Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Divergent reactivity of Acrylamides and *β*-Chloroenones under Base-Controlled Palladium Catalysis: Construction of Spirooxindoles and Furan-containing 3,3-Disubstituted Oxindoles

Jingli Zhang,‡[a] Weipeng Xu,‡[b] Du Wang,[a] Ye Yuan,[c] Yongqi Bai,[a] Minyan Wang,*[b] Guanbin Gao,*[ac] and Taolei Sun*[a]

[a]Hubei Key Laboratory of Nanomedicine for Neurodegenerative Diseases, School of Chemistry, Chemical Engineering and Life Science, Wuhan University of Technology, Wuhan 430070, China

[b]State Key Laboratory of Coordination Chemistry, School of Chemistry and Chemical Engineering, Nanjing University, Nanjing 210023, China

[c]State Key Laboratory of Advanced Technology for Materials Synthesis and Processing, Wuhan University of Technology, Wuhan 430070, China

E-Mail for Minyan Wang: wangmy@nju.edu.cn
E-Mail for Guanbin Gao: gbgao@whut.edu.cn
E-Mail for Taolei Sun: suntl@whut.edu.cn

Table of Contents

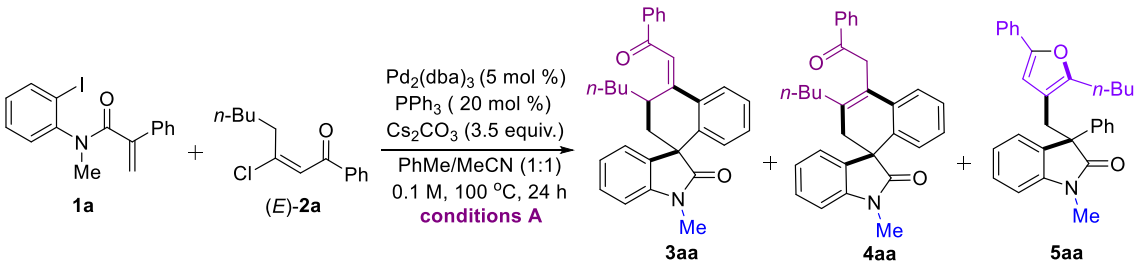
1) General Considerations

Unless stated otherwise, all reactions were carried out under an inert atmosphere of dry argon, using oven-dried glassware (120 ºC), while work-up and isolation of products from catalytic reactions were performed open to air on a benchtop using general techniques. Reaction monitoring was performed using thin-layer chromatography (TLC) on Merck KGaA TLC Silica Gel 60 F_{254} plates. The developed plates were visualized with UV light (254 nm) or $KMnO_4$. Solvent evaporation was carried out by a rotary evaporator at the appropriate temperature and pressure. Toluene was distilled over sodium (1% w:v) and benzophenone (1% w:v); 1,4-dioxane was purchased from Energy Chemical and stored with 3Å molecular sieves; anhydrous *N*,*N*-dimethylformamide was purchased from Aldrich and stored with 3Å molecular sieves; acetonitrile was purchased from Energy Chemical and stored with 3Å molecular sieves. Silica gel flash chromatography was performed on 200-300 mesh silica gel. NMR characterization data was collected at 298 K on a Bruker AVANCE III 500 or a Varian Mercury 400 operating at 400 or 500 MHz for ^{1}H-NMR, 100 or 125 MHz for ^{13}C-NMR, and 470 MHz for ^{19}F-NMR. ^{1}H-NMR chemical shifts were recorded in parts per million (ppm, δ) relative to TMS (δ = 0.00 ppm) with the solvent resonance as the internal standard ($CDCl_3$: δ = 7.26 ppm). Data for ^{1}H-NMR is reported as follows: chemical shift in ppm (δ), multiplicity (s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet), coupling constant (Hz) and integration. ^{13}C-NMR chemical shifts were reported in ppm with the solvent as the internal standard ($CDCl_3$: δ = 77.0 ppm). High-resolution mass spectra were obtained from the following spectrometers: Bruker micrOTOF-Q III (ESI) and JEOL-AccuTOF-DART. Infrared (IR) spectra were recorded on a VERTEX 80v FT-IR spectrophotometer. Data is presented in wavenumbers (cm^{-1}). Melting points were obtained on a SGW® X-4 Melting Point Apparatus and uncorrected.

2) Optimization of Conditions

Optimization procedure for 4aa or 5aa: A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1a** (72.6 mg, 0.20 mmol, 1.0 equiv), Pd catalyst (5 mol % or 10 mol %), ligand (20 mol %, 0.20 equiv.) and anhydrous base (3.0 or 3.5 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed solvent (1.0 mL) was added and the mixture was stirred at room temperature for 5 minutes. *β*-chloroenone (*E*)-**2a** (94.5 mg, 0.4 mmol, 2.0 equiv.) was dissolved in anhydrous solvent (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at the required temperature for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography (15:1 – 5:1 Pentanes: Et_2O) to afford products.

Table S1. Variation of reaction conditions for the formation of major product **4aa**.

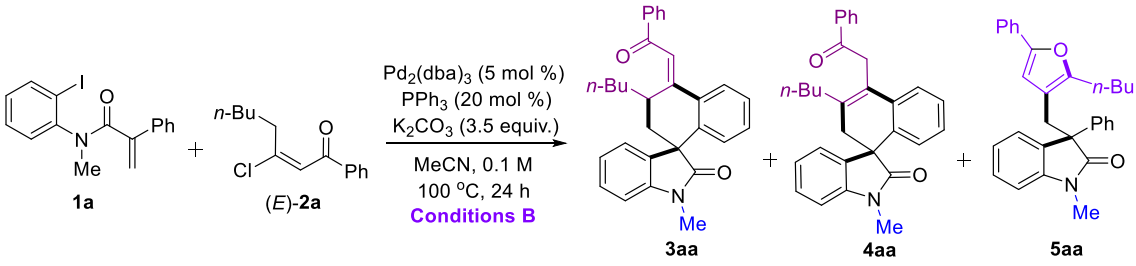


Entry	Variation from conditions A[a]	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[b]
1	none	< 1	(74)	2
2[c]	10 mol % $Pd(dba)_2$ instead of 5 mol % $Pd_2(dba)_3$	< 1	(61)	6
3[c]	10 mol % $Pd(OAc)_2$ instead of 5 mol % $Pd_2(dba)_3$	(13)	(59)	7
4[c]	10 mol % $Pd(PPh_3)_4$ instead of 5 mol % $Pd_2(dba)_3$ and 20 mol % PPh_3	< 1	(48)	3
5[d]	10 mol % $Pd(TFA)_2$ instead of 5 mol % $Pd_2(dba)_3$	(17)	(50)	7
6[d]	10 mol % $[PdCl(allyl)]_2$ instead of 5 mol % $Pd_2(dba)_3$	(28)	(27)	9
7[c]	DPPF instead of PPh_3	-	-	4
8[c]	DPPE instead of PPh_3	-	-	3
9[c]	P(*o*-tol)$_3$ instead of PPh_3	2	(46)	(29)
10[c]	K_2CO_3 instead of Cs_2CO_3	4	< 1	(70)
11[c]	EtN_3 instead of Cs_2CO_3	< 1	< 1	(66)
12[c]	C_sOPiv instead of Cs_2CO_3	4	2	(22)

13	PhMe instead of PhMe/MeCN (1: 1)	6	9	(14)
14	MeCN instead of PhMe/MeCN (1: 1)	5	(67)	8
15	Dioxane instead of PhMe/MeCN (1: 1)	< 1	(53)	8
16	DMF instead of PhMe/MeCN (1: 1)	1	(17)	2
17	2.5 mol % $Pd_2(dba)_3$ and 10 mol % PPh_3	5	(42)	(19)
18	3.0 equiv. Cs_2CO_3 instead of 3.5 equiv. Cs_2CO_3	(31)	(27)	4
19	0.05 M instead of 0.1 M	3	(47)	8
20	0.2 M instead of 0.1 M	< 1	(61)	6
21	80 °C instead of 100 °C	(12)	(61)	3
22	120 °C instead of 100 °C	< 1	8	(27)
23	-Br instead of -I	< 1	(68)	< 1
24[e]	(*Z*)-**2a** instead of (*E*)-**2a**	< 1	(28)	2

[a]Reaction conditions: **1a** (0.2 mmol), (*E*)-**2a** (0.4 mmol), catalyst (5 mol %), ligand (20 mol %), base (3.5 equiv.), solvent (2.0 mL), 100 °C, 24 h, sealed vial. [b]Yields were determined by ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard. Values in parentheses indicate isolated yields. [c]The reaction was performed in MeCN. [d]The reaction was performed at 90 °C. [e]Less reactivity observed of (*Z*)-**2a** might be due to the slower dehydrochlorination of (*Z*)-**2a.**[1]

Table S2. Variation of reaction conditions for the formation of major product **5aa**.



Entry	Variation from conditions B[a]	**3aa** (%)[b]	**4aa** (%)[b]	**5aa** (%)[b]
1	none	4	< 1	(70)
2[c]	10 mol % $Pd(OAc)_2$ and 20 mol % Johnphos	4	< 1	(40)
3[c]	10 mol % $Pd(dba)_2$ and 20 mol % P(*o*-CF_3Ph)$_3$	7	2	(58)
4[c]	10 mol % $[PdCl(allyl)]_2$ and 20 mol % P(*o*-CF_3Ph)$_3$	< 1	< 1	(41)
5[c]	5 mol % $Pd_2(dba)_3$ and 20 mol % P(*o*-CF_3Ph)$_3$	6	7	(54)
6	10 mol % $PdCl_2$ instead of 5 mol % $Pd_2(dba)_3$	< 1	< 1	(43)
7	EtN_3 instead of K_2CO_3	< 1	< 1	(66)
8	C_sOPiv instead of K_2CO_3	4	2	(22)
9	PhMe/MeCN (1: 1) instead of MeCN	2	3	(49)

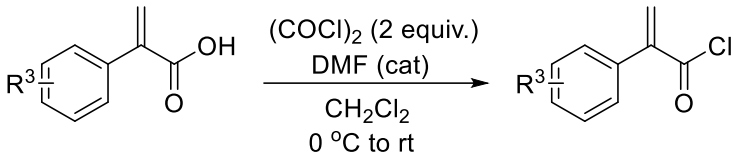
10	Dioxane instead of MeCN	2	2	(30)
11	2.5 mol % $Pd_2(dba)_3$ and 10 mol % PPh_3	< 1	< 1	(52)
12	3.0 equiv. K_2CO_3 instead of 3.5 equiv. K_2CO_3	< 1	3	(58)
13	0.05 M instead of 0.1 M	< 1	-	(69)
14	0.2 M instead of 0.1 M	2	4	(64)
15	80 °C instead of 100 °C	2	-	(43)
16	120 °C instead of 100 °C	3	2	(57)
17	-Br instead of -I	-	3	(33)
18[d]	(*Z*)-**2a** instead of (*E*)-**2a**	-	2	(10)

[a]Reaction conditions: **1a** (0.2 mmol), (*E*)-**2a** (0.4 mmol), catalyst (5 mol %), ligand (20 mol %), base (0.7 mmol), solvent (2.0 mL), 100 °C, 24 h, sealed vial. [b]Yields were determined by ^{1}H NMR analysis using 1,3,5-trimethoxybenzene as an internal standard. Values in parentheses indicate isolated yields. [c]Reaction conditions: **1a** (0.2 mmol), (*E*)-**2a** (0.4 mmol), catalyst (5 mol % or 10 mol %), ligand (20 mol %), Cs_2CO_3 (0.7 mmol), PhMe/MeCN (1:1, 2.0 mL), 90 °C, 22 h, sealed vial. [d]Less reactivity observed of (*Z*)-**2a** might be due to the slower dehydrochlorination of (*Z*)-**2a.**[1]

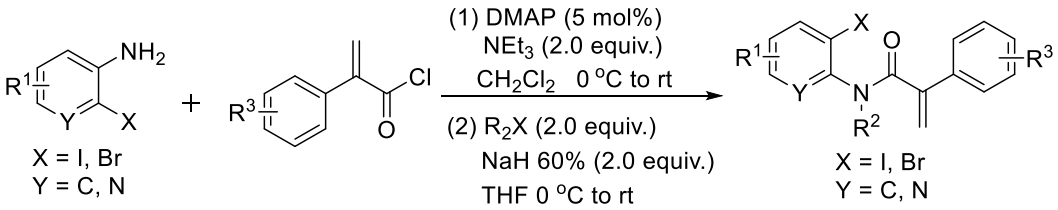
3) General procedures

All standard reagents were purchased from Sigma Aldrich, TCI, Aladdin, Energy Chemical, and were used without further purification. Acrylamides and *β*-chloroenones were prepared according to literature procedures.

General Procedure 1: Synthesis of acrylamides
The desired acrylamide was prepared following literature procedure.



Oxalyl chloride (2.0 equiv.) was added dropwise to a solution of substituted 2-phenylacrylic acid (1.0 equiv.) and DMF (4 drops) in CH_2Cl_2 (0.4 M) at 0°C. After 5 minutes, the reaction was allowed to warm to room temperature and stirred until the reaction was completed by TLC. The excess oxalyl chloride was removed under vacuum and the resulting acyl chloride was redissolved in CH_2Cl_2.

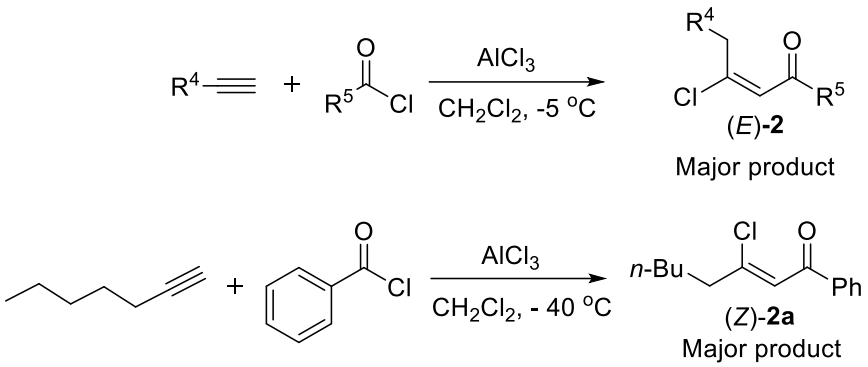


A solution of the substituted 2-iodoaniline or 2-bromoaniline (1.0 equiv.), DMAP (0.05 equiv.) and NEt_3 (2.0 equiv.) was prepared in CH_2Cl_2 (0.5 M) and cooled to 0 °C. The acyl chloride solution was added dropwise into the solution. After 5 minutes, the reaction was allowed to warm to room temperature and stirred overnight. The reaction was quenched with a saturated $NaHCO_3$ solution and extracted with CH_2Cl_2 (3x). The combined organic layers were washed with brine, dried over Na_2SO_4 and concentrated *in vacuo*. The crude unsubstituted acrylamide was used in the next step without further purification.

A solution of the unsubstituted acrylamide (1.0 equiv.) in THF (0.2 M) was prepared and cooled to 0 °C. NaH (60 % in mineral oil, 2.0 equiv.) was added to the solution and the mixture was stirred at 0 °C. After stirring for 20 min, R^2-X (2.0 equiv.) was added dropwise and the reaction mixture was allowed to warm to room temperature and stirred overnight. After completion of the reaction (monitored by TLC), the reaction was quenched with water and extracted with EtOAc (3x). The combined organic layers were washed with brine, dried with anhydrous Na_2SO_4 and concentrated *in vacuo*. The crude product was purified by silica gel flash column chromatography using the indicated mobile phase.

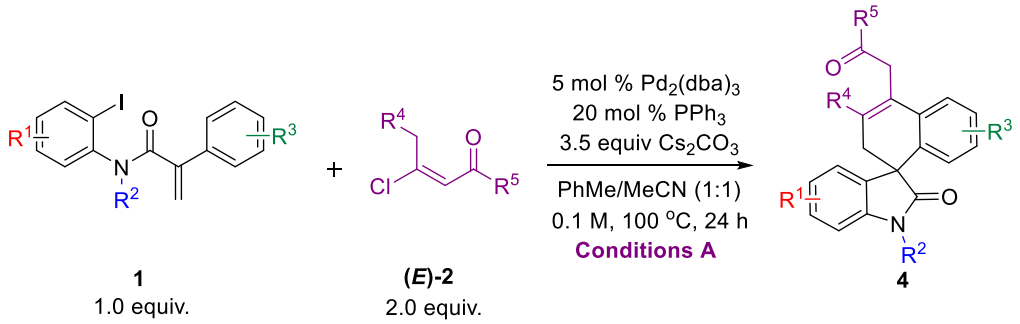
General Procedure 2: Synthesis of *β*-chloroenones

The desired *β*-chloroenone was prepared following literature procedure.



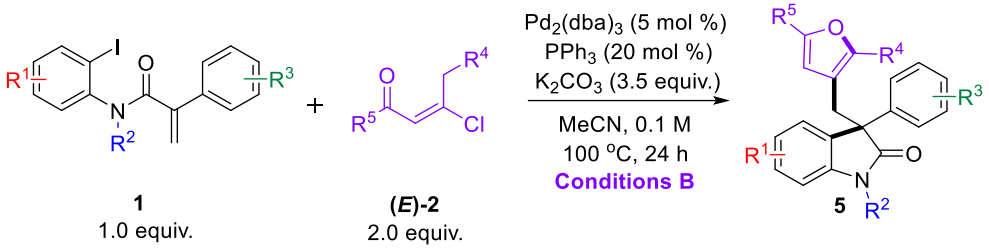
To a stirred suspension of aluminum chloride (1.47 g, 11 mmol, 1.1 equiv.) in dry dichloromethane (10 mL) at -5 °C (*E*-selective) or -40 °C (*Z*-selective) were added alkynes (10 mmol, 1.0 equiv.) and acyl chloride (10 mmol, 1.0 equiv.) dropwise at the same time. Stirring of the resulting solution was continued at the same temperature until the reaction was completed by TLC. The reaction was then quenched with H_2O, extracted with dichloromethane, and washed with brine. After drying over $MgSO_4$, the solution was concentrated under reduced pressure, and the crude product was purified by silica gel flash column chromatography using the indicated mobile phase.

General Procedure 3: Synthesis of spirooxindoles



A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1** (0.20 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol, 5 mol %), PPh_3 (10.5 mg, 0.04 mmol, 20 mol %) and Cs_2CO_3 (228.1 mg, 0.7 mmol, 3.5 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed PhMe (0.5 mL) and MeCN (0.5 mL) were added and the mixture was stirred at room temperature for 5 minutes. (*E*)-*β*-chloroenone **2** (0.4 mmol, 2.0 equiv.) was dissolved in anhydrous PhMe: MeCN (1:1) (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using the indicated mobile phase.

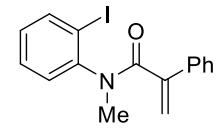
General Procedure 4: Synthesis of 3,3-disubstituted furan-containing oxindoles



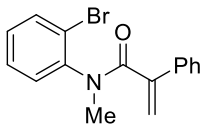
A flame-dried, 3-dram vial under argon atmosphere was charged with acrylamide **1** (0.20 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol, 5 mol %), PPh_3 (10.5 mg, 0.04 mmol, 20 mol %) and K_2CO_3 (96.7 mg, 0.7 mmol, 3.5 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed MeCN (1.0 mL) were added and the mixture was stirred at room temperature for 5 minutes. (*E*)-*β*-chloroenone **2** (0.4 mmol, 2.0 equiv.) was dissolved in anhydrous MeCN (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using the indicated mobile phase.

4) Synthesis of acrylamides

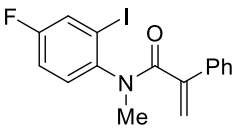
All acrylamides were synthesized according to literature procedures. [2]



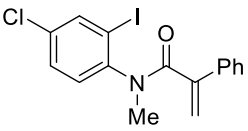
1a



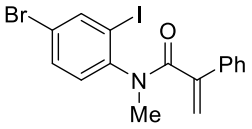
1a'



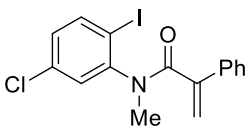
1b



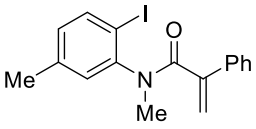
1c



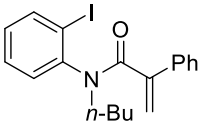
1d



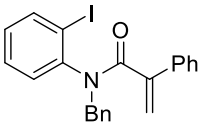
1e



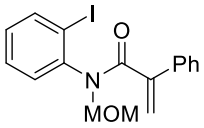
1f



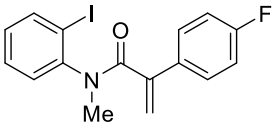
1g



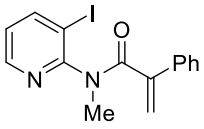
1h



1i



1j



1k

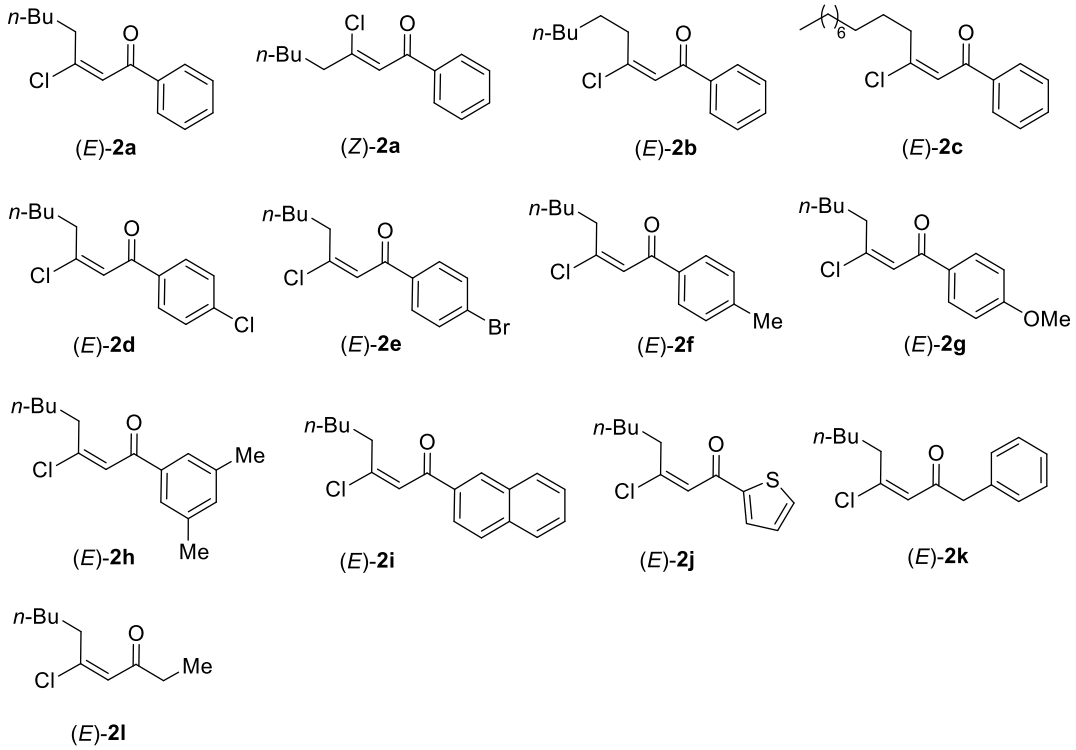
1a, **1b**, **1d**, **1e**, **1h**, **1i**, **1j:** H. Yoon, A. Lossouarn, F. Landau, M. Lautens, *Org. Lett.* **2016**, 18, 6324-6327.

1a', **1c**, **1f**, **1g:** C. Shao, Z. Wu, X. Ji, B. Zhou, Y. Zhang, *Chem. Commun*. **2017**, 53, 10429-10432.

1k: G. Xiao, L. Chen, G. Deng, J. Liu, Y. Liang, *Tetrahedron Lett*. **2018**, 59, 1836-1840.

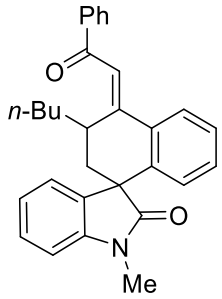
5) Synthesis of *β*-chloroenones

All *β*-chloroenones were synthesized according to literature procedures. [1,3]



(*E*)-**2a**, (*Z*)-**2a**, (*E*)-**2c**, (*E*)-**2e**, (*E*)-**2f**, (*E*)-**2g**, (*E*)-**2k**, (*E*)-**2l:** H. Y. Kim, J.-Y. Li, K. Oh, *J. Org. Chem.* **2012**, *77*, 11132-11145.
(*E*)-**2b:** T. Kashiwabara, M. Tanaka, *Adv. Synth. Catal.* **2011**, *353*, 1485-1490.
(*E*)-**2d**, (*E*)-**2h**: Y. Zhang, J. Zhang, Y. Yuan, L. Liu, B. Chen, T. Sun, *Eur. J. Org. Chem.* **2020**, 1976-1986.
(*E*)-**2i**, (*E*)-**2j:** R. Hou, Z. Wang, J. Peng, Y. Yuan, J. Zhang, D. Wang, T. Sun, *Asian J. Org. Chem.* **2021**, 10, 3334-3342.

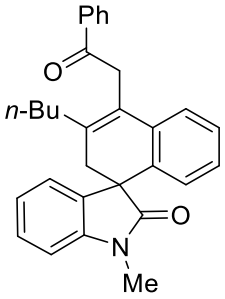
6) Synthesis of spirooxindoles



(*E*)-3'-Butyl-1-methyl-4'-(2-oxo-2-phenylethylidene)-3',4'-dihydro-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (3aa)

Prepared according to General Procedure **3** or **4** using starting material **1a** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (< 1% - 28 % yields).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.99 (d, J = 7.2 Hz, 2H), 7.41 (t, J = 7.4 Hz, 1H), 7.36-7.29 (m, 3H), 7.16 (d, J = 8.0 Hz, 1H), 7.12-7.06 (m, 2H), 6.95 (t, J = 7.6 Hz, 1H), 6.93 (t, J = 8.0 Hz, 1H), 6.84 (t, J = 7.6 Hz, 1H), 6.46 (d, J = 8.8 Hz, 2H), 3.41-3.33 (m, 1H), 3.27 (s, 3H), 2.42 (dd, J_1 = 13.6 Hz, J_2 = 4.6 Hz, 1H), 2.01 (dd, J_1 = 13.6 Hz, J_2 = 11.0 Hz, 1H), 1.89-1.80 (m, 1H), 1.56-1.48 (m, 1H), 1.47-1.32 (m, 4H), 0.92 (t, J = 7.2 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 196.5, 179.0, 153.0, 143.6, 137.8, 136.7, 135.7, 135.6, 132.5, 130.5, 129.3, 129.3, 128.3, 128.2, 127.0, 126.6, 124.0, 123.2, 121.6, 108.1, 52.1, 40.2, 38.7, 33.8, 29.1, 26.4, 22.8, 14.0. **IR** (neat, cm^{-1}): ν 3057, 3032, 2956, 2929, 2871, 1713, 1612, 1494, 1470, 1374, 1349, 1254, 1186, 1081, 1023, 949, 932, 813, 759, 694. **HRMS** (DART): *m/z* calcd for $C_{30}H_{29}NO_2$+H^+: 436.2271 $[M+H]^+$; found: 436.2279.

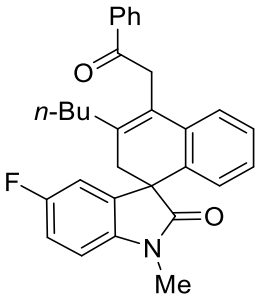


3'-Butyl-1-methyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4aa)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (64.4 mg, 0.148 mmol, 74 % yield, MP = 71-72 °C).

^{1}H NMR (400 MHz, $CDCl_3$) δ 8.13 (d, J = 8.0 Hz, 2H), 7.74 (d, J = 7.6 Hz, 1H), 7.63

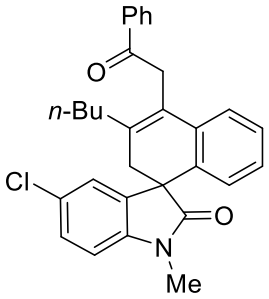
(t, J = 7.6 Hz, 1H), 7.54 (t, J = 7.6 Hz, 2H), 7.24 (t, J = 7.6 Hz, 1H), 7.07 (t, J = 8.0 Hz, 2H), 7.01 (d, J = 7.2 Hz, 1H), 6.97 (d, J = 7.2 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.77 (d, J = 7.6 Hz, 1H), 4.51 (d, J = 18.0 Hz, 1H), 4.30 (d, J = 18.0 Hz, 1H), 3.36 (s, 3H), 3.23 (d, J = 16.4 Hz, 1H), 2.34 (d, J = 16.4 Hz, 1H), 2.28-2.15 (m, 2H), 1.39-1.31 (m, 2H), 1.30-1.24 (m, 2H), 0.82 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 197.6, 180.3, 141.3, 137.0, 136.4, 135.0, 134.7, 134.2, 133.3, 128.8, 128.2, 128.0, 127.7, 127.1, 125.7, 124.4, 124.3, 123.5, 123.1, 108.1, 52.7, 38.5, 37.8, 34.5, 29.4, 26.6, 22.7, 13.9. **IR** (neat, cm^{-1}): ν 3056, 3025, 2955, 2929, 2869, 1712, 1686, 1609, 1597, 1491, 1469, 1373, 1348, 1212, 1128, 1090, 989, 754, 690. **HRMS** (DART): *m/z* calcd for $C_{30}H_{29}NO_2+H^+$: 436.2271 $[M+H]^+$; found: 436.2278.



3'-Butyl-5-fluoro-1-methyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ba)

Prepared according to General Procedure **3** using starting material **1b** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (67.1 mg, 0.148 mmol, 74 % yield, MP = 184-185 ºC).

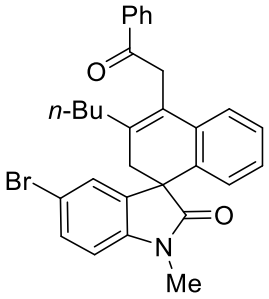
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.14 (d, J = 7.5 Hz, 2H), 7.71 (dd, J_1 = 8.5 Hz, J_2 = 2.5 Hz, 1H), 7.63 (t, J = 7.3 Hz, 1H), 7.54 (t, J = 7.5 Hz, 2H), 7.11 (t, J = 7.5 Hz, 1H), 7.06 (d, J = 7.5 Hz, 1H), 7.02 (t, J = 7.3 Hz, 1H), 6.94 (td, J_1 = 8.8 Hz, J_2 = 2.5 Hz, 1H), 6.80 (dd, J_1 = 8.8 Hz, J_2 = 4.0 Hz, 1H), 6.78 (d, J = 7.5 Hz, 1H), 4.53 (d, J = 17.5 Hz, 1H), 4.29 (d, J = 18.0 Hz, 1H), 3.35 (s, 3H), 3.26 (d, J = 16.5 Hz, 1H), 2.30 (d, J = 16.5 Hz, 1H), 2.26-2.15 (m, 2H), 1.40-1.31 (m, 2H), 1.30-1.25 (m, 2H), 0.83 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.4, 180.0, 159.4 (d, J = 239.0 Hz), 137.3 (d, J = 1.8 Hz), 136.9, 136.2, 135.5 (d, J = 8.6 Hz), 134.9, 134.2, 133.3, 128.8, 128.2, 128.0, 127.2, 125.7, 124.6, 123.6, 114.3 (d, J = 23.8 Hz), 112.8 (d, J = 25.4 Hz), 108.5 (d, J = 7.9 Hz), 53.1, 38.4, 37.6, 34.5, 29.4, 26.7, 22.7, 13.8. **^{19}F NMR** (470 MHz, $CDCl_3$): δ -114.49 – -114.53 (m, 1F). **IR** (neat, cm^{-1}): ν 3057, 2956, 2930, 2870, 1703, 1686, 1622, 1492, 1449, 1359, 1276, 1209, 1124, 994, 907, 818, 768, 688. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}FNO_2+Na^+$: 476.1996 $[M+Na]^+$; found: 476.1999.



3'-Butyl-5-chloro-1-methyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ca)

Prepared according to General Procedure **3** using starting material **1c** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (63.8 mg, 0. 136 mmol, 68 % yield, MP = 80-82 °C).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.5 Hz, 2H), 7.89 (d, *J* = 1.5 Hz, 1H), 7.63 (t, *J* = 7.3 Hz, 1H), 7.54 (t, *J* = 7.5 Hz, 2H), 7.22 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.5 Hz, 1H), 7.01 (t, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 8.5 Hz, 1H), 6.76 (d, *J* = 7.5 Hz, 1H), 4.52 (d, *J* = 17.5 Hz, 1H), 4.29 (d, *J* = 18.0 Hz, 1H), 3.34 (s, 3H), 3.24 (d, *J* = 16.0 Hz, 1H), 2.30 (d, *J* = 16.5 Hz, 1H), 2.26-2.14 (m, 2H), 1.39-1.32 (m, 2H), 1.31-1.26 (m, 2H), 0.83 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.3, 179.8, 140.0, 137.0, 136.2, 135.5, 135.1, 134.1, 133.3, 128.8, 128.3, 128.2, 128.1, 128.0, 127.2, 125.7, 125.0, 124.7, 123.7, 109.1, 52.9, 38.5, 37.7, 34.4, 29.5, 26.7, 22.7, 13.9. **IR** (neat, cm^{-1}): ν 3061, 3026, 2955, 2929, 2870, 1716, 1688, 1607, 1487, 1420, 1344, 1213, 1104, 989, 810, 754, 690. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}ClNO_2$+Na^+: 492.1701 $[M+Na]^+$; found: 492.1692.

