

Supporting Information for “Synthesis of a Water-soluble 1,3-*bis*(diphenylene)-2-phenylallyl (BDPA) Radical”

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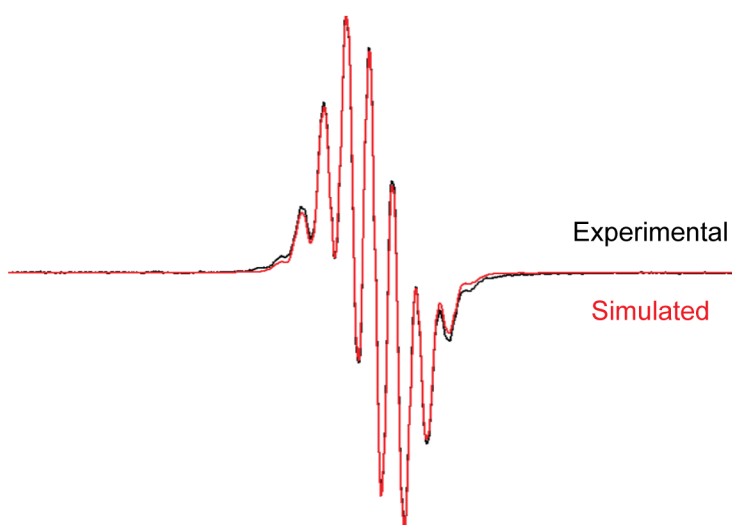
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Materials.

All chemicals, reagents, and solvents were used as received from commercial sources without further purification except dimethylacetamide, dimethylformamide, and dimethylsulfoxide, which were dried over oven-activated 4-Å molecular sieves.

WS-BDPA 9 GHz EPR Simulation



Experimental Parameters

[WS-BDPA] = 10 mM in 3:2 glycerol/water, rt, 2 mW, modulation amplitude 10 mT.

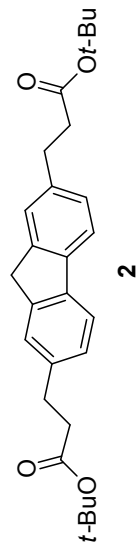
Simulation Parameters

Simulated using WinSim^a as a single radical with hyperfine couplings with 8 protons. (A1 = 1.986, A2 = 1.725, A3 = 1.894, A4 = 2.24, A5 = 1.717, A6 = 1.633, A7 = 2.164, A8 = 2.019).

^a Duling, D. R. *J. Magn. Reson., Series B* **1994**, *104*, 105.

Compound 2 ¹H-NMR

CD₂Cl₂, 500 MHz



7.65
7.63
7.36
7.19
7.19
7.19
7.18
7.18
7.17

3.82

2.95
2.94
2.92
2.55
2.54
2.52

1.39

2.00
1.89
2.07

2.18

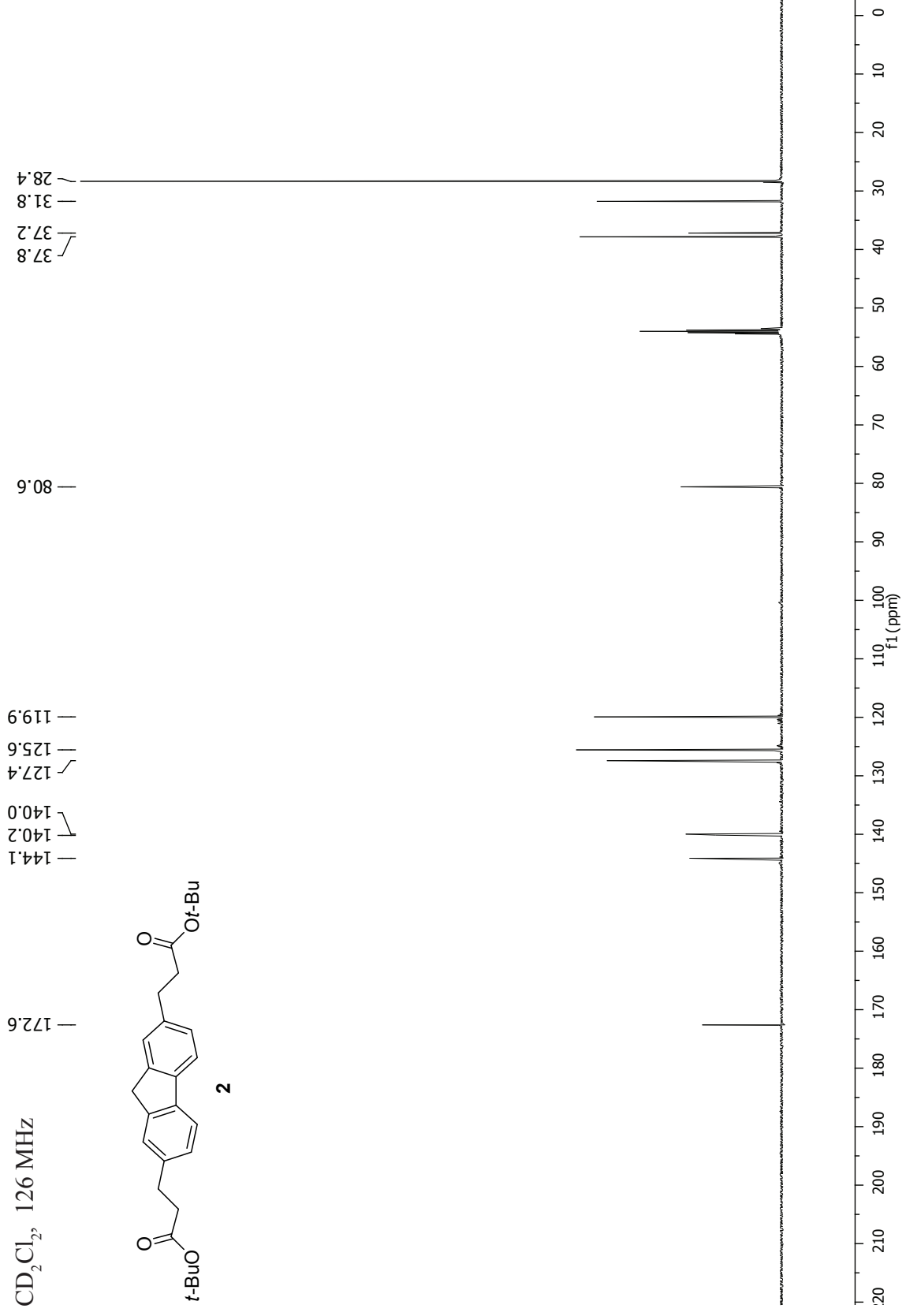
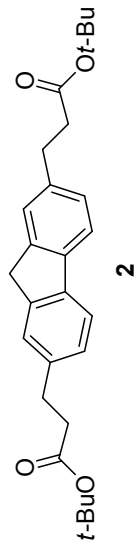
4.16

