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Supporting Information

Star Shaped Ferrocenyl Substituted Triphenylamines

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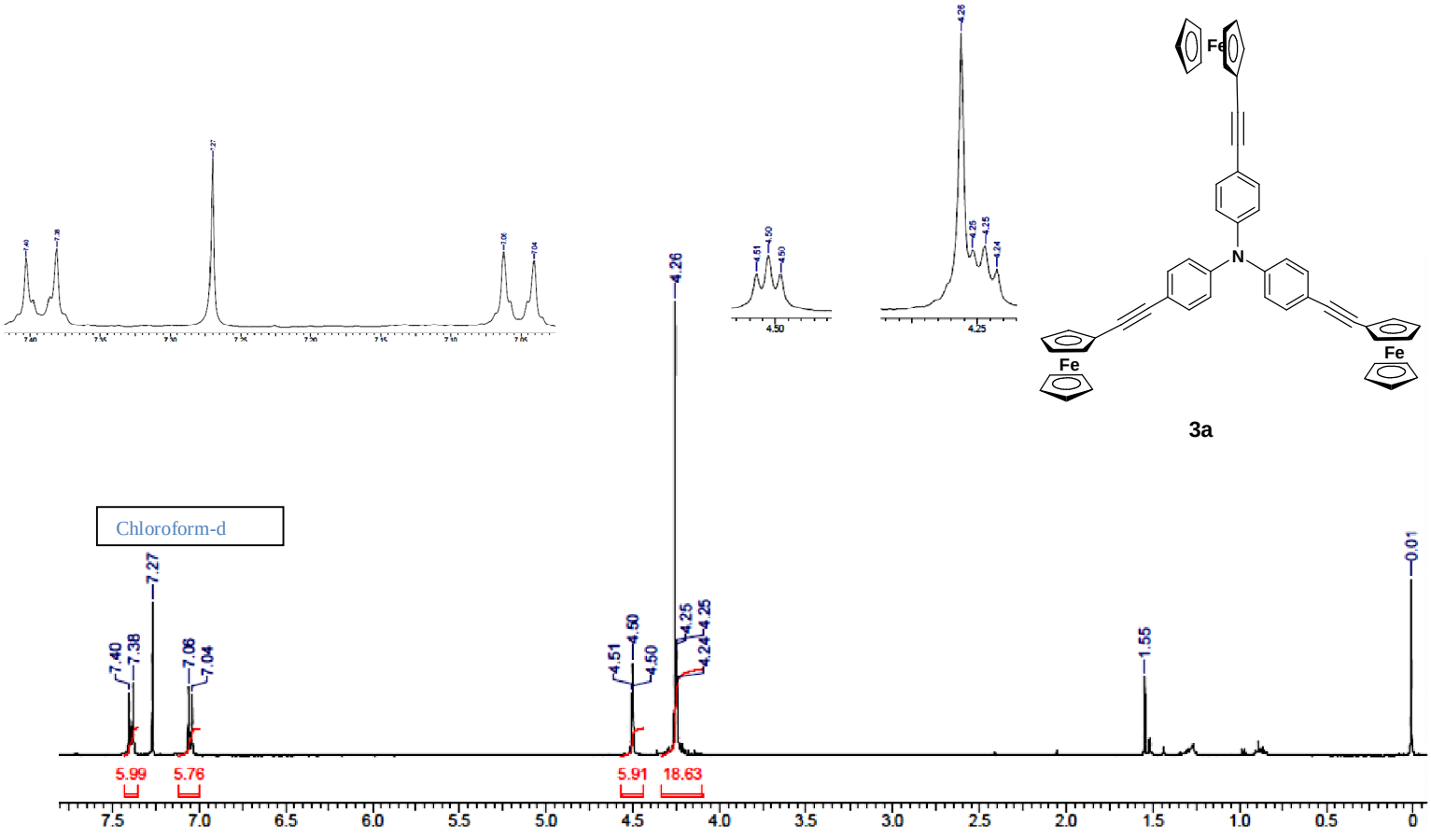


Figure S1. ^{1}H NMR Spectra of compound **3a**.

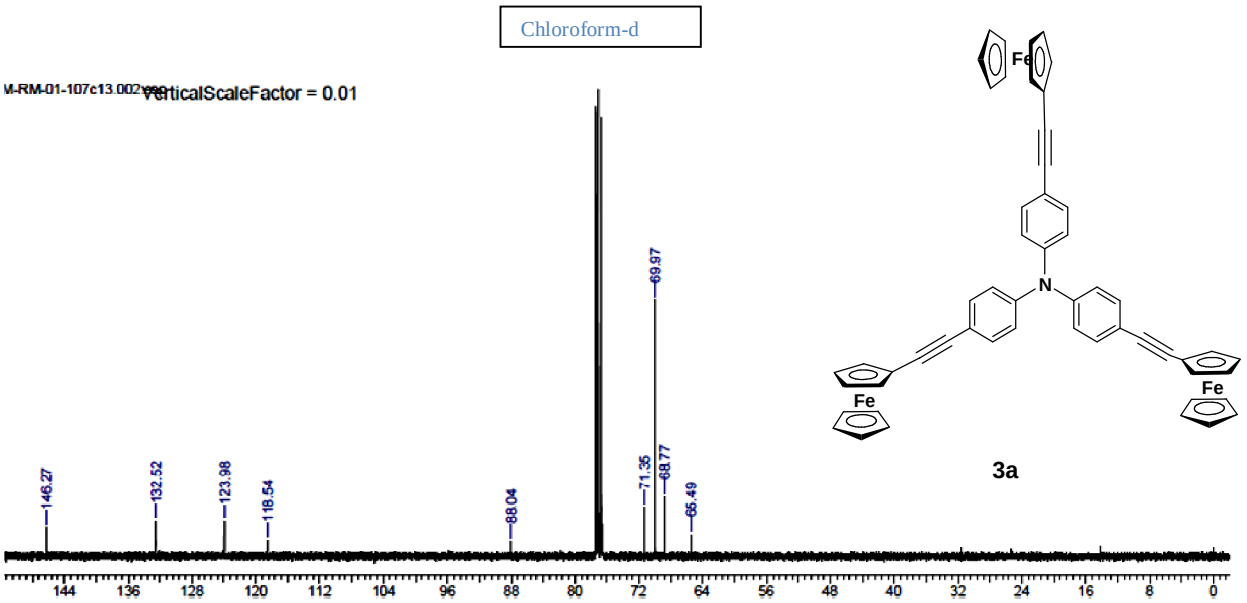


Figure S2. ^{13}C NMR Spectra of compound **3a**.

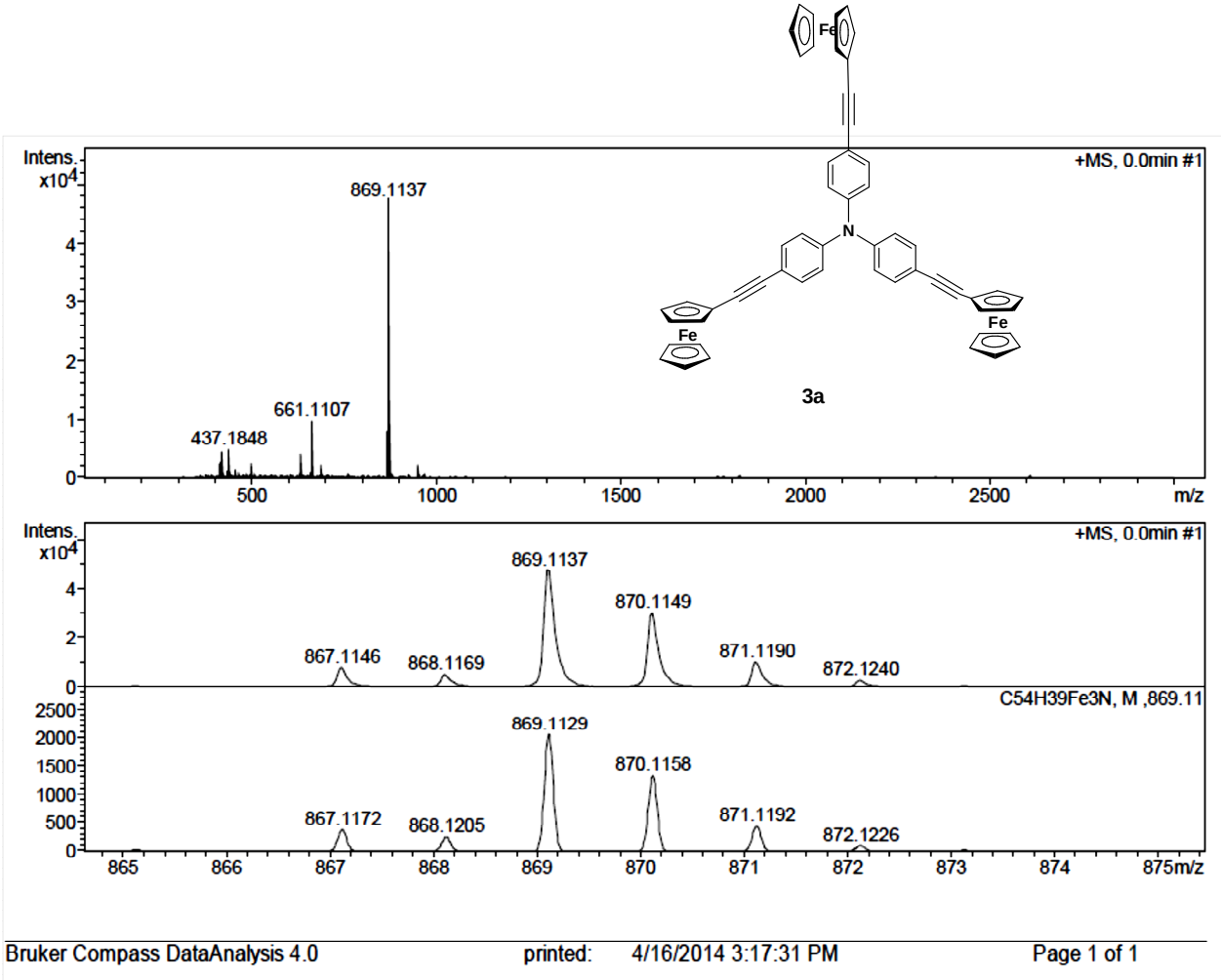


Figure S3. HRMS Spectra of **3a**.