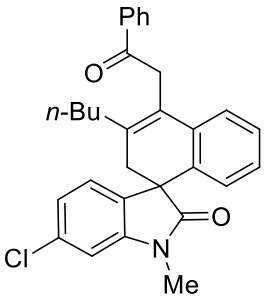


5-Bromo-3'-butyl-1-methyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4da)

Prepared according to General Procedure **3** using starting material **1d** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (50.3 mg, 0.098 mmol, 49 % yield, MP = 83-84 °C).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.15 (d, *J* = 7.5 Hz, 2H), 8.02 (d, *J* = 2.0 Hz, 1H), 7.63 (t, *J* = 7.5 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.38 (dd, J_1 = 8.3 Hz, J_2 = 2.0 Hz, 1H), 7.11 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.76 (d, *J* = 8.5 Hz, 1H), 6.75 (d, *J* = 8.5 Hz, 1H), 4.51 (d, *J* = 18.0 Hz, 1H), 4.29 (d, *J* = 18.5 Hz,

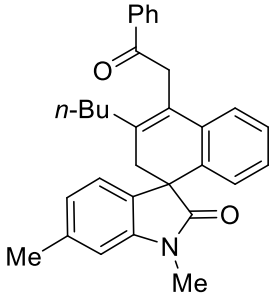
1H), 3.34 (s, 3H), 3.23 (d, J = 16.5 Hz, 1H), 2.30 (d, J = 16.0 Hz, 1H), 2.27-2.21 (m, 1H), 2.20-2.14 (m, 1H), 1.38-1.31 (m, 2H), 1.30-1.25 (m, 2H), 0.83 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.2, 179.7, 140.5, 137.0, 136.1, 135.8, 135.1, 134.0, 133.3, 130.9, 128.8, 128.2, 128.1, 127.7, 127.2, 125.7, 124.7, 123.7, 115.7, 109.6, 52.8, 38.5, 37.7, 34.4, 29.5, 26.7, 22.7, 13.9. **IR** (neat, cm^{-1}): ν 3060, 3026, 2955, 2928, 2869, 1716, 1687, 1604, 1485, 1417, 1342, 1250, 1212, 1103, 989, 808, 754, 690. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}BrNO_2$+Na^+: 536.1196 $[M+Na]^+$; found: 536.1194.



3'-Butyl-6-chloro-1-methyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ea)

Prepared according to General Procedure **3** using starting material **1e** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (61.9 mg, 0.132 mmol, 66 % yield, MP = 86-88 °C).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.11 (d, J = 7.0 Hz, 2H), 7.75 (d, J = 8.0 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.54 (t, J = 7.5 Hz, 2H), 7.10 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.06 (dd, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.01 (td, J_1 = 7.3 Hz, J_2 = 1.5 Hz, 1H), 6.95 (dd, J_1 = 8.0 Hz, J_2 = 2.0 Hz, 1H), 6.88 (d, J = 2.0 Hz, 1H), 6.75 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz, 1H), 4.52 (dd, J_1 = 18.0 Hz, J_2 = 2.0 Hz, 1H), 4.28 (d, J = 18.0 Hz, 1H), 3.34 (s, 3H), 3.22 (d, J = 16.5 Hz, 1H), 2.28 (d, J = 16.5 Hz, 1H), 2.25-2.13 (m, 2H), 1.37-1.30 (m, 2H), 1.29-1.25 (m, 2H), 0.82 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.3, 142.6, 136.9, 136.2, 134.9, 134.2, 133.8, 133.3, 132.5, 128.8, 128.1, 127.9, 127.2, 125.6, 125.5, 124.5, 123.6, 122.8, 108.8, 52.4, 38.5, 37.7, 34.4, 29.4, 26.7, 22.7, 13.8. **IR** (neat, cm^{-1}): ν 3060, 3026, 2955, 2928, 2870, 1719, 1686, 1605, 1492, 1447, 1369, 1322, 1245, 1212, 1078, 958, 840, 753, 690. **HRMS** (DART): *m/z* calcd for $C_{30}H_{28}ClNO_2$+H^+: 470.1881 $[M+H]^+$; found: 470.1889.

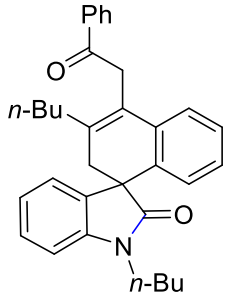


3'-Butyl-1,6-dimethyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-

naphthalen]-2-one (4fa)

General Procedure **3** using starting material **1f** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (66.5 mg, 0.148 mmol, 74 % yield, MP = 78-80 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 7.5 Hz, 2H), 7.63 (t, J = 7.5 Hz, 1H), 7.57 (d, J = 8.0 Hz, 1H), 7.53 (t, J = 7.5 Hz, 2H), 7.08 (td, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.05 (d, J = 6.5 Hz, 1H), 6.98 (td, J_1 = 7.5 Hz, J_2= 1.5 Hz, 1H), 6.78 (d, J = 7.5 Hz, 1H), 6.75 (d, J = 7.5 Hz, 1H), 6.71 (s, 1H), 4.49 (dd, J_1 = 18.0 Hz, J_2 = 1.0 Hz, 1H), 4.28 (d, J = 18.0 Hz, 1H), 3.34 (s, 3H), 3.20 (d, J = 16.0 Hz, 1H), 2.35 (s, 3H), 2.32 (d, J = 16.5 Hz, 1H), 2.26-2.15 (m, 2H), 1.39-1.32 (m, 2H), 1.31-1.24 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.6, 141.5, 138.0, 137.2, 136.5, 135.0, 135.0, 133.2, 131.5, 128.8, 128.2, 127.6, 127.1, 125.7, 124.3, 124.1, 123.5, 123.5, 109.0, 52.5, 38.6, 37.9, 34.5, 29.4, 26.5, 22.8, 21.8, 13.8. **IR** (neat, cm^{-1}): ν 3058, 3026, 2955, 2928, 2870, 1711, 1688, 1616, 1467, 1448, 1373, 1326, 1253, 1094, 989, 818, 755, 735, 690. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+Na^+: 472.2247 $[M+Na]^+$; found: 472.2247.

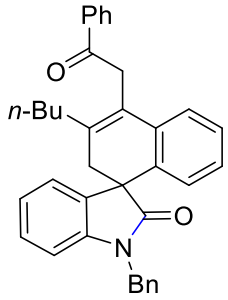


1,3'-Dibutyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ga)

Prepared according to General Procedure **3** using starting material **1g** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (70.5 mg, 0.148 mmol, 74 % yield, MP = 110-112 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 7.0 Hz, 2H), 7.72 (d, J = 7.0 Hz, 1H), 7.63 (t, J = 7.3 Hz, 1H), 7.53 (t, J = 7.5 Hz, 2H), 7.22 (td, J_1 = 7.8 Hz, J_2 = 1.0 Hz, 1H), 7.09 (td, J_1 = 7.3 Hz, J_2 = 1.0 Hz, 1H), 7.05 (d, J = 6.5 Hz, 1H), 7.00 (td, J_1 = 7.3 Hz, J_2= 1.0 Hz, 1H), 6.95 (td, J_1 = 7.5 Hz, J_2= 0.5 Hz, 1H), 6.89 (d, J = 7.5 Hz, 1H), 6.76 (dd, J_1 = 7.8 Hz, J_2= 1.0 Hz, 1H), 4.50 (dd, J_1 = 18.3 Hz, J_2= 1.0 Hz, 1H), 4.30 (d, J = 18.0 Hz, 1H), 3.90-3.78 (m, 2H), 3.22 (d, J = 16.5 Hz, 1H), 2.32 (d, J = 16.5 Hz, 1H), 2.25-2.15 (m, 2H), 1.81-1.74 (m, 2H), 1.51-1.44 (m, 2H), 1.39-1.32 (m, 2H), 1.31-1.23 (m, 2H), 1.01 (t, J = 7.5 Hz, 3H), 0.82 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.0, 140.8, 137.0, 136.4, 135.0, 134.8, 134.4, 133.2, 128.8, 128.2, 127.9, 127.7, 127.1, 125.7, 124.5, 124.2, 123.5, 122.7, 108.4, 52.5, 40.1, 38.6, 37.8, 34.5, 29.7, 29.4, 22.8, 20.3, 13.9, 13.8. **IR** (neat, cm^{-1}): ν 3055, 3027, 2956, 2927, 2869, 1707, 1686, 1607,

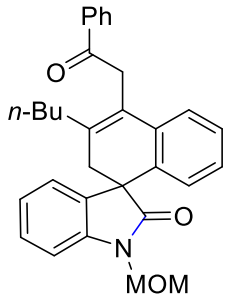
1486, 1464, 1447, 1359, 1208, 1098, 991, 931, 749, 689. **HRMS** (ESI): *m/z* calcd for $C_{33}H_{35}NO_2$+Na^+: 500.2560 $[M+Na]^+$; found: 500.2564.



1-Benzyl-3'-butyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ha)

Prepared according to General Procedure **3** using starting material **1h** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (71.6 mg, 0.14 mmol, 70 % yield, MP = 69-70 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (d, J = 7.5 Hz, 2H), 7.71 (d, J = 7.0 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.54 (t, J = 7.8 Hz, 2H), 7.38 (t, J = 7.3 Hz, 2H), 7.36 (t, J = 7.5 Hz, 2H), 7.30 (d, J = 7.0 Hz, 1H), 7.13 (dd, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 7.10 (dd, J_1 = 6.5 Hz, J_2= 1.5 Hz, 1H), 7.07 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 7.01 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 6.93 (td, J_1 = 7.5 Hz, J_2 = 0.5 Hz, 1H), 6.81 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.78 (d, J = 8.0 Hz, 1H), 5.07 (d, J = 15.5 Hz, 1H), 5.03 (d, J = 15.5 Hz, 1H), 4.51 (dd, J_1 = 18.0 Hz, J_2 = 1.5 Hz, 1H), 4.31 (d, J = 18.0 Hz, 1H), 3.27 (d, J = 16.5 Hz, 1H), 2.40 (d, J = 16.5 Hz, 1H), 2.25-2.19 (m, 2H), 1.40-1.32 (m, 2H), 1.31-1.26 (m, 2H), 0.83 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.3, 140.6, 137.0, 136.4, 136.1, 135.1, 134.7, 134.2, 133.3, 128.8, 128.8, 128.2, 127.9, 127.8, 127.6, 127.4, 127.2, 125.8, 124.5, 124.4, 123.6, 123.0, 109.1, 52.6, 44.0, 38.8, 37.9, 34.5, 29.4, 22.8, 13.9. **IR** (neat, cm^{-1}): ν 3059, 3028, 2955, 2927, 2857, 1712, 1688, 1609, 1597, 1486, 1465, 1448, 1380, 1347, 1210, 1105, 1080, 1001, 940, 755, 692. **HRMS** (ESI): *m/z* calcd for $C_{36}H_{33}NO_2$+H^+: 512.2584 $[M+H]^+$; found: 512.2580.

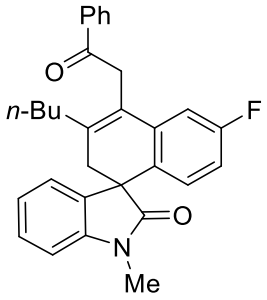


3'-Butyl-1-(methoxymethyl)-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ia)

Prepared according to General Procedure **3** using starting material **1i** and (*E*)-*β*-

chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (74.4 mg, 0.16 mmol, 80 % yield, MP = 58-60 ºC).

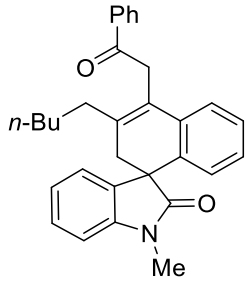
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (dd, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 2H), 7.72 (d, J = 7.5 Hz, 1H), 7.63 (t, J = 7.5 Hz, 1H), 7.54 (t, J = 7.5 Hz, 2H), 7.24 (td, J_1 = 7.5 Hz, J_2 =1.0 Hz, 1H), 7.11 (td, J_1 = 8.0 Hz, J_2 = 1.5 Hz, 1H), 7.07 (t, J = 7.5 Hz, 2H), 7.01 (t, J = 7.5 Hz, 2H), 6.78 (dd, J_1 = 7.8 Hz, J_2 = 1.0 Hz, 1H), 5.28 (d, J = 10.5 Hz, 1H), 5.25 (d, J = 11.0 Hz, 1H), 4.50 (dd, J_1 = 18.0 Hz, J_2 = 1.5 Hz, 1H), 4.31 (d, J = 18.0 Hz, 1H), 3.44 (s, 3H), 3.21 (d, J = 16.0 Hz, 1H), 2.41 (d, J = 16.5 Hz, 1H), 2.26-2.15 (m, 2H), 1.39-1.32 (m, 2H), 1.30-1.24 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.9, 139.7, 137.0, 136.2, 135.1, 134.4, 133.7, 133.3, 128.8, 128.2, 128.1, 127.9, 127.1, 125.8, 124.6, 124.4, 123.7, 123.5, 109.5, 71.6, 56.4, 53.0, 39.0, 37.9, 34.5, 29.4, 22.8, 13.9. **IR** (neat, cm^{-1}): ν 3059, 2930, 2865, 1718, 1685, 1603, 1459, 1340, 1207, 1077, 986, 914, 748, 689. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_3$+Na^+: 488.2196 $[M+Na]^+$; found: 488.2200.



3'-Butyl-6'-fluoro-1-methyl-4'-(2-oxo-2-phenylethyl)-2'H-spiro[indoline-3,1'-naphthalen]-2-one (4ja)

Prepared according to General Procedure **3** using starting material **1j** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (39.9 mg, 0.088 mmol, 44 % yield, MP = 125-126 ºC).

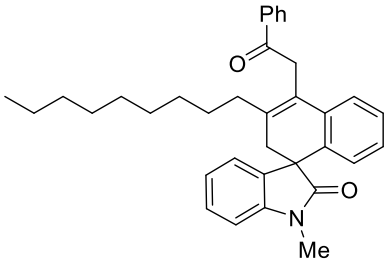
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, J = 7.5 Hz, 2H), 7.74 (d, J = 7.5 Hz, 1H), 7.64 (t, J = 7.5 Hz, 1H), 7.55 (t, J = 7.8 Hz, 2H), 7.26 (t, J = 7.5 Hz, 1H), 7.00 (t, J = 7.5 Hz, 1H), 6.89 (d, J = 7.5 Hz, 1H), 6.77-6.71 (m, 2H), 6.69 (td, J_1 = 8.5 Hz, J_2 = 2.0 Hz, 1H), 4.43 (d, J = 18.5 Hz, 1H), 4.30 (d, J = 18.5 Hz, 1H), 3.35 (s, 3H), 3.20 (d, J = 16.5 Hz, 1H), 2.36 (d, J = 16.5 Hz, 1H), 2.26-2.14 (m, 2H), 1.37-1.30 (m, 2H), 1.29-1.22 (m, 2H), 0.81 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.3, 180.0, 162.4 (d, J = 242.8 Hz), 141.3, 138.1, 137.5 (d, J = 7.4 Hz), 136.8, 134.0, 133.4, 130.3, 130.3, 128.9, 128.2, 127.2 (d, J = 8.4 Hz), 124.3, 123.8, 123.2, 113.4 (d, J = 21.4 Hz), 110.7 (d, J = 22.9 Hz), 108.2, 52.1, 38.7, 37.8, 34.5, 29.3, 26.6, 22.7, 13.8. **^{19}F NMR** (470 MHz, $CDCl_3$): δ -114.48 – -114.54 (m, 1F). **IR** (neat, cm^{-1}): ν 3058, 2956, 2930, 2870, 1709, 1686, 1607, 1493, 1471, 1374, 1350, 1216, 1171, 1129, 1091, 988, 908, 862, 759, 692. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}FNO_2$+Na^+: 476.1996 $[M+Na]^+$; found: 476.2001.



1-Methyl-4'-(2-oxo-2-phenylethyl)-3'-pentyl-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ab)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2b**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (65.3 mg, 0.145 mmol, 73 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (d, *J* = 8.0 Hz, 2H), 7.73 (d, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.23 (d, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.06 (d, *J* =7.5 Hz, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 6.97 (t, *J* = 7.3 Hz, 1H), 6.89 (d, *J* = 8.0 Hz, 1H), 6.76 (d, *J* = 7.5 Hz, 1H), 4.51 (d, *J* = 18.0 Hz, 1H), 4.30 (d, *J* = 18.0 Hz, 1H), 3.36 (s, 3H), 3.23 (d, *J* = 16.5 Hz, 1H), 2.33 (d, *J* = 16.0 Hz, 1H), 2.26-2.14 (m, 2H), 1.42-1.30 (m, 2H), 1.24-1.19 (m, 4H), 0.80 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.3, 141.3, 137.0, 136.5, 135.0, 134.7, 134.3, 133.3, 128.8, 128.2, 128.0, 127.8, 127.1, 125.8, 124.4, 124.3, 123.5, 123.1, 108.1, 52.7, 38.6, 37.8, 34.7, 31.8, 27.0, 26.6, 22.4, 13.9. **IR** (neat, cm^{-1}): ν 3058, 3025, 2954, 2927, 2857, 1707, 1687, 1608, 1490, 1469, 1448, 1373, 1349, 1254, 1211, 1128, 1090, 988, 908, 753, 730, 690. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+Na^+: 472.2247 $[M+Na]^+$; found: 472.2255.

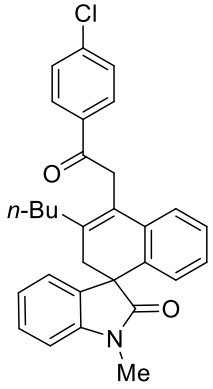


1-Methyl-3'-nonyl-4'-(2-oxo-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ac)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2c**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow oil (57.3 mg, 0.113 mmol, 57 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 8.13 (dd, J_1 = 8.5 Hz, J_2= 1.0 Hz, 2H), 7.74 (d, *J* = 7.5 Hz, 1H), 7.64 (t, *J* = 7.3 Hz, 1H), 7.54 (t, *J* = 7.8 Hz, 2H), 7.23 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 7.10 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 7.06 (dd, J_1 = 7.8 Hz, J_2 = 1.5 Hz,

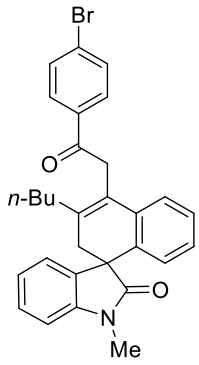
1H), 7.00 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.97 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.89 (d, J = 7.5 Hz, 1H), 6.76 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 4.51 (dd, J_1 = 18.5 Hz, J_2 = 1.5 Hz, 1H), 4.30 (d, J = 18.0 Hz, 1H), 3.36 (s, 3H), 3.23 (d, J = 16.5 Hz, 1H), 2.33 (d, J = 16.0 Hz, 1H), 2.26-2.13 (m, 2H), 1.40-1.31 (m, 2H), 1.25-1.20 (m, 4H), 1.18 (s, 8H), 0.85 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.6, 180.3, 141.3, 137.0, 136.5, 135.0, 134.7, 134.3, 133.3, 128.8, 128.2, 128.0, 127.8, 127.1, 125.7, 124.4, 124.3, 123.5, 123.1, 108.1, 52.7, 38.6, 37.8, 34.7, 31.8, 29.6, 29.5, 29.4, 29.3, 27.3, 26.6, 22.6, 14.1. **IR** (neat, cm^{-1}): ν 3058, 2922, 2852, 1711, 1689, 1609, 1469, 1372, 1348, 1253, 1211, 1091, 1024, 1000, 750, 689. **HRMS** (ESI): *m/z* calcd for $C_{35}H_{39}NO_2$+Na^+: 528.2873 $[M+Na]^+$; found: 528.2886.



3'-Butyl-4'-(2-(4-chlorophenyl)-2-oxoethyl)-1-methyl-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ad)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2d**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (54.5 mg, 0.116 mmol, 58 % yield, MP = 87-89 °C).

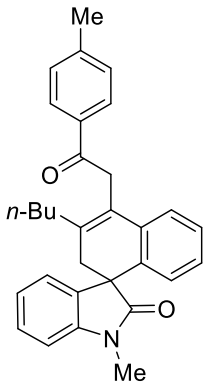
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.06 (d, J = 8.5 Hz, 2H), 7.70 (d, J = 7.0 Hz, 1H), 7.51 (d, J = 8.5 Hz, 2H), 7.24 (dd, J_1 = 8.0 Hz, J_2= 1.0 Hz, 1H), 7.10 (td, J_1 = 7.8 Hz, J_2= 1.0 Hz, 1H), 7.02 (d, J = 8.0 Hz, 1H), 7.01 (d, J = 7.5 Hz, 1H), 6.97 (t, J = 7.5 Hz, 1H), 6.89 (d, J = 8.0 Hz, 1H), 6.76 (d, J= 7.5 Hz, 1H), 4.46 (dd, J_1 = 18.0 Hz, J_2= 1.5 Hz, 1H), 4.25 (d, J = 18.0 Hz, 1H), 3.36 (s, 3H), 3.22 (d, J = 16.5 Hz, 1H), 2.34 (d, J = 16.5 Hz, 1H), 2.26-2.21 (m, 1H), 2.19-2.14 (m, 1H), 1.37-1.31 (m, 2H), 1.30-1.26 (m, 1H), 1.25-1.22 (m, 1H), 0.82 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.5, 180.2, 141.4, 139.8, 136.6, 135.3, 134.9, 134.7, 134.2, 129.6, 129.1, 128.0, 127.8, 127.2, 125.8, 124.3, 124.0, 123.4, 123.0, 108.1, 52.6, 38.5, 37.8, 34.5, 29.4, 26.6, 22.7, 13.9. **IR** (neat, cm^{-1}): ν 3058, 3023, 2955, 2927, 2858, 1707, 1687, 1608, 1587, 1489, 1468, 1372, 1348, 1208, 1089, 988, 908, 811, 749, 730, 693. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}ClNO_2$+H^+: 470.1881 $[M+H]^+$; found: 470.1876.



4'-(2-(4-Bromophenyl)-2-oxoethyl)-3'-butyl-1-methyl-2'H-spiro[indoline-3,1'-naphthalen]-2-one (4ae)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2e**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (35.9 mg, 0.07 mmol, 35 % yield, MP = 88-90 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.99 (d, *J* = 8.5 Hz, 2H), 7.69 (d, *J* = 7.5 Hz, 1H), 7.68 (d, *J* = 8.5 Hz, 2H), 7.25 (td, J_1 = 8.0 Hz, J_2= 1.0 Hz, 1H), 7.10 (td, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 7.01 (d, *J* = 8.5 Hz, 2H), 6.97 (td, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.76 (d, *J* = 8.0 Hz, 1H), 4.46 (dd, J_1 = 18.0 Hz, J_2= 1.5 Hz, 1H), 4.25 (d, *J* = 18.0 Hz, 1H), 3.36 (s, 3H), 3.21 (d, *J* = 16.0 Hz, 1H), 2.34 (d, *J* = 16.5 Hz, 1H), 2.27-2.21 (m, 1H), 2.19-2.13 (m, 1H), 1.37-1.31 (m, 2H), 1.30-1.27 (m, 1H), 1.25-1.22 (m, 1H), 0.82 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.7, 180.2, 141.4, 136.6, 135.7, 134.9, 134.7, 134.2, 132.1, 129.7, 128.5, 128.0, 127.8, 127.2, 125.8, 124.3, 124.0, 123.4, 123.0, 108.1, 52.6, 38.5, 37.8, 34.5, 29.4, 26.6, 22.7, 13.9. **IR** (neat, cm^{-1}): ν 3059, 3025, 2956, 2921, 2851, 1709, 1688, 1606, 1584, 1491, 1468, 1372, 1346, 1255, 1208, 1070, 988, 808, 749, 694. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}BrNO_2$+H^+: 514.1376 $[M+H]^+$; found: 514.1389.

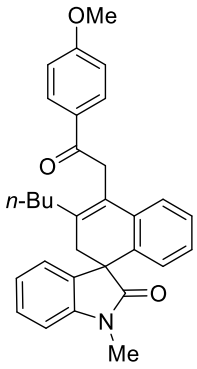


3'-Butyl-1-methyl-4'-(2-oxo-2-(p-tolyl)ethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4af)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2f**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as

a pale yellow solid (55.7 mg, 0.124 mmol, 62 % yield, MP = 145-147 ºC).

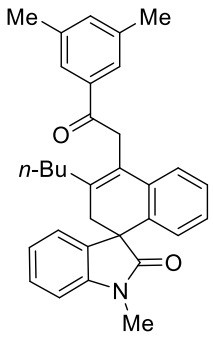
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.03 (d, *J* = 8.0 Hz, 2H), 7.76 (d, *J* = 7.0 Hz, 1H), 7.33 (d, *J* = 8.0 Hz, 2H), 7.24 (t, *J* = 7.8 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 7.0 Hz, 1H), 7.00 (d, *J* = 6.5 Hz, 1H), 6.97 (d, *J* = 7.0 Hz, 1H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.76 (d, *J* = 7.5 Hz, 1H), 4.49 (d, *J* = 18.0 Hz, 1H), 4.26 (d, *J* = 18.0 Hz, 1H), 3.36 (s, 3H), 3.22 (d, *J* = 16.0 Hz, 1H), 2.45 (s, 3H), 2.33 (d, *J* = 16.5 Hz, 1H), 2.27-2.21 (m, 1H), 2.20-2.14 (m, 1H), 1.38-1.31 (m, 2H), 1.29-1.22 (m, 2H), 0.81 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.3, 180.4, 144.1, 141.3, 136.3, 135.1, 134.6, 134.5, 134.3, 129.5, 128.3, 128.0, 127.7, 127.1, 125.7, 124.5, 124.4, 123.6, 123.1, 108.1, 52.7, 38.5, 37.7, 34.5, 29.4, 26.6, 22.7, 21.7, 13.9. **IR** (neat, cm^{-1}): ν 3054, 2957, 2922, 2855, 1704, 1683, 1605, 1491, 1467, 1373, 1349, 1254, 1203, 1172, 1090, 1025, 981, 812, 746. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+H^+: 450.2428 $[M+H]^+$; found: 450.2424.



3'-Butyl-4'-(2-(4-methoxyphenyl)-2-oxoethyl)-1-methyl-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ag)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2g**. The crude mixture was purified via silica-gel flash chromatography using 3:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (47.6 mg, 0.102 mmol, 51 % yield, MP = 131-132 ºC).

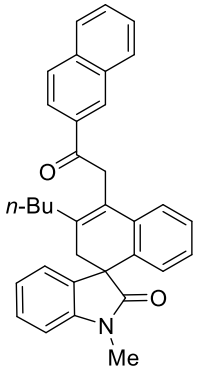
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.12 (d, *J* = 8.5 Hz, 2H), 7.76 (d, *J* = 7.5 Hz, 1H), 7.23 (d, *J* = 8.0 Hz, 1H), 7.09 (t, *J* = 8.0 Hz, 1H), 7.06 (d, *J* = 7.5 Hz, 1H), 7.01 (d, *J* = 9.0 Hz, 2H), 6.98 (t, *J* = 7.5 Hz, 2H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.75 (d, *J* = 7.5 Hz, 1H), 4.46 (d, *J* = 18.0 Hz, 1H), 4.23(d, *J* = 18.0 Hz, 1H), 3.91 (s, 3H), 3.36 (s, 3H), 3.22 (d, *J* = 16.5 Hz, 1H), 2.33 (d, *J* = 16.5 Hz, 1H), 2.26-2.17 (m, 2H), 1.41-1.34 (m, 2H), 1.31-1.22 (m, 2H), 0.82 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 196.2, 180.4, 163.6, 141.3, 136.2, 135.1, 134.7, 134.3, 130.5, 130.1, 128.0, 127.7, 127.1, 125.7, 124.6, 124.5, 123.6, 123.1, 113.9, 108.1, 55.5, 52.7, 38.6, 37.4, 34.5, 29.4, 26.6, 22.8, 13.9. **IR** (neat, cm^{-1}): ν 3060, 2955, 2919, 2850, 1709, 1678, 1598, 1494, 1465, 1373, 1346, 1250, 1168, 1024, 832, 750, 698. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_3$+H^+: 466.2377 $[M+H]^+$; found: 466.2390.



3'-Butyl-4'-(2-(3,5-dimethylphenyl)-2-oxoethyl)-1-methyl-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ah)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2h**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (50.3 mg, 0.108 mmol, 54 % yield, MP = 148-150 ºC).

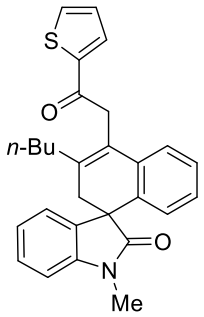
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.74 (d, J = 8.0 Hz, 1H), 7.73 (s, 2H), 7.27 (s, 1H), 7.23 (dd, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.09 (td, J_1 = 8.0 Hz, J_2= 1.0 Hz, 1H), 7.06 (d, J = 8.0 Hz, 1H), 6.99 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 6.97 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.89 (d, J = 7.5 Hz, 1H), 6.76 (d, J = 7.5 Hz, 1H), 4.49 (dd, J_1 = 18.0 Hz, J_2= 1.0 Hz, 1H), 4.26 (d, J = 18.0 Hz, 1H), 3.36 (s, 3H), 3.23 (d, J = 16.0 Hz, 1H), 2.42 (s, 6H), 2.32 (d, J = 16.5 Hz, 1H), 2.27-2.21 (m, 1H), 2.20-2.14 (m, 1H), 1.38-1.31 (m, 2H), 1.30-1.27 (m, 1H), 1.25-1.19 (m, 1H), 0.82 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 198.0, 180.4, 141.3, 138.4, 137.1, 136.3, 135.0, 134.9, 134.7, 134.3, 127.9, 127.7, 127.1, 126.0, 125.7, 124.4, 124.4, 123.6, 123.1, 108.1, 52.7, 38.5, 38.0, 34.5, 29.4, 26.6, 22.8, 21.3, 13.9. **IR** (neat, cm^{-1}): ν 3054, 3029, 2955, 2925, 2858, 1703, 1680, 1607, 1490, 1467, 1373, 1348, 1330, 1254, 1184, 1156, 1090, 910, 851, 749, 730, 686. **HRMS** (ESI): *m/z* calcd for $C_{32}H_{33}NO_2$+H^+: 464.2584 $[M+H]^+$; found 464.2600.



3'-Butyl-1-methyl-4'-(2-(naphthalen-2-yl)-2-oxoethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ai)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2i**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (86.8 mg, 0.178 mmol, 89 % yield, MP = 129-131 ºC).

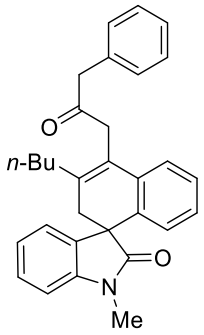
^{1}H NMR (500 MHz, $CDCl_3$) δ 8.69 (s, 1H), 8.15 (dd, J_1 = 8.5 Hz, J_2= 1.5 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 7.97 (d, J = 8.5 Hz, 1H), 7.93 (d, J = 8.5 Hz, 1H), 7.75 (d, J = 7.0 Hz, 1H), 7.64 (td, J_1 = 8.0 Hz, J_2= 1.0 Hz, 1H), 7.60 (td, J_1 = 7.0 Hz, J_2= 1.0 Hz, 1H), 7.23 (dd, J_1 = 7.8 Hz, J_2= 1.0 Hz, 1H), 7.11 (dd, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 7.09 (dd, J_1 = 7.0 Hz, J_2= 1.0 Hz, 1H), 7.00 (td, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 6.92 (td, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 6.89 (d, J = 7.5 Hz, 1H), 6.77 (d, J = 7.5 Hz, 1H), 4.66 (dd, J_1 = 18.0 Hz, J_2= 1.0 Hz, 1H), 4.43 (d, J = 17.5 Hz, 1H), 3.37 (s, 3H), 3.26 (d, J = 16.0 Hz, 1H), 2.35 (d, J = 16.5 Hz, 1H), 2.31-2.27 (m, 1H), 2.25-2.20 (m, 1H), 1.42-1.34 (m, 2H), 1.32-1.24 (m, 2H), 0.82 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 197.7, 180.3, 141.3, 136.5, 135.7, 135.0, 134.7, 134.3, 134.3, 132.6, 129.7, 129.6, 128.7, 128.6, 128.0, 127.8, 127.8, 127.1, 126.9, 125.8, 124.4, 124.4, 124.0, 123.6, 123.0, 108.1, 52.7, 38.6, 37.9, 34.6, 29.5, 26.6, 22.8, 13.9. **IR** (neat, cm^{-1}): ν 3059, 3025, 2955, 2928, 2870, 1706, 1681, 1608, 1490, 1468, 1372, 1350, 1252, 1182, 1124, 822, 727, 698. **HRMS** (ESI): *m/z* calcd for $C_{34}H_{31}NO_2$+H^+: 486.2428 $[M+H]^+$; found: 486.2442.



