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

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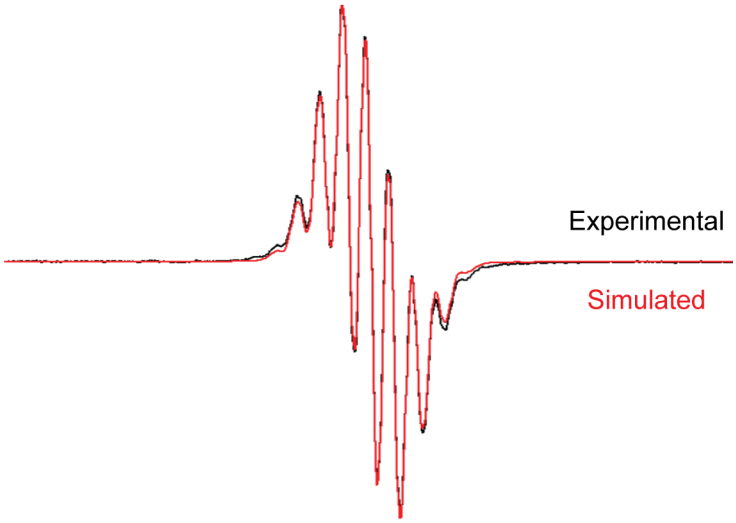
Materials.

All chemicals, reagents, and solvents were used as received from commercial sources without further purification except dimethylacetamide, dimethylformamide, and dimethylsufloxide, 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

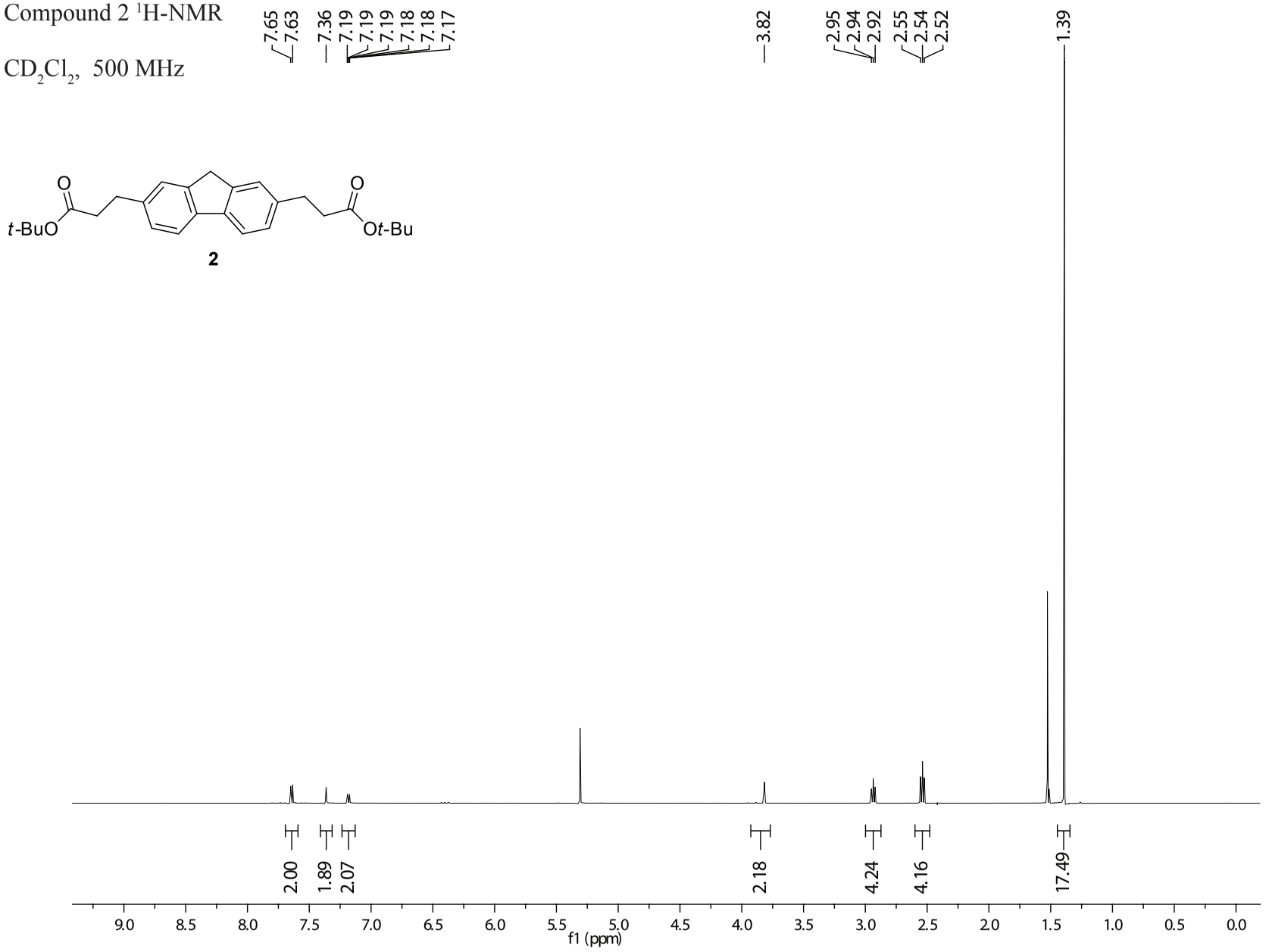
Simulated using WinSim[a] as a single radical with hyperfine couplings with 8 protons. (A1 = 1.986, A2 = 1.725, A3 = 1.894, A4 = 2.24, A5 = 1.717, A6 = 1.633, A7 = 2.164, A8 = 2.019).

