Supporting Information

Kinetic or Dynamic Control on a Bifurcating Potential Energy Surface? An Experimental and DFT Study of Gold-Catalyzed Ring Expansion and Spirocyclization of 2-Propargyl-β-tetrahydrocarbolines

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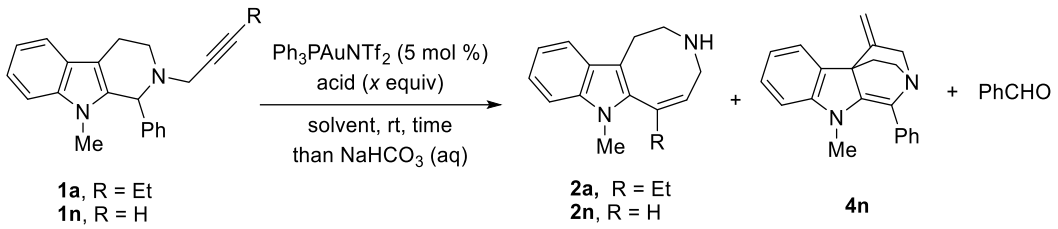
S1. General Information

All melting points were determined without correction. ^{1}H NMR spectra were obtained at 300 or 400 MHz. ^{13}C NMR spectra were obtained at 75 or 100 MHz. NMR spectra were recorded in $CDCl_3$, DMSO-d_6 or acetone-d_6 using the residual protonated solvent as the internal standard. *J* values were given in Hz.

S2. Experimental Details and Characterization Data

S2.1. Optimization of Reaction Conditions

Table S1. Effect of Acidic Additives on Gold-Catalyzed Transformations of 2-Propargyl-β-tetrahydrocarbolines[a]



1a, R = Et
1n, R = H

2a, R = Et
2n, R = H

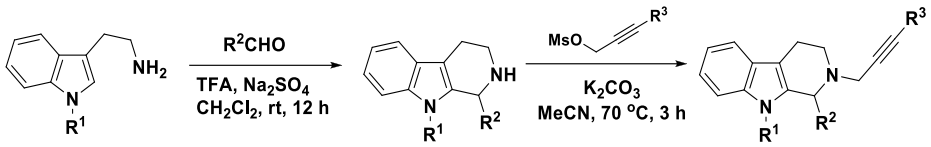
4n

entry	substrate	acid	*x*	solvent	time (h)	product, isolated yield (%)
1	**1a**	MsOH	0.1	PhMe	48	**2a**, 16
2	**1a**	MsOH	0.5	PhMe	48	**2a**, 40
3	**1a**	MsOH	1.0	PhMe	4	**2a**, 23
4	**1a**	MsOH	1.5	PhMe	4	**2a**, 90
5	**1a**	MsOH	1.8	PhMe	4	**2a**, 90
6	**1a**	MsOH	2.0	PhMe	4	**2a**, 92
7	**1a**	HOAc	2.0	PhMe	48	**2a**, 52
8	**1a**	CF_3CO_2H	2.0	PhMe	48	**2a**, 23
9	**1n**	MsOH	0.1	DCM	48	**4n**, 0
10	**1n**	MsOH	0.5	DCM	48	**4n**, 0
11	**1n**	MsOH	1.0	DCM	6	**4n**, 68
12	**1n**	MsOH	1.2	DCM	6	**4n**, 73
13	**1n**	MsOH	1.5	DCM	6	**4n**, 79
14	**1n**	MsOH	1.8	DCM	6	**4n**, 72
15	**1n**	MsOH	2.0	DCM	6	**4n**, 83
16	**1n**	HOAc	2.0	DCM	48	**4n**, 0
17	**1n**	CF_3CO_2H	2.0	DCM	48	**4n**, 58

[a]No reaction occurred in the absence of a gold catalyst.

S2.2. Synthesis of Substrates

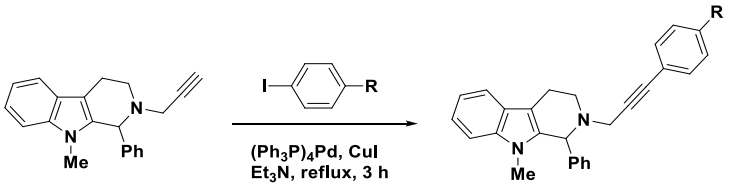
General Procedure A (for **1a–c**, **1j–u**, **1w**, and **1x**):



A mixture of tryptamine[1] (10.0 mmol), aldehyde (11.0 mmol), and anhydrous Na_2SO_4 (3.0 g) was stirred in CH_2Cl_2 (40 mL) at 0 °C. Then trifluoroacetic acid (16.0 mmol) was added dropwise over 15 min. The reaction mixture was allowed to stir at room temperature for another 12 h. Then saturated $NaHCO_3$ solution (20 mL) was added. The organic layer was separated and the aqueous layer was further extracted with CH_2Cl_2 (20 mL). The combined organic layer was washed with water (30 mL), then dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude 2-unsubstituted β-tetrahydrocarboline was used in the next step without further purification.

An oven-dried flask was charged with crude 2-unsubstituted β-tetrahydrocarboline (10.0 mmol), propargyl mesylate[2] (10.0 mmol), and anhydrous K_2CO_3 (50.0 mmol). Dry acetonitrile (20 mL) was added and the reaction mixture was stirred at 70 °C for 4 h. Then the reaction mixture was cooled to room temperature, filtered, and concentrated. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford the 2-propargyl-β-tetrahydrocarboline product.

General Procedure B (for **1d–f**):

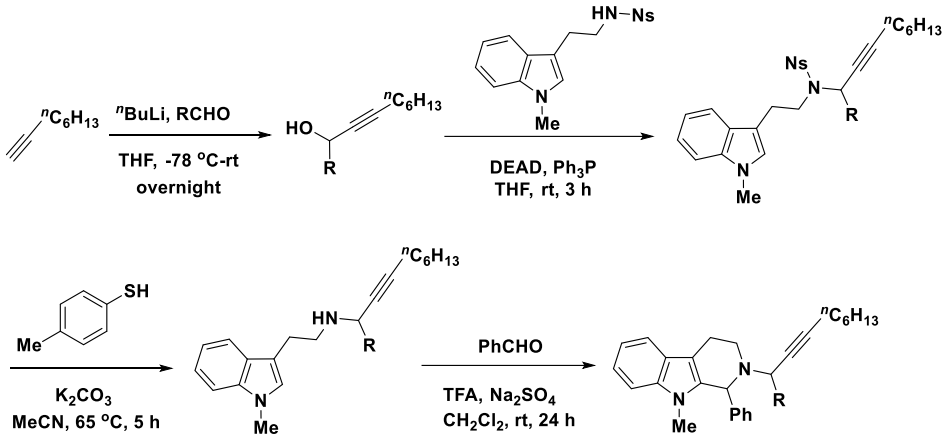


Under nitrogen atmosphere, a flame-dried 50 mL round-bottom flask equipped with a reflux condenser was charged with 2-propargyl-β-tetrahydrocarboline **1n** (4.0 mmol), aryl iodide (4.0 mmol), CuI (0.08 mmol), tetrakis(triphenylphosphine)palladium (0.08 mmol), and Et_3N (8.0 mL). The reaction mixture was heated to reflux for 3 h. Then the reaction mixture was cooled to room temperature, filtered, and concentrated. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford the 2-propargyl-β-tetrahydrocarboline product.

(1) For **1a–c**, **1j–u**: (a) Lygin, A. V.; de Meijere, A. *Eur. J. Org. Chem.* **2009**, 5138. (b) For **1w**: Jahangira, Brooka, M. A.; Macleana, D. B.; Hollandb, H. L. *Tetrahedron* **1987**, *43*, 5761. (c) For **1x**: Güngöra, T.; Malabrea, P.; Teulon, J. M. *Synth. Commun.* **1994**, *24*, 2247.

(2) For **1a**, **1j–m**: White, W. L.; Anzeveno, P. B.; Johnson, F. *J. Org. Chem.* **1982**, *47*, 2379. (b) For **1b**: Schelper, M.; de Meijere, A. *Eur. J. Org. Chem.* **2005**, 582. (c) For **1c**: Shirokova, E. A.; Tarussova, N. B.; Shipitsin, A. V.; Semizarov, D. G.; Krayevsky, A. A. *J. Med. Chem.* **1994**, *37*, 3739. (d) For **1n–u**, **1w**, and **1x**: Jackson, W. R.; Perlmutter, P.; Smallridge, A. J. *Aust. J. Chem.* **1988**, *41*, 1201.

General Procedure C (for **1g–i**):



Under nitrogen atmosphere, a flame-dried 50 mL round-bottom flask was charged with 1-octyne (20.0 mmol) and anhydrous THF (30 mL). *n*-Butyllithium (22.0 mmol) was added dropwise over 30 min at −78 °C, and the reaction mixture was stirred at −78 °C for an additional 1 h. Then aldehyde (20.0 mmol) was added dropwise over 30 min. After the addition was completed, the reaction mixture was allowed to stir at room temperature overnight, and then was quenched with saturated NH_4Cl solution (10 mL), extracted with CH_2Cl_2 (30 mL×3). The combined organic layer was washed with water (20 mL), dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was purified by column chromatography with petroleum ether/ethyl acetate as eluent to afford 1-substituted propargyl alcohol product.

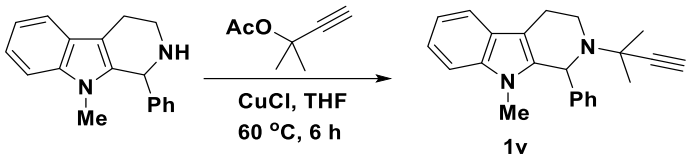
Under nitrogen atmosphere, an oven-dried 50 mL round-bottom flask was charged with 1-methyltryptamine nosylamide[3] (3.0 mmol), triphenylphosphine (3.6 mmol), 1-substituted propargyl alcohol (3.6 mmol), and anhydrous THF (15 mL). Diethyl azodicarboxylate (DEAD) was added dropwise over 30 min at 0 °C. After the addition was completed, the reaction mixture was allowed to stir at room temperature for 3 h. Then the reaction mixture was concentrated. The crude product was purified by column chromatography with petroleum ether/ethyl acetate as eluent to afford *N*-substituted-1-methyltryptamine nosylamide product.

Under nitrogen atmosphere, an oven-dried flask was charged with *N*-substituted-1-methyltryptamine nosylamide (2.8 mmol), K_2CO_3 (5.6 mmol), and *p*-toluenethiol (4.0 mmol). Dry acetonitrile (30 mL) was added and the reaction mixture was stirred at 65 °C for 5 h. Then the reaction mixture was cooled to room temperature, filtered, and concentrated. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate as eluent to afford the *N*-propargyl-1-methyltryptamine product.

A 50 mL round-bottom flask was charged with *N*-propargyl-1-methyltryptamine (8.0 mmol), anhydrous Na_2SO_4 (2.0 g), and CH_2Cl_2 (30 mL). Benzaldehyde (16.0 mmol) was added in one portion at 0 °C. Then trifluoroacetic acid (16.0 mmol) was added dropwise over 15 min. After the addition was completed, the mixture was allowed to stir at room temperature for 24 h. The reaction mixture was washed with saturated Na_2CO_3 solution (15 mL) and water (15 mL) successively. The obtained organic layer was dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was purified by column chromatography with petroleum ether/ethyl acetate as eluent to afford the 2-propargyl-β-tetrahydrocarboline product.

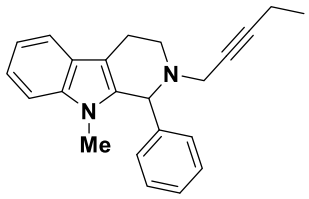
(3) Medley, J. W.; Movassaghi, M. *Angew. Chem., Int. Ed.* **2012**, *51*, 4572.

Procedure D (for **1v**):



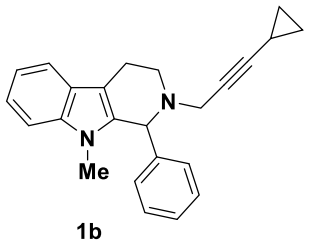
1v

A flame-dried 50 mL round-bottom flask was charged with 2-unsubstituted β-tetrahydrocarboline (10.0 mmol), 2-methylbut-3-yn-2-yl acetate[4] (5.0 mmol), CuCl (0.25 mmol), and anhydrous THF (10.0 mL). Under nitrogen atmosphere, the reaction mixture was stirred at 60 °C for 6 h. After cooling, the reaction mixture was quenched with saturated $NaHCO_3$ solution (15 mL), extracted with CH_2Cl_2 (20 mL×3). The combined organic layer was washed with water (30 mL), then dried over anhydrous Na_2SO_4, filtered, and concentrated. The crude product was purified by column chromatography with petroleum ether/ethyl acetate as eluent to afford 2-propargyl-β-tetrahydrocarboline **1v**.



1a

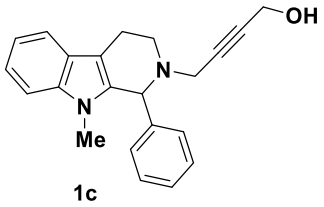
Compound **1a** was prepared in 72% yield according to the general procedure A. White solids; mp 113–116 °C; R_f (PE/EA, 10:1) = 0.7; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, J = 7.5 Hz, 1H), 7.32–7.26 (m, 5H), 7.21–7.19 (m, 2H), 7.15–7.10 (m, 1H), 5.10 (s, 1H), 3.41 (q, J = 2.9 Hz, 2H), 3.20 (s, 3H), 3.09–3.04 (m, 2H), 2.97–2.92 (m, 2H), 2.29 (qt, J_1 = 7.5 Hz, J_2 = 2.1 Hz, 2H), 1.20 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.2, 137.3, 134.9, 129.4, 128.4, 127.7, 126.3, 121.1, 118.9, 118.1, 108.8, 108.6, 87.1, 74.7, 60.0, 47.0, 43.1, 29.9, 20.5, 14.2, 12.5; IR (KBr) ν_{max}: 2800, 1471, 1375, 1149, 758, 737, 713 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{23}H_{25}N_2$: 329.2018 $[M+H]^+$; found: 329.2015.



1b

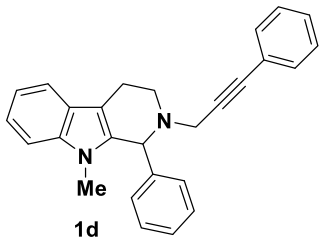
Compound **1b** was prepared in 83% yield according to the general procedure A. White solids; mp 120–122 °C; R_f (PE/EA, 10:1) = 0.7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, J = 7.7 Hz, 1H), 7.31–7.23 (m, 5H), 7.20–7.15 (m, 2H), 7.12–7.09 (m, 1H), 5.06 (s, 1H), 3.37 (s, 2H), 3.17 (s, 3H), 3.07–2.98 (m, 2H), 2.95–2.91(m, 2H), 1.31–1.28 (m, 1H), 0.80–0.73 (m, 2H), 0.71–0.68 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 137.3, 134.9, 129.4, 128.3, 127.7, 126.3, 121.1, 118.8, 118.1, 108.8, 108.7, 88.9, 70.7, 60.1, 47.1, 43.1, 29.9, 20.5, 8.28, 8.27; IR (KBr) ν_{max}: 1470, 1455, 1376, 739, 700 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{24}H_{25}N_2$: 341.2018 $[M+H]^+$; found: 341.2017.

(4) Bartels, A.; Mahrwald, R.; Müller, K. *Adv. Synth. Catal.* **2004**, *346*, 483.



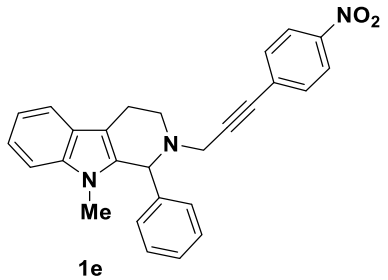
1c

Compound **1c** was prepared in 83% yield according to the general procedure A. Colorless oil; R_f (PE/EA, 2:1) = 0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.7 Hz, 1H), 7.32–7.24 (m, 6H), 7.21–7.16 (m, 2H), 7.14–7.10 (m, 1H), 5.05 (s, 1H), 4.33 (t, *J* = 1.7 Hz, 2H), 3.48 (d, *J* = 1.2 Hz, 2H), 3.19 (s, 3H), 3.11–3.01 (m, 2H), 2.97–2.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 137.3, 134.4, 129.4, 128.4, 127.9, 126.3, 121.2, 118.9, 118.2, 108.7, 108.6, 83.8, 81.2, 60.4, 50.9, 46.8, 43.0, 29.9, 20.3; IR (KBr) ν_{max}: 2905, 1470, 1452, 1013, 739, 701 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{22}H_{23}N_2O$: 331.1810 $[M+H]^+$; found: 331.1809.



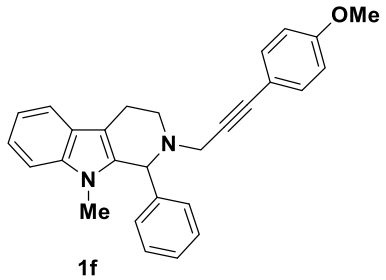
1d

Compound **1d** was prepared in 91% yield according to the general procedure B. White solids; mp 129–131 °C; R_f (PE/EA, 10:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.7 Hz, 1H), 7.50–7.46 (m, 2H), 7.35–7.27 (m, 8H), 7.22–7.17 (m, 2H), 7.14–7.10 (m, 1H), 5.17 (s, 1H), 3.70–3.62 (m, 2H), 3.19 (s, 3H), 3.15 (t, *J* = 5.8 Hz, 2H), 3.04–2.94 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.1, 137.4, 134.8, 131.7, 129.4, 128.4, 128.3, 128.1, 127.9, 126.3, 123.2, 121.2, 118.9, 118.2, 108.8, 108.7, 85.6, 85.1, 60.4, 47.4, 43.6, 30.0, 20.6; IR (KBr) ν_{max}: 1488, 1375, 1103, 754, 737, 701, 692 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{27}H_{25}N_2$: 377.2018 $[M+H]^+$; found: 377.2015.



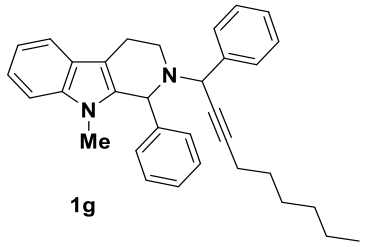
1e

Compound **1e** was prepared in 77% yield according to the general procedure B. White solids; mp 152–155 °C; R_f (PE/EA, 10:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.20–8.17 (m, 2H), 7.58 (d, *J* = 8.7 Hz, 3H), 7.37–7.28 (m, 5H), 7.24–7.18 (m, 2H), 7.16–7.12 (m, 1H), 5.11 (s, 1H), 3.72 (s, 2H), 3.20 (s, 3H), 3.19–3.09 (m, 2H), 3.06–2.96 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 146.9, 139.9, 137.4, 134.5, 132.4, 130.0, 129.4, 128.5, 128.0, 126.2, 123.5, 121.3, 118.9, 118.2, 108.8, 108.7, 91.3, 83.8, 60.9, 47.3, 43.7, 30.0, 20.6; IR (KBr) ν_{max}: 1592, 1516, 1342, 1105, 853, 702, 685 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{27}H_{24}N_3O_2$: 422.1869 $[M+H]^+$; found: 422.1865.



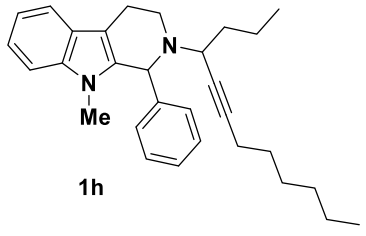
1f

Compound **1f** was prepared in 74% yield according to the general procedure B. White solids; mp 143–145 °C; R_f (PE/EA, 10:1) = 0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, J = 7.7 Hz, 1H), 7.44–7.40 (m, 2H), 7.35–7.29 (m, 5H), 7.23–7.17 (m, 2H), 7.15–7.10 (m, 1H), 6.87–6.83 (m, 2H), 5.18 (s, 1H), 3.82 (s, 3H), 3.65 (d, J = 2.4 Hz, 2H), 3.19 (s, 3H), 3.15 (t, J = 5.7 Hz, 2H), 3.01–2.97 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.4, 140.2, 137.4, 134.9, 133.1, 129.5, 128.4, 127.8, 126.3, 121.3, 118.8, 118.4, 115.3, 113.9, 108.8, 108.7, 85.4, 83.6, 60.4, 55.2, 47.3, 43.6, 29.9, 20.6; IR (KBr) ν_{max}: 1607, 1507, 1249, 826, 746, 733, 698 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{28}H_{27}N_2O$: 407.2123 $[M+H]^+$; found: 407.2123.



1g

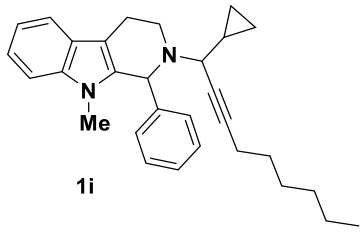
Compound **1g** was prepared in 72% yield according to the general procedure C. White solids; mp 141–143 °C; R_f (PE/EA, 20:1) = 0.7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 8.2 Hz, 1H), 7.51 (d, J = 7.2 Hz, 2H), 7.42 (d, J = 7.6 Hz, 2H), 7.35–7.26 (m, 6H), 7.19 (d, J = 6.8 Hz, 2H), 7.13–7.094 (m, 1H), 5.07 (s, 1H), 4.71 (s, 1H), 3.16 (s, 3H), 2.92–2.76 (m, 4H), 2.37 (td, J_1 = 6.9 Hz, J_2 = 1.3 Hz, 2H), 1.66–1.47 (m, 4H), 1.35–1.27 (m, 4H), 0.90 (t, J = 6.7 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.5, 140.3, 137.4, 136.0, 129.8, 128.4, 128.1, 128.0, 127.8, 127.2, 126.3, 120.9, 118.8, 118.2, 109.6, 108.6, 88.4, 75.6, 61.7, 55.3, 43.2, 31.3, 30.2, 29.1, 28.6, 23.0, 21.4, 18.9, 14.0; IR (KBr) ν_{max}: 2928, 1469, 1454, 1377, 738, 701 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{33}H_{37}N_2$: 461.2957 $[M+H]^+$; found: 461.2957.



1h

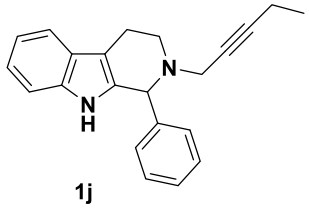
Compound **1h** was prepared in 79% yield according to the general procedure C, mixed diastereomers were obtained. Colorless oil; R_f (PE/EA, 20:1) = 0.8; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 7.6 Hz, 1.5H), 7.33–7.27 (m, 7H), 7.22–7.19 (m, 1.5 Hz), 7.17–7.13 (m, 2H), 7.11–7.07 (m, 1.5 Hz), 5.34 (s, 0.5H), 4.91 (s, 1H), 3.61–3.58 (m, 0.5H), 3.42 (t, J = 7.5 Hz, 1H), 3.31 (s, 1.5H), 3.16–3.09 (m, 4.5H), 3.03–2.96 (m, 2H), 2.89–2.85 (m, 1H), 2.81–2.70 (m, 1.5 H), 2.24 (td, J_1 = 6.9 Hz, J_2 = 2.0 Hz, 2H), 1.96–1.94 (m, 1H), 1.75–1.34 (m, 7H), 1.33–1.16 (m, 11H), 0.95 (t, J = 7.3 Hz, 1.5H), 0.90–0.86 (m, 4.5 Hz), 0.66 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 141.5, 137.4, 137.1, 136.7, 135.0, 130.0,

129.2, 128.13, 128.10, 127.7, 127.2, 126.8, 126.3, 120.9, 120.8, 118.7, 118.67, 118.1, 118.0, 109.7, 109.1, 108.6, 85.0, 84.8, 80.3, 78.3, 62.3, 58.7, 53.4, 50.6, 43.0, 41.6, 36.4, 36.3, 31.4, 31.3, 30.2, 29.4, 29.2, 28.8, 28.6, 28. 5, 22.7, 22.6, 22.0, 19.6, 19.3, 19.27, 18.7, 18.68, 14.0, 13.99, 13.97, 13.4; IR (KBr) ν_{max}: 2956, 2930, 1469, 1378, 737, 701 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{30}H_{39}N_2$: 427.3113 $[M+H]^+$; found: 427.3113.



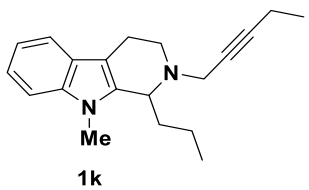
1i

Compound **1i** was prepared in 85% yield according to the general procedure C, mixed diastereomers were obtained. Colorless oil; R_f (PE/EA, 20:1) = 0.6; ^1H NMR (400 MHz, $CDCl_3$) δ 7.67–7.25 (m, 1.5H), 7.31–7.20 (m, 8H), 7.18–7.15 (m, 2.5 H), 7.13–7.07 (m, 1.5 Hz), 5.46 (s, 0.5H), 5.04 (s, 1H), 3.53–3.31 (m, 4.5H), 3.18–3.13 (m, 3.5H), 3.03–2.87 (m, 3.5H), 2.74–2.68 (m, 0.5H), 2.23 (td, J_1 = 6.9 Hz, J_2 = 2.0 Hz, 2H), 1.97 (s, 1H), 1.64–1.48 (m, 2H), 1.46–1.38 (m, 2H), 1.34–1.17 (m, 8.5H), 0.99–0.93 (m, 1H), 0.89–0.84 (m, 4.5H), 0.57–0.32 (m, 5H), 0.1–0.06 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 141.7, 141.6, 137.3, 137.1, 136.1, 134.7, 129.8, 129.1, 128.2, 128.1, 127.6, 127.2, 126.8, 126.3, 120.92, 120.88, 118.7, 118.66, 118.1, 109.6, 109.0, 108.6, 86.0, 85.1, 78.0, 75.5, 61.4, 58.3, 56.9, 55.0, 43.5, 41.6, 31.28, 31.26, 30.1, 29.4, 29.0, 28.7, 28.5, 28.46, 22.7, 22.6, 21.4, 19.2, 18.7, 18.6, 14.3, 14.1, 14.0, 13.99, 3.8, 3.5, 2.7, 2.2; IR (KBr) ν_{max}: 2930, 1470, 1378, 1028, 737, 702 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{30}H_{37}N_2$: 425.2957 $[M+H]^+$; found: 425.2955.



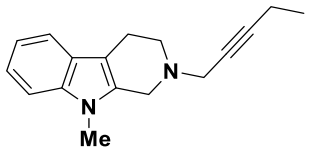
1j

Compound **1j** was prepared in 86% yield according to the general procedure A. White solids; mp 113–116 °C; R_f (PE/EA, 10:1) = 0.5; ^1H NMR (300 MHz, $CDCl_3$) δ 7.55–7.52 (m, 1H), 7.41–7.34 (m, 5H), 7.24 (s, 1H), 7.19–7.07 (m, 3H), 4.87 (s, 1H), 3.47–3.26 (m, 2H), 3.24–3.04 (m, 3H), 2.90–2.86 (m, 1H), 2.26 (qt, J_1 = 7.4 Hz, J_2 = 2.1 Hz, 2H), 1.19 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.3, 136.2, 134.9, 129.2, 128.3, 128.4, 127.0, 121.4, 119.3, 118.2, 110.7, 108.8, 87.6, 73.5, 62.2, 49.7, 43.7, 21.5, 14.3, 12.4; IR (KBr) ν_{max}: 3413, 2912, 1454, 1312, 1113, 749, 699 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{22}H_{23}N_2$: 315.1861 $[M+H]^+$; found: 315.1859.



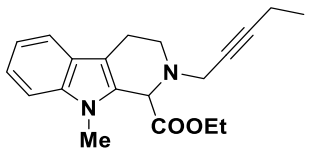
1k

Compound **1k** was prepared in 90% yield according to the general procedure A. White solids; mp 96–99 °C. R_f (PE/EA, 10:1) = 0.7; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.48 (d, *J* = 7.6 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.21–7.16 (m, 1H), 7.12–7.06 (m, 1H), 3.96 (d, *J* = 9.0 Hz, 1H), 3.64 (s, 3H), 3.39 (dt, J_1 = 6.2 Hz, J_2 = 2.2 Hz, 2H), 3.33–3.13 (m, 2H), 2.90–2.79 (m, 1H), 2.60–2.52 (m, 1H), 2.21 (qt, J_1 = 7.4 Hz, J_2 = 2.2 Hz, 2H), 1.84–1.55 (m, 4H), 1.14 (t, *J* = 7.5 Hz, 3H), 1.02 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.1, 136.3, 126.7, 120.9, 118.8, 117.9, 108.6, 106.0, 85.6, 76.4, 54.3, 43.4, 42.8, 36.5, 29.6, 19.8, 16.9, 14.0, 13.9, 12.4; IR (KBr) ν_{max}: 2929, 1473, 1356, 1011, 743 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{20}H_{27}N_2$: 295.2174 [M+H]$^+$; found: 295.2172.



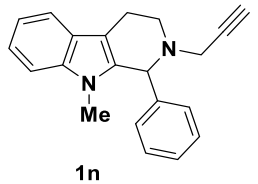
1l

Compound **1l** was prepared in 28% yield according to the general procedure A. White solids, mp 118–121 °C. R_f (PE:EA=10:1) = 0.4; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.5 Hz, 1H), 7.30 (d, *J* = 7.5 Hz, 1H), 7.26–7.17 (m, 1H), 7.15–7.08 (m, 1H), 3.86 (s, *J* = 1.7 Hz, 2H), 3.67–3.67 (m, *J* = 4.8 Hz, 5H), 3.07–2.70 (m, 4H), 2.28 (qt, J_1 = 7.3 Hz, J_2 = 2.0 Hz, 2H), 1.20 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.3, 133.4, 126.8, 120.9, 118.9, 118.1, 108.7, 107.1, 87.5, 74.1, 50.1, 48.2, 47.1, 29.3, 21.7, 14.3, 12.6. IR (KBr) ν_{max}: 3268, 2912, 1474, 1429, 1309, 1135, 735, 677, 649 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{17}H_{21}N_2$ ([M+H]$^+$) 253.1705, found 253.1702.



1m

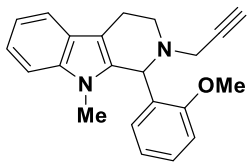
Compound **1m** was prepared in 88% yield according to the general procedure A. White solids; mp 49–53 °C; R_f (PE/EA, 10:1)= 0.7; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.24–7.19 (m, 1H), 7.13–7.07 (m, 1H), 4.84 (s, 1H), 4.22 (qd, J_1 = 7.1 Hz, J_2 = 1.2 Hz, 2H), 3.68 (s, 3H), 3.58–3.55 (m, 2H), 3.51–3.41 (m, 1H), 3.20–3.13 (m, 1H), 2.97–2.75 (m, 2H), 2.22 (qt, J_1 = 7.5 Hz, J_2 = 2.2 Hz, 2H), 1.29 (t, *J* = 7.1 Hz, 3H), 1.14 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.6, 137.5, 129.9, 126.3, 121.6, 118.9, 118.4, 108.9, 108.7, 86.9, 74.6, 61.3, 58.7, 45.5, 43.7, 29.9, 19.4, 14.1, 13.9, 12.4; IR (KBr) ν_{max}: 2976, 1743, 1471, 1209, 1042, 741 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{20}H_{25}N_2O_2$: 325.1916 [M+H]$^+$; found: 325.1913.



1n

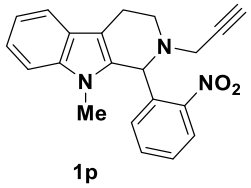
Compound **1n** was prepared in 81% yield according to the general procedure A. White solids; mp 127–129 °C; R_f (PE/EA, 10:1) = 0.7; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.58 (d, *J* = 7.6 Hz, 1H), 7.37–7.26 (m,

5H), 7.24–7.18 (m, 2H), 7.17–7.10 (m, 1H), 5.09 (s, 1H), 3.45 (d, J = 2.4 Hz, 2H), 3.19 (s, 3H), 3.14–3.05 (m, 2H), 3.05–2.87 (m, 2H), 2.35 (t, J = 2.4 Hz, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 140.1, 137.3, 134.8, 129.4, 128.6, 127.9, 126.2, 121.1, 118.8, 118.2, 108.7, 79.5, 73.4, 60.3, 47.4, 42.7, 30.0, 20.6; IR (KBr) ν_{max}: 3281, 2824, 1455, 1376, 1132, 733, 703, 662, 650 cm^{-1}; HRMS (ESI) m/z calculated for $C_{21}H_{21}N_2$: 301.1705 [M+H]$^+$; found: 301.1701.



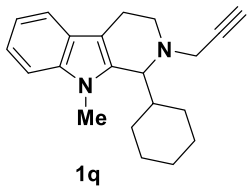
1o

Compound **1o** was prepared in 89% yield according to the general procedure A. White solids; mp 102–104 °C; R_f (PE/EA, 3:1) = 0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, J = 7.6 Hz, 1H), 7.27–7.16 (m, 3H), 7.14–7.10 (m, 1H), 6.95 (d, J = 8.2 Hz, 1H), 6.88 (dd, J_1 = 7.6 Hz, J_2 = 1.7 Hz, 1H), 6.80 (t, J = 7.4 Hz, 1H), 5.56 (s, 1H), 3.95 (s, 3H), 3.48 (qd, J_1 = 16.8 Hz, J_2 = 2.4 Hz, 2H), 3.19 (s, 3H), 3.17–3.11 (m, 2H), 2.95 (t, J = 5.4 Hz, 2H), 2.24 (t, J = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.6, 137.3, 135.3, 130.5, 128.9, 128.3, 126.6, 120.9, 120.6, 118.7, 118.0, 110.5, 108.7, 108.6, 80.3, 72.1, 55.6, 52.9, 46.1, 42.6, 29.3, 20.1; IR (KBr) ν_{max}: 3275, 1598, 1247, 1007, 764, 738 cm^{-1}; HRMS (ESI) m/z calculated for $C_{22}H_{23}N_2O$: 331.1810 [M+H]$^+$; found: 331.1809.



1p

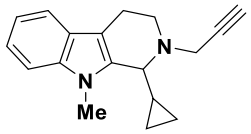
Compound **1p** was prepared in 89% yield according to the general procedure A. White solids; mp 134–136 °C; R_f (PE/EA, 3:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.84–7.82 (m, 1H), 7.58 (d, J = 7.8 Hz, 1H), 7.44–7.38 (m, 2H), 7.29 (d, J = 8.1 Hz, 1H), 7.27–7.23 (m, 1H), 7.18–7.14 (m, 1H), 6.98 (dd, J_1 = 7.3 Hz, J_2 = 1.9 Hz, 1H), 5.75 (s, 1H), 3.47 (qd, J_1 = 16.6 Hz, J_2 = 2.5 Hz, 2H), 3.41 (s, 3H), 3.20 (dt, J_1 = 12.6 Hz, J_2 = 4.6 Hz, 1H), 3.03–2.94 (m, 1H), 2.90–2.86 (m, 1H), 2.79 (dt, J_1 = 15.0, J_2 = 4.7 Hz, 1H), 2.25 (t, J = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.3, 137.4, 135.2, 132.2, 132.1, 130.8, 128.6, 126.4, 124.3, 121.7, 119.1, 118.4, 109.5, 108.9, 79.2, 73.0, 55.0, 44.0, 42.6, 29.6, 18.3; IR(KBr) ν_{max}: 3287, 1520, 1469, 1352, 1007, 750, 648 cm^{-1}; HRMS (ESI) m/z calculated for $C_{21}H_{20}N_3O_2$: 346.1556 [M+H]$^+$; found: 346.1552.



1q

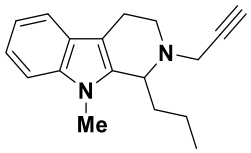
Compound **1q** was prepared in 85% yield according to the general procedure A. White solids; mp 102–104 °C; R_f (PE/EA, 10:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.7 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.23–7.19 (m, 1H), 7.11 (t, J = 7.7 Hz, 1H), 3.72 (d, J = 7.4 Hz, 1H), 3.64 (s, 3H), 3.43–3.24 (m,

3H), 3.14 (dd, J_1 = 14.2 Hz, J_2 = 6.2 Hz, 1H), 2.91–2.82 (m, 1H), 2.61 (dd, J_1 = 16.1 Hz, J_2 = 5.2 Hz, 1H), 2.22 (t, J = 2.4 Hz, 1H), 2.12–2.10 (m, 1H), 1.79–1.62 (m, 5H), 1.30–1.05 (m, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.5, 135.4, 126.9, 121.0, 118.8, 117.9, 108.8, 106.2, 81.4, 71.9, 60.0, 44.2, 43.6, 43.0, 31.1, 31.0, 30.9, 26.8, 26.7, 26.5, 17.0; IR (KBr) ν_{max}: 3200, 2920, 1470, 1450, 1362, 746 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{21}H_{27}N_2$: 307.2174 $[M+H]^+$; found: 307.2172.



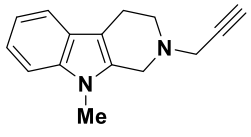
1r

Compound **1r** was prepared in 79% yield according to the general procedure A. White solids; mp 137–139 °C; R_f (PE/EA, 10:1) = 0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.50 (d, J = 7.8 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.23–7.19 (m, 1H), 7.11 (t, J = 7.2 Hz, 1H), 3.70 (s, 3H), 3.67 (d, J = 7.4 Hz, 1H), 3.55–3.34 (m, 3H), 3.23–3.19 (m, 1H), 2.93–2.85 (m, 1H), 2.69–2.63 (m, 1H), 2.25 (t, J = 2.4 Hz, 1H), 1.24–1.16 (m, 1H), 0.74–0.53 (m, 3H), 0.49–0.43 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 134.8, 126.6, 121.1, 119.0, 118.0, 108.8, 106.4, 81.0, 72.2, 57.9, 44.1, 42.4, 30.5, 17.4, 15.3, 5.2, 2.8; IR (KBr) ν_{max}: 3287, 1474, 1429, 1022, 748, 671, 647 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_2$: 265.1705 $[M+H]^+$; found: 265.1701.



1s

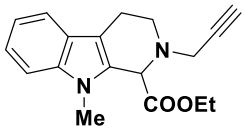
Compound **1s** was prepared in 80% yield according to the general procedure A. White solids; mp 81–83 °C; R_f (PE/EA, 10:1)= 0.6; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.49 (d, J = 7.7 Hz, 1H), 7.29 (d, J = 8.1 Hz, 1H), 7.22–7.17 (m, 1H), 7.13–7.07 (m, 1H), 3.94 (d, J = 9.3 Hz, 1H), 3.64 (s, 3H), 3.52–3.34 (m, 2H), 3.34–3.13 (m, 2H), 2.91–2.80 (m, 1H), 2.62–2.54 (m, 1H), 2.25 (t, J = 2.4 Hz, 1H), 1.80–1.56 (m, 4H), 1.02 (t, J = 7.0 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.1, 136.0, 126.7, 121.0, 118.9, 118.0, 108.6, 106.0, 81.3, 72.0, 54.7, 43.4, 42.5, 36.5, 29.6, 19.8, 16.9, 14.0; IR (KBr) ν_{max}: 3260, 2934, 1469, 1355, 1184, 747, 742, 687, 667 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{18}H_{23}N_2$: 267.1861 $[M+H]^+$; found: 267.1857.



1t

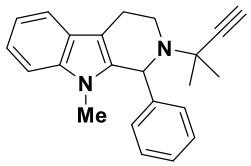
Compound **1t** was prepared in 79 % yield according to the general procedure A. White solids; mp 94–96 °C; R_f (PE/EA, 10:1) = 0.3; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (d, J = 7.8 Hz, 1H), 7.28 (d, J = 8.1 Hz, 1H), 7.20–7.16 (m, 1H), 7.11–7.08 (m, 1H), 3.84 (d, J = 1.3 Hz, 2H), 3.64 (d, J = 2.4 Hz, 2H), 3.62 (s, 3H), 2.97–2.94 (m, 2H), 2.90–2.87 (m, 2H), 2.32 (t, J = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.1, 133.0, 126.6, 120.7, 118.7, 117.9, 108.5, 106.8, 78.7, 73.5, 49.8, 47.9, 46.5, 29.0, 21.5; IR (KBr) ν_{max}:

3207, 1474, 1429, 1308, 1135, 735 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}N_2$: 225.1392 $[M+H]^+$; found: 225.1389.



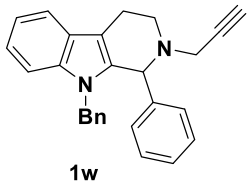
1u

Compound **1u** was prepared in 84% yield according to the general procedure A. White solids; mp 52–61 °C; R_f (PE/EA, 3:1) = 0.6; ^1H NMR (300 MHz, $CDCl_3$) δ 7.52 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.25–7.20 (m, 1H), 7.14–7.08 (m, 1H), 4.83 (s, 1H), 4.23 (qd, J_1 = 7.1 Hz, J_2 = 1.0 Hz, 2H), 3.68 (s, 3H), 3.61 (dd, J_1 = 4.1 Hz, J_2 = 2.5 Hz, 2H), 3.52–3.43 (m, 1H), 3.21–3.13 (m, 1H), 2.92–2.76 (m, 2H), 2.31 (t, *J* = 2.4 Hz, 1H), 1.29 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 170.4, 137.5, 129.7, 126.4, 121.6, 119.0, 118.4, 108.9, 108.6, 79.4, 73.2, 61.4, 58.7, 45.6, 43.4, 30.0, 19.4, 14.1; IR (KBr) ν_{max}: 3267, 1731, 1471, 1189, 1141, 1025, 739 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_2O_2$: 297.1603 $[M+H]^+$; found: 297.1600.



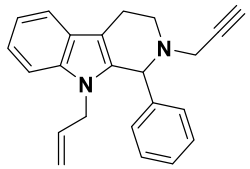
1v

Compound **1v** was prepared in 77% yield according to the procedure D. White solids; mp 125–128 °C; R_f (PE/EA, 10:1) = 0.7; ^1H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.8 Hz, 1H), 7.31–7.20 (m, 7H), 7.15–7.12 (m, 1H), 5.42 (s, 1H), 3.43–3.41 (m, 4H), 3.09–2.93 (m, 2H), 2.70–2.66 (m, 1H), 2.09 (d, *J* = 1.5 Hz, 1H), 1.64 (s, 3H), 1.50 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 142.2, 136.9, 135.3, 128.7, 128.2, 127.1, 126.9, 120.9, 118.6, 118.2, 109.7, 108.6, 89.6, 69.6, 55.4, 53.7, 38.9, 30.3, 29.5, 28.6, 20.4; IR (KBr) ν_{max}: 3203, 2980, 1469, 1382, 1164, 981, 739, 703 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{23}H_{25}N_2$: 329.2018 $[M+H]^+$; found: 329.2015.



1w

Compound **1w** was prepared in 89% yield according to the general procedure A. White solids; mp 102–104 °C; R_f (PE/EA, 10:1) = 0.7; ^1H NMR (400 MHz, $CDCl_3$) δ 7.62–7.60 (m, 1H), 7.36–7.24 (m, 3H), 7.22–7.12 (m, 8H), 6.83–6.73 (m, 2H), 5.06 (d, *J* = 17.0 Hz, 1H), 4.93 (s, 1H), 4.58 (d, *J* = 17.0 Hz, 1H), 3.36 (d, *J* = 2.0 Hz, 2H), 3.12–2.92 (m, 4H), 2.20 (t, *J* = 2.3 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 137.6, 137.4, 134.5, 129.4, 128.4, 128.3, 127.9, 126.9, 126.6, 126.0, 121.5, 119.2, 118.2, 109.5, 109.4, 79.4, 73.2, 60.1, 46.61, 46.57, 42.6, 20.4; IR (KBr) ν_{max}: 3281, 1465, 1452, 1131, 734, 702 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{27}H_{25}N_2$: 377.2018 $[M+H]^+$; found: 377.2016.



1x

Compound **1x** was prepared in 91% yield according to the general procedure A. White solids; mp 83–85 °C; R_f(PE/EA, 10:1) = 0.7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 7.1 Hz, 1H), 7.33–7.27 (m, 5H), 7.21–7.08 (m, 3H), 5.50–5.40 (m, 1H), 5.07 (s, 1H), 4.95 (dd, J_1 = 10.3 Hz, J_2 = 1.3 Hz, 1H), 4.77 (dd, J_1 = 17.1 Hz, J_2 = 1.4 Hz, 1H), 4.44–4.38 (m, 1H), 4.08–4.03 (m, 1H), 3.43–3.41 (m, 2H), 3.12–2.95 (m, 4H), 2.32 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.0, 136.9, 134.4, 133.0, 129.5, 128.4, 127.9, 126.5, 121.3, 119.0, 118.2, 116.2, 109.3, 109.1, 79.5, 73.3, 60.1, 46.9, 45.8, 42.7, 20.5; IR (KBr) ν_{max}: 3285, 1466, 1317, 1139, 736, 705, 634 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{22}H_{23}N_2$: 327.1861 $[M+H]^+$; found: 327.1860.

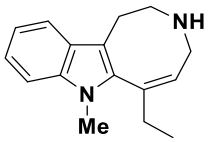
S2.3. Gold-Catalyzed Transformations of 2-Propargyl-β-tetrahydrocarbolines

General Procedure E: Gold-Catalyzed Ring Expansion of 2-Propargyl-β-tetrahydrocarbolines

To a stirred solution of 2-propargyl-β-tetrahydrocarboline (0.4 mmol) in toluene (8.0 mL), methanesulfonic acid (52 μL, 0.8 mmol) and triphenylphosphine gold(I) bis(trifluoromethanesulfonyl)imidate (3.0 mg, 0.004 mmol) were added successively. The reaction mixture was allowed to stir at room temperature for 12 h (monitored by TLC). After completion, the reaction mixture was diluted with CH_2Cl_2 (20 mL), washed with saturated $NaHCO_3$ solution (15 mL) and water (15 mL). The organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated. The crude product was purified by column chromatography on silica gel with CH_2Cl_2/MeOH (20:1, v:v) as the eluent to afford the azocinoindole product.

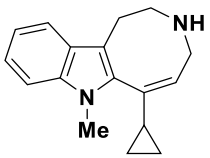
General Procedure F: Gold-Catalyzed Spirocyclization of 2-Propargyl-β-tetrahydrocarbolines

Cloro[2-(di-*tert*-butylphosphino)biphenyl]gold(I) (2.1 mg, 0.004 mmol) was added to a solution of $AgSbF_6$ (1.4 mg, 0.004 mmol) in CH_2Cl_2 (8.0 mL). After 10 min, 2-propargyl-β-tetrahydrocarboline (0.4 mmol) and methanesulfonic acid (52 μL, 0.8 mmol) were added successively at room temperature. The reaction mixture was allowed to stir for 30 min or 12 h (monitored by TLC). After completion, the reaction mixture was diluted with CH_2Cl_2 (20 mL), washed with saturated $NaHCO_3$ solution (15 mL) and water (15 mL). The organic layer was dried over anhydrous $MgSO_4$, filtered, and concentrated. The crude product was purified by column chromatography on silica gel with petroleum ether/ethyl acetate (20:1, v:v) as the eluent to give the spiroindoline product.



2a

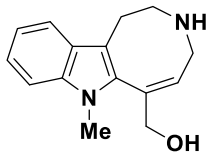
Compound **2a** was prepared in 90% yield according to the general procedure E. White solids; mp 53–55 °C; R_f (DCM/MeOH, 20:1) = 0.5; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.57 (d, J = 7.8 Hz, 1H), 7.32 (d, J = 8.0 Hz, 1H), 7.25 (t, J = 7.4 Hz, 1H), 7.14 (t, J = 7.3 Hz, 1H), 6.03 (t, J = 7.5 Hz, 1H), 3.68 (s, 3H), 3.47 (dd, J_1 = 13.8 Hz, J_2 = 6.6 Hz, 1H), 3.29–3.20 (m, 2H), 2.75 (dd, J_1 = 13.8 Hz, J_2 = 9.0 Hz, 1H), 2.57 (s, 1H), 2.52–2.35 (m, 4H), 0.97 (t, J = 7.5 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 137.8, 136.8, 134.8, 129.6, 127.1, 121.5, 118.8, 118.2, 114.7, 108.8, 46.4, 45.6, 31.2, 29.3, 27.1, 13.1; IR (KBr) ν_{max}: 2927, 2962, 1469, 1369, 1324, 742 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{16}H_{21}N_2$: 241.1705 $[M+H]^+$; found: 241.1702.



2b

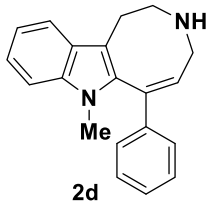
Compound **2b** was prepared in 95% yield according to the general procedure E. White solids; mp 87–89 °C; R_f (DCM/MeOH, 50:1) = 0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, J = 7.9 Hz, 1H), 7.32 (d, J = 8.1 Hz, 1H), 7.26–7.23 (m, 1H), 7.13 (t, J = 7.2 Hz, 1H), 5.86 (dd, J_1 = 8.7 Hz, J_2 = 7.0 Hz, 1H), 3.78 (s, 3H), 3.47 (dd, J_1 = 13.8 Hz, J_2 = 6.7 Hz, 1H), 3.27–3.20 (m, 2H), 2.72 (dd, J_1 = 13.7 Hz, J_2 = 9.1 Hz, 1H),

2.49–2.29 (m, 3H), 1.67–1.62 (m, 1H), 0.95–0.89 (m, 1H), 0.79–0.72 (m, 1H), 0.66–0.53 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 137.2, 135.3, 127.0, 125.8, 121.7, 118.9, 118.3, 114.0, 109.0, 46.1, 45.1, 31.4, 26.6, 15.5, 9.5, 6.9; IR (KBr) ν_{max}: 2924, 2849, 1469, 1365, 741, 714 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{17}H_{21}N_2$: 253.1705 $[M+H]^+$; found: 253.1702.



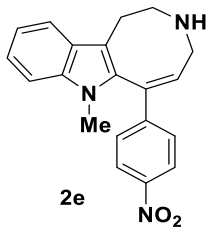
2c

Compound **2c** was prepared in 61% yield according to the general procedure E except that 5 mol % $Ph_3PAuNTf_2$ and CH_2Cl_2 were used. White solids; mp 155–158 °C; R_f (DCM/MeOH, 15:1) = 0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 7.9 Hz, 1H), 7.30 (d, J = 8.1 Hz, 1H), 7.27–7.23 (m, 1H), 7.15–7.11 (m, 1H), 6.23 (t, J = 7.6 Hz, 1H), 4.41–4.39 (m, 2H), 3.70 (s, 3H), 3.47 (dd, J_1 = 14.0 Hz, J_2 = 6.5 Hz, 1H), 3.25–3.15 (m, 2H), 2.90 (s, 2H), 2.84–2.74 (m, 1H), 2.45–2.32 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.1, 134.7, 133.6, 130.1, 127.0, 122.1, 119.1, 118.4, 115.4, 109.1, 64.9, 46.2, 45.3, 31.5, 26.5; IR (KBr) ν_{max}: 3388, 2924, 2880, 1602, 1510, 1463, 748, 704 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{15}H_{19}N_2O$: 243.1497 $[M+H]^+$; found: 243.1496.



2d

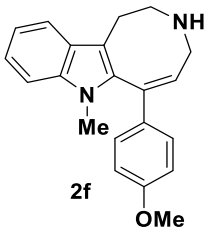
Compound **2d** was prepared in 90% yield according to the general procedure E. White solids; mp 185–187 °C; R_f (DCM/MeOH, 50:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.9 Hz, 1H), 7.32–7.26 (m, 5H), 7.23–7.20 (m, 2H), 7.18–7.14 (m, 1H), 6.42 (dd, J_1 = 8.6 Hz, J_2 = 6.8 Hz, 1H), 3.71 (dd, J_1 = 13.9 Hz, J_2 = 6.5 Hz, 1H), 3.38–3.28 (m, 2H), 3.24 (s, 3H), 3.22 (s, 1H), 2.97 (dd, J_1 = 13.7 Hz, J_2 = 9.1 Hz, 1H), 2.57–2.44 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 140.3, 137.8, 135.2, 134.3, 130.0, 128.6, 127.8, 126.92, 126.88, 122.0, 119.0, 118.5, 115.8, 109.1, 46.8, 44.9, 31.1, 26.8; IR (KBr) ν_{max}: 2927, 2726, 1467, 1370, 760, 741, 699 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{20}H_{21}N_2$: 289.1705 $[M+H]^+$; found: 289.1705.



2e

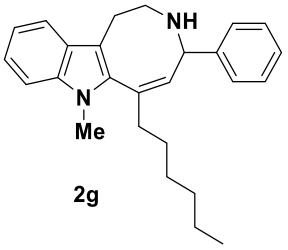
Compound **2e** was prepared in 91% yield according to the general procedure E. Yellow solids; mp 215–217 °C; R_f (DCM/MeOH, 50:1) = 0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.18–8.15 (m, 2H), 7.65 (d, J = 7.9 Hz, 1H), 7.38–7.35 (m, 2H), 7.31–7.28 (m, 2H), 7.21–7.17 (m, 1H), 6.55 (dd, J_1 = 8.6 Hz, J_2 = 6.6 Hz, 1H), 3.71 (dd, J_1 = 14.2 Hz, J_2 = 6.5 Hz, 1H), 3.38 (dd, J_1 = 14.4 Hz, J_2 = 5.2 Hz, 1H), 3.32–3.25 (m, 4H),

3.01 (dd, J_1 = 13.0 Hz, J_2 = 9.3 Hz, 1H), 2.55 (t, J = 11.8 Hz, 1H), 2.42 (t, J = 12.6 Hz, 1H), 1.86 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 147.1, 147.0, 137.9, 134.6, 133.9, 131.8, 127.4, 126.8, 123.8, 122.5, 119.2, 118.7, 116.6, 109.1, 47.2, 45.1, 31.2, 27.1; IR (KBr) ν_{max}: 2926, 1593, 1515, 1341, 853, 743 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{20}H_{20}N_3O_2$: 334.1556 [M+H]$^+$; found: 334.1554.



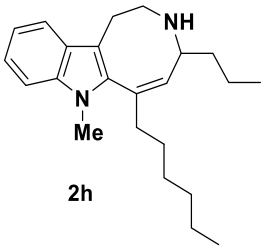
2f

Compound **2f** was prepared in 84% yield according to the general procedure E. Pale yellow solids; mp 193–196 °C; R_f (DCM/MeOH, 50:1) = 0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, J = 7.9 Hz, 1H), 7.29–7.24 (m, 2H), 7.18–7.13 (m, 3H), 6.85–6.83 (m, 2H), 6.34 (dd, J_1 = 9.0 Hz, J_2 = 6.7 Hz, 1H), 3.80 (s, 3H), 3.68 (dd, J_1 = 14.0 Hz, J_2 = 6.6 Hz, 1H), 3.39–3.26 (m, 5H), 2.92 (dd, J_1 = 13.9 Hz, J_2 = 9.1 Hz, 1H), 2.56–2.42 (m, 2H), 2.17 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.3, 137.8, 135.5, 133.5, 132.9, 128.6, 128.0, 126.9, 121.9, 118.9, 118.5, 115.7, 113.9, 109.0, 55.2, 46.8, 45.2, 31.1, 27.0; IR (KBr) ν_{max}: 2929, 1606, 1509, 1247, 853, 742 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{21}H_{23}N_2O$: 319.1810 [M+H]$^+$; found: 319.1810.



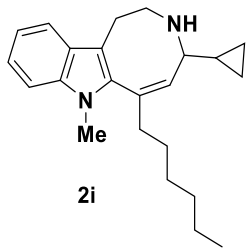
2g

Compound **2g** was prepared in 66% yield according to the general procedure E. White solids; mp 178–180 °C; R_f (DCM/MeOH, 50:1) = 0.7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, J = 7.8 Hz, 1H), 7.35–7.24 (m, 6 H), 7.23–7.19 (m, 1H), 7.17–7.13 (m, 1H), 5.98 (d, J = 8.8 Hz, 1H), 3.85 (d, J = 8.8 Hz, 1H), 3.72 (s, 3H), 3.42–3.32 (m, 2H), 2.64 (t, J = 11.6 Hz, 1H), 2.52–2.47 (m, 1H), 2.42–2.35 (m, 2H), 1.62 (s, 1H), 1.31–1.20 (m, 8H), 0.83 (t, J = 6.9 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 145.6, 138.0, 137.1, 135.5, 131.5, 128.6, 127.3, 126.8, 126.4, 121.7, 118.9, 118.3, 115.3, 109.0, 60.1, 45.9, 36.5, 31.6, 31.3, 29.1, 28.6, 27.8, 22.5, 14.0; IR (KBr) ν_{max}: 2926, 2854, 1467, 1366, 742, 700 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{26}H_{33}N_2$: 373.2644 [M+H]$^+$; found: 373.2644.



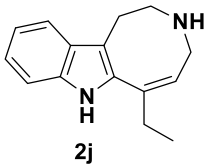
2h

Compound **2h** was prepared in 93% yield according to the general procedure E. White solids; mp 125–128 °C; R_f (DCM/MeOH, 50:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.55 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.25–7.21 (m, 1H), 7.14–7.10 (m, 1H), 5.65 (d, *J* = 8.6 Hz, 1H), 3.66 (s, 3H), 3.30–3.22 (m, 2H), 2.61 (dd, J_1 = 14.6 Hz, J_2 = 8.2 Hz, 1H), 2.53–2.43 (m, 2H), 2.41–2.34 (m, 1H), 2.31–2.24 (m, 1H), 1.53 (s, 1H), 1.49–1.33 (m, 2H), 1.29–1.11 (m, 10H), 0.83 (t, *J* = 6.9 Hz, 3H), 0.78 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.8, 137.5, 136.1, 131.6, 127.3, 121.4, 118.8, 118.3, 114.8, 108.8, 55.4, 46.0, 40.2, 36.4, 31.6, 31.2, 29.1, 28.7, 27.8, 22.5, 19.1, 14.0, 13.8; IR (KBr) ν_{max}: 2926, 2855, 1467, 1366, 741 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{23}H_{35}N_2$: 339.2800 $[M+H]^+$; found: 339.2799.



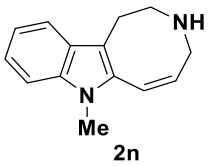
2i

Compound **2i** was prepared in 95% yield according to the general procedure E. White solids; mp 112–114 °C; R_f (DCM/MeOH, 50:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.25–7.21 (m, 1H), 7.14–7.10 (m, 1H), 5.88 (d, *J* = 8.6 Hz, 1H), 3.66 (s, 3H), 3.33–3.21 (m, 2H), 2.51–2.22 (m, 4H), 1.93–1.87 (m, 2H), 1.28–1.20 (m, 8H), 1.02–0.92 (m, 1H), 0.83 (t, *J* = 6.9 Hz, 3H), 0.46–0.41 (m, 2H), 0.08–0.03 (m, 1H), –0.07– –0.12 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.7, 137.3, 135.2, 131.1, 127.2, 121.5, 118.8, 118.2, 114.8, 108.8, 61.1, 46.2, 36.3, 31.5, 31.1, 29.1, 28.6, 27.2, 22.5, 18.5, 14.0, 3.1; IR (KBr) ν_{max}: 2927, 2854, 1467, 1366, 1014, 741 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{23}H_{33}N_2$: 337.2644 $[M+H]^+$; found: 337.2644.



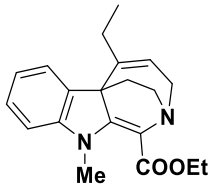
2j

Compound **2j** was prepared in 92% yield according to the general procedure E. White solids; mp 56–59 °C; R_f (DCM/MeOH, 20:1) = 0.5; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.14 (brs, 1H), 7.53 (d, *J* = 7.8 Hz, 1H), 7.34 (d, *J* = 8.0 Hz, 1H), 7.22–7.18 (m, 1H), 7.14–7.10 (m, 1H), 5.74 (t, *J* = 6.6 Hz, 1H), 3.35 (brs, 1H), 3.10–2.88 (m, 4H), 2.70–2.59 (m, 3H), 2.47 (q, *J* = 7.3 Hz, 2H), 1.03 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 136.4, 136.1, 133.6, 127.8, 124.4, 122.0, 119.1, 118.2, 113.4, 110.7, 46.0, 44.1, 29.6, , 25.7, 13.2; IR (KBr) ν_{max}: 3280, 2927, 1464, 1453, 742, 702 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{15}H_{19}N_2$: 227.1548 $[M+H]^+$; found: 227.1546.



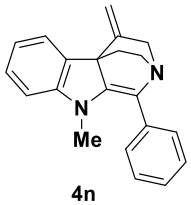
2n

Compound **2n** was obtained as a side product according to the general procedure F. Pale brown oil; R_f (DCM/MeOH, 20:1) = 0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.8 Hz, 1H), 7.29 (d, *J* = 8.1 Hz, 1H), 7.23 (t, *J* = 7.5 Hz, 1H), 7.12 (t, *J* = 7.3 Hz, 1H), 6.47 (d, *J* = 11.8 Hz, 1H), 5.88 (td, J_1 = 11.7 Hz, J_2 = 5.2 Hz, 1H), 3.69 (s, 3H), 3.62 (dd, J_1 = 3.8 Hz, J_2 = 1.3 Hz, 2H), 3.25 (s, 1H), 3.03 (s, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 137.2, 134.6, 131.9, 126.9, 121.9, 119.0, 118.5, 118.2, 111.1, 108.9, 48.2, 46.1, 29.9, 24.8; IR (KBr) ν_{max}: 3384, 2925, 1468, 1327, 1261, 803, 769, 743 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{13}H_{15}N_2$: 213.1392 [M+H]$^+$; found: 213.1392.



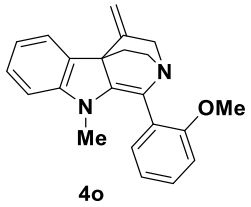
3m

Compound **3m** was obtained as a side product in 29% yield according to the general procedure E except that 5 mol % $Ph_3PAuNTf_2$ was used. White solids; mp 115–118 °C; R_f (PE/EA, 3:1) = 0.6; ^{1}H NMR (300 MHz, $CDCl_3$) δ 7.28–7.23 (m, 2H), 6.95 (t, *J* = 7.1 Hz, 1H), 6.83 (d, *J* = 7.6 Hz, 1H), 5.03 (s, 1H), 4.42–4.18 (m, 2H), 3.83–3.63 (m, 2H), 3.48 (s, 3H), 3.31–3.26 (m, 1H), 3.18–3.13 (m, 1H), 2.94–2.84 (m, 1H), 2.16–2.07 (m, 1H), 1.98–1.91 (m, 1H), 1.59–1.51 (m, 1H), 1.34 (t, *J* = 7.1 Hz, 3H), 0.66 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 165.6, 148.5, 144.3, 133.5, 127.9, 125.1, 121.6, 120.3, 108.1, 106.2, 59.6, 55.3, 52.4, 47.1, 44.0, 35.2, 29.5, 14.7, 12.4; IR (KBr) ν_{max}: 2960, 2932, 1682, 1577, 1486, 1218, 746 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{20}H_{25}N_2O_2$: 325.1916 [M+H]$^+$; found: 325.1916.



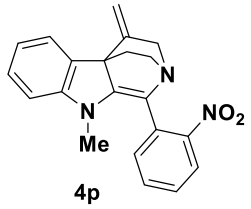
4n

Compound **4n** was prepared in 95% yield according to the general procedure F. White solids; mp 118–120 °C; R_f (PE/EA, 20:1) = 0.6; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.43–7.40 (m, 2H), 7.38–7.31 (m, 3H), 7.28 (td, J_1 = 7.8, J_2 = 1.3 Hz, 1H), 7.20–7.16 (m, 1H), 6.95–6.92 (m, 1H), 6.75 (d, *J* = 7.9 Hz, 1H), 4.86 (t, *J* = 2.4 Hz, 1H), 4.78 (t, *J* = 1.8 Hz, 1H), 3.70 (d, *J* = 16.3 Hz, 1H), 3.38 (dd, J_1 = 16.4, J_2 = 2.1 Hz, 1H), 3.14–3.08 (m, 1H), 3.07 (s, 3H), 2.81–2.73 (m, 1H), 2.33–2.27 (m, 1H), 1.83–1.76 (m, 1H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 151.6, 149.7, 147.3, 137.5, 130.4, 128.12, 128.11, 127.7, 125.6, 125.2, 118.9, 116.0, 107.3, 103.0, 55.2, 51.8, 47.1, 34.5, 33.2; IR (KBr) ν_{max}: 1654, 1608, 1485, 1461, 1352, 1102, 891, 757, 750, 733, 702 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{21}H_{21}N_2$: 301.1705 [M+H]$^+$; found: 301.1704.



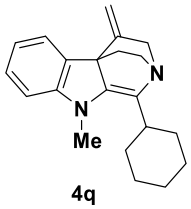
4o

Compound **4o** was prepared in 89% yield according to the general procedure F. White solids; mp 90–93 °C; R_f (PE/EA, 5:1) = 0.5; ^{1}H NMR (400 MHz, Acetone–d_6) δ 7.36–7.34 (m, 1H), 7.26–7.21 (m, 3H), 6.97 (d, J = 8.1 Hz, 1H), 6.90 (td, J_1 = 7.4, J_2 = 0.9 Hz, 1H), 6.88–6.84 (m, 1H), 6.73 (d, J = 7.9 Hz, 1H), 4.79 (t, J = 2.3 Hz, 1H), 4.74 (t, J = 1.7 Hz, 1H), 3.79 (s, 3H), 3.53 (d, J = 16.1 Hz, 1H), 3.22 (s, 2H), 2.97–2.91 (m, 1H), 2.84 (s, 3H), 2.27–2.21 (m, 1H), 1.69 (td, J_1 = 11.3 Hz, J_2 = 5.2 Hz, 1H); ^{13}C NMR (100 MHz, Acetone–d_6) δ 158.9, 153.6, 150.3, 148.2, 132.1, 131.2, 128.9, 128.8, 127.9, 125.9, 120.5, 119.2, 111.7, 107.5, 102.8, 55.7, 52.1, 47.2, 35.7, 31.5, 30.7; IR (KBr) ν_{max}: 1608, 1487, 1462, 1353, 1240, 1101, 750, 738 cm^{-1}; HRMS (ESI) m/z calculated for $C_{22}H_{23}N_2O$: 331.1810 [M+H]$^+$; found: 331.1807.



4p

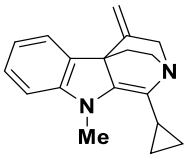
Compound **4p** was prepared in 76% yield according to the general procedure F. Dark yellow solids; mp 111–113 °C; R_f (PE/EA, 5:1) = 0.4; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, J_1 = 8.6, J_2 = 1.2 Hz, 1H), 7.50 (td, J_1 = 7.6, J_2 = 1.2 Hz, 1H), 7.37 (d, J = 7.2 Hz, 1H), 7.31–7.27 (m, 3H), 6.96 (t, J = 7.2 Hz, 1H), 6.77 (d, J = 7.9 Hz, 1H), 4.84 (t, J = 2.4 Hz, 1H), 4.77 (t, J = 1.8 Hz, 1H), 3.54 (d, J = 16.4 Hz, 1H), 3.32 (dd, J_1 = 16.5 Hz, J_2 = 2.1 Hz, 1H), 3.02 (s, 3H), 2.97–2.91 (m, 1H), 2.77–2.69 (m, 1H), 2.31–2.26 (m, 1H), 1.78 (td, J_1 = 11.1 Hz, J_2 = 5.2 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 151.3, 150.5, 148.9, 132.4, 131.8, 131.2, 130.3, 128.1, 126.3, 125.2, 124.2, 119.3, 110.1, 107.3, 103.2, 55.3, 52.0, 46.8, 34.5, 32.6; IR (KBr) ν_{max}: 1607, 1524, 1462, 1355, 752, 740, 723 cm^{-1}; HRMS (ESI) m/z calculated for $C_{21}H_{20}N_3O_2$: 346.1556 [M+H]$^+$; found: 346.1553.



4q

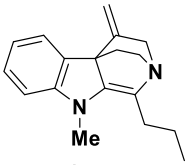
Compound **4q** was prepared in 90% yield according to the general procedure F. White solids; mp 101–103 °C; R_f (PE/EA, 10:1) = 0.7; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.27–7.25 (m, 1H), 7.22 (td, J_1 = 7.8 Hz, J_2 = 1.1 Hz, 1H), 6.83 (t, J = 7.3 Hz, 1H), 6.66 (d, J = 7.9 Hz, 1H), 4.77 (t, J = 2.3 Hz, 1H), 4.69 (t, J = 1.8 Hz, 1H), 3.62 (d, J = 16.2 Hz, 1H), 3.29 (s, 3H), 3.12–3.01 (m, 2H), 2.70–2.62 (m, 1H), 2.53–2.47 (m, 1H), 2.18–2.13 (m, 1H), 1.80–1.57 (m, 9H), 1.28–1.25 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 149.5, 143.1, 130.0, 127.9, 125.1, 121.8, 117.8, 106.0, 102.0, 55.8, 50.6, 47.7, 39.5, 34.9, 32.4, 30.9, 30.6,

26.41, 26.37, 25.7; IR (KBr) ν_{max}: 2922, 2843, 1674, 1609, 1488, 1102, 878, 749, 737 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{21}H_{27}N_2$: 307.2174 $[M+H]^+$; found: 307.2170.



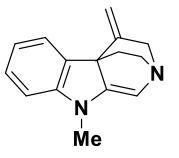
4r

Compound **4r** was prepared in 97% yield according to the general procedure F. White solids; mp 90–93 °C; R_f (PE/EA, 10:1) = 0.5; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28–7.25 (m, 1H), 7.23 (td, J_1 = 7.8 Hz, J_2 = 1.3 Hz, 1H), 6.82 (td, J_1 = 7.5 Hz, J_2 = 0.8 Hz, 1H), 6.66 (d, J = 7.9 Hz, 1H), 4.75 (t, J = 2.4 Hz, 1H), 4.67 (t, J = 1.8 Hz, 1H), 3.50 (d, J = 16.3 Hz, 1H), 3.41 (s, 3H), 3.04 (dd, J_1 = 16.3 Hz, J_2 = 2.1 Hz, 1H), 2.96–2.89 (m, 1H), 2.47–2.39 (m, 1H), 2.19–2.12 (m, 1H), 1.85–1.78 (m, 1H), 1.66 (td, J_1 = 11.2 Hz, J_2 = 5.0 Hz, 1H), 0.78–0.69 (m, 2H), 0.65–0.58 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 149.5, 145.9, 130.2, 127.9, 125.1, 117.7, 115.8, 106.0, 102.0, 55.1, 51.1, 47.1, 35.0, 32.3, 9.5, 3.91, 3.87; IR (KBr) ν_{max}: 1609, 1487, 1460, 1381, 1262, 1105, 884, 746, 733 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_2$: 265.1705 $[M+H]^+$; found: 265.1705.



4s

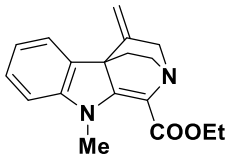
Compound **4s** was prepared in 90% yield according to the general procedure F. Colorless oil; R_f (PE/EA, 10:1) = 0.6; ^1H NMR (400 MHz, $CDCl_3$) δ 7.28 (dd, J_1 = 8.3, J_2 = 1.0 Hz, 1H), 7.22 (td, J_1 = 7.7 Hz, J_2 = 1.2 Hz, 1H), 6.84–6.81 (m, 1H), 6.65 (d, J = 7.9 Hz, 1H), 4.77 (t, J = 2.4 Hz, 1H), 4.69 (t, J = 1.8 Hz, 1H), 3.56 (dt, J_1 = 16.3 Hz, J_2 = 1.8 Hz, 1H), 3.28 (s, 3H), 3.17 (dd, J_1 = 16.3 Hz, J_2 = 2.2 Hz, 1H), 3.02–2.95 (m, 1H), 2.60–2.52 (m, 1H), 2.35 (t, J = 7.3 Hz, 2H), 2.21–2.14 (m, 1H), 1.70–1.55 (m, 3H), 0.96 (t, J = 7.4 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.1, 149.3, 144.8, 130.0, 127.9, 125.2, 117.8, 116.4, 105.9, 102.1, 55.0, 50.5, 46.9, 35.0, 32.8, 31.7, 21.9, 14.0; IR (KBr) ν_{max}: 2955, 2933, 1681, 1609, 1488, 1462, 1100, 881, 749, 737 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{18}H_{23}N_2$: 267.1861 $[M+H]^+$; found: 267.1856.



4t

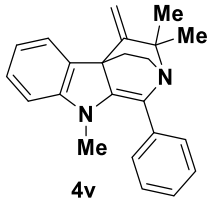
Compound **4t** was prepared in 90% yield according to the general procedure F. Colorless oil; R_f (PE/EA, 1:1) = 0.3; ^1H NMR (400 MHz, $CDCl_3$) δ 7.32 (d, J = 7.2 Hz, 1H), 7.26–7.22 (m, 1H), 6.86 (t, J = 7.4 Hz, 1H), 6.67 (d, J = 7.9 Hz, 1H), 5.58 (s, 1H), 4.83 (t, J = 2.4 Hz, 1H), 4.72 (t, J = 1.8 Hz, 1H), 3.57 (d, J = 16.2 Hz, 1H), 3.17 (dd, J_1 = 16.1 Hz, J_2 = 2.2 Hz, 1H), 3.07 (s, 3H), 3.03–2.96 (m, 1H), 2.61–2.52 (m, 1H), 2.23–2.17 (m, 1H), 1.65 (td, J_1 = 11.2 Hz, J_2 = 5.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 150.6, 148.6, 130.2, 128.1, 125.4, 118.2, 106.0, 103.0, 102.8, 55.5, 49.8, 47.4, 33.8, 29.1; IR (KBr) ν_{max}: 2922, 2844,

1675, 1608, 1488, 1102, 878, 748, 737 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{15}H_{17}N_2$: 225.1392 $[M+H]^+$; found: 225.1391.



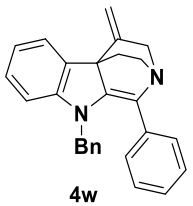
4u

Compound **4u** was prepared in 96% yield according to the general procedure F. White solids; mp 143–145 °C; R_f (PE/EA, 3:1) = 0.5; ^1H NMR (300 MHz, $CDCl_3$) δ 7.37–7.30 (m, 2H), 7.07–7.02 (m, 1H), 6.92 (d, *J* = 7.9 Hz, 1H), 4.83 (t, *J* = 2.5 Hz, 1H), 4.77 (t, *J* = 2.0 Hz, 1H), 4.30 (q, *J* = 7.1 Hz, 2H), 3.77 (s, 3H), 3.70–3.63 (m, 1H), 3.26 (dd, J_1 = 16.6 Hz, J_2 = 2.2 Hz, 1H), 3.13–3.04 (m, 1H), 2.73–2.63 (m, 1H), 2.30–2.19 (m, 1H), 1.64 (td, J_1 = 11.1 Hz, J_2 = 5.2 Hz, 1H), 1.33 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (75 MHz, $CDCl_3$) δ 164.3, 161.2, 148.7, 148.5, 130.6, 128.2, 124.8, 120.9, 108.7, 106.7, 104.9, 59.7, 54.7, 46.4, 33.7, 32.7, 29.6, 14.7; IR (KBr) ν_{max}: 1657, 1565, 1485, 1215, 1107, 747, 737 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{18}H_{21}N_2O_2$: 297.1603 $[M+H]^+$; found: 297.1599.



4v

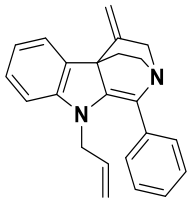
Compound **4v** was prepared in 91% yield according to the general procedure F. White solids; mp 112–115 °C; R_f (PE/EA, 10:1) = 0.6; ^1H NMR (400 MHz, $CDCl_3$) δ 7.46–7.44 (m, 2H), 7.35–7.31(m, 3H), 7.28–7.24 (m, 1H), 7.16 (t, *J* = 7.3 Hz, 1H), 6.91 (t, *J* = 7.1 Hz, 1H), 6.74 (d, *J* = 7.9 Hz, 1H), 4.83 (s, 1H), 4.71 (s, 1H), 3.52–3.47 (m, 1H), 3.05 (s, 3H), 2.62–2.55 (m, 1H), 2.26–2.19 (m, 1H), 1.73 (td, J_1 = 11.3 Hz, J_2 = 3.8 Hz, 1H), 1.54 (s, 3H), 1.26 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 160.5, 150.0, 146.0, 138.3, 131.0, 128.2, 128.1, 127.7, 125.4, 125.1, 118.8, 117.3, 107.4, 103.7, 59.7, 53.2, 42.1, 33.6, 32.5, 32.0, 29.4; IR (KBr) ν_{max}: 2975, 2926, 1608, 1462, 1350, 1098, 744, 700 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{23}H_{24}N_2$: 329.2018 $[M+H]^+$; found: 329.2018.



4w

Compound **4w** was prepared in 95% yield according to the general procedure F. White solids; mp 146–150 °C; R_f (PE/EA, 10:1) = 0.3; ^1H NMR (400 MHz, $CDCl_3$) δ 7.39 (d, *J* = 7.3 Hz, 1H), 7.26–7.21 (m, 2H), 7.21–7.09 (m, 7H), 6.96–6.89 (m, 3H), 6.68 (d, *J* = 7.9 Hz, 1H), 4.88 (t, *J* = 2.3 Hz, 1H), 4.80 (t, *J* = 1.8 Hz, 1H), 4.73 (s, 2H), 3.68 (d, *J* = 16.3 Hz, 1H), 3.34 (dd, J_1 = 16.4 Hz, J_2 = 2.0 Hz, 1H), 3.15–3.07 (m, 1H), 2.79–2.71 (m, 1H), 2.35–2.29 (m, 1H), 1.85–1.76 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.4,

149.2, 146.4, 137.5, 136.9, 130.5, 128.2, 128.0, 127.9, 127.6, 126.8, 126.4, 125.8, 125.3, 119.2, 117.0, 108.6, 103.2, 55.1, 52.0, 48.3, 47.1, 34.6; IR (KBr) ν_{max}: 1655, 1607, 1465, 1365, 1173, 755, 724, 697 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{27}H_{25}N_2$: 377.2018 $[M+H]^+$; found: 377.2016.



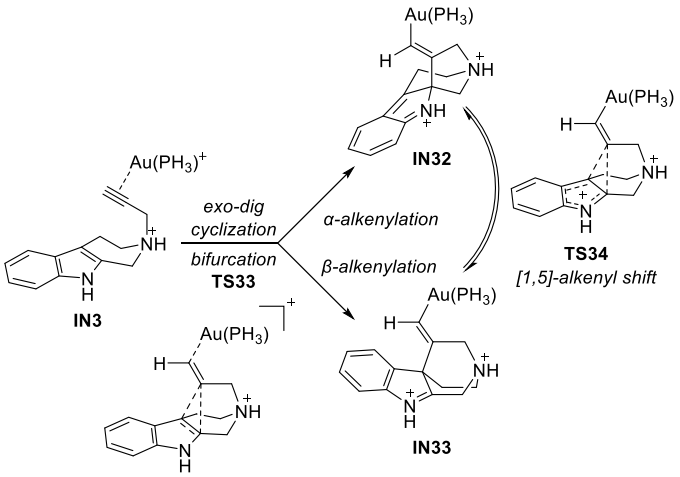
4x

Compound **4x** was prepared in 94% yield according to the general procedure F. White solids; mp 125–128 °C; R_f (PE/EA, 10:1) = 0.6; ^1H NMR (400 MHz, $CDCl_3$) δ 7.41 (dd, J_1 = 8.1 Hz, J_2 = 1.1 Hz, 2H), 7.37 (dd, J_1 = 7.3 Hz, J_2 = 0.8 Hz, 1H), 7.31 (t, J = 7.7 Hz, 2H), 7.25 (td, J_1 = 7.7 Hz, J_2 = 1.3 Hz, 2H), 7.21–7.14 (m, 1H), 6.94 (td, J_1 = 7.4 Hz, J_2 = 0.7 Hz, 1H), 6.76 (d, J = 7.9 Hz, 1H), 5.71–5.61 (m, 1H), 5.10 (dd, J_1 = 10.4 Hz, J_2 = 1.5 Hz, 1H), 4.97 (dd, J_1 = 17.2 Hz, J_2 = 1.5 Hz, 1H), 4.85 (t, J = 2.4 Hz, 1H), 4.78 (t, J = 1.8 Hz, 1H), 4.10 (dt, J_1 = 4.4 Hz, J_2 = 1.6 Hz, 2H), 3.68 (d, J = 16.3 Hz, 1H), 3.38 (dd, J_1 = 16.4 Hz, J_2 = 2.1 Hz, 1H), 3.14–3.08 (m, 1H), 2.82–2.75 (m, 1H), 2.34–2.28 (m, 1H), 1.81 (td, J_1 = 11.1 Hz, J_2 = 5.0 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.6, 149.0, 146.5, 137.7, 132.2, 130.6, 128.0, 127.96, 127.7, 125.9, 125.2, 119.1, 116.7, 116.5, 108.6, 103.1, 55.2, 51.9, 47.3, 47.1, 34.6; IR (KBr) ν_{max}: 2929, 1603, 1461, 759, 742, 699 cm^{-1}; HRMS (ESI) *m/z* calculated for $C_{23}H_{23}N_2$: 327.1861 $[M+H]^+$; found: 327.1861.

S3. DFT Studies

S3.1. Relaxed Potential Energy Surface Scans

Scheme S1. Transition States and Intermediates Involved in the *exo*-Dig Cyclization of IN3



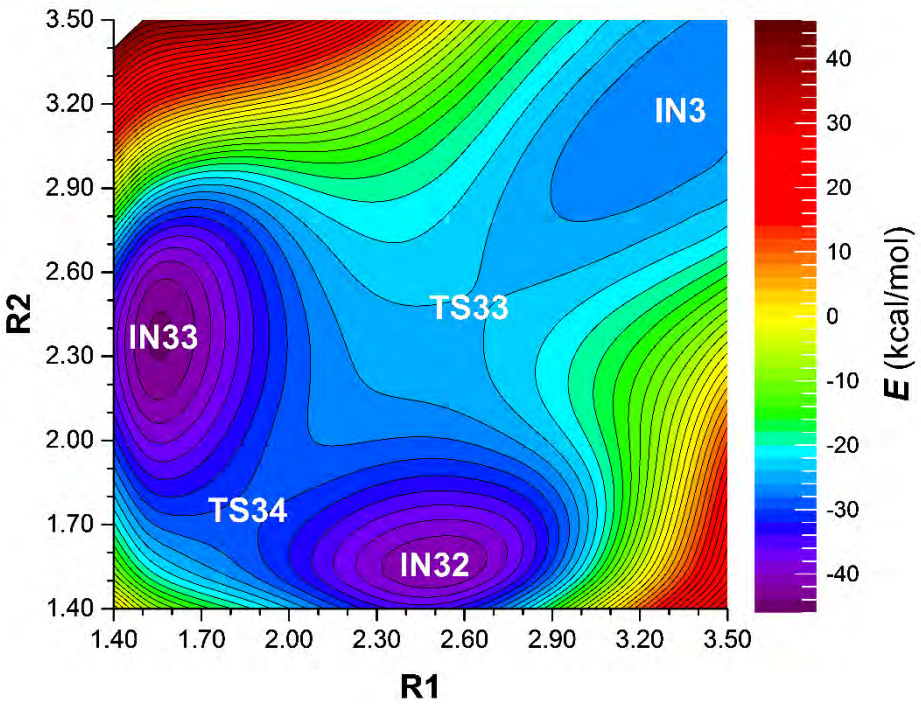
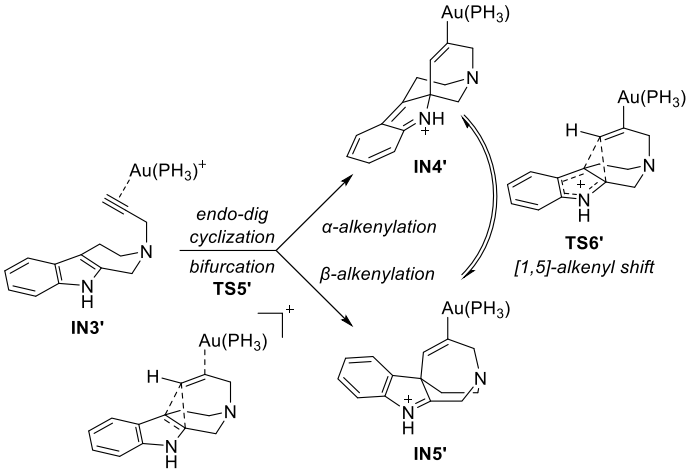
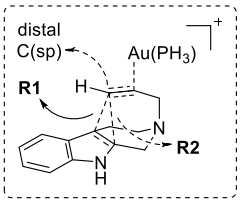


Figure S1. Potential energy surface for the *exo*-dig cyclization of **IN3**. Computed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM. Distances are given in Å. See Scheme S1 for the structures of transition states and intermediates.

Scheme S2. Transition States and Intermediates Involved in the *endo*-Dig Cyclization of IN3'





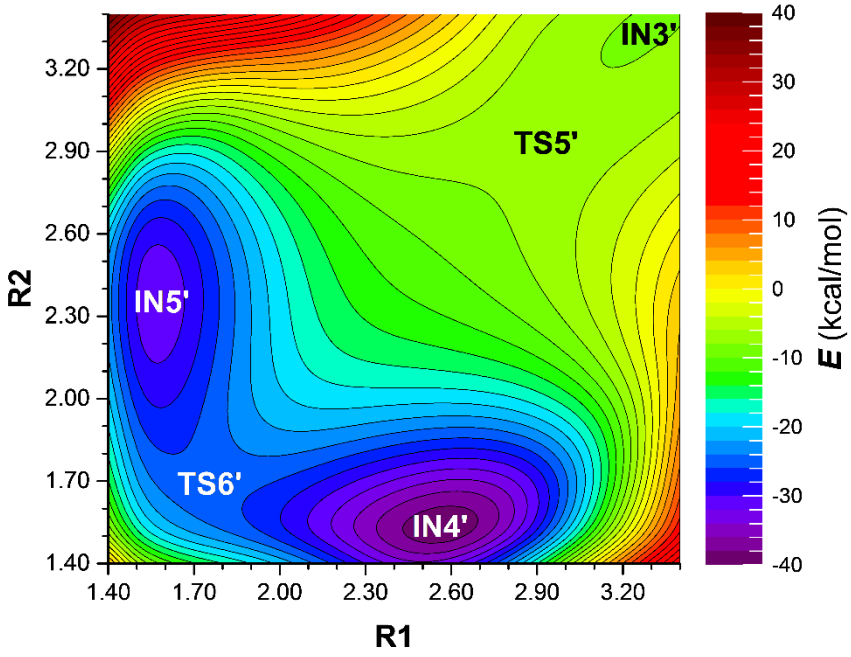
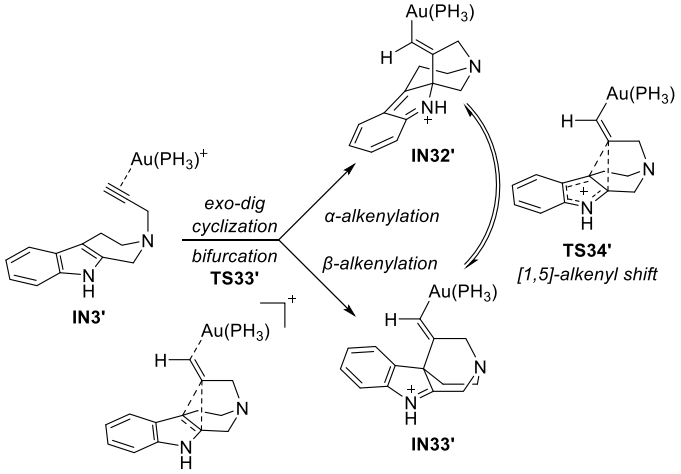
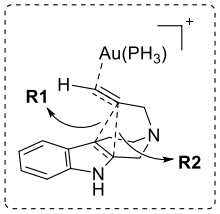


Figure S2. Potential energy surface for the *endo*-dig cyclization of **IN3'**. Computed at the B3LYP/SDD-6-31G(d) level in the gas phase. Distances are given in Å. See Scheme S2 for the structures of transition states and intermediates.

Scheme S3. Transition States and Intermediates Involved in the *exo*-Dig Cyclization of IN3'





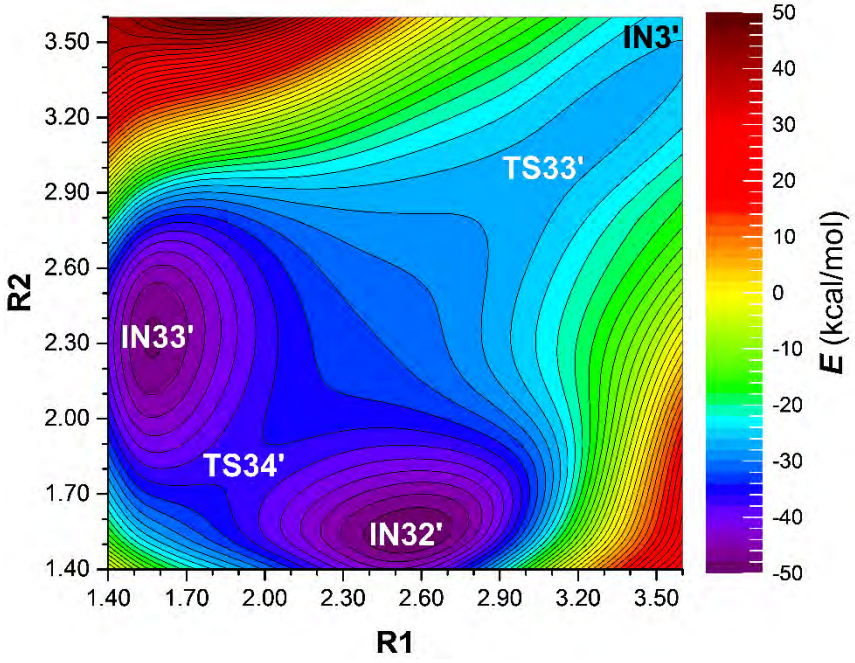
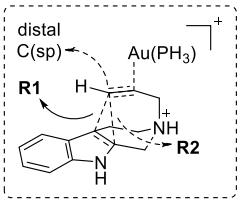


Figure S3. Potential energy surface for the *exo*-dig cyclization of **IN3'**. Computed at the B3LYP/SDD-6-31G(d) level in the gas phase. Distances are given in Å. See Scheme S3 for the structures of transition states and intermediates.

Table S2. Relaxed Potential Energy Surface Scan for the *endo*-Dig Cyclization of IN3[a]



R1 (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)
1.40	1.40	−1130.583324	1.50	1.40	−1130.599184	1.60	1.40	−1130.607049
1.40	1.50	−1130.597837	1.50	1.50	−1130.612720	1.60	1.50	−1130.619638
1.40	1.60	−1130.605591	1.50	1.60	−1130.619226	1.60	1.60	−1130.624905
1.40	1.70	−1130.610265	1.50	1.70	−1130.623018	1.60	1.70	−1130.627448
1.40	1.80	−1130.613984	1.50	1.80	−1130.626061	1.60	1.80	−1130.629391
1.40	1.90	−1130.617502	1.50	1.90	−1130.629101	1.60	1.90	−1130.631551
1.40	2.00	−1130.620907	1.50	2.00	−1130.632105	1.60	2.00	−1130.633908
1.40	2.10	−1130.624052	1.50	2.10	−1130.635029	1.60	2.10	−1130.636364
1.40	2.20	−1130.626788	1.50	2.20	−1130.637648	1.60	2.20	−1130.638712
1.40	2.30	−1130.628570	1.50	2.30	−1130.639418	1.60	2.30	−1130.640321
1.40	2.40	−1130.629453	1.50	2.40	−1130.640180	1.60	2.40	−1130.641117
1.40	2.50	−1130.628633	1.50	2.50	−1130.639831	1.60	2.50	−1130.640757
1.40	2.60	−1130.625310	1.50	2.60	−1130.637608	1.60	2.60	−1130.639207
1.40	2.70	−1130.618713	1.50	2.70	−1130.632867	1.60	2.70	−1130.635718
1.40	2.80	−1130.608743	1.50	2.80	−1130.624994	1.60	2.80	−1130.629799
1.40	2.90	−1130.596278	1.50	2.90	−1130.613823	1.60	2.90	−1130.620850
1.40	3.00	−1130.582575	1.50	3.00	−1130.600260	1.60	3.00	−1130.608696
1.40	3.10	−1130.568692	1.50	3.10	−1130.585472	1.60	3.10	−1130.594294
1.40	3.20	−1130.555425	1.50	3.20	−1130.570448	1.60	3.20	−1130.578694
1.40	3.30	−1130.543145	1.50	3.30	−1130.555956	1.60	3.30	−1130.562796
1.40	3.40	−1130.531765	1.50	3.40	−1130.542475	1.60	3.40	−1130.547409
1.40	3.50	−1130.521311	1.50	3.50	−1130.530017	1.60	3.50	−1130.533108
1.70	1.40	−1130.611226	1.80	1.40	−1130.614227	1.90	1.40	−1130.617382
1.70	1.50	−1130.622983	1.80	1.50	−1130.625289	1.90	1.50	−1130.627807
1.70	1.60	−1130.627058	1.80	1.60	−1130.628233	1.90	1.60	−1130.629732
1.70	1.70	−1130.628176	1.80	1.70	−1130.627933	1.90	1.70	−1130.628096
1.70	1.80	−1130.628796	1.80	1.80	−1130.627037	1.90	1.80	−1130.625673
1.70	1.90	−1130.629801	1.80	1.90	−1130.626725	1.90	1.90	−1130.623900
1.70	2.00	−1130.631228	1.80	2.00	−1130.627046	1.90	2.00	−1130.623030
1.70	2.10	−1130.632959	1.80	2.10	−1130.627893	1.90	2.10	−1130.622904
1.70	2.20	−1130.634838	1.80	2.20	−1130.629076	1.90	2.20	−1130.623293
1.70	2.30	−1130.636173	1.80	2.30	−1130.630011	1.90	2.30	−1130.623666
1.70	2.40	−1130.636811	1.80	2.40	−1130.630361	1.90	2.40	−1130.623696
1.70	2.50	−1130.636454	1.80	2.50	−1130.629968	1.90	2.50	−1130.623128
1.70	2.60	−1130.635027	1.80	2.60	−1130.628559	1.90	2.60	−1130.621744
1.70	2.70	−1130.632328	1.80	2.70	−1130.626039	1.90	2.70	−1130.619375

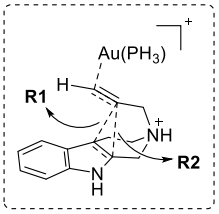
1.70	2.80	−1130.627734	1.80	2.80	−1130.622282	1.90	2.80	−1130.615845
1.70	2.90	−1130.620827	1.80	2.90	−1130.616744	1.90	2.90	−1130.611122
1.70	3.00	−1130.610893	1.80	3.00	−1130.608863	1.90	3.00	−1130.604680
1.70	3.10	−1130.597975	1.80	3.10	−1130.598110	1.90	3.10	−1130.595876
1.70	3.20	−1130.582938	1.80	3.20	−1130.584628	1.90	3.20	−1130.584510
1.70	3.30	−1130.566673	1.80	3.30	−1130.569027	1.90	3.30	−1130.570502
1.70	3.40	−1130.550139	1.80	3.40	−1130.552238	1.90	3.40	−1130.554403
1.70	3.50	−1130.534142	1.80	3.50	−1130.535264	1.90	3.50	−1130.537249
2.00	1.40	−1130.621241	2.10	1.40	−1130.625553	2.20	1.40	−1130.629943
2.00	1.50	−1130.631020	2.10	1.50	−1130.634744	2.20	1.50	−1130.638605
2.00	1.60	−1130.631973	2.10	1.60	−1130.634895	2.20	1.60	−1130.638119
2.00	1.70	−1130.629108	2.10	1.70	−1130.630948	2.20	1.70	−1130.633329
2.00	1.80	−1130.625287	2.10	1.80	−1130.625908	2.20	1.80	−1130.627269
2.00	1.90	−1130.622055	2.10	1.90	−1130.621395	2.20	1.90	−1130.621665
2.00	2.00	−1130.619928	2.10	2.00	−1130.618071	2.20	2.00	−1130.617315
2.00	2.10	−1130.618811	2.10	2.10	−1130.615977	2.20	2.10	−1130.614367
2.00	2.20	−1130.618413	2.10	2.20	−1130.614837	2.20	2.20	−1130.612579
2.00	2.30	−1130.618176	2.10	2.30	−1130.614053	2.20	2.30	−1130.611365
2.00	2.40	−1130.617830	2.10	2.40	−1130.613332	2.20	2.40	−1130.610358
2.00	2.50	−1130.617082	2.10	2.50	−1130.612413	2.20	2.50	−1130.609312
2.00	2.60	−1130.615646	2.10	2.60	−1130.610964	2.20	2.60	−1130.607905
2.00	2.70	−1130.613447	2.10	2.70	−1130.608900	2.20	2.70	−1130.605990
2.00	2.80	−1130.610124	2.10	2.80	−1130.605934	2.20	2.80	−1130.603407
2.00	2.90	−1130.605730	2.10	2.90	−1130.601896	2.20	2.90	−1130.599879
2.00	3.00	−1130.600169	2.10	3.00	−1130.596764	2.20	3.00	−1130.595365
2.00	3.10	−1130.592824	2.10	3.10	−1130.590453	2.20	3.10	−1130.589773
2.00	3.20	−1130.583298	2.10	3.20	−1130.582347	2.20	3.20	−1130.582826
2.00	3.30	−1130.571355	2.10	3.30	−1130.572203	2.20	3.30	−1130.574193
2.00	3.40	−1130.556812	2.10	3.40	−1130.559675	2.20	3.40	−1130.563412
2.00	3.50	−1130.540335	2.10	3.50	−1130.544596	2.20	3.50	−1130.550261
2.30	1.40	−1130.633377	2.40	1.40	−1130.635363	2.50	1.40	−1130.635154
2.30	1.50	−1130.641940	2.40	1.50	−1130.644068	2.50	1.50	−1130.644728
2.30	1.60	−1130.641003	2.40	1.60	−1130.643117	2.50	1.60	−1130.644094
2.30	1.70	−1130.635587	2.40	1.70	−1130.637326	2.50	1.70	−1130.638254
2.30	1.80	−1130.628774	2.40	1.80	−1130.629926	2.50	1.80	−1130.630543
2.30	1.90	−1130.622313	2.40	1.90	−1130.622848	2.50	1.90	−1130.622966
2.30	2.00	−1130.617112	2.40	2.00	−1130.617020	2.50	2.00	−1130.616704
2.30	2.10	−1130.613473	2.40	2.10	−1130.612864	2.50	2.10	−1130.612198
2.30	2.20	−1130.611187	2.40	2.20	−1130.610239	2.50	2.20	−1130.609373
2.30	2.30	−1130.609661	2.40	2.30	−1130.608564	2.50	2.30	−1130.607694
2.30	2.40	−1130.608513	2.40	2.40	−1130.607430	2.50	2.40	−1130.606739
2.30	2.50	−1130.607448	2.40	2.50	−1130.606510	2.50	2.50	−1130.606142
2.30	2.60	−1130.606181	2.40	2.60	−1130.605527	2.50	2.60	−1130.605628

2.30	2.70	−1130.604501	2.40	2.70	−1130.604206	2.50	2.70	−1130.604899
2.30	2.80	−1130.602307	2.40	2.80	−1130.602512	2.50	2.80	−1130.603774
2.30	2.90	−1130.599412	2.40	2.90	−1130.600287	2.50	2.90	−1130.602272
2.30	3.00	−1130.595670	2.40	3.00	−1130.597392	2.50	3.00	−1130.600281
2.30	3.10	−1130.590872	2.40	3.10	−1130.593704	2.50	3.10	−1130.597707
2.30	3.20	−1130.585068	2.40	3.20	−1130.589007	2.50	3.20	−1130.594320
2.30	3.30	−1130.577861	2.40	3.30	−1130.583392	2.50	3.30	−1130.590027
2.30	3.40	−1130.568858	2.40	3.40	−1130.576453	2.50	3.40	−1130.585044
2.30	3.50	−1130.557521	2.40	3.50	−1130.567716	2.50	3.50	−1130.578778
2.60	1.40	−1130.632104	2.70	1.40	−1130.626180	2.80	1.40	−1130.617393
2.60	1.50	−1130.643242	2.70	1.50	−1130.639071	2.80	1.50	−1130.632155
2.60	1.60	−1130.643525	2.70	1.60	−1130.640866	2.80	1.60	−1130.635798
2.60	1.70	−1130.638181	2.70	1.70	−1130.636459	2.80	1.70	−1130.632800
2.60	1.80	−1130.630411	2.70	1.80	−1130.629275	2.80	1.80	−1130.626561
2.60	1.90	−1130.622601	2.70	1.90	−1130.621475	2.80	1.90	−1130.619372
2.60	2.00	−1130.615949	2.70	2.00	−1130.614710	2.80	2.00	−1130.612679
2.60	2.10	−1130.611199	2.70	2.10	−1130.609759	2.80	2.10	−1130.607773
2.60	2.20	−1130.608305	2.70	2.20	−1130.606847	2.80	2.20	−1130.604949
2.60	2.30	−1130.606723	2.70	2.30	−1130.605464	2.80	2.30	−1130.603794
2.60	2.40	−1130.606084	2.70	2.40	−1130.605198	2.80	2.40	−1130.603968
2.60	2.50	−1130.605955	2.70	2.50	−1130.605605	2.80	2.50	−1130.604955
2.60	2.60	−1130.606023	2.70	2.60	−1130.606297	2.80	2.60	−1130.606251
2.60	2.70	−1130.605966	2.70	2.70	−1130.606874	2.80	2.70	−1130.607407
2.60	2.80	−1130.605509	2.70	2.80	−1130.607088	2.80	2.80	−1130.608216
2.60	2.90	−1130.604710	2.70	2.90	−1130.606902	2.80	2.90	−1130.608623
2.60	3.00	−1130.603536	2.70	3.00	−1130.606342	2.80	3.00	−1130.608556
2.60	3.10	−1130.601791	2.70	3.10	−1130.605304	2.80	3.10	−1130.608045
2.60	3.20	−1130.599431	2.70	3.20	−1130.603721	2.80	3.20	−1130.607055
2.60	3.30	−1130.596334	2.70	3.30	−1130.601577	2.80	3.30	−1130.605625
2.60	3.40	−1130.592603	2.70	3.40	−1130.598797	2.80	3.40	−1130.603590
2.60	3.50	−1130.588058	2.70	3.50	−1130.595327	2.80	3.50	−1130.601013
2.90	1.40	−1130.606531	3.00	1.40	−1130.594491	3.10	1.40	−1130.581995
2.90	1.50	−1130.622563	3.00	1.50	−1130.610960	3.10	1.50	−1130.598124
2.90	1.60	−1130.628172	3.00	1.60	−1130.617960	3.10	1.60	−1130.605875
2.90	1.70	−1130.627071	3.00	1.70	−1130.618801	3.10	1.70	−1130.608241
2.90	1.80	−1130.622102	3.00	1.80	−1130.615792	3.10	1.80	−1130.607052
2.90	1.90	−1130.615787	3.00	1.90	−1130.610725	3.10	1.90	−1130.603854
2.90	2.00	−1130.609758	3.00	2.00	−1130.605465	3.10	2.00	−1130.599896
2.90	2.10	−1130.605025	3.00	2.10	−1130.601475	3.10	2.10	−1130.596594
2.90	2.20	−1130.602453	3.00	2.20	−1130.599207	3.10	2.20	−1130.595173
2.90	2.30	−1130.601675	3.00	2.30	−1130.598945	3.10	2.30	−1130.595456
2.90	2.40	−1130.602276	3.00	2.40	−1130.600144	3.10	2.40	−1130.597466
2.90	2.50	−1130.603912	3.00	2.50	−1130.602400	3.10	2.50	−1130.600459

2.90	2.60	−1130.605826	3.00	2.60	−1130.604967	3.10	2.60	−1130.603674
2.90	2.70	−1130.607559	3.00	2.70	−1130.607239	3.10	2.70	−1130.606499
2.90	2.80	−1130.608857	3.00	2.80	−1130.609012	3.10	2.80	−1130.608707
2.90	2.90	−1130.609737	3.00	2.90	−1130.610285	3.10	2.90	−1130.610379
2.90	3.00	−1130.610176	3.00	3.00	−1130.611099	3.10	3.00	−1130.611513
2.90	3.10	−1130.610079	3.00	3.10	−1130.611472	3.10	3.10	−1130.612160
2.90	3.20	−1130.609536	3.00	3.20	−1130.611317	3.10	3.20	−1130.612429
2.90	3.30	−1130.608561	3.00	3.30	−1130.610711	3.10	3.30	−1130.612168
2.90	3.40	−1130.607166	3.00	3.40	−1130.609681	3.10	3.40	−1130.611492
2.90	3.50	−1130.605176	3.00	3.50	−1130.608270	3.10	3.50	−1130.610436
3.20	1.40	−1130.569638	3.30	1.40	−1130.558007	3.40	1.40	−1130.547335
3.20	1.50	−1130.584713	3.30	1.50	−1130.571382	3.40	1.50	−1130.558735
3.20	1.60	−1130.592425	3.30	1.60	−1130.578318	3.40	1.60	−1130.564258
3.20	1.70	−1130.595733	3.30	1.70	−1130.581810	3.40	1.70	−1130.567229
3.20	1.80	−1130.596218	3.30	1.80	−1130.583384	3.40	1.80	−1130.569165
3.20	1.90	−1130.594846	3.30	1.90	−1130.583727	3.40	1.90	−1130.570748
3.20	2.00	−1130.592589	3.30	2.00	−1130.583318	3.40	2.00	−1130.572123
3.20	2.10	−1130.590643	3.30	2.10	−1130.583028	3.40	2.10	−1130.573669
3.20	2.20	−1130.589916	3.30	2.20	−1130.583724	3.40	2.20	−1130.575933
3.20	2.30	−1130.591084	3.30	2.30	−1130.585862	3.40	2.30	−1130.579528
3.20	2.40	−1130.594039	3.30	2.40	−1130.589804	3.40	2.40	−1130.584854
3.20	2.50	−1130.598087	3.30	2.50	−1130.595056	3.40	2.50	−1130.591355
3.20	2.60	−1130.602070	3.30	2.60	−1130.600035	3.40	2.60	−1130.597291
3.20	2.70	−1130.605442	3.30	2.70	−1130.604113	3.40	2.70	−1130.602321
3.20	2.80	−1130.607924	3.30	2.80	−1130.607171	3.40	2.80	−1130.606033
3.20	2.90	−1130.610036	3.30	2.90	−1130.609422	3.40	2.90	−1130.608524
3.20	3.00	−1130.611506	3.30	3.00	−1130.611071	3.40	3.00	−1130.610457
3.20	3.10	−1130.612428	3.30	3.10	−1130.612316	3.40	3.10	−1130.611779
3.20	3.20	−1130.612884	3.30	3.20	−1130.613000	3.40	3.20	−1130.612794
3.20	3.30	−1130.613016	3.30	3.30	−1130.613375	3.40	3.30	−1130.613291
3.20	3.40	−1130.612695	3.30	3.40	−1130.613411	3.40	3.40	−1130.613570
3.20	3.50	−1130.611973	3.30	3.50	−1130.612978	3.40	3.50	−1130.613494
3.50	1.40	−1130.537774	3.50	2.20	−1130.566660	3.50	2.90	−1130.607604
3.50	1.50	−1130.547127	3.50	2.30	−1130.571743	3.50	3.00	−1130.609604
3.50	1.60	−1130.550815	3.50	2.40	−1130.578657	3.50	3.10	−1130.611163
3.50	1.70	−1130.552627	3.50	2.50	−1130.586842	3.50	3.20	−1130.612199
3.50	1.80	−1130.554251	3.50	2.60	−1130.594231	3.50	3.30	−1130.612986
3.50	1.90	−1130.556305	3.50	2.70	−1130.599974	3.50	3.40	−1130.613320
3.50	2.00	−1130.558967	3.50	2.80	−1130.604413	3.50	3.50	−1130.613476
3.50	2.10	−1130.562367						

[a]Computed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM. The SCF convergence criterion was set to 10^{-6} to accelerate the calculations.

