Supplementary Material For

Ferrocenyl Induced the One-Pot Synthesis of 3,3'-Ferrocenylbiindoles

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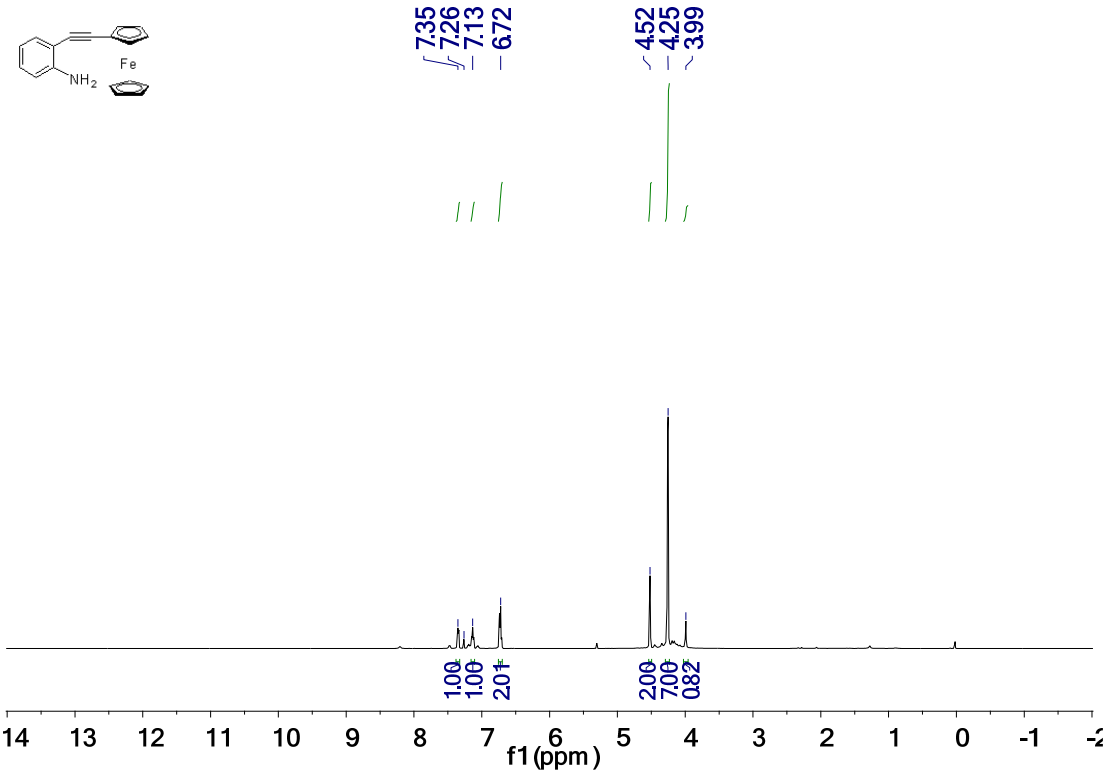
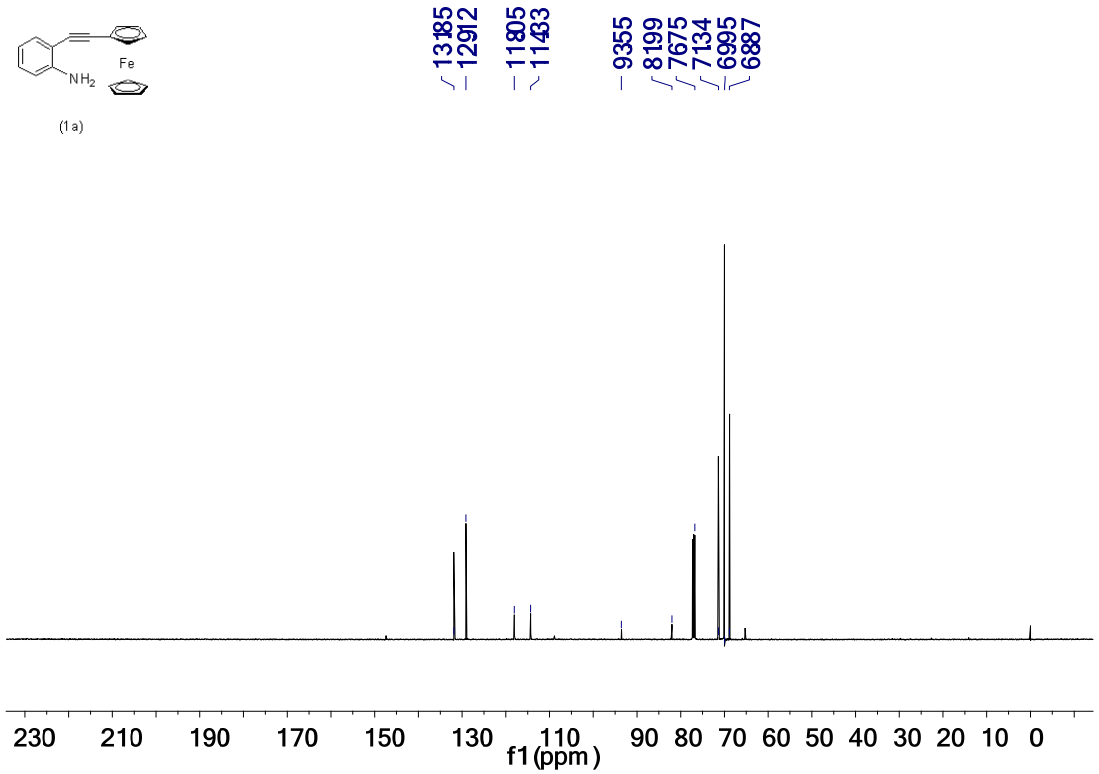
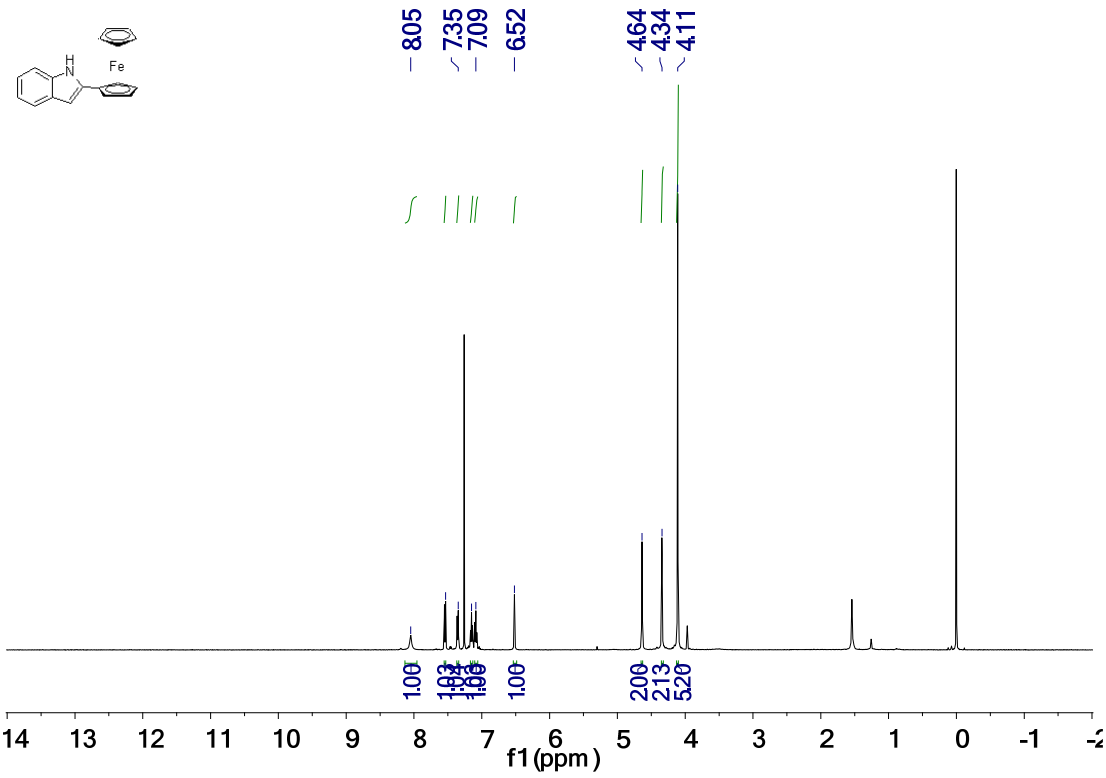
^{1}H and ^{13}C NMR spectra for 1a, 2a and 3a and the 2D COSY ,2D HSQC , 2D HMQC of 2-ferrocenylindoles (2a)