3'-Butyl-1-methyl-4'-(2-oxo-2-(thiophen-2-yl)ethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4aj)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2j**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (65.4 mg, 0.148 mmol, 74 % yield, MP = 149-151 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.95 (dd, J_1 = 3.5 Hz, J_2 = 1.0 Hz, 1H), 7.72 (d, J = 7.5 Hz, 1H), 7.69 (dd, J_1 = 5.0 Hz, J_2 = 1.0 Hz, 1H), 7.24 (td, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 7.21 (dd, J_1 = 5.0 Hz, J_2 = 3.5 Hz, 1H), 7.14 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 7.11 (td, J_1 = 8.0 Hz, J_2 = 1.0 Hz, 1H), 7.00 (td, J_1 = 7.5 Hz, J_2 = 1.5 Hz, 1H), 6.98 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.76 (dd, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 4.45 (dd, J_1 = 18.0 Hz, J_2= 1.5 Hz, 1H), 4.23 (d, J = 18.0 Hz, 1H), 3.36 (s, 3H), 3.22 (d, J = 16.5 Hz, 1H), 2.33 (d, J = 16.5 Hz, 1H), 2.28-2.17 (m, 2H), 1.40-1.32 (m, 2H), 1.31-1.24 (m, 2H), 0.82 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 190.5, 180.3, 144.0, 141.3, 136.9, 134.9, 134.7, 134.2, 133.8, 131.9, 128.3, 128.0, 127.8, 127.2, 125.8, 124.4, 123.9, 123.5, 123.1, 108.1, 52.7, 38.5, 38.5, 34.5, 29.4, 26.6, 22.8, 13.9. **IR** (neat, cm^{-1}): ν 3051, 3019, 2953, 2927, 2856, 1701, 1655, 1608, 1474, 1417, 1372, 1351, 1222, 1130, 1089, 925, 755, 732, 687. **HRMS** (ESI): *m/z* calcd for $C_{28}H_{27}NO_2S$+Na^+: 464.1655 $[M+Na]^+$; found: 464.1665.

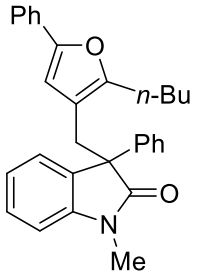


3'-Butyl-1-methyl-4'-(2-oxo-3-phenylpropyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (4ak)

Prepared according to General Procedure **3** using starting material **1a** and (*E*)-*β*-chloroenone **2k**. The crude mixture was purified via silica-gel flash chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (39.2 mg, 0.087 mmol, 44 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.55 (d, J = 7.5 Hz, 1H), 7.36 (t, J = 7.3 Hz, 2H), 7.31 (d, J = 7.5 Hz, 1H), 7.29 (d, J = 8.5 Hz, 2H), 7.23 (dd, J_1 = 7.8 Hz, J_2 = 1.0 Hz, 1H), 7.07 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 7.00 (dd, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 6.93 (td, J_1 = 7.5 Hz, J_2 = 0.5 Hz, 1H), 6.90 (d, J = 8.5 Hz, 1H), 6.88 (d, J = 8.0 Hz, 1H), 6.71 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 3.91 (dd, J_1 =18.5 Hz, J_2 = 1.5 Hz, 1H), 3.88 (s, 2H), 3.73 (d, J = 18.0 Hz, 1H), 3.32 (s, 3H), 3.08 (d, J = 16.5 Hz, 1H), 2.34 (d, J = 16.5 Hz, 1H), 2.15-2.08 (m, 1H), 2.07-2.01 (m, 1H), 1.37-1.19 (m, 4H), 0.81 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 206.3, 179.9, 141.6, 136.5, 134.9, 134.6, 134.3, 134.1, 129.5, 128.8, 128.6, 128.1, 127.8, 127.2, 125.8, 124.1, 123.9, 123.5, 123.0, 108.1, 52.4, 49.8, 41.5, 38.4, 34.3, 29.3, 26.5, 22.7, 13.8. **IR** (neat, cm^{-1}): ν 3058, 3027, 2953, 2924, 2856, 1707, 1609, 1491, 1469, 1372, 1347, 1252, 1170, 1089, 1024, 953, 869, 748, 699. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+Na^+: 472.2247 $[M+Na]^+$; found: 472.2257.

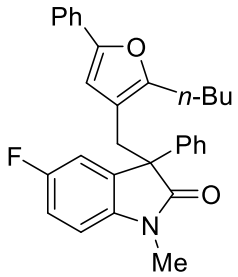
7) Synthesis of 3,3-disubstituted furan-containing oxindoles



3-((2-Butyl-5-phenylfuran-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5aa)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (60.9 mg, 0.14 mmol, 70 % yield, MP = 77-78 ºC).

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.51 (d, *J* = 6.8 Hz, 2H), 7.41 (d, *J* = 7.2 Hz, 2H), 7.34 (t, *J* = 8.0 Hz, 2H), 7.31-7.24 (m, 4H), 7.22 (d, *J* = 7.2 Hz, 1H), 7.15 (t, *J* = 7.4 Hz, 1H), 7.08 (t, *J* = 7.6 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.86 (s, 1H), 3.42 (d, *J* = 13.6 Hz, 1H), 3.28 (d, *J* = 13.6 Hz, 1H), 3.07 (s, 3H), 2.46-2.30 (m, 2H), 1.54-1.45 (m, 1H), 1.42-1.32 (m, 1H), 1.33-1.26 (m, 2H), 0.89 (t, *J* = 7.4 Hz, 3H). **^{13}C NMR** (100 MHz, $CDCl_3$) δ 178.1, 153.7, 150.5, 144.1, 139.7, 131.6, 131.1, 128.6, 128.5, 128.3, 127.4, 127.2, 126.5, 125.2, 123.1, 122.2, 115.0, 108.2, 107.0, 57.1, 33.7, 30.5, 26.2, 25.7, 22.5, 13.9. **IR** (neat, cm^{-1}): 3057, 3032, 2956, 2929, 2871, 1713, 1612, 1494, 1470, 1374, 1349, 1254, 1186, 1081, 932, 813, 759, 732, 694. **HRMS** (DART): *m/z* calcd for $C_{30}H_{29}NO_2+H^+$: 436.2271 $[M+H]^+$; found: 436.2273.

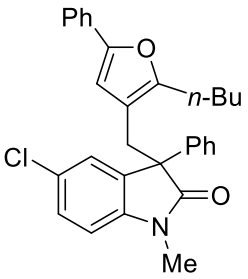


3-((2-Butyl-5-phenylfuran-3-yl)methyl)-5-fluoro-1-methyl-3-phenylindolin-2-one (5ba)

Prepared according to General Procedure **4** using starting material **1b** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (61.6 mg, 0.136 mmol, 68 % yield, MP = 111-113 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.5 Hz, 2H), 7.43 (d, *J* = 8.0 Hz, 2H), 7.35 (t, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 6.5 Hz, 1H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.15 (t, *J* = 7.5 Hz, 1H), 6.99-6.94 (m, 2H), 6.64 (dd, J_1 = 9.0 Hz, J_2= 4.0 Hz, 1H), 5.93 (s, 1H), 3.43 (d, *J* = 13.5 Hz, 1H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.06 (s, 3H), 2.47-2.33 (m, 2H), 1.56-

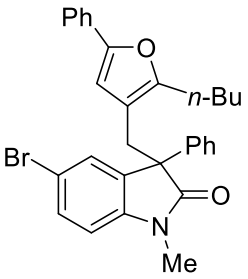
1.47 (m, 1H), 1.42-1.35 (m, 1H), 1.34-1.28 (m, 2H), 0.90 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 177.8, 159.0 (d, J = 239.1 Hz), 153.7, 150.8, 140.0 (d, J = 1.6 Hz), 139.1, 133.4 (d, J = 7.9 Hz), 131.0, 128.7, 128.5, 127.7, 127.0, 126.7, 123.1, 114.7, 114.5 (d, J = 23.4 Hz), 113.2 (d, J = 24.5 Hz), 108.7 (d, J = 8.1 Hz), 106.8, 57.6, 33.6, 30.5, 26.4, 25.7, 22.5, 13.8. **^{19}F NMR** (470 MHz, $CDCl_3$): δ -120.66 (s, 1F). **IR** (neat, cm^{-1}): ν 3056, 3030, 2958, 2931, 2871, 1707, 1600, 1491, 1445, 1351, 1271, 1257, 1143, 1101, 1036, 932, 892, 806, 762, 696. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}FNO_2$+Na^+: 476.1996 $[M+Na]^+$; found 476.1983.



3-((2-Butyl-5-phenylfuran-3-yl)methyl)-5-chloro-1-methyl-3-phenylindolin-2-one (5ca)

Prepared according to General Procedure **4** using starting material **1c** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (66.6 mg, 0.142 mmol, 71 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, J = 8.0 Hz, 2H), 7.44 (d, J = 7.5 Hz, 2H), 7.36 (t, J = 7.5 Hz, 2H), 7.31 (d, J = 7.0 Hz, 1H), 7.30 (t, J = 8.0 Hz, 2H), 7.23 (d, J = 2.0 Hz, 1H), 7.19 (d, J = 2.0 Hz, 1H), 7.17 (t, J = 7.5 Hz, 1H), 6.65 (d, J = 8.5 Hz, 1H), 5.96 (s, 1H), 3.44 (d, J = 14.0 Hz, 1H), 3.26 (d, J = 14.0 Hz, 1H), 3.07 (s, 3H), 2.46-2.39 (m, 1H), 2.38-2.32 (m, 1H), 1.55-1.48 (m, 1H), 1.43-1.36 (m, 1H), 1.35-1.29 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 177.7, 153.7, 150.8, 142.6, 139.0, 133.5, 131.0, 128.7, 128.5, 128.2, 127.7, 127.7, 127.0, 126.7, 125.5, 123.1, 114.6, 109.1, 106.7, 57.4, 33.6, 30.5, 26.4, 25.7, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3059, 3031, 2957, 2930, 2871, 1711, 1601, 1489, 1348, 1271, 1098, 1072, 908, 808, 761, 729, 694. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}ClNO_2$+H^+: 470.1881 $[M+H]^+$; found: 470.1883.

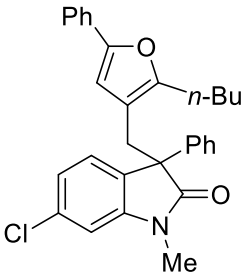


5-Bromo-3-((2-butyl-5-phenylfuran-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5da)

Prepared according to General Procedure **4** using starting material **1d** and (*E*)-*β*-

chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (66.7 mg, 0.13 mmol, 65 % yield, MP = 130-131 ºC).

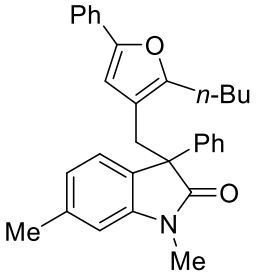
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.46 (d, *J* = 8.0 Hz, 2H), 7.44 (d, *J* = 7.0 Hz, 2H), 7.38 (dd, J_1 = 8.0 Hz, J_2= 2.0 Hz, 1H), 7.36 (t, *J* = 7.5 Hz, 2H), 7.32 (d, *J* = 2.0 Hz, 1H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.29 (t, *J* = 7.8 Hz, 2H), 7.16 (t, *J* = 7.3 Hz, 1H), 6.60 (d, *J* = 8.5 Hz, 1H), 5.97 (s, 1H), 3.44 (d, *J*= 14.0 Hz, 1H), 3.26 (d, *J* = 14.0 Hz, 1H), 3.06 (s, 3H), 2.46-2.39 (m, 1H), 2.37-2.30 (m, 1H), 1.55-1.47 (m, 1H), 1.44-1.37 (m, 1H), 1.36-1.29 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 177.6, 153.7, 150.8, 143.1, 138.9, 133.9, 131.1, 131.0, 128.7, 128.5, 128.2, 127.7, 127.0, 126.7, 123.1, 115.0, 114.5, 109.6, 106.8, 57.4, 33.6, 30.4, 26.4, 25.8, 22.6, 13.9. **IR** (neat, cm^{-1}): ν 3060, 2952, 2928, 2865, 1713, 1602, 1485, 1342, 1268, 1137, 1090, 924, 809, 758, 691. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}BrNO_2$+Na^+: 536.1196 $[M+Na]^+$; found 536.1199.



3-((2-Butyl-5-phenylfuran-3-yl)methyl)-6-chloro-1-methyl-3-phenylindolin-2-one (5ea)

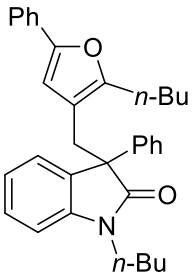
Prepared according to General Procedure **4** using starting material **1e** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow wax (52.5 mg, 0.112 mmol, 56 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.47 (d, *J* = 7.5 Hz, 2H), 7.44 (d, *J* = 7.0 Hz, 2H), 7.35 (t, *J* = 7.3 Hz, 2H), 7.30 (t, *J* = 7.8 Hz, 3H), 7.17 (t, *J* = 7.3 Hz, 1H), 7.11 (dd, J_1 = 7.5 Hz, J_2 = 2.0 Hz, 1H), 7.06 (dt, J_1 = 7.5 Hz, J_2 = 2.0 Hz, 1H), 6.75 (s, 1H), 5.90 (s, 1H), 3.39 (d, *J* = 13.5 Hz, 1H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.07 (s, 3H), 2.45-2.37 (m, 1H), 2.36-2.29 (m, 1H), 1.53-1.46 (m, 1H), 1.41-1.34 (m, 1H), 1.33-1.26 (m, 2H), 0.90 (d, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.1, 153.7, 150.8, 145.3, 139.1, 134.1, 131.0, 130.0, 128.7, 128.5, 127.7, 127.1, 126.7, 126.1, 123.2, 122.0, 114.8, 109.0, 106.8, 56.9, 33.7, 30.5, 26.4, 25.7, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3061, 3032, 2954, 2928, 2865, 1716, 1602, 1490, 1443, 1366, 1333, 1295, 1242, 1183, 1070, 812, 760, 694. **HRMS** (DART): *m/z* calcd for $C_{30}H_{28}ClNO_2$+H^+: 470.1881 $[M+H]^+$; found: 470.1888.



3-((2-Butyl-5-phenylfuran-3-yl)methyl)-1,6-dimethyl-3-phenylindolin-2-one (5fa)
Prepared according to General Procedure **4** using starting material **1f** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (62.0 mg, 0.138 mmol, 69 % yield).

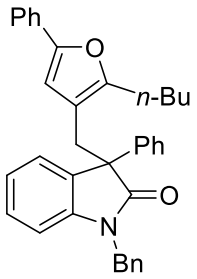
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.5 Hz, 2H), 7.42 (d, *J* = 7.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.27 (d, *J* = 2.0 Hz, 1H), 7.16 (t, *J* = 7.3 Hz, 1H), 7.08 (d, *J* = 7.5 Hz, 1H), 6.89 (d, *J* = 7.5 Hz, 1H), 6.56 (s, 1H), 5.91 (s, 1H), 3.39 (d, *J* = 13.5 Hz, 1H), 3.26 (d, *J* = 13.5 Hz, 1H), 3.06 (s, 3H), 2.45-2.38 (m, 1H), 2.37 (s, 3H), 2.36-2.30 (m, 1H), 1.52-1.45 (m, 1H), 1.38-1.33 (m, 1H), 1.32-1.27 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.4, 153.7, 150.4, 144.1, 139.9, 138.3, 131.2, 128.5, 128.5, 128.5, 127.3, 127.2, 126.5, 125.0, 123.1, 122.7, 115.2, 109.2, 107.1, 56.9, 33.8, 30.5, 26.2, 25.7, 22.5, 21.8, 13.9. **IR** (neat, cm^{-1}): ν 3057, 3029, 2956, 2928, 2871, 1712, 1620, 1600, 1554, 1467, 1448, 1373, 1338, 1256, 1191, 1088, 1037, 932, 813, 761, 735, 695. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+Na^+: 472.2247 $[M+Na]^+$; found 472.2262.



1-Butyl-3-((2-butyl-5-phenylfuran-3-yl)methyl)-3-phenylindolin-2-one (5ga)
Prepared according to General Procedure **4** using starting material **1g** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow oil (52.4 mg, 0.11 mmol, 55 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, *J* = 8.0 Hz, 2H), 7.38 (d, *J* = 8.0 Hz, 2H), 7.34 (t, *J* = 8.3 Hz, 2H), 7.29-7.24 (m, 5H), 7.13 (t, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.74 (s, 1H), 3.71-3.64 (m, 1H), 3.48 (d, *J* = 13.5 Hz, 1H), 3.44-3.37 (m, 1H), 3.25 (d, *J* = 13.5 Hz, 1H), 2.49-2.41 (m, 2H), 1.58-1.49 (m, 1H), 1.45-1.38 (m, 1H), 1.37-1.29 (m, 4H), 1.17-1.07 (m, 2H), 0.90 (t, *J* = 7.3 Hz, 3H), 0.72 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 177.8, 153.7, 150.4, 143.8, 140.1, 132.2, 131.1, 128.6, 128.4, 128.2, 127.3, 127.1, 126.4, 125.1, 123.1, 122.0, 115.0, 108.5,

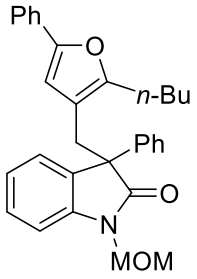
107.2, 57.1, 39.9, 33.6, 30.5, 29.3, 25.7, 22.5, 20.0, 13.9, 13.7. **IR** (neat, cm^{-1}): ν 3057, 3032, 2956, 2929, 2870, 1707, 1610, 1487, 1465, 1357, 1198, 1097, 1025, 932, 815, 756, 730, 692. **HRMS** (ESI): *m/z* calcd for $C_{33}H_{35}NO_2+H^+$: 478.2741 $[M+H]^+$; found 478.2742.



1-Benzyl-3-((2-butyl-5-phenylfuran-3-yl)methyl)-3-phenylindolin-2-one (5ha)

Prepared according to General Procedure **4** using starting material **1h** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow oil (61.4 mg, 0.12 mmol, 60 % yield).

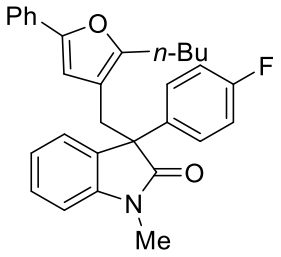
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.53 (d, *J* = 7.5 Hz, 2H), 7.37 (dd, J_1 = 7.5 Hz, J_2= 2.5 Hz, 3H), 7.34 (d, *J* = 6.5 Hz, 1H), 7.31 (d, *J* = 5.0 Hz, 1H), 7.29 (d, *J* = 5.5 Hz, 1H), 7.27 (s, 1H), 7.24 (d, *J* = 7.0 Hz, 1H), 7.17 (d, *J* = 6.5 Hz, 1H), 7.14 (d, *J* = 6.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.04-6.97 (m, 3H), 6.87 (d, *J* = 7.5 Hz, 2H), 6.56 (d, *J* = 8.0 Hz, 1H), 5.75 (s, 1H), 5.01 (d, *J* = 16.0 Hz, 1H), 4.58 (d, *J* = 16.0 Hz, 1H), 3.60 (d, *J* = 14.0 Hz, 1H), 3.31 (d, *J* = 14.0 Hz, 1H), 2.48 (t, *J* = 7.5 Hz, 2H), 1.54-1.46 (m, 1H), 1.44-1.36 (m, 1H), 1.35-1.27 (m, 2H), 0.86 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 154.0, 150.6, 143.5, 140.2, 135.4, 132.0, 131.1, 128.7, 128.6, 128.5, 128.3, 127.5, 127.1, 127.1, 126.6, 126.6, 125.1, 123.2, 122.3, 115.2, 109.5, 107.4, 57.3, 43.9, 33.5, 30.5, 25.8, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3058, 3032, 2956, 2928, 2870, 1715, 1611, 1488, 1466, 1359, 1265, 1223, 1189, 1073, 1036, 945, 932, 814, 759, 694. **HRMS** (ESI): *m/z* calcd for $C_{36}H_{33}NO_2+H^+$: 512.2584 $[M+H]^+$; found: 512.2579.



3-((2-Butyl-5-phenylfuran-3-yl)methyl)-1-(methoxymethyl)-3-phenylindolin-2-one (5ia)

Prepared according to General Procedure **4** using starting material **1i** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow oil (44.7 mg, 0.096 mmol, 48 % yield).

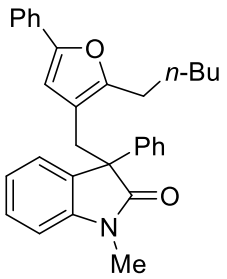
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.5 Hz, 2H), 7.35 (t, *J* = 8.3 Hz, 4H), 7.31 (d, *J* = 7.0 Hz, 1H), 7.30 (d, *J* = 7.0 Hz, 2H), 7.26 (d, *J* = 7.8 Hz, 2H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 7.3 Hz, 1H), 6.98 (d, *J* = 7.5 Hz, 1H), 5.72 (s, 1H), 5.02 (d, *J* = 11.0 Hz, 1H), 4.96 (d, *J* = 11.0 Hz, 1H), 3.52 (d, *J* = 14.0 Hz, 1H), 3.29 (d, *J* = 14.0 Hz, 1H), 2.96 (s, 3H), 2.47 (t, *J* = 7.5 Hz, 2H), 1.57-1.49 (m, 1H), 1.46-1.38 (m, 1H), 1.37-1.28 (m, 2H), 0.91 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.6, 153.8, 150.6, 142.6, 139.9, 131.3, 131.0, 128.7, 128.5, 128.5, 127.5, 127.1, 126.6, 125.3, 123.1, 122.8, 115.1, 109.9, 107.1, 71.5, 57.7, 55.5, 33.6, 30.5, 25.8, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3057, 2929, 2865, 1719, 1607, 1488, 1458, 1341, 1295, 1235, 1186, 1086, 918, 813, 756, 696. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_3+H^+$: 466.2377 $[M+H]^+$; found: 466.2379.



3-((2-Butyl-5-phenylfuran-3-yl)methyl)-3-(4-fluorophenyl)-1-methylindolin-2-one (5ja)

Prepared according to General Procedure **4** using starting material **1j** and (*E*)-*β*-chloroenone **2a**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (66.2 mg, 0.146 mmol, 73 % yield).

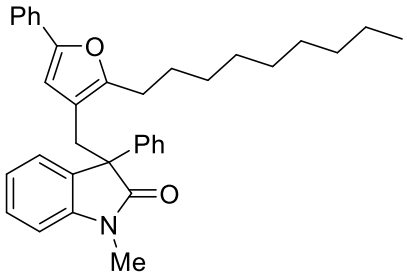
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.49-7.46 (m, 2H), 7.42 (dd, J_1 = 8.5 Hz, J_2= 1.0 Hz, 2H), 7.29 (t, *J* = 8.0 Hz, 3H), 7.20 (d, *J* = 7.5 Hz, 1H), 7.16 (t, *J* = 7.5 Hz, 1H), 7.10 (t, *J* = 7.5 Hz, 1H), 7.03 (t, *J* = 8.8 Hz, 2H), 6.75 (d, *J* = 7.5 Hz, 1H), 5.85 (s, 1H), 3.37 (d, *J* = 14.0 Hz, 1H), 3.24 (d, *J* = 14.0 Hz, 1H), 3.08 (s, 3H), 2.44-2.37 (m, 1H), 2.36-2.29 (m, 1H), 1.52-1.45 (m, 1H), 1.41-1.35 (m, 1H), 1.32-1.25 (m, 2H), 0.89 (d, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 177.9, 162.2 (d, *J* = 245.1 Hz), 153.7, 150.6, 144.1, 135.4 (d, *J* = 3.3 Hz), 131.3, 131.0, 129.0 (d, *J* = 7.9 Hz), 128.5, 128.5, 126.6, 125.2, 123.1, 122.3, 115.3 (d, *J* = 21.1 Hz), 114.8, 108.4, 106.9, 56.5, 34.1, 30.5, 26.3, 25.7, 22.5, 13.9. **^{19}F NMR** (470 MHz, $CDCl_3$): δ -115.28 – -115.35 (m, 1F). **IR** (neat, cm^{-1}): ν 3058, 2954, 2928, 2866, 1710, 1606, 1500, 1463, 1347, 1230, 1164, 1082, 1017, 813, 752, 693. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}FNO_2+H^+$: 454.2177 $[M+H]^+$; found: 454.2182.



1-Methyl-3-((2-pentyl-5-phenylfuran-3-yl)methyl)-3-phenylindolin-2-one (5ab)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2b**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (65.6 mg, 0.146 mmol, 73 % yield, MP = 77-78 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.5 Hz, 2H), 7.41 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.30-7.23 (m, 4H), 7.21 (d, *J* = 7.5 Hz, 1H), 7.14 (t, *J* = 7.5 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.72 (d, *J* = 7.5 Hz, 1H), 5.87 (s, 1H), 3.42 (d, *J* = 14.0 Hz, 1H), 3.28 (d, *J* = 14.0 Hz, 1H), 3.06 (s, 3H), 2.45-2.38 (m, 1H), 2.37-2.29 (m, 1H), 1.56-1.47 (m, 1H), 1.44-1.35 (m, 1H), 1.32-1.22 (m, 4H), 0.88 (t, *J* = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 153.7, 150.5, 144.1, 139.7, 131.6, 131.1, 128.5, 128.5, 128.3, 127.4, 127.2, 126.5, 125.2, 123.1, 122.2, 115.0, 108.2, 107.0, 57.1, 33.7, 31.5, 28.0, 26.2, 25.9, 22.5, 14.0. **IR** (neat, cm^{-1}): ν 3057, 3036, 2954, 2926, 2854, 1709, 1611, 1491, 1467, 1447, 1370, 1349, 1250, 1180, 1081, 930, 910, 807, 765, 750, 693. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+H^+: 450.2428 $[M+H]^+$; found: 450.2432.

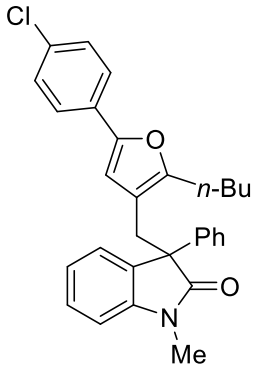


1-Methyl-3-((2-nonyl-5-phenylfuran-3-yl)methyl)-3-phenylindolin-2-one (5ac)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2c**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow sticky oil (90.9 mg, 0.18 mmol, 90 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.0 Hz, 2H), 7.41(d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.30-7.24 (m, 4H), 7.21(d, *J* = 7.0 Hz, 1H), 7.15 (t, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.73 (d, *J* = 7.5 Hz, 1H), 5.87 (s, 1H), 3.42 (d, *J* = 13.5 Hz, 1H), 3.28 (d, *J* = 14.0 Hz, 1H), 3.07 (s, 3H), 2.44-2.38 (m, 1H), 2.36-2.30 (m, 1H), 1.54-1.45 (m, 1H), 1.42-1.34 (m, 1H), 1.32-1.20 (m, 12H), 0.88 (t, *J* = 6.8 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 153.7, 150.5, 144.1, 139.7, 131.6, 131.1, 128.5, 128.5, 128.3, 127.4, 127.2, 126.5, 125.2, 123.1, 122.2, 115.0, 108.2, 107.0, 57.1, 33.7, 31.9, 29.5, 29.4, 29.4, 29.3, 28.3, 26.2, 26.0, 22.7, 14.1. **IR** (neat, cm^{-1}): ν 3058, 3030,

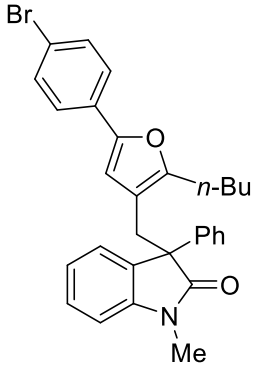
2952, 2923, 2853, 1711, 1611, 1492, 1469, 1373, 1348, 1254, 1182, 1079, 931, 811, 758, 694. **HRMS** (ESI): *m/z* calcd for $C_{35}H_{39}NO_2+H^+$: 506.3054 $[M+H]^+$; found: 506.3062.



3-((2-Butyl-5-(4-chlorophenyl)furan-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5ad)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2d**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (61.0 mg, 0.13 mmol, 65 % yield, MP = 125-126 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.5 Hz, 2H), 7.35 (d, *J* = 7.0 Hz, 2H), 7.33 (d, *J* = 2.5 Hz, 1H), 7.31 (t, *J* = 2.0 Hz, 1H), 7.29 (d, *J* = 5.0 Hz, 1H), 7.27 (d, *J* = 5.5 Hz, 1H), 7.24 (d, *J* = 2.0 Hz, 1H), 7.22 (d, *J* = 7.5 Hz, 2H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 8.0 Hz, 1H), 5.85 (s, 1H), 3.42 (d, *J* = 13.5 Hz, 1H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.06 (s, 3H), 2.45-2.38 (m, 1H), 2.37-2.29 (m, 1H), 1.52-1.44 (m, 1H), 1.40-1.34 (m, 1H), 1.33-1.28 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 154.1, 149.5, 144.1, 139.6, 132.0, 131.6, 129.5, 128.7, 128.6, 128.3, 127.5, 127.2, 125.2, 124.3, 122.2, 115.2, 108.2, 107.5, 57.1, 33.7, 30.4, 26.2, 25.7, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3055, 3029, 2952, 2925, 2857, 1707, 1599, 1485, 1468, 1373, 1349, 1253, 1189, 1088, 1011, 877, 838, 749, 697. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}ClNO_2+Na^+$: 492.1701 $[M+Na]^+$; found: 492.1698.

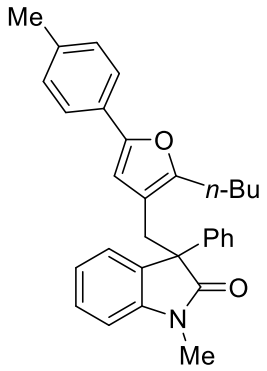


3-((5-(4-Bromophenyl)-2-butylfuran-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5ae)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-

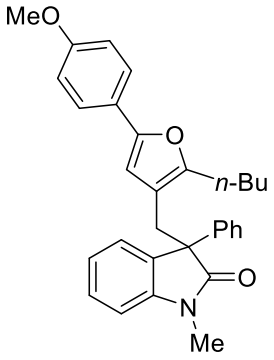
chloroenone **2e**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (51.3 mg, 0.10 mmol, 50 % yield, MP = 122 -123 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.5 Hz, 2H), 7.39 (d, *J* = 8.5 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.31-7.25 (m, 4H), 7.22 (d, *J* = 7.5 Hz, 1H), 7.09 (t, *J* = 7.5 Hz, 1H), 6.74 (d, *J* = 7.5 Hz, 1H), 5.86 (s, 1H), 3.42 (d, *J* = 14.0 Hz, 1H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.07 (s, 3H), 2.45-2.38 (m, 1H), 2.36-2.30 (m, 1H), 1.52-1.44 (m, 1H), 1.40-1.33 (m, 1H), 1.32-1.26 (m, 2H), 0.89 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 154.2, 149.5, 144.1, 139.6, 131.6, 131.6, 130.0, 128.6, 128.3, 127.5, 127.2, 125.2, 124.6, 122.2, 120.1, 115.3, 108.2, 107.6, 57.1, 33.7, 30.4, 26.2, 25.7, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3054, 3026, 2956, 2927, 2870, 1711, 1649, 1589, 1494, 1447, 1374, 1334, 1259, 1186, 1072, 980, 884, 759, 693. **HRMS** (ESI): *m/z* calcd for $C_{30}H_{28}BrNO_2$+H^+: 514.1376 $[M+H]^+$; found 514.1379.



3-((2-Butyl-5-(p-tolyl)furan-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5af)
Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2f**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (59.3 mg, 0.132 mmol, 66 % yield, MP = 116-117 ºC).

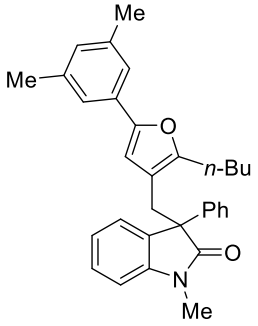
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (dd, J_1 = 8.5 Hz, J_2= 1.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.31 (d, *J* = 8.0 Hz, 2H), 7.29-7.24 (m, 2H), 7.21 (d, *J* = 7.0 Hz, 1H), 7.12-7.06 (m, 3H), 6.73 (d, *J* = 8.0 Hz, 1H), 5.80 (s, 1H), 3.41 (d, *J* = 14.0 Hz, 1H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.07 (s, 3H), 2.44-2.37 (m, 1H), 2.36-2.29 (m, 1H), 2.31 (s, 3H), 1.53-1.44 (m, 1H), 1.40-1.33 (m, 1H), 1.32-1.26 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.1, 153.3, 150.7, 144.1, 139.7, 136.3, 131.6, 129.2, 128.5, 128.4, 128.3, 127.4, 127.2, 125.2, 123.1, 122.2, 114.9, 108.2, 106.2, 57.1, 33.8, 30.5, 26.2, 25.7, 22.5, 21.2, 13.9. **IR** (neat, cm^{-1}): ν 3054, 3029, 2951, 2922, 2855, 1709, 1610, 1492, 1468, 1373, 1349, 1255, 1169, 1082, 1016, 929, 821, 755, 698. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+H^+: 450.2428 $[M+H]^+$; found: 450.2434.



