

Supporting Information

for

“Click-chemistry” approach for the synthesis of porphyrin dyads as sensitizers for dye- sensitized solar cells

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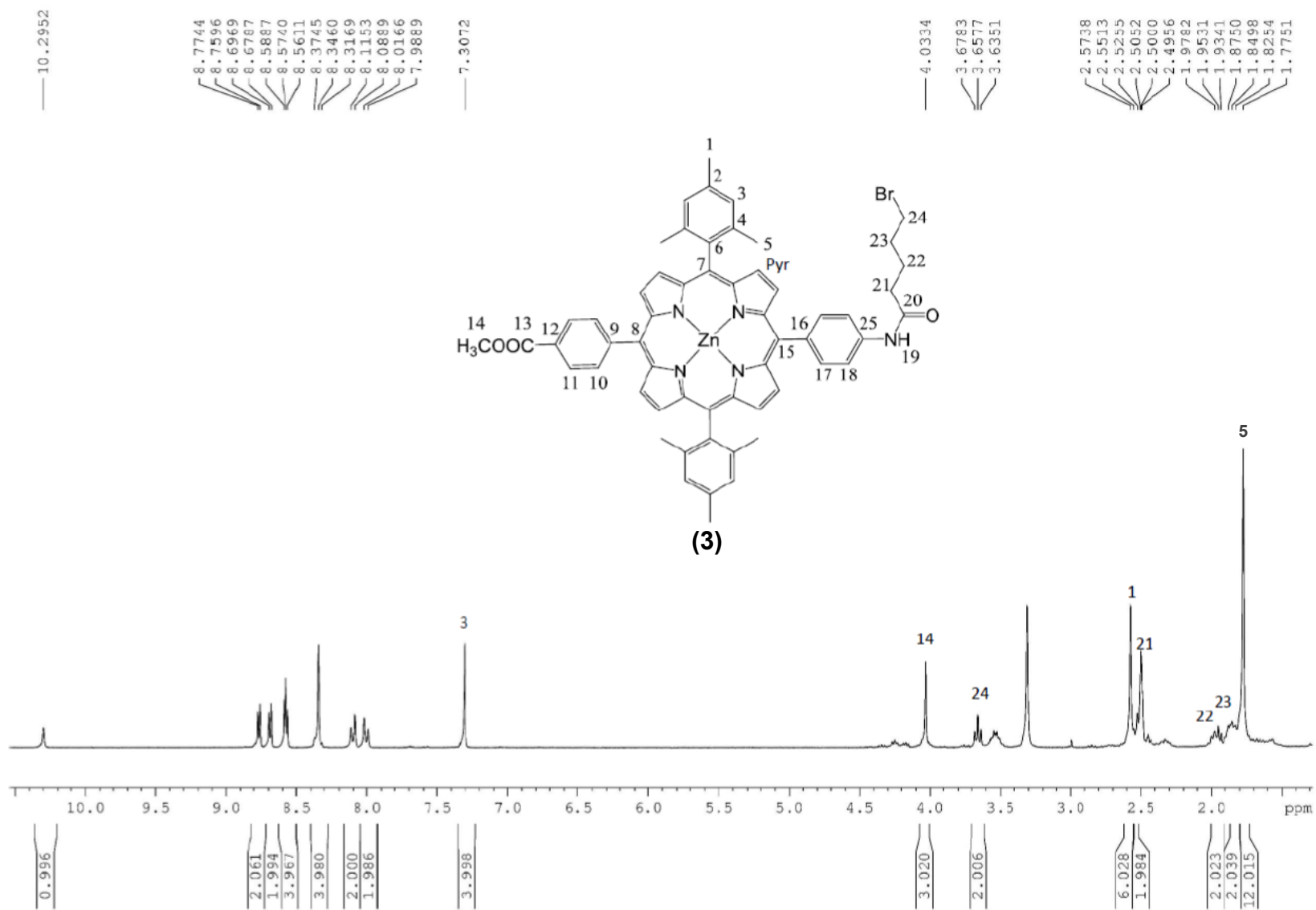


Figure S1: ¹H NMR spectrum of **3** (300MHz, DMSO-d₆).

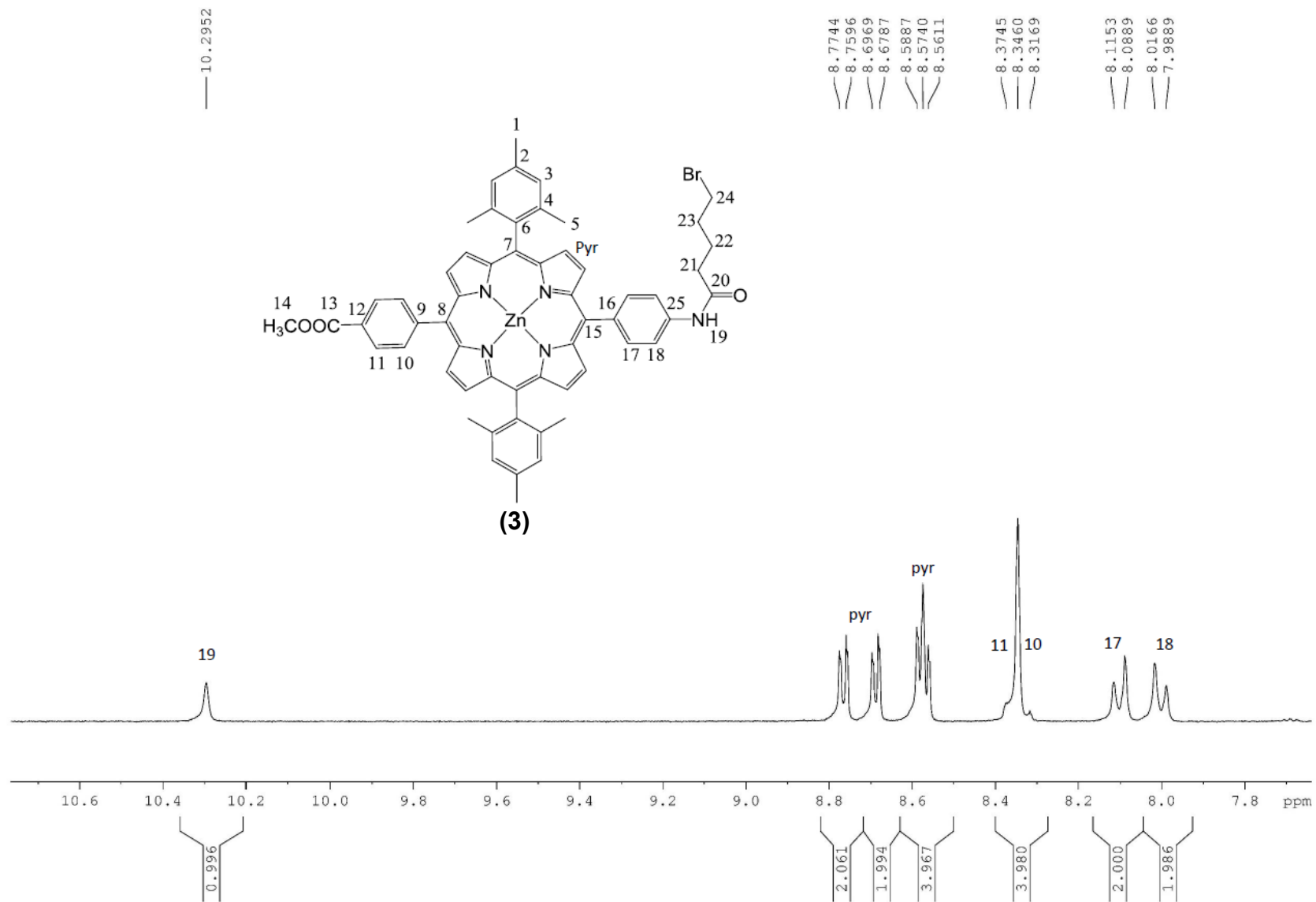


Figure S2: Focus on aromatic region of ^1H NMR spectrum of **3** (300MHz, DMSO-d_6).

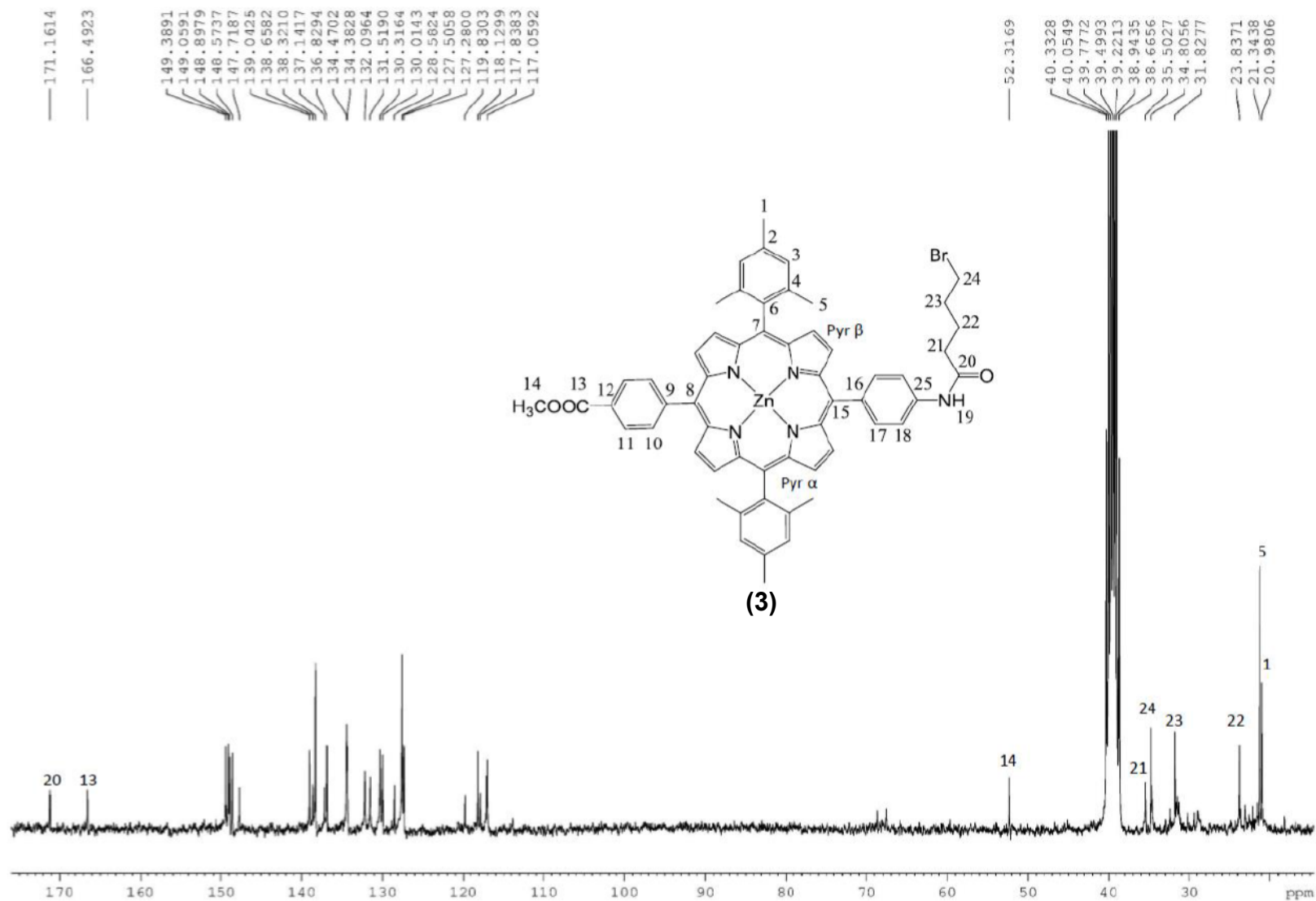


Figure S3: ¹³C NMR spectrum of **3** (75MHz, DMSO-d₆).

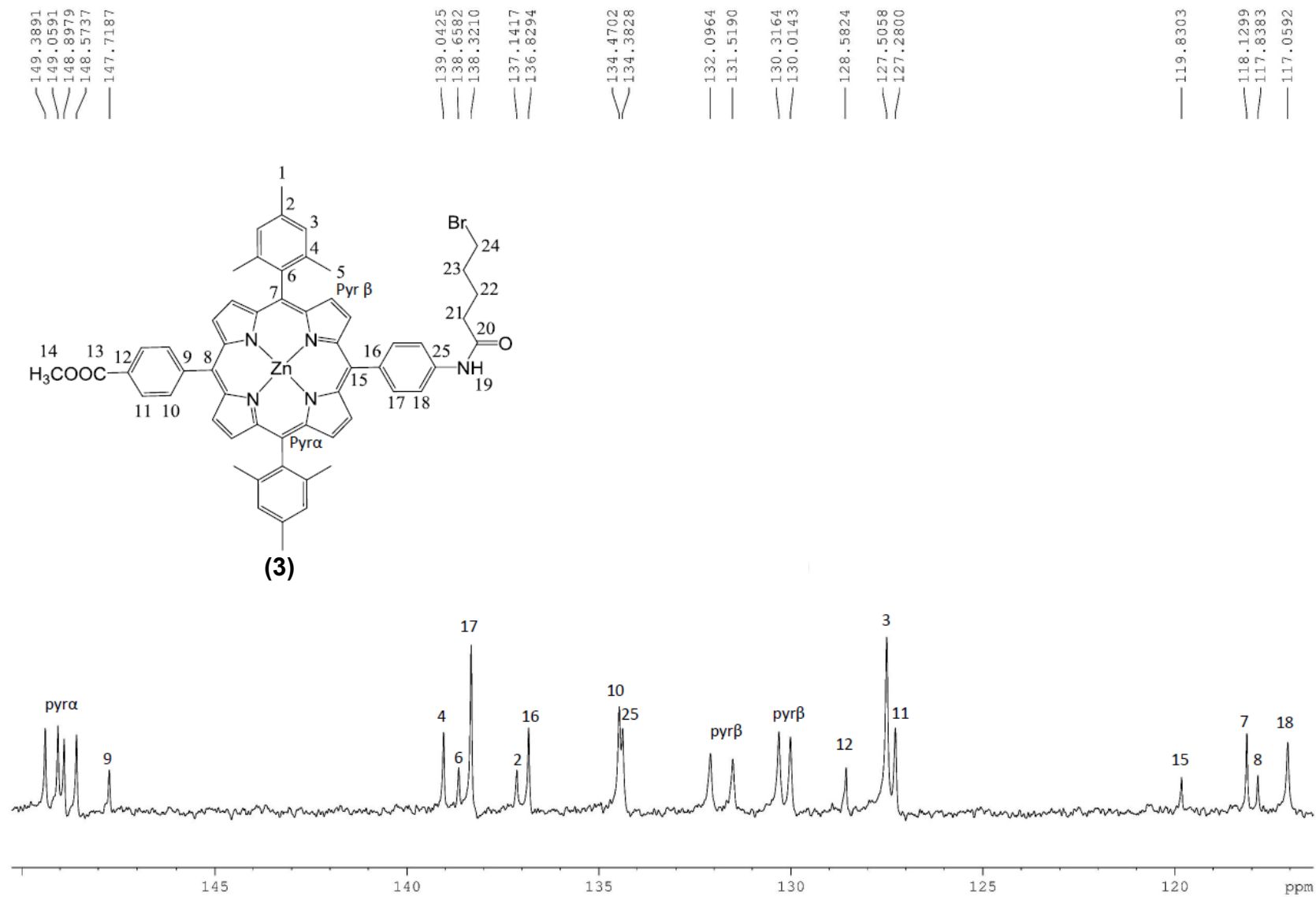


Figure S4: Focus on ¹³C NMR spectrum of **3** (75MHz, DMSO-d⁶).

