Supporting Information

Modifying Organic Phenoxazine Dyes for Efficient Dye-Sensitized Solar Cells

Haining Tian [a], Ilkay Bora [a,c], Xiao Jiang [b], Erik Gabrielsson [a], Karl Martin Karlsson [a], Anders Hagfeldt [b], Licheng Sun [a, d,*]

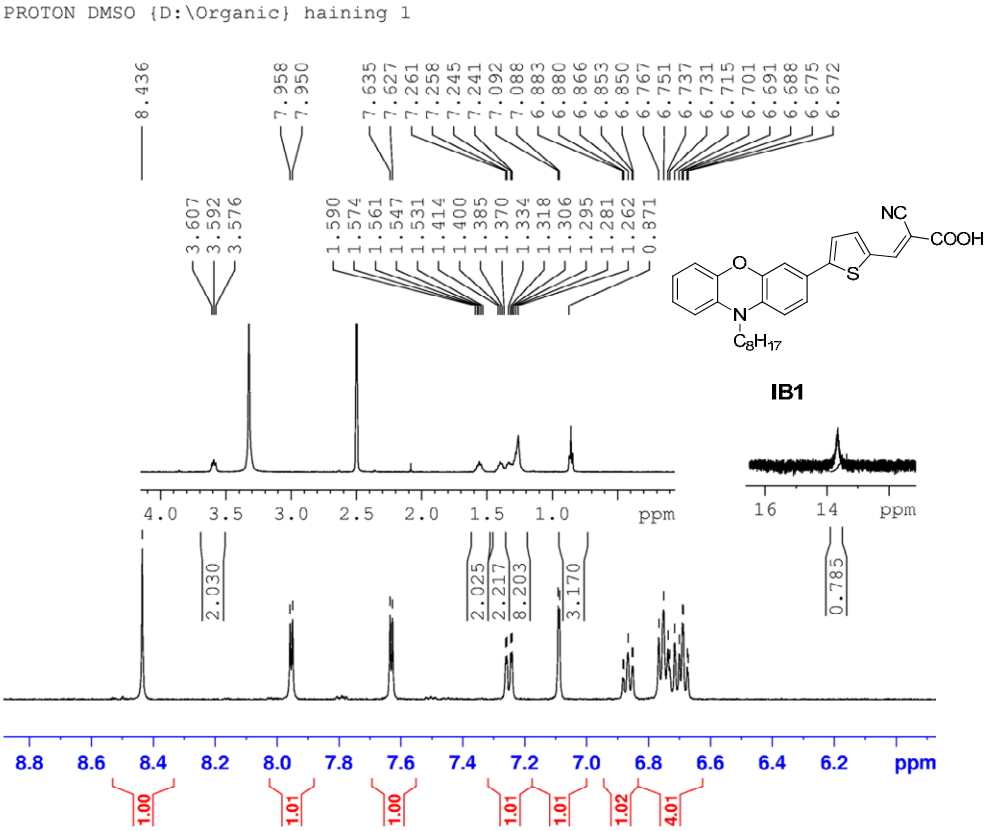
[a] Department of Chemistry, School of Chemical Science and Engineering, Center of Molecular Devices, Royal Institute of Technology (KTH), 10044 Stockholm, Sweden. E-mail: lichengs@kth.se

