Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Vapochromism of indolenine-based heptamethine cyanine dye adsorbed on silica gel

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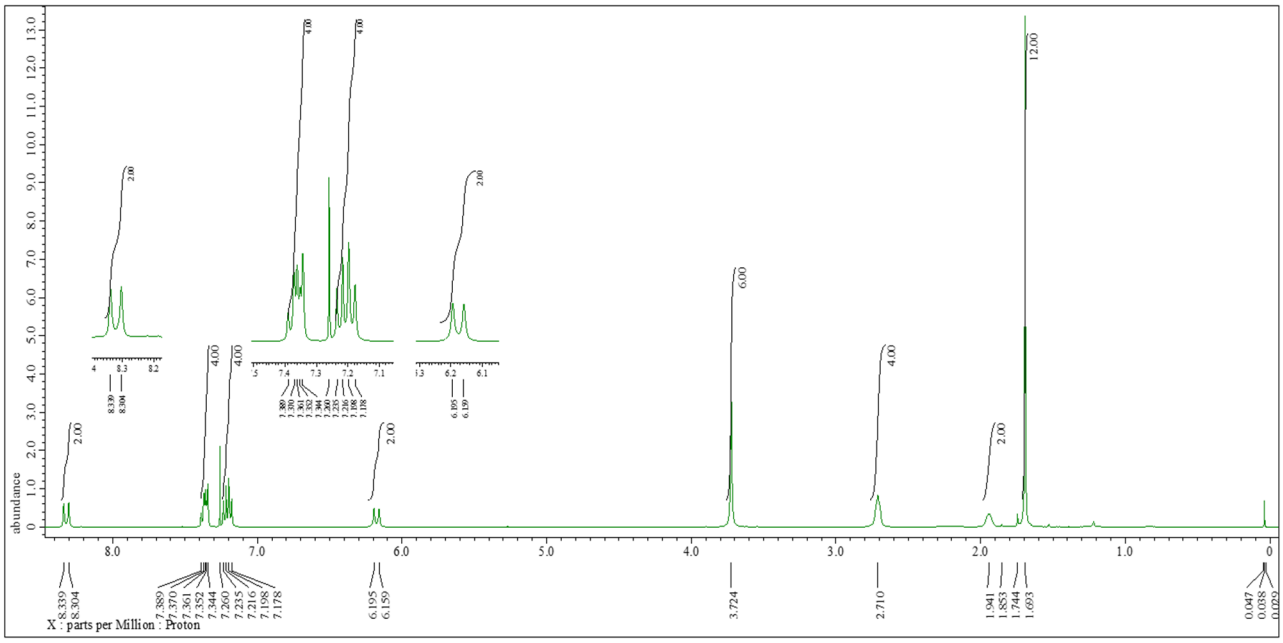
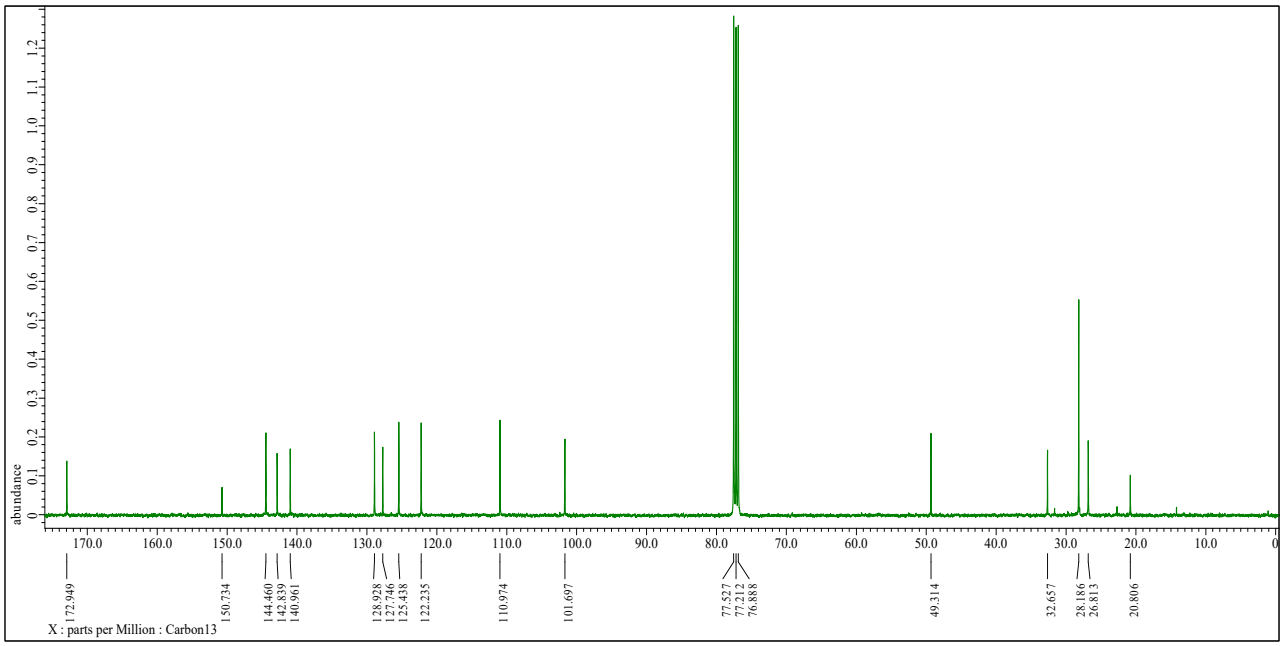
(Contents)