Table S3. Relaxed Potential Energy Surface Scan for the *exo*-Dig Cyclization of IN3[a]



R1 (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)
1.40	1.40	−1130.562975	1.50	1.40	−1130.578671	1.60	1.40	−1130.587433
1.40	1.50	−1130.581181	1.50	1.50	−1130.594632	1.60	1.50	−1130.601876
1.40	1.60	−1130.592162	1.50	1.60	−1130.604457	1.60	1.60	−1130.609596
1.40	1.70	−1130.600037	1.50	1.70	−1130.611534	1.60	1.70	−1130.615069
1.40	1.80	−1130.606796	1.50	1.80	−1130.617670	1.60	1.80	−1130.620030
1.40	1.90	−1130.613034	1.50	1.90	−1130.623467	1.60	1.90	−1130.624962
1.40	2.00	−1130.618529	1.50	2.00	−1130.628637	1.60	2.00	−1130.629577
1.40	2.10	−1130.623209	1.50	2.10	−1130.633138	1.60	2.10	−1130.633667
1.40	2.20	−1130.626398	1.50	2.20	−1130.636386	1.60	2.20	−1130.636796
1.40	2.30	−1130.627822	1.50	2.30	−1130.638056	1.60	2.30	−1130.638573
1.40	2.40	−1130.627409	1.50	2.40	−1130.638295	1.60	2.40	−1130.639087
1.40	2.50	−1130.624411	1.50	2.50	−1130.636356	1.60	2.50	−1130.637934
1.40	2.60	−1130.617648	1.50	2.60	−1130.631781	1.60	2.60	−1130.634817
1.40	2.70	−1130.606947	1.50	2.70	−1130.623446	1.60	2.70	−1130.628588
1.40	2.80	−1130.592975	1.50	2.80	−1130.611275	1.60	2.80	−1130.618969
1.40	2.90	−1130.577011	1.50	2.90	−1130.595939	1.60	2.90	−1130.605485
1.40	3.00	−1130.560347	1.50	3.00	−1130.578820	1.60	3.00	−1130.589132
1.40	3.10	−1130.543941	1.50	3.10	−1130.561114	1.60	3.10	−1130.571145
1.40	3.20	−1130.528515	1.50	3.20	−1130.543681	1.60	3.20	−1130.552518
1.40	3.30	−1130.514204	1.50	3.30	−1130.527300	1.60	3.30	−1130.534253
1.40	3.40	−1130.501491	1.50	3.40	−1130.512229	1.60	3.40	−1130.517175
1.40	3.50	N/A[b]	1.50	3.50	−1130.498985	1.60	3.50	−1130.501642
1.70	1.40	−1130.593023	1.80	1.40	−1130.597479	1.90	1.40	−1130.602013
1.70	1.50	−1130.606120	1.80	1.50	−1130.609667	1.90	1.50	−1130.613465
1.70	1.60	−1130.612183	1.80	1.60	−1130.614234	1.90	1.60	−1130.616794
1.70	1.70	−1130.615624	1.80	1.70	−1130.615858	1.90	1.70	−1130.616814
1.70	1.80	−1130.618930	1.80	1.80	−1130.617203	1.90	1.80	−1130.616295
1.70	1.90	−1130.622552	1.80	1.90	−1130.619256	1.90	1.90	−1130.616606
1.70	2.00	−1130.626264	1.80	2.00	−1130.621748	1.90	2.00	−1130.617742
1.70	2.10	−1130.629709	1.80	2.10	−1130.624306	1.90	2.10	−1130.619263
1.70	2.20	−1130.632487	1.80	2.20	−1130.626532	1.90	2.20	−1130.620764
1.70	2.30	−1130.634183	1.80	2.30	−1130.627906	1.90	2.30	−1130.621678
1.70	2.40	−1130.634748	1.80	2.40	−1130.628391	1.90	2.40	−1130.621952
1.70	2.50	−1130.633982	1.80	2.50	−1130.627786	1.90	2.50	−1130.621314
1.70	2.60	−1130.631729	1.80	2.60	−1130.625983	1.90	2.60	−1130.619690

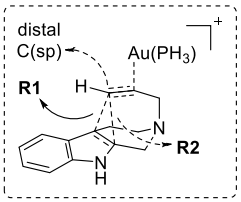
1.70	2.70	−1130.627225	1.80	2.70	−1130.622482	1.90	2.70	−1130.616895
1.70	2.80	−1130.619728	1.80	2.80	−1130.616740	1.90	2.80	−1130.612273
1.70	2.90	−1130.608797	1.80	2.90	−1130.608045	1.90	2.90	−1130.605399
1.70	3.00	−1130.594288	1.80	3.00	−1130.596036	1.90	3.00	−1130.595596
1.70	3.10	−1130.577114	1.80	3.10	−1130.580640	1.90	3.10	−1130.582581
1.70	3.20	−1130.558270	1.80	3.20	−1130.562621	1.90	3.20	−1130.566275
1.70	3.30	−1130.538855	1.80	3.30	−1130.542996	1.90	3.30	−1130.547428
1.70	3.40	−1130.519932	1.80	3.40	−1130.522901	1.90	3.40	−1130.527095
1.70	3.50	−1130.502380	1.80	3.50	−1130.503423	1.90	3.50	−1130.506391
2.00	1.40	−1130.607079	2.10	1.40	−1130.612468	2.20	1.40	−1130.617686
2.00	1.50	−1130.617813	2.10	1.50	−1130.622589	2.20	1.50	−1130.627292
2.00	1.60	−1130.620062	2.10	1.60	−1130.623910	2.20	1.60	−1130.627949
2.00	1.70	−1130.618741	2.10	1.70	−1130.621434	2.20	1.70	−1130.624538
2.00	1.80	−1130.616633	2.10	1.80	−1130.618028	2.20	1.80	−1130.620043
2.00	1.90	−1130.615207	2.10	1.90	−1130.615200	2.20	1.90	−1130.616099
2.00	2.00	−1130.614931	2.10	2.00	−1130.613522	2.20	2.00	−1130.613327
2.00	2.10	−1130.615379	2.10	2.10	−1130.612928	2.20	2.10	−1130.611788
2.00	2.20	−1130.616092	2.10	2.20	−1130.612885	2.20	2.20	−1130.611090
2.00	2.30	−1130.616511	2.10	2.30	−1130.612817	2.20	2.30	−1130.610596
2.00	2.40	−1130.616451	2.10	2.40	−1130.612434	2.20	2.40	−1130.609937
2.00	2.50	−1130.615710	2.10	2.50	−1130.611511	2.20	2.50	−1130.608871
2.00	2.60	−1130.614222	2.10	2.60	−1130.609997	2.20	2.60	−1130.607407
2.00	2.70	−1130.611759	2.10	2.70	−1130.608002	2.20	2.70	−1130.605562
2.00	2.80	−1130.608046	2.10	2.80	−1130.604748	2.20	2.80	−1130.602913
2.00	2.90	−1130.602454	2.10	2.90	−1130.600300	2.20	2.90	−1130.599302
2.00	3.00	−1130.594453	2.10	3.00	−1130.593756	2.20	3.00	−1130.594053
2.00	3.10	−1130.583555	2.10	3.10	−1130.584746	2.20	3.10	−1130.586862
2.00	3.20	−1130.569553	2.10	3.20	−1130.572810	2.20	3.20	−1130.576966
2.00	3.30	−1130.552332	2.10	3.30	−1130.557802	2.20	3.30	−1130.564039
2.00	3.40	−1130.532667	2.10	3.40	−1130.539662	2.20	3.40	−1130.548046
2.00	3.50	−1130.511617	2.10	3.50	−1130.519157	2.20	3.50	−1130.528958
2.30	1.40	−1130.621867	2.40	1.40	−1130.624277	2.50	1.40	−1130.624250
2.30	1.50	−1130.631217	2.40	1.50	−1130.633824	2.50	1.50	−1130.634759
2.30	1.60	−1130.631478	2.40	1.60	−1130.633934	2.50	1.60	−1130.635004
2.30	1.70	−1130.627439	2.40	1.70	−1130.629556	2.50	1.70	−1130.630552
2.30	1.80	−1130.622118	2.40	1.80	−1130.623720	2.50	1.80	−1130.624498
2.30	1.90	−1130.617264	2.40	1.90	−1130.618253	2.50	1.90	−1130.618653
2.30	2.00	−1130.613672	2.40	2.00	−1130.614049	2.50	2.00	−1130.614061
2.30	2.10	−1130.611418	2.40	2.10	−1130.611312	2.50	2.10	−1130.611042
2.30	2.20	−1130.610224	2.40	2.20	−1130.609796	2.50	2.20	−1130.609392
2.30	2.30	−1130.609441	2.40	2.30	−1130.608897	2.50	2.30	−1130.608504
2.30	2.40	−1130.608616	2.40	2.40	−1130.608091	2.50	2.40	−1130.607886
2.30	2.50	−1130.607520	2.40	2.50	−1130.607089	2.50	2.50	−1130.607161

2.30	2.60	−1130.606102	2.40	2.60	−1130.605852	2.50	2.60	−1130.606266
2.30	2.70	−1130.604376	2.40	2.70	−1130.604261	2.50	2.70	−1130.605068
2.30	2.80	−1130.602232	2.40	2.80	−1130.602492	2.50	2.80	−1130.603583
2.30	2.90	−1130.599400	2.40	2.90	−1130.600259	2.50	2.90	−1130.601647
2.30	3.00	−1130.595266	2.40	3.00	−1130.597080	2.50	3.00	−1130.599128
2.30	3.10	−1130.589592	2.40	3.10	−1130.592769	2.50	3.10	−1130.596036
2.30	3.20	−1130.581723	2.40	3.20	−1130.586571	2.50	3.20	−1130.591313
2.30	3.30	−1130.571125	2.40	3.30	−1130.578198	2.50	3.30	−1130.584779
2.30	3.40	−1130.557411	2.40	3.40	−1130.567091	2.50	3.40	−1130.576122
2.30	3.50	−1130.540593	2.40	3.50	−1130.553005	2.50	3.50	−1130.564847
2.60	1.40	−1130.621042	2.70	1.40	−1130.614939	2.80	1.40	−1130.605732
2.60	1.50	−1130.633145	2.70	1.50	−1130.628661	2.80	1.50	−1130.621520
2.60	1.60	−1130.634624	2.70	1.60	−1130.631755	2.80	1.60	−1130.626283
2.60	1.70	−1130.630421	2.70	1.70	−1130.628734	2.80	1.70	−1130.624757
2.60	1.80	−1130.624164	2.70	1.80	−1130.622978	2.80	1.80	−1130.620123
2.60	1.90	−1130.618226	2.70	1.90	−1130.616870	2.80	1.90	−1130.614617
2.60	2.00	−1130.613430	2.70	2.00	−1130.612038	2.80	2.00	−1130.609774
2.60	2.10	−1130.610265	2.70	2.10	−1130.608828	2.80	2.10	−1130.606671
2.60	2.20	−1130.608640	2.70	2.20	−1130.607287	2.80	2.20	−1130.605271
2.60	2.30	−1130.607942	2.70	2.30	−1130.606887	2.80	2.30	−1130.605163
2.60	2.40	−1130.607640	2.70	2.40	−1130.607041	2.80	2.40	−1130.605851
2.60	2.50	−1130.607325	2.70	2.50	−1130.607313	2.80	2.50	−1130.606853
2.60	2.60	−1130.606962	2.70	2.60	−1130.607541	2.80	2.60	−1130.607905
2.60	2.70	−1130.606338	2.70	2.70	−1130.607649	2.80	2.70	−1130.608737
2.60	2.80	−1130.605223	2.70	2.80	−1130.607283	2.80	2.80	−1130.609032
2.60	2.90	−1130.603739	2.70	2.90	−1130.606306	2.80	2.90	−1130.608728
2.60	3.00	−1130.601647	2.70	3.00	−1130.604585	2.80	3.00	−1130.607641
2.60	3.10	−1130.599184	2.70	3.10	−1130.602266	2.80	3.10	−1130.605739
2.60	3.20	−1130.595670	2.70	3.20	−1130.599662	2.80	3.20	−1130.603228
2.60	3.30	−1130.590802	2.70	3.30	−1130.596072	2.80	3.30	−1130.600355
2.60	3.40	−1130.584215	2.70	3.40	−1130.591088	2.80	3.40	−1130.596620
2.60	3.50	−1130.575439	2.70	3.50	−1130.584239	2.80	3.50	−1130.591417
2.90	1.40	−1130.594065	3.00	1.40	−1130.580989	3.10	1.40	−1130.567269
2.90	1.50	−1130.611279	3.00	1.50	−1130.598773	3.10	1.50	−1130.584798
2.90	1.60	−1130.618201	3.00	1.60	−1130.607259	3.10	1.60	−1130.594127
2.90	1.70	−1130.618511	3.00	1.70	−1130.609695	3.10	1.70	−1130.598287
2.90	1.80	−1130.615248	3.00	1.80	−1130.608414	3.10	1.80	−1130.599066
2.90	1.90	−1130.610789	3.00	1.90	−1130.605354	3.10	1.90	−1130.597941
2.90	2.00	−1130.606585	3.00	2.00	−1130.602091	3.10	2.00	−1130.596214
2.90	2.10	−1130.603698	3.00	2.10	−1130.599870	3.10	2.10	−1130.595036
2.90	2.20	−1130.602593	3.00	2.20	−1130.599344	3.10	2.20	−1130.595252
2.90	2.30	−1130.602903	3.00	2.30	−1130.600181	3.10	2.30	−1130.596811
2.90	2.40	−1130.604165	3.00	2.40	−1130.602003	3.10	2.40	−1130.599351

2.90	2.50	−1130.605843	3.00	2.50	−1130.604386	3.10	2.50	−1130.602402
2.90	2.60	−1130.607704	3.00	2.60	−1130.606860	3.10	2.60	−1130.605486
2.90	2.70	−1130.609254	3.00	2.70	−1130.609102	3.10	2.70	−1130.608361
2.90	2.80	−1130.610284	3.00	2.80	−1130.610732	3.10	2.80	−1130.610441
2.90	2.90	−1130.610538	3.00	2.90	−1130.611676	3.10	2.90	−1130.611971
2.90	3.00	−1130.610074	3.00	3.00	−1130.611771	3.10	3.00	−1130.612747
2.90	3.10	−1130.608763	3.00	3.10	−1130.611043	3.10	3.10	−1130.612596
2.90	3.20	−1130.606638	3.00	3.20	−1130.609450	3.10	3.20	−1130.611585
2.90	3.30	−1130.603866	3.00	3.30	−1130.607110	3.10	3.30	−1130.609679
2.90	3.40	−1130.600905	3.00	3.40	−1130.604066	3.10	3.40	−1130.607167
2.90	3.50	−1130.596935	3.00	3.50	−1130.600853	3.10	3.50	−1130.604429
3.20	1.40	−1130.553530	3.30	1.40	−1130.540409	3.40	1.40	−1130.528008
3.20	1.50	−1130.570074	3.30	1.50	−1130.555302	3.40	1.50	−1130.541091
3.20	1.60	−1130.579393	3.30	1.60	−1130.563894	3.40	1.60	−1130.548296
3.20	1.70	−1130.584569	3.30	1.70	−1130.569231	3.40	1.70	−1130.553117
3.20	1.80	−1130.587205	3.30	1.80	−1130.572994	3.40	1.80	−1130.557152
3.20	1.90	−1130.588106	3.30	1.90	−1130.575846	3.40	1.90	−1130.561145
3.20	2.00	−1130.588214	3.30	2.00	−1130.577994	3.40	2.00	−1130.565255
3.20	2.10	−1130.588619	3.30	2.10	−1130.580162	3.40	2.10	−1130.569610
3.20	2.20	−1130.590027	3.30	2.20	−1130.583187	3.40	2.20	−1130.574489
3.20	2.30	−1130.592596	3.30	2.30	−1130.587108	3.40	2.30	−1130.580175
3.20	2.40	−1130.596129	3.30	2.40	−1130.591878	3.40	2.40	−1130.586468
3.20	2.50	−1130.600071	3.30	2.50	−1130.597000	3.40	2.50	−1130.592990
3.20	2.60	−1130.603793	3.30	2.60	−1130.601735	3.40	2.60	−1130.599030
3.20	2.70	−1130.606996	3.30	2.70	−1130.605487	3.40	2.70	−1130.603857
3.20	2.80	−1130.609727	3.30	2.80	−1130.608505	3.40	2.80	−1130.606939
3.20	2.90	−1130.611604	3.30	2.90	−1130.610743	3.40	2.90	−1130.609533
3.20	3.00	−1130.612875	3.30	3.00	−1130.612345	3.40	3.00	−1130.611303
3.20	3.10	−1130.613386	3.30	3.10	−1130.613302	3.40	3.10	−1130.612583
3.20	3.20	−1130.612981	3.30	3.20	−1130.613580	3.40	3.20	−1130.613317
3.20	3.30	−1130.611660	3.30	3.30	−1130.612922	3.40	3.30	−1130.613337
3.20	3.40	−1130.609608	3.30	3.40	−1130.611419	3.40	3.40	−1130.612524
3.20	3.50	−1130.606814	3.30	3.50	−1130.609172	3.40	3.50	−1130.610875
3.50	1.40	−1130.516463	3.50	2.20	−1130.563450	3.50	2.90	−1130.608388
3.50	1.50	−1130.527720	3.50	2.30	−1130.571189	3.50	3.00	−1130.610069
3.50	1.60	−1130.533250	3.50	2.40	−1130.579396	3.50	3.10	−1130.611267
3.50	1.70	−1130.536861	3.50	2.50	−1130.587634	3.50	3.20	−1130.612424
3.50	1.80	−1130.540469	3.50	2.60	−1130.595216	3.50	3.30	−1130.612941
3.50	1.90	−1130.544829	3.50	2.70	−1130.601343	3.50	3.40	−1130.612797
3.50	2.00	−1130.550096	3.50	2.80	−1130.605366	3.50	3.50	−1130.611850
3.50	2.10	−1130.556346						

[a]Computed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM. The SCF convergence criterion was set to 10^{-6} to accelerate the calculations. [b]Not located.

Table S4. Relaxed Potential Energy Surface Scan for the *endo*-Dig Cyclization of IN3'[a]



R1 (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)
1.40	1.40	−1130.061114	1.50	1.40	−1130.077535	1.60	1.40	−1130.086038
1.40	1.50	−1130.077137	1.50	1.50	−1130.092125	1.60	1.50	−1130.099422
1.40	1.60	−1130.085777	1.50	1.60	−1130.099517	1.60	1.60	−1130.105380
1.40	1.70	−1130.090855	1.50	1.70	−1130.103691	1.60	1.70	−1130.108238
1.40	1.80	−1130.094450	1.50	1.80	−1130.106682	1.60	1.80	−1130.110172
1.40	1.90	−1130.097488	1.50	1.90	−1130.109329	1.60	1.90	−1130.112048
1.40	2.00	−1130.100205	1.50	2.00	−1130.111805	1.60	2.00	−1130.113997
1.40	2.10	−1130.102561	1.50	2.10	−1130.114027	1.60	2.10	−1130.115875
1.40	2.20	−1130.104353	1.50	2.20	−1130.115790	1.60	2.20	−1130.117447
1.40	2.30	−1130.105291	1.50	2.30	−1130.116807	1.60	2.30	−1130.118434
1.40	2.40	−1130.105246	1.50	2.40	−1130.116813	1.60	2.40	−1130.118533
1.40	2.50	−1130.103971	1.50	2.50	−1130.115698	1.60	2.50	−1130.117559
1.40	2.60	−1130.100484	1.50	2.60	−1130.113101	1.60	2.60	−1130.115362
1.40	2.70	−1130.093654	1.50	2.70	−1130.108115	1.60	2.70	−1130.111514
1.40	2.80	−1130.083474	1.50	2.80	−1130.099902	1.60	2.80	−1130.105236
1.40	2.90	−1130.070924	1.50	2.90	−1130.088516	1.60	2.90	−1130.095887
1.40	3.00	−1130.057268	1.50	3.00	−1130.074814	1.60	3.00	−1130.083516
1.40	3.10	−1130.043581	1.50	3.10	−1130.059965	1.60	3.10	−1130.068881
1.40	3.20	−1130.030515	1.50	3.20	−1130.045009	1.60	3.20	−1130.053085
1.40	3.30	−1130.018321	1.50	3.30	−1130.030646	1.60	3.30	−1130.037151
1.40	3.40	−1130.007083	1.50	3.40	−1130.017203	1.60	3.40	−1130.021795
1.70	1.40	−1130.090752	1.80	1.40	−1130.094123	1.90	1.40	−1130.097485
1.70	1.50	−1130.103195	1.80	1.50	−1130.105796	1.90	1.50	−1130.108466
1.70	1.60	−1130.107782	1.80	1.60	−1130.109178	1.90	1.60	−1130.110801
1.70	1.70	−1130.109161	1.80	1.70	−1130.109090	1.90	1.70	−1130.109367
1.70	1.80	−1130.109739	1.80	1.80	−1130.108203	1.90	1.80	−1130.107029
1.70	1.90	−1130.110515	1.80	1.90	−1130.107682	1.90	1.90	−1130.105154
1.70	2.00	−1130.111661	1.80	2.00	−1130.107798	1.90	2.00	−1130.104124
1.70	2.10	−1130.112981	1.80	2.10	−1130.108368	1.90	2.10	−1130.103802
1.70	2.20	−1130.114188	1.80	2.20	−1130.109058	1.90	2.20	−1130.103856
1.70	2.30	−1130.114996	1.80	2.30	−1130.109550	1.90	2.30	−1130.103929
1.70	2.40	−1130.115101	1.80	2.40	−1130.109546	1.90	2.40	−1130.103711
1.70	2.50	−1130.114254	1.80	2.50	−1130.108763	1.90	2.50	−1130.102918
1.70	2.60	−1130.112305	1.80	2.60	−1130.107015	1.90	2.60	−1130.101328
1.70	2.70	−1130.109043	1.80	2.70	−1130.104119	1.90	2.70	−1130.098746
1.70	2.80	−1130.104013	1.80	2.80	−1130.099816	1.90	2.80	−1130.094969

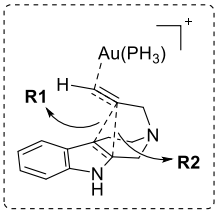
1.70	2.90	−1130.096599	1.80	2.90	−1130.093674	1.90	2.90	−1130.089684
1.70	3.00	−1130.086283	1.80	3.00	−1130.085241	1.90	3.00	−1130.082526
1.70	3.10	−1130.073074	1.80	3.10	−1130.074057	1.90	3.10	−1130.073146
1.70	3.20	−1130.057660	1.80	3.20	−1130.060105	1.90	3.20	−1130.061134
1.70	3.30	−1130.041096	1.80	3.30	−1130.044012	1.90	3.30	−1130.046477
1.70	3.40	−1130.024387	1.80	3.40	−1130.026790	1.90	3.40	−1130.029744
2.00	1.40	−1130.101429	2.10	1.40	−1130.106105	2.20	1.40	−1130.111332
2.00	1.50	−1130.111712	2.10	1.50	−1130.115595	2.20	1.50	−1130.119897
2.00	1.60	−1130.113108	2.10	1.60	−1130.116099	2.20	1.60	−1130.119528
2.00	1.70	−1130.110488	2.10	1.70	−1130.112430	2.20	1.70	−1130.114917
2.00	1.80	−1130.106811	2.10	1.80	−1130.107570	2.20	1.80	−1130.109025
2.00	1.90	−1130.103616	2.10	1.90	−1130.103167	2.20	1.90	−1130.103558
2.00	2.00	−1130.101421	2.10	2.00	−1130.099864	2.20	2.00	−1130.099261
2.00	2.10	−1130.100152	2.10	2.10	−1130.097661	2.20	2.10	−1130.096202
2.00	2.20	−1130.099491	2.10	2.20	−1130.096272	2.20	2.20	−1130.094127
2.00	2.30	−1130.099080	2.10	2.30	−1130.095342	2.20	2.30	−1130.092695
2.00	2.40	−1130.098580	2.10	2.40	−1130.094528	2.20	2.40	−1130.091566
2.00	2.50	−1130.097708	2.10	2.50	−1130.093531	2.20	2.50	−1130.090433
2.00	2.60	−1130.096224	2.10	2.60	−1130.092111	2.20	2.60	−1130.089047
2.00	2.70	−1130.093937	2.10	2.70	−1130.090066	2.20	2.70	−1130.087207
2.00	2.80	−1130.090622	2.10	2.80	−1130.087197	2.20	2.80	−1130.084730
2.00	2.90	−1130.086048	2.10	2.90	−1130.083271	2.20	2.90	−1130.081410
2.00	3.00	−1130.079902	2.10	3.00	−1130.078032	2.20	3.00	−1130.077001
2.00	3.10	−1130.071854	2.10	3.10	−1130.071170	2.20	3.10	−1130.071232
2.00	3.20	−1130.061577	2.10	3.20	−1130.062374	2.20	3.20	−1130.063815
2.00	3.30	−1130.048740	2.10	3.30	−1130.051275	2.20	3.30	−1130.054410
2.00	3.40	−1130.033347	2.10	3.40	−1130.037598	2.20	3.40	−1130.042593
2.30	1.40	−1130.116654	2.40	1.40	−1130.120719	2.50	1.40	−1130.122293
2.30	1.50	−1130.124302	2.40	1.50	−1130.128240	2.50	1.50	−1130.130607
2.30	1.60	−1130.123070	2.40	1.60	−1130.126394	2.50	1.60	−1130.128900
2.30	1.70	−1130.117591	2.40	1.70	−1130.120163	2.50	1.70	−1130.122303
2.30	1.80	−1130.110803	2.40	1.80	−1130.112567	2.50	1.80	−1130.114096
2.30	1.90	−1130.104420	2.40	1.90	−1130.105396	2.50	1.90	−1130.106230
2.30	2.00	−1130.099256	2.40	2.00	−1130.099497	2.50	2.00	−1130.099695
2.30	2.10	−1130.095457	2.40	2.10	−1130.095069	2.50	2.10	−1130.094745
2.30	2.20	−1130.092788	2.40	2.20	−1130.091914	2.50	2.20	−1130.091198
2.30	2.30	−1130.090916	2.40	2.30	−1130.089695	2.50	2.30	−1130.088721
2.30	2.40	−1130.089509	2.40	2.40	−1130.088074	2.50	2.40	−1130.086969
2.30	2.50	−1130.088260	2.40	2.50	−1130.086755	2.50	2.50	−1130.085633
2.30	2.60	−1130.086910	2.40	2.60	−1130.085471	2.50	2.60	−1130.084455
2.30	2.70	−1130.085254	2.40	2.70	−1130.084004	2.50	2.70	−1130.083208
2.30	2.80	−1130.083125	2.40	2.80	−1130.082201	2.50	2.80	−1130.081734
2.30	2.90	−1130.080351	2.40	2.90	−1130.079917	2.50	2.90	−1130.079909

2.30	3.00	−1130.076701	2.40	3.00	−1130.076959	2.50	3.00	−1130.077577
2.30	3.10	−1130.071936	2.40	3.10	−1130.073095	2.50	3.10	−1130.074536
2.30	3.20	−1130.065784	2.40	3.20	−1130.068097	2.50	3.20	−1130.070578
2.30	3.30	−1130.057960	2.40	3.30	−1130.061703	2.50	3.30	−1130.065483
2.30	3.40	−1130.048074	2.40	3.40	−1130.053609	2.50	3.40	−1130.059000
2.60	1.40	−1130.120369	2.70	1.40	−1130.114770	2.80	1.40	−1130.105787
2.60	1.50	−1130.130594	2.70	1.50	−1130.127373	2.80	1.50	−1130.120811
2.60	1.60	−1130.129785	2.70	1.60	−1130.128449	2.80	1.60	−1130.124224
2.60	1.70	−1130.123444	2.70	1.70	−1130.123032	2.80	1.70	−1130.120598
2.60	1.80	−1130.115056	2.70	1.80	−1130.114947	2.80	1.80	−1130.113409
2.60	1.90	−1130.106736	2.70	1.90	−1130.106587	2.80	1.90	−1130.105373
2.60	2.00	−1130.099674	2.70	2.00	−1130.099243	2.80	2.00	−1130.098105
2.60	2.10	−1130.094276	2.70	2.10	−1130.093524	2.80	2.10	−1130.092286
2.60	2.20	−1130.090418	2.70	2.20	−1130.089425	2.80	2.20	−1130.088088
2.60	2.30	−1130.087758	2.70	2.30	−1130.086645	2.80	2.30	−1130.085269
2.60	2.40	−1130.085940	2.70	2.40	−1130.084820	2.80	2.40	−1130.083492
2.60	2.50	−1130.084649	2.70	2.50	−1130.083618	2.80	2.50	−1130.082425
2.60	2.60	−1130.083613	2.70	2.60	−1130.082764	2.80	2.60	−1130.081780
2.60	2.70	−1130.082619	2.70	2.70	−1130.082047	2.80	2.70	−1130.081359
2.60	2.80	−1130.081501	2.70	2.80	−1130.081316	2.80	2.80	−1130.081033
2.60	2.90	−1130.080139	2.70	2.90	−1130.080440	2.80	2.90	−1130.080661
2.60	3.00	−1130.078398	2.70	3.00	−1130.079294	2.80	3.00	−1130.080105
2.60	3.10	−1130.076118	2.70	3.10	−1130.077750	2.80	3.10	−1130.079255
2.60	3.20	−1130.073135	2.70	3.20	−1130.075658	2.80	3.20	−1130.077959
2.60	3.30	−1130.069261	2.70	3.30	−1130.072925	2.80	3.30	−1130.076139
2.60	3.40	−1130.064301	2.70	3.40	−1130.069364	2.80	3.40	−1130.073704
2.90	1.40	−1130.094311	3.00	1.40	−1130.081515	3.10	1.40	−1130.068469
2.90	1.50	−1130.111104	3.00	1.50	−1130.098950	3.10	1.50	−1130.085410
2.90	1.60	−1130.116956	3.00	1.60	−1130.106705	3.10	1.60	−1130.094055
2.90	1.70	−1130.115573	3.00	1.70	−1130.107756	3.10	1.70	−1130.097096
2.90	1.80	−1130.110059	3.00	1.80	−1130.104381	3.10	1.80	−1130.096100
2.90	1.90	−1130.102871	3.00	1.90	−1130.098744	3.10	1.90	−1130.092503
2.90	2.00	−1130.095962	3.00	2.00	−1130.092639	3.10	2.00	−1130.087830
2.90	2.10	−1130.090323	3.00	2.10	−1130.087443	3.10	2.10	−1130.083424
2.90	2.20	−1130.086209	3.00	2.20	−1130.083615	3.10	2.20	−1130.080171
2.90	2.30	−1130.083496	3.00	2.30	−1130.081150	3.10	2.30	−1130.078117
2.90	2.40	−1130.081857	3.00	2.40	−1130.079783	3.10	2.40	−1130.077128
2.90	2.50	−1130.080976	3.00	2.50	−1130.079179	3.10	2.50	−1130.076924
2.90	2.60	−1130.080577	3.00	2.60	−1130.079073	3.10	2.60	−1130.077204
2.90	2.70	−1130.080460	3.00	2.70	−1130.079292	3.10	2.70	−1130.077808
2.90	2.80	−1130.080532	3.00	2.80	−1130.079760	3.10	2.80	−1130.078691
2.90	2.90	−1130.080651	3.00	2.90	−1130.080352	3.10	2.90	−1130.079565
2.90	3.00	−1130.080672	3.00	3.00	−1130.080843	3.10	3.00	−1130.080582

2.90	3.10	−1130.080404	3.00	3.10	−1130.081059	3.10	3.10	−1130.081200
2.90	3.20	−1130.079744	3.00	3.20	−1130.080910	3.10	3.20	−1130.081476
2.90	3.30	−1130.078648	3.00	3.30	−1130.080375	3.10	3.30	N/A[b]
2.90	3.40	N/A[b]	3.00	3.40	N/A[b]	3.10	3.40	N/A[b]
3.20	1.40	−1130.055911	3.30	1.40	−1130.044246	3.40	1.40	−1130.033646
3.20	1.50	−1130.071498	3.30	1.50	−1130.057956	3.40	1.50	−1130.045245
3.20	1.60	−1130.079961	3.30	1.60	−1130.065385	3.40	1.60	−1130.051066
3.20	1.70	−1130.084079	3.30	1.70	−1130.069558	3.40	1.70	−1130.054450
3.20	1.80	−1130.085115	3.30	1.80	−1130.071810	3.40	1.80	−1130.056929
3.20	1.90	−1130.083814	3.30	1.90	−1130.072544	3.40	1.90	−1130.058975
3.20	2.00	−1130.081081	3.30	2.00	−1130.072022	3.40	2.00	−1130.060468
3.20	2.10	−1130.078000	3.30	2.10	−1130.070791	3.40	2.10	−1130.061371
3.20	2.20	−1130.075582	3.30	2.20	−1130.069625	3.40	2.20	−1130.061993
3.20	2.30	−1130.074240	3.30	2.30	−1130.069215	3.40	2.30	−1130.062861
3.20	2.40	−1130.073793	3.30	2.40	−1130.069613	3.40	2.40	−1130.064293
3.20	2.50	−1130.074084	3.30	2.50	−1130.070562	3.40	2.50	−1130.066212
3.20	2.60	−1130.074881	3.30	2.60	−1130.071973	3.40	2.60	−1130.068366
3.20	2.70	−1130.075971	3.30	2.70	−1130.073676	3.40	2.70	−1130.070801
3.20	2.80	−1130.077300	3.30	2.80	−1130.075537	3.40	2.80	−1130.073337
3.20	2.90	−1130.078694	3.30	2.90	−1130.077365	3.40	2.90	−1130.075669
3.20	3.00	−1130.079932	3.30	3.00	−1130.078953	3.40	3.00	−1130.077640
3.20	3.10	−1130.080887	3.30	3.10	−1130.080208	3.40	3.10	−1130.079203
3.20	3.20	−1130.081542	3.30	3.20	−1130.081151	3.40	3.20	−1130.080412
3.20	3.30	−1130.081818	3.30	3.30	−1130.081714	3.40	3.30	−1130.081240
3.20	3.40	N/A[b]	3.30	3.40	−1130.081884	3.40	3.40	−1130.081687

[a]Computed at the B3LYP/SDD-6-31G(d) level in the gas phase. The SCF convergence criterion was set to 10^{-6} to accelerate the calculations. [b]These points are on the potential energy surface for the *exo*-dig cyclization of **IN3'**.

Table S5. Relaxed Potential Energy Surface Scan for the *exo*-Dig Cyclization of IN3'[a]



R1 (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)	**R1** (Å)	**R2** (Å)	*E* (a.u.)
1.40	1.40	−1130.040950	1.50	1.40	−1130.055224	1.60	1.40	−1130.065196
1.40	1.50	−1130.059355	1.50	1.50	−1130.072330	1.60	1.50	−1130.079801
1.40	1.60	−1130.070904	1.50	1.60	−1130.082978	1.60	1.60	−1130.088305
1.40	1.70	−1130.079255	1.50	1.70	−1130.090663	1.60	1.70	−1130.094397
1.40	1.80	−1130.086038	1.50	1.80	−1130.097020	1.60	1.80	−1130.099672
1.40	1.90	−1130.091858	1.50	1.90	−1130.102589	1.60	1.90	−1130.104546
1.40	2.00	−1130.096710	1.50	2.00	−1130.107329	1.60	2.00	−1130.108877
1.40	2.10	−1130.100354	1.50	2.10	−1130.110991	1.60	2.10	−1130.112353
1.40	2.20	−1130.102553	1.50	2.20	−1130.113335	1.60	2.20	−1130.114719
1.40	2.30	−1130.103266	1.50	2.30	−1130.114266	1.60	2.30	−1130.115841
1.40	2.40	−1130.102328	1.50	2.40	−1130.113662	1.60	2.40	−1130.115563
1.40	2.50	−1130.099004	1.50	2.50	−1130.111290	1.60	2.50	−1130.113742
1.40	2.60	−1130.092063	1.50	2.60	−1130.106251	1.60	2.60	−1130.109962
1.40	2.70	−1130.081153	1.50	2.70	−1130.097590	1.60	2.70	−1130.103351
1.40	2.80	−1130.067110	1.50	2.80	−1130.085133	1.60	2.80	−1130.093199
1.40	2.90	−1130.051389	1.50	2.90	−1130.069713	1.60	2.90	−1130.079435
1.40	3.00	−1130.035308	1.50	3.00	−1130.052702	1.60	3.00	−1130.062875
1.40	3.10	−1130.019729	1.50	3.10	−1130.035366	1.60	3.10	−1130.044813
1.40	3.20	−1130.005118	1.50	3.20	−1130.018607	1.60	3.20	−1130.026479
1.40	3.30	−1129.991807	1.50	3.30	−1130.002964	1.60	3.30	−1130.008786
1.40	3.40	−1129.980398	1.50	3.40	−1129.988863	1.60	3.40	−1129.992339
1.40	3.50	−1129.976811	1.50	3.50	−1129.976936	1.60	3.50	−1129.977675
1.40	3.60	−1129.974656	1.50	3.60	−1129.971637	1.60	3.60	−1129.965637
1.70	1.40	−1130.072057	1.80	1.40	−1130.077380	1.90	1.40	−1130.082323
1.70	1.50	−1130.085090	1.80	1.50	−1130.089501	1.90	1.50	−1130.093765
1.70	1.60	−1130.091363	1.80	1.60	−1130.094111	1.90	1.60	−1130.097155
1.70	1.70	−1130.095322	1.80	1.70	−1130.095990	1.90	1.70	−1130.097360
1.70	1.80	−1130.098928	1.80	1.80	−1130.097636	1.90	1.80	−1130.097132
1.70	1.90	−1130.102640	1.80	1.90	−1130.099827	1.90	1.90	−1130.097640
1.70	2.00	−1130.106228	1.80	2.00	−1130.102362	1.90	2.00	−1130.098919
1.70	2.10	−1130.109278	1.80	2.10	−1130.104758	1.90	2.10	−1130.100476
1.70	2.20	−1130.111476	1.80	2.20	−1130.106597	1.90	2.20	−1130.101806
1.70	2.30	−1130.112663	1.80	2.30	−1130.107669	1.90	2.30	−1130.102610
1.70	2.40	−1130.112627	1.80	2.40	−1130.107755	1.90	2.40	−1130.102665
1.70	2.50	−1130.111215	1.80	2.50	−1130.106639	1.90	2.50	−1130.101758

1.70	2.60	−1130.108204	1.80	2.60	−1130.104225	1.90	2.60	−1130.099808
1.70	2.70	−1130.103040	1.80	2.70	−1130.100050	1.90	2.70	−1130.096423
1.70	2.80	−1130.094982	1.80	2.80	−1130.093541	1.90	2.80	−1130.091094
1.70	2.90	−1130.083503	1.80	2.90	−1130.084128	1.90	2.90	−1130.083333
1.70	3.00	−1130.068604	1.80	3.00	−1130.071429	1.90	3.00	−1130.072667
1.70	3.10	−1130.051059	1.80	3.10	−1130.055488	1.90	3.10	−1130.058809
1.70	3.20	−1130.032094	1.80	3.20	−1130.037040	1.90	3.20	−1130.041862
1.70	3.30	−1130.012914	1.80	3.30	−1130.017258	1.90	3.30	−1130.022538
1.70	3.40	−1129.994441	1.80	3.40	−1129.997319	1.90	3.40	−1130.001964
1.70	3.50	−1129.977335	1.80	3.50	−1129.978156	1.90	3.50	−1129.981297
1.70	3.60	−1129.962275	1.80	3.60	−1129.960494	1.90	3.60	−1129.961489
2.00	1.40	−1130.087456	2.10	1.40	−1130.092916	2.20	1.40	−1130.098540
2.00	1.50	−1130.098237	2.10	1.50	−1130.102935	2.20	1.50	−1130.107684
2.00	1.60	−1130.100617	2.10	1.60	−1130.104407	2.20	1.60	−1130.108271
2.00	1.70	−1130.099484	2.10	1.70	−1130.102144	2.20	1.70	−1130.105038
2.00	1.80	−1130.097702	2.10	1.80	−1130.099083	2.20	1.80	−1130.100892
2.00	1.90	−1130.096640	2.10	1.90	−1130.096708	2.20	1.90	−1130.097424
2.00	2.00	−1130.096594	2.10	2.00	−1130.095455	2.20	2.00	−1130.095168
2.00	2.10	−1130.097207	2.10	2.10	−1130.095114	2.20	2.10	−1130.093989
2.00	2.20	−1130.097932	2.10	2.20	−1130.095193	2.20	2.20	−1130.093454
2.00	2.30	−1130.098369	2.10	2.30	−1130.095225	2.20	2.30	−1130.093093
2.00	2.40	−1130.098272	2.10	2.40	−1130.094921	2.20	2.40	−1130.092565
2.00	2.50	−1130.097455	2.10	2.50	−1130.094079	2.20	2.50	−1130.091676
2.00	2.60	−1130.095851	2.10	2.60	−1130.092696	2.20	2.60	−1130.090373
2.00	2.70	−1130.093093	2.10	2.70	−1130.090425	2.20	2.70	−1130.088492
2.00	2.80	−1130.088749	2.10	2.80	−1130.086915	2.20	2.80	−1130.085644
2.00	2.90	−1130.082375	2.10	2.90	−1130.081732	2.20	2.90	−1130.081495
2.00	3.00	−1130.073500	2.10	3.00	−1130.074445	2.20	3.00	−1130.075582
2.00	3.10	−1130.061699	2.10	3.10	−1130.064592	2.20	3.10	−1130.067515
2.00	3.20	−1130.046751	2.10	3.20	−1130.051785	2.20	3.20	−1130.056831
2.00	3.30	−1130.028810	2.10	3.30	−1130.035836	2.20	3.30	−1130.043151
2.00	3.40	−1130.008591	2.10	3.40	−1130.016925	2.20	3.40	−1130.026295
2.00	3.50	−1129.987195	2.10	3.50	−1129.995771	2.20	3.50	−1130.006453
2.00	3.60	−1129.965782	2.10	3.60	−1129.973489	2.20	3.60	−1129.984343
2.30	1.40	−1130.103748	2.40	1.40	−1130.107683	2.50	1.40	−1130.109017
2.30	1.50	−1130.112163	2.40	1.50	−1130.115831	2.50	1.50	−1130.117989
2.30	1.60	−1130.111917	2.40	1.60	−1130.115013	2.50	1.60	−1130.117166
2.30	1.70	−1130.107800	2.40	1.70	−1130.110154	2.50	1.70	−1130.111821
2.30	1.80	−1130.102746	2.40	1.80	−1130.104292	2.50	1.80	−1130.105324
2.30	1.90	−1130.098354	2.40	1.90	−1130.099137	2.50	1.90	−1130.099494
2.30	2.00	−1130.095267	2.40	2.00	−1130.095359	2.50	2.00	−1130.095156
2.30	2.10	−1130.093416	2.40	2.10	−1130.092974	2.50	2.10	−1130.092340
2.30	2.20	−1130.092386	2.40	2.20	−1130.091597	2.50	2.20	−1130.090717

2.30	2.30	−1130.091708	2.40	2.30	−1130.090725	2.50	2.30	−1130.089778
2.30	2.40	−1130.090993	2.40	2.40	−1130.089934	2.50	2.40	−1130.089042
2.30	2.50	−1130.090059	2.40	2.50	−1130.088974	2.50	2.50	−1130.088179
2.30	2.60	−1130.088808	2.40	2.60	−1130.087826	2.50	2.60	−1130.087147
2.30	2.70	−1130.087187	2.40	2.70	−1130.086372	2.50	2.70	−1130.085899
2.30	2.80	−1130.084855	2.40	2.80	−1130.084419	2.50	2.80	−1130.084224
2.30	2.90	−1130.081543	2.40	2.90	−1130.081742	2.50	2.90	−1130.082005
2.30	3.00	−1130.076800	2.40	3.00	−1130.077948	2.50	3.00	−1130.078949
2.30	3.10	−1130.070272	2.40	3.10	−1130.072701	2.50	3.10	−1130.074744
2.30	3.20	−1130.061553	2.40	3.20	−1130.065667	2.50	3.20	−1130.069092
2.30	3.30	−1130.050163	2.40	3.30	−1130.056372	2.50	3.30	−1130.061597
2.30	3.40	−1130.035736	2.40	3.40	−1130.044369	2.50	3.40	−1130.051784
2.30	3.50	−1130.018086	2.40	3.50	−1130.029302	2.50	3.50	−1130.039253
2.30	3.60	−1129.997392	2.40	3.60	−1130.010965	2.50	3.60	−1130.023638
2.60	1.40	−1130.107070	2.70	1.40	−1130.101056	2.80	1.40	−1130.091292
2.60	1.50	−1130.117576	2.70	1.50	−1130.114174	2.80	1.50	−1130.107068
2.60	1.60	−1130.117744	2.70	1.60	−1130.115974	2.80	1.60	−1130.111456
2.60	1.70	−1130.112553	2.70	1.70	−1130.111722	2.80	1.70	−1130.108876
2.60	1.80	−1130.105638	2.70	1.80	−1130.105059	2.80	1.80	−1130.103017
2.60	1.90	−1130.099291	2.70	1.90	−1130.098399	2.80	1.90	−1130.096651
2.60	2.00	−1130.094449	2.70	2.00	−1130.093166	2.80	2.00	−1130.091278
2.60	2.10	−1130.091299	2.70	2.10	−1130.089698	2.80	2.10	−1130.087558
2.60	2.20	−1130.089499	2.70	2.20	−1130.087786	2.80	2.20	−1130.085493
2.60	2.30	−1130.088564	2.70	2.30	−1130.086913	2.80	2.30	−1130.084698
2.60	2.40	−1130.087993	2.70	2.40	−1130.086548	2.80	2.40	−1130.084591
2.60	2.50	−1130.087378	2.70	2.50	−1130.086281	2.80	2.50	−1130.084685
2.60	2.60	−1130.086535	2.70	2.60	−1130.085803	2.80	2.60	−1130.084686
2.60	2.70	−1130.085540	2.70	2.70	−1130.085093	2.80	2.70	−1130.084393
2.60	2.80	−1130.084159	2.70	2.80	−1130.084080	2.80	2.80	−1130.083817
2.60	2.90	−1130.082287	2.70	2.90	−1130.082579	2.80	2.90	−1130.082788
2.60	3.00	−1130.079789	2.70	3.00	−1130.080504	2.80	3.00	−1130.081162
2.60	3.10	−1130.076397	2.70	3.10	−1130.077714	2.80	3.10	−1130.078844
2.60	3.20	−1130.071844	2.70	3.20	−1130.073991	2.80	3.20	−1130.075716
2.60	3.30	−1130.065819	2.70	3.30	−1130.069118	2.80	3.30	−1130.071675
2.60	3.40	−1130.057870	2.70	3.40	−1130.062693	2.80	3.40	−1130.066450
2.60	3.50	−1130.047599	2.70	3.50	−1130.054339	2.80	3.50	−1130.059663
2.60	3.60	−1130.034620	2.70	3.60	−1130.043709	2.80	3.60	−1130.051051
2.90	1.40	−1130.078904	3.00	1.40	−1130.065063	3.10	1.40	−1130.050820
2.90	1.50	−1130.096591	3.00	1.50	−1130.083538	3.10	1.50	−1130.068934
2.90	1.60	−1130.103557	3.00	1.60	−1130.092549	3.10	1.60	−1130.078934
2.90	1.70	−1130.103452	3.00	1.70	−1130.094992	3.10	1.70	−1130.083540
2.90	1.80	−1130.099274	3.00	1.80	−1130.093107	3.10	1.80	−1130.084208
2.90	1.90	−1130.093619	3.00	1.90	−1130.089076	3.10	1.90	−1130.082292

2.90	2.00	−1130.088522	3.00	2.00	−1130.084728	3.10	2.00	−1130.079431
2.90	2.10	−1130.084869	3.00	2.10	−1130.081349	3.10	2.10	−1130.076909
2.90	2.20	−1130.082751	3.00	2.20	−1130.079448	3.10	2.20	−1130.075426
2.90	2.30	−1130.081946	3.00	2.30	−1130.078805	3.10	2.30	−1130.075111
2.90	2.40	−1130.082042	3.00	2.40	−1130.079050	3.10	2.40	−1130.075639
2.90	2.50	−1130.082534	3.00	2.50	−1130.079803	3.10	2.50	−1130.076684
2.90	2.60	−1130.083015	3.00	2.60	−1130.080765	3.10	2.60	−1130.077960
2.90	2.70	−1130.083281	3.00	2.70	−1130.081616	3.10	2.70	−1130.079343
2.90	2.80	−1130.083216	3.00	2.80	−1130.082159	3.10	2.80	−1130.080570
2.90	2.90	−1130.082767	3.00	2.90	−1130.082359	3.10	2.90	−1130.081452
2.90	3.00	−1130.081719	3.00	3.00	−1130.082017	3.10	3.00	−1130.081921
2.90	3.10	−1130.079958	3.00	3.10	−1130.080949	3.10	3.10	−1130.081675
2.90	3.20	−1130.077374	3.00	3.20	−1130.079070	3.10	3.20	−1130.080558
2.90	3.30	−1130.073857	3.00	3.30	−1130.076227	3.10	3.30	−1130.078483
2.90	3.40	−1130.069430	3.00	3.40	−1130.072262	3.10	3.40	−1130.075333
2.90	3.50	−1130.063864	3.00	3.50	−1130.067245	3.10	3.50	−1130.071002
2.90	3.60	−1130.056896	3.00	3.60	−1130.061516	3.10	3.60	−1130.065472
3.20	1.40	−1130.036920	3.30	1.40	−1130.023825	3.40	1.40	−1130.011775
3.20	1.50	−1130.053820	3.30	1.50	−1130.038972	3.40	1.50	−1130.024891
3.20	1.60	−1130.063707	3.30	1.60	−1130.047901	3.40	1.60	−1130.032296
3.20	1.70	−1130.069465	3.30	1.70	−1130.053731	3.40	1.70	−1130.037342
3.20	1.80	−1130.072352	3.30	1.80	−1130.057892	3.40	1.80	−1130.041715
3.20	1.90	−1130.072978	3.30	1.90	−1130.060739	3.40	1.90	−1130.045911
3.20	2.00	−1130.072117	3.30	2.00	−1130.062341	3.40	2.00	−1130.049704
3.20	2.10	−1130.070963	3.30	2.10	−1130.063151	3.40	2.10	−1130.052877
3.20	2.20	−1130.070425	3.30	2.20	−1130.063992	3.40	2.20	−1130.055685
3.20	2.30	−1130.070804	3.30	2.30	−1130.065404	3.40	2.30	−1130.058557
3.20	2.40	−1130.071863	3.30	2.40	−1130.067322	3.40	2.40	−1130.061728
3.20	2.50	−1130.073250	3.30	2.50	−1130.069438	3.40	2.50	−1130.064919
3.20	2.60	−1130.074742	3.30	2.60	−1130.071445	3.40	2.60	−1130.067815
3.20	2.70	−1130.076515	3.30	2.70	−1130.073195	3.40	2.70	−1130.070171
3.20	2.80	−1130.078376	3.30	2.80	−1130.075594	3.40	2.80	−1130.072157
3.20	2.90	−1130.080011	3.30	2.90	−1130.078019	3.40	2.90	−1130.075378
3.20	3.00	−1130.081294	3.30	3.00	−1130.080040	3.40	3.00	−1130.078173
3.20	3.10	−1130.081882	3.30	3.10	−1130.081401	3.40	3.10	−1130.080222
3.20	3.20	−1130.081550	3.30	3.20	−1130.081847	3.40	3.20	−1130.081409
3.20	3.30	−1130.080229	3.30	3.30	−1130.081310	3.40	3.30	−1130.081655
3.20	3.40	−1130.077878	3.30	3.40	−1130.079747	3.40	3.40	−1130.080890
3.20	3.50	−1130.074396	3.30	3.50	−1130.077116	3.40	3.50	−1130.079087
3.20	3.60	−1130.069741	3.30	3.60	−1130.073354	3.40	3.60	−1130.076213
3.50	1.40	−1130.000904	3.50	3.00	−1130.075621	3.60	2.30	−1130.038454
3.50	1.50	−1130.011902	3.50	3.10	−1130.078390	3.60	2.40	−1130.045253
3.50	1.60	−1130.017425	3.50	3.20	−1130.080243	3.60	2.50	−1130.051684

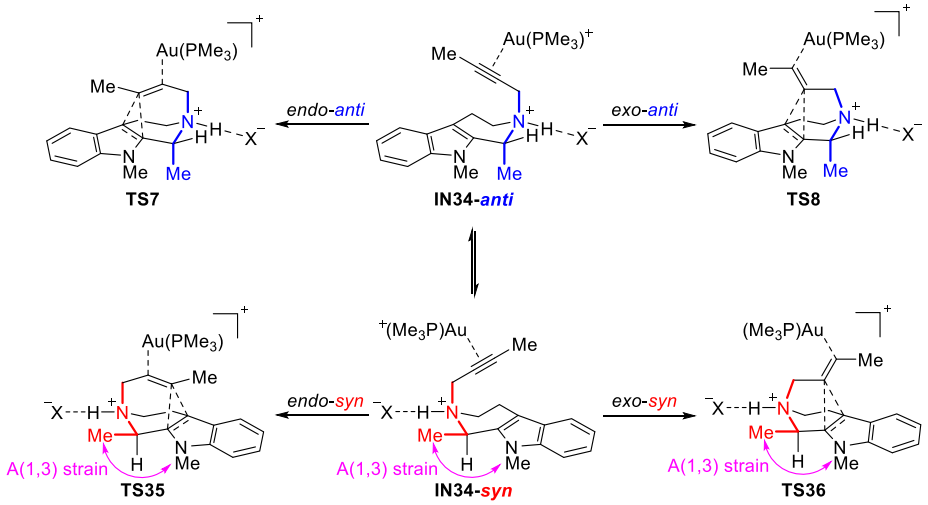
3.50	1.70	−1130.021102	3.50	3.30	−1130.081237	3.60	2.60	−1130.057440
3.50	1.80	−1130.024798	3.50	3.40	−1130.081270	3.60	2.70	−1130.062288
3.50	1.90	−1130.029302	3.50	3.50	−1130.080293	3.60	2.80	−1130.066123
3.50	2.00	−1130.034474	3.50	3.60	−1130.078283	3.60	2.90	−1130.068897
3.50	2.10	−1130.039787	3.60	1.40	−1129.991312	3.60	3.00	−1130.072300
3.50	2.20	−1130.044893	3.60	1.50	−1130.000221	3.60	3.10	−1130.075859
3.50	2.30	−1130.049740	3.60	1.60	−1130.003642	3.60	3.20	−1130.078429
3.50	2.40	−1130.054525	3.60	1.70	−1130.005564	3.60	3.30	−1130.080070
3.50	2.50	−1130.059170	3.60	1.80	−1130.007970	3.60	3.40	−1130.080868
3.50	2.60	−1130.063324	3.60	1.90	−1130.011870	3.60	3.50	−1130.080707
3.50	2.70	−1130.066746	3.60	2.00	−1130.017407	3.60	3.60	−1130.079555
3.50	2.80	−1130.069319	3.60	2.10	−1130.024099			
3.50	2.90	−1130.071983	3.60	2.20	−1130.031310			

[a]Computed at the B3LYP/SDD-6-31G(d) level in the gas phase. The SCF convergence criterion was set to 10^{-6} to accelerate the calculations.

S3.2. Diastereoselectivity of the Initial Intramolecular Cyclization

As shown in Tables S6 and S7, in all cases, the *anti*-attack transition state is favored over its *syn*-attack counterpart by ca. 3 kcal/mol. We reasoned that the *syn*-attack transition states suffer strong allylic 1,3-strain between the C1-methyl group and the methyl group on the indole nitrogen atom, which does not exist in the *anti*-attack transition states.

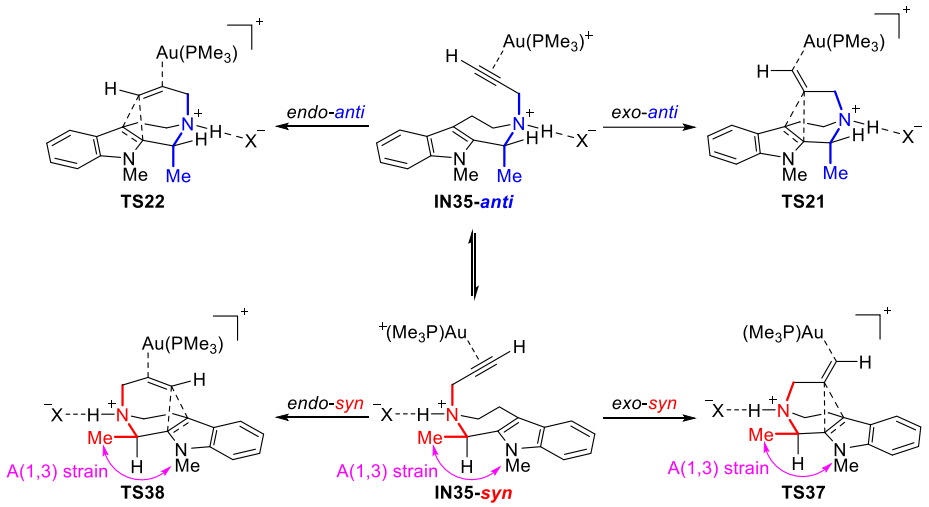
Table S6. Relative Gibbs Free Energies for *endo*- and *exo*-Dig Cyclizations of IN34[a]



entry	transition state	*exo*/*endo*	*syn*/*anti*	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
1	**TS7**	*endo*	*anti*	0.0
2	**TS35**	*endo*	*syn*	3.6
3	**TS8**	*exo*	*anti*	3.0
4	**TS36**	*exo*	*syn*	6.1

[a]Computed at the SMD(PhMe)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(PhMe)/B3LYP/SDD-6-31G(d) level in PhMe. A standard state of 298 K and 1 mol/L was used. X = OMs.

Table S7. Relative Gibbs Free Energies for *exo*- and *endo*-Dig Cyclizations of IN35[a]



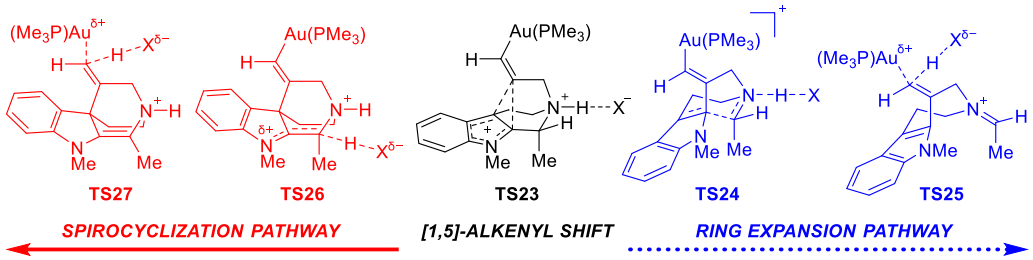
entry	transition state	*exo*/*endo*	*syn*/*anti*	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
1	**TS21**	*exo*	*anti*	0.0
2	**TS37**	*exo*	*syn*	2.7
3	**TS22**	*endo*	*anti*	0.5
4	**TS38**	*endo*	*syn*	3.7

[a]Computed at the SMD(DCM)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM. A standard state of 298 K and 1 mol/L was used. X = OMs.

S3.3. Assessment of Density Functionals for the Chemoselectivity

In addition to the B3LYP-D3(BJ) method, we have also tested the performance of other popular functionals, such as M06[5] and PBE0,[6] by doing solution-phase single point energy calculations using the optimized structures from the SMD(DCM)/B3LYP/SDD-6-31G(d) method. The DFT-computed relative Gibbs free energies were listed in Table S8. All of the functionals indicated that the [1,5]-alkenyl shift process is easier than the ring expansion and spirocyclization processes, suggesting that the chemoselectivity is under kinetic control (see Figures 1D and 7A for details). Moreover, all of the functionals suggested that the spirocyclization is favored over the ring expansion, which is in good accordance with our experiments (Tables 3 and 4, no ring expansion product **5** was observed in all cases). Therefore, different density functionals performed similarly in these gold-catalyzed transformations.

Table S8. Relative Gibbs Free Energies of TS23–27 in DCM by Three Density Functionals[a]



DF	TS27	TS26	TS23	TS24	TS25
B3LYP-D3(BJ)	1.2	1.1	0.0	2.9	−10.5
M06	4.2	4.6	0.0	6.0	−6.0
PBE0	2.4	2.9	0.0	4.9	−7.1

[a]Computed at the SMD(DCM)/DF/SDD-6-311+G(d,p)//SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM. A standard state of 298 K and 1 mol/L was used. Reported in kcal/mol. X = OMs.

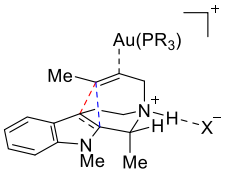
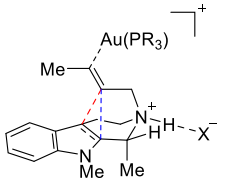
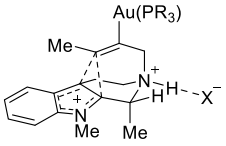
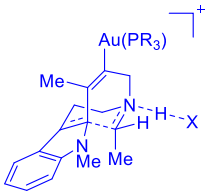
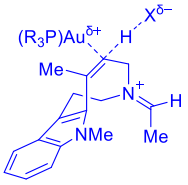
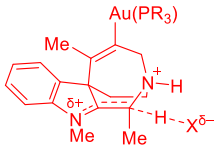
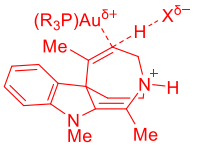
(5) Zhao, Y.; Truhlar, D. G. *Theor. Chem. Acc.* **2008**, *120*, 215.

(6) Adamo, C.; Barone, V. *J. Chem. Phys.* **1999**, *110*, 6158.

S3.4. DFT Investigations on the Ligand Effect

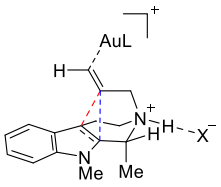
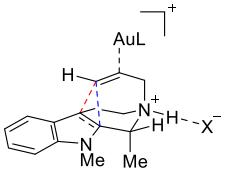
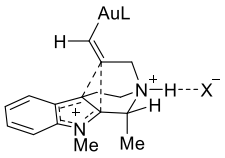
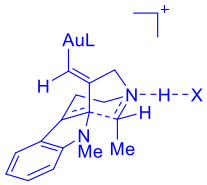
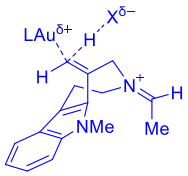
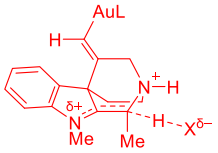
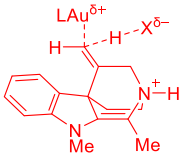
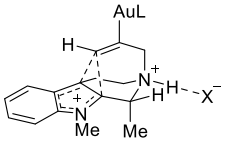
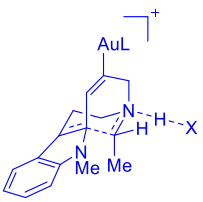
In addition to the model ligand, PMe_3, we have also performed optimizations for some key transition states with the real ligand PPh_3. The relative Gibbs free energies were listed in Tables S9 and S10. We found that the replacement of PPh_3 by simple PMe_3 did not change our discussions or conclusions.

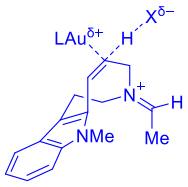
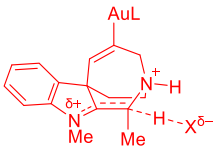
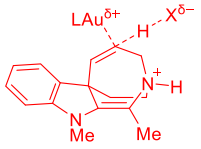
Table S9. Relative Gibbs Free Energies of TS7–13 in PhMe with Different Ligands[a]

transition state	structure	R = Me	R = Ph
TS7		0.4	−0.5
TS8		3.4	3.4
TS9		0.0	0.0
TS10		−2.9	−2.4
TS11		−9.6	−8.9
TS12		6.5	5.6
TS13		5.4	5.5

[a]Computed at the SMD(PhMe)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(PhMe)/B3LYP/SDD-6-31G(d) level in PhMe. A standard state of 298 K and 1 mol/L was used. Reported in kcal/mol. X = OMs.

Table S10. Relative Gibbs Free Energies of TS21–32 in DCM with Different Ligands[a]

transition state	structure	L = PMe_3	L = PPh_3	L = JohnPhos
TS21		0.6	−0.2	−0.6
TS22		1.1	2.6	−0.3
TS23		0.0	0.0	0.0
TS24		2.9	3.6	4.0
TS25		−10.5	−10.1	−10.8
TS26		1.1	1.3	1.3
TS27		1.2	1.9	0.6
TS28		−4.7	−3.6	−5.7
TS29		−2.5	−1.4	−1.2

TS30		−12.3	−11.6	−11.3
TS31		2.3	3.2	3.3
TS32		3.9	4.7	3.1

[a]Computed at the SMD(DCM)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM. A standard state of 298 K and 1 mol/L was used. Reported in kcal/mol. X = OMs.

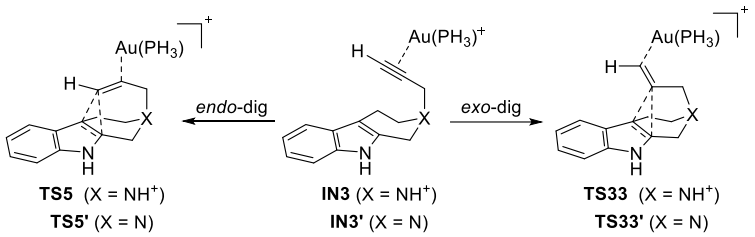
In principle, we may also understand why JohnPhos showed better chemoselectivity than PPh_3 (Table 3) by DFT studies if we can locate all the conformations for 12 transition states in Table S10. However, JohnPhos is large and does not have the C_3-axis as PMe_3 and PPh_3 do; and consequently, hundreds of transition states have to be optimized to give convincing conclusions for the chemoselectivities, which precluded our fully investigations of the reaction system.

During our studies, we located 61 conformers for these transition states with JohnPhos as the ligand. We found that rotation of the JohnPhos ligand may change the relative Gibbs energy of one certain transition state by as much as ca. 2 kcal/mol. Therefore, searching only limited numbers of transition states can not provide convincing conclusions. And consequently, we did not further investigate the ligand effect of JohnPhos on the chemoselectivity.

S3.5. DFT Investigations on the Additive Effect

Effects on the Regioselectivity of the Initial Cyclization. In addition to the roles of MsOH mentioned in the paper, another potential role of the acid is to increase the induction effect of the nitrogen atom in the regioselectivity-determining step. Although it is correct theoretically, we found that whether the nitrogen atom was protonated did not influence the energy difference of the *exo*- and *endo*-dig cyclizations significantly (1.4 kcal/mol for X = NH^+ versus 1.2 kcal/mol for X = N as shown in Table S11).

Table S11. Relative Gibbs Free Energies for *exo*- and *endo*-Dig Cyclizations of IN3 and IN3'[a]

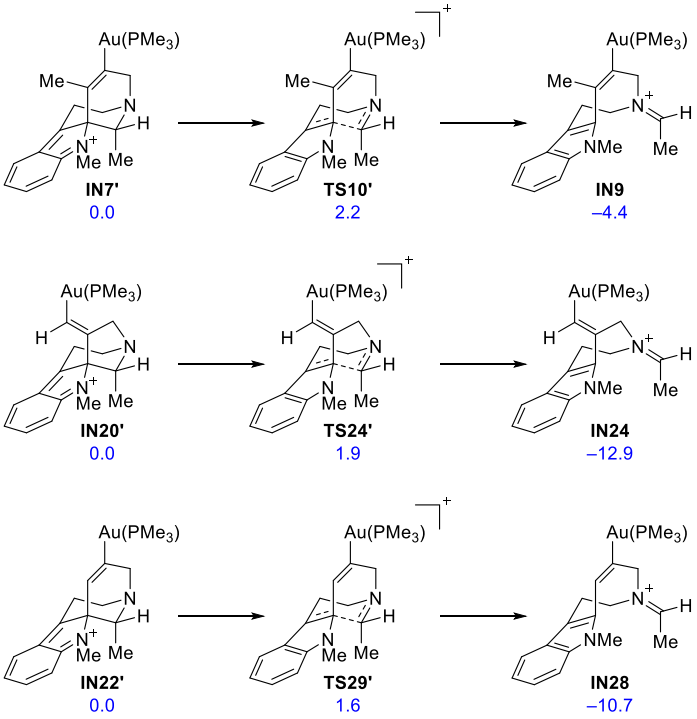


entry	X	intermediate	transition state	*exo*/*endo*	$\Delta\Delta G^{\ddagger}$ (kcal/mol)
1	NH^+	**IN3**	**TS33**	*exo*	3.8
2	NH^+	**IN3**	**TS5**	*endo*	5.2
3	N	**IN3'**	**TS33'**	*exo*	5.5
4	N	**IN3'**	**TS5'**	*endo*	6.7

[a]Computed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level in DCM.

Effects on the Fragmentation Process. DFT calculations indicated that if MsOH is not presented, the activation energy of the fragmentation process in the ring expansion pathway is only ca. 2 kcal/mol (Scheme S4). However, if MsOH is added as an additive, the fragmentation process needs a higher activation energy of ca. 8–13 kcal/mol (Figures 4, 5, and 7), making the spirocyclization pathway compete with the ring expansion pathway.

Scheme S4. Relative Gibbs Free Energies for Transition States and Intermediates Involved in the Fragmentation Processes in the Absence of MsOH[a]



[a]Computed at the SMD/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD/B3LYP/SDD-6-31G(d) level in solvent (PhMe for **IN7'**; DCM for **IN20'** and **IN22'**). A standard state of 298 K and 1 mol/L was used. Reported in kcal/mol.

S3.6. 3D Structures for Representative Intermediates and Transition States

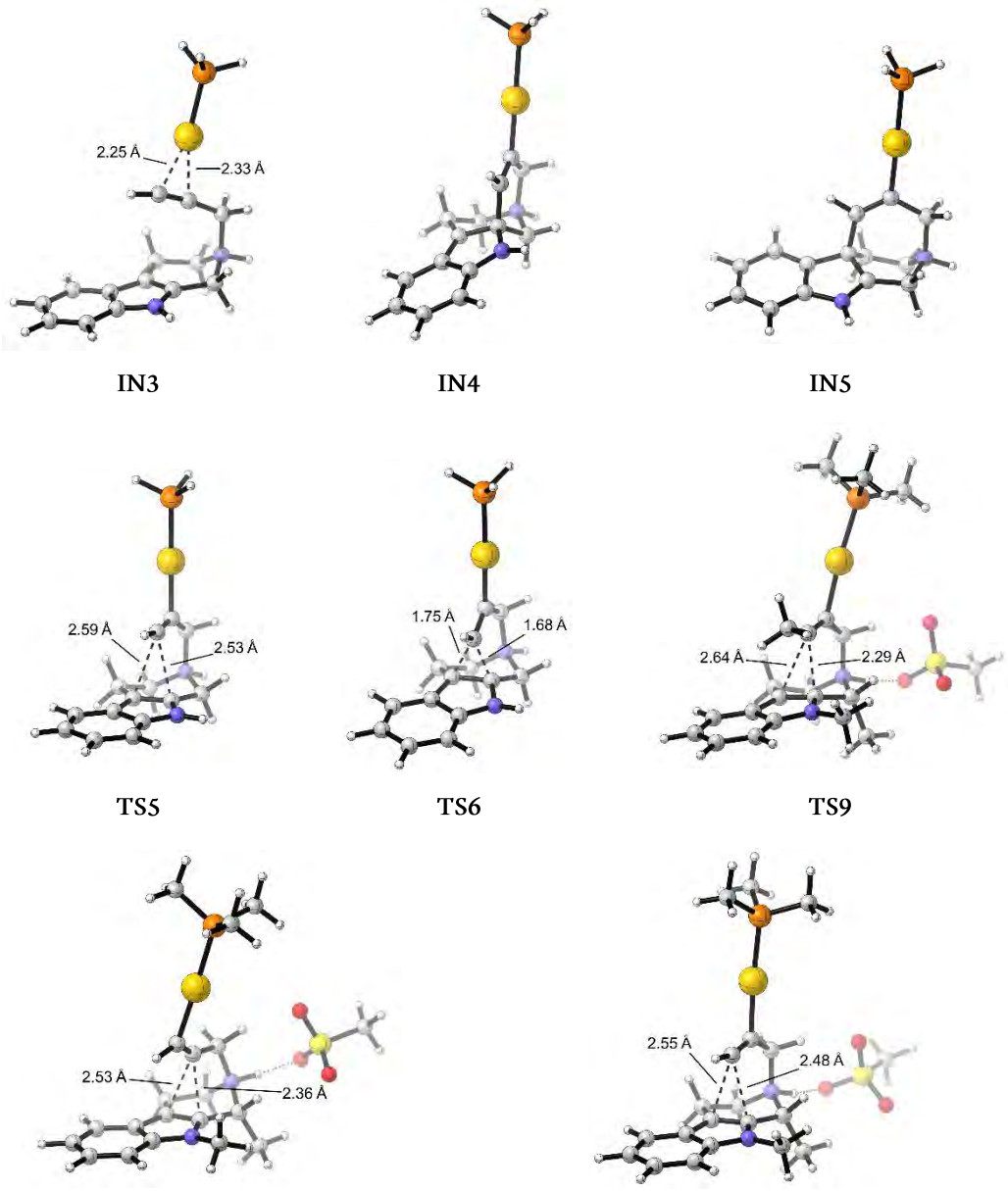


Figure S4. 3D structures for representative intermediates and transition states. Color scheme: H, white; C, gray; O, red; P, dark orange; S, yellow; Au, gold.[7]

(7) Legault, C. Y. *CYLview*, 1.0b; Université de Sherbrooke, 2009. http://www.cylview.org.

S3.7. Computed Energies of All Stationary Points

Table S12. Sum of Electronic and Thermal Enthalpies *H*, Sum of Electronic and Thermal Free Energies *G* (After Quasiharmonic Correction of Entropy[8]), Thermal Correction to Gibbs Free Energy *TCG* (After Quasiharmonic Correction of Entropy), and Single Point Energy in PhMe Using the B3LYP-D3(BJ) Functional E_{PhMe}

Figure 4 and Tables S6	*H* (a.u.)[a]	*G* (a.u.)[a]	*TCG* (a.u.)[a]	E_{PhMe} (a.u.)[b]
MsOH (in PhMe)	−664.240434	−664.276732	0.032226	−664.447692
IN7	−2029.874735	−2029.967336	0.461362	−2030.973654
IN8	−2029.869804	−2029.962239	0.462297	−2030.968856
IN9	−1365.626923	−1365.708698	0.400207	−1366.501677
IN10	−2029.884834	−2029.979201	0.459345	−2030.984899
IN11	−1365.605165	−1365.684942	0.403959	−1366.485921
IN12	−2029.858236	−2029.951528	0.462153	−2030.968298
TS7	−2029.852740	−2029.946388	0.458539	−2030.951737
TS8	−2029.848645	−2029.942171	0.459220	−2030.947572
TS9	−2029.858668	−2029.950463	0.460783	−2030.954574
TS10	−2029.863044	−2029.956928	0.457298	−2030.955745
TS11	−2029.871821	−2029.966918	0.452120	−2030.961288
TS12	−2029.847673	−2029.939035	0.458523	−2030.941937
TS13	−2029.845580	−2029.938114	0.456738	−2030.942002
TS35	−2029.846278	−2029.939266	0.459476	−2030.946955
TS36	−2029.844000	−2029.937372	0.459377	−2030.942876

[a]Computed at the SMD(PhMe)/B3LYP/SDD-6-31G(d) level. A standard state of 298 K and 1 atm was used. Conversion to the standard state of 298 K and 1 mol/L was achieved by adding 1.89 kcal/mol to the Gibbs free energy.[9] [b]Computed at the SMD(PhMe)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(PhMe)/B3LYP/SDD-6-31G(d) level.

(8) (a) Zhao, Y.; Truhlar, D. G. *Phys. Chem. Chem. Phys.* **2008**, *10*, 2813. (b) Ribeiro, R. F.; Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. *J. Phys. Chem. B* **2011**, *115*, 14556.

(9) Keith, J. A.; Carter, E. A. *J. Chem. Theory Comput.* **2012**, *8*, 3187.

Table S13. Sum of Electronic and Thermal Enthalpies *H*, Sum of Electronic and Thermal Free Energies *G* (After Quasiharmonic Correction of Entropy), Thermal Correction to Gibbs Free Energy *TCG* (After Quasiharmonic Correction of Entropy), and Single Point Energy in PhMe Using the B3LYP-D3(BJ) Functional E_{PhMe}

Figure 5	*H* (a.u.)[a]	*G* (a.u.)[a]	*TCG* (a.u.)[a]	E_{PhMe} (a.u.)[b]
MsOH (in PhMe)	−664.240434	−664.276732	0.032226	−664.447692
IN13	−2218.404903	−2218.503609	0.472709	−2219.590231
IN14	−2218.397592	−2218.495760	0.473878	−2219.582250
IN15	−1554.149022	−1554.236104	0.412386	−1555.113900
IN16	−2218.403444	−2218.502722	0.472527	−2219.589246
IN17	−1554.155304	−1554.240612	0.416488	−1555.121495
IN18	−2218.404891	−2218.503539	0.475018	−2219.600631
TS14	−2218.383011	−2218.482672	0.470304	−2219.568421
TS15	−2218.378696	−2218.478287	0.470610	−2219.563308
TS16	−2218.386836	−2218.484703	0.472176	−2219.568640
TS17	−2218.393710	−2218.493490	0.469275	−2219.574759
TS18	−2218.390917	−2218.490414	0.466053	−2219.566358
TS19	−2218.390731	−2218.487623	0.470975	−2219.570915
TS20	−2218.393630	−2218.491781	0.469242	−2219.575663

[a]Computed at the SMD(PhMe)/B3LYP/SDD-6-31G(d) level. A standard state of 298 K and 1 atm was used. Conversion to the standard state of 298 K and 1 mol/L was achieved by adding 1.89 kcal/mol to the Gibbs free energy. [b]Computed at the SMD(PhMe)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(PhMe)/B3LYP/SDD-6-31G(d) level.

Table S14. Sum of Electronic and Thermal Enthalpies *H*, Sum of Electronic and Thermal Free Energies *G* (After Quasiharmonic Correction of Entropy), Thermal Correction to Gibbs Free Energy *TCG* (After Quasiharmonic Correction of Entropy), and Single Point Energy in DCM Using the B3LYP-D3(BJ) Functional E_{DCM}

Figure 7 and Table S7	*H* (a.u.)[a]	*G* (a.u.)[a]	*TCG* (a.u.)[a]	E_{DCM} (a.u.)[b]
MsOH (in DCM)	−664.244720	−664.280437	0.032699	−664.453114
IN20	−1990.615284	−1990.705680	0.433748	−1991.663927
IN21	−1990.623210	−1990.712483	0.435866	−1991.672610
IN22	−1990.621802	−1990.711818	0.434855	−1991.672200
IN23	−1990.622146	−1990.711366	0.436508	−1991.673357
IN24	−1326.371322	−1326.449832	0.373841	−1327.194771
IN25	−1990.644873	−1990.736456	0.432683	−1991.690829
IN26	−1326.351197	−1326.428415	0.376054	−1327.181047
IN27	−1990.616694	−1990.707091	0.434559	−1991.673373
IN28	−1326.374519	−1326.453714	0.372878	−1327.199681
IN29	−1990.642026	−1990.734984	0.431047	−1991.689953
IN30	−1326.350216	−1326.427162	0.376961	−1327.181526
IN31	−1990.613863	−1990.704298	0.435194	−1991.672797
TS21	−1990.594877	−1990.685365	0.431621	−1991.644998
TS22	−1990.591253	−1990.683020	0.430184	−1991.642850
TS23	−1990.601298	−1990.690881	0.432771	−1991.647118
TS24	−1990.598548	−1990.690040	0.428860	−1991.638520
TS25	−1990.620243	−1990.711558	0.425811	−1991.656845
TS26	−1990.598648	−1990.687597	0.430658	−1991.643184
TS27	−1990.596754	−1990.686952	0.427981	−1991.640425
TS28	−1990.609878	−1990.698724	0.434298	−1991.656121
TS29	−1990.605815	−1990.697167	0.429327	−1991.647713
TS30	−1990.620496	−1990.712399	0.425569	−1991.659563
TS31	−1990.592761	−1990.681932	0.430937	−1991.641687
TS32	−1990.591307	−1990.681161	0.428938	−1991.637031
TS37	−1990.589861	−1990.680160	0.431577	−1991.640587
TS38	−1990.585043	−1990.676111	0.430865	−1991.638317

[a]Computed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level. A standard state of 298 K and 1 atm was used. Conversion to the standard state of 298 K and 1 mol/L was achieved by adding 1.89 kcal/mol to the Gibbs free energy. [b]Computed at the SMD(DCM)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(DCM)/B3LYP/SDD-6-31G(d) level.

Table S15. Sum of Electronic and Thermal Enthalpies *H*, Sum of Electronic and Thermal Free Energies *G* (After Quasiharmonic Correction of Entropy), Thermal Correction to Gibbs Free Energy *TCG* (After Quasiharmonic Correction of Entropy), and Single Point Energy in PhMe Using the B3LYP-D3(BJ) Functional E_{PhMe}

Table S9	*H* (a.u.)[a]	*G* (a.u.)[a]	*TCG* (a.u.)[a]	E_{PhMe} (a.u.)[b]
TS7 (L = PPh_3)	–2604.885279	–2604.996901	0.610767	–2606.372221
TS8 (L = PPh_3)	–2604.880456	–2604.992204	0.610895	–2606.366071
TS9 (L = PPh_3)	–2604.890811	–2604.999920	0.613699	–2606.374344
TS10 (L = PPh_3)	–2604.894861	–2605.006068	0.610158	–2606.374653
TS11 (L = PPh_3)	–2604.904019	–2605.016271	0.605125	–2606.380024
TS12 (L = PPh_3)	–2604.879755	–2604.989056	0.610442	–2606.362193
TS13 (L = PPh_3)	–2604.877675	–2604.988016	0.608800	–2606.360747

[a]Computed at the SMD(PhMe)/B3LYP/SDD-6-31G(d) level. A standard state of 298 K and 1 atm was used. Conversion to the standard state of 298 K and 1 mol/L was achieved by adding 1.89 kcal/mol to the Gibbs free energy. [b]Computed at the SMD(PhMe)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(PhMe)/B3LYP/SDD-6-31G(d) level.

Table S16. Sum of Electronic and Thermal Enthalpies *H*, Sum of Electronic and Thermal Free Energies *G* (After Quasiharmonic Correction of Entropy), Thermal Correction to Gibbs Free Energy *TCG* (After Quasiharmonic Correction of Entropy), and Single Point Energy in DCM Using the B3LYP-D3(BJ) Functional E_{DCM}

Table S10	*H* (a.u.)[a]	*G* (a.u.)[a]	*TCG* (a.u.)[a]	E_{DCM} (a.u.)[b]
TS21 (L = PPh_3)	−2565.626957	−2565.735585	0.583113	−2567.064782
TS22 (L = PPh_3)	−2565.622148	−2565.730937	0.583482	−2567.060686
TS23 (L = PPh_3)	−2565.633452	−2565.740288	0.585840	−2567.067224
TS24 (L = PPh_3)	−2565.630179	−2565.738696	0.582240	−2567.057886
TS25 (L = PPh_3)	−2565.651968	−2565.761169	0.577889	−2567.075389
TS26 (L = PPh_3)	−2565.630634	−2565.737048	0.583311	−2567.062650
TS27 (L = PPh_3)	−2565.627992	−2565.735944	0.580466	−2567.058795
TS28 (L = PPh_3)	−2565.641098	−2565.747222	0.587348	−2567.074410
TS29 (L = PPh_3)	−2565.637223	−2565.745748	0.582690	−2567.066260
TS30 (L = PPh_3)	−2565.651822	−2565.761493	0.578002	−2567.077927
TS31 (L = PPh_3)	−2565.624685	−2565.731718	0.583004	−2567.059248
TS32 (L = PPh_3)	−2565.622118	−2565.729885	0.581421	−2567.055336
TS21 (L = JohnPhos)	−2648.917133	−2649.036358	0.723121	−2650.576649
TS22 (L = JohnPhos)	−2648.914198	−2649.034197	0.722612	−2650.575553
TS23 (L = JohnPhos)	−2648.922093	−2649.040005	0.725295	−2650.577810
TS24 (L = JohnPhos)	−2648.918358	−2649.038062	0.721269	−2650.567373
TS25 (L = JohnPhos)	−2648.940493	−2649.060601	0.717567	−2650.587295
TS26 (L = JohnPhos)	−2648.918459	−2649.036207	0.722257	−2650.572754
TS27 (L = JohnPhos)	−2648.916175	−2649.034631	0.720559	−2650.572136
TS28 (L = JohnPhos)	−2648.931689	−2649.049269	0.726046	−2650.587571
TS29 (L = JohnPhos)	−2648.925714	−2649.044861	0.722518	−2650.576973
TS30 (L = JohnPhos)	−2648.938531	−2649.058640	0.718319	−2650.588898
TS31 (L = JohnPhos)	−2648.912011	−2649.030052	0.722425	−2650.569650
TS32 (L = JohnPhos)	−2648.911083	−2649.029816	0.720515	−2650.568027

[a]Computed at the SMD(DCM)/B3LYP/SDD-6-31G(d) level. A standard state of 298 K and 1 atm was used. Conversion to the standard state of 298 K and 1 mol/L was achieved by adding 1.89 kcal/mol to the Gibbs free energy. [b]Computed at the SMD(DCM)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD(DCM)/B3LYP/SDD-6-31G(d) level.

Table S17. Sum of Electronic and Thermal Enthalpies *H*, Sum of Electronic and Thermal Free Energies *G* (After Quasiharmonic Correction of Entropy), Thermal Correction to Gibbs Free Energy *TCG* (After Quasiharmonic Correction of Entropy), and Single Point Energy in Solvent Using the B3LYP-D3(BJ) Functional E_{sol}

Scheme S4	*H* (a.u.)[a]	*G* (a.u.)[a]	*TCG* (a.u.)[a]	E_{sol} (a.u.)[b]
IN7' (in PhMe)	−1365.620490	−1365.699727	0.402237	−1366.496762
IN9 (in PhMe)	−1365.626923	−1365.708698	0.400207	−1366.501677
IN20' (in DCM)	−1326.348687	−1326.426258	0.373217	−1327.173604
IN22' (in DCM)	−1326.358004	−1326.434650	0.374872	−1327.184584
IN24 (in DCM)	−1326.371322	−1326.449832	0.373841	−1327.194771
IN28 (in DCM)	−1326.374519	−1326.453714	0.372878	−1327.199681
TS10' (in PhMe)	−1365.616056	−1365.695561	0.400740	−1366.491792
TS24' (in DCM)	−1326.346555	−1326.423183	0.373478	−1327.170778
TS29' (in DCM)	−1326.355486	−1326.431758	0.374149	−1327.181385

[a]Computed at the SMD(solvent)/B3LYP/SDD-6-31G(d) level. A standard state of 298 K and 1 atm was used. Conversion to the standard state of 298 K and 1 mol/L was achieved by adding 1.89 kcal/mol to the Gibbs free energy. [b]Computed at the SMD(solvent)/B3LYP-D3(BJ)/SDD-6-311+G(d,p)//SMD (solvent)/B3LYP/SDD-6-31G(d) level.

S3.8. Cartesian Coordinates of All Stationary Points

MsOH (in PhMe)

S	−0.09844000	−0.14481400	−0.02764200
O	−0.60545100	1.31846500	0.53228100
O	−0.34634200	−1.15988200	0.99265600
O	−0.64815200	−0.31883900	−1.37359200
C	1.65106600	0.21690800	−0.09886200
H	−1.50095900	1.47457600	0.16701200
H	2.15167200	−0.69783200	−0.42613600
H	1.99609300	0.49782000	0.89833800
H	1.82139300	1.02305800	−0.81453200

MsOH (in DCM)

S	−0.08853300	−0.13802200	0.05669700
O	−0.78636900	1.10678600	−0.74773600
O	−0.33782700	−1.32060800	−0.76178500
O	−0.53972200	−0.09035500	1.44956400
C	1.64438800	0.29303000	−0.03241300
H	1.93310000	0.36796900	−1.08278700
H	2.20637900	−0.50475000	0.46035500
H	1.80178100	1.24252500	0.48381000
H	−1.07970900	1.77784000	−0.09440200

IN3

Au	−2.48800500	−0.39023100	0.01041500
P	−4.76258300	−0.85819700	−0.04380300
N	3.28530400	0.26069900	1.63667600
N	0.93190600	2.80114800	0.17972700
C	−0.24087200	−0.53560400	0.03767500
C	−0.41247900	0.68062600	0.06368400
C	−0.43710700	2.14815400	0.12040600
C	1.83141900	2.30008100	1.29905400
C	2.63709100	1.14602300	0.80314300
C	3.93121200	−0.68457500	0.86268100
C	4.71778000	−1.77838000	1.24345300
C	5.22975200	−2.58252600	0.22995200
C	4.96934200	−2.30560600	−1.13032000
C	4.19178600	−1.21613900	−1.50652700
C	3.66161200	−0.38173800	−0.50418400
C	2.83751200	0.79908300	−0.51079900
C	2.19847500	1.54580800	−1.64351500
C	1.67088300	2.89404500	−1.15738400
H	−5.10332800	−2.17315400	0.31098200
H	−5.39869200	−0.69901100	−1.28526100
H	−5.56501200	−0.09006400	0.81489300
H	3.33093500	0.32534400	2.64540400
H	0.71027000	3.77479500	0.42188700
H	0.13265500	−1.54396700	0.01138100
H	−0.94468600	2.56098900	−0.75464800
H	−0.96962900	2.47287500	1.01834000
H	1.19149400	2.04545700	2.14877300
H	2.45224900	3.15497200	1.58642500
H	4.91581800	−1.99119400	2.29027000
H	5.84238700	−3.44118000	0.49069500
H	5.38664600	−2.95687300	−1.89344600
H	3.99998300	−1.01004900	−2.55639500
H	1.39336100	0.96156100	−2.10835400
H	2.91756200	1.76141500	−2.44320600
H	0.97086200	3.35014800	−1.85897900
H	2.48934600	3.59070800	−0.96321900

IN4

Au	2.52702800	−0.25839900	0.02326700
P	4.67393500	−1.14764100	0.41126000
N	−2.70408000	−0.57635300	−1.47958300
N	−0.88592500	2.56703800	−0.55721900
C	−0.44547800	−0.25620700	−0.48431700
C	0.63615600	0.51858000	−0.30617300
C	0.54017400	2.01814100	−0.36709400
C	−1.68361200	1.69012100	−1.48192400
C	−1.83811300	0.33817500	−0.76052400
C	−3.74236000	−0.94608500	−0.72236700
C	−4.78360200	−1.85680600	−1.00975300
C	−5.74690600	−2.02343800	−0.04118800
C	−5.73049600	−1.32580300	1.21610900
C	−4.73064700	−0.44568600	1.51952700
C	−3.69668300	−0.23828800	0.54933200
C	−2.57654600	0.55618900	0.53163800
C	−2.04187100	1.57036500	1.47772400
C	−1.64468100	2.85363700	0.72281200
H	4.98728100	−1.52453900	1.73041200
H	5.77660100	−0.32790400	0.10692900
H	5.02279800	−2.32057700	−0.28387300
H	−2.46022500	−0.99255700	−2.37270900
H	−0.77955300	3.47455700	−1.02560000
H	−0.42230100	−1.33930100	−0.41148500
H	0.92043700	2.48777900	0.54304300
H	1.11430200	2.41052800	−1.21181900
H	−1.12695400	1.57918500	−2.41382300
H	−2.64513300	2.17141800	−1.66843500
H	−4.81607800	−2.39050800	−1.95320100
H	−6.56440700	−2.71331700	−0.23037000
H	−6.53124300	−1.51406300	1.92333800
H	−4.70161500	0.08558700	2.46509400
H	−1.16396100	1.15549500	1.98950500
H	−2.77554900	1.82997400	2.24465300
H	−1.00854600	3.49144900	1.33732100
H	−2.53210900	3.41279300	0.41882000

IN5

Au	2.34416800	−0.25486300	−0.02255200
P	4.45051700	−1.30090700	−0.17554200
N	−3.28433300	0.50236200	−1.52061400
N	−0.86822300	2.85224700	−0.03935900
C	−0.63167200	−0.10542100	0.27269500
C	0.47702900	0.63886500	0.11468800
C	0.49310400	2.13708400	0.03439500
C	−1.70394200	2.40738900	−1.20897700
C	−2.37431400	1.13469700	−0.83867700
C	−3.77711500	−0.62530000	−0.80361500
C	−4.75095600	−1.53322700	−1.19148000
C	−5.05307300	−2.54337900	−0.27152700
C	−4.39514500	−2.61851900	0.96326100
C	−3.40755800	−1.68994200	1.32294300
C	−3.10216800	−0.67675900	0.42293800
C	−2.08225500	0.44274100	0.45526500
C	−2.16497200	1.44125100	1.64266000
C	−1.65575200	2.84583700	1.25747300
H	4.92014000	−1.97642500	0.96612200
H	5.55866100	−0.48447800	−0.46869000
H	4.60106400	−2.30358500	−1.15146000

H	−3.60962800	0.77103500	−2.45074300
H	−0.63622400	3.83668500	−0.21971100
H	−0.57835200	−1.18942300	0.28151600
H	0.99701300	2.57863700	0.89932500
H	1.02064900	2.46909100	−0.86496300
H	−1.05502500	2.29939600	−2.08353400
H	−2.44557300	3.18460800	−1.41767300
H	−5.25168400	−1.46301200	−2.15151900
H	−5.81125500	−3.27887200	−0.52165500
H	−4.65405500	−3.41344400	1.65608700
H	−2.90056200	−1.76390200	2.28015400
H	−1.58060500	1.03076400	2.46837900
H	−3.20241700	1.53384100	1.97356900
H	−0.99356000	3.26610200	2.01485200
H	−2.48496000	3.53655900	1.09221500

IN6

Au	−2.29742700	−0.13445600	0.00313100
P	−4.60342900	−0.42466300	0.15544700
N	3.82808100	0.24896700	1.26533700
N	1.44878000	2.55555600	−0.57057700
C	0.38604600	−2.01673800	0.17048300
C	0.03223100	−0.61188900	−0.02324400
C	−0.12223300	0.59625000	−0.21101500
C	0.02118500	2.04463800	−0.42682100
C	2.37665900	2.23301500	0.62231900
C	3.26814700	3.45276100	0.88920800
C	3.11711000	0.96456300	0.31327400
C	4.01131300	0.56943200	2.67330900
C	4.41614600	−0.83493000	0.62929200
C	5.24776400	−1.83524700	1.15099300
C	5.68952600	−2.82085400	0.27512100
C	5.32013800	−2.81643400	−1.08718300
C	4.50152600	−1.82097100	−1.60464700
C	4.04133600	−0.80742600	−0.74265100
C	3.21518200	0.35535100	−0.91730600
C	2.51700700	0.86133500	−2.14215800
C	2.08906000	2.30921900	−1.93929800
C	−5.37585900	−0.85998900	−1.44639000
C	−5.05225300	−1.76423300	1.32036200
C	−5.46788700	1.07715300	0.74652700
H	1.32295800	3.57358600	−0.52996300
H	1.47029600	−2.12059200	0.04061400
H	−0.10963600	−2.65611800	−0.56705100
H	0.11903400	−2.35886400	1.17552200
H	−0.50472400	2.35699000	−1.33305800
H	−0.40697500	2.59186100	0.41782500
H	1.69703000	2.09933400	1.47151400
H	3.93546700	3.66081400	0.04761400
H	2.66425000	4.34225700	1.10653600
H	3.89261100	3.25944400	1.76532800
H	4.98495900	1.03894000	2.85596400
H	3.94701900	−0.34679700	3.26640400
H	3.22253300	1.24302600	3.01353600
H	5.54662600	−1.84274100	2.19460100
H	6.33783700	−3.60868600	0.64739300
H	5.68899500	−3.60259100	−1.73947500
H	4.22993700	−1.82094100	−2.65698700
H	1.65378700	0.23736200	−2.40913500
H	3.17981200	0.84842400	−3.01609000
H	1.35950800	2.64568100	−2.67872500
H	2.95100400	2.97816200	−1.96962300
H	−5.21235500	−0.05684800	−2.17157200
H	−6.45296200	−1.00839000	−1.31057200
H	−4.93388200	−1.78209000	−1.83624400
H	−4.60923100	−2.70958000	0.99235600
H	−6.14186500	−1.87331700	1.35725100
H	−4.68049300	−1.52860100	2.32218400
H	−5.10249600	1.35373000	1.74041800
H	−6.54561700	0.88744300	0.80053800
H	−5.28615000	1.90936000	0.05944200

IN7

Au	−2.32912200	−0.74554000	−0.07345400
S	0.54051700	4.39979600	0.31404600
P	−4.64427400	−1.16791800	0.09728600
O	1.24722700	4.03199400	−0.99110700
O	−0.88606900	3.98140600	0.30105100
O	1.31483700	3.93430900	1.49529200
N	3.02125100	−1.01096100	1.28216000
N	1.41465500	1.41310400	−1.09842500
C	0.56678900	6.19733600	0.32078800
C	0.52337100	−2.36618600	0.97481500
C	0.69393400	−1.01941500	0.31379100
C	−0.29756900	−0.29214200	−0.23158900
C	−0.04756700	0.99863900	−0.95885100
C	2.18217700	1.06390900	0.15008200
C	3.56264500	1.71717900	0.17856000
C	2.16893300	−0.49266800	0.21234000
C	2.85621300	−0.67772500	2.69294600
C	3.95951200	−1.81567600	0.76928500
C	4.97782400	−2.54046800	1.43684500
C	5.82643600	−3.29130000	0.65642700
C	5.72007900	−3.36330700	−0.77385800
C	4.74715900	−2.67231500	−1.44083000
C	3.83493400	−1.87536700	−0.67800700
C	2.78943700	−1.05164200	−1.02882200
C	2.27456700	−0.60442000	−2.35186200
C	2.07287200	0.92860300	−2.35163100
C	−5.27597100	−1.23240400	1.82257300
C	−5.18822900	−2.75930900	−0.64484800
C	−5.68969400	0.10020700	−0.72522500
H	1.38415700	2.50427000	−1.12456100
H	0.07155700	6.54527800	1.23062200
H	0.03366400	6.56297100	−0.55961700
H	1.60451900	6.53761000	0.30444000
H	−0.50695600	−2.70882800	0.84628600
H	1.18627800	−3.12418000	0.53625800
H	0.73334900	−2.33838600	2.05152000
H	−0.45006800	0.96301000	−1.97582900
H	−0.54028300	1.83683500	−0.45171700
H	1.59063700	1.46951100	0.97423600
H	4.27602500	1.26492500	−0.51613000
H	3.97757800	1.64500000	1.18760900
H	3.46067500	2.78086300	−0.05159900
H	2.87462600	−1.58665600	3.30025900
H	1.89419600	−0.18237500	2.82940000
H	3.65274500	−0.00427300	3.02655400
H	5.08641400	−2.50093700	2.51481100
H	6.61818800	−3.85705800	1.13940900
H	6.42939400	−3.97806900	−1.31798400
H	4.65559800	−2.71982400	−2.52121300
H	1.31366900	−1.09487100	−2.55091200
H	2.95561800	−0.88095300	−3.16118500

H	1.44379400	1.23548900	−3.18886200
H	3.03047900	1.44523900	−2.43727500
H	−4.75919500	−2.02209700	2.37756900
H	−6.35321100	−1.43279600	1.83438100
H	−5.08398200	−0.27738200	2.32221700
H	−4.93815800	−2.77453800	−1.71060700
H	−6.26954100	−2.89438300	−0.52968600
H	−4.67011600	−3.59161300	−0.15749700
H	−5.49274400	1.08289700	−0.28461500
H	−6.75342100	−0.13692700	−0.61164400
H	−5.44543300	0.14614100	−1.79144400

IN7'

Au	−2.25656500	0.01573000	0.02184400
P	−4.55065200	−0.50336100	−0.22513100
N	3.12396300	−0.80351400	1.06361100
N	1.40438900	2.45746100	0.43127300
C	0.63205800	−1.82366500	0.02917300
C	0.76654100	−0.33585600	0.26747400
C	−0.25193900	0.54391200	0.23152800
C	−0.00763600	2.04225500	0.38668100
C	2.18496600	1.57285000	1.24840600
C	3.55697700	2.11390700	1.64846400
C	2.23492800	0.15996700	0.43154200
C	2.93369900	−1.33846200	2.40368400
C	4.19947700	−1.02257600	0.28147700
C	5.33543800	−1.82760100	0.52687500
C	6.29917600	−1.87907100	−0.45921800
C	6.19057000	−1.15037400	−1.68354800
C	5.10176600	−0.35233300	−1.93210200
C	4.07903900	−0.26742600	−0.94342900
C	2.89301500	0.45333800	−0.86539600
C	2.32210600	1.50359800	−1.72695600
C	2.01512300	2.78495700	−0.83897300
C	−5.39333500	−1.01572400	1.32779500
C	−4.90816000	−1.87094000	−1.40201300
C	−5.56404000	0.90086500	−0.84580800
H	1.28544200	−2.15684400	−0.78929300
H	−0.39867800	−2.06762900	−0.24370200
H	0.89380800	−2.42335200	0.91023700
H	−0.49262400	2.59177100	−0.42653200
H	−0.48927900	2.38394500	1.31390300
H	1.61050100	1.35566900	2.15399100
H	4.25674200	2.19491000	0.81245800
H	4.01456000	1.47508500	2.40932600
H	3.42787800	3.11008200	2.08475000
H	3.07575500	−2.42327000	2.40239600
H	1.91623700	−1.11980300	2.73051300
H	3.63840300	−0.88861600	3.11289200
H	5.44282500	−2.38837400	1.44894500
H	7.17843900	−2.49757300	−0.30193000
H	6.98503700	−1.23714000	−2.41781900
H	5.01005900	0.20442500	−2.85956500
H	1.36270700	1.17002300	−2.13935800
H	2.98257300	1.76498700	−2.55893900
H	1.34986500	3.44590800	−1.39920300
H	2.95208500	3.32032600	−0.66647600
H	−4.90939200	−1.91109600	1.73133700
H	−6.45193200	−1.23252000	1.14533100
H	−5.31569800	−0.21740300	2.07300600
H	−4.52413500	−1.61354000	−2.39447200
H	−5.98602300	−2.05513200	−1.47260800
H	−4.41018700	−2.78691600	−1.06766300
H	−5.49543100	1.74093300	−0.14694700
H	−6.61509800	0.61033500	−0.95368400
H	−5.18309500	1.23123000	−1.81771500

IN8

Au	−2.05250300	−0.95618500	−0.14653400
S	−0.24411700	4.34515800	0.25534300
P	−4.30535000	−1.43900100	0.36356700
O	0.57368600	4.19211600	−1.02443300
O	−1.58378000	3.71456400	0.13933300
O	0.53888100	3.91056600	1.44802100
N	3.46850800	−0.25889500	1.21184300
N	1.36191900	1.66184800	−1.14417000
C	−0.49899100	6.11955500	0.40071000
C	0.85050900	−2.66083300	0.15681100
C	0.98335800	−1.26990700	−0.42015700
C	−0.06955000	−0.43688400	−0.57285000
C	−0.00025100	0.98357800	−1.04773000
C	2.15250000	1.59112700	0.14234100
C	3.28630400	2.63874400	0.13729200
C	2.68499300	0.20027100	0.26098900
C	3.75869300	0.35996100	2.50876600
C	4.03220900	−1.51507800	0.81455700
C	4.97659200	−2.28086200	1.48464500
C	5.41351900	−3.44128700	0.83553200
C	4.91449300	−3.79752300	−0.42265200
C	3.94807500	−3.01369200	−1.06712400
C	3.50245200	−1.85968900	−0.43373000
C	2.46968600	−0.82171700	−0.81026000
C	2.54678600	−0.26563200	−2.25412300
C	2.14937300	1.22322200	−2.33919300
C	−4.66383400	−1.45178000	2.16665900
C	−4.89620800	−3.07410000	−0.23519800
C	−5.50581500	−0.23473700	−0.33332700
H	1.10211000	2.70683300	−1.23025100
H	−1.08891400	6.31021300	1.30053700
H	−1.03677400	6.47294200	−0.48195900
H	0.47175800	6.61499400	0.47550700
H	−0.20374000	−2.87338800	0.35272500
H	1.23599000	−3.42689200	−0.52648500
H	1.39514700	−2.77307500	1.10300400
H	−0.44243100	1.08475100	−2.04570600
H	−0.58946000	1.63082400	−0.39111200
H	1.45310200	1.86563600	0.94069300
H	4.12528800	2.35183400	−0.50278900
H	3.65978600	2.78018600	1.15336400
H	2.87357100	3.59275900	−0.19801600
H	3.66462200	−0.40456800	3.28319900
H	3.04358500	1.15680800	2.70750800
H	4.77750100	0.75631300	2.50965400
H	5.37444900	−1.99597100	2.45266200
H	6.15940800	−4.06733900	1.31525700
H	5.28156100	−4.69715600	−0.90702400
H	3.56031000	−3.30579700	−2.03845300
H	1.89461100	−0.87311200	−2.88586900
H	3.56674100	−0.37450000	−2.63406600
H	1.52990600	1.42614100	−3.21446500
H	3.02746800	1.86775300	−2.39617000
H	−4.05662100	−2.21772200	2.65992900
H	−5.72353400	−1.65879100	2.35338500
H	−4.40727000	−0.47865800	2.59744100

H	−4.80905800	−3.12050600	−1.32549700
H	−5.94175600	−3.23987100	0.04778100
H	−4.27953400	−3.87087600	0.19321600
H	−5.27752900	0.77036500	0.03551300
H	−6.53104400	−0.49842300	−0.04983000
H	−5.42801500	−0.22566000	−1.42535200

IN9

Au	2.28012400	0.00455300	0.00287700
P	4.62764700	−0.25487100	0.10409900
N	−3.02851100	−1.51979800	−0.52208700
N	−1.51579400	2.22697500	−0.44836300
C	−0.16694900	−2.18643100	0.29619100
C	−0.67692700	−0.76714800	0.05501300
C	0.19871800	0.26334800	−0.07537600
C	−0.09620800	1.73150000	−0.34800000
C	−2.08846100	2.28146500	−1.60189100
C	−3.47272800	2.69140800	−1.93284800
C	−2.15404800	−0.64277100	0.12641200
C	−2.70071800	−2.47435200	−1.56976900
C	−4.32169800	−1.23961800	−0.11860300
C	−5.53216900	−1.83959600	−0.49177300
C	−6.70239800	−1.33679900	0.06898100
C	−6.67510000	−0.26302300	0.98378000
C	−5.47415100	0.32955800	1.35485700
C	−4.27348900	−0.15764400	0.80406800
C	−2.89045800	0.19614900	0.94985000
C	−2.30951000	1.33372500	1.72661900
C	−2.15800800	2.58756400	0.83570600
C	5.29449100	−0.38058800	1.81336600
C	5.58096600	1.12580100	−0.64893300
C	5.26673700	−1.75656900	−0.74353100
H	0.87179300	−2.16607000	0.63919700
H	−0.76877100	−2.69483000	1.05979600
H	−0.19816700	−2.80743000	−0.60661000
H	0.35989500	2.34686200	0.43244800
H	0.37928900	2.01900700	−1.29043400
H	−1.46375700	1.97459200	−2.43964200
H	−4.07133100	3.03604400	−1.09147200
H	−3.97570300	1.83295900	−2.39886800
H	−3.42889600	3.47468400	−2.70055900
H	−2.56903000	−3.48853500	−1.17569700
H	−1.78505100	−2.16655100	−2.07752900
H	−3.50746300	−2.48893300	−2.30795200
H	−5.56303700	−2.67535800	−1.18435800
H	−7.65494600	−1.78649400	−0.19714700
H	−7.60823700	0.10097100	1.40491000
H	−5.46389600	1.15247000	2.06574600
H	−1.32938600	1.06111800	2.13420400
H	−2.94534200	1.61512200	2.57310500
H	−1.52168900	3.34366800	1.30550500
H	−3.12875000	3.03261700	0.62874000
H	5.04685400	0.52637000	2.37453500
H	6.38263300	−0.50925700	1.80156600
H	4.83996000	−1.23477000	2.32571000
H	5.31088000	1.23072100	−1.70475600
H	6.65886300	0.94383800	−0.57336300
H	5.34018800	2.06355300	−0.13763800
H	4.82280000	−2.65241300	−0.29726000
H	6.35750300	−1.81855000	−0.65973000
H	4.99110600	−1.72811000	−1.80278000

IN10

Au	2.17351200	0.40721500	−0.02230000
S	−2.93913100	3.17437400	−0.39553700
P	4.44037500	−0.11089100	−0.19761700
O	−1.89682800	3.58075200	−1.37439300
O	−2.61030500	3.54032000	1.02533600
O	−3.32826700	1.72522800	−0.50297700
N	−2.02602600	−1.51116000	−1.46509900
N	−1.36258700	0.39342000	2.25087100
C	−4.42096600	4.11592400	−0.80821300
C	−0.34694700	0.83787600	−2.16909500
C	−0.48867100	0.33790500	−0.74682300
C	0.06645800	1.16515600	0.25043700
C	−0.35843800	1.34583000	1.71672700
C	−2.61384600	0.73142400	2.22979000
C	−3.77662900	−0.07939500	2.64950400
C	−1.15678400	−0.93020200	−0.52492600
C	−2.82929200	−0.81511900	−2.47655200
C	−2.30903800	−2.79484200	−1.05995600
C	−3.13948400	−3.76319000	−1.65159900
C	−3.23534900	−4.99583500	−1.02381100
C	−2.53478100	−5.27974700	0.17440600
C	−1.72626600	−4.32594600	0.76543700
C	−1.61051500	−3.05889800	0.15099800
C	−0.90559000	−1.87044600	0.48969300
C	−0.07443500	−1.67354500	1.71479300
C	−0.82584900	−0.87108600	2.79244000
C	4.89445200	−1.72629700	0.54211300
C	5.51771800	1.11987200	0.63269800
C	5.03808700	−0.18869500	−1.93022300
H	0.31121700	2.15216800	−0.15064400
H	−4.71638300	3.87872200	−1.83332000
H	−4.19708300	5.18206800	−0.72309600
H	−5.22271700	3.84601500	−0.11650600
H	0.51312700	1.50555600	−2.25815700
H	−0.23747200	0.02286500	−2.88771500
H	−1.22708600	1.43972500	−2.41840400
H	0.49832800	1.31983600	2.39358900
H	−0.81410100	2.33835100	1.77244200
H	−2.81355200	1.73866900	1.85642100
H	−3.57546300	−1.12519700	2.87903100
H	−4.51250400	−0.01681100	1.83808300
H	−4.24232800	0.40518100	3.51904500
H	−2.32924600	−0.79562500	−3.44906600
H	−3.04836900	0.19746600	−2.13356400
H	−3.77781600	−1.34484400	−2.58322200
H	−3.67057600	−3.57042400	−2.57779000
H	−3.85847900	−5.76749800	−1.46688000
H	−2.63802700	−6.26034100	0.62960700
H	−1.19220000	−4.54637300	1.68598500
H	0.87248400	−1.16760100	1.47413100
H	0.19139400	−2.63904300	2.15772300
H	−0.15611000	−0.60325100	3.61630900
H	−1.64792900	−1.45612700	3.19897200
H	4.65104900	−1.72849900	1.60935700
H	5.96707200	−1.91389700	0.42007200
H	4.33289900	−2.52901500	0.05389300
H	5.36504800	2.10783900	0.18693300
H	6.57116500	0.83724700	0.52772100
H	5.26702000	1.17620400	1.69669200
H	4.49019900	−0.96172600	−2.47814700
H	6.10843900	−0.42251800	−1.95173600

H	4.87152000	0.77363800	−2.42436100

IN11

Au	−2.10736500	0.01194800	−0.04695100
P	−4.37202300	−0.52880400	0.36701600
N	3.68680400	0.43438600	1.23851000
N	1.45340200	2.53218200	−0.86360900
C	0.61400900	−1.87848000	−0.43529400
C	0.89398300	−0.39274600	−0.50379600
C	−0.10571900	0.51120800	−0.39655500
C	0.06135500	2.00433200	−0.49034800
C	2.44424700	2.32988700	0.22904800
C	2.76484800	3.57276200	1.00436100
C	2.83485300	1.04271300	0.33790300
C	4.20205900	0.99572100	2.47379300
C	4.10656600	−0.80626200	0.72324200
C	5.09591200	−1.65297000	1.21808200
C	5.37395700	−2.82204000	0.49669200
C	4.69483700	−3.12038500	−0.68554400
C	3.69964100	−2.25500200	−1.16548200
C	3.39664900	−1.10409700	−0.45045000
C	2.39213400	0.01259900	−0.71684200
C	2.59779600	0.64911500	−2.11529600
C	1.90727500	2.01838000	−2.22459200
C	−4.71622500	−1.05978100	2.09443800
C	−5.02527400	−1.90239700	−0.66637200
C	−5.54932100	0.85484500	0.07694000
H	1.33703100	3.54403200	−0.97129500
H	−0.45787100	−2.05458700	−0.30604400
H	0.92794400	−2.39719800	−1.35046600
H	1.14327800	−2.36167700	0.39481300
H	−0.60478600	2.41862600	−1.25508200
H	−0.18127200	2.49309900	0.45974200
H	3.63072600	3.42716600	1.65091200
H	3.01387100	4.40016800	0.32388300
H	1.93158200	3.91245900	1.63671000
H	4.41823500	0.18024400	3.16883000
H	3.44478900	1.63286800	2.93468100
H	5.12202100	1.57534900	2.32045600
H	5.65556000	−1.41443100	2.11654400
H	6.14483200	−3.49530100	0.86122800
H	4.93760600	−4.02209000	−1.23971000
H	3.17718700	−2.48974800	−2.08842000
H	2.21002000	−0.01917000	−2.88940500
H	3.67090900	0.76776900	−2.29095800
H	1.01314600	1.98988100	−2.84920600
H	2.58610600	2.77493800	−2.62178200
H	−4.11149000	−1.93916200	2.33847300
H	−5.77589600	−1.30585500	2.22596400
H	−4.44751600	−0.25601100	2.78756000
H	−4.95338200	−1.63453200	−1.72553900
H	−6.07197400	−2.11532200	−0.42163000
H	−4.42900800	−2.80543100	−0.49990400
H	−5.28870900	1.70195500	0.71983900
H	−6.57901300	0.54762700	0.29172200
H	−5.48467600	1.18207900	−0.96591100

IN12

Au	−1.11326100	1.17625100	−0.10890800
S	4.45015900	1.16856400	−0.50237400
P	−3.23235000	2.13157200	−0.29658800
O	3.54583400	2.28888500	−0.90325400
O	4.55936800	1.01767600	0.99002800
O	4.13425700	−0.12615800	−1.18169300
N	−1.38340800	−2.40605100	1.00261900
N	1.61140800	−0.63527900	2.32890100
C	6.09983000	1.63635500	−1.06125000
C	0.99743500	−0.09967700	−2.02648300
C	0.82268500	−0.26762300	−0.53741000
C	1.12460900	0.79883700	0.28885000
C	1.52754900	0.75756600	1.74258600
C	0.28506300	−1.29734900	2.47191600
C	−0.23268500	−1.31482000	3.87946600
C	−0.19417800	−1.76338600	1.29846000
C	−2.49789300	−2.62911300	1.90558500
C	−1.28668800	−3.02647600	−0.25908400
C	−2.18380800	−3.91170000	−0.85335300
C	−1.84800900	−4.43355300	−2.10978400
C	−0.64852800	−4.09442700	−2.73825900
C	0.24363000	−3.20355300	−2.12292000
C	−0.08771000	−2.65986500	−0.88794800
C	0.67032100	−1.70466500	0.02402700
C	2.09963800	−2.21136100	0.38351500
C	2.66320800	−1.50794900	1.62906100
C	−4.53967100	1.27983700	0.66662200
C	−3.83648200	2.15638100	−2.02679700
C	−3.26772700	3.87642700	0.26557100
H	1.97593100	−0.49490200	3.27603300
H	1.51260800	1.69273100	−0.20359000
H	6.80195500	0.84037300	−0.80130000
H	6.39179500	2.56737900	−0.56929200
H	6.08028300	1.77729500	−2.14481300
H	1.94927500	−0.57066200	−2.30477800
H	1.08375400	0.95658400	−2.29064200
H	0.19186000	−0.55891600	−2.60295300
H	2.54372000	1.16974600	1.79440400
H	0.86409200	1.33568500	2.39060500
H	−1.08464500	−1.98461300	3.99227300
H	0.54507700	−1.67431700	4.56859500
H	−0.54073500	−0.31918700	4.23047700
H	−3.40089800	−2.79848200	1.31453500
H	−2.66445100	−1.74114200	2.51893000
H	−2.34124100	−3.49862900	2.55719000
H	−3.10032400	−4.21661800	−0.35955900
H	−2.52985400	−5.13019400	−2.58931000
H	−0.39806800	−4.52715800	−3.70182900
H	1.18181300	−2.95262500	−2.60791700
H	2.78166800	−2.03073000	−0.45103600
H	2.03745700	−3.28880800	0.55553700
H	3.49217700	−0.83682400	1.38935800
H	2.97688800	−2.23095500	2.38375300
H	−4.62906700	0.24169500	0.33199800
H	−5.50211900	1.78499600	0.52801300
H	−4.28319900	1.28549300	1.73065100
H	−3.14062300	2.72235700	−2.65390100
H	−4.82707600	2.62187400	−2.07813900
H	−3.89952200	1.13387600	−2.41204800
H	−2.98570200	3.93280100	1.32156200
H	−4.27235500	4.29486000	0.13860100
H	−2.55531900	4.46933100	−0.31643500