4.24

17.49

Compound 2 ¹³C-NMR

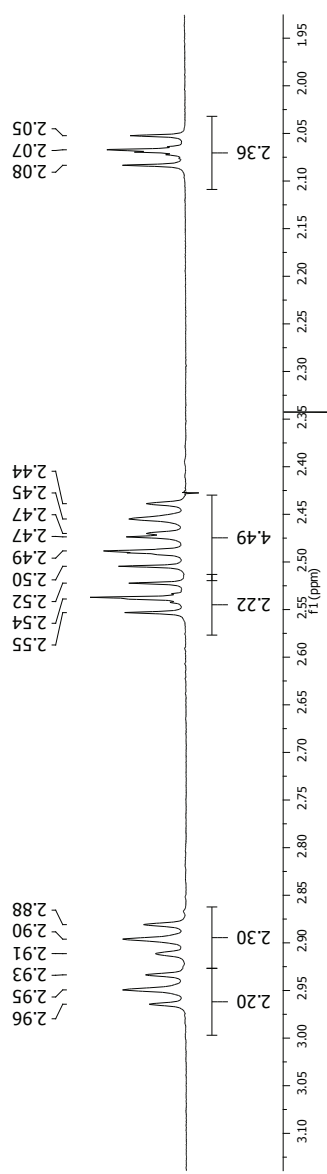
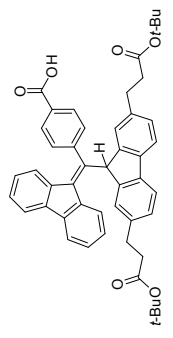
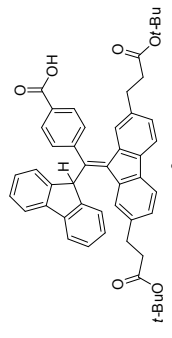
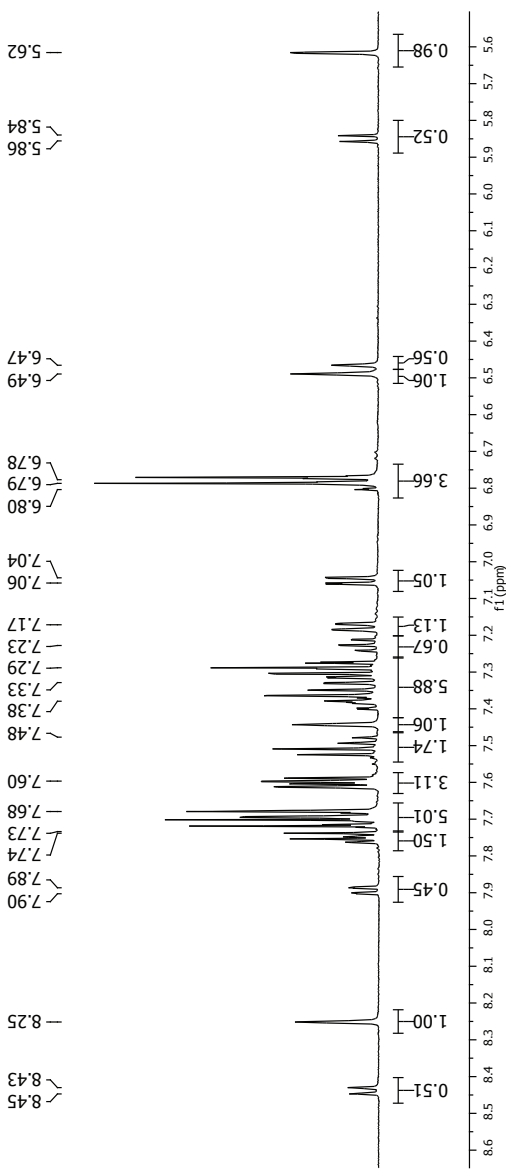
CD₂Cl₂, 126 MHz



