Supporting Information

Deep Learning Optical Spectroscopy Based on Experimental Database: Potential Applications to Molecular Design

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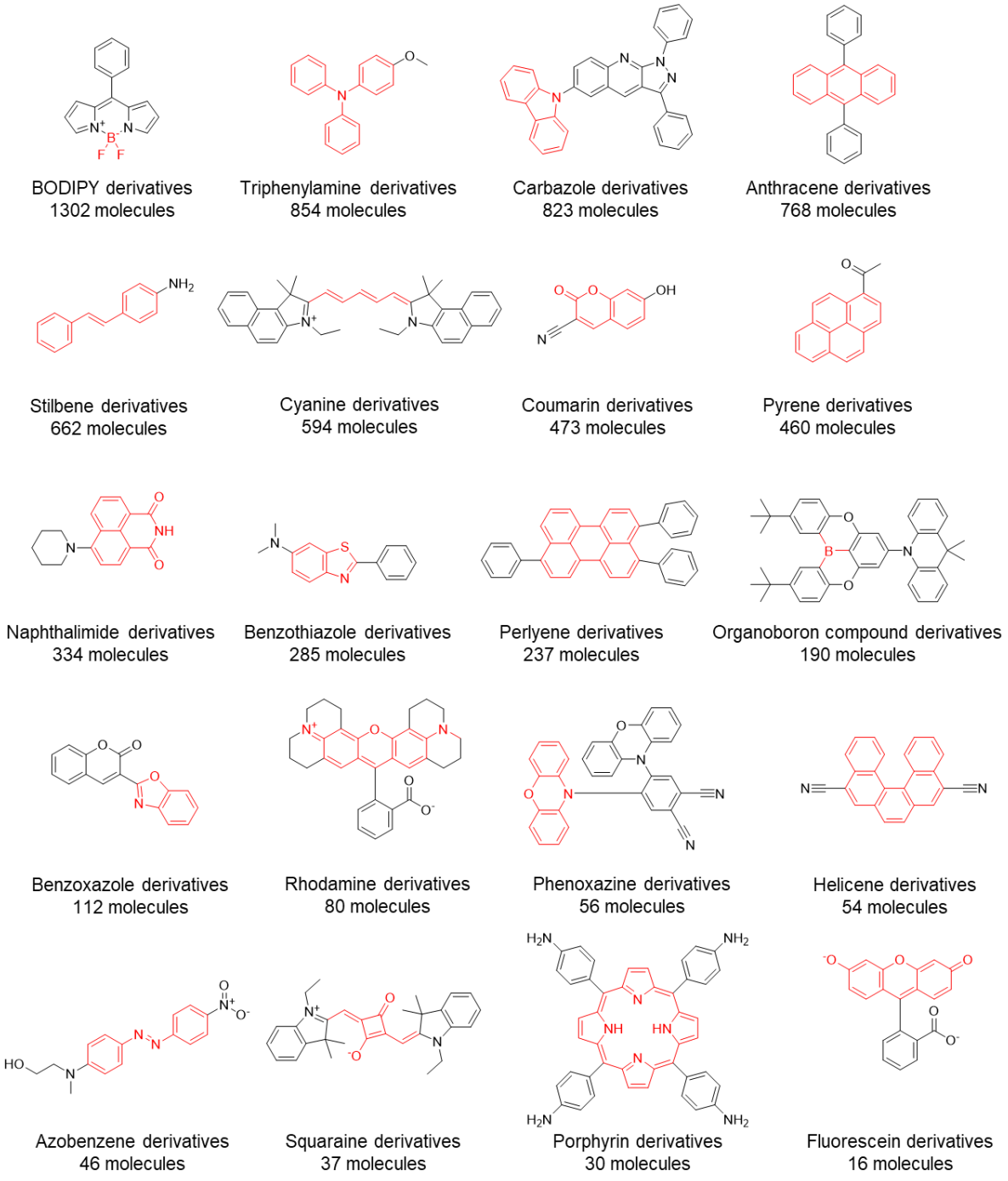


Figure S1. Examples of various chromophores included in our database. The molecular structures of chromophores and the number of chromophores that contain the core structures in red. Note that the chromophores, which are structurally similar but do not contain the exact core structures in red, are not taken into account.

1. Deep learning model

Algorithm of our deep learning model. The detailed algorithm of our deep learning (DL) model is described in Algorithm 1. A_j and X_j are the adjacency and feature matrices of j, respectively, H_j is the hidden matrix which is an updated feature matrix of j, *reduce_sum* represents the summation over all nodes, *concat* represents the concatenation of vectors, MLP stands for a multi-layer perceptron, and ○ denotes the function composition.

Algorithm 1. Deep learning model algorithm

	Input : A_{chm},X_{chm},A_{sol},X_{sol}	# Chromophore and solvent graphs
	Output : Properties y	
1	$H_{chm}^{(0)} \leftarrow X_{chm}$	
2	$H_{sol}^{(0)} \leftarrow X_{sol}$	
3	**for** k in range(Number of GCN layers)	# GCN layers
4	$H_{chm} \leftarrow GCN^{chm}_k(A_{chm},H_{chm})$	
5	$H_{sol} \leftarrow GCN^{sol}_k(A_{sol}, H_{sol})$	
6	**endfor**	
7	$z_{chm}^{(0)} \leftarrow$ *reduce_sum*(H_{chm})	# Chemical space layers
8	$z_{sol}^{(0)} \leftarrow$ *reduce_sum*(H_{sol})	
9	**for** l in range(Number of MLPs)	
10	$z_{chm} \leftarrow MLP_{chm}^{l}(z_{chm})$	
11	$z_{sol} \leftarrow MLP_{sol}^{l}(z_{sol})$	
12	**endfor**	
13	**for** m in range(Number of interaction layers)	# Interaction layers
14	$z \leftarrow MLP_m \circ$ *concat*(z_{chm}, z_{sol})	
15	**endfor**	
16	$y \leftarrow MLP(z)$	# Output
17	return y	

Graph representation of molecules. Molecules and their structural features can be represented by using an adjacency matrix and a feature matrix. The adjacency matrix describes the connectivity of atoms in a given molecule. The single, aromatic, double, and triple bonds are encoded as 1, 1.5, 2, and 3 in the adjacency matrix, respectively. In addition, the diagonal elements are encoded as 1 to represent the atom itself. In our deep learning model, the maximum number of atoms is 150, which can be readily extended if necessary, giving the adjacency matrix of 150×150 elements. The feature matrix consists of one-hot encoded 16 kinds of atoms, the number of hydrogen atoms, the number of connected heavy atoms, aromaticity, hybridization state, ring, and formal charge. The total feature matrix size is 150×43. The example of the adjacency and feature matrices for phenol is shown in Figure S2.

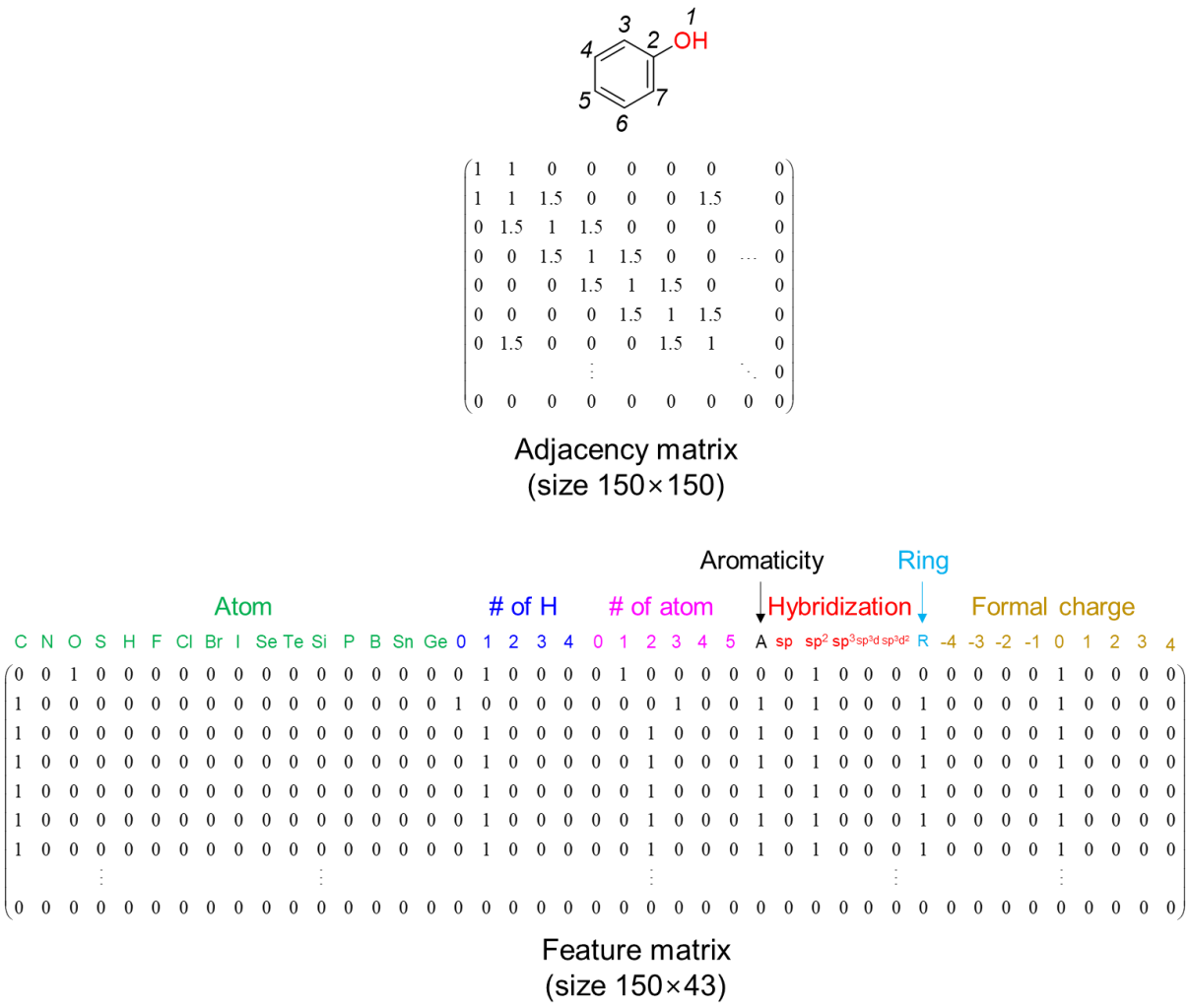


Figure S2. Schematic illustration of the adjacency and feature matrices for phenol.

GCN layer. The graph convolutional network (GCN) is the simplest version of the message passing neural network.[1-6] The GCN as an extension of the convolutional neural networks was found to effectively deal with graph structures like molecular structures because the GCN bypasses the conformational isomerism and maintains rotational and translational invariances. Furthermore, the GCN is a cost-efficient method because it utilizes a small number of weight parameters. A single graph convolution of adjacency matrix (A_j) and updated feature matrix (H_j^l) updates the atom's features, producing a new feature matrix of the l+1-th layer, H_j^{l+1}, which contains all information on the nearest neighbor atoms as follows,

$$H^{l+1} = \sigma\left(AH^lW^l + B^l + H^l\right) \quad \text{(S1)}$$

where $\sigma(x)$, A, W^l, and B^l denote the activation function, adjacency matrix, convolution weights, and bias of the l-th GCN layer, respectively. To explain Eq. S1 in detail, H^l is a set of each atom's features, h_i^l is a row vector of H^l. Thus, $H^l = \left\{h_1^l, h_2^l, ..., h_N^l\right\}, h_i^l \in \mathbb{R}^F$, where N is the number of atoms, F is the number of features.

As an example of the phenol molecule in Figure S2, the carbon atom in the second row (^{2}C) of the feature matrix is bonded to ^{1}O, ^{3}C, and ^{7}C atoms. The single graph convolution of each atom is drawn schematically in Figure 2. Operation of the single graph convolution on the second row of l-th layer in the feature matrix (h_2^l) gives h_2^{l+1} as in the follow equation

$$h_2^{l+1} = \sigma\left\{(a_{22}h_2^l + a_{21}h_1^l + a_{23}h_3^l + a_{27}h_7^l)\cdot W^l + b_2^l + h_2^l\right\} \quad \text{(S2)}$$

where $a_{i,j}$ and b_i^l denote elements of A and a row vector of B^l, respectively. Thus, the features of ^{2}C is updated based on the features of bonded atoms.

In our deep learning model, the rectified linear unit (ReLU), $ReLU(x)=max(0, x)$, is used as the activation function. Multiple graph convolutions are applied to reflect the atom's features at a long distance from a specific central atom. However, deeply stacked layers have side-effects such as the vanishing gradient problem. Using skip-connection in each hidden layer is a common solution to avoid the problem. In our deep learning model, the feature matrix of the l-th layer, H^l, is added to $AH^lW^l + B^l$ as represented in Eq. S1. For a given molecule, several GCN layers (ReLU activation, size 150×43 for feature matrix, 150×150 for adjacency matrix) are stacked to treat the molecular structures of chromophores and solvents simultaneously.

Chemical space layer. Chemical space layers are to extract molecular information from the GCN. The final feature matrix of GCN layers, $H^{(f)}$, is summed over all nodes to produce one row vector, which guarantees permutation invariance. To explain this summation in equation, a row vector, $z^{(0)}$, is obtained by $z = \sum_i h_i$. The row vector passes through multi-layer perceptrons (MLPs, ReLU activation) to produce a chemical space vector, $z^{(f)}$.

Interaction layer. Since the optical properties of chromophore are substantially influenced by the local environments, two parallel GCN and chemical space layers are used for both chromophore and solvent. The chemical space vectors of chromophore and solvent are concatenated and passes through the MLPs (ReLU activation) to obtain an interaction vector which is expected to contain all information of chromophore affected by solvent. Finally, the interaction vector passes through the MLPs to obtain seven optical properties (λ_{abs}, λ_{emi}, σ_{abs}, σ_{emi}, ε, Φ, and τ).

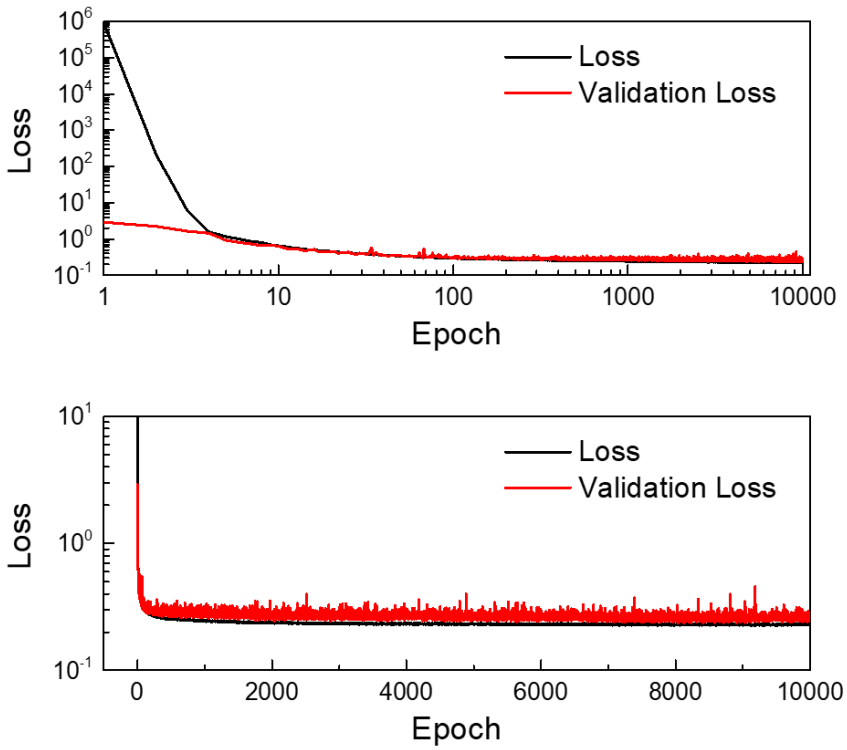


Figure S3. The loss functions for training and validation of our deep learning (DL) model as a function of epoch.