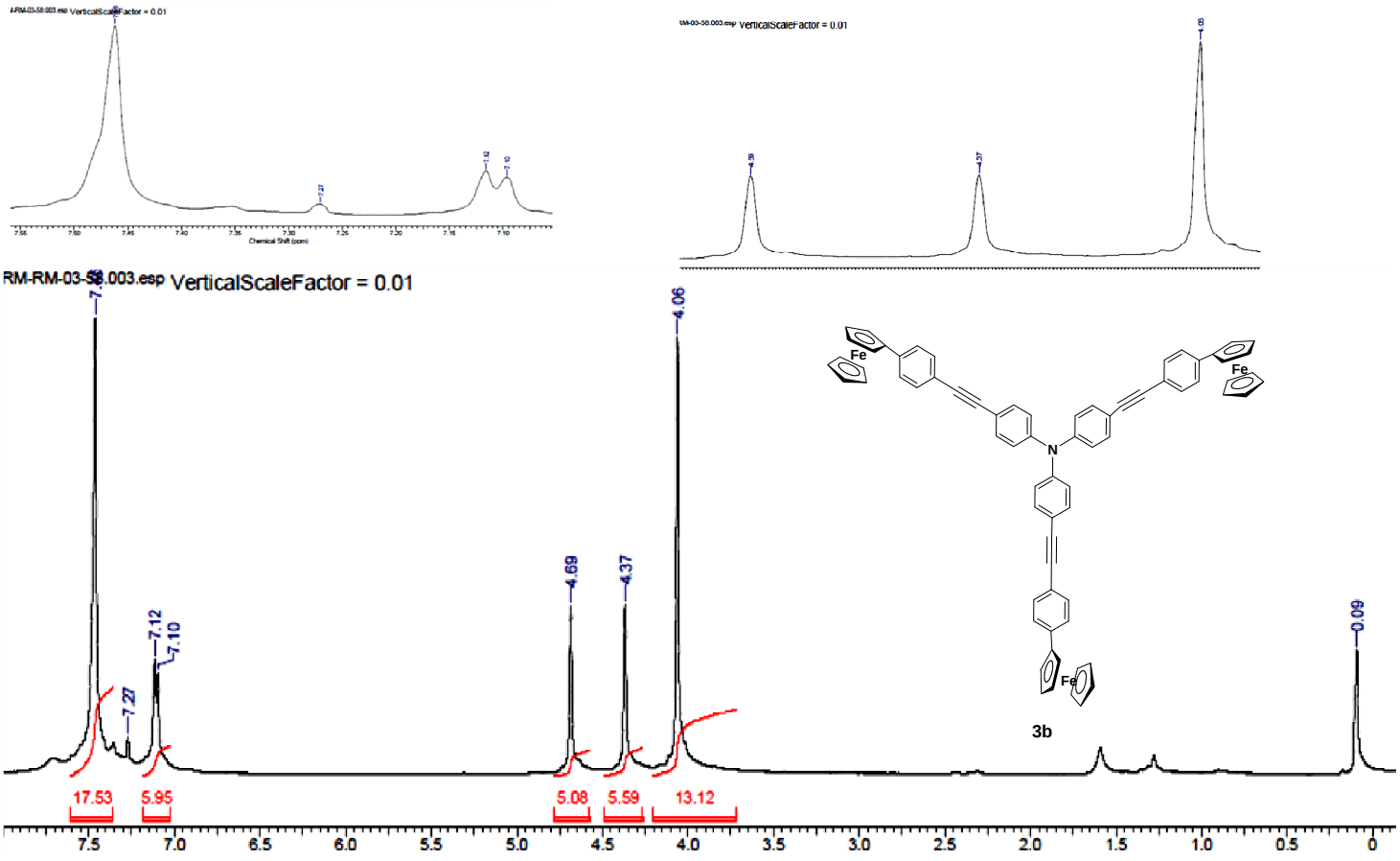


Figure S4. [1] H NMR spectra of **3b**

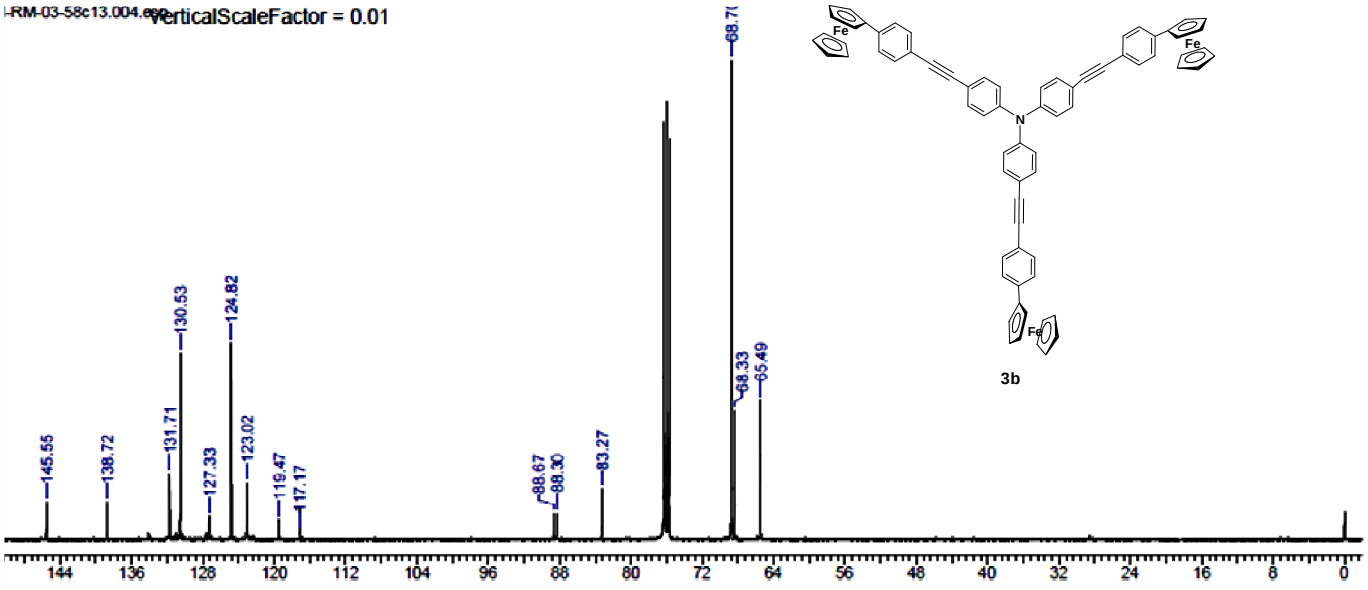


Figure S5. ^{13}C NMR Spectra of compound **3b**.

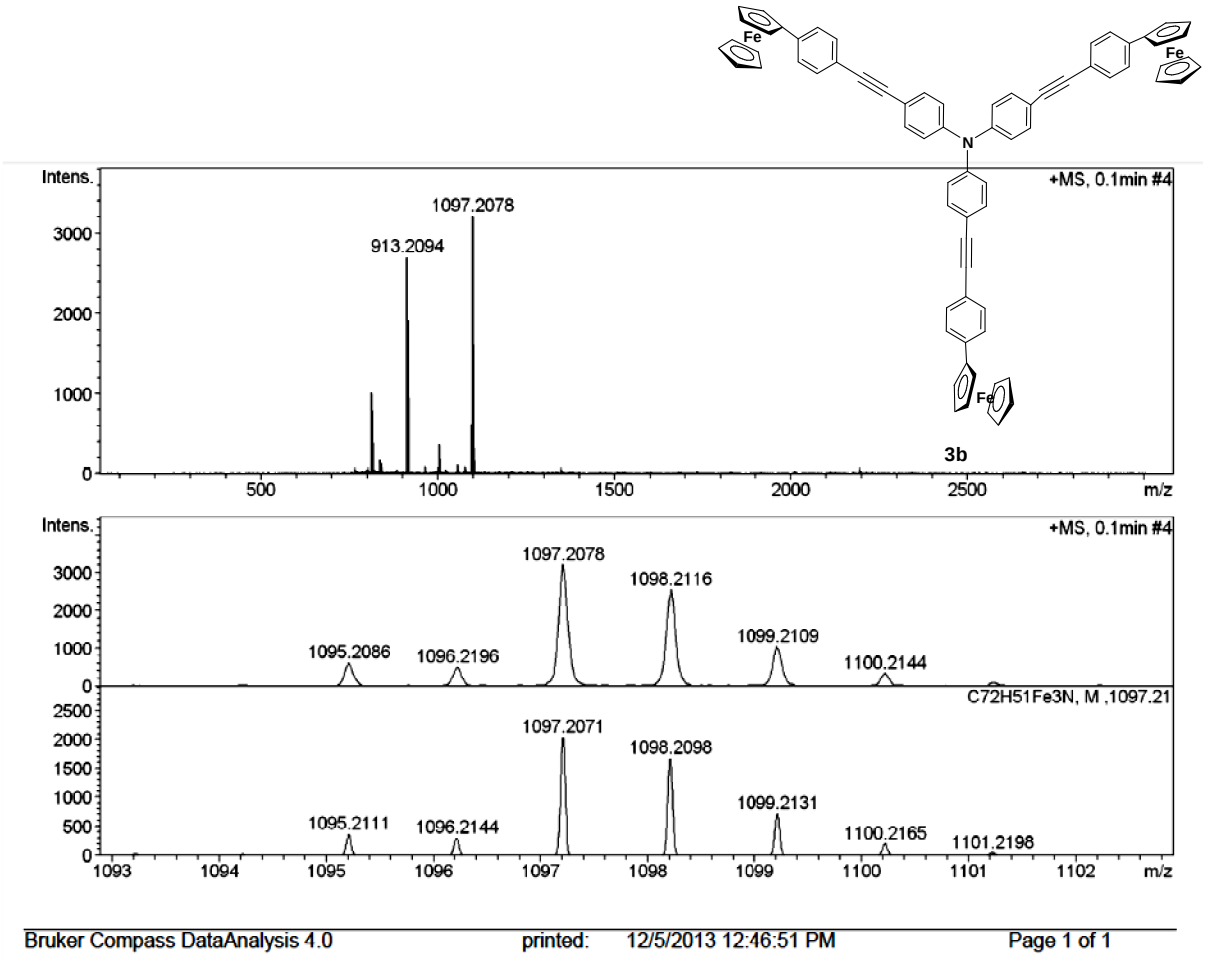


Figure S6. HRMS Spectra of **3b**.

