Electronic Supplementary Material (ESI) for Organic Biomolecular Chemistry

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Supporting Information for

Imides Modified Benzopicenes: Synthesis, Solid Structure and Optoelectronic Properties

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1. X‐ray crystallographic structures of **1b** and **1d**

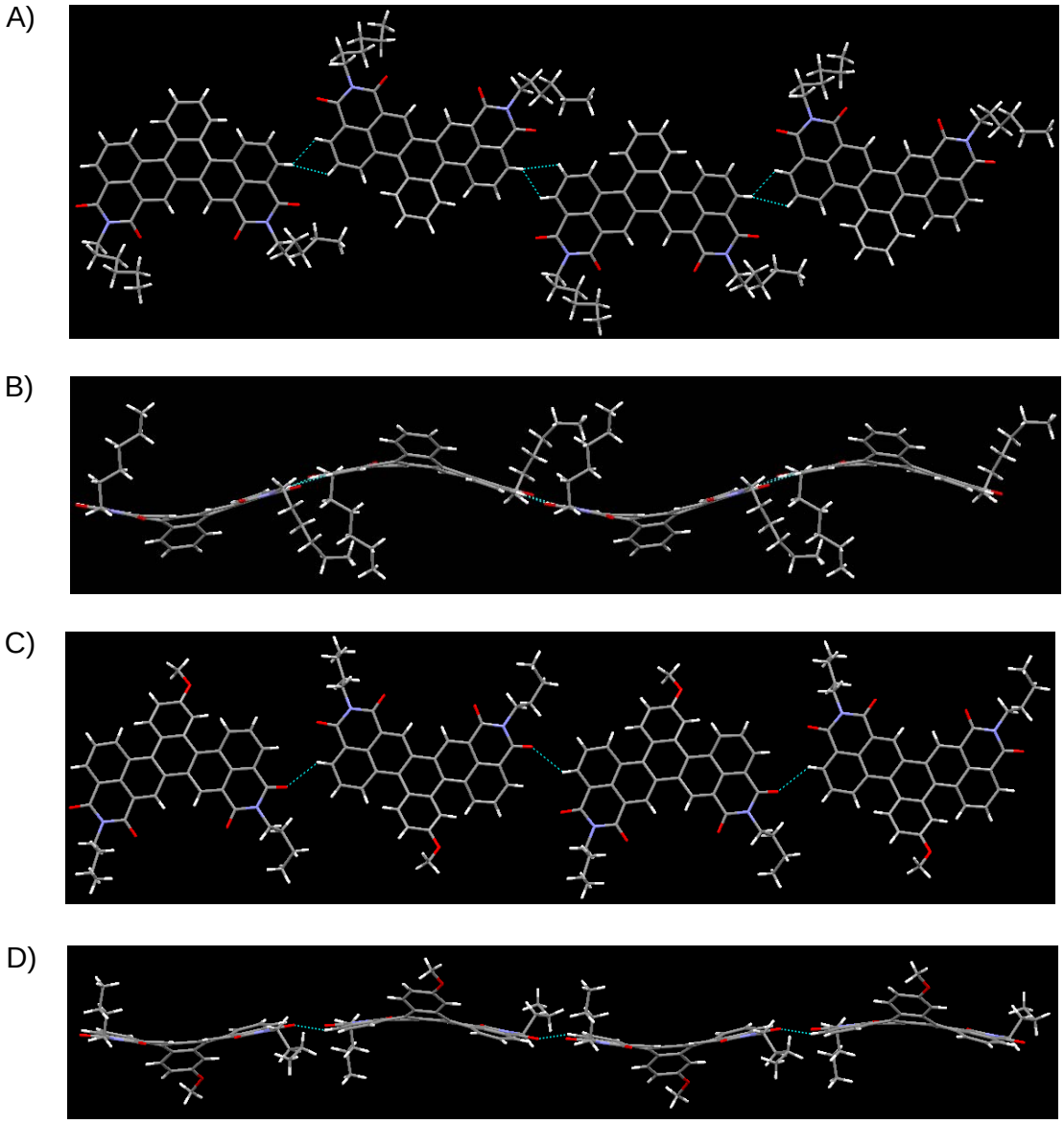


Figure S1. Packing views (along b axis) of **1b** and **1d**. **1b**: A) top view, B) side view; **1d**: C) top view, D) side view.

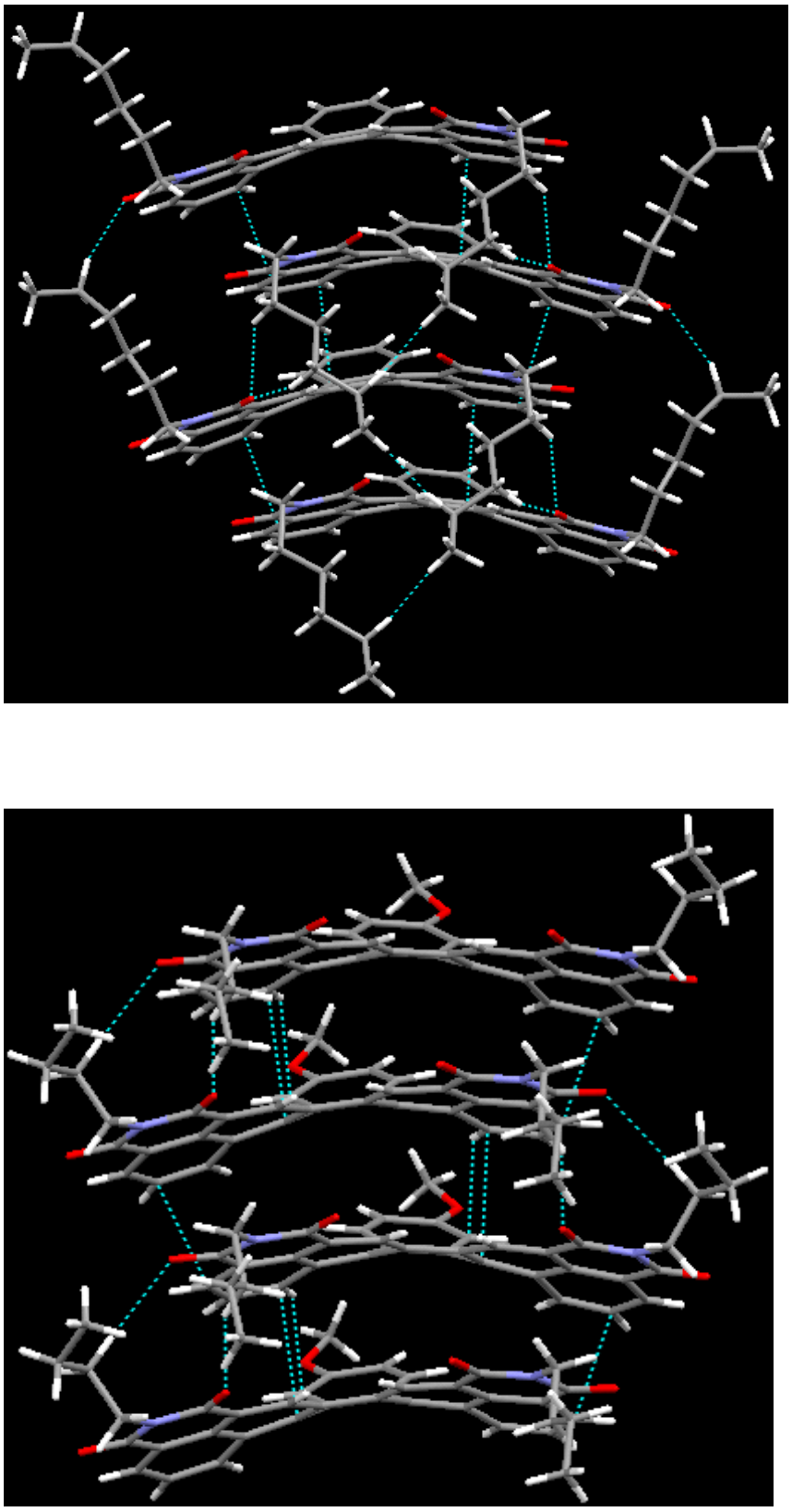


Figure S2. Packing views (along c axis) of **1b** (top) and **1d** (bottom)**.**

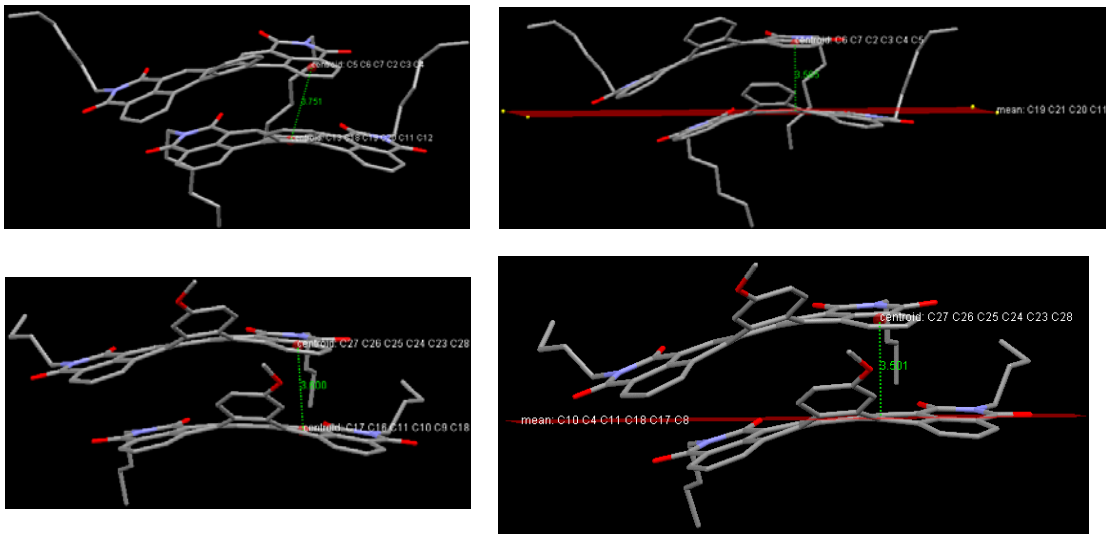


Figure S3. π···π interaction in **1b** (top) and **1d** (bottom).

2. Photophysical properties

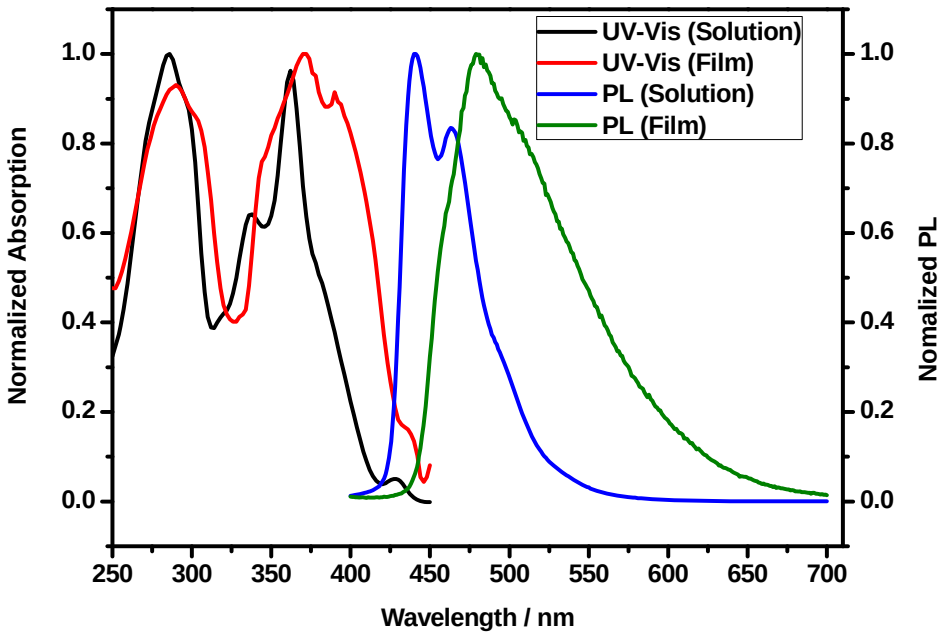


Figure S4. Normalized UV−vis absorption and photoluminescence spectra of **1b** in DCM (1.0×10^{-5} M) and in thin film.

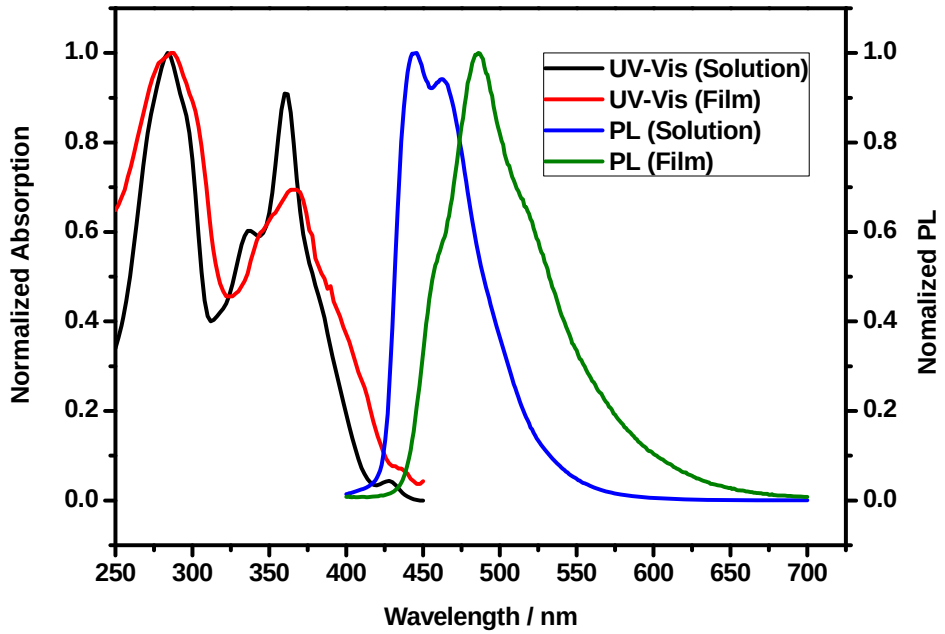


Figure S5. Normalized UV−vis absorption and photoluminescence spectra of **1c** in DCM (1.0×10^{-5} M) and in thin film.