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

Compound 2 ^{1}H-NMR

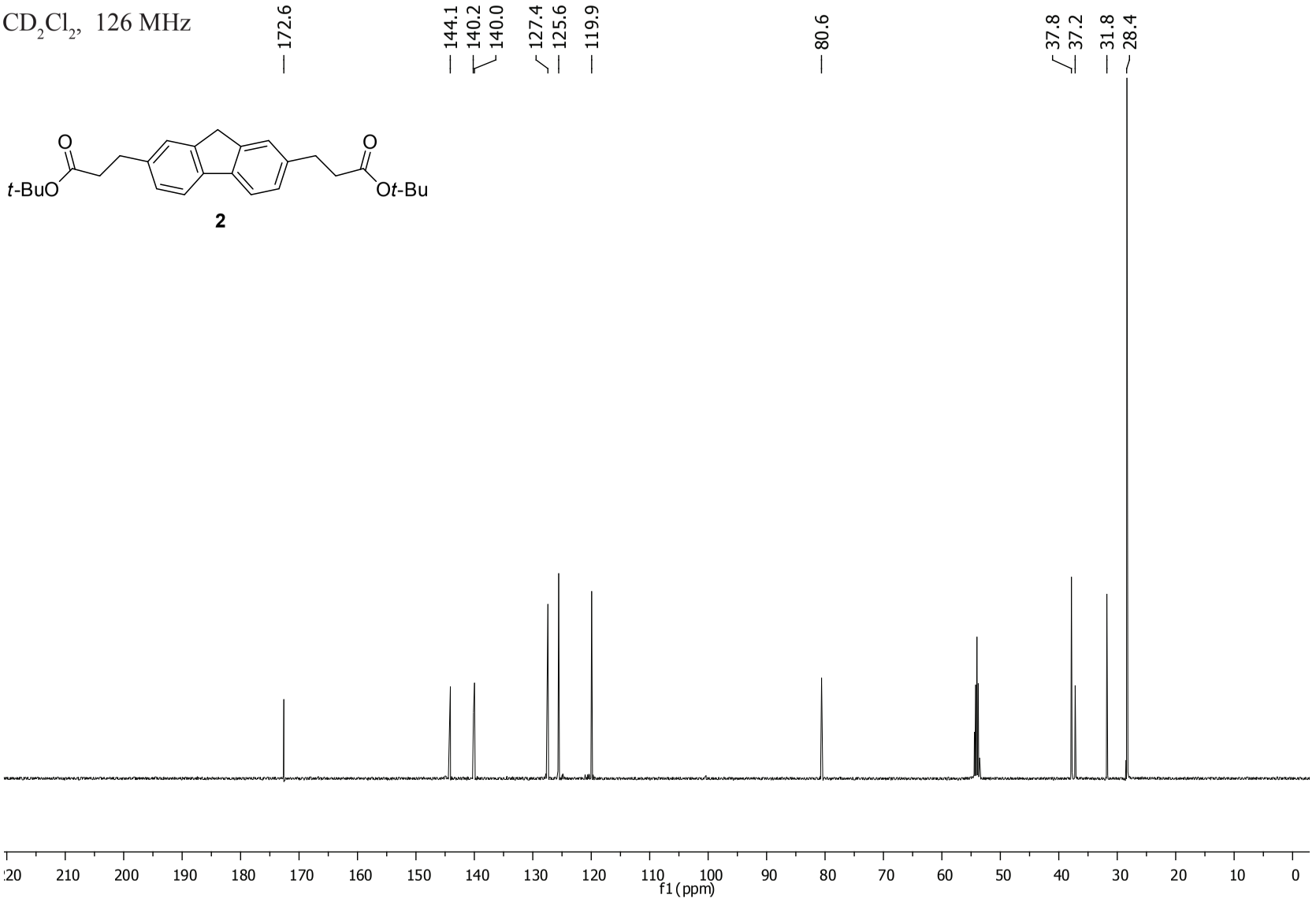
CD_2Cl_2, 500 MHz

2



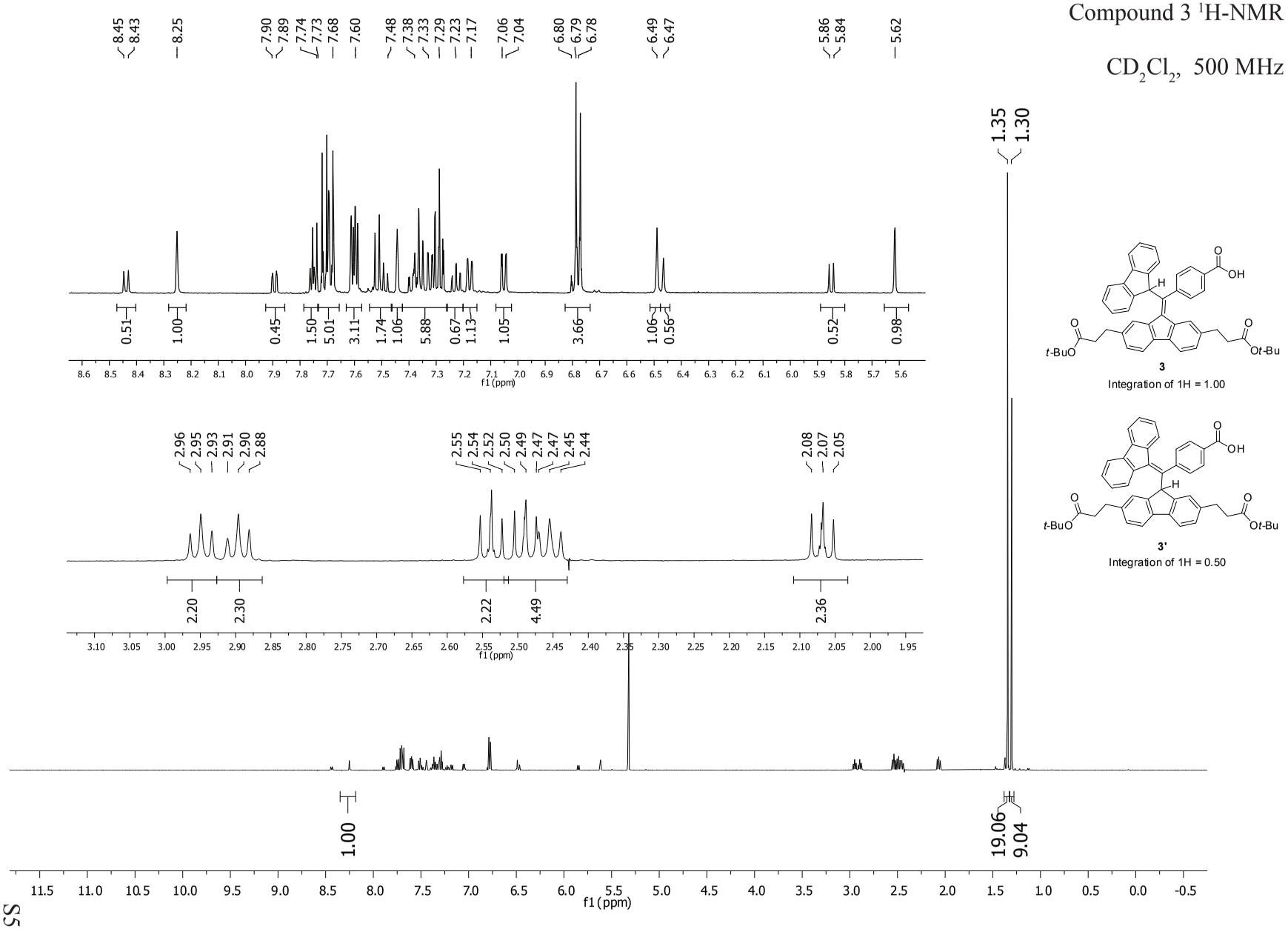
Compound 2 ^{13}C-NMR

CD_2Cl_2, 126 MHz



Compound 3 ^{1}H-NMR

CD_2Cl_2, 500 MHz



