Supplementary Information

A concise Friedländer/Buchwald-Hartwig approach to the total synthesis of quindoline, a bioactive natural indoloquinoline alkaloid, and toward the unnatural 10-methylquindoline

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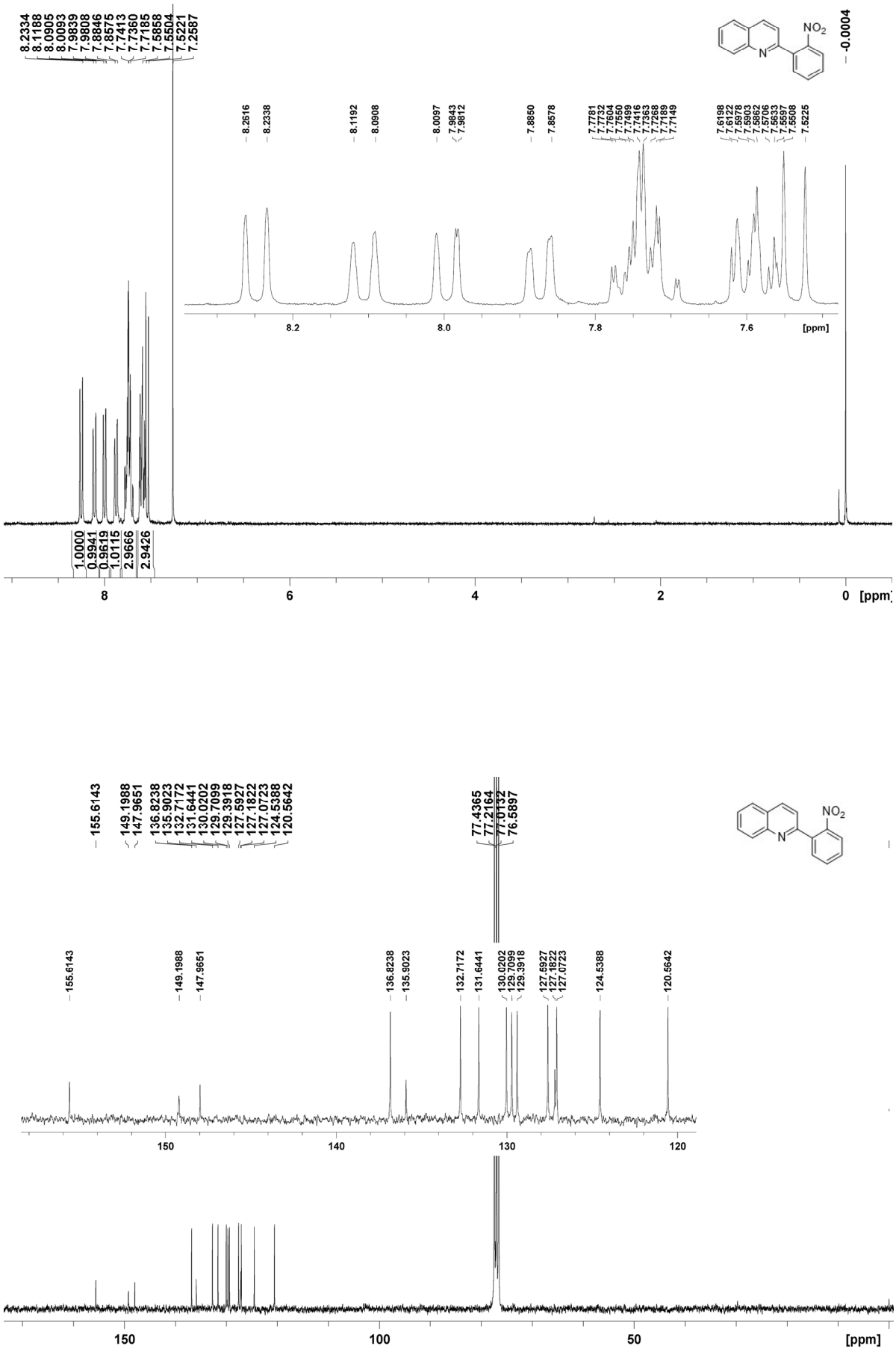


Figure S1. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **17** in $CDCl_3$.

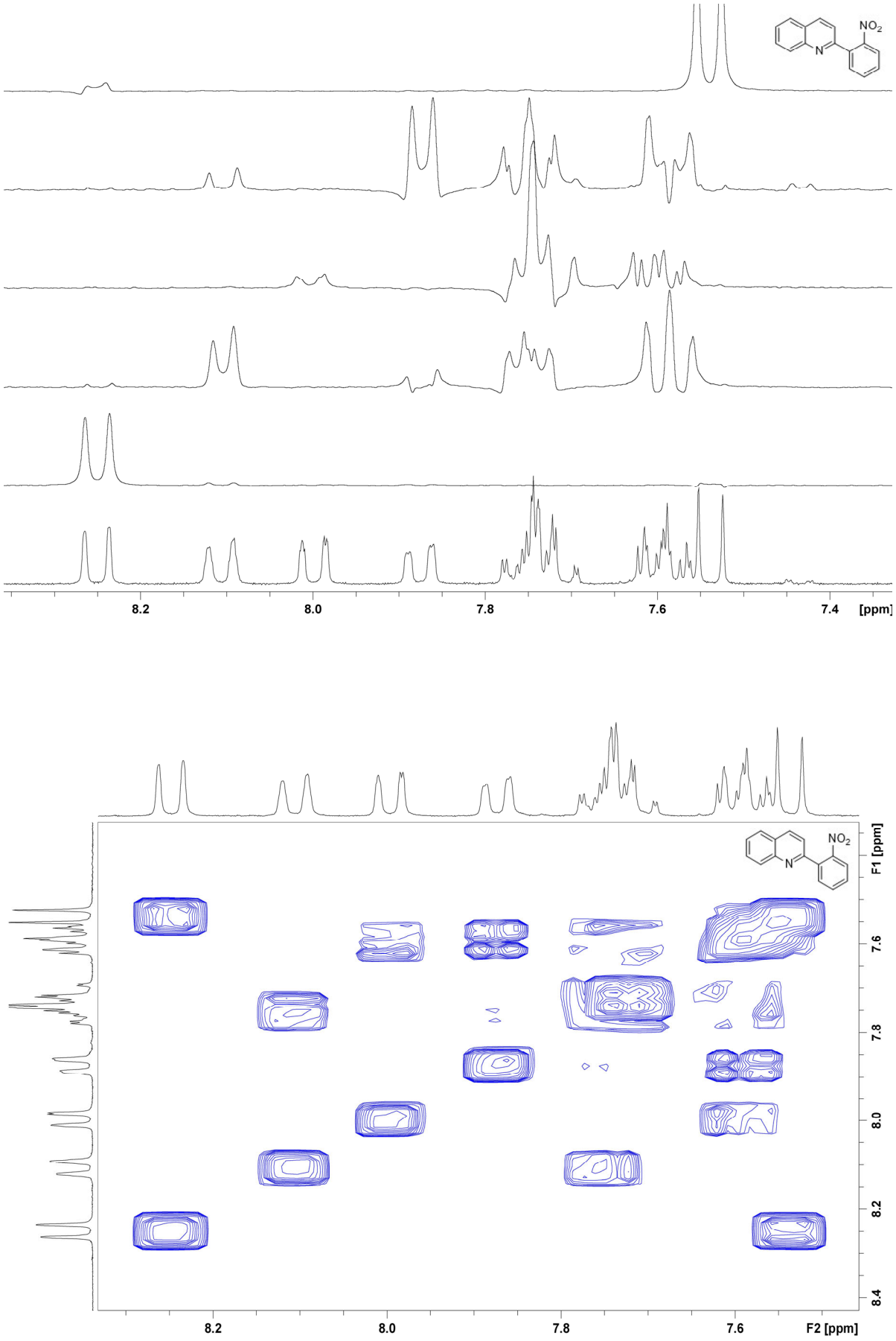


Figure S2. TOCSY NMR spectrum (top) and COSY NMR spectrum (bottom) of **17** in $CDCl_3$.

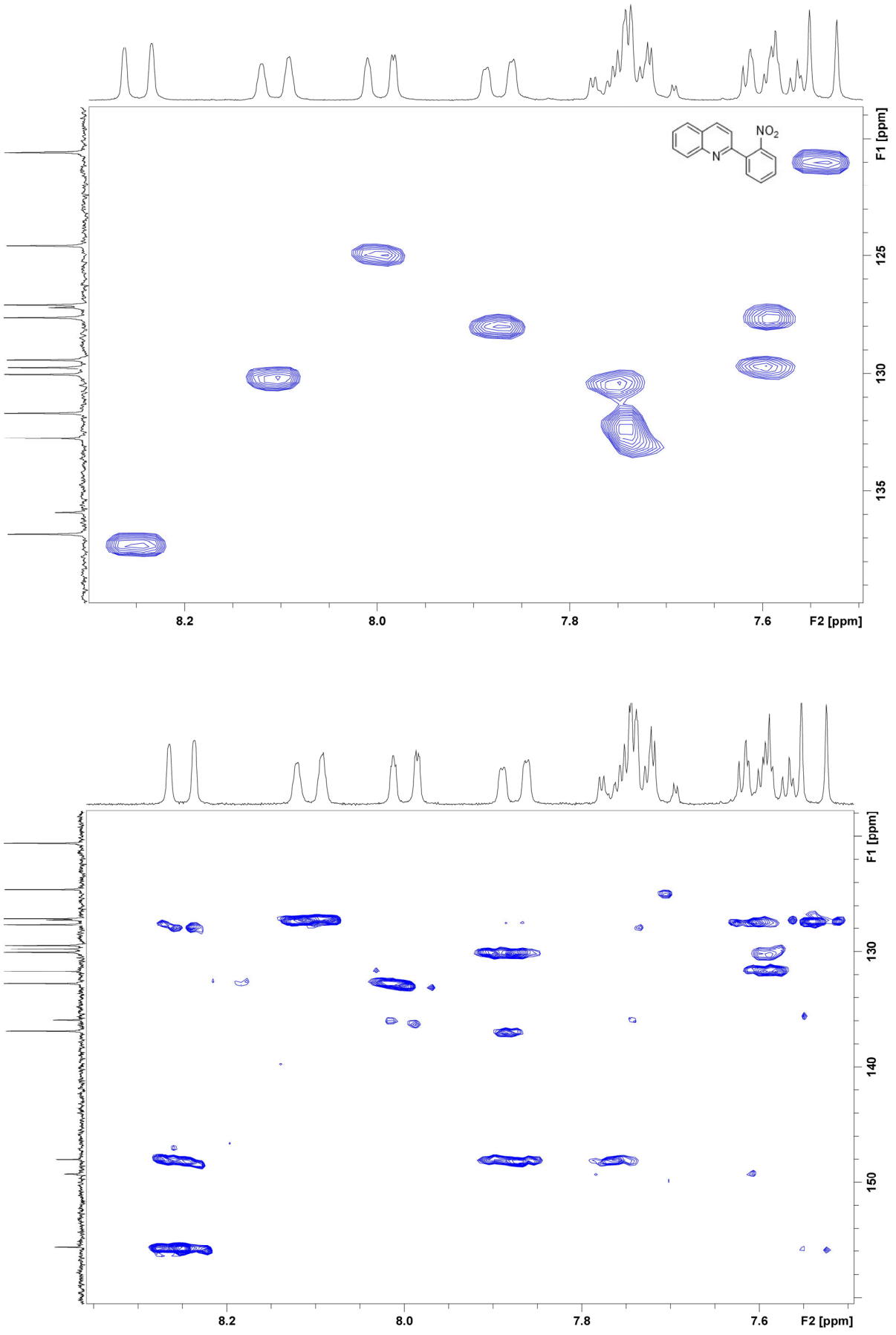


Figure S3. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **17** in $CDCl_3$.

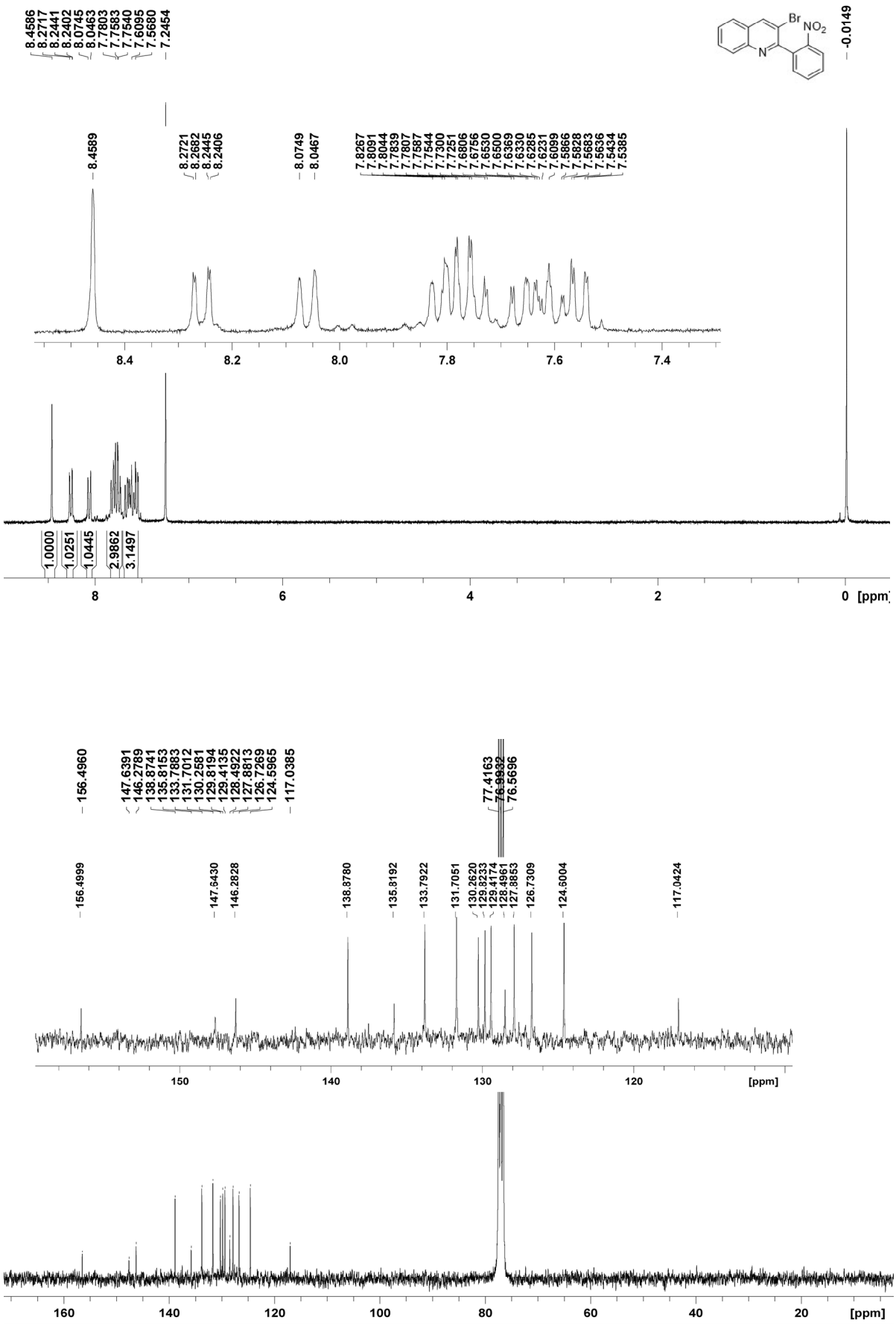


Figure S4. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **21** in $CDCl_3$.

