Electronic Supplementary Material (ESI) for RSC Advances.

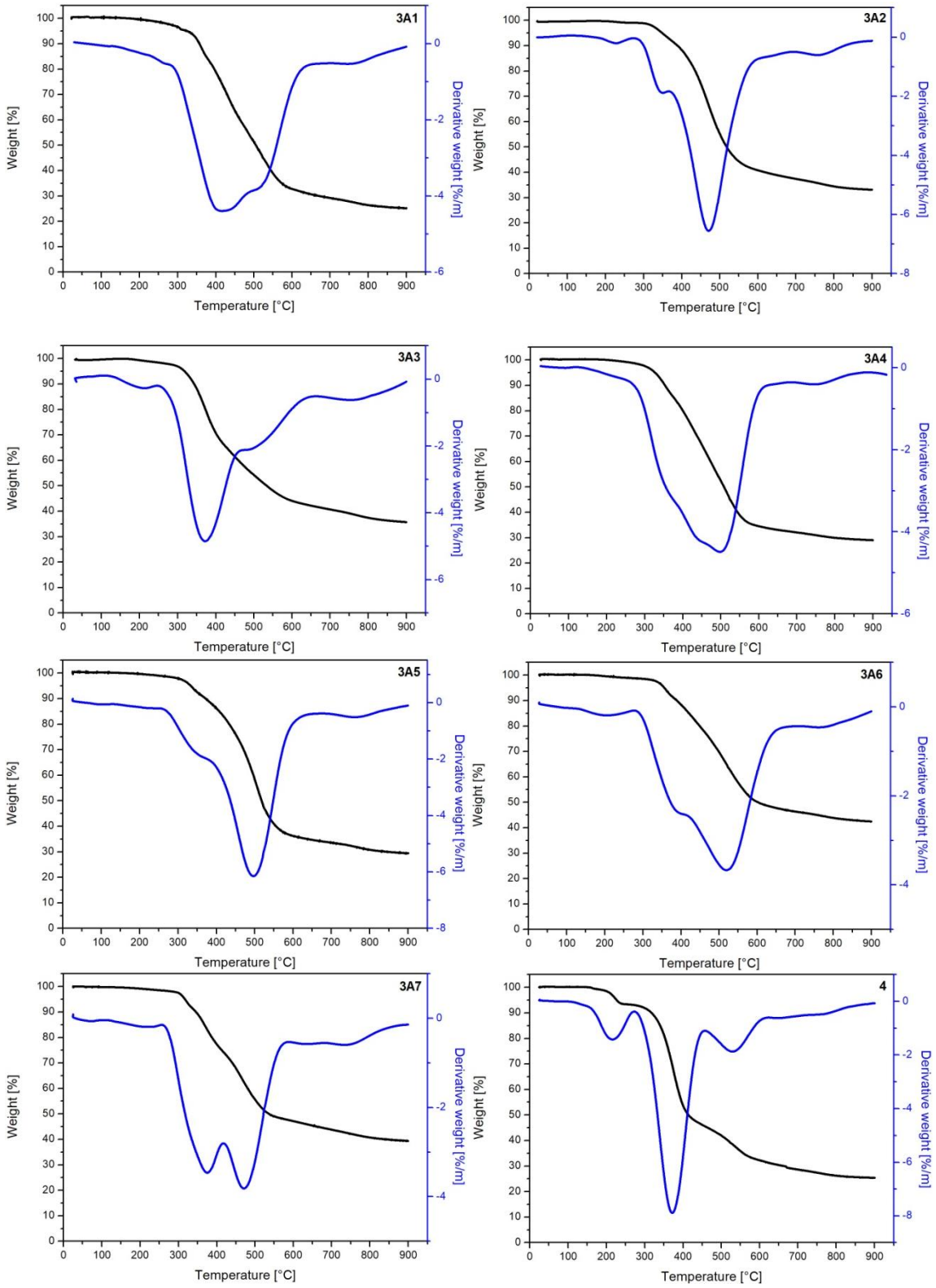


Figure S1. TGA and DTG curves of **3A1**-**3A7** and **4**.

Table S1. Wavelength maxima [nm] of absorption spectra together with oscillator strengths calculated for **3A2-3A6** molecules with the TD-DFT method.

Code	Calculated wavelengths [nm] (oscillator strengths)	Transitions
3A2	351.34 (0.31)	HOMO->LUMO (98%)
	297.56 (0.15)	H-1->LUMO (83%)
	287.98 (0.28)	HOMO->L+2 (91%)
	283.38 (0.17)	H-4->LUMO (14%), H-3->L+1 (45%), H-2->LUMO (17%)
	280.88 (0.98)	H-3->L+1 (16%), H-2->LUMO (63%)
	263.40 (0.16)	H-1->L+1 (69%)
	262.16 (0.15)	H-7->LUMO (10%), H-2->L+1 (67%)
	256.98 (0.12)	HOMO->L+4 (32%), HOMO->L+5 (16%), HOMO->L+6 (20%)
	251.04 (0.23)	H-1->L+2 (86%)
3A3	304.66 (1.02)	HOMO->LUMO (95%)
	299.31 (0.13)	H-1->LUMO (84%)
	269.37 (0.65)	H-4->LUMO (17%), H-2->LUMO (50%), H-1->L+1 (11%), HOMO->L+2 (10%)
	253.48 (0.19)	H-1->L+2 (67%), H-1->L+3 (22%)
	250.30 (0.19)	H-5->L+1 (17%), H-2->L+1 (54%)
	248.10 (0.04)	HOMO->L+3 (72%)
3A4	352.97 (0.49)	HOMO->LUMO (97%)
	308.80 (1.17)	HOMO->L+2 (89%)
	297.99 (0.15)	H-1->LUMO (84%)
	279.82 (0.49)	H-5->L+1 (10%), H-2->LUMO (71%)
	262.91 (0.15)	H-2->L+1 (61%)
	252.92 (0.23)	H-1->L+2 (50%), H-1->L+3 (39%)
	244.36 (0.11)	H-9->L+1 (11%), H-7->L+1 (43%)
3A5	381.65 (0.19)	HOMO->LUMO (98%)
	307.01 (0.22)	HOMO->L+2 (51%), HOMO->L+3 (40%)
	299.04 (0.13)	H-3->LUMO (80%)
	292.92 (0.34)	HOMO->L+4 (35%), HOMO->L+7 (24%)
	288.29 (0.96)	H-2->LUMO (68%), H-1->L+3 (10%)
	273.39 (0.29)	H-1->L+2 (49%), HOMO->L+6 (16%), HOMO->L+7 (13%)
	266.99 (0.28)	H-4->LUMO (51%), H-1->L+3 (15%)
	266.16 (0.15)	H-4->L+1 (12%), H-2->L+1 (69%)
	264.17 (0.36)	H-3->L+1 (24%), H-1->L+3 (37%), HOMO->L+7 (21%)
	263.51 (0.15)	H-8->L+1 (10%), H-4->LUMO (21%), H-3->L+1 (50%)
3A6	341.99 (0.32)	HOMO->LUMO (96%)
	302.68 (0.13)	H-2->LUMO (33%), H-1->LUMO (30%), HOMO->L+1 (23%)
	302.27 (0.12)	H-2->LUMO (18%), H-1->LUMO (49%), HOMO->L+1 (16%)
	287.29 (1.20)	H-3->LUMO (40%), HOMO->L+3 (30%), HOMO->L+4 (11%)
	281.30 (0.10)	H-3->LUMO (37%), HOMO->L+3 (31%)
	267.69 (0.11)	H-1->L+2 (13%), HOMO->L+4 (30%), HOMO->L+5 (25%)
	264.57 (0.33)	H-1->L+2 (16%), HOMO->L+5 (22%)
	252.78 (0.22)	H-2->L+2 (41%), H-2->L+3 (43%)

	246.15 (0.27)	H-3->L+2 (25%), H-1->L+3 (10%), H-1->L+4 (23%), HOMO->L+8 (14%)

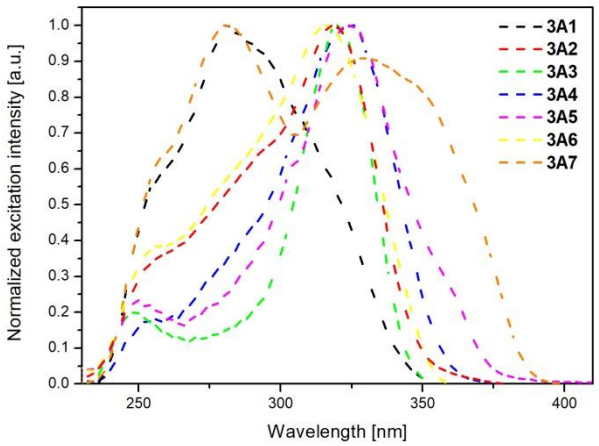
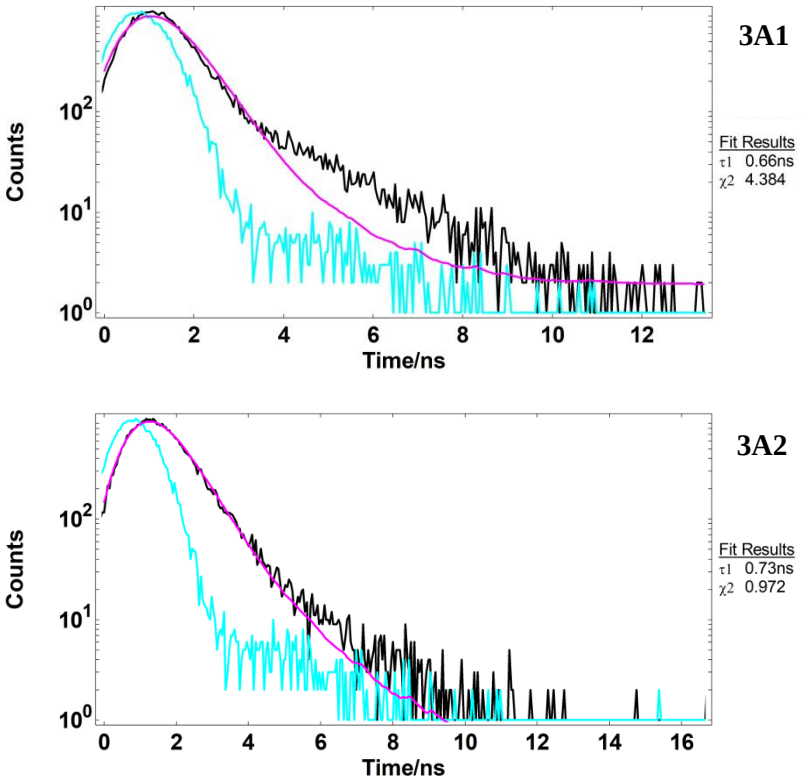
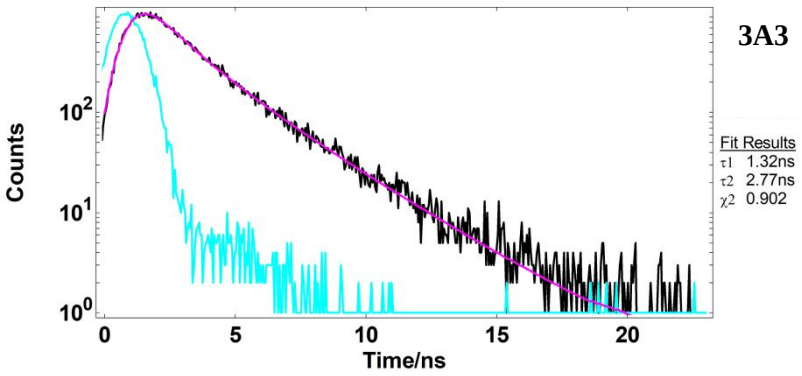


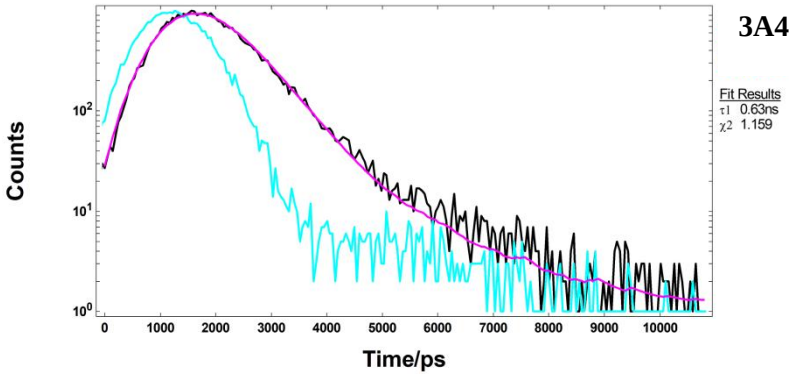
Figure S2. Normalized excitation spectra of **3A1**-**3A7**.



