

Fluorene-Based Sensitizers with Phenothiazine Donor: Effect of Mode of Donor Tethering on the Performance of Dye-Sensitized Solar Cells

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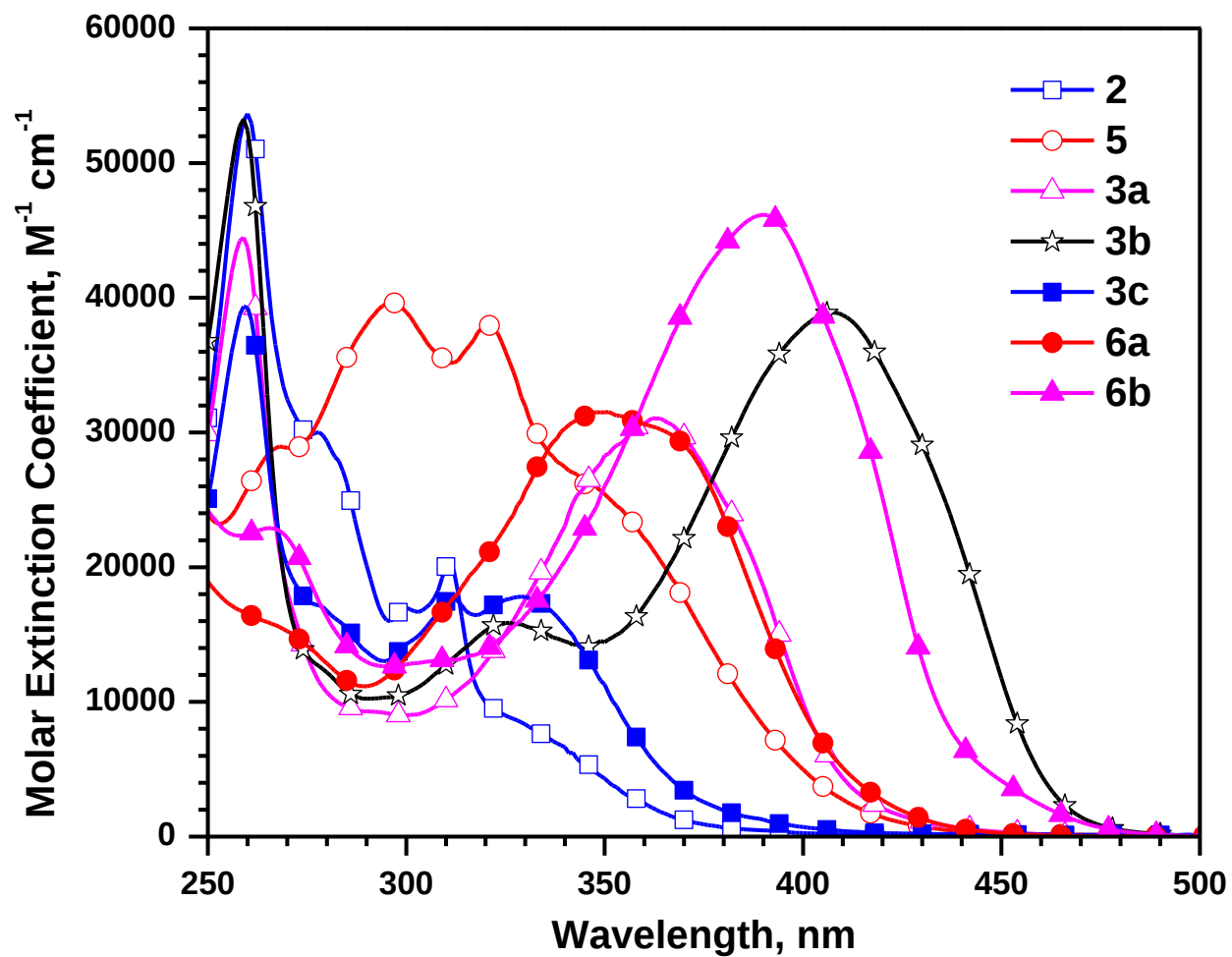


Figure S1. Absorption spectra of the precursor bromo and aldehydes derivatives recorded in DCM solutions.

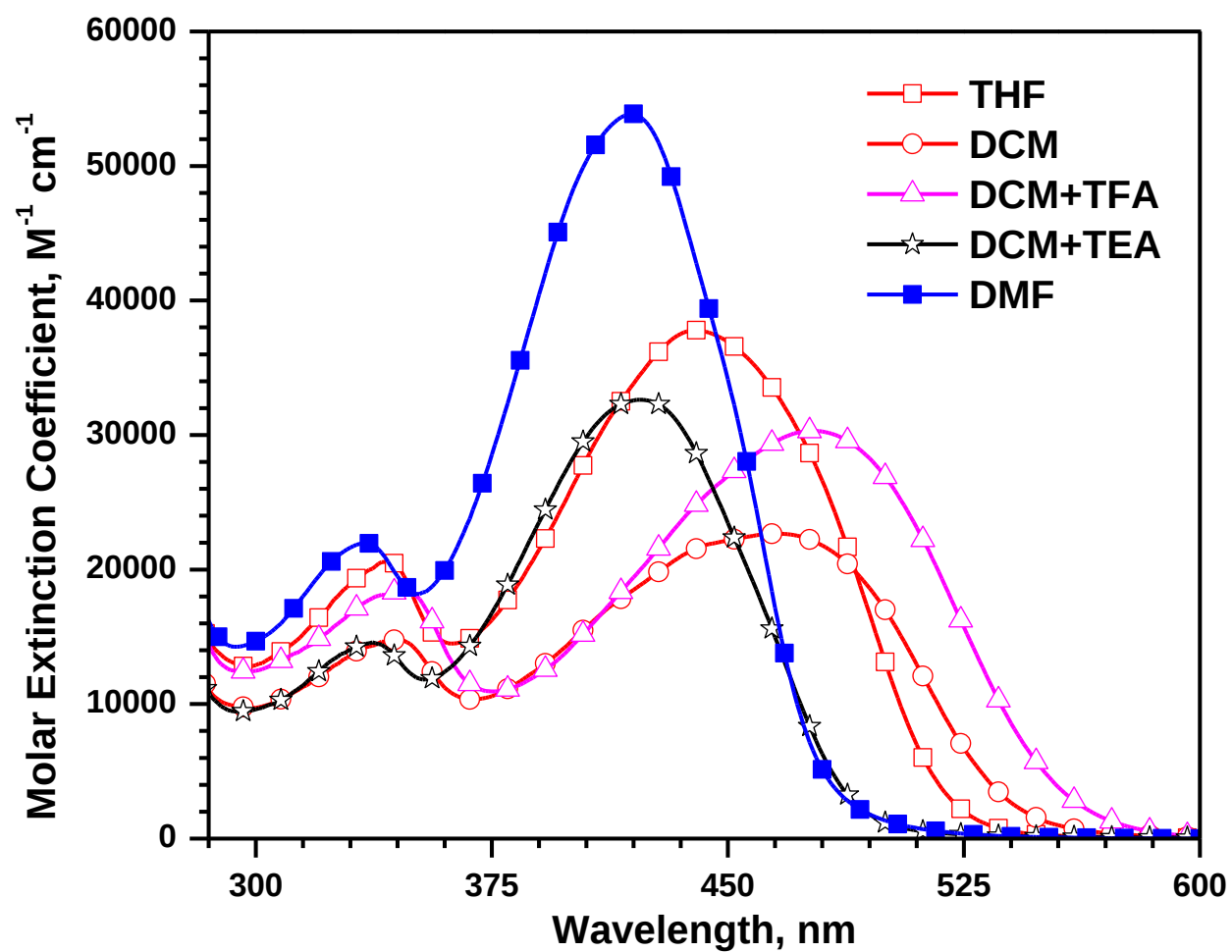


Figure S2. Absorption spectra of the dye **4b** recorded in different solvents.

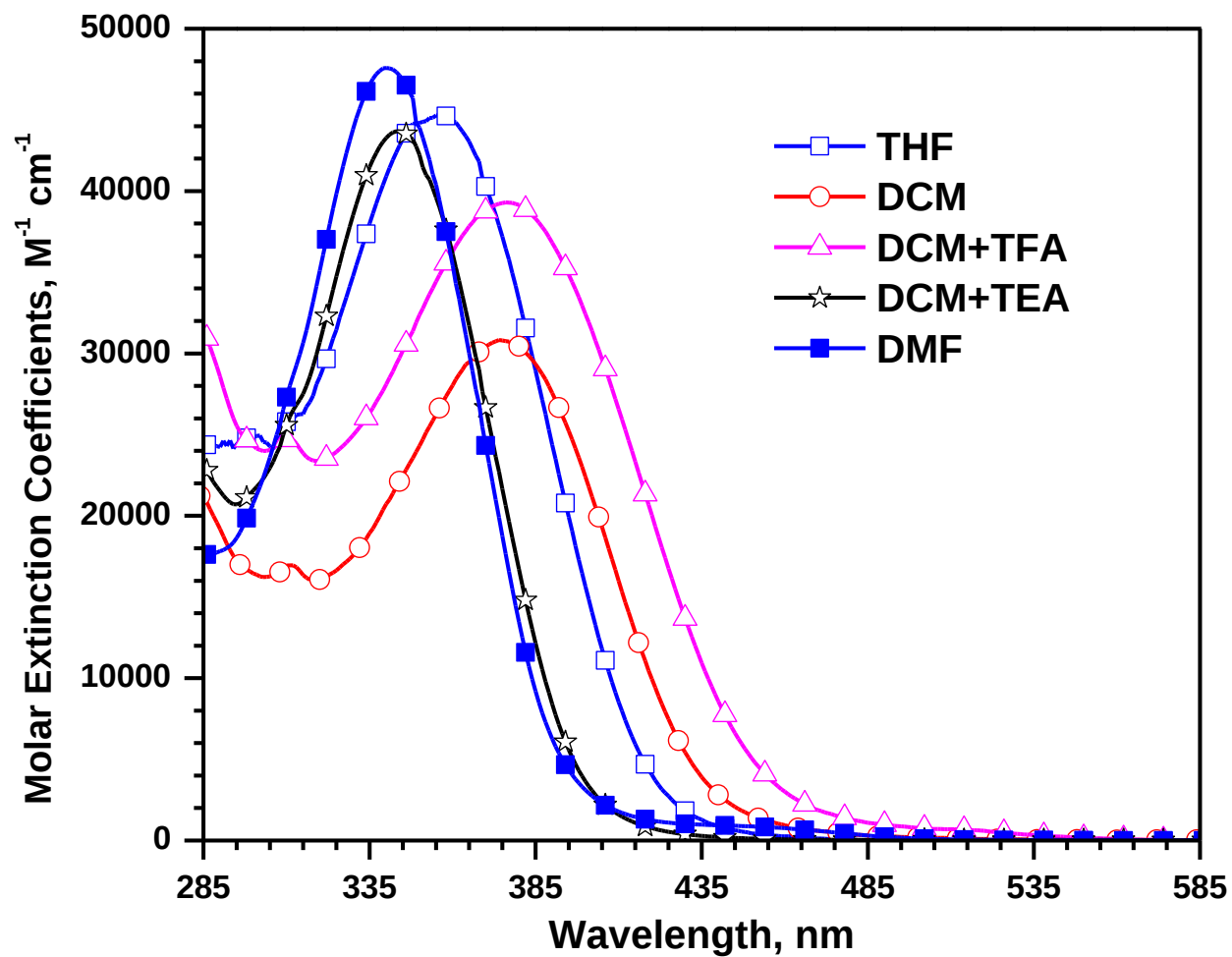


Figure S3. Absorption spectra of the dye 4c recorded in different solvents.

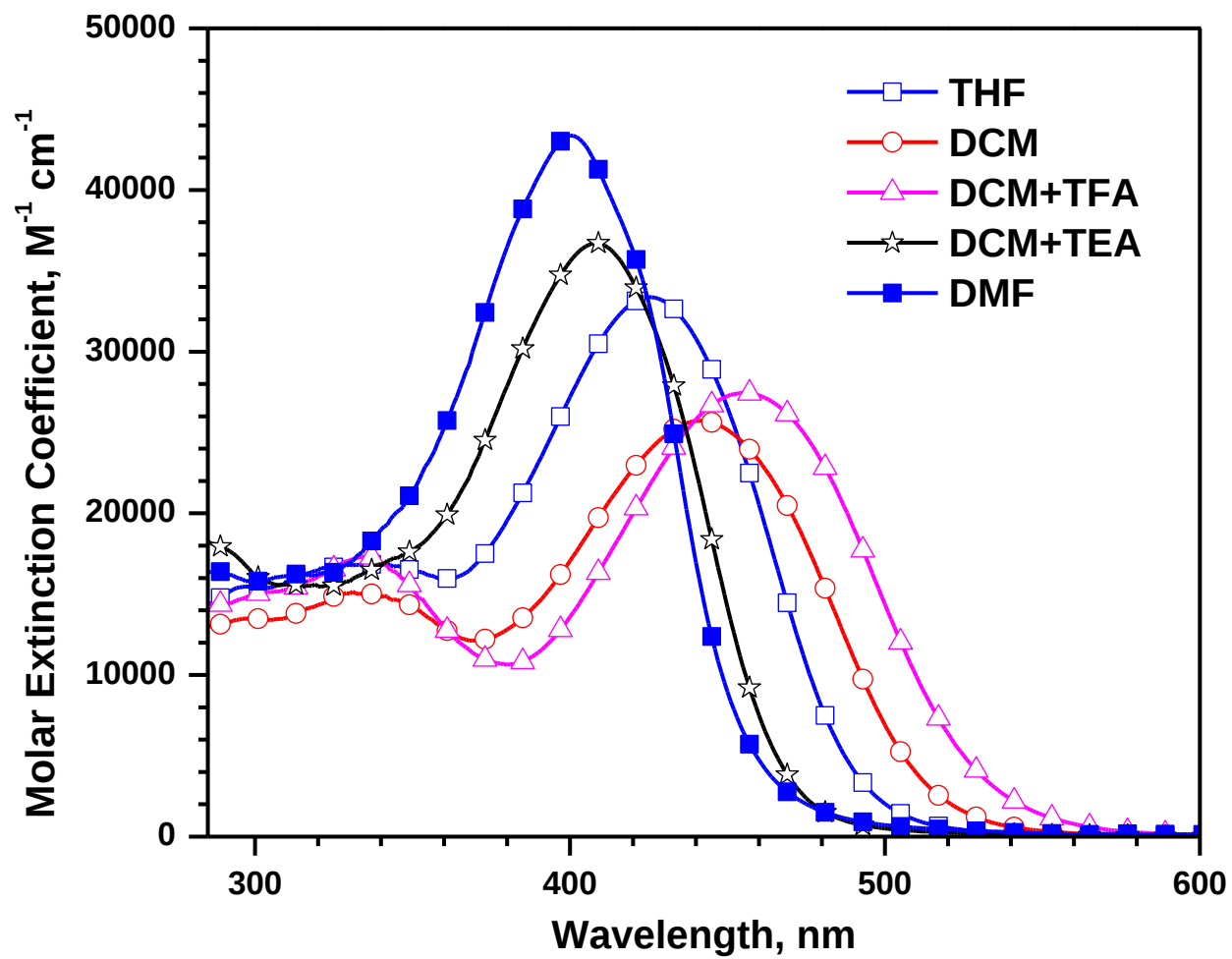


Figure S4. Absorption spectra of the dye 7a recorded in different solvents.

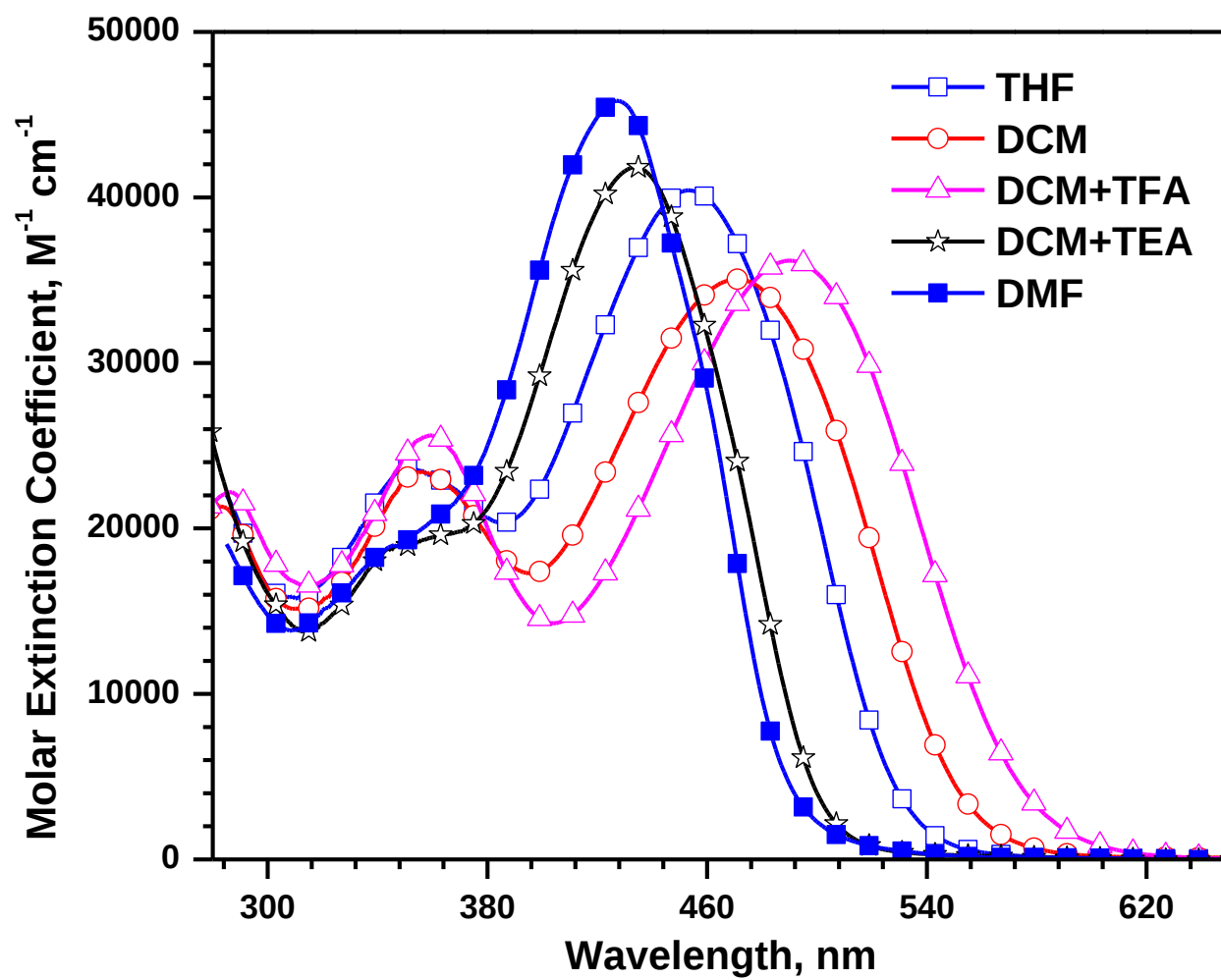


Figure S5. Absorption spectra of the dye **7b** recorded in different solvents.