2-((*E*)-2-((*E*)-2-chloro-3-(2-((*E*)-1,3,3-trimethylindolin-2-ylidene)ethylidene)cyclohex-1-en-1-yl)vinyl)-1,3,3-trimethyl-3*H*-indol-1-ium iodide (3)

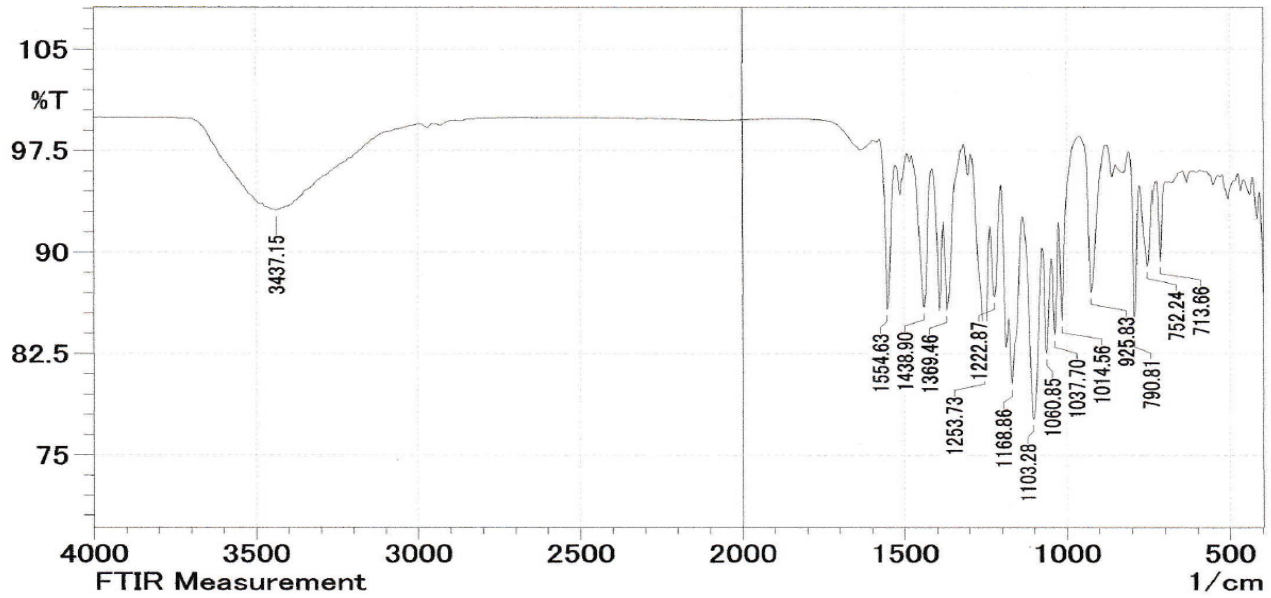
^{1}H NMR



^{13}C NMR



IR

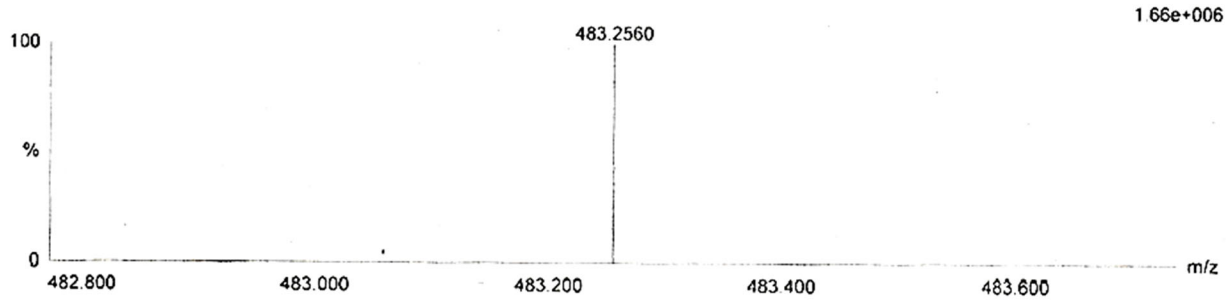


HRMS

Elemental Composition Report **Page 1**

Single Mass Analysis
Tolerance = 15.0 mDa / DBE: min = -1.5, max = 50.0
Element prediction: Off
Number of isotope peaks used for i-FIT = 3

