Structure-property relationship of isomeric diphenylethenyl-disubstituted dimethoxycarbazoles

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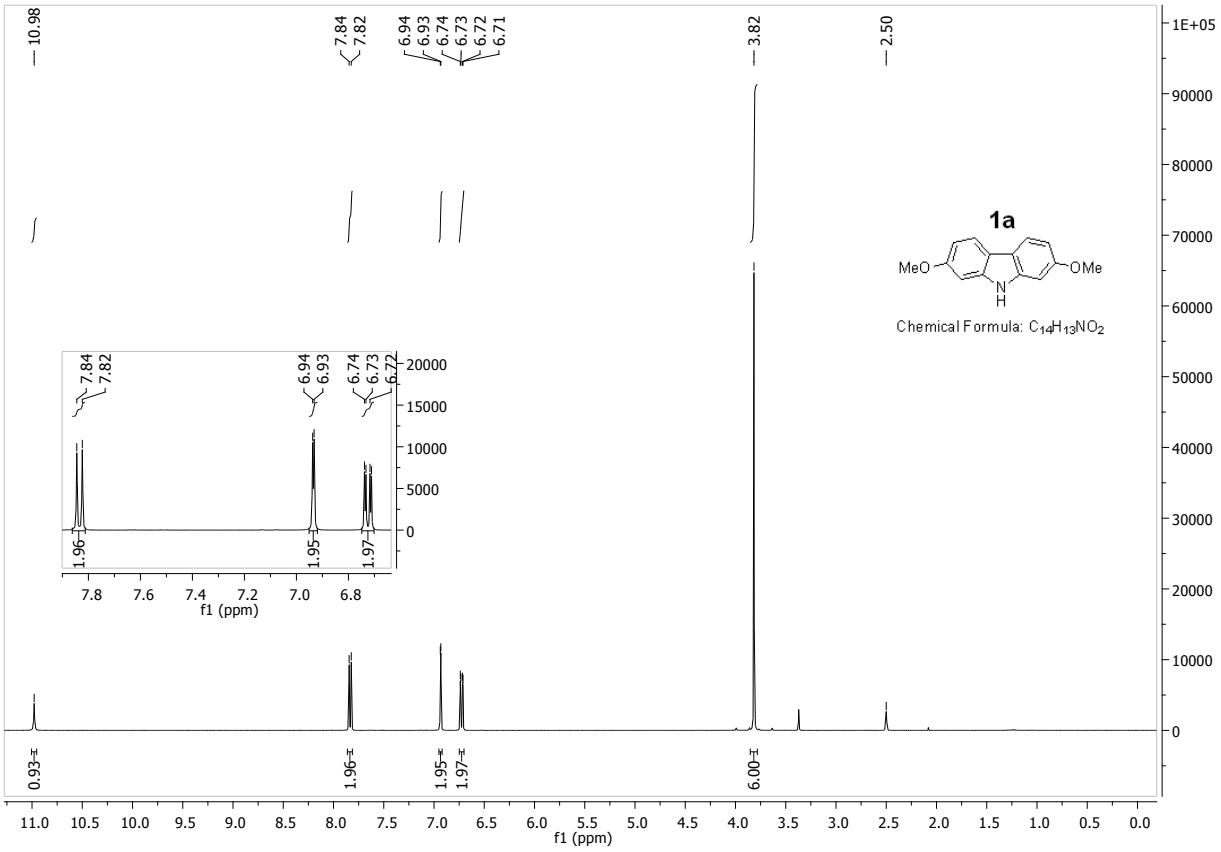
Supplementary information

