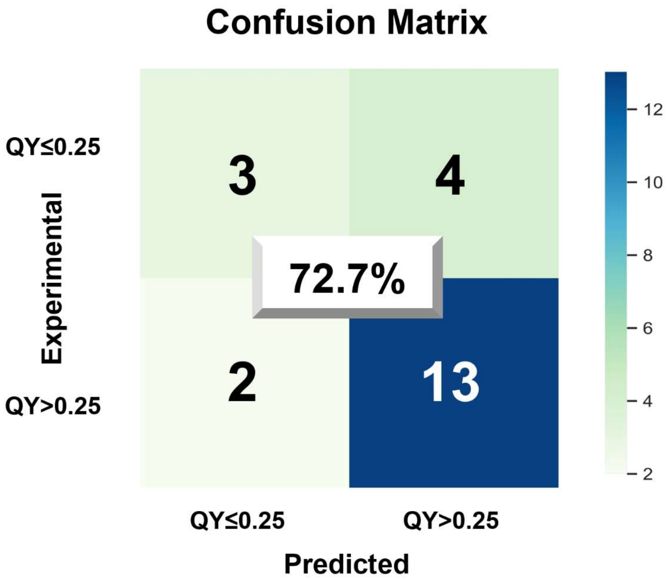


Figure S24. Confusion Matrix of ***22*** selected molecules with threshold = 0.25.

4. Comparison with TD-DFT

4.1. Comparsion with data in DFT benchmark studies.

Table S14. The emission energies (eV) of 116 selected molecules achieved by different method. (The lack is because move into training set.)

Experimental[1]	Predicted1[2]	Predicted2[3]	TD-DFT[4]	Solvent	Reference (DOI)
2.140	1.875	1.874	2.340	water	10.1021/jp3021485
2.170	1.912	1.915	2.350	water	10.1021/jp3021485
2.180	2.158	2.165	2.410	MeCN	10.1021/jp3021485
2.180	2.183	2.187	2.400	MeCN	10.1021/jp3021485
2.180	2.194	2.197	2.400	MeCN	10.1021/jp3021485
2.330	2.067	2.060	2.510	EtOH	10.1021/jp3021485
2.230	2.157	2.138	2.360	MeCN	10.1021/jp3021485
2.110	2.062	2.092	2.260	EtOH	10.1021/jp3021485
2.280	2.272	2.254	2.320	MeOH	10.1021/jp3021485
2.080	2.051	2.062	2.100	MeCN	10.1021/jp3021485
2.080	2.034	2.048	2.210	MeCN	10.1021/jp3021485
1.997	2.095	2.153	2.130	EtOH	10.1021/ct500328t
1.890	2.115	2.177	2.080	EtOH	10.1021/ct500328t
2.226	2.320	2.390	2.150	THF	10.1021/ct500328t
2.318	2.321	2.363	2.230	THF	10.1021/ct500328t
2.638	2.195	2.355	2.740	MeOH	10.1021/ct500328t
2.348	2.120	2.274	2.250	MeOH	10.1021/ct500328t
2.134	2.130	2.082	2.080	THF	10.1021/ct500328t
2.050	2.110	2.021	2.060	THF	10.1021/ct500328t
2.309	2.189	2.069	2.270	THF	10.1021/ct500328t
2.322	2.151	2.020	2.270	THF	10.1021/ct500328t
2.202	2.118	2.102	2.400	MeOH	10.1021/ct500328t
2.006	1.922	1.892	2.355	CH_2Cl_2	10.1039/C4RA09494H
1.764	1.808	1.829	2.109	CH_2Cl_2	10.1039/C4RA09494H
1.442	1.762	1.751	1.944	CH_2Cl_2	10.1039/C4RA09494H
1.946	1.740	1.763	2.187	CH_2Cl_2	10.1039/C4RA09494H
1.962	1.877	1.855	2.348	CH_2Cl_2	10.1039/C4RA09494H
1.931	1.825	1.811	2.250	CH_2Cl_2	10.1039/C4RA09494H
1.977	1.837	1.859	2.320	CH_2Cl_2	10.1039/C4RA09494H
1.943	1.849	1.792	2.238	CH_2Cl_2	10.1039/C4RA09494H
1.864	1.840	1.826	2.175	CH_2Cl_2	10.1039/C4RA09494H
1.807	1.839	1.824	2.113	CH_2Cl_2	10.1039/C4RA09494H
1.815	1.828	1.806	2.089	CH_2Cl_2	10.1039/C4RA09494H
1.664	1.802	1.742	2.189	CH_2Cl_2	10.1039/C4RA09494H
3.523	3.009	3.091	3.553	EtOH	10.1063/1.2361290
2.818	2.549	2.856	3.196	Water	10.1063/1.2361290
3.017	2.598	2.701	3.298	EtOH	10.1063/1.2361290