3-((2-Butyl-5-(4-methoxyphenyl)furan-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5ag)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2g**. The crude mixture was purified via silica-gel flash chromatography using 12:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (80.9 mg, 0.174 mmol, 87 % yield, MP = 121-123 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.51 (d, *J* = 7.0 Hz, 2H), 7.36-7.32 (m, 4H), 7.28 (d, *J* = 7.0 Hz, 1H), 7.25 (dd, J_1 = 7.5 Hz, J_2= 1.0 Hz, 1H), 7.21 (d, *J* = 7.0 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 6.83 (d, *J* = 8.5 Hz, 2H), 6.73 (d, *J* = 7.5 Hz, 1H), 5.73 (s, 1H), 3.78 (s, 3H), 3.40 (d, *J* = 13.5 Hz, 1H), 3.27 (d, *J* = 13.5 Hz, 1H), 3.07 (s, 3H), 2.44-2.37 (m, 1H), 2.35-2.28 (m, 1H), 1.52-1.44 (m, 1H), 1.40-1.33 (m, 1H), 1.32-1.26 (m, 2H), 0.88 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.1, 158.5, 152.9, 150.5, 144.1, 139.7, 131.6, 128.5, 128.2, 127.4, 127.2, 125.2, 124.5, 124.3, 122.2, 114.8, 114.0, 108.2, 105.4, 57.1, 55.3, 33.8, 30.5, 26.2, 25.6, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3055, 3031, 2951, 2924, 2860, 1705, 1609, 1499, 1461, 1375, 1350, 1243, 1177, 1083, 1030, 928, 836, 754, 699. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_3$+Na^+: 488.2196 $[M+Na]^+$; found: 488.2208.

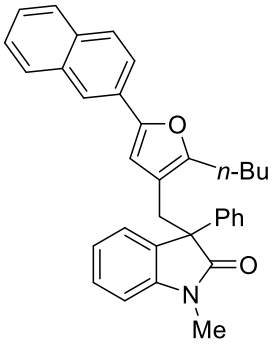


3-((2-Butyl-5-(3,5-dimethylphenyl)furan-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5ah)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2h**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow wax (72.3 mg, 0.156 mmol, 78 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, *J* = 7.0 Hz, 2H), 7.34 (t, *J* = 7.5 Hz, 2H), 7.28 (t, *J* = 7.5 Hz, 1H), 7.25 (t, *J* = 7.5 Hz, 1H), 7.21 (d, *J* =7.0 Hz, 1H), 7.08 (t, *J* = 7.5 Hz,

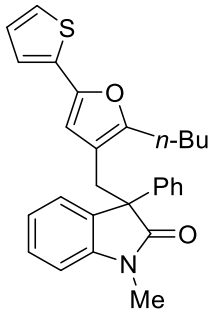
1H), 7.05 (s, 2H), 6.80 (s, 1H), 6.72 (d, J = 7.5 Hz, 1H), 5.89 (s, 1H), 3.43 (d, J = 13.5 Hz, 1H), 3.27 (d, J = 14.0 Hz, 1H), 3.07 (s, 3H), 2.43-2.36 (m, 1H), 2.34-2.30 (m, 1H), 2.28 (s, 6H), 1.53-1.44 (m, 1H), 1.38-1.32 (m, 1H), 1.31-1.25 (m, 2H), 0.89 (t, J = 7.0 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.1, 153.4, 150.8, 144.1, 139.7, 138.0, 131.6, 131.0, 129.0, 128.6, 128.4, 128.3, 128.2, 127.4, 127.2, 125.1, 122.2, 120.9, 114.8, 108.2, 106.8, 57.2, 33.7, 30.5, 26.3, 25.7, 22.5, 21.3, 21.3, 13.9. **IR** (neat, cm^{-1}): ν 3054, 3029, 2955, 2925, 2869, 1711, 1610, 1494, 1469, 1373, 1347, 1253, 1184, 1080, 948, 846, 752, 696. **HRMS** (ESI): *m/z* calcd for $C_{32}H_{33}NO_2$+Na^+: 486.2404 $[M+Na]^+$; found: 486.2424.



3-((2-Butyl-5-(naphthalen-2-yl)furan-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5ai)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2i**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a pale yellow solid (61.1 mg, 0.126 mmol, 63 % yield, MP = 128-130 ºC).

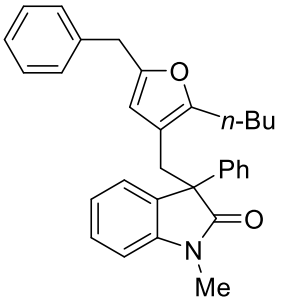
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.89 (s, 1H), 7.78 (d, J = 8.0 Hz, 1H), 7.73 (t, J = 8.0 Hz, 2H), 7.52 (dd, J_1 = 7.0 Hz, J_2= 1.5 Hz, 2H), 7.48 (dd, J_1 = 8.5 Hz, J_2 = 1.5 Hz, 1H), 7.43 (td, J_1 = 8.0 Hz, J_2= 1.0 Hz, 1H), 7.39 (dd, J_1 = 8.0 Hz, J_2= 1.0 Hz, 1H), 7.35 (t, J = 7.5 Hz, 2H), 7.32-7.22 (m, 3H), 7.10 (t, J = 7.5 Hz, 1H), 6.72 (d, J = 7.5 Hz, 1H), 6.00 (s, 1H), 3.46 (d, J = 13.5 Hz, 1H), 3.31 (d, J = 13.5 Hz, 1H), 3.07 (s, 3H), 2.49-2.42 (m, 1H), 2.41-2.34 (m, 1H), 1.59-1.50 (m, 1H), 1.45-1.38 (m, 1H), 1.37-1.29 (m, 2H), 0.91 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 154.1, 150.6, 144.1, 139.7, 133.5, 132.3, 131.6, 128.6, 128.4, 128.3, 128.1, 127.9, 127.7, 127.4, 127.2, 126.3, 125.5, 125.2, 122.2, 122.0, 121.0, 115.2, 108.2, 107.8, 57.2, 33.8, 30.5, 26.3, 25.8, 22.5, 13.9. **IR** (neat, cm^{-1}): ν 3052, 3029, 2956, 2921, 2851, 1712, 1601, 1491, 1465, 1370, 1346, 1256, 1130, 1081, 1019, 949, 893, 822, 752, 699. **HRMS** (ESI): *m/z* calcd for $C_{34}H_{31}NO_2$+H^+: 486.2428 $[M+H]^+$; found: 486.2441.



3-((2-Butyl-5-(thiophen-2-yl)furan-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5aj)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2j**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow solid (65.3 mg, 0.148 mmol, 74 % yield, MP = 133-135 °C).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.50 (d, J = 7.5 Hz, 2H), 7.33 (t, J = 7.5 Hz, 2H), 7.30-7.24 (m, 2H), 7.21 (d, J = 7.5 Hz, 1H), 7.10-7.05 (m, 2H), 6.99 (dd, J_1 = 8.5 Hz, J_2 = 1.0 Hz, 1H), 6.93 (dd, J_1 = 5.0 Hz, J_2 = 3.5 Hz, 1H), 6.74 (d, J = 7.5 Hz, 1H), 5.72 (s, 1H), 3.41 (d, J = 14.0 Hz, 1H), 3.25 (d, J = 13.5 Hz, 1H), 3.08 (s, 3H), 2.43-2.36 (m, 1H), 2.35-2.28 (m, 1H), 1.51-1.43 (m, 1H), 1.39-1.32 (m, 1H), 1.31-1.25 (m, 2H), 0.88 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.0, 153.3, 146.2, 144.1, 139.6, 134.2, 131.5, 128.6, 128.3, 127.4, 127.4, 127.2, 125.1, 123.1, 122.2, 121.3, 115.0, 108.2, 107.0, 57.1, 33.7, 30.4, 26.2, 25.6, 22.4, 13.9. **IR** (neat, cm^{-1}): ν 3066, 2953, 2931, 2869, 1705, 1610, 1493, 1465, 1374, 1349, 1254, 1133, 1085, 949, 850, 809, 749, 701, 644. **HRMS** (ESI): *m/z* calcd for $C_{28}H_{27}NO_2S+H^+$: 442.1835 $[M+H]^+$; found: 442.1850.

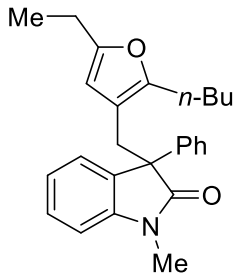


3-((5-Benzyl-2-butylfuran-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5ak)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2k**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow oil (30.5 mg, 0.068 mmol, 34 % yield).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.45 (d, J = 7.0 Hz, 2H), 7.31 (t, J = 7.5 Hz, 2H), 7.26 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 2H), 7.24 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 2H), 7.19 (d, J = 7.5 Hz, 1H), 7.16 (d, J = 7.5 Hz, 1H), 7.04 (t, J = 7.5 Hz, 1H), 6.97 (d, J = 7.0 Hz, 2H), 6.71 (d, J = 8.0 Hz, 1H), 5.16 (s, 1H), 3.71 (d, J = 16.5 Hz, 1H), 3.68 (d, J = 16.5 Hz, 1H), 3.38 (d, J = 14.0 Hz, 1H), 3.18 (d, J = 13.5 Hz, 1H), 2.98 (s, 3H), 2.36-2.23 (m,

2H), 1.44-1.37 (m, 1H), 1.33-1.28 (m, 1H), 1.24-1.19 (m, 2H), 0.85 (t, J = 7.3 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.1, 152.5, 150.9, 144.1, 139.8, 138.8, 131.8, 128.5, 128.4, 128.2, 128.1, 127.3, 127.2, 126.1, 125.1, 122.2, 113.4, 108.2, 108.0, 57.2, 34.1, 33.8, 30.5, 26.1, 25.6, 22.4, 13.9. **IR** (neat, cm^{-1}): ν 3059, 3028, 2955, 2925, 2856, 1710, 1611, 1494, 1469, 1373, 1348, 1254, 1128, 1079, 977, 801, 751, 696. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{31}NO_2$+Na^+: 472.2247 $[M+Na]^+$; found 472.2228.



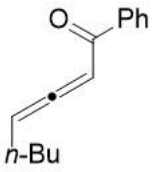
3-((2-Butyl-5-ethylfuran-3-yl)methyl)-1-methyl-3-phenylindolin-2-one (5al)

Prepared according to General Procedure **4** using starting material **1a** and (*E*)-*β*-chloroenone **2l**. The crude mixture was purified via silica-gel flash chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase. The title compound was obtained as a yellow oil (51.9 mg, 0.134 mmol, 67 % yield).

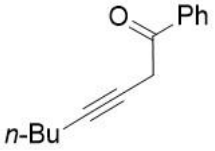
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.48 (d, J = 7.5 Hz, 2H), 7.32 (t, J = 7.5 Hz, 2H), 7.26 (t, J = 7.5 Hz, 2H), 7.16 (d, J = 7.5 Hz, 1H), 7.05 (t, J = 7.5 Hz, 1H), 6.74 (d, J = 7.5 Hz, 1H), 5.17 (s, 1H), 3.34 (d, J = 13.5 Hz, 1H), 3.21 (d, J = 13.5 Hz, 1H), 3.07 (s, 3H), 2.38 (q, J = 7.5 Hz, 2H), 2.33-2.26 (m, 1H), 2.25-2.18 (m, 1H), 1.43-1.35 (m, 1H), 1.31-1.26 (m, 1H), 1.25-1.20 (m, 2H), 1.02 (t, J = 7.5 Hz, 3H), 0.86 (t, J = 7.5 Hz, 3H). **^{13}C NMR** (125 MHz, $CDCl_3$) δ 178.2, 154.4, 151.6, 144.1, 139.8, 131.8, 128.5, 128.1, 127.3, 127.2, 125.2, 122.1, 113.0, 108.0, 105.6, 57.2, 33.8, 30.6, 26.2, 25.6, 22.5, 21.1, 13.9, 12.2. **IR** (neat, cm^{-1}): ν 3055, 3028, 2957, 2928, 2871, 1710, 1611, 1494, 1469, 1373, 1347, 1254, 1186, 1080, 947, 811, 752, 697. **HRMS** (ESI): *m/z* calcd for $C_{26}H_{29}NO_2$+H^+: 388.2271 $[M+H]^+$; found: 388.2267.

8) Mechanistic studies

Synthesis of 6, 7, 3aa-Pd, 8

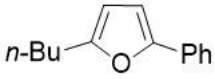


Phenylocta-2,3-dien-1-one (6):
Prepared according to literature procedure.[1]



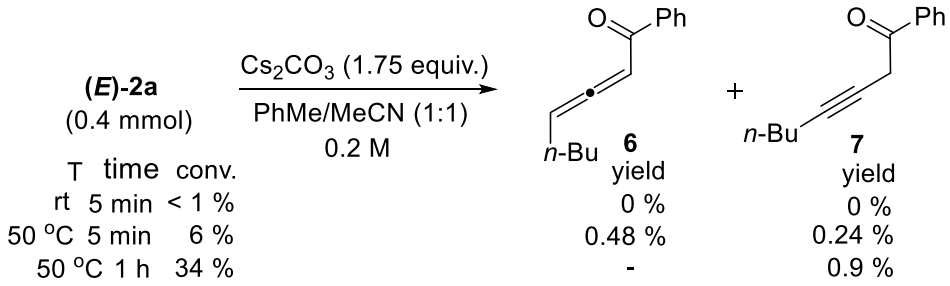
Phenyloct-3-yn-1-one (7):
Prepared according to literature procedure.[1]

Palladacycle 3aa-Pd:
Prepared according to literature procedure.[2a]



2-butyl-5-phenylfuran (8):
Prepared according to literature procedure.[1]

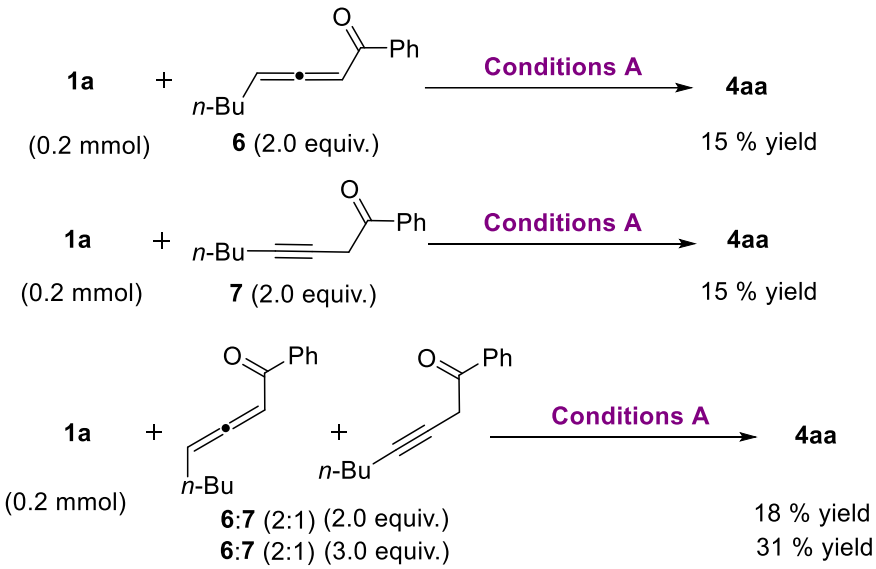
Confirmation of (*E*)-2a as a precursor in the spirocyclizations



T	time	conv.	6 yield	7 yield
rt	5 min	< 1 %	0 %	0 %
50 °C	5 min	6 %	0.48 %	0.24 %
50 °C	1 h	34 %	-	0.9 %

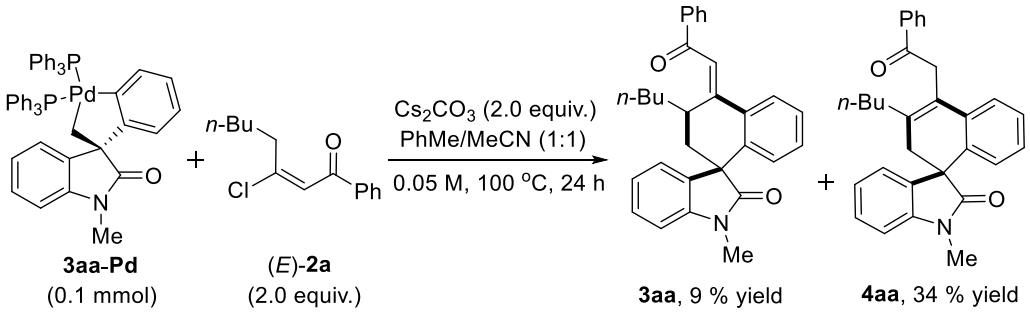
To three flame-dried, 3-dram vial charged with (*E*)-*β*-chloroenone **2a** (94.5 mg, 0.4 mmol, 1.0 equiv.) under argon were added dry PhMe/MeCN (1:1, 2.0 mL) and Cs_2CO_3 (228.1 mg, 0.7 mmol, 1.75 equiv.), respectively. The three vials were stirred at: (1) room temperature, 5 minutes; (2) 50 °C, 5 minutes; (3) 50 °C, 1h. The reactions were each passed through a pad of silica gel washing with EtOAc. The filtrates were concentrated under reduced pressure and the residue were purified by silica gel flash column chromatography using 20:1 Pentanes: Et_2O v:v as the mobile phase. The conversions of (*E*)-**2a**, the yields of **6** and **7** were determined by ^1H NMR analysis of the purified mixture of (*E*)-**2a**, **6**, and **7**.

Spirocyclizations synthesized from allenyl ketone 6, alkynyl ketone 7



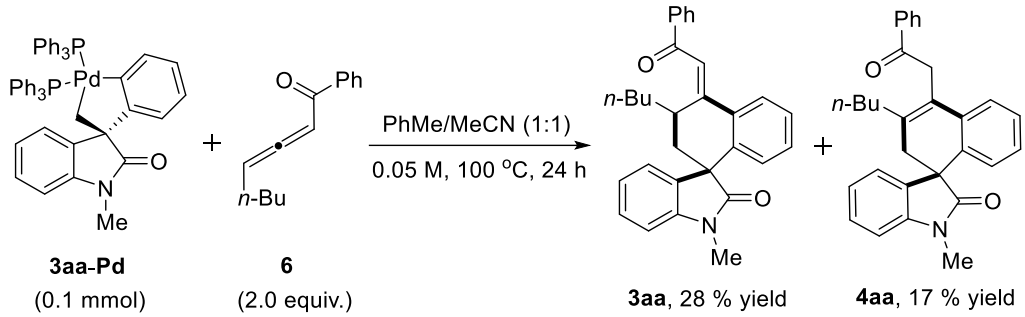
A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1a** (72.6 mg, 0.20 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol, 5 mol %), PPh_3 (10.5 mg, 0.04 mmol, 20 mol %) and Cs_2CO_3 (228.1 mg, 0.7 mmol, 3.5 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed PhMe (0.5 mL) and MeCN (0.5 mL) were added and the mixture was stirred at room temperature for 5 minutes. Allenyl ketone **6** (80mg, 0.4 mmol, 2.0 equiv.) or alkynyl ketone **7** (80mg, 0.4 mmol, 2.0 equiv.), or the mixture of **6** and **7** (80mg, 0.4 mmol, 2.0 equiv.) was dissolved in anhydrous PhMe: MeCN (1:1) (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase, affording the corresponding product **4aa** in 15 % (13.1 mg), 15 % (12.7 mg), 18 % (15.7 mg), 31 % (27 mg) yields.

Palladacycle as an intermediate in the spirocyclizations



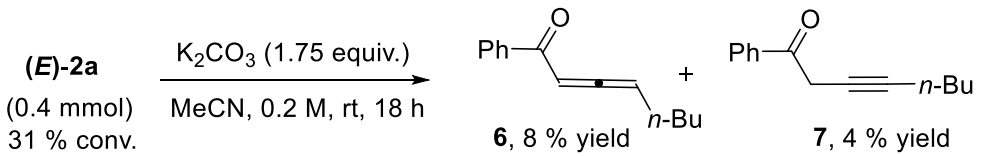
A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, palladacycle **3aa-Pd** (86.5 mg, 0.10 mmol, 1.0 equiv.), and Cs_2CO_3 (65.2 mg, 0.2 mmol, 2.0 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed PhMe

(0.5 mL) and MeCN (0.5 mL) were added and the mixture was stirred at room temperature for 5 minutes. (*E*)-*β*-chloroenone **2a** (47.2 mg, 0.2 mmol, 2.0 equiv.) was dissolved in anhydrous PhMe: MeCN (1:1) (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. Obtained 4 mg of **3aa** (9 % yield) and 14.8 mg of **4aa** (34 % yield).



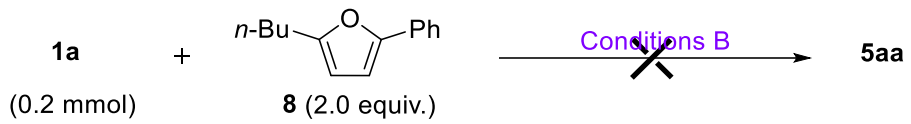
A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, palladacycle **3aa-Pd** (86.5 mg, 0.10 mmol, 1.0 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed PhMe (0.5 mL) and MeCN (0.5 mL) were added and the mixture was stirred at room temperature for 5 minutes. Allenyl ketone **6** (40 mg, 0.2 mmol, 2.0 equiv.) was dissolved in anhydrous PhMe: MeCN (1:1) (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using 5:1 Pentanes: Et_2O v:v as the mobile phase. Obtained 12.2 mg of **3aa** (28 % yield) and 7.4 mg of **4aa** (17 % yield).

Confirmation of (*E*)-2a as a precursor in the cascade cyclizations



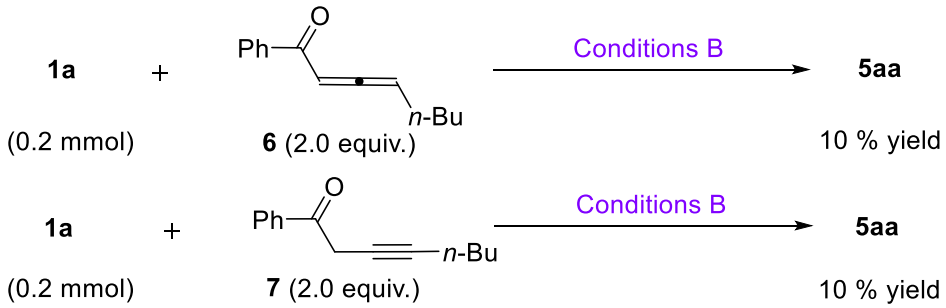
To a flame-dried, 3-dram vial charged with (*E*)-*β*-chloroenone **2a** (94.5 mg, 0.4 mmol, 1.0 equiv.) under argon were added dry MeCN (2.0 mL) and K_2CO_3 (96.7 mg, 0.7 mmol, 1.75 equiv.) at ambient temperature. The solution was stirred for 18 h and concentrated under reduced pressure. The crude product was purified by silica gel flash column chromatography using 20:1 Pentanes: Et_2O v:v as the mobile phase, affording the mixture of allenyl ketone **6** and alkynyl ketone **7** in 12 % yield. The ratio of **6**/**7** was analyzed by ^1H NMR spectroscopy.

Determining whether the cycloisomerized furan of (*E*)-2a was a catalytically active intermediate



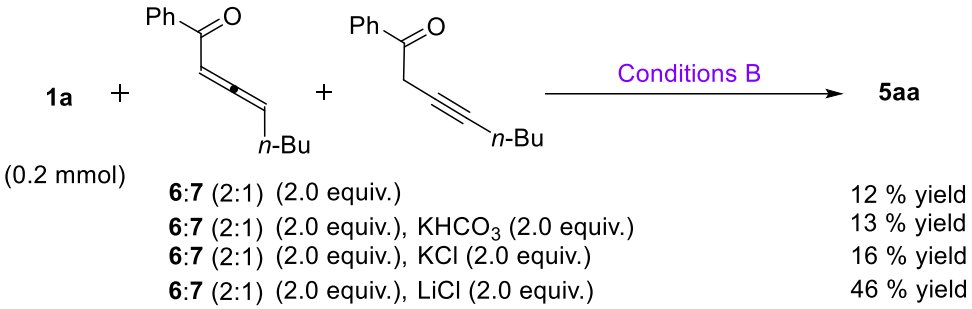
A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1a** (72.6 mg, 0.20 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol, 5 mol %), PPh_3 (10.5 mg, 0.04 mmol, 20 mol %) and K_2CO_3 (96.7 mg, 0.7 mmol, 3.5 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed MeCN (1.0 mL) were added and the mixture was stirred at room temperature for 5 minutes. 2-Butyl-5-phenylfuran **8** (80 mg, 0.4 mmol, 2.0 equiv.) was dissolved in anhydrous MeCN (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was monitored, no corresponding product **5aa** was obtained.

Cascade cyclizations synthesized from allenyl ketone 6, alkynyl ketone 7



A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1a** (72.6 mg, 0.20 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol, 5 mol %), PPh_3 (10.5 mg, 0.04 mmol, 20 mol %) and K_2CO_3 (96.7 mg, 0.7 mmol, 3.5 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed MeCN (1.0 mL) were added and the mixture was stirred at room temperature for 5 minutes. Allenyl ketone **6** (80 mg, 0.4 mmol, 2.0 equiv.) or alkynyl ketone **7** (80 mg, 0.4 mmol, 2.0 equiv.) was dissolved in anhydrous MeCN (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase, affording the corresponding product **5aa** in 10 % (9.1 mg), 10 % (8.5 mg) yield, respectively.

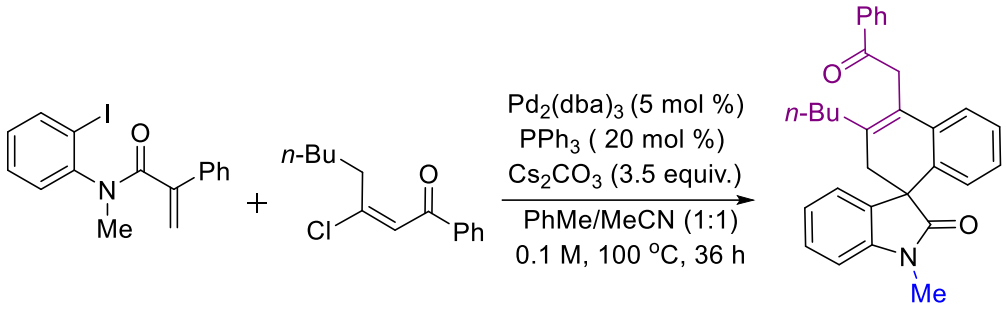
Cascade cyclizations employing allenyl ketone 6 and alkynyl ketone 7 without or with additives



A flame-dried, 3-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1a** (72.6 mg, 0.20 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (9.2 mg, 0.01 mmol, 5 mol %), PPh_3 (10.5 mg, 0.04 mmol, 20 mol %), K_2CO_3 (96.7 mg, 0.7 mmol, 3.5 equiv.) and additive (0.40 mmol, 2.0 equiv.), and was purged with argon for 5 minutes. Anhydrous and degassed MeCN (1.0 mL) were added and the mixture was stirred at room temperature for 5 minutes. The mixture of allenyl ketone **6** and alkynyl ketone **7** (80 mg, 0.4 mmol, 2.0 equiv.) was dissolved in anhydrous MeCN (1.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 3-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using 15:1 Pentanes: Et_2O v:v as the mobile phase, affording the corresponding product **5aa** in 12 % (10.4 mg), 13 % (11.3 mg), 16 % (13.9 mg), 46 % (40 mg) yields.

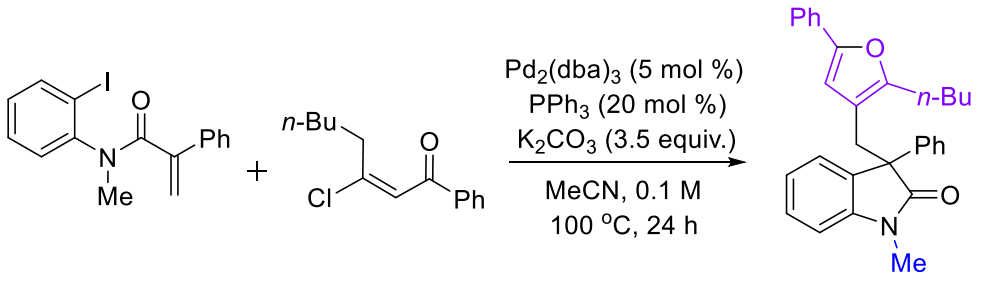
9) Scale up and product derivatization experiments

Scale up



1a **(*E*)-2a** **4aa**

A flame-dried, 9.5-dram vial under argon atmosphere was charged with a stir bar, acrylamide **1a** (363 mg, 1.0 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (46 mg, 0.05 mmol, 5 mol %), PPh_3 (53 mg, 0.2 mmol, 20 mol %) and Cs_2CO_3 (1.14 g, 3.5 mmol, 3.5 equiv.), and was purged with argon for 10 minutes. Anhydrous and degassed PhMe (3.0 mL) and MeCN (3.0 mL) were added and the mixture was stirred at room temperature for 10 minutes. *β*-chloroenone (*E*)-**2a** (472 mg, 2.0 mmol, 2.0 equiv.) was dissolved in anhydrous PhMe: MeCN (1:1) (4.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 9.5-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 36 hours. The reaction mixture was then cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using the indicated mobile phase.

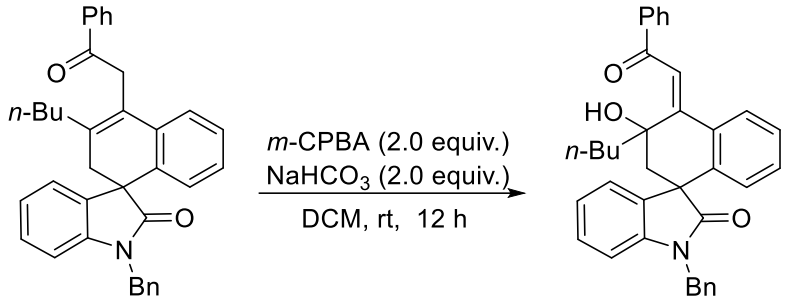


1a **(*E*)-2a** **5aa**

A flame-dried, 9.5-dram vial under argon atmosphere was charged with acrylamide **1a** (363 mg, 1.0 mmol, 1.0 equiv.), $Pd_2(dba)_3$ (46 mg, 0.05 mmol, 5 mol %), PPh_3 (53 mg, 0.2 mmol, 20 mol %) and K_2CO_3 (484 mg, 3.5 mmol, 3.5 equiv.), and was purged with argon for 10 minutes. Anhydrous and degassed MeCN (6.0 mL) were added and the mixture was stirred at room temperature for 10 minutes. *β*-chloroenone (*E*)-**2a** (472 mg, 2.0 mmol, 2.0 equiv.) was dissolved in anhydrous MeCN (4.0 mL) and transferred to the vial via syringe, and the vial was then purged with argon for 5 minutes. A Teflon lined screw cap was fitted on the 9.5-dram vial. The vial was sealed with Teflon tape and placed in a preheated oil bath at 100 °C for 24 hours. The reaction mixture was then

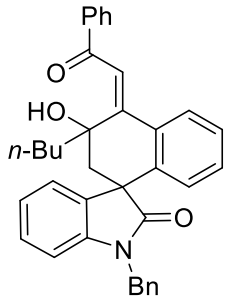
cooled down to room temperature and was filtered through a plug of silica gel using EtOAc. The filtrate was concentrated under reduced pressure and the residue was purified by silica gel flash column chromatography using the indicated mobile phase.

Product derivatization experiments



4ha **9**

m-CPBA (51.8 mg, 0.3 mmol, 2.0 equiv) and $NaHCO_3$ (25.3 mg, 0.3 mmol, 2.0 equiv.) were dissolved in 5.0 mL dichloromethane at room temperature and stirred for 5min. Spirooxindole **4ha** (76.8 mg, 0.15 mmol) was added and the mixture was stirred at room temperature for 12 h. The reaction mixture was concentrated and purified by silica gel column chromatography using the specified solvent.

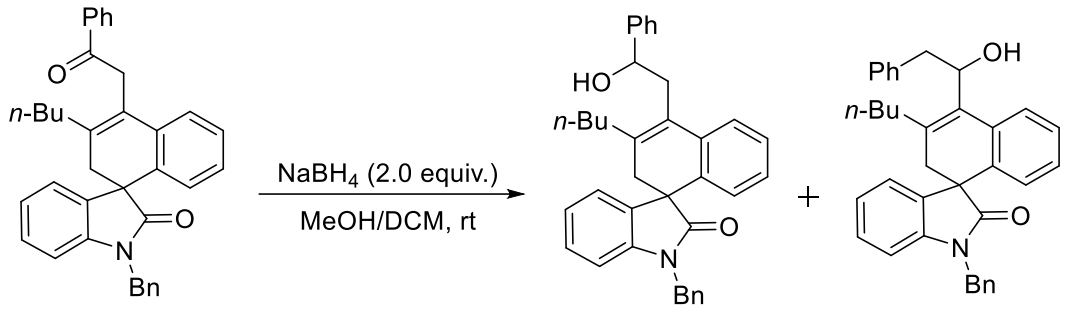


(Z)-1-benzyl-3'-butyl-3'-hydroxy-4'-(2-oxo-2-phenylethylidene)-3',4'-dihydro-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (9)

The crude material was purified via silica-gel flash chromatography using 8:1 Pentanes: EtOAc v:v as the mobile phase. The title compound was obtained as a pale yellow solid (61.7 mg, 0.12 mmol, 78 % yield, MP = 182-183 ºC).

