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Electronic Supplementary Information

Solid-state red fluorescence of intramolecular ring-fused donor-π-acceptor-type fluorinated diphenylacetylenes achieved by enhancing intramolecular charge transfer properties

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Experimental

General

A Bruker AVANCE III 400 NMR spectrometer (^{1}H: 400 MHz and ^{13}C: 100 MHz) was used for recording ^{1}H and ^{13}C NMR spectra in chloroform-*d* ($CDCl_3$) solutions, and chemical shifts were reported in parts per million (ppm) using residual protons in the NMR solvent. The Bruker AVANCE III 400 NMR spectrometer was used for recording ^{19}F NMR (376 MHz) spectra in $CDCl_3$ solutions with $CFCl_3$ (δ_F = 0.0 ppm) or hexafluorobenzene (δ_F = –163 ppm) as the internal standard. IR spectra were recorded using the KBr method with a JASCO FT/IR-4100 type spectrometer; all spectra are reported in wavenumbers (cm^{-1}). HRMS data were recorded by a JEOL JMS-700MS spectrometer using the fast atom bombardment method. Dried glassware and a magnetic stirrer were used for all reactions. Reagent-grade chemicals were used after purification in the usual manner. Silica gel (Wakogel® 60N, 38-100 μm) was used for column chromatography and silica gel TLC plates (Merck, Silica gel $60F_{254}$) were used for TLC analysis.

Synthesis of IndCBZ-F through nucleophilic aromatic substitution

2-Ethynylindlo[3,2,1-*jk*]carbazole (0.3 g, 1.1 mmol) was placed in a two-necked round bottomed flask containing THF (11 mL). The flask was equipped with a Teflon®-coated stirring bar and cooled to 0 ºC. Subsequently, a solution of *n*-BuLi (1.6 mol L^{-1} hexane solution, 0.70 mL, 1.1 mmol) was slowly added to the mixture. After stirring for 30 min, pentafluorobenzonitrile (1.57 g/mL, 0.21 mL, 1.7 mmol) was gradually added to the mixture. Subsequently, after stirring for 1 h, the reaction mixture was heated to room temperature, stirred for 18 h, and poured into a saturated NH_4Cl solution. The crude product was extracted with EtOAc (thrice) and the combined organic layer was washed with brine (once). The organic layer was subsequently dried over anhydrous Na_2SO_4 and separated via filtration. The filtrate was evaporated in vacuo and purified by silica-gel column chromatography (hexane/CH_2Cl_2 = 1/1) to generate the corresponding product **IndCBZ-F** (0.053 g, 0.12 mmol) in 11% isolated yield as a yellow solid. Further recrystallization from CH_2Cl_2/hexane produced yellow crystals that were sufficiently pure for photophysical analysis.

2-[2-(4-Cyano-2,3,5,6-tetrafluorophenyl)ethyn-1yl]indro[3,2,1-jk]carbazole (IndCBZ-F)

Yield: 11% (yellow solid); M.p.: 272.0–273.9 ºC; ^{1}H NMR ($CDCl_3$): δ8.32 (s, 2H), 8.15 (d, *J* = 7.5 Hz, 2H), 7.93 (d, *J* = 8.1 Hz, 2H), 7.62 (td, *J* = 7.8, 1.1 Hz, 2H), 7.41 (td, *J* = 7.8, 1.1 Hz, 2H); The ^{13}C NMR spectrum was not obtained due to extremely low solubility in the common deuterated NMR solvents; ^{19}F NMR ($CDCl_3$): δ –134.25 (m, Ar*F*), –135.31 (m, Ar*F*); IR (KBr): ν3058, 2373, 2348, 2245, 2211, 1644, 1589, 1489, 1452, 1360, 1163, 1139, 1094, 1037 cm^{-1}; HRMS: (FAB+) *m*/*z* $[M]^+$ calcd for $C_{27}H_{10}F_4N_2$: 438.0780; found: 438.0777.

4-[2-(4-Cyano-2,3,5,6-tetrafluorophenyl)ethyn-1-yl]julolidine (JLD-F)

Yield: 13% (orange solid); M.p.: 197.6–199.9 ºC; ^{1}H NMR ($CDCl_3$): δ7.02 (s, 2H), 3.25 (t, *J* = 5.7 Hz, 4H), 2.73 (t, *J* = 7.1 Hz, 4H), 1.97 (quin, *J* = 6.1 Hz, 4H); ^{13}C NMR ($CDCl_3$): δ145.9–148.5 (dm, *J* = 259.3 Hz), 148.3–145.7 (dm, *J* = 259.0 Hz), 144.7, 131.2, 120.9, 111.3, 108.0, 107.9, 105.2, 91.0, 73.0, 49.9, 27.5, 21.4; ^{19}F NMR ($CDCl_3$): δ –135.17 (ddd, *J* = 25.0, 16.4, 5.7 Hz, 2F), –134.90 (ddd, *J* = 24.8, 16.2, 5.8 Hz, 2F); IR (KBr): ν3435, 2941, 2847, 2200, 1598, 1521, 1491, 1335, 1312, 1098, 984 cm^{-1}; HRMS: (FAB+) *m*/*z* $[M]^+$ calcd for $C_{21}H_{14}F_4N_2$: 370.1093; found: 370.1104.

9-[2-(4-Cyano-2,3,5,6-tetrafluorophenyl)ethyn-1-yl]-1,1,7,7-tetramethyljulolidine (TMeJLD-F)

Yield: 41% (orange solid); M.p.: 242.1–243.3 ºC; ^{1}H NMR ($CDCl_3$): δ 7.25 (s, 2H), 3.28 (t, *J* = 6.1 Hz, 4H), 1.74 (t, *J* = 6.1 Hz, 4H), 1.30 (s, 12H); ^{13}C NMR ($CDCl_3$): δ 145.8–148.5 (dm, *J* = 264.0 Hz), 144.8–147.1 (dm, *J* = 234.7 Hz), 142.6, 130.2, 128.3, 112.1, 112.1, 108.1, 105.4, 78.2, 72.3, 53.6, 46.8, 35.9, 32.3, 30.5; ^{19}F NMR ($CDCl_3$): δ –135.36 (m, 2F), –136.62 (m, 2F); IR (KBr): ν 2962, 2924, 2853, 2185, 1646, 1595, 1523, 1333, 1310, 1095, 984 cm^{-1}; HRMS: (FAB+) *m*/*z* [M]$^{+}$ calcd for $C_{25}H_{22}F_4N_2$: 426.1719; found: 426.1723.

Synthesis of IndCBZ-H through Pd(0)-catalyzed Sonogashira cross-coupling reaction

2-Ethynylindlo[3,2,1-*jk*]carbazole (0.27 g, 1.1 mmol), $Cl_2Pd(PPh_3)_2$ (0.036 g, 0.057 mmol), PPh_3 (0.13 g, 0.057 mmol), CuI (0.020 g, 0.11 mmol), and 4-bromobenzonitrile (0.26 g, 1.6 mmol) in Et_3N (5.0 mL) were placed in a two-necked round-bottomed flask equipped with a Teflon®-coated stirring bar. The reaction mixture was stirred at 80 ºC for 6 h; the precipitate formed during the reaction was separated by atmospheric filtration and the filtrate was poured into a saturated aqueous solution of NH_4Cl. The crude product was extracted with EtOAc (thrice) and the combined organic layer was washed with brine (once). The organic layer was dried over anhydrous Na_2SO_4 and separated via filtration. The filtrate was evaporated in vacuo and purified using silica-gel column chromatography (hexane/CH_2Cl_2 = 2/5) to generate the corresponding product **IndCBZ-H** (0.17 g, 0.46 mmol) in 42% isolated yield as a white solid. Further recrystallization from CH_2Cl_2/hexane produced white crystals that were sufficiently pure for photophysical analysis.

2-[2-(4-Cyanophenyl)ethyn-1yl]indro[3,2,1-jk]carbazole (IndCBZ-H)

Yield: 42% (white solid); M.p.: 240.1–241.6 ºC; ^{1}H NMR ($CDCl_3$): δ 8.23 (s, 2H), 8.11 (d, *J* = 8.0 Hz, 2H), 7.90 (d, *J* = 8.0 Hz, 2H), 7.65 (s, 4H), 7.58 (td, *J* = 7.8, 1.2 Hz, 2H), 7.38 (td, *J* = 7.6, 0.9 Hz, 2H); ^{13}C NMR ($CDCl_3$): δ 143.6, 139.2, 132.1, 131.9, 129.4, 128.8, 127.5, 123.7, 123.4, 122.3, 118.7, 118.5, 116.5, 112.4, 111.0, 96.3, 86.1; IR (KBr): ν 3055, 2225, 2204, 1916, 1647, 1647, 1603, 1589, 1455, 1427, 1164, 1134, 1112, 1087, 1038, 1011 cm^{-1}; HRMS: (FAB+) *m/z* [M]$^{+}$ calcd for $C_{27}H_{14}N_2$: 366.1157; found: 366.1151.

4-[2-(4-Cyanophenyl)ethyn-1-yl]julolidine (JLD-H)

Yield: 34% (white solid); M.p.: 162.9–163.5 ºC; ^{1}H NMR ($CDCl_3$): δ 7.57 (d, *J* = 8.8 Hz, 2H), 7.50 (d, *J* = 8.8 Hz, 2H), 6.98 (s, 2H), 3.21 (t, *J* = 5.7 Hz, 4H), 2.72 (t, *J* = 6.4 Hz, 4H), 1.97 (quin, *J* = 6.1 Hz, 4H); ^{13}C NMR ($CDCl_3$): δ 143.6, 131.9, 131.4, 130.6, 129.6, 121.0, 119.0, 109.9, 107.3, 96.6, 86.0, 49.9, 27.5, 21.6; IR (KBr): ν 3397, 3084, 2949, 2932, 2850, 2836, 2221. 2190, 1593, 1519, 1337, 1309, 1201, 1131, 974 cm^{-1}; HRMS: (FAB+) *m/z* [M]$^{+}$ calcd for $C_{21}H_{18}N_2$: 298.1470; found: 298.1468.

9-[2-(4-Cyanophenyl)ethyn-1-yl]-1,1,7,7-tetramethyljulolidine (TMeJLD-H)

Yield: 8% (white solid); M.p.: 192.2–193.4 ºC; ^{1}H NMR ($CDCl_3$): δ 7.61–7.53 (m, 4H), 7.21 (s, 2H), 3.23 (t, *J* = 6.1 Hz, 4H), 1.74 (t, *J* = 6.1 Hz, 4H); ^{13}C NMR ($CDCl_3$): δ 141.3, 131.9, 131.4, 130.0, 129.6, 127.7, 119.0, 109.9, 107.1, 97.2, 85.7, 46.7, 36.2, 32.2, 30.7; IR (KBr): ν 3089, 3050, 2957, 2925, 2851, 2225, 2198 1671, 1595, 1507, 1456, 1330, 1309, 1159, 1020 cm^{-1}; HRMS: (FAB+) *m/z* [M]$^{+}$ calcd for $C_{25}H_{26}N_2$: 354.2096; found: 354.2100.

NMR Spectra

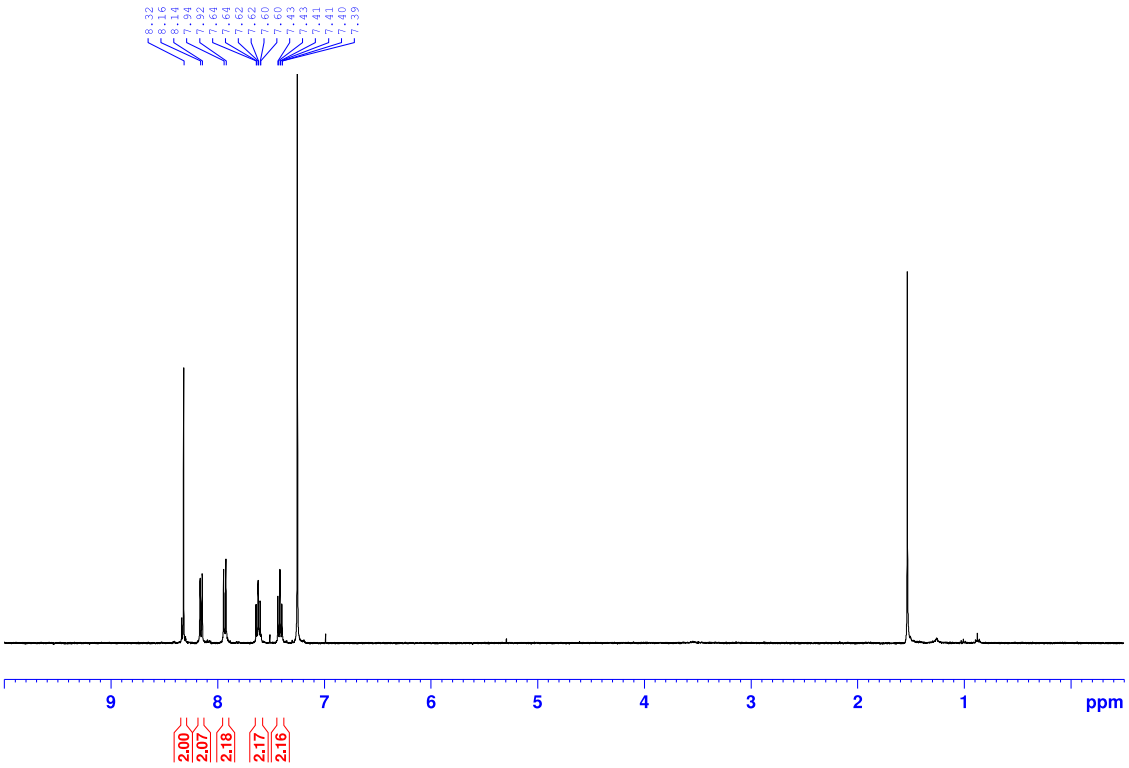


Figure S1. ^{1}H NMR spectrum of **IndCBZ-F** (400 MHz, $CDCl_3$)

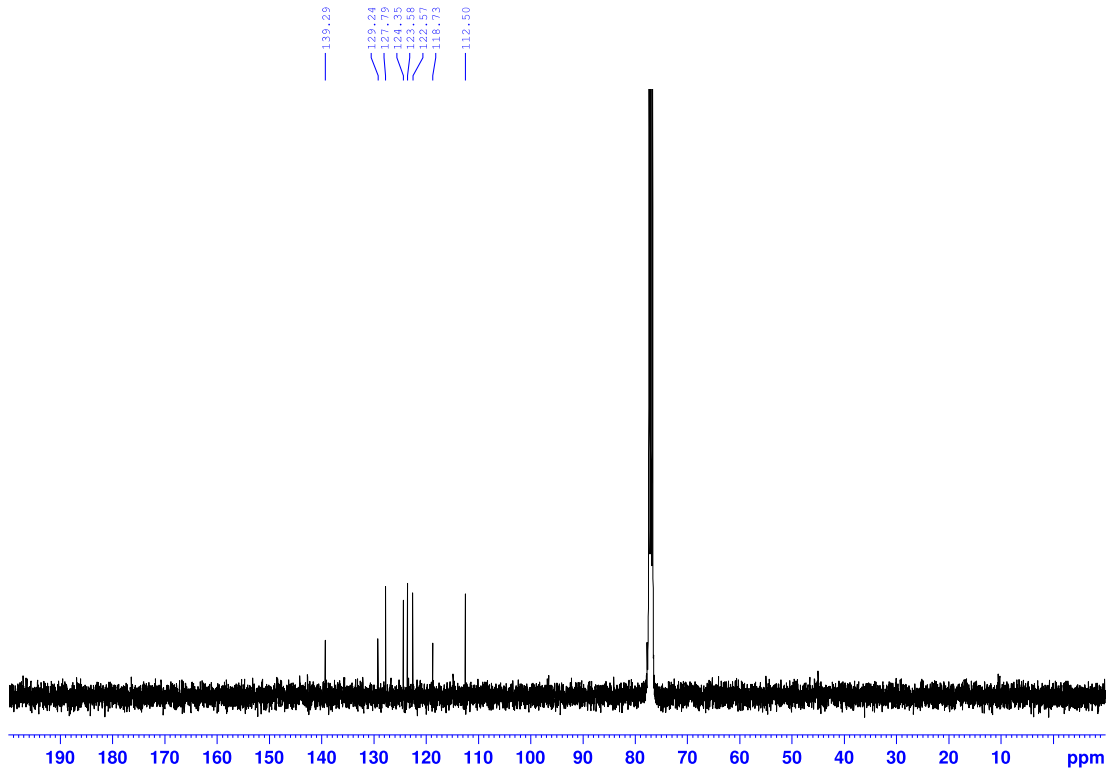


Figure S2. ^{13}C NMR spectrum of **IndCBZ-F** (100 MHz, $CDCl_3$)

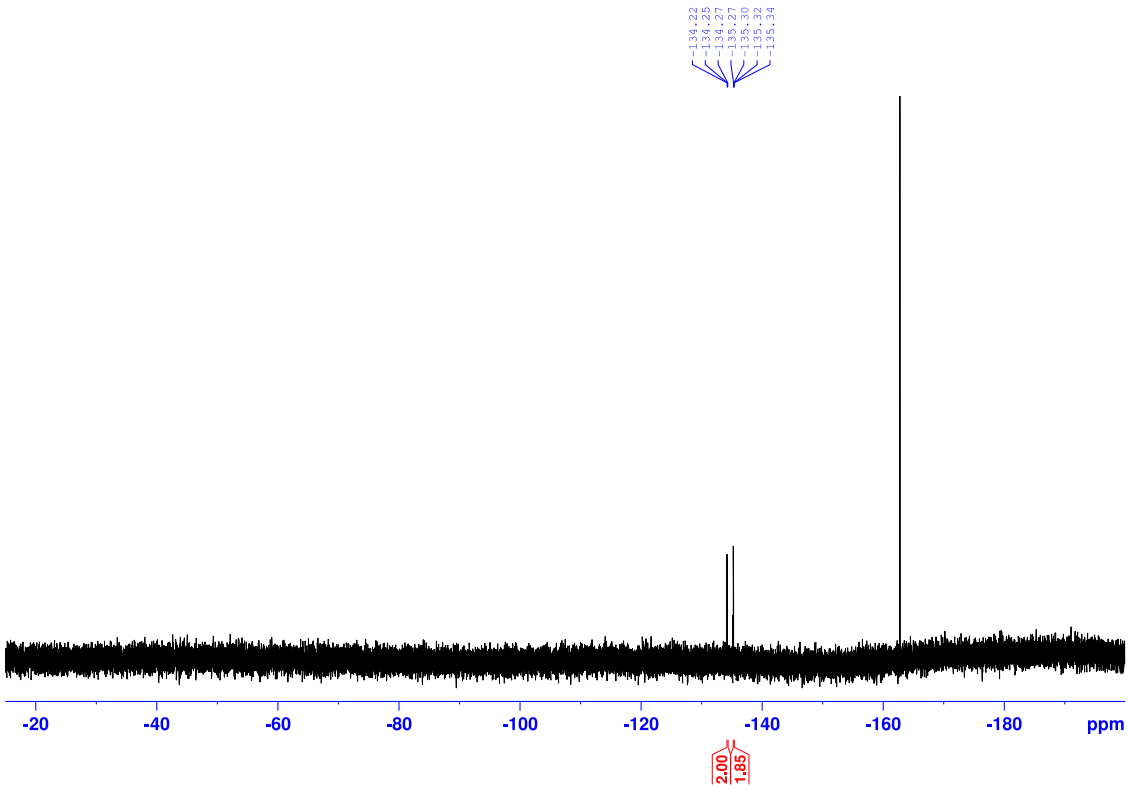


Figure S3. ^{19}F NMR spectrum of **IndCBZ-F** (376 MHz, $CDCl_3$, hexafluoro benzene)

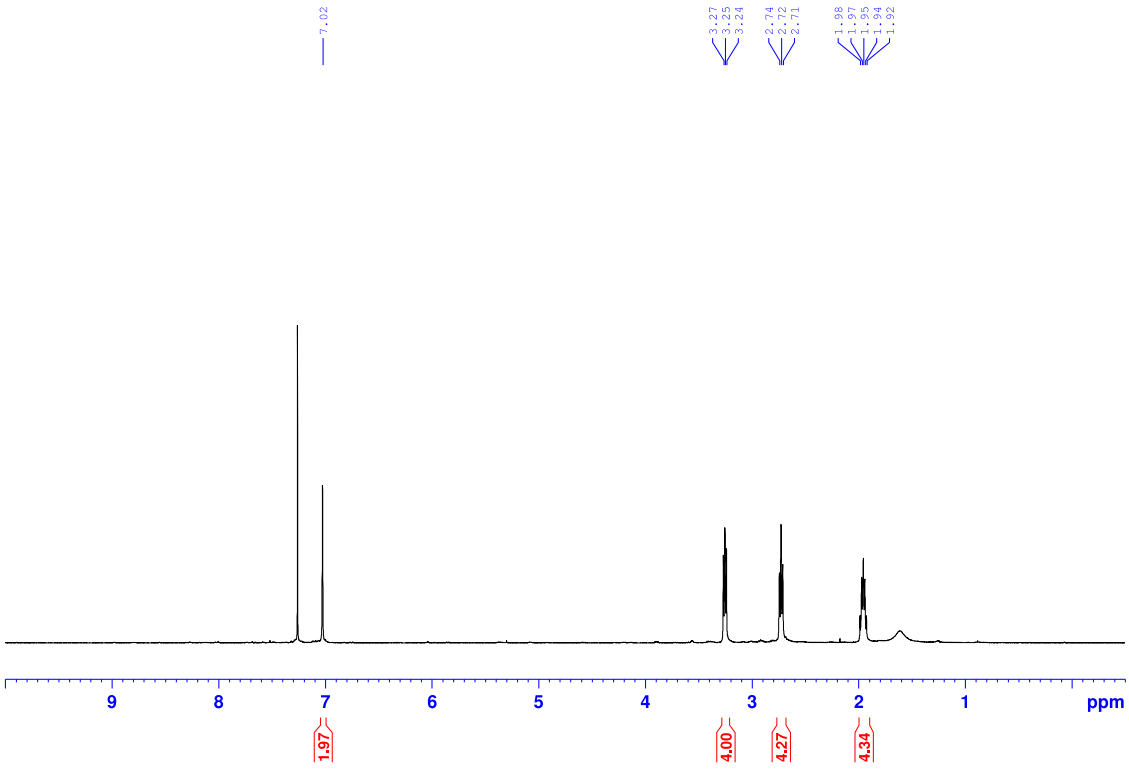


Figure S4. ^{1}H NMR spectrum of **JLD-F** (400 MHz, $CDCl_3$)