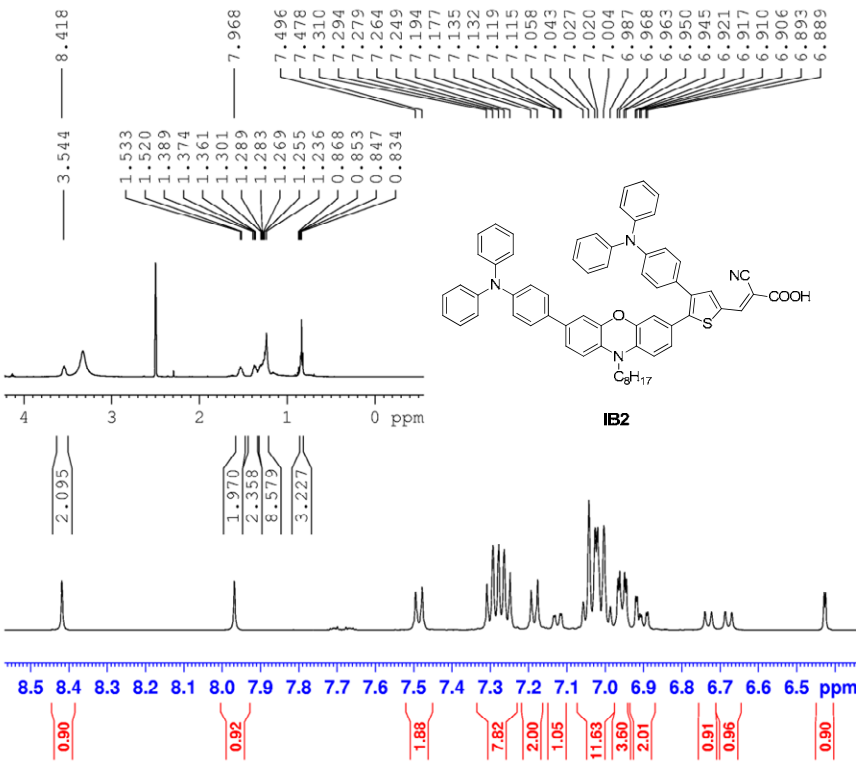
[b] Department of Physical and Analytical Chemistry, Center of Molecular Devices, Uppsala University, 75105 Uppsala, Sweden

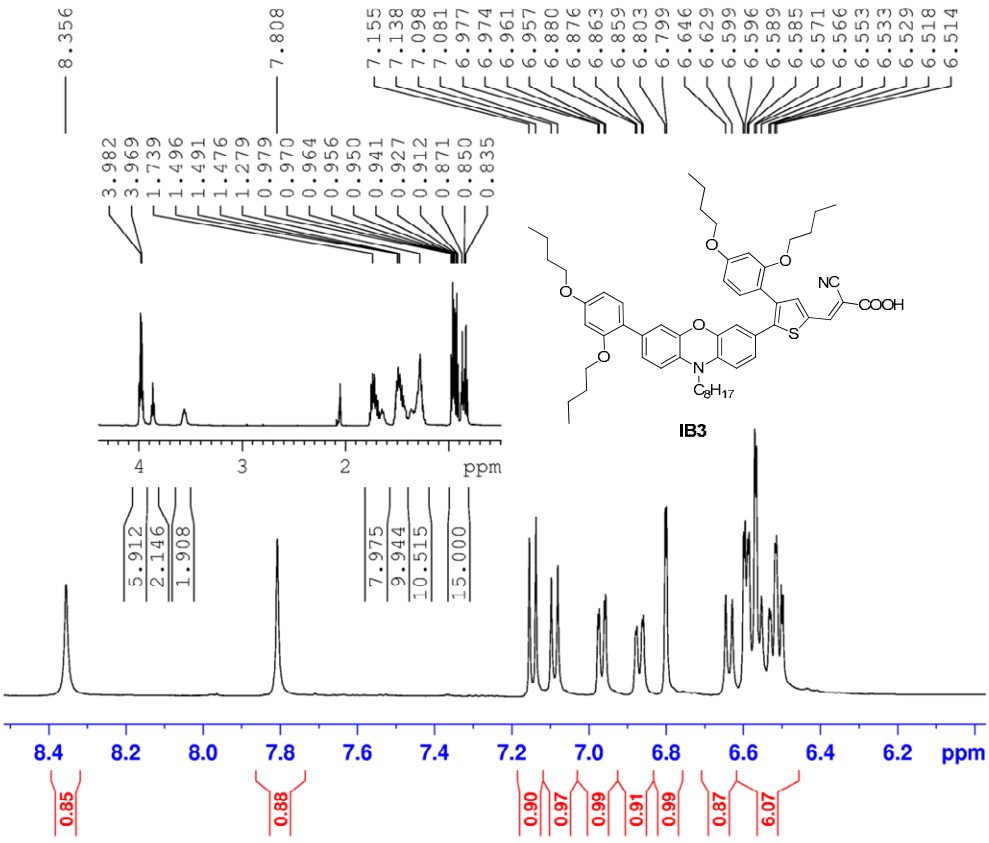
[c] Institute of Organic Chemistry, University of Stuttgart, 70049 Stuttgart, Germany