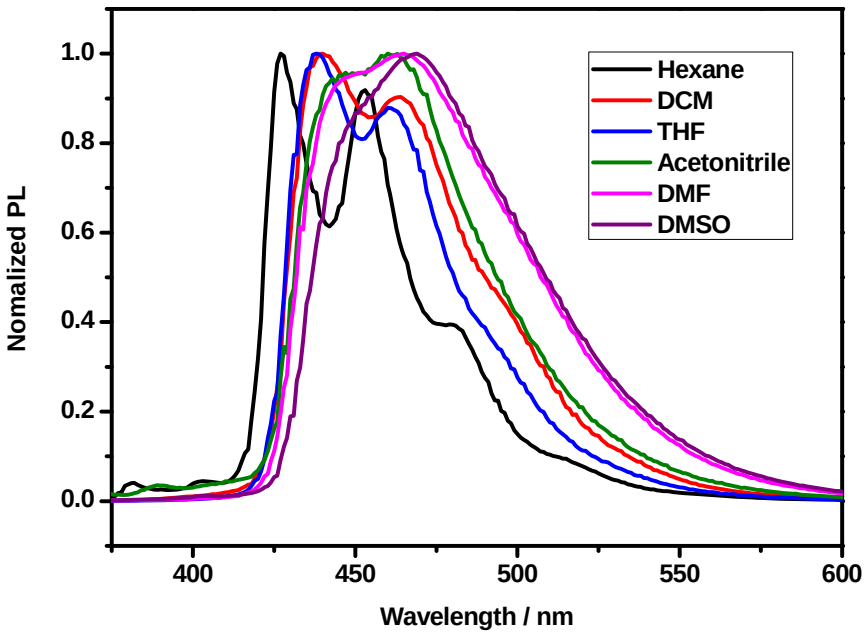


Figure S6. Normalized photoluminescence spectra of **1a** in different solvents (1.0×10^{-5} M).

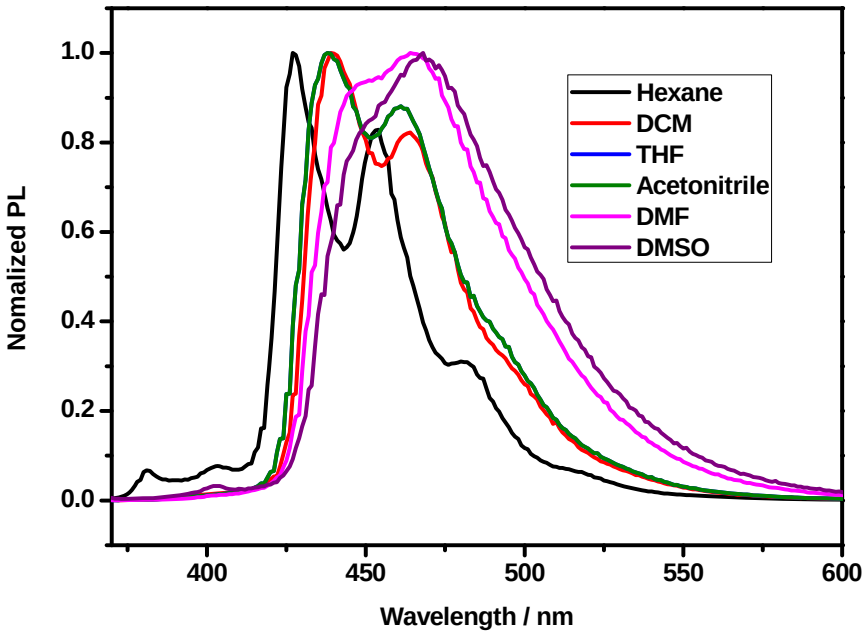


Figure S7. Normalized photoluminescence spectra of **1b** in different solvents (1.0×10^{-5} M).

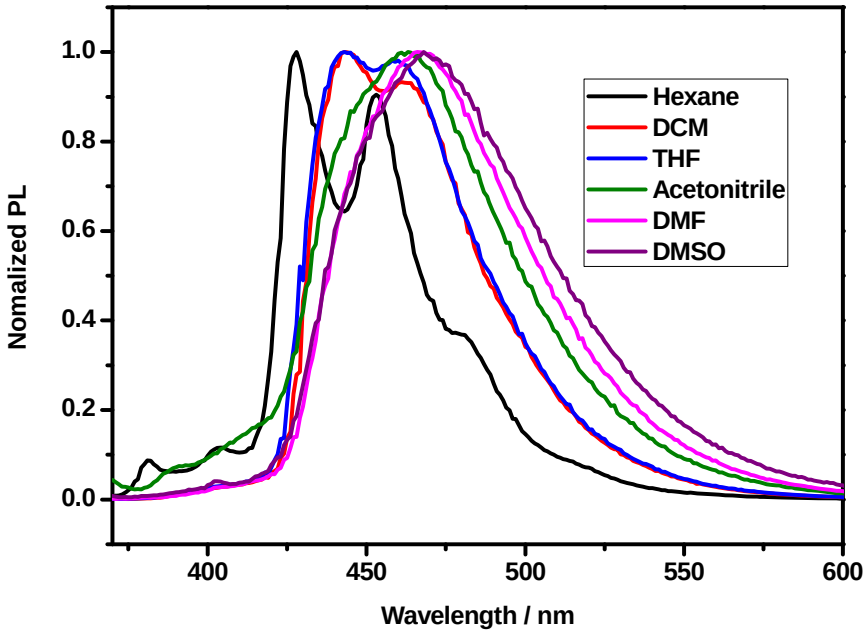


Figure S8. Normalized photoluminescence spectra of **1c** in different solvents (1.0×10^{-5} M).

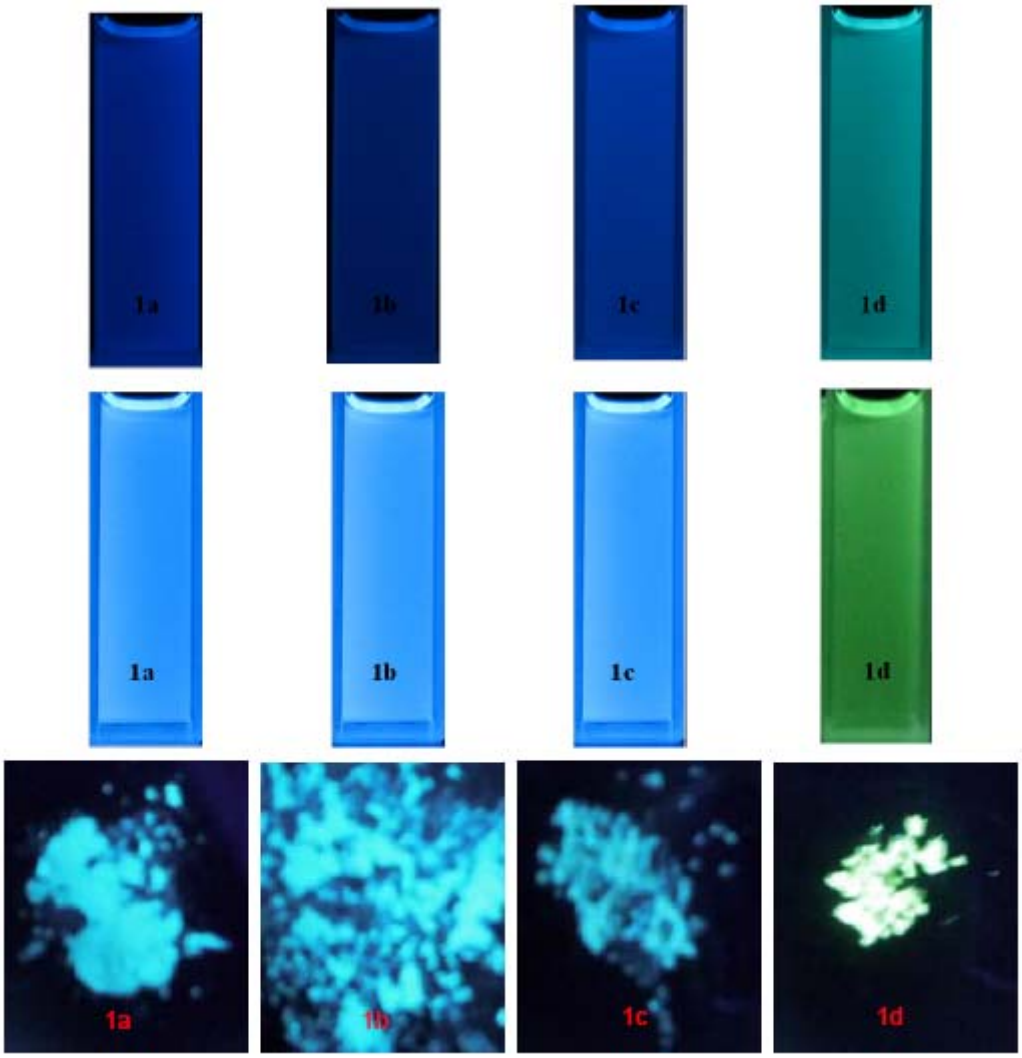
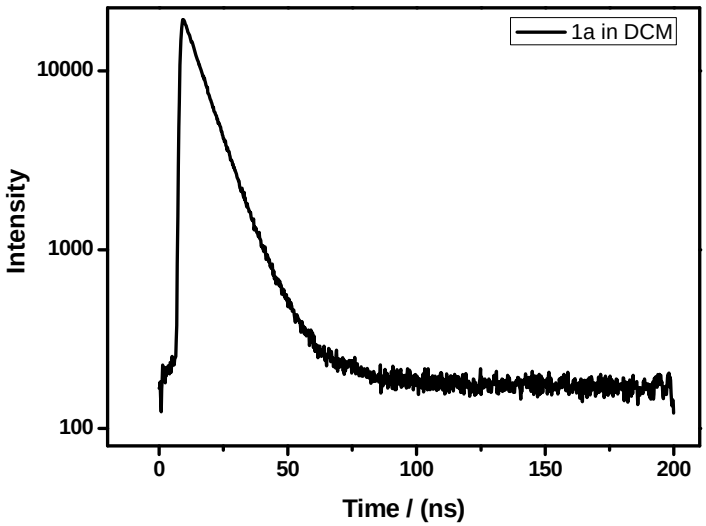
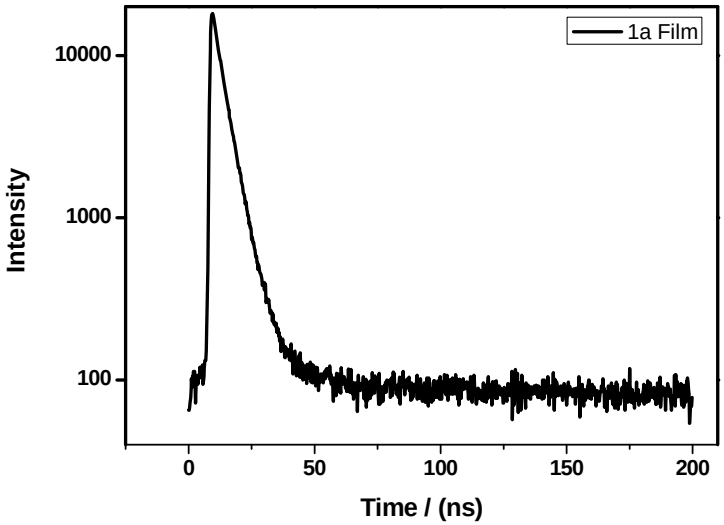


Figure S9. Colours in DCM (top), DMSO (middle) (1.0×10^{-5} M) and solid state (bottom) after irradiation of **1** in UV light ($\lambda = 365$ nm) under a UV-transilluminator.


1a in DCM
10000
1000
100
Intensity
0
50
100
150
200
Time / (ns)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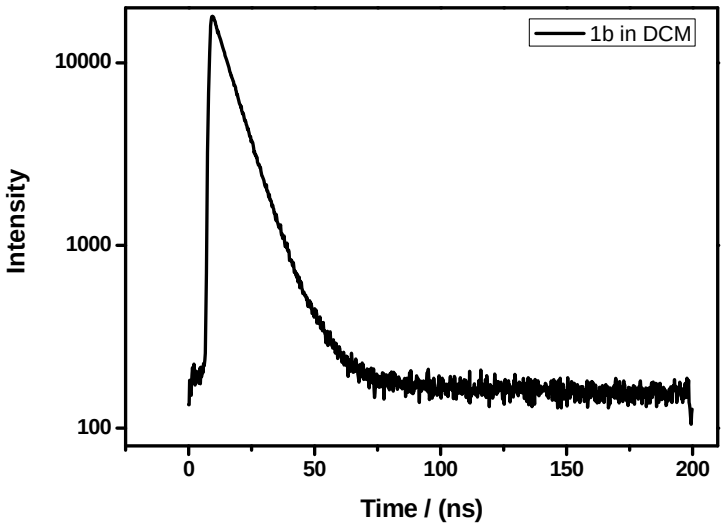
1000
100
Intensity
0
50
100
150
200
Time / (ns)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Intensity
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100
150
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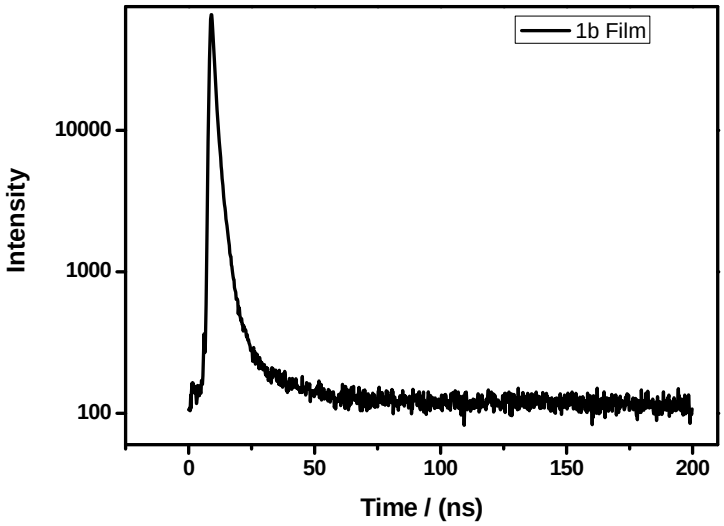
Time / (ns)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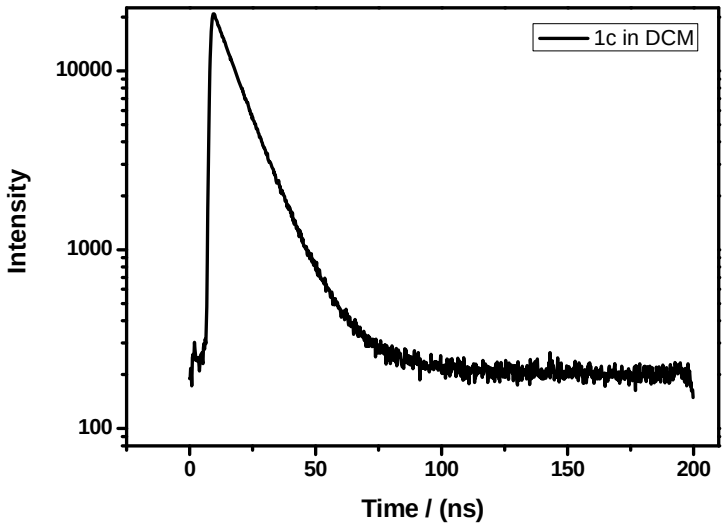
10000
1000
100
Intensity
0
50
100
150
200
Time / (ns)