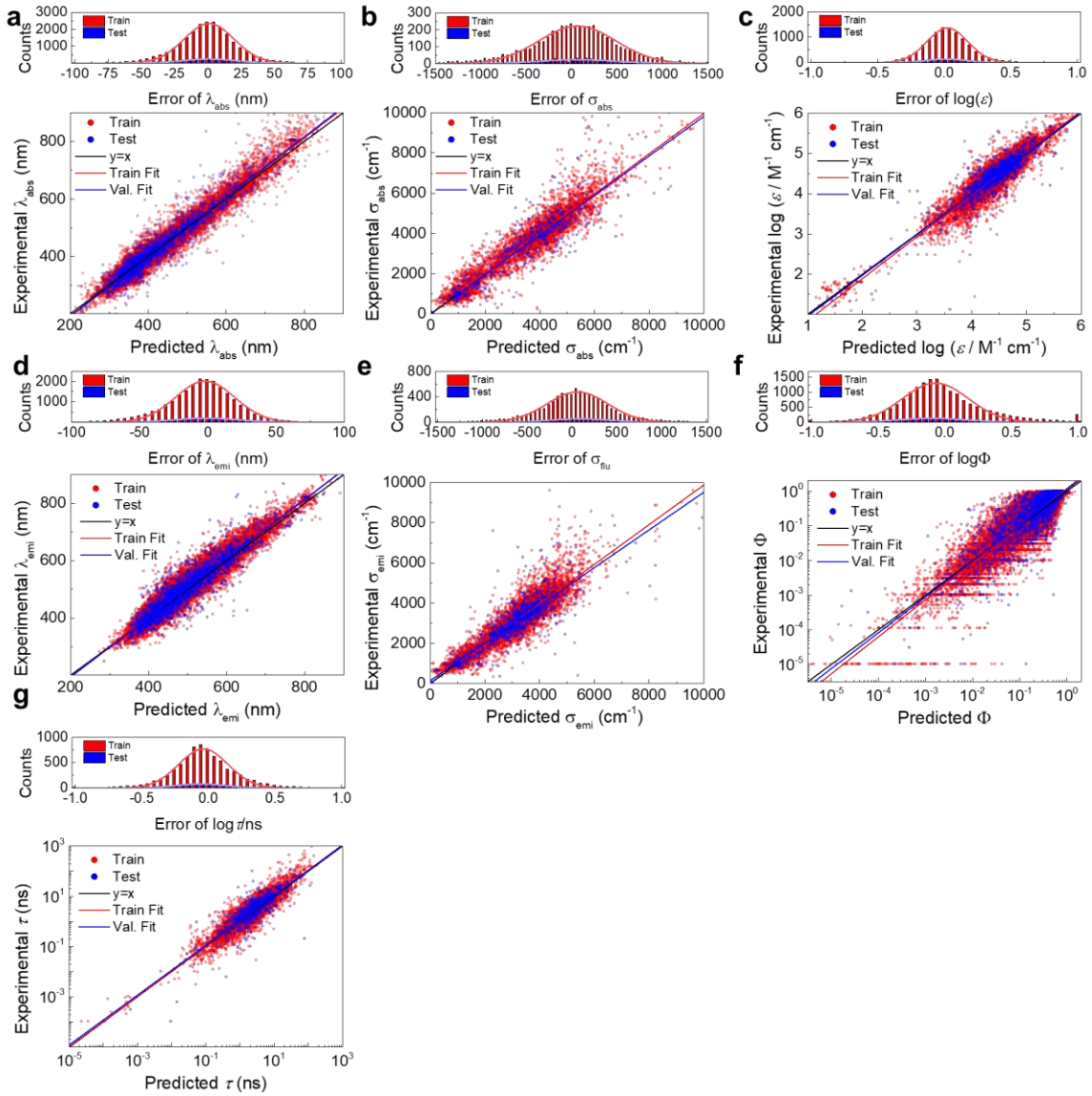


Figure S4. a-g. Results of our DL model for the first absorption peak position (λ_{abs}), and absorption bandwidth in FWHM (σ_{abs}), extinction coefficient (ε), emission peak position (λ_{emi}), emission bandwidth in FWHM (σ_{emi}), photoluminescence quantum yield (Φ), and lifetime (τ).

Table S1. Root mean square error (RMSE) in our DL model.

	Train and validation set	Test set
λ_{abs}	26.0 nm	31.6 nm
σ_{abs}	593 cm^{-1}	692 cm^{-1}
log ε	0.200	0.240
λ_{emi}	27.4 nm	32.6 nm
σ_{emi}	528 cm^{-1}	566 cm^{-1}
log Φ	0.363	0.431
log τ	0.255	0.318

Table S2. Square of the Pearson correlation coefficient (R^2) in our DL model.

	Train and validation set	Test set
λ_{abs}	0.951	0.926
σ_{abs}	0.889	0.836
log ε	0.880	0.795
λ_{emi}	0.926	0.892
σ_{emi}	0.818	0.769
log Φ	0.804	0.714
log τ	0.829	0.743

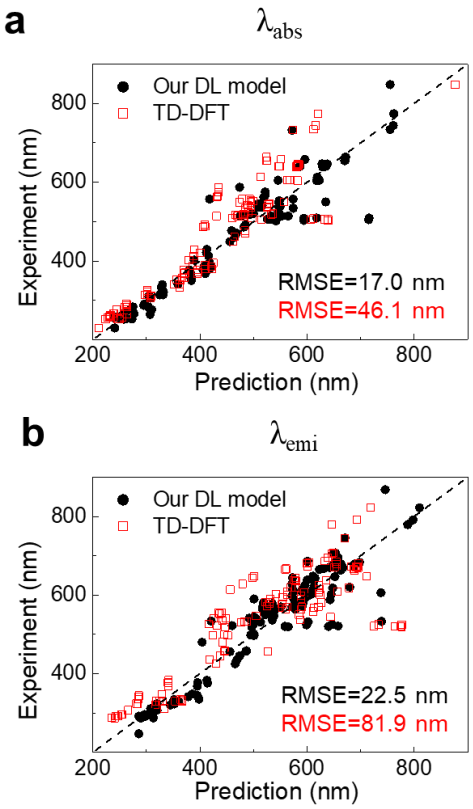


Figure S5. **a** and **b**. Comparison of the predictions obtained using our DL model and TD-DFT for molecules in Table S6.

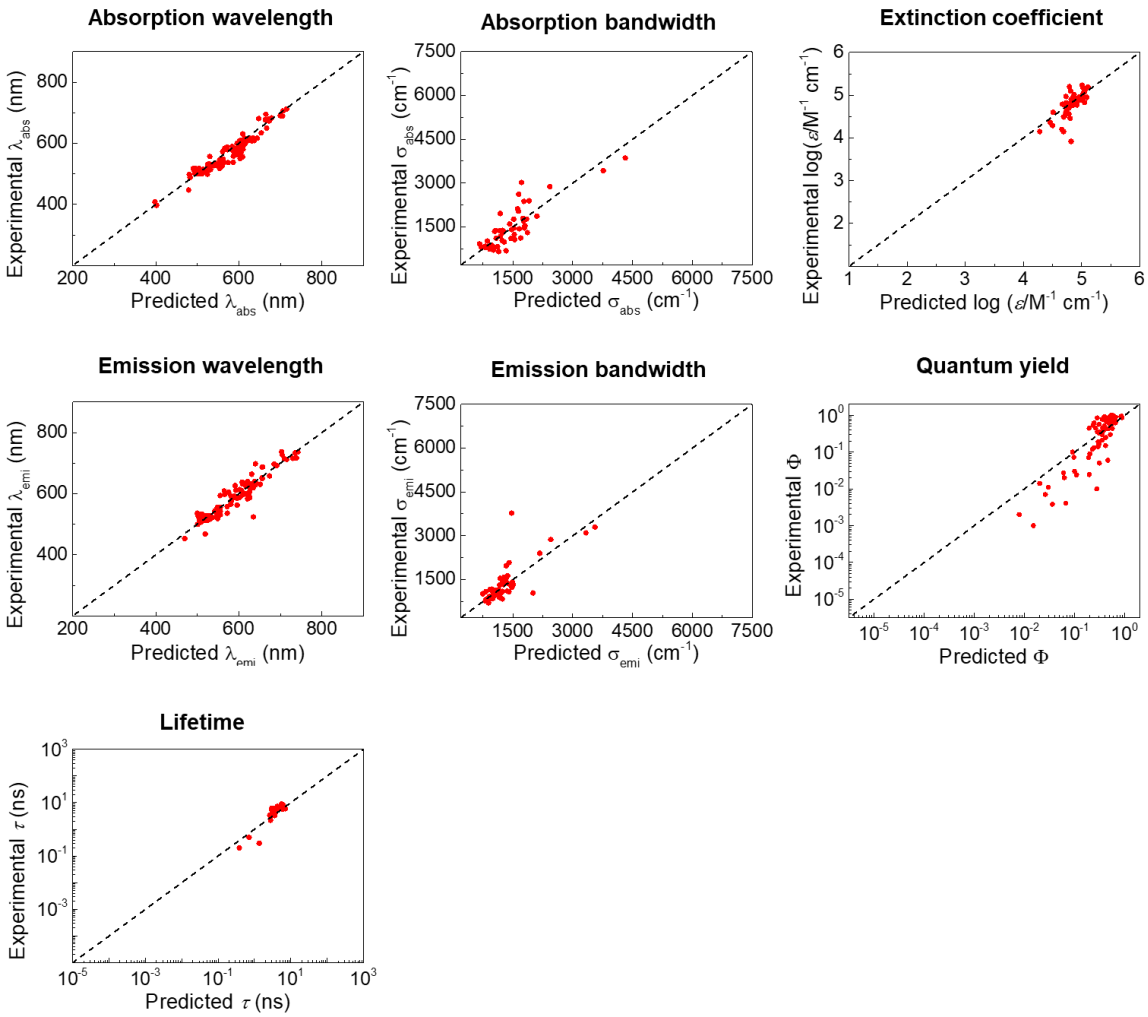


Figure S6. Results of our DL model for 97 chromophores in dichloromethane in Table S7.

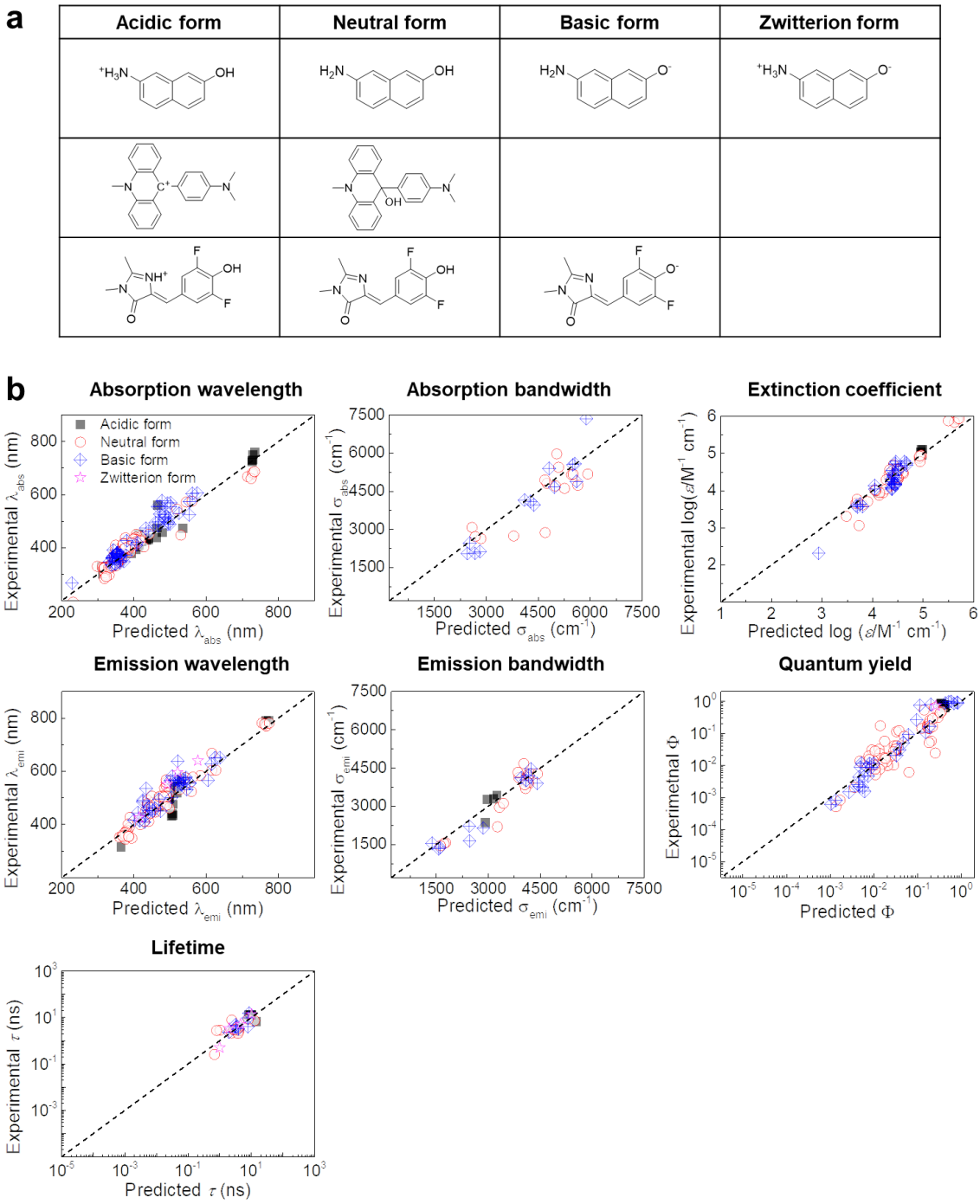


Figure S7. **a**. Molecular structures of protonated (acidic) and deprotonated (basic) forms of 3 molecules. **b**. Results of our DL model for 59 cores chromophores (129 acid/base combinations) in different environments.

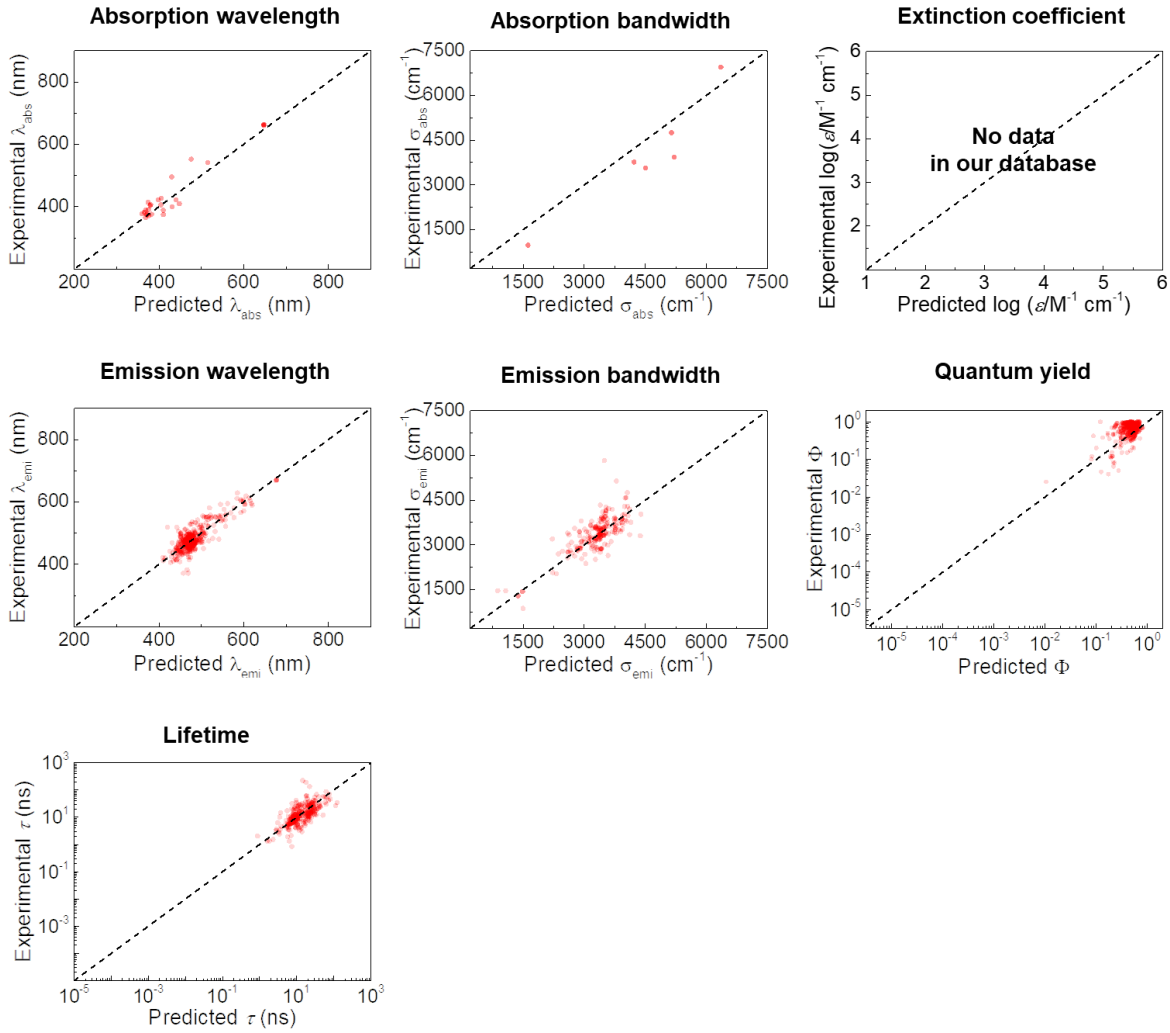


Figure S8. Results of our DL model for 361 chromophore-host systems.