3.017	2.631	2.702	3.289	MeOH	10.1063/1.2361290
2.756	2.440	2.546	2.918	Water	10.1063/1.2361290
2.995	2.999		3.272	EtOH	10.1063/1.2361290
3.010	3.036	2.998	3.272	MeOH	10.1063/1.2361290
3.054	2.994	2.988	3.263	Water	10.1063/1.2361290
3.307	2.952	2.987	3.594	EtOH	10.1063/1.2361290
3.333	2.944	3.146	3.351	MeOH	10.1063/1.2361290
3.255	2.895	3.141	3.333	Water	10.1063/1.2361290
2.918	2.527		3.155	Water	10.1063/1.2361290
3.962	2.938	3.185	3.473	EtOH	10.1063/1.2361290
3.238	2.991	3.156	3.605	EtOH	10.1063/1.2361290
2.967	2.815	3.021	3.039	EtOH	10.1063/1.2361290
3.263	2.889	3.108	3.626	EtOH	10.1063/1.2361290
3.263	2.902	3.080	3.615	Water	10.1063/1.2361290
3.221	2.843		3.553	EtOH	10.1063/1.2361290
3.221	2.885	3.190	3.553	MeOH	10.1063/1.2361290
3.221	2.843	3.063	3.533	Water	10.1063/1.2361290
2.557	2.622	2.532	2.644	EtOH	10.1063/1.2361290
2.562	2.623	2.540	2.650	MeOH	10.1063/1.2361290
2.557	2.619	2.565	2.661	Water	10.1063/1.2361290
2.952	2.498		3.316	EtOH	10.1063/1.2361290
2.952	2.535	2.932	3.316	MeOH	10.1063/1.2361290
2.918	2.515	2.876	3.307	Water	10.1063/1.2361290
2.787	2.816	2.966	3.024	EtOH	10.1063/1.2361290
2.787	2.852	2.933	3.024	MeOH	10.1063/1.2361290
2.756	2.806	2.917	3.024	Water	10.1063/1.2361290
3.163	3.062		3.553	EtOH	10.1063/1.2361290
3.246	3.114	3.173	3.543	MeOH	10.1063/1.2361290
3.212	3.037	3.136	3.533	Water	10.1063/1.2361290
3.010	2.635	2.883	3.360	Water	10.1063/1.2361290
2.952	3.074	2.963	3.379	EtOH	10.1063/1.2361290
3.212	2.772	3.096	3.533	EtOH	10.1063/1.2361290
3.163	2.814		3.523	MeOH	10.1063/1.2361290
3.123	2.787	3.043	3.503	Water	10.1063/1.2361290
2.583	2.626	2.608	2.678	EtOH	10.1063/1.2361290
2.594	2.620	2.644	2.690	Water	10.1063/1.2361290
2.877	2.431	2.831	3.280	Water	10.1063/1.2361290
2.812	2.808	2.851	3.024	EtOH	10.1063/1.2361290
2.818	2.839		3.024	MeOH	10.1063/1.2361290
2.756	2.807	2.870	3.017	Water	10.1063/1.2361290
3.246	3.063	3.099	3.523	EtOH	10.1063/1.2361290
3.221	3.105	3.147	3.513	MeOH	10.1063/1.2361290
3.155	3.059	3.171	3.513	Water	10.1063/1.2361290
3.179	3.051	3.161	3.503	MeOH	10.1063/1.2361290