Content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6.93
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6.71
3.82
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OMe
N
H
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1.95
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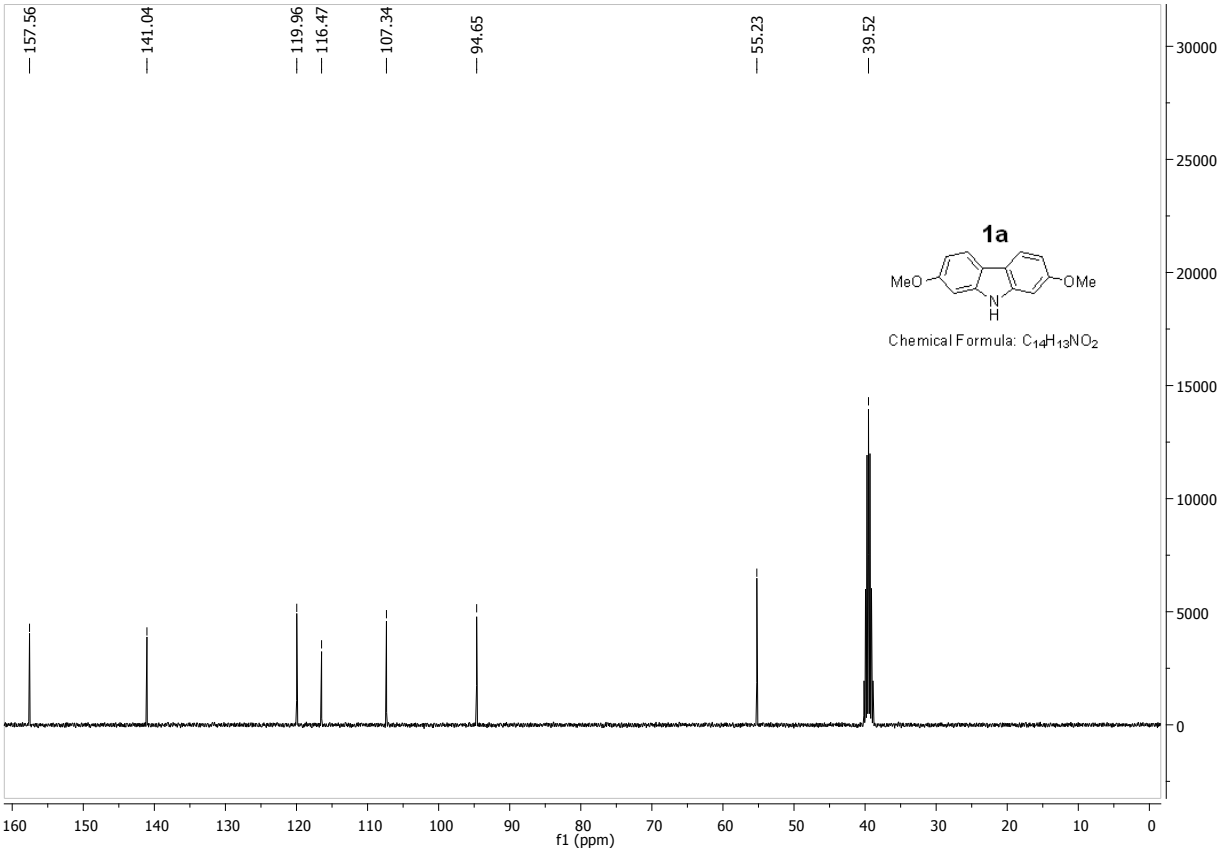
6.00
f1 (ppm)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141.04
119.96
116.47
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39.52
1a
MeO
OMe
N
H
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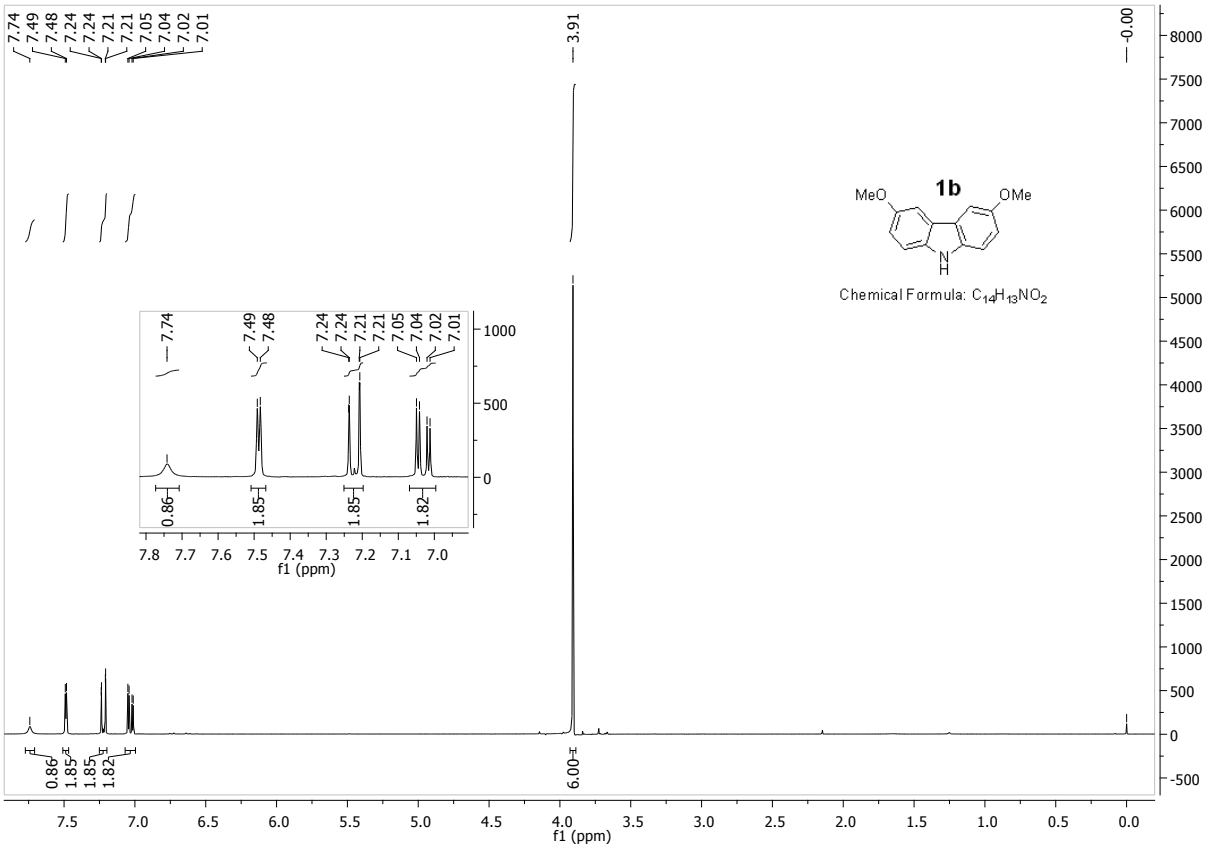
f1 (ppm)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7.49
7.48
7.24
7.24
7.21
7.21
7.05
7.04
7.02
7.01
