Supporting Information

Intermolecular Cascade Annulations of *N*-(Arysulfonyl)acrylamides with Dual C(sp^3)-H Bonds: Divergent Access to Indanes and Pyrrolidin-2-ones

Ming Hu,[+] Ling-Yu Guo,[+] Ying Han,* Fang-Lin Tan, Ren-Jie Song, and Jin-Heng Li*

[a] *College of Chemistry & Chemical Engineering, Yangzhou University, Yangzhou 225002, China,* [b] *State Key Laboratory of Chemo/Biosensing and Chemometrics Hunan University Changsha 410082, China, and* [c] *Key Laboratory of Jiangxi Province for Persistent Pollutants Control and Resources Recycle Nanchang Hangkong University Nanchang 330063, China*

hanying@yzu.edu.cn and jhli@hnu.edu.cn

List of Contents

(A) General Experimental Procedures

(a) Preparation of Substrates 1:

Substrates **1** were prepared according to literature procedures.[1]

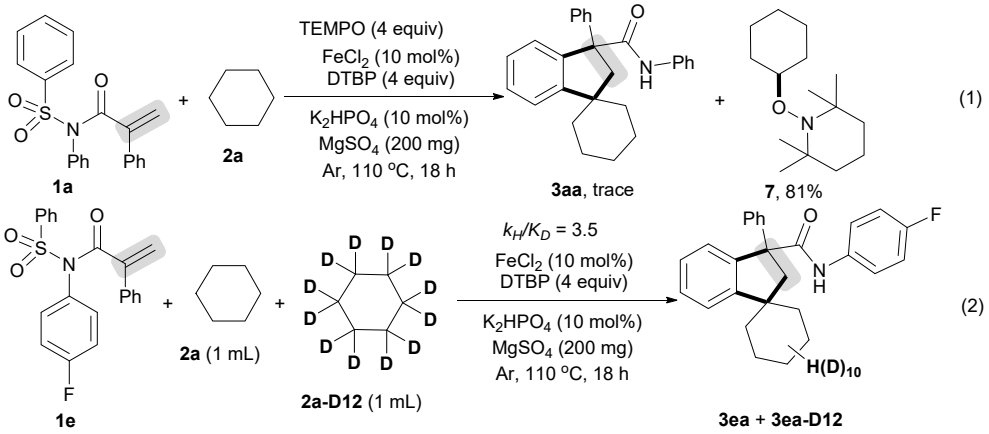
(b) General Procedures for the Syntehsis of Indanes (3):

To a Schlenk tube were added **1** (0.2 mmol), **2** (2 mL), $FeCl_2$ (10 mol%), DTBP (4 equiv), K_2HPO_4 (10 mol%), and $MgSO_4$ (200 mg). Then the mixture was stirred at 110 °C (oil bath temperature) under argon atmosphere for 18 h until complete consumption of starting material as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was washed with brine. The aqueous phase was re-extracted with EtOAc (3×10 mL). The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by silica gel flash column chromatography (hexane/ethyl acetate = 30 : 1) to afford indanes **3**.

(c) General Procedures for the Syntehsis of Pyrrolidin-2-ones (4):

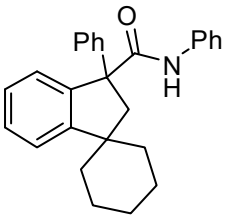
To a Schlenk tube were added **1** (0.2 mmol), **2** (2 mL), K_2HPO_4 (10 mol%), and TBPB (3 equiv). Then the mixture was stirred at 100 °C (oil bath temperature) under argon atmosphere (1 atm) for 12 h until complete consumption of starting material as monitored by TLC and GC-MS analysis. After the reaction was finished, the reaction mixture was washed with brine. The aqueous phase was re-extracted with EtOAc (3×10 mL). The combined organic extracts were dried over Na_2SO_4 and concentrated in vacuum. The residue was purified by silica gel flash column chromatography (hexane/ethyl acetate = 15 : 1) to afford pyrrolidin-2-ones **4**.

(d) Control Experiments



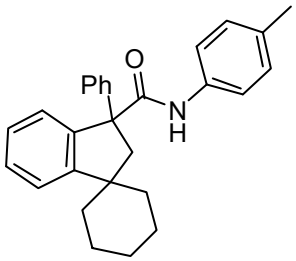
(B) Analytical data

N,3'-Diphenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3aa):



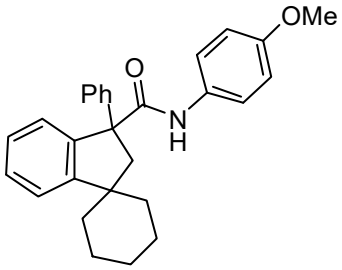
White solid, mp 87.7-89.0 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39 (d, *J* =8.4 Hz, 3H), 7.37-7.26 (m, 11H), 7.07 (t, *J* =7.6 Hz, 1H), 3.53 (d, *J* =13.6 Hz, 1H), 2.30 (d, *J* =13.6 Hz, 1H), 1.72 (d, *J* =10.4 Hz, 3H), 1.64-1.58 (m, 3H), 1.54-1.48 (m, 1H), 1.40 (d, *J* =16.0 Hz, 1H), 1.34-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 154.0, 144.8, 143.3, 137.8, 128.9 (2C), 128.6, 127.6, 127.4, 127.0, 125.3, 124.4, 123.8, 119.7, 65.2, 50.0, 47.3, 38.7, 37.9, 25.8, 23.5, 23.1; LRMS (EI, 70 eV) *m/z* (%): 381 (M^+, 32), 261 (100), 207 (21); HRMS *m/z* (ESI) calcd for $C_{27}H_{29}NO$ $(M+H)^+$ 382.2165, found 382.2172.

3'-Phenyl-*N*-(*p*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ba):



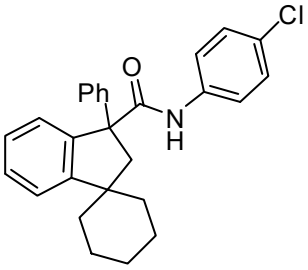
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.38-7.22 (m, 12H), 7.07 (d, *J* =8.4 Hz, 2H), 3.52 (d, *J* =13.2 Hz, 1H), 2.30 (d, *J* =14.4 Hz, 1H), 2.28 (s, 3H), 1.71 (d, *J* =10.4 Hz, 3H), 1.64-1.59 (m, 3H), 1.54-1.48 (m, 1H), 1.40 (d, *J* =15.2 Hz, 1H), 1.34-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 154.0, 144.9, 143.4, 135.2, 134.0, 129.4 (2C), 128.6, 127.7, 127.4, 127.0, 125.3, 123.8, 119.8, 65.1, 50.0, 47.3, 38.7, 37.7, 25.8, 23.5, 23.1, 20.8; LRMS (EI, 70 eV) *m/z* (%): 395 (M^+, 9), 261 (100), 207 (46); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO$ $(M+H)^+$ 396.2322, found 396.2321.

***N*-(4-Methoxyphenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ca):**



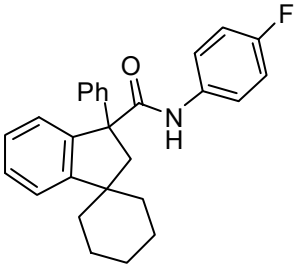
White solid, mp 98.8-100.6 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39-7.23 (m, 12H), 6.81 (d, *J* =8.8 Hz, 2H), 3.76 (s, 3H), 3.52 (d, *J* =13.6 Hz, 1H), 2.30 (d, *J* =13.6 Hz, 1H), 1.71 (d, *J* =10.4 Hz, 3H), 1.64-1.58 (m, 3H), 1.54-1.48 (m, 1H), 1.40 (d, *J* =15.2 Hz, 1H), 1.34-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 156.5, 154.0, 144.9, 143.5, 130.9, 128.6 (2C), 127.7, 127.4, 127.0, 125.3, 123.8, 121.7, 114.1, 65.0, 55.5, 50.0, 47.3, 38.7, 37.9, 25.8, 23.5, 23.1; LRMS (EI, 70 eV) *m/z* (%): 411 (M^+, 22), 261 (100), 183 (20), 169 (20); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO_2$ $(M+H)^+$ 412.2271, found 412.2279.

***N*-(4-Chlorophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3da):**



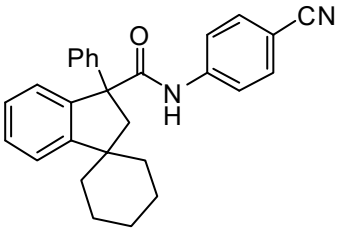
White solid, mp 109.8-111.0 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.21 (m, 14H), 3.50 (d, *J* = 13.2 Hz, 1H), 2.30 (d, *J* = 13.2 Hz, 1H), 1.73-1.49 (m, 6H), 1.40-1.26 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.6, 154.0, 144.6, 143.0, 136.3, 129.4, 128.9, 128.8, 128.7, 127.6, 127.5, 127.1, 125.2, 123.9, 121.0, 65.2, 50.0, 47.3, 38.7, 37.9, 25.8, 23.5, 23.1; LRMS (EI, 70 eV) *m/z* (%): 417 (M^++2, 2), 415 (M^+, 6), 261 (100), 169 (12); HRMS *m/z* (ESI) calcd for $C_{27}H_{27}{}^{35}ClNO$ $(M+H)^+$ 416.1776, found 416.1785.

***N*-(4-Fluorophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car boxamide (3ea):**



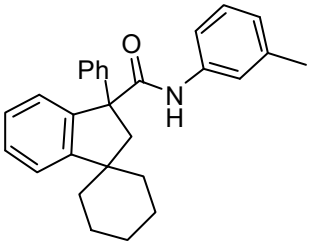
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.23 (m, 12H), 6.96 (t, *J* = 8.4 Hz, 2H), 3.51 (d, *J* = 13.6 Hz, 1H), 2.30 (d, *J* = 13.2 Hz, 1H), 1.74-1.68 (m, 3H), 1.65-1.51 (m, 4H), 1.41-1.28 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.6, 159.5 (d, *J* = 242.1 Hz, 1C), 154.0, 144.7, 143.2, 133.8 (d, *J* = 2.7 Hz, 1C), 128.7 (2C), 127.6, 127.4, 127.1, 125.3, 123.9, 121.7 ((d, *J* = 7.8 Hz, 1C), 115.5 ((d, *J* = 22.4 Hz, 1C), 65.1, 50.0, 47.3, 38.7, 37.9, 25.8, 23.5, 23.1; ^{19}F NMR (375 MHz, $CDCl_3$) δ: -117.9; LRMS (EI, 70 eV) *m/z* (%): 399 (M^+, 2), 261 (100), 207 (13); HRMS *m/z* (ESI) calcd for $C_{27}H_{27}{}^{19}FNO$ $(M+H)^+$ 400.2071, found 400.2074.

***N*-(4-Cyanophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car boxamide (3fa):**



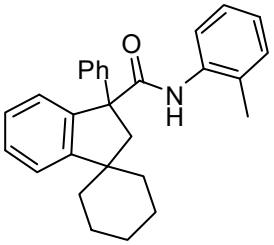
White solid, mp 137.3-139.1 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.59-7.52 (m, 5H), 7.42-7.24 (m, 9H), 3.49 (d, *J* = 13.6 Hz, 1H), 2.30 (d, *J* = 13.2 Hz, 1H), 1.74-1.49 (m, 7H), 1.40-1.26 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.9, 154.1, 144.1, 142.5, 141.7, 133.2, 129.0, 128.9, 128.6, 127.6, 127.5, 127.4, 125.1, 124.1, 119.5, 107.3, 65.4, 49.9, 47.4, 38.7, 37.9, 25.8, 23.5, 23.1; LRMS (EI, 70 eV) *m/z* (%): 406 (M^+, 1), 261 (100), 183 (15), 169 (13); HRMS *m/z* (ESI) calcd for $C_{28}H_{27}N_2O$ $(M+H)^+$ 407.2118, found 407.2116.

3'-Phenyl-*N*-(*m*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ga):



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.37-7.25 (m, 11H), 7.16-7.13 (m, 2H), 6.89 (s, 1H), 3.52 (d, *J* = 13.6 Hz, 1H), 2.30 (d, *J* = 10.0 Hz, 4H), 1.71 (d, *J* = 10.4 Hz, 3H), 1.64-1.48 (m, 4H), 1.39 (d, *J* = 14.4 Hz, 1H), 1.34-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 154.0, 144.8, 143.3, 138.9, 137.7, 128.7, 128.6 (2C), 127.6, 127.4, 127.0, 125.3, 125.2, 123.8, 120.3, 116.8, 65.2, 50.0, 47.3, 38.7, 37.9, 25.8, 23.5, 23.1, 21.4; LRMS (EI, 70 eV) *m/z* (%): 395 (M^+, 6) 261 (100), 207 (41); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO$ ($[M+H]^+$) 396.2322, found 396.2319.

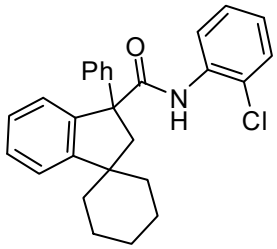
3'-Phenyl-*N*-(*o*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ha):



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, *J* = 8.0 Hz, 1H), 7.38-7.25 (m, 10H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.07 (d,

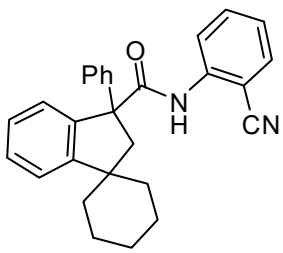
J = 7.2 Hz, 1H), 7.00 (t, *J* = 7.6 Hz, 1H), 3.53 (d, *J* = 13.6 Hz, 1H), 2.36 (d, *J* = 13.2 Hz, 1H), 1.82 (s, 3H), 1.74-1.69 (m, 3H), 1.66-1.53 (m, 4H), 1.46-1.26 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 154.0, 144.8, 143.5, 136.0, 130.3, 128.7, 128.6, 127.7, 127.6, 127.3, 127.0, 126.8, 125.4, 124.6, 123.9, 121.5, 65.3, 50.0, 47.3, 38.8, 37.8, 25.8, 23.5, 23.1, 17.2; LRMS (EI, 70 eV) *m/z* (%): 395 (M^+, 7), 261 (100), 207 (36); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO$ $(M+H)^+$ 396.2322, found 396.2321.

_N_-(2-Chlorophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ia):



White solid, mp 113.5-115.2 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.43 (d, *J* = 8.0 Hz, 1H), 8.06 (s, 1H), 7.40-7.31 (m, 7H), 7.29-7.23 (m, 4H), 6.99 (t, *J* = 7.2 Hz, 1H), 3.51 (d, *J* = 13.6 Hz, 1H), 2.36 (d, *J* = 13.2 Hz, 1H), 1.74-1.66 (m, 3H), 1.63-1.54 (m, 4H), 1.41-1.29 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.8, 153.9, 144.4, 142.8, 134.8, 128.9, 128.7 (2C), 127.2 (2C), 127.4, 127.1, 125.8, 124.5, 123.7, 122.9, 121.1, 65.5, 49.8, 47.3, 38.7, 37.9, 25.8, 23.5, 23.1; LRMS (EI, 70 eV) *m/z* (%): 417 (M^+, 2), 415 (M^+, 5), 261 (100), 169 (15); HRMS *m/z* (ESI) calcd for $C_{27}H_{27}{}^{35}ClNO$ $(M+H)^+$ 416.1776, found 416.1784.

_N_-(2-Cyanophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ja):

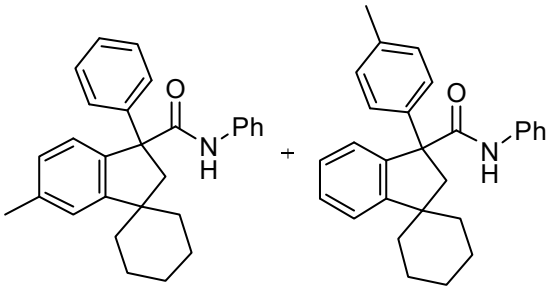


Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.46 (d, *J* = 8.4 Hz, 1H), 8.06 (s, 1H), 7.56 (d, *J* = 8.0 Hz, 1H), 7.48 (d, *J* = 8.0 Hz, 1H), 7.42-7.28 (m, 9H), 7.12 (t, *J* = 7.6 Hz, 1H), 3.52

(d, *J* = 13.2 Hz, 1H), 2.33 (d, *J* = 13.2 Hz, 1H), 1.71 (t, *J* = 12.0 Hz, 3H), 1.65-1.54 (m, 4H),1.42-1.29 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 173.1, 153.9, 143.9, 142.1, 140.7, 134.0, 132.2, 128.9 (2C), 127.9, 127.4 (2C), 125.8, 124.1, 123.8, 120.8, 115.8, 102.1, 65.5, 49.9, 47.3, 38.8, 37.9, 25.8, 23.5, 23.1; LRMS (EI, 70 eV) *m/z* (%): 406 (M^+, 2), 261 (100), 207 (17); HRMS *m/z* (ESI) calcd for $C_{28}H_{27}N_2O$ $(M+H)^+$ 407.2118, found 407.2131.

6'-Methyl-*N*,3'-diphenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ka) and *N*-phenyl-3'-(*p*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ka'):

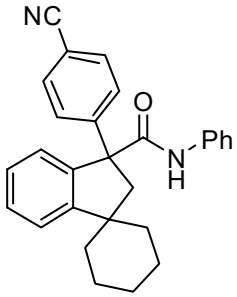
3ka:**3ka'** = 1:1;



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.42-7.36 (m, 6.1H), 7.34-7.25 (m, 14.3H), 7.20 (d, *J* = 8.0 Hz, 2.0H), 7.13-7.10 (m, 4.0H), 7.09-7.05 (m, 2.0H), 3.53-3.47 (m, 2.0H), 2.40 (s, 3.0H), 2.33 (s, 3.0H), 2.30-2.26 (m, 2.0H), 1.72 (t, *J* = 8.0 Hz, 6.0H), 1.64-1.54 (m, 8.1H), 1.40 (d, *J* = 13.2 Hz, 2.1H), 1.33-1.25 (m, 4.0H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.7, 172.6, 154.1, 153.9, 144.9, 143.4, 141.8, 140.4, 138.5, 137.8, 136.7, 129.3, 128.9 (3C), 128.6, 128.5, 128.4, 127.6, 127.5, 127.3, 126.9, 125.3, 125.0, 124.4, 124.3 (2C), 123.8, 119.7 (2C), 64.9, 64.8, 50.3, 49.8, 47.3, 47.1, 38.8, 38.7, 37.9, 37.8, 25.9, 25.8, 23.5 (2C), 23.1 (2C), 21.5, 20.9; LRMS (EI, 70 eV)

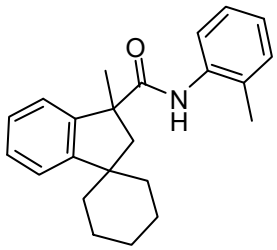
m/z (%): 395 (M^+, 2), 275 (100), 207 (8); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO$ $(M+H)^+$ 396.2322, found 396.2330.

3'-(4-Cyanophenyl)-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3la):



White solid, mp 131.8-133.5 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.60 (d, *J* = 8.4 Hz, 2H), 7.47 (d, *J* = 8.0 Hz, 2H), 7.43-7.34 (m, 6H), 7.30 (t, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 1H), 7.11 (t, *J* = 7.2 Hz, 1H), 3.53 (d, *J* = 13.6 Hz, 1H), 2.22 (d, *J* = 13.6 Hz, 1H), 1.79-1.58 (m, 6H), 1.47 (t, *J* = 12.8 Hz, 2H), 1.38-1.30 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 171.2, 154.3, 150.2, 142.3, 137.3, 132.3, 129.3, 129.0, 128.5, 128.0, 125.1, 124.8, 124.3, 119.9, 118.7, 110.8, 65.3, 51.2, 47.5, 38.8, 37.6, 25.7, 23.5, 22.9; LRMS (EI, 70 eV) *m/z* (%): 406 (M^+, 4), 312 (52), 289 (56), 206 (100); HRMS *m/z* (ESI) calcd for $C_{28}H_{27}N_2O$ $(M+H)^+$ 407.2118, found 407.2123.

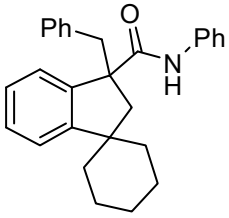
3'-Methyl-*N*-(*o*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ma):



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.94 (d, *J* = 8.0 Hz, 1H), 7.38-7.34 (m, 3H), 7.29 (d, *J* = 6.8 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 7.06 (t, *J* = 7.2 Hz, 2H), 6.98 (t, *J* = 7.2 Hz, 1H), 2.97 (d, *J* = 13.6 Hz, 1H), 1.91 (d, *J* = 13.6 Hz, 1H), 1.81 (s, 3H), 1.75 (d, *J* = 12.0 Hz, 2H), 1.70 (s, 3H), 1.65-1.59 (m, 2H), 1.56-1.44 (m, 4H), 1.31-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 175.6, 153.8, 144.2, 135.9, 130.2, 128.7, 127.6 (2C), 126.8, 124.5, 124.0, 123.8, 121.4, 55.2, 49.8, 47.0, 39.4, 38.1, 26.4,

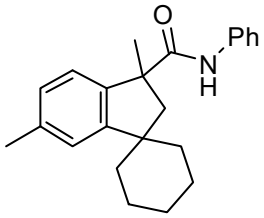
25.8, 23.6, 23.0, 17.1; LRMS (EI, 70 eV) *m/z* (%): 333 (M^+, 2), 199 (100), 131 (20); HRMS *m/z* (ESI) calcd for $C_{23}H_{28}NO$ $(M+H)^+$ 334.2165, found 334.2167.

3'-Benzyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3na):



White solid, mp 100.3-102.2 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34 (t, *J* = 7.2 Hz, 3H), 7.27 (t, *J* = 7.6 Hz, 3H), 7.22-7.15 (m, 5H), 7.09-7.02 (m, 4H), 3.63 (d, *J* = 13.2 Hz, 1H), 3.19 (d, *J* = 13.2 Hz, 1H), 2.61 (d, *J* = 14.0 Hz, 1H), 2.23 (d, *J* = 14.0 Hz, 1H), 1.69 (d, *J* = 12.4 Hz, 1H), 1.64-1.59 (m, 2H), 1.53-1.18 (m, 6H), 1.02 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.8, 154.6, 141.8, 137.8, 137.7, 130.7, 128.9, 128.7, 127.9, 127.2, 126.5, 125.4, 124.3, 123.9, 119.9, 60.5, 46.8, 46.7, 44.8, 39.4, 38.6, 25.7, 23.4, 23.0; IR ν CO (KBr, cm^{-1}): 1676, 1596, 1462, 1095; LRMS (EI, 70 eV) *m/z* (%): 395 (M^+, 16), 304 (42), 275 (776), 91 (100); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO$ $(M+H)^+$ 396.2322, found 396.2325.

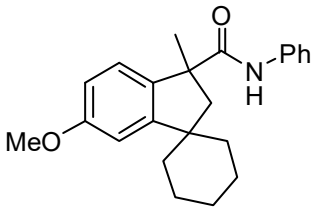
3',6'-Dimethyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3oa):



White solid, mp 107.4-109.2 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, *J* =8.0 Hz, 2H), 7.27-7.14 (m, 5H), 7.05 (t, *J* =8.0 Hz, 2H), 2.91 (d, *J* =13.6 Hz, 1H), 2.41 (s, 3H), 1.91 (d, *J* =13.6 Hz, 1H), 1.72 (t, *J* =10.0 Hz, 3H), 1.64 (d, *J* =11.6 Hz, 4H), 1.55-1.43 (m, 4H), 1.30-1.24 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 175.8, 153.9, 141.2, 138.5, 137.8, 128.8, 128.7, 124.6, 124.2, 123.5, 119.7, 54.6, 50.0, 46.9, 39.3, 38.2,

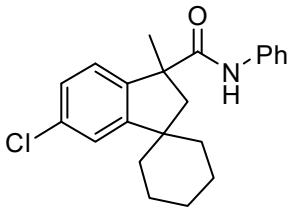
26.8, 25.8, 23.5, 23.0, 21.5; LRMS (EI, 70 eV) *m/z* (%): 333 (M^+, 5), 213 (100), 171 (7), 145 (18); HRMS *m/z* (ESI) calcd for $C_{23}H_{28}NO$ $(M+H)^+$ 334.2165, found 334.2168.

6'-Methoxy-3'-methyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3pa):



Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, *J* = 8.0 Hz, 2H), 7.29-7.23 (m, 3H), 7.19 (s, 1H), 7.06 (t, *J* = 7.6 Hz, 1H), 6.88 (d, *J* = 8.4 Hz, 1H), 6.79 (s, 1H), 3.86 (s, 3H), 2.91 (d, *J* = 13.6 Hz, 1H), 1.92 (d, *J* = 13.6 Hz, 1H), 1.76-1.69 (m, 3H), 1.64-1.42 (m, 8H) , 1.30-1.21 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 176.0, 160.4, 155.6, 137.8, 136.1, 128.9, 124.5, 124.2, 119.7, 113.7, 109.2, 55.4, 54.3, 50.2, 47.0, 39.2, 38.1, 26.8, 25.7, 23.5, 23.0; LRMS (EI, 70 eV) *m/z* (%): 349 (M^+, 1), 229(100), 161 (13), 147 (7); HRMS *m/z* (ESI) calcd for $C_{23}H_{28}NO_2$ $(M+H)^+$ 350.2115, found 350.2119.

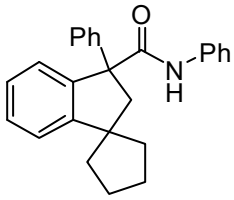
6'-Chloro-3'-methyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3qa):



Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.36-7.24 (m, 7H), 7.08 (t, *J* = 7.2 Hz, 2H), 2.92 (d, *J* = 13.6 Hz, 1H), 1.94 (d, *J* = 13.6 Hz, 1H), 1.74-1.43 (m, 11H), 1.30-1.26 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 175.0, 155.8, 142.7, 137.6, 134.5, 128.9, 128.0, 125.0, 124.5, 124.4, 119.8, 54.6, 49.8, 47.2, 39.2, 38.1, 26.8, 25.6, 23.4, 22.9; LRMS (EI, 70

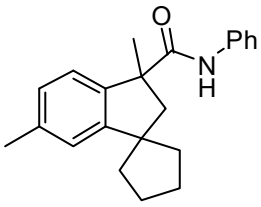
eV) *m/z* (%): 355 (M^++2, 3), 353 (M^+, 8), 233 (100), 207 (11), 165 (39); HRMS *m/z* (ESI) calcd for $C_{22}H_{25}{}^{35}ClNO$ $(M+H)^+$ 354.1619, found 354.1616.

_N_,3'-Diphenyl-2',3'-dihydrospiro[cyclopentane-1,1'-indene]-3'-carboxamide (3ab):



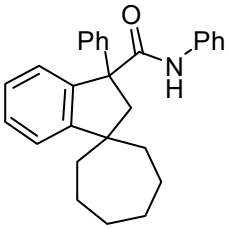
Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.23 (m, 14H), 7.08 (t, *J* = 7.2 Hz, 1H), 3.39 (d, *J* = 12.8 Hz, 1H), 2.37 (d, *J* = 12.8 Hz, 1H), 1.97-1.94 (m, 1H), 1.79 (s, 4H), 1.73-1.66 (m, 1H), 1.56-1.50 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.5, 153.0, 144.3, 143.8, 137.8, 128.9, 128.8, 128.6, 127.8, 127.1 (2C), 124.9, 124.4, 123.6, 119.8, 65.6, 54.6, 53.9, 41.0, 40.7, 25.2 (2C); LRMS (EI, 70 eV) *m/z* (%): 367 (M^+, 2), 247 (100), 169 (24); HRMS *m/z* (ESI) calcd for $C_{26}H_{26}NO$ $(M+H)^+$ 368.2009, found 368.2020.

3',6'-Dimethyl-_N_-phenyl-2',3'-dihydrospiro[cyclopentane-1,1'-indene]-3'-carboxamide (3ob):



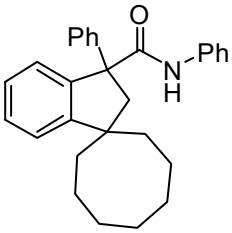
Colorless oil; ^1H NMR (400 MHz, $CDCl_3$) δ: 7.35 (d, *J* = 8.4 Hz, 2H), 7.27-7.21 (m, 3H), 7.14 (d, *J* = 6.8 Hz, 2H), 7.05 (t, *J* = 7.2 Hz, 2H), 2.75 (d, *J* = 13.2 Hz, 1H), 2.41 (s, 3H), 2.03-1.97 (m, 2H), 1.84-1.59 (m, 10H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 175.8, 152.8, 141.7, 138.7, 137.7, 128.8 (2C), 128.4, 124.2, 123.2, 119.7, 54.9 (2C), 53.4, 41.4, 41.3, 25.8, 25.3, 25.2, 21.5; LRMS (EI, 70 eV) *m/z* (%): 319 (M^+, 6), 199 (100), 171 (3), 157 (21); HRMS *m/z* (ESI) calcd for $C_{22}H_{26}NO$ $(M+H)^+$ 320.2009, found 320.2016.

***N*,3'-Diphenyl-2',3'-dihydrospiro[cycloheptane-1,1'-indene]-3'-carboxamide (3ac):**



White solid, m.p. 108.6-110.0 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (t, *J* =8.0 Hz, 3H), 7.36-7.22 (m, 11H), 7.08 (t, *J* =7.2 Hz, 1H), 3.47 (d, *J* =13.2 Hz, 1H), 2.35 (d, *J* =13.2 Hz, 1H), 1.86-1.47 (m, 10H), 1.36-1.22 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.4, 155.5, 144.6, 142.7, 137.8, 128.9, 128.8, 128.6, 127.7, 127.2, 127.0, 125.2, 124.4, 123.7, 119.8, 65.0, 52.4, 50.0, 41.6, 41.4, 29.2, 29.1, 24.4, 24.0; LRMS (EI, 70 eV) *m/z* (%): 395 (M^+, 2), 275 (100), 193 (36); HRMS *m/z* (ESI) calcd for $C_{28}H_{30}NO$ $(M+H)^+$ 396.2322, found 396.2328.

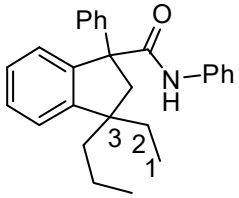
***N*,3'-Diphenyl-2',3'-dihydrospiro[cyclooctane-1,1'-indene]-3'-carboxamide (3ad):**



White solid, m.p. 102.0-103.8 °C (uncorrected); ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.24 (m, 13H), 7.07 (t, *J* = 7.2 Hz, 1H), 6.47 (s, 1H), 3.53 (d, *J* = 13.6 Hz, 1H), 2.31 (d, *J* = 13.2 Hz, 1H), 1.71 (d, *J* = 10.0 Hz, 1H), 1.64-1.52 (m, 7H), 1.62-1.26 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 178.3, 144.0, 141.9, 134.8, 131.9, 129.5, 129.0, 128.5, 128.0, 127.9, 127.2, 126.8, 126.5, 125.7, 122.8, 56.5, 46.2, 34.2, 34.0, 32.4, 27.1, 27.0, 26.4, 25.2, 25.1; LRMS (EI, 70 eV) *m/z* (%): 409 (M^+, 2), 289 (100), 193 (27); HRMS *m/z* (ESI) calcd for $C_{29}H_{32}NO$ $(M+H)^+$ 410.2478, found 410.2483.

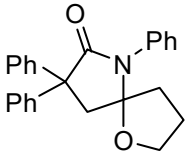
Product (3ae):

1°/2°/3° = 1.3:1:1;



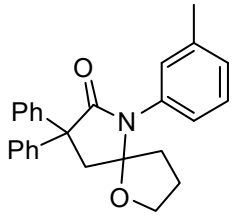
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41-7.23 (m, 14.1H), 7.08 (d, *J* = 7.6 Hz, 1.0H), 3.50 (d, *J* = 13.2 Hz, 0.3H), 3.43-3.38 (m, 0.4H), 3.25 (d, *J* = 13.2 Hz, 0.3H), 2.41 (d, *J* = 13.2 Hz, 0.3H), 2.32 (d, *J* = 13.6 Hz, 0.4H), 2.24 (d, *J* = 13.2 Hz, 0.3H), 1.63-1.52 (m, 3.1H), 1.27-1.07 (m, 5.1H), 0.91-0.84 (m, 2.1H), 0.80- 0.70 (m, 2.0H).

6,8,8-Triphenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4af):



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50-7.45 (m, 4H), 7.41-7.19 (m, 11H), 3.80-3.69 (m, 2H), 3.29 (d, *J* = 13.6 Hz, 1H), 2.96 (d, *J* = 13.2 Hz, 1H), 2.03-1.94 (m, 1H), 1.85-1.78 (m, 1H), 1.76-1.67 (m, 1H), 1.39-1.29 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.6, 144.4, 143.0, 136.1, 129.2, 129.0, 128.4, 128.2, 128.0 (2C), 127.7, 126.7, 126.6, 98.9, 68.3, 57.1, 49.5, 36.0, 25.4; LRMS (EI, 70 eV) *m/z* (%): 369 (M^+, 2), 250 (100), 207 (30); HRMS *m/z* (ESI) calcd for $C_{25}H_{24}NO_2$ $(M+H)^+$ 370.1802, found 370.1803.

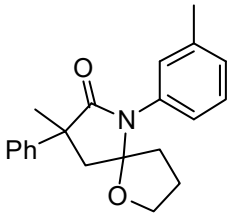
8,8-Diphenyl-6-(*m*-tolyl)-1-oxa-6-azaspiro[4.4]nonan-7-one (4gf):



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.49 (d, *J* = 7.6 Hz, 2H), 7.45 (d, *J* = 7.6 Hz, 2H), 7.36-7.20 (m, 7H), 7.16-7.11 (m, 3H), 3.81-3.70 (m, 2H), 3.29 (d, *J* = 13.6 Hz, 1H), 2.96 (d, *J* = 13.6 Hz, 1H), 2.36 (s, 3H), 2.05-1.98 (m, 1H), 1.87-1.80 (m, 1H), 1.78-1.69 (m, 1H), 1.43-1.33 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.7, 144.6, 143.1, 138.9, 136.0, 129.8, 128.8 (2C), 128.4, 128.2, 128.0, 127.8, 126.7 (2C), 126.2, 98.9, 68.3, 57.1, 49.6, 36.0, 25.4, 21.3; LRMS (EI, 70 eV) *m/z* (%): 383 (M^+, 7), 365 (29), 250 (100); HRMS *m/z* (ESI) calcd for $C_{26}H_{26}NO_2$ $(M+H)^+$ 384.1958, found 384.1967.