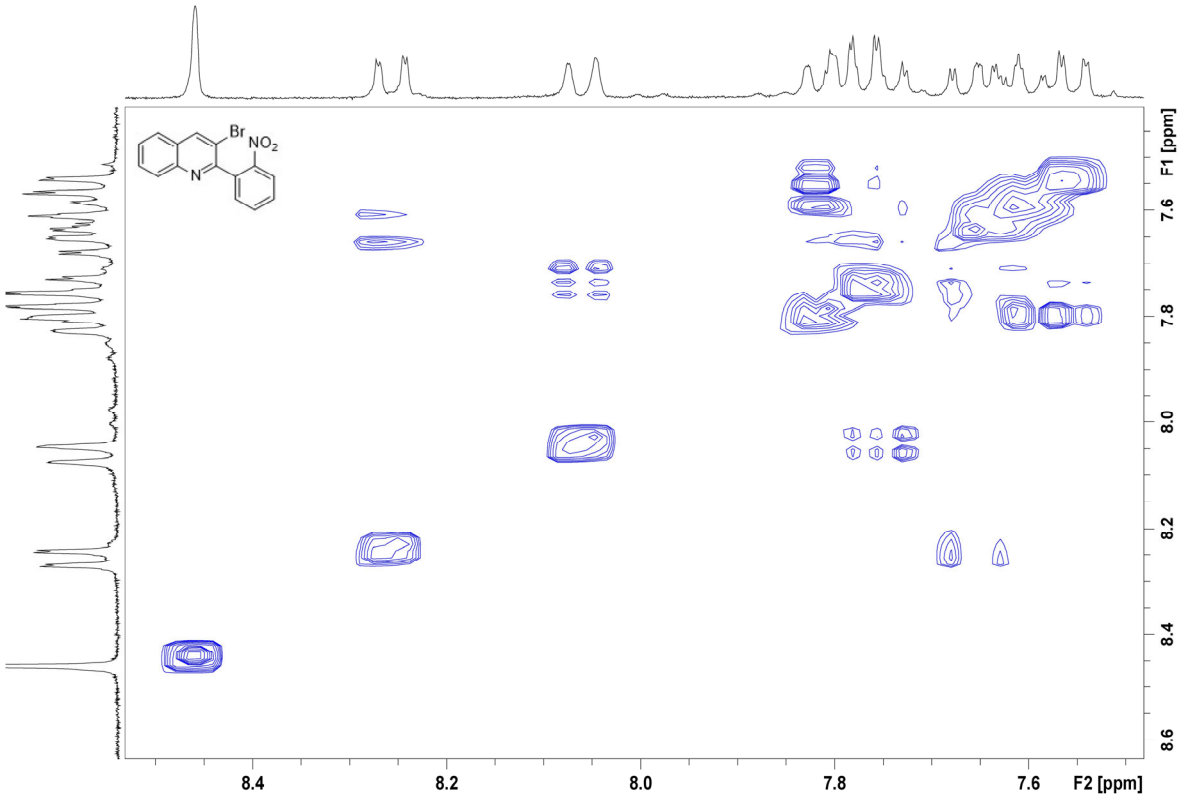


Figure S5. COSY NMR spectrum of **21** in $CDCl_3$.

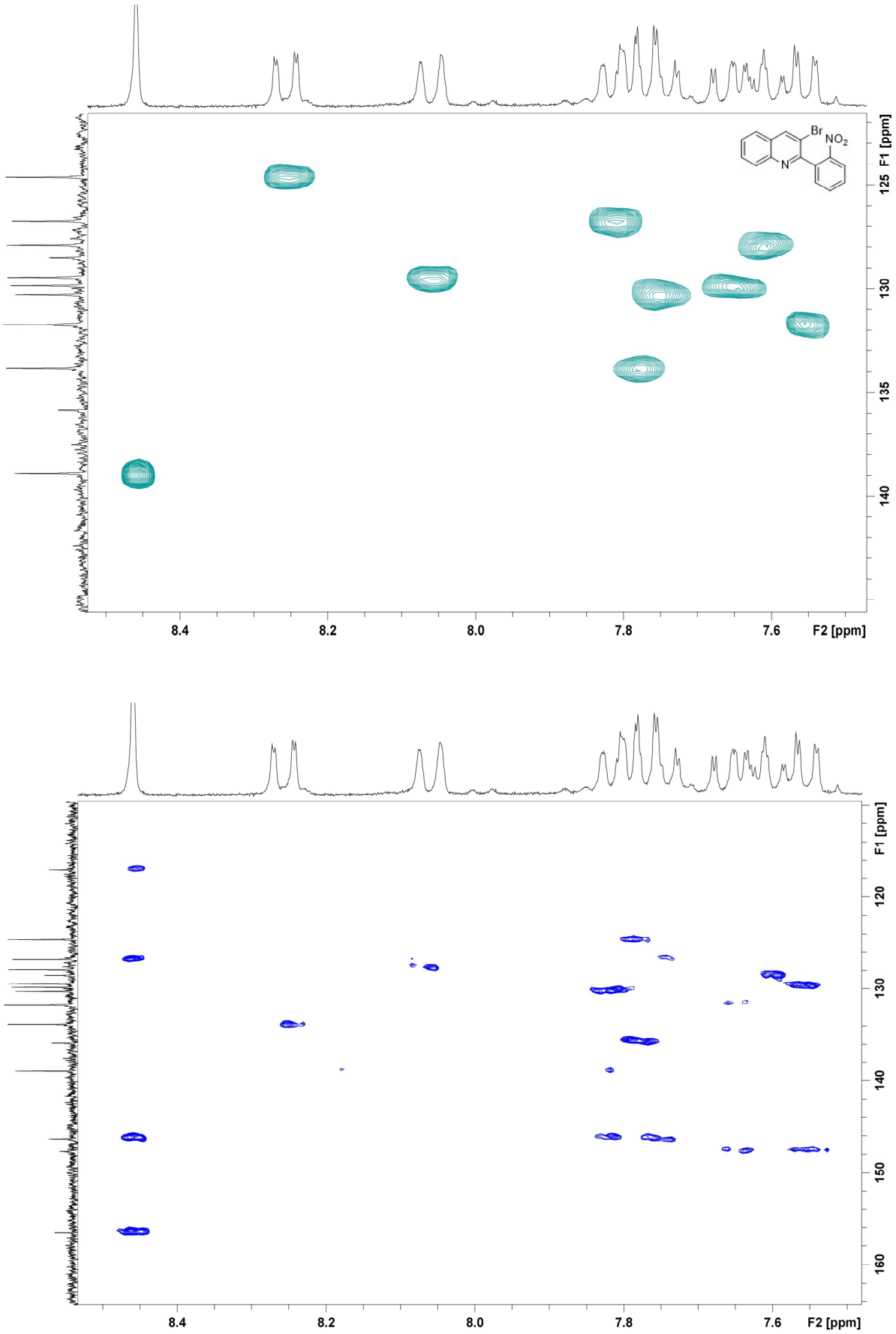


Figure S6. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **21** in $CDCl_3$.

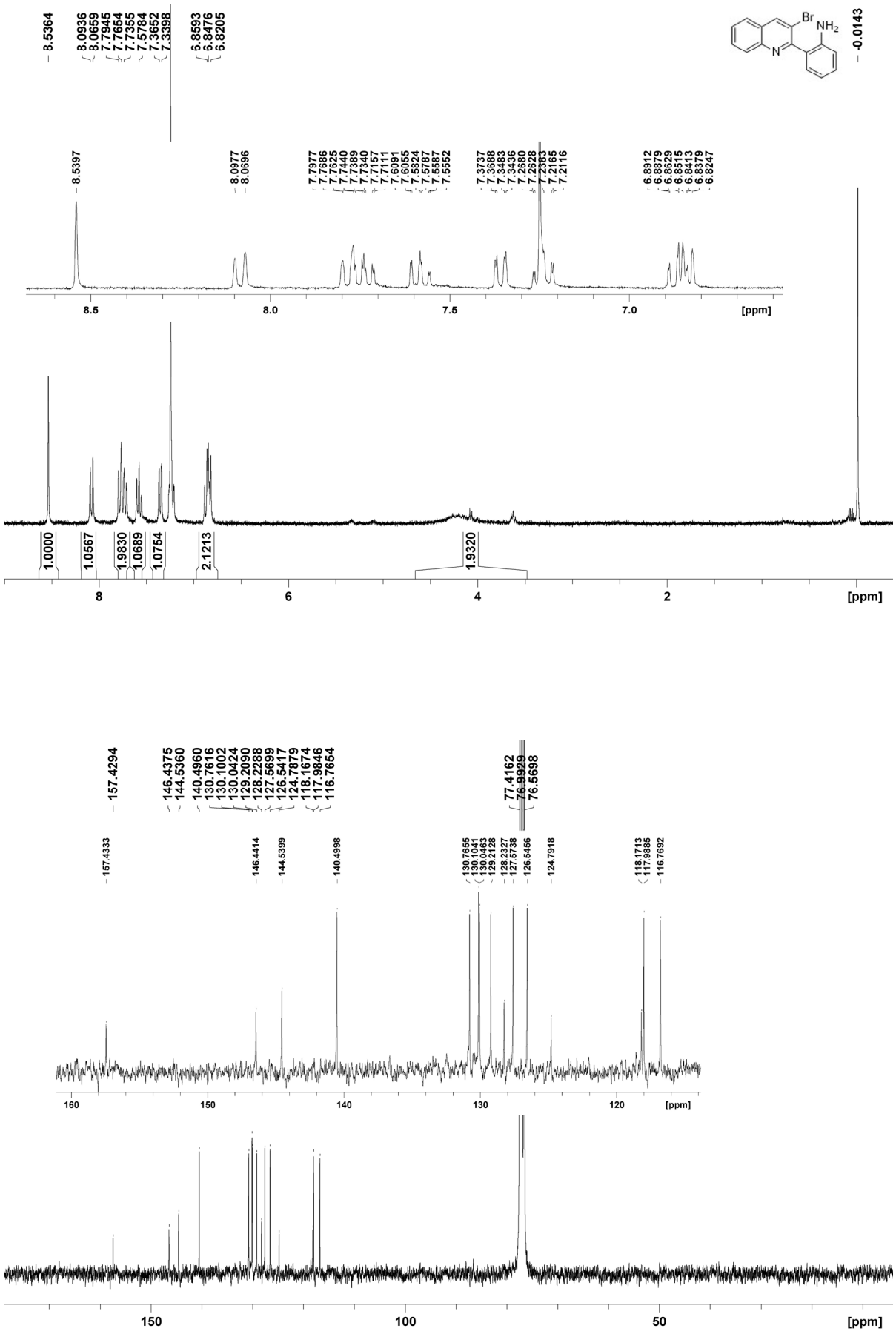


Figure S7. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **22** in $CDCl_3$.

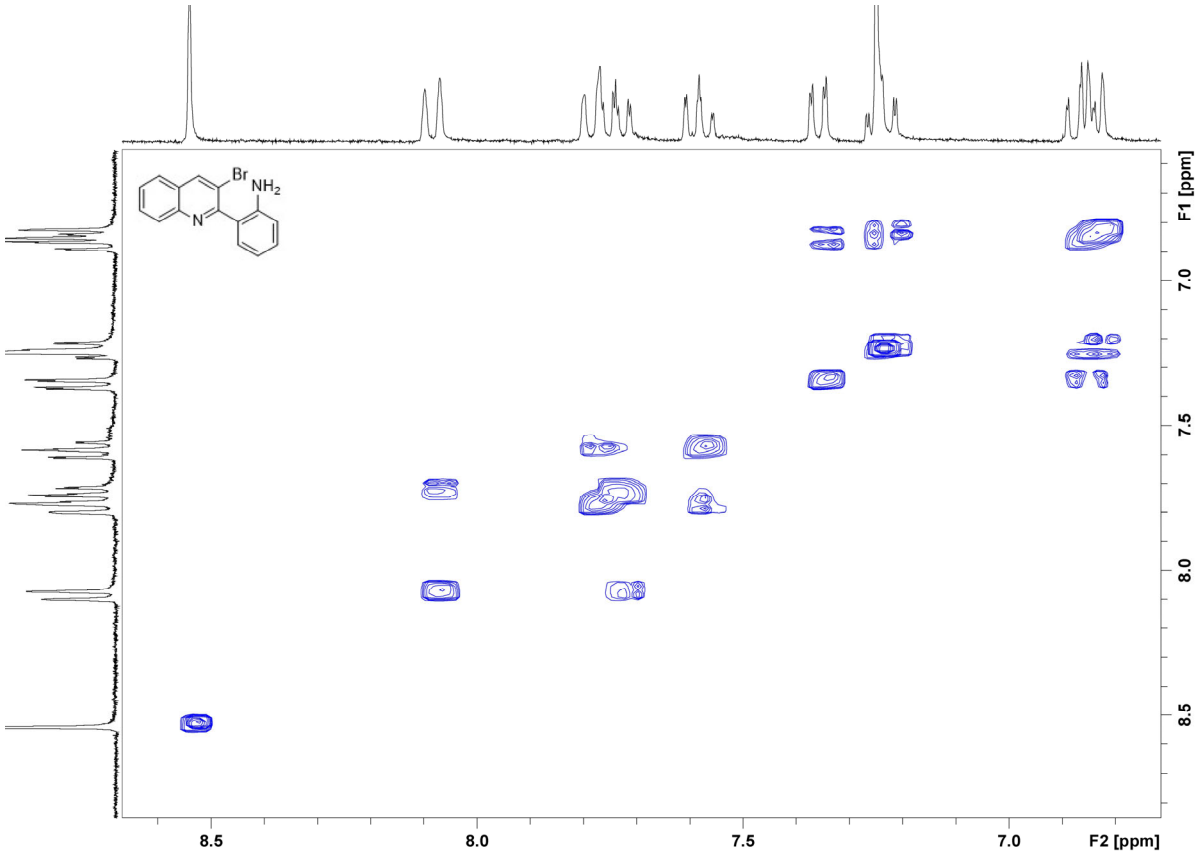


Figure S8. COSY NMR spectrum of **22** in $CDCl_3$.