3.91
-0.00
1b
MeO
OMe
N
H
Chemical Formula: C14H13NO2
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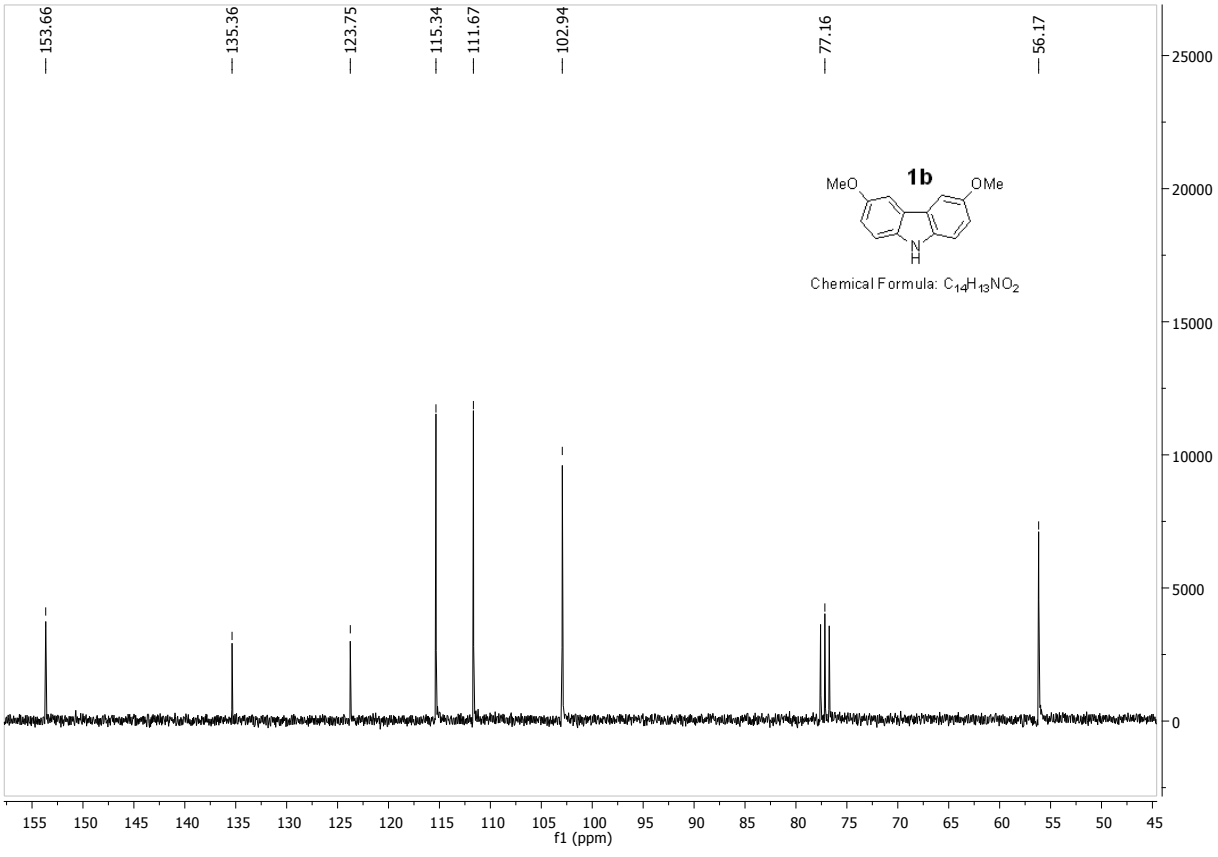
1.85
1.85
1.82
6.00
f1 (ppm)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135.36
123.75
115.34
111.67
102.94
77.16
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MeO
OMe
N
H
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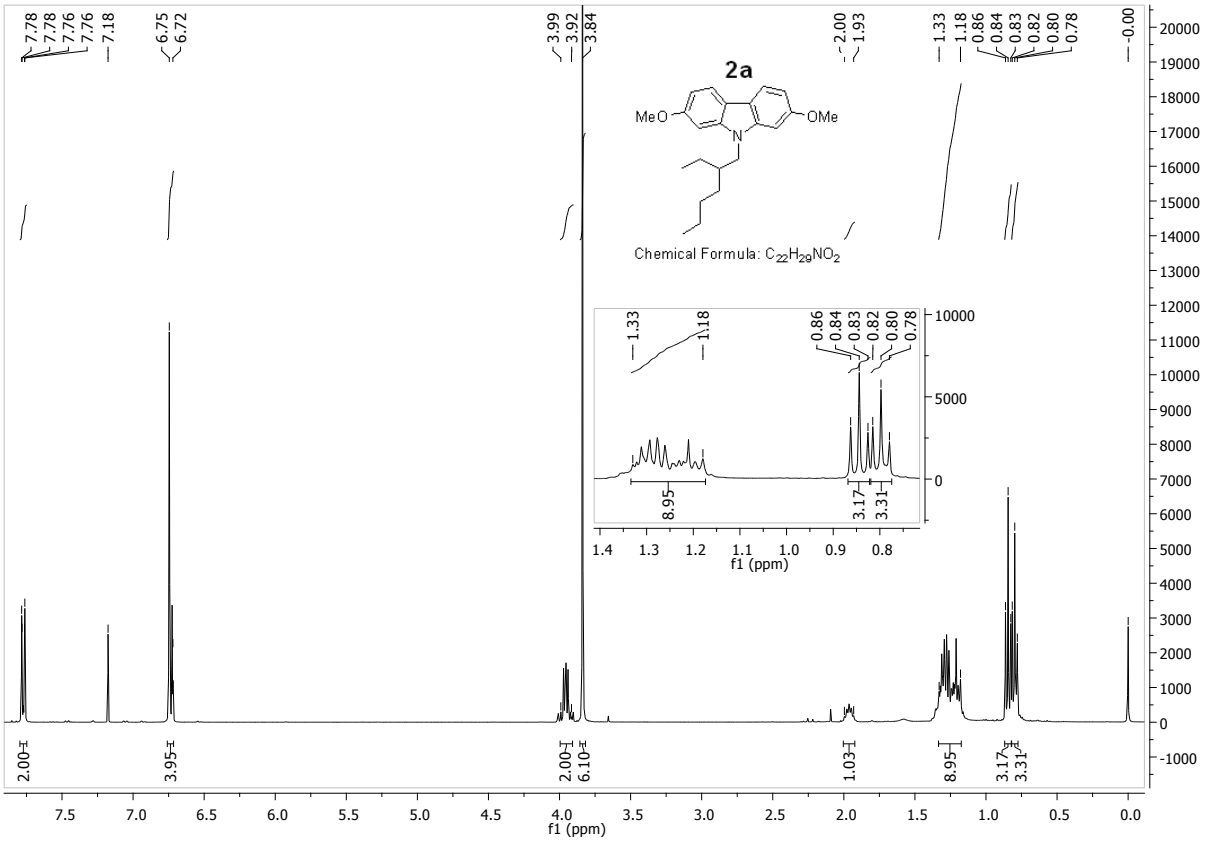
f1 (ppm)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MeO
OMe
N
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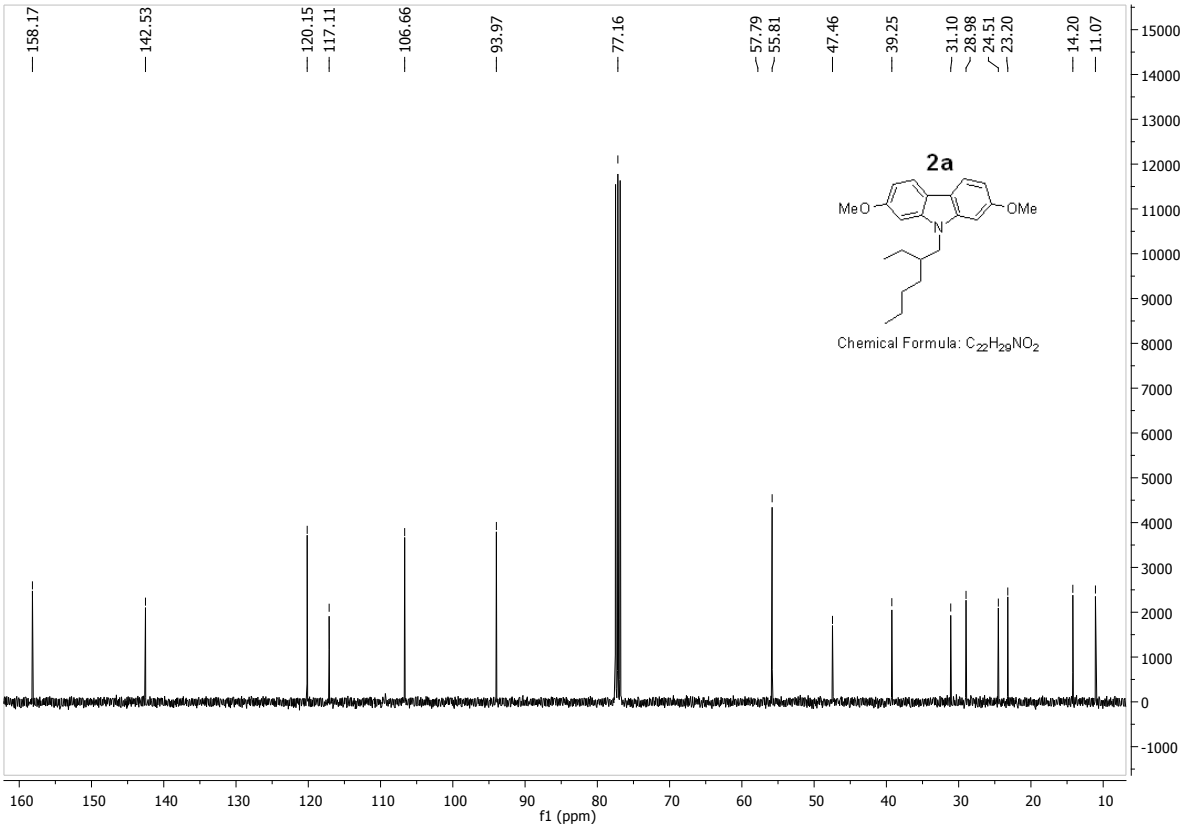
f1 (ppm)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MeO
OMe
N