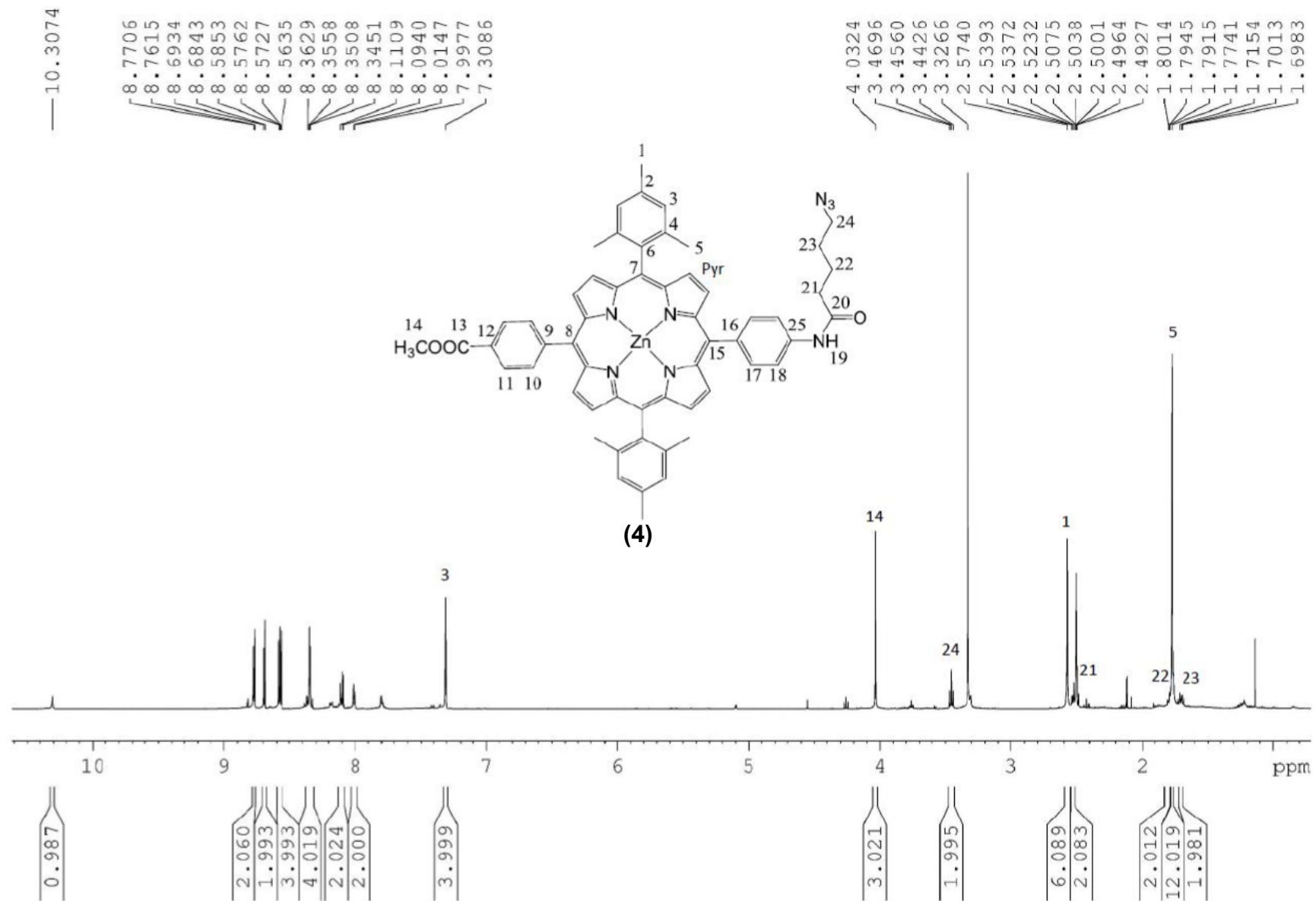


Figure S5: ^1H NMR spectrum of **4** (500MHz, DMSO-d_6).

—10.3074

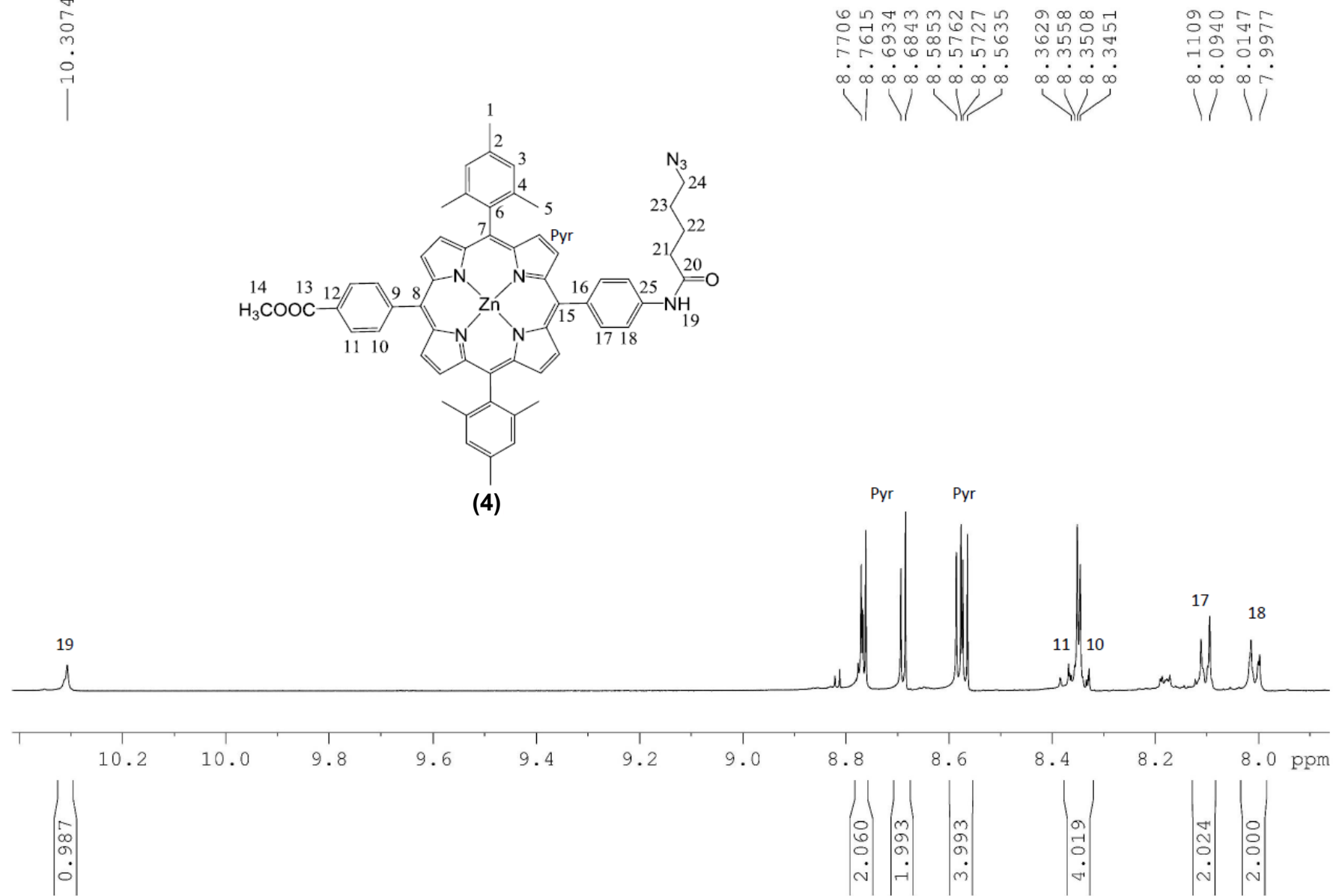


Figure S6: Focus on aromatic region of ¹H NMR spectrum of **4** (500MHz, DMSO-d₆).

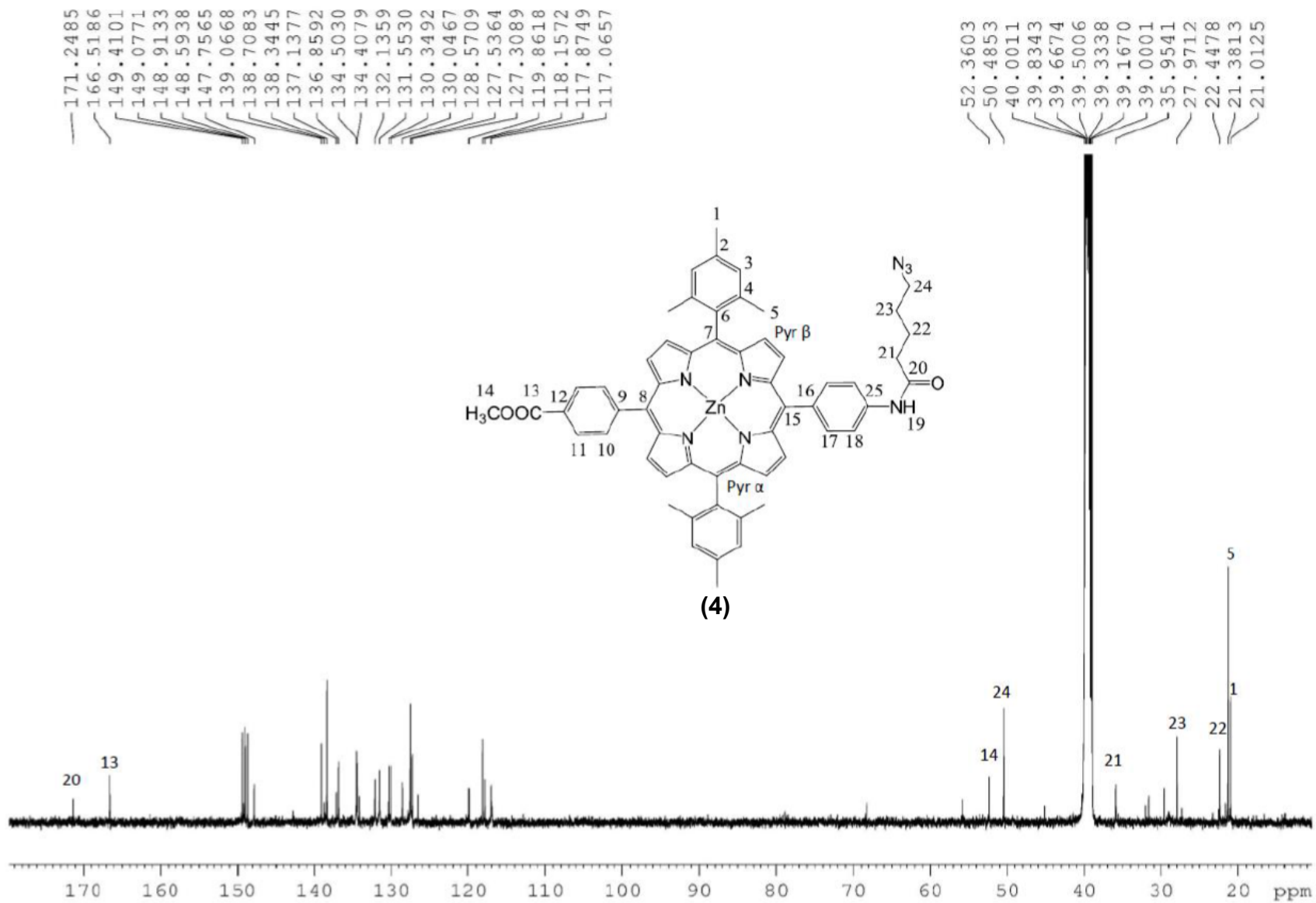


Figure S7: ¹³C NMR spectrum of **4** (125MHz, DMSO-d₆).

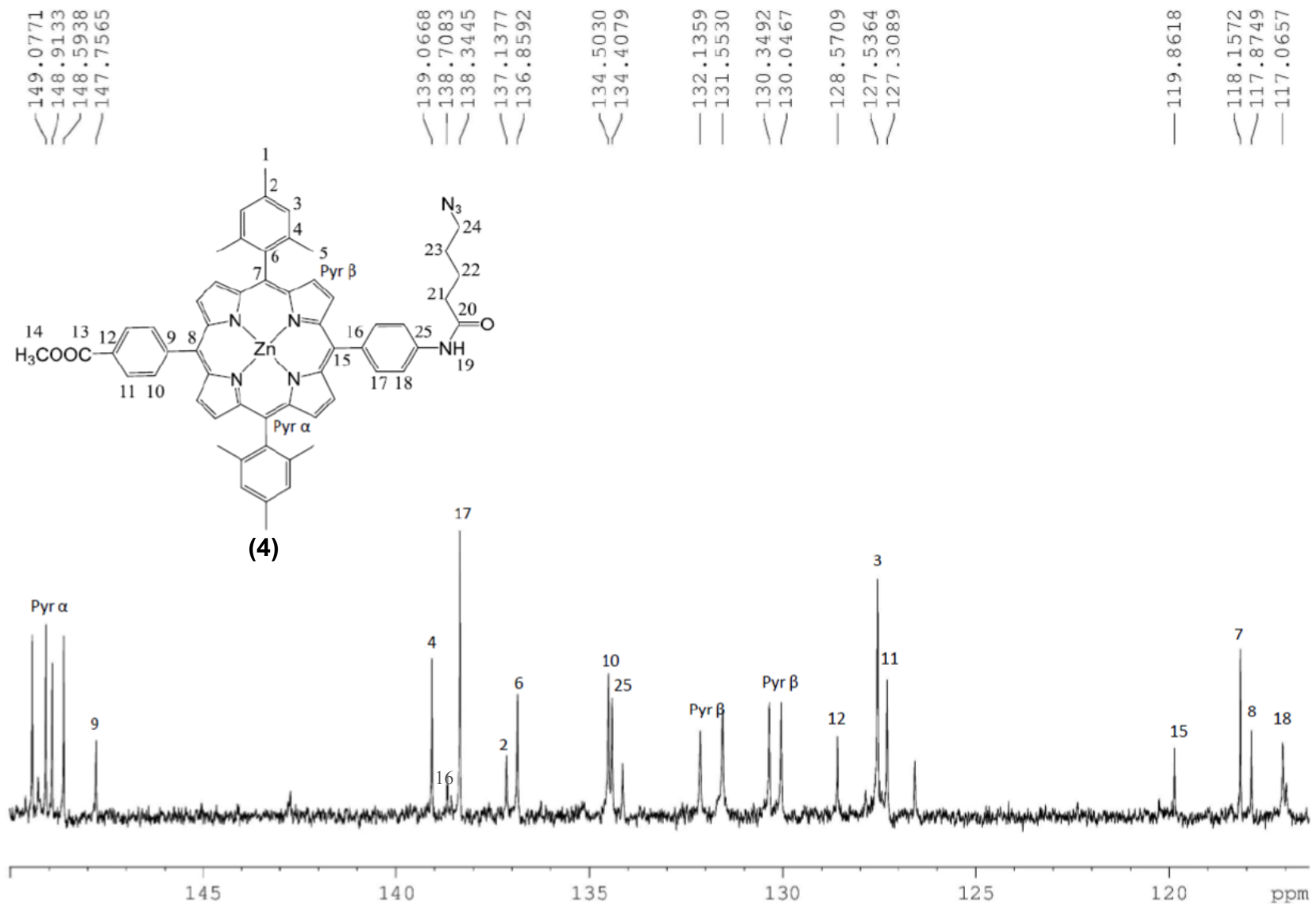


Figure S8: Focus on ^{13}C NMR spectrum of **4** (125MHz, DMSO- d_6).

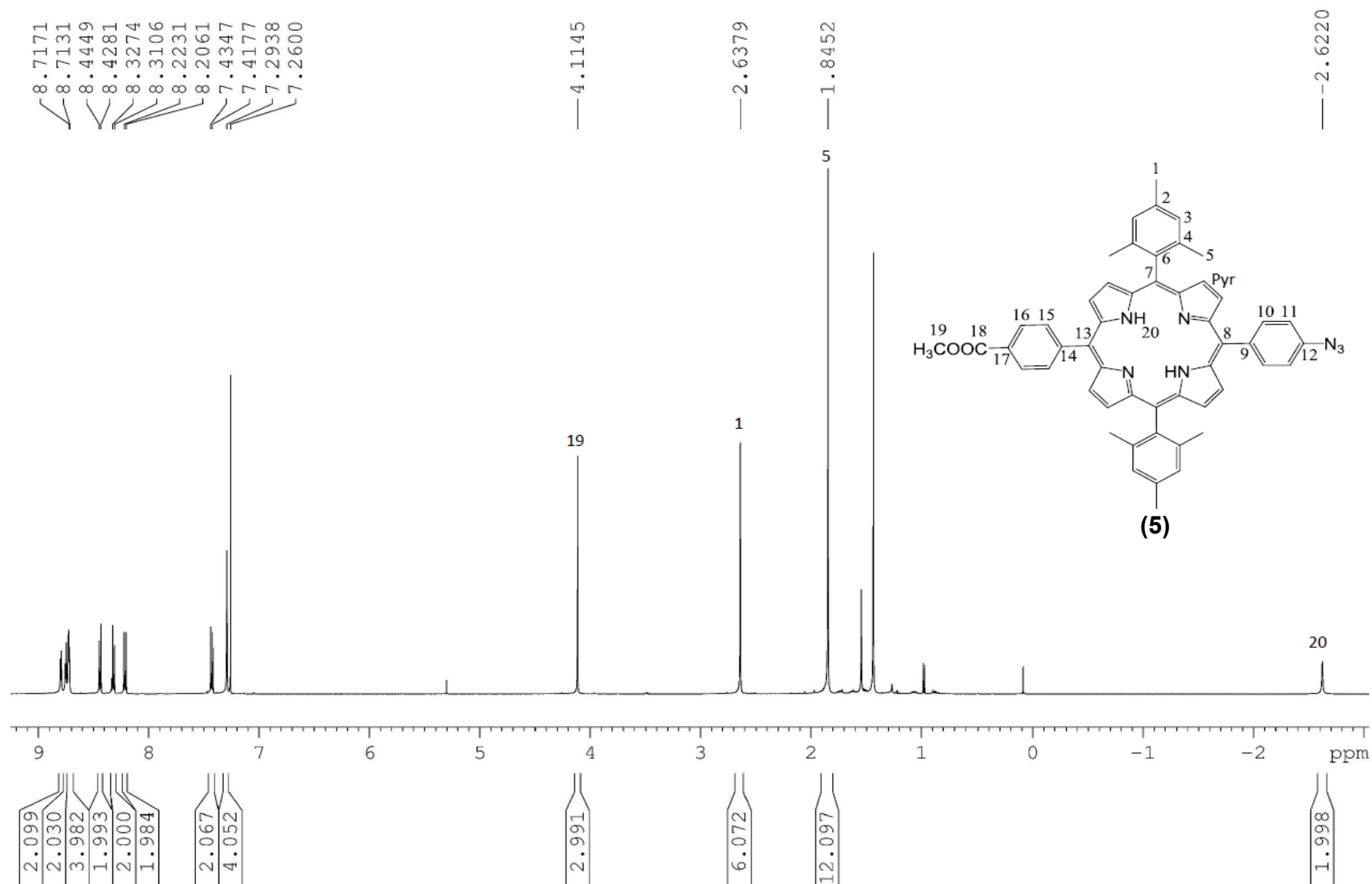


Figure S9: ¹H NMR spectrum of **5** (500MHz, CDCl₃).