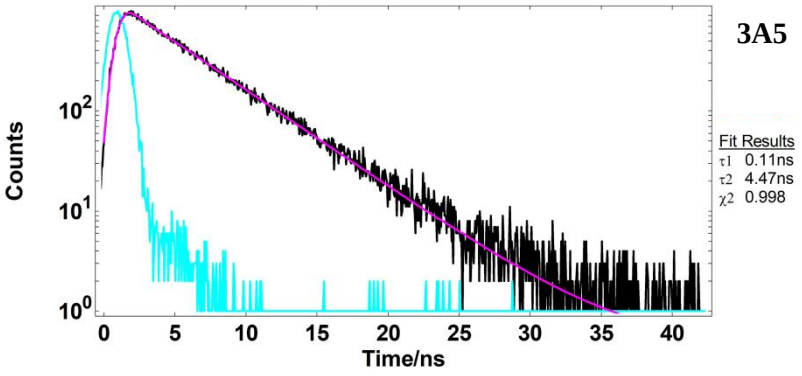
3A3



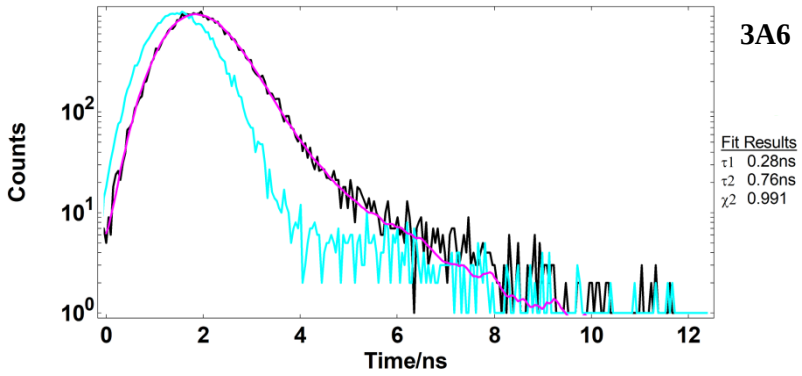
3A4



3A5



3A6



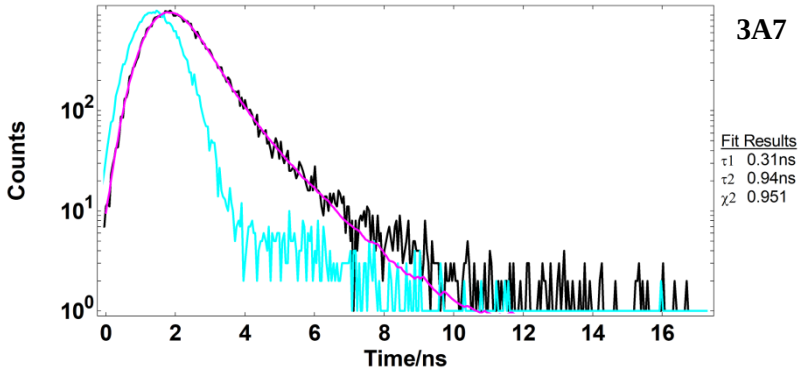
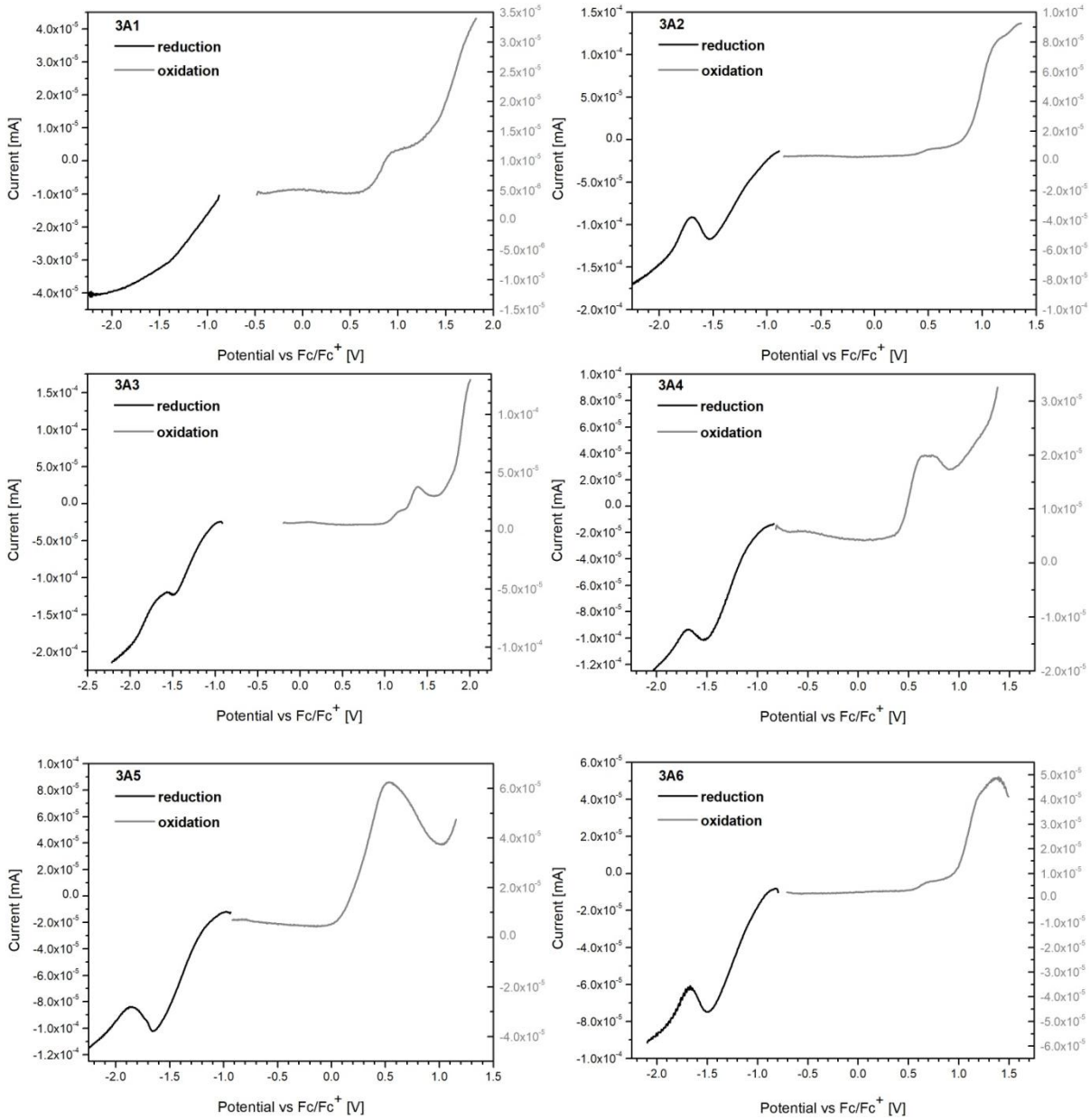


Figure S3. Decay curves of compounds **3A1**-**3A7** in chloroform solution.



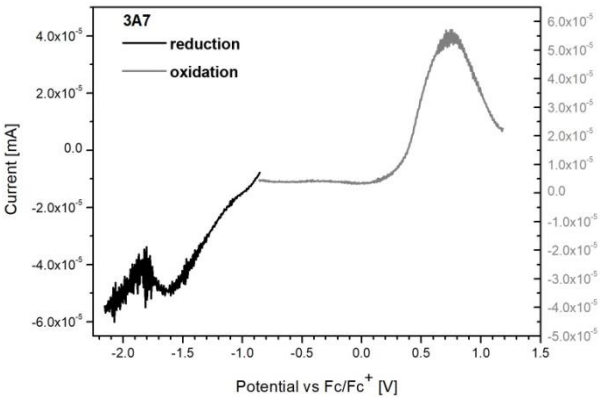
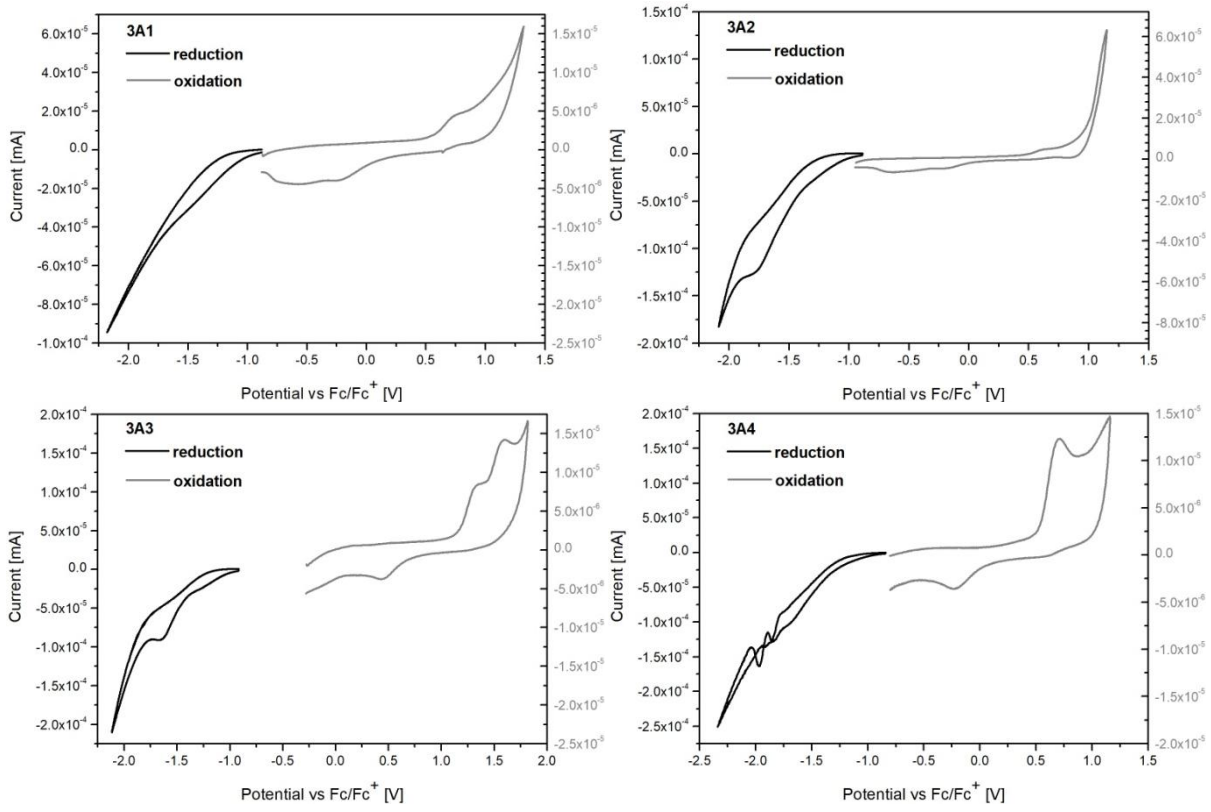


Figure S4. Differential pulse voltammetry (DPV) reduction and oxidation of **3A1-3A7**.



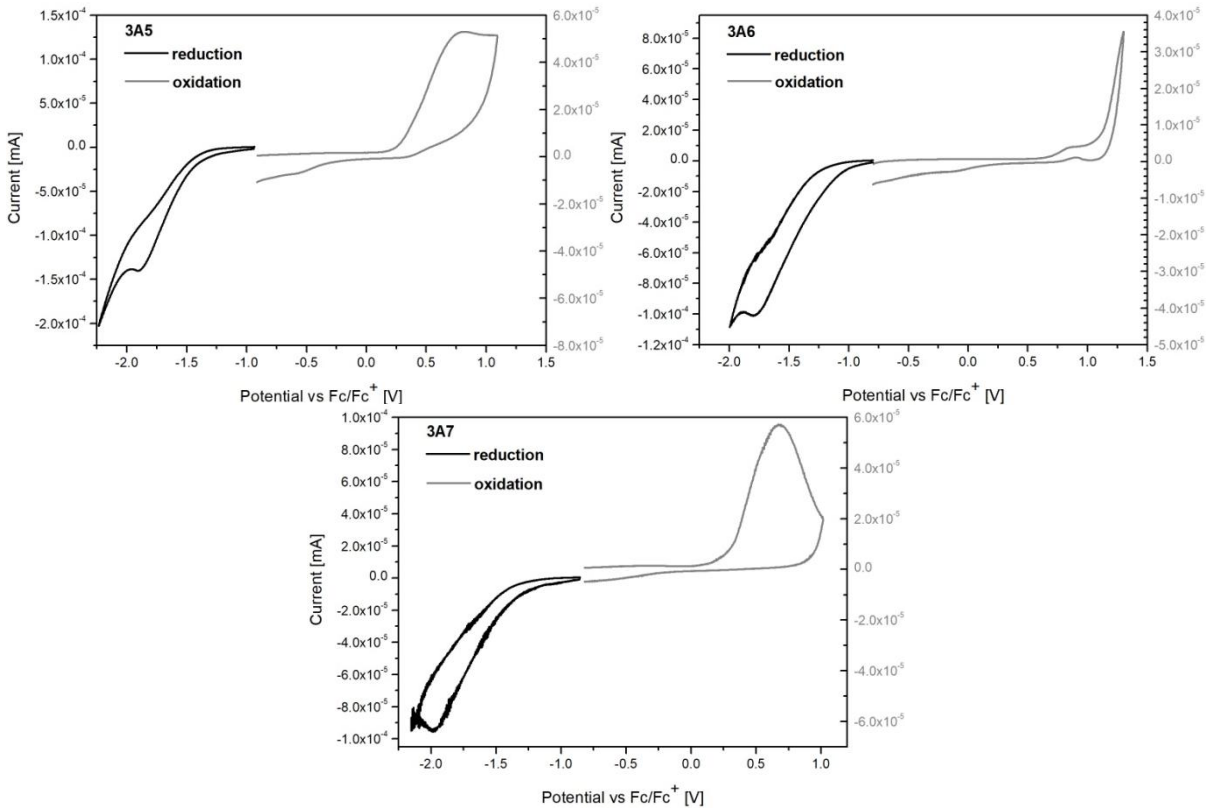


Figure S5. Cyclic voltammetry (CV) reduction and oxidation of **3A1-3A7**.

^{1}H NMR and ^{13}C NMR spectra of target compounds 3A1-3A7 and 4

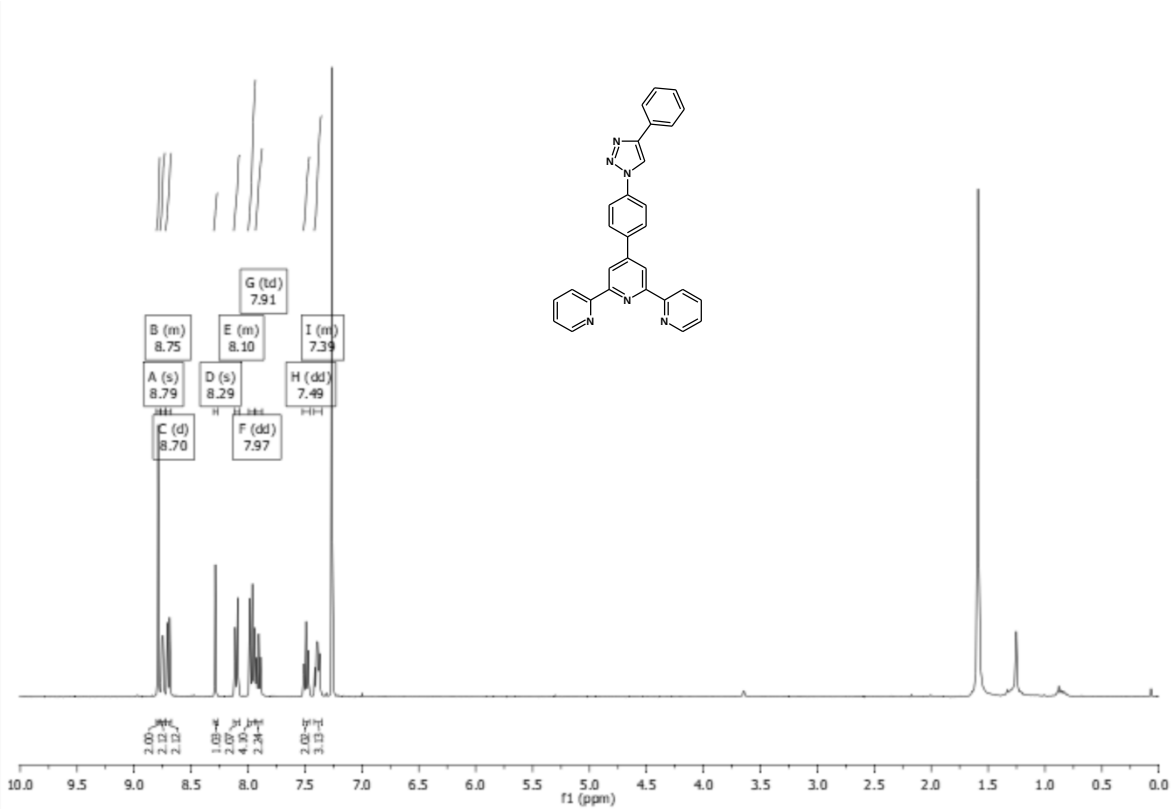


Figure S6. ^{1}H NMR plot of **3A1**.