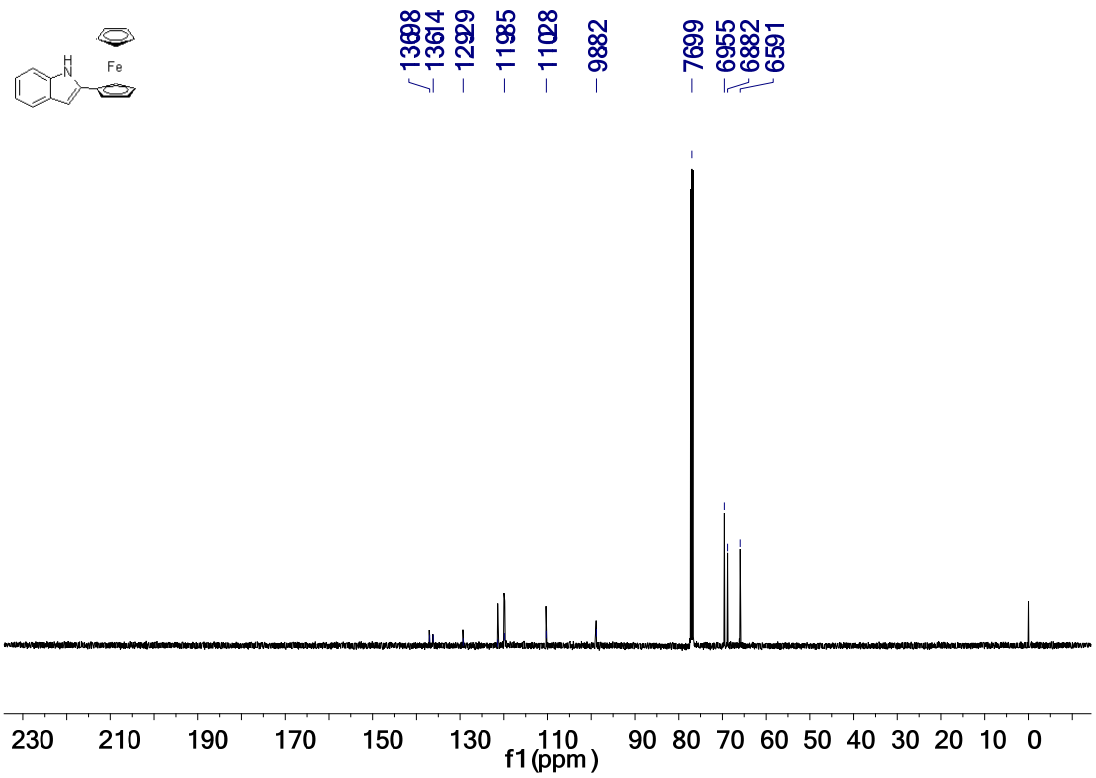
^{1}H-NMR spectrum of2-Ferrocenethynylanilines (**1a**)in $CDCl_3$ at 25℃