1c in DCM
Intensity
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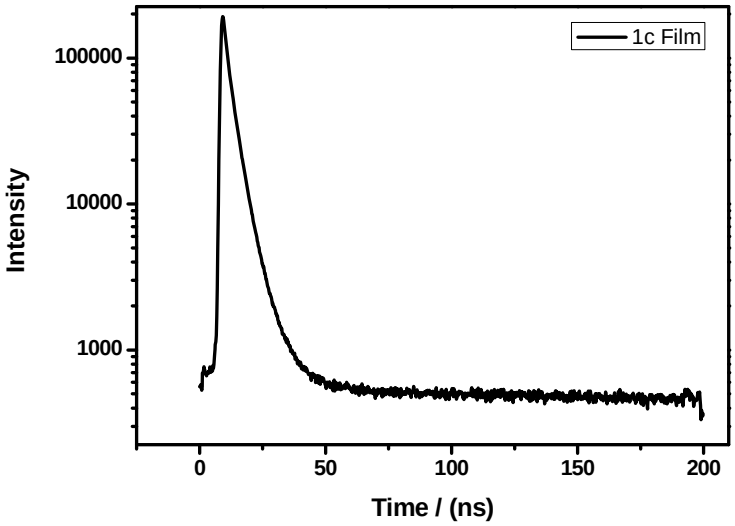
0
50
100
150
200
Time / (ns)


1c Film
Intensity
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10000
1000
0
50
100
150
200
Time / (ns)

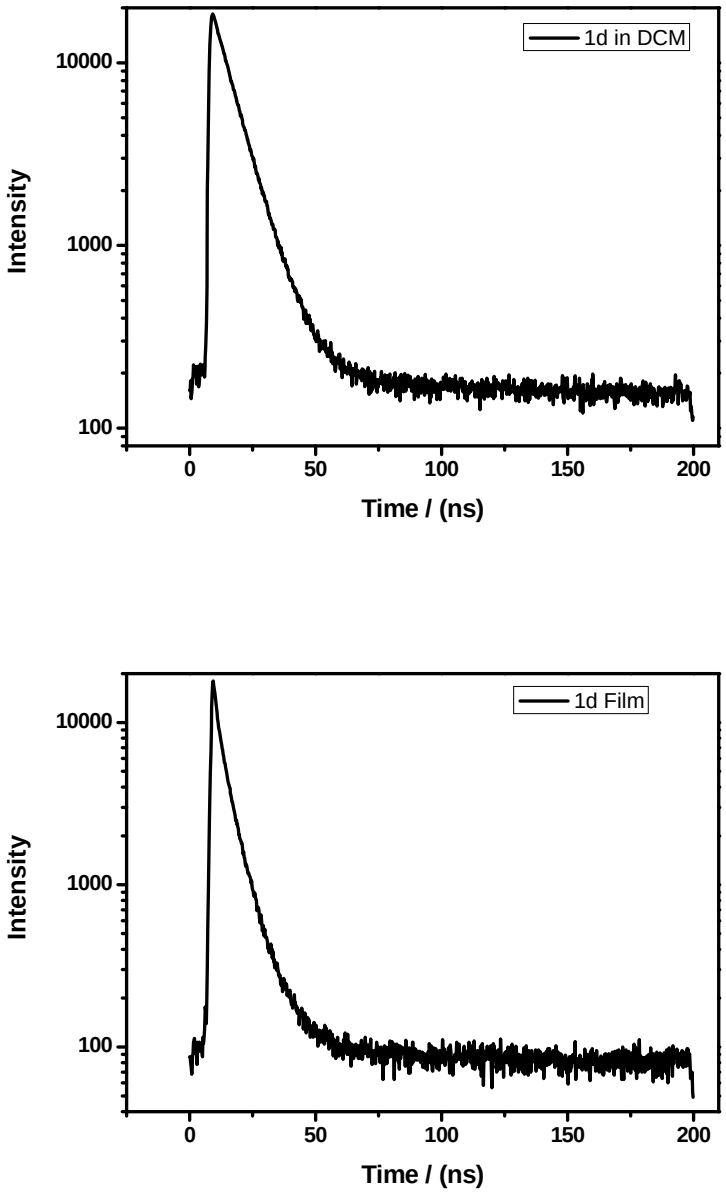


Figure S10. Time-resolved luminescence of **1a-d** in dichloromethane and in film state measured by Edinburgh Instruments FLS900.

	1a	**1b**	**1c**	**1d**
Hexane	42.4%	40.5%	46.7%	43.2%
DCM	54.9%	56.9%	66.1%	62.9%
THF	60.5%	61.2%	65.2%	64.5%
Acetonitrile	77.4%	76.9%	76.5%	77.1%
DMF	69.8%	67.9%	64.3%	66.8%
DMSO	52.6%	54.5%	52.1%	51.9%
Film	45.6%	46.5%	35.9%	46.7%

Table S1 The absolute fluorescence quantum yields of **1a-d** in different solvents and film state measured by Edinburgh Instruments FLS900

3. Computational studies for **1a**, **1b**, **1c** and **1d**

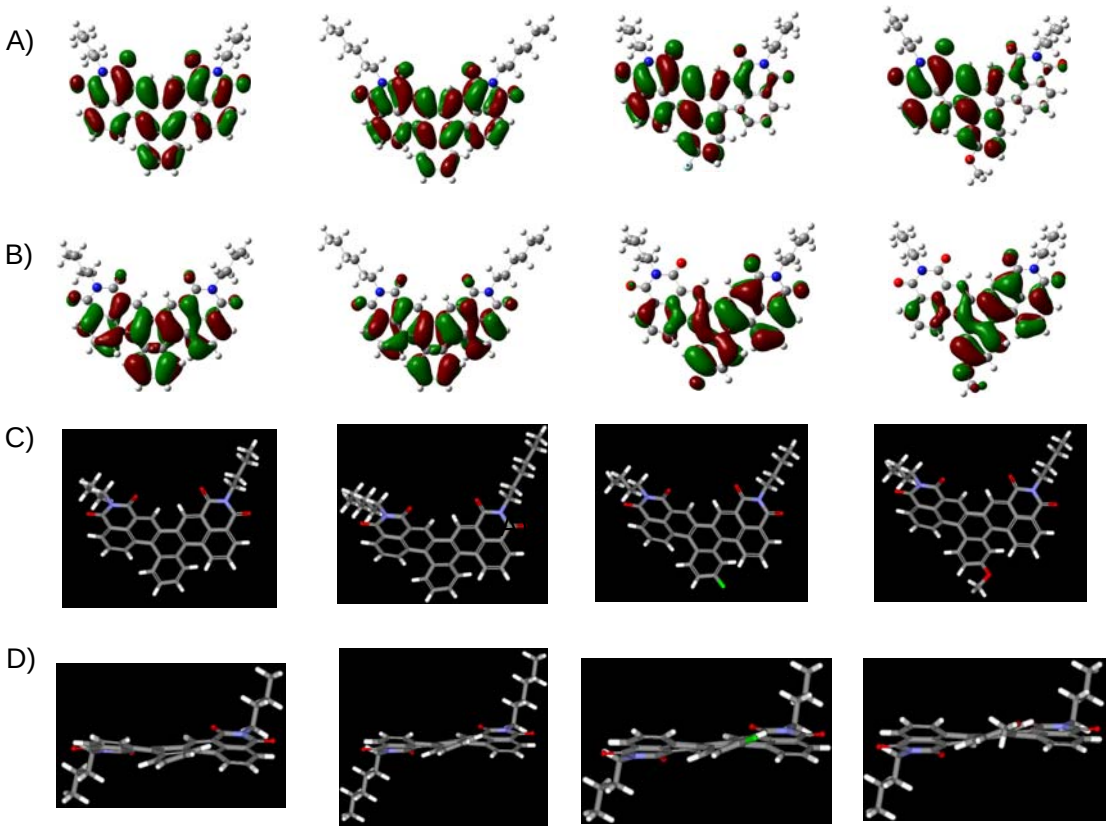
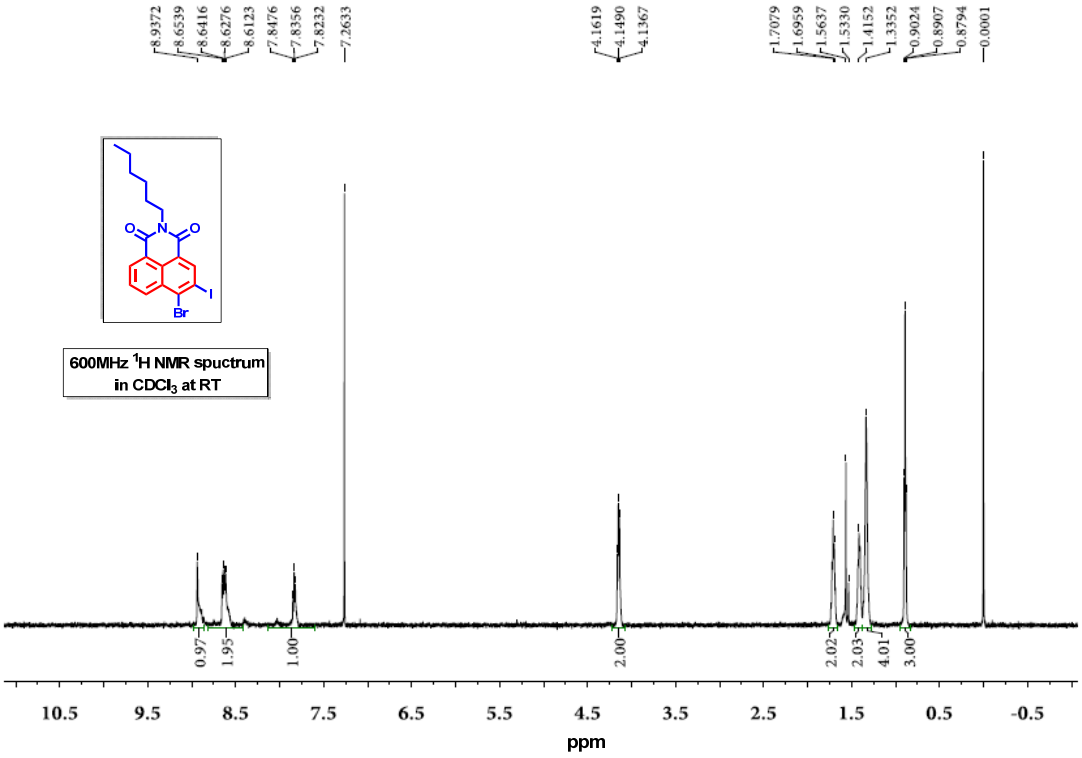
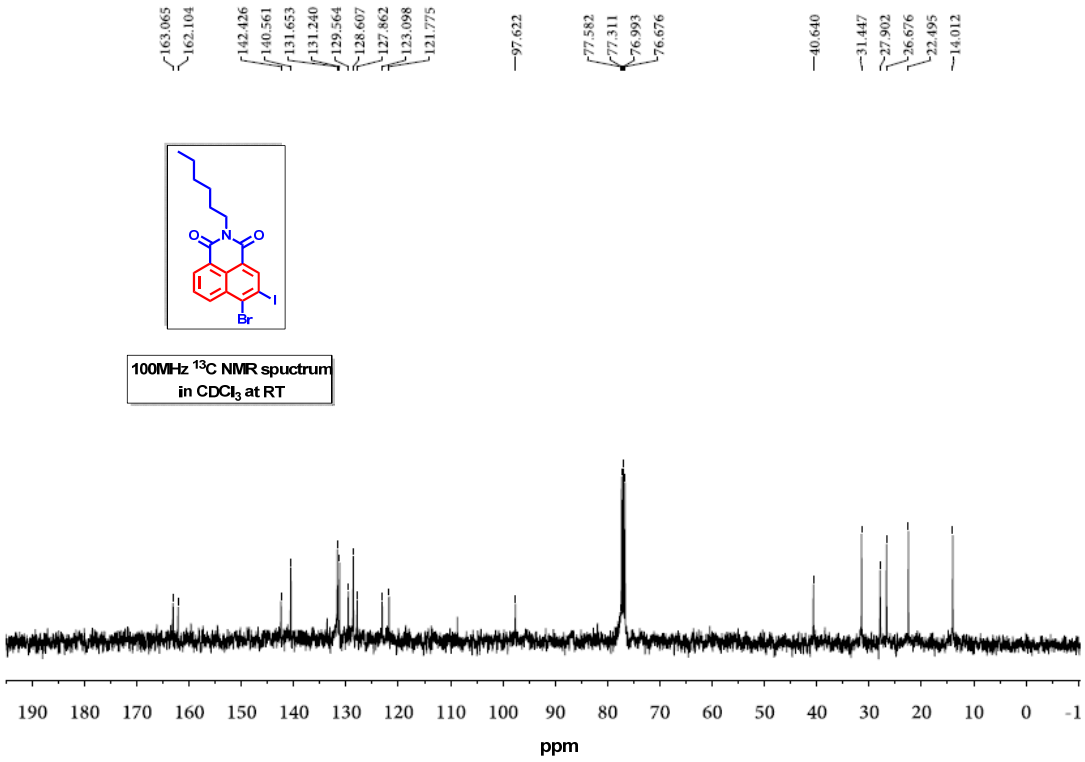
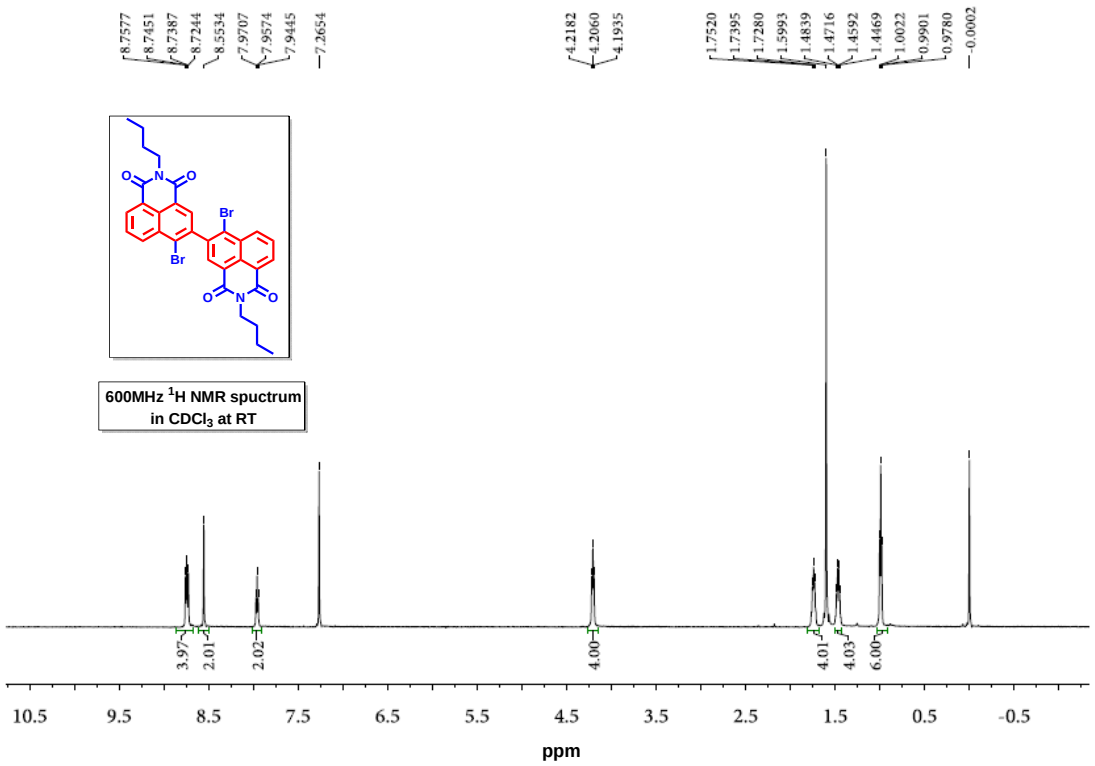