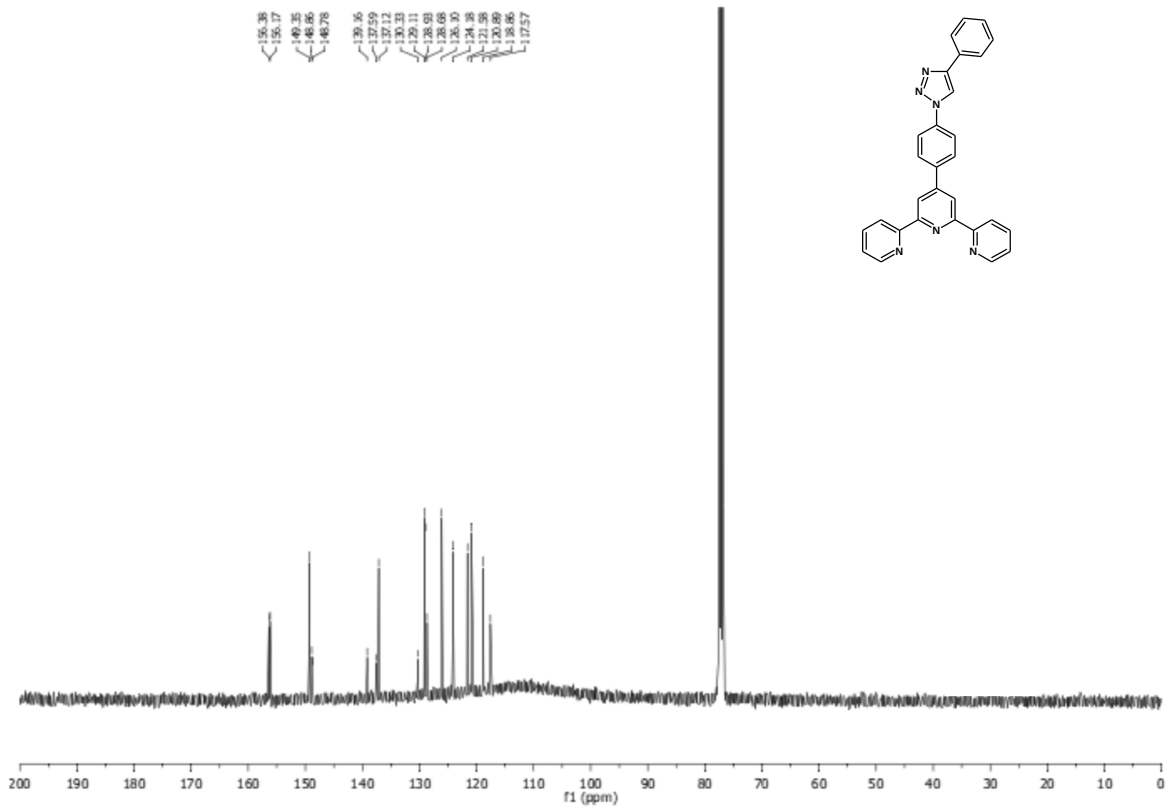


Figure S7. ^{13}C NMR plot of **3A1**.

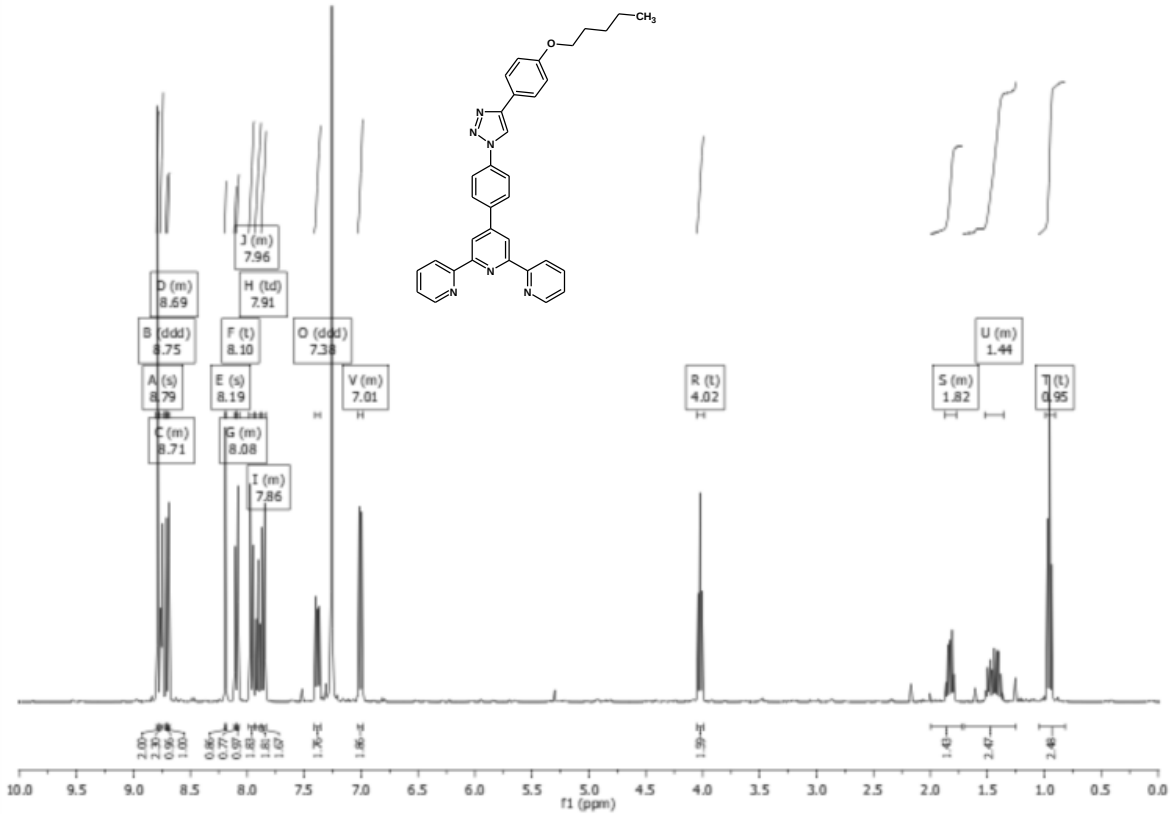


Figure S8. ^{1}H NMR plot of **3A2**.

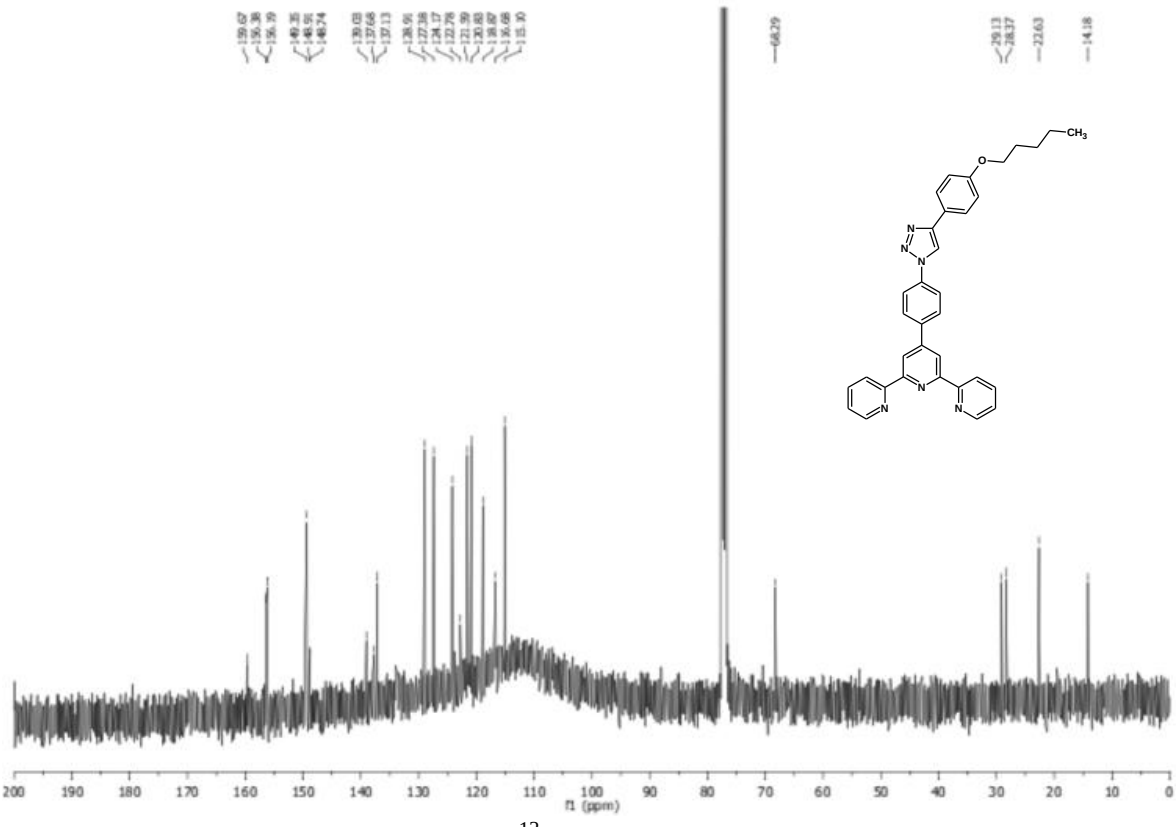


Figure S9. ^{13}C NMR plot of **3A2**.

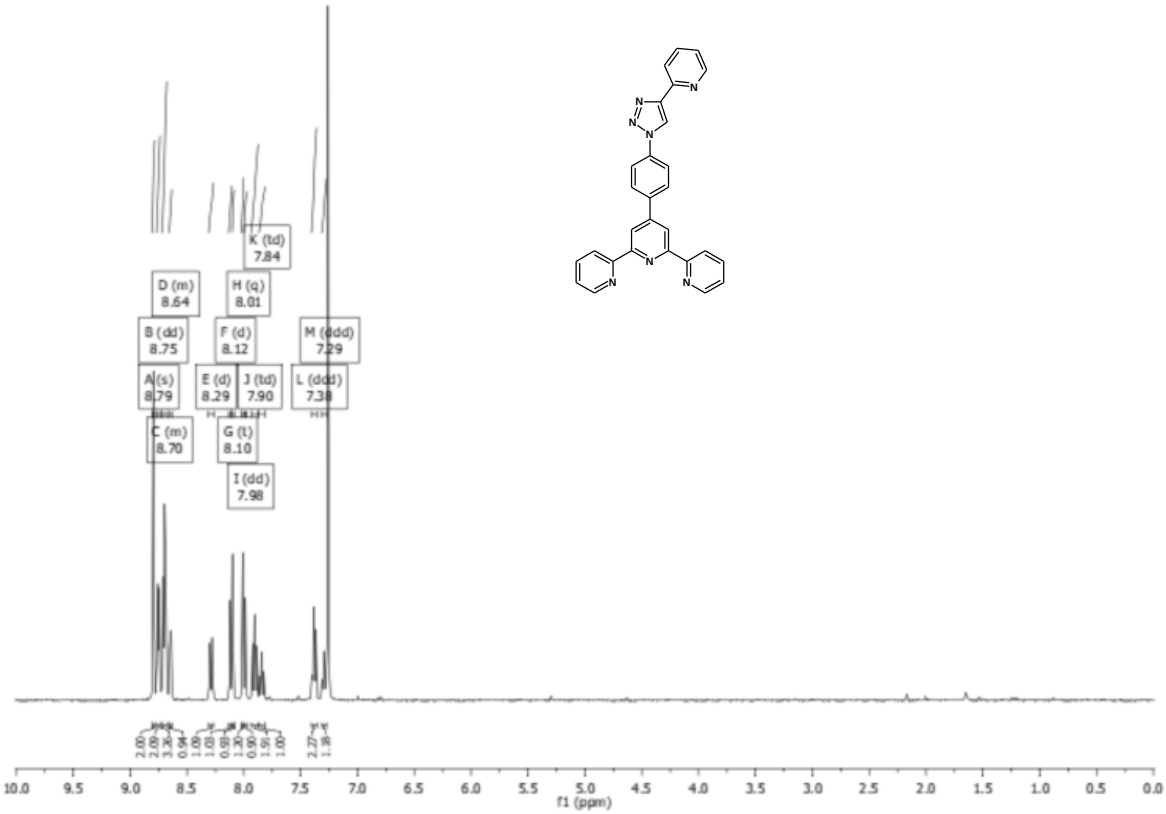


Figure S10. ^{1}H NMR plot of **3A3**.

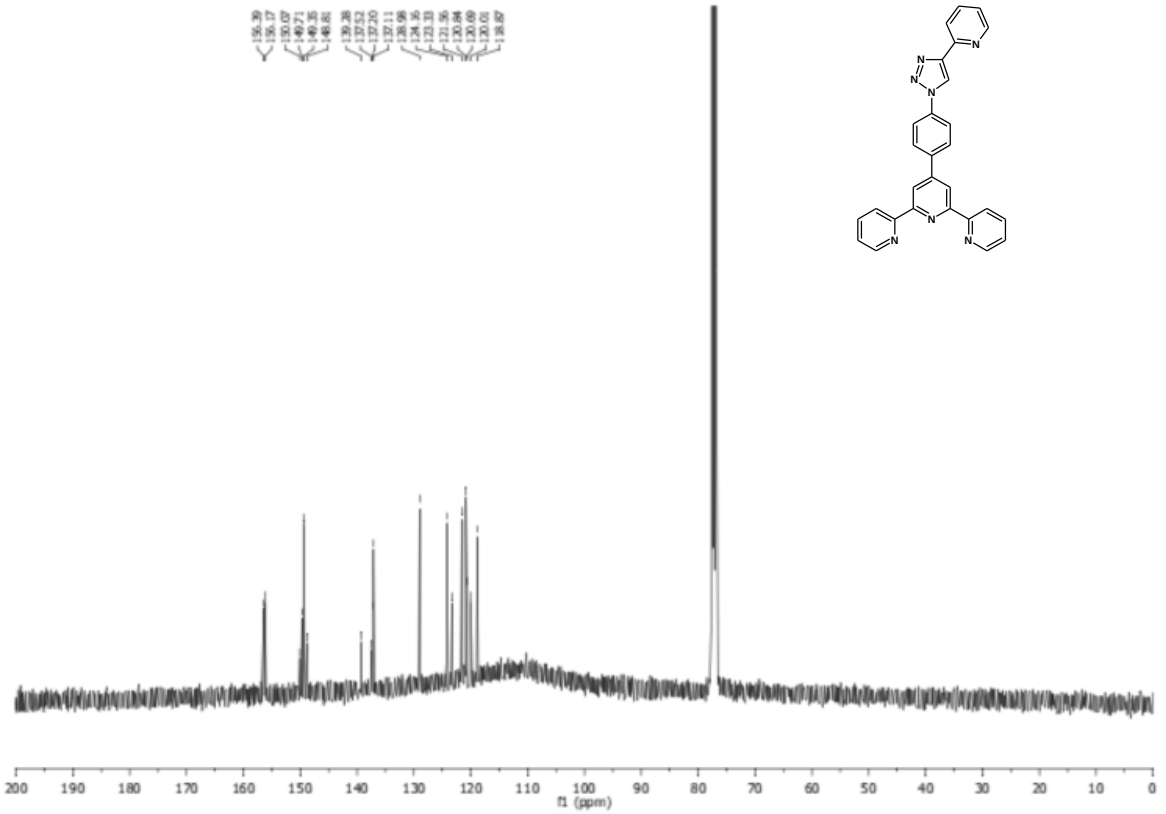


Figure S11. ^{13}C NMR plot of **3A3**.