8-Methyl-8-phenyl-6-(*m*-tolyl)-1-oxa-6-azaspiro[4.4]nonan-7-one (4mf):

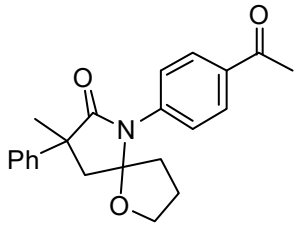
d.r. = 5:1;



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.52 (d, *J* = 7.6 Hz, 2.0H), 7.39-7.34 (m, 2.1H), 7.32-7.23 (m, 2.0H), 7.17-7.14 (m, 3.0H), 3.78 (t, *J* = 6.4 Hz, 2.0H), 2.65 (d, *J* = 13.2 Hz, 1.0H), 2.55 (d, *J* = 13.2 Hz, 1.0H), 2.38 (s, 3.0H), 2.04-1.99 (m, 1.1H), 1.83-1.61 (m, 5.0H), 1.40-1.33 (m, 1.0H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 177.7, 177.6, 144.8, 138.9, 136.2, 133.4, 129.8, 128.8 (2C), 128.5, 128.4, 126.9, 126.6, 126.2, 126.1, 99.9, 99.3, 68.3, 50.7, 48.2, 35.8, 26.5, 25.3, 21.3; LRMS (EI, 70 eV) *m/z* (%): 321 (M^+, 36), 187 (64), 173 (100); HRMS *m/z* (ESI) calcd for $C_{21}H_{24}NO_2$ $(M+H)^+$ 322.1802, found 322.1810.

6-(4-Acetylphenyl)-8-methyl-8-phenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4rf):

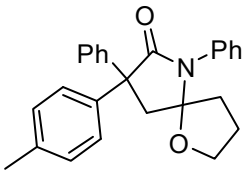
d.r. = 3:1;



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.01 (d, *J* = 8.0 Hz, 1.5H), 7.87 (d, *J* = 7.6 Hz, 0.5H), 7.52-7.47 (m, 4.0H), 7.38 (t, *J* = 7.2 Hz, 2.1H), 7.26 (t, *J* = 7.2 Hz, 1.0H), 3.85-3.81 (m, 2.0H), 2.69-2.55 (m, 5.0H), 2.00-1.92 (m, 1.1H), 1.85-1.72 (m, 5.0H), 1.50-1.41 (m, 1.1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 197.5, 197.4, 177.5, 144.4, 141.0, 136.2, 129.6, 129.1, 128.9, 128.8, 128.6, 126.7 (2C), 126.1, 99.5 (2C), 68.1, 50.6, 48.3, 35.7, 26.6 (2C), 25.3; LRMS (EI, 70 eV) *m/z* (%): 349 (M^+, 37), 187 (68), 173 (100); HRMS *m/z* (ESI) calcd for $C_{22}H_{24}NO_3$ $(M+H)^+$ 350.1751, found 350.1762.

6, 8-Diphenyl-8-(*p*-tolyl)-1-oxa-6-azaspiro[4.4]nonan-7-one (4kf):

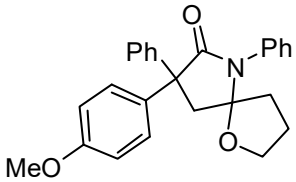
d.r. = 1:1;



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 8.10 (d, *J* = 7.6 Hz, 1.1H), 7.60 (t, *J* = 7.6 Hz, 1.0H), 7.46 (t, *J* = 8.0 Hz, 3.1H), 7.41-7.32 (m, 6.0H), 7.27 (d, *J* = 8.0 Hz, 1.1H), 7.15 (d, *J* = 8.0 Hz, 1.0H), 7.10 (d, *J* = 8.0 Hz, 1.0H), 3.78-3.70 (m, 2.0H), 3.30-3.25 (m, 1.0H), 2.99-2.93 (m, 1.0H), 2.33 (s, 1.5H), 2.30 (s, 1.5H), 1.98-1.93 (m, 1.1H), 1.86-1.78 (m, 1.1H), 1.75-1.67 (m, 1.0H), 1.40-1.29 (m, 1.0H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.9, 174.8, 144.7, 143.2, 141.2, 139.9, 136.4, 136.2 (2C), 133.6, 130.1, 129.2, 129.1, 129.0, 128.8, 128.4 (2C), 128.1, 128.0 (3C), 127.7, 127.6, 126.6 (2C), 99.0 (2C), 68.3, 68.2, 56.8 (2C), 49.6, 49.5, 36.0, 35.9, 25.4 (2C), 20.9 (2C); LRMS (EI, 70 eV) *m/z* (%): 383 (M^+, 5), 264 (100), 221 (26); HRMS *m/z* (ESI) calcd for $C_{26}H_{26}NO_2$ $(M+H)^+$ 384.1958, found 384.1966.

8-(4-Methoxyphenyl)-6, 8-diphenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4sf):

d.r. = 1.3:1;

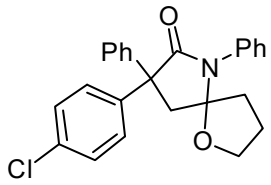


Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46-7.38 (m, 5.0H), 7.36-7.21 (m, 7.1H), 6.88 (d, *J* = 8.8 Hz, 1.0H), 6.83 (d, *J* = 8.8 Hz, 1.0H), 3.81 (s, 1.5H), 3.77-3.71 (m, 3.5H), 3.29-3.11 (m, 2.0H), 2.99-2.90 (m, 1.0H), 2.01-1.94 (m, 1.0H), 1.85-1.80 (m, 1.0H), 1.75-1.70 (m, 1.0H), 1.42-1.34 (m, 1.0H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.9, 174.8, 159.6, 158.3, 145.0, 143.6, 136.3, 135.0, 129.3, 129.2 (2C), 129.0, 128.9, 128.5, 128.1, 128.0 (2C), 127.7, 126.7, 126.6, 113.8, 113.4, 99.0, 98.9, 68.3 (2C), 56.5 (2C), 55.2 (2C), 49.7 (2C), 36.0 (2C), 25.4 (2C); LRMS (EI, 70 eV) *m/z* (%): 399 (M^+, 23),

381 (64), 280 (100); HRMS *m/z* (ESI) calcd for $C_{26}H_{26}NO_3$ $(M+H)^+$ 400.1907, found 400.1918.

8-(4-Chlorophenyl)-6, 8-diphenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4tf):

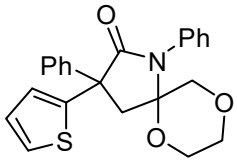
d.r. = 1:1;



Yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.46-7.24 (m, 14.3H), 3.76-3.73 (m, 2.0H), 3.29-3.23 (m, 1.0H), 2.95-2.90 (m, 1.0H), 2.03-1.97 (m, 1.0H), 1.87-1.79 (m, 1.0H), 1.75-1.71 (m, 1.1H), 1.39-1.31 (m, 1.0H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 174.4, 174.3, 144.2, 143.0, 142.7, 141.4, 136.0, 132.7, 129.7, 129.2, 129.1, 129.0, 128.6, 128.5, 128.1 (2C), 128.0, 127.6, 126.9, 126.8, 98.9, 98.8, 68.4, 68.4, 56.6 (2C), 49.3, 49.2, 36.1, 35.9, 25.3 (2C); LRMS (EI, 70 eV) *m/z* (%): 403 (M^+, 2), 283 (100), 178 (26); HRMS *m/z* (ESI) calcd for $C_{25}H_{23}{}^{35}ClNO_2(M+H)^+$ 404.1412, found 404.1418.

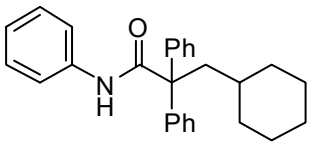
1,3-Diphenyl-3-(thiophen-2-yl)-6,9-dioxa-1-azaspiro[4.5]decan-2-one (4ug):

d.r. > 20:1;



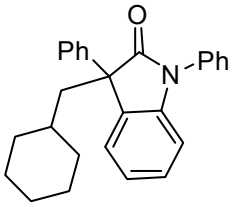
Light yellow oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.41 (d, *J* = 8.0 Hz, 2H), 7.35-7.26 (m, 7H), 7.19 (t, *J* = 7.6 Hz, 1H), 7.09-7.05 (m, 3H), 3.69 (d, *J* = 12.0 Hz, 1H), 3.60-3.52 (m, 2H), 3.38 (t, *J* = 10.4 Hz, 1H), 3.27-3.17 (m, 2H), 2.86 (t, *J* = 12.4 Hz, 1H), 2.16 (d, *J* = 12.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 178.1, 144.5, 140.3, 135.6, 130.2, 128.6 (2C), 127.5, 126.8, 125.7, 125.2, 123.8, 123.7, 123.1, 109.8, 73.0, 70.7, 66.5, 66.2, 53.7, 39.6; LRMS (EI, 70 eV) *m/z* (%): 391 (M^+, 43), 291 (100), 262 (28), 207 (35); HRMS *m/z* (ESI) calcd for $C_{23}H_{22}NO_3S$ $(M+H)^+$ 392.1315, found 392.1312.

3-Cyclohexyl-*N*,2,2-triphenylpropanamide (5aa):



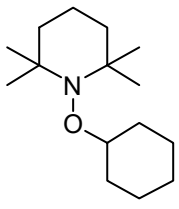
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.44 (d, *J* = 7.6 Hz, 4H), 7.37-7.31 (m, 5H), 7.30-7.23 (m, 5H), 7.18 (s, 1H), 7.05 (d, *J* = 7.2 Hz, 1H), 2.38 (s, 2H), 1.54-1.49 (m, 2H), 1.32-1.26 (m, 4H), 1.05-1.00 (m, 2H), 0.92-0.83 (m, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 172.5, 143.2, 137.9, 129.1, 128.9, 128.4, 127.1, 124.2, 119.7, 61.8, 45.9, 35.1, 34.6, 26.5, 26.3; LRMS (EI, 70 eV) *m/z* (%): 383 (M^+, 27), 264 (100), 121 (20); HRMS *m/z* (ESI) calcd for $C_{27}H_{30}NO$ $(M+H)^+$ 384.2322, found 384.2326.

3-(Cyclohexylmethyl)-1,3-diphenylindolin-2-one (6aa):



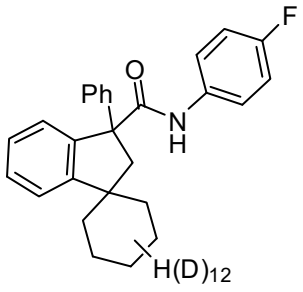
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.50 (t, *J* = 7.6 Hz, 2H), 7.44 (d, *J* = 8.0 Hz, 2H), 7.38 (t, *J* = 6.8 Hz, 3H), 7.29 (t, *J* = 7.2 Hz, 3H), 7.23 (t, *J* = 8.0 Hz, 2H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 2.56-2.51 (m, 1H), 2.24-2.19 (m, 1H), 1.60-1.51 (m, 4H), 1.35-1.21 (m, 2H), 1.04 (t, *J* = 8.0 Hz, 4H), 0.94-0.86 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 178.3, 143.8, 141.7, 134.7, 132.0, 129.5, 128.5, 127.9 (2C), 127.2, 126.7, 126.5, 125.5, 122.8, 109.6, 56.0, 45.6, 35.0, 34.6, 33.6, 26.2, 26.1 (2C); LRMS (EI, 70 eV) *m/z* (%): 381 (M^+, 12), 285 (100), 256 (21), 207 (9); HRMS *m/z* (ESI) calcd for $C_{27}H_{28}NO$ $(M+H)^+$ 382.2165, found 382.2168.

1-(Cyclohexyloxy)-2,2,6,6-tetramethylpiperidine (7):



Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.58 (s, 1H), 2.05 (s, 2H), 1.74 (s, 2H), 1.58-1.46 (m, 6H), 1.31-1.13 (m, 18H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 81.7, 59.6, 40.2, 32.9, 25.9, 25.1, 17.3.

Product (3ea + 3ea-D12):



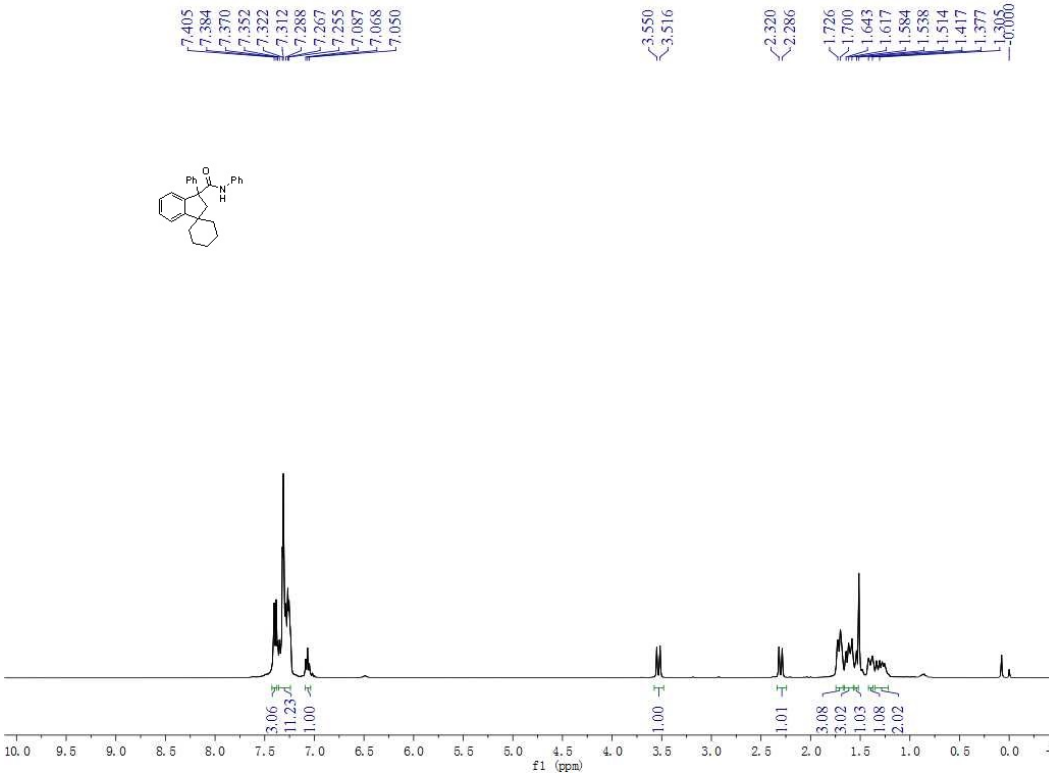
Colorless oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40-7.23 (m, 12.0H), 6.96 (t, *J* = 8.4 Hz, 2.0H), 3.51 (d, *J* = 13.6 Hz, 1.0H), 2.30 (d, *J* = 13.2 Hz, 1.0H), 1.73-1.68 (m, 2.4H), 1.65-1.60 (m, 1.6H), 1.53-1.51 (m, 0.8H), 1.41-1.28 (m, 3.0H).

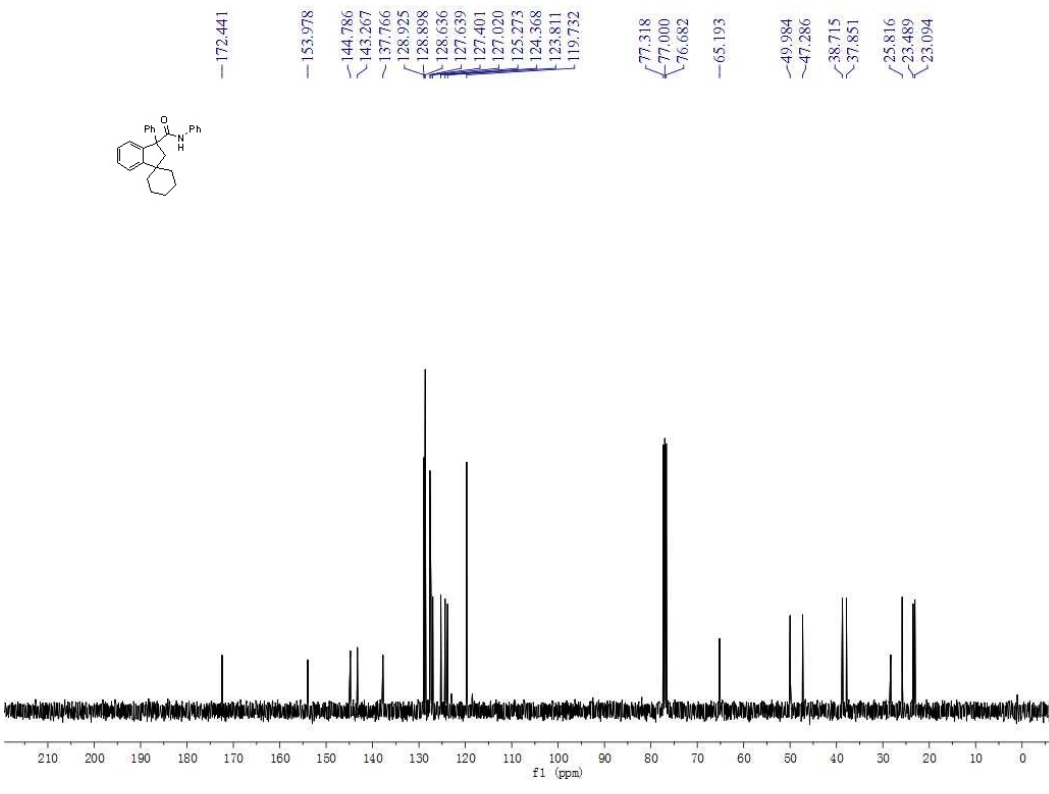
(C) Reference

[1] X. Mu, T. Wu, H.-Y. Wang, Y.-l. Guo, G. Liu, *J. Am. Chem. Soc.* **2012**, *134*, 878; W. Kong, M. Casimiro, E. Merino, C. Nevado, *J. Am. Chem. Soc.* **2013**, *135*, 14480; W. Kong, M. Casimiro, N. Fuentes, E. Merino, C. Nevado, *Angew. Chem. Int. Ed*. **2013**, *52*, 13086; W. Kong, E. Merino, C. Nevado, *Angew. Chem. Int. Ed*. **2014**, *53*, 5078.

(D) Spectra

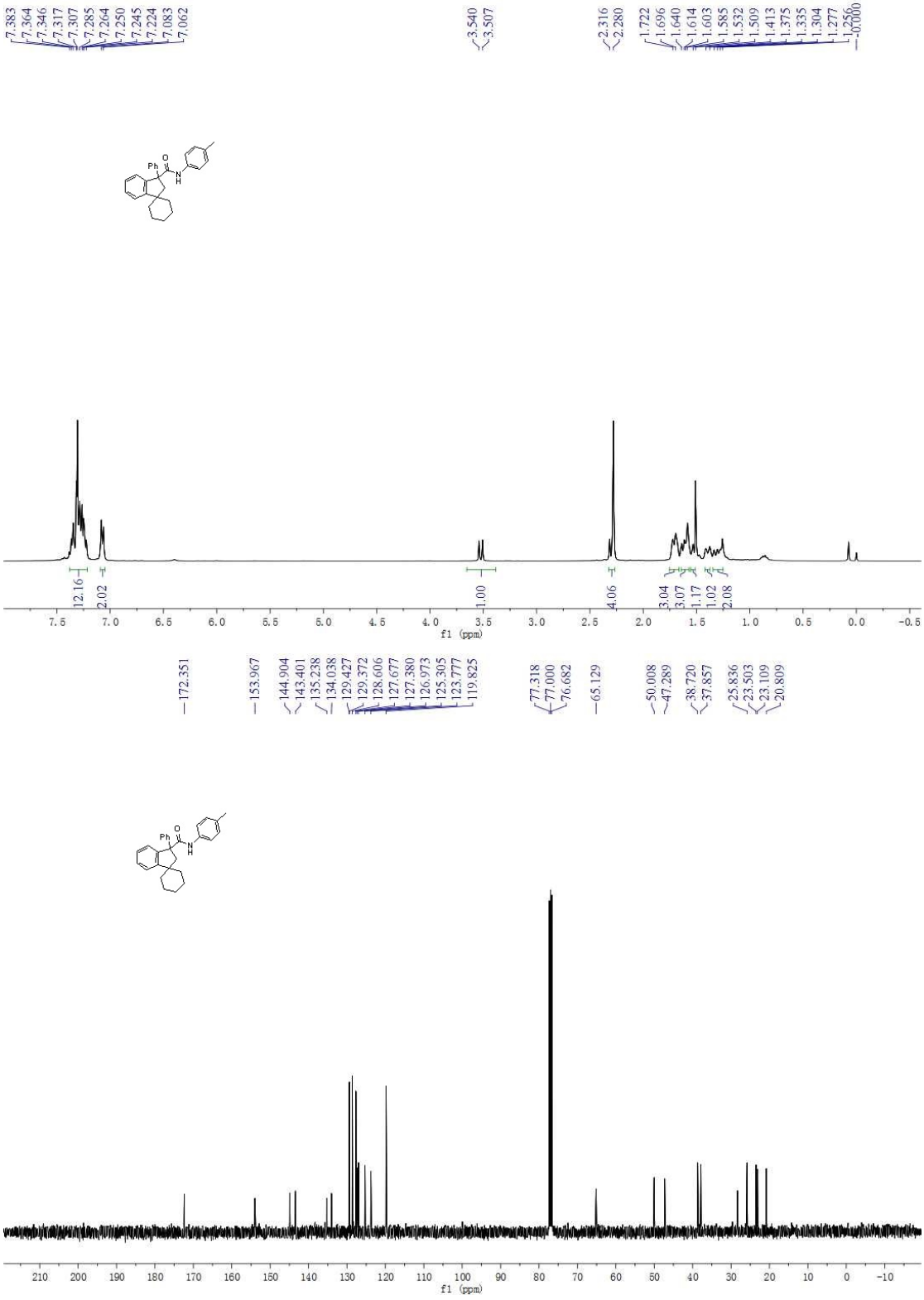
N,3'-Diphenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3aa)



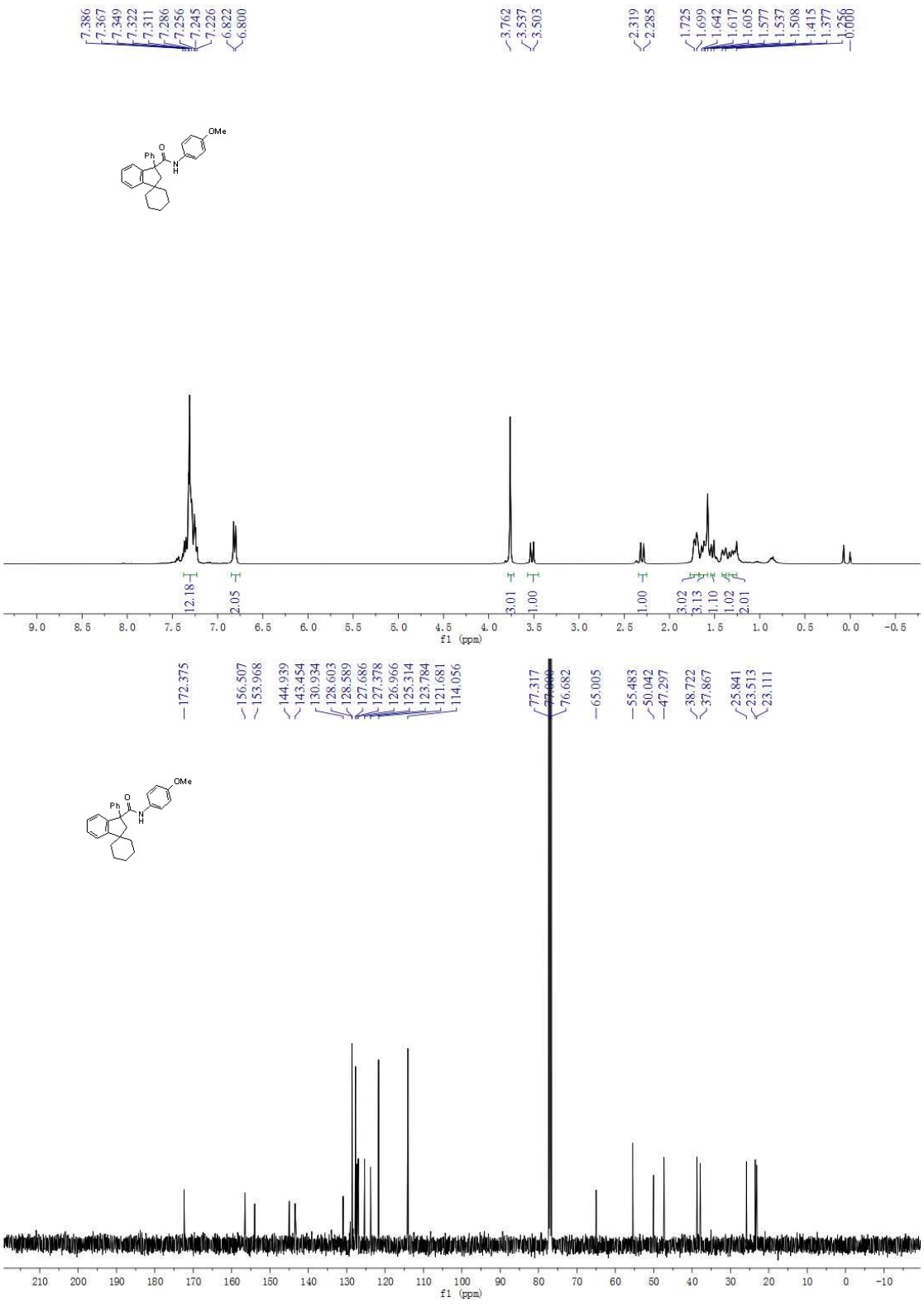


3'-Phenyl-*N*-(*p*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamid

e (3ba)

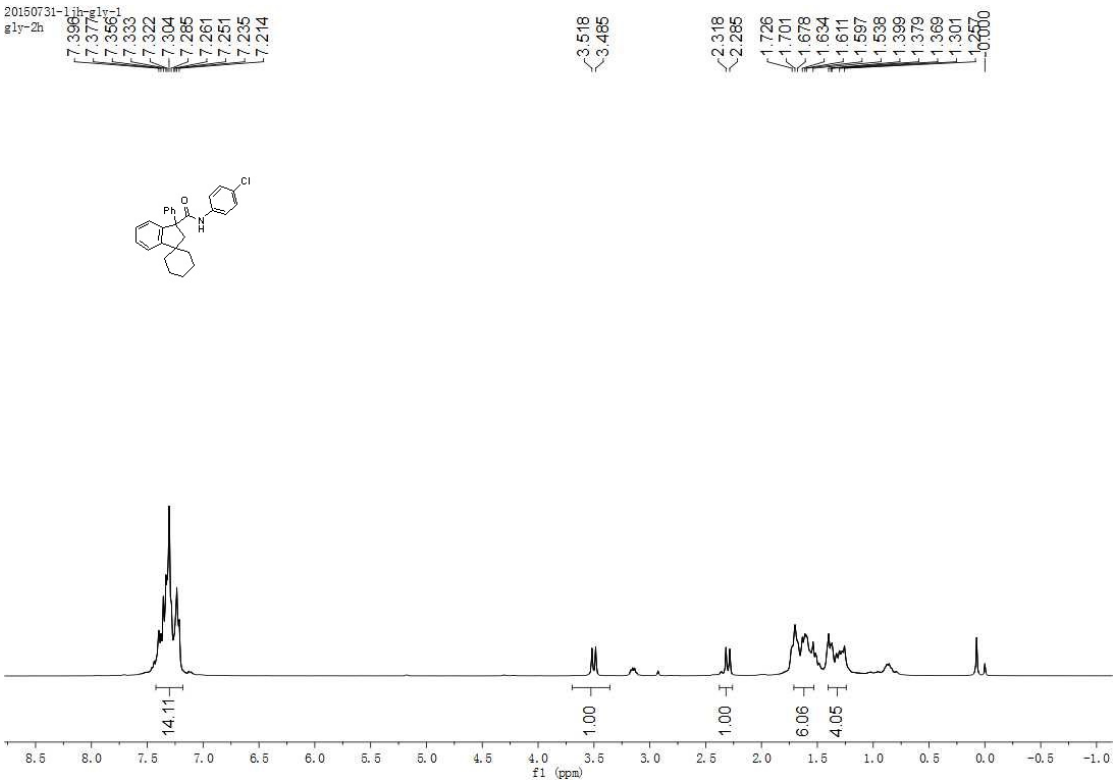


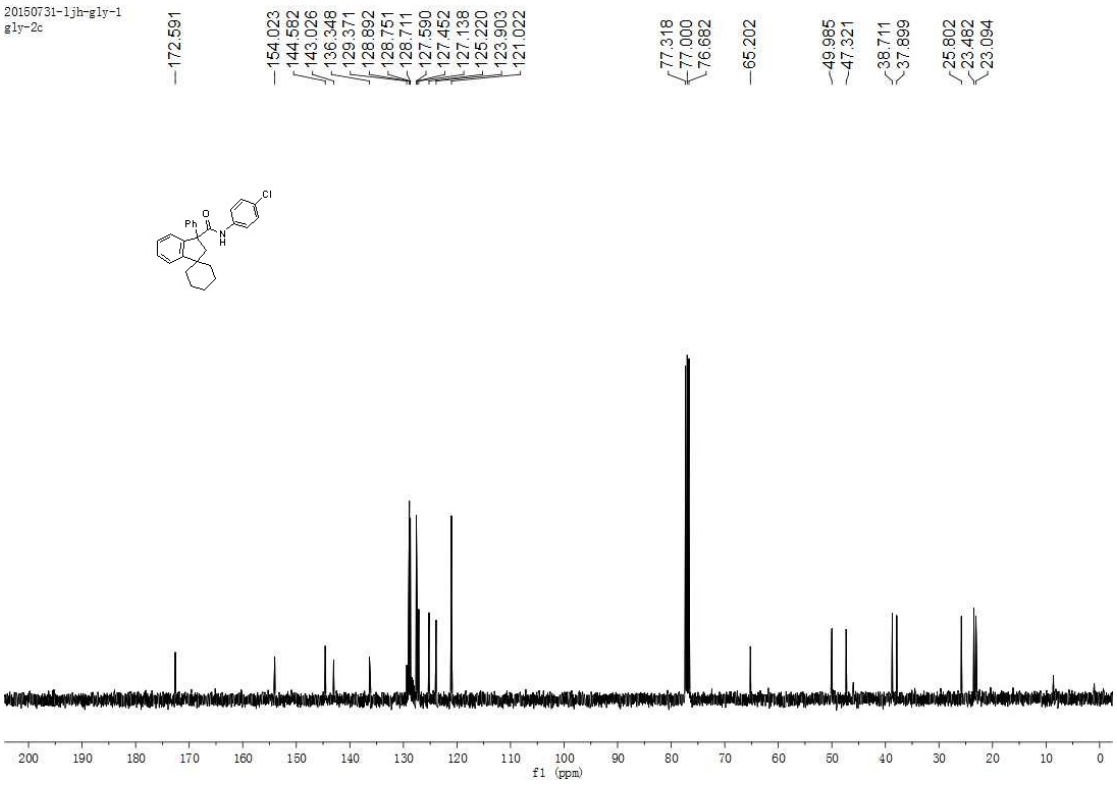
_N_-(4-Methoxyphenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ca)



_N_-(4-Chlorophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

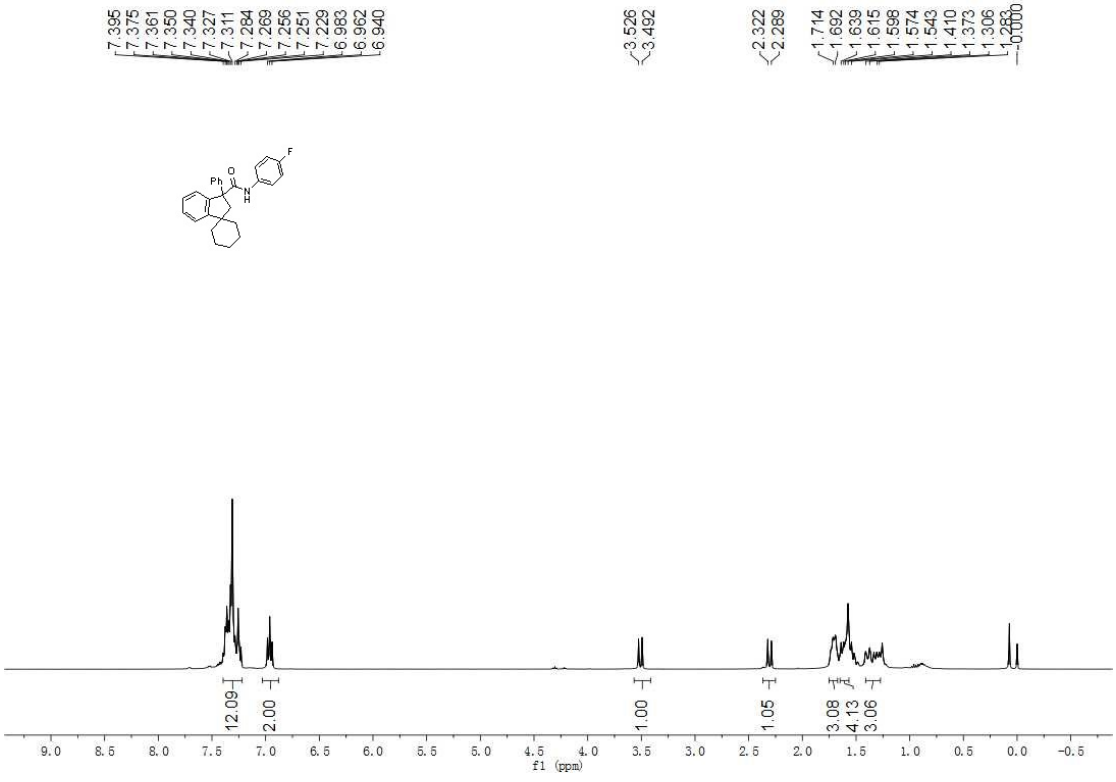
boxamide(3da)