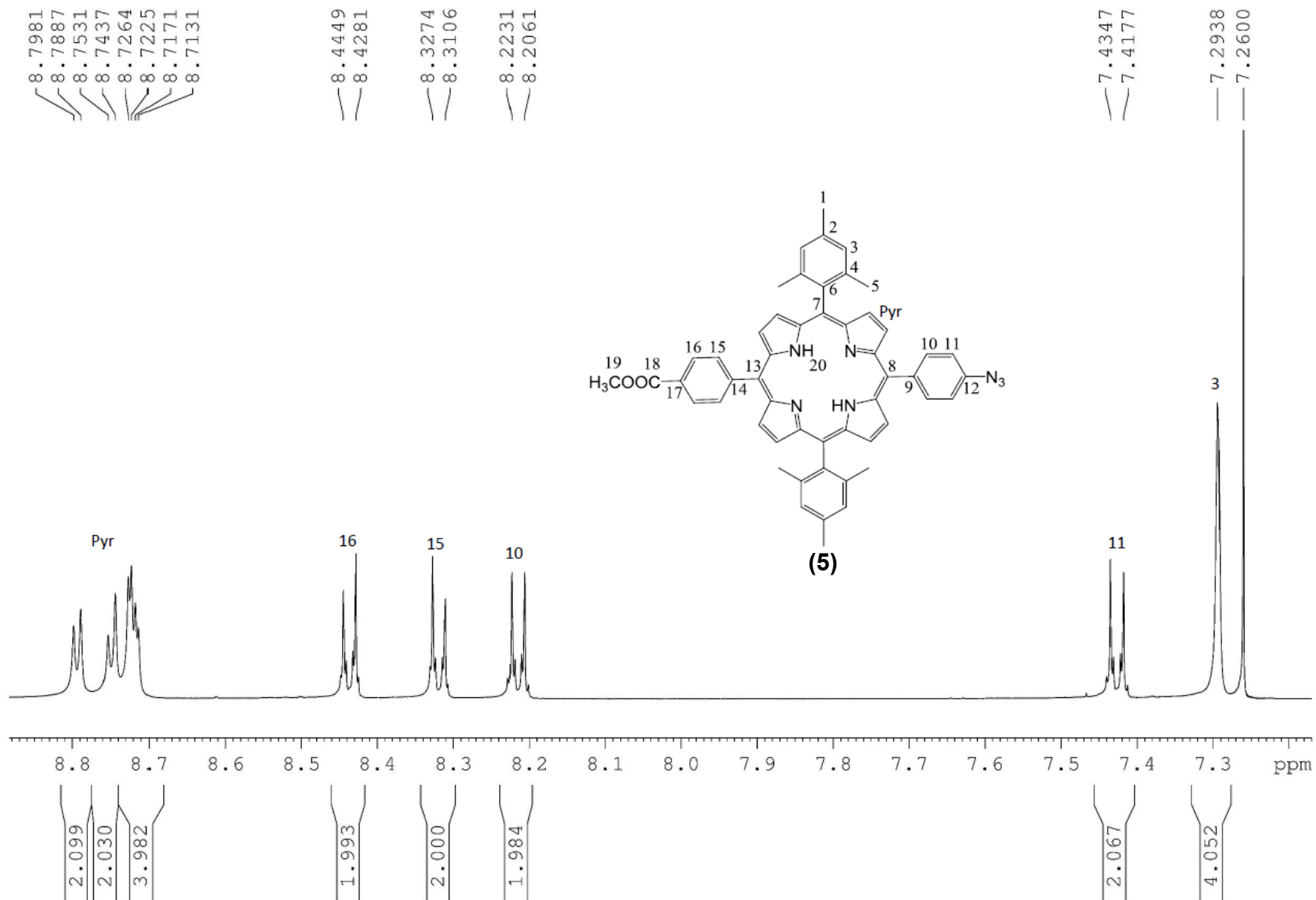


Figure S10: Focus on aromatic region of ^1H NMR spectrum of **5** (500MHz, CDCl_3).

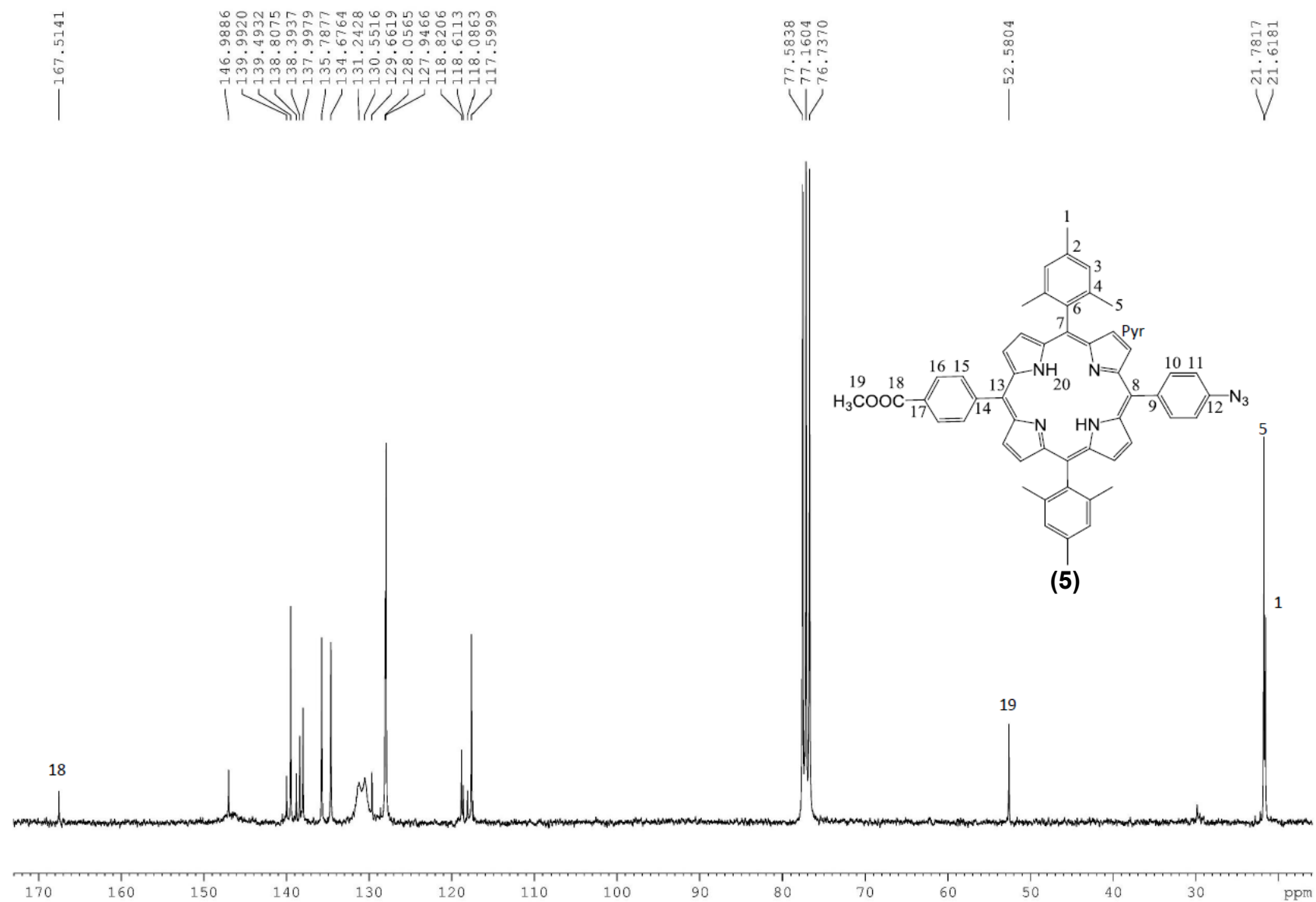


Figure S11: ^{13}C NMR spectrum of **5** (125MHz, CDCl_3).

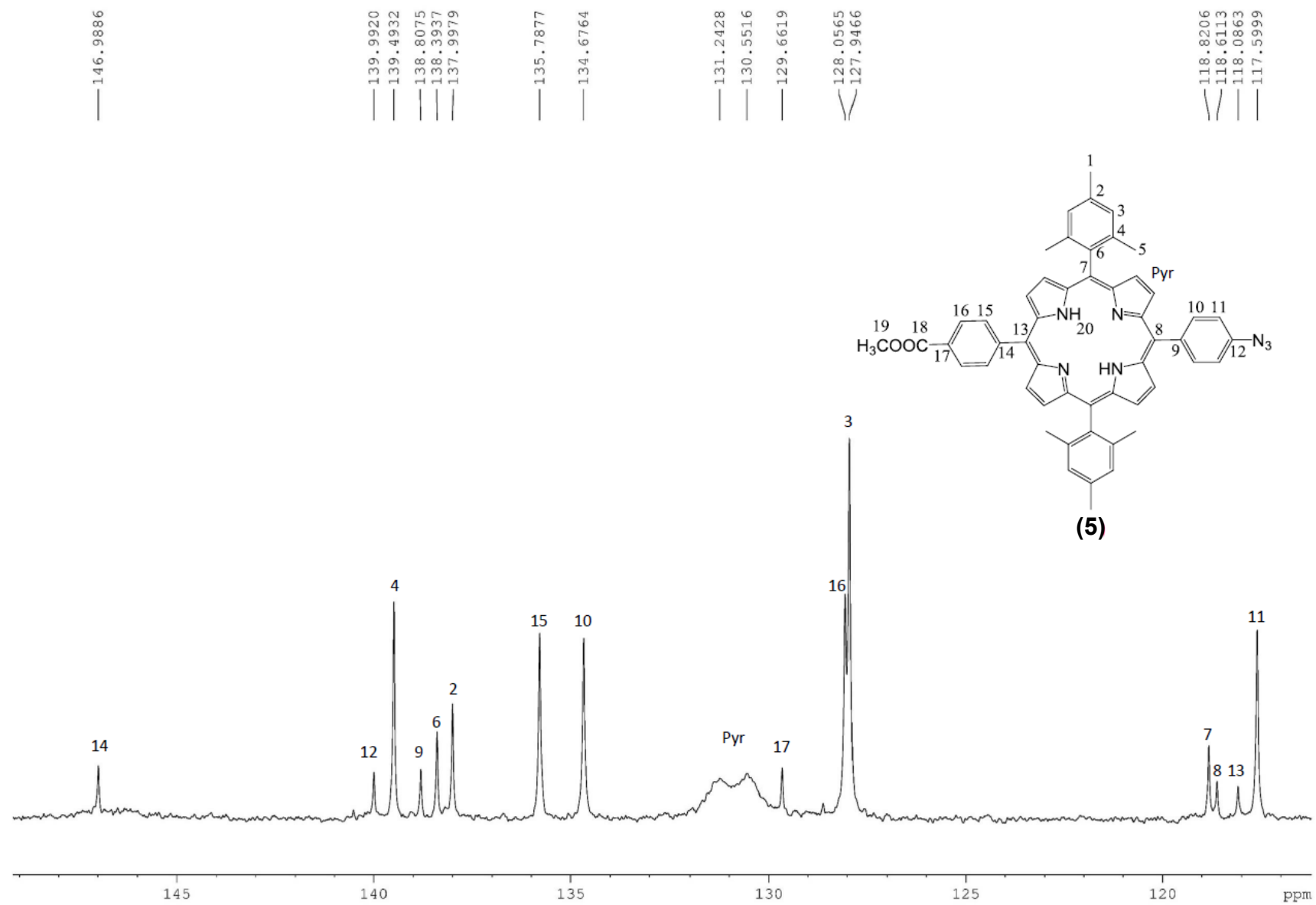


Figure S12: Focus on ¹³C NMR spectrum of **5** (125MHz, CDCl₃).

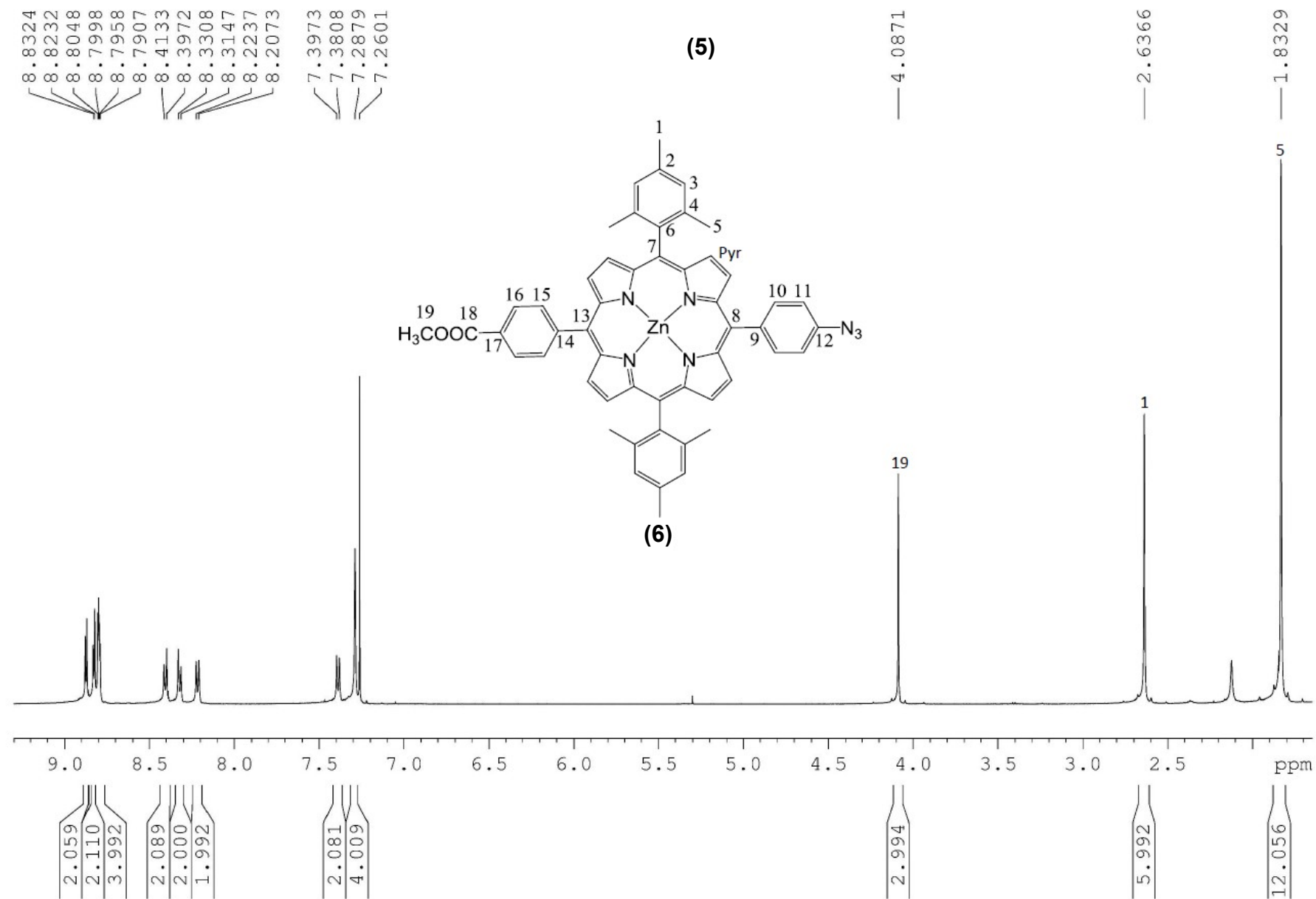


Figure S13: ^1H NMR spectrum of **6** (500MHz, CDCl_3).