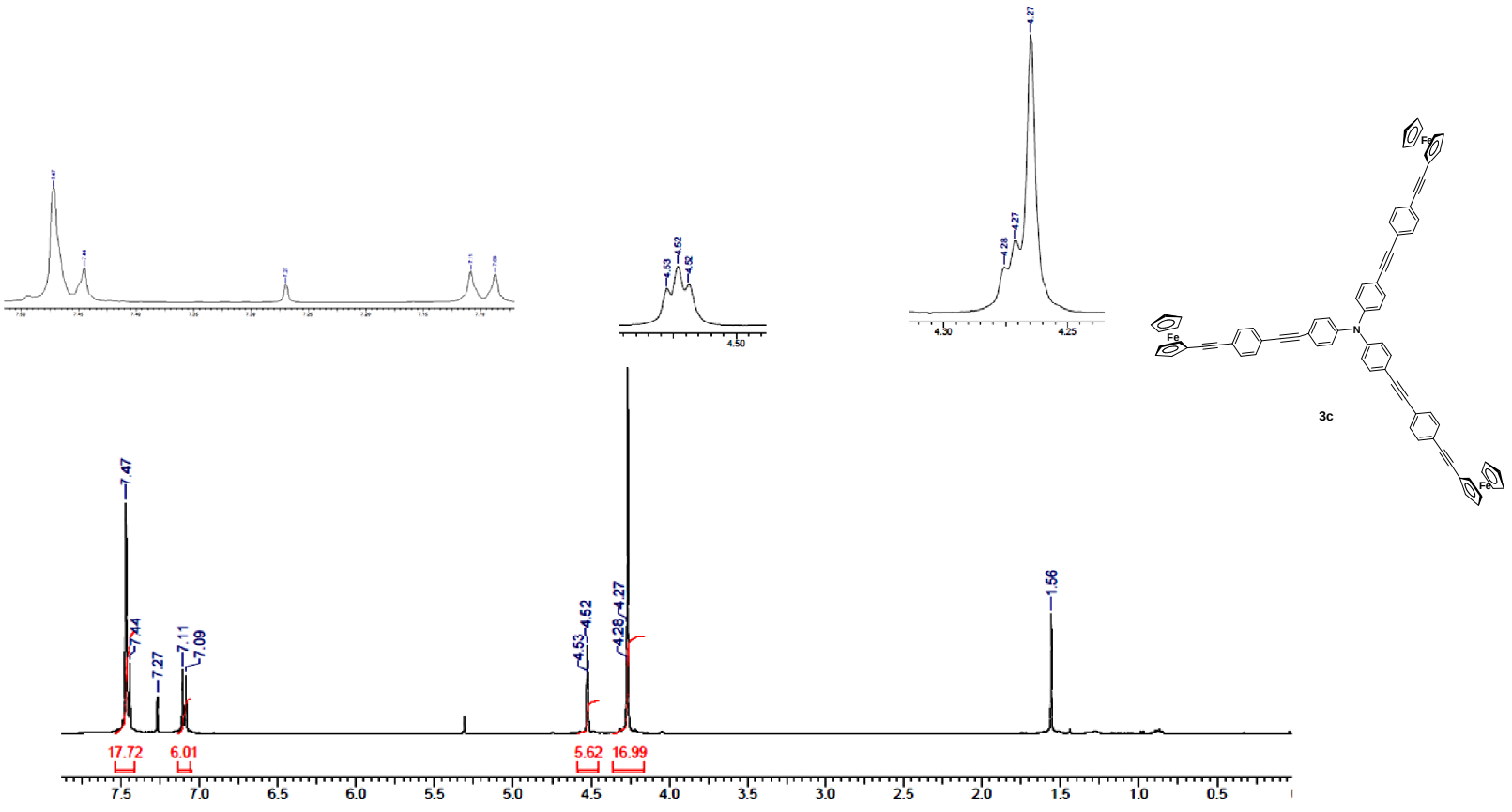


Figure S7. ^{1}H NMR Spectra of compound **3c**

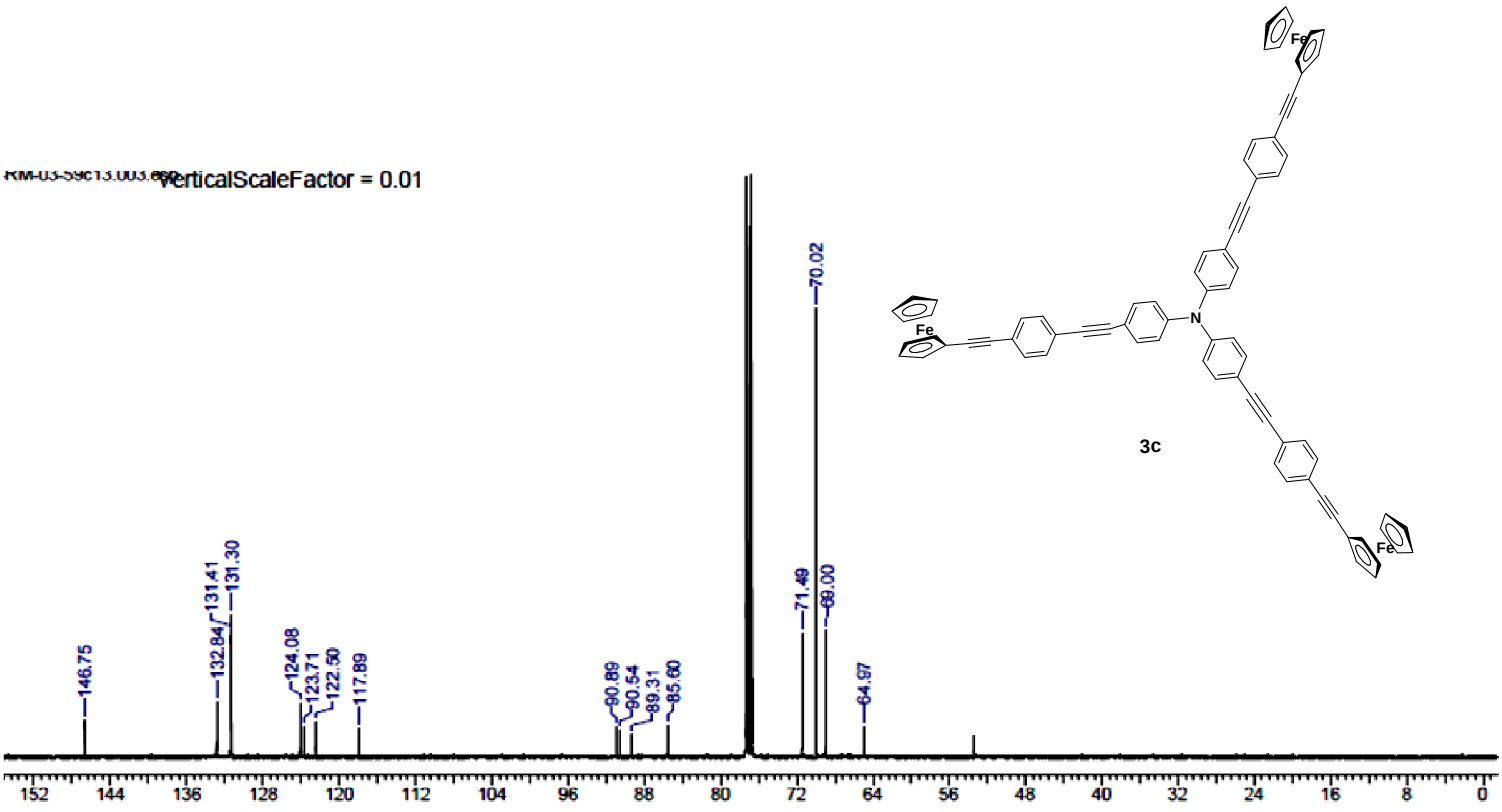


Figure S8. ^{13}C NMR Spectra of compound **3c.**

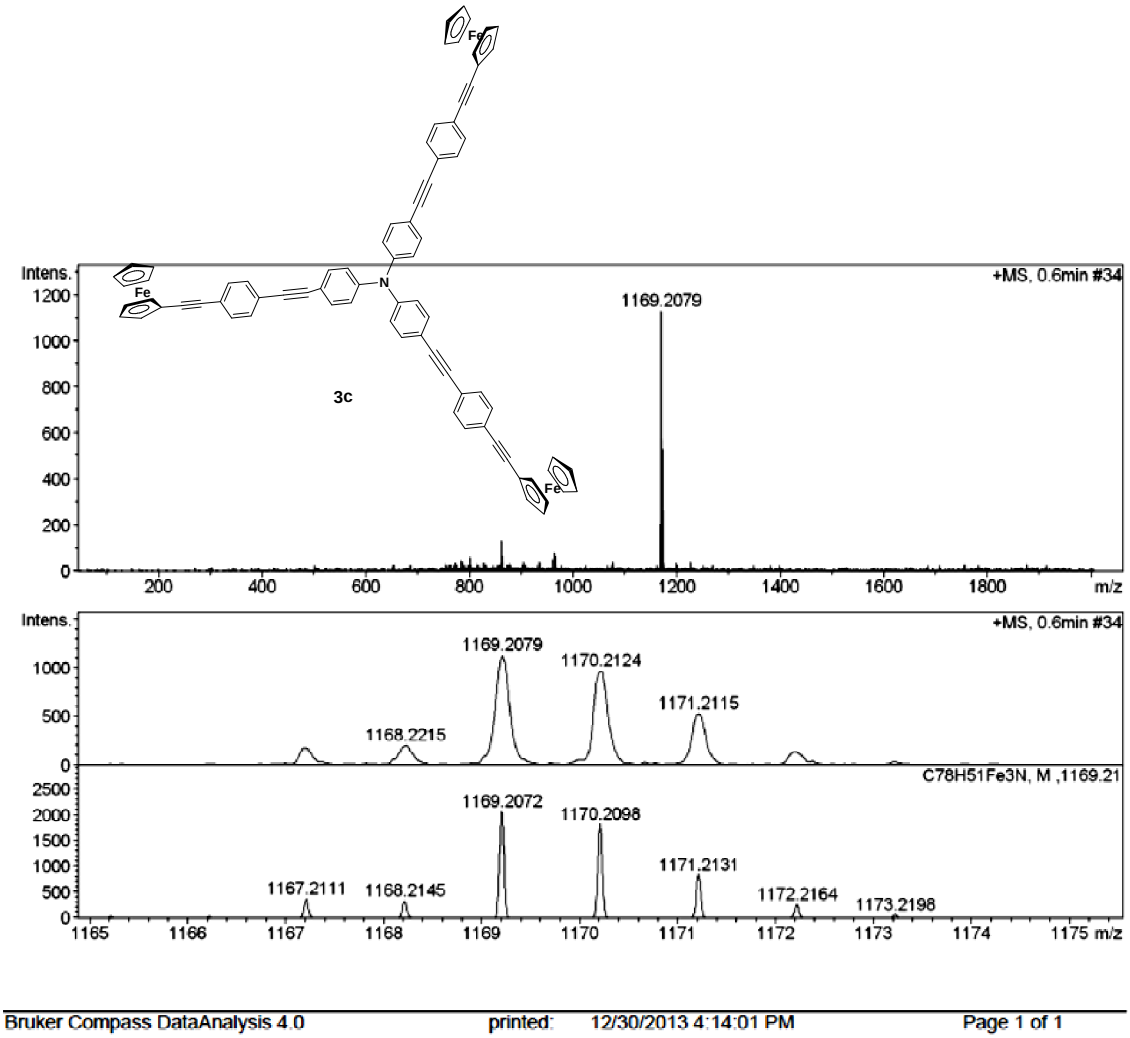


Figure S9. HRMS Spectra of **3c**.

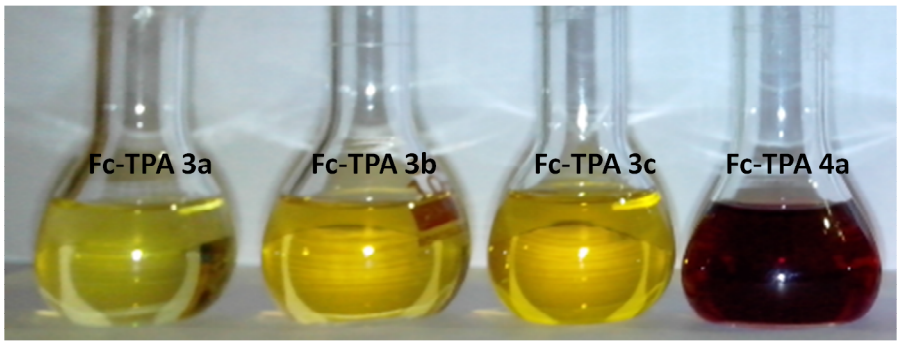


Figure S10. The Fc-TPA **3a-3c** in dichloromethane at 10^{-4} M concentration.

II. Cyclic voltammogram of the FC-TPA 3b and 3c

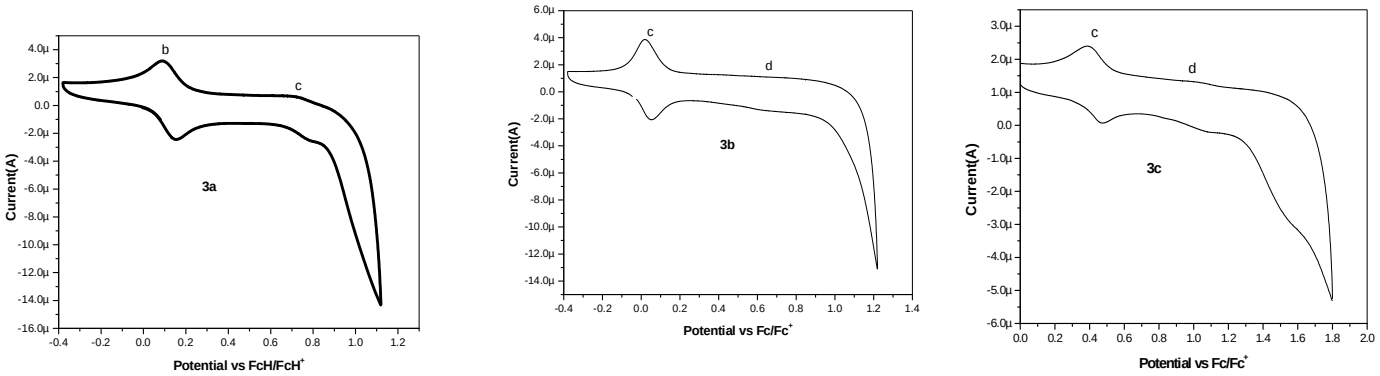
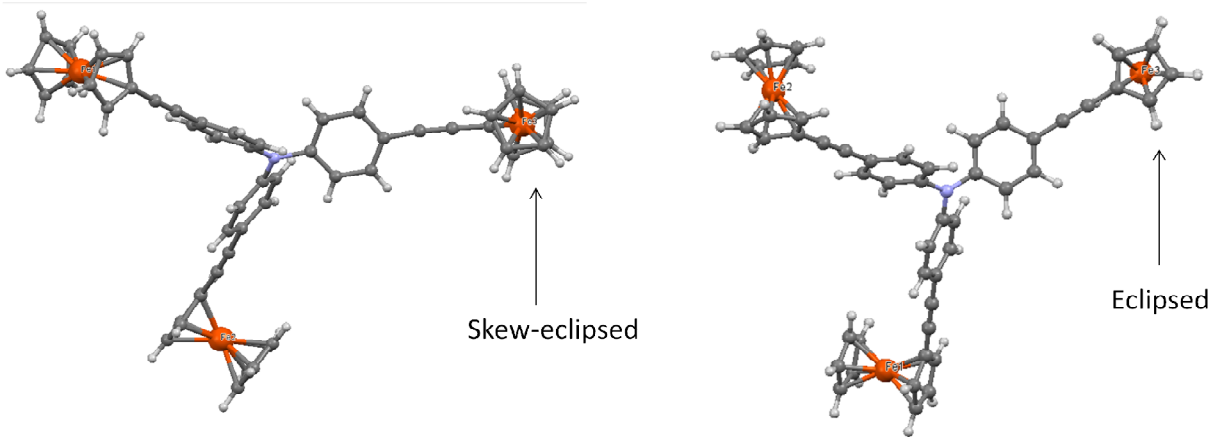
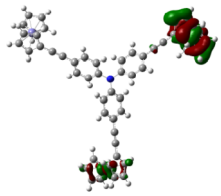
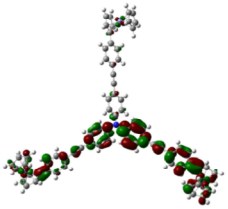
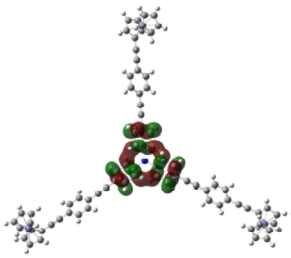
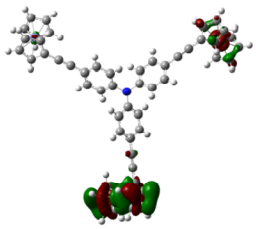