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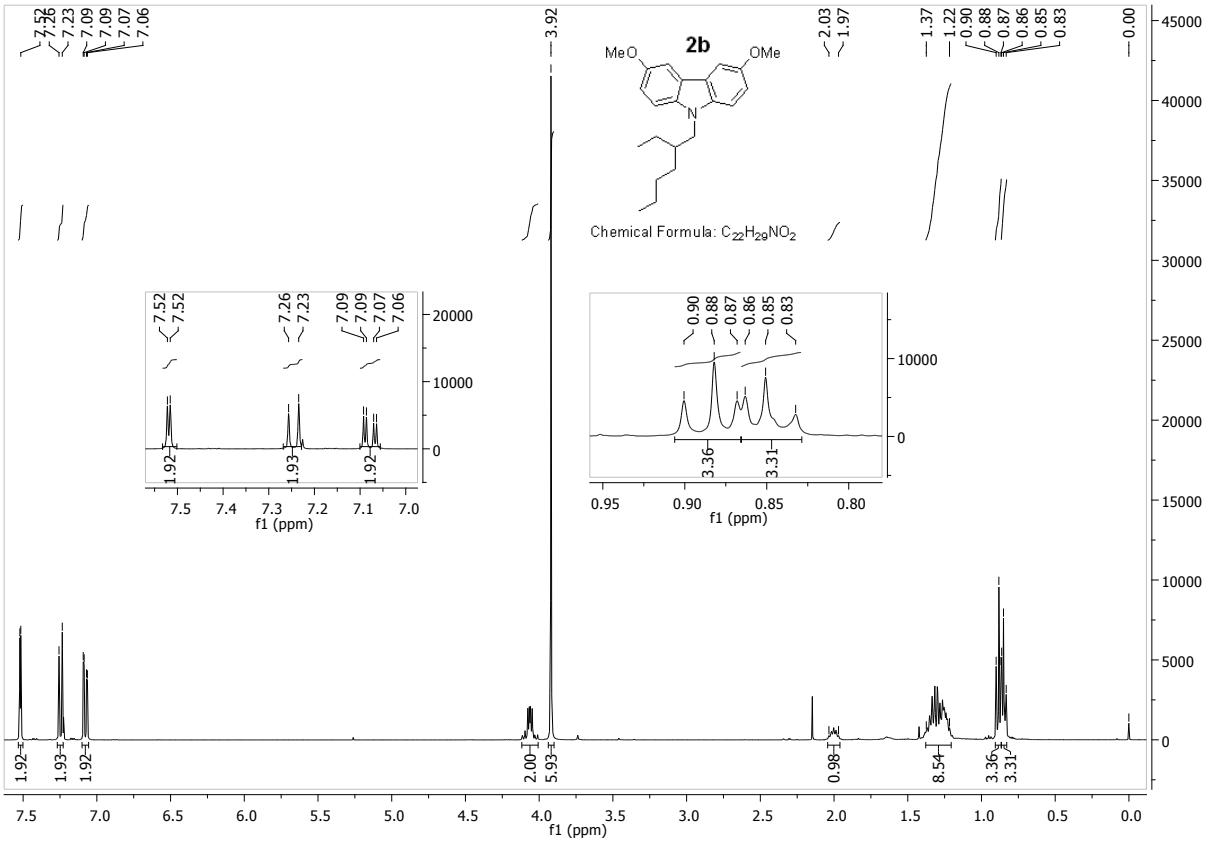
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OMe
N
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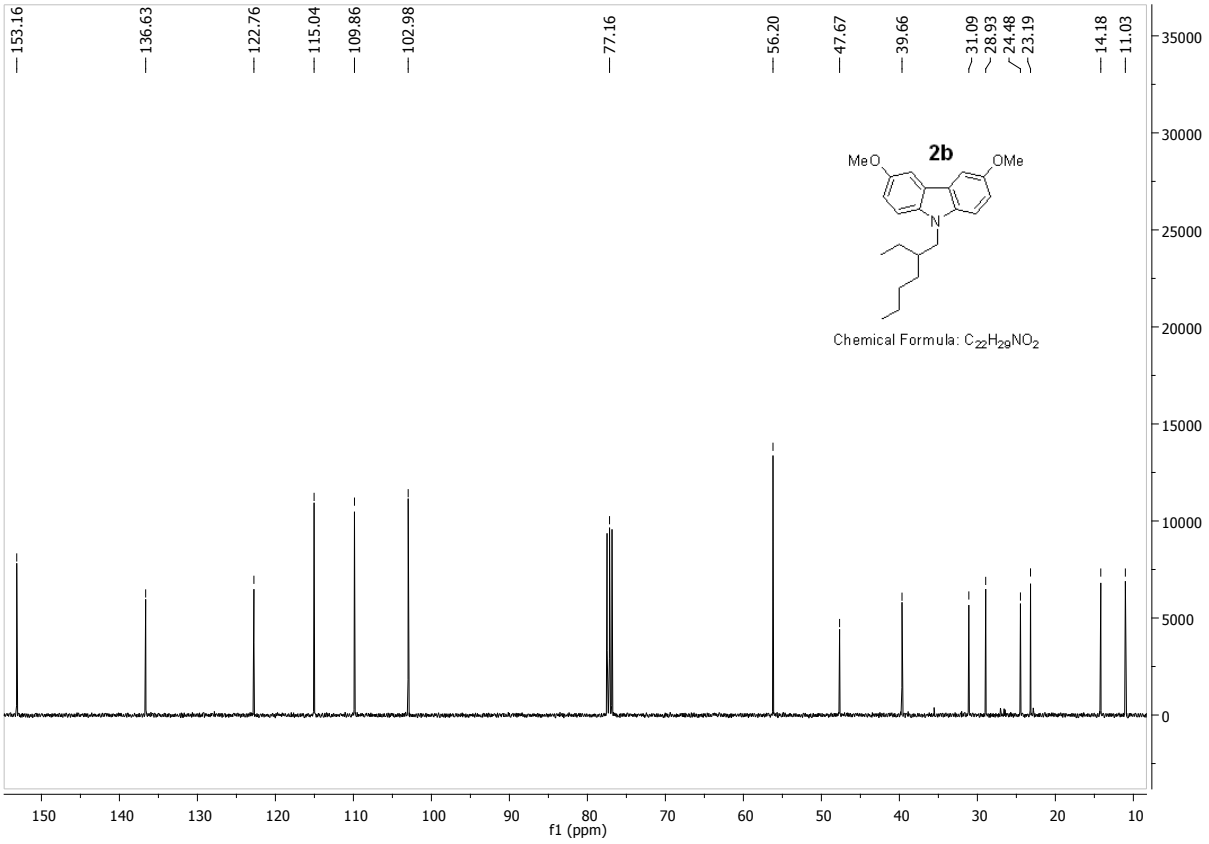
f1 (ppm)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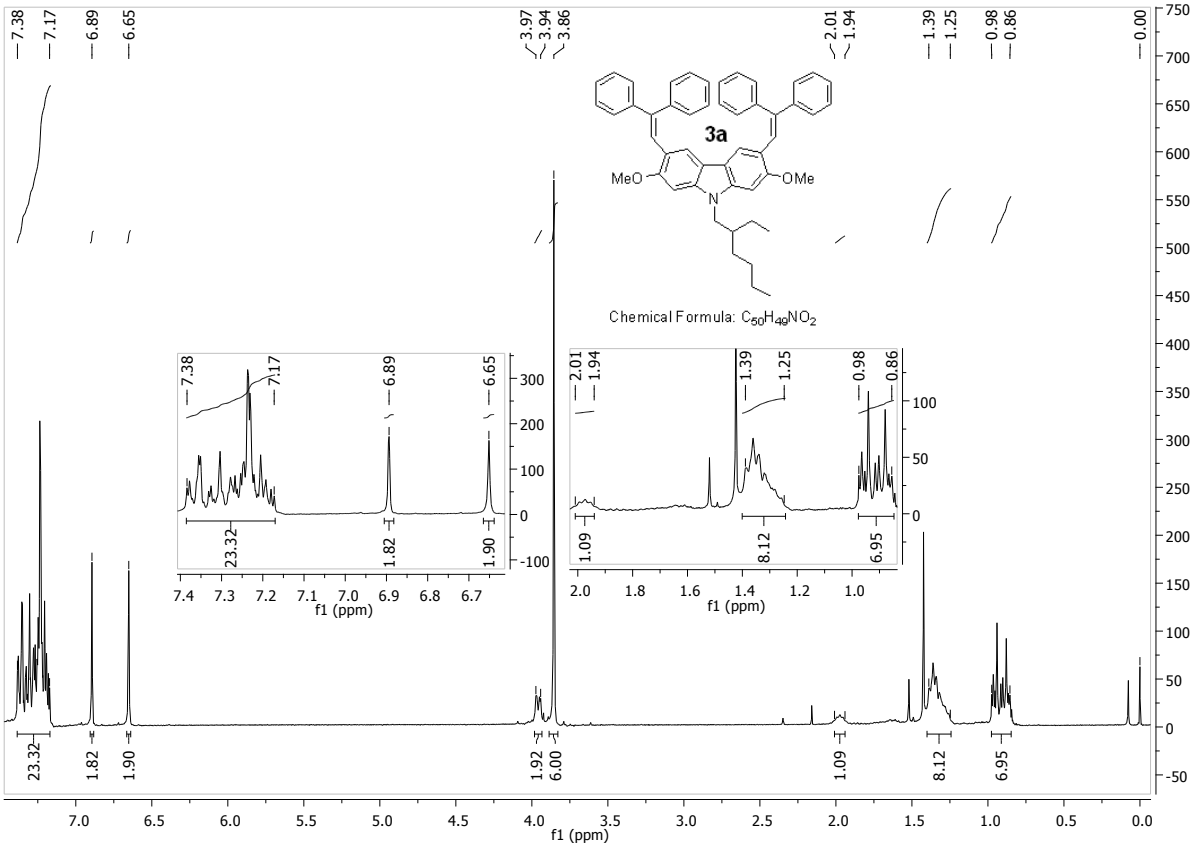
MeO
OMe
N
Chemical Formula: C22H29NO2
f1 (ppm)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6.89
6.65
3.97
3.94
3.86
2.01
1.94
1.39
1.25
0.98
0.86
0.00
3a
MeO
OMe
N
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23.32
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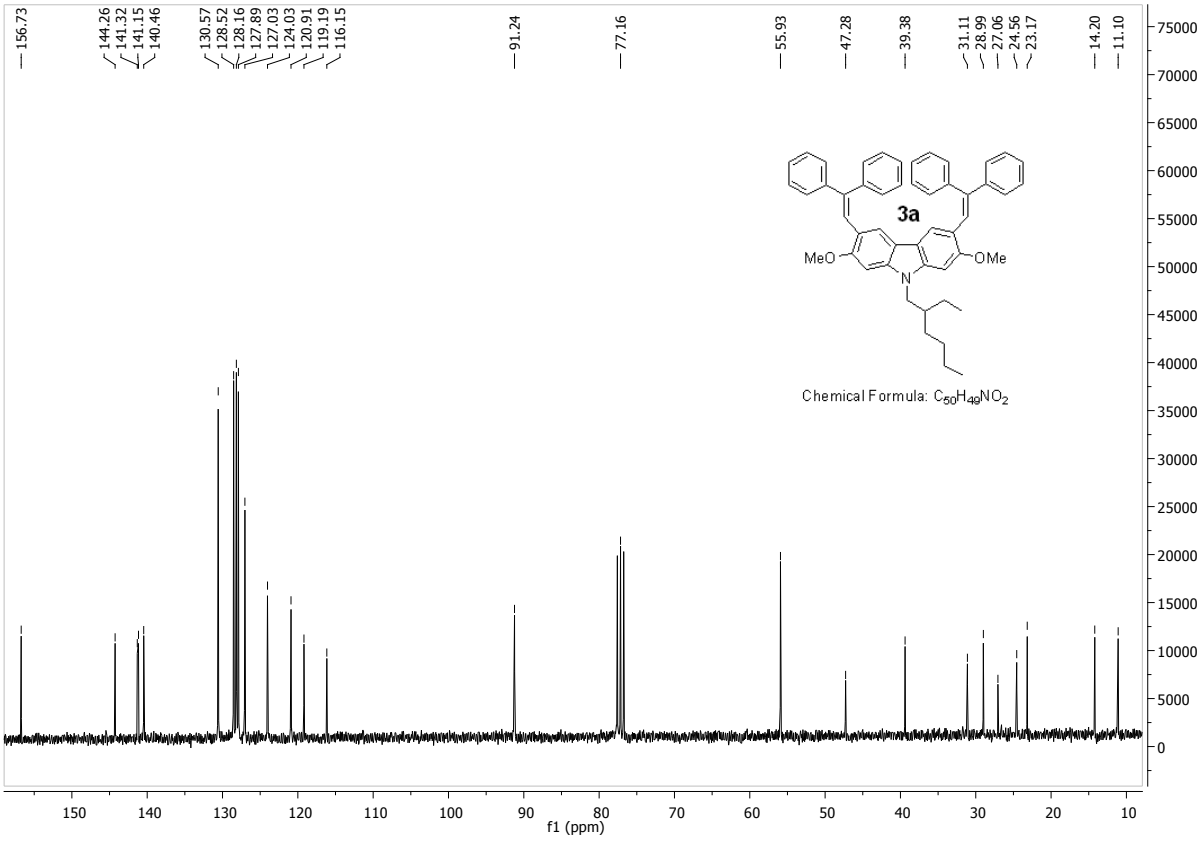
1.90
1.92
6.00
1.09
8.12
6.95
f1 (ppm)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140.46
