SUPPORTING INFORMATION

Naphthalene Imides as Novel p-type Sensitizers for NiO based p-type Dye Sensitized Solar Cells

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Geometry optimized structures and electronic properties of both synthesized molecules were performed by using Gaussian 09 package program with DFT/B3LYP method and 6−31+G(d) basis set.

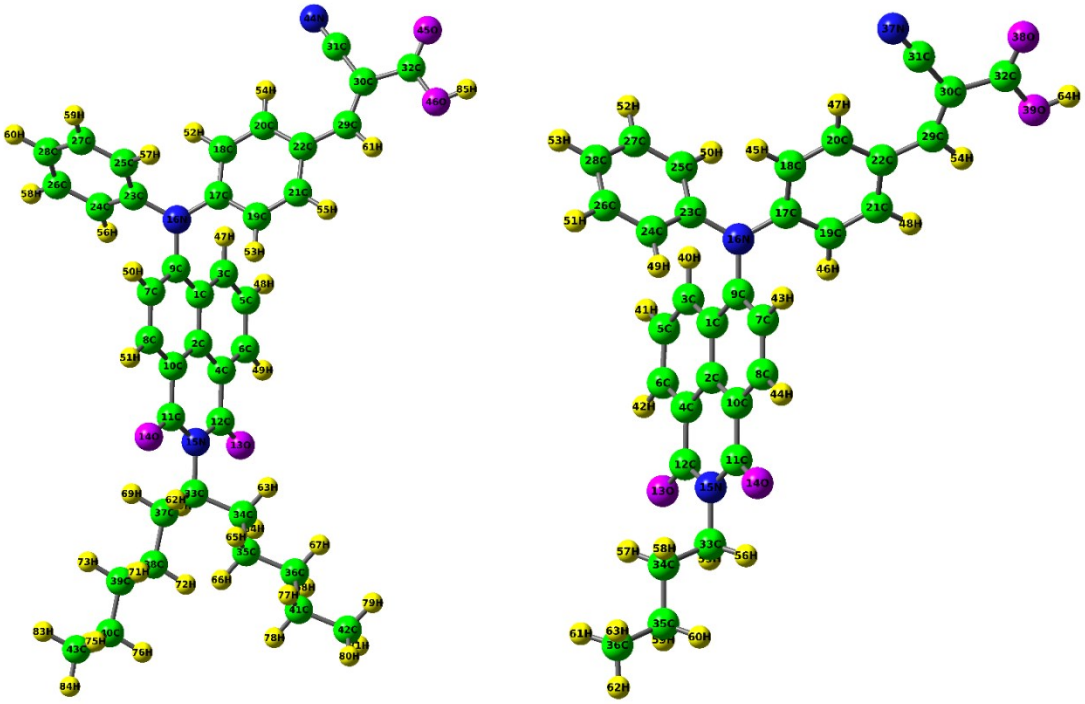


Fig. S-1 Schematic plot of the molecular structures with labels and atomic symbols: the first molecule (left) and the second molecule (right).

Table S-1 Bond lengths, bond angles and dihedral angles of optimized geometry for the first synthesized molecule (85 atoms) are calculated at DFT/B3LYP/6−31+G(d).

	Bond length (Å)		Bond angle (°)		Dihedral angle (°)
1C − 2C	1.432	2C − 1C − 3C	118.277	3C − 1C − 2C − 4C	1.803
1C − 3C	1.421	1C − 2C − 4C	119.790	2C − 1C − 3C − 5C	−1.377
2C − 4C	1.419	1C − 3C − 5C	120.831	1C − 2C − 4C − 6C	−0.874
3C − 5C	1.382	2C − 4C − 6C	120.308	5C − 3C − 1C − 7C	−175.638
4C − 6C	1.385	3C − 1C − 7C	152.965	3C − 1C − 7C − 8C	174.090
1C − 7C	2.444	1C − 7C − 8C	90.590	3C − 1C − 7C − 9C	−7.211
7C − 8C	1.406	1C − 7C − 9C	30.562	1C − 7C − 8C − 10C	1.129
7C − 9C	1.388	7C − 8C − 10C	120.498	7C − 8C − 10C − 11C	179.202
8C − 10C	1.386	8C − 10C − 11C	119.408	1C − 2C − 4C − 12C	179.632
10C − 11C	1.485	2C − 4C − 12C	120.490	2C − 4C − 12C − 13O	−179.663
4C − 12C	1.488	4C − 12C − 13O	121.500	8C − 10C − 11C − 14O	0.328
12C − 13O	1.226	10C − 11C − 14O	121.362	2C − 4C − 12C − 15N	0.132
11C − 14O	1.227	4C − 12C − 15N	117.684	1C − 7C − 9C − 16N	178.281
12C − 15N	1.402	7C − 9C − 16N	119.528	7C − 9C − 16N − 17C	117.892
9C − 16N	1.429	9C − 16N − 17C	120.725	9C − 16N − 17C − 18C	158.377
16N − 17C	1.403	16N − 17C − 18C	120.689	9C − 16N − 17C − 19C	−20.611
17C − 18C	1.414	16N − 17C − 19C	121.037	16N − 17C − 18C − 20C	−179.234
17C − 19C	1.410	17C − 18C − 20C	121.087	16N − 17C − 19C − 21C	178.977
18C − 20C	1.385	17C − 19C − 21C	120.250	17C − 19C − 21C − 22C	0.266
19C − 21C	1.386	19C − 21C − 22C	122.142	7C − 9C − 16N − 23C	−52.147
21C − 22C	1.415	9C − 16N − 23C	117.438	9C − 16N − 23C − 24C	−53.584
16N − 23C	1.434	16N − 23C − 24C	119.436	9C − 16N − 23C − 25C	125.109
23C − 24C	1.402	16N − 23C − 25C	120.897	16N − 23C − 24C − 26C	178.596
23C − 25C	1.403	23C − 24C − 26C	120.050	16N − 23C − 25C − 27C	−179.341
24C − 26C	1.396	23C − 25C − 27C	119.959	23C − 24C − 26C − 28C	0.682
25C − 27C	1.396	24C − 26C − 28C	120.353	19C − 21C − 22C − 29C	179.798
26C − 28C	1.398	21C − 22C − 29C	117.193	21C − 22C − 29C − 30C	−179.895
22C − 29C	1.447	22C − 29C − 30C	131.999	22C − 29C − 30C − 31C	−0.045
29C − 30C	1.370	29C − 30C − 31C	124.240	22C − 29C − 30C − 32C	179.963
30C − 31C	1.430	29C − 30C − 32C	121.337	4C − 12C − 15N − 33C	179.835
30C − 32C	1.485	12C − 15N − 33C	118.717	12C − 15N − 33C − 34C	59.448
15N − 33C	1.499	15N − 33C − 34C	111.759	15N − 33C − 34C − 35C	133.899
33C − 34C	1.551	33C − 34C − 35C	113.215	33C − 34C − 35C − 36C	−179.834
34C − 35C	1.538	34C − 35C − 36C	112.761	12C − 15N − 33C − 37C	−70.154
35C − 36C	1.535	15N − 33C − 37C	109.729	15N − 33C − 37C − 38C	−170.504
33C − 37C	1.543	33C − 37C − 38C	114.140	33C − 37C − 38C − 39C	174.640
37C − 38C	1.536	37C − 38C − 39C	112.476	37C − 38C − 39C − 40C	178.677
38C − 39C	1.536	38C − 39C − 40C	113.559	34C − 35C − 36C − 41C	179.733
39C − 40C	1.535	35C − 36C − 41C	113.607	35C − 36C − 41C − 42C	−179.385
36C − 41C	1.535	36C − 41C − 42C	113.211	38C − 39C − 40C − 43C	179.732
41C − 42C	1.534	39C − 40C − 43C	113.211	29C − 30C − 31C − 44N	−0.087
40C − 43C	1.534	30C − 31C − 44N	178.926	29C − 30C − 32C − 45O	179.987
31C − 44N	1.164	30C − 32C − 45O	124.582	29C − 30C − 32C − 46O	−0.009
32C − 45O	1.215	30C − 32C − 46O	113.275	2C − 1C − 3C − 47H	178.255
32C − 46O	1.362	1C − 3C − 47H	119.422	1C − 3C − 5C − 48H	179.803
3C − 47H	1.084	3C − 5C − 48H	119.779	2C − 4C − 6C − 49H	−179.903
5C − 48H	1.086	4C − 6C − 49H	118.808	3C − 1C − 7C − 50H	−5.451
6C − 49H	1.085	1C − 7C − 50H	149.668	1C − 7C − 8C − 51H	−179.932
7C − 50H	1.086	7C − 8C − 51H	120.566	16N − 17C − 18C − 52H	0.180
8C − 51H	1.085	17C − 18C − 52H	119.622	16N − 17C − 19C − 53H	−1.631
18C − 52H	1.085	17C − 19C − 53H	119.993	17C − 18C − 20C − 54H	179.455
19C − 53H	1.085	18C − 20C − 54H	118.353	17C − 19C − 21C − 55H	179.473
20C − 54H	1.083	19C − 21C − 55H	118.798	16N − 23C − 24C − 56H	−1.324