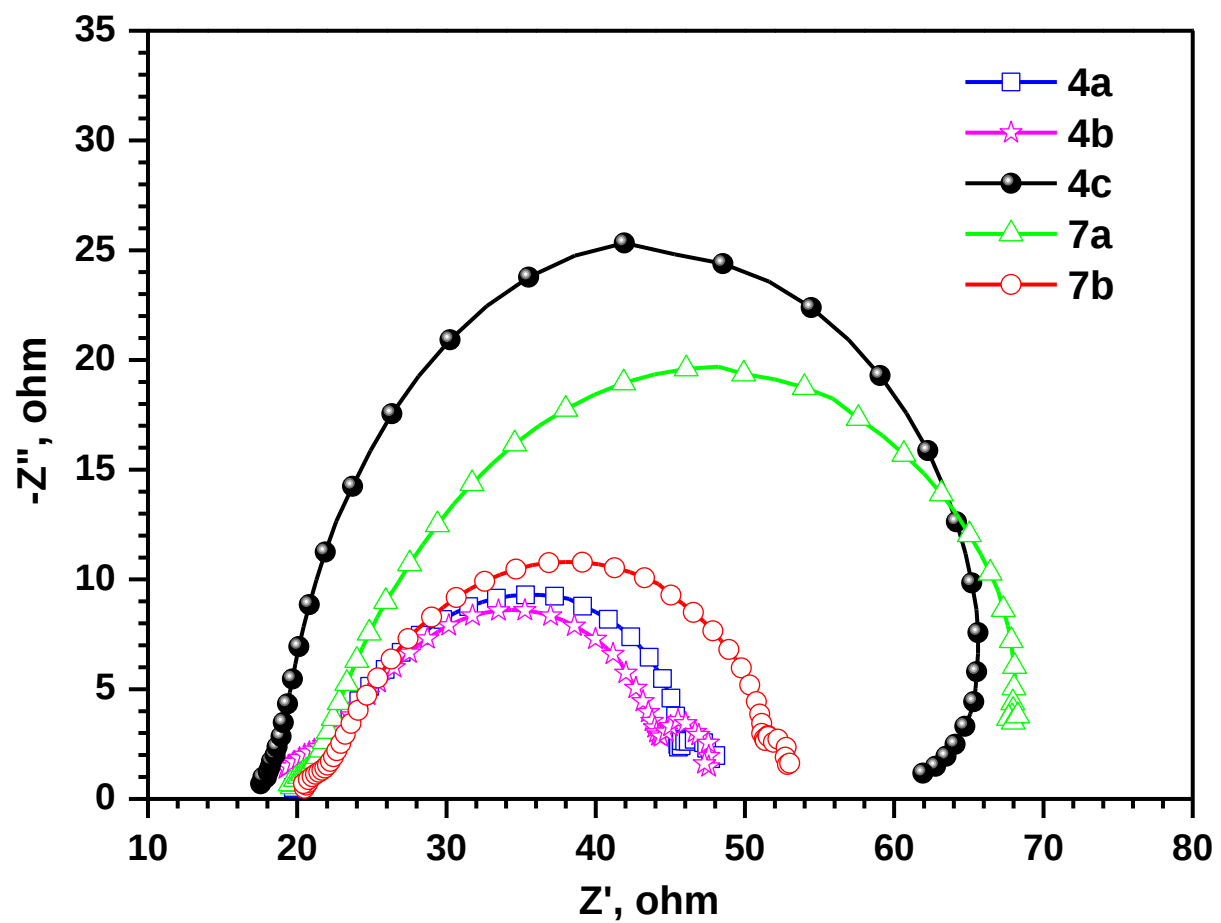


Figure S6. Nyquist plots for the DSSC measured under illumination.

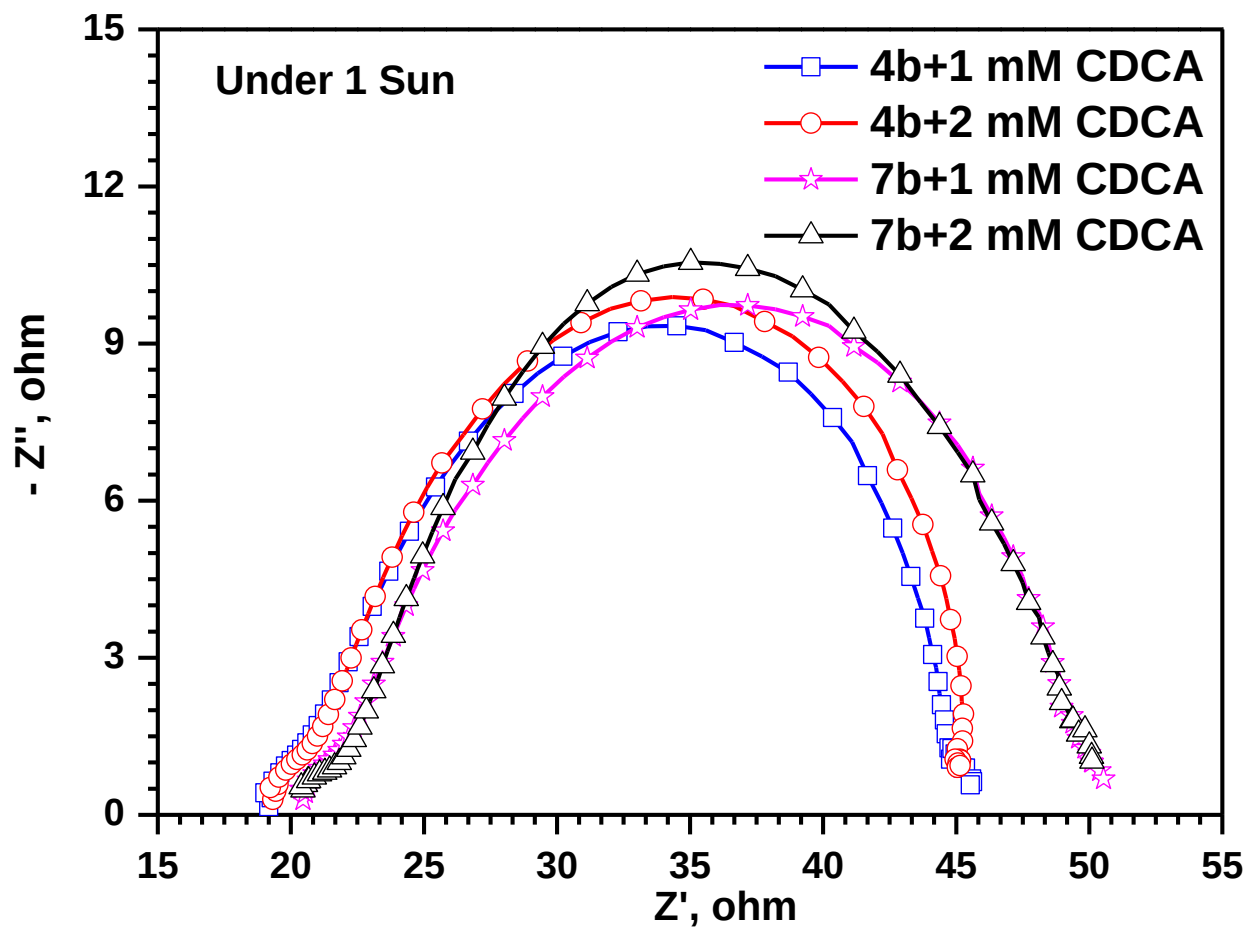


Figure S7. Nyquist plots for the DSSC using the dyes **4b** and **7b** co-adsorbed with CDCA measured under illumination.

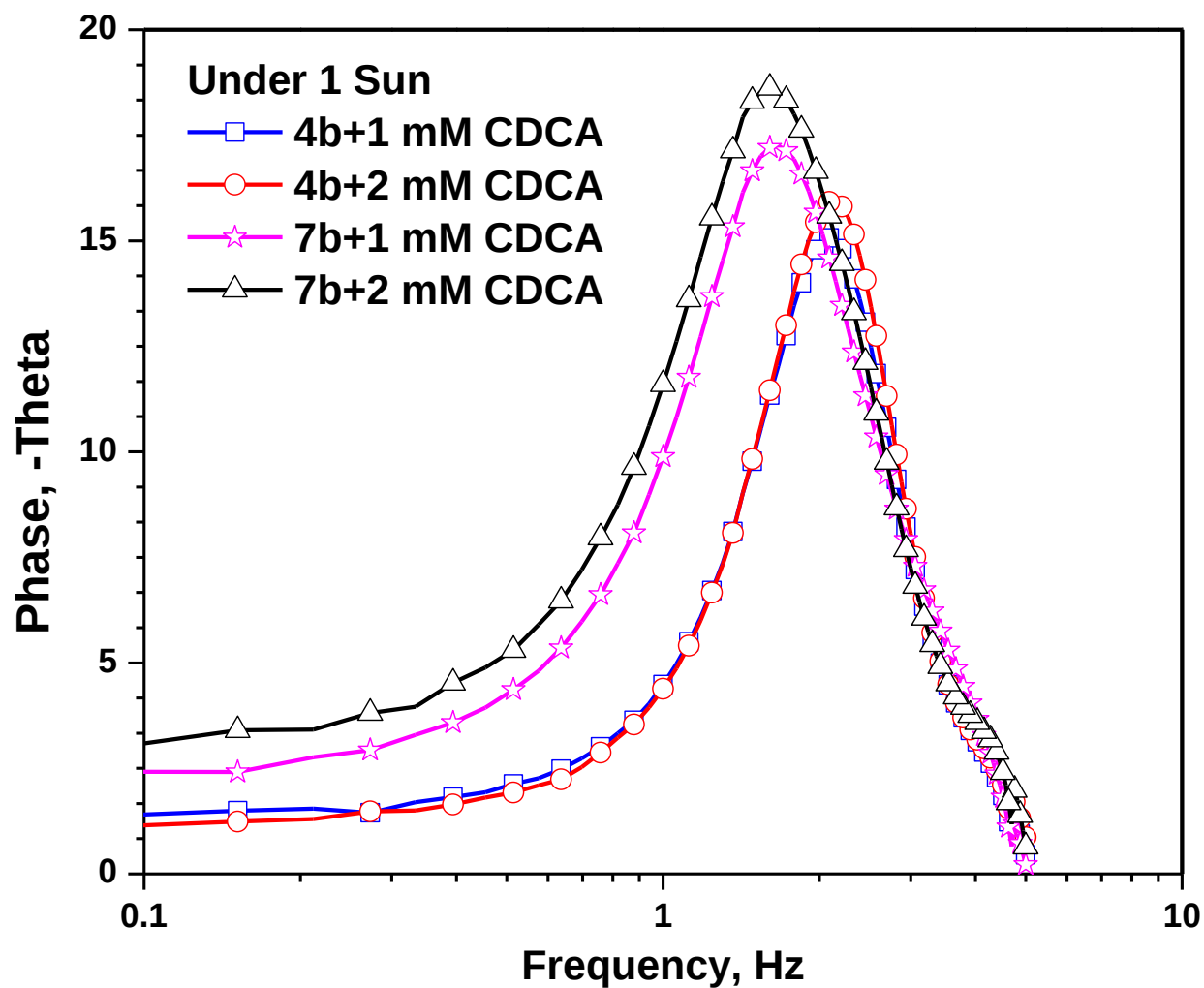


Figure S8. Bode phase plots for the DSSC using the dyes **4b** and **7b** co-adsorbed with CDCA measured under illumination.

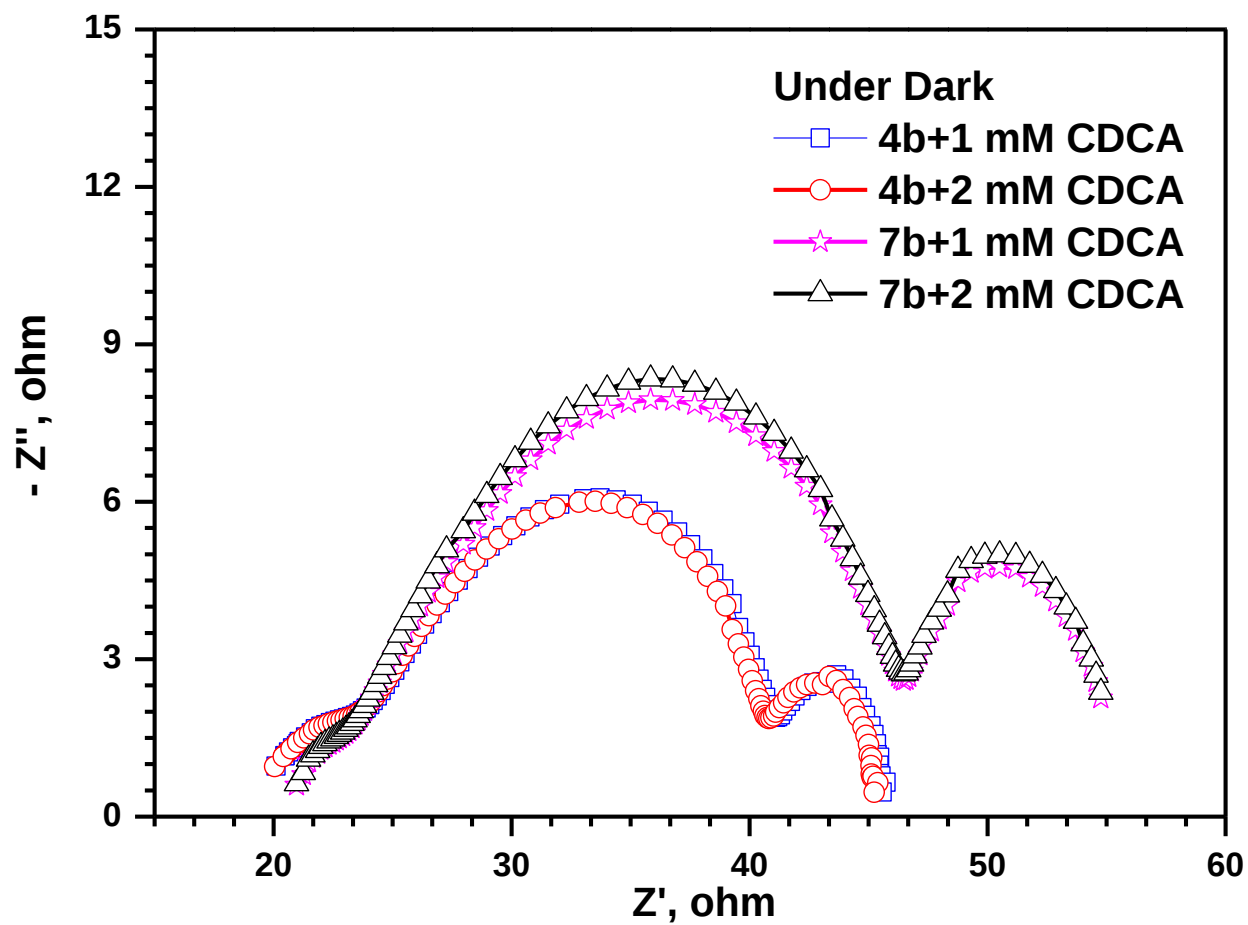


Figure S9. Nyquist plots for the DSSC using the dyes **4b** and **7b** co-adsorbed with CDCA measured under dark.