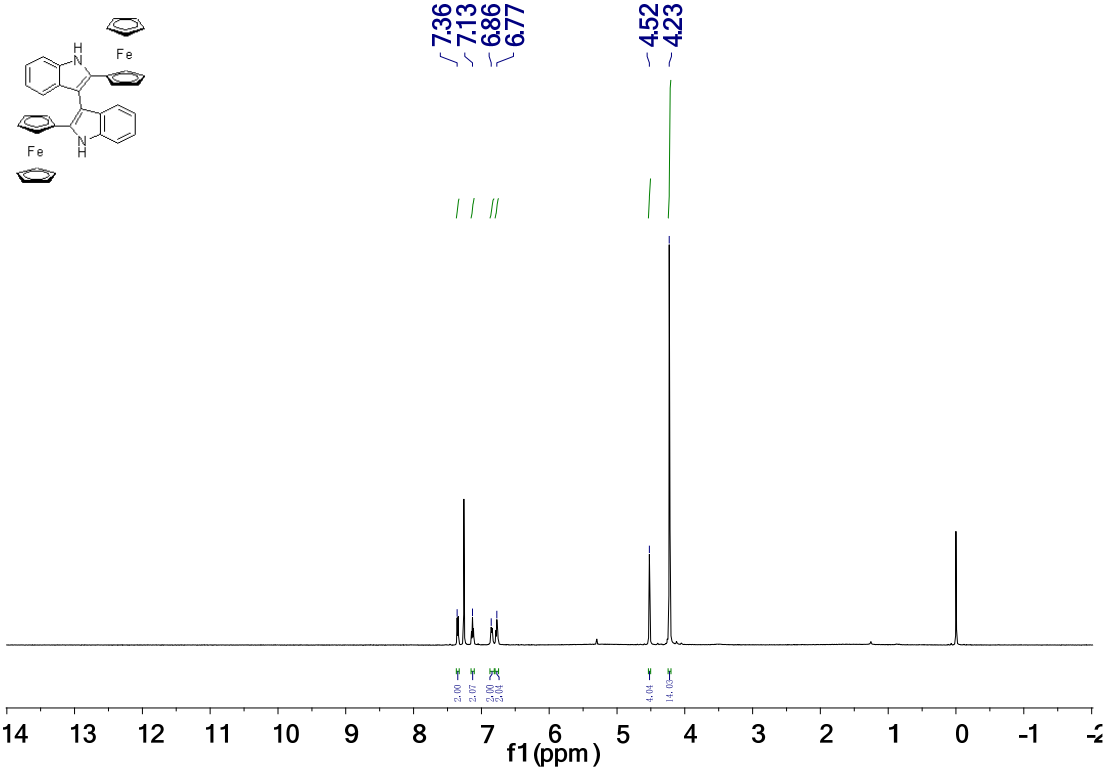
^{13}C-NMR spectrum of2-Ferrocenethynylanilines (**1a**)in $CDCl_3$ at 25℃