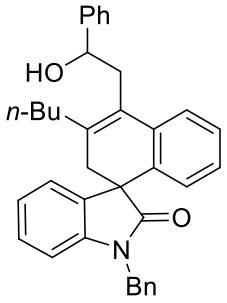
^{1}H NMR (500 MHz, $CDCl_3$) δ 7.97 (d, J = 7.5 Hz, 2H), 7.33 (t, J = 7.0 Hz, 2H), 7.31 -7.26 (m, 5H), 7.22 (d, J = 8.0 Hz, 1H), 7.15-7.10 (m, 3H), 7.07 (d, J = 7.0 Hz, 1H), 6.98 (s, 1H), 6.92 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.87 (d, J = 8.0 Hz, 1H), 6.84 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.47 (d, J = 7.5 Hz, 1H), 5.08 (d, J = 16.0 Hz, 1H), 4.85 (d, J = 15.5 Hz, 1H), 4.67 (s, 1H), 2.43 (d, J = 14.5 Hz, 1H), 2.35 (d, J = 14.5 Hz, 1H), 2.02-1.94 (m, 1H), 1.91-1.84 (m, 1H), 1.51-1.43 (m, 1H), 1.41-1.33 (m, 3H), 0.91 (t, J = 7.0 Hz, 3H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ 198.2, 179.8, 153.8, 142.7, 137.4, 137.1, 135.5, 134.4, 132.5, 132.4, 130.9, 129.4, 129.0, 128.9, 128.8, 127.9, 127.8, 127.2, 127.1, 125.8, 125.6, 124.3, 123.6, 109.6, 73.6, 52.2, 44.7, 44.1, 43.9, 26.2, 23.1, 14.0. **IR** (neat, cm^{-1}): ν 3444, 3062, 3033, 3005, 2959, 2924, 2856, 1681, 1633, 1490, 1467, 1371, 1349, 1268, 1216, 1174, 1082, 954, 855, 779, 745, 693. **HRMS** (ESI): *m/z* calcd for

$C_{36}H_{33}NO_3$+H^+: 528.2533 $[M+H]^+$; found: 528.2538.



4ha **10** **11**

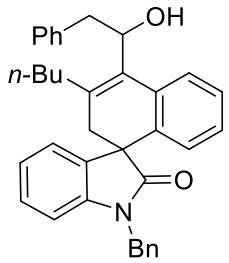
A solution of **4ha** (204.8 mg, 0.4 mmol) in 4.0 mL MeOH and 2.0 mL DCM was cooled to 0°C, and then $NaBH_4$ (30.3 mg, 0.8 mmol) was added successively. The reaction mixture was stirred at 0 °C until the complete consumption of **4ha** as monitored by thin layer chromatography. Then, saturated aq. NH_4Cl solution was added. The mixture was extracted with CH_2Cl_2. The combined organic phase was dried over $MgSO_4$, filtered, concentrated and purified by silica gel column chromatography using the specified solvent.



1-Benzyl-3'-butyl-4'-(2-hydroxy-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (10)

The crude material was purified via silica-gel flash chromatography using 5:1 Pentanes: EtOAc v:v as the mobile phase. The title compound was obtained as a pale yellow solid (67.7 mg, 0.13 mmol, 33 % yield, MP = 65-67 °C).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.60-7.56 (m, 3H), 7.42 (t, J = 7.5 Hz, 2H), 7.37 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 7.33-7.25 (m, 8H), 7.14 (td, J_1 = 7.5 Hz, J_2 = 0.5 Hz, 1H), 7.09 (td, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 6.86 (d, J = 8.0 Hz, 1H), 6.71 (dd, J_1 = 7.5 Hz, J_2 = 1.0 Hz, 1H), 4.97-4.93 (m, 1H), 4.94 (d, J = 15.5 Hz, 1H), 4.83 (d, J = 15.5 Hz, 1H), 3.17-3.03 (m, 2H), 3.11 (d, J = 16.5 Hz, 1H), 2.47-2.35 (m, 2H), 2.43 (d, J = 16.5 Hz, 1H), 1.71-1.61 (m, 1H), 1.46-1.34 (m, 3H), 0.94 (t, J = 7.0 Hz, 3H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ 177.5, 144.8, 142.7, 136.0, 135.8, 135.8, 135.0, 133.2, 128.7, 128.3, 128.3, 128.2, 127.6, 127.5, 127.3, 126.9, 126.8, 126.1, 125.6, 124.4, 124.3, 123.1, 109.3, 70.6, 51.4, 43.6, 39.7, 38.5, 34.3, 30.1, 23.0, 14.0. **IR** (neat, cm^{-1}): ν 3433, 3087, 3061, 3028, 2956, 2927, 2859, 2245, 1693, 1611, 1484, 1454, 1435, 1378, 1359, 1346, 1301, 1270, 1239, 1200, 1169, 1104, 1080, 1053, 1028, 1012, 976, 946, 908, 873, 729, 699,670, 647, 633, 611. **HRMS** (ESI): *m/z* calcd for $C_{36}H_{35}NO_2$+H^+: 514.2741 $[M+H]^+$; found: 514.2754.

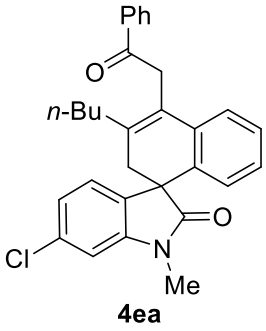


1-benzyl-3'-butyl-4'-(1-hydroxy-2-phenylethyl)-2'*H*-spiro[indoline-3,1'-naphthalen]-2-one (11)

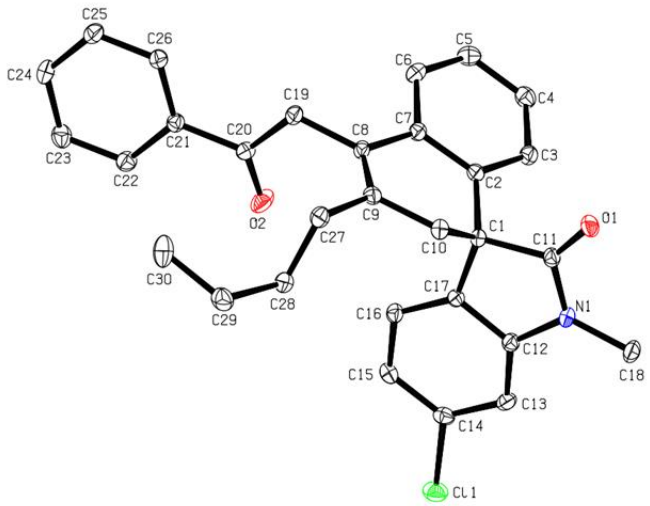
The crude material was purified via silica-gel flash chromatography using 5:1 Pentanes: EtOAc v:v as the mobile phase. The title compound was obtained as a pale yellow solid (128.6 mg, 0.25 mmol, 63 % yield, MP = 61-63 ºC).

^{1}H NMR (500 MHz, $CDCl_3$) δ 7.56 (d, *J* = 7.0 Hz, 1H), 7.54 (d, *J* = 7.0 Hz, 2H), 7.45 (d, *J* = 7.5 Hz, 1H), 7.41 (t, *J* = 7.5 Hz, 2H), 7.39-7.35 (m, 4H), 7.34-7.30 (m, 2H), 7.29 (d, *J* = 8.0 Hz, 1H), 7.22 (t, *J* = 7.8 Hz, 1H), 7.08 (t, *J* = 7.5 Hz, 1H), 7.02 (t, *J* = 7.5 Hz, 1H), 6.86 (d, *J* = 7.5 Hz, 1H), 6.80 (d, *J* = 7.5 Hz, 1H), 5.16-5.12 (m, 1H), 5.02 (d, *J* = 14.5 Hz, 1H), 4.99 (d, *J* = 14.5 Hz, 1H), 3.23-3.10 (m, 2H), 2.88 (d, *J* = 16.5 Hz, 1H), 2.74 (d, *J* = 16.5 Hz, 1H), 2.46-2.34 (m, 2H), 1.55-1.36 (m, 4H), 0.96 (t, *J* = 7.3 Hz, 3H). **^{13}C NMR (**125 MHz, $CDCl_3$) δ 179.1, 144.9, 141.6, 136.6, 135.9, 134.7, 134.5, 133.6, 128.7, 128.3, 128.1, 127.9, 127.7, 127.6, 127.3, 127.1, 126.7, 125.6, 125.5, 124.6, 124.1, 122.9, 109.2, 73.5, 52.0, 43.7, 38.8, 37.7, 34.1, 29.6, 22.8, 13.9. **IR** (neat, cm^{-1}): ν 3434, 3034, 3059, 3029, 2954, 2925, 2862, 1692, 1607, 1486, 1461, 1348, 1301, 1200, 1169, 1081, 1046, 1029, 941, 908, 869, 749, 729, 697, 650, 608. **HRMS** (ESI): *m/z* calcd for $C_{36}H_{35}NO_2$+Na^+: 526.2560 $[M+Na]^+$; found: 536.2565.

10) X-Ray Crystal Structure



4ea



Product 4ea CCDC 2179947

Table S3. Crystal data and structure refinement for d18163_a.

Identification code	d18163_a	
Empirical formula	C30 H28 Cl N O2	
Formula weight	469.98	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	C2/c	
Unit cell dimensions	a = 24.9121(14) Å	α= 90°.
	b = 12.9260(8) Å	β= 105.923(2)°.
	c = 15.4180(8) Å	γ = 90°.
Volume	4774.3(5) $Å^3$	
Z	8	
Density (calculated)	1.308 Mg/m^3	
Absorption coefficient	0.189 mm^{-1}	
F(000)	1984	
Crystal size	0.290 x 0.200 x 0.100 mm^3	
Theta range for data collection	1.700 to 27.560°.	
Index ranges	-31<=h<=32, -16<=k<=16, -20<=l<=19	
Reflections collected	45414	
Independent reflections	5513 [R(int) = 0.0502]	
Completeness to theta = 25.242°	100.0 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7456 and 0.6962	

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	5513 / 0 / 317
Goodness-of-fit on F^2	1.008
Final R indices [I>2sigma(I)]	R1 = 0.0403, wR2 = 0.0897
R indices (all data)	R1 = 0.0752, wR2 = 0.1071
Extinction coefficient	n/a
Largest diff. peak and hole	0.290 and -0.323 e.$Å^{-3}$

Table S4. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for d18163_a. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Cl(1)	4789(1)	8705(1)	4667(1)	36(1)
O(1)	6662(1)	9209(1)	1704(1)	30(1)
O(2)	6444(1)	4666(1)	4054(1)	41(1)
N(1)	6070(1)	9459(1)	2593(1)	24(1)
C(1)	6452(1)	7778(1)	2614(1)	21(1)
C(2)	7037(1)	7524(1)	3191(1)	21(1)
C(3)	7383(1)	8296(1)	3675(1)	25(1)
C(4)	7907(1)	8064(2)	4238(1)	29(1)
C(5)	8091(1)	7050(2)	4302(1)	30(1)
C(6)	7750(1)	6275(1)	3825(1)	27(1)
C(7)	7216(1)	6486(1)	3265(1)	22(1)
C(8)	6851(1)	5663(1)	2742(1)	22(1)
C(9)	6414(1)	5921(1)	2046(1)	23(1)
C(10)	6283(1)	7038(1)	1804(1)	24(1)
C(11)	6422(1)	8889(1)	2241(1)	24(1)
C(12)	5837(1)	8846(1)	3148(1)	23(1)
C(13)	5462(1)	9143(1)	3617(1)	26(1)
C(14)	5282(1)	8375(1)	4102(1)	26(1)
C(15)	5475(1)	7368(1)	4145(1)	26(1)
C(16)	5862(1)	7090(1)	3679(1)	24(1)
C(17)	6040(1)	7832(1)	3175(1)	22(1)
C(18)	5930(1)	10533(1)	2341(1)	31(1)
C(19)	6988(1)	4546(1)	2997(1)	26(1)
C(20)	6718(1)	4121(1)	3692(1)	24(1)
C(21)	6795(1)	2992(1)	3914(1)	22(1)
C(22)	6469(1)	2540(1)	4416(1)	27(1)
C(23)	6542(1)	1507(1)	4664(1)	32(1)
C(24)	6943(1)	923(1)	4419(1)	30(1)
C(25)	7265(1)	1360(1)	3914(1)	32(1)
C(26)	7188(1)	2392(1)	3658(1)	28(1)
C(27)	6019(1)	5156(1)	1454(1)	28(1)
C(28)	5491(1)	4994(1)	1764(1)	28(1)
C(29)	5132(1)	4090(2)	1294(1)	36(1)
C(30)	5398(1)	3043(2)	1595(2)	51(1)

Table S5. Bond lengths [Å] and angles [°] for d18163_a.

Cl(1)-C(14)	1.7440(18)
O(1)-C(11)	1.217(2)
O(2)-C(20)	1.218(2)
N(1)-C(11)	1.367(2)
N(1)-C(12)	1.404(2)
N(1)-C(18)	1.458(2)
C(1)-C(17)	1.514(2)
C(1)-C(2)	1.521(2)
C(1)-C(10)	1.538(2)
C(1)-C(11)	1.541(2)
C(2)-C(3)	1.393(2)
C(2)-C(7)	1.408(2)
C(3)-C(4)	1.388(2)
C(3)-H(3A)	0.9500
C(4)-C(5)	1.383(3)
C(4)-H(4A)	0.9500
C(5)-C(6)	1.387(3)
C(5)-H(5A)	0.9500
C(6)-C(7)	1.401(2)
C(6)-H(6A)	0.9500
C(7)-C(8)	1.485(2)
C(8)-C(9)	1.345(2)
C(8)-C(19)	1.511(2)
C(9)-C(10)	1.504(2)
C(9)-C(27)	1.511(2)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(12)-C(13)	1.384(2)
C(12)-C(17)	1.402(2)
C(13)-C(14)	1.389(2)
C(13)-H(13A)	0.9500
C(14)-C(15)	1.383(2)
C(15)-C(16)	1.398(2)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.382(2)
C(16)-H(16A)	0.9500

C(18)-H(18A)	0.9800
C(18)-H(18B)	0.9800
C(18)-H(18C)	0.9800
C(19)-C(20)	1.516(2)
C(19)-H(19A)	0.97(2)
C(19)-H(19B)	0.96(2)
C(20)-C(21)	1.499(2)
C(21)-C(26)	1.389(2)
C(21)-C(22)	1.394(2)
C(22)-C(23)	1.386(3)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.386(3)
C(23)-H(23A)	0.9500
C(24)-C(25)	1.382(3)
C(24)-H(24A)	0.9500
C(25)-C(26)	1.390(2)
C(25)-H(25A)	0.9500
C(26)-H(26A)	0.9500
C(27)-C(28)	1.532(3)
C(27)-H(27A)	0.9900
C(27)-H(27B)	0.9900
C(28)-C(29)	1.529(2)
C(28)-H(28A)	0.9900
C(28)-H(28B)	0.9900
C(29)-C(30)	1.523(3)
C(29)-H(29A)	0.9900
C(29)-H(29B)	0.9900
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800

C(11)-N(1)-C(12)	110.81(14)
C(11)-N(1)-C(18)	122.76(14)
C(12)-N(1)-C(18)	126.21(15)
C(17)-C(1)-C(2)	111.48(13)
C(17)-C(1)-C(10)	114.55(13)
C(2)-C(1)-C(10)	110.21(14)
C(17)-C(1)-C(11)	101.53(13)

C(2)-C(1)-C(11)	111.10(13)
C(10)-C(1)-C(11)	107.61(13)
C(3)-C(2)-C(7)	120.24(16)
C(3)-C(2)-C(1)	120.76(15)
C(7)-C(2)-C(1)	118.92(15)
C(4)-C(3)-C(2)	121.23(16)
C(4)-C(3)-H(3A)	119.4
C(2)-C(3)-H(3A)	119.4
C(5)-C(4)-C(3)	118.97(17)
C(5)-C(4)-H(4A)	120.5
C(3)-C(4)-H(4A)	120.5
C(4)-C(5)-C(6)	120.34(17)
C(4)-C(5)-H(5A)	119.8
C(6)-C(5)-H(5A)	119.8
C(5)-C(6)-C(7)	121.73(16)
C(5)-C(6)-H(6A)	119.1
C(7)-C(6)-H(6A)	119.1
C(6)-C(7)-C(2)	117.46(15)
C(6)-C(7)-C(8)	122.10(15)
C(2)-C(7)-C(8)	120.41(15)
C(9)-C(8)-C(7)	119.80(15)
C(9)-C(8)-C(19)	121.35(16)
C(7)-C(8)-C(19)	118.83(15)
C(8)-C(9)-C(10)	120.53(15)
C(8)-C(9)-C(27)	124.77(16)
C(10)-C(9)-C(27)	114.70(14)
C(9)-C(10)-C(1)	113.80(13)
C(9)-C(10)-H(10A)	108.8
C(1)-C(10)-H(10A)	108.8
C(9)-C(10)-H(10B)	108.8
C(1)-C(10)-H(10B)	108.8
H(10A)-C(10)-H(10B)	107.7
O(1)-C(11)-N(1)	125.02(16)
O(1)-C(11)-C(1)	126.01(16)
N(1)-C(11)-C(1)	108.95(14)
C(13)-C(12)-C(17)	122.28(16)
C(13)-C(12)-N(1)	127.85(16)
C(17)-C(12)-N(1)	109.87(15)

C(12)-C(13)-C(14)	116.56(16)
C(12)-C(13)-H(13A)	121.7
C(14)-C(13)-H(13A)	121.7
C(15)-C(14)-C(13)	122.65(16)
C(15)-C(14)-Cl(1)	119.29(14)
C(13)-C(14)-Cl(1)	118.06(14)
C(14)-C(15)-C(16)	119.76(16)
C(14)-C(15)-H(15A)	120.1
C(16)-C(15)-H(15A)	120.1
C(17)-C(16)-C(15)	118.98(16)
C(17)-C(16)-H(16A)	120.5
C(15)-C(16)-H(16A)	120.5
C(16)-C(17)-C(12)	119.73(16)
C(16)-C(17)-C(1)	131.49(15)
C(12)-C(17)-C(1)	108.76(14)
N(1)-C(18)-H(18A)	109.5
N(1)-C(18)-H(18B)	109.5
H(18A)-C(18)-H(18B)	109.5
N(1)-C(18)-H(18C)	109.5
H(18A)-C(18)-H(18C)	109.5
H(18B)-C(18)-H(18C)	109.5
C(8)-C(19)-C(20)	114.66(14)
C(8)-C(19)-H(19A)	112.0(12)
C(20)-C(19)-H(19A)	107.0(12)
C(8)-C(19)-H(19B)	112.8(11)
C(20)-C(19)-H(19B)	104.9(11)
H(19A)-C(19)-H(19B)	104.6(17)
O(2)-C(20)-C(21)	120.70(15)
O(2)-C(20)-C(19)	121.89(16)
C(21)-C(20)-C(19)	117.41(14)
C(26)-C(21)-C(22)	119.10(16)
C(26)-C(21)-C(20)	122.33(15)
C(22)-C(21)-C(20)	118.55(15)
C(23)-C(22)-C(21)	120.36(16)
C(23)-C(22)-H(22A)	119.8
C(21)-C(22)-H(22A)	119.8
C(24)-C(23)-C(22)	119.95(17)
C(24)-C(23)-H(23A)	120.0

C(22)-C(23)-H(23A)	120.0
C(25)-C(24)-C(23)	120.21(17)
C(25)-C(24)-H(24A)	119.9
C(23)-C(24)-H(24A)	119.9
C(24)-C(25)-C(26)	119.82(17)
C(24)-C(25)-H(25A)	120.1
C(26)-C(25)-H(25A)	120.1
C(21)-C(26)-C(25)	120.54(16)
C(21)-C(26)-H(26A)	119.7
C(25)-C(26)-H(26A)	119.7
C(9)-C(27)-C(28)	111.92(14)
C(9)-C(27)-H(27A)	109.2
C(28)-C(27)-H(27A)	109.2
C(9)-C(27)-H(27B)	109.2
C(28)-C(27)-H(27B)	109.2
H(27A)-C(27)-H(27B)	107.9
C(29)-C(28)-C(27)	113.39(15)
C(29)-C(28)-H(28A)	108.9
C(27)-C(28)-H(28A)	108.9
C(29)-C(28)-H(28B)	108.9
C(27)-C(28)-H(28B)	108.9
H(28A)-C(28)-H(28B)	107.7
C(30)-C(29)-C(28)	112.66(16)
C(30)-C(29)-H(29A)	109.1
C(28)-C(29)-H(29A)	109.1
C(30)-C(29)-H(29B)	109.1
C(28)-C(29)-H(29B)	109.1
H(29A)-C(29)-H(29B)	107.8
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S6. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for d18163_a. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Cl(1)	30(1)	41(1)	41(1)	-8(1)	17(1)	1(1)
O(1)	30(1)	27(1)	33(1)	7(1)	11(1)	-4(1)
O(2)	57(1)	29(1)	48(1)	9(1)	34(1)	17(1)
N(1)	28(1)	16(1)	30(1)	4(1)	8(1)	1(1)
C(1)	22(1)	18(1)	24(1)	2(1)	7(1)	0(1)
C(2)	22(1)	22(1)	22(1)	2(1)	10(1)	-1(1)
C(3)	28(1)	21(1)	29(1)	-1(1)	11(1)	0(1)
C(4)	28(1)	30(1)	28(1)	-4(1)	7(1)	-5(1)
C(5)	24(1)	37(1)	28(1)	-1(1)	4(1)	3(1)
C(6)	30(1)	24(1)	28(1)	2(1)	9(1)	7(1)
C(7)	25(1)	21(1)	21(1)	2(1)	10(1)	1(1)
C(8)	27(1)	16(1)	28(1)	0(1)	14(1)	1(1)
C(9)	25(1)	22(1)	25(1)	-2(1)	12(1)	-1(1)
C(10)	27(1)	22(1)	24(1)	0(1)	7(1)	-1(1)
C(11)	22(1)	21(1)	26(1)	2(1)	2(1)	-3(1)
C(12)	21(1)	20(1)	25(1)	0(1)	3(1)	-1(1)
C(13)	22(1)	22(1)	31(1)	-4(1)	4(1)	4(1)
C(14)	19(1)	31(1)	26(1)	-5(1)	5(1)	-1(1)
C(15)	25(1)	26(1)	27(1)	-1(1)	8(1)	-6(1)
C(16)	25(1)	18(1)	27(1)	-2(1)	6(1)	-2(1)
C(17)	19(1)	20(1)	25(1)	-1(1)	4(1)	-1(1)
C(18)	32(1)	18(1)	38(1)	5(1)	3(1)	2(1)
C(19)	29(1)	19(1)	32(1)	0(1)	12(1)	2(1)
C(20)	23(1)	23(1)	27(1)	0(1)	7(1)	3(1)
C(21)	23(1)	21(1)	23(1)	-1(1)	5(1)	0(1)
C(22)	30(1)	28(1)	26(1)	1(1)	12(1)	3(1)
C(23)	39(1)	30(1)	28(1)	3(1)	14(1)	-3(1)
C(24)	40(1)	18(1)	30(1)	3(1)	8(1)	1(1)
C(25)	34(1)	24(1)	40(1)	1(1)	16(1)	6(1)
C(26)	29(1)	23(1)	36(1)	3(1)	15(1)	1(1)
C(27)	31(1)	23(1)	30(1)	-6(1)	9(1)	-1(1)
C(28)	29(1)	22(1)	34(1)	-3(1)	9(1)	-1(1)
C(29)	32(1)	34(1)	39(1)	-8(1)	8(1)	-7(1)
C(30)	67(2)	27(1)	57(1)	-7(1)	15(1)	-12(1)

Table S7. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for d18163_a.

	x	y	z	U(eq)
H(3A)	7258	8993	3618	31
H(4A)	8137	8595	4574	35
H(5A)	8452	6883	4676	36
H(6A)	7883	5582	3879	32
H(10A)	5878	7108	1519	29
H(10B)	6479	7247	1353	29
H(13A)	5334	9836	3608	31
H(15A)	5345	6867	4491	31
H(16A)	5999	6402	3707	28
H(18A)	6205	10821	2060	46
H(18B)	5932	10935	2881	46
H(18C)	5558	10565	1913	46
H(19A)	7388(9)	4433(16)	3231(14)	41(6)
H(19B)	6874(8)	4084(15)	2492(13)	32(5)
H(22A)	6196	2941	4589	33
H(23A)	6317	1201	5002	38
H(24A)	6998	219	4600	36
H(25A)	7537	956	3742	38
H(26A)	7406	2690	3305	34
H(27A)	6212	4485	1466	34
H(27B)	5912	5411	825	34
H(28A)	5600	4870	2423	34
H(28B)	5265	5635	1648	34
H(29A)	4764	4122	1422	43
H(29B)	5068	4159	634	43
H(30A)	5134	2491	1331	76
H(30B)	5496	2997	2254	76
H(30C)	5736	2967	1392	76

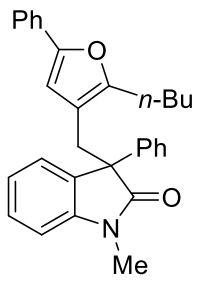
Table S8. Torsion angles [°] for d18163_a.

C(17)-C(1)-C(2)-C(3)	-82.12(18)
C(10)-C(1)-C(2)-C(3)	149.52(15)
C(11)-C(1)-C(2)-C(3)	30.3(2)
C(17)-C(1)-C(2)-C(7)	94.83(17)
C(10)-C(1)-C(2)-C(7)	-33.53(19)
C(11)-C(1)-C(2)-C(7)	-152.71(14)
C(7)-C(2)-C(3)-C(4)	-0.1(2)
C(1)-C(2)-C(3)-C(4)	176.85(15)
C(2)-C(3)-C(4)-C(5)	1.2(3)
C(3)-C(4)-C(5)-C(6)	-1.3(3)
C(4)-C(5)-C(6)-C(7)	0.2(3)
C(5)-C(6)-C(7)-C(2)	1.0(2)
C(5)-C(6)-C(7)-C(8)	179.19(16)
C(3)-C(2)-C(7)-C(6)	-1.0(2)
C(1)-C(2)-C(7)-C(6)	-177.98(14)
C(3)-C(2)-C(7)-C(8)	-179.28(15)
C(1)-C(2)-C(7)-C(8)	3.8(2)
C(6)-C(7)-C(8)-C(9)	-162.54(16)
C(2)-C(7)-C(8)-C(9)	15.6(2)
C(6)-C(7)-C(8)-C(19)	16.3(2)
C(2)-C(7)-C(8)-C(19)	-165.51(15)
C(7)-C(8)-C(9)-C(10)	-1.3(2)
C(19)-C(8)-C(9)-C(10)	179.92(15)
C(7)-C(8)-C(9)-C(27)	178.93(15)
C(19)-C(8)-C(9)-C(27)	0.1(3)
C(8)-C(9)-C(10)-C(1)	-30.3(2)
C(27)-C(9)-C(10)-C(1)	149.51(14)
C(17)-C(1)-C(10)-C(9)	-80.88(18)
C(2)-C(1)-C(10)-C(9)	45.78(19)
C(11)-C(1)-C(10)-C(9)	167.07(14)
C(12)-N(1)-C(11)-O(1)	176.42(15)
C(18)-N(1)-C(11)-O(1)	1.5(3)
C(12)-N(1)-C(11)-C(1)	-2.11(18)
C(18)-N(1)-C(11)-C(1)	-176.99(14)
C(17)-C(1)-C(11)-O(1)	-175.64(16)
C(2)-C(1)-C(11)-O(1)	65.7(2)

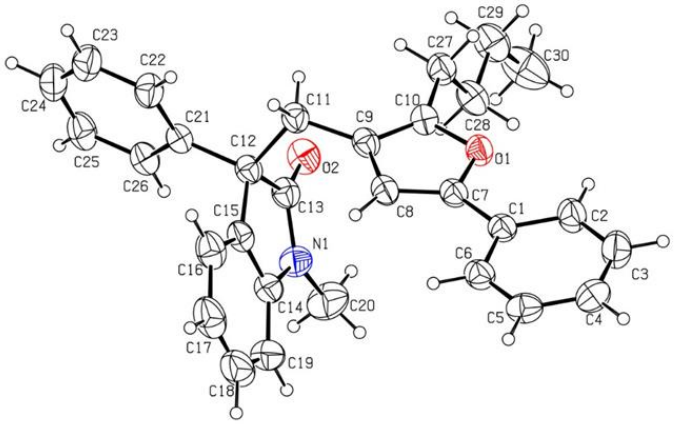
C(10)-C(1)-C(11)-O(1)	-55.0(2)
C(17)-C(1)-C(11)-N(1)	2.87(16)
C(2)-C(1)-C(11)-N(1)	-115.77(15)
C(10)-C(1)-C(11)-N(1)	123.50(15)
C(11)-N(1)-C(12)-C(13)	-179.70(16)
C(18)-N(1)-C(12)-C(13)	-5.0(3)
C(11)-N(1)-C(12)-C(17)	0.33(19)
C(18)-N(1)-C(12)-C(17)	175.00(15)
C(17)-C(12)-C(13)-C(14)	-1.7(2)
N(1)-C(12)-C(13)-C(14)	178.29(15)
C(12)-C(13)-C(14)-C(15)	1.9(2)
C(12)-C(13)-C(14)-Cl(1)	-177.49(12)
C(13)-C(14)-C(15)-C(16)	-0.8(3)
Cl(1)-C(14)-C(15)-C(16)	178.58(12)
C(14)-C(15)-C(16)-C(17)	-0.5(2)
C(15)-C(16)-C(17)-C(12)	0.6(2)
C(15)-C(16)-C(17)-C(1)	179.23(16)
C(13)-C(12)-C(17)-C(16)	0.5(2)
N(1)-C(12)-C(17)-C(16)	-179.50(14)
C(13)-C(12)-C(17)-C(1)	-178.35(15)
N(1)-C(12)-C(17)-C(1)	1.62(18)
C(2)-C(1)-C(17)-C(16)	-63.0(2)
C(10)-C(1)-C(17)-C(16)	63.0(2)
C(11)-C(1)-C(17)-C(16)	178.64(17)
C(2)-C(1)-C(17)-C(12)	115.71(15)
C(10)-C(1)-C(17)-C(12)	-118.28(15)
C(11)-C(1)-C(17)-C(12)	-2.65(17)
C(9)-C(8)-C(19)-C(20)	-91.2(2)
C(7)-C(8)-C(19)-C(20)	89.93(19)
C(8)-C(19)-C(20)-O(2)	-4.7(3)
C(8)-C(19)-C(20)-C(21)	174.71(15)
O(2)-C(20)-C(21)-C(26)	-167.04(18)
C(19)-C(20)-C(21)-C(26)	13.5(2)
O(2)-C(20)-C(21)-C(22)	11.3(2)
C(19)-C(20)-C(21)-C(22)	-168.10(15)
C(26)-C(21)-C(22)-C(23)	0.8(3)
C(20)-C(21)-C(22)-C(23)	-177.65(16)
C(21)-C(22)-C(23)-C(24)	0.5(3)

C(22)-C(23)-C(24)-C(25)	-1.2(3)
C(23)-C(24)-C(25)-C(26)	0.6(3)
C(22)-C(21)-C(26)-C(25)	-1.4(3)
C(20)-C(21)-C(26)-C(25)	177.01(16)
C(24)-C(25)-C(26)-C(21)	0.7(3)
C(8)-C(9)-C(27)-C(28)	96.1(2)
C(10)-C(9)-C(27)-C(28)	-83.70(18)
C(9)-C(27)-C(28)-C(29)	-169.65(15)
C(27)-C(28)-C(29)-C(30)	70.9(2)

Symmetry transformations used to generate equivalent atoms:



5aa



Product 5aa CCDC 2179949

Table S9. Crystal data and structure refinement for T.

Identification code	t	
Empirical formula	C30 H29 N O2	
Formula weight	435.54	
Temperature	294(1) K	
Wavelength	1.34139 Å	
Crystal system	Monoclinic	
Space group	P 1 21/c 1	
Unit cell dimensions	a = 10.1015(8) Å	α= 90°.
	b = 12.1620(11) Å	β= 90.612(3)°.
	c = 19.767(2) Å	γ = 90°.
Volume	2428.3(4) $Å^3$	
Z	4	
Density (calculated)	1.191 Mg/m^3	
Absorption coefficient	0.367 mm^{-1}	
F(000)	928	
Crystal size	0.3 x 0.2 x 0.2 mm^3	
Theta range for data collection	3.712 to 59.615°.	
Index ranges	-12<=h<=12, -14<=k<=15, -25<=l<=25	
Reflections collected	26848	
Independent reflections	5312 [R(int) = 0.0808]	
Completeness to theta = 53.594°	99.1 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	0.7516 and 0.5761	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5312 / 0 / 301	
Goodness-of-fit on F^2	1.092	

Final R indices [I>2sigma(I)]	R1 = 0.0541, wR2 = 0.1528
R indices (all data)	R1 = 0.0686, wR2 = 0.1641
Extinction coefficient	0.024(3)
Largest diff. peak and hole	0.300 and -0.167 e.Å^{-3}

Table S10. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for T. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
C(1)	6924(1)	8489(1)	5228(1)	54(1)
C(2)	8176(2)	8516(2)	5529(1)	70(1)
C(3)	8361(2)	9033(2)	6146(1)	82(1)
C(4)	7320(2)	9526(2)	6467(1)	74(1)
C(5)	6083(2)	9510(1)	6172(1)	71(1)
C(6)	5887(2)	8996(1)	5559(1)	63(1)
C(7)	6692(1)	7950(1)	4579(1)	54(1)
C(8)	5634(1)	7905(1)	4151(1)	56(1)
C(9)	6034(1)	7328(1)	3562(1)	54(1)
C(10)	7312(1)	7034(1)	3667(1)	57(1)
C(11)	5235(1)	7172(1)	2924(1)	57(1)
C(12)	4087(1)	6330(1)	2971(1)	52(1)
C(13)	4674(1)	5241(1)	3228(1)	57(1)
C(14)	3144(2)	5787(1)	4006(1)	65(1)
C(15)	3108(1)	6603(1)	3522(1)	58(1)
C(16)	2252(2)	7472(2)	3589(1)	76(1)
C(17)	1431(2)	7513(2)	4154(1)	98(1)
C(18)	1482(2)	6688(3)	4626(1)	105(1)
C(19)	2334(2)	5812(2)	4566(1)	93(1)
C(20)	4375(3)	3997(2)	4205(1)	105(1)
C(21)	3384(1)	6167(1)	2288(1)	53(1)
C(22)	3250(2)	7025(1)	1830(1)	68(1)
C(23)	2623(2)	6863(2)	1214(1)	81(1)
C(24)	2106(2)	5857(2)	1044(1)	80(1)
C(25)	2203(2)	5004(2)	1500(1)	75(1)
C(26)	2842(1)	5157(1)	2115(1)	63(1)
C(27)	8323(2)	6459(2)	3260(1)	66(1)
C(28)	8753(2)	5348(2)	3527(1)	74(1)
C(29)	9837(2)	4843(2)	3103(1)	89(1)
C(30)	10342(3)	3758(2)	3358(2)	123(1)
N(1)	4087(1)	4989(1)	3827(1)	68(1)
O(1)	7736(1)	7406(1)	4292(1)	59(1)
O(2)	5525(1)	4695(1)	2952(1)	71(1)

Table S11. Bond lengths [Å] and angles [°] for T.