Compound 3 ¹H-NMR

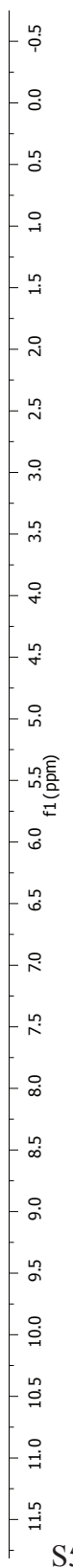
CD₂Cl₂, 500 MHz

1.30
1.35



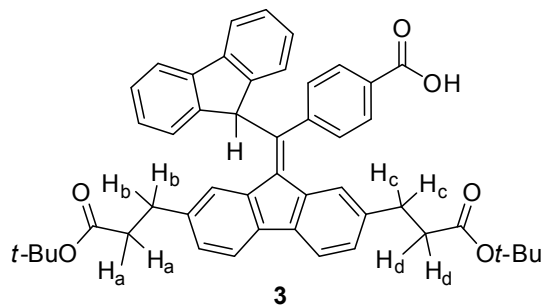
19.06
9.04

1.00

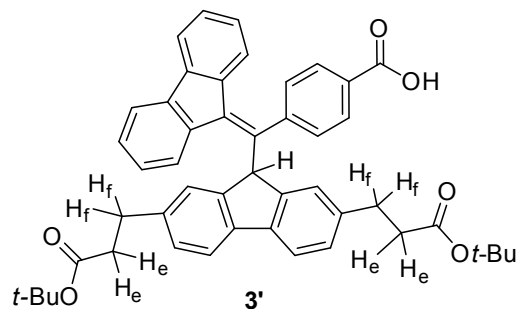


Compound 3 g-COSY 2D-NMR

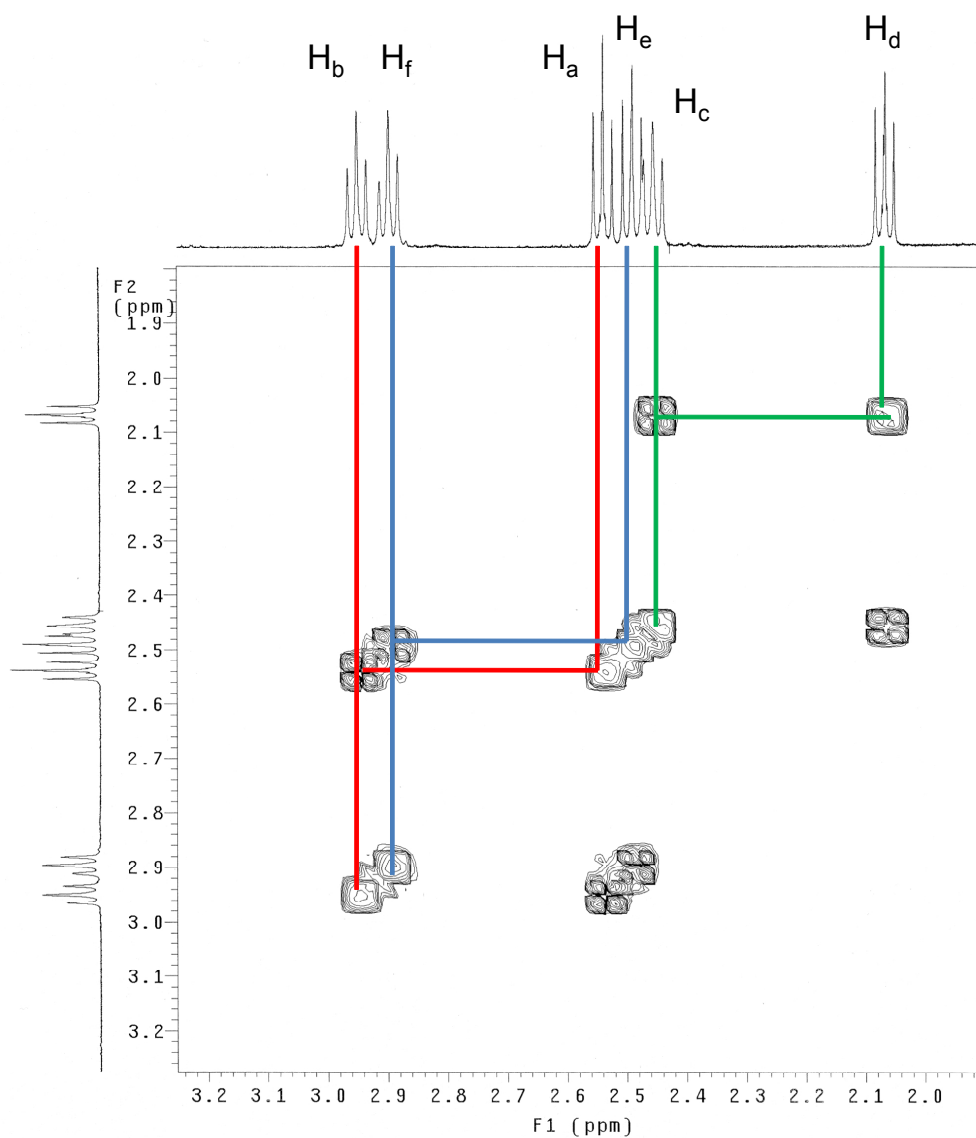
CD₂Cl₂, 500 MHz



Integration of 1H = 1.00