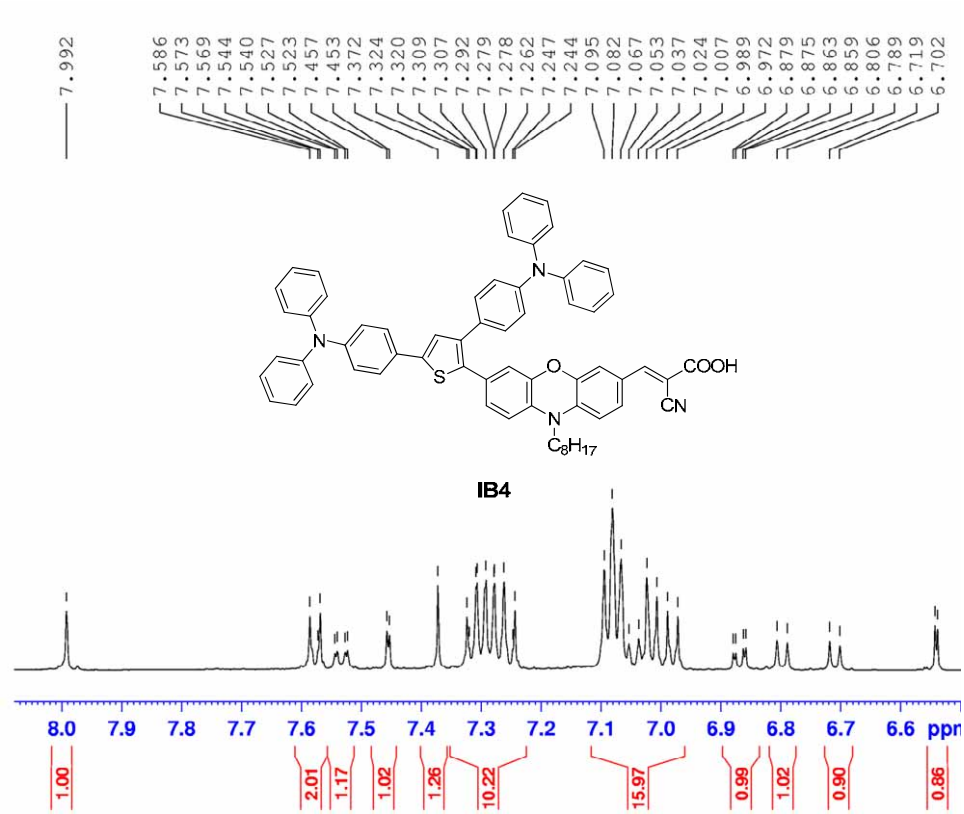
[d] State Key Laboratory of Fine Chemicals, DUT-KTH Joint Education and Research Center for Molecular Devices, Dalian University of Technology (DUT), 116024 Dalian, China