C(1)-C(2)	1.392(2)
C(1)-C(6)	1.387(2)
C(1)-C(7)	1.457(2)
C(2)-H(2)	0.9300
C(2)-C(3)	1.384(2)
C(3)-H(3)	0.9300
C(3)-C(4)	1.372(3)
C(4)-H(4)	0.9300
C(4)-C(5)	1.373(2)
C(5)-H(5)	0.9300
C(5)-C(6)	1.376(2)
C(6)-H(6)	0.9300
C(7)-C(8)	1.3574(19)
C(7)-O(1)	1.3731(16)
C(8)-H(8)	0.9300
C(8)-C(9)	1.422(2)
C(9)-C(10)	1.353(2)
C(9)-C(11)	1.5027(19)
C(10)-C(27)	1.482(2)
C(10)-O(1)	1.3798(16)
C(11)-H(11A)	0.9700
C(11)-H(11B)	0.9700
C(11)-C(12)	1.5504(18)
C(12)-C(13)	1.5357(18)
C(12)-C(15)	1.516(2)
C(12)-C(21)	1.5311(18)
C(13)-N(1)	1.3654(19)
C(13)-O(2)	1.2186(17)
C(14)-C(15)	1.378(2)
C(14)-C(19)	1.383(2)
C(14)-N(1)	1.408(2)
C(15)-C(16)	1.373(2)
C(16)-H(16)	0.9300
C(16)-C(17)	1.399(3)
C(17)-H(17)	0.9300
C(17)-C(18)	1.371(4)

C(18)-H(18)	0.9300
C(18)-C(19)	1.376(4)
C(19)-H(19)	0.9300
C(20)-H(20A)	0.9600
C(20)-H(20B)	0.9600
C(20)-H(20C)	0.9600
C(20)-N(1)	1.447(2)
C(21)-C(22)	1.388(2)
C(21)-C(26)	1.3861(19)
C(22)-H(22)	0.9300
C(22)-C(23)	1.380(2)
C(23)-H(23)	0.9300
C(23)-C(24)	1.371(3)
C(24)-H(24)	0.9300
C(24)-C(25)	1.376(3)
C(25)-H(25)	0.9300
C(25)-C(26)	1.383(2)
C(26)-H(26)	0.9300
C(27)-H(27A)	0.9700
C(27)-H(27B)	0.9700
C(27)-C(28)	1.513(2)
C(28)-H(28A)	0.9700
C(28)-H(28B)	0.9700
C(28)-C(29)	1.516(2)
C(29)-H(29A)	0.9700
C(29)-H(29B)	0.9700
C(29)-C(30)	1.500(3)
C(30)-H(30A)	0.9600
C(30)-H(30B)	0.9600
C(30)-H(30C)	0.9600

C(2)-C(1)-C(7)	121.59(13)
C(6)-C(1)-C(2)	118.38(14)
C(6)-C(1)-C(7)	120.03(13)
C(1)-C(2)-H(2)	120.0
C(3)-C(2)-C(1)	120.09(15)
C(3)-C(2)-H(2)	120.0
C(2)-C(3)-H(3)	119.7

C(4)-C(3)-C(2)	120.62(16)
C(4)-C(3)-H(3)	119.7
C(3)-C(4)-H(4)	120.1
C(3)-C(4)-C(5)	119.72(15)
C(5)-C(4)-H(4)	120.1
C(4)-C(5)-H(5)	119.9
C(4)-C(5)-C(6)	120.17(15)
C(6)-C(5)-H(5)	119.9
C(1)-C(6)-H(6)	119.5
C(5)-C(6)-C(1)	121.02(15)
C(5)-C(6)-H(6)	119.5
C(8)-C(7)-C(1)	133.25(13)
C(8)-C(7)-O(1)	109.02(12)
O(1)-C(7)-C(1)	117.63(11)
C(7)-C(8)-H(8)	126.2
C(7)-C(8)-C(9)	107.56(13)
C(9)-C(8)-H(8)	126.2
C(8)-C(9)-C(11)	126.56(13)
C(10)-C(9)-C(8)	106.51(12)
C(10)-C(9)-C(11)	126.69(13)
C(9)-C(10)-C(27)	134.71(13)
C(9)-C(10)-O(1)	109.69(12)
O(1)-C(10)-C(27)	115.56(12)
C(9)-C(11)-H(11A)	108.4
C(9)-C(11)-H(11B)	108.4
C(9)-C(11)-C(12)	115.33(11)
H(11A)-C(11)-H(11B)	107.5
C(12)-C(11)-H(11A)	108.4
C(12)-C(11)-H(11B)	108.4
C(13)-C(12)-C(11)	107.66(10)
C(15)-C(12)-C(11)	113.18(11)
C(15)-C(12)-C(13)	101.75(11)
C(15)-C(12)-C(21)	111.18(11)
C(21)-C(12)-C(11)	111.87(11)
C(21)-C(12)-C(13)	110.67(11)
N(1)-C(13)-C(12)	108.10(12)
O(2)-C(13)-C(12)	126.44(13)
O(2)-C(13)-N(1)	125.46(13)

C(15)-C(14)-C(19)	121.89(18)
C(15)-C(14)-N(1)	109.55(13)
C(19)-C(14)-N(1)	128.56(17)
C(14)-C(15)-C(12)	109.20(13)
C(16)-C(15)-C(12)	130.81(15)
C(16)-C(15)-C(14)	119.97(15)
C(15)-C(16)-H(16)	120.5
C(15)-C(16)-C(17)	118.9(2)
C(17)-C(16)-H(16)	120.5
C(16)-C(17)-H(17)	120.0
C(18)-C(17)-C(16)	119.9(2)
C(18)-C(17)-H(17)	120.0
C(17)-C(18)-H(18)	119.1
C(17)-C(18)-C(19)	121.80(19)
C(19)-C(18)-H(18)	119.1
C(14)-C(19)-H(19)	121.3
C(18)-C(19)-C(14)	117.5(2)
C(18)-C(19)-H(19)	121.3
H(20A)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
N(1)-C(20)-H(20A)	109.5
N(1)-C(20)-H(20B)	109.5
N(1)-C(20)-H(20C)	109.5
C(22)-C(21)-C(12)	121.28(12)
C(26)-C(21)-C(12)	120.71(12)
C(26)-C(21)-C(22)	118.00(13)
C(21)-C(22)-H(22)	119.7
C(23)-C(22)-C(21)	120.61(16)
C(23)-C(22)-H(22)	119.7
C(22)-C(23)-H(23)	119.5
C(24)-C(23)-C(22)	120.90(17)
C(24)-C(23)-H(23)	119.5
C(23)-C(24)-H(24)	120.4
C(23)-C(24)-C(25)	119.20(15)
C(25)-C(24)-H(24)	120.4
C(24)-C(25)-H(25)	119.9
C(24)-C(25)-C(26)	120.24(16)

C(26)-C(25)-H(25)	119.9
C(21)-C(26)-H(26)	119.5
C(25)-C(26)-C(21)	121.02(15)
C(25)-C(26)-H(26)	119.5
C(10)-C(27)-H(27A)	108.4
C(10)-C(27)-H(27B)	108.4
C(10)-C(27)-C(28)	115.40(14)
H(27A)-C(27)-H(27B)	107.5
C(28)-C(27)-H(27A)	108.4
C(28)-C(27)-H(27B)	108.4
C(27)-C(28)-H(28A)	109.2
C(27)-C(28)-H(28B)	109.2
C(27)-C(28)-C(29)	112.05(16)
H(28A)-C(28)-H(28B)	107.9
C(29)-C(28)-H(28A)	109.2
C(29)-C(28)-H(28B)	109.2
C(28)-C(29)-H(29A)	108.6
C(28)-C(29)-H(29B)	108.6
H(29A)-C(29)-H(29B)	107.6
C(30)-C(29)-C(28)	114.60(19)
C(30)-C(29)-H(29A)	108.6
C(30)-C(29)-H(29B)	108.6
C(29)-C(30)-H(30A)	109.5
C(29)-C(30)-H(30B)	109.5
C(29)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(13)-N(1)-C(14)	111.38(12)
C(13)-N(1)-C(20)	123.27(16)
C(14)-N(1)-C(20)	125.29(16)
C(7)-O(1)-C(10)	107.21(10)

Symmetry transformations used to generate equivalent atoms:

Table S12. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for T. The anisotropic displacement factor exponent takes the form: $-2\pi^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
C(1)	51(1)	51(1)	60(1)	6(1)	2(1)	0(1)
C(2)	53(1)	86(1)	71(1)	-10(1)	-4(1)	9(1)
C(3)	70(1)	100(1)	76(1)	-14(1)	-13(1)	5(1)
C(4)	90(1)	68(1)	63(1)	-2(1)	1(1)	4(1)
C(5)	78(1)	64(1)	71(1)	4(1)	16(1)	11(1)
C(6)	55(1)	66(1)	70(1)	6(1)	4(1)	5(1)
C(7)	46(1)	53(1)	63(1)	4(1)	2(1)	1(1)
C(8)	46(1)	54(1)	68(1)	5(1)	-3(1)	-1(1)
C(9)	48(1)	46(1)	69(1)	4(1)	-2(1)	-4(1)
C(10)	53(1)	58(1)	60(1)	-2(1)	-3(1)	-1(1)
C(11)	52(1)	53(1)	66(1)	7(1)	-6(1)	-6(1)
C(12)	47(1)	47(1)	61(1)	2(1)	-1(1)	-2(1)
C(13)	53(1)	49(1)	68(1)	3(1)	-4(1)	-3(1)
C(14)	56(1)	78(1)	62(1)	-2(1)	0(1)	-14(1)
C(15)	46(1)	61(1)	65(1)	-9(1)	-3(1)	-5(1)
C(16)	60(1)	77(1)	89(1)	-22(1)	-7(1)	7(1)
C(17)	60(1)	132(2)	101(1)	-50(1)	1(1)	11(1)
C(18)	66(1)	166(3)	82(1)	-39(2)	12(1)	-10(1)
C(19)	79(1)	134(2)	66(1)	-1(1)	8(1)	-25(1)
C(20)	130(2)	83(1)	103(1)	41(1)	-5(1)	0(1)
C(21)	43(1)	54(1)	61(1)	-2(1)	0(1)	1(1)
C(22)	66(1)	64(1)	75(1)	5(1)	-14(1)	0(1)
C(23)	73(1)	90(1)	78(1)	11(1)	-18(1)	4(1)
C(24)	60(1)	105(1)	72(1)	-16(1)	-14(1)	9(1)
C(25)	58(1)	78(1)	90(1)	-28(1)	-7(1)	-1(1)
C(26)	54(1)	59(1)	76(1)	-7(1)	-2(1)	-3(1)
C(27)	54(1)	78(1)	66(1)	-8(1)	0(1)	2(1)
C(28)	54(1)	73(1)	96(1)	-6(1)	5(1)	4(1)
C(29)	68(1)	88(1)	111(1)	-13(1)	9(1)	15(1)
C(30)	90(2)	88(2)	191(3)	9(2)	36(2)	20(1)
N(1)	75(1)	60(1)	69(1)	15(1)	-1(1)	-5(1)
O(1)	47(1)	66(1)	62(1)	-3(1)	-3(1)	5(1)
O(2)	67(1)	57(1)	88(1)	1(1)	-1(1)	12(1)

Table S13. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^{3}) for T.

	x	y	z	U(eq)
H(2)	8889	8186	5315	84
H(3)	9199	9046	6346	98
H(4)	7452	9870	6883	88
H(5)	5377	9847	6387	85
H(6)	5045	8989	5364	76
H(8)	4799	8199	4229	68
H(11A)	5827	6937	2568	68
H(11B)	4868	7877	2790	68
H(16)	2219	8025	3264	91
H(17)	851	8100	4209	117
H(18)	925	6722	4997	126
H(19)	2365	5257	4890	111
H(20A)	3662	3483	4146	158
H(20B)	4473	4173	4677	158
H(20C)	5181	3676	4044	158
H(22)	3585	7716	1938	82
H(23)	2550	7444	910	97
H(24)	1694	5751	626	95
H(25)	1837	4323	1394	90
H(26)	2910	4573	2417	76
H(27A)	9098	6927	3230	80
H(27B)	7975	6362	2804	80
H(28A)	7996	4858	3532	89
H(28B)	9071	5430	3989	89
H(29A)	9502	4744	2646	107
H(29B)	10572	5354	3084	107
H(30A)	10711	3850	3804	184
H(30B)	11012	3489	3060	184
H(30C)	9625	3240	3374	184

Table S14. Torsion angles [°] for T.

C(1)-C(2)-C(3)-C(4)	-0.2(3)
C(1)-C(7)-C(8)-C(9)	174.92(14)
C(1)-C(7)-O(1)-C(10)	-175.86(12)
C(2)-C(1)-C(6)-C(5)	-0.3(2)
C(2)-C(1)-C(7)-C(8)	-171.88(16)
C(2)-C(1)-C(7)-O(1)	4.0(2)
C(2)-C(3)-C(4)-C(5)	-0.2(3)
C(3)-C(4)-C(5)-C(6)	0.4(3)
C(4)-C(5)-C(6)-C(1)	-0.1(2)
C(6)-C(1)-C(2)-C(3)	0.5(3)
C(6)-C(1)-C(7)-C(8)	7.8(2)
C(6)-C(1)-C(7)-O(1)	-176.31(12)
C(7)-C(1)-C(2)-C(3)	-179.87(16)
C(7)-C(1)-C(6)-C(5)	-179.98(14)
C(7)-C(8)-C(9)-C(10)	1.02(16)
C(7)-C(8)-C(9)-C(11)	-173.65(12)
C(8)-C(7)-O(1)-C(10)	1.00(15)
C(8)-C(9)-C(10)-C(27)	-177.78(17)
C(8)-C(9)-C(10)-O(1)	-0.42(16)
C(8)-C(9)-C(11)-C(12)	-74.19(17)
C(9)-C(10)-C(27)-C(28)	-113.66(19)
C(9)-C(10)-O(1)-C(7)	-0.34(15)
C(9)-C(11)-C(12)-C(13)	-54.52(15)
C(9)-C(11)-C(12)-C(15)	57.13(16)
C(9)-C(11)-C(12)-C(21)	-176.32(11)
C(10)-C(9)-C(11)-C(12)	112.18(16)
C(10)-C(27)-C(28)-C(29)	-177.07(14)
C(11)-C(9)-C(10)-C(27)	-3.1(3)
C(11)-C(9)-C(10)-O(1)	174.25(12)
C(11)-C(12)-C(13)-N(1)	118.96(13)
C(11)-C(12)-C(13)-O(2)	-60.37(17)
C(11)-C(12)-C(15)-C(14)	-115.47(13)
C(11)-C(12)-C(15)-C(16)	65.55(18)
C(11)-C(12)-C(21)-C(22)	-33.49(18)
C(11)-C(12)-C(21)-C(26)	147.56(13)
C(12)-C(13)-N(1)-C(14)	0.69(16)

C(12)-C(13)-N(1)-C(20)	178.20(16)
C(12)-C(15)-C(16)-C(17)	179.09(15)
C(12)-C(21)-C(22)-C(23)	179.47(15)
C(12)-C(21)-C(26)-C(25)	179.85(13)
C(13)-C(12)-C(15)-C(14)	-0.25(14)
C(13)-C(12)-C(15)-C(16)	-179.23(15)
C(13)-C(12)-C(21)-C(22)	-153.55(13)
C(13)-C(12)-C(21)-C(26)	27.50(17)
C(14)-C(15)-C(16)-C(17)	0.2(2)
C(15)-C(12)-C(13)-N(1)	-0.26(14)
C(15)-C(12)-C(13)-O(2)	-179.59(13)
C(15)-C(12)-C(21)-C(22)	94.14(16)
C(15)-C(12)-C(21)-C(26)	-84.82(16)
C(15)-C(14)-C(19)-C(18)	-0.1(3)
C(15)-C(14)-N(1)-C(13)	-0.87(17)
C(15)-C(14)-N(1)-C(20)	-178.32(17)
C(15)-C(16)-C(17)-C(18)	-0.6(3)
C(16)-C(17)-C(18)-C(19)	0.6(3)
C(17)-C(18)-C(19)-C(14)	-0.3(3)
C(19)-C(14)-C(15)-C(12)	-178.98(14)
C(19)-C(14)-C(15)-C(16)	0.1(2)
C(19)-C(14)-N(1)-C(13)	178.74(16)
C(19)-C(14)-N(1)-C(20)	1.3(3)
C(21)-C(12)-C(13)-N(1)	-118.49(13)
C(21)-C(12)-C(13)-O(2)	62.18(18)
C(21)-C(12)-C(15)-C(14)	117.61(12)
C(21)-C(12)-C(15)-C(16)	-61.37(19)
C(21)-C(22)-C(23)-C(24)	0.7(3)
C(22)-C(21)-C(26)-C(25)	0.9(2)
C(22)-C(23)-C(24)-C(25)	0.8(3)
C(23)-C(24)-C(25)-C(26)	-1.5(3)
C(24)-C(25)-C(26)-C(21)	0.7(2)
C(26)-C(21)-C(22)-C(23)	-1.6(2)
C(27)-C(10)-O(1)-C(7)	177.59(12)
C(27)-C(28)-C(29)-C(30)	177.83(19)
N(1)-C(14)-C(15)-C(12)	0.66(16)
N(1)-C(14)-C(15)-C(16)	179.77(13)
N(1)-C(14)-C(19)-C(18)	-179.68(17)

O(1)-C(7)-C(8)-C(9)	-1.25(15)
O(1)-C(10)-C(27)-C(28)	69.09(18)
O(2)-C(13)-N(1)-C(14)	-179.98(13)
O(2)-C(13)-N(1)-C(20)	-2.5(3)

Symmetry transformations used to generate equivalent atoms:

Table S15. Hydrogen bonds for T [Å and °].

D-H...A	d(D-H)	d(H...A)	d(D...A)	<(DHA)

11) Computational Studies

Computational Details

Density functional theory (DFT) calculations were performed using Gaussian 09 program.[4] The B3LYP[5] functional with Grimme D3 correction[6] was employed for all geometry optimizations a mixed basis set of SDD[7] (Pd, I, K, and Cs) and 6-31G(d)[8] (C, H, N, O, P, and Cl). Frequency analyses were carried out at the same level of theory to determine the intermediates to be minima (no imaginary frequency) or transition states (only one imaginary frequency) and to acquire the thermal corrections to free energies. Single-point solvation energies were calculated at M06-D3[9]/6-311+G(d,p)[10]-SDD level of theory with SMD[11] continuum model in MeCN solvent. The sum of the thermal correction to free energy and the single-point energy is taken as the Gibbs free energy for intermediates or transition states to provide more accurate energetics. The calculated 3D optimized structures are visualized utilizing CYLview program.[12]

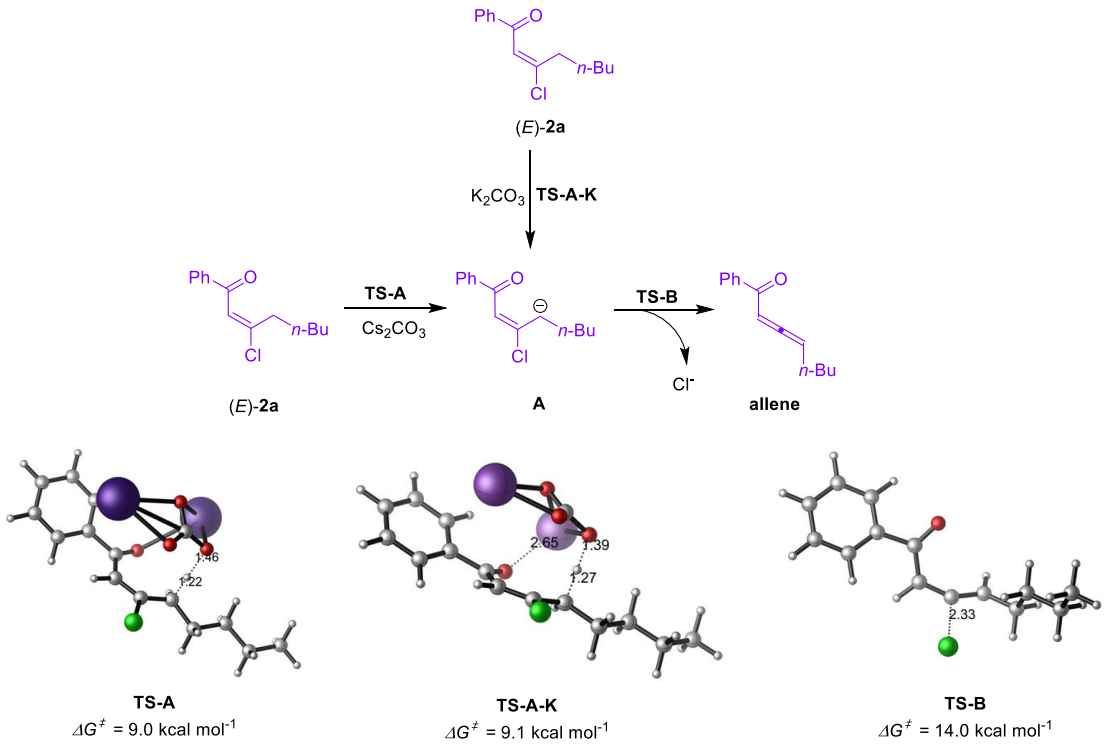


Figure S1. The generation of allene form substrate **(*E*)-2a**.

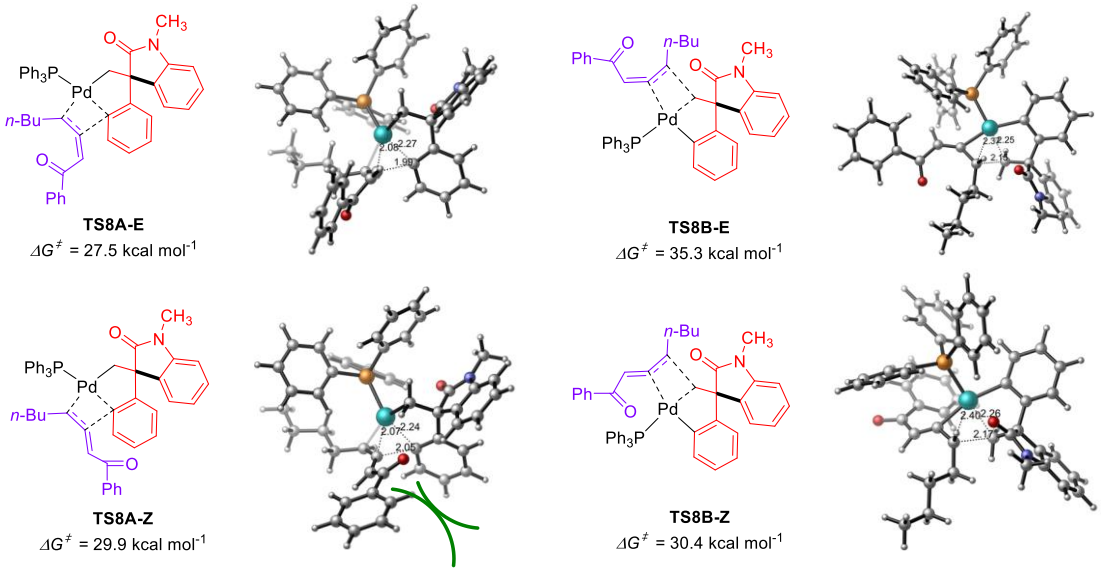


Figure S2. Activation energies for the migratory insertion step with allenyl ketone **6** and transition state structures.

Comment: The electron-rich double bond of the *in-situ* generated allene is kinetically more favorable to undergo migratory insertion into the Pd(II)-Csp^2 bond of **INT7A** through transition state **TS8A-E** with a surmountable activation energy of 27.5 kcal mol^{-1}, which is significantly lower than the migratory insertion into Pd-Csp^3 bond via transition states **TS8B-E** and **TS8B-Z** (27.5 vs 35.3 and 30.4 kcal mol^{-1}). The energy barrier of transition state **TS8A-Z** is 29.9 kcal mol^{-1}, which is 2.4 kcal mol^{-1} higher than that of **TS8A-E**. This difference in energy can be attributed to the noticeable increase in steric hindrance between phenylacetyl group of **6** and phenyl attached to palladium.

Table S16. The calculated energies of stationary points (in Hartree/Particle).

Structure	ZPE	H_{corr}	G_{corr}	E_{ele}	H_{sol}	G_{sol}
INT1A	0.551608	0.588175	0.473910	-2199.847233	-2199.259058	-2199.373323
1a	0.259615	0.277904	0.212223	-759.151676	-758.873772	-758.939453
TS2A	0.813555	0.867576	0.721879	-2959.012470	-2958.144894	-2958.290591
INT2A	0.815166	0.869647	0.721991	-2959.068711	-2958.199064	-2958.346720
INT3A	0.815502	0.867426	0.726782	-2947.481327	-2946.613901	-2946.754545
I^-	0.000000	0.002360	-0.016848	-11.572844	-11.570484	-11.589692
INT3B	0.538085	0.575227	0.466719	-1923.100643	-1922.525416	-1922.633924
PPh_3	0.274431	0.291257	0.228011	-1035.926986	-1035.635729	-1035.698975
TS4A	0.814348	0.865574	0.727593	-2947.470905	-2946.605331	-2946.743312
INT4A	0.817253	0.868571	0.729212	-2947.516132	-2946.647561	-2946.786920

TS4B	0.816727	0.867117	0.733763	-2947.442359	-2946.575242	-2946.708596
INT4B	0.817961	0.869118	0.731714	-2947.513206	-2946.644088	-2946.781492
TS4C	0.536765	0.573261	0.465612	-1923.082831	-1922.509570	-1922.617219
INT4C	0.539489	0.576342	0.466878	-1923.122875	-1922.546533	-1922.655997
TS4D	0.537786	0.574004	0.467284	-1923.065062	-1922.491058	-1922.597778
INT4D	0.540300	0.576687	0.469331	-1923.137996	-1922.561309	-1922.668665
(*E*)-**2a**	0.278348	0.295639	0.230935	-1078.847697	-1078.552058	-1078.616762
Cs_2CO_3	0.015395	0.023708	-0.022110	-304.180657	-304.156949	-304.202767
TS-A	0.290415	0.316099	0.228609	-1383.033765	-1382.717666	-1382.805156
K_2CO_3	0.016389	0.024110	-0.016839	-320.510336	-320.486226	-320.527175
TS-A-K	0.290461	0.315548	0.232345	-1399.361731	-1399.046183	-1399.129386
A	0.263156	0.280365	0.216849	-1078.358106	-1078.077741	-1078.141257
TS-B	0.290415	0.316099	0.228609	-1078.347600	-1078.031501	-1078.118991
6	0.263065	0.278966	0.218261	-618.007985	-617.729019	-617.789724
INT5A	0.556898	0.599786	0.475635	-2215.778297	-2215.178511	-2215.302662
TS6A	0.551070	0.593944	0.468084	-2215.748422	-2215.154478	-2215.280338
INT6A	0.555708	0.599091	0.473419	-2215.781538	-2215.182447	-2215.308119
INT7A	0.791238	0.841733	0.702082	-2529.098858	-2528.257125	-2528.396776
$Cs_2CO_3H^+$	0.028067	0.036917	-0.010438	-304.694550	-304.657633	-304.704988
INT7B	0.804183	0.854974	0.719032	-2947.045562	-2946.190588	-2946.326530
TS8A-E	0.790291	0.839763	0.702686	-2529.055621	-2528.215858	-2528.352935
INT8A-E	0.793848	0.843076	0.707000	-2529.120308	-2528.277232	-2528.413308
TS8A-Z	0.790948	0.840049	0.706023	-2529.055092	-2528.215043	-2528.349069
INT8A-Z	0.794232	0.843276	0.708672	-2529.124245	-2528.280969	-2528.415573
TS8B-E	0.792002	0.841121	0.705999	-2529.046492	-2528.205371	-2528.340493
INT8B-E	0.793753	0.843365	0.706210	-2529.106010	-2528.262645	-2528.399800
TS8B-Z	0.791291	0.840387	0.706938	-2529.055333	-2528.214946	-2528.348395
INT8B-Z	0.795800	0.844657	0.711261	-2529.138212	-2528.293555	-2528.426951
TS9A	0.791683	0.840987	0.702899	-2529.096766	-2528.255779	-2528.393867

3aa	0.519951	0.549661	0.458428	-1365.268211	-1364.718550	-1364.809783
4aa	0.519429	0.549343	0.456486	-1365.272064	-1364.722721	-1364.815578
INT5C	0.804837	0.855198	0.716954	-2529.567750	-2528.712552	-2528.850796
TS6C	0.805941	0.855091	0.721174	-2529.562913	-2528.707822	-2528.841739
INT6C	0.808709	0.857456	0.724368	-2529.581637	-2528.724181	-2528.857269
TS6D	0.805115	0.854781	0.717765	-2529.543512	-2528.688731	-2528.825747
INT6D	0.808512	0.858089	0.721568	-2529.615649	-2528.757560	-2528.894081
TS7C	0.806578	0.855686	0.719456	-2529.558944	-2528.703258	-2528.839488
INT7C	0.809329	0.858393	0.723287	-2529.628953	-2528.770560	-2528.905666
TS8C	0.804346	0.853340	0.716935	-2529.598812	-2528.745472	-2528.881877
INT8C	0.561765	0.600315	0.484136	-2660.683616	-2660.083301	-2660.199480
TS9C	0.559069	0.597122	0.484263	-2660.657282	-2660.060160	-2660.173019
HCl	0.006665	0.009970	-0.011228	-460.798303	-460.788333	-460.809531
INT8D	0.561264	0.600128	0.483114	-2211.887936	-2211.287808	-2211.404822
TS9D	0.558212	0.596801	0.479892	-2211.859550	-2211.262749	-2211.379658
HI	0.004933	0.008238	-0.015230	-11.989499	-11.981261	-12.004729
5aa	0.519344	0.549210	0.457143	-1365.267022	-1364.717812	-1364.809879

Note: ZPE = zero-point vibrational energy in the gas phase; H_{corr} = thermal correction to enthalpy in the gas phase; G_{corr} = thermal correction to Gibbs free energy in the gas phase; E_{ele} = the electronic energies in solvent; H_{sol} = ethalpies in solvent; G_{sol} = Gibbs free energies in solvent.

