

T. Kataoka, Y. Tsuchido, H. Kawai

Supporting Information for

Turn-Off Fluorescence Sensing of Benzenediols via Guest-Induced π -Conjugation Switching in Bisimidazole-Based Hydrindacene Allosteric Receptors

Takayuki Kataoka, Yoshitaka Tsuchido, and Hidetoshi Kawai*

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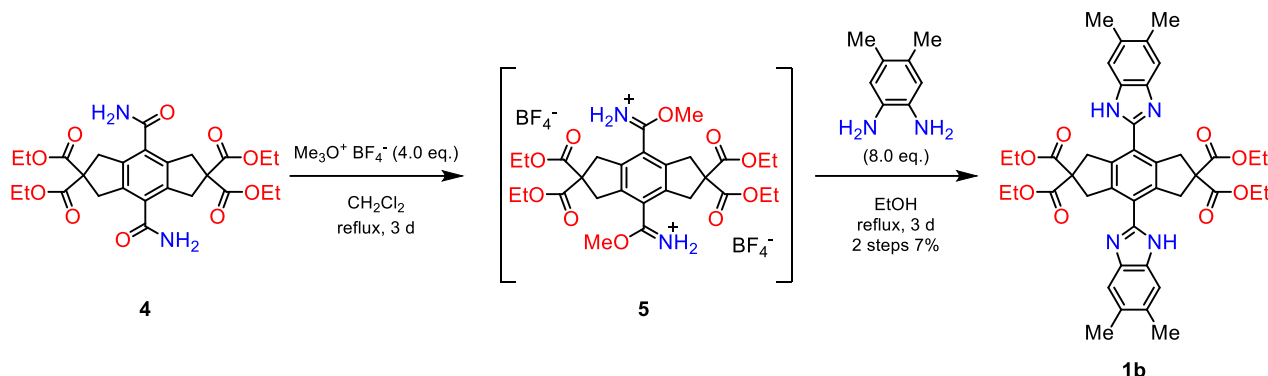
1. General information

^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were recorded on a Bruker BioSpin AVANCE NEO 400 spectrometer (^1H : 400 MHz, ^{13}C : 100 MHz). The chemical shifts in ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR were referenced with respect to TMS for CDCl_3 (^1H NMR: δ 0.00), or residual peaks of the solvents used for CDCl_3 (^{13}C NMR: δ 77.16) and DMSO (^1H NMR: δ 2.50, ^{13}C NMR: δ 39.52). IR spectra were recorded on a JASCO FT-IR-4600 (ATR) spectrometer. Mass spectra were recorded on a JEOL JMS-S3000 SpiralTOF (MALDI-TOF) spectrometer. UV/Vis absorption spectra were recorded on a JASCO V-630 spectrometer. Fluorescence spectra were recorded on a JASCO FP-8300 spectrometer. All melting points were recorded on a METTLER TOLEDO MP90. The X-ray analysis data were obtained by using a Bruker D8 QUEST (MoK α radiation, λ = 0.71073 Å). Thin-layer chromatography (TLC) was performed on silica gel 60 (Merck) of particle size 5-20 μm . Column chromatography was performed on silica gel 60 (YMC) of particle size 40-63 μm . All commercially available compounds were used without further purification.

Tetraethyl 4,8-bis(1*H*-benzo[*d*]imidazole-2-yl)-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**1a**),³⁵ Tetraethyl 4,8-diiodo-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**3**),³⁵ Tetraethyl 4,8-dicyano-*s*-hydrindacene-2,2,6,6-tetracarboxylate,³⁵ Tetraethyl 4,8-dicarbamoyl-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**4**),³⁵ and 4,5-Dimethoxy-1,2-phenylenediamine⁵⁵ were synthesized according to previously reported procedures.

2. Synthetic procedure and characterization

Tetraethyl 4,8-bis(5,6-dimethyl-1*H*-benzo[*d*]imidazol-2-yl)-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**1b**)



Trimethyloxonium tetrafluoroborate (296 mg, 2.0 mmol) was added to a solution of **4** (266 mg, 0.50 mmol) in dry CH_2Cl_2 (4.0 mL). The mixture was refluxed for 3 days, then cooled to room temperature, and concentrated *in vacuo*. 4,5-dimethyl-1,2-phenylenediamine (545 mg, 4.0 mmol) and dry EtOH (1.0 mL) were added to the residue, and the mixture was refluxed for an additional 3 days. After cooling to room temperature, the resulting solid was removed by filtration, and the filtrate was concentrated *in vacuo*. The residue was purified by silica gel chromatography using hexane/EtOAc (1:2) as the eluent and washed with MeCN to give **1b** as a yellowish white solid (24.6 mg, 7%).

Mp 281.9-290.2°C (*decomp.*); IR (ATR): 3398, 2978, 2933, 2861, 1722, 1443, 1366, 1288, 1239, 1200, 1180, 1157, 1075, 1050, 1000, 852, 717, 618, 562, 437 cm^{-1} ; ^1H NMR (400 MHz, $\text{DMSO}-d_6$) δ 12.21 (s, 2H), 7.53 (s, 2H), 7.37 (s, 2H), 4.11 (q, $J = 7.1$ Hz, 8H), 3.76 (s, 8H), 2.37 (s, 6H), 2.34 (s, 6H), 1.11 ppm (t, $J = 7.1$ Hz, 12H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, $\text{DMSO}-d_6$) δ 170.81, 148.16, 142.15, 138.98, 132.99, 131.52, 130.21, 124.45, 119.13, 111.65, 61.55, 59.67, 20.00, 13.77 ppm; HR-MS (MALDI: matrix DCTB) (m/z): calcd. for $\text{C}_{42}\text{H}_{46}\text{N}_4\text{O}_8\text{Na}$: 757.3208, found 757.3237.

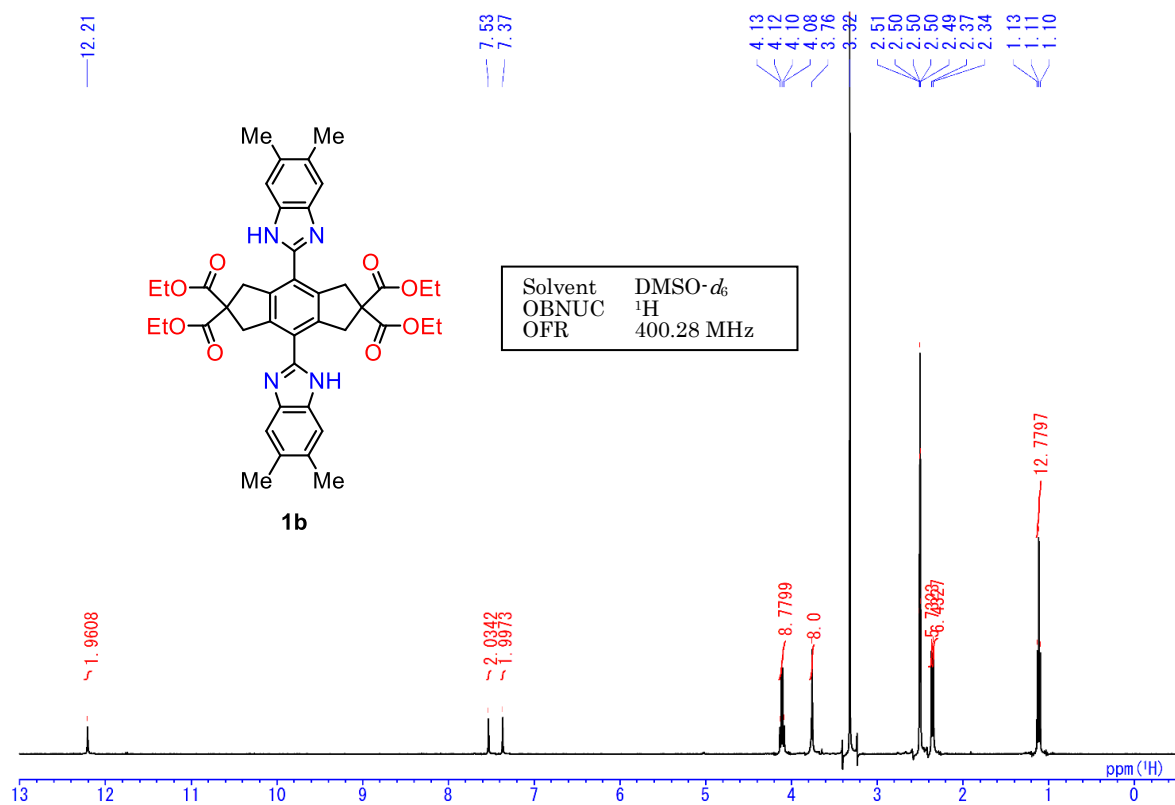


Figure S1. ^1H NMR spectrum of **1b**.

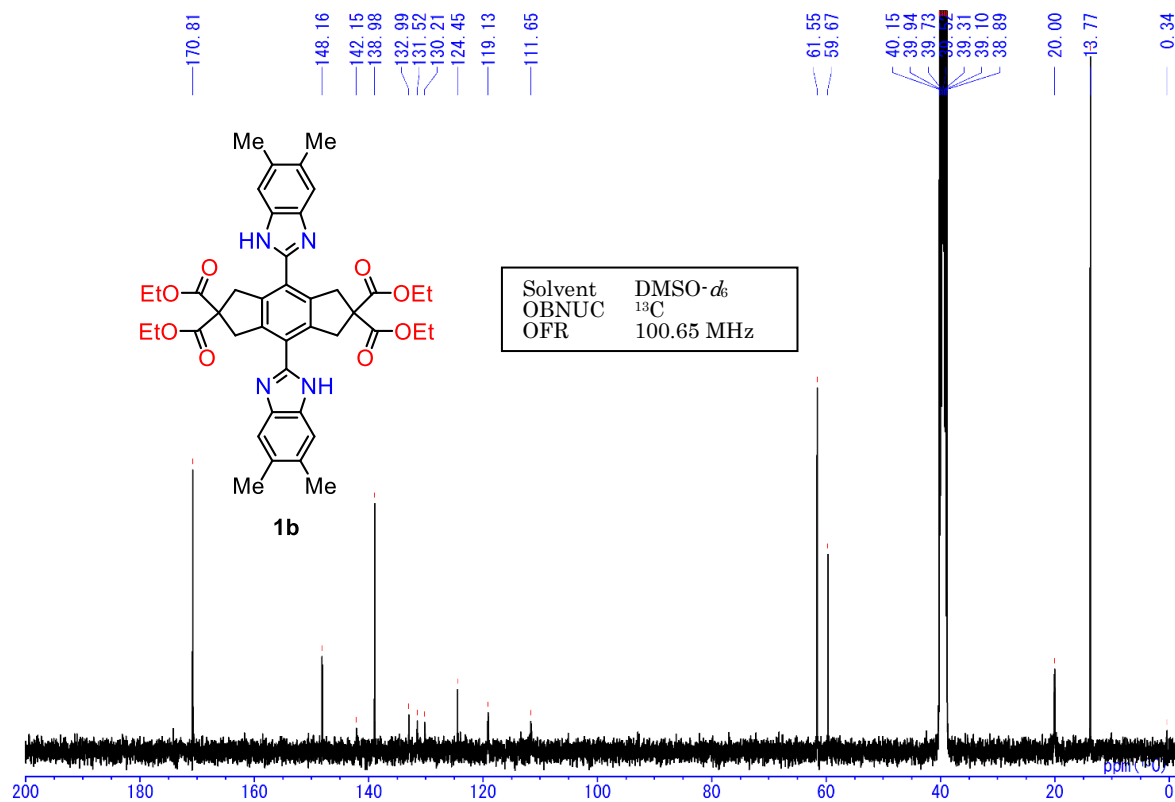
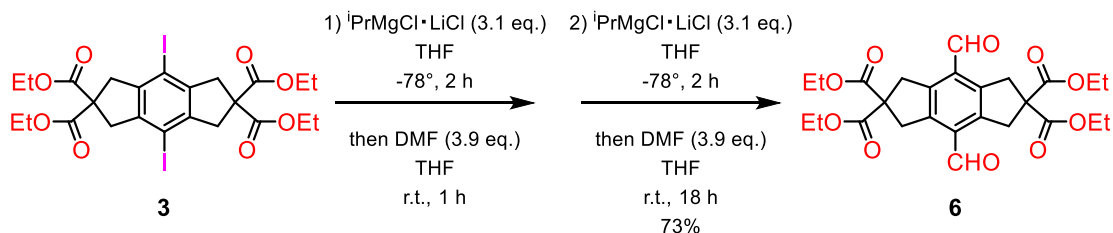


Figure S2. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1b**.

Tetraethyl 4,8-diformyl-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**6**)

A solution of isopropylmagnesium chloride-lithium chloride complex (1.3 M in THF, 7.2 mL, 9.4 mmol) was added to a solution of **3** (2.10 g, 3.0 mmol) in dry THF (60 mL) at -78°C . The mixture was stirred for 2 hours at -78°C , followed by the addition of dry DMF (0.9 mL, 12 mmol). After stirring for 1 hour at room temperature, the reaction mixture was cooled again to -78°C , and the isopropylmagnesium chloride-lithium chloride complex (7.2 mL, 9.4 mmol) was added. After stirring for 2 hours at -78°C , dry DMF (0.9 mL, 12 mmol) was added again, and the mixture was stirred for 18 hours at room temperature. The reaction mixture was quenched with saturated aqueous NH_4Cl , and the aqueous phase was extracted with MTBE. The combined organic phases were washed with water and brine, dried over MgSO_4 , and concentrated *in vacuo*. The residue was washed with MeOH to give **6** as a white solid (1.10 g, 73%).

Mp $166.5\text{--}175.4^\circ\text{C}$; IR (ATR): 2981, 2926, 2872, 1722, 1681, 1444, 1367, 1278, 1236, 1187, 1160, 1070, 1052, 1006, 958, 859, 718, 678 cm^{-1} ; ^1H NMR (400 MHz, CDCl_3) δ 10.39 (s, 2H), 4.23 (q, $J = 7.1$ Hz, 8H), 3.91 (s, 8H), 1.28 ppm (t, $J = 7.1$ Hz, 12H); $^{13}\text{C}\{^1\text{H}\}$ NMR (100 MHz, CDCl_3) δ 190.72, 171.28, 143.79, 130.53, 62.28, 60.73, 38.72, 14.16 ppm; HR-MS (MALDI: matrix DCTB) (m/z): calcd. for $\text{C}_{26}\text{H}_{30}\text{O}_{10}\text{Na}$: 525.1731, found 525.1736.

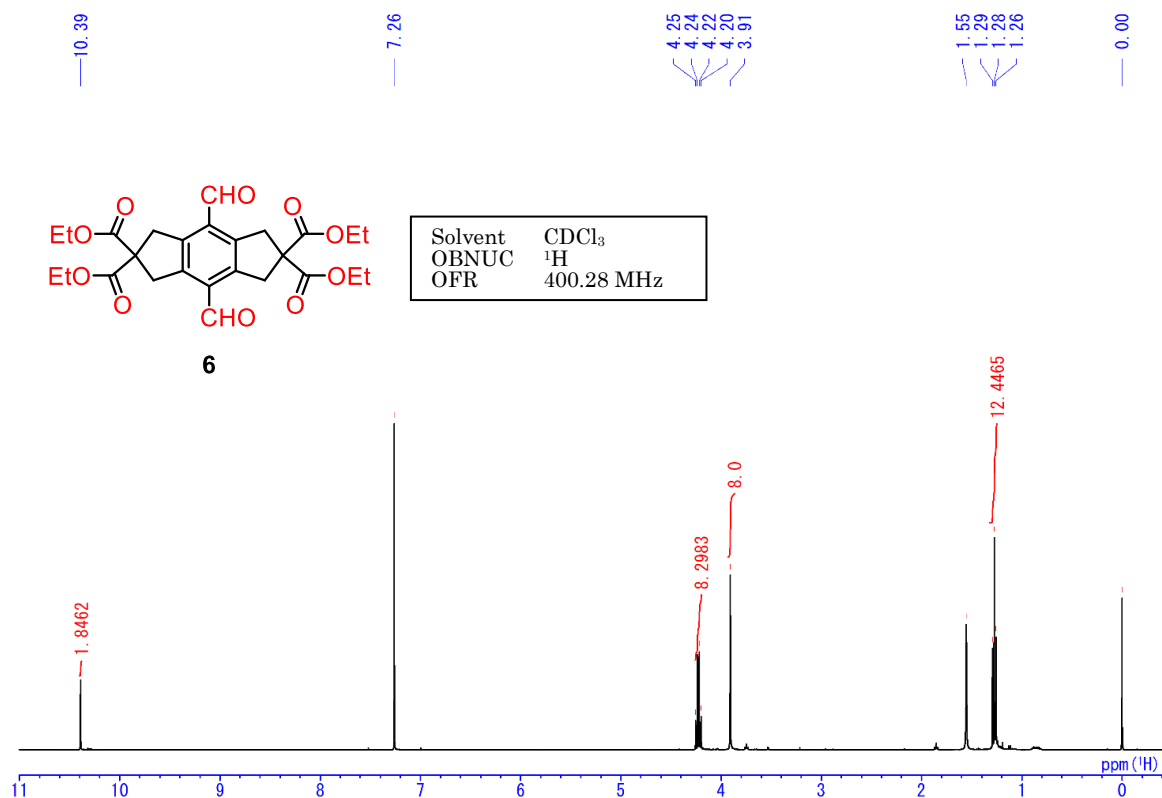


Figure S3. ^1H NMR spectrum of **6**.