3.179	3.001		3.483	Water	10.1063/1.2361290
2.931	2.527	2.840	3.298	Water	10.1063/1.2361290
3.298	3.242	3.356	3.360	nHex	10.1016/j.chemphys.2010.04.032
3.280	3.076	3.302	3.238	DCM	10.1016/j.chemphys.2010.04.032
3.229	2.963	3.083	3.196	EtOH	10.1016/j.chemphys.2010.04.032
3.289	3.102		3.204	MeCN	10.1016/j.chemphys.2010.04.032
3.407	3.132	3.171	3.351	nHex	10.1016/j.chemphys.2010.04.032
3.280	3.039	3.153	3.229	DCM	10.1016/j.chemphys.2010.04.032
3.212	2.871	2.941	3.204	EtOH	10.1016/j.chemphys.2010.04.032
3.298	2.989	3.070	3.196	MeCN	10.1016/j.chemphys.2010.04.032
3.017	2.881		2.959	DCM	10.1016/j.chemphys.2010.04.032
2.818	2.908	3.015	3.002	DCM	10.1016/j.chemphys.2010.04.032
3.351	2.862	2.922	3.196	EtOH	10.1016/j.chemphys.2010.04.032
3.263	2.777	2.863	3.047	EtOH	10.1016/j.chemphys.2010.04.032
3.263	2.777	2.863	2.974	EtOH	10.1016/j.chemphys.2010.04.032
2.340	2.413	2.315	2.557	EtOH	10.1016/j.chemphys.2010.04.032
2.353	2.438		2.557	EtOH	10.1016/j.chemphys.2010.04.032
2.371	2.502	2.445	2.589	EtOH	10.1016/j.chemphys.2010.04.032
2.296	2.510	2.403	2.567	EtOH	10.1016/j.chemphys.2010.04.032
2.296	2.475	2.328	2.562	EtOH	10.1016/j.chemphys.2010.04.032
2.385	2.526	2.344	2.573	EtOH	10.1016/j.chemphys.2010.04.032
2.375	2.618	2.525	2.627	EtOH	10.1016/j.chemphys.2010.04.032
2.318	2.390		2.546	EtOH	10.1016/j.chemphys.2010.04.032
2.667	2.502	2.423	2.831	EtOH	10.1016/j.chemphys.2010.04.032
2.375	2.608	2.566	2.353	EtOH	10.1016/j.chemphys.2010.04.032
2.296	2.618	2.525	2.510	EtOH	10.1016/j.chemphys.2010.04.032
2.925	3.013	2.806	3.229	nHex	10.1021/jp2079296
3.351	2.709	2.824	2.981	nHex	10.1021/jp2079296
3.054	3.115	3.049	3.280	nHex	10.1021/jp2079296
3.307	2.989	3.013	3.155	nHex	10.1021/jp2079296
2.375	2.895	2.545	3.039	nHex	10.1021/jp2079296
2.475	2.443	2.459	2.296	nHex	10.1021/jp2079296
2.385	2.624	2.460	2.787	nHex	10.1021/jp2079296
2.362	2.446	2.555	2.605	nHex	10.1021/jp2079296
2.371	2.627	2.466	2.713	nHex	10.1021/jp2079296

The SMILES of tested molecules could be found in file stored for test molecules.

[1] The experimental data were collected for the reported work.

[2] The ‘predicted1’ data were predicted by ML-model directly, as Figure 5a.

[3] The ‘predicted2’ data were predicted by ML-model with the inclusion of a few additional unfamiliar molecules into the training set, as Figure 5b. The lack molecules were put into training set.

[4] The TD-DFT data were collected for the reported work, with best level chosen for each skeleton.

4.2. Comparsion of time cost in other external dataset.

4.2.1. Computational Details.

Using Grimme's xTB code[S10], initial geometries were optimized at the level of GFN2-xTB[S11]. Then, all time-dependent density functional theory (TD-DFT) calculations were performed in the Gaussian 16 software package [S12]. The xTB geometries were optimized in S_1 state at the TD-CAM-B3LYP[S13]/6-31G(d)[S14]/LR-PCM(DCM)[S15] level of theory. Single-point calculations were performed with the PBE0[S16], ωB97X-D[S17], M06-2X[S18] and CAM-B3LYP[S13] functionals in combination with the 6-311+G(d) basis set[S14b][S19] and the LR-PCM(DCM) model for solvent effects.