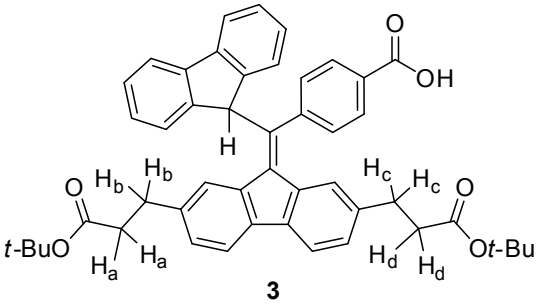
3

Integration of 1H = 1.00

3'

Integration of 1H = 0.50

Compound 3 g-COSY 2D-NMR
CD_2Cl_2, 500 MHz



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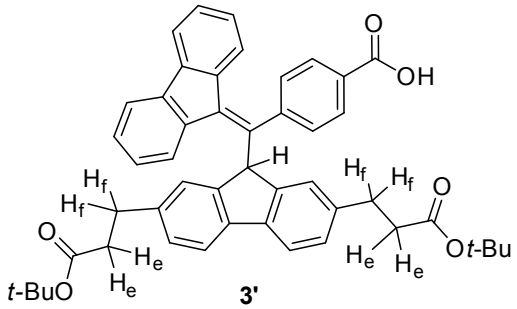
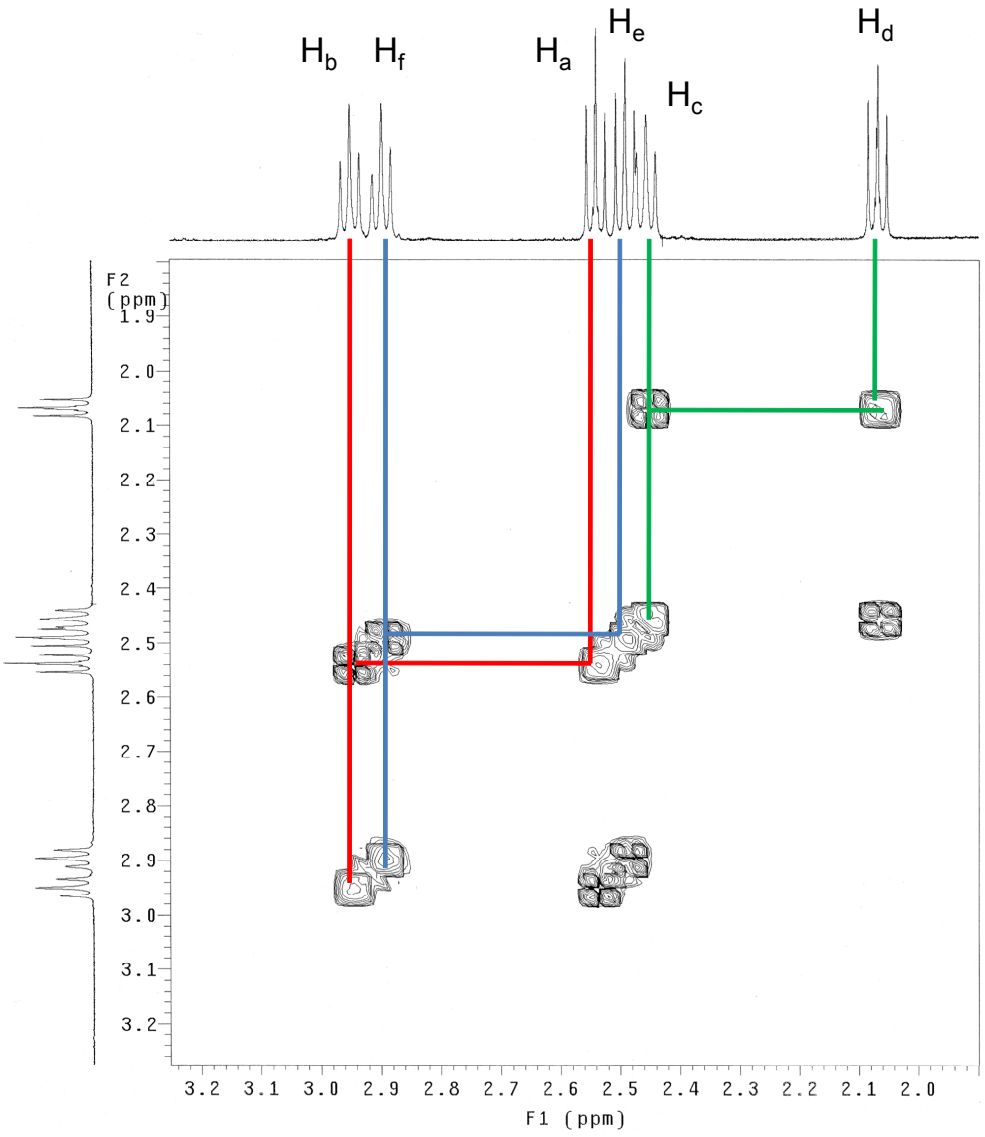


