Supporting Information

Beyond Woodward-Fieser Rules: Design Principles of Property-Oriented Chromophores Based on Explainable Deep Learning Optical Spectroscopy

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Methods

Extended experimental database and improved prediction accuracy of DLOS

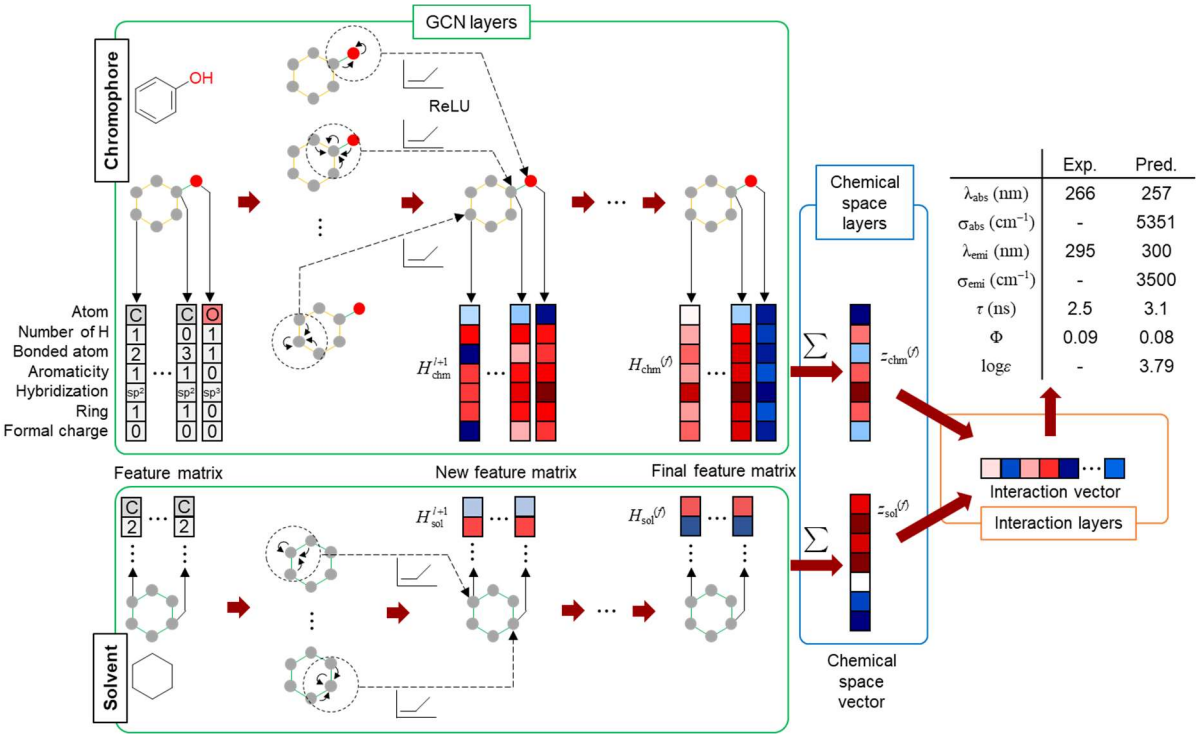


Figure S1. Schematic illustration of deep learning optical spectroscopy (DLOS). Reproduced with permission from Ref. 1. Copyright 2021 American Chemical Society.

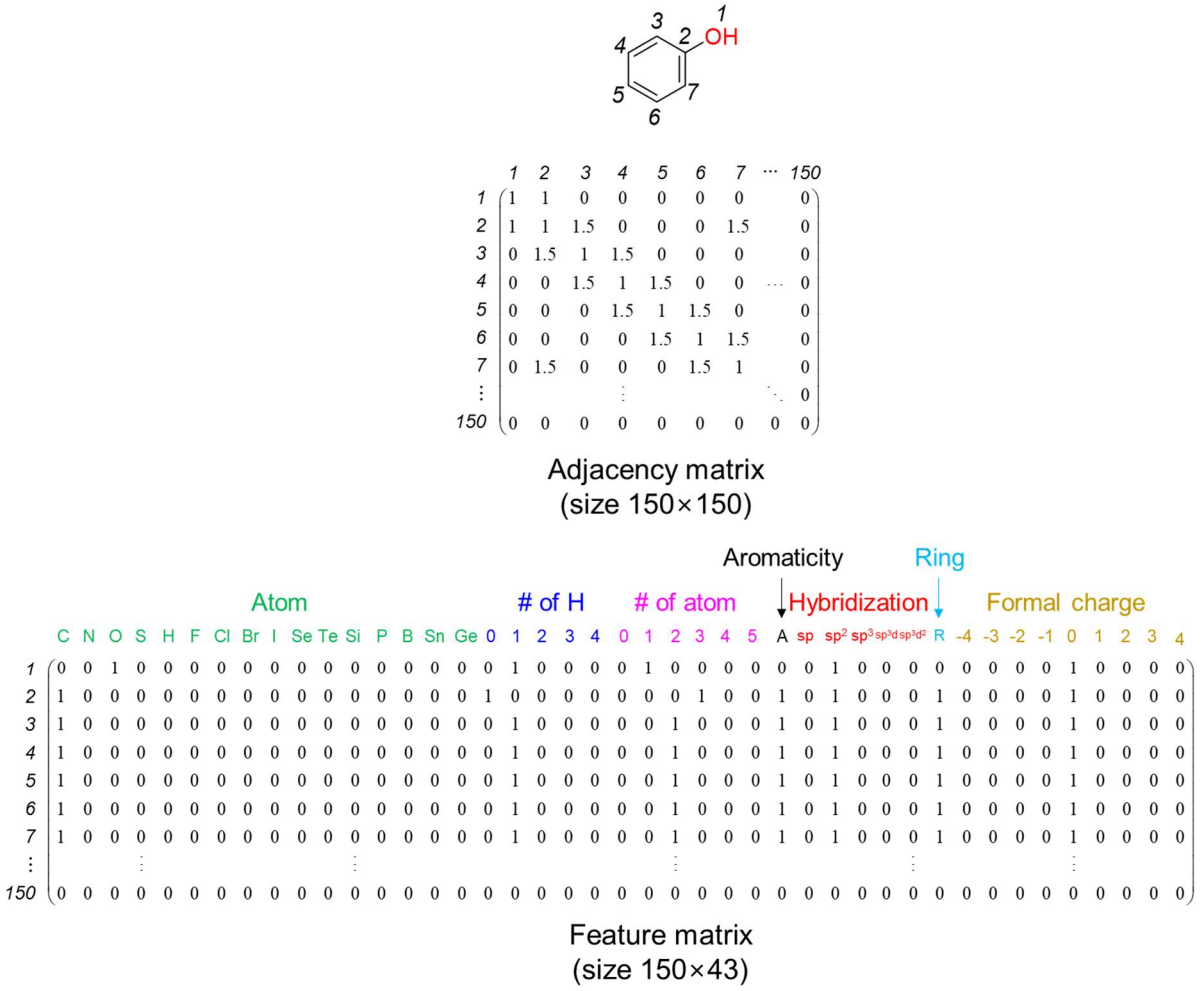


Figure S2. Schematic illustration of the adjacency and feature matrices for phenol. Reproduced with permission from Ref. 1. Copyright 2021 American Chemical Society.

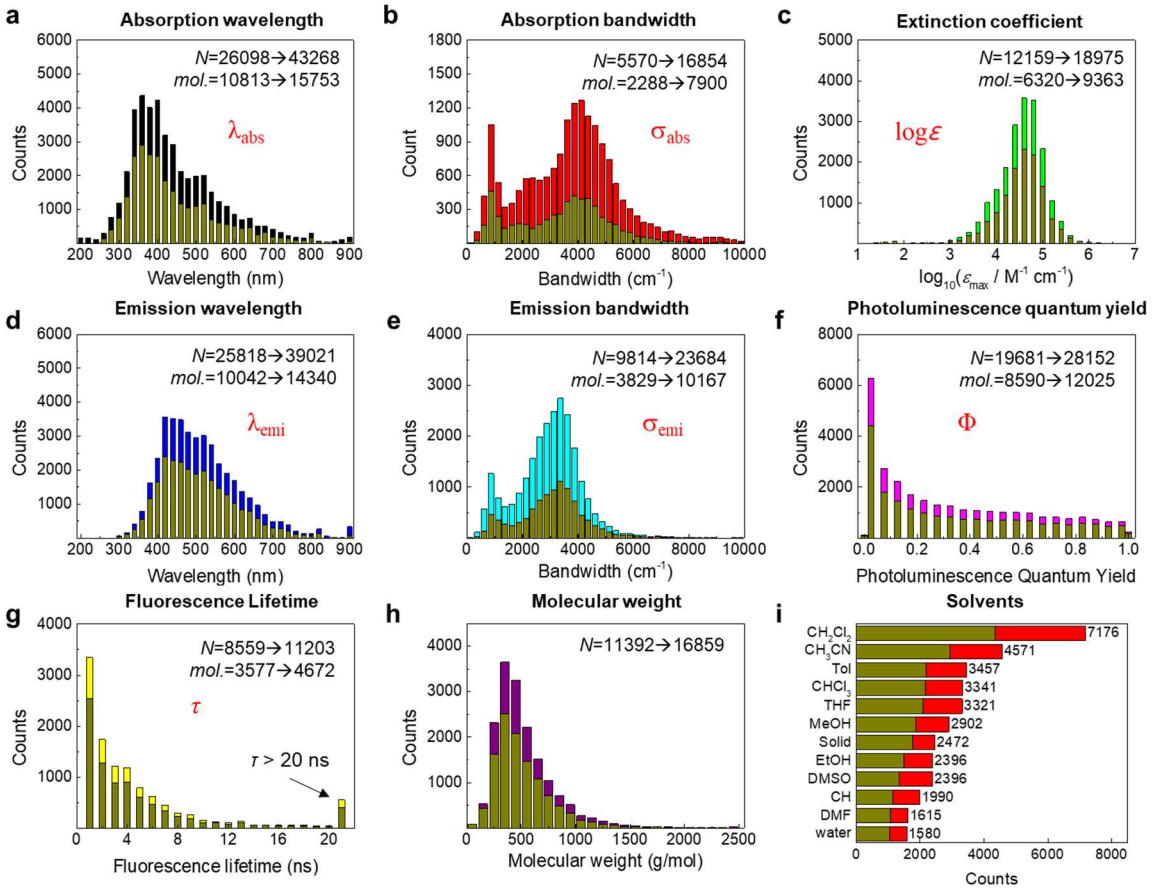


Figure S3. Database of the optical properties of organic compounds. Histograms of (a) first absorption peak position (λ_{abs}), (b) bandwidth in full width at half maximum (σ_{abs}), (c) extinction coefficient in logarithm (log ε), (d) emission peak position (λ_{emi}), (e) bandwidth in full width at half maximum (σ_{emi}), (f) photoluminescence quantum yield (Φ), (g) lifetime (τ), (h) the molecular weights of chromophores, and (i) solvents (CH_2Cl_2: dichloromethane, CH_3CN: acetonitrile, Tol: toluene, $CHCl_3$: chloroform, THF: tetrahydrofuran, MeOH: methanol, EtOH: ethanol, DMSO: dimethyl sulfoxide, CH: cyclohexane, and DMF: *N*,*N*-dimethylformamide). The histograms in gold represent the database used in Ref. 2,3. The number of data points (*N*= size of Ref. 1→ In this study) and the number of unique chromophores (*mol.* = size of Ref. 1 → In this study) are included in each graph.

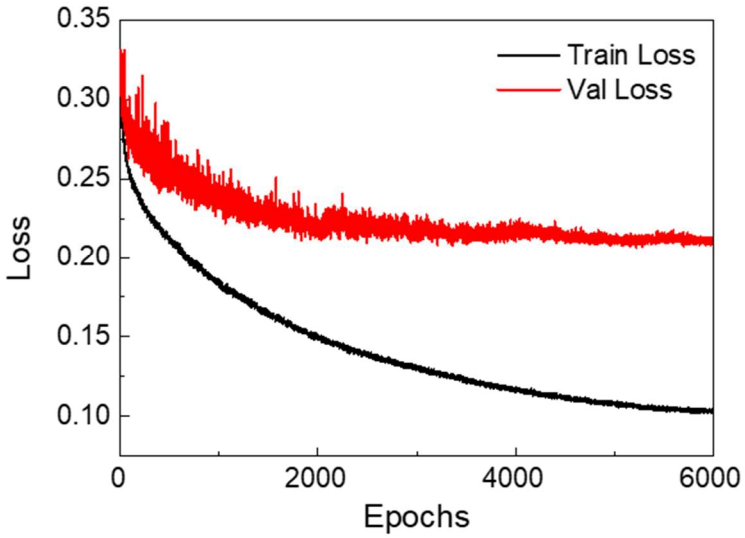


Figure S4. The losses for training and validation of DLOS as a function of epoch.

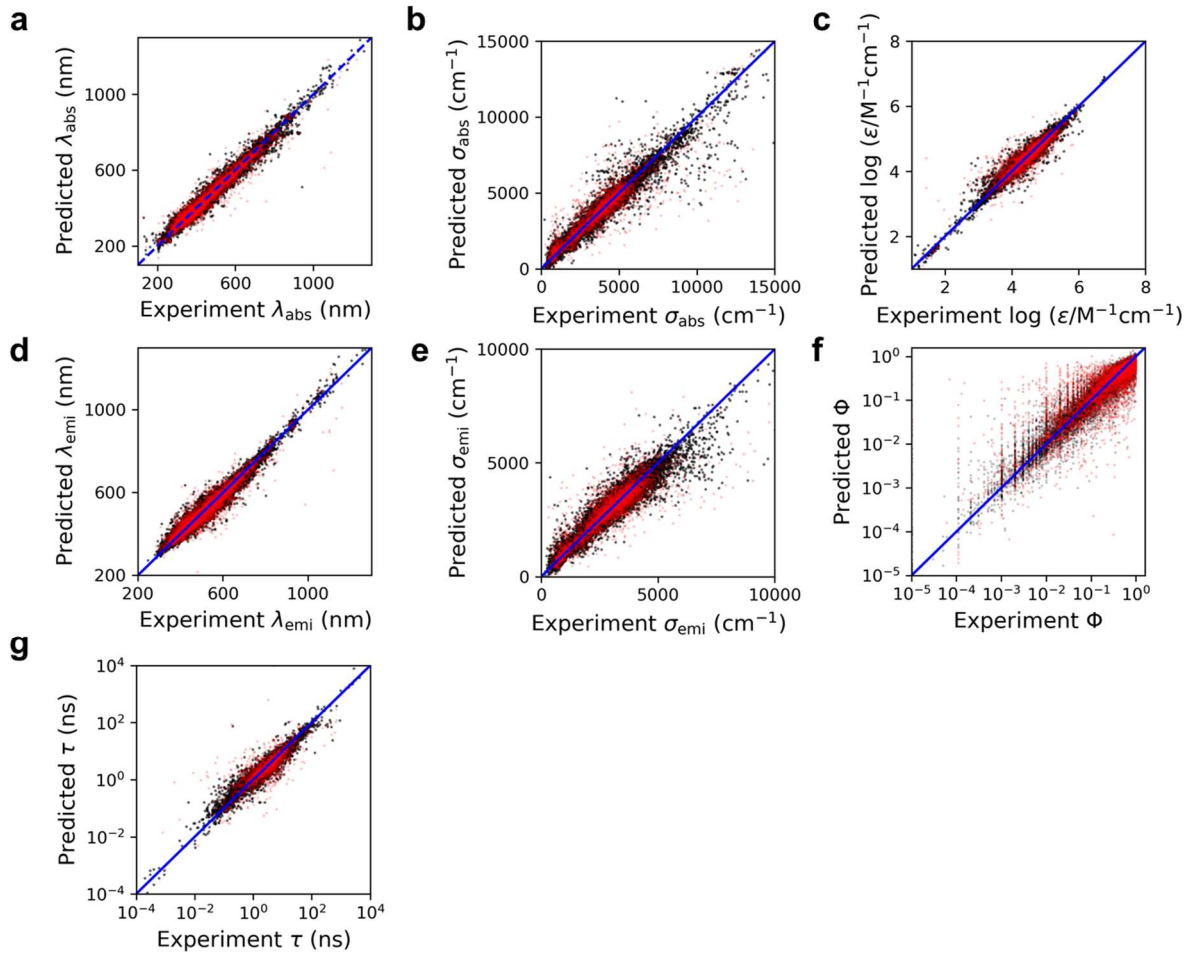


Figure S5. a-g. Results of our DL model for the first absorption peak position (λ_{abs}), and absorption bandwidth in FWHM (σ_{abs}), extinction coefficient (ε), emission peak position (λ_{emi}), emission bandwidth in FWHM (σ_{emi}), photoluminescence quantum yield (Φ), and lifetime (τ). Training and test datasets are in black and red dots, respectively.