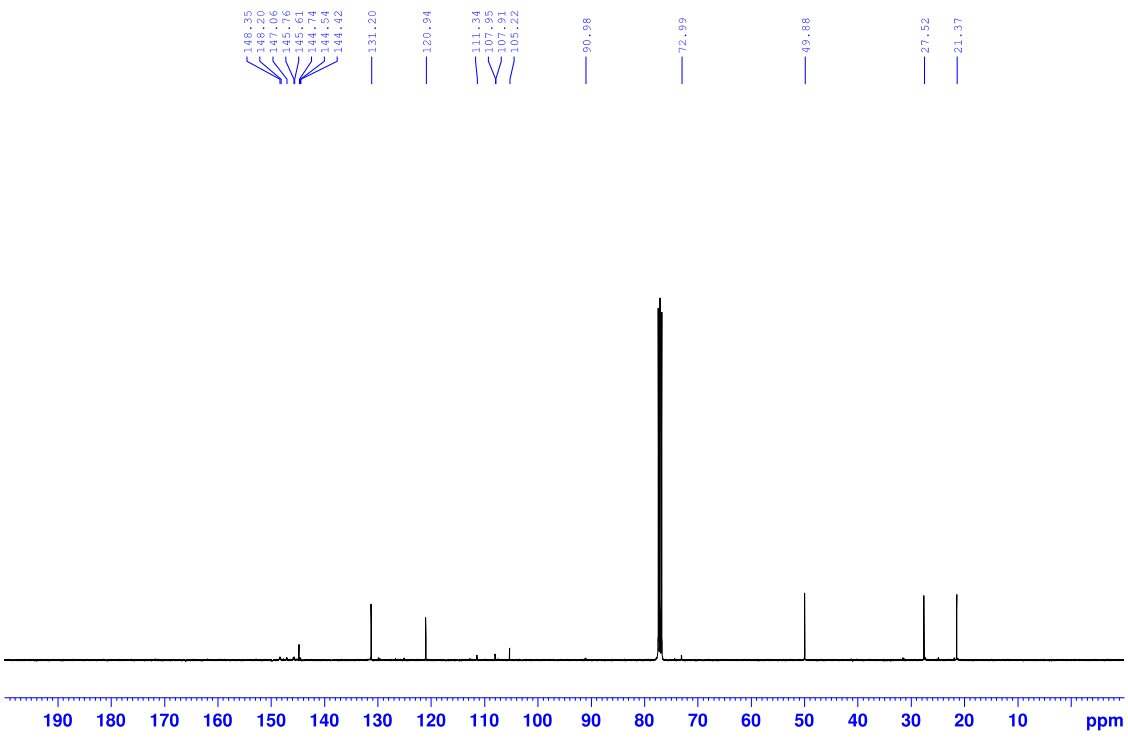


Figure S5. ^{13}C NMR spectrum of **JLD-F** (100 MHz, $CDCl_3$)

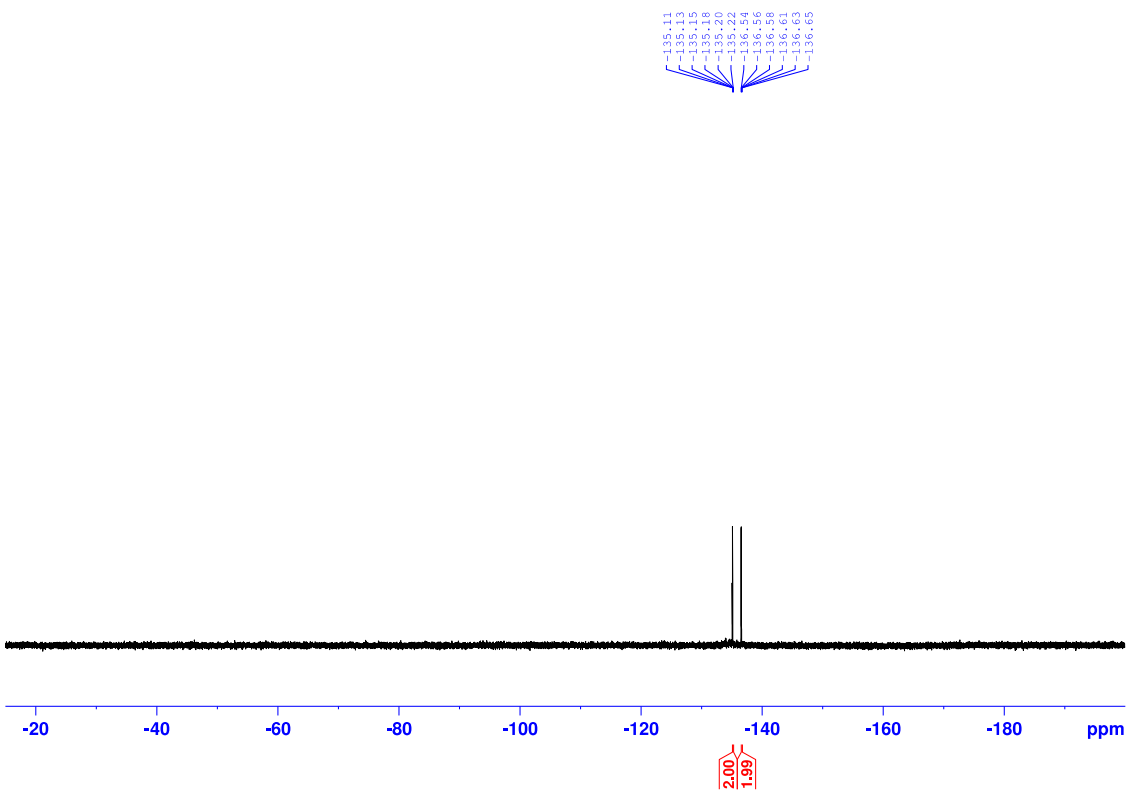


Figure S6. ^{19}F NMR spectrum of **JLD-F** (376 MHz, $CDCl_3$, hexafluoro benzene)

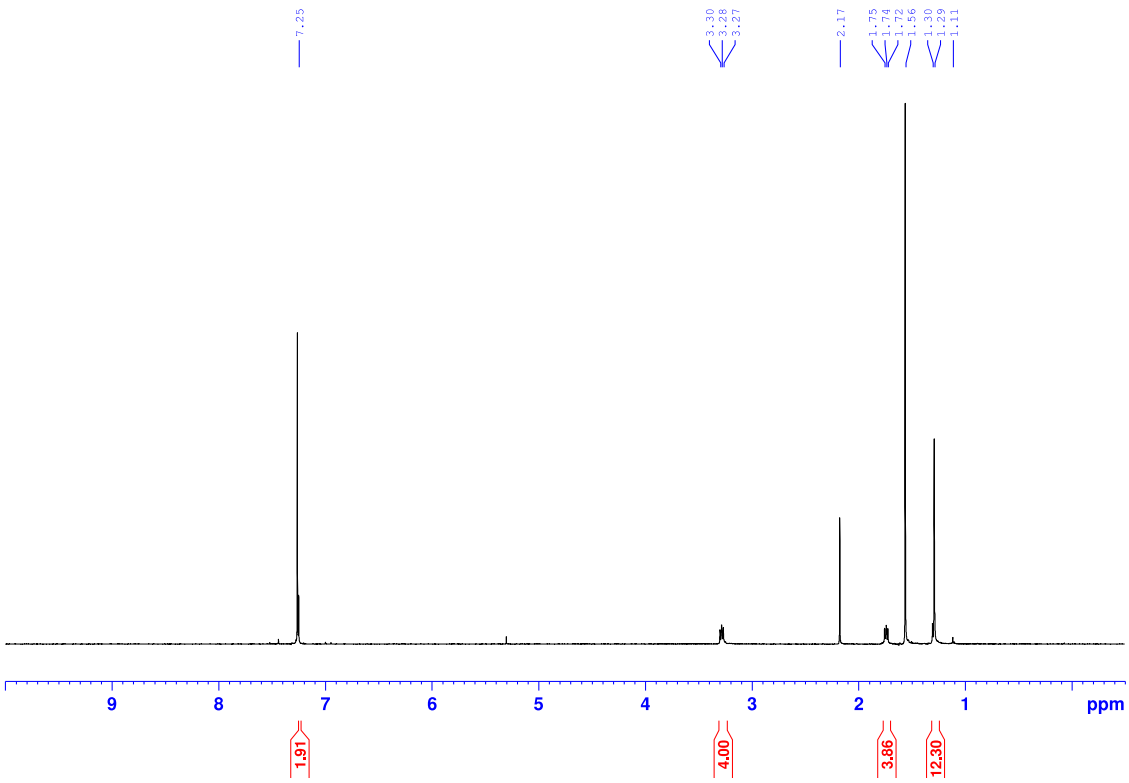


Figure S7. ^{1}H NMR spectrum of **TMeJLD-F** (400 MHz, $CDCl_3$)

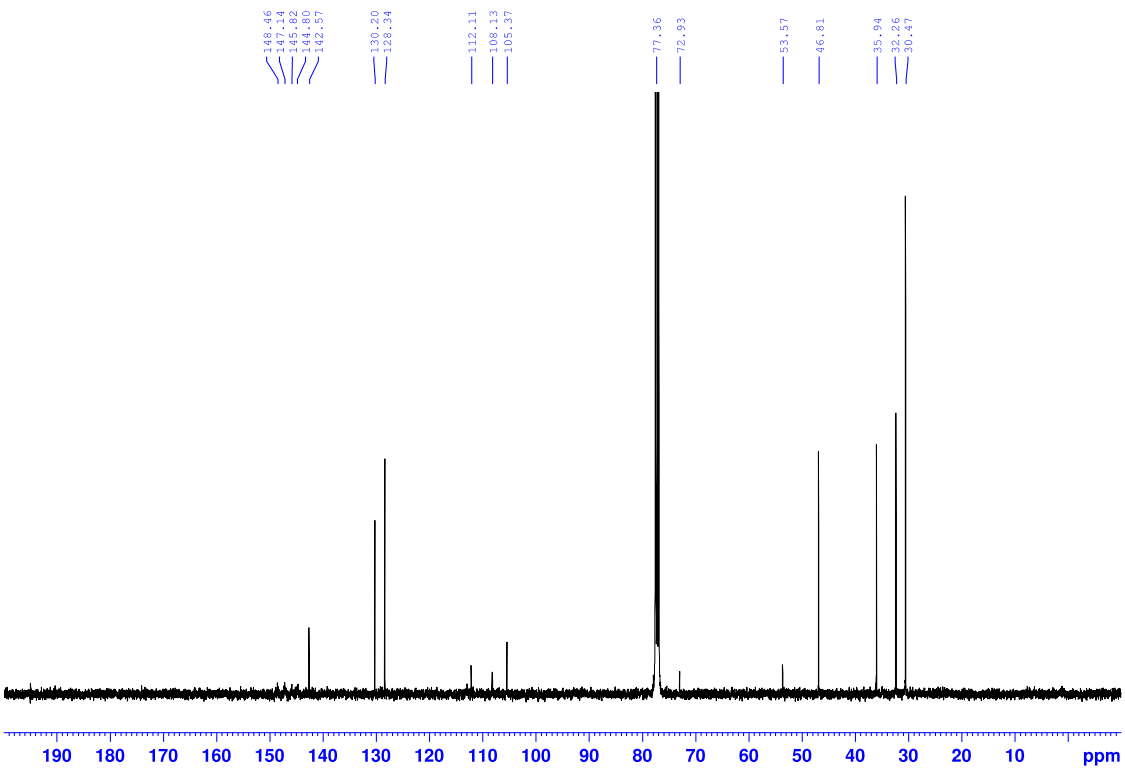


Figure S8. ^{13}C NMR spectrum of **TMeJLD-F** (100 MHz, $CDCl_3$)

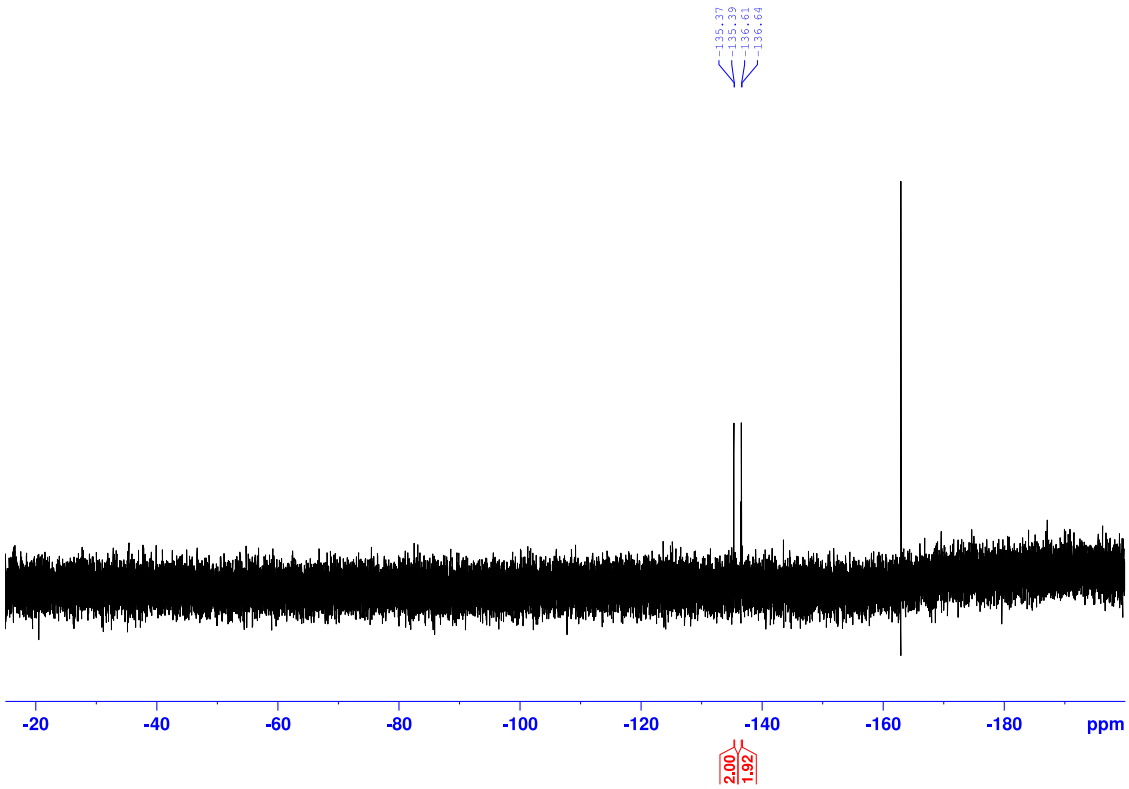


Figure S9. ^{19}F NMR spectrum of **TMeJLD-F** (376 MHz, $CDCl_3$, hexafluoro benzene)

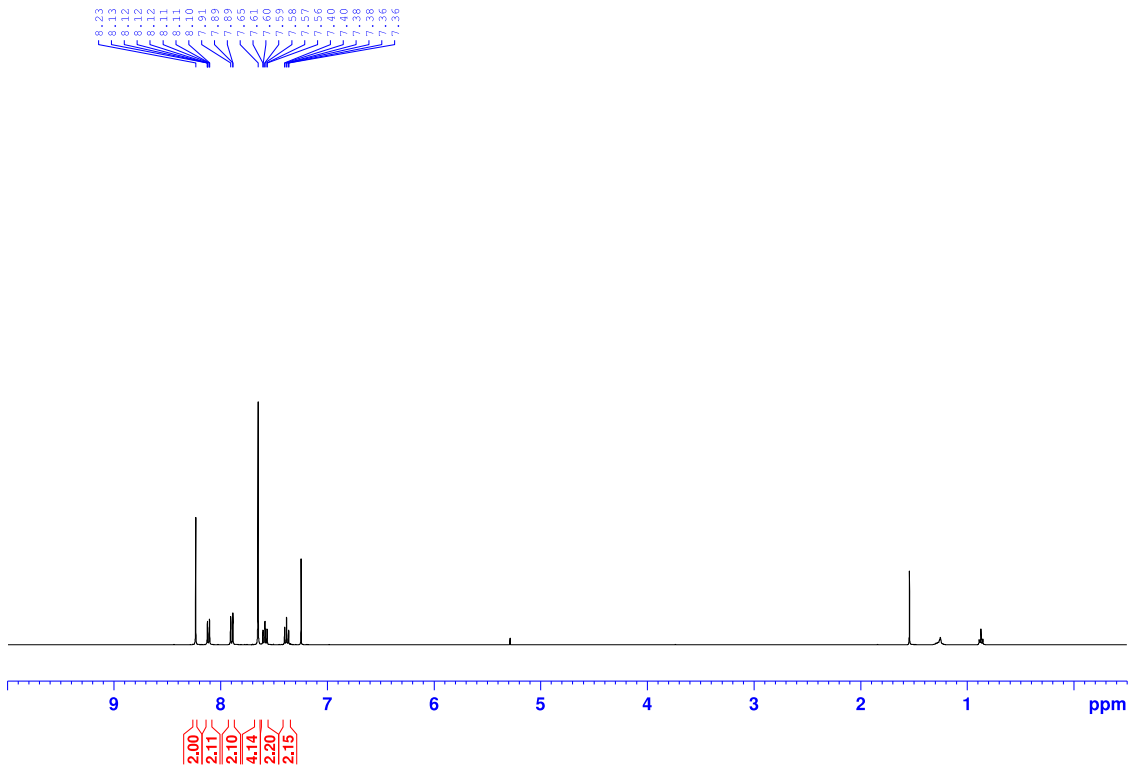


Figure S10. ^{1}H NMR spectrum of **IndCBZ-H** (400 MHz, $CDCl_3$)

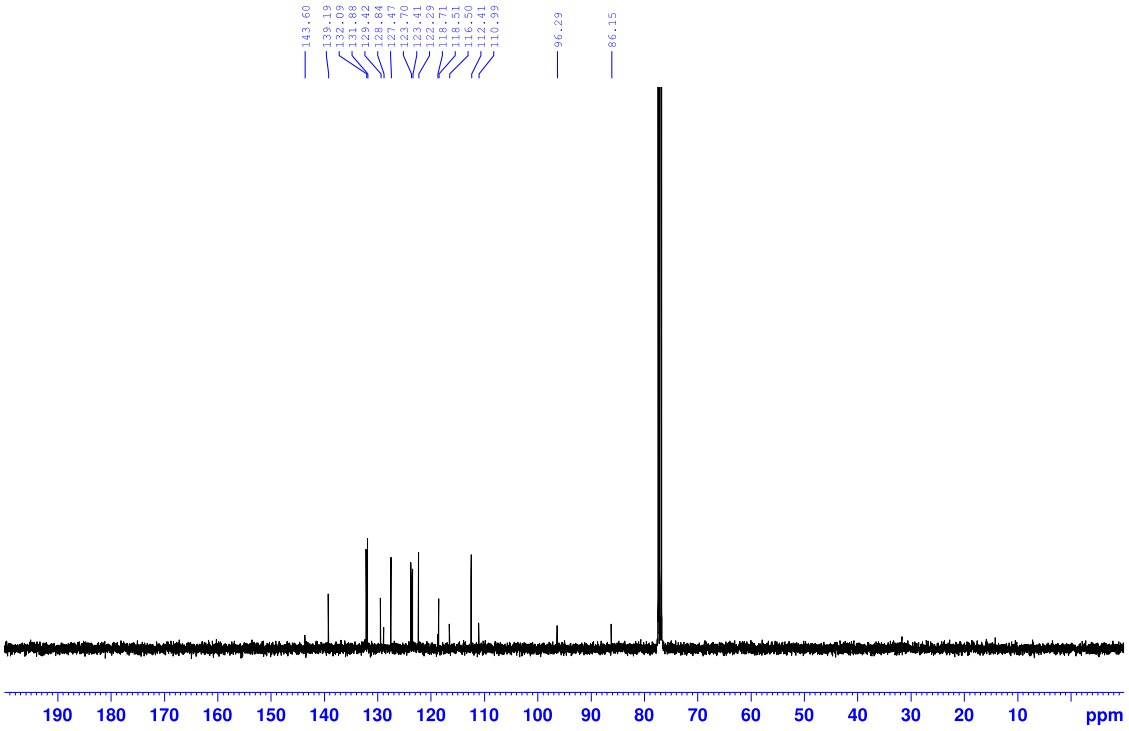


Figure S11. ^{13}C NMR spectrum of **IndCBZ-H** (100 MHz, $CDCl_3$)