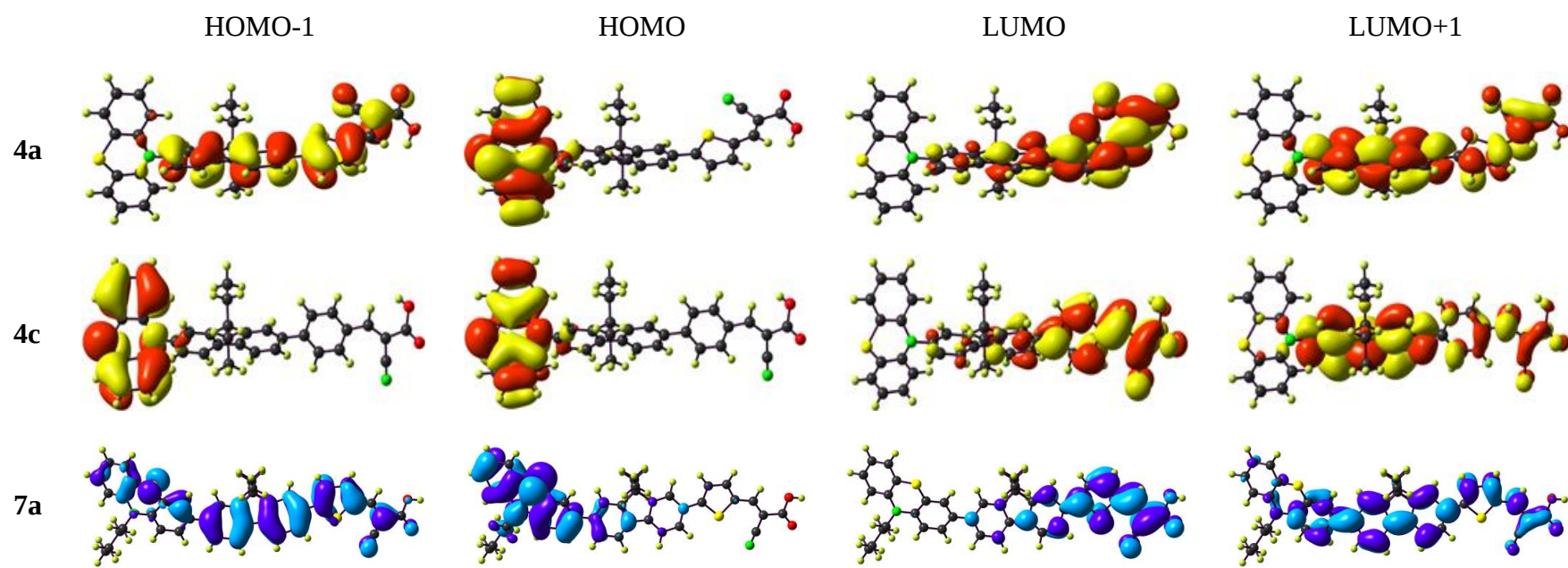


Figure S10. Electronic distribution in the frontier molecular orbitals of the dyes (**4a**, **4c** and **7a**).

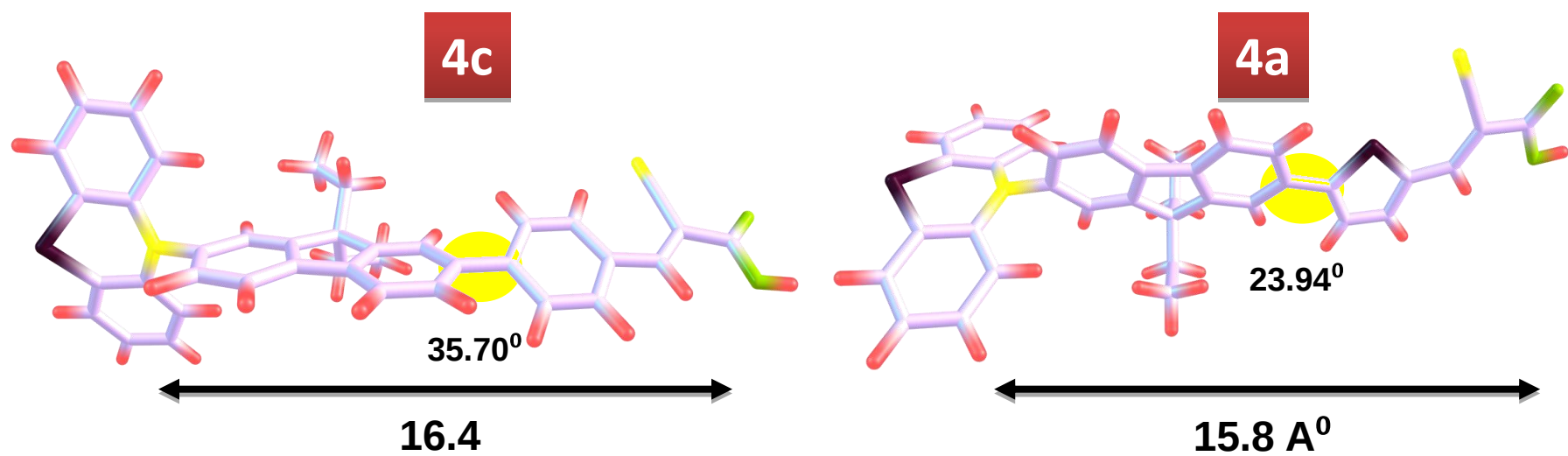


Figure S11. Molecular geometries of the dyes showing center-to-center distance between phenothizine nitrogen atom and carboxylic acid carbon and the dihedral angle between the π -spacer and fluorene core.

Table S1. Optical data of dyes recorded in different solvents.

Dye	λ_{abs} , nm (ϵ , $\text{M}^{-1}\text{cm}^{-1} \times 10^3$)			
	DCM+TEA	DCM+TFA	THF	DMF
4a	396 (37.9)	444 (47.3)	412 (37.1)	388 (43.1)
4b	422 (32.5),	476 (30.3),	440 (37.8),	420 (53.9),
	337 (14.6)	348 (18.4)	342 (20.7)	335 (21.9)
4c	344 (43.7)	376 (39.2)	356 (44.7)	340 (47.6)
7a	409 (36.7)	456 (27.4)	426 (33.3)	400 (43.4)
7b	434 (41.8),	489 (36.1)	453 (40.4),	428 (45.8)
	359 (25.6)		351 (23.7)	

Table S2. Calculated vertical transition energies and their oscillator strengths and configurations for the dyes.

Dye	λ_{exp} , nm	λ_{calc} , nm	f	Configuration	HOMO, eV	LUMO, eV	Band gap, eV
4a	429	433.1	1.00	HOMO-1→LUMO (98%)	-5.041	-2.914	2.127
4b	465	488.7	1.38	HOMO-1→LUMO (99%)	-5.042	-2.974	2.068
4c	374	411.2	0.39	HOMO→LUMO+1 (44%)	-5.049	-2.833	2.216
				HOMO-2→LUMO (36%)			
				HOMO-1→LUMO (18%)			
			0.50	HOMO-2→LUMO (60%)			
				HOMO→LUMO+1 (37%)			
7a	441	593.4	0.20	HOMO→LUMO (100%)	-4.944	2.648	2.296
		446.4	1.09	HOMO-1→LUMO (98%)			
		395.4	0.22	HOMO→LUMO+1 (86%)			
7b	471	623.6	0.20	HOMO→LUMO (100%)	-4.917	-2.753	2.164
		497.0	1.34	HOMO-1→LUMO (98%)			
		420.0	0.35	HOMO→LUMO+1 (86%)			

Table S3. Cartesian coordinates for the optimized geometry of **4a**.

Energy = -2483.1278461 Ha

Atom	X	Y	Z
C	-4.767104000	2.437862000	0.484876000
C	-5.296478000	3.719575000	0.638588000
C	-6.672400000	3.929765000	0.585954000
C	-7.517923000	2.836722000	0.395630000
C	-6.997866000	1.546662000	0.283379000
C	-7.145883000	-0.943227000	-0.770609000
C	-7.798380000	-1.861754000	-1.593929000
C	-7.077877000	-2.841698000	-2.276952000
C	-5.691947000	-2.877857000	-2.143763000
C	-5.028853000	-1.936217000	-1.356038000
C	-5.741389000	-0.949772000	-0.656438000
C	-5.606479000	1.327403000	0.304270000
C	-3.720475000	-0.225638000	0.543053000
C	-2.655610000	0.054016000	-0.329783000
C	-1.352328000	-0.186433000	0.088722000
C	-0.046513000	0.036937000	-0.673688000
C	0.977977000	-0.420170000	0.363820000
C	2.358925000	-0.456402000	0.257811000
C	3.139111000	-0.918735000	1.340545000
C	2.486322000	-1.338931000	2.519104000
C	1.099640000	-1.310208000	2.626785000
C	0.341903000	-0.848793000	1.547405000
C	-1.105947000	-0.702849000	1.377850000
C	-2.162983000	-0.981849000	2.247035000
C	-3.469379000	-0.740316000	1.821433000
C	0.150741000	1.531730000	-1.065635000
C	0.131505000	2.539280000	0.087818000
C	0.018517000	-0.819050000	-1.973293000
C	-0.132342000	-2.332233000	-1.790918000

N	-5.085486000	0.012921000	0.157431000
S	-8.114528000	0.160531000	0.236536000
H	-3.693347000	2.299152000	0.518391000
H	-4.619084000	4.555692000	0.788703000
H	-7.087098000	4.927618000	0.693018000
H	-8.594883000	2.974067000	0.354312000
H	-8.880691000	-1.815630000	-1.677068000
H	-7.596141000	-3.564874000	-2.899511000
H	-5.110377000	-3.634919000	-2.662596000
H	-3.949573000	-1.977506000	-1.275524000
H	-2.869230000	0.455620000	-1.317068000
H	2.846076000	-0.147612000	-0.663930000
H	3.077926000	-1.666626000	3.368181000
H	0.621783000	-1.634010000	3.547496000
H	-1.979977000	-1.379860000	3.241552000
H	-4.312867000	-0.945076000	2.473255000
H	1.104096000	1.615465000	-1.604047000
H	-0.630386000	1.792829000	-1.792192000
H	-0.818857000	2.513444000	0.631928000
H	0.268453000	3.555589000	-0.297093000
H	0.934649000	2.345013000	0.806240000
H	-0.762040000	-0.452998000	-2.653641000
H	0.974852000	-0.606322000	-2.469610000
H	0.665392000	-2.743919000	-1.163876000
H	-0.086406000	-2.836262000	-2.762506000
H	-1.090126000	-2.590283000	-1.326208000
C	4.599276000	-0.964452000	1.258682000
C	5.474882000	-1.745949000	1.998845000
S	5.472270000	0.051894000	0.137136000
C	6.823446000	-1.539745000	1.663826000
H	5.144868000	-2.466581000	2.737718000

C	7.018976000	-0.597749000	0.658749000
H	7.649327000	-2.068932000	2.129034000
C	8.302867000	-0.237121000	0.146521000
C	8.669575000	0.660197000	-0.819884000
H	9.115367000	-0.757967000	0.651957000
C	7.724009000	1.479217000	-1.505755000
C	10.107873000	0.933819000	-1.148884000
N	6.939440000	2.126822000	-2.072563000
O	10.496031000	1.993701000	-1.570678000
O	10.984737000	-0.085231000	-0.919567000
H	10.506261000	-0.926094000	-0.838568000

Table S4. Cartesian coordinates for the optimized geometry of **4b**.

Energy = -3034.9434262 Ha

Atom	X	Y	Z
C	-6.587292000	2.451064000	0.328383000
C	-7.146615000	3.727547000	0.395995000
C	-8.527183000	3.901410000	0.336971000
C	-9.346679000	2.777686000	0.229733000
C	-8.796549000	1.495472000	0.204605000
C	-8.896448000	-1.069553000	-0.658553000
C	-9.534316000	-2.064776000	-1.400217000
C	-8.797085000	-3.078073000	-2.013087000
C	-7.409440000	-3.070915000	-1.893948000
C	-6.761979000	-2.055242000	-1.189726000
C	-7.491301000	-1.034335000	-0.560235000
C	-7.399906000	1.310548000	0.229332000
C	-5.468254000	-0.175657000	0.535392000
C	-4.432095000	0.094792000	-0.374401000
C	-3.113359000	-0.091249000	0.021836000
C	-1.832387000	0.134515000	-0.781371000
C	-0.770903000	-0.254643000	0.246854000
C	0.608075000	-0.260172000	0.106276000
C	1.427244000	-0.660130000	1.184172000
C	0.815059000	-1.049651000	2.394444000
C	-0.569137000	-1.052602000	2.536774000
C	-1.366084000	-0.652014000	1.461517000
C	-2.821567000	-0.548555000	1.323863000
C	-3.850008000	-0.818173000	2.229334000
C	-5.172738000	-0.628432000	1.827051000
C	-1.685050000	1.617144000	-1.235072000
C	-1.702173000	2.667823000	-0.120771000
C	-1.775970000	-0.768253000	-2.048806000
C	-1.883206000	-2.276853000	-1.807085000

N	-6.848126000	0.002258000	0.168857000
S	-9.882715000	0.086209000	0.269679000
H	-5.510452000	2.341225000	0.366408000
H	-6.488537000	4.587597000	0.484516000
H	-8.965390000	4.894150000	0.376910000
H	-10.426922000	2.885985000	0.187247000
H	-10.618203000	-2.050702000	-1.474073000
H	-9.303836000	-3.860004000	-2.570720000
H	-6.814665000	-3.852373000	-2.358832000
H	-5.681360000	-2.064258000	-1.118206000
H	-4.680493000	0.444626000	-1.373268000
H	1.064958000	0.021069000	-0.839667000
H	1.438147000	-1.328551000	3.238502000
H	-1.014766000	-1.352717000	3.481464000
H	-3.632788000	-1.170140000	3.234279000
H	-5.994243000	-0.828310000	2.507877000
H	-0.747338000	1.703629000	-1.800500000
H	-2.490242000	1.830730000	-1.950945000
H	-2.636606000	2.636312000	0.449747000
H	-1.605495000	3.672537000	-0.546833000
H	-0.875803000	2.522740000	0.582822000
H	-2.581125000	-0.448140000	-2.723835000
H	-0.836651000	-0.551181000	-2.575364000
H	-1.063225000	-2.643675000	-1.181067000
H	-1.842764000	-2.815889000	-2.759978000
H	-2.825017000	-2.541175000	-1.314248000
C	2.886022000	-0.677353000	1.067276000
C	3.797773000	-1.443389000	1.768356000
S	3.723098000	0.370068000	-0.061619000
C	5.142632000	-1.209769000	1.404946000
H	3.501378000	-2.182168000	2.504193000

C	5.293347000	-0.255623000	0.414892000
H	5.980302000	-1.741017000	1.844934000
C	6.503914000	0.228573000	-0.196886000
C	6.639207000	1.117381000	-1.257442000
S	8.069105000	-0.295401000	0.384386000
C	7.975976000	1.370674000	-1.597633000
H	5.792486000	1.560094000	-1.770030000
C	8.902011000	0.687729000	-0.813957000
H	8.278309000	2.034066000	-2.401837000
C	10.315009000	0.796040000	-0.977448000
C	11.349626000	0.179203000	-0.324741000
H	10.591249000	1.467238000	-1.789888000
C	11.139966000	-0.794429000	0.696214000
C	12.780802000	0.394286000	-0.717845000
N	10.952914000	-1.573127000	1.541924000
O	13.639508000	-0.436471000	-0.560224000
O	13.073370000	1.592107000	-1.301554000
H	12.367114000	2.233001000	-1.119938000

Table S5. Cartesian coordinates for the optimized geometry of **4c**.

Energy = - 2162.36773091 Ha

Atom	X	Y	Z
C	5.146710000	-2.342710000	-0.711705000
C	5.751443000	-3.514758000	-1.167040000
C	7.136159000	-3.659881000	-1.127997000
C	7.911463000	-2.622992000	-0.608747000
C	7.310480000	-1.465513000	-0.112393000
C	7.389909000	1.209417000	0.302823000
C	8.061668000	2.425837000	0.174608000
C	7.352787000	3.615045000	0.003674000
C	5.962190000	3.569987000	-0.060552000
C	5.286006000	2.352452000	0.024014000
C	5.985531000	1.148974000	0.205217000
C	5.913311000	-1.295750000	-0.176224000
C	3.899124000	-0.100288000	0.564553000
C	2.964953000	0.098879000	-0.465871000
C	1.608089000	0.088451000	-0.165120000
C	0.418420000	0.280852000	-1.105150000
C	-0.749948000	0.155953000	-0.127972000
C	-2.109863000	0.239099000	-0.387834000
C	-3.041847000	0.079835000	0.659037000
C	-2.562256000	-0.161307000	1.961706000
C	-1.197766000	-0.241511000	2.230331000
C	-0.288764000	-0.083318000	1.182418000
C	1.176927000	-0.121674000	1.161082000
C	2.103702000	-0.320007000	2.186479000
C	3.464843000	-0.307488000	1.879758000
C	-4.495639000	0.165193000	0.394092000
C	-5.009977000	1.054128000	-0.568076000
C	-6.372896000	1.128615000	-0.812314000
C	-7.293834000	0.319703000	-0.112074000

C	-6.778792000	-0.571075000	0.854601000
C	-5.414547000	-0.640563000	1.095304000
C	0.369444000	-0.814480000	-2.212041000
C	0.318017000	-2.264373000	-1.721136000
C	0.448061000	1.673296000	-1.801745000
C	0.479527000	2.889494000	-0.871246000
C	-8.700658000	0.479465000	-0.441053000
C	-9.820392000	-0.173224000	-0.016467000
C	-11.178853000	0.140685000	-0.588232000
C	-9.811998000	-1.271142000	0.898168000
N	5.313715000	-0.099401000	0.302402000
N	-9.810040000	-2.151767000	1.659203000
O	-11.373658000	1.418223000	-1.016251000
O	-12.050328000	-0.683969000	-0.692479000
S	8.316430000	-0.253402000	0.718041000
H	4.068933000	-2.247591000	-0.761292000
H	5.127347000	-4.310709000	-1.563887000
H	7.611136000	-4.565762000	-1.492585000
H	8.993242000	-2.713461000	-0.563902000
H	9.146572000	2.434884000	0.232614000
H	7.883155000	4.559376000	-0.074514000
H	5.388974000	4.484082000	-0.188733000
H	4.204799000	2.340139000	-0.037930000
H	3.319918000	0.257405000	-1.481109000
H	-2.466319000	0.394752000	-1.402905000
H	-3.270106000	-0.257185000	2.779625000
H	-0.854896000	-0.418020000	3.246380000
H	1.779044000	-0.482108000	3.210813000
H	4.209548000	-0.458229000	2.654998000
H	-4.335300000	1.712383000	-1.106694000
H	-6.742383000	1.831473000	-1.555543000

H	-7.442880000	-1.218489000	1.413134000
H	-5.047428000	-1.356558000	1.824048000
H	-0.506010000	-0.613580000	-2.844301000
H	1.246833000	-0.677915000	-2.858533000
H	1.191889000	-2.514916000	-1.110178000
H	0.298521000	-2.952266000	-2.573567000
H	-0.576497000	-2.453802000	-1.118786000
H	1.322180000	1.697841000	-2.466362000
H	-0.431167000	1.739448000	-2.456990000
H	-0.405208000	2.925416000	-0.226991000
H	0.505280000	3.814898000	-1.457214000
H	1.363181000	2.879902000	-0.224162000
H	-8.875861000	1.246485000	-1.194797000
H	-10.687593000	2.000864000	-0.651943000

Table S6. Cartesian coordinates for the optimized geometry of **7a**.