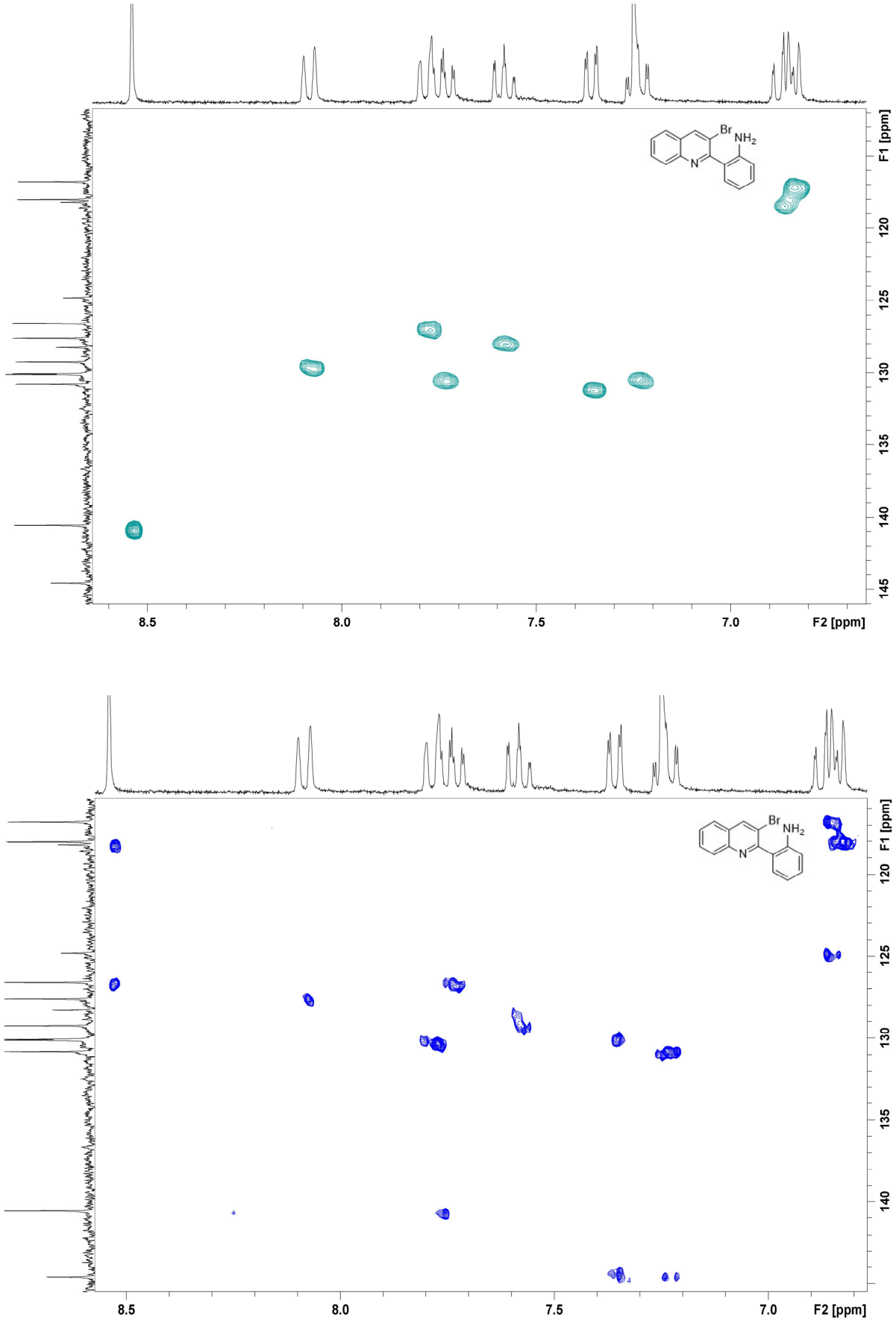


Figure S9. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **22** in $CDCl_3$.

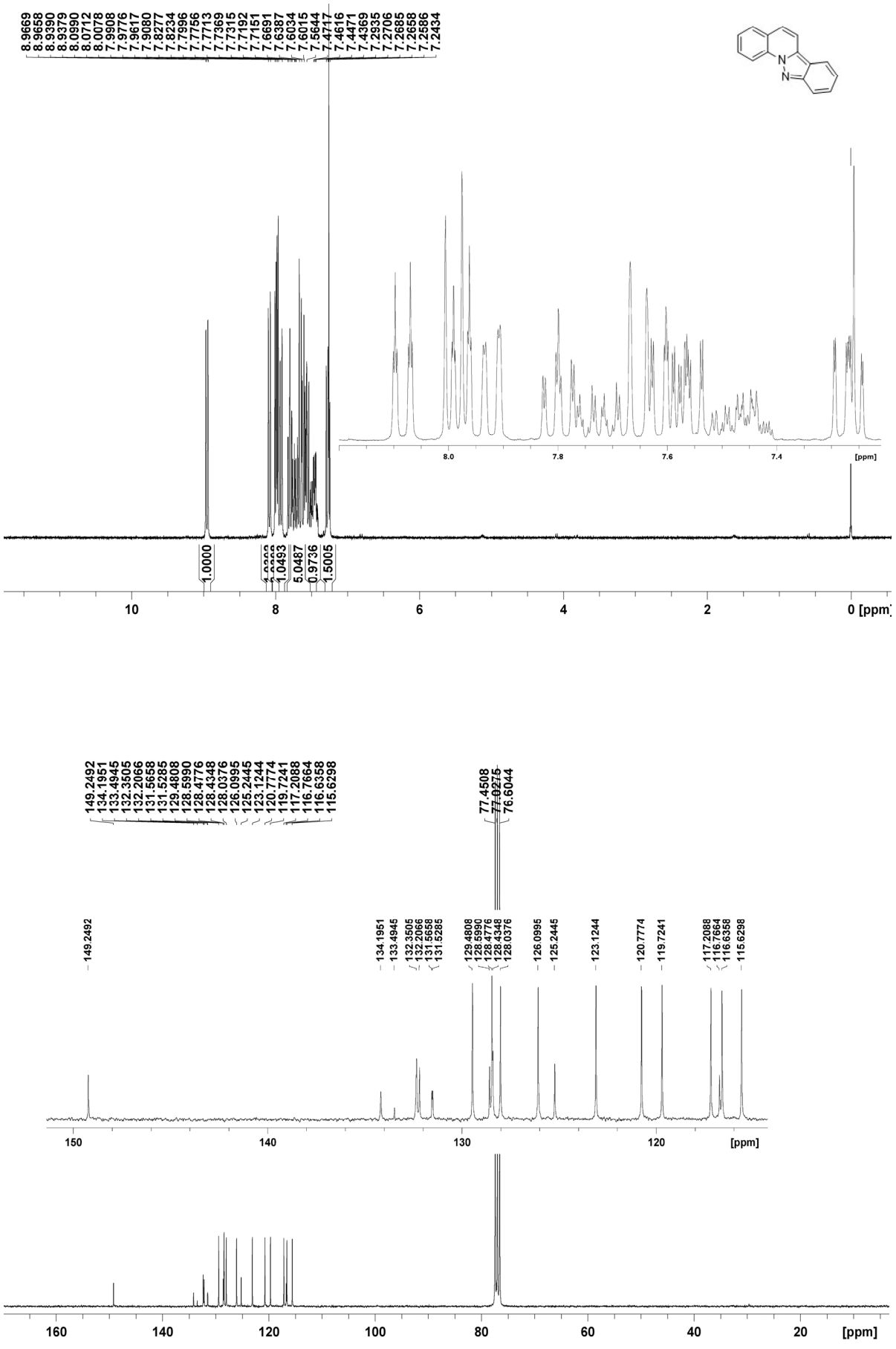


Figure S10. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **18** in $CDCl_3$.

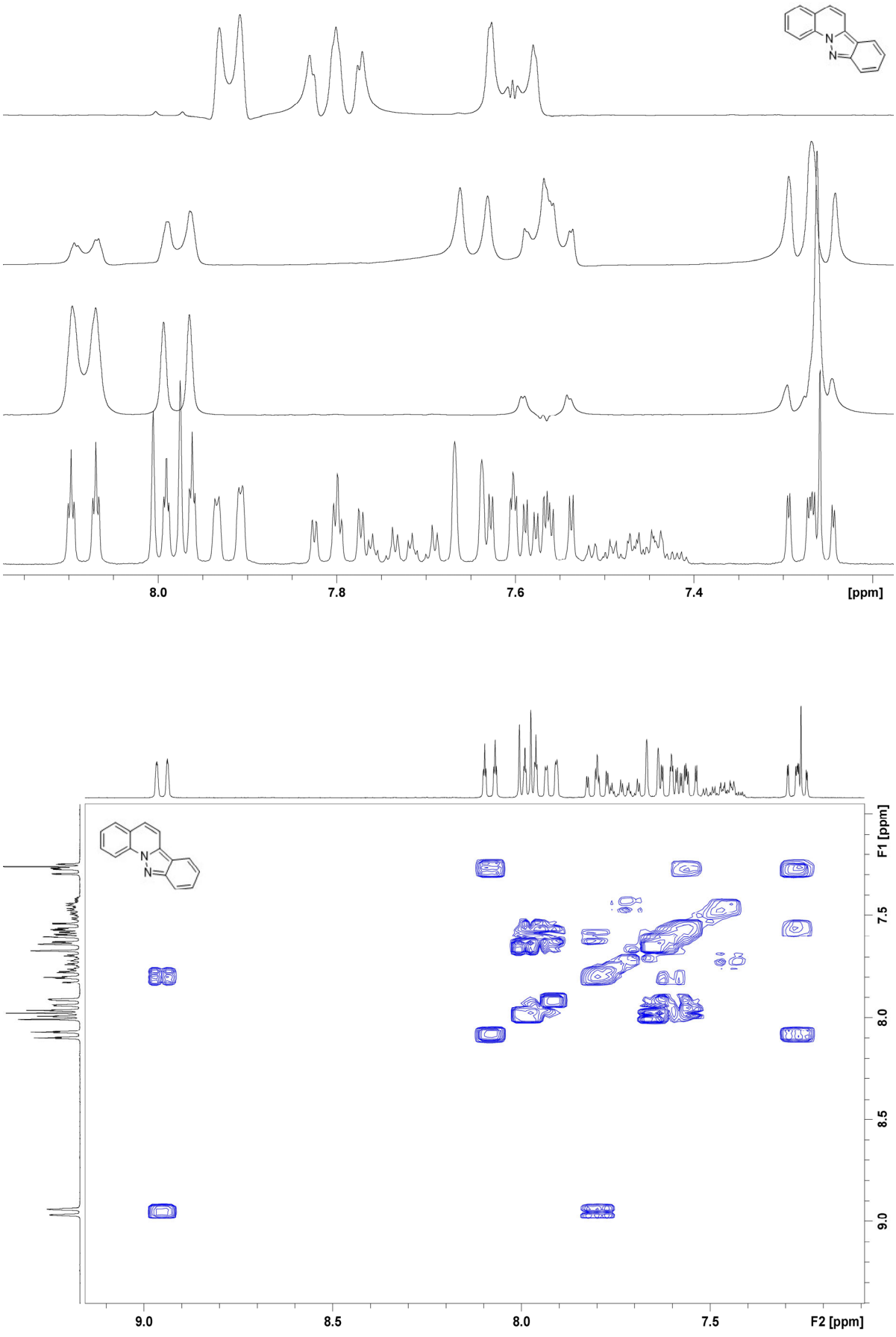


Figure S11. TOCSY NMR spectrum (top) and COSY NMR spectrum (bottom) of **18** in $CDCl_3$.

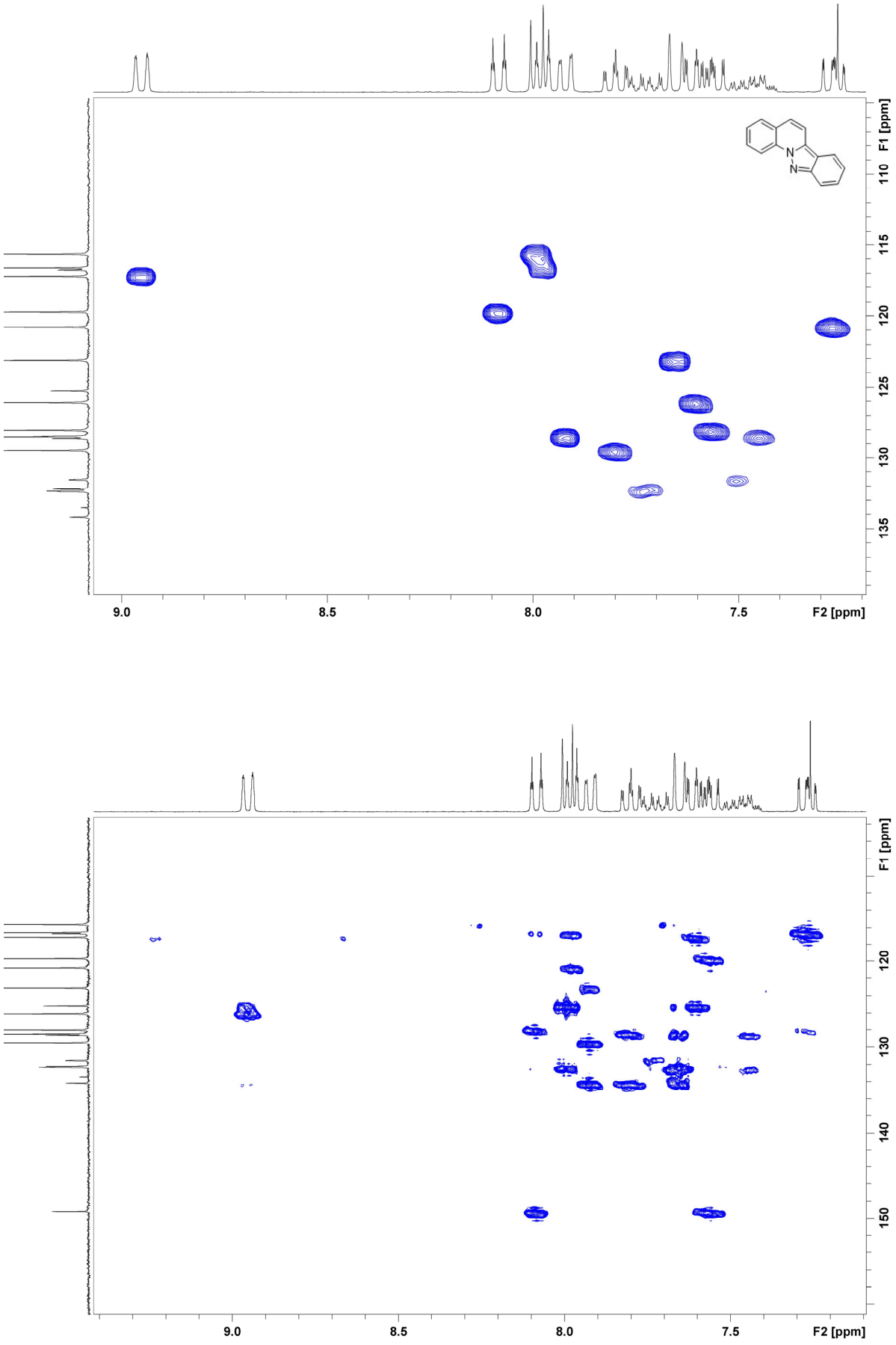


Figure S12. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **18** in $CDCl_3$.