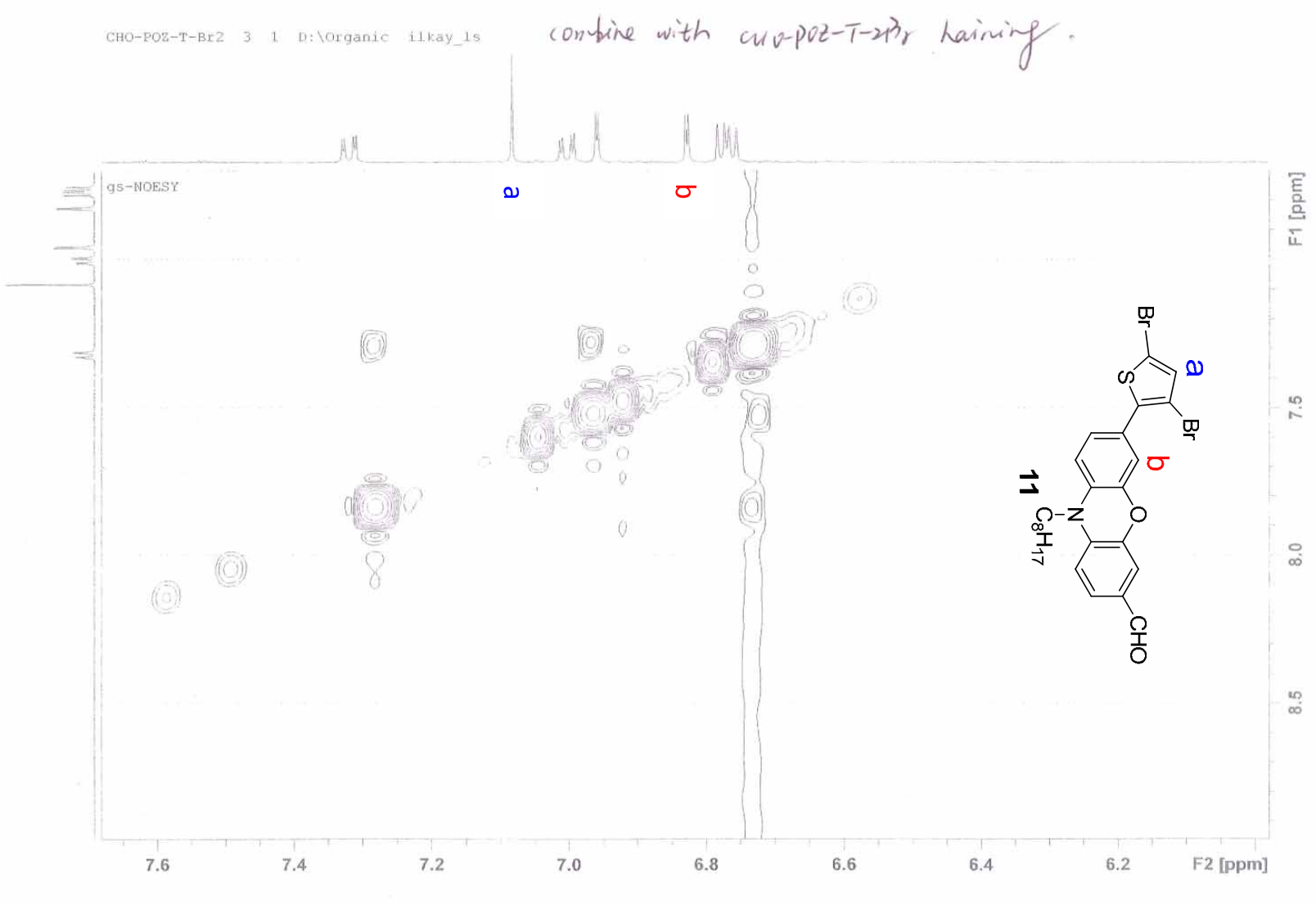
NMR and NOESY spectra




8.418
7.968
7.496
7.478
7.310
7.294
7.279
7.264
7.249
7.194
7.177
7.135
7.132
7.119
7.115
7.058
7.043
7.027
7.020
7.004
6.987
6.968
6.963
6.950
6.945
6.921
6.917
6.910
6.906
6.893
6.889
3.544
1.533
1.520
1.389
1.374
1.361
1.301
1.289
1.283
1.269
1.255
1.236
0.868
0.853
0.847
0.834
NC
COOH
S
O
N
C8H17
IB2
4
3
2
1
0 ppm
2.095
1.970
2.358
8.579
3.227
8.5 8.4 8.3 8.2 8.1 8.0 7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 ppm
0.90
0.92
1.88
7.82
2.00
1.05
11.63
3.60
2.01
0.91
0.96
0.90


8.356
7.808
7.155
7.138
7.098
7.081
6.977
6.974
6.961
6.957
6.880
6.876
6.863
6.859
6.803
6.799
6.646
6.629
6.599
6.596
6.589
6.585
6.571
6.566
6.553
6.533
6.529
6.518
6.514
3.982
3.969
1.739
1.496
1.491
1.476
1.279
0.979
0.970
0.964
0.956
0.950
0.941
0.927
0.912
0.871
0.850
0.835
NC
COOH
S
O
N
C8H17
IB3
4
3
2
ppm
5.912
2.146
1.908
7.975
9.944
10.515
15.000
8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 ppm
0.85
0.88
0.90
0.97
0.99
0.91
0.99
0.87
6.07