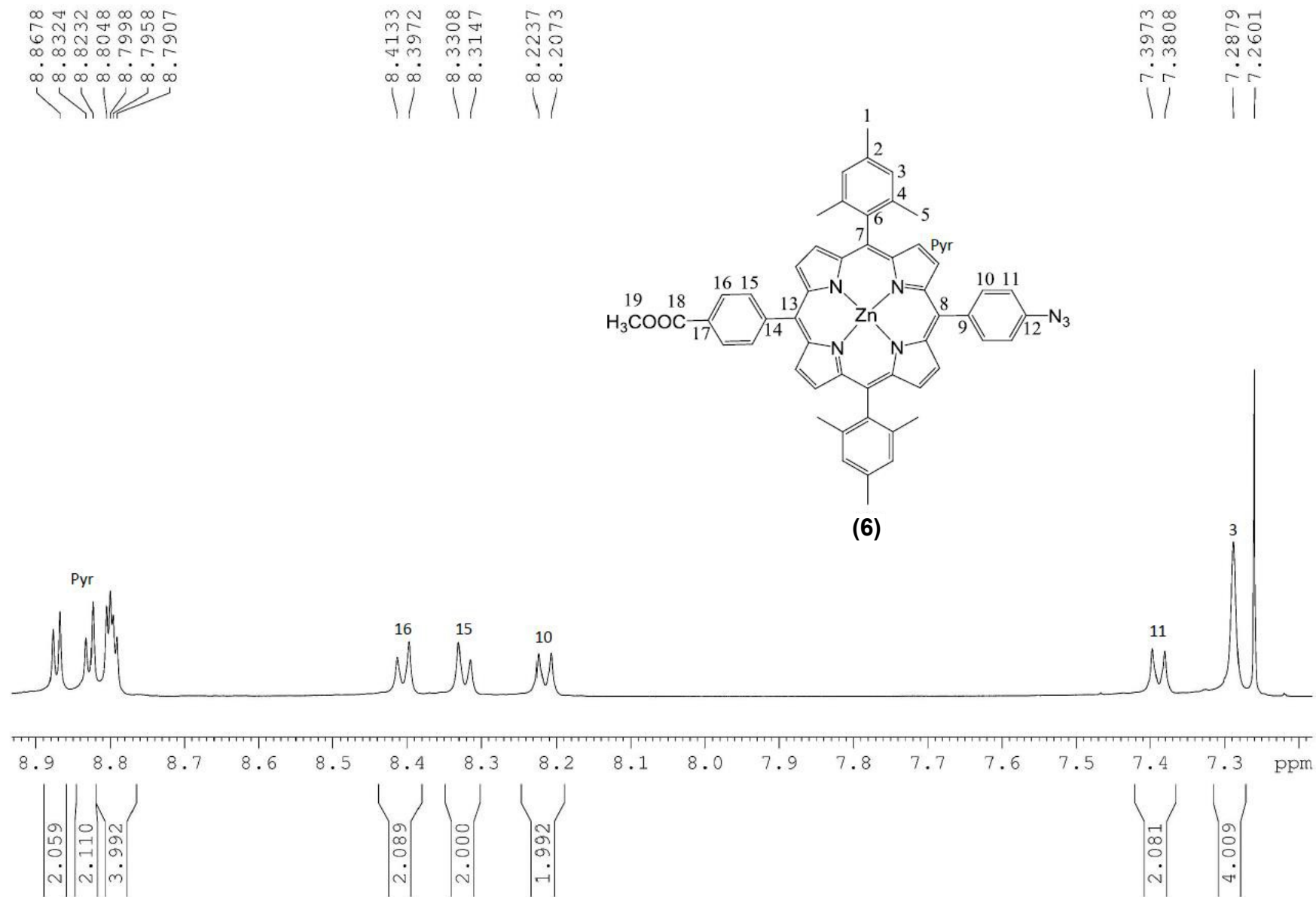


Figure S14: Focus on aromatic region of ^1H NMR spectrum of **6** (500MHz, CDCl_3).

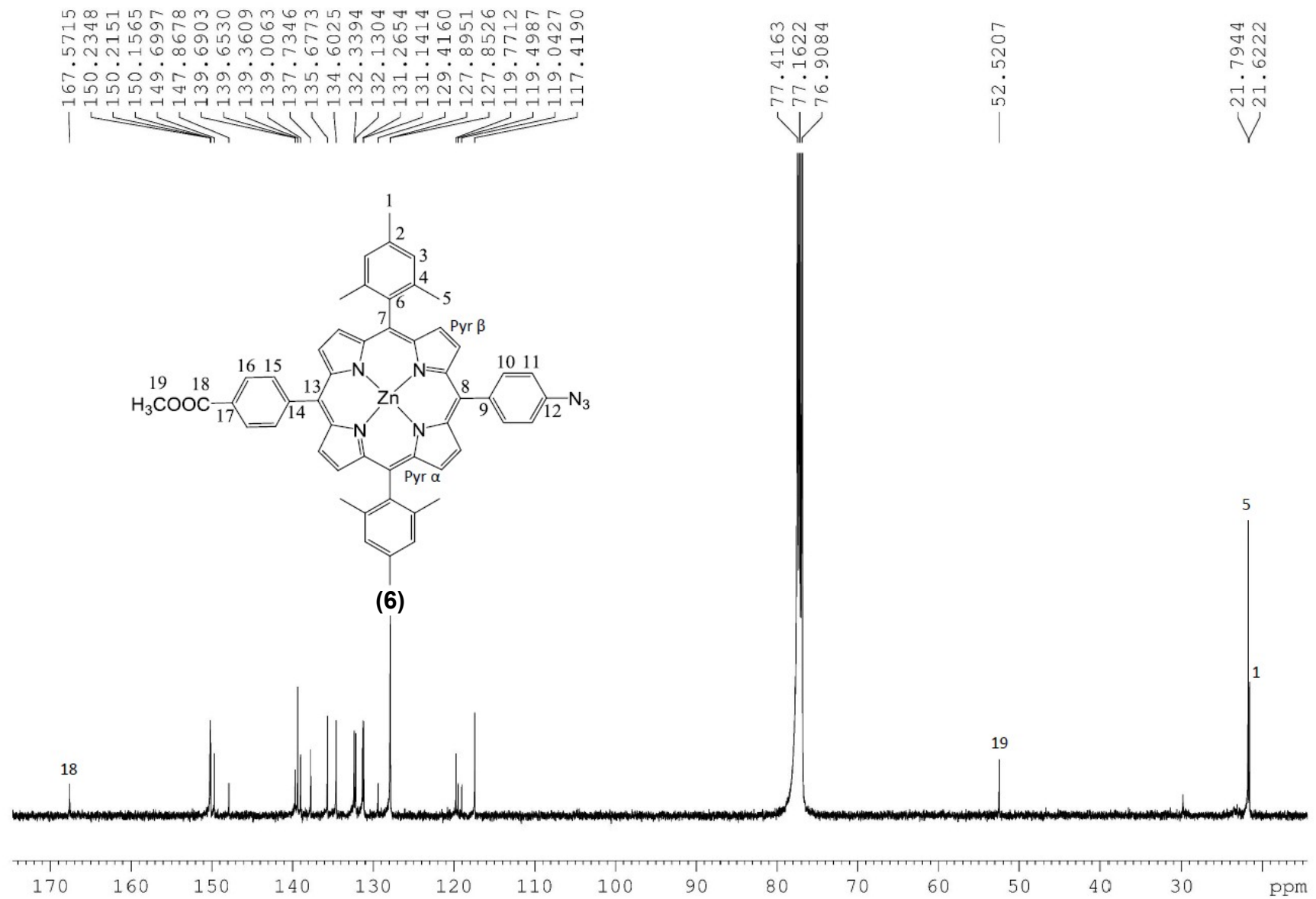


Figure S15: ¹³C NMR spectrum of **6** (125MHz, CDCl₃).

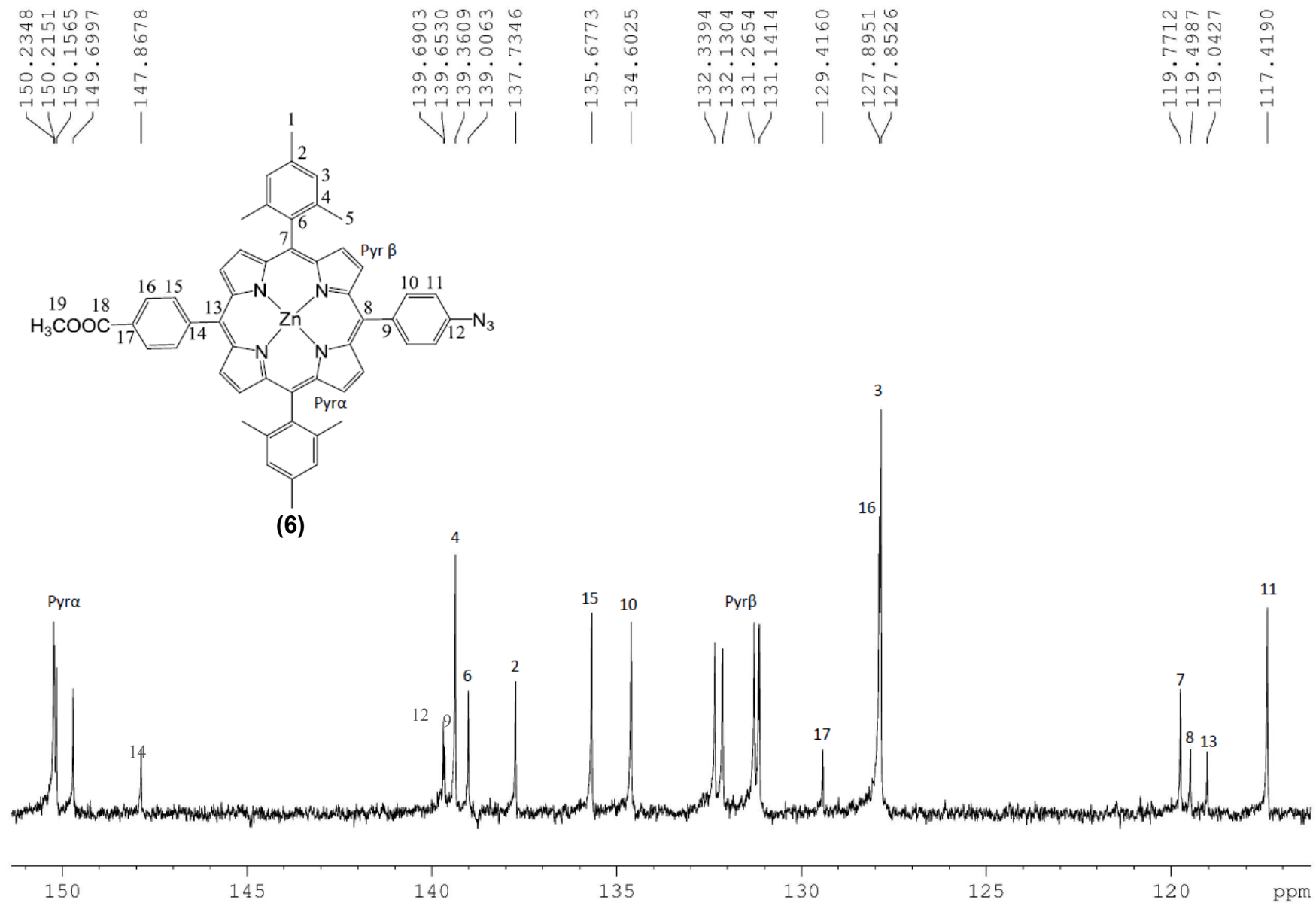


Figure S16: Focus on ¹³C NMR spectrum of **6** (125MHz, CDCl₃).

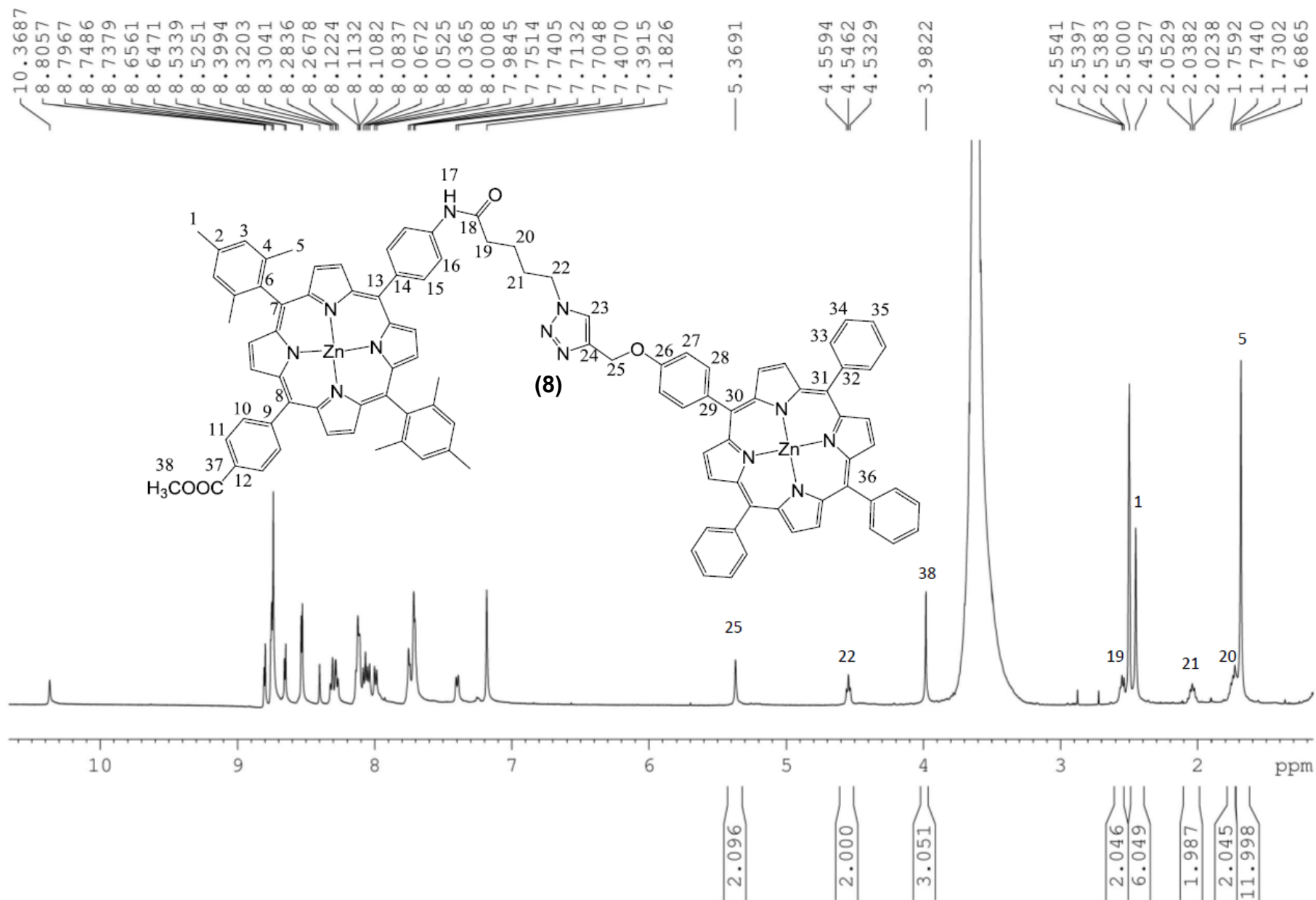


Figure S17: ¹H NMR spectrum of **8** (500MHz, DMSO-d₆).

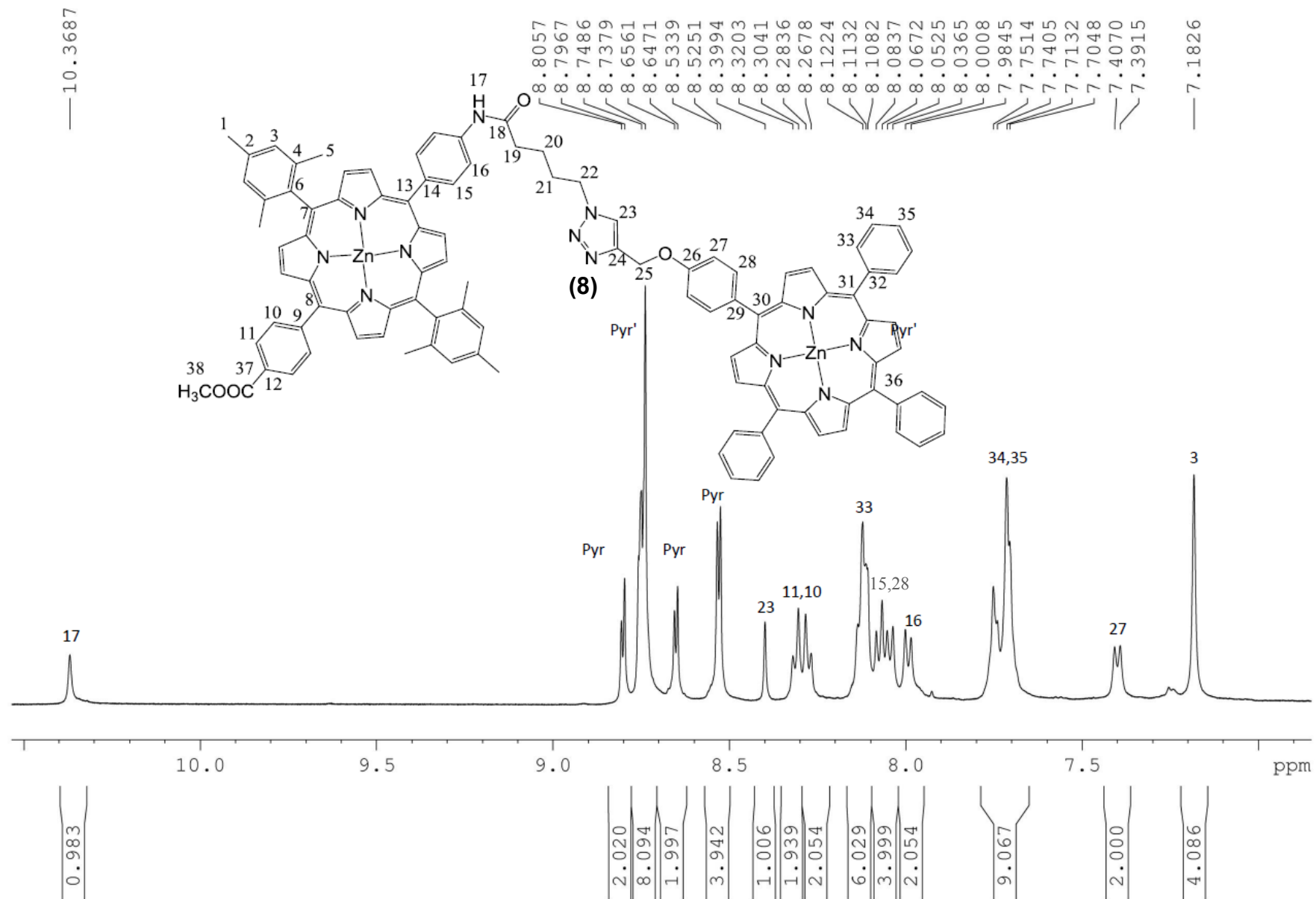


Figure S18: Focus on aromatic region of ^1H NMR spectrum of **8** (500MHz, DMSO-d_6).