Figure S11. Frontier molecular orbital profiles and optimized structures based on DFT (B3LYP/6-31G*) calculations; A) HOMO, B) LUMO, C) top view, D) side view; **1a**, **1b**, **1c** and **1d** from left to right.

4. Copies of the NMR spectra and mass spectrum



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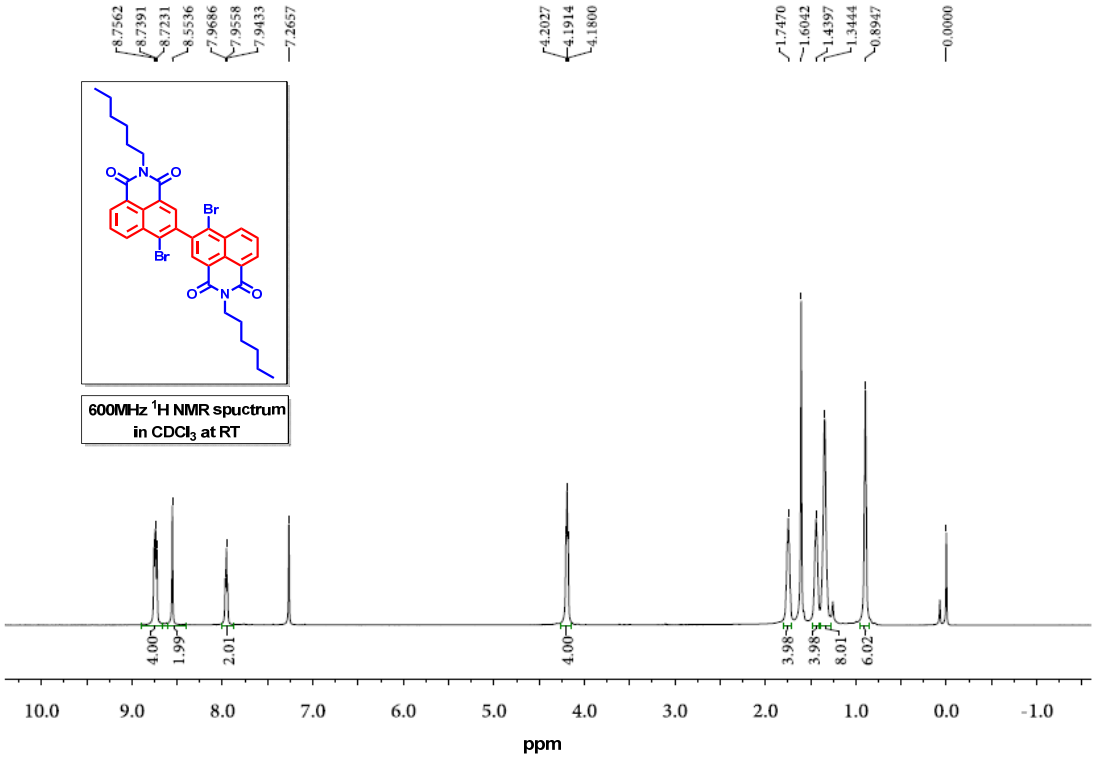
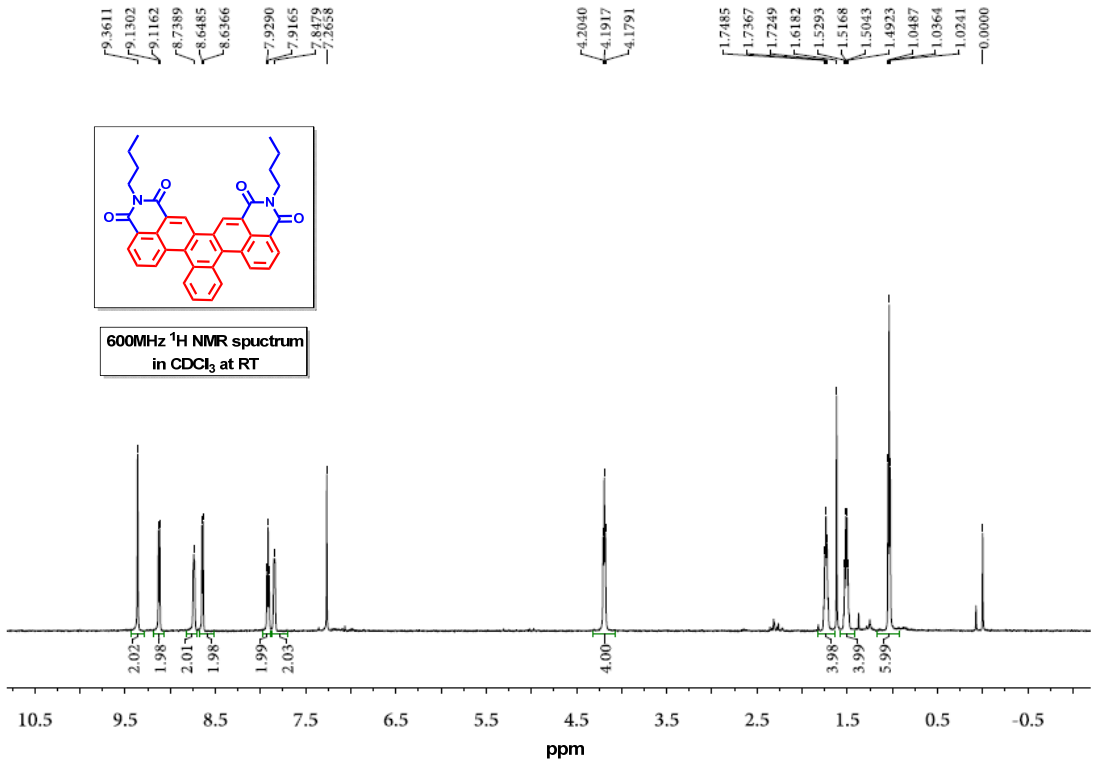
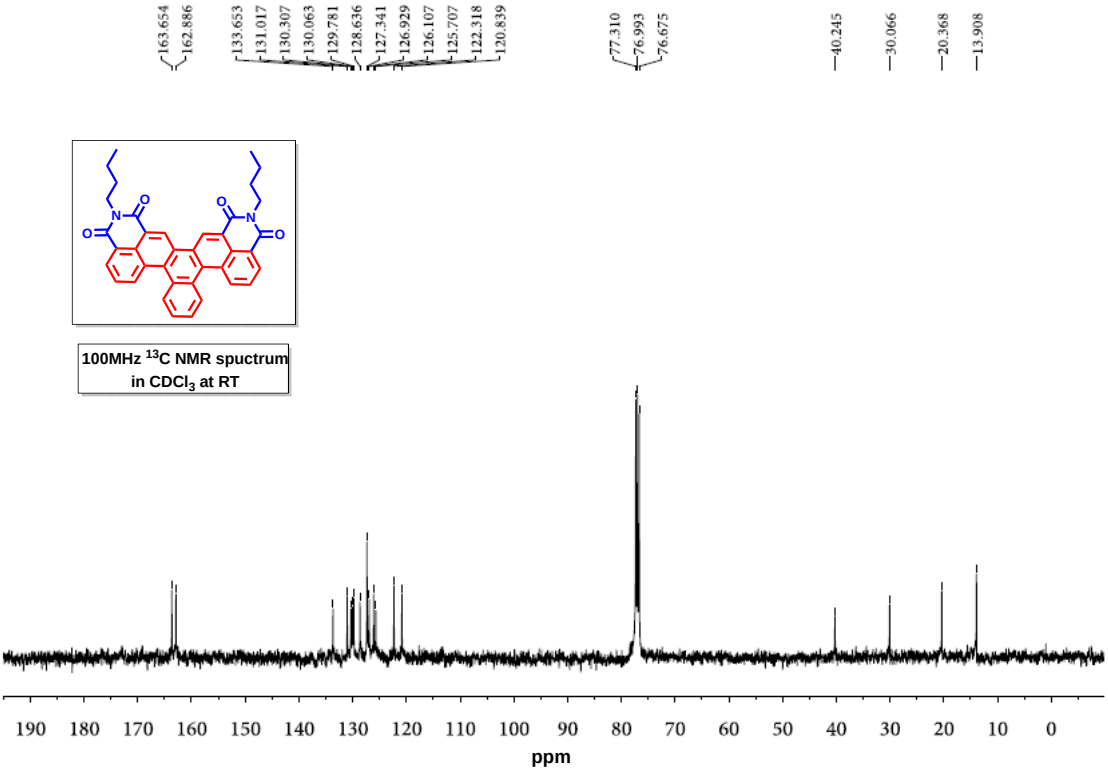
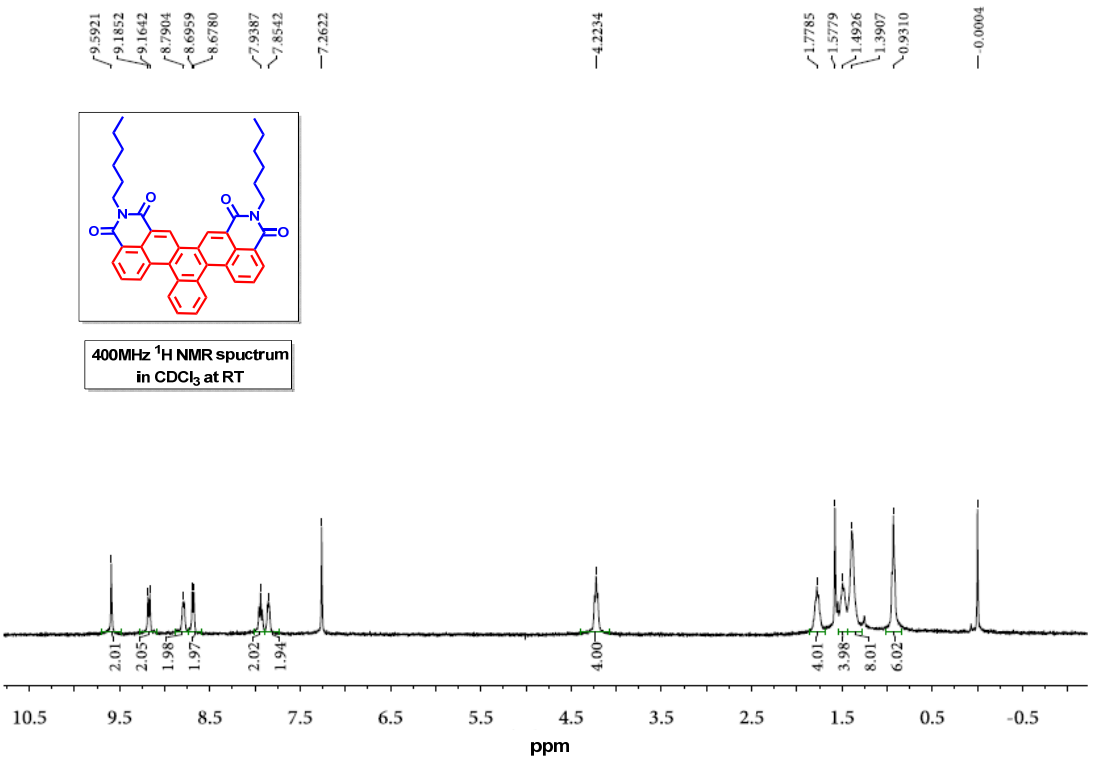
8.7387
8.7244
8.5534
7.9707
7.9574
7.9445
7.2654
4.2182
4.2060
4.1935
1.7520
1.7395
1.7280
1.5993
1.4839
1.4716
1.4592
1.4469
1.0022
0.9901
0.9780
-0.0002
Br
Br
600MHz ^{1}H NMR spuctrum
in CDCl$_3$ at RT
3.97
2.01
2.02
4.00
4.01
4.03
6.00
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
ppm