DFT-Computed Cartesian Coordinate (unit: angstrom)

1a				H	2.247867	2.941503	1.701640
C	1.371969	2.445429	1.295016	H	1.810363	0.551430	2.229986
C	1.125050	1.112650	1.604190	H	-1.304703	3.021657	-0.725403
C	0.020642	0.433940	1.069371	H	0.690636	4.167839	0.183661
C	-0.862540	1.149556	0.247543	I	-2.651757	0.225293	-0.516148
C	-0.619516	2.485758	-0.077864	N	-0.169930	-0.940325	1.404592
C	0.503164	3.129629	0.442722	C	0.004540	-1.970450	0.491123

O	-0.410209	-3.101268	0.710442	H	-5.080489	-0.087903	-1.310904
C	0.739943	-1.623527	-0.785710	H	-1.677406	-2.695394	-0.935460
C	0.206673	-2.044829	-1.939702	H	-2.973873	-4.535942	-1.979865
H	-0.732021	-2.588409	-1.953311	H	-5.320686	-4.145613	-2.711231
H	0.700092	-1.862824	-2.890270	C	-3.160485	1.581963	-0.573528
C	2.025954	-0.886019	-0.714396	C	-4.218146	2.066918	0.210092
C	2.995353	-1.249298	0.234413	C	-2.760901	2.310640	-1.705505
C	2.293012	0.187343	-1.576806	C	-4.868615	3.252808	-0.138215
C	4.201257	-0.554869	0.318124	H	-4.531027	1.521782	1.095758
H	2.797470	-2.081355	0.905317	C	-3.417997	3.489876	-2.057209
C	3.497316	0.884831	-1.489952	H	-1.924438	1.951544	-2.300870
H	1.531755	0.494208	-2.288054	C	-4.472967	3.964041	-1.273040
C	4.454585	0.517983	-0.541062	H	-5.684196	3.620984	0.478923
H	4.944682	-0.851469	1.053455	H	-3.099338	4.043888	-2.936320
H	3.683261	1.723481	-2.155703	H	-4.979378	4.887546	-1.541280
H	5.391101	1.064640	-0.470268	C	-2.613487	-0.269408	1.585839
C	-0.884206	-1.224018	2.650310	C	-1.708656	0.256601	2.523201
H	-0.467388	-0.607984	3.452398	C	-3.728643	-0.985166	2.046064
H	-1.954290	-1.003959	2.547840	C	-1.918699	0.077559	3.890143
H	-0.763681	-2.281527	2.884974	H	-0.827825	0.788446	2.173432
				C	-3.934714	-1.167676	3.416068
INT1A				H	-4.433380	-1.407123	1.335647
C	-5.340308	-2.091023	-2.054990	C	-3.032306	-0.637128	4.340183
C	-4.616036	-1.059200	-1.452540	H	-1.203259	0.484737	4.599885
C	-3.294062	-1.271867	-1.035196	H	-4.800229	-1.728544	3.759528
C	-2.709516	-2.533027	-1.238265	H	-3.192494	-0.785427	5.404982
C	-3.437918	-3.564577	-1.830011	P	-2.258039	0.014184	-0.208256
C	-4.755366	-3.344990	-2.241453	C	4.994494	-3.126835	-0.587467
H	-6.362769	-1.912976	-2.378284	C	4.303332	-2.024128	-0.080498

C	3.217944	-1.482348	-0.785712	H	6.299229	2.350459	-2.045859
C	2.832038	-2.071368	-2.000510	H	5.164604	4.562224	-2.104740
C	3.529527	-3.166896	-2.509886	P	2.260840	-0.013241	-0.211621
C	4.612139	-3.697354	-1.803510	Pd	0.000985	0.002056	-0.610684
H	5.831359	-3.540416	-0.030511				
H	4.606059	-1.588498	0.867338	**TS2A**			
H	1.974307	-1.671168	-2.536379	C	-3.825638	2.247139	2.050519
H	3.220955	-3.613174	-3.451638	C	-2.794648	2.455661	1.131998
H	5.150415	-4.556499	-2.195145	C	-1.483627	2.072235	1.442703
C	2.609413	0.029935	1.605276	C	-1.226344	1.488068	2.695070
C	3.680799	0.737529	2.169982	C	-2.255017	1.298365	3.615202
C	1.739660	-0.676727	2.453006	C	-3.563096	1.668851	3.292308
C	3.877924	0.735698	3.553586	H	-4.840259	2.527767	1.782930
H	4.358315	1.298116	1.532772	H	-3.029260	2.885352	0.165431
C	1.941318	-0.681850	3.832776	H	-0.220026	1.176484	2.949727
H	0.891525	-1.205028	2.025294	H	-2.030864	0.844658	4.577057
C	3.010792	0.027074	4.387307	H	-4.372025	1.498100	3.997365
H	4.709073	1.292709	3.978549	C	-0.658456	3.350322	-1.026877
H	1.253199	-1.227739	4.473009	C	-0.199156	4.675068	-1.040834
H	3.163479	0.032264	5.463435	C	-1.572898	2.934881	-2.007379
C	3.245340	1.412012	-0.851440	C	-0.648713	5.564174	-2.019547
C	2.608809	2.663408	-0.899427	H	0.506342	5.013310	-0.287962
C	4.580350	1.311510	-1.269694	C	-2.038738	3.829961	-2.969564
C	3.298543	3.792720	-1.339966	H	-1.928097	1.910937	-2.000087
H	1.567241	2.741874	-0.595548	C	-1.570330	5.146315	-2.982603
C	5.266175	2.442185	-1.720241	H	-0.282809	6.587818	-2.024448
H	5.085422	0.350480	-1.247972	H	-2.760503	3.495691	-3.710164
C	4.629252	3.684205	-1.752963	H	-1.921126	5.842886	-3.739571
H	2.794138	4.755002	-1.370476	C	1.264534	2.934747	1.087860

C	2.545048	2.803987	0.531289	C	1.025322	-0.183085	5.021030
C	1.120093	3.659984	2.279363	H	2.547000	1.345875	4.952055
C	3.663697	3.348045	1.160648	H	-0.460280	-1.725110	4.737663
H	2.665502	2.247961	-0.390503	H	0.716164	0.048057	6.036671
C	2.239361	4.203719	2.914646	C	3.876637	-0.402238	0.299659
H	0.138070	3.785165	2.723355	C	4.109279	0.242278	-0.923519
C	3.513433	4.042103	2.364250	C	4.943491	-0.554932	1.199366
H	4.647156	3.205220	0.720940	C	5.371859	0.757741	-1.227801
H	2.113485	4.753491	3.844016	H	3.292332	0.346077	-1.633932
H	4.382266	4.456810	2.868814	C	6.200328	-0.028323	0.902920
P	-0.119565	2.089023	0.201764	H	4.788298	-1.083436	2.135597
C	2.656955	-5.235267	1.290201	C	6.416218	0.633776	-0.309841
C	2.347361	-3.887884	1.497915	H	5.534965	1.257998	-2.178755
C	2.681118	-2.918994	0.541569	H	7.014387	-0.141499	1.614115
C	3.358977	-3.340624	-0.618243	H	7.397203	1.040688	-0.540740
C	3.669080	-4.682963	-0.825164	P	2.198787	-1.121727	0.608251
C	3.310287	-5.641805	0.127022	Pd	0.496778	-0.061629	-0.647433
H	2.390569	-5.966149	2.049626	I	0.394274	-0.006504	-3.484457
H	1.862745	-3.601430	2.423540	C	-1.370048	-4.211653	-1.339218
H	3.659073	-2.607981	-1.363351	C	-2.222187	-3.120416	-1.465140
H	4.194896	-4.979529	-1.729137	C	-1.751138	-1.855897	-1.856800
H	3.548455	-6.689933	-0.032356	C	-0.371277	-1.713911	-2.132716
C	1.838404	-0.787657	2.387822	C	0.465867	-2.841020	-2.093714
C	2.464844	0.237708	3.114528	C	-0.014350	-4.068778	-1.655520
C	0.756778	-1.462888	2.985410	H	-1.764245	-5.172170	-1.020283
C	2.057161	0.537062	4.416919	H	-3.280830	-3.218398	-1.243600
H	3.252906	0.828912	2.662261	H	1.506415	-2.735402	-2.368730
C	0.370544	-1.182048	4.295073	H	0.674994	-4.902841	-1.561560
H	0.193137	-2.193401	2.412637	N	-2.684142	-0.778486	-1.969388

C	-3.441498	-0.272051	-0.930864	H	4.008019	5.089522	-1.226954
O	-4.208175	0.666506	-1.152202	H	2.131988	4.356366	0.195196
C	-3.394459	-0.920538	0.432316	H	1.015336	1.453263	-2.781770
C	-2.261042	-1.093814	1.123285	H	2.900979	2.175282	-4.195146
H	-1.285187	-0.830031	0.720999	H	4.413373	3.998824	-3.426140
H	-2.284145	-1.467009	2.142065	C	0.300768	2.994530	1.457691
C	-4.703199	-1.351792	1.001923	C	-0.558925	3.849021	2.159716
C	-5.859037	-0.553235	0.954222	C	1.441323	2.484658	2.097936
C	-4.783458	-2.608831	1.627127	C	-0.266266	4.195528	3.480545
C	-7.047430	-0.996183	1.534134	H	-1.461200	4.223184	1.689373
H	-5.808515	0.409778	0.463127	C	1.724766	2.823034	3.418946
C	-5.973417	-3.048130	2.207736	H	2.114383	1.820748	1.569931
H	-3.905289	-3.248972	1.640021	C	0.869272	3.683464	4.112569
C	-7.111699	-2.241141	2.165326	H	-0.938778	4.856993	4.019846
H	-7.929178	-0.361423	1.494778	H	2.605815	2.400251	3.892499
H	-6.012783	-4.025386	2.682394	H	1.083336	3.949448	5.144343
H	-8.041745	-2.581757	2.612957	C	-1.295308	3.504106	-0.988749
C	-3.087975	-0.339718	-3.316648	C	-2.406758	2.988629	-1.667731
H	-2.783833	0.689217	-3.519354	C	-1.085368	4.891862	-0.970029
H	-2.617502	-0.997749	-4.047464	C	-3.297940	3.847688	-2.312821
H	-4.176912	-0.399350	-3.403120	H	-2.590133	1.919887	-1.666465
				C	-1.984973	5.749037	-1.602184
INT2A				H	-0.219055	5.303046	-0.460278
C	3.350691	4.296492	-1.572844	C	-3.092310	5.227617	-2.276948
C	2.285362	3.885607	-0.770024	H	-4.160463	3.435986	-2.829698
C	1.432429	2.853970	-1.195635	H	-1.818937	6.822479	-1.571672
C	1.659439	2.254590	-2.442681	H	-3.791638	5.896145	-2.771898
C	2.728747	2.663208	-3.239813	P	-0.061510	2.369419	-0.225924
C	3.577395	3.684340	-2.807198	C	-1.143912	-4.572225	-3.260575

C	-1.763189	-3.642280	-2.421453	H	-1.741726	-2.355385	4.865009
C	-1.175935	-3.291818	-1.198726	H	-2.589140	-6.016891	2.764411
C	0.036008	-3.897233	-0.827442	H	-2.241323	-4.793948	4.903521
C	0.651562	-4.821451	-1.666079	P	-1.891790	-2.003013	-0.091030
C	0.064303	-5.160274	-2.888293	Pd	-0.836936	0.139162	-0.078923
H	-1.612127	-4.835945	-4.205252	I	-2.999601	1.115229	1.427990
H	-2.704263	-3.195828	-2.723598	C	2.696546	-2.100625	-2.576666
H	0.508898	-3.636363	0.113205	C	2.902613	-1.827107	-1.229162
H	1.596539	-5.267630	-1.370085	C	1.976598	-1.073190	-0.486834
H	0.547742	-5.878764	-3.544725	C	0.758010	-0.674932	-1.077337
C	-3.610226	-1.807916	-0.710190	C	0.569637	-0.982823	-2.436877
C	-4.709107	-2.441775	-0.120975	C	1.525807	-1.659190	-3.193355
C	-3.812239	-0.969210	-1.818460	H	3.434803	-2.675176	-3.129371
C	-5.992198	-2.239102	-0.634639	H	3.795012	-2.198115	-0.737446
H	-4.572100	-3.075999	0.748433	H	-0.364070	-0.699714	-2.917900
C	-5.090963	-0.779827	-2.337225	H	1.335609	-1.875123	-4.241473
H	-2.965314	-0.454031	-2.265025	N	2.301075	-0.767458	0.881773
C	-6.186103	-1.412558	-1.741982	C	3.507648	-0.259784	1.313843
H	-6.841323	-2.725258	-0.162154	O	3.709339	-0.034053	2.510692
H	-5.235094	-0.127193	-3.194096	C	4.612556	0.028319	0.325693
H	-7.186312	-1.254865	-2.136034	C	4.522546	1.073217	-0.504090
C	-2.006398	-2.896461	1.512242	H	3.623219	1.668378	-0.573796
C	-1.811837	-2.214106	2.721938	H	5.354704	1.365512	-1.137741
C	-2.283612	-4.275060	1.540248	C	5.815154	-0.844116	0.394677
C	-1.896367	-2.897366	3.936303	C	6.310020	-1.340943	1.612904
H	-1.608755	-1.149873	2.715737	C	6.472311	-1.205759	-0.795347
C	-2.372622	-4.952075	2.756066	C	7.443017	-2.154411	1.635324
H	-2.419668	-4.820816	0.611615	H	5.808615	-1.068252	2.534485
C	-2.177401	-4.264296	3.956758	C	7.605817	-2.017105	-0.768302

H	6.069426	-0.865570	-1.745260	H	2.698493	0.730162	-1.925840
C	8.097601	-2.493895	0.449009	C	4.140053	-0.886306	0.696212
H	7.817839	-2.522061	2.587133	H	3.072100	-2.039314	2.173091
H	8.097048	-2.287298	-1.699648	H	4.917971	0.317120	-0.917350
H	8.978211	-3.130454	0.471832	H	5.116270	-1.077120	1.134200
C	1.335761	-1.087766	1.940534	C	-1.148996	-1.195829	-0.437330
H	0.702287	-0.228963	2.187397	C	-1.277886	-2.466409	-1.022223
H	0.706596	-1.911940	1.611156	C	-1.887942	-0.910107	0.720881
H	1.884299	-1.377347	2.838169	C	-2.109903	-3.432227	-0.456342
				H	-0.722026	-2.699755	-1.927688
PPh_3				C	-2.729491	-1.873462	1.280916
C	-0.258514	3.304581	1.275245	H	-1.805311	0.067038	1.186832
C	0.159799	2.095595	0.715366	C	-2.840428	-3.136611	0.696841
C	-0.459562	1.593051	-0.439082	H	-2.194486	-4.411739	-0.919868
C	-1.502496	2.332917	-1.020470	H	-3.297003	-1.636332	2.177337
C	-1.928006	3.534386	-0.454342	H	-3.496005	-3.884897	1.134486
C	-1.304325	4.024826	0.695196				
H	0.232686	3.681952	2.168659	**INT3A**			
H	0.970157	1.540992	1.178699	C	1.245533	4.267813	3.165732
H	-1.984385	1.964082	-1.923285	C	0.804110	3.825105	1.919326
H	-2.739667	4.091629	-0.914937	C	0.597865	2.453812	1.689760
H	-1.628600	4.965123	1.133287	C	0.801926	1.544015	2.737224
P	0.001501	-0.001009	-1.261950	C	1.233647	1.991265	3.986532
C	1.612298	-0.398322	-0.438455	C	1.463035	3.352103	4.199495
C	1.736562	-1.183593	0.717796	H	1.409535	5.328243	3.332919
C	2.775732	0.130522	-1.021522	H	0.609398	4.544768	1.129712
C	2.992211	-1.427331	1.278125	H	0.629655	0.483983	2.576574
H	0.850704	-1.605563	1.182624	H	1.387754	1.276889	4.790159
C	4.028660	-0.103720	-0.455311	H	1.798976	3.701257	5.171543

C	-1.319724	3.038120	-0.379842	H	4.358704	-3.588566	3.689714
C	-1.437732	3.574367	-1.670658	H	4.219813	-2.358833	1.549572
C	-2.262063	3.394945	0.599937	H	-0.059596	-2.098674	1.990214
C	-2.484841	4.447487	-1.975223	H	0.085540	-3.319632	4.133802
H	-0.717564	3.325649	-2.441265	H	2.297138	-4.070268	4.992003
C	-3.306834	4.261146	0.288733	C	3.395043	-0.122510	0.074405
H	-2.190255	2.985921	1.600946	C	4.257070	0.041421	-1.018678
C	-3.422999	4.789201	-1.000381	C	3.648673	0.601077	1.251911
H	-2.561094	4.860701	-2.976855	C	5.344734	0.912524	-0.933856
H	-4.032152	4.519805	1.054304	H	4.095926	-0.510899	-1.936753
H	-4.237112	5.466810	-1.240889	C	4.729966	1.476688	1.329526
C	1.310610	2.189174	-1.206910	H	3.016409	0.470097	2.121049
C	1.139833	1.591707	-2.469634	C	5.583048	1.635716	0.234997
C	2.400308	3.038214	-0.984854	H	6.005788	1.022851	-1.788579
C	2.039151	1.863666	-3.500219	H	4.908489	2.025197	2.250147
H	0.297859	0.926668	-2.653474	H	6.431388	2.311365	0.296557
C	3.299391	3.300921	-2.019946	C	2.342856	-2.451510	-1.304581
H	2.566497	3.475877	-0.007436	C	2.192153	-2.037680	-2.640898
C	3.119141	2.722225	-3.276738	C	2.732639	-3.770601	-1.037742
H	1.893646	1.406876	-4.475081	C	2.449470	-2.921336	-3.687686
H	4.148806	3.951582	-1.836207	H	1.867443	-1.024941	-2.863192
H	3.821342	2.932270	-4.078231	C	2.980402	-4.655336	-2.090863
P	0.025625	1.861674	0.058529	H	2.840203	-4.116025	-0.015028
C	3.391266	-3.266275	3.315774	C	2.843190	-4.234255	-3.413975
C	3.313082	-2.577868	2.105426	H	2.329727	-2.588861	-4.714669
C	2.067792	-2.157232	1.608059	H	3.279951	-5.676286	-1.872303
C	0.910074	-2.432081	2.353216	H	3.034326	-4.926159	-4.228856
C	0.989970	-3.117303	3.567048	P	1.931202	-1.245406	0.017550
C	2.231336	-3.537017	4.048109	Pd	-0.404463	-0.402112	-0.018719

C	-4.829267	0.901257	1.538215	H	-4.785155	0.703877	-2.963434
C	-4.628495	0.726083	0.169697	H	-3.793050	2.020860	-2.276974
C	-3.373622	0.340819	-0.315569	H	-3.146389	0.993537	-3.586309
C	-2.299154	0.161562	0.571304				
C	-2.524340	0.296109	1.943813	**INT3B**			
C	-3.784600	0.663040	2.431526	C	3.359458	2.072692	3.497978
H	-5.807536	1.197674	1.904704	C	2.856207	1.957604	2.201715
H	-5.454210	0.853669	-0.523944	C	2.136651	0.812659	1.821666
H	-1.709338	0.155154	2.648466	C	1.933302	-0.214728	2.756517
H	-3.937060	0.780473	3.500835	C	2.439719	-0.094044	4.051139
N	-3.189900	0.098615	-1.703035	C	3.150354	1.048545	4.424702
C	-2.434167	-0.964202	-2.146081	H	3.913287	2.963079	3.782730
O	-2.027387	-1.063939	-3.299579	H	3.017540	2.761183	1.490008
C	-2.128917	-2.057990	-1.117972	H	1.395488	-1.112073	2.465780
C	-0.878722	-2.603633	-1.174314	H	2.277873	-0.896119	4.765693
H	-0.217611	-2.331348	-1.986758	H	3.540937	1.141294	5.434460
H	-0.609161	-3.473185	-0.583552	C	1.165515	2.302192	-0.498179
C	-3.215789	-2.629368	-0.287098	C	1.438494	2.638375	-1.832948
C	-4.525815	-2.665928	-0.789933	C	0.553441	3.257353	0.330571
C	-2.956300	-3.202009	0.968284	C	1.107387	3.901838	-2.326112
C	-5.547526	-3.271406	-0.059771	H	1.915008	1.921510	-2.492300
H	-4.744612	-2.231858	-1.761199	C	0.227111	4.518425	-0.164871
C	-3.979121	-3.795646	1.701707	H	0.314526	3.014078	1.359094
H	-1.951675	-3.163524	1.378961	C	0.501170	4.845632	-1.495131
C	-5.279400	-3.833798	1.189162	H	1.327625	4.145608	-3.361805
H	-6.553608	-3.301562	-0.467590	H	-0.253173	5.239637	0.490207
H	-3.764952	-4.224942	2.676353	H	0.244167	5.828510	-1.880816
H	-6.077403	-4.297055	1.761896	C	2.911851	0.042474	-0.910131
C	-3.768468	1.012560	-2.691180	C	2.648551	-0.546680	-2.156964

C	4.238102	0.228820	-0.501126	C	-3.625194	-1.785159	1.082975
C	3.699379	-0.924205	-2.990548	C	-4.822976	-0.503931	-0.577660
H	1.623459	-0.729550	-2.466239	C	-4.750807	-1.775796	1.902286
C	5.287620	-0.165860	-1.333315	H	-2.709852	-2.261201	1.424528
H	4.457801	0.665765	0.467412	C	-5.951044	-0.497302	0.243194
C	5.021332	-0.737566	-2.578328	H	-4.857341	-0.007993	-1.543551
H	3.484123	-1.383765	-3.950876	C	-5.919464	-1.131507	1.485687
H	6.313789	-0.029579	-1.003200	H	-4.712234	-2.262649	2.872984
H	5.840479	-1.046329	-3.221925	H	-6.854332	0.005987	-0.090740
P	1.494749	0.593890	0.120159	H	-6.795727	-1.120268	2.128007
Pd	-0.293640	-0.861048	-0.069516	C	-2.289029	2.252247	-2.698391
C	-2.930828	2.884252	1.535757	H	-3.301069	2.643244	-2.864741
C	-2.958249	2.582373	0.174707	H	-1.640569	3.060394	-2.353912
C	-2.218885	1.503332	-0.325990	H	-1.912906	1.847425	-3.637803
C	-1.421822	0.733579	0.536897	I	1.259214	-3.153734	0.102599
C	-1.445258	1.014653	1.906003				
C	-2.190804	2.087553	2.409542	**TS4A**			
H	-3.507507	3.724708	1.912027	C	1.910842	3.975549	3.281461
H	-3.575924	3.168595	-0.499384	C	1.401547	3.656960	2.022904
H	-0.844787	0.422136	2.591098	C	0.989528	2.343849	1.736314
H	-2.176207	2.303481	3.474701	C	1.054698	1.373474	2.747811
N	-2.290501	1.178941	-1.705301	C	1.556975	1.695799	4.009734
C	-2.279863	-0.128775	-2.146074	C	1.994222	2.994874	4.274755
O	-2.146867	-0.426915	-3.329113	H	2.233879	4.991265	3.490270
C	-2.477896	-1.213690	-1.091003	H	1.307150	4.433674	1.269913
C	-1.736892	-2.358031	-1.236088	H	0.720887	0.359698	2.546304
H	-1.072297	-2.477168	-2.084247	H	1.605364	0.932489	4.781208
H	-1.943313	-3.244496	-0.647623	H	2.387189	3.247607	5.255307
C	-3.648722	-1.153144	-0.170468	C	-0.982239	3.155046	-0.202603

C	-1.314253	3.543053	-1.510986	H	4.076952	-2.698885	1.347981
C	-1.681062	3.724439	0.872099	H	-0.126196	-2.125009	2.096165
C	-2.318098	4.485651	-1.734971	H	0.085058	-3.363292	4.228816
H	-0.779500	3.129811	-2.359442	H	2.289835	-4.283754	4.919751
C	-2.680488	4.670911	0.643372	C	3.325464	-0.416722	-0.079103
H	-1.450484	3.432054	1.890569	C	4.082817	-0.298765	-1.253124
C	-3.003716	5.053854	-0.658441	C	3.754760	0.251578	1.079781
H	-2.551735	4.787955	-2.752261	C	5.247978	0.468682	-1.262692
H	-3.207725	5.105748	1.487696	H	3.777751	-0.809017	-2.159254
H	-3.778428	5.794608	-0.834315	C	4.916654	1.021270	1.063488
C	1.556746	2.203552	-1.198803	H	3.196591	0.160317	2.003557
C	1.310228	1.640785	-2.464584	C	5.668898	1.129621	-0.107983
C	2.697923	2.992531	-1.015946	H	5.825895	0.548051	-2.178649
C	2.170170	1.892052	-3.533205	H	5.235095	1.527639	1.970233
H	0.439206	1.006013	-2.615174	H	6.578775	1.722907	-0.120033
C	3.560225	3.236532	-2.086468	C	1.984456	-2.644357	-1.374066
H	2.935983	3.396865	-0.039438	C	1.669033	-2.227609	-2.679682
C	3.295811	2.697705	-3.346237	C	2.397640	-3.965096	-1.156778
H	1.962525	1.457190	-4.506946	C	1.786699	-3.111416	-3.750766
H	4.447160	3.843135	-1.929271	H	1.324010	-1.212236	-2.855418
H	3.969223	2.893874	-4.175514	C	2.504443	-4.850302	-2.232664
P	0.305234	1.870688	0.106631	H	2.629658	-4.311695	-0.155395
C	3.314114	-3.554731	3.167057	C	2.203706	-4.426784	-3.527740
C	3.198191	-2.854860	1.966375	H	1.538242	-2.778506	-4.754188
C	1.953828	-2.340718	1.561679	H	2.820917	-5.873850	-2.053982
C	0.837381	-2.531126	2.390828	H	2.284851	-5.119786	-4.359920
C	0.956991	-3.226430	3.595373	P	1.782576	-1.422056	-0.020397
C	2.194911	-3.741797	3.983335	Pd	-0.364037	-0.408861	-0.061676
H	4.280026	-3.949963	3.467669	C	-4.450225	1.833813	1.306259

C	-4.329403	1.626526	-0.065116	H	-3.462947	2.112071	-2.896494
C	-3.336112	0.758899	-0.531842	H	-3.375310	0.629738	-3.899575
C	-2.436393	0.143591	0.353708				
C	-2.633356	0.292959	1.734393	**INT4A**			
C	-3.617039	1.158925	2.209345	C	-0.101087	-5.452151	1.096243
H	-5.219686	2.503676	1.678058	C	-0.761519	-4.428139	0.415279
H	-5.016863	2.099641	-0.758144	C	-0.505155	-3.088109	0.739137
H	-1.999676	-0.238886	2.439623	C	0.420814	-2.785929	1.750918
H	-3.735585	1.310671	3.278219	C	1.071600	-3.813197	2.433826
N	-3.266033	0.308349	-1.857617	C	0.813247	-5.146653	2.107097
C	-2.734139	-0.950404	-2.029363	H	-0.303675	-6.487737	0.838114
O	-2.491942	-1.458541	-3.112889	H	-1.473775	-4.672724	-0.366941
C	-2.445308	-1.671604	-0.704190	H	0.650470	-1.753436	2.001385
C	-1.158862	-2.297583	-0.661334	H	1.787203	-3.564763	3.211079
H	-0.682839	-2.428748	-1.629639	H	1.324196	-5.945674	2.637002
H	-1.014570	-3.136641	0.014077	C	-1.960791	-2.404281	-1.699963
C	-3.600964	-2.270942	0.032963	C	-3.268759	-2.867159	-1.904639
C	-4.893506	-2.214934	-0.508037	C	-1.043127	-2.439394	-2.765835
C	-3.407451	-2.925641	1.260416	C	-3.656232	-3.345607	-3.158662
C	-5.965871	-2.807426	0.160151	H	-3.987541	-2.849198	-1.092196
H	-5.066799	-1.725127	-1.460885	C	-1.435016	-2.921560	-4.014049
C	-4.479256	-3.506804	1.929722	H	-0.024016	-2.095264	-2.614847
H	-2.416666	-2.964710	1.703535	C	-2.743731	-3.370243	-4.214897
C	-5.764662	-3.451026	1.380877	H	-4.672442	-3.699659	-3.307075
H	-6.958425	-2.765591	-0.278509	H	-0.719918	-2.943254	-4.831748
H	-4.314120	-4.005651	2.880413	H	-3.049063	-3.739703	-5.189708
H	-6.600349	-3.908809	1.901738	C	-2.913181	-1.491706	0.898047
C	-3.779986	1.070379	-2.987890	C	-3.880061	-0.567799	0.467661
H	-4.874932	1.026801	-3.026187	C	-3.124040	-2.196994	2.091673

C	-5.033830	-0.355152	1.218064	C	2.209618	0.862938	2.188219
H	-3.735978	-0.015736	-0.456052	C	3.521852	-1.298185	3.361549
C	-4.279880	-1.975915	2.843356	H	4.254735	-1.729519	1.390702
H	-2.391448	-2.919020	2.435837	C	2.085951	0.628131	3.561272
C	-5.234786	-1.055824	2.410568	H	1.707120	1.719948	1.756469
H	-5.771213	0.365212	0.876310	C	2.733560	-0.456636	4.152121
H	-4.432922	-2.528714	3.765923	H	4.045930	-2.136986	3.811141
H	-6.132761	-0.884697	2.997327	H	1.481708	1.300471	4.164475
P	-1.388072	-1.714655	-0.095230	H	2.637855	-0.638787	5.218548
Pd	0.268482	0.046495	-0.452418	C	4.085078	-2.780277	-2.207685
C	7.171228	0.405108	-1.449108	H	4.324826	-2.529456	-3.246319
C	6.330800	-0.683679	-1.724839	H	4.868572	-3.428997	-1.804614
C	5.029562	-0.611349	-1.251249	H	3.125055	-3.296151	-2.165189
C	4.548114	0.490143	-0.527844	C	-3.812202	2.724410	2.689336
C	5.391668	1.554288	-0.251357	C	-3.111185	2.721775	1.484429
C	6.711401	1.508021	-0.724966	C	-1.963498	1.928645	1.338863
H	8.196968	0.384270	-1.804421	C	-1.526181	1.146828	2.418394
H	6.689274	-1.541687	-2.284543	C	-2.230819	1.152171	3.622169
H	5.036076	2.405405	0.322556	C	-3.376026	1.938389	3.758504
H	7.383708	2.336271	-0.523486	H	-4.704600	3.335394	2.790104
N	3.986198	-1.569309	-1.408892	H	-3.473164	3.324014	0.658420
C	2.851016	-1.104466	-0.852793	H	-0.642218	0.524587	2.315606
O	1.710461	-1.608765	-0.964721	H	-1.891160	0.531136	4.445830
C	3.104259	0.217324	-0.137108	H	-3.930243	1.935063	4.692557
C	2.031751	1.164561	-0.720900	C	-2.122639	2.201307	-1.612042
H	2.078711	2.151006	-0.262898	C	-2.719780	3.455213	-1.834644
H	2.166917	1.279806	-1.802948	C	-2.428003	1.138025	-2.475914
C	2.974896	0.009156	1.384510	C	-3.630392	3.624712	-2.877350
C	3.639863	-1.065709	1.992452	H	-2.459874	4.303380	-1.208734

C	-3.340629	1.311470	-3.517669	H	-1.854341	0.000617	-4.479660
H	-1.950759	0.174142	-2.347477	H	-1.459540	2.163089	-5.656102
C	-3.948314	2.552293	-3.715700	C	2.885558	0.417520	-1.509066
H	-4.086366	4.597176	-3.038897	C	4.048184	1.196549	-1.470306
H	-3.565953	0.474803	-4.172681	C	2.899217	-0.807946	-2.193500
H	-4.657010	2.689243	-4.527313	C	5.216947	0.736304	-2.080486
C	-0.043359	3.520072	-0.101369	H	4.054346	2.151604	-0.956642
C	0.472407	4.101100	-1.272279	C	4.066185	-1.262200	-2.803659
C	0.247732	4.101709	1.141308	H	1.998231	-1.414048	-2.237671
C	1.258113	5.250047	-1.198399	C	5.232302	-0.494317	-2.739359
H	0.256241	3.657550	-2.240227	H	6.117181	1.342836	-2.038124
C	1.040872	5.249466	1.209894	H	4.070329	-2.217754	-3.319460
H	-0.151409	3.669671	2.053685	H	6.145606	-0.852027	-3.205399
C	1.546371	5.825010	0.043118	C	1.608532	2.450654	0.194214
H	1.645857	5.696172	-2.109647	C	2.586055	2.369793	1.202724
H	1.255310	5.696373	2.176395	C	0.874558	3.636661	0.050550
H	2.159333	6.719876	0.098728	C	2.838388	3.460519	2.031814
P	-0.971335	1.940624	-0.205402	H	3.163279	1.464855	1.329504
				C	1.136194	4.727405	0.881977
TS4B				H	0.091334	3.717588	-0.691636
C	-0.029593	2.863130	-4.199692	C	2.116560	4.646152	1.871221
C	0.640977	2.586974	-3.008283	H	3.602927	3.377591	2.798732
C	0.386200	1.393146	-2.316297	H	0.558771	5.638001	0.754937
C	-0.495681	0.457447	-2.875628	H	2.315962	5.498857	2.513948
C	-1.159083	0.729357	-4.072984	P	1.280702	0.933967	-0.776045
C	-0.938295	1.941615	-4.729315	C	-5.702675	-0.003225	-1.505164
H	0.163370	3.797000	-4.719819	C	-4.674682	0.412260	-0.660380
H	1.357871	3.302741	-2.619298	C	-3.430873	-0.246042	-0.672766
H	-0.674015	-0.485608	-2.370263	C	-3.233329	-1.308657	-1.566622

C	-4.260952	-1.714461	-2.419310	P	-2.072275	0.350202	0.410201
C	-5.497250	-1.067701	-2.387189	Pd	0.055400	-0.842704	0.394732
H	-6.659332	0.510366	-1.481301	C	-2.306150	-4.954452	-0.418814
H	-4.833930	1.261523	-0.002622	C	-0.993641	-4.739550	-0.845248
H	-2.285344	-1.831995	-1.593379	C	-0.253946	-3.630760	-0.396996
H	-4.093070	-2.540965	-3.103724	C	-0.916663	-2.687284	0.422535
H	-6.296872	-1.386838	-3.049411	C	-2.181269	-2.969664	0.932243
C	-2.198049	2.178135	0.171151	C	-2.894844	-4.089553	0.498376
C	-2.144517	3.070554	1.252496	H	-2.842104	-5.828520	-0.776215
C	-2.397622	2.690143	-1.123901	H	-0.532879	-5.475967	-1.491833
C	-2.295457	4.442603	1.044327	H	-2.635681	-2.300886	1.652060
H	-2.001162	2.706359	2.262951	H	-3.898104	-4.270136	0.872018
C	-2.539692	4.061663	-1.327135	N	1.132922	-3.529954	-0.738101
H	-2.459371	2.022421	-1.974605	C	2.159266	-3.048483	0.094337
C	-2.491308	4.943196	-0.243194	O	3.310404	-3.397518	-0.116403
H	-2.260239	5.117564	1.894414	C	1.836639	-2.039167	1.189658
H	-2.693322	4.437276	-2.334452	C	2.949541	-1.197008	1.742484
H	-2.612552	6.010926	-0.402065	C	4.154712	-0.982605	1.045005
C	-2.595066	0.134796	2.165399	C	2.836124	-0.623027	3.027676
C	-1.616120	0.329673	3.157840	C	5.190177	-0.239050	1.612056
C	-3.892740	-0.227989	2.550877	H	4.299985	-1.409879	0.066113
C	-1.933841	0.173969	4.506577	C	3.869529	0.122294	3.588790
H	-0.603744	0.610853	2.873930	H	1.940873	-0.763680	3.622343
C	-4.203412	-0.395940	3.902956	C	5.060040	0.317441	2.884411
H	-4.658554	-0.399127	1.801979	H	6.103696	-0.096969	1.042616
C	-3.228921	-0.195070	4.881632	H	3.745923	0.540346	4.583679
H	-1.171432	0.337815	5.263041	H	5.873199	0.887701	3.323906
H	-5.210374	-0.685939	4.188646	C	1.609736	-4.320205	-1.881332
H	-3.475328	-0.325754	5.931147	H	1.761028	-5.374663	-1.623704