IN13

Au	2.80144300	−0.45362900	0.03215500
S	−1.20088300	4.18828700	−0.13586800

P	5.14933900	−0.52053300	−0.19926600
O	−1.36455200	3.66594000	1.29123300
O	0.21098300	4.12989700	−0.58877100
O	−2.17454900	3.52513900	−1.04905100
O	−4.04219600	1.34134500	0.93778800
O	−3.88978400	1.00414000	−1.28815200
N	−2.45737500	−1.60388200	−1.17009500
N	−1.20984100	1.07534100	1.16621300
C	−1.65790700	5.92145100	−0.01385500
C	0.22442000	−2.55547300	−0.84080900
C	−0.14639200	−1.21999100	−0.24073000
C	0.72908700	−0.31803000	0.23878000
C	0.28970100	0.94596900	0.92258400
C	−1.93356600	0.59507600	−0.05093900
C	−3.40841100	1.03071300	−0.04762900
C	−5.22979600	1.52318800	−1.45595600
C	−1.68713100	−0.94704500	−0.11442500
C	−2.31480000	−1.32515100	−2.59657100
C	−3.26489800	−2.52714400	−0.63352700
C	−4.16085900	−3.41120600	−1.28247900
C	−4.88876600	−4.26247500	−0.48317400
C	−4.77403300	−4.28610100	0.94841400
C	−3.91355000	−3.44587600	1.59756500
C	−3.12920600	−2.53950100	0.81434600
C	−2.20377200	−1.57695600	1.14306600
C	−1.70277600	−1.07125600	2.44727500
C	−1.68746700	0.47386900	2.45967900
C	5.74732500	−0.16562100	−1.90106700
C	5.91577200	−2.13567200	0.22909900
C	6.03018200	0.70017300	0.85537300
H	−1.36697300	2.16715700	1.24401300
H	−1.56416700	6.37530200	−1.00351600
H	−0.98305700	6.41507100	0.68901800
H	−2.68934500	5.99452000	0.33755900
H	1.29744100	−2.72431200	−0.71715000
H	−0.30379900	−3.38303200	−0.34881000
H	−0.00149500	−2.61856000	−1.91240200
H	0.76078400	1.05087600	1.90378500
H	0.56847000	1.83053600	0.33761600
H	−1.46466100	1.07740000	−0.91012800
H	−5.44646900	1.42230200	−2.51921500
H	−5.25354700	2.57352800	−1.15921700
H	−5.94185800	0.94713500	−0.86036100
H	−2.08669900	−2.24710200	−3.13891100
H	−1.49593700	−0.61930800	−2.73838800
H	−3.23261300	−0.88190000	−2.99013900
H	−4.27183600	−3.41274400	−2.36074800
H	−5.58739100	−4.95018300	−0.95144900
H	−5.38588700	−4.98622500	1.50748200
H	−3.81623900	−3.45435600	2.67825100
H	−0.68516400	−1.45026300	2.60491000
H	−2.31740100	−1.42868800	3.27792200
H	−1.02540900	0.84791900	3.24209100
H	−2.69016200	0.86230600	2.62244400
H	5.34693300	−0.90798300	−2.59914100
H	6.84207600	−0.18896000	−1.94112100
H	5.39900200	0.82380900	−2.21484800
H	5.68709100	−2.38919000	1.26943100
H	7.00335100	−2.10035300	0.10029200
H	5.50569400	−2.92094500	−0.41428700
H	5.69197300	1.71182400	0.60899100
H	7.11334500	0.63820100	0.70163100
H	5.80635900	0.50877300	1.90974300

IN14

Au	2.60428100	−0.43001200	0.09041900
S	−0.93750200	4.11597500	−0.11804100
P	4.89331300	−0.22632300	−0.44311800
O	−1.19793500	3.65900900	1.31010100
O	0.47673700	3.92095700	−0.52433600
O	−1.93078500	3.50958800	−1.05800100
O	−3.98409700	1.98671800	1.06455300
O	−4.19321700	1.37931300	−1.09978300
N	−2.86973400	−1.44273500	−1.11618700
N	−1.40518300	1.03640800	1.22621400
C	−1.25070400	5.88500600	−0.08092700
C	0.33347300	−2.92522800	−0.13606400
C	−0.19299100	−1.63466700	0.44941200
C	0.56542400	−0.52236500	0.56435100
C	0.09023800	0.82198700	1.02253300
C	−2.18469900	0.72980600	−0.01708600
C	−3.56867900	1.44921900	0.06749600
C	−5.42546000	2.14001400	−1.20297800
C	−2.28603100	−0.75693000	−0.15494200
C	−3.25307000	−0.99630500	−2.46073100
C	−3.01287900	−2.80992700	−0.71117000
C	−3.66755800	−3.83535200	−1.38080000
C	−3.72150700	−5.07189300	−0.72795100
C	−3.13865600	−5.25056800	0.53223900
C	−2.46596300	−4.20269600	1.17449400
C	−2.40342500	−2.96925900	0.53742300
C	−1.73669200	−1.66431100	0.90220600
C	−1.91497800	−1.17559200	2.35463600
C	−1.93110200	0.36207700	2.46284300
C	6.02396900	−0.41371000	0.99449800
C	5.33778900	1.40214900	−1.16797400
C	5.50437600	−1.45379500	−1.66802600
H	−1.46468800	2.11687200	1.35287100
H	−1.08493000	6.28831800	−1.08276500
H	−0.56188700	6.34947600	0.62831500
H	−2.28392600	6.05617000	0.22911700
H	1.39745400	−2.81626500	−0.36113800
H	0.21087500	−3.76887900	0.55309400
H	−0.17757600	−3.19699300	−1.06833600
H	0.54735000	1.09757500	1.97857600
H	0.39001200	1.59579800	0.30781800
H	−1.67080800	1.21313900	−0.85656500
H	−5.78595800	1.96336600	−2.21570600
H	−5.20941500	3.19867300	−1.04905300
H	−6.15006100	1.78784400	−0.46579300
H	−2.81739500	−1.69532500	−3.17870800
H	−2.87161100	0.00468500	−2.64331900
H	−4.34086500	−1.00020000	−2.55614800
H	−4.13176000	−3.69216900	−2.35060400
H	−4.23354300	−5.90112800	−1.20604700
H	−3.20761500	−6.21809000	1.02000800
H	−2.00560000	−4.35645300	2.14578100
H	−1.10724400	−1.59760500	2.95673500
H	−2.85818200	−1.55999700	2.75395500
H	−1.30776700	0.71760100	3.28467000
H	−2.93899000	0.74345200	2.61020400
H	5.80179900	0.35707000	1.73947000
H	7.06999800	−0.31974800	0.68173700
H	5.87652100	−1.39388100	1.45951300

H	4.77177500	1.56074500	−2.09156200
H	6.40971900	1.45050500	−1.38963300
H	5.07979200	2.20298200	−0.46758400
H	5.36894900	−2.46752600	−1.27710000
H	6.56680700	−1.29272700	−1.88249000
H	4.93446500	−1.36343400	−2.59831800

IN15

Au	−2.68149600	0.03470500	−0.01674200
P	−5.03204000	−0.18557200	0.07458400
O	4.12229300	2.64236300	0.23795700
O	3.87300200	1.23536300	1.99913000
N	2.58636500	−1.61507400	0.50424700
N	1.20372000	2.10406500	−0.16608800
C	−0.28802200	−2.24341900	−0.06904500
C	0.25391100	−0.81642400	−0.06688300
C	−0.59500000	0.24551900	−0.08936400
C	−0.23996600	1.72769100	−0.08715900
C	1.96411500	1.70079800	0.81606900
C	3.43980300	1.92183700	0.93764600
C	5.27846000	1.37430400	2.31614800
C	1.74073800	−0.76111500	−0.18905100
C	2.29863200	−2.31638600	1.74905600
C	3.85745100	−1.54509700	−0.04804600
C	5.02986200	−2.21617600	0.31894000
C	6.17929600	−1.94990700	−0.42081500
C	6.16911600	−1.03575100	−1.49573000
C	5.00584700	−0.36554900	−1.85237100
C	3.82777500	−0.62127600	−1.12601300
C	2.48529600	−0.12664100	−1.20784000
C	1.91900400	0.86421400	−2.15554100
C	1.75414500	2.29450100	−1.49929900
C	−5.67677600	−1.69230300	−0.75888200
C	−5.96507200	1.19390100	−0.70334800
C	−5.71217500	−0.28220700	1.78032200
H	−1.35245900	−2.24103200	−0.32047500
H	0.23619400	−2.86167600	−0.80909500
H	−0.18422400	−2.74364300	0.90072300
H	−0.72980600	2.23361300	−0.92155400
H	−0.62452900	2.18504400	0.83071200
H	1.46461300	1.33949500	1.70895100
H	5.44986800	0.70636100	3.15950500
H	5.89461200	1.08607700	1.46251800
H	5.49484400	2.40862500	2.59533000
H	2.12991100	−3.38514300	1.57982000
H	1.41670100	−1.88238500	2.22079400
H	3.14365800	−2.19554300	2.43252700
H	5.04634600	−2.93063000	1.13605000
H	7.10207100	−2.46538100	−0.17004500
H	7.08572700	−0.85703700	−2.05030900
H	5.00439000	0.33833700	−2.68006400
H	0.93100700	0.54410800	−2.50307800
H	2.56190000	0.99563800	−3.03078500
H	1.06516200	2.90532400	−2.08343200
H	2.71903100	2.78740900	−1.41945200
H	−5.39116700	−1.68016000	−1.81573200
H	−6.76880700	−1.74275600	−0.68443200
H	−5.24573200	−2.58634600	−0.29668700
H	−5.71792000	2.13636400	−0.20398800
H	−7.04509300	1.02333200	−0.63147700
H	−5.68716800	1.28082400	−1.75869500
H	−5.27254200	−1.13592900	2.30618100
H	−6.80171200	−0.39726800	1.76118800
H	−5.45766400	0.62846500	2.33229500

IN16

Au	−2.49232800	0.01646000	−0.10307900
S	1.53489000	3.86130100	0.59462400
P	−4.70561000	−0.71147200	−0.11186000
O	0.04606700	3.95469000	0.60290300
O	2.08869300	2.95375300	1.64413900
O	2.08488500	3.55356900	−0.77618600
O	3.89525300	−0.54136400	−3.13699800
O	4.60055600	0.33426000	−1.16428800
N	1.87632800	−1.12073600	1.87917900
N	1.25821800	0.34876300	−1.98825400
C	2.13990800	5.51299700	0.98274100
C	−0.29120600	0.87571100	2.26786700
C	0.09175100	0.34564300	0.90329900
C	−0.47665900	1.01086600	−0.19938000
C	0.08308200	1.18143100	−1.61934300
C	2.43787200	0.82059700	−1.77761600
C	3.71592600	0.09707500	−2.12179300
C	5.91093600	−0.26809700	−1.33363400
C	1.00407000	−0.77930600	0.83383400
C	2.43893600	−0.21699000	2.88894000
C	2.42571100	−2.35121400	1.60161800
C	3.37038200	−3.09789000	2.32694800
C	3.74881000	−4.32745500	1.80944100
C	3.21827400	−4.82005100	0.59155100
C	2.29848400	−4.08222800	−0.13141100
C	1.89459300	−2.82414200	0.36879100
C	1.01746500	−1.81469100	−0.11871200
C	0.26719300	−1.85077600	−1.40923900
C	0.95940100	−1.00565300	−2.50297200
C	−5.88767100	0.67638200	0.09001500
C	−5.10606900	−1.88869800	1.23689800
C	−5.20827500	−1.55715400	−1.66003200
H	−0.88412200	1.98279200	0.10040500
H	3.23258800	5.50516100	0.97849300
H	1.77279300	5.79805200	1.97193600
H	1.76752800	6.21375300	0.23163000
H	−1.25281900	1.39130400	2.22533900
H	−0.34254400	0.08456000	3.01972500
H	0.45318500	1.62397700	2.56524500
H	−0.67465300	0.99930700	−2.38324100
H	0.41274800	2.22210300	−1.68923000
H	2.50461100	1.83151300	−1.33702100
H	6.47629600	0.03173800	−0.45261800
H	5.81789000	−1.35522800	−1.38460900
H	6.37878400	0.11286300	−2.24393700
H	1.87921700	−0.26185900	3.82776600
H	2.45128500	0.80674500	2.51099800
H	3.47047700	−0.51776500	3.08254300
H	3.77505800	−2.74335400	3.26900600
H	4.46566100	−4.93311600	2.35653000
H	3.54256900	−5.79002600	0.22637100
H	1.89692600	−4.46117900	−1.06740700
H	−0.76772700	−1.50397700	−1.27452700
H	0.21188300	−2.87400500	−1.79459700
H	0.30872000	−0.87743700	−3.37240900
H	1.89067800	−1.46406800	−2.82351800
H	−5.69963400	1.19000900	1.03819900
H	−6.91862900	0.30511400	0.08145100

H	−5.75903500	1.39564000	−0.72486400
H	−4.49113400	−2.78896800	1.14064000
H	−6.16422200	−2.17046700	1.19443100
H	−4.89705400	−1.42613300	2.20653400
H	−5.06121600	−0.88877400	−2.51412100
H	−6.26326600	−1.84859000	−1.60949100
H	−4.59600100	−2.45236000	−1.80838800

IN17

Au	2.41225800	−0.03502400	−0.02583000
P	4.71922100	0.04014700	0.48520600
O	−2.71241400	−3.90386100	−0.50610000
O	−4.10013100	−2.80889200	0.90592300
N	−3.42144100	0.32047400	1.00202100
N	−1.44152600	−1.77871800	−1.33788400
C	0.02281600	2.30045400	−0.11513200
C	−0.46612000	0.91482600	−0.48071000
C	0.37726900	−0.14137400	−0.50139500
C	−0.00906300	−1.54847000	−0.86375500
C	−2.44002800	−1.59080700	−0.26512200
C	−3.07859300	−2.86415300	0.04514100
C	−4.76465500	−4.06274000	1.17902400
C	−2.65280400	−0.27238500	0.05669100
C	−3.97574600	−0.25732400	2.22098900
C	−3.59593600	1.69182000	0.68388100
C	−4.43799200	2.60753600	1.30457400
C	−4.48981600	3.90045500	0.76626400
C	−3.73214800	4.24494400	−0.35494800
C	−2.88179800	3.30513900	−0.95640100
C	−2.80815400	2.02462000	−0.42338200
C	−1.99618700	0.80305400	−0.82851300
C	−2.21211600	0.41989800	−2.31440800
C	−1.76178000	−1.02276100	−2.61165100
C	5.12009300	−0.15174000	2.27022500
C	5.54526500	1.61113600	0.00376000
C	5.71140500	−1.26743800	−0.34492500
H	−1.51524700	−2.79114500	−1.54036300
H	1.09754600	2.27543000	0.08611200
H	−0.14836300	3.02350600	−0.92273300
H	−0.48108500	2.69706900	0.77470300
H	0.61665800	−1.92337200	−1.68071700
H	0.11976500	−2.22689800	−0.01347900
H	−4.06542500	−4.78011700	1.61530500
H	−5.55365700	−3.81847400	1.89038800
H	−5.19209600	−4.47585800	0.26246700
H	−3.86676700	0.47658200	3.02439900
H	−3.42113700	−1.15445000	2.48475800
H	−5.03419300	−0.50804200	2.10339600
H	−5.05135200	2.33579500	2.15700200
H	−5.14345700	4.63749700	1.22358300
H	−3.80172500	5.24684000	−0.76763400
H	−2.29456100	3.58218900	−1.82679700
H	−1.66228100	1.11824500	−2.95105500
H	−3.27469900	0.52580100	−2.55225600
H	−0.86159300	−1.06287000	−3.22671900
H	−2.55010100	−1.58957000	−3.10998100
H	4.63653800	0.64529900	2.84431600
H	6.20230900	−0.10685800	2.43642000
H	4.74276900	−1.11319600	2.63355000
H	5.43338000	1.77227200	−1.07342200
H	6.61224300	1.58742900	0.25249500
H	5.07478600	2.45014000	0.52679500
H	5.35350000	−2.25511600	−0.03612500
H	6.77317000	−1.17671200	−0.09010700
H	5.59600200	−1.18516200	−1.43060400

IN18

Au	−0.96830900	−1.44175000	−0.15727400
S	4.57387100	−1.11964100	−0.15203500
P	−2.97052300	−2.61930200	−0.35086000
O	3.73852600	−2.35978600	−0.16254900
O	4.47279000	−0.34103700	−1.43374300
O	4.35250200	−0.26134800	1.05339500
O	0.11889700	2.88552800	−3.54908200
O	−1.62153400	3.53553000	−2.26119000
N	−1.47944100	2.20607600	0.64581700
N	1.34407800	1.52665700	−1.68423400
C	6.28571100	−1.67931900	−0.05868500
C	1.32437400	−1.00425300	1.94568800
C	0.96126600	−0.18215300	0.73335600
C	1.18800400	−0.71594100	−0.52066200
C	1.38880000	0.02529600	−1.81687400
C	0.00626200	2.06549100	−1.35646800
C	−0.50038500	2.84591600	−2.48686100
C	−2.08448600	4.36577600	−3.35168600
C	−0.34977500	1.89681900	−0.04062400
C	−2.80295700	2.53340500	0.12776800
C	−1.22947700	2.15209200	2.04163400
C	−2.07618700	2.54798200	3.07183700
C	−1.58080000	2.46092100	4.37973400
C	−0.28375400	2.00905700	4.63118300
C	0.55037400	1.61158900	3.57589300
C	0.06320200	1.67383000	2.27605600
C	0.70363500	1.33694600	0.93933600
C	2.04891100	2.08414600	0.69487500
C	2.45567900	2.07610000	−0.79015200
C	−4.37049200	−1.64382900	−1.02094400
C	−3.56153500	−3.30602700	1.24265600
C	−2.79105000	−4.05938500	−1.47057500
H	1.66118900	−1.69987800	−0.53884400
H	1.51197700	1.89035200	−2.63858000
H	6.94613900	−0.80879900	−0.04997600
H	6.50332700	−2.30507400	−0.92762500
H	6.41859300	−2.25714000	0.85930700
H	2.27920900	−0.62422000	2.33219500
H	1.49777400	−2.04545800	1.66619200
H	0.57247500	−0.95241800	2.73594700
H	2.40286200	−0.21915500	−2.15643900
H	0.66701800	−0.24957600	−2.58994200
H	−3.00470300	4.82470000	−2.99014900
H	−1.34286600	5.13287600	−3.58569500
H	−2.28125800	3.75927600	−4.23861200
H	−2.97183500	3.61398300	0.10674300
H	−3.54633400	2.06898100	0.78164300
H	−2.91386300	2.13496900	−0.87753700
H	−3.07103700	2.93605900	2.88148300
H	−2.21435900	2.76975900	5.20595600
H	0.08772100	1.97118700	5.65051300
H	1.56019700	1.27034900	3.77929700
H	2.84232800	1.60460100	1.27429100
H	1.92959900	3.11132600	1.05016900
H	3.32926100	1.44461600	−0.97383600
H	2.64283600	3.08711300	−1.15531300
H	−4.58231900	−0.79711200	−0.36065900

H	−5.26582500	−2.27039300	−1.09998300
H	−4.11329600	−1.25916500	−2.01275500
H	−2.79769800	−3.96470700	1.66749500
H	−4.48345400	−3.87793200	1.08816900
H	−3.75533200	−2.49435100	1.95084700
H	−2.49720000	−3.72200900	−2.46946100
H	−3.73737000	−4.60735500	−1.54086400
H	−2.01529000	−4.73039400	−1.08849900

IN19

Au	−2.21214400	−0.17377000	0.02021700
P	−4.51761100	−0.46485800	0.13654800
N	3.75390200	0.09615200	1.26494700
N	1.55500100	2.57665500	−0.52891400
C	0.02372600	−0.58040300	0.04439200
C	0.00105200	0.63065200	−0.15043000
C	0.12972100	2.07704300	−0.36394700
C	2.49469300	2.21262900	0.63516500
C	3.47647300	3.36670600	0.86879700
C	3.13696100	0.89508500	0.31330100
C	3.95647400	0.39320200	2.67596400
C	4.23269200	−1.03369800	0.62294600
C	4.94620900	−2.12397800	1.13973800
C	5.29239600	−3.14249800	0.25683200
C	4.94476800	−3.08100400	−1.11032700
C	4.24488300	−1.99495400	−1.62355200
C	3.88369300	−0.94763400	−0.75524000
C	3.19039600	0.29837900	−0.92548100
C	2.53214600	0.87282200	−2.14282200
C	2.16342300	2.33373100	−1.90929600
C	−5.27879000	−0.89089300	−1.47303600
C	−4.97812000	−1.81583900	1.28327500
C	−5.39980800	1.02519700	0.73111000
H	1.44056000	3.59609000	−0.47027400
H	0.26661600	−1.61618900	0.19989400
H	−0.41440900	2.38468000	−1.26033600
H	−0.28425800	2.61430700	0.49357400
H	1.83852200	2.12892600	1.50722500
H	4.13871200	3.51820500	0.01169700
H	2.93719700	4.29657800	1.08358700
H	4.09817500	3.13153800	1.73718700
H	4.95401800	0.80927900	2.85946600
H	3.84402800	−0.52470100	3.25839300
H	3.20521500	1.10596200	3.02019600
H	5.22237200	−2.17612100	2.18848300
H	5.84498200	−4.00128100	0.62813900
H	5.23371700	−3.89523900	−1.76935100
H	3.98647400	−1.95265500	−2.67859500
H	1.64391300	0.29293200	−2.42652700
H	3.20026000	0.85034200	−3.01247200
H	1.43314300	2.70476000	−2.63002200
H	3.04633900	2.97326600	−1.94362600
H	−5.10812000	−0.08062500	−2.18846900
H	−6.35631400	−1.04218700	−1.34451100
H	−4.82825000	−1.80883400	−1.86280900
H	−4.51864900	−2.75267900	0.95363600
H	−6.06737700	−1.93260400	1.29954100
H	−4.62242100	−1.58124700	2.29114500
H	−5.04293700	1.29306400	1.73037500
H	−6.47645100	0.82622800	0.77111900
H	−5.21172000	1.86196600	0.05142300

IN20

Au	2.34249600	−0.94226200	−0.09763800
S	−0.95806300	4.63906900	−0.22690700
P	4.67852400	−0.63880700	0.11647700
O	−1.89058400	4.13846000	0.86392500
O	0.14821900	5.47122900	0.30041800
O	−0.52800800	3.51364000	−1.11203100
N	−2.60174300	−1.35814700	−1.25906500
N	−1.86584600	1.46721400	1.00835000
C	−1.98748600	5.71448400	−1.23957700
C	0.31336300	−1.22867500	−0.32293300
C	−0.64647100	−0.39524600	0.08862200
C	−0.46629500	0.91665000	0.84145500
C	−2.59321300	0.97892500	−0.22679400
C	−4.07053500	1.32668900	−0.28442500
C	−2.18027100	−0.52183600	−0.15526700
C	−2.26510200	−1.08980900	−2.65237300
C	−3.34892300	−2.37071500	−0.79598300
C	−3.97224200	−3.42308200	−1.50981700
C	−4.69083400	−4.33857700	−0.77555500
C	−4.83379000	−4.26592200	0.65179500
C	−4.24616300	−3.25784000	1.36363300
C	−3.48628100	−2.27726600	0.64946800
C	−2.80759900	−1.15084900	1.04857300
C	−2.61533900	−0.51473500	2.38300000
C	−2.52768900	1.02558600	2.28356600
C	5.38060900	−1.21922700	1.71396000
C	5.21799300	1.11359300	−0.01088900
C	5.67104300	−1.51188800	−1.16081500
H	−1.84241800	2.53844700	0.98613000
H	−1.37956800	6.11587900	−2.05438700
H	−2.36758800	6.53210600	−0.62216800
H	−2.81947800	5.13374900	−1.64518200
H	−0.02489800	−2.12528800	−0.84974800
H	−0.00573200	0.80862100	1.82491400
H	0.08842600	1.65206700	0.25408200
H	−2.07056300	1.44978700	−1.06365900
H	−4.67234000	0.82615500	0.47777600
H	−4.19554000	2.40956200	−0.18188200
H	−4.45886300	1.03690100	−1.26589500
H	−1.32562100	−0.53597500	−2.68686300
H	−3.05260500	−0.50097600	−3.13487700
H	−2.13773100	−2.03315300	−3.18740300
H	−3.88912500	−3.50175500	−2.58753900
H	−5.17932700	−5.15703500	−1.29681100
H	−5.41998600	−5.02752000	1.15534500
H	−4.34486100	−3.18552000	2.44191500
H	−1.68170400	−0.90251500	2.81337600
H	−3.41688300	−0.79474900	3.07180400
H	−1.93865800	1.43499100	3.10510600
H	−3.51636100	1.48494900	2.30464400
H	4.90779600	−0.68023900	2.54145400
H	6.46260400	−1.04926900	1.74501300
H	5.17995000	−2.28863000	1.83604600
H	4.90753500	1.52433300	−0.97710200
H	6.30712600	1.19170200	0.08032700
H	4.74663900	1.70204900	0.78306100
H	5.48564300	−2.58931300	−1.10003800
H	6.74002800	−1.32059700	−1.01573700
H	5.37548100	−1.16470400	−2.15628700

IN20'

Au	−2.16155100	−0.31499600	0.02421800
P	−4.51731700	−0.23048000	−0.20391500
N	2.83196200	−0.67785600	1.11343600
N	1.77266900	2.77464300	0.30621900
C	−0.11338800	−0.43680400	0.21326100
C	0.75520400	0.57874200	0.27696100
C	0.46614900	2.09269500	0.20917000
C	2.55419400	1.91636200	1.17516200
C	4.00275400	2.30456400	1.42568800
C	2.28787100	0.47958900	0.44690000
C	2.44248000	−1.11960200	2.44565600
C	3.81259300	−1.21340800	0.36207600
C	4.65394600	−2.31525800	0.64334300
C	5.58199100	−2.66064300	−0.31597300
C	5.72445200	−1.94949200	−1.54981800
C	4.92652100	−0.87099100	−1.83543300
C	3.94856400	−0.47621500	−0.87518100
C	3.01715900	0.54971600	−0.84140400
C	2.70274600	1.65123600	−1.77790000
C	2.41060300	2.98996100	−0.99171800
C	−5.44452900	−1.03261100	1.16565500
C	−5.15864600	−1.05267200	−1.71842800
C	−5.21643900	1.46814100	−0.28081600
H	0.32261500	−1.43901000	0.27128100
H	−0.04764000	2.38446500	−0.71064100
H	−0.16360200	2.39294500	1.05519300
H	2.03717700	1.83787100	2.13768600
H	4.62333300	2.30961000	0.52620800
H	4.45106200	1.60600200	2.13962300
H	4.03410600	3.30422400	1.87333500
H	3.17793800	−0.80530900	3.19472800
H	2.35463600	−2.20936700	2.46330700
H	1.47169100	−0.68613000	2.68803400
H	4.56941400	−2.86598100	1.57348800
H	6.23628000	−3.50820000	−0.13110200
H	6.47852200	−2.27773600	−2.25815000
H	5.02597900	−0.32167600	−2.76651200
H	1.78300500	1.38837900	−2.31846600
H	3.49069400	1.79180900	−2.52389600
H	1.75882700	3.61913000	−1.60163200
H	3.34570900	3.53278300	−0.83740800
H	−5.15900700	−2.08723900	1.23580500
H	−6.52459400	−0.96349600	0.99412000
H	−5.19832500	−0.54291400	2.11347000
H	−4.73342600	−0.57439600	−2.60678000
H	−6.25152300	−0.98625200	−1.76220800
H	−4.86262600	−2.10676100	−1.71667400
H	−4.96755700	2.01044300	0.63729100
H	−6.30563400	1.43463700	−0.39571200
H	−4.78252800	2.00669300	−1.12963000

IN21

Au	−2.20560800	−0.96828800	−0.04595300
S	0.72426700	4.46623800	0.21139400
P	−4.47621400	−0.37070200	0.25845700
O	1.55936300	4.09653300	−1.00387000
O	−0.64886300	4.89616000	−0.14278700
O	0.78877800	3.38941500	1.24807900
N	3.50610300	−1.05210200	1.13681000
N	1.95159500	1.44490200	−1.04305800
C	1.56019900	5.89962600	0.90848000
C	−0.23436800	−1.51158800	−0.29958400
C	0.77456100	−0.69040000	−0.62867400
C	0.60100400	0.80945900	−0.82024200
C	2.84992300	1.19657000	0.15405600
C	4.19686800	1.92204600	0.01562900
C	2.94178800	−0.29289100	0.23858400
C	4.15431000	−0.63845000	2.38674500
C	3.37576000	−2.43064600	0.75499300
C	3.88316000	−3.54616600	1.40636700
C	3.63385200	−4.78569600	0.80564300
C	2.90993900	−4.87878800	−0.38919100
C	2.40498900	−3.73489000	−1.02283200
C	2.64562500	−2.49745600	−0.43788800
C	2.26561200	−1.09851500	−0.83214400
C	2.74398700	−0.60280000	−2.22716900
C	2.53333400	0.92657700	−2.33346200
C	−4.73836600	1.05836600	1.38525200
C	−5.52465400	−1.70624700	0.96425200
C	−5.34002300	0.11188100	−1.29111700
H	1.80395100	2.50320100	−1.09855800
H	1.01774400	6.22094600	1.80137200
H	1.56511600	6.70259200	0.16732700
H	2.58471600	5.62576100	1.17144000
H	0.02749300	−2.56374000	−0.17027800
H	−0.00270100	1.05478300	−1.69787400
H	0.16549000	1.29825300	0.05361900
H	2.30350800	1.61376600	1.00897800
H	4.84017200	1.46845200	−0.74210800
H	4.72086800	1.89836800	0.97404100
H	4.00670200	2.96710000	−0.24489100
H	5.23529600	−0.76539600	2.28959700
H	3.77885300	−1.27193100	3.19249300
H	3.91260800	0.40137700	2.59938000
H	4.45000800	−3.47011200	2.32786700
H	4.01501100	−5.68723800	1.27528400
H	2.73651100	−5.85416900	−0.83384500
H	1.84468200	−3.81676700	−1.94896000
H	2.16844600	−1.12847400	−2.99259300
H	3.79964900	−0.85307600	−2.36154500
H	1.81790700	1.19381700	−3.11199600
H	3.46347800	1.46158300	−2.52210200
H	−4.32829100	0.82767800	2.37387100
H	−5.80621100	1.28400300	1.48217200
H	−4.21869500	1.93780000	0.99105500
H	−5.51091100	−2.57610000	0.29949200
H	−6.55792900	−1.36277800	1.08678200
H	−5.12854300	−2.00887900	1.93917700
H	−4.83561600	0.97375000	−1.74015700
H	−6.38461200	0.37221900	−1.08676000
H	−5.30982000	−0.71772300	−2.00501200

IN22

Au	−2.31490800	−0.72505900	−0.06559500
S	0.72291100	4.47883000	0.30914500
P	−4.61434600	−1.21593200	0.13632000
O	1.43593700	4.03617600	−0.95824300
O	−0.72226000	4.11708900	0.28970300
O	1.44559700	4.04254900	1.53483800
N	2.93853800	−1.17825800	1.33211700
N	1.51615000	1.34678300	−1.07959200
C	0.80980800	6.27562100	0.25145800
C	0.67979800	−1.00832600	0.31342500

C	−0.29411100	−0.26821400	−0.23750200
C	0.02708400	1.00248000	−0.97310200
C	2.25482700	0.96473100	0.18475500
C	3.66171600	1.55238600	0.23740300
C	2.16610500	−0.58643400	0.24193900
C	2.65698100	−0.95728900	2.74715100
C	3.79767000	−2.07770900	0.83939000
C	4.68931800	−2.93209600	1.53397200
C	5.48680700	−3.75492000	0.77274400
C	5.44559300	−3.78123400	−0.66344500
C	4.58666300	−2.97422300	−1.35580400
C	3.73014000	−2.10048900	−0.61271700
C	2.77765000	−1.18374400	−0.98850200
C	2.32583900	−0.70236300	−2.32145400
C	2.17930100	0.83322400	−2.32627500
C	−5.21321500	−1.33086300	1.86995100
C	−5.11809500	−2.81021600	−0.62463500
C	−5.71240800	0.03305600	−0.64545300
H	1.53904700	2.41506600	−1.11069900
H	0.30995600	6.67767200	1.13641800
H	0.30786400	6.62728700	−0.65305700
H	1.85870200	6.58131200	0.24335000
H	0.50438200	−1.95387100	0.81847700
H	−0.35058700	0.97463900	−1.99902900
H	−0.43483000	1.86559100	−0.48152600
H	1.66496100	1.38928600	1.00041300
H	4.35609100	1.08297700	−0.46445400
H	4.05972900	1.42433300	1.24824100
H	3.61603100	2.62542900	0.03161900
H	2.12650600	−1.81460000	3.17506800
H	2.03827400	−0.06609900	2.85422300
H	3.59425600	−0.80442900	3.28846300
H	4.73987000	−2.93417900	2.61674700
H	6.18363500	−4.41949600	1.27589200
H	6.11000000	−4.45862900	−1.18985500
H	4.53948100	−2.98534300	−2.43990600
H	1.35529000	−1.15932800	−2.55365900
H	3.02222500	−1.00122200	−3.10914200
H	1.57288500	1.16169100	−3.17144500
H	3.15462500	1.31696100	−2.39276600
H	−4.67062600	−2.12330300	2.39561300
H	−6.28589800	−1.55344500	1.89104400
H	−5.03265000	−0.38258600	2.38655000
H	−4.89145600	−2.79505600	−1.69570500
H	−6.19143200	−2.98165700	−0.48606700
H	−4.56042100	−3.63124000	−0.16259500
H	−5.54908300	1.00972000	−0.17827700
H	−6.76432900	−0.25075800	−0.52911400
H	−5.47797600	0.11420200	−1.71178800

IN22'

Au	−2.21554400	0.02184500	0.01830600
P	−4.47395100	−0.64041500	−0.21471500
N	3.06874200	−0.83136100	1.10579500
N	1.47927900	2.48736500	0.35465200
C	0.77525300	−0.25896800	0.30075200
C	−0.23603200	0.62028300	0.20397900
C	0.05252200	2.11535900	0.28372500
C	2.22464100	1.60709500	1.21617900
C	3.60503200	2.11712000	1.62383100
C	2.24725100	0.16791100	0.44510900
C	2.75158400	−1.43611400	2.39194400
C	4.11718300	−1.15473000	0.32700500
C	5.16448700	−2.07377500	0.57258700
C	6.12530400	−2.21279400	−0.40729200
C	6.09776000	−1.46922900	−1.62878200
C	5.09056200	−0.57180600	−1.88282700
C	4.06992900	−0.39885300	−0.90298800
C	2.93441500	0.39931000	−0.85010700
C	2.42596300	1.44862500	−1.75102600
C	2.12901600	2.75925400	−0.91323800
C	−5.16454800	−1.54859100	1.22718500
C	−4.79739800	−1.75064200	−1.64451700
C	−5.63708400	0.76164200	−0.46429800
H	0.63074500	−1.33478600	0.23818900
H	−0.38906300	2.63767600	−0.57088600
H	−0.44653400	2.51456000	1.17816300
H	1.63110300	1.43325700	2.11833000
H	4.31548000	2.16728700	0.79427800
H	4.03117400	1.46875500	2.39514000
H	3.50084900	3.12161700	2.04833800
H	3.62306300	−1.40083900	3.05259300
H	2.44014900	−2.47921700	2.26655100
H	1.93621300	−0.87894400	2.85490800
H	5.20507200	−2.64916700	1.49095200
H	6.93745800	−2.91729800	−0.25007900
H	6.88738400	−1.62753300	−2.35643300
H	5.05606300	−0.00568900	−2.80860600
H	1.47137400	1.12863300	−2.18696800
H	3.12105000	1.66311300	−2.56776800
H	1.49353900	3.41826200	−1.50902000
H	3.07430800	3.27705000	−0.73319200
H	−4.58948600	−2.46521600	1.39397200
H	−6.21427500	−1.80924900	1.05186500
H	−5.09330400	−0.92548500	2.12458300
H	−4.48979900	−1.25597900	−2.57151300
H	−5.86242300	−2.00106400	−1.70536100
H	−4.21740900	−2.67261300	−1.53358300
H	−5.58288700	1.44424400	0.38989900
H	−6.66516100	0.39684100	−0.56829900
H	−5.35863900	1.31367200	−1.36796800

IN23

Au	−2.28914300	−0.45719400	−0.09625200
S	1.31609500	4.53732400	0.20653500
P	−4.60799900	−0.55982400	0.33700100
O	1.90701800	3.93036800	−1.05615300
O	−0.00645500	5.16628300	−0.02136400
O	1.35285400	3.55437800	1.33210300
N	3.30003800	−1.36986200	1.15916200
N	1.74942100	1.24304500	−0.93978700
C	2.45390400	5.86319500	0.64047700
C	0.53208800	−1.43095700	−0.56091100
C	−0.24416200	−0.33653700	−0.46504000
C	0.27263600	1.06414300	−0.59936900
C	2.66926200	0.86124700	0.19433500
C	4.07949000	1.44075100	−0.03640700
C	2.68722500	−0.63102100	0.27249100
C	3.92513400	−0.93823100	2.41438400
C	3.29417000	−2.74285100	0.74137500
C	3.86441300	−3.83482100	1.38132200
C	3.73401900	−5.07117300	0.73784200
C	3.05473100	−5.18469000	−0.48128200
C	2.47761900	−4.06541400	−1.09747600

C	2.61388300	−2.83011700	−0.47677000
C	2.07167100	−1.46102000	−0.81704300
C	2.46030100	−0.86982100	−2.19048300
C	2.12234700	0.63690400	−2.27464200
C	−5.04860600	−0.36366700	2.11028900
C	−5.40910300	−2.13673600	−0.16143200
C	−5.58044500	0.74201600	−0.52118800
H	1.84743000	2.30331400	−1.03148200
H	2.09611700	6.34507200	1.55390600
H	2.47959800	6.58940500	−0.17588300
H	3.45079300	5.44687700	0.80346000
H	0.10755400	−2.42156600	−0.42648200
H	−0.25731900	1.59489400	−1.39603900
H	0.12153100	1.63526200	0.32202400
H	2.24106500	1.32239400	1.09037500
H	4.59960300	0.94779500	−0.86195900
H	4.67871100	1.32572500	0.86947800
H	3.98770700	2.50766000	−0.25588900
H	3.56024300	−1.58402500	3.21581500
H	3.65216200	0.09332100	2.62815300
H	5.01014400	−1.03520600	2.32803100
H	4.38835800	−3.74407700	2.32654000
H	4.16972700	−5.95415000	1.19523300
H	2.97297200	−6.15687200	−0.95819400
H	1.94444400	−4.16416700	−2.03822000
H	1.92509800	−1.41402400	−2.97263700
H	3.53224200	−1.01993400	−2.35216300
H	1.27313400	0.82771200	−2.93101200
H	2.97384500	1.20544100	−2.65097300
H	−4.57945600	−1.16089300	2.69595100
H	−6.13503300	−0.40762600	2.24618000
H	−4.67981600	0.59970800	2.47722400
H	−5.26619800	−2.29803300	−1.23493800
H	−6.48214600	−2.11324600	0.05923500
H	−4.94838600	−2.96995500	0.37916600
H	−5.23204400	1.73032100	−0.20372400
H	−6.64668100	0.64426600	−0.28877900
H	−5.43765400	0.65542600	−1.60324400

IN24

Au	2.21722000	−0.46089900	0.08158100
P	4.56589600	−0.14378400	0.05460500
N	−2.81178700	−1.37157900	−0.50147700
N	−1.50544300	2.50267200	−0.08493100
C	0.18727200	−0.80786100	0.07849400
C	−0.84022900	0.07076300	0.20093800
C	−0.51426700	1.53994000	0.47926600
C	−1.30845300	3.00033000	−1.25842500
C	−2.13828700	3.98757200	−1.98230400
C	−2.26873200	−0.27548400	0.17773600
C	−2.15618800	−2.23881000	−1.47188700
C	−4.17289100	−1.40521200	−0.26487400
C	−5.14204100	−2.31271900	−0.71736600
C	−6.46018800	−2.10086900	−0.32391100
C	−6.81375700	−1.01207900	0.50365800
C	−5.85302300	−0.11411700	0.95247800
C	−4.51061000	−0.29991900	0.56665900
C	−3.29345500	0.40592300	0.82770500
C	−3.12481400	1.65960500	1.63833400
C	−2.66200100	2.85371800	0.78821500
C	5.30449200	0.24758100	1.69258400
C	5.12931700	1.22878900	−1.03162800
C	5.51933400	−1.60217400	−0.53252300
H	−0.10941900	−1.85525000	0.00330800
H	−0.46783500	1.75071200	1.55070400
H	0.46188300	1.77673100	0.05557000
H	−0.41272700	2.65068900	−1.76821400
H	−3.02020400	4.33629700	−1.44746000
H	−1.49803700	4.84588100	−2.22700000
H	−2.43467000	3.54562400	−2.94301800
H	−1.31702300	−1.71566400	−1.93216100
H	−2.87341500	−2.49525300	−2.25567300
H	−1.79129700	−3.16495600	−1.01331000
H	−4.87842100	−3.15990700	−1.34314500
H	−7.23111700	−2.79116100	−0.65581800
H	−7.85268500	−0.88008100	0.79444900
H	−6.13248500	0.71982400	1.59185500
H	−2.43776700	1.50787600	2.47903000
H	−4.08172400	1.95472600	2.08073200
H	−2.34186200	3.68805500	1.42150700
H	−3.47528300	3.18795400	0.14699800
H	4.85538600	1.16360200	2.09019900
H	6.38808500	0.38612400	1.60657600
H	5.10015500	−0.57012300	2.39142300
H	4.82009700	1.03121600	−2.06326600
H	6.21985900	1.32929000	−0.99657400
H	4.67151400	2.16847400	−0.70562900
H	5.31597200	−2.46004500	0.11671100
H	6.59471000	−1.39185100	−0.52430100
H	5.21123700	−1.85850400	−1.55151900

IN25

Au	0.93279200	−1.24431600	−0.20159400
S	3.55682700	2.24733900	−0.38231900
P	2.01116500	−3.07462300	0.74368800
O	3.44784300	1.40329800	−1.60980100
O	3.13516100	1.53374400	0.86535000
O	2.89266200	3.58358000	−0.52749400
N	−2.83478000	−0.60662700	−1.02983800
N	−0.82207200	3.04947300	0.64888600
C	5.31408600	2.60439900	−0.17542700
C	0.07478800	0.48073700	−1.40722000
C	−0.80059300	0.76684100	−0.36575200
C	−0.26283600	1.67571700	0.74300200
C	−0.08119800	4.00443300	0.18808600
C	−0.49069200	5.41616100	0.03747500
C	−2.18369900	0.35900300	−0.24341600
C	−2.25868900	−1.51061900	−2.01891500
C	−4.15675500	−0.65558600	−0.65168900
C	−5.20678300	−1.46010100	−1.13199200
C	−6.45812700	−1.29241000	−0.55796500
C	−6.68602600	−0.34712100	0.47275600
C	−5.65658800	0.44679300	0.94579100
C	−4.36775200	0.29570600	0.38569600
C	−3.11645400	0.92396600	0.64128200
C	−2.91006200	2.02424400	1.64585300
C	−2.22681300	3.27976300	1.10541700
C	0.87528700	−4.23355700	1.59708600
C	3.26907600	−2.61109000	1.99211300
C	2.90105600	−4.09053200	−0.49523300
H	1.00521700	1.04304000	−1.48375000
H	5.67656500	3.13622800	−1.05893400
H	5.85832600	1.66356400	−0.05927200
H	5.44963400	3.22461500	0.71424900

H	−0.27274900	0.01592200	−2.32285400
H	−0.50348500	1.28497300	1.73162200
H	0.82285200	1.75193900	0.67135500
H	0.94286600	3.74399900	−0.10376200
H	−1.52776100	5.63076500	0.29146900
H	0.17691100	6.02802000	0.66043600
H	−0.29018700	5.71653300	−0.99959000
H	−2.10732400	−1.01151900	−2.98209000
H	−2.94295900	−2.34675200	−2.16418900
H	−1.30830600	−1.91432400	−1.66217700
H	−5.05910100	−2.18021400	−1.92973200
H	−7.28722900	−1.89827400	−0.91309000
H	−7.68347200	−0.24823100	0.89132700
H	−5.83429700	1.16979100	1.73710200
H	−2.38726300	1.66520000	2.54111000
H	−3.89041100	2.36084300	1.99690900
H	−2.19098300	4.04335100	1.88637900
H	−2.78599700	3.67452200	0.25388700
H	0.35261100	−3.71107600	2.40428900
H	1.44035900	−5.07432700	2.01480600
H	0.13511500	−4.61375800	0.88610600
H	4.02321000	−1.96619200	1.53052700
H	3.75382100	−3.50878400	2.39192300
H	2.79138100	−2.06169700	2.80930400
H	2.19159000	−4.47555100	−1.23442900
H	3.40292600	−4.93055100	−0.00236800
H	3.64615700	−3.47452100	−1.00829500

IN26

Au	2.04516200	0.30139000	−0.03827700
P	4.37416200	0.05506000	0.32679700
N	−3.92527900	−0.17368300	1.11394600
N	−1.88495700	−2.64784300	−0.70267700
C	0.02456900	0.55650700	−0.34301500
C	−0.90898400	−0.39213000	−0.51633100
C	−0.58652400	−1.87962400	−0.50350800
C	−2.87213200	−2.32997800	0.37276300
C	−3.33024900	−3.49644000	1.18826800
C	−3.13066400	−1.00489200	0.35416900
C	−4.71618800	−0.57588800	2.26496100
C	−3.88328200	1.13122000	0.58796200
C	−4.59428400	2.25709500	1.00255600
C	−4.38404800	3.45654200	0.30800700
C	−3.50372400	3.52762300	−0.77437700
C	−2.80312600	2.38292300	−1.18664500
C	−2.99305700	1.19011100	−0.50145000
C	−2.42214200	−0.18630900	−0.73016900
C	−2.80349500	−0.82041100	−2.10588900
C	−2.44257200	−2.31933900	−2.08269000
C	5.41411300	0.22729600	−1.18010100
C	4.86331900	−1.57696400	1.01929600
C	5.09192200	1.26917900	1.50573900
H	−1.67209000	−3.64935300	−0.67271100
H	−0.34881200	1.58349400	−0.36206900
H	0.08472700	−2.17744000	−1.31324000
H	−0.16944300	−2.21510600	0.44835300
H	−3.70845300	−4.30373600	0.54521400
H	−2.51741600	−3.91766100	1.79709900
H	−4.13898200	−3.21184300	1.86327200
H	−4.99968200	0.31126300	2.83327100
H	−4.12321200	−1.21895000	2.92108900
H	−5.62787400	−1.10770300	1.96588700
H	−5.29710000	2.21836500	1.82828400
H	−4.92925900	4.34412800	0.61803700
H	−3.36364600	4.46672100	−1.30157800
H	−2.12716900	2.42989900	−2.03601200
H	−2.26524600	−0.30617400	−2.90636600
H	−3.87544300	−0.69184900	−2.27747000
H	−1.66588000	−2.58241700	−2.80310800
H	−3.30557000	−2.96874400	−2.22971500
H	5.11866700	−0.52478000	−1.91893500
H	6.47443100	0.09520000	−0.93698600
H	5.26710800	1.21948400	−1.61923400
H	4.35496500	−1.73881700	1.97544300
H	5.94678900	−1.62137600	1.17678400
H	4.56815600	−2.37487700	0.32991700
H	4.94256100	2.28517400	1.12595500
H	6.16438400	1.08946300	1.64051200
H	4.58822600	1.18345300	2.47407300

IN27

Au	−0.51783400	1.27055700	−0.14112900
S	4.78147400	0.36079100	−0.47599300
P	−1.91721700	3.01659100	0.49682100
O	4.69503800	−0.86412000	0.38505100
O	4.88789100	0.06058000	−1.93002600
O	3.70809100	1.35911700	−0.15461900
N	−2.31431100	−2.15684800	0.79800300
N	1.24143900	−2.24989500	1.76135100
C	6.32929400	1.16648200	−0.01295200
C	1.03908200	−0.00302400	−1.21190600
C	0.74542000	−0.87722500	−0.19904100
C	1.57674000	−0.94171100	1.07255800
C	−0.19947400	−2.31453100	2.14443400
C	−0.46870900	−2.49930600	3.60315700
C	−0.95638700	−2.18848800	1.03440100
C	−3.34492900	−2.28665700	1.81553800
C	−2.55407000	−2.08862800	−0.58696500
C	−3.77748200	−2.08736200	−1.25728900
C	−3.75823700	−2.02392100	−2.65724400
C	−2.55723100	−1.98023000	−3.37016100
C	−1.33300000	−1.98871600	−2.68445900
C	−1.33757400	−2.02832900	−1.29563800
C	−0.20774700	−2.07222100	−0.29678600
C	0.72892200	−3.32406700	−0.41395600
C	1.62779700	−3.40083700	0.83544500
C	−1.21654000	4.65261700	0.06292500
C	−2.23581900	3.07961700	2.30125800
C	−3.56740300	2.96561100	−0.29868400
H	1.92084400	0.63427100	−1.12543200
H	1.81739000	−2.31261600	2.60737000
H	6.44305200	2.08146700	−0.60043300
H	7.16302000	0.48973300	−0.21803100
H	6.30364300	1.41083400	1.05220800
H	0.57034500	−0.11328400	−2.18617300
H	2.65235000	−0.93217500	0.85622900
H	1.33851000	−0.14215800	1.77528600
H	0.07767700	−3.36923800	3.99305700
H	−0.15501900	−1.62482900	4.19066500
H	−1.53008200	−2.66669500	3.79149500
H	−4.31030300	−2.01564600	1.38712200
H	−3.14193700	−1.60485700	2.64619400
H	−3.40523300	−3.31297600	2.19732400
H	−4.72141600	−2.14689400	−0.72616100

H	−4.70301400	−2.02441200	−3.19413900
H	−2.56858300	−1.94957400	−4.45553500
H	−0.39755300	−1.97563500	−3.23639500
H	1.33144300	−3.24636200	−1.32244500
H	0.10135000	−4.21462100	−0.49087500
H	2.68596800	−3.26847500	0.60484300
H	1.48733700	−4.31853100	1.40601400
H	−0.25660900	4.78855100	0.57050100
H	−1.90517700	5.44818600	0.36844400
H	−1.05343400	4.70858100	−1.01781300
H	−2.72987900	2.15703300	2.62162600
H	−2.87769400	3.93537800	2.53856000
H	−1.28729900	3.17792300	2.83844200
H	−3.45048400	2.98285400	−1.38669000
H	−4.16186500	3.83088600	0.01545000
H	−4.08778800	2.04586000	−0.01449200

IN28

Au	−2.25509500	0.01884600	−0.03330700
P	−4.56206400	−0.49180500	−0.11084300
N	2.91503900	−1.58713900	0.51685200
N	1.51382800	2.33912700	0.36537700
C	0.67925100	−0.60044300	0.01766000
C	−0.21040700	0.42618200	0.03199800
C	0.09493800	1.91116300	0.11448900
C	1.95023400	2.37373900	1.57861300
C	3.30876900	2.70325400	2.06419300
C	2.14157600	−0.60023400	−0.09793000
C	2.42859400	−2.63819800	1.39632600
C	4.23198500	−1.42328400	0.13747000
C	5.37107000	−2.16485700	0.48221900
C	6.59157200	−1.76151400	−0.05275300
C	6.68154100	−0.64981100	−0.91893700
C	5.55111500	0.08246300	−1.26396500
C	4.30152500	−0.29961800	−0.73780400
C	2.96474900	0.19852700	−0.88145000
C	2.49640400	1.36793700	−1.69084100
C	2.32234500	2.63883200	−0.83490300
C	−5.11525200	−1.28524900	−1.67433800
C	−5.67125000	0.96224100	0.07531000
C	−5.11137700	−1.65239000	1.20516800
H	0.25403500	−1.60391500	0.04371100
H	−0.21663200	2.41722200	−0.80361300
H	−0.48890600	2.34715600	0.92941100
H	1.21426200	2.11980900	2.33940900
H	4.03502000	2.95217000	1.29243100
H	3.67260100	1.84265200	2.64167900
H	3.22486600	3.53441500	2.77671600
H	2.19145500	−3.55379400	0.84042700
H	1.53214800	−2.29691600	1.91772400
H	3.19156300	−2.86821600	2.14420400
H	5.30871200	−3.02771000	1.13874400
H	7.49114500	−2.31846500	0.19572800
H	7.65093400	−0.36477300	−1.31948500
H	5.62952200	0.93602400	−1.93326600
H	1.54336700	1.13382800	−2.18081800
H	3.21170600	1.61191700	−2.48366100
H	1.79279300	3.42100700	−1.38622500
H	3.28728000	3.02919900	−0.52073900
H	−4.90785600	−0.62009900	−2.51887900
H	−6.18916700	−1.50020400	−1.63984500
H	−4.56600900	−2.22022600	−1.82560100
H	−5.47134800	1.46085300	1.02935600
H	−6.72175400	0.65220500	0.04534600
H	−5.48270600	1.67389300	−0.73504600
H	−4.56013700	−2.59436000	1.11882300
H	−6.18510900	−1.85422300	1.12007800
H	−4.90466300	−1.21760400	2.18852000

IN29

Au	0.86746500	1.57857100	−0.00361600
S	3.28483000	−3.30436800	0.69102200
P	1.34785700	3.85414300	−0.09013100
O	3.64731900	−1.85059500	0.69766000
O	2.47870400	−3.68744000	−0.51953600
O	2.68582700	−3.77650600	1.96815600
N	−2.47163400	−0.64185800	1.64346100
N	−0.40648300	−2.04680000	−1.95922200
C	4.84998600	−4.18273900	0.50416200
C	−0.20058300	−0.50608700	0.70377700
C	0.83357400	−0.72191900	−0.19754800
C	0.79700900	−1.23368500	−1.62908500
C	−0.43836900	−3.28260800	−1.57919600
C	−1.52069500	−4.26756000	−1.78658900
C	−1.63882000	−0.50045400	0.52819700
C	−2.02941300	−0.86434100	3.01480600
C	−3.77964100	−0.56795600	1.22627600
C	−4.97623400	−0.65720800	1.95943800
C	−6.16893500	−0.53655900	1.26087400
C	−6.19307500	−0.33044000	−0.14049400
C	−5.01693200	−0.24287000	−0.86619000
C	−3.78516700	−0.36295700	−0.18580400
C	−2.42483500	−0.31774700	−0.61138800
C	−1.92870500	−0.07245700	−2.00464800
C	−1.46076400	−1.34765700	−2.72678700
C	−0.12910800	4.91928400	−0.29860200
C	2.46895100	4.29352700	−1.47169600
C	2.17724600	4.45832300	1.42819500
H	1.81676300	−0.87489900	0.25390800
H	5.49752500	−3.94257200	1.35158800
H	5.32832400	−3.86957500	−0.42725200
H	4.65720600	−5.25846500	0.47934500
H	0.12566900	−0.43730300	1.73969600
H	0.86666800	−0.43785100	−2.37123000
H	1.66278200	−1.88888200	−1.74391500
H	0.46096100	−3.62222000	−1.05625900
H	−2.45514200	−3.86694200	−2.17663200
H	−1.70346500	−4.77367600	−0.83073300
H	−1.14200200	−5.04071500	−2.47070800
H	−1.49567600	0.00961500	3.40328900
H	−1.37845000	−1.74178600	3.07590300
H	−2.90242300	−1.04224200	3.64231300
H	−4.97735300	−0.81209700	3.03355500
H	−7.10835700	−0.59982800	1.80329400
H	−7.14997700	−0.24165600	−0.64730500
H	−5.03805600	−0.08592600	−1.94144300
H	−1.11762400	0.66779300	−1.99366300
H	−2.72865200	0.35451600	−2.61849800
H	−1.02525000	−1.09769500	−3.69948800
H	−2.29375000	−2.02897800	−2.88438900
H	−0.64357700	4.66058700	−1.22927000
H	0.17004400	5.97282300	−0.33006800
H	−0.81614300	4.76237600	0.53861400
H	3.41155200	3.74705600	−1.36895400

H	2.67109100	5.37043600	−1.46202500
H	2.00503400	4.01999100	−2.42443100
H	1.53080600	4.28745400	2.29454400
H	2.39075900	5.52939600	1.33978000
H	3.11492800	3.91350300	1.57557700

IN30

Au	2.05705200	−0.05270300	−0.04894400
P	4.29245200	0.61630300	0.33479600
N	−3.79454000	−0.21365300	1.15825000
N	−1.59199700	−2.55955200	−0.71480800
C	−0.89732200	0.28660200	−0.56008800
C	0.08211600	−0.61880800	−0.37299600
C	−0.16818300	−2.10335700	−0.36277600
C	−2.59294700	−2.23624800	0.34213100
C	−3.00637000	−3.41321700	1.17297400
C	−2.93654300	−0.93185800	0.34380500
C	−4.38640800	−0.66401400	2.40656600
C	−4.03117300	1.05424200	0.60045900
C	−4.89880600	2.05111400	1.04584200
C	−4.94633800	3.24834400	0.31656700
C	−4.15851900	3.44031000	−0.82071400
C	−3.29338400	2.42291600	−1.25737700
C	−3.24054600	1.23252000	−0.54708800
C	−2.39493900	−0.00865400	−0.75809500
C	−2.64641700	−0.71815900	−2.11267900
C	−2.01179700	−2.11987500	−2.11598600
C	4.62988900	1.16146100	2.05806500
C	4.85189300	2.02622400	−0.70336800
C	5.53791500	−0.69888700	0.01950900
H	−1.53202000	−3.58181600	−0.75647400
H	−0.65178700	1.34682900	−0.57125200
H	0.47275200	−2.60985200	−1.09162800
H	0.03921100	−2.53882100	0.62046800
H	−3.87450900	−3.18178900	1.79112400
H	−3.28481700	−4.25876200	0.52774600
H	−2.20383300	−3.76338600	1.83771400
H	−4.60326400	0.20646000	3.03008900
H	−3.67532600	−1.29286200	2.94700700
H	−5.31746600	−1.22256000	2.24830700
H	−5.52729400	1.91322100	1.91951800
H	−5.61718900	4.03735800	0.64620600
H	−4.21625100	4.37500200	−1.37093200
H	−2.67835700	2.56791600	−2.14212100
H	−2.22773700	−0.12376700	−2.92993400
H	−3.72527100	−0.79973400	−2.27595400
H	−1.11142200	−2.17111400	−2.72929300
H	−2.71620800	−2.87579100	−2.46520300
H	3.98480300	2.01051100	2.30651200
H	5.67804700	1.45935600	2.17300500
H	4.40984500	0.34355900	2.75184900
H	4.77393000	1.75801800	−1.76202600
H	5.89095400	2.28778300	−0.47392700
H	4.21340600	2.89610100	−0.51782700
H	5.33971400	−1.55764300	0.66913200
H	6.55110800	−0.32883300	0.21240000
H	5.46816300	−1.02786800	−1.02245400

IN31

Au	0.63227200	−1.25801000	0.01060500
S	−4.77319900	−0.48640700	−0.67772400
P	2.28604500	−2.90106500	0.03029100
O	−3.91631200	−1.70673100	−0.52046000
O	−4.53559300	0.52421500	0.40668700
O	−4.73185500	0.09671900	−2.04669500
N	2.13165500	2.18902000	0.79629900
N	−1.34779700	1.75749700	2.06524800
C	−6.46540500	−1.06338500	−0.42561800
C	−0.64645300	0.63327200	−0.54933200
C	−1.38653600	−0.09350100	0.34806200
C	−1.70403600	0.31480400	1.76012200
C	0.11611900	1.98478900	2.24424300
C	0.53164400	2.13050500	3.67678600
C	0.78564400	2.02125100	1.07309000
C	3.21743900	2.18995000	1.76246500
C	2.31414200	2.43124500	−0.57664100
C	3.49249500	2.73564000	−1.25829400
C	3.41451200	2.91739700	−2.64668000
C	2.20142300	2.80613200	−3.33112500
C	1.02318800	2.50558000	−2.62885800
C	1.08942100	2.32572200	−1.25480500
C	0.00737900	1.98087800	−0.25104700
C	−1.12938100	3.03481900	−0.13352500
C	−2.02006000	2.73627200	1.08582500
C	3.82914900	−2.39783000	0.88016100
C	2.78969200	−3.39705100	−1.66016100
C	1.74853500	−4.44273900	0.86245700
H	−2.03235300	−0.89172100	−0.02569000
H	−1.78544200	1.94536500	2.97346400
H	−7.15074600	−0.21667400	−0.51786200
H	−6.55180200	−1.50263700	0.57165500
H	−6.70313400	−1.81498800	−1.18302700
H	−0.73914400	0.38525300	−1.60594200
H	−2.78914400	0.23421900	1.87374000
H	−1.21265700	−0.30721400	2.51215100
H	1.56161400	2.47505500	3.76597100
H	−0.10443400	2.87176700	4.18158900
H	0.43922500	1.18840800	4.23543500
H	4.14842800	1.94250900	1.24841300
H	3.04054400	1.42392100	2.52083400
H	3.33489100	3.16482300	2.25163900
H	4.44113700	2.84229600	−0.74294800
H	4.32128300	3.15744600	−3.19545900
H	2.16679500	2.95828800	−4.40575700
H	0.07534500	2.42166600	−3.15452600
H	−1.74361200	3.03259800	−1.03892300
H	−0.67059300	4.02262500	−0.04033600
H	−2.96705700	2.26977200	0.80726700
H	−2.21566000	3.63903400	1.66497600
H	4.24533500	−1.50915000	0.39578300
H	4.56304200	−3.21043800	0.83770400
H	3.61208300	−2.16146200	1.92653900
H	1.92030700	−3.77902300	−2.20422900
H	3.55896200	−4.17575800	−1.61008600
H	3.18600200	−2.52842200	−2.19521900
H	1.50327300	−4.22989400	1.90758300
H	2.54989300	−5.18902500	0.82228600
H	0.85821400	−4.83912000	0.36453000

IN32

Au	2.47093400	−0.40335300	0.03620100
P	4.80756400	−0.49685600	0.37298200
N	−2.37810800	−0.50169800	−1.43566600
N	−1.26438600	2.88816000	−0.53734000

C	0.44813000	−0.39682800	−0.30362500
C	−0.35878800	0.66346900	−0.39208600
C	0.02098300	2.12899500	−0.23057000
C	−2.00415200	2.00171400	−1.50438300
C	−1.86867400	0.65669700	−0.75485400
C	−3.33772900	−1.09473400	−0.71342100
C	−4.07352000	−2.26593300	−0.99309000
C	−5.02431900	−2.63668400	−0.06859500
C	−5.28686300	−1.89441900	1.13386500
C	−4.58436600	−0.75972800	1.42753200
C	−3.57840400	−0.33057400	0.50229900
C	−2.71205500	0.73505000	0.48755700
C	−2.49258800	1.87121600	1.42593800
C	−2.11748800	3.17109000	0.68338900
H	5.42623900	−1.74960100	0.20170400
H	5.30770700	−0.13536400	1.63808800
H	5.61502900	0.30231200	−0.45822400
H	−1.97319600	−0.87852400	−2.28666000
H	−1.04472700	3.78663900	−0.98149500
H	−0.02825900	−1.36834900	−0.45696500
H	0.35591300	2.40487400	0.77031500
H	0.76747100	2.44860900	−0.96078700
H	−1.46569500	1.98639500	−2.45319900
H	−3.02602100	2.35686200	−1.63791200
H	−3.89396200	−2.83864000	−1.89634900
H	−5.61019900	−3.53274500	−0.25324500
H	−6.05702000	−2.25497900	1.80751500
H	−4.76883100	−0.18917700	2.33174700
H	−1.67912100	1.59233000	2.11038300
H	−3.37541400	2.05458100	2.04376900
H	−1.54772900	3.84208500	1.32648000
H	−3.00294400	3.68921700	0.31151800

IN33

Au	−2.28517200	−0.33489400	0.01032100
P	−4.64048100	−0.38647000	0.22769200
N	3.36798900	0.31776100	1.51437400
N	1.36680300	3.00773500	0.07475200
C	−0.24434700	−0.36949700	−0.18598000
C	0.59314800	0.67663000	−0.22197900
C	0.13846800	2.12140100	−0.05749700
C	2.22747100	2.55391800	1.22427800
C	2.64104300	1.17362700	0.86249700
C	3.50118700	−0.89908700	0.78240300
C	4.21765500	−2.03336500	1.13239000
C	4.19091100	−3.08805400	0.21339200
C	3.47974500	−2.98227300	−0.98897100
C	2.76341300	−1.82148600	−1.31502400
C	2.77515300	−0.76665600	−0.41063200
C	2.13587900	0.59810700	−0.42539100
C	2.53348900	1.55438600	−1.59113900
C	2.14958400	3.00705900	−1.22805500
H	−5.24496600	−1.64956900	0.37121800
H	−5.40312500	0.14239500	−0.83081900
H	−5.21300200	0.29571500	1.31777600
H	3.77604500	0.47419000	2.43737300
H	1.05970400	3.96828700	0.26769200
H	0.21505800	−1.35143400	−0.30833800
H	−0.41247900	2.49866500	−0.92258800
H	−0.46234700	2.27019700	0.84193700
H	1.63627800	2.58882900	2.14459800
H	3.08158200	3.23137100	1.31841400
H	4.76874300	−2.09762400	2.06483400
H	4.73562700	−4.00001700	0.43688100
H	3.48245100	−3.81652800	−1.68386900
H	2.21708000	−1.75313100	−2.25033000
H	2.00857400	1.22505300	−2.49041400
H	3.60816100	1.48875700	−1.77457500
H	1.50044600	3.47004800	−1.97125300
H	3.02165300	3.64176000	−1.06495900

TS5

Au	2.36451500	−0.27702000	−0.00759600
P	4.41676600	−1.37424100	0.09216900
N	−2.99974100	0.13445200	−1.64828600
N	−0.91219100	2.90534900	−0.19559500
C	−0.23812800	−0.11114100	−0.13988000
C	0.54549300	0.86764600	−0.06813600
C	0.49971100	2.34737600	−0.05050500
C	−1.70486900	2.28478400	−1.33210000
C	−2.38041400	1.04645500	−0.83517400
C	−3.62862800	−0.81671600	−0.86046200
C	−4.36621400	−1.94621400	−1.23131500
C	−4.88712400	−2.73021600	−0.20681300
C	−4.67943600	−2.40392100	1.15162900
C	−3.94099000	−1.28513300	1.51701900
C	−3.40360600	−0.47127300	0.50231700
C	−2.60231700	0.72467700	0.49959800
C	−2.13748500	1.60294500	1.62393600
C	−1.72412100	2.97797900	1.09583500
H	4.64084000	−2.18092700	1.22023400
H	5.54665700	−0.53948800	0.10126000
H	4.71141400	−2.25294300	−0.96370400
H	−2.96788500	0.13193700	−2.66038000
H	−0.76284000	3.88418200	−0.46811200
H	−0.62798900	−1.11070900	−0.20872600
H	0.90743700	2.75143100	0.87874700
H	1.07458700	2.75329200	−0.88652600
H	−1.01405400	2.09665800	−2.15795000
H	−2.43043900	3.03806300	−1.65353400
H	−4.52525400	−2.19732000	−2.27586200
H	−5.46832900	−3.61305300	−0.45773600
H	−5.10509400	−3.04177800	1.92094400
H	−3.78400000	−1.04032700	2.56382400
H	−1.31582000	1.14126200	2.18318800
H	−2.94624800	1.76816300	2.34524700
H	−1.11024200	3.52811400	1.81026600
H	−2.59862300	3.57951700	0.83784200

TS6

Au	2.26858600	−0.26762100	−0.00140400
P	4.33245000	−1.40263000	0.07295700
N	−2.82275700	0.10253100	−1.67949800
N	−0.83401700	2.90646400	−0.18770000
C	−0.71588500	0.05073600	−0.22567000
C	0.46183000	0.72000000	−0.04392100
C	0.50367800	2.20982800	0.06521600
C	−1.56603500	2.28191100	−1.34798100
C	−1.99045600	0.90558200	−0.91016900
C	−3.48404200	−0.80088800	−0.85997800
C	−4.34803500	−1.84353800	−1.20935500
C	−4.91711000	−2.56812700	−0.16611500
C	−4.62945400	−2.28181600	1.18487100
C	−3.74657200	−1.26239500	1.52570700

C	−3.16592200	−0.51801000	0.49164500
C	−2.21386300	0.59036500	0.49158600
C	−2.00702100	1.59478900	1.60622300
C	−1.70937200	2.98924200	1.04652000
H	4.70436200	−1.96329400	1.30798700
H	5.48113500	−0.65432000	−0.24145400
H	4.48577700	−2.50770600	−0.78314900
H	−2.72027600	−0.01001500	−2.68264500
H	−0.61466600	3.87221000	−0.46084300
H	−0.76155900	−1.01686100	−0.40336500
H	0.85212200	2.53456900	1.05099600
H	1.19708500	2.61337700	−0.67858900
H	−0.89544900	2.26784300	−2.20972300
H	−2.43797200	2.90269000	−1.56468000
H	−4.57367200	−2.06616900	−2.24725200
H	−5.60452800	−3.37596200	−0.39988000
H	−5.10039900	−2.87089200	1.96560800
H	−3.51233000	−1.04717900	2.56387400
H	−1.21434400	1.26532300	2.28242800
H	−2.92642200	1.65619100	2.19584600
H	−1.17716600	3.60971300	1.76866800
H	−2.61980700	3.50294200	0.73162500

TS7

Au	−2.04622300	−1.10641000	−0.13611400
S	−0.69589000	4.22645000	0.30746700
P	−4.27899800	−1.71244100	0.18496900
O	0.19335600	4.14499100	−0.92943000
O	−1.87668800	3.32318600	0.19187000
O	0.08872800	4.05536300	1.55752100
N	3.42630800	−0.29813800	1.26910900
N	1.27043000	1.73452400	−1.06357000
C	−1.32316600	5.91100400	0.27886100
C	1.21610600	−2.34643000	0.74892700
C	0.83226400	−1.10652700	0.06468500
C	−0.06487000	−0.35640500	−0.45725900
C	−0.05111500	0.98546800	−1.10320300
C	2.01360800	1.56395800	0.25084400
C	2.99959900	2.71864200	0.47594500
C	2.69673100	0.21826000	0.20490600
C	3.27204800	0.03311400	2.68031800
C	4.29655600	−1.25011700	0.77728000
C	5.20898600	−2.06395100	1.46507700
C	5.97244600	−2.94267900	0.70811000
C	5.83573300	−3.03116400	−0.69815400
C	4.92568600	−2.23919800	−1.37747600
C	4.13946200	−1.32784200	−0.63926800
C	3.14160300	−0.37589100	−0.99168600
C	2.65967500	0.06911200	−2.34015400
C	2.13513900	1.50748300	−2.27331500
C	−5.00877300	−2.64943200	−1.21385800
C	−4.56436500	−2.76270400	1.66280100
C	−5.37083400	−0.25629900	0.41338200
H	0.93540800	2.76416200	−1.06646800
H	−1.97008700	6.05358200	1.14788500
H	−1.89172200	6.06220500	−0.64140800
H	−0.48095600	6.60546000	0.32131500
H	2.15133400	−2.75857500	0.35846100
H	0.43221000	−3.09127300	0.56722300
H	1.31606800	−2.20716900	1.83036400
H	−0.34035300	0.91127200	−2.15544900
H	−0.77978400	1.64336800	−0.61595900
H	1.24305700	1.62138700	1.02341700
H	3.83659100	2.69422100	−0.22753700
H	2.47414900	3.67327500	0.39999300
H	3.40808400	2.64490800	1.48780400
H	4.14422400	0.58299000	3.04904300
H	3.15503400	−0.88166300	3.26941800
H	2.38103600	0.64661600	2.81888300
H	5.32730500	−2.00255100	2.54209600
H	6.69790400	−3.57788200	1.20819500
H	6.45652500	−3.73311400	−1.24658100
H	4.82121100	−2.31141900	−2.45626700
H	1.87845200	−0.60150200	−2.71983100
H	3.47670400	0.03132500	−3.06919600
H	1.52883100	1.76066500	−3.14535600
H	2.95600500	2.22393500	−2.21235600
H	−4.94256900	−2.05701700	−2.13190200
H	−6.06040100	−2.88099600	−1.01110100
H	−4.45803600	−3.58365900	−1.36240000
H	−4.00461700	−3.69852000	1.56804300
H	−5.63057200	−2.99223600	1.76893000
H	−4.21954900	−2.24018800	2.56061100
H	−5.04742400	0.31372100	1.29000100
H	−6.40984300	−0.57499900	0.55319800
H	−5.30885200	0.39608000	−0.46309200

TS7 (L = PPh_3)

Au	−0.78410300	−0.56521100	−0.25903300
S	1.21397300	4.23254300	0.30633800
P	−3.10763400	−0.57404300	0.03654400
O	2.21936400	4.16206800	−0.83541700
O	−0.10955500	3.67012600	−0.09024500
O	1.76722000	3.66094500	1.56355600
N	4.70235100	−0.70566600	1.25751800
N	2.96542000	1.62293300	−1.14913400
C	0.97343100	5.99517300	0.56879600
C	2.21027700	−2.36912000	0.71418100
C	2.05933300	−1.09859800	−0.00458200
C	1.30509800	−0.23097500	−0.56989500
C	1.55376000	1.06396800	−1.26084400
C	3.62297500	1.34348100	0.19372500
C	4.77101500	2.33069200	0.44846500
C	4.08678800	−0.09333300	0.17132300
C	4.55956800	−0.34306900	2.66241400
C	5.43650900	−1.77786900	0.79321500
C	6.20086800	−2.71303800	1.50739000
C	6.84956600	−3.69692600	0.77350000
C	6.74144000	−3.77222400	−0.63628700
C	5.97581100	−2.86007800	−1.34193200
C	5.31023400	−1.84000000	−0.62753800
C	4.47738900	−0.75201400	−1.01143600
C	4.12170400	−0.23724000	−2.37448100
C	3.83861700	1.26888000	−2.32119100
C	−3.60148300	0.68877100	1.26794400
C	−4.66780400	0.47344800	2.15532700
C	−5.03180800	1.46879100	3.06436500
C	−4.33840100	2.68078000	3.09303500
C	−3.27489100	2.89772800	2.21319100
C	−2.89983600	1.90688400	1.30569200
C	−3.77011200	−2.18267400	0.61386400
C	−5.01165100	−2.67046100	0.17884700
C	−5.48947800	−3.89200100	0.65863400
C	−4.73643700	−4.63134900	1.57278000

C	−3.49900100	−4.15023900	2.00952600
C	−3.01418300	−2.93379100	1.52972000
C	−3.97720100	−0.17498600	−1.52724100
C	−5.11173600	0.64957300	−1.55440800
C	−5.75388100	0.91480500	−2.76619300
C	−5.27061300	0.36195700	−3.95358000
C	−4.14056400	−0.46036900	−3.93219100
C	−3.49180200	−0.72440100	−2.72640200
H	2.78212000	2.68201100	−1.13513400
H	0.25204300	6.13115100	1.37821300
H	0.59436200	6.44305700	−0.35242500
H	1.92987100	6.44638200	0.84237800
H	3.08752000	−2.92863700	0.37595700
H	1.32957800	−2.98656100	0.50165100
H	2.28000100	−2.22496400	1.79760600
H	1.33144400	0.97772700	−2.32846500
H	0.89139300	1.83734400	−0.86050800
H	2.84360600	1.53479000	0.93512500
H	5.63706200	2.14155100	−0.19220800
H	4.41885100	3.35478500	0.30080000
H	5.09570300	2.23803800	1.48861400
H	5.48038700	0.10985700	3.04507900
H	4.33104400	−1.23373700	3.25537400
H	3.73960800	0.36700400	2.77757900
H	6.29683700	−2.66411100	2.58718800
H	7.46049300	−4.42811800	1.29497300
H	7.26853400	−4.55998000	−1.16583600
H	5.89201300	−2.92181500	−2.42316300
H	3.25409500	−0.76983500	−2.78399100
H	4.94617800	−0.41080300	−3.07448100
H	3.32219500	1.61798900	−3.21749600
H	4.76129100	1.84169600	−2.21590100
H	−5.21279600	−0.46524900	2.14203400
H	−5.85667800	1.29438300	3.74946000
H	−4.62302100	3.45269900	3.80260300
H	−2.72567200	3.83434800	2.23387400
H	−2.06098900	2.09233800	0.63917400
H	−5.60408800	−2.10369200	−0.53243300
H	−6.45061400	−4.26397900	0.31523400
H	−5.11044200	−5.58230400	1.94150400
H	−2.90918000	−4.72423300	2.71860000
H	−2.04808500	−2.56575000	1.86669000
H	−5.49401500	1.08666200	−0.63745200
H	−6.62983200	1.55708700	−2.77953200
H	−5.77108200	0.57318100	−4.89437200
H	−3.75893900	−0.88878600	−4.85469000
H	−2.60737500	−1.35689800	−2.71583200

TS8

Au	−1.55346900	−1.53250200	−0.08168000
S	−1.66810200	3.45244400	0.29063800
P	−3.88379700	−1.53503000	0.10300300
O	−0.72342500	3.95847500	−0.78989700
O	−2.58825800	2.39939500	−0.22415500
O	−0.92777100	3.05683500	1.52191100
N	3.37027700	0.40126900	1.30431300
N	1.16004100	2.11592300	−1.10269800
C	−2.67814400	4.88164400	0.70206300
C	1.30494800	−2.70313400	0.33881600
C	0.60002500	−1.48076100	−0.16474300
C	0.93027500	−0.32327100	−0.62640500
C	0.28859200	0.89297600	−1.21247800
C	1.85295300	2.15560000	0.24725700
C	2.55101000	3.49888700	0.48968500
C	2.75223900	0.95867500	0.23571900
C	3.16949800	0.72528900	2.71318100
C	4.16642700	−0.66104600	0.85391800
C	4.98768800	−1.51843900	1.58616100
C	5.69368500	−2.48476800	0.86977700
C	5.58538300	−2.58782200	−0.53008500
C	4.74983900	−1.73817000	−1.25044900
C	4.01612300	−0.77139600	−0.54909900
C	3.07316700	0.25567100	−0.95101800
C	2.91248300	0.85321800	−2.33186600
C	2.12370900	2.17141700	−2.25631200
C	−4.68915900	−3.13041300	−0.31381900
C	−4.66348200	−0.28487900	−0.98889800
C	−4.47274100	−1.12534900	1.79218600
H	0.47447000	2.94512800	−1.10475100
H	−3.39061600	4.59062800	1.47773900
H	−3.21015000	5.20914200	−0.19395500
H	−2.03046200	5.68053900	1.06980800
H	0.87082100	−3.60214200	−0.11099800
H	1.16696900	−2.79680000	1.42271200
H	2.37550100	−2.68882600	0.12398200
H	0.06004100	0.76070900	−2.27363700
H	−0.65037400	1.11151300	−0.69638500
H	1.04081300	2.06235000	0.97743000
H	3.43500300	3.64115300	−0.13726900
H	2.87160700	3.54435500	1.53456200
H	1.84312100	4.31529800	0.32038200
H	4.10385300	1.08692400	3.15277600
H	2.83709200	−0.16538100	3.25475300
H	2.40725800	1.49811100	2.81067900
H	5.08672600	−1.43571000	2.66371000
H	6.34932100	−3.16568400	1.40443600
H	6.16165300	−3.34498200	−1.05327300
H	4.66314900	−1.82980000	−2.32928100
H	2.42232600	0.14376100	−3.00648600
H	3.89948600	1.05831700	−2.76185000
H	1.53385300	2.35212500	−3.15664500
H	2.77431400	3.03091900	−2.09647400
H	−4.44588600	−3.41016000	−1.34384100
H	−5.77725300	−3.05123200	−0.21211200
H	−4.32303900	−3.91666600	0.35408700
H	−4.24612800	0.70150800	−0.76027300
H	−5.74975200	−0.27256900	−0.84406400
H	−4.44422300	−0.52311600	−2.03494100
H	−4.09359600	−1.85974000	2.50986700
H	−5.56808700	−1.12158500	1.82533400
H	−4.10091200	−0.13566800	2.07574200

TS8 (L = PPh_3)

Au	−0.67267900	−0.87704900	−0.12141000
S	1.18757900	4.12593800	0.32641900
P	−2.97681900	−0.44033900	0.01892100
O	2.15929000	4.18752700	−0.84448600
O	−0.00543100	3.28970400	0.00052800
O	1.87029600	3.74142400	1.59064400
N	4.66808000	−0.60781300	1.27755300
N	3.15319500	1.75152400	−1.12116700
C	0.61128700	5.81827100	0.50975100
C	1.67668000	−2.81771000	0.35354100
C	1.40131900	−1.43557200	−0.16054900

C	2.09741200	−0.45217300	−0.62071200
C	1.90064500	0.91830100	−1.18706600
C	3.84838600	1.55809700	0.21357200
C	4.98873700	2.56252500	0.41755700
C	4.26228400	0.11967200	0.20934600
C	4.62923500	−0.21524400	2.68281200
C	5.04135100	−1.88289500	0.83100800
C	5.52605500	−2.96655800	1.56360500
C	5.83877600	−4.12415800	0.85102400
C	5.67790400	−4.19450900	−0.54588000
C	5.17879800	−3.11280800	−1.26653200
C	4.83863000	−1.94573900	−0.56850000
C	4.30021200	−0.66005000	−0.97205500
C	4.33225000	−0.05617900	−2.35890400
C	4.04687100	1.45342300	−2.29313000
C	−3.40684000	0.69060400	1.39541800
C	−4.53359800	0.47205000	2.20341500
C	−4.83496300	1.36096200	3.23729500
C	−4.01870800	2.46969200	3.46981600
C	−2.89777800	2.69125700	2.66537800
C	−2.58476900	1.80623500	1.63300000
C	−3.92923100	−1.98478100	0.29175400
C	−5.17024600	−2.20953600	−0.32247600
C	−5.87278900	−3.39001000	−0.06952200
C	−5.34653400	−4.34966800	0.79726300
C	−4.11114900	−4.13085600	1.41335300
C	−3.40220200	−2.95702900	1.15909300
C	−3.63483000	0.31221200	−1.51777600
C	−4.63941900	1.29107100	−1.49041600
C	−5.13459500	1.81778100	−2.68544200
C	−4.63493300	1.37185700	−3.91056600
C	−3.63234800	0.39861900	−3.94362200
C	−3.12932600	−0.12627200	−2.75344200
H	2.81774900	2.77774500	−1.12926900
H	−0.10330100	5.85377900	1.33556100
H	0.12835100	6.13087300	−0.41861400
H	1.46740100	6.46135500	0.72579200
H	0.95815100	−3.52991800	−0.06456400
H	1.54819000	−2.84358400	1.44243100
H	2.68486000	−3.16126200	0.11463500
H	1.59688200	0.88501100	−2.23712300
H	1.12494700	1.45665200	−0.63148100
H	3.08026000	1.76881000	0.96556000
H	5.84440100	2.37466000	−0.23614400
H	5.33590700	2.49241700	1.45251500
H	4.61464000	3.57723400	0.25718000
H	5.64511500	−0.13927800	3.08251900
H	4.07011800	−0.95859400	3.25821500
H	4.13197500	0.74920800	2.78536800
H	5.66637300	−2.91537600	2.63851500
H	6.22538600	−4.98649300	1.38612700
H	5.94495800	−5.10938500	−1.06629100
H	5.04639400	−3.17670900	−2.34267100
H	3.61724500	−0.55967900	−3.01735700
H	5.32249000	−0.20749800	−2.80363200
H	3.53279000	1.81620300	−3.18498100
H	4.95800900	2.03711600	−2.16302600
H	−5.17511100	−0.38630800	2.03160500
H	−5.70790800	1.18366700	3.85932000
H	−4.25430200	3.15767300	4.27711900
H	−2.25820400	3.55148600	2.84149800
H	−1.70806000	1.99975000	1.01938400
H	−5.58961400	−1.46935900	−0.99646700
H	−6.83146700	−3.55740000	−0.55239200
H	−5.89525700	−5.26723600	0.99027200
H	−3.69645000	−4.87592500	2.08647100
H	−2.43898000	−2.79398500	1.63664100
H	−5.03411800	1.64410600	−0.54298400
H	−5.91053700	2.57755800	−2.65605100
H	−5.02200400	1.78479800	−4.83784900
H	−3.23810800	0.05250300	−4.89494100
H	−2.34415100	−0.87813100	−2.78264000

TS9

Au	−1.98765000	−0.97533600	−0.13600600
S	−0.36597800	4.36278300	0.28382500
P	−4.22431400	−1.63002900	0.22933900
O	0.55966200	4.26622600	−0.92659100
O	−1.62880200	3.60263100	0.06650800
O	0.34607600	4.02252500	1.54419900
N	3.28758000	−0.38358400	1.26851200
N	1.32899800	1.75254600	−1.10899900
C	−0.80139800	6.10439900	0.35725200
C	1.04261200	−2.26960000	0.74126400
C	1.08486600	−0.95062200	0.00056300
C	−0.03952100	−0.30342900	−0.44278900
C	−0.00887900	1.03976400	−1.09334000
C	2.05042900	1.56324500	0.20833300
C	3.26516500	2.48951000	0.31884800
C	2.41673400	0.09235900	0.28250500
C	3.25771400	−0.01218800	2.67924400
C	3.99446200	−1.46477200	0.76504700
C	4.92753000	−2.28466100	1.41167400
C	5.51271400	−3.29713800	0.65721000
C	5.17333300	−3.51214700	−0.69447300
C	4.22352300	−2.71513600	−1.32307600
C	3.62727200	−1.68282000	−0.58614800
C	2.63186700	−0.68141400	−0.93069700
C	2.38759400	−0.14363600	−2.32703500
C	2.15152900	1.37269100	−2.29907700
C	−4.66376200	−1.76967900	2.00793700
C	−4.67408400	−3.26131300	−0.48530800
C	−5.45528000	−0.45698200	−0.46426000
H	1.07613500	2.80806700	−1.13906000
H	−1.46799500	6.25843900	1.20930800
H	−1.30577900	6.38486800	−0.57004000
H	0.11015700	6.69240900	0.48468800
H	−0.00096400	−2.49965600	0.97033800
H	1.45125700	−3.09490500	0.14927900
H	1.58460300	−2.23927700	1.69085200
H	−0.35370200	0.97573100	−2.13248400
H	−0.70689900	1.71822100	−0.58464600
H	1.32552500	1.85089600	0.97435800
H	4.10517700	2.16901500	−0.30380200
H	3.60500600	2.51265400	1.35736200
H	2.97265200	3.50680500	0.04548500
H	2.92083600	−0.85302100	3.29585300
H	2.57031200	0.82197900	2.82296600
H	4.25605700	0.29313200	3.00722900
H	5.19633700	−2.13243200	2.45157400
H	6.25401400	−3.93945000	1.12378000
H	5.65738200	−4.31284100	−1.24459000
H	3.95037400	−2.88669700	−2.36021700
H	1.54719600	−0.65818300	−2.80059700

H	3.26960200	−0.35132800	−2.94077300
H	1.60880200	1.70891900	−3.18510300
H	3.08879800	1.92731700	−2.24364200
H	−4.01305200	−2.50338400	2.49454100
H	−5.70708000	−2.08333000	2.12462700
H	−4.52370000	−0.80211300	2.50072700
H	−4.51899600	−3.24814000	−1.56893300
H	−5.72303300	−3.49895400	−0.27605300
H	−4.03808100	−4.04214200	−0.05585600
H	−5.30247400	0.53690100	−0.03129600
H	−6.47559100	−0.79102200	−0.24548100
H	−5.32621800	−0.38342400	−1.54882100

TS9 (L = PPh_3)

Au	−0.76652400	−0.33513600	−0.21721100
S	2.09311500	4.43340600	0.25534300
P	−3.11933700	−0.38919000	0.04873500
O	2.98403500	4.12496600	−0.94478100
O	0.67740600	4.04742200	−0.00156600
O	2.66194300	3.87883200	1.51315700
N	4.48036300	−1.05732800	1.25857500
N	3.12417200	1.49387400	−1.13190700
C	2.14066700	6.22560300	0.38234000
C	1.84512400	−2.33160900	0.71588700
C	2.21616400	−1.06615000	−0.02652700
C	1.28926600	−0.16482200	−0.48134800
C	1.65296100	1.12957200	−1.12959500
C	3.76735400	1.13389900	0.19195300
C	5.16911600	1.73901900	0.31074000
C	3.76115800	−0.38208800	0.26582800
C	4.52954700	−0.68864800	2.66925500
C	4.90112200	−2.28062900	0.76033700
C	5.59312600	−3.30740100	1.41478000
C	5.91498800	−4.43421500	0.66406600
C	5.54790000	−4.55810200	−0.69181500
C	4.83371500	−3.54949200	−1.32840500
C	4.50598300	−2.40108200	−0.59517100
C	3.79083400	−1.18567200	−0.94627800
C	3.69965500	−0.60463300	−2.34384600
C	3.83888900	0.92412400	−2.31641800
C	−3.70053100	−1.78245500	1.09249600
C	−4.85130700	−2.52187600	0.78232000
C	−5.26109400	−3.56285800	1.61914900
C	−4.53042600	−3.87044500	2.76830100
C	−3.38320300	−3.13645400	3.08289000
C	−2.96603600	−2.10044900	2.24780800
C	−3.98134900	−0.55287800	−1.56325100
C	−5.12322200	0.19642600	−1.88143100
C	−5.74493900	0.03255800	−3.12179100
C	−5.23684200	−0.87942600	−4.04847800
C	−4.09919400	−1.62960500	−3.73694100
C	−3.46970700	−1.46422900	−2.50370400
C	−3.74298000	1.14315600	0.83701600
C	−4.90286100	1.14918000	1.62834300
C	−5.36059600	2.34322700	2.18813600
C	−4.66632300	3.53518100	1.96588700
C	−3.50830600	3.53423300	1.18470300
C	−3.04422700	2.34345000	0.62479100
H	3.13665300	2.57729800	−1.16250700
H	1.51766800	6.52918300	1.22711700
H	1.75566900	6.65868100	−0.54350700
H	3.17309000	6.54239900	0.54626500
H	0.77092500	−2.30694700	0.91555300
H	2.06210700	−3.23549700	0.13772700
H	2.35390900	−2.42026700	1.68009400
H	1.31233100	1.15109500	−2.17159700
H	1.13729100	1.95741700	−0.62553500
H	3.12777700	1.59201100	0.95134200
H	5.91283300	1.22423300	−0.30424800
H	5.49693600	1.68552700	1.35206500
H	5.13182500	2.79567100	0.03250800
H	3.97107700	−1.40661400	3.28051500
H	4.08911800	0.29957600	2.80429700
H	5.56829900	−0.66022500	3.01207300
H	5.87905100	−3.22797300	2.45822700
H	6.46631600	−5.24157900	1.13741800
H	5.82157400	−5.45487400	−1.23867300
H	4.53680500	−3.64809400	−2.36841800
H	2.76528300	−0.89890600	−2.82938400
H	4.51153100	−1.02066600	−2.94830600
H	3.40108500	1.38097500	−3.20647000
H	4.88235800	1.23386100	−2.25309600
H	−5.42752100	−2.29098900	−0.10823400
H	−6.15281800	−4.13160100	1.37091400
H	−4.85182800	−4.68117500	3.41612500
H	−2.81081600	−3.37310400	3.97550200
H	−2.07044300	−1.53538100	2.49498100
H	−5.52816900	0.90750500	−1.16856500
H	−6.62728800	0.61950600	−3.36079700
H	−5.72308500	−1.00363500	−5.01201300
H	−3.69813000	−2.33829800	−4.45612100
H	−2.58057500	−2.04521700	−2.27035200
H	−5.44707400	0.22746200	1.81080200
H	−6.25822700	2.34018800	2.80008100
H	−5.02411400	4.46168200	2.40618800
H	−2.95634300	4.45469700	1.01797300
H	−2.13486400	2.34912400	0.02988100

TS10

Au	−2.45541800	−0.71056700	−0.09054600
S	0.79688700	4.57044700	0.47220000
P	−4.80652300	−0.92010500	0.02341700
O	1.18194300	4.14949000	−1.06083100
O	−0.55971900	4.10331100	0.77233100
O	1.89158500	4.15012100	1.35512800
N	2.84182400	−1.73586900	1.21941500
N	1.45725100	1.16472400	−0.93048800
C	0.80520300	6.34203800	0.24893700
C	0.06177800	−2.72875300	0.86479400
C	0.50210300	−1.38500400	0.30211300
C	−0.38071800	−0.47981200	−0.18040400
C	−0.00328100	0.86296700	−0.77762600
C	2.19345900	0.92308800	0.18459700
C	3.62905000	1.30902300	0.33198100
C	2.00062000	−1.25650300	0.20173400
C	2.54878800	−1.75247100	2.64702800
C	4.07127400	−2.04107800	0.68434900
C	5.23208700	−2.51251900	1.32010300
C	6.34812600	−2.73396000	0.52618400
C	6.33590800	−2.48651800	−0.86882100
C	5.19908000	−2.00859800	−1.49525100
C	4.04128000	−1.78088500	−0.71783500
C	2.73750600	−1.30777500	−1.01920000
C	2.19720700	−0.77810200	−2.29261300

C	2.05048100	0.78914000	−2.21352800
C	−5.50249900	−2.27765500	−1.00324400
C	−5.72961800	0.57478500	−0.52029900
C	−5.44737900	−1.25917000	1.71370200
H	1.34963600	3.17410900	−1.06705800
H	0.53962100	6.78291700	1.21316600
H	0.06219600	6.60614100	−0.50603000
H	1.80504400	6.65895300	−0.05298300
H	−1.00619500	−2.87867600	0.68261700
H	0.60966700	−3.55278400	0.38813600
H	0.22741800	−2.81666700	1.94496500
H	−0.44481600	0.97286300	−1.77160600
H	−0.42948500	1.66193400	−0.16005800
H	1.61455400	0.98828400	1.10256700
H	4.21726700	1.25186400	−0.58317200
H	4.10734900	0.69335900	1.09866300
H	3.64068900	2.34345800	0.70362900
H	2.43090100	−2.77668600	3.01627400
H	1.62883700	−1.19756700	2.83400100
H	3.36148700	−1.27010100	3.19912400
H	5.25476000	−2.71333100	2.38621600
H	7.25631600	−3.11380900	0.98549400
H	7.23410700	−2.67829500	−1.44803900
H	5.19003700	−1.82225400	−2.56550300
H	1.20456000	−1.19505100	−2.49466100
H	2.84828400	−1.01467400	−3.13904100
H	1.40929800	1.15041300	−3.01922500
H	3.02855700	1.25997700	−2.31647800
H	−5.24568700	−2.11470800	−2.05501000
H	−6.59287700	−2.32367200	−0.90518000
H	−5.07484600	−3.23571300	−0.69025600
H	−5.45671100	1.42791300	0.10939400
H	−6.81120500	0.41197500	−0.45422500
H	−5.46803200	0.81498600	−1.55602500
H	−5.01456700	−2.19052500	2.09330300
H	−6.53958300	−1.34744600	1.70988600
H	−5.15759800	−0.44676100	2.38809700

TS10 (L = PPh_3)

Au	1.04378900	−0.31754100	0.09733400
S	−2.93026300	4.53940500	−0.45970300
P	3.41474900	−0.27816700	0.01162000
O	−3.18200000	4.07287400	1.08836300
O	−1.56722000	4.16982300	−0.85314800
O	−4.04787100	4.05717200	−1.27903400
N	−4.09235000	−1.97074000	−1.21273300
N	−3.06449600	1.06541000	0.95059400
C	−3.04960600	6.30257400	−0.20407500
C	−1.20658800	−2.61587500	−0.87683600
C	−1.80716300	−1.33692900	−0.31130000
C	−1.04258100	−0.33126500	0.17392300
C	−1.58000500	0.95426900	0.77392300
C	−3.78259500	0.74304700	−0.15492700
C	−5.25823600	0.94170900	−0.27741600
C	−3.30827000	−1.39941800	−0.19889900
C	−3.81541400	−1.93299300	−2.64289900
C	−5.27065400	−2.42768800	−0.67015800
C	−6.37205100	−3.02804200	−1.30246700
C	−7.44782400	−3.38673900	−0.50283300
C	−7.45263400	−3.15212100	0.89425100
C	−6.37489900	−2.54858500	1.51742000
C	−5.25939600	−2.17706400	0.73398000
C	−4.02068600	−1.54774300	1.02798400
C	−3.53428800	−0.96748600	2.30126000
C	−3.58486900	0.60683100	2.23827300
C	4.09975800	1.41280200	−0.19024400
C	5.26176200	1.66573400	−0.93554000
C	5.75460100	2.96780500	−1.04573100
C	5.09575300	4.02462300	−0.41371400
C	3.93759800	3.77983700	0.32864200
C	3.43822800	2.48181900	0.43719800
C	4.06546000	−1.26267800	−1.39612400
C	5.20336400	−2.07585700	−1.28742600
C	5.65376900	−2.80324200	−2.39188800
C	4.97803600	−2.72222300	−3.61082900
C	3.84452500	−1.91269700	−3.72635500
C	3.38615800	−1.19050900	−2.62472500
C	4.19471500	−0.97086700	1.52397400
C	5.37052000	−0.43953800	2.07464900
C	5.92748500	−1.00911000	3.22205100
C	5.32030600	−2.11238000	3.82498800
C	4.14868000	−2.64657200	3.28189400
C	3.58401400	−2.07616700	2.14109300
H	−3.21565000	3.08416700	1.09797900
H	−2.89877400	6.77391100	−1.17865300
H	−2.26939700	6.61292700	0.49349100
H	−4.04239200	6.53863600	0.18347000
H	−0.12406200	−2.62296400	−0.72120000
H	−1.62988900	−3.49955300	−0.37988100
H	−1.38631300	−2.73694500	−1.95162800
H	−1.14113400	1.12509100	1.76021200
H	−1.27203800	1.79809700	0.14593800
H	−3.23146200	0.88686000	−1.08127400
H	−5.81712100	0.82714000	0.65102100
H	−5.67156900	0.25740800	−1.02388500
H	−5.40824800	1.96013300	−0.66338600
H	−3.59482700	−2.93325500	−3.03009300
H	−2.96039100	−1.28200800	−2.82752800
H	−4.68036000	−1.52937300	−3.17901500
H	−6.37923200	−3.21940100	−2.37062400
H	−8.30930700	−3.86554200	−0.95964300
H	−8.31698700	−3.45317000	1.47848000
H	−6.38005300	−2.37162200	2.58926300
H	−2.49542600	−1.26055100	2.48870500
H	−4.14121100	−1.29051300	3.15188400
H	−2.98129100	1.03895800	3.03812600
H	−4.61249700	0.94931300	2.36054600
H	5.78108700	0.85210200	−1.43245900
H	6.65347900	3.15434400	−1.62675700
H	5.48011300	5.03682200	−0.50334800
H	3.41806600	4.59971400	0.81666200
H	2.53123800	2.29766800	1.00769800
H	5.73710600	−2.14838900	−0.34502700
H	6.53409300	−3.43270900	−2.29649900
H	5.33021400	−3.29080100	−4.46695300
H	3.31304700	−1.84817600	−4.67173000
H	2.49709800	−0.57142300	−2.71761800
H	5.85193200	0.41736900	1.61403800
H	6.83641300	−0.58836700	3.64299300
H	5.75575400	−2.55231300	4.71787100
H	3.67020700	−3.50234100	3.75000300
H	2.66627100	−2.48867400	1.72924300

TS10'

Au	−2.30068000	0.03094900	0.01974000
P	−4.61699900	−0.36195300	−0.24210700
N	3.07219300	−1.22050100	0.66903700
N	1.45161600	2.22259100	0.78892500
C	0.41653900	−1.92364300	−0.40278100
C	0.70588300	−0.51276400	0.08249200
C	−0.26242800	0.41525200	0.25453700
C	0.02207800	1.84729300	0.68589900
C	2.20572700	1.33876100	1.49337200
C	3.61321700	1.65226100	1.92168300
C	2.19481400	−0.22319300	0.18097300
C	2.81233000	−2.10696500	1.79455900
C	4.28950700	−1.09308200	0.05598300
C	5.48034300	−1.80804700	0.27725400
C	6.58442200	−1.45679700	−0.48359000
C	6.53575800	−0.41026000	−1.44042700
C	5.37308000	0.30567800	−1.65091400
C	4.22345800	−0.02890700	−0.89655500
C	2.90989300	0.49299300	−0.83816700
C	2.33162800	1.69109900	−1.48069900
C	2.05715000	2.81061500	−0.38834800
C	−5.33313300	−1.54401100	0.97053700
C	−5.08336700	−1.06319300	−1.87702200
C	−5.66808300	1.13820400	−0.08087300
H	0.98224300	−2.14478900	−1.31862100
H	−0.64874500	−2.03438000	−0.62508600
H	0.68577400	−2.69411300	0.32940100
H	−0.44659500	2.55171600	−0.00637400
H	−0.43505200	2.02915200	1.66656800
H	1.63141000	0.81357600	2.25442400
H	4.24860100	2.06512600	1.13809700
H	4.09473500	0.75737900	2.32328600
H	3.55519200	2.38324200	2.73968500
H	2.84767300	−3.15627100	1.48356300
H	1.82262500	−1.89236000	2.19947500
H	3.55475700	−1.94897100	2.58465900
H	5.53279800	−2.61158000	1.00445500
H	7.51506300	−2.00017200	−0.34658500
H	7.42819800	−0.17612600	−2.01281100
H	5.33630600	1.10496500	−2.38564500
H	1.36876700	1.45547300	−1.94778400
H	2.99372700	2.10793900	−2.24489500
H	1.38806400	3.56790200	−0.80000400
H	2.99713400	3.29449000	−0.12014800
H	−4.81928000	−2.50779100	0.89523900
H	−6.40277100	−1.69330900	0.78540900
H	−5.19640500	−1.16063200	1.98693400
H	−4.78705900	−0.37435700	−2.67478700
H	−6.16416200	−1.23395600	−1.93511500
H	−4.56284600	−2.01362400	−2.03356300
H	−5.53069600	1.58379100	0.90980800
H	−6.72701000	0.89192500	−0.21813700
H	−5.37334700	1.87769400	−0.83251100

TS11

Au	2.22354200	−0.50389300	−0.00788600
S	−0.01828200	3.65895000	−0.16300400
P	4.34782600	−1.44247100	−0.22588700
O	1.14298100	2.62346600	−0.27094500
O	−0.57462800	3.66983000	1.21435000
O	−1.00002500	3.47717500	−1.25169500
N	−3.13277500	−0.15279200	−1.46029700
N	−1.48861300	0.21357000	2.28720600
C	0.84294400	5.21029800	−0.42056300
C	−0.25183400	0.15164900	−2.17275400
C	−0.71312200	−0.03395600	−0.73599500
C	0.18997800	0.22142300	0.28022400
C	−0.08544000	0.33610100	1.78546100
C	−2.23819100	1.26385300	2.34792100
C	−3.64828100	1.35471400	2.78891300
C	−2.09878000	−0.49019600	−0.57682300
C	−3.19771800	1.00701800	−2.34756600
C	−4.22665100	−0.94371900	−1.17709900
C	−5.49866200	−0.96738000	−1.77107400
C	−6.42094500	−1.88238100	−1.27962400
C	−6.10093800	−2.75842300	−0.21704100
C	−4.84807500	−2.73035300	0.37574600
C	−3.89052600	−1.81120500	−0.10085500
C	−2.54558900	−1.50431300	0.27133200
C	−1.78270000	−2.08353900	1.41912700
C	−1.89057500	−1.16127200	2.65214000
C	4.37531300	−3.25605500	0.05881800
C	5.58918500	−0.76272500	0.94341200
C	5.09063800	−1.21432000	−1.88950800
H	0.76528200	1.42555100	−0.07974000
H	1.29944400	5.19929500	−1.41235800
H	1.60472500	5.32900500	0.35241600
H	0.10581300	6.01446400	−0.35395600
H	0.83633800	0.08927400	−2.24636900
H	−0.68843900	−0.60601000	−2.83161500
H	−0.54465400	1.13819400	−2.54806100
H	0.48453300	−0.41184900	2.34081400
H	0.26735100	1.31753500	2.11392300
H	−1.76041300	2.19084600	2.01846200
H	−4.10954300	0.42114200	3.10753200
H	−4.23046300	1.78214300	1.96138600
H	−3.70309100	2.08885400	3.60391100
H	−2.91353800	0.74949700	−3.37336000
H	−2.55183900	1.80408600	−1.97577200
H	−4.22345000	1.38353300	−2.35550200
H	−5.75412200	−0.31164900	−2.59726700
H	−7.40899300	−1.93162900	−1.72862700
H	−6.84986800	−3.46187700	0.13535200
H	−4.60870700	−3.40713800	1.19205700
H	−0.72789300	−2.23376700	1.16078100
H	−2.18323100	−3.06098900	1.70770800
H	−1.22410900	−1.48705800	3.45675800
H	−2.91040200	−1.14781300	3.02974400
H	4.01283700	−3.47757000	1.06772200
H	5.39139200	−3.65106200	−0.05144900
H	3.71741300	−3.75255200	−0.66153800
H	5.70211900	0.31332500	0.77722000
H	6.55965400	−1.25185100	0.80277300
H	5.25359300	−0.92038700	1.97328400
H	4.45072000	−1.67733800	−2.64736400
H	6.08638000	−1.66943500	−1.93379400
H	5.17338400	−0.14590700	−2.11290000

TS11 (L = PPh_3)

Au	−0.88015000	0.06593100	−0.07999300
S	1.96302200	3.81006400	0.18982700
P	−3.15889500	−0.45195800	0.06073500
O	0.66889300	2.94571600	0.27820200

O	2.52837900	3.75736800	−1.18263500
O	2.90013700	3.48582000	1.28469100
N	4.44839000	−0.44099500	1.48435900
N	2.94024700	0.20740100	−2.30345500
C	1.32030600	5.46323500	0.45436800
C	1.62337000	0.25840700	2.14660400
C	2.08741800	0.03004900	0.71605300
C	1.25442300	0.43410600	−0.31126800
C	1.56091700	0.51462400	−1.81147800
C	3.81933300	1.15141900	−2.37045000
C	5.22709100	1.05674900	−2.81847900
C	3.39623000	−0.61775800	0.57567200
C	4.64493400	0.67543300	2.40696100
C	5.43311400	−1.36340100	1.19984700
C	6.67861500	−1.57006600	1.81409400
C	7.47996000	−2.58943200	1.31636000
C	7.06669600	−3.39248400	0.22841800
C	5.84054500	−3.18429200	−0.38394800
C	5.00571200	−2.15479700	0.09768100
C	3.72107800	−1.66324500	−0.28908500
C	2.90623800	−2.11884100	−1.45742700
C	3.15763700	−1.20718500	−2.67581300
C	−3.91005100	0.17291000	1.61236900
C	−4.93051700	−0.52300800	2.27840900
C	−5.48617800	0.00207100	3.44726600
C	−5.03031200	1.21977500	3.95685700
C	−4.01333400	1.91598700	3.29827500
C	−3.45093000	1.39453500	2.13330400
C	−3.47175500	−2.25836900	0.01649400
C	−4.58753100	−2.80584300	−0.63476400
C	−4.79782300	−4.18670800	−0.62044100
C	−3.90180900	−5.02763400	0.04266300
C	−2.78781300	−4.48790800	0.69155100
C	−2.56920800	−3.11064800	0.67535100
C	−4.11356300	0.28157000	−1.32314300
C	−5.39658200	0.81882600	−1.14050400
C	−6.08865600	1.36182700	−2.22568600
C	−5.51005200	1.36998800	−3.49611900
C	−4.23245800	0.83530600	−3.68441100
C	−3.53452900	0.29774400	−2.60353100
H	0.86750500	1.70292100	0.06213100
H	0.84854800	5.50565700	1.43828700
H	0.59554600	5.69221800	−0.32941500
H	2.16077800	6.16052300	0.40913300
H	0.53354500	0.31079300	2.19821400
H	1.96136800	−0.54500500	2.80870100
H	2.01330200	1.20608400	2.53422200
H	0.90283900	−0.15087000	−2.37459400
H	1.34365500	1.53433300	−2.14118100
H	3.46833200	2.13399400	−2.04330700
H	5.56532400	0.06662600	−3.12029100
H	5.86382200	1.42525500	−2.00298500
H	5.36727700	1.76101300	−3.64960000
H	4.29416400	0.43459700	3.41596700
H	4.12838700	1.56369700	2.03998800
H	5.71210200	0.90497800	2.45539100
H	7.00252200	−0.97233200	2.66003700
H	8.44349600	−2.77973100	1.78073200
H	7.72176600	−4.18261800	−0.12736900
H	5.52751900	−3.80509700	−1.21971700
H	1.83688300	−2.13056200	−1.21678300
H	3.17712700	−3.13765600	−1.75386400
H	2.46687500	−1.43188700	−3.49455800
H	4.17600800	−1.32881300	−3.03749700
H	−5.29018100	−1.47145000	1.89153100
H	−6.27409700	−0.54313000	3.95916700
H	−5.46284800	1.62369300	4.86788700
H	−3.65171400	2.86071800	3.69422900
H	−2.65305100	1.93402200	1.62934500
H	−5.29018300	−2.16139700	−1.15402600
H	−5.66312300	−4.60317000	−1.12833400
H	−4.06831700	−6.10110000	0.05071000
H	−2.08582500	−5.13896600	1.20493200
H	−1.69671100	−2.69582100	1.17417800
H	−5.85599200	0.82088500	−0.15706400
H	−7.08008700	1.77937900	−2.07470800
H	−6.04993300	1.79640900	−4.33683700
H	−3.77635600	0.84430700	−4.67037000
H	−2.53612700	−0.10638600	−2.75179900

TS12

Au	2.04030700	−0.88308600	0.18955300
S	0.51887300	3.65102100	−0.47473600
P	4.30130400	−1.17442500	−0.41501600
O	−0.53441800	2.68498900	−1.14653800
O	1.88664100	3.19288300	−0.74730100
O	0.14031900	3.85072400	0.94562500
N	−3.68300500	0.33313400	−0.85669100
N	−1.41256600	1.31373700	1.87594500
C	0.25187800	5.18760600	−1.35904500
C	−0.85332600	−2.41895000	−0.65104100
C	−1.00370600	−1.25170600	0.29773100
C	0.05022700	−0.53142900	0.72960900
C	−0.03721700	0.65627700	1.64436700
C	−2.19069000	1.64889700	0.61808600
C	−3.02729200	2.91334200	0.83123800
C	−2.79216100	0.46091700	0.13282200
C	−4.09956200	1.35879400	−1.81095100
C	−4.19848600	−0.99646400	−0.88614300
C	−5.22158800	−1.50058700	−1.67882800
C	−5.58443300	−2.83810900	−1.47364900
C	−4.94500100	−3.61853200	−0.50676800
C	−3.91128500	−3.08531600	0.27614100
C	−3.53554400	−1.76265300	0.07722300
C	−2.47741100	−0.89926900	0.73771000
C	−2.59967300	−0.84674400	2.29494100
C	−2.24623700	0.53704200	2.86393500
C	4.69748500	−0.57251200	−2.10676800
C	4.90405900	−2.91234100	−0.40139300
C	5.48060900	−0.27546700	0.67268600
H	−1.18002600	2.22207200	2.29299400
H	0.44485600	5.01889700	−2.42063500
H	0.95370500	5.92525000	−0.96191200
H	−0.77655700	5.51850900	−1.20196800
H	0.20380000	−2.56800100	−0.88742600
H	−1.24046100	−3.35234800	−0.22426600
H	−1.39053500	−2.25625100	−1.59444200
H	0.32288400	0.40625200	2.64949700
H	0.58790500	1.47038500	1.28044000
H	−1.21695100	2.16107700	−0.36662200
H	−3.48141800	3.25138400	−0.10147600
H	−3.83646100	2.77103200	1.55990600
H	−2.38058100	3.72481600	1.17828400
H	−4.31951300	0.87242000	−2.76312600

H	−3.28292600	2.06367000	−1.96991800
H	−4.99256300	1.88620600	−1.46185100
H	−5.73680200	−0.89172900	−2.41386500
H	−6.38362600	−3.26668200	−2.07090400
H	−5.25243700	−4.64914700	−0.35765800
H	−3.41852300	−3.69993300	1.02381700
H	−1.94498900	−1.61354600	2.71498400
H	−3.62394300	−1.08824400	2.59180800
H	−1.67444900	0.46607100	3.79155000
H	−3.13912200	1.13614200	3.05202400
H	4.09406200	−1.11390500	−2.84262500
H	5.75904100	−0.71911000	−2.33624400
H	4.45722900	0.49275200	−2.18311600
H	4.79040100	−3.33707300	0.60128100
H	5.95871000	−2.96153900	−0.69435300
H	4.31111900	−3.51453400	−1.09753100
H	5.24158300	0.79298900	0.66991900
H	6.51230400	−0.41232500	0.32976100
H	5.39325600	−0.64539400	1.69954000

TS12 (L = PPh_3)