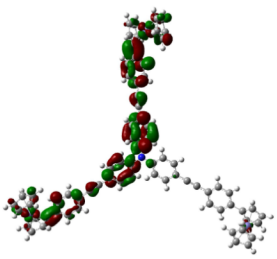
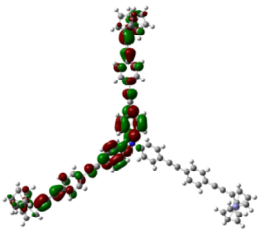


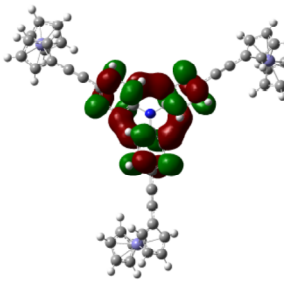
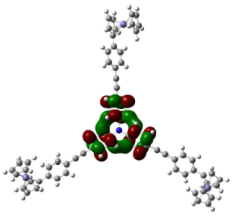
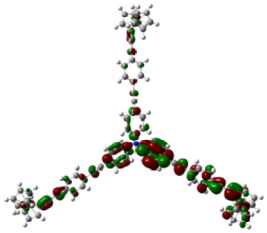
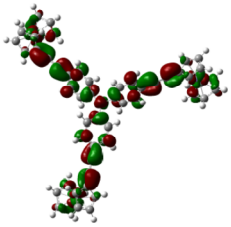
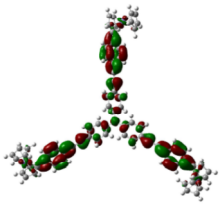
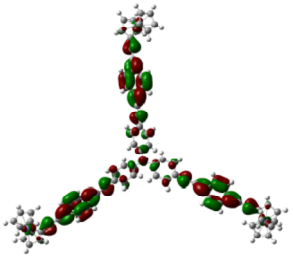
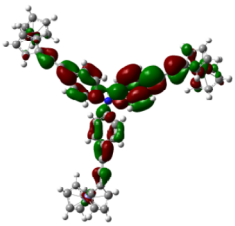
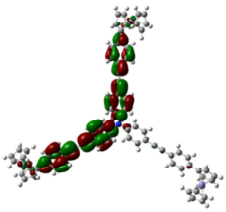
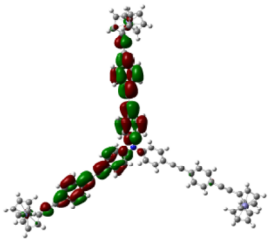
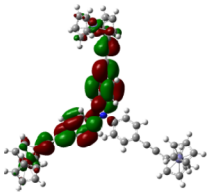
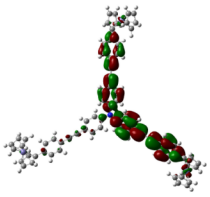
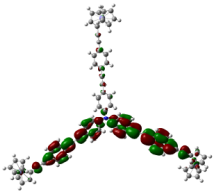
Figure S11. The Cyclic voltammograms of the FC-TPA **3a** and **3c**.