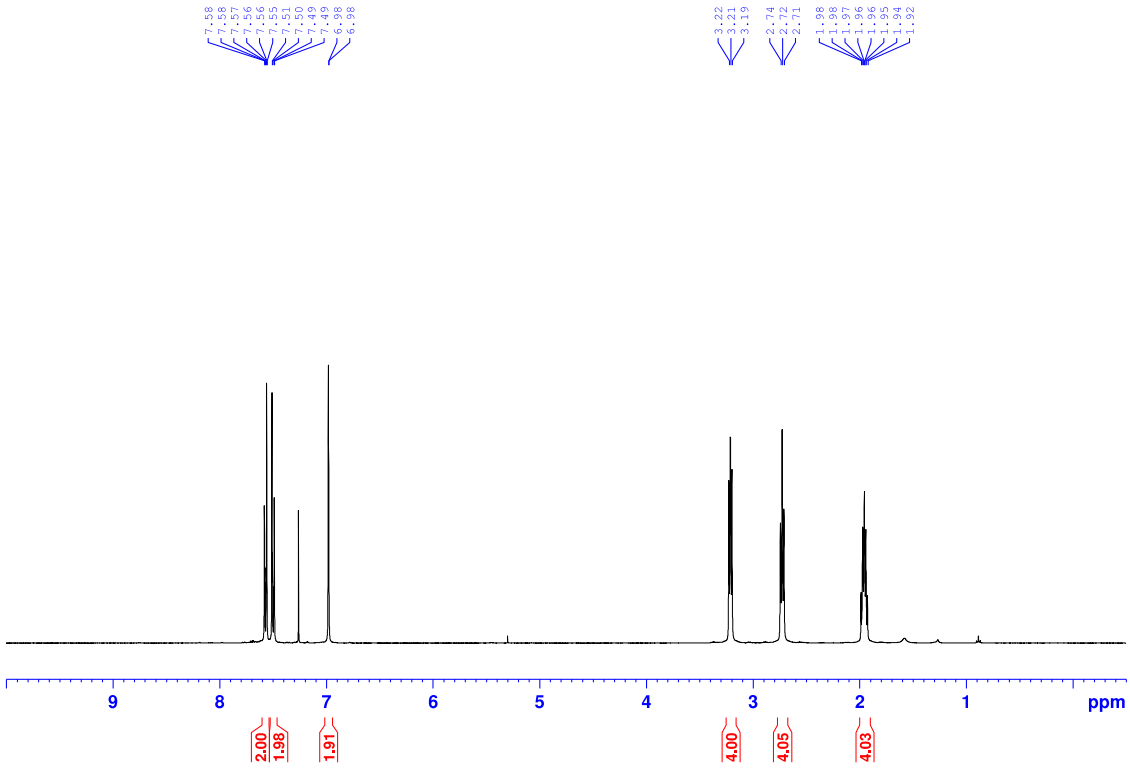


Figure S12. ^{1}H NMR spectrum of **JLD-H** (400 MHz, $CDCl_3$)

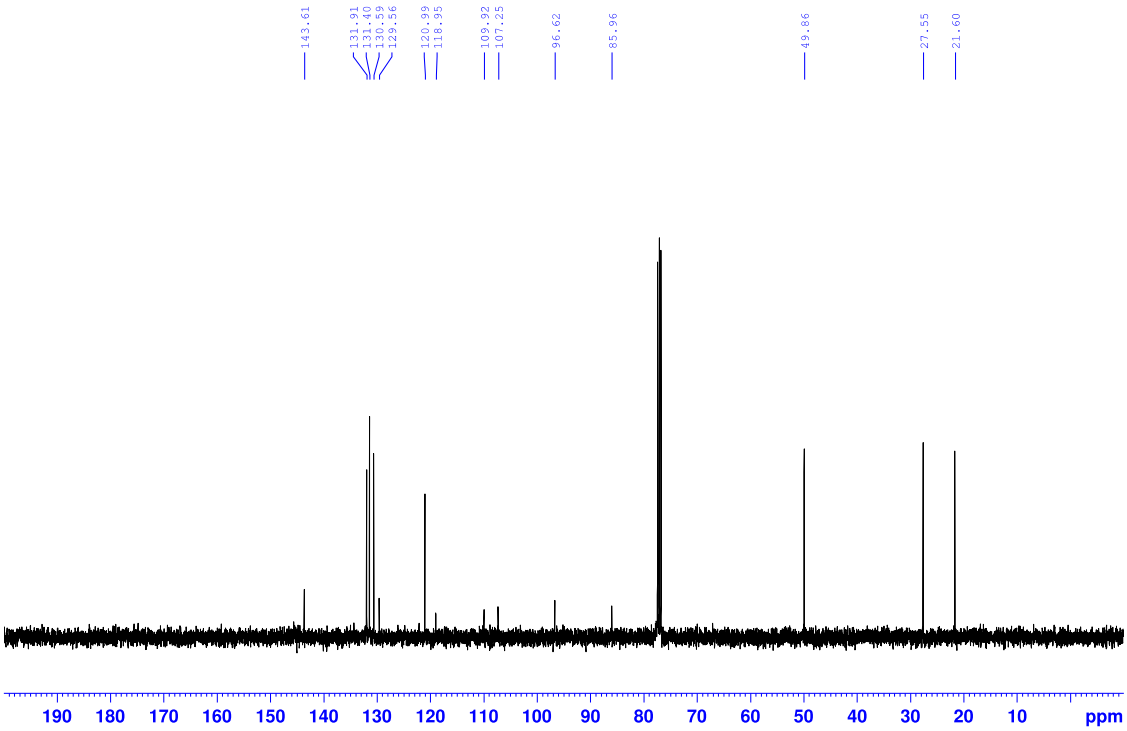


Figure S13. ^{13}C NMR spectrum of **JLD-H** (100 MHz, $CDCl_3$)

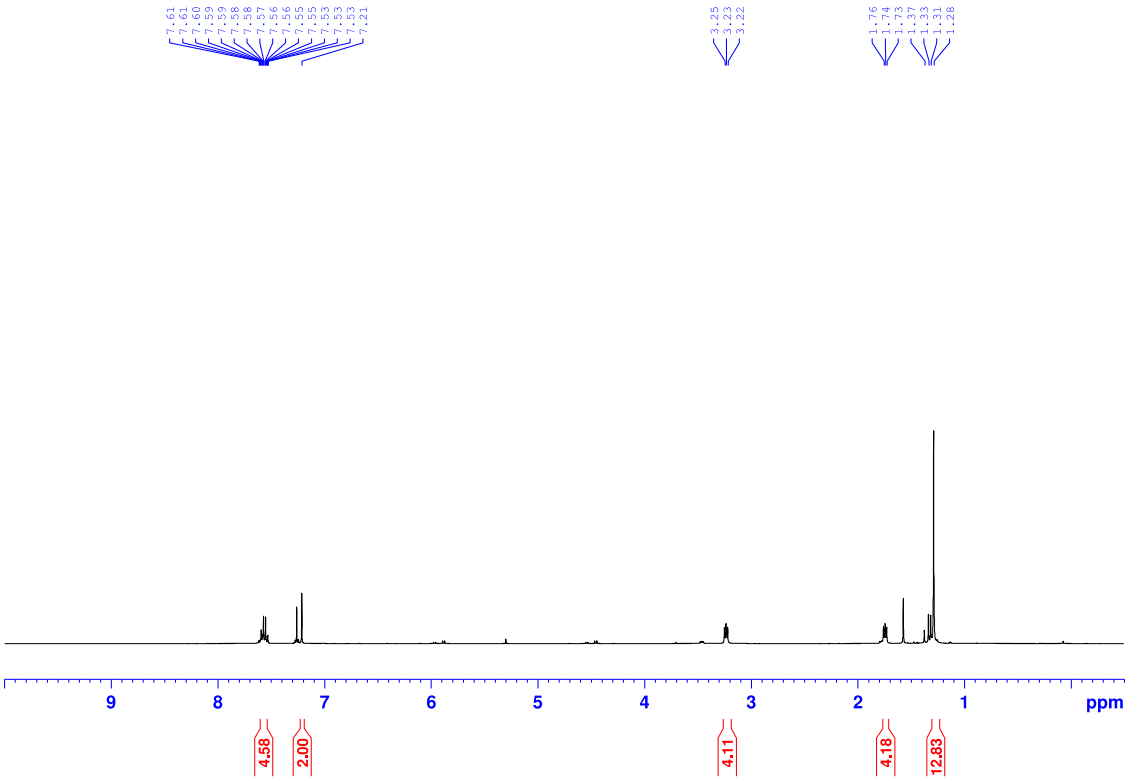


Figure S14. ^{1}H NMR spectrum of **TMeJLD-H** (400 MHz, $CDCl_3$)

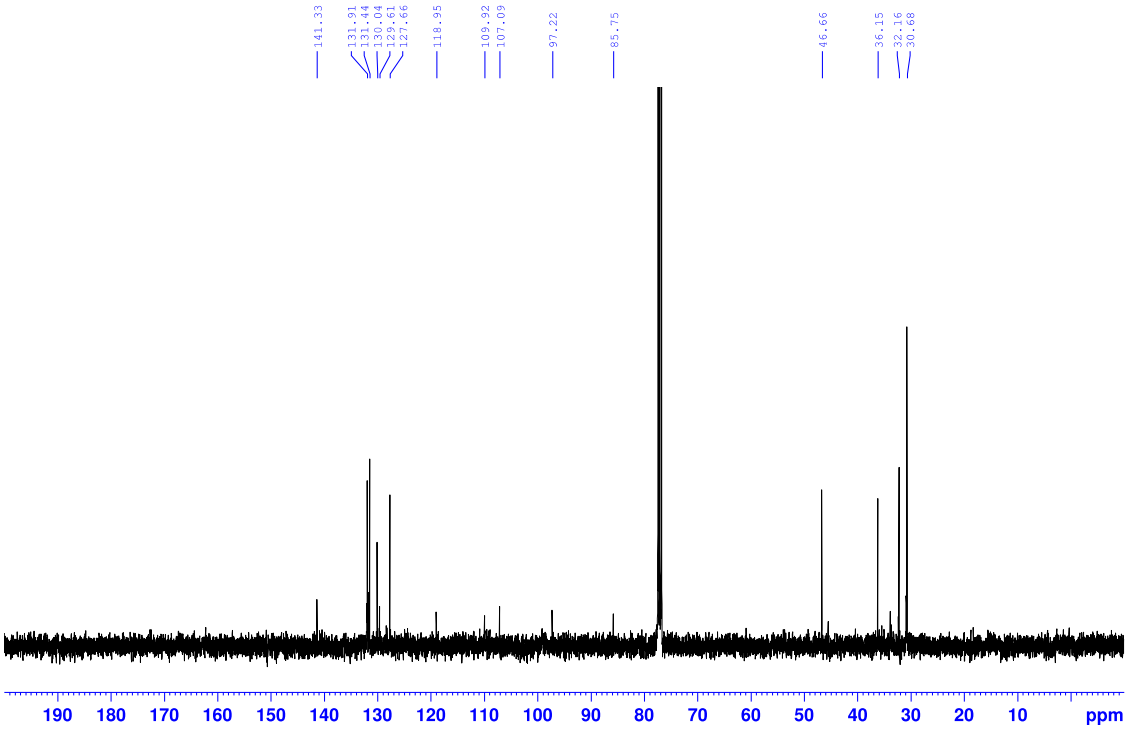


Figure S15. ^{13}C NMR spectrum of **TMeJLD-H** (100 MHz, $CDCl_3$)

Crystallographic analysis

Single crystal X-ray diffractions were recorded on an XtaLab AFC11 diffractometer (Rigaku). The reflection data were integrated, scaled, and averaged using CrysAlisPro (ver. 1.171.39.43a, Rigaku). Empirical absorption corrections were applied using the SCALE 3 ABSPACK scaling algorithm (CrysAlisPro). The structure was identified by a direct method (SHELXT-2018/2) and refined using a full matrix least square method (SHELXL-2014/7) visualized by Olex2. The crystallographic data were deposited into the Cambridge Crystallographic Data Centre (CCDC) database.

Table S1. Crystallographic data of **JLD-F**.

Compound	**JLD-F**	**JLD-H**	**TMeJLD-F**	**TMeJLD-H**
CCDC #	2369867	2401628	2402070	2401629
Empirical Formula	$C_{21}H_{14}F_4N_2$	$C_{21}H_{18}N_2$	$C_{25}H_{22}F_4N_2$	$C_{25}H_{26}N_2$
Formula weight	370.34	298.37	426.44	354.48
Temperature [K]	200	173	173	173
Crystal Color / Habit	Orange / Plate	Yellow / Block	yellow / Plate	Yellow / Block
Crystal Size [mm]	0.32x0.13x0.06	0.395x0.337x0.114	0.244x0.176x0.043	0.266x0.16x0.113
Crystal System	Triclinic	Monoclinic	Triclinic	Orthorhombic
Space Group	$P\,\bar{1}$	$P2_1/c$	$P\,\bar{1}$	$Pna2_1$
a [Å]	6.7485(5)	13.5475(8)	6.3253(5)	18.4085(10)
b [Å]	8.3818(7)	8.1404(3)	16.5547(18)	6.3801(3)
c [Å]	15.2313(16)	15.4286(8)	21.013(3)	33.690(2)
α [°]	93.866(8)	90	70.720(11)	90
β [°]	91.617(8)	111.086(6)	89.417(9)	90
γ [°]	97.057(7)	90	89.860(8)	90
V [Å^3]	852.50(13)	1587.57(15)	2076.8(4)	3956.9(4)
Z	2	4	4	8
R [$F^2 > 2\sigma(F^2)$] [a]	0.1578	0.0427	0.2994	0.0783
wR_2 (F^2) [b]	0.4750	0.1239	0.7073	0.2117

[a] $R = \Sigma||F_o| - |F_c|| \,/\, \Sigma|F_o|$. [b] $wR = \{[\Sigma w(|F_o| - |F_c|)]/\Sigma w|F_o|\}^{1/2}$.

DFT calculation

All computations were carried out using density functional theory (DFT) with the Gaussian 16 (Rev. B.01)[1] package. Geometry optimizations were executed using the CAM-B3LYP hybrid functional and 6-31+G(d,p) basis set.[2] Vertical excitations were also calculated using a TD-DFT method at the same level of theory except for geometry optimizations at excited state.

Table S2. Dipole moment (debye) of all derivatives at the S_1 state.

	Dipole moment (debye)
IndCBZ-F	X= –9.5318/ Y= 0.0000/ Z= -0.0001/ Tot= 9.5313
JLD-F	X= -11.4218/ Y= 0.0000/ Z= 0.0000/ Tot= 11.4218
TMeJLD-F	X= 11.2173/ Y= 0.0000/ Z= 0.0000/ Tot= 11.2173
IndCBZ-H	X= 7.4547/ Y= -0.0002/ Z= -0.0001/ Tot= 7.4547
JLD-H	X= -10.7299/ Y= 0.0000/ Z= 0.0001/ Tot= 10.7299
TMeJLD-H	X= 10.5814/ Y= 0.0000/ Z= 0.0001/ Tot= 10.5814

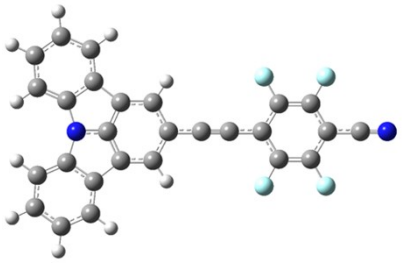
Table S3. Vertical transition behavior from structure optimized at the S_0 state corresponding to absorption process.

Sample	Transition	Transition Energy (eV)	Theoretical Absorption (nm)	Oscillator strength / f
IndCBZ-F	HOMO → LUMO	3.7895	327.15	1.3790
JLD-F	HOMO → LUMO	3.4297	361.50	1.3097
TMeJLD-F	HOMO → LUMO	3.4260	361.90	1.3072
IndCBZ-H	HOMO → LUMO	3.9397	314.71	0.1308
JLD-H	HOMO → LUMO	3.6840	336.54	1.3273
TMeJLD-H	HOMO → LUMO	3.6885	336.14	1.3303

Table S4. Vertical transition behavior from structure optimized at the S_1 state corresponding to emission process.

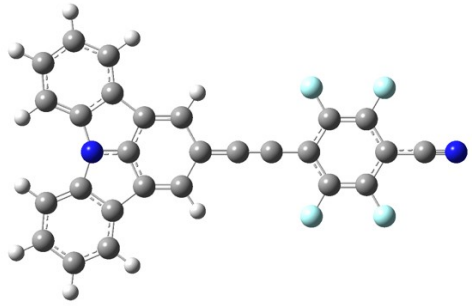
Sample	Transition	Transition Energy (eV)	Theoretical Absorption (nm)	Oscillator strength / f
IndCBZ-F	HOMO → LUMO	3.3479	370.34	1.5476
JLD-F (twist-bent)	HOMO → LUMO	2.0575	602.59	0.0001
JLD-F (planar)	HOMO → LUMO	3.1601	392.34	1.4764
TMeJLD-F (twist-bent)	HOMO → LUMO	2.0488	605.16	0.0001
TMeJLD-F (planar)	HOMO → LUMO	3.5395	350.29	1.2873
IndCBZ-H	HOMO → LUMO	3.7421	331.32	0.1578
JLD-H	HOMO → LUMO	3.3113	374.73	1.4853
TMeJLD-H	HOMO → LUMO	3.3086	374.73	1.4874

Table S5. Cartesian coordinate for **IndCBZ-F** at the optimized geometry in S_0 state using CAM-B3LYP/6-31+G(d,p) level of theory.



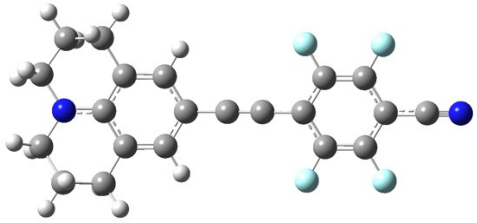
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.473079	-1.258162	-0.000008
2	6	0	-1.083572	-1.249615	-0.000008
3	6	0	-0.4128	-0.000065	0.000049
4	6	0	-1.08352	1.249513	0.000097
5	6	0	-2.473027	1.258118	0.000105
6	6	0	-3.043927	-0.00001	0.000063
7	6	0	1.013353	-0.000097	0.000049
8	6	0	2.221703	-0.000094	0.00004
9	6	0	3.637069	-0.000054	0.000017
10	6	0	4.363037	1.195772	-0.000211
11	6	0	5.744644	1.197639	-0.000231
12	6	0	6.460927	0.000026	-0.000023
13	6	0	5.744711	-1.197627	0.000206
14	6	0	4.363104	-1.195838	0.000225
15	6	0	7.887446	0.000067	-0.000046
16	7	0	9.043141	0.000073	-0.000047
17	9	0	3.718101	-2.359511	0.000446
18	9	0	6.39582	-2.355269	0.000408
19	9	0	3.717969	2.359409	-0.000413
20	9	0	6.395688	2.355318	-0.000451
21	7	0	-4.400155	0.000019	0.000043
22	6	0	-4.808444	-1.342331	-0.000063
23	6	0	-4.808387	1.342387	0.000072
24	6	0	-3.634678	2.157225	0.000116
25	6	0	-3.774942	-3.539458	-0.000199
26	6	0	-5.04973	-4.093955	-0.000282
27	6	0	-6.183627	-3.279966	-0.000256
28	6	0	-6.079822	-1.89289	-0.000147
29	6	0	-6.079742	1.892999	0.000088
30	6	0	-6.183489	3.280079	0.000143
31	6	0	-5.049557	4.094021	0.000187
32	6	0	-3.774793	3.539469	0.000177
33	6	0	-3.634769	-2.157219	-0.000087
34	1	0	-0.490481	-2.157511	-0.000047
35	1	0	-0.490391	2.157384	0.000116
36	1	0	-2.897441	-4.178484	-0.000222
37	1	0	-5.165458	-5.172669	-0.00037
38	1	0	-7.168618	-3.735583	-0.000325
39	1	0	-6.965167	-1.26702	-0.000129
40	1	0	-6.965114	1.267167	0.000059
41	1	0	-7.16846	3.735738	0.000154
42	1	0	-5.165239	5.17274	0.000233
43	1	0	-2.897265	4.178459	0.000214

Table S6. Cartesian coordinate for **IndCBZ-F** at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.