Au	0.77575200	−0.44108300	0.39189300
S	−1.54835000	3.86478300	−0.43278200
P	3.09506000	−0.37773200	−0.09473400
O	−2.35754000	2.70872400	−1.14557100
O	−0.10389300	3.65736400	−0.59599800
O	−2.05632700	4.01439000	0.95188900
N	−5.01159000	−0.22185300	−0.90862700
N	−3.05763300	1.22433000	1.86091000
C	−2.02455800	5.30684200	−1.38507200
C	−1.78491400	−2.48135400	−0.44763000
C	−2.16788300	−1.30188700	0.41668100
C	−1.26579100	−0.39529300	0.84168800
C	−1.58444300	0.81236900	1.67712200
C	−3.84843000	1.37613200	0.57680600
C	−4.92144700	2.45976400	0.72786900
C	−4.20474300	0.08698100	0.11346500
C	−5.52570400	0.68608700	−1.93136400
C	−5.30139000	−1.61747100	−0.90150100
C	−6.18907300	−2.31241800	−1.71297900
C	−6.34172700	−3.68229400	−1.46149400
C	−5.63487000	−4.30999300	−0.43254000
C	−4.73933500	−3.58546000	0.36717600
C	−4.57154800	−2.22801100	0.12334900
C	−3.69692200	−1.17904900	0.78645600
C	−3.88617600	−1.09201300	2.33491500
C	−3.76788800	0.34823100	2.86322500
C	3.50484400	0.80546700	−1.43662500
C	4.56539000	0.58343000	−2.32967000
C	4.84876100	1.51875100	−3.32695400
C	4.07956200	2.67933800	−3.44073300
C	3.02163500	2.90358800	−2.55665200
C	2.72950200	1.97055100	−1.56090900
C	3.77935400	−1.99800800	−0.62761000
C	5.02582000	−2.46952700	−0.19014400
C	5.50394100	−3.70472400	−0.63486400
C	4.74663700	−4.47494900	−1.51920300
C	3.50446600	−4.01021900	−1.96037900
C	3.01998600	−2.78103000	−1.51385000
C	4.08536500	0.13317100	1.36653200
C	5.19229800	0.98855600	1.26350800
C	5.91580400	1.34058300	2.40559400
C	5.54322400	0.84260200	3.65552100
C	4.44138300	−0.01006900	3.76534900
C	3.71097100	−0.35813900	2.62916700
H	−2.99647100	2.17348000	2.24728300
H	−1.73511000	5.14940200	−2.42627700
H	−1.49372300	6.16826000	−0.97219700
H	−3.10375700	5.44954800	−1.30278700
H	−0.70895700	−2.46291800	−0.63928700
H	−2.02806900	−3.43939600	0.02831300
H	−2.30175900	−2.47022800	−1.41570600
H	−1.20179500	0.69563000	2.69791300
H	−1.10597100	1.69966100	1.26446900
H	−2.95016800	2.06624600	−0.39699800
H	−5.40874800	2.66796100	−0.22596600
H	−5.70586900	2.18308400	1.44473400
H	−4.45761900	3.39414700	1.05695500
H	−5.57566400	0.14437300	−2.87809300
H	−4.83766300	1.52318400	−2.05334000
H	−6.52444000	1.05194500	−1.67362000
H	−6.75857500	−1.82501500	−2.49716800
H	−7.03117500	−4.25795500	−2.07176900
H	−5.78100700	−5.36985200	−0.24749900
H	−4.19194700	−4.08214200	1.16296300
H	−3.13949400	−1.73573600	2.80523400
H	−4.87200900	−1.47754500	2.60822600
H	−3.20574900	0.39861300	3.79809400
H	−4.74841500	0.80008400	3.02387500
H	5.16749000	−0.31664300	−2.25248200
H	5.66989800	1.33809500	−4.01514400
H	4.30114100	3.40365400	−4.21978900
H	2.41289200	3.79899600	−2.64267500
H	1.89400600	2.15342500	−0.89107300
H	5.62343700	−1.87835700	0.49647300
H	6.46960300	−4.06247200	−0.28851600
H	5.12071400	−5.43570700	−1.86186000
H	2.91030500	−4.60668200	−2.64712000
H	2.05076600	−2.42691000	−1.85612900
H	5.49168600	1.38232600	0.29730600
H	6.76973900	2.00616600	2.31548500
H	6.10736100	1.11934800	4.54183100
H	4.14481000	−0.39690600	4.73638500
H	2.84761000	−1.01255400	2.72186100

TS13

Au	−1.92423200	−0.57117900	−0.01160100
S	−0.45399000	3.84873300	−0.31229700
P	−3.85376300	−1.83048100	−0.33183800
O	−1.37258600	2.60495400	−0.50074500
O	−0.17966700	4.07550900	1.12873700
O	0.73527000	3.77000200	−1.18704900
N	3.27000300	−1.94777900	0.71814300
N	1.51752200	0.85603400	2.42319200
C	−1.50279000	5.18296600	−0.89608000
C	0.71469500	0.18785200	−1.93971200
C	0.97484900	0.24979900	−0.46021600
C	−0.05695600	0.49687600	0.40362500
C	0.09336400	0.74476800	1.89173400
C	2.22859800	−0.45221200	2.40581500
C	2.33968200	−1.10299000	3.75227200
C	2.62527400	−0.81041400	1.16695600
C	3.51710800	−3.16499800	1.46939800
C	3.82450400	−1.70538800	−0.55319300

C	4.69994700	−2.51112300	−1.27789100
C	5.15803900	−2.03050300	−2.51189800
C	4.76609700	−0.77980200	−2.99193500
C	3.88320000	0.01703300	−2.24774300
C	3.40142600	−0.45697800	−1.03438100
C	2.45985800	0.16842300	−0.01108500
C	2.92415500	1.58337800	0.43768500
C	2.30895200	1.99530900	1.78624000
C	−3.84537300	−3.43579900	0.55864900
C	−4.15592200	−2.26667900	−2.08903100
C	−5.39064900	−0.98825000	0.21316400
H	1.41084400	1.11970300	3.40745000
H	−0.79825800	1.49969900	−0.12250800
H	−0.94139000	6.11550400	−0.79716300
H	−2.40800900	5.22061500	−0.28643600
H	−1.75243000	5.00303700	−1.94380700
H	1.25993800	0.98900100	−2.45349700
H	−0.34935300	0.30636300	−2.15776100
H	1.05724300	−0.76014500	−2.36885500
H	−0.39006600	1.69323000	2.14831600
H	−0.36863200	−0.04843200	2.48663800
H	3.04106200	−1.93746300	3.73962000
H	2.71633500	−0.38543900	4.49558300
H	1.37653800	−1.48105900	4.12487700
H	3.61975300	−3.99691200	0.76829200
H	2.66512200	−3.38092200	2.11719400
H	4.43097700	−3.10544000	2.07513500
H	5.04218900	−3.46860500	−0.89952500
H	5.84549200	−2.63981200	−3.09192600
H	5.14885700	−0.41682100	−3.94090500
H	3.58985700	0.99397600	−2.62040600
H	2.65126000	2.31954200	−0.32337700
H	4.01392300	1.56895700	0.52075500
H	1.61466100	2.83319100	1.69296900
H	3.08401900	2.24746800	2.51190500
H	−2.97976300	−4.02862900	0.24625500
H	−4.76113600	−3.99929400	0.34719200
H	−3.77524300	−3.26127800	1.63706400
H	−4.26703000	−1.35332800	−2.68177600
H	−5.06687900	−2.86856900	−2.18247500
H	−3.30759600	−2.83495100	−2.48331600
H	−5.33249800	−0.75969200	1.28197600
H	−6.26388700	−1.62368100	0.02800700
H	−5.50646500	−0.04830700	−0.33578700

TS13 (L = PPh_3)

Au	−0.68771000	0.21051300	0.09806100
S	1.88072100	4.07038500	−0.37464800
P	−2.92114400	−0.44730200	−0.08043000
O	0.67827700	3.09347700	−0.53361800
O	2.21854300	4.24704500	1.06025000
O	3.00411900	3.68275800	−1.25364100
N	3.98394400	−2.48908700	0.75936800
N	3.09166600	0.73510500	2.38548000
C	1.19163100	5.61417900	−0.97614000
C	1.98925100	0.14324000	−1.92487900
C	2.31044100	0.19446200	−0.45682100
C	1.41128600	0.73800300	0.41963000
C	1.67110900	0.98546400	1.89334500
C	3.43466500	−0.71366700	2.40646100
C	3.43403300	−1.32032600	3.77752400
C	3.67722900	−1.20688500	1.17441800
C	3.92554300	−3.69993000	1.55760500
C	4.54029400	−2.44579200	−0.53326600
C	5.15033300	−3.47833500	−1.24200500
C	5.67978000	−3.17809200	−2.50415100
C	5.61563500	−1.88545700	−3.02714400
C	4.99597600	−0.85896500	−2.29856200
C	4.44518900	−1.14717700	−1.05654500
C	3.73623300	−0.26032200	−0.03909400
C	4.57441700	0.99310600	0.34156300
C	4.13062400	1.60388200	1.68146600
C	−3.14452800	−2.25992400	0.08103400
C	−4.12284600	−2.95361500	−0.64757900
C	−4.27479000	−4.33173300	−0.47925400
C	−3.45776100	−5.02503300	0.41591400
C	−2.48232100	−4.33927100	1.14486100
C	−2.32142800	−2.96427600	0.97564300
C	−3.65304000	0.02763000	−1.69335200
C	−4.92377700	0.61325300	−1.79024000
C	−5.44224500	0.95488900	−3.04176100
C	−4.70242000	0.71140900	−4.19991400
C	−3.43585600	0.12646000	−4.10903100
C	−2.90923100	−0.20892300	−2.86250700
C	−3.94959800	0.33167600	1.22209100
C	−5.03585400	−0.33470600	1.80985200
C	−5.80256800	0.30489100	2.78634800
C	−5.49500200	1.60903500	3.17981000
C	−4.41529700	2.27776100	2.59678000
C	−3.64140500	1.64204600	1.62599300
H	3.09062200	1.05095900	3.35994800
H	0.94866100	1.88633500	−0.12817200
H	1.97326500	6.37559700	−0.91204000
H	0.34020100	5.89317200	−0.35213100
H	0.87959400	5.48299200	−2.01428200
H	2.72056900	0.72589200	−2.49773500
H	0.99530000	0.55141700	−2.12325700
H	2.02877600	−0.88275200	−2.30774700
H	1.46289600	2.03550100	2.12419100
H	1.03667900	0.36168100	2.52958500
H	3.88373600	−2.31323800	3.77887600
H	4.02589700	−0.70406400	4.46992400
H	2.42469300	−1.40964800	4.20475700
H	3.78601100	−4.55482900	0.89146300
H	3.06561500	−3.65927500	2.22930800
H	4.83988100	−3.86049100	2.14389000
H	5.23994400	−4.47852500	−0.83168200
H	6.16476400	−3.96659000	−3.07275800
H	6.05150200	−1.66913100	−3.99772400
H	4.95850000	0.14758600	−2.70459000
H	4.48635600	1.74873400	−0.44371700
H	5.62241000	0.68889300	0.40448600
H	3.67328000	2.58822100	1.56237400
H	4.96696000	1.67586800	2.37880100
H	−4.76355800	−2.42528900	−1.34663800
H	−5.03229700	−4.86143000	−1.04986000
H	−3.57731500	−6.09735400	0.54234800
H	−1.84186200	−4.87586800	1.83923900
H	−1.55422000	−2.43599100	1.53638000
H	−5.50906600	0.80651400	−0.89704100
H	−6.42554200	1.41187200	−3.10756600
H	−5.10788600	0.98062300	−5.17110800
H	−2.85483700	−0.06092900	−5.00752800
H	−1.91983700	−0.65474800	−2.79838100

H	−5.28473500	−1.34861400	1.51231400
H	−6.63990100	−0.21847400	3.23914000
H	−6.09253100	2.10225300	3.94132300
H	−4.16998900	3.29115100	2.90163800
H	−2.79679800	2.16270000	1.18153600

TS14

Au	2.58740700	−0.74762300	0.06788400
S	−0.20177700	4.10215500	−0.06457400
P	4.88853900	−0.83697000	−0.32287900
O	−0.72869900	3.74566200	1.31891400
O	1.19450400	3.62476300	−0.26273100
O	−1.15228700	3.66906400	−1.12788500
O	−3.73500300	2.38872100	0.83169400
O	−3.69762000	1.81336600	−1.35185400
N	−2.97589900	−1.20515300	−1.11717200
N	−1.26427000	1.17081100	1.27522200
C	−0.15606500	5.89850900	−0.07284000
C	−0.32714600	−2.68171200	−0.76716100
C	−0.22782200	−1.40260700	−0.05218900
C	0.50109000	−0.48941600	0.47643000
C	0.20340100	0.78599900	1.18504500
C	−1.99530800	0.88717600	−0.01091800
C	−3.24206200	1.79959000	−0.10347300
C	−4.82682100	2.68340400	−1.60408300
C	−2.34133500	−0.58544200	−0.04255200
C	−2.89579900	−0.84068900	−2.52821300
C	−3.57513200	−2.35642200	−0.65331600
C	−4.28652500	−3.33652300	−1.36329000
C	−4.79241600	−4.40457300	−0.63620200
C	−4.59393000	−4.52136700	0.76188600
C	−3.87688000	−3.56742400	1.46129100
C	−3.35411700	−2.46193700	0.75320800
C	−2.59548400	−1.32333900	1.13319400
C	−2.14904200	−0.86409200	2.48717200
C	−1.96586600	0.65549400	2.50940600
C	5.81862300	−1.82022400	0.91675200
C	5.33541100	−1.56403500	−1.94771500
C	5.66548200	0.82429300	−0.30655900
H	−1.19917500	2.25563400	1.35360700
H	0.21547400	6.23132700	−1.04512100
H	0.51203400	6.23954900	0.72121000
H	−1.16625900	6.27861700	0.09438400
H	−1.09035800	−3.33562500	−0.33501300
H	0.63508100	−3.19801100	−0.66897000
H	−0.53767200	−2.54732000	−1.83301700
H	0.58056500	0.76044300	2.21087300
H	0.70024600	1.62072200	0.67886900
H	−1.33274600	1.18919700	−0.82442500
H	−5.04098200	2.57509000	−2.66698200
H	−4.55679600	3.71499700	−1.36996800
H	−5.68644900	2.37483100	−1.00435500
H	−3.88764100	−0.59067600	−2.91459000
H	−2.48551000	−1.67574500	−3.10525200
H	−2.24912900	0.02640400	−2.65041800
H	−4.45015800	−3.25819700	−2.43300300
H	−5.36061700	−5.17279000	−1.15272400
H	−5.01278400	−5.37530600	1.28530400
H	−3.72205600	−3.66019900	2.53228200
H	−1.21881000	−1.36794700	2.77795800
H	−2.89352900	−1.13105900	3.24513400
H	−1.36432700	0.98007200	3.36062900
H	−2.92384600	1.17146500	2.54136300
H	5.65967100	−1.40146300	1.91548600
H	6.89059500	−1.80797100	0.68974000
H	5.46242000	−2.85524900	0.91270700
H	4.96429700	−2.59196800	−2.00972500
H	6.42291400	−1.56754800	−2.08166000
H	4.87650500	−0.98011100	−2.75181000
H	5.20349000	1.45533500	−1.07229300
H	6.74105700	0.74852000	−0.50178200
H	5.51014500	1.29704700	0.66839200

TS15

Au	2.22010800	−1.25813200	0.00452400
S	0.81653600	3.57826800	−0.11866500
P	4.44308500	−0.57922700	−0.25000800
O	0.12064400	3.59364200	1.23005100
O	2.03363100	2.71800100	−0.11068500
O	−0.13833500	3.25834400	−1.22178000
O	−3.25601900	3.33687700	0.81733700
O	−3.83162600	2.38786500	−1.15381000
N	−3.09123300	−0.70893400	−1.12973300
N	−1.36364200	1.40425800	1.35712700
C	1.36684900	5.27034900	−0.36574100
C	−0.19931800	−3.16509300	−0.42742500
C	0.14464900	−1.82319000	0.14540000
C	−0.48714400	−0.84103400	0.69507500
C	−0.17444300	0.47983700	1.32578700
C	−2.10431500	1.33340800	0.05068600
C	−3.13733400	2.47625700	−0.02321500
C	−4.79088100	3.44979100	−1.39879700
C	−2.63689500	−0.06346700	−0.03124900
C	−3.02796200	−0.26856300	−2.52130200
C	−3.50083200	−1.99491100	−0.74685400
C	−4.04861400	−3.01190000	−1.52948600
C	−4.39099500	−4.19639400	−0.87820300
C	−4.19843300	−4.35702600	0.50737100
C	−3.63482700	−3.34267100	1.27651200
C	−3.26385200	−2.15124600	0.63837700
C	−2.65767700	−0.91674000	1.10201700
C	−2.61855600	−0.40297400	2.52392900
C	−2.24234100	1.08671600	2.54355500
C	5.70142000	−1.84785300	0.17393500
C	4.83836400	0.87986400	0.78819500
C	4.83921500	−0.06199600	−1.96558600
H	−0.93069300	2.38992500	1.42028800
H	1.88326500	5.33247700	−1.32668600
H	2.04729000	5.54156600	0.44455000
H	0.49595600	5.92938800	−0.36330100
H	0.53689300	−3.91247600	−0.11529000
H	−0.16327900	−3.12526400	−1.52302200
H	−1.19139200	−3.50865600	−0.12692900
H	0.15962500	0.37083000	2.36089700
H	0.61887300	0.98681200	0.76974400
H	−1.36857400	1.56429400	−0.73317900
H	−5.24086700	3.21045000	−2.36152600
H	−4.27679200	4.41208900	−1.44125100
H	−5.54683500	3.46088800	−0.61070800
H	−4.03807400	−0.17917300	−2.93059000
H	−2.46187900	−0.99817800	−3.10746800
H	−2.53612600	0.69981600	−2.58404300
H	−4.21400600	−2.89014200	−2.59493500
H	−4.82683100	−5.00862400	−1.45229200

H	−4.49253300	−5.28922800	0.98013900
H	−3.47858700	−3.47597800	2.34299600
H	−1.92121200	−0.99423800	3.12554700
H	−3.60566200	−0.51927200	2.98575600
H	−1.67387900	1.36060700	3.43379600
H	−3.11189300	1.73683700	2.47531800
H	5.56915300	−2.16855400	1.21217100
H	6.71236800	−1.44376700	0.05022600
H	5.58144600	−2.72100100	−0.47535600
H	4.12913100	1.68374900	0.56392100
H	5.86162100	1.22137600	0.59451600
H	4.74388200	0.61587800	1.84674600
H	4.67526000	−0.89623200	−2.65498900
H	5.88261700	0.26494600	−2.03742500
H	4.18363300	0.76529800	−2.25484000

TS16

Au	−2.51697900	−0.54544300	−0.06575600
S	0.62272300	4.17272800	0.06062100
P	−4.83619500	−0.55909000	0.36496700
O	1.08058800	3.76969800	−1.33628100
O	−0.78660800	3.76720700	0.31577800
O	1.58935400	3.70741900	1.09512800
O	4.00207500	1.98389400	−0.87572700
O	3.91762400	1.44927900	1.31484800
N	2.79263900	−1.36813200	1.11171200
N	1.35904000	1.16815500	−1.26370100
C	0.66942900	5.96812700	0.03877100
C	0.09901300	−2.58882700	0.73301400
C	0.45462100	−1.34447600	−0.05137000
C	−0.47399500	−0.42572500	−0.46332600
C	−0.12012100	0.85342800	−1.14548300
C	2.04597400	0.82459900	0.02707700
C	3.44268200	1.48626900	0.07505000
C	5.17307600	2.13814500	1.53459800
C	2.04658100	−0.69350100	0.14129200
C	2.85039400	−1.03181800	2.53352100
C	3.14930900	−2.61484600	0.61368400
C	3.84431600	−3.64803000	1.25392200
C	4.08994500	−4.80053600	0.51345400
C	3.64484500	−4.94160700	−0.81706500
C	2.92628600	−3.92575000	−1.43669700
C	2.67390500	−2.75293200	−0.71216700
C	1.97090300	−1.52646900	−1.04962400
C	1.79551300	−0.98609700	−2.45389000
C	1.97731800	0.53462800	−2.47827100
C	−5.25830900	−0.35757100	2.14132700
C	−5.69812900	−2.09734700	−0.15065000
C	−5.73906400	0.79428600	−0.48634200
H	1.38522200	2.25781700	−1.35910400
H	0.35400300	6.33510700	1.01848100
H	−0.01086100	6.33104800	−0.73488600
H	1.69043200	6.29290400	−0.17320000
H	−0.94859600	−2.51389400	1.03489100
H	0.21905900	−3.50196500	0.14109700
H	0.69227100	−2.70119300	1.64402900
H	−0.53567900	0.88661900	−2.15917700
H	−0.56399500	1.69758400	−0.60104600
H	1.46790900	1.29451800	0.82681400
H	5.39774800	1.99293700	2.59081500
H	5.05280600	3.19979200	1.30993900
H	5.95822600	1.70697300	0.90959800
H	2.32381300	−1.78936700	3.12440300
H	2.38622300	−0.06180700	2.70040700
H	3.89154200	−0.97849200	2.86213100
H	4.19129800	−3.55386900	2.27730000
H	4.64308500	−5.61382200	0.97428100
H	3.86232900	−5.85726700	−1.35784500
H	2.56987200	−4.03720800	−2.45642800
H	0.82265800	−1.27535600	−2.85974800
H	2.55478800	−1.43742400	−3.09993500
H	1.48838500	0.98427500	−3.34497900
H	3.02638900	0.82146300	−2.48110600
H	−4.81732500	−1.17431100	2.72176800
H	−6.34460200	−0.36137100	2.28465000
H	−4.85128400	0.58849200	2.51252900
H	−5.55613800	−2.25883400	−1.22410800
H	−6.77097600	−2.03195100	0.06231200
H	−5.27876600	−2.95476800	0.38559000
H	−5.34112000	1.76236700	−0.16533400
H	−6.80938400	0.75164300	−0.25580900
H	−5.60156200	0.70824100	−1.56903100

TS17

Au	2.86528100	−0.57070700	0.07586400
S	−0.99751300	4.34836200	−0.35669400
P	5.21755200	−0.53681900	−0.14216300
O	−1.38046400	4.12910200	1.22139100
O	0.43338800	4.09934900	−0.54651700
O	−1.95483700	3.58471300	−1.16709300
O	−4.02083400	1.44828800	0.88144700
O	−3.83491200	0.62922000	−1.22130500
N	−2.32999500	−2.07584200	−1.10469700
N	−1.14453700	0.93589600	1.11820500
C	−1.33313400	6.09958000	−0.44707900
C	0.52818600	−2.80528700	−0.81305200
C	−0.02860400	−1.51700700	−0.22036400
C	0.78114400	−0.54084400	0.25887500
C	0.32355800	0.75741400	0.90136400
C	−1.88904900	0.69136900	0.02784900
C	−3.36445000	0.96065500	−0.01734000
C	−5.23967200	0.89454600	−1.44400300
C	−1.52711900	−1.54176500	−0.10103000
C	−2.06626000	−2.02835100	−2.53789500
C	−3.54918900	−2.44064700	−0.56891900
C	−4.67481600	−2.98367600	−1.20371000
C	−5.78284800	−3.25791100	−0.41081200
C	−5.79130300	−2.99145200	0.97877500
C	−4.68444600	−2.44185100	1.60369900
C	−3.54079600	−2.16022900	0.82651500
C	−2.26480600	−1.60484900	1.12523400
C	−1.73234700	−1.09623300	2.40701900
C	−1.66593600	0.48421500	2.40502100
C	6.09991700	−1.76494000	0.90439000
C	5.98831400	1.07325000	0.29683600
C	5.82238700	−0.88031300	−1.84472800
H	−1.51781800	3.16568500	1.35960600
H	−1.09241200	6.41578500	−1.46500500
H	−0.69414200	6.61748000	0.27105300
H	−2.38916500	6.27189900	−0.23137600
H	1.60877400	−2.85281200	−0.65139900
H	0.07301200	−3.68397800	−0.33645200
H	0.35099500	−2.89716500	−1.89087700
H	0.79450400	0.88021200	1.87975900

H	0.65680800	1.60083700	0.28603900
H	−1.38609500	0.80693100	−0.92560700
H	−5.45349800	0.49953200	−2.43642200
H	−5.84816500	0.39386000	−0.68841200
H	−5.42108500	1.97167800	−1.41354900
H	−1.91842500	−3.03350400	−2.94531900
H	−1.17335500	−1.43085900	−2.72146500
H	−2.90903500	−1.55367100	−3.04858300
H	−4.68055100	−3.19794600	−2.26744700
H	−6.66570900	−3.69391600	−0.86967900
H	−6.67979500	−3.22411800	1.55788300
H	−4.69139800	−2.23730400	2.67036600
H	−0.71692000	−1.46974400	2.57580200
H	−2.35858200	−1.39778100	3.25111300
H	−1.00618800	0.83655700	3.19894600
H	−2.66443400	0.89038500	2.54890600
H	5.87489800	−1.58147600	1.95991500
H	7.18329500	−1.70115700	0.75256700
H	5.76367500	−2.77571700	0.65129500
H	5.57806200	1.86328800	−0.34051500
H	7.07579000	1.03745200	0.16708400
H	5.76032400	1.32050900	1.33885000
H	5.47719100	−1.86789200	−2.16798800
H	6.91719500	−0.85509100	−1.88226200
H	5.42261400	−0.13341600	−2.53835200

TS18

Au	−2.60452400	−0.40785700	−0.09540400
S	−0.02884400	3.46052300	0.74283000
P	−4.82879300	−1.10205700	−0.18325700
O	−1.27834400	2.53237900	0.66065500
O	0.64410000	3.53133500	−0.58162200
O	0.83508700	3.09833100	1.88412800
O	4.15126400	0.45626300	−3.02331400
O	4.27233500	2.01312900	−1.37881800
N	2.60433300	−0.75247400	1.84302600
N	1.35199700	0.20648200	−1.97416800
C	−0.77122400	5.06022100	1.06350400
C	−0.29366700	−0.25798200	2.33158200
C	0.28854400	−0.32421500	0.92841800
C	−0.49262800	0.13143500	−0.11895900
C	−0.08063800	0.39023500	−1.57501800
C	2.17987900	1.17552400	−1.80587900
C	3.64750500	1.13729400	−2.15577100
C	5.70676600	2.12668300	−1.56582200
C	1.64097000	−0.88106700	0.83370900
C	2.67356600	0.28195600	2.87453700
C	3.65958200	−1.59051800	1.55011000
C	4.86168800	−1.80152000	2.24444000
C	5.75655700	−2.72193300	1.71449100
C	5.47884300	−3.42216400	0.51753100
C	4.29663800	−3.20841700	−0.17337400
C	3.36884100	−2.27843900	0.33956700
C	2.09367700	−1.81180900	−0.10324000
C	1.39737600	−2.18663000	−1.37168100
C	1.68781000	−1.14685400	−2.47649000
C	−5.03154000	−2.87501800	−0.61517900
C	−5.83387300	−0.19705000	−1.42469900
C	−5.73093900	−0.89396500	1.40225000
H	−0.98686800	1.33322000	0.34153900
H	−1.31032200	5.01441600	2.01189400
H	−1.45106900	5.30688700	0.24560300
H	0.03512600	5.79583300	1.12112300
H	−1.38576500	−0.24914400	2.30193900
H	0.02995800	−1.11061000	2.93703800
H	0.02521400	0.65984700	2.83735800
H	−0.64518200	−0.24454400	−2.26007600
H	−0.32384400	1.42967400	−1.81130500
H	1.78762200	2.10258600	−1.37540900
H	6.03091000	2.86869100	−0.83785900
H	6.18484200	1.16259400	−1.37840400
H	5.92257900	2.45970000	−2.58343200
H	2.26222500	−0.06706300	3.82743200
H	2.14059000	1.17682000	2.54905000
H	3.72101600	0.55298100	3.02637100
H	5.08206200	−1.28344400	3.17222800
H	6.68899700	−2.91511600	2.23758100
H	6.20462400	−4.13615600	0.13900400
H	4.08820800	−3.74758300	−1.09400400
H	0.31619600	−2.28173900	−1.22024400
H	1.75539500	−3.15109500	−1.74667000
H	1.06493900	−1.31373700	−3.36047800
H	2.73307700	−1.15818900	−2.76989500
H	−4.58657200	−3.06988900	−1.59615700
H	−6.09243700	−3.14751500	−0.64323100
H	−4.52144300	−3.49757100	0.12669600
H	−5.83173200	0.87276100	−1.19299400
H	−6.86681100	−0.56259700	−1.42486600
H	−5.40403000	−0.33570100	−2.42184200
H	−5.23283800	−1.46812800	2.19001400
H	−6.76660400	−1.23894200	1.30686100
H	−5.72949200	0.16181400	1.69122100

TS19

Au	2.41471800	−0.66936800	0.27568400
S	0.28814400	3.27968000	−0.87671500
P	4.69314600	−0.51171700	−0.30936200
O	−0.82758200	2.25530800	−1.27083400
O	1.56819100	2.93240300	−1.51308800
O	0.28629700	3.45221400	0.59573400
O	−3.07925800	2.84805300	1.87787700
O	−4.18533800	2.14772500	0.03799000
N	−3.22521500	−0.51646000	−1.00086800
N	−1.38650500	0.84472500	1.90746100
C	−0.29282400	4.81199900	−1.61299000
C	−0.14648800	−2.67210300	−0.64706800
C	−0.51349900	−1.58095700	0.33279500
C	0.38848300	−0.69230200	0.79868100
C	0.08372000	0.46119800	1.70978200
C	−2.15021800	1.04894800	0.62706400
C	−3.19386100	2.09955800	0.92230100
C	−5.16401700	3.19996800	0.24153300
C	−2.52256700	−0.24468100	0.08741600
C	−3.58665300	0.37684700	−2.10658000
C	−3.53202300	−1.91461800	−1.04061900
C	−4.35165900	−2.58178300	−1.94062800
C	−4.53931800	−3.95254600	−1.72329700
C	−3.92655800	−4.60335900	−0.64768100
C	−3.09135300	−3.90629900	0.23639100
C	−2.89489400	−2.54659500	0.03010600
C	−2.05111800	−1.51886600	0.75267600
C	−2.20753500	−1.49492900	2.29614200
C	−2.11339300	−0.07072800	2.86254900
C	4.97916700	0.07044200	−2.02898000

C	5.64436200	−2.08136600	−0.19138600
C	5.63219700	0.67300100	0.73631600
H	−1.39173500	1.78261100	2.33699500
H	−0.37680000	4.67655400	−2.69348600
H	0.43984000	5.59115300	−1.38851300
H	−1.26178000	5.07103700	−1.18090600
H	0.92813500	−2.63970000	−0.84479500
H	−0.39554100	−3.67018300	−0.26731300
H	−0.66704200	−2.55697900	−1.60659600
H	0.46760100	0.28211700	2.72068600
H	0.54548900	1.37906100	1.34210900
H	−1.37787500	1.68440600	−0.29050600
H	−4.67923400	4.17698400	0.19056200
H	−5.88131200	3.08447700	−0.57030300
H	−5.65468600	3.07634900	1.20928500
H	−3.32465500	−0.13048000	−3.03842100
H	−3.02205800	1.30306300	−2.03333700
H	−4.65801200	0.58649100	−2.09025400
H	−4.83975700	−2.07345500	−2.76495800
H	−5.17975300	−4.51266600	−2.39771200
H	−4.09880700	−5.66445400	−0.49518600
H	−2.61093200	−4.42282900	1.06206900
H	−1.43337600	−2.13321800	2.72784000
H	−3.17715000	−1.91312700	2.58004400
H	−1.57107500	−0.03878900	3.80940500
H	−3.09917400	0.37302700	3.01442300
H	4.52695300	−0.63237900	−2.73634000
H	6.05093300	0.15281400	−2.24163800
H	4.50701700	1.04813900	−2.16795500
H	5.58575200	−2.47335000	0.82920100
H	6.69658000	−1.92294700	−0.45295800
H	5.21526800	−2.82543200	−0.87050700
H	5.17876200	1.66662400	0.66054800
H	6.67943100	0.73199400	0.41920800
H	5.59257200	0.35555600	1.78341700

TS20

Au	2.08703400	−0.66926400	0.16187400
S	1.13043600	3.81615300	−0.76575200
P	3.89095300	−2.07910700	0.55852000
O	1.95568700	2.57592600	−0.31523000
O	0.60375200	3.61771000	−2.13939600
O	0.12875100	4.19263700	0.25579800
O	−2.54398800	−1.29394700	−3.79748000
O	−3.79124400	−2.41362100	−2.27907100
N	−3.24222300	−1.34575800	0.68765800
N	−1.55270400	0.43482600	−2.10688600
C	2.38385000	5.09857300	−0.83596600
C	−0.07105900	1.05287400	2.07726000
C	−0.58121800	0.70771300	0.70491000
C	0.30126100	0.51397400	−0.32084900
C	−0.07866200	0.31137100	−1.77199200
C	−2.36944200	−0.66351700	−1.54854800
C	−2.89090300	−1.49240000	−2.63304500
C	−4.35006200	−3.19861900	−3.35749600
C	−2.59692700	−0.54903000	−0.20034800
C	−3.59736600	−2.75441400	0.55504400
C	−3.51796700	−0.61821800	1.87443100
C	−4.29960500	−1.01585700	2.95352200
C	−4.48277700	−0.09015100	3.98953600
C	−3.91192800	1.18277300	3.92951500
C	−3.12102900	1.55842600	2.83369000
C	−2.91561200	0.64264600	1.80941100
C	−2.12826700	0.73629000	0.51098300
C	−2.51382200	1.97761000	−0.34417100
C	−2.12767200	1.81286800	−1.82675600
C	3.51793000	−3.85357300	0.27337400
C	4.52448600	−1.99952600	2.27894200
C	5.34309500	−1.72058300	−0.50509700
H	1.22519800	1.48366000	−0.24526200
H	−1.61751800	0.27309200	−3.12710400
H	1.89700300	6.02269400	−1.15750100
H	3.15128600	4.80603800	−1.55537000
H	2.81789000	5.22749800	0.15786000
H	−0.43619000	2.03990200	2.38440600
H	1.02130000	1.07470900	2.09105700
H	−0.41479600	0.33296000	2.82832000
H	0.42463200	1.06456800	−2.38662600
H	0.21284000	−0.67810800	−2.13548000
H	−5.05446100	−3.87943200	−2.87954600
H	−4.86678500	−2.55188000	−4.07030500
H	−3.56415000	−3.75851700	−3.86992700
H	−4.64311400	−2.88159400	0.26073700
H	−3.43418000	−3.23702000	1.52251600
H	−2.95591800	−3.22479200	−0.18672900
H	−4.77432200	−1.99042100	2.98987900
H	−5.09396900	−0.36717200	4.84348700
H	−4.08483400	1.89157300	4.73344100
H	−2.68514900	2.55186100	2.79186100
H	−2.01506200	2.86029500	0.06555900
H	−3.59338800	2.12706200	−0.25850900
H	−1.36827200	2.53360400	−2.13680800
H	−3.00052600	1.89933200	−2.47590100
H	2.70284700	−4.17199600	0.93092800
H	4.40228900	−4.46847800	0.47436200
H	3.20492300	−4.00552800	−0.76449800
H	4.84856200	−0.97924800	2.50721100
H	5.37090700	−2.68313400	2.40915200
H	3.72927300	−2.27464500	2.97902700
H	5.06442000	−1.81886600	−1.55906800
H	6.16360200	−2.41227300	−0.28354600
H	5.68174700	−0.69424800	−0.33192500

TS21

Au	1.86215900	1.23705600	−0.07299200
S	0.42897100	−4.17529700	0.34220800
P	4.19597700	1.27176000	0.01086600
O	−0.62013400	−4.30492900	−0.74672700
O	1.46529200	−3.15681000	−0.01131700
O	−0.17644300	−3.97626400	1.68558900
N	−3.10664800	0.56076300	1.36592400
N	−1.83890900	−1.92269300	−1.04654200
C	1.25914000	−5.77083000	0.35558100
C	−0.26581900	1.31360100	−0.09294500
C	−0.76518600	0.25721300	−0.58853900
C	−0.62158700	−1.05538900	−1.25107600
C	−2.43521800	−1.68057000	0.33297000
C	−3.50996100	−2.71363500	0.68126700
C	−2.89755400	−0.25437400	0.28172900
C	−2.68604300	0.29803600	2.73651700
C	−3.56351100	1.78737400	0.89719800
C	−3.87959500	2.95294700	1.60795600
C	−4.34148200	4.04140300	0.87497600
C	−4.48616700	3.98356700	−0.52922300

C	−4.16564800	2.83059700	−1.23325800
C	−3.69439600	1.71345700	−0.51819300
C	−3.26909900	0.40104500	−0.90170300
C	−3.27282700	−0.25563100	−2.25395500
C	−2.84305900	−1.72804400	−2.15627200
C	4.94988200	2.48670200	−1.13795900
C	4.96547700	−0.33693200	−0.41654300
C	4.85878000	1.69614800	1.66756300
H	−1.47272100	−2.92296400	−1.04324600
H	2.03412600	−5.75361300	1.12606900
H	1.70821100	−5.94704200	−0.62464500
H	0.52683100	−6.54995300	0.58011400
H	−0.73214500	2.20183300	0.32223000
H	−0.46384100	−0.94974300	−2.32737400
H	0.23607900	−1.59091700	−0.82011100
H	−1.60300600	−1.80763600	1.03161400
H	−4.41987600	−2.59273300	0.08850200
H	−3.77497200	−2.58843100	1.73550400
H	−3.11343900	−3.72446500	0.54858600
H	−3.38768500	0.77311300	3.42541100
H	−1.67834300	0.69000500	2.91921300
H	−2.69494600	−0.77588900	2.92616800
H	−3.77026400	3.00937400	2.68616000
H	−4.59629400	4.95953300	1.39701900
H	−4.85274200	4.85659800	−1.06146900
H	−4.27583700	2.78844600	−2.31319400
H	−2.61679900	0.29116500	−2.94157500
H	−4.27557200	−0.21972700	−2.69532900
H	−2.36502700	−2.07452400	−3.07382900
H	−3.68431400	−2.38501700	−1.93671100
H	4.65611800	2.25116200	−2.16572400
H	6.04228100	2.45564300	−1.05867500
H	4.59786700	3.49367400	−0.89282800
H	4.61935600	−1.10575000	0.28129800
H	6.05736900	−0.26232500	−0.36283200
H	4.67316700	−0.62752000	−1.43060800
H	4.50267500	2.68763900	1.96472400
H	5.95440500	1.69535600	1.65025900
H	4.50799900	0.96303800	2.40073800

TS21 (L = PPh_3)

Au	0.65860700	−0.83717100	0.23266900
S	−1.58778700	4.20079700	−0.33396800
P	2.94919500	−0.39310300	0.01642500
O	−2.76401700	4.17377200	0.62382900
O	−0.43846400	3.39504000	0.18684100
O	−1.98186800	3.85469400	−1.72447900
N	−4.19631100	−1.14655700	−1.38049400
N	−3.57563200	1.62852600	0.96392700
C	−1.05398600	5.91780500	−0.33321900
C	−1.40663500	−1.32198900	0.30922900
C	−2.10685600	−0.34686000	0.71970300
C	−2.25260900	0.99323800	1.31804400
C	−4.00280000	1.22270400	−0.43991600
C	−5.20084300	2.03736900	−0.93480600
C	−4.22765000	−0.25652300	−0.33731700
C	−3.70334000	−0.88611700	−2.72702100
C	−4.47855700	−2.41045500	−0.87346500
C	−4.52963300	−3.64456500	−1.53451300
C	−4.86161500	−4.76178800	−0.77441700
C	−5.13414500	−4.66363800	0.60816800
C	−5.07564500	−3.44043100	1.26327400
C	−4.74047300	−2.29299300	0.52022800
C	−4.57993400	−0.90878900	0.85270000
C	−4.82277500	−0.19752700	2.15460500
C	−4.62854700	1.31986600	2.00166400
C	3.27411000	0.90532400	−1.23836000
C	4.37080500	0.84022400	−2.11164900
C	4.57941500	1.85582200	−3.04839700
C	3.70149000	2.93999000	−3.11747200
C	2.60916600	3.00892100	−2.24795300
C	2.39037000	1.99598300	−1.31364000
C	3.88753700	−1.88051700	−0.50353000
C	5.18621500	−2.14050700	−0.03998900
C	5.87155600	−3.27564300	−0.47999400
C	5.26925700	−4.15493000	−1.38286900
C	3.97506900	−3.90134600	−1.84667200
C	3.28359500	−2.77219800	−1.40675900
C	3.69587200	0.18899100	1.58636300
C	4.75099700	1.11444500	1.60664800
C	5.30020400	1.52146100	2.82479100
C	4.80355200	1.00962100	4.02612000
C	3.75190900	0.08897300	4.01145100
C	3.19648000	−0.31825700	2.79783800
H	−3.38321700	2.67562100	0.92765700
H	−0.19213300	6.01816100	−0.99770400
H	−0.77790600	6.20377200	0.68438300
H	−1.87559300	6.54331600	−0.69034600
H	−1.69055700	−2.30398800	−0.05648700
H	−2.17820200	0.95794600	2.40769100
H	−1.46022200	1.65157700	0.93394600
H	−3.14531700	1.45386900	−1.07868300
H	−6.12095800	1.80630400	−0.39267200
H	−5.36236800	1.79888100	−1.99045500
H	−4.98555100	3.10704500	−0.85603900
H	−4.29481800	−1.45798400	−3.44587000
H	−2.64860000	−1.17134500	−2.81897600
H	−3.80967400	0.17343900	−2.96118700
H	−4.31988600	−3.73022800	−2.59588200
H	−4.91177700	−5.73367100	−1.25737200
H	−5.39119600	−5.56086900	1.16385100
H	−5.28438100	−3.36805300	2.32703100
H	−4.16011300	−0.59349500	2.93312600
H	−5.84619200	−0.37778000	2.50365200
H	−4.29524700	1.78369100	2.93115300
H	−5.54158300	1.81772700	1.67660200
H	5.06019100	0.00283700	−2.06827000
H	5.42865700	1.79637500	−3.72343700
H	3.86461700	3.72607200	−3.84962200
H	1.91918000	3.84655700	−2.29933500
H	1.53053900	2.06125700	−0.65146400
H	5.66458900	−1.46351200	0.66076700
H	6.87626700	−3.47060700	−0.11551900
H	5.80460400	−5.03781700	−1.72101400
H	3.50072200	−4.58549300	−2.54472900
H	2.27360700	−2.58330800	−1.76233700
H	5.14279500	1.51939200	0.67875900
H	6.11499100	2.24018400	2.83254300
H	5.23048500	1.33193800	4.97181500
H	3.35872000	−0.30706900	4.94361100
H	2.37131600	−1.02627700	2.79027800

TS21 (L = JohnPhos)

Au	0.86796400	−0.15678800	0.15602400

S	−2.86969700	4.21863900	−0.59656700
P	2.98828200	0.89882600	0.13488900
O	−3.86179000	3.93605900	0.51683100
O	−1.47826300	3.84192800	−0.20130700
O	−3.30359600	3.64006900	−1.89629300
N	−3.94970500	−1.65758300	−1.22866400
N	−3.85490700	1.28365100	0.99345600
C	−2.89108500	6.00831700	−0.77192300
C	−1.05516200	−1.04857400	0.19277000
C	−1.96738200	−0.26465800	0.60690600
C	−2.37693300	1.04239200	1.16940700
C	−4.31577100	0.71452900	−0.34034600
C	−5.75148200	1.12272700	−0.67866300
C	−4.08537400	−0.76078000	−0.19759200
C	−3.69765000	−1.33596000	−2.62775000
C	−3.84104300	−2.92848000	−0.67811000
C	−3.64764300	−4.16213400	−1.31441700
C	−3.60446000	−5.29526000	−0.50835800
C	−3.74158200	−5.21396200	0.89600800
C	−3.92212700	−3.99022400	1.52601400
C	−3.97069300	−2.82592000	0.73566900
C	−4.13456300	−1.43588800	1.03295800
C	−4.40176900	−0.75914900	2.34832700
C	−4.64705500	0.74727800	2.16109300
C	4.43537800	−0.25055200	−0.05774400
C	5.72872300	0.30395800	0.04438200
C	6.87997400	−0.47799300	−0.01204900
C	6.76503800	−1.85786700	−0.17053100
C	5.49940100	−2.42639900	−0.28198200
C	4.32306400	−1.65369500	−0.23755900
C	3.05677800	−2.43976900	−0.41007100
C	2.44142800	−2.54082000	−1.66937100
C	1.36562700	−3.41041100	−1.86891500
C	0.88824300	−4.19407800	−0.81411100
C	1.49347000	−4.10192500	0.44274100
C	2.57326300	−3.23717900	0.64137800
C	3.03242400	2.09937400	−1.35976100
C	2.62412800	1.26348400	−2.59143500
C	4.40289600	2.74161500	−1.64342100
C	1.98608300	3.20821400	−1.13551600
C	3.20022000	1.76274900	1.84723200
C	1.83326500	2.34434900	2.27060900
C	4.23927400	2.89836900	1.89579200
C	3.58788900	0.66131900	2.85521400
H	−3.96576400	2.34113000	0.92358600
H	−2.19159900	6.28878800	−1.56341400
H	−2.58789200	6.46311100	0.17401000
H	−3.90216600	6.32686400	−1.03654300
H	−1.11722800	−2.07860800	−0.14746400
H	−2.15271900	1.11001800	2.23674900
H	−1.85079500	1.85377600	0.64940900
H	−3.64923400	1.15950400	−1.08457800
H	−6.49046800	0.64320200	−0.03214300
H	−5.95761200	0.81952000	−1.70971500
H	−5.85615900	2.20984200	−0.61638700
H	−4.20540900	−2.06513500	−3.26337400
H	−2.62313200	−1.35297700	−2.84487600
H	−4.09418200	−0.34600200	−2.85518600
H	−3.54086100	−4.23510900	−2.39192800
H	−3.46300700	−6.26773900	−0.97173600
H	−3.70442400	−6.12491700	1.48637400
H	−4.02554400	−3.92939000	2.60578200
H	−3.56563400	−0.92994000	3.03661700
H	−5.28621600	−1.19385700	2.82796100
H	−4.33901300	1.32132300	3.03635100
H	−5.69396100	0.96697000	1.95480800
H	5.84947000	1.37085900	0.17395200
H	7.85521500	−0.00688700	0.07152800
H	7.64949800	−2.48746800	−0.21171300
H	5.40515500	−3.50010100	−0.41731400
H	2.82425800	−1.95615100	−2.50114000
H	0.91185900	−3.48573700	−2.85380400
H	0.05849600	−4.87764100	−0.97251800
H	1.13801600	−4.71580400	1.26630800
H	3.05750100	−3.19138800	1.61334000
H	1.61622800	0.84676600	−2.48624300
H	3.32312900	0.44086000	−2.77759100
H	2.63143500	1.91286500	−3.47635800
H	4.28557100	3.43659500	−2.48502000
H	5.15255600	2.00119400	−1.93567600
H	4.78812200	3.31545300	−0.79665100
H	0.99411700	2.80925000	−0.89943900
H	1.89626100	3.79444400	−2.05933400
H	2.28183800	3.89703300	−0.33848600
H	1.06329400	1.56762800	2.33147300
H	1.47842300	3.12481500	1.59251600
H	1.94189300	2.79312000	3.26653400
H	4.25686300	3.30145400	2.91683800
H	3.98195600	3.72216900	1.22410500
H	5.25345600	2.56237900	1.66807400
H	2.88052100	−0.17664100	2.83722800
H	3.56934900	1.08865500	3.86584900
H	4.59306500	0.26866800	2.67641900

TS22

Au	2.15586100	0.88561200	−0.08118000
S	−0.44373700	−4.76532700	0.25890300
P	4.42540700	1.34155700	0.21297200
O	−1.16719800	−4.19464900	−0.94887600
O	0.69929200	−3.89872900	0.67316800
O	−1.37686000	−5.11693300	1.35933800
N	−3.29296100	1.03645400	1.29432800
N	−1.59606300	−1.54871600	−0.86447700
C	0.26379200	−6.30537300	−0.34623800
C	−0.53579500	1.24375000	−0.09617700
C	0.13306200	0.22824200	−0.42017000
C	−0.12762400	−1.16543900	−0.85245600
C	−2.33744600	−1.15971500	0.41292300
C	−3.48165700	−2.14475600	0.68941800
C	−2.79205000	0.26795900	0.26506200
C	−3.31049700	0.71766500	2.71716900
C	−3.75454000	2.23038400	0.75652300
C	−4.34124900	3.32814000	1.39854600
C	−4.71815100	4.40675400	0.60345500
C	−4.51629900	4.40048600	−0.79384900
C	−3.92747000	3.31262200	−1.42762800
C	−3.53936400	2.20693700	−0.64931700
C	−2.91821600	0.94656500	−0.94795400
C	−2.55569200	0.33531800	−2.26960200
C	−2.33929400	−1.17320200	−2.12633700
C	4.80624500	3.12371000	0.41684500
C	5.14340400	0.51798600	1.68540700
C	5.44814300	0.78657200	−1.20345500
H	−1.53355100	−2.61677500	−0.86550800

H	0.80651600	−6.78703700	0.47116100
H	0.94565700	−6.08645600	−1.17137200
H	−0.54440900	−6.95552600	−0.69010300
H	−0.76256300	2.23672900	0.24741700
H	0.25674700	−1.34212400	−1.86019800
H	0.35873300	−1.88039800	−0.17976300
H	−1.59699200	−1.25382100	1.21282600
H	−4.23201300	−2.13405200	−0.10604500
H	−3.08577900	−3.15783100	0.80788600
H	−3.97766200	−1.86368200	1.62293800
H	−4.32240300	0.45962600	3.04702900
H	−2.95903000	1.58132500	3.28853000
H	−2.64363400	−0.12103300	2.91850400
H	−4.50508900	3.33776100	2.47156100
H	−5.18183500	5.27171500	1.06966400
H	−4.82669000	5.26137000	−1.37936400
H	−3.77256100	3.31284200	−2.50307100
H	−1.66429500	0.81150100	−2.69454800
H	−3.36181000	0.48689600	−2.99714000
H	−1.76230900	−1.58360500	−2.95697000
H	−3.29306500	−1.70096300	−2.07817000
H	4.47797000	3.67388800	−0.47051500
H	5.88445500	3.26375700	0.55326900
H	4.27683700	3.51561500	1.29093400
H	4.63406700	0.86923100	2.58824900
H	6.21244900	0.74593200	1.76093700
H	5.00827500	−0.56509600	1.60433100
H	5.32502300	−0.29136700	−1.34758500
H	6.50448000	1.00902300	−1.01600800
H	5.12565600	1.30181600	−2.11366500

TS22 (L = PPh_3)

Au	0.86599800	−0.23332900	0.17265200
S	−3.19160100	4.56856800	−0.25185200
P	3.19682200	−0.18576800	−0.04824900
O	−3.73362000	3.82223300	0.95531900
O	−1.88376900	4.00423300	−0.70032700
O	−4.20236700	4.70484500	−1.33074700
N	−4.32408800	−1.79160900	−1.28518600
N	−3.40498600	1.16212500	0.87304800
C	−2.85865300	6.22341200	0.37294500
C	−1.62346000	−1.24302900	0.11613500
C	−1.25973000	−0.08660900	0.45184800
C	−1.88760300	1.18745800	0.87616200
C	−4.00074400	0.58328900	−0.40872600
C	−5.36596200	1.22055700	−0.70372000
C	−4.05731500	−0.91385700	−0.25538800
C	−4.39197800	−1.49495300	−2.71114500
C	−4.45578200	−3.06308200	−0.74509200
C	−4.71806300	−4.27979000	−1.38746400
C	−4.79882900	−5.41804900	−0.59065600
C	−4.62208200	−5.35416500	0.80878300
C	−4.35628300	−4.14646800	1.44322500
C	−4.27247100	−2.97831900	0.66322200
C	−4.01612600	−1.59673500	0.96065900
C	−3.83366600	−0.90571900	2.28002600
C	−4.03193200	0.60429600	2.13064200
C	3.77697300	1.39201600	−0.77568200
C	4.89683900	1.45097400	−1.61962100
C	5.31846400	2.67905300	−2.13463900
C	4.62838200	3.85039600	−1.81307200
C	3.51170500	3.79644800	−0.97388100
C	3.08231900	2.57226300	−0.46039800
C	3.80887600	−1.53278200	−1.13077000
C	5.00282100	−2.21877000	−0.86154500
C	5.43734700	−3.22840800	−1.72412700
C	4.68867800	−3.55680800	−2.85661500
C	3.49839200	−2.87570800	−3.12883000
C	3.05557800	−1.87121400	−2.26812600
C	4.03466200	−0.37648700	1.57093000
C	5.22096100	0.30615100	1.87950000
C	5.83498700	0.11402700	3.11963400
C	5.27415300	−0.75884700	4.05472700
C	4.09207700	−1.44134300	3.75218100
C	3.47029900	−1.24831200	2.51827400
H	−3.63472300	2.20729500	0.86931600
H	−2.46174800	6.83231300	−0.44337900
H	−2.12626900	6.16124300	1.18152200
H	−3.79108500	6.65759600	0.74169500
H	−1.57896100	−2.26089600	−0.22623300
H	−1.57331300	1.46142400	1.88648400
H	−1.60590300	2.00507000	0.20343700
H	−3.30499100	0.87213400	−1.20203300
H	−6.09915800	0.99750900	0.07645200
H	−5.26288500	2.30425800	−0.81189400
H	−5.74868800	0.82238700	−1.64794700
H	−5.42432900	−1.55086300	−3.07211400
H	−3.78108900	−2.21395100	−3.26455800
H	−4.00198900	−0.49465800	−2.90006300
H	−4.85964100	−4.33517900	−2.46225500
H	−5.00647000	−6.37711600	−1.05714800
H	−4.69570100	−6.26577600	1.39515500
H	−4.22003100	−4.10293400	2.52035700
H	−2.84698100	−1.12219000	2.70612400
H	−4.56911500	−1.26626800	3.00874300
H	−3.59610200	1.15795900	2.96415600
H	−5.09221600	0.85523000	2.07038300
H	5.43958800	0.54621900	−1.87529400
H	6.18488200	2.71756400	−2.78892900
H	4.95769000	4.80327500	−2.21798900
H	2.96860700	4.70443600	−0.72719100
H	2.20683100	2.53180200	0.18314900
H	5.59331200	−1.97168800	0.01515400
H	6.36148900	−3.75732100	−1.50820200
H	5.02900600	−4.34420000	−3.52343800
H	2.91089300	−3.13042100	−4.00655000
H	2.12455700	−1.35017700	−2.47788300
H	5.66672500	0.98552300	1.15996700
H	6.75172200	0.64862900	3.35225300
H	5.75446000	−0.90415700	5.01841800
H	3.64975200	−2.11756500	4.47838200
H	2.54582600	−1.77347000	2.29043700

TS22 (L = JohnPhos)

Au	−0.99447300	−0.38987900	−0.45392500
S	3.02094200	4.58998400	−0.38358000
P	−3.34589300	−0.51256700	−0.67144300
O	3.67506100	3.64528400	−1.37701300
O	1.62851200	4.16001200	−0.05453000
O	3.87910400	4.84771700	0.79958300
N	4.15200900	−1.72987100	1.43017100
N	3.29424500	1.02549100	−0.99873900
C	2.88141700	6.13880200	−1.28966100
C	1.54602400	−1.32643200	−0.11145600

C	1.14464200	−0.21762800	−0.56032100
C	1.77751900	1.02559500	−1.06600900
C	3.84064300	0.56251900	0.34847000
C	5.18859300	1.23559900	0.64389400
C	3.90931600	−0.94177000	0.32413800
C	4.16408700	−1.32199300	2.83016200
C	4.32307700	−3.03757800	0.99890600
C	4.58084500	−4.19493500	1.74480400
C	4.71690300	−5.38946800	1.04370100
C	4.59589600	−5.43962500	−0.36241400
C	4.33180400	−4.29175200	−1.09956300
C	4.19396700	−3.06886400	−0.41748300
C	3.92923500	−1.72179700	−0.83473700
C	3.80261200	−1.14408000	−2.21308100
C	3.97705900	0.37607900	−2.18080300
C	−4.33683500	0.11458100	0.77011700
C	−5.74040400	−0.00976900	0.69124800
C	−6.57975200	0.35867100	1.73975600
C	−6.02710900	0.86358400	2.91517300
C	−4.64539900	0.99750400	3.01458900
C	−3.77737600	0.64078100	1.96412500
C	−2.32511900	0.87752300	2.25141300
C	−1.63476900	1.96525800	1.68931100
C	−0.33345500	2.27467300	2.09820100
C	0.29724000	1.49712100	3.07455100
C	−0.37601200	0.40862800	3.63622900
C	−1.67952800	0.10630600	3.23278900
C	−3.79916900	0.58337300	−2.17921000
C	−3.17035500	1.96773700	−1.90975700
C	−5.30667200	0.78180900	−2.42360300
C	−3.15520500	−0.02772900	−3.43923300
C	−3.79877100	−2.37596900	−0.87957500
C	−2.70291300	−3.05924400	−1.72751700
C	−5.16019800	−2.65321200	−1.54254600
C	−3.77377800	−2.99754400	0.53240300
H	3.51861200	2.06880300	−1.07948000
H	2.41614200	6.88500500	−0.64054200
H	2.26447500	5.97871700	−2.17706700
H	3.88075700	6.47032800	−1.58199100
H	1.48949500	−2.31210600	0.31412300
H	1.50587800	1.20790300	−2.10886300
H	1.45443300	1.89426400	−0.48340300
H	3.11128000	0.90853900	1.08615800
H	5.95707700	0.94976600	−0.07976300
H	5.07459500	2.32367600	0.64538500
H	5.53120900	0.92926500	1.63648500
H	5.17897200	−1.37024600	3.23834800
H	3.51288700	−1.98129100	3.41146600
H	3.79263600	−0.30113100	2.92142100
H	4.67885200	−4.16420800	2.82539100
H	4.92386000	−6.30437700	1.59203700
H	4.71161400	−6.39211300	−0.87189900
H	4.23879100	−4.33433100	−2.18127900
H	2.83964600	−1.40936400	−2.66459300
H	4.57598200	−1.55491600	−2.87257300
H	3.56686500	0.85255300	−3.07276100
H	5.03099600	0.64797900	−2.10218500
H	−6.19791000	−0.40837200	−0.20382300
H	−7.65493100	0.24551800	1.63407500
H	−6.66250000	1.15398000	3.74724800
H	−4.21159900	1.40027100	3.92524400
H	−2.12963600	2.58974500	0.95131600
H	0.18557800	3.12003200	1.65376400
H	1.30202400	1.74828600	3.40451900
H	0.10238300	−0.19379800	4.40427800
H	−2.20958300	−0.72312700	3.69383100
H	−2.07968100	1.91274500	−1.81870100
H	−3.57156700	2.43037200	−1.00138400
H	−3.40661500	2.63049900	−2.75226200
H	−5.42603100	1.37039100	−3.34233700
H	−5.78259400	1.34216700	−1.61445600
H	−5.84490000	−0.15886800	−2.56285100
H	−2.08635700	−0.22667900	−3.29998800
H	−3.25936200	0.68553900	−4.26687000
H	−3.64728500	−0.95695900	−3.74125300
H	−1.71025800	−2.95019100	−1.27758600
H	−2.65997700	−2.67473000	−2.75000100
H	−2.93058400	−4.13142400	−1.78621100
H	−5.29887000	−3.74091200	−1.59525800
H	−5.20591800	−2.26788000	−2.56501200
H	−6.00343100	−2.25131100	−0.97613200
H	−2.81969000	−2.81984800	1.04350800
H	−3.90203600	−4.08320900	0.43768000
H	−4.58063300	−2.61971800	1.16679500

TS23

Au	1.82431200	−1.18771700	0.05180600
S	0.16706900	4.31621700	−0.33383200
P	4.18412400	−1.10748700	0.00331700
O	−0.84092700	4.34984600	0.80105400
O	1.35845400	3.48446200	0.00106000
O	−0.47058600	3.96475700	−1.63335700
N	−2.96527900	−0.66969200	−1.36864200
N	−1.87662700	1.88696600	1.07075900
C	0.73925800	6.01601800	−0.46752400
C	−0.23206600	−1.26849100	0.03221100
C	−1.04386000	−0.28068700	0.44712000
C	−0.64444600	1.02038000	1.10395000
C	−2.52307500	1.61518900	−0.27460000
C	−3.86517600	2.30757900	−0.48007700
C	−2.57809300	0.09997700	−0.27967400
C	−2.49956500	−0.42183900	−2.72740000
C	−3.33421700	−1.92798700	−0.89389300
C	−3.70081000	−3.07103700	−1.61562400
C	−4.06629200	−4.19646100	−0.88229600
C	−4.06030200	−4.20458100	0.52813300
C	−3.67037500	−3.07739600	1.24206500
C	−3.29936100	−1.93280600	0.52355300
C	−2.83655500	−0.62708500	0.94023100
C	−3.03179800	0.03272200	2.28545700
C	−2.76803300	1.55415400	2.23503100
C	4.84763500	0.38632700	−0.83346300
C	4.96163400	−2.51746100	−0.88033500
C	4.97562700	−1.10175100	1.66090500
H	−1.56403600	2.90705300	1.08350100
H	1.47353600	6.07346500	−1.27506600
H	1.19934200	6.31385300	0.47763800
H	−0.11312500	6.66218800	−0.69058800
H	−0.71336000	−2.15987300	−0.37606100
H	−0.32636700	0.90901600	2.14254000
H	0.14471600	1.52913100	0.54427600
H	−1.80777300	1.98821400	−1.01342900
H	−4.66120600	1.89662700	0.14613400
H	−4.15863300	2.18220400	−1.52670500

H	−3.76338600	3.37981500	−0.28480900
H	−3.17352600	−0.90868700	−3.43446700
H	−1.48161200	−0.81299000	−2.86428800
H	−2.50328800	0.65033000	−2.92907200
H	−3.70803700	−3.08343200	−2.70011900
H	−4.36447900	−5.09543200	−1.41438100
H	−4.35601300	−5.10502300	1.05766000
H	−3.64871000	−3.08074300	2.32767400
H	−2.39188400	−0.44919900	3.03038200
H	−4.06659000	−0.14292800	2.59778900
H	−2.24982400	1.89973800	3.13037100
H	−3.68612400	2.12925200	2.12311000
H	4.49338200	0.41458800	−1.86893200
H	5.94331100	0.37724100	−0.82683100
H	4.49056700	1.28462000	−0.31973900
H	4.68497100	−3.45712200	−0.39154700
H	6.05270600	−2.41664300	−0.87835200
H	4.60413500	−2.54415300	−1.91470700
H	4.63834400	−0.22626800	2.22513000
H	6.06656800	−1.07069900	1.56363700
H	4.68782800	−2.00367600	2.21066200

TS23 (L = PPh_3)

Au	0.67127000	−0.83109900	0.01540300
S	−2.14660600	4.30905700	−0.28724800
P	2.97126300	−0.24944200	0.00655300
O	−3.12589300	4.06748700	0.84796300
O	−0.75275600	3.94042300	0.09108900
O	−2.61245200	3.69285300	−1.56132500
N	−4.15719600	−1.31797600	−1.35856600
N	−3.56537600	1.42942700	1.04439000
C	−2.17117500	6.09204300	−0.52133200
C	−1.32071700	−1.33007900	−0.00573300
C	−2.31281800	−0.52282600	0.40797200
C	−2.17927800	0.84157200	1.04637500
C	−4.17492100	1.01904300	−0.28249300
C	−5.63813700	1.41146600	−0.44870600
C	−3.91208500	−0.47485700	−0.28315400
C	−3.79813900	−0.98946400	−2.73321600
C	−4.23867900	−2.62199100	−0.87058100
C	−4.37379400	−3.82259600	−1.57902300
C	−4.47071400	−4.99408400	−0.83338600
C	−4.42310900	−4.98932500	0.57634100
C	−4.26255000	−3.79919700	1.27625400
C	−4.16592600	−2.60756400	0.54516300
C	−3.97881400	−1.23010000	0.94588800
C	−4.27362700	−0.61585800	2.29494900
C	−4.33480700	0.92575200	2.23379600
C	3.26800900	1.39165700	−0.75968000
C	4.44222300	1.68710500	−1.47042100
C	4.62130400	2.95489100	−2.02907900
C	3.63507900	3.93452600	−1.88318600
C	2.46345000	3.64588100	−1.17832400
C	2.27836100	2.37956900	−0.62167500
C	3.99710400	−1.45034400	−0.92975200
C	5.28722400	−1.81983800	−0.52037300
C	6.02857600	−2.73048000	−1.27776100
C	5.49138600	−3.27558500	−2.44621800
C	4.20626800	−2.91153000	−2.85898100
C	3.45919800	−2.00772700	−2.10271700
C	3.67304100	−0.17744400	1.70161100
C	4.65744100	0.75289600	2.06877400
C	5.16814300	0.75613700	3.36921600
C	4.70335100	−0.16618300	4.30987600
C	3.72156200	−1.09411600	3.95080700
C	3.20393900	−1.09784400	2.65486600
H	−3.47870800	2.49457500	1.05719300
H	−1.48532900	6.34589400	−1.33359400
H	−1.85052700	6.57780500	0.40335000
H	−3.18628800	6.40386400	−0.77820600
H	−1.61118200	−2.30839100	−0.39416100
H	−1.81565900	0.81132700	2.07533600
H	−1.52961400	1.49458300	0.45974500
H	−3.57219800	1.53038200	−1.03894500
H	−6.30687300	0.85440100	0.21240600
H	−5.93429600	1.20831100	−1.48227400
H	−5.75669000	2.48435200	−0.26737700
H	−4.37573800	−1.61566900	−3.41544500
H	−2.72530100	−1.15630000	−2.90325600
H	−4.03710000	0.05542800	−2.93634500
H	−4.40850900	−3.84445100	−2.66280700
H	−4.58674900	−5.94008000	−1.35473800
H	−4.50584800	−5.92778800	1.11583200
H	−4.21056700	−3.78903800	2.36080500
H	−3.52779900	−0.94734800	3.02310300
H	−5.24030700	−1.00093800	2.63629400
H	−3.87712500	1.37933900	3.11373700
H	−5.35543800	1.29540600	2.14623800
H	5.21434100	0.93358600	−1.59213200
H	5.53178900	3.17457300	−2.57995800
H	3.77732800	4.91763600	−2.32382800
H	1.68145500	4.39076600	−1.06406500
H	1.35721700	2.16432300	−0.08756900
H	5.71624600	−1.40237800	0.38523700
H	7.02608000	−3.01263400	−0.95225200
H	6.06991400	−3.98531900	−3.03116600
H	3.78172600	−3.33663600	−3.76431500
H	2.45581000	−1.73557500	−2.42113500
H	5.02503900	1.47510100	1.34639900
H	5.92875000	1.48117500	3.64541200
H	5.10115200	−0.15908900	5.32094800
H	3.35279200	−1.80986800	4.68037200
H	2.43327000	−1.81508200	2.38282000

TS23 (L = JohnPhos)

Au	−0.80266300	0.15412000	0.12698600
S	3.17574000	−4.15133900	−0.55904800
P	−2.89519100	−1.01177800	0.12031400
O	4.06347200	−3.79195700	0.61925400
O	1.72826000	−4.02701000	−0.22627700
O	3.57715600	−3.42796300	−1.79816900
N	3.77637500	1.78247100	−1.24245400
N	3.88436900	−1.14107900	1.01621900
C	3.50122200	−5.89768700	−0.83883800
C	1.03856300	1.06593100	0.12174900
C	2.19951400	0.49352500	0.49104300
C	2.39854100	−0.89378100	1.05974900
C	4.35389100	−0.53346800	−0.29137800
C	5.86501600	−0.55860300	−0.49033900
C	3.74474400	0.85197500	−0.21193000
C	3.49458600	1.44660000	−2.63234500
C	3.57164800	3.04501500	−0.68798900
C	3.43289200	4.28067000	−1.33278100
C	3.29000200	5.40714900	−0.52677300

C	3.26942200	5.32139300	0.88079500
C	3.37789000	4.08994600	1.51754400
C	3.52396700	2.94373700	0.72529800
C	3.65690200	1.54013100	1.05526900
C	4.11555700	0.94684500	2.36828400
C	4.53948800	−0.53075700	2.22351600
C	−4.42834800	0.03121600	−0.04334400
C	−5.67882000	−0.61387100	0.06198000
C	−6.88351300	0.08419700	0.02256600
C	−6.86888400	1.47035000	−0.12127100
C	−5.64781500	2.12865700	−0.23439900
C	−4.41929800	1.44085700	−0.20727600
C	−3.21248000	2.31667700	−0.37562600
C	−2.61700700	2.48400600	−1.63671400
C	−1.59964700	3.42370500	−1.82554400
C	−1.16150100	4.21171600	−0.75708100
C	−1.74752800	4.05354500	0.50214600
C	−2.76952000	3.11849100	0.68936000
C	−2.88655600	−2.19599600	−1.39105200
C	−2.56828600	−1.31305100	−2.61697400
C	−4.20712600	−2.93951500	−1.66149200
C	−1.75162600	−3.22220200	−1.20696400
C	−3.04346200	−1.91741900	1.81861500
C	−1.63582100	−2.40526500	2.22807800
C	−3.99539100	−3.12713100	1.85958700
C	−3.50382300	−0.86223700	2.84609200
H	4.04816400	−2.19446500	0.96778800
H	2.90180200	−6.23396100	−1.68864100
H	3.22763300	−6.46029700	0.05702300
H	4.56365700	−6.03151800	−1.05593900
H	1.09731700	2.10140900	−0.22104100
H	2.06125300	−0.99920100	2.09271700
H	1.90857600	−1.65443700	0.44704300
H	3.87685400	−1.13561100	−1.07062600
H	6.39599800	0.11704800	0.18516600
H	6.08116400	−0.25244900	−1.51828300
H	6.23916100	−1.57840400	−0.35601000
H	3.92498900	2.21027700	−3.28284300
H	2.41112600	1.38698900	−2.80568200
H	3.95240900	0.48643300	−2.87531500
H	3.44555800	4.36391400	−2.41416600
H	3.19380000	6.38114000	−0.99822100
H	3.16044400	6.22743900	1.46891200
H	3.34909200	4.01462900	2.60047200
H	3.32626100	1.05293500	3.11806200
H	4.96917000	1.53418600	2.72271000
H	4.22155000	−1.12385300	3.08198800
H	5.61656400	−0.64267200	2.10592600
H	−5.72255500	−1.68756200	0.18189100
H	−7.82208200	−0.45601200	0.10893900
H	−7.79640000	2.03554600	−0.14883600
H	−5.63140200	3.20789900	−0.35685900
H	−2.96879700	1.89353400	−2.47805600
H	−1.16093300	3.54910500	−2.81219500
H	−0.37775400	4.94945200	−0.90642900
H	−1.42380500	4.67011000	1.33675400
H	−3.24037300	3.02119700	1.66409000
H	−1.59168700	−0.82498500	−2.52378900
H	−3.32951400	−0.54126500	−2.77611400
H	−2.54543600	−1.94646900	−3.51339600
H	−4.05132000	−3.61173800	−2.51549300
H	−5.01658400	−2.25562800	−1.93110700
H	−4.53272300	−3.55247200	−0.81729100
H	−0.78931300	−2.74721600	−0.98962500
H	−1.63856000	−3.79042200	−2.13945000
H	−1.97238100	−3.93936800	−0.41107300
H	−0.92582500	−1.57488000	2.30381500
H	−1.22590300	−3.14256400	1.53262500
H	−1.70713500	−2.88240300	3.21434600
H	−3.98313100	−3.53770000	2.87788100
H	−3.67626600	−3.92527500	1.18335600
H	−5.03206200	−2.86809900	1.63269500
H	−2.86423500	0.02879100	2.83427800
H	−3.44293100	−1.29977800	3.85081900
H	−4.53772000	−0.54509600	2.68116400

TS24

Au	2.17628800	−1.39026400	0.00700700
S	0.53806400	4.58476200	−0.31342500
P	4.53811800	−1.25141700	0.12379900
O	−0.96925900	4.38892700	0.25996100
O	1.46345200	4.79381600	0.80331600
O	0.82060400	3.49247700	−1.25696200
N	−2.87406500	−1.52187500	−1.03112400
N	−1.66352100	1.63604800	0.63734500
C	0.29774500	6.12085300	−1.19152500
C	0.12755300	−1.55467700	−0.12932100
C	−0.78249200	−0.59572100	0.11804300
C	−0.41697600	0.82551200	0.58731600
C	−2.45379700	1.27987800	−0.43998600
C	−3.83838800	1.80088500	−0.65815000
C	−2.26194400	−0.73753400	−0.04292700
C	−2.32883100	−1.83598600	−2.34694500
C	−4.15031500	−1.82097000	−0.63069400
C	−5.15450900	−2.53371100	−1.31028600
C	−6.37199700	−2.68637700	−0.66506400
C	−6.61690100	−2.14382700	0.62405400
C	−5.63877100	−1.43281400	1.29161400
C	−4.38166300	−1.25969400	0.66463600
C	−3.18969200	−0.60453400	1.04463100
C	−2.84853900	0.15492100	2.27468000
C	−2.34549000	1.60972700	1.93755000
C	5.30571100	−2.38694200	1.34962200
C	5.18812500	0.40889600	0.57214000
C	5.38445500	−1.65574100	−1.45760700
H	−1.16400800	3.41310200	0.36894800
H	1.26792100	6.40935500	−1.60404200
H	−0.05233600	6.87843600	−0.48702600
H	−0.42769900	5.96405100	−1.99186100
H	−0.27920500	−2.51976300	−0.44416200
H	0.04690200	0.83927400	1.57551800
H	0.27272400	1.29126900	−0.12160200
H	−1.88111600	1.17796300	−1.36015200
H	−4.46082500	1.83955400	0.23585200
H	−3.75336000	2.81529800	−1.07411900
H	−4.33822200	1.18592400	−1.41300800
H	−1.37841000	−1.31822000	−2.47169600
H	−3.02225500	−1.50548300	−3.12646800
H	−2.16125500	−2.91297200	−2.44952900
H	−4.98188800	−2.95614700	−2.29466400
H	−7.16452000	−3.24160300	−1.15913900
H	−7.58818000	−2.29519600	1.08535500
H	−5.82146000	−1.01814000	2.27875800
H	−2.03690500	−0.35784400	2.80465900

H	−3.70334700	0.21887900	2.95318600
H	−1.64608500	1.94999700	2.70172500
H	−3.18460000	2.30548100	1.90965800
H	4.92898300	−2.15579900	2.35130700
H	6.39665800	−2.28500600	1.34234600
H	5.04006400	−3.42132200	1.10803900
H	4.84339500	1.14758200	−0.15879600
H	6.28377000	0.40456200	0.59033400
H	4.81253700	0.69673400	1.55957900
H	5.12143600	−2.67274500	−1.76632700
H	6.47216400	−1.58445000	−1.34571500
H	5.05654100	−0.96069800	−2.23744100

TS24 (L = PPh_3)

Au	−0.90325700	−0.98200500	0.11749900
S	1.64603400	4.66824300	0.31354500
P	−3.22392200	−0.48358100	−0.03573500
O	3.05626500	4.24987100	−0.37675600
O	0.66421300	4.98058600	−0.72812400
O	1.30084200	3.64641600	1.31349300
N	4.10053700	−1.83952500	1.07933300
N	3.32554900	1.40935600	−0.66820700
C	2.17273200	6.17400400	1.11688600
C	1.09501500	−1.44662300	0.25658700
C	2.13172500	−0.64350800	−0.04188700
C	1.97174100	0.80471400	−0.54310700
C	4.09488200	0.97253200	0.39342300
C	5.55201300	1.27418100	0.54199200
C	3.57568800	−1.00762500	0.08100800
C	3.57596900	−2.00417300	2.43015200
C	5.30412000	−2.33729300	0.65108400
C	6.21674500	−3.16742900	1.32603500
C	7.37174400	−3.52440100	0.64711700
C	7.64381700	−3.07213900	−0.67089900
C	6.75750100	−2.24548100	−1.33400600
C	5.56593600	−1.86367800	−0.67293300
C	4.46920500	−1.05295300	−1.04087600
C	4.19438600	−0.29366200	−2.28720300
C	3.94182100	1.23360800	−1.98931400
C	−3.93447700	0.10575600	1.55272500
C	−5.22808700	−0.23699100	1.97445000
C	−5.71963400	0.24342100	3.19099500
C	−4.92828300	1.06983800	3.99225800
C	−3.63883600	1.41566600	3.57752900
C	−3.14073000	0.93196000	2.36712800
C	−4.23107400	−1.93626200	−0.53601500
C	−5.37499600	−1.81783600	−1.34056800
C	−6.11289800	−2.95378500	−1.68273500
C	−5.71732400	−4.21331000	−1.22564600
C	−4.57843300	−4.33836200	−0.42504100
C	−3.83464000	−3.20719300	−0.08545900
C	−3.57970800	0.82804300	−1.27287800
C	−4.55399600	1.81730300	−1.07144100
C	−4.77901600	2.78911900	−2.05030900
C	−4.03952100	2.77950100	−3.23518600
C	−3.06825500	1.79548000	−3.44261500
C	−2.83496100	0.82755900	−2.46516100
H	3.10885500	3.25349400	−0.45320300
H	1.29588200	6.59863400	1.61224200
H	2.54993900	6.86510300	0.35979800
H	2.94680000	5.93246900	1.84731600
H	1.35622400	−2.45348200	0.59310000
H	1.47050000	0.86547400	−1.51106900
H	1.39570600	1.38975800	0.17864600
H	3.55372300	0.98657200	1.33770700
H	6.12997900	1.20312500	−0.37920500
H	5.64496900	2.29437600	0.94169500
H	5.98451700	0.59817800	1.28647000
H	2.67255600	−1.40445100	2.53503500
H	4.31711700	−1.67126100	3.16401500
H	3.32877000	−3.05336800	2.62020600
H	6.02244900	−3.52282800	2.33248600
H	8.09158200	−4.17428500	1.13698300
H	8.56298200	−3.38457100	−1.15721300
H	6.96068900	−1.89868700	−2.34303600
H	3.28825500	−0.68855100	−2.76196400
H	5.01632600	−0.38787200	−3.00182100
H	3.27475500	1.65590900	−2.74133600
H	4.88069900	1.78686600	−2.01671100
H	−5.85242600	−0.87708300	1.35894100
H	−6.72166800	−0.02994100	3.51017300
H	−5.31287200	1.44001300	4.93869600
H	−3.01743000	2.05463400	4.19897400
H	−2.13323900	1.19466100	2.05398100
H	−5.69194200	−0.84430400	−1.70181900
H	−6.99613800	−2.85195400	−2.30732100
H	−6.29218600	−5.09511400	−1.49510400
H	−4.26328700	−5.31638100	−0.07182300
H	−2.94302900	−3.31084400	0.52809100
H	−5.13579400	1.83515100	−0.15523500
H	−5.53336000	3.55333200	−1.88455300
H	−4.21543700	3.53816900	−3.99281400
H	−2.48741000	1.78538400	−4.36080000
H	−2.07162400	0.07023700	−2.62595200

TS24 (L = JohnPhos)

Au	−1.01669400	−0.96210100	−0.22931400
S	1.79145000	4.73662100	−0.26667300
P	−3.34296100	−0.70171000	−0.78914300
O	3.10957200	4.20324900	−1.05027600
O	0.66720400	4.83376700	−1.20182700
O	1.61834300	3.92293400	0.94633900
N	3.92160900	−1.72307700	1.14307500
N	3.31804900	1.35044600	−0.95530900
C	2.36818100	6.37267800	0.15473300
C	0.97549200	−1.37046000	0.10304600
C	2.04237000	−0.60791500	−0.19770900
C	1.94362000	0.79401200	−0.83042500
C	4.02920000	1.00380200	0.17835600
C	5.48610200	1.28861800	0.36082900
C	3.46994600	−0.98421800	0.04115900
C	3.32049300	−1.75465100	2.47109300
C	5.13456900	−2.28222400	0.83323000
C	5.99157500	−3.05287500	1.63873100
C	7.17548500	−3.49255200	1.06649000
C	7.52868900	−3.17851800	−0.27221600
C	6.69632900	−2.41116500	−1.06439100
C	5.47776600	−1.94762700	−0.51423800
C	4.42069400	−1.15792000	−1.01957800
C	4.22636900	−0.52493500	−2.34902500
C	3.98609700	1.02776900	−2.22283200
C	−4.49346000	0.01281500	0.49089000
C	−5.85761000	0.14060000	0.15471800
C	−6.81065600	0.59827000	1.06178600

C	−6.41859400	0.93500200	2.35610600
C	−5.07545900	0.83374400	2.70685300
C	−4.09328900	0.39570900	1.79717000
C	−2.69152000	0.43866400	2.32804600
C	−1.85242000	1.52315800	2.02159900
C	−0.61363000	1.66812800	2.65153500
C	−0.19318400	0.72682900	3.59603900
C	−1.01581600	−0.36077600	3.90293000
C	−2.25943900	−0.49921700	3.27969400
C	−3.46921000	0.44417300	−2.33602300
C	−3.36506700	1.89296000	−1.81525500
C	−4.74116000	0.29550400	−3.19007500
C	−2.24940600	0.17001000	−3.24328500
C	−3.98754900	−2.48865300	−1.09696000
C	−3.19937900	−3.09076200	−2.27774700
C	−5.49461700	−2.64291300	−1.37176800
C	−3.64912600	−3.28037500	0.18548300
H	3.15831800	3.20570100	−0.97376400
H	1.54609000	6.88160200	0.66452500
H	2.62855000	6.90314400	−0.76367700
H	3.23310400	6.28427200	0.81449800
H	1.20918500	−2.34334200	0.54541000
H	1.47922800	0.78371800	−1.81826100
H	1.36022000	1.45572100	−0.18394400
H	3.44816000	1.12794300	1.09042500
H	6.10137100	1.10871400	−0.52077400
H	5.58842500	2.34293700	0.65596200
H	5.86890000	0.68538300	1.19000300
H	2.41818800	−1.14464000	2.46848400
H	4.02262300	−1.35731500	3.21138500
H	3.05258800	−2.77998800	2.74524600
H	5.73469300	−3.30085700	2.66328700
H	7.85465900	−4.09882700	1.65956600
H	8.46773000	−3.55006800	−0.67142000
H	6.96275500	−2.16918800	−2.08919300
H	3.33894700	−0.95573800	−2.82825500
H	5.08229700	−0.70337600	−3.00520200
H	3.35830000	1.37748000	−3.04295100
H	4.93451200	1.56387100	−2.26685100
H	−6.19292100	−0.12948600	−0.83663700
H	−7.84984400	0.68168900	0.75605500
H	−7.14602300	1.28391400	3.08391000
H	−4.76141200	1.11778300	3.70724400
H	−2.18539700	2.27088500	1.30701200
H	0.01560600	2.51972400	2.40705400
H	0.76302700	0.84720600	4.09864900
H	−0.70054800	−1.09222700	4.64269000
H	−2.90735300	−1.33076800	3.54460700
H	−2.46798400	2.04310600	−1.20315500
H	−4.23816400	2.18556000	−1.22418500
H	−3.29828400	2.57327200	−2.67406600
H	−4.68030900	1.00924500	−4.02253700
H	−5.65684300	0.52561200	−2.63988000
H	−4.83256600	−0.70433400	−3.62411600
H	−1.30432200	0.31492800	−2.70955200
H	−2.27616000	0.87508400	−4.08463600
H	−2.25426000	−0.84122900	−3.65957400
H	−2.11668500	−2.98161500	−2.14758900
H	−3.48370500	−2.63953800	−3.23326400
H	−3.42293100	−4.16391900	−2.33971500
H	−5.69375600	−3.69907800	−1.59658900
H	−5.83650400	−2.05617500	−2.22805600
H	−6.10139100	−2.37789600	−0.50206200
H	−2.57210500	−3.28747900	0.38796800
H	−3.97870000	−4.31990700	0.05864300
H	−4.16214100	−2.87508600	1.06484000

TS24'

Au	−2.25236300	−0.34255100	−0.04581200
P	−4.60823600	−0.13230100	−0.18412200
N	2.80312900	−1.01580400	0.80139000
N	1.72682100	2.55127900	0.64664500
C	−0.20772800	−0.57654100	0.04669400
C	0.71782200	0.37696900	0.23893200
C	0.42594000	1.87938200	0.45443800
C	2.51725900	1.69972000	1.40208000
C	3.95350800	2.00935500	1.72549700
C	2.21267000	0.16066900	0.28605800
C	2.33954900	−1.76262300	1.96377700
C	3.98894900	−1.23349300	0.16307500
C	4.95574300	−2.23290000	0.38977700
C	6.08110400	−2.22173500	−0.41663000
C	6.28138700	−1.24160100	−1.42815100
C	5.34823500	−0.24975800	−1.64669500
C	4.17923300	−0.23062400	−0.84463400
C	3.05605200	0.61399600	−0.79664100
C	2.70991900	1.83621300	−1.55643200
C	2.34677600	3.03305300	−0.57960400
C	−5.53489000	−1.18406600	1.00582500
C	−5.31320700	−0.57877000	−1.82296500
C	−5.24205100	1.56473400	0.13268900
H	0.18164100	−1.58956400	−0.09204300
H	−0.09928100	2.33260600	−0.38895800
H	−0.18605300	2.02182400	1.35137200
H	1.98081300	1.30793900	2.26700300
H	4.55007200	2.34241900	0.87545800
H	4.42779100	1.12204200	2.15585000
H	3.97048100	2.79279300	2.49475200
H	3.04647200	−1.66003800	2.79432400
H	2.23196300	−2.82271200	1.71440300
H	1.36773800	−1.37518100	2.26858700
H	4.82039100	−2.98654900	1.15839000
H	6.83851900	−2.98771700	−0.27475800
H	7.18392800	−1.28247500	−2.03028500
H	5.49472300	0.50120900	−2.41751100
H	1.81778800	1.64305100	−2.16484200
H	3.51788700	2.14013500	−2.22767300
H	1.65599800	3.71068000	−1.08317600
H	3.24923100	3.59152500	−0.32867400
H	−5.29685700	−2.23803600	0.82953900
H	−6.61461700	−1.03521000	0.89271700
H	−5.24269100	−0.92751500	2.02933500
H	−4.88509100	0.06811600	−2.59565700
H	−6.40301500	−0.46503300	−1.82141500
H	−5.06079400	−1.61735400	−2.06107800
H	−4.93209200	1.89313000	1.13023200
H	−6.33583700	1.58740300	0.07178400
H	−4.82615600	2.25839200	−0.60547600

TS25

Au	2.14123800	−0.65642600	−0.27273400
S	0.28108000	3.58924100	−0.64959100
P	4.26024800	−1.55407300	0.13417800
O	1.21151100	2.38346500	−1.01148000

O	0.14099600	3.71560300	0.82119900
O	−0.97805500	3.53845400	−1.41875500
N	−2.85819000	−0.42129000	−1.37168900
N	−1.65534700	0.60113900	2.44422300
C	1.25991700	4.97263900	−1.23102000
C	0.15428800	−0.02335300	−0.74934400
C	−0.86063500	−0.16842600	0.16639300
C	−0.52621200	0.05588700	1.64036700
C	−1.77160600	1.87994000	2.58681800
C	−2.79137400	2.60696800	3.37244100
C	−2.22851900	−0.56599600	−0.13035800
C	−2.44399600	0.42395600	−2.48864400
C	−4.09017700	−1.03502100	−1.30662200
C	−5.08549300	−1.16024500	−2.29013300
C	−6.24251900	−1.84980100	−1.95022700
C	−6.42181000	−2.40686100	−0.66152500
C	−5.44350600	−2.27820800	0.31240600
C	−4.25778100	−1.58044500	−0.00101900
C	−3.07987800	−1.25810400	0.73572800
C	−2.77370500	−1.62336000	2.15960400
C	−2.57167000	−0.39549700	3.06143900
C	4.21211200	−3.25884700	0.81459700
C	5.26519300	−0.59904900	1.33821100
C	5.31317200	−1.67586600	−1.36489200
H	0.75862800	1.27127200	−0.77820100
H	1.43025500	4.86077300	−2.30389900
H	2.20825400	4.99125700	−0.68988200
H	0.69308200	5.88605600	−1.03209100
H	−0.11716100	−0.28003000	−1.77369600
H	−0.21833300	−0.87475300	2.12249200
H	0.30935800	0.75243400	1.71514300
H	−1.03272400	2.48591000	2.05813400
H	−3.46230900	1.98579600	3.96371400
H	−2.26498400	3.30907000	4.03196700
H	−3.37407200	3.22694200	2.67654700
H	−1.85956400	1.26987400	−2.12390600
H	−3.33816200	0.81692600	−2.97799900
H	−1.85956400	−0.13661400	−3.22644400
H	−4.95477700	−0.74946700	−3.28613300
H	−7.02531400	−1.97034200	−2.69421500
H	−7.34014700	−2.94269700	−0.43760600
H	−5.58560400	−2.70700000	1.30103300
H	−1.90026500	−2.28335400	2.22201900
H	−3.60762200	−2.18675100	2.58944500
H	−2.13523300	−0.68796400	4.02204700
H	−3.52643300	0.09477300	3.23979200
H	3.65120400	−3.26511100	1.75463500
H	5.22738000	−3.62765700	0.99809900
H	3.71014000	−3.92362600	0.10426800
H	5.41908900	0.41778100	0.96286000
H	6.23820600	−1.07909100	1.49164500
H	4.73584400	−0.54155000	2.29477100
H	4.81830000	−2.30519600	−2.11148500
H	6.28798400	−2.10918100	−1.11510400
H	5.46010800	−0.67861400	−1.79192500

TS25 (L = PPh_3)

Au	−0.81282900	−0.03888300	0.41426500
S	1.68720500	3.77360100	0.63051100
P	−3.07520500	−0.49593800	0.00563700
O	0.70077600	2.73622200	1.25763000
O	1.57807400	3.76258800	−0.85018000
O	3.05023900	3.61294500	1.17509100
N	4.18315200	−0.65934700	1.42313900
N	3.07766200	0.52657000	−2.37054800
C	1.00224100	5.31844100	1.22720200
C	1.25948000	0.19149000	0.86627200
C	2.21796800	−0.10827700	−0.07365600
C	1.89344700	0.18116400	−1.53815300
C	3.39833400	1.76477500	−2.55046600
C	4.54210600	2.23620900	−3.37122600
C	3.51016800	−0.71664400	0.19710300
C	3.92665100	0.25193300	2.53574800
C	5.31649700	−1.43774800	1.33067500
C	6.31927900	−1.68424800	2.28351000
C	7.36806200	−2.51608800	1.91265700
C	7.43340500	−3.09899800	0.62446100
C	6.44698700	−2.85494200	−0.31827400
C	5.37119600	−2.00895400	0.02615800
C	4.23093500	−1.52870700	−0.68267800
C	3.84060700	−1.84375900	−2.09747400
C	3.82669500	−0.59728300	−2.99351600
C	−3.92570100	0.85782500	−0.89701000
C	−5.25605900	1.21498400	−0.62960000
C	−5.86273600	2.24680700	−1.35038700
C	−5.15016400	2.92571200	−2.34145800
C	−3.82436700	2.57419900	−2.61219300
C	−3.21156000	1.54921300	−1.89076800
C	−4.02028700	−0.76320400	1.55599400
C	−5.08165800	−1.67775900	1.63864200
C	−5.77864000	−1.83476700	2.83916300
C	−5.42535600	−1.08162600	3.96145800
C	−4.36832500	−0.17018100	3.88545500
C	−3.66498600	−0.01344700	2.69048000
C	−3.29353400	−2.01128700	−1.00749700
C	−4.33082100	−2.14357800	−1.94354700
C	−4.46518600	−3.32459300	−2.67776800
C	−3.56899700	−4.37871300	−2.48497900
C	−2.53352600	−4.25259400	−1.55439100
C	−2.39151400	−3.07314300	−0.82232000
H	0.91060000	1.55760800	0.94482500
H	1.02069600	5.31517100	2.31919400
H	−0.02104600	5.42012500	0.86017700
H	1.62565900	6.12914900	0.84122300
H	1.50282000	−0.12714300	1.88014500
H	1.41409200	−0.67987900	−2.01031700
H	1.19151600	1.01447200	−1.58794200
H	2.77192500	2.49824400	−2.03912200
H	5.48827000	1.98469600	−2.87111100
H	4.55663300	1.76756200	−4.36088700
H	4.48970800	3.32052900	−3.48209600
H	3.47642700	1.17556300	2.16851300
H	4.87979300	0.50447100	3.00561700
H	3.27370900	−0.20096500	3.28946600
H	6.27647600	−1.25484900	3.27936700
H	8.15383300	−2.73006400	2.63202300
H	8.27021700	−3.74621000	0.37677800
H	6.50064200	−3.30349400	−1.30682900
H	2.86720400	−2.34663900	−2.13929100
H	4.56062200	−2.53804600	−2.54109100
H	3.34891000	−0.81231700	−3.95555500
H	4.84503300	−0.25375000	−3.17283800
H	−5.81988800	0.69432400	0.13807700
H	−6.89232900	2.51849000	−1.13452400

H	−5.62435800	3.72935200	−2.89811600
H	−3.26439300	3.10296600	−3.37861900
H	−2.17702200	1.28619000	−2.09712700
H	−5.36499800	−2.26924800	0.77363200
H	−6.59697500	−2.54729900	2.89505000
H	−5.96796300	−1.20869900	4.89416200
H	−4.08599400	0.41380300	4.75706200
H	−2.83603600	0.68819000	2.63851800
H	−5.03298000	−1.33103900	−2.10228100
H	−5.27003200	−3.41782700	−3.40168900
H	−3.67538400	−5.29486000	−3.05939100
H	−1.83151600	−5.06802500	−1.40338100
H	−1.57984400	−2.97521300	−0.10547500

TS25 (L = JohnPhos)

Au	0.88179000	−0.04917300	−0.00378900
S	−1.64659900	−2.86594000	2.49063900
P	3.06794800	−0.28431500	−0.89125600
O	−0.67024400	−1.64631400	2.42857900
O	−1.60333800	−3.62349900	1.21352200
O	−2.98792100	−2.45903000	2.95199700
N	−4.01563500	1.39208500	0.68554000
N	−3.25526000	−1.84414200	−1.73533400
C	−0.87769100	−3.87061900	3.76101100
C	−1.15892700	0.18805900	0.60117300
C	−2.18143500	−0.06356500	−0.28142700
C	−1.99125200	−1.18600300	−1.29913100
C	−3.64132600	−2.92255900	−1.13764500
C	−4.82947500	−3.74684900	−1.44415600
C	−3.42789400	0.68448300	−0.36822100
C	−3.72596900	1.26275300	2.11077600
C	−5.11437800	2.06520200	0.19466300
C	−6.03144500	2.89632100	0.85881100
C	−7.05848500	3.45253300	0.10607300
C	−7.18473900	3.19503100	−1.27944300
C	−6.28339200	2.37034300	−1.93563000
C	−5.23239100	1.78645600	−1.19782700
C	−4.16675800	0.89858700	−1.53283800
C	−3.85766100	0.30669500	−2.87716200
C	−3.97002500	−1.22578000	−2.88604500
C	4.35688100	0.90398400	−0.26976200
C	5.64167300	0.84019200	−0.84930200
C	6.66530400	1.71324500	−0.48920200
C	6.42502800	2.69222200	0.47329400
C	5.16507400	2.77457400	1.05906900
C	4.11762700	1.89911200	0.71273900
C	2.83734000	2.13443600	1.45829700
C	2.50767500	1.37122500	2.59040600
C	1.40440200	1.70810300	3.37961100
C	0.61374500	2.81284100	3.05015500
C	0.93110600	3.57778000	1.92412500
C	2.03806200	3.24489400	1.13875200
C	3.68770200	−2.04042000	−0.41602700
C	3.56842600	−2.12886500	1.12030800
C	5.14109900	−2.36744100	−0.80441900
C	2.74457900	−3.08024200	−1.05248600
C	2.94077100	0.01179900	−2.79569700
C	1.58298600	−0.54200800	−3.28232900
C	4.04898100	−0.63095600	−3.65033800
C	2.93969400	1.53926800	−3.01267600
H	−0.83416400	−0.89215100	1.47521500
H	−0.85653100	−3.30394900	4.69443100
H	0.13507200	−4.13126000	3.44682300
H	−1.48254200	−4.77343300	3.88028400
H	−1.31749000	1.06092200	1.23539500
H	−1.50108100	−0.81872900	−2.20365300
H	−1.34742800	−1.95118600	−0.86498200
H	−3.00554800	−3.25575400	−0.31486600
H	−5.40420600	−3.43932100	−2.31631600
H	−4.49046100	−4.78294000	−1.57520500
H	−5.47592600	−3.75215500	−0.55540900
H	−3.31123900	0.27566900	2.32005800
H	−4.66040200	1.36328400	2.66785800
H	−3.02737600	2.03239400	2.45564400
H	−5.93888100	3.11215400	1.91857600
H	−7.77738500	4.10656600	0.59217500
H	−8.00015600	3.65296200	−1.83258400
H	−6.38418700	2.17403200	−2.99997900
H	−2.86487200	0.61234300	−3.22855600
H	−4.56943300	0.67306600	−3.62337000
H	−3.53279800	−1.64213300	−3.79953100
H	−5.01577700	−1.52089700	−2.82680900
H	5.85657800	0.09537400	−1.60289900
H	7.63882400	1.62630000	−0.96332600
H	7.20848900	3.38472300	0.76837500
H	4.97451000	3.53249000	1.81350500
H	3.13159200	0.52649100	2.86811200
H	1.17263800	1.11447600	4.26017500
H	−0.23479800	3.08278000	3.67318700
H	0.32946900	4.44536800	1.66553100
H	2.29679800	3.86092300	0.28132400
H	2.53718400	−1.98202700	1.45765900
H	4.20666500	−1.39389600	1.62318000
H	3.89262200	−3.12684600	1.44308000
H	5.34299900	−3.40781300	−0.51766100
H	5.86029200	−1.73968700	−0.27173400
H	5.32910800	−2.28244000	−1.87736800
H	1.69440100	−2.88396800	−0.80851400
H	3.00019800	−4.07270300	−0.65935800
H	2.84829400	−3.12031400	−2.14110900
H	0.74353100	−0.04962900	−2.78015500
H	1.48962800	−1.62082900	−3.12872300
H	1.49501100	−0.34951700	−4.35955600
H	3.86460000	−0.37256000	−4.70148900
H	4.04307800	−1.72223700	−3.57714500
H	5.04890600	−0.26800200	−3.40208100
H	2.17417400	2.03960500	−2.40730000
H	2.71286400	1.74314200	−4.06703400
H	3.90894700	1.99192100	−2.78519400

TS26

Au	2.10340300	−0.98565800	0.07004300
S	−0.18464700	3.77678500	−0.50495400
P	4.41145800	−0.53860700	−0.22252000
O	−0.65118200	3.92769700	0.89410600
O	1.23829900	3.46562400	−0.70352500
O	−1.07661400	2.69057300	−1.22891900
N	−3.71771200	−0.30747200	−0.92708800
N	−1.88128300	1.37420900	1.75855400
C	−0.58070000	5.26806800	−1.41193000
C	0.09897000	−1.42045700	0.25587100
C	−0.84892900	−0.67402600	0.84289800
C	−0.56356700	0.65501300	1.51802600
C	−2.70235600	1.49424300	0.49002200

C	−3.74222000	2.60529300	0.56626900
C	−2.99261100	0.17478600	0.08483700
C	−4.40902500	0.47164100	−1.95323800
C	−3.68939100	−1.73386700	−0.90877400
C	−4.34747000	−2.61654800	−1.75677300
C	−4.15907500	−3.98567400	−1.52439300
C	−3.34815500	−4.43949300	−0.47982600
C	−2.69937400	−3.52991300	0.36812200
C	−2.87657300	−2.16973700	0.14695900
C	−2.36210600	−0.95881500	0.87629500
C	−2.88283300	−0.81172600	2.34791200
C	−2.63150200	0.62786100	2.84719300
C	5.24691100	−1.67905600	−1.39826200
C	5.41616200	−0.65718900	1.31280900
C	4.78716500	1.13734200	−0.87791100
H	−1.65563000	2.32997400	2.06364800
H	−0.32161600	5.11796400	−2.46229300
H	0.01096200	6.08366800	−0.98854200
H	−1.64753800	5.47432600	−1.30403100
H	−0.25173300	−2.35456300	−0.18923800
H	−0.09920200	0.54131900	2.50205300
H	0.07147200	1.29967100	0.91328300
H	−1.74595800	2.11734900	−0.51135200
H	−4.53240600	2.39150500	1.29744500
H	−3.26130200	3.54879900	0.84196700
H	−4.21800100	2.75332100	−0.40550200
H	−4.44423400	−0.11343300	−2.87315000
H	−3.85066600	1.38760500	−2.15032600
H	−5.42836600	0.71413200	−1.63864600
H	−4.98865100	−2.27369100	−2.56169800
H	−4.65932400	−4.70299800	−2.16862700
H	−3.22291500	−5.50617100	−0.31905600
H	−2.07502800	−3.88419400	1.18301500
H	−2.36204900	−1.54002500	2.97441500
H	−3.95118300	−1.03879300	2.37850800
H	−2.00935100	0.66325300	3.74252300
H	−3.55538300	1.17555800	3.03296600
H	5.15434600	−2.70975300	−1.04043000
H	6.30851400	−1.42633100	−1.49715500
H	4.76819500	−1.60874100	−2.38043600
H	5.04479500	0.06197900	2.05030300
H	6.47117300	−0.44643000	1.10454400
H	5.32690600	−1.66354500	1.73488900
H	4.29858600	1.27046700	−1.84863700
H	5.86775000	1.27421300	−0.99693500
H	4.40048800	1.89626500	−0.19001100

TS26 (L = PPh_3)

Au	−0.74842400	−0.86403400	−0.16056300
S	1.76822700	3.67859500	0.53658200
P	−3.04044100	−0.26312500	0.04831000
O	2.24268700	3.85029000	−0.85711400
O	0.33601500	3.40209600	0.72298900
O	2.62838100	2.55196100	1.23509100
N	5.09194500	−0.54915100	0.91881500
N	3.38298800	1.23911900	−1.78184900
C	2.20023300	5.13577200	1.48298900
C	1.22455700	−1.42733100	−0.29867500
C	2.22230000	−0.74233700	−0.87740500
C	2.02263900	0.59871500	−1.55821000
C	4.19407200	1.31063700	−0.50307800
C	5.28883500	2.36856900	−0.56294600
C	4.40681400	−0.02469100	−0.09950400
C	5.82101800	0.18945000	1.94926700
C	4.97778100	−1.97171600	0.90018100
C	5.57511500	−2.89247600	1.75271100
C	5.30854800	−4.24787400	1.51653400
C	4.48253800	−4.65228700	0.46361300
C	3.89613400	−3.70538300	−0.38877700
C	4.15045900	−2.35816600	−0.16360500
C	3.71578300	−1.11824700	−0.89676300
C	4.25354800	−1.00405200	−2.36505100
C	4.10253400	0.45028900	−2.86179900
C	−3.55761800	−0.01279600	1.79414000
C	−4.85765900	−0.29725000	2.24107500
C	−5.20377300	−0.08163200	3.57705800
C	−4.25825400	0.41772200	4.47643400
C	−2.96186900	0.70187100	4.03859200
C	−2.61006000	0.48396300	2.70538100
C	−4.17012200	−1.54624400	−0.62811400
C	−5.35824400	−1.22795300	−1.30355000
C	−6.18661800	−2.24564600	−1.78404500
C	−5.83833000	−3.58492500	−1.59358900
C	−4.65545900	−3.90884200	−0.92268400
C	−3.82146500	−2.89605500	−0.44738100
C	−3.45356200	1.29151800	−0.84115300
C	−4.36886700	2.22991400	−0.34116000
C	−4.64769600	3.39293100	−1.06390700
C	−4.01908600	3.62724900	−2.28900300
C	−3.10591600	2.69641100	−2.79300100
C	−2.81899700	1.53717400	−2.07119100
H	3.21956200	2.20504500	−2.09208000
H	1.93456000	4.96467600	2.52848300
H	1.63055000	5.97713500	1.08034400
H	3.27232300	5.31704000	1.38266200
H	1.50673400	−2.38039700	0.15406800
H	1.56574200	0.50958000	−2.54828500
H	1.41924800	1.28183600	−0.96374600
H	3.26841400	1.96117900	0.49758800
H	6.07230800	2.12074000	−1.29043200
H	4.85669600	3.33669300	−0.83467300
H	5.76417100	2.48537000	0.41334400
H	5.82960900	−0.40281300	2.86509700
H	5.30699400	1.12963800	2.15353400
H	6.85009800	0.38533800	1.63420400
H	6.22738100	−2.58944000	2.56450100
H	5.75952300	−4.99393400	2.16439400
H	4.29624900	−5.70959900	0.30010600
H	3.26024800	−4.02196400	−1.21015400
H	3.68690900	−1.69414300	−2.99498200
H	5.30421800	−1.30231700	−2.39235900
H	3.49896700	0.52847200	−3.76716600
H	5.06222200	0.93929500	−3.02915800
H	−5.60013100	−0.68767800	1.55194500
H	−6.21228000	−0.30663500	3.91322300
H	−4.52959100	0.58066400	5.51596000
H	−2.22129900	1.08565200	4.73492800
H	−1.59777100	0.69790900	2.37163000
H	−5.63989500	−0.19066300	−1.45636600
H	−7.10355400	−1.98946000	−2.30780200
H	−6.48386400	−4.37378300	−1.96996400
H	−4.37692400	−4.94891400	−0.77674200
H	−2.89757200	−3.15302500	0.06517700
H	−4.86438600	2.05839900	0.60936500

H	−5.35622000	4.11460300	−0.66661000
H	−4.23598100	4.53386100	−2.84738800
H	−2.60969700	2.87638800	−3.74286200
H	−2.10014500	0.82108400	−2.46201700

TS26 (L = JohnPhos)

Au	−0.97528900	−0.70538900	−0.59865400
S	2.15276100	3.91541200	0.62269100
P	−3.29180400	−0.06599600	−0.72112300
O	2.48144200	3.95210000	−0.82176300
O	0.73853500	4.04004700	0.99771200
O	2.74889400	2.58925800	1.24794500
N	4.90440500	−0.75054400	0.80678500
N	3.38574400	1.30990200	−1.80995200
C	3.07963600	5.20285700	1.45379700
C	0.99104400	−1.32234800	−0.63109400
C	2.06094500	−0.63951600	−1.06505400
C	1.97818600	0.77584300	−1.61005700
C	4.19409200	1.24680800	−0.52984600
C	5.39202800	2.18859800	−0.54614700
C	4.28132100	−0.11993900	−0.19129700
C	5.66784000	−0.13203500	1.88951500
C	4.68192200	−2.15599800	0.70802200
C	5.18196200	−3.16240300	1.52547700
C	4.81513800	−4.47863900	1.21358300
C	3.98857100	−4.76205300	0.12206200
C	3.50076100	−3.72967100	−0.69276100
C	3.85274600	−2.41980000	−0.39123400
C	3.52715600	−1.11214300	−1.06030600
C	4.10525700	−0.95499700	−2.50987900
C	4.04083400	0.52816300	−2.93481100
C	−4.23626300	0.08870400	0.87735000
C	−5.61476800	0.38075300	0.80558900
C	−6.42240100	0.45416800	1.93833500
C	−5.86300200	0.22984600	3.19495700
C	−4.50405900	−0.05542300	3.29223100
C	−3.66902800	−0.12638700	2.16040200
C	−2.23092400	−0.42730200	2.46331600
C	−1.27679600	0.60045100	2.53999300
C	0.02596400	0.33227000	2.96930000
C	0.39456700	−0.96647200	3.33134000
C	−0.54726400	−1.99654300	3.26100800
C	−1.85163800	−1.72706800	2.83772900
C	−3.37226900	1.66481300	−1.54905500
C	−2.45272400	2.57277200	−0.70405200
C	−4.76033300	2.32766100	−1.62184000
C	−2.79420900	1.55104700	−2.97395300
C	−4.19218400	−1.44814500	−1.72706300
C	−3.24737200	−1.92791400	−2.85250600
C	−5.53614800	−1.06079600	−2.37063900
C	−4.40854300	−2.62602000	−0.75416400
H	3.30058000	2.30183900	−2.06423000
H	2.89875700	5.12515800	2.52820600
H	2.72330300	6.16616800	1.07996900
H	4.14115100	5.07674500	1.23098800
H	1.19928500	−2.32767100	−0.25748800
H	1.48859500	0.82992300	−2.58676500
H	1.46652600	1.45336900	−0.92922600
H	3.32834000	1.96274000	0.50024200
H	6.16107000	1.87662500	−1.26425000
H	5.06928000	3.20172700	−0.80557600
H	5.85655200	2.23689000	0.44124700
H	5.57053300	−0.74996200	2.78334100
H	5.25525700	0.85389500	2.10640500
H	6.72507000	−0.04532800	1.62169400
H	5.83545700	−2.95103800	2.36493500
H	5.18806600	−5.29020700	1.83173000
H	3.72476300	−5.79156200	−0.10116700
H	2.86439500	−3.95246900	−1.54404200
H	3.51619900	−1.58070600	−3.18484000
H	5.13881300	−1.30894100	−2.53225500
H	3.43283600	0.68727000	−3.82648700
H	5.02786200	0.96277600	−3.09340400
H	−6.07731200	0.55314100	−0.15616700
H	−7.47934800	0.68234600	1.83294700
H	−6.47420000	0.27832000	4.09198600
H	−4.06110000	−0.22336000	4.26978800
H	−1.55870600	1.61644700	2.27888000
H	0.75070200	1.14021500	3.02255600
H	1.40524100	−1.17272600	3.67377300
H	−0.27383300	−3.00792700	3.55078800
H	−2.58651800	−2.52750100	2.80991400
H	−1.41906600	2.21224700	−0.69383200
H	−2.80004700	2.65465900	0.33185900
H	−2.45581000	3.58260200	−1.13484500
H	−4.65715800	3.27644200	−2.16485900
H	−5.15529200	2.56536000	−0.63049000
H	−5.49813100	1.72373000	−2.15631400
H	−1.82071100	1.04756100	−2.98527600
H	−2.65432600	2.56136100	−3.38041100
H	−3.46980000	1.01616100	−3.64845100
H	−2.29045100	−2.28587200	−2.45819800
H	−3.04112300	−1.14824400	−3.59067500
H	−3.73027600	−2.76172900	−3.37899400
H	−5.92310400	−1.93528500	−2.91070500
H	−5.42809300	−0.25144600	−3.09859700
H	−6.29660500	−0.77709700	−1.63936500
H	−3.47374600	−2.93206400	−0.26920300
H	−4.78467900	−3.48764600	−1.32077200
H	−5.14080100	−2.39341300	0.02458400

TS27

Au	−1.95447500	−0.48975900	−0.18140500
S	−0.15885800	3.80988500	−0.33279300
P	−3.98826300	−1.58332400	0.13687300
O	0.21099800	3.80391300	1.10422400
O	0.97105100	3.78249800	−1.28645100
O	−1.18362000	2.67529700	−0.64098900
N	3.52084200	−2.03387500	0.41284000
N	2.08208800	0.64005000	2.50155300
C	−1.13423100	5.28240900	−0.64948000
C	−0.00412800	0.31552400	−0.58994100
C	0.98613900	0.28417500	0.33585200
C	0.73844900	0.58134800	1.80085100
C	2.79945300	−0.66582000	2.39262000
C	3.16530400	−1.31063600	3.69045400
C	2.97213500	−0.96550300	1.08777700
C	4.04500600	−3.24289600	1.02652000
C	3.51773700	−1.77433300	−0.97066700
C	4.03145900	−2.55959900	−2.00209800
C	3.91568900	−2.07546900	−3.31257100
C	3.31881400	−0.84211700	−3.58575200
C	2.81200500	−0.05883600	−2.53704700
C	2.90419100	−0.53500900	−1.23564900

C	2.48221500	0.07601100	0.07561800
C	3.18028500	1.43422300	0.42473200
C	2.90017900	1.78109600	1.89921900
C	−5.46456300	−0.53162100	−0.15098500
C	−4.21452800	−2.26415000	1.82636700
C	−4.20860800	−3.01669300	−0.98817800
H	−0.70462500	1.49825100	−0.52655400
H	1.91804200	0.84941500	3.49113100
H	−1.45563300	5.27726500	−1.69315200
H	−0.49766000	6.14955600	−0.45475300
H	−1.99802000	5.29063500	0.01861200
H	0.31612000	0.12045700	−1.61482000
H	0.24796200	1.55026400	1.93542100
H	0.15686100	−0.19998300	2.29298600
H	3.73039700	−0.61553900	4.32718500
H	2.27800500	−1.62687300	4.25709100
H	3.79128000	−2.18964000	3.52915100
H	4.09708900	−4.03228600	0.27505300
H	3.37253000	−3.57865600	1.82049900
H	5.04735500	−3.08616500	1.44355600
H	4.51939200	−3.50948100	−1.81107800
H	4.31123100	−2.67421900	−4.12869600
H	3.25285500	−0.48410800	−4.60882000
H	2.36039500	0.90807800	−2.74029100
H	2.79682100	2.21837800	−0.23300800
H	4.25370600	1.32527600	0.25260000
H	2.29827200	2.68479400	2.00734800
H	3.80541500	1.86122700	2.50054700
H	−5.45822000	0.31135000	0.54714600
H	−6.38042500	−1.11529100	−0.00550600
H	−5.44377400	−0.14038100	−1.17302700
H	−3.40224700	−2.96185300	2.05369700
H	−5.17307400	−2.78966400	1.90158400
H	−4.19155600	−1.44947400	2.55731200
H	−4.15903700	−2.67681700	−2.02758200
H	−5.17763400	−3.49672300	−0.81144800
H	−3.40859500	−3.74459200	−0.82044300

TS27 (L = PPh_3)