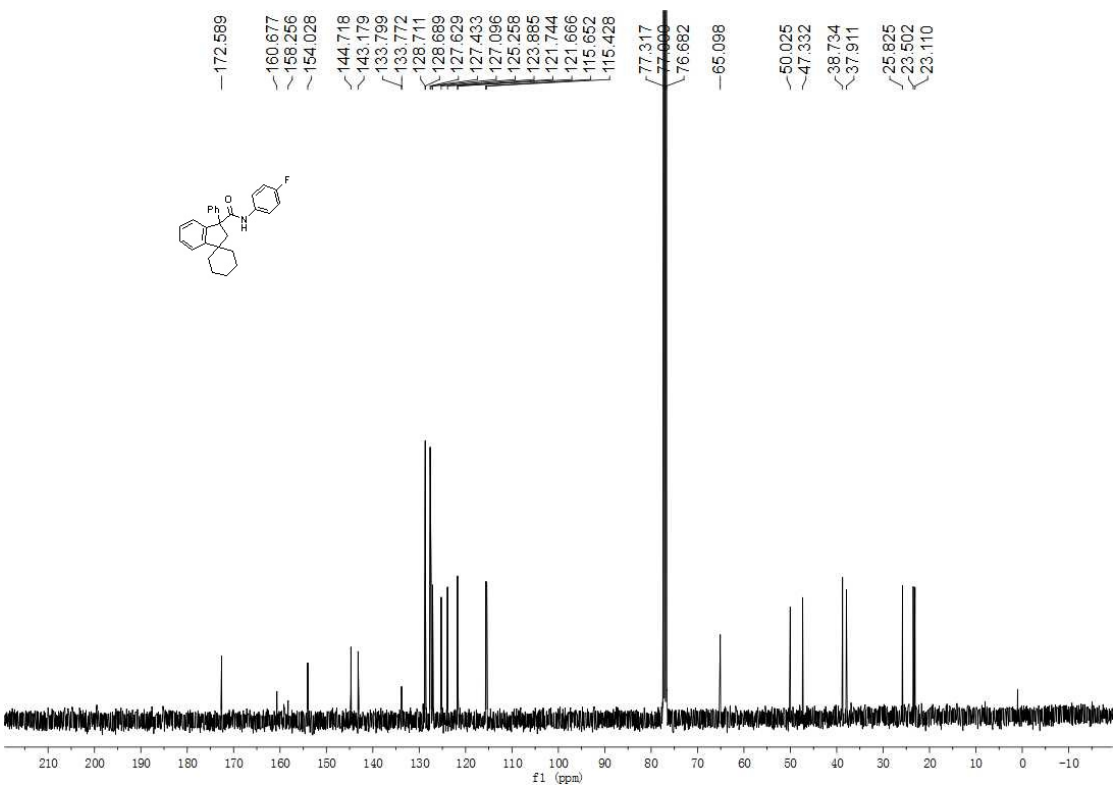




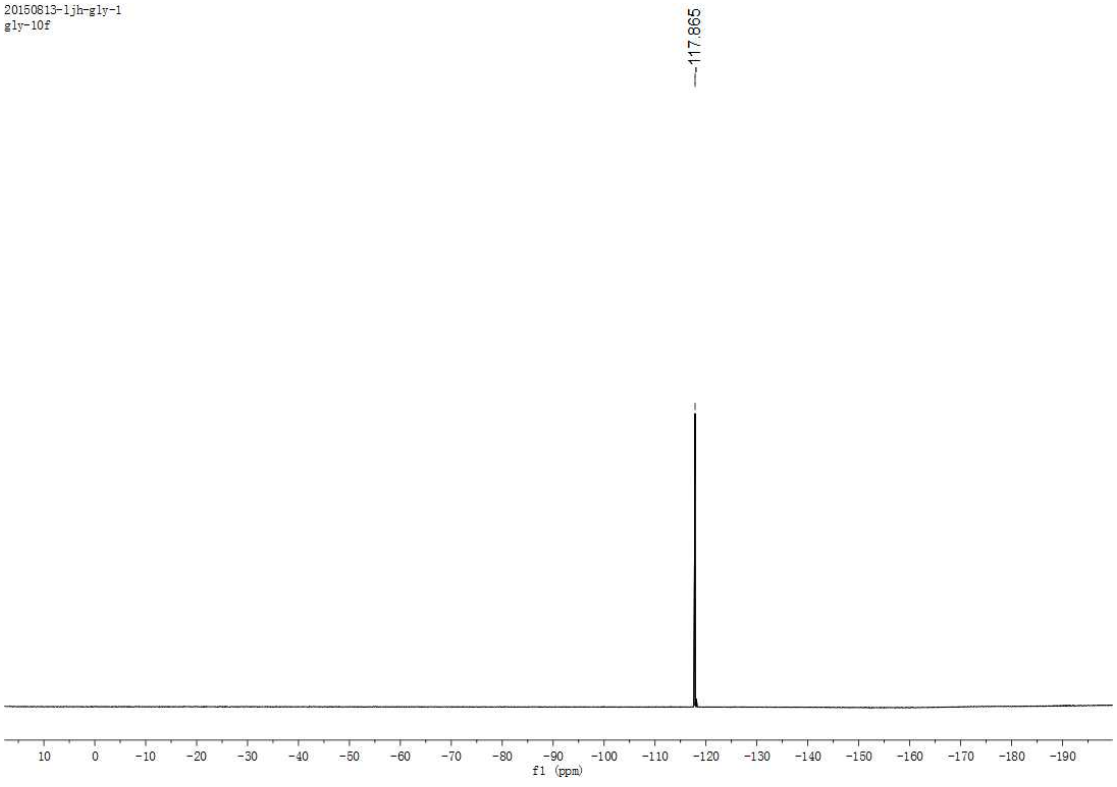
_N_-(4-Fluorophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

boxamide(3ea)



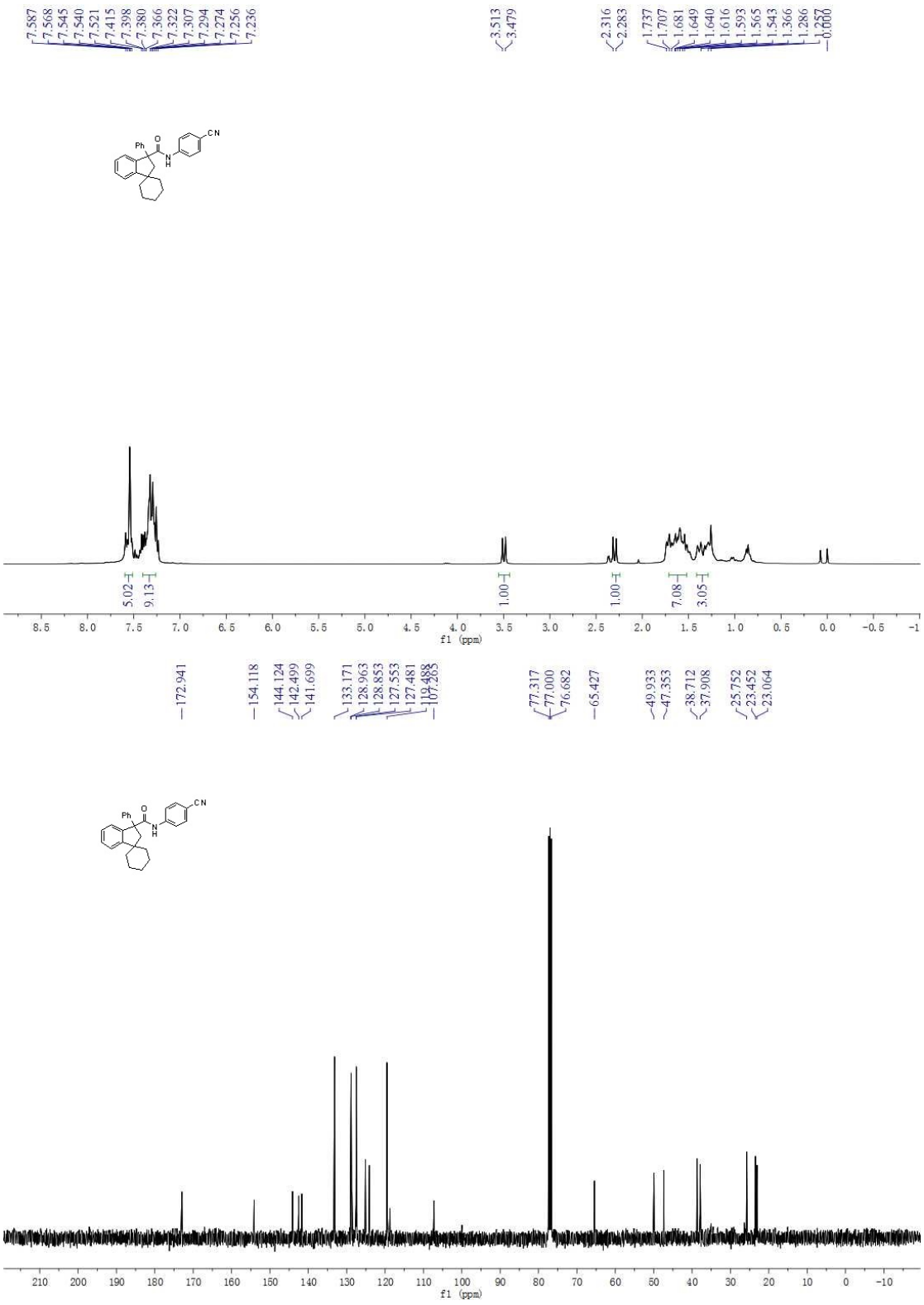


20150813-ljh-gly-1
gly-10f

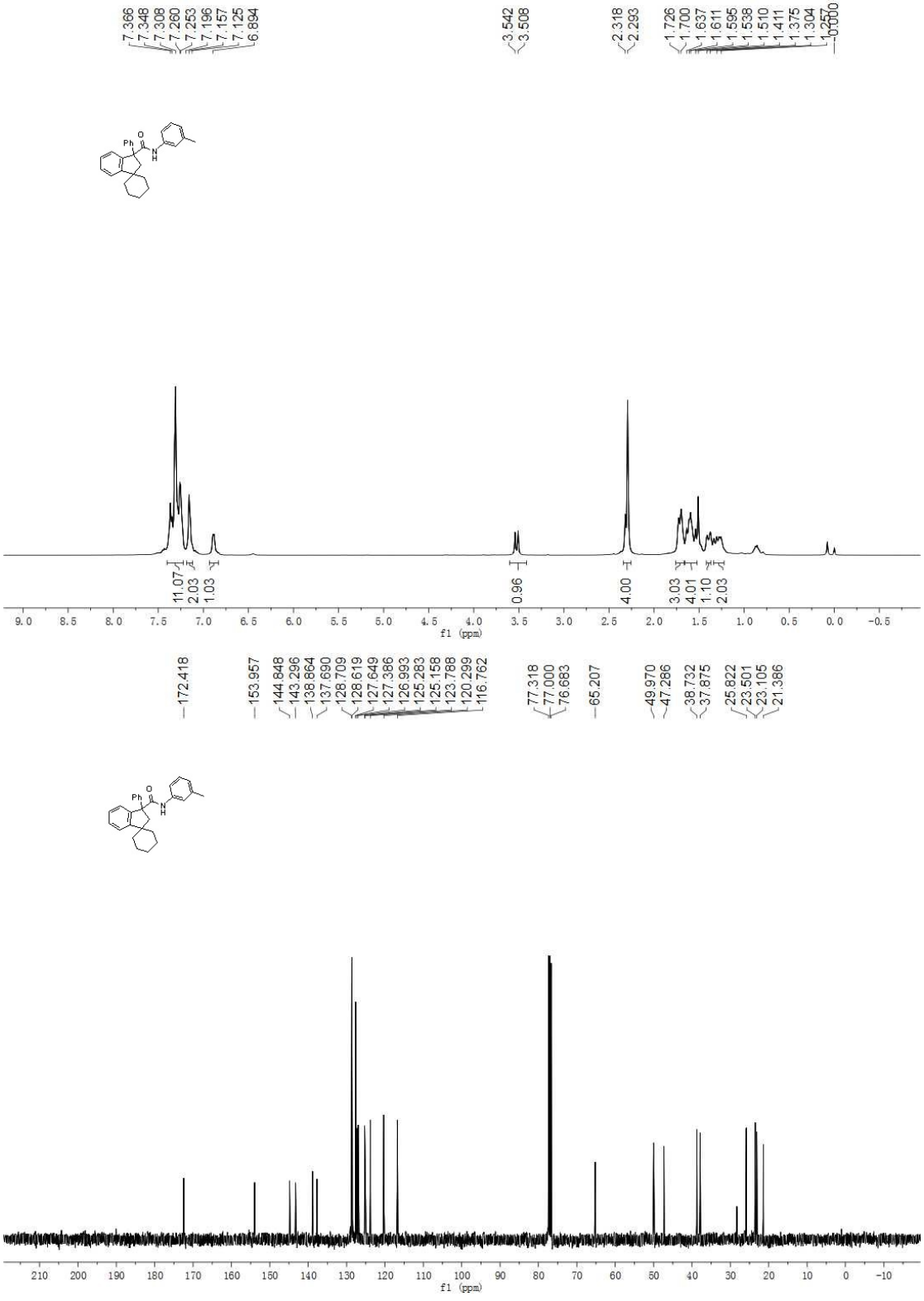


_N_-(4-Cyanophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

boxamide (3fa)

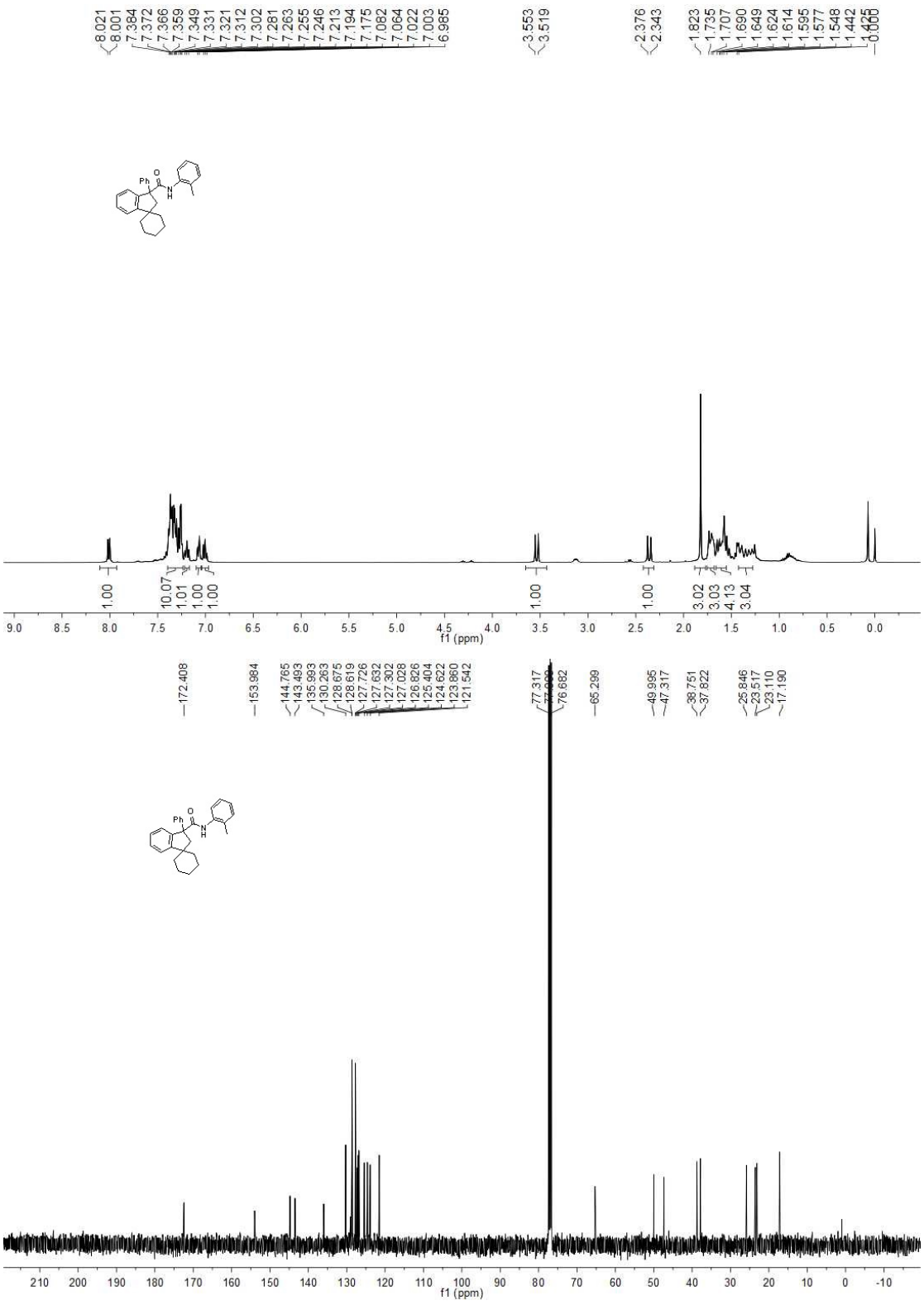


3'-Phenyl-*N*-(*m*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3ga)



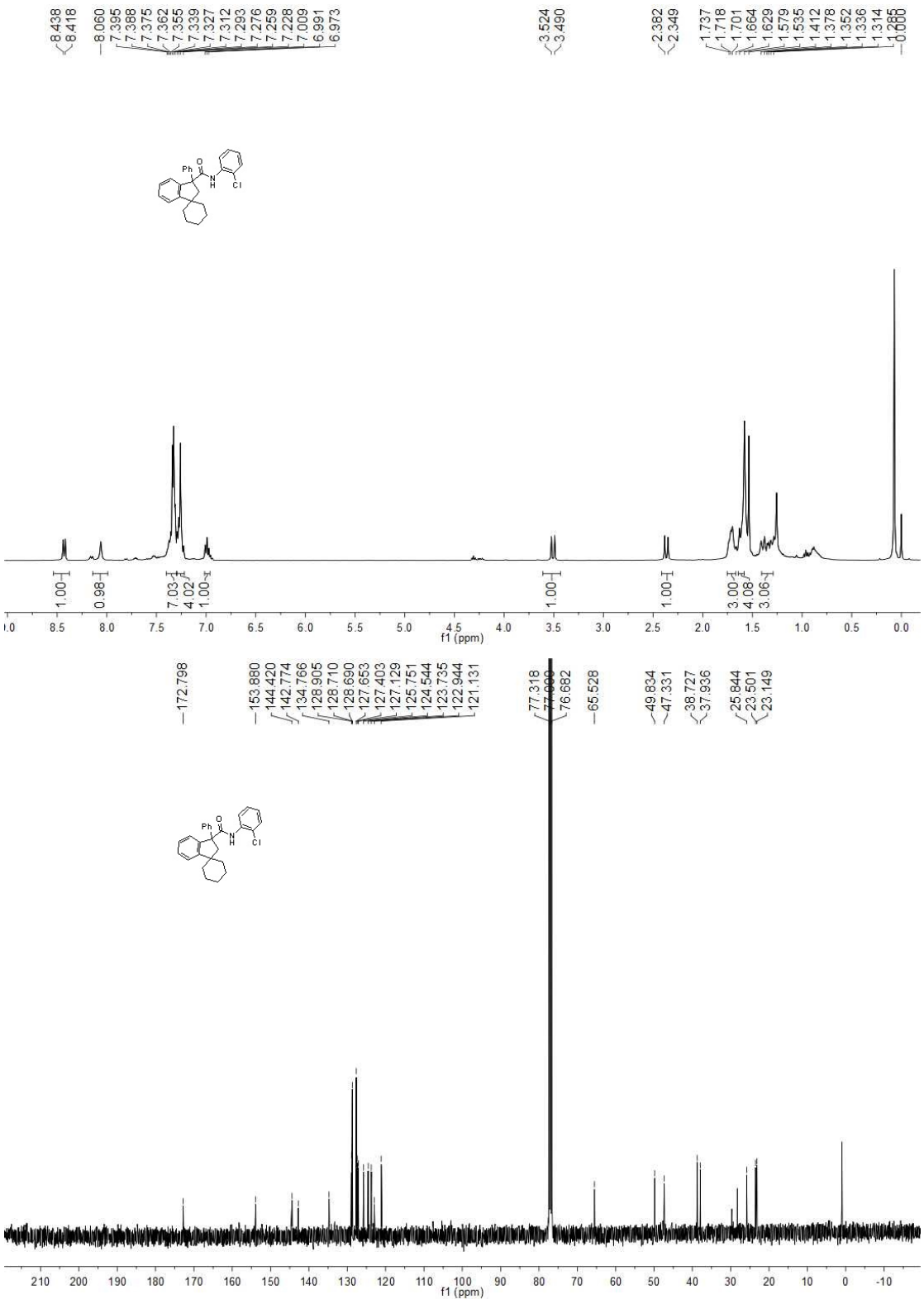
3'-Phenyl-*N*-(*o*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamid

e (3ha)



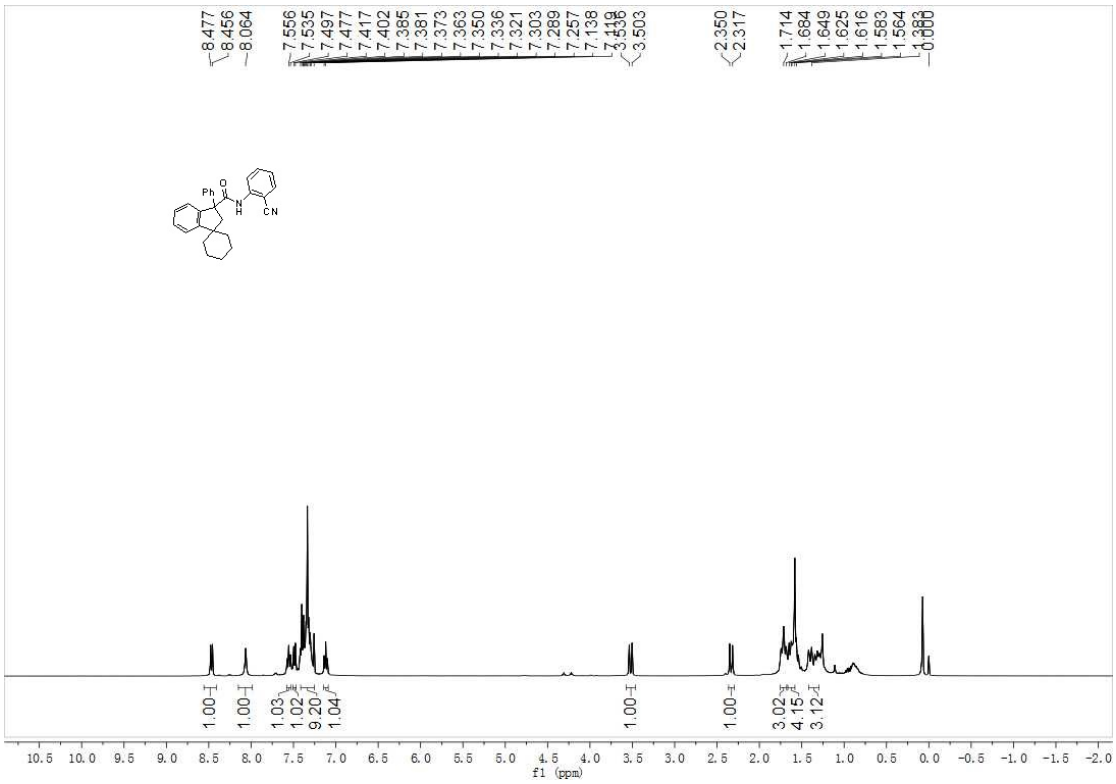
_N_-(2-Chlorophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

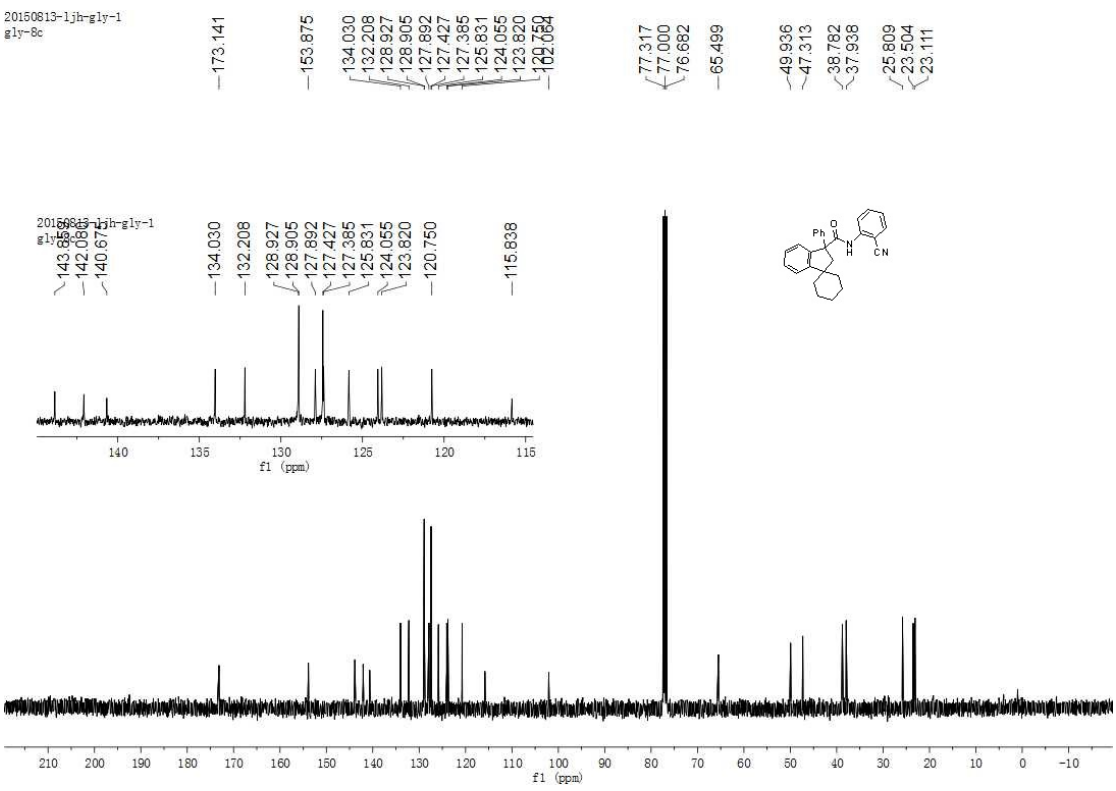
boxamide (3ia):



_N_-(2-Cyanophenyl)-3'-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

boxamide(3ja)

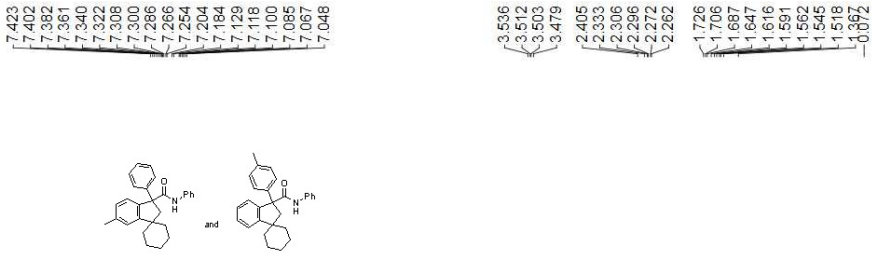


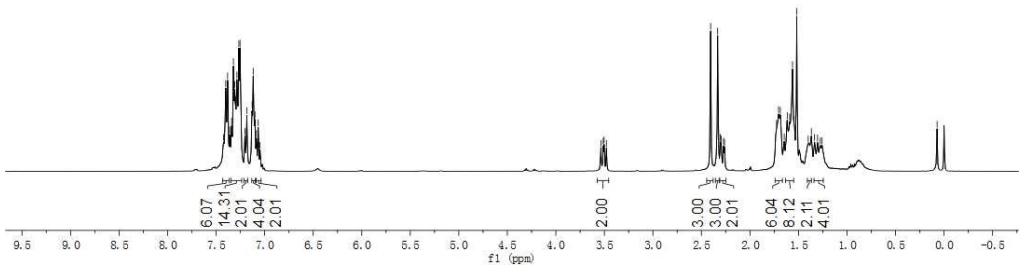


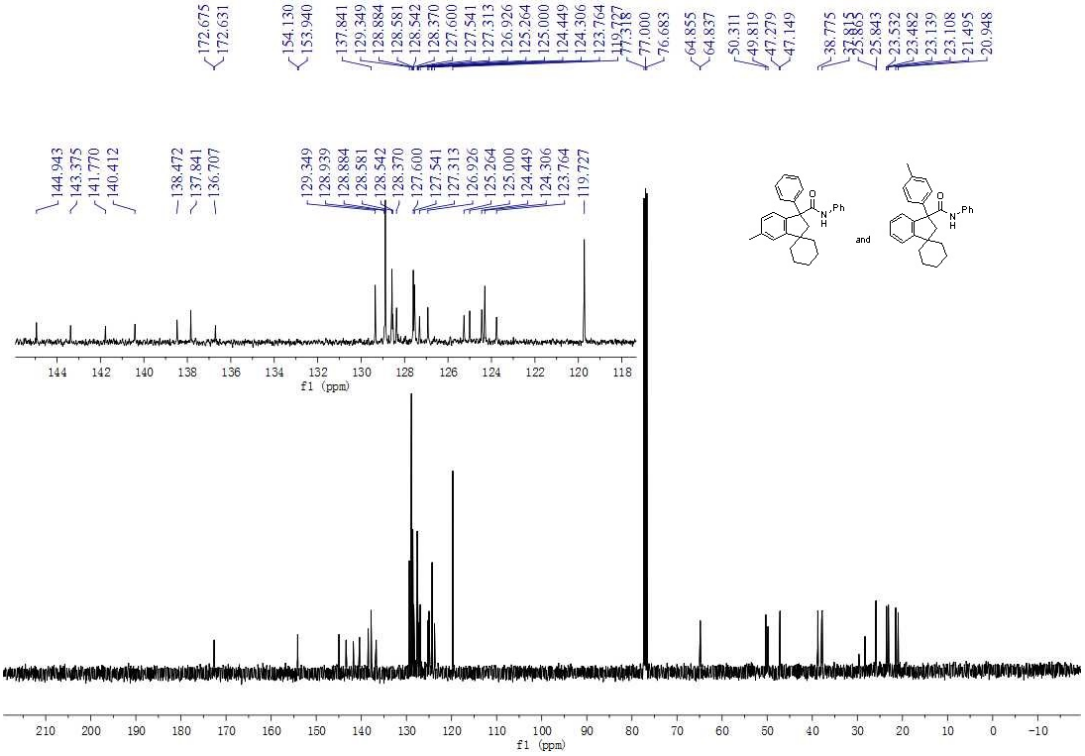
6'-Methyl-*N*,3'-diphenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxa

mide (3ka) and *N*-Phenyl-3'-(*p*-tolyl)-2',3'-dihydrospiro

[cyclohexane-1,1'-indene]-3'-carboxamide (3ka'):