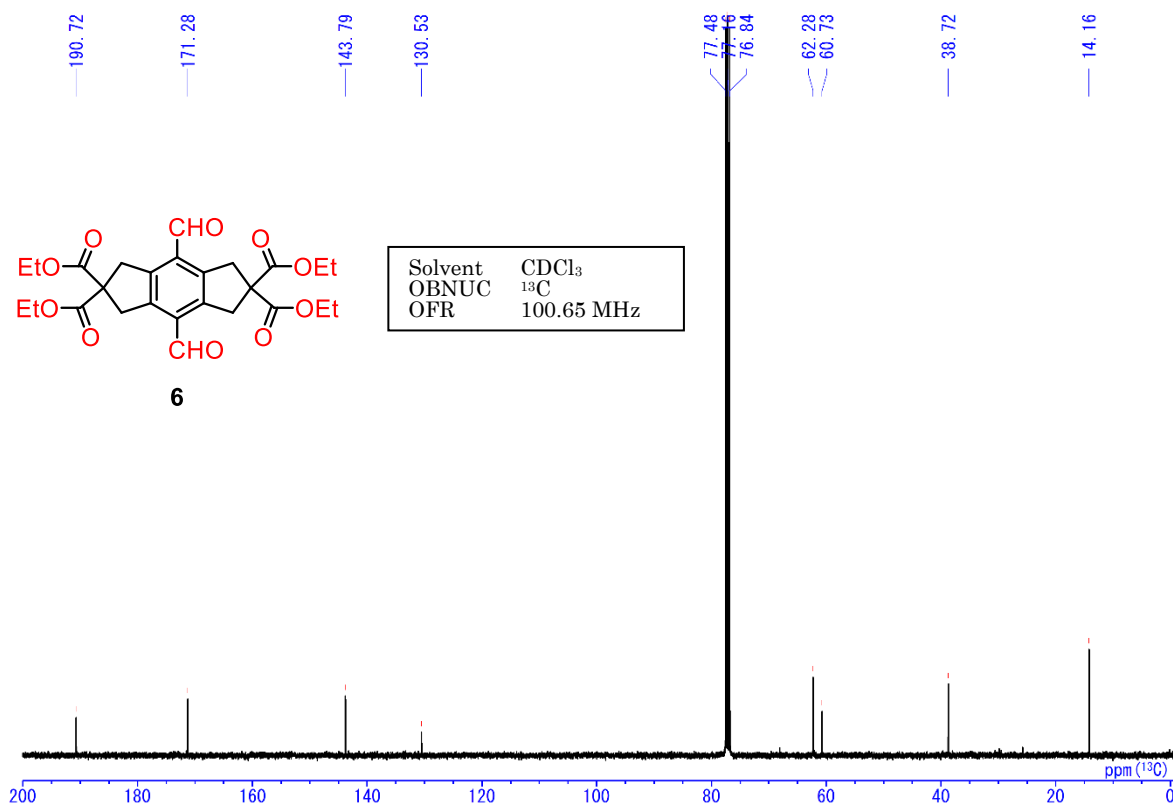
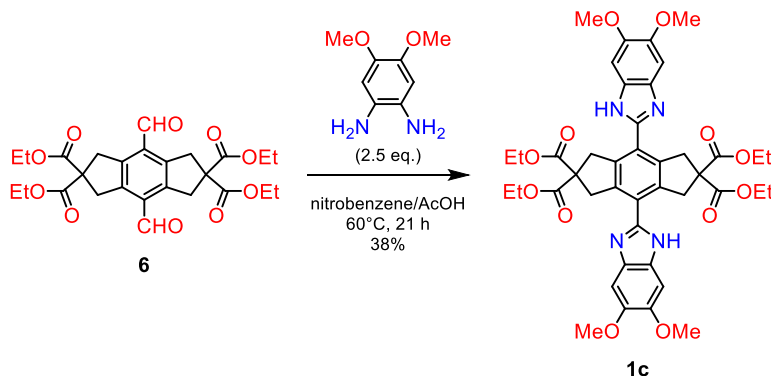


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **6**.

Tetraethyl 4,8-bis(5,6-dimethoxy-1*H*-benzo[*d*]imidazol-2-yl)-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**1c**)



4,5-Dimethoxy-1,2-phenylenediamine (80.0 mg, 0.48 mmol) was added to a solution of **6** (100 mg, 0.20 mmol) in 10:1 nitrobenzene/AcOH (1.1 mL). The mixture was stirred for 21 hours at 60°C, then cooled to room temperature. The resulting mixture was suspended in hexane, filtered, and washed with MeOH. The residue was purified by silica gel chromatography using CHCl₃/MeOH (19:1) as the eluent, then recrystallized from EtOH to give **1c** as a yellowish white solid (59.9 mg, 38%).

Mp 270.9-275.3°C (*decomp.*); IR (ATR): 3352, 2986, 2963, 2939, 2838, 1710, 1587, 1481, 1442, 1368, 1332, 1283, 1242, 1196, 1160, 1132, 1071, 887, 836, 733, 630, 542, 418 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.14 (s, 2H), 7.33 (s, 2H), 7.11 (s, 2H), 4.12 (q, *J* = 7.0 Hz, 8H), 3.85 (s, 6H), 3.83 (s, 6H), 3.79 (s, 8H), 1.13 ppm (t, *J* = 7.0 Hz, 12H); ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆) δ 170.91, 147.34, 147.26, 146.48, 138.71, 137.07, 128.15, 124.16, 101.64, 94.61, 61.60, 59.72, 55.91, 55.87, 13.83 ppm (methylene signal of the five-membered ring is overlapped with the solvent signal); HR-MS (MALDI: matrix DCTB) (*m/z*): calcd. for C₄₂H₄₆N₄O₁₂Na: 821.3004, found 821.2995.

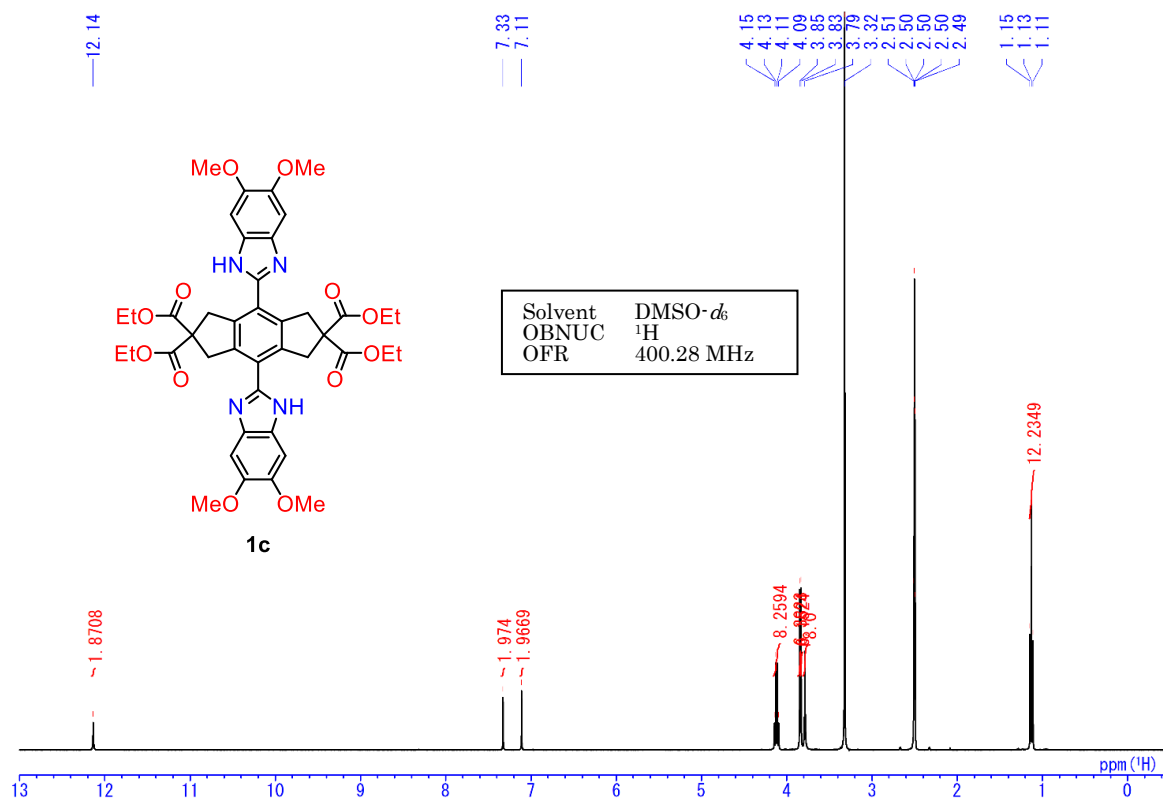


Figure S5. ^1H NMR spectrum of **1c**.

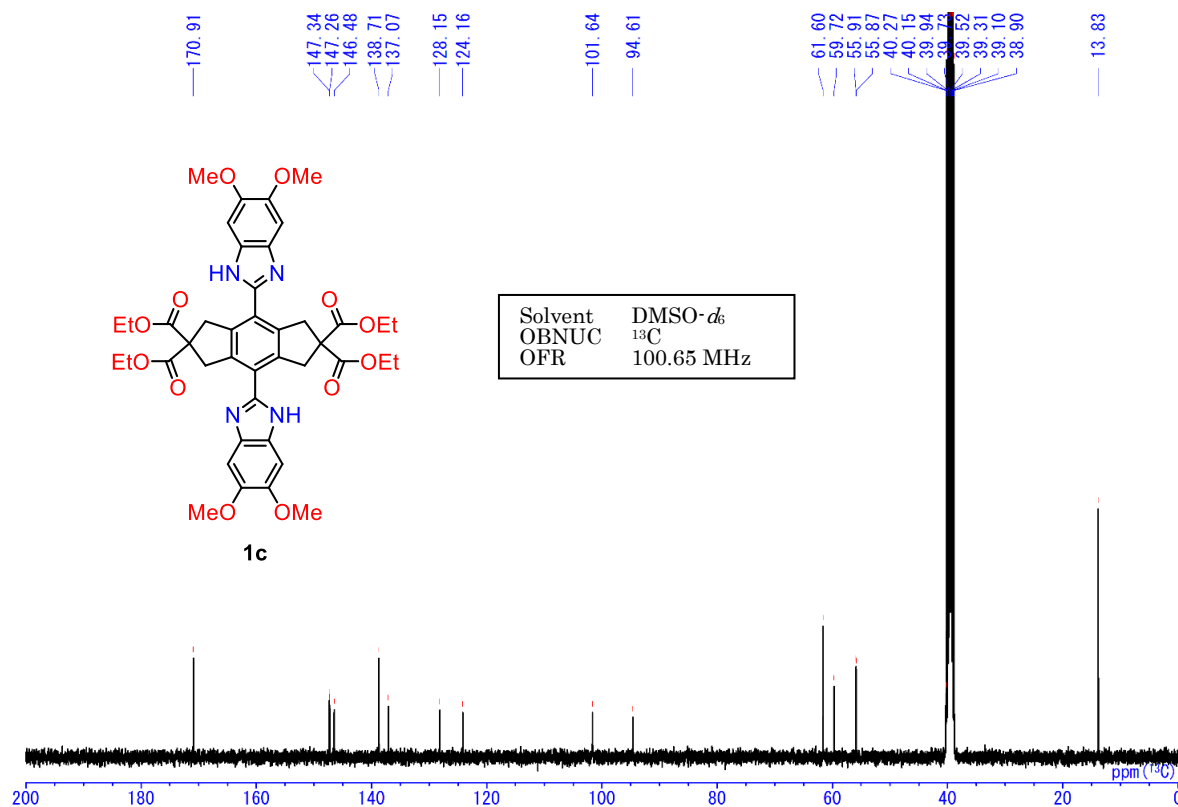
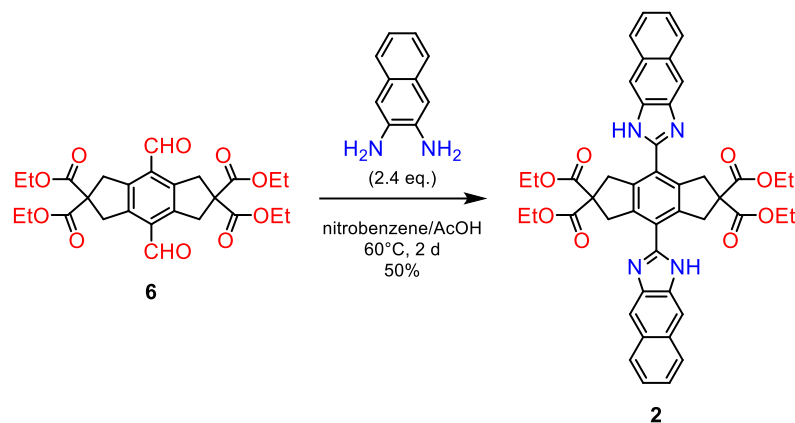


Figure S6. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **1c**.

Tetraethyl 4,8-bis(1*H*-naphtho[2,3-*d*]imidazole-2-yl)-*s*-hydrindacene-2,2,6,6-tetracarboxylate (**2**)

2,3-Diaminonaphthalene (38.0 mg, 0.24 mmol) was added to a solution of **6** (50.0 mg, 0.10 mmol) in 10:1 nitrobenzene/AcOH (0.55 mL). The mixture was stirred for 2 days at 60°C, then cooled to room temperature. The resulting mixture was suspended in hexane and filtered. The residue was purified by silica gel chromatography using CHCl₃/MeOH (100:3) as the eluent, then washed with MeCN to give **2** as a yellow solid (38.7 mg, 50%).

Mp 280.2-288.4°C (*decomp.*); IR (ATR): 3508, 3403, 3055, 2979, 1723, 1450, 1409, 1366, 1290, 1245, 1201, 1183, 1076, 1010, 856, 741, 614, 555, 473, 419 cm⁻¹; ¹H NMR (400 MHz, DMSO-*d*₆) δ 12.59 (s, 2H), 8.35 (s, 2H), 8.10 (s, 2H), 8.07-8.04 (m, 4H), 7.46-7.39 (m, 4H), 4.12 (q, *J* = 7.1 Hz, 8H), 3.87 (s, 8H), 1.12 ppm (t, *J* = 7.1 Hz, 12H); ¹³C{¹H} NMR (100 MHz, DMSO-*d*₆) δ 170.75, 153.32, 143.87, 139.73, 135.14, 130.37, 129.79, 128.17, 127.49, 124.75, 124.06, 123.25, 115.75, 107.12, 61.62, 59.70, 13.77 ppm (methylene signal of the five-membered ring is overlapped with the solvent signal); HR-MS (MALDI: matrix DCTB) (*m/z*): calcd. for C₄₆H₄₂N₄O₈Na: 801.2895, found 801.2931.