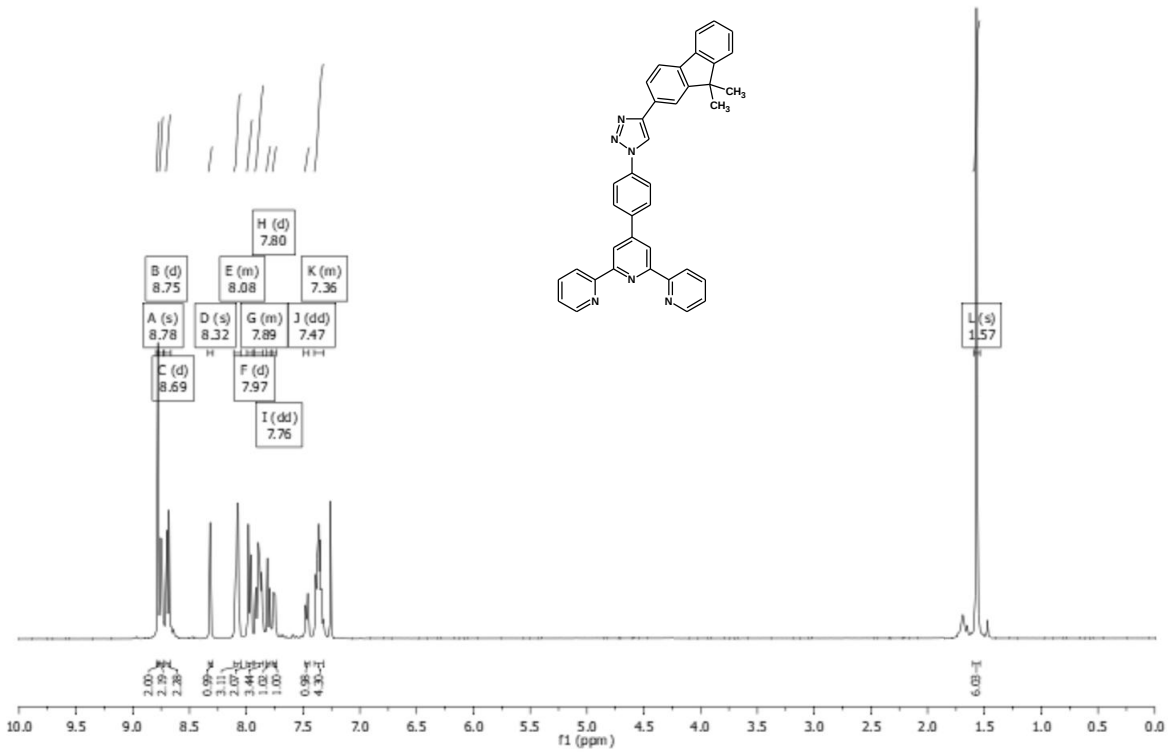


Figure S12. ^{1}H NMR plot of **3A4**.

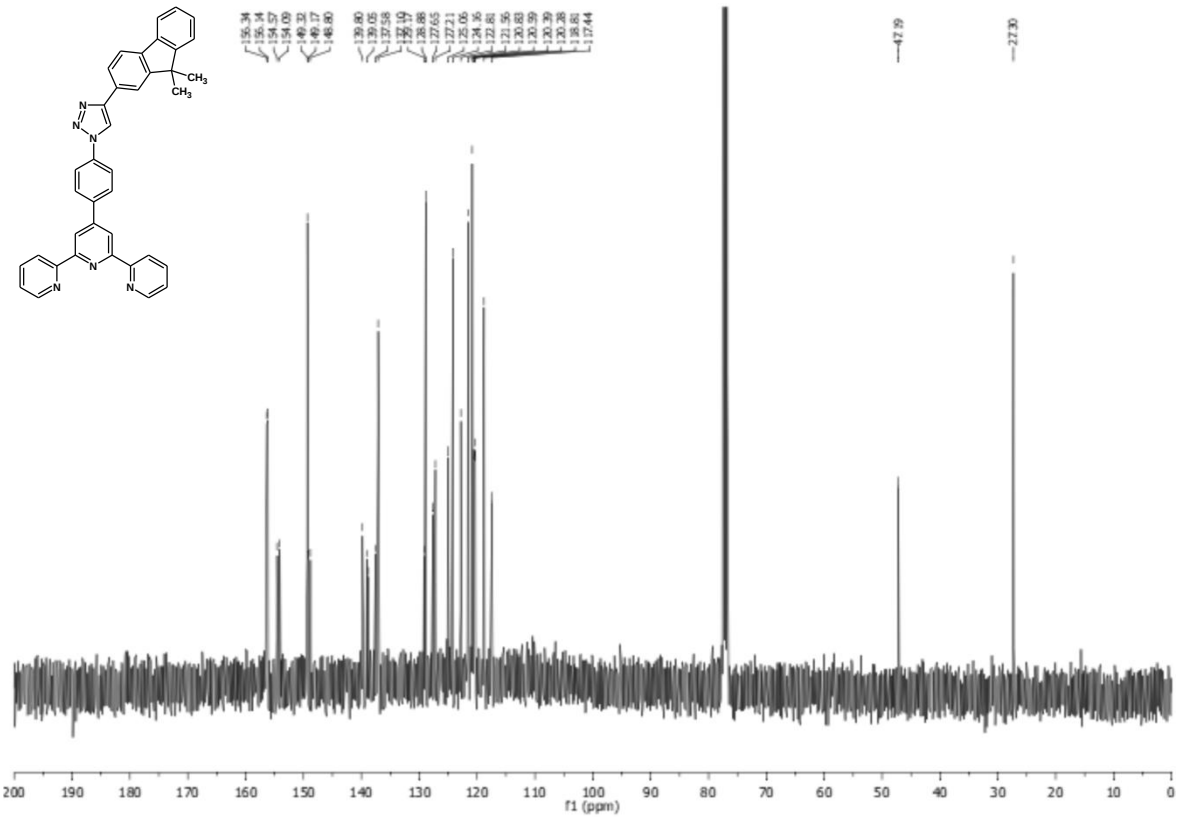


Figure S13. ^{13}C NMR plot of **3A4**.

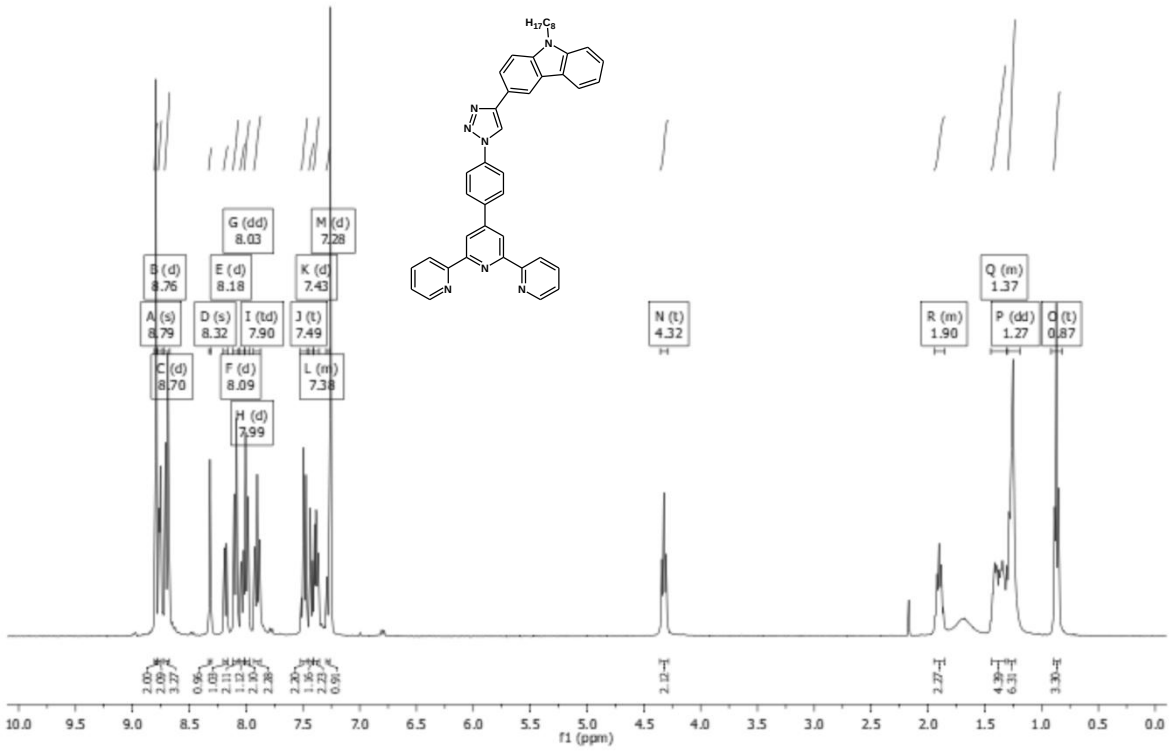


Figure S14. ^{1}H NMR plot of **3A5**.

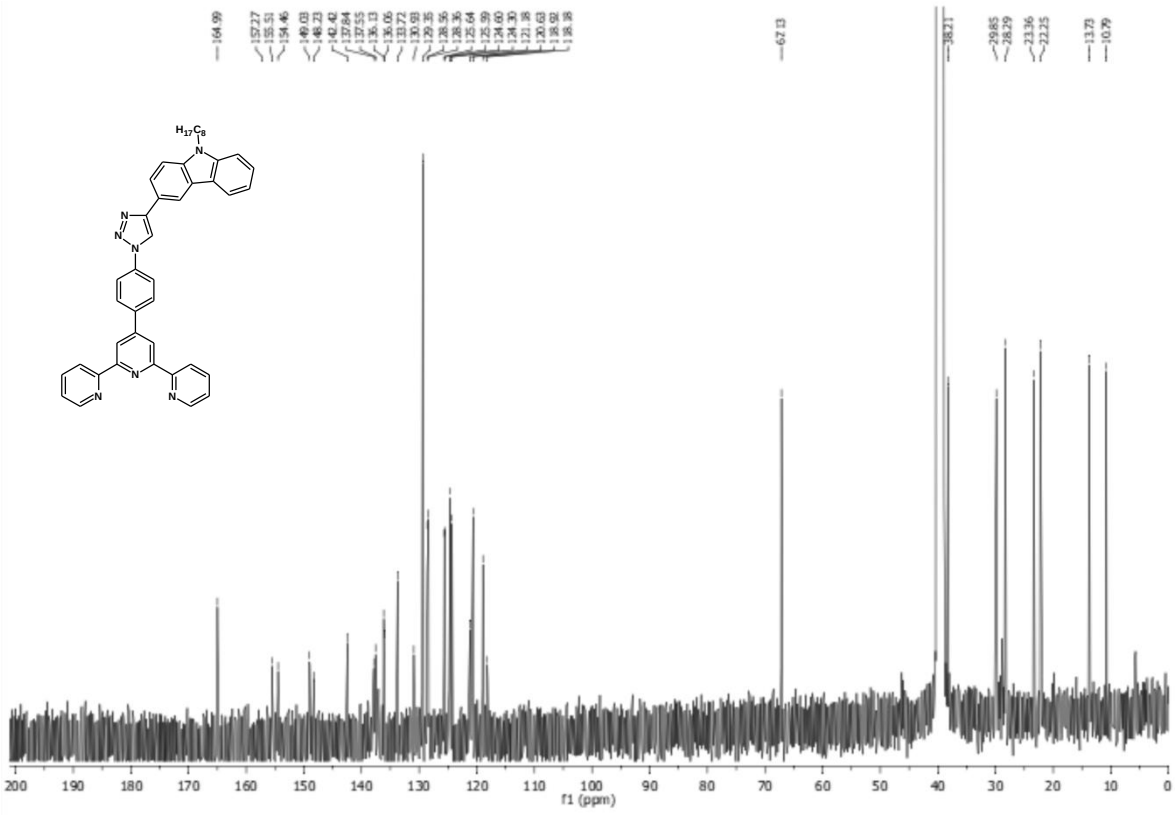


Figure S15. ^{13}C NMR plot of **3A5**.

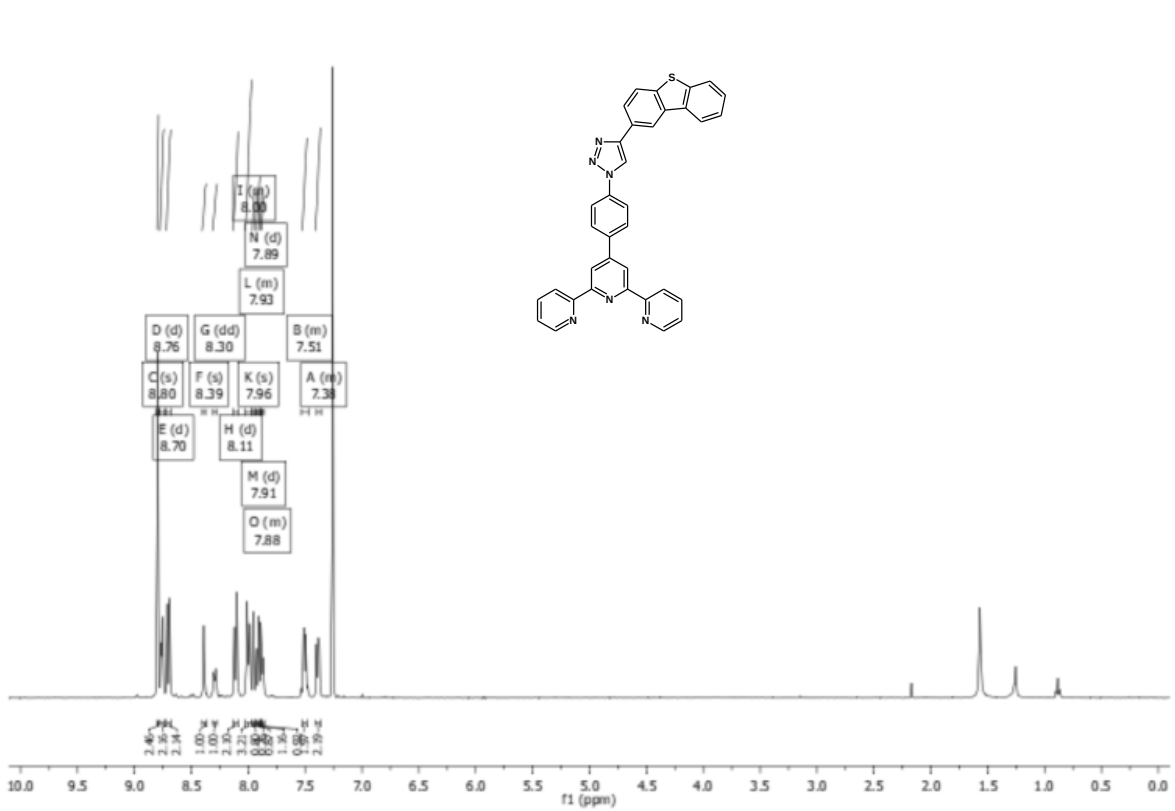


Figure S16. ^{1}H NMR plot of **3A6**.