Monoisotopic Mass, Even Electron Ions
1 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass)
Elements Used:
C: 32-32 H: 36-36 N: 2-2 Cl: 1-1
20220826_06 12 (0.421)
1: TOF MS ES+



Minimum:				-1.5			
Maximum:		15.0	10.0	50.0			
Mass	Calc. Mass	mDa	PPM	DBE	i-FIT	i-FIT (Norm)	Formula
483.2560	483.2567	-0.7	-1.4	15.5	43.1	0.0	C32 H36 N2 Cl

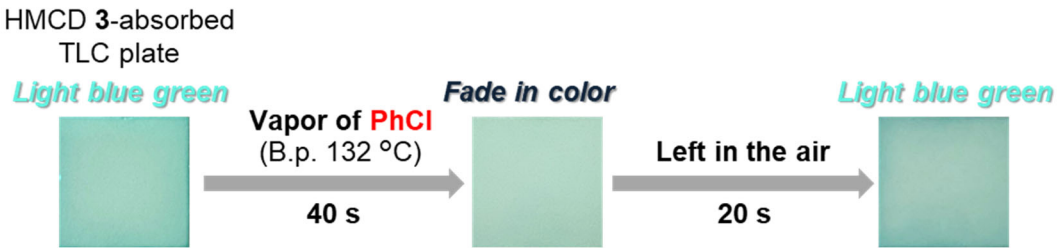


Figure S1. Photographs of the TLC plates adsorbed with HMCD **3** using an acetone solution and exposed to PhCl vapor and left in the air.