Au	0.65004700	0.18001900	0.30067200
S	−2.00449500	3.98955700	0.35401000
P	2.89818100	−0.38402400	−0.00373100
O	−2.26748500	3.85743900	−1.10085700
O	−3.17376600	3.79337300	1.23734700
O	−0.81275800	3.07995500	0.78170100
N	−4.30915700	−2.56349900	−0.43505700
N	−3.43804200	0.37542600	−2.48254300
C	−1.33498300	5.62755700	0.64851700
C	−1.43565200	0.51560700	0.67672500
C	−2.36312900	0.26721100	−0.28155400
C	−2.14089400	0.62163500	−1.73725100
C	−3.84118600	−1.06029700	−2.39510000
C	−3.99725900	−1.76465200	−3.70452500
C	−3.98796100	−1.39786300	−1.09606400
C	−4.53975400	−3.85747000	−1.05593300
C	−4.42114900	−2.31186000	0.94524500
C	−4.80328400	−3.19121300	1.95786900
C	−4.84857900	−2.69814400	3.26924800
C	−4.53693200	−1.36762100	3.56044200
C	−4.16420700	−0.49079900	2.52967900
C	−4.10043500	−0.97067400	1.22781400
C	−3.77962800	−0.27641200	−0.07075100
C	−4.75753700	0.88886100	−0.44719300
C	−4.51492900	1.29641800	−1.91256500
C	3.42358300	−0.26462900	−1.75842700
C	4.30993700	−1.18394300	−2.33956600
C	4.68778100	−1.04329500	−3.67750700
C	4.18913300	0.01357300	−4.44209600
C	3.30638700	0.93350300	−3.86815900
C	2.91992400	0.79368000	−2.53484900
C	3.25503700	−2.09980300	0.54040200
C	4.49947300	−2.46881800	1.07512900
C	4.73236200	−3.79176600	1.45801900
C	3.73014400	−4.75379000	1.30960800
C	2.48823700	−4.39179900	0.78033600
C	2.24855500	−3.07044100	0.40073900
C	4.01790500	0.70992700	0.95376100
C	5.26879800	1.11638500	0.46475800
C	6.08834700	1.94081000	1.24009400
C	5.66842200	2.36247100	2.50385600
C	4.42314500	1.96031200	2.99562300
C	3.59794200	1.14230200	2.22340000
H	−1.02154100	1.82463200	0.63805300
H	−3.29296600	0.62306000	−3.46629600
H	−1.09729000	5.72931200	1.70947700
H	−2.09770700	6.35612200	0.36165700
H	−0.43822000	5.75986100	0.03956300
H	−1.73215800	0.24223700	1.69052100
H	−1.88071300	1.67831800	−1.85420600
H	−1.37978900	−0.00335100	−2.20759500
H	−4.66167000	−1.20104700	−4.37424200
H	−3.03612000	−1.88795300	−4.22349400
H	−4.43421900	−2.75539100	−3.56968600
H	−4.39750900	−4.64282100	−0.31141300
H	−3.81332900	−4.02004900	−1.85570200
H	−5.55405300	−3.93832200	−1.46574200
H	−5.07169200	−4.22153300	1.74951100
H	−5.14441400	−3.36897100	4.07141200
H	−4.59035300	−1.00754700	4.58350700
H	−3.93878500	0.54954500	2.74689000
H	−4.58735900	1.73703800	0.22088400
H	−5.78286900	0.53712400	−0.31078000
H	−4.13189300	2.31378200	−2.00534300
H	−5.39428400	1.16918500	−2.54338000
H	4.70615800	−2.00900500	−1.75631400
H	5.37241200	−1.76200400	−4.11930300
H	4.48355600	0.11853400	−5.48270100
H	2.91283000	1.75571700	−4.45946400
H	2.22579600	1.50642200	−2.09621300
H	5.28586600	−1.73003300	1.19472000
H	5.69778800	−4.06847000	1.87247800
H	3.91405900	−5.78134400	1.61105700
H	1.70338500	−5.13504700	0.67032500
H	1.27783200	−2.78845900	0.00051900
H	5.60546500	0.79545900	−0.51616100
H	7.05443200	2.25350700	0.85354800
H	6.30719000	3.00635300	3.10211400
H	4.08948500	2.28995800	3.97564000
H	2.62494700	0.84173400	2.60418900

TS27 (L = JohnPhos)

Au	−0.79665900	0.35957400	−0.16270400
S	2.06638900	3.74825300	−1.45328800
P	−3.08480100	0.40628600	0.45277600

O	2.30315400	4.05475300	−0.02020100
O	3.24266800	3.26411300	−2.20760400
O	0.85012500	2.78846300	−1.61842100
N	4.15693200	−2.27530400	1.30857000
N	3.36461800	1.15659700	2.39772600
C	1.46059600	5.23901300	−2.24658000
C	1.30837100	0.38091900	−0.63636300
C	2.25246900	0.41903600	0.33660100
C	2.06182600	1.19835800	1.62154900
C	3.73836500	−0.24970700	2.73666800
C	3.89325500	−0.53921700	4.19499900
C	3.86154000	−0.95986200	1.59536200
C	4.38765200	−3.32352600	2.28901300
C	4.26018000	−2.44595400	−0.08485200
C	4.61817800	−3.59174300	−0.79489200
C	4.66680600	−3.50559300	−2.19373000
C	4.37884500	−2.31279600	−2.86290700
C	4.02571400	−1.16580300	−2.13457900
C	3.95844100	−1.24230700	−0.74978600
C	3.65843500	−0.19012400	0.28618900
C	4.66043000	1.01467500	0.29090600
C	4.45021300	1.84285500	1.57210200
C	−4.10189700	−1.10387200	0.07266700
C	−5.47911700	−1.06149700	0.37800600
C	−6.33593400	−2.12433700	0.10215900
C	−5.82932900	−3.27626100	−0.49681100
C	−4.47417700	−3.34078600	−0.80724900
C	−3.59058800	−2.27850800	−0.53519000
C	−2.16801400	−2.53660300	−0.93574400
C	−1.24913900	−3.07000300	−0.01725800
C	0.02041600	−3.47769500	−0.43606600
C	0.39068400	−3.35928700	−1.77871100
C	−0.51513400	−2.82721100	−2.70022200
C	−1.78672300	−2.42453300	−2.28303200
C	−3.13522700	0.61302100	2.36218500
C	−2.27672900	−0.53559900	2.93414200
C	−4.52901700	0.53730500	3.01364900
C	−2.48341700	1.96118500	2.72796400
C	−3.89959900	1.86486600	−0.51416200
C	−2.88434400	3.02502300	−0.60388300
C	−5.20264400	2.41832000	0.09098600
C	−4.16984600	1.35091200	−1.94338200
H	0.96495100	1.65077400	−1.03173100
H	3.23525900	1.68731100	3.26472400
H	1.22750100	5.01535800	−3.28982200
H	2.25058300	5.99272800	−2.19119900
H	0.56880200	5.58580300	−1.72025500
H	1.57667200	−0.20563600	−1.51643600
H	1.82011700	2.24673100	1.42265600
H	1.30022100	0.75619200	2.26502600
H	4.60106000	0.16064200	4.66079100
H	2.93960700	−0.44843400	4.73442100
H	4.27452800	−1.54843500	4.35825100
H	4.29147300	−4.29573800	1.80337600
H	3.63402100	−3.26685200	3.07888200
H	5.38666800	−3.24919200	2.73582600
H	4.86859500	−4.52058500	−0.29327400
H	4.94716200	−4.38758900	−2.76347100
H	4.43612700	−2.26914800	−3.94647600
H	3.81574000	−0.23081800	−2.64661200
H	4.49107500	1.63020600	−0.59629800
H	5.67758000	0.61768300	0.25324800
H	4.08898000	2.85064800	1.36191800
H	5.33660500	1.88778600	2.20457400
H	−5.90140500	−0.18119500	0.84214000
H	−7.38947100	−2.04605400	0.35519100
H	−6.47934600	−4.11737500	−0.72149500
H	−4.07341200	−4.23738200	−1.27144800
H	−1.53908200	−3.19026800	1.02303900
H	0.71431200	−3.90184500	0.28513700
H	1.37251800	−3.68899100	−2.10618500
H	−0.24068500	−2.74077400	−3.74843100
H	−2.49720100	−2.04070900	−3.01046400
H	−1.24397100	−0.49432800	2.57020700
H	−2.69188800	−1.51848000	2.68491400
H	−2.25636200	−0.45120000	4.02850900
H	−4.41101900	0.72336000	4.08920400
H	−4.98178300	−0.45173700	2.90390700
H	−5.22476900	1.28643400	2.62718000
H	−1.50405300	2.08967000	2.25365100
H	−2.33741600	1.99642700	3.81538400
H	−3.11650100	2.81037200	2.45318100
H	−1.95632400	2.72070600	−1.09743500
H	−2.63119200	3.43848800	0.37612300
H	−3.33455400	3.83196700	−1.19662000
H	−5.55860100	3.23377800	−0.55225400
H	−5.04738000	2.83546800	1.09007300
H	−6.00344600	1.67704700	0.13830800
H	−3.26313900	0.94917900	−2.41136000
H	−4.51400800	2.19223800	−2.55841200
H	−4.94493900	0.57940400	−1.96833600

TS28

Au	−2.05954200	−0.71230500	−0.12768000
S	0.47548700	4.56825900	0.30012100
P	−4.32019800	−1.28531600	0.23363400
O	1.35367000	4.22031800	−0.89044000
O	−0.90476800	4.02401000	0.14681000
O	1.12581100	4.22322500	1.59251500
N	3.08891300	−1.00842900	1.32376900
N	1.65793500	1.55157000	−1.04288000
C	0.33621500	6.36036800	0.23265300
C	0.94865200	−1.01911800	−0.03153000
C	−0.07714200	−0.21452900	−0.44184300
C	0.19872400	1.11824600	−1.05012900
C	2.33408400	1.19980400	0.27280800
C	3.70135400	1.87081200	0.40733300
C	2.40017600	−0.31613700	0.31111400
C	2.94943300	−0.72547200	2.74881100
C	3.49536700	−2.23515700	0.81955900
C	4.12064900	−3.29733500	1.48654300
C	4.46749500	−4.41018400	0.72577800
C	4.18934000	−4.48860100	−0.65490900
C	3.53634100	−3.44820000	−1.30660700
C	3.18142500	−2.31695500	−0.56080400
C	2.49468900	−1.08692800	−0.92006800
C	2.40882900	−0.47921200	−2.30351700
C	2.40882400	1.05497100	−2.24494700
C	−4.77435300	−1.42684200	2.00763300
C	−4.80075800	−2.90059500	−0.49496700
C	−5.52079200	−0.08262700	−0.46140900
H	1.61907300	2.61905000	−1.06663100
H	−0.29235700	6.69347000	1.06250100
H	−0.11785700	6.64771500	−0.71859500

H	1.33301500	6.79912000	0.32126200
H	0.79306800	−1.96469300	0.47386500
H	−0.14161800	1.15570300	−2.09126100
H	−0.35194700	1.90037000	−0.51279700
H	1.66840600	1.58758500	1.04830900
H	4.46201400	1.41875400	−0.23489000
H	4.03649000	1.78053700	1.44439900
H	3.61453900	2.93563300	0.17374000
H	2.14901200	−1.32823600	3.19497800
H	2.72058900	0.33149000	2.88931000
H	3.89203500	−0.94752500	3.25518700
H	4.33884500	−3.25219600	2.54810100
H	4.96831200	−5.24312100	1.21125600
H	4.48112400	−5.37562800	−1.20874500
H	3.30265800	−3.50804100	−2.36539100
H	1.52506400	−0.84821800	−2.83059800
H	3.28060600	−0.80628700	−2.87867500
H	1.92367700	1.48699800	−3.12179900
H	3.42070200	1.45393900	−2.17982500
H	−4.14632900	−2.18292300	2.48968600
H	−5.82703300	−1.71278000	2.11021000
H	−4.61185300	−0.46664100	2.50787300
H	−4.63882800	−2.88066100	−1.57749000
H	−5.85609300	−3.11356900	−0.29132200
H	−4.18330400	−3.69586200	−0.06511300
H	−5.35546100	0.90293900	−0.01425200
H	−6.54776800	−0.40424500	−0.25564600
H	−5.37670400	−0.00325100	−1.54367100

TS28 (L = PPh_3)

Au	−0.74738700	−0.13766100	−0.21406300
S	2.99963100	4.39906500	0.28830100
P	−3.10185200	−0.17455900	0.05043800
O	3.75286300	3.84779000	−0.91132300
O	1.52959200	4.17638700	0.16759000
O	3.58235600	3.93325100	1.57471400
N	4.17055400	−1.64273900	1.31388100
N	3.40677600	1.18732900	−1.05696500
C	3.26676000	6.17538600	0.19172500
C	2.10145400	−1.14304900	−0.06147100
C	1.29936400	−0.11760100	−0.47880800
C	1.88757200	1.11437600	−1.07679600
C	3.96933600	0.68562100	0.26329100
C	5.45388300	1.02120600	0.40942700
C	3.67718500	−0.80365300	0.29844000
C	4.08480200	−1.33770800	2.73873400
C	4.26852800	−2.93252600	0.80888300
C	4.60616300	−4.11737800	1.47710200
C	4.67519500	−5.28044400	0.71548600
C	4.39961200	−5.28620600	−0.66766600
C	4.02874100	−4.11602100	−1.32104300
C	3.95588100	−2.93369300	−0.57369400
C	3.58890300	−1.57332500	−0.93404000
C	3.66337600	−0.96358600	−2.31672800
C	4.02799900	0.52625800	−2.25418400
C	−3.63355600	−1.18293400	1.48924700
C	−4.79442700	−1.97091400	1.46658400
C	−5.15686200	−2.71643000	2.59141500
C	−4.36776500	−2.68058000	3.74348100
C	−3.21090600	−1.89622900	3.77235900
C	−2.84120000	−1.15424500	2.64992900
C	−3.93547600	−0.88926000	−1.42127500
C	−5.13692900	−0.37513000	−1.93113200
C	−5.72848500	−0.96035500	−3.05387000
C	−5.13031100	−2.06123600	−3.67091900
C	−3.93336600	−2.57867800	−3.16654200
C	−3.33421400	−1.99299700	−2.05110200
C	−3.80716300	1.49959700	0.29881700
C	−4.95425500	1.71884900	1.07779200
C	−5.46095600	3.01163400	1.22899500
C	−4.83031900	4.09150600	0.60567900
C	−3.68763500	3.87933400	−0.17061000
C	−3.17438300	2.59027900	−0.32139600
H	3.62450700	2.23369800	−1.08030600
H	2.74644500	6.65358400	1.02552900
H	2.87093400	6.54524800	−0.75711600
H	4.33878500	6.37789800	0.25494100
H	1.71959300	−2.02356100	0.44088700
H	1.57287900	1.23698800	−2.11930700
H	1.53438100	2.00174800	−0.53634500
H	3.40683300	1.21592800	1.03605800
H	6.09169200	0.41429700	−0.23836800
H	5.75600200	0.84232100	1.44508900
H	5.61484000	2.08036600	0.19054100
H	3.12366100	−1.66183300	3.15666300
H	4.19924300	−0.26399900	2.89212100
H	4.89557000	−1.84887700	3.26266100
H	4.81776500	−4.13068100	2.54079400
H	4.94968600	−6.21171600	1.20307200
H	4.46999400	−6.21700100	−1.22204400
H	3.79714300	−4.11508200	−2.38202200
H	2.72172100	−1.11354700	−2.85153400
H	4.43814400	−1.48821800	−2.88441600
H	3.66692200	1.06237500	−3.13353800
H	5.10524600	0.67312500	−2.17972200
H	−5.41528700	−2.00758200	0.57683300
H	−6.05617000	−3.32546600	2.56411600
H	−4.65058600	−3.26454200	4.61500300
H	−2.59203000	−1.86747600	4.66488000
H	−1.93515700	−0.55371100	2.67417300
H	−5.61230700	0.47882100	−1.45901100
H	−6.65733600	−0.55359000	−3.44404900
H	−5.59215500	−2.51252600	−4.54476800
H	−3.46186200	−3.43237300	−3.64551700
H	−2.39733200	−2.39114100	−1.66919700
H	−5.45119500	0.88744700	1.56820200
H	−6.34796000	3.17326400	1.83529600
H	−5.22485400	5.09639300	0.72856400
H	−3.19025300	4.71679200	−0.65187800
H	−2.27934300	2.43041300	−0.91763300

TS28 (L = JohnPhos)

Au	−0.88604600	−0.34627800	−0.45798000
S	3.07215900	4.32661000	−0.49065400
P	−3.26847300	−0.56892200	−0.60594600
O	3.83593800	3.49950300	−1.51156700
O	1.60008700	4.27053300	−0.72469500
O	3.48157900	4.00730300	0.90331000
N	3.94994800	−1.60513600	1.54182900
N	3.33004700	0.88120100	−1.22187000
C	3.58817900	6.01695700	−0.82689900
C	1.94975200	−1.28369900	0.01682100
C	1.17595700	−0.31661700	−0.56728400
C	1.81121000	0.82479000	−1.28949500

C	3.83167500	0.55709700	0.17546700
C	5.31736200	0.88168100	0.33606700
C	3.50816400	−0.90811900	0.40270400
C	3.81752200	−1.10949000	2.90803300
C	4.05434000	−2.95173600	1.22114300
C	4.35867600	−4.03486100	2.05648900
C	4.44791500	−5.29152600	1.46349100
C	4.22493200	−5.48478000	0.08482800
C	3.88734100	−4.41279500	−0.73511900
C	3.79587900	−3.13992000	−0.15951100
C	3.45786100	−1.83792500	−0.71767500
C	3.60385200	−1.42521900	−2.16678000
C	3.98313100	0.05622800	−2.29347700
C	−4.30802300	0.23260200	0.71330500
C	−5.70352900	0.02967800	0.65938200
C	−6.56629500	0.52149700	1.63619600
C	−6.04636600	1.23671900	2.71340900
C	−4.67360600	1.45350200	2.78595400
C	−3.78427300	0.97389100	1.80455700
C	−2.34748100	1.33056500	2.03750800
C	−1.72783000	2.36013600	1.30987600
C	−0.44084900	2.79496200	1.64022500
C	0.24648100	2.20373400	2.70486200
C	−0.35847800	1.17706900	3.43515700
C	−1.64785100	0.74800300	3.10779200
C	−3.77550500	0.24444400	−2.26961000
C	−3.21403700	1.68163000	−2.22686100
C	−5.28787300	0.32707700	−2.54541200
C	−3.09258800	−0.52434300	−3.41839100
C	−3.65073100	−2.45801600	−0.50629700
C	−2.52136400	−3.22544800	−1.22974800
C	−4.99363000	−2.90755400	−1.11090100
C	−3.60409700	−2.83570100	0.98963000
H	3.57843800	1.90902000	−1.38658500
H	3.07658700	6.68385800	−0.12833300
H	3.32102000	6.27470900	−1.85461000
H	4.66955100	6.09168500	−0.68947700
H	1.53312200	−2.08676000	0.61279900
H	1.53781800	0.82131100	−2.35048700
H	1.45285800	1.77468700	−0.87631800
H	3.24999800	1.19990400	0.84100200
H	5.96414100	0.17774600	−0.19428800
H	5.57334900	0.84217900	1.39862600
H	5.51343400	1.89636600	−0.02109100
H	2.86276100	−1.41915800	3.35045900
H	3.87513500	−0.02043200	2.90910000
H	4.63838300	−1.50128700	3.51374400
H	4.53056600	−3.90236500	3.11927000
H	4.69838000	−6.14813300	2.08302200
H	4.30865800	−6.48224200	−0.33539100
H	3.69670300	−4.55592500	−1.79464400
H	2.68487300	−1.64059500	−2.71833800
H	4.39631600	−2.02819600	−2.62076600
H	3.65995100	0.46979300	−3.25021400
H	5.05883700	0.20514100	−2.20067000
H	−6.13660000	−0.52845100	−0.15933200
H	−7.63405400	0.33986900	1.55249600
H	−6.70024200	1.62634100	3.48874500
H	−4.26466500	2.02077200	3.61715100
H	−2.26701000	2.83977900	0.49809200
H	0.02848000	3.58594900	1.06140700
H	1.24347300	2.54954100	2.96525800
H	0.16330400	0.71953400	4.27196700
H	−2.12359300	−0.03289800	3.69559600
H	−2.12450100	1.69001400	−2.11204700
H	−3.65373100	2.26986500	−1.41394600
H	−3.46035500	2.18459500	−3.17105200
H	−5.42924500	0.76156900	−3.54380900
H	−5.79990800	0.97987300	−1.83340800
H	−5.77881100	−0.64954200	−2.54161100
H	−2.01477000	−0.63723400	−3.25385300
H	−3.23223300	0.04022700	−4.34931600
H	−3.52905200	−1.51667800	−3.56625400
H	−1.53993400	−3.01541000	−0.79122000
H	−2.47450300	−2.99776400	−2.29799900
H	−2.71440400	−4.30142900	−1.12885400
H	−5.08240600	−3.99403400	−0.97870500
H	−5.05173800	−2.70360300	−2.18395900
H	−5.85863000	−2.45540400	−0.62021900
H	−2.67324300	−2.50579500	1.46723000
H	−3.65325200	−3.92856900	1.07809000
H	−4.44480400	−2.41662500	1.55005500

TS29

Au	−2.49591300	−0.69637700	−0.08440000
S	1.10808800	4.68766300	0.46595100
P	−4.84157100	−0.94230400	0.06291600
O	1.49260100	4.00884300	−0.96384600
O	−0.27270400	4.32987700	0.81307100
O	2.16558000	4.38142500	1.43742100
N	2.66074300	−2.00710200	1.19936500
N	1.51337000	1.08883900	−0.81084100
C	1.19733400	6.39592700	−0.04216900
C	0.42357300	−1.40440700	0.25413400
C	−0.43335100	−0.46719100	−0.20328300
C	0.03204800	0.86252200	−0.76077000
C	2.18125000	0.69819000	0.32165200
C	3.61910400	1.03990700	0.56941700
C	1.91689900	−1.37518100	0.18821200
C	2.21964200	−2.21768500	2.57149800
C	3.87903800	−2.38244800	0.69857600
C	4.96075800	−3.00710000	1.34536100
C	6.09253100	−3.26467100	0.58688000
C	6.17558500	−2.91080000	−0.78511800
C	5.11822600	−2.29005100	−1.42343200
C	3.94367900	−2.01928100	−0.68262100
C	2.70358600	−1.41980400	−1.00960600
C	2.25851300	−0.78275200	−2.26881500
C	2.15978200	0.77713200	−2.08621500
C	−5.52805800	−2.31523800	−0.94807800
C	−5.78805600	0.53694600	−0.48056700
C	−5.45792400	−1.27908800	1.76185000
H	1.56209000	3.02267500	−0.84413800
H	0.94362300	7.00092900	0.83201600
H	0.47657200	6.56592900	−0.84437600
H	2.21447100	6.61348100	−0.37379600
H	0.03729300	−2.31979800	0.69986500
H	−0.34516200	1.01377200	−1.77536300
H	−0.39150700	1.66660400	−0.14783600
H	1.56269100	0.75639300	1.21433100
H	4.26418500	0.97491300	−0.30643000
H	4.02305300	0.40020700	1.35892200
H	3.64013200	2.07099200	0.95021600
H	1.98142300	−3.27235100	2.74961000

H	1.32924100	−1.61571500	2.75676500
H	3.00444700	−1.90676600	3.26732800
H	4.90963700	−3.28557500	2.39285400
H	6.94148600	−3.75519200	1.05512500
H	7.08506300	−3.13500400	−1.33470800
H	5.17870500	−2.02152000	−2.47425600
H	1.26427200	−1.14803000	−2.55129000
H	2.94896500	−0.98803100	−3.09139100
H	1.57461300	1.21511100	−2.89615600
H	3.15761500	1.21607000	−2.10674400
H	−5.28761900	−2.15124600	−2.00354700
H	−6.61602800	−2.37361500	−0.83212000
H	−5.08126100	−3.26395400	−0.63347400
H	−5.52058300	1.39577700	0.14374500
H	−6.86596300	0.35622700	−0.40215400
H	−5.53849700	0.77231400	−1.52035700
H	−5.00109400	−2.19821200	2.14311700
H	−6.54794200	−1.39062200	1.76411700
H	−5.18022300	−0.45288000	2.42451900

TS29 (L = PPh_3)

Au	1.01964900	−0.27689900	0.11928100
S	−3.14361100	4.61824400	−0.48405500
P	3.38907100	−0.30247400	0.00337100
O	−3.47156100	3.93304200	0.95676800
O	−1.76682600	4.28391000	−0.87107000
O	−4.22187800	4.29495000	−1.42599100
N	−3.93566400	−2.18057200	−1.19476200
N	−3.17498800	1.02257900	0.83565200
C	−3.25028500	6.32413900	0.02879000
C	−1.78696900	−1.30776400	−0.25446600
C	−1.05363400	−0.27740100	0.21661000
C	−1.67723300	0.98116100	0.78397700
C	−3.79144600	0.56159000	−0.29884500
C	−5.26226500	0.71795700	−0.53652000
C	−3.27154500	−1.46591700	−0.18333800
C	−3.47748500	−2.32894100	−2.56936100
C	−5.09195900	−2.71279900	−0.68931900
C	−6.08715200	−3.47017600	−1.33302800
C	−7.16992300	−3.87743300	−0.56860400
C	−7.28841400	−3.54539100	0.80632400
C	−6.31641500	−2.79558600	1.44169500
C	−5.19267000	−2.37024100	0.69483800
C	−4.03702300	−1.61962100	1.01935800
C	−3.67324000	−0.93693900	2.28098200
C	−3.77751400	0.62346500	2.10799700
C	4.04164000	−1.94733000	−0.49291100
C	5.23068500	−2.48049100	0.02725800
C	5.68433700	−3.73139900	−0.39953500
C	4.95918700	−4.45726200	−1.34727800
C	3.77253700	−3.93298400	−1.86803700
C	3.31186700	−2.68747400	−1.43960000
C	4.18711600	0.11108900	1.60529200
C	5.43930200	0.74161000	1.68160900
C	6.00983300	1.01940800	2.92587300
C	5.33728900	0.67401600	4.10097700
C	4.08943400	0.04857800	4.03231200
C	3.51356900	−0.22782000	2.79105300
C	4.05931000	0.89754500	−1.21686300
C	5.18252300	0.61929600	−2.01045800
C	5.65764500	1.57435500	−2.91311400
C	5.01922400	2.81127400	−3.02915100
C	3.89848800	3.09399700	−2.24281800
C	3.41640600	2.14104400	−1.34452000
H	−3.44427000	2.94279100	0.85798800
H	−3.04561300	6.93490000	−0.85411300
H	−2.50225000	6.50985100	0.80193100
H	−4.25803500	6.51892800	0.40086500
H	−1.28995000	−2.16275300	−0.71025900
H	−1.32031500	1.17086400	1.79940900
H	−1.35642900	1.83481000	0.17587600
H	−3.18760200	0.70439700	−1.19221200
H	−5.88733400	0.55053700	0.34017000
H	−5.58222900	0.04650500	−1.33785700
H	−5.42126500	1.74533700	−0.89413900
H	−3.07291200	−3.33250800	−2.74287900
H	−2.69900200	−1.59164800	−2.76945400
H	−4.30910600	−2.15563500	−3.25826400
H	−6.00744700	−3.73477100	−2.38237100
H	−7.95095100	−4.47225600	−1.03425900
H	−8.15665000	−3.88990800	1.36024000
H	−6.40258000	−2.54325800	2.49476100
H	−2.63914500	−1.17165900	2.55892700
H	−4.32900300	−1.23481400	3.10372500
H	−3.25588700	1.12853200	2.92230700
H	−4.82391400	0.92937700	2.12747700
H	5.80379900	−1.92614000	0.76377800
H	6.60533100	−4.13661800	0.01057200
H	5.31437800	−5.43009600	−1.67605700
H	3.20181800	−4.49548900	−2.60186900
H	2.38290300	−2.28818900	−1.83946300
H	5.97072400	1.01674600	0.77567500
H	6.97885800	1.50840100	2.97510500
H	5.78300400	0.89506800	5.06701100
H	3.55973400	−0.21654500	4.94320400
H	2.53808300	−0.70518700	2.74014000
H	5.68783500	−0.33792600	−1.92772900
H	6.52759700	1.34908200	−3.52396100
H	5.39048200	3.55098500	−3.73319900
H	3.39424400	4.05217400	−2.33388100
H	2.53790300	2.36170000	−0.74306200

TS29 (L = JohnPhos)

Au	−1.11812000	−0.45863000	−0.44676800
S	2.95466800	4.60655600	−0.28178500
P	−3.49564600	−0.63277700	−0.69392400
O	3.43504300	3.70407200	−1.54910800
O	1.51990700	4.38888700	−0.05293700
O	3.87294900	4.38569800	0.84169900
N	3.78275900	−2.06467200	1.40515500
N	3.10169300	0.83294200	−1.06269100
C	3.22463400	6.21287700	−1.01056200
C	1.68224600	−1.36912900	0.23459100
C	0.96168100	−0.42340000	−0.40467000
C	1.60302600	0.76269900	−1.09474900
C	3.65557800	0.53418100	0.15483300
C	5.10811900	0.74798500	0.45458700
C	3.17050400	−1.50353800	0.27138600
C	3.23637400	−2.05699600	2.75519600
C	4.97759500	−2.62806800	1.04282600
C	5.94282300	−3.27343600	1.83665600
C	7.07725500	−3.75005200	1.19739500
C	7.27551500	−3.59387900	−0.19910800
C	6.33305500	−2.95428600	−0.98264700

C	5.15885900	−2.46276400	−0.36541300
C	4.01242000	−1.78992500	−0.85256100
C	3.71492000	−1.28461100	−2.21099800
C	3.78609200	0.28740100	−2.23553900
C	−4.56401600	−0.07257800	0.72566800
C	−5.95452000	−0.29251600	0.62905400
C	−6.83126400	0.00024600	1.67105200
C	−6.32988900	0.52289300	2.86169900
C	−4.96333800	0.75958200	2.97731100
C	−4.06143900	0.48653500	1.92984000
C	−2.63807300	0.85657700	2.22315900
C	−2.07233400	2.02962600	1.69614200
C	−0.80732200	2.45901700	2.10720900
C	−0.08744600	1.72139500	3.05177000
C	−0.63969000	0.55215000	3.58232100
C	−1.90754900	0.12720300	3.17600400
C	−4.00036300	0.44658200	−2.20038700
C	−3.44629300	1.85984200	−1.91679000
C	−5.51224800	0.57112000	−2.46283000
C	−3.30933800	−0.11713600	−3.45743500
C	−3.88427900	−2.51142300	−0.92996400
C	−2.74206500	−3.14519000	−1.75675700
C	−5.21352200	−2.85122100	−1.62820600
C	−3.86392200	−3.14701400	0.47627000
H	3.37059300	2.74001000	−1.30831100
H	2.92539500	6.95390900	−0.26499900
H	2.60644300	6.30312800	−1.90599000
H	4.28417400	6.32070600	−1.24997100
H	1.17182600	−2.17175000	0.76512000
H	1.30845600	0.80809400	−2.14633400
H	1.23284300	1.68213700	−0.62735800
H	2.99818300	0.77592200	0.98669100
H	5.78740300	0.48210300	−0.35497800
H	5.38871000	0.19038200	1.35249400
H	5.23419900	1.81504600	0.68717000
H	2.85009000	−3.04549500	3.02868700
H	2.42437400	−1.33090900	2.80802000
H	4.01298500	−1.76806400	3.46910500
H	5.80275100	−3.40349500	2.90478500
H	7.83656200	−4.26249100	1.78177400
H	8.18109100	−3.98704300	−0.65161000
H	6.48067400	−2.83811200	−2.05265400
H	2.70282200	−1.57653500	−2.51498700
H	4.42340800	−1.67098100	−2.94879400
H	3.30833800	0.67310600	−3.13720700
H	4.82744500	0.61016200	−2.23136800
H	−6.37040800	−0.70856800	−0.27801800
H	−7.89443700	−0.18733400	1.54980100
H	−6.99329300	0.75113800	3.69134900
H	−4.57081700	1.18216000	3.89773200
H	−2.63683800	2.62128000	0.98152500
H	−0.38522600	3.37049300	1.69232300
H	0.89077500	2.06262800	3.38050500
H	−0.09390200	−0.02074300	4.32774700
H	−2.34291200	−0.76875800	3.61118300
H	−2.35670100	1.85791100	−1.80267500
H	−3.88781900	2.29894800	−1.01541600
H	−3.69762100	2.51423300	−2.76188700
H	−5.65394100	1.16792200	−3.37357700
H	−6.02688700	1.09187300	−1.65057400
H	−5.99953900	−0.39385600	−2.62286000
H	−2.23322400	−0.25801300	−3.30486700
H	−3.44155600	0.59475100	−4.28268800
H	−3.74385200	−1.07046800	−3.77257500
H	−1.76624500	−3.00793900	−1.27926400
H	−2.68420500	−2.74436700	−2.77261100
H	−2.93074100	−4.22378600	−1.83752200
H	−5.29347300	−3.94404700	−1.70051600
H	−5.25706800	−2.45376600	−2.64621900
H	−6.09137100	−2.50468000	−1.07829400
H	−2.93856800	−2.91606500	1.01822000
H	−3.92165100	−4.23785200	0.36976300
H	−4.71087000	−2.82602800	1.08961100

TS29'

Au	2.27298600	0.01926600	0.00795900
P	4.56611000	−0.49853000	0.25859100
N	−3.00378000	−1.26767800	−0.66453900
N	−1.49943200	2.22731700	−0.78126500
C	−0.71131300	−0.43870600	−0.09016800
C	0.26131700	0.48554900	−0.22137900
C	−0.05911700	1.91920400	−0.61580100
C	−2.20167000	1.27549200	−1.47838500
C	−3.59636700	1.55445000	−1.97961800
C	−2.19671900	−0.19937300	−0.19831200
C	−2.60449100	−2.24673700	−1.66529600
C	−4.22125200	−1.21928800	−0.05230500
C	−5.35192900	−2.03842600	−0.23758900
C	−6.47698000	−1.75003300	0.51727100
C	−6.51176400	−0.66936400	1.43976900
C	−5.40950900	0.14156900	1.62295500
C	−4.23625400	−0.12824700	0.87612100
C	−2.96507300	0.48014800	0.81852500
C	−2.46326000	1.71062100	1.45942100
C	−2.17300900	2.81511600	0.35788700
C	5.21036100	−1.71041700	−0.96408800
C	5.01420300	−1.22354200	1.88704100
C	5.68243200	0.95208800	0.08714200
H	−0.46499000	−1.47041700	0.15559200
H	0.34605300	2.62205500	0.11729300
H	0.43783100	2.14290800	−1.56817900
H	−1.58377500	0.78213800	−2.22691700
H	−4.28257100	1.93976400	−1.22498400
H	−4.02518200	0.64553900	−2.40934500
H	−3.51948800	2.29424600	−2.78723700
H	−3.36836900	−2.32347600	−2.44533400
H	−2.45742600	−3.23359200	−1.21202700
H	−1.66732200	−1.92557100	−2.12195300
H	−5.34034800	−2.86734600	−0.93767100
H	−7.36197300	−2.37023300	0.40375600
H	−7.42096000	−0.48703800	2.00498300
H	−5.43091300	0.96543200	2.33057300
H	−1.51363200	1.51665600	1.97195200
H	−3.17464600	2.11444700	2.18512000
H	−1.54573600	3.59814700	0.78662300
H	−3.11586000	3.26419700	0.04283700
H	4.65354600	−2.64937000	−0.88133300
H	6.27424900	−1.90571600	−0.78871600
H	5.07952400	−1.31663000	−1.97731200
H	4.74732600	−0.52675300	2.68825200
H	6.08900900	−1.43120200	1.93415000
H	4.46027500	−2.15572600	2.03868100
H	5.53887600	1.41578900	−0.89431600
H	6.72999200	0.64778800	0.19116300

H	5.44379200	1.69182000	0.85819900

TS30

Au	−2.16006600	−0.55934700	−0.05054400
S	−0.16916000	3.63613300	0.48256500
P	−4.24936600	−1.53341900	0.30980300
O	−1.23450300	2.51973200	0.21173500
O	0.57032100	3.95947100	−0.76015200
O	0.65437500	3.30792700	1.66352400
N	2.96240400	−0.33129200	1.57158600
N	1.53963700	0.42500000	−2.38768500
C	−1.21880100	5.03283200	0.88389500
C	0.73654900	−0.11473000	0.52163100
C	−0.16789600	0.18570000	−0.46811000
C	0.11031500	0.26130400	−1.96597800
C	2.08749000	1.59237700	−2.32003000
C	3.47371700	1.97472500	−2.66715300
C	2.11223800	−0.56620100	0.48548500
C	2.64371400	0.46739300	2.74834600
C	4.15595600	−0.97411300	1.34557400
C	5.31649900	−1.03744200	2.13581300
C	6.38392400	−1.78279000	1.65273200
C	6.31509400	−2.45726200	0.40980900
C	5.17272000	−2.39429900	−0.37289400
C	4.07038200	−1.64210100	0.08707900
C	2.77159400	−1.37512000	−0.44155200
C	2.19848000	−1.87822600	−1.73172900
C	2.21144400	−0.81190200	−2.84254500
C	−4.26159200	−3.34639700	0.02383200
C	−5.57736400	−0.87624900	−0.77365900
C	−4.88367100	−1.32053100	2.01931600
H	−0.78558500	1.40689100	−0.04074900
H	−1.81327000	4.78938900	1.76713200
H	−1.86655300	5.24905600	0.03176500
H	−0.56853700	5.88708100	1.09038300
H	0.35942200	0.02536900	1.53421100
H	−0.26358900	−0.62255900	−2.48738400
H	−0.42447200	1.12114100	−2.37774600
H	1.44420300	2.39343400	−1.94981600
H	4.11745000	1.16532100	−3.00759000
H	3.91831900	2.45356100	−1.78457400
H	3.42316700	2.75401200	−3.43982900
H	2.08570200	−0.11836000	3.48891400
H	2.05710800	1.34346800	2.46156300
H	3.57268600	0.81349600	3.20484100
H	5.37884700	−0.53362100	3.09531200
H	7.29215700	−1.85404900	2.24513100
H	7.17229200	−3.03195900	0.06981600
H	5.12543500	−2.91360200	−1.32663400
H	1.17516300	−2.24224700	−1.58319300
H	2.78093900	−2.72751700	−2.10372900
H	1.66771900	−1.16201600	−3.72517000
H	3.23216300	−0.57524500	−3.13268800
H	−3.95390600	−3.55832200	−1.00515400
H	−5.26497800	−3.75345700	0.19130800
H	−3.55615300	−3.83054000	0.70662800
H	−5.69147300	0.19914700	−0.60394200
H	−6.52746400	−1.37842000	−0.55945800
H	−5.31233800	−1.03917100	−1.82326600
H	−4.17509300	−1.75540800	2.73143900
H	−5.85572100	−1.81406400	2.12911400
H	−4.99194000	−0.25400100	2.24092800

TS30 (L = PPh_3)

Au	−0.82082200	0.10351700	−0.19142500
S	1.88140900	3.85444500	0.51969700
P	−3.07366600	−0.47311200	0.07716900
O	0.65028300	2.97331900	0.11702100
O	2.76345700	4.08097500	−0.64948000
O	2.53471100	3.32786000	1.73505100
N	4.19986700	−0.64586000	1.56878600
N	3.06052900	0.45922500	−2.39615400
C	1.08151800	5.40647900	0.92302800
C	2.08006100	−0.00356000	0.47015200
C	1.27810600	0.48131800	−0.53622200
C	1.61179500	0.54590100	−2.02322700
C	3.80953900	1.50340700	−2.26833300
C	5.25702400	1.62817900	−2.54757200
C	3.35104500	−0.69680500	0.45725000
C	3.99795600	0.16847200	2.76102100
C	5.26603900	−1.48478200	1.34910200
C	6.37678000	−1.77472200	2.16015600
C	7.31258700	−2.67666300	1.67107800
C	7.16119500	−3.29032900	0.40394200
C	6.06626600	−3.00748500	−0.39754200
C	5.09832800	−2.09193000	0.06825700
C	3.88261200	−1.58480900	−0.47994400
C	3.26792000	−1.94052400	−1.79877000
C	3.51202100	−0.86541000	−2.87308900
C	−4.19036600	0.98326900	0.04433300
C	−5.36640800	1.03865200	0.80828200
C	−6.19177700	2.16378100	0.74258000
C	−5.85165500	3.23790400	−0.08328200
C	−4.68188200	3.18821700	−0.84689100
C	−3.85101400	2.06899600	−0.78099700
C	−3.38735500	−1.33917200	1.66379000
C	−4.35983400	−2.34386100	1.78629000
C	−4.57430000	−2.96385100	3.01966800
C	−3.82325500	−2.58762400	4.13594800
C	−2.85290200	−1.58821200	4.01943500
C	−2.63144800	−0.96830800	2.78893700
C	−3.64376100	−1.60160100	−1.25390300
C	−4.91748000	−1.49560500	−1.83218300
C	−5.30583700	−2.38399300	−2.83855800
C	−4.43078300	−3.38270500	−3.27129600
C	−3.16046200	−3.49380400	−2.69759800
C	−2.76496600	−2.60516700	−1.69754000
H	0.88865900	1.78750300	−0.10829000
H	0.39550300	5.24405600	1.75708000
H	0.54223700	5.76817100	0.04502300
H	1.86038000	6.11848500	1.20818400
H	1.70056200	0.17940000	1.47488300
H	1.10142700	−0.24024800	−2.58378400
H	1.25507900	1.50017100	−2.41953200
H	3.30744700	2.40046300	−1.90080300
H	5.77805800	0.69594000	−2.76071300
H	5.72203500	2.12289500	−1.68593800
H	5.37904700	2.31695100	−3.39566800
H	3.33247900	−0.32943800	3.47643000
H	3.57531300	1.13774600	2.48656000
H	4.96221700	0.34139800	3.24250800
H	6.50079500	−1.32043500	3.13798000
H	8.17984900	−2.92167700	2.27838400
H	7.91633000	−3.99186100	0.06006700
H	5.95311600	−3.48096300	−1.36950700

H	2.19084600	−2.11153400	−1.68743600
H	3.69460600	−2.87313100	−2.18212400
H	2.94295400	−1.08489100	−3.78143800
H	4.56720700	−0.80974100	−3.13006400
H	−5.63998300	0.21029200	1.45421200
H	−7.09904000	2.19919700	1.33914200
H	−6.49401600	4.11296600	−0.12888500
H	−4.41094800	4.02341500	−1.48678300
H	−2.93600800	2.03873800	−1.36731300
H	−4.94879200	−2.64525200	0.92549700
H	−5.32791300	−3.74178800	3.10516100
H	−3.99004100	−3.07510000	5.09253700
H	−2.26260300	−1.29600100	4.88350400
H	−1.86905200	−0.19815100	2.70023800
H	−5.60634500	−0.72395500	−1.50334200
H	−6.29302200	−2.29246800	−3.28301100
H	−4.73543300	−4.07000000	−4.05571300
H	−2.47496200	−4.26703700	−3.03343200
H	−1.77286600	−2.68908100	−1.26066300

TS30 (L = JohnPhos)

Au	0.97049700	0.31327200	0.18458200
S	−1.82226900	3.90177000	−0.75551100
P	3.33717000	0.28899400	−0.01674000
O	−0.58930500	3.03937400	−0.32351600
O	−2.70167300	4.17316500	0.40618200
O	−2.47867100	3.33027800	−1.94877500
N	−4.13332500	−0.59407200	−1.49304300
N	−2.93141100	0.69919500	2.38846200
C	−1.02740000	5.43958800	−1.22033100
C	−1.98524600	0.04622000	−0.45260900
C	−1.16327400	0.57881000	0.51075900
C	−1.48377200	0.72893600	1.99533800
C	−3.65887500	1.74996200	2.20454700
C	−5.09850000	1.92873100	2.49628500
C	−3.27697400	−0.60845200	−0.38600300
C	−3.91057500	0.13822800	−2.73386600
C	−5.22626300	−1.38054600	−1.21708800
C	−6.35437200	−1.67743800	−2.00110500
C	−7.31463800	−2.51927300	−1.45548000
C	−7.17122200	−3.06567800	−0.15717000
C	−6.06050000	−2.77358300	0.61912900
C	−5.06757400	−1.91784300	0.09562800
C	−3.83055900	−1.42099500	0.60530100
C	−3.21686900	−1.72234800	1.93852000
C	−3.40940500	−0.58057400	2.95205100
C	4.20654200	−1.35026800	−0.15716200
C	5.61780000	−1.34014200	−0.14036300
C	6.37411200	−2.50951300	−0.14945200
C	5.72738400	−3.74362200	−0.17017800
C	4.33694100	−3.77953800	−0.20025700
C	3.55310400	−2.60852800	−0.20405400
C	2.07842100	−2.86041400	−0.29255900
C	1.39321300	−2.70816400	−1.50934600
C	0.07366500	−3.14719800	−1.64326500
C	−0.58333000	−3.74266500	−0.56264800
C	0.08427700	−3.88738900	0.65683900
C	1.40692600	−3.45575600	0.78836500
C	3.76630900	1.26717200	−1.61207700
C	2.97522200	0.59458800	−2.75403800
C	5.25609800	1.27994000	−2.00052600
C	3.27210400	2.71792000	−1.45016200
C	4.01177800	1.10304200	1.60292100
C	3.05320300	2.23963300	2.02518900
C	5.43069600	1.69801000	1.52225600
C	3.96723500	0.01169600	2.69310600
H	−0.80733600	1.86338600	−0.01212600
H	−0.34482000	5.24828800	−2.05100600
H	−0.48542500	5.83517700	−0.35883100
H	−1.80923800	6.13877800	−1.52837000
H	−1.61413700	0.15780800	−1.47072300
H	−0.98919300	−0.04245600	2.58954900
H	−1.10031300	1.69181600	2.34240900
H	−3.14589200	2.61002300	1.77052900
H	−5.63051000	1.03561600	2.82052700
H	−5.57349200	2.33464500	1.59415900
H	−5.19060500	2.70933000	3.26460200
H	−3.23557100	−0.40838800	−3.40337200
H	−3.48976500	1.12340500	−2.51901200
H	−4.86648400	0.27793800	−3.24160700
H	−6.47285400	−1.27467300	−3.00199700
H	−8.19507200	−2.76859800	−2.04175100
H	−7.94506000	−3.72223600	0.23113200
H	−5.95417700	−3.19433600	1.61590600
H	−2.14831900	−1.93855200	1.82883100
H	−3.67331400	−2.61545400	2.37762000
H	−2.82902500	−0.76417100	3.86126600
H	−4.45701100	−0.47849200	3.22452100
H	6.14955500	−0.39972500	−0.11673000
H	7.45868000	−2.44930000	−0.13543300
H	6.29578400	−4.66955500	−0.17131700
H	3.82813800	−4.73843000	−0.23626200
H	1.90760500	−2.27967800	−2.36427200
H	−0.43380600	−3.04081000	−2.59863700
H	−1.60414700	−4.09812800	−0.67295000
H	−0.41420600	−4.35812600	1.50016800
H	1.93284000	−3.60322500	1.72819600
H	1.89538900	0.61508600	−2.56929200
H	3.28264700	−0.44546800	−2.90849100
H	3.17058200	1.14054400	−3.68617000
H	5.36855100	1.90513000	−2.89594000
H	5.62462500	0.28202000	−2.25301400
H	5.89584200	1.70344800	−1.22202100
H	2.21955400	2.76416000	−1.15050900
H	3.36848000	3.22831300	−2.41733400
H	3.86895500	3.27668300	−0.72330000
H	2.03114500	1.87785200	2.17788300
H	3.02209400	3.05668000	1.29970100
H	3.41029600	2.65475200	2.97662400
H	5.67256700	2.13347200	2.50072200
H	5.49954900	2.50136700	0.78323100
H	6.20199700	0.95537900	1.30732300
H	2.97568100	−0.45167300	2.76877700
H	4.19129800	0.47413800	3.66287500
H	4.70365200	−0.77915600	2.52314300

TS31

Au	2.23899900	−0.51604900	0.24129000
S	−0.86968400	3.18419600	−1.00652400
P	4.47092200	−0.46443800	−0.53123600
O	−0.90727800	2.91277500	0.54880600
O	−1.43317100	2.02453300	−1.72626800
O	−1.44977000	4.50450800	−1.29720000
N	−3.75467100	0.15409900	−0.29560700

N	−1.46616500	0.34462700	2.60291600
C	0.89295000	3.26256700	−1.32499900
C	−0.68628400	−1.24058300	0.25001200
C	0.26873500	−0.56292300	0.90981400
C	−0.00401200	0.24204900	2.14692300
C	−2.39592200	1.01676500	1.60484600
C	−3.36319000	1.94746400	2.33239600
C	−2.81886600	0.05801200	0.65340300
C	−4.54150500	1.33205700	−0.65970500
C	−3.90114900	−1.08978400	−0.97617900
C	−4.79255900	−1.41751300	−1.99142400
C	−4.73294000	−2.72464300	−2.49346100
C	−3.81576600	−3.65351200	−1.99224200
C	−2.92898700	−3.29885500	−0.96488600
C	−2.98736900	−2.00903600	−0.45373200
C	−2.18095100	−1.32560600	0.62601100
C	−2.37596200	−1.95449500	2.03814500
C	−2.01258600	−0.95984000	3.15548700
C	4.71017400	0.46414200	−2.09920100
C	5.19288200	−2.11975700	−0.87674700
C	5.65155100	0.31452200	0.64262800
H	−1.42747800	0.98180200	3.40535800
H	1.34583200	2.30671300	−1.05021800
H	1.32336400	4.07526200	−0.73527200
H	1.03197000	3.45854500	−2.39158600
H	−0.43539100	−1.79747600	−0.64914800
H	0.53169500	−0.16756300	3.00978600
H	0.32092700	1.27722000	2.01661600
H	−1.56710000	2.01063600	0.87446700
H	−3.97597100	2.51559800	1.63198900
H	−4.03650300	1.40072300	3.00568800
H	−2.79991400	2.67726100	2.92516300
H	−4.74943300	1.28977300	−1.72959300
H	−3.96917100	2.23554900	−0.46487900
H	−5.48564700	1.35220600	−0.10732100
H	−5.51043400	−0.70511800	−2.38303600
H	−5.41548100	−3.01618900	−3.28645800
H	−3.79137900	−4.66016900	−2.39906500
H	−2.21755800	−4.02163100	−0.57541100
H	−1.75728800	−2.85248500	2.10301200
H	−3.42003100	−2.25735900	2.15733300
H	−1.25218600	−1.34988800	3.83375500
H	−2.89225000	−0.68409500	3.73931000
H	4.11206900	0.00521300	−2.89317900
H	5.76550700	0.45696700	−2.39418100
H	4.37942000	1.49966900	−1.97049600
H	5.19428300	−2.72059500	0.03840800
H	6.21984900	−2.02291100	−1.24640600
H	4.58670900	−2.63389100	−1.62968500
H	5.34710600	1.34765400	0.83976000
H	6.66712300	0.31086000	0.23132900
H	5.64567500	−0.23674800	1.58856900

TS31 (L = PPh_3)

Au	−0.84556900	−0.32532000	−0.49687200
S	2.58284300	3.17651000	1.05053800
P	−3.13229100	−0.18334000	0.11989400
O	2.65787500	2.94310000	−0.51012100
O	2.71932800	1.88778500	1.75792800
O	3.50259200	4.25535900	1.44692300
N	5.13335500	−0.11087000	0.35788400
N	3.01351400	0.39369800	−2.63122000
C	0.90211200	3.77103600	1.23142300
C	2.01514600	−1.25717900	−0.41360400
C	1.14735200	−0.45978800	−1.05952900
C	1.53732800	0.41531100	−2.21445300
C	3.97158900	0.92946200	−1.58132100
C	5.05995000	1.77135000	−2.24446100
C	4.25525300	−0.09691300	−0.64945500
C	5.97409700	0.98589700	0.83662900
C	5.15357400	−1.39239600	0.98053100
C	5.95793800	−1.82662600	2.02766600
C	5.78462400	−3.14980000	2.45577100
C	4.84284400	−3.98932300	1.85289100
C	4.04383900	−3.52679800	0.79659000
C	4.21521000	−2.22020800	0.35835300
C	3.51732900	−1.42847800	−0.72359400
C	3.74239400	−1.99429200	−2.15566600
C	3.43975000	−0.93670200	−3.23383100
C	−3.41040000	−0.27018900	1.93269900
C	−4.57946500	−0.81390700	2.48844300
C	−4.74806000	−0.84480400	3.87462900
C	−3.75539200	−0.33490400	4.71559900
C	−2.58814600	0.20522400	4.16908800
C	−2.41285100	0.23379400	2.78458100
C	−4.13383400	−1.53843400	−0.61308100
C	−5.44112100	−1.34298000	−1.08383100
C	−6.15879700	−2.41271200	−1.62569900
C	−5.58138600	−3.68254900	−1.69838500
C	−4.27924300	−3.88381800	−1.23143000
C	−3.55595100	−2.81725100	−0.69630100
C	−3.90203000	1.38428900	−0.45202200
C	−4.84820000	2.08799100	0.30786800
C	−5.40137800	3.27354800	−0.18409300
C	−5.01866600	3.76297400	−1.43495200
C	−4.07562200	3.06690100	−2.19703600
C	−3.51497300	1.88713800	−1.70669700
H	3.05748000	1.06505800	−3.40512600
H	0.20960500	3.00097600	0.88440700
H	0.78542800	4.68555000	0.64546100
H	0.73582600	3.98140400	2.29123300
H	1.67830200	−1.85893500	0.42645100
H	0.98663900	0.14044100	−3.11998200
H	1.31937500	1.46450900	−1.99930900
H	3.22953000	1.98457600	−0.84365100
H	5.74220600	2.19853600	−1.50946700
H	5.65782600	1.18392700	−2.95388200
H	4.60638000	2.60997200	−2.78455500
H	6.00922900	0.94275100	1.92666200
H	5.54309500	1.94212100	0.55129700
H	6.98854000	0.89664500	0.43612600
H	6.69420500	−1.18219300	2.49561800
H	6.39756300	−3.52478500	3.27026200
H	4.73060100	−5.01128300	2.20280900
H	3.31258600	−4.18082300	0.32984000
H	3.10201700	−2.86975200	−2.28689000
H	4.78168400	−2.32143400	−2.25228200
H	2.63410300	−1.24042800	−3.90353400
H	4.32602300	−0.71897900	−3.83166500
H	−5.35690400	−1.21482900	1.84527200
H	−5.65505300	−1.26944600	4.29605300
H	−3.88892100	−0.36310900	5.79353400
H	−1.81015300	0.59652100	4.81885600
H	−1.49798500	0.64306500	2.36357000

H	−5.90165100	−0.36126700	−1.03226600
H	−7.16998600	−2.25113100	−1.98905500
H	−6.14167800	−4.51168200	−2.12169700
H	−3.82300900	−4.86818500	−1.29030500
H	−2.53887700	−2.97624700	−0.34605400
H	−5.15524300	1.71736300	1.28086600
H	−6.13207800	3.81260800	0.41261100
H	−5.44984100	4.68558200	−1.81379800
H	−3.77028800	3.44515300	−3.16885000
H	−2.77305500	1.35504700	−2.29709800

TS31 (L = JohnPhos)

Au	−0.93384900	0.04946100	−0.12411400
S	3.21598900	3.41135000	−0.40933500
P	−3.10571300	0.83945400	0.52459900
O	2.90615700	2.46395300	−1.63467000
O	3.65663400	2.60185300	0.74427500
O	4.09322500	4.51366400	−0.83436600
N	5.19202400	−0.24796500	0.34218600
N	2.81247300	−0.75750400	−2.44376400
C	1.59496600	4.08337400	−0.05105600
C	1.84352100	−1.04936000	0.31279300
C	1.00724100	−0.53147300	−0.60340300
C	1.38879500	−0.34460800	−2.04123000
C	3.92682900	0.04121700	−1.78578800
C	5.01684700	0.35465700	−2.80859600
C	4.19369200	−0.50665300	−0.50863300
C	6.26531900	0.73538400	0.19461700
C	5.10031100	−1.09252100	1.48665900
C	5.95776700	−1.16285900	2.57895400
C	5.64251100	−2.09358500	3.57792500
C	4.51434500	−2.91319800	3.47648700
C	3.66582800	−2.82514600	2.36314500
C	3.97390600	−1.91047900	1.36446900
C	3.27353900	−1.57562100	0.06863100
C	3.26705900	−2.75732200	−0.94951600
C	3.03056500	−2.26021000	−2.38791400
C	−4.57181800	−0.25838700	0.18600700
C	−5.85384500	0.25983000	0.46617600
C	−7.02180800	−0.45042300	0.19989700
C	−6.93660300	−1.72062400	−0.36729600
C	−5.68284500	−2.25637700	−0.64711200
C	−4.48987600	−1.55653500	−0.37960400
C	−3.24048100	−2.30976400	−0.73230600
C	−2.56791900	−3.07744200	0.23232000
C	−1.51733500	−3.92260500	−0.13534000
C	−1.12474700	−4.01711300	−1.47371600
C	−1.78565900	−3.25560700	−2.44201600
C	−2.83829700	−2.41279600	−2.07438300
C	−3.06219100	1.07509900	2.43005100
C	−2.60780800	−0.28149400	3.01050900
C	−4.39709100	1.45465100	3.09762600
C	−2.00236600	2.14220400	2.77005300
C	−3.43823000	2.47476200	−0.44797400
C	−2.09480300	3.22272100	−0.60125600
C	−4.45063800	3.44909500	0.18230600
C	−3.91682800	2.06581300	−1.85670800
H	2.86226100	−0.51501400	−3.43859200
H	0.93006000	3.26404700	0.22576900
H	1.22066300	4.60414500	−0.93514100
H	1.70204900	4.78495700	0.78060800
H	1.52027900	−1.15232100	1.34572700
H	0.73537200	−0.92547000	−2.69987800
H	1.30498900	0.70547500	−2.33303700
H	3.36917400	1.39864000	−1.55464400
H	5.78815100	1.00055200	−2.38856600
H	5.50405800	−0.55470500	−3.18491800
H	4.58175100	0.89176700	−3.65905600
H	6.54479500	1.09215600	1.18638800
H	5.91092800	1.58895200	−0.37680600
H	7.13736400	0.28385800	−0.28791000
H	6.83893000	−0.53650400	2.66516800
H	6.29203700	−2.17582500	4.44452700
H	4.29471400	−3.62717600	4.26479700
H	2.79024800	−3.46348100	2.28406600
H	2.48726300	−3.46193200	−0.65176700
H	4.22700600	−3.27953600	−0.90346300
H	2.15420800	−2.71661700	−2.85000100
H	3.89904500	−2.45378000	−3.01914200
H	−5.94994100	1.24527900	0.89971900
H	−7.98649800	−0.00779300	0.43175300
H	−7.83404500	−2.29200900	−0.58786400
H	−5.61119100	−3.24954700	−1.08145900
H	−2.88418200	−3.03079400	1.27054700
H	−1.01840500	−4.52055300	0.62303100
H	−0.32031800	−4.68896800	−1.76143600
H	−1.49781100	−3.33142000	−3.48757200
H	−3.36758600	−1.84546400	−2.83571900
H	−1.61857700	−0.57336200	2.64075900
H	−3.31555600	−1.08467800	2.77731000
H	−2.55094000	−0.19692100	4.10360700
H	−4.21366500	1.59400600	4.17120800
H	−5.14586300	0.66394500	2.99785000
H	−4.82068200	2.38703300	2.71545600
H	−1.03782500	1.92828400	2.29576300
H	−1.84586300	2.14944600	3.85672100
H	−2.31950200	3.14750600	2.47624100
H	−1.35411800	2.61799000	−1.13394100
H	−1.66791400	3.52152800	0.35986700
H	−2.26965300	4.13607400	−1.18511900
H	−4.52828100	4.33064500	−0.46787100
H	−4.12654600	3.79840400	1.16672100
H	−5.45625500	3.03191400	0.27223200
H	−3.22909500	1.35440600	−2.33040300
H	−3.95475000	2.96165900	−2.48994900
H	−4.91704900	1.62330600	−1.84571700

TS32

Au	−1.72834700	−0.70897900	0.02259300
S	−1.09793300	3.87706300	−0.56727800
P	−3.41227300	−2.29183300	−0.21568800
O	−1.70073600	2.43593700	−0.63496800
O	−0.52655100	4.13165200	0.77758800
O	−0.20475400	4.14035500	−1.71200700
N	3.51282300	−1.56291100	0.71283600
N	1.60118700	1.22529200	2.28072800
C	−2.56848000	4.88759100	−0.74636300
C	0.97847200	0.40348200	−0.45593200
C	−0.04960500	0.64128700	0.39650500
C	0.15363600	0.98314200	1.85516600
C	2.41058200	−0.02629100	2.33522500
C	2.64760300	−0.53733200	3.72434900
C	2.78453000	−0.45551400	1.11221200
C	3.91138100	−2.68220900	1.54996400

C	3.87185800	−1.43825100	−0.64055000
C	4.67915200	−2.27730000	−1.40825500
C	4.87916100	−1.93815600	−2.75420900
C	4.29755800	−0.79794000	−3.31414300
C	3.49138200	0.03902200	−2.52561100
C	3.29069800	−0.28473000	−1.19182600
C	2.46895400	0.40563200	−0.12120900
C	2.92006300	1.85778000	0.19838500
C	2.26730900	2.35956600	1.49863600
C	−2.98891700	−3.90746300	0.54405000
C	−3.82840900	−2.68116300	−1.95957500
C	−5.00251300	−1.80555900	0.55942300
H	−0.97254700	1.51785900	−0.19260500
H	1.53288800	1.57018900	3.24383900
H	−2.25975800	5.93581200	−0.71766800
H	−3.25119800	4.67147100	0.07790600
H	−3.04085600	4.66207400	−1.70490800
H	0.75231100	0.23932100	−1.50813000
H	−0.37702000	1.90924600	2.09718000
H	−0.21725300	0.19347200	2.51498100
H	3.38353900	−1.34129800	3.73631800
H	3.03474700	0.26666500	4.36670300
H	1.72806500	−0.91415800	4.19405600
H	4.09050400	−3.55289700	0.91575500
H	3.10413200	−2.93394800	2.24149000
H	4.82458900	−2.46931300	2.11957100
H	5.15022900	−3.15974300	−0.98820600
H	5.50709600	−2.57843400	−3.36808700
H	4.47182000	−0.55448600	−4.35807200
H	3.03713800	0.92880200	−2.95433100
H	2.65212000	2.52343600	−0.62711300
H	4.00915400	1.86401600	0.29648200
H	1.48415200	3.09700100	1.31569600
H	3.00976200	2.78277900	2.17628600
H	−2.08511100	−4.30928400	0.07513600
H	−3.81175600	−4.61855700	0.41101100
H	−2.79831100	−3.77217300	1.61342200
H	−4.17398900	−1.77502600	−2.46704400
H	−4.61621100	−3.44177300	−1.99868400
H	−2.93817300	−3.05417900	−2.47559700
H	−4.84991300	−1.62320400	1.62786700
H	−5.74726600	−2.59884200	0.43050400
H	−5.37066200	−0.88478700	0.09588700

TS32 (L = PPh_3)

Au	−0.58445800	0.34077700	0.14374600
S	1.91595200	4.21336100	−0.57280700
P	−2.77962600	−0.41884700	−0.05472800
O	0.72669400	3.19999400	−0.55966600
O	2.53045500	4.30385300	0.77418700
O	2.84254600	3.93806900	−1.68924700
N	3.87250800	−2.57344700	0.70193200
N	3.29815900	0.74673600	2.29535900
C	1.06940700	5.75992500	−0.90354200
C	2.32239300	0.25024200	−0.41670700
C	1.50245700	0.88363100	0.45923900
C	1.86771400	1.11911000	1.90770700
C	3.52720000	−0.72668500	2.33885600
C	3.56252600	−1.29277300	3.72609800
C	3.66608900	−1.26730800	1.11071500
C	3.81015400	−3.75850800	1.54086200
C	4.21654400	−2.60078000	−0.66115400
C	4.59555900	−3.69207100	−1.44275200
C	4.88280200	−3.45806300	−2.79517000
C	4.80081500	−2.17781800	−3.34834400
C	4.42295100	−1.08887300	−2.54622000
C	4.14001800	−1.30874300	−1.20606800
C	3.69546300	−0.34864900	−0.12075900
C	4.70070100	0.79922400	0.17297200
C	4.34946600	1.51224800	1.49102100
C	−3.66390700	0.35209700	−1.46485400
C	−5.03190900	0.66013000	−1.41046100
C	−5.66414800	1.23134200	−2.51770700
C	−4.93996500	1.49619200	−3.68239200
C	−3.57675200	1.19198400	−3.74132200
C	−2.93848300	0.62711500	−2.63679000
C	−3.76348700	−0.06120000	1.45219900
C	−4.75370300	−0.93754900	1.92204900
C	−5.48623100	−0.61588800	3.06736500
C	−5.23772500	0.57786400	3.74881100
C	−4.25184600	1.45413000	3.28562700
C	−3.51334200	1.13568700	2.14538000
C	−2.85412800	−2.23332400	−0.31719600
C	−3.84685800	−2.83205800	−1.10831700
C	−3.87285400	−4.21987700	−1.26651500
C	−2.91391500	−5.01763100	−0.63789000
C	−1.92228500	−4.42653800	0.15042100
C	−1.88784800	−3.04043900	0.30707500
H	1.00812100	2.04923600	−0.11965900
H	3.39887900	1.08522200	3.25767200
H	1.82313100	6.55106200	−0.93651400
H	0.35292200	5.95473300	−0.10282400
H	0.55800700	5.68672900	−1.86575600
H	2.01978100	0.19296100	−1.46085300
H	1.77119500	2.18301300	2.14552600
H	1.22403100	0.55613800	2.58945500
H	3.89215600	−2.33160400	3.72883000
H	4.26639500	−0.72709900	4.35330600
H	2.58094000	−1.24880800	4.21872600
H	3.62063800	−4.62980800	0.91082600
H	2.98030000	−3.67102200	2.24583400
H	4.74237100	−3.92196500	2.09569500
H	4.68008500	−4.69150000	−1.02929700
H	5.18165700	−4.29581600	−3.41958100
H	5.03374900	−2.02216900	−4.39755900
H	4.35965100	−0.08942000	−2.96914800
H	4.69123900	1.52159000	−0.64801200
H	5.70394800	0.36859900	0.23242700
H	3.93654600	2.50928400	1.32876300
H	5.21957900	1.58461200	2.14452300
H	−5.60464900	0.45932900	−0.51042300
H	−6.72293600	1.46975500	−2.46682700
H	−5.43449000	1.94345000	−4.54023300
H	−3.00793600	1.40195900	−4.64287400
H	−1.87548300	0.40335200	−2.68223100
H	−4.95445700	−1.86864900	1.40135900
H	−6.24961300	−1.30077700	3.42595300
H	−5.80737700	0.82293400	4.64101400
H	−4.05184400	2.38135200	3.81551400
H	−2.74028200	1.81442400	1.79333500
H	−4.59700100	−2.22218800	−1.60206600
H	−4.64307400	−4.67512900	−1.88287500
H	−2.93564700	−6.09636800	−0.76584100
H	−1.17061000	−5.04249700	0.63628800

H	−1.10809900	−2.58257900	0.91083800

TS32 (L = JohnPhos)

Au	0.68397300	0.46385800	−0.34327500
S	−1.94932600	3.97986000	1.29167200
P	2.93150200	−0.10034600	−0.79589400
O	−0.72117200	3.07665700	0.93425800
O	−2.76490300	4.24242800	0.08193300
O	−2.67449900	3.45486400	2.46485200
N	−3.62743300	−2.52769500	−1.38318700
N	−3.32630000	1.09548600	−2.19635100
C	−1.13601900	5.50797400	1.75913600
C	−2.20064900	0.07147800	0.30046100
C	−1.45377400	0.93201500	−0.43423100
C	−1.90113300	1.45964400	−1.77999600
C	−3.47549400	−0.34161000	−2.56787300
C	−3.54948600	−0.58523000	−4.04473900
C	−3.52148000	−1.15183200	−1.49062500
C	−3.48697600	−3.49330700	−2.46017100
C	−3.90526200	−2.88417700	−0.05237200
C	−4.17176300	−4.14893800	0.47162100
C	−4.40897600	−4.24726600	1.85030100
C	−4.38837000	−3.12057500	2.67640400
C	−4.12332600	−1.85359200	2.13096800
C	−3.88808200	−1.74461600	0.76827100
C	−3.55105900	−0.53610900	−0.08315100
C	−4.63943600	0.57094000	−0.08251200
C	−4.37979600	1.59116000	−1.20406800
C	3.93150300	−0.90763700	0.54919300
C	5.28592400	−1.18404200	0.26665500
C	6.11218800	−1.85916600	1.16172600
C	5.59162300	−2.29488100	2.37865200
C	4.26163700	−2.02350500	2.68464900
C	3.41416100	−1.32131200	1.80451900
C	2.04015900	−1.06571200	2.34243000
C	1.18147400	−2.14682900	2.60375700
C	−0.02829700	−1.95305100	3.27562800
C	−0.39027800	−0.67622500	3.71405300
C	0.45503500	0.40751800	3.45870000
C	1.65785800	0.21629800	2.77321400
C	2.83887900	−1.40409400	−2.20520600
C	1.96104500	−2.55106500	−1.65997100
C	4.18382900	−2.00133700	−2.65776400
C	2.13371800	−0.76030300	−3.41447300
C	3.84764800	1.52800500	−1.28324100
C	2.84328400	2.46049000	−1.99625300
C	5.06816700	1.35675800	−2.20794700
C	4.28503300	2.20543300	0.03185200
H	−0.97598200	2.01534000	0.35174200
H	−3.49039200	1.63578600	−3.05207100
H	−1.91194700	6.22672300	2.03518300
H	−0.55992700	5.88118100	0.90998200
H	−0.48210500	5.31541400	2.61253100
H	−1.84714800	−0.20641300	1.29092000
H	−1.87325400	2.55378900	−1.78017500
H	−1.26029400	1.10341400	−2.59135100
H	−3.84373000	−1.61094700	−4.26846200
H	−4.29934100	0.07541500	−4.50306500
H	−2.59289300	−0.39065500	−4.55023600
H	−3.18643900	−4.45398300	−2.03636500
H	−2.70140900	−3.17063900	−3.14729300
H	−4.42177100	−3.63297400	−3.01689600
H	−4.20675200	−5.03239200	−0.15724600
H	−4.62064800	−5.22385900	2.27757800
H	−4.58333500	−3.22178800	3.73998000
H	−4.10739400	−0.97276900	2.76770900
H	−4.65156300	1.08299500	0.88386100
H	−5.61344800	0.09416300	−0.22361300
H	−4.00938400	2.54365400	−0.82215600
H	−5.27900200	1.76598900	−1.79614600
H	5.71335000	−0.87615100	−0.67768100
H	7.14996600	−2.04597300	0.90067500
H	6.21426200	−2.83173300	3.08898000
H	3.85835100	−2.34128300	3.64176300
H	1.47347000	−3.14706200	2.29397000
H	−0.67911900	−2.80162200	3.46934500
H	−1.31916600	−0.52693400	4.25770400
H	0.18386900	1.40260800	3.80081500
H	2.32231500	1.05887200	2.60369200
H	0.96612900	−2.19944900	−1.36430600
H	2.42165600	−3.04552600	−0.79755500
H	1.83617700	−3.30549600	−2.44764200
H	3.98608500	−2.70300700	−3.47858800
H	4.67207600	−2.56552000	−1.85893600
H	4.88262200	−1.24952100	−3.03258300
H	1.17444100	−0.31158400	−3.13240500
H	1.93479200	−1.53876300	−4.16235100
H	2.75102700	0.00735500	−3.89082000
H	1.98537700	2.69829900	−1.35887200
H	2.46868500	2.03812000	−2.93335300
H	3.35610200	3.40049600	−2.23848300
H	5.49864200	2.35044800	−2.38888500
H	4.79230900	0.93898300	−3.18024700
H	5.85880500	0.74093700	−1.77337300
H	3.44456800	2.34385200	0.72235500
H	4.68718100	3.19888800	−0.20393100
H	5.06670600	1.64200500	0.54949200

TS33

Au	2.32355700	−0.29955300	0.00534300
P	4.63764300	−0.54069500	0.11910200
N	−2.80669000	−0.06381500	−1.68033000
N	−1.45387400	3.03383100	−0.23519000
C	0.19763100	−0.29685000	−0.08339600
C	−0.22091600	0.88815800	−0.04632600
C	−0.12737400	2.36185700	0.03431400
C	−2.17686300	2.38169300	−1.39047900
C	−2.57611500	1.03391500	−0.89603500
C	−3.19557000	−1.11682900	−0.87120800
C	−3.53786000	−2.43140200	−1.20949900
C	−3.90532900	−3.27836600	−0.17003700
C	−3.93219700	−2.83704600	1.17338700
C	−3.59251200	−1.53357600	1.50703900
C	−3.22050700	−0.64847700	0.47494000
C	−2.83305400	0.73004300	0.44068900
C	−2.69252700	1.73156600	1.55076200
C	−2.35359400	3.11976400	0.99479300
H	5.13037000	−1.80856800	−0.23246900
H	5.22882800	−0.34030700	1.37828600
H	5.40705300	0.30401900	−0.69934500
H	−2.67106600	−0.10959000	−2.68286300
H	−1.23891700	4.00137100	−0.50638500
H	−0.24727400	−1.28420500	−0.14231000
H	0.21342800	2.68592200	1.02024800

H	0.57214000	2.72476600	−0.72393700
H	−1.49881500	2.34616700	−2.24636400
H	−3.02645300	3.02639200	−1.63341900
H	−3.51904700	−2.77091100	−2.24065900
H	−4.17970300	−4.30494900	−0.39570600
H	−4.22711200	−3.53306200	1.95329800
H	−3.61958500	−1.19836000	2.53995900
H	−1.92980400	1.40625800	2.26829800
H	−3.62612200	1.82515000	2.11759600
H	−1.82477000	3.73856500	1.72066500
H	−3.24416800	3.64962800	0.65143100

TS34

Au	2.18734900	−0.31184600	−0.01931500
P	4.53720300	−0.45294700	0.16554200
N	−2.66113400	−0.04571900	−1.68505900
N	−1.43403600	3.09277200	−0.20300900
C	0.14626300	−0.26290100	−0.15816900
C	−0.63577100	0.82760200	−0.11850200
C	−0.19599500	2.26558600	0.06191800
C	−2.13354500	2.43181600	−1.35903400
C	−2.20764300	0.99643400	−0.90918300
C	−3.02131300	−1.10367200	−0.85828700
C	−3.46203500	−2.38469000	−1.20313500
C	−3.80163900	−3.23725500	−0.15667200
C	−3.70069100	−2.83998900	1.19379700
C	−3.24330700	−1.57152500	1.53181400
C	−2.89782300	−0.69505200	0.49385600
C	−2.40194200	0.66786500	0.48424900
C	−2.53579100	1.70942100	1.57116300
C	−2.32366600	3.13417900	1.02602500
H	5.11779200	−1.71864800	−0.03372900
H	5.10012100	−0.09273500	1.40346400
H	5.30366900	0.33440100	−0.71301500
H	−2.45644700	−0.14008200	−2.67422500
H	−1.17559900	4.05334600	−0.45609100
H	−0.36348100	−1.22316600	−0.25842500
H	0.16691900	2.50192700	1.06327300
H	0.55800500	2.54131200	−0.67743900
H	−1.53150400	2.56292500	−2.26024800
H	−3.12008600	2.88020300	−1.48913100
H	−3.54280800	−2.69422600	−2.24006100
H	−4.15607200	−4.23771500	−0.38734100
H	−3.98097300	−3.53853300	1.97596300
H	−3.15524000	−1.26566100	2.56977700
H	−1.83986800	1.49378300	2.38644400
H	−3.54601700	1.63939300	1.98708200
H	−1.82391200	3.77546900	1.75222200
H	−3.25752700	3.60175100	0.71166700

TS35

Au	2.68555900	−0.13393400	0.02328100
S	−3.79902200	−3.73175700	−0.05609400
P	4.98383600	−0.54042400	−0.10747000
O	−2.36951800	−3.61798000	0.47841000
O	−4.56478700	−2.49319100	0.27787000
O	−3.83804000	−4.13402800	−1.47734100
N	−2.74447900	2.02368700	−1.22313100
N	−1.67122500	−1.10752800	0.58706700
C	−4.51941800	−5.06991200	0.90623300
C	0.50685900	2.65631700	−0.49223300
C	0.21211200	1.29475400	−0.03946400
C	0.55767300	0.08509200	0.19260800
C	−0.16800700	−1.17583900	0.54003700
C	−2.33658300	−0.42755100	−0.60149600
C	−1.76301700	−0.97040700	−1.91640100
C	−2.29907100	1.06100200	−0.35386200
C	−3.21294600	1.83280100	−2.59436200
C	−2.76415400	3.25290400	−0.55317800
C	−3.12966900	4.52188200	−1.01568400
C	−3.06989400	5.57541500	−0.10732900
C	−2.65289700	5.38031400	1.22504500
C	−2.27784400	4.12113700	1.67681600
C	−2.33084800	3.04085200	0.77934000
C	−2.02195300	1.64184100	0.89904200
C	−1.84897400	0.83986000	2.15997900
C	−2.22114600	−0.61844500	1.89827800
C	5.73934500	−0.02994300	−1.69984300
C	5.40120200	−2.31733600	0.07561300
C	5.95841700	0.31874100	1.18841000
H	−1.98686200	−2.15584000	0.52625200
H	−3.93940300	−5.98009600	0.73663500
H	−4.50131100	−4.80162600	1.96490400
H	−5.54983700	−5.21792700	0.57387600
H	0.50476800	3.37887700	0.32911600
H	1.49677000	2.65712100	−0.96465900
H	−0.21312500	2.98874700	−1.24781900
H	0.15257800	−1.54815700	1.51705100
H	0.08363200	−1.95000200	−0.18847100
H	−3.37794900	−0.76993300	−0.53100700
H	−0.75572800	−0.60197500	−2.12768500
H	−2.41313500	−0.69244200	−2.74688300
H	−1.75505600	−2.06403500	−1.88239700
H	−3.89278200	0.97967600	−2.64814200
H	−3.76780600	2.72107900	−2.89587700
H	−2.37875700	1.68550100	−3.28658600
H	−3.44927400	4.69339300	−2.03823200
H	−3.35474300	6.57093100	−0.43493300
H	−2.62561300	6.22741000	1.90391300
H	−1.95548700	3.97277500	2.70372000
H	−0.83193100	0.91636800	2.55975300
H	−2.51664700	1.23014200	2.93688400
H	−1.83933600	−1.28776900	2.67223200
H	−3.30207900	−0.75911000	1.82766400
H	5.58967800	1.04335300	−1.85454600
H	6.81360400	−0.24565100	−1.70145100
H	5.26346200	−0.56928700	−2.52494000
H	4.91531000	−2.89557000	−0.71664200
H	6.48519600	−2.46518900	0.01490700
H	5.04396600	−2.68592500	1.04240600
H	5.62127700	−0.00236900	2.17912700
H	7.02446800	0.08976400	1.08074000
H	5.81336800	1.40066300	1.10709800

TS36

Au	−1.32627100	−1.68502000	0.03809100
S	−2.26543700	3.49742600	0.23336800
P	−3.64045600	−1.95914700	−0.13619100
O	−1.07122300	3.94010100	−0.60758000
O	−1.84346200	3.20771100	1.63252400
O	−3.03263900	2.40303600	−0.42061500
N	3.79565600	0.48486800	−1.33787500
N	0.94015900	2.37605800	0.07714500
C	−3.33447500	4.94298000	0.27921300

C	1.67081700	−2.61991600	0.09735900
C	0.81861200	−1.39265000	0.15716200
C	0.95969600	−0.12172000	0.27713200
C	0.14279600	1.12860400	0.33217900
C	1.89893700	2.20814400	−1.08213600
C	1.12200600	1.90890700	−2.37177500
C	2.88708800	1.17589300	−0.59907600
C	4.02044800	0.55825600	−2.77922200
C	4.50670400	−0.37130300	−0.48408400
C	5.51854500	−1.28674400	−0.78285700
C	6.07756600	−1.98852800	0.28423900
C	5.64508500	−1.78368400	1.60861400
C	4.62179500	−0.88584300	1.89550100
C	4.02986900	−0.18561900	0.83452100
C	2.96613100	0.79352600	0.76195200
C	2.46928900	1.66466000	1.89470400
C	1.64163500	2.82540300	1.32959300
C	−4.56029300	−0.62238700	0.71823300
C	−4.24127200	−1.92661000	−1.87041900
C	−4.28430800	−3.53150500	0.55863800
H	0.19460100	3.11493300	−0.19223500
H	−4.21999500	4.70123300	0.87212800
H	−2.78959700	5.77020600	0.73947100
H	−3.62508500	5.20298400	−0.74110700
H	1.34653400	−3.34486300	0.85196700
H	1.55753300	−3.10899400	−0.87725800
H	2.72894800	−2.40082000	0.25638700
H	−0.34721100	1.27012600	1.29725200
H	−0.64452500	1.09479000	−0.42300200
H	2.38990100	3.18280800	−1.18575700
H	0.76309900	0.87704600	−2.41114000
H	0.26579100	2.58699900	−2.44037900
H	1.75402600	2.08959400	−3.24291900
H	5.04538900	0.24663800	−2.98425600
H	3.33190800	−0.09389600	−3.32558900
H	3.90927000	1.58677600	−3.12409200
H	5.86562300	−1.45299500	−1.79729500
H	6.87004600	−2.70454900	0.08758200
H	6.11531700	−2.33975000	2.41406200
H	4.28159600	−0.73963300	2.91661200
H	1.88750300	1.08096000	2.61506300
H	3.32491000	2.07393300	2.44398400
H	0.86384700	3.16726700	2.01463300
H	2.26689300	3.67647000	1.04938800
H	−4.22952000	0.35337600	0.34391000
H	−5.63788000	−0.73550800	0.55261400
H	−4.35611500	−0.66738200	1.79317700
H	−3.76339100	−2.72509600	−2.44672300
H	−5.32805300	−2.06356200	−1.89922500
H	−3.98819800	−0.96511000	−2.32807300
H	−4.03358300	−3.59839000	1.62186700
H	−5.37280600	−3.58156800	0.44259900
H	−3.82971900	−4.38150600	0.03981600

TS37

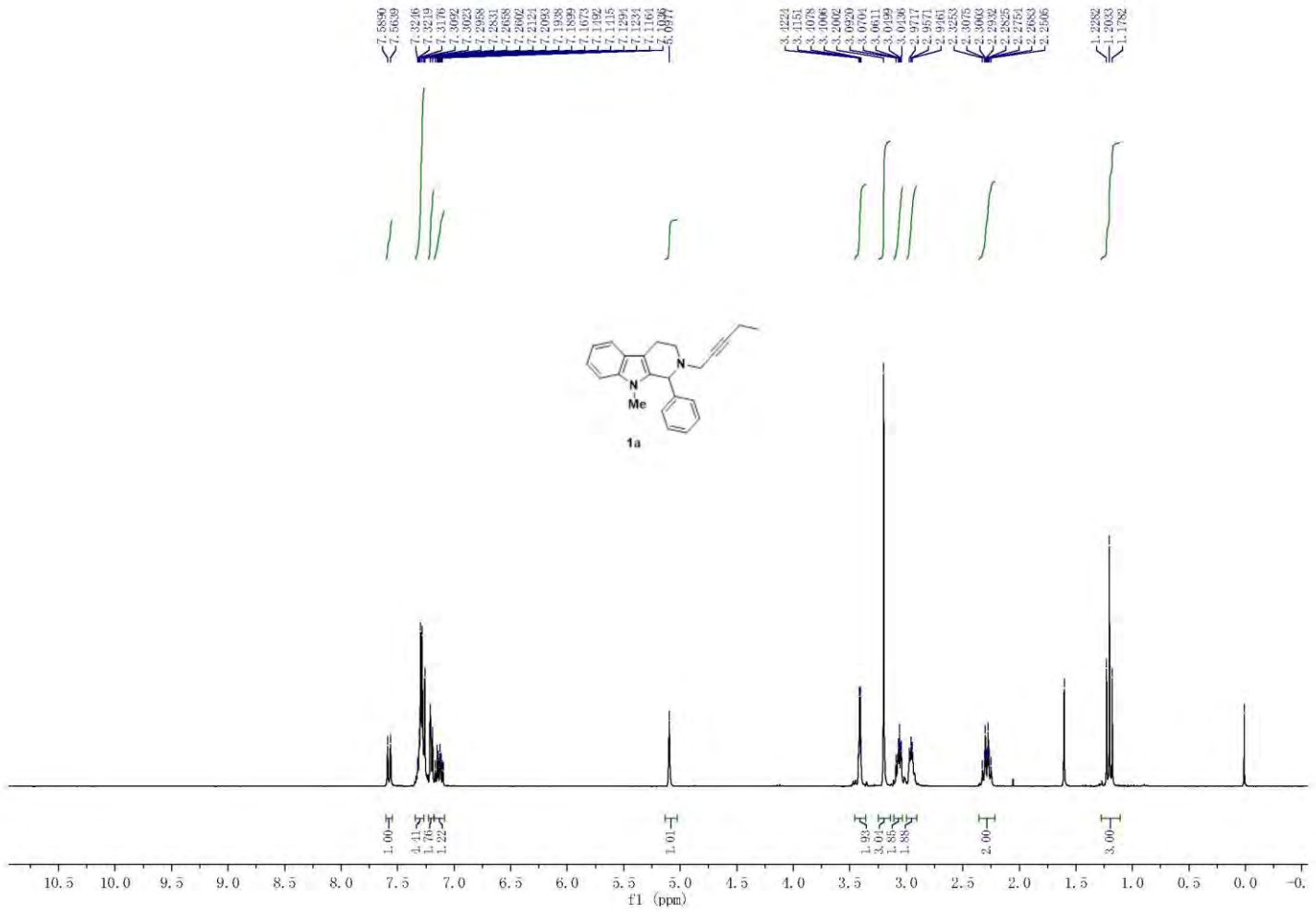
Au	−1.68409000	−1.46621700	0.00991300
S	−0.91565100	4.59981700	−0.13358200
P	−3.98380300	−1.86895700	0.00716400
O	0.41998600	4.53003000	0.58629600
O	−1.73181600	3.37049600	0.10032000
O	−0.76708000	4.97267400	−1.56276300
N	3.40902300	−0.44961000	−1.35282300
N	1.67315200	2.17255300	0.61807000
C	−1.77459900	5.95443200	0.68111900
C	0.44282100	−1.29322600	−0.00093500
C	0.78519300	−0.12989900	0.35735100
C	0.50280600	1.24390800	0.81678100
C	2.45330100	1.86256700	−0.65338200
C	1.58482200	2.11092300	−1.88780000
C	3.00869800	0.47694800	−0.41308200
C	3.32039000	−0.34801000	−2.80711300
C	3.89869000	−1.56454400	−0.67943900
C	4.40028400	−2.77430900	−1.18302800
C	4.84284500	−3.71800900	−0.26254700
C	4.79255600	−3.48110300	1.12963900
C	4.29342300	−2.28670700	1.62849300
C	3.83934100	−1.31283100	0.71802500
C	3.28221100	−0.00756700	0.87627100
C	3.09073000	0.78214000	2.13953100
C	2.58329000	2.19209600	1.82154100
C	−4.50893500	−2.98471500	1.36469500
C	−5.01088700	−0.36153000	0.19532200
C	−4.57802200	−2.66993700	−1.53154100
H	1.23859100	3.14771900	0.53067600
H	−2.75532800	6.07969300	0.21522200
H	−1.89190000	5.71883300	1.74150300
H	−1.18707600	6.86803200	0.56187900
H	0.99885400	−2.18033100	−0.28420300
H	0.24941200	1.26068100	1.87980700
H	−0.34736100	1.66419700	0.26571500
H	3.26817800	2.59502300	−0.65295700
H	0.81108700	1.35080300	−2.02374700
H	1.10738600	3.09209000	−1.80769500
H	2.21295200	2.13086700	−2.77987600
H	3.89370100	−1.16513800	−3.24422500
H	2.28392200	−0.42094300	−3.14924400
H	3.75718200	0.59155800	−3.15113700
H	4.44386000	−2.97950100	−2.24752600
H	5.23644300	−4.66329500	−0.62578200
H	5.15002900	−4.24606800	1.81285500
H	4.25467700	−2.10124200	2.69826200
H	2.39997100	0.26384000	2.81545200
H	4.03920200	0.87106200	2.68191400
H	2.00979700	2.62064600	2.64527100
H	3.39896900	2.87220100	1.56912900
H	−4.24976600	−2.53737200	2.32939200
H	−5.59122500	−3.15058400	1.32175700
H	−3.99165500	−3.94486700	1.27276100
H	−4.81113400	0.32419500	−0.63400300
H	−6.07389600	−0.62703600	0.19934800
H	−4.75943500	0.14158100	1.13419200
H	−4.05617900	−3.62115500	−1.67601200
H	−5.65618300	−2.85558800	−1.47056400
H	−4.37024300	−2.02145800	−2.38844400

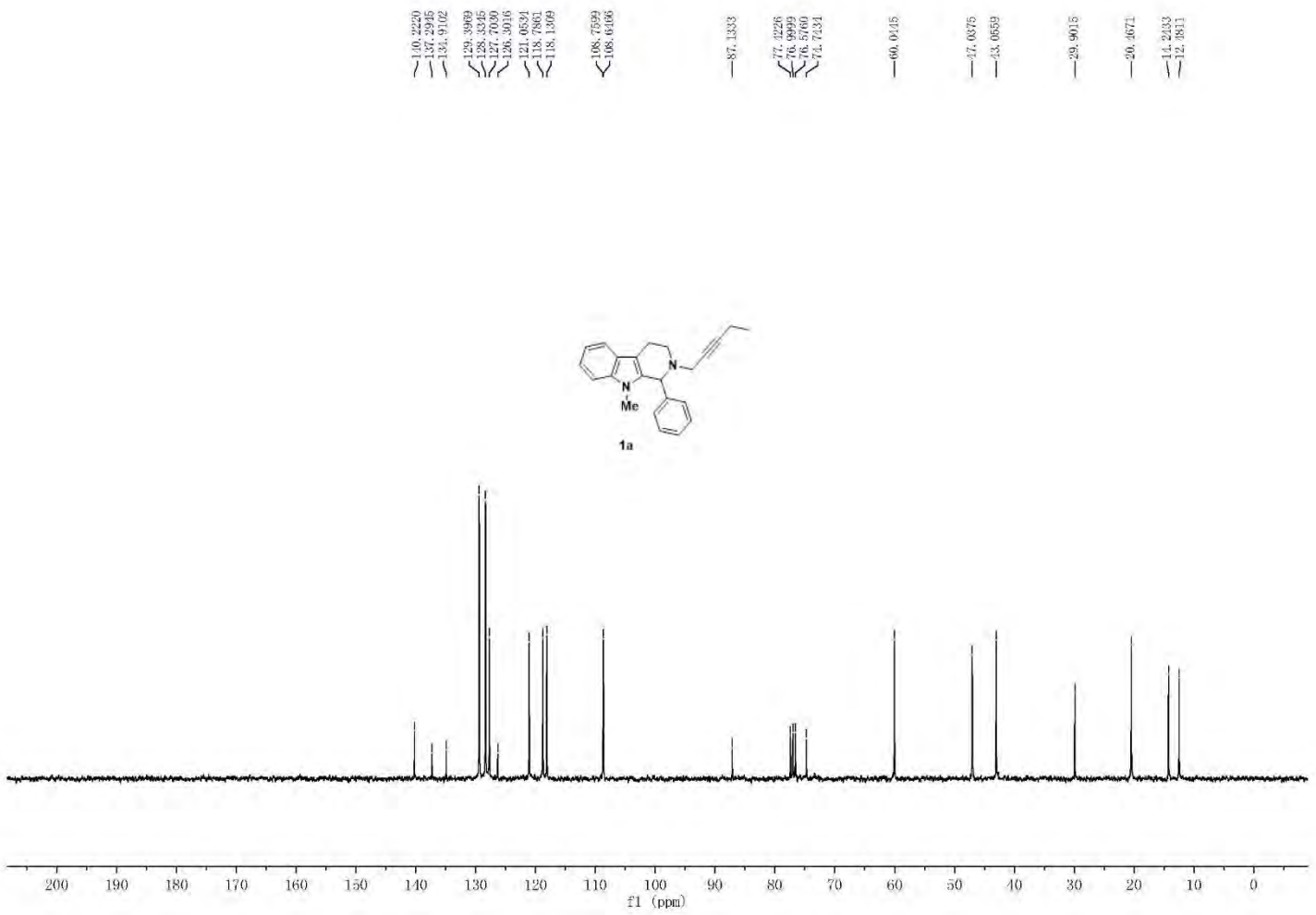
TS38

Au	2.64122300	−0.41317000	0.04126700
S	−4.56770800	−3.17456700	−0.06747200
P	4.91385100	−0.92647800	−0.09728000
O	−3.05824200	−3.26796800	0.10553600
O	−5.03535200	−1.77086200	0.13512600
O	−5.03516800	−3.81728100	−1.31674700
N	−2.15515000	2.47719700	−1.29788400
N	−1.88626600	−0.89686800	0.41452100

C	−5.23436300	−4.13742200	1.29964900
C	0.46178800	1.10885700	0.05226000
C	0.50626400	−0.13546600	0.21287800
C	−0.42284600	−1.27294400	0.42621700
C	−2.35618200	−0.03738400	−0.76292200
C	−1.81628500	−0.61166300	−2.07756700
C	−2.06490100	1.41034600	−0.42640400
C	−2.47214400	2.44184200	−2.72325400
C	−1.94185500	3.64943100	−0.57664900
C	−1.91457200	4.98215600	−1.00917000
C	−1.70196200	5.96626500	−0.04772700
C	−1.51357800	5.64271400	1.31286700
C	−1.52802200	4.32022200	1.73894300
C	−1.74094700	3.30669100	0.78719300
C	−1.82061400	1.87584700	0.86781600
C	−1.85063800	1.00021000	2.08673700
C	−2.40776800	−0.37823900	1.73386300
C	5.67616900	−0.43909200	−1.69145700
C	5.25561600	−2.71933000	0.07659500
C	5.91999100	−0.10734700	1.19803000
H	−2.38721300	−1.83741500	0.27650700
H	−4.87802500	−5.16734400	1.21823600
H	−4.89959700	−3.69981900	2.24326700
H	−6.32596000	−4.11663900	1.24561800
H	0.75460100	2.12421500	−0.14073000
H	−0.23050000	−1.75901400	1.38611200
H	−0.27517300	−2.02301700	−0.35304900
H	−3.44201700	−0.19336600	−0.75479000
H	−0.75808400	−0.39197300	−2.24015200
H	−2.38558600	−0.20931400	−2.91616100
H	−1.96560400	−1.69606900	−2.08354400
H	−3.33424800	1.79659500	−2.90488800
H	−2.73504800	3.44975200	−3.04415600
H	−1.62037000	2.09480000	−3.31566100
H	−2.05417000	5.25099900	−2.05116500
H	−1.68089900	7.00830800	−0.35476200
H	−1.35434000	6.44036200	2.03310300
H	−1.38026600	4.07126900	2.78632100
H	−0.85973700	0.91255800	2.54703800
H	−2.50565700	1.43807000	2.84953000
H	−2.15569100	−1.12798900	2.48624100
H	−3.49298400	−0.35636500	1.61513100
H	5.56579200	0.63990300	−1.83819300
H	6.74102200	−0.69715100	−1.69481700
H	5.17413500	−0.95933400	−2.51321100
H	4.74163100	−3.27107600	−0.71670300
H	6.33315100	−2.90512300	0.00656500
H	4.89050000	−3.07390500	1.04555000
H	5.57232600	−0.42132100	2.18727700
H	6.97582600	−0.37628100	1.08296900
H	5.81223000	0.97874000	1.11600100

