Electronic Supplementary Information

Argentivorous Molecules with Chromophores: Dependence of Fluorescence Intensity on the Distance between Donor and Acceptor

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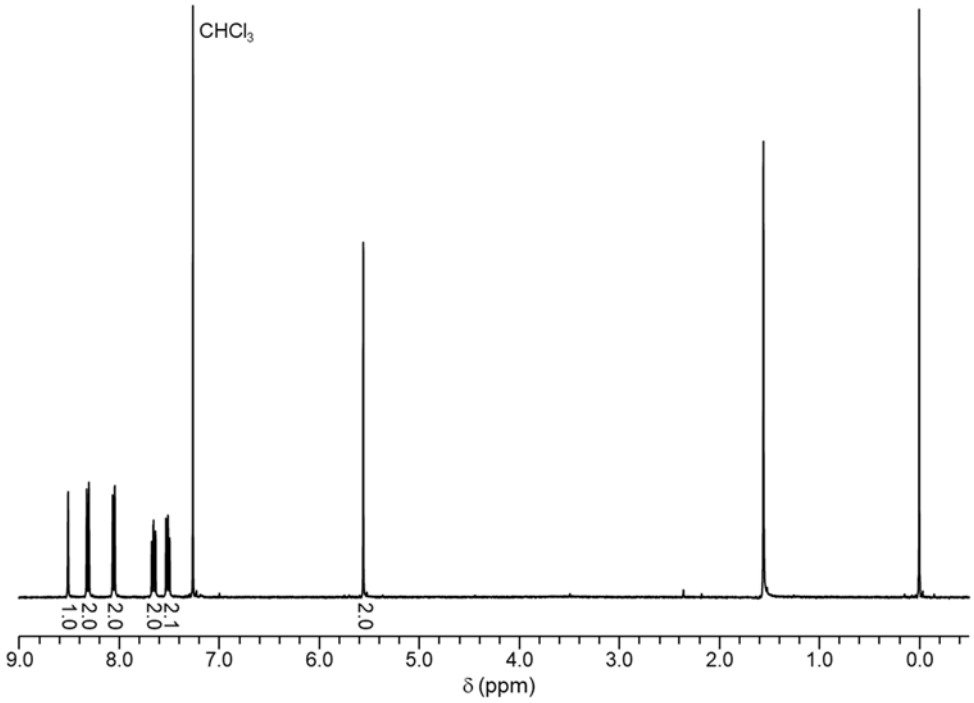


Fig. S1. ^{1}H NMR spectrum of **2** in $CDCl_3$.

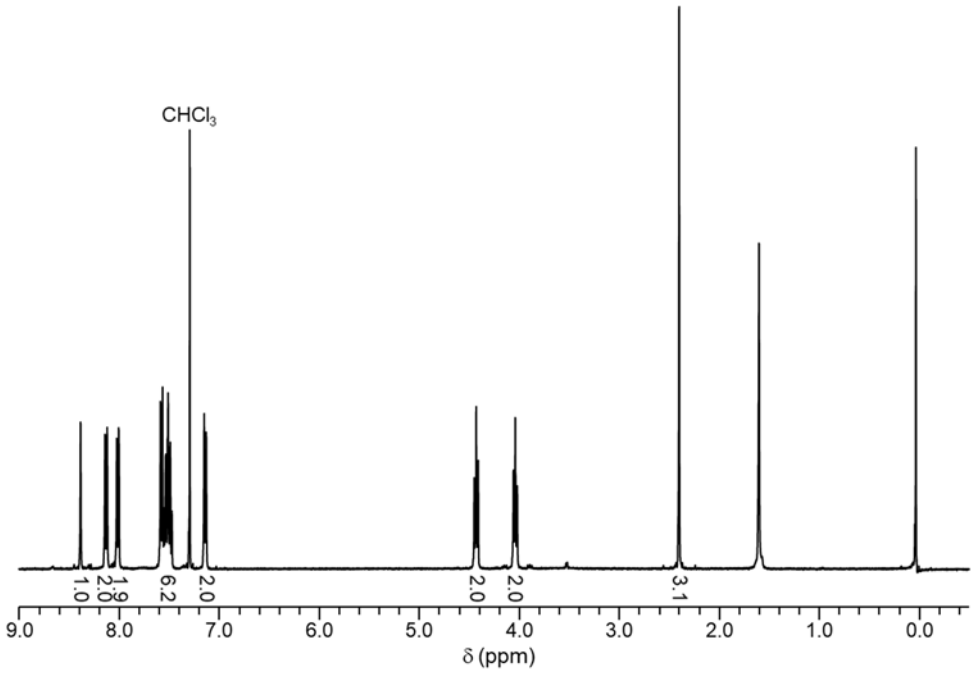
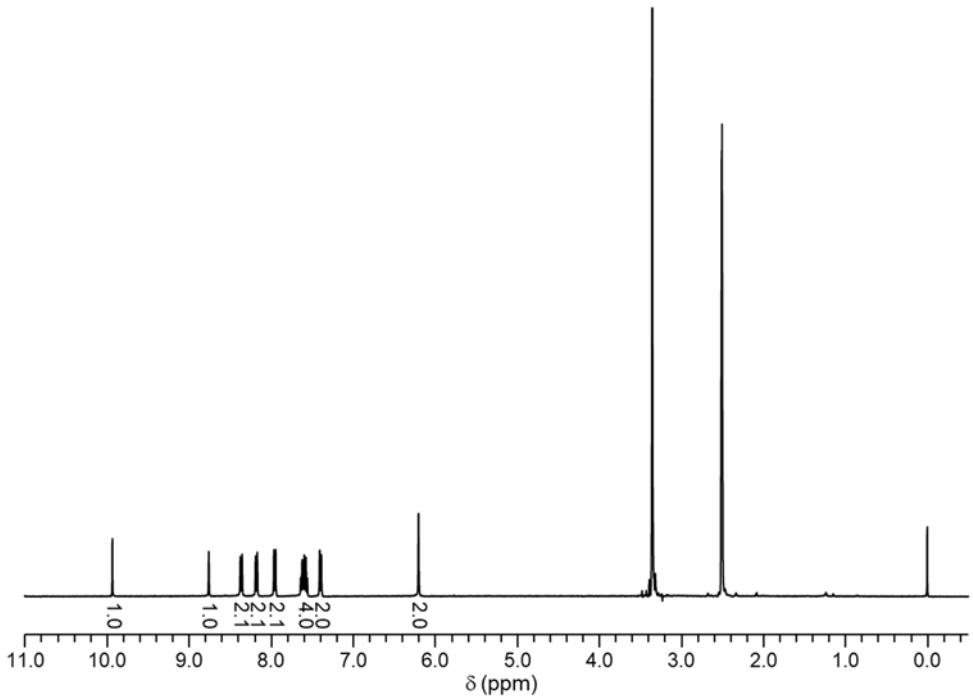
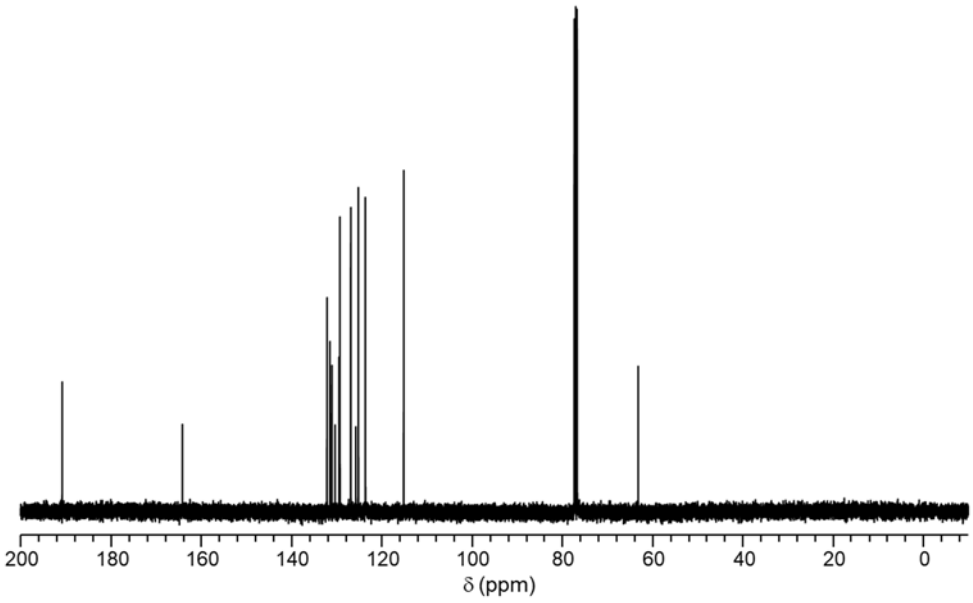


Fig. S2. ^{1}H NMR spectrum of **3** in $CDCl_3$.

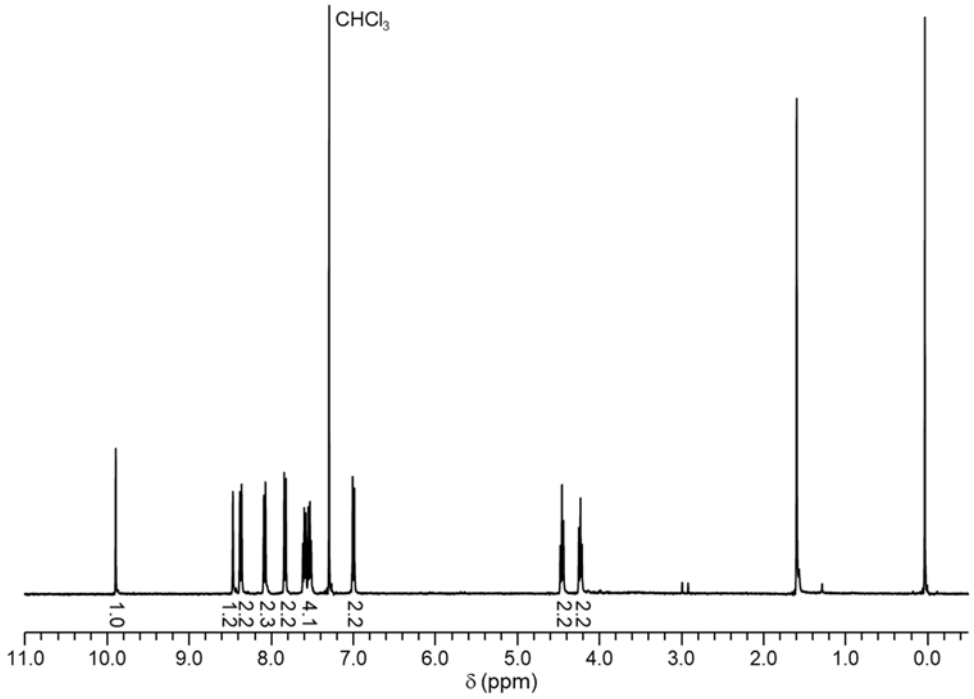


(a)