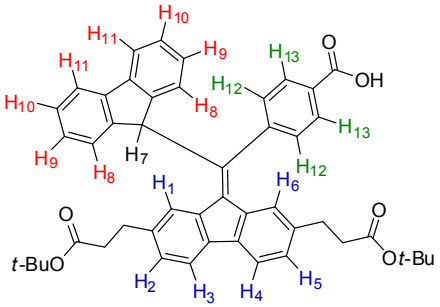
3'

Integration of 1H = 0.50



Compound 3 g-COSY 2D-NMR

CD_2Cl_2, 500 MHz



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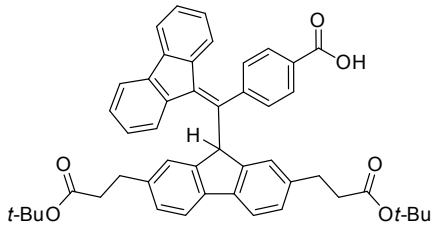

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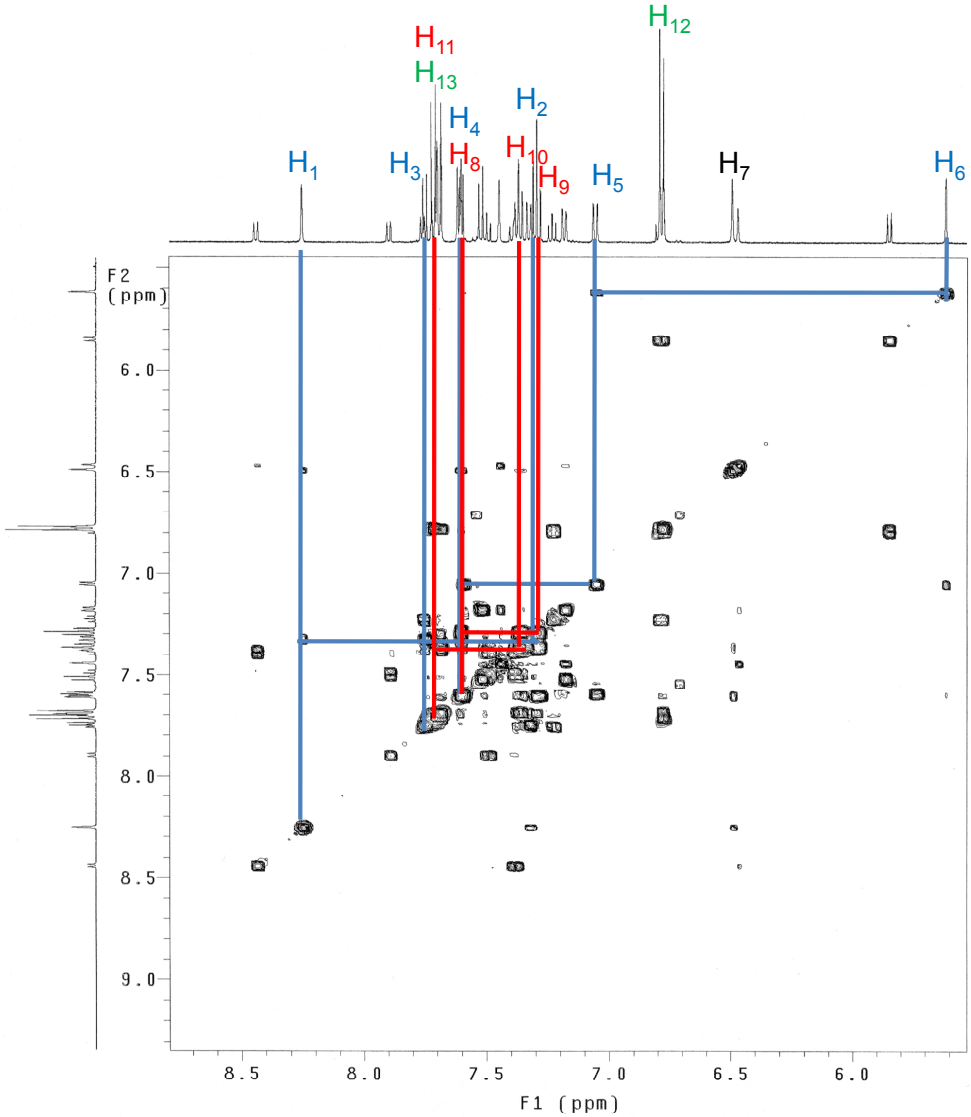
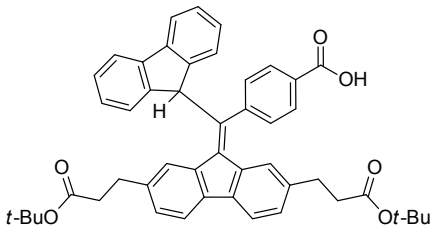
Integration of 1H = 0.50



Compound 3 g-COSY 2D-NMR
CD_2Cl_2, 500 MHz



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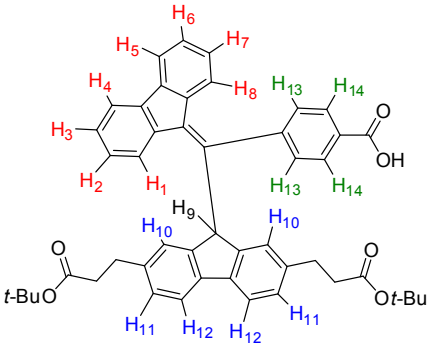
Integration of 1H = 1.00