4.2.2. Dataset and prediction results.

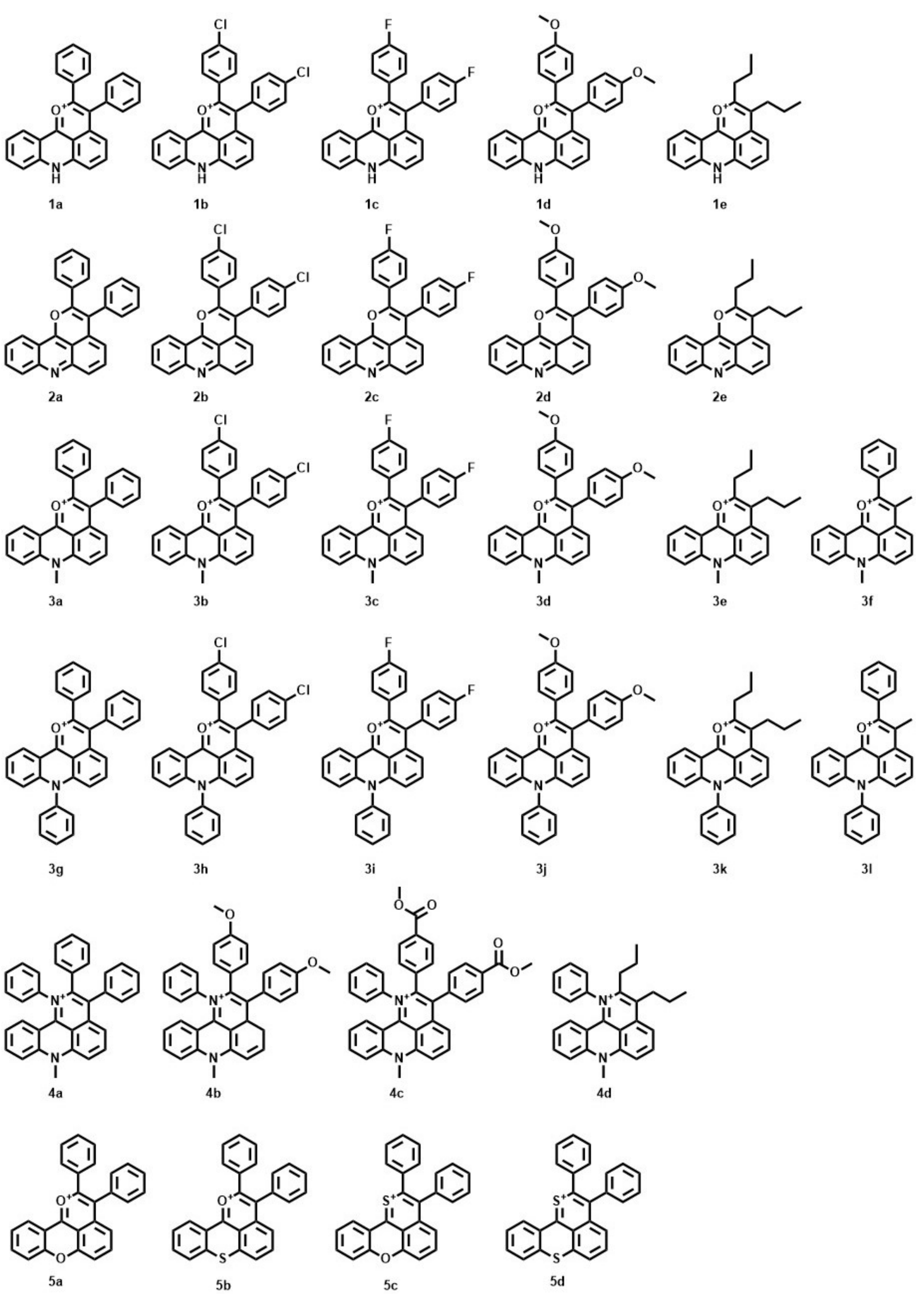


Figure S25. Chemical structure of 30 heterocycle dyes.

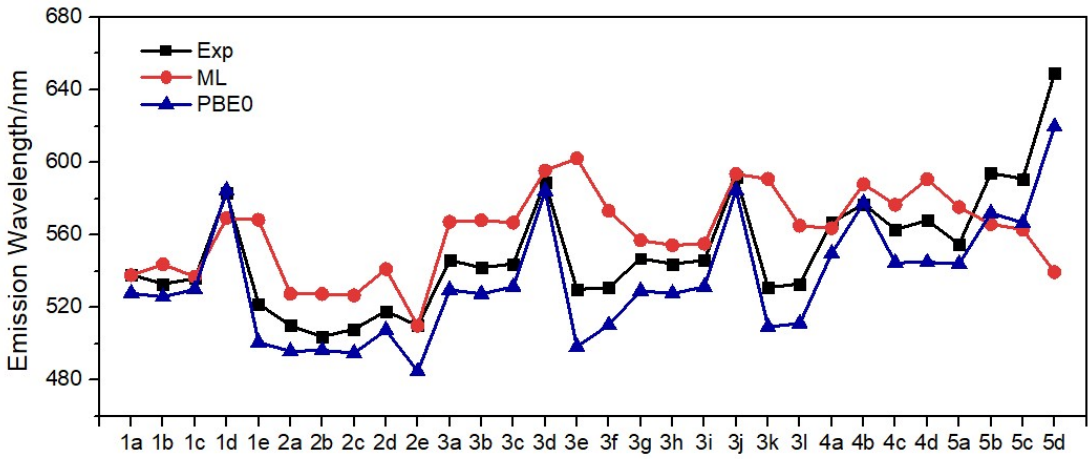


Figure S26. The prediction result of emission wavelength of heterocycle dyes with ML model(GBRT/FSD_CDK) and PBE0/6-311+G* in DCM.