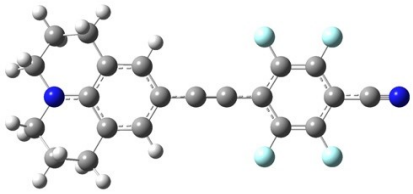
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.460076	0.268739	0.000006
2	6	0	-1.084863	-1.271829	-0.000015
3	6	0	-0.38733	-0.000001	-0.000021
4	6	0	-1.084863	1.271828	-0.000015
5	6	0	-2.460076	1.268739	0.000007
6	6	0	-3.035512	0	0.000023
7	6	0	0.99342	-0.000001	-0.000039
8	6	0	2.232375	-0.000002	-0.000055
9	6	0	3.610183	-0.000002	-0.000033
10	6	0	4.365811	1.213483	-0.000021
11	6	0	5.731715	1.208577	0.000003
12	6	0	6.465288	-0.000001	0.000017
13	6	0	5.731716	-1.208579	0.000006
14	6	0	4.365812	-1.213487	-0.000018
15	6	0	7.877436	0	0.000042
16	7	0	9.038451	0.00001	0.000061
17	9	0	3.70473	-2.37328	-0.000028
18	9	0	6.395896	-2.364918	0.000018
19	9	0	3.704728	2.373277	-0.000035
20	9	0	6.395894	2.364917	0.000012
21	7	0	-4.380056	0.000001	0.000031
22	6	0	-4.79929	-1.345211	0.000017
23	6	0	-4.799289	1.345212	0.000018
24	6	0	-3.629708	2.163542	0.000006
25	6	0	-3.77471	-3.542283	-0.000008
26	6	0	-5.056001	-4.090684	-0.000009
27	6	0	-6.184293	-3.273067	0.000004
28	6	0	-6.072705	-1.883681	0.000017
29	6	0	-6.072703	1.883683	0.000019
30	6	0	-6.18429	3.27307	0.000007
31	6	0	-5.055998	4.090686	-0.000005
32	6	0	-3.774707	3.542283	-0.000004
33	6	0	-3.62971	-2.163542	0.000004
34	1	0	-0.489031	-2.177296	-0.000031
35	1	0	-0.48903	2.177294	-0.000032
36	1	0	-2.901256	-4.186408	-0.000017
37	1	0	-5.176203	-5.168721	-0.000018
38	1	0	-7.171613	-3.722947	0.000003
39	1	0	-6.954808	-1.253582	0.000027
40	1	0	-6.954807	1.253585	0.000028
41	1	0	-7.17161	3.72295	0.000006
42	1	0	-5.176199	5.168723	-0.000014
43	1	0	-2.901253	4.186408	-0.000013

Table S7. Cartesian coordinate for **JLD-F** at the optimized geometry in S_0 state using CAM-B3LYP/6-31G+(d,p) level of theory.



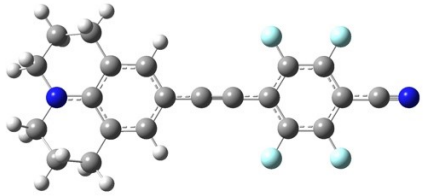
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.07945	-1.199256	-0.69486
2	6	0	-3.460497	-1.217166	-0.085814
3	6	0	-4.176963	0.000001	-0.000005
4	6	0	-3.460499	1.217167	0.085824
5	6	0	-2.079452	1.199255	0.069536
6	6	0	-1.359017	0	0.000037
7	6	0	0.060395	-0.000001	0.000061
8	6	0	1.270386	-0.000002	0.000061
9	6	0	2.683389	-0.000001	0.000035
10	6	0	3.411888	1.193055	0.074825
11	6	0	4.792912	1.194744	0.074905
12	6	0	5.510642	-0.000001	-0.000022
13	6	0	4.792909	-1.194746	-0.074917
14	6	0	3.411886	-1.193057	-0.074785
15	6	0	6.936696	-0.000001	-0.000046
16	7	0	8.092569	0.000004	-0.00007
17	9	0	5.444204	-2.35089	-0.147487
18	9	0	2.76758	-2.355675	-0.147684
19	9	0	5.444208	2.350888	0.14745
20	9	0	2.767584	2.355672	0.147752
21	7	0	-5.55488	0.000001	-0.000024
22	6	0	-6.33854	1.222748	-0.074068
23	6	0	-5.530378	2.396861	-0.603369
24	6	0	-4.225506	2.512714	0.177471
25	6	0	-4.225504	-2.512712	-0.177484
26	6	0	-5.530393	-2.396859	0.603327
27	6	0	-6.338543	-1.222745	0.07401
28	1	0	-1.53748	-2.138952	-0.12136
29	1	0	-1.537482	2.138951	0.121425
30	1	0	-6.747049	1.466416	0.919467
31	1	0	-7.198072	1.035056	-0.729938
32	1	0	-6.126998	3.310139	-0.520317
33	1	0	-5.310254	2.243034	-1.665627
34	1	0	-4.453371	2.747407	1.226468
35	1	0	-3.613851	3.337355	-0.201025
36	1	0	-3.613859	-3.337355	0.201022
37	1	0	-4.453346	-2.747399	-1.226487
38	1	0	-5.310292	-2.243034	1.66559
39	1	0	-6.127011	-3.310137	0.520261
40	1	0	-6.747036	-1.466414	-0.919532
41	1	0	-7.198086	-1.035051	0.729865

Table S8. Cartesian coordinate for **JLD-F** at the optimized geometry in S_0 state using B3LYP/6-31G+(d,p) level of theory.



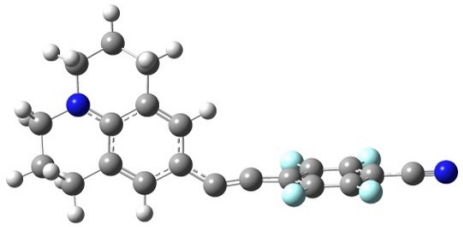
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.086887	-1.207736	-0.066216
2	6	0	-3.472892	-1.225894	-0.082716
3	6	0	-4.194827	0.000001	0.000014
4	6	0	-3.472826	1.225863	0.082639
5	6	0	-2.086824	1.207644	0.065934
6	6	0	-1.358975	-0.000062	-0.000198
7	6	0	0.054407	-0.000094	-0.000316
8	6	0	1.275189	-0.000095	-0.000316
9	6	0	2.682339	-0.000052	-0.000174
10	6	0	3.425906	1.19753	0.073604
11	6	0	4.810582	1.198832	0.073797
12	6	0	5.541627	0.000033	0.000107
13	6	0	4.810669	-1.19881	-0.073725
14	6	0	3.425992	-1.19759	-0.073802
15	6	0	6.966137	0.000075	0.000244
16	7	0	8.129661	0.000139	0.000353
17	9	0	5.465358	-2.366278	-0.145579
18	9	0	2.776797	-2.37112	-0.146079
19	9	0	5.465188	2.36634	0.145772
20	9	0	2.776626	2.371021	0.145754
21	7	0	-5.575077	0.000032	0.000114
22	6	0	-6.363409	1.230826	-0.066829
23	6	0	-5.556618	2.412805	-0.59673
24	6	0	-4.238957	2.526288	0.175341
25	6	0	-4.239094	-2.526286	-0.175304
26	6	0	-5.556639	-2.412741	0.596957
27	6	0	-6.363454	-1.230728	0.067171
28	1	0	-1.544296	-2.147707	-0.115498
29	1	0	-1.544184	2.147592	0.115131
30	1	0	-6.766118	1.466671	0.932163
31	1	0	-7.226198	1.042436	-0.71935
32	1	0	-6.154195	3.325298	-0.499941
33	1	0	-5.347055	2.268732	-1.663712
34	1	0	-4.45688	2.763288	1.227305
35	1	0	-3.628308	3.349381	-0.210144
36	1	0	-3.628426	-3.349403	0.210097
37	1	0	-4.457179	-2.76328	-1.227235
38	1	0	-5.346915	-2.268676	1.663909
39	1	0	-6.15427	-3.325208	0.500256
40	1	0	-6.766317	-1.466556	-0.931763
41	1	0	-7.226141	-1.042298	0.719816

Table S9. Cartesian coordinate for **JLD-F** at the optimized geometry in S_0 state using B3LYP/cc-PVDZ level of theory.



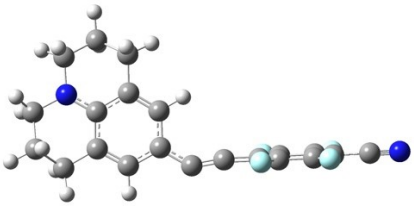
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.088881	-1.207579	-0.065997
2	6	0	-3.476474	-1.226391	-0.082213
3	6	0	-4.199235	0.000006	0.000009
4	6	0	-3.476344	1.226332	0.082154
5	6	0	-2.088755	1.207382	0.065786
6	6	0	-1.36012	-0.000134	-0.000148
7	6	0	0.056615	-0.000208	-0.000237
8	6	0	1.28	-0.000214	-0.00023
9	6	0	2.691545	-0.000118	-0.000124
10	6	0	3.428196	1.201545	0.073236
11	6	0	4.815456	1.202789	0.073439
12	6	0	5.540367	0.000069	0.000081
13	6	0	4.815625	-1.202747	-0.073385
14	6	0	3.428365	-1.201684	-0.07338
15	6	0	6.967241	0.000161	0.000182
16	7	0	8.131071	0.000296	0.000262
17	9	0	5.47298	-2.364034	-0.144317
18	9	0	2.776702	-2.368843	-0.144652
19	9	0	5.47265	2.364162	0.144462
20	9	0	2.776368	2.368618	0.144416
21	7	0	-5.580522	0.000075	0.000083
22	6	0	-6.365149	1.23067	-0.059764
23	6	0	-5.561081	2.410428	-0.595074
24	6	0	-4.243004	2.526525	0.172426
25	6	0	-4.243273	-2.526509	-0.172401
26	6	0	-5.561256	-2.410279	0.595239
27	6	0	-6.365264	-1.230442	0.060013
28	1	0	-1.543074	-2.152494	-0.115072
29	1	0	-1.542849	2.152243	0.114796
30	1	0	-6.765228	1.470641	0.94707
31	1	0	-7.240098	1.045229	-0.707473
32	1	0	-6.162469	3.327884	-0.500268
33	1	0	-5.353073	2.261164	-1.668396
34	1	0	-4.460137	2.76621	1.230664
35	1	0	-3.630167	3.354438	-0.216089
36	1	0	-3.630476	-3.35448	0.216051
37	1	0	-4.460542	-2.766176	-1.230615
38	1	0	-5.353119	-2.261034	1.668539
39	1	0	-6.162745	-3.327676	0.500499
40	1	0	-6.765473	-1.470375	-0.946779
41	1	0	-7.240127	-1.044914	0.707814

Table S10. Cartesian coordinate for **JLD-F** (twist-bent) at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.



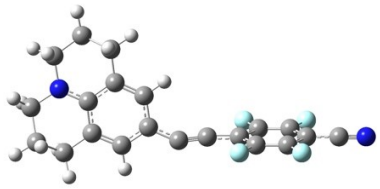
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.09164	-1.030132	0.647104
2	6	0	3.45597	-1.046516	0.670308
3	6	0	4.177556	0.000042	-0.000041
4	6	0	3.455669	1.046343	-0.670465
5	6	0	2.091342	1.029477	-0.6474
6	6	0	1.348104	-0.000456	-0.00018
7	6	0	-0.036611	-0.000715	-0.000266
8	6	0	-1.280646	-0.000787	-0.000409
9	6	0	-2.660028	-0.000459	-0.000194
10	6	0	-3.42267	-0.645119	-1.023527
11	6	0	-4.783079	-0.641576	-1.018162
12	6	0	-5.533397	0.000265	0.000214
13	6	0	-4.782467	0.641729	1.018377
14	6	0	-3.422055	0.64459	1.023351
15	6	0	-6.940151	0.000613	0.000418
16	7	0	-8.102934	0.000898	0.000586
17	9	0	-5.440207	1.263767	2.005174
18	9	0	-2.750659	1.267206	2.011388
19	9	0	-5.441412	-1.263295	-2.004764
20	9	0	-2.751872	-1.268077	-2.011754
21	7	0	5.525153	0.000279	0.000027
22	6	0	6.323079	1.097482	-0.554063
23	6	0	5.537801	2.391884	-0.65714
24	6	0	4.223856	2.128188	-1.381646
25	6	0	4.224467	-2.128092	1.381563
26	6	0	5.538578	-2.391321	0.657189
27	6	0	6.32341	-1.096642	0.554195
28	1	0	1.535239	-1.818593	1.142331
29	1	0	1.534713	1.817735	-1.142692
30	1	0	6.696804	0.791355	-1.540426
31	1	0	7.194103	1.221823	0.096957
32	1	0	6.142206	3.132882	-1.18654
33	1	0	5.340002	2.785373	0.345759
34	1	0	4.433153	1.81971	-2.414791
35	1	0	3.616609	3.034732	-1.442334
36	1	0	3.617534	-3.034851	1.442187
37	1	0	4.433552	-1.819544	2.41473
38	1	0	5.34102	-2.784878	-0.345731
39	1	0	6.143192	-3.132108	1.186649
40	1	0	6.696928	-0.790385	1.540596
41	1	0	7.194544	-1.220674	-0.096738

Table S11. Cartesian coordinate for **JLD-F** at the optimized geometry in S_1 state using CAM-B3LYP/6-31G+(d,p) level of theory.



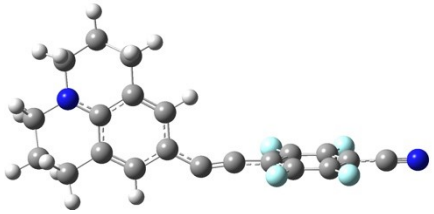
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.64375	-0.548282	0.223507
2	6	0	2.929753	-0.969326	0.404127
3	6	0	4.008459	-0.095242	0.028718
4	6	0	3.715772	1.202815	-0.51512
5	6	0	2.410821	1.584588	-0.655339
6	6	0	1.325189	0.737682	-0.303452
7	6	0	-0.006291	1.159106	-0.47115
8	6	0	-1.186319	0.730852	-0.293505
9	6	0	-2.524091	0.450249	-0.176205
10	6	0	-3.268565	0.740209	1.008516
11	6	0	-4.592662	0.43769	1.128058
12	6	0	-5.322484	-0.181705	0.08742
13	6	0	-4.596801	-0.469906	-1.091366
14	6	0	-3.272766	-0.171898	-1.222306
15	6	0	-6.693046	-0.495958	0.218477
16	7	0	-7.81962	-0.756688	0.327157
17	9	0	-5.235746	-1.057797	-2.114038
18	9	0	-2.627778	-0.476157	-2.367298
19	9	0	-5.227598	0.735701	2.271623
20	9	0	-2.619561	1.324655	2.036493
21	7	0	5.287824	-0.491824	0.186054
22	6	0	6.431932	0.390564	-0.060362
23	6	0	6.053482	1.859087	-0.01171
24	6	0	4.853506	2.101917	-0.918309
25	6	0	3.249998	-2.319505	0.987805
26	6	0	4.545311	-2.850221	0.386839
27	6	0	5.65667	-1.843385	0.617561
28	1	0	0.820578	-1.201239	0.494315
29	1	0	2.173812	2.564228	-1.056519
30	1	0	6.86447	0.134892	-1.037184
31	1	0	7.186074	0.158702	0.697912
32	1	0	6.913739	2.457616	-0.321524
33	1	0	5.808439	2.144704	1.016991
34	1	0	5.136437	1.898774	-1.959757
35	1	0	4.531139	3.144909	-0.878006
36	1	0	2.419205	-3.005404	0.807511
37	1	0	3.360343	-2.236411	2.077135
38	1	0	4.416614	-3.020824	-0.687485
39	1	0	4.831433	-3.803754	0.83753
40	1	0	5.930195	-1.806303	1.680756
41	1	0	6.55652	-2.123921	0.061611

Table S12. Cartesian coordinate for **JLD-F** at the optimized geometry in S_1 state using B3LYP/6-31+G(d,p) level of theory.



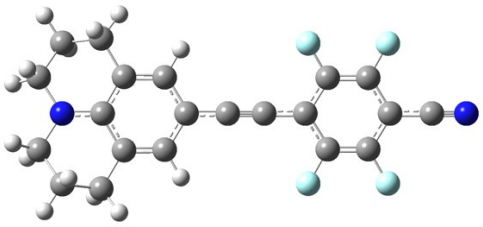
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.766377	0.6628	-0.333446
2	6	0	3.095721	0.983561	-0.505952
3	6	0	4.09777	0.068189	-0.0273
4	6	0	3.69993	-1.159169	0.608606
5	6	0	2.353707	-1.435546	0.740437
6	6	0	1.349707	-0.546364	0.285138
7	6	0	-0.034836	-0.862553	0.446418
8	6	0	-1.222303	-0.542601	0.278248
9	6	0	-2.593256	-0.319654	0.159922
10	6	0	-3.346524	-0.756985	-0.976538
11	6	0	-4.6927	-0.54488	-1.088876
12	6	0	-5.447274	0.128959	-0.078463
13	6	0	-4.69675	0.569251	1.056092
14	6	0	-3.350596	0.357365	1.169044
15	6	0	-6.830102	0.346465	-0.194042
16	7	0	-7.983827	0.53067	-0.291869
17	9	0	-5.347216	1.221594	2.045308
18	9	0	-2.69169	0.805555	2.267454
19	9	0	-5.33925	-0.98018	-2.193262
20	9	0	-2.683709	-1.396989	-1.972787
21	7	0	5.421196	0.363952	-0.175697
22	6	0	6.491438	-0.575804	0.19244
23	6	0	6.010243	-2.01997	0.246933
24	6	0	4.755221	-2.109384	1.117101
25	6	0	3.520868	2.263047	-1.182997
26	6	0	4.848371	2.751907	-0.600895
27	6	0	5.892742	1.649059	-0.715325
28	1	0	1.000854	1.347847	-0.68226
29	1	0	2.038601	-2.360908	1.211131
30	1	0	6.896628	-0.265256	1.167127
31	1	0	7.293649	-0.454697	-0.543165
32	1	0	6.81465	-2.645069	0.645383
33	1	0	5.790101	-2.375577	-0.766552
34	1	0	5.010813	-1.855168	2.156414
35	1	0	4.357851	-3.127904	1.1346
36	1	0	2.738069	3.018061	-1.071108
37	1	0	3.63597	2.088769	-2.262906
38	1	0	4.716902	3.03014	0.451419
39	1	0	5.211604	3.63756	-1.13026
40	1	0	6.177428	1.492259	-1.766444
41	1	0	6.805538	1.911618	-0.170103

Table S13. Cartesian coordinate for **JLD-F** at the optimized geometry in S_1 state using B3LYP/cc-PVDZ level of theory.



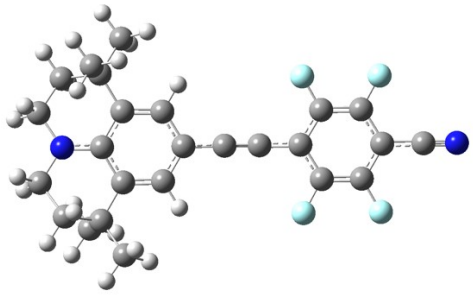
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.712832	-0.611773	-0.279704
2	6	0	-3.029438	-0.980837	-0.46139
3	6	0	-4.068483	-0.082039	-0.029588
4	6	0	-3.719086	1.178568	0.570678
5	6	0	-2.38333	1.501892	0.713193
6	6	0	-1.341211	0.631321	0.303645
7	6	0	0.030473	1.003049	0.476955
8	6	0	1.21376	0.63809	0.300455
9	6	0	2.577595	0.387305	0.177771
10	6	0	3.319876	0.766094	-0.988918
11	6	0	4.659417	0.507493	-1.113057
12	6	0	5.400835	-0.156423	-0.087864
13	6	0	4.664534	-0.535684	1.076422
14	6	0	3.325032	-0.278728	1.204142
15	6	0	6.777377	-0.424261	-0.2187
16	7	0	7.922166	-0.649173	-0.328376
17	9	0	5.316191	-1.167432	2.071883
18	9	0	2.668609	-0.662704	2.32199
19	9	0	5.306158	0.883897	-2.233206
20	9	0	2.658606	1.391233	-1.988785
21	7	0	-5.38021	-0.424768	-0.188415
22	6	0	-6.482307	0.492014	0.131613
23	6	0	-6.047787	1.950591	0.142781
24	6	0	-4.81362	2.1094	1.029696
25	6	0	-3.405794	-2.29483	-1.100423
26	6	0	-4.724844	-2.80381	-0.520895
27	6	0	-5.799834	-1.739978	-0.691089
28	1	0	-0.916001	-1.287006	-0.594867
29	1	0	-2.102729	2.4573	1.159073
30	1	0	-6.897381	0.200973	1.115857
31	1	0	-7.275598	0.319644	-0.61276
32	1	0	-6.883668	2.567033	0.504981
33	1	0	-5.817936	2.277431	-0.885246
34	1	0	-5.081014	1.875792	2.07764
35	1	0	-4.448092	3.146219	1.024732
36	1	0	-2.597025	-3.025105	-0.955745
37	1	0	-3.512695	-2.156687	-2.192872
38	1	0	-4.600949	-3.038789	0.549606
39	1	0	-5.054834	-3.724788	-1.023676
40	1	0	-6.073549	-1.628761	-1.757992
41	1	0	-6.720305	-2.015348	-0.152474

Table S14. Cartesian coordinate for **JLD-F** (planar) at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.