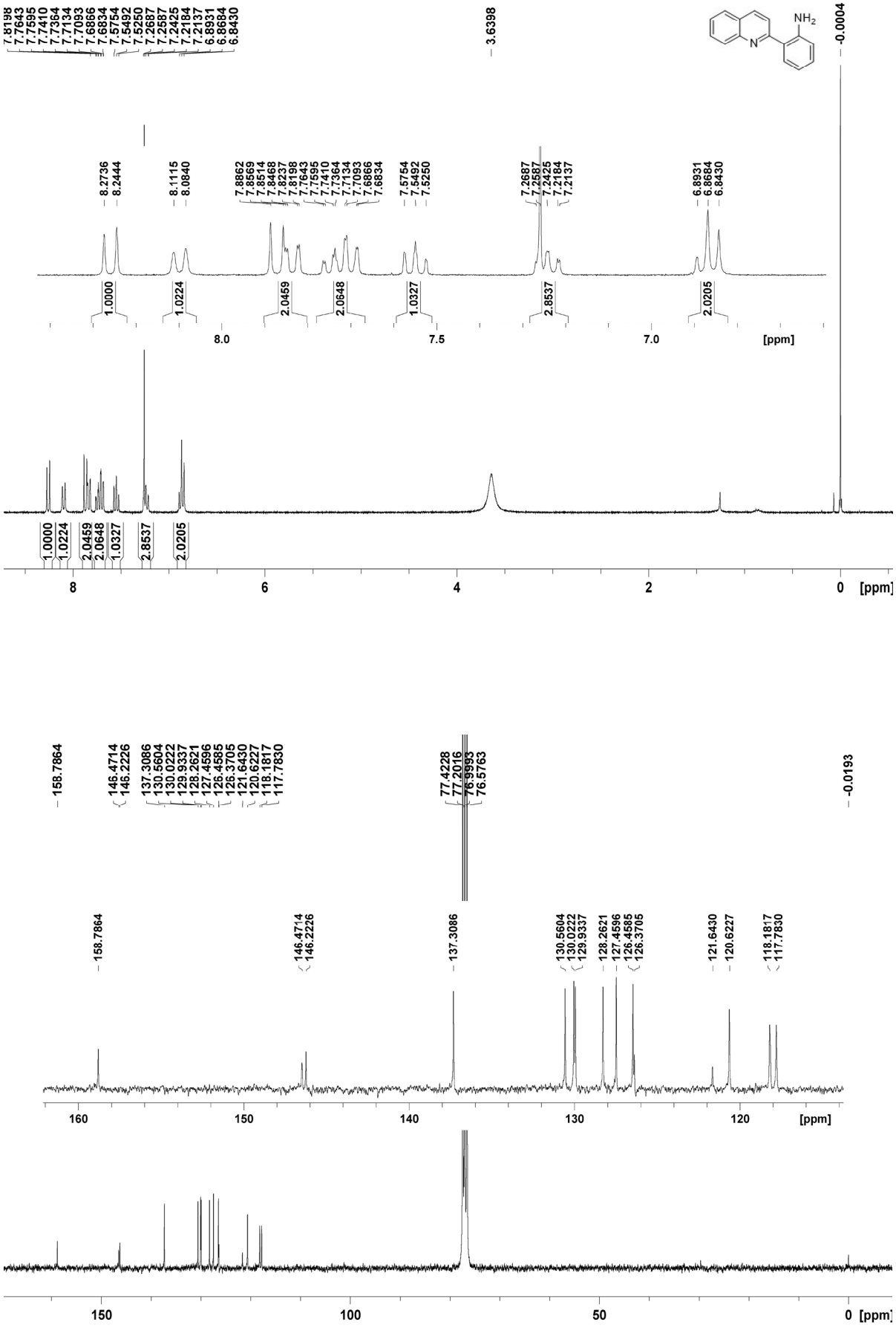


Figure S13. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **23** in $CDCl_3$.

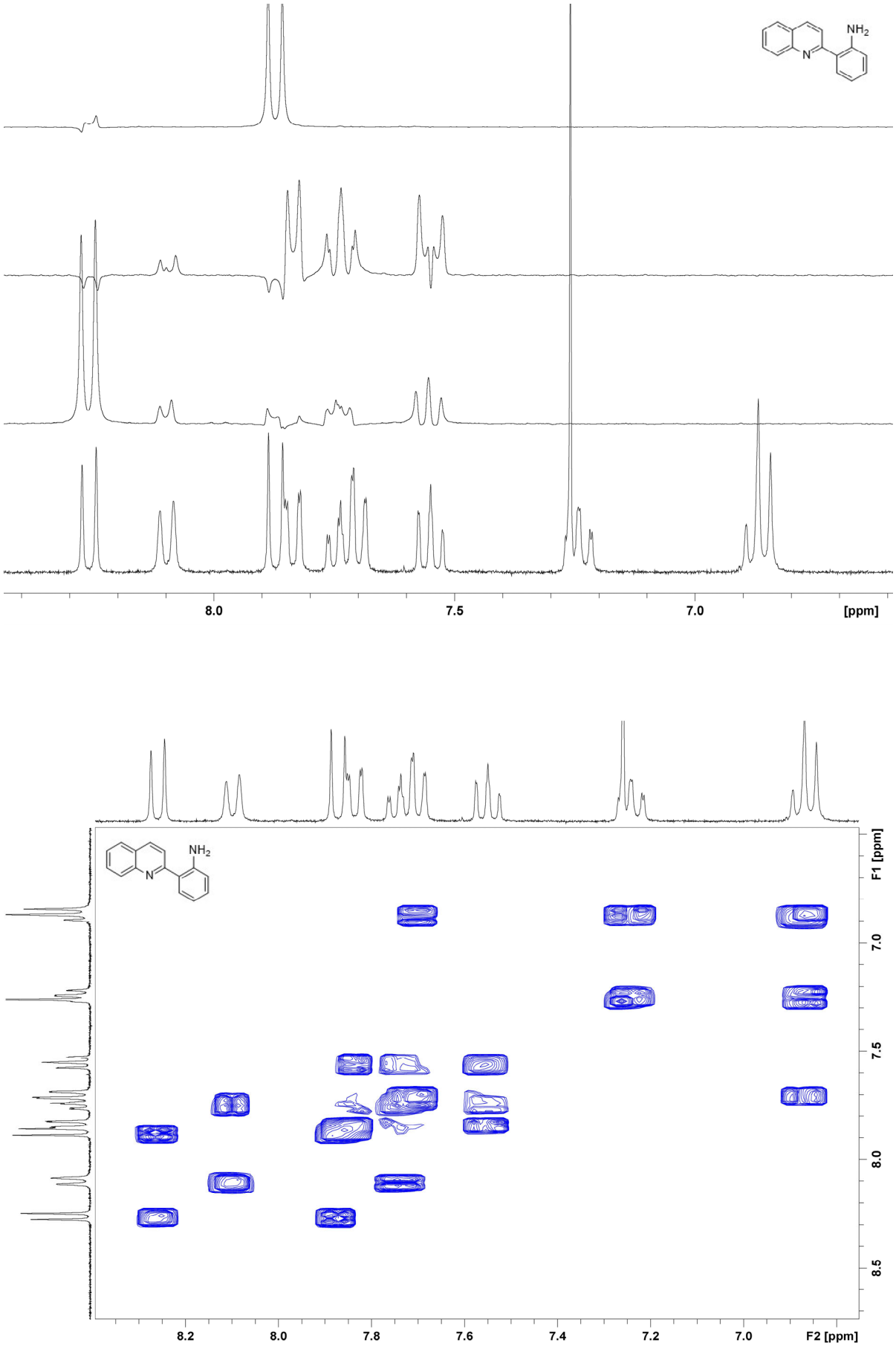


Figure S14. TOCSY NMR spectrum (top) and COSY NMR spectrum (bottom) of **23** in $CDCl_3$.

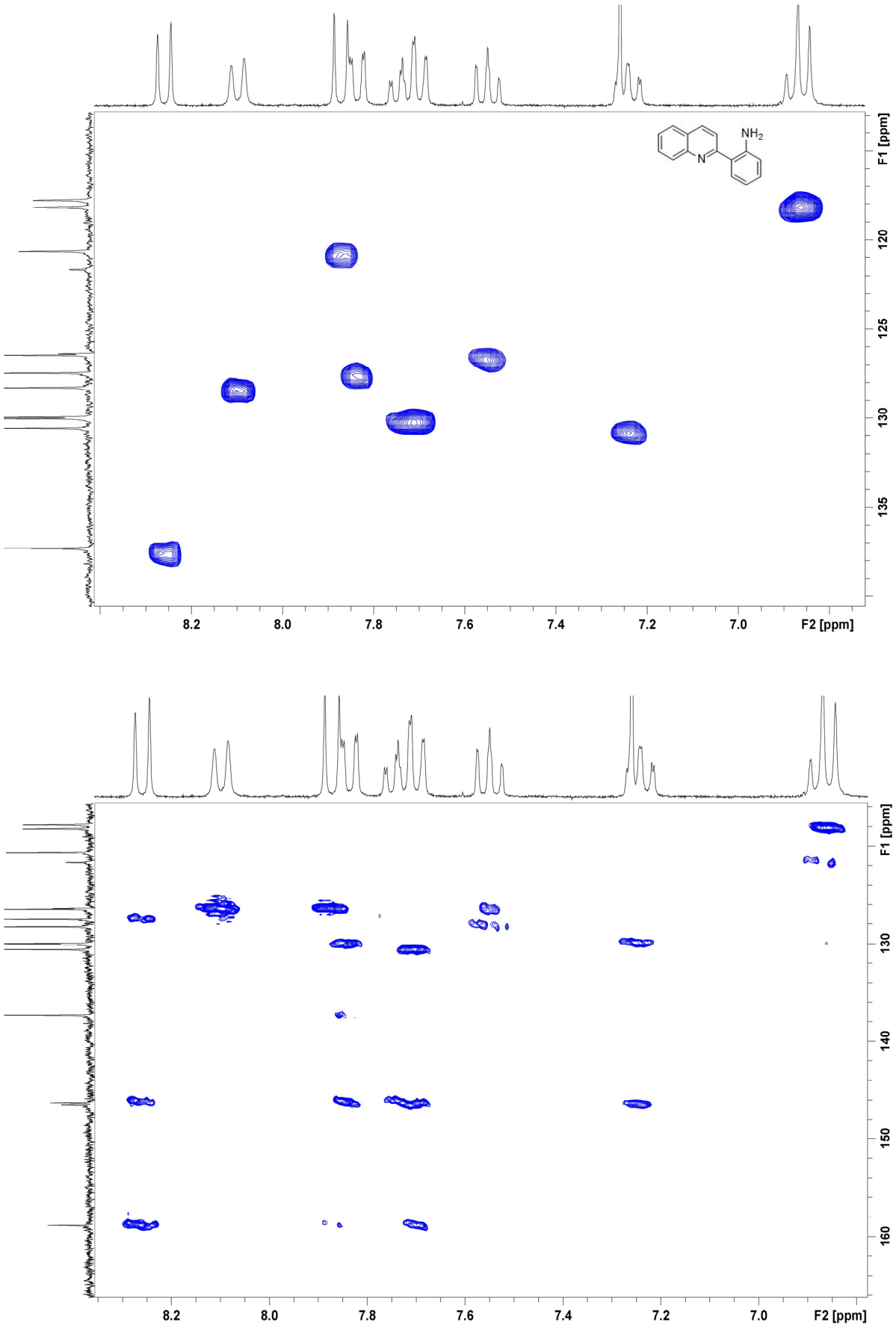


Figure S15. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **23** in $CDCl_3$.

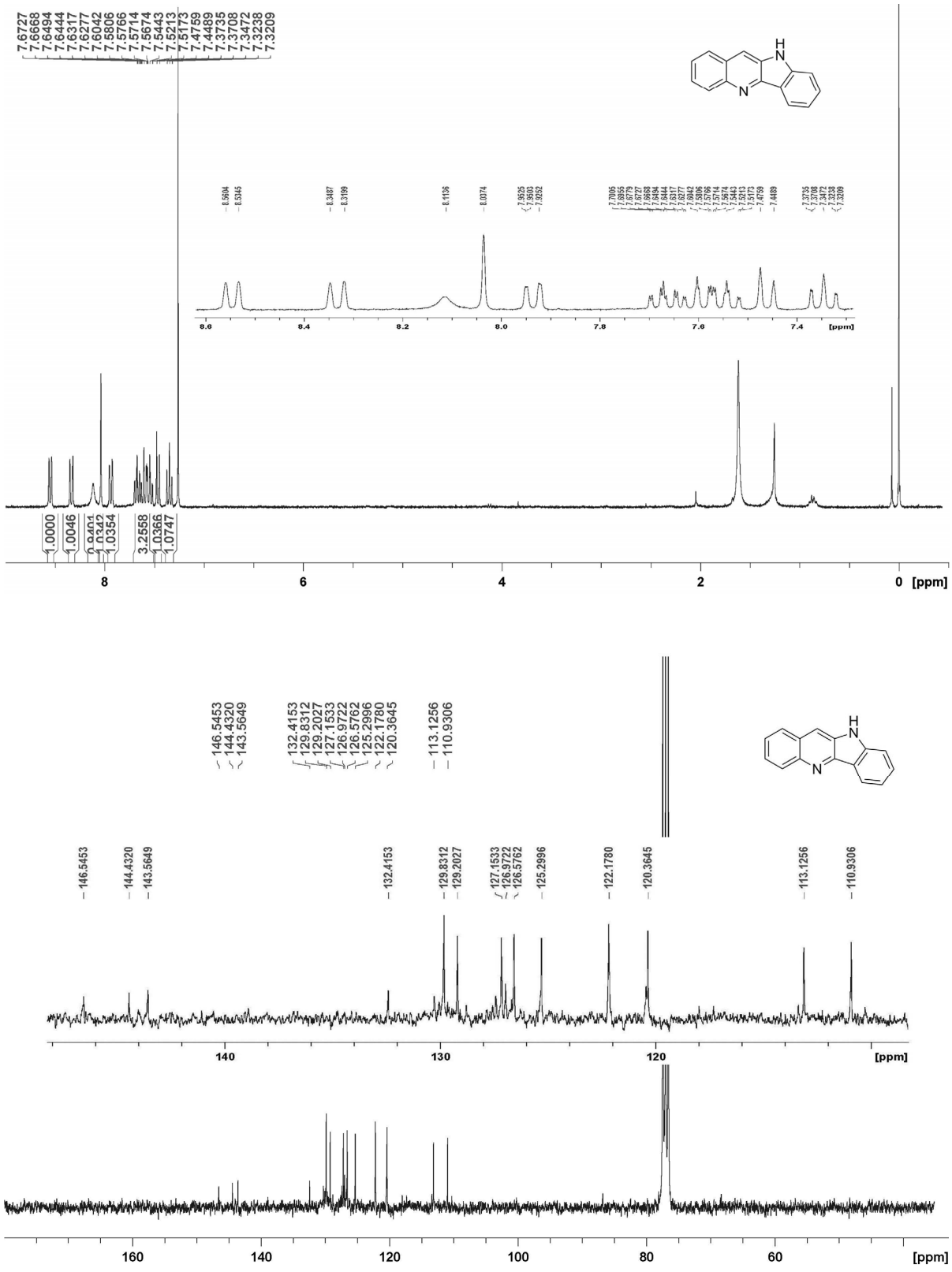


Figure S16. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **1** in $CDCl_3$.