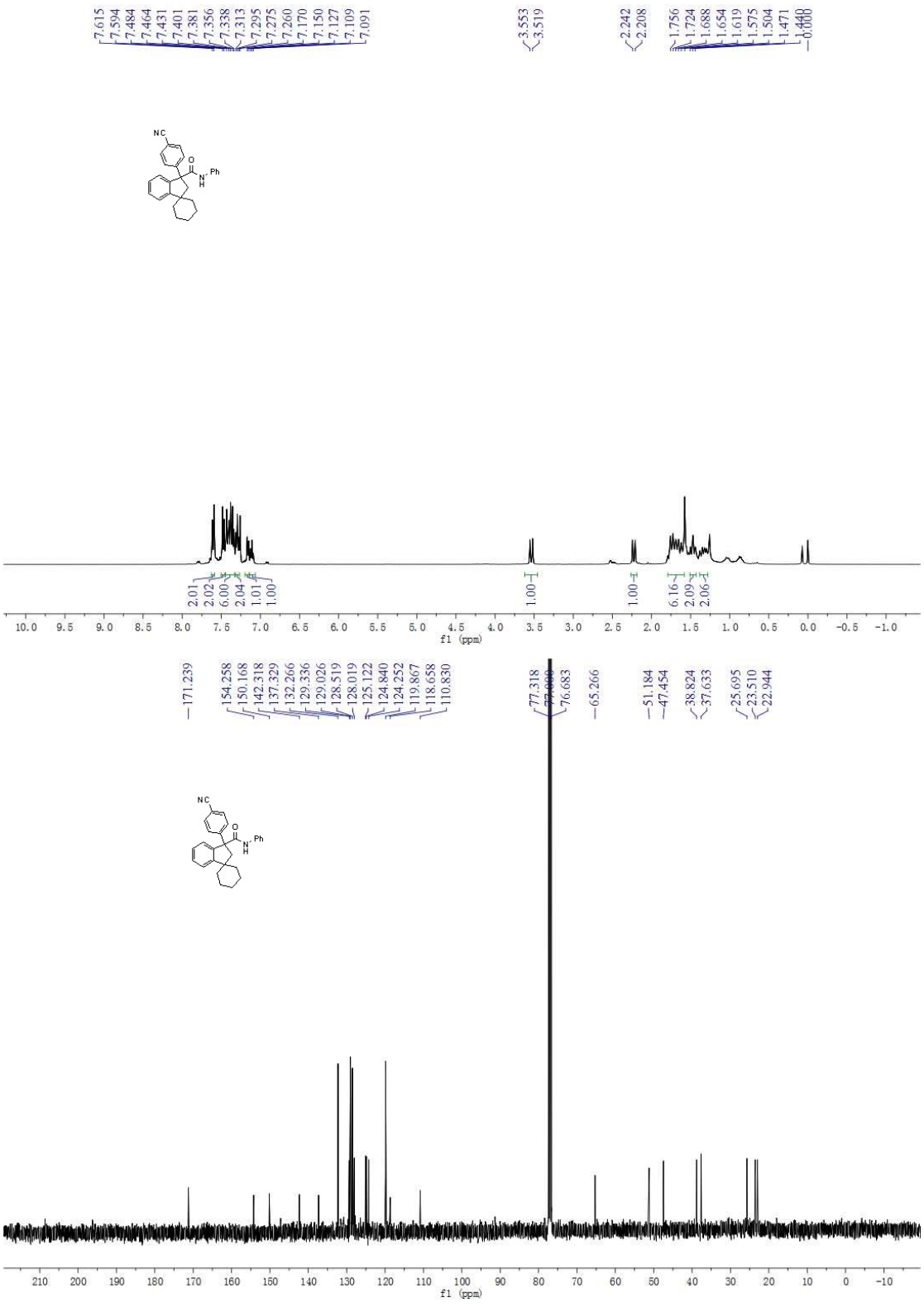






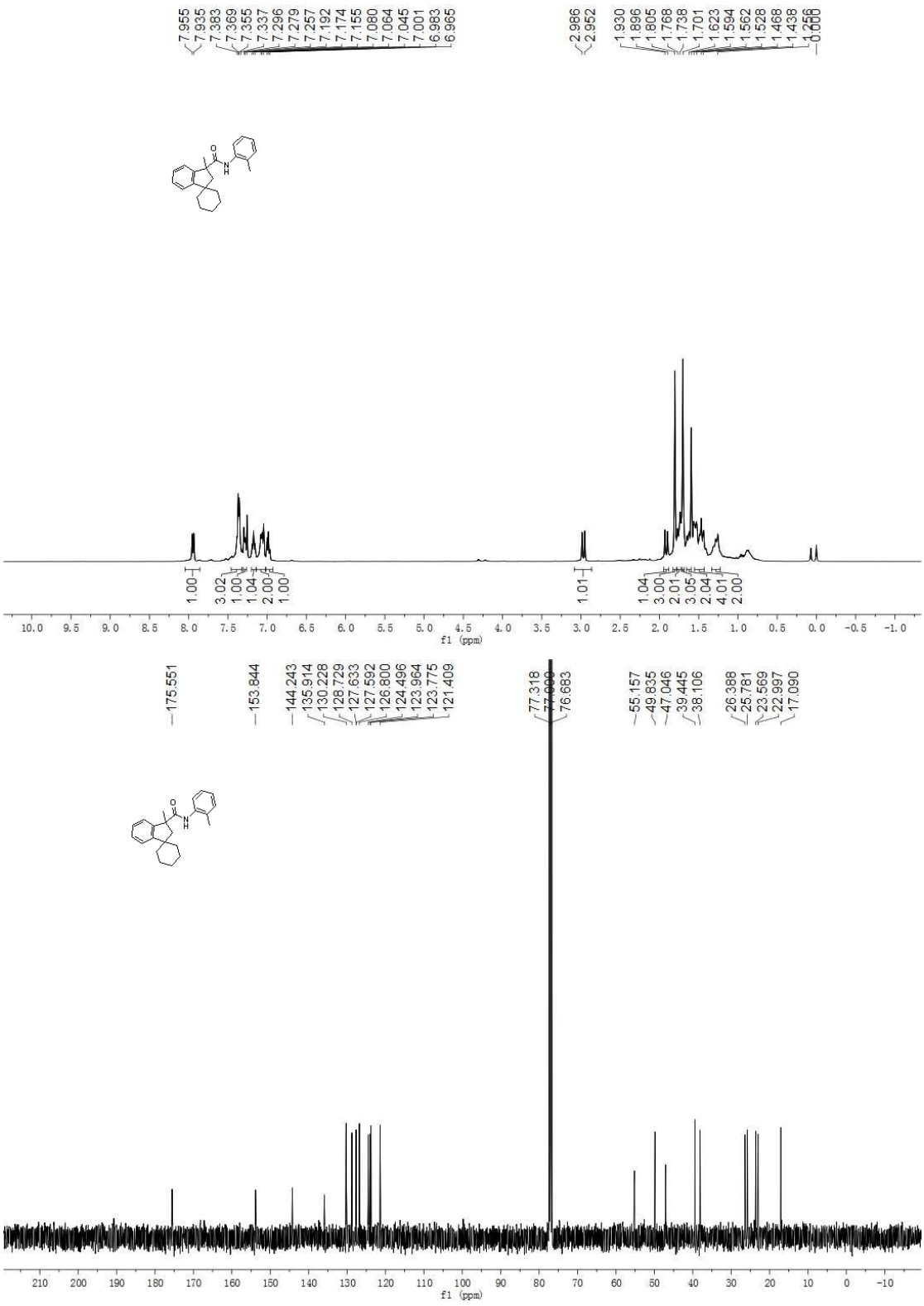
3'-(4-Cyanophenyl)-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

boxamide (3la)



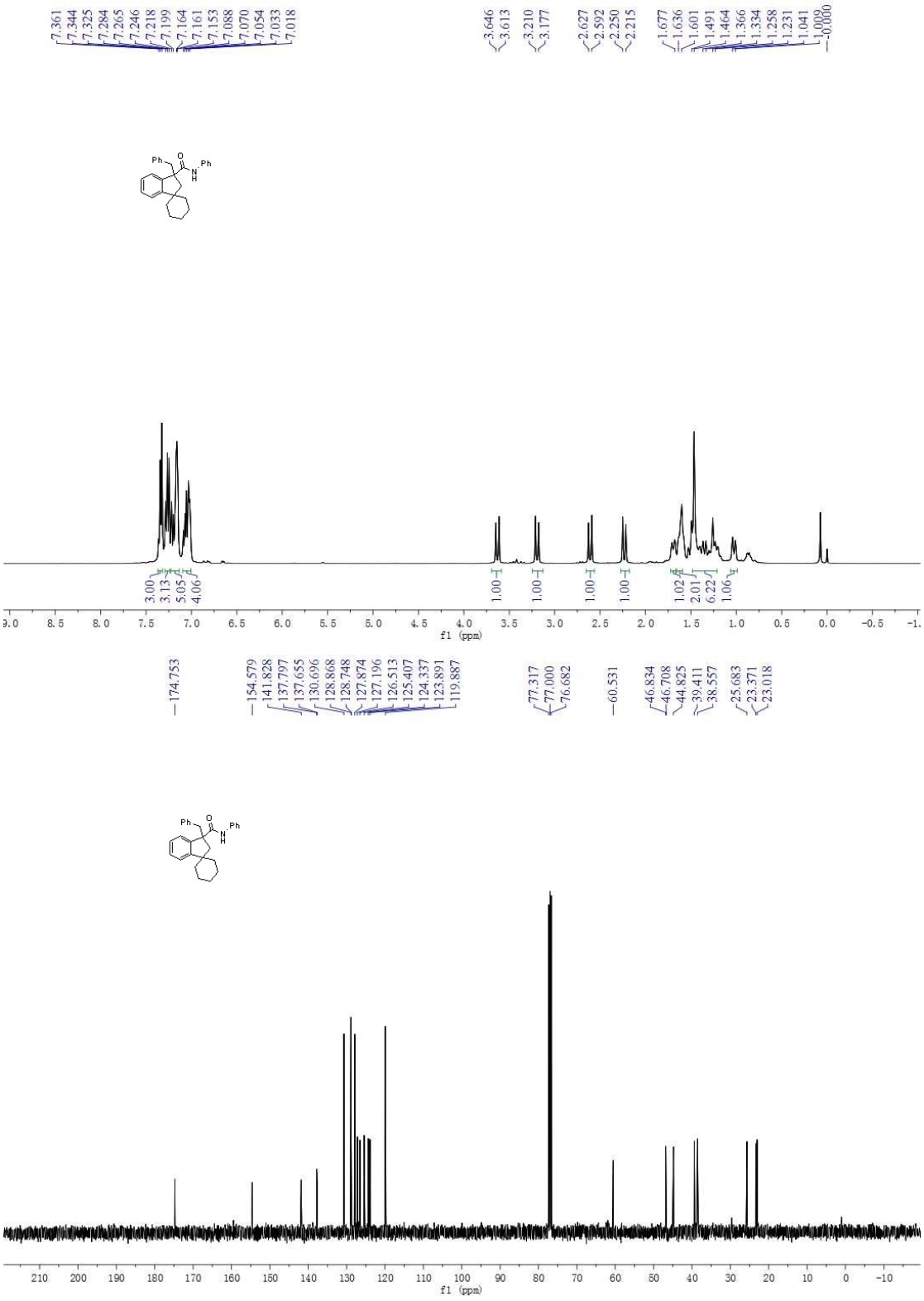
3'-Methyl-*N*-(*o*-tolyl)-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamid

e (3ma)



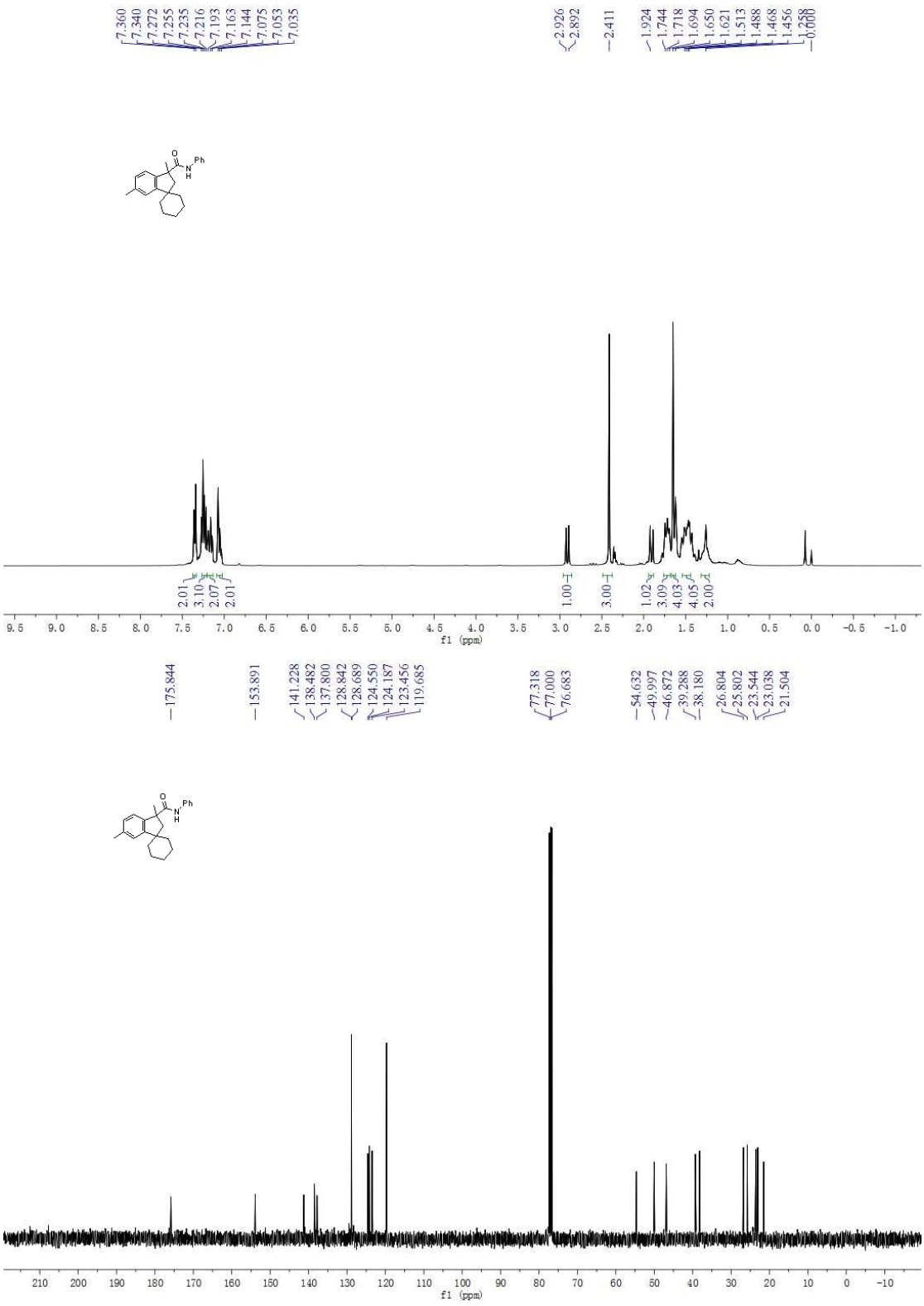
3'-Benzyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide

(3na)

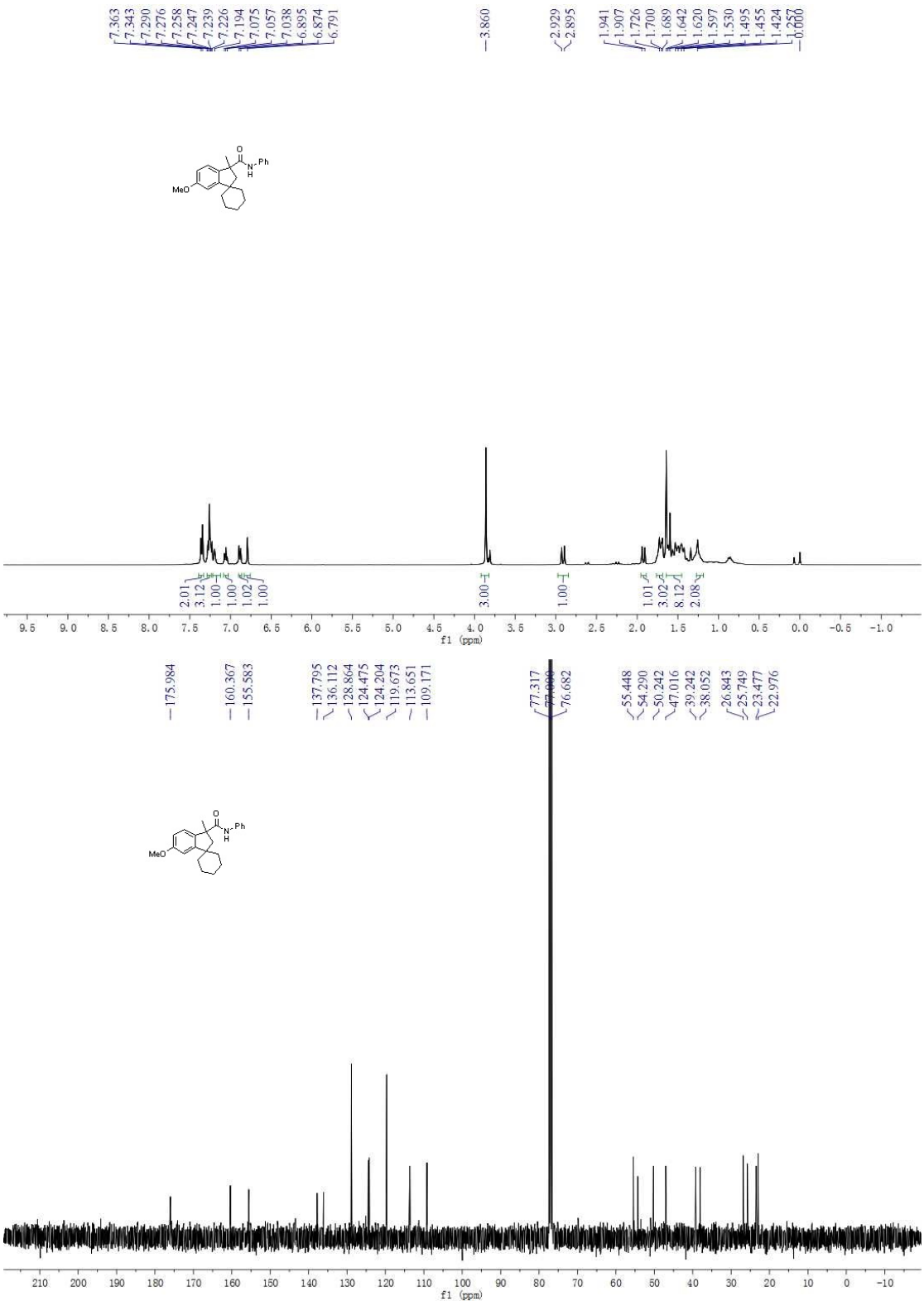


3',6'-Dimethyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxa

mide (3oa)

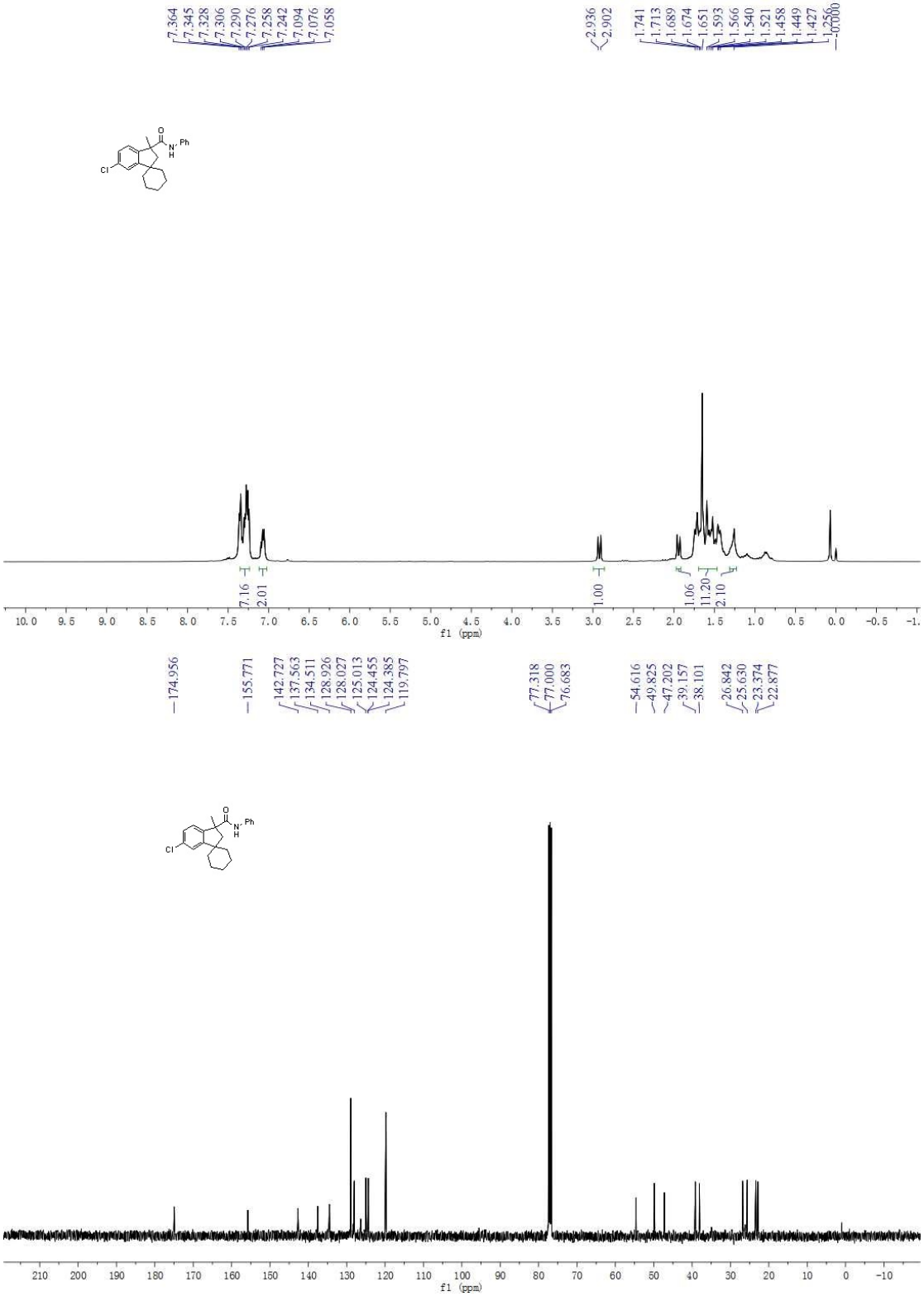


6'-Methoxy-3'-methyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-carboxamide (3pa)



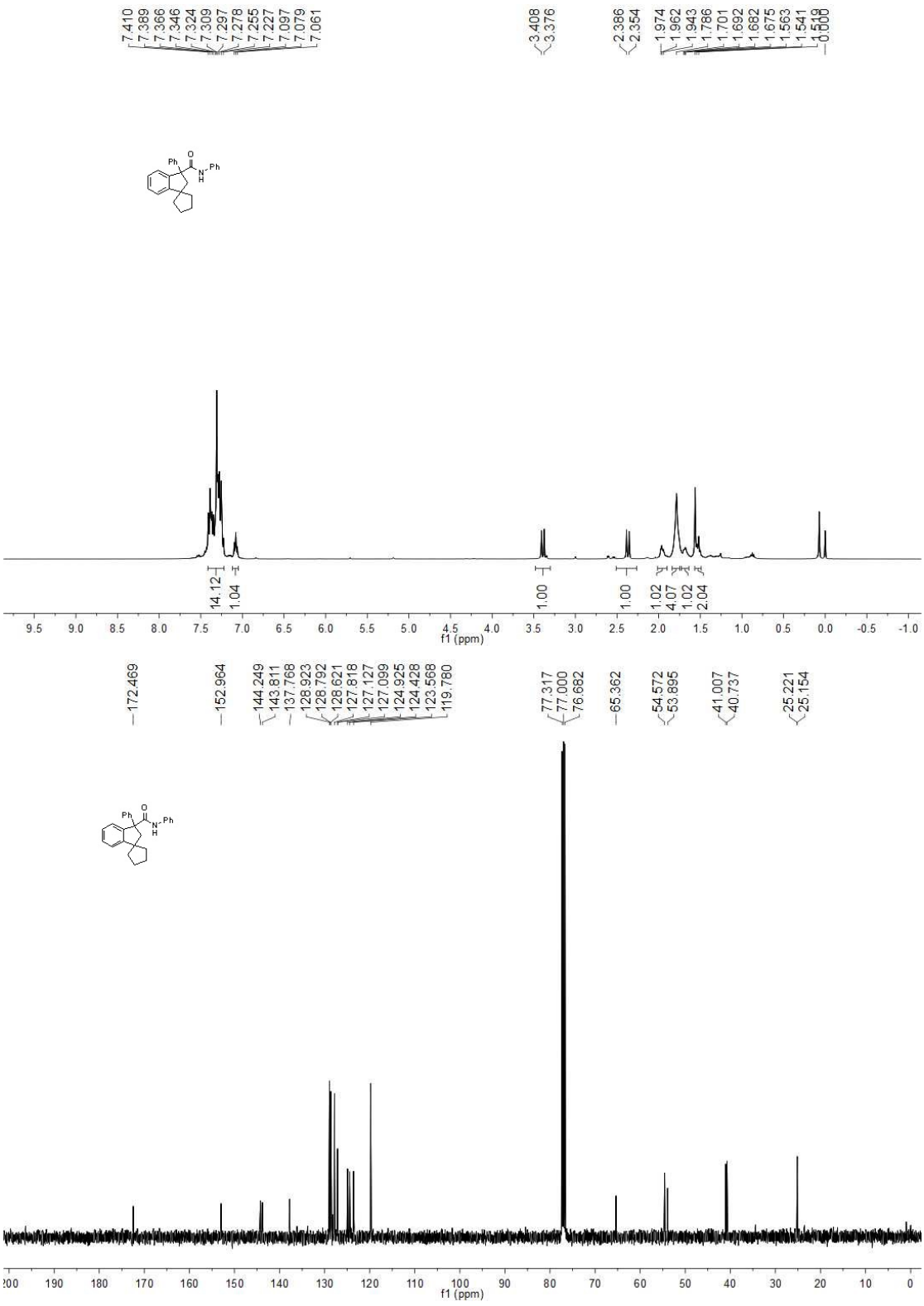
6'-Chloro-3'-methyl-*N*-phenyl-2',3'-dihydrospiro[cyclohexane-1,1'-indene]-3'-car

boxamide (3qa)



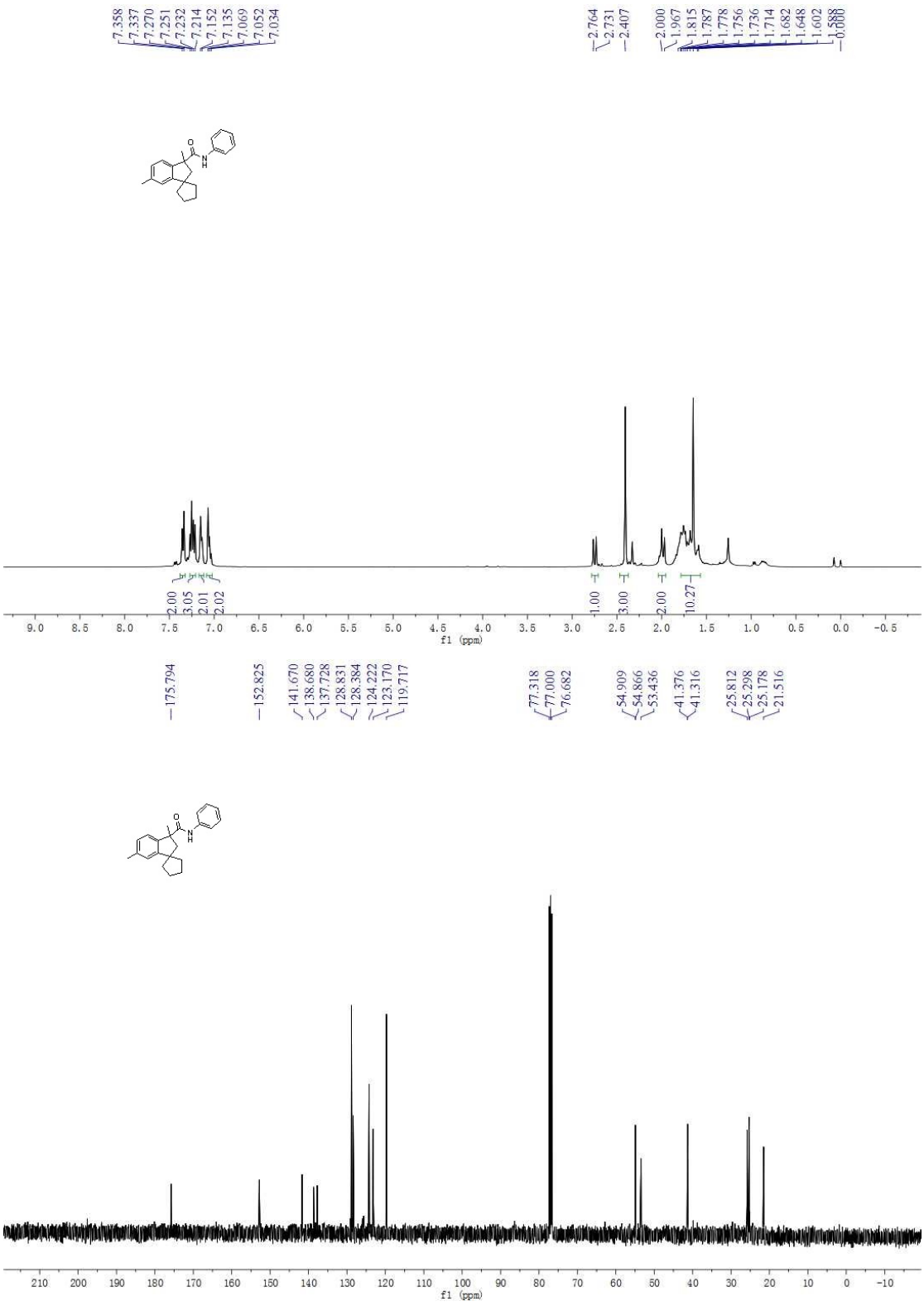
_N_,3'-Diphenyl-2',3'-dihydrospiro[cyclopentane-1,1'-indene]-3'-carboxamide

(3ab)



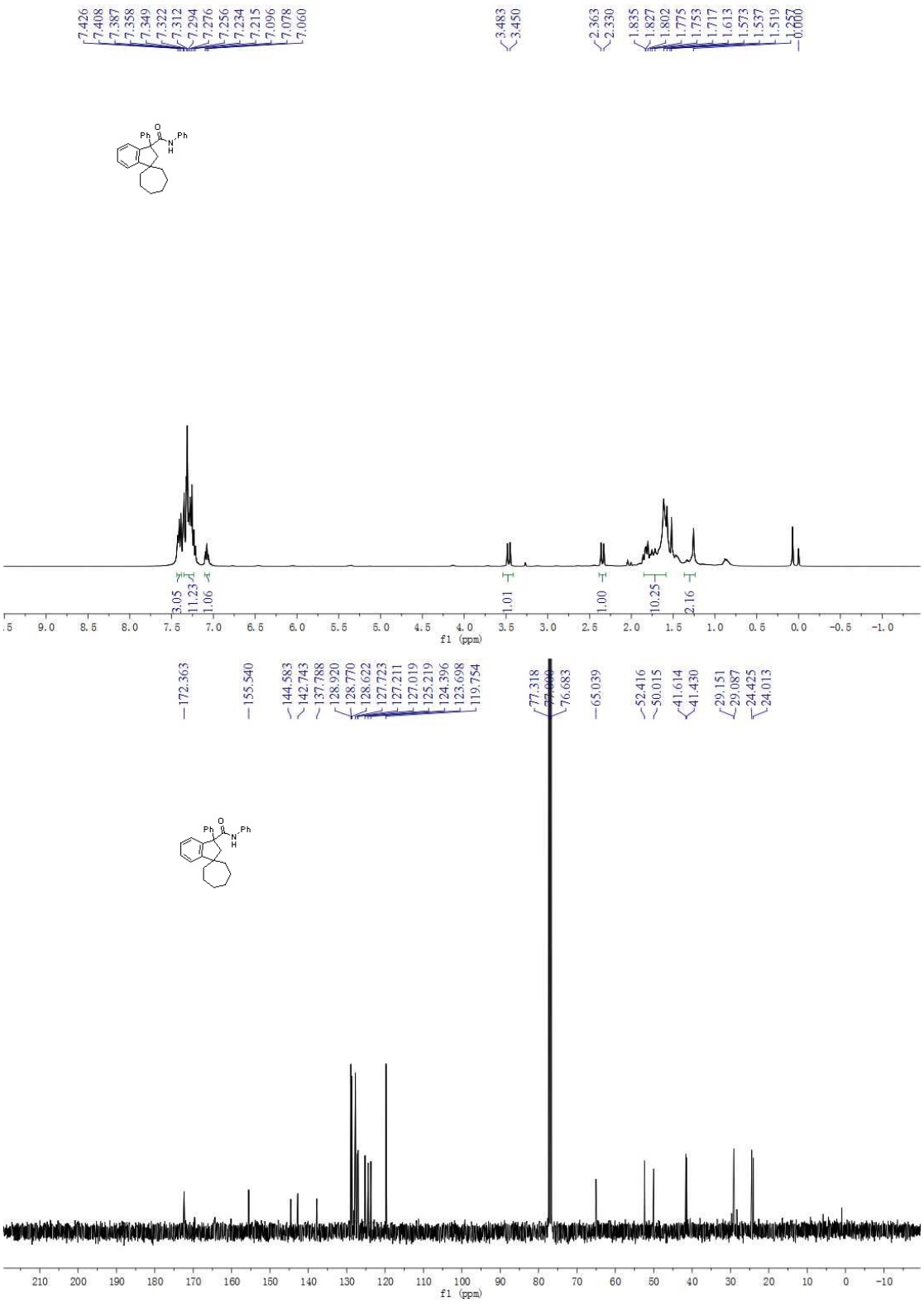
3',6'-Dimethyl-*N*-phenyl-2',3'-dihydrospiro[cyclopentane-1,1'-indene]-3'-carboxa

mide (3ob)