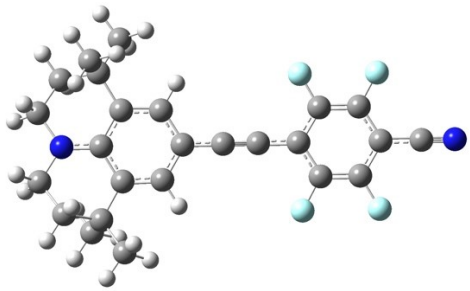
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.082809	-1.217146	-0.018903
2	6	0	-3.453338	-1.233174	-0.035364
3	6	0	-4.174983	0	-0.000001
4	6	0	-3.453336	1.233173	0.035363
5	6	0	-2.082807	1.217143	0.018905
6	6	0	-1.34508	-0.000002	0.000001
7	6	0	0.043815	-0.000003	0.000004
8	6	0	1.275724	-0.000003	0.000004
9	6	0	2.662257	-0.000002	0.000004
10	6	0	3.416147	1.203844	0.1233
11	6	0	4.782657	1.2005	0.124542
12	6	0	5.519248	0.000001	-0.000002
13	6	0	4.782658	-1.2005	-0.124543
14	6	0	3.416148	-1.203846	-0.123296
15	6	0	6.930806	0.000002	-0.000006
16	7	0	8.092282	0.000006	-0.000008
17	9	0	5.444829	-2.353783	-0.242746
18	9	0	2.756766	-2.360825	-0.242141
19	9	0	5.444826	2.353784	0.242744
20	9	0	2.756763	2.360821	0.242151
21	7	0	-5.54181	0.000001	-0.000002
22	6	0	-6.328849	1.222519	-0.104605
23	6	0	-5.531524	2.378384	-0.684531
24	6	0	-4.222018	2.526984	0.08147
25	6	0	-4.222022	-2.526983	-0.081472
26	6	0	-5.531528	-2.378381	0.684528
27	6	0	-6.328851	-1.222515	0.104601
28	1	0	-1.534779	-2.153654	-0.030827
29	1	0	-1.534776	2.15365	0.030831
30	1	0	-6.713219	1.489761	0.892066
31	1	0	-7.20039	1.002995	-0.732252
32	1	0	-6.132107	3.290441	-0.626227
33	1	0	-5.323428	2.188775	-1.743285
34	1	0	-4.440523	2.79684	1.123929
35	1	0	-3.613472	3.336758	-0.330372
36	1	0	-3.613478	-3.336759	0.33037
37	1	0	-4.440526	-2.796838	-1.123931
38	1	0	-5.323433	-2.188773	1.743282
39	1	0	-6.132113	-3.290437	0.626223
40	1	0	-6.713222	-1.489757	-0.892069
41	1	0	-7.200392	-1.00299	0.732249

Table S15. Cartesian coordinate for **TMeJLD-F** at the optimized geometry in S_0 state using CAM-B3LYP/6-31+G(d,p) level of theory.



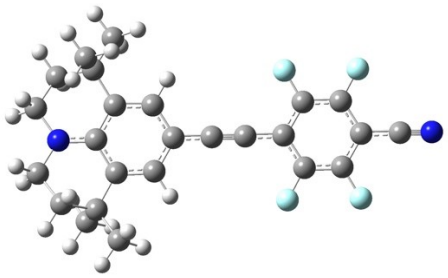
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.885672	1.2277	0.008553
2	6	0	1.503752	1.200889	0.017232
3	6	0	0.78661	-0.000023	0.000026
4	6	0	1.503777	-1.200919	-0.017201
5	6	0	2.885698	-1.227702	-0.008552
6	6	0	3.6004	0.000006	0
7	6	0	-0.632965	-0.000038	0.000051
8	6	0	-1.843077	-0.000039	0.000048
9	6	0	-3.255965	-0.000024	0.000033
10	6	0	-3.984629	-1.195304	-0.012575
11	6	0	-5.365615	-1.196993	-0.012637
12	6	0	-6.083444	0.000008	-0.000017
13	6	0	-5.365589	1.196992	0.012632
14	6	0	-3.984603	1.195272	0.012614
15	6	0	-7.509449	0.000023	-0.000037
16	7	0	-8.665331	0.000036	-0.000054
17	9	0	-3.340254	2.36019	0.024846
18	9	0	-6.016836	2.355403	0.024814
19	9	0	-3.340305	-2.360236	-0.024782
20	9	0	-6.016887	-2.355389	-0.02484
21	6	0	3.656341	-2.543738	0.02563
22	6	0	4.941863	-2.335096	-0.787335
23	6	0	5.77262	-1.190167	-0.242675
24	7	0	4.979326	0.000023	-0.000006
25	6	0	5.772596	1.190225	0.242687
26	6	0	4.94181	2.335145	0.787324
27	6	0	3.65629	2.543747	-0.025655
28	6	0	2.87721	-3.704354	-0.602445
29	6	0	3.988829	-2.903235	1.485528
30	6	0	2.877134	3.704364	0.602385
31	6	0	3.988781	2.903214	-1.48556
32	1	0	0.946795	2.129933	0.028123
33	1	0	0.946839	-2.129975	-0.028083
34	1	0	5.548054	-3.247564	-0.783139
35	1	0	4.670796	-2.131173	-1.829771
36	1	0	6.280816	-1.491648	0.685442
37	1	0	6.566302	-0.934353	-0.958045
38	1	0	6.566263	0.934423	0.958079
39	1	0	6.280812	1.491711	-0.685416
40	1	0	4.670738	2.131231	1.829761
41	1	0	5.547983	3.247625	0.783121
42	1	0	2.553583	-3.465279	-1.620302
43	1	0	3.514522	-4.593651	-0.648374
44	1	0	1.993146	-3.973304	-0.017837
45	1	0	3.069821	-3.103143	2.044473
46	1	0	4.617551	-3.800339	1.531571
47	1	0	4.512021	-2.091725	1.99869
48	1	0	2.553513	3.465314	1.62025
49	1	0	3.514426	4.593678	0.648286
50	1	0	1.993063	3.973275	0.017769
51	1	0	3.069773	3.103103	-2.044513
52	1	0	4.617495	3.800323	-1.53162
53	1	0	4.511982	2.091697	-1.998701

Table S16. Cartesian coordinate for **TMeJLD-F** at the optimized geometry in S_0 state using B3LYP/6-31G+(d,p) level of theory.



No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.898436	1.237024	0.010535
2	6	0	1.511781	1.208541	0.018313
3	6	0	0.787144	-0.000037	0.000035
4	6	0	1.511819	-1.208591	-0.018267
5	6	0	2.898475	-1.237031	-0.010526
6	6	0	3.619461	0.000008	-0.000004
7	6	0	-0.62641	-0.000061	0.000051
8	6	0	-1.84734	-0.000064	0.000045
9	6	0	-3.254329	-0.000038	0.000021
10	6	0	-3.998126	-1.199733	-0.013259
11	6	0	-5.382745	-1.20099	-0.013285
12	6	0	-6.113838	0.000012	-0.000015
13	6	0	-5.382704	1.200988	0.013276
14	6	0	-3.998084	1.199683	0.013286
15	6	0	-7.538312	0.000037	-0.000034
16	7	0	-8.701851	0.000058	-0.000049
17	9	0	-3.348739	2.37543	0.026203
18	9	0	-6.037312	2.370689	0.026148
19	9	0	-3.348822	-2.375503	-0.026155
20	9	0	-6.037394	-2.370668	-0.026175
21	6	0	3.666105	-2.56326	0.023912
22	6	0	4.972965	-2.354132	-0.769653
23	6	0	5.797522	-1.202279	-0.217227
24	7	0	4.999849	0.000031	-0.000021
25	6	0	5.797489	1.202364	0.217177
26	6	0	4.972906	2.354191	0.76962
27	6	0	3.666022	2.563277	-0.02392
28	6	0	2.88978	-3.721378	-0.632473
29	6	0	3.972749	-2.944233	1.494154
30	6	0	2.889672	3.721369	0.63248
31	6	0	3.972625	2.944257	-1.494168
32	1	0	0.953773	2.137187	0.028889
33	1	0	0.953839	-2.137254	-0.028828
34	1	0	5.580694	-3.266277	-0.749128
35	1	0	4.720569	-2.156841	-1.819003
36	1	0	6.287403	-1.492622	0.725512
37	1	0	6.604639	-0.952138	-0.920415
38	1	0	6.604624	0.952246	0.920352
39	1	0	6.287346	1.492725	-0.725569
40	1	0	4.720536	2.156891	1.818975
41	1	0	5.580604	3.266355	0.749083
42	1	0	2.589465	-3.473944	-1.656166
43	1	0	3.524911	-4.613483	-0.670701
44	1	0	1.991789	-3.99164	-0.06921
45	1	0	3.042298	-3.143022	2.035359
46	1	0	4.592481	-3.848576	1.53807
47	1	0	4.495433	-2.144962	2.027815
48	1	0	2.589396	3.473931	1.656183
49	1	0	3.524768	4.6135	0.670683
50	1	0	1.991653	3.991591	0.069241
51	1	0	3.042156	3.143012	-2.035355
52	1	0	4.592323	3.848622	-1.538097
53	1	0	4.495327	2.145004	-2.027838

Table S17. Cartesian coordinate for **TMeJLD-F** at the optimized geometry in S_0 state using B3LYP/cc-PVDZ level of theory.



No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.901559	1.236935	0.008795
2	6	0	1.513277	1.208574	0.018421
3	6	0	0.787684	0.00003	0.000001
4	6	0	1.513247	-1.208533	-0.01842
5	6	0	2.901528	-1.236929	-0.008796
6	6	0	3.623248	-0.000006	-0.000001
7	6	0	-0.629128	0.00005	0.000003
8	6	0	-1.852652	0.000053	0.000002
9	6	0	-3.264015	0.000031	0.000002
10	6	0	-4.000918	-1.203685	-0.014816
11	6	0	-5.388129	-1.204897	-0.014851
12	6	0	-6.113088	-0.000011	-0.000001
13	6	0	-5.388164	1.204896	0.014851
14	6	0	-4.000953	1.203725	0.014818
15	6	0	-7.539925	-0.000031	-0.000002
16	7	0	-8.703769	-0.000047	-0.000003
17	9	0	-3.349081	2.373029	0.029169
18	9	0	-6.045452	2.368354	0.029172
19	9	0	-3.349012	-2.372969	-0.029166
20	9	0	-6.045383	-2.368373	-0.029173
21	6	0	3.670347	-2.563201	0.025642
22	6	0	4.974383	-2.351855	-0.770578
23	6	0	5.799133	-1.201754	-0.217866
24	7	0	5.004814	-0.000022	-0.000003
25	6	0	5.799162	1.201689	0.217869
26	6	0	4.974439	2.35181	0.770579
27	6	0	3.67041	2.563188	-0.025643
28	6	0	2.892692	-3.719334	-0.627578
29	6	0	3.977957	-2.938255	1.494864
30	6	0	2.892783	3.719341	0.627574
31	6	0	3.978032	2.938232	-1.494865
32	1	0	0.952424	2.142296	0.027759
33	1	0	0.952371	-2.142241	-0.027756
34	1	0	5.587021	-3.267954	-0.756064
35	1	0	4.716313	-2.150541	-1.824213
36	1	0	6.294573	-1.496632	0.72839
37	1	0	6.613238	-0.952246	-0.923041
38	1	0	6.613257	0.952158	0.923048
39	1	0	6.294616	1.496556	-0.728383
40	1	0	4.716362	2.150502	1.824214
41	1	0	5.5871	3.267894	0.756067
42	1	0	2.590357	-3.47184	-1.657289
43	1	0	3.527367	-4.619551	-0.665541
44	1	0	1.988456	-3.987388	-0.060956
45	1	0	3.042919	-3.136462	2.041676
46	1	0	4.602582	-3.846949	1.545168
47	1	0	4.502204	-2.131438	2.029224
48	1	0	2.590441	3.471856	1.657285
49	1	0	3.527479	4.619542	0.665534
50	1	0	1.988554	3.987415	0.060951
51	1	0	3.043	3.136463	-2.041679
52	1	0	4.602681	3.84691	-1.545169
53	1	0	4.50226	2.1314	-2.029224

Table S18. Cartesian coordinate for **TMeJLD-F** (twist-bent) at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.

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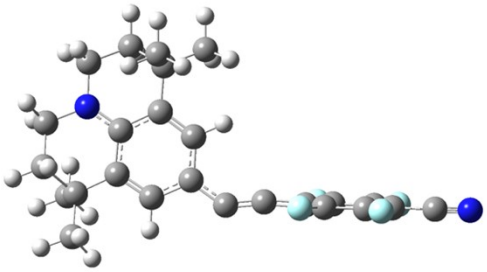
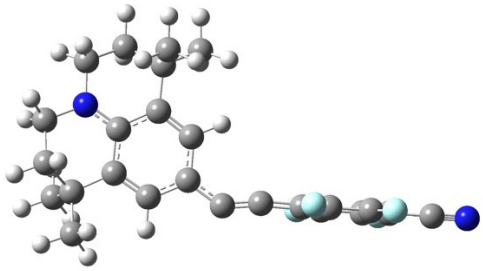


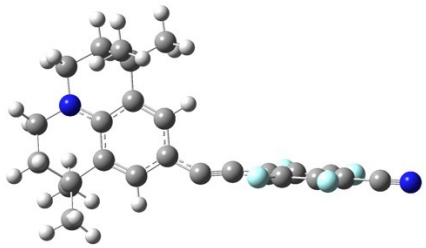
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.336246	1.124622	0.033336
2	6	0	1.070515	0.613504	0.023538
3	6	0	0.80069	-0.782927	-0.022728
4	6	0	1.916414	-1.658671	-0.055988
5	6	0	3.209394	-1.21616	-0.040949
6	6	0	3.449147	0.205734	0.00422
7	6	0	-0.509786	-1.286175	-0.036977
8	6	0	-1.706911	-0.862233	-0.022712
9	6	0	-3.053126	-0.609265	-0.014553
10	6	0	-3.796785	-0.400765	-1.216384
11	6	0	-5.126661	-0.101631	-1.199968
12	6	0	-5.852233	0.02524	0.005673
13	6	0	-5.127118	-0.180309	1.200715
14	6	0	-3.797234	-0.479875	1.19808
15	6	0	-7.227835	0.339354	0.015674
16	7	0	-8.358979	0.600368	0.023956
17	9	0	-3.148002	-0.661424	2.361051
18	9	0	-5.768738	-0.074695	2.368918
19	9	0	-3.147029	-0.505633	-2.388537
20	9	0	-5.767778	0.080273	-2.359031
21	6	0	4.385462	-2.18562	-0.017955
22	6	0	5.543615	-1.514635	-0.766008
23	6	0	5.88962	-0.168408	-0.168519
24	7	0	4.713727	0.677237	0.019429
25	6	0	5.04587	2.084535	0.22703
26	6	0	3.889702	2.872895	0.802156
27	6	0	2.593114	2.627352	0.021418
28	6	0	4.065552	-3.510162	-0.719839
29	6	0	4.772982	-2.478402	1.444083
30	6	0	1.468447	3.418893	0.697856
31	6	0	2.731132	3.105968	-1.43643
32	1	0	0.213234	1.274362	0.0429
33	1	0	1.698713	-2.718499	-0.086849
34	1	0	6.433723	-2.151135	-0.73945
35	1	0	5.266879	-1.389247	-1.819207
36	1	0	6.396271	-0.282115	0.79811
37	1	0	6.578607	0.376065	-0.823562
38	1	0	5.906942	2.117364	0.903645
39	1	0	5.378453	2.508988	-0.728541
40	1	0	3.73728	2.591193	1.850456
41	1	0	4.147225	3.936635	0.787837
42	1	0	3.705642	-3.346949	-1.740104
43	1	0	4.970227	-4.124105	-0.771642
44	1	0	3.31341	-4.091894	-0.181449
45	1	0	3.958054	-3.000088	1.953277
46	1	0	5.663303	-3.115618	1.485124
47	1	0	4.978985	-1.56716	2.013292
48	1	0	1.277119	3.057866	1.712816
49	1	0	1.750746	4.474575	0.759397
50	1	0	0.532628	3.369851	0.136
51	1	0	1.785643	2.971579	-1.968794
52	1	0	2.990986	4.169823	-1.46808
53	1	0	3.495341	2.551427	-1.989103

Table S19. Cartesian coordinate for **TMeJLD-F** at the optimized geometry in S_1 state using CAM-B3LYP/6-31+G(d,p) level of theory.



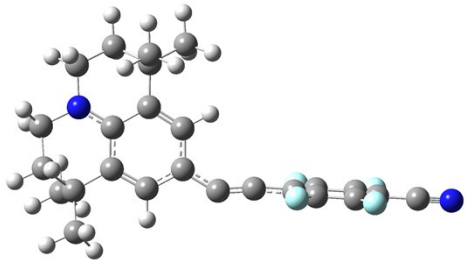
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.210094	1.221703	-0.047827
2	6	0	-1.91394	1.656173	-0.068421
3	6	0	-0.804846	0.771601	-0.031252
4	6	0	-1.081708	-0.623944	0.024321
5	6	0	-2.350931	-1.127287	0.037505
6	6	0	-3.459518	-0.200289	0.004353
7	6	0	0.512921	1.262118	-0.049727
8	6	0	1.707714	0.838834	-0.030567
9	6	0	3.05445	0.577328	-0.018671
10	6	0	3.806035	0.471447	1.192187
11	6	0	5.139763	0.188651	1.198593
12	6	0	5.873797	-0.01706	0.007661
13	6	0	5.141141	0.088847	-1.197084
14	6	0	3.807419	0.371068	-1.21567
15	6	0	7.254452	-0.313309	0.020759
16	7	0	8.389499	-0.559475	0.031582
17	9	0	3.156501	0.452467	-2.394568
18	9	0	5.783433	-0.096611	-2.360329
19	9	0	3.153915	0.650913	2.359445
20	9	0	5.780786	0.100712	2.373924
21	6	0	-2.617356	-2.628436	0.031404
22	6	0	-3.916195	-2.861999	0.812743
23	6	0	-5.066888	-2.068709	0.235012
24	7	0	-4.725888	-0.663082	0.022203
25	6	0	-5.897365	0.18995	-0.169267
26	6	0	-5.543223	1.532031	-0.769833
27	6	0	-4.380294	2.198209	-0.024178
28	6	0	-1.497648	-3.425291	0.710895
29	6	0	-2.757909	-3.111534	-1.425836
30	6	0	-4.054275	3.521151	-0.727195
31	6	0	-4.763756	2.494309	1.43941
32	1	0	-1.690228	2.714314	-0.105116
33	1	0	-0.229584	-1.29098	0.046417
34	1	0	-4.180144	-3.92381	0.801418
35	1	0	-3.760891	-2.578551	1.859936
36	1	0	-5.401673	-2.493186	-0.719649
37	1	0	-5.927759	-2.092916	0.91156
38	1	0	-6.588273	-0.3526	-0.823204
39	1	0	-6.402829	0.308547	0.797255
40	1	0	-5.267707	1.404089	-1.822826
41	1	0	-6.428772	2.174207	-0.743313
42	1	0	-1.305962	-3.064647	1.725441
43	1	0	-1.787033	-4.478489	0.773041
44	1	0	-0.56109	-3.383696	0.15094
45	1	0	-1.810052	-2.990627	-1.956039
46	1	0	-3.029338	-4.172136	-1.452201
47	1	0	-3.513807	-2.551439	-1.983022
48	1	0	-3.699697	3.356454	-1.748616
49	1	0	-4.955633	4.139372	-0.775033
50	1	0	-3.297704	4.098736	-0.19188
51	1	0	-3.947709	3.017105	1.944417
52	1	0	-5.653201	3.131921	1.480041
53	1	0	-4.968385	1.585538	2.011805

Table S20. Cartesian coordinate for **TMeJLD-F** at the optimized geometry in S_1 state using B3LYP/6-31+G(d,p) level of theory.



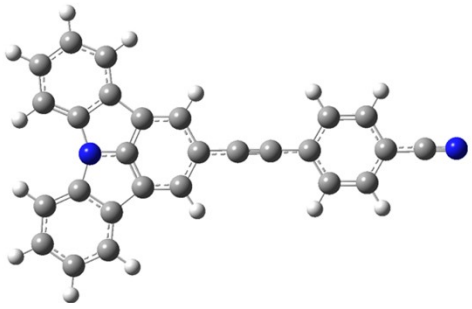
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.175226	-1.244698	0.033069
2	6	0	-1.832596	-1.567786	0.0385
3	6	0	-0.81098	-0.590316	0.010438
4	6	0	-1.198457	0.77379	-0.023774
5	6	0	-2.517551	1.174689	-0.029431
6	6	0	-3.542985	0.15387	-0.001512
7	6	0	0.565948	-0.97194	0.01726
8	6	0	1.763183	-0.645255	0.009925
9	6	0	3.140648	-0.429158	0.005846
10	6	0	3.900042	-0.338177	-1.204644
11	6	0	5.251828	-0.132343	-1.208068
12	6	0	6.007126	0.006436	-0.001857
13	6	0	5.250573	-0.081176	1.208356
14	6	0	3.898806	-0.287061	1.212196
15	6	0	7.39563	0.217683	-0.005583
16	7	0	8.554315	0.397073	-0.008712
17	9	0	3.23482	-0.353532	2.394068
18	9	0	5.901346	0.050262	2.386008
19	9	0	3.237335	-0.454774	-2.383302
20	9	0	5.903872	-0.050923	-2.389524
21	6	0	-2.899841	2.656454	-0.014953
22	6	0	-4.238571	2.794295	-0.766244
23	6	0	-5.313677	1.894878	-0.184301
24	7	0	-4.858414	0.511231	-0.0085
25	6	0	-5.952666	-0.451371	0.157941
26	6	0	-5.486337	-1.769061	0.749288
27	6	0	-4.253705	-2.329695	0.012972
28	6	0	-1.857663	3.540999	-0.727508
29	6	0	-3.035374	3.131863	1.454908
30	6	0	-3.809181	-3.616618	0.736069
31	6	0	-4.596098	-2.678449	-1.458879
32	1	0	-1.521234	-2.603978	0.061433
33	1	0	-0.406726	1.511222	-0.041657
34	1	0	-4.590942	3.830429	-0.726704
35	1	0	-4.085385	2.546046	-1.823706
36	1	0	-5.659904	2.265446	0.79041
37	1	0	-6.191885	1.864408	-0.839582
38	1	0	-6.702174	0.020655	0.803647
39	1	0	-6.428254	-0.599183	-0.821511
40	1	0	-5.239693	-1.628476	1.808871
41	1	0	-6.31372	-2.485066	0.703519
42	1	0	-1.662579	3.192557	-1.746652
43	1	0	-2.232056	4.568444	-0.784717
44	1	0	-0.906559	3.576179	-0.190594
45	1	0	-2.06921	3.068206	1.963296
46	1	0	-3.368333	4.175529	1.48681
47	1	0	-3.744789	2.528901	2.030442
48	1	0	-3.474507	-3.409467	1.757457
49	1	0	-4.65261	-4.313063	0.788537
50	1	0	-3.001211	-4.130366	0.209256
51	1	0	-3.724778	-3.11317	-1.956786
52	1	0	-5.41007	-3.411428	-1.495517
53	1	0	-4.898304	-1.802363	-2.041108

Table S21. Cartesian coordinate for **TMeJLD-F** at the optimized geometry in S_1 state using B3LYP/cc-PVDZ level of theory.