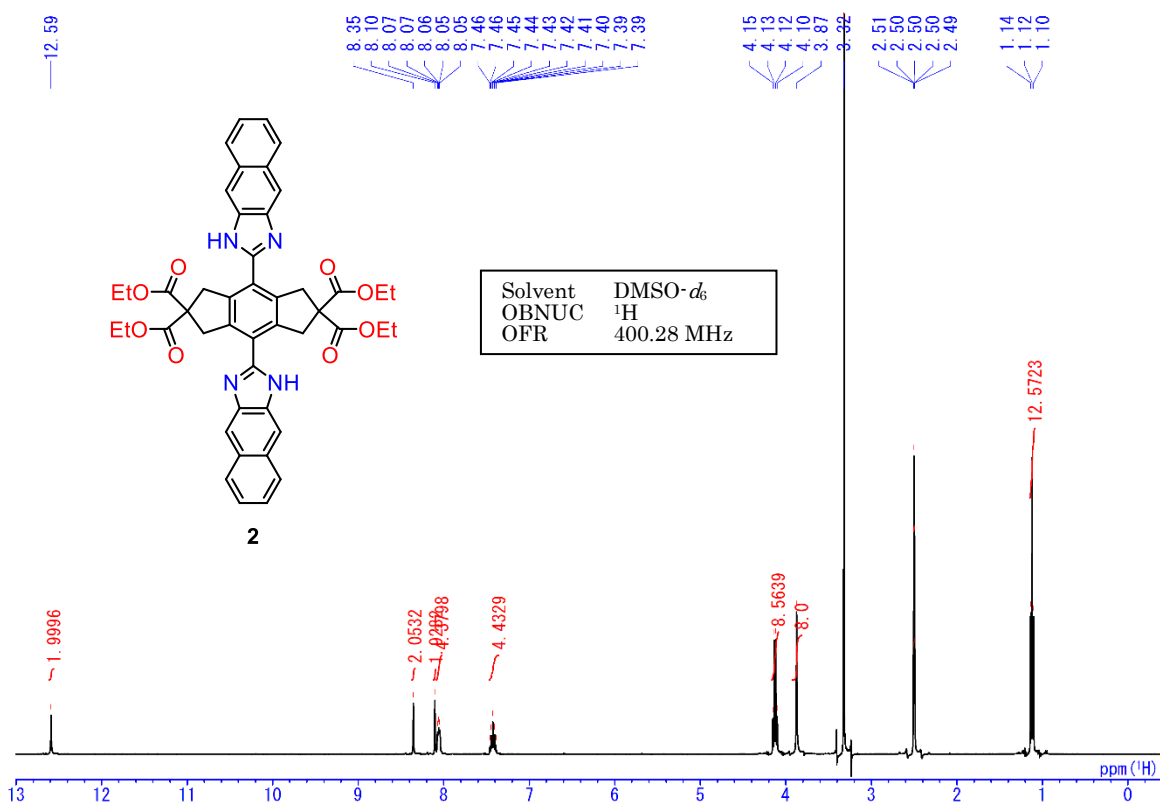


Figure S7. ^1H NMR spectrum of **2**.

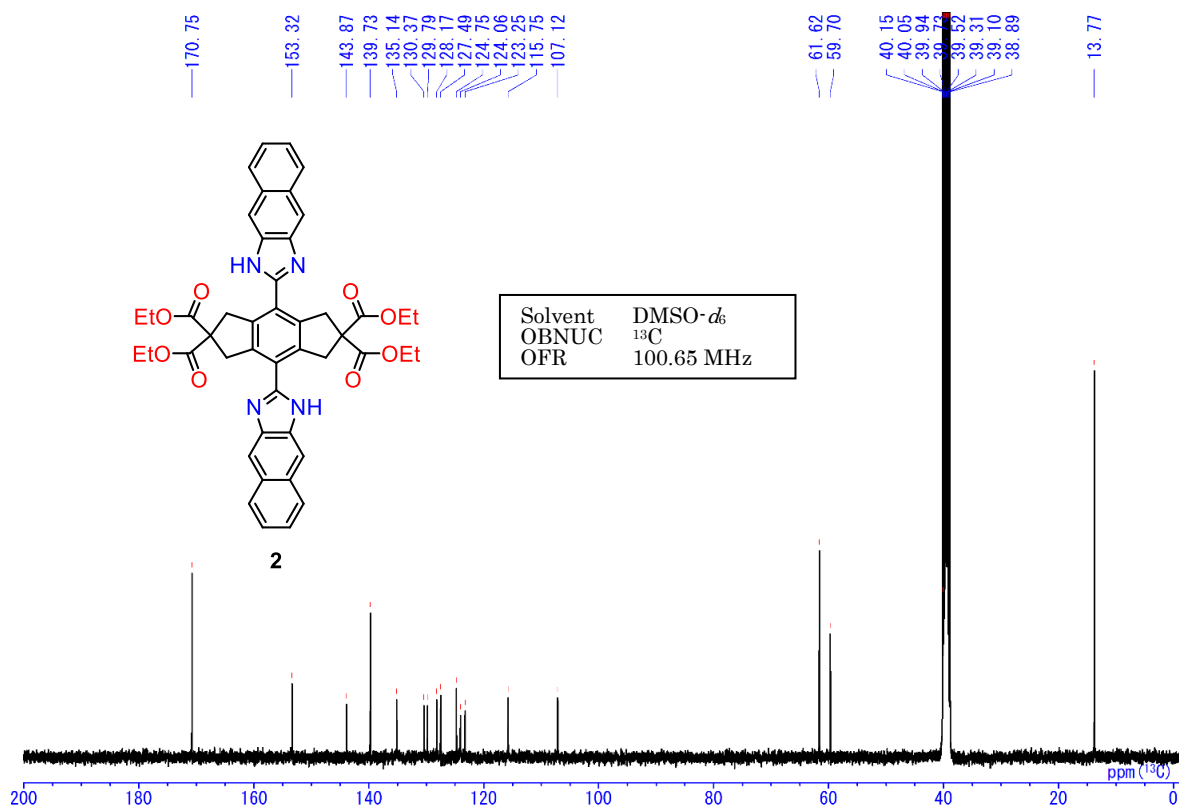


Figure S8. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2**.

3. Single crystal X-ray structural analysis

A suitable crystal of **2** was obtained by diffusion method from a DMSO/methanol mixture. Single X-ray structure determination was performed on Bruker D8 QUEST (MoK α radiation, $\lambda = 0.71073$ Å). Crystallographic data collection and refinement information is listed in Table S1.

Table S1. Crystal data and structure refinement parameters for **2**·(MeOH)₂.

Compound	2 ·(MeOH) ₂
Data deposition	CCDC 2490135
Empirical formula	C ₄₈ H ₅₀ N ₄ O ₁₀
Formula weight	842.92
Crystal habit	Orangish yellow plate
Crystal size	0.60×0.2×0.10 mm ³
Temperature	90 K
Wavelength	0.71073 Å
Crystal system	Triclinic
Space group	<i>P</i> 1
Unit cell dimensions	<i>a</i> 7.6813(12) Å
	<i>b</i> 10.6712(17) Å
	<i>c</i> 14.613(2) Å
	<i>a</i> 111.251(5)°
	<i>b</i> 101.585(5)°
	<i>g</i> 94.648(5)°
Volume	1078.0(3) Å ³
<i>Z</i>	1
Density	1.298 g cm ⁻³
Absorption coefficient μ	0.092 mm ⁻¹
<i>F</i> (000)	446
Theta range for data collection	2.052° to 25.025°
Index ranges	-9 ≤ <i>h</i> ≤ 9
	-12 ≤ <i>k</i> ≤ 12
	-17 ≤ <i>l</i> ≤ 16
Reflections collected	9187
Refinement method	Full-matrix least-squares on <i>F</i> ²
Data/restraints/parameters	3657/0/284
Goodness-of-fit on <i>F</i> ²	1.100
Final <i>R</i> indices ⁵⁶	<i>R</i> ₁ = 0.1084 [<i>I</i> > 2σ(<i>I</i>)]
	<i>wR</i> ₂ = 0.2945 (all data)

4. NMR titration

The known amount of the **1a** (1.7 mg, 2.5×10^{-3} mmol) was dissolved in 5.0 mL of solvent as a guest solution ($[1a] = 0.50$ mM). Then, 500 μ L of the host solution was added to the NMR tube and a catechol (19.8 mg, 0.18 mmol) was dissolved in the rest of the host solution (4.5 mL) to make a guest stock solution ($[1a] = 0.50$ mM, $[catechol] = 40.0$ mM, host : guest = 1 : 80). NMR titrations were carried out by adding the guest stock solution to the host solution in the NMR tube, and the chemical shifts of the host were measured and recorded after each addition. The changes in chemical shift of the host signals as a function of guest concentration were then analyzed as a 1:2 association model by BindFit.⁴⁶ At least two titration experiments were performed and titration data for six different signals were used to determine the binding constants. Errors are quoted as twice the standard error from the weighted mean (weighting based on the observed change in chemical shift).

Note that the titration results of **1a** with an orcinol as a guest molecule have already been reported.³⁵

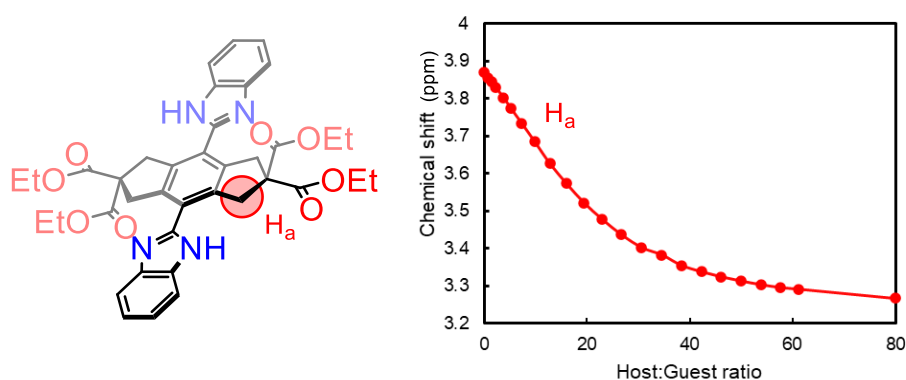


Figure S9. NMR titration curve for **1a** with catechol in $CDCl_3$ at 25°C.

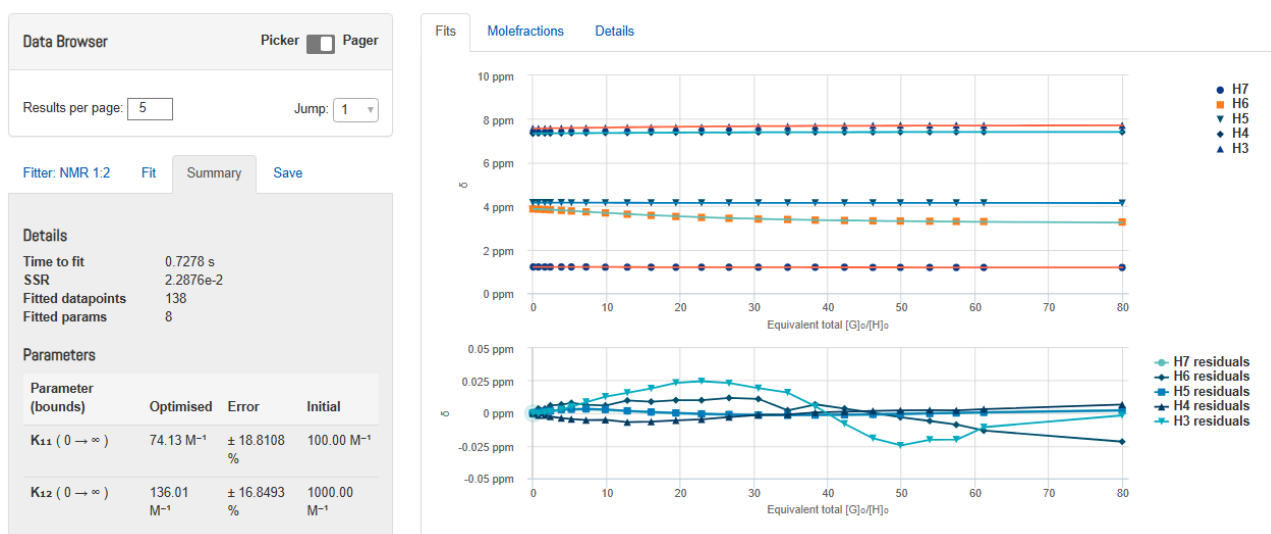


Figure S10. Curve fitting of 1H NMR titration result for **1a** with catechol ($CDCl_3$, 298 K) to a 1:2 association model by BindFit.

5. Additional UV/Vis and fluorescence spectra

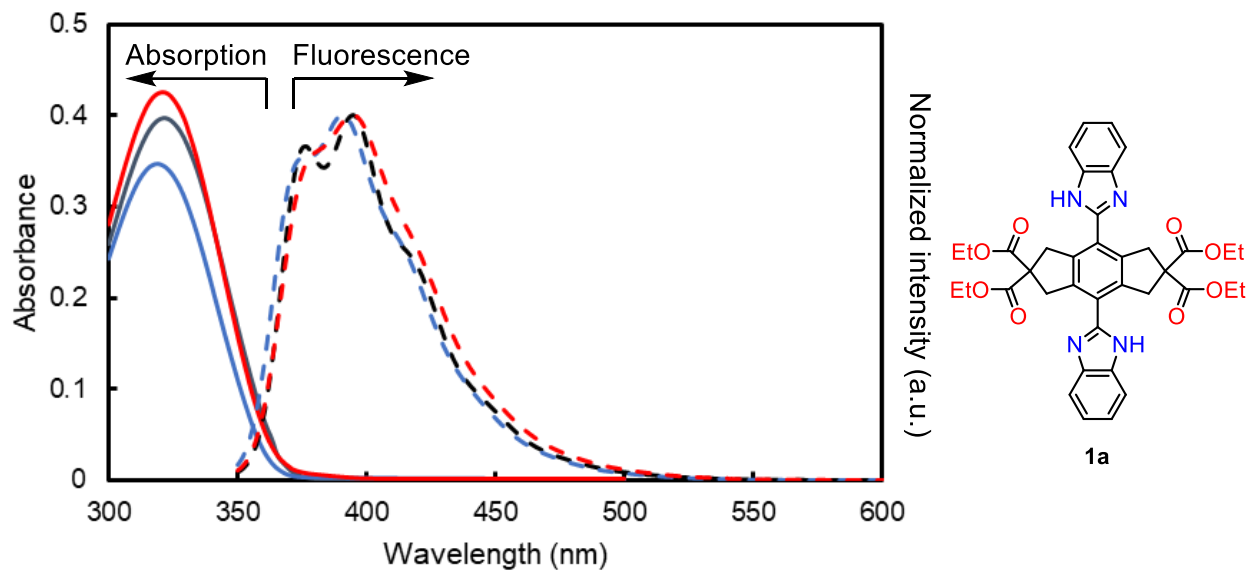


Figure S11. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **1a** in CH_2Cl_2 (black), MeCN (blue), and DMSO (red) (10 μM).

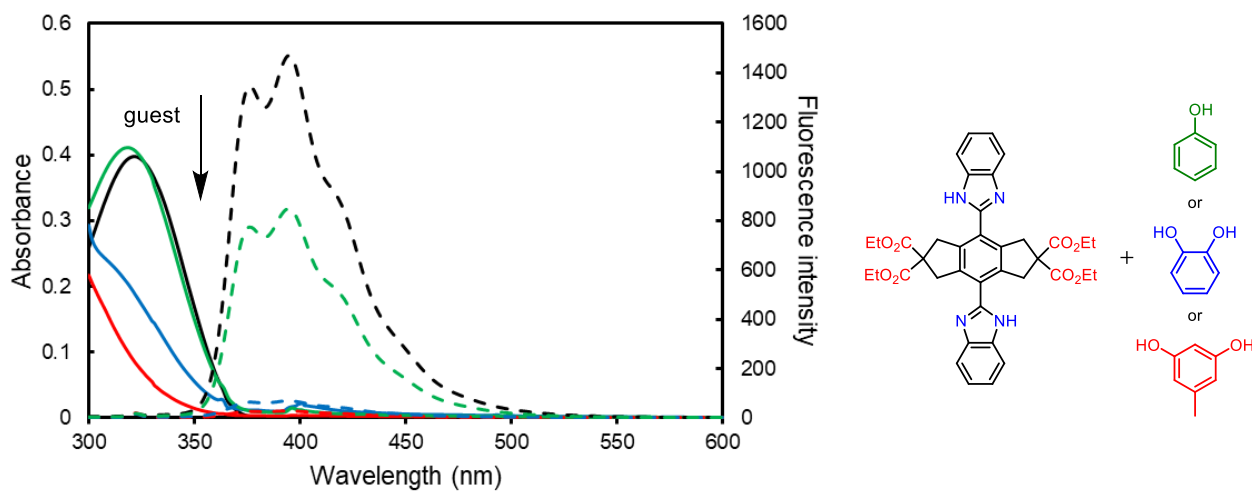


Figure S12. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **1a** (black), **1a** with orcinol (red), **1a** with catechol (blue), and **1a** with phenol (green) in CH_2Cl_2 (**1a**: 10 μM ; orcinol, catechol, and phenol: 30 mM).