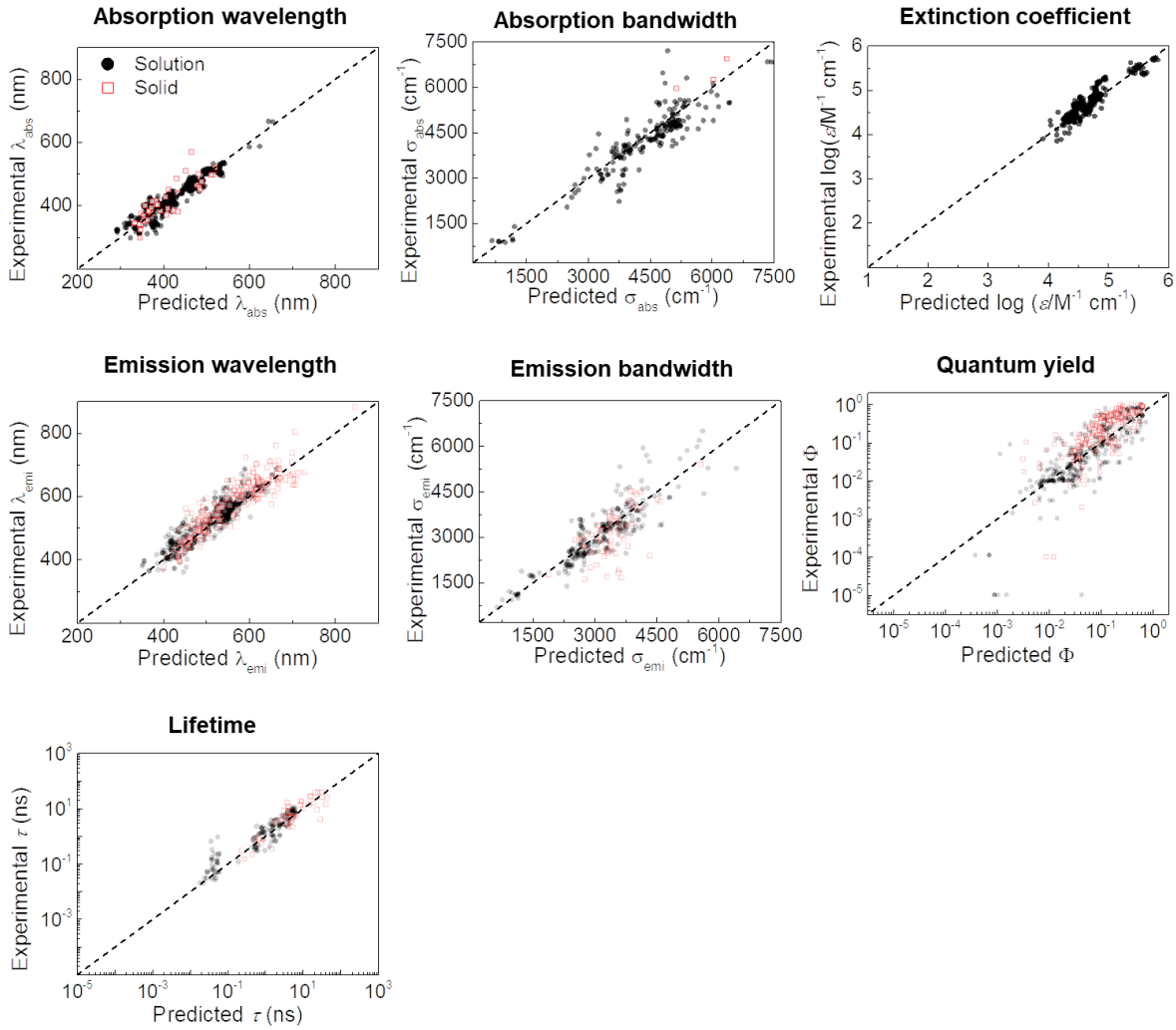
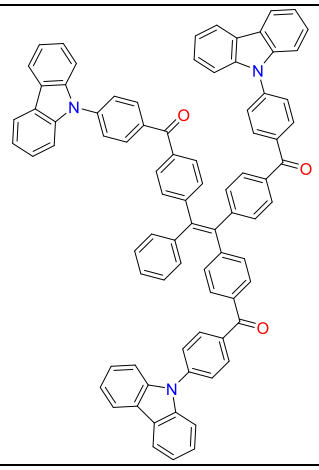
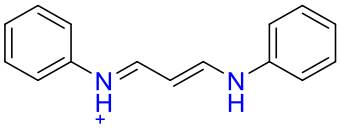
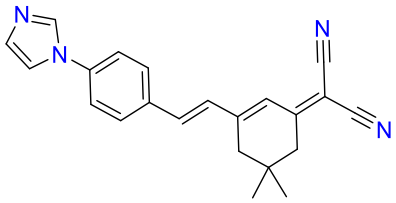
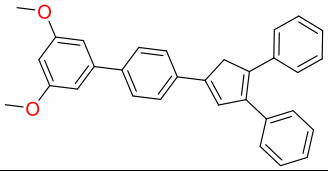
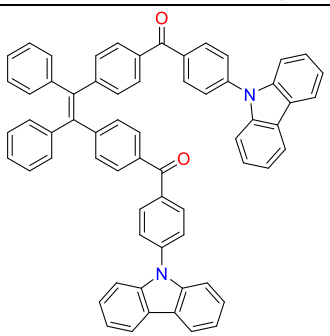


Figure S9. Results of our DL model for 730 examples of chromophores in different environments exhibiting aggregation-induced emission (AIE).

Table S3. Examples of molecules exhibiting AIE and their PLQY (Φ).

Molecule	Solvent	Solution		Solid	
		Φ_{exp}	Φ_{pred}	Φ_{exp}	Φ_{pred}
	THF	0.2973	0.2979	0.6671	0.5596
	Dimethyl sulfoxide	0.08	0.09	0.18	0.103
	Ethanol	0.001	0.0004	0.027	0.031
	CH_2Cl_2	0.0575	0.0348	0.19	0.11
	THF	0.2681	0.106	0.6491	0.5129

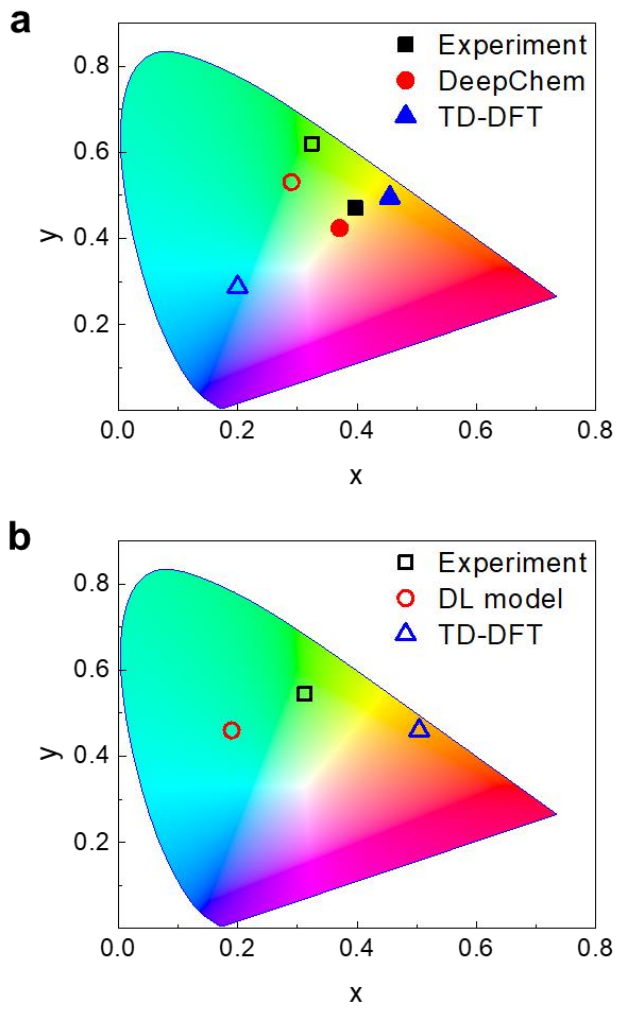


Figure S10. Representation of the CIE 1931 *xy* chromaticity space. Filled and empty circles indicate absorption and emission, respectively. **a.** Coumarin 153 in ethanol. **b.** BPCP-2CPC in C-2PC.

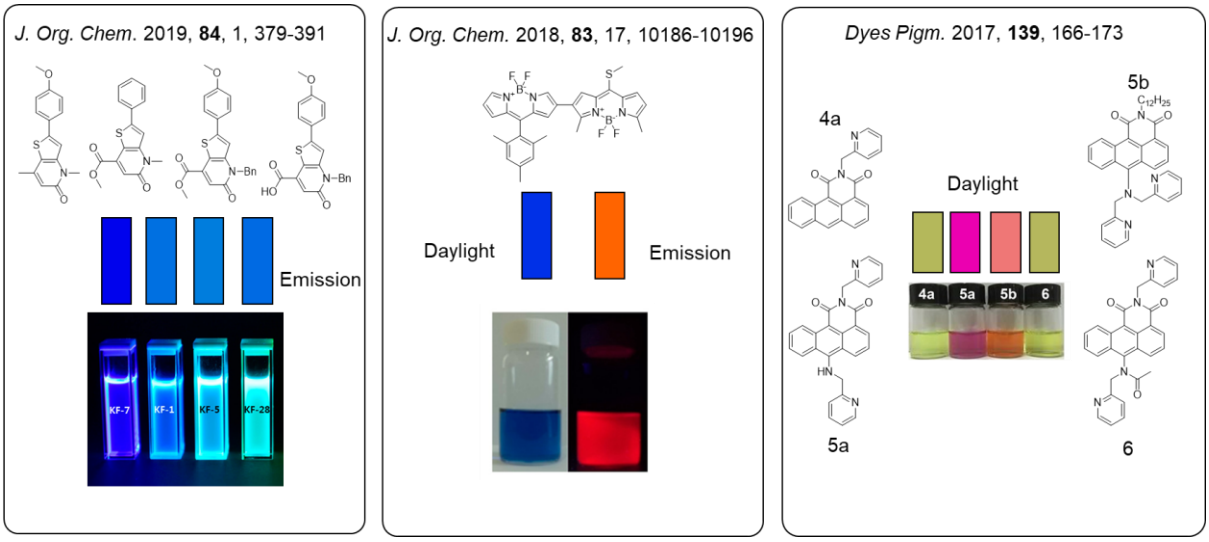
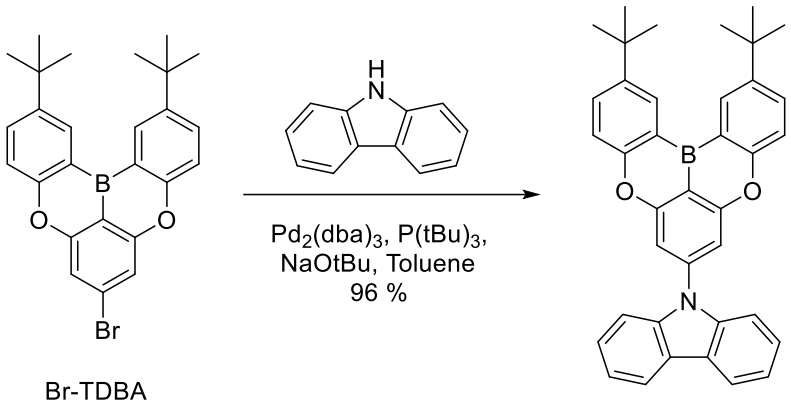


Figure S11. The filled box indicates the daylight and emission color reconstructed based on the absorption and emission spectra of molecules predicted by our DL model.[7-9] Reprinted with permission from Ref. 7 and 8. © 2019, 2018 American Chemical Society. Reprinted with permission from Ref. 9. © 2016 Published by Elsevier Ltd.

2. Synthesis and measurements of 9-(2,12-di-tert-butyl-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracen-7-yl)-9H-carbazole (1)



Br-TDBA

Br-TDBA (0.1 g, 0.21 mmol) and carbazole (0.042 g, 0.25 mmol) were dissolved in toluene (15 mL), and NaO^{t}Bu(0.060 g, 0.60 mmol, 5 mL) was added and purged with nitrogen (N_2) for 15 min. Subsequently, $Pd_2(dba)_3$ (0.023 g, 0.021 mmol) as the catalyst and P(^{t}Bu)$_3$ as the ligand was added under N_2, and the resulting mixture was stirred at 80 °C for 3h. After complete conversion to the product, the mixture was cooled to RT, and the organic layer was extracted with dichloromethane(MC), dried, filtered, and subjected to silica gel column chromatography for purification using hexane: MC (9:1, *v*/*v*) as the eluent. Moreover, the product was further purified via precipitation in Hexane: ethanol (1:4, *v*/*v*) solvent mixture to afford a white solid (0.11 g, 96% yield). ^{1}H NMR (500 MHz, CDCl3): δ (ppm) 8.80 (d, J = 2.4 Hz, 2H), 8.18 (d, J = 7.7 Hz, 2H), 7.81 (dd, J = 8.7, 2.4 Hz, 2H), 7.71 (d, J = 8.2 Hz, 2H), 7.53 (d, J = 8.7 Hz, 2H), 7.50 – 7.42 (m, 4H), 7.34 (t, J = 7.4 Hz, 2H), 1.52 (s, 18H). UV−visible absorption spectrum was taken by using a UV−visible spectrometer (Cary 100, Varian) in the wavelength range of 200−800 nm. The baselines were corrected by the absorption spectrum of the reference solution. Steady-state fluorescence spectrum was recorded by using a fluorimeter (F-7000, Hitachi). Time-resolved fluorescence spectrum was collected at by using a time-correlated single-photon

counting (TCSPC) technique. The sample solution was excited by a 375 nm pulse (LDH-P-C-375, Picoquant). The fluorescence from the sample solution was measured by a single photon detector (ID100, Idqeantique) with a rising time of 50 ps. The instrumental response function (IRF) of our TCSPC setup was measured to be about 80 ps in FWHM.

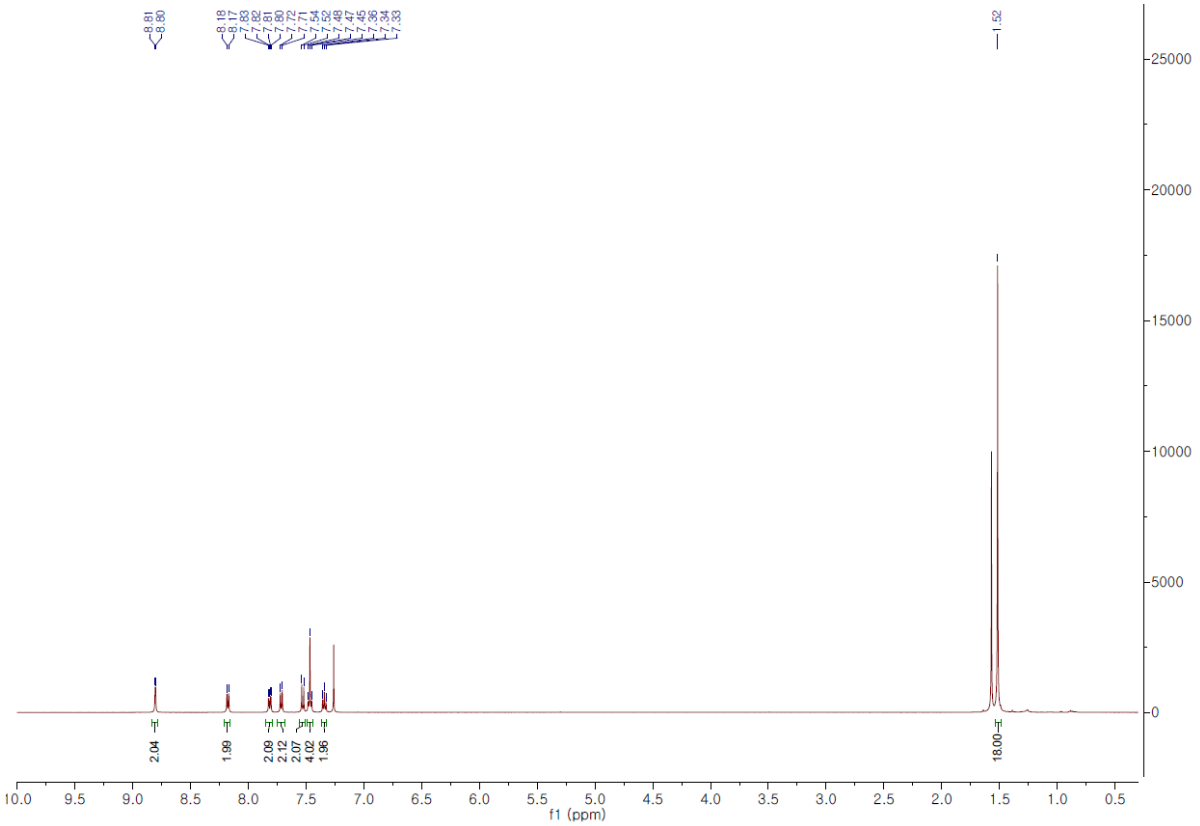


Figure S12. ^{1}H NMR spectrum of 9-(2,12-di-tert-butyl-5,9-dioxa-13b-boranaphtho[3,2,1-de]anthracen-7-yl)-9H-carbazole (**1**).