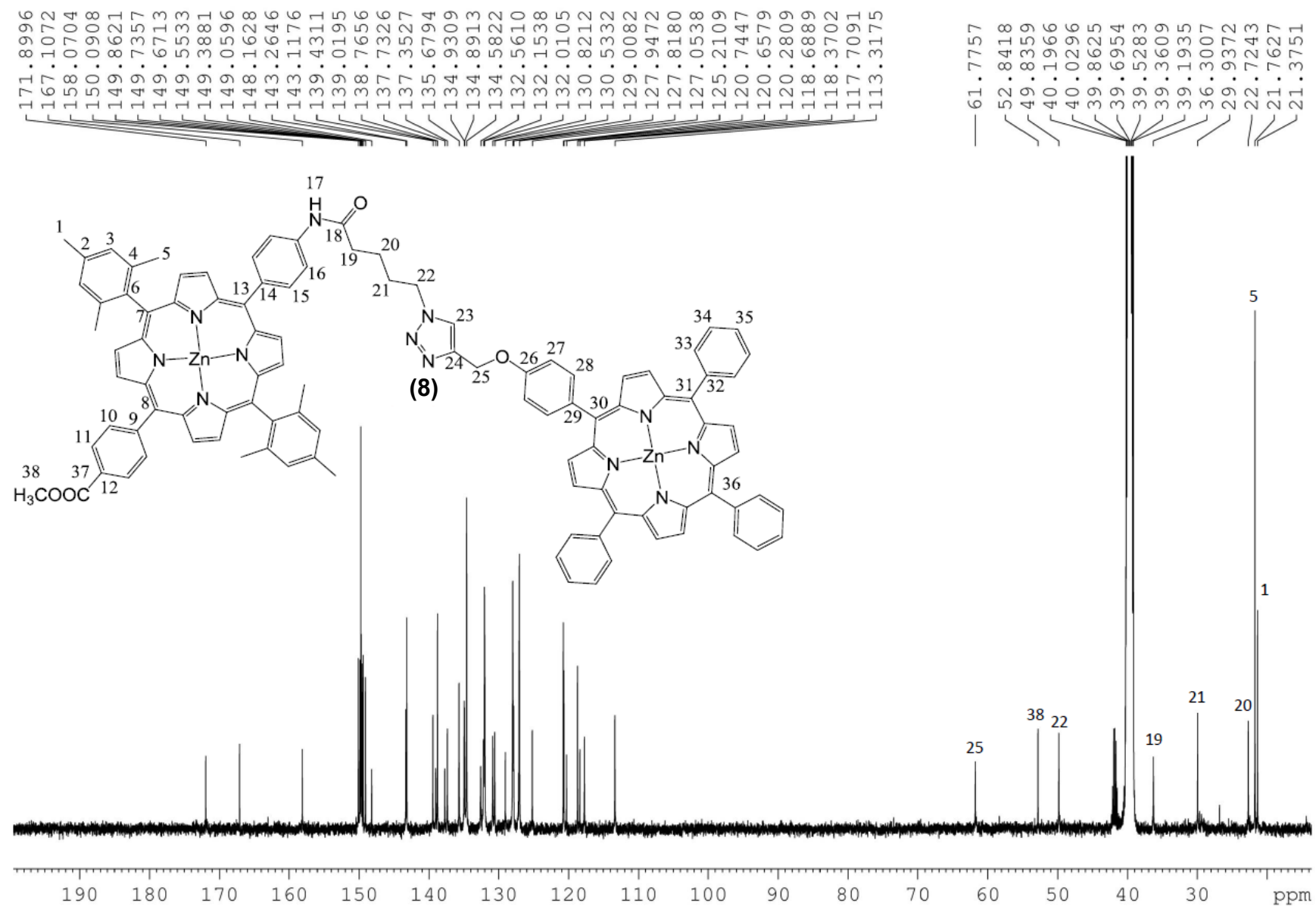


Figure S19: ¹³C NMR spectrum of **8** (125MHz, DMSO-d₆).

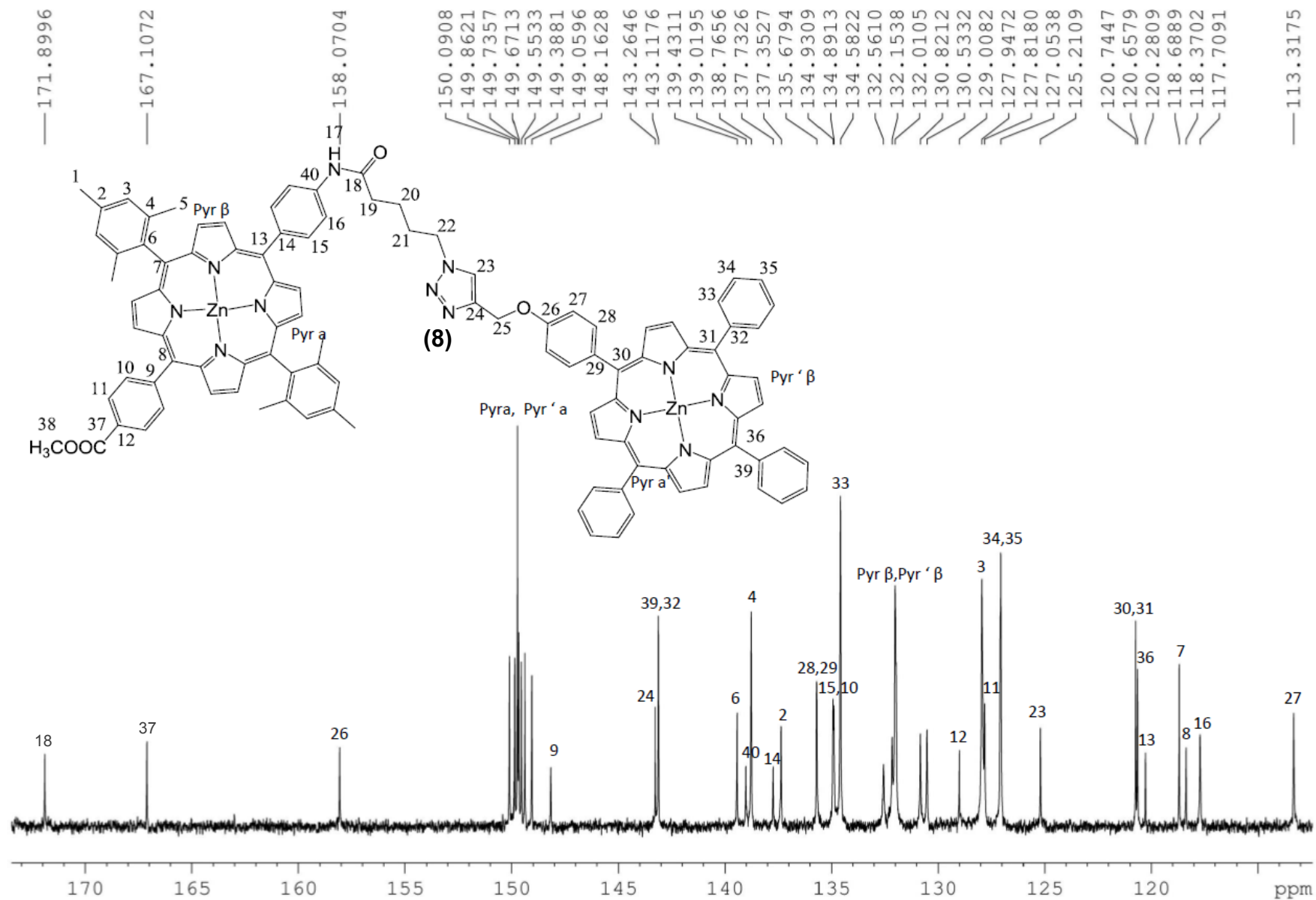


Figure S20: Focus on ^{13}C NMR spectrum of **8** (125MHz, DMSO- d_6).

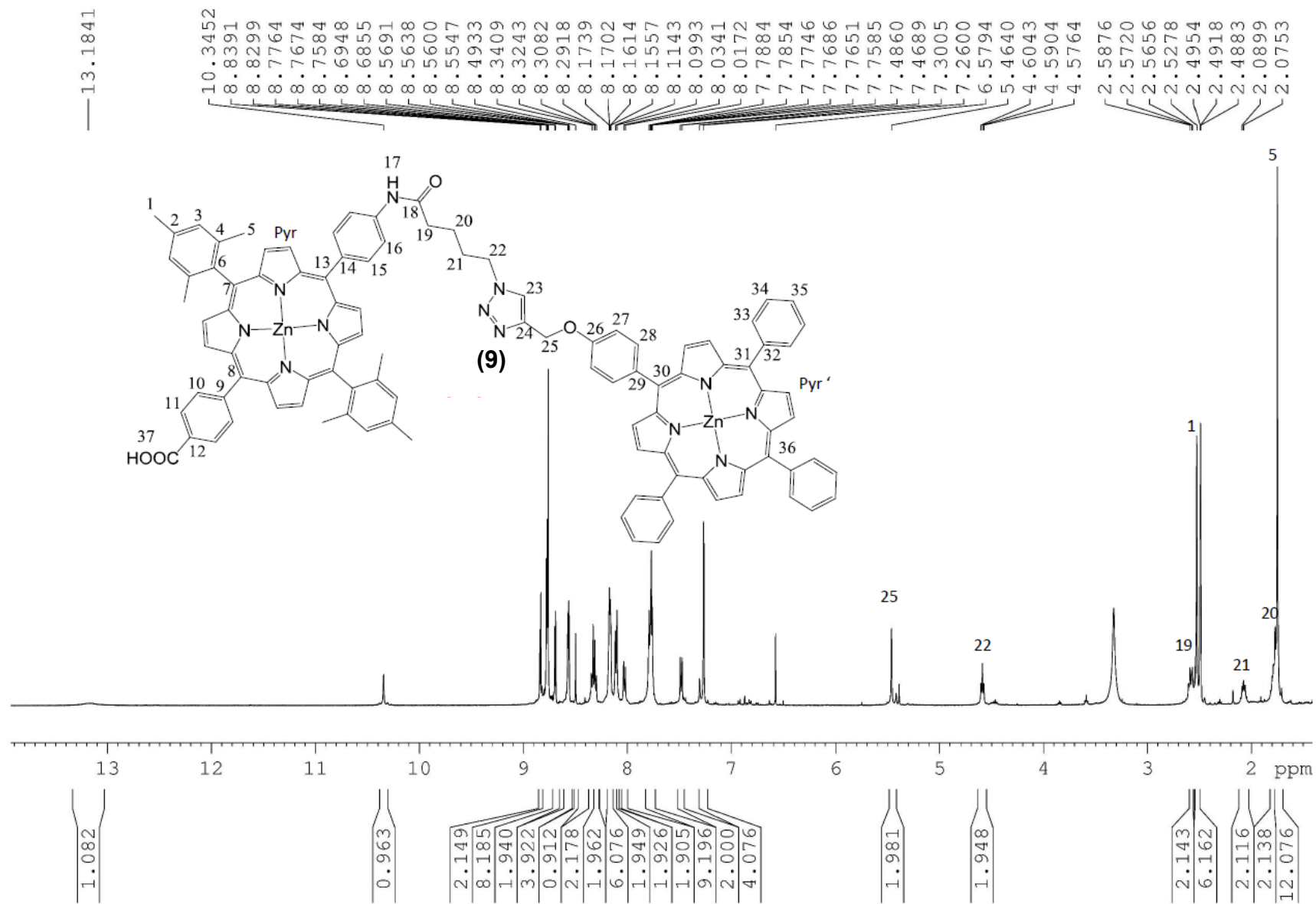


Figure S21: ¹H NMR spectrum of **9** (500MHz, DMSO-d₆).

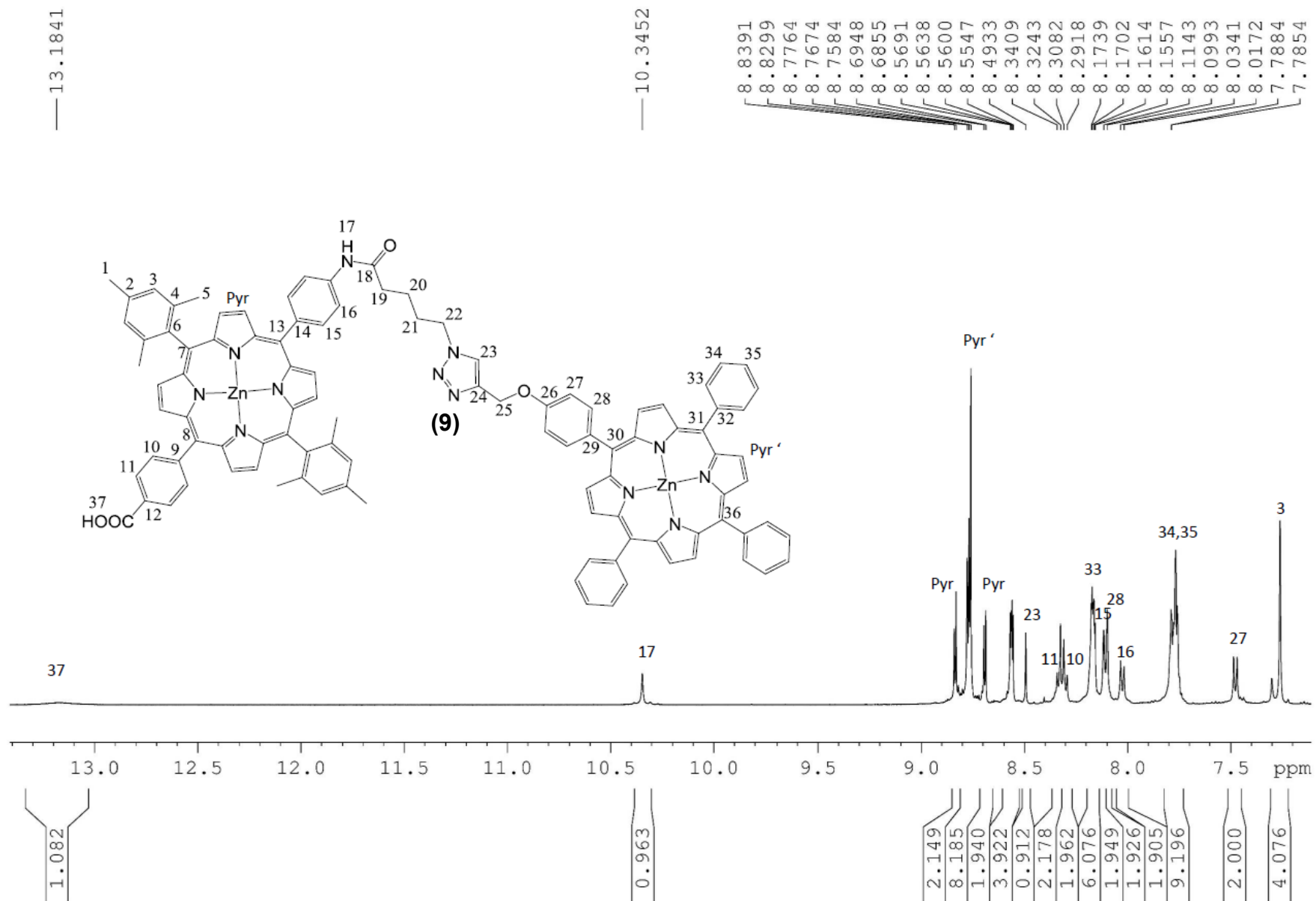


Figure S22: Focus on aromatic region of ^1H NMR spectrum of **9** (500MHz, DMSO- d_6).