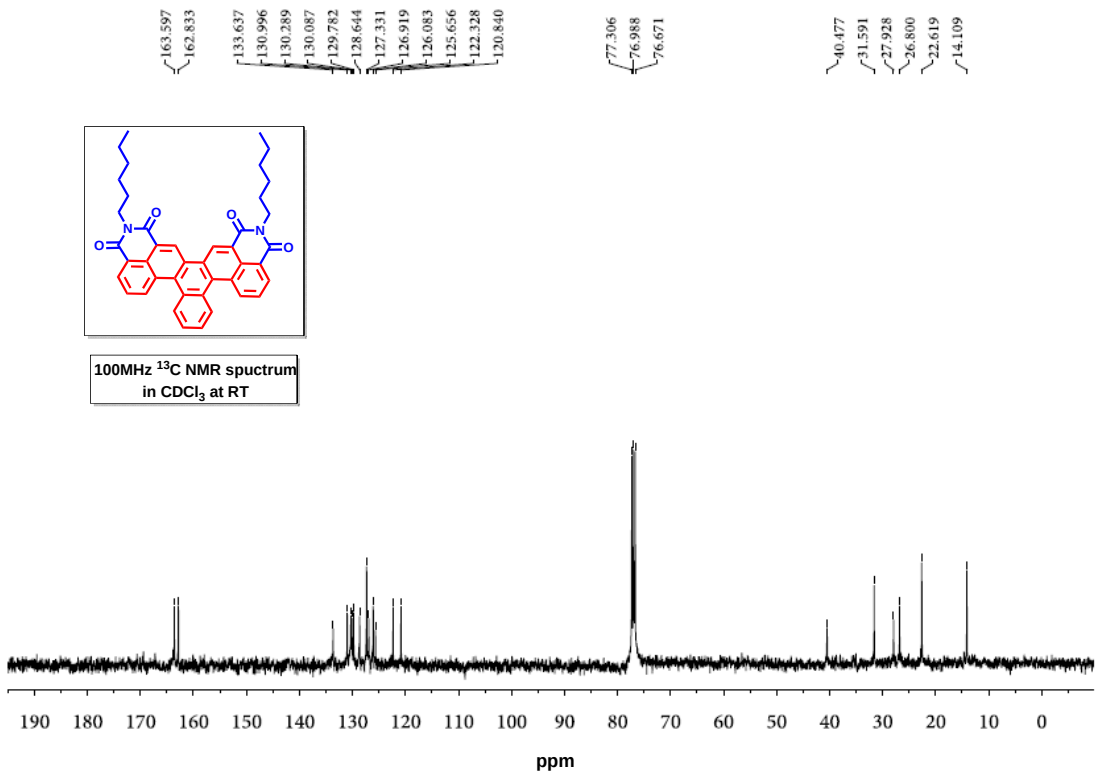

8.7562
8.7391
8.7231
8.5536
7.9686
7.9558
7.9433
7.2657
4.2027
4.1914
4.1800
1.7470
1.6042
1.4397
1.3444
0.8947
0.0000
Br
Br
600MHz ^{1}H NMR spuctrum
in CDCl$_3$ at RT
4.00
1.99
2.01
4.00
3.98
3.98
8.01
6.02
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
ppm


9.3611
9.1302
9.1162
8.7389
8.6485
8.6366
7.9290
7.9165
7.8479
7.2658
4.2040
4.1917
4.1791
1.7485
1.7367
1.7249
1.6182
1.5293
1.5168
1.5043
1.4923
1.0487
1.0364
1.0241
0.0000
600MHz ^{1}H NMR spuctrum in CDCl$_3$ at RT
2.02
1.98
2.01
1.98
1.99
2.03
4.00
3.98
3.99
5.99
10.5
9.5
8.5
7.5
6.5
5.5
4.5
3.5
2.5
1.5
0.5
-0.5
ppm

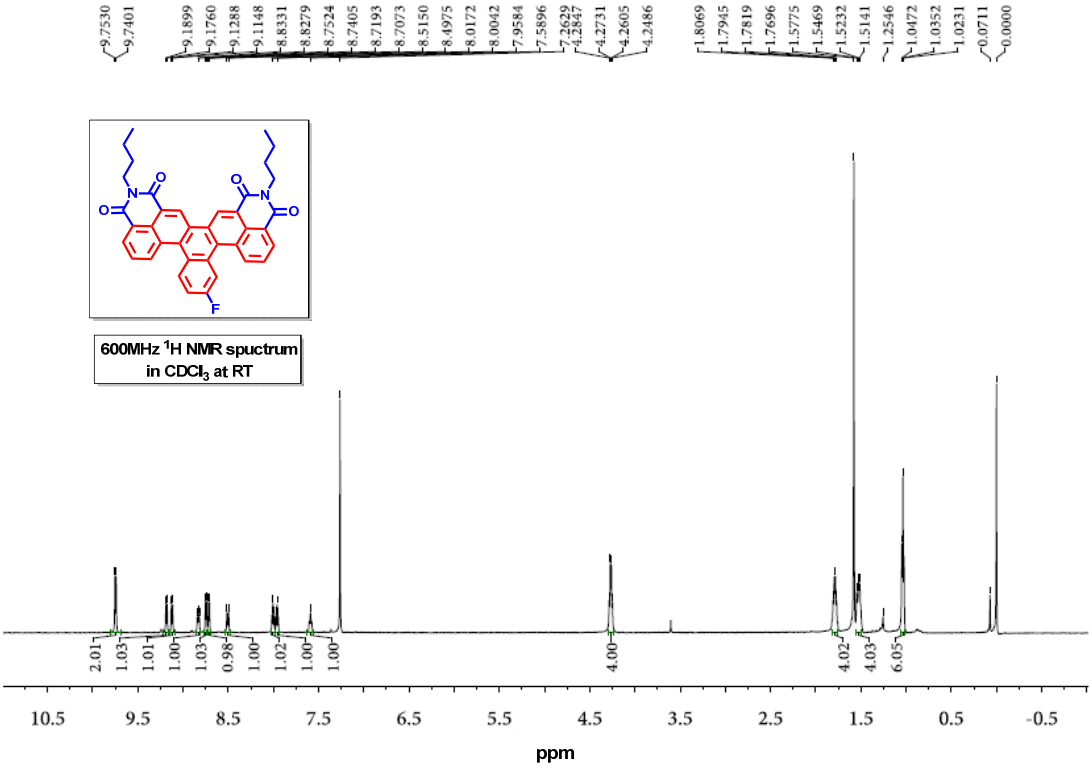

163.654
162.886
133.653
131.017
130.307
130.063
129.781
128.636
127.341
126.929
126.107
125.707
122.318
120.839
77.310
76.993
76.675
40.245
30.066
20.368
13.908
100MHz ^{13}C NMR spuctrum in CDCl$_3$ at RT
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
ppm



400MHz ^{1}H NMR spuctrum in $CDCl_3$ at RT



100MHz ^{13}C NMR spuctrum in $CDCl_3$ at RT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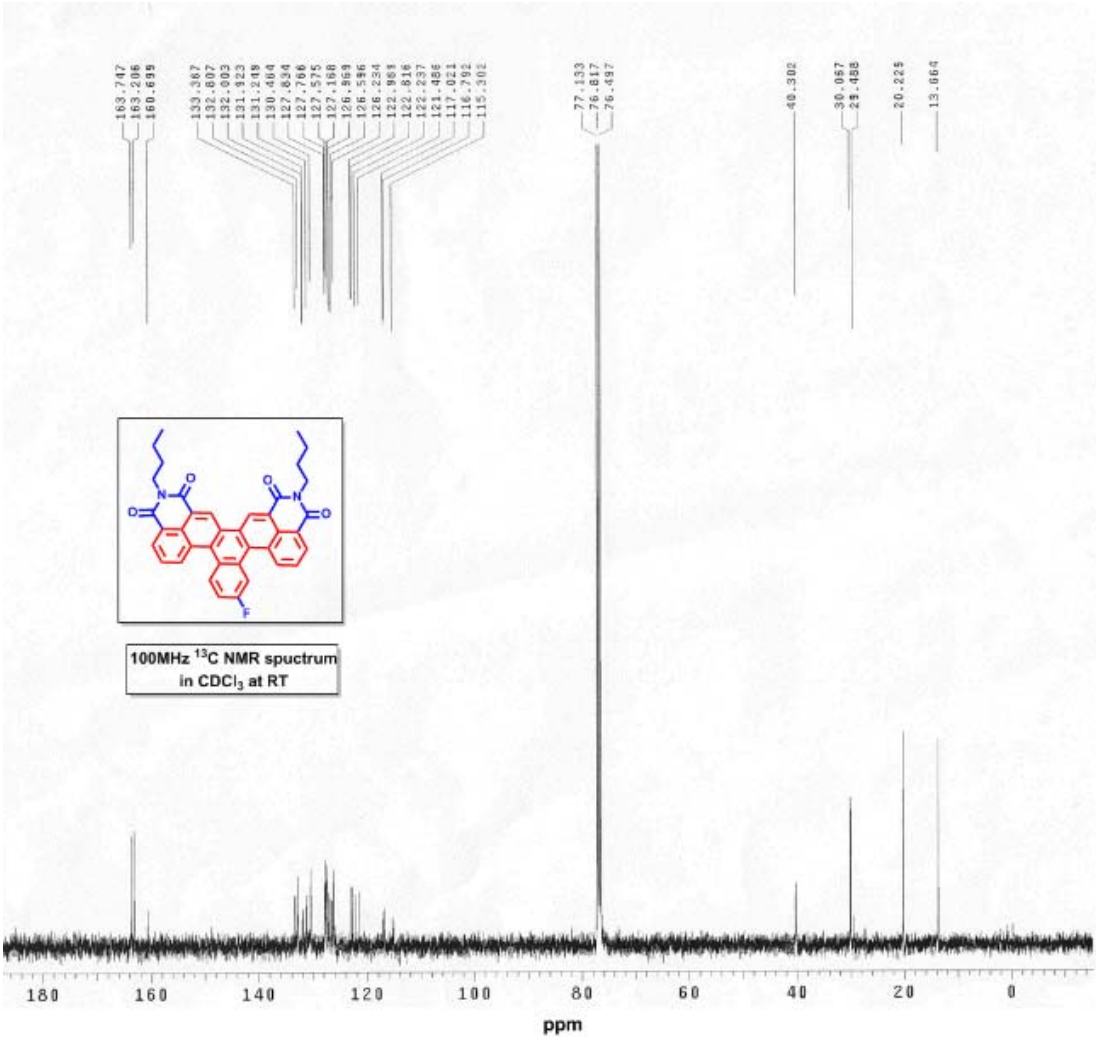
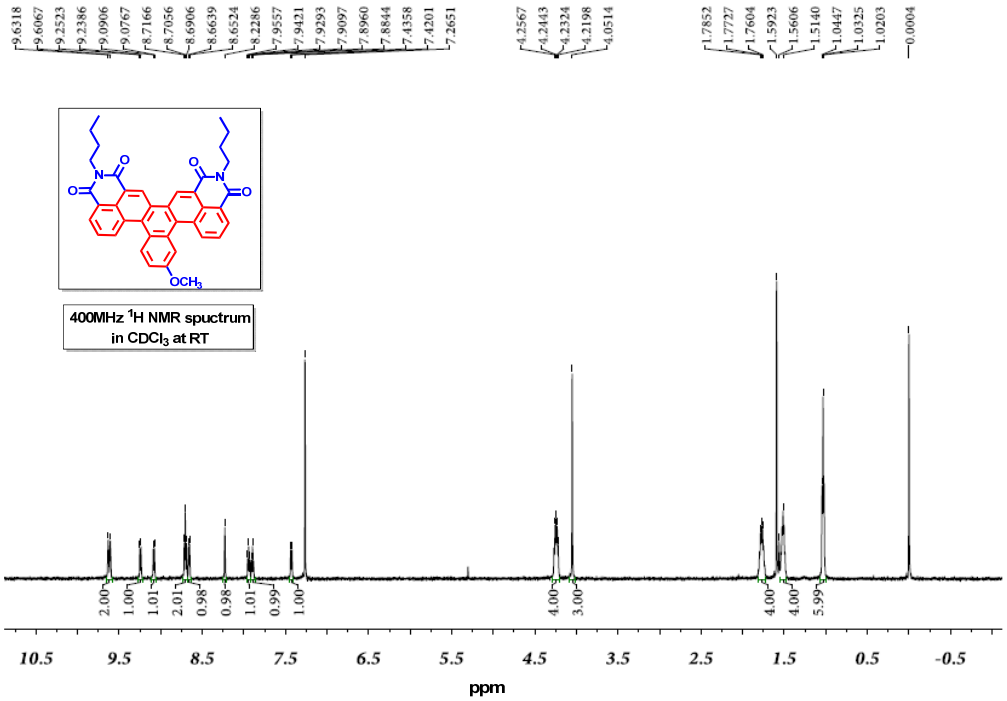