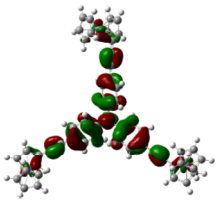
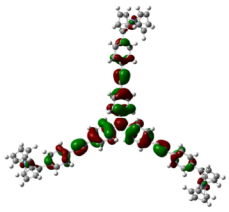
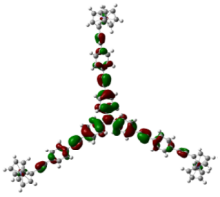
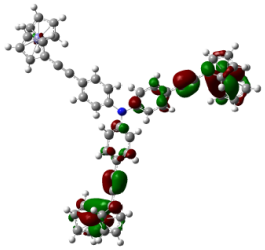
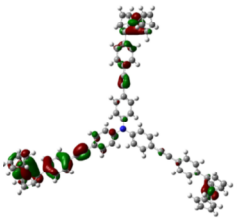
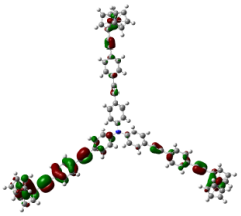
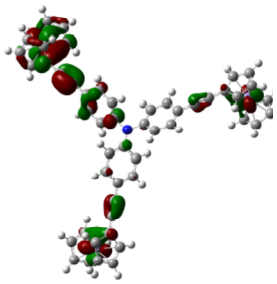
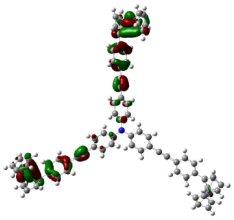
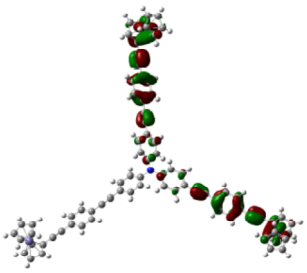
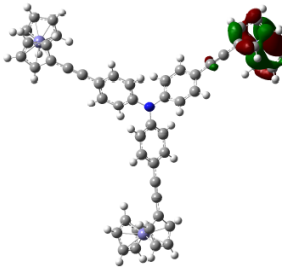
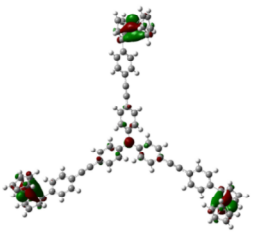
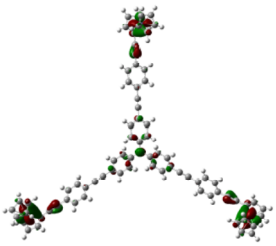


(a) **(b)**

Figure S12. Conformation comparison of (a) crystal structure and (b) CAM-B3LYP optimized structure of Fc-TPA **3a**.

Fc-TPA **3a**	**3a**	**3b**	**3c**
LUMO +5			
LUMO +4			

LUMO +3			
LUMO +2			
LUMO +1			
LUMO			

HOMO			
HOMO-1			
HOMO-2			
HOMO-3			

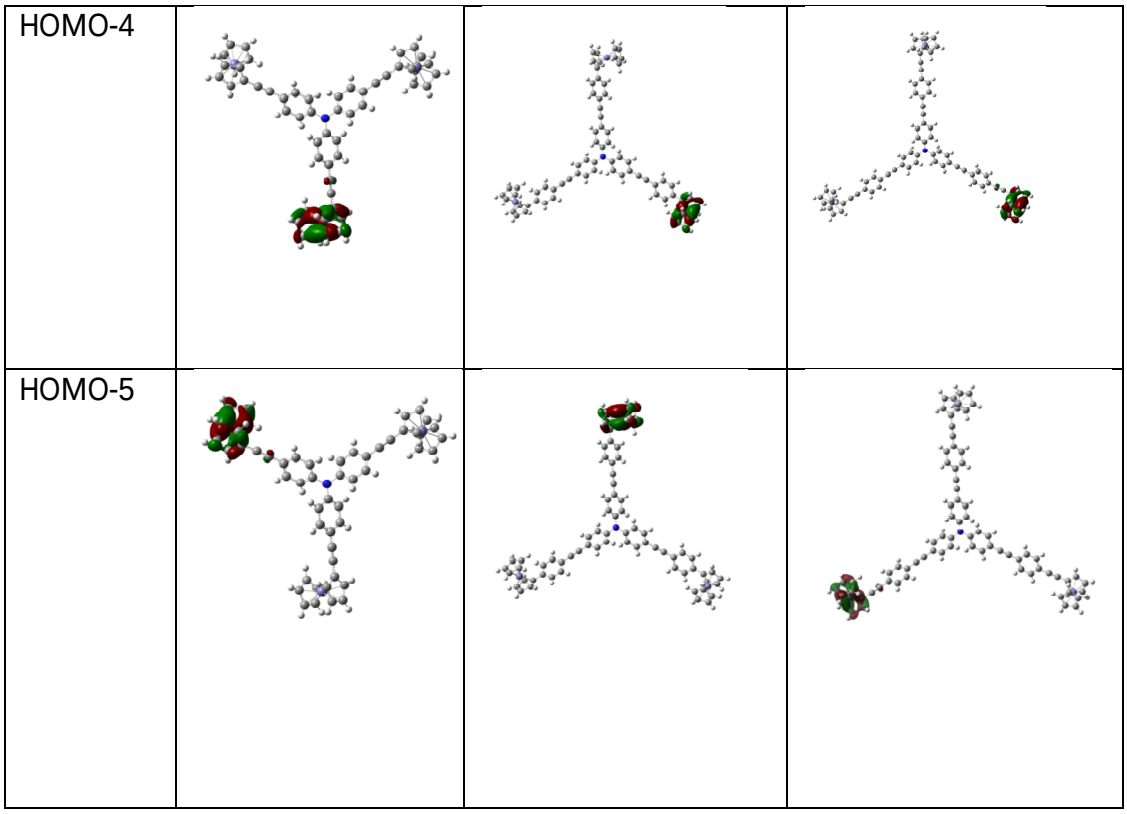


Figure S13. The molecular orbital surfaces in the optimized ground-state structure for Fc-TPA **3a–3c** and 4a using TD-DFT, CAM-B3LYP level of theory.

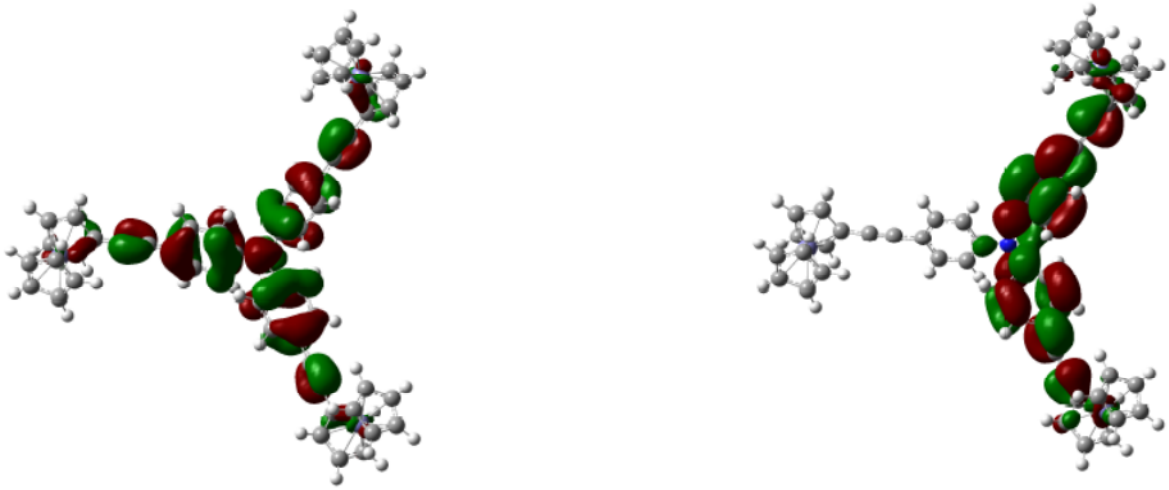


Figure S14. The calculated $\pi \rightarrow \pi^*$ transition band (328.73 nm with oscillator strength of 1.4958) between HOMO to LUMO of compound **3a** using CAM-B3LYP Theory.

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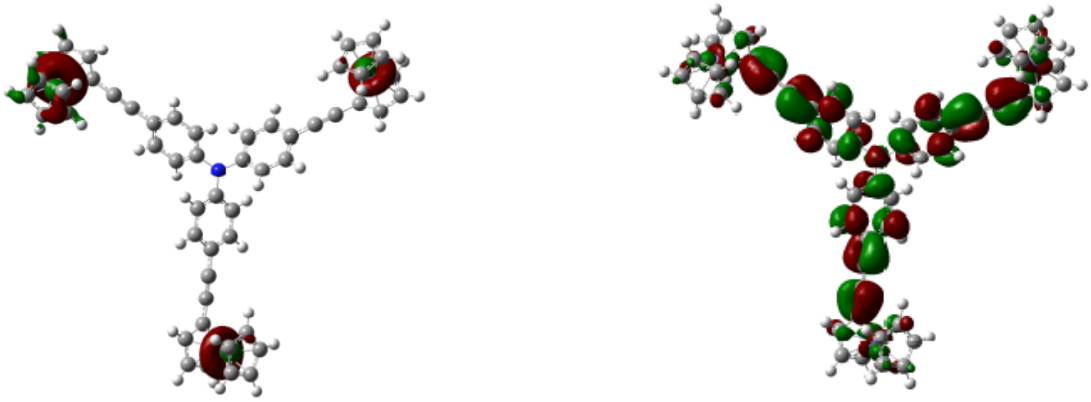

Figure S15. The calculated d-d transition band (473.08 nm with oscillator strength 0.0043) between HOMO-17 to LUMO+2 (expansion coefficient 0.21) of compound **3a** using CAM-B3LYP Theory.