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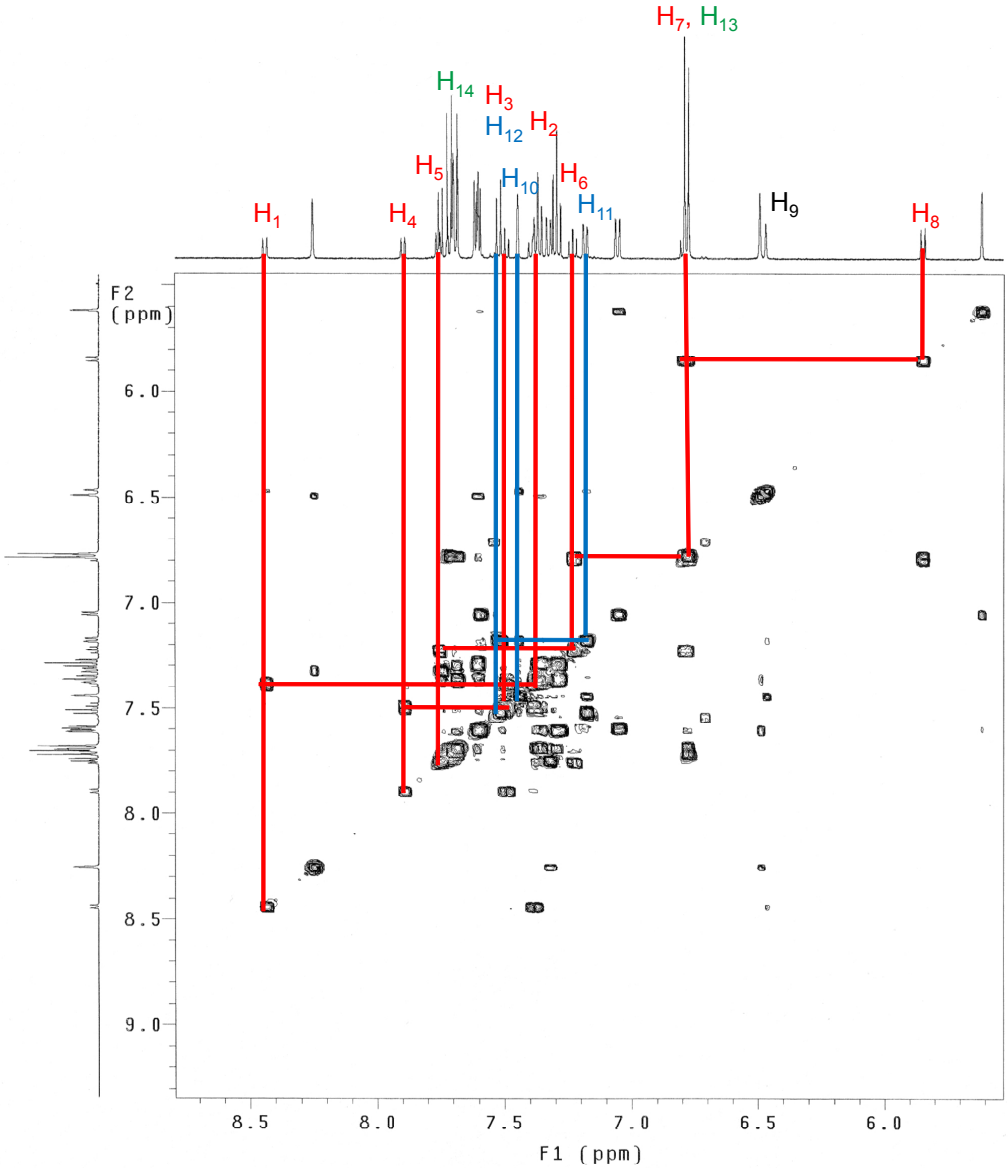
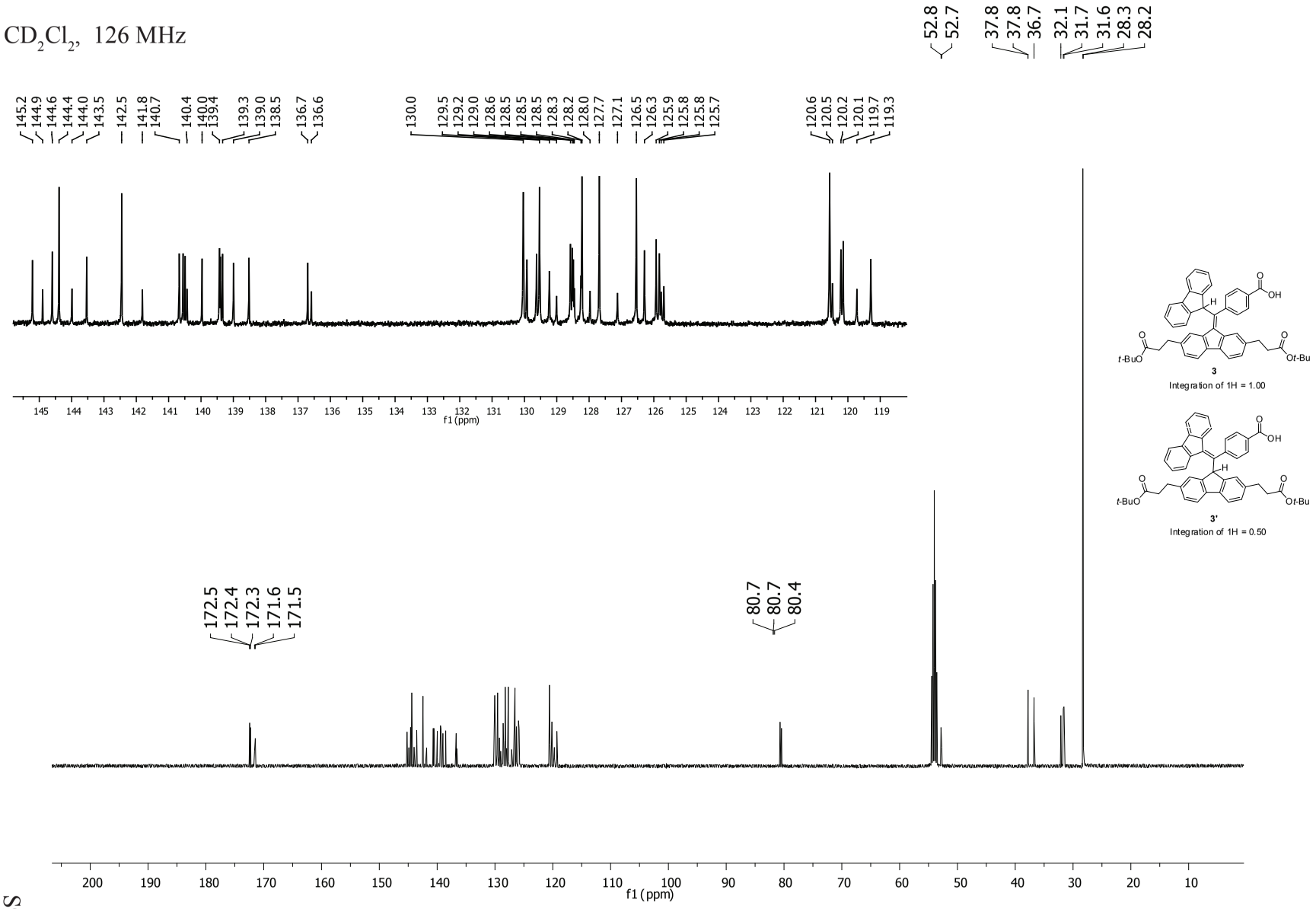
Integration of 1H = 0.50