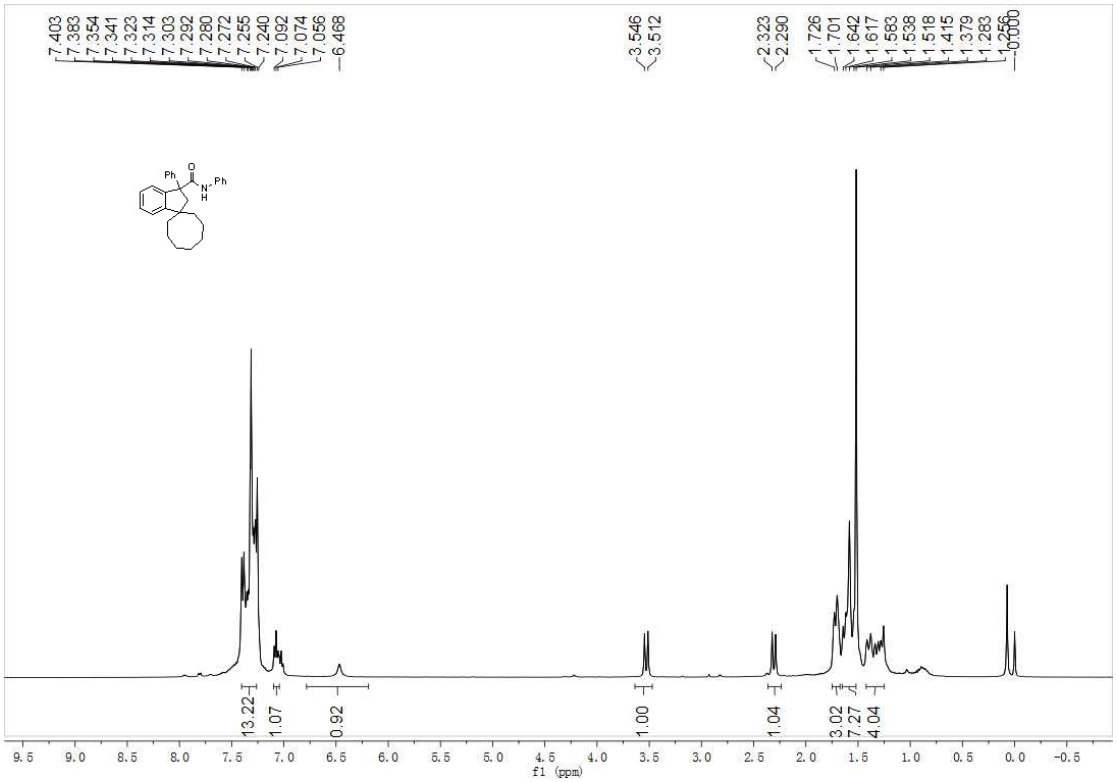


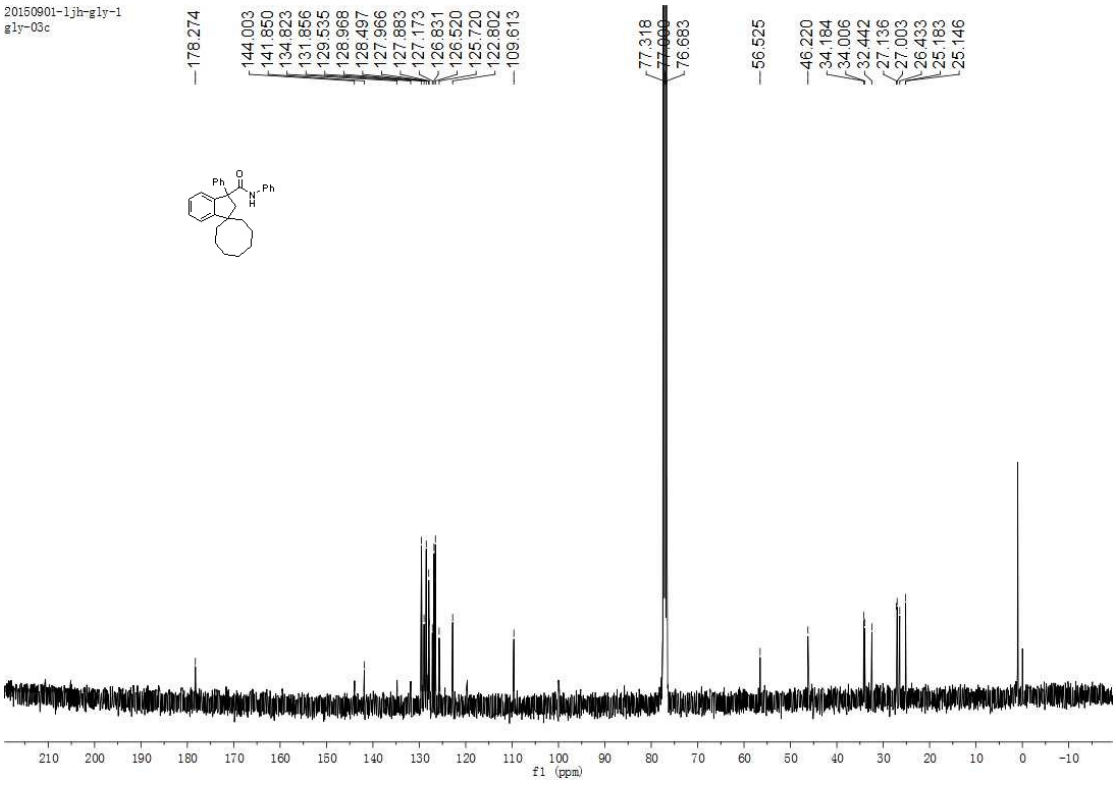
_N_,3'-Diphenyl-2',3'-dihydrospiro[cycloheptane-1,1'-indene]-3'-carboxamide

(3ac)

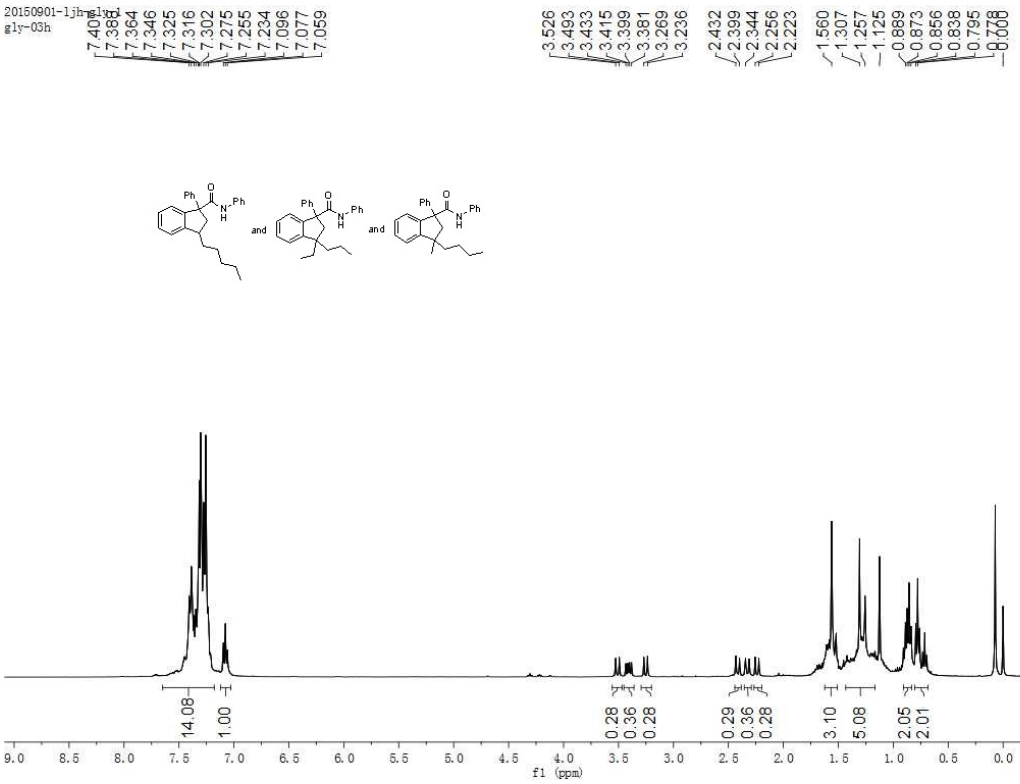


_N_,3'-Diphenyl-2',3'-dihydrospiro[cyclooctane-1,1'-indene]-3'-carboxamide (3ad)

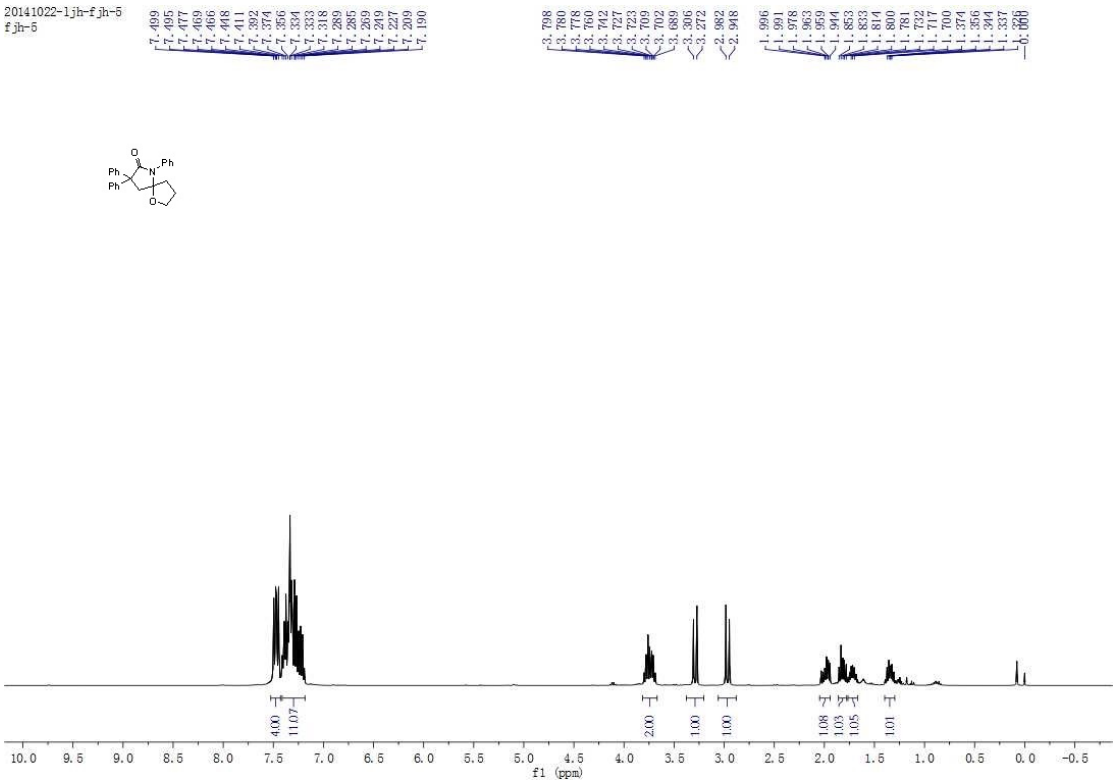


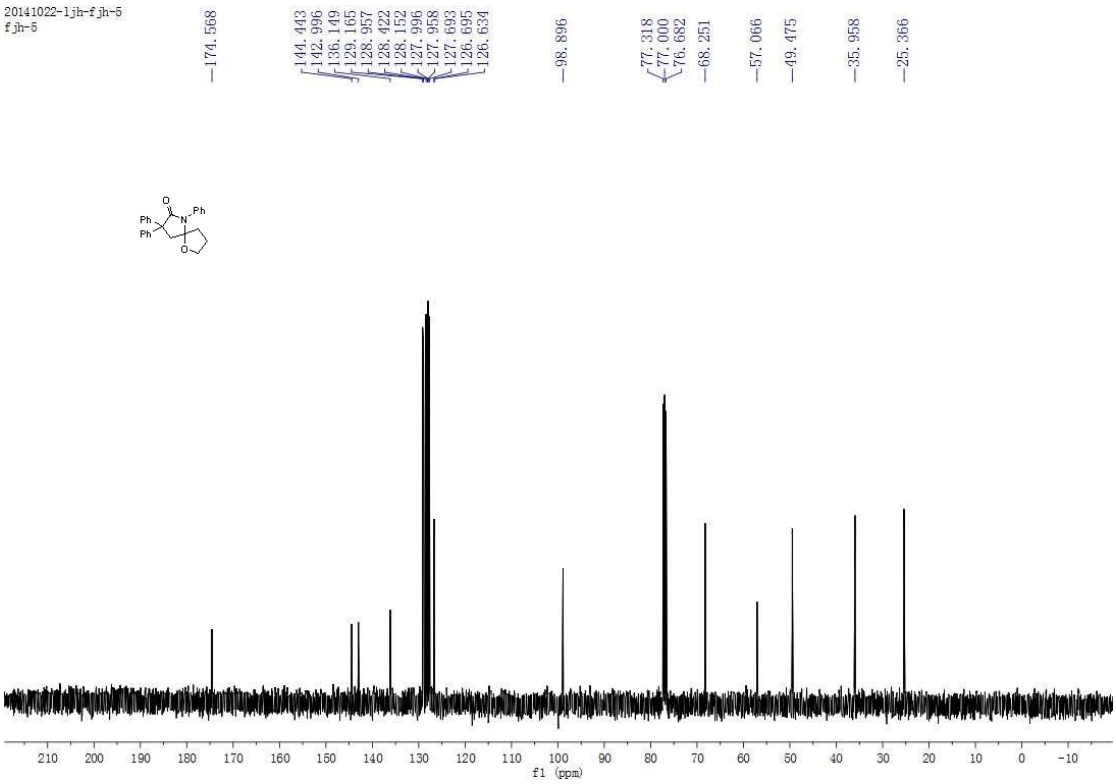


Product (3ae)


20150901-ljh-glyxl
gly-03h
7.409
7.388
7.364
7.346
7.325
7.316
7.302
7.275
7.255
7.234
7.096
7.077
7.059
3.526
3.493
3.433
3.415
3.399
3.381
3.269
3.236
2.432
2.399
2.344
2.256
2.223
1.560
1.307
1.257
1.125
0.889
0.873
0.856
0.838
0.795
0.778
0.000
Ph
O
N
H
Ph
and
Ph
O
N
H
Ph
and
Ph
O
N
H
Ph
14.08
1.00
0.28
0.36
0.28
0.29
0.36
0.28
3.10
5.08
2.05
2.01
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
-0.5
f1 (ppm)

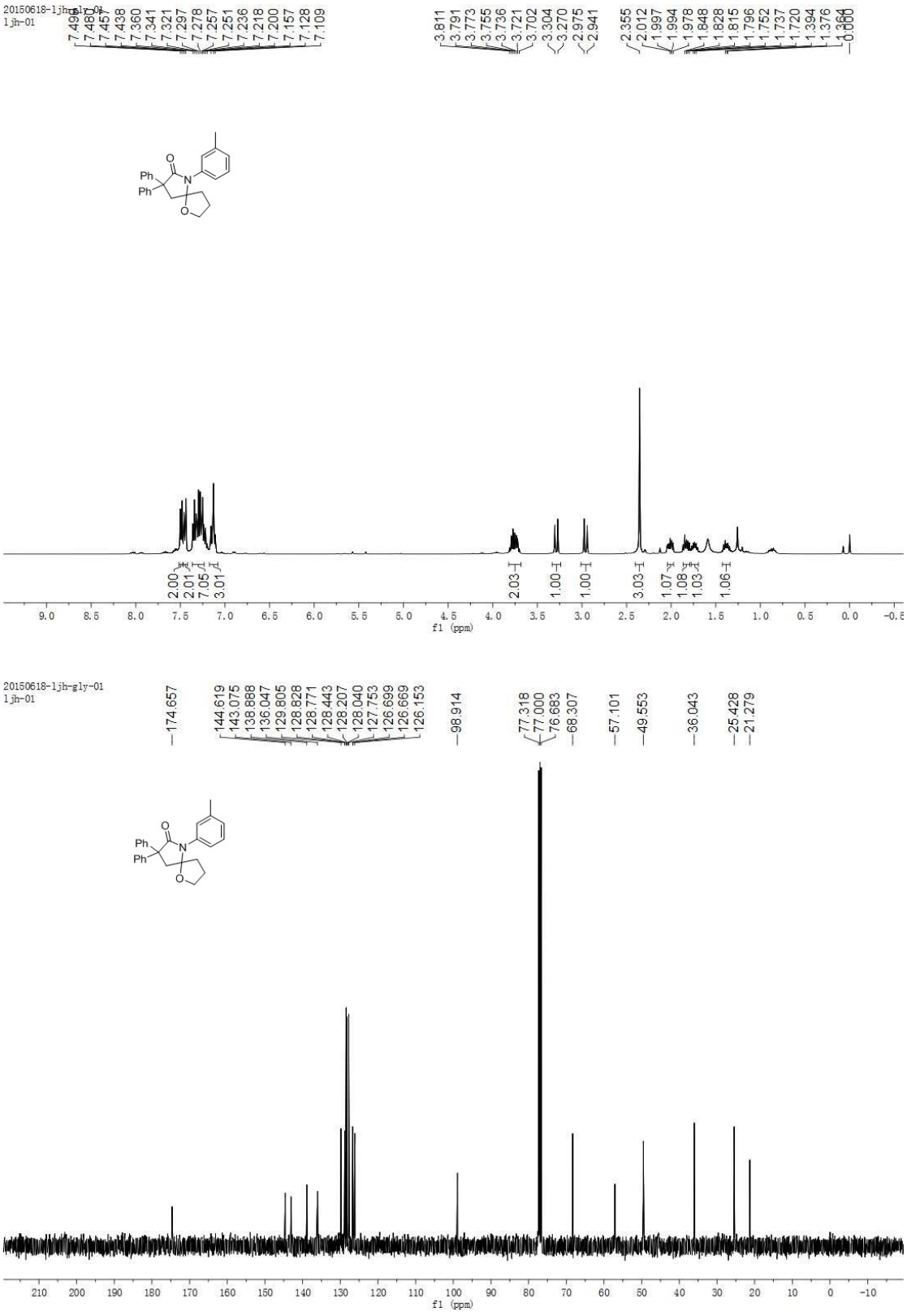
6,8,8-Triphenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4af)



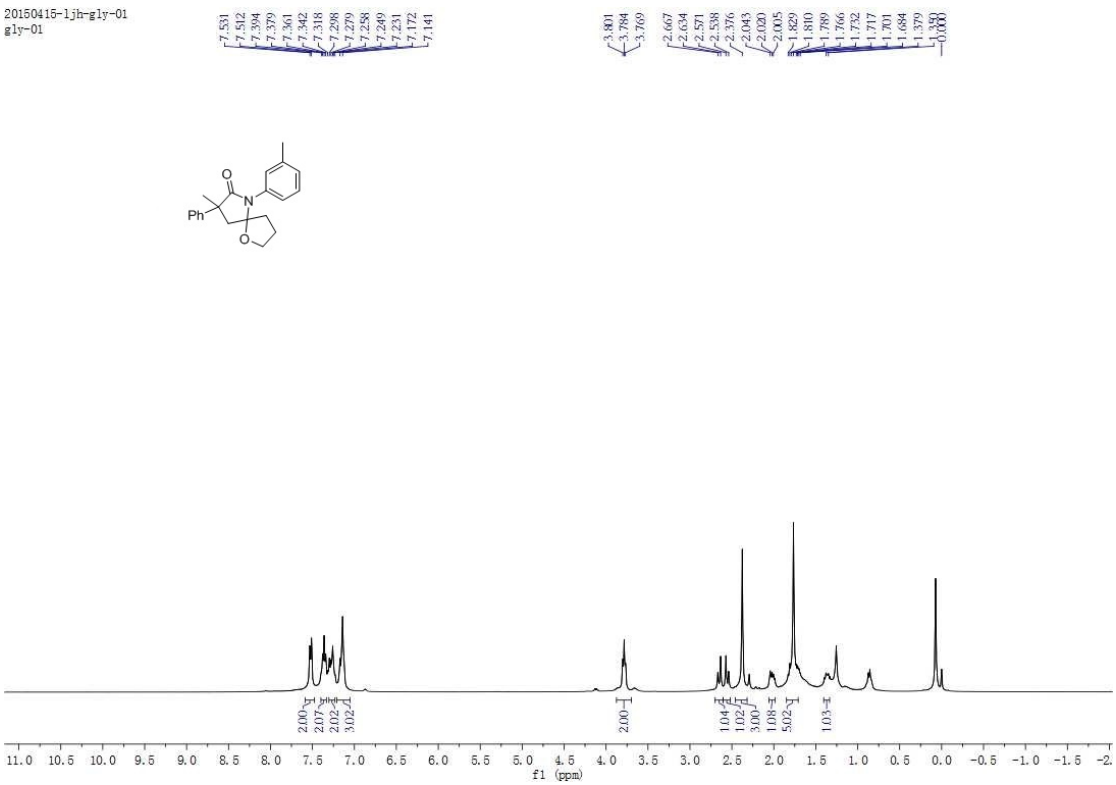


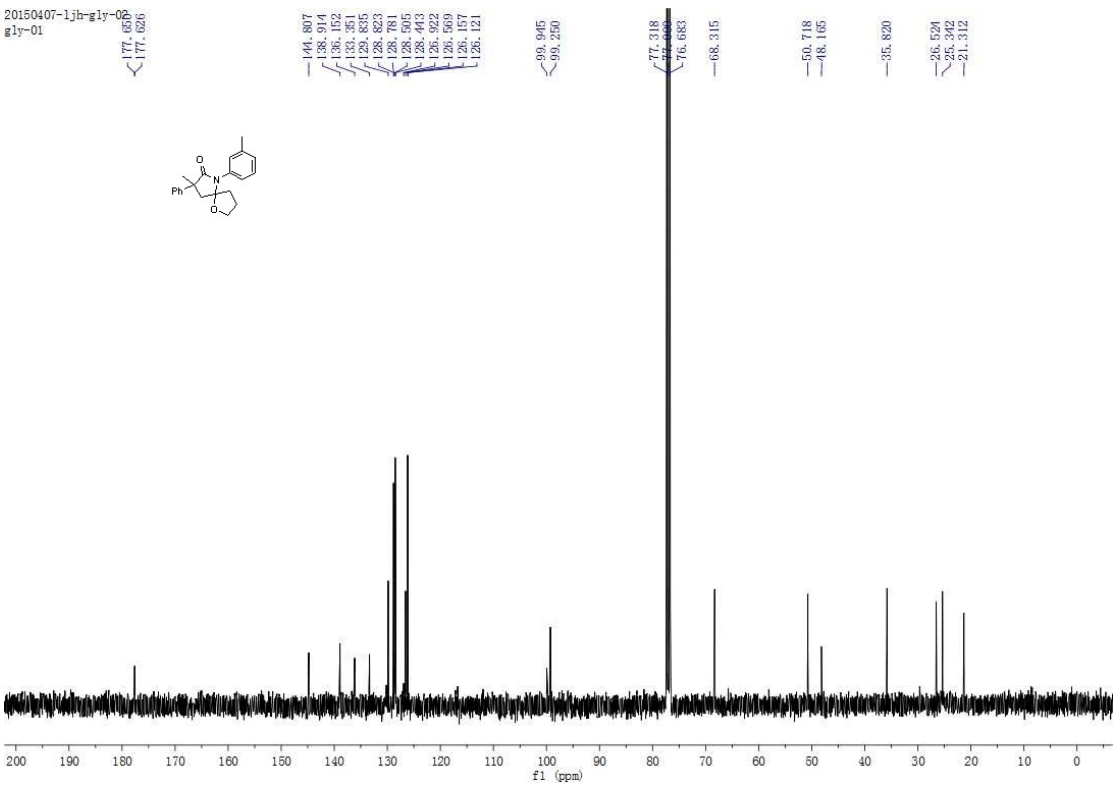
8,8-Diphenyl-6-(*m*-tolyl)-1-oxa-6-azaspiro[4.4]nonan-7-one

(4gf)

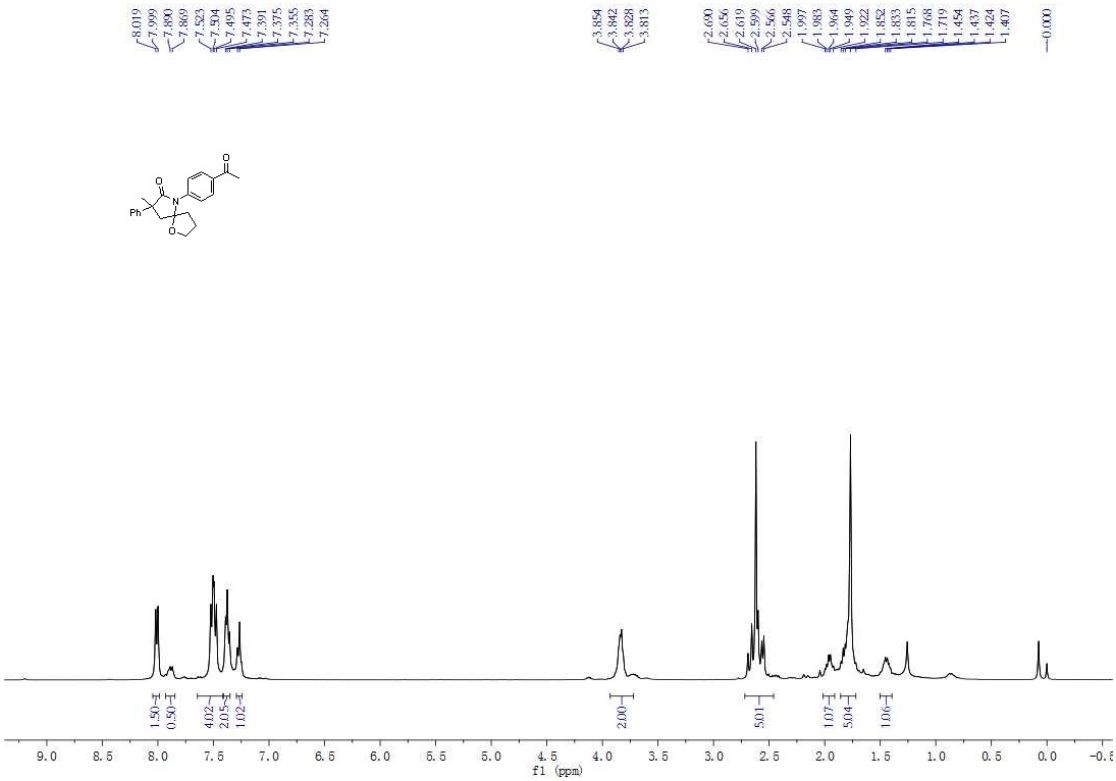


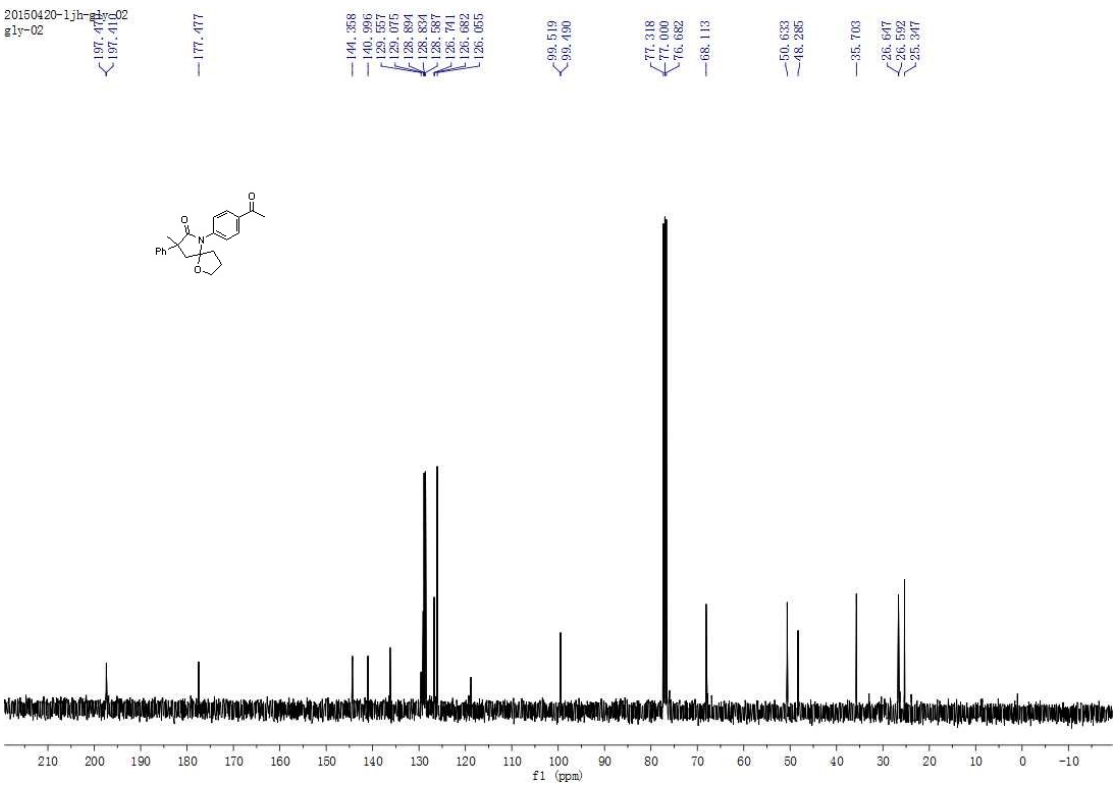
8-Methyl-8-phenyl-6-(*m*-tolyl)-1-oxa-6-azaspiro[4.4]nonan-7-one (4mf):



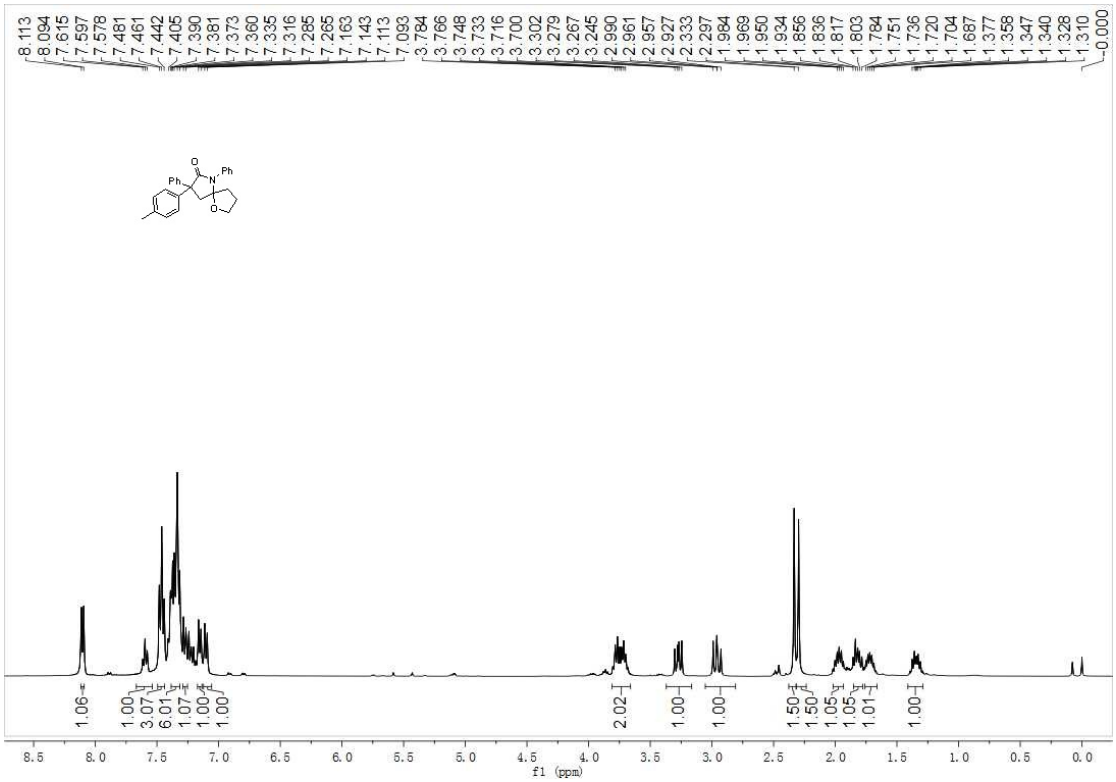


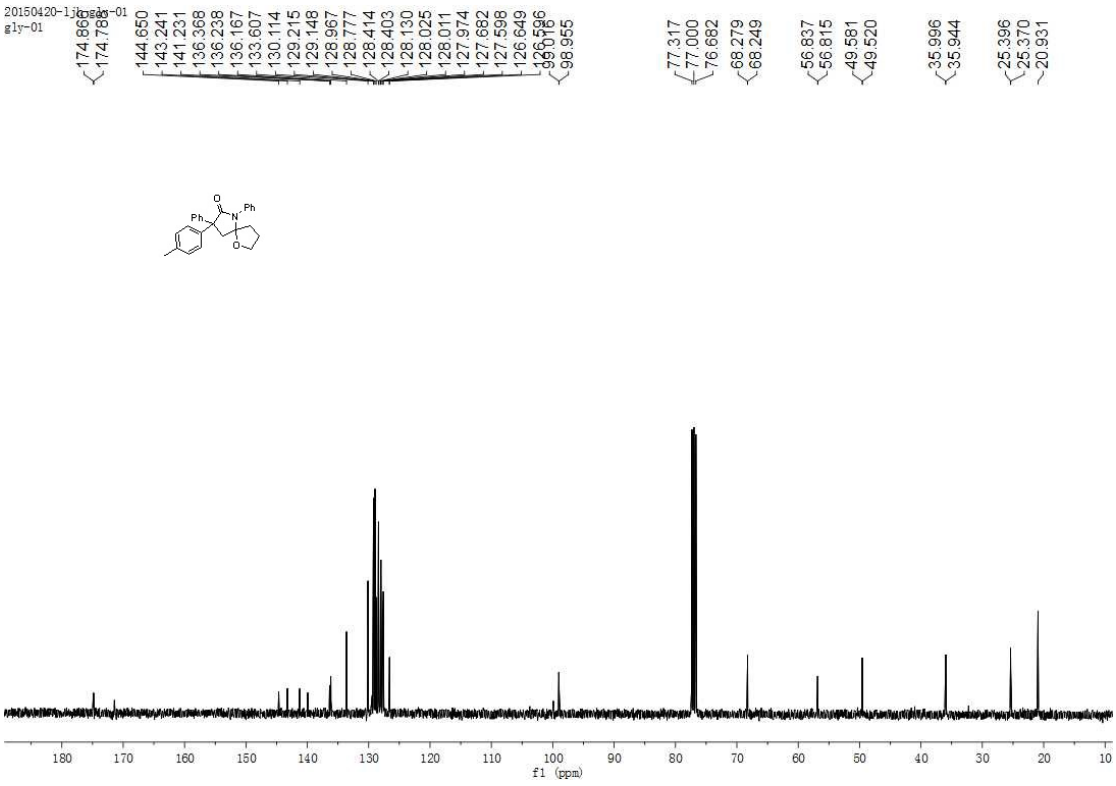
6-(4-Acetylphenyl)-8-methyl-8-phenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4rf)