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128.52
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127.03
124.03
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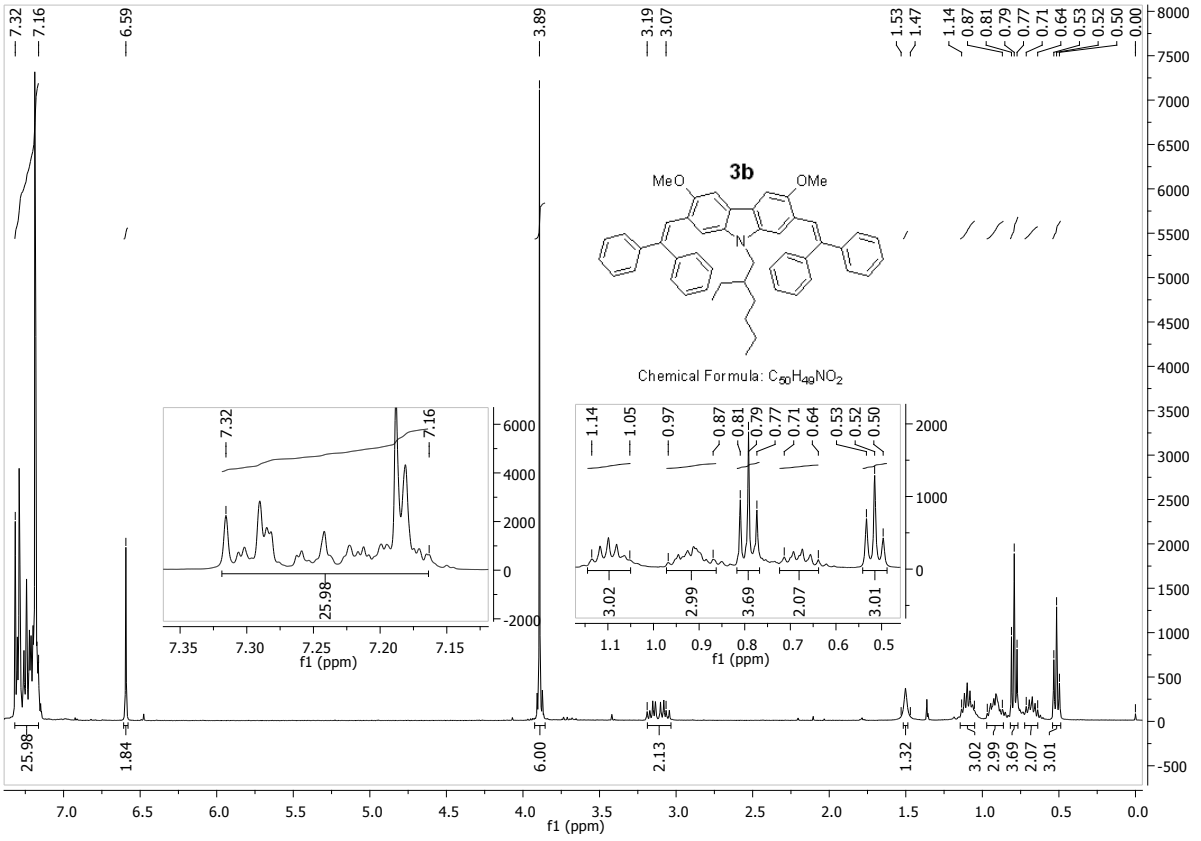
116.15
91.24
77.16
55.93
47.28
39.38
31.11
28.99
27.06
24.56
23.17
14.20
11.10
3a
MeO
OMe
N
Chemical Formula: C50H49NO2
f1 (ppm)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MeO
OMe
N
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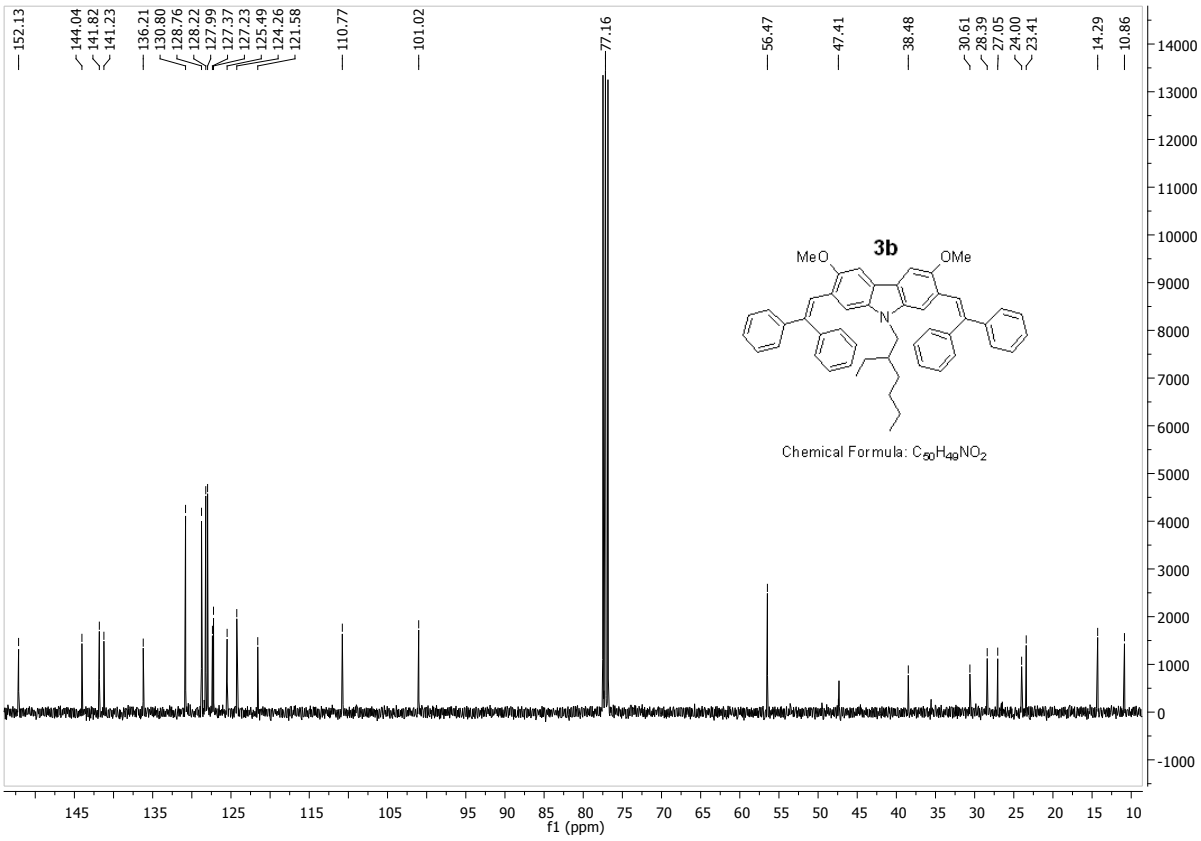
f1 (ppm)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OMe
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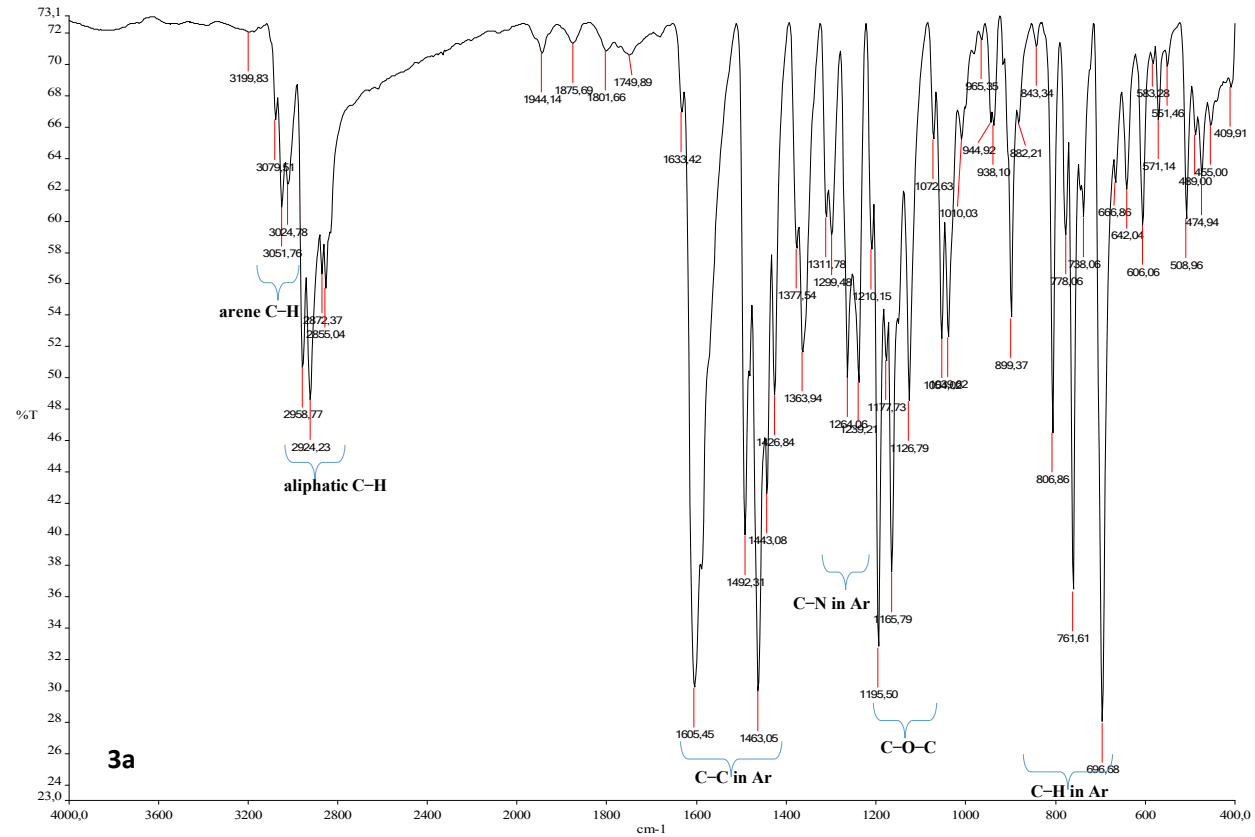
f1 (ppm)