21C − 55H	1.088	23C − 24C − 56H	119.567	16N − 23C − 25C − 57H	0.721
24C − 56H	1.086	23C − 25C − 57H	119.768	23C − 24C − 26C − 58H	−179.984
25C − 57H	1.086	24C − 26C − 58H	119.477	23C − 25C − 27C − 59H	−179.883
26C − 58H	1.087	25C − 27C − 59H	119.432	24C − 26C − 28C − 60H	179.559
27C − 59H	1.087	26C − 28C − 60H	120.233	21C − 22C − 29C − 61H	0.103
28C − 60H	1.086	22C − 29C − 61H	114.038	12C − 15N − 33C − 62H	175.392
29C − 61H	1.087	15N − 33C − 62H	103.001	15N − 33C − 34C − 63H	13.273
33C − 62H	1.091	33C − 34C − 63H	109.196	15N − 33C − 34C − 64H	−102.275
34C − 63H	1.097	33C − 34C − 64H	109.944	33C − 34C − 35C − 65H	−58.210
34C − 64H	1.096	34C − 35C − 65H	109.137	33C − 34C − 35C − 66H	57.911
35C − 65H	1.100	34C − 35C − 66H	110.199	34C − 35C − 36C − 67H	57.563
35C − 66H	1.099	35C − 36C − 67H	109.222	34C − 35C − 36C − 68H	−58.009
36C − 67H	1.101	35C − 36C − 68H	109.343	15N − 33C − 37C − 69H	−49.853
36C − 68H	1.101	33C − 37C − 69H	107.689	15N − 33C − 37C − 70H	66.344
37C − 69H	1.099	33C − 37C − 70H	109.455	33C − 37C − 38C − 71H	52.869
37C − 70H	1.095	37C − 38C − 71H	109.775	33C − 37C − 38C − 72H	−63.911
38C − 71H	1.100	37C − 38C − 72H	109.899	37C − 38C − 39C − 73H	−59.148
38C − 72H	1.099	38C − 39C − 73H	109.245	37C − 38C − 39C − 74H	56.523
39C − 73H	1.101	38C − 39C − 74H	109.248	38C − 39C − 40C − 75H	57.543
39C − 74H	1.101	39C − 40C − 75H	109.256	38C − 39C − 40C − 76H	−58.124
40C − 75H	1.100	39C − 40C − 76H	109.191	35C − 36C − 41C − 77H	−57.201
40C − 76H	1.100	36C − 41C − 77H	109.229	35C − 36C − 41C − 78H	58.433
41C − 77H	1.100	36C − 41C − 78H	109.223	36C − 41C − 42C − 79H	59.960
41C − 78H	1.100	41C − 42C − 79H	111.145	36C − 41C − 42C − 80H	−179.927
42C − 79H	1.098	41C − 42C − 80H	111.443	36C − 41C − 42C − 81H	−59.783
42C − 80H	1.097	41C − 42C − 81H	111.193	39C − 40C − 43C − 82H	59.707
42C − 81H	1.098	40C − 43C − 82H	111.177	39C − 40C − 43C − 83H	−60.073
43C − 82H	1.098	40C − 43C − 83H	111.173	39C − 40C − 43C − 84H	179.827
43C − 83H	1.098	40C − 43C − 84H	111.423	30C − 32C − 46O − 85H	−179.981
43C − 84H	1.097	32C − 46O − 85H	106.279		
46O − 85H	0.975				

Table S-2 Bond lengths, bond angles and dihedral angles of optimized geometry for the second synthesized molecule (64 atoms) are calculated at DFT/B3LYP/6−31+G(d).

	Bond length (Å)		Bond angle (°)		Dihedral angle (°)
1C − 2C	1.432	2C − 1C − 3C	118.313	3C − 1C − 2C − 4C	−1.603
1C − 3C	1.421	1C − 2C − 4C	119.687	2C − 1C − 3C − 5C	1.162
2C − 4C	1.420	1C − 3C − 5C	120.873	1C − 2C − 4C − 6C	0.790
3C − 5C	1.382	2C − 4C − 6C	120.347	5C − 3C − 1C − 7C	176.154
4C − 6C	1.385	3C − 1C − 7C	152.891	3C − 1C − 7C − 8C	−174.935
1C − 7C	2.444	1C − 7C − 8C	90.599	3C − 1C − 7C − 9C	6.050
7C − 8C	1.406	1C − 7C − 9C	30.550	1C − 7C − 8C − 10C	−0.890
7C − 9C	1.389	7C − 8C − 10C	120.476	7C − 8C − 10C − 11C	−179.141
8C − 10C	1.385	8C − 10C − 11C	119.472	1C − 2C − 4C − 12C	−179.545
10C − 11C	1.484	2C − 4C − 12C	120.417	2C − 4C − 12C − 13O	178.628
4C − 12C	1.486	4C − 12C − 13O	122.203	8C − 10C − 11C − 14O	0.952
12C − 13O	1.226	10C − 11C − 14O	122.250	2C − 4C − 12C − 15N	−1.619
11C − 14O	1.227	4C − 12C − 15N	117.171	1C − 7C − 9C − 16N	179.851
12C − 15N	1.403	7C − 9C − 16N	119.533	7C − 9C − 16N − 17C	52.762
9C − 16N	1.429	9C − 16N − 17C	119.287	9C − 16N − 17C − 18C	−143.614
16N − 17C	1.407	16N − 17C − 18C	121.551	9C − 16N − 17C − 19C	36.449
17C − 18C	1.412	16N − 17C − 19C	120.128	16N − 17C − 18C − 20C	−179.579
17C − 19C	1.411	17C − 18C − 20C	121.035	16N − 17C − 19C − 21C	179.814

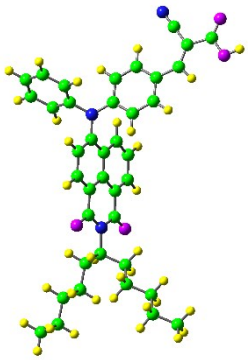
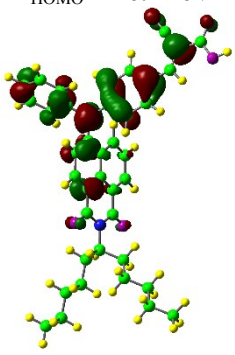
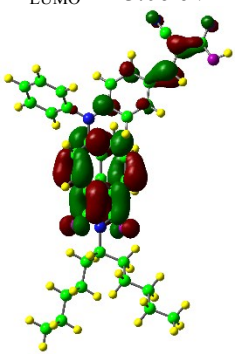
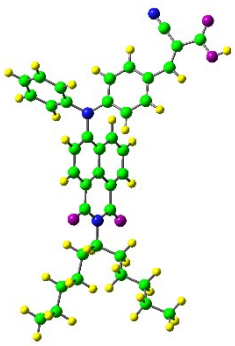
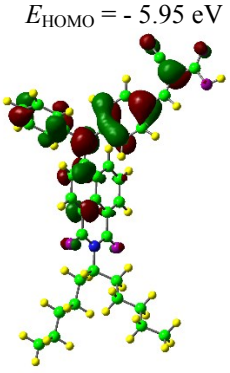
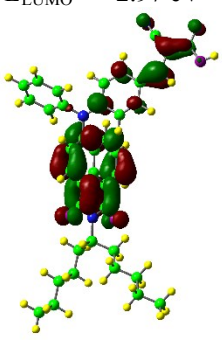
18C − 20C	1.387	17C − 19C − 21C	120.296	17C − 18C − 20C − 22C	−0.213
19C − 21C	1.385	18C − 20C − 22C	121.220	7C − 9C − 16N − 23C	−115.870
20C − 22C	1.415	9C − 16N − 23C	118.626	9C − 16N − 23C − 24C	36.352
16N − 23C	1.432	16N − 23C − 24C	120.392	9C − 16N − 23C − 25C	−142.219
23C − 24C	1.402	16N − 23C − 25C	120.132	16N − 23C − 24C − 26C	−178.524
23C − 25C	1.405	23C − 24C − 26C	120.066	16N − 23C − 25C − 27C	179.343
24C − 26C	1.397	23C − 25C − 27C	120.100	23C − 24C − 26C − 28C	−0.685
25C − 27C	1.395	24C − 26C − 28C	120.490	18C − 20C − 22C − 29C	179.939
26C − 28C	1.397	20C − 22C − 29C	125.781	20C − 22C − 29C − 30C	−0.594
22C − 29C	1.447	22C − 29C − 30C	132.024	22C − 29C − 30C − 31C	−0.055
29C − 30C	1.370	29C − 30C − 31C	124.255	22C − 29C − 30C − 32C	−179.962
30C − 31C	1.430	29C − 30C − 32C	121.315	4C − 12C − 15N − 33C	−179.443
30C − 32C	1.486	12C − 15N − 33C	117.639	12C − 15N − 33C − 34C	−89.186
15N − 33C	1.478	15N − 33C − 34C	112.700	15N − 33C − 34C − 35C	179.820
33C − 34C	1.534	33C − 34C − 35C	111.873	33C − 34C − 35C − 36C	179.946
34C − 35C	1.535	34C − 35C − 36C	112.854	29C − 30C − 31C − 37N	−1.772
35C − 36C	1.534	30C − 31C − 37N	178.927	29C − 30C − 32C − 38O	179.904
31C − 37N	1.164	30C − 32C − 38O	124.566	29C − 30C − 32C − 39O	−0.096
32C − 38O	1.215	30C − 32C − 39O	113.258	2C − 1C − 3C − 40H	−178.762
32C − 39O	1.362	1C − 3C − 40H	119.330	1C − 3C − 5C − 41H	−179.813
3C − 40H	1.084	3C − 5C − 41H	119.803	2C − 4C − 6C − 42H	179.989
5C − 41H	1.086	4C − 6C − 42H	118.798	3C − 1C − 7C − 43H	5.533
6C − 42H	1.085	1C − 7C − 43H	149.702	1C − 7C − 8C − 44H	−179.660
7C − 43H	1.086	7C − 8C − 44H	120.589	16N − 17C − 18C − 45H	1.163
8C − 44H	1.085	17C − 18C − 45H	119.726	16N − 17C − 19C − 46H	0.352
18C − 45H	1.085	17C − 19C − 46H	119.815	17C − 18C − 20C − 47H	−179.232
19C − 46H	1.085	18C − 20C − 47H	118.317	17C − 19C − 21C − 48H	−179.398
20C − 47H	1.083	19C − 21C − 48H	118.895	16N − 23C − 24C − 49H	1.553
21C − 48H	1.088	23C − 24C − 49H	119.790	16N − 23C − 25C − 50H	−0.699
24C − 49H	1.086	23C − 25C − 50H	119.671	23C − 24C − 26C − 51H	179.954
25C − 50H	1.086	24C − 26C − 51H	119.345	23C − 25C − 27C − 52H	179.770
26C − 51H	1.087	25C − 27C − 52H	119.392	24C − 26C − 28C − 53H	−179.611
27C − 52H	1.087	26C − 28C − 53H	120.320	20C − 22C − 29C − 54H	179.482
28C − 53H	1.086	22C − 29C − 54H	114.022	12C − 15N − 33C − 55H	32.298
29C − 54H	1.087	15N − 33C − 55H	106.785	12C − 15N − 33C − 56H	149.319
33C − 55H	1.091	15N − 33C − 56H	106.759	15N − 33C − 34C − 57H	58.363
33C − 56H	1.091	33C − 34C − 57H	109.061	15N − 33C − 34C − 58H	−58.710
34C − 57H	1.098	33C − 34C − 58H	109.072	33C − 34C − 35C − 59H	−58.079
34C − 58H	1.098	34C − 35C − 59H	109.292	33C − 34C − 35C − 60H	57.965
35C − 59H	1.100	34C − 35C − 60H	109.302	34C − 35C − 36C − 61H	59.901
35C − 60H	1.100	35C − 36C − 61H	111.162	34C − 35C − 36C − 62H	179.942
36C − 61H	1.098	35C − 36C − 62H	111.270	34C − 35C − 36C − 63H	−60.018
36C − 62H	1.097	35C − 36C − 63H	111.164	30C − 32C − 39O − 64H	−179.966
36C − 63H	1.098	32C − 39O − 64H	106.304		
39O − 64H	0.975				