Table S4. Optical and photophysical properties of Compound **1**, **2** and **3** in toluene predicted by DL spectroscopy.

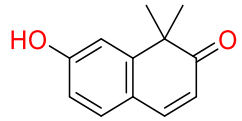
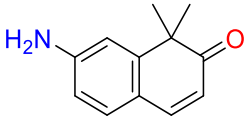
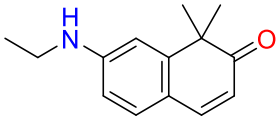
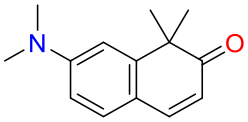
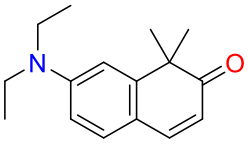
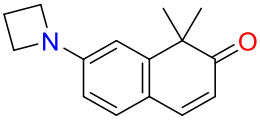
In toluene	**1**	**2**	**3**
λ_{abs} (nm)	411	478	540
σ_{abs} (cm^{-1})	1877	1869	1536
log ε	4.735	4.548	4.507
λ_{emi} (nm)	428	509	563
σ_{emi} (cm^{-1})	1563	1673	1228
Φ	0.682	0.698	0.669
τ (ns)	6.3	8.5	6.4

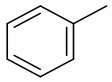
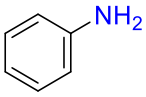
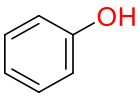
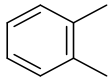
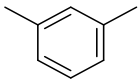
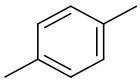
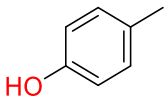
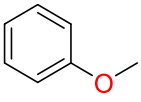
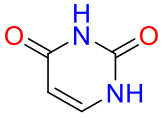
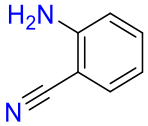
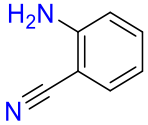
Table S5. Comparison of experimental and predicted optical and photophysical properties of **1** in toluene.

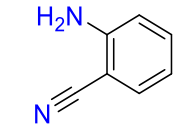
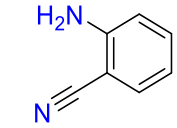
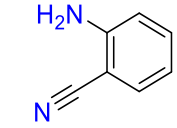
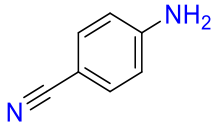
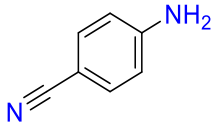
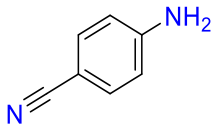
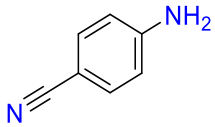
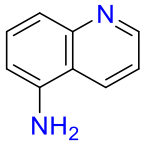
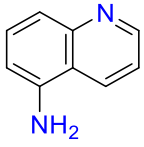
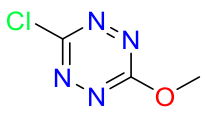
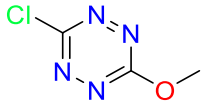
1 in toluene	Experiments	Predicted values
λ_{abs} (nm)	379	411
σ_{abs} (cm^{-1})	N.D.[a]	1877
σ_{abs} (nm)	N.D.[a]	32
log ε	4.296	4.735
λ_{emi} (nm)	393	428
σ_{emi} (cm^{-1})	1401	1563
σ_{emi} (nm)	22	29
Φ	0.543	0.682
τ (ns)	5.1	6.3

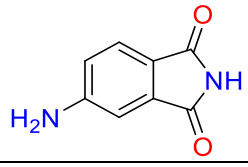
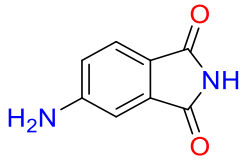
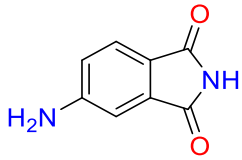
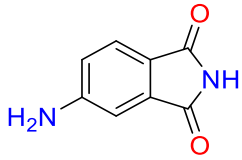
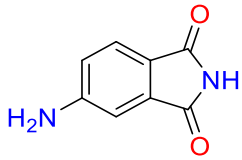
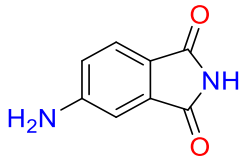
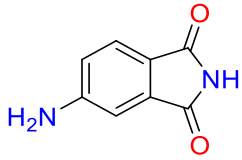
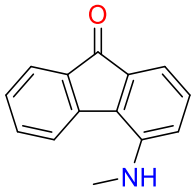
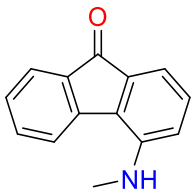
[a] Not determined. The σ_{abs} cannot be experimentally measured because the S_1 transition is overlapped with higher electronic transitions.

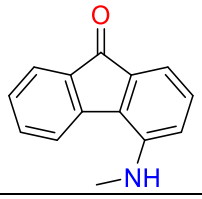
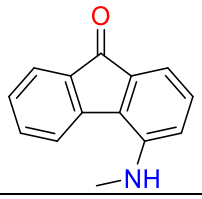
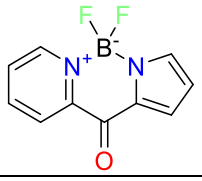
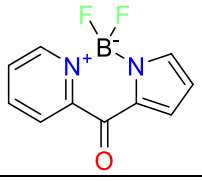
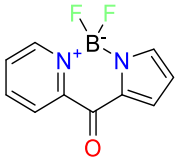
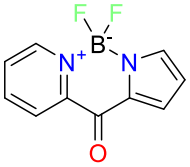
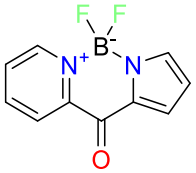
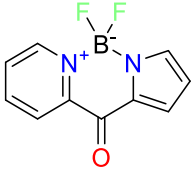
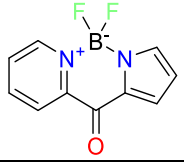
Table S6. Comparison of the optical and photophysical properties by experimentally-measured, predicted by our DL model, and obtained by TD-DFT calculations.

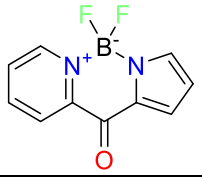
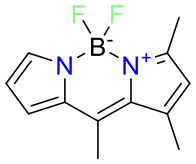
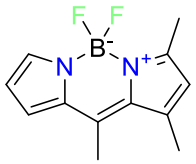
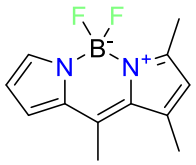
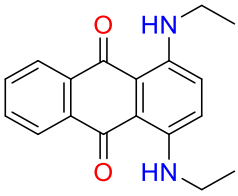
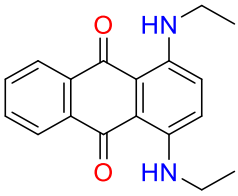
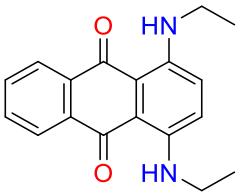
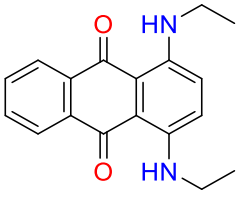
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Water	341		522	
		359	352.16	460	431.27
		5.28%	3.27%	11.88%	17.38%
	Water	377		526	
		380	369.26	500	416.35
		0.80%	2.05%	4.94%	20.85%
	Water	402		541	
		389	379.52	492	425.64
		3.23%	5.59%	9.06%	21.32%
	Water	413		554	
		416	388.42	537	434.67
		0.73%	5.95%	3.07%	21.54%
	Water	429		552	
		413	388.91	523	436.87
		3.73%	9.34%	5.25%	20.86%
	Water	387		555	
		408	386.75	537	440.71
		5.43%	0.06%	3.24%	20.59%
	Cyclohexane	253		287	
		273	223.78	313	235.33
		8.11%	11.38%	8.92%	18.11%
	Methyl-cyclohexane	252		NaN	
		258	250.19	307	307.39
		2.38%	0.72%		
	Chloroform	253		NaN	
		262	248.07	309	304.91
		3.56%	1.95%		
	Water	253		NaN	
		252	246.04	312	302.59
		0.40%	2.75%		

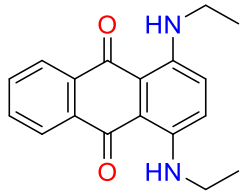
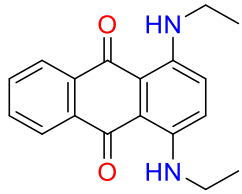
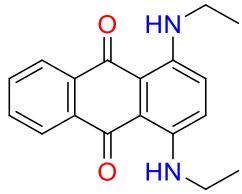
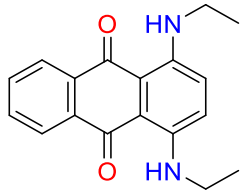
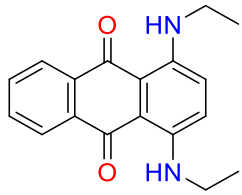
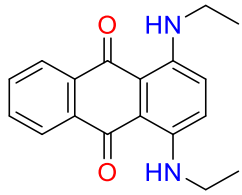
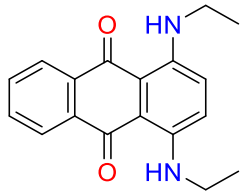
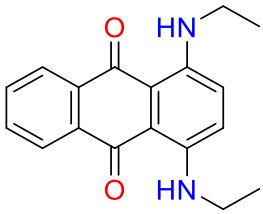
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	CH_2Cl_2	230		247	
		241	211.45	286	1653.58
		4.78%	8.07%	15.79%	569.47 %
	Cyclohexane	256		287	
		252	228.31	289	240.77
		1.75%	10.98%	0.83%	16.00%
	Cyclohexane	283		323	
		275	260.34	320	281.35
		2.87%	8.05%	1.06%	13.01%
	Cyclohexane	266		295	
		277	238.52	311	253.87
		4.15%	10.32%	5.43%	13.94%
	Cyclohexane	258		291	
		245	230.2	286	242.56
		5.14%	10.87%	1.84%	16.75%
	Cyclohexane	260		292	
		256	232.23	297	245.86
		1.44%	10.59%	1.87%	15.67%
	Cyclohexane	263		292	
		256	233.17	299	246.94
		2.62%	11.30%	2.38%	15.45%
	Water	276		307	
		270	244.54	320	265.73
		2.17%	11.40%	4.23%	13.44%
	Cyclohexane	267		296	
		259	239.85	297	255.22
		3.08%	10.25%	0.45%	13.68%
	Acetonitrile	256		311	
		239	254.2	308	334.02
		6.64%	0.70%	0.96%	7.40%
	Cyclohexane	314		348	
		325	297.64	386	329.03
		3.50%	5.21%	10.92%	5.45%
	Acetonitrile	321		368	
		332	301.71	395	340.93
		3.43%	6.01%	7.34%	7.36%

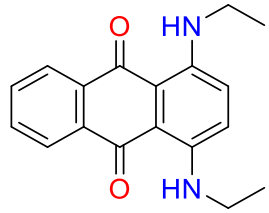
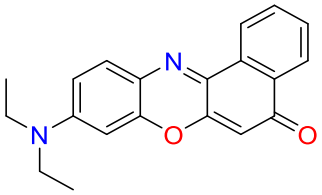
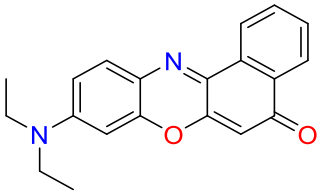
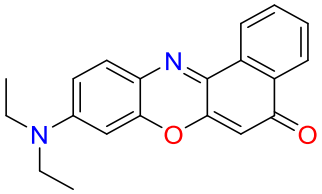
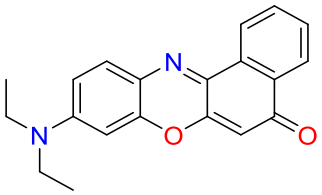
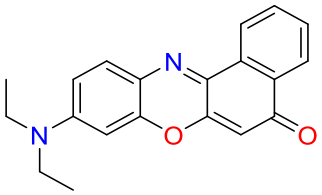
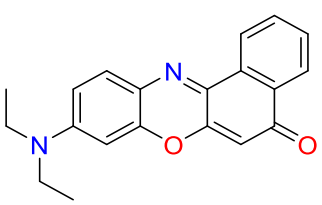
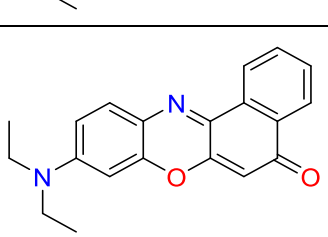
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Ethanol	325		377	
		331	301.67	396	340.49
		1.85%	7.18%	5.04%	9.68%
	Trifluoro-ethanol	314		376	
		331	301.24	414	340.59
		5.41%	4.06%	10.11%	9.42%
	Water	315		383	
		329	301.84	413	341.49
		4.44%	4.18%	7.83%	10.84%
	Cyclohexane	283		323	
		304	263.28	352	283.62
		7.42%	6.97%	8.98%	12.19%
	Ethanol	276		341	
		310	263.93	378	284.97
		12.32%	4.37%	10.85%	16.43%
	Trifluoroethanol	264		335	
		307	263.79	398	285.1
		16.29%	0.08%	18.81%	14.90%
	Water	283		344	
		304	263.94	395	286.31
		7.42%	6.73%	14.83%	16.77%
	Acetonitrile	340		480	
		330	362.51	404	442.13
		2.94%	6.62%	15.83%	7.89%
	Water	333		534	
		328	362.72	421	442.62
		1.50%	8.92%	21.16%	17.11%
	Trifluoro-ethanol	518		558	
		494	533.34	538	611.01
		4.63%	2.96%	3.58%	9.50%
	CH_2Cl_2	520		567	
		500	536.27	539	613.28
		3.85%	3.13%	4.94%	8.16%

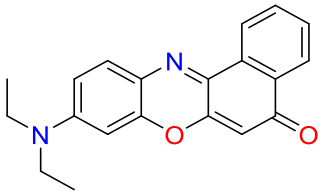
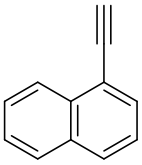
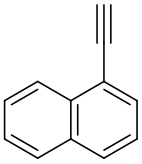
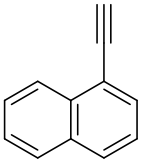
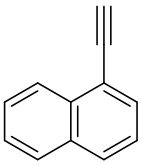
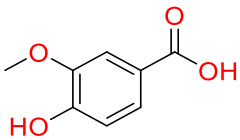
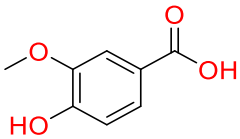
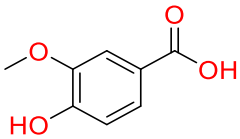
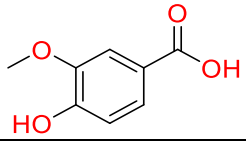
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Diethylether	350		425	
		384	362.94	466	430.54
		9.71%	3.70%	9.65%	1.30%
	1,4-dioxane	352		435	
		384	356.29	469	417.75
		9.09%	1.22%	7.82%	3.97%
	THF	357		445	
		384	367.23	474	438.01
		7.56%	2.87%	6.52%	1.57%
	Acetone	357		457	
		384	370.66	486	445.38
		7.56%	3.83%	6.35%	2.54%
	Acetonitrile	357		458	
		383	371.53	487	447.33
		7.28%	4.07%	6.33%	2.33%
	Methanol	368		518	
		383	371.28	497	447.08
		4.08%	0.89%	4.05%	13.69%
	Water	370		540	
		382	372.17	504	448.82
		3.24%	0.59%	6.67%	16.89%
	Cyclohexane	449		536	
		456	462.34	535	586.97
		1.56%	2.97%	0.19%	9.51%
	Benzene	461		570	
		465	464.72	551	590.93
		0.87%	0.81%	3.33%	3.67%