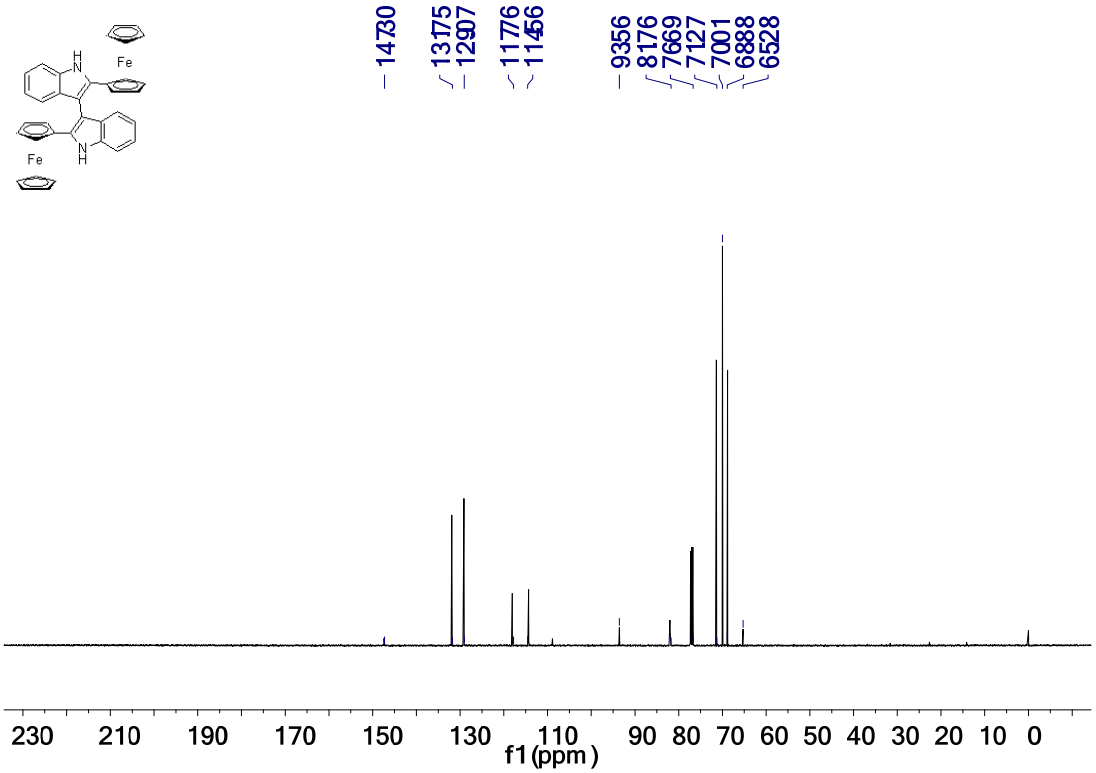
^{1}H-NMR spectrum of2-Ferrocenylindoles (**2a**)in $CDCl_3$ at 25℃



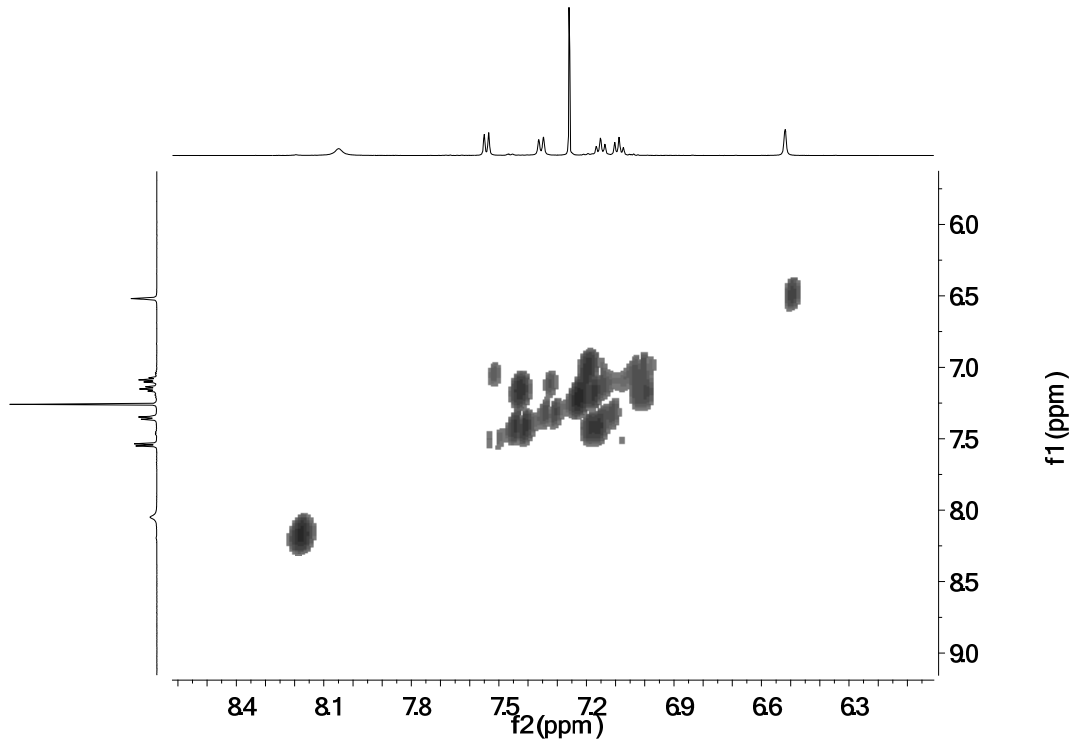
^{13}C-NMR spectrum of 2-Ferrocenylindoles (**2a**)in $CDCl_3$ at 25℃