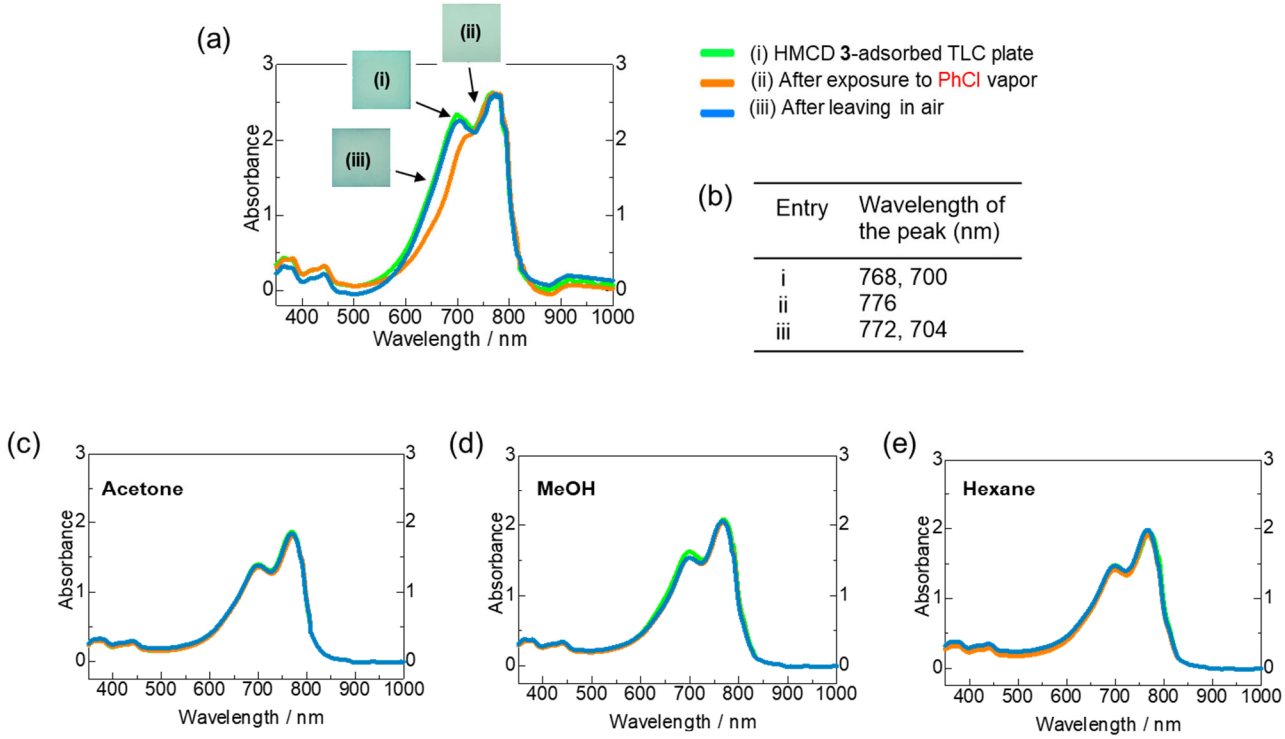


Figure S2. UV-Vis-NIR spectrum of TLC plates adsorbed with HMCD **3** using an acetone solution and exposed to solvents. (a) PhCl, (b) acetone, (c) MeOH, and (d) hexane vapor, and (b) wavelengths of the peaks in UV-Vis-NIR spectrum of HMCD **3**-adsorbed TLC plates and exposed to PhCl vapor.

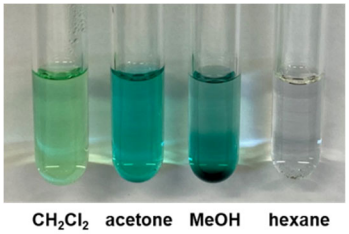


Figure S3. Photograph of various solutions (0.5 ml) including HMCD **3** (31 mg).

Computational Details. All calculations were performed using computational chemistry software package Gaussian 16 ver. B.01[2] using Super Computers at Research Center for Computational Science, Okazaki, Japan.

a) Ground State Details.

Ground state geometries of **3** and **3'** were computed at RB3LYP/6-31+G(d,p) level of theory. At the optimized structures, no imaginary frequency was found through the frequency analysis. All coordinates are reported as XYZ Cartesian coordinates. And computed E (RB3LYP) and sum of zero-point and thermal correction energies of optimized structures are shown.

3

E (RB3LYP) = -1810.682746 a.u.

Sum of electronic and thermal Energies = -1810.044293 a.u.

Imaginary Frequency = 0

Table S1. Cartesian coordinates of the optimized **3**.

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	7.205471	0.07864	-0.18412
C	6.674557	-1.20701	-0.04791
C	7.523434	-2.30607	-0.0221
C	8.905616	-2.0978	-0.13413
C	9.419682	-0.80411	-0.26973
C	8.574457	0.311587	-0.29721
C	4.934923	0.395936	-0.04864
H	7.131595	-3.31364	0.083054
H	9.581508	-2.94643	-0.11534
H	10.4915	-0.65701	-0.35538
H	8.990493	1.307233	-0.4027
N	6.139476	1.01029	-0.18151
C	6.318352	2.451829	-0.30385
H	7.377986	2.676764	-0.40194
H	5.798495	2.828084	-1.19032
H	5.934116	2.962252	0.584852
C	5.159641	-1.12338	0.050302
C	4.503407	-1.87946	-1.13303

H	4.791873	-2.93386	-1.09266
H	3.413007	-1.82665	-1.09597
H	4.836063	-1.47445	-2.09288
C	4.676757	-1.68803	1.410411
H	3.591064	-1.62715	1.514061
H	4.965154	-2.74036	1.488211
H	5.133572	-1.14965	2.245536
C	3.740644	1.121192	-0.01712
H	3.824943	2.19743	-0.10919
C	2.459674	0.568663	0.111755
H	2.381547	-0.5069	0.183346
C	1.254205	1.283781	0.137449
C	-0.000007	0.634044	0.201922
C	-1.25421	1.283798	0.137661
C	-2.45968	0.56867	0.111953
H	-2.38153	-0.50691	0.183307
C	-3.74066	1.121216	-0.0167
H	-3.82497	2.19747	-0.10858
C	-4.93494	0.395957	-0.0483
C	-5.15964	-1.12337	0.050391
C	-6.67454	-1.20703	-0.04807
C	-7.20547	0.078644	-0.18404
C	-7.52339	-2.30611	-0.02262
C	-8.57444	0.311585	-0.29724
C	-8.90556	-2.09785	-0.13477
H	-7.13154	-3.31369	0.082356
C	-9.41965	-0.80414	-0.27013
H	-8.99049	1.307245	-0.40256
H	-9.58144	-2.9465	-0.11625
H	-10.4915	-0.65704	-0.35587
N	-6.13949	1.010316	-0.18112
C	-4.67699	-1.68821	1.410514
H	-4.96542	-2.74055	1.488129
H	-3.59132	-1.62737	1.514362
H	-5.13394	-1.14993	2.245628
C	-4.50317	-1.87927	-1.13292
H	-3.41278	-1.82639	-1.09567
H	-4.79157	-2.93369	-1.09273