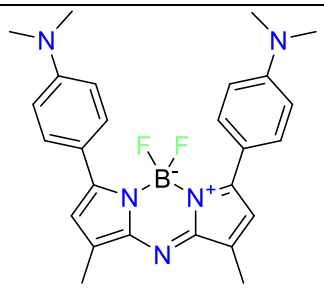
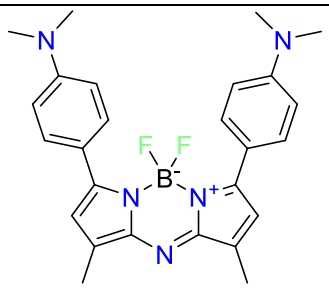
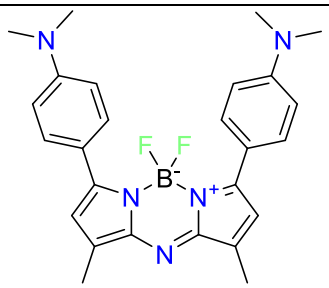
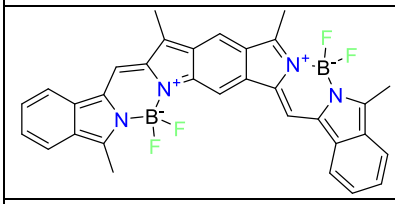
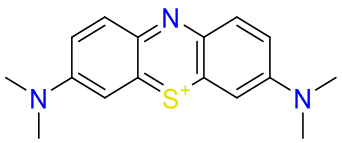
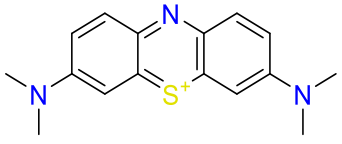
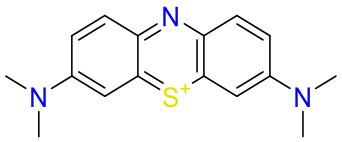
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Acetonitrile	471		638	
		468	484.58	600	635.18
		0.64%	2.88%	5.96%	0.44%
	Ethanol	477		686	
		459	483.85	601	633.26
		3.77%	1.44%	12.39%	7.69%
	Cyclohexane	395		544	
		418	424.97	501	643.86
		5.82%	7.59%	7.90%	18.36%
	Toluene	386		570	
		421	421.58	517	621.32
		9.07%	9.22%	9.30%	9.00%
	1,4-dioxane	379		581	
		416	422.68	519	626.96
		9.76%	11.53%	10.67%	7.91%
	Chloroform	389		550	
		419	409.1	522	584.79
		7.71%	5.17%	5.09%	6.33%
	Diethylether	379		563	
		418	409.78	517	588.82
		10.29%	8.12%	8.17%	4.59%
	DMF	372		577	
		410	396.3	535	553.32
		10.22%	6.53%	7.28%	4.10%
	Acetonitrile	368		578	
		410	395.61	535	553.51
		11.41%	7.50%	7.44%	4.24%

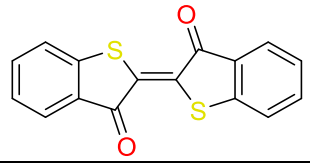
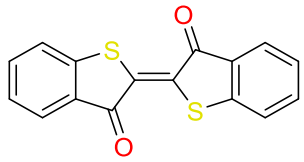
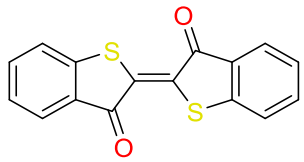
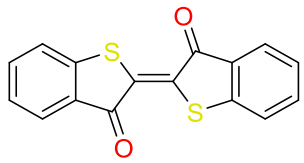
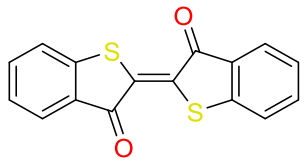
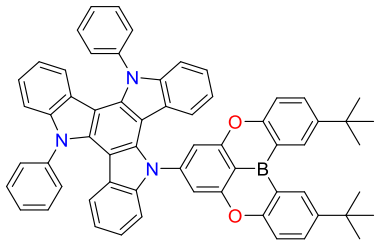
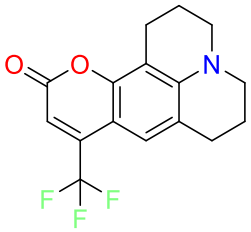
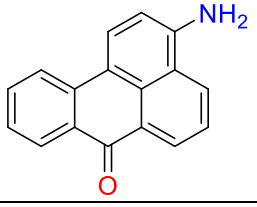
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Methanol	377		568	
		406	395.66	530	553.96
		7.69%	4.95%	6.69%	2.47%
	Hexane	492		498	
		485	409.49	495	423.69
		1.42%	16.77%	0.60%	14.92%
	CH_2Cl_2	488		500	
		483	409.59	501	445.17
		1.02%	16.07%	0.20%	10.97%
	Methanol	486		497	
		482	406.15	501	451.95
		0.82%	16.43%	0.80%	9.06%
	Cyclohexane	643		670	
		631	582.12	642	651.65
		1.87%	9.47%	4.18%	2.74%
	Benzene	646		670	
		636	584.79	652	655.28
		1.55%	9.48%	2.69%	2.20%
	1,4-dioxane	642		684	
		636	582.19	654	654.46
		0.93%	9.32%	4.39%	4.32%
	CCl_4	646		679	
		638	583.46	650	654.71
		1.24%	9.68%	4.27%	3.58%

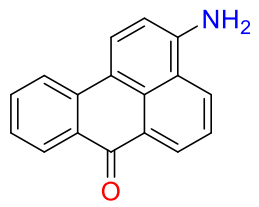
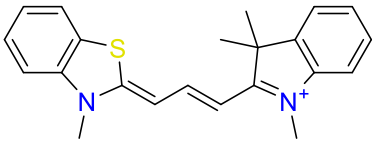
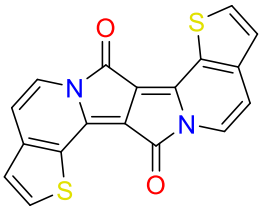
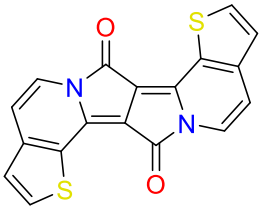
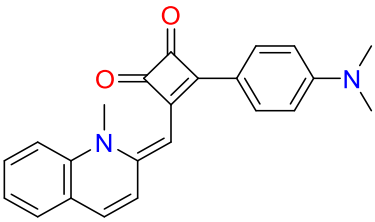
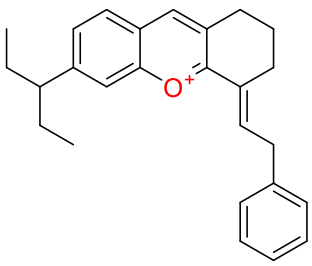
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Acetone	640		671	
		634	580.76	662	692.6
		0.94%	9.26%	1.34%	3.22%
	DMF	641		680	
		633	583.38	663	695.59
		1.25%	8.99%	2.50%	2.29%
	Dimethyl-sulfoxide	644		672	
		632	582.9	662	696.36
		1.86%	9.49%	1.49%	3.63%
	Methanol	639		669	
		629	579.58	667	695.14
		1.56%	9.30%	0.30%	3.91%
	Ethanol	641		672	
		630	580.85	665	693.79
		1.72%	9.38%	1.04%	3.24%
	n-Butanol	644		670	
		630	582.28	663	691.44
		2.17%	9.58%	1.04%	3.20%
	n-Hexanol	645		663	
		630	582.93	663	688.49
		2.33%	9.62%	0.00%	3.84%
	n-Heptanol	646		666	
		629	583.18	663	687.44
		2.63%	9.72%	0.45%	3.22%

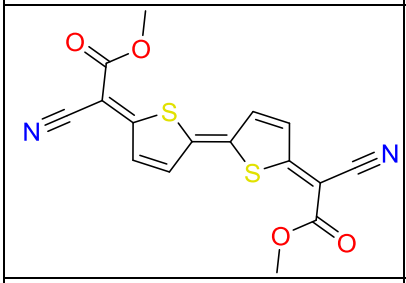
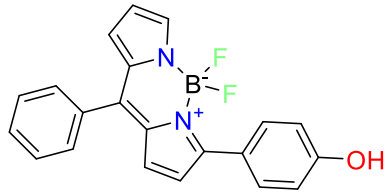
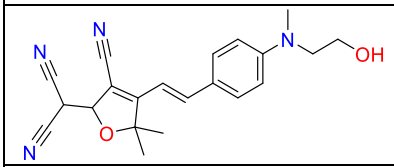
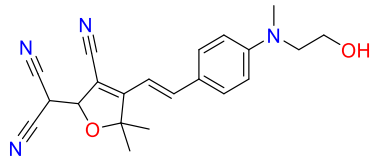
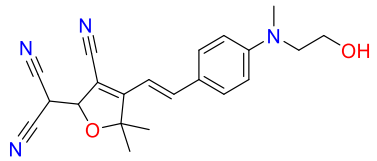
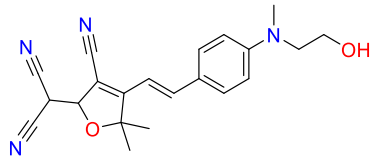
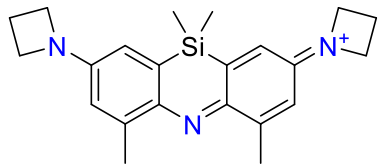
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	n-Decanol	647		672	
		628	583.56	664	682.14
		2.94%	9.81%	1.19%	1.51%
	Toluene	524		572	
		547	485.12	591	524.96
		4.39%	7.42%	3.32%	8.22%
	1,4-Dioxane	519		582	
		546	481.59	593	522.1
		5.20%	7.21%	1.89%	10.29%
	Ethyl acetate	524		594	
		546	490.43	597	554.68
		4.20%	6.41%	0.51%	6.62%
	CH_2Cl_2	539		608	
		550	494.9	607	563.22
		2.04%	8.18%	0.16%	7.37%
	Dimethyl sulfoxide	552		635	
		548	498.96	613	579.77
		0.72%	9.61%	3.46%	8.70%
	Acetonitrile	535		620	
		548	495.46	613	578.43
		2.43%	7.39%	1.13%	6.70%
	Ethanol	549		638	
		547	495.62	612	576.04
		0.36%	9.72%	4.08%	9.71%

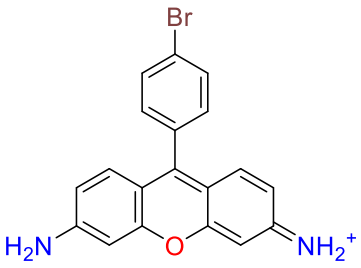
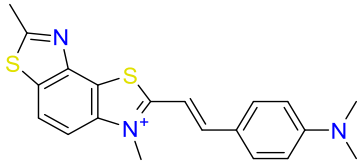
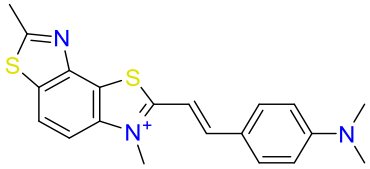
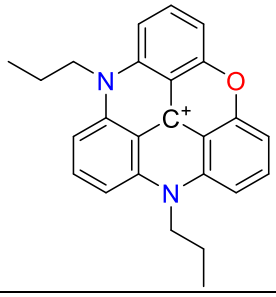
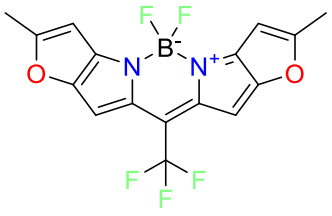
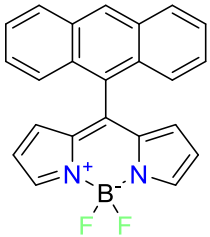
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Methanol	553		643	
		548	494.63	615	577.91
		0.90%	10.56%	4.35%	10.12%
	Cyclohexane	310		330	
		305	308.84	352	353.85
		1.61%	0.37%	6.67%	7.23%
	CH_2Cl_2	312		334	
		305	308.69	352	363.91
		2.24%	1.06%	5.39%	8.96%
	Methanol	309		332	
		305	307.91	351	367
		1.29%	0.35%	5.72%	10.54%
	Acetonitrile	306		329	
		307	308.04	353	367.11
		0.33%	0.67%	7.29%	11.58%
	Cyclohexane	287		320	
		295	263.13	345	316.94
		2.72%	8.38%	7.81%	0.96%
	1,4-Dioxane	290		330	
		296	263.1	354	317.8
		2.07%	9.28%	7.27%	3.70%
	Ethyl acetate	291		330	
		296	262.77	356	324.93
		1.89%	9.55%	7.88%	1.54%
	Acetonitrile	290		330	
		296	262.45	360	329.79
		2.07%	9.50%	9.09%	0.06%

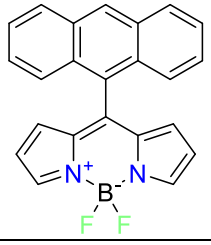
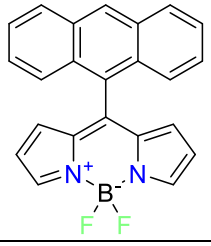
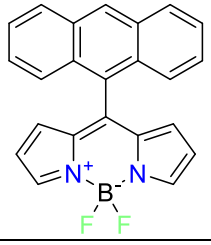
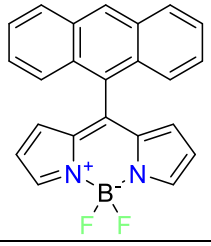
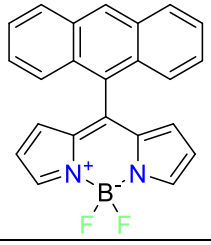
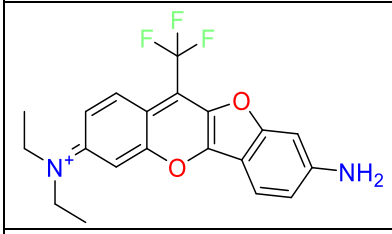
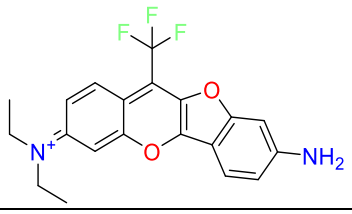
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Dimethyl sulfoxide	774		822	
		762	620	810	718.99
		1.55%	19.90%	1.46%	12.53%
	THF	744		791	
		761	616.26	798	692.72
		2.28%	17.17%	0.88%	12.42%
	Toluene	734		779	
		755	612.34	788	646.22
		2.86%	16.57%	1.16%	17.04%
	Chloroform	848		868	
		755	876.52	746	1128.01
		10.97%	3.36%	14.06%	29.96%
	Water	664		683	
		672	524.2	698	604.04
		1.20%	21.05%	2.20%	11.56%
	Acetonitrile	655		672	
		670	524.63	688	601.17
		2.29%	19.90%	2.38%	10.54%
	Ethanol	655		680	
		671	525.43	690	598.94
		2.44%	19.78%	1.47%	11.92%

Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Dimethyl sulfoxide	545		614	
		509	529.57	591	623.06
		6.61%	2.83%	3.75%	1.48%
	1,4-Dioxane	536		590	
		513	525.74	575	588.47
		4.29%	1.91%	2.54%	0.26%
	DMF	543		607	
		511	529.79	591	622.44
		5.89%	2.43%	2.64%	2.54%
	Benzene	544		598	
		512	527.44	572	589.18
		5.88%	3.04%	4.35%	1.47%
	Methanol	538		624	
		508	527.44	596	622.02
		5.58%	1.96%	4.49%	0.32%
	Toluene	NaN		456	
		396	444.63	456	527.23
				0.00%	15.62%
	Ethanol	421		531	
		412	400.82	513	476.48
		2.14%	4.79%	3.39%	10.27%
	i-Propanol	517		665	
		479	481.86	623	559.26
		7.36%	6.81%	6.30%	15.89%

Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Methanol	514		667	
		475	481.99	631	561.15
		7.61%	6.25%	5.41%	15.88%
	Dimethyl sulfoxide	549		569	
		565	474.21	602	563.02
		2.91%	13.62%	5.80%	1.05%
	Chloroform	605		609	
		574	567.73	605	656.44
		5.12%	6.16%	0.66%	7.79%
	DMF	605		618	
		574	563.19	609	678.12
		5.12%	6.91%	1.46%	9.73%
	Dichloromethane	509		588	
		418	497.56	501	2186.27
		17.88%	2.25%	14.80%	271.81 %
	Ethanol	604		647	
		619	582.43	680	711.78
		2.48%	3.57%	5.10%	10.01%

Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Toluene	550		601	
		526	556.61	599	624.27
		4.36%	1.20%	0.33%	3.87%
	Chloroform	541		564	
		531	489.37	559	559.69
		1.85%	9.54%	0.89%	0.76%
	Toluene	562		614	
		594	432.12	640	456.45
		5.69%	23.11%	4.23%	25.66%
	Ethyl Acetate	565		628	
		594	433	647	479.55
		5.13%	23.36%	3.03%	23.64%
	Methanol	575		644	
		587	434.61	649	498.31
		2.09%	24.42%	0.78%	22.62%
	Water	587		648	
		586	435.21	653	501.01
		0.17%	25.86%	0.77%	22.68%
	Ethanol	732		745	
		715	573.26	738	670.07
		2.32%	21.69%	0.94%	10.06%

Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Ethanol	514		532	
		481	430.86	538	482.93
		6.42%	16.18%	1.13%	9.22%
	Methanol	534		600	
		533	484.35	587	563.12
		0.19%	9.30%	2.17%	6.15%
	Chloroform	557		603	
		552	492.69	592	541.43
		0.90%	11.55%	1.82%	10.21%
	Acetonitrile	557		590	
		538	479.06	587	531.25
		3.41%	13.99%	0.51%	9.96%
	Chloroform	613		620	
		663	513.25	667	570.02
		8.16%	16.27%	7.58%	8.06%
	DMF	506		524	
		498	639.46	532	776.7
		1.58%	26.38%	1.53%	48.23%

Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Dichloro-methane	506		520	
		502	632.2	527	764.19
		0.79%	24.94%	1.35%	46.96%
	Acetonitrile	502		519	
		497	639.35	533	776.52
		1.00%	27.36%	2.70%	49.62%
	Ethanol	503		520	
		495	638.28	526	774.63
		1.59%	26.89%	1.15%	48.97%
	Toluene	508		525	
		498	611.92	525	733.38
		1.97%	20.46%	0.00%	39.69%
	Hexane	505		521	
		486	606.52	513	725.12
		3.76%	20.10%	1.54%	39.18%
	Dichloro-methane	658		695	
		640	551.58	673	638.79
		2.74%	16.17%	3.17%	8.09%
	Ethanol	640		706	
		632	548.67	672	646.2
		1.25%	14.27%	4.82%	8.47%

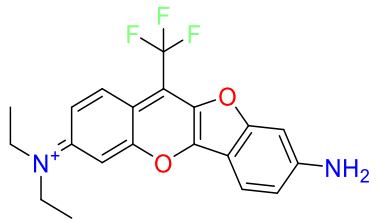
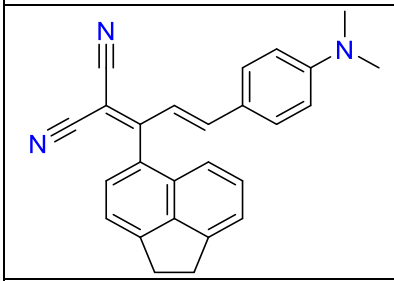
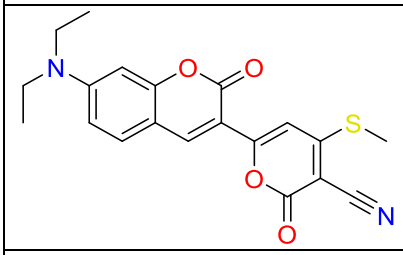
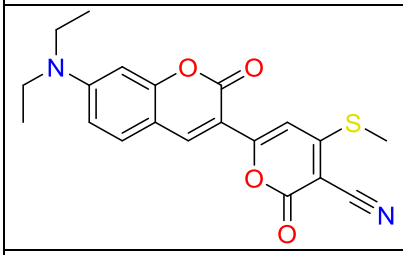
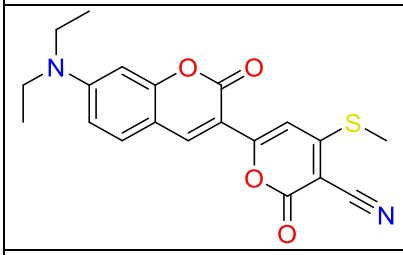
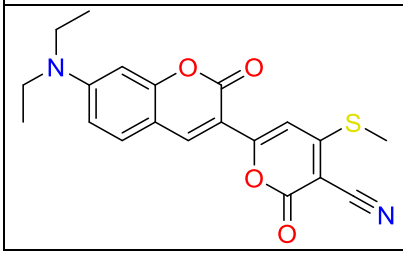
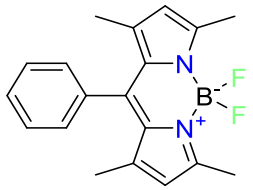
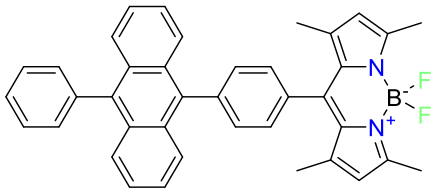
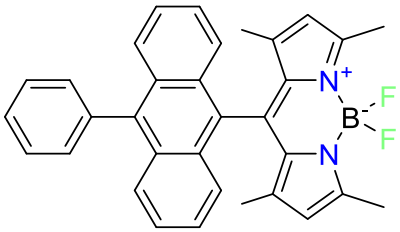
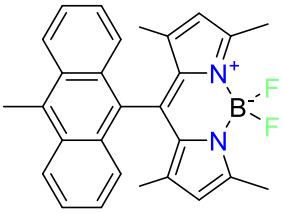
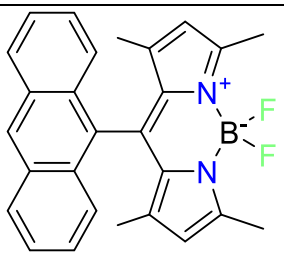
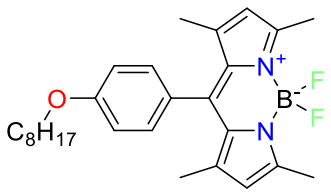
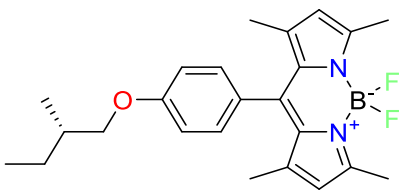
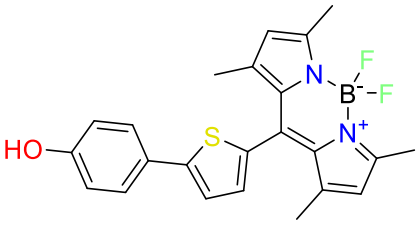
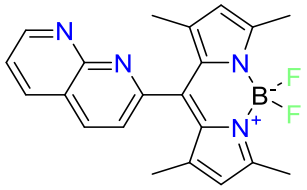
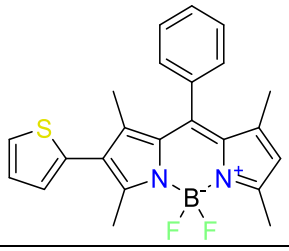
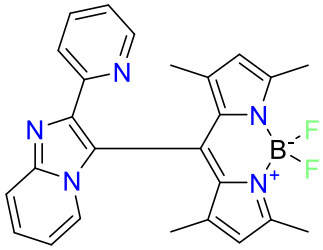
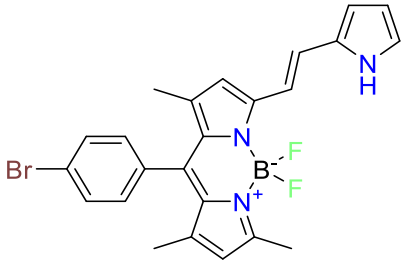
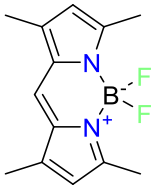
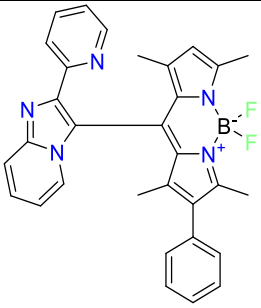
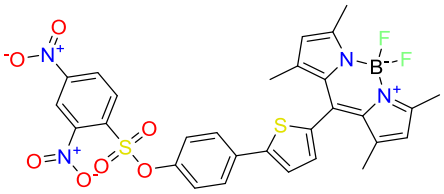
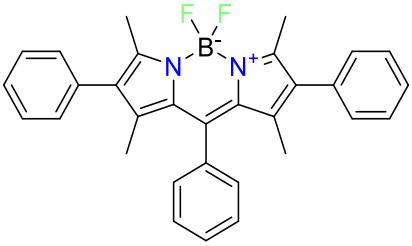
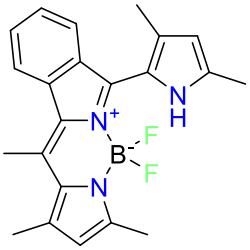
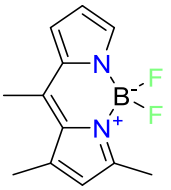
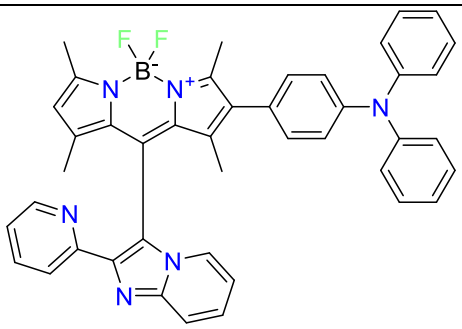
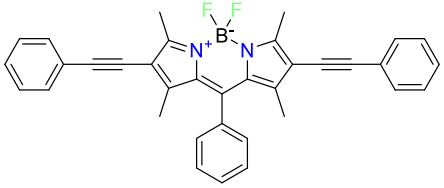
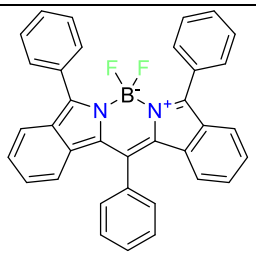
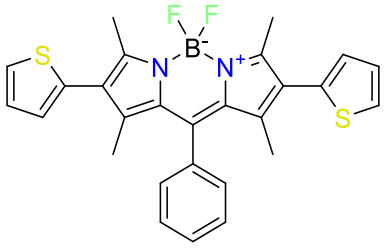
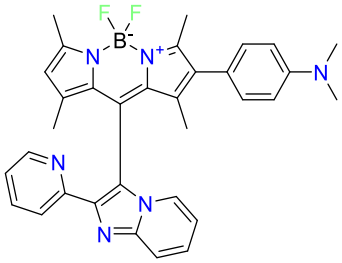
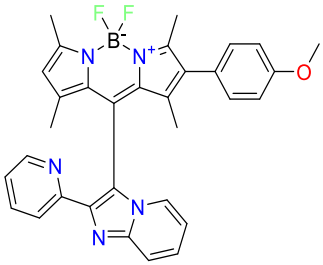
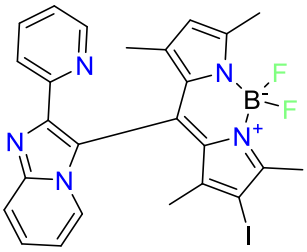
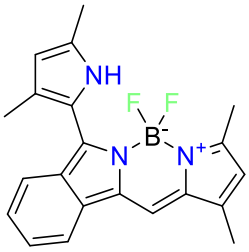
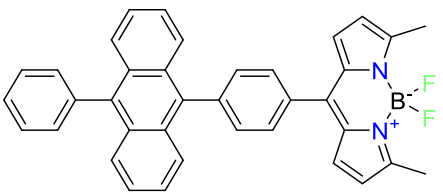
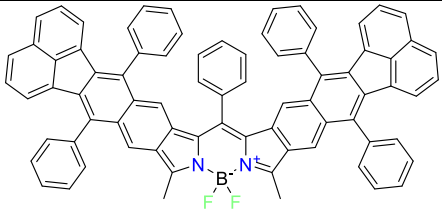
Molecule	Solvent	Exp. λ_{abs} (nm)		Exp. λ_{emi} (nm)	
		DL	DFT	DL	DFT
		Error	Error	Error	Error
	Water	640		707	
		630	547.31	684	649.65
		1.56%	14.48%	3.25%	8.11%
	DMF	505		606	
		493	514.94	591	595.15
		2.38%	1.97%	2.48%	1.79%
	Toluene	509		533	
		525	460.14	565	488.13
		3.14%	9.60%	6.00%	8.42%
	Chloroform	517		547	
		527	466.11	571	505.03
		1.93%	9.84%	4.39%	7.67%
	Methanol	514		582	
		533	470.16	594	529.25
		3.70%	8.53%	2.06%	9.06%
	Acetonitrile	514		578	
		530	470.94	586	529.69
		3.11%	8.38%	1.38%	8.36%

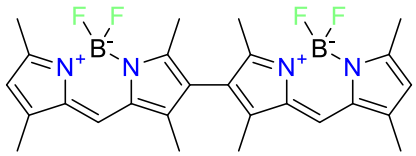
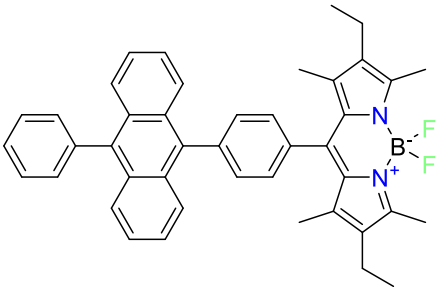
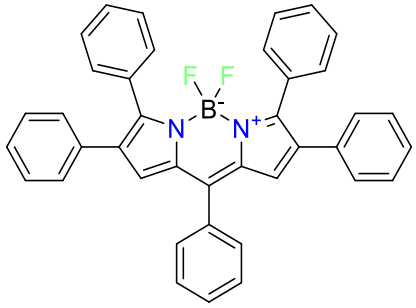
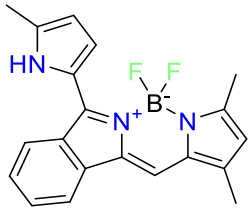
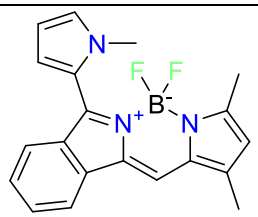
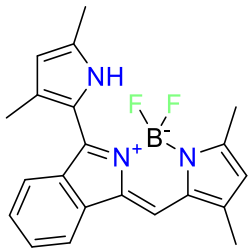
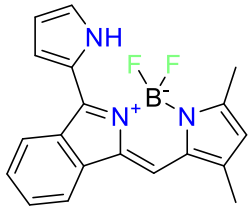
Table S7. Comparison of the optical properties of 97 molecules in dichloromethane that are experimentally measured and predicted by our DL model. λ_{abs} and λ_{emi} are in nm, τ in ns, σ_{abs} and σ_{emi} are in cm^{-1}.