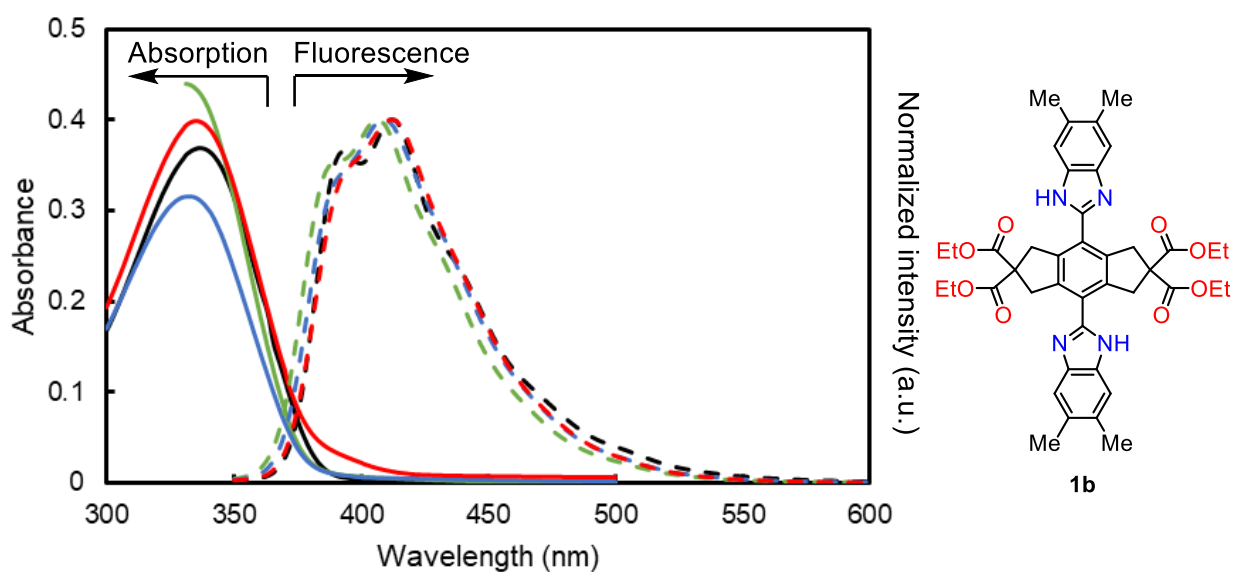


Figure S13. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **1b** in CH_2Cl_2 (black), MeCN (blue), acetone (green), and DMSO (red) (10 μM).

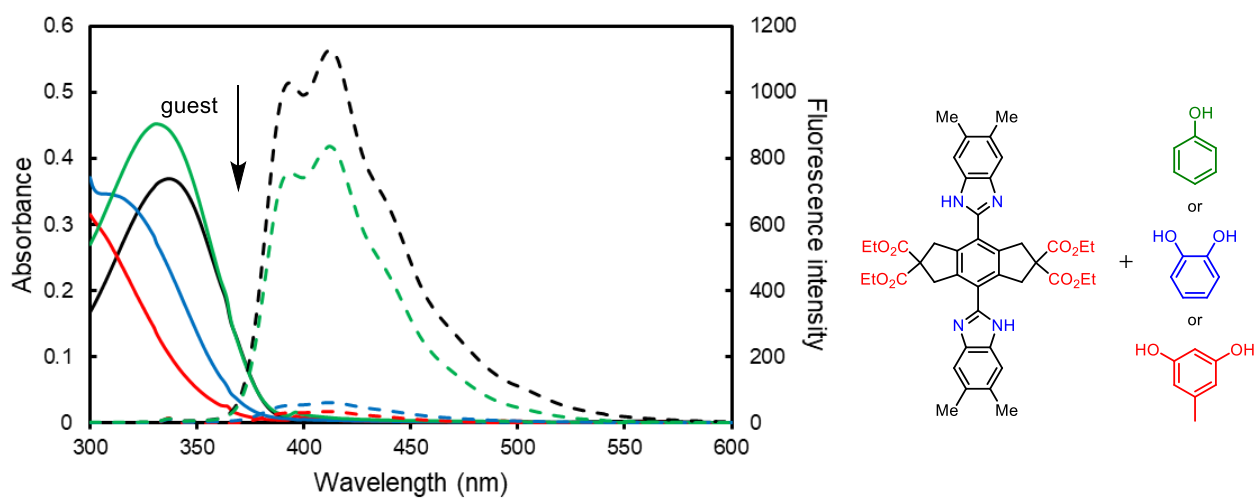


Figure S14. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **1b** (black), **1b** with orcinol (red), **1b** with catechol (blue), and **1b** with phenol (green) in CH_2Cl_2 (**1b**: 10 μM ; orcinol, catechol, and phenol: 30 mM).

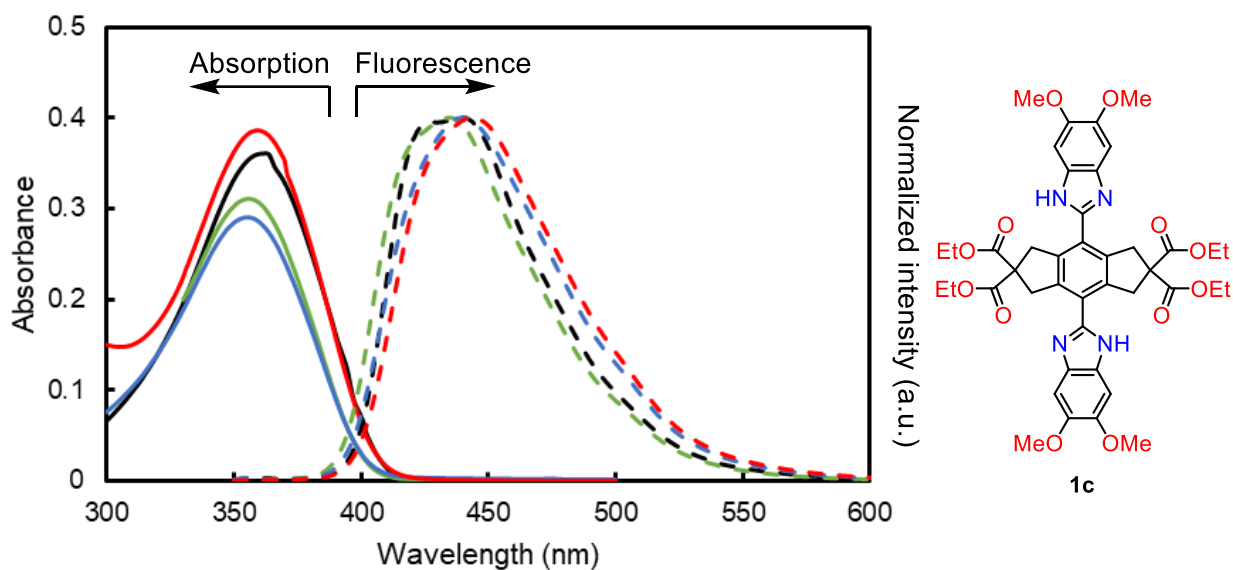


Figure S15. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **1c** in CH_2Cl_2 (black), MeCN (blue), acetone (green), and DMSO (red) (10 μM).

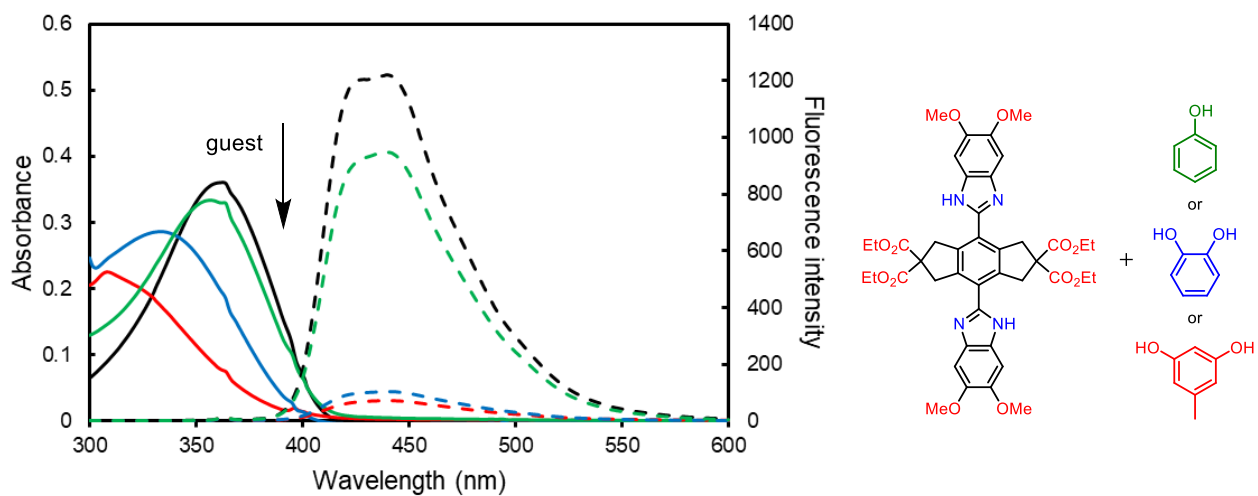


Figure S16. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **1c** (black), **1c** with orcinol (red), **1c** with catechol (blue), and **1c** with phenol (green) in CH_2Cl_2 (**1c**: 10 μM ; orcinol, catechol, and phenol: 30 mM).

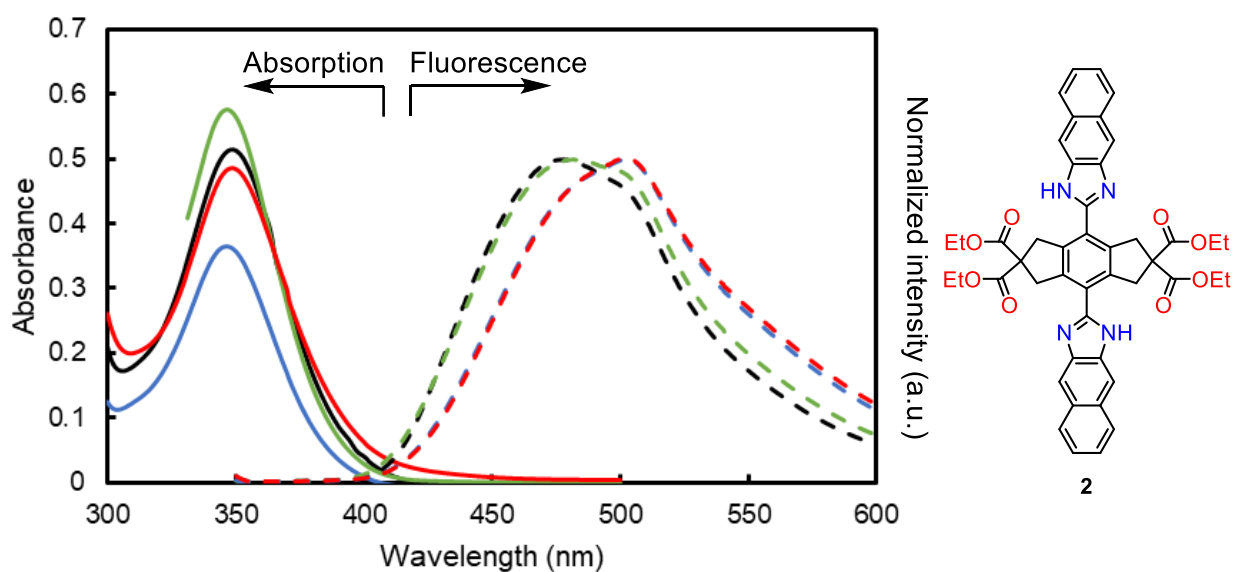


Figure S17. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **2** in CH_2Cl_2 (black), MeCN (blue), acetone (green), and DMSO (red) (10 μM).

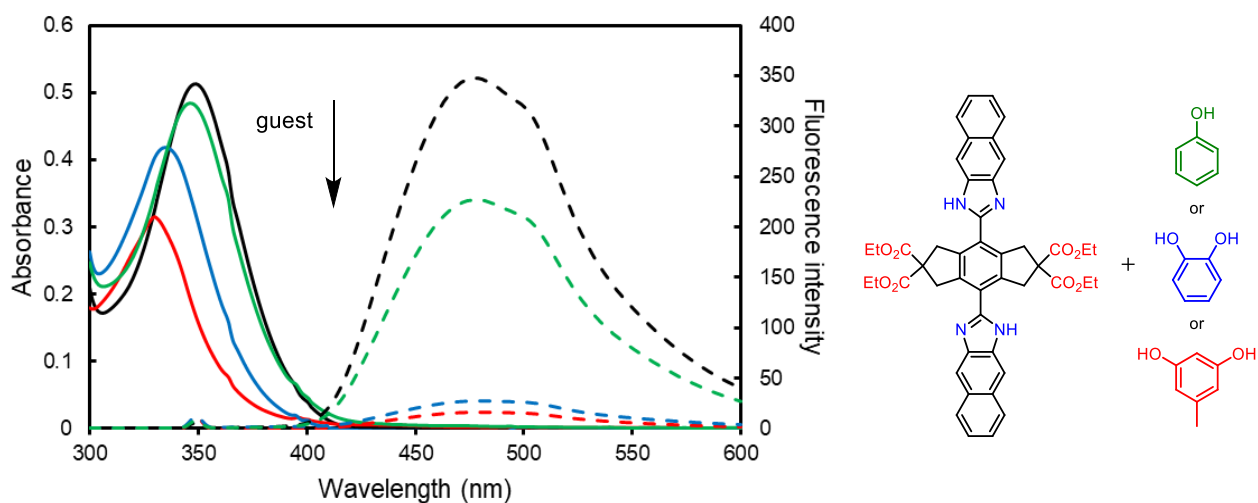


Figure S18. UV-Vis absorption (solid lines) and fluorescence (dotted lines) spectra of receptor **2** (black), **2** with orcinol (red), **2** with catechol (blue), and **2** with phenol (green) in CH_2Cl_2 (**2**: 10 μM ; orcinol, catechol, and phenol: 30 mM).