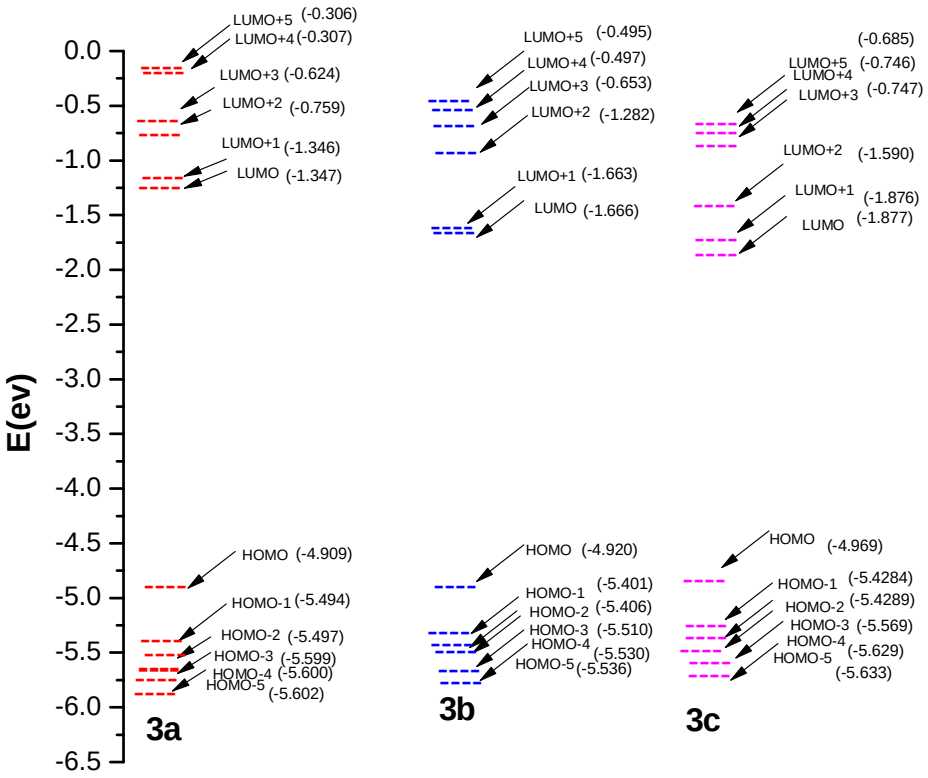

Figure S16. The energy level diagram of the frontier molecular orbitals (HOMO-5 to LUMO+5) of the Fc-TPA **3a-3c**, and **4a** calculated using B3LYP level of TD-DFT theory

Table S1. Selected bond lengths of intermolecular interactions in the crystal structure of **3a**

Compound 3a			
Bond lengths (Å)		**Bond angles °**	
Fe(1)-C(31)	1.97(2)	C(31)-Fe(1)-C(30)	38.4(8)
Fe(2)-C(42)	1.95(4)	C(42)-Fe(2)-C(40)	40.7(18)
Fe(3)-C(45)	1.990(17)	C(45)-Fe(3)-C(50)	128.4(10)
N(1)-C(9)	1.407(18)	C(9)-N(1)-C(1)	119.9(15)
C(20)-C(23)	1.43(2)	C(14)-C(9)-N(1)	118.8(19)
Cl(2)-C(111)	1.77(3)	C(8)-C(25)-Fe(1)	126.7(12)
C(51)-C(52)	1.35(2)	C(51)-C(52)-C(53)	108.9(17)
C(29)-C(34)	3.33(1)	C(29)-Fe(1)-C(34)	110.01(1)
C(11)-C(37)	3.26(2)	C(11)-Fe(2)-C(37)	108.14(2)
C(47)-C(52)	3.25(3)	C(47)-Fe(3)-C(52)	109.42(3)

The separation distance between the cyclopenta dienyl ligands almost similar (3.266 to 3.331 Å) in all ferrocenyl groups in crystal structure of **3a** as shown Figure S17.

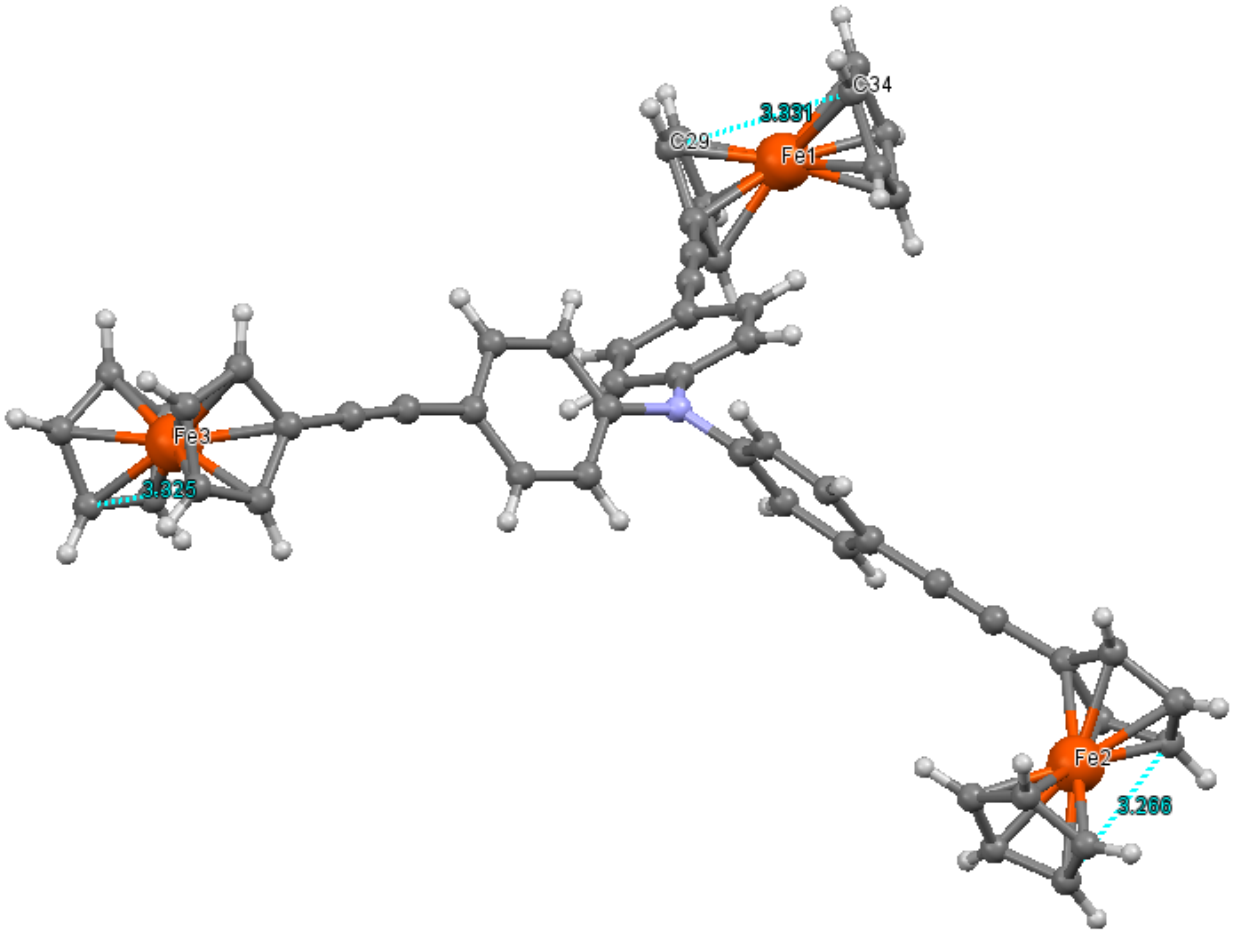

Figure S17. The separation distance between the cyclopenta dienyl ligands in crystal structure of **3a**

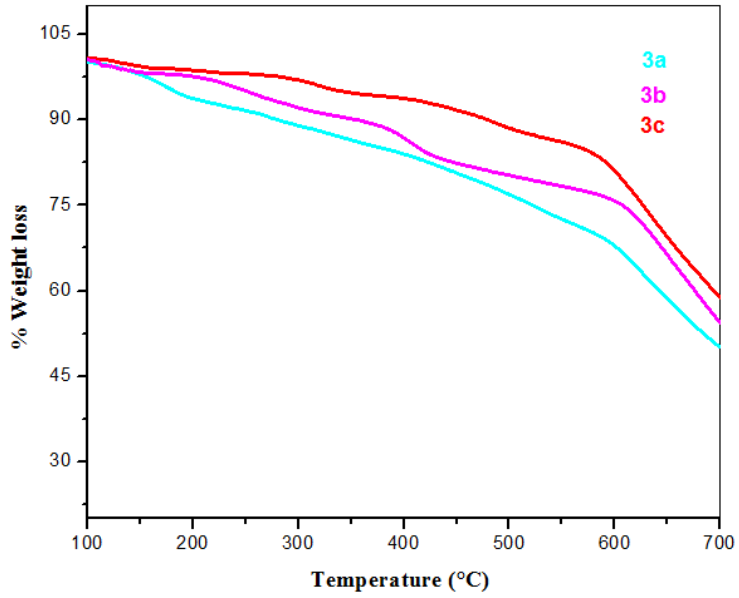

Figure S18. TGA plots of ferrocene substituted Fc-TPA **3a**–**3c**.