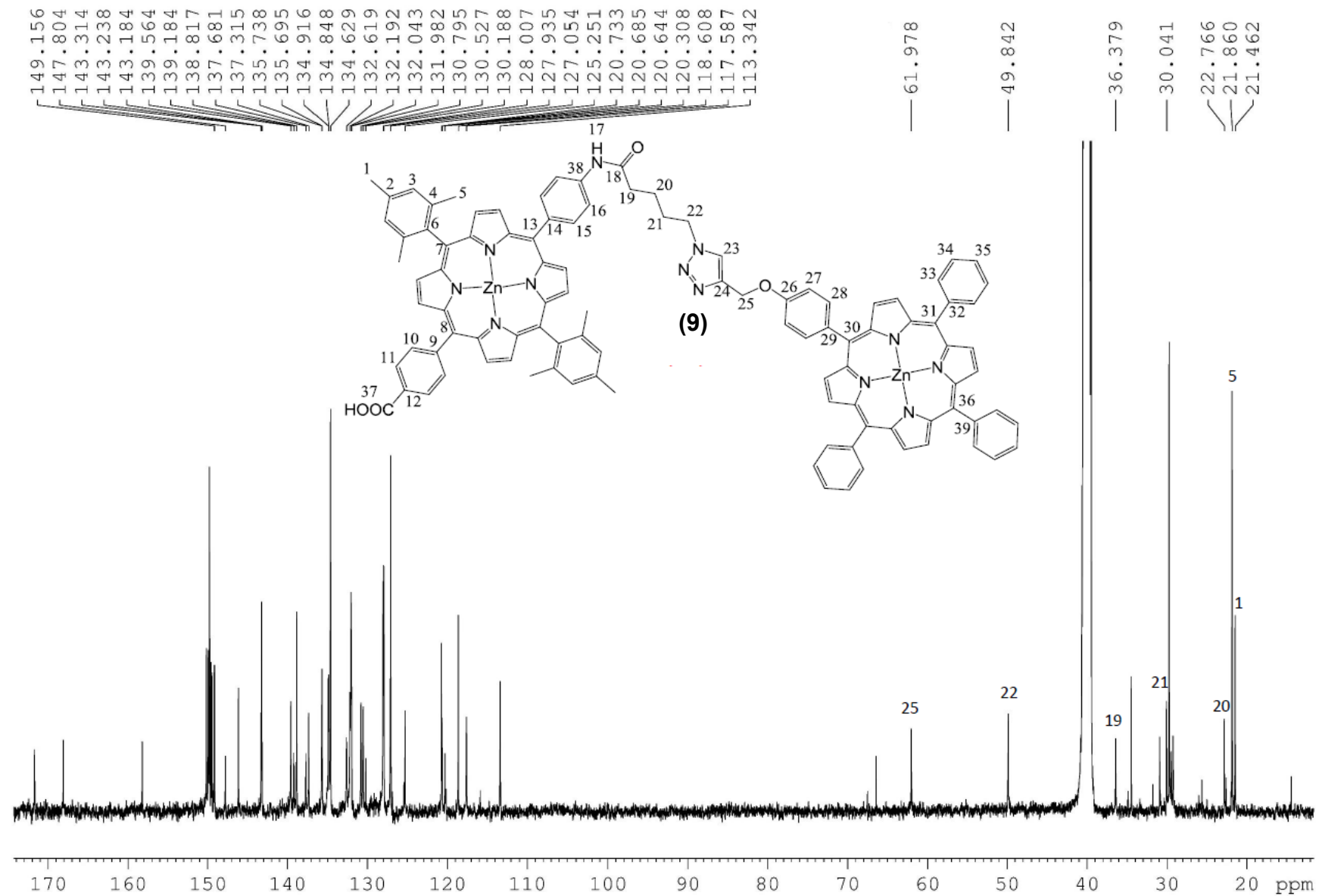


Figure S23: ¹³C NMR spectrum of **9** (125MHz, DMSO-d⁶).

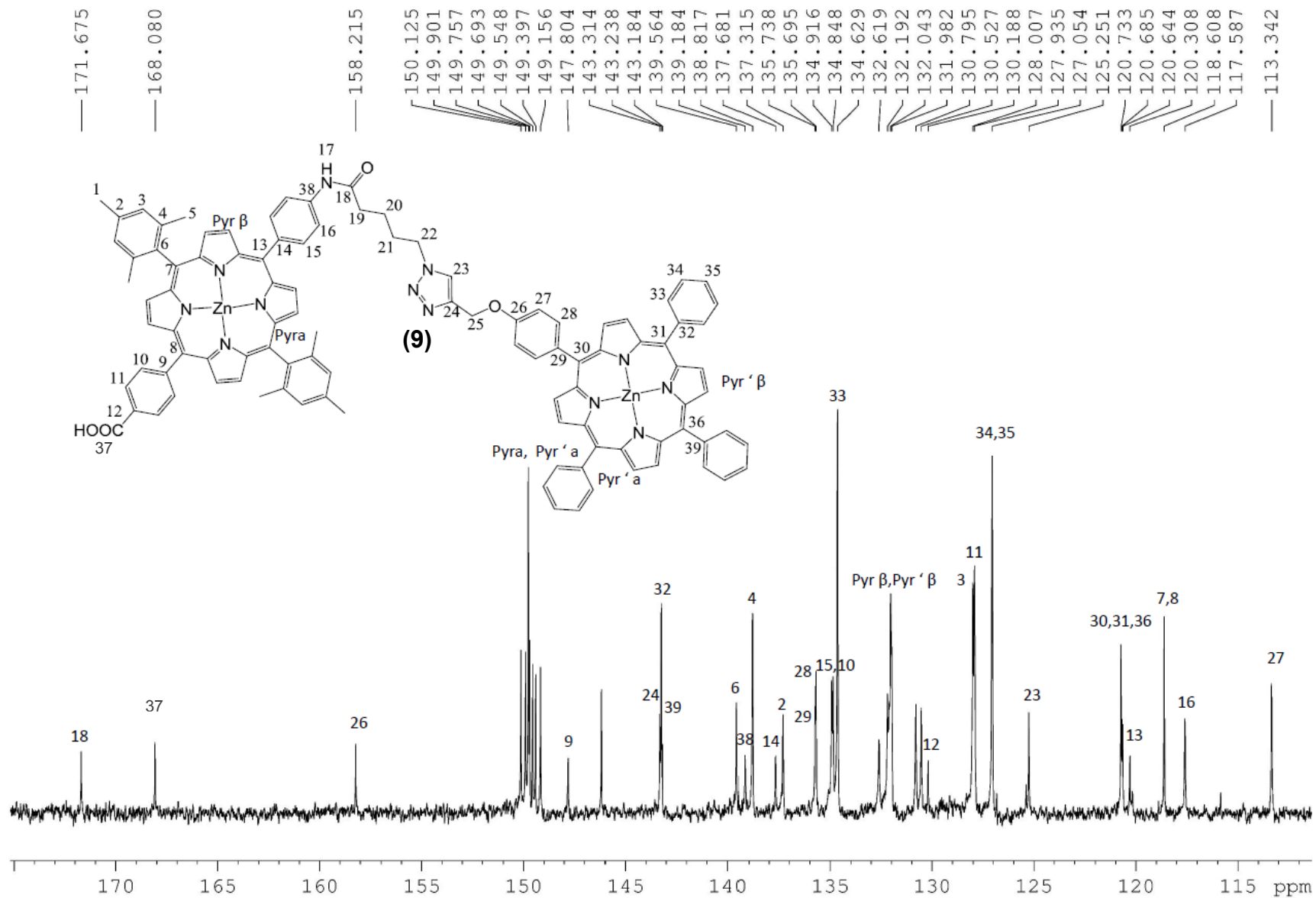


Figure S24: Focus on ¹³C NMR spectrum of **9** (125MHz, DMSO-d₆).

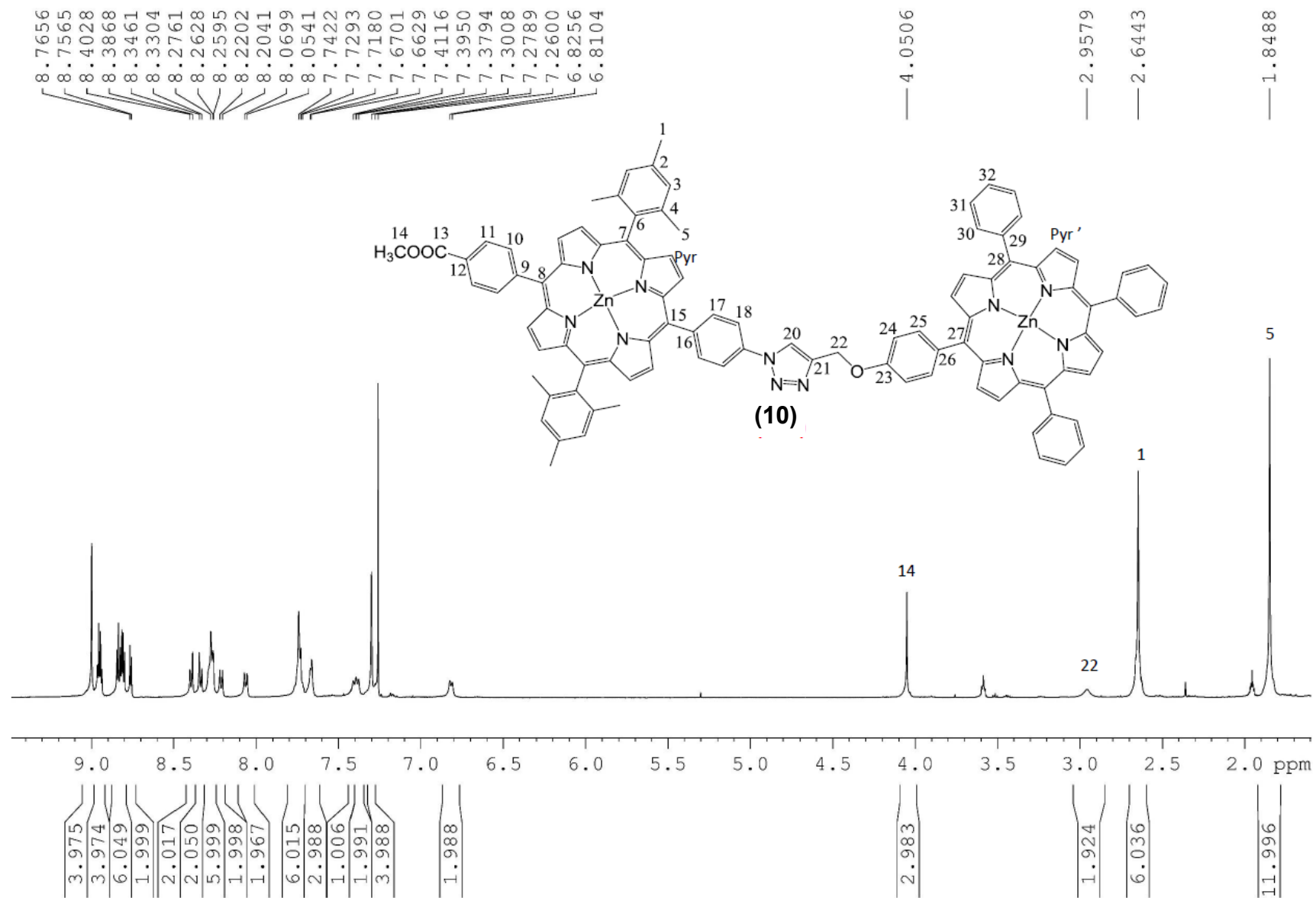


Figure S25: ¹H NMR spectrum of **10** (500MHz, CDCl₃).

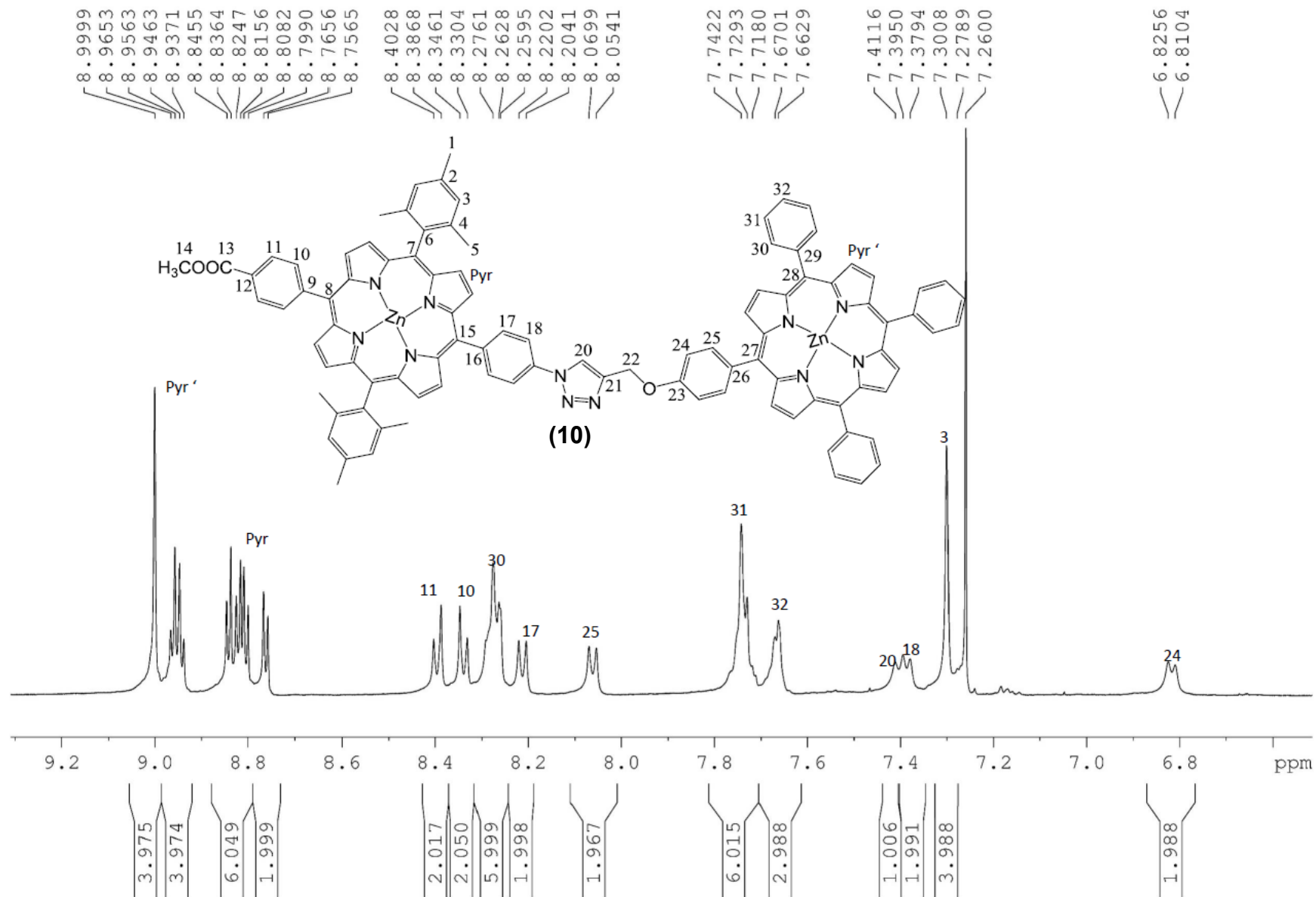


Figure S26: Focus on aromatic region of ¹H NMR spectrum of **10** (500MHz, CDCl₃).

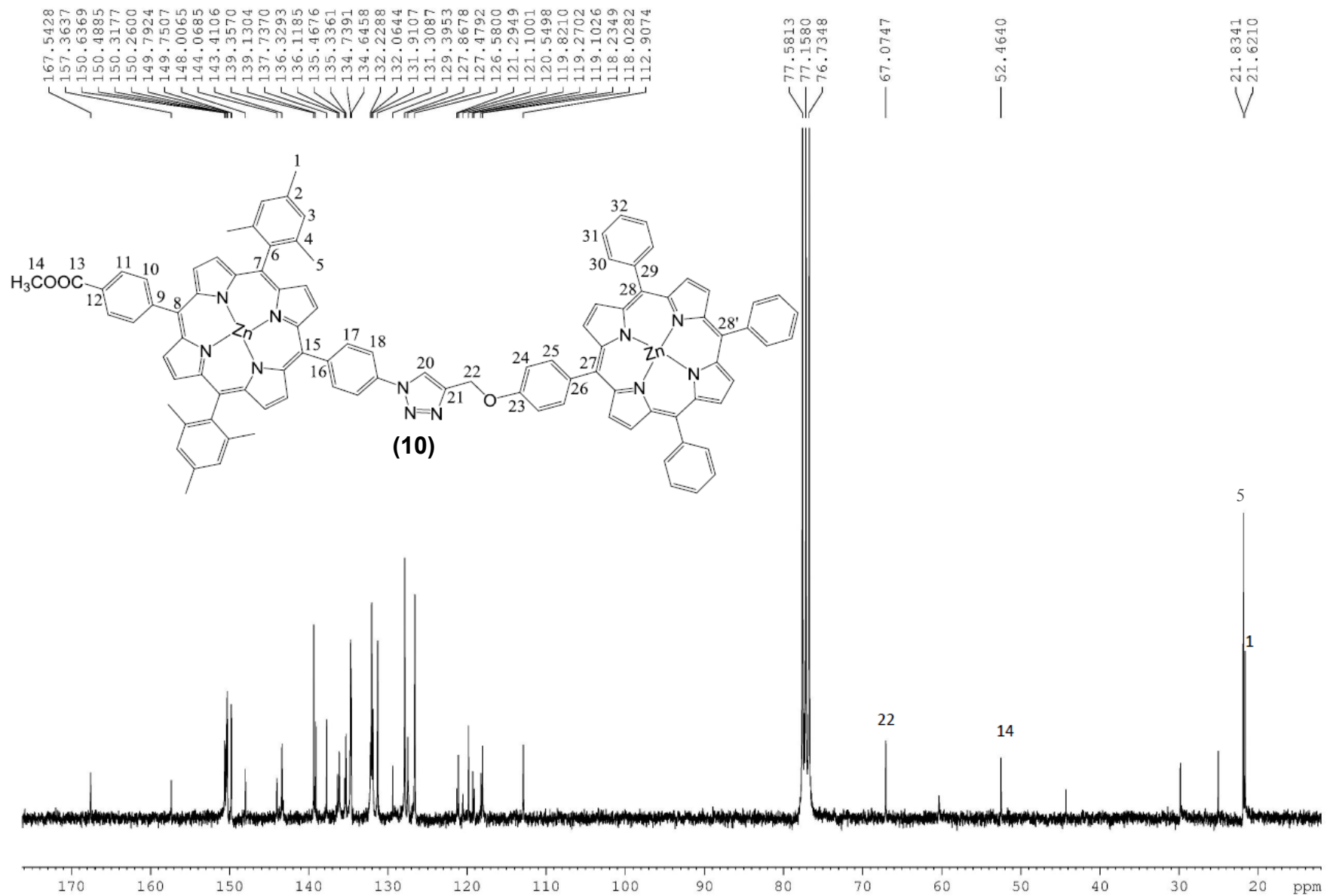


Figure S27: ¹³C NMR spectrum of **10** (125MHz, CDCl₃).