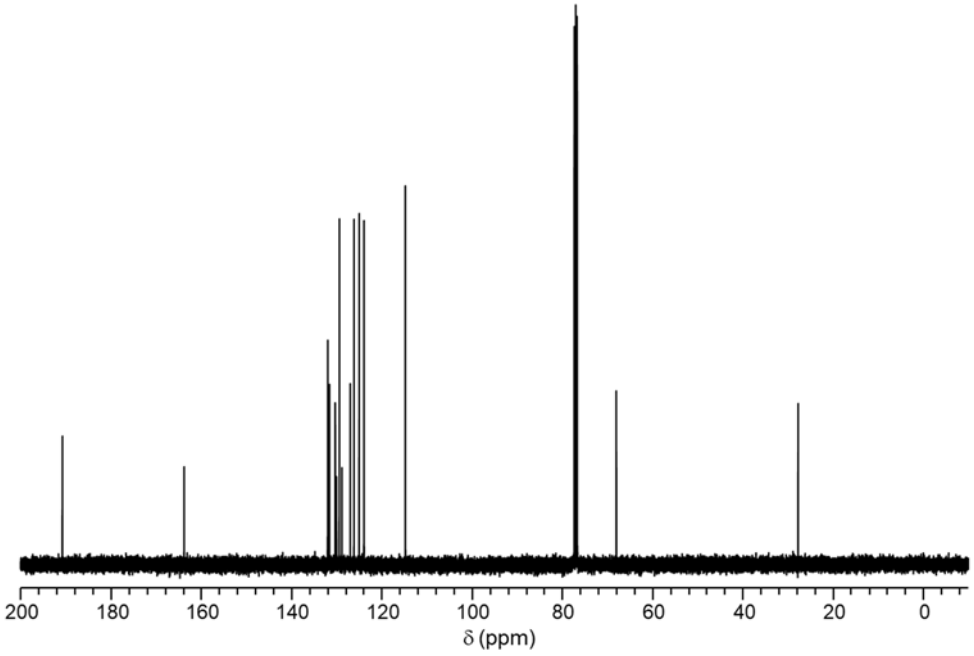


(b)

Fig. S3. (a) ^{1}H (in DMSO-d_6) and (b) ^{13}C (in $CDCl_3$) NMR spectra of **5**.

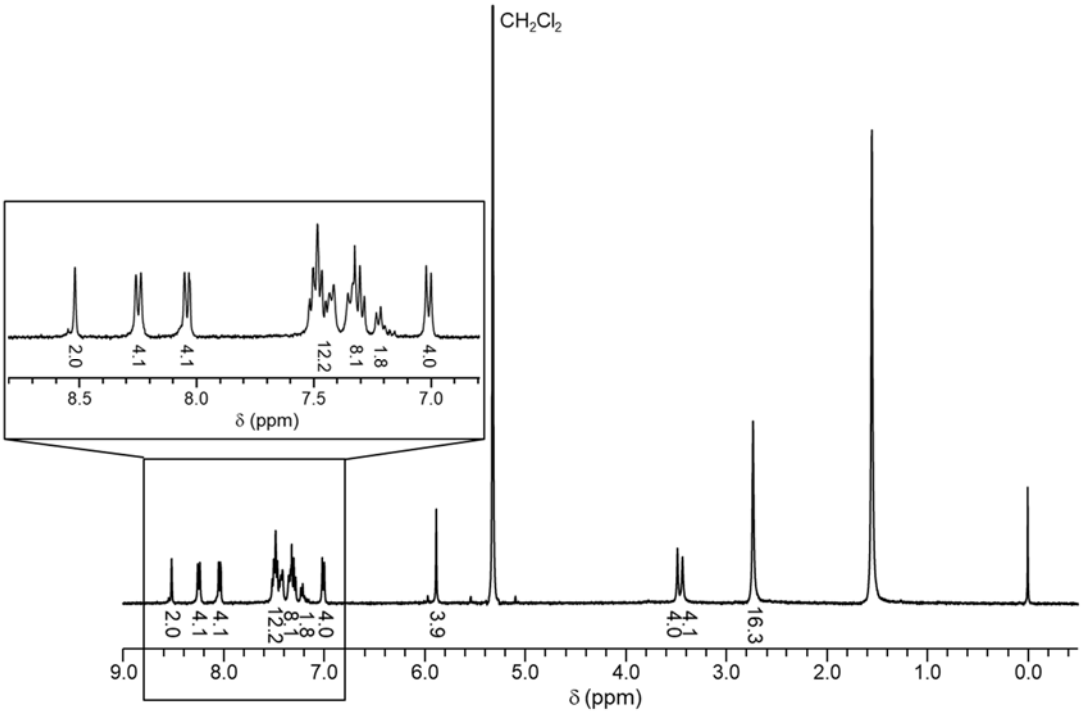


(a)

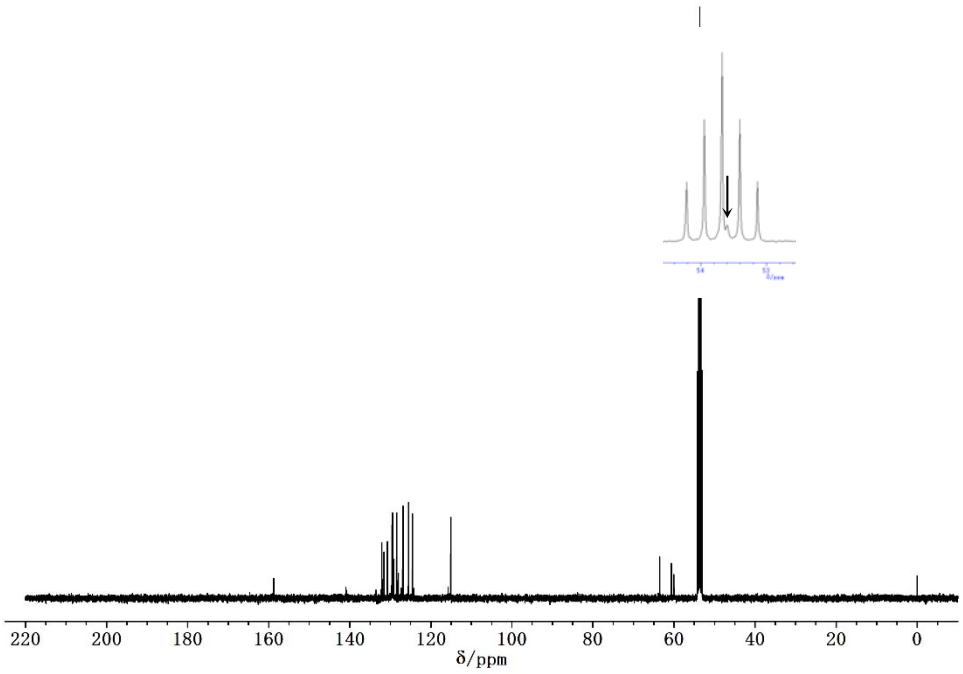


(b)

Fig. S4. (a) ^{1}H and (b) ^{13}C NMR spectra of **6** in $CDCl_3$.

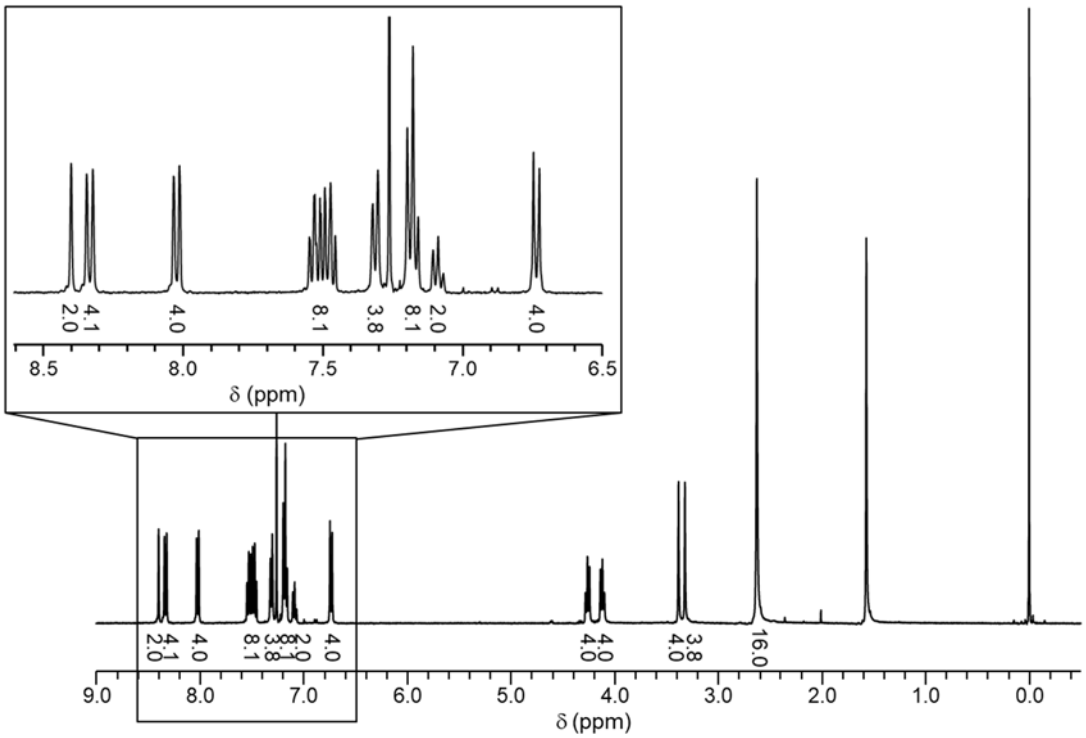


(a)

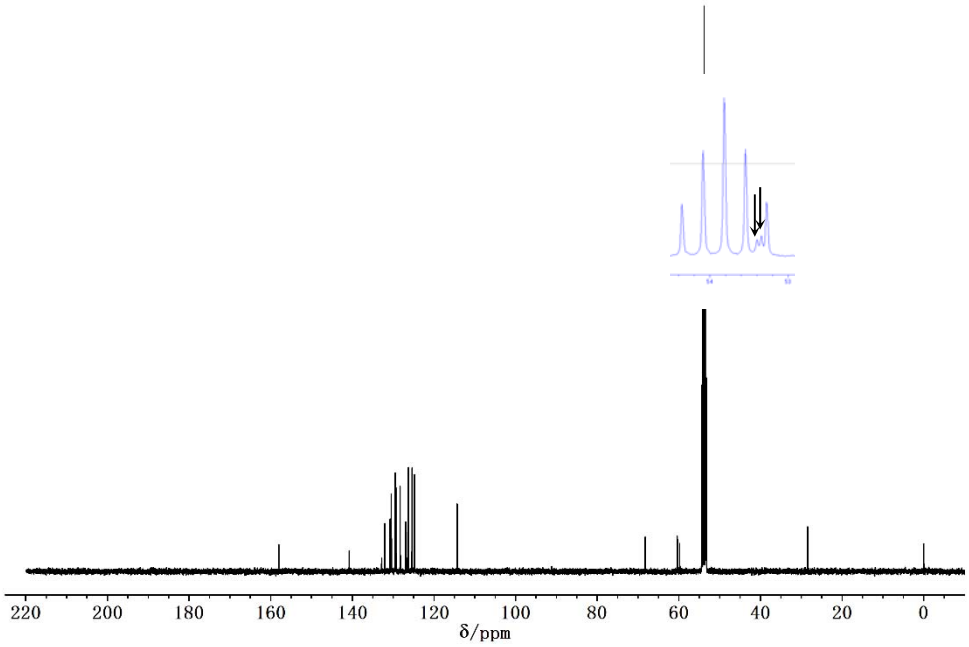


(b)

Fig. S5. (a) ^{1}H NMR and (b) ^{13}C NMR of **L²** in CD_2Cl_2.