3a
%T
cm-1
arene C−H
aliphatic C−H
C−C in Ar
C−N in Ar
C−O−C
C−H in Ar
3199,83
3079,61
3051,76
3024,78
2958,77
2924,23
2872,37
2855,04
1944,14
1875,69
1801,66
1749,89
1633,42
1605,45
1492,31
1463,05
1443,08
1426,84
1377,54
1363,94
1311,78
1299,48
1264,06
1239,21
1210,15
1195,50
1165,79
1126,79
1072,63
1010,03
965,35
944,92
938,10
899,37
882,21
843,34
806,86
761,61
738,06
696,68
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642,04
606,06
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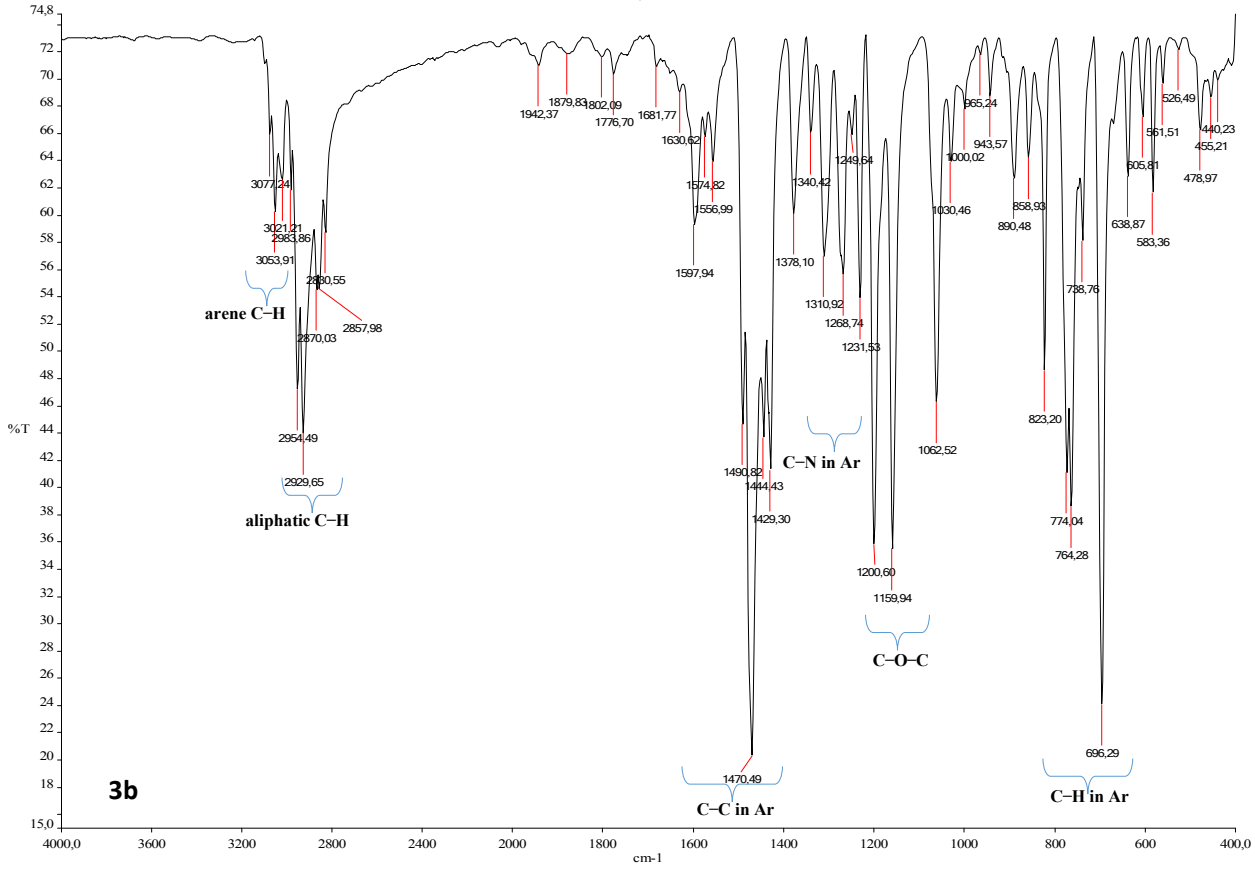
489,00
474,94
455,00
409,91