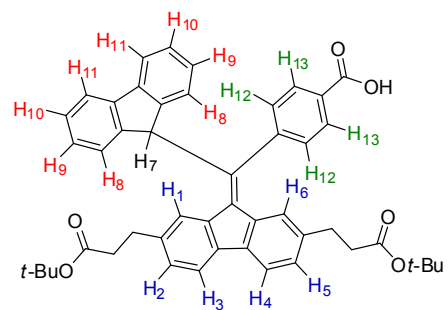


Integration of 1H = 0.50

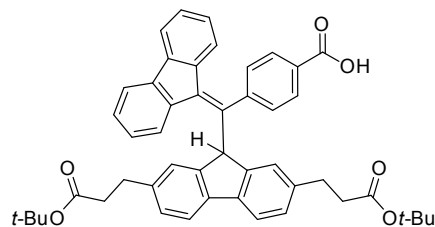


Compound 3 g-COSY 2D-NMR

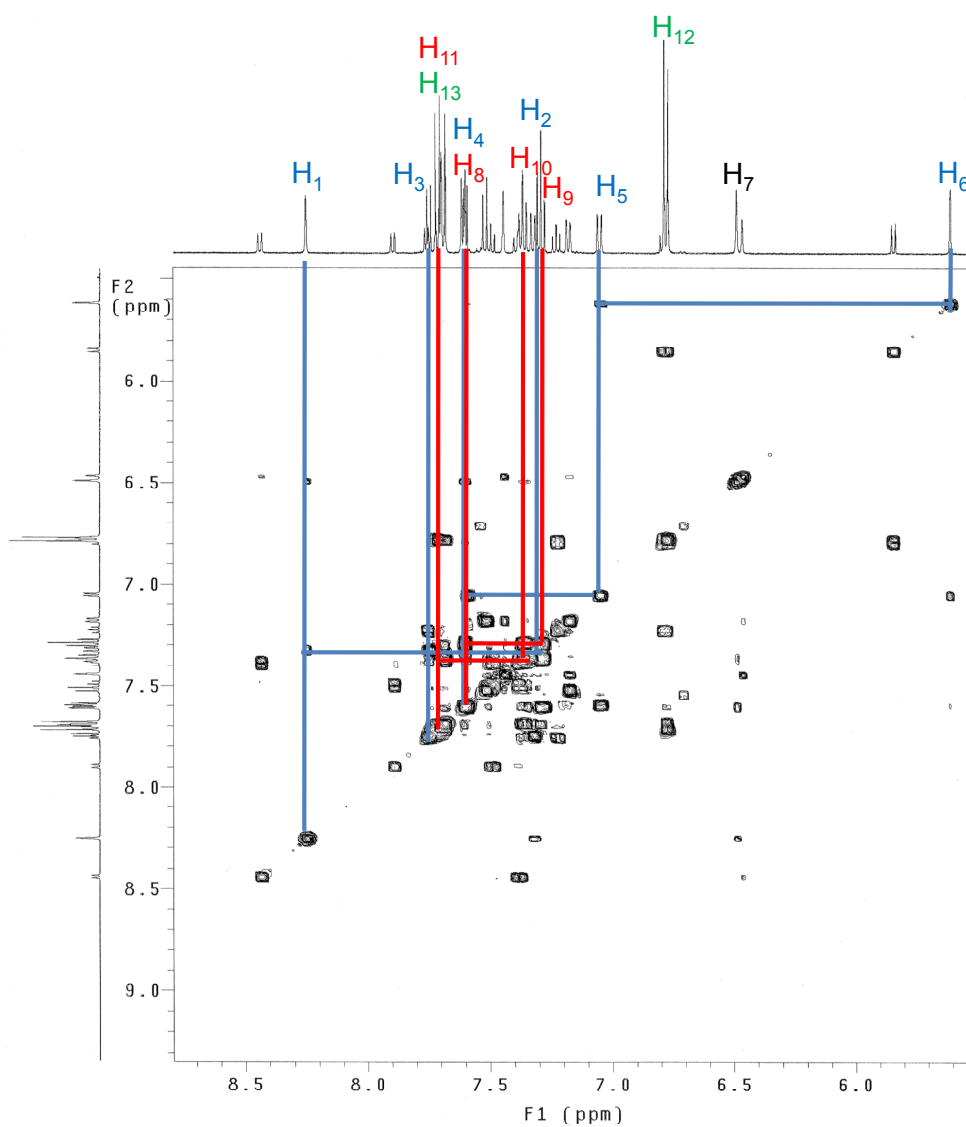
CD₂Cl₂, 500 MHz



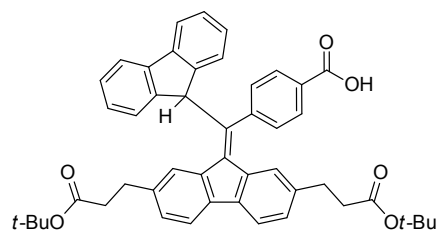
Integration of 1H = 1.00



Integration of 1H = 0.50