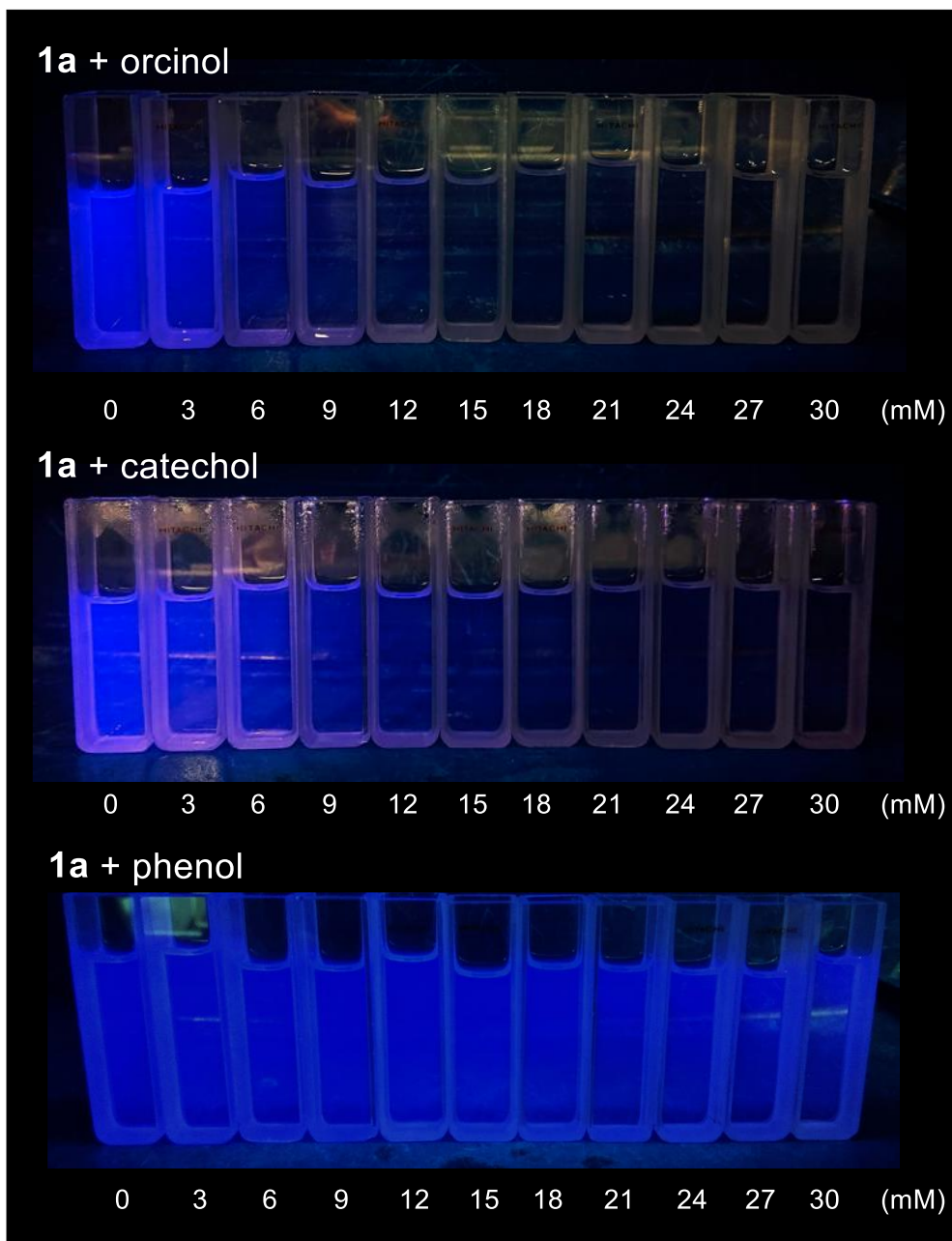


Figure S19. Photographs showing the fluorescence emission of receptor **1a** upon adding orcinol, catechol, and phenol under UV light (365 nm) in CH_2Cl_2 (**1a**: 10 μ M; orcinol, catechol, and phenol: 0–30 mM).

6. Determination of limit of detection (LOD)

The limit of detection (LOD) can be calculated via the following equation²⁷

$$\text{LOD} = 3\sigma/K_{\text{sv}}$$

where σ is the standard deviation of blank measurements and Stern-Volmer quenching constant (K_{sv}) is the slope of a plot of fluorescence intensity ratio (I_0/I) against guest concentrations.

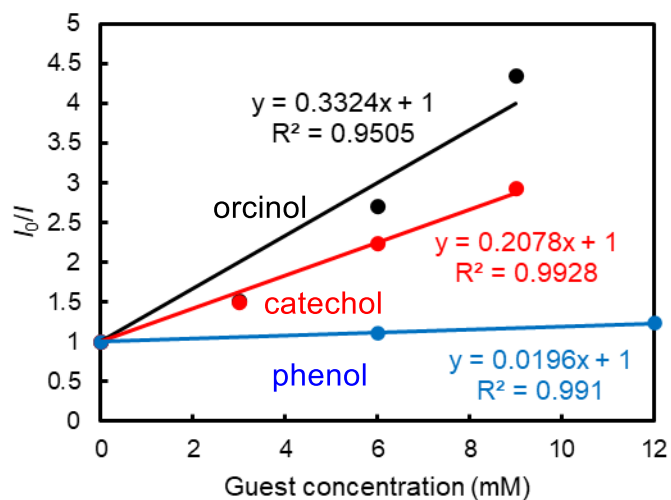


Figure S20. The fluorescence intensity ratio of I_0/I against guest concentrations.

7. Quenching efficiency and selectivity determination

The relative quenching efficiency of orcinol against catechol and phenol, which serve as an index of selectivity, is defined as follows:

$$\text{Selectivity} = \{(I_0/D)_{\text{orcinol}} - 1\} / \{(I_0/D)_{\text{catechol}} - 1\}$$

$$\text{or } \{(I_0/D)_{\text{orcinol}} - 1\} / \{(I_0/D)_{\text{phenol}} - 1\}$$

When the quenching efficiency ratio is plotted as a function of guest concentration, the value remains constant if there is no selectivity amplification. In contrast, the value changes with concentration when the quenching selectivity is amplified.

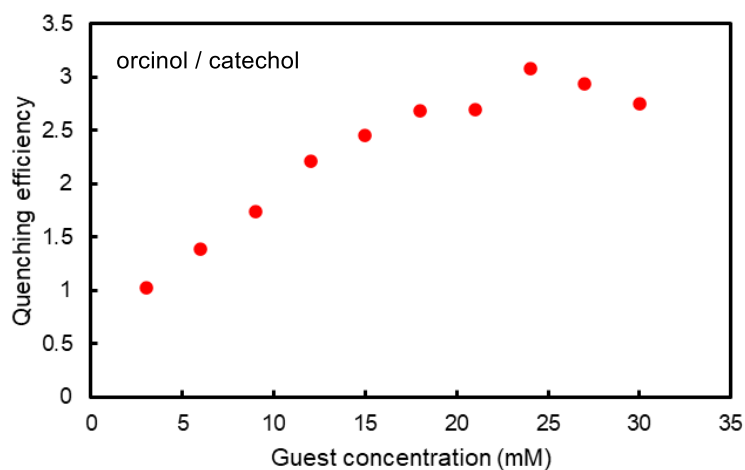


Figure S21. Quenching efficiency ratio of orcinol relative to catechol as a guest concentration.

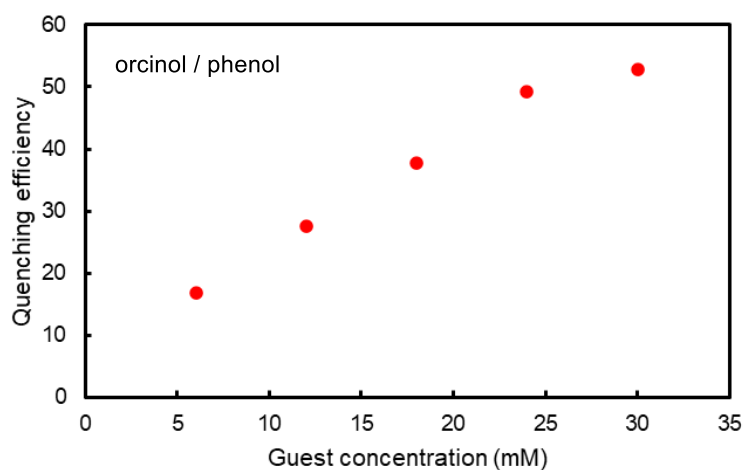


Figure S22. Quenching efficiency ratio of orcinol relative to phenol as a guest concentration.

8. Fluorescence lifetime measurement

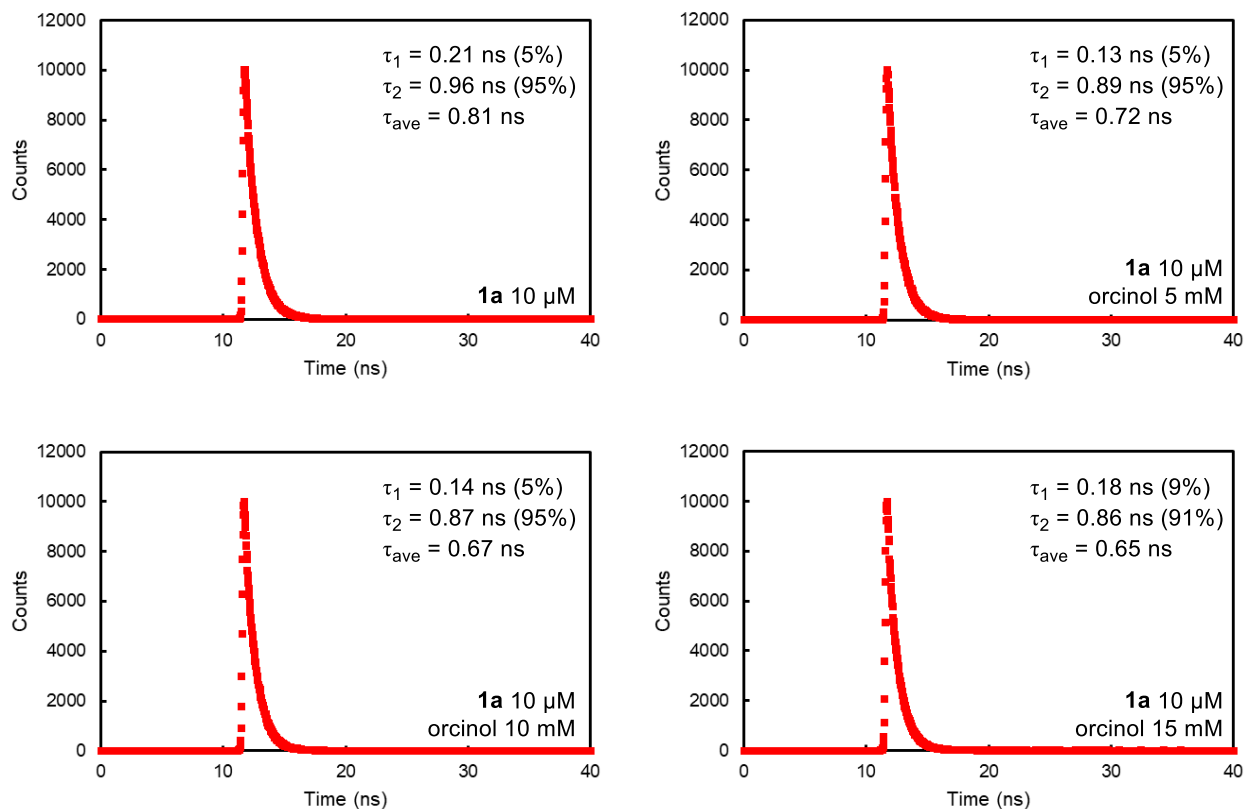


Figure S23. Fluorescence lifetime measurement of a) **1a** only (10 μ M), **1a** (10 μ M) with orcinol (5 mM), **1a** (10 μ M) with orcinol (10 mM), and **1a** (10 μ M) with orcinol (15 mM) in CH_2Cl_2 .

The dynamic quenching constant (K_D) can be calculated via the following Stern-Volmer equation

$$\tau_0/\tau = 1 + K_D[\text{Q}]$$

where τ is the measured fluorescence lifetime and $[\text{Q}]$ is the concentration of the quencher.⁵³ From this, $K_D = 0.0183 \text{ mM}^{-1}$ was estimated.

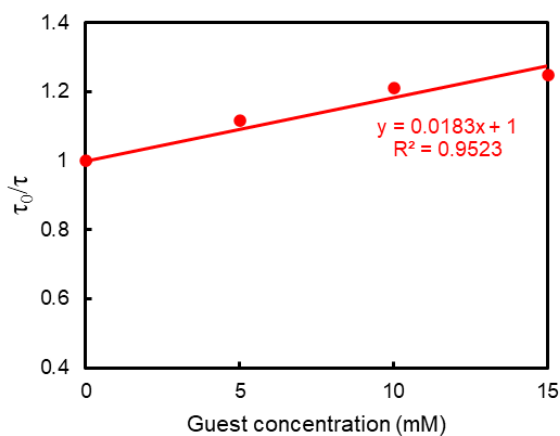


Figure S24. Plot of the ratio of fluorescence lifetimes versus guest concentration.

When the quenching process is purely dynamic, the ratio of the fluorescence lifetimes (τ_0/τ) is equal to the ratio of the fluorescence intensities (I_0/I). In contrast, for purely static quenching, τ_0/τ remains unity. The dynamic contribution ratio (f_{dyn}) and static contribution ratio (f_{stat}) can be defined as follows.

$$f_{\text{dyn}} = \{(\tau_0/\tau) - 1\} / \{(I_0/I) - 1\}$$

$$f_{\text{stat}} = 1 - f_{\text{dyn}}$$

Table S2. Dynamic contribution ratio (f_{dyn}) and static contribution ratio (f_{stat}) relative to guest concentration.

[Q] (mM)	$(\tau_0/\tau) - 1$	$(I_0/I) - 1$	f_{dyn}	f_{stat}
3	0.055	0.503	0.109	0.891
6	0.110	1.704	0.065	0.935
9	0.165	3.350	0.049	0.951
12	0.220	6.698	0.033	0.967
15	0.274	10.802	0.025	0.975
18	0.329	16.825	0.020	0.980
21	0.384	22.089	0.017	0.983
24	0.439	32.176	0.014	0.986
27	0.494	39.014	0.013	0.987
30	0.549	46.054	0.012	0.988

9. Theoretical calculations

The conformers of **1a**, **1b**, **1c**, **2** were optimized at the DFT level using the r²SCAN-3c/def2-mTZVPP.⁵⁷ The calculations were performed using ORCA software version 5.0.4.⁵⁸ The X-ray crystal structure of **1a**³⁵ (CCDC 2325723) and **2** were used as the initial conformation for geometry optimization.