Table S15. The emission wavelength(nm) of 30 dyes in DCM predicted by different method and various functionals.

No	Exp	ML	PBE0	wB97xd	CAM-B3LYP	M062X
1a	*538*	537.768	527.81	476.8	482.68	484.97
1b	*533*	543.798	525.91	473.78	479.67	482.14
1c	*536*	536.986	529.99	476.66	482.46	484.95
1d	*583*	569.205	584.52	498.77	509.29	512.58
1e	*522*	568.321	500.75	463.68	467.09	469.6
2a	*510*	527.502	495.83	457.87	463.49	463.24
2b	*504*	527.425	496.34	457.51	463.39	463.13
2c	*508*	526.716	494.9	456.86	462.36	462.02
2d	*518*	541.153	507.49	463.92	470.28	470.26
2e	*510*	509.842	484.76	449.5	454.02	454.16
3a	*546*	567.207	529.77	480.25	485.91	488.63
3b	*542*	568.051	527.53	477.18	482.89	485.77
3c	*544*	566.731	531.41	480.01	485.65	488.51
3d	*589*	595.536	584.22	501.18	511.42	514.93
3e	*530*	602.134	498.31	462.74	465.83	468.67
3f	*531*	573.16	510.46	469.54	473.89	476.45
3g	*547*	556.987	529.17	479.47	485.07	487.66
3h	*544*	554.296	527.68	476.74	482.38	485.16
3i	*546*	555.109	531.41	479.48	485.02	487.8
3j	*592*	593.591	584.52	500.51	510.6	514.3
3k	*531*	590.913	509.32	471.3	474.77	477.7
3l	*533*	565.037	511.22	469.95	474.23	476.68
4a	*567*	563.672	549.77	503.92	507.42	513.45
4b	*577*	587.971	577.63	515.82	521.2	527.58
4c	*563*	576.532	544.7	500.22	503.47	509.55

4d	*568*	590.707	544.89	503.48	506.28	511.67
5a	*555*	575.282	544.11	480.82	488.53	489.3
5b	*594*	565.918	572.08	516.96	523.16	525
5c	*591*	562.891	566.63	508.23	514.23	516.38
5d	*649*	539.442	619.62	563.9	569.16	573.85

Table S16. Quantum yield of 30 dyes achieved by ML regressor and classifier.

No	Exp	ML Classifier	ML Regressor [1]
1a	*0.59*	1	0.553
1b	*0.69*	1	0.501
1c	*0.54*	1	0.626
1d	*0.47*	0	0.281
1e	*0.6*	1	0.594
2a	*0.24*	0	0.125
2b	*0.25*	0	0.118
2c	*0.19*	0	0.094
2d	*0.23*	0	0.101
2e	*0.65*	1	0.538
3a	*0.82*	1	0.508
3b	*0.68*	1	0.473
3c	*0.75*	1	0.573
3d	*0.68*	0	0.180
3e	*0.83*	1	0.541
3f	*0.72*	1	0.522
3g	*0.71*	1	0.605
3h	*0.76*	1	0.560
3i	*0.87*	1	0.662
3j	*0.58*	0	0.268
3k	*0.85*	0	0.561
3l	*0.82*	1	0.555
4a	*0.77*	1	0.437
4b	*0.79*	0	0.210
4c	*0.76*	1	0.348
4d	*0.77*	1	0.510
5a	*0.55*	1	0.331
5b	*0.65*	1	0.597
5c	*0.36*	0	0.274
5d	*0.37*	1	0.485

[1] Oversample mentioned in SI3.3.1 have been applied.