3b
%T
cm-1
arene C−H
aliphatic C−H
C−C in Ar
C−N in Ar
C−O−C
C−H in Ar
3077,24
3053,91
3021,21
2983,86
2954,49
2929,65
2870,03
2857,98
2830,55
1942,37
1879,83
1802,09
1776,70
1681,77
1630,62
1597,94
1574,82
1556,99
1490,82
1470,49
1444,43
1429,30
1378,10
1340,42
1310,92
1268,74
1249,64
1231,53
1200,60
1159,94
1062,52
1030,46
1000,02
965,24
943,57
890,48
858,93
823,20
774,04
764,28
738,76
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561,51
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478,97
455,21
440,23

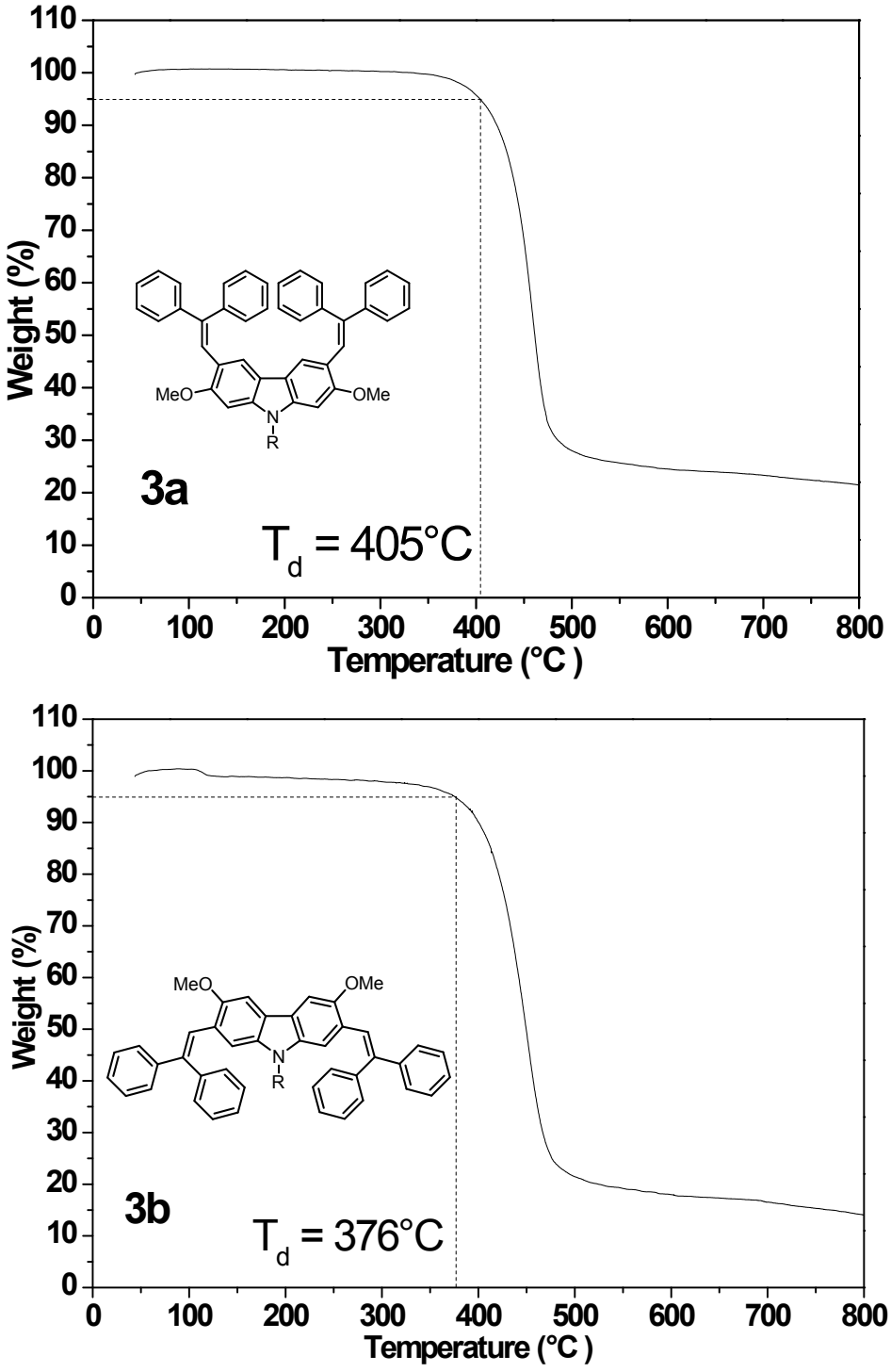


Figure S1. TGA curves of **3a** and **3b** (heating rate 10 °C/min, N_2 atmosphere).

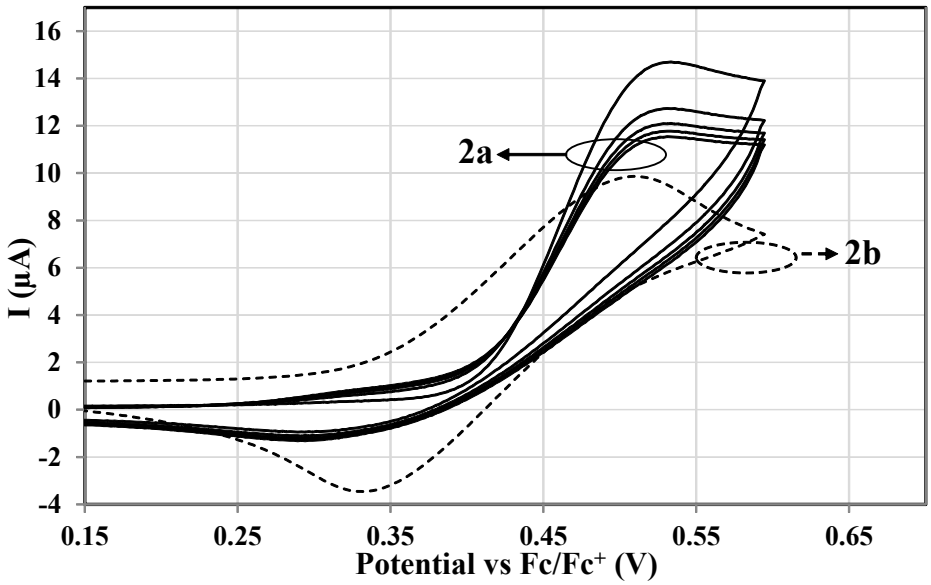


Figure S2. Cyclic voltammograms of **2a-b** at 10^{-3} mol L^{-1} in a solution of in argon-purged TBAP (0.1 M) in CH_2Cl_2. v = 50 mV/s.