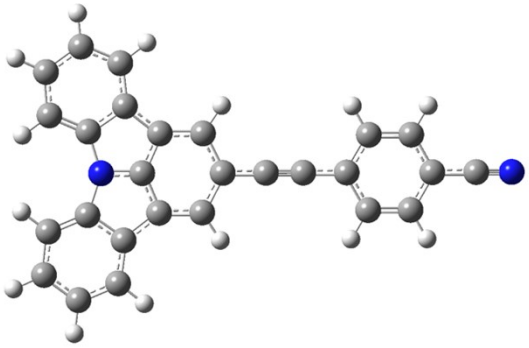
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.199891	-1.235344	0.032898
2	6	0	-1.868293	-1.604968	0.040055
3	6	0	-0.809892	-0.664169	0.009894
4	6	0	-1.153206	0.713816	-0.027045
5	6	0	-2.458904	1.159757	-0.030714
6	6	0	-3.519955	0.175278	-0.002099
7	6	0	0.552864	-1.100221	0.018296
8	6	0	1.748538	-0.734742	0.01025
9	6	0	3.121071	-0.498927	0.006517
10	6	0	3.872759	-0.391486	-1.209598
11	6	0	5.220832	-0.148074	-1.2114
12	6	0	5.96297	0.01473	-0.001153
13	6	0	5.21716	-0.091348	1.21312
14	6	0	3.869116	-0.334786	1.218562
15	6	0	7.348333	0.267907	-0.004938
16	7	0	8.500726	0.480835	-0.008085
17	9	0	3.204537	-0.420062	2.393155
18	9	0	5.868758	0.057154	2.382984
19	9	0	3.211754	-0.531695	-2.380871
20	9	0	5.876029	-0.054403	-2.384913
21	6	0	-2.791775	2.654399	-0.017063
22	6	0	-4.122555	2.833906	-0.772054
23	6	0	-5.227807	1.974574	-0.188883
24	7	0	-4.823152	0.578024	-0.00901
25	6	0	-5.946662	-0.346221	0.161511
26	6	0	-5.524921	-1.677138	0.753952
27	6	0	-4.316734	-2.282123	0.01399
28	6	0	-1.719173	3.500971	-0.725958
29	6	0	-2.915529	3.129905	1.451395
30	6	0	-3.91501	-3.582289	0.733852
31	6	0	-4.672324	-2.613278	-1.456374
32	1	0	-1.59106	-2.657025	0.063685
33	1	0	-0.332268	1.427804	-0.045342
34	1	0	-4.443204	3.886787	-0.740742
35	1	0	-3.973403	2.572266	-1.833244
36	1	0	-5.565539	2.363238	0.789175
37	1	0	-6.112259	1.974557	-0.846848
38	1	0	-6.684302	0.154398	0.809858
39	1	0	-6.434375	-0.480259	-0.821352
40	1	0	-5.265346	-1.541141	1.817391
41	1	0	-6.383033	-2.366027	0.715998
42	1	0	-1.535029	3.145581	-1.751482
43	1	0	-2.055831	4.548156	-0.782298
44	1	0	-0.761949	3.499018	-0.185765
45	1	0	-1.947717	3.032903	1.965736
46	1	0	-3.216849	4.189948	1.488262
47	1	0	-3.6487	2.54446	2.027983
48	1	0	-3.572684	-3.386689	1.761716
49	1	0	-4.784034	-4.257083	0.785356
50	1	0	-3.117796	-4.122772	0.204143
51	1	0	-3.812521	-3.079841	-1.960146
52	1	0	-5.517496	-3.320302	-1.497767
53	1	0	-4.943412	-1.719693	-2.039913

Table S22. Cartesian coordinate for **IndCBZ-H** at the optimized geometry in S_0 state using CAM-B3LYP/6-31+G(d,p) level of theory.



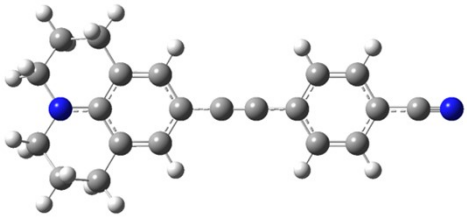
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.784041	2.156306	0.000016
2	6	0	2.924271	3.538566	0.00001
3	6	0	4.198723	4.093978	0
4	6	0	5.333048	3.280596	0
5	6	0	5.229655	1.893505	0.00001
6	6	0	3.958589	1.341865	0.000016
7	7	0	3.551268	-0.00001	0.000037
8	6	0	2.193766	0.000003	0.00004
9	6	0	3.958562	-1.341894	0.000006
10	6	0	5.229617	-1.893559	-0.000016
11	6	0	5.332982	-3.280652	-0.000046
12	6	0	4.198641	-4.094011	-0.000051
13	6	0	2.9242	-3.538573	-0.000028
14	6	0	2.783998	-2.156311	0.000001
15	6	0	1.622398	-1.256996	0.000019
16	6	0	0.232091	-1.247511	0.000008
17	6	0	-0.441585	0.00003	0.000008
18	6	0	0.232115	1.247557	0.000014
19	6	0	1.622423	1.257014	0.00003
20	6	0	-1.870433	0.000045	-0.000005
21	6	0	-3.079596	0.000041	-0.000012
22	6	0	-4.505018	0.000027	-0.000008
23	6	0	-5.21698	1.208406	-0.000108
24	6	0	-6.600242	1.210081	-0.000105
25	6	0	-7.300698	-0.000001	-0.000002
26	6	0	-6.600218	-1.210069	0.000097
27	6	0	-5.216956	-1.208367	0.000095
28	6	0	-8.735043	-0.000014	0.000002
29	7	0	-9.891972	-0.000034	-0.000001
30	1	0	2.046445	4.177229	0.000011
31	1	0	4.313862	5.172805	-0.000006
32	1	0	6.317888	3.736629	-0.000007
33	1	0	6.115285	1.267968	0.000012
34	1	0	6.11526	-1.26804	-0.000012
35	1	0	6.317813	-3.736705	-0.000064
36	1	0	4.313759	-5.17284	-0.000075
37	1	0	2.046361	-4.17722	-0.000033
38	1	0	-0.359693	-2.156247	-0.000007
39	1	0	-0.359651	2.156305	0.000004
40	1	0	-4.670912	2.144931	-0.000186
41	1	0	-7.147386	2.146263	-0.000182
42	1	0	-7.147343	-2.146262	0.000177
43	1	0	-4.670869	-2.144881	0.000172

Table S23. Cartesian coordinate for **IndCBZ-H** at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.



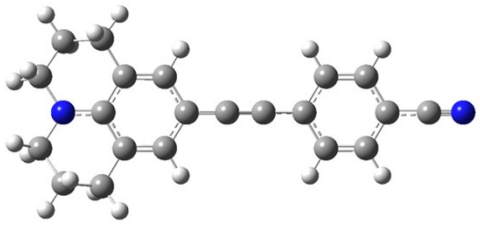
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.761521	2.160672	-0.000006
2	6	0	2.927391	3.545627	-0.000007
3	6	0	4.216655	4.082678	0.000038
4	6	0	5.348801	3.270092	0.000084
5	6	0	5.220124	1.872763	0.000087
6	6	0	3.94962	1.345354	0.000042
7	7	0	3.519505	0.00012	0.000033
8	6	0	2.176923	-0.000039	-0.000017
9	6	0	3.949938	-1.345012	0.000042
10	6	0	5.220567	-1.872121	0.000088
11	6	0	5.349574	-3.26942	0.000086
12	6	0	4.217619	-4.082273	0.00004
13	6	0	2.928229	-3.545527	-0.000005
14	6	0	2.762032	-2.16061	-0.000005
15	6	0	1.614807	-1.280124	-0.000044
16	6	0	0.207656	-1.273424	-0.000104
17	6	0	-0.449517	-0.000349	-0.00013
18	6	0	0.207356	1.272881	-0.000104
19	6	0	1.614504	1.279914	-0.000044
20	6	0	-1.85981	-0.000516	-0.000197
21	6	0	-3.074661	-0.000599	-0.000232
22	6	0	-4.494034	-0.00038	-0.000121
23	6	0	-5.205168	1.210657	-0.000069
24	6	0	-6.587545	1.211803	0.000028
25	6	0	-7.286549	0.000045	0.000074
26	6	0	-6.587913	-1.211925	0.000021
27	6	0	-5.205536	-1.2112	-0.000075
28	6	0	-8.720786	0.000263	0.000175
29	7	0	-9.877606	0.000434	0.000255
30	1	0	2.063184	4.202163	-0.000042
31	1	0	4.337265	5.16151	0.000037
32	1	0	6.337573	3.714911	0.000119
33	1	0	6.097033	1.23455	0.000122
34	1	0	6.097325	-1.233701	0.000123
35	1	0	6.338451	-3.714005	0.000121
36	1	0	4.338485	-5.161077	0.000039
37	1	0	2.064177	-4.202267	-0.000041
38	1	0	-0.394362	-2.172746	-0.000131
39	1	0	-0.394875	2.17206	-0.000133
40	1	0	-4.657568	2.146163	-0.000107
41	1	0	-7.135949	2.147073	0.000068
42	1	0	-7.1366	-2.147028	0.000056
43	1	0	-4.65822	-2.146872	-0.000118

Table S24. Cartesian coordinate for **JLD-H** at the optimized geometry in S_0 state using CAM-B3LYP/6-31G+(d,p) level of theory.



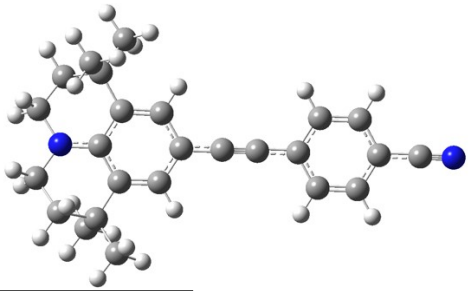
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.630491	1.211391	0.12999
2	6	0	-1.248183	1.193742	0.112773
3	6	0	-0.525588	0.00001	-0.000078
4	6	0	-1.24818	-1.193728	-0.112887
5	6	0	-2.630488	-1.211388	-0.13003
6	6	0	-3.346911	-0.000002	0.000001
7	6	0	0.897709	0.000015	-0.00012
8	6	0	2.108106	0.000016	-0.000117
9	6	0	3.531743	0.00001	-0.000061
10	6	0	4.245799	-1.202335	-0.118346
11	6	0	5.628765	-1.203961	-0.118427
12	6	0	6.330275	-0.000002	0.000036
13	6	0	5.628767	1.203963	0.11845
14	6	0	4.245801	1.202349	0.118272
15	6	0	-3.395563	-2.502849	-0.267874
16	6	0	-4.699271	-2.41585	0.518936
17	6	0	-5.509907	-1.2242	0.033599
18	7	0	-4.727604	-0.000008	0.000037
19	6	0	-5.509918	1.224179	-0.033463
20	6	0	-4.699324	2.415835	-0.518854
21	6	0	-3.395566	2.502848	0.267871
22	6	0	7.764248	-0.000008	0.000086
23	7	0	8.921365	-0.000016	0.000126
24	1	0	-0.707763	2.131975	0.198598
25	1	0	-0.707757	-2.131957	-0.198746
26	1	0	3.699748	-2.134395	-0.210136
27	1	0	6.175687	-2.135885	-0.210115
28	1	0	6.175691	2.135883	0.210175
29	1	0	3.699752	2.134414	0.210023
30	1	0	-2.783503	-3.340966	0.079456
31	1	0	-3.62558	-2.699592	-1.324287
32	1	0	-5.29544	-3.326233	0.405097
33	1	0	-4.476664	-2.299364	1.58545
34	1	0	-5.92202	-1.434756	-0.966386
35	1	0	-6.368038	-1.061653	0.698438
36	1	0	-6.368095	1.061628	-0.698239
37	1	0	-5.92196	1.43473	0.966553
38	1	0	-5.295493	3.326213	-0.40498
39	1	0	-4.476785	2.299348	-1.585383
40	1	0	-2.783534	3.340966	-0.079505
41	1	0	-3.625517	2.699599	1.324297

Table S25. Cartesian coordinate for **JLD-H** at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.



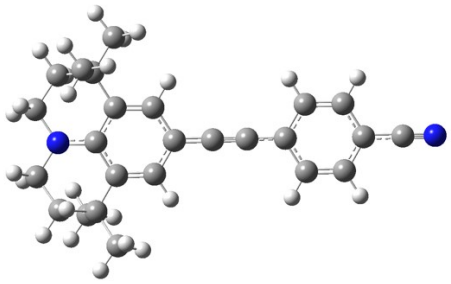
No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.619407	1.226141	0.125064
2	6	0	-1.249526	1.213046	0.110274
3	6	0	-0.504869	0.000036	0.000144
4	6	0	-1.24948	-1.212996	-0.110063
5	6	0	-2.61936	-1.226129	-0.125004
6	6	0	-3.34142	-0.000003	-0.00001
7	6	0	0.877548	0.000054	0.000226
8	6	0	2.116254	0.000064	0.000287
9	6	0	3.502683	0.000038	0.000168
10	6	0	4.241406	-1.220594	-0.118793
11	6	0	5.611055	-1.21503	-0.118511
12	6	0	6.329454	-0.000014	-0.000078
13	6	0	5.61112	1.215028	0.11848
14	6	0	4.241471	1.220643	0.118999
15	6	0	-3.39098	-2.51204	-0.263891
16	6	0	-4.69545	-2.418656	0.519629
17	6	0	-5.497599	-1.22569	0.027032
18	7	0	-4.711759	-0.000022	-0.000083
19	6	0	-5.497629	1.225624	-0.027284
20	6	0	-4.69546	2.418612	-0.519793
21	6	0	-3.391078	2.512031	0.263869
22	6	0	7.748333	-0.00004	-0.000201
23	7	0	8.910993	-0.000061	-0.000303
24	1	0	-0.704039	2.147592	0.193226
25	1	0	-0.70396	-2.147527	-0.192953
26	1	0	3.696411	-2.15422	-0.209749
27	1	0	6.161027	-2.145786	-0.209342
28	1	0	6.161142	2.145763	0.209217
29	1	0	3.696527	2.154288	0.21005
30	1	0	-2.782073	-3.351931	0.082256
31	1	0	-3.618343	-2.702856	-1.321909
32	1	0	-5.296292	-3.325147	0.40282
33	1	0	-4.479152	-2.302467	1.587365
34	1	0	-5.891424	-1.427335	-0.981865
35	1	0	-6.364622	-1.052355	0.675884
36	1	0	-6.364578	1.052265	-0.676231
37	1	0	-5.89157	1.427258	0.98157
38	1	0	-5.29634	3.325087	-0.403048
39	1	0	-4.479043	2.30243	-1.587505
40	1	0	-2.782156	3.351939	-0.082211
41	1	0	-3.618561	2.70284	1.321863

Table S26. Cartesian coordinate for **TMeJLD-H** at the optimized geometry in S_0 state using CAM-B3LYP/6-31G+(d,p) level of theory.



No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.098355	1.225789	0.010529
2	6	0	0.715109	1.198723	0.01948
3	6	0	-0.004102	-0.00001	0.000003
4	6	0	0.715119	-1.198739	-0.019474
5	6	0	2.098365	-1.225793	-0.010524
6	6	0	2.812862	0.000001	0
7	6	0	-1.427691	-0.000016	0.000002
8	6	0	-2.638178	-0.000016	0.000003
9	6	0	-4.06178	-0.000012	0.000001
10	6	0	-4.77597	-1.207906	-0.023021
11	6	0	-6.158927	-1.209537	-0.023055
12	6	0	-6.860492	-0.000005	-0.000003
13	6	0	-6.158921	1.209524	0.023051
14	6	0	-4.775964	1.207886	0.023021
15	6	0	2.870148	-2.541273	0.020005
16	6	0	4.152889	-2.330937	-0.797296
17	6	0	4.986684	-1.187698	-0.252883
18	7	0	4.194644	0.000002	0.000007
19	6	0	4.986676	1.187722	0.25282
20	6	0	4.15289	2.330952	0.797263
21	6	0	2.870118	2.541281	-0.019992
22	6	0	-8.294438	-0.000001	-0.000005
23	7	0	-9.451559	0.000009	-0.000006
24	6	0	2.090386	-3.702386	-0.606268
25	6	0	3.208325	-2.901938	1.478269
26	6	0	2.090349	3.702359	0.606336
27	6	0	3.208234	2.90199	-1.478259
28	1	0	0.159448	2.128588	0.032491
29	1	0	0.159464	-2.128607	-0.032484
30	1	0	-4.229966	-2.144338	-0.040923
31	1	0	-6.705833	-2.145806	-0.040911
32	1	0	-6.705821	2.145797	0.040905
33	1	0	-4.229954	2.144315	0.040922
34	1	0	3.877282	-2.123836	-1.837922
35	1	0	4.758753	-3.243762	-0.79842
36	1	0	5.501186	-1.494348	0.670452
37	1	0	5.776617	-0.929909	-0.972221
38	1	0	5.776659	0.929963	0.972112
39	1	0	5.501115	1.494367	-0.670554
40	1	0	4.758745	3.243784	0.798367
41	1	0	3.877323	2.123845	1.837897
42	1	0	1.763011	-3.462668	-1.622797
43	1	0	2.7283	-4.591207	-0.654967
44	1	0	1.208413	-3.971995	-0.018715
45	1	0	2.291387	-3.102527	2.040438
46	1	0	3.838	-3.798636	1.521743
47	1	0	3.732664	-2.090056	1.989563
48	1	0	1.763023	3.462612	1.622874
49	1	0	2.72824	4.591197	0.655027
50	1	0	1.208343	3.971957	0.018825
51	1	0	2.291271	3.102576	-2.04039
52	1	0	3.83789	3.798702	-1.521733
53	1	0	3.73257	2.090133	-1.989595

Table S27. Cartesian coordinate for **TMeJLD-H** at the optimized geometry in S_1 state using CAM-B3LYP/6-31G(d) level of theory.