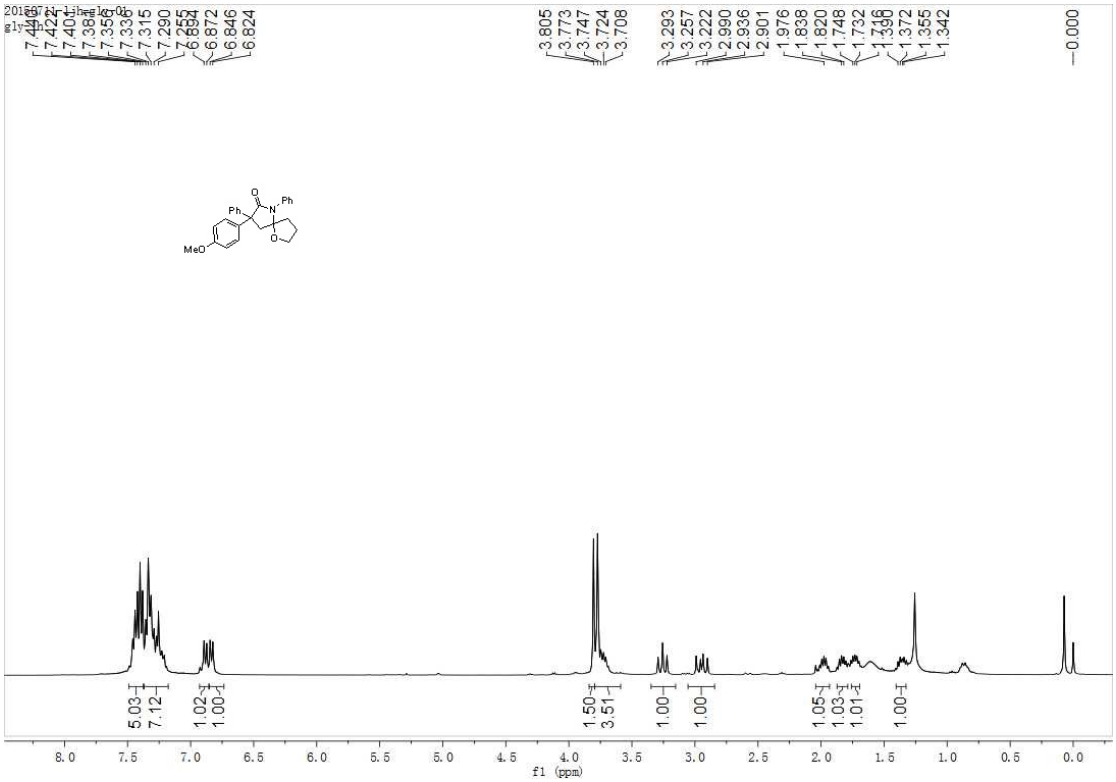


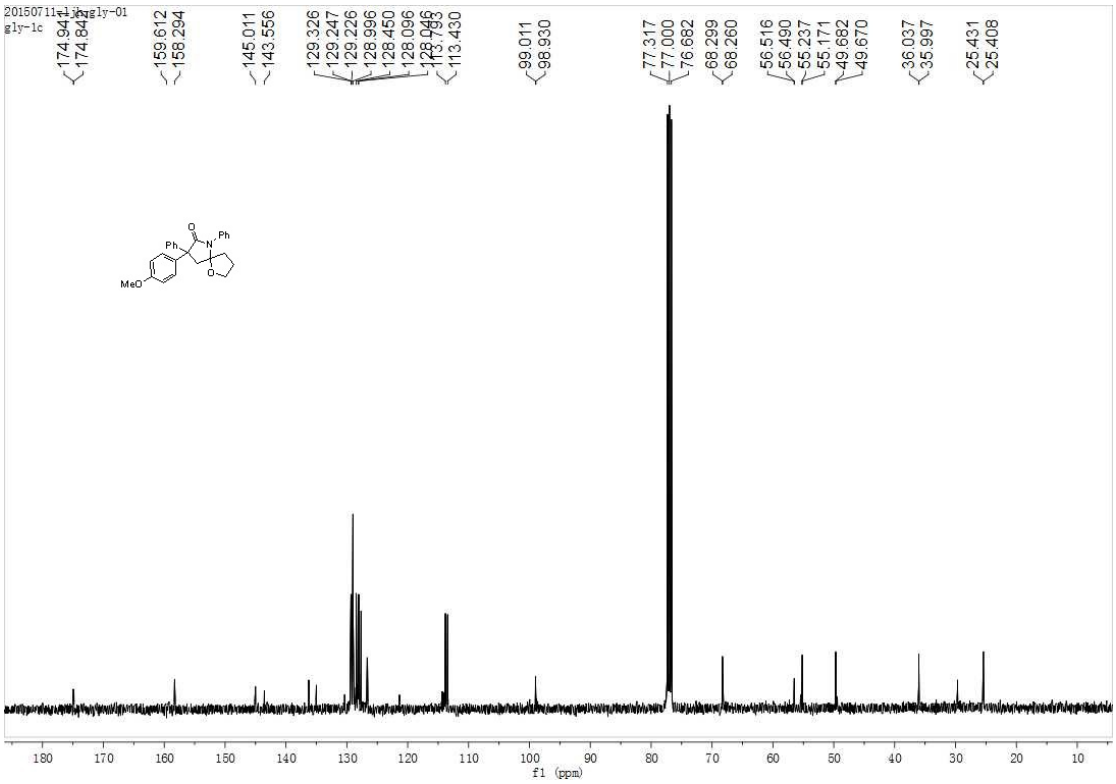
6, 8-Diphenyl-8-(*p*-tolyl)-1-oxa-6-azaspiro[4.4]nonan-7-one (4kf)



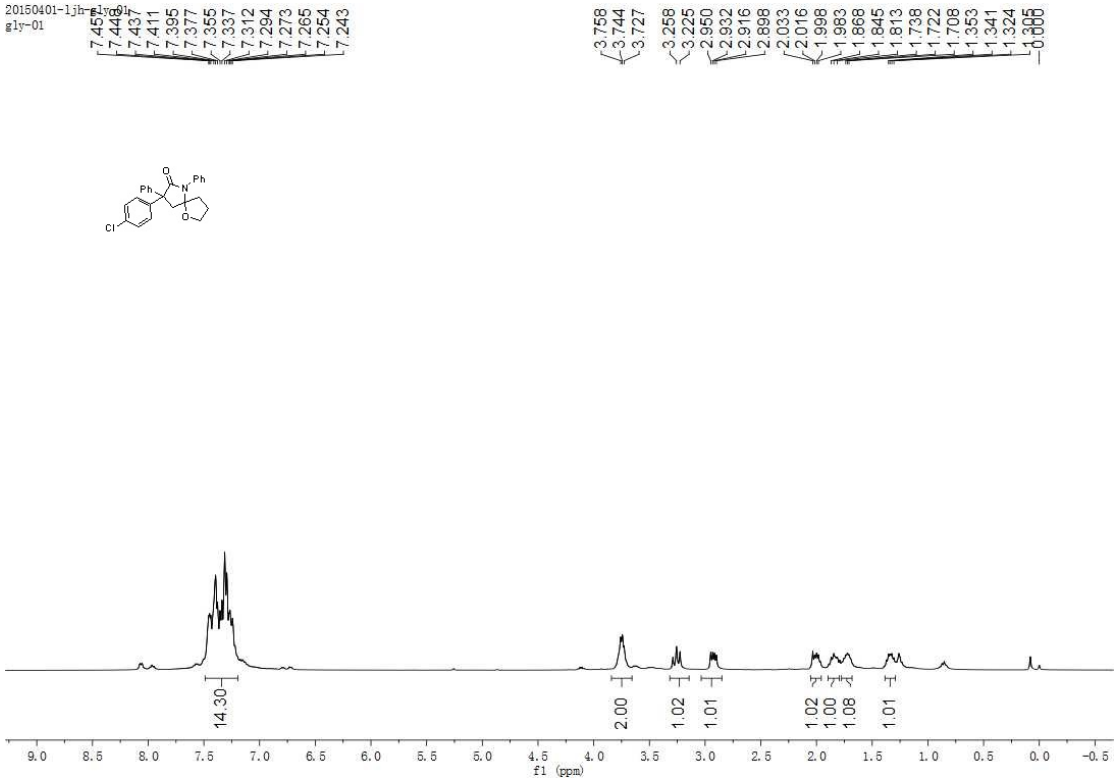


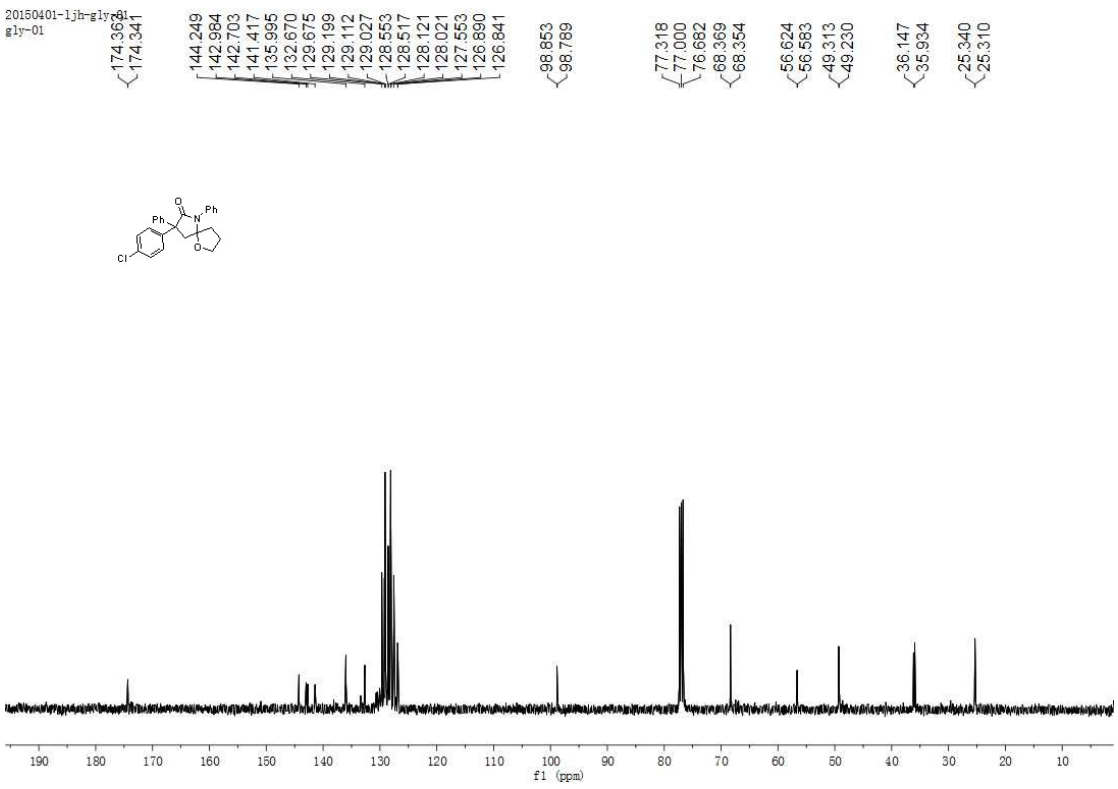
8-(4-Methoxyphenyl)-6, 8-diphenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4sf)



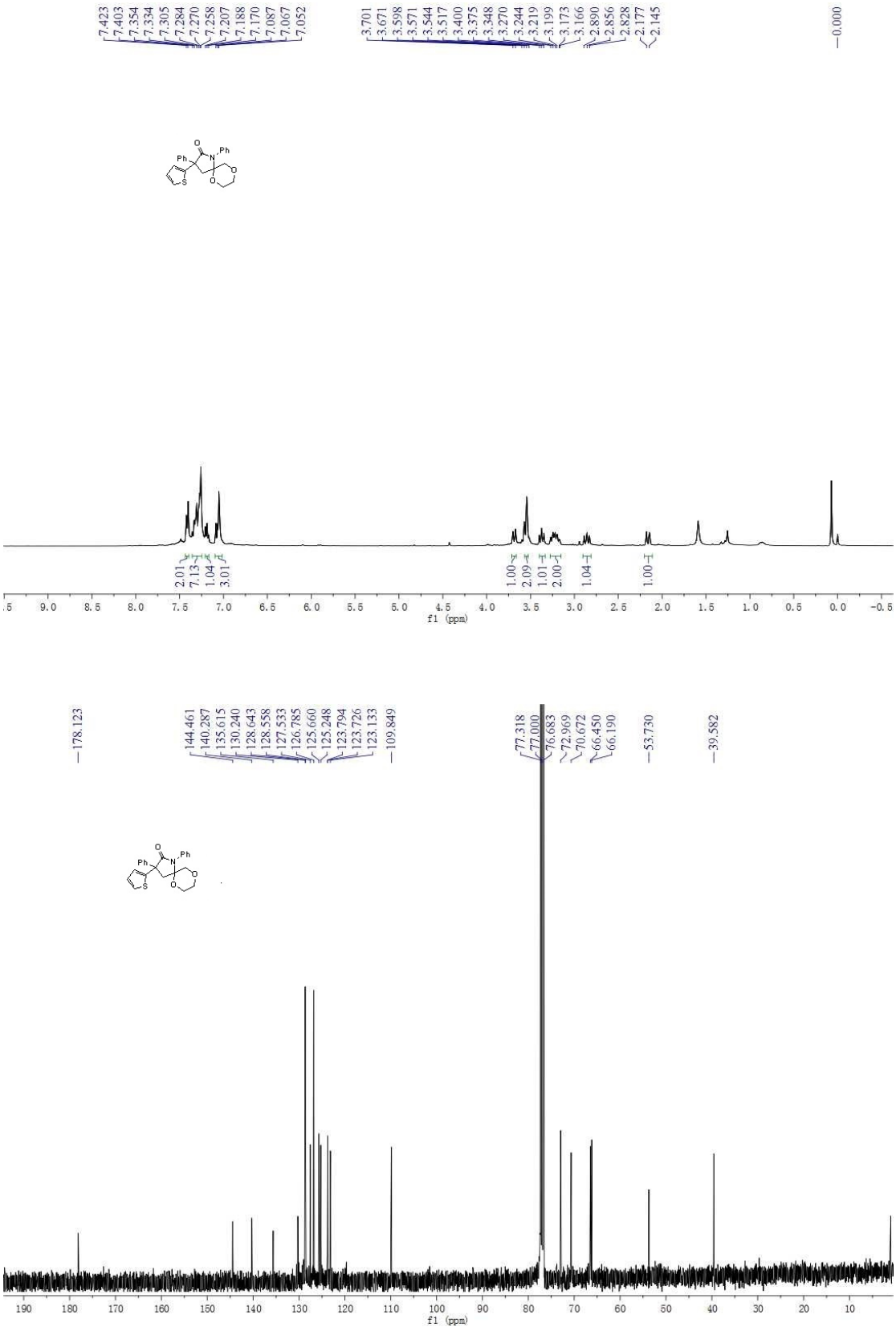


8-(4-Chlorophenyl)-6, 8-diphenyl-1-oxa-6-azaspiro[4.4]nonan-7-one (4tf)

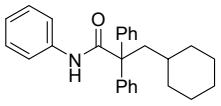


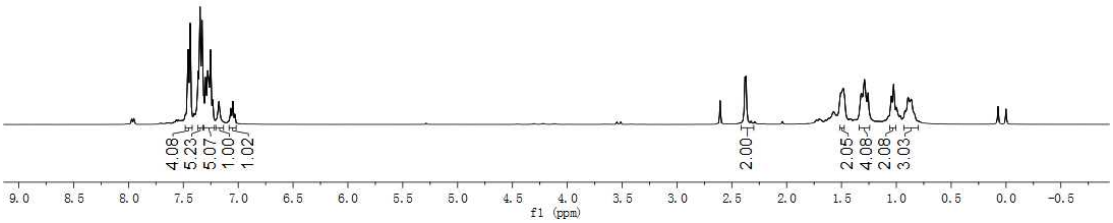


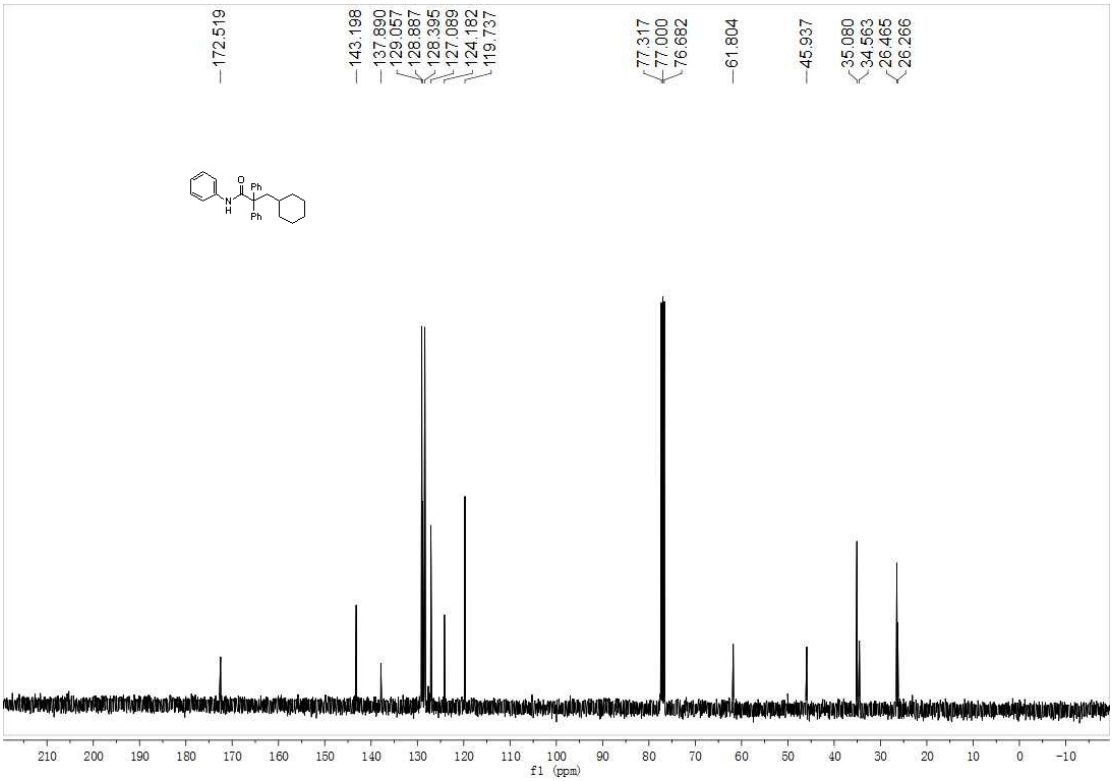
1,3-Diphenyl-3-(thiophen-2-yl)-6,9-dioxa-1-azaspiro[4.5]decan-2-one (4ug)



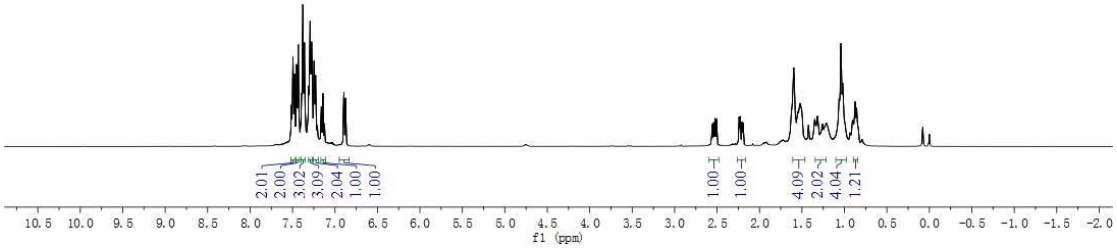
3-Cyclohexyl-*N*,2,2-triphenylpropanamide (5aa)

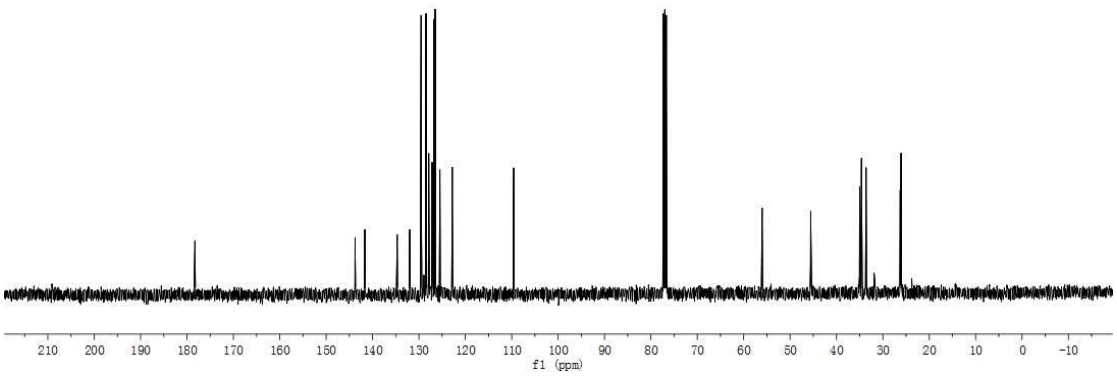




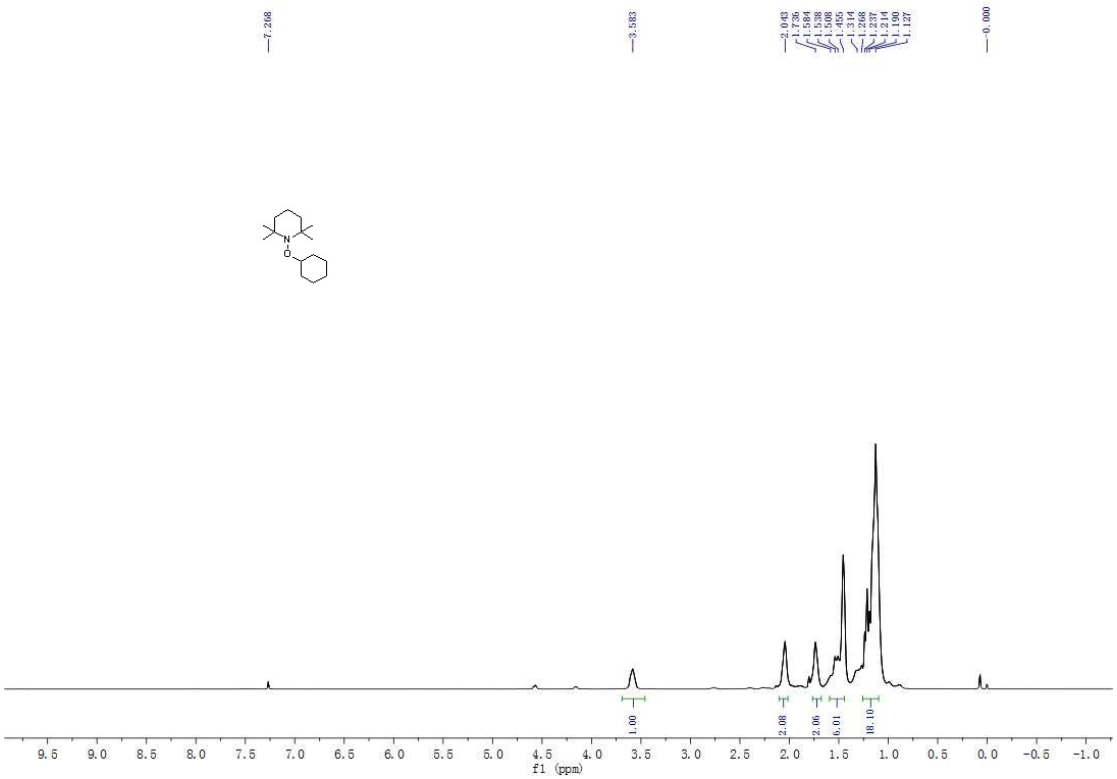


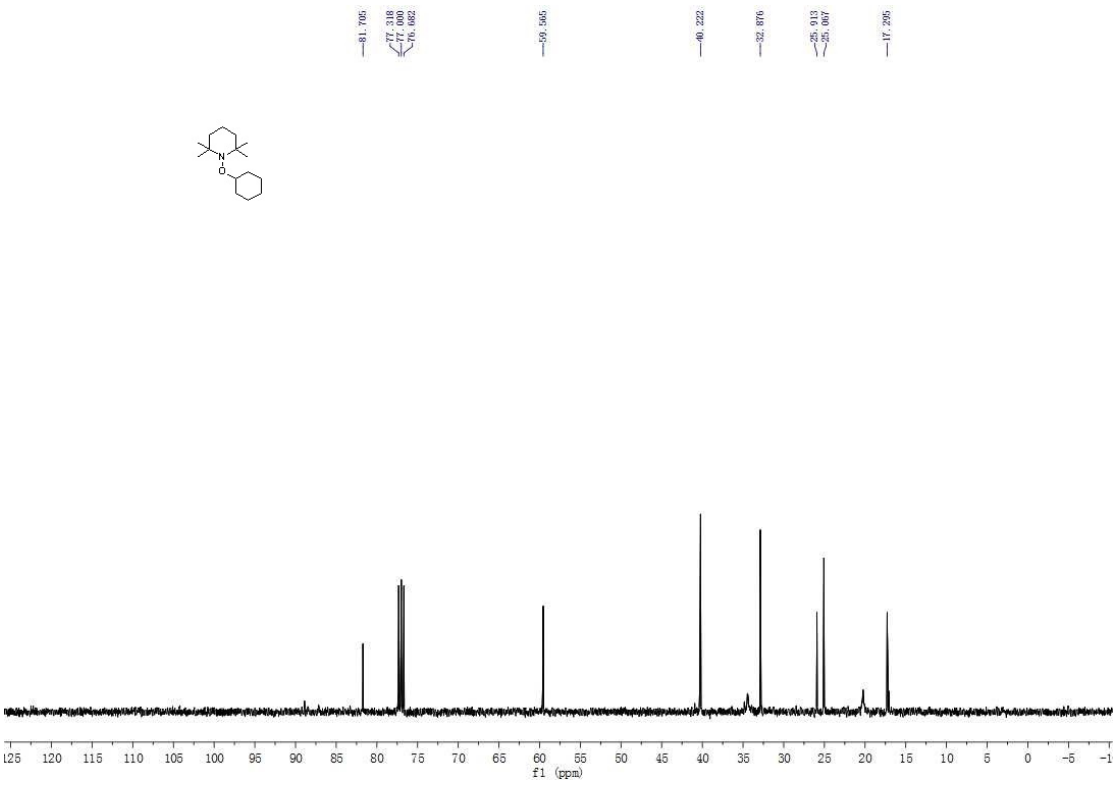
3-(Cyclohexylmethyl)-1,3-diphenylindolin-2-one (6aa)



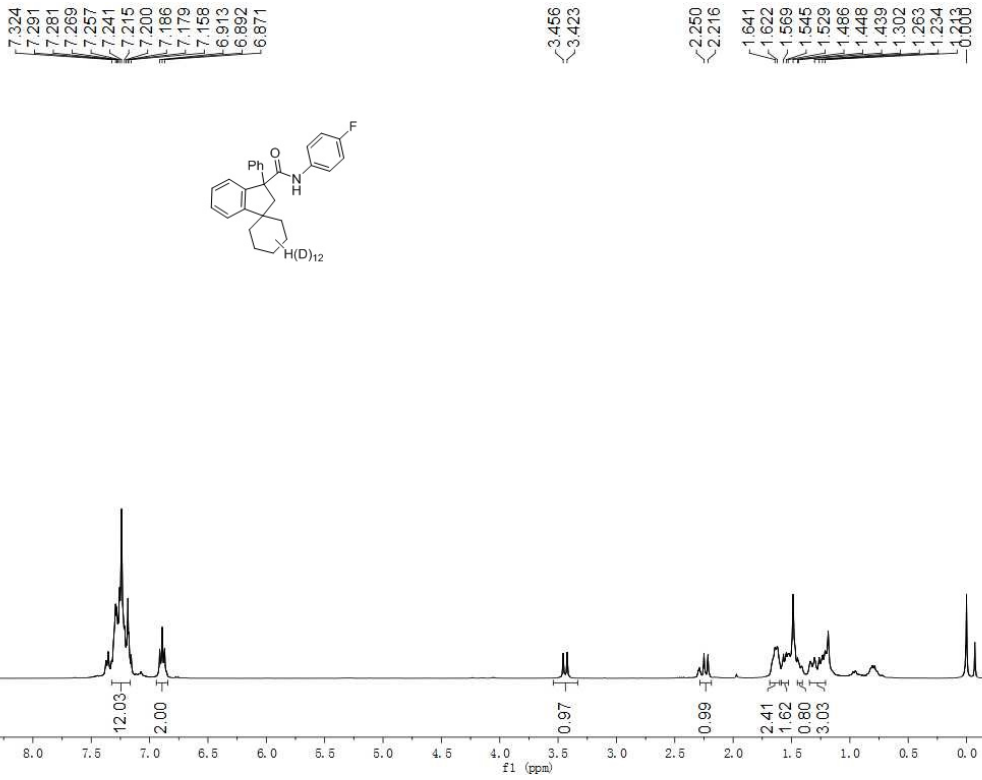


1-(Cyclohexyloxy)-2,2,6,6-tetramethylpiperidine (7)

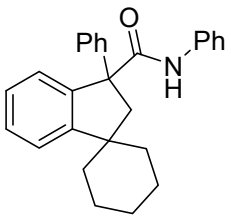


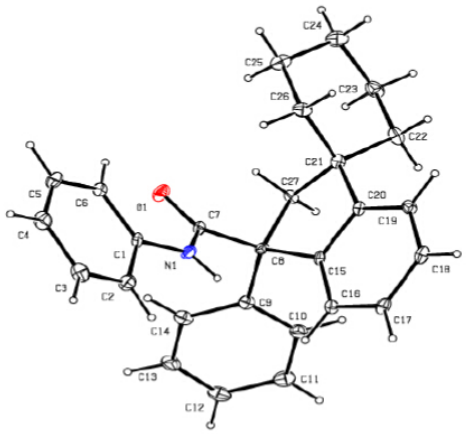


Product (3ea + 3ea-D12)



(E) The X-ray single-crystal diffraction analysis of 3aa





3aa

Crystal data and structure refinement for **3aa**:

Identification code	**3aa**
Empirical formula	C27 H27 N O
Formula weight	381.50
Temperature	296(2) K
Wavelength	0.71073 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 13.803(4) A alpha = 90 deg.
	b = 14.747(5) A beta = 108.236(5) deg.
	c = 21.885(7) A gamma = 90 deg.
Volume	4231(2) A^3
Z, Calculated density	8, 1.198 Mg/m^3
Absorption coefficient	0.072 mm^-1
F(000)	1632
Crystal size	0.23 x 0.21 x 0.20 mm
Theta range for data collection	0.98 to 25.00 deg.
Limiting indices	-15<=h<=16, -17<=k<=15, -26<=l<=22
Reflections collected / unique	20326 / 11613 [R(int) = 0.0397]
Completeness to theta = 25.00	99.0 %
Absorption correction	Semi-empirical from equivalents

Max. and min. transmission	0.9858 and 0.9837
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	11613 / 1 / 1046
Goodness-of-fit on F^2	1.423
Final R indices [I>2sigma(I)]	R1 = 0.1329, wR2 = 0.3425
R indices (all data)	R1 = 0.1501, wR2 = 0.3549
Absolute structure parameter	-2(4)
Extinction coefficient	0.040(5)
Largest diff. peak and hole	1.155 and -0.649 e.A^-3

Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters (A^2 x 10^3) for ljh021_0m. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	-3757(4)	6090(4)	4752(2)	53(1)
N(1)	-2111(4)	5961(5)	4791(2)	41(1)
C(1)	-2190(5)	6023(5)	4133(3)	40(2)
N(2)	2825(4)	6208(5)	4779(3)	41(1)
O(2)	1195(4)	6323(5)	4740(3)	68(2)
C(2)	-1299(6)	6254(6)	3997(4)	52(2)
N(3)	3105(5)	7591(5)	172(3)	48(2)
O(3)	1515(5)	7377(6)	203(3)	73(2)
C(3)	-1307(8)	6281(7)	3369(4)	60(2)
N(4)	8113(5)	7333(5)	198(3)	50(2)
O(4)	6545(5)	7221(6)	282(3)	84(2)
C(4)	-2209(8)	6088(7)	2871(4)	67(3)
C(5)	-3058(7)	5855(7)	3012(3)	63(2)

C(6)	-3079(7)	5841(6)	3642(3)	54(2)
C(7)	-2875(5)	5979(5)	5069(3)	37(2)
C(8)	-2536(4)	5845(5)	5799(3)	30(1)
C(9)	-2308(5)	6770(5)	6133(3)	37(2)
C(10)	-1871(6)	6782(6)	6794(4)	52(2)
C(11)	-1721(7)	7632(7)	7116(5)	64(2)
C(12)	-2051(8)	8429(7)	6777(5)	70(3)
C(13)	-2515(7)	8389(6)	6157(5)	67(3)
C(14)	-2627(6)	7557(6)	5816(4)	53(2)
C(15)	-1646(4)	5162(5)	6012(3)	30(1)
C(16)	-616(5)	5325(5)	6123(3)	36(2)
C(17)	68(5)	4612(6)	6275(3)	43(2)
C(18)	-301(5)	3736(6)	6310(3)	45(2)
C(19)	-1313(5)	3587(5)	6198(3)	42(2)
C(20)	-2005(5)	4301(5)	6066(3)	33(1)
C(21)	-3128(5)	4278(5)	5945(3)	37(2)
C(22)	-3425(7)	3743(6)	6449(4)	54(2)
C(23)	-4565(6)	3735(7)	6330(5)	61(2)
C(24)	-5113(7)	3332(9)	5640(5)	77(3)
C(25)	-4839(6)	3838(7)	5141(4)	58(2)
C(26)	-3705(6)	3862(6)	5277(4)	49(2)
C(27)	-3347(5)	5297(5)	5981(3)	34(1)
C(28)	2765(6)	6097(5)	4135(3)	42(2)
C(29)	3677(6)	6069(6)	3995(4)	48(2)
C(30)	3653(8)	5984(8)	3371(5)	74(3)
C(31)	2754(8)	5980(9)	2873(4)	77(3)
C(32)	1894(8)	5988(8)	3011(4)	69(3)
C(33)	1840(6)	6077(6)	3633(3)	48(2)
C(34)	2089(5)	6278(5)	5060(3)	41(2)
C(35)	2432(5)	6251(5)	5796(3)	34(2)

C(36)	2544(5)	5254(5)	6009(3)	38(2)
C(37)	2134(6)	4545(5)	5590(3)	44(2)
C(38)	2212(6)	3660(6)	5811(4)	57(2)
C(39)	2680(7)	3470(6)	6453(4)	57(2)
C(40)	3075(6)	4153(6)	6863(4)	53(2)
C(41)	3040(6)	5044(5)	6658(4)	49(2)
C(42)	3400(5)	6802(5)	6082(3)	35(2)
C(43)	4390(5)	6580(6)	6178(3)	42(2)
C(44)	5141(6)	7207(7)	6413(4)	54(2)
C(45)	4932(6)	8042(6)	6588(4)	55(2)
C(46)	3919(5)	8267(5)	6522(4)	44(2)
C(47)	3150(5)	7658(5)	6275(3)	35(1)
C(48)	2011(5)	7754(5)	6156(3)	34(2)
C(49)	1763(6)	8163(6)	6740(4)	48(2)
C(50)	664(7)	8294(6)	6635(4)	58(2)
C(51)	181(8)	8888(8)	6046(5)	76(3)
C(52)	410(6)	8529(7)	5451(4)	62(2)
C(53)	1536(5)	8373(5)	5585(3)	43(2)
C(54)	1658(5)	6761(5)	6054(3)	35(1)
C(55)	3673(6)	7518(6)	827(4)	48(2)
C(56)	4724(6)	7332(7)	971(4)	57(2)
C(57)	5334(7)	7318(7)	1609(5)	68(3)
C(58)	4881(9)	7465(7)	2099(4)	74(3)
C(59)	3895(9)	7610(7)	1956(4)	68(3)
C(60)	3281(7)	7632(7)	1324(4)	58(2)
C(61)	2071(6)	7541(6)	-94(3)	46(2)
C(62)	1669(5)	7738(5)	-828(3)	39(2)
C(63)	1483(5)	6829(5)	-1183(3)	38(2)
C(64)	1491(6)	6001(6)	-880(4)	50(2)
C(65)	1297(7)	5209(6)	-1249(5)	68(3)

C(66)	1008(8)	5265(7)	-1925(5)	72(3)
C(67)	991(8)	6051(8)	-2203(4)	70(3)
C(68)	1235(8)	6857(7)	-1851(4)	64(2)
C(69)	2317(5)	8411(5)	-1043(3)	37(2)
C(70)	3206(5)	8243(7)	-1205(4)	53(2)
C(71)	3725(6)	8953(7)	-1347(5)	62(2)
C(72)	3392(6)	9842(7)	-1328(4)	62(2)
C(73)	2507(6)	9995(5)	-1223(4)	49(2)
C(74)	1935(5)	9279(6)	-1056(3)	43(2)
C(75)	934(5)	9307(6)	-932(3)	44(2)
C(76)	138(6)	9890(8)	-1381(4)	64(2)
C(77)	-865(6)	9894(8)	-1264(4)	62(2)
C(78)	-737(8)	10215(10)	-605(7)	98(4)
C(79)	85(8)	9730(8)	-96(5)	73(3)
C(80)	1067(6)	9688(8)	-262(4)	63(2)
C(81)	650(5)	8301(6)	-979(4)	47(2)
C(82)	8709(6)	7498(6)	846(3)	45(2)
C(83)	9778(7)	7537(8)	981(4)	69(3)
C(84)	10379(8)	7672(10)	1589(5)	83(3)
C(85)	9999(11)	7789(9)	2072(5)	93(4)
C(86)	8995(9)	7726(8)	1961(4)	74(3)
C(87)	8325(8)	7561(7)	1345(4)	63(2)
C(88)	7071(6)	7269(6)	-45(3)	47(2)
C(89)	6652(6)	7282(5)	-793(3)	44(2)
C(90)	6582(6)	8261(6)	-1014(4)	48(2)
C(91)	6396(8)	8462(7)	-1651(4)	66(3)
C(92)	6233(10)	9330(8)	-1880(5)	83(3)
C(93)	6238(7)	10065(6)	-1463(4)	61(2)
C(94)	6452(6)	9870(7)	-836(5)	63(2)
C(95)	6600(6)	8990(6)	-594(4)	55(2)

C(96)	7261(5)	6691(5)	-1098(3)	40(2)
C(97)	8151(6)	6847(6)	-1207(4)	50(2)
C(98)	8654(6)	6181(8)	-1473(4)	61(2)
C(99)	8166(6)	5371(7)	-1678(4)	58(2)
C(100)	7233(6)	5207(6)	-1591(4)	52(2)
C(101)	6780(5)	5845(5)	-1291(3)	39(2)
C(102)	5783(5)	5794(5)	-1157(3)	41(2)
C(103)	4915(6)	5424(7)	-1689(5)	59(2)
C(104)	3927(5)	5358(7)	-1526(4)	56(2)
C(105)	4076(8)	4744(7)	-958(6)	84(3)
C(106)	4955(7)	5030(8)	-390(5)	72(3)
C(107)	5935(6)	5170(8)	-569(5)	67(3)
C(108)	5605(5)	6793(5)	-1027(4)	42(2)

Bond lengths [A] and angles [deg] for ljh021_0m.