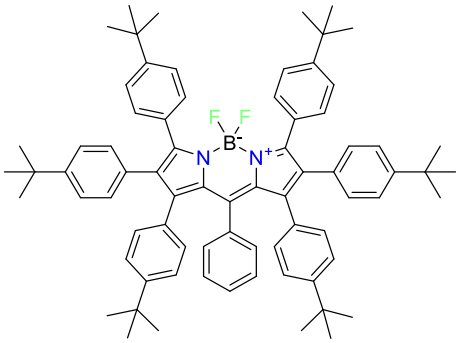
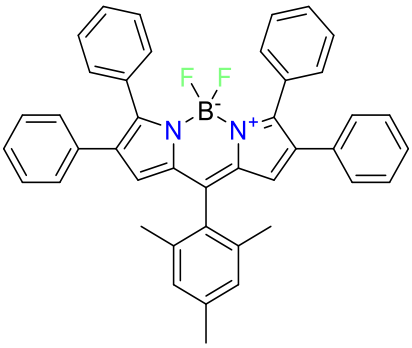
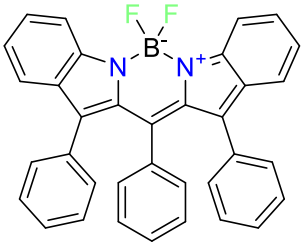
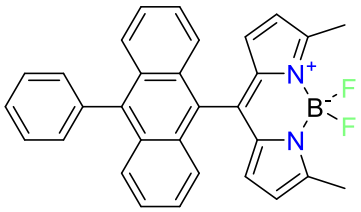
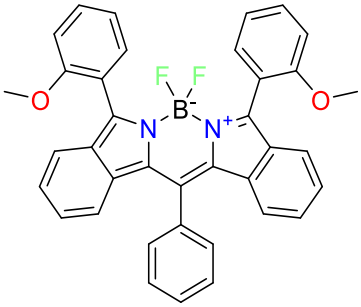
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	501	513	3.970	0.630			
	Pred.	512	517	3.689	0.591	4.89	675	1186
	Error	11	4	-0.281	-0.039			
	Exp.	502	512		0.570			
	Pred.	494	506	2.454	0.308	4.77	782	1175
	Error	-8	-6		-0.262			
	Exp.	507	515		0.024			
	Pred.	497	511	1.557	0.110	4.75	827	1092
	Error	-10	-4		0.086			
	Exp.	506	519		0.011			
	Pred.	499	505	0.644	0.030	4.78	599	1078
	Error	-7	-14		0.019			
	Exp.	506	517		0.072			
	Pred.	518	531	1.991	0.097	4.82	898	1156
	Error	12	14		0.025			
	Exp.	500	513		0.760		810	836
	Pred.	501	507	3.295	0.531	4.87	712	1236
	Error	1	-6		-0.229		-98	401
	Exp.	501	520		0.870		918	969
	Pred.	508	513	3.427	0.517	4.89	666	1146
	Error	7	-7		-0.353		-252	176

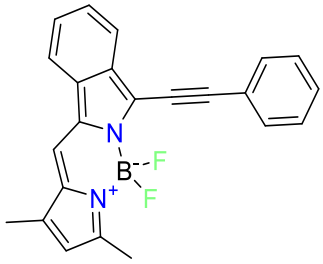
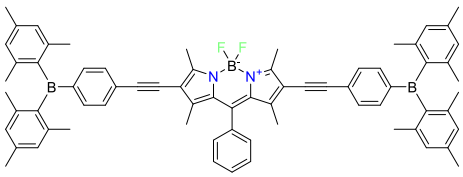
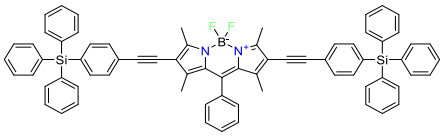
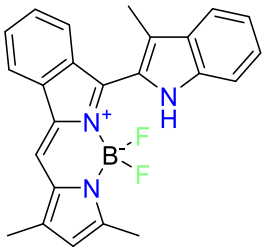
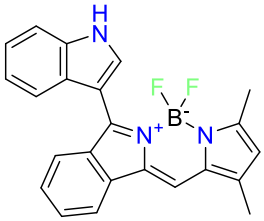
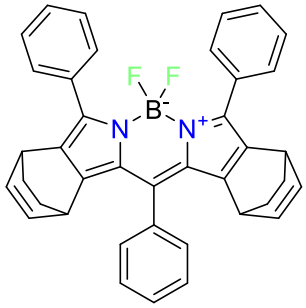
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	514	525			4.95		
	Pred.	532	546	3.691	0.185	4.85	750	1056
	Error	18	21			-0.10		
	Exp.	506	522		0.060	4.78	815	1543
	Pred.	521	537	3.471	0.461	4.89	960	1184
	Error	15	15		0.401	0.11	145	-359
	Exp.	511	594			4.82		
	Pred.	526	555	3.089	0.314	4.73	1478	1454
	Error	15	-39			-0.09		
	Exp.	518	536	6.900	0.635	4.90	787	1141
	Pred.	554	572	4.815	0.576	4.86	968	1078
	Error	36	36	-2.085	-0.059	-0.04	181	-63
	Exp.	590	613		0.250			
	Pred.	584	602	3.521	0.422	4.85	991	923
	Error	-6	-11		0.172			
	Exp.	506	513	5.730	0.920			
	Pred.	497	524	5.890	0.835	4.85	1826	1730
	Error	-9	11	0.160	-0.085			
	Exp.	532	566	6.200	0.739	5.10	1119	1238
	Pred.	550	581	2.998	0.425	4.81	1696	1476
	Error	18	15	-3.202	-0.314	-0.29	577	238

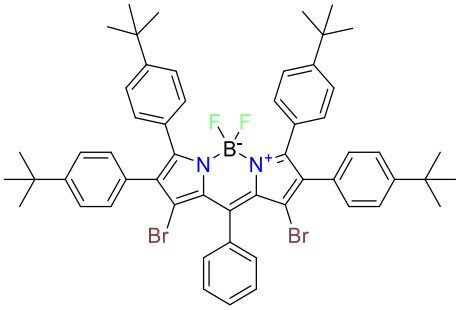
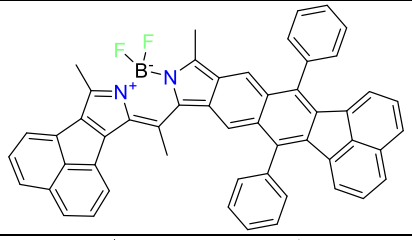
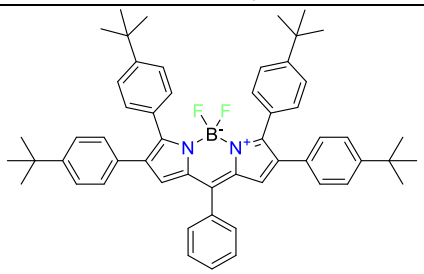
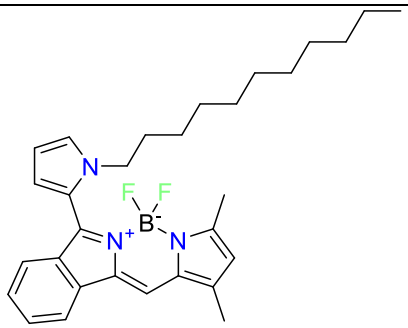
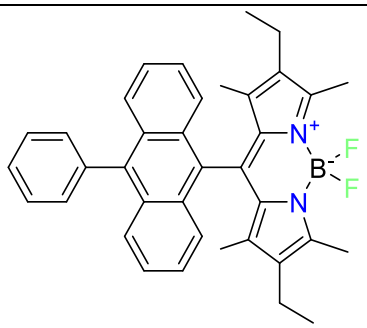
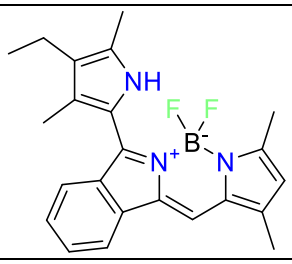
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	515	528			4.90		
	Pred.	514	530	1.605	0.056	4.90	845	1059
	Error	-1	2			0.00		
	Exp.	528	555			4.60		
	Pred.	527	548	3.481	0.496	4.74	1493	1515
	Error	-1	-7			0.14		
	Exp.	599	625	7.300	0.800	4.96	1957	1053
	Pred.	601	628	4.257	0.424	4.96	1184	1021
	Error	2	3	-3.043	-0.376	0.00	-773	-33
	Exp.	488	500	5.930	0.950			
	Pred.	483	501	6.469	0.863	4.65	1620	1638
	Error	-5	1	0.539	-0.087			
	Exp.	537	698	0.200	0.004	4.60	1868	2868
	Pred.	574	640	0.385	0.036	4.51	2102	2450
	Error	37	-58	0.185	0.032	-0.09	235	-418
	Exp.	561	594		0.820			
	Pred.	599	624	2.381	0.433	4.91	1504	1120
	Error	38	30		-0.387			
	Exp.	631	664	5.200	0.930	5.01	979	851
	Pred.	609	631	3.027	0.396	4.87	1282	995
	Error	-22	-33	-2.173	-0.534	-0.14	303	144

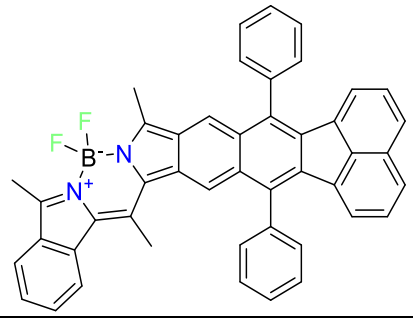
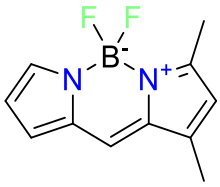
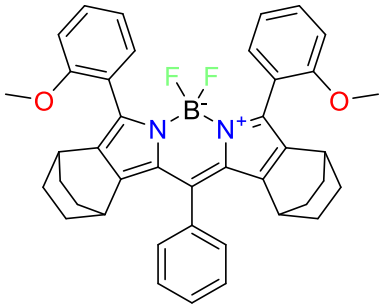
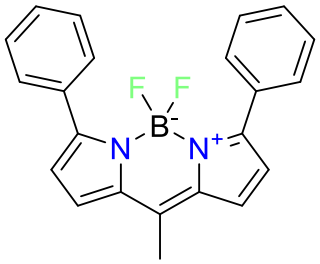
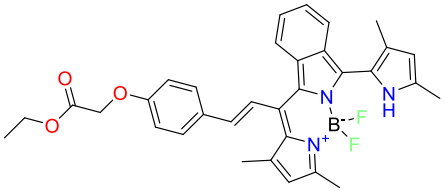
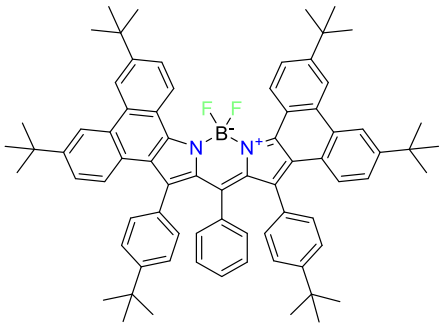
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	527	609			4.20	2116	2078
	Pred.	540	565	4.873	0.558	4.66	1618	1406
	Error	13	-44			0.46	-498	-671
	Exp.	538	524	0.500	0.004	4.70	2391	1040
	Pred.	586	635	0.709	0.067	4.73	1907	2007
	Error	48	111	0.209	0.063	0.03	-484	967
	Exp.	535	592	2.200	0.212	5.20	1407	1973
	Pred.	563	589	2.780	0.359	4.79	1469	1333
	Error	28	-3	0.580	0.147	-0.41	61	-641
	Exp.	534	558	0.300	0.025	4.70		
	Pred.	545	572	1.355	0.197	4.78	1542	1509
	Error	11	14	1.055	0.172	0.08		
	Exp.	609	631		0.610			
	Pred.	637	651	4.548	0.581	4.94	868	592
	Error	28	20		-0.029			
	Exp.	513	526		0.027			
	Pred.	492	502	1.263	0.060	4.69	761	1226
	Error	-21	-24		0.033			
	Exp.	765	783		0.320	5.30		
	Pred.	668	695	2.189	0.236	4.94	1340	884
	Error	-97	-88		-0.084	-0.36		

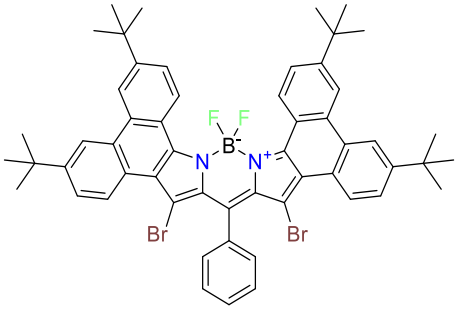
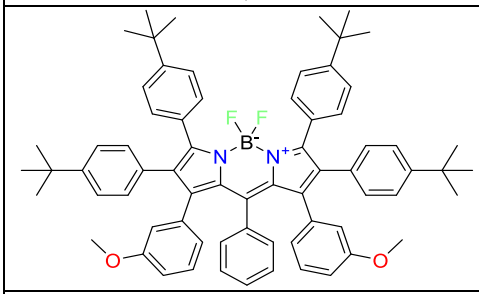
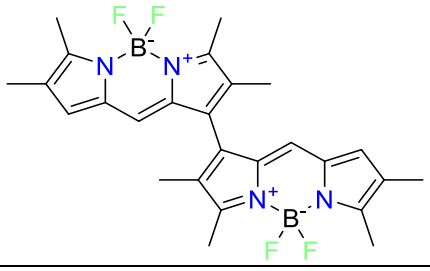
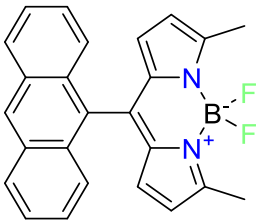
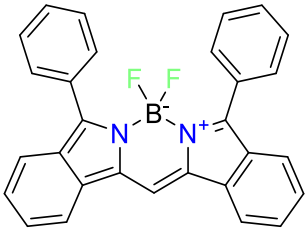
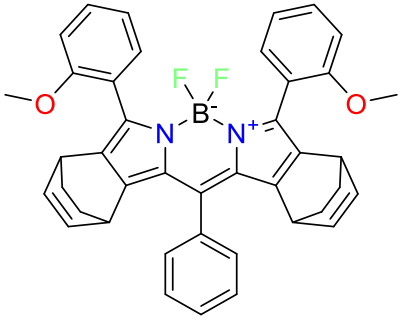
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	526	563		0.660	5.18		
	Pred.	560	596	3.055	0.444	5.02	1709	1392
	Error	34	33		-0.216	-0.16		
	Exp.	527	540		0.744			
	Pred.	530	544	5.067	0.599	4.70	1001	1280
	Error	3	4		-0.145			
	Exp.	584	628		0.400	4.77		
	Pred.	602	632	2.457	0.388	4.83	1690	1321
	Error	18	4		-0.012	0.06		
	Exp.	608	629	6.650	0.890	4.79	874	918
	Pred.	611	630	5.718	0.538	4.89	955	908
	Error	3	1	-0.932	-0.352	0.10	80	-10
	Exp.	585	611	6.910	0.990	4.83	1374	1061
	Pred.	586	606	5.498	0.574	4.92	1069	1003
	Error	1	-5	-1.412	-0.416	0.09	-304	-58
	Exp.	609	631	6.400	0.610	4.87	820	939
	Pred.	606	630	5.243	0.504	4.93	1114	957
	Error	-3	-1	-1.157	-0.106	0.06	294	19
	Exp.	602	621	7.280	0.870	4.93	842	1009
	Pred.	611	626	6.338	0.641	4.98	814	744
	Error	9	5	-0.942	-0.229	0.05	-29	-265

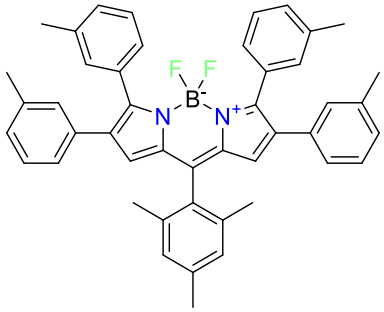
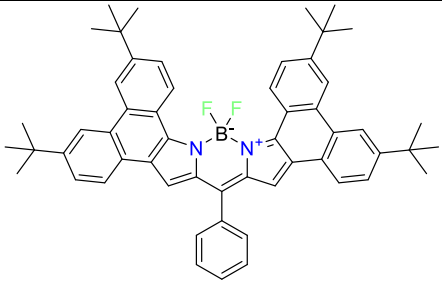
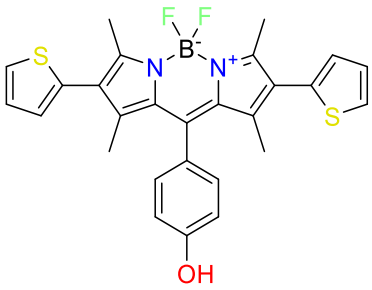
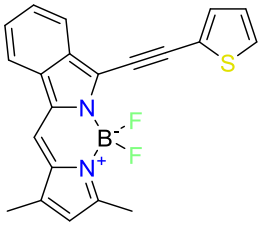
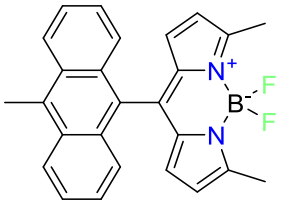
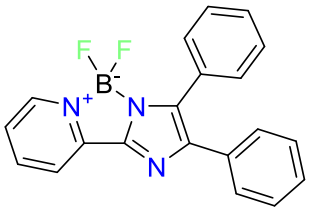
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	579	636		0.450	4.77	1767	1368
	Pred.	584	622	2.532	0.364	4.86	1845	1454
	Error	5	-14		-0.086	0.09	78	86
	Exp.	585	626		0.740	4.80	1457	1309
	Pred.	609	637	2.502	0.411	4.87	1523	1170
	Error	24	11		-0.329	0.07	66	-139
	Exp.	568			0.000	4.56		
	Pred.	605	601	1.924	0.001	4.78	1329	773
	Error	37			0.001	0.22		
	Exp.	518	533		0.007		738	1583
	Pred.	494	511	0.741	0.026	4.68	922	1283
	Error	-24	-22		0.019		184	-300
	Exp.	617	652	5.800	0.910	5.01	881	924
	Pred.	644	656	3.225	0.496	5.02	950	534
	Error	27	4	-2.575	-0.414	0.01	69	-390