<optimized geometries >

88				O	3.53490181697048	-1.29894010790441	-2.89289465755571
1a				C	3.26864214271689	-1.36471855605705	-4.31978153513691
C	1.23074814375896	0.12362644670565	0.46460587371247	H	-2.13282619884293	-2.93217786419166	2.19738724324575
C	1.31186656492148	-1.26419538996623	0.37759546999137	H	-2.88020083958135	-2.34540856152259	0.68266571315206
C	0.21431396340976	-2.08101591794721	0.69638274255640	H	-2.37464856138545	1.21449806608975	2.38581284366467
C	-0.96318351812291	-1.43456802951606	1.10838946835406	H	-3.03822069839513	0.70588245857770	0.85061075497932
C	-1.04430329277073	-0.04674590343991	1.19540070090881	H	3.14775879133637	1.03447032844387	0.89035613643047
C	0.05324818996683	0.77007514688619	0.87660622385513	H	2.40040317426628	1.62123963968690	-0.62437498883906
C	-2.26486550552877	-2.05985799453614	1.55149566987252	H	3.30577637931978	-2.01683925823113	0.72239198870073
C	-2.97660155227790	-0.91225835679884	2.30751092327363	H	2.64221322763140	-2.52543040571022	-0.81282179043987
C	-2.40273326076768	0.38039760315353	1.68230311370025	H	1.95628671436239	2.75991195967465	1.40959019791310
C	2.53243418259716	0.74891984912822	0.02151840641430	H	-1.68872310084162	-4.07084044887981	0.16337009462306
C	3.24418017254361	-0.39867748618421	-0.73448962994009	H	-2.72041040467159	5.27886382869112	0.80518127368739
C	2.67029842364088	-1.69133832814465	-0.10930093469308	H	-1.64239153503492	7.49559101712990	1.18282306952405
C	-0.06433804708505	2.21960493253995	0.96950037187071	H	0.77784609990838	7.67336326324823	1.59691765996329
C	0.33189870447796	-3.53054362482175	0.60347853969207	H	2.22589537983608	5.65759701984903	1.64483404637851
N	-1.19236276083144	2.89564363128975	0.85174942815823	H	2.98796681921974	-6.58980785152511	0.76775678217260
C	-0.85034572929827	4.22072582192638	1.01931880940383	H	1.90994523002957	-8.80652999724755	0.39009206646103
C	0.53935751740887	4.34420236519685	1.25206782011200	H	-0.51029449826907	-8.98429468349082	-0.02400178408404
N	1.01668530489627	3.05336271315525	1.20411633719818	H	-1.95834098231896	-6.96852495442976	-0.07189399379757
N	1.45992292646089	-4.20658506728618	0.72121182625202	C	-6.70302914816054	-3.38671419403701	3.80786733571731
C	1.11790336191174	-5.53166515826606	0.55363319255970	H	-6.65327864037262	-2.50535828105278	1.81799574492832
C	-0.27179990849305	-5.65513708006354	0.32088471161835	H	-6.90588301142083	-1.33122444034074	3.12024544500117
N	-0.74912527129073	-4.36429699737519	0.36885047662162	C	-3.82663434748808	1.19036811261812	6.44698432984879
C	-1.65384348603194	5.36298147808130	0.98859321592809	H	-1.92709576748482	0.20924873214641	6.04000804339886
C	-1.04310213433690	6.59025326556695	1.20000254275495	H	-3.26666816381433	-0.91139362002255	6.34007114806807
C	0.33906021998788	6.69328225463728	1.43609685899685	H	6.92093876421732	1.19430034002073	-0.24503495491341
C	1.15811081069760	5.57126725352401	1.46594762880659	C	6.97066657349202	2.07565406244342	-2.23490853711220
C	1.92139944018192	-6.67392231002933	0.58434635222139	H	7.17344517998901	0.02015466903382	-1.54729296670816
C	1.31065657877873	-7.90119124136700	0.37292419469411	C	4.09353169284632	-2.50193932284612	-4.87377210891764
C	-0.07150697454230	-8.00421591339509	0.13683020530634	H	3.53380337177818	-0.40009967906443	-4.76714612622124
C	-0.89055603256731	-6.88219899052376	0.10699263806509	H	2.19416510857464	-1.52054777209125	-4.46665220035320
C	-4.48777314677574	-1.02409894535434	2.14940368181045	H	5.16047969339094	-2.32953622323380	-4.70513355434289
O	-5.17162166457273	-0.36257094507856	1.40720036524792	H	3.92336458995079	-2.58734386622539	-5.95149554601871
O	-4.95664012044822	-2.02475310074179	2.92270801094654	H	3.81673541691485	-3.45015043666515	-4.40405015045195
C	-6.38947186510756	-2.25972726610552	2.85280478751323	H	-6.16825997716840	-4.29871133918992	3.52732318686437
C	-2.61107705229121	-0.97522474425375	3.79207095984407	H	-7.77702658120938	-3.59603567035987	3.78810466114344
O	-1.83424291718864	-1.75032385801782	4.29531121434385	H	-6.42166744624088	-3.12115984757659	4.83092988531201
O	-3.26754120781814	-0.01221045321302	4.46598257734449	H	6.68925838880901	1.81011364259970	-3.25796192638123
C	-3.00153174015261	0.05333441844964	5.89292696230341	H	8.04467470613623	2.28492382151823	-2.21518115749180
C	4.75534730645747	-0.28683474579612	-0.57634856055861	H	6.43595054384692	2.98767678554727	-1.95434644468075
O	5.43919600021181	-0.94843718307132	0.16578830053788	H	-3.54985853124228	2.13869271969491	5.97747931792125
O	5.22424142545019	0.71377698741661	-1.34969148417371	H	-3.65665643967729	1.27559680823787	7.52475160632742
C	6.65708677737538	0.94868215715707	-1.27983560283798	H	-4.89353602414889	1.01788408445752	6.27813619420976
C	2.87869243707563	-0.33570179392889	-2.21905686838128				
O	2.10167982831462	0.43923652259426	-2.72226986839672	100			

1b				H	1.97119380658399	2.76579291183522	1.34870524589825
C	1.22728277513689	0.12009965444789	0.45570930466755	H	-1.70751426193640	-4.07993377898089	0.21800728896252
C	1.30590431777903	-1.26766035455896	0.36711042513885	H	-2.71810132340920	5.27691697822458	0.89045907882025
C	0.20991752226511	-2.08496423633516	0.69275636500378	C	-1.90165415661865	7.84869928204366	1.22711524144068
C	-0.96330995151917	-1.43542999630291	1.11398465168465	C	0.98223872897632	8.06619733442276	1.62045178951849
C	-1.04194999398967	-0.04763623517019	1.20253150514214	H	2.23253688052414	5.66528746184687	1.56759814941778
C	0.05390991945980	0.76966581368917	0.87670587044154	H	2.98058539738744	-6.59292176562393	0.67727899605236
C	-2.26327312805027	-2.05946104959465	1.56374685702891	C	2.16338399713455	-9.16438579555509	0.33916843161720
C	-2.97481128050062	-0.91082541960079	2.31821915975377	C	-0.72039505737134	-9.38065663440188	-0.05579650010731
C	-2.39713138054893	0.38177427869508	1.69653976244749	H	-1.97005709883462	-6.97961629175217	-0.00096290126130
C	2.52709308766309	0.74437185678525	0.00611524393068	C	-6.70802568923890	-3.39162836594098	3.79193429507409
C	3.24031738147337	-0.40436327699250	-0.74647016681622	H	-6.65078278454251	-2.49577260642484	1.80877873746551
C	2.66090307793007	-1.69737127837749	-0.12699212672362	H	-6.90764692908797	-1.33117015280242	3.11849172494351
C	-0.06168644832641	2.21858814437670	0.97200254507556	C	-3.84149645090158	1.19168421738504	6.45364943070043
C	0.32514856717594	-3.53384751489976	0.59680066144463	H	-1.94092555139117	0.20942646273823	6.05454856164696
N	-1.19389857701849	2.89463106591345	0.88776983930956	H	-3.28209454053213	-0.91043088347340	6.34987040145999
C	-0.84652445025849	4.21961656691602	1.04375643073030	H	6.91643332892168	1.17594699020226	-0.21623187893535
C	0.54433429189564	4.34510948004495	1.23260280930906	C	6.96965687352450	2.10080963098690	-2.18609221640612
N	1.02474633475735	3.05559793287347	1.17294283761171	H	7.17046999438764	0.03067741316569	-1.54338276954261
N	1.45714085658627	-4.21027076874199	0.68083533865990	C	4.13992955361567	-2.49021800465654	-4.88305857438984
C	1.10939872904785	-5.53506047231325	0.52388551948428	H	3.55391092565829	-0.39548178601628	-4.77807324052359
C	-0.28150103363952	-5.65998690581738	0.33461572778171	H	2.22656752364933	-1.53243243240523	-4.48546698071336
N	-0.76156048839714	-4.37039081356074	0.39543086330285	H	5.20377381311624	-2.30479028455401	-4.70859804549771
C	-1.64540083657999	5.36476056850372	1.03915764470325	H	3.97651961143340	-2.57713671600586	-5.96172698096245
C	-1.05135981617658	6.60622014858397	1.22749000488561	H	3.87231766390065	-3.44189851765979	-4.41503126971894
C	0.35452120114898	6.71363332136213	1.42032878716441	H	-6.17214850442508	-4.30156897348285	3.50680452157777
C	1.15868537013359	5.57720232851443	1.42302294516927	H	-7.78197841166341	-3.60067016824566	3.76639449401264
C	1.90792016059916	-6.68041090478038	0.52812767446169	H	-6.43057173005975	-3.13362265275653	4.81799973759885
C	1.31352321476061	-7.92159578478640	0.33890149598627	H	6.68954484577902	1.85809630805302	-3.21516681232314
C	-0.09228672829272	-8.02846020621994	0.14571016621952	H	8.04376514484512	2.30899606538131	-2.16011164855916
C	-0.89618256976309	-6.89177744267041	0.14355236257759	H	6.43494907146969	3.00671126981197	-1.88625153142422
C	-4.48548360232022	-1.02053422429917	2.15503341421270	H	-3.56229490765224	2.13950118460408	5.98454249122380
O	-5.16744941316312	-0.35607889181903	1.41369671934372	H	-3.67578747275239	1.27739349558021	7.53206580320121
O	-4.95805740781795	-2.02413625647663	2.92317307436434	H	-4.90781372558823	1.01969260476500	6.28052477510599
C	-6.39029355663745	-2.25780563378157	2.84624189792342	H	0.79324016767631	8.72792144034876	0.76665699677958
C	-2.61642006552714	-0.97530901521995	3.80419087759154	H	2.06458974607354	7.98163249539255	1.74695727970800
O	-1.84326823692317	-1.75120712976812	4.31176506374252	H	0.57847551029712	8.57109929384709	2.50643740259294
O	-3.27535050849331	-0.01159324058503	4.47563119568029	H	-1.80322397359338	-9.29602080818069	-0.17810985902232
C	-3.01484642843438	0.05394027910704	5.90310330397168	H	-0.52824677147594	-10.04462981031838	0.79552663455406
C	4.75077537343290	-0.29585650586827	-0.58147248951144	H	-0.31969526173518	-9.88301110853059	-0.94462680593355
O	5.43449066480824	-0.97182621803649	0.14763312401838	H	1.86946348539788	-9.85601958150694	1.13808912276060
O	5.22134860173271	0.72080870368766	-1.33387354922375	H	3.21694249854258	-8.91382721371152	0.48477030777116
C	6.65370457414695	0.95323285246943	-1.25653255707508	H	2.07543939466189	-9.71511251280569	-0.60510291704321
C	2.88505983216612	-0.34075444990046	-2.23314480849546	H	-2.95471786978341	7.59797156204885	1.07825985445321
O	2.10410842619127	0.42710389859332	-2.74091522452645	H	-1.60582269914268	8.54188281801768	0.43027004159133
O	3.55617921481290	-1.29601911090351	-2.90463502338822	H	-1.81657844712005	8.39777647325394	2.17263631032065
C	3.29825376395796	-1.36354008347337	-4.33252258785942				
H	-2.12832716952328	-2.92864429341435	2.21340971246358	104			
H	-2.88103269207857	-2.34988667886955	0.69813790780309	1c			
H	-2.36297574931596	1.21278891353822	2.40331318978885	C	1.27450721318487	0.05815702836617	0.60052103684501
H	-3.03424740324331	0.71447862709927	0.86904936898227	C	1.32095565632036	-1.32764686349799	0.47439721006843
H	3.14414767523780	1.03674103180180	0.87158245498143	C	0.19942865918711	-2.12831743280173	0.75358029646458
H	2.39178466090658	1.61279404904803	-0.64449889028313	C	-0.96621212841971	-1.45939172124644	1.16835159098018
H	3.29769646485167	-2.03259295658918	0.69970513721015	C	-1.01267152782905	-0.07357137204759	1.29421680647858
H	2.62609851178027	-2.52727901448677	-0.83515403119759	C	0.10891599950529	0.72702835936221	1.01532366765641

C	-2.28926541404939	-2.06316492655936	1.57651976149519	O	1.79920017492594	-9.17510267673357	0.22238410889452
C	-2.98626761109892	-0.91858473555604	2.35046896144450	O	-0.72173204241100	-9.28784691345523	-0.18236990631047
C	-2.36634621445408	0.37594788088103	1.77441687435105	H	-2.09532511961656	-6.92899821186967	-0.11844715680638
C	2.59739937138759	0.66209217876645	0.19218347436077	C	-6.79819203792431	-3.35778476527239	3.68392195082573
C	3.29352876553909	-0.48202840202379	-0.58313360351874	H	-6.69318605323824	-2.39623517946954	1.73381254119126
C	2.67453635092359	-1.77672459878792	-0.00656902088906	H	-6.93654106426376	-1.27103349052277	3.07982117809586
C	0.02753864570179	2.17293655976146	1.14980645427838	C	-3.88550531700034	1.08041240243930	6.53059698424758
C	0.28103186615608	-3.57419646713627	0.61933055964586	H	-1.99317991165713	0.08264013322636	6.13169898308811
N	-1.08445530136779	2.88504889025348	1.06363195813429	H	-3.35401692550320	-1.02572137819272	6.37493388042957
C	-0.70471336777005	4.19239866364282	1.26474580455658	H	7.00129572033147	0.99612022433592	0.02702288387054
C	0.68005109140572	4.27555699280800	1.48462245361221	C	7.10437057524036	1.95455897815173	-1.92472108162002
N	1.13032826052318	2.97758672081251	1.39505178755052	H	7.24317613093767	-0.13124848695779	-1.31743187816502
N	1.39361864162361	-4.28575014199696	0.70324676132029	C	4.18308776332644	-2.48218372521132	-4.76483607789375
C	1.01419627544038	-5.59331472621826	0.50339530803378	H	3.65735353550076	-0.37469192202406	-4.60788790395737
C	-0.37099932859406	-5.67730752430891	0.28647976445081	H	2.29381701265827	-1.47951358958959	-4.36373149669397
N	-0.82179033916843	-4.37958700196632	0.37662747231212	H	5.24960262262899	-2.33345376634165	-4.57231323929096
C	-1.48755618208576	5.35573970026794	1.27176125350161	H	4.03124575211016	-2.53406660536205	-5.84745740826270
C	-0.85865286167041	6.56573545433616	1.50763972966799	H	3.88146667548098	-3.43819567319436	-4.32729225620819
C	0.55202761910774	6.63064002342659	1.73674246698356	H	-6.28266940645262	-4.27124789099524	3.37355655561142
C	1.33473032832106	5.48361037470873	1.72625629880762	H	-7.87683944395757	-3.53746888724278	3.63927677669762
C	1.79765215925436	-6.75625405496661	0.49502761690265	H	-6.52638962623616	-3.14261899964554	4.72132478544145
C	1.16890466092892	-7.96665452432385	0.26087067538040	H	6.83140693213608	1.73778376400498	-2.96148388886535
C	-0.24223693242684	-8.03238724828010	0.03476886419634	H	8.18308756166207	2.13417908510668	-1.88153746327179
C	-1.02554415332131	-6.88578433314147	0.04662140644582	H	6.58927417585776	2.86856156401713	-1.61524405085128
C	-4.49609244576601	-0.98567616546705	2.16200242251324	H	-3.58599571764928	2.03708225980614	6.09304401205181
O	-5.15314017415771	-0.27589925822147	1.44032585165072	H	-3.73488850665601	1.13305344174468	7.61335270821467
O	-5.00311302077716	-2.00768724510300	2.88352638922191	H	-4.95142645896661	0.92877705220919	6.33705825568935
C	-6.43938181459443	-2.20082285903878	2.78185301223803	C	3.20046709156140	-9.17603542957834	0.45910427898695
C	-2.65508785905438	-1.03218855186861	3.83966091376750	H	3.51208311853307	-10.22015355123970	0.39825224265711
O	-1.90757971169127	-1.83805436586321	4.33862997373572	H	3.43771025797353	-8.78009254187765	1.45626500017607
O	-3.30598050905246	-0.07385194010525	4.52744417543081	H	3.73570575191435	-8.58965866070869	-0.30074513620934
C	-3.06672475120496	-0.05305786175438	5.95970955887276	C	-2.11746693395935	-9.42089359444179	-0.40755214129775
C	4.80361262958393	-0.41486294941362	-0.39663848458845	H	-2.29524606063249	-10.48726266189780	-0.55627213370067
O	5.46134968298018	-1.12364772360443	0.32540252296685	H	-2.43324729961322	-8.87037225679279	-1.30508172003140
O	5.31001231388919	0.60589594262192	-1.12032542582871	H	-2.69808612614419	-9.07199511385113	0.45810286587825
C	6.74639819892865	0.79905840170988	-1.02044390807162	C	-2.88931693842920	7.77615139431754	1.30648790941742
C	2.96046434017039	-0.36761961324167	-2.07189832880404	H	-3.20060313740201	8.82035732329843	1.36752705096975
O	2.21424309169974	0.44006452435477	-2.56983451965097	H	-3.42579778900683	7.18952514644269	2.06526515261885
O	3.60858809625071	-1.32711105038414	-2.76070757866600	H	-3.12541691619715	7.38092727617325	0.30876279398661
C	3.36788470643784	-1.34674591086379	-4.19273624094004	C	2.42721382976936	8.01813878328708	2.18242883249443
H	-2.18686823851382	-2.95328739979292	2.20345811789506	H	2.60530666992206	9.08443238825975	2.33132469279186
H	-2.89823618045321	-2.31471887073493	0.69249052695597	H	3.00890023340212	7.66885312768108	1.31764924456663
H	-2.32550830411777	1.18697208100615	2.50376107329104	H	2.74146272405084	7.46759361487703	3.08048752006443
H	-2.98091857142663	0.74499169438222	0.94539753180903				
H	3.20705788964448	0.91264840504824	1.07602313065591	100			
H	2.49474493623312	1.55303508108805	-0.43352805039213	2			
H	3.28975981235146	-2.14536928238491	0.82216522911472	C	1.18605829132211	0.11718059188218	0.51769492704960
H	2.63362993461317	-2.58792657933284	-0.73568143719481	C	1.26650147034490	-1.26923953109330	0.40875690031771
H	2.06326053005836	2.65738031360074	1.58903545465727	C	0.16933450550330	-2.08946714503906	0.72022374885975
H	-1.75534279612013	-4.06007843144167	0.18451730840683	C	-1.00729736286439	-1.45156006243430	1.14749453518177
H	-2.55365331795654	5.28361259416111	1.09520841212280	C	-1.08774112705899	-0.06513993246079	1.25643951613542
O	-1.48837674710394	7.77451900341889	1.54507011851238	C	0.00944008022318	0.75509049939816	0.94498269295482
O	1.03174274685800	7.88578301902223	1.95522994563674	C	-2.30644253209813	-2.08358849462840	1.58787869794606
H	2.40417051296009	5.52613958053530	1.89370833030916	C	-3.01402458898901	-0.94797112997309	2.36474146235294
H	2.86409934006969	-6.68349932177747	0.66920203333305	C	-2.44321176128407	0.35442252893323	1.75723208590476