7.992
7.586
7.573
7.569
7.544
7.540
7.527
7.523
7.457
7.453
7.372
7.324
7.320
7.309
7.307
7.292
7.279
7.278
7.262
7.247
7.244
7.095
7.082
7.067
7.053
7.037
7.024
7.007
6.989
6.972
6.879
6.875
6.863
6.859
6.806
6.789
6.719
6.702
N
N
S
O
N
COOH
CN
C8H17
IB4
8.0
7.9
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
6.8
6.7
6.6
ppm
1.00
2.01
1.17
1.02
1.26
10.22
15.97
0.99
1.02
0.90
0.86


CHO-POZ-T-Br2 3 1 D:\Organic ilkay_ls
combine with cho-poz-T-2Br staining.
gs-NOESY
a
b
F1 [ppm]
7.5
8.0
8.5
7.6
7.4
7.2
7.0
6.8
6.6
6.4
6.2
F2 [ppm]
Br
S
Br
a
b
N
O
CHO
11
C8H17

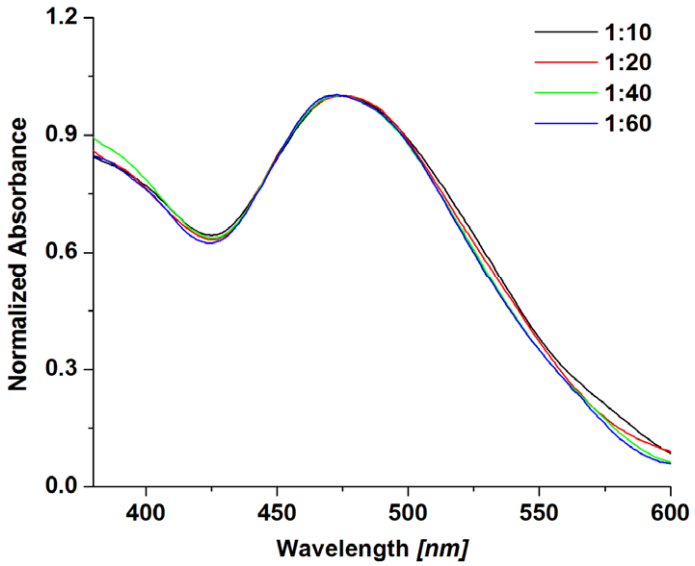


Figure S1. The absorption spectra of **IB4**-sensitized TiO_2 with different ratio of **IB4**/CDCA (mol/mol) in dye bath

(TiO_2: ~2 μm; Sensitization time: 30 min)

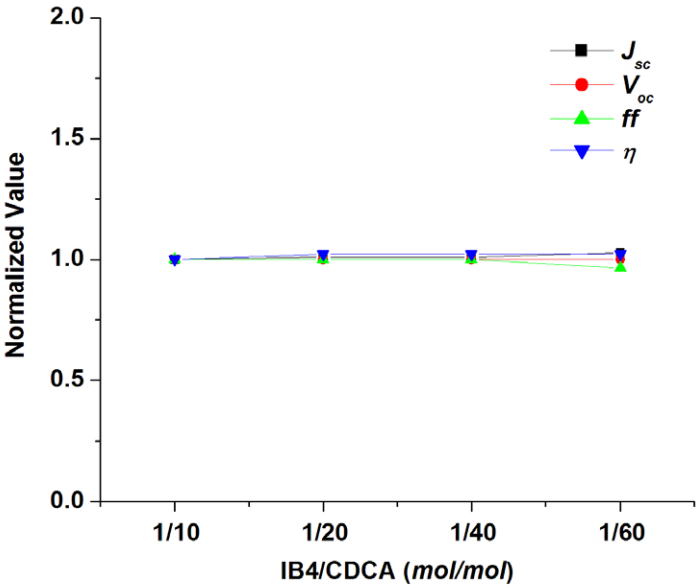


Figure S2. The effect of different ratio of **IB4**/CDCA on DSCs performance

(TiO_2: 6 μm transparent layer + 4 μm scattering layer; Pt CEs: Heptachroma Co. Ldt. Pt-paste; Sensitization time: 17 h)