100MHz ^{13}C NMR spuctrum
in $CDCl_3$ at RT
ppm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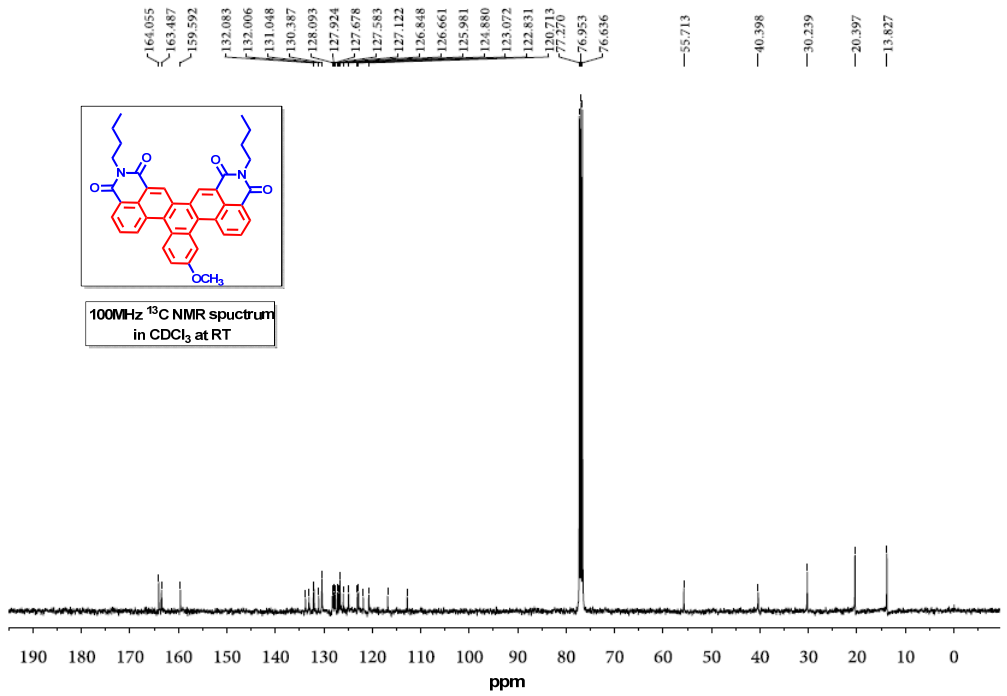
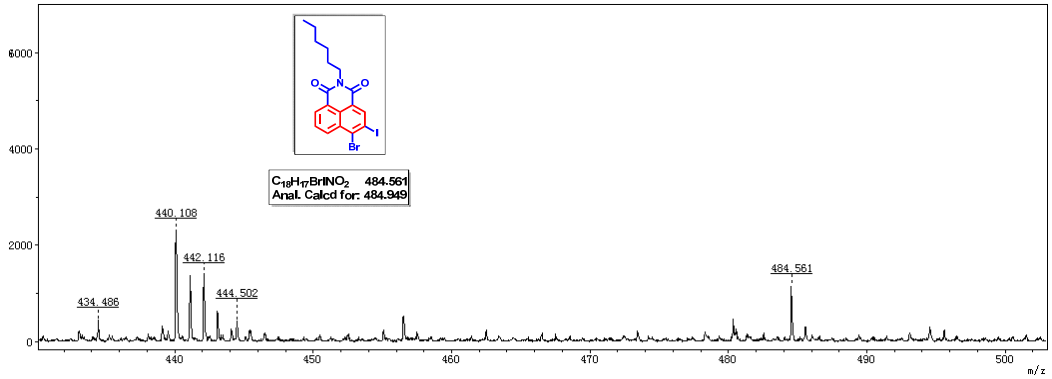
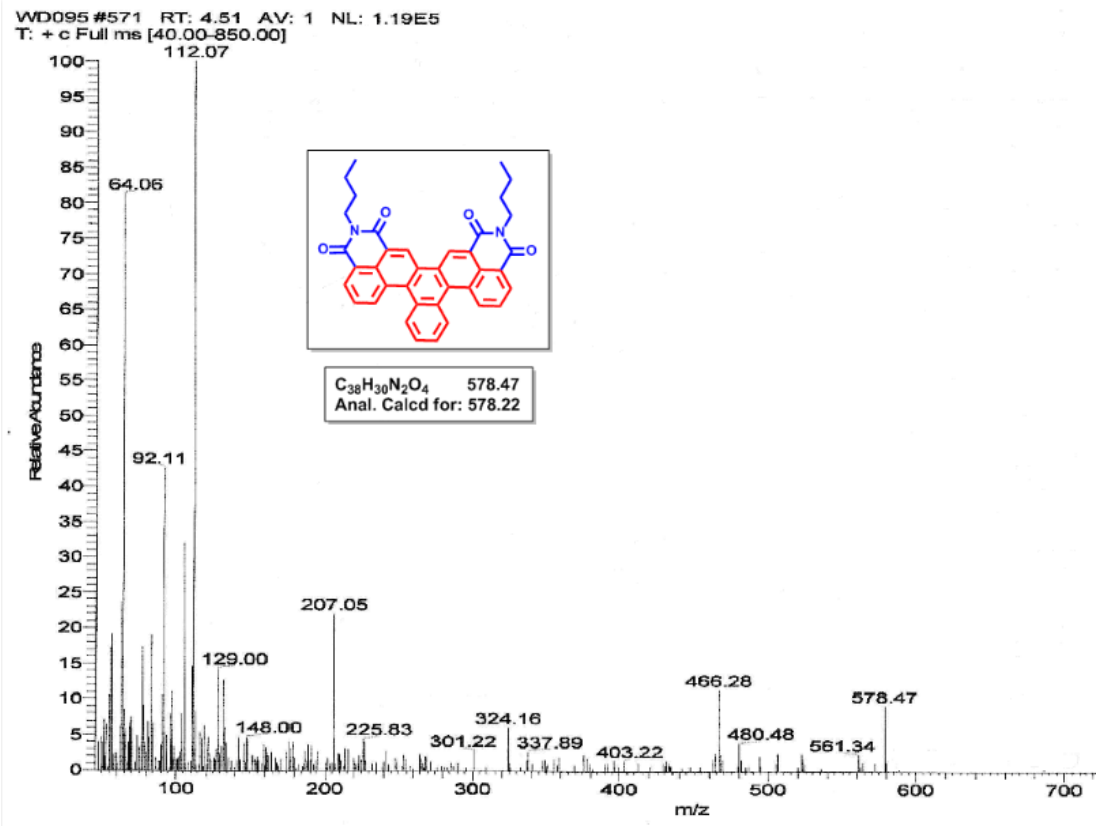

100MHz ^{13}C NMR spuctrum
in $CDCl_3$ at RT
ppm


$C_{18}H_{17}BrINO_2$ 484.561
Anal. Calcd for: 484.949
440.108
442.116
444.502
434.486
484.561
m/z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Relative Abundance
m/z
112.07
64.06
92.11
207.05
129.00
148.00
225.83
301.22
324.16
337.89
403.22
466.28
480.48
561.34
578.47
C38H30N2O4 578.47
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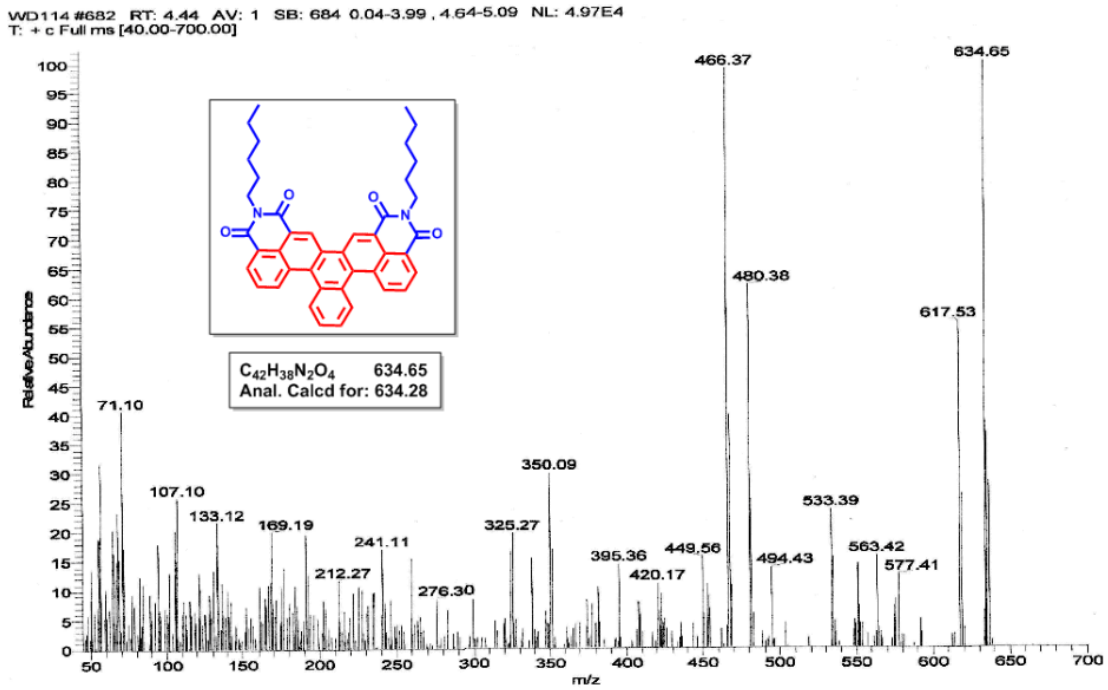
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107.10
133.12
169.19
212.27
241.11
276.30
325.27
350.09
395.36
420.17
449.56
466.37
480.38
494.43
533.39
563.42
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634.65
C42H38N2O4 634.65
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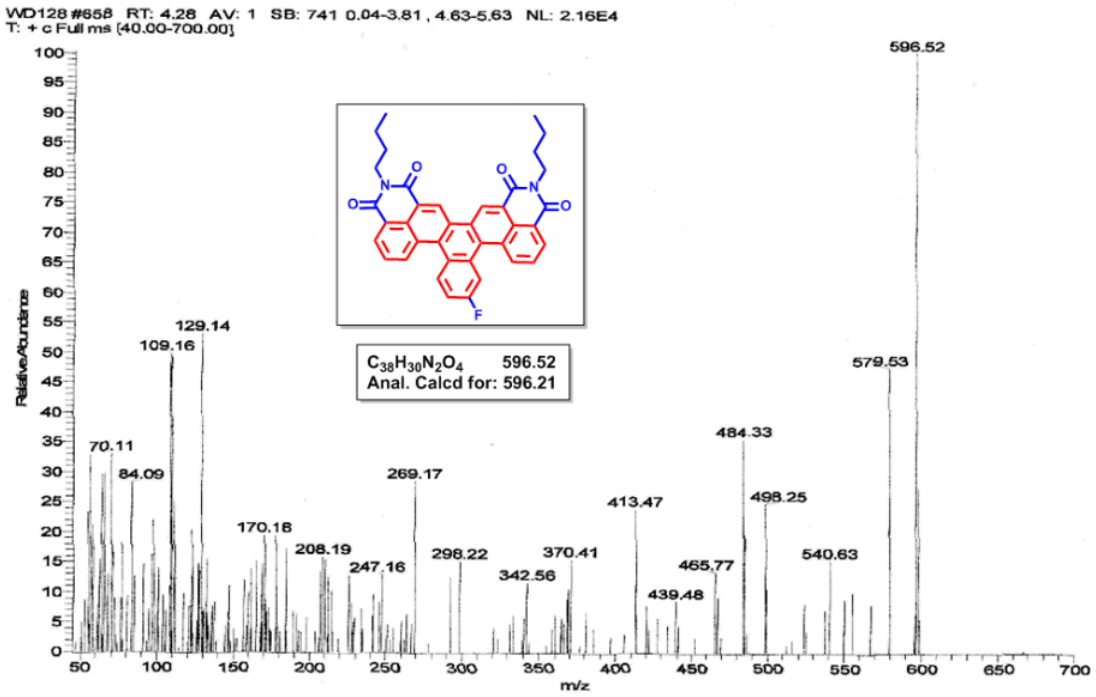
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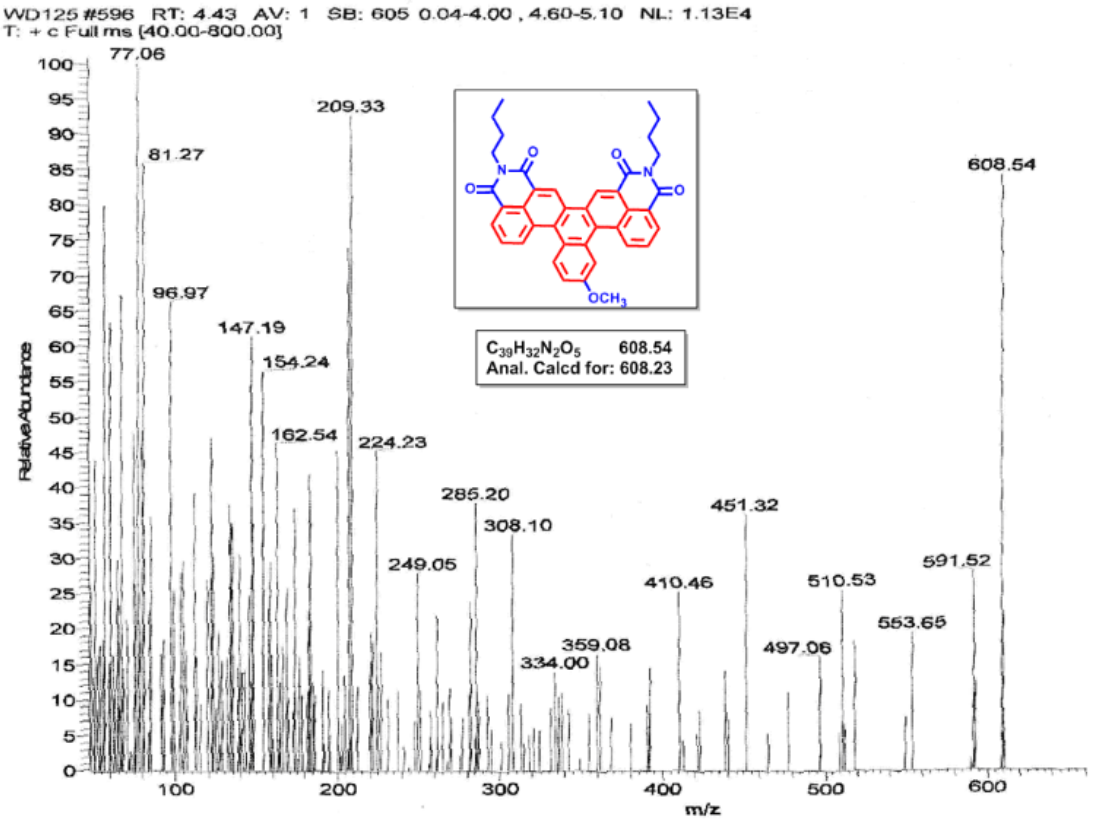
129.14
109.16
579.53
70.11
84.09
484.33
269.17
413.47
498.25
170.18
208.19
298.22
370.41
247.16
342.56
465.77
540.63
439.48
C38H30N2O4 596.52
Anal. Calcd for: 596.21
Relative Abundance
m/z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209.33
608.54
81.27
96.97
147.19
154.24
162.54
224.23
285.20
308.10
451.32
249.05
591.52
410.46
510.53
553.65
359.08
334.00
497.06
OCH3
C39H32N2O5 608.54
Anal. Calcd for: 608.23
Relative Abundance
m/z