Energy = - 2640.4616267 Ha

Atom	X	Y	Z
C	-2.096263000	0.681577000	-0.675886000
C	-1.456917000	1.764541000	-1.312405000
H	-2.062835000	2.533810000	-1.780783000
C	-0.069104000	1.852962000	-1.383846000
H	0.395678000	2.696500000	-1.886508000
C	0.706281000	0.839498000	-0.815509000
C	0.085385000	-0.253491000	-0.177677000
C	-1.297869000	-0.331424000	-0.105735000
H	-1.775791000	-1.157266000	0.413676000
C	2.156363000	0.663849000	-0.733277000
C	3.209245000	1.456708000	-1.196897000
H	3.018429000	2.382190000	-1.732030000
C	4.519203000	1.043648000	-0.975455000
H	5.336466000	1.647554000	-1.358088000
C	4.804535000	-0.155033000	-0.289214000
C	3.729048000	-0.943837000	0.179426000
H	3.933712000	-1.853307000	0.736395000
C	2.424322000	-0.538759000	-0.043925000
C	1.125571000	-1.227811000	0.375568000
C	0.989009000	-2.643434000	-0.258016000
H	1.769220000	-3.282652000	0.175543000
H	0.033090000	-3.067676000	0.074778000
C	1.069338000	-2.705917000	-1.785676000
H	0.963211000	-3.739709000	-2.129412000
H	2.028294000	-2.328854000	-2.153306000
H	0.275623000	-2.116009000	-2.253178000
C	1.019420000	-1.375408000	1.921800000
H	0.064365000	-1.867836000	2.145553000
H	1.801635000	-2.073215000	2.248010000

C	1.123612000	-0.078484000	2.728439000
H	1.032959000	-0.289338000	3.798662000
H	0.330541000	0.624843000	2.458536000
H	2.084229000	0.419800000	2.567502000
C	6.182060000	-0.589735000	-0.060961000
C	6.640761000	-1.877936000	0.178942000
S	7.505027000	0.550772000	-0.055881000
C	8.031733000	-1.949229000	0.353330000
H	5.988964000	-2.742641000	0.193683000
C	8.679588000	-0.721182000	0.252448000
H	8.573419000	-2.871009000	0.536533000
C	10.089239000	-0.558840000	0.388709000
C	10.876844000	0.558558000	0.304389000
H	10.619620000	-1.484627000	0.593991000
C	10.355728000	1.860427000	0.038361000
C	12.346662000	0.491541000	0.483928000
N	9.905236000	2.911712000	-0.180671000
O	13.093434000	1.445202000	0.418479000
O	12.792958000	-0.768653000	0.735180000
H	13.755571000	-0.686559000	0.832517000
C	-3.573927000	0.609615000	-0.606470000
C	-4.248132000	-0.620681000	-0.681183000
C	-4.364554000	1.756598000	-0.463291000
C	-5.636046000	-0.701388000	-0.634191000
H	-3.684055000	-1.535588000	-0.834405000
C	-5.751868000	1.680062000	-0.370576000
H	-3.891920000	2.729746000	-0.375912000
C	-6.430963000	0.450648000	-0.447318000
S	-6.398934000	-2.269795000	-0.982656000
H	-6.301941000	2.599756000	-0.226376000
N	-7.837048000	0.368035000	-0.367043000

C	-7.898338000	-2.072691000	-0.046774000
C	-8.489681000	-0.799327000	0.097166000
C	-8.621904000	1.598102000	-0.522262000
C	-8.529803000	-3.217209000	0.439409000
C	-9.758259000	-0.743823000	0.701347000
C	-8.813825000	2.471528000	0.733713000
H	-9.600501000	1.309320000	-0.919108000
H	-8.140836000	2.190352000	-1.307454000
H	-8.032106000	-4.175920000	0.327650000
C	-9.791240000	-3.141853000	1.029603000
C	-10.403941000	-1.898478000	1.145588000
H	-10.259085000	0.205475000	0.830886000
C	-9.626848000	3.734949000	0.423106000
H	-9.313264000	1.896533000	1.520873000
H	-7.840512000	2.752572000	1.150464000
H	-10.281690000	-4.041257000	1.387246000
H	-11.387276000	-1.810237000	1.597458000
C	-9.848920000	4.623152000	1.650926000
H	-9.116431000	4.312978000	-0.359463000
H	-10.598823000	3.447379000	-0.000933000
H	-10.433002000	5.513463000	1.397793000
H	-10.387880000	4.083757000	2.437702000
H	-8.896297000	4.959483000	2.074889000

Table S7. Cartesian coordinates for the optimized geometry of **7b**.

Energy = - 3192.2805507 Ha

Atom	X	Y	Z
C	3.899826000	-0.892474000	-0.640469000
C	3.373602000	-2.065803000	-1.216642000
H	4.056323000	-2.811483000	-1.611771000
C	2.000511000	-2.273208000	-1.323954000
H	1.623500000	-3.183791000	-1.781255000
C	1.125936000	-1.291528000	-0.852449000
C	1.633497000	-0.111275000	-0.272146000
C	3.002572000	0.086382000	-0.165767000
H	3.394260000	0.982742000	0.306971000
C	-0.336229000	-1.228535000	-0.832340000
C	-1.305497000	-2.130382000	-1.277640000
H	-1.021923000	-3.070919000	-1.741036000
C	-2.651655000	-1.806539000	-1.134833000
H	-3.404873000	-2.493936000	-1.508379000
C	-3.056476000	-0.592058000	-0.544138000
C	-2.064632000	0.305614000	-0.088364000
H	-2.362747000	1.229369000	0.398867000
C	-0.724305000	-0.008924000	-0.237291000
C	0.498660000	0.806369000	0.183181000
C	0.546117000	2.190015000	-0.528002000
H	-0.302313000	2.784022000	-0.163967000
H	1.448122000	2.712833000	-0.185077000
C	0.526481000	2.158452000	-2.058759000
H	0.559605000	3.176288000	-2.460085000
H	-0.380804000	1.679545000	-2.438928000
H	1.386376000	1.613815000	-2.459645000
C	0.531097000	1.048670000	1.721163000
H	1.434717000	1.628266000	1.949326000
H	-0.316415000	1.697662000	1.977103000

C	0.496020000	-0.206110000	2.597691000
H	0.526335000	0.069718000	3.656492000
H	1.351647000	-0.857377000	2.397238000
H	-0.415775000	-0.787026000	2.430438000
C	-4.471112000	-0.246766000	-0.403724000
C	-5.043788000	1.007333000	-0.305676000
S	-5.712995000	-1.481439000	-0.325878000
C	-6.450368000	0.988043000	-0.183386000
H	-4.464400000	1.921215000	-0.356564000
C	-6.991329000	-0.284956000	-0.184193000
H	-7.055874000	1.885111000	-0.115173000
C	-8.372757000	-0.678426000	-0.085851000
C	-8.914297000	-1.956087000	-0.181206000
S	-9.623513000	0.513050000	0.191120000
C	-10.308419000	-1.975708000	-0.038708000
H	-8.313205000	-2.840561000	-0.356047000
C	-10.878745000	-0.722024000	0.168606000
H	-10.908926000	-2.877596000	-0.086843000
C	-12.276251000	-0.507137000	0.335144000
C	-12.989514000	0.645356000	0.539896000
H	-12.868748000	-1.416732000	0.290581000
C	-12.379018000	1.932256000	0.625339000
C	-14.463614000	0.633617000	0.687844000
N	-11.853410000	2.969551000	0.690660000
O	-15.146658000	1.619652000	0.869515000
O	-14.995117000	-0.615657000	0.599178000
H	-15.952454000	-0.496717000	0.709552000
C	5.363694000	-0.690783000	-0.537834000
C	5.936858000	0.580976000	-0.703534000
C	6.240202000	-1.750682000	-0.275176000
C	7.311701000	0.781923000	-0.632679000

H	5.303837000	1.428390000	-0.948462000
C	7.613166000	-1.549634000	-0.157208000
H	5.846158000	-2.749205000	-0.114400000
C	8.191909000	-0.279204000	-0.327906000
S	7.952972000	2.373123000	-1.100919000
H	8.232428000	-2.403355000	0.080837000
N	9.584339000	-0.074012000	-0.225938000
C	9.440535000	2.382367000	-0.125911000
C	10.129210000	1.179802000	0.141652000
C	10.467704000	-1.245252000	-0.241135000
C	9.965551000	3.613586000	0.265913000
C	11.383921000	1.283288000	0.768439000
C	10.685998000	-1.971758000	1.101210000
H	11.432759000	-0.917390000	-0.640623000
H	10.061225000	-1.948380000	-0.975302000
H	9.394593000	4.514155000	0.060217000
C	11.214673000	3.695436000	0.881017000
C	11.923256000	2.522190000	1.117505000
H	11.958106000	0.394403000	0.990443000
C	11.631053000	-3.170973000	0.950674000
H	11.089660000	-1.275853000	1.844626000
H	9.726370000	-2.309129000	1.508053000
H	11.621974000	4.660346000	1.164580000
H	12.899939000	2.555812000	1.590708000
C	11.871499000	-3.914676000	2.267693000
H	11.220202000	-3.867512000	0.206820000
H	12.592295000	-2.828514000	0.543221000
H	12.548160000	-4.763404000	2.127436000
H	12.316902000	-3.254531000	3.020122000
H	10.933791000	-4.301387000	2.681883000

AB-1-344

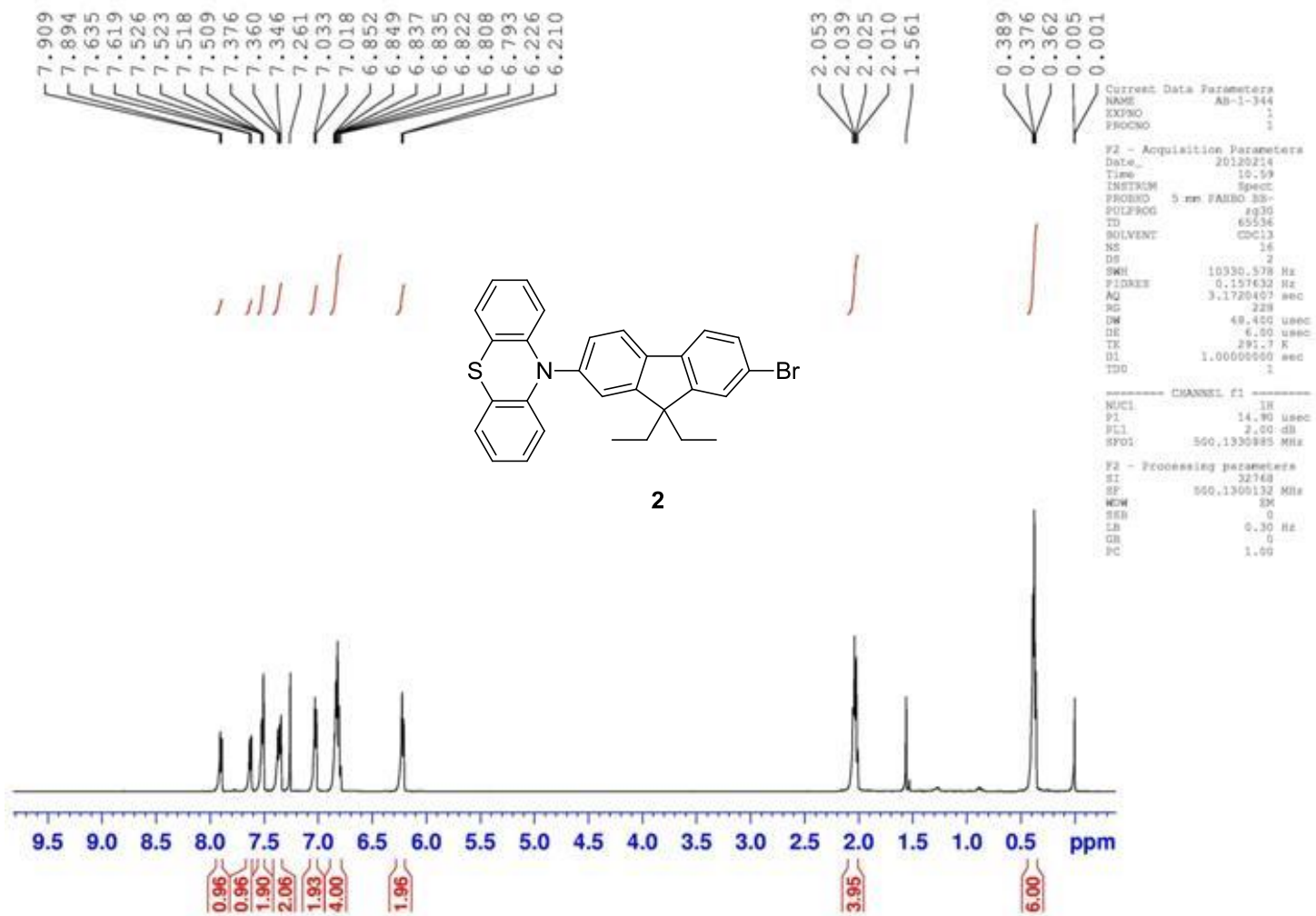


Figure S12. ¹H NMR spectra of 2 in CDCl₃.

344 13C

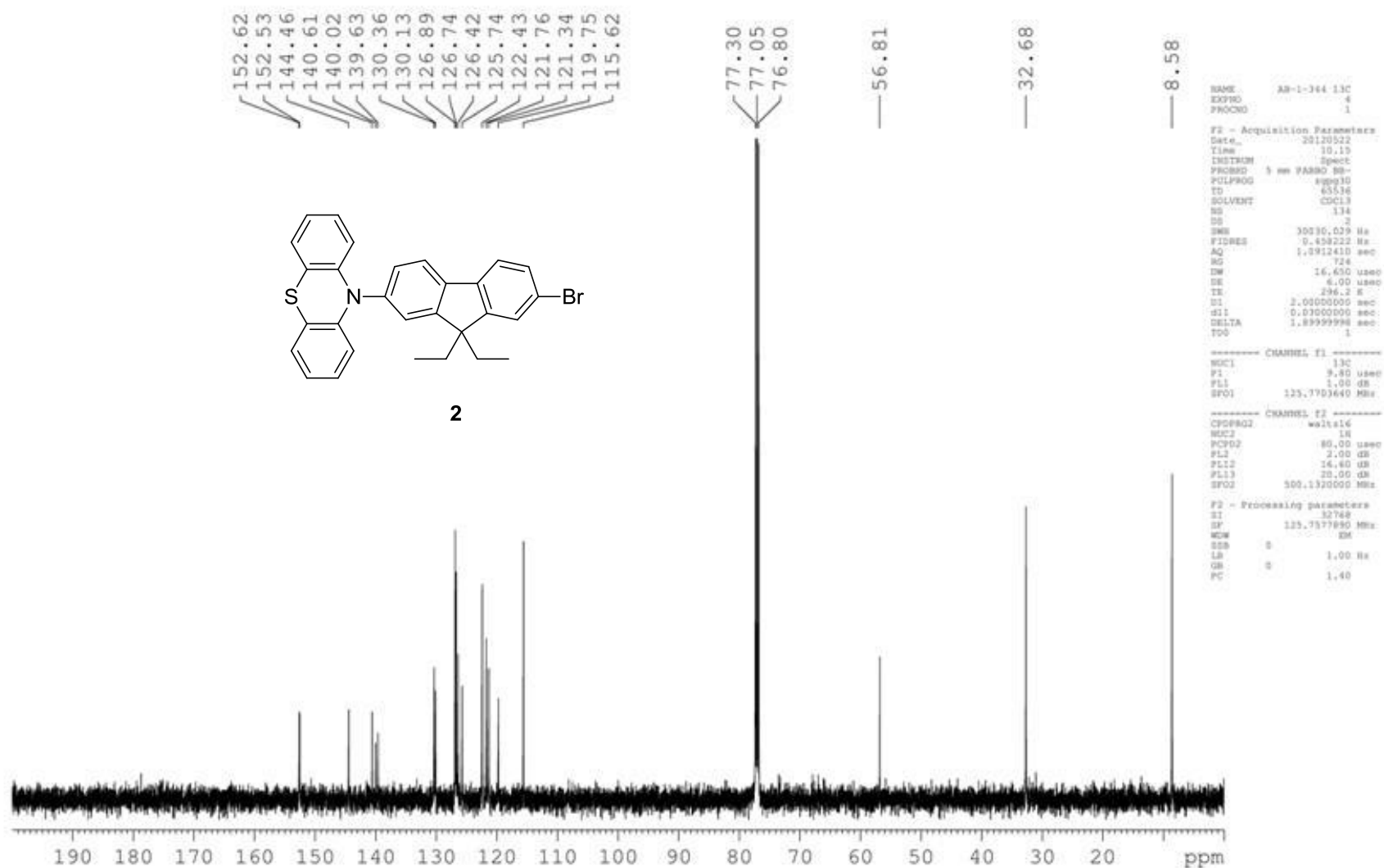
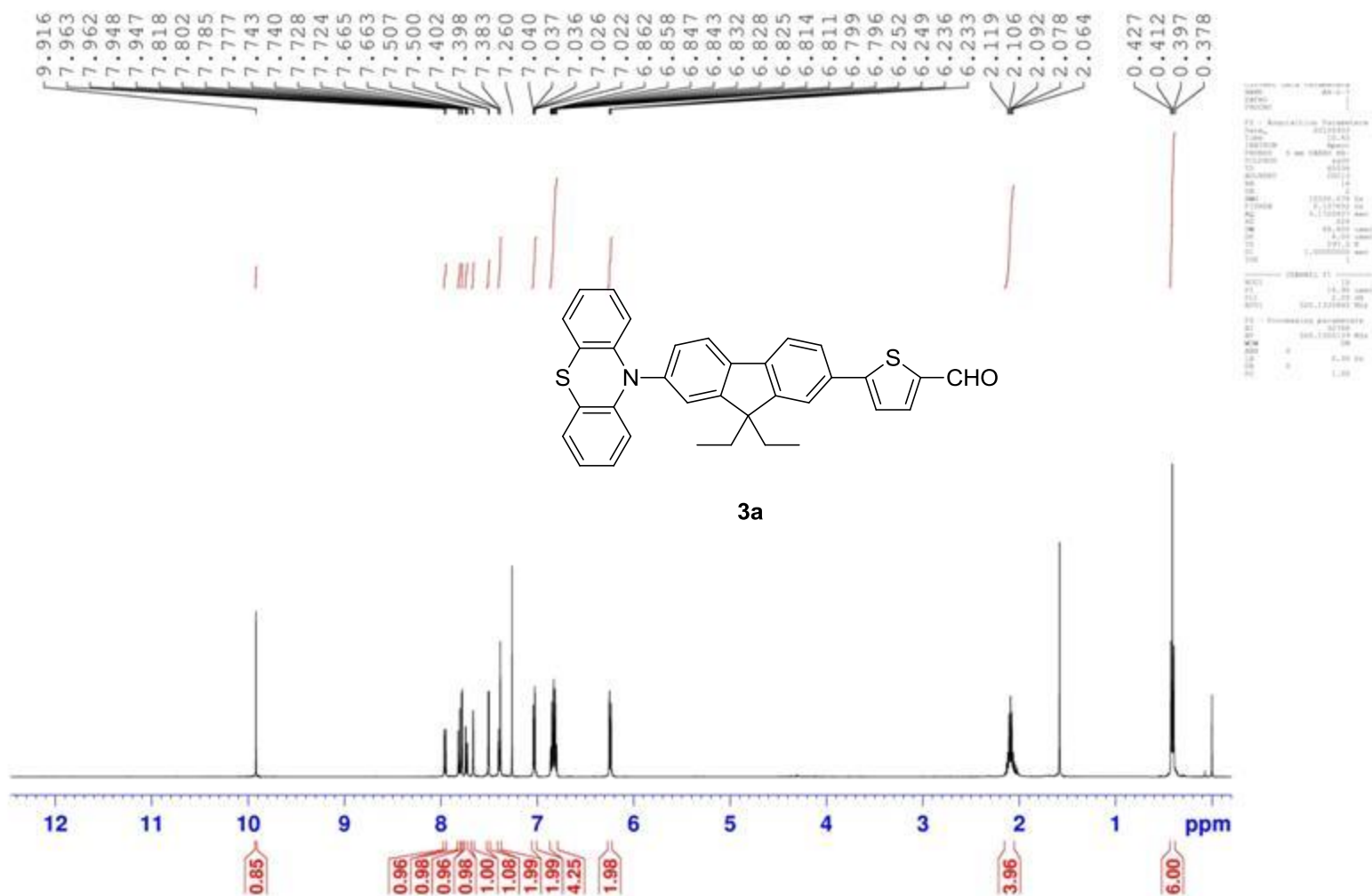