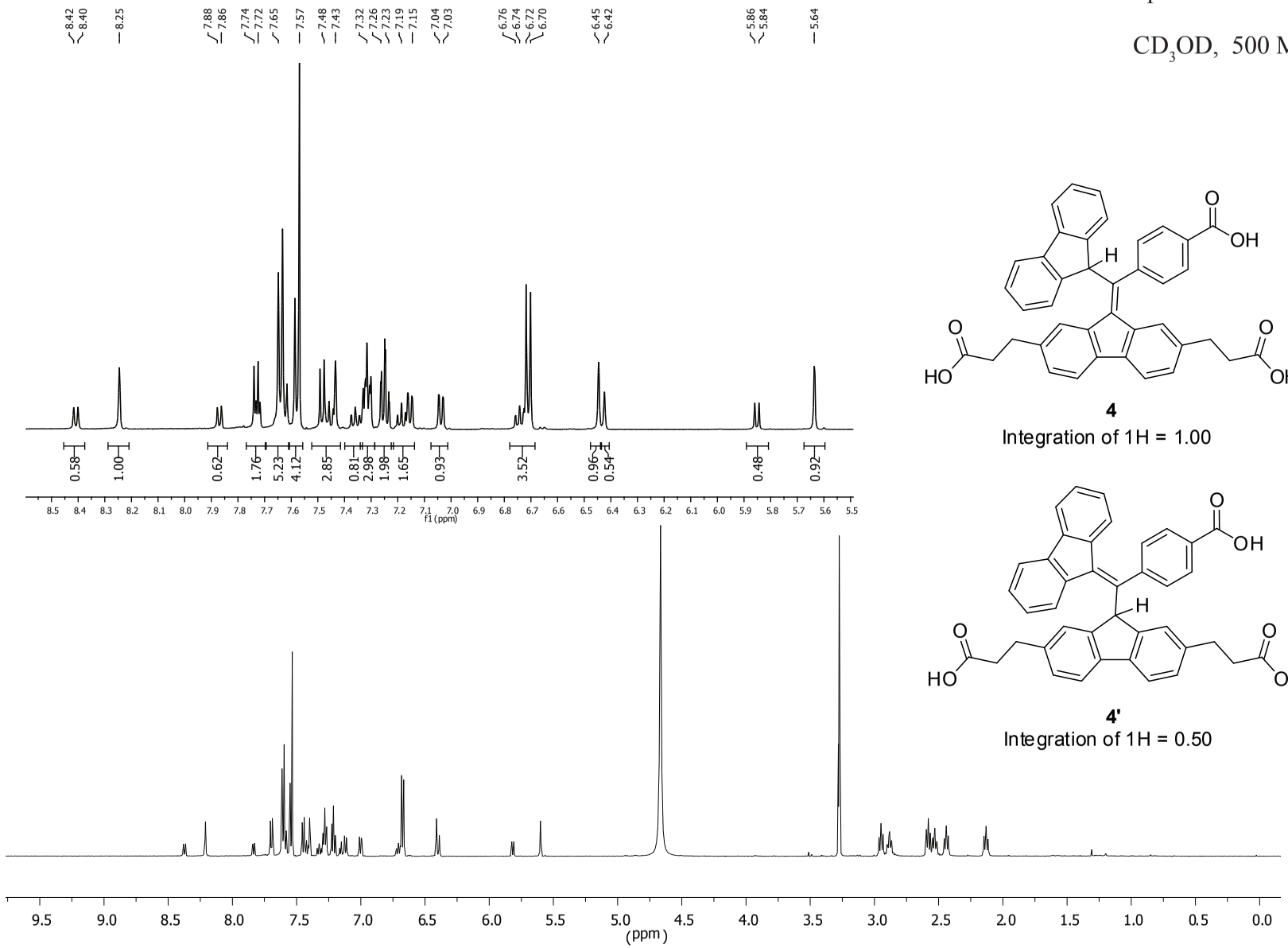
Compound 3 ^{13}C-NMR

CD_2Cl_2, 126 MHz



Compound 4 ^{1}H-NMR

CD_3OD, 500 MHz



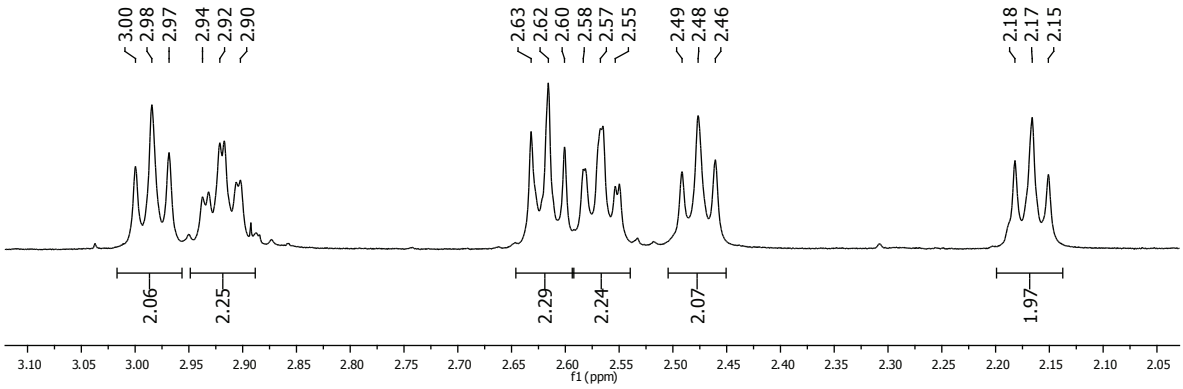
4

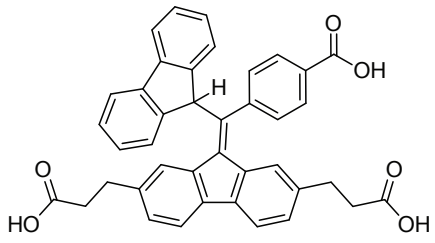
Integration of 1H = 1.00

4'