In the gas phase, ionization energy is the minimum energy required to remove an electron from a molecule. Electron affinity is defined as the energy given off when an electron is added to a molecule. According to Koopman's theorem [S-1]. ionization energy (I) is $I = -E_{HOMO}$ and electron affinity (A) is defined as $A = -E_{LUMO}$. Electronegativity ( ) is defined as $\chi = \frac{I+A}{2}$. Chemical hardness ( ) is $\eta = \frac{I-A}{2}$. Chemical softness (S) is $S = \frac{1}{\eta}$. Electron chemical potential (μ) is defined as $\mu = -\chi$ [S-1].

Table S-3 The electronic properties of the synthesized molecules (85 and 64 atoms) are calculated with DFT/B3LYP/6−31+G(d) in the gas-phase. These values depend on the energy levels of HOMO and LUMO for both molecules.

Property	85 atoms	64 atoms
E_{HOMO} (eV)	−6.11059	−6.10433
E_{LUMO} (eV)	−3.05938	−3.11081
ΔE_{gap} (eV)	3.05121	2.99352
I (eV)	6.11059	6.10433
A (eV)	3.05938	3.11081
χ (eV)	4.58499	4.60757
η (eV)	1.52561	1.49676
S (eV^{-1})	0.65548	0.66811
μ (eV)	-4.58499	-4.60757

Table S-4 The total energies of the synthesized molecules (85 atoms) are calculated with solvents and gas-phase (default) at DFT/B3LYP/6−31+G(d) method.

Solvent	Optimized Geometry	HOMO(163)	LUMO(164)
Gas-phase (default)		E_{HOMO} = - 6.11 eV 	E_{LUMO} = - 3.06 eV 
Chlorobenzene		E_{HOMO} = - 5.95 eV 	E_{LUMO} = - 2.97 eV 

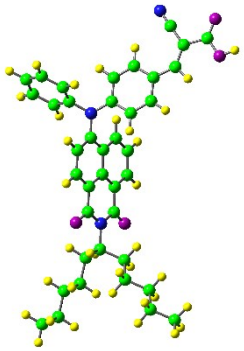
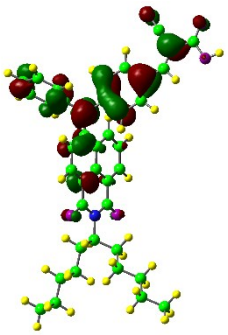
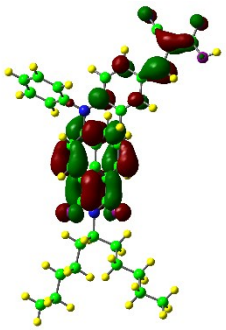
Acetonitrile		E_{HOMO} = - 5.90 eV 	E_{LUMO} = - 2.95 eV 

Table S-5 The total energies of the synthesized molecules (64 atoms) are calculated with solvents and gas-phase (default) at DFT/B3LYP/6−31+G(d) method.

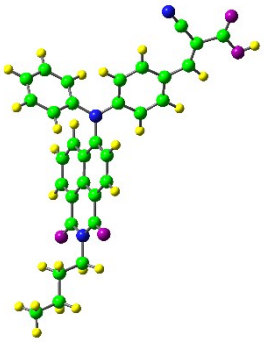
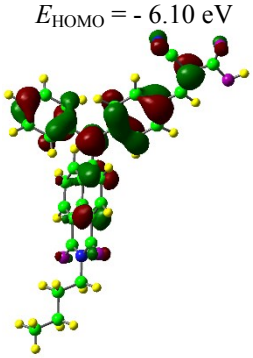
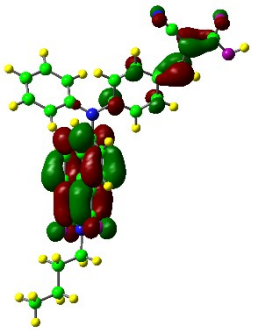
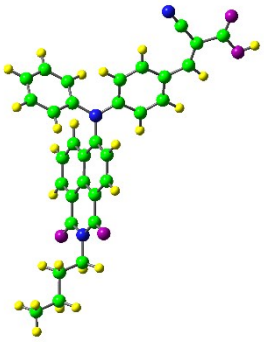
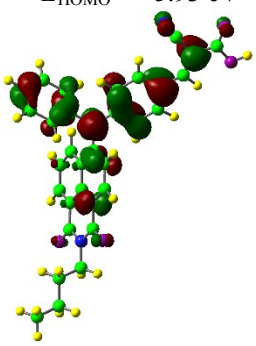
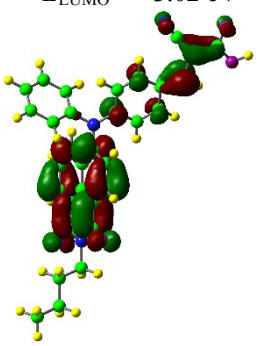
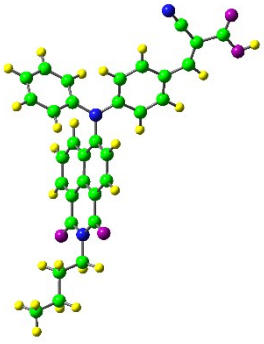
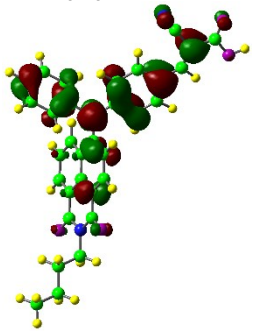
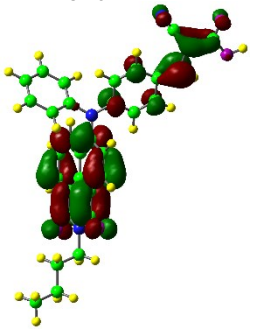
Solvent	Optimized Geometry	HOMO(135)	LUMO(136)
Gas-phase (default)		E_{HOMO} = - 6.10 eV 	E_{LUMO} = - 3.11 eV 
Chlorobenzene		E_{HOMO} = - 5.93 eV 	E_{LUMO} = - 3.02 eV 
Acetonitrile		E_{HOMO} = - 5.90 eV 	E_{LUMO} = - 3.01 eV 

Table S-6 In the solvent of chlorobenzene, the excitation energies and absorption results of the first synthesized molecule (85 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	503.03	2.4647	0.4813	HOMO → LUMO (95.20%) HOMO → LUMO+1 (3.90%)	5.9410
2nd ($S_0 \rightarrow S_2$)	432.85	2.8644	0.5337	HOMO → LUMO (4.00%) HOMO → LUMO+1 (93.60%)	
3rd ($S_0 \rightarrow S_3$)	353.01	3.5122	0.1259	HOMO−1 → LUMO (95.40%)	
4th ($S_0 \rightarrow S_4$)	334.79	3.7034	0.2535	HOMO−1 → LUMO+1 (96.66%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref.S-2, [e] Dipole moment