Table S2. Crystallographic data and structure refinement detail for compounds Fc-TPA 3a

Compound	**3a**
Empirical formula	$C_{55}\ H_{41}\ Cl_2\ Fe_3\ N$
Formula weight	954.34
Crystal system	Monoclinic
Space group	P 21/c
Unit cell dimensions	
a (A°)	a = 13.9874(10) A
b (A°)	b = 20.9683(12) A
c (A°)	c = 16.3109(13) A
Volume	4463.4(5) A^3

Z, Calculated density	4, 1.420 Mg/m^3
Absorption coefficient	9.107 mm^-1
Max. and min. transmission F (000)	1960
Crystal size	0.33 x 0.26 x 0.21 mm
Theta range for data collection	3.39 to 39.99 deg
Completeness to theta	39.99 100.0 %
Reflections collected / unique	11025 / 2706 [R(int) = 0.0698]
Data / restraints / parameters	8692 / 42 / 551
Goodness-of-fit on F^2	1.128
Refinement method	Full-matrix least-squares on F^2
Final R indices [I>2sigma (I)]	R1 = 0.1217, wR2 = 0.3216
R indices (all data)	R1 = 0.1715, wR2 = 0.3849
Largest diff. peak and hole	1.184 and -0.753 e.A^-3
Extinction coefficient	0.0029 (4)

VII. DFT Calculations.

TD-DFT calculation data of the FC-TPA **3a-3c**. Calculation method:TD-DFT/CAM-B3LYP/6-31+G** for C, H, N and Lanl2DZ for Fe with Gaussian 09[1].

Data for compound **3a**:

26	-4.236805000	8.663352000	0.414613000
26	-5.577328000	-7.898317000	0.418240000
26	9.723240000	-0.765459000	0.427317000
7	0.058368000	-0.001977000	-0.742525000
6	-0.420263000	1.334830000	-0.744113000
6	-1.513266000	1.703570000	-1.547780000
1	-1.988286000	0.960630000	-2.179415000
6	-1.987089000	3.009069000	-1.542081000
1	-2.829676000	3.277701000	-2.171185000
6	-1.376422000	3.999297000	-0.743936000
6	-0.274638000	3.623167000	0.053241000
1	0.205507000	4.366605000	0.681456000
6	0.190073000	2.314488000	0.058517000
1	1.029309000	2.043335000	0.690020000
6	-1.857798000	5.339492000	-0.741259000
6	-2.261777000	6.488164000	-0.742144000
6	1.454891000	-0.255680000	-0.741821000
6	2.324361000	0.519566000	-1.529154000
1	1.921736000	1.313671000	-2.148727000
6	3.691262000	0.274138000	-1.524762000

1	4.347706000	0.878688000	-2.142408000
6	4.239779000	-0.765480000	-0.744403000
6	3.360105000	-1.542423000	0.038739000
1	3.760744000	-2.341428000	0.654349000
6	1.994984000	-1.287559000	0.045881000
1	1.338042000	-1.887802000	0.666136000
6	5.639879000	-1.025370000	-0.749390000
6	6.835138000	-1.257385000	-0.764695000
6	-0.861087000	-1.083466000	-0.752019000
6	-0.627007000	-2.217240000	-1.549825000
1	0.262497000	-2.262594000	-2.168967000
6	-1.526890000	-3.275071000	-1.557105000
1	-1.333881000	-4.140261000	-2.183265000
6	-2.702981000	-3.233337000	-0.778861000
6	-2.932711000	-2.090271000	0.015763000
1	-3.825806000	-2.040496000	0.630416000
6	-2.025514000	-1.039027000	0.034705000
1	-2.214648000	-0.175324000	0.663057000
6	-3.634287000	-4.310467000	-0.798314000
6	-4.440375000	-5.222644000	-0.827140000
6	-2.717170000	7.831459000	-0.748423000
6	-2.204161000	8.909943000	0.059438000
1	-1.429220000	8.814233000	0.807006000
6	-2.903086000	10.099336000	-0.291407000
1	-2.759732000	11.072504000	0.157701000

6	-3.856594000	9.775306000	-1.304791000
1	-4.560564000	10.460555000	-1.756617000
6	-3.752350000	8.383541000	-1.586565000
1	-4.346733000	7.822257000	-2.293840000
6	-5.047950000	7.181050000	1.626906000
1	-4.714095000	6.152243000	1.619930000
6	-4.509451000	8.231859000	2.430348000
1	-3.705838000	8.135519000	3.147734000
6	-5.192477000	9.440334000	2.091093000
1	-4.994430000	10.419996000	2.504345000
6	-6.151562000	9.135836000	1.077713000
1	-6.806989000	9.844389000	0.589721000
6	-6.061488000	7.739226000	0.789804000
1	-6.638646000	7.204374000	0.047809000
6	-5.390933000	-6.274084000	-0.878238000
6	-6.692046000	-6.280622000	-0.256921000
1	-7.085957000	-5.494642000	0.372046000
6	-7.345075000	-7.496066000	-0.606648000
1	-8.327839000	-7.803321000	-0.276245000
6	-6.462191000	-8.256472000	-1.433247000
1	-6.659546000	-9.240455000	-1.836036000
6	-5.258007000	-7.515464000	-1.599307000
1	-4.383721000	-7.822353000	-2.156051000
6	-5.129474000	-9.734304000	1.287435000
1	-5.310279000	-10.691124000	0.816551000

6	-6.051540000	-9.015263000	2.107497000
1	-7.053136000	-9.331933000	2.365184000
6	-3.943561000	-8.947446000	1.161443000
1	-3.068078000	-9.205462000	0.581233000
6	-4.132692000	-7.743253000	1.905598000
1	-3.430670000	-6.923359000	1.975339000
6	-5.435515000	-7.783681000	2.489293000
1	-5.887697000	-7.005993000	3.089693000
6	8.224050000	-1.542850000	-0.798728000
6	8.896876000	-2.601449000	-0.087754000
1	8.425339000	-3.284193000	0.605186000
6	10.273750000	-2.573549000	-0.448423000
1	11.041874000	-3.229087000	-0.061720000
6	10.472761000	-1.501281000	-1.371536000
1	11.417361000	-1.204665000	-1.806399000
6	9.219980000	-0.860349000	-1.586958000
1	9.034616000	-0.003727000	-2.219749000
6	9.885575000	1.234185000	0.976113000
1	9.735004000	2.065928000	0.301438000
6	11.122123000	0.558424000	1.213378000
1	12.071114000	0.787401000	0.747816000
6	10.875629000	-0.500963000	2.138805000
1	11.605414000	-1.214571000	2.496541000
6	9.486807000	-0.480532000	2.473940000
1	8.981203000	-1.173867000	3.132245000

6	8.876083000	0.592691000	1.756237000
1	7.824573000	0.845932000	1.766088000

Total Energy, E(TD-HF/TD-KS) = -2506.10729703

Data for compound **3b**:

7	-0.032105000	-0.041160000	-0.388239000
6	-1.271261000	-0.732314000	-0.401691000
6	-2.336062000	-0.280412000	-1.201596000
1	-2.204704000	0.598800000	-1.822948000
6	-3.551344000	-0.951676000	-1.205443000
1	-4.362276000	-0.591964000	-1.830506000
6	-3.744092000	-2.108858000	-0.421047000
6	-2.667558000	-2.561743000	0.370950000
1	-2.796498000	-3.444570000	0.988762000
6	-1.456798000	-1.882496000	0.386017000
1	-0.647578000	-2.237953000	1.014659000
6	1.186393000	-0.770183000	-0.369574000
6	1.349013000	-1.913527000	-1.171456000
1	0.537617000	-2.236711000	-1.814696000
6	2.540348000	-2.626550000	-1.151539000
1	2.652916000	-3.503589000	-1.780663000
6	3.618558000	-2.214972000	-0.339442000
6	3.448361000	-1.064361000	0.459795000
1	4.261130000	-0.736560000	1.099800000

6	2.252394000	-0.359231000	0.449930000
1	2.136652000	0.515048000	1.081469000
6	-0.006972000	1.377691000	-0.398448000
6	-0.926158000	2.116904000	0.367363000
1	-1.654979000	1.596610000	0.979306000
6	-0.905239000	3.505108000	0.350483000
1	-1.618804000	4.060829000	0.950217000
6	0.045555000	4.207415000	-0.420338000
6	0.969525000	3.458302000	-1.179759000
1	1.703240000	3.977953000	-1.787478000
6	0.939022000	2.070372000	-1.174939000
1	1.647895000	1.513914000	-1.778468000
6	4.844865000	-2.936414000	-0.329936000
6	5.897948000	-3.549010000	-0.324902000
6	7.130565000	-4.260654000	-0.323843000
6	7.318929000	-5.386088000	-1.154799000
6	8.199782000	-3.857010000	0.501870000
6	8.524795000	-6.074074000	-1.154174000
1	6.507174000	-5.714302000	-1.796253000
6	9.405196000	-4.549114000	0.490972000
1	8.078263000	-2.989858000	1.143229000
6	9.596270000	-5.673821000	-0.332430000
1	8.634594000	-6.944531000	-1.793297000
1	10.218165000	-4.199737000	1.119589000
6	0.074030000	5.629809000	-0.432122000

6	0.102729000	6.847768000	-0.444068000
6	0.142422000	8.270359000	-0.459991000
6	1.128241000	8.958376000	-1.199884000
6	-0.800216000	9.032115000	0.260559000
6	1.168429000	10.345939000	-1.209235000
1	1.863510000	8.390487000	-1.761144000
6	-0.755210000	10.421277000	0.239814000
1	-1.572068000	8.523206000	0.829186000
6	0.231516000	11.111400000	-0.488198000
1	1.948357000	10.845583000	-1.774909000
1	-1.507887000	10.979716000	0.787281000
6	-4.989753000	-2.796213000	-0.426623000
6	-6.058809000	-3.380593000	-0.429446000
6	-7.311901000	-4.055395000	-0.433303000
6	-7.514268000	-5.217851000	0.338451000
6	-8.388387000	-3.576992000	-1.211185000
6	-8.741910000	-5.869874000	0.330662000
1	-6.697112000	-5.607712000	0.937063000
6	-9.612346000	-4.231857000	-1.207492000
1	-8.252903000	-2.683315000	-1.812125000
6	-9.820898000	-5.390868000	-0.434942000
1	-8.860639000	-6.774690000	0.918353000
1	-10.425300000	-3.830225000	-1.804093000
6	10.887308000	-6.383713000	-0.354482000
6	11.906268000	-6.344074000	0.658569000