Integration of 1H = 0.50

Compound 4 ^{1}H-NMR (con't.) and g-COSY 2D-NMR
CD_3OD, 500 MHz





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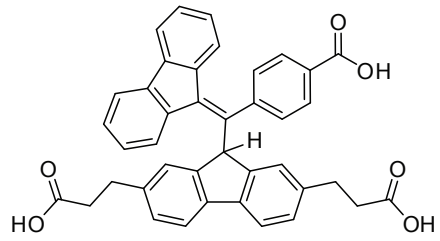
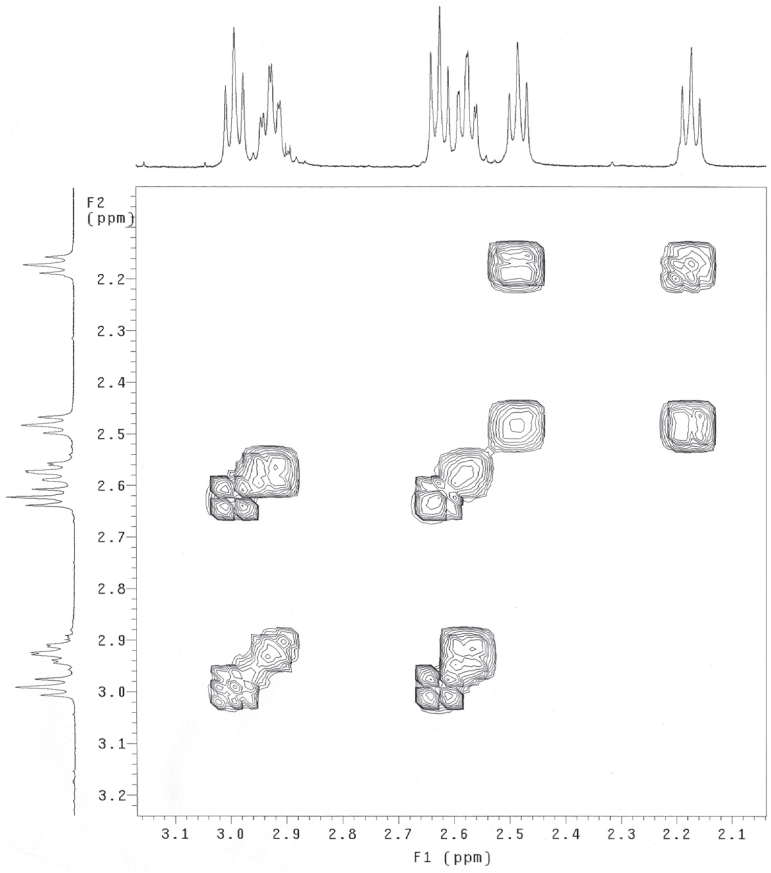
Integration of 1H = 1.00

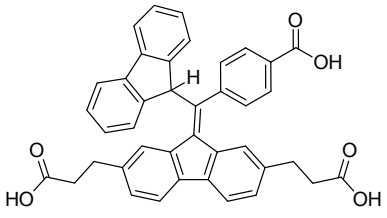


4'

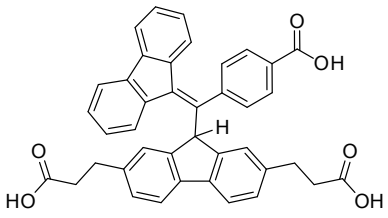
Integration of 1H = 0.50



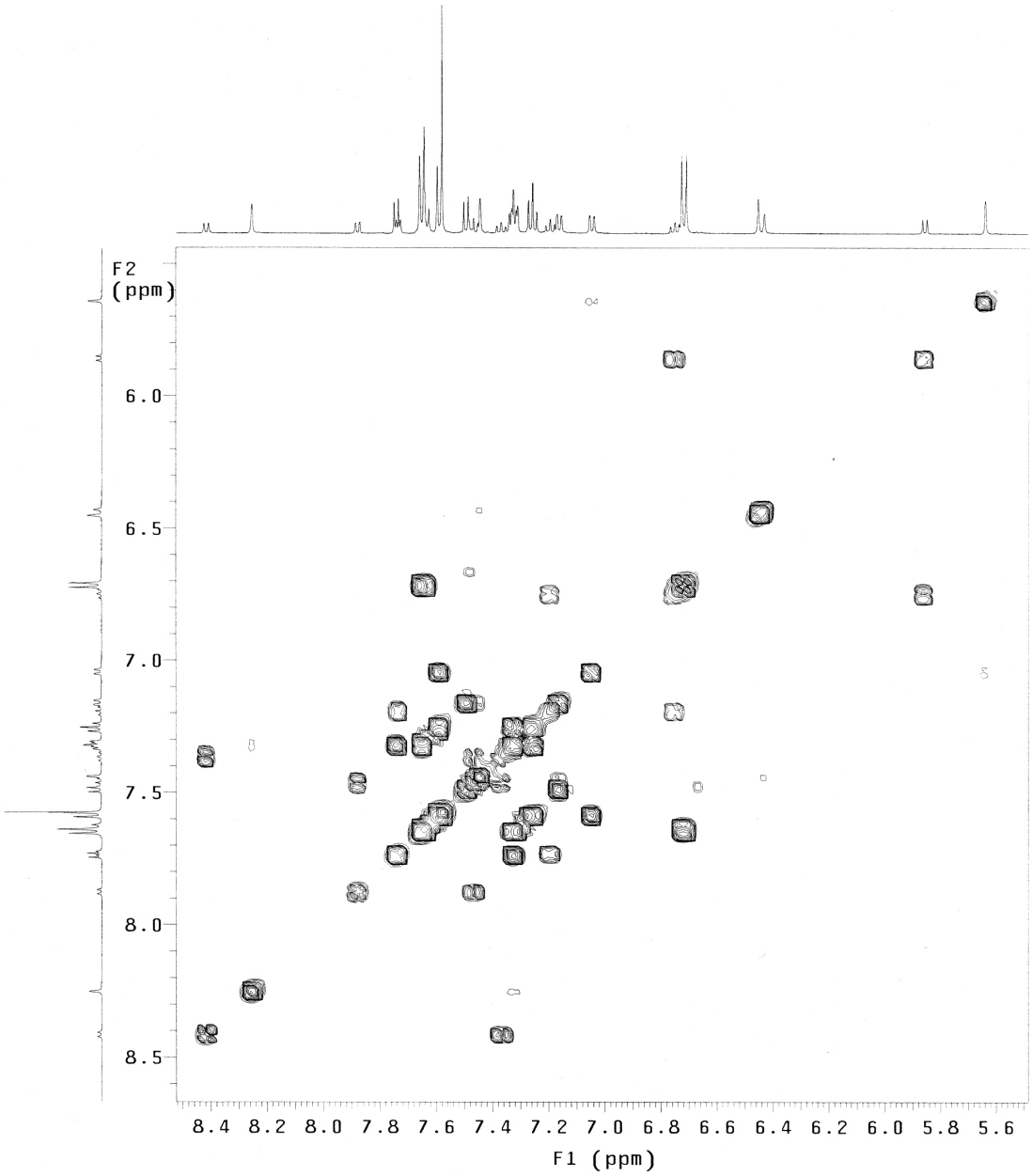
Compound 4 g-COSY 2D-NMR
CD_3OD, 500 MHz