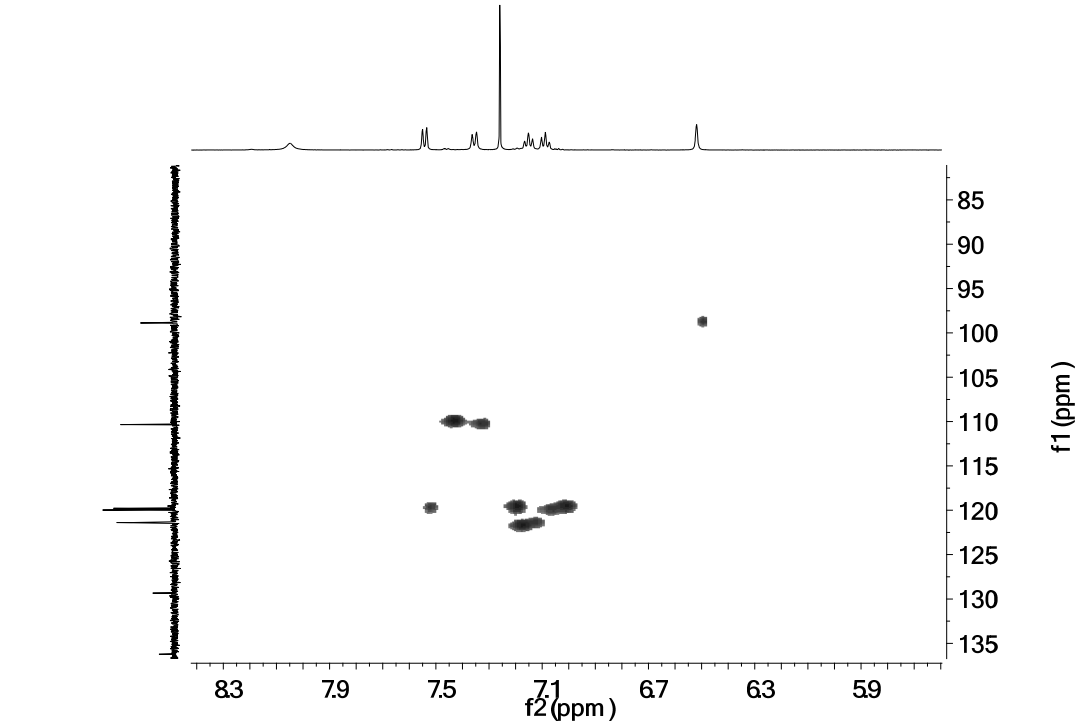
^{1}H-NMR spectrum of3,3'-Ferrocenylbiindoles (**3a**)in $CDCl_3$ at 25℃



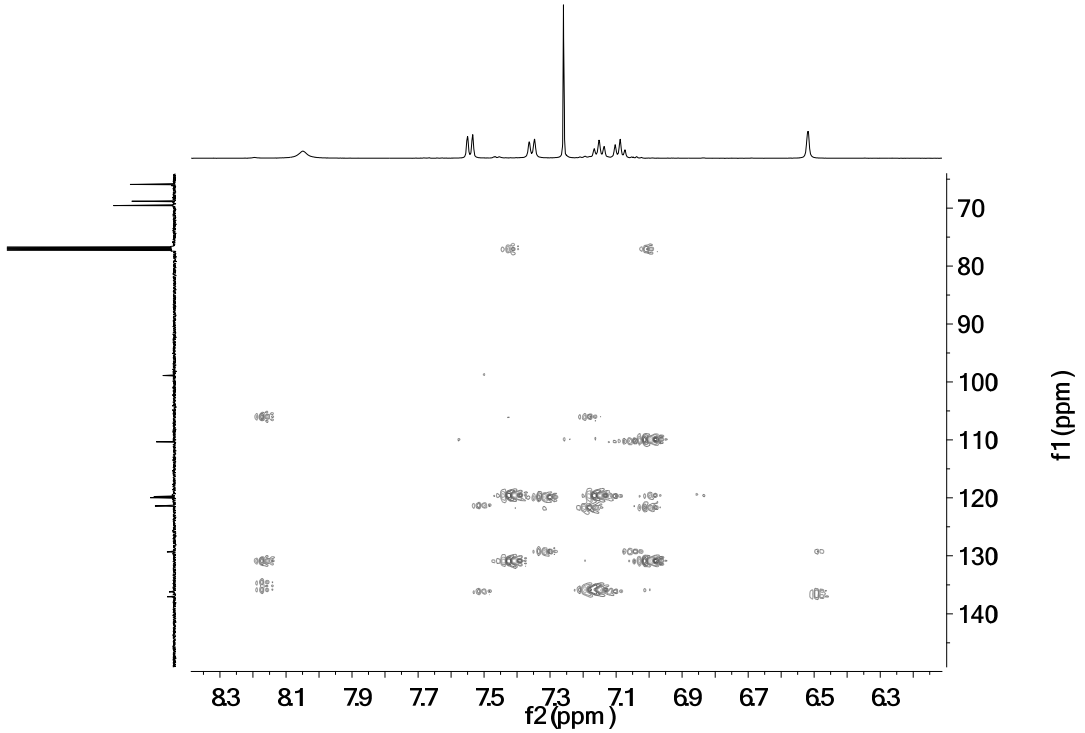
^{13}C-NMR spectrum of 3,3'-Ferrocenylbiindoles (**3a**)in $CDCl_3$ at 25℃



2D COSY of 2-ferrocenylindoles (**2a**)



2D HSQC of 2-ferrocenylindoles (2a)



The 2D HMQC of 2-ferrocenylindoles (**2a**)

All calculations were performed by using gaussian09 program. The geometry optimizations, frequency analysis and thermodynamic corrections were performed at the B3LYP(D3BJ)//MDF10 (for Fe)/Def2SVP(for others) level of theory.