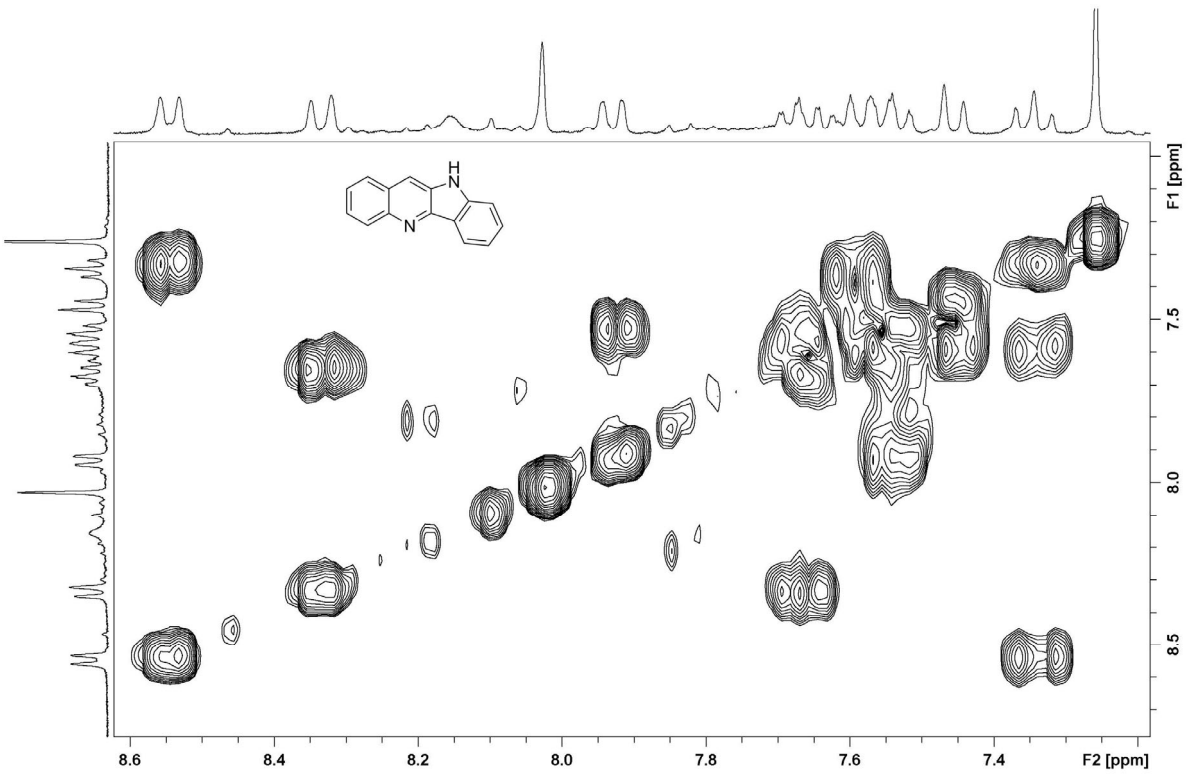


Figure S17. COSY NMR spectrum of **1** in $CDCl_3$.

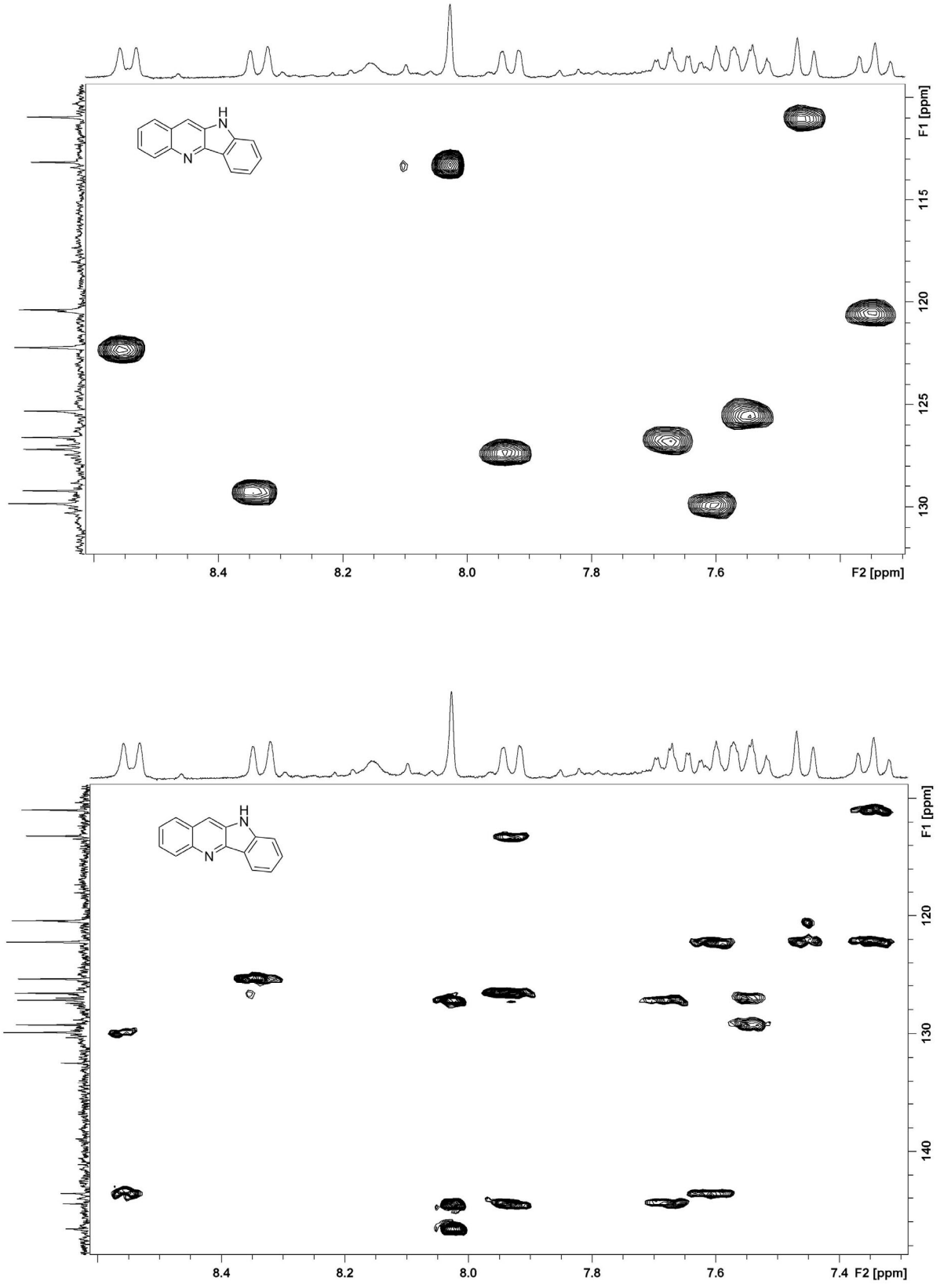


Figure S18. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **1** in $CDCl_3$.

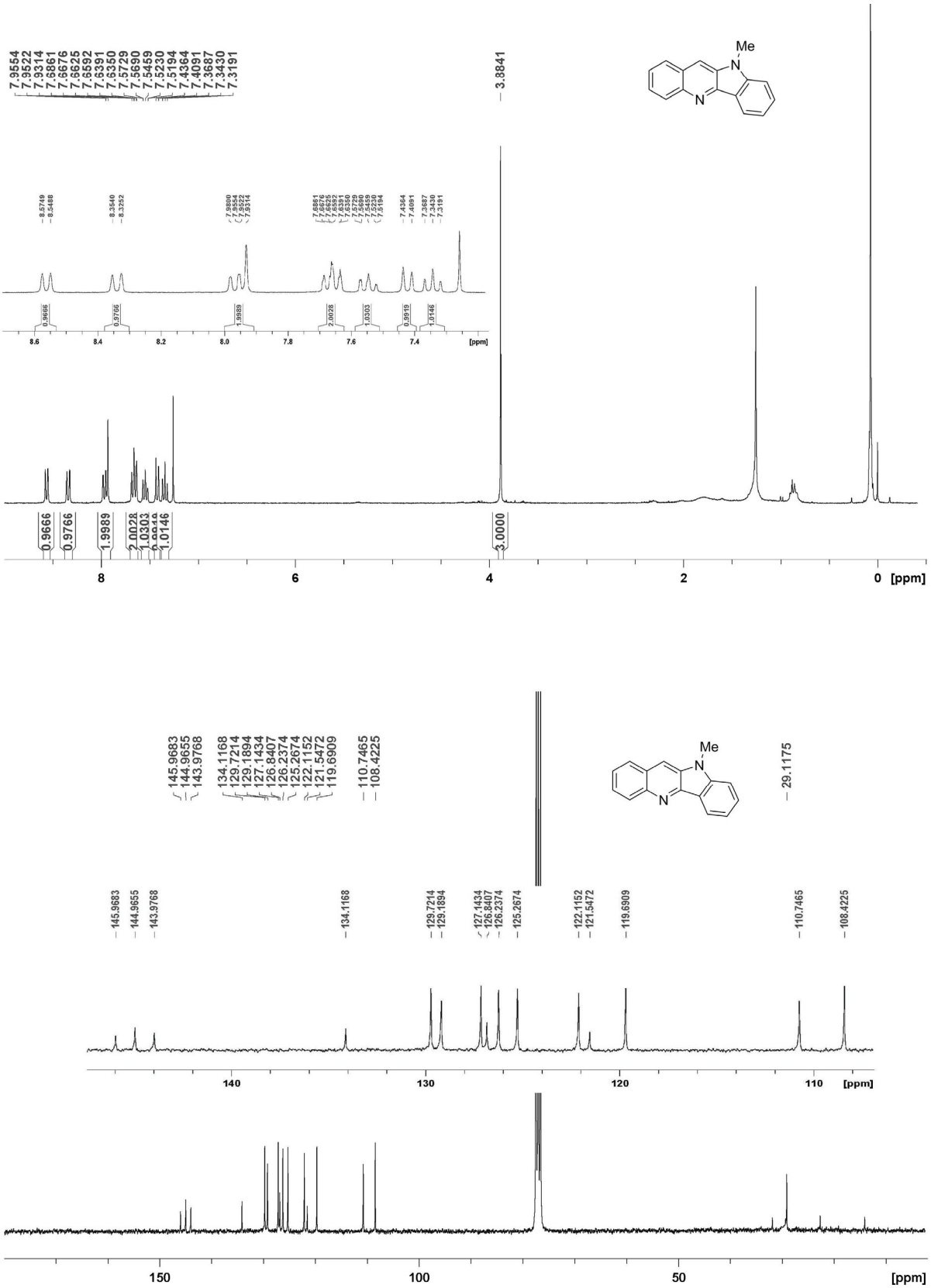


Figure S19. 300 MHz ^{1}H NMR spectrum (top) and 75 MHz ^{13}C NMR spectrum (bottom) of **14** in $CDCl_3$.

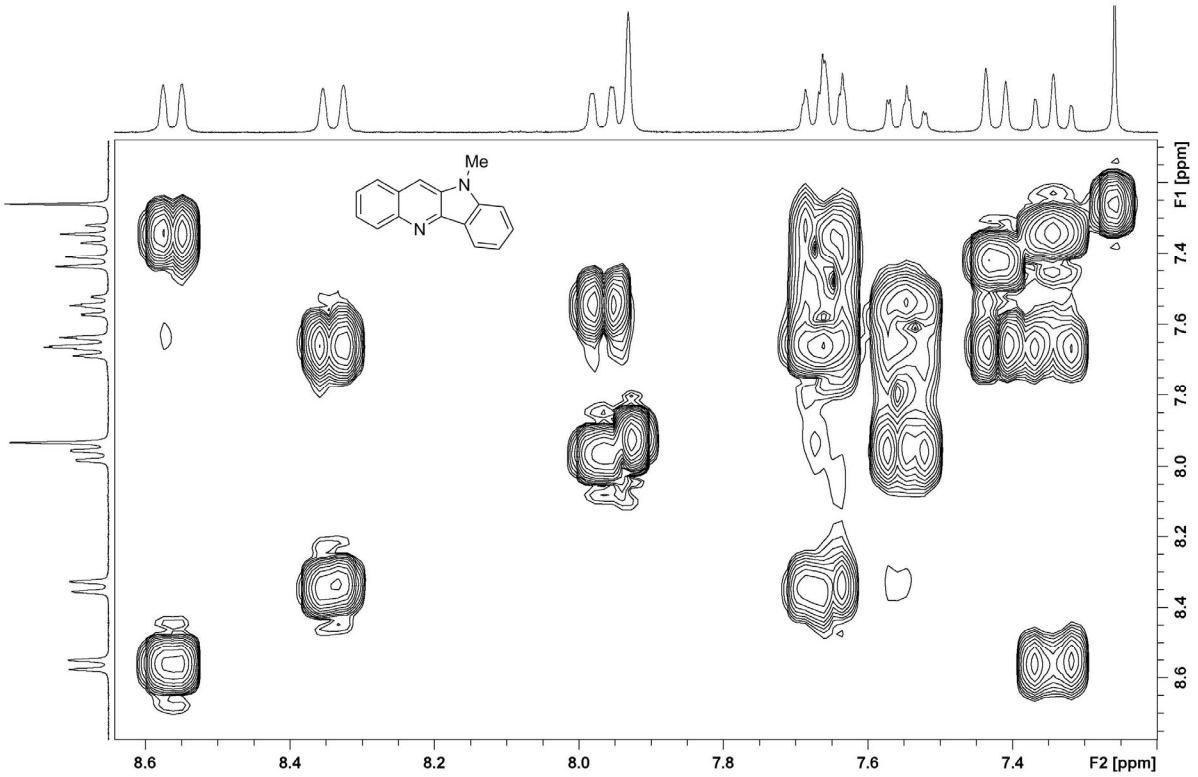


Figure S20. COSY NMR spectrum of **14** in $CDCl_3$.