Table S1. The RMSEs of predicted properties by the DLOS model.

RMSEs	λ_{abs} (nm)	σ_{abs} (cm^{-1})	log ε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	log Φ	log τ
Previous study[1]	19.8	656	0.151	21.3	422	0.288	0.218
This study	17.9	547	0.123	18.7	365	0.233	0.177
R^2	0.974	0.897	0.921	0.961	0.875	0.864	0.873

[1] The RMSEs of DLOS model used in Reference 1. The DLOS model in the previous study was trained with 30,094 chromophore/solvent combinations, while the DLOS model in this study was trained with 49,500 chromophore/solvent combinations.

The explainable DLOS model

In our DLOS model, shown in Figure S1, the atoms in a molecule are described by seven features, namely atom identity, the number of bonded hydrogen atoms, the number of bonded heavy atoms, aromaticity, hybridization, ring, and formal charge, as shown in Figure S2. In addition, the adjacency matrix contains the connectivity and bond order. All the elements in the adjacency and feature matrices have the attribution to each property. For example, the attributions to the λ_{abs} of benzaldehyde in cyclohexane are calculated for each feature, as shown in Figure S6. By summing all the attributions from the elements in the feature matrix into each atom, the total attribution of the features for the atom in benzaldehyde is established to range from −7.1 to +6.0 nm. In addition, the attributions of the adjacency matrix are calculated for the diagonal element (atom itself) and the off-diagonal component (bond), as shown in Figure S7. Since it is difficult to understand the attributions of the adjacency and feature matrices when the molecule is large, the attribution of the atom is calculated by summing the attributions of the adjacency and feature matrices, and $A_i = \sum_j B_{ij} / 2$, where A_i is the attribution of atom i, and B_{ij} is the attribution of the bond between atoms i and j. The attributions of an atom of benzaldehyde in cyclohexane to λ_{abs} are calculated to range from −20.6 to +24.8 nm. Similarly, the attributions of the atoms in cyclohexane to λ_{abs} are calculated as −3.47 nm. The completeness can be evaluated by summing all the attributions and the value of the references: −34.0 nm − 3.3 nm × 6 + 385 nm = 330.2 nm. The predicted λ_{abs} of benzaldehyde in cyclohexane is 330.0 nm. The error between the predicted value and the summation of the attributions originates from the Riemann approximation of the integral. We established that the errors are negligible.

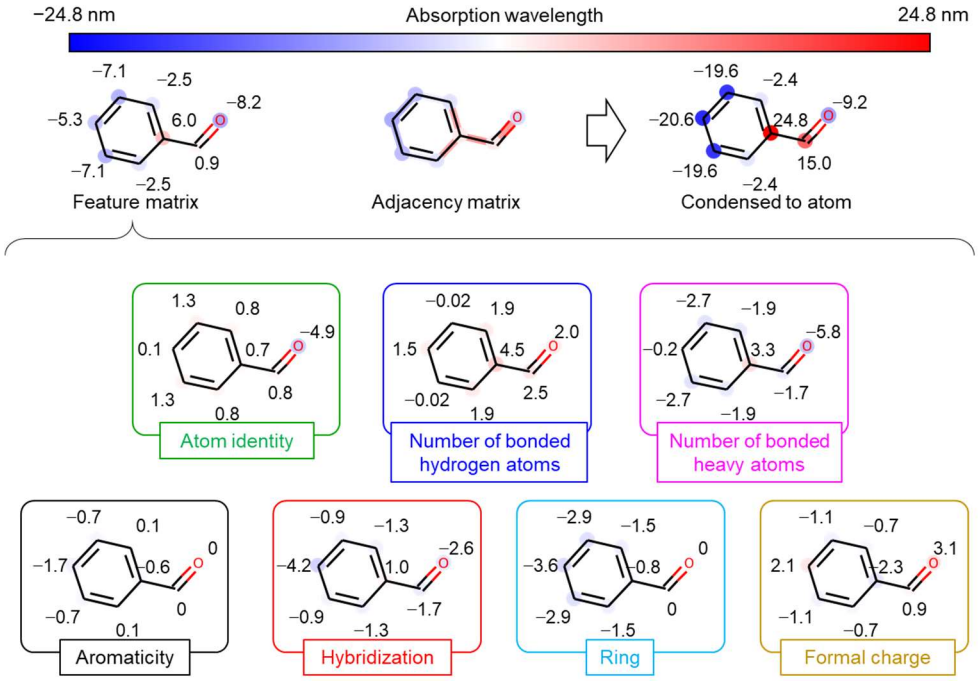


Figure S6. Attribution of all elements in the adjacency and feature matrices to the λ_{abs} of benzaldehyde in cyclohexane.

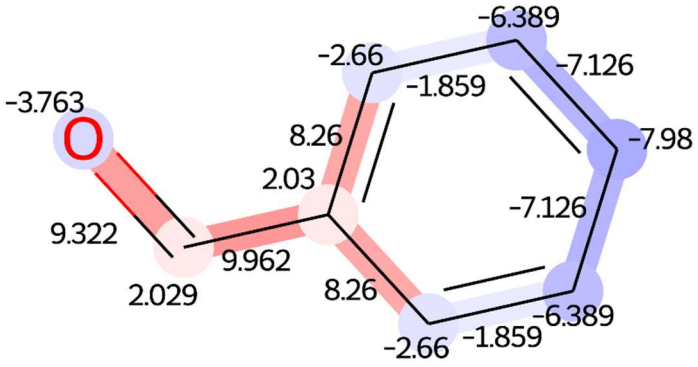


Figure S7. The attributions of the adjacency matrix to λ_{abs} of benzaldehyde in cyclohexane.

As illustrated in Figure S6, the integrated gradients method enables the quantification of the attributions of functional groups, core structures, and solvent molecules to specific properties. For example, cyclohexane shifts the λ_{abs} of benzaldehyde by −20.8 nm. Similarly, we can quantify the attributions of the carbon atom in benzene to logΦ, as shown in Figure S8. The attributions of benzene and cyclohexane to logΦ are calculated to be 0.516 and −0.480, respectively (Note that the attributions are in the $\log_{10}$ scale). The predicted and experimental values of Φ are 0.099 and 0.14, respectively, which are in good agreement. Notably, the accuracy of the attributions is within the prediction accuracy of the DLOS model.

Using the integrated gradients method, the attributions of functional groups and solvent molecules can be readily quantified. As shown in Table S4, we selected 54 functional groups: 7 alkyls, 2 alkenyls, 2 alkynyls, 11 phenyls, 4 hydroxyls, 10 amines, 2 ketones, 5 esters, 4 halogens, 1 amide, 2 perfluorinated groups, and 4 other groups. The number of unique chromophores containing at least one of the functional groups in Table S4 is 15,922 (out of 16,859) in our experimental database, which corresponds to 96% of our experimental data. In addition, we selected nine solvent molecules. 1) Nonpolar and weakly polar solvents: cyclohexane (CH), toluene (Tol), and dichloromethane (DCM); 2) polar aprotic solvents: acetonitrile (ACN), *N*,*N*-dimethylformamide (DMF), and dimethyl sulfoxide (DMSO); and 3) polar protic solvents: ethanol (EtOH), methanol (MeOH), and water (H_2O). The nine solvents covered 56.7% of the 49,500 chromophore/solvent combinations in our experimental database. The attributions were calculated with 143,298 chromophore/solvent combinations (i.e., 15,922 chromophores and 9 solvents). The attributions of the functional groups in a chromophore were calculated by comparison with a molecule without those functional groups, as a reference (Figure S9).

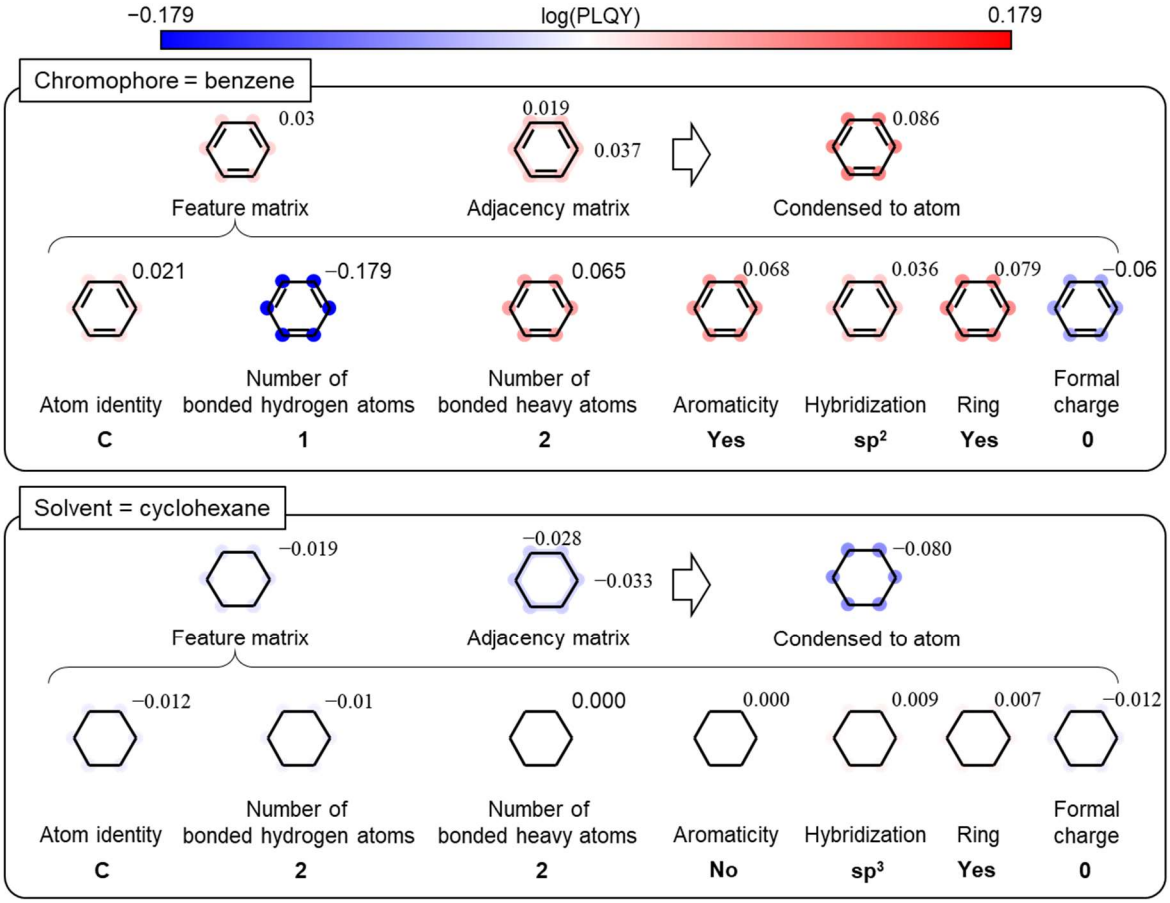


Figure S8. The attributions to $\log_{10}\Phi$ of benzene in cyclohexane. The results show that the rigid structure of benzene would enhance the PLQY and additionally cyclohexane is not good for the PLQY. The predicted PLQY can be calculated by summing all attributions and the value of the references; $\log_{10}\Phi = 0.086\times6 - 0.080\times6 - 1.05 = -1.014$, $\Phi = 10^{-1.014} = 0.097$.

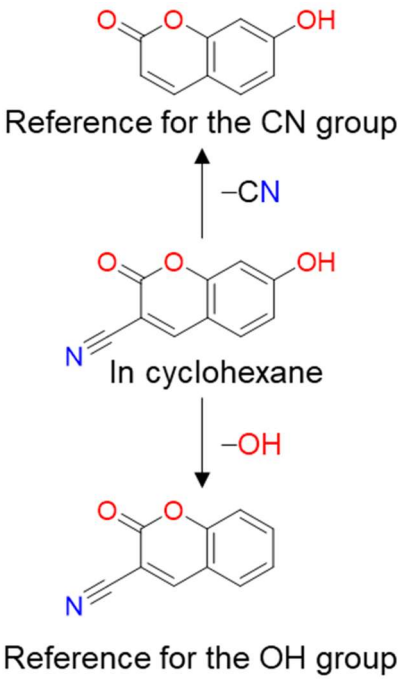


Figure S9. Illustration how to set the reference molecule to calculate the attribution of specific functional groups.

Reconstruction of absorption and emission spectra.

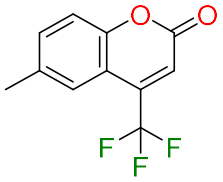
Absorption and emission spectra, $S_j(\omega)$, were calculated as a single peak using the normalized Gaussian function and predicted values by our DL model

$$S_j(\omega) = \exp\left[-4\ln(2)\cdot\left(\frac{10^7/\omega - 10^7/\lambda_j}{\sigma_j}\right)^2\right] \quad (1)$$

where λ_j is the absorption or emission peak position in nm and σ_j is the bandwidth. The vibronic features and asymmetric nature of the spectroscopic peaks were not reflected in Equation (S1). The absorption intensity is directly related to the extinction coefficient by Beer's law ($A = \varepsilon bc$); thus, the absorption spectrum can be approximated as $\varepsilon \cdot S_{\text{abs}}(\omega)$. Similarly, the emission intensity is proportional to the absorption intensity and PLQY, and thus, the emission spectrum can be obtained as $\varepsilon \cdot \Phi \cdot S_{\text{emi}}(\omega)$. The product of PLQY and extinction coefficient (i.e., $\Phi \cdot \varepsilon$) is known as the brightness. Using the optical and photophysical properties (λ_{abs}, λ_{emi}, σ_{abs}, σ_{emi}, ε, and Φ) predicted by the DL model, the absorption or emission spectra of a molecule were readily calculated. Furthermore, the CIE 1931 color space was computed using the calculated absorption and emission spectra. The CIE Standard Illuminant D65 was used for a daylight color.

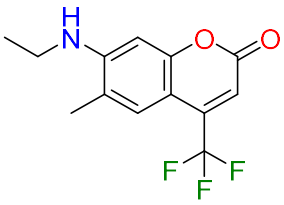
Property-oriented chromophore design

Using the average attributions in Table S13-S21, the optical and photophysical properties of chromophore can be estimated when a specific functional group is introduced. For example, the optical properties of the below molecule in an acetonitrile solvent are predicted using our DLOS, and the prediction results are summarized in table below.



	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ (ns)
Predicted properties	341.0	4509	4.122	416	4117	0.1981	2.3

If one decides to introduce the ethyl amine group to the molecule as shown below, the optical and photophysical properties of a new molecule could be estimated using the average attributions.