4.2.3. Cartesian Coordinates for Optimized Structures in Excited States

1a

C	4.1735443493	-0.433656914	0.0068370669
N	3.8208760392	-1.6301204279	0.602974777
C	5.5114366203	-0.1055502658	-0.1979706171
C	5.8400498054	1.09981796	-0.8063754431
C	4.8360745498	1.9810755837	-1.2093260639
C	3.4978961222	1.6679662021	-1.0061392753
C	3.1407469378	0.4603865164	-0.396810406
C	1.8044117158	0.0499263592	-0.141094961
O	0.7992717717	0.9096610842	-0.5162250818
C	-0.4930935701	0.6199451477	-0.2689148254
C	-1.35947872	1.705674955	-0.7257148406
C	-0.9739030744	2.4351439495	-1.8635084871
C	-1.7515779789	3.4878811752	-2.3160241061
C	-2.9066729238	3.8483545025	-1.6266119833
C	-3.2822192153	3.1493588079	-0.4821754178
C	-2.5221250522	2.0812372586	-0.0340856002
C	-0.8735246515	-0.5743320093	0.3357258309
C	-2.3044561226	-0.9093259838	0.5399365421
C	-2.8072698496	-1.0989190936	1.8320388123
C	-4.1448635678	-1.4234885305	2.0237019012
C	-4.9895693927	-1.5753361919	0.9289667133
C	-4.4934068467	-1.3996471113	-0.3596814935
C	-3.1602164617	-1.0655722705	-0.5550585222
C	0.1440480799	-1.5083994487	0.7291936068
C	-0.1293071815	-2.7749035281	1.3072265792
C	0.9017646236	-3.6212572514	1.6747758494
C	2.23410834	-3.250228358	1.4594529403
C	2.5343045072	-2.0219810019	0.8577679768
C	1.4899743641	-1.1492783558	0.4872709118
H	4.5722719208	-2.2606889998	0.8591920236
H	6.2866095564	-0.7932958592	0.1243738734
H	6.882447173	1.3518622875	-0.9650348403
H	5.0989956752	2.9205420722	-1.683130423
H	2.71758804	2.3543643457	-1.3123507301
H	-0.073748779	2.1557863476	-2.3981063917
H	-1.4555087677	4.0313353313	-3.2068038421
H	-3.5109842028	4.6784445947	-1.9775699632
H	-4.1700586818	3.4417095698	0.0679795738
H	-2.8130084007	1.5590519567	0.8677015556
H	-2.1520725278	-0.9705658046	2.6881599041
H	-4.526515019	-1.5563269515	3.0306594261
H	-6.0333471603	-1.831032441	1.0793230894
H	-5.1469296644	-1.5240594103	-1.2168649031
H	-2.7758253454	-0.9295632061	-1.5605493963
H	-1.156976786	-3.0797066641	1.4551191203
H	0.6817987011	-4.582656488	2.1220943385
H	3.0385410508	-3.9197334406	1.7453552014

1b

Cl	-4.4057866596	4.9918842086	-1.3613114884
C	-3.2915484231	3.7028882005	-1.0106668748
C	-3.6435266651	2.3937486242	-1.3225611968
C	-2.7620714041	1.3669630917	-1.033072673
C	-2.0627306931	4.0019822264	-0.4315922169
C	-1.1776710702	2.9733735643	-0.1625311584
C	-1.5198403737	1.6398430745	-0.4406208575
C	-0.5361755386	0.5943122588	-0.160906584
C	-0.7793474941	-0.7089778588	0.2575063502
C	-2.159042038	-1.1805411549	0.5338105238
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C	1.8065289249	0.2393161977	-0.1862216031
C	3.0858555395	0.7989539481	-0.4540903653
C	3.3057829989	2.1160194635	-0.8684663363
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C	4.2085230914	-0.0610563006	-0.2835344183
N	3.9919422306	-1.3631967816	0.1262427839
O	0.7135078442	1.0564995361	-0.3544972437
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H	-0.2181162912	3.2003806656	0.2860113222
H	-2.1423994607	-2.6804816037	-1.0148961764

H	-4.428449868	-3.484601277	-0.5355184298
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H	-2.494493989	0.2005215776	2.1526057813
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H	4.7542930627	3.5939207972	-1.4253096145
H	6.6962188195	2.0800309699	-1.1189821595
H	6.3429030233	-0.2627042032	-0.3901266715
H	4.8073999777	-1.9537965284	0.2467742418

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C	2.9423493403	2.5761552799	0.7900470136
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C	2.4040878556	-1.1324949402	-1.1144173522
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H	2.032950625	-0.5357377407	-1.9404505796
H	0.2193214167	-3.653795668	-0.1123968643
H	-1.7534692077	-5.1322880571	-0.0797307872
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F	5.4098818068	-2.8553888479	-0.1216343832