Table S-7 In the solvent of acetonitrile, the excitation energies and absorption results of the first synthesized molecule (85 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	504.03	2.4599	0.4602	HOMO → LUMO (93.46%) HOMO → LUMO+1 (5.64%)	6.2803
2nd ($S_0 \rightarrow S_2$)	433.80	2.8581	0.5056	HOMO → LUMO (5.80%) HOMO → LUMO+1 (91.52%)	
3rd ($S_0 \rightarrow S_3$)	353.41	3.5082	0.1178	HOMO−1 → LUMO (95.04%)	
4th ($S_0 \rightarrow S_4$)	336.13	3.6886	0.2474	HOMO−1 → LUMO+1 (96.68%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-8 In the solvent of tetrahydrofuran (thf), the excitation energies and absorption results of the first synthesized molecule (85 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	502.41	2.4678	0.4625	HOMO → LUMO (94.44%) HOMO → LUMO+1 (4.64%)	6.0277
2nd ($S_0 \rightarrow S_2$)	432.06	2.8696	0.5216	HOMO → LUMO (4.78%) HOMO → LUMO+1 (92.64%)	
3rd ($S_0 \rightarrow S_3$)	352.67	3.5156	0.1219	HOMO−1 → LUMO (95.10%)	
4th ($S_0 \rightarrow S_4$)	334.95	3.7015	0.2479	HOMO−1 → LUMO+1 (96.48%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-9 In the solvent of chloroform, the excitation energies and absorption results of the first synthesized molecule (85 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	501.32	2.4732	0.4632	HOMO → LUMO (95.02%) HOMO → LUMO+1 (4.06%)	5.8670
2nd ($S_0 \rightarrow S_2$)	430.85	2.8777	0.5327	HOMO → LUMO (4.18%) HOMO → LUMO+1 (93.30%)	
3rd ($S_0 \rightarrow S_3$)	352.23	3.5200	0.1249	HOMO−1 → LUMO (95.10%)	
4th ($S_0 \rightarrow S_4$)	334.18	3.7101	0.2474	HOMO−1 → LUMO+1 (96.14%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-10 In the solvent of chlorobenzene, the excitation energies and absorption results of the first synthesized molecule (64 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	512.98	2.4169	0.5458	HOMO → LUMO (93.46%) HOMO → LUMO+1 (5.64%)	6.3793
2nd ($S_0 \rightarrow S_2$)	436.17	2.8425	0.5135	HOMO → LUMO (5.80%) HOMO → LUMO+1 (91.52%)	
3rd ($S_0 \rightarrow S_3$)	351.20	3.5304	0.1256	HOMO−1 → LUMO (95.04%)	
4th ($S_0 \rightarrow S_4$)	330.10	3.7559	0.0052	HOMO−5 → LUMO (26.62%) HOMO−5 → LUMO+1 (7.16%) HOMO−4 → LUMO (10.68%) HOMO−2 → LUMO (31.70%) HOMO−1 → LUMO+1 (3.92%) HOMO → LUMO+2 (10.74%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-11 In the solvent of acetonitrile, the excitation energies and absorption results of the first synthesized molecule (64 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	513.96	2.4123	0.5191	HOMO → LUMO (94.10%) HOMO → LUMO+1 (4.98%)	6.7348
2nd ($S_0 \rightarrow S_2$)	437.30	2.8352	0.4947	HOMO → LUMO (5.14%) HOMO → LUMO+1 (92.62%)	
3rd ($S_0 \rightarrow S_3$)	352.23	3.5200	0.1126	HOMO−1 → LUMO (93.98%)	
4th ($S_0 \rightarrow S_4$)	330.34	3.7533	0.0094	HOMO−4 → LUMO (17.58%) HOMO−2 → LUMO (47.84%) HOMO−2 → LUMO+1 (2.88%) HOMO−1 → LUMO+1 (7.66%) HOMO → LUMO+2 (13.88%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-12 In the solvent of tetrahydrofuran (thf), the excitation energies and absorption results of the second synthesized molecule (64 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	512.20	2.4206	0.5239	HOMO → LUMO (94.90%) HOMO → LUMO+1 (4.16%)	6.4706
2nd ($S_0 \rightarrow S_2$)	435.43	2.8474	0.5067	HOMO → LUMO (4.32%) HOMO → LUMO+1 (93.50%)	
3rd ($S_0 \rightarrow S_3$)	351.12	3.5311	0.1184	HOMO−1 → LUMO (93.98%)	
4th ($S_0 \rightarrow S_4$)	329.87	3.7586	0.0079	HOMO−6 → LUMO (3.80%) HOMO−6 → LUMO+1 (2.70%) HOMO−5 → LUMO (3.96%) HOMO−4 → LUMO (16.28%) HOMO−2 → LUMO (41.80%) HOMO−2 → LUMO+1 (2.34%) HOMO−1 → LUMO+1 (5.76%) HOMO → LUMO+2 (15.30%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-13 In the solvent of chloroform, the excitation energies and absorption results of the second synthesized molecule (64 atoms) are calculated by using time−dependent density functional theory (TD−DFT) with B3LYP/6−31+G(d).

Excited States	λ^a (nm)	E^b (eV)	f^c	Transitions[d]	$\Delta\mu^e$ (Debye)
1st ($S_0 \rightarrow S_1$)	511.00	2.4263	0.5263	HOMO → LUMO (95.38%) HOMO → LUMO+1 (3.68%)	6.3012
2nd ($S_0 \rightarrow S_2$)	434.14	2.8558	0.5154	HOMO−2 → LUMO (3.82%) HOMO−1 → LUMO+1 (94.04%)	
3rd ($S_0 \rightarrow S_3$)	350.40	3.5383	0.1220	HOMO → LUMO (2.02%) HOMO → LUMO+1 (93.96%)	
4th ($S_0 \rightarrow S_4$)	330.62	3.7500	0.0015	HOMO−5 → LUMO (58.84%) HOMO−5 → LUMO+1 (16.10%) HOMO−4 → LUMO (2.66%) HOMO−2 → LUMO (12.30%) HOMO → LUMO+2 (3.12%)	

[a] Wavelength of excited states, [b] Excitation energy, [c] Oscillator strength, [d] Data given in parentheses are (CI coefficient)^2×100% Ref. S-2, [e] Dipole moment

Table S-14 The total energies of the synthesized molecules (85 and 64 atoms) are calculated with four solvents and gas-phase (default) at DFT/B3LYP/6−31+G(d) method.

(85 atoms)		(64 atoms)	
Solvent	Total Energy	Solvent	Total Energy
Gas-phase (default)	−53736.83 eV	Gas-phase (default)	−46248.54 eV
Chlorobenzene	−53737.45 eV	Chlorobenzene	−46249.18 eV
Acetonitrile	−53737.61 eV	Acetonitrile	−46249.34 eV
Tetrahydrofuran	−53737.49 eV	Tetrahydrofuran	−46249.22 eV
Chloroform	−53737.40 eV	Chloroform	−46249.14 eV

Table S-15 The light-harvesting efficiencies of the synthesized molecules (85 and 64 atoms) are calculated with solvents and gas-phase (default) at DFT/B3LYP/6−31+G(d) method.

Molecules	Solvent	λ (nm)	Oscillator strength	LHE(%) ($S_0 \rightarrow S_1$)
85 atoms	Gas-phase	484.74	0.3054	51
	Chlorobenzene	503.03	0.4813	67
	Acetonitrile	504.03	0.4602	65
	Tetrahydrofuran	502.41	0.4625	66
	Chloroform	501.32	0.4632	66
64 atoms	Gas-phase	491.32	0.3559	56
	Chlorobenzene	512.98	0.5458	72
	Acetonitrile	513.96	0.5191	70
	Tetrahydrofuran	512.20	0.5239	70
	Chloroform	511.00	0.5263	70

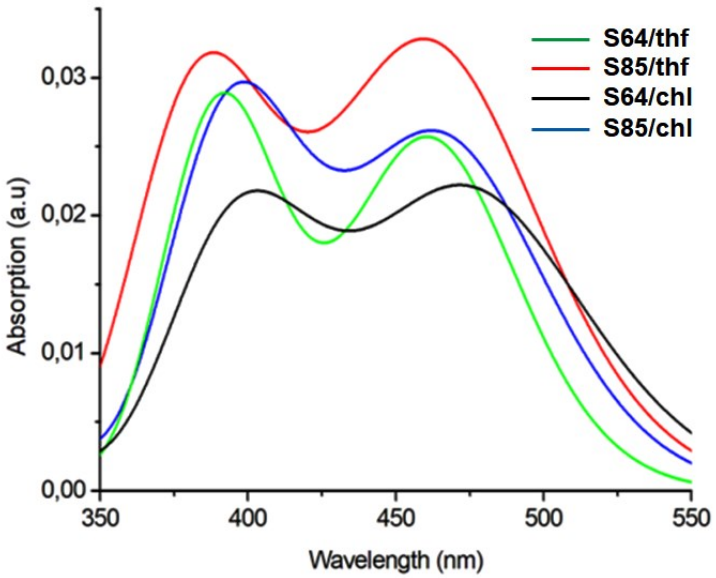


Fig. S-2 For synthesized molecules (64 atoms) and (85 atoms). Plot of absorption versus wavelength are calculated by using TD-DFT with B3LYP/6-31+G(d) in solvents of tetrahydrofuran (thf) and chloroform (chl).