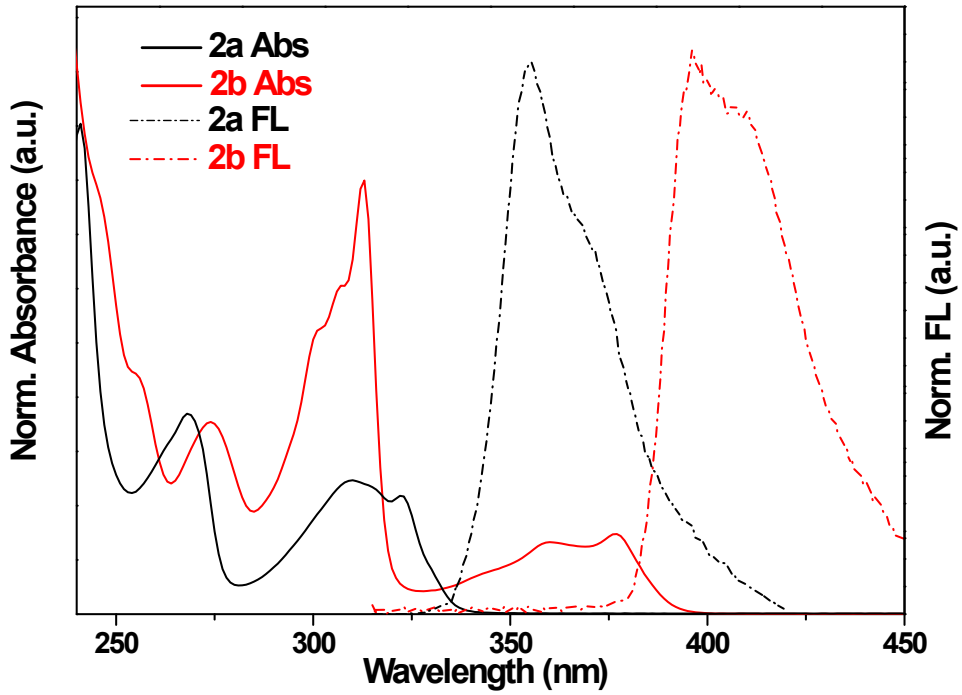
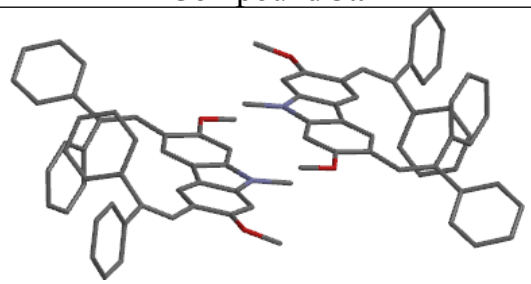
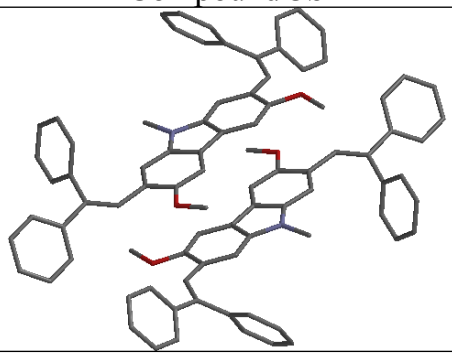
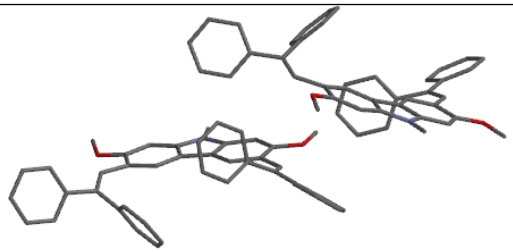
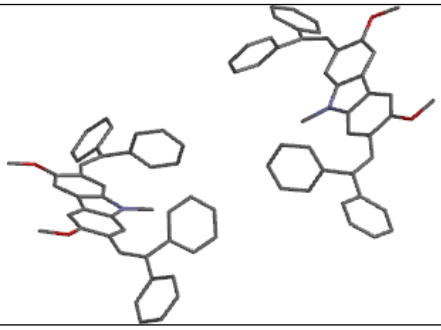


Figure S3. UV-vis and fluorescence spectra of dilute THF solutions (10^{-5} M) of compounds **2a**, **2b**. λ_{ex}= 350 nm.

Table S1. Crystalographic data of **3a** and **3b**

	3a	**3b**
Chemical formula	$C_{50}H_{49}NO_2$	$C_{50}H_{49}NO_2$. ½ CH_3OH
Crystal system	orthorhombic	monoclinic
Formula weight	695.93	695.93
Shape	yellow plate	yellow plate
Space group	P b c a	P 21/n
***a* / Å**	16.3265(2)	20.8163(5)
***b* / Å**	18.2018(2)	7.6277(2)
***c* / Å**	26.5776(3)	26.4292(5)
***α* / º**	90.00	90.00
***β* / º**	90.00	91.0202(15)
***γ* / º**	90.00	90.00
***V* / Å^3**	7898.1(2)	4195.78(17)
Z	8	2
***D* / g cm^{-3}**	1.171	1.118
***Temperature* / K**	173	193

Compound **3a**	Compound **3b**
	
Channel 1	Channel 1
	
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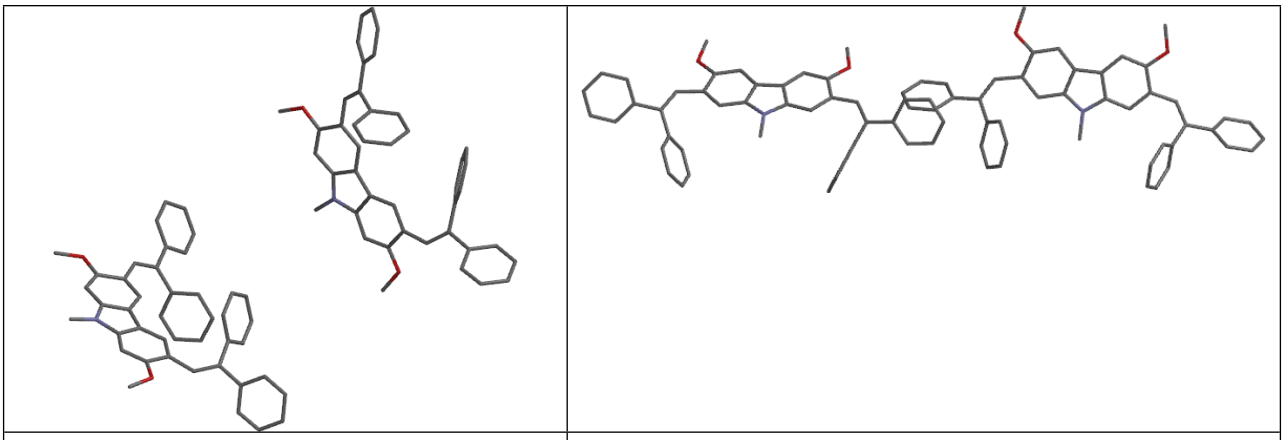
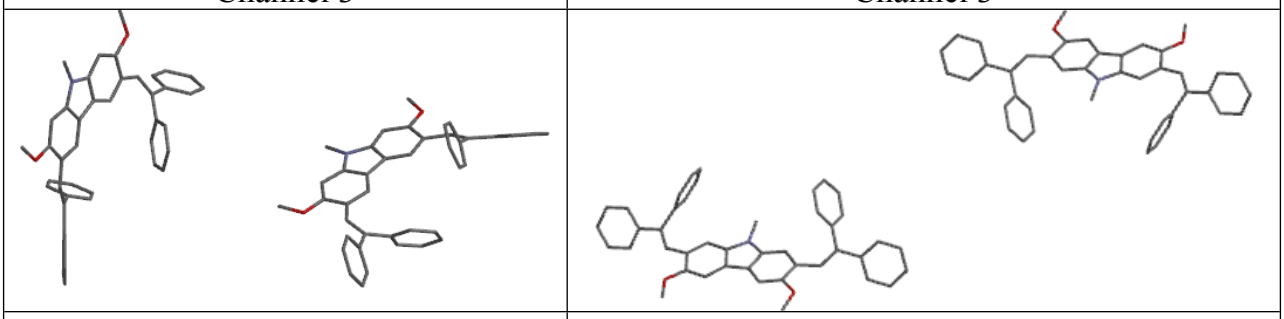


Channel 3	Channel 3



Channel 4	Channel 4

Figure S4. The intermolecular charge-hopping channels for **3a-b** generated from X-ray data.