In table S16, the average attributions of the ethylamine group in acetonitrile can be found as follows:

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Ethyl amine	70.8	-860	0.277	48.1	-751	0.353	0.145

The optical and photophysical properties of a new molecule can be estimated by simply adding the attributions and the properties of the original molecule. For example, the absorption wavelength can be calculated as λ_{abs} = 341 nm +70.8 nm = 411.8 nm. Other properties can be calculated in the same way. However, the PLQY and fluorescence lifetime should be taken a logarithm before adding the attribution as follows:

1. Check the PLQY of the original molecule: $\Phi = 0.1981$
2. Take a logarithm with base 10: $\log_{10}\Phi = -0.703$
3. Add the average attribution: $\log_{10}\Phi = -0.703 + 0.353 = -0.350$
4. Take an exponent with base 10: $\Phi = 0.45$

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ (ns)
Calculated properties using attribution	412	3649	4.40	464	3366	0.45	3.2
Predicted properties	387	4085	4.29	478	2966	0.52	4.9
Error	25	-436	0.11	-14	400	-0.07	-1.7
Experimental properties	383	-	-	481	-	-	-

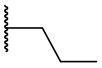
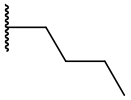
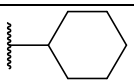
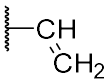
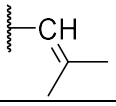
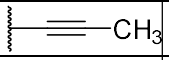
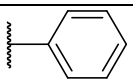
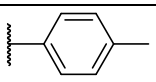
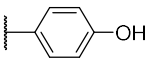
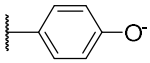
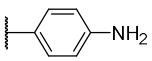
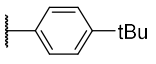
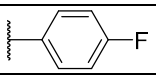
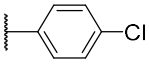
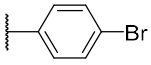
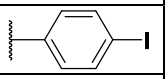
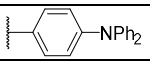
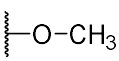
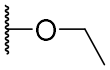
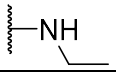
Table S2. The predicted values of the optical properties of a reference (zero matrix).

λ_{abs} (nm)	σ_{abs} (cm^{-1})	log ε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	log Φ	log τ
385.0	4391	4.14	464.0	3413	–1.05	0.39

Table S3. The average attribution of various solvents.

Solvent	λ_{abs} (nm)	σ_{abs} (cm^{-1})	log ε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	log Φ	log (τ / ns)
Cyclohexane	−17.1	46	−0.273	−59.8	−57	−0.465	−0.211
Toluene	−10.9	134	−0.280	−42.0	37	−0.321	−0.117
CH_2Cl_2	−8.3	132	−0.180	−19.5	91	−0.187	0.009
Acetonitrile	−12.6	240	−0.157	−11.6	264	−0.278	−0.013
DMF	−14.8	367	−0.208	−14.0	378	−0.328	0.022
DMSO	−9.3	327	−0.205	−6.0	303	−0.309	−0.011
Ethanol	−26.0	328	−0.178	−16.2	307	−0.218	0.010
Methanol	−21.6	583	−0.215	−16.2	366	−0.297	−0.042
Water	−21.7	795	−0.238	−3.6	383	−0.538	−0.235

Table S4. The selected functional groups to be investigated.

Alkyl group (7)	Name	Methyl	Ethyl	Propyl	Butyl	*i*-propyl
	Counts	15,161	1,963	777	4,335	1,772
	Structure					
	Name	*t*-butyl	Cyclohexyl			
	Counts	1,909	83			
	Structure					
Alkenyl group (2)	Name	Ethene	Dimethyl-ethene			
	Counts	94	27			
	Structure					
Alkynyl group (2)	Name	Ethyne	Methyl-ethyne			
	Counts	91	13			
	Structure					
Phenyl group (11)	Name	Phenyl	*p*-tolyl	Phenol	Phenolate	Anilne
	Counts	6,961	892	140	36	81
	Structure					
	Name	tBuPh	PhF	PhCl	PhBr	PhI
	Counts	729	242	232	235	84
	Structure					
	Name	$PhNPh_2$				
	Counts	707				
	Structure					
Hydroxyl group (4)	Name	Hydroxyl	Hydroxylate	methoxy	Ethoxy	
	Counts	1,967	406	4,684	175	
	Structure					
Amine group (10)	Name	Amine	protonated amine	methyl amine	Dimethylamine	Ethyl amine
	Counts	839	28	86	1,665	58
	Structure					

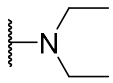
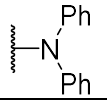
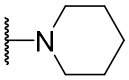
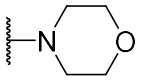
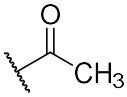
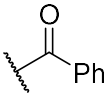
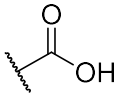
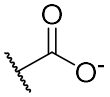
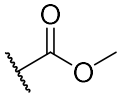
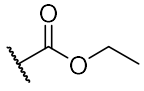
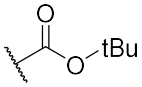
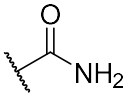
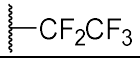
	Name	diethylamine	NPh_2	NHPh	piperidine	morpholine
	Counts	694	264	82	252	192
	Structure					
Ketone group (2)	Name	acetyl	phenyl ketone			
	Counts	517	138			
	Structure					
Ester group (5)	Name	Acetic acid	acetate	COOMe	COOEt	COOtBu
	Counts	554	115	724	881	200
	Structure					
Halide group (4)	Name	Fluorine	Chlorine	Bromine	Iodine	
	Counts	7,661	1,177	989	223	
	Structure					
Amide group (1)	Name	$CONH_2$				
	Counts	42				
	Structure					
Other (4)	Name	nitrile	nitro	Sulfonyl	Sulfonate	
	Counts	3677	809	81	220	
	Structure					
Perfluorinated group (2)	Name	CF_2	CF_3			
	Counts	860	129			
	Structure					

Table S5. Average attribution to the absorption wavelength of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	3.4	3.1	2.8	2.6	2.5	2.4	2.4	2.3	2.3
Ethyl	4.7	4.7	4.3	3.9	4.0	3.9	3.6	3.5	3.5
Propyl	22.9	22.7	22.6	21.3	21.2	20.9	18.8	18.3	18.6
Butyl	2.0	2.1	2.3	2.3	2.3	2.4	2.4	2.3	2.3
Isopropyl	5.5	5.3	4.7	4.5	4.3	4.4	4.4	4.5	4.7
t-Butyl	5.7	5.7	5.9	5.8	5.7	5.5	5.7	5.7	5.8
cyclohexyl	-0.6	-0.1	0.3	-0.2	-0.1	-0.6	-1.3	-1.7	-1.8
ethene	-2.1	-1.8	-1.3	-0.6	-0.9	-0.5	-0.6	-0.7	-0.7
dimethylethene	4.0	4.4	5.6	7.0	7.0	7.0	5.4	5.3	5.4
Ethyne	-1.9	-2.2	-2.4	-3.0	-3.1	-3.5	-3.1	-2.9	-2.8
methylethyne	5.7	5.7	5.1	4.3	3.4	4.2	4.7	4.3	2.6
Phenyl	10.7	10.7	10.6	10.5	10.6	10.3	10.0	10.0	10.2
p-tolyl	8.5	8.4	8.5	8.5	8.6	8.2	8.2	8.3	8.4
Phenol	15.6	15.6	16.5	17.7	17.6	17.0	17.4	18.0	18.7
Phenolate	132.4	135.9	136.9	128.7	132.8	125.9	104.9	101.3	100.2
Anilne	18.4	19.2	20.9	22.9	23.0	22.4	22.8	22.9	23.3
tBuPh	8.0	8.2	8.7	9.0	8.9	8.8	8.6	8.6	8.7
PhF	2.7	2.3	3.0	4.0	3.9	3.5	3.9	4.3	4.5
PhCl	3.0	3.0	3.1	3.7	3.7	3.3	3.4	3.5	3.6
PhBr	13.5	13.3	12.8	12.3	12.6	12.2	12.0	12.3	12.5
PhI	8.4	7.2	6.3	6.2	6.2	5.7	6.2	6.5	6.5
$PhNPh_2$	22.7	22.5	23.9	23.7	24.0	22.8	23.0	22.5	21.9
Hydroxyl	5.6	5.5	5.6	5.4	5.4	5.3	5.2	5.0	4.9
Hydroxylate	36.0	35.9	34.3	31.9	32.4	31.4	28.6	27.8	27.9
methoxy	3.6	3.6	4.0	4.0	4.0	3.8	3.8	3.7	3.5
Ethoxy	-2.3	-2.7	-3.0	-3.1	-3.3	-3.4	-2.2	-2.2	-2.4
Amine	16.0	16.0	16.7	17.0	16.9	16.7	17.0	17.1	17.3
protonated amine	-1.5	-1.7	-1.4	0.1	-0.1	0.2	0.6	0.5	0.8
methyl amine	22.4	23.7	26.3	27.2	27.4	26.6	25.9	25.1	24.3
Dimethylamine	36.9	37.9	39.9	39.9	40.3	39.5	39.0	38.4	38.1
Ethyl amine	70.1	69.4	71.4	70.8	70.3	69.8	69.6	68.9	68.5
diethylamine	51.7	52.1	54.3	54.5	54.5	54.3	55.0	54.6	54.6
NPh_2	30.5	31.1	32.0	30.8	31.4	30.6	29.1	28.4	28.2
NHPh	13.9	14.5	12.8	9.9	10.4	9.5	7.3	6.1	5.6

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
piperidine	42.8	42.5	43.2	42.9	42.9	42.3	42.1	41.7	41.7
morpholine	29.7	31.0	32.7	32.2	32.5	32.1	31.2	30.9	31.1
acetyl	18.6	18.2	18.1	18.1	18.2	17.5	15.9	15.6	15.3
phenyl ketone	20.9	21.2	23.7	24.7	24.8	23.8	24.2	23.8	23.5
Acetic acid	6.0	5.9	5.2	4.7	4.8	4.6	4.2	4.3	4.5
acetate	6.2	5.8	5.4	4.3	4.3	4.1	3.4	3.5	3.8
COOMe	4.2	4.2	4.3	4.3	4.3	3.8	3.8	4.0	4.1
COOEt	-1.5	-1.6	-1.9	-2.2	-2.2	-2.7	-2.8	-2.7	-2.7
COOtBu	-3.5	-4.2	-4.2	-4.2	-4.4	-4.9	-4.5	-4.2	-4.0
Fluorine	23.1	22.6	20.6	19.6	19.5	19.6	19.5	19.6	19.9
Chlorine	13.4	13.7	14.0	13.8	13.9	13.7	12.9	12.7	12.5
Bromine	9.6	9.7	9.9	9.6	9.8	9.4	8.9	8.8	8.7
Iodine	8.7	8.7	9.1	8.9	9.1	8.8	8.5	8.9	9.2
$CONH_2$	1.1	1.0	1.4	1.6	0.9	2.0	3.8	4.4	5.2
nitrile	25.8	26.0	26.1	25.4	25.7	25.1	24.3	24.3	24.6
nitro	23.9	25.6	27.5	26.8	27.5	27.0	24.4	23.8	23.9
Sulfonyl	-6.1	-6.8	-7.5	-8.5	-8.6	-8.6	-8.7	-8.5	-8.2
Sulfonate	1.8	1.5	1.4	1.9	1.8	2.2	2.6	2.6	2.7
CF_3	6.1	6.5	7.0	7.0	7.2	7.0	6.8	6.9	7.0
CF_2CF_3	-5.1	-5.4	-5.6	-6.1	-6.2	-6.3	-6.2	-6.4	-6.8

Table S6. Average attribution to the absorption bandwidth of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	-55	-52	-48	-48	-48	-47	-54	-59	-67
Ethyl	44	45	50	53	52	51	55	58	62
Propyl	23	13	7	8	12	2	-13	-14	-8
Butyl	-33	-33	-32	-31	-32	-31	-32	-34	-38
Isopropyl	-120	-116	-109	-112	-111	-109	-120	-127	-137
t-Butyl	-35	-36	-35	-34	-34	-31	-34	-36	-41
cyclohexyl	30	41	52	54	51	56	46	36	22
ethene	231	231	210	205	210	194	210	209	210
dimethylethene	-326	-344	-334	-350	-353	-352	-352	-353	-364
Ethyne	-35	-44	-53	-54	-55	-51	-57	-58	-63
methylethyne	-918	-892	-942	-945	-934	-931	-955	-956	-949
Phenyl	-32	-29	-21	-22	-26	-22	-25	-35	-47
p-tolyl	40	37	51	50	45	49	53	48	37
Phenol	-327	-341	-317	-326	-331	-328	-326	-343	-375
Phenolate	-470	-506	-387	-384	-450	-429	-313	-367	-482
Anilne	-165	-191	-161	-166	-172	-167	-160	-165	-184
tBuPh	126	125	120	118	119	112	122	119	113
PhF	166	157	148	134	134	136	129	118	99
PhCl	203	201	209	207	201	206	212	204	194
PhBr	-39	-40	-36	-42	-45	-43	-40	-46	-53
PhI	-169	-160	-153	-154	-156	-149	-156	-164	-178
$PhNPh_2$	9	32	88	121	110	116	108	92	64
Hydroxyl	-45	-45	-42	-41	-41	-40	-44	-48	-54
Hydroxylate	-462	-463	-446	-433	-441	-436	-425	-439	-472
methoxy	-44	-41	-37	-34	-36	-34	-34	-37	-44
Ethoxy	-80	-72	-70	-74	-76	-72	-75	-77	-86
Amine	-337	-324	-296	-288	-292	-284	-311	-336	-368
protonated amine	-227	-238	-241	-248	-250	-245	-242	-251	-268
methyl amine	-70	-64	-59	-69	-80	-74	-79	-96	-123
Dimethylamine	-399	-373	-314	-279	-289	-282	-295	-313	-343
Ethyl amine	-920	-905	-878	-860	-855	-868	-904	-951	-1027
diethylamine	-813	-792	-748	-707	-708	-707	-734	-755	-802
NPh_2	-302	-268	-214	-192	-202	-193	-216	-240	-275
NHPh	75	73	110	125	121	113	125	135	148

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
piperidine	-449	-424	-380	-367	-371	-370	-400	-431	-474
morpholine	-73	-66	-52	-44	-45	-49	-66	-72	-79
acetyl	-256	-253	-234	-243	-251	-237	-237	-248	-267
phenyl ketone	-170	-189	-179	-193	-206	-193	-176	-189	-220
Acetic acid	-28	-27	-24	-25	-27	-28	-27	-31	-34
acetate	52	47	44	40	43	41	30	28	25
COOMe	11	13	16	9	5	9	7	-3	-18
COOEt	149	143	134	122	118	120	129	124	114
COOtBu	134	129	96	84	85	89	86	83	81
Fluorine	-569	-549	-526	-504	-499	-497	-520	-532	-547
Chlorine	-190	-192	-186	-182	-186	-184	-176	-174	-176
Bromine	-89	-90	-83	-82	-86	-80	-79	-82	-89
Iodine	-126	-132	-119	-118	-123	-113	-107	-109	-115
$CONH_2$	-804	-796	-777	-784	-780	-775	-812	-844	-887
nitrile	-120	-110	-93	-92	-97	-91	-102	-113	-130
nitro	364	362	394	415	408	399	419	428	432
Sulfonyl	-171	-154	-158	-162	-161	-154	-169	-179	-187
Sulfonate	-83	-80	-72	-65	-66	-63	-66	-69	-72
CF_3	-55	-53	-40	-38	-40	-38	-42	-47	-54
CF_2CF_3	121	125	125	126	129	128	124	126	126