S4. ^{1}H and ^{13}C NMR Spectra of All New Compounds

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N
Me
1a
200
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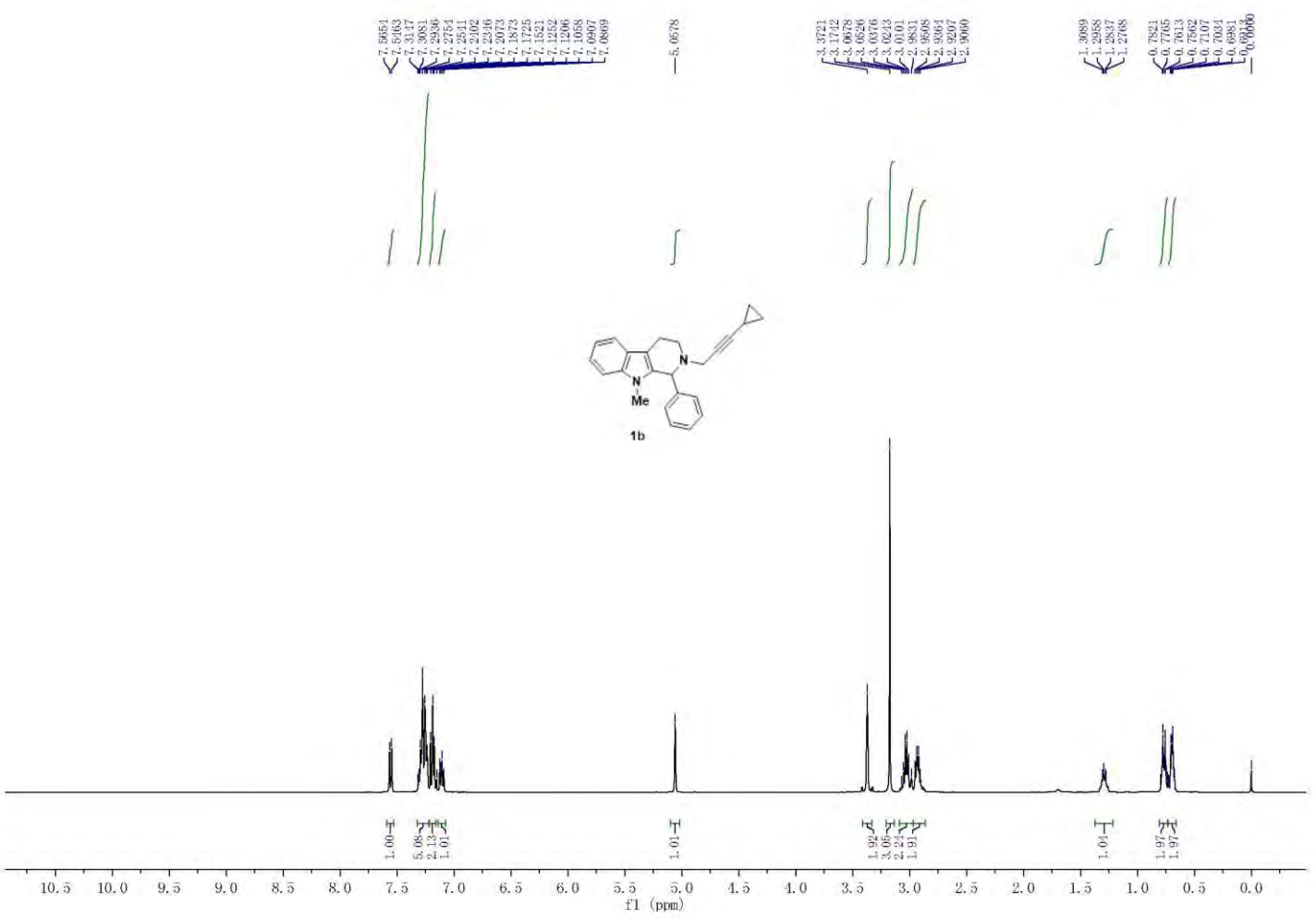
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3.1742
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2.9207
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1.2958
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1.2768
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Me
1b
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1.01
1.01
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3.05
2.21
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1.04
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6.0
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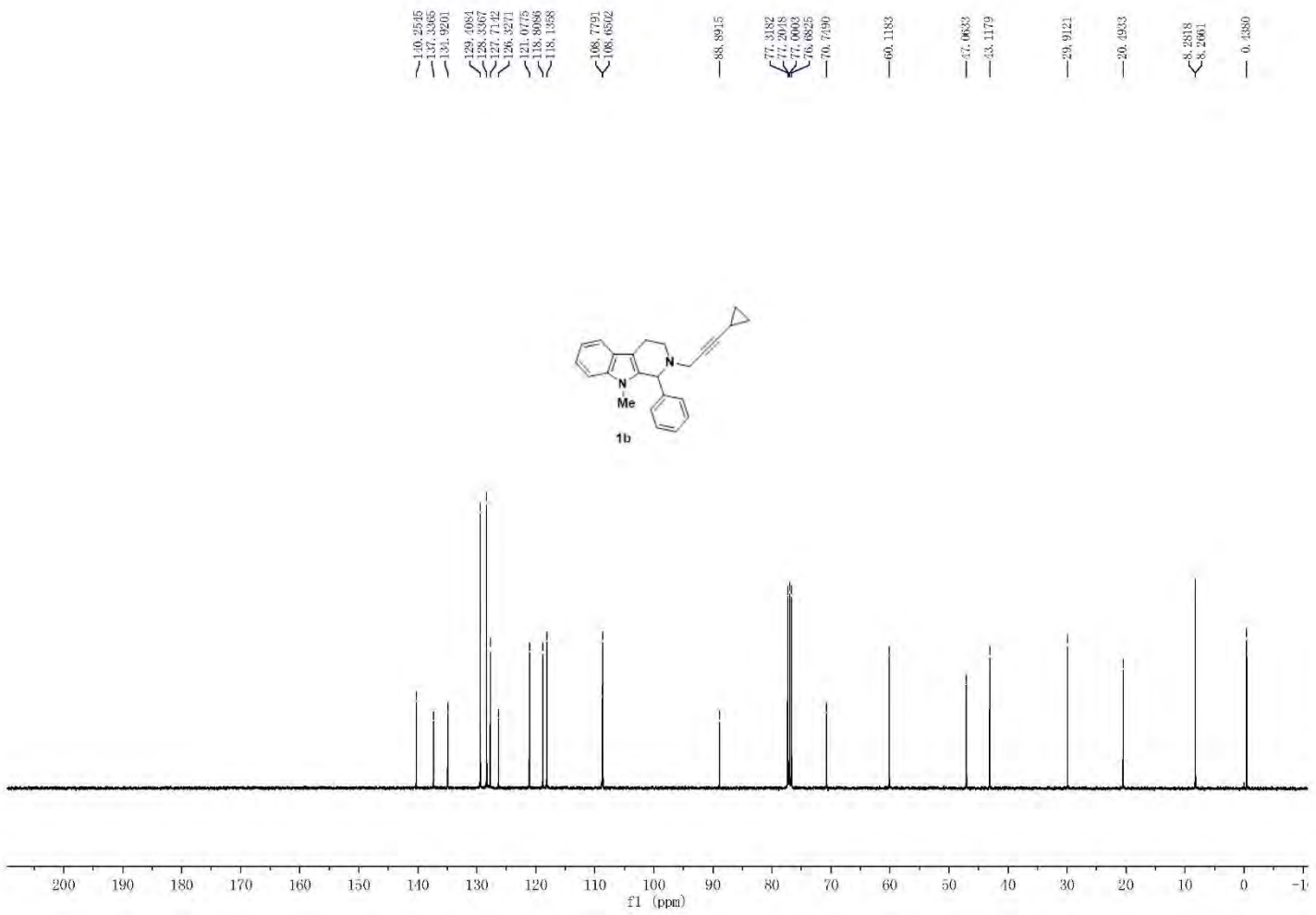
f1 (ppm)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76.8625
70.7790
60.1183
47.0633
43.1179
29.9121
20.4933
8.2818
8.2061
0.4380
N
N
Me
1b
200
190
180
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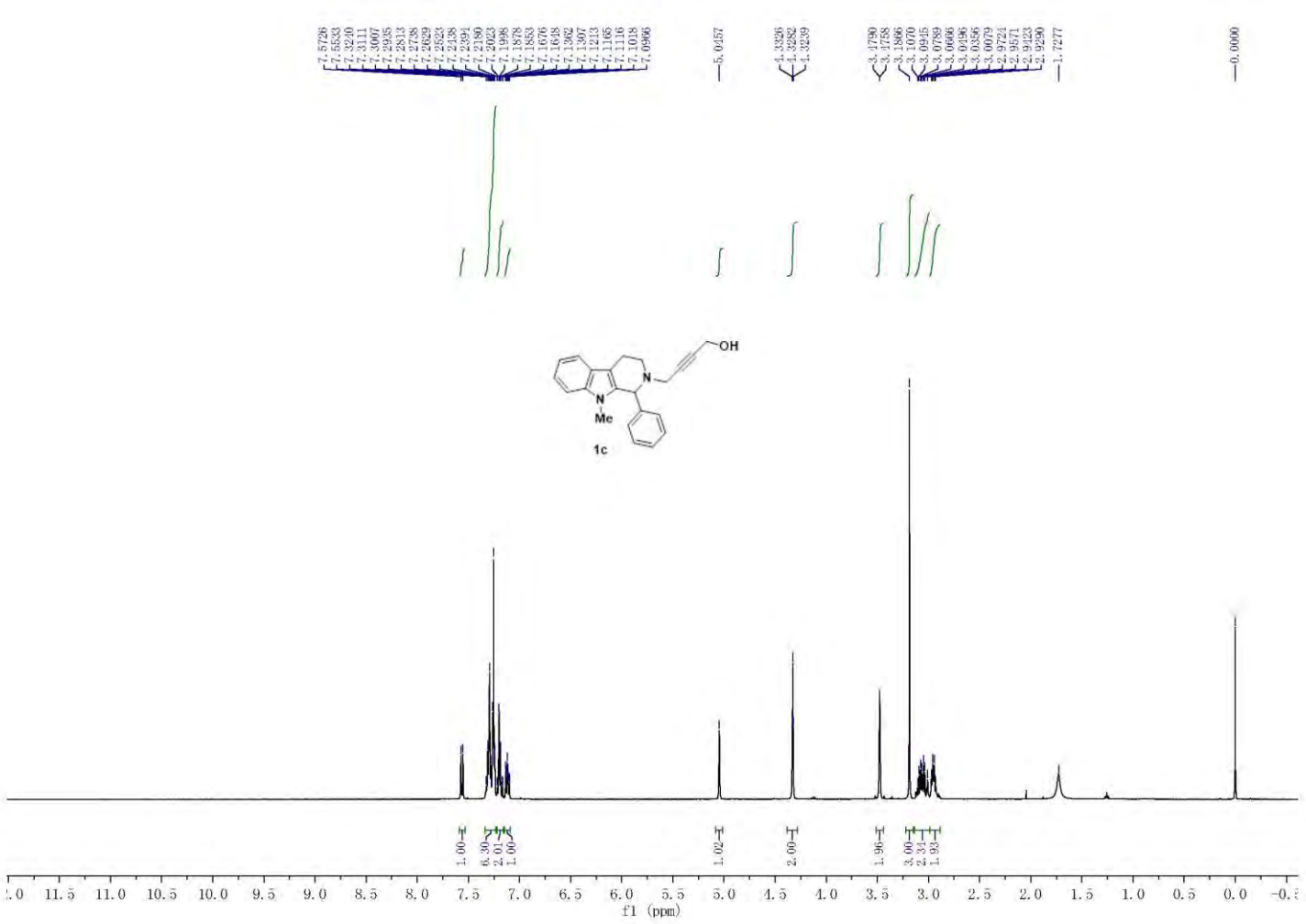
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7.2023
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7.1307
7.1213
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7.1116
7.1018
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4.3282
4.3239
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3.4758
3.1866
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2.9721
2.9571
2.9423
2.9290
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OH
N
N
Me
1c
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1.00
1.02
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3.00
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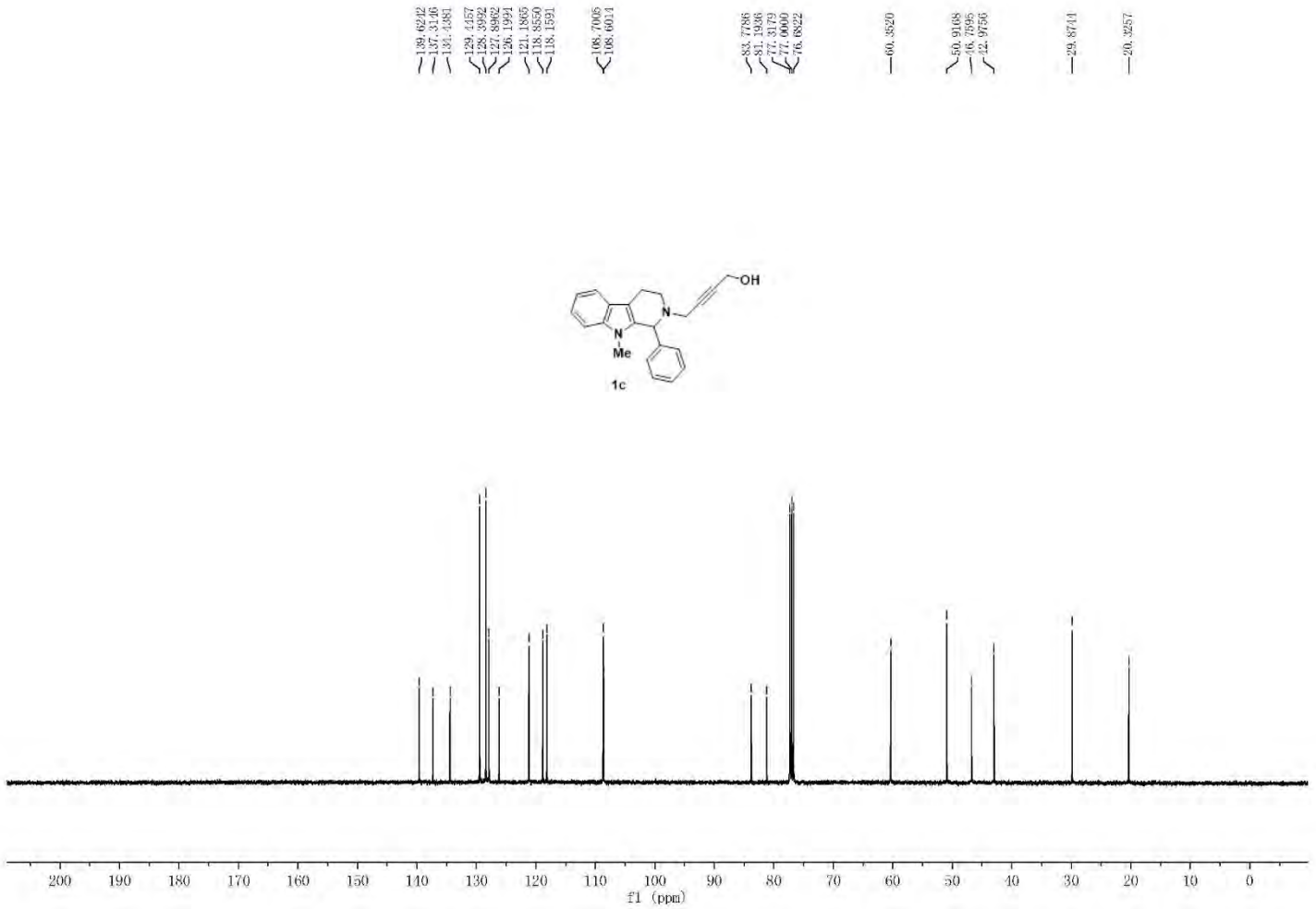
1.93
f1 (ppm)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OH
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N
Me
1c
200
190
180
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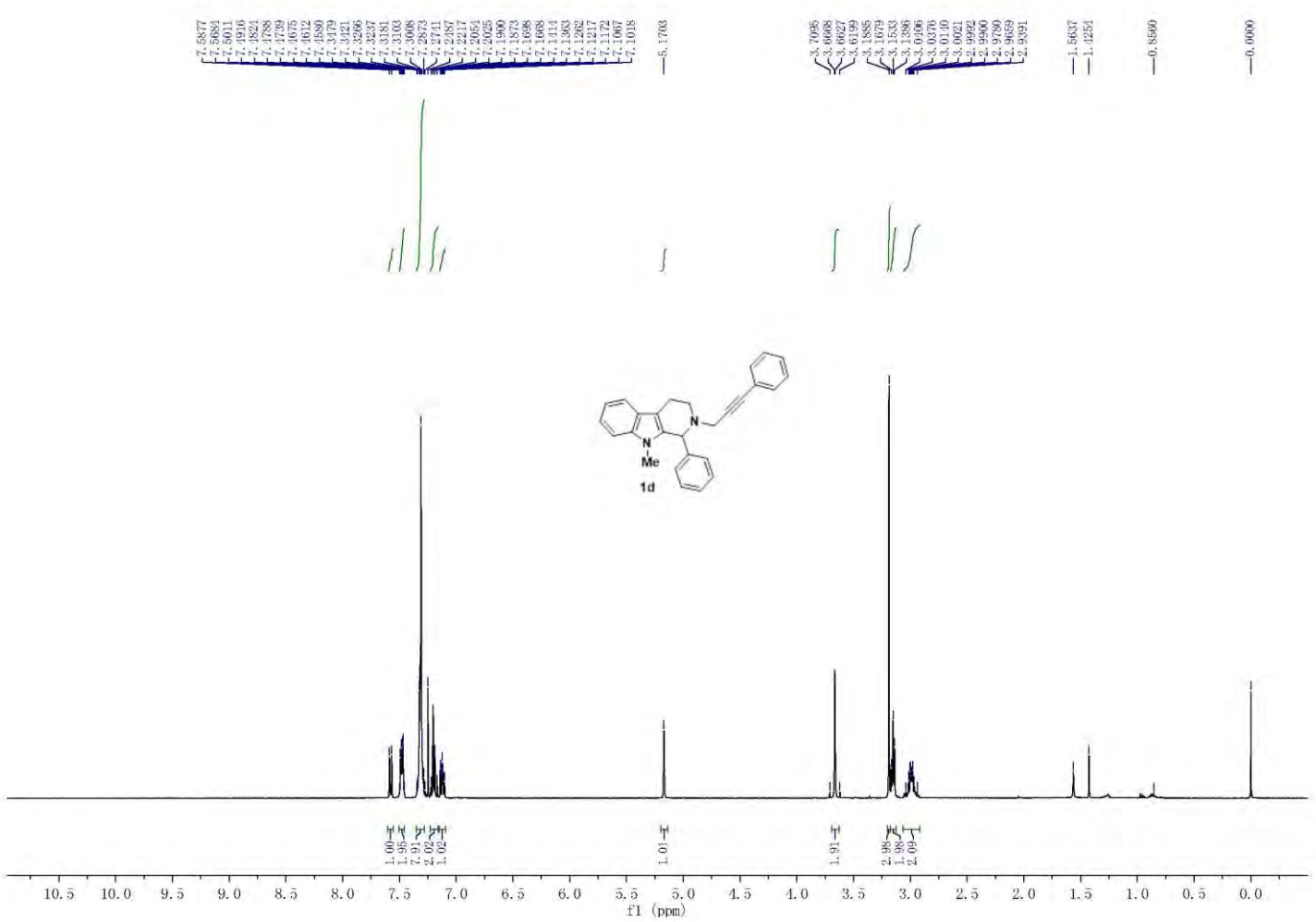
f1 (ppm)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7.3257
7.3181
7.3103
7.3008
7.2573
7.2711
7.2357
7.2217
7.2051
7.2025
7.1900
7.1873
7.1698
7.1668
7.1414
7.1363
7.1262
7.1217
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7.1067
7.1018
5.1703
3.7095
3.6668
3.6627
3.6199
3.1885
3.1679
3.1533
3.1398
3.0406
3.0376
3.0140
3.0021
2.9992
2.9960
2.9780
2.9659
2.9391
1.5637
1.4251
0.8560
0.0000
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N
Me
1d
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1.95
5.91
2.02
1.02
1.01
1.91
2.98
1.98
2.09
10.5
10.0
9.5
9.0
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8.0
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6.0
5.5
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2.0
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1.0
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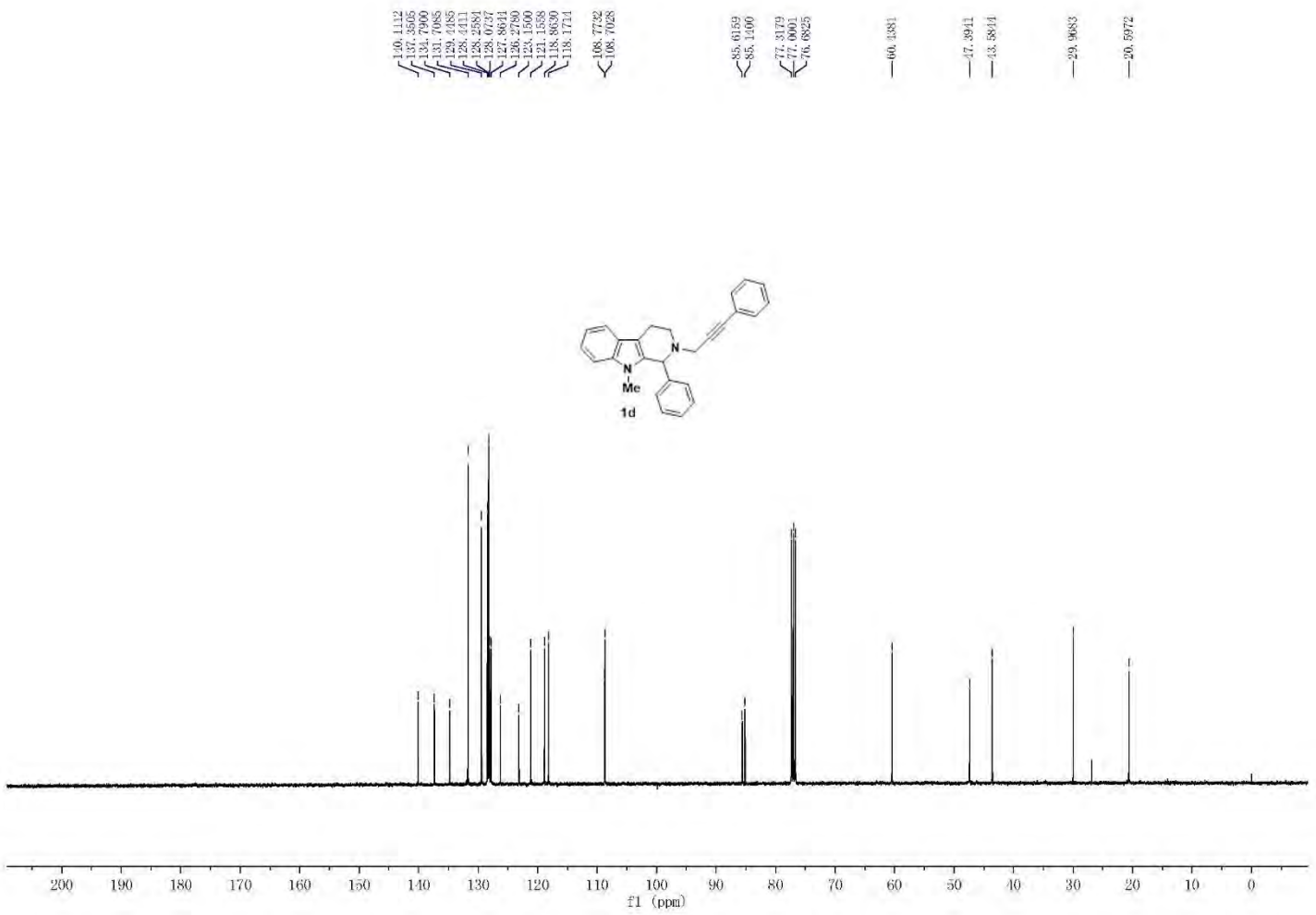
0.0
f1 (ppm)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108.7732
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85.6159
85.1200
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77.0001
76.6825
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47.3941
43.5844
29.9683
20.5972
Me
1d
200
190
180
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150
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130
120
110
100
90
80
70
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50
40
30
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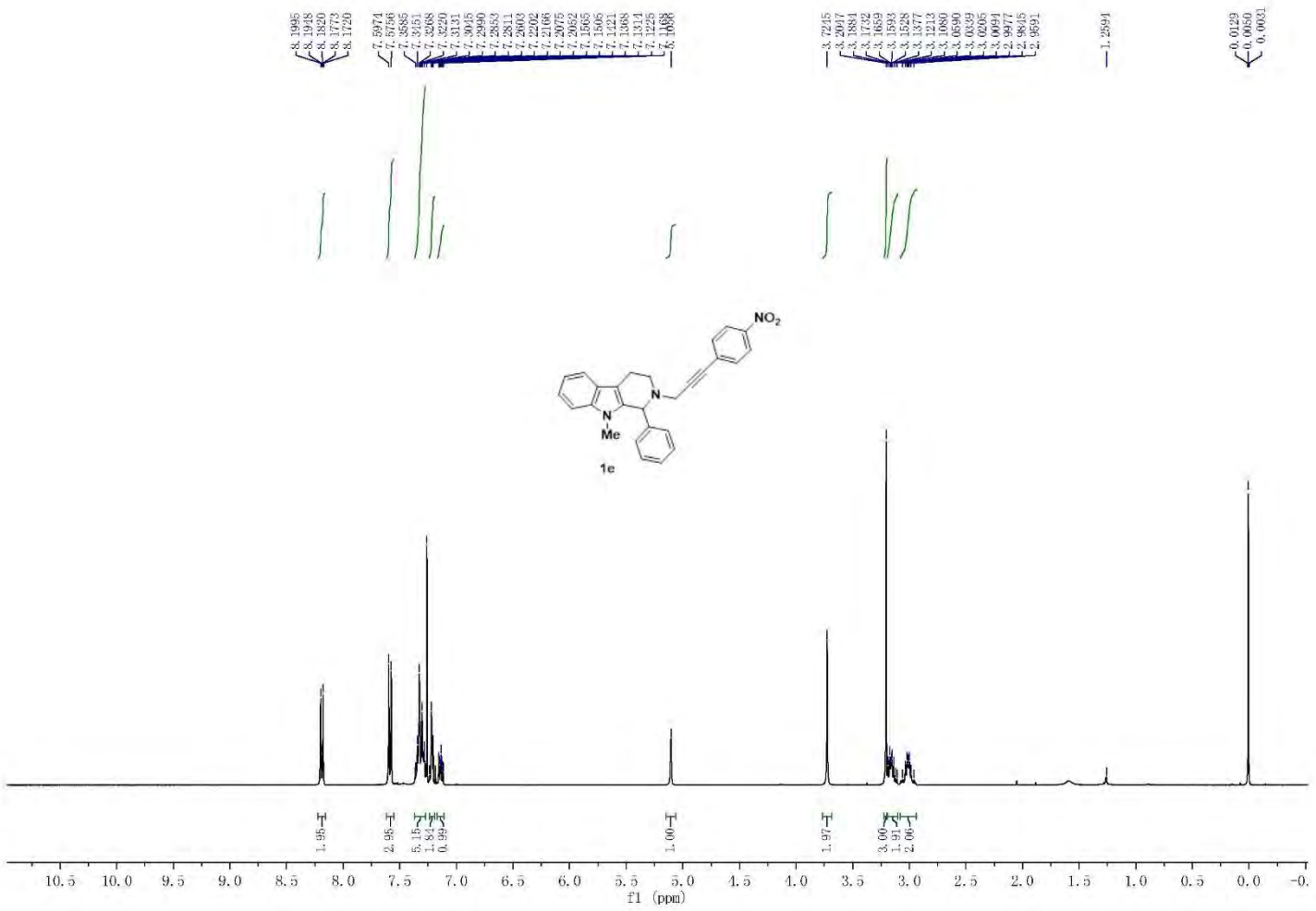
10
0
f1 (ppm)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7.3131
7.3045
7.2990
7.2853
7.2811
7.2603
7.2202
7.2166
7.2075
7.2052
7.1565
7.1505
7.1421
7.1368
7.1314
7.1225
7.1168
7.1088
3.7245
3.2047
3.1881
3.1732
3.1659
3.1593
3.1528
3.1377
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3.1080
3.0690
3.0339
3.0205
3.0094
2.9977
2.9845
2.9691
1.2594
0.0129
0.0050
0.0031
NO2
N
N
Me
1e
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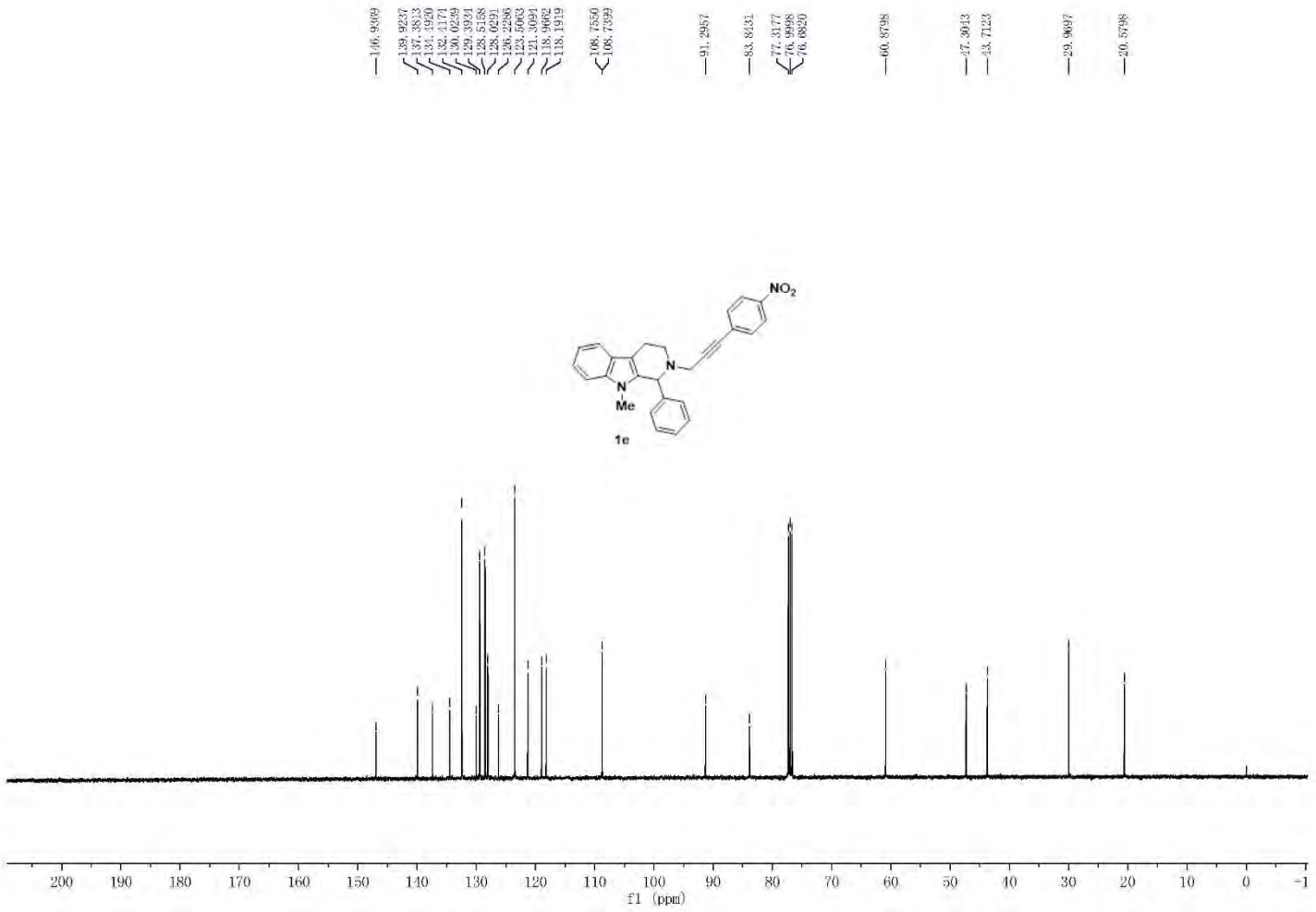
2.95
5.15
1.84
0.99
1.00
1.97
3.60
1.91
2.06
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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91.2957
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76.9998
76.6820
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47.3013
43.7123
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20.5798
NO2
N
N
Me
1e
200
190
180
170
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120
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100
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80
70
60
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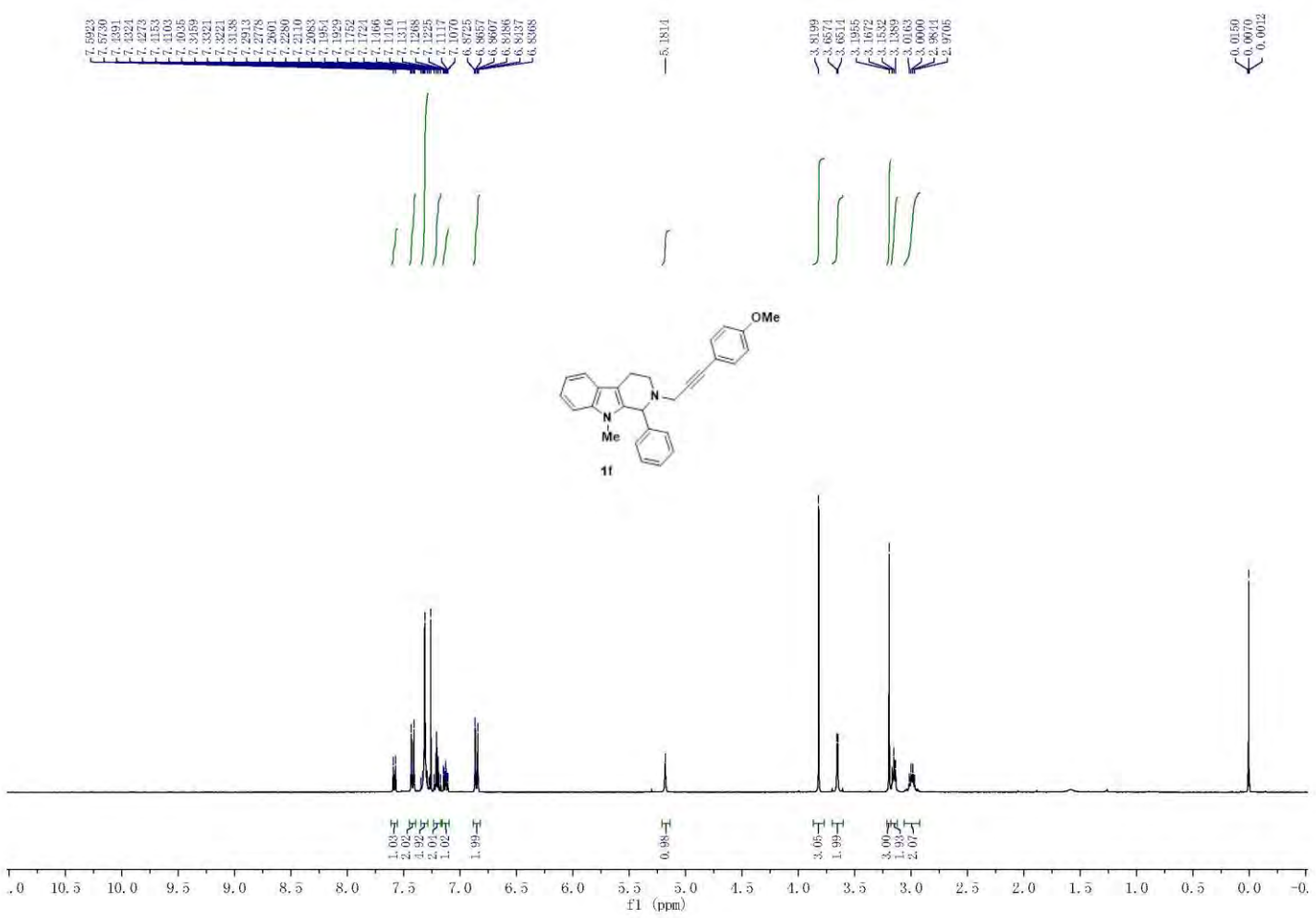
40
30
20
10
0
-1
f1 (ppm)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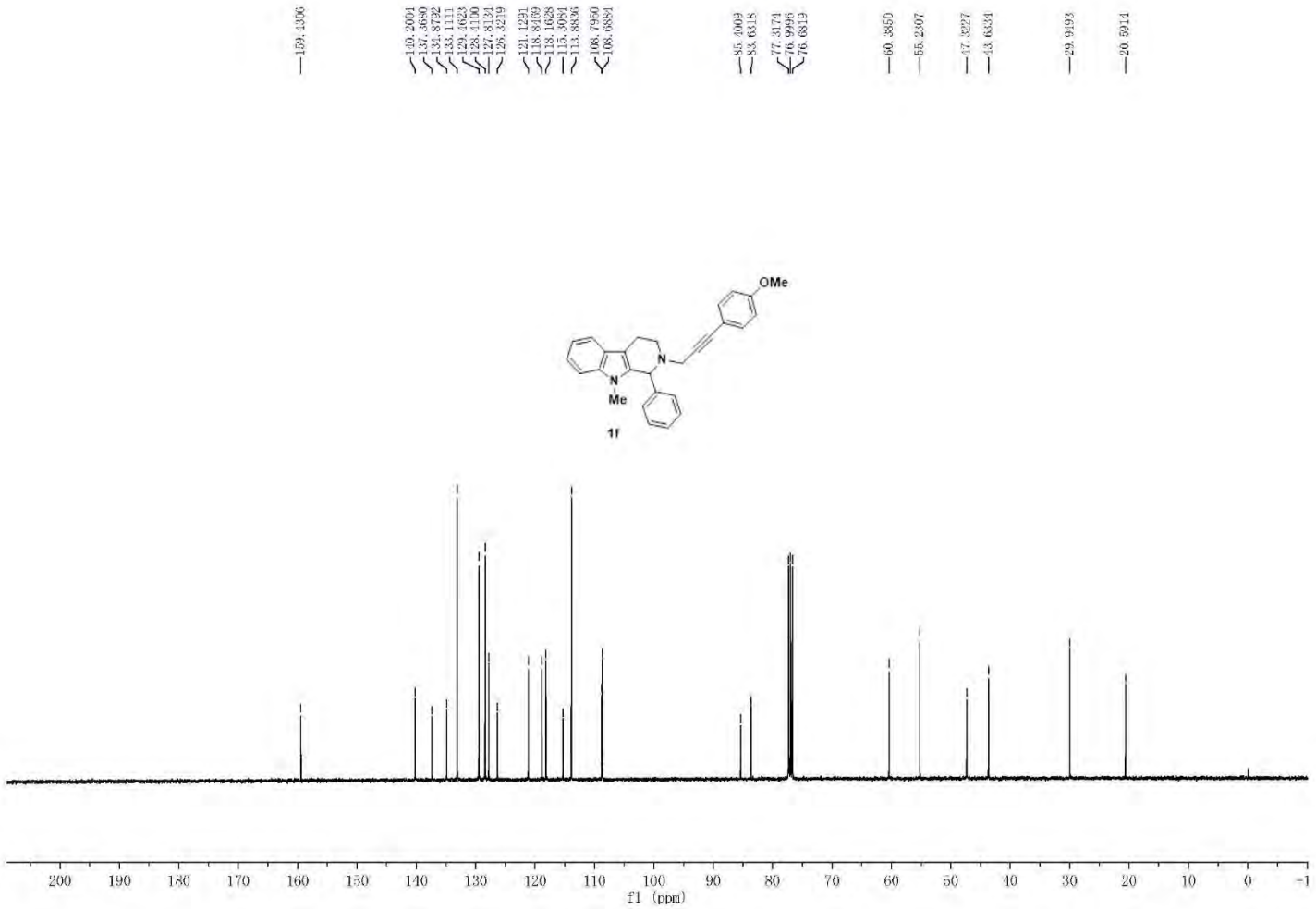
N
Me
1f
f1 (ppm)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76.9996
76.6819
60.3850
55.2307
47.3227
43.6834
29.9193
20.6914
OMe
N
N
Me
1f
200
190
180
170
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120
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100
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80
70
60
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40
30
20
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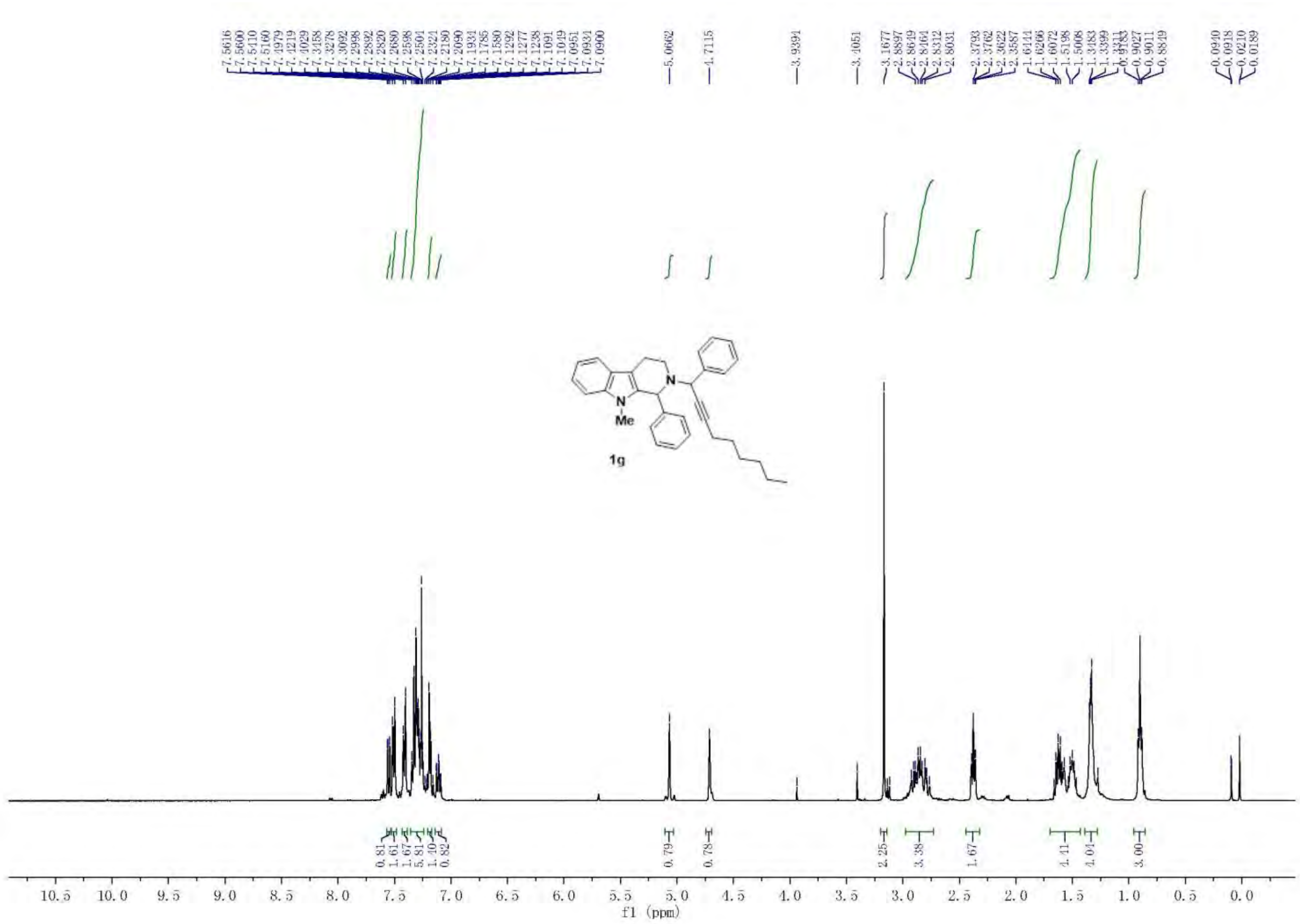
-1
f1 (ppm)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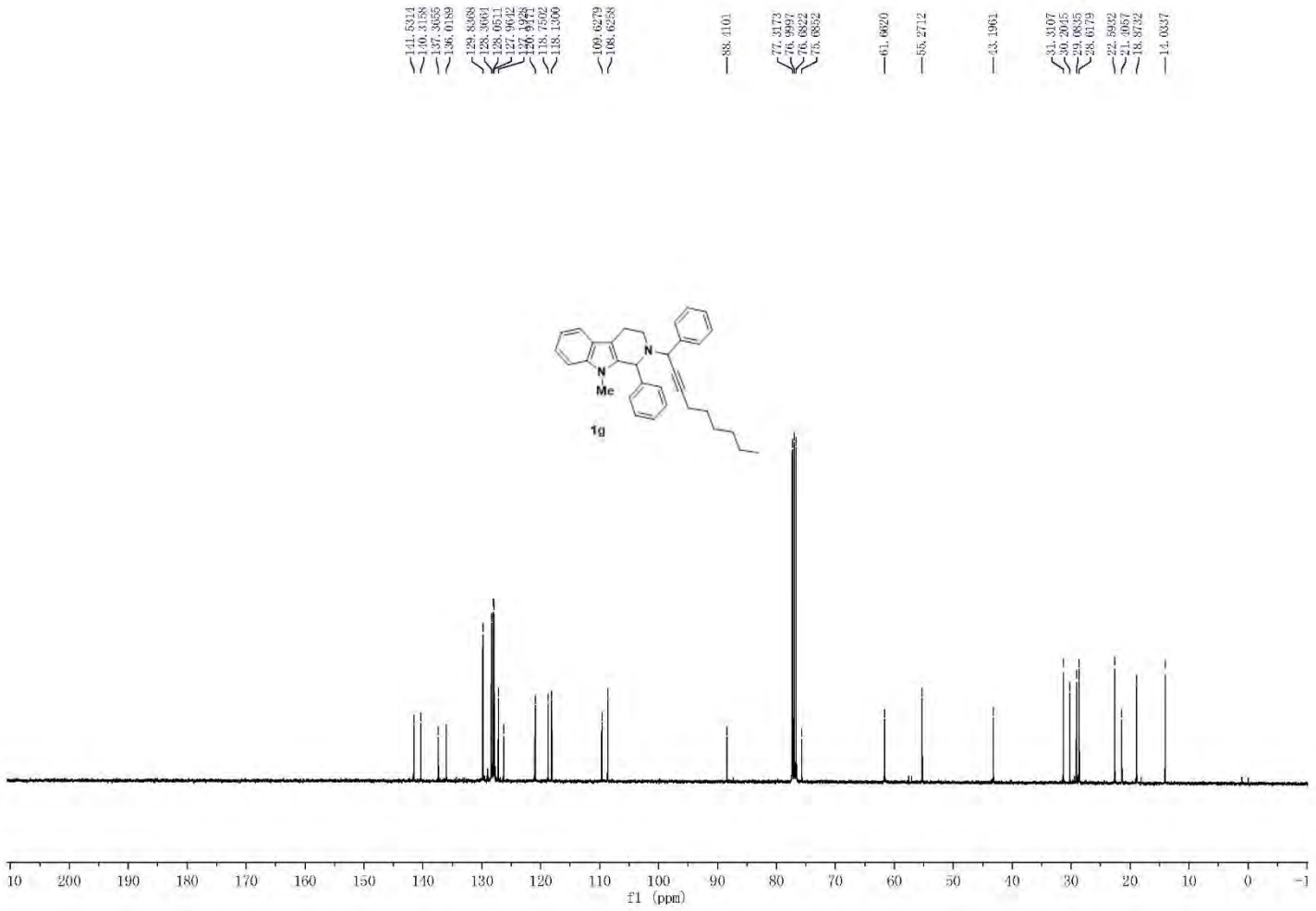
Me
1g
f1 (ppm)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31.3107
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21.3057
18.8732
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N
N
Me
1g
10
200
190
180
170
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100
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80
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40
30
20
10
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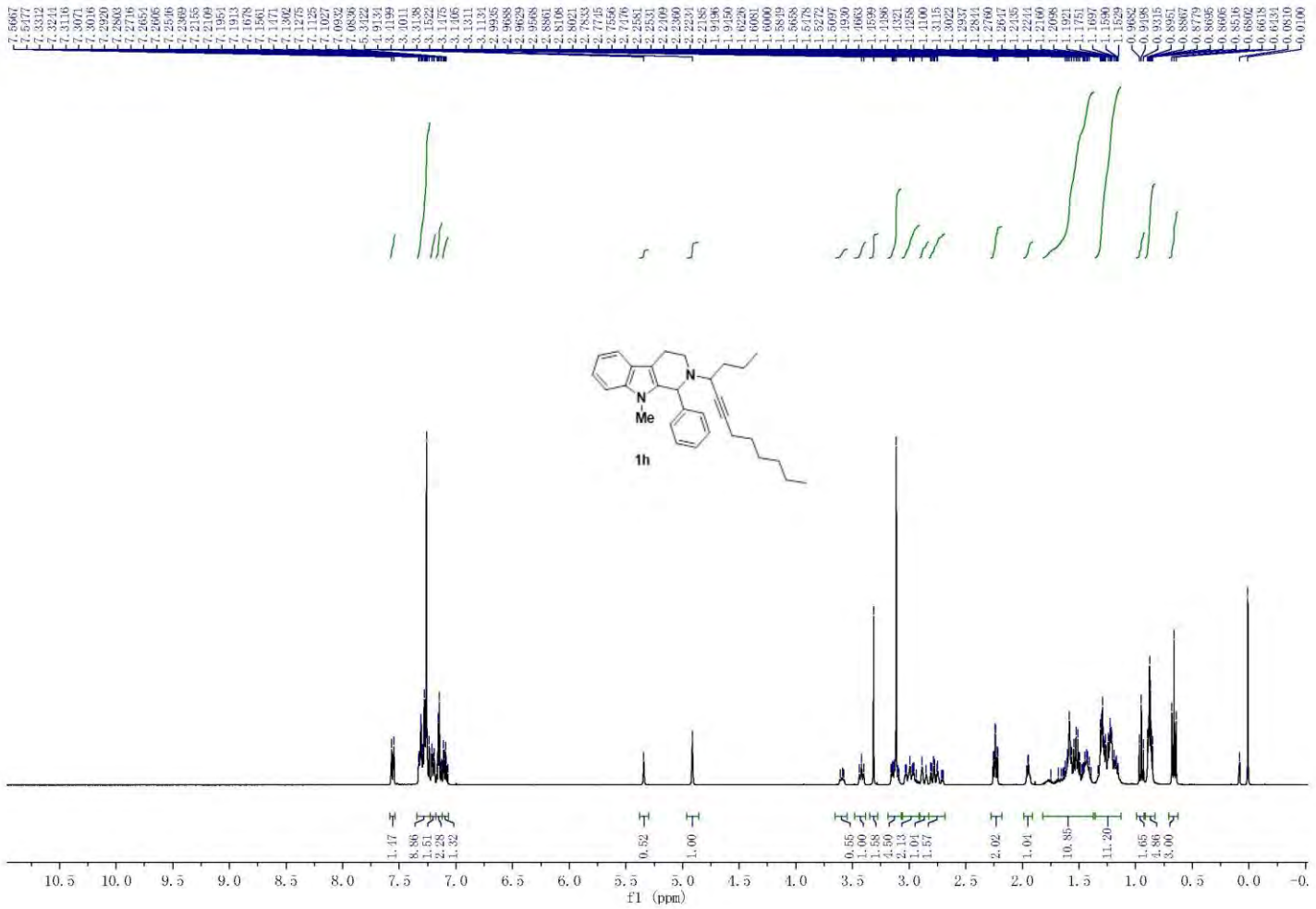
-1
f1 (ppm)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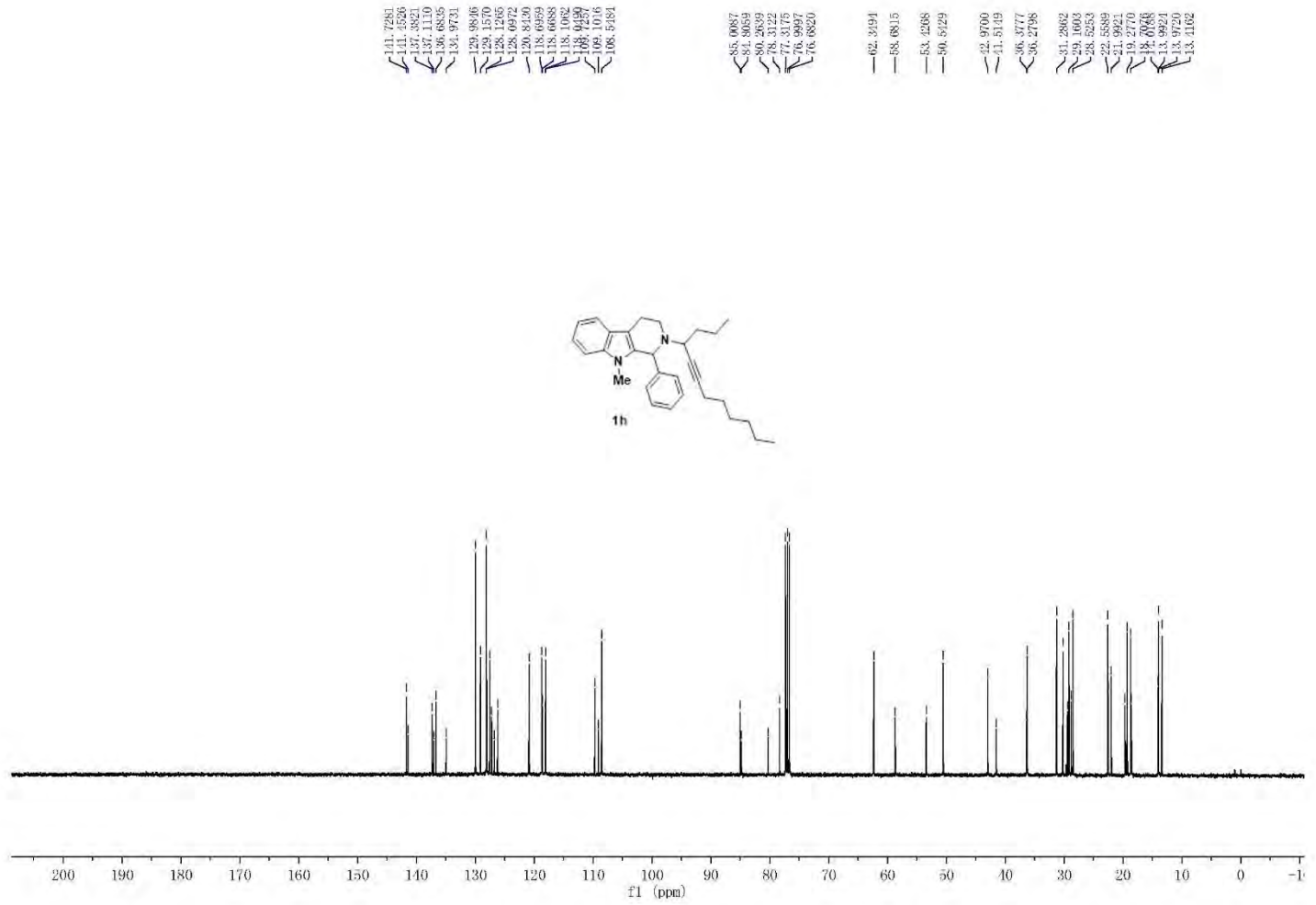
Me
1h
f1 (ppm)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36.2798
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29.1603
28.5253
22.5589
21.9921
19.2770
13.9921
13.9720
13.2162
N
N
Me
1h
200
190
180
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110
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90
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50
40
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20
10
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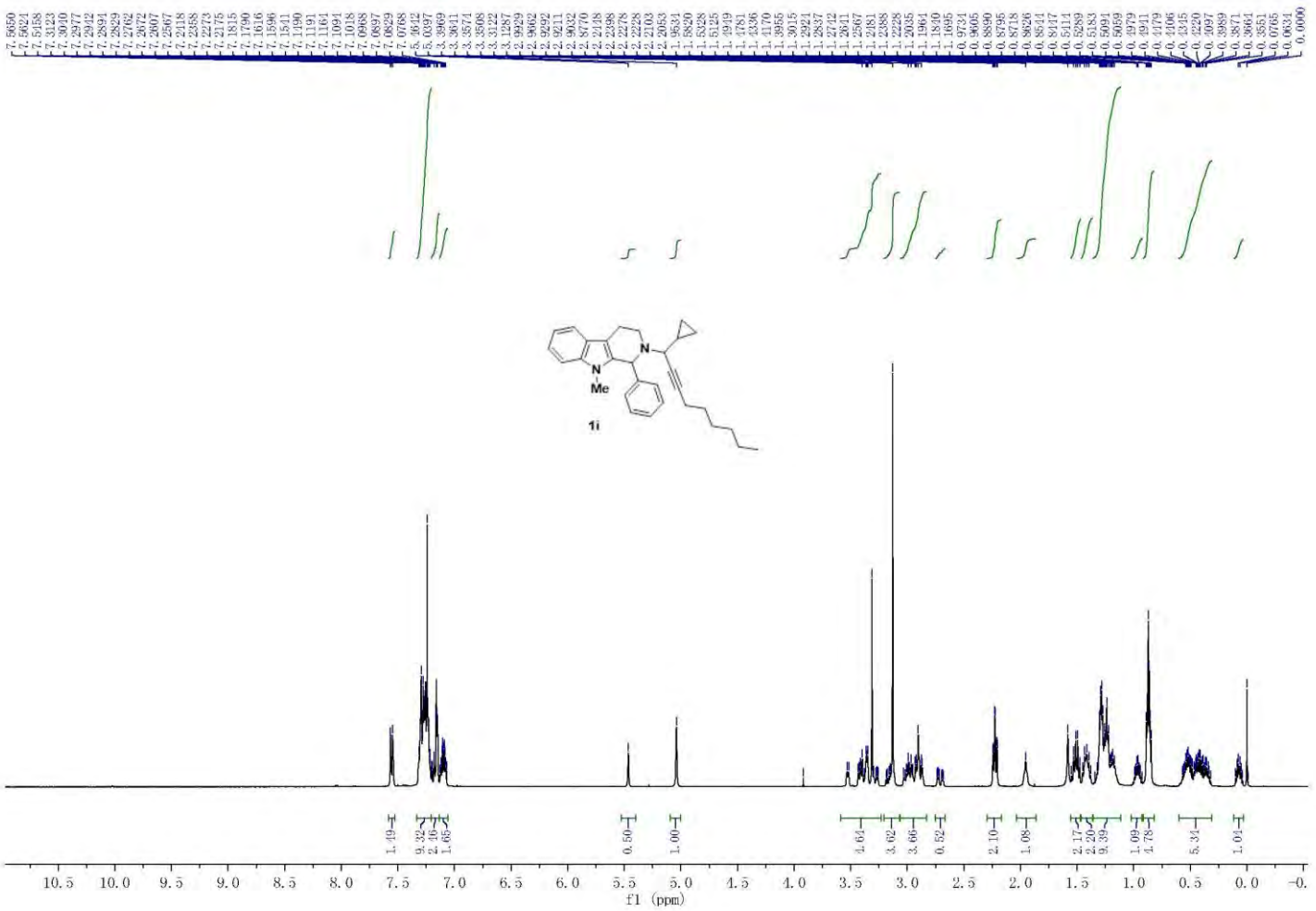
f1 (ppm)


Me
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2.17
2.20
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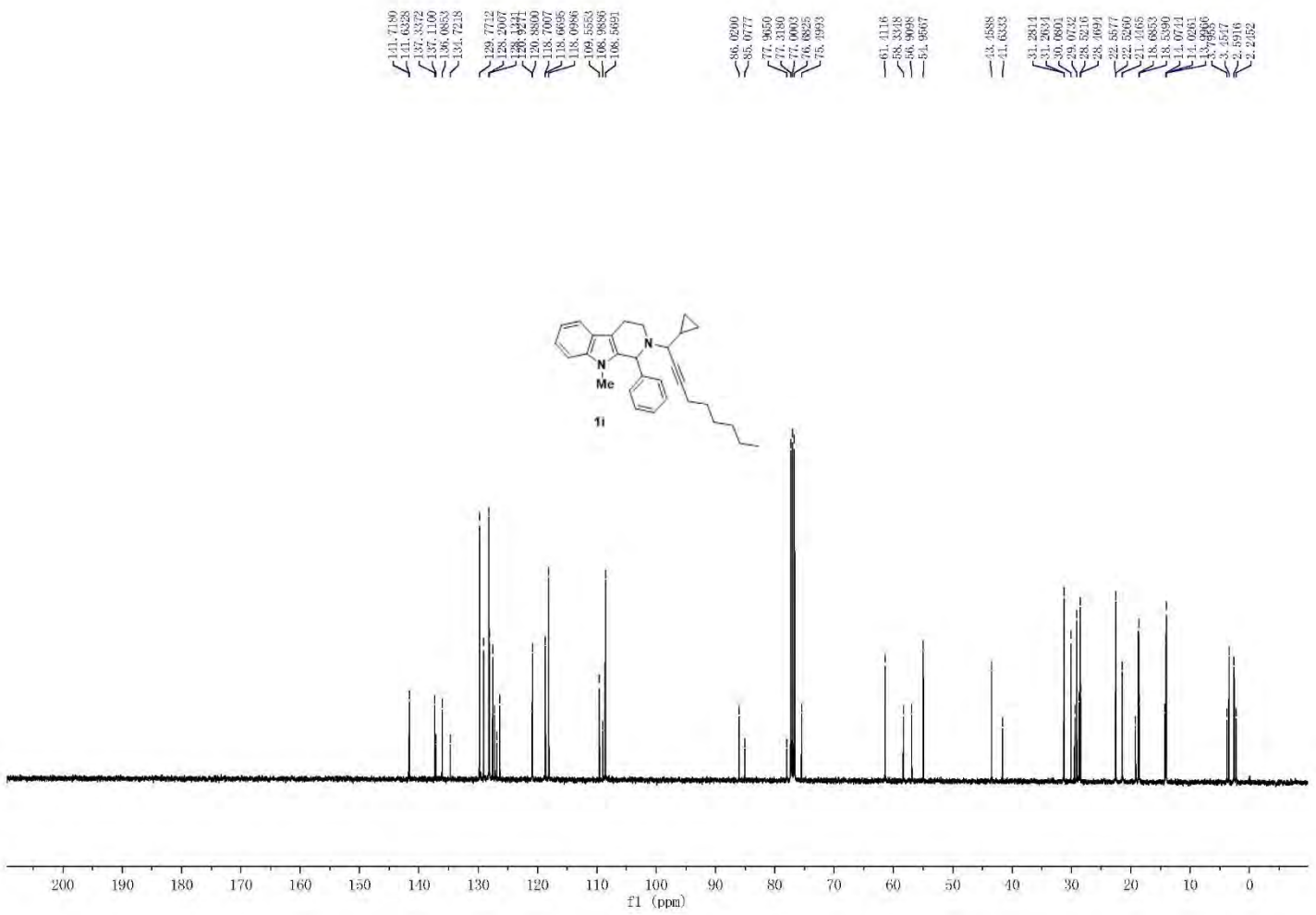
4.78
5.34
1.01
f1 (ppm)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3.4567
3.1917
2.6916
2.2452
N
N
Me
1i
200
190
180
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150
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130
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110
100
90
80
70
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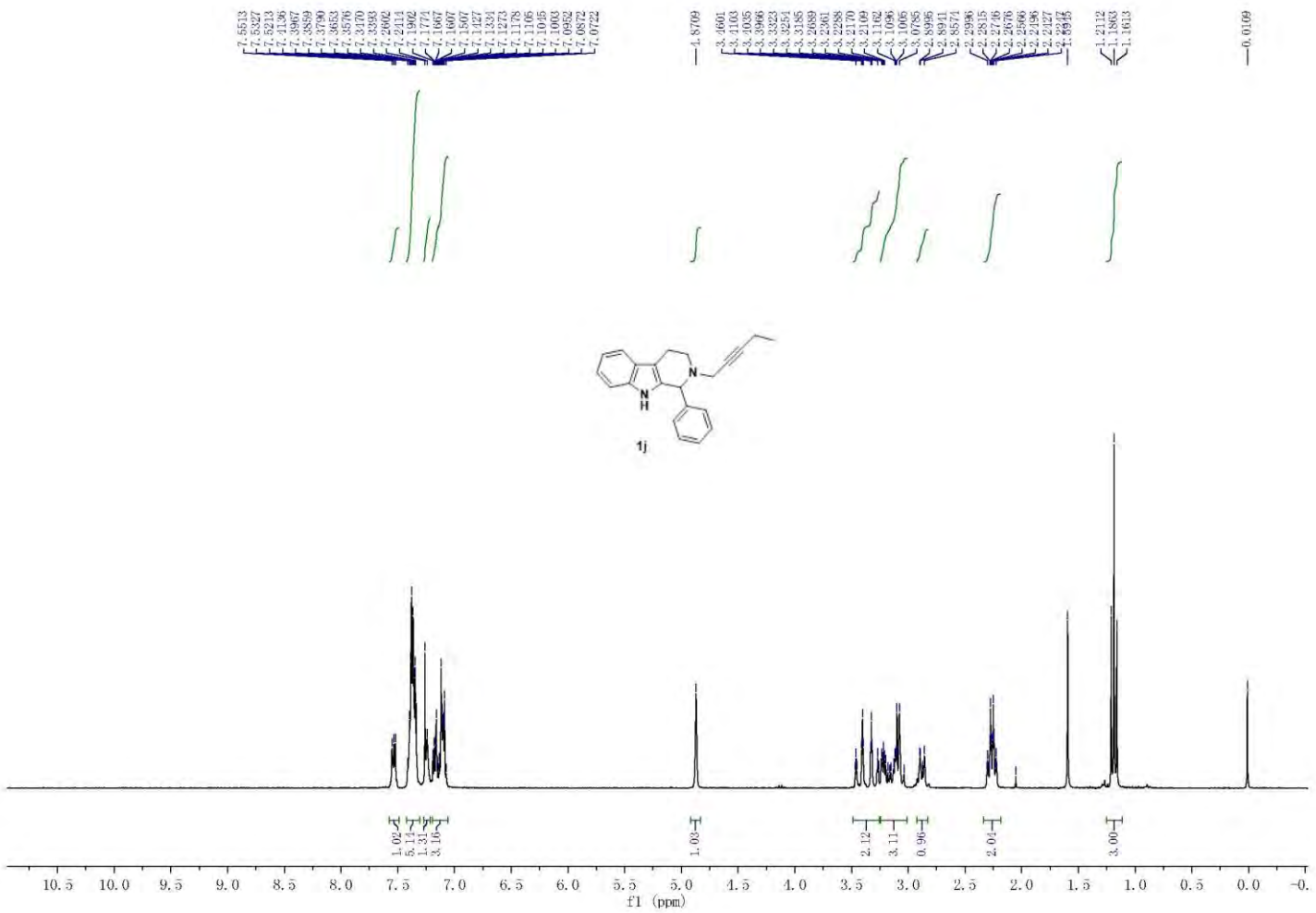
50
40
30
20
10
0
f1 (ppm)


1j
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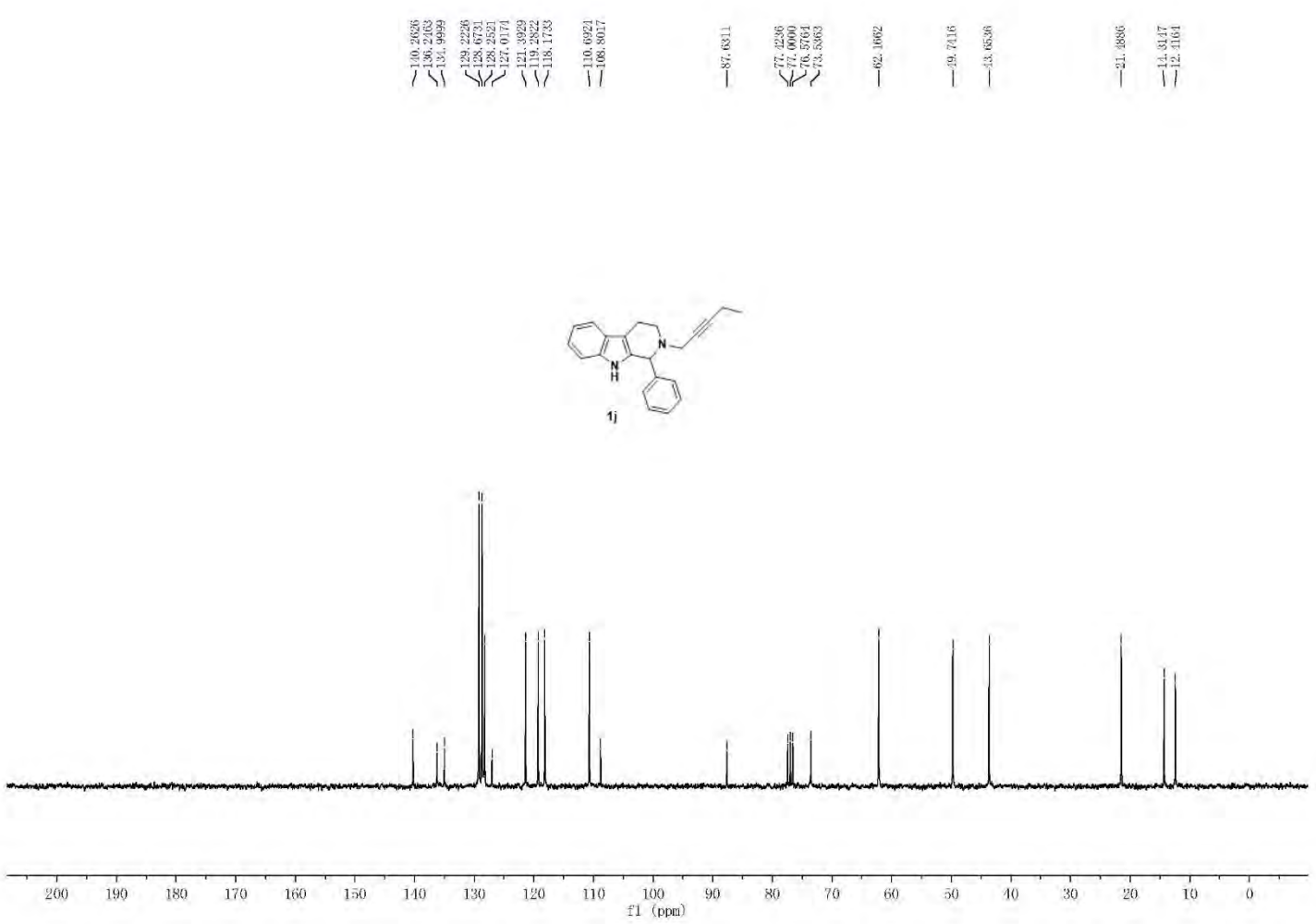
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77.4236
77.0000
76.5764
73.5363
62.1662
39.7416
43.6536
21.0886
11.3147
12.2164
1j
200
190
180
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150
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130
120
110
100
90
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50
40
30
20
10
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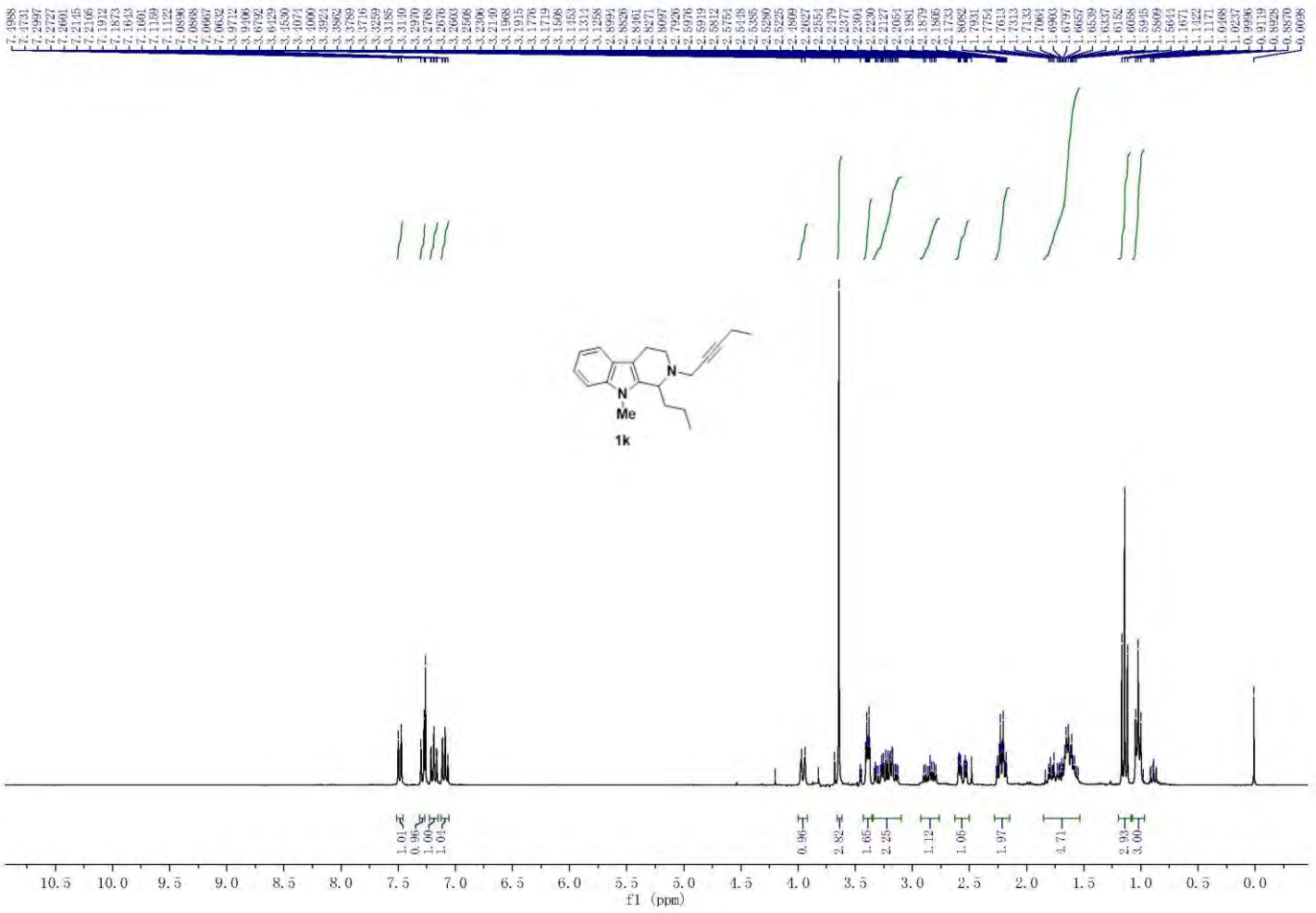
f1 (ppm)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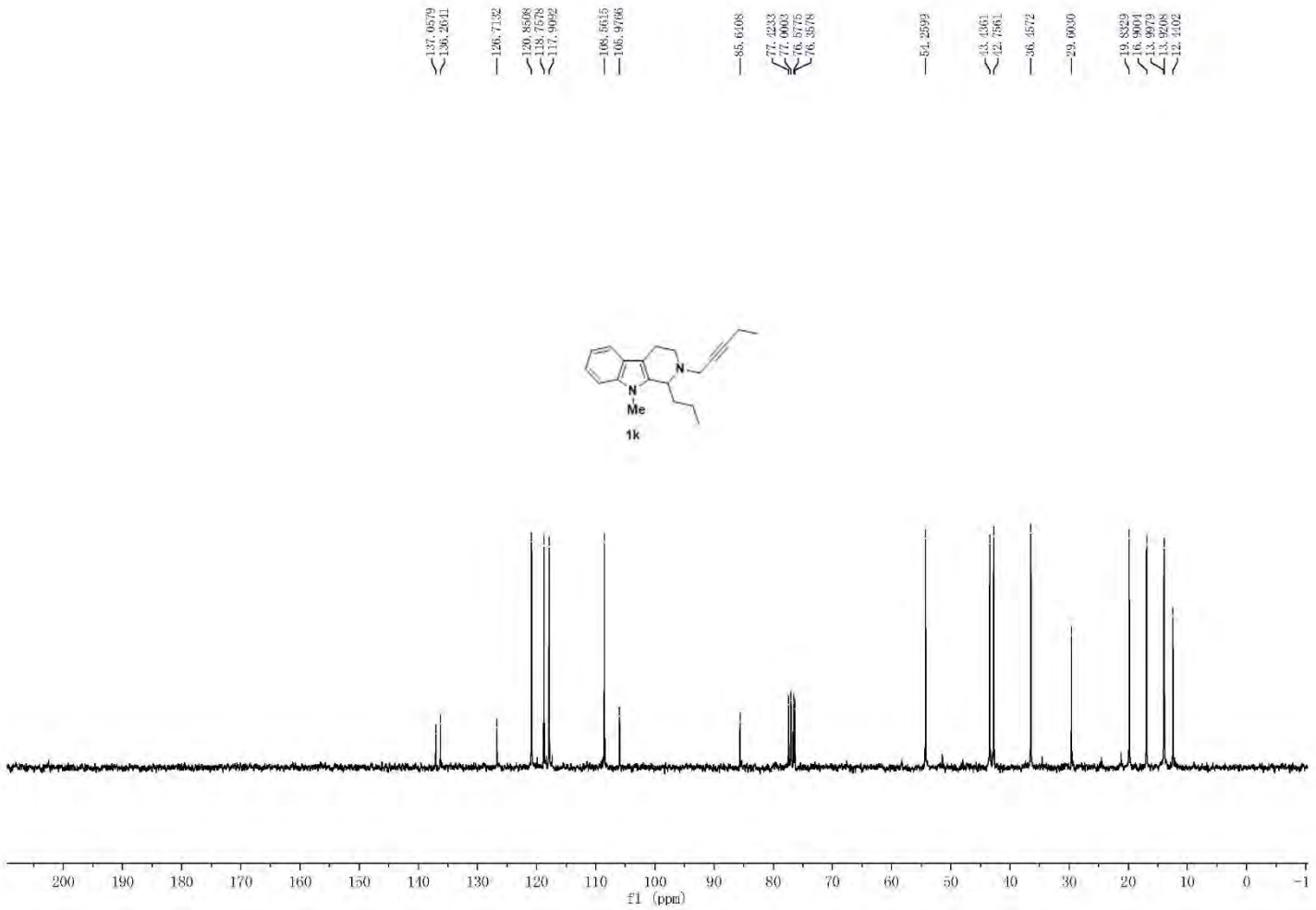
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29.6030
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13.9208
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Me
1k
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190
180
170
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100
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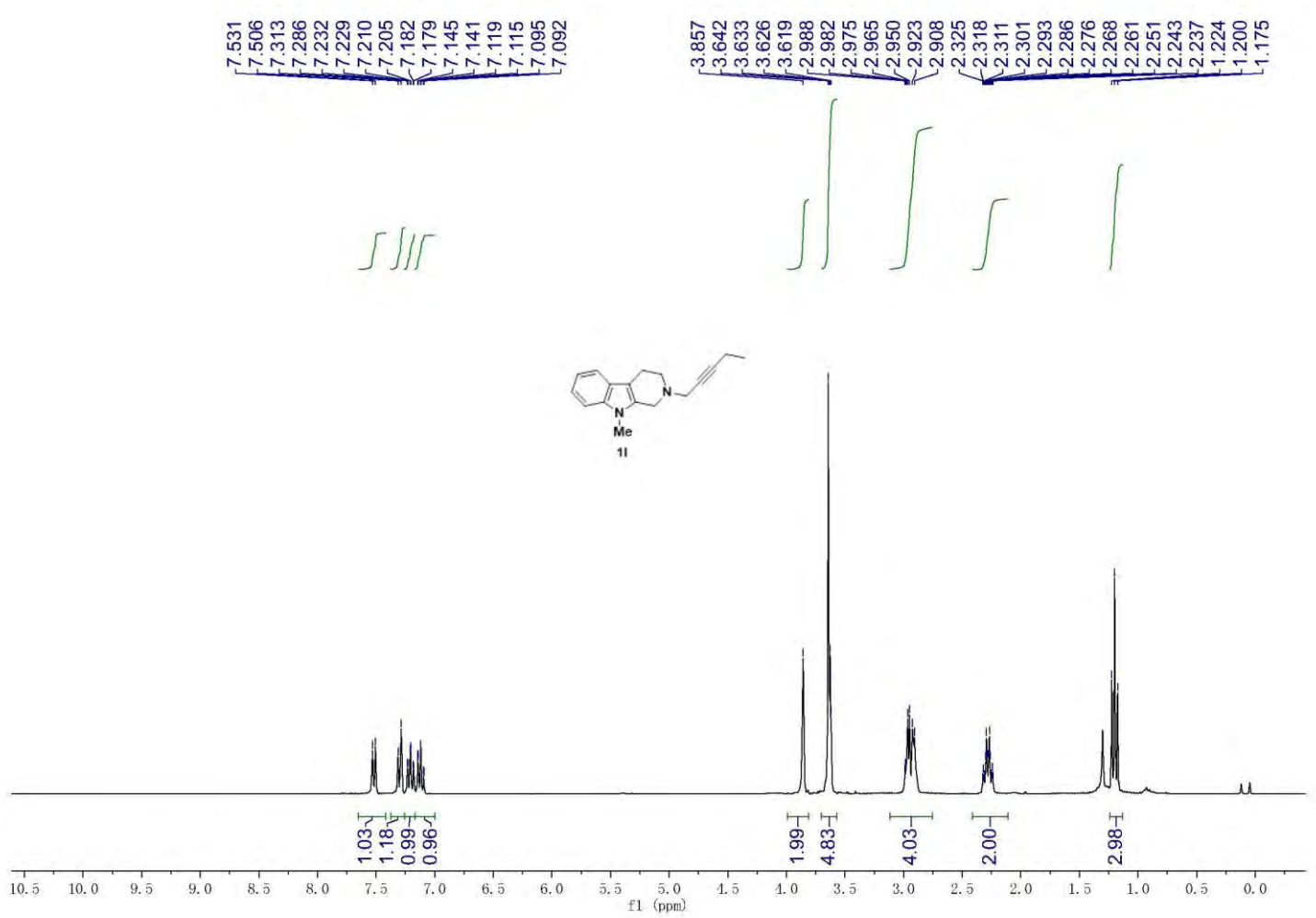
f1 (ppm)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7.141
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7.115
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7.092
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3.642
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3.626
3.619
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2.982
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2.965
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2.261
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2.237
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1.200
1.175
N
N
Me
1l
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1.18
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0.96
1.99
4.83
4.03
2.00
2.98
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
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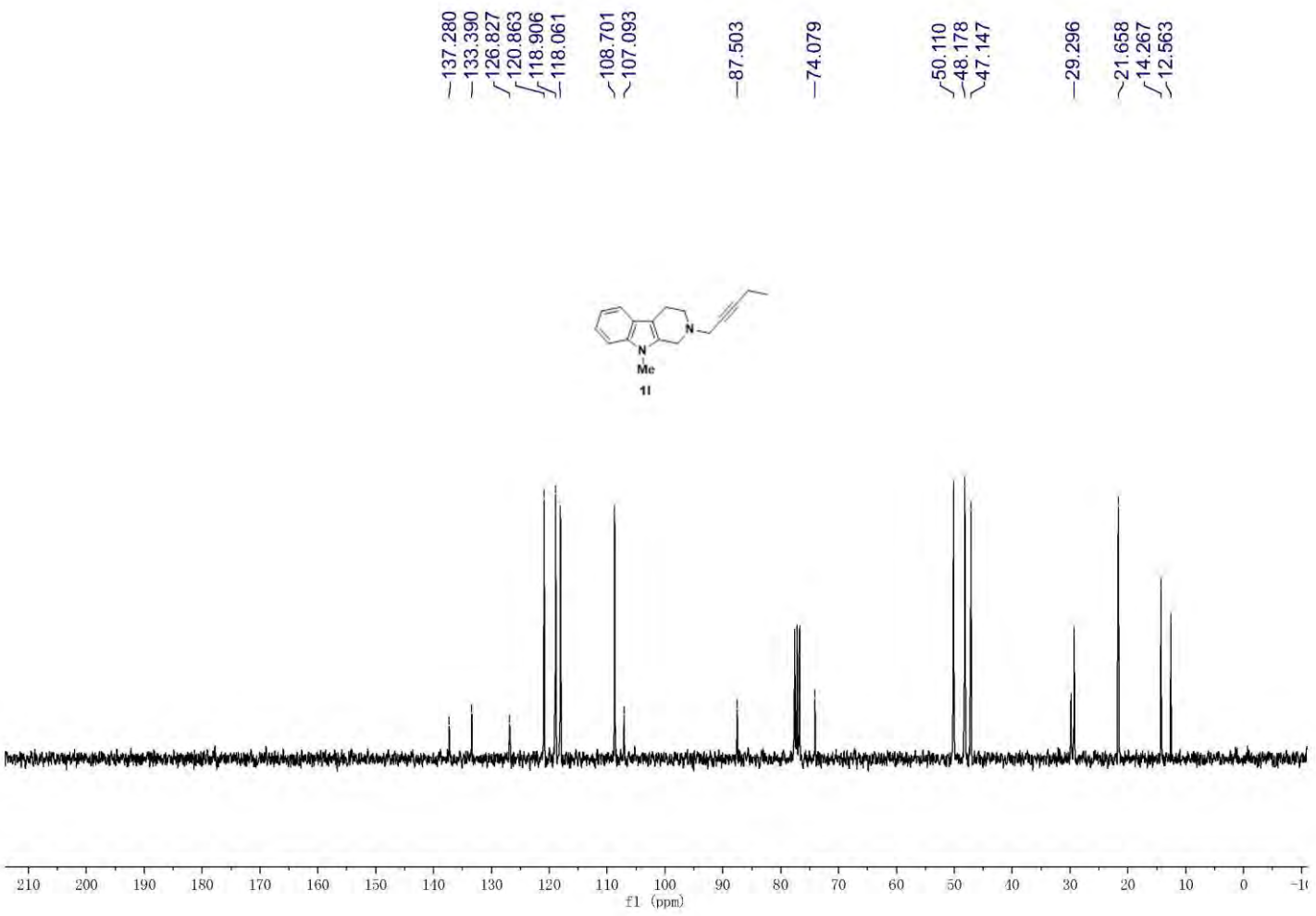
3.0
2.5
2.0
1.5
1.0
0.5
0.0
f1 (ppm)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29.296
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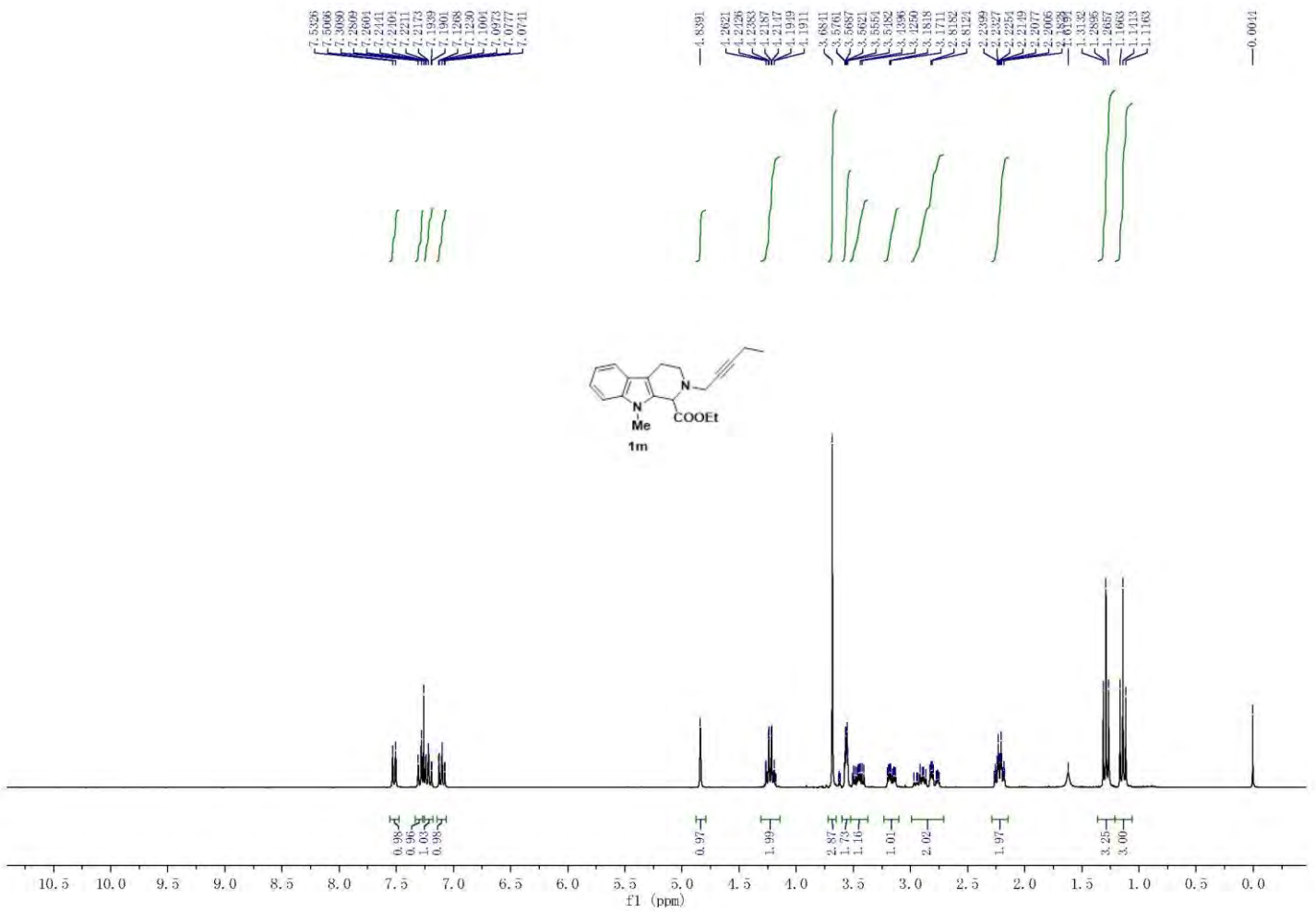
Me
1l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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7.2173
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7.1268
7.1230
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4.1911
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2.2399
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N
Me
COOEt
1m
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0.96
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0.98
0.97
1.99
2.87
1.73
1.16
1.01
2.02
1.97
3.25
3.00
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9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
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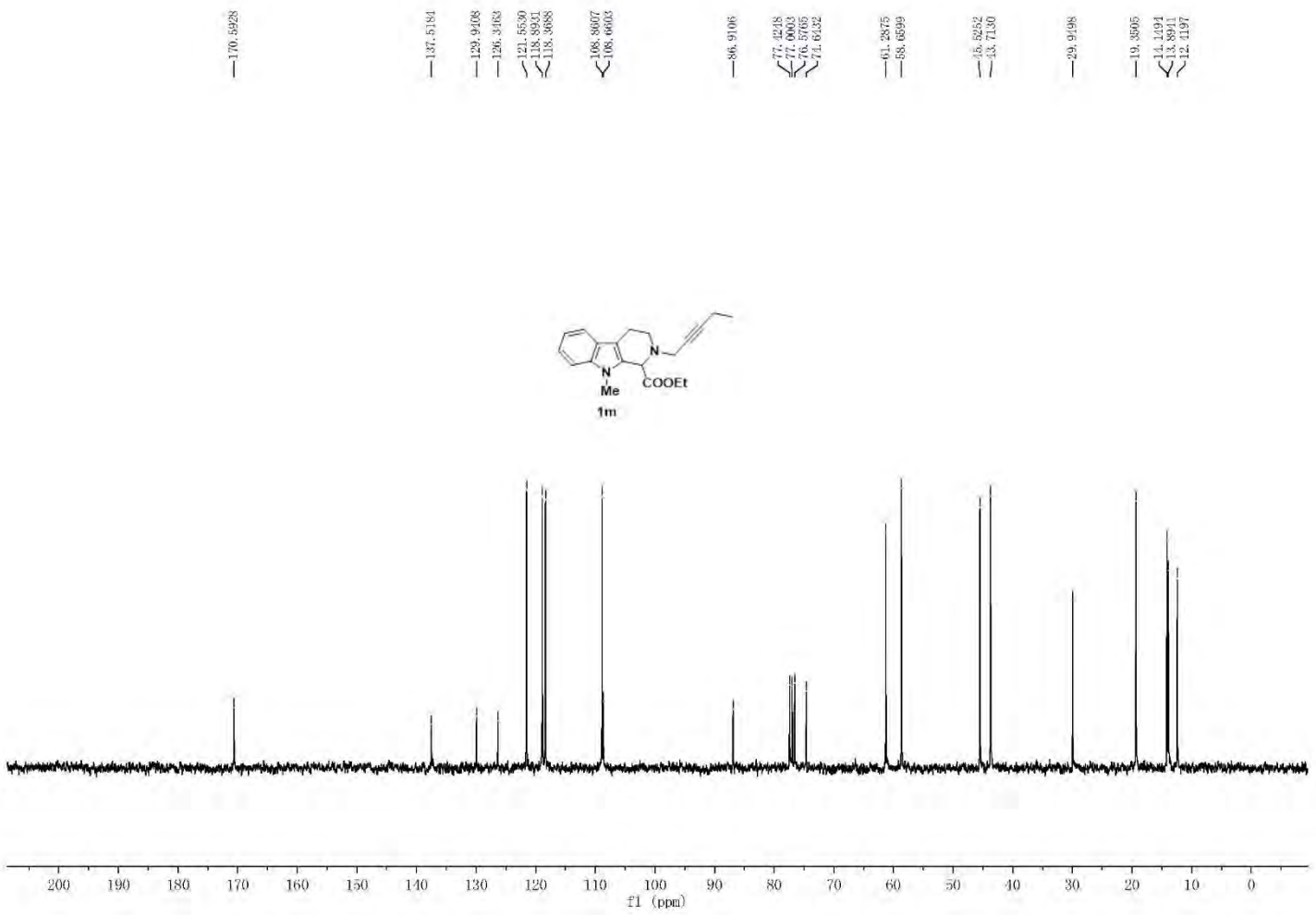
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74.6432
61.2875
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45.6252
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29.9198
19.3505
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13.8941
12.1197
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N
Me
COOEt
1m
200
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180
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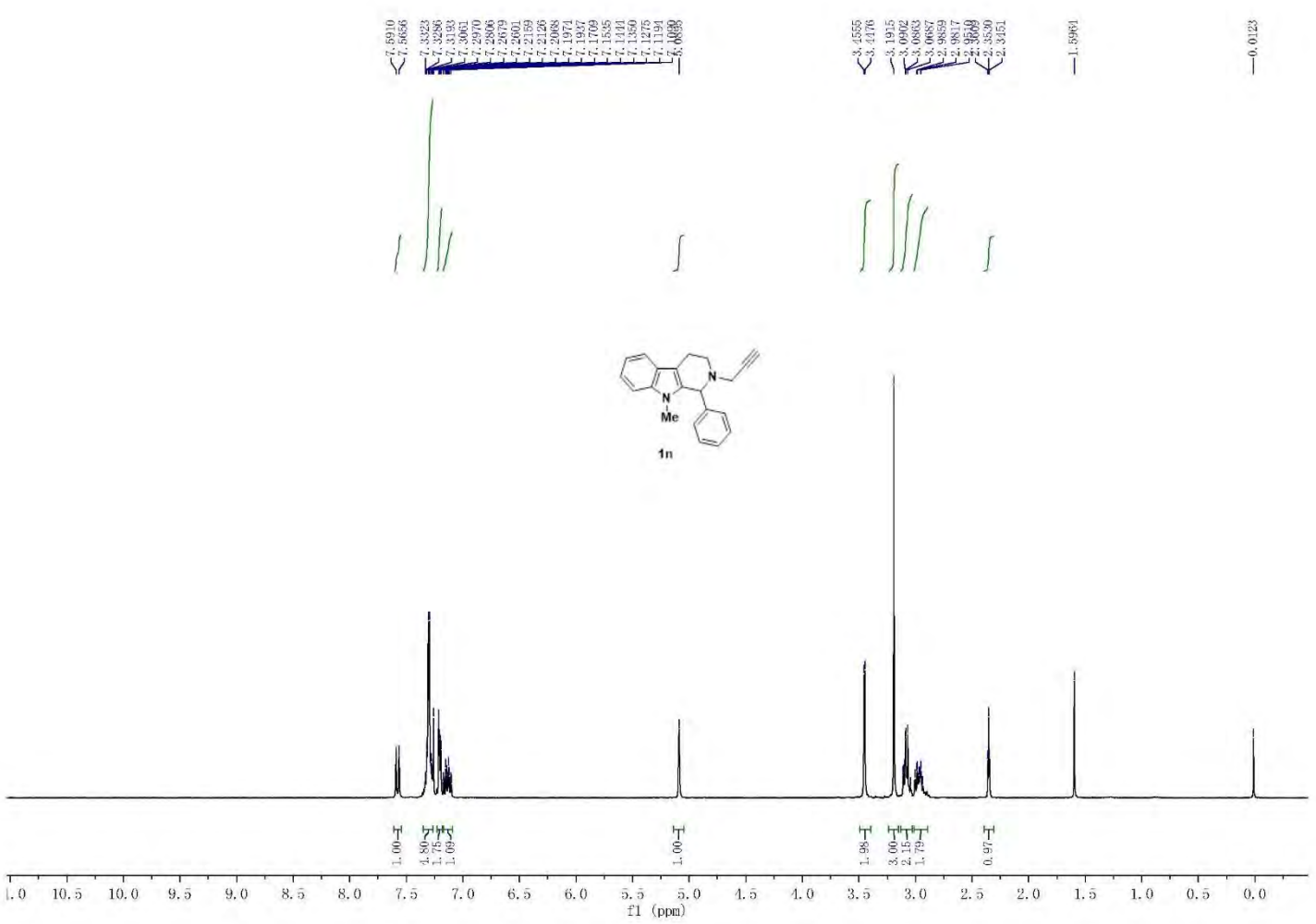
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7.2068
7.1971
7.1937
7.1709
7.1535
7.1441
7.1350
7.1275
7.1194
3.4555
3.4476
3.1915
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3.0687
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2.3530
2.3451
1.5961
0.0123
N
N
Me
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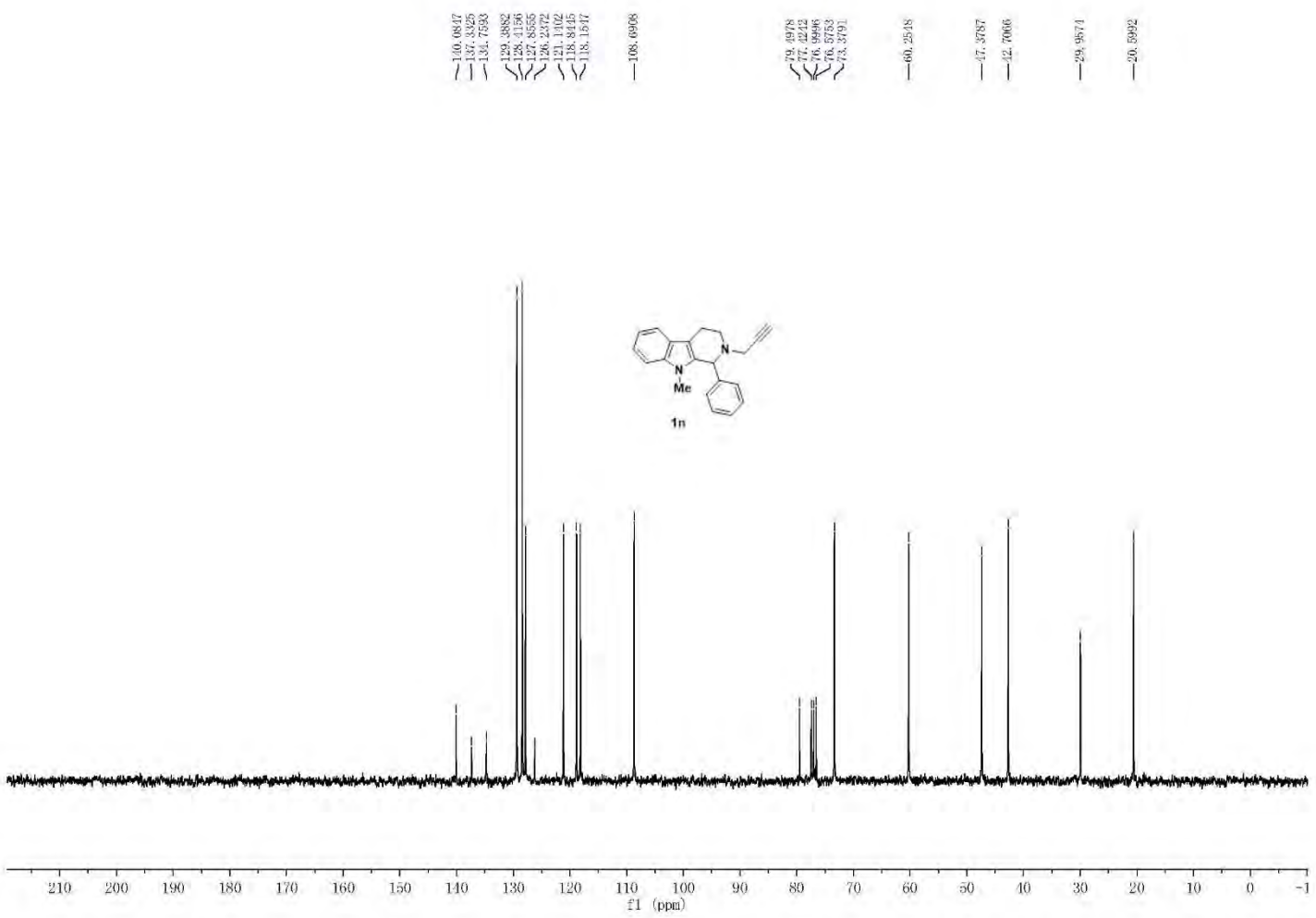
f1 (ppm)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77.4242
76.9996
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73.3791
60.2548
47.3787
42.7066
29.9571
20.5992
N
N
Me
1n
210
200
190
180
170
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100
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80
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40
30
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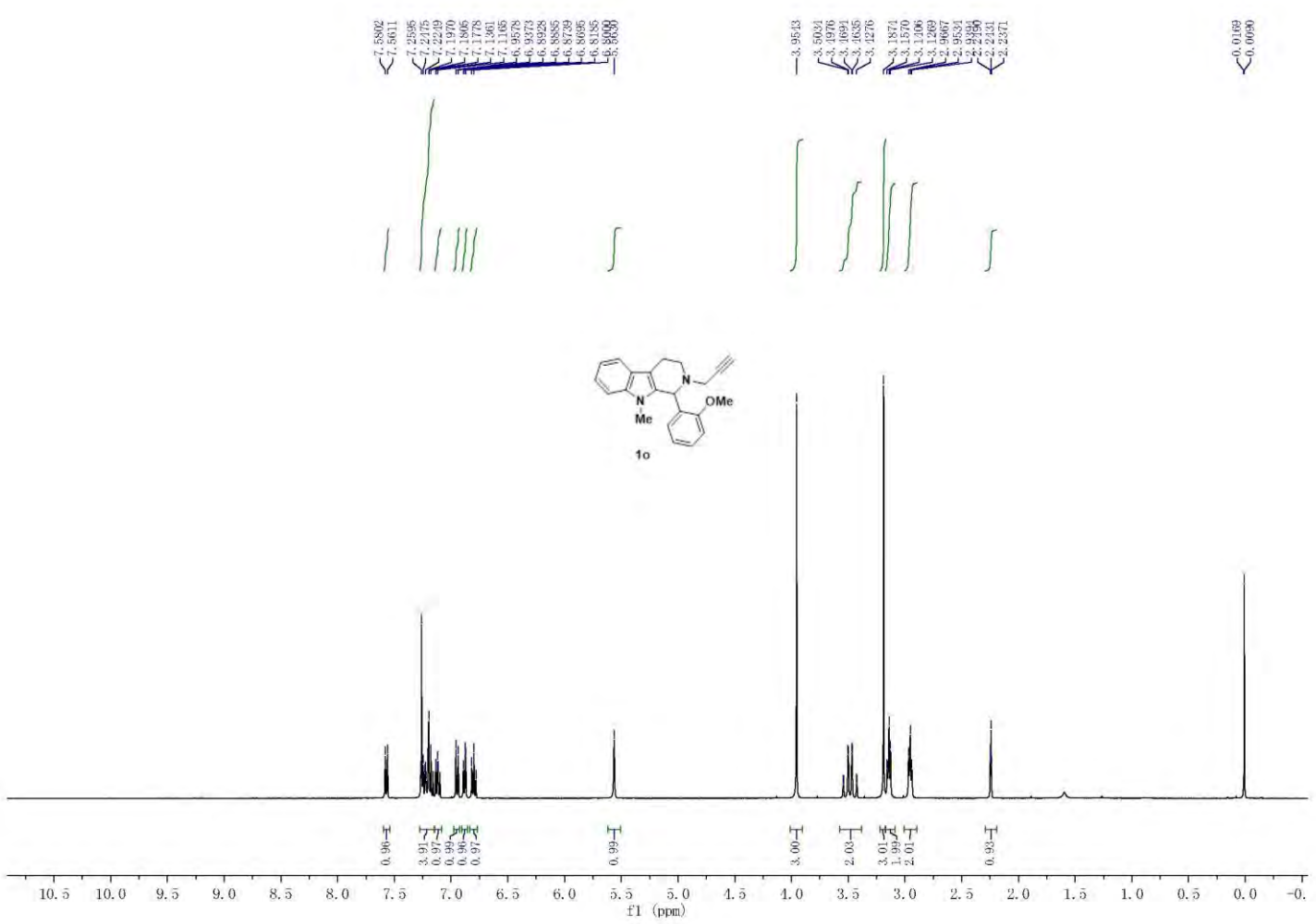
f1 (ppm)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3.0276
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3.1306
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2.2371
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0.0000
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N
Me
OMe
1o
0.96
3.91
0.97
0.99
0.96
0.97
0.99
3.00
2.03
3.01
1.99
2.01
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9.0
8.5
8.0
7.5
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6.5
6.0
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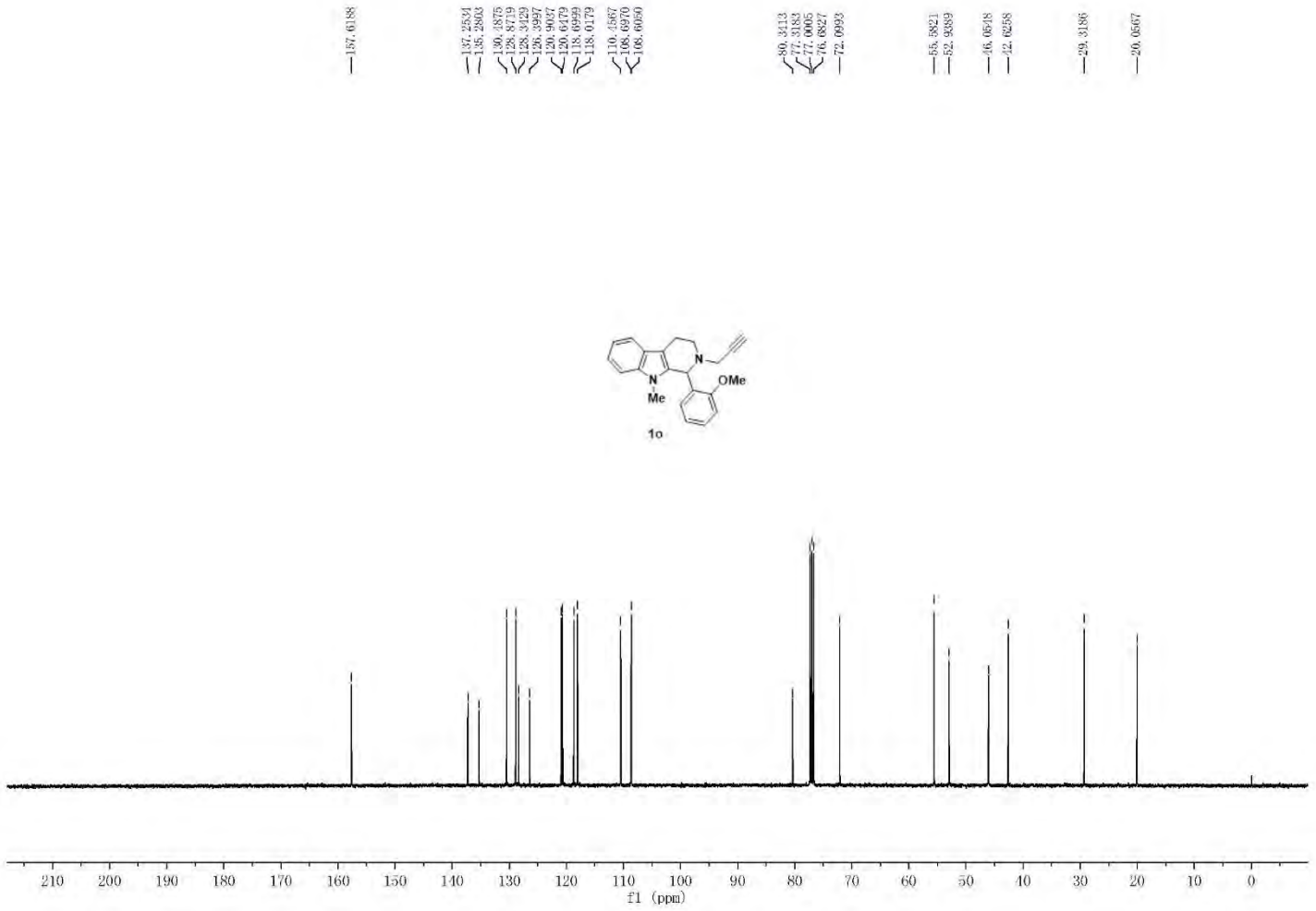
-0.
f1 (ppm)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46.0648
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29.3186
20.0667
N
N
Me
OMe
1o
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200
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180
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80
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50
40
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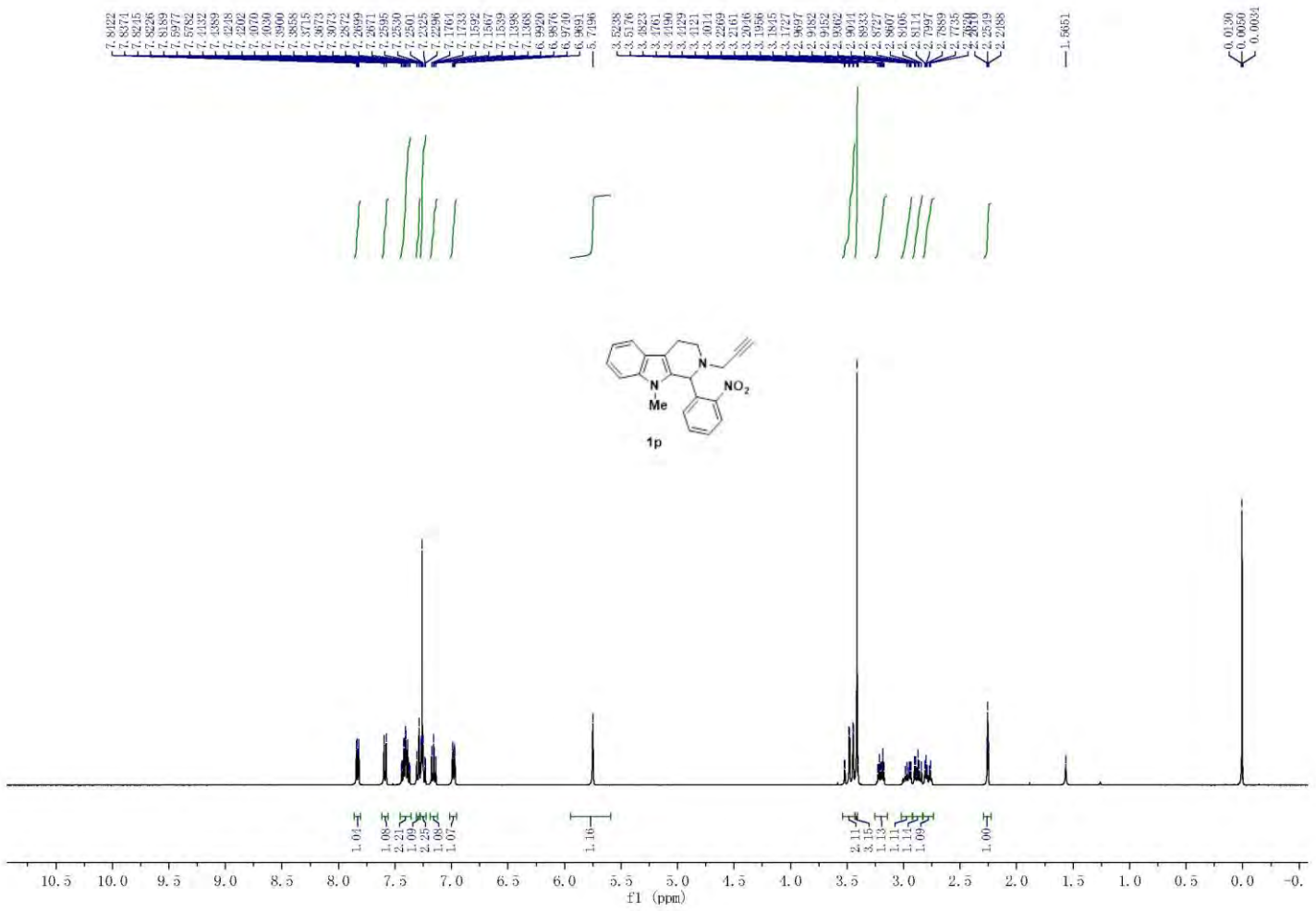
f1 (ppm)


NO2
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Me
1p
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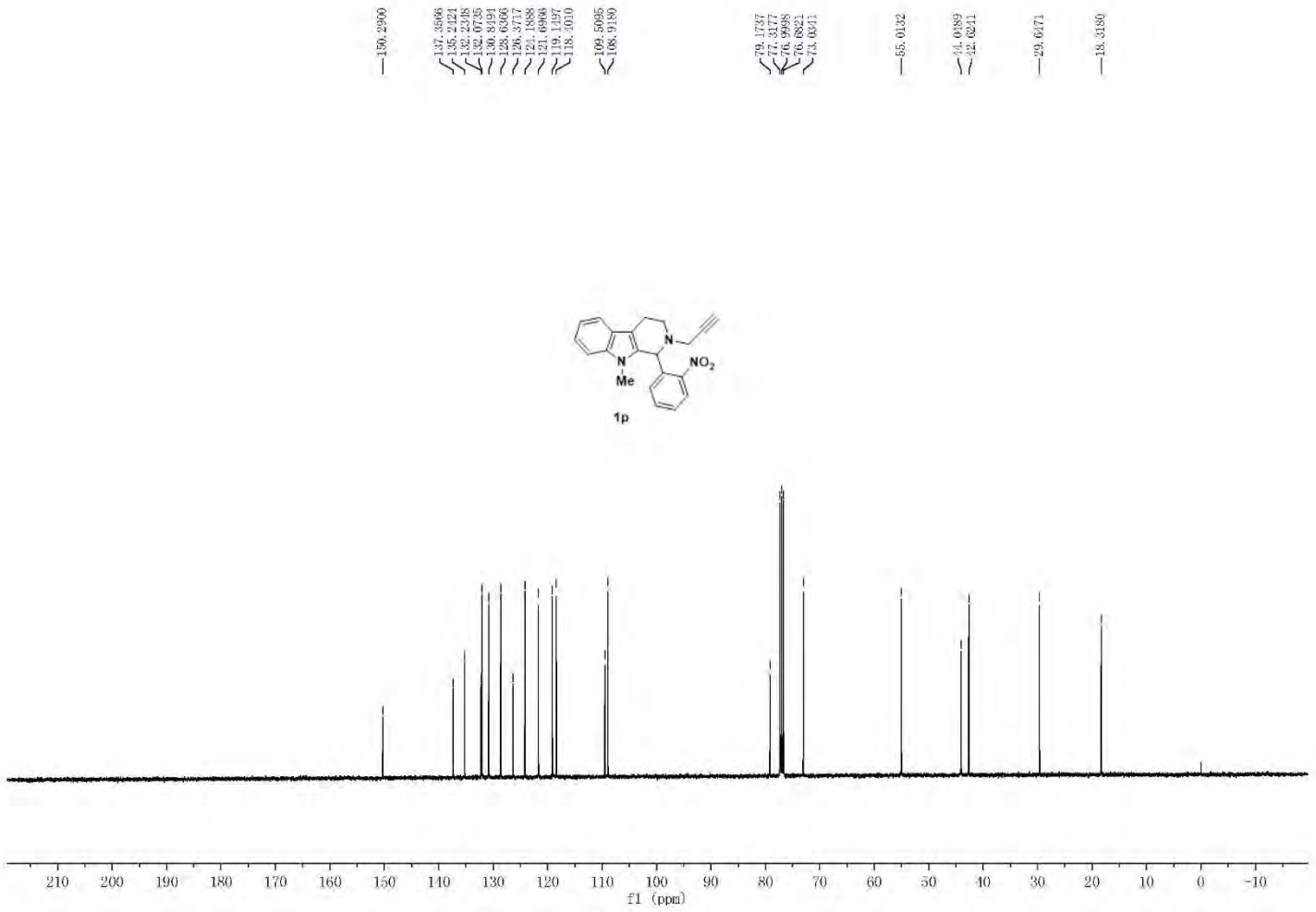
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77.3177
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76.6821
73.0041
55.0132
44.0189
42.6241
29.6471
18.3190
N
N
Me
NO2
1p
210
200
190
180
170
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140
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120
110
100
90
80
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60
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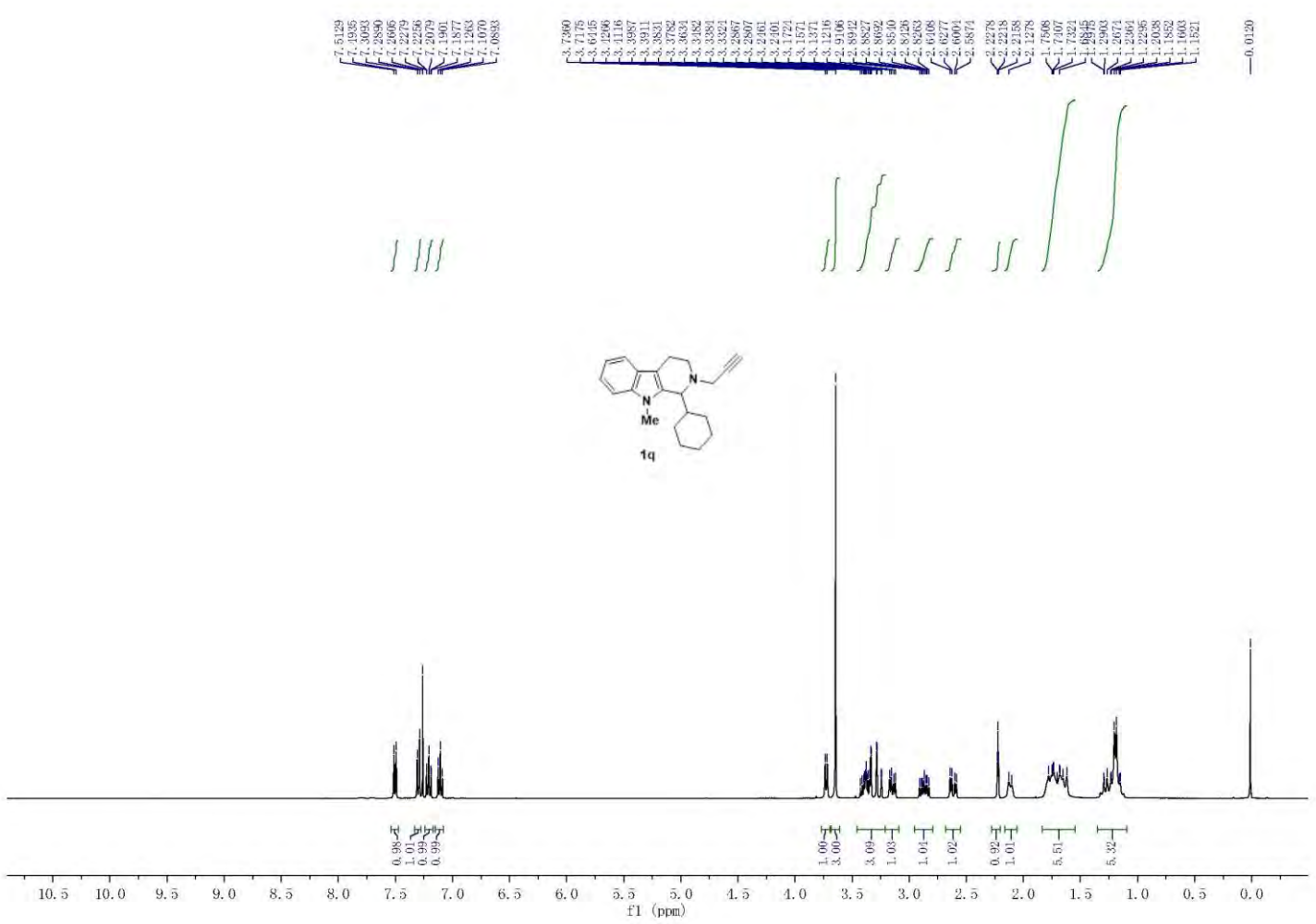
40
30
20
10
0
-10
f1 (ppm)