C	2.48521639363110	0.74918514454532	0.07731898401627	C	-6.72035181827024	-3.49089762717851	3.79535236397559
C	3.19273544818615	-0.38642784803069	-0.69961864384477	H	-6.69763359763972	-2.52072041737067	1.84677032200262
C	2.62197338328536	-1.68880400272162	-0.09203335503601	H	-6.92986575834933	-1.40625265509108	3.20388978454054
C	-0.10816675079401	2.20320418205208	1.06099871179602	C	-3.88271699892062	1.05511791521844	6.54959134578837
C	0.28699250710685	-3.53758092340869	0.60427838459131	H	-1.96119332251583	0.13337898259336	6.10796997448910
N	-1.23586058299159	2.87510049567925	0.95484969156686	H	-3.26708214954707	-1.02840260872857	6.39948425685114
C	-0.89867324345745	4.20254611632452	1.14504281615792	H	6.87554278010392	1.18709450399741	-0.18030201298355
C	0.50491507749953	4.32392756653579	1.38179198446143	C	6.89841306927972	2.15848775469742	-2.12827718184171
N	0.97814677228141	3.03001303167480	1.30727750622440	H	7.10874865092085	0.07357970054085	-1.53803571497884
N	1.41468598508910	-4.20944297752465	0.71061708316165	C	4.06545036725835	-2.38532679665946	-4.88568807061342
C	1.07752685662880	-5.53692262535598	0.52059144363171	H	3.44807548323384	-0.30245456415596	-4.73375373871981
C	-0.32604003865292	-5.65835382688680	0.28374976224328	H	2.14280873420493	-1.46557016512066	-4.44479053387751
N	-0.79928566738727	-4.36442903181043	0.35799248949581	H	5.12851897849051	-2.18602976652388	-4.72237417436525
C	-1.69976191944519	5.32505085306129	1.13451677424457	H	3.88853777690306	-2.45464403324208	-5.96346260310643
C	-1.10683501337990	6.58174910744963	1.37099674156089	H	3.81928849958262	-3.34989823424400	-4.43257133900081
C	0.31245022405648	6.68579328131734	1.61645565368841	H	-6.19168143004236	-4.39005051039970	3.46602523648682
C	1.12196112837119	5.52796784401361	1.61799477893888	H	-7.79492373343917	-3.69767996842428	3.78175762648983
C	1.87862244578868	-6.65941841112807	0.53134905882975	H	-6.42379110857408	-3.27214239237591	4.82516926800723
C	1.28571911572022	-7.91616041428991	0.29503527944180	H	6.60226975648806	1.94022944581237	-3.15831976371381
C	-0.13354434219405	-8.02025338266126	0.04947178751287	H	7.97288300590236	2.36576806647521	-2.11422800632601
C	-0.94305897078610	-6.86242917670998	0.04765849564228	H	6.36921753701496	3.05718690915615	-1.79855552145012
C	-4.52648323453269	-1.05451882952633	2.21718587309238	H	-3.63623355568470	2.01897932226360	6.09514017767863
O	-5.21974971892640	-0.35748849857977	1.51750717523455	H	-3.70475739082976	1.12553555214356	7.62712206080790
O	-4.98451214505827	-2.09167587282028	2.94737848082220	H	-4.94608881378809	0.85645069030914	6.38748701501206
C	-6.41880381180358	-2.32231419578826	2.88776869763455	C	0.08147605029217	9.09494211623696	1.84623888362839
C	-2.63784585127235	-1.03173192827845	3.84561662748927	C	-1.30875053025705	8.99481850262895	1.60599507874890
O	-1.83804679917023	-1.79742943170778	4.32685093649754	H	1.93509281661867	8.04948756816133	2.03485965859874
O	-3.30984430846953	-0.09637215995580	4.54185580026919	H	0.52694024084079	10.06877446621644	2.02755759468487
C	-3.03242241005526	-0.04888276319781	5.96790254849539	H	-2.95038411737467	7.69186090504269	1.18974088911772
C	4.70521152861613	-0.27990125607359	-0.55227809340282	H	-1.92033656236956	9.89223190498711	1.60445490953438
O	5.39849086973691	-0.97655848157655	0.14775931213100	C	1.48766511796259	-10.32926690060121	0.06045753416591
O	5.16298031525973	0.75789872450560	-1.28172429200836	C	0.09745867526770	-10.42943988985361	-0.17988087694711
C	6.59714182298571	0.98919786445349	-1.22151165840215	H	3.12925625707412	-9.02623590396852	0.47664339484052
C	2.81634611274284	-0.30266190490703	-2.18044125131346	H	2.09925686251962	-11.22667646255962	0.06219779543154
O	2.01739453704667	0.46387787813169	-2.66174399924091	H	-1.75615178221778	-9.38402601070343	-0.36881004168350
O	3.48981514074068	-1.23660473683767	-2.87715675063305	H	-0.34798588418439	-11.40330598689537	-0.36106762501864
C	3.21376752587442	-1.28265068200217	-4.30351878170998				
H	-2.17145805024162	-2.96652675321305	2.21819165020884	122			
H	-2.92615279829905	-2.35597358913554	0.71802997023039	1a (orcinol) ₂			
H	-2.41184538822746	1.17765539975193	2.47341677270940	C	0.96401290469669	0.25428614256328	0.31470383731027
H	-3.08337059662548	0.69334479752196	0.93449224106259	C	1.10150035942426	-1.12988423931733	0.26189688084877
H	3.10494969419610	1.02148875877673	0.94717671302591	C	0.18703795983711	-1.96322049680027	0.90461833568727
H	2.35025769364123	1.63216349702708	-0.55294658524427	C	-0.87478824044467	-1.37157286572362	1.58761665334619
H	3.26216544500972	-2.02763504032363	0.73071806094248	C	-1.01227890221464	0.01259210163551	1.64042183947268
H	2.59061539837873	-2.51207870472839	-0.80816330970910	C	-0.09780355713902	0.84593252724764	0.99771869014494
H	1.91295030004033	2.72865246364729	1.52159074725448	C	-2.04013611433778	-2.05872660446586	2.23914004221617
H	-1.73410468672682	-4.06313177563663	0.14366336147334	C	-2.73625551398457	-0.91731711885800	3.03372389871998
H	-2.76699775288730	5.24277092016167	0.94992679342285	C	-2.27695594808463	0.40172581752342	2.35480538048848
C	-1.88216245377109	7.77197575638433	1.37556190584632	C	2.12935514845339	0.94142790992173	-0.33684961895875
C	0.86622342828981	7.97090738693003	1.85067741098646	C	2.82543333365794	-0.19998960826229	-1.13146588129756
H	2.19039103508147	5.61152261135709	1.79837297518566	C	2.36615366781848	-1.51902533697575	-0.45252480768389
H	2.94583980991035	-6.57710585041794	0.71603015072911	C	-0.27004304930153	2.30497877629671	0.98426108483268
C	2.06105220570621	-9.10638324783889	0.29073517467992	C	0.35928531711420	-3.42226726721828	0.91811000100394
C	-0.68729494088901	-9.30540929225167	-0.18457099338930	N	-0.63187023655164	2.99908957874632	-0.08031380512562
H	-2.01147580591060	-6.94601680294628	-0.13278171565290	C	-0.68638315966626	4.31617851237351	0.35420414563954

C	-0.33562109018104	4.38517262357465	1.72268581236821	H	-1.39461058942466	-2.45583154361693	6.49399336352066
N	-0.08298885535344	3.08014924291676	2.09376411654322	H	6.73221557526715	-1.15358118160587	-0.84296514389361
N	0.72120374136422	-4.11633096684172	1.98267997449853	H	6.67105548330246	-0.20963925053311	-2.34230001127053
C	0.77568091048070	-5.43343999229538	1.54821651735626	C	6.72189612206944	-2.36530500588910	-2.64966018668458
C	0.42476793296171	-5.50249710505749	0.17978592768402	H	1.48365748902050	1.33845890998316	-4.59169636696570
N	0.17211546351694	-4.19748780986201	-0.19133005639598	C	3.42109387006497	2.12354271641026	-5.19878312812070
C	-1.01814906762218	5.47911219729778	-0.34092892658404	H	2.61143012859366	0.10171173293920	-5.18129532226701
C	-0.98115050864022	6.68008532147935	0.35393364784409	C	-2.90390704625296	-2.59143694685294	-1.52799628949297
C	-0.62354914136809	6.73338566943955	1.71165765843848	H	-2.87413907197725	-3.66508080848068	-1.69301443383963
C	-0.29399885820490	5.58624635329076	2.42257750354894	C	-1.80254322674407	-1.81557033906558	-1.87758777876978
C	1.10752333951031	-6.59634019671737	2.24336107989129	O	-0.71096216100655	-2.47488729087509	-2.38718394581809
C	1.07043463291278	-7.79734773576519	1.54856697105594	H	0.01100331436654	-1.84014257753316	-2.56522888197801
C	0.71266647542021	-7.85071406171945	0.19090437310329	C	-1.80443672431012	-0.43300651953287	-1.70169971694818
C	0.38304792714628	-6.70360865146327	-0.52003235918293	H	-0.93595970746650	0.16275980160855	-1.96759091701219
C	-4.25531813708841	-1.04591517073451	3.03060236050361	C	-2.92637444040131	0.16548115335800	-1.12655291039666
O	-4.89414744244159	-1.92504476675755	2.50704693473500	O	-2.99465993944354	1.49759545503221	-0.87048464949722
O	-4.79294738831500	-0.00332671599459	3.69276916188629	H	-2.11247061288891	1.92507781238056	-0.90248573757514
C	-6.24487313228348	0.01855775308251	3.76565900606245	C	-4.03981556040956	-0.60411005879587	-0.77569676104962
C	-2.23596169393218	-0.99226953166603	4.46999179741472	H	-4.90318227431626	-0.10884916787938	-0.34055514517814
O	-1.31558180269166	-0.34759221026734	4.93742873517152	C	-4.03793829849784	-1.98028782812063	-0.98849442373458
O	-2.89955001505492	-1.92062067140381	5.16131342882198	C	-5.25064879704135	-2.80590832865211	-0.65700896228646
C	-2.44873384207369	-2.15991396285058	6.52794869696380	H	-5.91180198605698	-2.28007572377476	0.03475800494312
C	4.34449683828317	-0.07142433162731	-1.12840471587709	H	-5.81585612348745	-3.03629839621754	-1.56845966790639
O	4.98339582143114	0.80762104829451	-0.60472859729612	H	-4.96851009470154	-3.75659311156301	-0.19386389139376
O	4.88205961900338	-1.11396493368659	-1.79070976065472	C	2.99299162818454	1.47430773520897	3.43044990003060
C	6.33397920540309	-1.13592348778951	-1.86363065759631	H	2.96313570870876	2.54794570672075	3.59549428769766
C	2.32508503198750	-0.12505128406409	-2.56771029043908	C	1.89168500191057	0.69834198230546	3.78003533124114
O	1.40469717698547	-0.76974272141335	-3.03510829066687	O	0.80005938017307	1.35756930716275	4.28964916439374
O	2.98866611232185	0.80325883453208	-3.25908282790253	H	0.07809358785838	0.72279735938503	4.46760188723340
C	2.53777059955396	1.04254266114600	-4.62568649342180	C	1.89368967286094	-0.68421241294004	3.60409080029745
H	-1.75678507612143	-2.90582672432382	2.87158167938541	H	1.02526563886737	-1.28006106113307	3.86997674251654
H	-2.73467985655064	-2.43711424071216	1.47764864038003	C	3.01566457115739	-1.28259153149624	3.02886912453626
H	-2.15253174145130	1.20790893129068	3.08339715386646	O	3.08403925537775	-2.61469133612971	2.77271330649095
H	-3.02450790505941	0.73256992550260	1.62205272091712	H	2.20184779818441	-3.04223542559778	2.80477529392511
H	2.82392720216780	1.31981323836949	0.42462150831452	C	4.12904354003748	-0.51290362157703	2.67801049537124
H	1.84598331299400	1.78853407575451	-0.96928135678327	H	4.99244084727016	-1.00808240874123	2.24280023086306
H	3.11372416969612	-1.84987684877526	0.28020483232766	C	4.12705942611153	0.86326685269479	2.89088489612427
H	2.24169120386376	-2.32520794054558	-1.18111229119162	C	5.33971760104521	1.68897498123098	2.55941163047589
H	0.23173558891168	2.71148840756084	2.99089813493042	H	5.90523241773795	1.91888000855540	3.47079504509785
H	-0.14267715772107	-3.82885815872105	-1.08844961219391	H	6.00061894945568	1.16342600932815	1.86718450672331
H	-1.29494514704457	5.43624055791890	-1.38977977727756	H	5.05749119385175	2.63990595164794	2.09682297798446
H	-1.23347985985000	7.60229211384370	-0.16070478865861	H	-3.24957556665968	-4.16265695049048	6.51840401932866
H	-0.60520729761564	7.69386313356163	2.21768825428853	H	-4.37955194219617	-2.92657759635120	7.11069511082085
H	-0.01954662797648	5.62912663997583	3.47218999062344	H	-3.02542085314262	-3.45335365839442	8.12966488534736
H	1.38444378678584	-6.55341849150476	3.29216515110111	H	-6.27536059307943	2.15611498397142	4.05725552906194
H	1.32282195865905	-8.71952931055409	2.06321699949767	H	-6.21638753765507	1.21437903407897	5.56219375915463
H	0.69424992466612	-8.81121870545534	-0.31506818436310	H	-7.72305184120856	1.30411311834482	4.62903878451992
H	0.10846863336028	-6.74654236999697	-1.56959829875693	H	6.30539461414161	-2.33110281196654	-3.66060430662411
H	-6.58188429480500	-0.90758630477026	4.24461664864956	H	6.36417871825929	-3.27339746543072	-2.15598952498287
H	-6.64305905242746	0.03584649267186	2.74497537775945	H	7.81201708934693	-2.42139430075505	-2.72741694066503
C	-6.63292989107602	1.24815844399556	4.55126469382541	H	3.11438134568999	2.33593776022233	-6.22744461477888
C	-3.33208939608032	-3.24094330817499	7.10099003196197	H	4.46855204843811	1.80916484403409	-5.20851276461025
H	-2.52243291390486	-1.21908372380613	7.08356686948912	H	3.33861958528519	3.04525239221972	-4.61621843657234

<Kohn-Sham orbitals>

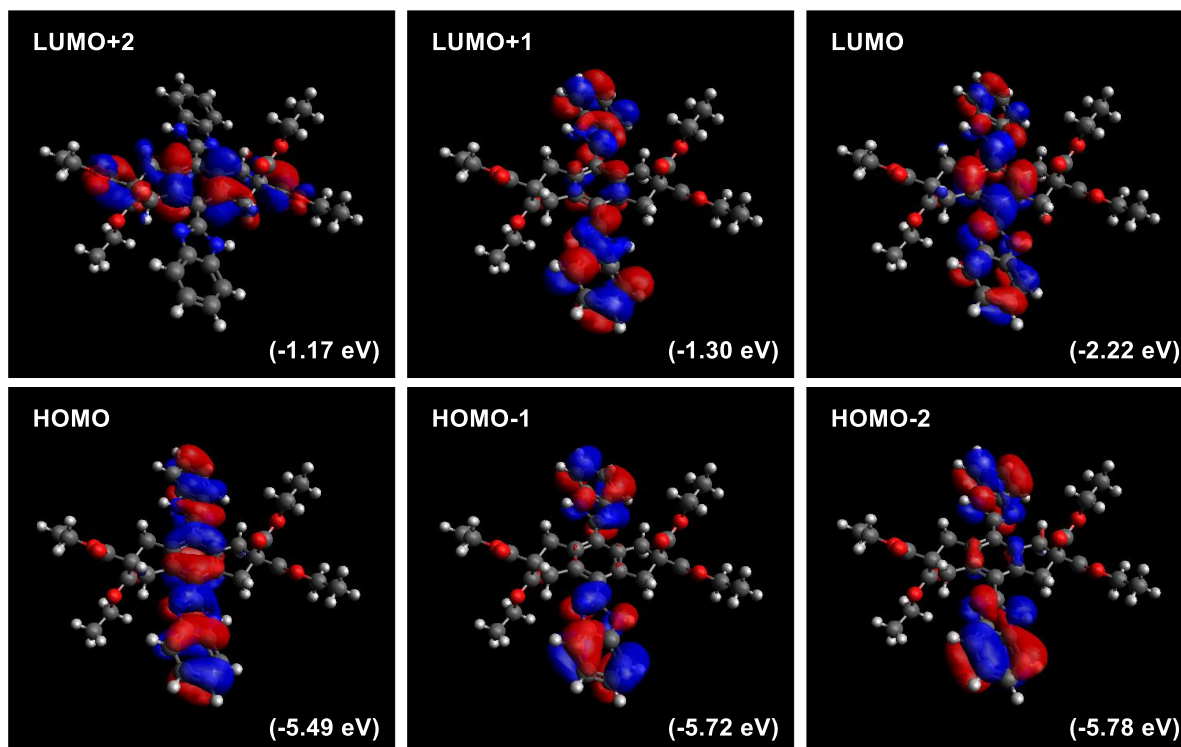


Figure S25. Kohn-Sham orbitals of receptor **1a** calculated at the r^2 SCAN-3c/def2-mTZVPP level.