H	-4.83569	-1.47417	-2.09278
C	-6.31838	2.451875	-0.3032
H	-5.93425	2.962137	0.585629
H	-5.79844	2.828307	-1.18956
H	-7.37801	2.676807	-0.40137
C	1.257056	2.802177	0.052552
H	2.138969	3.193901	0.568894
H	1.349366	3.109592	-0.99982
C	-1.25712	2.802212	0.053005
H	-1.34991	3.109786	-0.99928
H	-2.13882	3.193823	0.569796
C	0.000087	3.420397	0.66324
H	0.000068	4.504162	0.508242
H	0.000287	3.249795	1.746983
Cl	-0.000038	-1.1364	0.341466

3'

E (RB3LYP) = -1810.955053 a.u.

Sum of electronic and thermal Energies = -1810.303001 a.u.

Imaginary Frequency = 0

Table S2. Cartesian coordinates of the optimized **3'**.

	Coordinates (Angstroms)		
Atom	X	Y	Z
C	-7.23676	0.132693	0.268329
C	-6.70638	-1.13771	0.118094
C	-7.57222	-2.22945	0.218863
C	-8.92745	-2.00101	0.473557
C	-9.42597	-0.70074	0.632963
C	-8.575	0.402637	0.526792
C	-4.88516	0.37263	-0.01314
H	-7.2045	-3.24447	0.106929
H	-9.60507	-2.84463	0.554733
H	-10.4794	-0.54518	0.839515
H	-8.95668	1.411847	0.648685
N	-6.17781	1.160412	0.093298

C	-6.44201	2.068383	-1.09273
H	-7.39714	2.570375	-0.93712
H	-5.63691	2.798463	-1.16687
H	-6.48157	1.446917	-1.9861
C	-5.2024	-1.12208	-0.11982
C	-4.48401	-1.94573	0.980332
H	-4.82775	-2.98293	0.939969
H	-3.40129	-1.95385	0.839677
H	-4.70164	-1.55417	1.977643
C	-4.85643	-1.68372	-1.52488
H	-3.78194	-1.63118	-1.71887
H	-5.15735	-2.73343	-1.58562
H	-5.37636	-1.13812	-2.31732
C	-3.73513	1.076315	0.027306
H	-3.81523	2.152298	0.165231
C	-2.4029	0.529886	-0.10151
H	-2.33091	-0.52761	-0.31238
C	-1.23818	1.237432	0.019853
C	0.064577	0.582405	-0.10428
C	1.274958	1.24424	-0.03425
C	2.523267	0.522928	-0.04602
H	2.451953	-0.55108	-0.14241
C	3.764978	1.091988	0.075144
H	3.838008	2.16786	0.180694
C	5.000259	0.373159	0.07564
C	5.249822	-1.13027	-0.08428
C	6.764178	-1.18404	-0.01304
C	7.267494	0.107204	0.165982
C	7.642176	-2.25795	-0.09586
C	8.630164	0.384812	0.2643
C	9.017124	-2.00687	0.001819
H	7.282116	-3.27276	-0.23402
C	9.501939	-0.70354	0.178527
H	9.020753	1.387005	0.397586
H	9.717961	-2.83273	-0.06122
H	10.57086	-0.53304	0.249426
N	6.167009	1.007131	0.21923
C	4.752891	-1.64914	-1.46051

H	5.063904	-2.69012	-1.5803
H	3.66435	-1.612	-1.5411
H	5.183071	-1.07197	-2.2835
C	4.624482	-1.94027	1.083956
H	3.532913	-1.91374	1.060376
H	4.937248	-2.98405	0.998034
H	4.961613	-1.56601	2.054416
C	6.331081	2.455583	0.402107
H	6.040887	2.985581	-0.50867
H	5.727229	2.797196	1.244815
H	7.374583	2.669691	0.617025
C	-1.19596	2.720578	0.338122
H	-2.12809	3.205916	0.040526
H	-1.11115	2.844551	1.427514
C	1.299046	2.759036	0.077402
H	1.538292	3.035109	1.114838
H	2.11163	3.150482	-0.54329
C	-0.01552	3.410689	-0.34671
H	-0.0028	4.474486	-0.09252
H	-0.12933	3.340688	-1.43516
Cl	0.051577	-1.16823	-0.32249
H	-6.13526	1.7512	0.93111

Reference

[1] Gaussian 16, Revision B.01, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.