O(1)-C(7)	1.209(8)
N(1)-C(7)	1.374(9)
N(1)-C(1)	1.412(9)
N(1)-H(1A)	0.8600
C(1)-C(6)	1.382(10)
C(1)-C(2)	1.394(11)
N(2)-C(34)	1.346(9)
N(2)-C(28)	1.395(9)
N(2)-H(2A)	0.8600
O(2)-C(34)	1.215(8)
C(2)-C(3)	1.372(11)
C(2)-H(2)	0.9300

N(3)-C(61)	1.364(10)
N(3)-C(55)	1.406(10)
N(3)-H(3A)	0.8600
O(3)-C(61)	1.177(9)
C(3)-C(4)	1.403(13)
C(3)-H(3)	0.9300
N(4)-C(88)	1.372(10)
N(4)-C(82)	1.420(9)
N(4)-H(4A)	0.8600
O(4)-C(88)	1.172(9)
C(4)-C(5)	1.347(13)
C(4)-H(4)	0.9300
C(5)-C(6)	1.387(12)
C(5)-H(5)	0.9300
C(6)-H(6)	0.9300
C(7)-C(8)	1.529(9)
C(8)-C(27)	1.530(9)
C(8)-C(9)	1.534(10)
C(8)-C(15)	1.543(8)
C(9)-C(14)	1.353(12)
C(9)-C(10)	1.384(11)
C(10)-C(11)	1.422(13)
C(10)-H(10)	0.9300
C(11)-C(12)	1.389(15)
C(11)-H(11)	0.9300
C(12)-C(13)	1.307(14)
C(12)-H(12)	0.9300
C(13)-C(14)	1.420(13)
C(13)-H(13)	0.9300
C(14)-H(14)	0.9300

C(15)-C(20)	1.381(10)
C(15)-C(16)	1.386(9)
C(16)-C(17)	1.382(10)
C(16)-H(16)	0.9300
C(17)-C(18)	1.400(12)
C(17)-H(17)	0.9300
C(18)-C(19)	1.358(10)
C(18)-H(18)	0.9300
C(19)-C(20)	1.390(10)
C(19)-H(19)	0.9300
C(20)-C(21)	1.489(9)
C(21)-C(22)	1.515(10)
C(21)-C(27)	1.539(10)
C(21)-C(26)	1.556(10)
C(22)-C(23)	1.513(12)
C(22)-H(22A)	0.9700
C(22)-H(22B)	0.9700
C(23)-C(24)	1.578(15)
C(23)-H(23A)	0.9700
C(23)-H(23B)	0.9700
C(24)-C(25)	1.469(14)
C(24)-H(24A)	0.9700
C(24)-H(24B)	0.9700
C(25)-C(26)	1.499(11)
C(25)-H(25A)	0.9700
C(25)-H(25B)	0.9700
C(26)-H(26A)	0.9700
C(26)-H(26B)	0.9700
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700

C(28)-C(29)	1.386(11)
C(28)-C(33)	1.401(10)
C(29)-C(30)	1.360(12)
C(29)-H(29)	0.9300
C(30)-C(31)	1.371(14)
C(30)-H(30)	0.9300
C(31)-C(32)	1.314(14)
C(31)-H(31)	0.9300
C(32)-C(33)	1.393(12)
C(32)-H(32)	0.9300
C(33)-H(33)	0.9300
C(34)-C(35)	1.531(9)
C(35)-C(42)	1.521(9)
C(35)-C(36)	1.535(10)
C(35)-C(54)	1.550(9)
C(36)-C(37)	1.388(10)
C(36)-C(41)	1.404(10)
C(37)-C(38)	1.384(12)
C(37)-H(37)	0.9300
C(38)-C(39)	1.380(12)
C(38)-H(38)	0.9300
C(39)-C(40)	1.345(13)
C(39)-H(39)	0.9300
C(40)-C(41)	1.384(11)
C(40)-H(40)	0.9300
C(41)-H(41)	0.9300
C(42)-C(43)	1.357(9)
C(42)-C(47)	1.407(10)
C(43)-C(44)	1.363(11)
C(43)-H(43)	0.9300

C(44)-C(45)	1.347(13)
C(44)-H(44)	0.9300
C(45)-C(46)	1.400(11)
C(45)-H(45)	0.9300
C(46)-C(47)	1.366(10)
C(46)-H(46)	0.9300
C(47)-C(48)	1.518(9)
C(48)-C(53)	1.521(9)
C(48)-C(54)	1.537(10)
C(48)-C(49)	1.546(9)
C(49)-C(50)	1.473(11)
C(49)-H(49A)	0.9700
C(49)-H(49B)	0.9700
C(50)-C(51)	1.529(13)
C(50)-H(50A)	0.9700
C(50)-H(50B)	0.9700
C(51)-C(52)	1.527(14)
C(51)-H(51A)	0.9700
C(51)-H(51B)	0.9700
C(52)-C(53)	1.506(10)
C(52)-H(52A)	0.9700
C(52)-H(52B)	0.9700
C(53)-H(53A)	0.9700
C(53)-H(53B)	0.9700
C(54)-H(54A)	0.9700
C(54)-H(54B)	0.9700
C(55)-C(60)	1.371(12)
C(55)-C(56)	1.410(11)
C(56)-C(57)	1.387(12)
C(56)-H(56)	0.9300

C(57)-C(58)	1.417(16)
C(57)-H(57)	0.9300
C(58)-C(59)	1.315(15)
C(58)-H(58)	0.9300
C(59)-C(60)	1.378(12)
C(59)-H(59)	0.9300
C(60)-H(60)	0.9300
C(61)-C(62)	1.553(10)
C(62)-C(69)	1.508(10)
C(62)-C(63)	1.531(10)
C(62)-C(81)	1.576(11)
C(63)-C(64)	1.388(11)
C(63)-C(68)	1.394(11)
C(64)-C(65)	1.398(13)
C(64)-H(64)	0.9300
C(65)-C(66)	1.410(14)
C(65)-H(65)	0.9300
C(66)-C(67)	1.306(15)
C(66)-H(66)	0.9300
C(67)-C(68)	1.400(13)
C(67)-H(67)	0.9300
C(68)-H(68)	0.9300
C(69)-C(74)	1.380(11)
C(69)-C(70)	1.401(11)
C(70)-C(71)	1.357(12)
C(70)-H(70)	0.9300
C(71)-C(72)	1.394(15)
C(71)-H(71)	0.9300
C(72)-C(73)	1.331(12)
C(72)-H(72)	0.9300

C(73)-C(74)	1.433(11)
C(73)-H(73)	0.9300
C(74)-C(75)	1.489(10)
C(75)-C(76)	1.494(12)
C(75)-C(80)	1.528(11)
C(75)-C(81)	1.530(12)
C(76)-C(77)	1.485(12)
C(76)-H(76A)	0.9700
C(76)-H(76B)	0.9700
C(77)-C(78)	1.474(17)
C(77)-H(77A)	0.9700
C(77)-H(77B)	0.9700
C(78)-C(79)	1.500(17)
C(78)-H(78A)	0.9700
C(78)-H(78B)	0.9700
C(79)-C(80)	1.510(12)
C(79)-H(79A)	0.9700
C(79)-H(79B)	0.9700
C(80)-H(80A)	0.9700
C(80)-H(80B)	0.9700
C(81)-H(81A)	0.9700
C(81)-H(81B)	0.9700
C(82)-C(87)	1.358(12)
C(82)-C(83)	1.413(12)
C(83)-C(84)	1.345(13)
C(83)-H(83)	0.9300
C(84)-C(85)	1.329(17)
C(84)-H(84)	0.9300
C(85)-C(86)	1.333(17)
C(85)-H(85)	0.9300

C(86)-C(87)	1.398(13)
C(86)-H(86)	0.9300
C(87)-H(87)	0.9300
C(88)-C(89)	1.555(10)
C(89)-C(96)	1.504(11)
C(89)-C(90)	1.517(12)
C(89)-C(108)	1.552(10)
C(90)-C(91)	1.367(12)
C(90)-C(95)	1.409(12)
C(91)-C(92)	1.367(14)
C(91)-H(91)	0.9300
C(92)-C(93)	1.416(15)
C(92)-H(92)	0.9300
C(93)-C(94)	1.340(13)
C(93)-H(93)	0.9300
C(94)-C(95)	1.393(14)
C(94)-H(94)	0.9300
C(95)-H(95)	0.9300
C(96)-C(97)	1.343(10)
C(96)-C(101)	1.414(11)
C(97)-C(98)	1.428(13)
C(97)-H(97)	0.9300
C(98)-C(99)	1.376(14)
C(98)-H(98)	0.9300
C(99)-C(100)	1.381(12)
C(99)-H(99)	0.9300
C(100)-C(101)	1.401(10)
C(100)-H(100)	0.9300
C(101)-C(102)	1.497(9)
C(102)-C(103)	1.489(10)

C(102)-C(108)	1.535(11)
C(102)-C(107)	1.541(12)
C(103)-C(104)	1.516(11)
C(103)-H(10A)	0.9700
C(103)-H(10B)	0.9700
C(104)-C(105)	1.499(14)
C(104)-H(10C)	0.9700
C(104)-H(10D)	0.9700
C(105)-C(106)	1.501(15)
C(105)-H(10E)	0.9700
C(105)-H(10F)	0.9700
C(106)-C(107)	1.536(13)
C(106)-H(10G)	0.9700
C(106)-H(10H)	0.9700
C(107)-H(10I)	0.9700
C(107)-H(10J)	0.9700
C(108)-H(10K)	0.9700
C(108)-H(10L)	0.9700

C(7)-N(1)-C(1)	128.8(6)
C(7)-N(1)-H(1A)	115.6
C(1)-N(1)-H(1A)	115.6
C(6)-C(1)-C(2)	120.6(7)
C(6)-C(1)-N(1)	123.2(7)
C(2)-C(1)-N(1)	116.2(6)
C(34)-N(2)-C(28)	131.0(6)
C(34)-N(2)-H(2A)	114.5
C(28)-N(2)-H(2A)	114.5
C(3)-C(2)-C(1)	119.4(8)
C(3)-C(2)-H(2)	120.3

C(1)-C(2)-H(2)	120.3
C(61)-N(3)-C(55)	127.3(6)
C(61)-N(3)-H(3A)	116.3
C(55)-N(3)-H(3A)	116.3
C(2)-C(3)-C(4)	119.9(8)
C(2)-C(3)-H(3)	120.1
C(4)-C(3)-H(3)	120.1
C(88)-N(4)-C(82)	127.4(6)
C(88)-N(4)-H(4A)	116.3
C(82)-N(4)-H(4A)	116.3
C(5)-C(4)-C(3)	119.9(7)
C(5)-C(4)-H(4)	120.0
C(3)-C(4)-H(4)	120.0
C(4)-C(5)-C(6)	121.4(8)
C(4)-C(5)-H(5)	119.3
C(6)-C(5)-H(5)	119.3
C(1)-C(6)-C(5)	118.7(8)
C(1)-C(6)-H(6)	120.6
C(5)-C(6)-H(6)	120.6
O(1)-C(7)-N(1)	121.4(6)
O(1)-C(7)-C(8)	122.9(6)
N(1)-C(7)-C(8)	115.7(5)
C(7)-C(8)-C(27)	109.3(5)
C(7)-C(8)-C(9)	109.4(6)
C(27)-C(8)-C(9)	113.8(5)
C(7)-C(8)-C(15)	110.9(5)
C(27)-C(8)-C(15)	98.9(5)
C(9)-C(8)-C(15)	114.2(5)
C(14)-C(9)-C(10)	119.4(8)
C(14)-C(9)-C(8)	122.3(6)

C(10)-C(9)-C(8)	117.8(7)
C(9)-C(10)-C(11)	118.5(9)
C(9)-C(10)-H(10)	120.7
C(11)-C(10)-H(10)	120.7
C(12)-C(11)-C(10)	120.6(8)
C(12)-C(11)-H(11)	119.7
C(10)-C(11)-H(11)	119.7
C(13)-C(12)-C(11)	119.3(9)
C(13)-C(12)-H(12)	120.3
C(11)-C(12)-H(12)	120.3
C(12)-C(13)-C(14)	121.5(9)
C(12)-C(13)-H(13)	119.3
C(14)-C(13)-H(13)	119.3
C(9)-C(14)-C(13)	120.5(8)
C(9)-C(14)-H(14)	119.7
C(13)-C(14)-H(14)	119.7
C(20)-C(15)-C(16)	121.3(6)
C(20)-C(15)-C(8)	110.6(5)
C(16)-C(15)-C(8)	128.0(6)
C(17)-C(16)-C(15)	119.8(7)
C(17)-C(16)-H(16)	120.1
C(15)-C(16)-H(16)	120.1
C(16)-C(17)-C(18)	118.8(6)
C(16)-C(17)-H(17)	120.6
C(18)-C(17)-H(17)	120.6
C(19)-C(18)-C(17)	120.7(7)
C(19)-C(18)-H(18)	119.7
C(17)-C(18)-H(18)	119.7
C(18)-C(19)-C(20)	121.1(7)
C(18)-C(19)-H(19)	119.5

C(20)-C(19)-H(19)	119.5
C(15)-C(20)-C(19)	118.2(6)
C(15)-C(20)-C(21)	112.8(6)
C(19)-C(20)-C(21)	128.9(7)
C(20)-C(21)-C(22)	112.8(6)
C(20)-C(21)-C(27)	100.3(6)
C(22)-C(21)-C(27)	111.7(6)
C(20)-C(21)-C(26)	112.0(5)
C(22)-C(21)-C(26)	107.6(7)
C(27)-C(21)-C(26)	112.5(6)
C(23)-C(22)-C(21)	112.5(7)
C(23)-C(22)-H(22A)	109.1
C(21)-C(22)-H(22A)	109.1
C(23)-C(22)-H(22B)	109.1
C(21)-C(22)-H(22B)	109.1
H(22A)-C(22)-H(22B)	107.8
C(22)-C(23)-C(24)	109.2(8)
C(22)-C(23)-H(23A)	109.8
C(24)-C(23)-H(23A)	109.8
C(22)-C(23)-H(23B)	109.8
C(24)-C(23)-H(23B)	109.8
H(23A)-C(23)-H(23B)	108.3
C(25)-C(24)-C(23)	111.3(8)
C(25)-C(24)-H(24A)	109.4
C(23)-C(24)-H(24A)	109.4
C(25)-C(24)-H(24B)	109.4
C(23)-C(24)-H(24B)	109.4
H(24A)-C(24)-H(24B)	108.0
C(24)-C(25)-C(26)	111.1(7)
C(24)-C(25)-H(25A)	109.4

C(26)-C(25)-H(25A)	109.4
C(24)-C(25)-H(25B)	109.4
C(26)-C(25)-H(25B)	109.4
H(25A)-C(25)-H(25B)	108.0
C(25)-C(26)-C(21)	113.0(6)
C(25)-C(26)-H(26A)	109.0
C(21)-C(26)-H(26A)	109.0
C(25)-C(26)-H(26B)	109.0
C(21)-C(26)-H(26B)	109.0
H(26A)-C(26)-H(26B)	107.8
C(8)-C(27)-C(21)	109.3(5)
C(8)-C(27)-H(27A)	109.8
C(21)-C(27)-H(27A)	109.8
C(8)-C(27)-H(27B)	109.8
C(21)-C(27)-H(27B)	109.8
H(27A)-C(27)-H(27B)	108.3
C(29)-C(28)-N(2)	117.2(6)
C(29)-C(28)-C(33)	119.6(7)
N(2)-C(28)-C(33)	123.1(7)
C(30)-C(29)-C(28)	119.1(8)
C(30)-C(29)-H(29)	120.5
C(28)-C(29)-H(29)	120.5
C(29)-C(30)-C(31)	122.0(9)
C(29)-C(30)-H(30)	119.0
C(31)-C(30)-H(30)	119.0
C(32)-C(31)-C(30)	118.3(8)
C(32)-C(31)-H(31)	120.8
C(30)-C(31)-H(31)	120.8
C(31)-C(32)-C(33)	123.7(9)
C(31)-C(32)-H(32)	118.2

C(33)-C(32)-H(32)	118.2
C(32)-C(33)-C(28)	117.0(8)
C(32)-C(33)-H(33)	121.5
C(28)-C(33)-H(33)	121.5
O(2)-C(34)-N(2)	121.1(6)
O(2)-C(34)-C(35)	122.1(7)
N(2)-C(34)-C(35)	116.7(5)
C(42)-C(35)-C(34)	111.2(5)
C(42)-C(35)-C(36)	113.3(6)
C(34)-C(35)-C(36)	108.2(5)
C(42)-C(35)-C(54)	102.0(5)
C(34)-C(35)-C(54)	110.4(6)
C(36)-C(35)-C(54)	111.7(5)
C(37)-C(36)-C(41)	118.1(7)
C(37)-C(36)-C(35)	122.6(6)
C(41)-C(36)-C(35)	119.2(6)
C(38)-C(37)-C(36)	120.6(7)
C(38)-C(37)-H(37)	119.7
C(36)-C(37)-H(37)	119.7
C(39)-C(38)-C(37)	120.4(8)
C(39)-C(38)-H(38)	119.8
C(37)-C(38)-H(38)	119.8
C(40)-C(39)-C(38)	119.3(8)
C(40)-C(39)-H(39)	120.3
C(38)-C(39)-H(39)	120.3
C(39)-C(40)-C(41)	121.9(8)
C(39)-C(40)-H(40)	119.0
C(41)-C(40)-H(40)	119.0
C(40)-C(41)-C(36)	119.6(7)
C(40)-C(41)-H(41)	120.2

C(36)-C(41)-H(41)	120.2
C(43)-C(42)-C(47)	119.9(6)
C(43)-C(42)-C(35)	130.4(7)
C(47)-C(42)-C(35)	109.7(6)
C(42)-C(43)-C(44)	120.3(8)
C(42)-C(43)-H(43)	119.8
C(44)-C(43)-H(43)	119.8
C(45)-C(44)-C(43)	121.5(8)
C(45)-C(44)-H(44)	119.3
C(43)-C(44)-H(44)	119.3
C(44)-C(45)-C(46)	118.9(7)
C(44)-C(45)-H(45)	120.5
C(46)-C(45)-H(45)	120.5
C(47)-C(46)-C(45)	120.8(7)
C(47)-C(46)-H(46)	119.6
C(45)-C(46)-H(46)	119.6
C(46)-C(47)-C(42)	118.4(6)
C(46)-C(47)-C(48)	129.9(6)
C(42)-C(47)-C(48)	111.7(6)
C(47)-C(48)-C(53)	110.7(5)
C(47)-C(48)-C(54)	101.5(5)
C(53)-C(48)-C(54)	114.7(6)
C(47)-C(48)-C(49)	112.4(6)
C(53)-C(48)-C(49)	107.1(6)
C(54)-C(48)-C(49)	110.4(6)
C(50)-C(49)-C(48)	114.0(7)
C(50)-C(49)-H(49A)	108.8
C(48)-C(49)-H(49A)	108.8
C(50)-C(49)-H(49B)	108.8
C(48)-C(49)-H(49B)	108.8

H(49A)-C(49)-H(49B)	107.6
C(49)-C(50)-C(51)	111.2(7)
C(49)-C(50)-H(50A)	109.4
C(51)-C(50)-H(50A)	109.4
C(49)-C(50)-H(50B)	109.4
C(51)-C(50)-H(50B)	109.4
H(50A)-C(50)-H(50B)	108.0
C(52)-C(51)-C(50)	111.6(8)
C(52)-C(51)-H(51A)	109.3
C(50)-C(51)-H(51A)	109.3
C(52)-C(51)-H(51B)	109.3
C(50)-C(51)-H(51B)	109.3
H(51A)-C(51)-H(51B)	108.0
C(53)-C(52)-C(51)	111.3(8)
C(53)-C(52)-H(52A)	109.4
C(51)-C(52)-H(52A)	109.4
C(53)-C(52)-H(52B)	109.4
C(51)-C(52)-H(52B)	109.4
H(52A)-C(52)-H(52B)	108.0
C(52)-C(53)-C(48)	113.9(6)
C(52)-C(53)-H(53A)	108.8
C(48)-C(53)-H(53A)	108.8
C(52)-C(53)-H(53B)	108.8
C(48)-C(53)-H(53B)	108.8
H(53A)-C(53)-H(53B)	107.7
C(48)-C(54)-C(35)	107.0(5)
C(48)-C(54)-H(54A)	110.3
C(35)-C(54)-H(54A)	110.3
C(48)-C(54)-H(54B)	110.3
C(35)-C(54)-H(54B)	110.3

H(54A)-C(54)-H(54B)	108.6
C(60)-C(55)-N(3)	124.6(7)
C(60)-C(55)-C(56)	118.7(8)
N(3)-C(55)-C(56)	116.8(7)
C(57)-C(56)-C(55)	119.2(9)
C(57)-C(56)-H(56)	120.4
C(55)-C(56)-H(56)	120.4
C(56)-C(57)-C(58)	119.1(9)
C(56)-C(57)-H(57)	120.5
C(58)-C(57)-H(57)	120.5
C(59)-C(58)-C(57)	120.9(8)
C(59)-C(58)-H(58)	119.5
C(57)-C(58)-H(58)	119.5
C(58)-C(59)-C(60)	120.6(9)
C(58)-C(59)-H(59)	119.7
C(60)-C(59)-H(59)	119.7
C(55)-C(60)-C(59)	121.5(9)
C(55)-C(60)-H(60)	119.3
C(59)-C(60)-H(60)	119.3
O(3)-C(61)-N(3)	123.5(7)
O(3)-C(61)-C(62)	121.7(7)
N(3)-C(61)-C(62)	114.8(6)
C(69)-C(62)-C(63)	116.0(6)
C(69)-C(62)-C(61)	113.0(6)
C(63)-C(62)-C(61)	108.0(6)
C(69)-C(62)-C(81)	99.5(6)
C(63)-C(62)-C(81)	111.0(5)
C(61)-C(62)-C(81)	108.9(6)
C(64)-C(63)-C(68)	119.4(7)
C(64)-C(63)-C(62)	123.5(6)

C(68)-C(63)-C(62)	117.0(7)
C(63)-C(64)-C(65)	119.2(8)
C(63)-C(64)-H(64)	120.4
C(65)-C(64)-H(64)	120.4
C(64)-C(65)-C(66)	119.8(9)
C(64)-C(65)-H(65)	120.1
C(66)-C(65)-H(65)	120.1
C(67)-C(66)-C(65)	119.9(9)
C(67)-C(66)-H(66)	120.0
C(65)-C(66)-H(66)	120.0
C(66)-C(67)-C(68)	122.2(9)
C(66)-C(67)-H(67)	118.9
C(68)-C(67)-H(67)	118.9
C(63)-C(68)-C(67)	119.3(9)
C(63)-C(68)-H(68)	120.4
C(67)-C(68)-H(68)	120.4
C(74)-C(69)-C(70)	121.2(7)
C(74)-C(69)-C(62)	110.8(6)
C(70)-C(69)-C(62)	128.0(7)
C(71)-C(70)-C(69)	119.2(9)
C(71)-C(70)-H(70)	120.4
C(69)-C(70)-H(70)	120.4
C(70)-C(71)-C(72)	121.1(8)
C(70)-C(71)-H(71)	119.5
C(72)-C(71)-H(71)	119.5
C(73)-C(72)-C(71)	119.5(8)
C(73)-C(72)-H(72)	120.2
C(71)-C(72)-H(72)	120.2
C(72)-C(73)-C(74)	121.9(8)
C(72)-C(73)-H(73)	119.1

C(74)-C(73)-H(73)	119.1
C(69)-C(74)-C(73)	116.8(7)
C(69)-C(74)-C(75)	113.2(7)
C(73)-C(74)-C(75)	129.9(8)
C(74)-C(75)-C(76)	115.5(7)
C(74)-C(75)-C(80)	110.2(6)
C(76)-C(75)-C(80)	105.2(8)
C(74)-C(75)-C(81)	101.1(6)
C(76)-C(75)-C(81)	113.2(7)
C(80)-C(75)-C(81)	111.8(7)
C(77)-C(76)-C(75)	115.0(8)
C(77)-C(76)-H(76A)	108.5
C(75)-C(76)-H(76A)	108.5
C(77)-C(76)-H(76B)	108.5
C(75)-C(76)-H(76B)	108.5
H(76A)-C(76)-H(76B)	107.5
C(78)-C(77)-C(76)	109.7(8)
C(78)-C(77)-H(77A)	109.7
C(76)-C(77)-H(77A)	109.7
C(78)-C(77)-H(77B)	109.7
C(76)-C(77)-H(77B)	109.7
H(77A)-C(77)-H(77B)	108.2
C(77)-C(78)-C(79)	113.9(10)
C(77)-C(78)-H(78A)	108.8
C(79)-C(78)-H(78A)	108.8
C(77)-C(78)-H(78B)	108.8
C(79)-C(78)-H(78B)	108.8
H(78A)-C(78)-H(78B)	107.7
C(78)-C(79)-C(80)	111.6(9)
C(78)-C(79)-H(79A)	109.3

C(80)-C(79)-H(79A)	109.3
C(78)-C(79)-H(79B)	109.3
C(80)-C(79)-H(79B)	109.3
H(79A)-C(79)-H(79B)	108.0
C(79)-C(80)-C(75)	113.5(7)
C(79)-C(80)-H(80A)	108.9
C(75)-C(80)-H(80A)	108.9
C(79)-C(80)-H(80B)	108.9
C(75)-C(80)-H(80B)	108.9
H(80A)-C(80)-H(80B)	107.7
C(75)-C(81)-C(62)	107.7(6)
C(75)-C(81)-H(81A)	110.2
C(62)-C(81)-H(81A)	110.2
C(75)-C(81)-H(81B)	110.2
C(62)-C(81)-H(81B)	110.2
H(81A)-C(81)-H(81B)	108.5
C(87)-C(82)-C(83)	118.3(8)
C(87)-C(82)-N(4)	124.4(8)
C(83)-C(82)-N(4)	117.1(7)
C(84)-C(83)-C(82)	119.6(9)
C(84)-C(83)-H(83)	120.2
C(82)-C(83)-H(83)	120.2
C(85)-C(84)-C(83)	122.1(11)
C(85)-C(84)-H(84)	119.0
C(83)-C(84)-H(84)	119.0
C(84)-C(85)-C(86)	119.6(10)
C(84)-C(85)-H(85)	120.2
C(86)-C(85)-H(85)	120.2
C(85)-C(86)-C(87)	121.5(10)
C(85)-C(86)-H(86)	119.2

C(87)-C(86)-H(86)	119.2
C(82)-C(87)-C(86)	118.8(10)
C(82)-C(87)-H(87)	120.6
C(86)-C(87)-H(87)	120.6
O(4)-C(88)-N(4)	122.8(7)
O(4)-C(88)-C(89)	123.2(8)
N(4)-C(88)-C(89)	114.0(6)
C(96)-C(89)-C(90)	113.5(6)
C(96)-C(89)-C(108)	100.2(6)
C(90)-C(89)-C(108)	112.1(6)
C(96)-C(89)-C(88)	112.6(6)
C(90)-C(89)-C(88)	108.2(6)
C(108)-C(89)-C(88)	110.1(6)
C(91)-C(90)-C(95)	117.2(9)
C(91)-C(90)-C(89)	120.3(7)
C(95)-C(90)-C(89)	122.1(7)
C(92)-C(91)-C(90)	122.3(9)
C(92)-C(91)-H(91)	118.8
C(90)-C(91)-H(91)	118.8
C(91)-C(92)-C(93)	120.8(9)
C(91)-C(92)-H(92)	119.6
C(93)-C(92)-H(92)	119.6
C(94)-C(93)-C(92)	116.8(8)
C(94)-C(93)-H(93)	121.6
C(92)-C(93)-H(93)	121.6
C(93)-C(94)-C(95)	123.2(8)
C(93)-C(94)-H(94)	118.4
C(95)-C(94)-H(94)	118.4
C(94)-C(95)-C(90)	119.5(8)
C(94)-C(95)-H(95)	120.2

C(90)-C(95)-H(95)	120.2
C(97)-C(96)-C(101)	117.9(7)
C(97)-C(96)-C(89)	130.5(7)
C(101)-C(96)-C(89)	111.6(6)
C(96)-C(97)-C(98)	122.9(8)
C(96)-C(97)-H(97)	118.6
C(98)-C(97)-H(97)	118.6
C(99)-C(98)-C(97)	118.7(8)
C(99)-C(98)-H(98)	120.7
C(97)-C(98)-H(98)	120.7
C(98)-C(99)-C(100)	119.3(8)
C(98)-C(99)-H(99)	120.4
C(100)-C(99)-H(99)	120.4
C(99)-C(100)-C(101)	121.3(8)
C(99)-C(100)-H(100)	119.3
C(101)-C(100)-H(100)	119.3
C(100)-C(101)-C(96)	119.7(7)
C(100)-C(101)-C(102)	129.1(7)
C(96)-C(101)-C(102)	111.1(6)
C(103)-C(102)-C(101)	115.4(6)
C(103)-C(102)-C(108)	111.1(7)
C(101)-C(102)-C(108)	101.5(6)
C(103)-C(102)-C(107)	107.5(7)
C(101)-C(102)-C(107)	107.4(6)
C(108)-C(102)-C(107)	114.0(7)
C(102)-C(103)-C(104)	113.7(7)
C(102)-C(103)-H(10A)	108.8
C(104)-C(103)-H(10A)	108.8
C(102)-C(103)-H(10B)	108.8
C(104)-C(103)-H(10B)	108.8

H(10A)-C(103)-H(10B)	107.7
C(105)-C(104)-C(103)	109.5(7)
C(105)-C(104)-H(10C)	109.8
C(103)-C(104)-H(10C)	109.8
C(105)-C(104)-H(10D)	109.8
C(103)-C(104)-H(10D)	109.8
H(10C)-C(104)-H(10D)	108.2
C(104)-C(105)-C(106)	112.5(8)
C(104)-C(105)-H(10E)	109.1
C(106)-C(105)-H(10E)	109.1
C(104)-C(105)-H(10F)	109.1
C(106)-C(105)-H(10F)	109.1
H(10E)-C(105)-H(10F)	107.8
C(105)-C(106)-C(107)	112.0(9)
C(105)-C(106)-H(10G)	109.2
C(107)-C(106)-H(10G)	109.2
C(105)-C(106)-H(10H)	109.2
C(107)-C(106)-H(10H)	109.2
H(10G)-C(106)-H(10H)	107.9
C(106)-C(107)-C(102)	113.1(7)
C(106)-C(107)-H(10I)	109.0
C(102)-C(107)-H(10I)	109.0
C(106)-C(107)-H(10J)	109.0
C(102)-C(107)-H(10J)	109.0
H(10I)-C(107)-H(10J)	107.8
C(102)-C(108)-C(89)	108.6(6)
C(102)-C(108)-H(10K)	110.0
C(89)-C(108)-H(10K)	110.0
C(102)-C(108)-H(10L)	110.0
C(89)-C(108)-H(10L)	110.0