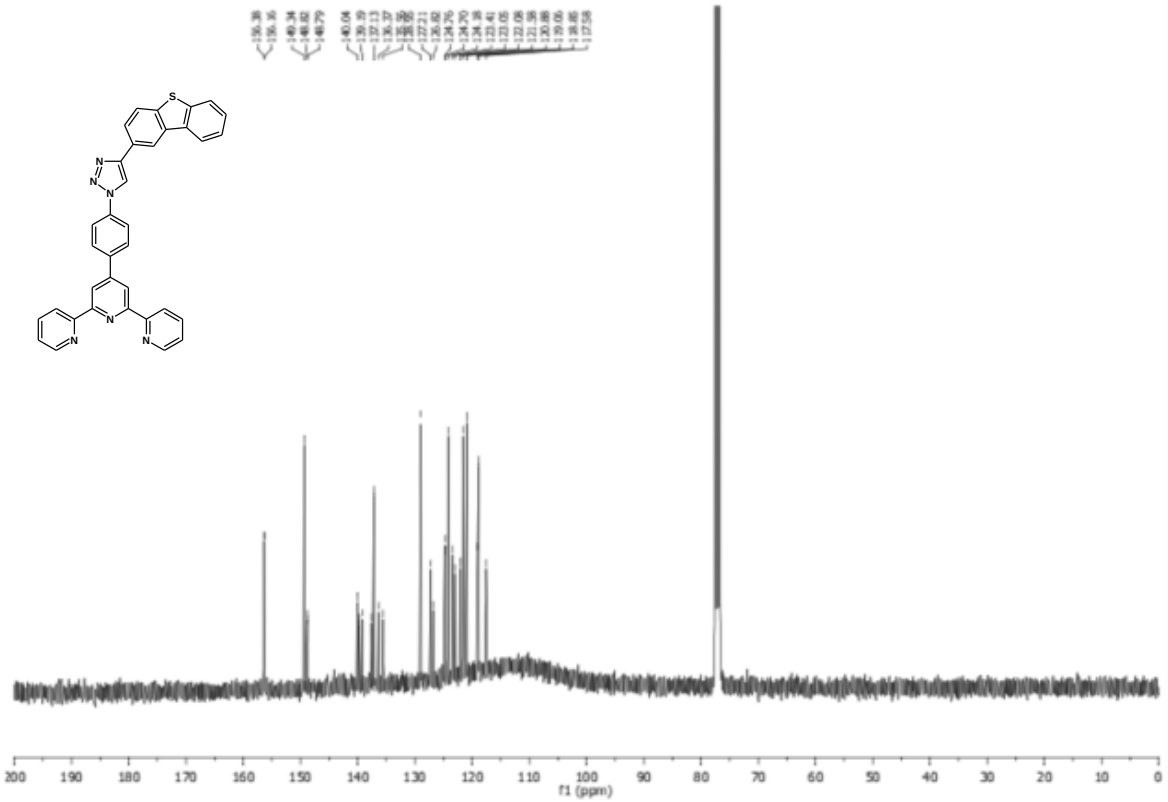


Figure S17. ^{13}C NMR plot of **3A6**.

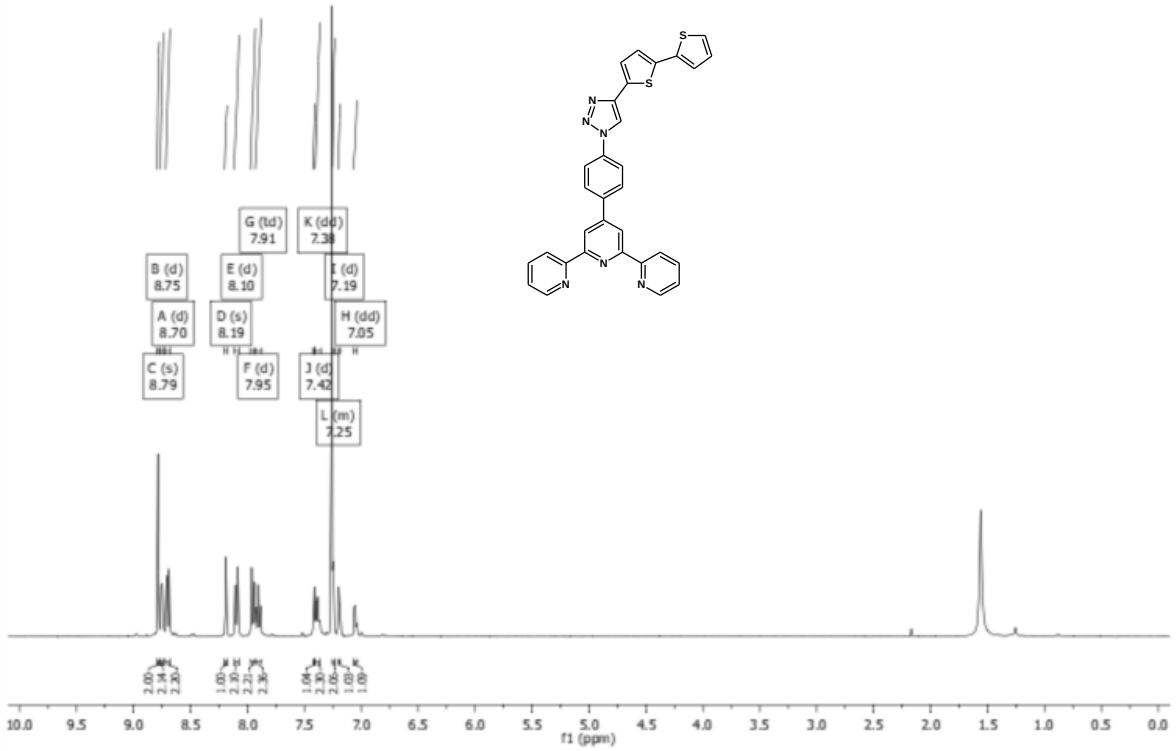


Figure S18. ^{1}H NMR plot of **3A7**.

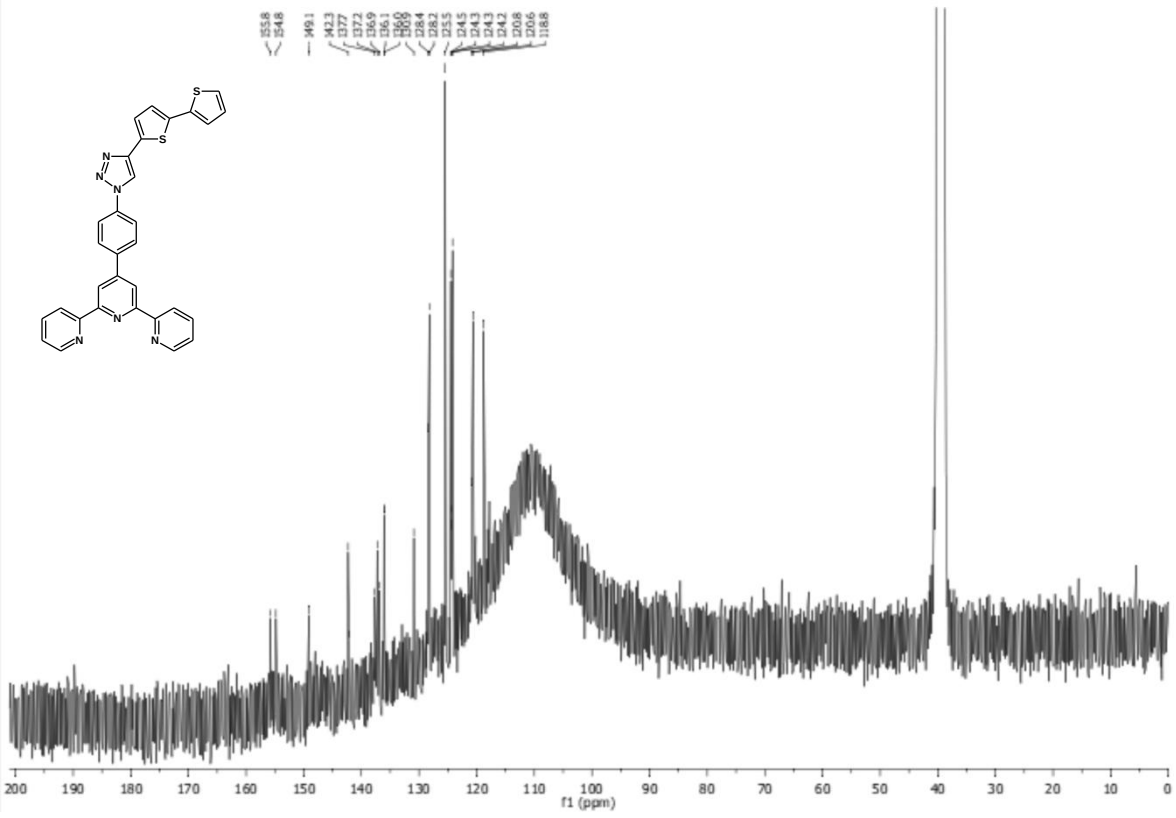


Figure S19. ^{13}C NMR plot of **3A7**.

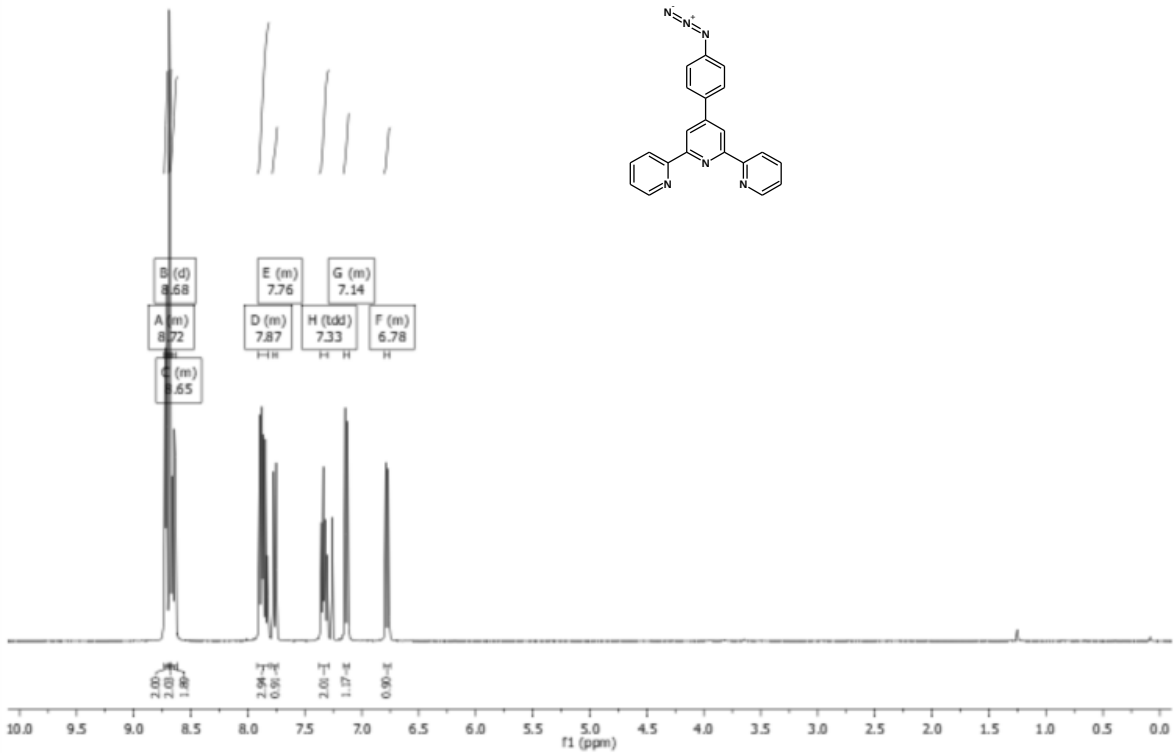


Figure S20. ^{1}H NMR plot of **4**.

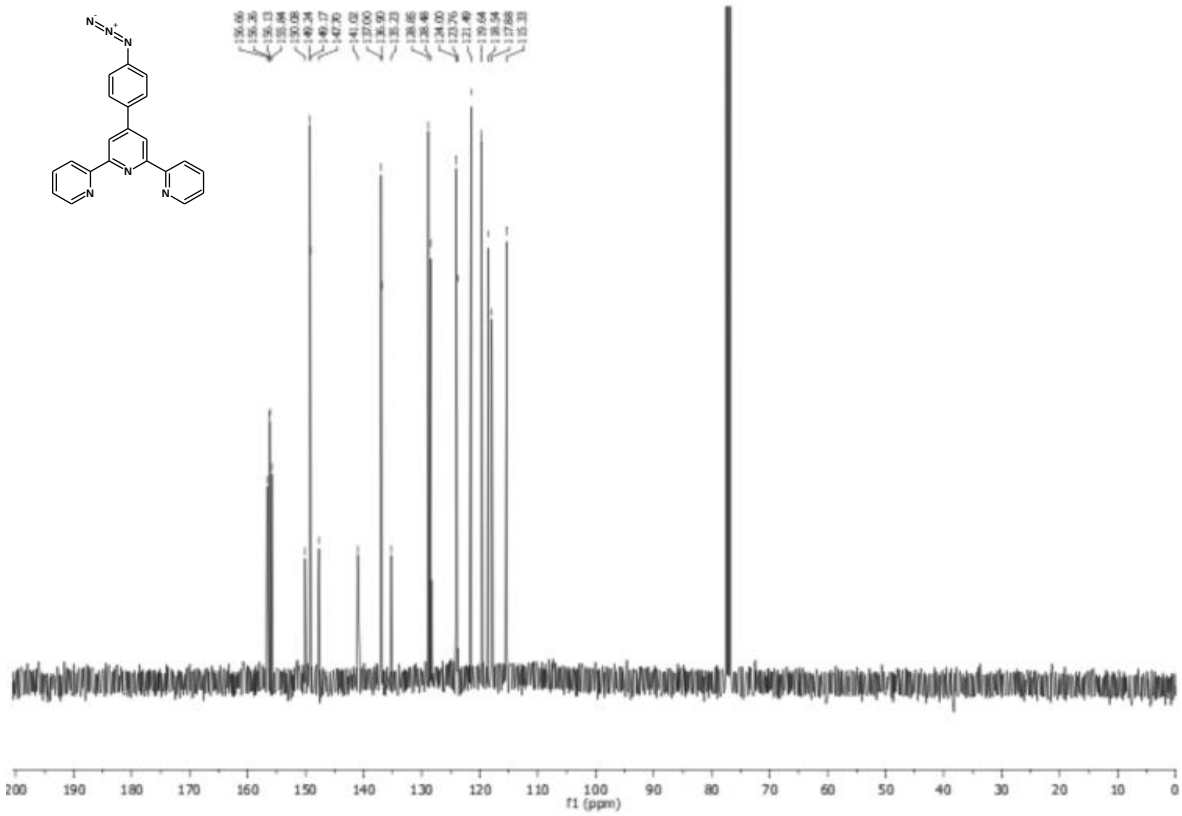


Figure S21. ^{13}C NMR plot of **4**.