(a)



(b)

Fig. S6. (a) ^{1}H NMR (in $CDCl_3$) and (b) ^{13}C NMR (in CD_2Cl_2) of **L³**.

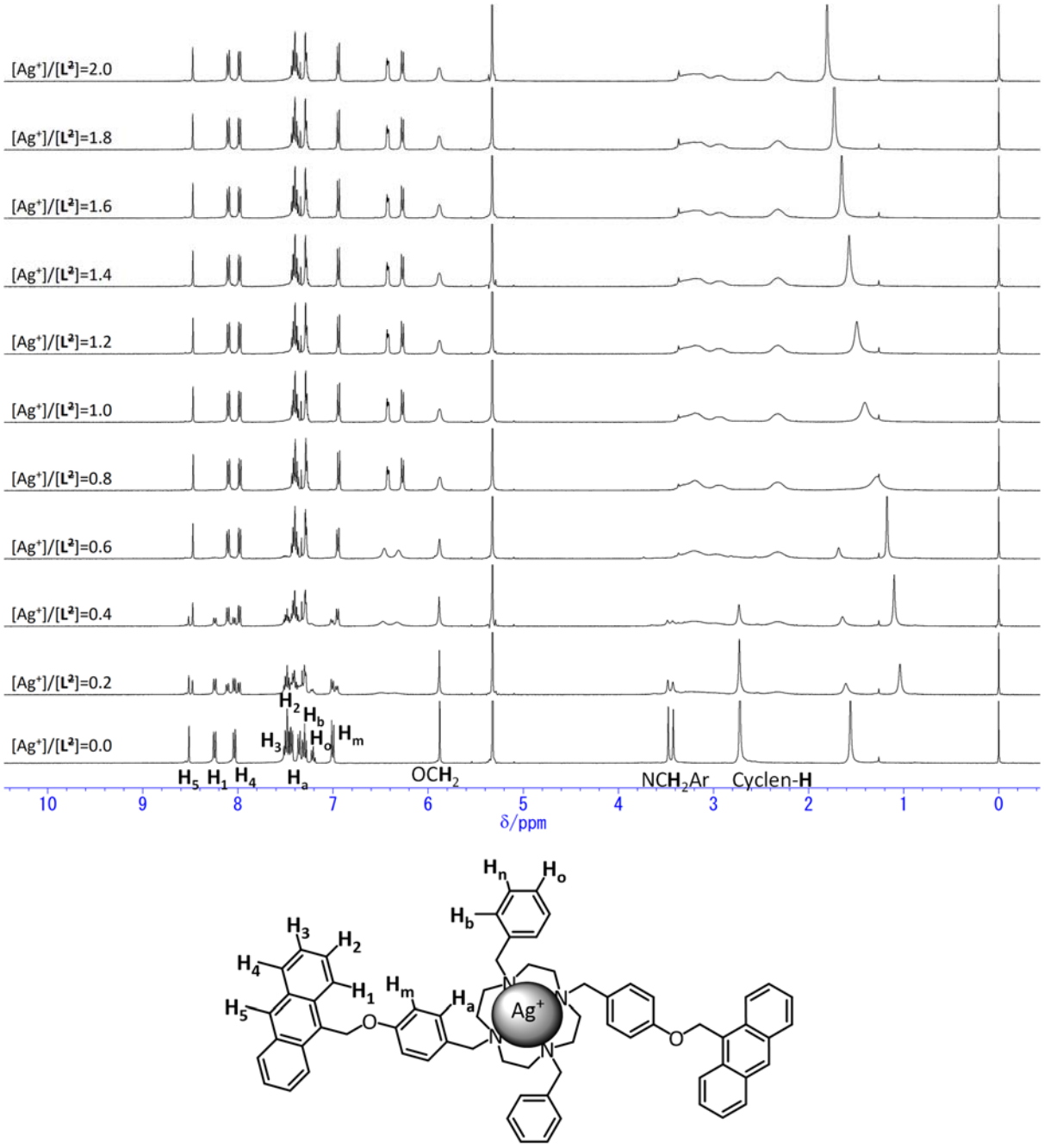


Fig. S7 Ag^+ ion-induced ^1H NMR spectral changes of **L²** in CD_2Cl_2/CD_3OD. ([**L²**] = 5.0 x 10^{-5} M).

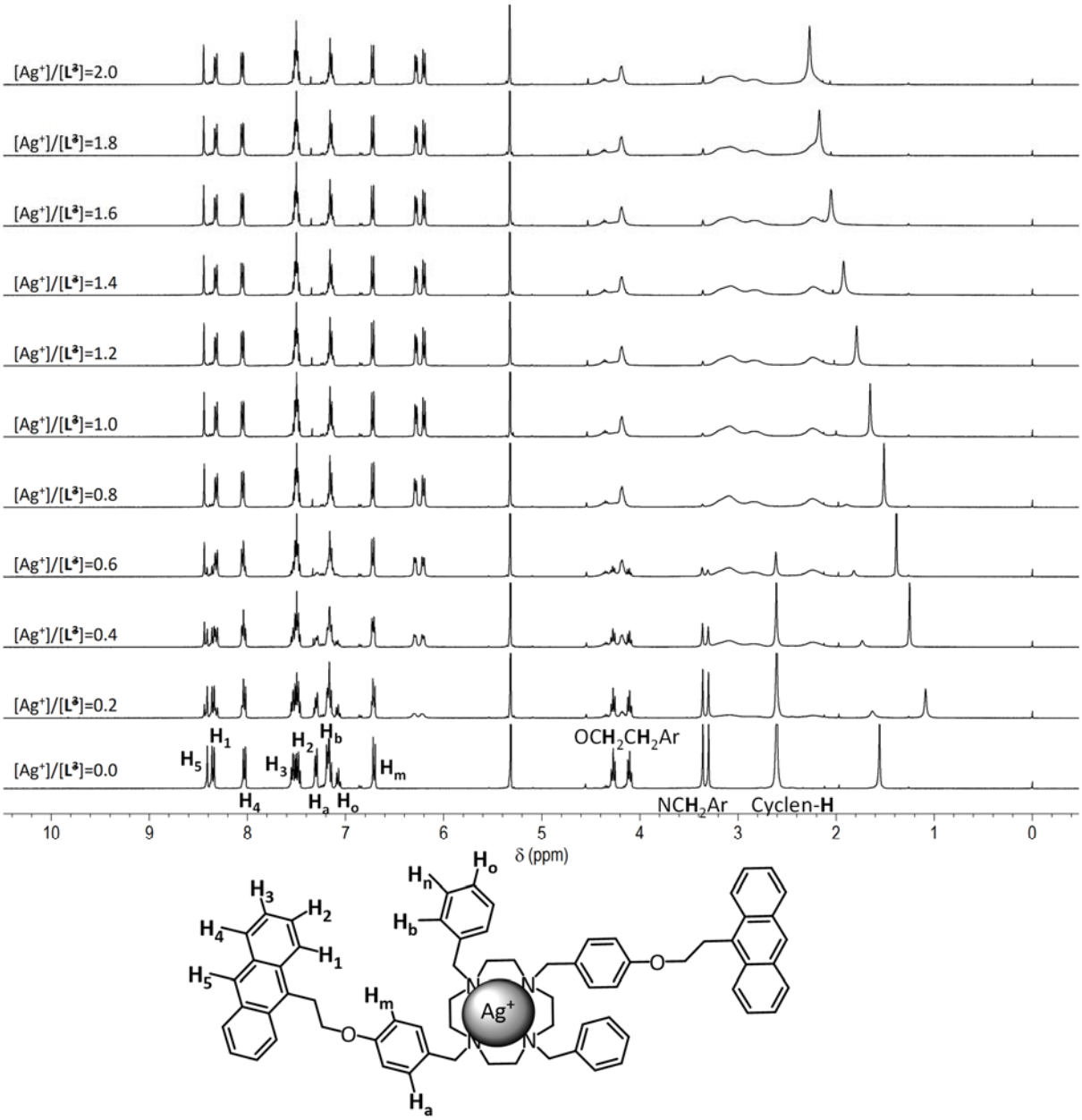


Figure S8. Ag^+ ion-induced ^1H NMR spectral changes of **L³** in CD_2Cl_2/CD_3OD ([**L³**] = 5.0 x 10^{-5} M).

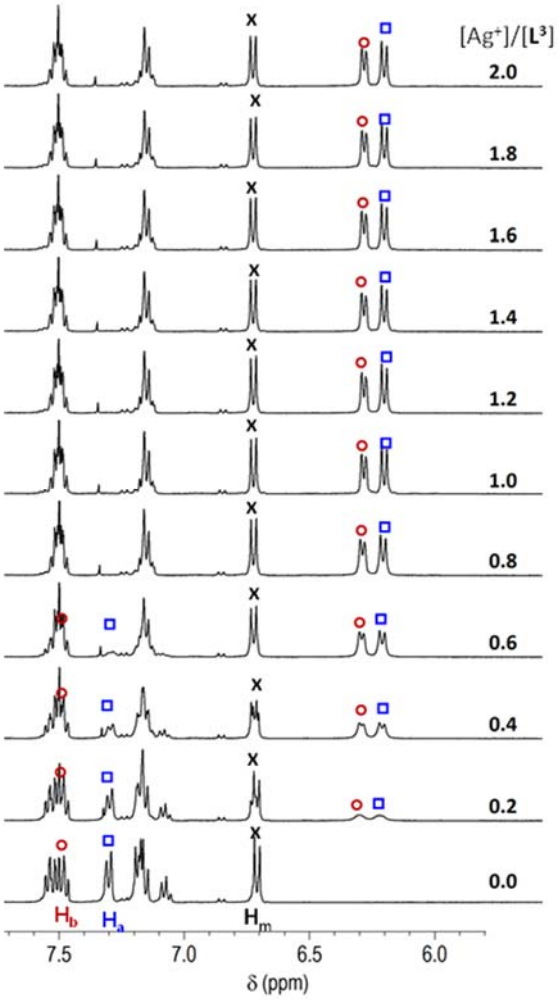
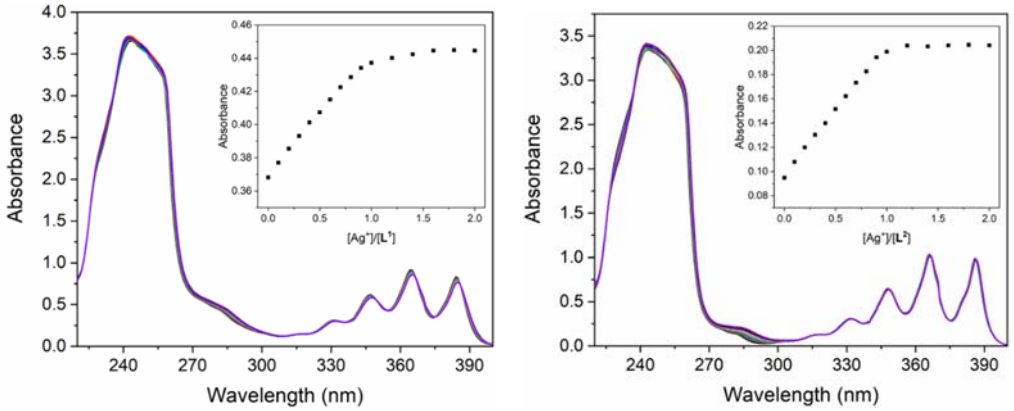
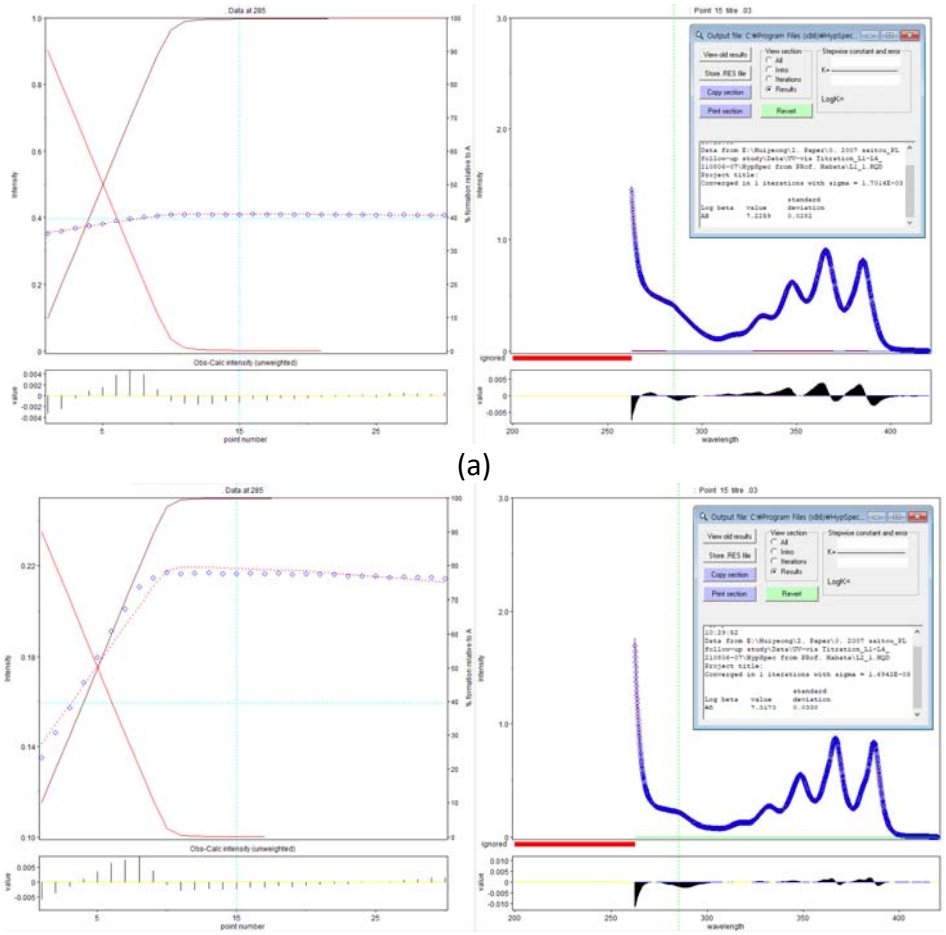