Table S7. Average attribution to the extinction coefficients of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	0.013	0.013	0.013	0.013	0.013	0.013	0.014	0.015	0.016
Ethyl	0.012	0.012	0.013	0.013	0.013	0.012	0.013	0.013	0.012
Propyl	-0.001	0.000	-0.002	0.002	0.002	0.002	0.006	0.007	0.006
Butyl	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.010	0.010
Isopropyl	-0.021	-0.022	-0.025	-0.026	-0.026	-0.025	-0.025	-0.023	-0.022
t-Butyl	0.011	0.012	0.012	0.013	0.013	0.013	0.013	0.014	0.015
cyclohexyl	-0.038	-0.037	-0.038	-0.037	-0.036	-0.037	-0.039	-0.038	-0.040
ethene	-0.054	-0.058	-0.052	-0.052	-0.052	-0.052	-0.054	-0.054	-0.054
dimethylethene	0.001	0.005	0.009	0.013	0.015	0.016	0.015	0.016	0.018
Ethyne	0.034	0.034	0.025	0.021	0.020	0.023	0.024	0.026	0.028
methylethyne	0.099	0.088	0.091	0.087	0.083	0.082	0.083	0.087	0.091
Phenyl	0.006	0.006	0.005	0.006	0.006	0.005	0.006	0.006	0.006
p-tolyl	0.044	0.044	0.042	0.044	0.045	0.044	0.045	0.045	0.044
Phenol	0.134	0.139	0.141	0.137	0.137	0.134	0.137	0.134	0.132
Phenolate	0.162	0.170	0.174	0.189	0.199	0.195	0.215	0.215	0.209
Anilne	0.150	0.155	0.152	0.152	0.154	0.152	0.152	0.151	0.151
tBuPh	0.018	0.020	0.022	0.024	0.025	0.025	0.024	0.024	0.026
PhF	0.031	0.031	0.031	0.034	0.034	0.032	0.036	0.036	0.037
PhCl	0.000	-0.002	-0.001	0.001	0.003	-0.001	0.000	0.000	0.000
PhBr	0.002	0.003	0.006	0.008	0.009	0.008	0.008	0.009	0.010
PhI	0.025	0.025	0.017	0.013	0.014	0.016	0.014	0.014	0.017
$PhNPh_2$	0.163	0.158	0.151	0.145	0.146	0.139	0.143	0.141	0.137
Hydroxyl	0.017	0.017	0.016	0.017	0.017	0.017	0.017	0.018	0.019
Hydroxylate	0.067	0.069	0.070	0.071	0.071	0.072	0.075	0.076	0.078
methoxy	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009	0.009
Ethoxy	-0.020	-0.023	-0.025	-0.027	-0.027	-0.028	-0.027	-0.027	-0.025
Amine	0.056	0.055	0.053	0.050	0.050	0.049	0.053	0.053	0.054
protonated amine	0.040	0.040	0.040	0.038	0.038	0.037	0.037	0.037	0.037
methyl amine	-0.087	-0.090	-0.094	-0.094	-0.093	-0.091	-0.090	-0.089	-0.088
Dimethylamine	0.130	0.125	0.116	0.108	0.108	0.104	0.109	0.106	0.102
Ethyl amine	0.321	0.318	0.297	0.277	0.275	0.269	0.279	0.281	0.287
diethylamine	0.257	0.255	0.236	0.219	0.217	0.213	0.219	0.215	0.211
NPh_2	-0.004	-0.008	-0.011	-0.012	-0.013	-0.011	-0.009	-0.010	-0.010
NHPh	-0.013	-0.014	-0.007	0.000	0.001	-0.001	0.002	0.001	-0.003

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
piperidine	0.157	0.147	0.132	0.121	0.121	0.116	0.120	0.119	0.116
morpholine	0.025	0.020	0.018	0.017	0.016	0.014	0.020	0.017	0.011
acetyl	-0.047	-0.047	-0.045	-0.043	-0.042	-0.041	-0.037	-0.036	-0.035
phenyl ketone	-0.017	-0.014	-0.018	-0.022	-0.020	-0.023	-0.022	-0.022	-0.023
Acetic acid	0.017	0.017	0.017	0.017	0.018	0.017	0.017	0.018	0.018
acetate	-0.026	-0.025	-0.023	-0.020	-0.021	-0.018	-0.015	-0.013	-0.010
COOMe	-0.007	-0.007	-0.007	-0.005	-0.004	-0.003	-0.003	-0.001	0.002
COOEt	-0.038	-0.039	-0.037	-0.033	-0.032	-0.033	-0.033	-0.031	-0.029
COOtBu	-0.074	-0.076	-0.077	-0.076	-0.075	-0.073	-0.075	-0.072	-0.069
Fluorine	0.090	0.088	0.091	0.090	0.088	0.088	0.089	0.090	0.091
Chlorine	-0.003	-0.004	-0.007	-0.008	-0.008	-0.007	-0.007	-0.007	-0.006
Bromine	-0.002	0.000	-0.001	0.001	0.002	0.002	0.002	0.002	0.003
Iodine	0.005	0.009	0.007	0.006	0.008	0.009	0.008	0.007	0.007
$CONH_2$	0.024	0.028	0.047	0.050	0.048	0.050	0.052	0.055	0.061
nitrile	-0.039	-0.038	-0.039	-0.038	-0.038	-0.036	-0.033	-0.032	-0.032
nitro	0.019	0.024	0.030	0.035	0.036	0.035	0.040	0.038	0.034
Sulfonyl	-0.223	-0.226	-0.230	-0.233	-0.234	-0.231	-0.231	-0.230	-0.229
Sulfonate	0.008	0.010	0.010	0.007	0.008	0.006	0.004	0.005	0.007
CF_3	0.006	0.006	0.004	0.004	0.004	0.003	0.004	0.004	0.003
CF_2CF_3	-0.005	-0.007	-0.008	-0.008	-0.008	-0.007	-0.005	-0.004	-0.004

Table S8. Average attribution to the emission wavelength of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	2.3	2.2	2.2	1.9	1.9	1.7	1.6	1.5	1.1
Ethyl	4.9	5.2	5.2	4.9	5.0	5.0	4.7	4.7	4.8
Propyl	18.7	18.5	18.3	17.5	17.7	17.0	15.5	15.0	15.0
Butyl	1.7	1.8	2.0	2.0	2.0	2.1	2.1	2.0	1.9
Isopropyl	3.9	3.6	2.0	0.8	0.9	0.6	0.4	0.2	-0.3
t-Butyl	6.1	6.1	6.1	6.1	6.1	5.9	6.0	6.0	5.7
cyclohexyl	0.6	1.1	3.0	3.6	3.2	3.4	3.4	3.4	3.4
ethene	0.9	1.2	0.4	-0.1	-0.1	-0.2	-0.3	-0.6	-0.9
dimethylethene	-0.5	-1.2	-2.3	-3.5	-3.3	-3.7	-4.7	-5.0	-5.1
Ethyne	-3.8	-4.8	-7.4	-8.7	-8.6	-9.1	-9.0	-8.9	-9.4
methylethyne	-16.5	-17.6	-20.9	-22.5	-23.3	-22.3	-21.9	-23.0	-25.3
Phenyl	12.3	12.6	14.0	14.6	14.5	14.3	14.3	14.4	14.5
p-tolyl	11.7	11.9	13.7	14.3	14.3	14.0	14.5	14.7	14.9
Phenol	15.1	14.1	14.1	14.8	14.7	13.8	14.6	15.0	15.0
Phenolate	128.4	132.2	137.7	135.4	137.2	133.0	122.6	120.6	119.6
Anilne	22.9	23.4	28.7	31.4	31.1	30.9	32.3	33.2	34.1
tBuPh	9.8	10.2	10.4	10.6	10.5	10.4	10.2	9.8	9.2
PhF	4.2	3.7	4.8	5.5	5.6	5.0	5.4	5.2	4.9
PhCl	8.3	8.8	11.7	13.8	13.4	13.4	14.2	14.4	14.7
PhBr	13.6	13.8	14.9	15.0	15.0	14.9	14.7	14.6	14.6
PhI	6.5	5.6	5.3	5.3	5.4	4.9	5.6	6.3	6.5
$PhNPh_2$	32.4	34.8	44.6	50.6	49.8	49.8	51.6	52.0	52.3
Hydroxyl	5.0	5.1	5.4	5.2	5.2	5.0	4.9	4.6	4.3
Hydroxylate	26.4	26.4	26.5	25.7	26.0	25.3	23.7	23.0	22.3
methoxy	4.4	4.6	5.5	6.2	6.0	6.1	6.4	6.3	6.2
Ethoxy	-1.2	-0.9	-0.1	0.2	-0.3	0.0	1.3	1.3	1.0
Amine	14.1	13.7	14.1	13.9	14.0	13.4	13.7	13.6	13.4
protonated amine	-5.8	-6.6	-7.6	-8.1	-8.1	-8.0	-7.3	-7.5	-7.7
methyl amine	23.3	25.1	26.9	26.8	26.8	26.3	26.3	25.8	25.3
Dimethylamine	39.3	42.2	49.7	53.7	53.4	53.4	54.2	54.5	54.8
Ethyl amine	54.3	52.5	50.7	48.1	48.8	46.7	45.4	44.1	41.3
diethylamine	42.9	43.6	45.7	47.2	47.5	46.8	47.6	47.9	47.7
NPh_2	35.7	38.8	44.8	47.0	46.9	46.6	46.4	46.5	46.9
NHPh	18.4	20.2	24.4	24.4	24.3	24.2	23.7	23.8	24.8

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
piperidine	43.3	43.8	45.3	45.1	45.1	44.0	44.1	43.9	43.6
morpholine	34.7	36.7	39.1	39.9	39.7	39.5	39.3	39.1	39.5
acetyl	16.4	17.0	19.6	20.1	19.9	19.6	19.3	19.5	19.6
phenyl ketone	24.6	25.3	29.6	32.3	31.6	31.2	33.1	33.9	34.3
Acetic acid	5.8	5.7	5.3	4.5	4.7	4.4	3.7	3.4	3.2
acetate	1.7	1.1	-0.2	-1.6	-1.4	-1.8	-2.6	-2.9	-3.5
COOMe	5.3	5.2	6.1	6.0	6.0	5.5	5.3	5.0	4.5
COOEt	1.4	1.5	1.9	1.8	1.6	1.2	1.4	1.2	0.6
COOtBu	-0.4	-0.5	0.3	0.1	-0.2	-0.5	0.3	0.5	0.9
Fluorine	12.1	11.7	9.8	7.8	8.3	7.6	6.4	5.6	4.5
Chlorine	11.9	12.5	13.2	13.4	13.4	13.3	12.9	12.8	12.8
Bromine	10.0	10.4	11.3	11.6	11.6	11.5	11.6	11.7	11.7
Iodine	9.6	9.5	10.4	11.0	10.8	11.0	11.5	11.9	12.3
$CONH_2$	-4.9	-6.9	-14.7	-20.3	-19.4	-20.7	-22.0	-23.9	-27.3
nitrile	28.3	29.6	31.2	31.0	31.1	30.5	30.1	30.0	30.1
nitro	30.9	34.7	40.7	44.0	43.9	44.1	43.4	43.2	43.3
Sulfonyl	-8.4	-9.2	-11.5	-13.7	-13.7	-14.0	-14.1	-14.4	-15.0
Sulfonate	2.6	2.4	2.5	2.4	2.4	2.7	2.6	2.3	2.0
CF_3	7.1	7.7	9.4	10.1	10.1	10.1	10.1	10.2	10.4
CF_2CF_3	-4.9	-5.1	-4.6	-4.7	-4.9	-4.6	-4.4	-4.5	-4.5

Table S9. Average attribution to the emission bandwidth of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	-35	-31	-25	-25	-23	-25	-32	-33	-34
Ethyl	-28	-29	-26	-29	-30	-30	-32	-33	-36
Propyl	-94	-93	-108	-147	-147	-150	-197	-200	-200
Butyl	-17	-17	-14	-14	-13	-14	-14	-14	-14
Isopropyl	-59	-59	-66	-73	-71	-74	-77	-75	-73
t-Butyl	-27	-29	-32	-40	-40	-39	-46	-50	-54
cyclohexyl	4	9	37	43	43	47	43	44	43
ethene	14	9	-21	-67	-70	-72	-78	-86	-91
dimethylethene	72	59	19	-17	-16	-16	-19	-13	-3
Ethyne	-56	-45	-54	-80	-79	-78	-93	-102	-112
methylethyne	-629	-593	-592	-612	-600	-615	-650	-657	-661
Phenyl	-59	-59	-52	-52	-52	-49	-49	-49	-50
p-tolyl	-22	-29	-32	-33	-35	-31	-31	-32	-36
Phenol	-99	-105	-112	-133	-132	-126	-127	-125	-123
Phenolate	17	-30	-30	-65	-66	-109	-159	-151	-141
Anilne	-78	-97	-69	-59	-63	-59	-46	-40	-39
tBuPh	-6	-11	-21	-37	-39	-41	-48	-55	-63
PhF	-34	-41	-45	-67	-65	-62	-68	-76	-84
PhCl	59	51	46	35	31	39	45	44	39
PhBr	-52	-59	-82	-110	-113	-114	-115	-123	-134
PhI	-33	-26	-19	-23	-21	-23	-26	-27	-27
$PhNPh_2$	-207	-186	-110	-64	-66	-51	-59	-62	-67
Hydroxyl	-45	-45	-45	-50	-48	-50	-56	-58	-60
Hydroxylate	-220	-219	-182	-178	-175	-180	-201	-203	-209
methoxy	-28	-26	-17	-11	-12	-10	-9	-9	-9
Ethoxy	-77	-78	-71	-73	-73	-67	-68	-67	-68
Amine	-154	-153	-163	-160	-155	-150	-162	-158	-155
protonated amine	-77	-65	-8	4	4	6	13	17	23
methyl amine	-248	-261	-285	-312	-313	-307	-312	-308	-311
Dimethylamine	-395	-383	-342	-318	-318	-304	-314	-310	-310
Ethyl amine	-860	-823	-779	-751	-727	-728	-793	-801	-824
diethylamine	-723	-696	-668	-664	-656	-642	-678	-680	-683
NPh_2	-217	-208	-155	-114	-116	-110	-113	-112	-119
NHPh	19	21	85	136	134	140	159	175	189

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
piperidine	-470	-452	-436	-434	-431	-420	-439	-437	-438
morpholine	-328	-329	-344	-358	-362	-342	-352	-356	-361
acetyl	-89	-87	-67	-76	-78	-77	-92	-83	-71
phenyl ketone	-103	-126	-143	-172	-182	-166	-152	-147	-149
Acetic acid	-18	-20	-27	-39	-37	-40	-45	-50	-55
acetate	-46	-50	-64	-101	-98	-106	-126	-135	-141
COOMe	7	1	-8	-29	-30	-34	-39	-46	-54
COOEt	154	143	140	125	124	120	123	120	116
COOtBu	60	62	50	-4	-7	-4	-21	-36	-51
Fluorine	-347	-328	-318	-322	-313	-317	-344	-352	-360
Chlorine	-81	-84	-88	-99	-100	-101	-105	-103	-102
Bromine	-43	-51	-58	-64	-67	-65	-62	-63	-65
Iodine	58	48	44	34	29	30	38	35	33
$CONH_2$	57	62	35	32	45	27	13	16	25
nitrile	-133	-141	-153	-179	-181	-182	-197	-206	-216
nitro	-52	-69	-60	-47	-55	-47	-45	-46	-50
Sulfonyl	23	31	22	19	18	19	15	13	10
Sulfonate	-26	-27	-20	-21	-23	-20	-19	-22	-27
CF_3	-32	-32	-16	1	1	2	6	10	13
CF_2CF_3	24	20	23	13	13	11	7	4	3