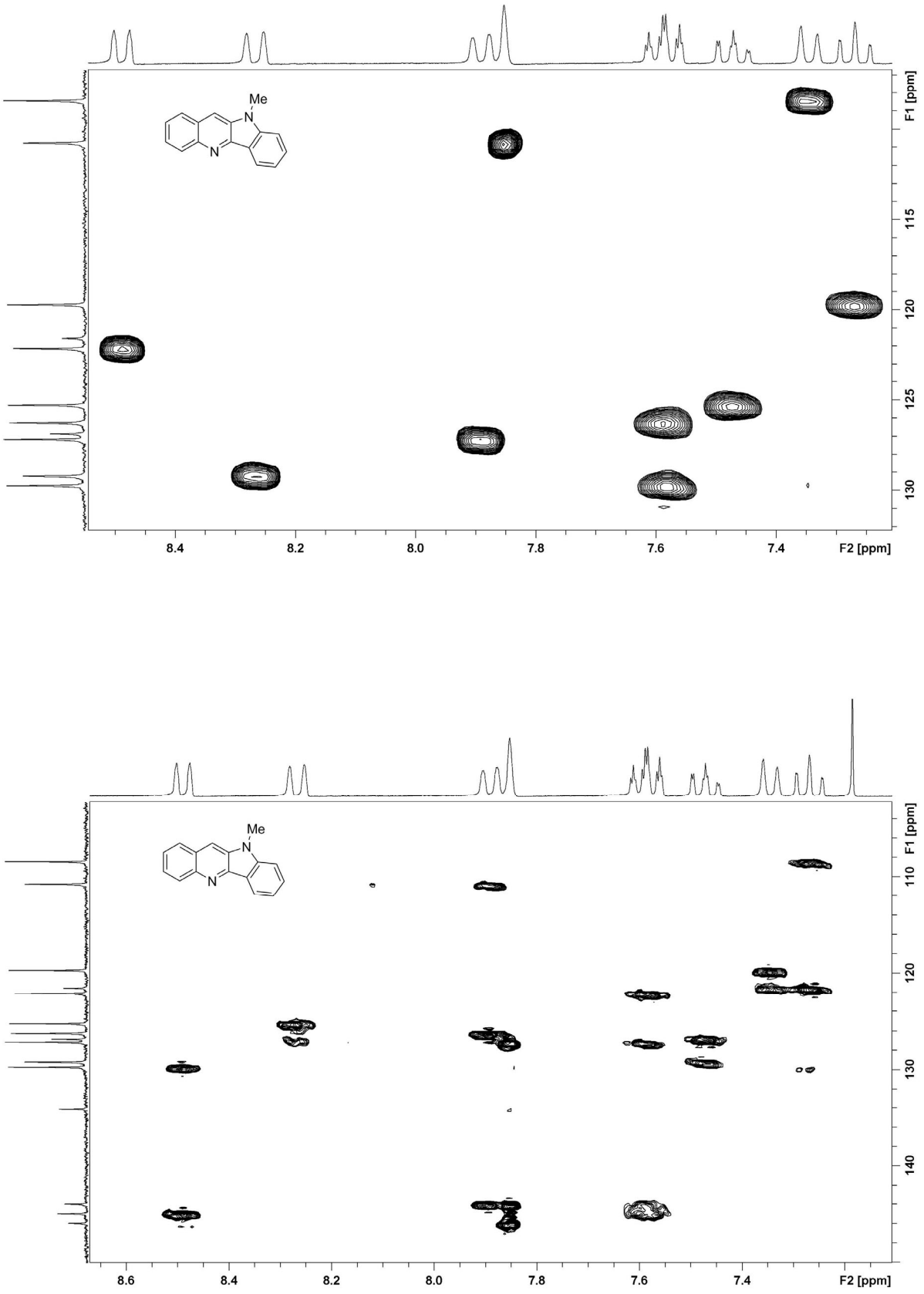


Figure S21. HSQC NMR spectrum (top) and HMBC NMR spectrum (bottom) of **14** in $CDCl_3$.

Computational methods

Conformational searches for the reactants, the transition structures (TSs) and the products were run to locate the global minima at the B3LYP/6-31G* level of theory. Initially, a large number of geometries was generated using the conformational search module of Hyperchem with the MM+ method.[1] Selected structures were then successively reoptimized at the B3LYP/6-31G* and B3LYP/6-311+G** levels of theory.[2]

The geometries for all structures were fully optimized and normal mode analysis was used to confirm the nature of the stationary points and to evaluate the thermochemical properties. Reported thermochemical properties include zero-point energies (ZPEs) without scaling and were calculated at 1 atm and 298.15 K and 383.15 K, temperature where the reaction was carried out.

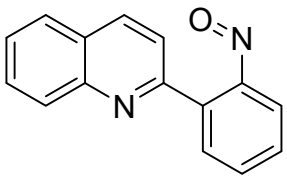
The molecular orbitals of the reactants were calculated to analyze the frontier orbital interactions. Intrinsic reaction coordinate (IRCs) calculations were run to verify the connectivity between reactants, TSs and products. To examine the more important interactions in the TSs we performed natural bond orbital calculations and Wiberg bond indexes (WBIs) were analyzed.

To interpret the presence of hydrogen bonds and the energy value, Second Order Perturbation analysis was carried out of the transition state at different level theories. Free energies in solution were computed on the structures optimized in the gas phase at the B3LYP/6-31G* with PPh_3 and PPh_3O as the phosphines and B3LYP/6-311+G** with the simplest PMe_3 and PMe_3O levels of theory with the polarizable continuum model (PCM)[3] using toluene as solvent ($\varepsilon_{toluene}$= 2.379).

1 Hyperchem Professional Release 7.52, Hypercube, Inc., 2005.

2 Gaussian 09, Revision D.01: M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2013.

3 (a) S. Miertš, E Scrocco and J. Tomasi, *J. Chem. Phys.,* 1981, **55**, 117-129. (b) B. Mennucci and J. Tomasi, *J. Chem. Phys.,* 1997, **106**, 5151-5158. (c) J. Tomasi, B., Mennucci and R. Cammi, *Chem. Rev.,* 2005, **105**, 2999-3094.

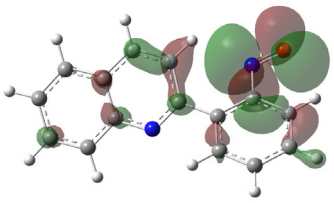


19

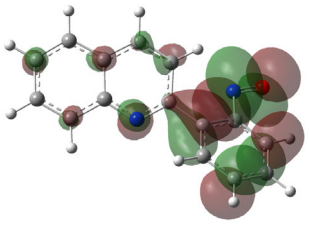
LUMO **19**: -0.1012

ΔeV: 0.11 eV

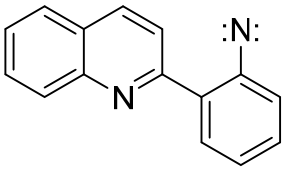
HOMO **19**: -0.2157



HOMO **19**



LUMO **19**

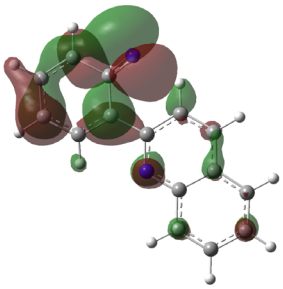


A

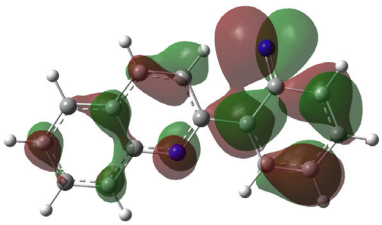
LUMO **A**: -0.1281

ΔeV: 0.055 eV

HOMO **A**: -0.1833



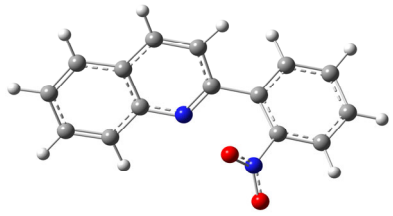
HOMO **A**



LUMO **A**

Figure S22. Shapes and energies (in eV) of FMOs of the nitroso derivative **19** and the nitrene **A**.

2-(2-Nitrophenyl)-quinoline (**17**).-



17

B3LYP/6-31G* Energy + ZPE: -837.261791.

B3LYP/6-31G* Free Energy: -837.303915.

B3LYP/6-31G* Free Energy in Toluene: -837.309017.

B3LYP/6-31G* Free Energy in Toluene (383.15K): -837.326372.

B3LYP/6-311+G** Energy + ZPE: -837.481615.

B3LYP/6-311+G** Free Energy: -837.523908.

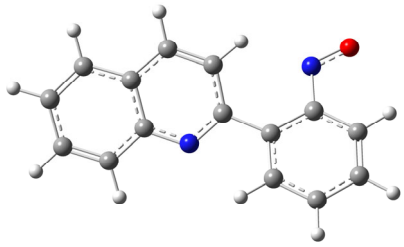
B3LYP/6-311+G** Free Energy in Toluene: -837.529682.

B3LYP/6-311+G** Free Energy in Toluene (383.15K): -837.547097.

Number of Imaginary Frequencies: 0

C	4.77624700	0.20173400	-0.25436600
C	4.07752200	-0.81433400	0.35782000
C	2.65972600	-0.84251500	0.30552100
C	1.96378000	0.19725100	-0.39119100
C	2.71288400	1.23170300	-1.01291700
C	4.08747600	1.23189800	-0.94371500
C	1.87351100	-1.85260400	0.91353000
C	0.50477100	-1.80120100	0.81266100
C	-0.09279000	-0.72543200	0.09707900
N	0.60601800	0.23331000	-0.48487900
C	-1.57334700	-0.67156300	-0.07128800
C	-2.32950400	0.50095300	0.08876900
C	-3.69061400	0.55505600	-0.19890100
C	-4.34865100	-0.59770100	-0.62251900
C	-3.63221600	-1.78568700	-0.76650600
C	-2.26272600	-1.81369800	-0.50226000
N	-1.73438400	1.72823000	0.65139600
O	-2.11451100	2.80024800	0.18271300
O	-0.94974600	1.60344700	1.58695200
H	5.86170800	0.21906900	-0.21060500
H	4.60094600	-1.60576500	0.88933000
H	2.16319500	2.01045400	-1.53184600
H	4.65474600	2.02749500	-1.41894600
H	2.36210300	-2.65460500	1.46214100
H	-0.12128600	-2.55024300	1.28687900
H	-4.21691400	1.49380600	-0.07071000
H	-5.41289200	-0.56493300	-0.83506800
H	-4.13378600	-2.68914900	-1.10132200
H	-1.70161000	-2.72962900	-0.66308800

2-(2-Nitrosophenyl)-quinoline (**19**).-



19

B3LYP/6-31G* Energy + ZPE: -762.064507.

B3LYP/6-31G* Free Energy: -762.105299.

B3LYP/6-31G* Free Energy in Toluene: -762.108963.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -762.098029.

B3LYP/6-311+G** Energy + ZPE: -762.257213.

B3LYP/6-311+G** Free Energy: -762.298163.

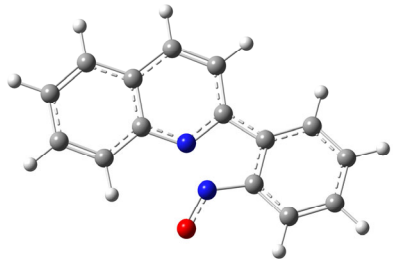
B3LYP/6-311+G** Free Energy in Toluene: -762.302423.

B3LYP/6-311+G** Free Energy in Toluene (383.15K): -762.319252.

Number of Imaginary Frequencies: 0

C	4.85762900	0.05578100	0.11502500
C	4.39375900	-1.20209400	0.57654400
C	3.04693500	-1.48485400	0.60290300
C	2.10122600	-0.51796400	0.16689200
C	2.57077200	0.75127600	-0.29825800
C	3.96491100	1.01263000	-0.31408300
N	0.77916700	-0.83774300	0.20824900
C	-0.11447900	0.06025600	-0.18325200
C	0.26049600	1.34394300	-0.68072600
C	1.59066000	1.67799400	-0.73300900
C	-1.53531000	-0.39599600	-0.14074900
C	-2.64006700	0.43713500	0.15429400
C	-3.95252800	-0.06357300	0.14533900
C	-4.18786400	-1.39627000	-0.14862600
C	-3.10174800	-2.24103900	-0.42111100
C	-1.80092300	-1.74891400	-0.41179500
N	-2.36634600	1.79551900	0.53970000
H	5.92431500	0.26188700	0.10210800
H	5.11171800	-1.94547400	0.91217000
H	2.66785300	-2.43967400	0.95368800
H	4.31555900	1.97880900	-0.66941200
H	-0.49855900	2.03966000	-1.01216300
H	1.90193000	2.64856100	-1.11222500
H	-4.75539500	0.62320100	0.39138600
H	-5.20168800	-1.78650500	-0.15742900
H	-3.27496800	-3.29059100	-0.64364100
H	-0.96083200	-2.40275900	-0.61651700
O	-3.35506200	2.48482300	0.75500900

19TSB.-



19TSB

B3LYP/6-31G* Energy + ZPE: -762.039378.

B3LYP/6-31G* Free Energy: -762.077899.

B3LYP/6-31G* Free Energy in Toluene: -762.082280.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -762.098029.

B3LYP/6-311+G** Energy + ZPE: -762.232265.

B3LYP/6-311+G** Free Energy: -762.270903.

B3LYP/6-311+G** Free Energy in Toluene: -762.276148.

B3LYP/6-311+G** Free Energy in Toluene (383.15K): -762.291958.

Number of Imaginary Frequencies: 1 (-353.97)

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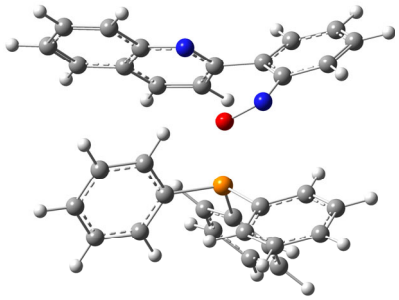
C	-2.34061000	1.45418600	0.13997400
C	-1.65879400	0.21918600	0.10030500
C	-2.37779300	-1.00716100	-0.03167700
C	-3.78843000	-0.95144000	-0.11229400
C	-1.63571100	-2.22907300	-0.07499500
C	-0.26715100	-2.21847700	-0.00878100
C	0.40915500	-0.97779900	0.13192100
N	-0.29313000	0.16948600	0.21802000
C	1.81122000	-0.67693700	0.07730200
C	1.98993700	0.72250800	-0.03992300
C	3.27236600	1.29189100	-0.09827700
C	4.36406100	0.43976000	-0.06345700
C	4.20002600	-0.96205100	0.01410900
C	2.93355900	-1.52228400	0.07747000
N	0.81610000	1.44041200	-0.29070200
O	0.62483400	2.61971800	0.05800200
H	-5.53154600	0.29295500	-0.14644600
H	-4.24984900	2.41320600	0.06035600
H	-1.76205500	2.36670900	0.22502000
H	-4.34489200	-1.88047000	-0.20930000
H	-2.17563700	-3.16611900	-0.18072500
H	0.30932100	-3.13567900	-0.07168900
H	3.37517000	2.36953200	-0.16662700
H	5.36751500	0.85611500	-0.08998100
H	5.07630500	-1.60313000	0.03451000
H	2.81070700	-2.59946200	0.15308900

17TSA.-



17TSA

B3LYP/6-31G* Energy + ZPE: -1798.050766.