Fig. S9. ^{1}H NMR spectral changes of **L^{3}** depending on the addition of AgOTf in CD_2Cl_2/CD_3OD ([**L^{2}**] and [**L^{3}**] = 5.0 x 10^{-5} M). The chemical shift at the 2,6-positions of the phenyl groups was predicted to appear at higher fields.



(a) (b)

Fig. S10. Ag(I)-induced UV-vis spectral changes of (a) $\mathbf{L^2}$ and (b) $\mathbf{L^3}$ in $CHCl_3$/MeOH (1:19, [$\mathbf{L^2}$] and [$\mathbf{L^3}$] = 5.0 x 10^{-5} M). The insets show the absorbance at 290 nm.



(a)

(b)

Fig. S11. HypSpec^{TM} output for UV-Vis spectral titration of **L** upon addition of silver(I) triflate in $CHCl_3$/MeOH (1:19): (a) [$\mathbf{L^2}$] = 5.0 × 10^{-5} M and (b) [$\mathbf{L^3}$] = 5.0 × 10^{-5} M.

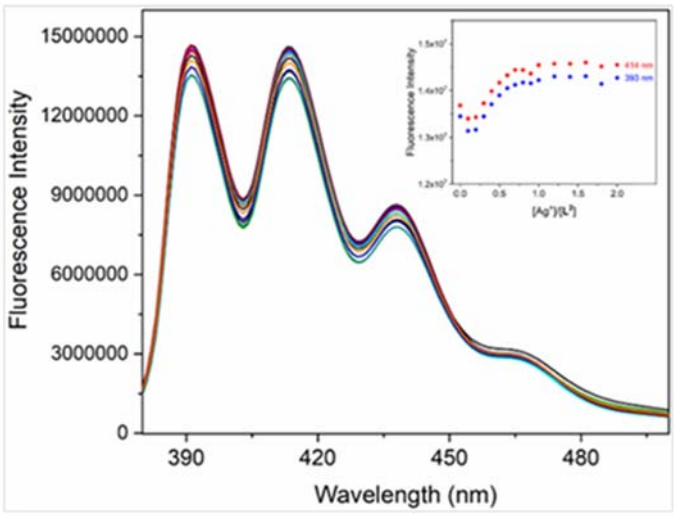


Fig. S12 Ag(I)-induced fluorescence spectral changes of $\mathbf{L^2}$ in THF. ([$\mathbf{L^2}$] = 2.0×10^{-7} M). λ_{ex}=363 nm

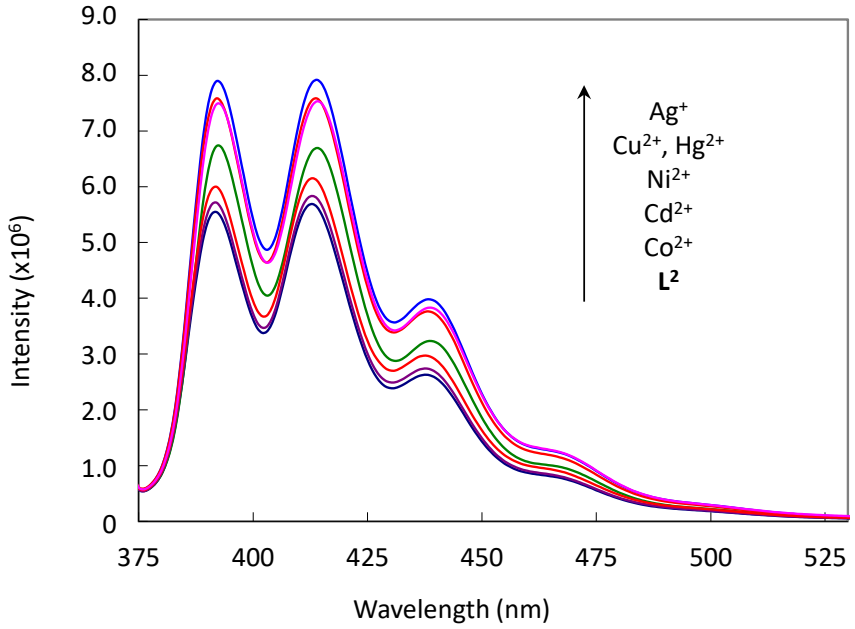
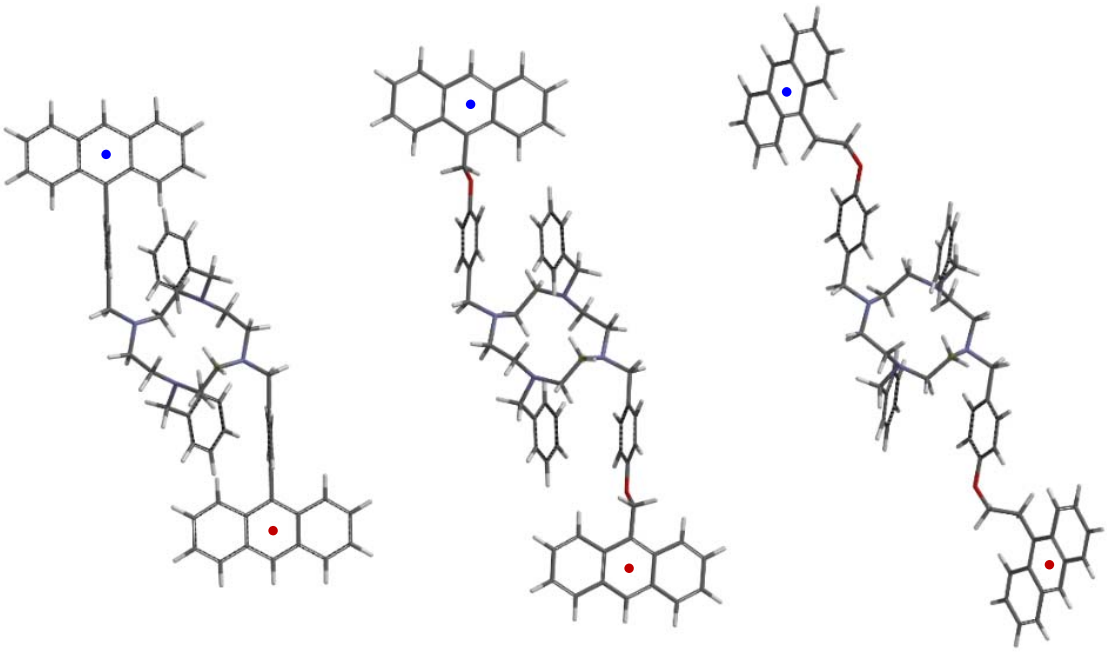


Fig. S13. Metal ion-induced fluorescence spectral changes of $\mathbf{L^3}$ in THF. [$\mathbf{L^3}$]=[metal ion]=2.0 x 10^{-7} M. λ_{ex}=363 nm



L¹ **L²** **L³**

Fig. S14. Structures of **L¹**–**L³** optimized by DFT (B3LYP/6-311G). The positions of points 1 and 2 in each compounds are indicated by ● and ●, respectively.