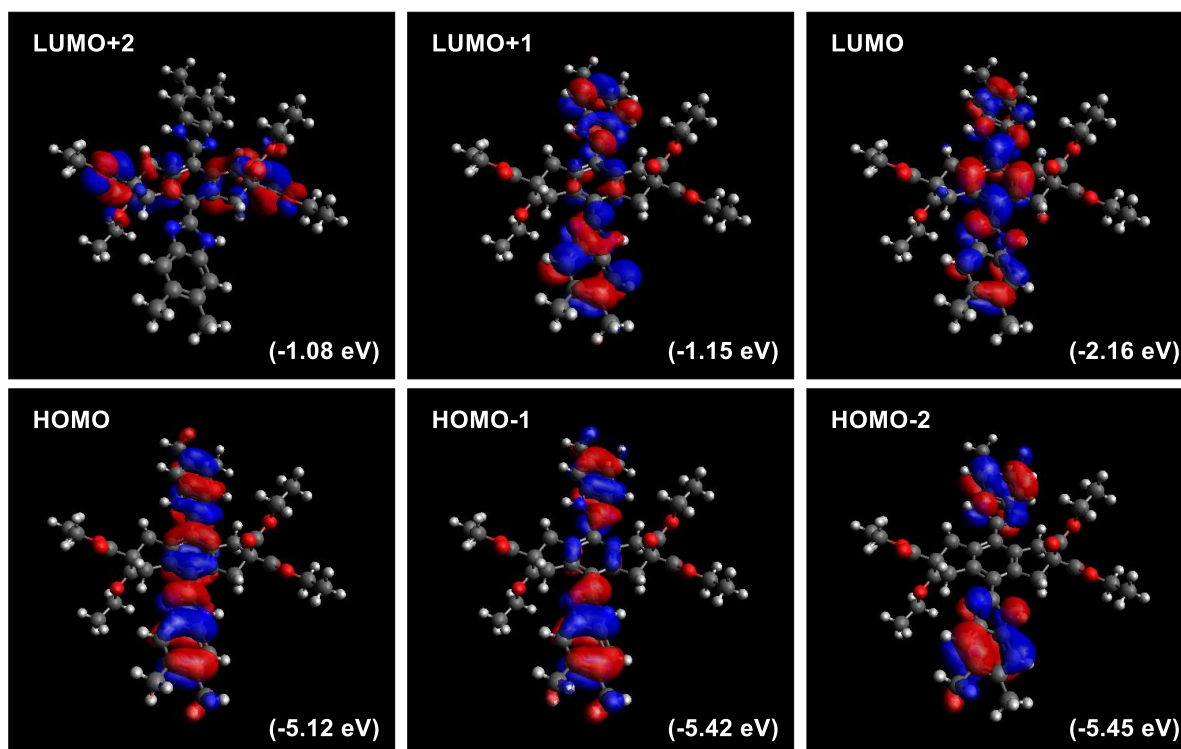


Figure S26. Kohn-Sham orbitals of receptor **1b** calculated at the r^2 SCAN-3c/def2-mTZVPP level.

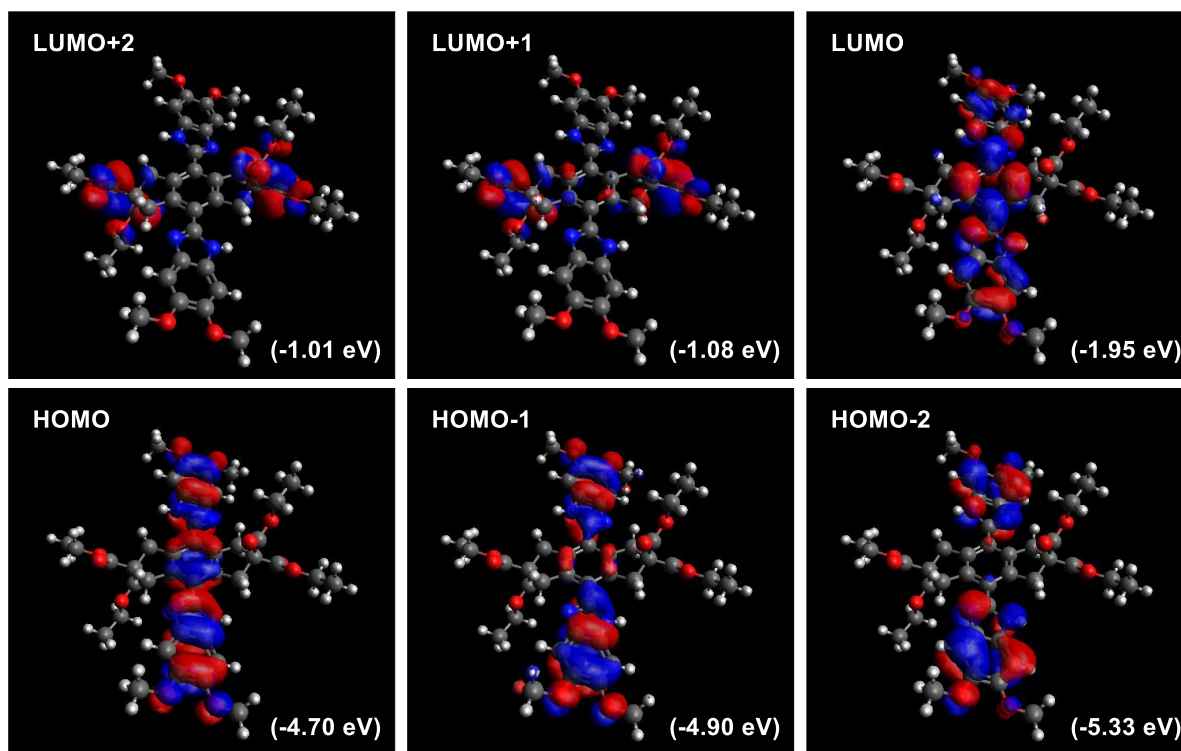


Figure S27. Kohn-Sham orbitals of receptor **1c** calculated at the r^2 SCAN-3c/def2-mTZVPP level.

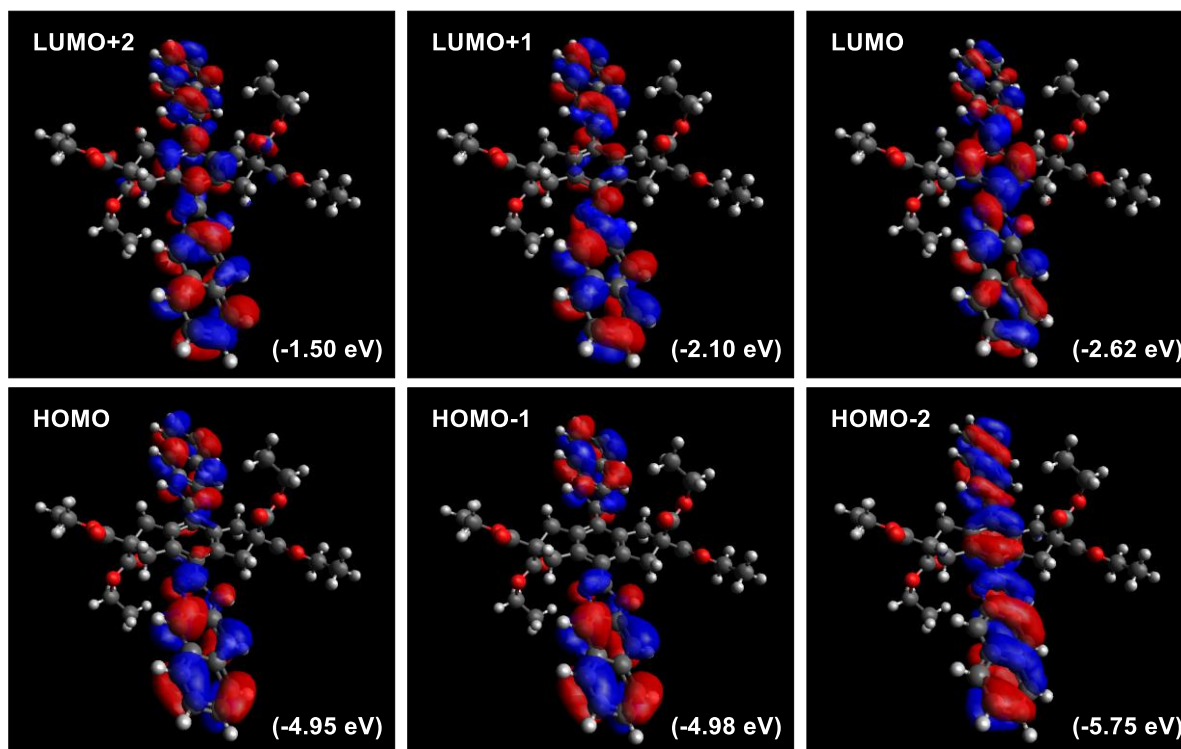


Figure S28. Kohn-Sham orbitals of receptor **2** calculated at the r^2 SCAN-3c/def2-mTZVPP level.

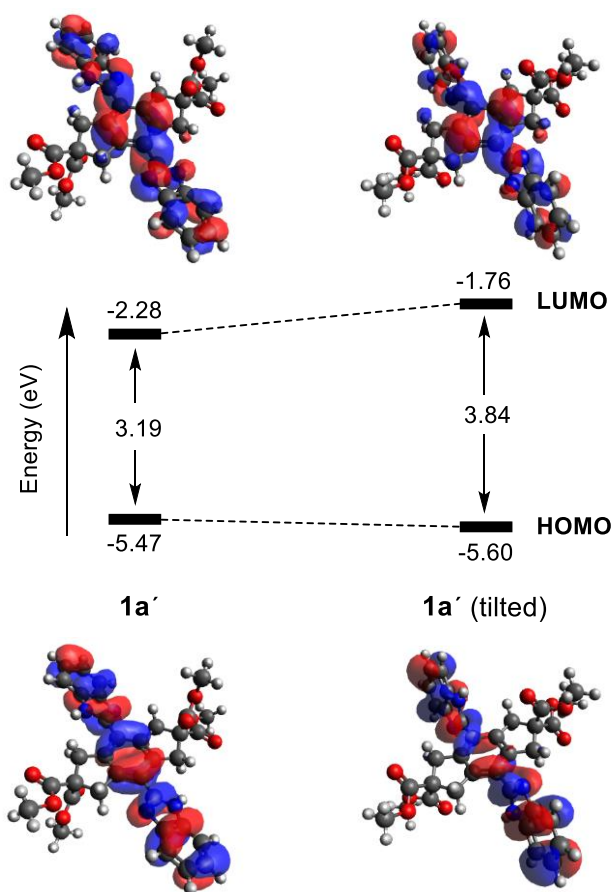


Figure S29. HOMO and LUMO energy levels and Kohn-Sham orbitals of receptor model **1a'**, where the ethyl ester groups at the 2,6-positions were replaced with methyl ester groups, was calculated at the r2SCAN-3c/def2-mTZVPP level. (left) The optimized conformation. (right) The hypothetical conformation where the benzimidazole units have the same dihedral angles as the optimized host-guest complex (**1a'**·(orcinol)₂).

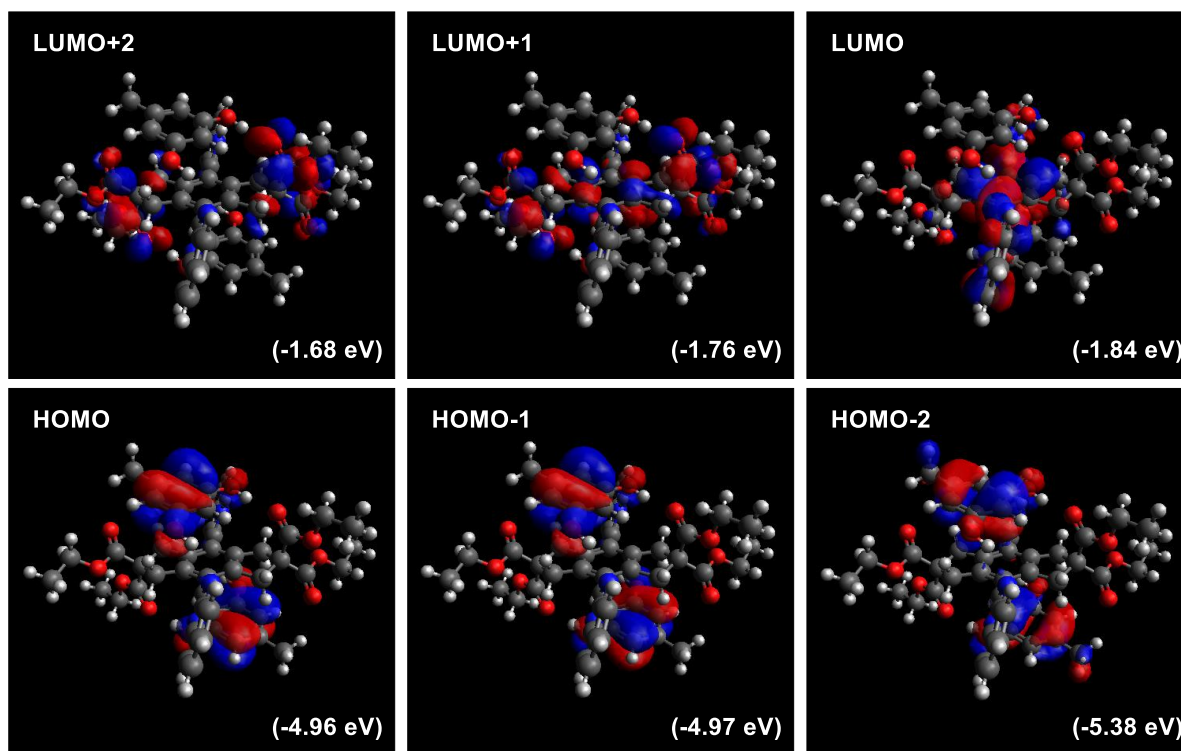


Figure S30. Kohn-Sham orbitals of receptor **1a** binding with orcinol calculated at the r²SCAN-3c/def2-mTZVPP level.

10. Additional references

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