Me
1q
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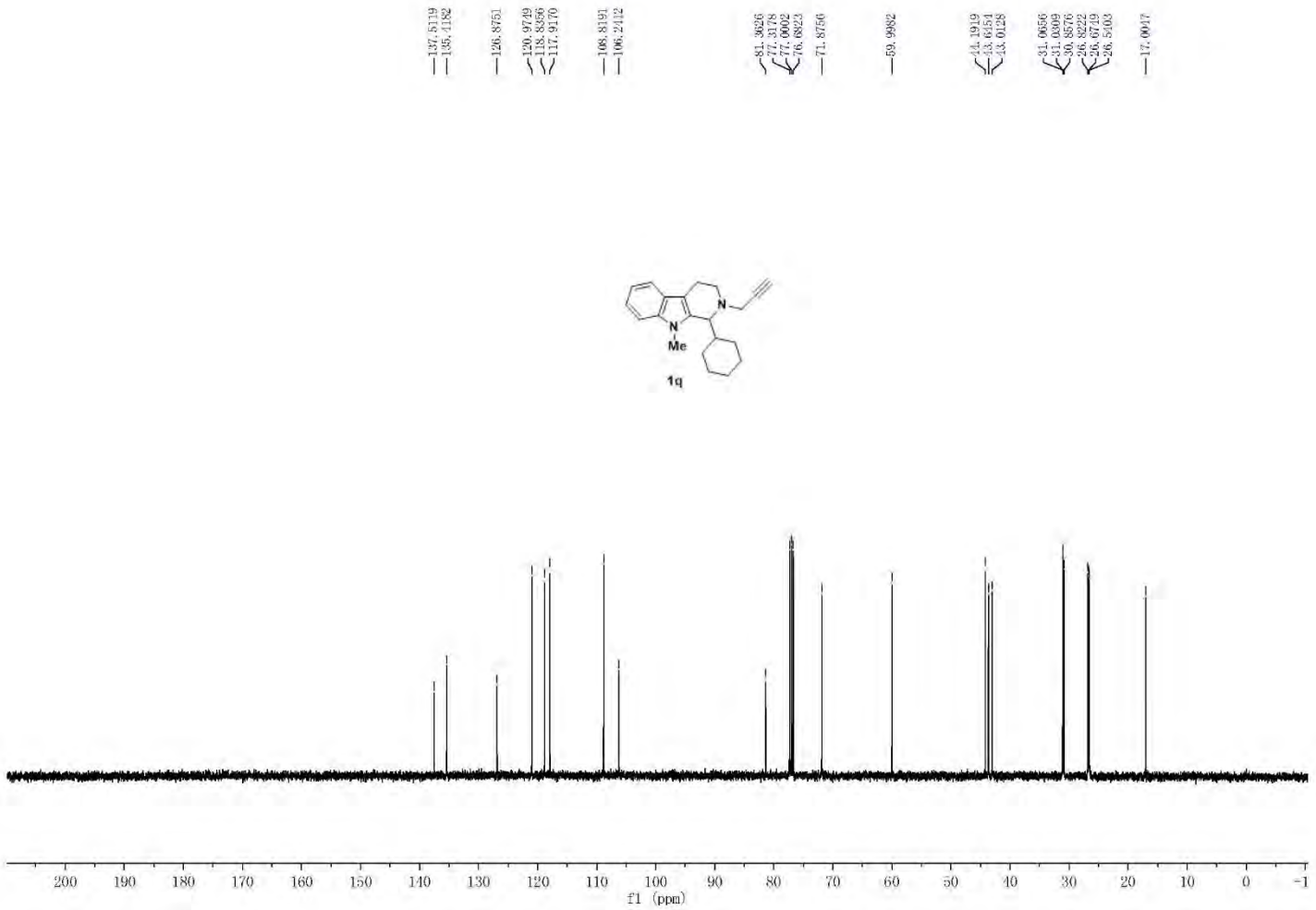
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59.9982
44.1919
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43.0128
31.0656
31.0099
30.8576
26.8222
26.6749
26.5103
17.0017
N
N
Me
1q
200
190
180
170
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120
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100
90
80
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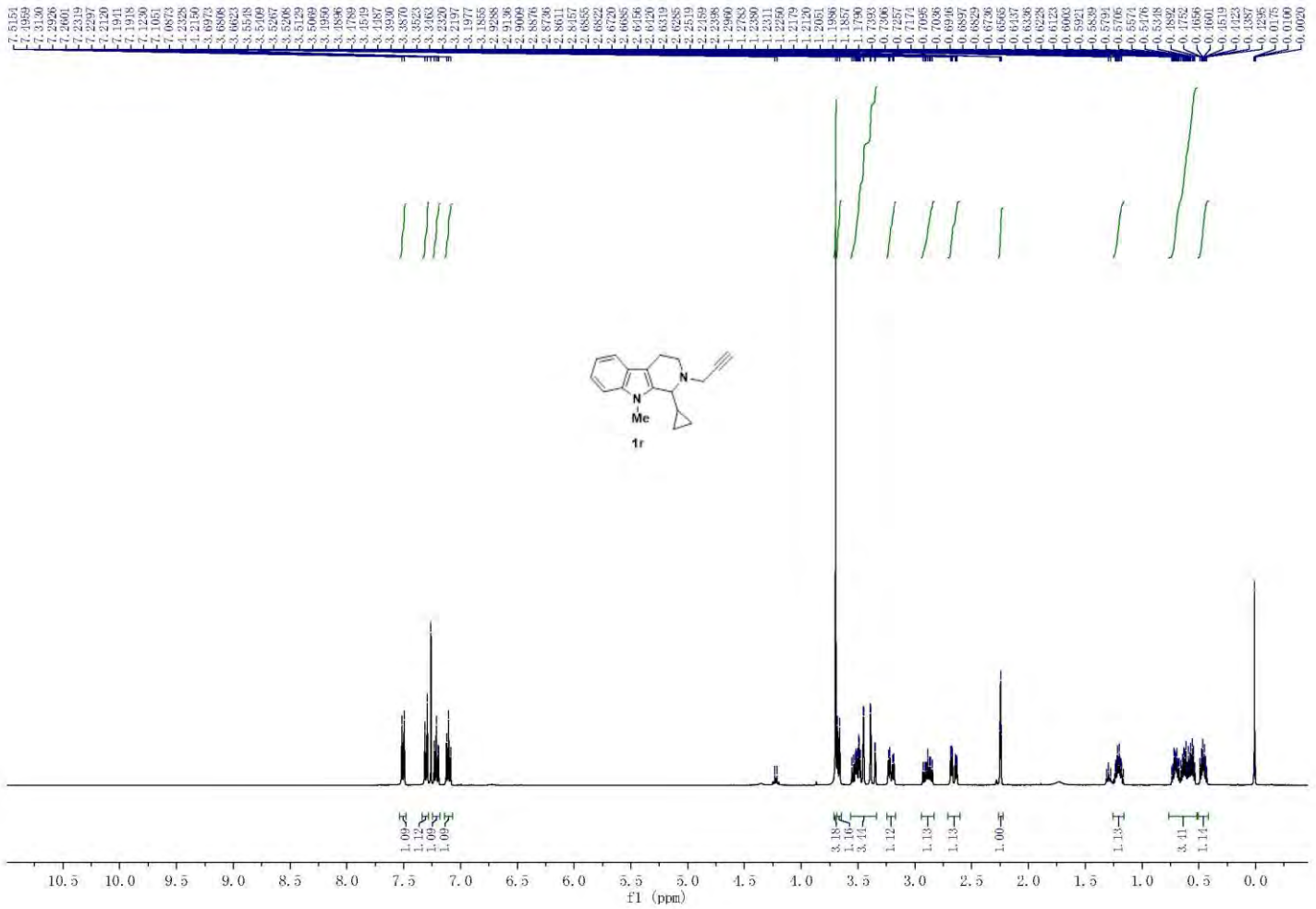
40
30
20
10
0
-1
f1 (ppm)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1.13
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1.13
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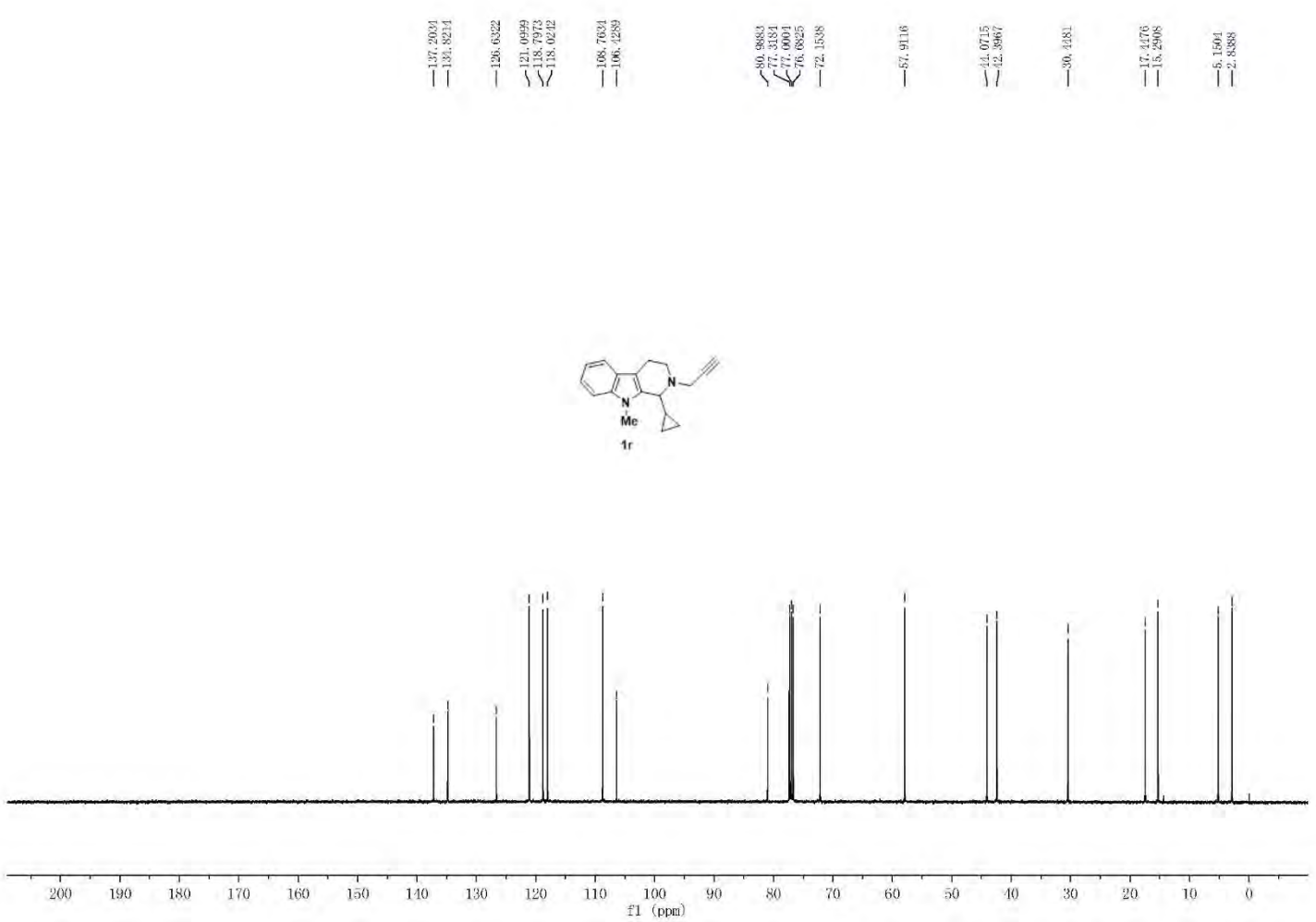
1.14
f1 (ppm)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42.3967
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17.4476
15.2908
5.1501
2.8388
Me
1r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
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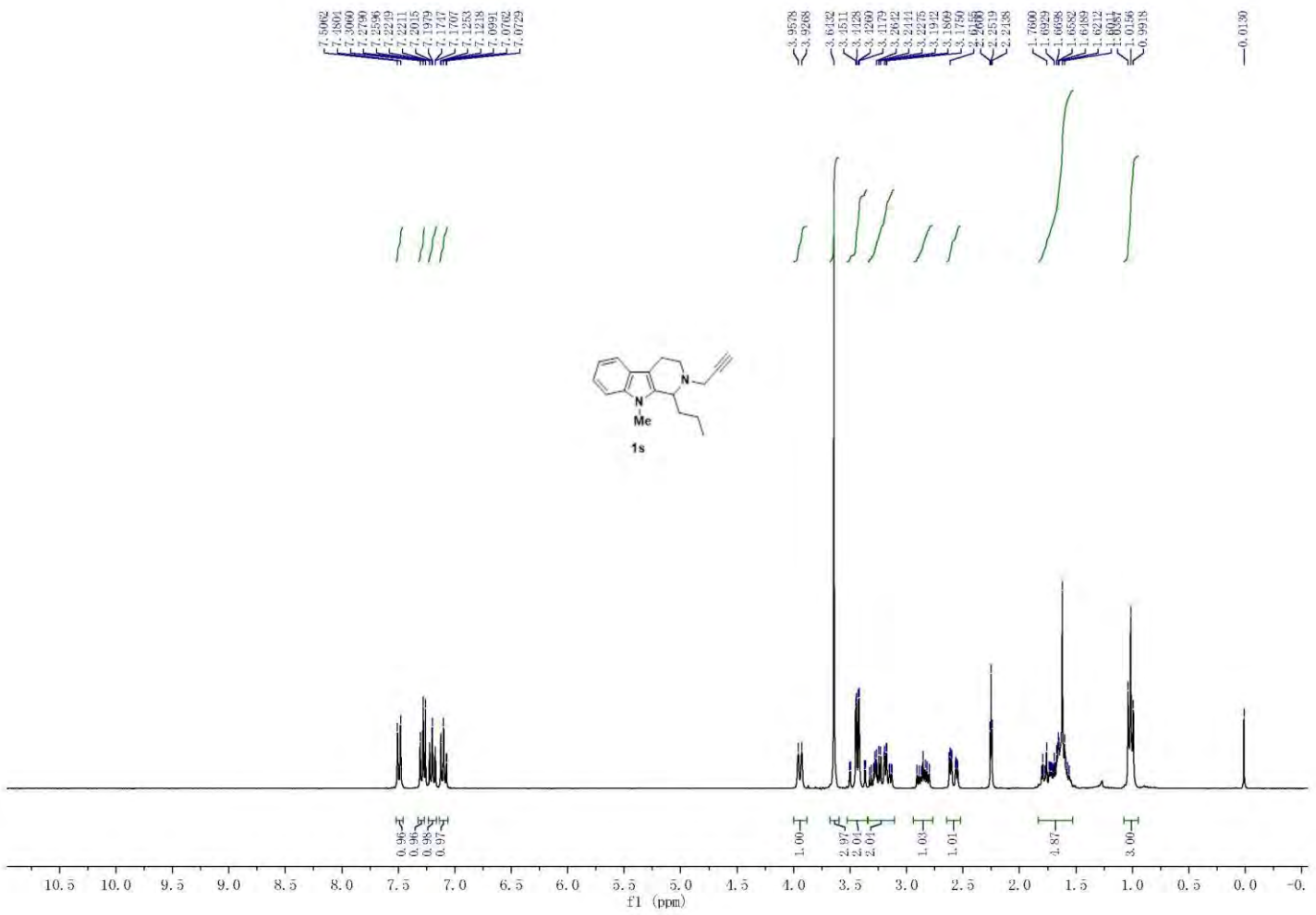
50
40
30
20
10
0
f1 (ppm)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3.9268
3.6432
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3.4428
3.4266
3.4179
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3.2441
3.2275
3.1942
3.1869
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2.2619
2.2438
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1.6489
1.6212
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0.0130
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N
Me
1s
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0.96
0.98
0.97
1.00
2.97
2.01
2.01
1.03
1.01
1.87
3.00
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
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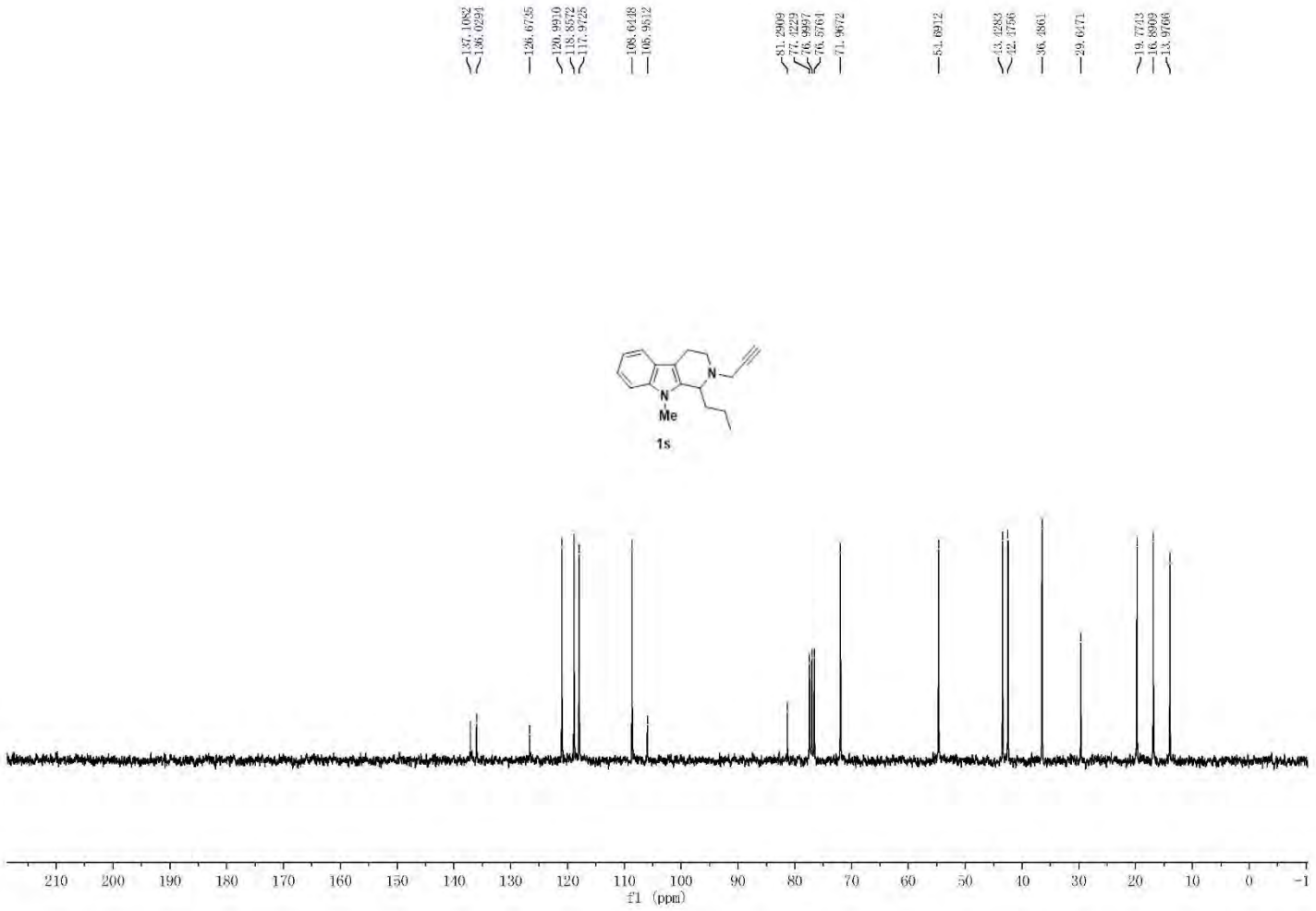
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53.6912
43.4283
42.3756
36.4861
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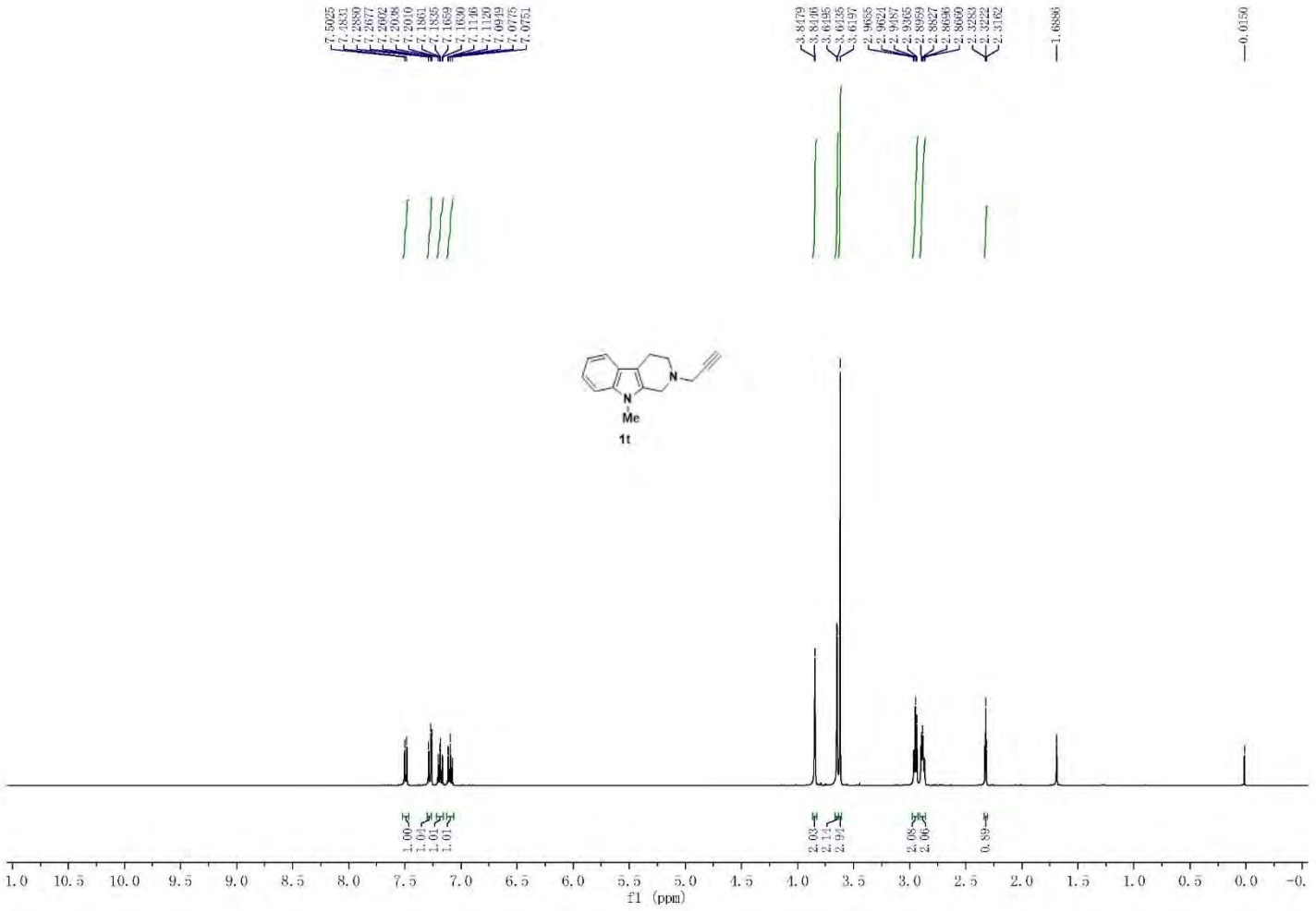
f1 (ppm)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7.1861
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7.1640
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7.1126
7.0949
7.0775
7.0751
3.8479
3.8406
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3.6135
3.6197
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Me
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1.01
1.01
2.03
2.13
2.97
2.08
2.06
0.89
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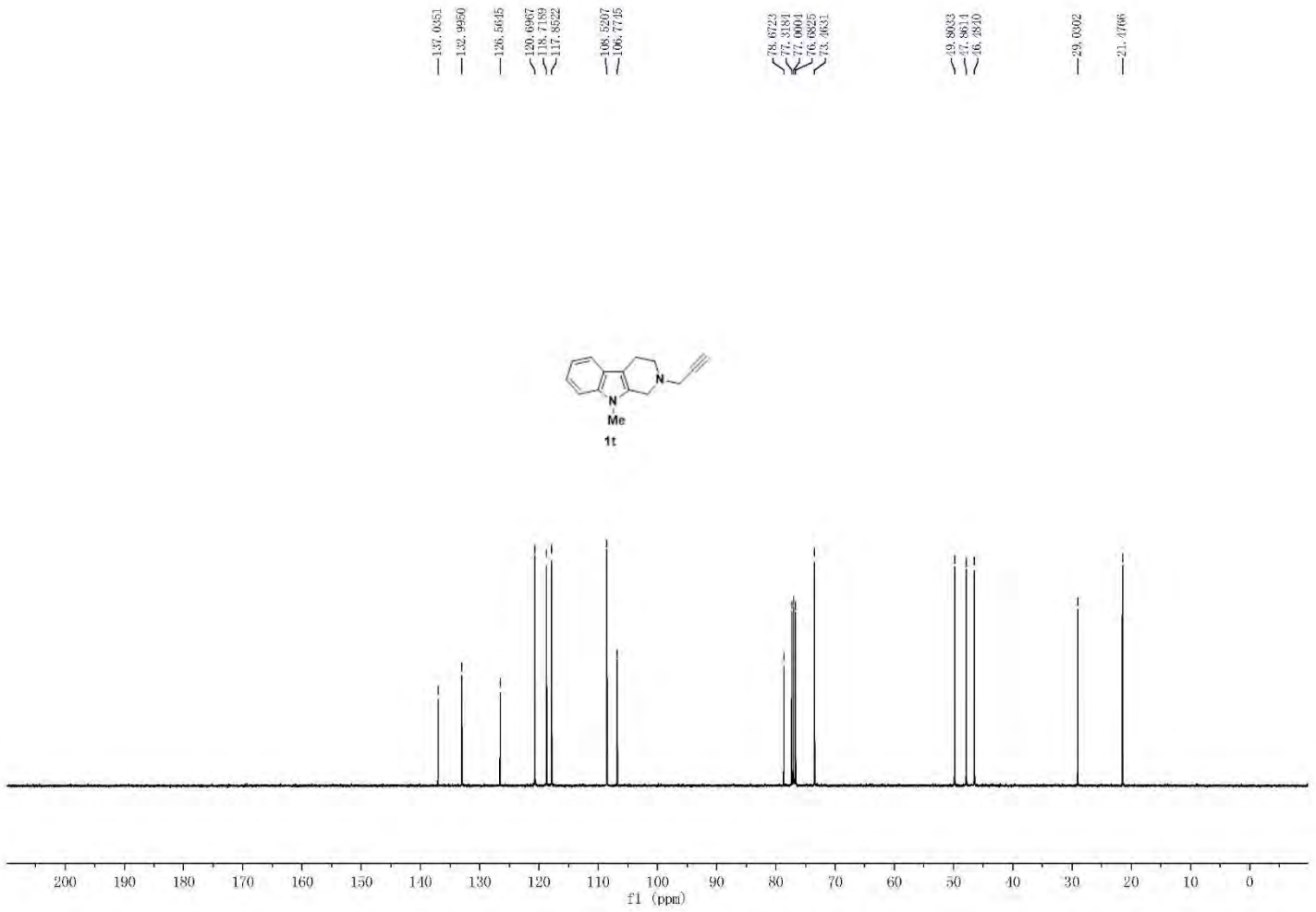
f1 (ppm)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50
40
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10
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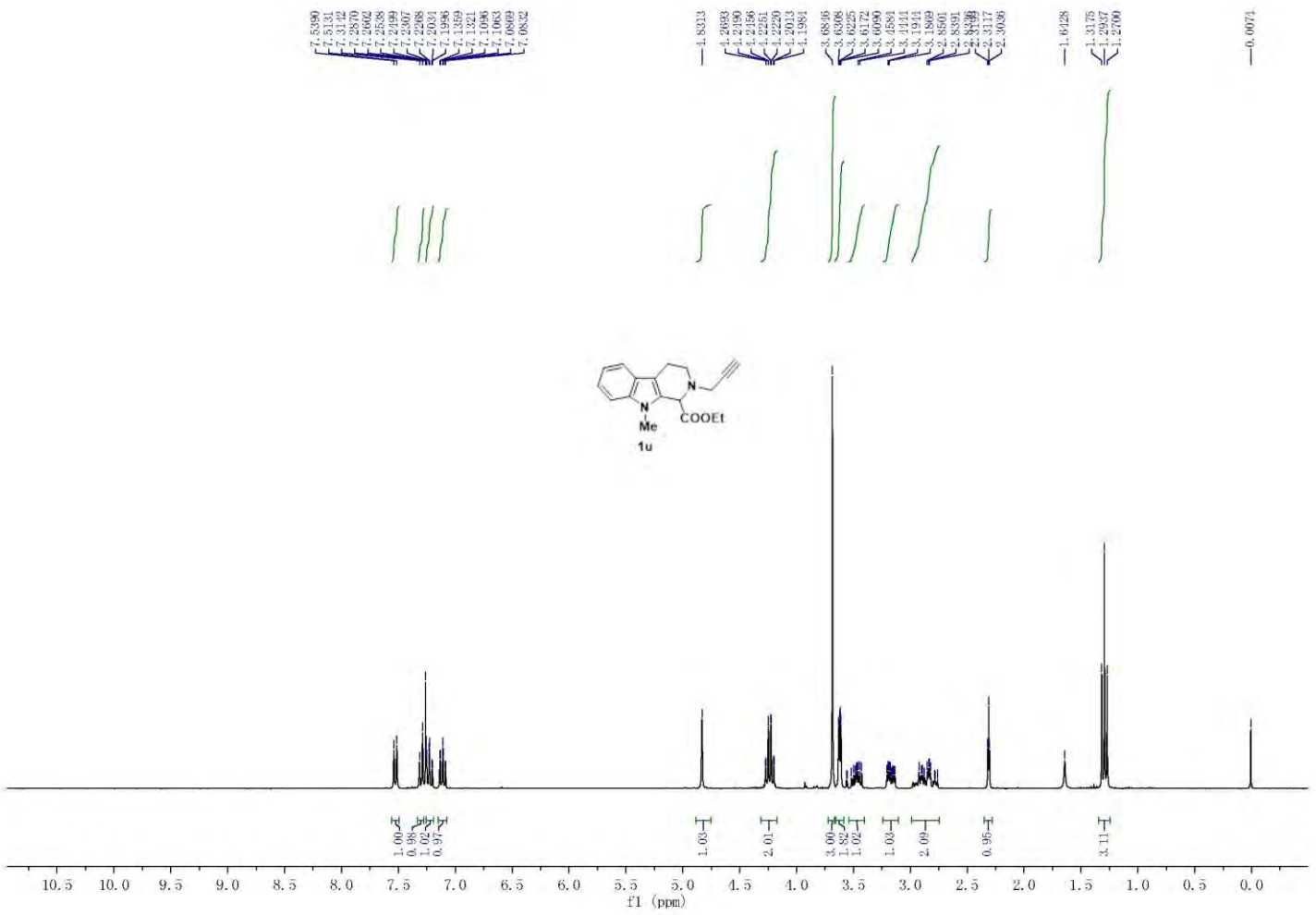
f1 (ppm)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7.1321
7.1096
7.1063
7.0869
7.0832
1.8313
1.2693
1.2590
1.2456
1.2251
1.2220
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3.1241
3.1169
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N
Me
COOEt
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1.02
0.97
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3.00
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1.02
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8.0
7.5
7.0
6.5
6.0
5.5
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4.5
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2.5
2.0
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1.0
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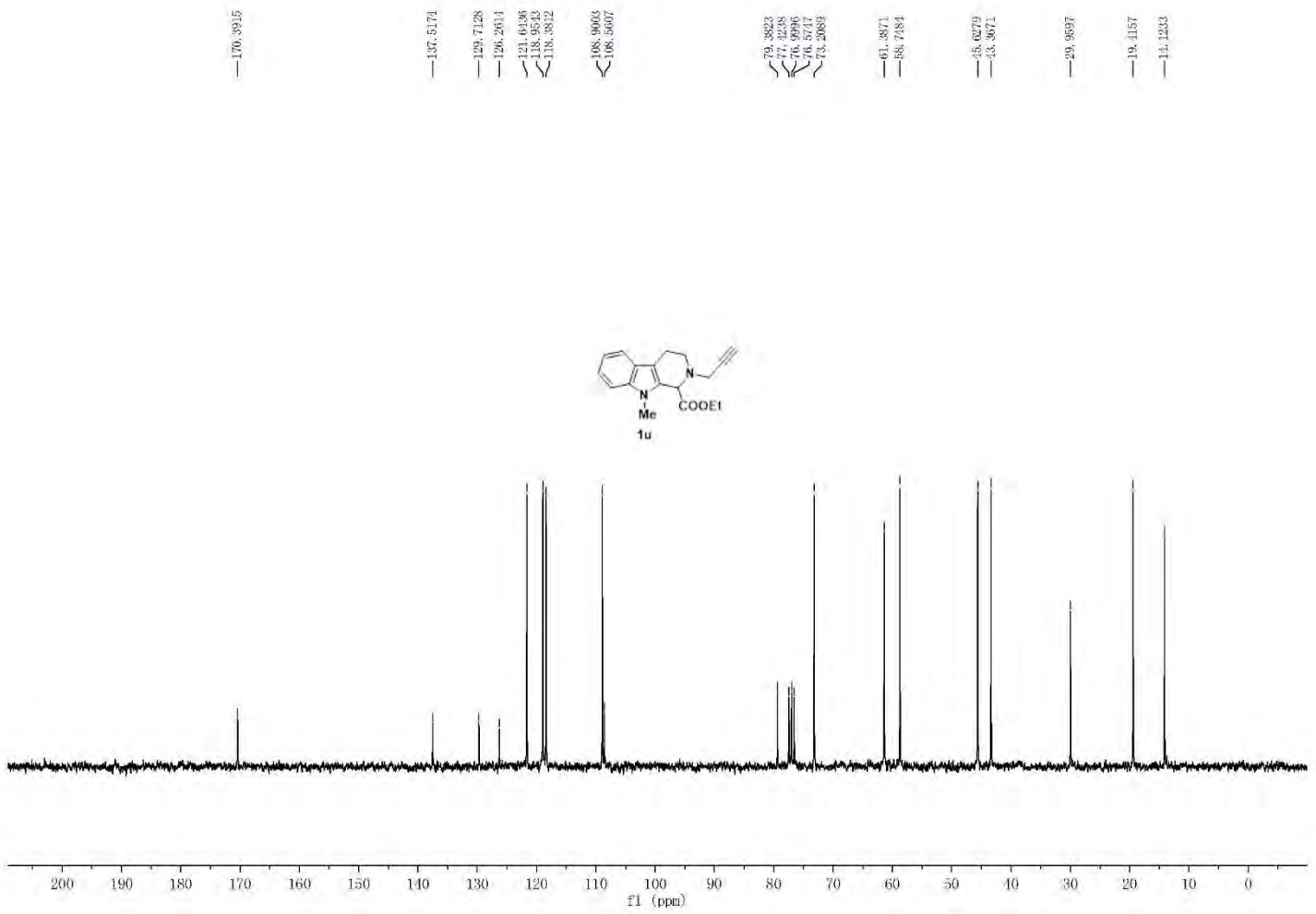
0.0
f1 (ppm)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N
N
Me
COOEt
1u
200
190
180
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50
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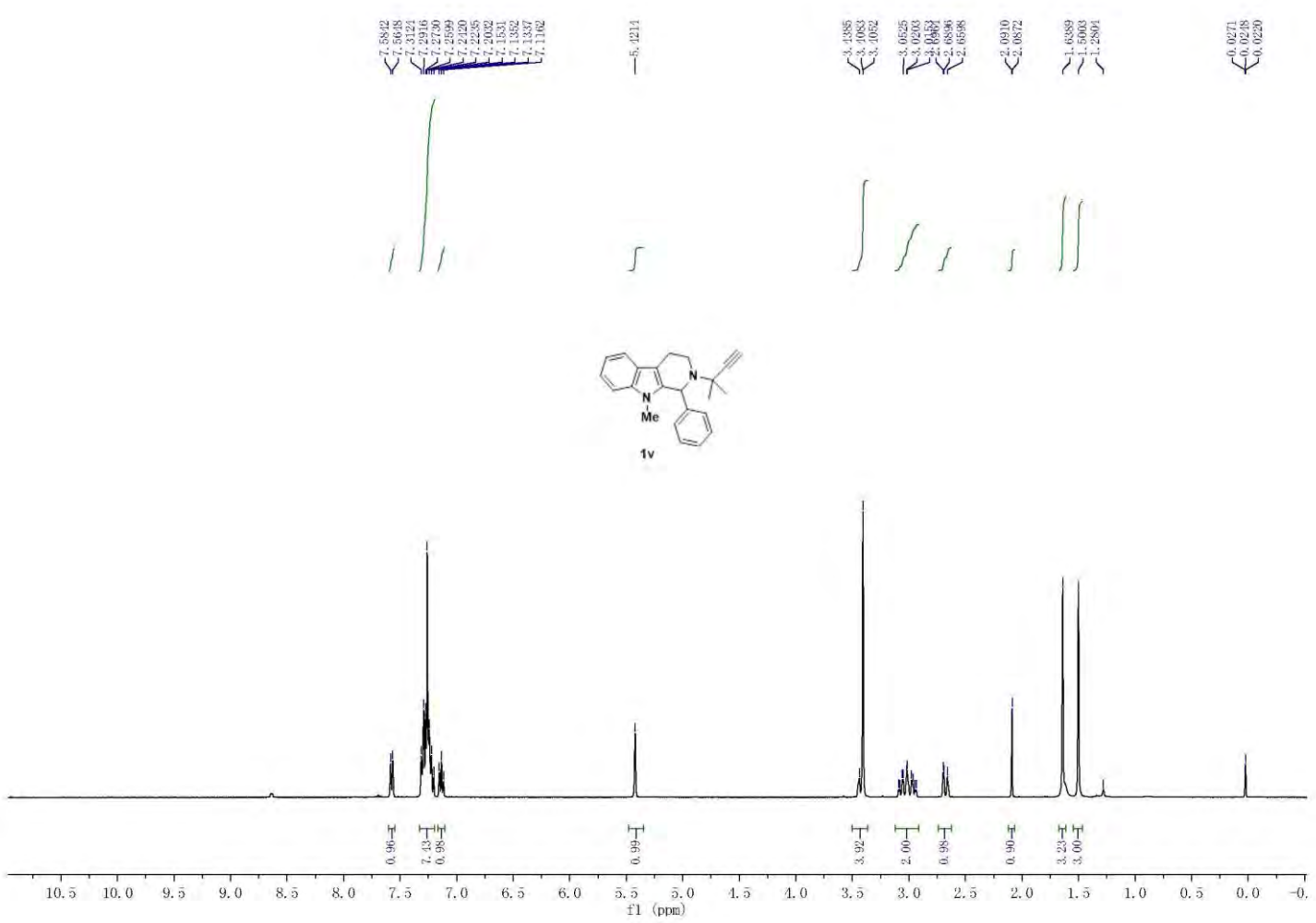
f1 (ppm)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7.1337
7.1162
5.1211
4.1385
4.1083
4.1052
3.0525
3.0203
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2.6598
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1.2891
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0.0220
Me
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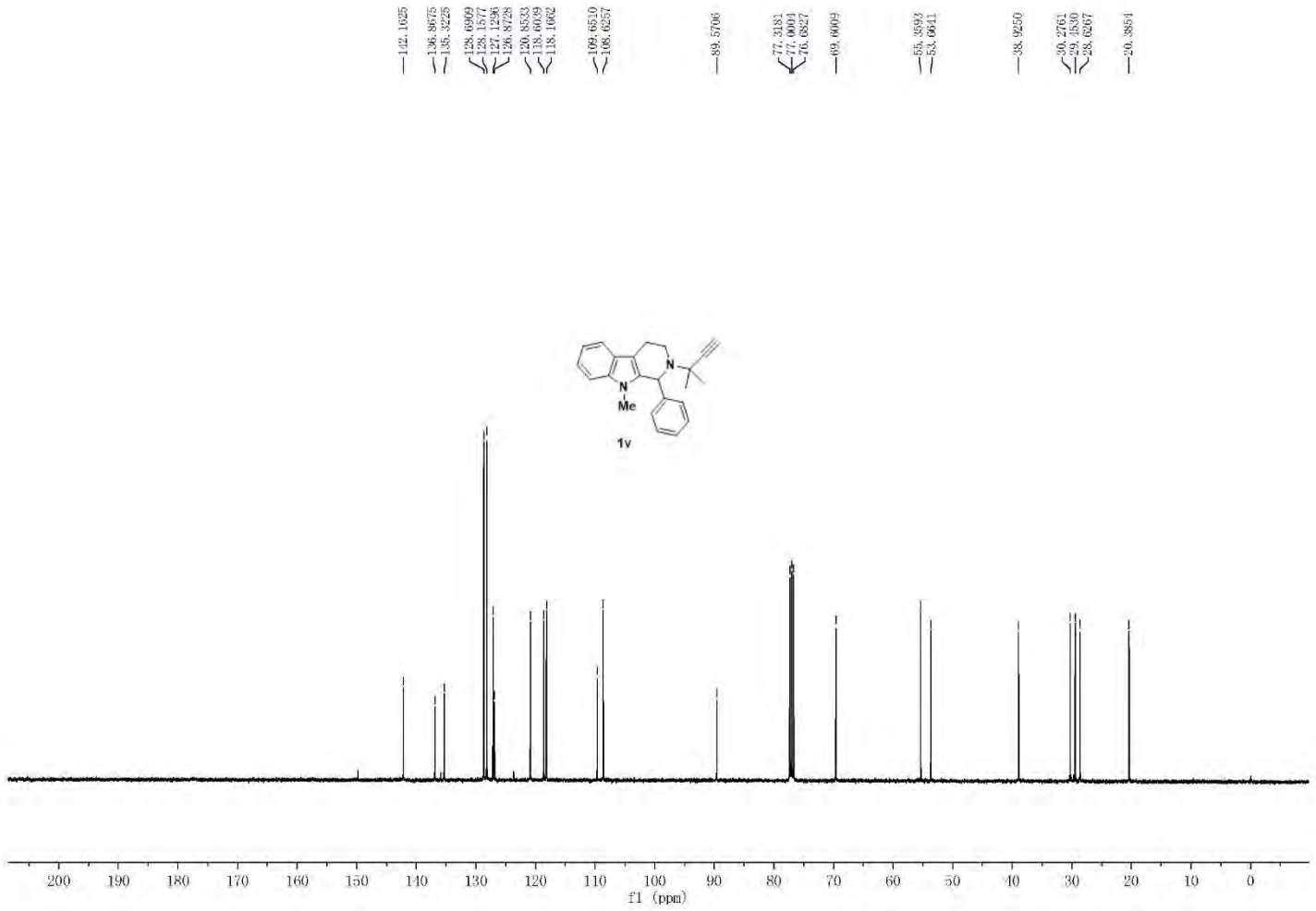
3.00
f1 (ppm)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53.0641
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29.1530
28.6267
20.3851
Me
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180
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130
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110
100
90
80
70
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50
40
30
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10
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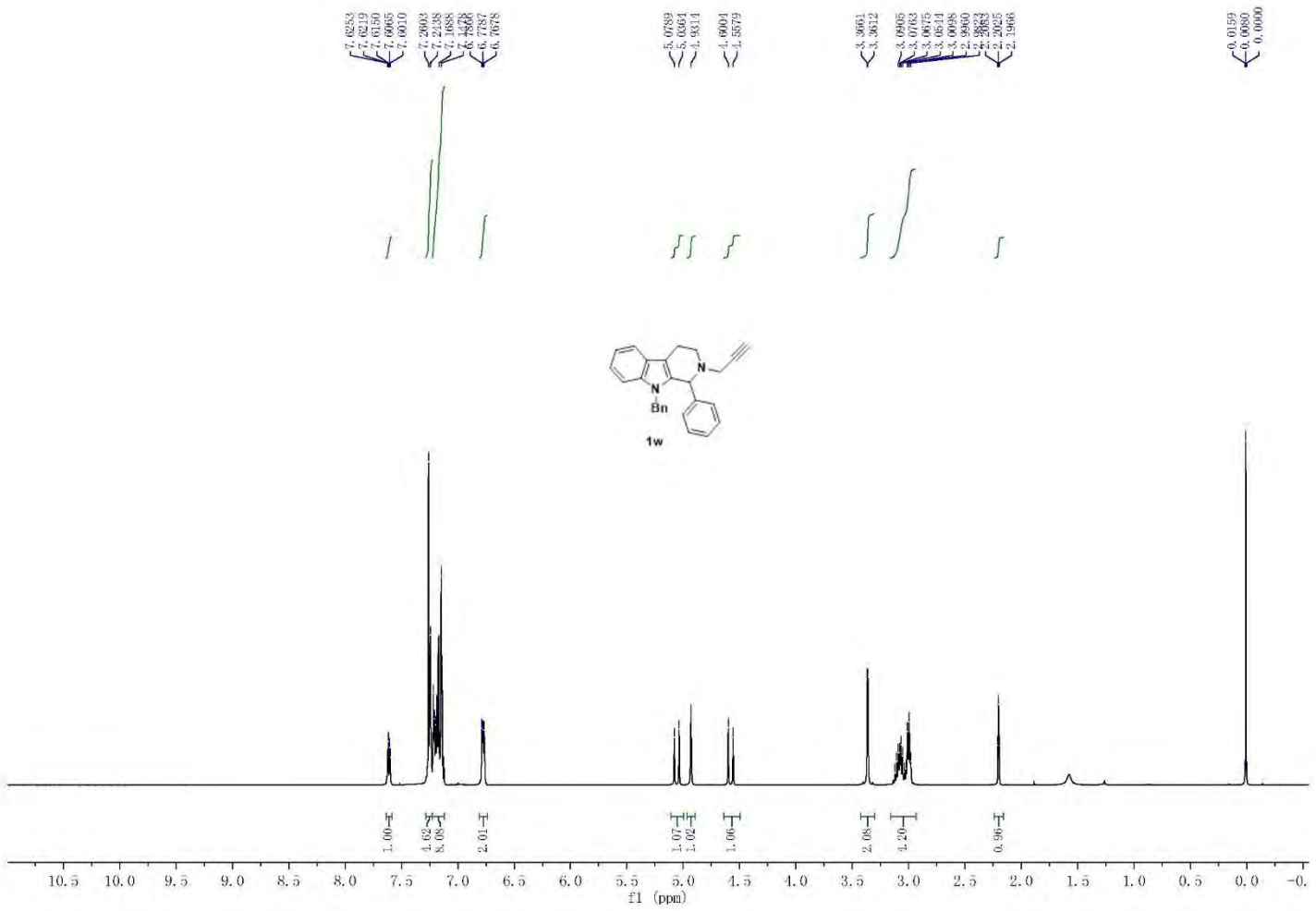
f1 (ppm)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3.0675
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0.0000
Bn
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3.09
2.01
1.07
1.02
1.06
2.08
4.20
0.96
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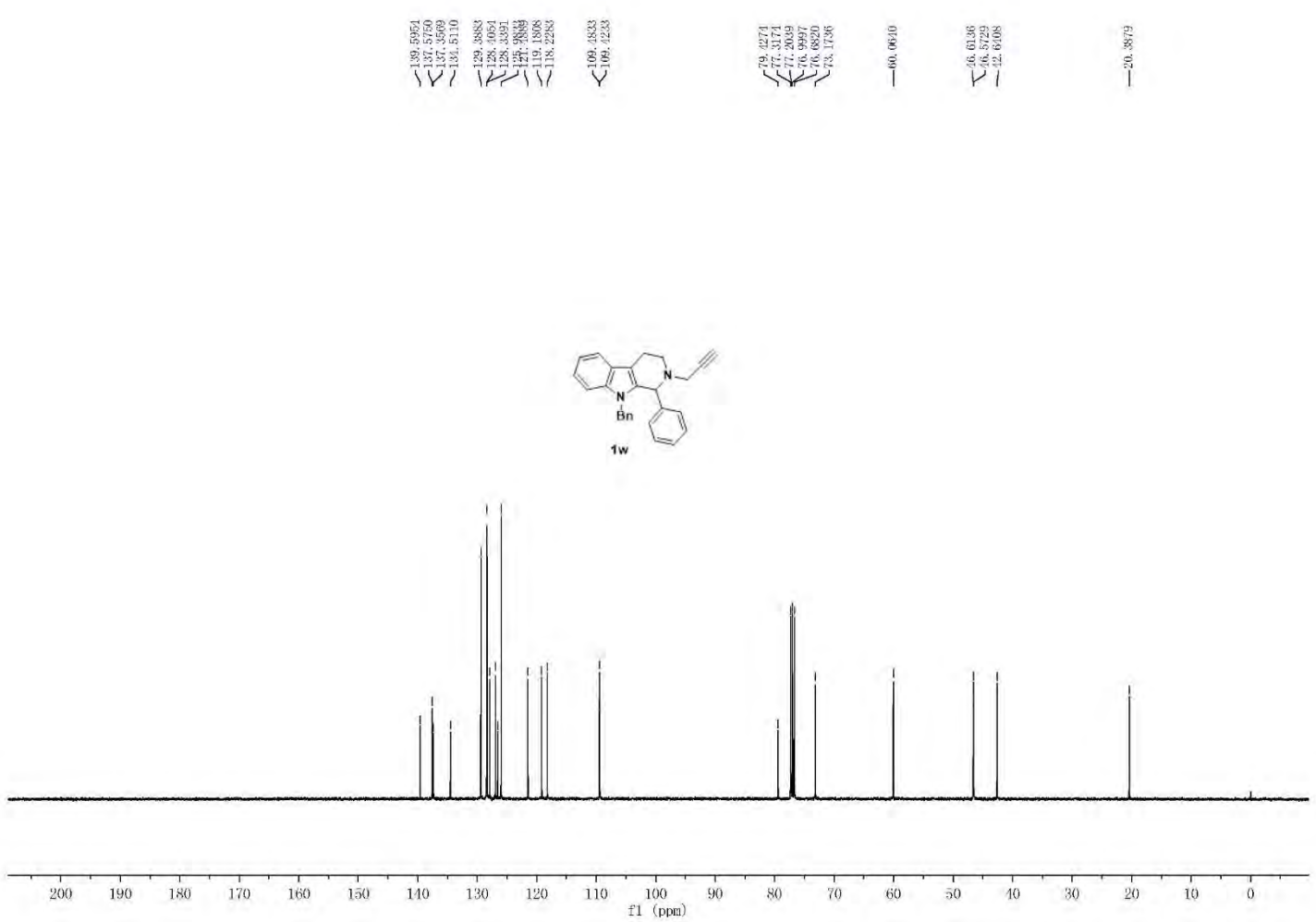
f1 (ppm)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60.0610
46.6136
46.5729
42.6408
20.3879
Bn
1w
200
190
180
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70
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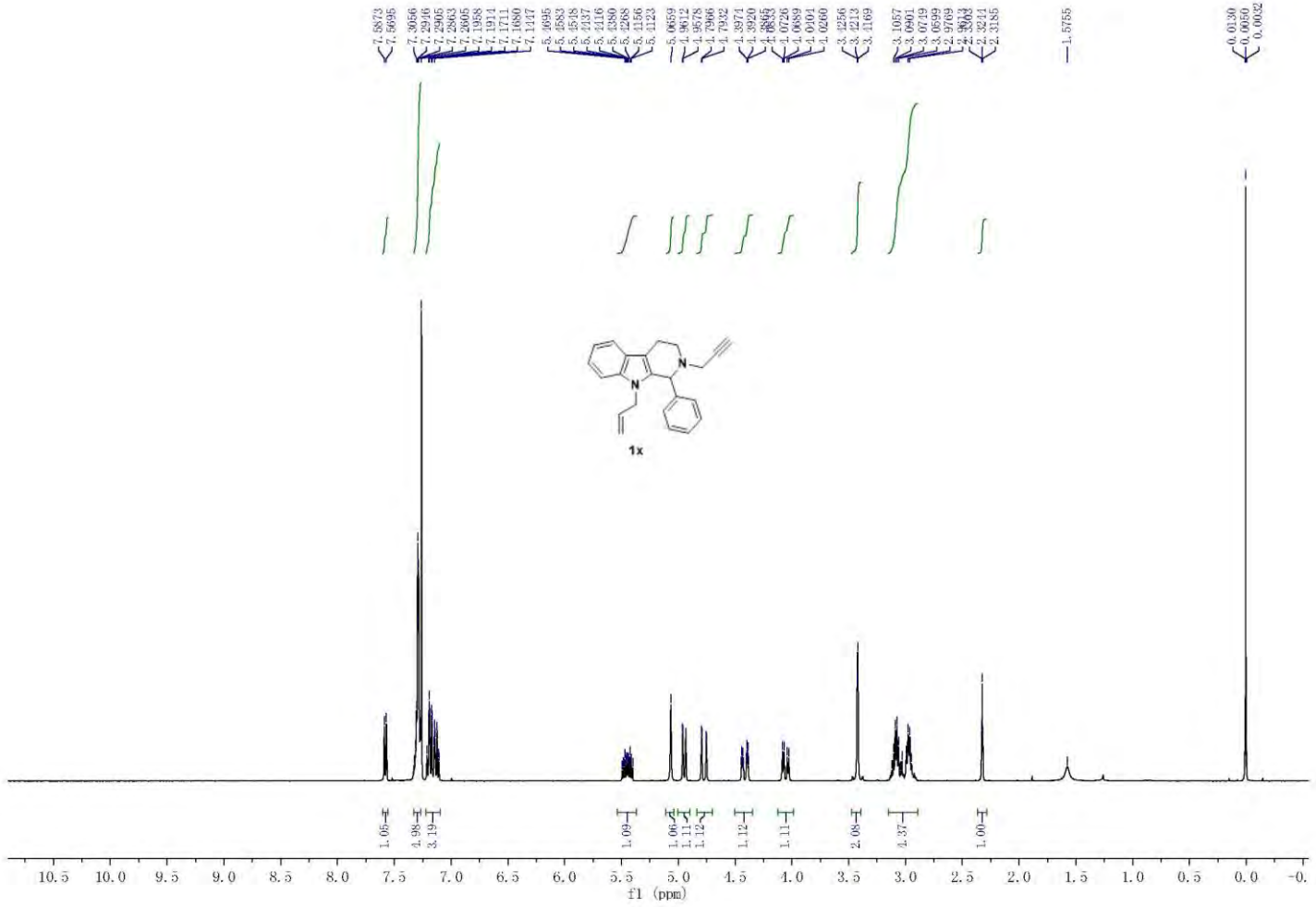
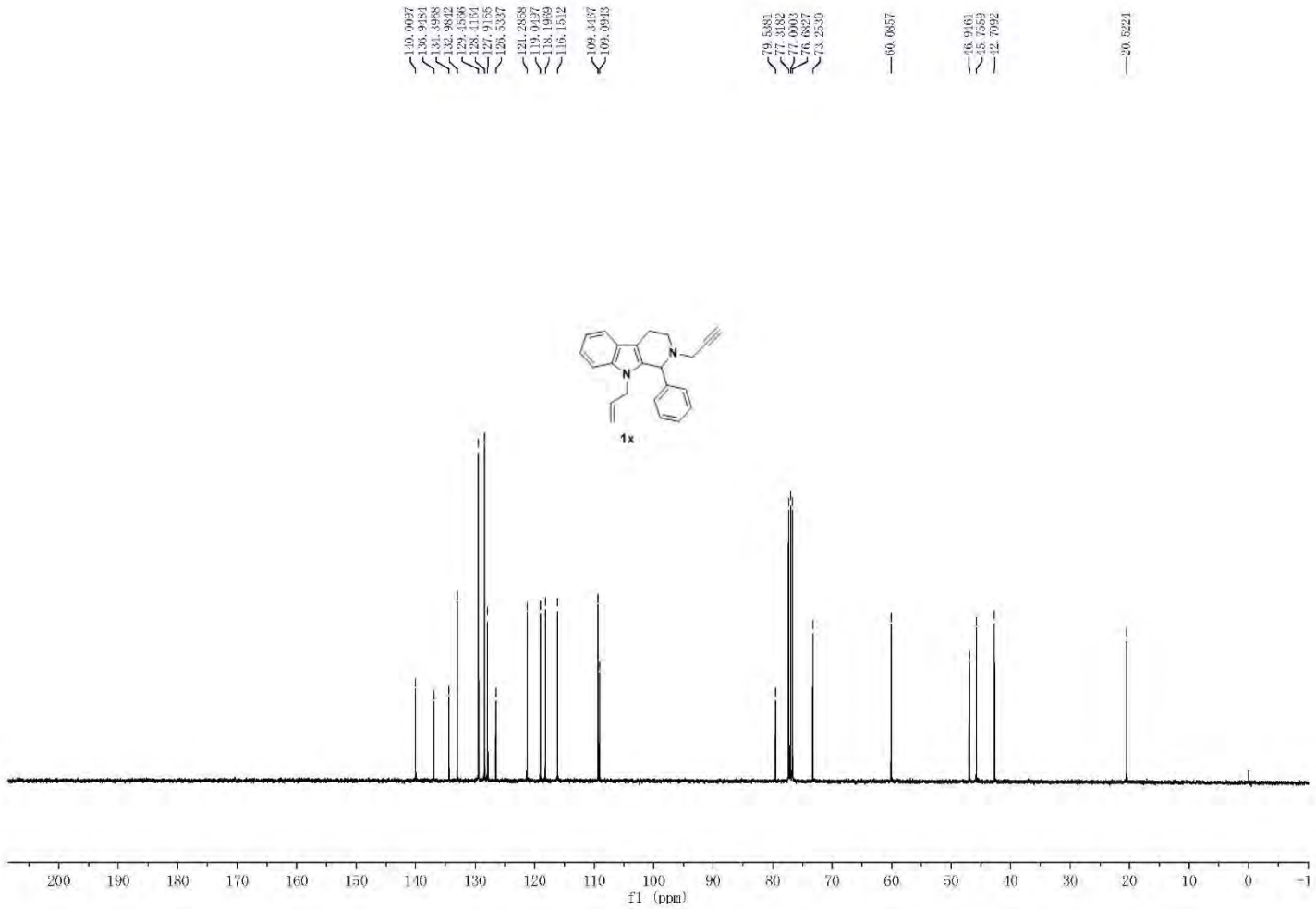
50
40
30
20
10
0
f1 (ppm)


1x
f1 (ppm)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118.1969
116.1512
109.3467
109.0943
79.5381
77.3182
77.0003
76.6827
73.2530
60.0857
46.9461
45.7659
42.7092
20.5224
1x
200
190
180
170
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80
70
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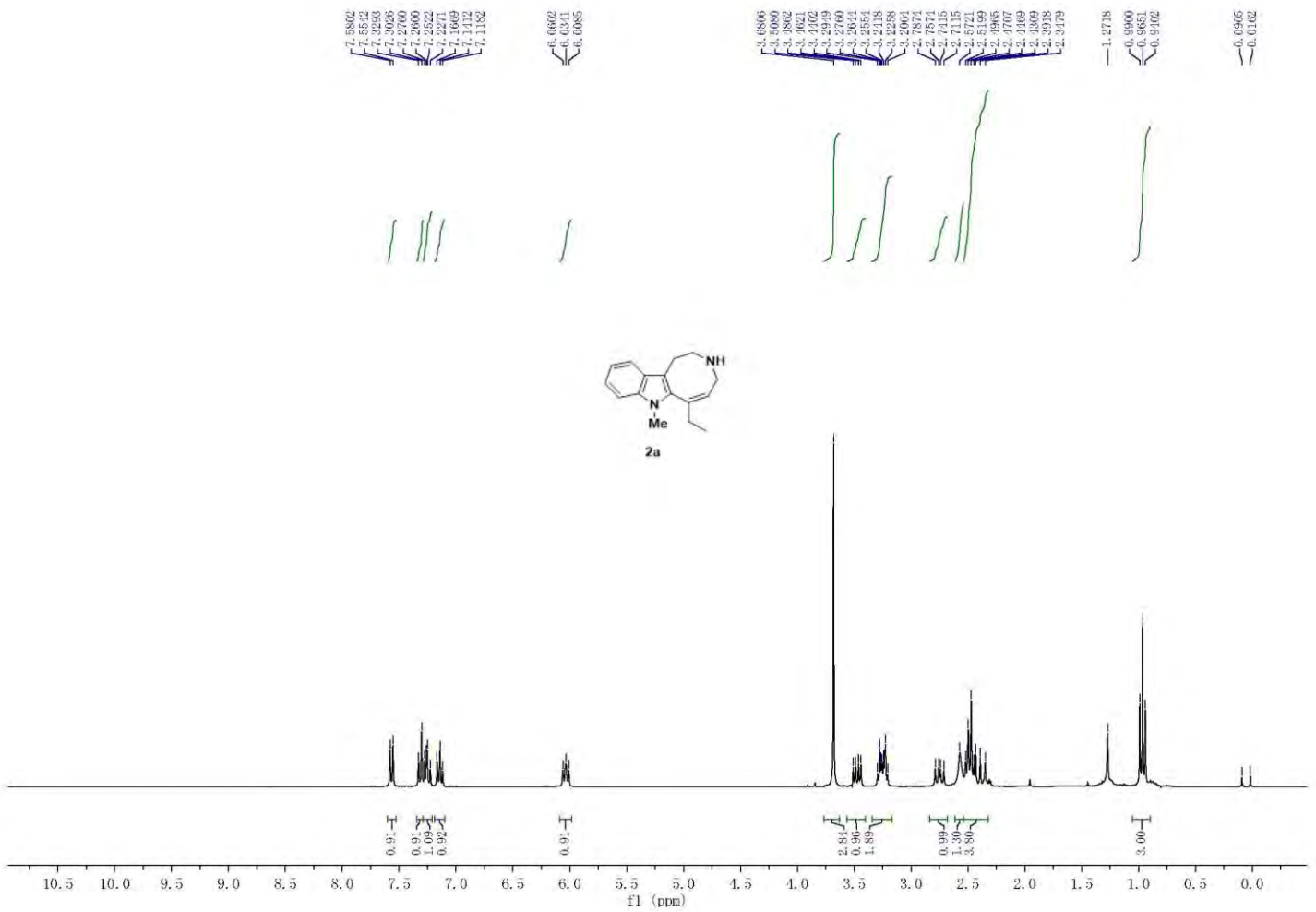
30
20
10
0
-1
f1 (ppm)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7.1182
6.0602
6.0411
6.0085
3.6806
3.5080
3.1862
3.1621
3.1102
3.0919
3.0760
3.0641
3.0551
3.0418
3.0258
3.0061
2.7871
2.7571
2.7115
2.6721
2.6199
2.1965
2.1707
2.1169
2.1069
2.0918
2.0479
1.2718
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0.9651
0.9102
0.0966
0.0102
NH
N
Me
2a
0.91
0.91
1.09
0.92
0.91
2.84
0.96
1.89
0.99
1.39
3.80
3.00
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10.0
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8.0
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6.0
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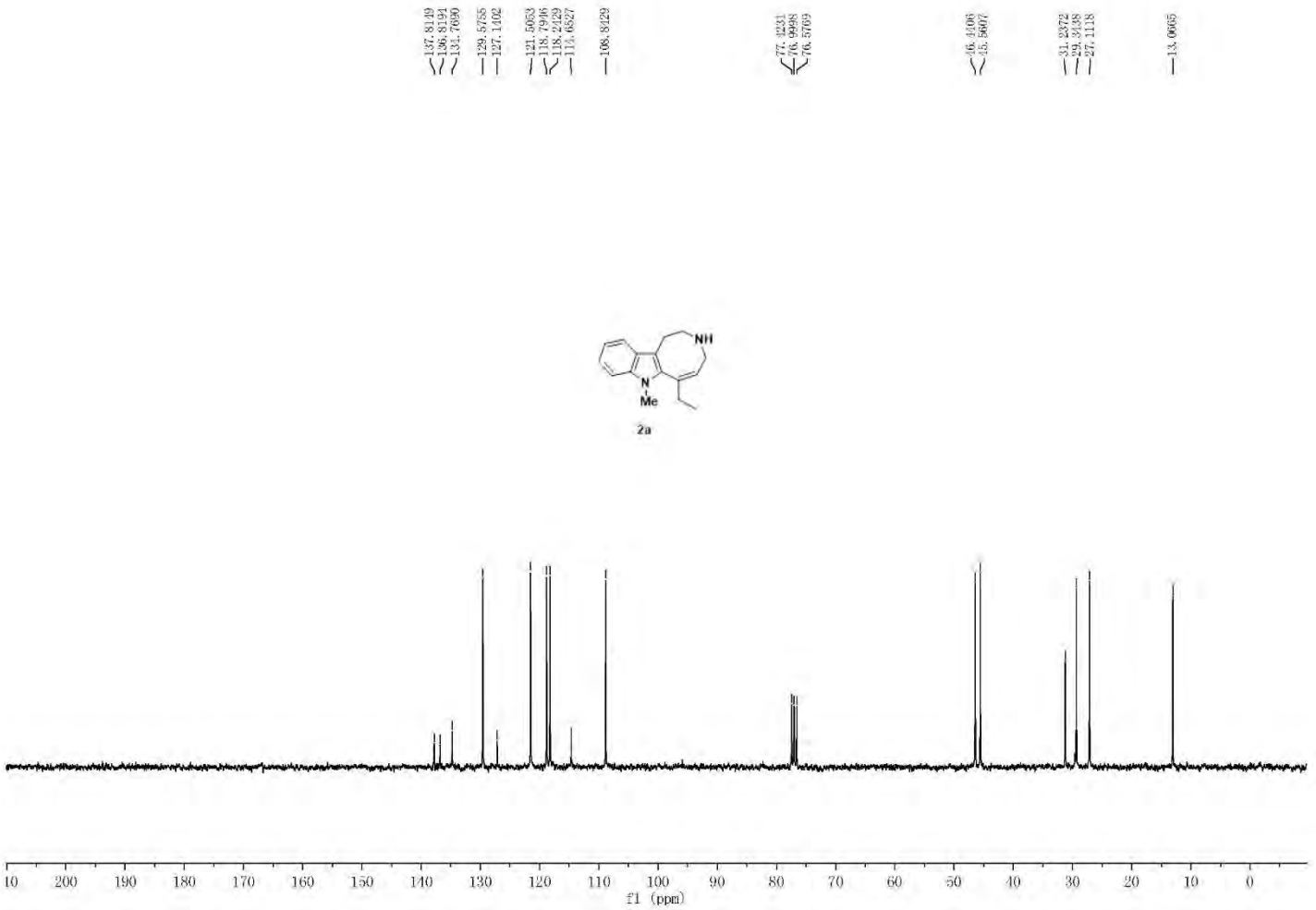
f1 (ppm)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76.9998
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31.2372
29.3435
27.1118
13.9665
NH
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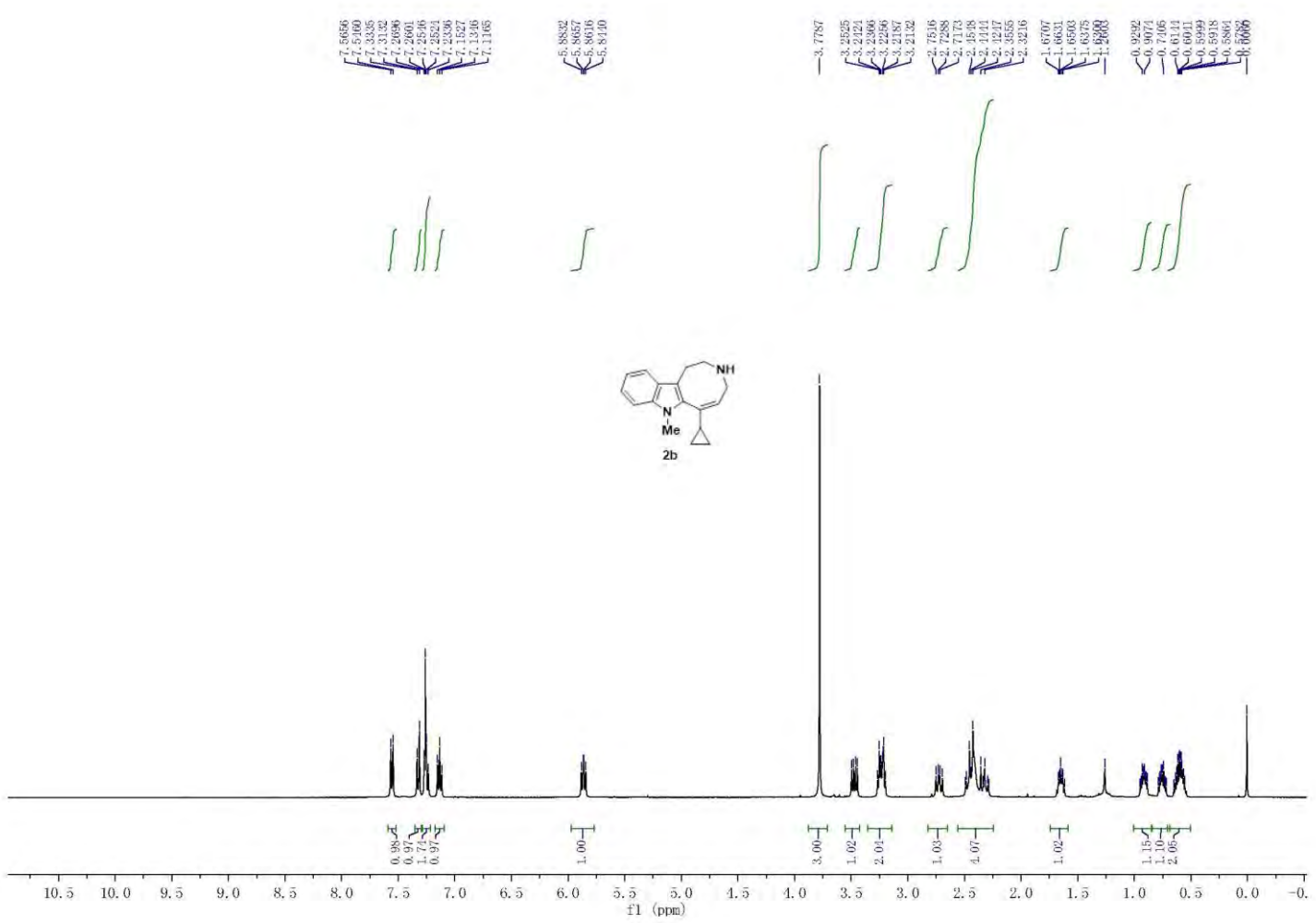
Me
2a
f1 (ppm)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Me
2b
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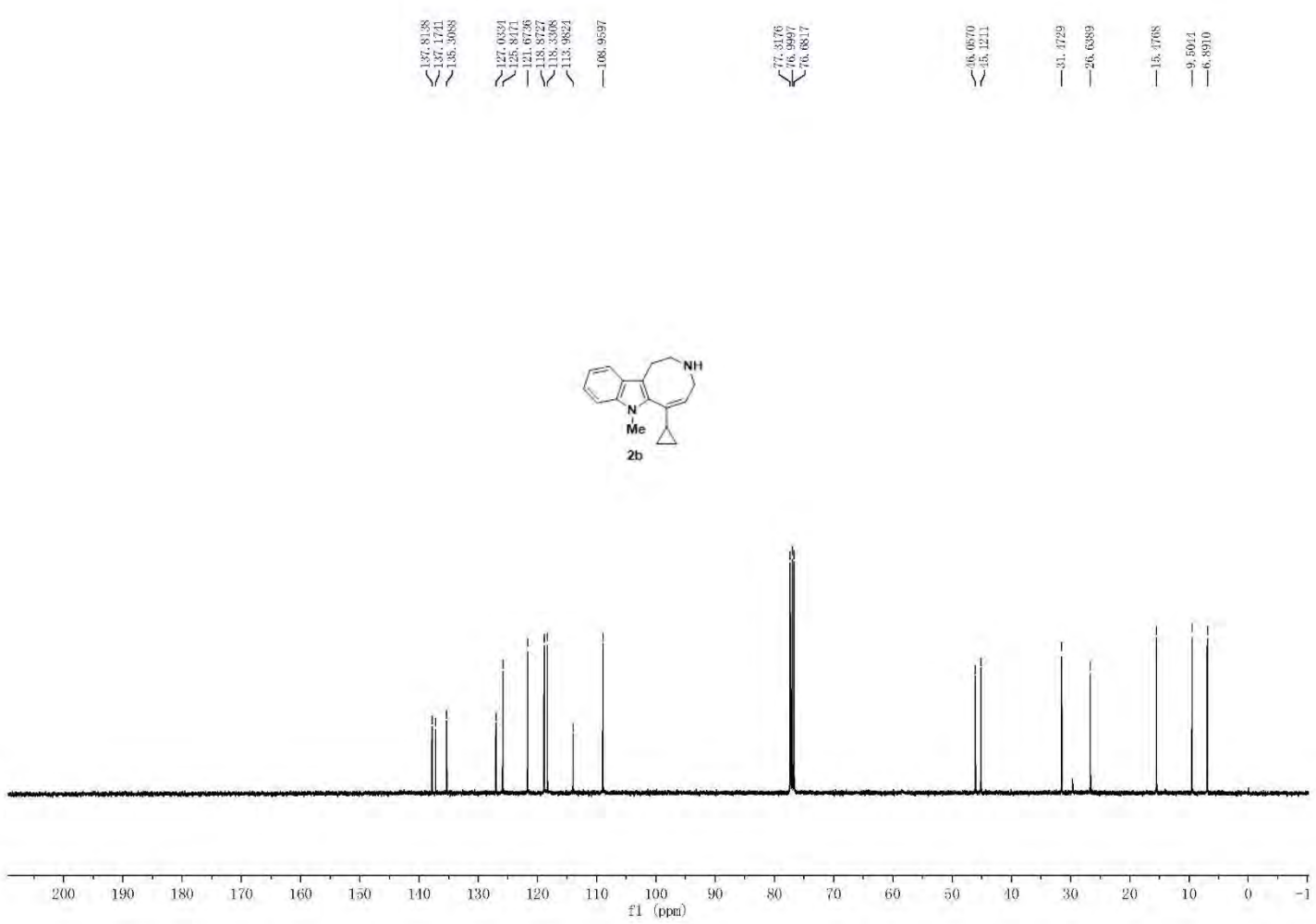
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76.9997
76.6817
36.0570
35.1211
31.4729
26.6389
15.5768
9.5044
6.8910
NH
N
Me
2b
200
190
180
170
160
150
140
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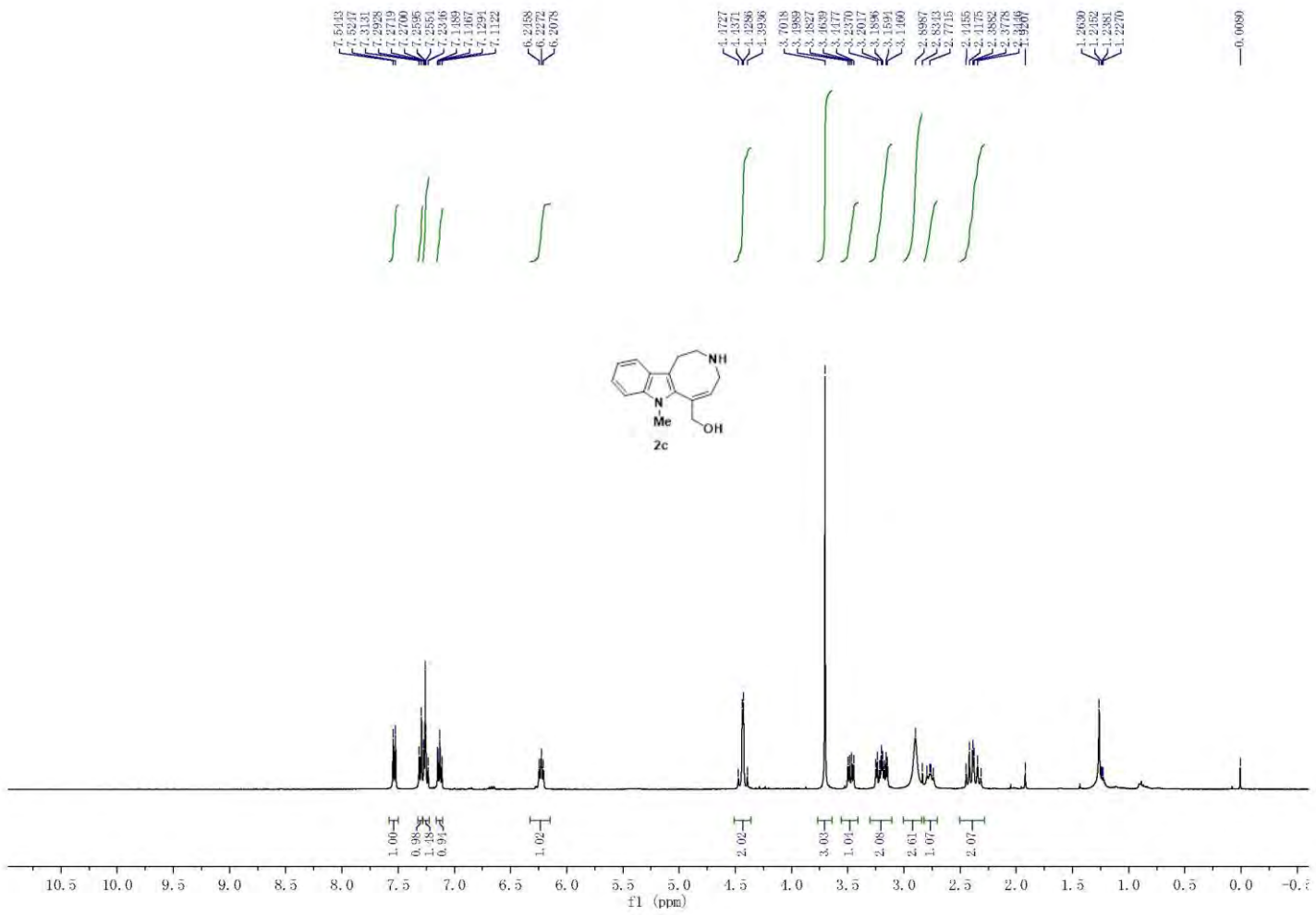
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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OH
2c
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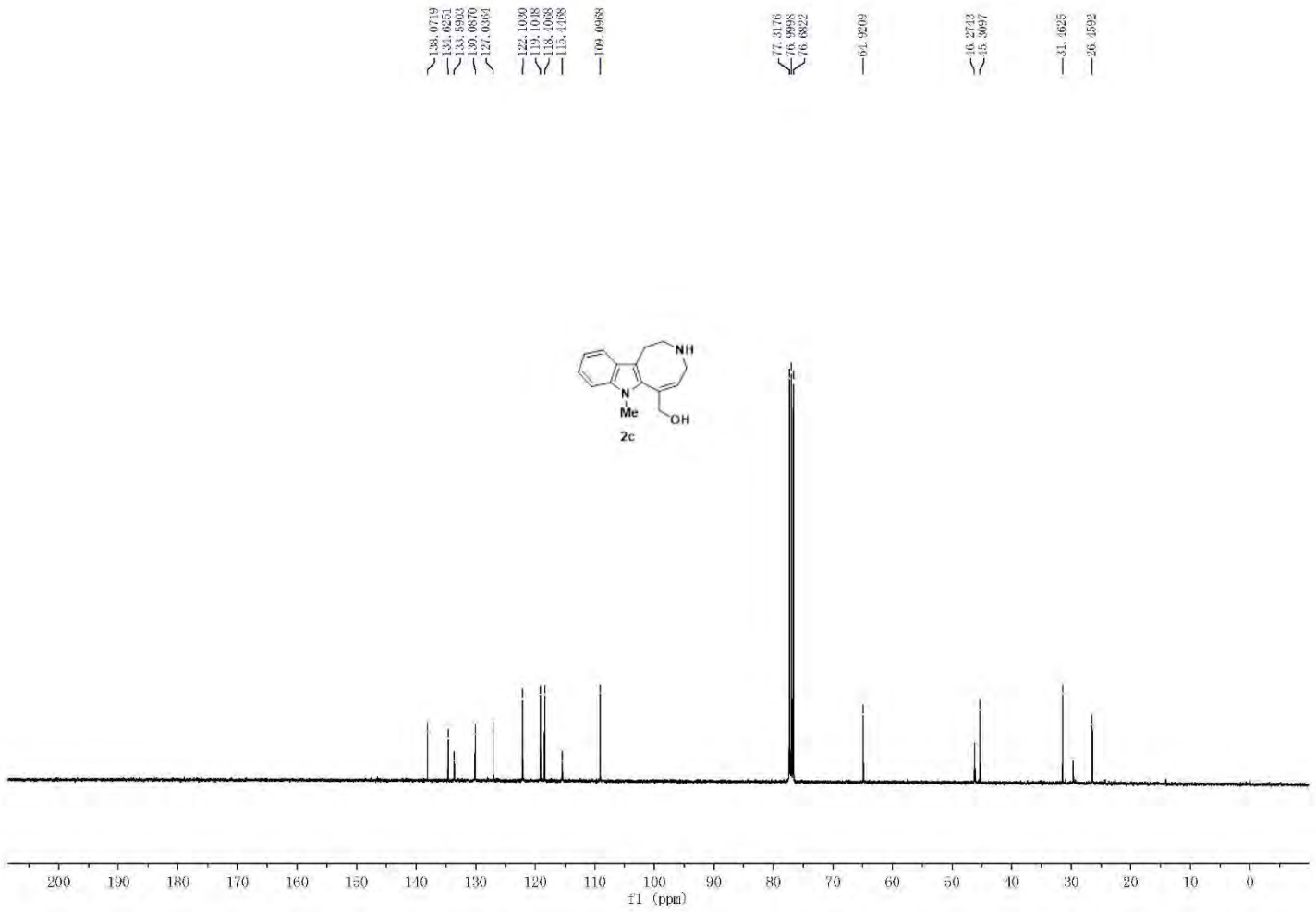
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76.9998
76.6822
61.9209
46.2743
45.3097
31.4625
26.0592
NH
N
Me
OH
2c
200
190
180
170
160
150
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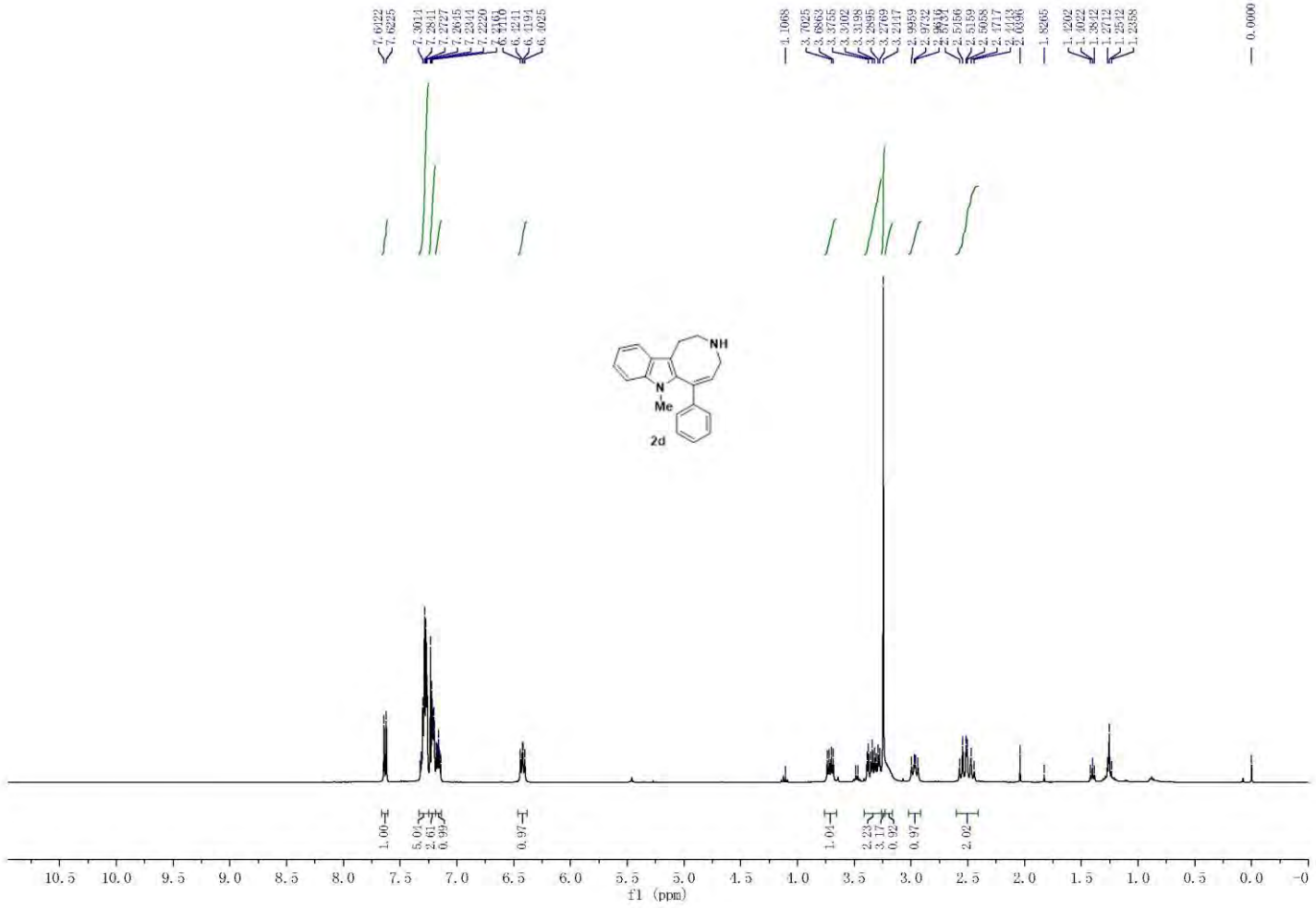
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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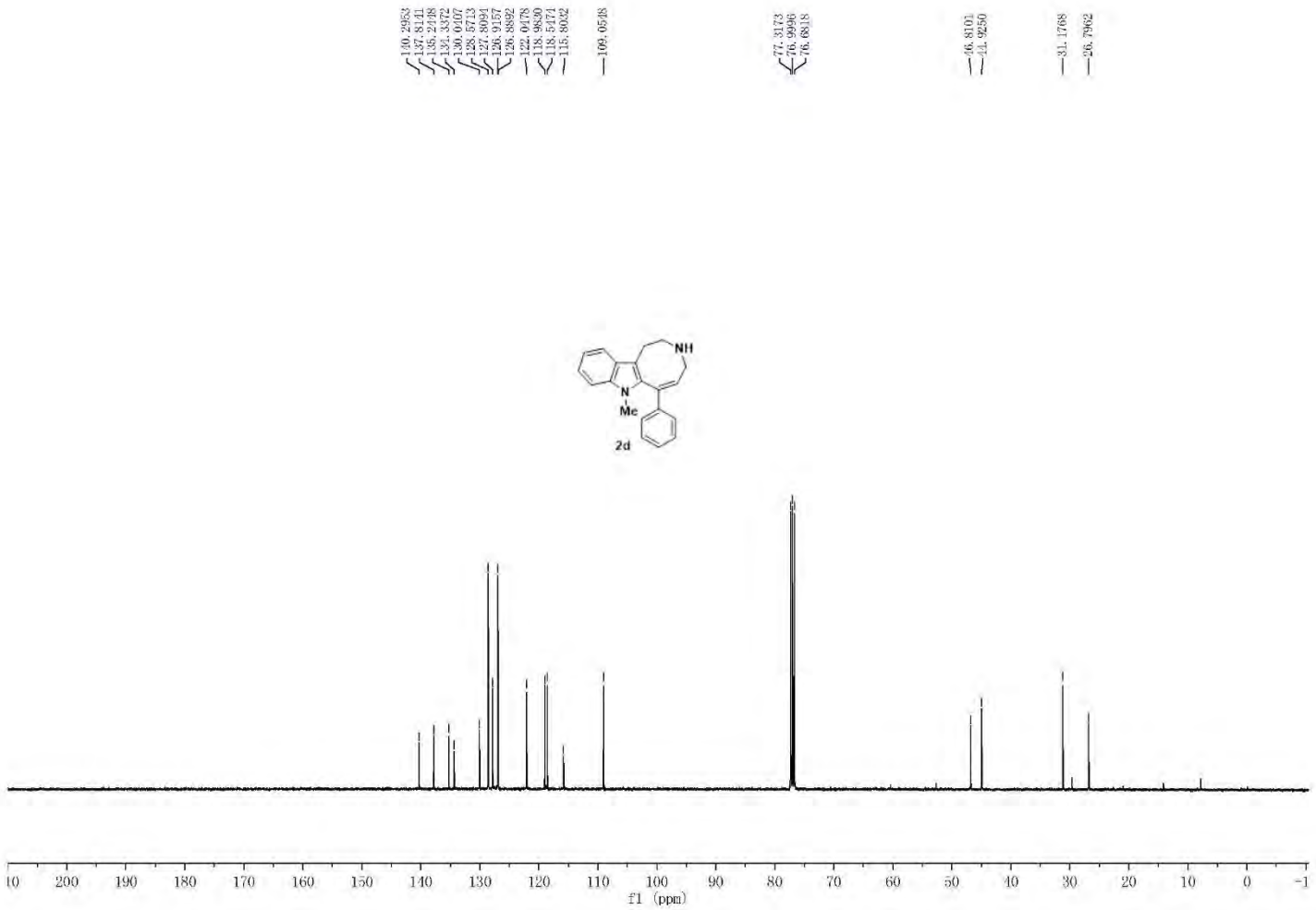
Me
2d
f1 (ppm)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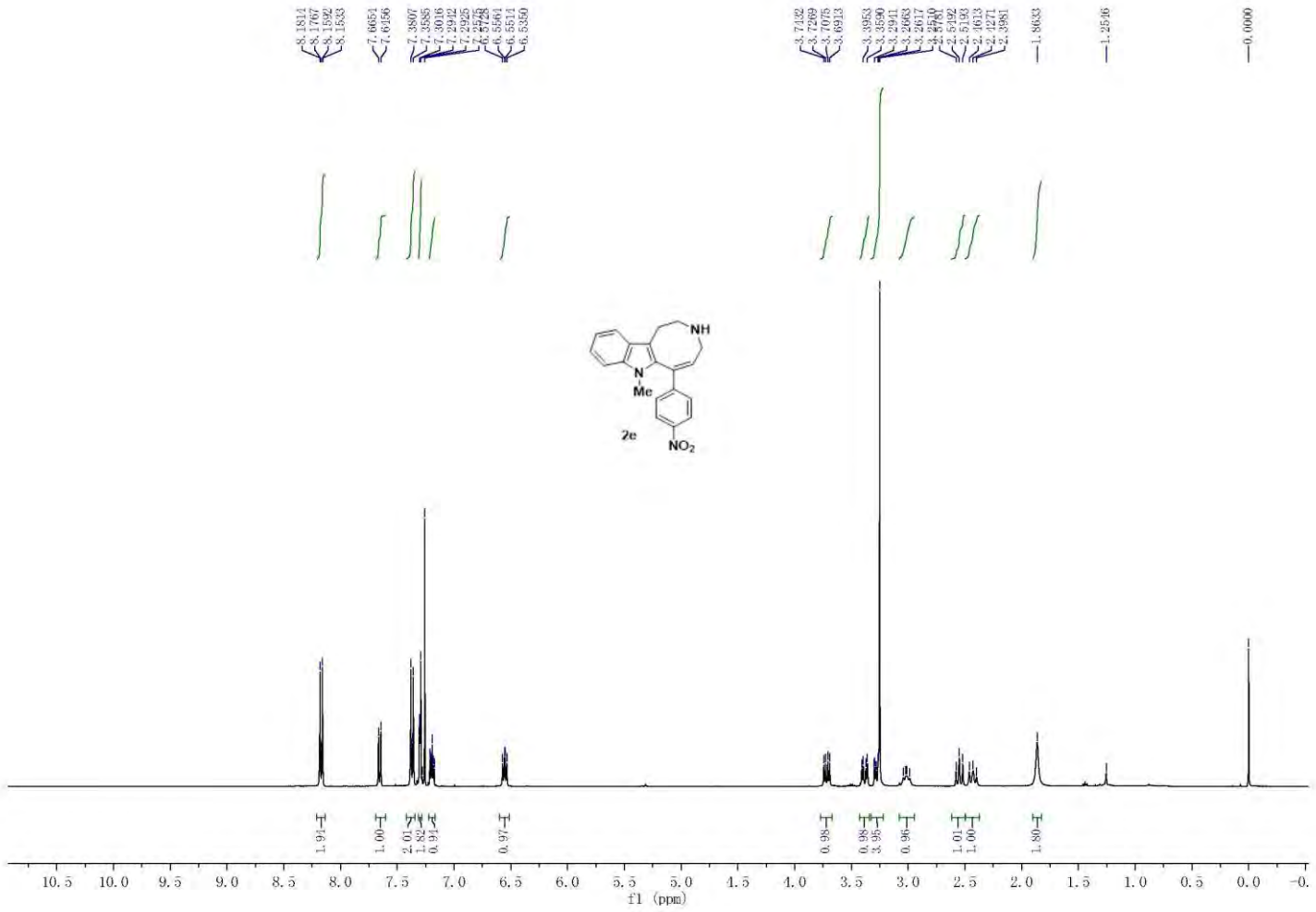
118.9859
118.5471
115.8052
109.0548
77.3173
76.9996
76.6818
46.8101
41.9250
31.1768
26.7962
NH
N
Me
2d
f1 (ppm)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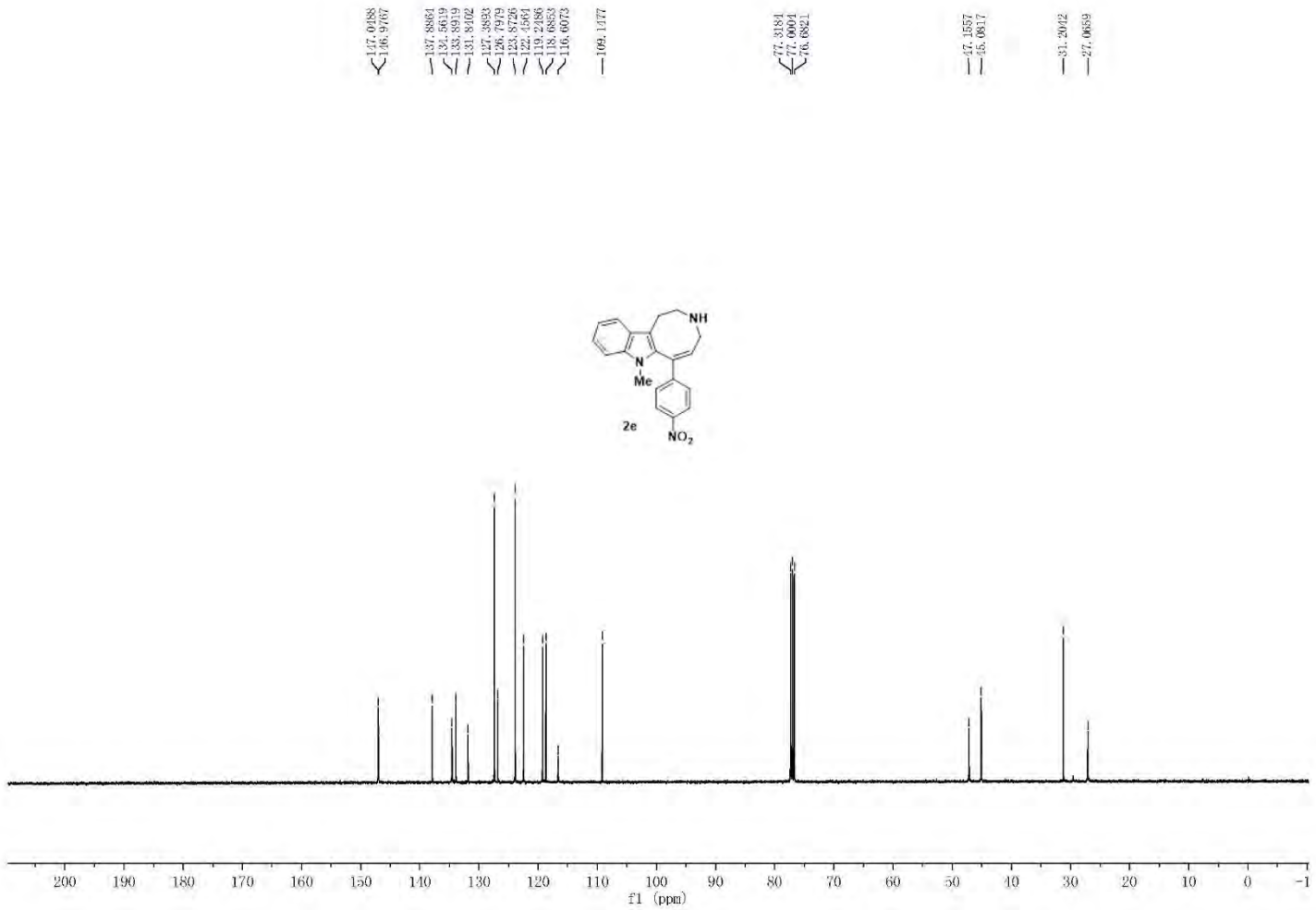
8.1592
8.1533
7.6651
7.6456
7.3807
7.3585
7.3016
7.2942
7.2925
6.5661
6.5511
6.5359
3.7432
3.7269
3.7075
3.6913
3.3953
3.3590
3.2941
3.2663
3.2617
2.6192
2.6130
2.1271
2.1081
1.8633
1.2546
0.0000
NH
N
Me
2e
NO2
1.94
1.00
2.01
1.82
0.94
0.97
0.98
0.98
3.95
0.96
1.01
1.00
1.80
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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118.6983
116.6073
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77.0004
76.6821
47.1557
45.0617
31.2042
27.0659
NH
N
Me
2e
NO2
200
190
180
170
160
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140
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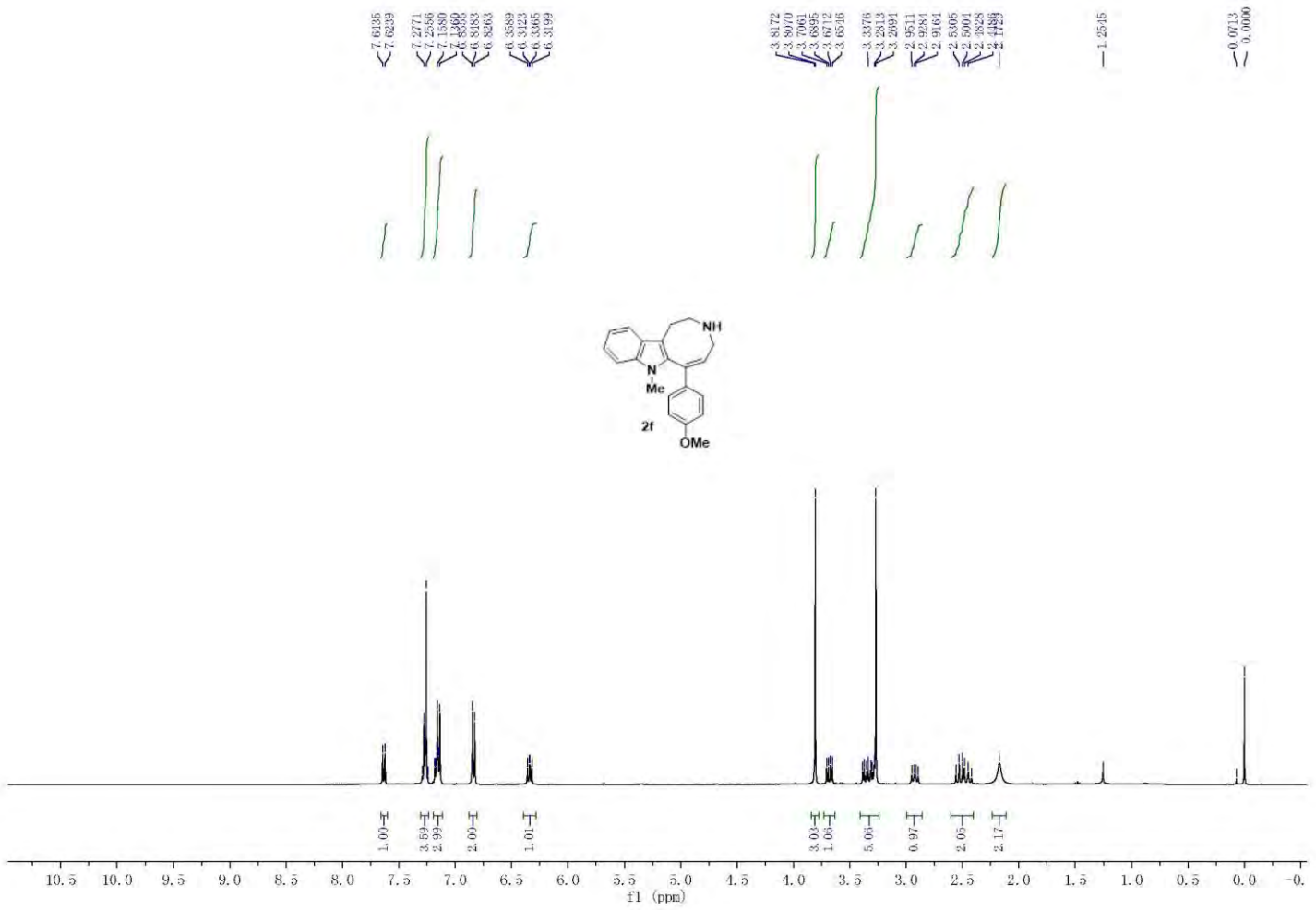
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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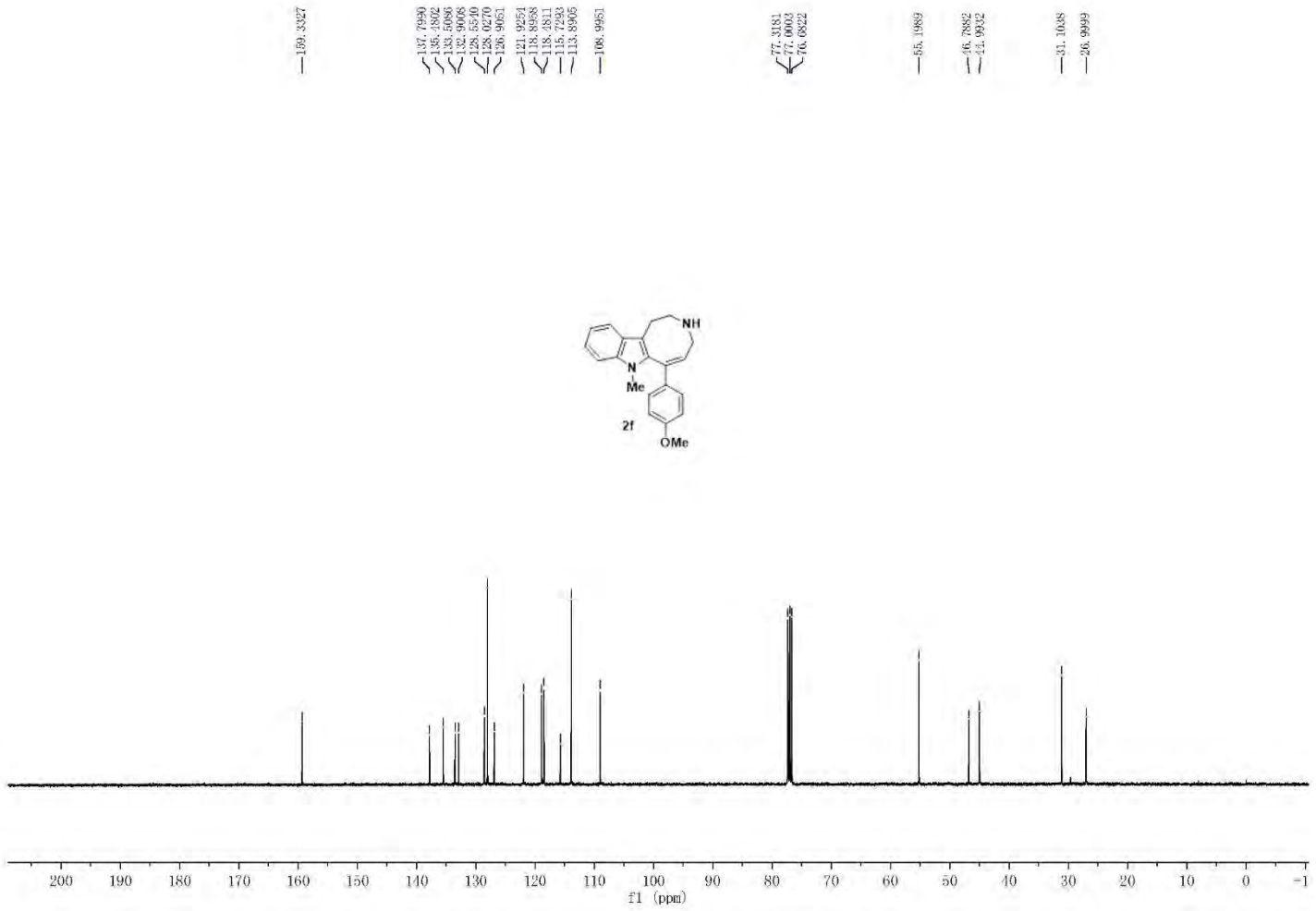
7.1580
7.1360
6.8858
6.8183
6.8263
6.3589
6.3323
6.3365
6.3199
3.8172
3.8070
3.7061
3.6895
3.6712
3.6536
3.3376
3.2813
3.2694
2.9511
2.9284
2.9161
2.5305
2.5091
2.1628
2.1499
1.2545
0.0713
0.0000
NH
N
Me
2f
OMe
1.00
3.59
2.99
2.00
1.01
3.03
1.06
5.06
0.97
2.05
2.17
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.
f1 (ppm)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77.3181
77.0003
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NH
N
Me
2f
OMe
200
190
180
170
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120
110
100
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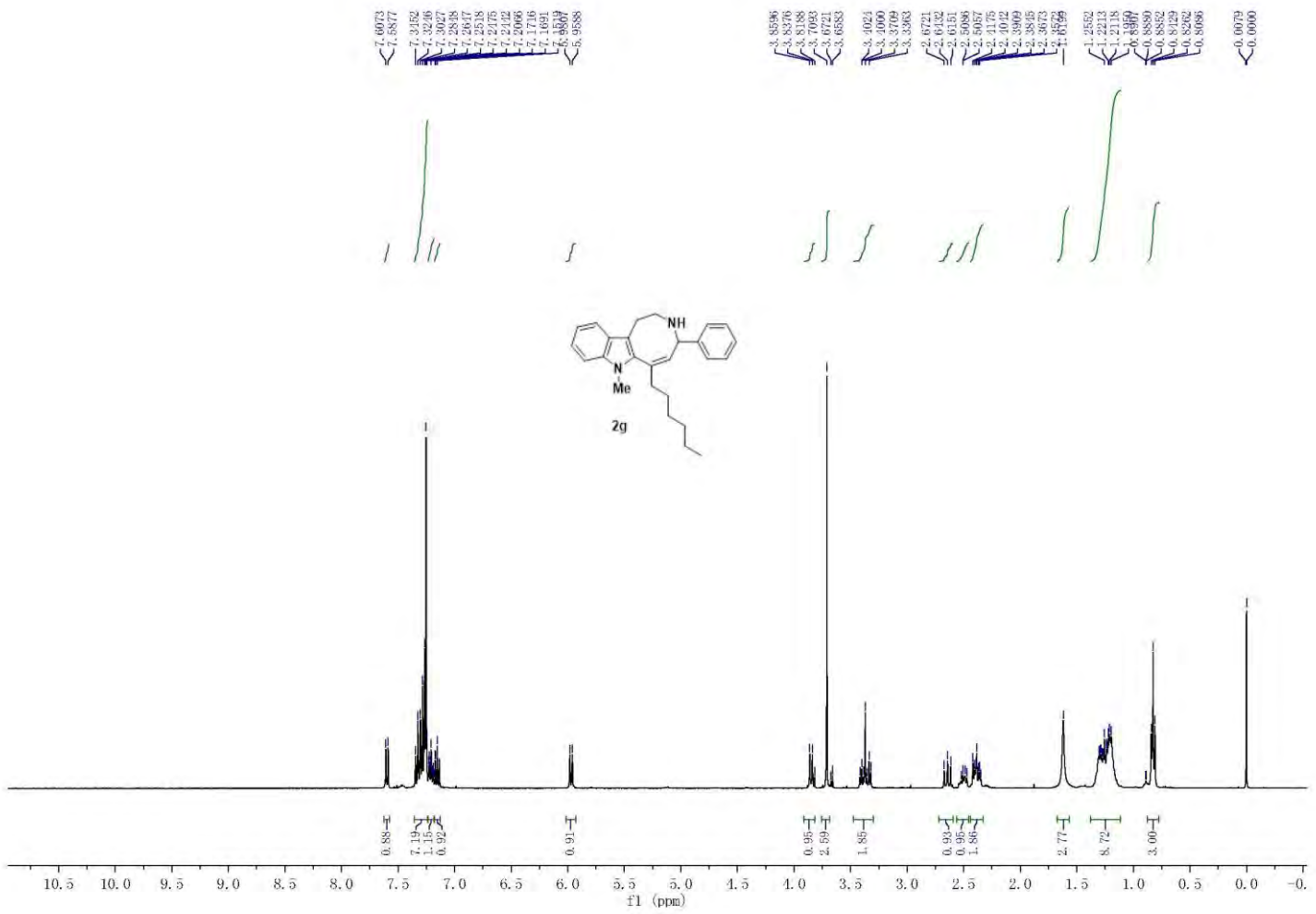
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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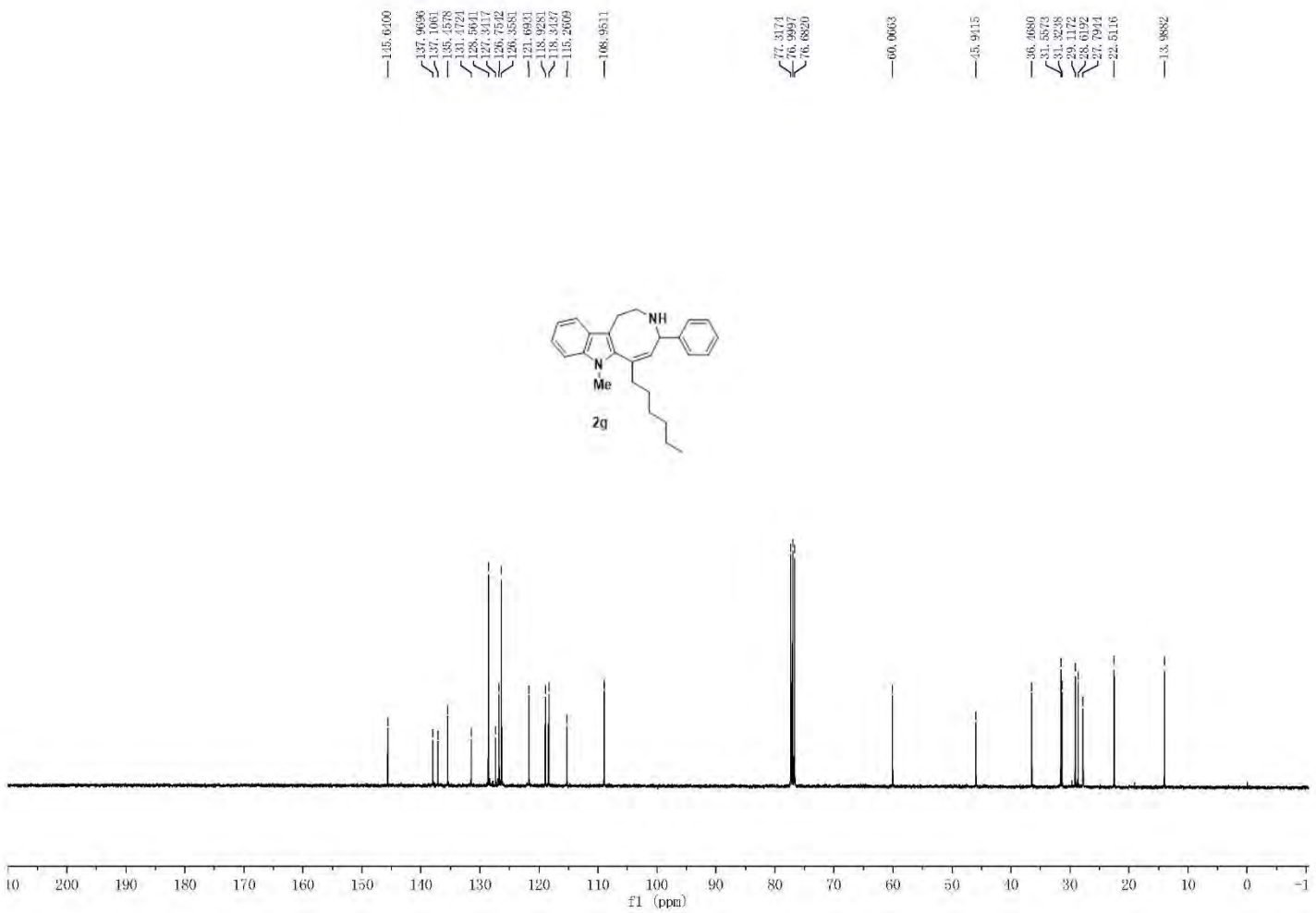
Me
2g
f1 (ppm)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108.9511
77.3171
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76.6820
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45.9415
36.4689
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22.6116
13.9882
NH
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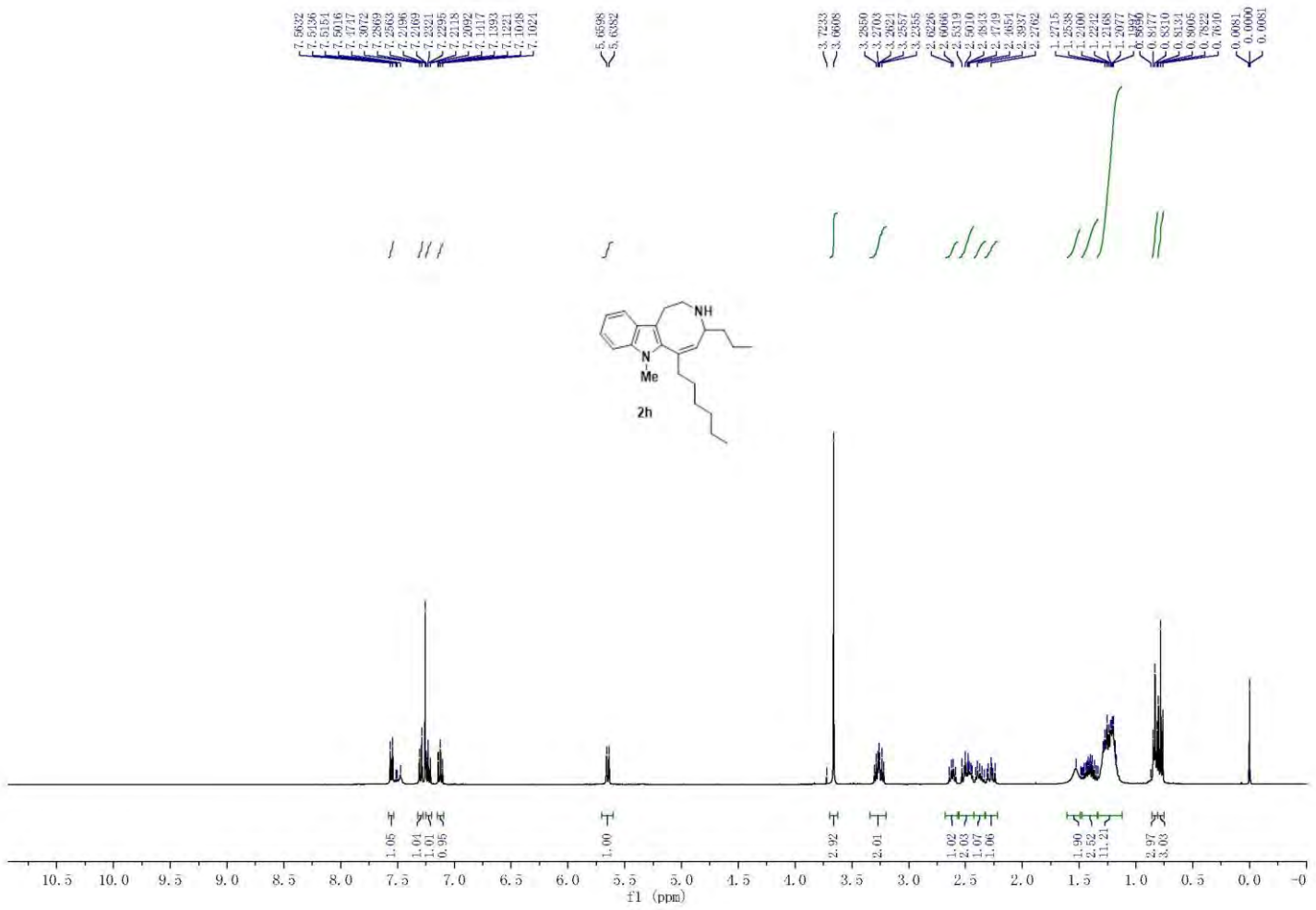
Me
2g
f1 (ppm)