Table S1. Fluorescence Intensities and the average distances between the center of chromophores and nitrogen atoms in **L¹**, **L²**, and **L³**

	L¹	**L²**	**L³**
Intensity (I)	60000	4000000	14000000
Log *I*	4.778	6.602	7.146
	Average distances between the center of chromophores and N atoms		
N1-Point1	8.0 Å	9.9 Å	10.2 Å
N2-Point1	11.2 Å	9.4 Å	10.5 Å
N3-Point1	11.6 Å	12.8 Å	13.7 Å
N4-Point1	8.2 Å	12.9 Å	13.2 Å
N1-Point2	11.6 Å	12.8 Å	13.6 Å
N2-Point2	8.2 Å	12.9 Å	13.2 Å
N3-Point2	8.0 Å	9.9 Å	10.1 Å
N4-Point2	11.0 Å	9.5 Å	10.5 Å
Average	9.7 Å	11.3 Å	11.9 Å

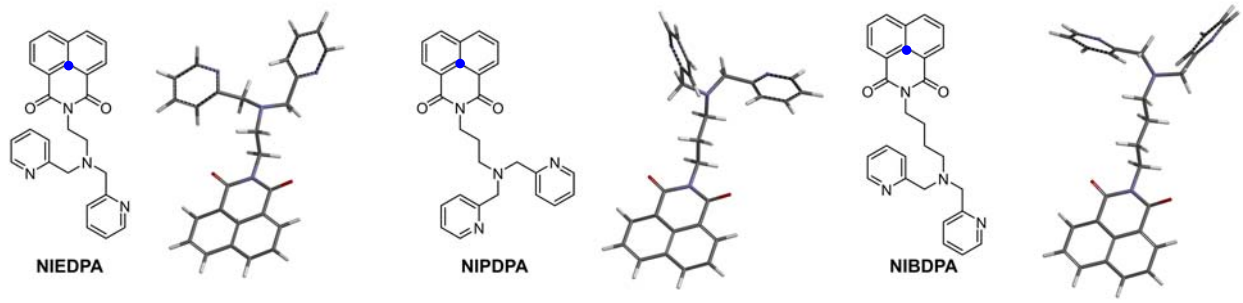


Fig. S15. Structures of **NIEDPA**, **NIPDPA**, and **NIBDPA**[S1] optimized by DFT (B3LYP/6-311G). The position of point 1 in each compound is indicated by ●

Table S2. Fluorescence Intensities at 394 nm and the average distances between the center of chromophores and nitrogen atoms in **NIEDPA**, **NIPDPA**, and **NIBDPA** optimized by DFT calculation (B3LYP/6-311G).[S1]

	NIEDPA	**NIPDPA**	**NIBDPA**
Intensity (I)	38.78	145.0	176.8
Log ***I***	1.589	2.161	2.247
	Average distances between the center of chromophores and N atoms		
N3-Point1	8.4 Å	10.0 Å	10.3 Å
N4-Point1	8.1 Å	9.9 Å	11.9 Å
Average	8.3 Å	10.0 Å	11.1 Å

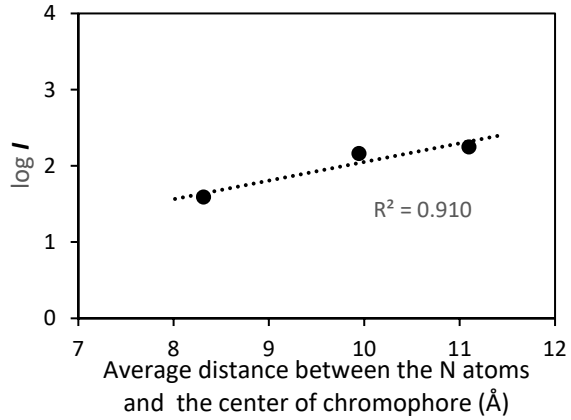


Fig. S16. Correlation between the average distances between donors (nitrogen atoms in the pyridine) and the center of naphthalimide of **NIEDPA**, **NIPDPA**, and **NIBDPA**[S1] optimized by DFT (B3LYP/6-311G) and fluorescence intensities at 394 nm.

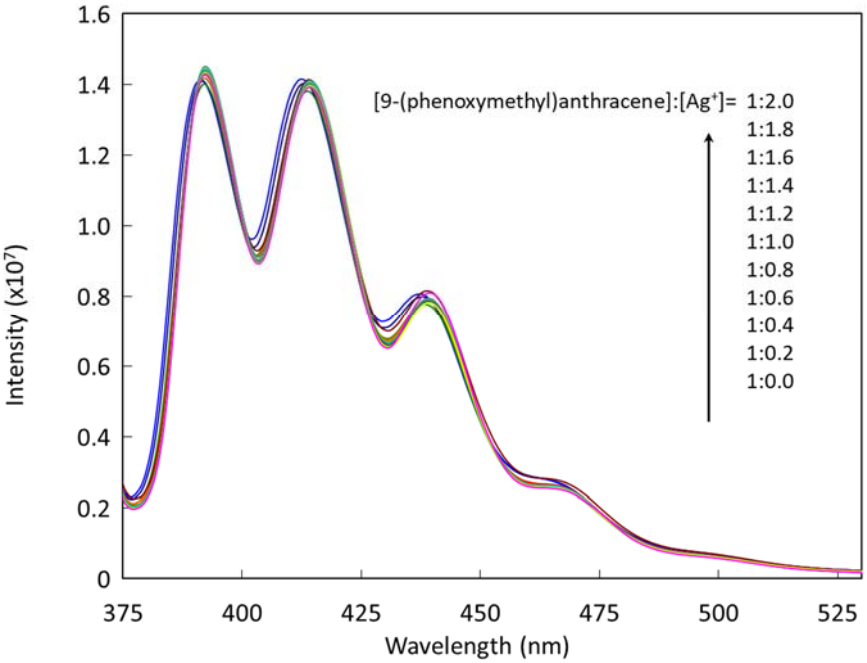


Fig. S17. Ag^+ ion-induced fluorescence spectral changes. [9-(phenoxymethyl)amthracene[S2]] = [metal ion]=4.0 x 10^{-7} M in THF. λ_{ex}=363 nm.

Table S3 Cartesian coordinates of **L^1-L^3**, **NIEDPA**,[S1] **NIPDPA**,[S1] and **NIBDPA**[S1] optimized by DFT calculations (B3LYP/6-311G)

.

Cartesian Coordinates (Angstroms) of L1

	Atom	X	Y	Z
1	N1	1.8762509	0.4067796	-1.8618576
2	N2	-1.357222	-0.4485303	-1.4740208
3	C1	2.61139	0.9221219	-0.6991339
4	H1A	3.1979721	1.7746693	-1.0528061
5	H1B	3.3465571	0.1854607	-0.3278528
6	C2	1.1362983	-0.8364017	-1.568907
7	H2A	0.9828744	-0.8853164	-0.4919367
8	H2B	1.7527259	-1.7120594	-1.8334345
9	C3	-0.2245827	-0.9394122	-2.2798144
10	H3A	-0.1886935	-0.3565722	-3.1964925
11	H3B	-0.4085476	-1.9876232	-2.5819094
12	C4	-1.7285948	-1.4389894	-0.4503674
13	H4A	-0.8167332	-1.8369503	-0.003187
14	H4B	-2.2359562	-2.297098	-0.9311899
15	C5	2.807446	0.2439202	-2.9878922
16	H5A	3.5068148	-0.5913119	-2.7982097
17	H5B	3.418979	1.1507651	-3.0368445
18	C6	2.1653745	0.0445855	-4.3460113
19	C7	1.3326185	1.0274525	-4.891806
20	H7	1.0912285	1.9092057	-4.3071948
21	C8	0.7854196	0.8750408	-6.1602624
22	H8	0.1341333	1.6464105	-6.5571908
23	C9	1.0562496	-0.2654437	-6.928774
24	C10	1.8864327	-1.2478031	-6.3836883
25	H10	2.1077665	-2.1406629	-6.9603812
26	C11	2.4313189	-1.0929261	-5.1088889
27	H11	3.0747152	-1.8703849	-4.7057952
28	C12	0.4710903	-0.4189773	-8.2976124
29	C13	-0.7932983	-1.0254885	-8.4587102
30	C14	-1.5509483	-1.5273734	-7.3526969
31	H14	-1.1372385	-1.4381425	-6.3556031
32	C15	-2.7732249	-2.1128178	-7.5373772
33	H15	-3.3258976	-2.4922796	-6.6835503
34	C16	-3.3307294	-2.235399	-8.840725
35	H16	-4.3026799	-2.7015663	-8.9672643
36	C17	-2.643068	-1.7704664	-9.9250723
37	H17	-3.0610978	-1.8622079	-10.9233719
38	C18	-1.3611763	-1.1556323	-9.7794423
39	C19	-0.6481332	-0.6815973	-10.8815201
40	H19	-1.0793498	-0.7813086	-11.874309
41	C20	0.6055731	-0.0845373	-10.7400321
42	C21	1.3355575	0.3976556	-11.8695724
43	H21	0.8913114	0.2900202	-12.854996
44	C22	2.5619823	0.9799532	-11.720781
45	H22	3.1056676	1.342	-12.5875237
46	C23	3.1345082	1.114446	-10.4253037
47	H23	4.1102388	1.5779219	-10.3189643
48	C24	2.4692405	0.6675694	-9.3175415
49	H24	2.9178625	0.7769512	-8.337695
50	C25	1.1817064	0.0504831	-9.4231755
51	C26	-2.4995535	-0.1397932	-2.3415029
52	H26A	-3.382838	-0.0170919	-1.708192
53	H26B	-2.7280546	-0.9914309	-3.0096635
54	C27	-2.3426769	1.1203067	-3.1712441
55	C28	-1.7624674	2.2725837	-2.6317903
56	H28	-1.3557653	2.2349476	-1.6281419
57	C29	-1.6920529	3.4479138	-3.3746501
58	H29	-1.2382629	4.3333032	-2.939678
59	C30	-2.2025491	3.4918125	-4.6716963
60	H30	-2.1495327	4.4088269	-5.2499381
61	C31	-2.7770872	2.3482742	-5.2209784
62	H31	-3.1688432	2.3651185	-6.2334827
63	C32	-2.8417874	1.1723042	-4.4752528
64	H32	-3.283281	0.2840042	-4.9182303
65	N1	-1.8744827	-0.4136556	1.8617329
66	N2	1.358564	0.442442	1.474128
67	C1	-2.6095369	-0.9296858	0.6992423
68	H1A	-3.1949331	-1.7828503	1.0532688

69	H1B	-3.345577	-0.1936719	0.3283109
70	C2	-1.1350913	0.8297463	1.5686455
71	H2A	-0.9816291	0.8786878	0.4914951
72	H2B	-1.7516341	1.705391	1.833386
73	C3	0.2259037	0.933571	2.2795209
74	H3A	0.1902188	0.3515147	3.1967656
75	H3B	0.4090477	1.981949	2.5809969
76	C4	1.7302391	1.4321652	0.450085
77	H4A	0.818552	1.8301214	0.0029276
78	H4B	2.2376199	2.2901947	0.9305256
79	C5	-2.8057809	-0.2510249	2.9876179
80	H5A	-3.5060873	0.5835715	2.7978258
81	H5B	-3.4164568	-1.1585594	3.0369543
82	C6	-2.1643017	-0.049529	4.3457124
83	C7	-1.3291678	-1.0299059	4.8923982
84	H7	-1.0848915	-1.9113169	4.3084528
85	C8	-0.7827119	-0.8751099	6.1609045
86	H8	-0.1296495	-1.6445085	6.5586005
87	C9	-1.0565946	0.2652879	6.928395
88	C10	-1.8892955	1.2450427	6.3824695
89	H10	-2.1133904	2.1377749	6.9582919
90	C11	-2.4333803	1.0878291	5.1077163
91	H11	-3.0787685	1.863302	4.7039759
92	C12	-0.4715784	0.4223215	8.2968787
93	C13	0.7905475	1.0340151	8.4566236
94	C14	1.5456711	1.5373213	7.3496114
95	H14	1.1324801	1.4447407	6.3524751
96	C15	2.7652603	2.128529	7.5331379
97	H15	3.3157006	2.5091672	6.6783679
98	C16	3.3225221	2.2555573	8.8361812
99	H16	4.2924108	2.7263184	8.961621
100	C17	2.6374132	1.7890782	9.921443
101	H17	3.0554	1.8841527	10.9196935
102	C18	1.3582487	1.1686765	9.7770377
103	C19	0.6474083	0.6938672	10.880225
104	H19	1.0779688	0.7974147	11.8728996
105	C20	-0.6042093	0.0917477	10.740093
106	C21	-1.3324195	-0.3904134	11.8707192
107	H21	-0.8887948	-0.2790877	12.855917
108	C22	-2.5568376	-0.9769924	11.7230836
109	H22	-3.099392	-1.3385513	12.5907045
110	C23	-3.1289474	-1.1162273	10.4278645
111	H23	-4.1030443	-1.5831798	10.3224777
112	C24	-2.4654348	-0.6695587	9.3191133
113	H24	-2.9138392	-0.7824485	8.3396099
114	C25	-1.18012	-0.047945	9.4234921
115	C26	2.500785	0.1336007	2.3416257
116	H26A	3.3837642	0.0095875	1.7085423
117	H26B	2.7300665	0.9855028	3.0088591
118	C27	2.3431174	-1.1255914	3.1725333
119	C28	1.762818	-2.2781229	2.6339284
120	H28	1.3567868	-2.2410823	1.6300573
121	C29	1.6915406	-3.4525951	3.3779807
122	H29	1.2376177	-4.3382304	2.9435103
123	C30	2.2011482	-3.4952606	4.6753921
124	H30	2.147331	-4.4116423	5.2546774
125	C31	2.7756666	-2.3513736	5.2238526
126	H31	3.1667738	-2.3674733	6.2364863
127	C32	2.8412969	-1.1762828	4.4769599
128	H32	3.2827084	-0.2875249	4.9191093