2a

Sum of electronic and thermal Free Energies= -872.957735 Hartree

C	5.07406000	1.09542500	-0.44760800
C	5.34641600	0.20048200	0.60903900
C	4.36775900	-0.66410400	1.08995500
C	3.08579100	-0.63828400	0.50953200
C	2.83502100	0.27017000	-0.56343100
C	3.81746900	1.14091600	-1.04815400
C	1.86094600	-1.35254700	0.74210400
C	0.92645800	-0.88126500	-0.15930400
N	1.52447800	0.08837800	-0.95236900
H	5.86246600	1.76338700	-0.80241000
H	6.34387000	0.18958800	1.05476400
H	4.58805700	-1.35323600	1.90894000
H	3.60822700	1.83162200	-1.86862000
H	1.68977800	-2.14014400	1.47191600
H	1.02850300	0.65425600	-1.62660200
C	-0.47192800	-1.24381300	-0.33992100
C	-1.33720300	-1.79244100	0.66408300
C	-1.25716100	-1.07023300	-1.53151400
C	-2.63385700	-1.96141200	0.09508000
C	-2.58549800	-1.51459800	-1.26019900
H	-0.89911200	-0.67700100	-2.48135300
H	-3.51455300	-2.33456700	0.61403500
H	-3.41927800	-1.49551700	-1.95940000
H	-1.05122800	-2.00449200	1.69201400
Fe	-2.06126900	0.02474900	0.01297600
C	-2.09960800	1.28088300	1.64922600
C	-3.41451700	1.13695700	1.10899000
C	-1.25903800	1.82199700	0.62962500
H	-1.78434600	0.99877800	2.65209400
C	-3.38747600	1.58906100	-0.24547000
H	-4.27884300	0.72803700	1.62914000
C	-2.05536600	2.01305100	-0.54154700
H	-0.19059800	2.01142100	0.71874100
H	-4.22796200	1.58894500	-0.93718200
H	-1.70695100	2.39533800	-1.49978500

INT1

Sum of electronic and thermal Free Energies= -872.735544Hartree

C	-5.28724100	0.55311300	-0.79796600
C	-5.32428000	0.73905700	0.60765000
C	-4.22333900	0.45481700	1.39670500

C	-3.04969500	-0.02728200	0.77214000
C	-3.03342500	-0.20092000	-0.64816400
C	-4.15124500	0.08316500	-1.44469800
C	-1.77055200	-0.42480700	1.25017300
C	-1.01248600	-0.82125800	0.14824700
N	-1.78701400	-0.66845700	-0.99562800
H	-6.17735700	0.78503200	-1.38667100
H	-6.24172300	1.10980700	1.06853400
H	-4.25669000	0.59388400	2.47916600
H	-4.13357400	-0.05851500	-2.52702900
H	-1.43360500	-0.42157900	2.28436800
H	-1.52672500	-0.96510100	-1.92638000
C	0.34448700	-1.28551900	0.11146100
C	1.14097300	-1.55943600	-1.05294600
C	1.21948100	-1.42722900	1.24528000
C	2.44920400	-1.94724500	-0.63613700
H	0.80859400	-1.49824700	-2.08775500
C	2.49540000	-1.87070600	0.78884400
H	0.93899500	-1.25366500	2.28198100
H	3.26562100	-2.24094300	-1.29362200
H	3.35463300	-2.09552900	1.41834300
Fe	2.11537900	-0.00091300	-0.00953500
C	1.56246400	2.07743200	-0.08251800
C	2.30224600	1.72649500	-1.24534000
C	2.37324000	1.81308000	1.05588600
H	0.52963500	2.42398200	-0.06256200
C	3.58520300	1.25343300	-0.83076700
H	1.94602100	1.79134300	-2.27246700
C	3.62970000	1.30558000	0.59692900
H	2.08133000	1.95759200	2.09499700
H	4.38331300	0.91050400	-1.48717000
H	4.46994700	1.01373200	1.22490900

INT2

Sum of electronic and thermal Free Energies= -1745.669100Hartree

C	-1.00739200	-3.80894700	2.78789900
C	-0.82848100	-4.58745300	1.63837100
C	-0.21510500	-4.06251700	0.49258400
C	0.20435900	-2.73721900	0.54639400
C	0.03758300	-1.94264700	1.69196500
C	-0.57099300	-2.47365100	2.82045400
N	0.80912600	-1.95906200	-0.45045700
C	1.05801100	-0.68768000	-0.04045200