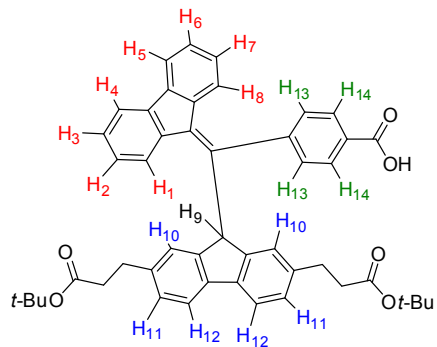


Compound 3 g-COSY 2D-NMR
CD₂Cl₂, 500 MHz



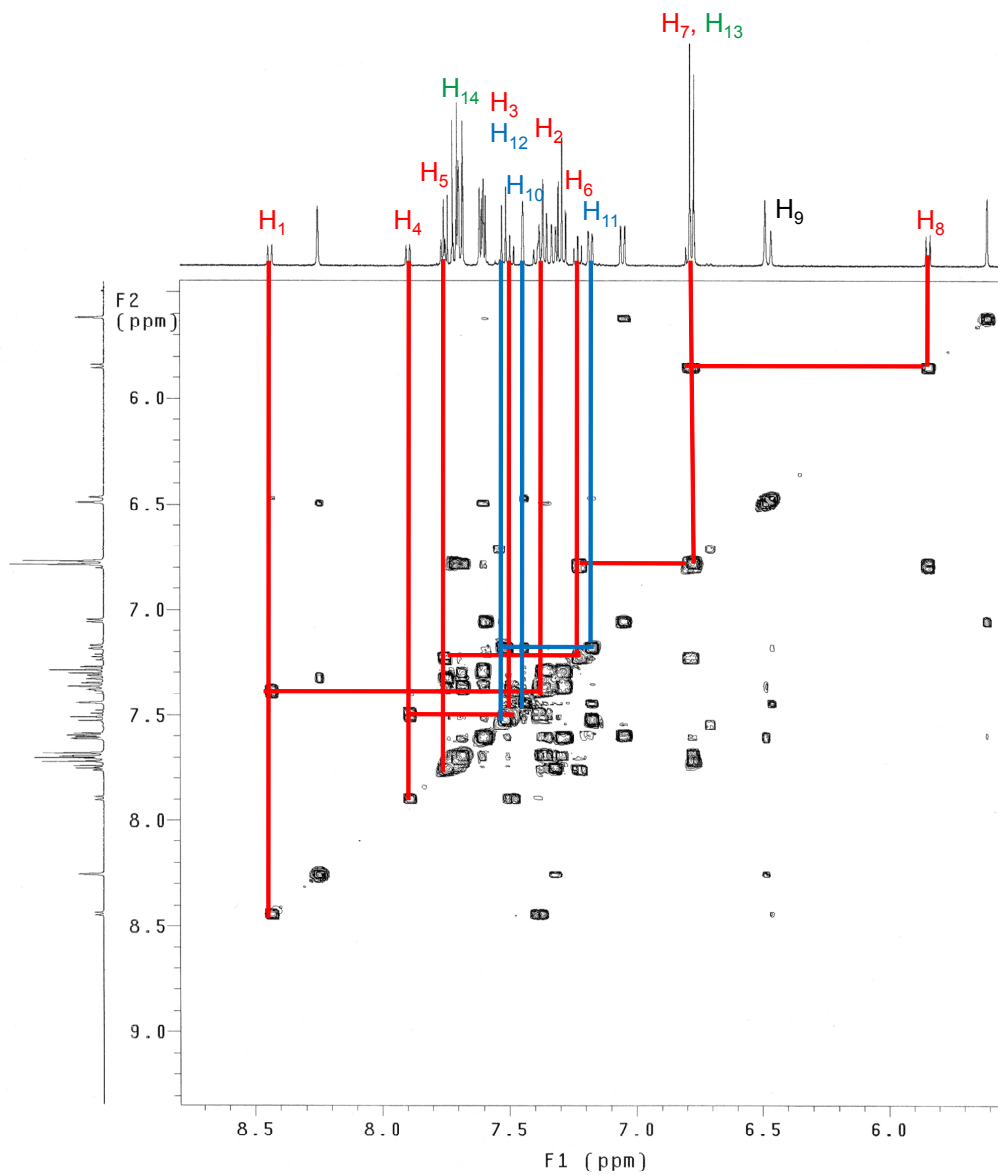
3

Integration of 1H = 1.00



3'

Integration of 1H = 0.50

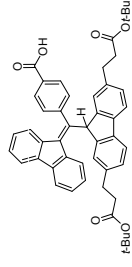
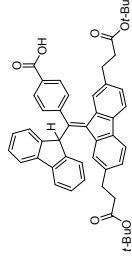
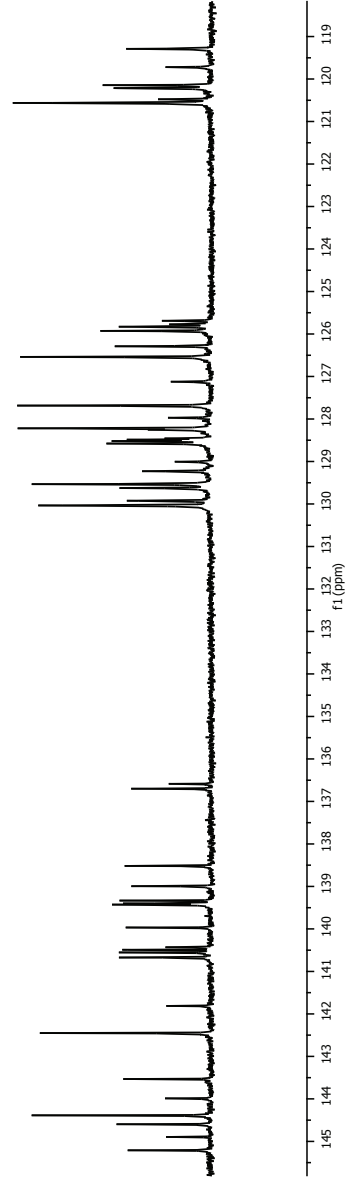