Table S10. Average attribution to $\log_{10}$(PLQY) of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	0.018	0.012	0.014	0.029	0.029	0.029	0.033	0.041	0.055
Ethyl	-0.046	-0.042	-0.040	-0.038	-0.038	-0.034	-0.033	-0.030	-0.027
Propyl	-0.044	-0.051	-0.052	0.011	0.011	0.028	0.056	0.078	0.102
Butyl	-0.003	-0.005	-0.012	-0.014	-0.014	-0.015	-0.015	-0.013	-0.011
Isopropyl	-0.007	-0.012	-0.016	0.003	0.001	0.007	0.014	0.024	0.038
t-Butyl	-0.020	-0.024	-0.023	-0.011	-0.011	-0.009	-0.005	0.004	0.020
cyclohexyl	0.092	0.079	0.026	0.047	0.051	0.035	0.028	0.017	0.013
ethene	0.038	0.038	0.028	0.035	0.034	0.034	0.035	0.037	0.031
dimethylethene	-0.191	-0.177	-0.155	-0.098	-0.100	-0.077	-0.057	-0.050	-0.042
Ethyne	0.020	0.007	0.002	0.018	0.016	0.021	0.033	0.048	0.071
methylethyne	0.482	0.438	0.477	0.632	0.635	0.620	0.617	0.677	0.813
Phenyl	0.015	0.006	-0.025	-0.050	-0.048	-0.056	-0.059	-0.062	-0.064
p-tolyl	-0.030	-0.036	-0.047	-0.045	-0.044	-0.044	-0.043	-0.041	-0.040
Phenol	-0.004	-0.010	-0.047	-0.110	-0.108	-0.122	-0.123	-0.141	-0.167
Phenolate	-0.632	-0.678	-0.815	-0.859	-0.829	-0.829	-0.761	-0.799	-0.862
Anilne	-0.005	-0.020	-0.068	-0.126	-0.120	-0.130	-0.142	-0.165	-0.197
tBuPh	-0.023	-0.024	-0.022	-0.010	-0.008	-0.008	-0.006	0.002	0.018
PhF	0.051	0.038	0.034	0.052	0.049	0.047	0.055	0.072	0.101
PhCl	-0.037	-0.039	-0.044	-0.050	-0.047	-0.053	-0.053	-0.053	-0.044
PhBr	-0.073	-0.070	-0.061	-0.065	-0.062	-0.060	-0.059	-0.050	-0.041
PhI	-0.022	-0.030	-0.016	-0.026	-0.026	-0.040	-0.039	-0.051	-0.054
$PhNPh_2$	0.217	0.167	0.052	-0.098	-0.087	-0.136	-0.156	-0.181	-0.199
Hydroxyl	0.016	0.012	0.011	0.026	0.025	0.025	0.029	0.036	0.048
Hydroxylate	-0.083	-0.087	-0.108	-0.096	-0.095	-0.094	-0.073	-0.063	-0.044
methoxy	0.029	0.022	0.009	-0.008	-0.007	-0.015	-0.020	-0.023	-0.022
Ethoxy	0.070	0.063	0.057	0.035	0.040	0.023	0.017	0.021	0.028
Amine	0.065	0.054	0.023	0.009	0.009	0.002	0.005	0.001	-0.006
protonated amine	0.086	0.070	0.046	0.021	0.027	0.000	-0.014	-0.039	-0.062
methyl amine	0.192	0.175	0.129	0.122	0.122	0.091	0.090	0.081	0.084
Dimethylamine	0.140	0.103	0.005	-0.113	-0.107	-0.146	-0.159	-0.185	-0.207
Ethyl amine	0.510	0.440	0.363	0.353	0.343	0.298	0.313	0.343	0.429
diethylamine	0.267	0.220	0.138	0.043	0.042	0.000	-0.009	-0.038	-0.070
NPh_2	0.119	0.091	0.012	-0.082	-0.079	-0.114	-0.124	-0.150	-0.168
NHPh	-0.106	-0.102	-0.148	-0.172	-0.170	-0.167	-0.169	-0.191	-0.222
piperidine	0.228	0.187	0.104	0.040	0.037	0.010	0.008	-0.006	-0.016
morpholine	-0.031	-0.058	-0.163	-0.260	-0.257	-0.265	-0.266	-0.278	-0.292

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
acetyl	-0.066	-0.080	-0.078	-0.075	-0.070	-0.078	-0.070	-0.083	-0.097
phenyl ketone	0.029	0.019	-0.050	-0.175	-0.166	-0.202	-0.223	-0.257	-0.286
Acetic acid	-0.023	-0.021	-0.018	-0.007	-0.007	-0.005	0.001	0.010	0.024
acetate	-0.095	-0.091	-0.062	-0.005	-0.005	0.013	0.030	0.053	0.088
COOMe	0.018	0.013	0.016	0.053	0.054	0.056	0.068	0.088	0.114
COOEt	-0.047	-0.047	-0.047	-0.029	-0.027	-0.026	-0.023	-0.009	0.024
COOtBu	0.040	0.025	0.028	0.067	0.067	0.068	0.075	0.097	0.127
Fluorine	0.173	0.164	0.226	0.315	0.308	0.314	0.325	0.358	0.406
Chlorine	-0.023	-0.028	-0.043	-0.055	-0.053	-0.059	-0.059	-0.063	-0.059
Bromine	-0.100	-0.100	-0.111	-0.120	-0.119	-0.119	-0.116	-0.119	-0.119
Iodine	-0.185	-0.179	-0.203	-0.248	-0.242	-0.243	-0.248	-0.260	-0.271
$CONH_2$	-0.067	-0.063	-0.009	0.070	0.065	0.077	0.096	0.127	0.170
nitrile	-0.122	-0.131	-0.161	-0.165	-0.162	-0.159	-0.146	-0.139	-0.129
nitro	-0.282	-0.284	-0.373	-0.461	-0.449	-0.453	-0.462	-0.475	-0.484
Sulfonyl	-0.027	-0.033	-0.064	-0.062	-0.062	-0.059	-0.055	-0.047	-0.021
Sulfonate	0.051	0.054	0.047	0.039	0.040	0.039	0.041	0.053	0.074
CF_3	-0.006	-0.014	-0.059	-0.097	-0.096	-0.102	-0.106	-0.115	-0.124
CF_2CF_3	-0.013	-0.008	-0.006	0.011	0.014	0.018	0.020	0.034	0.043

Table S11. Average attribution to $\log_{10}$(fluorescence lifetime) of functional groups in various solvents.

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
Methyl	0.015	0.012	0.011	0.021	0.021	0.022	0.025	0.031	0.042
Ethyl	-0.012	-0.012	-0.008	-0.007	-0.008	-0.007	-0.006	-0.004	-0.004
Propyl	-0.019	-0.025	-0.026	0.015	0.012	0.025	0.039	0.055	0.073
Butyl	-0.003	-0.004	-0.008	-0.010	-0.010	-0.011	-0.010	-0.009	-0.008
Isopropyl	0.029	0.025	0.020	0.032	0.030	0.033	0.039	0.047	0.057
t-Butyl	-0.006	-0.008	-0.010	-0.004	-0.005	-0.003	0.000	0.005	0.017
cyclohexyl	0.068	0.063	0.035	0.052	0.056	0.044	0.037	0.030	0.031
ethene	0.066	0.071	0.065	0.060	0.060	0.057	0.056	0.058	0.053
dimethylethene	-0.119	-0.118	-0.094	-0.053	-0.056	-0.050	-0.034	-0.031	-0.026
Ethyne	-0.064	-0.072	-0.088	-0.084	-0.084	-0.077	-0.069	-0.057	-0.040
methylethyne	0.348	0.323	0.322	0.418	0.422	0.414	0.426	0.473	0.571
Phenyl	0.015	0.011	-0.007	-0.027	-0.026	-0.029	-0.033	-0.037	-0.039
p-tolyl	-0.060	-0.061	-0.067	-0.068	-0.069	-0.064	-0.065	-0.065	-0.066
Phenol	-0.060	-0.066	-0.083	-0.136	-0.137	-0.146	-0.148	-0.166	-0.192
Phenolate	-0.382	-0.385	-0.485	-0.583	-0.567	-0.565	-0.571	-0.601	-0.632
Anilne	-0.137	-0.140	-0.162	-0.205	-0.204	-0.203	-0.215	-0.235	-0.259
tBuPh	-0.020	-0.019	-0.018	-0.014	-0.013	-0.014	-0.015	-0.011	-0.001
PhF	-0.005	-0.011	-0.015	-0.008	-0.011	-0.007	-0.005	0.007	0.027
PhCl	-0.038	-0.036	-0.028	-0.033	-0.034	-0.035	-0.036	-0.039	-0.036
PhBr	-0.053	-0.050	-0.044	-0.054	-0.053	-0.050	-0.052	-0.049	-0.045
PhI	-0.078	-0.080	-0.084	-0.096	-0.097	-0.096	-0.095	-0.105	-0.107
$PhNPh_2$	0.071	0.055	-0.001	-0.107	-0.102	-0.126	-0.147	-0.167	-0.180
Hydroxyl	0.003	0.002	-0.004	0.003	0.002	0.003	0.005	0.010	0.019
Hydroxylate	-0.061	-0.063	-0.077	-0.071	-0.070	-0.068	-0.061	-0.053	-0.039
methoxy	0.019	0.017	0.007	-0.007	-0.006	-0.010	-0.013	-0.015	-0.013
Ethoxy	0.054	0.052	0.057	0.045	0.047	0.037	0.034	0.038	0.044
Amine	0.058	0.051	0.033	0.019	0.018	0.013	0.014	0.010	0.003
protonated amine	0.008	0.004	-0.001	-0.030	-0.026	-0.038	-0.049	-0.068	-0.088
methyl amine	0.115	0.120	0.077	0.055	0.053	0.048	0.046	0.044	0.056
Dimethylamine	0.058	0.046	-0.012	-0.101	-0.098	-0.116	-0.132	-0.151	-0.164
Ethyl amine	0.255	0.220	0.157	0.145	0.144	0.125	0.124	0.154	0.220
diethylamine	0.049	0.024	-0.034	-0.112	-0.112	-0.132	-0.145	-0.165	-0.190
NPh_2	0.115	0.109	0.047	-0.026	-0.024	-0.038	-0.052	-0.072	-0.082
NHPh	-0.017	-0.010	-0.018	-0.019	-0.020	-0.022	-0.022	-0.036	-0.051

	Cyclo-hexane	Toluene	CH_2Cl_2	ACN	DMF	DMSO	Ethanol	Methanol	Water
piperidine	0.153	0.134	0.081	0.032	0.028	0.015	0.010	-0.001	-0.009
morpholine	0.120	0.110	0.060	-0.008	-0.008	-0.022	-0.025	-0.036	-0.046
acetyl	-0.009	-0.011	-0.014	-0.025	-0.023	-0.022	-0.022	-0.031	-0.037
phenyl ketone	-0.082	-0.081	-0.131	-0.234	-0.230	-0.246	-0.265	-0.292	-0.311
Acetic acid	0.001	0.002	0.004	0.007	0.007	0.008	0.010	0.016	0.025
acetate	-0.041	-0.038	-0.023	0.007	0.008	0.017	0.025	0.042	0.065
COOMe	-0.011	-0.010	-0.017	0.000	-0.001	0.005	0.011	0.025	0.045
COOEt	-0.013	-0.010	-0.015	-0.008	-0.007	-0.005	-0.005	0.003	0.028
COOtBu	0.010	0.005	-0.004	0.007	0.006	0.015	0.018	0.031	0.051
Fluorine	0.177	0.171	0.221	0.283	0.280	0.281	0.288	0.313	0.345
Chlorine	-0.012	-0.013	-0.024	-0.040	-0.039	-0.041	-0.043	-0.046	-0.042
Bromine	-0.087	-0.086	-0.099	-0.112	-0.112	-0.109	-0.105	-0.108	-0.109
Iodine	-0.174	-0.172	-0.199	-0.238	-0.235	-0.234	-0.238	-0.250	-0.262
$CONH_2$	0.132	0.118	0.117	0.150	0.149	0.146	0.166	0.187	0.209
nitrile	-0.026	-0.028	-0.056	-0.076	-0.075	-0.073	-0.066	-0.065	-0.059
nitro	-0.102	-0.097	-0.150	-0.223	-0.218	-0.224	-0.233	-0.245	-0.252
Sulfonyl	0.109	0.103	0.080	0.079	0.079	0.077	0.083	0.088	0.104
Sulfonate	0.054	0.058	0.059	0.055	0.055	0.053	0.055	0.063	0.077
CF_3	0.000	-0.004	-0.029	-0.054	-0.054	-0.057	-0.061	-0.068	-0.074
CF_2CF_3	-0.023	-0.021	-0.024	-0.011	-0.009	-0.006	-0.004	0.006	0.014

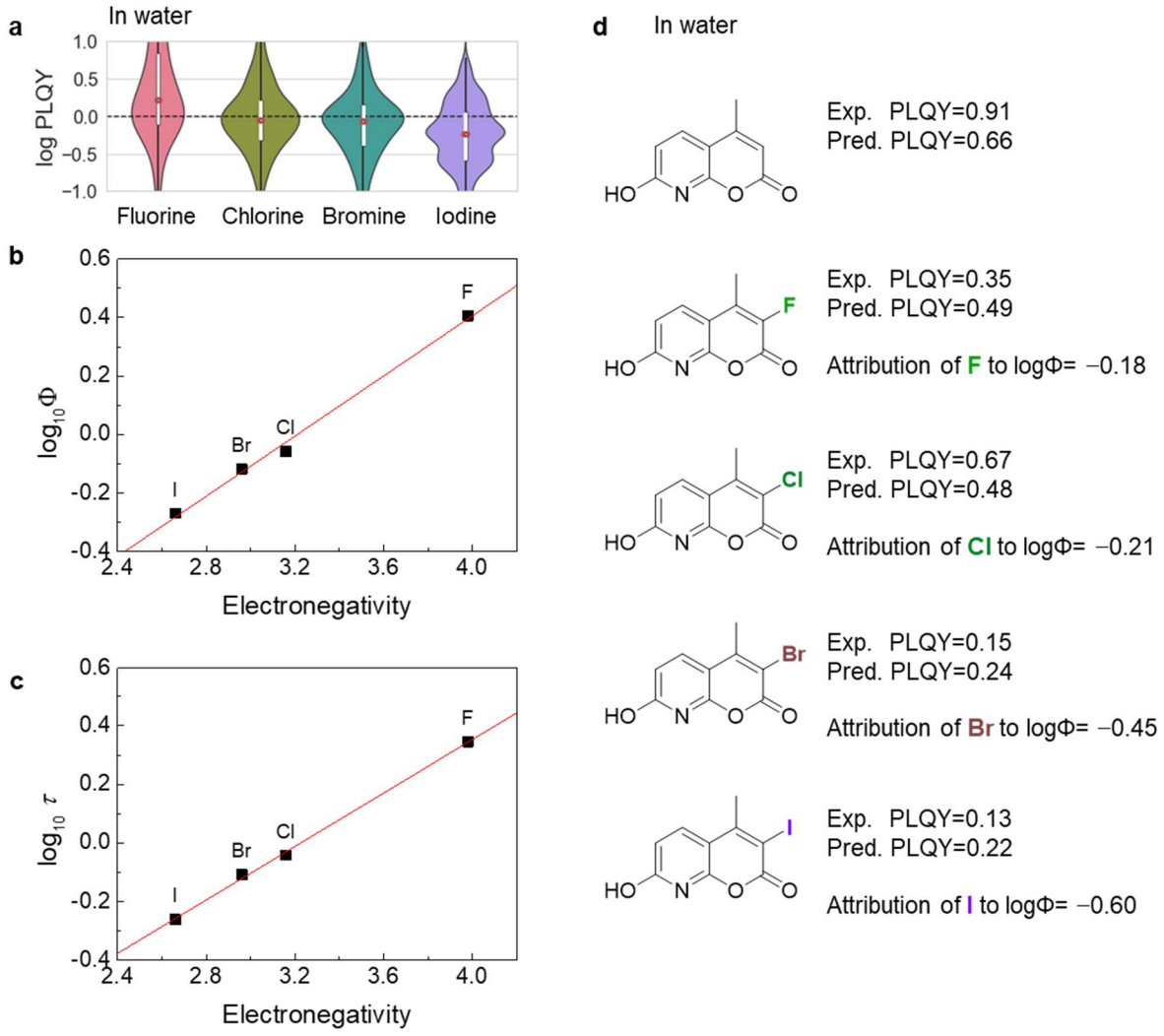


Figure S10. **a**. The violin plots of the attribution of halogen groups in water to log Φ. **b**. The plot of average attribution to log Φ versus the electronegativity in the Pauling scale. **c**. The plot of average attribution to log τ versus the electronegativity in the Pauling scale. **d**. The experimental and predicted PLQYs of 8-aza-coumarin derivatives with the attributions of halogen groups to log Φ.