C	0.55152000	-0.54701600	1.39901900
C	-0.03727000	1.94279100	1.69196000
C	0.57152900	2.47378500	2.82033200
C	1.00791900	3.80908200	2.78770000
C	0.82876500	4.58760000	1.63821800
C	0.21514800	4.06267800	0.49255500
C	-0.20428900	2.73737300	0.54643600
N	-0.80927300	1.95922000	-0.45029200
C	-1.05805100	0.68783700	-0.04025000
C	-0.55127600	0.54716400	1.39911700
H	-1.48495900	-4.24428100	3.66743200
H	-1.17168500	-5.62403100	1.63101400
H	-0.08429400	-4.66871100	-0.40557700
H	-0.71167200	-1.86930200	3.71995400
H	1.37045200	-0.26395600	2.08430400
H	0.71239100	1.86942700	3.71979800
H	1.48566800	4.24440800	3.66713900
H	1.17196400	5.62418000	1.63080000
H	0.08414400	4.66888400	-0.40557000
H	-1.09006300	2.32172800	-1.35302200
H	-1.37007100	0.26411000	2.08456800
H	1.08961600	-2.32154600	-1.35328900
C	1.89743000	0.21104300	-0.76168100
C	2.54556100	1.39653900	-0.24436700
C	2.38951600	0.01550300	-2.11017100
C	3.37614900	1.92741000	-1.26721300
H	2.42763300	1.80377700	0.75491300
C	3.27965600	1.08156900	-2.41376900
H	2.11511300	-0.78907200	-2.79004800
H	4.00815200	2.80819400	-1.17542600
H	3.81879200	1.21021100	-3.35008900
Fe	3.94957800	-0.00694700	-0.77575300
C	4.46693300	-1.58347700	0.46866800
C	5.11183200	-0.38394900	0.89610300
C	4.87919900	-1.85478300	-0.87100900
H	3.76127400	-2.17322700	1.05233500
C	5.93030600	0.08204300	-0.17772600
H	4.99154700	0.09929400	1.86400700
C	5.78697200	-0.82529100	-1.26888100
H	4.55965700	-2.69564800	-1.48410700
H	6.53754100	0.98537500	-0.17306400
H	6.26743100	-0.73652800	-2.24144600
C	-1.89753400	-0.21089800	-0.76141400
C	-2.54558800	-1.39645600	-0.24415300

C	-2.38951900	-0.01542900	-2.10995000
C	-3.37605100	-1.92741200	-1.26707000
H	-2.42769900	-1.80368800	0.75513000
C	-3.27952900	-1.08157200	-2.41362500
H	-2.11509300	0.78915000	-2.78981400
H	-4.00797800	-2.80825600	-1.17532300
H	-3.81857100	-1.21028000	-3.34999000
C	-4.87980000	1.85446200	-0.87124500
C	-4.46730200	1.58355400	0.46844800
C	-5.78736100	0.82464400	-1.26878200
H	-4.56055400	2.69526800	-1.48457800
C	-5.11186100	0.38396700	0.89622700
H	-3.76173500	2.17362900	1.05189300
C	-5.93033700	-0.08247100	-0.17739500
H	-6.26791400	0.73555200	-2.24127100
H	-4.99134300	-0.09901900	1.86423000
H	-6.53734300	-0.98595500	-0.17246200
Fe	-3.94970400	0.00687600	-0.77566900

INT3

Sum of electronic and thermal Free Energies= -1745.388615Hartree

C	-1.07741800	-3.81351400	2.39819400
C	-0.83760700	-4.58415400	1.25218100
C	-0.15044300	-4.05416700	0.15129500
C	0.27221900	-2.73511500	0.25654900
C	0.03502900	-1.94455800	1.38713600
C	-0.64360000	-2.48040100	2.47513400
N	0.98030300	-1.94822400	-0.68056000
C	1.26571900	-0.72593400	-0.22587700
C	0.56541800	-0.55444200	1.12095600
C	-0.03471000	1.94497700	1.38707400
C	0.64422700	2.48084400	2.47486900
C	1.07794800	3.81398000	2.39781200
C	0.83772900	4.58462300	1.25188600
C	0.15023800	4.05461800	0.15121400
C	-0.27231700	2.73553900	0.25658000
N	-0.98067500	1.94862400	-0.68030600
C	-1.26578100	0.72627900	-0.22559600
C	-0.56515800	0.55485300	1.12107100
H	-1.60284900	-4.25889500	3.24494300
H	-1.18432100	-5.61873300	1.21675800
H	0.04019500	-4.65572000	-0.73924300
H	-0.83624900	-1.89003200	3.37423300
H	1.30022200	-0.24205900	1.87781400