Figure S13. ¹³C NMR spectra of **2** in CDCl₃.

2-7

Figure S14. ¹H NMR spectra of **3a** in CDCl₃.

2-7 13C

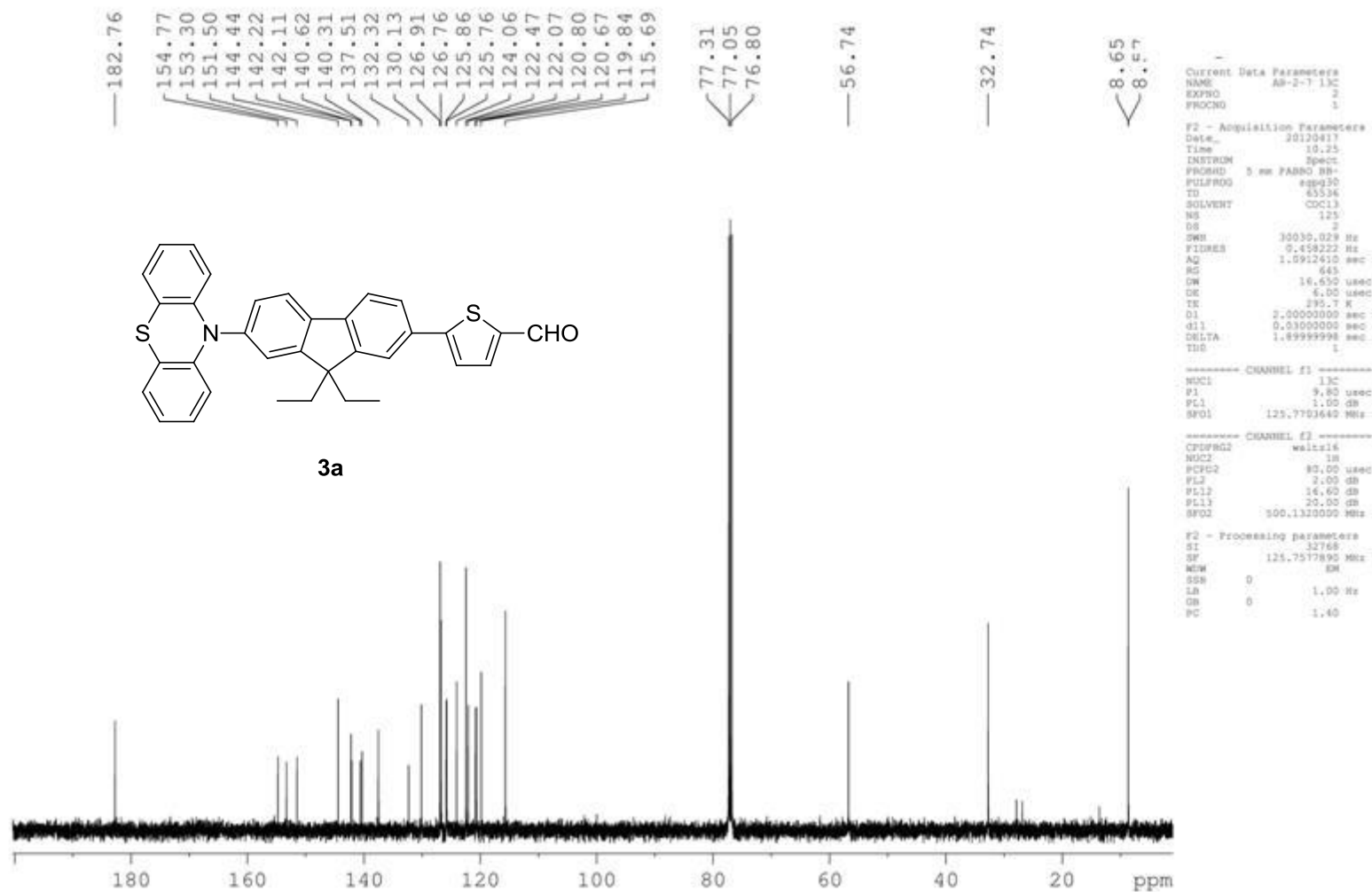


Figure S15. ¹³C NMR spectra of **3a** in CDCl₃.

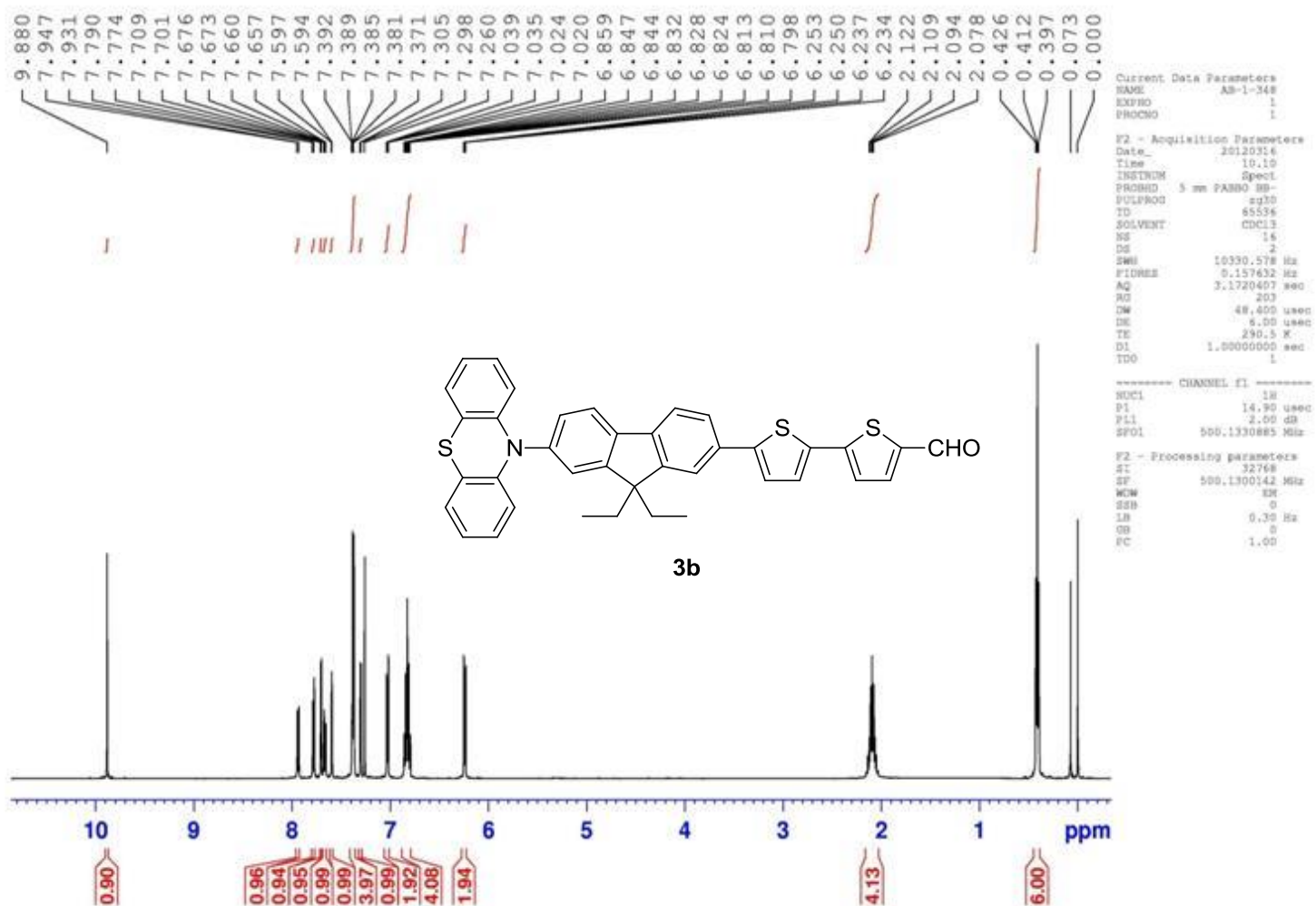
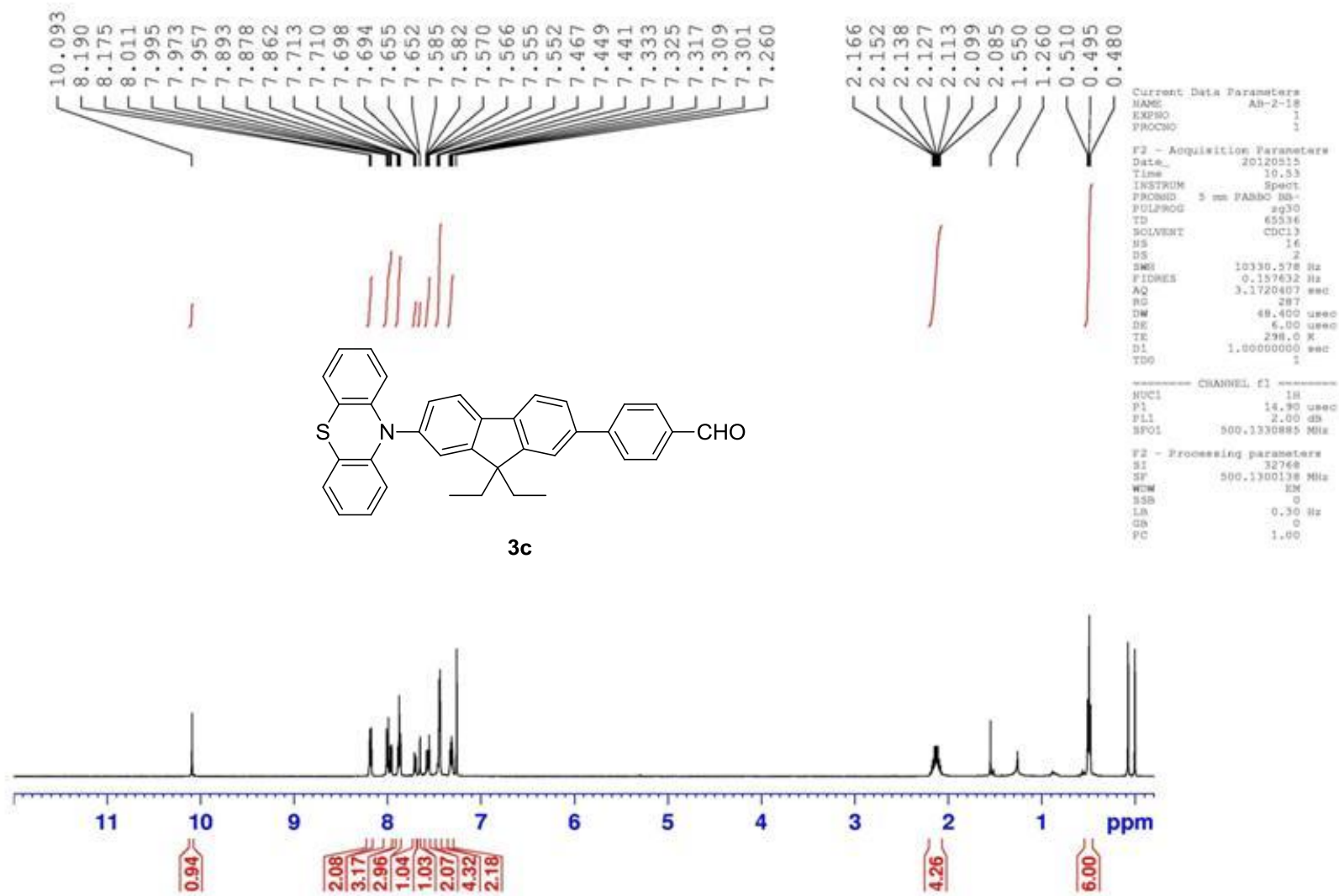


Figure S16. ¹H NMR spectra of **4b** in CDCl₃.

2-18

Figure S18. ¹H NMR spectra of **3c** in CDCl₃.

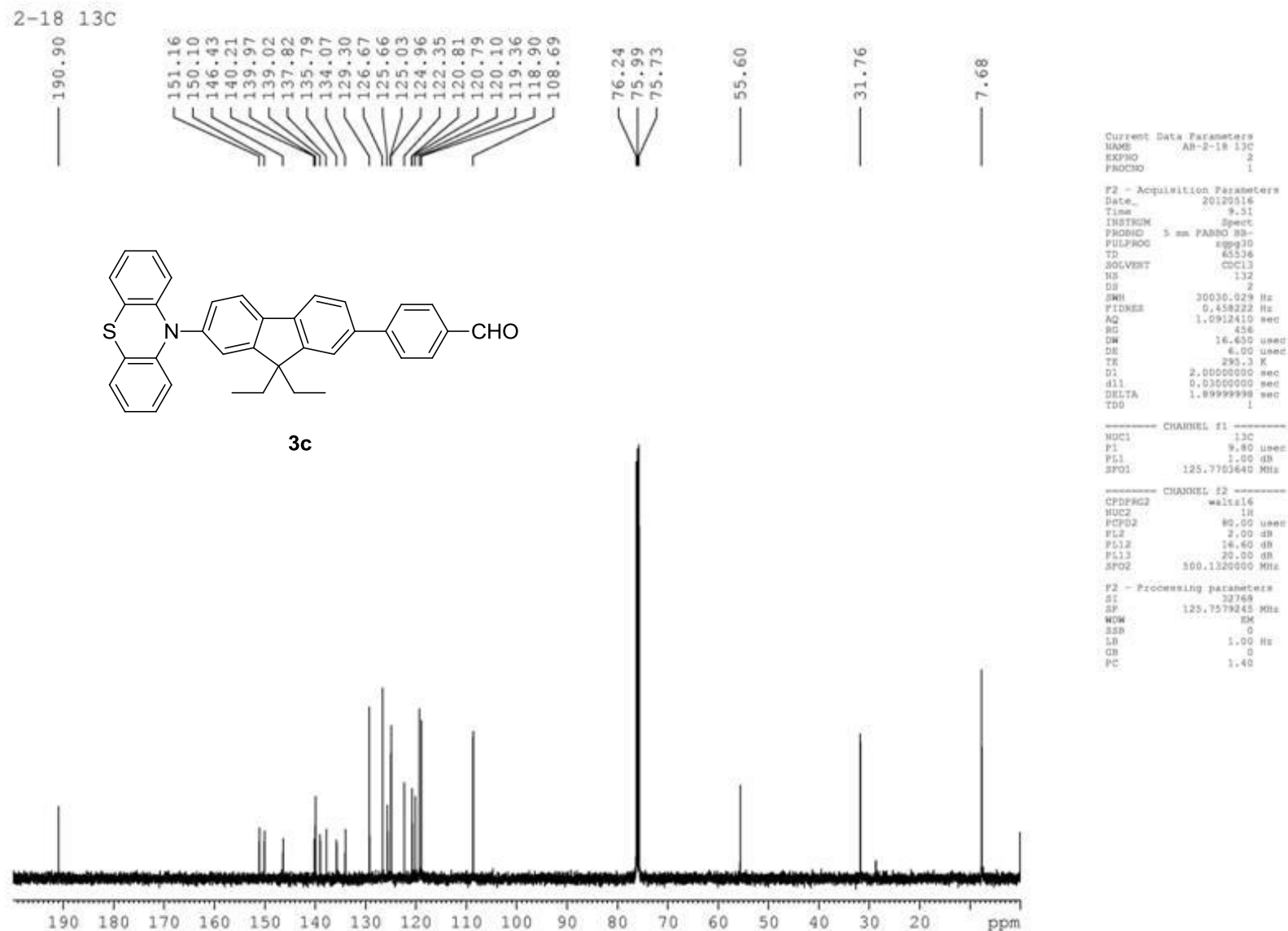


Figure S19. ^{13}C NMR spectra of **3c** in CDCl_3 .