Table S12. Tuning the optical properties based on the attributions of functional groups.

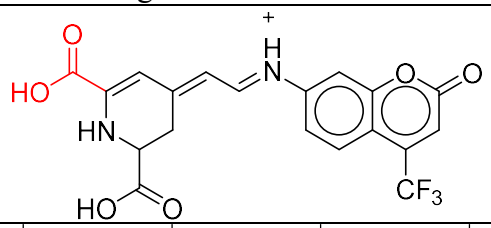
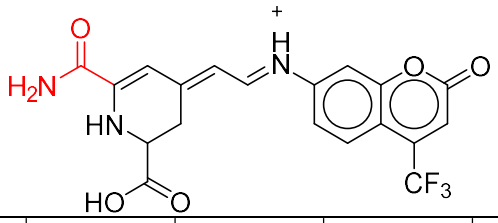
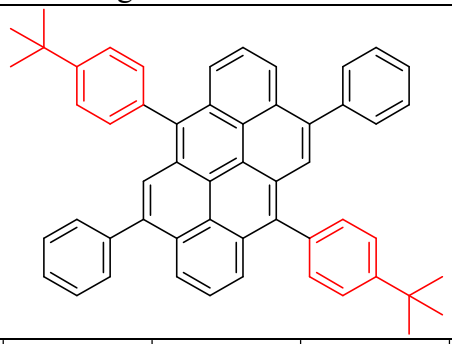
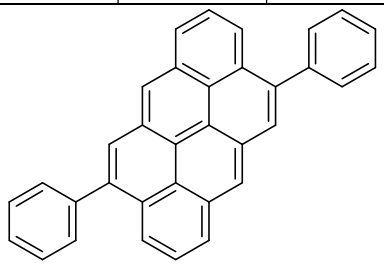
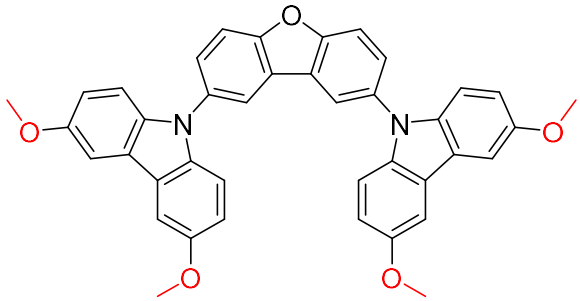
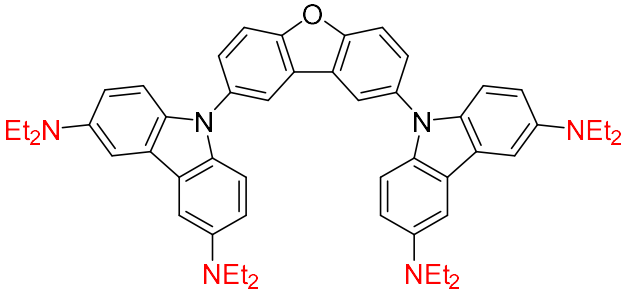
Figure 5a							
Structure							
Property	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ
Pred.	519	2751	4.77	**581**	1675	0.03	0.11
Exp.	519	2867	4.81	**570**	1815	0.02	0.10
Structure							
Property	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ
Pred.	490	3088	4.83	**557**	1873	0.02	0.11
Exp.	-	-	-	**-**	-	-	-
Figure 5c							
Structure							
Property	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ
Pred.	463	2287	4.71	483	**1554**	0.29	3.10
Exp.	454	2322	4.87	465	**1316**	0.26	2.98
Structure							
Property	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ
Pred.	438	595	4.58	449	**864**	0.37	4.80
Exp.	439	925	4.68	442	**692**	0.33	4.21

Figure 5e							
Structure							
Property	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ
Pred.	319	6368	4.14		2955	**0.353**	7.9
Exp.	-	-	-	-	-	-	-
Structure							
Property	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi} (cm^{-1})	Φ	τ
Pred.	390	4461	4.35		3194	**0.718**	4.0
Exp.	-	-	-	-	-	-	-

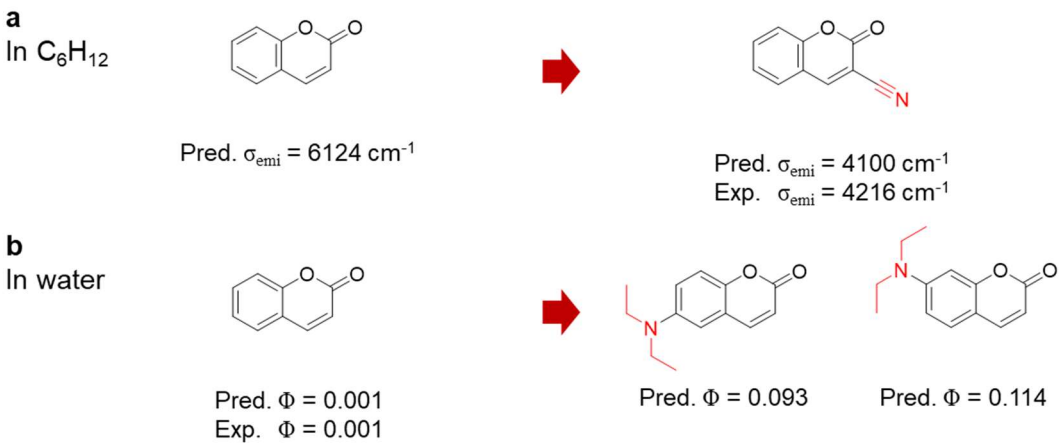


Figure S11. Tuning the optical properties based on the attributions of functional groups. **a** and **b**. Addition of functional groups.

Table S13. Average attribution of functional groups in cyclohexane.

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	3.4	-52	0.013	2.3	-35	0.018	0.015
Ethyl	4.7	45	0.012	4.9	-28	-0.046	-0.012
Propyl	22.9	13	-0.001	18.7	-94	-0.044	-0.019
Butyl	2.0	-33	0.009	1.7	-17	-0.003	-0.003
Isopropyl	5.5	-116	-0.021	3.9	-59	-0.007	0.029
t-Butyl	5.7	-36	0.011	6.1	-27	-0.020	-0.006
cyclohexyl	-0.6	41	-0.038	0.6	4	0.092	0.068
ethene	-2.1	231	-0.054	0.9	14	0.038	0.066
dimethylethene	4.0	-344	0.001	-0.5	72	-0.191	-0.119
Ethyne	-1.9	-44	0.034	-3.8	-56	0.020	-0.064
methylethyne	5.7	-892	0.099	-16.5	-629	0.482	0.348
Phenyl	10.7	-29	0.006	12.3	-59	0.015	0.015
p-tolyl	8.5	37	0.044	11.7	-22	-0.030	-0.060
Phenol	15.6	-341	0.134	15.1	-99	-0.004	-0.060
Phenolate	132.4	-506	0.162	128.4	17	-0.632	-0.382
Anilne	18.4	-191	0.150	22.9	-78	-0.005	-0.137
tBuPh	8.0	125	0.018	9.8	-6	-0.023	-0.020
PhF	2.7	157	0.031	4.2	-34	0.051	-0.005
PhCl	3.0	201	0.000	8.3	59	-0.037	-0.038
PhBr	13.5	-40	0.002	13.6	-52	-0.073	-0.053
PhI	8.4	-160	0.025	6.5	-33	-0.022	-0.078
$PhNPh_2$	22.7	32	0.163	32.4	-207	0.217	0.071
Hydroxyl	5.6	-45	0.017	5.0	-45	0.016	0.003
Hydroxylate	36.0	-463	0.067	26.4	-220	-0.083	-0.061
methoxy	3.6	-41	0.009	4.4	-28	0.029	0.019
Ethoxy	-2.3	-72	-0.020	-1.2	-77	0.070	0.054
Amine	16.0	-324	0.056	14.1	-154	0.065	0.058
protonated amine	-1.5	-238	0.040	-5.8	-77	0.086	0.008
methyl amine	22.4	-64	-0.087	23.3	-248	0.192	0.115
Dimethylamine	36.9	-373	0.130	39.3	-395	0.140	0.058
Ethyl amine	70.1	-905	0.321	54.3	-860	0.510	0.255
diethylamine	51.7	-792	0.257	42.9	-723	0.267	0.049
NPh_2	30.5	-268	-0.004	35.7	-217	0.119	0.115
NHPh	13.9	73	-0.013	18.4	19	-0.106	-0.017
piperidine	42.8	-424	0.157	43.3	-470	0.228	0.153
morpholine	29.7	-66	0.025	34.7	-328	-0.031	0.120

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	18.6	-253	-0.047	16.4	-89	-0.066	-0.009
phenyl ketone	20.9	-189	-0.017	24.6	-103	0.029	-0.082
Acetic acid	6.0	-27	0.017	5.8	-18	-0.023	0.001
acetate	6.2	47	-0.026	1.7	-46	-0.095	-0.041
COOMe	4.2	13	-0.007	5.3	7	0.018	-0.011
COOEt	-1.5	143	-0.038	1.4	154	-0.047	-0.013
COOtBu	-3.5	129	-0.074	-0.4	60	0.040	0.010
Fluorine	23.1	-549	0.090	12.1	-347	0.173	0.177
Chlorine	13.4	-192	-0.003	11.9	-81	-0.023	-0.012
Bromine	9.6	-90	-0.002	10.0	-43	-0.100	-0.087
Iodine	8.7	-132	0.005	9.6	58	-0.185	-0.174
CONH2	1.1	-796	0.024	-4.9	57	-0.067	0.132
nitrile	25.8	-110	-0.039	28.3	-133	-0.122	-0.026
nitro	23.9	362	0.019	30.9	-52	-0.282	-0.102
Sulfonyl	-6.1	-154	-0.223	-8.4	23	-0.027	0.109
Sulfonate	1.8	-80	0.008	2.6	-26	0.051	0.054
CF_3	6.1	-53	0.006	7.1	-32	-0.006	0.000
CF_2CF_3	-5.1	125	-0.005	-4.9	24	-0.013	-0.023

Table S14. Average attribution of functional groups in toluene.

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	3.1	-52	0.013	2.2	-31	0.012	0.012
Ethyl	4.7	45	0.012	5.2	-29	-0.042	-0.012
Propyl	22.7	13	0.000	18.5	-93	-0.051	-0.025
Butyl	2.1	-33	0.009	1.8	-17	-0.005	-0.004
Isopropyl	5.3	-116	-0.022	3.6	-59	-0.012	0.025
t-Butyl	5.7	-36	0.012	6.1	-29	-0.024	-0.008
cyclohexyl	-0.1	41	-0.037	1.1	9	0.079	0.063
ethene	-1.8	231	-0.058	1.2	9	0.038	0.071
dimethylethene	4.4	-344	0.005	-1.2	59	-0.177	-0.118
Ethyne	-2.2	-44	0.034	-4.8	-45	0.007	-0.072
methylethyne	5.7	-892	0.088	-17.6	-593	0.438	0.323
Phenyl	10.7	-29	0.006	12.6	-59	0.006	0.011
p-tolyl	8.4	37	0.044	11.9	-29	-0.036	-0.061
Phenol	15.6	-341	0.139	14.1	-105	-0.010	-0.066
Phenolate	135.9	-506	0.170	132.2	-30	-0.678	-0.385
Anilne	19.2	-191	0.155	23.4	-97	-0.020	-0.140
tBuPh	8.2	125	0.020	10.2	-11	-0.024	-0.019
PhF	2.3	157	0.031	3.7	-41	0.038	-0.011
PhCl	3.0	201	-0.002	8.8	51	-0.039	-0.036
PhBr	13.3	-40	0.003	13.8	-59	-0.070	-0.050
PhI	7.2	-160	0.025	5.6	-26	-0.030	-0.080
$PhNPh_2$	22.5	32	0.158	34.8	-186	0.167	0.055
Hydroxyl	5.5	-45	0.017	5.1	-45	0.012	0.002
Hydroxylate	35.9	-463	0.069	26.4	-219	-0.087	-0.063
methoxy	3.6	-41	0.009	4.6	-26	0.022	0.017
Ethoxy	-2.7	-72	-0.023	-0.9	-78	0.063	0.052
Amine	16.0	-324	0.055	13.7	-153	0.054	0.051
protonated amine	-1.7	-238	0.040	-6.6	-65	0.070	0.004
methyl amine	23.7	-64	-0.090	25.1	-261	0.175	0.120
Dimethylamine	37.9	-373	0.125	42.2	-383	0.103	0.046
Ethyl amine	69.4	-905	0.318	52.5	-823	0.440	0.220
diethylamine	52.1	-792	0.255	43.6	-696	0.220	0.024
NPh_2	31.1	-268	-0.008	38.8	-208	0.091	0.109
NHPh	14.5	73	-0.014	20.2	21	-0.102	-0.010
piperidine	42.5	-424	0.147	43.8	-452	0.187	0.134
morpholine	31.0	-66	0.020	36.7	-329	-0.058	0.110

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	18.2	-253	-0.047	17.0	-87	-0.080	-0.011
phenyl ketone	21.2	-189	-0.014	25.3	-126	0.019	-0.081
Acetic acid	5.9	-27	0.017	5.7	-20	-0.021	0.002
acetate	5.8	47	-0.025	1.1	-50	-0.091	-0.038
COOMe	4.2	13	-0.007	5.2	1	0.013	-0.010
COOEt	-1.6	143	-0.039	1.5	143	-0.047	-0.010
COOtBu	-4.2	129	-0.076	-0.5	62	0.025	0.005
Fluorine	22.6	-549	0.088	11.7	-328	0.164	0.171
Chlorine	13.7	-192	-0.004	12.5	-84	-0.028	-0.013
Bromine	9.7	-90	0.000	10.4	-51	-0.100	-0.086
Iodine	8.7	-132	0.009	9.5	48	-0.179	-0.172
CONH2	1.0	-796	0.028	-6.9	62	-0.063	0.118
nitrile	26.0	-110	-0.038	29.6	-141	-0.131	-0.028
nitro	25.6	362	0.024	34.7	-69	-0.284	-0.097
Sulfonyl	-6.8	-154	-0.226	-9.2	31	-0.033	0.103
Sulfonate	1.5	-80	0.010	2.4	-27	0.054	0.058
CF_3	6.5	-53	0.006	7.7	-32	-0.014	-0.004
CF_2CF_3	-5.4	125	-0.007	-5.1	20	-0.008	-0.021

Table S15. Average attribution of functional groups in dichloromethane (CH_2Cl_2).