1d

C	-2.4819010456	3.8541700829	-0.2248381851
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C	-2.0817566541	1.5274307913	-0.7190274238
C	-1.2479674254	3.9349299638	0.4351334462
C	-0.4390158586	2.8187301646	0.5008394621
C	-0.8372693191	1.5837279709	-0.0492613913
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C	-3.4963219719	-2.6298864795	-0.791527721
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C	-3.7865981675	-1.3943780571	1.2672683993
C	-2.4817213141	-0.9557394389	1.1930045005
C	0.821464801	-1.8643681597	0.0737989712
C	0.6211102935	-3.2611086687	0.1654569061
C	1.6965142459	-4.1332125946	0.1377069031
C	3.0054659314	-3.6458988237	0.0488212178
C	3.2398692308	-2.2694610985	0.0054393037
C	2.1499959306	-1.370263952	0.0248581986
C	2.4022010603	-0.0061181155	0.0333655331
C	3.7146905602	0.5361877858	-0.0239428526
C	4.0058071777	1.9068611991	-0.0429671751
C	5.3209882019	2.3432554826	-0.1010244267
C	6.3698065184	1.4227030113	-0.144387803
C	6.1081668038	0.0589988114	-0.1286810165

C	4.7915672865	-0.3924079289	-0.0667978709
N	4.5057810468	-1.7441670559	-0.0424688227
O	1.3591035616	0.8890503249	0.0693882286
H	-3.8247387941	2.6085067969	-1.3417108118
H	-2.3978755956	0.6142036278	-1.2038490879
H	-0.9198113962	4.8585888814	0.8932830103
H	0.5122560677	2.8885756348	1.013589292
H	-1.5580131976	-2.5011391655	-1.6828855954
H	-3.8764216859	-3.2700840595	-1.5771714166
H	-4.4297113727	-1.1045414283	2.0907499184
H	-2.0901615511	-0.3094175722	1.9714032238
H	-0.3836578004	-3.6496859479	0.2665683222
H	1.5291671414	-5.2016586608	0.1988337269
H	3.8439517552	-4.3345742619	0.0338272962
H	3.1889167373	2.6178746668	-0.0169832614
H	5.533126041	3.4067997981	-0.1151486223
H	7.3963432733	1.7688216024	-0.1916744584
H	6.9189372647	-0.6614507909	-0.1672895714
H	5.2892005623	-2.3863354646	-0.048476513
O	-3.3373998098	4.8730735503	-0.3581540181
O	-5.5973055825	-2.5968097869	0.4285998553
C	-2.9961950195	6.1430496433	0.190675351
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H	-2.0820469207	6.5330156361	-0.2661673863
H	-2.8730531087	6.0792740469	1.2756226034
C	-6.1855135791	-3.4479550079	-0.5444684266
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H	-5.6644673683	-4.4093865156	-0.5956700686
H	-6.1857621644	-2.9776952862	-1.5331068662

1e

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C	-0.4652897161	-3.6398588716	0.6548793402
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C	0.9101170989	0.2497711234	-0.1447563021
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C	4.5744476562	-0.3409676275	-0.2462267042
C	3.2014034265	-0.5425900971	-0.1298624766
N	2.690938457	-1.8002158476	0.1324073424
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H	-3.6855918667	-1.0709945478	-0.5351711869

2a

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H	3.0428481575	-4.3888658199	-0.2139731492

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H	-0.9793879991	-2.849185405	-2.012313549
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3a

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C	5.2670720322	2.2477564256	0.2500642943
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H	5.5728177646	-1.2789824475	-1.836227119
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5a

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H	-6.2521906696	-0.6640075564	-0.6496148838
H	-5.1553380844	-0.5249546397	1.5706467103
H	-2.6933775752	-0.4464803084	1.7334277302

5c

C	4.3979049023	-0.9033589739	0.1720094377
O	3.8260932433	-2.1184465139	0.3971785652
C	2.4899079203	-2.2735187791	0.4488074455
C	1.6096837181	-1.1954059416	0.2452398247
C	0.21262167	-1.4655961593	0.3107773298
C	-0.2090857326	-2.7770759306	0.6511275046
C	0.6875176009	-3.8171035755	0.8397766602
C	2.0482691846	-3.5698911586	0.7293477391
C	5.7819598999	-0.8591701847	0.1499556092
C	6.4099833646	0.3585856616	-0.0654571607
C	5.6467105153	1.5148533933	-0.2551451818
C	4.2635549902	1.4622727202	-0.2327658332
C	3.5929007918	0.2444112943	-0.0192274239
C	2.1732462757	0.0777370147	0.019034903