AB-13

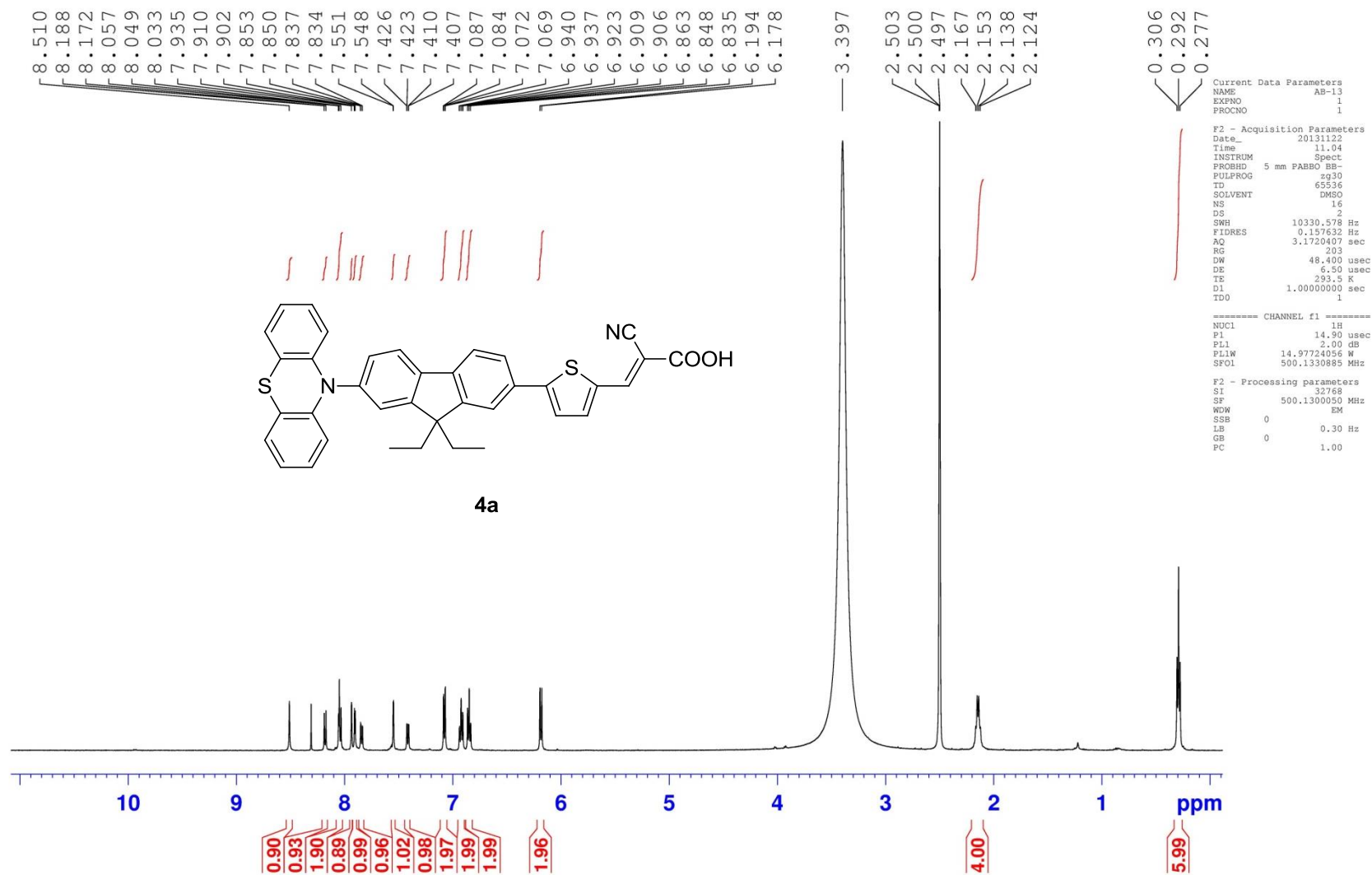


Figure S20. ^1H NMR spectra of **4a** in $\text{DMSO}-d_6$.

2-13 13C

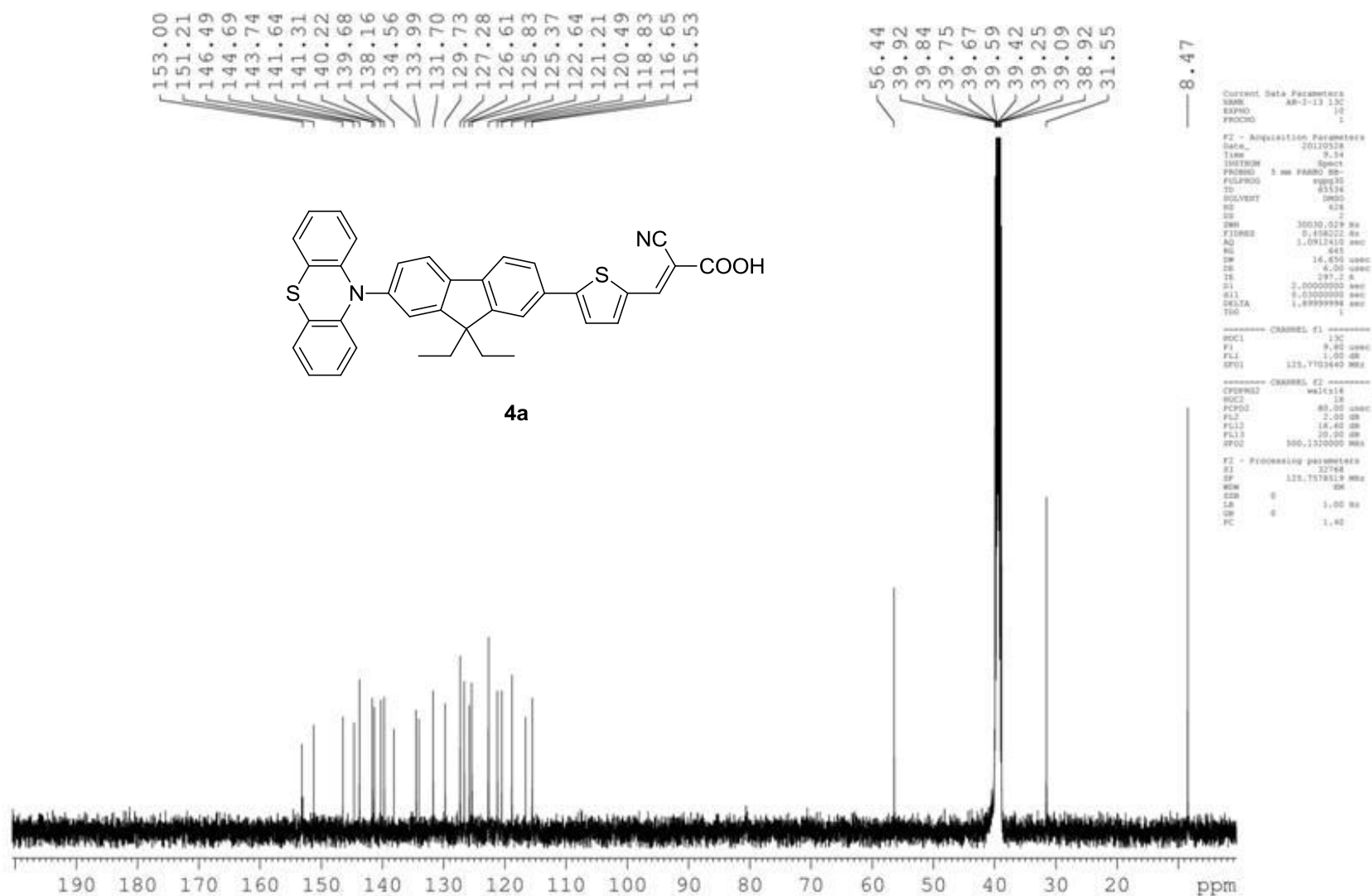


Figure S21. ^{13}C NMR spectra of **4a** in $\text{DMSO}-d_6$.

2-4

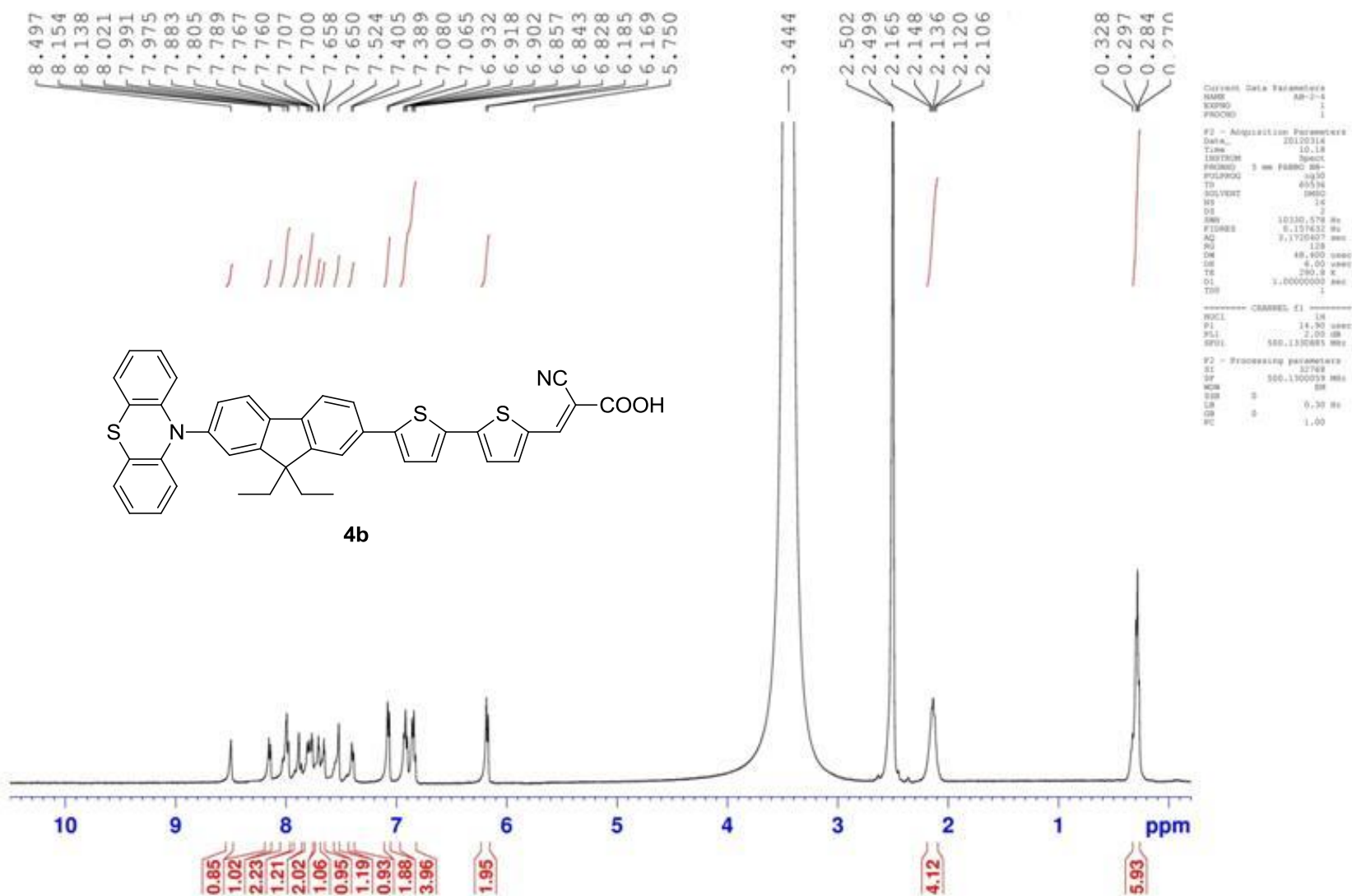


Figure S22. ¹H NMR spectra of **4b** in DMSO-*d*₆.

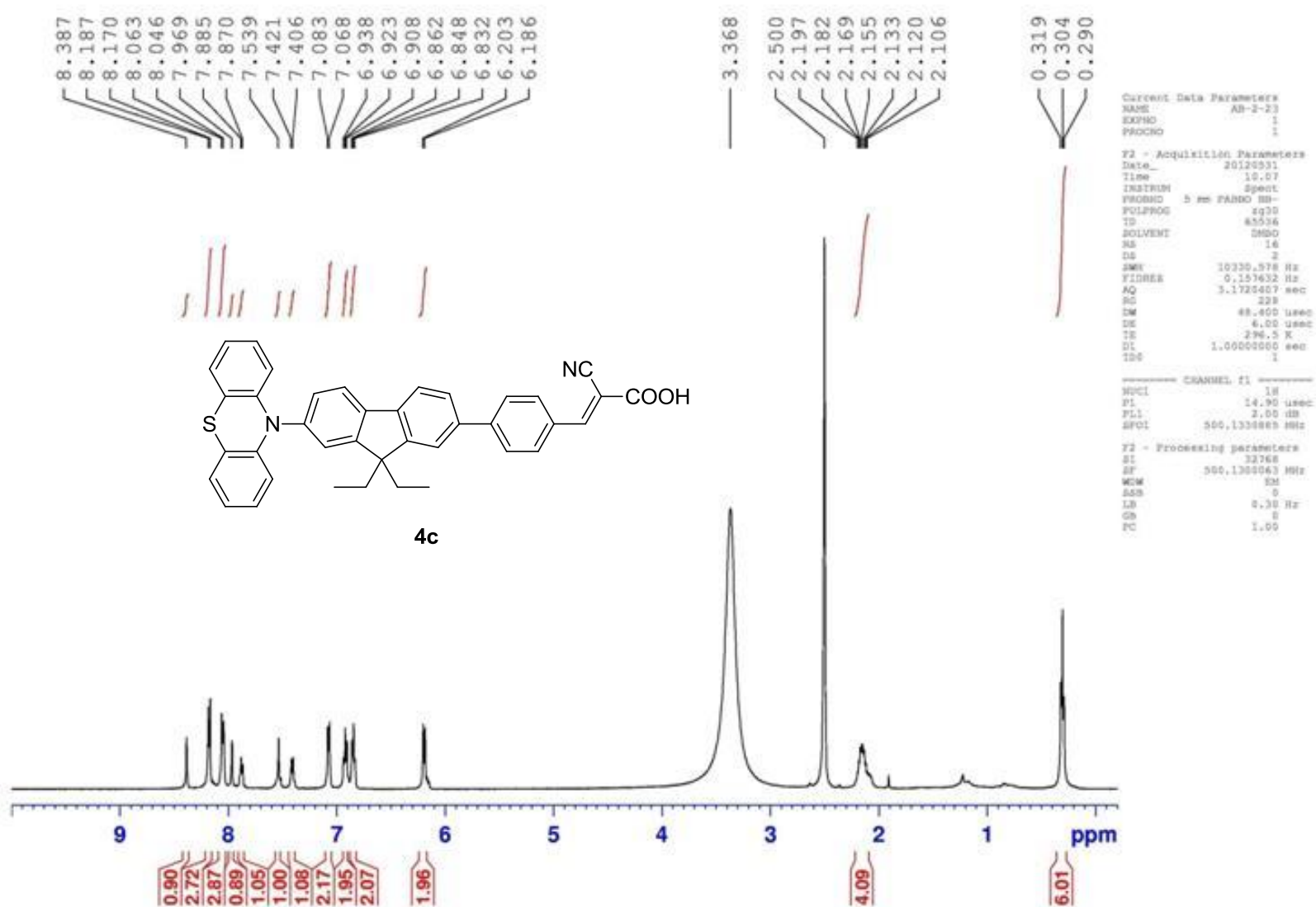
Chemical structure of compound **4b** is shown above the spectrum. The structure is a complex molecule with a central fluorene core, a thiophene ring, and a carboxylic acid group.

13C NMR Spectrum (DMSO-d₆):

- Chemical Shifts (ppm): 152.85, 145.52, 143.78, 141.64, 140.51, 139.29, 138.14, 135.78, 133.98, 132.23, 129.69, 128.40, 127.27, 126.59, 125.70, 125.35, 124.91, 122.58, 122.37, 121.01, 119.93, 118.73, 116.71, 115.46, 56.37, 39.97, 39.80, 39.64, 39.47, 39.30, 39.14, 38.97, 31.57, 8.48.

S41

2-23

Figure S24. ¹H NMR spectra of 4c in DMSO-*d*₆.