Cartesian Coordinates (Angstroms) of L^2

	Atom	X	Y	Z
1	N1	1.8855622	1.1140727	-1.5212386
2	N2	-0.854928	-0.8257462	-1.69886
3	C1	2.2094276	1.7695117	-0.2479559
4	H1A	2.5443191	2.7813478	-0.4923972
5	H1B	3.0645459	1.28203	0.2540811
6	C2	1.6054244	-0.3264057	-1.3683349
7	H2A	1.3311234	-0.5038957	-0.3292346
8	H2B	2.5265512	-0.9071262	-1.5447545
9	C3	0.4965289	-0.8639311	-2.2896629
10	H3A	0.4820471	-0.2789021	-3.2057475
11	H3B	0.7408385	-1.9014188	-2.5850376
12	C4	-1.0203998	-1.9141698	-0.7206265
13	H4A	-0.1160758	-1.9862102	-0.1150978
14	H4B	-1.1093921	-2.8798355	-1.2536365
15	C5	2.958217	1.37219	-2.4971589

16	H5A	3.8795663	0.8251466	-2.2224437
17	H5B	3.2018802	2.4374949	-2.4324975
18	C6	2.6033777	1.0491519	-3.9320927
19	C7	1.6006342	1.7616786	-4.589694
20	H7	1.0569393	2.5350469	-4.0563384
21	C8	1.2449744	1.4797844	-5.90611
22	H8	0.4484	2.0509751	-6.3641985
23	C9	1.9012807	0.4563536	-6.5979151
24	C10	2.9239593	-0.2529298	-5.9604655
25	H10	3.4288212	-1.0403959	-6.50941
26	C11	3.2642001	0.0447171	-4.6468028
27	H11	4.0554829	-0.5235746	-4.1654607
28	C26	-1.8688855	-0.9386041	-2.7524218
29	H26A	-2.8202073	-1.2020151	-2.2805434
30	H26B	-1.6341976	-1.7812421	-3.4301803
31	C27	-2.1035632	0.3142983	-3.5751765
32	C28	-1.9352514	1.5925974	-3.0382604
33	H28	-1.5487739	1.6906989	-2.0314841
34	C29	-2.2513562	2.7258492	-3.7857481
35	H29	-2.1147249	3.7112835	-3.3502929
36	C30	-2.7464242	2.6000169	-5.08248
37	H30	-2.9997393	3.4829536	-5.66115
38	C31	-2.913902	1.3288438	-5.6296412
39	H31	-3.298349	1.2151814	-6.6388147
40	C32	-2.5876023	0.199181	-4.8824038
41	H32	-2.7198315	-0.7871562	-5.3197958
42	N3	-1.8818629	-1.1192588	1.521784
43	N4	0.8605878	0.8185953	1.6993748
44	C12	-2.2049144	-1.7747759	0.2483259
45	H1	-2.5410939	-2.786232	0.4925271
46	H2	-3.0588426	-1.286466	-0.2548912
47	C13	-1.5996849	0.3207572	1.3685194
48	H3	-1.3242445	0.4975009	0.329575
49	H4	-2.5201891	0.9027149	1.5439795
50	C14	-0.4907012	0.8568229	2.2906089
51	H5	-0.4765202	0.2705991	3.2059536
52	H6	-0.7344706	1.8940577	2.5872543
53	C15	1.0261181	1.9082147	0.7224595
54	H9	0.1212001	1.9821284	0.1180125
55	H12	1.1166949	2.8729639	1.256876
56	C16	-2.9556751	-1.3753155	2.4968634
57	H13	-3.8762195	-0.8276831	2.220626
58	H14	-3.2003764	-2.4404592	2.433303
59	C17	-2.6017943	-1.0504999	3.9316533
60	C18	-1.5993211	-1.7619561	4.5908639
61	H15	-1.0550206	-2.5358431	4.0588851
62	C19	-1.2450987	-1.4786985	5.9073895
63	H16	-0.4489955	-2.0493971	6.3669123
64	C20	-1.9024345	-0.4548296	6.5975875
65	C21	-2.9246437	0.2535443	5.9584216
66	H17	-3.4303529	1.0413388	6.5061115
67	C22	-3.263527	-0.0455172	4.6447155
68	H18	-4.0546051	0.5219824	4.1620982
69	C23	1.8751459	0.9297043	2.7525584
70	H19	2.826794	1.1910217	2.280167
71	H20	1.642325	1.7729482	3.4302091
72	C24	2.1075193	-0.3235034	3.5754223
73	C25	1.9387372	-1.6015047	3.0378306
74	H21	1.5535268	-1.6989589	2.0304947
75	C33	2.2526915	-2.735284	3.7853576
76	H22	2.1157104	-3.7204477	3.3494015
77	C34	2.7459488	-2.6103436	5.0828994
78	H23	2.9974815	-3.493737	5.6616461
79	C35	2.9137937	-1.3395361	5.6307337
80	H24	3.2967753	-1.2265468	6.6405418
81	C36	2.5897261	-0.2092825	4.8833565
82	H25	2.7222324	0.7767701	5.3213046
83	O1	1.6116008	0.0734148	-7.8778219
84	O2	-1.6145694	-0.0709968	7.8776616
85	C37	0.5067299	0.7051474	-8.5389046
86	H26	-0.3834317	0.6407752	-7.9076096
87	H27	0.7178579	1.7684589	-8.6773873
88	C38	-0.5083131	-0.6995812	8.5394503
89	H33	0.3816921	-0.6340942	7.9080854
90	H34	-0.7171482	-1.7631986	8.6792599
91	H35	-2.2548574	-3.3208902	-7.8936066
92	C39	-1.8867554	-2.8574693	-8.8035603
93	H36	-0.7979248	-1.3800558	-7.7497206

94	C40	-1.0785675	-1.7568028	-8.7251375
95	C41	-1.7581191	-2.8572343	-11.2121281
96	C42	-0.5594903	-1.1273242	-9.9019892
97	C43	-2.2432171	-3.412625	-10.0631811
98	C44	-0.900045	-1.7155199	-11.1747257
99	C45	0.262054	0.0212336	-9.8598928
100	H37	-2.8910331	-4.2822684	-10.1037367
101	H38	-0.6533166	-1.5928957	-13.3028748
102	H39	-2.0127769	-3.2795586	-12.1798686
103	C46	0.8283552	0.5341126	-11.0468516
104	C47	1.7540493	1.6270455	-11.0670688
105	C48	0.4799025	-0.0615307	-12.3159697
106	H40	0.7451549	0.0261677	-14.4640672
107	C49	-0.383485	-1.1569587	-12.344447
108	C50	2.2664387	2.1073939	-12.2401019
109	H41	2.0894068	2.0606285	-10.1332576
110	H42	2.9753577	2.9291213	-12.2206207
111	C51	1.8918504	1.5368379	-13.4877711
112	H43	2.3042041	1.9374922	-14.4081013
113	C52	1.0281483	0.4803833	-13.5189367
114	H44	2.2548382	3.3255361	7.8929906
115	C53	1.8855244	2.8631737	8.8029914
116	H45	0.7976708	1.384884	7.7493852
117	C54	1.0771956	1.7625988	8.7247631
118	C55	1.753813	2.8656265	11.2113872
119	C56	0.5564477	1.1345359	9.9016323
120	C57	2.2405572	3.419608	10.0624596
121	C58	0.8954496	1.7241148	11.1741609
122	C59	-0.2652628	-0.01387	9.8597946
123	H46	2.8885816	4.2891057	10.1028896
124	H47	0.6457802	1.6041155	13.3021062
125	H48	2.0073187	3.2889686	12.1789857
126	C60	-0.8334338	-0.5251025	11.046594
127	C61	-1.7595511	-1.6176787	11.0667097
128	C62	-0.4866494	0.071963	12.3154719
129	H49	-0.7551153	-0.0130459	14.4632837
130	C63	0.3771002	1.1671279	12.343833
131	C64	-2.273811	-2.0964542	12.2395772
132	H50	-2.0937702	-2.0521214	10.1328895
133	H51	-2.9830003	-2.9179463	12.2200634
134	C65	-1.9008353	-1.5245321	13.4870992
135	H52	-2.3146843	-1.9239344	14.4073033
136	C66	-1.0368327	-0.4683154	13.5182811

Cartesian Coordinates (Angstroms) of L^3

	Atom	X	Y	Z
1	N1	-0.6795983	-1.739956	1.9178026
2	N2	-1.1128448	1.4439966	0.9425407
3	C1	-0.0319029	-2.6632474	0.9776778
4	H1A	-0.5862547	-3.6041727	1.0291766
5	H1B	0.998658	-2.903911	1.2952623
6	C2	0.070057	-0.4803892	2.0857335
7	H2A	0.7311245	-0.3698265	1.2270642
8	H2B	0.7245739	-0.5509012	2.9705986
9	C3	-0.811704	0.7723486	2.2202546
10	H3A	-1.7547577	0.4917759	2.682258
11	H3B	-0.3261307	1.4883617	2.9094249
12	C4	0.0537418	2.2153282	0.482405
13	H4A	0.9481956	1.6053682	0.6124351
14	H4B	0.1903924	3.1042414	1.1275951
15	C5	-0.9095056	-2.425428	3.1997081
16	H5A	0.047802	-2.6105849	3.7230799
17	H5B	-1.3247979	-3.4114406	2.9668477
18	C6	-1.857283	-1.7261552	4.1516529
19	C7	-3.184076	-1.4859397	3.7910859
20	H7	-3.5228539	-1.7462855	2.7937627
21	C8	-4.0838564	-0.8862147	4.6681922
22	H8	-5.0932481	-0.6997048	4.3263248
23	C9	-3.665334	-0.5122515	5.9495049
24	C10	-2.3393308	-0.7458655	6.324574
25	H10	-2.0223547	-0.4489252	7.3184666
26	C11	-1.4541105	-1.3417816	5.4335647
27	H11	-0.427493	-1.5132019	5.7457892
28	C26	-2.2768178	2.3226472	1.1005726
29	H26A	-2.3172913	2.9907764	0.2354695
30	H26B	-2.1538006	2.9816687	1.9803565
31	C27	-3.6124217	1.6097464	1.1947863
32	C28	-3.8764099	0.4513397	0.458065
33	H28	-3.0817936	0.0137403	-0.1340814
34	C29	-5.136327	-0.1420312	0.4943622
35	H29	-5.3233408	-1.0419927	-0.0844009
36	C30	-6.1552987	0.413278	1.2677277
37	H30	-7.1371642	-0.0483314	1.2975294
38	C31	-5.9011543	1.5654723	2.0088957
39	H31	-6.6860022	2.0061712	2.6160424
40	C32	-4.6380062	2.1523986	1.9745755
41	H32	-4.4458843	3.0455986	2.5633169