4
Integration of 1H = 1.00

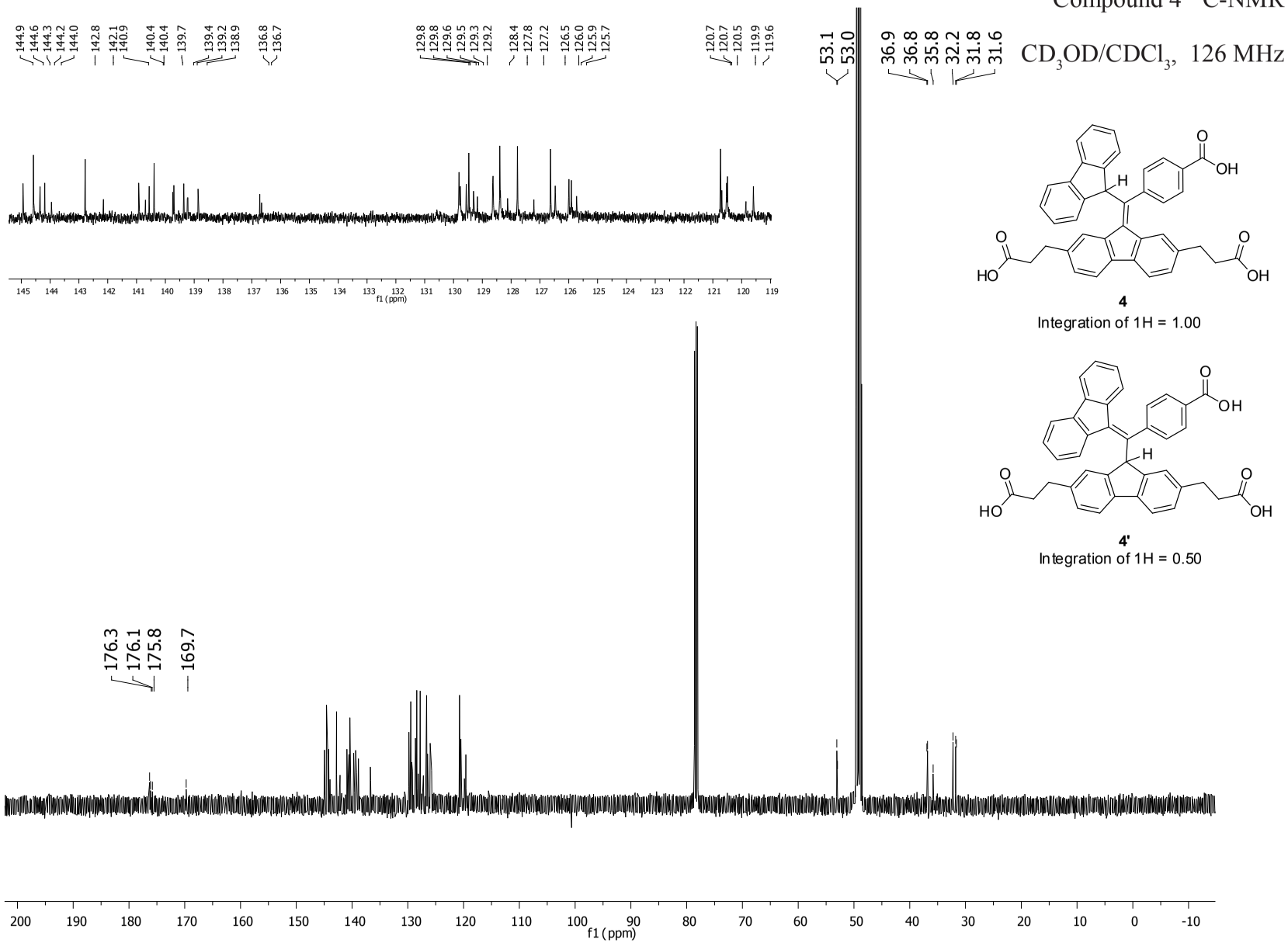


4'
Integration of 1H = 0.50



Compound 4 ^{13}C-NMR

$CD_3OD/CDCl_3$, 126 MHz



4

Integration of 1H = 1.00

4'

Integration of 1H = 0.50

WS-BDPA ^{1}H-NMR
CD_3OD, 500 MHz