B3LYP/6-31G* Free Energy: -1798.115947.

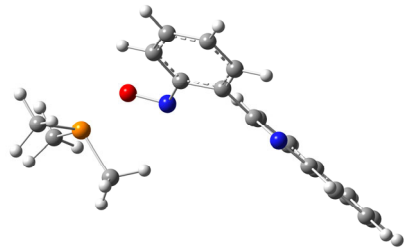
B3LYP/6-31G* Free Energy in Toluene: -1798.123538.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -1798.153236.

Number of Imaginary Frequencies: 1 (-289.89)

C	5.63894900	-1.43856300	-0.34713200
C	5.20852200	-1.11011600	-1.65742000
C	4.17751400	-0.21909700	-1.85402000
C	3.52491100	0.38804100	-0.74631700
C	3.96399800	0.05636700	0.57585700
C	5.02859300	-0.86582900	0.74659300
N	2.51650800	1.26791500	-0.99271900
C	1.89960100	1.83513700	0.03189000
C	2.27153000	1.57096200	1.38662200
C	3.29218500	0.69158400	1.65116100
C	0.86290000	2.86948100	-0.25883000
C	-0.26116300	2.68123500	-1.12275400
C	-1.03020100	3.82096100	-1.47251000
C	-0.75847900	5.07829800	-0.95873500
C	0.29669000	5.24688900	-0.05452500
C	1.08657600	4.14727100	0.27623900
N	-0.74302900	1.50659800	-1.67667500
O	-0.21621800	0.40982300	-1.11600700
P	-1.26618600	-0.67474900	0.04484200
C	-0.47499900	-2.25886400	-0.33598100
C	-0.49844100	-3.33711700	0.56730100
C	0.17378600	-2.41393800	-1.57553000
C	0.11714100	-4.54307600	0.23777900
C	0.78840600	-3.62448200	-1.89438300
C	0.76231200	-4.68919600	-0.99262000
C	-1.47260600	-0.57293300	1.85111700
C	-0.33154600	-0.73054800	2.66694800
C	-2.69050000	-0.20619000	2.45612400
C	-0.42015000	-0.55850800	4.04540900
C	-2.76583300	-0.02397300	3.83593800
C	-1.63578700	-0.20200000	4.63663300
C	-2.90320800	-0.59189700	-0.71399900
C	-3.54806900	0.65745200	-0.77371100
C	-3.49954600	-1.70717500	-1.32464600
C	-4.78677300	0.77246400	-1.40614900
C	-4.73482900	-1.58191900	-1.95706500
C	-5.38057600	-0.34336500	-1.99671700
H	6.45528400	-2.14265900	-0.20984400
H	5.70152100	-1.56748400	-2.51144600
H	3.83170800	0.04979000	-2.84736200

17TSA modelled with PMe_3.-



B3LYP/6-311+G** Energy + ZPE: -1223.281546.

B3LYP/6-311+G** Free Energy: -1223.332617.

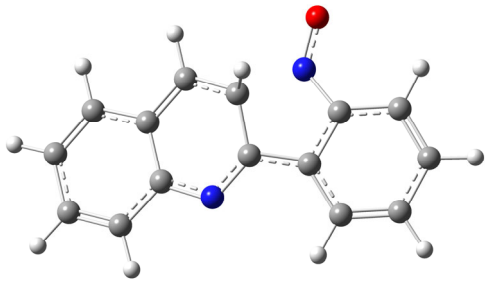
B3LYP/6-311+G** Free Energy in Toluene: -1223.341539.

B3LYP/6-311+G** Free Energy in Toluene (383.15 K): -1223.364055.

Number of Imaginary Frequencies: 1 (-301.05)

P	-3.77929700	-1.21742600	0.36855800
C	-2.47844600	-1.80978400	1.49020400
C	-5.13449800	-0.51473400	1.41331900
C	-4.53333300	-2.63530100	-0.49382200
C	5.77217700	-1.44560700	0.36775600
C	5.55785400	-0.47591400	1.37658700
C	4.39586200	0.25963200	1.40548000
C	3.39024500	0.05858400	0.42330000
C	3.60764600	-0.92176000	-0.59213900
C	4.81569700	-1.66285100	-0.59726600
N	2.25378900	0.80569700	0.48743200
C	1.30261200	0.62086200	-0.41634600
C	1.43890900	-0.33479800	-1.46883700
C	2.57849100	-1.08817900	-1.55268300
C	0.11184700	1.50780200	-0.32478500
C	-1.21606300	1.06513100	-0.61806000
C	-2.27552200	1.99890500	-0.52308700
C	-2.04268800	3.31157900	-0.13182700
C	-0.74942600	3.73779500	0.17005400
C	0.30672000	2.83314700	0.07018900
N	-1.41701000	-0.27737600	-0.89790000
O	-2.69312800	-0.55734500	-1.15336400
H	6.69427100	-2.01571800	0.35910900
H	6.31959100	-0.31404000	2.13125800
H	4.21637100	1.00583700	2.17076400
H	4.97415000	-2.40397400	-1.37420700
H	0.63946000	-0.44872000	-2.18581500
H	2.70493400	-1.81181200	-2.35191400
H	-3.27391800	1.67260100	-0.77770400
H	-2.87307700	4.00789300	-0.07196600
H	-0.56114000	4.76262900	0.46856300
H	1.31664800	3.14989900	0.29959300
H	-2.56390800	-1.32597500	2.46308500
H	-1.52143300	-1.53257000	1.02672400
H	-2.51822100	-2.89327900	1.61290500
H	-4.73716900	0.30238800	2.01587700
H	-5.55457600	-1.28401800	2.07017500
H	-5.92296700	-0.12555400	0.76723500
H	-5.07482000	-3.27884900	0.20385600
H	-3.74858600	-3.20519200	-0.99137400
H	-5.22710500	-2.26668900	-1.25255400

19TSC.-



19TSC

B3LYP/6-31G* Energy + ZPE: -762.012189.

B3LYP/6-31G* Free Energy: -762.050631.

B3LYP/6-31G* Free Energy in Toluene: -762.054624.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -762.070339.

B3LYP/6-311+G** Energy + ZPE: -762.205884.

B3LYP/6-311+G** Free Energy: -762.244433.

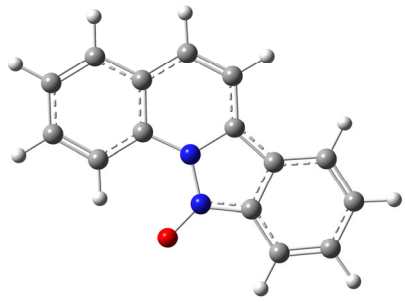
B3LYP/6-311+G** Free Energy in Toluene: -762.25498.

B3LYP/6-311+G** Free Energy in Toluene (383.15K): -762.265032.

Number of Imaginary Frequencies: 1 (-304.38)

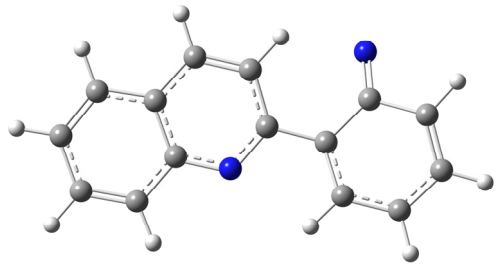
C	-4.63084000	0.18667000	-0.34580700
C	-4.36209400	-1.21424100	-0.26442500
C	-3.08492800	-1.66601200	-0.04876800
C	-2.00246000	-0.75390300	0.10519600
C	-2.27154400	0.67881900	0.04014300
C	-3.62455200	1.10072300	-0.20108500
N	-0.75548800	-1.25044200	0.25092700
C	0.23464600	-0.39082800	0.43055300
C	0.06894000	1.07564700	0.59500900
C	-1.24157100	1.57882600	0.26200100
C	1.61449600	-0.68852100	0.21623300
C	2.34467100	0.51166900	-0.02889600
C	3.73176300	0.49973300	-0.29235700
C	4.36262100	-0.72533600	-0.33424900
C	3.64159400	-1.93435800	-0.12796500
C	2.28460700	-1.92580800	0.13303800
N	1.51604600	1.61228700	-0.15569800
O	1.89847300	2.79683400	-0.16167200
H	-5.64842800	0.52316300	-0.52490400
H	-5.17878000	-1.92097000	-0.38112300
H	-2.85371500	-2.72547200	0.00405300
H	-3.82954400	2.16703000	-0.25698300
H	0.45270100	1.46479100	1.54789800
H	-1.43261500	2.64825400	0.28462100
H	4.25208500	1.43557000	-0.46487300
H	5.43013700	-0.77457200	-0.53034900
H	4.17509800	-2.87943600	-0.17557300
H	1.72928900	-2.84441100	0.29227600

Intermediate B.-

 B	B3LYP/6-31G* Energy + ZPE: -762.062349. B3LYP/6-31G* Free Energy: -762.100893. B3LYP/6-31G* Free Energy in Toluene: -762.100893 B3LYP/6-31G* Free Energy in Toluene (383.15 K): -762.116707. B3LYP/6-311+G** Energy + ZPE: -762.250996. B3LYP/6-311+G** Free Energy: -762.298573. B3LYP/6-311+G** Free Energy in Toluene: -762.294545. B3LYP/6-311+G** Free Energy in Toluene (383.15K): -762.310454. Number of Imaginary Frequencies: 0

C	4.41322300	-0.24849300	0.00000600
C	3.70066900	-1.45763800	0.00000400
C	2.31241200	-1.46944000	0.00000200
C	1.61262000	-0.24960900	0.00000200
C	2.31550500	0.99236400	0.00000400
C	3.72714000	0.95294400	0.00000600
C	1.60045400	2.23659400	0.00000400
C	0.23486800	2.25583700	0.00000200
C	-0.49011700	1.04579600	0.00000000
N	0.21059800	-0.16311100	0.00000000
C	-1.86131700	0.72173400	-0.00000200
C	-1.93708500	-0.69542400	-0.00000300
C	-3.15859300	-1.39584000	-0.00000600
C	-4.30804100	-0.63488600	-0.00000600
C	-4.26019700	0.79032200	-0.00000500
C	-3.06084800	1.47170600	-0.00000300
N	-0.67755000	-1.22490500	-0.00000200
O	-0.33827600	-2.45864600	-0.00000300
H	5.49935200	-0.25504300	0.00000700
H	4.23478400	-2.40319200	0.00000400
H	1.75483200	-2.39303900	0.00000100
H	4.26729500	1.89592900	0.00000700
H	2.16834400	3.16152600	0.00000500
H	-0.32205300	3.18682900	0.00000200
H	-3.16771700	-2.47974300	-0.00000700
H	-5.27579800	-1.12803200	-0.00000800
H	-5.19285100	1.34671700	-0.00000600
H	-3.03547100	2.55752400	-0.00000200

Intermediate A.-



A

B3LYP/6-31G* Energy + ZPE: -686.800712.

B3LYP/6-31G* Free Energy: -686.840338.

B3LYP/6-31G* Free Energy in Toluene: -686.844595.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -686.860698.

B3LYP/6-311+G** Energy + ZPE: -686.970237.

B3LYP/6-311+G** Free Energy: -687.010053.

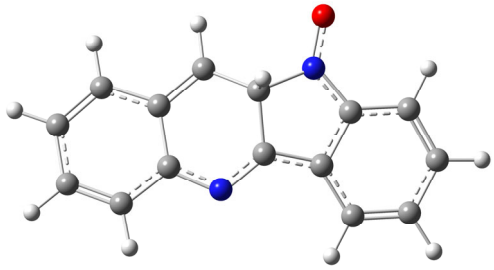
B3LYP/6-311+G** Free Energy in Toluene: -687.015138.

B3LYP/6-311+G** Free Energy in Toluene (383.15K): -687.031355.

Number of Imaginary Frequencies: 0

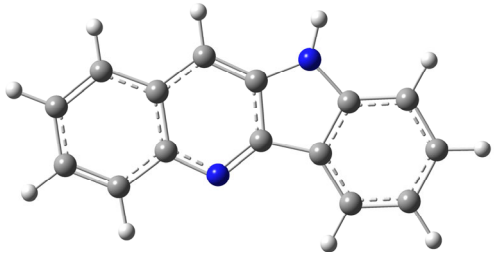
C	-3.55029200	-1.79067800	-0.06574700
C	-2.18668600	-1.46804800	-0.15358600
C	-1.74214700	-0.15907300	-0.04735400
C	-2.74922100	0.91035400	0.10331800
C	-4.15615800	0.53640400	-0.04520400
C	-4.53359900	-0.79286400	0.01746900
N	-2.57734100	2.10314500	0.54667300
C	-0.31989700	0.18377100	-0.11950100
N	0.54744300	-0.82488100	-0.00755500
C	1.87180600	-0.55096900	0.01284900
C	2.38821500	0.78641300	-0.07441400
C	1.44616000	1.83194200	-0.21226500
C	0.10326000	1.54059900	-0.26047700
C	2.78922200	-1.63484400	0.13292100
C	4.14281500	-1.40075900	0.16140900
C	4.65064300	-0.07677600	0.07471900
C	3.79267000	0.99221000	-0.04216100
H	-3.84818900	-2.83480300	-0.10889800
H	-1.44501400	-2.25084000	-0.27468400
H	-4.87316000	1.34893800	-0.04552300
H	-5.58539900	-1.06648500	0.03903800
H	1.79326000	2.85826800	-0.30472200
H	-0.62831400	2.32567100	-0.41722200
H	2.37807800	-2.63720300	0.19982000
H	4.83644200	-2.23213800	0.25284800
H	5.72422700	0.08729700	0.10332900
H	4.17660300	2.00736000	-0.10966800

Intermediate C.-

 **C**	B3LYP/6-31G* Energy + ZPE: -762.015765. B3LYP/6-31G* Free Energy: -762.054569. B3LYP/6-31G* Free Energy in Toluene: -762.058932 B3LYP/6-31G* Free Energy in Toluene (383.15 K): -762.074867. B3LYP/6-311+G** Energy + ZPE: -762.210429. B3LYP/6-311+G** Free Energy: -762.249320. B3LYP/6-311+G** Free Energy in Toluene: -762.254698. B3LYP/6-311+G** Free Energy in Toluene (383.15K): -762.270683. Number of Imaginary Frequencies: 0