2-23 13C

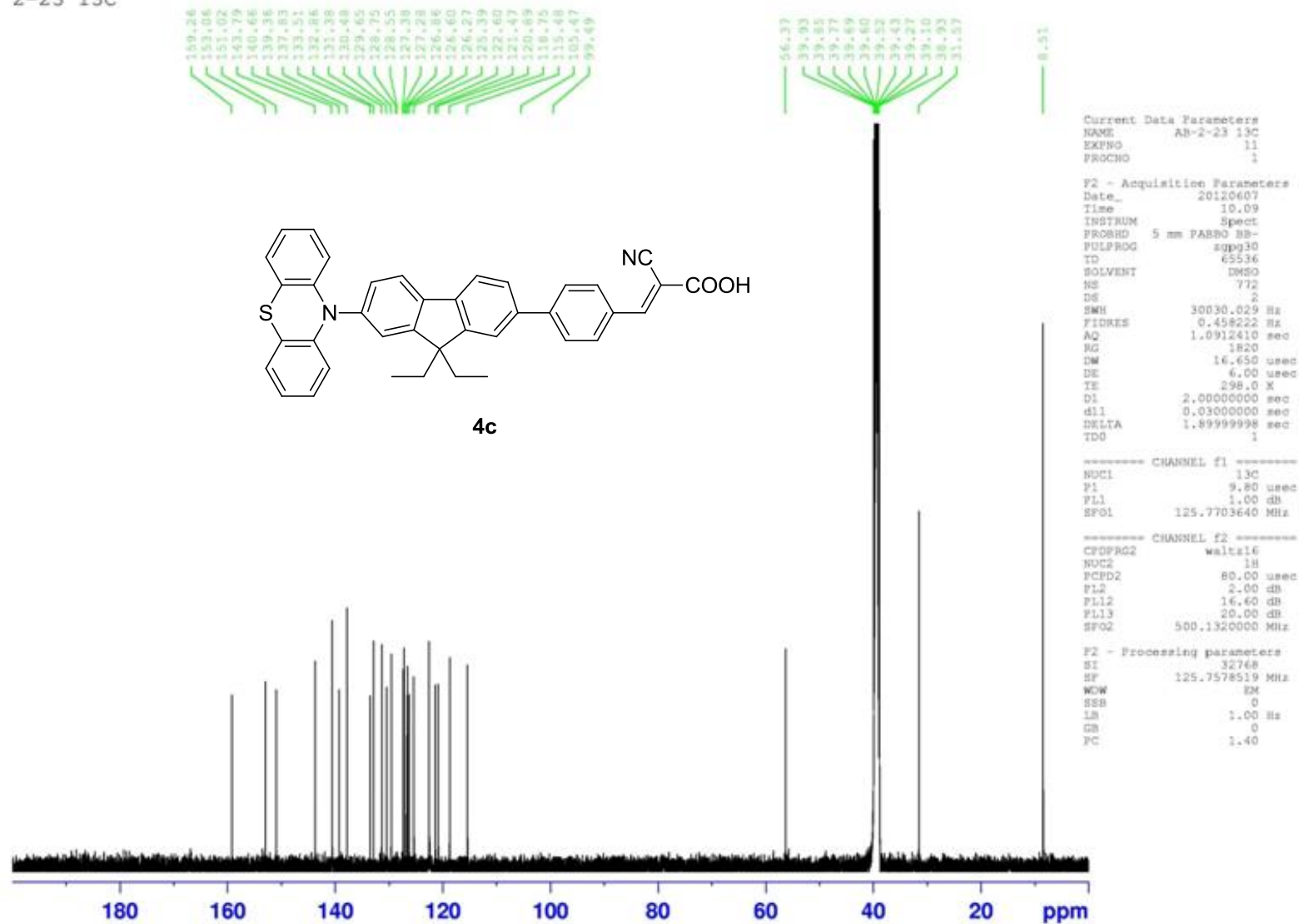


Figure S25. ^{13}C NMR spectra of **4c** in $\text{DMSO}-d_6$.

AB-2-117

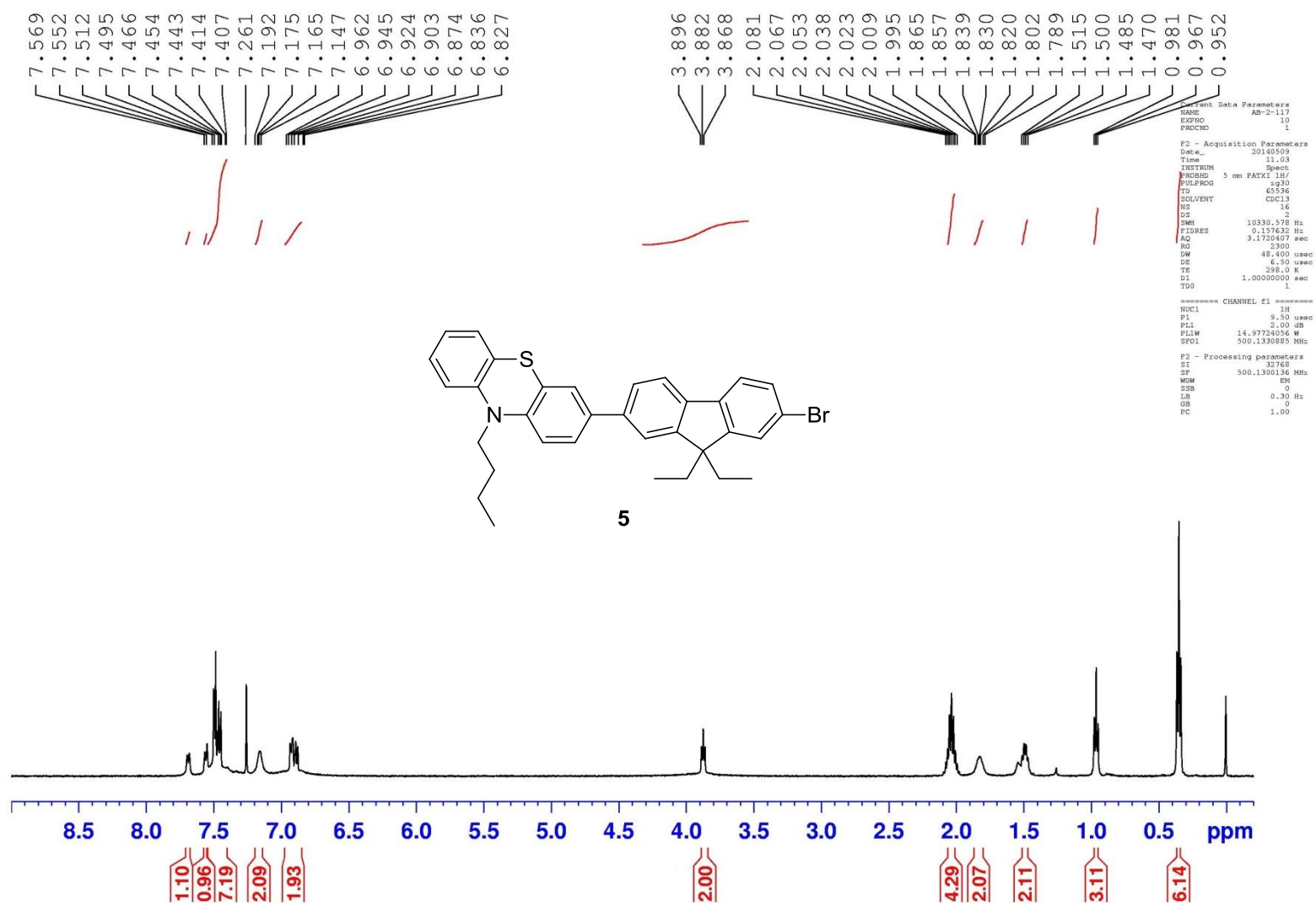


Figure S26. ^1H NMR spectra of 5 in CDCl_3 .

AD-117-13C

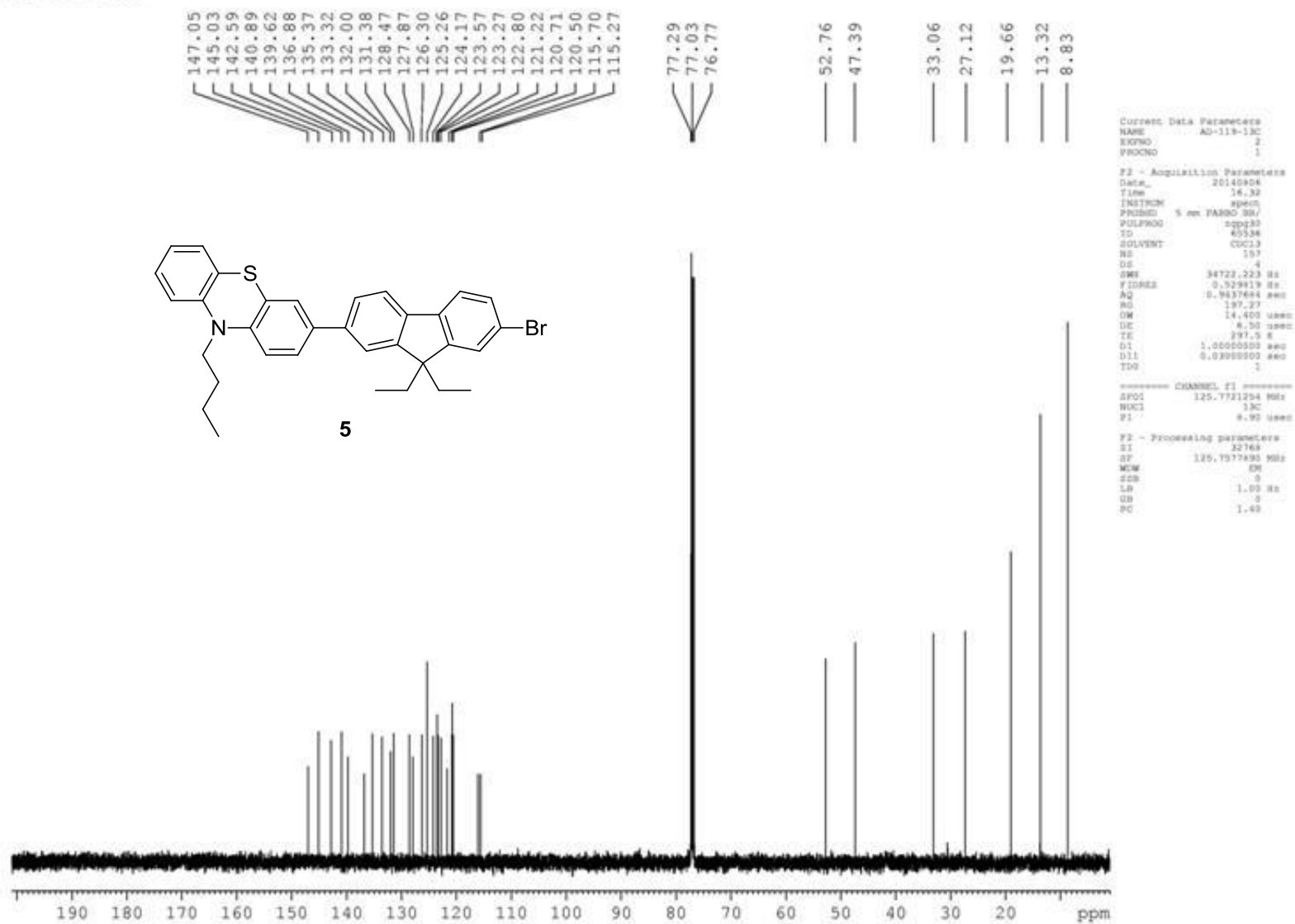


Figure S27. ¹³C NMR spectra of 5 in CDCl₃.

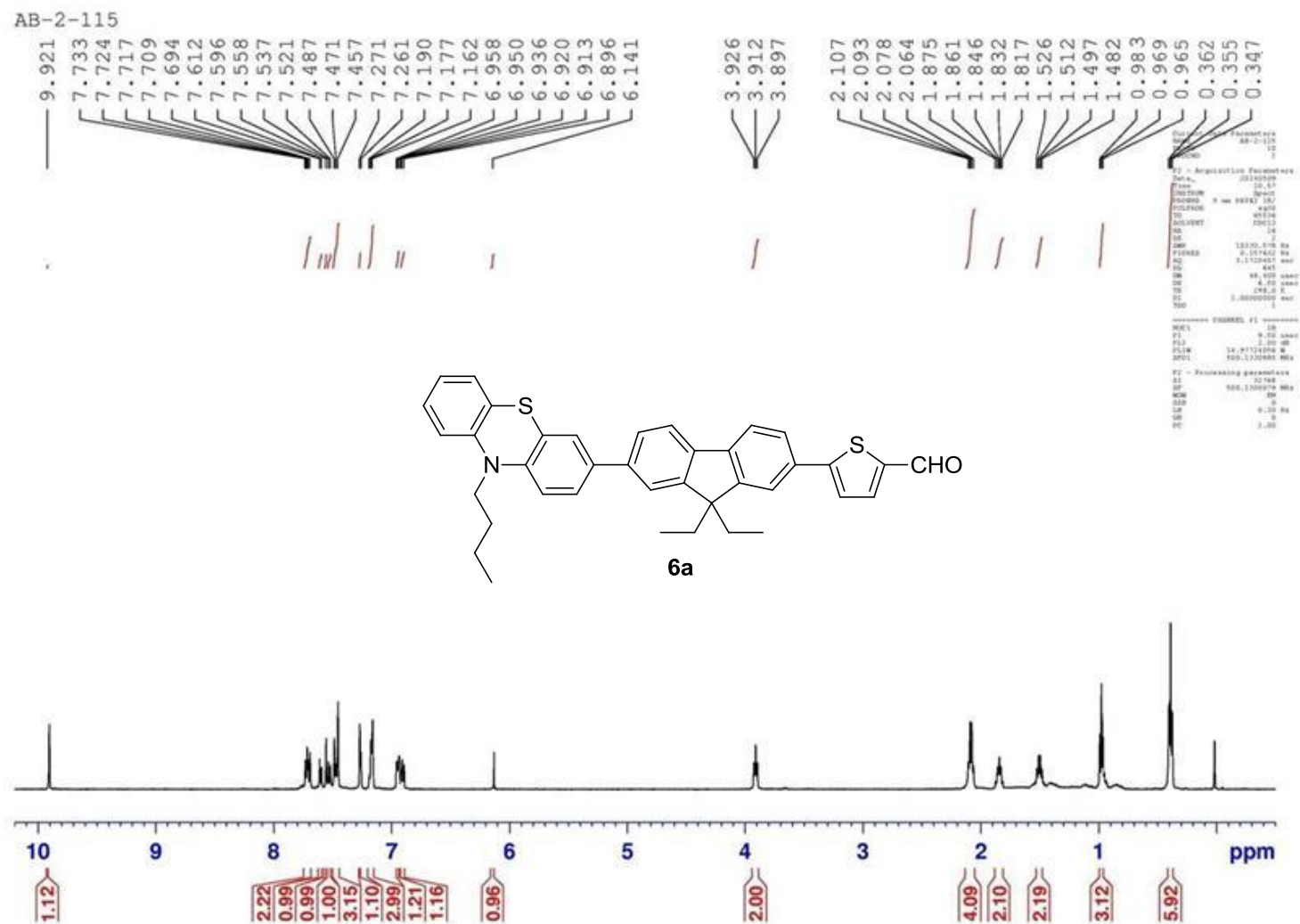


Figure S28. ^1H NMR spectra of **6a** in CDCl_3 .

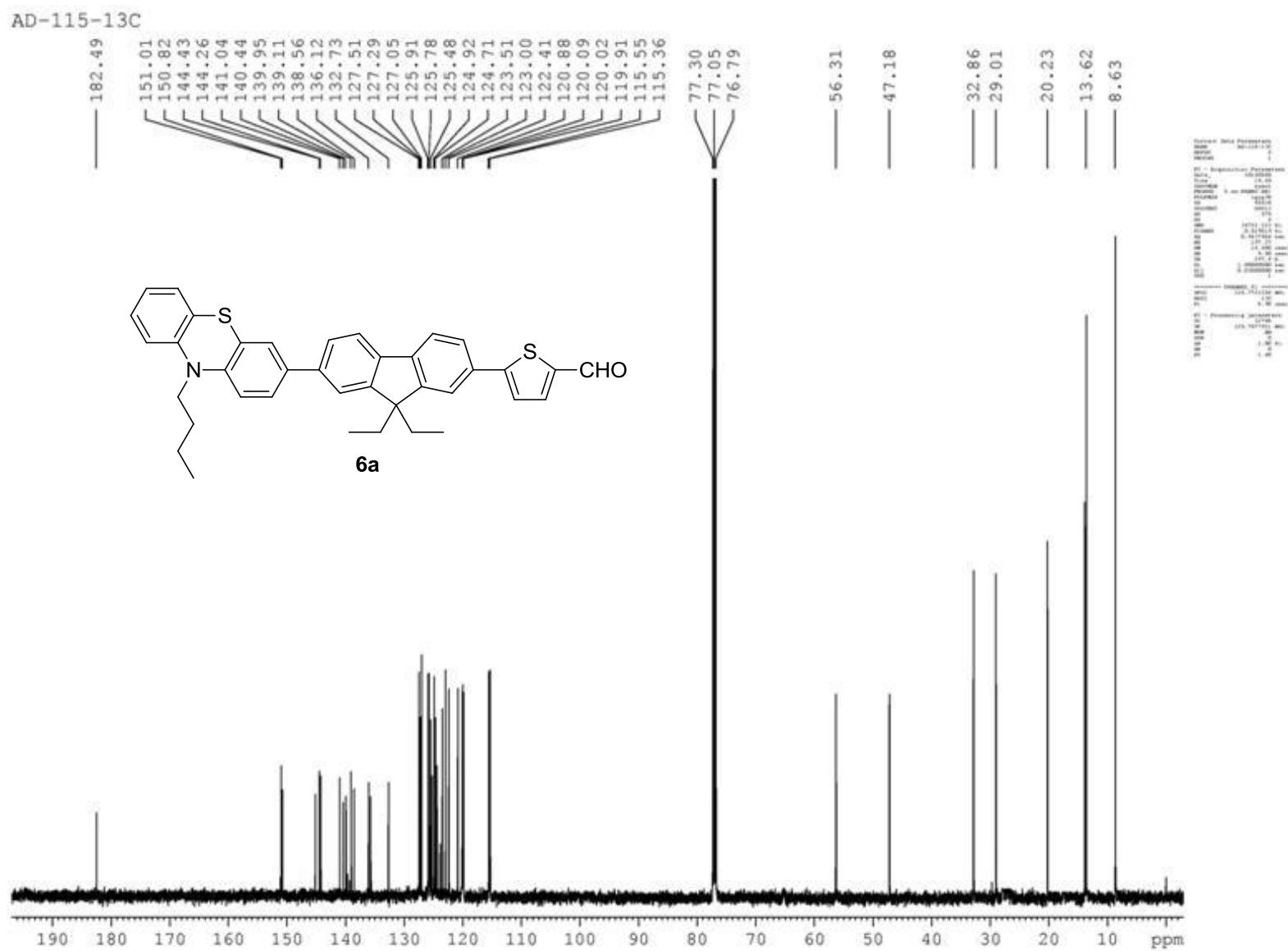


Figure S29. ^{13}C NMR spectra of **6a** in CDCl_3 .