5. Tables for crystal data

Table S2 X-ray crystallographic structure and data for **1b**

formula	$C_{42}H_{38}N_2O_4$
fw	634.74
temp (K)	298(2)
cryst syst	Monoclinic
Space group	P2(1)/c
a (Å)	15.263(3)
b (Å)	28.289(5)
c (Å)	7.5628(13)
α (°)	90.00
β (°)	93.171(10)
γ (°)	90.00
V (Å^3)	3260.4(10)
Z	4
D (calcl.) (mg/m^3)	1.293
Absor.coeff. (mm^{-1})	0.658
F(000)	1344
Crystal size (mm^3)	0.15 x 0.12 x 0.10
θ Range (°)	3.29 to 42.79
Index ranges	-13≤h≤13, -24≤k≤24, -6≤l≤6
Reflections collected	13094
Independent reflec.	2278 [R(int)= 0.0757]
Max. and min. transm.	0.9371 and 0.9078
Data / restr. / param.	2278 / 22 / 436
Goodness-of-fit / F2	1.412
Final R indices [I>2sigma(I)]	R1 = 0.1105, wR2 = 0.3010
*R*ind (all data)	R1 = 0.1270, wR2 = 0.3210
diff. peak and hole	0.566 and - 0.317e.$^{-3}$

Table S3. Selective bond lengths [Å] and angles [°] of **1b**

O(3)-C(29)	1.240(10)	C(16)-H(16)	0.9300
O(4)-C(30)	1.208(10)	C(15)-C(14)	1.373(10)
C(25)-C(26)	1.376(10)	C(15)-H(15)	0.9300
C(25)-C(24)	1.427(11)	C(14)-C(13)	1.385(10)
C(25)-H(25)	0.9300	C(14)-H(14)	0.9300
C(26)-C(27)	1.374(12)	C(5)-C(4)	1.371(10)
C(26)-H(26)	0.9300	C(5)-C(6)	1.416(10)
C(27)-C(28)	1.393(12)	C(5)-H(5)	0.9300
C(27)-H(27)	0.9300	C(4)-C(3)	1.413(11)
C(17)-C(16)	1.367(10)	C(4)-H(4)	0.9300
C(17)-C(18)	1.402(11)	C(3)-C(2)	1.357(10)
C(17)-H(17)	0.9300	C(3)-H(3)	0.9300
C(16)-C(15)	1.389(11)	O(1)-C(1)	1.231(9)
O(2)-C(9)	1.212(10)	C(40)-C(41)	1.492(17)
N(2)-C(30)	1.390(11)	C(40)-C(39)	1.529(15)

N(2)-C(29)	1.403(12)	C(40)-H(40A)	0.9700
N(2)-C(37)	1.458(10)	C(40)-H(40B)	0.9700
C(10)-C(8)	1.382(9)	C(39)-H(39A)	0.9700
C(10)-C(11)	1.426(10)	C(39)-H(39B)	0.9700
C(10)-H(10)	0.9300	C(42)-C(41)	1.370(17)
C(8)-C(7)	1.403(10)	C(42)-H(42A)	0.9600
C(8)-C(9)	1.471(12)	C(42)-H(42B)	0.9600
N(1)-C(1)	1.372(11)	C(42)-H(42C)	0.9600
N(1)-C(9)	1.394(11)	C(41)-H(41A)	0.9700
N(1)-C(31)	1.475(9)	C(41)-H(41B)	0.9700
C(23)-C(22)	1.389(11)	C(26)-C(25)-C(24)	122.4(8)
C(23)-C(28)	1.414(11)	C(26)-C(25)-H(25)	118.8
C(23)-C(24)	1.422(11)	C(24)-C(25)-H(25)	118.8
C(24)-C(19)	1.453(11)	C(27)-C(26)-C(25)	119.7(8)
C(28)-C(29)	1.463(12)	C(27)-C(26)-H(26)	120.2
C(18)-C(13)	1.431(10)	C(25)-C(26)-H(26)	120.2
C(18)-C(19)	1.442(10)	C(26)-C(27)-C(28)	121.0(9)
C(13)-C(12)	1.461(10)	C(26)-C(27)-H(27)	119.5
C(2)-C(7)	1.435(10)	C(28)-C(27)-H(27)	119.5
C(2)-C(1)	1.487(11)	C(16)-C(17)-C(18)	124.0(8)
C(7)-C(6)	1.409(10)	C(16)-C(17)-H(17)	118.0
C(30)-C(22)	1.492(12)	C(18)-C(17)-H(17)	118.0
C(22)-C(21)	1.360(10)	C(17)-C(16)-C(15)	119.2(8)
C(21)-C(20)	1.428(11)	C(17)-C(16)-H(16)	120.4
C(21)-H(21)	0.9300	C(15)-C(16)-H(16)	120.4
C(20)-C(19)	1.376(10)	C(14)-C(15)-C(16)	118.9(7)
C(20)-C(11)	1.484(10)	C(14)-C(15)-H(15)	120.5
C(11)-C(12)	1.371(9)	C(16)-C(15)-H(15)	120.5
C(31)-C(32)	1.545(11)	C(15)-C(14)-C(13)	122.6(8)
C(31)-H(31A)	0.9700	C(15)-C(14)-H(14)	118.7
C(31)-H(31B)	0.9700	C(13)-C(14)-H(14)	118.7
C(32)-C(33)	1.470(11)	C(4)-C(5)-C(6)	121.5(8)
C(32)-H(32A)	0.9700	C(4)-C(5)-H(5)	119.2
C(32)-H(32B)	0.9700	C(6)-C(5)-H(5)	119.2
C(33)-C(34)	1.520(13)	C(5)-C(4)-C(3)	120.0(7)
C(33)-H(33A)	0.9700	C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0	O(3)-C(29)-C(28)	122.0(12)
C(2)-C(3)-C(4)	119.8(8)	N(2)-C(29)-C(28)	118.0(10)

C(2)-C(3)-H(3)	120.1	O(4)-C(30)-N(2)	120.5(10)
C(4)-C(3)-H(3)	120.1	O(4)-C(30)-C(22)	122.3(10)
C(30)-N(2)-C(29)	123.4(9)	N(2)-C(30)-C(22)	117.1(10)
C(30)-N(2)-C(37)	117.8(9)	C(21)-C(22)-C(23)	120.7(9)
C(29)-N(2)-C(37)	118.6(9)	C(21)-C(22)-C(30)	118.1(11)
C(8)-C(10)-C(11)	119.8(7)	C(23)-C(22)-C(30)	121.0(10)
C(8)-C(10)-H(10)	120.1	C(22)-C(21)-C(20)	121.1(8)
C(11)-C(10)-H(10)	120.1	C(22)-C(21)-H(21)	119.5
C(10)-C(8)-C(7)	119.9(8)	C(20)-C(21)-H(21)	119.5
C(10)-C(8)-C(9)	119.9(10)	C(19)-C(20)-C(21)	119.5(8)
C(7)-C(8)-C(9)	120.1(11)	C(19)-C(20)-C(11)	119.3(9)
C(1)-N(1)-C(9)	123.3(8)	C(21)-C(20)-C(11)	121.1(10)
C(1)-N(1)-C(31)	118.3(9)	C(12)-C(11)-C(10)	121.0(8)
C(9)-N(1)-C(31)	118.3(9)	C(12)-C(11)-C(20)	120.6(9)
C(22)-C(23)-C(28)	119.7(11)	C(10)-C(11)-C(20)	118.4(10)
C(22)-C(23)-C(24)	120.2(9)	O(2)-C(9)-N(1)	120.2(10)
C(28)-C(23)-C(24)	120.0(11)	O(2)-C(9)-C(8)	121.8(10)
C(23)-C(24)-C(25)	116.6(9)	N(1)-C(9)-C(8)	117.9(10)
C(23)-C(24)-C(19)	118.1(9)	N(1)-C(31)-C(32)	111.3(7)
C(25)-C(24)-C(19)	125.0(11)	N(1)-C(31)-H(31A)	109.4
C(27)-C(28)-C(23)	119.9(10)	C(32)-C(31)-H(31A)	109.4
C(27)-C(28)-C(29)	119.5(11)	N(1)-C(31)-H(31B)	109.4
C(23)-C(28)-C(29)	120.6(11)	C(32)-C(31)-H(31B)	109.4
C(17)-C(18)-C(13)	115.6(8)	H(31A)-C(31)-H(31B)	108.0
C(17)-C(18)-C(19)	124.6(10)	C(33)-C(32)-C(31)	115.0(8)
C(13)-C(18)-C(19)	119.1(8)	C(33)-C(32)-H(32A)	108.5
C(14)-C(13)-C(18)	119.5(8)	C(31)-C(32)-H(32A)	108.5
C(14)-C(13)-C(12)	120.3(10)	C(33)-C(32)-H(32B)	108.5
C(18)-C(13)-C(12)	119.6(8)	C(31)-C(32)-H(32B)	108.5
C(3)-C(2)-C(7)	121.6(9)	H(32A)-C(32)-H(32B)	107.5
C(3)-C(2)-C(1)	120.9(11)	C(32)-C(33)-C(34)	114.6(10)
C(7)-C(2)-C(1)	117.4(10)	C(32)-C(33)-H(33A)	108.6
C(8)-C(7)-C(6)	120.7(9)	C(34)-C(33)-H(33A)	108.6
C(8)-C(7)-C(2)	120.9(10)	C(32)-C(33)-H(33B)	108.6
C(6)-C(7)-C(2)	118.4(10)	C(34)-C(33)-H(33B)	108.6
O(3)-C(29)-N(2)	120.0(11)	H(33A)-C(33)-H(33B)	107.6
C(33)-C(34)-C(35)	111.8(12)	H(36A)-C(36)-H(36B)	109.5
C(33)-C(34)-H(34A)	109.3	C(35)-C(36)-H(36C)	109.5

C(35)-C(34)-H(34A)	109.3	H(36A)-C(36)-H(36C)	109.5
C(33)-C(34)-H(34B)	109.3	H(36B)-C(36)-H(36C)	109.5
C(35)-C(34)-H(34B)	109.3	C(41)-C(40)-C(39)	107.5(16)
H(34A)-C(34)-H(34B)	107.9	C(41)-C(40)-H(40A)	110.2
C(20)-C(19)-C(18)	118.8(9)	C(39)-C(40)-H(40A)	110.2
C(20)-C(19)-C(24)	119.4(8)	C(41)-C(40)-H(40B)	110.2
C(18)-C(19)-C(24)	121.7(10)	C(39)-C(40)-H(40B)	110.2
C(11)-C(12)-C(6)	118.2(9)	H(40A)-C(40)-H(40B)	108.5
C(11)-C(12)-C(13)	117.1(9)	C(38)-C(39)-C(40)	117.1(16)
C(6)-C(12)-C(13)	124.7(10)	C(38)-C(39)-H(39A)	108.0
C(7)-C(6)-C(5)	118.6(9)	C(40)-C(39)-H(39A)	108.0
C(7)-C(6)-C(12)	118.5(9)	C(38)-C(39)-H(39B)	108.0
C(5)-C(6)-C(12)	122.6(10)	C(40)-C(39)-H(39B)	108.0
O(1)-C(1)-N(1)	120.6(10)	H(39A)-C(39)-H(39B)	107.3
O(1)-C(1)-C(2)	119.5(11)	C(41)-C(42)-H(42A)	109.5
N(1)-C(1)-C(2)	119.9(9)	C(41)-C(42)-H(42B)	109.5
N(2)-C(37)-C(38)	114.8(9)	H(42A)-C(42)-H(42B)	109.5
N(2)-C(37)-H(37A)	108.6	C(41)-C(42)-H(42C)	109.5
C(38)-C(37)-H(37A)	108.6	H(42A)-C(42)-H(42C)	109.5
N(2)-C(37)-H(37B)	108.6	H(42B)-C(42)-H(42C)	109.5
C(38)-C(37)-H(37B)	108.6	C(42)-C(41)-C(40)	121.8(18)
H(37A)-C(37)-H(37B)	107.5	C(42)-C(41)-H(41A)	106.9
C(39)-C(38)-C(37)	124.5(14)	C(40)-C(41)-H(41A)	106.9
C(39)-C(38)-H(38A)	106.2	C(42)-C(41)-H(41B)	106.9
C(37)-C(38)-H(38A)	106.2	C(40)-C(41)-H(41B)	106.9
C(39)-C(38)-H(38B)	106.2	H(41A)-C(41)-H(41B)	106.7
C(37)-C(38)-H(38B)	106.2		
H(38A)-C(38)-H(38B)	106.4		
C(36)-C(35)-C(34)	114.9(15)		
C(36)-C(35)-H(35A)	108.5		
C(34)-C(35)-H(35A)	108.5		
C(36)-C(35)-H(35B)	108.5		
C(34)-C(35)-H(35B)	108.5		
H(35A)-C(35)-H(35B)	107.5		
C(35)-C(36)-H(36A)	109.5		
C(35)-C(36)-H(36B)	109.5		