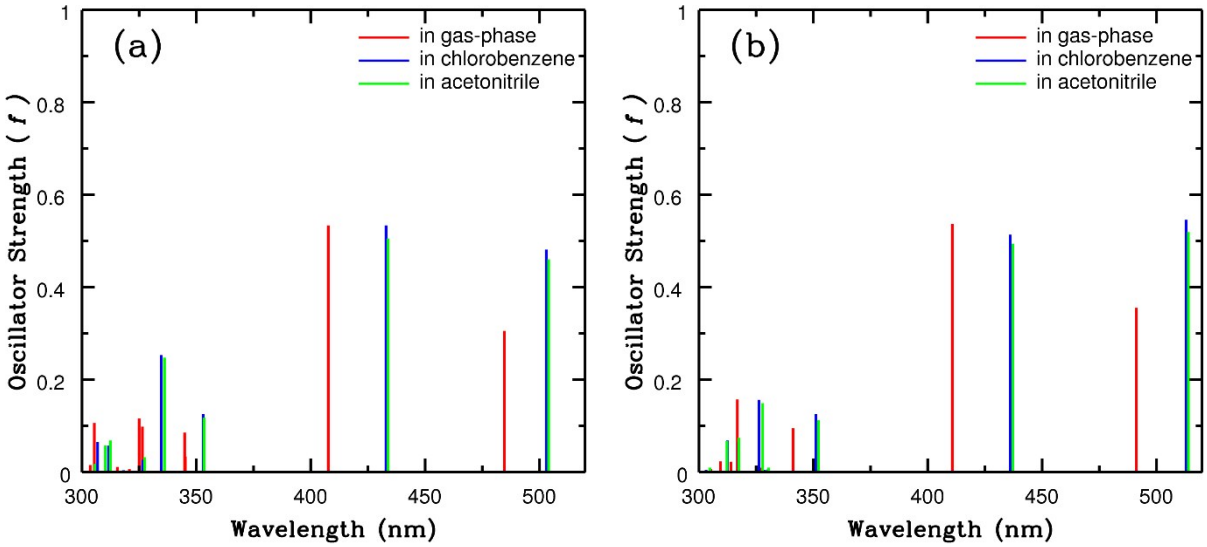


Fig. S-3 For synthesized molecules (a) 85 atoms and (b) 64 atoms. Plots of oscillator strength versus wavelength are calculated by using TD-DFT with B3LYP/6-31+G(d) in gas-phase (default) and in solvents of chlorobenzene and acetonitrile for the first ten excited states.

Table S-16 The Cartesian coordinates (Å) for the optimized structures of the synthesized molecules (85 and 64 atoms) by using DFT/B3LYP/6−31+G(d) method.

85 atoms				64 atoms			
C	0.68745700	0.88433400	-0.50503700	C	1.32849400	0.81323300	0.71730300
C	-0.70622900	0.59976700	-0.34242200	C	2.55842700	0.09268300	0.58063500
C	1.30512000	0.54111700	-1.73750700	C	1.22254900	1.77401700	1.75844200
C	-1.42049300	-0.04452800	-1.38537500	C	3.64070400	0.37625900	1.45546000
C	0.58561500	-0.07771000	-2.74226600	C	2.28728900	2.02487300	2.60293000
C	-0.78019100	-0.38258600	-2.56562900	C	3.50609700	1.33258100	2.44773900
C	0.67901600	1.90359000	1.71611400	C	0.41933000	-0.49689400	-1.13480500
C	-0.69484700	1.63477600	1.85018000	C	1.62805800	-1.20637600	-1.24568400
C	1.37582100	1.52883200	0.57581500	C	0.25879700	0.50465000	-0.18632800
C	-1.38463500	0.97931800	0.84311400	C	2.69329300	-0.91463700	-0.40937000
C	-2.83119900	0.69197600	1.01768900	C	3.96512700	-1.66425900	-0.55851600
C	-2.86746100	-0.35506800	-1.22972600	C	4.92804600	-0.35476400	1.32158900
O	-3.50124900	-0.91677700	-2.11661600	O	5.89151200	-0.11909100	2.04281700
O	-3.43109500	1.02845000	2.03399400	O	4.11812400	-2.53030500	-1.41384400
N	-3.48714600	0.01332100	-0.02694500	N	5.00309700	-1.34342900	0.32927300
N	2.77002100	1.82294300	0.47421800	N	-0.97472900	1.22274500	-0.12224500
C	3.71408300	0.79097800	0.36270200	C	-2.18279400	0.50817600	-0.02148900
C	4.99523900	1.04056200	-0.18117700	C	-3.35745500	0.94794800	-0.66950800
C	3.40545500	-0.52402500	0.76887800	C	-2.24290000	-0.67745100	0.74136400
C	5.92793700	0.02473200	-0.30959200	C	-4.54440900	0.24003900	-0.55590400
C	4.34337100	-1.53556600	0.63178300	C	-3.43113900	-1.38151100	0.84605600
C	5.63077800	-1.30056400	0.09396200	C	-4.61932900	-0.94876800	0.20865200
C	3.17851800	3.17730400	0.70945800	C	-0.96748300	2.62587600	-0.40876600
C	2.57298600	4.21521000	-0.01342700	C	-0.12131500	3.14303200	-1.39954700
C	4.15452800	3.47857900	1.67070900	C	-1.78840200	3.49927800	0.32344000
C	2.93989100	5.54054500	0.22614900	C	-0.09729200	4.51706700	-1.65230200
C	4.52768000	4.80554100	1.89340200	C	-1.77069200	4.86748100	0.05309200
C	3.92130100	5.84146500	1.17582400	C	-0.92313600	5.38459000	-0.93329800
C	6.52649600	-2.43314100	0.00385900	C	-5.80207800	-1.76209700	0.39484900

C	7.81237800	-2.55078800	-0.45405400
C	8.58137100	-1.46622700	-0.98049100
C	8.52242900	-3.85515900	-0.43603200
C	-4.94532700	-0.28515100	0.15306200
C	-5.23950000	-1.80331300	0.04000900
C	-6.16207500	-2.32686400	1.15420800
C	-6.44307200	-3.83125900	1.03465300
C	-5.78143400	0.62664400	-0.76938700
C	-7.29327600	0.57128500	-0.50453800
C	-8.07525900	1.58697400	-1.35079900
C	-9.59329700	1.53079900	-1.12917000
C	-7.35718300	-4.37579500	2.14134900
C	-7.61977100	-5.88213000	2.02181900
C	-10.36555800	2.55241700	-1.97299000
N	9.19068100	-0.56966100	-1.40578800
O	9.65996800	-4.02648700	-0.82666800
O	7.76906200	-4.87115300	0.06958100
H	2.35304000	0.77417600	-1.89132900
H	1.07428400	-0.32966700	-3.67911500
H	-1.35030200	-0.87330600	-3.34787300
H	1.21051200	2.40551900	2.51894900
H	-1.22803600	1.92184200	2.75071400
H	5.25134000	2.04129400	-0.51285200
H	2.43460000	-0.74479700	1.19948300
H	6.89241500	0.26351400	-0.74031400
H	4.08345500	-2.53915600	0.96066800
H	1.81762400	3.98020200	-0.75796000
H	4.61781100	2.67690000	2.23841600
H	2.46444800	6.33758800	-0.33923500
H	5.28618300	5.02907600	2.63892400
H	4.21045500	6.87313000	1.35561900
H	6.10034100	-3.36455500	0.36703900
H	-5.13366900	0.02293300	1.18273000
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H	-5.66644400	-2.02918300	-0.94398400
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H	-7.11491200	-1.78023600	1.14581700
H	-5.48904500	-4.38055200	1.05016600
H	-6.89759500	-4.04047800	0.05413700
H	-5.43675100	1.65977500	-0.61944700
H	-5.58312700	0.36798200	-1.81514300
H	-7.49168100	0.75988400	0.56122900
H	-7.67376100	-0.43699000	-0.71856000
H	-7.71358100	2.60182000	-1.12545400
H	-7.85844400	1.41500900	-2.41608200
H	-9.81078400	1.69763400	-0.06396600
H	-9.95513400	0.51811800	-1.35989900
H	-6.90752400	-4.15971400	3.12156400
H	-8.31455300	-3.83485500	2.11908100
H	-6.68366200	-6.45292700	2.07720600
H	-8.27590600	-6.23972200	2.82469900
H	-8.09977100	-6.12663400	1.06528100
H	-10.19431700	2.39149200	-3.04528900
H	-10.05260400	3.57812500	-1.73823400
H	-11.44559500	2.48489900	-1.79439000
H	8.32763800	-5.66928800	0.03425400
C	-7.08664400	-1.63036400	-0.06176000
C	-7.54063200	-0.55595300	-0.88887200
C	-8.13441700	-2.62571300	0.28260800
C	6.27435100	-2.08550500	0.19546500
C	7.25647300	-1.40808300	-0.76812300
C	8.57091500	-2.19159900	-0.88943400
C	9.56983300	-1.53406600	-1.84949900
N	-7.89041500	0.32780300	-1.56155200
O	-9.28983200	-2.56624500	-0.08766500
O	-7.67644500	-3.63800400	1.07028100
H	0.29216100	2.31441000	1.88955800
H	2.18618100	2.76110100	3.39521500
H	4.34918700	1.52901400	3.10234100
H	-0.40112800	-0.72307200	-1.80940800
H	1.74881900	-1.97727400	-2.00014900
H	-3.33263600	1.84645900	-1.27631300
H	-1.35606000	-1.03399400	1.25515500
H	-5.41572300	0.61030600	-1.08179100
H	-3.45415200	-2.28706100	1.44797300
H	0.51393100	2.47246700	-1.97025400
H	-2.43684700	3.10358300	1.10000700
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H	6.70630600	-2.15367300	1.19551600
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H	7.46483600	-0.39088000	-0.41129800
H	6.78647800	-1.32043000	-1.75655400
H	9.02949000	-2.28801800	0.10525600
H	8.35439500	-3.21395900	-1.23134200
H	9.83146600	-0.52148400	-1.51669000
H	10.49835200	-2.11363500	-1.91575400
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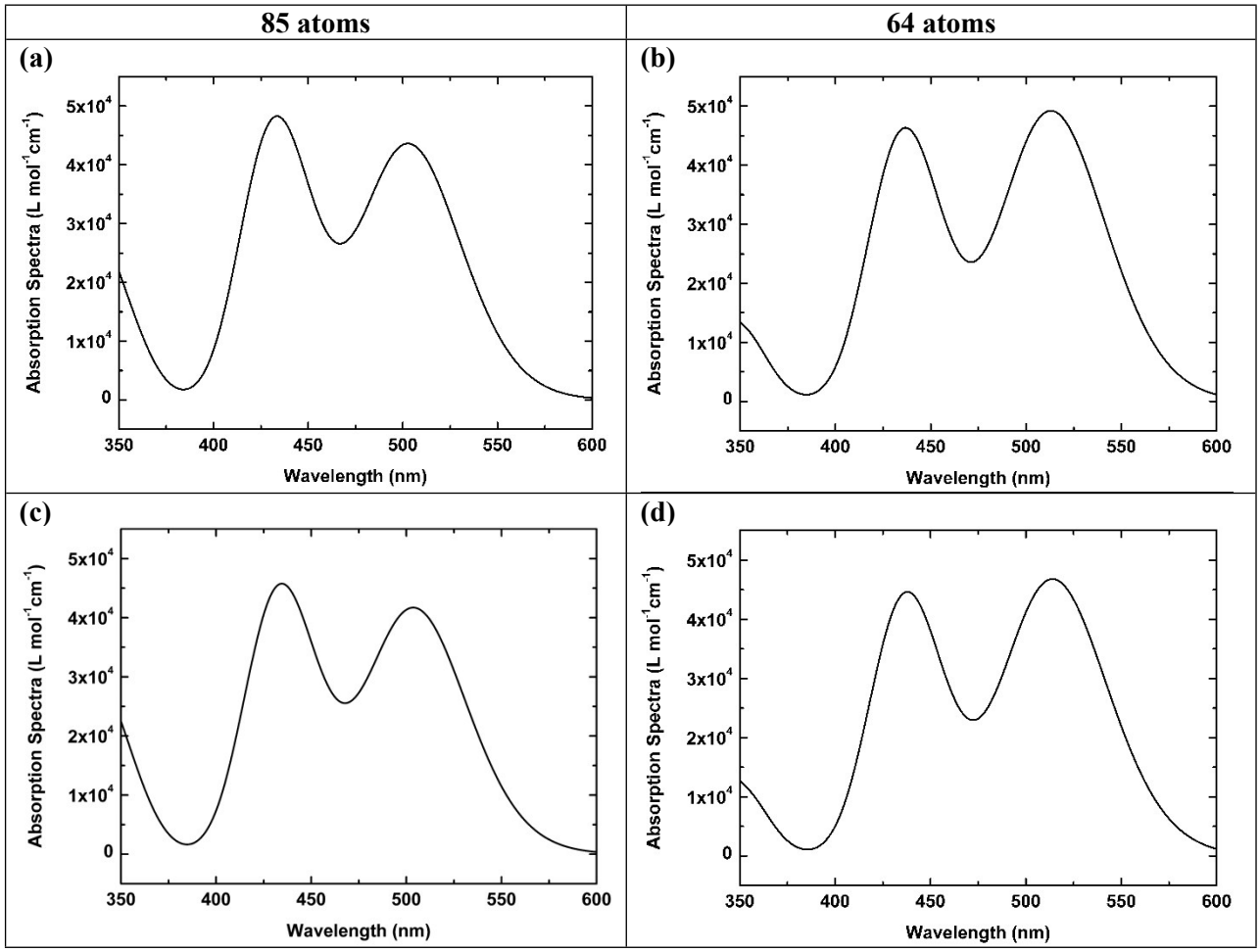