AD-118-13C

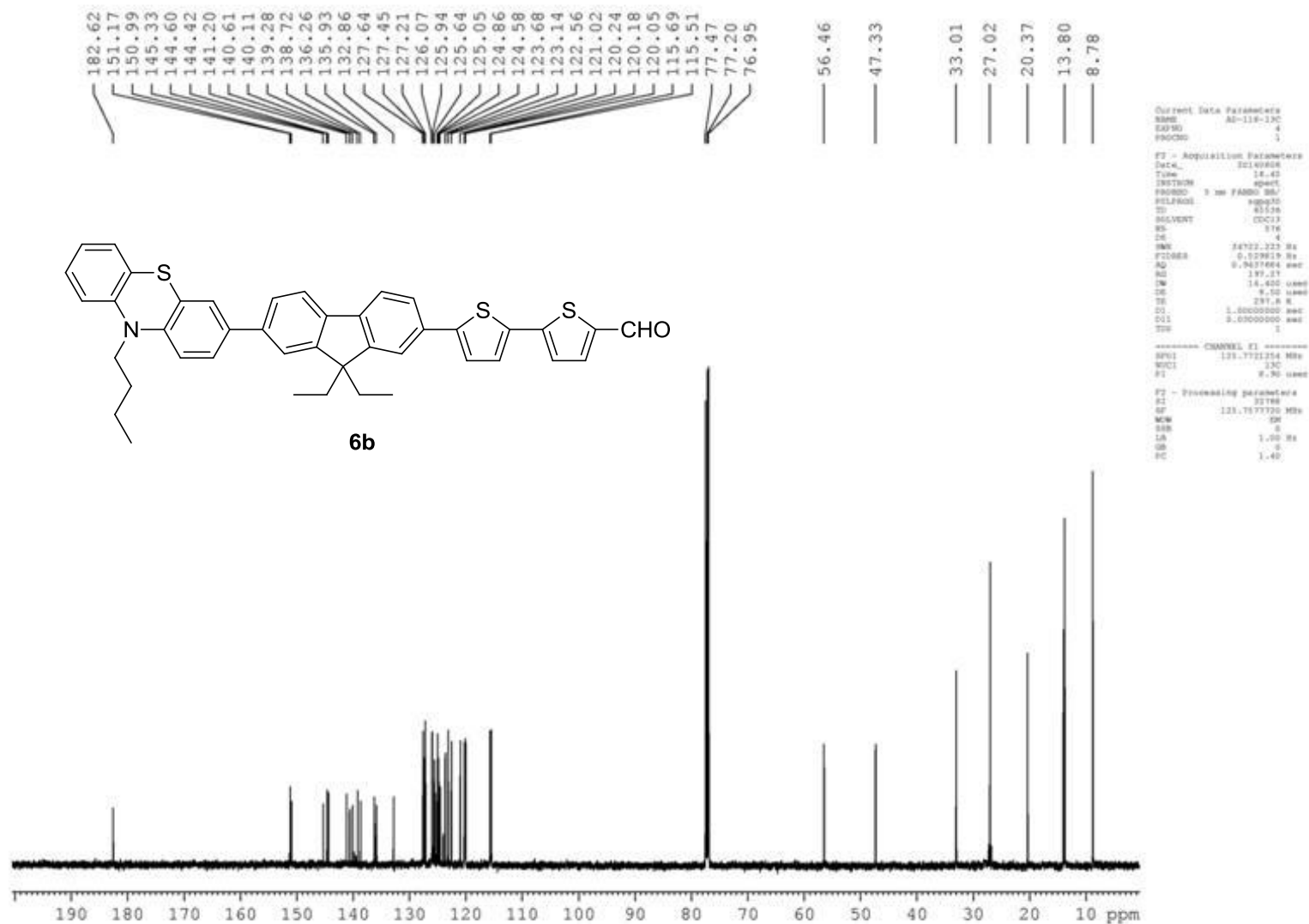


Figure S31. ^{13}C NMR spectra of **6b** in CDCl_3 .

AD-119-1H

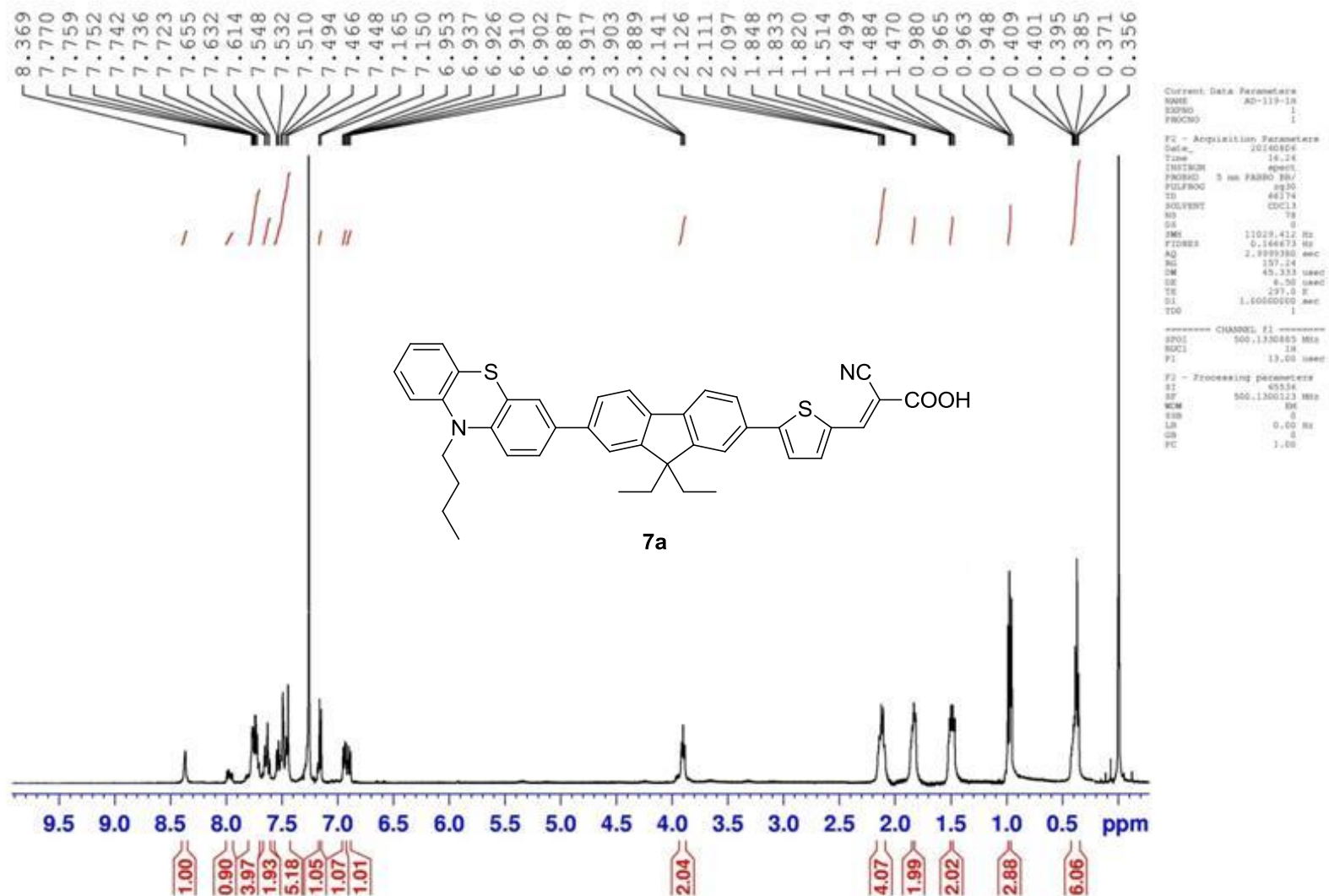


Figure S32. ^1H NMR spectra of **7a** in CDCl_3 .

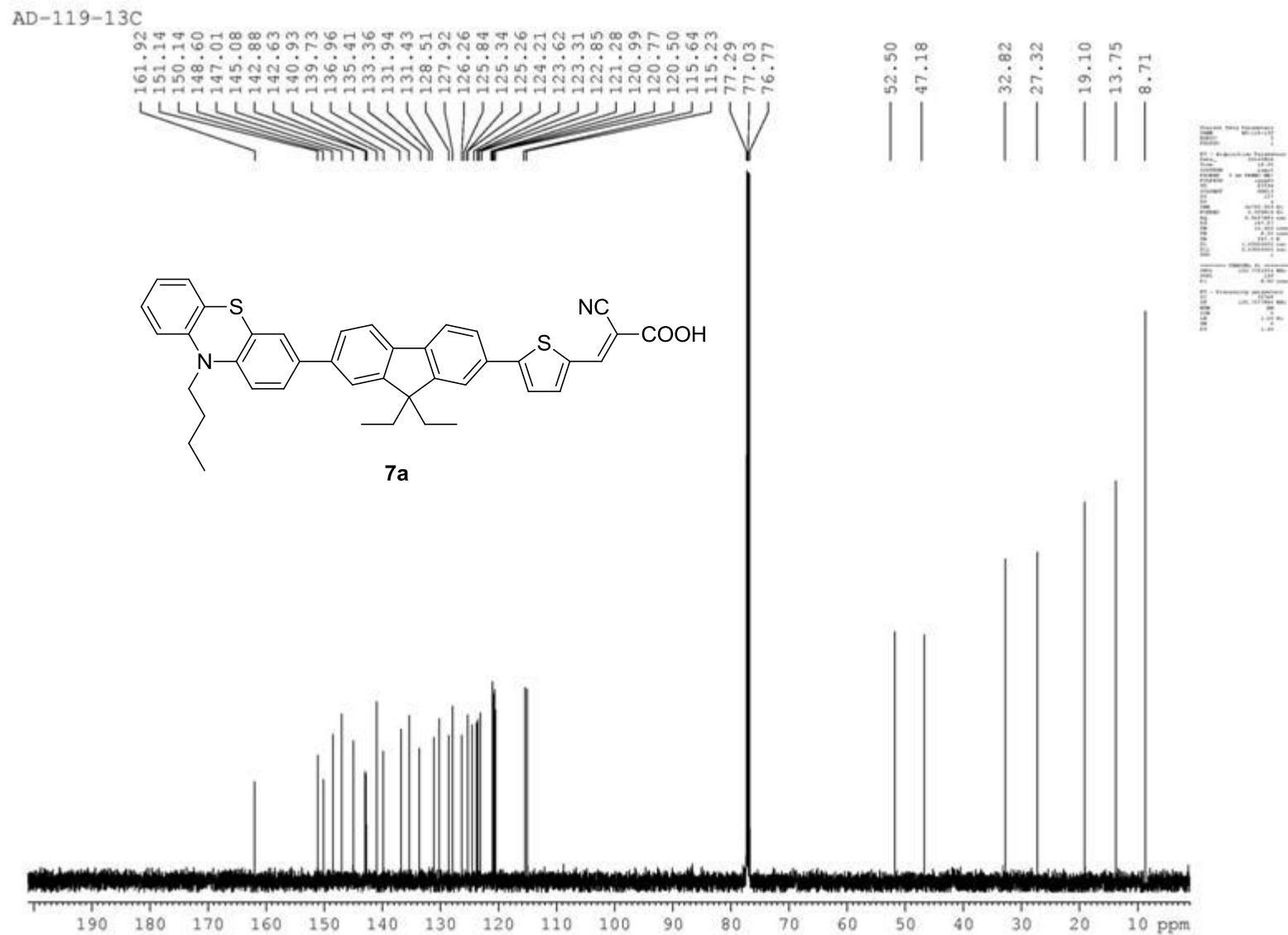


Figure S33. ^{13}C NMR spectra of **7a** in CDCl_3 .

AD-120-1H

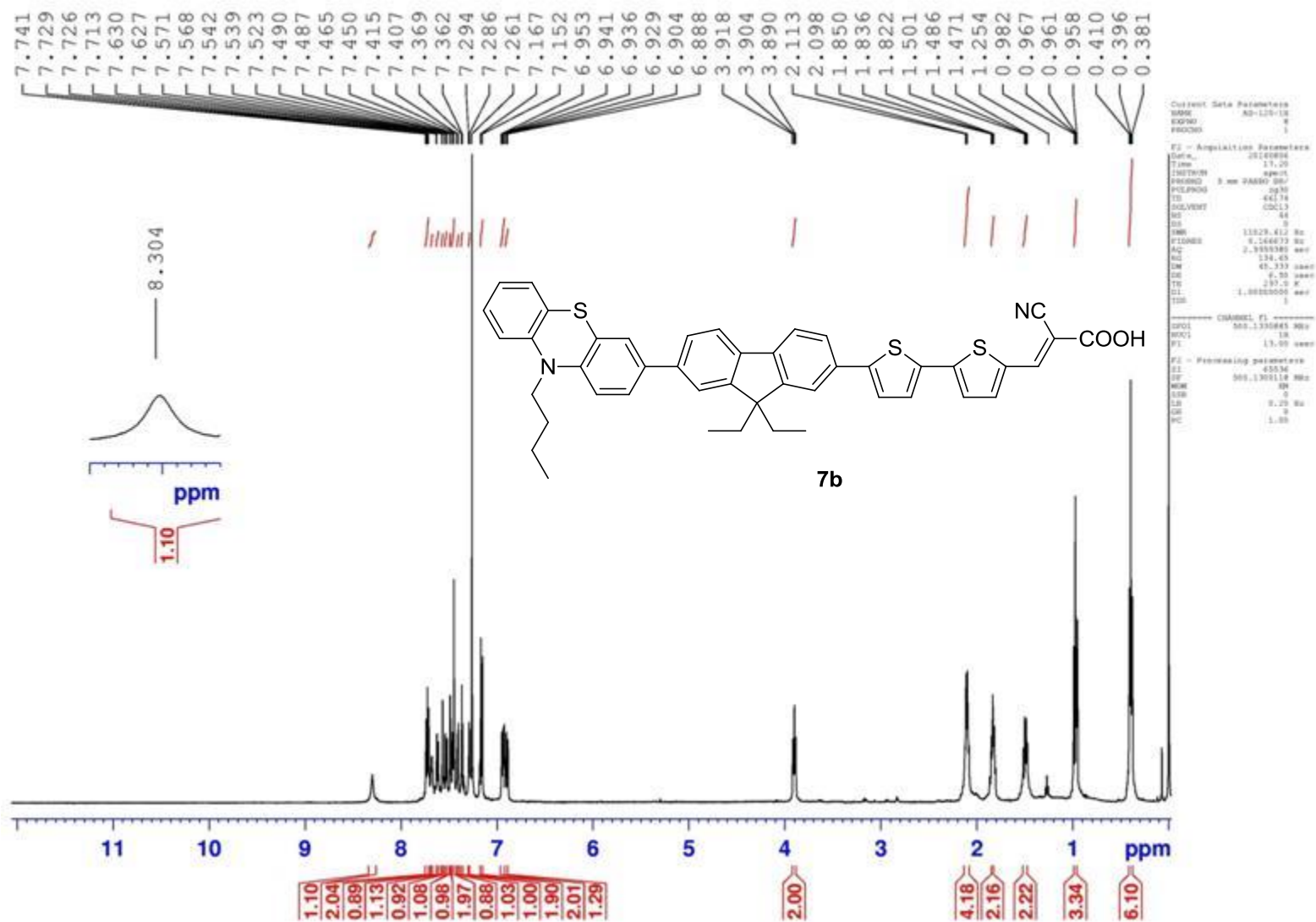


Figure S34. ^1H NMR spectra of **7b** in CDCl_3 .

Chemical structure of **7b** is shown above the spectrum.

7b

Chemical shifts (ppm): 159.89, 151.23, 150.93, 145.16, 144.51, 143.28, 141.81, 139.74, 139.39, 138.30, 135.69, 134.44, 134.11, 132.09, 127.48, 127.29, 125.80, 125.55, 125.34, 124.94, 124.43, 124.11, 122.43, 122.89, 120.13, 115.52, 115.38, 77.23, 76.98, 76.73, 56.43, 47.30, 32.88, 29.74, 20.20, 13.80, 8.63.

Current Data Parameters
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EXPNO: 1
PROCNO: 1

F2 - Acquisition Parameters
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Time : 9.18
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PROBHD : 5 mm QNP5B 90°
PULPROG : zgpg30
TD : 65536
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NS : 1800
DS : 4
SWH : 22961.304 Hz
FIDRES : 0.4946291 Hz
AQ : 1.1007068 sec
RG : 197.27
CH : 16.800 usec
SE : 6.50 usec
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D11 : 0.00000000 sec
TD0 : 1

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NUC1 : 125.7604637 MHz
P1 : 8.00 usec
PC : 0.00

F2 - Processing parameters
SI : 32768
SF : 125.7577711 MHz
WDW : EM
SSB : 0
LB : 1.00 Hz
GB : 0
PC : 1.00

S53