Compound 3 ¹³C-NMR

CD₂Cl₂, 126 MHz

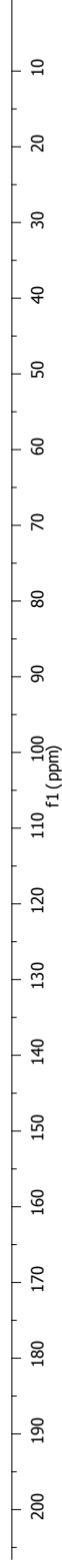
52.8
52.7
37.8
37.8
36.7
32.1
31.7
31.6
28.3
28.2

145.2
144.9
144.6
144.4
144.0
143.5
142.5
141.8
140.7
140.4
140.0
139.4
139.3
139.0
138.5
136.7
136.6
130.0
129.5
129.2
129.0
128.6
128.5
128.5
128.5
128.3
128.2
128.0
127.7
127.1
126.5
126.3
125.9
125.8
125.8
125.7
120.6
120.5
120.5
120.2
120.1
119.7
119.3



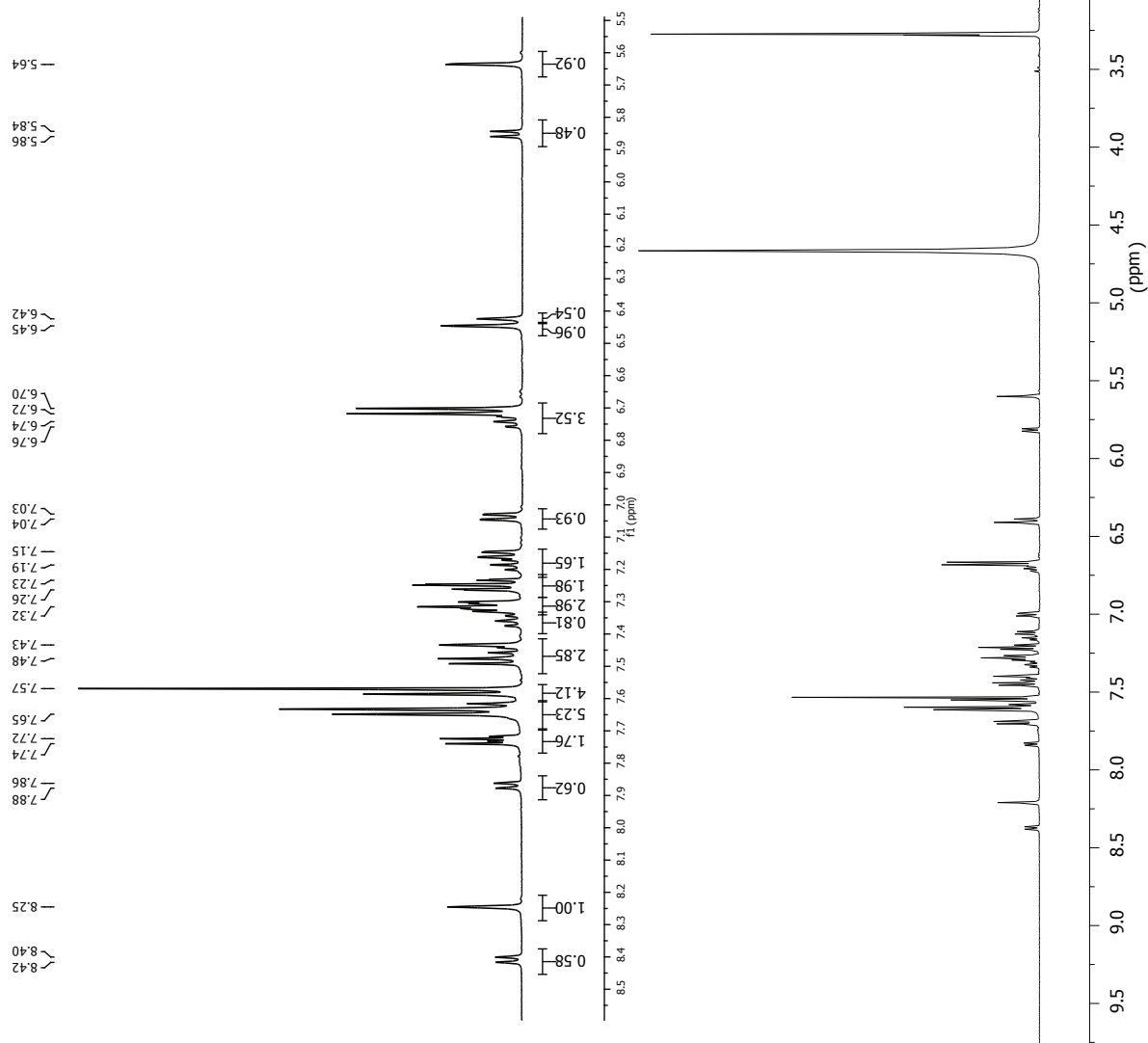
80.7
80.7
80.4

172.5
172.4
172.3
171.6
171.5

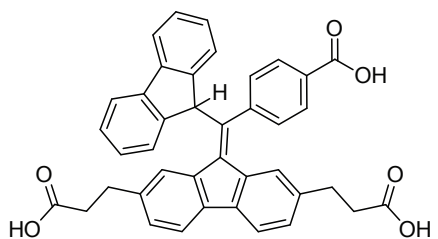
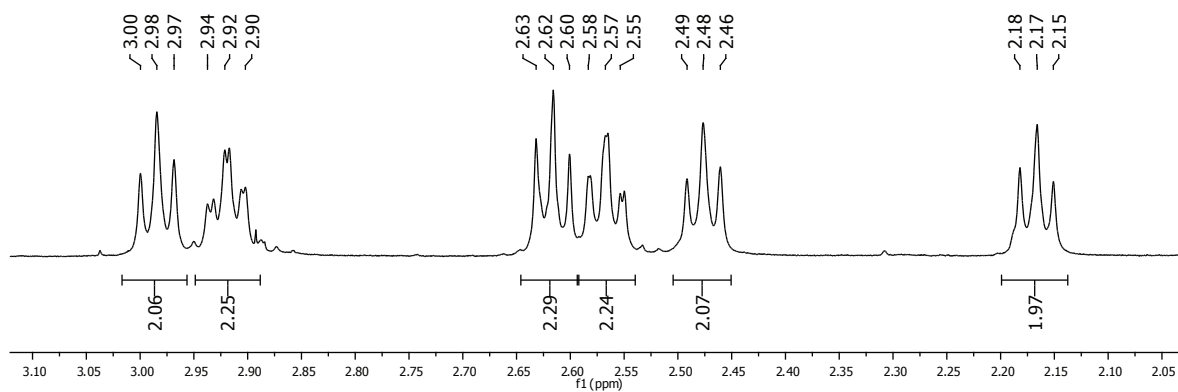


Compound 4 ¹H-NMR

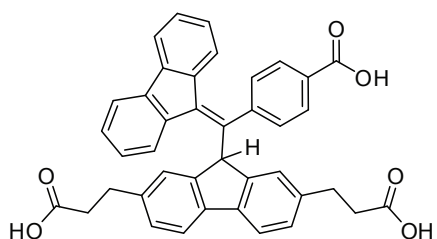
CD₃OD, 500 MHz



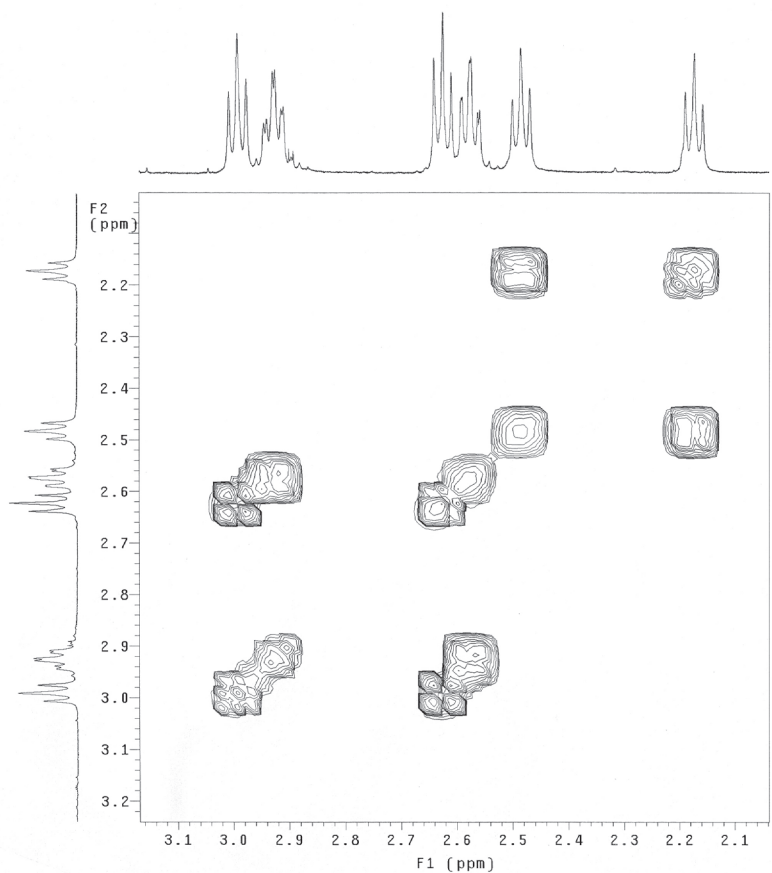
Compound 4 ¹H-NMR (con't.) and g-COSY 2D-NMR
 CD₃OD, 500 MHz