NH
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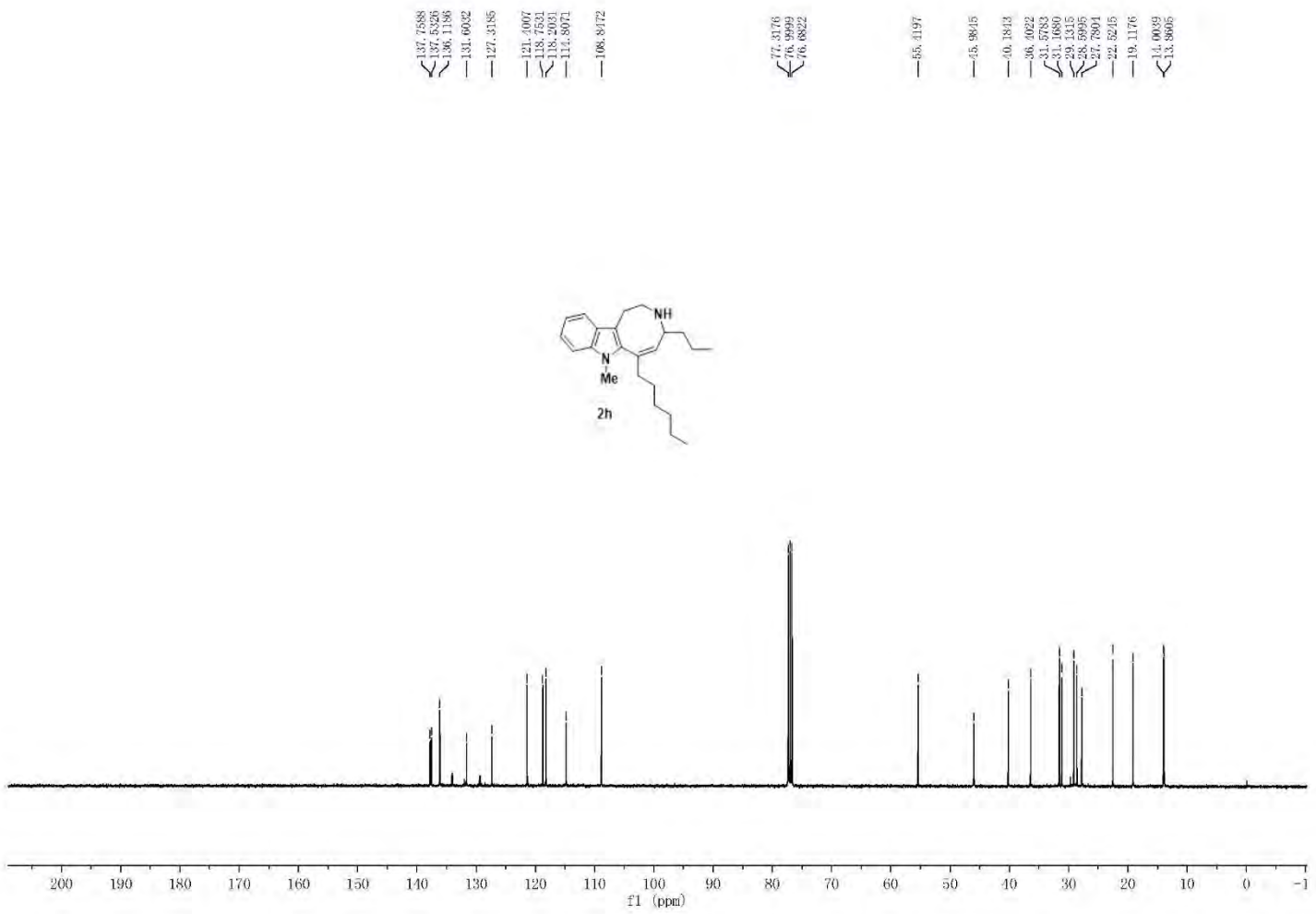
Me
2h
f1 (ppm)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108.8172
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76.9999
76.6822
55.4197
45.9845
40.1843
36.4022
31.5783
31.1080
29.3315
28.5995
27.7801
22.5245
19.1176
14.0039
13.9605
NH
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Me
2h
200
190
180
170
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140
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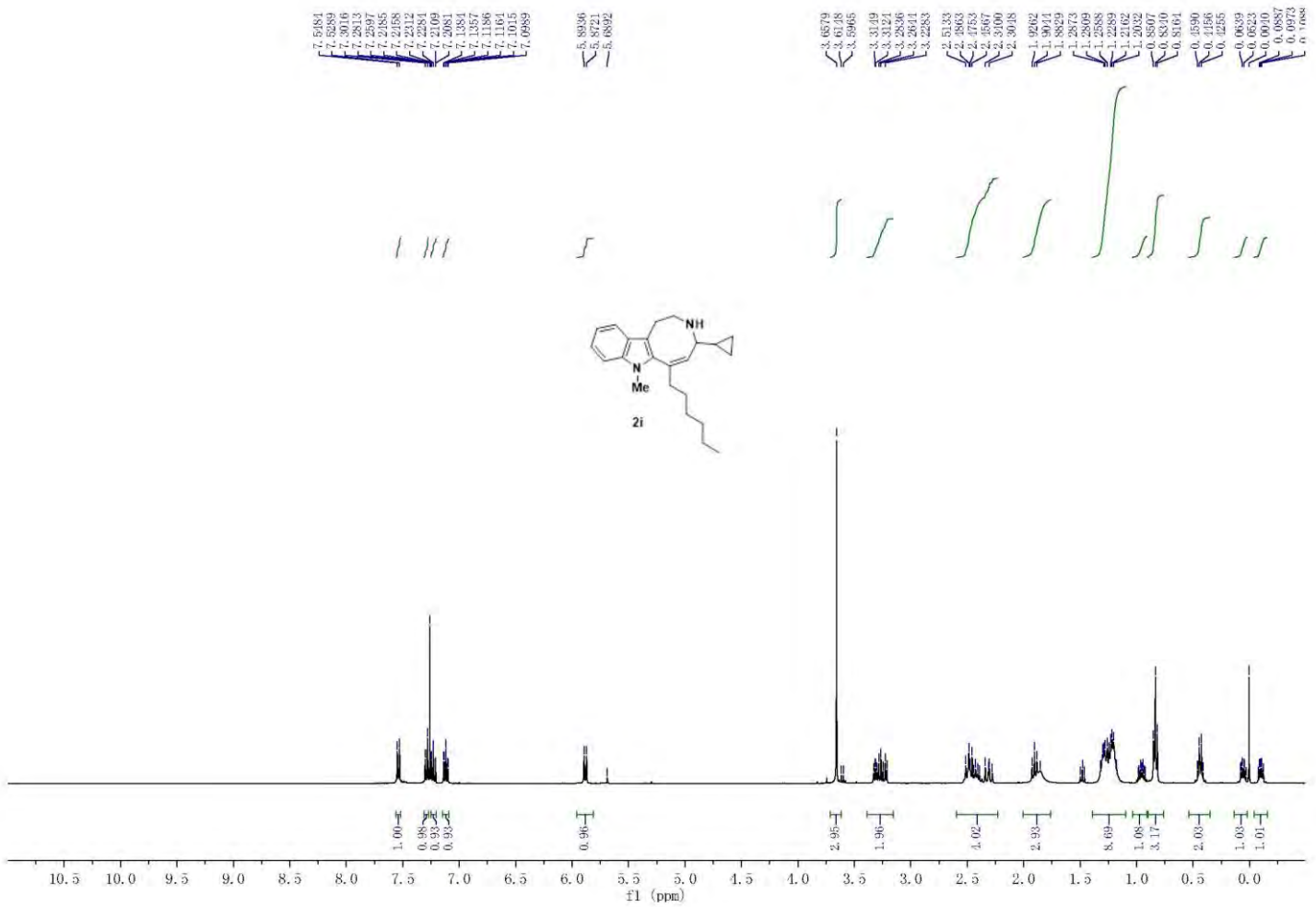
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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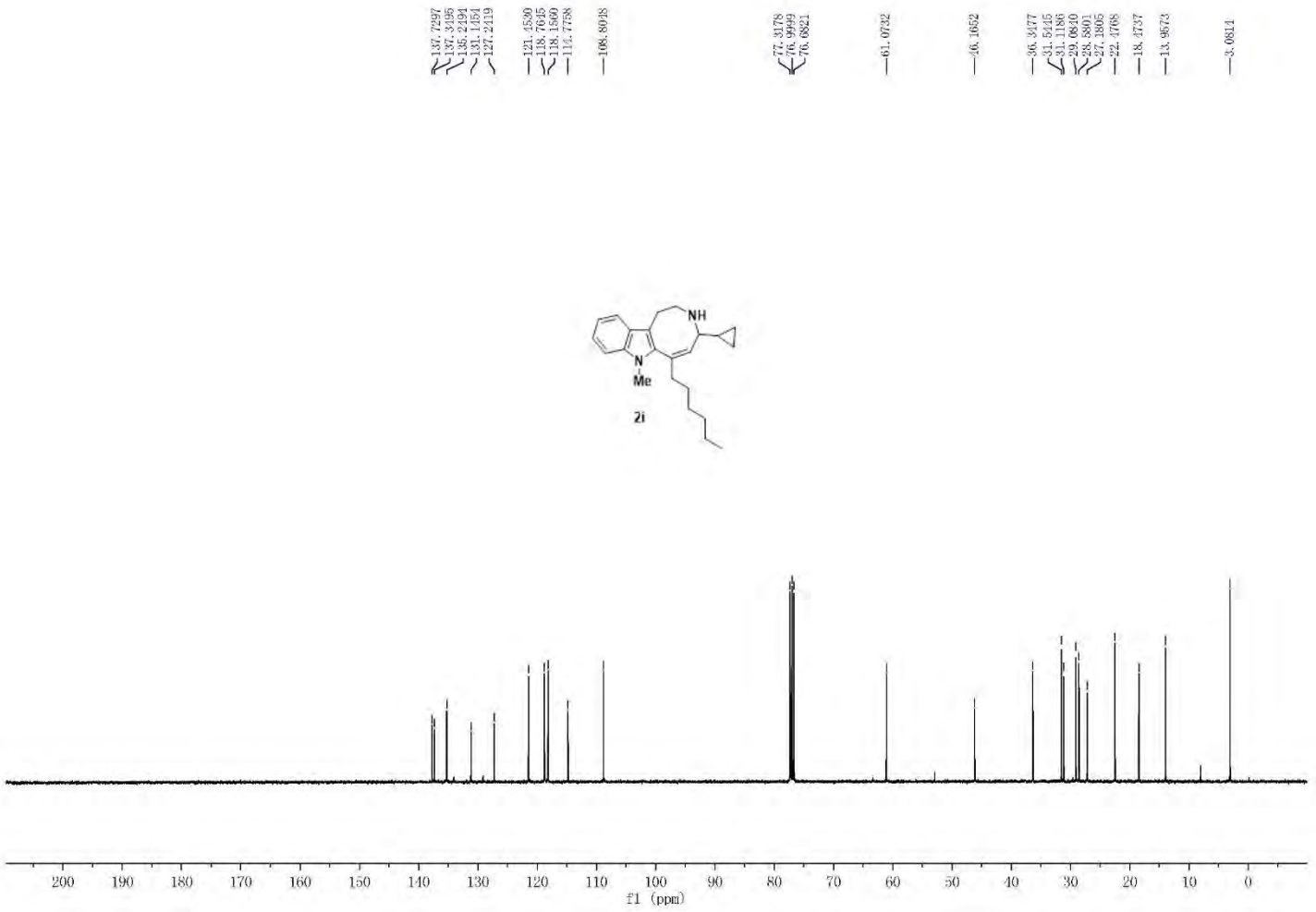
Me
2i
f1 (ppm)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46.1652
36.3477
31.5445
31.1186
29.0840
28.8801
27.1805
22.4768
18.4737
13.9573
3.0814
NH
N
Me
2i
200
190
180
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130
120
110
100
90
80
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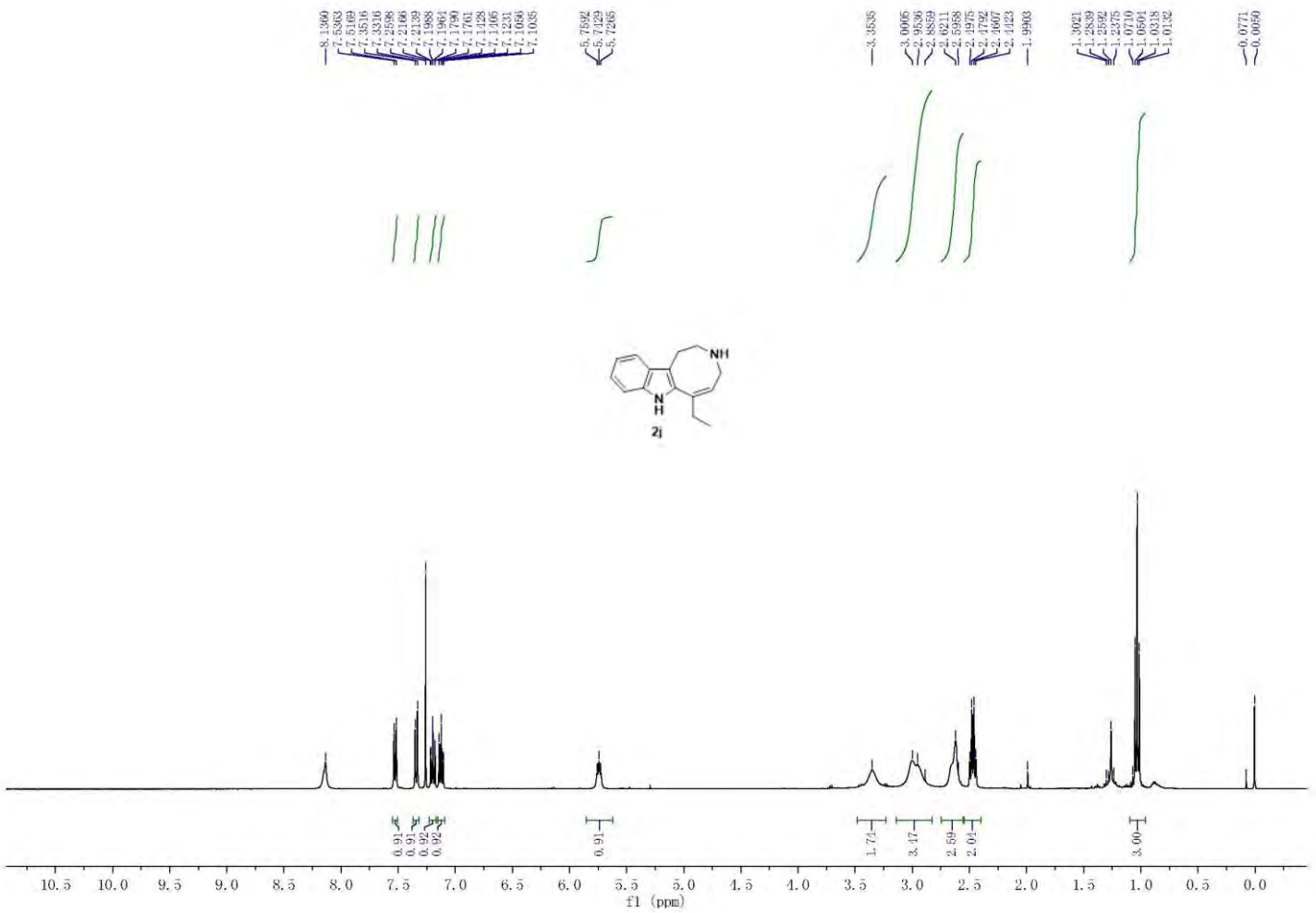
50
40
30
20
10
0
f1 (ppm)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1.2375
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1.0318
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0.0050
NH
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H
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0.91
0.92
0.92
0.91
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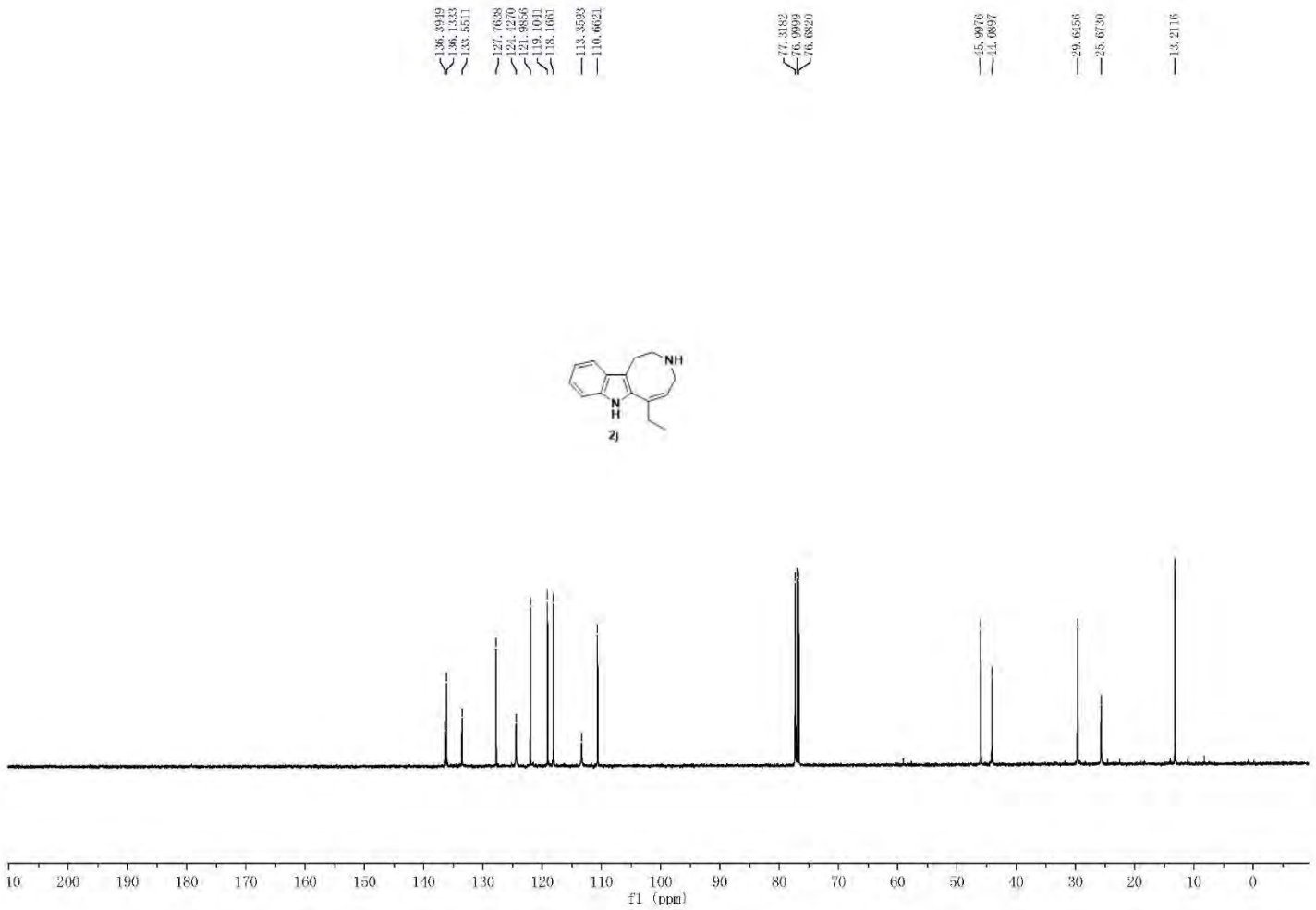
f1 (ppm)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25.6730
13.2116
NH
N
H
2j
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180
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10
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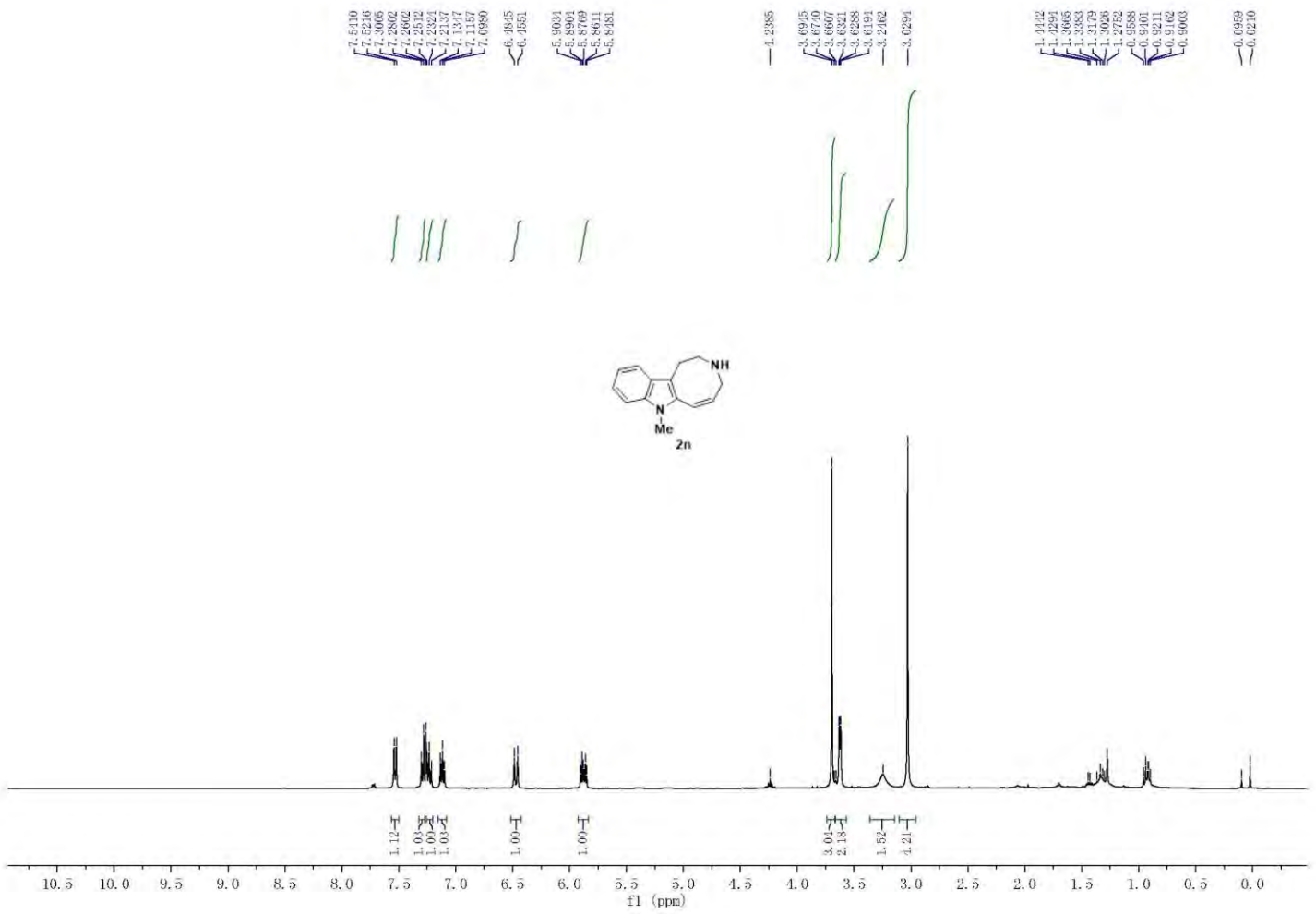
f1 (ppm)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6.4551
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5.8901
5.8769
5.8611
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4.2385
3.6945
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1.3026
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Me
2n
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1.03
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1.03
1.00
1.00
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1.52
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8.0
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6.5
6.0
5.5
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3.5
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2.5
2.0
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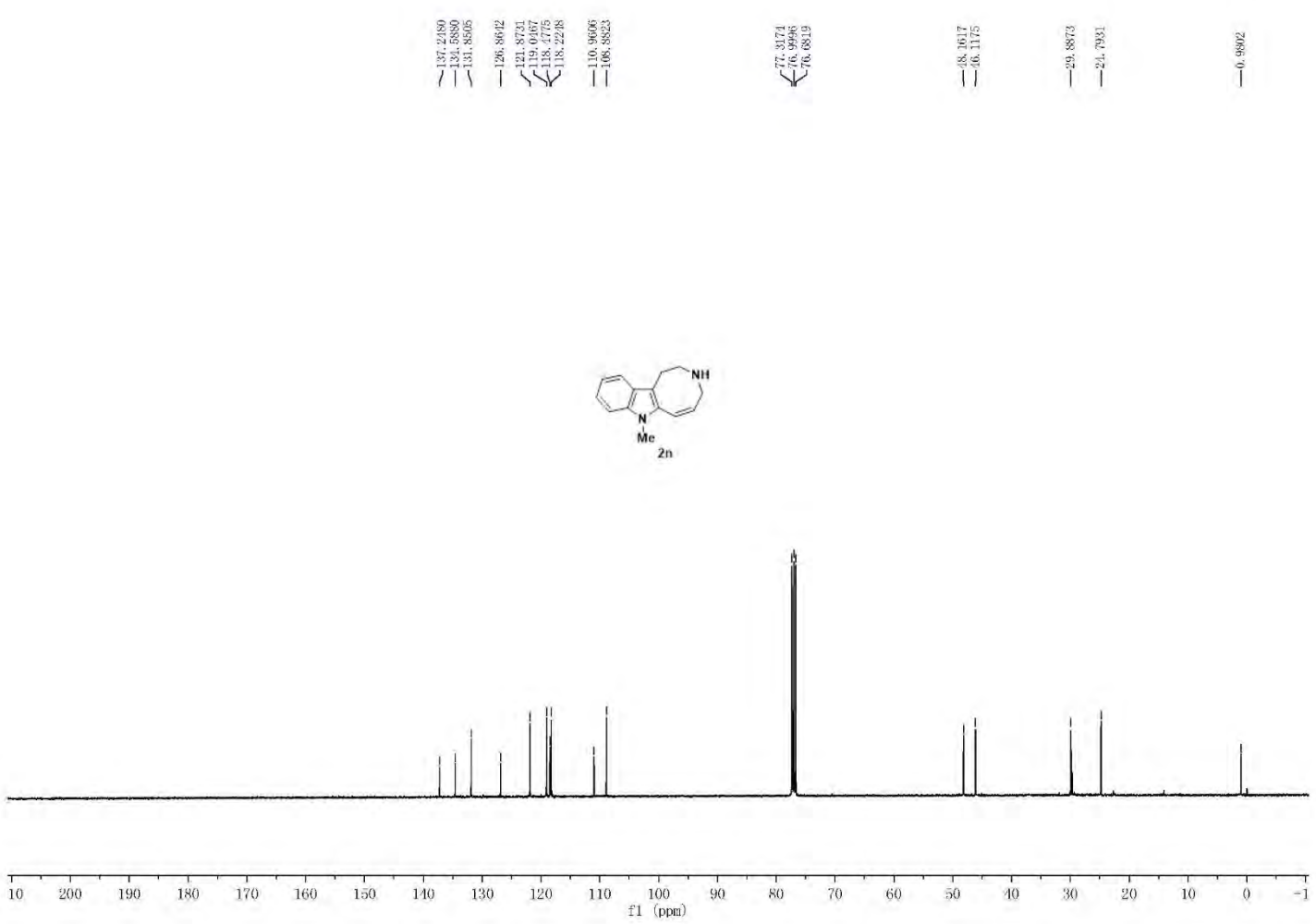
f1 (ppm)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76.9996
76.6819
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46.1175
29.8873
24.7931
0.9892
NH
N
Me
2n
10
200
190
180
170
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120
110
100
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80
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60
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30
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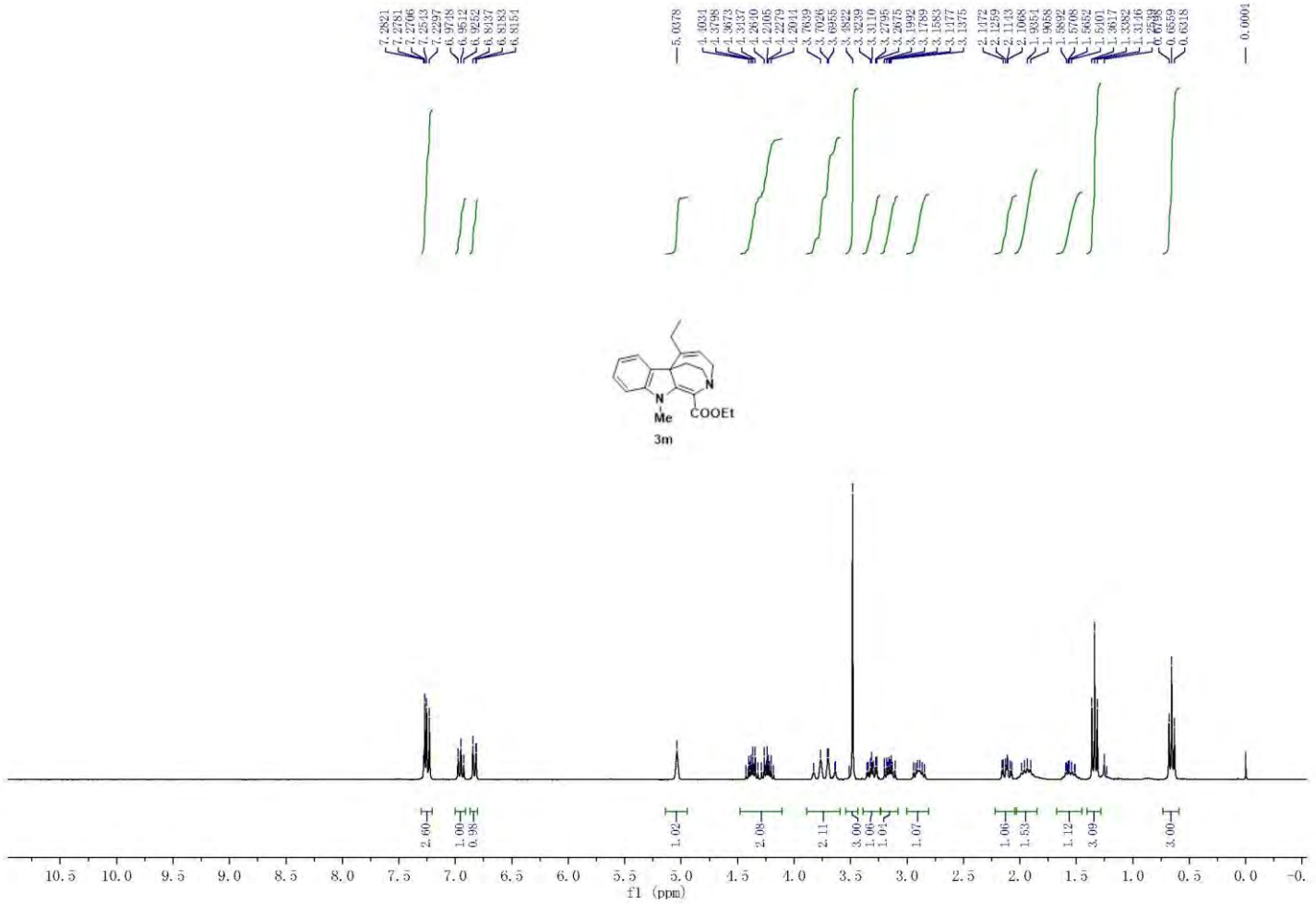
f1 (ppm)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6.9252
6.8137
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1.0031
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1.3673
1.3437
1.2610
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1.2279
1.2041
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Me
COOEt
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3.00
1.06
1.04
1.07
1.06
1.53
1.12
3.09
3.00
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10.0
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8.0
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7.0
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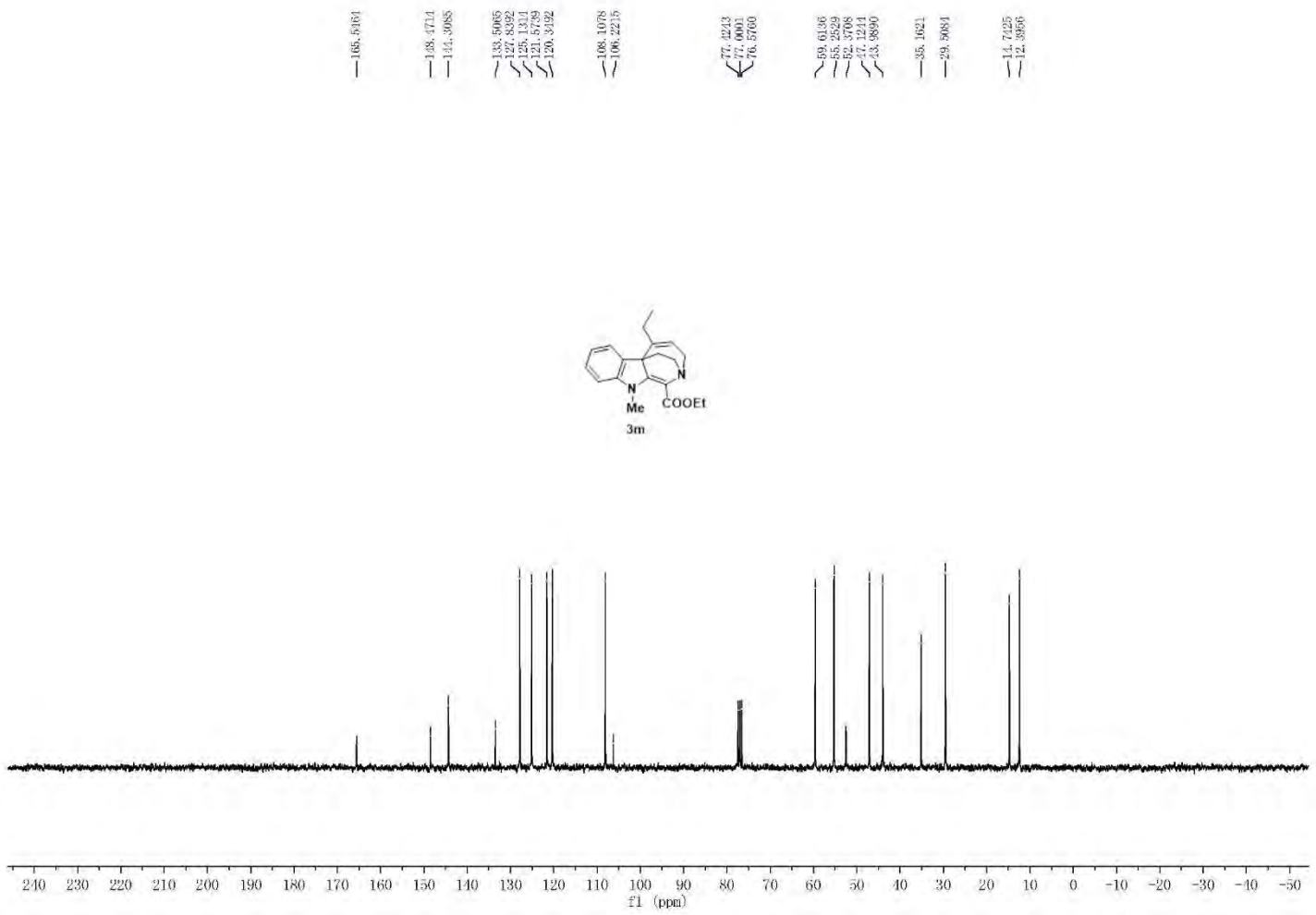
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.
f1 (ppm)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121.5739
120.3192
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77.4243
77.0001
76.5760
59.6136
55.2529
52.5706
47.1244
43.3890
35.1621
29.9084
14.7425
12.3956
N
N
Me
COOEt
3m
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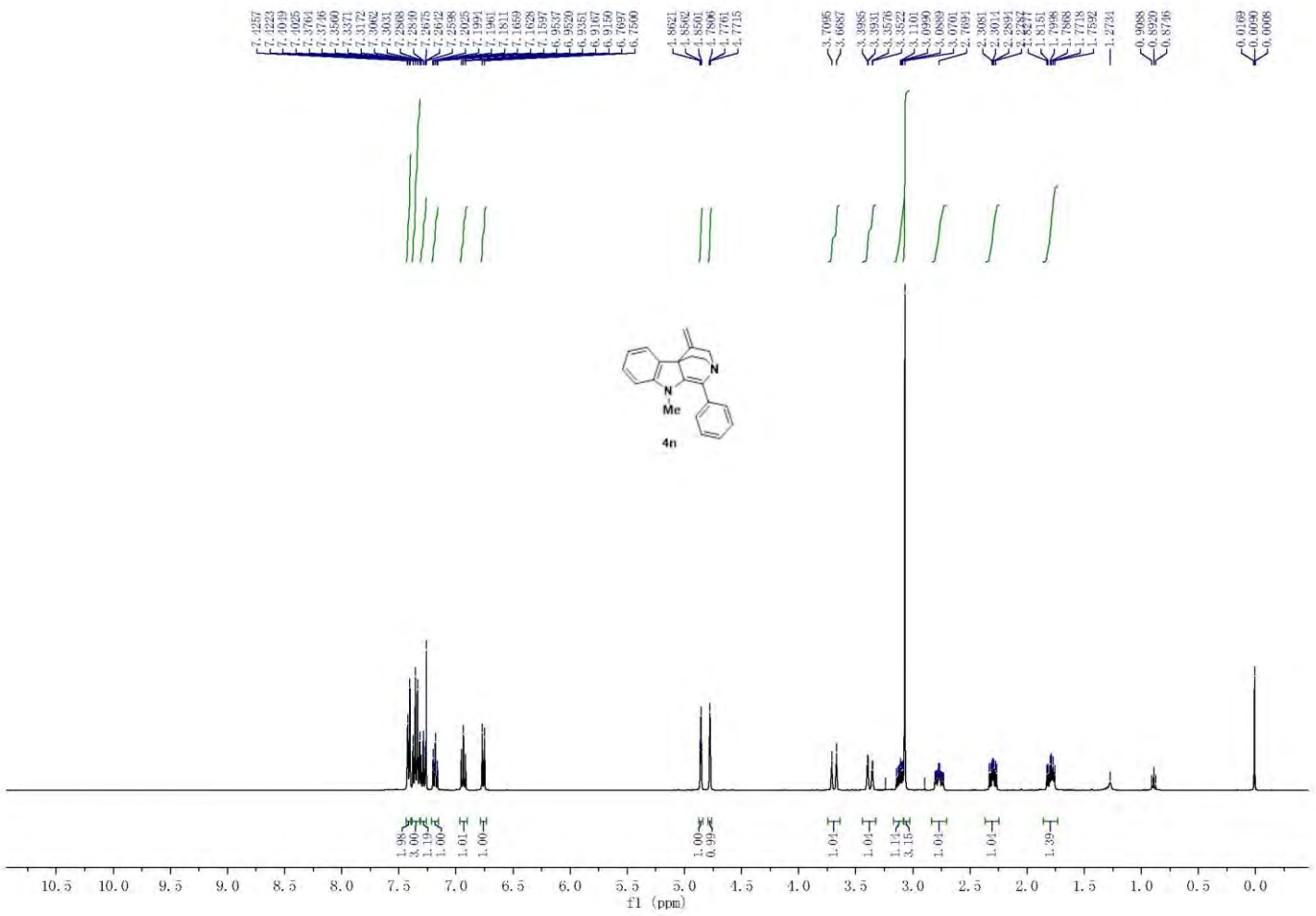
f1 (ppm)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Me
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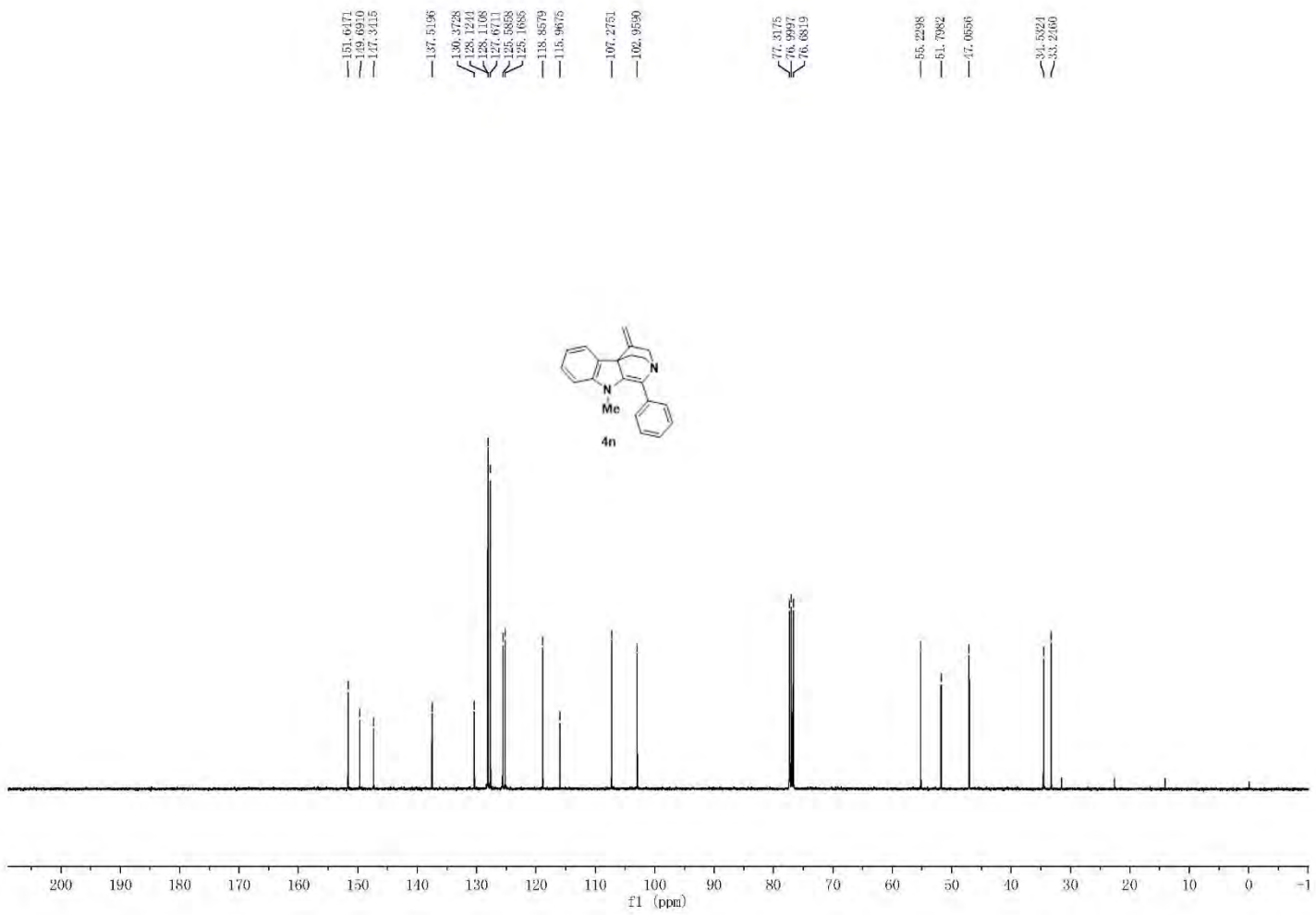
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118.8579
115.9675
107.2751
102.9590
77.3175
76.9997
76.6819
55.2298
51.7982
47.0656
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33.2460
N
N
Me
4n
200
190
180
170
160
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140
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120
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100
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80
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60
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40
30
20
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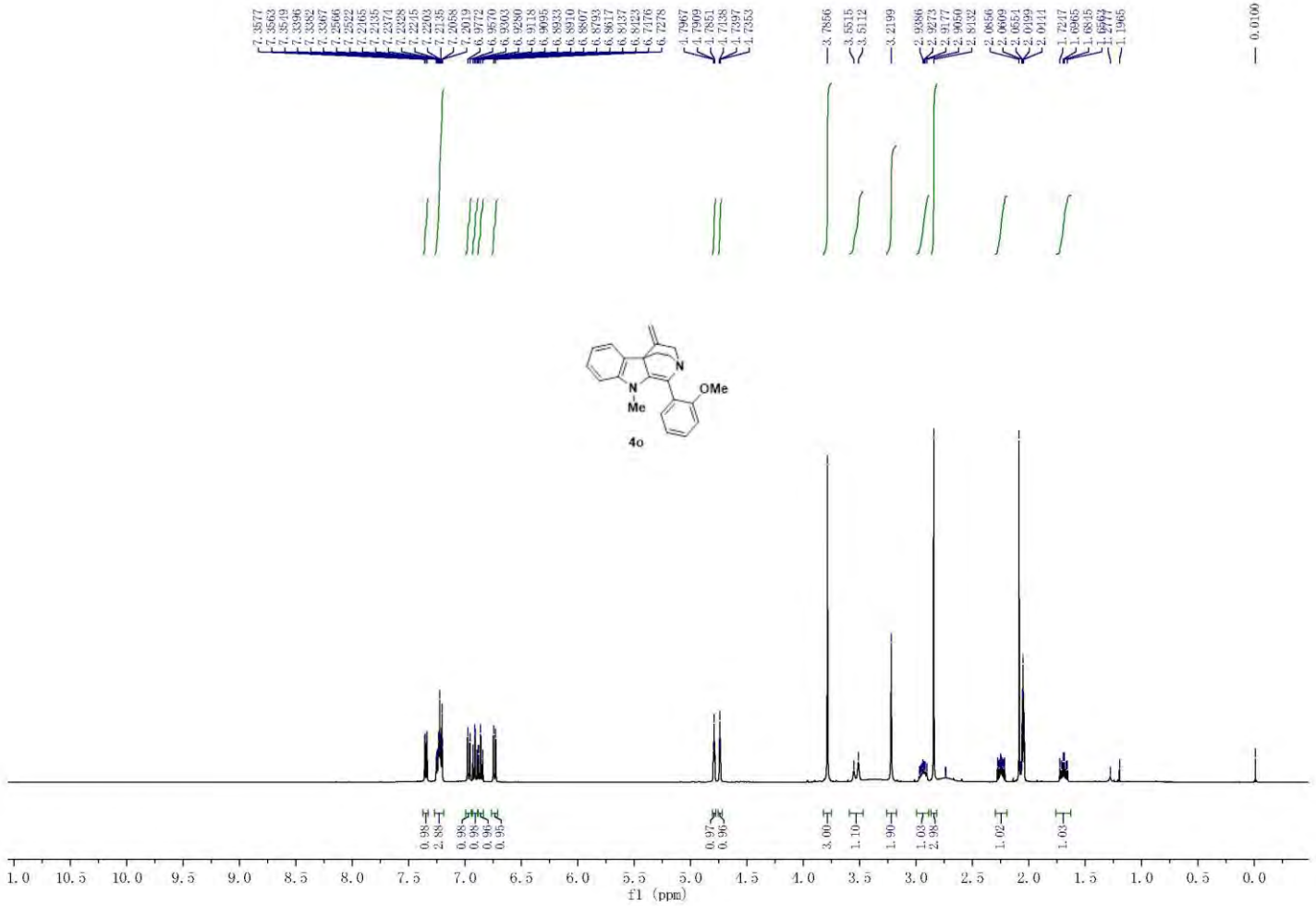
-1
f1 (ppm)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N
N
Me
4o
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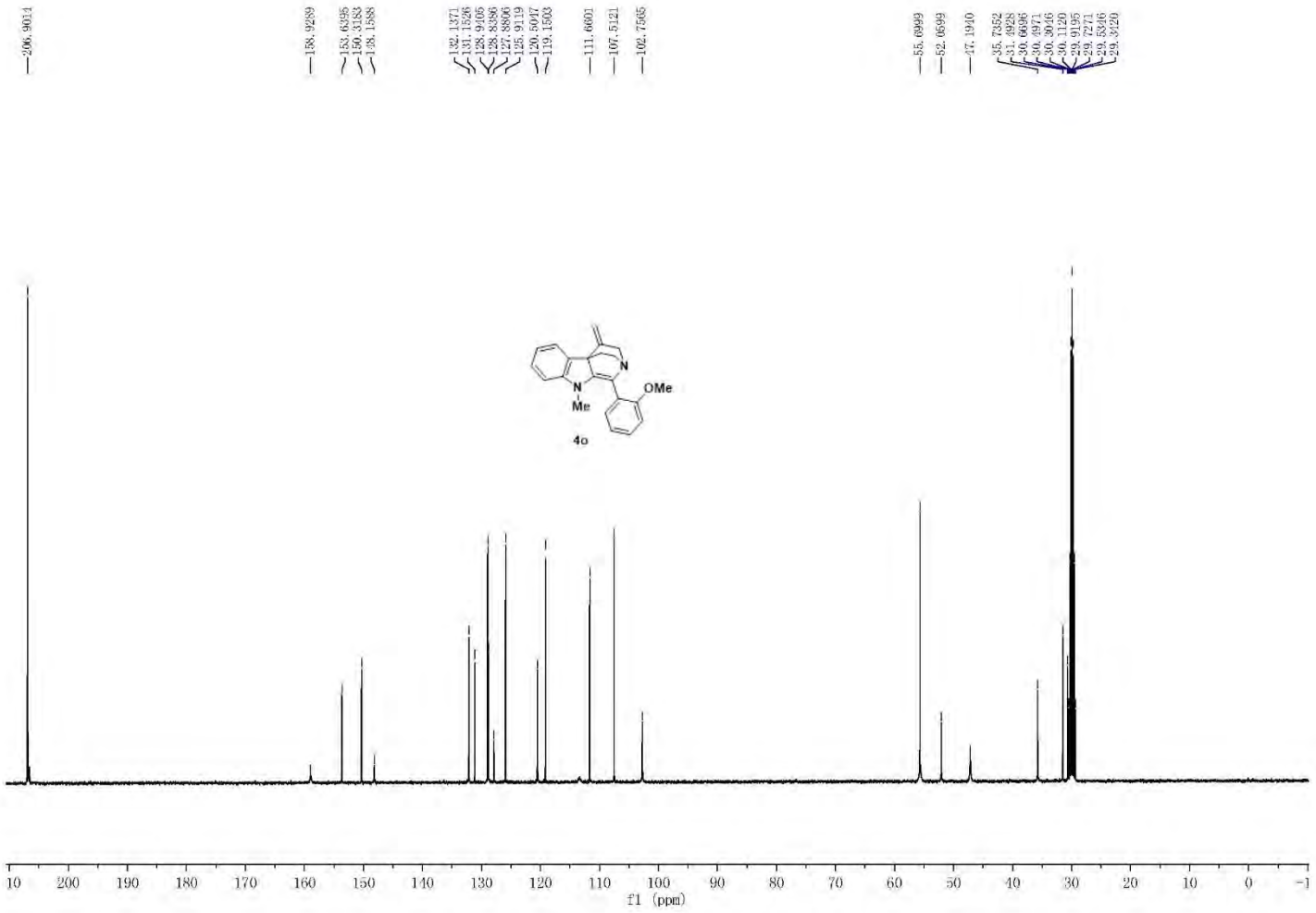
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111.6601
107.5121
102.7565
55.6999
52.0699
47.1940
35.7352
31.3928
30.6696
30.4971
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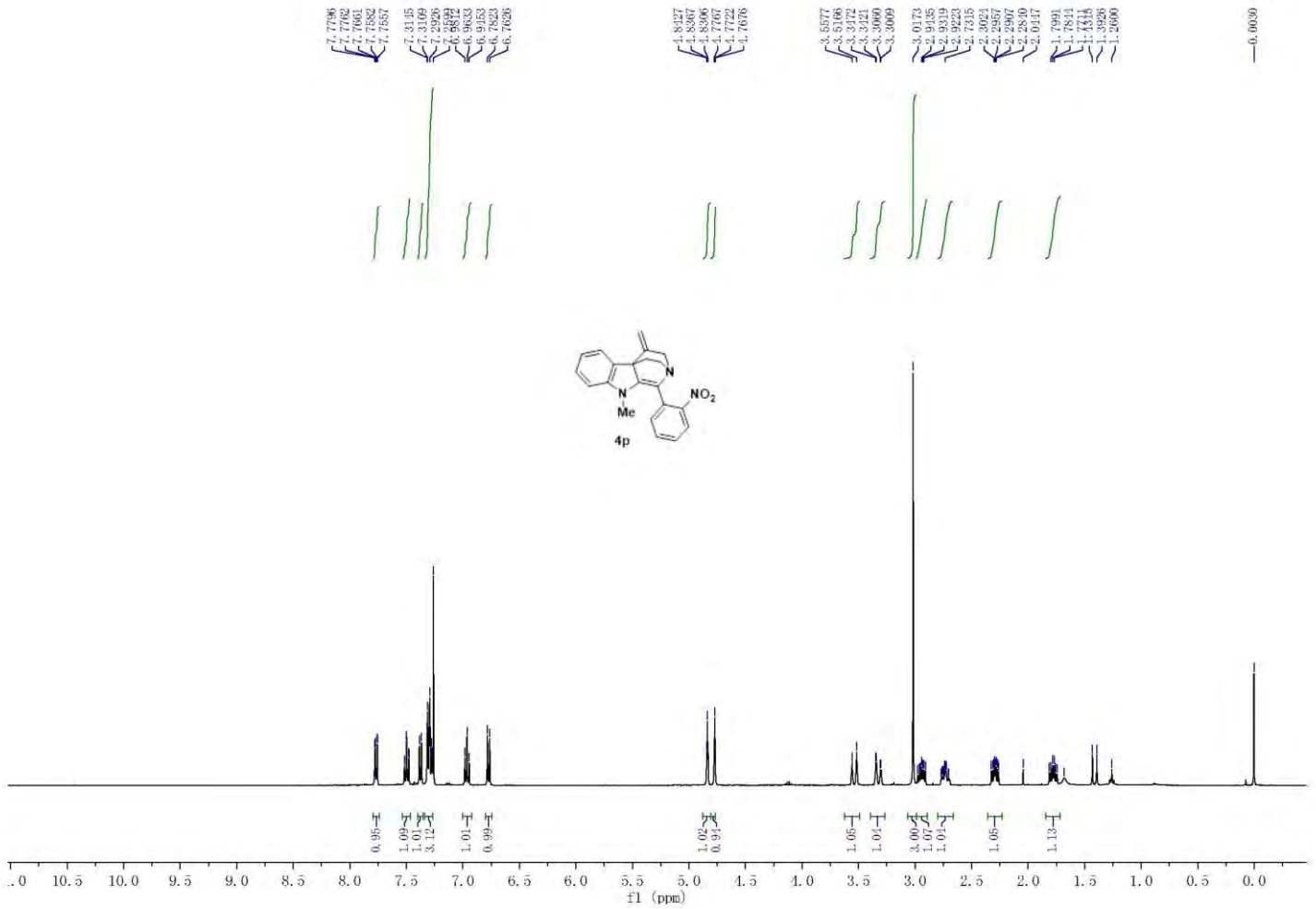
29.9195
29.7271
29.5346
29.3420
OMe
N
N
Me
4o
f1 (ppm)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7.3145
7.3109
7.2926
6.9633
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6.7823
6.7626
1.8127
1.8367
1.8306
1.7767
1.7722
1.7676
3.5577
3.5106
3.3372
3.3421
3.3069
3.3009
3.0173
2.9435
2.9319
2.9223
2.7315
2.3021
2.2957
2.2907
2.2840
2.0417
1.7991
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1.7771
1.7434
1.3926
1.2600
0.0000
N
N
Me
NO2
4p
0.95
1.09
1.01
3.12
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0.94
1.05
1.04
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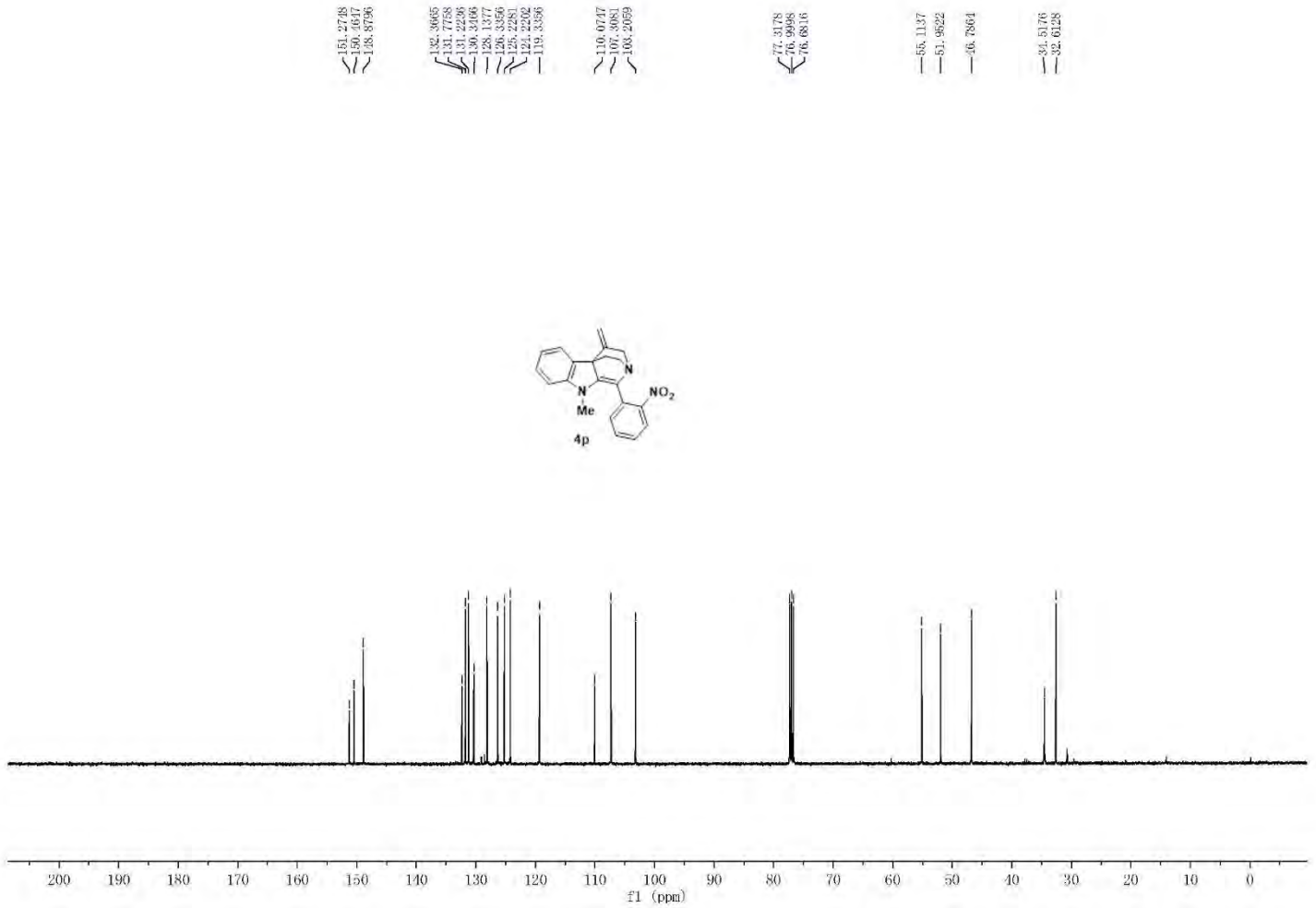
1.07
1.01
1.05
1.13
f1 (ppm)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119.3356
110.6747
107.3081
101.2059
77.3178
76.9998
76.6816
55.1137
51.9622
46.7864
34.5176
32.6128
NO2
N
N
Me
4p
200
190
180
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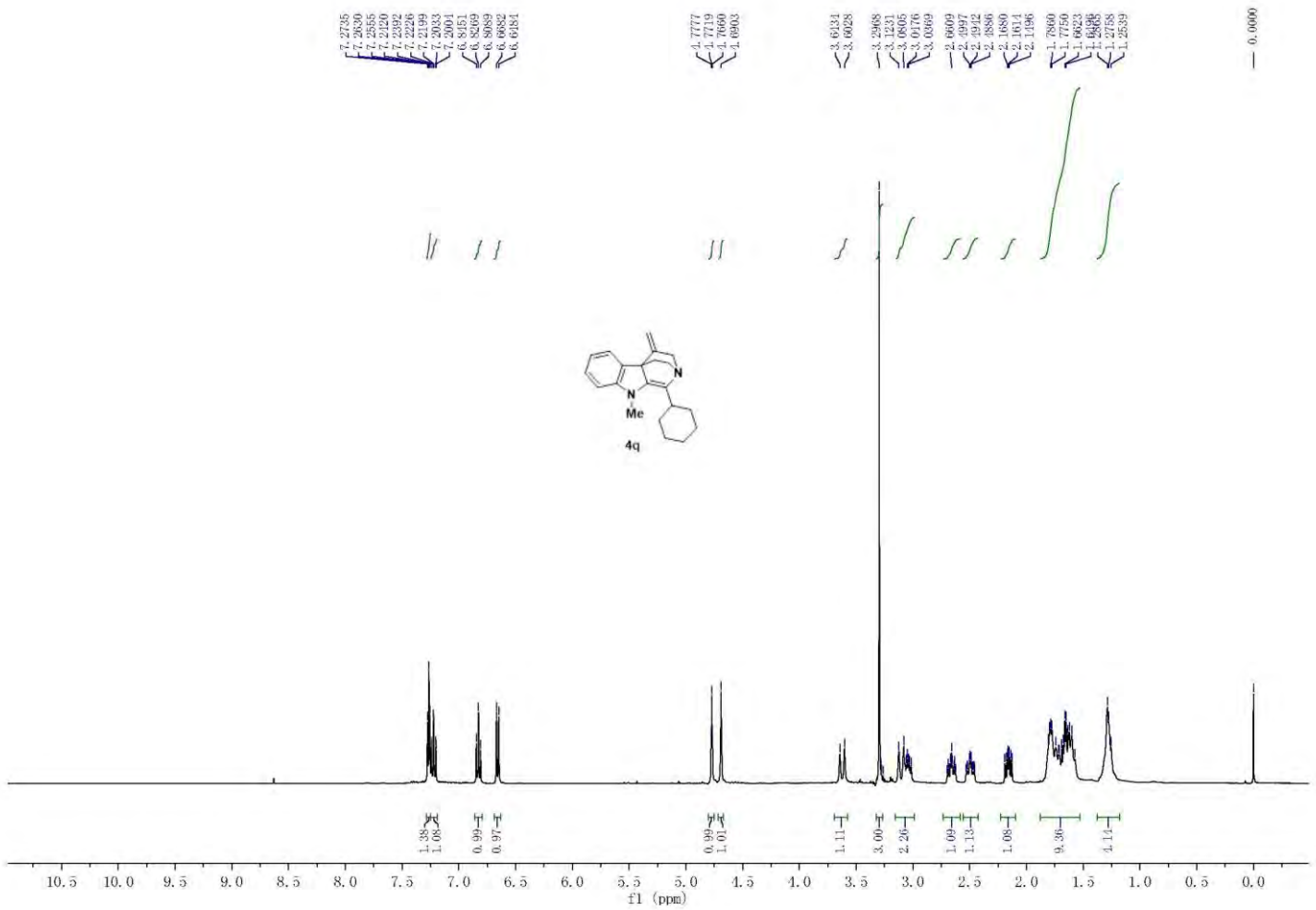
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)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7.2120
7.2092
7.2226
7.2199
7.2033
7.2091
6.9151
6.9209
6.9089
6.9052
6.9181
1.7777
1.7719
1.7060
1.6903
3.6134
3.6028
3.2968
3.1231
3.0805
3.0176
3.0369
2.6609
2.4997
2.3942
2.3886
2.1680
2.1614
2.1196
1.7860
1.7750
1.6923
1.6436
1.2883
1.2735
1.2539
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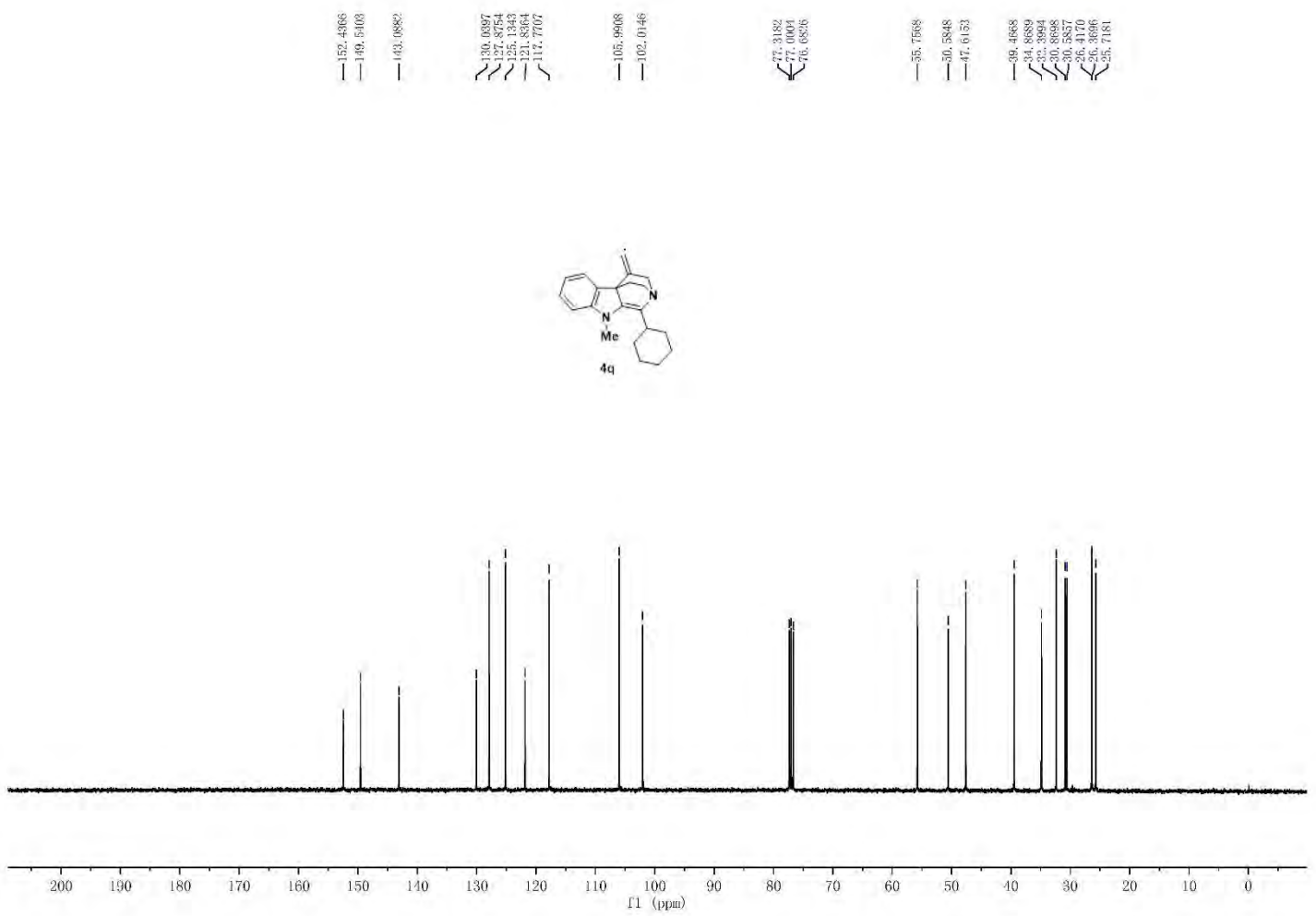
Me
4q
1.38
1.08
0.99
0.97
0.99
1.01
1.11
3.00
2.26
1.09
1.13
1.08
9.36
4.14
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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50.5948
47.6153
39.4668
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30.8894
30.5837
26.4170
26.3886
25.7161
Me
4q
200
190
180
170
160
150
140
130
120
110
100
90
80
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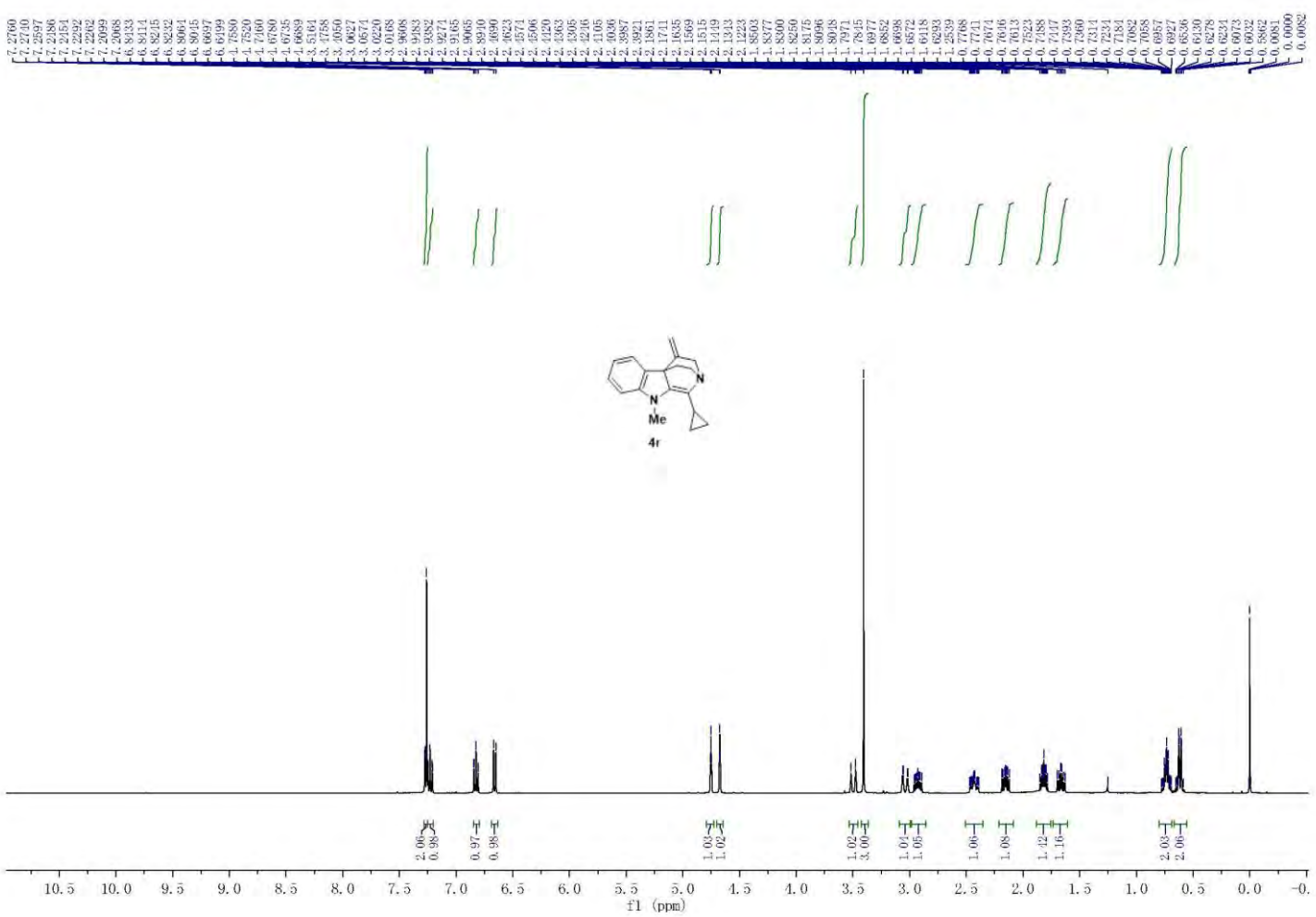
50
40
30
20
10
0
f1 (ppm)


Me
4r
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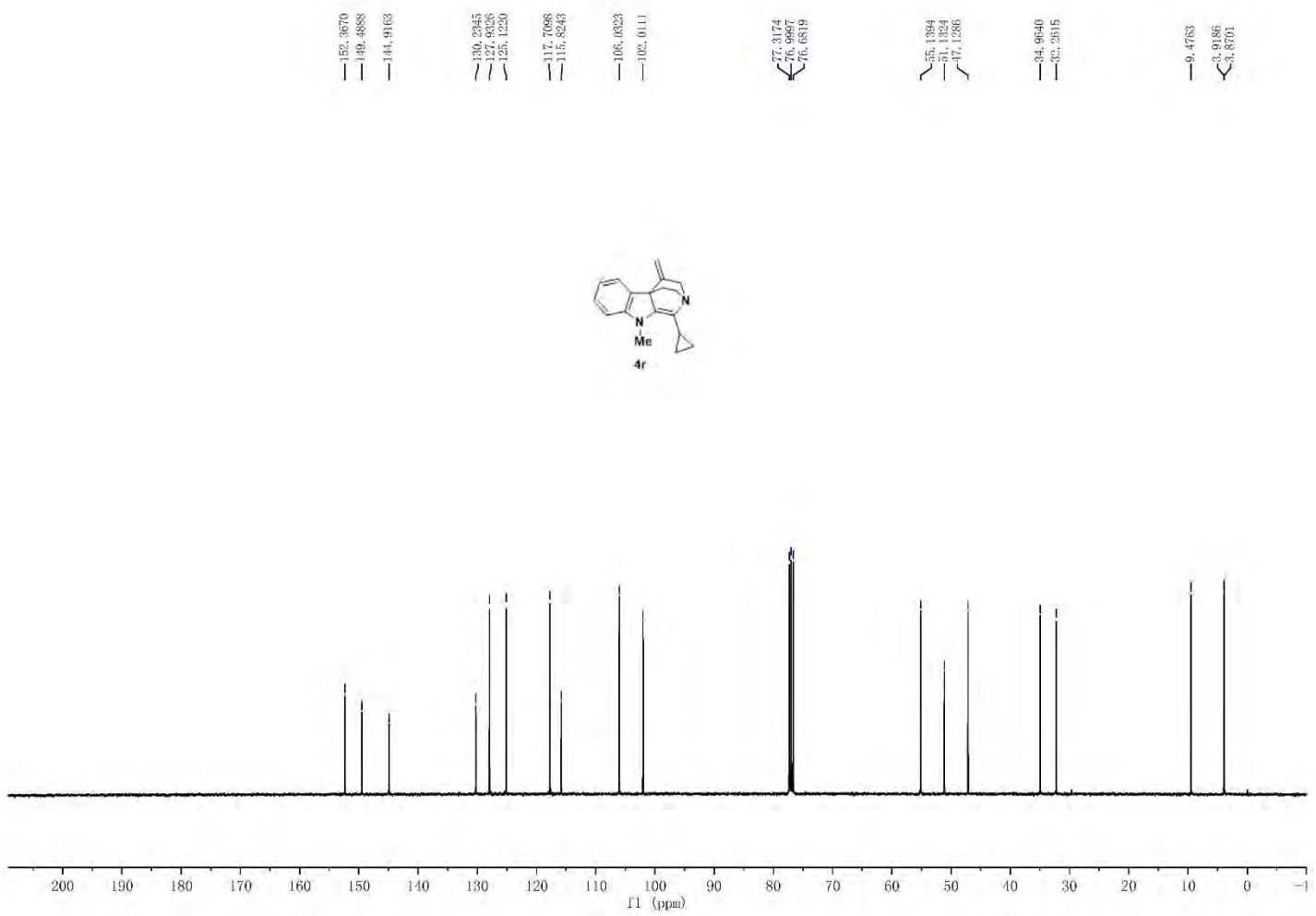
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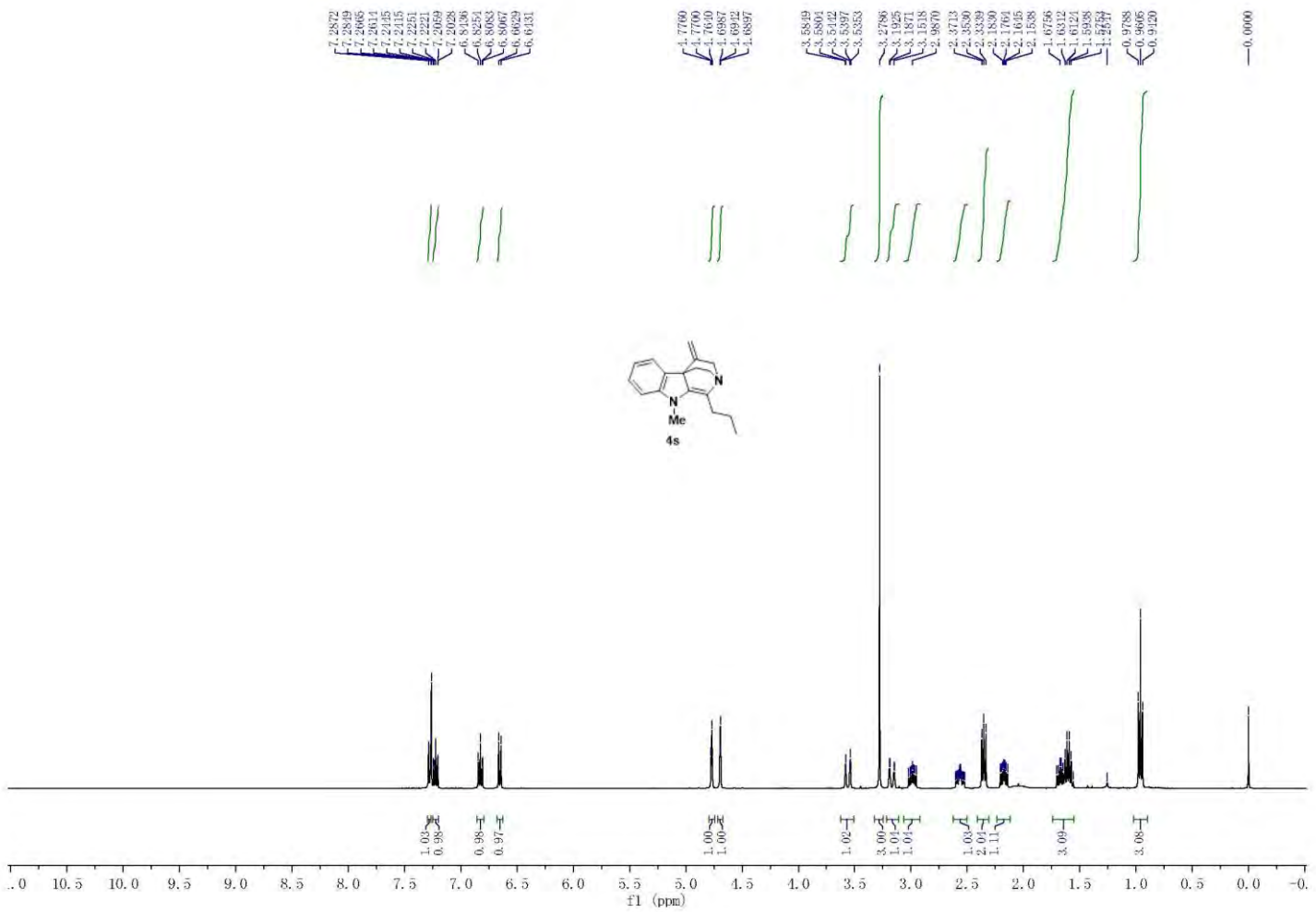
76.9997
76.6819
55.1394
51.1324
47.1286
34.9040
32.2615
9.4763
3.9186
3.8701
N
N
Me
4r
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-1
f1 (ppm)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7.2445
7.2415
7.2251
7.2221
7.2059
7.2028
6.8136
6.8251
6.8063
6.8067
6.6629
6.6431
1.7700
1.7690
1.7640
1.6987
1.6942
1.6897
3.5849
3.5801
3.5402
3.5397
3.5353
3.2786
3.1925
3.1871
3.1518
2.9870
2.3713
2.3530
2.3339
2.1800
2.1761
2.1615
2.1538
1.6756
1.6312
1.6121
1.5938
1.2517
0.9788
0.9605
0.9420
0.0000
N
N
Me
4s
1.03
0.98
0.98
0.97
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1.00
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3.00
1.01
1.01
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2.01
1.11
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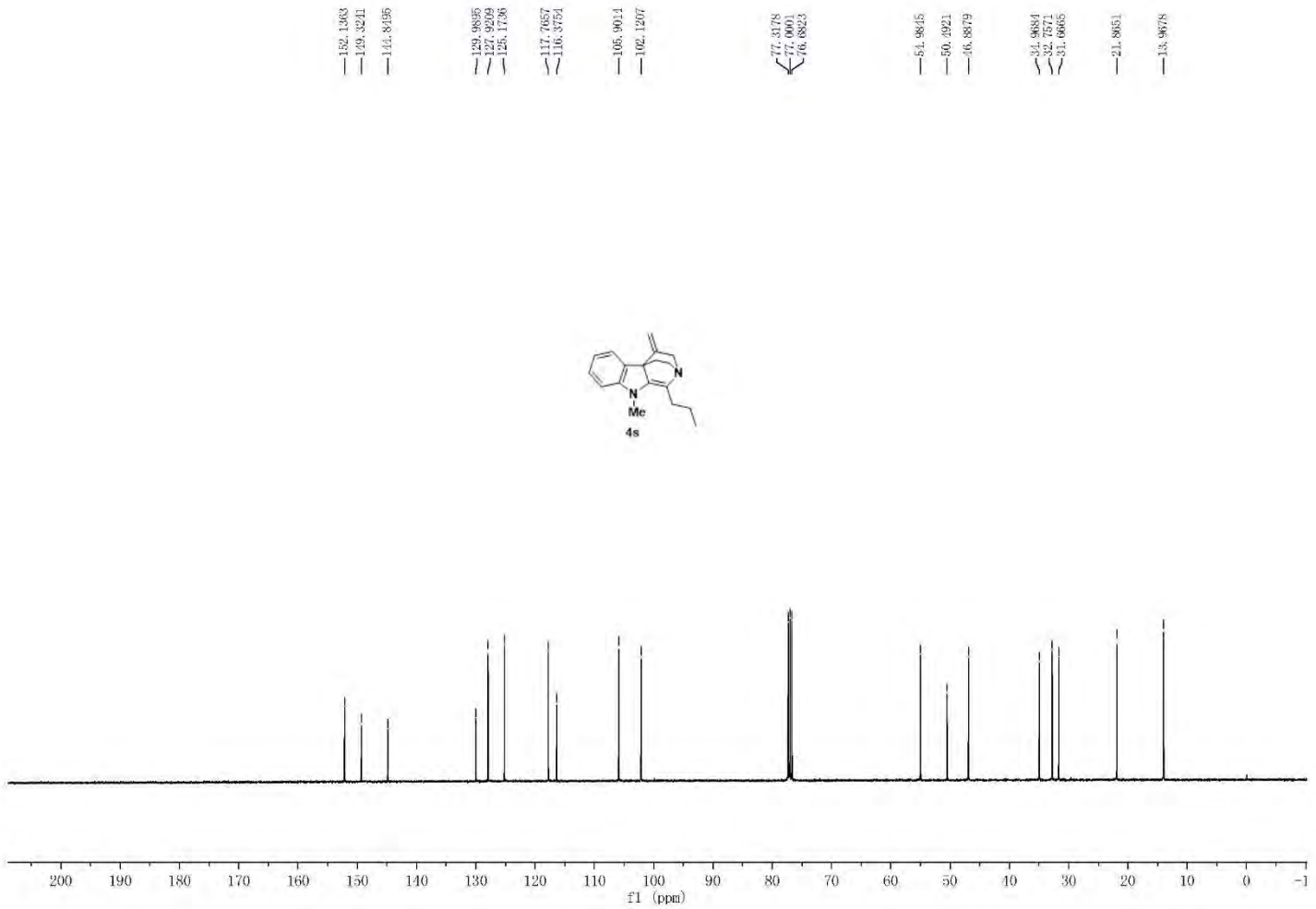
3.08
f1 (ppm)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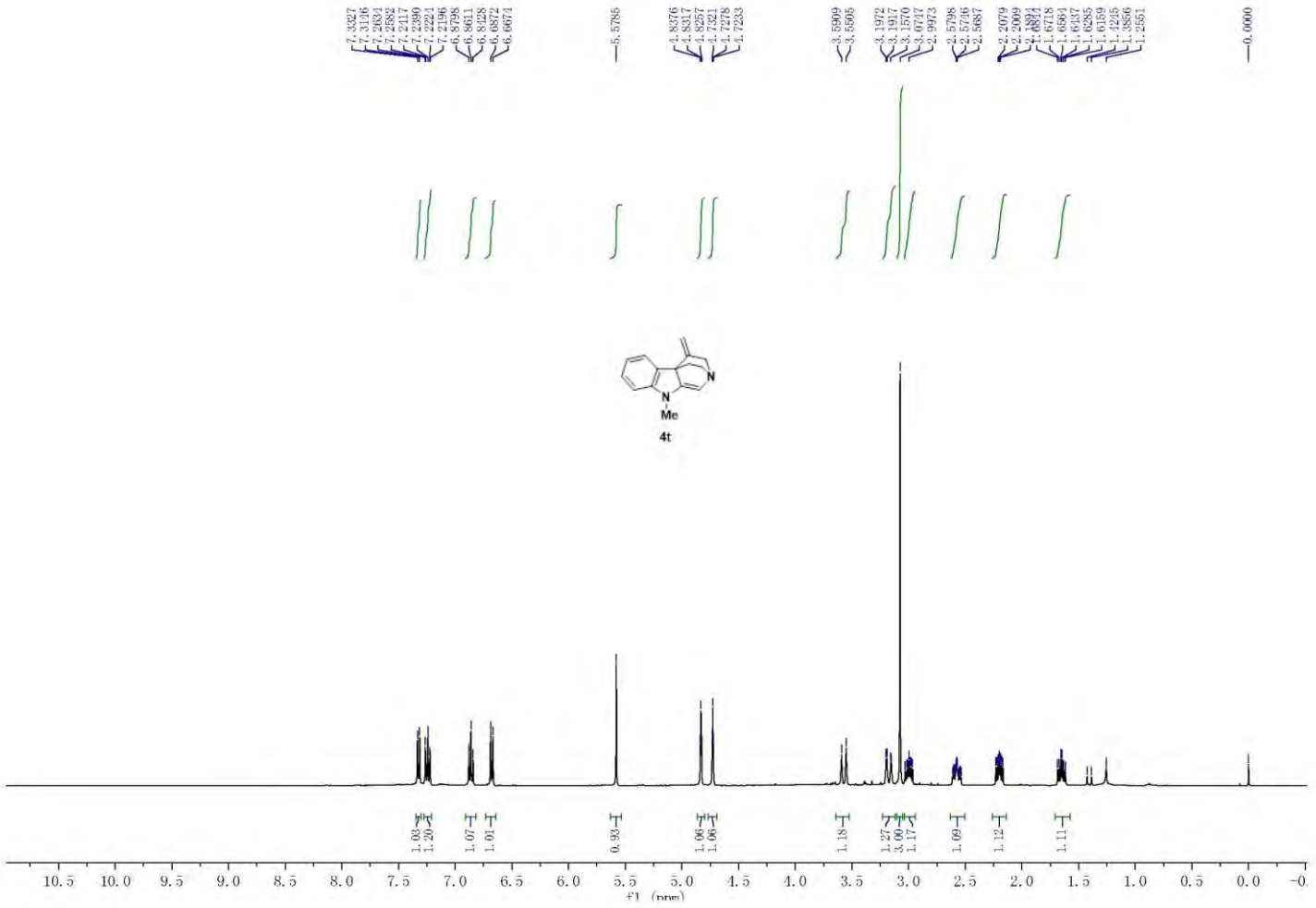
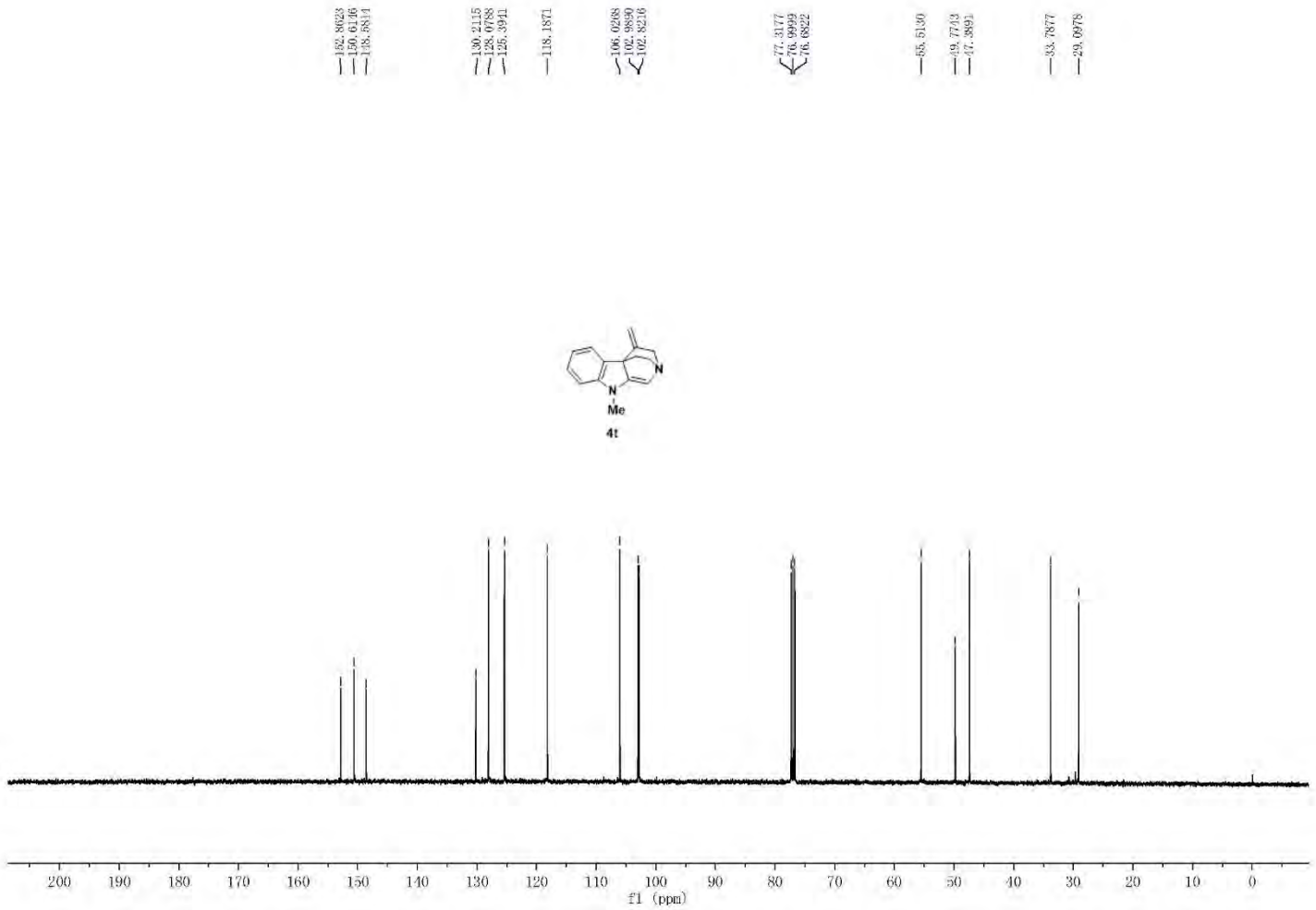
77.0001
76.6823
54.9845
50.2921
46.8879
34.9684
32.7571
31.6665
21.9651
13.9678
N
N
Me
4s
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)


Me
4t
f1 (ppm)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76.9999
76.6822
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49.7713
47.3991
33.7877
29.0978
N
N
Me
4t
200
190
180
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90
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50
40
30
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10
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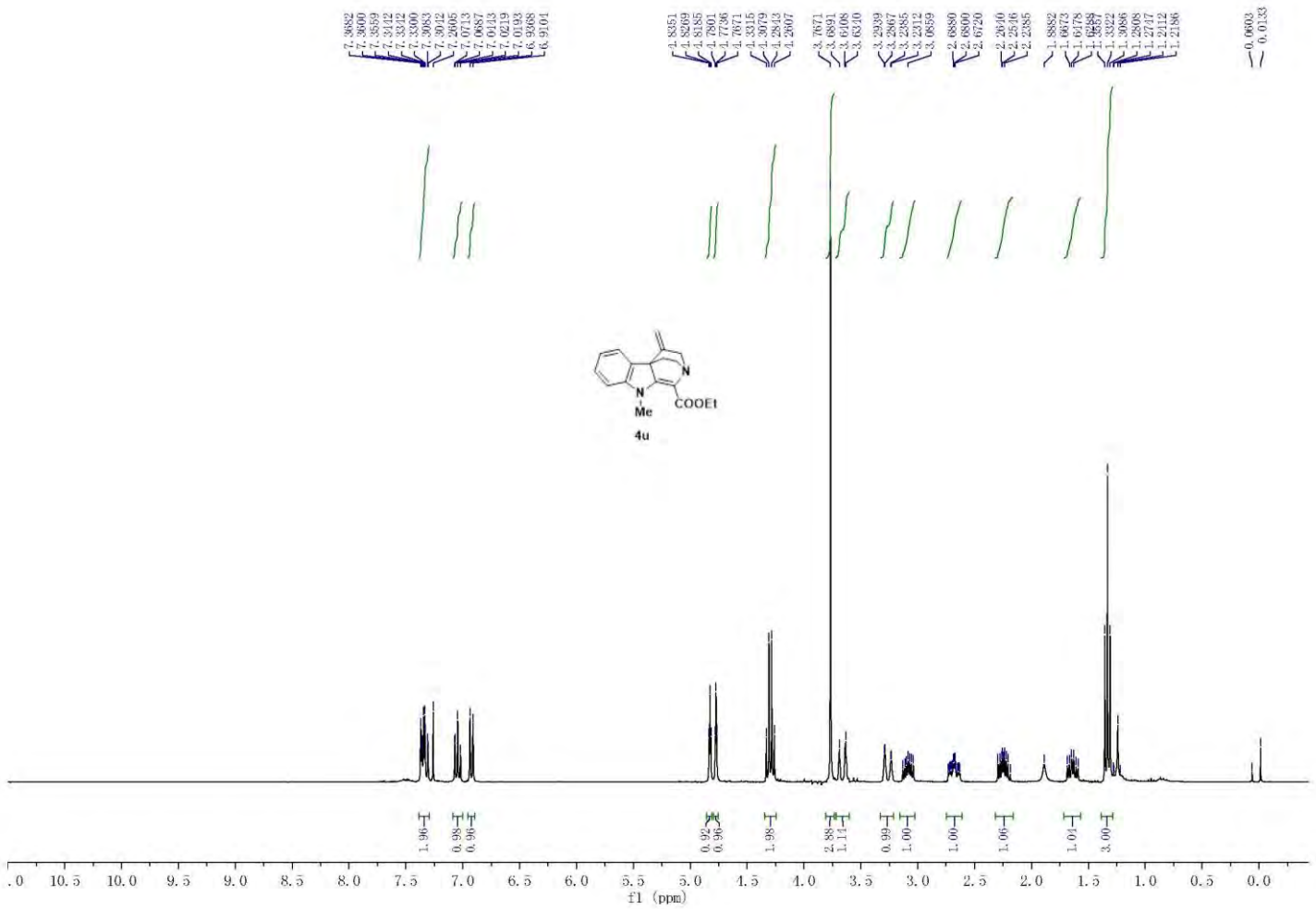
f1 (ppm)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7.2605
7.0713
7.0687
7.0413
7.0219
7.0193
6.9368
6.9104
4.8351
4.8269
4.8185
4.7901
4.7736
4.7671
4.3315
4.3079
4.2843
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3.7671
3.6891
3.6108
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3.2939
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N
N
Me
COOEt
4u
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0.98
0.96
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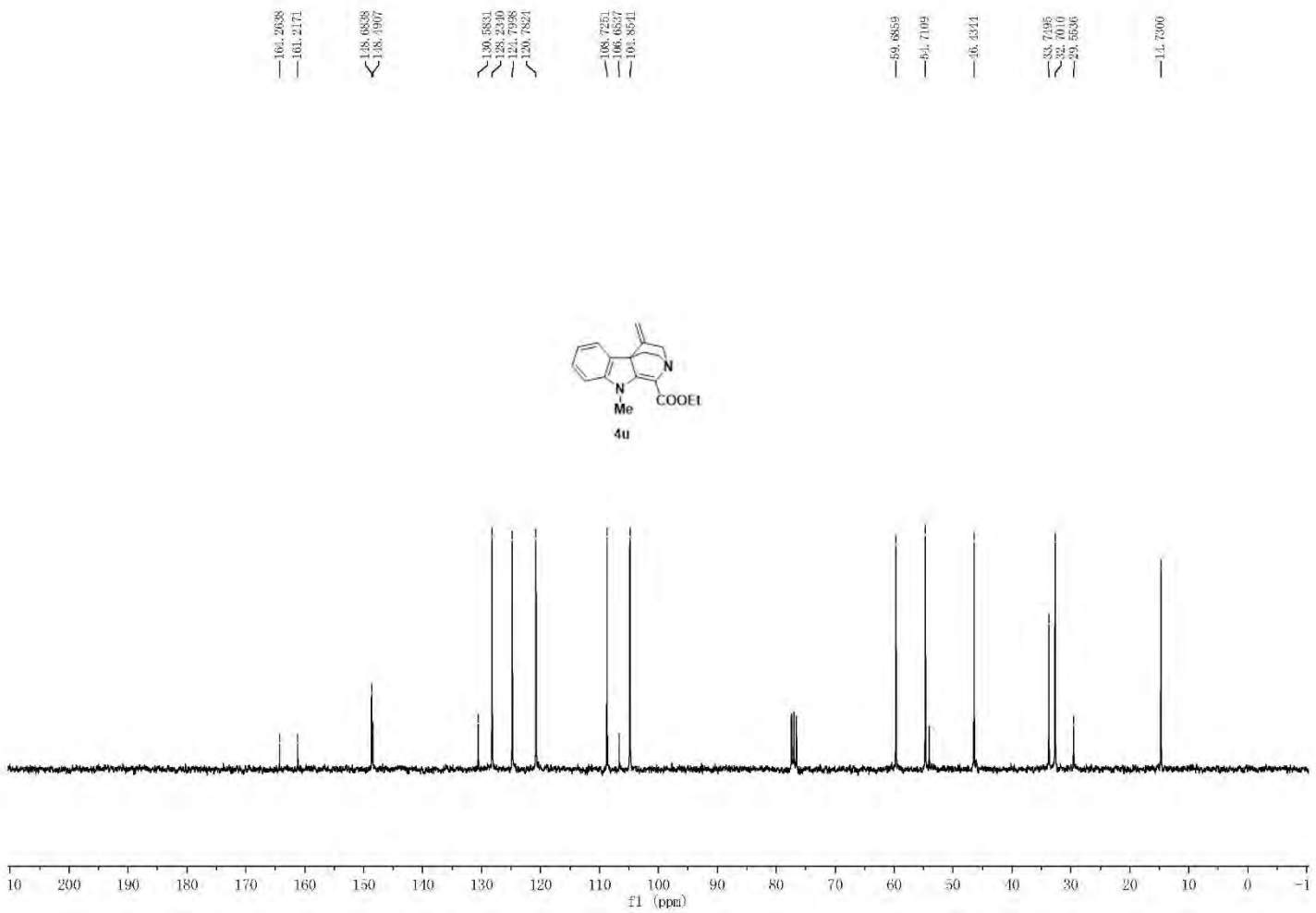
1.00
1.00
1.06
1.04
3.00
f1 (ppm)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59.6859
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14.7300
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N
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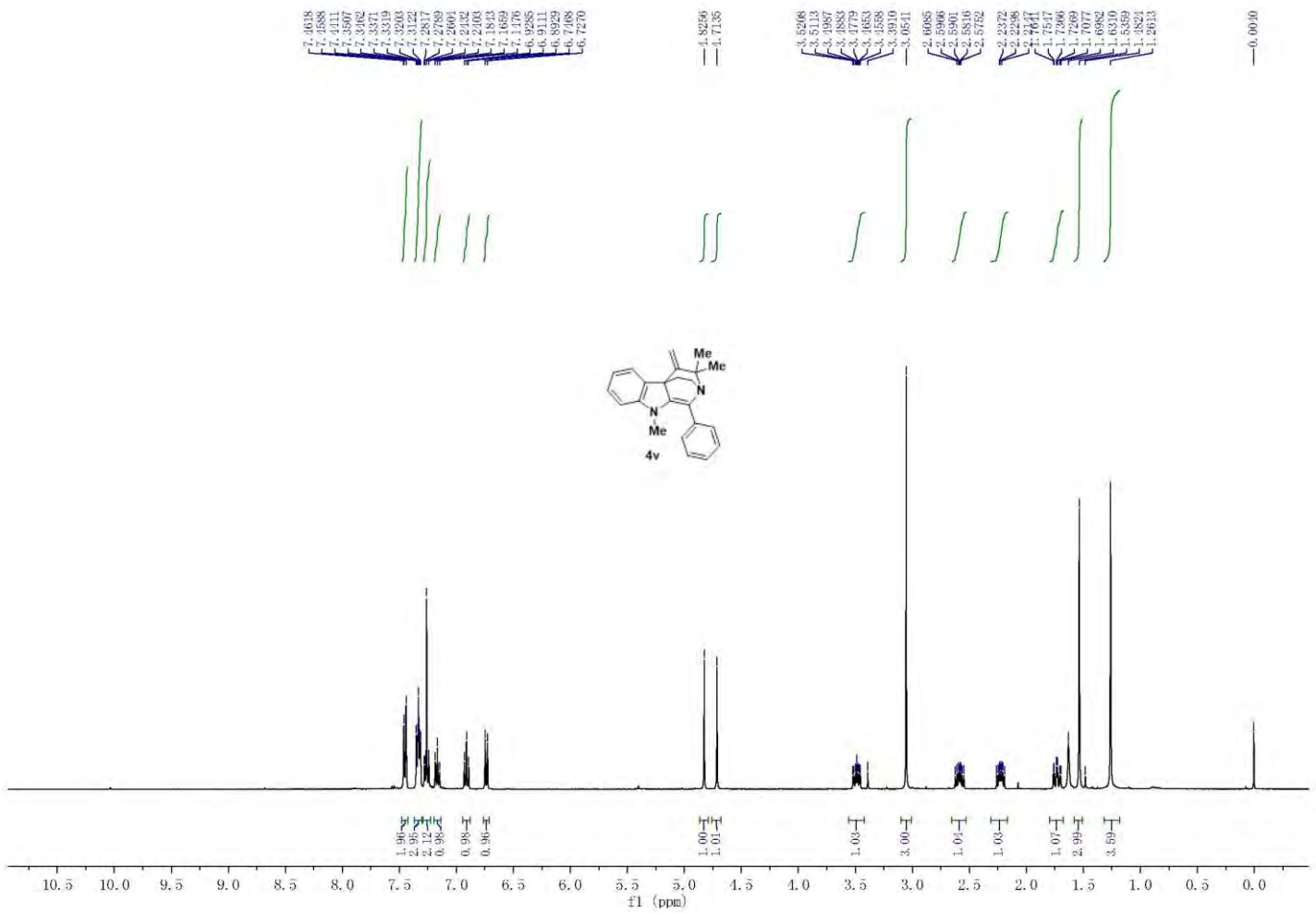
COOEt
4u
f1 (ppm)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Me
N
N
Me
4v
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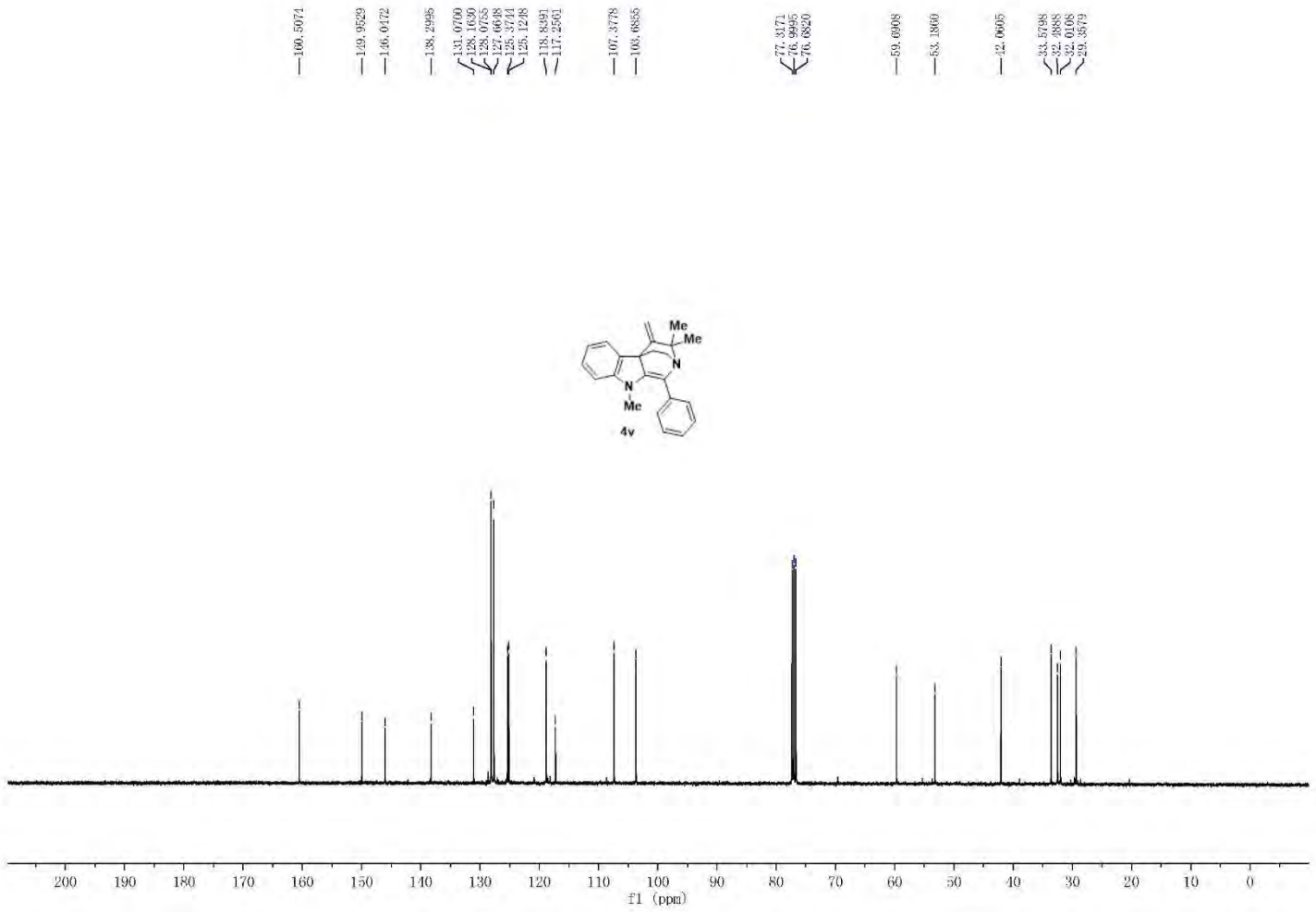
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107.3778
103.6855
77.3171
76.9995
76.6820
59.6908
53.1860
42.0605
33.5798
32.3988
32.0198
29.3879
Me
Me
N
N
Me
4v
200
190
180
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150
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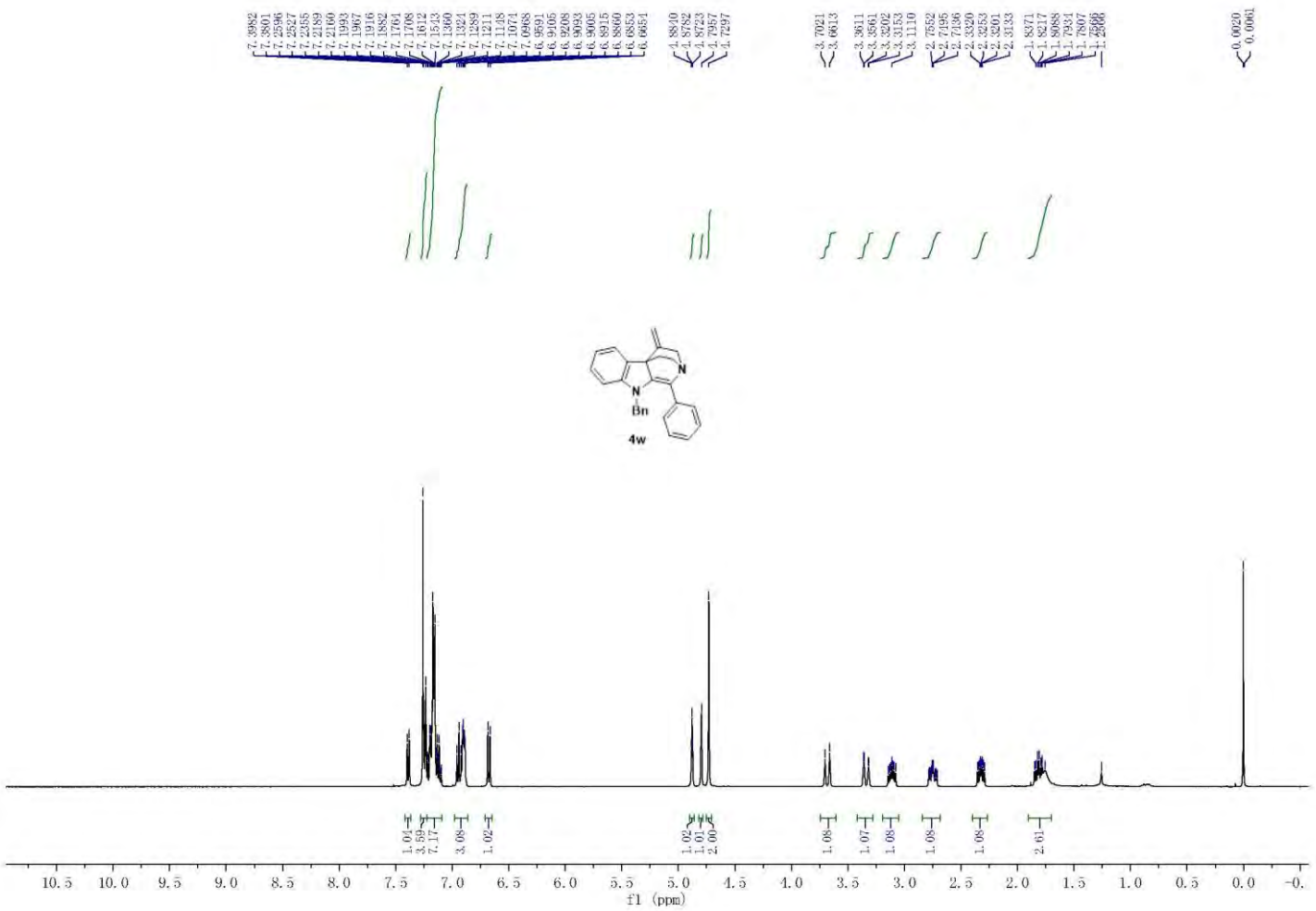
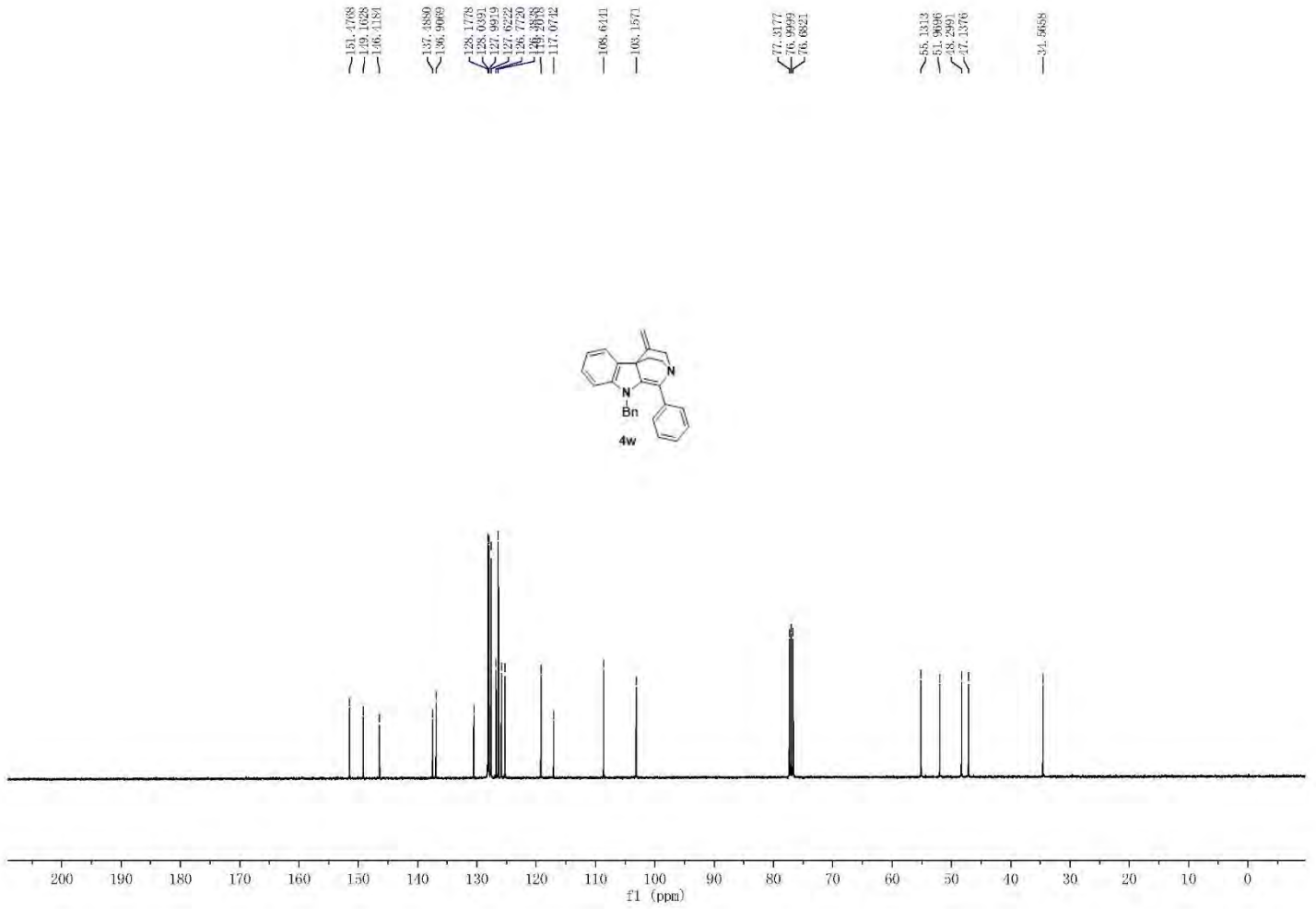
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)


4w
f1 (ppm)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119.2018
117.0742
108.6411
103.1571
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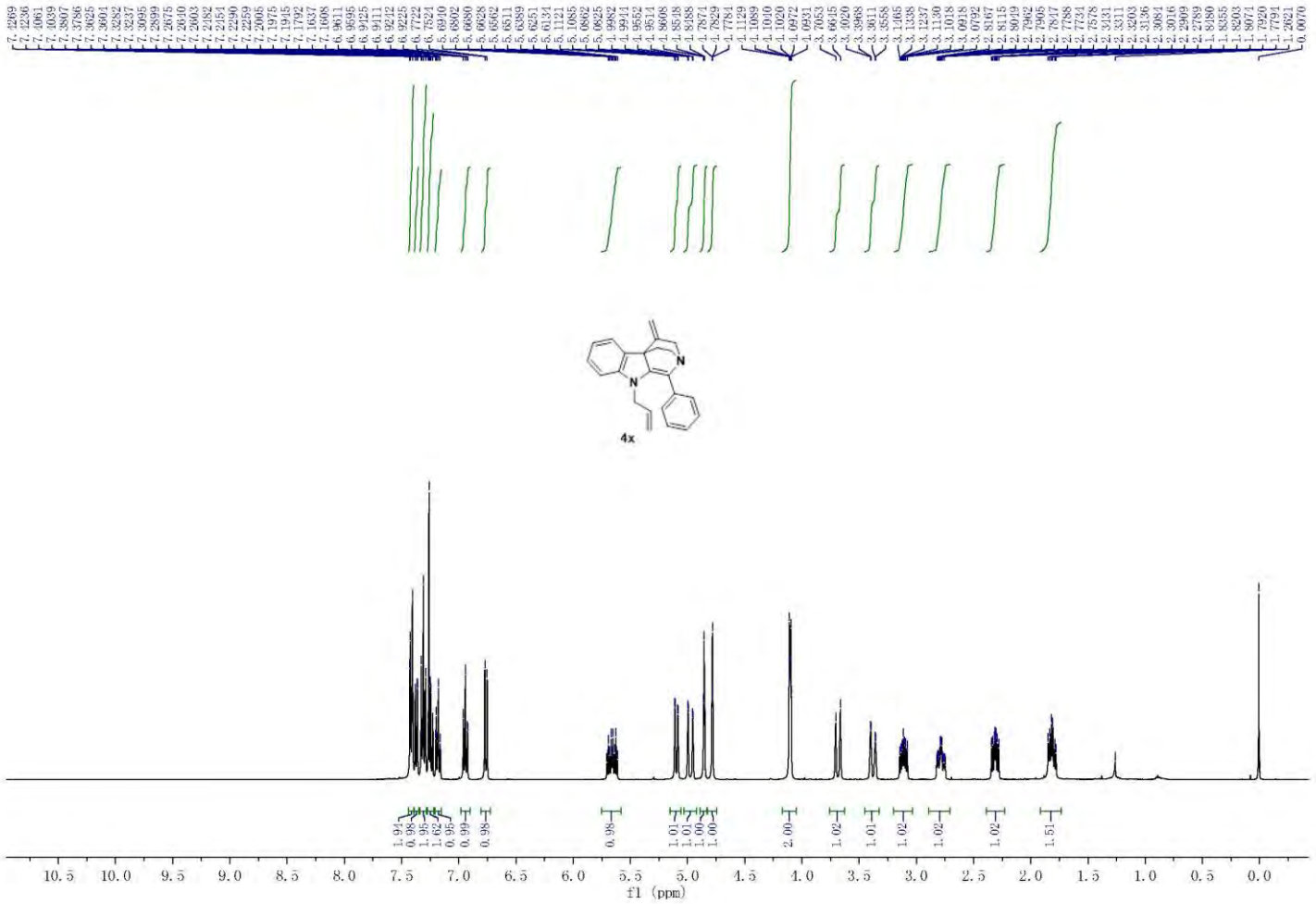
Bn
4w
f1 (ppm)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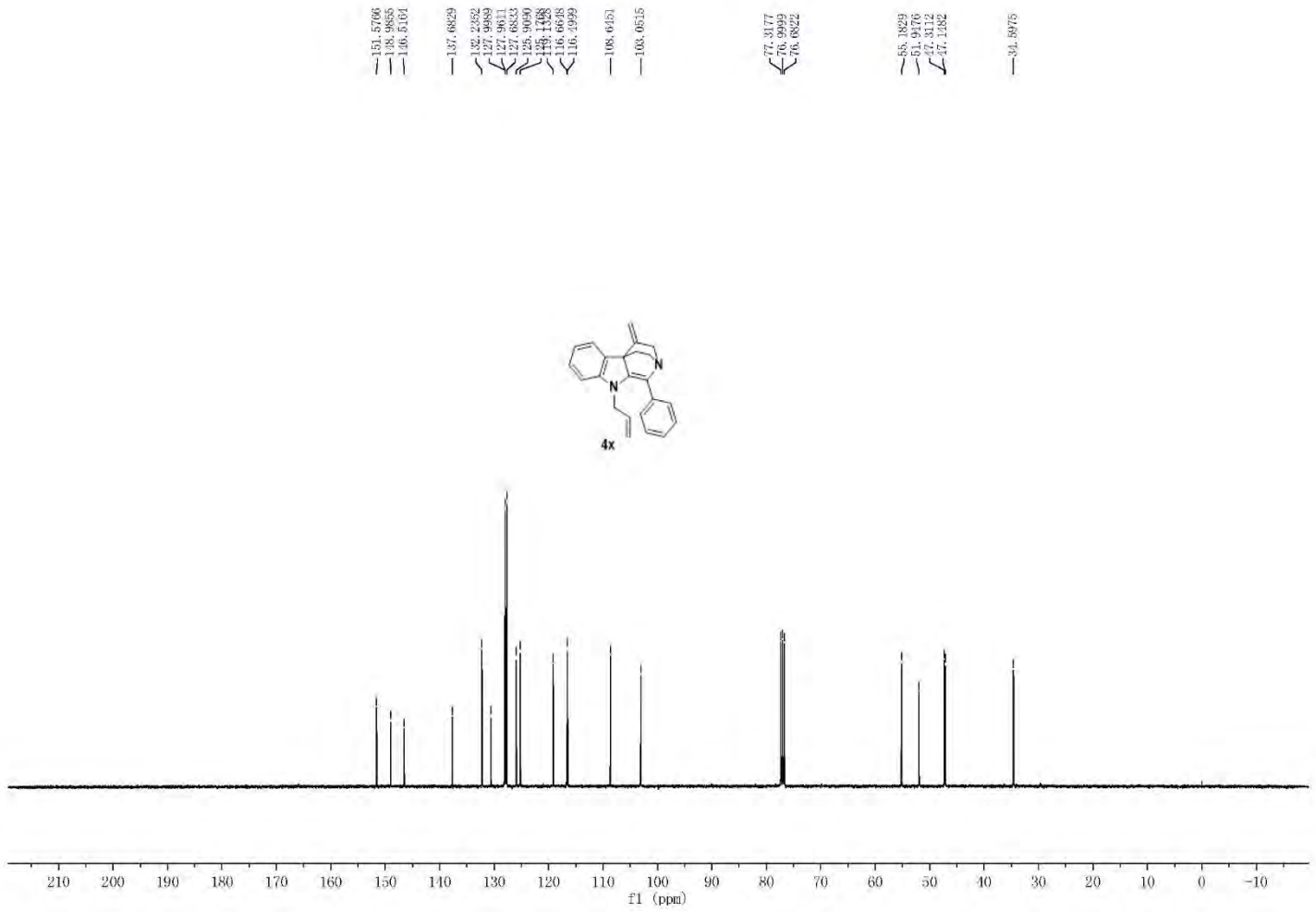
0.95
0.99
0.98
0.98
1.01
1.01
1.00
1.00
2.00
1.02
1.01
1.02
1.02
1.02
1.51
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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137.6829
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127.9611
127.6533
125.9099
116.6648
116.4999
108.6451
103.0515
77.3177
76.9999
76.6822
55.1829
51.9176
47.3112
47.1282
34.5975
4x
N
N
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)