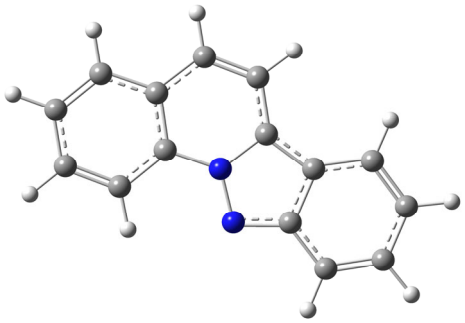
C	-4.60446800	0.22039500	-0.36396000
C	-4.38557900	-1.17447900	-0.12209300
C	-3.12367900	-1.65083600	0.11934300
C	-1.99833000	-0.77660200	0.15388300
C	-2.21981000	0.66454700	-0.05220600
C	-3.56552800	1.10332900	-0.33726600
N	-0.76941600	-1.31797900	0.27214000
C	0.25548500	-0.48170900	0.34336400
C	0.11644800	1.01040000	0.52503000
C	-1.16189200	1.54066900	0.01041900
C	1.62861200	-0.74037000	0.14841100
C	2.31718200	0.51727600	0.03215600
C	3.70839300	0.59355900	-0.22067600
C	4.38830100	-0.59315300	-0.34931400
C	3.72240300	-1.85572700	-0.23874400
C	2.36930400	-1.93825800	0.00031000
N	1.44123000	1.55638800	0.10406900
O	1.67697800	2.79380800	0.01147100
H	-5.61229000	0.57228200	-0.56670900
H	-5.23069900	-1.85662400	-0.14453300
H	-2.93342300	-2.70774600	0.27876700
H	-3.73173000	2.16397800	-0.50893400
H	0.16851300	1.24558300	1.60678800
H	-1.27320600	2.60708700	-0.16061500
H	4.18768900	1.56201500	-0.30954300
H	5.45761100	-0.58126100	-0.54074600
H	4.30638400	-2.76473800	-0.35063300
H	1.86157900	-2.89414400	0.07899000

Quindoline (**1**).-

 **1**	B3LYP/6-31G* Energy + ZPE: -686.940400. B3LYP/6-31G* Free Energy: -686.977819. B3LYP/6-31G* Free Energy in Toluene: -686.818220. B3LYP/6-31G* Free Energy in Toluene (383.15 K): -686.997547. B3LYP/6-311+G** Energy + ZPE: -687.109936. B3LYP/6-311+G** Free Energy: -687.147472. B3LYP/6-311+G** Free Energy in Toluene: -687.152319. B3LYP/6-311+G** Free Energy in Toluene (383.15K): -687.16759. Number of Imaginary Frequencies: 0

C	-4.56391000	0.19643100	-0.00001100
C	-4.26032800	-1.18909200	0.00005200
C	-2.95196700	-1.61271900	0.00004500
C	-1.88097800	-0.67740400	0.00000000
C	-2.18945200	0.73134700	-0.00003700
C	-3.55395000	1.13068600	-0.00005500
N	-0.60671500	-1.15920700	0.00000100
C	0.36267600	-0.26616800	-0.00001700
C	0.15349100	1.16160800	0.00000000
C	-1.12418900	1.66745000	-0.00001300
C	1.80047600	-0.47399200	-0.00001600
C	2.60310500	-1.61737200	-0.00004500
C	3.98746500	-1.46488700	-0.00003500
C	4.56513900	-0.18331200	0.00001400
C	3.78299300	0.97160100	0.00004100
C	2.39681200	0.81111500	0.00001800
H	-5.60157900	0.51915000	-0.00002900
H	-5.06859700	-1.91525300	0.00010500
H	-2.69157700	-2.66670900	0.00007500
H	-3.78610100	2.19350300	-0.00009000
H	-1.33222300	2.73486100	0.00000200
H	4.62920000	-2.34104400	-0.00006400
H	5.64753600	-0.08657200	0.00003300
H	4.23936600	1.95770000	0.00008200
H	2.14213600	-2.60048800	-0.00008000
H	1.54998200	2.77228600	-0.00010800
N	1.39351100	1.77646600	0.00006000

Indazolo[2,3-*a*]quinoline (**18**).-



18

B3LYP/6-31G* Energy + ZPE: -686.914461.

B3LYP/6-31G* Free Energy: -686.951543.

B3LYP/6-31G* Free Energy in Toluene -686.954645.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -686.969643.

B3LYP/6-311+G** Energy + ZPE: -687.080783.

B3LYP/6-311+G** Free Energy: -687.117972.

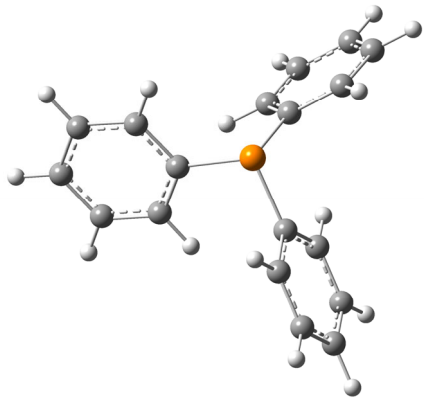
B3LYP/6-311+G** Free Energy in Toluene: -687.121417.

B3LYP/6-311+G** Free Energy in Toluene (383.15K): -687.136532.

Number of Imaginary Frequencies: 0

C	4.34494700	-0.43798500	0.00001400
C	3.60228800	-1.63435600	0.00000900
C	2.21784400	-1.60513000	-0.00000300
C	1.55910200	-0.36542600	-0.00000500
C	2.28254200	0.85666100	-0.00000100
C	3.69412900	0.78219700	0.00000800
N	0.16740300	-0.29455400	-0.00002200
C	-0.52203800	0.90908000	-0.00000800
C	0.20639500	2.12584000	-0.00000600
C	1.57181600	2.10400500	-0.00000300
C	-1.88706300	0.54983800	-0.00000300
C	-1.87742900	-0.88251000	-0.00000500
C	-3.09579100	-1.60461100	0.00000200
C	-4.27164400	-0.88602900	0.00001100
C	-4.28204800	0.53813100	0.00001200
C	-3.10682900	1.26067800	0.00000500
N	-0.62219400	-1.38906200	-0.00001400
H	5.43051300	-0.47459100	0.00002100
H	4.11750800	-2.59060700	0.00001300
H	1.62359800	-2.51083100	-0.00000900
H	4.26224700	1.70897800	0.00001100
H	-0.34484100	3.06065100	-0.00000200
H	2.14155100	3.02853300	0.00000300
H	-3.08628400	-2.69002700	0.00000000
H	-5.22110900	-1.41505300	0.00001700
H	-5.23568200	1.05841100	0.00001800
H	-3.12129400	2.34754000	0.00000600

Triphenylphosphine.-



PPh_3

B3LYP/6-31G* Energy + ZPE: -1036.023972.

B3LYP/6-31G* Free Energy: -1036.070407.

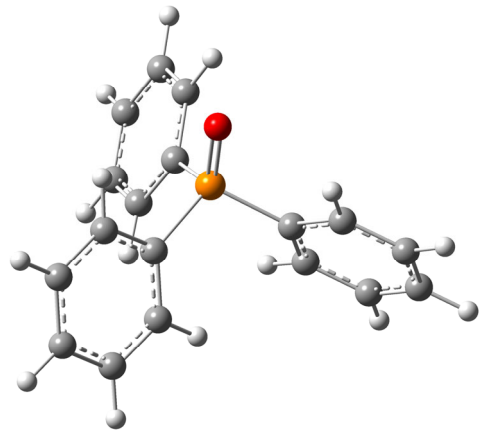
B3LYP/6-31G* Free Energy in Toluene -1036.073107.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -1036.092422.

Number of Imaginary Frequencies: 0

P	0.00001100	0.00025900	-1.20670500
C	1.59595200	0.49386200	-0.40243500
C	2.33813600	1.50620300	-1.03403000
C	2.11799500	-0.09288800	0.76036600
C	3.55631100	1.93539100	-0.50778100
H	1.95911900	1.95729900	-1.94828500
C	3.34340800	0.32860000	1.28122000
H	1.56791200	-0.88505200	1.25918500
C	4.06352700	1.34501000	0.65165800
H	4.11419900	2.72239300	-1.00858300
H	3.73456800	-0.13872400	2.18146700
H	5.01745100	1.67080200	1.05794500
C	-0.37092800	-1.62887000	-0.40296900
C	-1.14046400	-1.78775500	0.75969500
C	0.13553500	-2.77771200	-1.03401700
C	-1.38668900	-3.05969200	1.28134500
H	-1.55282400	-0.91553300	1.25786400
C	-0.10068700	-4.04723700	-0.50709300
H	0.71576300	-2.67514000	-1.94825800
C	-0.86512100	-4.19136200	0.65264700
H	-1.98698100	-3.16488800	2.18158100
H	0.30273500	-4.92378200	-1.00742000
H	-1.05871600	-5.18028500	1.05974600
C	-1.22572300	1.13551100	-0.40288000
C	-2.47505600	1.26850200	-1.03217100
C	-0.97738000	1.88396700	0.75775600
C	-3.45614600	2.10838300	-0.50577800
H	-2.67728600	0.71201200	-1.94454800
C	-1.95551600	2.73393100	1.27875300
H	-0.01513800	1.80605700	1.25482900
C	-3.19729600	2.84590100	0.65147100
H	-4.41788200	2.19517700	-1.00471400
H	-1.74552700	3.30865400	2.17732900
H	-3.95671700	3.50867600	1.05789900

Triphenylphosphine Oxide.-



PPh_3O

B3LYP/6-31G* Energy + ZPE: -1111.271894.

B3LYP/6-31G* Free Energy: -1111.318342.

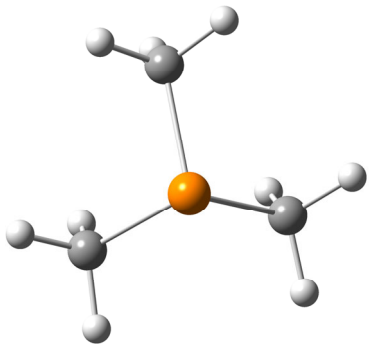
B3LYP/6-31G* Free Energy in Toluene: -1111.323867.

B3LYP/6-31G* Free Energy in Toluene (383.15 K): -1111.344066.

Number of Imaginary Frequencies: 0

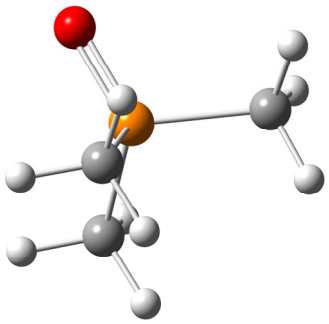
P	-0.00029200	0.00072500	0.91438300
C	-1.63849900	0.42882100	0.21516000
C	-2.47873700	1.21691100	1.01575000
C	-2.08361800	0.01185400	-1.04756000
C	-3.73732500	1.59771200	0.55060200
H	-2.14265700	1.50917200	2.00621900
C	-3.34270100	0.39693900	-1.51114100
H	-1.45882100	-0.62901700	-1.66361400
C	-4.16847700	1.19239700	-0.71437100
H	-4.38382900	2.20587900	1.17760300
H	-3.68199000	0.06753900	-2.48966700
H	-5.15020100	1.48776000	-1.07522800
C	0.44755000	-1.63210700	0.21488600
C	1.02675100	-1.80915400	-1.04989000
C	0.18915900	-2.75359700	1.01697100
C	1.32207700	-3.09200300	-1.51416100
H	1.26644500	-0.94749800	-1.66689900
C	0.48785100	-4.03391500	0.55113700
H	-0.22822100	-2.60834700	2.00896900
C	1.04982100	-4.20476700	-0.71590400
H	1.77348000	-3.22113300	-2.49431700
H	0.28740400	-4.89780100	1.17922300
H	1.28424900	-5.20264100	-1.07719600
C	1.19023800	1.20454200	0.21473300
C	2.29425700	1.53566100	1.01444000
C	1.05180700	1.79929400	-1.04766100
C	3.25479800	2.43336200	0.54878600
H	2.37936400	1.09781900	2.00460800
C	2.01615200	2.69557300	-1.51161900
H	0.18362300	1.58045000	-1.66329500
C	3.11931800	3.01037700	-0.71576000
H	4.10591700	2.68700400	1.17506400
H	1.90050600	3.15479800	-2.48982500
H	3.86705800	3.71154700	-1.07697500
O	-0.00006000	0.00077600	2.41790000

Trimethylphosphine.-

 PMe_3	B3LYP/6-311+G** Energy + ZPE: -461.052399. B3LYP/6-311+G** Free Energy: -461.081733. B3LYP/6-311+G** Free Energy in Toluene: -461.083105. B3LYP/6-311+G** Free Energy in Toluene (383.15 K): -461.094192. Number of Imaginary Frequencies: 0

P	-0.00005100	-0.00036900	-0.59820100
C	0.11733900	1.63794700	0.27738800
C	-1.47776000	-0.71721600	0.27743000
C	1.36044100	-0.92032400	0.27763100
H	0.11095900	1.52889900	1.36669300
H	-0.72268200	2.27073200	-0.01928600
H	1.03765200	2.14568700	-0.02138200
H	-2.37725000	-0.17378500	-0.02197100
H	-1.38043300	-0.66773200	1.36668600
H	-1.60612200	-1.76110000	-0.01900800
H	1.27046800	-0.85869300	1.36692600
H	2.32802500	-0.50932400	-0.02056100
H	1.34003200	-1.97159100	-0.01977300

Trimethylphosphine oxide.-

 PMe_3O	B3LYP/6-311+G** Energy + ZPE: -536.328209. B3LYP/6-311+G** Free Energy: -536.358809. B3LYP/6-31G* Free Energy in Toluene: -536.365835. B3LYP/6-311+G** Free Energy in Toluene (383.15 K): -536.377494. Number of Imaginary Frequencies: 0

P	-0.00009600	-0.00020300	0.17446200
C	-1.37901900	-0.95332000	-0.55110700
C	1.51548300	-0.71670900	-0.55117500
C	-0.13663000	1.67136000	-0.54954700
H	-1.31565200	-1.98806600	-0.20879800
H	-1.35150700	-0.93154400	-1.64293400
H	-2.32442800	-0.53082100	-0.20529500
H	1.48426000	-0.70288800	-1.64310100
H	1.62296300	-1.74704000	-0.20639500
H	2.37926400	-0.14423200	-0.20752900
H	-1.06300800	2.13466900	-0.20430900
H	-0.13480400	1.63784000	-1.64149200
H	0.70355200	2.27781100	-0.20563800
O	0.00022300	-0.00133300	1.68244200