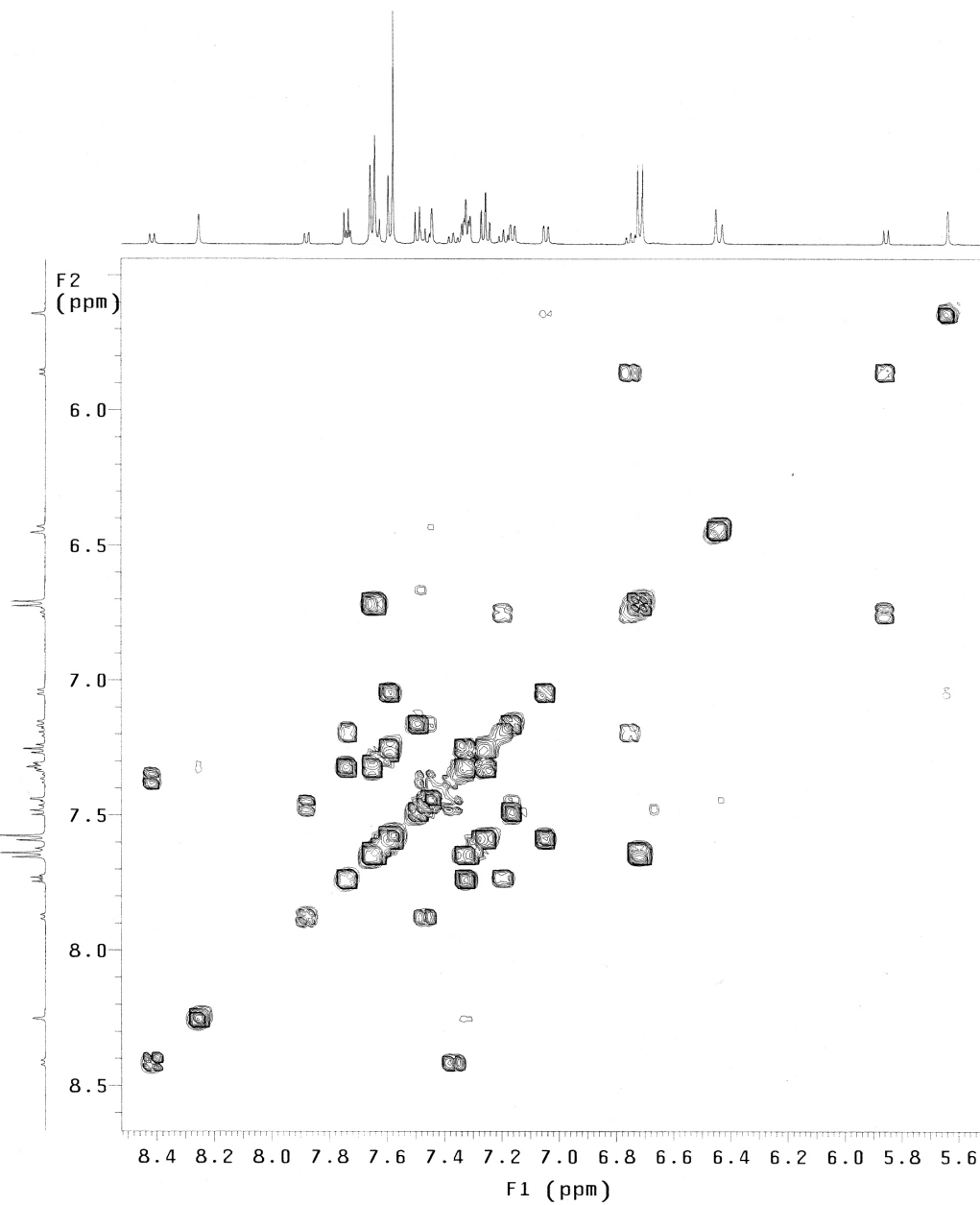
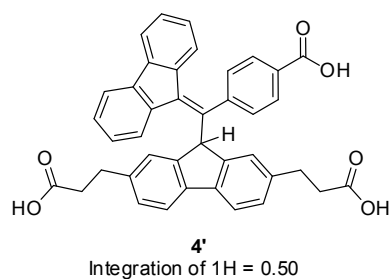
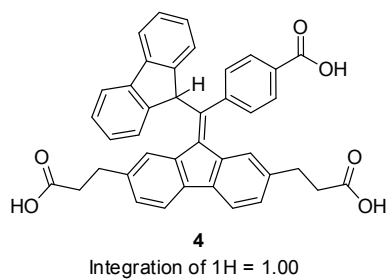
Integration of 1H = 1.00



Integration of 1H = 0.50



Compound 4 g-COSY 2D-NMR
CD₃OD, 500 MHz



Compound 4 ¹³C-NMR

CD₃OD/CDCl₃, 126 MHz

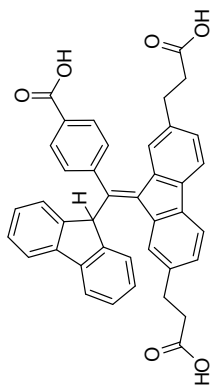
31.6
31.8
32.2
35.8
36.8
36.9

53.0
53.1

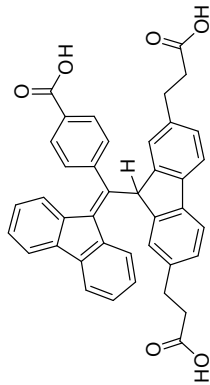
119.6
119.9
120.5
120.7
120.7

125.7
125.9
126.0
126.5
127.2
127.8
128.4
129.2
129.3
129.5
129.6
129.8

136.7
136.8
138.9
139.2
139.4
139.7
140.4
140.4
140.9
142.1
142.8
144.0
144.2
144.3
144.6
144.9

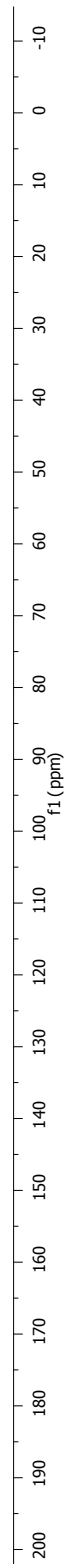


Integration of 1H = 1.00



Integration of 1H = 0.50

176.3
176.1
175.8
169.7



WS-BDPA ¹H-NMR
CD₃OD, 500 MHz