6	11.383294000	-7.225596000	-1.409913000
26	11.299808000	-8.310416000	0.356493000
6	13.010544000	-7.134070000	0.224756000
1	11.835728000	-5.831591000	1.608013000
6	12.687841000	-7.677382000	-1.055399000
1	10.858343000	-7.471166000	-2.322625000
6	11.352424000	-10.389696000	0.431164000
6	10.041963000	-9.942298000	0.078971000
6	9.554953000	-9.122752000	1.142759000
6	11.675381000	-9.845138000	1.711420000
6	10.564243000	-9.062035000	2.151593000
1	13.916818000	-7.318173000	0.785340000
1	13.309814000	-8.339673000	-1.642004000
1	11.999860000	-11.004248000	-0.179599000
1	9.521418000	-10.162830000	-0.843102000
1	8.606064000	-8.604026000	1.160497000
1	12.609372000	-9.976963000	2.240741000
1	10.508941000	-8.498406000	3.073010000
6	0.263649000	12.584312000	-0.513520000
6	-0.376737000	13.472993000	0.417613000
6	0.925986000	13.410747000	-1.487000000
26	1.670250000	13.835530000	0.402221000
6	-0.123570000	14.816056000	0.013050000
1	-0.929881000	13.177242000	1.298176000
6	0.681077000	14.777451000	-1.165388000

1	1.509908000	13.057505000	-2.325583000
6	3.451065000	14.851669000	0.758455000
6	3.721130000	13.493426000	0.406372000
6	3.080528000	12.652967000	1.367287000
6	2.643275000	14.849882000	1.936317000
6	2.413415000	13.490719000	2.312424000
1	-0.453386000	15.706637000	0.530393000
1	1.062642000	15.633169000	-1.705633000
1	3.774404000	15.726620000	0.210812000
1	4.287008000	13.159967000	-0.452987000
1	3.065723000	11.571544000	1.355063000
1	2.247708000	15.723515000	2.436535000
1	1.815335000	13.155057000	3.148641000
6	-11.114428000	-6.096459000	-0.445956000
6	-11.582425000	-7.047045000	0.525920000
6	-12.143805000	-5.982188000	-1.443953000
26	-12.915949000	-5.456997000	0.409277000
6	-12.866198000	-7.516777000	0.121746000
1	-11.065597000	-7.333165000	1.431359000
6	-13.212634000	-6.859038000	-1.097017000
1	-12.113853000	-5.341223000	-2.313959000
6	-14.679383000	-4.378328000	0.650431000
6	-13.604647000	-3.496800000	0.319614000
6	-12.605699000	-3.619575000	1.333086000
6	-14.343382000	-5.046476000	1.867278000

6	-13.061422000	-4.577544000	2.289260000
1	-13.484394000	-8.218221000	0.665169000
1	-14.135785000	-6.981041000	-1.646969000
1	-15.574894000	-4.536689000	0.064947000
1	-13.545463000	-2.867898000	-0.558309000
1	-11.652246000	-3.109160000	1.348862000
1	-14.940385000	-5.798739000	2.364794000
1	-12.518344000	-4.910906000	3.163149000

Total Energy, E(TD-HF/TD-KS) = -3199.29055022

Data for compound **3c**:

7	-0.003483000	-0.040789000	-0.774334000
6	1.289872000	-0.625478000	-0.755049000
6	1.576664000	-1.753369000	-1.544405000
1	0.804517000	-2.172871000	-2.180220000
6	2.839741000	-2.329238000	-1.520774000
1	3.047267000	-3.196590000	-2.139000000
6	3.867301000	-1.789980000	-0.717794000
6	3.573232000	-0.654141000	0.066569000
1	4.346329000	-0.230124000	0.699098000
6	2.306400000	-0.086944000	0.053661000
1	2.096275000	0.776366000	0.675622000
6	-0.142946000	1.371432000	-0.769582000
6	0.711888000	2.176852000	-1.543252000

1	1.475237000	1.712564000	-2.158106000
6	0.583977000	3.559051000	-1.530004000
1	1.249221000	4.166638000	-2.134866000
6	-0.413589000	4.187716000	-0.754624000
6	-1.273571000	3.372272000	0.011585000
1	-2.041406000	3.835621000	0.622574000
6	-1.136029000	1.990930000	0.010147000
1	-1.796211000	1.383605000	0.619624000
6	-1.156181000	-0.868704000	-0.773811000
6	-1.205870000	-2.026126000	0.023386000
1	-0.357834000	-2.283859000	0.648437000
6	-2.333517000	-2.835708000	0.023264000
1	-2.359345000	-3.722187000	0.648618000
6	-3.459582000	-2.510940000	-0.762915000
6	-3.403199000	-1.346206000	-1.557812000
1	-4.253808000	-1.083938000	-2.178502000
6	-2.270095000	-0.544250000	-1.568578000
1	-2.241319000	0.339254000	-2.197011000
6	-0.547483000	5.603594000	-0.742995000
6	-0.661650000	6.816548000	-0.729294000
6	-0.795820000	8.232211000	-0.707925000
6	0.095254000	9.054234000	-1.431930000
6	-1.822873000	8.847916000	0.040539000
6	-0.034301000	10.435338000	-1.406944000
1	0.888934000	8.594810000	-2.012041000

6	-1.952502000	10.228868000	0.065214000
1	-2.515302000	8.228420000	0.601158000
6	-1.060360000	11.051072000	-0.657349000
1	0.658029000	11.054694000	-1.967913000
1	-2.746441000	10.688307000	0.645005000
6	-4.620283000	-3.332742000	-0.749336000
6	-5.615214000	-4.035754000	-0.730481000
6	-6.776829000	-4.855717000	-0.701352000
6	-7.915339000	-4.524756000	-1.468260000
6	-6.818653000	-6.018393000	0.098990000
6	-9.049938000	-5.322535000	-1.434543000
1	-7.897112000	-3.634448000	-2.088370000
6	-7.953124000	-6.816021000	0.132577000
1	-5.950673000	-6.285315000	0.693025000
6	-9.092514000	-6.483969000	-0.632641000
1	-9.917798000	-5.055528000	-2.028778000
1	-7.971273000	-7.706493000	0.752527000
6	5.164732000	-2.372358000	-0.697233000
6	6.278814000	-2.865076000	-0.674545000
6	7.583169000	-3.430797000	-0.638959000
6	8.581654000	-2.881033000	0.194749000
6	7.910685000	-4.551272000	-1.433251000
6	9.855111000	-3.429413000	0.232834000
1	8.343804000	-2.019619000	0.810292000
6	9.184790000	-5.099595000	-1.395305000

1	7.153393000	-4.984030000	-2.078808000
6	10.182948000	-4.549988000	-0.561578000
1	10.612754000	-2.996385000	0.877852000
1	9.422498000	-5.960572000	-2.011588000
6	-1.192178000	12.467650000	-0.628758000
6	-1.310565000	13.679470000	-0.607911000
6	-1.460579000	15.089121000	-0.594641000
6	-2.501240000	15.831103000	0.073607000
6	-0.621010000	16.047140000	-1.270765000
26	-0.639648000	16.433866000	0.770124000
6	-2.308133000	17.213432000	-0.204579000
1	-3.280255000	15.398075000	0.685249000
6	-1.150721000	17.346493000	-1.031937000
1	0.261540000	15.805714000	-1.846252000
6	0.791556000	17.615710000	1.709823000
6	1.307833000	16.302232000	1.486026000
6	0.467826000	15.375545000	2.175375000
6	-0.367728000	17.499683000	2.535709000
6	-0.568826000	16.114364000	2.822755000
1	-2.913917000	18.024868000	0.174724000
1	-0.728535000	18.276346000	-1.387417000
1	1.189397000	18.533715000	1.299003000
1	2.165913000	16.051367000	0.877499000
1	0.570562000	14.298825000	2.168265000
1	-1.001543000	18.314210000	2.859196000

1	-1.379608000	15.696178000	3.403634000
6	-10.256767000	-7.301200000	-0.593713000
6	-11.248746000	-8.006829000	-0.561937000
6	-12.395920000	-8.839282000	-0.534190000
6	-12.542893000	-10.066253000	0.209304000
6	-13.620829000	-8.636152000	-1.267711000
26	-14.017786000	-8.714407000	0.770317000
6	-13.827308000	-10.607440000	-0.078391000
1	-11.800807000	-10.483992000	0.875045000
6	-14.490885000	-9.727244000	-0.987719000
1	-13.831576000	-7.790351000	-1.906961000
6	-15.794349000	-8.051642000	1.626446000
6	-14.945278000	-6.940298000	1.333374000
6	-13.729276000	-7.110896000	2.062483000
6	-15.102077000	-8.908739000	2.535135000
6	-13.824682000	-8.327750000	2.804104000
1	-14.241856000	-11.511386000	0.346151000
1	-15.495102000	-9.849073000	-1.369684000
1	-16.775290000	-8.230150000	1.207334000
1	-15.171873000	-6.128518000	0.655661000
1	-12.868228000	-6.457479000	2.023090000
1	-15.467405000	-9.849174000	2.924926000
1	-13.053999000	-8.749658000	3.434661000
6	11.490931000	-5.108948000	-0.519404000
6	12.616556000	-5.572109000	-0.481659000

6	13.935529000	-6.089978000	-0.438633000
6	15.000891000	-5.632438000	0.418901000
6	14.475240000	-7.142324000	-1.264060000
26	14.646844000	-7.654728000	0.742029000
6	16.170921000	-6.381101000	0.110328000
1	14.907734000	-4.860846000	1.170150000
6	15.847533000	-7.310613000	-0.925635000
1	13.918475000	-7.704251000	-2.000718000
6	15.018011000	-9.589469000	1.409059000
6	13.641253000	-9.447824000	1.053595000
6	13.078392000	-8.421968000	1.872155000
6	15.305195000	-8.650079000	2.445731000
6	14.106093000	-7.927332000	2.731672000
1	17.129840000	-6.285566000	0.600815000
1	16.519410000	-8.040823000	-1.355270000
1	15.726954000	-10.264795000	0.949629000
1	13.124063000	-9.999478000	0.280422000
1	12.063416000	-8.052024000	1.818310000
1	16.269256000	-8.490186000	2.909108000
1	14.002196000	-7.126723000	3.451325000

Total Energy, E(TD-HF/TD-KS) = -3427.75497756

1. a) A. D. Becke. *J. Chem. Phys.* 1993, **98**, 5648-5652; b) C. T. Lee, W. T. Yang, R. G. Parr. *Phys. Rev. B.* 1988, **37**, 785-789.