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.8	-48	0.013	2.2	-25	0.014	0.011
Ethyl	4.3	50	0.013	5.2	-26	-0.040	-0.008
Propyl	22.6	7	-0.002	18.3	-108	-0.052	-0.026
Butyl	2.3	-32	0.009	2.0	-14	-0.012	-0.008
Isopropyl	4.7	-109	-0.025	2.0	-66	-0.016	0.020
t-Butyl	5.9	-35	0.012	6.1	-32	-0.023	-0.010
cyclohexyl	0.3	52	-0.038	3.0	37	0.026	0.035
ethene	-1.3	210	-0.052	0.4	-21	0.028	0.065
dimethylethene	5.6	-334	0.009	-2.3	19	-0.155	-0.094
Ethyne	-2.4	-53	0.025	-7.4	-54	0.002	-0.088
methylethyne	5.1	-942	0.091	-20.9	-592	0.477	0.322
Phenyl	10.6	-21	0.005	14.0	-52	-0.025	-0.007
p-tolyl	8.5	51	0.042	13.7	-32	-0.047	-0.067
Phenol	16.5	-317	0.141	14.1	-112	-0.047	-0.083
Phenolate	136.9	-387	0.174	137.7	-30	-0.815	-0.485
Anilne	20.9	-161	0.152	28.7	-69	-0.068	-0.162
tBuPh	8.7	120	0.022	10.4	-21	-0.022	-0.018
PhF	3.0	148	0.031	4.8	-45	0.034	-0.015
PhCl	3.1	209	-0.001	11.7	46	-0.044	-0.028
PhBr	12.8	-36	0.006	14.9	-82	-0.061	-0.044
PhI	6.3	-153	0.017	5.3	-19	-0.016	-0.084
$PhNPh_2$	23.9	88	0.151	44.6	-110	0.052	-0.001
Hydroxyl	5.6	-42	0.016	5.4	-45	0.011	-0.004
Hydroxylate	34.3	-446	0.070	26.5	-182	-0.108	-0.077
methoxy	4.0	-37	0.009	5.5	-17	0.009	0.007
Ethoxy	-3.0	-70	-0.025	-0.1	-71	0.057	0.057
Amine	16.7	-296	0.053	14.1	-163	0.023	0.033
protonated amine	-1.4	-241	0.040	-7.6	-8	0.046	-0.001
methyl amine	26.3	-59	-0.094	26.9	-285	0.129	0.077
Dimethylamine	39.9	-314	0.116	49.7	-342	0.005	-0.012
Ethyl amine	71.4	-878	0.297	50.7	-779	0.363	0.157
diethylamine	54.3	-748	0.236	45.7	-668	0.138	-0.034
NPh_2	32.0	-214	-0.011	44.8	-155	0.012	0.047
NHPh	12.8	110	-0.007	24.4	85	-0.148	-0.018
piperidine	43.2	-380	0.132	45.3	-436	0.104	0.081
morpholine	32.7	-52	0.018	39.1	-344	-0.163	0.060

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	18.1	-234	-0.045	19.6	-67	-0.078	-0.014
phenyl ketone	23.7	-179	-0.018	29.6	-143	-0.050	-0.131
Acetic acid	5.2	-24	0.017	5.3	-27	-0.018	0.004
acetate	5.4	44	-0.023	-0.2	-64	-0.062	-0.023
COOMe	4.3	16	-0.007	6.1	-8	0.016	-0.017
COOEt	-1.9	134	-0.037	1.9	140	-0.047	-0.015
COOtBu	-4.2	96	-0.077	0.3	50	0.028	-0.004
Fluorine	20.6	-526	0.091	9.8	-318	0.226	0.221
Chlorine	14.0	-186	-0.007	13.2	-88	-0.043	-0.024
Bromine	9.9	-83	-0.001	11.3	-58	-0.111	-0.099
Iodine	9.1	-119	0.007	10.4	44	-0.203	-0.199
CONH2	1.4	-777	0.047	-14.7	35	-0.009	0.117
nitrile	26.1	-93	-0.039	31.2	-153	-0.161	-0.056
nitro	27.5	394	0.030	40.7	-60	-0.373	-0.150
Sulfonyl	-7.5	-158	-0.230	-11.5	22	-0.064	0.080
Sulfonate	1.4	-72	0.010	2.5	-20	0.047	0.059
CF_3	7.0	-40	0.004	9.4	-16	-0.059	-0.029
CF_2CF_3	-5.6	125	-0.008	-4.6	23	-0.006	-0.024

Table S16. Average attribution of functional groups in acetonitrile (ACN).

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.6	-48	0.013	1.9	-25	0.029	0.021
Ethyl	3.9	53	0.013	4.9	-29	-0.038	-0.007
Propyl	21.3	8	0.002	17.5	-147	0.011	0.015
Butyl	2.3	-31	0.009	2.0	-14	-0.014	-0.010
Isopropyl	4.5	-112	-0.026	0.8	-73	0.003	0.032
t-Butyl	5.8	-34	0.013	6.1	-40	-0.011	-0.004
cyclohexyl	-0.2	54	-0.037	3.6	43	0.047	0.052
ethene	-0.6	205	-0.052	-0.1	-67	0.035	0.060
dimethylethene	7.0	-350	0.013	-3.5	-17	-0.098	-0.053
Ethyne	-3.0	-54	0.021	-8.7	-80	0.018	-0.084
methylethyne	4.3	-945	0.087	-22.5	-612	0.632	0.418
Phenyl	10.5	-22	0.006	14.6	-52	-0.050	-0.027
p-tolyl	8.5	50	0.044	14.3	-33	-0.045	-0.068
Phenol	17.7	-326	0.137	14.8	-133	-0.110	-0.136
Phenolate	128.7	-384	0.189	135.4	-65	-0.859	-0.583
Anilne	22.9	-166	0.152	31.4	-59	-0.126	-0.205
tBuPh	9.0	118	0.024	10.6	-37	-0.010	-0.014
PhF	4.0	134	0.034	5.5	-67	0.052	-0.008
PhCl	3.7	207	0.001	13.8	35	-0.050	-0.033
PhBr	12.3	-42	0.008	15.0	-110	-0.065	-0.054
PhI	6.2	-154	0.013	5.3	-23	-0.026	-0.096
$PhNPh_2$	23.7	121	0.145	50.6	-64	-0.098	-0.107
Hydroxyl	5.4	-41	0.017	5.2	-50	0.026	0.003
Hydroxylate	31.9	-433	0.071	25.7	-178	-0.096	-0.071
methoxy	4.0	-34	0.009	6.2	-11	-0.008	-0.007
Ethoxy	-3.1	-74	-0.027	0.2	-73	0.035	0.045
Amine	17.0	-288	0.050	13.9	-160	0.009	0.019
protonated amine	0.1	-248	0.038	-8.1	4	0.021	-0.030
methyl amine	27.2	-69	-0.094	26.8	-312	0.122	0.055
Dimethylamine	39.9	-279	0.108	53.7	-318	-0.113	-0.101
Ethyl amine	70.8	-860	0.277	48.1	-751	0.353	0.145
diethylamine	54.5	-707	0.219	47.2	-664	0.043	-0.112
NPh_2	30.8	-192	-0.012	47.0	-114	-0.082	-0.026
NHPh	9.9	125	0.000	24.4	136	-0.172	-0.019
piperidine	42.9	-367	0.121	45.1	-434	0.040	0.032
morpholine	32.2	-44	0.017	39.9	-358	-0.260	-0.008

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	18.1	-243	-0.043	20.1	-76	-0.075	-0.025
phenyl ketone	24.7	-193	-0.022	32.3	-172	-0.175	-0.234
Acetic acid	4.7	-25	0.017	4.5	-39	-0.007	0.007
acetate	4.3	40	-0.020	-1.6	-101	-0.005	0.007
COOMe	4.3	9	-0.005	6.0	-29	0.053	0.000
COOEt	-2.2	122	-0.033	1.8	125	-0.029	-0.008
COOtBu	-4.2	84	-0.076	0.1	-4	0.067	0.007
Fluorine	19.6	-504	0.090	7.8	-322	0.315	0.283
Chlorine	13.8	-182	-0.008	13.4	-99	-0.055	-0.040
Bromine	9.6	-82	0.001	11.6	-64	-0.120	-0.112
Iodine	8.9	-118	0.006	11.0	34	-0.248	-0.238
CONH2	1.6	-784	0.050	-20.3	32	0.070	0.150
nitrile	25.4	-92	-0.038	31.0	-179	-0.165	-0.076
nitro	26.8	415	0.035	44.0	-47	-0.461	-0.223
Sulfonyl	-8.5	-162	-0.233	-13.7	19	-0.062	0.079
Sulfonate	1.9	-65	0.007	2.4	-21	0.039	0.055
CF_3	7.0	-38	0.004	10.1	1	-0.097	-0.054
CF_2CF_3	-6.1	126	-0.008	-4.7	13	0.011	-0.011

Table S17. Average attribution of functional groups in *N*,*N*-dimethylforamide (DMF).

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.5	-48	0.013	1.9	-23	0.029	0.021
Ethyl	4.0	52	0.013	5.0	-30	-0.038	-0.008
Propyl	21.2	12	0.002	17.7	-147	0.011	0.012
Butyl	2.3	-32	0.009	2.0	-13	-0.014	-0.010
Isopropyl	4.3	-111	-0.026	0.9	-71	0.001	0.030
t-Butyl	5.7	-34	0.013	6.1	-40	-0.011	-0.005
cyclohexyl	-0.1	51	-0.036	3.2	43	0.051	0.056
ethene	-0.9	210	-0.052	-0.1	-70	0.034	0.060
dimethylethene	7.0	-353	0.015	-3.3	-16	-0.100	-0.056
Ethyne	-3.1	-55	0.020	-8.6	-79	0.016	-0.084
methylethyne	3.4	-934	0.083	-23.3	-600	0.635	0.422
Phenyl	10.6	-26	0.006	14.5	-52	-0.048	-0.026
p-tolyl	8.6	45	0.045	14.3	-35	-0.044	-0.069
Phenol	17.6	-331	0.137	14.7	-132	-0.108	-0.137
Phenolate	132.8	-450	0.199	137.2	-66	-0.829	-0.567
Anilne	23.0	-172	0.154	31.1	-63	-0.120	-0.204
tBuPh	8.9	119	0.025	10.5	-39	-0.008	-0.013
PhF	3.9	134	0.034	5.6	-65	0.049	-0.011
PhCl	3.7	201	0.003	13.4	31	-0.047	-0.034
PhBr	12.6	-45	0.009	15.0	-113	-0.062	-0.053
PhI	6.2	-156	0.014	5.4	-21	-0.026	-0.097
$PhNPh_2$	24.0	110	0.146	49.8	-66	-0.087	-0.102
Hydroxyl	5.4	-41	0.017	5.2	-48	0.025	0.002
Hydroxylate	32.4	-441	0.071	26.0	-175	-0.095	-0.070
methoxy	4.0	-36	0.009	6.0	-12	-0.007	-0.006
Ethoxy	-3.3	-76	-0.027	-0.3	-73	0.040	0.047
Amine	16.9	-292	0.050	14.0	-155	0.009	0.018
protonated amine	-0.1	-250	0.038	-8.1	4	0.027	-0.026
methyl amine	27.4	-80	-0.093	26.8	-313	0.122	0.053
Dimethylamine	40.3	-289	0.108	53.4	-318	-0.107	-0.098
Ethyl amine	70.3	-855	0.275	48.8	-727	0.343	0.144
diethylamine	54.5	-708	0.217	47.5	-656	0.042	-0.112
NPh_2	31.4	-202	-0.013	46.9	-116	-0.079	-0.024
NHPh	10.4	121	0.001	24.3	134	-0.170	-0.020
piperidine	42.9	-371	0.121	45.1	-431	0.037	0.028
morpholine	32.5	-45	0.016	39.7	-362	-0.257	-0.008

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	18.2	-251	-0.042	19.9	-78	-0.070	-0.023
phenyl ketone	24.8	-206	-0.020	31.6	-182	-0.166	-0.230
Acetic acid	4.8	-27	0.018	4.7	-37	-0.007	0.007
acetate	4.3	43	-0.021	-1.4	-98	-0.005	0.008
COOMe	4.3	5	-0.004	6.0	-30	0.054	-0.001
COOEt	-2.2	118	-0.032	1.6	124	-0.027	-0.007
COOtBu	-4.4	85	-0.075	-0.2	-7	0.067	0.006
Fluorine	19.5	-499	0.088	8.3	-313	0.308	0.280
Chlorine	13.9	-186	-0.008	13.4	-100	-0.053	-0.039
Bromine	9.8	-86	0.002	11.6	-67	-0.119	-0.112
Iodine	9.1	-123	0.008	10.8	29	-0.242	-0.235
CONH2	0.9	-780	0.048	-19.4	45	0.065	0.149
nitrile	25.7	-97	-0.038	31.1	-181	-0.162	-0.075
nitro	27.5	408	0.036	43.9	-55	-0.449	-0.218
Sulfonyl	-8.6	-161	-0.234	-13.7	18	-0.062	0.079
Sulfonate	1.8	-66	0.008	2.4	-23	0.040	0.055
CF_3	7.2	-40	0.004	10.1	1	-0.096	-0.054
CF_2CF_3	-6.2	129	-0.008	-4.9	13	0.014	-0.009

Table S18. Average attribution of functional groups in dimethyl sulfoxide (DMSO).

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.4	-47	0.013	1.7	-25	0.029	0.022
Ethyl	3.9	51	0.012	5.0	-30	-0.034	-0.007
Propyl	20.9	2	0.002	17.0	-150	0.028	0.025
Butyl	2.4	-31	0.009	2.1	-14	-0.015	-0.011
Isopropyl	4.4	-109	-0.025	0.6	-74	0.007	0.033
t-Butyl	5.5	-31	0.013	5.9	-39	-0.009	-0.003
cyclohexyl	-0.6	56	-0.037	3.4	47	0.035	0.044
ethene	-0.5	194	-0.052	-0.2	-72	0.034	0.057
dimethylethene	7.0	-352	0.016	-3.7	-16	-0.077	-0.050
Ethyne	-3.5	-51	0.023	-9.1	-78	0.021	-0.077
methylethyne	4.2	-931	0.082	-22.3	-615	0.620	0.414
Phenyl	10.3	-22	0.005	14.3	-49	-0.056	-0.029
p-tolyl	8.2	49	0.044	14.0	-31	-0.044	-0.064
Phenol	17.0	-328	0.134	13.8	-126	-0.122	-0.146
Phenolate	125.9	-429	0.195	133.0	-109	-0.829	-0.565
Anilne	22.4	-167	0.152	30.9	-59	-0.130	-0.203
tBuPh	8.8	112	0.025	10.4	-41	-0.008	-0.014
PhF	3.5	136	0.032	5.0	-62	0.047	-0.007
PhCl	3.3	206	-0.001	13.4	39	-0.053	-0.035
PhBr	12.2	-43	0.008	14.9	-114	-0.060	-0.050
PhI	5.7	-149	0.016	4.9	-23	-0.040	-0.096
$PhNPh_2$	22.8	116	0.139	49.8	-51	-0.136	-0.126
Hydroxyl	5.3	-40	0.017	5.0	-50	0.025	0.003
Hydroxylate	31.4	-436	0.072	25.3	-180	-0.094	-0.068
methoxy	3.8	-34	0.009	6.1	-10	-0.015	-0.010
Ethoxy	-3.4	-72	-0.028	0.0	-67	0.023	0.037
Amine	16.7	-284	0.049	13.4	-150	0.002	0.013
protonated amine	0.2	-245	0.037	-8.0	6	0.000	-0.038
methyl amine	26.6	-74	-0.091	26.3	-307	0.091	0.048
Dimethylamine	39.5	-282	0.104	53.4	-304	-0.146	-0.116
Ethyl amine	69.8	-868	0.269	46.7	-728	0.298	0.125
diethylamine	54.3	-707	0.213	46.8	-642	0.000	-0.132
NPh_2	30.6	-193	-0.011	46.6	-110	-0.114	-0.038
NHPh	9.5	113	-0.001	24.2	140	-0.167	-0.022
piperidine	42.3	-370	0.116	44.0	-420	0.010	0.015
morpholine	32.1	-49	0.014	39.5	-342	-0.265	-0.022

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	17.5	-237	-0.041	19.6	-77	-0.078	-0.022
phenyl ketone	23.8	-193	-0.023	31.2	-166	-0.202	-0.246
Acetic acid	4.6	-28	0.017	4.4	-40	-0.005	0.008
acetate	4.1	41	-0.018	-1.8	-106	0.013	0.017
COOMe	3.8	9	-0.003	5.5	-34	0.056	0.005
COOEt	-2.7	120	-0.033	1.2	120	-0.026	-0.005
COOtBu	-4.9	89	-0.073	-0.5	-4	0.068	0.015
Fluorine	19.6	-497	0.088	7.6	-317	0.314	0.281
Chlorine	13.7	-184	-0.007	13.3	-101	-0.059	-0.041
Bromine	9.4	-80	0.002	11.5	-65	-0.119	-0.109
Iodine	8.8	-113	0.009	11.0	30	-0.243	-0.234
CONH2	2.0	-775	0.050	-20.7	27	0.077	0.146
nitrile	25.1	-91	-0.036	30.5	-182	-0.159	-0.073
nitro	27.0	399	0.035	44.1	-47	-0.453	-0.224
Sulfonyl	-8.6	-154	-0.231	-14.0	19	-0.059	0.077
Sulfonate	2.2	-63	0.006	2.7	-20	0.039	0.053
CF_3	7.0	-38	0.003	10.1	2	-0.102	-0.057
CF_2CF_3	-6.3	128	-0.007	-4.6	11	0.018	-0.006

Table S19. Average attribution of functional groups in ethanol.