H(10K)-C(108)-H(10L) 108.3

Symmetry transformations used to generate equivalent atoms:

Anisotropic displacement parameters (A^2 x 10^3) for ljh021_0m. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	30(2)	73(4)	51(3)	9(3)	5(2)	11(3)
N(1)	32(3)	54(4)	31(3)	4(3)	3(2)	-3(3)
C(1)	48(4)	39(4)	28(3)	8(3)	6(3)	10(3)
N(2)	29(3)	60(4)	33(3)	4(3)	7(2)	-9(3)
O(2)	31(3)	103(6)	60(3)	-17(3)	2(2)	16(3)
C(2)	46(4)	60(6)	47(4)	4(4)	11(3)	1(4)
N(3)	54(4)	60(4)	31(3)	12(3)	16(3)	11(3)
O(3)	59(4)	104(6)	64(4)	10(4)	30(3)	-5(4)
C(3)	83(6)	59(6)	52(5)	5(4)	39(4)	5(5)
N(4)	60(4)	62(5)	27(3)	-1(3)	12(3)	0(3)
O(4)	77(4)	128(7)	57(4)	-18(4)	36(3)	-38(4)
C(4)	105(7)	66(6)	29(4)	-1(4)	21(4)	-11(6)
C(5)	74(6)	78(7)	25(3)	2(4)	-2(3)	-13(5)
C(6)	61(5)	50(5)	39(4)	7(3)	0(3)	-14(4)
C(7)	34(3)	37(4)	35(3)	10(3)	3(3)	9(3)
C(8)	22(3)	33(4)	31(3)	-1(3)	4(2)	0(3)
C(9)	28(3)	39(4)	46(4)	-1(3)	15(3)	7(3)
C(10)	48(4)	43(5)	61(5)	-8(4)	10(4)	-4(4)

C(11)	60(5)	65(6)	68(5)	-22(5)	20(4)	-6(5)
C(12)	85(7)	48(6)	83(7)	-26(5)	31(5)	-20(5)
C(13)	60(5)	28(4)	104(8)	-3(4)	11(5)	2(4)
C(14)	49(4)	43(5)	72(5)	-7(4)	24(4)	-5(4)
C(15)	28(3)	33(4)	29(3)	9(2)	7(2)	13(3)
C(16)	36(3)	41(4)	35(3)	2(3)	17(3)	1(3)
C(17)	30(3)	64(5)	34(3)	7(3)	11(3)	12(3)
C(18)	43(4)	57(5)	35(3)	6(3)	10(3)	19(4)
C(19)	44(4)	31(4)	51(4)	0(3)	16(3)	5(3)
C(20)	36(3)	36(4)	26(3)	5(3)	9(2)	8(3)
C(21)	34(3)	38(4)	39(3)	0(3)	13(3)	6(3)
C(22)	67(5)	47(5)	55(5)	14(4)	29(4)	3(4)
C(23)	51(5)	51(5)	89(6)	10(4)	35(4)	-1(4)
C(24)	45(5)	91(8)	95(7)	0(6)	20(5)	-19(5)
C(25)	45(4)	66(6)	59(5)	-12(4)	10(4)	-1(4)
C(26)	51(4)	42(4)	56(4)	-14(3)	22(4)	-1(4)
C(27)	35(3)	32(4)	42(3)	1(3)	23(3)	1(3)
C(28)	56(4)	24(3)	38(4)	-3(3)	2(3)	-9(3)
C(29)	43(4)	47(5)	52(4)	-4(4)	12(3)	-5(4)
C(30)	83(6)	89(8)	66(6)	-15(5)	47(5)	5(6)
C(31)	86(7)	104(9)	46(5)	-16(5)	26(5)	6(6)
C(32)	78(6)	74(7)	42(4)	-13(4)	-1(4)	9(5)
C(33)	62(5)	46(5)	34(4)	-4(3)	11(3)	-2(4)
C(34)	40(4)	40(4)	35(3)	4(3)	-1(3)	1(3)
C(35)	37(3)	34(4)	32(3)	-5(3)	11(3)	-11(3)
C(36)	32(3)	34(4)	44(4)	-8(3)	9(3)	-1(3)
C(37)	57(4)	34(4)	44(4)	-4(3)	19(3)	-7(3)
C(38)	58(5)	41(5)	76(6)	-19(4)	26(4)	-14(4)
C(39)	67(5)	44(5)	59(5)	6(4)	20(4)	1(4)
C(40)	55(5)	39(5)	55(4)	7(4)	4(3)	-1(4)

C(41)	55(4)	33(4)	49(4)	5(3)	3(3)	-1(3)
C(42)	34(3)	34(4)	33(3)	2(3)	2(3)	-6(3)
C(43)	33(3)	55(5)	40(4)	0(3)	15(3)	-11(3)
C(44)	37(4)	67(6)	51(4)	-9(4)	3(3)	-20(4)
C(45)	46(4)	52(5)	64(5)	-11(4)	15(4)	-21(4)
C(46)	43(4)	34(4)	63(4)	-17(3)	27(3)	-15(3)
C(47)	36(3)	31(4)	38(3)	-3(3)	13(3)	-2(3)
C(48)	34(3)	36(4)	39(3)	4(3)	19(3)	3(3)
C(49)	73(5)	40(4)	50(4)	-3(3)	45(4)	5(4)
C(50)	68(5)	46(5)	71(5)	10(4)	36(4)	12(4)
C(51)	74(6)	67(7)	104(7)	41(6)	53(6)	39(5)
C(52)	45(4)	76(7)	62(5)	33(5)	14(4)	15(4)
C(53)	43(4)	38(4)	52(4)	14(3)	21(3)	0(3)
C(54)	35(3)	33(4)	41(3)	0(3)	19(3)	0(3)
C(55)	38(4)	50(5)	54(4)	0(4)	14(3)	-7(4)
C(56)	45(4)	59(6)	63(5)	9(4)	10(4)	-3(4)
C(57)	53(5)	64(6)	66(6)	-8(5)	-12(4)	-5(5)
C(58)	94(8)	65(7)	48(5)	10(4)	-1(5)	-9(6)
C(59)	92(7)	61(6)	53(5)	-1(4)	25(5)	2(5)
C(60)	56(5)	71(6)	45(4)	0(4)	14(4)	1(4)
C(61)	56(4)	46(5)	42(4)	-4(3)	26(3)	-5(4)
C(62)	33(3)	44(4)	36(3)	-1(3)	6(3)	-12(3)
C(63)	34(3)	34(4)	47(4)	-6(3)	15(3)	-10(3)
C(64)	41(4)	52(5)	57(4)	1(4)	16(3)	0(4)
C(65)	70(6)	34(5)	95(7)	-1(4)	20(5)	-8(4)
C(66)	91(7)	59(7)	75(6)	-31(5)	37(5)	-17(5)
C(67)	93(7)	64(7)	55(5)	-15(5)	23(5)	-18(6)
C(68)	94(7)	47(5)	46(4)	-9(4)	18(4)	-25(5)
C(69)	41(4)	33(4)	38(3)	4(3)	15(3)	1(3)
C(70)	36(4)	53(5)	67(5)	17(4)	13(3)	-11(4)

C(71)	47(4)	65(6)	82(6)	16(5)	32(4)	0(4)
C(72)	46(4)	59(6)	74(5)	17(4)	8(4)	-14(4)
C(73)	51(4)	29(4)	66(5)	2(3)	17(4)	0(3)
C(74)	42(4)	55(5)	32(3)	11(3)	13(3)	-3(4)
C(75)	35(4)	46(5)	48(4)	-14(3)	10(3)	-5(3)
C(76)	56(5)	74(7)	68(5)	24(5)	28(4)	21(5)
C(77)	42(4)	78(7)	61(5)	13(5)	11(4)	6(4)
C(78)	61(6)	88(9)	154(12)	1(8)	47(7)	14(6)
C(79)	74(6)	86(8)	69(6)	-25(5)	38(5)	-20(6)
C(80)	50(5)	73(7)	67(5)	-23(5)	19(4)	-10(4)
C(81)	31(3)	60(5)	48(4)	-11(3)	11(3)	-8(3)
C(82)	45(4)	51(5)	41(4)	11(3)	16(3)	7(4)
C(83)	54(5)	100(8)	53(5)	-12(5)	17(4)	-5(5)
C(84)	65(6)	122(11)	56(5)	-7(6)	10(4)	-7(6)
C(85)	119(10)	80(8)	65(6)	-24(6)	9(6)	-28(7)
C(86)	103(8)	80(7)	41(5)	6(4)	26(5)	-12(6)
C(87)	93(7)	53(5)	49(5)	-2(4)	30(4)	0(5)
C(88)	61(5)	51(5)	39(4)	-7(3)	29(3)	-15(4)
C(89)	55(4)	43(4)	32(4)	-4(3)	13(3)	2(4)
C(90)	42(4)	48(5)	58(5)	-5(4)	19(3)	-5(3)
C(91)	111(8)	48(5)	52(5)	-1(4)	43(5)	-12(5)
C(92)	136(10)	53(6)	54(5)	-1(4)	20(5)	-15(6)
C(93)	81(6)	36(4)	73(6)	16(4)	36(5)	10(4)
C(94)	53(5)	51(6)	87(6)	-29(5)	23(4)	-5(4)
C(95)	57(5)	51(5)	55(4)	-4(4)	16(4)	2(4)
C(96)	38(4)	46(4)	31(3)	-2(3)	6(3)	-10(3)
C(97)	47(4)	45(5)	57(4)	-6(4)	17(3)	0(4)
C(98)	45(4)	80(7)	67(5)	6(5)	27(4)	0(5)
C(99)	52(5)	61(6)	69(5)	8(4)	29(4)	21(4)
C(100)	54(5)	51(5)	56(4)	-17(4)	23(4)	1(4)

C(101)	41(4)	39(4)	40(3)	3(3)	18(3)	4(3)
C(102)	33(3)	42(4)	54(4)	-14(3)	21(3)	-8(3)
C(103)	39(4)	60(6)	77(5)	-22(4)	16(4)	-3(4)
C(104)	28(4)	73(6)	59(5)	-6(4)	2(3)	-5(4)
C(105)	66(6)	37(5)	145(10)	9(6)	25(6)	-13(5)
C(106)	65(6)	77(7)	78(6)	29(5)	30(5)	18(5)
C(107)	47(5)	78(7)	69(5)	13(5)	9(4)	3(5)
C(108)	33(3)	38(4)	56(4)	-4(3)	18(3)	-3(3)

Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for ljh021_0m.

	x	y	z	U(eq)
H(1A)	-1502	5904	5052	49
H(2A)	3436	6237	5041	50
H(2)	-706	6389	4329	62
H(3A)	3448	7676	-91	57
H(3)	-714	6426	3273	72
H(4A)	8444	7266	-74	60
H(4)	-2221	6121	2445	80
H(5)	-3643	5699	2681	75
H(6)	-3680	5713	3732	65
H(10)	-1680	6245	7023	63
H(11)	-1399	7655	7558	77
H(12)	-1943	8985	6988	85
H(13)	-2776	8918	5935	81

H(14)	-2923	7553	5371	64
H(16)	-386	5911	6096	43
H(17)	761	4712	6352	51
H(18)	151	3250	6411	54
H(19)	-1547	2998	6210	50
H(22A)	-3186	3124	6453	65
H(22B)	-3090	4004	6870	65
H(23A)	-4805	4347	6358	73
H(23B)	-4724	3368	6655	73
H(24A)	-4919	2701	5629	93
H(24B)	-5846	3356	5554	93
H(25A)	-5096	4453	5121	70
H(25B)	-5155	3555	4726	70
H(26A)	-3550	4213	4945	58
H(26B)	-3461	3249	5258	58
H(27A)	-4018	5439	5688	40
H(27B)	-3336	5454	6413	40
H(29)	4297	6109	4322	58
H(30)	4265	5927	3280	88
H(31)	2754	5972	2448	93
H(32)	1287	5932	2675	83
H(33)	1217	6121	3712	58
H(37)	1803	4666	5158	53
H(38)	1947	3190	5524	68
H(39)	2721	2876	6602	68
H(40)	3381	4023	7296	63
H(41)	3343	5501	6947	59
H(43)	4558	5998	6083	50
H(44)	5812	7055	6454	65
H(45)	5452	8462	6749	66

H(46)	3768	8838	6648	53
H(49A)	2036	7767	7107	58
H(49B)	2104	8744	6844	58
H(50A)	569	8577	7013	70
H(50B)	327	7709	6576	70
H(51A)	-552	8908	5962	91
H(51B)	441	9502	6134	91
H(52A)	47	7963	5317	74
H(52B)	169	8961	5102	74
H(53A)	1883	8954	5664	51
H(53B)	1645	8112	5205	51
H(54A)	978	6725	5746	42
H(54B)	1644	6496	6457	42
H(56)	5003	7221	643	68
H(57)	6032	7213	1714	82
H(58)	5286	7459	2528	89
H(59)	3610	7699	2284	82
H(60)	2584	7726	1234	69
H(64)	1625	5974	-436	60
H(65)	1357	4646	-1049	81
H(66)	831	4742	-2173	87
H(67)	809	6075	-2649	85
H(68)	1233	7406	-2061	76
H(70)	3437	7653	-1216	63
H(71)	4311	8844	-1458	74
H(72)	3785	10325	-1388	74
H(73)	2252	10583	-1259	59
H(76A)	392	10508	-1348	77
H(76B)	38	9686	-1817	77
H(77A)	-1334	10288	-1572	74

H(77B)	-1148	9286	-1318	74
H(78A)	-1378	10140	-516	117
H(78B)	-580	10857	-582	117
H(79A)	-140	9119	-47	87
H(79B)	207	10042	312	87
H(80A)	1552	9314	54	76
H(80B)	1351	10294	-234	76
H(81A)	204	8160	-1408	56
H(81B)	297	8154	-672	56
H(83)	10064	7469	651	83
H(84)	11083	7685	1674	99
H(85)	10430	7914	2483	111
H(86)	8734	7794	2302	89
H(87)	7629	7495	1278	76
H(91)	6379	7993	-1937	79
H(92)	6117	9439	-2316	100
H(93)	6099	10655	-1616	73
H(94)	6504	10346	-549	76
H(95)	6711	8884	-159	66
H(97)	8454	7414	-1104	59
H(98)	9298	6293	-1508	74
H(99)	8462	4938	-1873	70
H(100)	6898	4663	-1735	63
H(10A)	5096	4825	-1800	70
H(10B)	4805	5808	-2064	70
H(10C)	3724	5956	-1427	67
H(10D)	3391	5121	-1892	67
H(10E)	4194	4131	-1080	101
H(10F)	3458	4739	-837	101
H(10G)	5075	4570	-57	86

H(10H)	4782	5591	-217	86
H(10I)	6180	4585	-660	80
H(10J)	6454	5430	-204	80
H(10K)	5265	6836	-701	50
H(10L)	5174	7078	-1417	50

Torsion angles [deg] for ljh021_0m.

C(7)-N(1)-C(1)-C(6)	-20.4(13)
C(7)-N(1)-C(1)-C(2)	161.6(8)
C(6)-C(1)-C(2)-C(3)	-1.5(13)
N(1)-C(1)-C(2)-C(3)	176.6(8)
C(1)-C(2)-C(3)-C(4)	0.9(14)
C(2)-C(3)-C(4)-C(5)	-1.7(15)
C(3)-C(4)-C(5)-C(6)	3.1(16)
C(2)-C(1)-C(6)-C(5)	2.8(13)
N(1)-C(1)-C(6)-C(5)	-175.2(8)
C(4)-C(5)-C(6)-C(1)	-3.7(15)
C(1)-N(1)-C(7)-O(1)	-2.7(13)
C(1)-N(1)-C(7)-C(8)	176.8(7)
O(1)-C(7)-C(8)-C(27)	35.6(10)
N(1)-C(7)-C(8)-C(27)	-143.9(6)
O(1)-C(7)-C(8)-C(9)	-89.6(8)
N(1)-C(7)-C(8)-C(9)	91.0(7)
O(1)-C(7)-C(8)-C(15)	143.6(7)
N(1)-C(7)-C(8)-C(15)	-35.9(8)
C(7)-C(8)-C(9)-C(14)	15.7(9)
C(27)-C(8)-C(9)-C(14)	-106.8(8)

C(15)-C(8)-C(9)-C(14)	140.6(7)
C(7)-C(8)-C(9)-C(10)	-172.3(6)
C(27)-C(8)-C(9)-C(10)	65.2(8)
C(15)-C(8)-C(9)-C(10)	-47.3(8)
C(14)-C(9)-C(10)-C(11)	-3.4(11)
C(8)-C(9)-C(10)-C(11)	-175.7(7)
C(9)-C(10)-C(11)-C(12)	3.0(13)
C(10)-C(11)-C(12)-C(13)	0.9(15)
C(11)-C(12)-C(13)-C(14)	-4.4(16)
C(10)-C(9)-C(14)-C(13)	0.1(12)
C(8)-C(9)-C(14)-C(13)	172.0(7)
C(12)-C(13)-C(14)-C(9)	4.0(14)
C(7)-C(8)-C(15)-C(20)	-95.4(6)
C(27)-C(8)-C(15)-C(20)	19.3(6)
C(9)-C(8)-C(15)-C(20)	140.5(6)
C(7)-C(8)-C(15)-C(16)	82.5(8)
C(27)-C(8)-C(15)-C(16)	-162.9(6)
C(9)-C(8)-C(15)-C(16)	-41.7(9)
C(20)-C(15)-C(16)-C(17)	1.6(9)
C(8)-C(15)-C(16)-C(17)	-175.9(6)
C(15)-C(16)-C(17)-C(18)	0.3(10)
C(16)-C(17)-C(18)-C(19)	-0.1(10)
C(17)-C(18)-C(19)-C(20)	-2.0(11)
C(16)-C(15)-C(20)-C(19)	-3.7(9)
C(8)-C(15)-C(20)-C(19)	174.3(5)
C(16)-C(15)-C(20)-C(21)	178.4(5)
C(8)-C(15)-C(20)-C(21)	-3.6(7)
C(18)-C(19)-C(20)-C(15)	3.8(10)
C(18)-C(19)-C(20)-C(21)	-178.6(6)
C(15)-C(20)-C(21)-C(22)	-132.8(7)

C(19)-C(20)-C(21)-C(22)	49.6(9)
C(15)-C(20)-C(21)-C(27)	-13.8(7)
C(19)-C(20)-C(21)-C(27)	168.5(6)
C(15)-C(20)-C(21)-C(26)	105.6(7)
C(19)-C(20)-C(21)-C(26)	-72.0(9)
C(20)-C(21)-C(22)-C(23)	179.0(7)
C(27)-C(21)-C(22)-C(23)	67.0(9)
C(26)-C(21)-C(22)-C(23)	-57.0(9)
C(21)-C(22)-C(23)-C(24)	57.5(10)
C(22)-C(23)-C(24)-C(25)	-56.0(11)
C(23)-C(24)-C(25)-C(26)	55.9(11)
C(24)-C(25)-C(26)-C(21)	-57.2(11)
C(20)-C(21)-C(26)-C(25)	-179.5(7)
C(22)-C(21)-C(26)-C(25)	56.0(9)
C(27)-C(21)-C(26)-C(25)	-67.4(9)
C(7)-C(8)-C(27)-C(21)	87.8(6)
C(9)-C(8)-C(27)-C(21)	-149.6(5)
C(15)-C(8)-C(27)-C(21)	-28.1(6)
C(20)-C(21)-C(27)-C(8)	26.6(6)
C(22)-C(21)-C(27)-C(8)	146.3(6)
C(26)-C(21)-C(27)-C(8)	-92.5(6)
C(34)-N(2)-C(28)-C(29)	178.4(8)
C(34)-N(2)-C(28)-C(33)	3.0(13)
N(2)-C(28)-C(29)-C(30)	-178.4(9)
C(33)-C(28)-C(29)-C(30)	-2.8(12)
C(28)-C(29)-C(30)-C(31)	4.1(16)
C(29)-C(30)-C(31)-C(32)	-5.4(19)
C(30)-C(31)-C(32)-C(33)	5.6(19)
C(31)-C(32)-C(33)-C(28)	-4.4(16)
C(29)-C(28)-C(33)-C(32)	2.8(12)

N(2)-C(28)-C(33)-C(32)	178.1(8)
C(28)-N(2)-C(34)-O(2)	-6.2(13)
C(28)-N(2)-C(34)-C(35)	171.0(7)
O(2)-C(34)-C(35)-C(42)	-141.5(8)
N(2)-C(34)-C(35)-C(42)	41.4(9)
O(2)-C(34)-C(35)-C(36)	93.5(9)
N(2)-C(34)-C(35)-C(36)	-83.6(8)
O(2)-C(34)-C(35)-C(54)	-29.1(10)
N(2)-C(34)-C(35)-C(54)	153.8(6)
C(42)-C(35)-C(36)-C(37)	-139.1(7)
C(34)-C(35)-C(36)-C(37)	-15.4(9)
C(54)-C(35)-C(36)-C(37)	106.4(7)
C(42)-C(35)-C(36)-C(41)	43.8(9)
C(34)-C(35)-C(36)-C(41)	167.5(6)
C(54)-C(35)-C(36)-C(41)	-70.7(8)
C(41)-C(36)-C(37)-C(38)	0.2(11)
C(35)-C(36)-C(37)-C(38)	-176.9(7)
C(36)-C(37)-C(38)-C(39)	1.4(13)
C(37)-C(38)-C(39)-C(40)	-1.1(13)
C(38)-C(39)-C(40)-C(41)	-0.9(14)
C(39)-C(40)-C(41)-C(36)	2.6(13)
C(37)-C(36)-C(41)-C(40)	-2.2(12)
C(35)-C(36)-C(41)-C(40)	175.0(7)
C(34)-C(35)-C(42)-C(43)	-81.9(9)
C(36)-C(35)-C(42)-C(43)	40.2(9)
C(54)-C(35)-C(42)-C(43)	160.4(7)
C(34)-C(35)-C(42)-C(47)	99.6(7)
C(36)-C(35)-C(42)-C(47)	-138.3(6)
C(54)-C(35)-C(42)-C(47)	-18.1(7)
C(47)-C(42)-C(43)-C(44)	-5.3(10)

C(35)-C(42)-C(43)-C(44)	176.4(7)
C(42)-C(43)-C(44)-C(45)	3.5(12)
C(43)-C(44)-C(45)-C(46)	-0.3(13)
C(44)-C(45)-C(46)-C(47)	-1.1(12)
C(45)-C(46)-C(47)-C(42)	-0.6(11)
C(45)-C(46)-C(47)-C(48)	-179.5(7)
C(43)-C(42)-C(47)-C(46)	3.8(10)
C(35)-C(42)-C(47)-C(46)	-177.6(6)
C(43)-C(42)-C(47)-C(48)	-177.1(6)
C(35)-C(42)-C(47)-C(48)	1.5(7)
C(46)-C(47)-C(48)-C(53)	72.6(9)
C(42)-C(47)-C(48)-C(53)	-106.3(7)
C(46)-C(47)-C(48)-C(54)	-165.2(7)
C(42)-C(47)-C(48)-C(54)	15.9(7)
C(46)-C(47)-C(48)-C(49)	-47.2(10)
C(42)-C(47)-C(48)-C(49)	133.9(6)
C(47)-C(48)-C(49)-C(50)	178.2(7)
C(53)-C(48)-C(49)-C(50)	56.3(9)
C(54)-C(48)-C(49)-C(50)	-69.2(8)
C(48)-C(49)-C(50)-C(51)	-56.5(11)
C(49)-C(50)-C(51)-C(52)	52.8(12)
C(50)-C(51)-C(52)-C(53)	-51.8(12)
C(51)-C(52)-C(53)-C(48)	55.1(10)
C(47)-C(48)-C(53)-C(52)	-177.9(7)
C(54)-C(48)-C(53)-C(52)	67.9(9)
C(49)-C(48)-C(53)-C(52)	-55.1(9)
C(47)-C(48)-C(54)-C(35)	-26.8(6)
C(53)-C(48)-C(54)-C(35)	92.6(6)
C(49)-C(48)-C(54)-C(35)	-146.2(6)
C(42)-C(35)-C(54)-C(48)	27.9(6)

C(34)-C(35)-C(54)-C(48)	-90.3(6)
C(36)-C(35)-C(54)-C(48)	149.2(5)
C(61)-N(3)-C(55)-C(60)	-18.9(14)
C(61)-N(3)-C(55)-C(56)	162.4(8)
C(60)-C(55)-C(56)-C(57)	-3.4(13)
N(3)-C(55)-C(56)-C(57)	175.4(8)
C(55)-C(56)-C(57)-C(58)	1.8(15)
C(56)-C(57)-C(58)-C(59)	0.3(16)
C(57)-C(58)-C(59)-C(60)	-0.7(17)
N(3)-C(55)-C(60)-C(59)	-175.7(9)
C(56)-C(55)-C(60)-C(59)	3.0(14)
C(58)-C(59)-C(60)-C(55)	-1.0(16)
C(55)-N(3)-C(61)-O(3)	-4.3(14)
C(55)-N(3)-C(61)-C(62)	174.4(7)
O(3)-C(61)-C(62)-C(69)	147.0(8)
N(3)-C(61)-C(62)-C(69)	-31.8(10)
O(3)-C(61)-C(62)-C(63)	-83.2(10)
N(3)-C(61)-C(62)-C(63)	98.0(8)
O(3)-C(61)-C(62)-C(81)	37.4(11)
N(3)-C(61)-C(62)-C(81)	-141.4(7)
C(69)-C(62)-C(63)-C(64)	139.5(7)
C(61)-C(62)-C(63)-C(64)	11.4(9)
C(81)-C(62)-C(63)-C(64)	-107.9(8)
C(69)-C(62)-C(63)-C(68)	-44.4(9)
C(61)-C(62)-C(63)-C(68)	-172.5(7)
C(81)-C(62)-C(63)-C(68)	68.2(9)
C(68)-C(63)-C(64)-C(65)	2.9(12)
C(62)-C(63)-C(64)-C(65)	178.9(7)
C(63)-C(64)-C(65)-C(66)	-5.5(13)
C(64)-C(65)-C(66)-C(67)	4.6(16)

C(65)-C(66)-C(67)-C(68)	-1.0(17)
C(64)-C(63)-C(68)-C(67)	0.6(14)
C(62)-C(63)-C(68)-C(67)	-175.7(9)
C(66)-C(67)-C(68)-C(63)	-1.6(17)
C(63)-C(62)-C(69)-C(74)	140.0(6)
C(61)-C(62)-C(69)-C(74)	-94.4(7)
C(81)-C(62)-C(69)-C(74)	20.9(7)
C(63)-C(62)-C(69)-C(70)	-41.2(10)
C(61)-C(62)-C(69)-C(70)	84.4(9)
C(81)-C(62)-C(69)-C(70)	-160.3(7)
C(74)-C(69)-C(70)-C(71)	3.2(12)
C(62)-C(69)-C(70)-C(71)	-175.5(8)
C(69)-C(70)-C(71)-C(72)	0.6(14)
C(70)-C(71)-C(72)-C(73)	-5.8(15)
C(71)-C(72)-C(73)-C(74)	7.3(13)
C(70)-C(69)-C(74)-C(73)	-1.8(10)
C(62)-C(69)-C(74)-C(73)	177.1(6)
C(70)-C(69)-C(74)-C(75)	174.3(6)
C(62)-C(69)-C(74)-C(75)	-6.9(8)
C(72)-C(73)-C(74)-C(69)	-3.5(11)
C(72)-C(73)-C(74)-C(75)	-178.8(8)
C(69)-C(74)-C(75)-C(76)	-133.8(8)
C(73)-C(74)-C(75)-C(76)	41.6(11)
C(69)-C(74)-C(75)-C(80)	107.3(8)
C(73)-C(74)-C(75)-C(80)	-77.4(10)
C(69)-C(74)-C(75)-C(81)	-11.2(8)
C(73)-C(74)-C(75)-C(81)	164.2(8)
C(74)-C(75)-C(76)-C(77)	178.4(8)
C(80)-C(75)-C(76)-C(77)	-59.9(11)
C(81)-C(75)-C(76)-C(77)	62.5(11)

C(75)-C(76)-C(77)-C(78)	59.1(13)
C(76)-C(77)-C(78)-C(79)	-51.2(13)
C(77)-C(78)-C(79)-C(80)	49.2(14)
C(78)-C(79)-C(80)-C(75)	-52.3(13)
C(74)-C(75)-C(80)-C(79)	-179.3(9)
C(76)-C(75)-C(80)-C(79)	55.6(11)
C(81)-C(75)-C(80)-C(79)	-67.6(11)
C(74)-C(75)-C(81)-C(62)	24.2(7)
C(76)-C(75)-C(81)-C(62)	148.3(7)
C(80)-C(75)-C(81)-C(62)	-93.1(7)
C(69)-C(62)-C(81)-C(75)	-27.6(7)
C(63)-C(62)-C(81)-C(75)	-150.4(6)
C(61)-C(62)-C(81)-C(75)	90.8(7)
C(88)-N(4)-C(82)-C(87)	4.5(14)
C(88)-N(4)-C(82)-C(83)	-179.9(9)
C(87)-C(82)-C(83)-C(84)	-2.8(16)
N(4)-C(82)-C(83)-C(84)	-178.7(11)
C(82)-C(83)-C(84)-C(85)	-1(2)
C(83)-C(84)-C(85)-C(86)	3(2)
C(84)-C(85)-C(86)-C(87)	-1.5(19)
C(83)-C(82)-C(87)-C(86)	4.5(14)
N(4)-C(82)-C(87)-C(86)	-179.9(9)
C(85)-C(86)-C(87)-C(82)	-2.5(16)
C(82)-N(4)-C(88)-O(4)	-11.0(15)
C(82)-N(4)-C(88)-C(89)	168.1(7)
O(4)-C(88)-C(89)-C(96)	-137.0(9)
N(4)-C(88)-C(89)-C(96)	43.9(10)
O(4)-C(88)-C(89)-C(90)	96.7(10)
N(4)-C(88)-C(89)-C(90)	-82.4(8)
O(4)-C(88)-C(89)-C(108)	-26.1(12)

N(4)-C(88)-C(89)-C(108)	154.7(7)
C(96)-C(89)-C(90)-C(91)	43.5(10)
C(108)-C(89)-C(90)-C(91)	-69.2(10)
C(88)-C(89)-C(90)-C(91)	169.3(8)
C(96)-C(89)-C(90)-C(95)	-143.1(7)
C(108)-C(89)-C(90)-C(95)	104.3(8)
C(88)-C(89)-C(90)-C(95)	-17.3(10)
C(95)-C(90)-C(91)-C(92)	0.1(15)
C(89)-C(90)-C(91)-C(92)	173.8(10)
C(90)-C(91)-C(92)-C(93)	-0.8(19)
C(91)-C(92)-C(93)-C(94)	2.8(17)
C(92)-C(93)-C(94)-C(95)	-4.1(15)
C(93)-C(94)-C(95)-C(90)	3.5(14)
C(91)-C(90)-C(95)-C(94)	-1.3(12)
C(89)-C(90)-C(95)-C(94)	-174.9(8)
C(90)-C(89)-C(96)-C(97)	43.3(10)
C(108)-C(89)-C(96)-C(97)	163.0(8)
C(88)-C(89)-C(96)-C(97)	-80.1(10)
C(90)-C(89)-C(96)-C(101)	-136.7(6)
C(108)-C(89)-C(96)-C(101)	-17.0(7)
C(88)-C(89)-C(96)-C(101)	99.9(7)
C(101)-C(96)-C(97)-C(98)	-3.6(11)
C(89)-C(96)-C(97)-C(98)	176.3(8)
C(96)-C(97)-C(98)-C(99)	5.6(13)
C(97)-C(98)-C(99)-C(100)	-3.2(13)
C(98)-C(99)-C(100)-C(101)	-0.9(13)
C(99)-C(100)-C(101)-C(96)	3.0(11)
C(99)-C(100)-C(101)-C(102)	179.7(8)
C(97)-C(96)-C(101)-C(100)	-0.7(10)
C(89)-C(96)-C(101)-C(100)	179.4(7)

C(97)-C(96)-C(101)-C(102)	-178.0(7)
C(89)-C(96)-C(101)-C(102)	2.1(8)
C(100)-C(101)-C(102)-C(103)	-42.6(12)
C(96)-C(101)-C(102)-C(103)	134.4(7)
C(100)-C(101)-C(102)-C(108)	-162.8(8)
C(96)-C(101)-C(102)-C(108)	14.2(8)
C(100)-C(101)-C(102)-C(107)	77.3(10)
C(96)-C(101)-C(102)-C(107)	-105.7(7)
C(101)-C(102)-C(103)-C(104)	178.3(8)
C(108)-C(102)-C(103)-C(104)	-66.9(10)
C(107)-C(102)-C(103)-C(104)	58.4(10)
C(102)-C(103)-C(104)-C(105)	-60.2(11)
C(103)-C(104)-C(105)-C(106)	54.7(12)
C(104)-C(105)-C(106)-C(107)	-51.5(12)
C(105)-C(106)-C(107)-C(102)	51.2(12)
C(103)-C(102)-C(107)-C(106)	-53.3(10)
C(101)-C(102)-C(107)-C(106)	-178.1(8)
C(108)-C(102)-C(107)-C(106)	70.3(10)
C(103)-C(102)-C(108)-C(89)	-148.2(6)
C(101)-C(102)-C(108)-C(89)	-25.0(7)
C(107)-C(102)-C(108)-C(89)	90.1(7)
C(96)-C(89)-C(108)-C(102)	25.9(7)
C(90)-C(89)-C(108)-C(102)	146.5(6)
C(88)-C(89)-C(108)-C(102)	-92.9(7)