MS spectra of target compounds 3A1-3A7 and 4

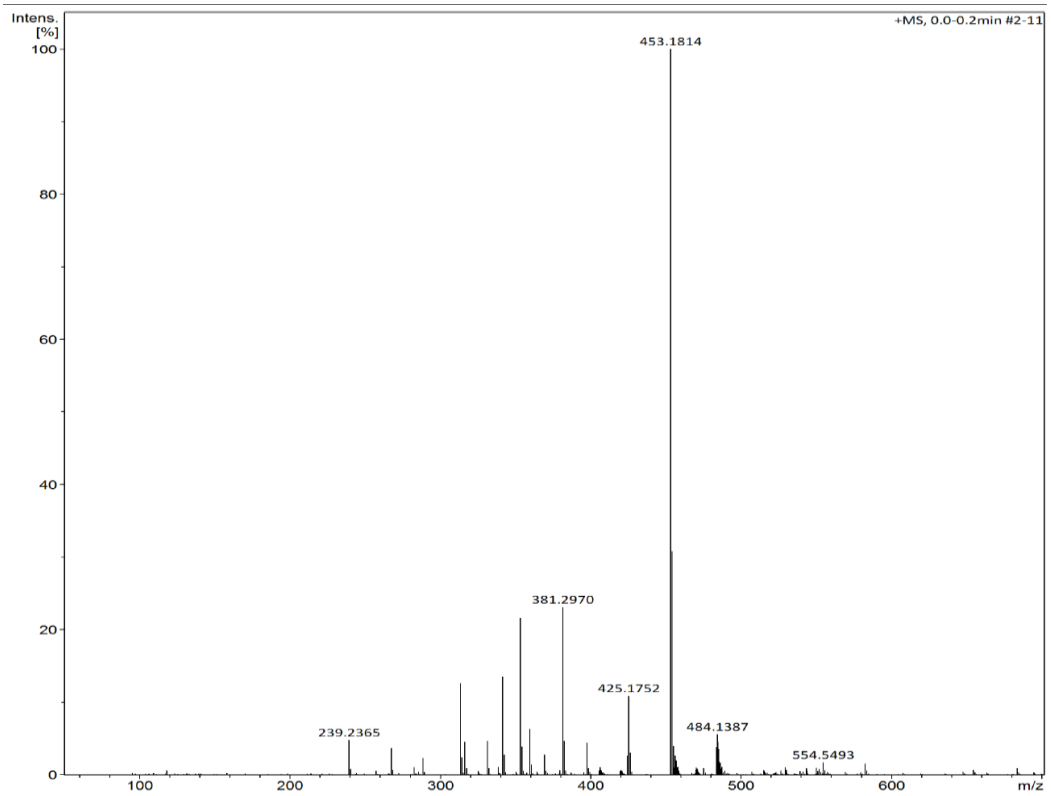


Figure S22. MS spectrum of **3A1**.

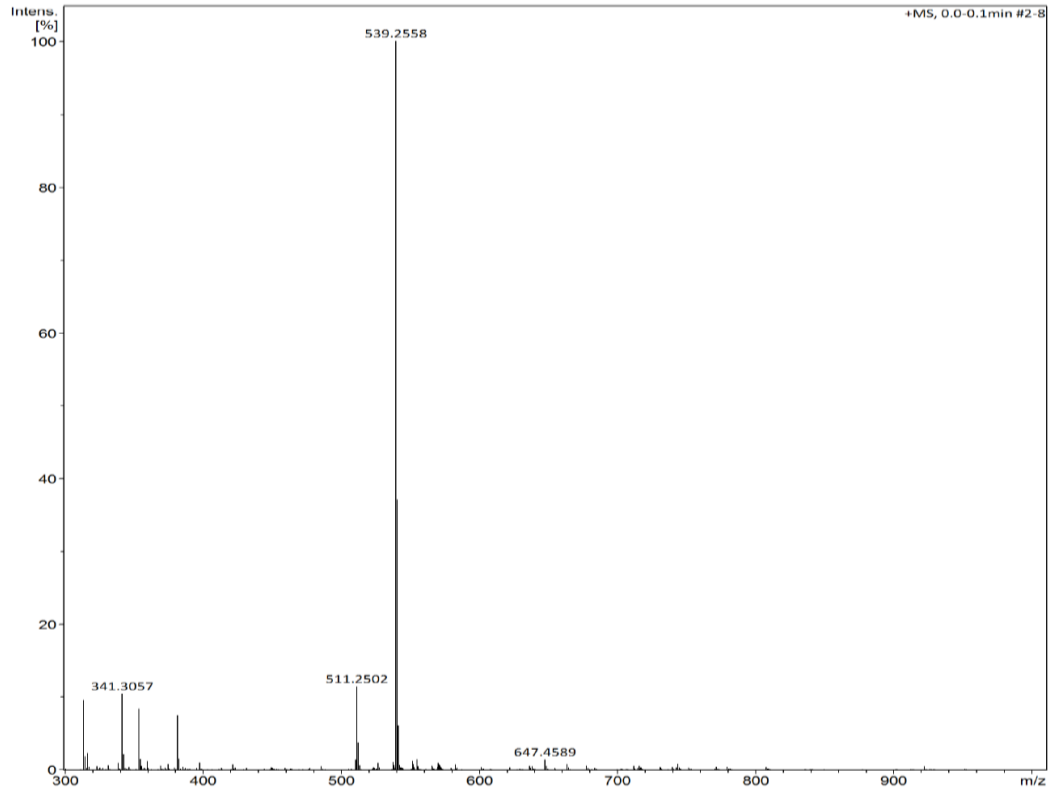


Figure S23. MS spectrum of **3A2**.

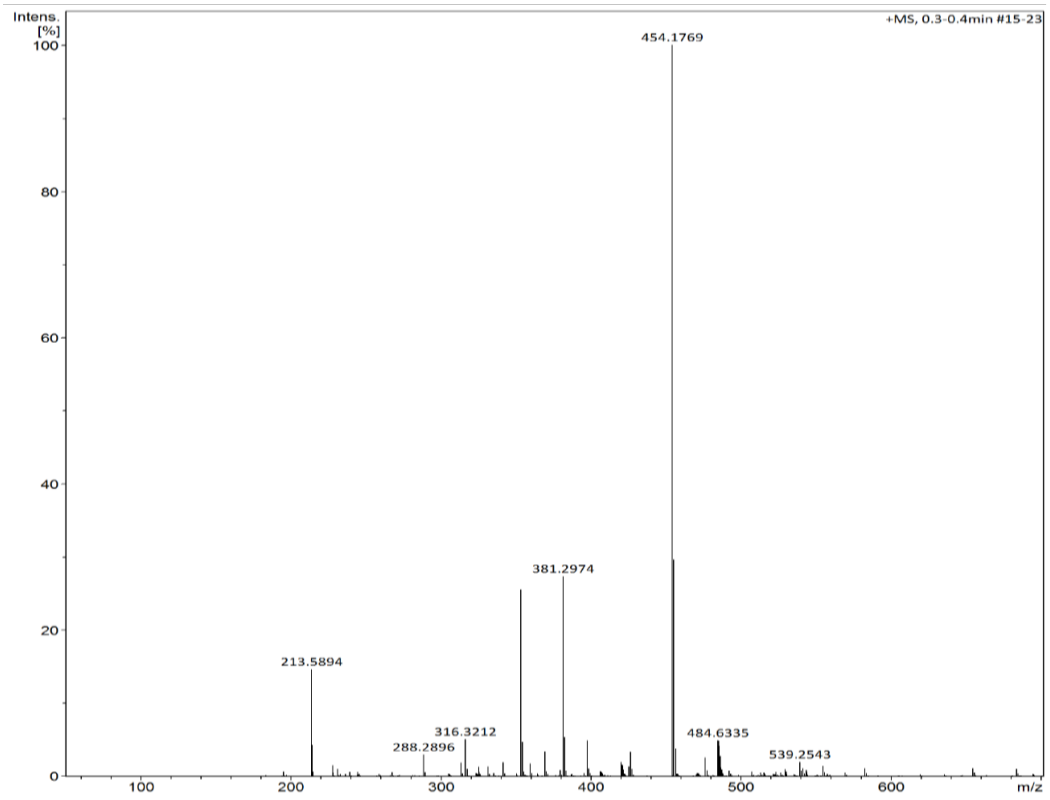


Figure S24. MS spectrum of **3A3**.

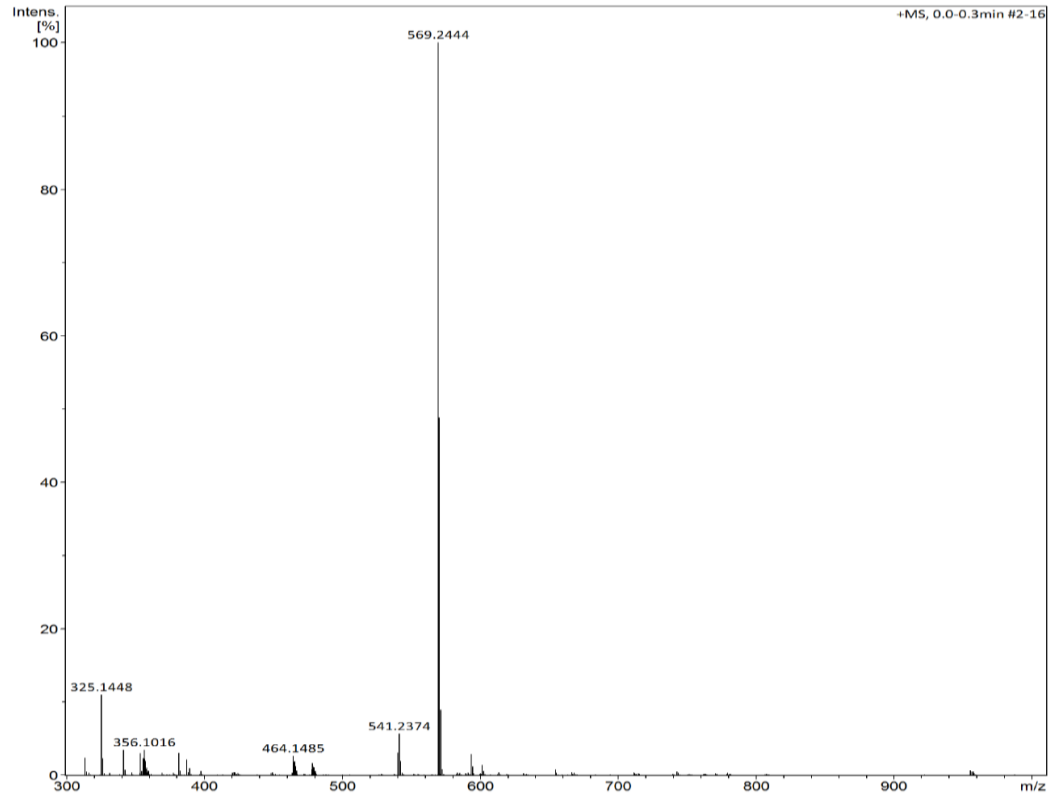


Figure S25. MS spectrum of **3A4**.

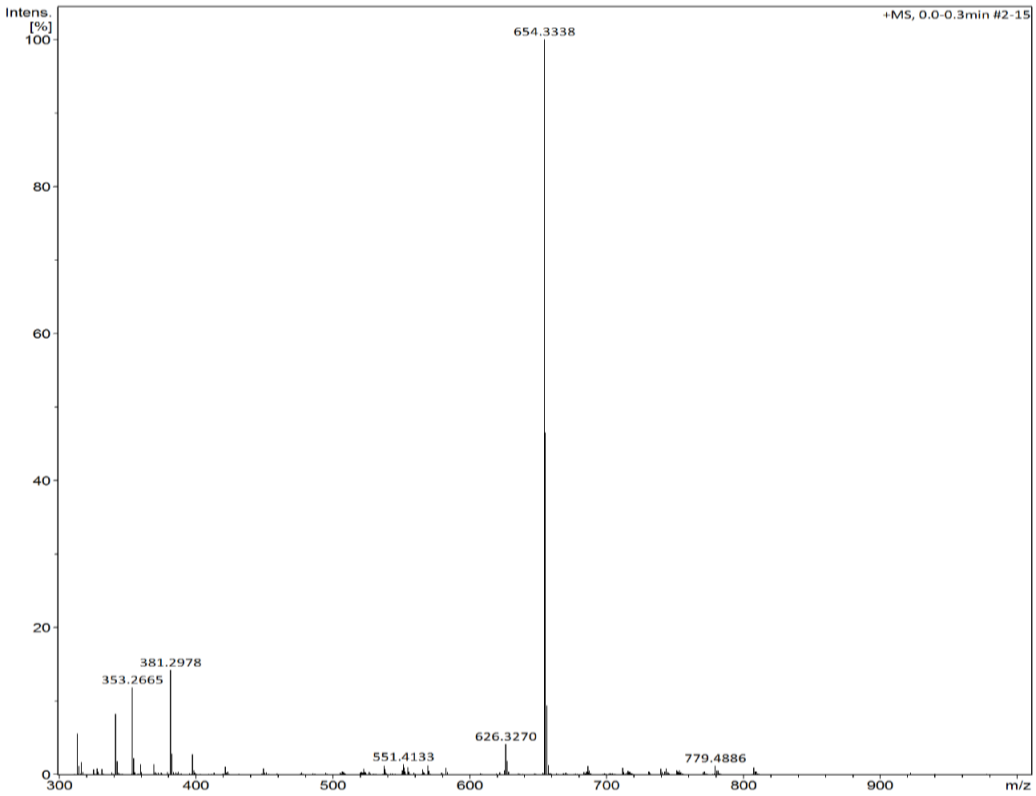


Figure S26. MS spectrum of **3A5**.

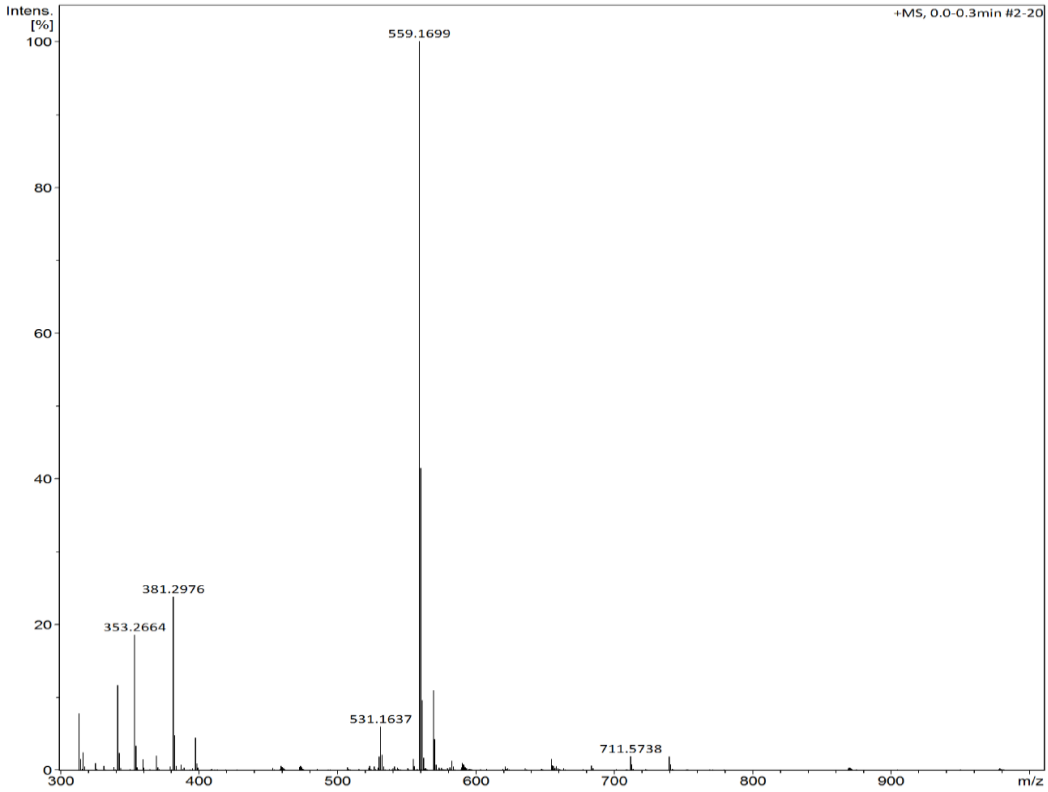


Figure S27. MS spectrum of **3A6**.