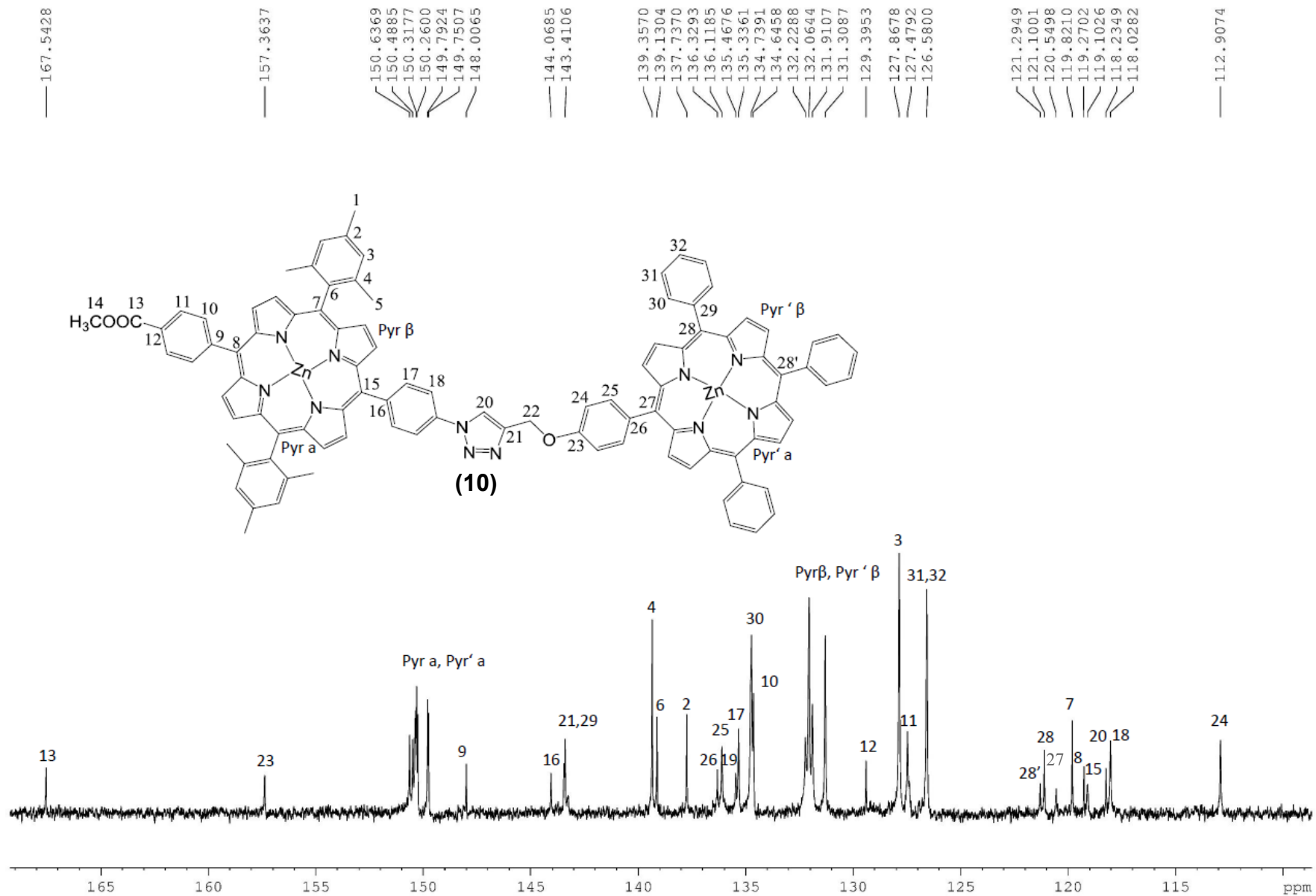


Figure S28: Focus on ¹³C NMR spectrum of **10** (125MHz, CDCl₃).

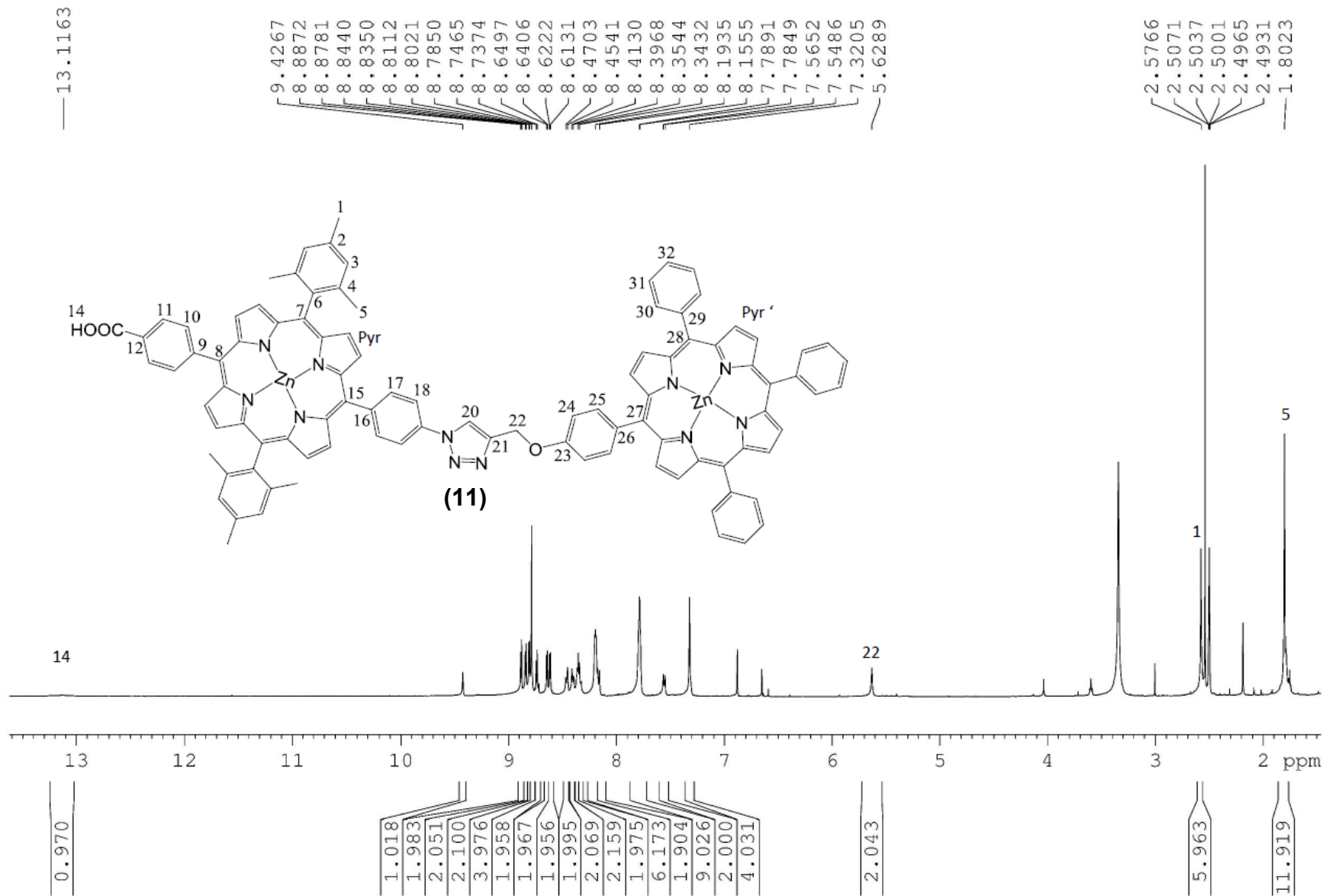


Figure S29: ^1H NMR spectrum of **11** (500MHz, DMSO- d_6).

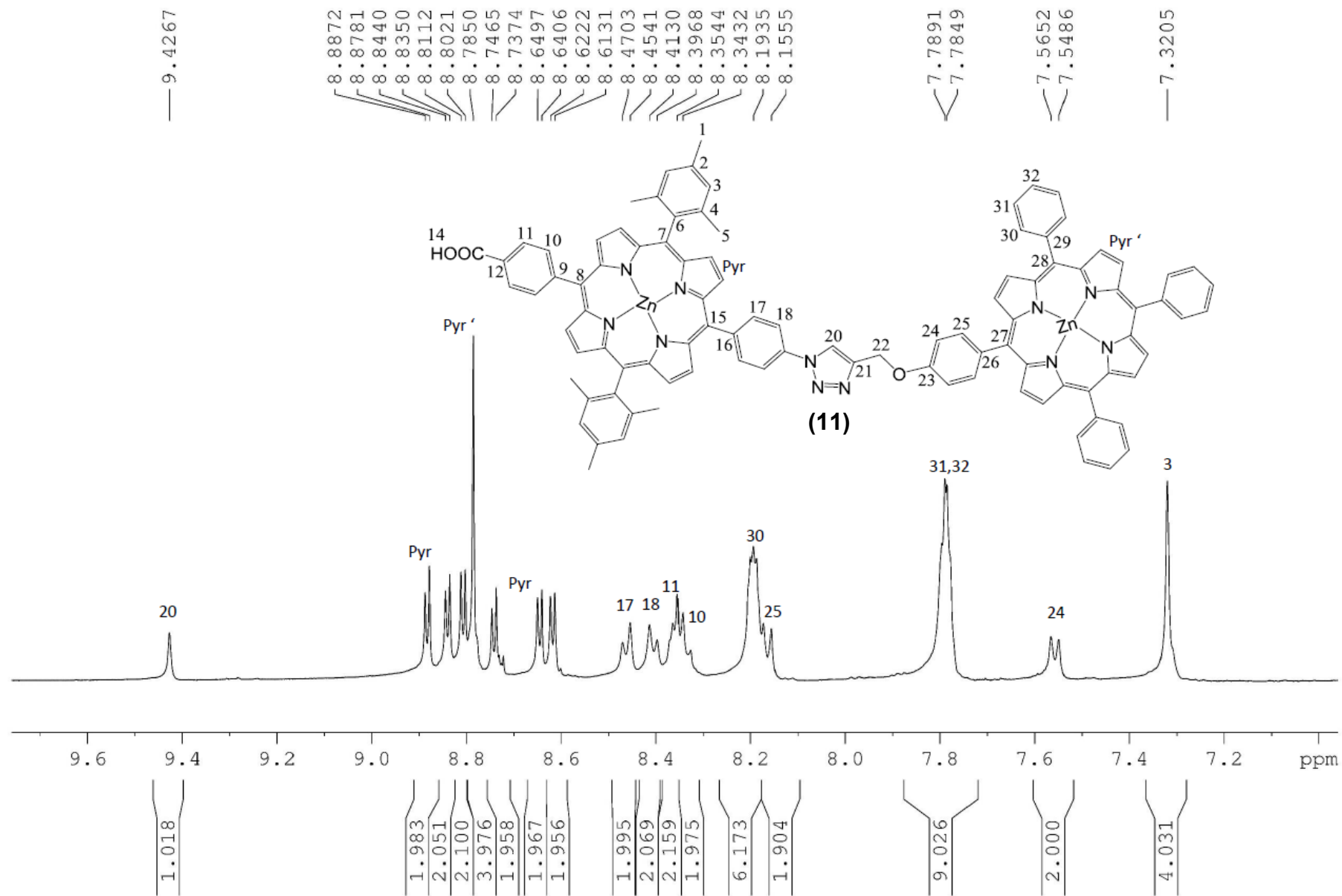


Figure S30: Focus on aromatic region of ^1H NMR spectrum of **11** (500MHz, DMSO-d_6).