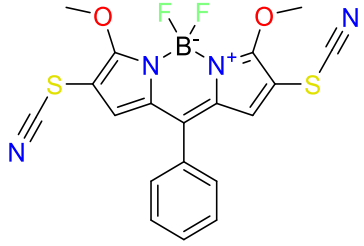
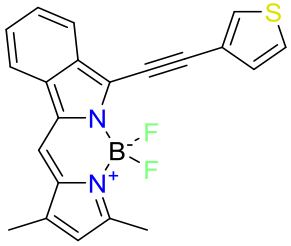
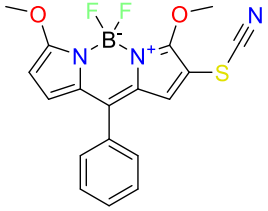
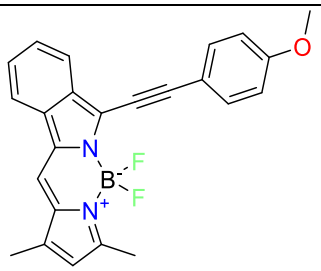
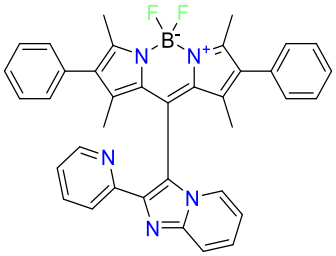
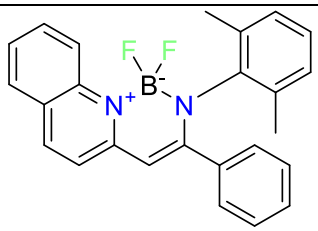
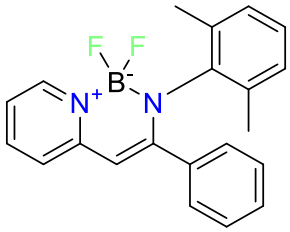
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	612	629		0.890	4.69		
	Pred.	617	627	5.148	0.658	4.75	1193	595
	Error	5	-2		-0.232	0.06		
	Exp.	576	602		0.650	5.23		
	Pred.	592	611	3.136	0.484	5.01	1118	1005
	Error	16	9		-0.166	-0.22		
	Exp.	575	600		0.150	4.83		
	Pred.	587	617	2.295	0.414	4.87	1693	1308
	Error	12	17		0.264	0.04		
	Exp.	608	631	3.270	0.850	4.90	1032	975
	Pred.	602	631	3.589	0.282	5.02	1235	1088
	Error	-6	0	0.319	-0.568	0.12	203	113
	Exp.	581	606	6.420	0.980	4.89	1017	1086
	Pred.	610	626	6.036	0.594	4.99	859	825
	Error	29	20	-0.384	-0.386	0.10	-158	-261
	Exp.	558	588	6.100	0.870	4.85	1291	1054
	Pred.	587	602	3.188	0.556	4.92	1241	1047
	Error	29	14	-2.912	-0.314	0.07	-50	-8

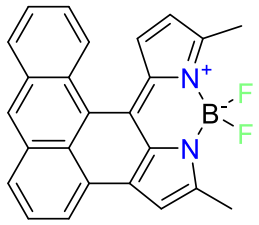
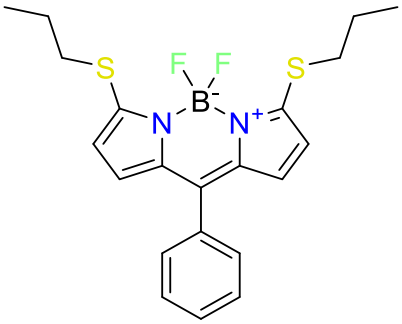
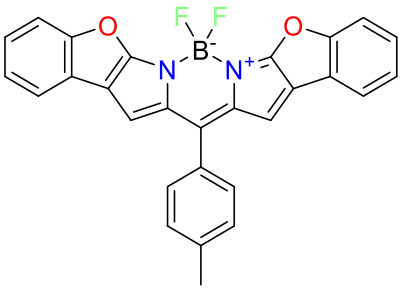
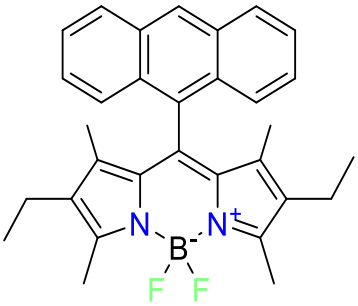
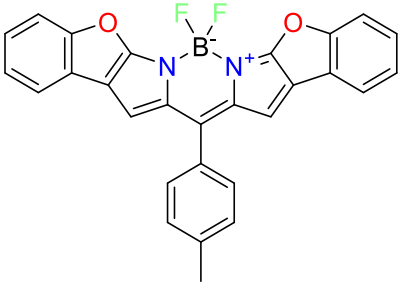
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	572	619		0.090	4.90	1788	1357
	Pred.	597	634	2.135	0.202	4.82	1752	1394
	Error	25	15		0.112	-0.08	-36	38
	Exp.	658	695		0.700	4.90		
	Pred.	593	618	3.461	0.343	4.61	1369	1130
	Error	-65	-77		-0.357	-0.29		
	Exp.	598	649		0.300	4.77	1699	1449
	Pred.	615	656	2.675	0.356	4.92	1772	1305
	Error	17	7		0.056	0.15	73	-144
	Exp.	584	611	8.890	0.990	4.72	1597	1089
	Pred.	566	593	5.612	0.559	4.74	1421	1240
	Error	-18	-18	-3.278	-0.431	0.02	-176	151
	Exp.	532	543		0.833			
	Pred.	529	544	5.411	0.628	4.74	1121	1280
	Error	-3	1		-0.205			
	Exp.	616	640	4.930	0.860	4.95	856	704
	Pred.	615	638	3.909	0.427	5.09	984	890
	Error	-1	-2	-1.021	-0.433	0.14	128	186

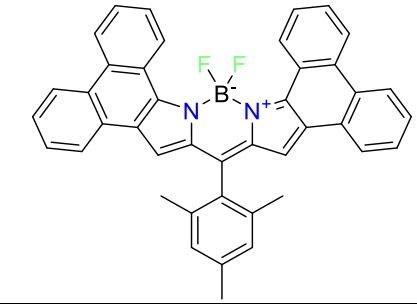
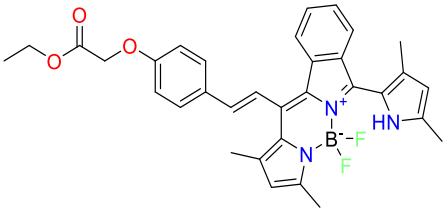
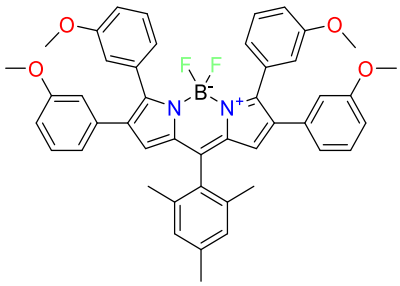
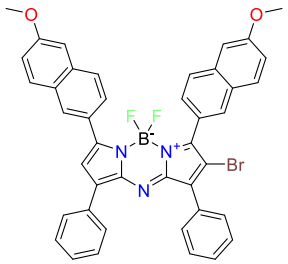
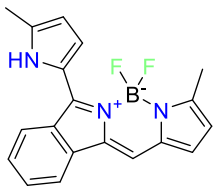
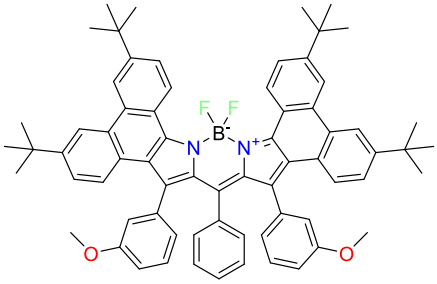
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	681	697		0.360	4.96		
	Pred.	648	685	3.359	0.283	4.86	1519	1021
	Error	-33	-12		-0.077	-0.10		
	Exp.	498	507	5.890	0.870			
	Pred.	481	509	7.148	0.884	4.56	2206	1724
	Error	-17	2	1.258	0.014			
	Exp.	550	583	4.500	0.770	4.81	1380	1174
	Pred.	603	621	3.557	0.579	4.90	1248	975
	Error	53	38	-0.943	-0.191	0.09	-132	-199
	Exp.	544	577		0.640	4.76		
	Pred.	561	582	3.758	0.536	4.84	1341	1150
	Error	17	5		-0.104	0.08		
	Exp.	608	687		0.010			
	Pred.	632	656	3.682	0.277	4.85	949	723
	Error	24	-31		0.267			
	Exp.	683	712		0.450	4.83	682	939
	Pred.	679	715	1.859	0.262	5.05	1330	1023
	Error	-4	3		-0.188	0.22	648	84

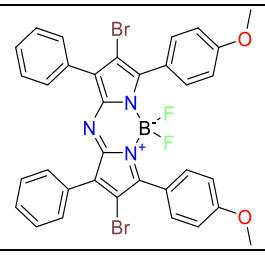
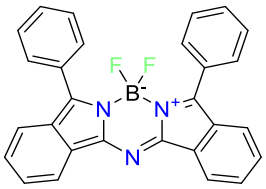
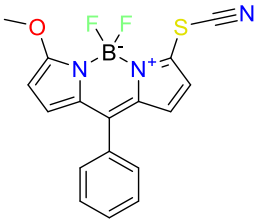
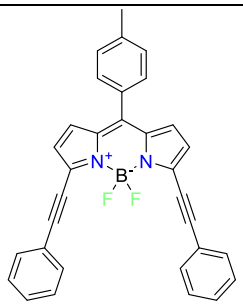
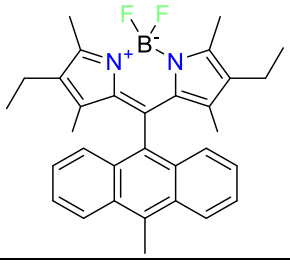
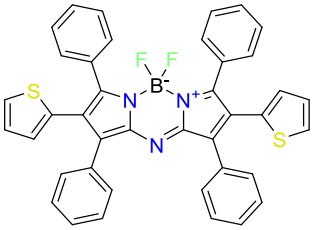
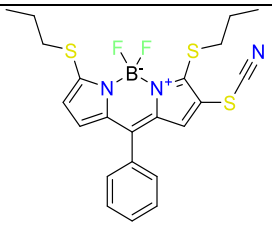
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	689	717		0.030	5.08	656	844
	Pred.	705	739	1.047	0.099	5.05	1148	950
	Error	16	22		0.069	-0.03	492	106
	Exp.	583	640		0.580	4.77	1763	1353
	Pred.	592	621	3.392	0.499	4.84	1522	1216
	Error	9	-19		-0.082	0.07	-241	-137
	Exp.	557	598		0.050	4.90		
	Pred.	530	566	1.591	0.311	4.94	2043	1812
	Error	-27	-32		0.261	0.04		
	Exp.	518	528		0.001	4.74	733	3772
	Pred.	504	517	0.586	0.015	4.80	1005	1472
	Error	-14	-11		0.014	0.06	272	-2300
	Exp.	634	658		0.880	5.04		
	Pred.	654	674	2.626	0.380	5.03	979	709
	Error	20	16		-0.500	-0.01		
	Exp.	556	587	5.100	0.870	4.79	1363	1158
	Pred.	609	626	3.261	0.535	4.90	1173	927
	Error	53	39	-1.839	-0.335	0.11	-190	-231

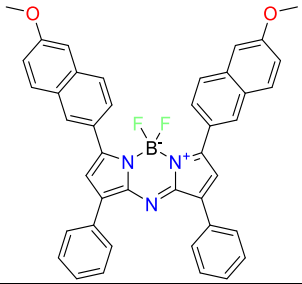
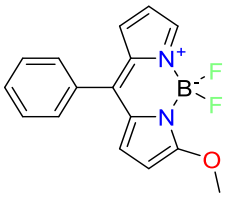
Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	573	627		0.300	4.93	2040	1529
	Pred.	561	591	3.533	0.515	4.85	1640	1327
	Error	-12	-36		0.215	-0.08	-400	-202
	Exp.	691	716		0.620	5.19	705	763
	Pred.	700	730	1.768	0.244	5.11	1014	817
	Error	9	14		-0.376	-0.08	309	53
	Exp.	528	605			4.79		
	Pred.	547	575	4.394	0.516	4.67	1628	1408
	Error	19	-30			-0.12		
	Exp.	618	631		0.440	4.15		
	Pred.	634	652	5.180	0.564	4.69	1372	605
	Error	16	21		0.124	0.54		
	Exp.	517	536		0.002		797	1629
	Pred.	490	500	0.345	0.008	4.71	820	1372
	Error	-27	-36		0.006		23	-257
	Exp.	408	528		0.150	4.15	3859	3297
	Pred.	398	524	4.607	0.297	4.28	4316	3559
	Error	-10	-4		0.147	0.13	457	262

Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	518	555		0.170		1103	1327
	Pred.	530	555	2.407	0.309	4.68	1453	1261
	Error	12	0		0.139		350	-66
	Exp.	612	628		0.800	4.97		
	Pred.	622	636	5.445	0.638	4.73	1281	542
	Error	10	8		-0.162	-0.24		
	Exp.	515	543		0.190		1464	1415
	Pred.	522	555	1.853	0.296	4.60	1789	1488
	Error	7	12		0.106		325	73
	Exp.	616	633		0.630	4.53		
	Pred.	627	643	4.840	0.577	4.72	1232	609
	Error	11	10		-0.053	0.19		
	Exp.	548	585	3.400	0.785	4.80	1303	1331
	Pred.	562	596	2.654	0.358	4.77	1866	1509
	Error	14	11	-0.746	-0.427	-0.03	563	177
	Exp.	447	468		0.620	4.49	2877	2404
	Pred.	479	519	2.317	0.524	4.69	2423	2175
	Error	32	51		-0.096	0.20	-454	-229
	Exp.	397	453		0.360	4.29	3425	3097
	Pred.	402	470	1.579	0.321	4.50	3766	3331
	Error	5	17		-0.039	0.21	341	234

Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	583	638		0.450	4.36	2373	1107
	Pred.	568	608	3.516	0.196	4.46	1777	1356
	Error	-15	-30		-0.254	0.10	-596	249
	Exp.	579	593		0.430		743	822
	Pred.	572	581	2.976	0.460	4.82	942	828
	Error	-7	-12		0.030		199	6
	Exp.	583	597		0.630			
	Pred.	597	609	3.499	0.659	5.21	924	698
	Error	14	12		0.029			
	Exp.	531	543		0.799			
	Pred.	532	544	4.995	0.625	4.83	1089	1247
	Error	1	1		-0.174			
	Exp.	583	597		0.630			
	Pred.	597	609	3.499	0.659	5.21	924	698
	Error	14	12		0.029			

Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	673	692		0.510	5.15		
	Pred.	673	691	2.923	0.391	5.07	702	583
	Error	0	-1		-0.119	-0.08		
	Exp.	608	687	3.070	0.014	3.92	1362	888
	Pred.	621	657	2.786	0.020	4.82	1252	1164
	Error	13	-30	-0.284	0.006	0.90	-110	276
	Exp.	588	632		0.830	4.87	1539	1333
	Pred.	572	609	3.542	0.496	4.83	1801	1472
	Error	-16	-23		-0.334	-0.04	262	138
	Exp.	695	728		0.120	4.91	1432	
	Pred.	665	704	2.358	0.226	4.88	1662	1060
	Error	-30	-24		0.106	-0.03	230	
	Exp.	600	624	8.110	0.790	4.46	1112	965
	Pred.	596	617	6.205	0.579	4.80	1082	1065
	Error	-4	-7	-1.905	-0.211	0.34	-30	100
	Exp.	677	737		0.540	4.96	1059	1011
	Pred.	664	703	1.871	0.234	4.96	1546	1185
	Error	-13	-34		-0.306	0.00	487	174

Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	679	714		0.100	4.88	1239	
	Pred.	672	710	0.800	0.091	4.85	1536	1166
	Error	-7	-4		-0.009	-0.03	298	
	Exp.	712	736		0.140	4.98		
	Pred.	715	742	2.277	0.296	5.03	938	628
	Error	3	6		0.156	0.05		
	Exp.	508	531		0.070		3021	1085
	Pred.	520	555	1.423	0.190	4.52	1720	1403
	Error	12	24		0.120		-1301	318
	Exp.	614	628		1.000			
	Pred.	629	639	3.710	0.532	4.83	939	661
	Error	15	11		-0.468			
	Exp.	531	543		0.667			
	Pred.	525	542	4.578	0.576	4.78	1208	1352
	Error	-6	-1		-0.091			
	Exp.	650			0.000	4.60		
	Pred.	667	711	0.161	0.002	4.73	2021	1669
	Error	17			0.002	0.13		
	Exp.	545	586		0.130		2616	1341
	Pred.	554	586	2.126	0.243	4.72	1645	1215
	Error	9	0		0.113		-971	-126

Molecular structure		λ_{abs}	λ_{emi}	τ	Φ	log ε	σ_{abs}	σ_{emi}
	Exp.	706	733		0.330	4.95	1347	
	Pred.	706	735	2.359	0.308	4.99	1045	668
	Error	0	2		-0.023	0.04	-302	
	Exp.	499	518		0.020		1173	1140
	Pred.	524	549	0.490	0.062	4.75	1190	1152
	Error	25	31		0.042		17	12

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