No.	Atom	Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.088967	1.240526	0.014069
2	6	0	0.718505	1.217392	0.020746
3	6	0	-0.023052	0.000052	0.000134
4	6	0	0.718448	-1.217323	-0.02055
5	6	0	2.088909	-1.240519	-0.014017
6	6	0	2.809666	-0.000013	-0.000012
7	6	0	-1.405555	0.000083	0.000213
8	6	0	-2.644461	0.000102	0.000278
9	6	0	-4.030724	0.000067	0.000161
10	6	0	-4.769858	-1.2259	-0.033453
11	6	0	-6.139403	-1.220297	-0.033669
12	6	0	-6.858083	-0.000002	-0.000071
13	6	0	-6.139468	1.220328	0.033644
14	6	0	-4.769924	1.225998	0.033651
15	6	0	2.864944	-2.552468	0.020662
16	6	0	4.150299	-2.337477	-0.790202
17	6	0	4.975973	-1.190924	-0.243497
18	7	0	4.180256	-0.000044	-0.000083
19	6	0	4.976052	1.190799	0.243249
20	6	0	4.150488	2.337389	0.790041
21	6	0	2.865058	2.55244	-0.020687
22	6	0	-8.276809	-0.000035	-0.000185
23	7	0	-9.439523	-0.000065	-0.000277
24	6	0	2.090686	-3.715181	-0.609284
25	6	0	3.193292	-2.909743	1.482595
26	6	0	2.090918	3.715186	0.609343
27	6	0	3.193268	2.909705	-1.482654
28	1	0	0.157768	2.143326	0.032589
29	1	0	0.157667	-2.143231	-0.03233
30	1	0	-4.224947	-2.163665	-0.059173
31	1	0	-6.6894	-2.155131	-0.059459
32	1	0	-6.689515	2.155134	0.059348
33	1	0	-4.225063	2.16379	0.059463
34	1	0	3.882491	-2.134622	-1.833642
35	1	0	4.761268	-3.246395	-0.784137
36	1	0	5.478198	-1.484723	0.689943
37	1	0	5.772753	-0.926002	-0.951523
38	1	0	5.772894	0.925841	0.951191
39	1	0	5.478193	1.484577	-0.690244
40	1	0	4.761497	3.24628	0.783914
41	1	0	3.882779	2.134545	1.833509
42	1	0	1.767297	-3.476734	-1.627057
43	1	0	2.731649	-4.601736	-0.653806
44	1	0	1.207383	-3.986337	-0.025244
45	1	0	2.272189	-3.110355	2.037037
46	1	0	3.821964	-3.806396	1.529738
47	1	0	3.713951	-2.099197	2.000397
48	1	0	1.767624	3.47675	1.627149
49	1	0	2.731925	4.601712	0.653801
50	1	0	1.207565	3.986384	0.025397
51	1	0	2.272116	3.11036	-2.036998
52	1	0	3.821976	3.806329	-1.52986
53	1	0	3.713835	2.099136	-2.000514

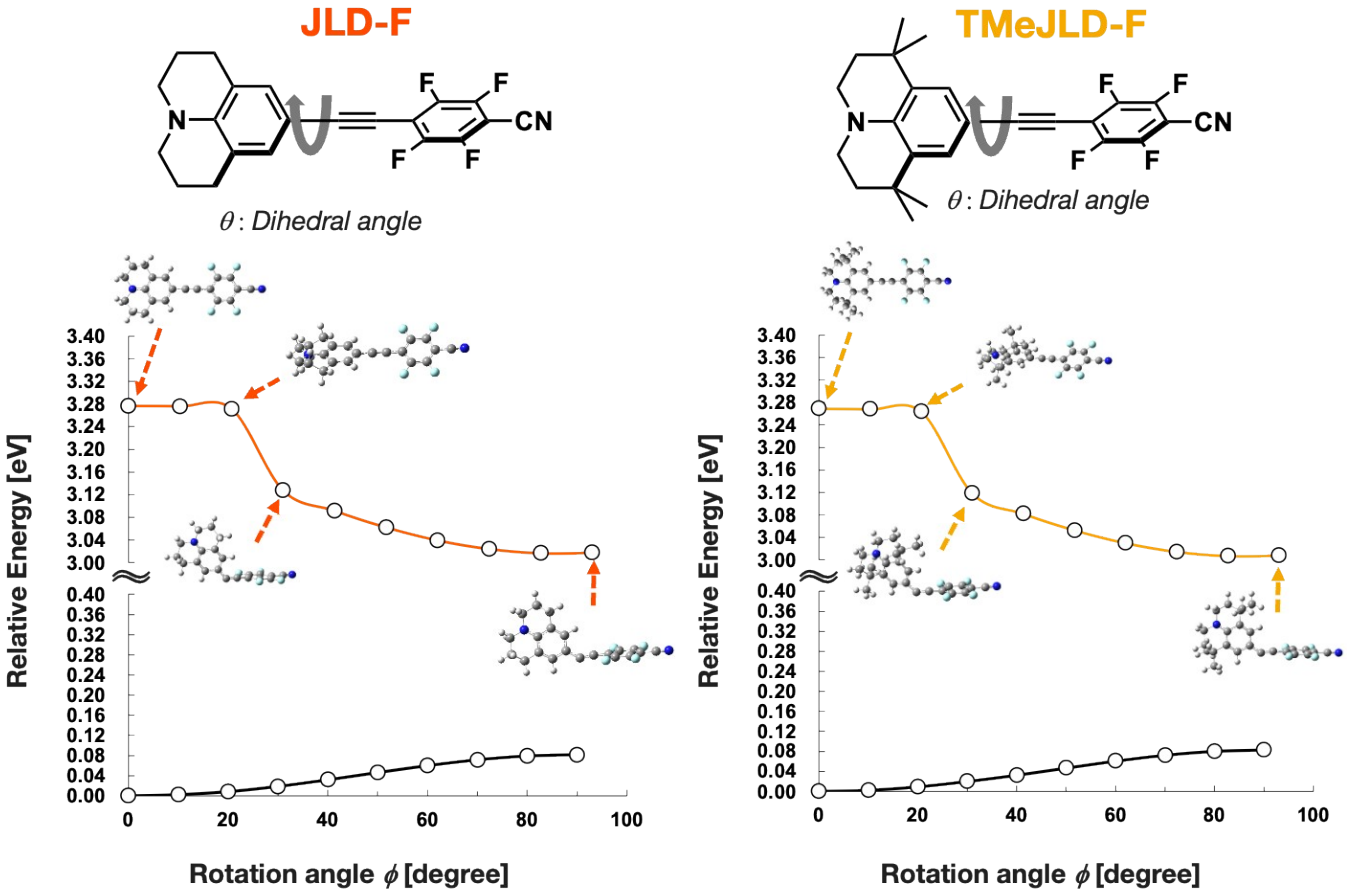


Figure S16. The energy profile of (a) **JLD-F** and (b) **TMeJLD-F** in S_0 and S_1. These are gained by performing constrained structural optimization using (TD)-DFT at the CAMB3LYP/6-31G+(d,p)//CAM-B3LYP/6-31G+(d,p) level.

Table S28. S_1-S_0 Excitation energies and oscillator strength for **JLD-F** and **TMeJLD-F**.

compound	functional	basis set	excitation energy [nm]	oscillator strength
JLD-F	CAM-B3LYP	6-31G(d)	602	0.002
	CAM-B3LYP	6-31+G(d,p)	600	0.001
	B3LYP	6-31+G(d,p)	745	0.000
	B3LYP	cc-PVDZ	771	0.000
TMeJLD-F	CAM-B3LYP	6-31G(d)	605	0.000
	CAM-B3LYP	6-31+G(d,p)	603	0.001
	B3LYP	6-31+G(d,p)	772	0.000
	B3LYP	cc-PVDZ	743	0.000

Photophysical Characteristics

UV-vis absorption spectra were recorded using a JASCO V-530 and V-750 absorption spectrometer (JASCO, Japan). PL spectra of the solution was measured using a Rf-6000 (Shimadzu, Japan). Photoluminescence quantum yields were measured using Quantaurus-QY C11347-01 series (Hamamatsu Photonics, Japan). PL lifetime was measured using a Quantaurus-Tau fluorescence lifetime spectrometer C11367-34 (Hamamatsu Photonics, Japan).

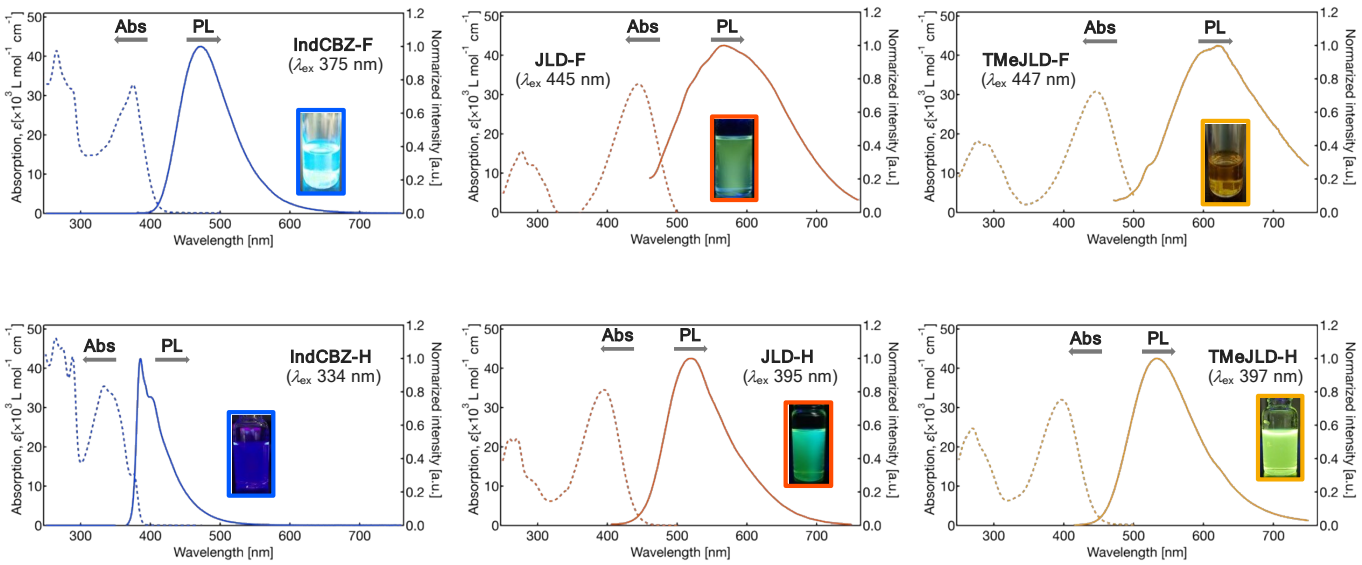


Figure S17. UV-vis and PL spectra of all derivatives in dichloromethane. Concentration: 1.0×10^{-5} mol L^{-1} for UV-vis and PL.

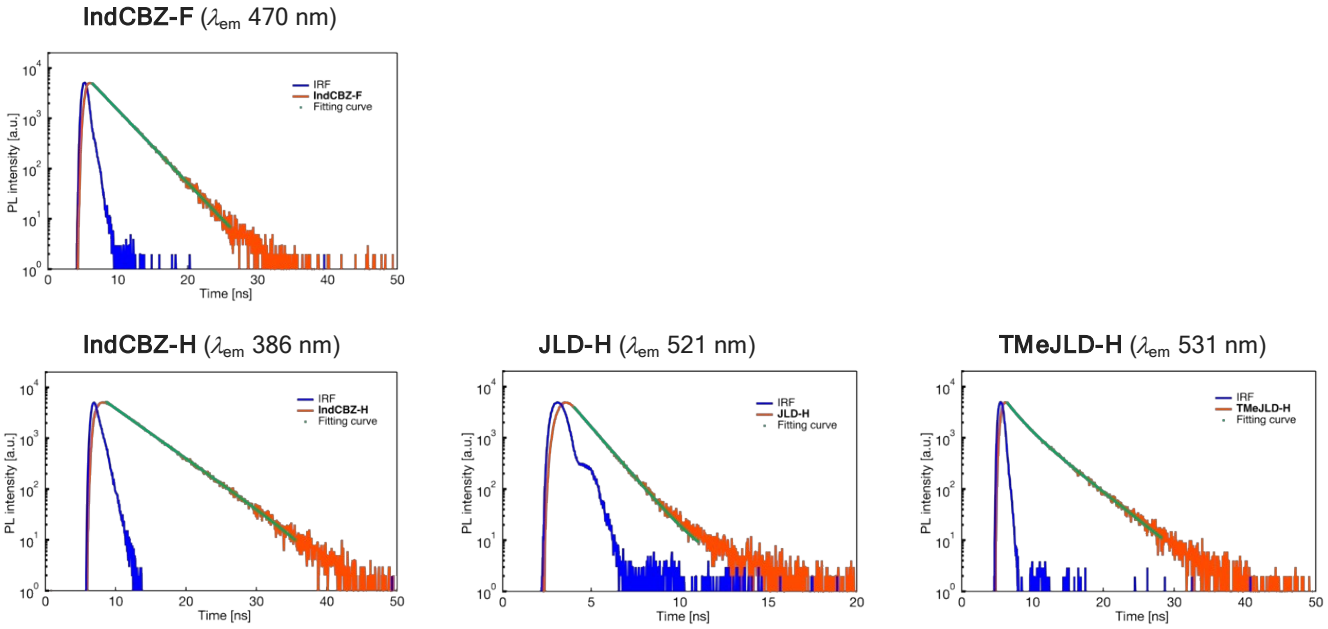


Figure S18. Transient photoluminescence decay curves of **IndCBZ-F**, **IndCBZ-H**, **JLD-H** and **TMeJLD-H** in dichloromethane.

Table S29. Photophysical properties of synthetic derivatives in dichloromethane.

compound	λ_{abs} (ε) [nm]	λ_{em}[a] (Φ_{em}[b]) [nm]	τ [ns]	k_r [10^7 s^{-1}]	k_{nr} [10^7 s^{-1}]
IndCBZ-F	375 (31.5)	470 (0.96)	2.99	32.1	1.34
IndCBZ-H	334 (34.0)	386 (0.54)	4.42	12.2	10.4
JLD-F	445 (32.7)	568 (0.01>)	-	-	-
JLD-H	395 (34.5)	521 (0.07)	1.08	6.48	86.1
TMeJLD-F	447 (31.1)	627 (0.01>)	-	-	-
TMeJLD-H	397 (32.0)	531 (0.18)	3.24	5.56	25.3

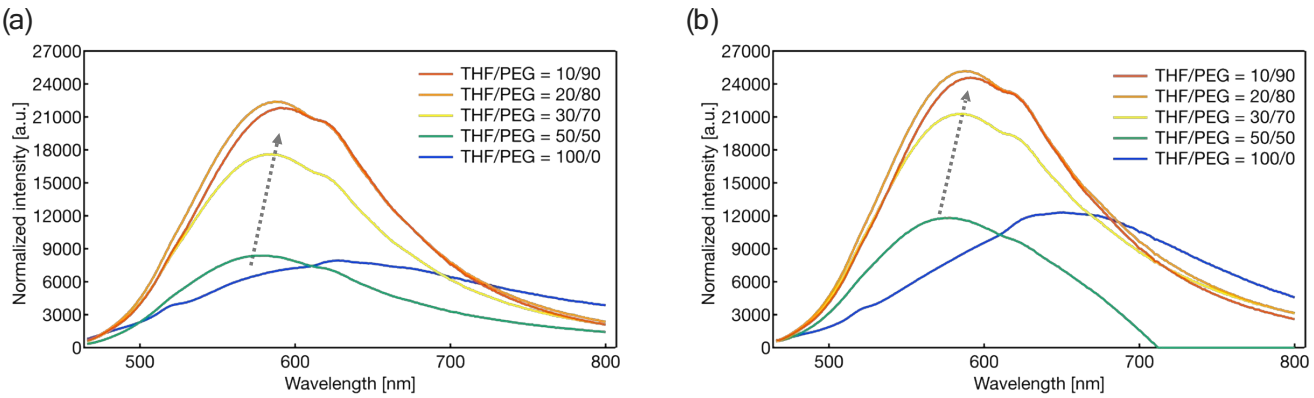


Figure S19. Emission spectra of (a) **JLD-F** and (b) **TMeJLD-F** in 10^{-5} mol/L THF and PEG 400 mixed solution. Excited wavelength was 450nm.

Table S30. Photophysical properties of **JLD-F** in THF and PEG 400 mixed solution

PEG ratio [%]	PL intensity [a.u.]	λ_{max} [nm]	Φ_{em}
0	7937	628	<0.01
50	8377	576	<0.01
70	17622	585	<0.01
80	22401	591	<0.01
90	21825	591	<0.01

Table S31. Photophysical properties of **TMeJLD-F** in THF and PEG 400 mixed solution

PEG ratio [%]	PL intensity [a.u.]	λ_{max} [nm]	Φ_{em}
0	12316	651	<0.01
50	11808	578	<0.01
70	21288	586	<0.01
80	25176	588	<0.01
90	24563	591	<0.01

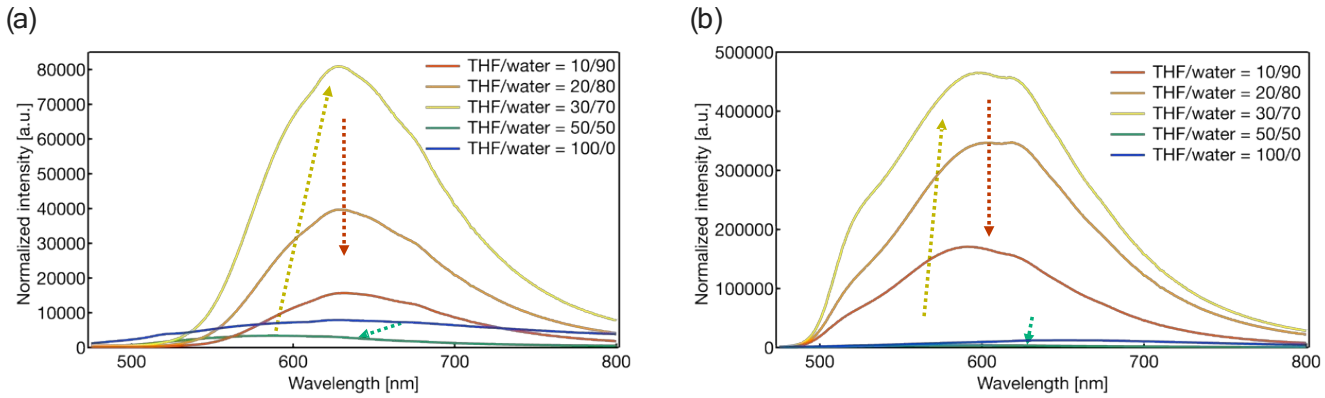


Figure S20. Emission spectra of (a) **JLD-F** and (b) **TMeJLD-F** in 10^{-5} mol/L THF and water mixed solution. Excited wavelength was 450nm.

Table S32. Photophysical properties of **JLD-F** in THF and water mixed solution.

Water ratio [%]	PL intensity [a.u.]	λ_{max} [nm]	Φ_{em}
0	7937	628	<0.01
50	3433	588	<0.01
70	80894	628	0.04
80	39701	628	0.03
90	15696	632	0.03

Table S33. Photophysical properties of **TMeJLD-F** in THF and water mixed solution.

Water ratio [%]	PL intensity [a.u.]	λ_{max} [nm]	Φ_{em}
0	12316	651	<0.01
50	3884	590	<0.01
70	465015	597	0.12
80	346916	619	0.09
90	170794	591	

Lippert-Mataga Plot [3]

$$\Delta\nu = \frac{2(\mu_e - \mu_g)^2}{hca^3}\left(\frac{\varepsilon - 1}{2\varepsilon + 1} - \frac{n^2 - 1}{2n^2 + 1}\right) = \frac{2(\mu_e - \mu_g)^2}{hca^3}\Delta f + const.$$

Where *h* is the Plank's constant, *c* is the velocity of light, and a_0 is Onsager cavity radius. The solvent parameters ε and *n* are solvent dielectric constant and refraction index, respectively. The Onsager radius (a_0 = 6.00 Å for **IndCBZ-F,** 5.74 Å for **JLD-F** and 5.86 Å for **TMeJLD-F**) was calculated from DFT optimization.

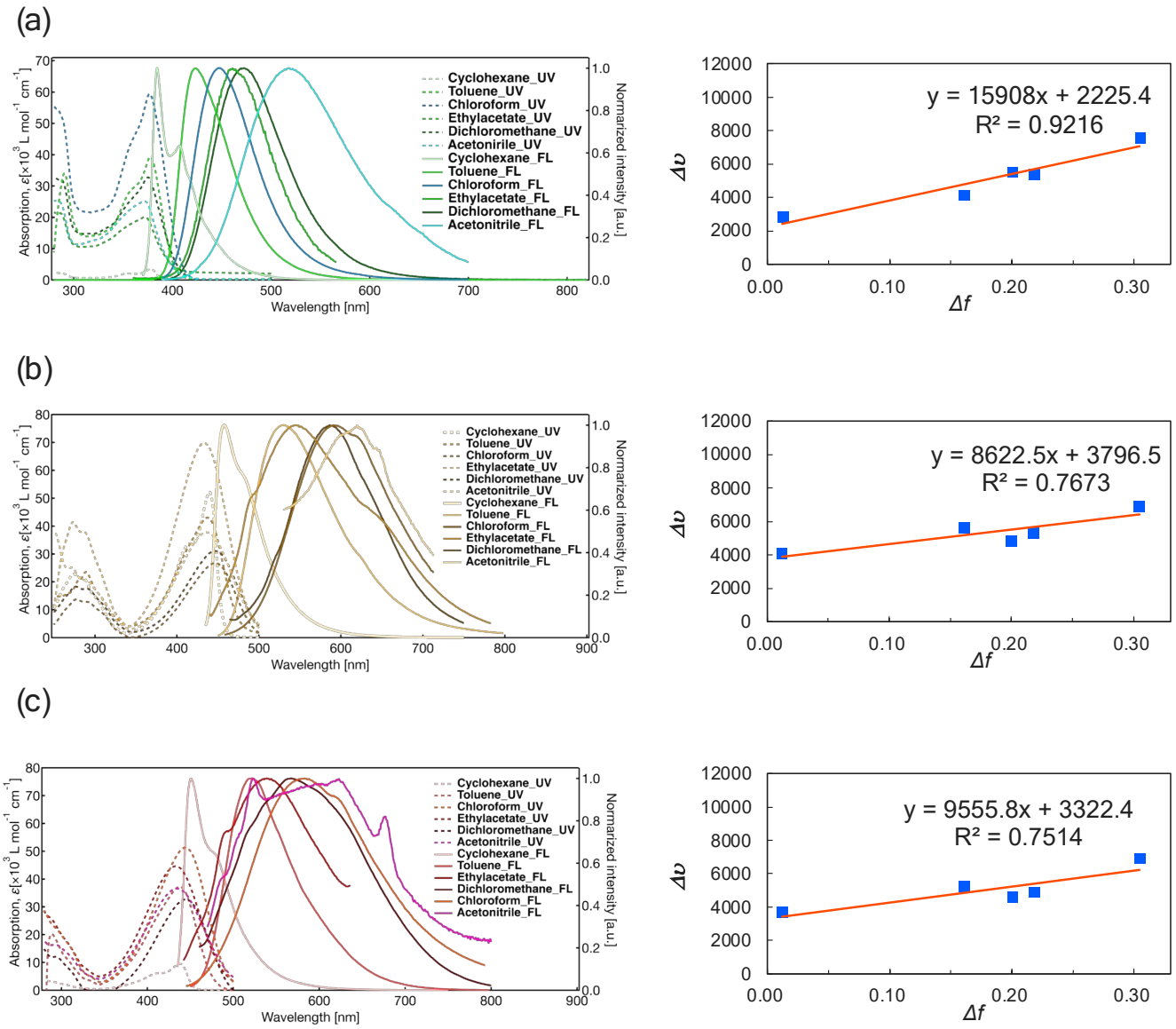


Figure S21. UV-vis absorption and fluorescence spectra in various solvents and Lippert-Mataga Plot of (a) **IndCBZ-F**, (b) **JLD-F** and (c) **TMeJLD-F**. Excited at the longest absorption maxima. Lippert-Mataga plot was created excluding values in cyclohexane or hexane.

Table S34. Photophysical properties of **IndCBZ-F** in various solvents.