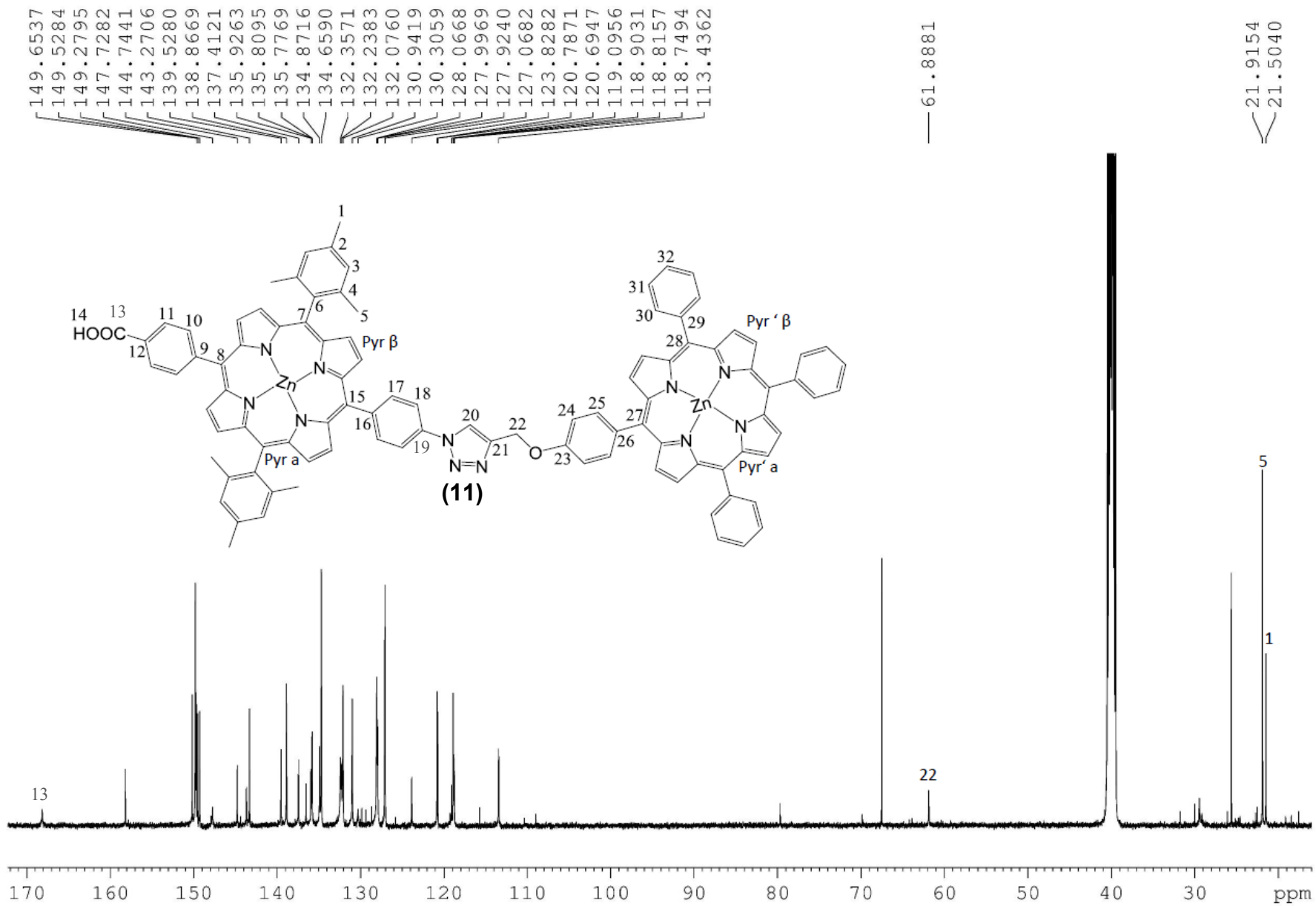


Figure S31: ^{13}C NMR spectrum of **11** (125MHz, DMSO-d_6). 13 170

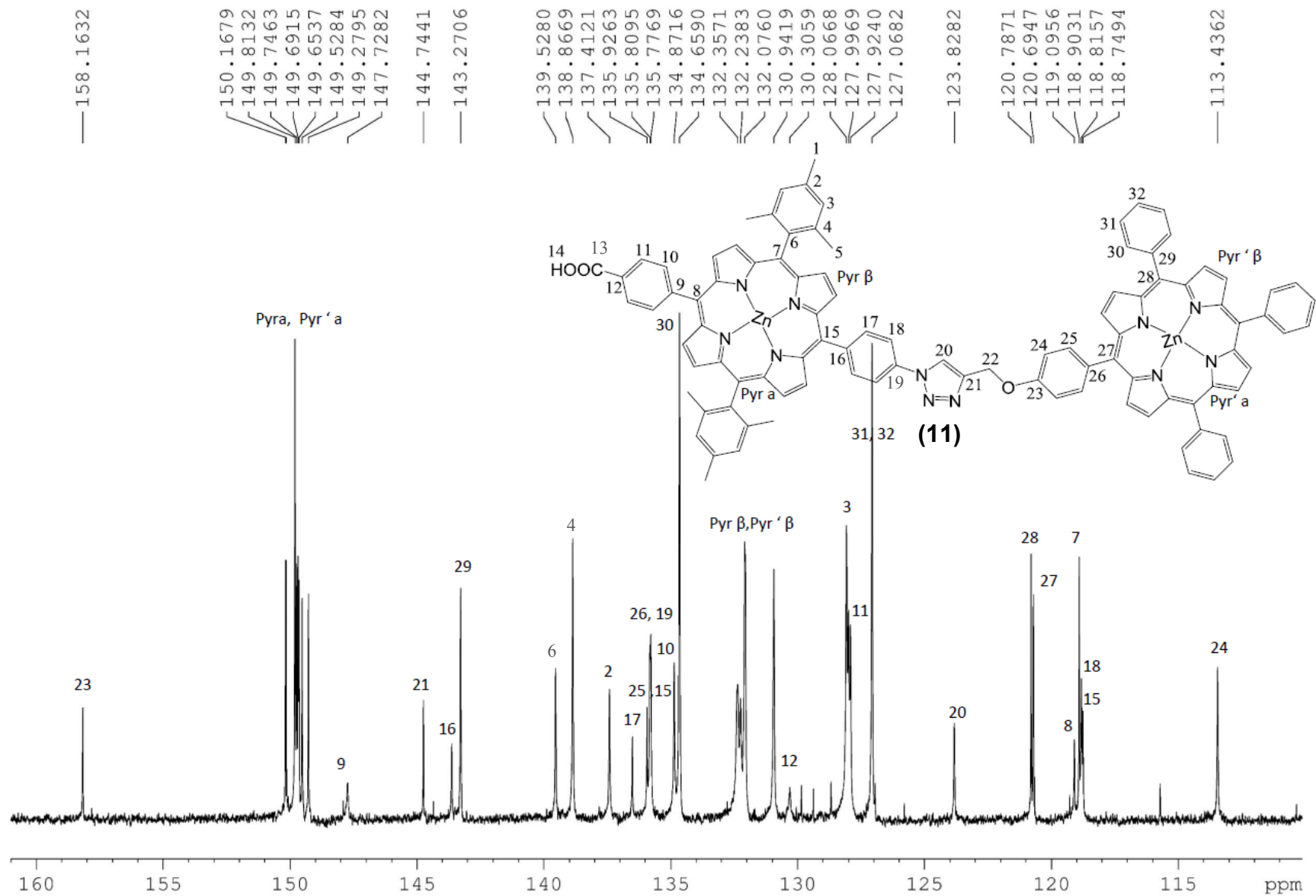


Figure S32: Focus on ^{13}C NMR spectrum of **11** (125MHz, DMSO-d_6).

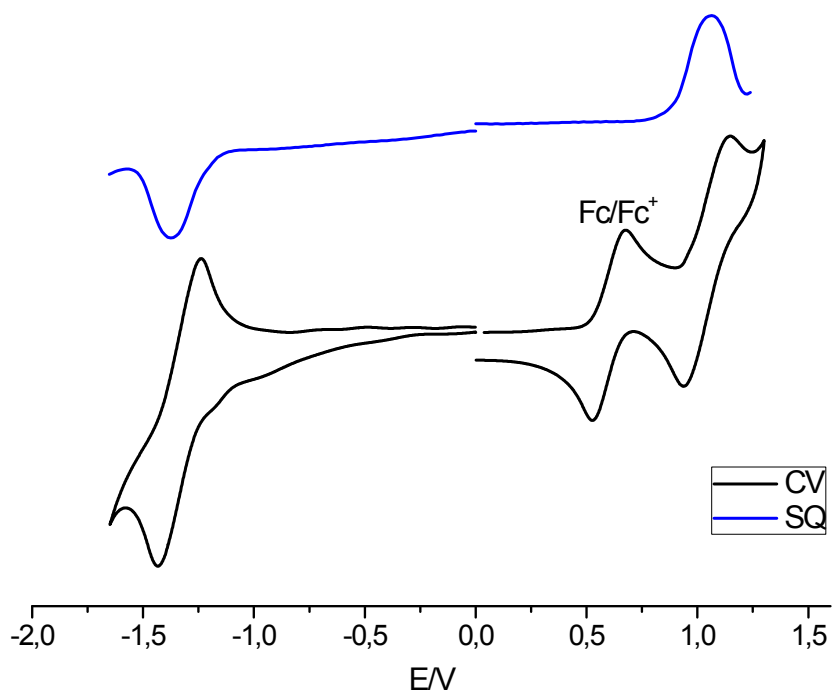
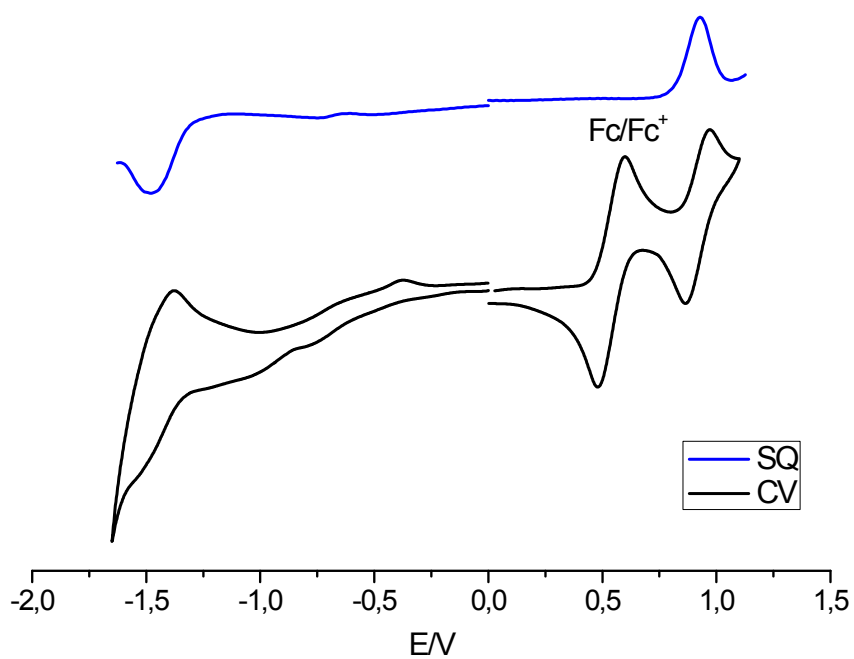


Figure S33: Cyclic and Square-wave voltammograms of **9** (upper part) and **11** (lower part).

Table S1. Coordinates of gas phase geometry optimized structure of **9** (phenyl and mesityl groups are omitted) calculated by DFT at the B3LYP/LANL2DG/6-31G(d) level. E = -3670.11707528 Hartree / particle.

Zn	-9.822080000	9.703813000	-13.982198000
N	-9.764780000	10.859364000	-12.269613000
N	-11.313316000	10.902008000	-14.772318000
C	-8.980133000	10.662673000	-11.158254000
C	-9.324920000	11.654265000	-10.156902000
H	-8.881858000	11.728902000	-9.174514000
C	-10.304549000	12.439959000	-10.689360000
H	-10.807739000	13.279869000	-10.226562000
C	-10.580114000	11.934311000	-12.013208000
C	-11.543166000	12.455966000	-12.886006000
C	-11.884255000	11.987092000	-14.158226000
C	-12.891534000	12.556494000	-15.027805000
H	-13.498792000	13.422030000	-14.793595000
C	-12.911741000	11.798472000	-16.162642000
H	-13.539215000	11.923403000	-17.036408000
C	-11.917934000	10.759230000	-15.995238000
C	-8.009158000	9.645606000	-11.005305000
H	-12.093851000	13.321310000	-12.527188000
C	-7.232274000	9.621671000	-9.726650000
C	-7.357800000	8.554002000	-8.818294000
H	-8.033988000	7.736043000	-9.050299000
C	-6.646108000	8.533859000	-7.625586000
H	-6.753102000	7.714531000	-6.921339000
C	-5.780611000	9.589136000	-7.302348000
C	-5.636964000	10.659595000	-8.192252000
H	-4.971801000	11.486822000	-7.972631000
C	-6.360473000	10.664157000	-9.388088000
H	-6.237242000	11.496846000	-10.074842000
N	-9.860577000	8.554261000	-15.702538000

N	-8.347529000	8.498331000	-13.178464000
C	-10.667501000	8.741595000	-16.795846000
C	-10.379622000	7.723460000	-17.783827000
H	-10.871000000	7.633380000	-18.744692000
C	-9.394241000	6.933035000	-17.266906000
H	-8.923506000	6.070751000	-17.722622000
C	-9.072929000	7.461133000	-15.958221000
C	-8.107792000	6.949983000	-15.085219000
C	-7.765095000	7.429840000	-13.814884000
C	-6.726064000	6.880831000	-12.976233000
H	-6.099670000	6.035686000	-13.233515000
C	-6.689424000	7.634375000	-11.839712000
H	-6.023097000	7.523100000	-10.996629000
C	-7.718129000	8.649324000	-11.965900000
C	-11.617444000	9.760747000	-16.928517000
H	-7.552547000	6.083548000	-15.434316000
H	-12.183022000	9.778239000	-17.856163000
Zn	6.334589000	1.049950000	8.174306000
N	8.175912000	0.137901000	8.416083000
N	5.838804000	0.439326000	10.088149000
C	9.149031000	0.066910000	7.449912000
C	10.265786000	-0.701413000	7.946728000
H	11.168708000	-0.919931000	7.390313000
C	9.948696000	-1.092321000	9.214022000
H	10.542999000	-1.696273000	9.884311000
C	8.632887000	-0.556542000	9.509710000
C	7.921145000	-0.745480000	10.715986000
C	6.617535000	-0.264855000	10.973991000
C	5.898835000	-0.406499000	12.226745000
H	6.274694000	-0.900631000	13.110939000
C	4.692270000	0.208960000	12.069186000
H	3.895872000	0.306090000	12.796455000

C	4.661554000	0.740656000	10.727319000
C	9.067525000	0.631883000	6.173734000
C	8.601034000	-1.514651000	11.804524000
C	8.101081000	-2.758429000	12.226894000
H	7.215364000	-3.164018000	11.746871000
C	8.731590000	-3.478612000	13.238458000
H	8.338821000	-4.440317000	13.549741000
C	9.882371000	-2.965368000	13.852658000
C	10.389275000	-1.725642000	13.440105000
H	11.276729000	-1.337003000	13.928817000
C	9.756266000	-1.010972000	12.428512000
H	10.148618000	-0.046689000	12.119370000
H	9.928580000	0.479481000	5.528595000
N	4.494478000	1.963160000	7.933366000
N	6.831238000	1.661352000	6.261265000
C	3.523545000	2.037758000	8.900641000
C	2.412195000	2.816729000	8.409110000
H	1.512002000	3.039889000	8.968121000
C	2.731299000	3.211809000	7.143468000
H	2.142123000	3.823864000	6.476271000
C	4.041422000	2.665879000	6.842571000
C	4.747950000	2.848990000	5.631735000
C	6.048220000	2.358381000	5.372578000
C	6.761339000	2.487636000	4.115913000
H	6.379203000	2.971316000	3.228760000
C	7.969436000	1.874609000	4.274041000
H	8.762528000	1.769790000	3.544175000
C	8.005453000	1.354847000	5.620111000
C	3.602449000	1.467509000	10.175620000
C	4.069205000	3.622209000	4.546327000
C	4.580072000	4.852723000	4.102931000
H	5.481637000	5.252520000	4.557933000

C	3.941453000	5.575559000	3.101066000
H	4.354356000	6.531334000	2.783288000
C	2.765775000	5.090697000	2.506324000
C	2.242693000	3.860490000	2.933215000
H	1.341307000	3.477509000	2.476453000
C	2.895681000	3.149319000	3.938655000
H	2.484945000	2.194646000	4.254928000
H	2.740865000	1.619426000	10.820147000
O	-5.134317000	9.480895000	-6.103364000
C	10.596887000	-3.687737000	14.936002000
O	11.598423000	-3.288654000	15.497528000
O	10.017445000	-4.873501000	15.258515000
H	10.569241000	-5.248571000	15.969833000
N	-3.031038000	9.230753000	-2.545616000
N	-2.734036000	10.544327000	-2.454492000
C	-3.628964000	8.953577000	-3.733350000
C	-3.694590000	10.173936000	-4.370174000
N	-3.139616000	11.116736000	-3.557574000
C	-4.246945000	10.524889000	-5.715007000
H	-3.964303000	7.967211000	-4.011316000
H	-4.771208000	11.488359000	-5.659079000
H	-3.441834000	10.627838000	-6.458230000
N	2.172431000	5.882920000	1.499917000
H	2.671179000	6.734672000	1.281166000
C	1.015258000	5.658028000	0.787231000
O	0.290173000	4.685053000	0.946260000
C	0.702650000	6.728339000	-0.260981000
H	1.019245000	6.327698000	-1.234617000
H	1.288146000	7.641626000	-0.092405000
C	-0.796672000	7.051628000	-0.304901000
H	-1.345755000	6.106023000	-0.376351000
H	-1.093854000	7.511645000	0.647673000

C	-1.168030000	7.980952000	-1.465654000
H	-0.910620000	7.509170000	-2.423561000
H	-0.599380000	8.917268000	-1.409845000
C	-2.661981000	8.327320000	-1.459838000
H	-3.276060000	7.426947000	-1.558823000
H	-2.937442000	8.821408000	-0.523437000

Table S2. Coordinates of gas phase geometry optimized structure of **11** (phenyl and mesityl groups are omitted) calculated by DFT at the B3LYP/LANL2DG/6-31G(d) level. E = -3344.15685811 Hartree / particle.

Zn	-10.919700000	2.644190000	-0.227194000
N	-9.432534000	4.079207000	-0.272164000
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H	-13.320702000	7.063724000	1.415812000
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H	-15.258517000	5.186867000	1.439335000
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C	-7.530907000	2.685113000	-1.041058000
H	-10.727049000	7.036082000	0.792451000
C	-6.075340000	2.701128000	-1.388764000
C	-5.137928000	1.980714000	-0.625569000
H	-5.478726000	1.411271000	0.234452000
C	-3.785786000	1.992719000	-0.944214000
H	-3.063677000	1.441214000	-0.349992000
C	-3.328024000	2.730354000	-2.045299000
C	-4.241931000	3.453333000	-2.819698000
H	-3.918879000	4.025584000	-3.681809000
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H	-6.301374000	3.990141000	-3.096254000
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C	-14.430866000	0.135816000	0.030828000
H	-15.481371000	-0.007877000	0.251306000
C	-13.530980000	-0.790738000	-0.410348000
H	-13.702463000	-1.839213000	-0.620318000
C	-12.261828000	-0.110266000	-0.555478000
C	-11.067780000	-0.692284000	-0.991951000
C	-9.822029000	-0.071751000	-1.147789000
C	-8.631224000	-0.720828000	-1.642927000
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C	-8.217918000	1.455971000	-1.170899000
C	-14.274061000	2.603106000	0.581051000
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C	10.885012000	-3.231779000	-0.736265000
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H	13.045055000	2.598757000	3.455383000

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C	15.884576000	-2.842892000	3.862904000
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C	16.790748000	-2.819842000	1.617885000
H	17.629261000	-2.994778000	0.951742000
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H	15.457060000	-2.147632000	0.071641000
H	9.562898000	-4.263743000	-2.023781000
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N	8.673858000	-1.144734000	-1.019898000
C	9.385456000	2.376201000	1.249276000
C	8.391768000	3.416025000	1.125504000
H	8.440995000	4.385590000	1.605170000
C	7.421353000	2.942692000	0.292492000
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C	7.083783000	0.754149000	-0.965430000
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H	5.764880000	-1.219322000	-2.649161000
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H	4.802561000	1.296508000	0.428601000
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C	18.272368000	-3.574412000	3.452869000
O	19.228677000	-3.792290000	2.734994000
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H	19.221082000	-4.104506000	4.977896000
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C	0.832846000	2.565069000	-2.481183000
C	0.025447000	3.209310000	-3.387478000
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H	0.612875000	2.025977000	-1.575437000
H	-1.696671000	4.480593000	-3.274461000
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