42	N3	0.6796949	1.7501565	-1.9250315
43	N4	1.1136298	-1.4346346	-0.9504782
44	C12	0.0327587	2.6736955	-0.9846555
45	H1	0.5877203	3.6142662	-1.0362637
46	H2	-0.9976835	2.9148791	-1.3021603
47	C13	-0.0700067	0.4903827	-2.09267
48	H3	-0.7309944	0.3794601	-1.2339838
49	H4	-0.724716	0.5611264	-2.9773994
50	C14	0.8113783	-0.7626582	-2.2278402
51	H5	1.7541502	-0.4827589	-2.6908439
52	H6	0.3246688	-1.4783972	-2.9164749
53	C15	-0.0533535	-2.2047388	-0.489343
54	H9	-0.9472157	-1.5937525	-0.6187091
55	H12	-0.1914411	-3.0934134	-1.1345466
56	C16	0.9084772	2.4357559	-3.2070237
57	H13	-0.0491772	2.6198098	-3.7300707
58	H14	1.3227999	3.4223545	-2.9747066
59	C17	1.8563149	1.7367418	-4.1591139
60	C18	3.1808763	1.4890742	-3.7954562
61	H15	3.5178741	1.743545	-2.7960635
62	C19	4.08001	0.8873907	-4.6717402
63	H16	5.0868225	0.6928973	-4.3266325
64	C20	3.6636475	0.5203055	-5.9556549
65	C21	2.3403354	0.7624911	-6.334396
66	H17	2.0247898	0.4705102	-7.3302115
67	C22	1.4552983	1.3593821	-5.4437714
68	H18	0.4303908	1.5366267	-5.7584123
69	C23	2.2762209	-2.3150524	-1.1098753
70	H19	2.318639	-2.9807407	-0.2429784
71	H20	2.1496486	-2.9764708	-1.9873193
72	C24	3.612125	-1.6036123	-1.2110886
73	C25	3.8815165	-0.4466196	-0.4740585
74	H21	3.0910244	-0.0096393	0.1240582
75	C33	5.1412874	0.1464922	-0.5178404
76	H22	5.3324065	1.0454369	0.0611582
77	C34	6.1547986	-0.4075721	-1.2993156
78	H23	7.1362293	0.0544554	-1.336164
79	C35	5.8954459	-1.5586669	-2.0403068
80	H24	6.6761749	-1.9985263	-2.6533656
81	C36	4.6324829	-2.1455638	-1.998169
82	H25	4.436285	-3.0379677	-2.5867359
83	O1	-4.4506818	0.0990651	6.8881094
84	O2	4.4487906	-0.09435	-6.8922104
85	C37	-5.857082	0.2262679	6.6774825
86	H26	-6.1625846	1.0302121	7.3480965
87	H27	-6.0752716	0.5546484	5.6573474
88	C38	5.85387	-0.2264628	-6.6766663
89	H33	6.158074	-1.0315439	-7.3463985
90	H34	6.0670107	-0.5560719	-5.6558202
91	C39	-6.606717	-1.0713038	7.0234832
92	H35	-6.3262881	-1.3609935	8.0381829
93	H36	-6.2422183	-1.8771073	6.3871111
94	C40	6.6104619	1.0680309	-7.0192281
95	H37	6.2456345	1.8754922	-6.3851715
96	H38	6.3367731	1.3583101	-8.0356148
97	H39	-8.4638961	0.9274058	11.1345562
98	C41	-8.9608494	0.6175746	10.2207262
99	H40	-7.1590867	-0.0344204	9.3326234
100	C42	-8.2282719	0.0741605	9.2015232
101	C43	-10.9981961	0.3910658	8.9529639
102	C44	-8.8408141	-0.351313	7.9775931
103	C45	-10.3674997	0.7809643	10.0990388
104	C46	-10.2701242	-0.1794406	7.8641493
105	C47	-8.1101539	-0.9186968	6.9060284
106	H41	-10.9326016	1.213428	10.9183578
107	H42	-11.9928129	-0.440589	6.6112158
108	H43	-12.0728604	0.508616	8.8472894
109	C48	-8.7858835	-1.3067705	5.724257
110	C49	-8.1223547	-1.88195	4.5917168
111	C50	-10.2169047	-1.1293785	5.623823
112	H44	-11.9691681	-1.385733	4.377571
113	C51	-10.9171138	-0.5725073	6.6930517
114	C52	-8.8072075	-2.2519356	3.4668089
115	H45	-7.0516861	-2.0358014	4.6157234
116	H46	-8.2702012	-2.6908318	2.6318597
117	C53	-10.2146159	-2.0732759	3.3790876
118	H47	-10.7415811	-2.3732466	2.4791192
119	C54	-10.8935169	-1.5274983	4.4297833
120	H48	8.4799	-0.9486145	-11.1154074
121	C55	8.9735815	-0.638268	-10.1999798
122	H49	7.1700782	0.0233136	-9.3225696
123	C56	8.2381901	-0.0891119	-9.185904
124	C57	11.0055637	-0.4166801	-8.9227448
125	C58	8.8464371	0.3371099	-7.9600773
126	C59	10.3789402	-0.8070931	-10.0708751
127	C60	10.2744219	0.159696	-7.839066
128	C61	8.1126176	0.909775	-6.8935603
129	H50	10.9462769	-1.2441912	-10.8861708
130	H51	11.9918888	0.4172551	-6.5781914
131	H52	12.0791839	-0.5384186	-8.8113584
132	C62	8.7839254	1.2977257	-5.7091568
133	C63	8.1170228	1.877762	-4.5810903
134	C64	10.2137496	1.1152045	-5.6012865
135	H53	11.960868	1.3679601	-4.3470914
136	C65	10.9171303	0.5531315	-6.6657349
137	C66	8.7977989	2.2479986	-3.4537543
138	H54	7.0470496	2.0353656	-4.610567
139	H55	8.2583259	2.6909674	-2.6225617
140	C67	10.2041004	2.0645047	-3.3588107
141	H56	10.7278184	2.3647572	-2.4570469

142	C68	10.8860293	1.5136608	-4.4049106

Cartesian Coordinates (Angstroms) of NIEDPA

	Atom	X	Y	Z
1	H1	-3.0450617	-2.1195054	-5.6674005
2	C1	-2.1725515	-1.632661	-5.2416639
3	H6	-0.9030135	-2.1096316	-6.9034755
4	C6	-0.9772945	-1.627338	-5.9319165
5	C3	-1.1706612	-0.3819837	-3.4227135
6	C5	0.1735592	-0.9968343	-5.3901877
7	C2	-2.271604	-1.007227	-3.9813967
8	C4	0.0672269	-0.3662188	-4.1131928
9	C10	1.4254613	-0.9642083	-6.0590884
10	H2	-3.2058016	-1.0037993	-3.4294916
11	C9	2.5164194	-0.3399999	-5.4886876
12	H10	1.51309	-1.4413657	-7.0321701
13	H9	3.4683662	-0.3228298	-6.0110887
14	C8	2.4061304	0.2784031	-4.2257657
15	H8	3.2574058	0.769695	-3.7658716
16	C7	1.2005493	0.2682819	-3.5463171
17	C11	1.1056428	0.9247159	-2.2196833
18	C12	-1.2967667	0.2721098	-2.0970674
19	N1	-0.1529449	0.9051365	-1.5908677
20	O1	2.0609188	1.4695623	-1.6840971
21	O2	-2.3519702	0.2860334	-1.4719039
22	C13	-0.2614106	1.5546697	-0.2739423
23	H4	-1.2884961	1.906911	-0.1810642
24	H5	0.4206958	2.4043938	-0.2785075
25	C14	0.0889068	0.572538	0.8708829
26	H3	1.1552456	0.3288014	0.8101693
27	H7	-0.4668689	-0.3586283	0.7113278
28	N2	-0.2025196	1.0629925	2.2065534
29	C15	-1.6146754	1.1529154	2.561183
30	H12	-2.2117513	1.7443626	1.8437312
31	H13	-1.6810251	1.657131	3.5299223
32	C16	0.708532	2.0753911	2.721937
33	H11	1.0422402	2.7961066	1.9599971
34	H16	0.1784704	2.6665971	3.4793263
35	C17	-2.2452233	-0.2219457	2.7135271
36	C18	-3.3203231	-2.7183743	3.084162
37	N4	-1.8953955	-0.9158329	3.8118835
38	C20	-3.1275581	-0.7291635	1.7544792
39	C21	-3.6722629	-1.9996817	1.9442697
40	C22	-2.4262848	-2.1300126	3.9819692
41	H17	-3.359538	-0.1495597	0.8659871
42	H18	-4.3566027	-2.4181306	1.2108179
43	H19	-2.1254579	-2.6607025	4.8846725
44	H20	-3.7211411	-3.7089296	3.2780855
45	C23	1.9564979	1.4847422	3.3682023
46	C24	4.2363504	0.5608714	4.5716002
47	C25	1.9304457	0.2282147	3.9855783
48	N3	3.050937	2.2606173	3.3402828
49	C27	4.1582448	1.7981908	3.9335165
50	C28	3.0924492	-0.2375164	4.5965
51	H15	1.0100747	-0.3469092	3.9780956
52	H22	5.0291439	2.4513168	3.8905617
53	H23	3.1058985	-1.2079566	5.0866754
54	H24	5.1652901	0.2362447	5.0316648

Cartesian Coordinates (Angstroms) of NIPDPA

	Atom	X	Y	Z
1	H1	4.2213493	5.2744804	3.7933728
2	C1	3.6488517	5.0324688	2.9028126
3	H6	3.0604384	7.0634452	2.5412417
4	C6	3.0010909	6.031203	2.2047246
5	C3	2.8502963	3.3651107	1.3348405
6	C5	2.2482469	5.7327435	1.0388787
7	C2	3.5732257	3.6925871	2.4683306
8	C4	2.1775623	4.3748605	0.6021161
9	C10	1.5625781	6.7224042	0.2870459
10	H2	4.0762488	2.8982303	3.0099031
11	C9	0.8425481	6.3813573	-0.8399475
12	H10	1.6133525	7.7581812	0.6140029
13	H9	0.322261	7.1483928	-1.4058422
14	C8	0.7752181	5.0382545	-1.2655853
15	H8	0.2120105	4.7572803	-2.1494548
16	C7	1.4320254	4.0473414	-0.5580254
17	C11	1.3442001	2.6399517	-1.0204392
18	C12	2.7801509	1.9488735	0.8969817
19	N1	2.0516423	1.6836902	-0.2742551
20	O1	0.6931601	2.3092173	-2.0029585
21	O2	3.3249979	1.0421686	1.5132492
22	C13	1.9718912	0.2816808	-0.7215084
23	H4	2.9013869	-0.1999243	-0.4153201
24	H5	1.9101185	0.2985302	-1.8109041
25	C14	0.7627023	-0.4484923	-0.1252401
26	H3	-0.1575114	0.0651413	-0.4241214
27	H7	0.8329651	-0.3991139	0.9675757
28	C15	0.69513	-1.9014713	-0.6058636
29	H12	1.6266468	-2.4379684	-0.3410154
30	H13	0.6377434	-1.9011129	-1.6999057
31	N2	-0.4894267	-2.616169	-0.1066123