Table S4 X-ray crystallographic structure and data for **1d**

formula	$C_{39}H_{32}N_2O_5$
fw	608.67
temp (K)	298(2)
cryst syst	Monoclinic
Space group	Pc
a (Å)	12.7675(2)
b (Å)	31.0308(5)
c (Å)	7.55930(10)
α (°)	90.00
β (°)	93.9960(10)
γ (°)	90.00
V (Å^3)	2987.61(8)
Z	4
D (calcl.) (mg/m^3)	1.353
Absor.coeff. (mm^{-1})	0.722
F(000)	1280
Crystal size (mm^3)	0.15 x 0.12 x 0.10
θ Range (°)	2.85 to 51.28
Index ranges	-12≤h≤12, -31≤k≤31, -7≤l≤7
Reflections collected	20731
Independent reflec.	3177 [R(int)= 0.0266]
Max. and min. transm.	0.9313 and 0.8894
Data / restr. / param.	3177 / 26 / 468
Goodness-of-fit / F2	1.115
Final R indices [I>2sigma(I)]	R1 = 0.0625, wR2 = 0.1466
*R*ind (all data)	R1 = 0.0650, wR2 = 0.1483
diff. peak and hole	0.312 and -0.212e.$^{-3}$

Table S5. Selective bond lengths [Å] and angles [°] of **1d**

C(1)-O(1')	1.316(8)	C(8)-C(21)	1.405(5)
C(1)-C(6)	1.357(6)	C(8)-C(9)	1.460(5)
C(1)-C(2)	1.382(6)	C(9)-C(10)	1.400(5)
C(1)-H(1)	0.9482	C(9)-C(18)	1.412(5)
C(2)-O(1)	1.356(5)	C(10)-C(11)	1.447(5)
C(2)-C(3)	1.380(6)	C(11)-C(12)	1.406(5)
C(2)-H(2)	0.9563	C(11)-C(16)	1.416(5)
C(3)-C(4)	1.409(5)	C(12)-C(13)	1.370(5)
C(3)-H(3)	0.9300	C(12)-H(12)	0.9300
C(4)-C(5)	1.417(5)	C(13)-C(14)	1.384(6)
C(4)-C(10)	1.455(5)	C(13)-H(13)	0.9300
C(5)-C(6)	1.398(5)	C(14)-C(15)	1.368(6)
C(5)-C(7)	1.449(5)	C(14)-H(14)	0.9300
C(6)-H(6)	0.9300	C(15)-C(16)	1.412(5)
C(7)-C(8)	1.403(5)	C(15)-C(20)	1.478(6)
C(7)-C(24)	1.447(5)	C(16)-C(17)	1.412(5)
C(29)-N(1)	1.391(6)	C(17)-C(18)	1.364(5)
C(30)-O(5)	1.215(5)	C(17)-C(19)	1.472(5)

C(30)-N(1)	1.396(5)	C(18)-H(18)	0.9300
C(31)-N(2)	1.496(5)	C(19)-O(2)	1.216(5)
C(31)-C(32')	1.497(15)	C(19)-N(2)	1.396(5)
C(31)-C(32)	1.500(9)	C(20)-O(3)	1.213(5)
C(31)-H(31A)	0.9700	C(20)-N(2)	1.396(5)
C(31)-H(31B)	0.9700	C(21)-C(22)	1.366(5)
C(31)-H(31C)	0.9700	C(21)-H(21)	0.9300
C(31)-H(31D)	0.9700	C(22)-C(23)	1.408(5)
C(32)-C(33)	1.530(10)	C(22)-C(30)	1.463(6)
C(32)-H(32A)	0.9700	C(23)-C(28)	1.412(5)
C(32)-H(32B)	0.9700	C(23)-C(24)	1.414(5)
C(33)-C(34)	1.502(10)	C(24)-C(25)	1.418(5)
C(33)-H(33A)	0.9700	C(25)-C(26)	1.368(6)
C(33)-H(33B)	0.9700	C(25)-H(25)	0.9300
C(34)-H(34A)	0.9600	C(26)-C(27)	1.394(6)
C(34)-H(34B)	0.9600	C(26)-H(26)	0.9300
C(34)-H(34C)	0.9600	C(27)-C(28)	1.371(6)
C(32')-C(33')	1.544(17)	C(27)-H(27)	0.9300
C(32')-H(32C)	0.9700	C(28)-C(29)	1.470(6)
C(32')-H(32D)	0.9700	C(29)-O(4)	1.225(5)
C(33')-C(34')	1.464(19)	C(38)-H(38A)	0.9600
C(33')-H(33C)	0.9700	C(38)-H(38B)	0.9600
C(33')-H(33D)	0.9700	C(38)-H(38C)	0.9600
C(34')-H(34D)	0.9600	C(76)-O(1)	1.435(6)
C(34')-H(34E)	0.9600	C(76)-H(76A)	0.9600
C(34')-H(34F)	0.9600	C(76)-H(76B)	0.9600
C(35)-N(1)	1.471(5)	C(76)-H(76C)	0.9600
C(35)-C(36)	1.558(6)	O(1)-H(2)	0.4060
C(35)-H(35A)	0.9700	C(76')-O(1')	1.415(10)
C(35)-H(35B)	0.9700	C(76')-H(76D)	0.9600
C(36)-C(37)	1.427(6)	C(76')-H(76E)	0.9600
C(36)-H(36A)	0.9700	C(76')-H(76F)	0.9600
C(36)-H(36B)	0.9700	O(1')-H(1)	0.4381
C(37)-C(38)	1.510(7)	O(1')-C(1)-C(6)	132.0(7)
C(37)-H(37A)	0.9700	O(1')-C(1)-C(2)	108.6(6)
C(37)-H(37B)	0.9700	C(6)-C(1)-C(2)	119.3(4)
C(11)-C(12)-H(12)	119.2	O(1')-C(1)-H(1)	12.2
C(12)-C(13)-C(14)	121.1(4)	C(6)-C(1)-H(1)	120.7

C(12)-C(13)-H(13)	119.5	C(2)-C(1)-H(1)	120.0
C(14)-C(13)-H(13)	119.5	O(1)-C(2)-C(3)	118.9(5)
C(15)-C(14)-C(13)	119.5(4)	O(1)-C(2)-C(1)	120.9(5)
C(15)-C(14)-H(14)	120.3	C(3)-C(2)-C(1)	120.0(4)
C(13)-C(14)-H(14)	120.3	O(1)-C(2)-H(2)	3.6
C(14)-C(15)-C(16)	120.3(4)	C(3)-C(2)-H(2)	121.3
C(14)-C(15)-C(20)	119.6(4)	C(1)-C(2)-H(2)	118.8
C(16)-C(15)-C(20)	120.1(4)	C(2)-C(3)-C(4)	121.6(4)
C(15)-C(16)-C(17)	119.6(4)	C(2)-C(3)-H(3)	119.2
C(15)-C(16)-C(11)	120.5(4)	C(4)-C(3)-H(3)	119.2
C(17)-C(16)-C(11)	119.9(3)	C(3)-C(4)-C(5)	117.8(4)
C(18)-C(17)-C(16)	119.9(4)	C(3)-C(4)-C(10)	121.6(4)
C(18)-C(17)-C(19)	118.8(4)	C(5)-C(4)-C(10)	119.9(3)
C(16)-C(17)-C(19)	121.2(3)	C(6)-C(5)-C(4)	118.2(4)
C(17)-C(18)-C(9)	121.9(3)	C(6)-C(5)-C(7)	121.2(4)
C(17)-C(18)-H(18)	119.1	C(4)-C(5)-C(7)	119.9(3)
C(9)-C(18)-H(18)	119.1	C(1)-C(6)-C(5)	123.0(4)
O(2)-C(19)-N(2)	120.4(4)	C(1)-C(6)-H(6)	118.5
O(2)-C(19)-C(17)	122.5(4)	C(5)-C(6)-H(6)	118.5
N(2)-C(19)-C(17)	117.1(4)	C(8)-C(7)-C(24)	118.5(3)
O(3)-C(20)-N(2)	119.2(4)	C(8)-C(7)-C(5)	117.3(3)
O(3)-C(20)-C(15)	122.9(4)	C(24)-C(7)-C(5)	124.1(3)
N(2)-C(20)-C(15)	117.9(4)	C(7)-C(8)-C(21)	119.0(3)
C(22)-C(21)-C(8)	122.3(4)	C(7)-C(8)-C(9)	120.0(3)
C(22)-C(21)-H(21)	118.8	C(21)-C(8)-C(9)	121.0(3)
C(8)-C(21)-H(21)	118.8	C(10)-C(9)-C(18)	119.5(3)
C(21)-C(22)-C(23)	119.7(4)	C(10)-C(9)-C(8)	120.2(3)
C(21)-C(22)-C(30)	119.3(4)	C(18)-C(9)-C(8)	120.3(3)
C(23)-C(22)-C(30)	121.0(4)	C(9)-C(10)-C(11)	118.6(3)
C(22)-C(23)-C(28)	119.6(4)	C(9)-C(10)-C(4)	117.3(3)
C(22)-C(23)-C(24)	119.8(3)	C(11)-C(10)-C(4)	123.9(3)
C(28)-C(23)-C(24)	120.6(4)	C(12)-C(11)-C(16)	116.7(3)
C(23)-C(24)-C(25)	116.8(3)	C(12)-C(11)-C(10)	124.4(4)
C(23)-C(24)-C(7)	119.0(3)	C(16)-C(11)-C(10)	118.9(3)
C(25)-C(24)-C(7)	124.0(4)	C(13)-C(12)-C(11)	121.6(4)
C(26)-C(25)-C(24)	121.6(4)	C(13)-C(12)-H(12)	119.2
C(26)-C(25)-H(25)	119.2	C(31)-C(32)-C(33)	110.7(12)
C(24)-C(25)-H(25)	119.2	C(31)-C(32)-H(32A)	109.5

C(25)-C(26)-C(27)	120.8(4)	C(33)-C(32)-H(32A)	109.5
C(25)-C(26)-H(26)	119.6	C(31)-C(32)-H(32B)	109.5
C(27)-C(26)-H(26)	119.6	C(33)-C(32)-H(32B)	109.5
C(28)-C(27)-C(26)	119.6(4)	H(32A)-C(32)-H(32B)	108.1
C(28)-C(27)-H(27)	120.2	C(34)-C(33)-C(32)	109.9(14)
C(26)-C(27)-H(27)	120.2	C(34)-C(33)-H(33A)	109.7
C(27)-C(28)-C(23)	120.3(4)	C(32)-C(33)-H(33A)	109.7
C(27)-C(28)-C(29)	119.6(4)	C(34)-C(33)-H(33B)	109.7
C(23)-C(28)-C(29)	120.0(4)	C(32)-C(33)-H(33B)	109.7
O(4)-C(29)-N(1)	119.5(4)	H(33A)-C(33)-H(33B)	108.2
O(4)-C(29)-C(28)	122.4(5)	C(31)-C(32')-C(33')	114.1(14)
N(1)-C(29)-C(28)	118.1(4)	C(31)-C(32')-H(32C)	108.7
O(5)-C(30)-N(1)	119.7(4)	C(33')-C(32')-H(32C)	108.7
O(5)-C(30)-C(22)	122.8(4)	C(31)-C(32')-H(32D)	108.7
N(1)-C(30)-C(22)	117.5(4)	C(33')-C(32')-H(32D)	108.7
N(2)-C(31)-C(32')	108.3(10)	H(32C)-C(32')-H(32D)	107.6
N(2)-C(31)-C(32)	110.9(6)	C(34')-C(33')-C(32')	110(2)
C(32')-C(31)-C(32)	15(2)	C(34')-C(33')-H(33C)	109.6
N(2)-C(31)-H(31A)	109.5	C(32')-C(33')-H(33C)	109.6
C(32')-C(31)-H(31A)	97.3	C(34')-C(33')-H(33D)	109.6
C(32)-C(31)-H(31A)	109.5	C(32')-C(33')-H(33D)	109.6
N(2)-C(31)-H(31B)	109.5	H(33C)-C(33')-H(33D)	108.1
C(32')-C(31)-H(31B)	123.2	C(33')-C(34')-H(34D)	109.5
C(32)-C(31)-H(31B)	109.5	C(33')-C(34')-H(34E)	109.5
H(31A)-C(31)-H(31B)	108.0	H(34D)-C(34')-H(34E)	109.5
N(2)-C(31)-H(31C)	109.7	C(33')-C(34')-H(34F)	109.5
C(32')-C(31)-H(31C)	111.4	H(34D)-C(34')-H(34F)	109.5
C(32)-C(31)-H(31C)	122.0	H(34E)-C(34')-H(34F)	109.5
H(31A)-C(31)-H(31C)	15.9	N(1)-C(35)-C(36)	108.8(4)
H(31B)-C(31)-H(31C)	93.6	N(1)-C(35)-H(35A)	109.9
N(2)-C(31)-H(31D)	110.3	C(36)-C(35)-H(35A)	109.9
C(32')-C(31)-H(31D)	108.9	N(1)-C(35)-H(35B)	109.9
C(32)-C(31)-H(31D)	94.4	C(36)-C(35)-H(35B)	109.9
H(31A)-C(31)-H(31D)	121.3	H(35A)-C(35)-H(35B)	108.3
H(31B)-C(31)-H(31D)	16.6	C(37)-C(36)-C(35)	116.0(5)
H(31C)-C(31)-H(31D)	108.2	C(37)-C(36)-H(36A)	108.3