Solvent	λ_{abs} [nm]	λ_{em} [nm]	Φ_{PL}	Δf	$\Delta \nu$ [cm^{-1}]
Cyclohexane	378	385	0.80	0.0004	481
Toluene	378	423	0.96	0.012	2814
Chloroform	377	446	0.83	0.161	4245
Ethyl acetate	372	468	0.73	0.201	5514
Dichloromethane	375	470	0.96	0.219	5390
Acetonitrile	372	518	0.47	0.305	7362

Table S35. Photophysical properties of **JLD-F** in various solvents.

Solvent	λ_{abs} [nm]	λ_{em} [nm]	Φ_{PL}	Δf	$\Delta \nu$ [cm^{-1}]
Cyclohexane	438	451	0.49	0.0004	658
Toluene	438	522	0.13	0.012	3674
Chloroform	447	583	0.06	0.161	5574
Ethyl acetate	433	539	<0.01	0.201	4542
Dichloromethane	445	568	<0.01	0.219	4866
Acetonitrile	436	623	<0.01	0.305	6990

Table S36. Photophysical properties of **TMeJLD-F** in various solvents.

Solvent	λ_{abs} [nm]	λ_{em} [nm]	Φ_{PL}	Δf	$\Delta \nu$ [cm^{-1}]
Cyclohexane	440	458	0.38	0.0004	893
Toluene	437	531	0.24	0.012	4051
Chloroform	444	591		0.161	5807
Ethyl acetate	433	548	<0.01	0.201	4847
Dichloromethane	447	586	<0.01	0.219	5307
Acetonitrile	434	620	<0.01	0.305	6598

PMMA film

Thin films of synthetic derivatives were prepared using Opticoat MS-B100 spin coater (MIKASA, Japan). The solutions of PMMA (100 mg) in $CHCl_3$ (3 mL) containing varying amounts of derivatives in the range from 1.0 weight per weight were prepared. Then, the thoroughly cleaned glass slide was mounted and clamped on the top rotating plate of a spin coater. Few drops of a solution of PMMA in $CHCl_3$ containing calculated amounts of derivatives were placed on the glass slide and the top plate of spin coater kept rotating at the speed of 500 revolutions per minute (rpm) for 5 seconds, then at 750 rpm for an additional 5 seconds, and finally at 1200 rpm for 10 seconds. The solvent evaporates and a thin smooth film was seen deposited on a glass slide. The prepared films were used for photophysical measurements without further drying the solvent.

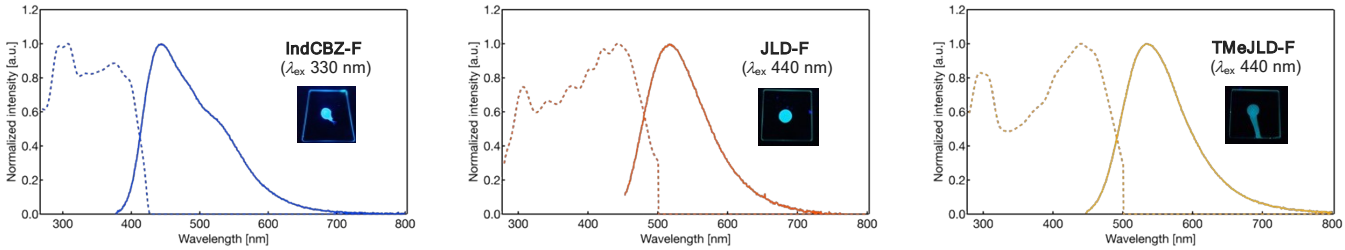
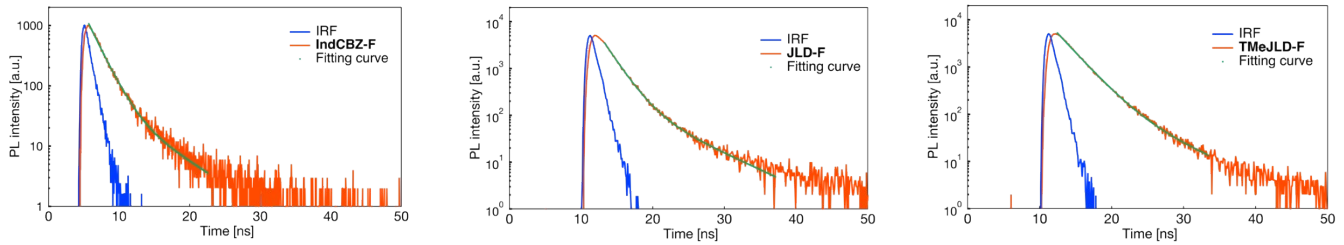


Figure S22. PL spectra of **IndCBZ-F**, **JLD-F** and **TMeJLD-F** in PMMA film 1wt%.

Figure S23. Transient photoluminescence decay curves of **IndCBZ-F**, **JLD-F** and **TMeJLD-F** in PMMA film



1wt%.

Table S37. Photophysical properties of **IndCBZ-F**, **JLD-F** and **TMeJLD-F** in PMMA film 1wt%.

compound	λ_{em} (Φ_{em}) [nm]	τ [ns]	k_r [$10^7 s^{-1}$]	k_{nr} [$10^7 s^{-1}$]
IndCBZ-F	447 (1.0)	2.43	2.58	0.45
JLD-F	517 (0.54)	2.26	23.9	20.4
TMeJLD-F	534 (0.66)	3.73	17.7	9.12

λ_{ex}: 330 nm for **IndCBZ-F**,440 nm for **JLD-F** and **TMeJLD-F**.

Solid-states

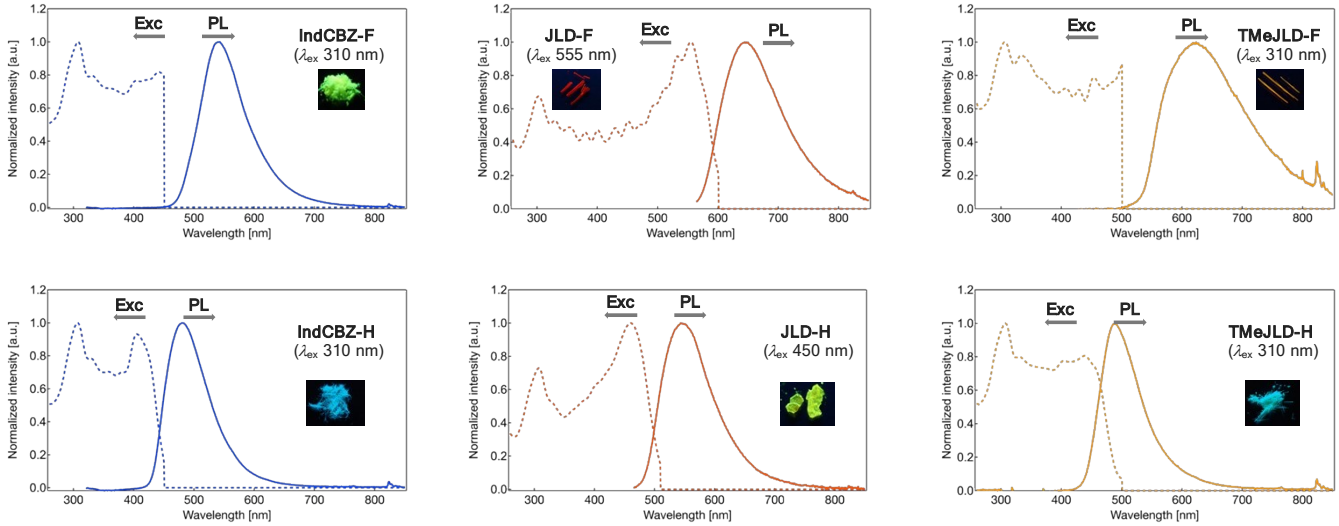


Figure S24. Excitation and PL spectra of all derivatives in the solid states. Excitation spectra were obtained by monitoring PL at the maximum PL wavelength.

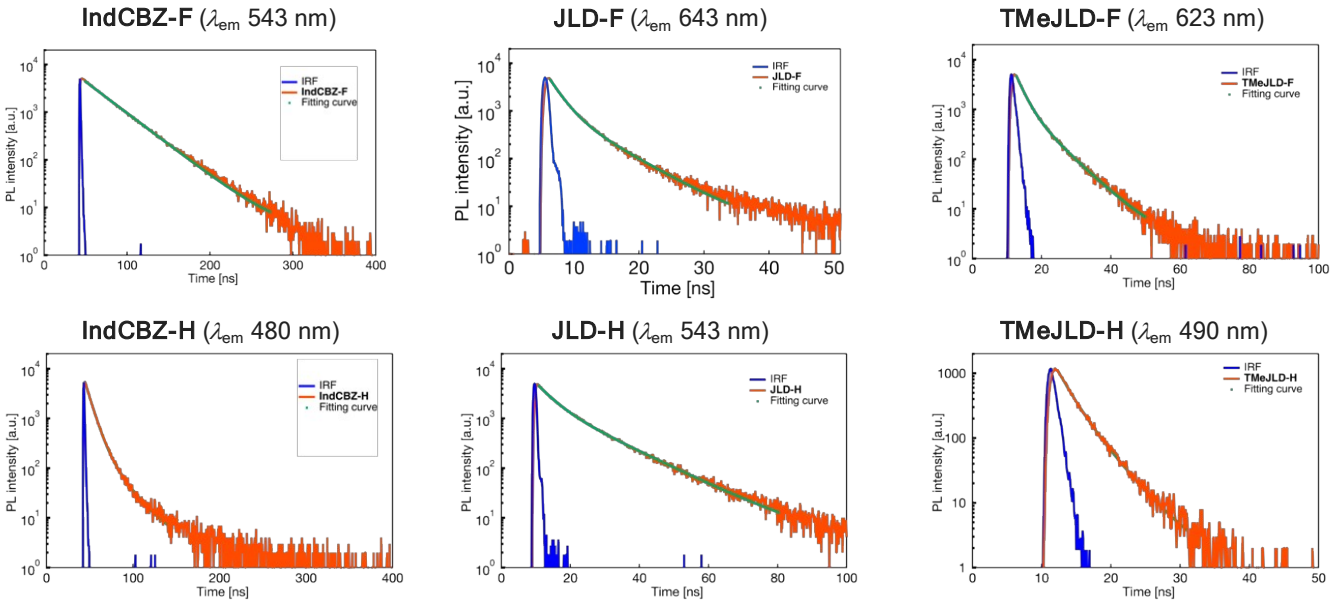


Figure S25. Transient photoluminescence decay curves of all derivatives in crystalline state.

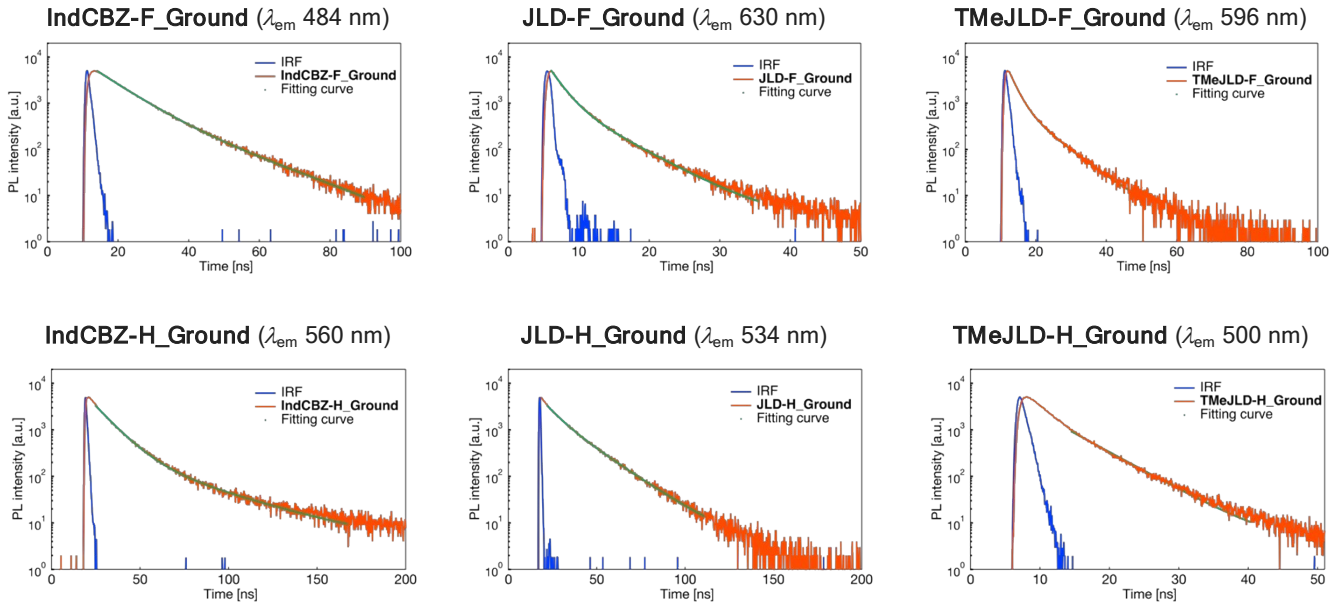


Figure S26. Transient photoluminescence decay curves of all ground sample.

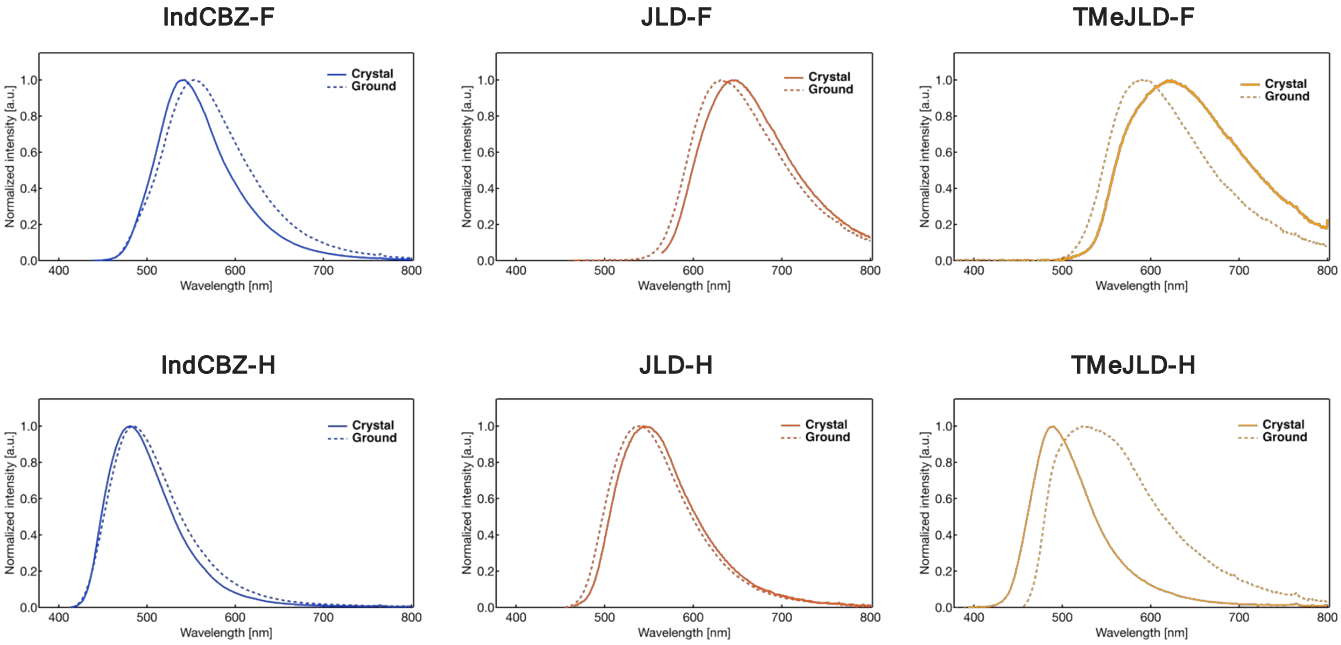


Figure S27. Fluorescence spectra of all derivatives (**Crystal** and **Ground**).

Table S38. Photophysical properties of derivatives in solid state.

compound	λ_{em} (Φ_{em})	τ					k_r	k_{nr}	χ^2
	[nm]	τ_{AVE} [ns]	τ_1 [ns]	τ_2 [ns]	A_1	A_2	[$10^7 s^{-1}$]	[$10^7 s^{-1}$]	[-]
IndCBZ-F	543 (0.85)	33.0	–	–			2.58	0.45	1.57
JLD-F	643 (0.08)	2.51	1.79	5.67	2337.7	192.3	3.19	36.7	1.35
TMeJLD-F	623 (0.20)	3.15	2.32	6.76	347.4	78.6	6.35	25.4	1.15
IndCBZ-H	480 (0.37)	8.02	7.00	20.3	361.3	233.0	4.61	7.86	1.21
JLD-H	543 (0.18)	7.79	4.34	13.1	677.5	155.8	2.31	10.5	1.15
TMeJLD-H	490 (0.22)	2.44	1.86	3.74	110.6	50.0	9.02	32.0	1.10
IndCBZ-F (ground)	553 (0.40)	9.21	7.78	16.2	439.6	89.4	4.34	6.51	1.00
JLD-F (ground)	630 (0.20)	2.20	1.69	5.29	413.4	95.7	9.09	36.4	1.27
TMeJLD-F (ground)	596 (0.25)	2.95	2.16	7.34	766.8	139.1	8.47	25.4	1.21
IndCBZ-H (ground)	484 (0.71)	11.9	10.1	36.6	757.1	53.8	5.97	2.44	1.24
JLD-H (ground)	543 (0.25)	11.8	6.83	17.3	530.9	484.3	2.12	6.35	1.19
TMeJLD-H (ground)	523 (0.21)	3.80	2.93	6.68	216.7	65.4	5.53	20.8	1.11

λ_{ex}: 310 nm for **IndCBZ-F**, **IndCBZ-H**, **TMeJLD-F** and **TMeJLD-H**, 450 nm for **JLD-H**, 555 nm for **JLD-F**. Amplitude average lifetime $\tau_{AVE} = \Sigma A_i\tau_i/\Sigma A_i$[4].

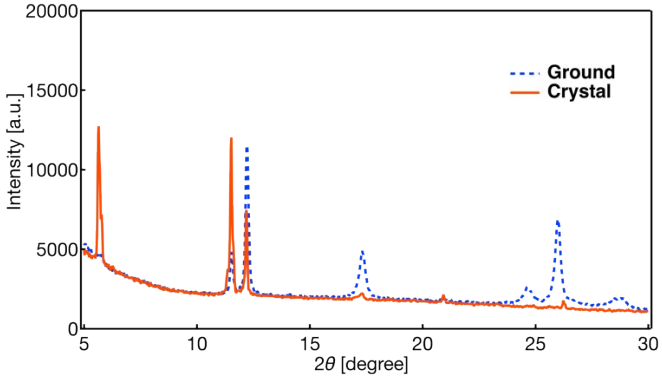


Figure S28. PXRD pattern of **JLD-F** (**Crystal** and **Ground**).

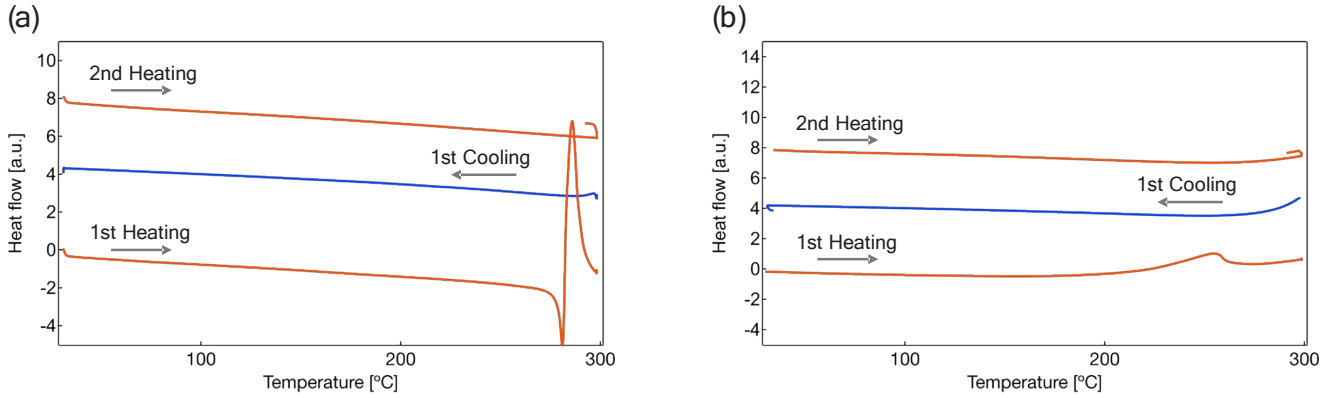


Figure S29. DSC curve of **JLD-F** ((a). **Crystal** and (b). **Ground**).

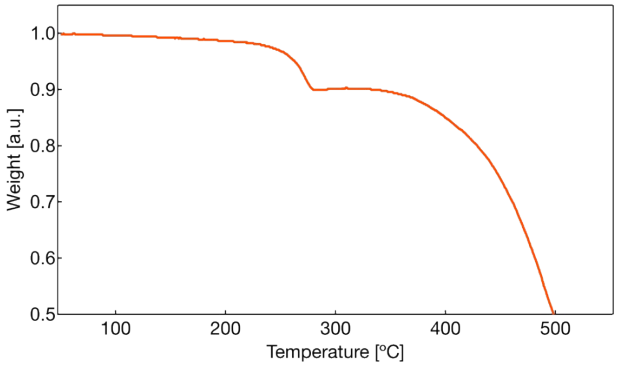


Figure S30. DSC curve of **JLD-F**.

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