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.4	-54	0.014	1.6	-32	0.033	0.025
Ethyl	3.6	55	0.013	4.7	-32	-0.033	-0.006
Propyl	18.8	-13	0.006	15.5	-197	0.056	0.039
Butyl	2.4	-32	0.009	2.1	-14	-0.015	-0.010
Isopropyl	4.4	-120	-0.025	0.4	-77	0.014	0.039
t-Butyl	5.7	-34	0.013	6.0	-46	-0.005	0.000
cyclohexyl	-1.3	46	-0.039	3.4	43	0.028	0.037
ethene	-0.6	210	-0.054	-0.3	-78	0.035	0.056
dimethylethene	5.4	-352	0.015	-4.7	-19	-0.057	-0.034
Ethyne	-3.1	-57	0.024	-9.0	-93	0.033	-0.069
methylethyne	4.7	-955	0.083	-21.9	-650	0.617	0.426
Phenyl	10.0	-25	0.006	14.3	-49	-0.059	-0.033
p-tolyl	8.2	53	0.045	14.5	-31	-0.043	-0.065
Phenol	17.4	-326	0.137	14.6	-127	-0.123	-0.148
Phenolate	104.9	-313	0.215	122.6	-159	-0.761	-0.571
Anilne	22.8	-160	0.152	32.3	-46	-0.142	-0.215
tBuPh	8.6	122	0.024	10.2	-48	-0.006	-0.015
PhF	3.9	129	0.036	5.4	-68	0.055	-0.005
PhCl	3.4	212	0.000	14.2	45	-0.053	-0.036
PhBr	12.0	-40	0.008	14.7	-115	-0.059	-0.052
PhI	6.2	-156	0.014	5.6	-26	-0.039	-0.095
$PhNPh_2$	23.0	108	0.143	51.6	-59	-0.156	-0.147
Hydroxyl	5.2	-44	0.017	4.9	-56	0.029	0.005
Hydroxylate	28.6	-425	0.075	23.7	-201	-0.073	-0.061
methoxy	3.8	-34	0.009	6.4	-9	-0.020	-0.013
Ethoxy	-2.2	-75	-0.027	1.3	-68	0.017	0.034
Amine	17.0	-311	0.053	13.7	-162	0.005	0.014
protonated amine	0.6	-242	0.037	-7.3	13	-0.014	-0.049
methyl amine	25.9	-79	-0.090	26.3	-312	0.090	0.046
Dimethylamine	39.0	-295	0.109	54.2	-314	-0.159	-0.132
Ethyl amine	69.6	-904	0.279	45.4	-793	0.313	0.124
diethylamine	55.0	-734	0.219	47.6	-678	-0.009	-0.145
NPh_2	29.1	-216	-0.009	46.4	-113	-0.124	-0.052
NHPh	7.3	125	0.002	23.7	159	-0.169	-0.022
piperidine	42.1	-400	0.120	44.1	-439	0.008	0.010
morpholine	31.2	-66	0.020	39.3	-352	-0.266	-0.025

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	15.9	-237	-0.037	19.3	-92	-0.070	-0.022
phenyl ketone	24.2	-176	-0.022	33.1	-152	-0.223	-0.265
Acetic acid	4.2	-27	0.017	3.7	-45	0.001	0.010
acetate	3.4	30	-0.015	-2.6	-126	0.030	0.025
COOMe	3.8	7	-0.003	5.3	-39	0.068	0.011
COOEt	-2.8	129	-0.033	1.4	123	-0.023	-0.005
COOtBu	-4.5	86	-0.075	0.3	-21	0.075	0.018
Fluorine	19.5	-520	0.089	6.4	-344	0.325	0.288
Chlorine	12.9	-176	-0.007	12.9	-105	-0.059	-0.043
Bromine	8.9	-79	0.002	11.6	-62	-0.116	-0.105
Iodine	8.5	-107	0.008	11.5	38	-0.248	-0.238
CONH2	3.8	-812	0.052	-22.0	13	0.096	0.166
nitrile	24.3	-102	-0.033	30.1	-197	-0.146	-0.066
nitro	24.4	419	0.040	43.4	-45	-0.462	-0.233
Sulfonyl	-8.7	-169	-0.231	-14.1	15	-0.055	0.083
Sulfonate	2.6	-66	0.004	2.6	-19	0.041	0.055
CF_3	6.8	-42	0.004	10.1	6	-0.106	-0.061
CF_2CF_3	-6.2	124	-0.005	-4.4	7	0.020	-0.004

Table S20. Average attribution of functional groups in methanol.

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.3	-59	0.015	1.5	-33	0.041	0.031
Ethyl	3.5	58	0.013	4.7	-33	-0.030	-0.004
Propyl	18.3	-14	0.007	15.0	-200	0.078	0.055
Butyl	2.3	-34	0.010	2.0	-14	-0.013	-0.009
Isopropyl	4.5	-127	-0.023	0.2	-75	0.024	0.047
t-Butyl	5.7	-36	0.014	6.0	-50	0.004	0.005
cyclohexyl	-1.7	36	-0.038	3.4	44	0.017	0.030
ethene	-0.7	209	-0.054	-0.6	-86	0.037	0.058
dimethylethene	5.3	-353	0.016	-5.0	-13	-0.050	-0.031
Ethyne	-2.9	-58	0.026	-8.9	-102	0.048	-0.057
methylethyne	4.3	-956	0.087	-23.0	-657	0.677	0.473
Phenyl	10.0	-35	0.006	14.4	-49	-0.062	-0.037
p-tolyl	8.3	48	0.045	14.7	-32	-0.041	-0.065
Phenol	18.0	-343	0.134	15.0	-125	-0.141	-0.166
Phenolate	101.3	-367	0.215	120.6	-151	-0.799	-0.601
Anilne	22.9	-165	0.151	33.2	-40	-0.165	-0.235
tBuPh	8.6	119	0.024	9.8	-55	0.002	-0.011
PhF	4.3	118	0.036	5.2	-76	0.072	0.007
PhCl	3.5	204	0.000	14.4	44	-0.053	-0.039
PhBr	12.3	-46	0.009	14.6	-123	-0.050	-0.049
PhI	6.5	-164	0.014	6.3	-27	-0.051	-0.105
$PhNPh_2$	22.5	92	0.141	52.0	-62	-0.181	-0.167
Hydroxyl	5.0	-48	0.018	4.6	-58	0.036	0.010
Hydroxylate	27.8	-439	0.076	23.0	-203	-0.063	-0.053
methoxy	3.7	-37	0.009	6.3	-9	-0.023	-0.015
Ethoxy	-2.2	-77	-0.027	1.3	-67	0.021	0.038
Amine	17.1	-336	0.053	13.6	-158	0.001	0.010
protonated amine	0.5	-251	0.037	-7.5	17	-0.039	-0.068
methyl amine	25.1	-96	-0.089	25.8	-308	0.081	0.044
Dimethylamine	38.4	-313	0.106	54.5	-310	-0.185	-0.151
Ethyl amine	68.9	-951	0.281	44.1	-801	0.343	0.154
diethylamine	54.6	-755	0.215	47.9	-680	-0.038	-0.165
NPh_2	28.4	-240	-0.010	46.5	-112	-0.150	-0.072
NHPh	6.1	135	0.001	23.8	175	-0.191	-0.036
piperidine	41.7	-431	0.119	43.9	-437	-0.006	-0.001
morpholine	30.9	-72	0.017	39.1	-356	-0.278	-0.036

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	15.6	-248	-0.036	19.5	-83	-0.083	-0.031
phenyl ketone	23.8	-189	-0.022	33.9	-147	-0.257	-0.292
Acetic acid	4.3	-31	0.018	3.4	-50	0.010	0.016
acetate	3.5	28	-0.013	-2.9	-135	0.053	0.042
COOMe	4.0	-3	-0.001	5.0	-46	0.088	0.025
COOEt	-2.7	124	-0.031	1.2	120	-0.009	0.003
COOtBu	-4.2	83	-0.072	0.5	-36	0.097	0.031
Fluorine	19.6	-532	0.090	5.6	-352	0.358	0.313
Chlorine	12.7	-174	-0.007	12.8	-103	-0.063	-0.046
Bromine	8.8	-82	0.002	11.7	-63	-0.119	-0.108
Iodine	8.9	-109	0.007	11.9	35	-0.260	-0.250
CONH2	4.4	-844	0.055	-23.9	16	0.127	0.187
nitrile	24.3	-113	-0.032	30.0	-206	-0.139	-0.065
nitro	23.8	428	0.038	43.2	-46	-0.475	-0.245
Sulfonyl	-8.5	-179	-0.230	-14.4	13	-0.047	0.088
Sulfonate	2.6	-69	0.005	2.3	-22	0.053	0.063
CF_3	6.9	-47	0.004	10.2	10	-0.115	-0.068
CF_2CF_3	-6.4	126	-0.004	-4.5	4	0.034	0.006

Table S21. Average attribution of functional groups in water.

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
Methyl	2.3	-67	0.016	1.1	-34	0.055	0.042
Ethyl	3.5	62	0.012	4.8	-36	-0.027	-0.004
Propyl	18.6	-8	0.006	15.0	-200	0.102	0.073
Butyl	2.3	-38	0.010	1.9	-14	-0.011	-0.008
Isopropyl	4.7	-137	-0.022	-0.3	-73	0.038	0.057
t-Butyl	5.8	-41	0.015	5.7	-54	0.020	0.017
cyclohexyl	-1.8	22	-0.040	3.4	43	0.013	0.031
ethene	-0.7	210	-0.054	-0.9	-91	0.031	0.053
dimethylethene	5.4	-364	0.018	-5.1	-3	-0.042	-0.026
Ethyne	-2.8	-63	0.028	-9.4	-112	0.071	-0.040
methylethyne	2.6	-949	0.091	-25.3	-661	0.813	0.571
Phenyl	10.2	-47	0.006	14.5	-50	-0.064	-0.039
p-tolyl	8.4	37	0.044	14.9	-36	-0.040	-0.066
Phenol	18.7	-375	0.132	15.0	-123	-0.167	-0.192
Phenolate	100.2	-482	0.209	119.6	-141	-0.862	-0.632
Anilne	23.3	-184	0.151	34.1	-39	-0.197	-0.259
tBuPh	8.7	113	0.026	9.2	-63	0.018	-0.001
PhF	4.5	99	0.037	4.9	-84	0.101	0.027
PhCl	3.6	194	0.000	14.7	39	-0.044	-0.036
PhBr	12.5	-53	0.010	14.6	-134	-0.041	-0.045
PhI	6.5	-178	0.017	6.5	-27	-0.054	-0.107
$PhNPh_2$	21.9	64	0.137	52.3	-67	-0.199	-0.180
Hydroxyl	4.9	-54	0.019	4.3	-60	0.048	0.019
Hydroxylate	27.9	-472	0.078	22.3	-209	-0.044	-0.039
methoxy	3.5	-44	0.009	6.2	-9	-0.022	-0.013
Ethoxy	-2.4	-86	-0.025	1.0	-68	0.028	0.044
Amine	17.3	-368	0.054	13.4	-155	-0.006	0.003
protonated amine	0.8	-268	0.037	-7.7	23	-0.062	-0.088
methyl amine	24.3	-123	-0.088	25.3	-311	0.084	0.056
Dimethylamine	38.1	-343	0.102	54.8	-310	-0.207	-0.164
Ethyl amine	68.5	-1027	0.287	41.3	-824	0.429	0.220
diethylamine	54.6	-802	0.211	47.7	-683	-0.070	-0.190
NPh_2	28.2	-275	-0.010	46.9	-119	-0.168	-0.082
NHPh	5.6	148	-0.003	24.8	189	-0.222	-0.051
piperidine	41.7	-474	0.116	43.6	-438	-0.016	-0.009
morpholine	31.1	-79	0.011	39.5	-361	-0.292	-0.046

	λ_{abs} (nm)	σ_{abs} (cm^{-1})	logε	λ_{emi} (nm)	σ_{emi}(cm^{-1})	logΦ	logτ
acetyl	15.3	-267	-0.035	19.6	-71	-0.097	-0.037
phenyl ketone	23.5	-220	-0.023	34.3	-149	-0.286	-0.311
Acetic acid	4.5	-34	0.018	3.2	-55	0.024	0.025
acetate	3.8	25	-0.010	-3.5	-141	0.088	0.065
COOMe	4.1	-18	0.002	4.5	-54	0.114	0.045
COOEt	-2.7	114	-0.029	0.6	116	0.024	0.028
COOtBu	-4.0	81	-0.069	0.9	-51	0.127	0.051
Fluorine	19.9	-547	0.091	4.5	-360	0.406	0.345
Chlorine	12.5	-176	-0.006	12.8	-102	-0.059	-0.042
Bromine	8.7	-89	0.003	11.7	-65	-0.119	-0.109
Iodine	9.2	-115	0.007	12.3	33	-0.271	-0.262
CONH2	5.2	-887	0.061	-27.3	25	0.170	0.209
nitrile	24.6	-130	-0.032	30.1	-216	-0.129	-0.059
nitro	23.9	432	0.034	43.3	-50	-0.484	-0.252
Sulfonyl	-8.2	-187	-0.229	-15.0	10	-0.021	0.104
Sulfonate	2.7	-72	0.007	2.0	-27	0.074	0.077
CF_3	7.0	-54	0.003	10.4	13	-0.124	-0.074
CF_2CF_3	-6.8	126	-0.004	-4.5	3	0.043	0.014

References

(1) Joung, J. F.; Han, M.; Hwang, J.; Jeong, M.; Choi, D. H.; Park, S. Deep Learning Optical Spectroscopy Based on Experimental Database: Potential Applications to Molecular Design. *JACS Au* **2021,** *1*, 427.

(2) Joung, J. F.; Han, M.; Jeong, M.; Park, S. figshare, 2020, DOI:https://doi.org/10.6084/m9.figshare.12045567.v2.

(3) Joung, J. F.; Han, M.; Jeong, M.; Park, S. Experimental database of optical properties of organic compounds. *Sci. Data* **2020,** *7*, 295.