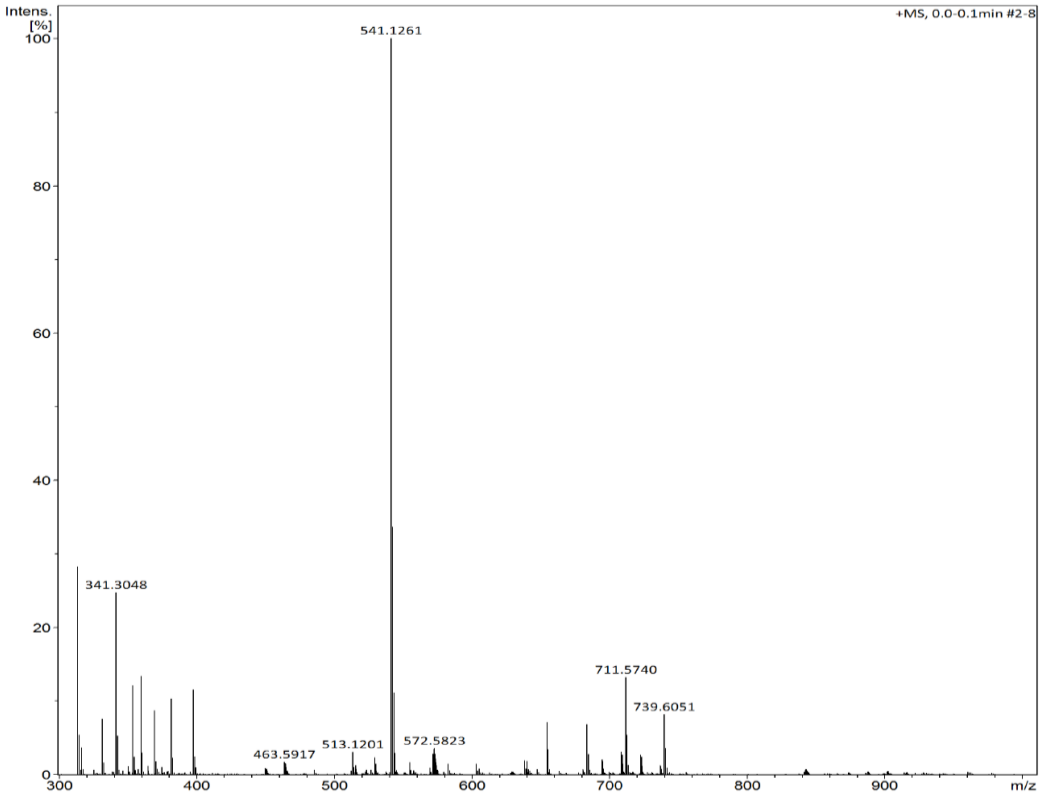


Figure S28. MS spectrum of **3A7**.

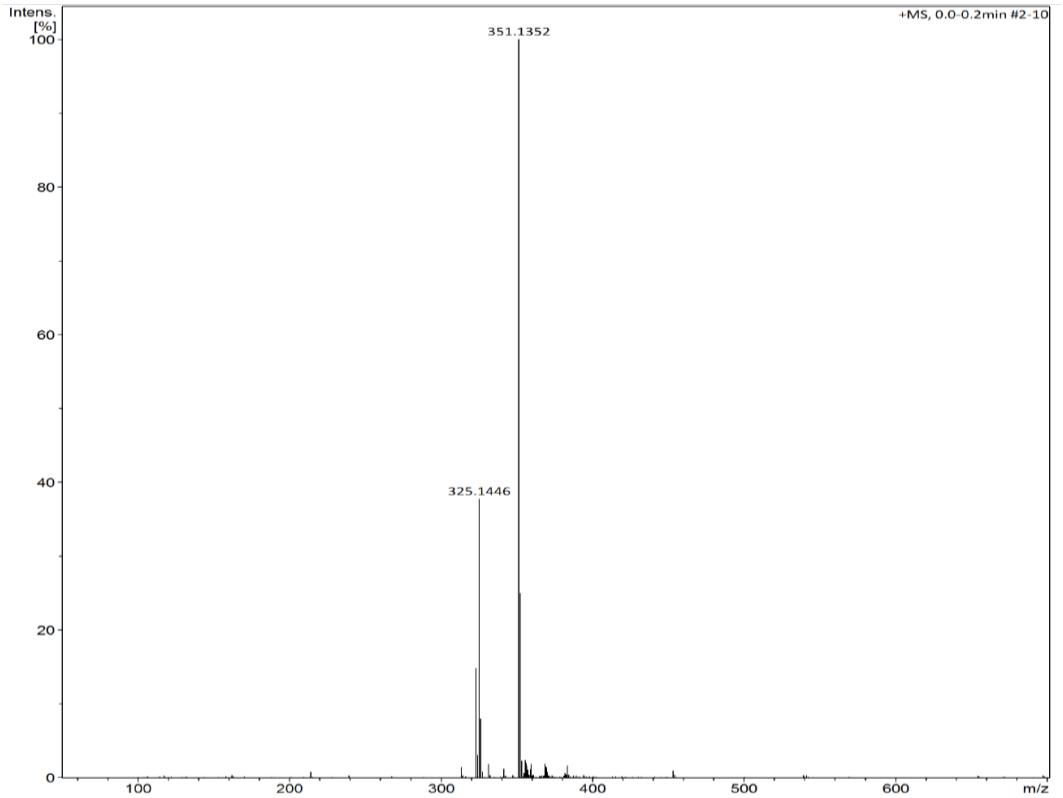


Figure S29. MS spectrum of **4**.

Cartesian coordinates of DFT-optimized structure of **3A1** by B3LYP /6-31G**/$CHCl_3$:
Charge = 0; multiplicity=1

C	-4.175717000	-0.054245000	0.001640000
C	-5.177481000	-1.024635000	0.127018000
C	-6.522988000	-0.633768000	0.146166000
N	-6.905239000	0.649410000	0.062987000
C	-5.954300000	1.588818000	-0.049367000
C	-4.587608000	1.281082000	-0.090132000
C	-7.607015000	-1.655123000	0.278124000
C	-7.482794000	-2.915365000	-0.326085000
C	-8.515150000	-3.839595000	-0.183027000
C	-9.639248000	-3.479990000	0.557145000
C	-9.674478000	-2.201624000	1.117948000
N	-8.693288000	-1.302915000	0.989513000
C	-6.414289000	3.008089000	-0.151695000
N	-7.555914000	3.232065000	-0.827521000
C	-7.981525000	4.494762000	-0.934173000
C	-7.314249000	5.591469000	-0.384655000
C	-6.136255000	5.355308000	0.320444000
C	-5.677607000	4.045323000	0.439943000
C	-2.740452000	-0.427690000	-0.034007000
C	-2.318217000	-1.610045000	-0.665593000
C	-0.975088000	-1.965778000	-0.710001000
C	-0.024950000	-1.139725000	-0.102264000
C	-0.419843000	0.035523000	0.542636000
C	-1.766032000	0.387072000	0.564681000
N	1.348013000	-1.506713000	-0.142240000
C	2.450581000	-0.711241000	-0.110518000
C	3.521461000	-1.584105000	-0.170910000
N	3.012010000	-2.857197000	-0.235104000
N	1.712732000	-2.815281000	-0.217132000
C	4.965692000	-1.317899000	-0.179786000
C	5.876754000	-2.384312000	-0.259341000
C	7.248939000	-2.142655000	-0.269494000
C	7.736363000	-0.835385000	-0.201533000
C	6.837830000	0.231150000	-0.122346000
C	5.464831000	-0.006651000	-0.111136000
H	-4.912955000	-2.068374000	0.251873000
H	-3.857530000	2.068929000	-0.237343000
H	-6.606463000	-3.157729000	-0.917317000
H	-8.444832000	-4.817686000	-0.649112000
H	-10.469491000	-4.164407000	0.696000000
H	-10.536390000	-1.885887000	1.703169000
H	-8.905336000	4.640856000	-1.491213000
H	-7.712001000	6.593659000	-0.504788000
H	-5.587523000	6.173168000	0.777475000
H	-4.776737000	3.826987000	1.003065000
H	-3.045414000	-2.245737000	-1.159873000
H	-0.655165000	-2.868110000	-1.216084000

H	0.309793000	0.658207000	1.048351000
H	-2.064478000	1.288804000	1.088884000
H	2.385999000	0.363402000	-0.079408000
H	5.496427000	-3.398472000	-0.312510000
H	7.939759000	-2.978416000	-0.331057000
H	7.206004000	1.251407000	-0.068762000
H	4.779859000	0.833826000	-0.048288000
H	8.806025000	-0.648953000	-0.210047000

Cartesian coordinates of DFT-optimized structure of **3A2** by B3LYP /6-31G**/$CHCl_3$:
Charge = 0; multiplicity=1

C	-2.044175000	-1.042298000	0.018224000
C	-3.259358000	-1.717028000	-0.152511000
C	-3.277737000	-3.117933000	-0.174438000
N	-2.165470000	-3.858368000	-0.049294000
C	-0.994031000	-3.222929000	0.108972000
C	-0.891648000	-1.826002000	0.154278000
C	-4.565603000	-3.854783000	-0.361556000
C	-5.759370000	-3.363079000	0.187690000
C	-6.940316000	-4.074754000	-0.011243000
C	-6.895967000	-5.254403000	-0.751103000
C	-5.660650000	-5.668057000	-1.253600000
N	-4.518147000	-4.997754000	-1.070672000
C	0.224796000	-4.076822000	0.257597000
N	0.076524000	-5.244424000	0.910575000
C	1.155532000	-6.020493000	1.057284000
C	2.423098000	-5.692828000	0.571917000
C	2.571632000	-4.486828000	-0.109581000
C	1.457925000	-3.665562000	-0.270369000
C	-1.982545000	0.439394000	0.051634000
C	-3.012282000	1.191032000	0.643085000
C	-2.961437000	2.579663000	0.682312000
C	-1.873603000	3.244579000	0.108154000
C	-0.841470000	2.520611000	-0.495236000
C	-0.897142000	1.130236000	-0.511251000
N	-1.827442000	4.665145000	0.138374000
C	-0.745076000	5.489899000	0.117830000
C	-1.270667000	6.768871000	0.155847000
N	-2.638008000	6.650330000	0.198390000
N	-2.974043000	5.392787000	0.186593000
C	-0.599974000	8.073426000	0.161084000
C	-1.345082000	9.255266000	0.334332000
C	-0.725980000	10.495848000	0.338927000
C	0.664816000	10.597146000	0.170423000
C	1.421959000	9.430518000	-0.002229000
C	0.786334000	8.188627000	-0.006725000
H	-4.174971000	-1.158978000	-0.310862000
H	0.068416000	-1.356953000	0.336588000
H	-5.758776000	-2.453959000	0.778785000
H	-7.874283000	-3.717197000	0.411200000
H	-7.788495000	-5.843506000	-0.933293000
H	-5.587844000	-6.585068000	-1.835676000
H	1.001673000	-6.954886000	1.594171000
H	3.260272000	-6.366157000	0.722235000
H	3.533924000	-4.192454000	-0.516981000
H	1.537870000	-2.732620000	-0.817331000
H	-3.849858000	0.683764000	1.110160000
H	-3.748264000	3.150847000	1.158920000

H	-0.014605000	3.033776000	-0.973284000
H	-0.102626000	0.579127000	-1.003256000
H	0.265356000	5.116925000	0.114342000
H	-2.419541000	9.187471000	0.464984000
H	-1.301100000	11.406449000	0.472043000
H	2.495594000	9.476151000	-0.136234000
O	1.175900000	11.859260000	0.188380000
C	2.584990000	12.038644000	-0.004875000
C	2.872051000	13.532365000	0.030515000
C	4.356829000	13.847298000	-0.189358000
C	4.662234000	15.350137000	-0.162609000
C	6.143050000	15.666036000	-0.392426000
H	1.392588000	7.299077000	-0.150958000
H	2.884661000	11.606898000	-0.969606000
H	3.138496000	11.515096000	0.786640000
H	2.541936000	13.933417000	0.996657000
H	2.266747000	14.024341000	-0.740810000
H	4.680810000	13.430073000	-1.153049000
H	4.957908000	13.342835000	0.580126000
H	4.342827000	15.766154000	0.802195000
H	4.056524000	15.854392000	-0.927377000
H	6.771185000	15.202811000	0.377049000
H	6.329369000	16.744607000	-0.368974000
H	6.480939000	15.290574000	-1.365025000

Cartesian coordinates of DFT-optimized structure of **3A3** by B3LYP /6-31G**/$CHCl_3$:
Charge = 0; multiplicity=1

C	-4.158496000	-0.067576000	-0.014122000
C	-5.165145000	-1.031271000	0.122521000
C	-6.507803000	-0.631340000	0.153119000
N	-6.882280000	0.654034000	0.068561000
C	-5.926451000	1.586899000	-0.056157000
C	-4.562155000	1.270106000	-0.106863000
C	-7.597336000	-1.644653000	0.300575000
C	-7.487571000	-2.909013000	-0.297802000
C	-8.524508000	-3.825545000	-0.139093000
C	-9.638688000	-3.454415000	0.610334000
C	-9.659834000	-2.172725000	1.164196000
N	-8.674072000	-1.281315000	1.020814000
C	-6.378160000	3.008650000	-0.161455000
N	-7.525277000	3.236377000	-0.826685000
C	-7.943397000	4.501297000	-0.936637000
C	-7.262944000	5.596691000	-0.400860000
C	-6.079300000	5.356707000	0.293417000
C	-5.628346000	4.044363000	0.416219000
C	-2.725908000	-0.449955000	-0.059461000
C	-2.313874000	-1.629680000	-0.702256000
C	-0.973052000	-1.993262000	-0.755353000
C	-0.015594000	-1.178133000	-0.144421000
C	-0.400377000	-0.005781000	0.511675000
C	-1.744126000	0.354051000	0.541581000
N	1.355796000	-1.552258000	-0.192376000
C	2.462085000	-0.768028000	-0.121717000
C	3.520829000	-1.649745000	-0.210939000
N	3.010359000	-2.915012000	-0.330721000
N	1.711284000	-2.863276000	-0.318462000
C	4.959035000	-1.360844000	-0.194050000
C	5.904745000	-2.389040000	-0.315319000
C	7.255997000	-2.057265000	-0.291708000
C	7.621341000	-0.718426000	-0.149462000
C	6.605960000	0.232773000	-0.036774000
N	5.302291000	-0.065109000	-0.056514000
H	-4.905771000	-2.076264000	0.247974000
H	-3.827734000	2.052237000	-0.262617000
H	-6.618885000	-3.160579000	-0.896436000
H	-8.465312000	-4.806694000	-0.600275000
H	-10.471924000	-4.132559000	0.761483000
H	-10.513732000	-1.847933000	1.756185000
H	-8.871975000	4.650362000	-1.484903000
H	-7.655005000	6.600863000	-0.523133000
H	-5.520144000	6.173529000	0.739526000
H	-4.723035000	3.823460000	0.971163000
H	-3.047391000	-2.257017000	-1.197940000
H	-0.661183000	-2.893448000	-1.270043000

H	0.334750000	0.609544000	1.018167000
H	-2.034879000	1.253986000	1.073173000
H	2.430239000	0.305015000	-0.044638000
H	5.572041000	-3.414823000	-0.423783000
H	8.011693000	-2.831495000	-0.383049000
H	6.853033000	1.286792000	0.075235000
H	8.662500000	-0.414927000	-0.125996000