Fig. S-4 For 85 and 64 atoms, DFT(B3LYP) results on absorption spectra versus wavelength. These results are obtained by using **(a)** and **(b)** chlorobenzene solvent, **(c)** and **(d)** acetonitrile solvent for 85 and 64 atoms.

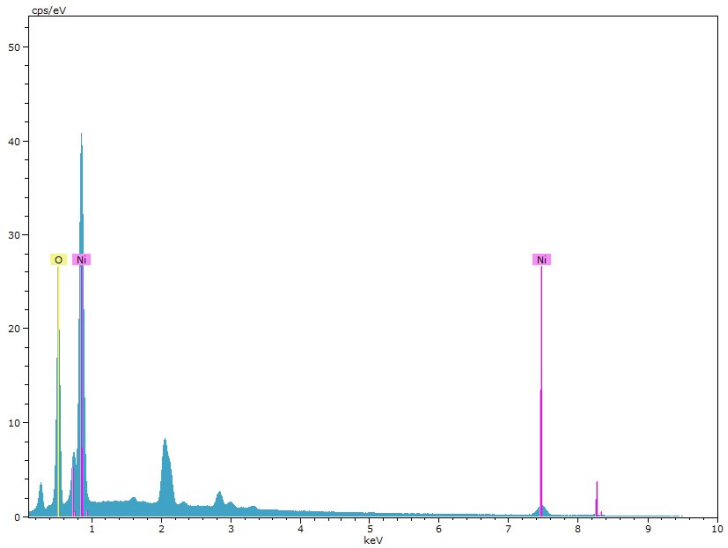


Fig. S5. EDX spectra of NiO

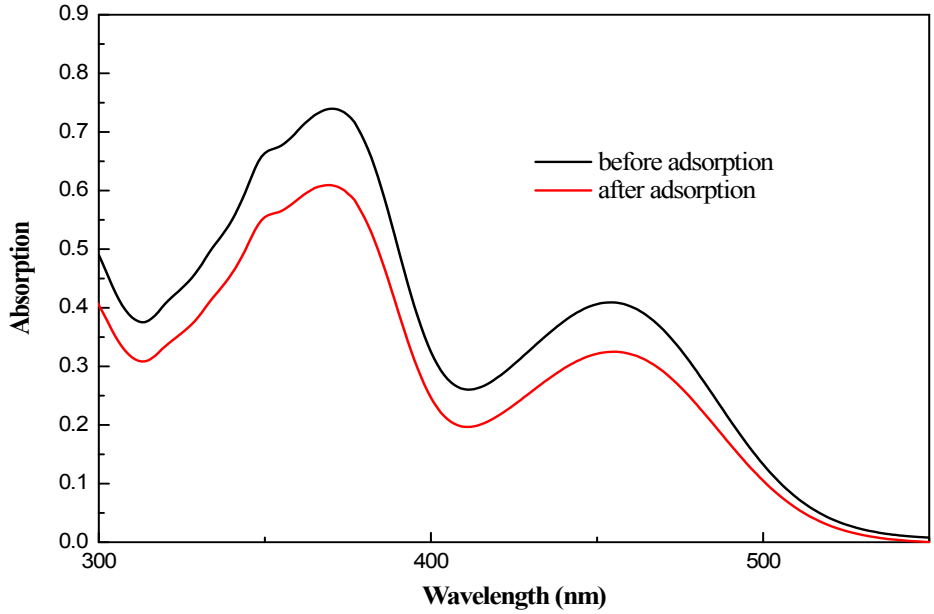
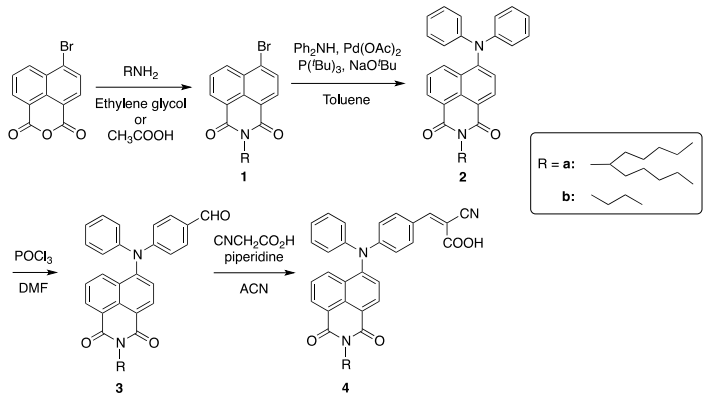


Fig. S6. Absorbance of S85 dye before and after adsorbing on NiO.

General procedure of the synthesis of the compound 2.[3-5]

To a two-necked flask were added the compound 1 (1.0 mmol), $Pd(OAc)_2$ (0.02 mmol), diphenylamine (1.2 mmol), NaO^{t}Bu (1.5 mmol) and toluene (3 mL). The mixture was refluxed for overnight under argon atmosphere. After cooling to room temperature, water (3 mL) and EtOAc (20 mL) were added. The organic layer was separated and washed with water and brine, and then dried over $MgSO_4$. The solvent was removed in vacuum. The residue was purified by column chromatography (hexane/EtOAc, 95/5).



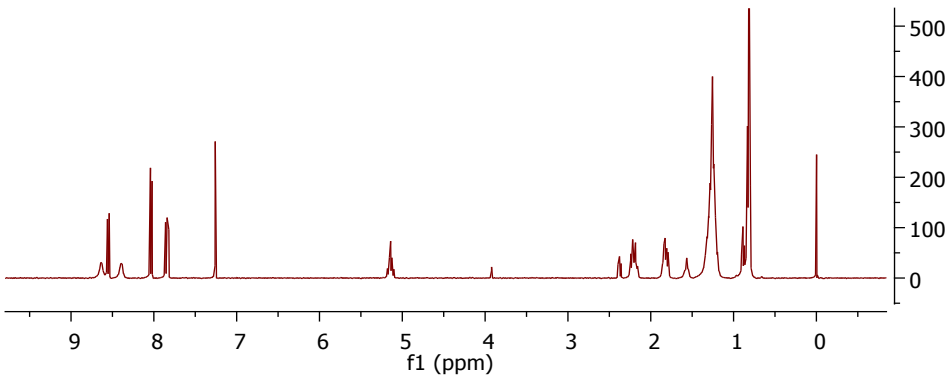


Fig. S7. ^{1}H NMR spectrum of compound 1a (N-(1-Hexylpentyl)-4-bromonaphthalene-1,8-dicarboxmonoimide).