S	1.1845463673	1.4951131008	-0.2573669361
C	-0.4340294973	0.8925993906	-0.1409151848
C	-1.4095788002	1.9778678767	-0.3616653358
C	-2.4213693062	1.8597730846	-1.3269718754
C	-3.2869650136	2.9157108788	-1.5605128765
C	-3.1699051761	4.0955945611	-0.8290717062
C	-2.1711056004	4.2223567302	0.1308084711
C	-1.2857523268	3.1781099115	0.3546892861
C	-0.7730298094	-0.4355289205	0.0871202845
C	-2.2143647039	-0.8040847558	0.1252467859
C	-3.057909405	-0.2786516011	1.1092654319
C	-4.3992990908	-0.6335716249	1.1425891936
C	-4.9177700186	-1.5032838286	0.1870731901
C	-4.0866826596	-2.0273754024	-0.7978264156
C	-2.7400477231	-1.6880835493	-0.82520725
H	-1.2654963131	-2.9673023791	0.7775448059
H	0.3296205686	-4.8086577344	1.0869289439
H	2.7895197402	-4.3471523981	0.874243508
H	6.3399025395	-1.7756729997	0.3028501736
H	7.4925937184	0.4101718221	-0.0851317193
H	6.1405344602	2.4656298338	-0.4224165465
H	3.6948245638	2.373344946	-0.3821106225
H	-2.5120405578	0.9495926494	-1.9066653922
H	-4.0559960644	2.8191378643	-2.3193468194
H	-3.8569409712	4.9158119787	-1.0092702593
H	-2.079842456	5.1362387024	0.7077929994
H	-0.5158461663	3.278009303	1.1124512791
H	-2.6576463779	0.4018951459	1.8534101487
H	-5.0424960705	-0.2286717334	1.9168640058
H	-5.9687441918	-1.7720610461	0.2106281016
H	-4.4858377805	-2.7023716377	-1.5475902346
H	-2.094214222	-2.0929810358	-1.5981968547

5d

C	4.5475158696	-0.9214979759	0.248070407
S	4.0818872551	-2.4956132054	0.8177193134
C	2.3505425279	-2.4758262294	0.8047386674
C	1.5695244787	-1.3283833625	0.5291023732
C	0.1491619852	-1.5036055968	0.537672943
C	-0.3917885845	-2.7565810928	0.9225440054
C	0.39992422	-3.8511094191	1.212541449
C	1.7755199753	-3.7127591463	1.1369861473
C	5.9147392594	-0.731816698	0.0427701927
C	6.3924871203	0.4956529632	-0.3803621799
C	5.4898518226	1.5354947272	-0.6043107413
C	4.1328769884	1.3498835042	-0.4069759988
C	3.6050642373	0.1187264824	0.0335092006
C	2.19040295	-0.0796860993	0.251514129
S	1.2415512353	1.3929240132	0.1746190231
C	-0.3950996966	0.8649583565	0.0669507825
C	-1.3112453001	1.9999993942	-0.1897700907
C	-2.1665321274	1.993881441	-1.2987231497
C	-2.9769687147	3.0888231136	-1.5573863907
C	-2.9536994639	4.1951593986	-0.7120290834
C	-2.106659019	4.208379155	0.3907495284
C	-1.2798731889	3.1225261437	0.6467124654
C	-0.7840574994	-0.4515888556	0.2000523735
C	-2.2207570586	-0.800181873	0.0214634398
C	-3.1989675046	-0.2875771471	0.8785659209
C	-4.5335140256	-0.6249162244	0.6982625666
C	-4.9086169088	-1.4659898182	-0.3457572024
C	-3.9419080666	-1.9789869431	-1.2045921968
C	-2.603753308	-1.6559800444	-1.0183429868
H	-1.465748146	-2.8514125596	0.9997064955
H	-0.0453221108	-4.795334722	1.4999726324
H	2.4228204706	-4.556922923	1.3519791802
H	6.5993017092	-1.5560047177	0.2161952512
H	7.4548934345	0.6417135044	-0.5373971578
H	5.8470891581	2.501941873	-0.942597869
H	3.4689147317	2.1786824672	-0.6181530125
H	-2.1841328727	1.1377363289	-1.9627346034
H	-3.6289589406	3.0790149881	-2.4244318235
H	-3.5954180388	5.0463856825	-0.9144010981
H	-2.0879595081	5.065248196	1.0556926124
H	-0.6271102588	3.1343196496	1.513762392
H	-2.9105152465	0.370873083	1.6910129014
H	-5.2834001997	-0.2290179745	1.3751468694
H	-5.95337549	-1.722065882	-0.4884325289
H	-4.2283895551	-2.6334578771	-2.0211854564
H	-1.8504985953	-2.0556080784	-1.6904296924

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