H	0.83718400	1.89047300	3.37390100
H	1.60362400	4.25937800	3.24440000
H	1.18437400	5.61922200	1.21636700
H	-0.04073100	4.65618000	-0.73924800
H	-1.32912700	2.31234400	-1.56261000
H	-1.29978200	0.24250300	1.87812200
H	1.32851000	-2.31197800	-1.56294200
C	2.08624500	0.20300800	-0.90729200
C	2.66247900	1.41967300	-0.34713100
C	2.79231900	-0.06477700	-2.15456700
C	3.63399000	1.89238500	-1.25838400
H	2.39781300	1.88353700	0.59670300
C	3.71346800	0.98773200	-2.36176700
H	2.62633500	-0.89655500	-2.83697700
H	4.25392600	2.77563800	-1.11841100
H	4.39849600	1.07075000	-3.20349100
Fe	4.08540000	-0.03531400	-0.56477400
C	4.48753400	-1.53386900	0.82121200
C	5.03887300	-0.29345600	1.26068400
C	5.06504900	-1.85857300	-0.44334700
H	3.74206600	-2.12557800	1.35181400
C	5.96923900	0.14423900	0.27016500
H	4.79737000	0.22749000	2.18544000
C	5.98595500	-0.82030700	-0.77978000
H	4.85494700	-2.74362800	-1.04126300
H	6.54783000	1.06598500	0.29879900
H	6.58034400	-0.76243300	-1.69005100
C	-2.08621500	-0.20281700	-0.90690500
C	-2.66220800	-1.41957300	-0.34669500
C	-2.79224200	0.06466000	-2.15429000
C	-3.63350900	-1.89262900	-1.25799400
H	-2.39759100	-1.88326400	0.59723200
C	-3.71307000	-0.98811200	-2.36147700
H	-2.62635400	0.89641000	-2.83675700
H	-4.25325200	-2.77601300	-1.11799100
H	-4.39799200	-1.07138900	-3.20326300
C	-5.06545400	1.85812100	-0.44362200
C	-4.48816700	1.53363300	0.82109600
C	-5.98611700	0.81965800	-0.78016600
H	-4.85536200	2.74314900	-1.04158200
C	-5.03942500	0.29319200	1.26055800
H	-3.74289400	2.12550900	1.35178200
C	-5.96947800	-0.14479300	0.26987700
H	-6.58027600	0.76156000	-1.69057200

H	-4.79805500	-0.22762300	2.18542200
H	-6.54791100	-1.06663900	0.29847800
Fe	-4.08549300	0.03503200	-0.56467500

3a

Sum of electronic and thermal Free Energies= -1744.742008 Hartree

C	2.07070200	0.65277900	4.11726200
C	1.13659500	0.11474700	5.02940500
C	-0.19894900	-0.07024400	4.67355800
C	-0.58062300	0.29245400	3.37652100
C	0.34831800	0.83537000	2.44262500
C	1.68752700	1.01521900	2.82873300
N	-1.79955400	0.22249200	2.73611200
C	-1.68304000	0.68595800	1.43188200
C	-0.36644800	1.07214300	1.21283900
C	0.19219800	2.95262000	-0.49349400
C	-0.36164600	4.13582500	0.02454000
C	-0.20762000	5.31893500	-0.69201600
C	0.48942700	5.34174800	-1.91959200
C	1.04303500	4.18203700	-2.45964200
C	0.88433200	2.99318500	-1.73822300
N	1.29939300	1.70661100	-2.01179600
C	0.91093500	0.85210300	-0.98740500
C	0.22096700	1.58603000	-0.03093300
H	3.10763700	0.78972700	4.43355600
H	1.46533400	-0.16007000	6.03438400
H	-0.91933900	-0.48515100	5.38266800
H	2.40402500	1.43562600	2.12028900
H	-2.65036600	-0.14108400	3.14025500
H	-0.90071200	4.11418200	0.97429700
H	-0.63062400	6.24766500	-0.30197100
H	0.59553500	6.28616200	-2.45865400
H	1.57848200	4.20209800	-3.41195300
H	1.87806800	1.43368800	-2.79314500
C	-2.82258700	0.67605000	0.52715000
C	-2.79947600	0.95154700	-0.88324700
C	-4.17800600	0.33423900	0.86948500
C	-4.12012400	0.79020200	-1.39157800
H	-1.91650200	1.21724500	-1.45567200
C	-4.97224100	0.40799400	-0.31247300
H	-4.54668700	0.06072600	1.85662700
H	-4.41907700	0.90943700	-2.43107800
H	-6.03598500	0.18873700	-0.37921700
H	-1.47209500	-2.47571600	0.77991200

C	-2.23909700	-2.54550800	0.01230400
C	-2.05568000	-2.24669800	-1.37148500
C	-3.61117900	-2.88767300	0.21493100
C	-3.31645200	-2.40356700	-2.02532200
H	-1.12303100	-1.92551100	-1.82886100
C	-4.27844100	-2.80047500	-1.04598500
H	-4.07437500	-3.14409900	1.16630900
H	-3.51660100	-2.22337900	-3.08010400
H	-5.33769000	-2.97783200	-1.22363200
Fe	-3.45323700	-0.97445400	-0.54095000
C	1.21121100	-0.56994500	-1.05051600
C	1.66555200	-1.28383000	-2.21536600
C	1.14787100	-1.51789400	0.02743300
C	1.86801400	-2.64901900	-1.85556700
H	1.82378100	-0.86371600	-3.20702400
C	1.54633300	-2.79133600	-0.47290100
H	0.87367500	-1.28692700	1.05168400
H	2.22376800	-3.43598300	-2.51747900
H	1.61821600	-3.70782900	0.10913300
H	3.97992200	1.16954900	-0.06072200
C	4.30611400	0.13471600	-0.15449800
C	4.79725300	-0.48664800	-1.34421100
C	4.25925800	-0.85559300	0.87375200
C	5.05208700	-1.86223900	-1.05187800
H	4.93458500	-0.00368100	-2.31028700
C	4.72026700	-2.08883900	0.31894800
H	3.89147700	-0.70628600	1.88696900
H	5.41170800	-2.61069800	-1.75588300
H	4.77734000	-3.04191600	0.84176000
Fe	3.06409700	-1.40889400	-0.7106880