Cartesian coordinates of DFT-optimized structure of **3A4** by B3LYP /6-31G**/$CHCl_3$:
Charge = 0; multiplicity=1

C	-4.335933000	-0.860298000	-0.845813000
C	-5.491282000	-1.336606000	-1.461445000
C	-5.397014000	-2.448059000	-2.296198000
C	-4.141566000	-3.033940000	-2.469930000
N	-3.023450000	-2.590152000	-1.885944000
C	-3.116988000	-1.512605000	-1.084974000
C	-1.854239000	-1.030684000	-0.445113000
C	-1.637445000	0.339756000	-0.250400000
C	-0.448501000	0.775240000	0.347629000
C	0.477614000	-0.207632000	0.718293000
C	0.190332000	-1.557828000	0.475808000
N	-0.955922000	-1.963064000	-0.092499000
C	1.165271000	-2.622643000	0.866500000
N	0.653406000	-3.793975000	1.288159000
C	1.508434000	-4.757507000	1.646575000
C	2.897554000	-4.621556000	1.606264000
C	3.424197000	-3.410830000	1.161906000
C	2.547498000	-2.395487000	0.786032000
C	-0.184257000	2.217411000	0.575673000
C	-1.225499000	3.094489000	0.924593000
C	-0.990562000	4.450021000	1.125318000
C	0.307632000	4.950051000	0.987960000
C	1.363013000	4.096657000	0.655767000
C	1.111040000	2.744096000	0.446292000
N	0.546425000	6.337647000	1.190144000
N	-0.224874000	7.053835000	2.051104000
N	0.209109000	8.280115000	2.035446000
C	1.268533000	8.389936000	1.168870000
C	1.488594000	7.137490000	0.623039000
C	1.960663000	9.662629000	0.934293000
C	1.536388000	10.824730000	1.605810000
C	2.171742000	12.047565000	1.400993000
C	3.247112000	12.116333000	0.511780000
C	3.680737000	10.958650000	-0.166227000
C	3.047179000	9.742449000	0.040752000
H	-4.382419000	-0.011791000	-0.172047000
H	-6.446846000	-0.852743000	-1.284261000
H	-6.268151000	-2.856416000	-2.797384000
H	-4.030136000	-3.903874000	-3.114741000
H	-2.367737000	1.060162000	-0.600129000
H	1.392571000	0.070756000	1.228406000
H	1.061250000	-5.689595000	1.987509000
H	3.539181000	-5.441923000	1.909801000
H	4.497505000	-3.259722000	1.100164000
H	2.928968000	-1.451011000	0.414098000
H	-2.232602000	2.712011000	1.053055000
H	-1.798652000	5.120789000	1.389726000

H	2.374300000	4.478221000	0.570199000
H	1.933323000	2.094598000	0.165364000
H	2.186692000	6.774565000	-0.112676000
C	4.093307000	13.242318000	0.101222000
C	5.043891000	12.769997000	-0.827258000
C	4.864748000	11.273100000	-1.081278000
C	4.073045000	14.587499000	0.479285000
C	5.012727000	15.457644000	-0.078792000
C	5.957283000	14.990275000	-0.999786000
C	5.976686000	13.641984000	-1.378663000
C	4.523771000	10.989771000	-2.561932000
C	6.123033000	10.475741000	-0.669824000
H	0.699566000	10.754342000	2.291690000
H	1.827502000	12.931252000	1.930620000
H	3.386802000	8.853655000	-0.484003000
H	3.341817000	14.954846000	1.193869000
H	5.010421000	16.506134000	0.204480000
H	6.681411000	15.679210000	-1.424690000
H	6.714295000	13.290023000	-2.095079000
H	3.631925000	11.540811000	-2.873874000
H	4.339361000	9.921801000	-2.717869000
H	5.354071000	11.285530000	-3.211335000
H	6.384596000	10.662708000	0.375646000
H	6.977944000	10.757573000	-1.292915000
H	5.956232000	9.400873000	-0.794535000

Cartesian coordinates of DFT-optimized structure of **3A5** by B3LYP /6-31G**/$CHCl_3$:
Charge = 0; multiplicity=1

C	-1.861609000	-0.907393000	0.142530000
C	-2.996007000	-1.477144000	-0.449100000
C	-3.038131000	-2.858660000	-0.680514000
N	-2.018323000	-3.675021000	-0.373263000
C	-0.922700000	-3.139987000	0.186920000
C	-0.808980000	-1.772024000	0.467822000
C	-4.241980000	-3.485825000	-1.308449000
C	-5.528265000	-2.988767000	-1.049035000
C	-6.625082000	-3.597887000	-1.654568000
C	-6.407548000	-4.683918000	-2.499632000
C	-5.092601000	-5.112036000	-2.692588000
N	-4.029344000	-4.539487000	-2.118533000
C	0.191990000	-4.077754000	0.525494000
N	-0.151866000	-5.316848000	0.922926000
C	0.830559000	-6.168511000	1.235225000
C	2.188449000	-5.849829000	1.170410000
C	2.541235000	-4.568969000	0.750992000
C	1.530210000	-3.668391000	0.423048000
C	-1.777689000	0.548958000	0.412894000
C	-2.915512000	1.281270000	0.792595000
C	-2.846140000	2.647634000	1.040103000
C	-1.618790000	3.307032000	0.921279000
C	-0.470355000	2.599347000	0.555804000
C	-0.557584000	1.234765000	0.298532000
N	-1.545248000	4.703378000	1.178000000
C	-0.664686000	5.619658000	0.690643000
C	-1.039464000	6.818702000	1.269886000
N	-2.124518000	6.565144000	2.072498000
N	-2.428680000	5.300055000	2.020278000
C	-0.467717000	8.162827000	1.123112000
C	-1.141038000	9.274448000	1.682513000
C	-0.644860000	10.567425000	1.571325000
C	0.559578000	10.754723000	0.882743000
C	1.253710000	9.654197000	0.308464000
C	0.736477000	8.363771000	0.436435000
H	-3.820558000	-0.848236000	-0.764301000
H	0.072099000	-1.393002000	0.972442000
H	-5.669452000	-2.156748000	-0.368060000
H	-7.629918000	-3.234825000	-1.461901000
H	-7.229035000	-5.191463000	-2.994002000
H	-4.884583000	-5.958062000	-3.345297000
H	0.517747000	-7.160032000	1.557774000
H	2.939138000	-6.586285000	1.436770000
H	3.583708000	-4.276346000	0.671916000
H	1.775204000	-2.672330000	0.070946000
H	-3.867816000	0.775230000	0.910835000
H	-3.728356000	3.204870000	1.329600000

H	0.487294000	3.102031000	0.481038000
H	0.336226000	0.701426000	-0.007195000
H	0.098221000	5.364064000	-0.025294000
H	-2.072679000	9.102460000	2.209750000
H	-1.187146000	11.400227000	2.006232000
H	1.274496000	7.521861000	0.010526000
C	2.441654000	10.197757000	-0.316917000
C	2.408795000	11.601011000	-0.091795000
N	1.272108000	11.920485000	0.644066000
C	3.419266000	12.441467000	-0.572156000
C	4.469563000	11.855958000	-1.276696000
C	4.518116000	10.468816000	-1.504917000
C	3.508571000	9.635950000	-1.028790000
C	0.867937000	13.264159000	1.038480000
C	0.028544000	13.993505000	-0.020361000
C	-0.358796000	15.409543000	0.421255000
C	-1.195018000	16.162094000	-0.621341000
C	-1.574615000	17.582835000	-0.186700000
C	-2.409303000	18.339889000	-1.226837000
C	-2.784138000	19.762665000	-0.794328000
C	-3.617041000	20.512938000	-1.838180000
H	3.392429000	13.513683000	-0.408844000
H	5.265881000	12.487653000	-1.659168000
H	5.350592000	10.046230000	-2.058935000
H	3.548204000	8.565152000	-1.207756000
H	1.774663000	13.835190000	1.263653000
H	0.311184000	13.185569000	1.977504000
H	-0.874425000	13.405829000	-0.228191000
H	0.596493000	14.037254000	-0.958119000
H	0.552341000	15.984688000	0.638624000
H	-0.918359000	15.356825000	1.365847000
H	-2.108902000	15.589887000	-0.834305000
H	-0.637612000	16.208284000	-1.567508000
H	-0.659158000	18.152753000	0.027406000
H	-2.131068000	17.535895000	0.760296000
H	-3.326901000	17.772620000	-1.439293000
H	-1.854574000	18.384676000	-2.175129000
H	-1.866948000	20.328956000	-0.582200000
H	-3.338572000	19.717863000	0.153007000
H	-3.074778000	20.603365000	-2.786450000
H	-3.866978000	21.524101000	-1.500410000
H	-4.557367000	19.989131000	-2.045066000

Cartesian coordinates of DFT-optimized structure of **3A6** by B3LYP /6-31G**/$CHCl_3$:

Charge = 0; multiplicity=1

C	-4.349675000	-1.101380000	0.347882000
C	-5.579763000	-1.738488000	0.200526000
C	-5.643041000	-2.908543000	-0.553042000
C	-4.460979000	-3.388546000	-1.120561000
N	-3.272620000	-2.790144000	-0.987644000
C	-3.216141000	-1.655832000	-0.265659000
C	-1.878823000	-0.998812000	-0.136789000
C	-1.778443000	0.398264000	-0.096883000
C	-0.519037000	0.999529000	0.016784000
C	0.590583000	0.149116000	0.093292000
C	0.404909000	-1.239021000	0.046724000
N	-0.806733000	-1.803881000	-0.073559000
C	1.577515000	-2.163321000	0.137636000
N	1.511459000	-3.303669000	-0.574252000
C	2.550225000	-4.143093000	-0.508854000
C	3.695025000	-3.908495000	0.255464000
C	3.757108000	-2.730724000	0.996960000
C	2.684299000	-1.843855000	0.938811000
C	-0.367739000	2.475335000	0.036599000
C	-1.320003000	3.287826000	0.675326000
C	-1.184775000	4.671126000	0.705089000
C	-0.089256000	5.267846000	0.074226000
C	0.865721000	4.483396000	-0.578018000
C	0.726491000	3.098766000	-0.584958000
N	0.044624000	6.683717000	0.098839000
N	-1.054020000	7.481019000	0.174368000
N	-0.640476000	8.714568000	0.181253000
C	0.729480000	8.747551000	0.108625000
C	1.174316000	7.438868000	0.055070000
C	1.480568000	10.009360000	0.106797000
C	0.788577000	11.232825000	0.243395000
C	1.464305000	12.446377000	0.247936000
C	2.854833000	12.442856000	0.115394000
C	3.573987000	11.234122000	-0.022908000
C	2.872972000	10.022100000	-0.026583000
H	-4.265545000	-0.201861000	0.947651000
H	-6.468600000	-1.331493000	0.672681000
H	-6.577365000	-3.440726000	-0.696798000
H	-4.472076000	-4.300470000	-1.714922000
H	-2.666590000	1.009639000	-0.207050000
H	1.588650000	0.561992000	0.183152000
H	2.466347000	-5.052815000	-1.100760000
H	4.504771000	-4.630276000	0.268409000
H	4.619995000	-2.508033000	1.617019000
H	2.695093000	-0.931103000	1.524267000
H	-2.161832000	2.832287000	1.185966000
H	-1.911089000	5.289321000	1.217894000
H	1.695992000	4.946162000	-1.099760000

H	1.460003000	2.500568000	-1.115082000
H	2.158818000	7.003010000	0.023752000
H	-0.290286000	11.214750000	0.346566000
H	3.420151000	9.090806000	-0.136668000
C	5.007505000	11.459117000	-0.147205000
C	5.336887000	12.832793000	-0.098503000
S	3.908681000	13.860853000	0.096966000
C	6.658252000	13.273944000	-0.198885000
C	7.665083000	12.323081000	-0.350874000
C	7.357597000	10.954213000	-0.401734000
C	6.039852000	10.520605000	-0.300979000
H	0.916131000	13.376845000	0.353918000
H	6.896912000	14.331924000	-0.159883000
H	8.698039000	12.647475000	-0.430646000
H	8.155527000	10.227963000	-0.520660000
H	5.810213000	9.459969000	-0.341076000

Cartesian coordinates of DFT-optimized structure of **3A7** by B3LYP /6-31G**/$CHCl_3$:
Charge = 0; multiplicity=1

C	-1.702793000	-1.223116000	-0.213231000
C	-2.942421000	-1.714740000	0.213855000

C	-3.111822000	-3.091601000	0.412970000
N	-2.122040000	-3.977420000	0.221095000
C	-0.931557000	-3.518915000	-0.195340000
C	-0.682872000	-2.159171000	-0.423560000
C	-4.430748000	-3.634410000	0.863415000
C	-5.631317000	-3.039247000	0.446926000
C	-6.840647000	-3.571502000	0.888292000
C	-6.817608000	-4.681342000	1.730088000
C	-5.574833000	-5.209389000	2.085791000
N	-4.405578000	-4.711361000	1.670418000
C	0.145337000	-4.532758000	-0.417683000
N	0.165124000	-5.591991000	0.412380000
C	1.123140000	-6.507853000	0.234998000
C	2.099443000	-6.431652000	-0.760354000
C	2.071083000	-5.338139000	-1.623044000
C	1.080624000	-4.373587000	-1.451470000
C	-1.475986000	0.228707000	-0.420286000
C	-2.497833000	1.053998000	-0.920225000
C	-2.295845000	2.415632000	-1.115487000
C	-1.048885000	2.974291000	-0.819969000
C	-0.013293000	2.174198000	-0.330179000
C	-0.234213000	0.815430000	-0.127422000
N	-0.839477000	4.366253000	-1.026733000
C	0.020260000	5.208133000	-0.392419000
C	-0.182674000	6.436689000	-0.995154000
N	-1.150643000	6.276505000	-1.958115000
N	-1.542854000	5.036985000	-1.977403000
H	-3.752369000	-1.030255000	0.437024000
H	0.295747000	-1.834227000	-0.757093000
H	-5.619757000	-2.191142000	-0.228759000
H	-7.781540000	-3.131559000	0.572399000
H	-7.732527000	-5.132053000	2.099695000
H	-5.518039000	-6.076819000	2.741022000
H	1.113431000	-7.348463000	0.926574000
H	2.850655000	-7.208661000	-0.854075000
H	2.800307000	-5.239767000	-2.421288000
H	1.019744000	-3.524489000	-2.123320000
H	-3.461831000	0.625850000	-1.174093000
H	-3.089231000	3.045167000	-1.498732000
H	0.961073000	2.599824000	-0.118300000
H	0.569687000	0.208654000	0.275424000
H	0.653810000	4.893633000	0.420376000
C	0.433549000	7.727473000	-0.753285000
C	0.118136000	8.928860000	-1.345710000
C	0.907687000	10.011605000	-0.881544000
C	1.838895000	9.654030000	0.071076000
S	1.744695000	7.927203000	0.390929000
C	2.804990000	10.480920000	0.764846000
S	3.219844000	12.080080000	0.162311000
C	4.331553000	12.342909000	1.469914000

C	4.388199000	11.263672000	2.308273000
C	3.521898000	10.205620000	1.910504000
H	-0.667362000	9.021661000	-2.085296000
H	0.781929000	11.031694000	-1.226422000
H	4.870989000	13.277466000	1.534489000
H	5.021125000	11.224282000	3.187111000
H	3.417589000	9.277883000	2.461979000