2a: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.49 (s, 2H), 8.15 (dd, *J* = 8 Hz, 1H), 7.48 (dd, , *J* = 8 Hz, 1H), 7.37 (d, *J* = 8 Hz, 1H), 7.28-7.23 (m, 4H), 7.08-7.03 (m, 6H), 5.20-5.12 (m, 1H), 2.28-2.19 (m, 2H), 1.84-1.81 (m, 2H), 1.36-1.26 (m, 12H), 0.84 (t, *J* = 8 Hz, 3H).

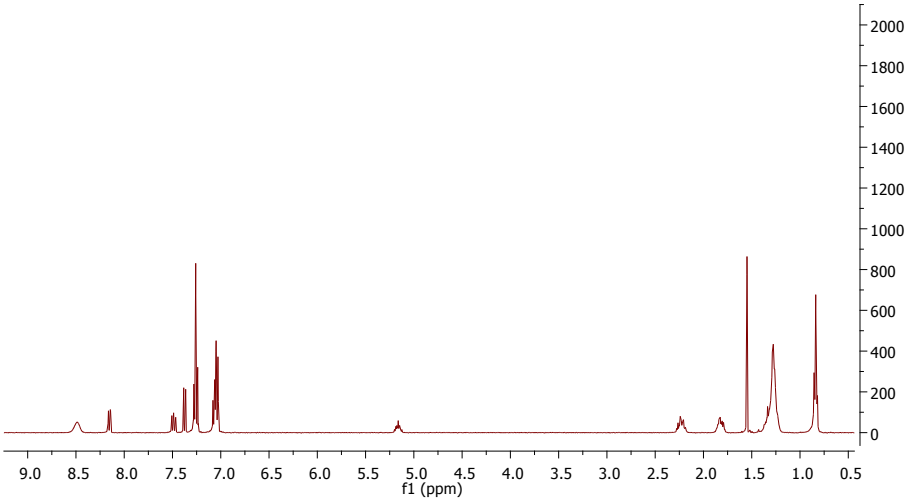


Fig. S8: ^{1}H NMR spectrum of compound 2a.

2b: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54-8.49 (m, 2H), 8.18 (dd, *J* = 4 Hz, 1H), 7.49 (dd, , *J* = 8 Hz, 1H), 7.37 (d, *J* = 8 Hz, 1H), 7.28-7.24 (m, 4H), 7.08-6.98 (m, 6H), 4.19 (t, *J* = 8 Hz, 2H), 1.76-1.69 (m, 2H), 1.56-1.41 (m, 2H), 0.99 (t, *J* = 8 Hz, 3H).

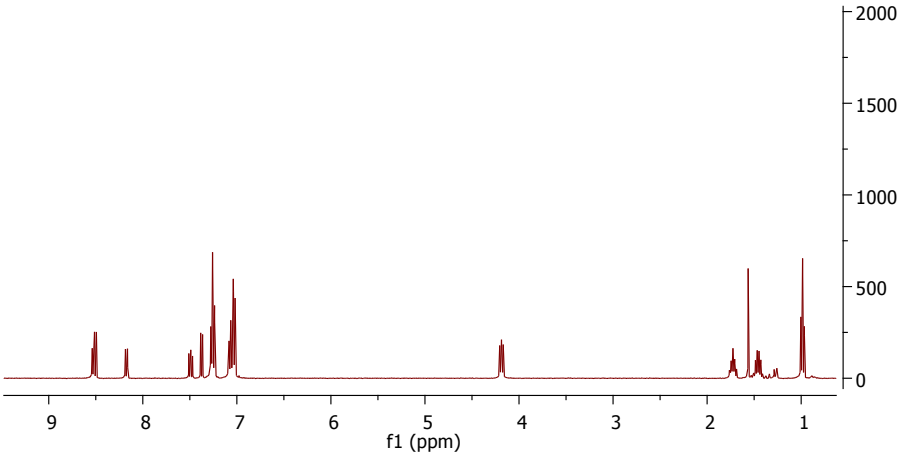


Fig. S9: ^{1}H NMR spectrum of compound 2b.

General procedure of the synthesis of the compound 3.[6]

$POCl_3$ (1.36 mmol, 0.2 g) is stirred in a two-necked flask at 0 °C for 1 h in dried DMF under argon atmosphere. After additional stirring for 1 h at room temperature, the compound 2 was added to this solution. The reaction mixture was stirred at 90 °C for 5 h. After cooling to room temperature, the solution was poured into water. The solution was neutralized with 2 M NaOH solution and extracted with CH_2Cl_2. The combined organic layer was washed with water and brine, dried over Na_2SO_4. The solvent was evaporated and purified using column chromatography (hexane/EtOAc, 10/1).

3a: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.85 (s, 1H), 8.55 (s, 2H), 8.12 (d, *J* = 8 Hz, 1H), 7.71 (d, *J* = 8 Hz, 2H), 7.58 (t, *J* = 8 Hz, 1H), 7.51 (d, *J* = 8 Hz, 1H), 7.35 (t, *J* = 8 Hz, 2H), 7.19 (d, *J* = 8 Hz, 2H), 6.98 (d, *J* = 8 Hz, 2H), 5.20-5.13 (m, 1H), 2.34-2.21 (m, 2H), 1.86-1.80 (m, 2H), 1.29-1.21 (m, 12H), 0.84 (t, *J* = 8 Hz, 3H).

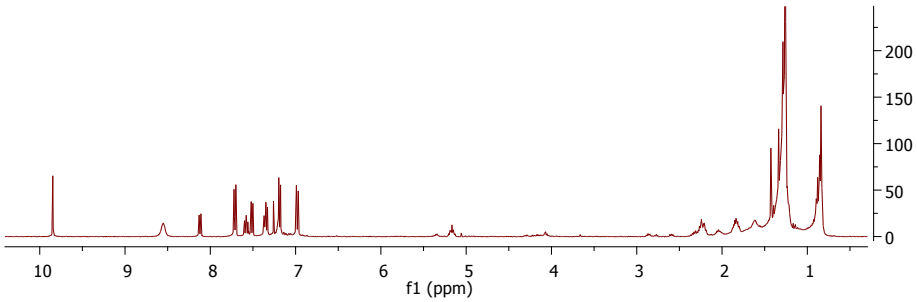


Fig. S10. ^{1}H NMR spectrum of compound 3a.

3b: ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.84 (s, 1H), 8.57 (d, *J* = 8 Hz, 2H), 8.14 (dd, *J* = 4 Hz, 1H), 7.80 (d, *J* = 8 Hz, 2H), 7.60-7.56 (m, 1H), 7.51 (d, *J* = 8 Hz, 1H), 7.36-7.32 (m, 2H), 7.21-7.16 (m, 2H), 6.98-6.95 (m, 2H), 4.19 (t, *J* = 8 Hz, 2H), 1.76-1.69 (m, 2H), 1.50-1.39 (m, 2H), 0.98 (t, *J* = 8 Hz, 3H).

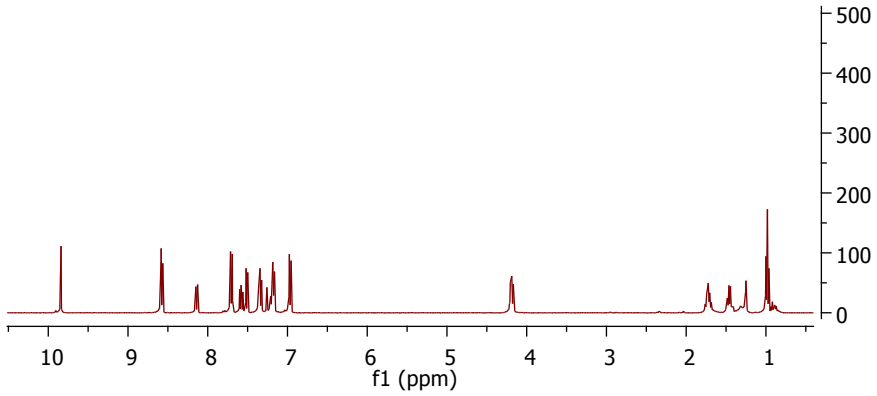


Fig. S11. ^{1}H NMR spectrum of compound 3b.

General procedure of the synthesis of the compound 4.[6c]

The compound 3 (0.25 mmol) is dissolved in a little amount of acetonirile in a two-necked flask. Cyano-acetic acid (0.50 mmol) and catalytic amount of piperidine is placed in a flask and stirred at 40 ^{o}C for overnight under argon atmosphere. After the reaction is finished, the solvent was evaporated. The residue was extracted with chloroform and 0.1 M HCl solution. The organic phase was dired over $MgSO_4$. The crude product was purified by column chromatography ($CHCl_3$: MeOH).

4a: ^{1}H NMR (400 MHz, $CDCl_3$). 8.57 (s, 2H), 8.15-8.11 (m, 2H), 7.90 (d, J = 12 Hz, 2H), 7.62 (t, J = 8 Hz, 1H), 7.54 (d, J = 8 Hz, 1H), 7.37 (t, J = 8 Hz, 2H), 7.24-7.20 (m, 3H), 6.94 (d, J = 8 Hz, 2H), 5.21-5.13 (m, 1H), 2.27-2.21 (m, 2H), 1.85-1.80 (m, 2H), 1.28-1.25 (m, 12H), 0.83 (t, J = 8 Hz, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 178.3, 154.9, 152.8, 147.4, 145.7, 133.6, 131.6, 132.3, 130.2, 129.8, 128.4, 127.4, 125.9, 125.5, 124.3, 119.8, 54.5, 32.2, 31.6, 29.6, 26.6, 22.4, 13.9. Exact mass (HRMS) found 613.002. Anal. Calc. for $C_{39}H_{39}N_3O_4$: C, 76.32; H, 6.40; N, 6.85. Found: C, 76.21; H, 6.42; N, 6.89.