32	C16	-0.3358872	-3.040227	1.290085
33	H14	0.1465699	-2.2241475	1.840478
34	H15	0.3170947	-3.9228016	1.3967853
35	C17	-0.8283897	-3.7590754	-0.9611364
36	H16	0.0368308	-4.4166911	-1.1534321
37	H17	-1.5643512	-4.3698725	-0.422512
38	C18	-1.659347	-3.3526388	1.9650688
39	C19	-3.9868189	-3.9539415	3.2880219
40	N4	-1.7015093	-4.4659585	2.7128287
41	C20	-2.7584872	-2.4925282	1.8348425
42	C21	-3.9382355	-2.7990558	2.5059076
43	C22	-2.8425948	-4.7469923	3.3562649
44	H18	-2.6740857	-1.6079155	1.2120637
45	H19	-4.8053716	-2.1487985	2.4219002
46	H20	-2.8389442	-5.6589924	3.9515973
47	H21	-4.8858312	-4.2351465	3.8285819
48	C23	-1.4287307	-3.3688568	-2.2999615
49	C24	-2.5403532	-2.8277708	-4.7498986
50	C25	-2.2386932	-2.2352757	-2.4436237
51	N3	-1.1718124	-4.2042012	-3.3194876
52	C27	-1.7243586	-3.9326488	-4.5079934
53	C28	-2.7984205	-1.9603494	-3.688649
54	H22	-2.4075805	-1.5893441	-1.588904
55	H23	-1.4945608	-4.6335081	-5.3096497
56	H24	-3.425092	-1.0830552	-3.8283297
57	H25	-2.9537583	-2.6535492	-5.7389255

Cartesian Coordinates (Angstroms) of NIBDPA

	Atom	X	Y	Z
1	H1	-3.1831302	-2.8614529	-6.9575275
2	C1	-2.6036656	-2.0094879	-6.6144965
3	H6	-1.9168676	-1.4878761	-8.579091
4	C6	-1.8975291	-1.2434645	-7.5197156
5	C3	-1.8460736	-0.6134156	-4.7834604
6	C5	-1.1347379	-0.1265857	-7.0883044
7	C2	-2.5777606	-1.6955632	-5.2395812
8	C4	-1.1145032	0.1879416	-5.6954343
9	C10	-0.3898349	0.6911626	-7.9782077
10	H2	-3.1266541	-2.2916655	-4.517891
11	C9	0.3383932	1.7656026	-7.5090498
12	H10	-0.4014276	0.4568086	-9.0399396
13	H9	0.9044341	2.3830813	-8.20042
14	C8	0.3563843	2.0699471	-6.13174
15	H8	0.9278125	2.9100577	-5.7506003
16	C7	-0.3597274	1.296313	-5.2354868
17	C11	-0.3245458	1.6315526	-3.7897345
18	C12	-1.8268467	-0.3043148	-3.3322413
19	N1	-1.082104	0.8170084	-2.9328099
20	O1	0.336596	2.5614254	-3.3458041
21	O2	-2.4266922	-0.9818298	-2.5075321
22	C13	-1.0468496	1.1264499	-1.491589
23	H4	-2.0165791	0.8376295	-1.0837128
24	H5	-0.9175016	2.2059048	-1.4033362
25	C14	0.0804397	0.3860675	-0.7637206
26	H3	1.0423323	0.6825535	-1.2006453
27	H7	-0.0396353	-0.6913453	-0.9323205
28	C15	0.0784073	0.6769991	0.7426593
29	H12	-0.8928553	0.4031729	1.1751838
30	H13	0.2001969	1.7570746	0.9030908
31	C16	1.1727002	-0.1054221	1.4764906
32	H11	2.1622934	0.1170422	1.0338731
33	H14	0.9943522	-1.1734905	1.3134373
34	N2	1.1820171	0.124449	2.9300113
35	C17	1.8393226	1.3884672	3.2801572
36	H16	1.5183481	2.1476309	2.5564008
37	H17	2.9386469	1.3282646	3.2041598
38	C18	1.8059123	-0.9945246	3.6462946
39	H18	2.8028616	-1.2506141	3.2486485
40	H19	1.958975	-0.6764092	4.6855975
41	C19	1.4962098	1.8887222	4.6723453
42	C20	0.9662883	2.9123564	7.1618249
43	N4	2.5071368	2.4273339	5.3720319
44	C21	0.1866251	1.8290971	5.1672541
45	C22	-0.0799687	2.347881	6.4311589
46	C23	2.2351243	2.9264967	6.5845177
47	H20	-0.5912956	1.3776064	4.5607632
48	H21	-1.0868943	2.3137748	6.8400226
49	H22	3.0804531	3.3544718	7.1218918
50	H23	0.8063997	3.3278426	8.1525052
51	C24	0.9659452	-2.2587024	3.6555075
52	C25	-0.4420306	-4.6118016	3.7654727
53	C26	-0.4298282	-2.2119725	3.766337
54	N3	1.6447703	-3.4155307	3.5950929
55	C27	0.9466728	-4.5564409	3.6539825
56	C28	-1.1425345	-3.4066179	3.8200078
57	H24	-0.9284369	-1.2496407	3.7995508
58	H25	1.532018	-5.4737648	3.6022969
59	H26	-2.2264948	-3.3980579	3.9031204
60	H27	-0.9551417	-5.5681984	3.8027035

Table S4. Crystallographic Data and Structure Refinement.

	[**L**^{2}·Ag]OTf	[**L**^{3}·Ag]OTf·DCE
formula	$C_{67}H_{64}AgF_3N_4O_5S$	$C_{71}H_{72}AgCl_2F_3N_4O_5S$
formula weight	1202.15	1329.15
Temperature (K)	90	90
crystal system	Triclinic	Orthorhombic
space group	*P*-1	$Pna2_1$
Z	2	4
a (Å)	14.5272(13)	19.4648(13)
b (Å)	14.5290(14)	21.0751(14)
c (Å)	15.8434(15)	14.7014(10)
α (°)	94.4274(19)	90
β (°)	99.9833(18)	90
γ (°)	116.5991(15)	90
V (Å^3)	2898.9(5)	6030.8(7)
D_{calc}(g/cm^3)	1.377	1.464
μ (mm^{-1})	0.448	0.524
$2\vartheta_{max}$ (°)	52	52
reflections collected	18392	37170
independent reflections	11337 [R_{int} = 0.0324]	11194 [R_{int} = 0.0278]
goodness-of-fit on F^2	1.038	1.010
R_1, wR_2[$I > 2\sigma(I)$]	0.0493, 0.1134	0.0281, 0.0713
R_1, wR_2[all data]	0.0603, 0.1202	0.0296, 0.0724

Table S5. Selected Bond Lengths (Å) and Bond Angles (deg) for [**L**^{2}·Ag]OTf.

Ag1-N1	2.470(3)	Ag1-N2	2.429(3)

Ag1-N3	2.480(3)	Ag1-N4	2.428(2)
N1-Ag1-N2	76.20(9)	N1-Ag1-N3	122.54(8)
N1-Ag1-N4	76.58(9)	N2-Ag1-N3	76.58(9)
N2-Ag1-N4	123.02(8)	N3-Ag1-N4	77.63(8)

Table S6. Selected Bond Lengths (Å) and Bond Angles (deg) for [$\mathbf{L^3}$·Ag]OTf·DCE.

Ag1-N1	2.473(3)	Ag1-N2	2.495(2)
Ag1-N3	2.397(3)	Ag1-N4	2.478(3)
N1-Ag1-N2	75.40(9)	N1-Ag1-N3	122.12(9)
N1-Ag1-N4	76.19(10)	N2-Ag1-N3	77.40(9)
N2-Ag1-N4	122.75(9)	N3-Ag1-N4	77.43(9)

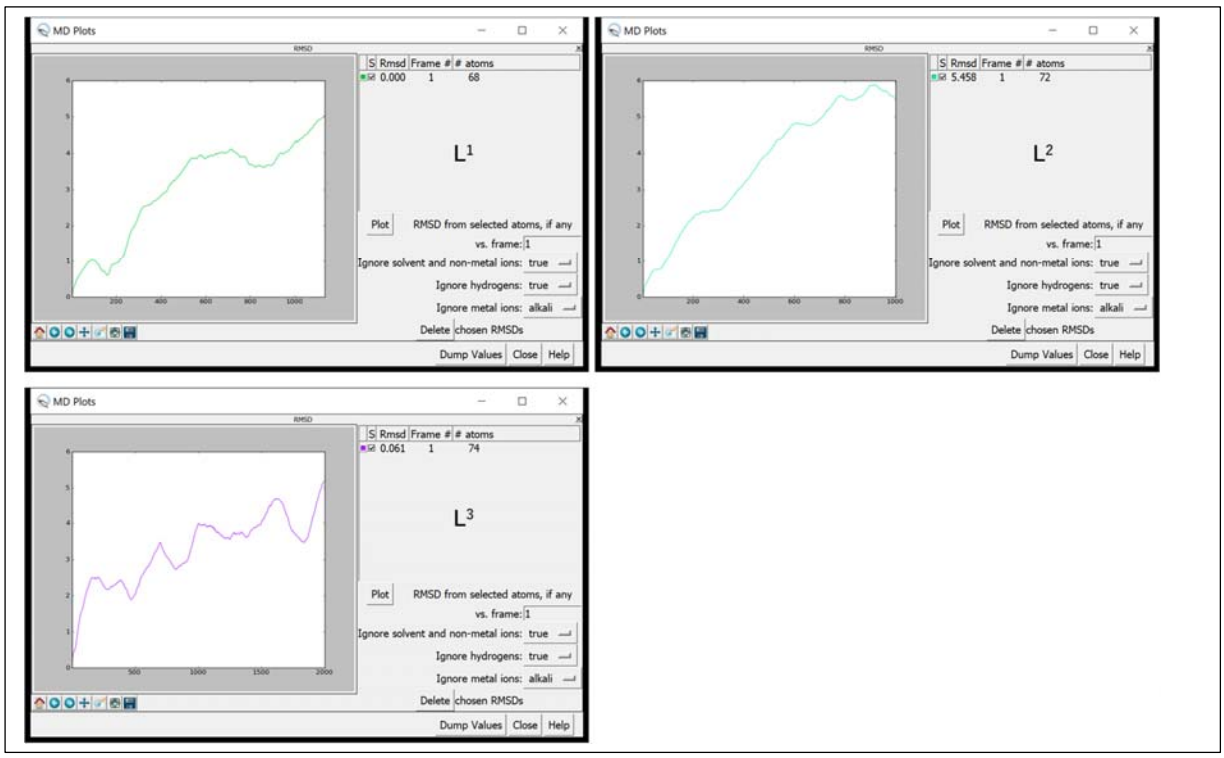


Figure S18. Time-dependent RMSD plots for $\mathbf{L^1}$ — $\mathbf{L^3}$. X and y axis are steps (fs) and time-dependent root-mean-squar-deviation for all atoms, respectively.

References

S1 S. Y. Kim and J. -I. Hong, Naphthalimide-based fluorescent Zn^{2+} chemosensors showing PET effect according to their linker length in water. *Tetrahedron Lett.* 2009, **50**, 2822-2824.

S2 9-(Phenoxymethyl)anthracene was prepared according to the literature. A. M. Sarotti, M. M. Joullie, R. A. Spanevello, and A. G. Suarez, *Org. Lett.*, 2006, **8**, 5561-5564.