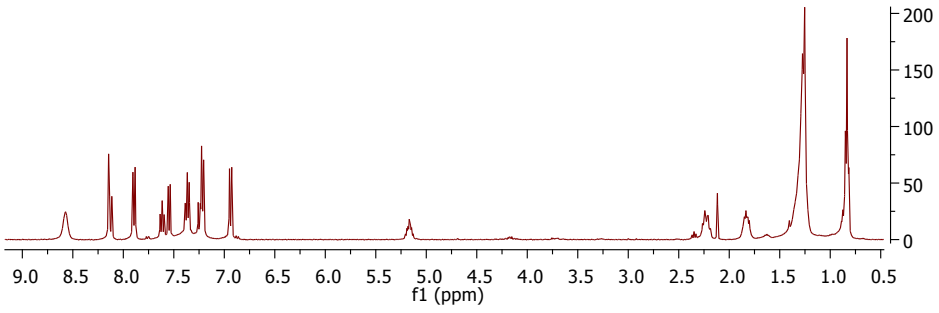


Fig. S12. ^{1}H NMR spectrum of compound 4a (S64)

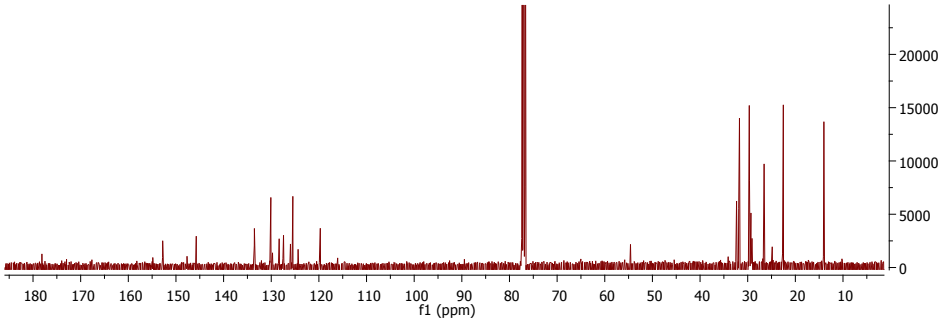


Fig. S13. ^{13}C NMR spectrum of compound 4a (S64).

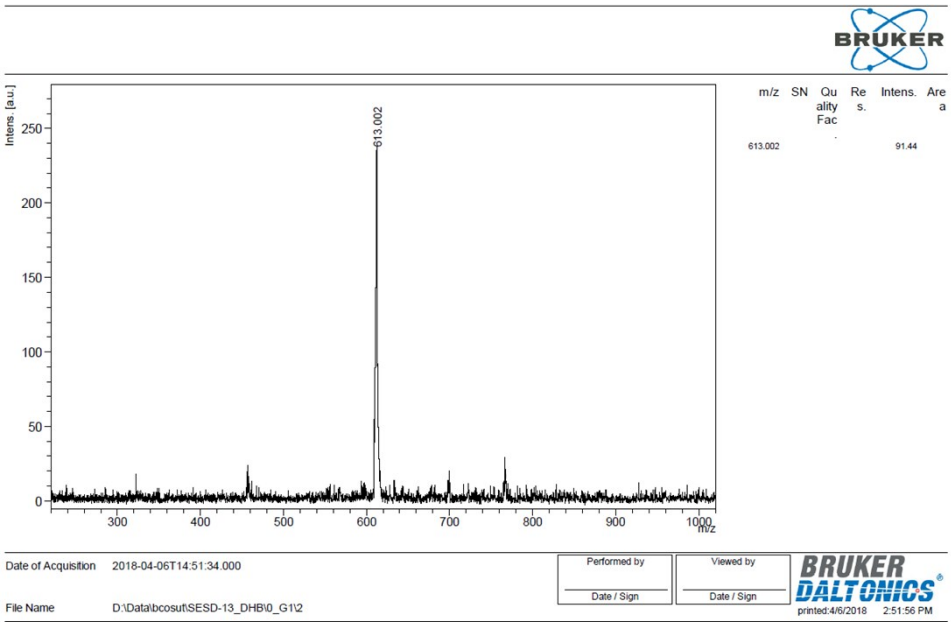
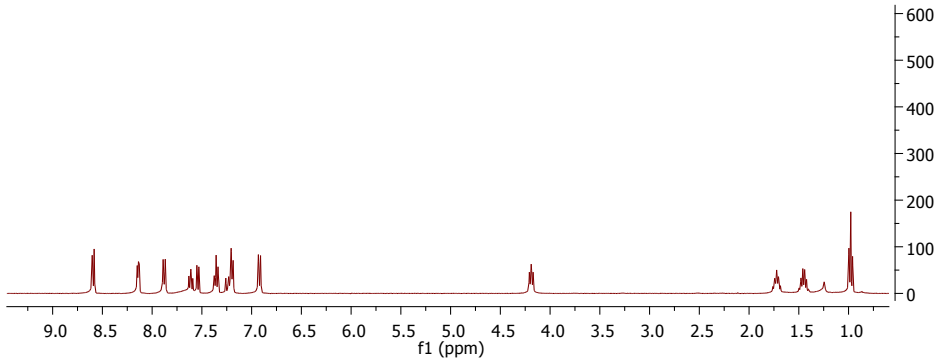


Fig. S14: (a) Mass spectrum of compound 4a (S85)

4b: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.59 (d, J = 8 Hz, 2H), 8.14 (t, J = 4 Hz, 2H), 7.78 (d, J = 8 Hz, 2H), 7.61 (t, J = 8 Hz, 1H), 7.54 (d, J = 8 Hz, 1H), 7.21 (t, J = 8 Hz, 3H), 6.92 (d, J = 8 Hz, 2H), 4.19 (t, J = 8 Hz, 2H), 1.76-1.68 (m, 2H), 1.50-1.40 (m, 2H), 0.98 (t, J = 8 Hz, 3H). ^{13}C NMR (400 MHz, $CDCl_3$) δ 163.9, 163.5, 154.9, 152.8, 147.9, 145.7, 133.6, 132.0, 131.7, 130.1, 128.5, 127.4, 126.0, 125.5, 123.6, 120.9, 119.8, 40.3, 30.2, 20.3, 13.8. Exact mass (HRMS) found 515.159. Anal. Calc. for $C_{32}H_{25}N_3O_4$: C, 74.55; H, 4.89; N, 8.15. Found: C, 75.03; H, 4.69; N, 8.09.

a)



b)

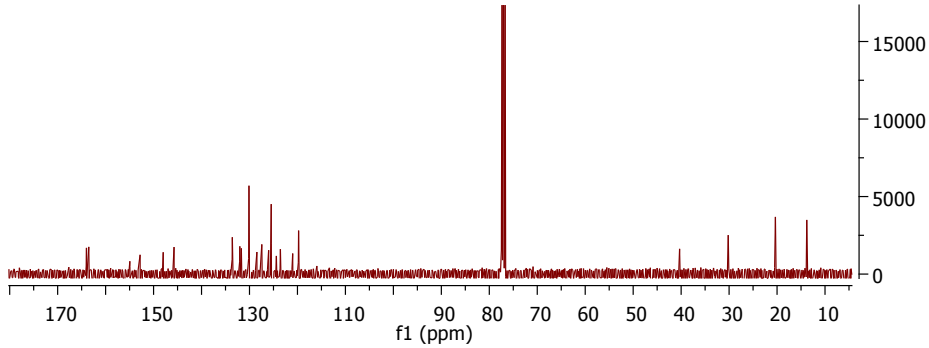


Fig. S15. (a) ^{1}H NMR spectrum of compound 4b (S64) and (b) ^{13}C NMR spectrum of compound 4b (S64) .

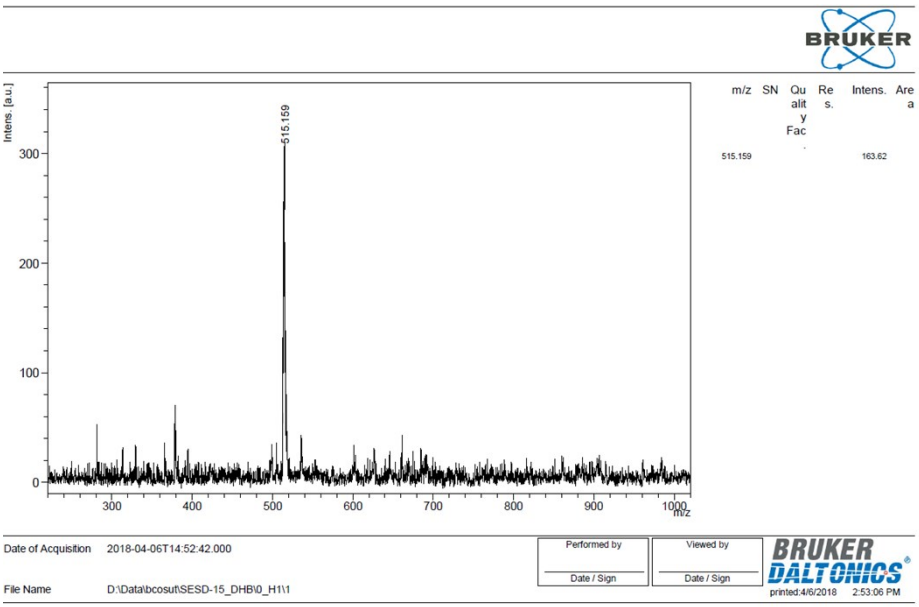


Fig. S16. Mass spectrum of compound 4a (S64)

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