H	0.882646	-4.239615	-2.692217	C	1.389492	2.299950	0.351415
H	2.566872	-3.917087	-2.205902	C	1.804459	2.058306	1.673396
C	0.717693	-2.342801	1.999124	C	1.026033	3.597942	-0.029292
H	0.489146	-1.754046	2.880865	C	1.864515	3.103837	2.592946
H	0.338363	-3.351516	2.061643	H	2.096265	1.062760	1.983240
				C	1.086511	4.639259	0.898275
INT4B				H	0.672269	3.801762	-1.031804
C	0.739842	2.866178	-4.330620	C	1.505225	4.397710	2.207205
C	1.272887	2.439403	-3.115375	H	2.198977	2.901860	3.606478
C	0.646153	1.409174	-2.391532	H	0.791490	5.638764	0.594892
C	-0.481943	0.782187	-2.935475	H	1.549894	5.212899	2.923710
C	-1.010007	1.205868	-4.156675	P	1.357779	0.865382	-0.789508
C	-0.406826	2.256226	-4.849842	C	-5.659362	0.384961	-1.523306
H	1.225584	3.668666	-4.877995	C	-4.614377	0.762031	-0.681343
H	2.179169	2.900566	-2.733901	C	-3.400466	0.052759	-0.702085
H	-0.949988	-0.038750	-2.407599	C	-3.253331	-1.033285	-1.575187
H	-1.890085	0.712156	-4.558852	C	-4.300012	-1.404260	-2.420959
H	-0.816924	2.590047	-5.798556	C	-5.502071	-0.695720	-2.397433
C	3.099005	0.568485	-1.245303	H	-6.594419	0.937079	-1.501887
C	4.165529	1.255844	-0.645082	H	-4.736683	1.612120	-0.016954
C	3.358239	-0.360121	-2.267014	H	-2.326539	-1.597716	-1.591434
C	5.472202	1.015944	-1.069180	H	-4.173151	-2.248988	-3.091567
H	3.980850	1.974441	0.145029	H	-6.315898	-0.982114	-3.057413
C	4.665274	-0.596123	-2.684156	C	-2.112376	2.351011	0.428841
H	2.538824	-0.899126	-2.733061	C	-2.122288	3.074725	1.628709
C	5.724099	0.089168	-2.083723	C	-2.198561	3.042970	-0.792870
H	6.293528	1.555246	-0.606123	C	-2.224895	4.466938	1.606631
H	4.857521	-1.324403	-3.465772	H	-2.064576	2.561230	2.582147
H	6.744013	-0.098436	-2.406598	C	-2.304706	4.432238	-0.807509

H	-2.197601	2.498330	-1.731510	C	2.070548	-2.879261	-0.400097
C	-2.320011	5.148180	0.392608	O	3.230486	-2.792156	-0.785629
H	-2.237333	5.016632	2.543273	C	1.529297	-2.192792	0.828582
H	-2.380445	4.953711	-1.757499	C	2.475016	-1.544369	1.789502
H	-2.409077	6.230733	0.380566	C	3.792508	-1.160858	1.452004
C	-2.423838	-0.065966	2.073611	C	2.037544	-1.232996	3.100749
C	-1.438316	0.046419	3.074849	C	4.606764	-0.494826	2.366926
C	-3.627981	-0.721006	2.367555	H	4.177497	-1.396908	0.473392
C	-1.659924	-0.487322	4.344190	C	2.856344	-0.569936	4.011501
H	-0.497721	0.550228	2.863560	H	1.036125	-1.488078	3.423507
C	-3.841991	-1.257015	3.639610	C	4.150302	-0.188325	3.649118
H	-4.391594	-0.824511	1.603567	H	5.611604	-0.214090	2.064396
C	-2.859911	-1.146462	4.627036	H	2.479660	-0.352506	5.007516
H	-0.894952	-0.390779	5.109724	H	4.791969	0.328846	4.356567
H	-4.778044	-1.762961	3.858107	C	1.645032	-4.253500	-2.388440
H	-3.029660	-1.568670	5.613113	H	1.281081	-5.281283	-2.469626
P	-2.003393	0.519226	0.382165	H	1.310187	-3.682286	-3.264169
Pd	0.046117	-0.758127	0.183129	H	2.732045	-4.251163	-2.361556
C	-2.501257	-4.310030	-1.398251	C	0.432303	-3.051511	1.469124
C	-1.162060	-4.179663	-1.774785	H	-0.019516	-2.581666	2.345180
C	-0.213793	-3.715248	-0.849015	H	0.882396	-3.993354	1.830524
C	-0.642319	-3.357325	0.451030				
C	-1.995056	-3.463712	0.794434	**TS4C**			
C	-2.929884	-3.945233	-0.121203	C	3.718650	1.692763	3.537727
H	-3.215950	-4.691551	-2.121880	C	3.169042	1.690715	2.255707
H	-0.863359	-4.464436	-2.776068	C	2.349831	0.628872	1.834066
H	-2.301794	-3.184270	1.798424	C	2.092719	-0.428392	2.721013
H	-3.975360	-4.031184	0.155731	C	2.646974	-0.423612	4.002553
N	1.157610	-3.651709	-1.147731	C	3.458290	0.635365	4.413415

H	4.349583	2.519882	3.852010	C	-2.396491	3.077178	1.394403
H	3.367787	2.522502	1.586570	C	-2.461158	2.875824	0.017553
H	1.476650	-1.262531	2.399521	C	-2.140340	1.615056	-0.494990
H	2.444275	-1.251050	4.676853	C	-1.716390	0.569946	0.343691
H	3.887168	0.638295	5.411929	C	-1.748412	0.769036	1.733200
C	1.256973	2.292736	-0.302093	C	-2.052643	2.026397	2.254601
C	1.276018	2.673962	-1.654425	H	-2.640530	4.053920	1.802652
C	0.866778	3.237369	0.657321	H	-2.782754	3.673577	-0.643574
C	0.926957	3.970591	-2.032518	H	-1.500554	-0.047560	2.405428
H	1.578123	1.961430	-2.415755	H	-2.024262	2.187464	3.328606
C	0.528629	4.537367	0.277778	N	-2.378321	1.235066	-1.821361
H	0.814743	2.959789	1.704282	C	-2.624245	-0.108383	-2.011407
C	0.556533	4.909927	-1.065887	O	-2.820017	-0.623948	-3.100428
H	0.959388	4.249968	-3.082543	C	-2.628656	-0.901926	-0.698227
H	0.231592	5.255126	1.037729	C	-1.861121	-2.116217	-0.745597
H	0.293556	5.922595	-1.359515	H	-1.510758	-2.431360	-1.725888
C	3.010731	0.118864	-0.982293	H	-2.134360	-2.934973	-0.087363
C	2.695854	-0.471562	-2.216492	C	-3.913382	-0.892767	0.086383
C	4.351088	0.391732	-0.678267	C	-5.046595	-0.237059	-0.411417
C	3.700856	-0.758538	-3.140026	C	-4.002945	-1.561381	1.317189
H	1.666586	-0.735572	-2.441791	C	-6.245731	-0.254198	0.304315
C	5.356467	0.089552	-1.598127	H	-5.004661	0.274176	-1.368066
H	4.619115	0.823361	0.280255	C	-5.197464	-1.573221	2.031061
C	5.033850	-0.479516	-2.831778	H	-3.127466	-2.058998	1.724294
H	3.442604	-1.221734	-4.088156	C	-6.326120	-0.918565	1.527341
H	6.393483	0.295648	-1.346859	H	-7.117258	0.252415	-0.101154
H	5.819142	-0.716298	-3.544586	H	-5.247785	-2.092870	2.984013
P	1.620387	0.538156	0.151407	H	-7.258628	-0.929421	2.084626
Pd	-0.225914	-0.950742	-0.104975	C	-2.447593	2.181206	-2.922029

H	-3.369311	2.774913	-2.876755	C	1.781241	0.440988	2.855151
H	-1.583923	2.851227	-2.880354	C	2.743943	2.275210	1.601503
H	-2.438384	1.609601	-3.850811	C	1.920043	1.171527	4.035367
I	1.256033	-3.213025	-0.092403	H	1.341261	-0.553386	2.880803
				C	2.876055	3.005600	2.784267
INT4C				H	3.043588	2.721100	0.659819
C	3.965308	2.247824	-2.629117	C	2.465234	2.457820	4.001235
C	3.661042	1.474926	-1.511004	H	1.594423	0.739345	4.977412
C	2.357032	0.979377	-1.329936	H	3.297055	4.006970	2.751777
C	1.376372	1.227851	-2.298291	H	2.565094	3.031489	4.918518
C	1.690881	2.001660	-3.418380	P	1.940011	-0.042438	0.129855
C	2.976299	2.516911	-3.581701	Pd	0.057131	-1.341176	0.065094
H	4.972864	2.632190	-2.763117	C	-5.905625	1.220655	1.641241
H	4.435607	1.245681	-0.783744	C	-5.598317	0.451937	0.508829
H	0.378147	0.816887	-2.188466	C	-4.288622	0.486734	0.045317
H	0.922498	2.197638	-4.160378	C	-3.299886	1.252393	0.683914
H	3.215428	3.118419	-4.454778	C	-3.614082	2.012012	1.798126
C	3.310333	-1.271483	0.170365	C	-4.933776	1.996971	2.276572
C	4.279580	-1.318963	1.181512	H	-6.922131	1.212055	2.024755
C	3.345200	-2.224727	-0.863806	H	-6.356729	-0.145819	0.013562
C	5.269014	-2.304678	1.156147	H	-2.851241	2.616700	2.281237
H	4.266535	-0.590552	1.986020	H	-5.199446	2.591933	3.145435
C	4.333024	-3.207633	-0.882193	N	-3.743336	-0.153327	-1.076449
H	2.602312	-2.194808	-1.658374	C	-2.420853	0.182336	-1.254165
C	5.296610	-3.249923	0.129313	O	-1.734606	-0.119170	-2.218682
H	6.018993	-2.331742	1.942094	C	-1.966101	0.995381	-0.010460
H	4.346797	-3.941662	-1.682777	C	-1.197513	0.034251	0.932401
H	6.065027	-4.017858	0.116805	H	-0.636831	0.579721	1.690824
C	2.196024	0.985801	1.627394	H	-1.901039	-0.637408	1.424066

C	-1.241188	2.282374	-0.388070	C	1.409130	1.194859	1.705386
C	-1.483556	2.898494	-1.625921	C	2.749377	1.597353	1.764792
C	-0.386295	2.929528	0.512690	C	0.411692	2.055041	2.192767
C	-0.864152	4.100277	-1.963902	C	3.082973	2.848326	2.290734
H	-2.138152	2.421015	-2.346880	H	3.529150	0.944060	1.387503
C	0.236749	4.133337	0.175522	C	0.746804	3.301031	2.716196
H	-0.185275	2.499857	1.487080	H	-0.630796	1.752330	2.139295
C	0.007077	4.721709	-1.066756	C	2.085313	3.703708	2.760609
H	-1.058478	4.548008	-2.934933	H	4.125082	3.154758	2.326688
H	0.907070	4.601216	0.891098	H	-0.035296	3.964578	3.073500
H	0.497591	5.653826	-1.333444	H	2.346547	4.680862	3.157169
C	-4.463726	-1.056687	-1.950761	C	2.429256	-1.195479	0.430101
H	-4.776637	-1.945762	-1.393278	C	2.935093	-0.886309	-0.841798
H	-5.342125	-0.559513	-2.378547	C	3.138226	-2.070082	1.264210
H	-3.782900	-1.357082	-2.747707	C	4.144508	-1.433897	-1.266087
I	-1.651085	-3.390564	-0.039185	H	2.385069	-0.224142	-1.502078
				C	4.342836	-2.625792	0.829220
TS4D				H	2.749211	-2.324167	2.245348
C	0.243427	-1.840543	4.746256	C	4.848769	-2.306638	-0.432978
C	0.734224	-1.111577	3.663104	H	4.526197	-1.186445	-2.252641
C	0.220689	-1.326086	2.372197	H	4.883664	-3.310927	1.476504
C	-0.796512	-2.275201	2.187305	H	5.785542	-2.743234	-0.768893
C	-1.285429	-2.999622	3.276027	P	0.868637	-0.382418	0.932705
C	-0.768282	-2.785241	4.554740	Pd	-0.776291	-0.134009	-0.812410
H	0.649355	-1.667834	5.739473	C	-5.276550	0.095108	0.577833
H	1.512801	-0.371397	3.822005	C	-4.453837	1.205841	0.772095
H	-1.196511	-2.457275	1.195835	C	-3.211452	1.320997	0.120773
H	-2.073297	-3.731103	3.119231	C	-2.805383	0.227420	-0.679165
H	-1.152603	-3.349395	5.400401	C	-3.663969	-0.838147	-0.945938

C	-4.896776	-0.921708	-0.293117
H	-6.229944	0.049415	1.096320
H	-4.808461	2.000019	1.415733
H	-3.346685	-1.622037	-1.622067
H	-5.540372	-1.778776	-0.467970
N	-2.449169	2.512456	0.259807
C	-1.305779	2.874470	-0.471021
O	-0.786432	3.971062	-0.294013
C	-0.737548	1.897932	-1.466467
C	0.661235	2.088985	-1.952302
C	1.631913	2.763135	-1.179902
C	1.082199	1.516595	-3.172784
C	2.955012	2.839982	-1.604803
H	1.351119	3.223095	-0.245080
C	2.407507	1.602368	-3.595550
H	0.381212	0.980835	-3.801428
C	3.355484	2.261229	-2.811103
H	3.678160	3.352700	-0.977006
H	2.695367	1.145487	-4.538208
H	4.390524	2.323438	-3.135455
C	-2.911719	3.504121	1.234262
H	-3.872583	3.936881	0.934185
H	-3.019290	3.037804	2.219073
H	-2.168905	4.295818	1.281514
C	-1.724305	1.201873	-2.273221
H	-1.425874	0.670177	-3.171399
H	-2.715003	1.629944	-2.374354
I	-0.591069	-2.768581	-1.737617

INT4D

C	-4.470175	0.782318	3.199929
C	-3.969536	0.699137	1.901291
C	-2.590339	0.535331	1.678214
C	-1.726794	0.439811	2.780204
C	-2.233723	0.521137	4.079153
C	-3.601814	0.695241	4.291670
H	-5.537654	0.909708	3.358763
H	-4.654753	0.742621	1.059686
H	-0.661105	0.309878	2.625151
H	-1.553439	0.445666	4.922721
H	-3.993134	0.757053	5.303641
C	-3.160188	-0.527162	-0.948863
C	-3.394582	-0.267614	-2.308326
C	-3.802876	-1.620384	-0.346798
C	-4.255541	-1.080864	-3.046006
H	-2.910702	0.576531	-2.790579
C	-4.676396	-2.422186	-1.083013
H	-3.620285	-1.846517	0.698916
C	-4.901812	-2.159568	-2.435442
H	-4.430919	-0.863578	-4.096323
H	-5.174220	-3.258112	-0.598570
H	-5.578623	-2.786780	-3.009192
C	-2.013531	2.117822	-0.748103
C	-1.132465	2.440774	-1.792017
C	-2.956230	3.066983	-0.330474
C	-1.211281	3.681273	-2.424946
H	-0.364860	1.731073	-2.086795
C	-3.023020	4.312912	-0.955617

H	-3.627091	2.847754	0.493180	H	-1.062549	-5.006877	1.257073
C	-2.156603	4.620104	-2.006855	H	-1.871440	-3.010155	-2.463331
H	-0.518996	3.920703	-3.227261	H	-2.533671	-4.642189	-0.719937
H	-3.750568	5.045478	-0.616574	C	4.745765	-0.914943	2.219657
H	-2.209651	5.592180	-2.489681	H	5.821052	-0.990201	2.036275
P	-1.891734	0.434081	-0.018264	H	4.519244	0.048046	2.693575
Pd	0.273822	-0.508264	-0.114289	H	4.425765	-1.714706	2.883184
C	5.704937	1.580506	-1.084092	C	2.865314	-1.603948	-1.518547
C	5.362096	0.784774	0.009526	H	2.256762	-1.480182	-2.416707
C	4.416133	-0.239639	-0.135313	H	3.432518	-2.541999	-1.663175
C	3.831359	-0.463811	-1.391597	I	1.488684	1.696136	0.845232
C	4.178440	0.344684	-2.470617				
C	5.114119	1.370927	-2.329270	(*E*)-**2a**			
H	6.431569	2.377302	-0.950767	C	-0.657982	1.550762	0.179814
H	5.808996	0.994149	0.973148	C	0.586026	1.151497	-0.144937
H	3.708702	0.162753	-3.435078	H	1.251736	1.864821	-0.616479
H	5.375459	1.996256	-3.177893	C	1.093513	-0.223630	0.081001
N	4.025502	-1.051186	0.955618	O	0.343057	-1.175175	0.297832
C	2.802709	-1.720348	1.010464	C	2.576401	-0.442225	0.008185
O	2.414183	-2.212543	2.071593	C	3.034788	-1.763744	-0.118991
C	2.017224	-1.787178	-0.264549	C	3.514295	0.598660	0.093793
C	0.847002	-2.667551	-0.355340	C	4.397600	-2.036829	-0.178130
C	0.410169	-3.591285	0.646748	H	2.299627	-2.560128	-0.169516
C	-0.024412	-2.469943	-1.482900	C	4.880748	0.323005	0.045510
C	-0.770800	-4.289686	0.494237	H	3.187200	1.625226	0.225092
H	1.034243	-3.732183	1.517012	C	5.324570	-0.992855	-0.096936
C	-1.232712	-3.187375	-1.603690	H	4.740630	-3.062226	-0.285567
H	0.303513	-1.890525	-2.339559	H	5.597925	1.135605	0.121361
C	-1.603136	-4.090379	-0.626891	H	6.389425	-1.205415	-0.141063

Cl	-1.116604	3.208091	-0.234537
C	-1.756845	0.753833	0.815744
C	-2.652485	0.076329	-0.242034
H	-2.360377	1.412271	1.450379
H	-1.305932	-0.020866	1.440860
C	-3.773035	-0.748774	0.397768
H	-3.080832	0.841867	-0.902779
H	-2.018959	-0.572128	-0.857678
C	-4.674122	-1.436235	-0.634825
H	-3.329261	-1.509024	1.056743
H	-4.386235	-0.101108	1.042367
H	-5.117748	-0.675283	-1.292582
H	-4.057584	-2.077080	-1.280520
C	-5.785866	-2.271643	0.007722
H	-6.415453	-2.752899	-0.749388
H	-5.367119	-3.060068	0.645317
H	-6.434867	-1.648605	0.635828

K_2CO_3

C	-0.000118	0.809588	0.000063
O	-0.000001	-0.539503	-0.000094
O	1.126696	1.428044	0.000043
O	-1.127154	1.427669	0.000261
K	2.524389	-0.615400	0.000061
K	-2.524158	-0.615506	-0.000170

Cs_2CO_3

C	0.000000	-1.199420	0.000001
O	-0.000002	0.138357	-0.000166
O	-1.125771	-1.827196	0.000189
O	1.125773	-1.827193	0.000160
Cs	2.831928	0.321134	-0.000093
Cs	-2.831928	0.321134	0.000066

TS-A

C	-0.841779	1.953373	-1.044274
C	0.401059	1.526419	-1.481235
H	1.199360	2.257072	-1.447549
C	0.756361	0.177385	-1.806982
O	-0.024732	-0.796960	-1.893226
C	2.243286	-0.102046	-1.925580
C	2.695348	-1.380695	-1.557266
C	3.199092	0.855227	-2.309395
C	4.056510	-1.682553	-1.525182
H	1.953991	-2.122607	-1.281767
C	4.561749	0.550789	-2.294424
H	2.877153	1.838005	-2.640302
C	4.998133	-0.714420	-1.888896
H	4.384507	-2.674553	-1.223503
H	5.283939	1.300053	-2.609127
H	6.059370	-0.948768	-1.874672
Cl	-0.897368	3.656315	-0.564273
C	-2.043741	1.182110	-0.868663
C	-3.412723	1.855178	-0.775479
H	-1.909034	0.628122	0.212473
H	-2.030703	0.350954	-1.580474
C	-4.500624	0.811099	-0.489927
H	-3.404976	2.589114	0.038035

H	-3.652721	2.405663	-1.697988	H	3.061129	2.430606	-1.320558
C	-5.902871	1.411956	-0.348897	C	5.470753	0.070873	-0.867270
H	-4.510437	0.062681	-1.299961	H	5.112512	-2.055691	-0.762010
H	-4.231180	0.277393	0.431477	H	5.505347	2.220747	-1.054438
H	-5.894083	2.156211	0.459644	H	6.547299	-0.019409	-0.749704
H	-6.161547	1.959540	-1.266926	Cl	-1.162441	3.095500	0.629927
C	-6.975690	0.356305	-0.060435	C	-1.862003	0.728169	-0.549840
H	-7.970782	0.805074	0.043329	C	-3.321422	1.162942	-0.442370
H	-7.026383	-0.384367	-0.869430	H	-1.732200	-0.162027	0.342603
H	-6.752705	-0.183053	0.868976	H	-1.646785	0.153783	-1.456019
C	-0.545423	0.012932	1.759280	C	-4.263678	-0.029001	-0.655702
O	0.248380	-1.002227	1.911685	H	-3.504817	1.586790	0.551477
O	-0.163531	1.222212	1.869817	H	-3.552879	1.956157	-1.169818
O	-1.803930	-0.234890	1.389191	C	-5.746130	0.342150	-0.542901
Cs	2.613958	0.752721	1.730108	H	-4.077403	-0.469893	-1.648805
Cs	-1.361961	-2.695582	0.066525	H	-4.019075	-0.804082	0.083221
				H	-5.930839	0.784090	0.446291
TS-A-K				H	-5.983852	1.125456	-1.277275
C	-0.787798	1.637482	-0.302518	C	-6.678015	-0.856482	-0.749326
C	0.558927	1.502222	-0.621039	H	-7.732600	-0.570761	-0.657569
H	1.218475	2.280996	-0.259189	H	-6.537462	-1.298725	-1.744297
C	1.161188	0.360946	-1.232429	H	-6.477353	-1.640096	-0.007839
O	0.560635	-0.638878	-1.696915	C	-0.414981	-1.056762	1.749145
C	2.675973	0.308595	-1.175012	O	0.539111	-1.933124	1.619888
C	3.283740	-0.952097	-1.040791	O	-0.272372	0.038489	2.371777
C	3.500466	1.447774	-1.178807	K	-0.470495	-2.828379	-0.627663
C	4.664269	-1.071569	-0.875181	K	2.260012	-0.074425	2.253541
H	2.649474	-1.831515	-1.052166	O	-1.563484	-1.304509	1.109396
C	4.883808	1.329344	-1.032213				

A

C	-0.821403	0.518770	-0.493997
C	0.583278	0.607218	-0.246836
H	1.000693	1.599081	-0.140094
C	1.428166	-0.516045	-0.204713
O	1.094277	-1.722895	-0.390370
C	2.905113	-0.256795	0.063802
C	3.809766	-1.282175	-0.260252
C	3.428534	0.913084	0.641058
C	5.179606	-1.136837	-0.048039
H	3.389130	-2.193209	-0.674655
C	4.798741	1.061275	0.861525
H	2.753085	1.707681	0.944079
C	5.686402	0.039046	0.513200
H	5.858023	-1.945498	-0.317553
H	5.174842	1.976622	1.316421
H	6.754999	0.154063	0.686148
Cl	-1.633423	2.172852	-0.491358
C	-1.620491	-0.550352	-0.720238
C	-3.107137	-0.550124	-0.934312
H	-1.083360	-1.494857	-0.692478
C	-3.921668	-0.580191	0.376537
H	-3.419080	0.333852	-1.508398
H	-3.389572	-1.427374	-1.537619
C	-5.438480	-0.594032	0.153009
H	-3.627238	-1.461331	0.965289
H	-3.643583	0.297549	0.974742
H	-5.723483	0.289320	-0.437381
H	-5.709638	-1.467953	-0.458749
C	-6.241746	-0.615979	1.458141
H	-7.324507	-0.621583	1.275307
H	-5.998258	-1.505344	2.053866
H	-6.010157	0.262481	2.073824

TS-B

C	0.801487	0.744651	0.944280
C	-0.547333	0.754870	0.720764
H	-1.068727	1.705507	0.716729
C	-1.271903	-0.452666	0.431071
O	-0.823856	-1.611711	0.507127
C	-2.740541	-0.295121	0.056796
C	-3.583630	-1.401908	0.237093
C	-3.285391	0.871555	-0.500079
C	-4.934668	-1.339482	-0.098453
H	-3.139063	-2.307549	0.638443
C	-4.636500	0.934957	-0.847651
H	-2.642213	1.726023	-0.687444
C	-5.469322	-0.167241	-0.641699
H	-5.573921	-2.206674	0.058199
H	-5.037863	1.846064	-1.287243
H	-6.522858	-0.116322	-0.909759
Cl	1.747030	2.383012	-0.414708
C	1.776716	0.115571	1.582395
C	3.240742	0.055461	1.233959
H	1.431878	-0.466532	2.439213
C	3.520077	-0.752007	-0.046035
H	3.610875	1.076974	1.086187
H	3.799533	-0.384314	2.073798

C	5.007947	-0.803983	-0.409012
H	3.126720	-1.772413	0.069439
H	2.955099	-0.284971	-0.860926
H	5.382740	0.222890	-0.527198
H	5.578319	-1.244788	0.423777
C	5.281506	-1.597750	-1.691210
H	6.350549	-1.618823	-1.941569
H	4.939833	-2.636238	-1.590927
H	4.745311	-1.157795	-2.541028

6

C	-0.048580	-2.175998	0.521611
C	-1.254123	-1.900830	0.939657
H	-1.434341	-1.835926	2.014729
C	1.160573	-2.422772	0.065025
H	1.476831	-3.444937	-0.140058
C	-2.415775	-1.557174	0.032816
C	-2.805241	-0.073162	0.163901
H	-3.279262	-2.186676	0.290538
H	-2.152496	-1.781819	-1.007107
C	-3.979831	0.318347	-0.739741
H	-3.060321	0.144878	1.211484
H	-1.928924	0.545440	-0.072862
C	-4.360265	1.796283	-0.606159
H	-3.720742	0.097229	-1.784684
H	-4.849064	-0.310566	-0.500020
H	-5.197829	2.055763	-1.263388
H	-4.655455	2.035785	0.422936
H	-3.515146	2.444776	-0.867495
C	2.158802	-1.400527	-0.371338
C	1.985885	0.049493	-0.027716
C	2.520566	0.990761	-0.921269
C	1.356586	0.498449	1.142629
C	2.396151	2.354137	-0.669343
H	3.028014	0.628916	-1.809741
C	1.245131	1.864875	1.401043
H	0.974505	-0.217333	1.860601
C	1.754738	2.794344	0.492280
H	2.801913	3.074848	-1.374143
H	0.764403	2.203139	2.314982
H	1.660010	3.858499	0.692004
O	3.100026	-1.766173	-1.066018

INT5A

C	0.135310	2.654014	4.201174
C	0.022181	2.806582	2.817741
C	0.674091	1.917009	1.955989
C	1.426931	0.858693	2.499029
C	1.536017	0.712273	3.881795
C	0.892094	1.611359	4.737169
H	-0.380096	3.347393	4.859756
H	-0.599237	3.597281	2.414986
H	1.909018	0.144779	1.835735
H	2.118137	-0.109217	4.292330
H	0.973782	1.494480	5.814224
C	-0.329883	3.559862	-0.293717
C	0.163378	4.792151	0.166676
C	-1.461599	3.543259	-1.117763

C	-0.483839	5.980313	-0.170260	H	-4.149960	-2.030221	-2.183186
H	1.053745	4.824327	0.788442	H	-6.341556	-1.616984	-3.287886
C	-2.102510	4.734207	-1.463034	N	-4.287930	1.738819	0.169020
H	-1.842769	2.601295	-1.487445	C	-3.086929	1.169322	0.527495
C	-1.619830	5.953248	-0.984285	O	-2.281229	1.680075	1.292495
H	-0.097992	6.927206	0.196665	C	-2.940454	-0.182900	-0.224359
H	-2.977282	4.706533	-2.107016	C	-1.785505	-0.088428	-1.268575
H	-2.119825	6.880357	-1.250052	H	-1.800929	-1.021012	-1.850116
C	2.265947	2.405398	-0.416657	H	-2.018413	0.722363	-1.967406
C	2.570646	2.292445	-1.784826	C	-2.736305	-1.310605	0.801334
C	3.267890	2.832367	0.466614	C	-1.703698	-1.210383	1.753755
C	3.844271	2.609366	-2.260096	C	-3.569012	-2.437756	0.853636
H	1.806847	1.946071	-2.476799	C	-1.510893	-2.201631	2.716753
C	4.548563	3.141797	-0.007518	H	-1.072316	-0.332142	1.766083
H	3.052634	2.927045	1.526389	C	-3.376055	-3.437541	1.816941
C	4.840205	3.035016	-1.370864	H	-4.401030	-2.529068	0.164929
H	4.056984	2.535754	-3.323710	C	-2.345863	-3.325350	2.755331
H	5.309382	3.489124	0.687291	H	-0.721107	-2.075882	3.453533
H	5.826758	3.302038	-1.741787	H	-4.058297	-4.284018	1.851871
P	0.533956	1.996302	0.123662	H	-2.218012	-4.082515	3.525829
Pd	0.175496	-0.092155	-0.689177	C	-4.733311	3.033418	0.645128
C	-6.689892	0.247817	-2.267456	H	-4.867010	3.725363	-0.193780
C	-6.208284	1.191617	-1.350480	H	-5.680743	2.938771	1.187039
C	-4.988307	0.929801	-0.737499	H	-3.963331	3.421401	1.312819
C	-4.250871	-0.235009	-0.998459	O	2.511104	-3.065545	-0.579320
C	-4.727429	-1.143639	-1.934491	C	1.766218	-2.065510	-0.667667
C	-5.958822	-0.904613	-2.563261	O	2.140320	-0.854674	-0.292053
H	-7.641740	0.424273	-2.759907	Cs	4.975940	-0.878020	-0.635820
H	-6.766675	2.096711	-1.133354	O	0.527031	-2.122808	-1.127082

Cs	-0.243215	-4.717486	-0.089553	H	5.194681	4.894157	0.964356
				H	6.502220	3.756650	0.543972
TS6A				H	5.558145	4.547029	-0.750849
C	4.196570	1.405399	3.558321	Pd	0.178544	0.421242	-0.735377
C	4.696804	2.314846	2.616996	C	1.456643	2.019627	-0.757878
C	4.206214	2.235648	1.317496	H	1.196634	2.772082	-0.007635
C	3.242488	1.286023	0.936245	H	1.398252	2.470085	-1.755673
C	2.755589	0.391007	1.879602	C	-0.282230	-2.359070	0.118978
C	3.239873	0.455069	3.197099	O	-0.773462	-3.491870	0.379203
H	4.561067	1.446220	4.581068	O	-0.939319	-1.459446	-0.568669
H	5.440065	3.055652	2.894269	O	0.940584	-2.053222	0.526766
H	2.015212	-0.354476	1.611589	C	-4.202712	0.545203	2.992111
H	2.860430	-0.239500	3.942198	C	-3.702927	1.133935	1.826946
N	4.553774	3.035266	0.221527	C	-2.353464	0.970270	1.467693
C	3.865158	2.656762	-0.916412	C	-1.510825	0.219467	2.306004
O	3.985236	3.169116	-2.016111	C	-2.012442	-0.366808	3.471056
C	2.903304	1.502522	-0.533435	C	-3.358671	-0.210528	3.814063
C	3.073365	0.275108	-1.414275	H	-5.245496	0.687496	3.263996
C	4.165867	0.066225	-2.260501	H	-4.368882	1.712789	1.194400
C	1.978016	-0.621859	-1.432885	H	-0.469967	0.074533	2.031131
C	4.175727	-1.017059	-3.143951	H	-1.349363	-0.945000	4.108513
H	4.990601	0.771116	-2.273943	H	-3.746432	-0.662070	4.723405
C	1.989960	-1.675158	-2.369358	C	-3.038458	1.521275	-1.302950
H	1.396303	-1.137939	-0.319643	C	-4.091861	2.449932	-1.327179
C	3.079704	-1.883736	-3.215587	C	-3.048084	0.450009	-2.213551
H	5.027681	-1.162504	-3.802990	C	-5.154189	2.289310	-2.218853
H	1.122221	-2.332265	-2.422271	H	-4.072160	3.309603	-0.663097
H	3.070774	-2.692784	-3.942954	C	-4.114653	0.292061	-3.102316
C	5.510424	4.122067	0.253103	H	-2.213585	-0.245418	-2.233317

C	-5.171887	1.206540	-3.102364	H	3.108926	-0.130584	3.751599
H	-5.960822	3.016859	-2.232290	N	4.795315	2.547717	-0.428038
H	-4.103700	-0.527397	-3.816889	C	3.754157	2.426316	-1.348357
H	-5.993460	1.090924	-3.803775	O	3.691197	3.013102	-2.410190
C	-1.486431	3.453182	0.186011	C	2.751251	1.386542	-0.792792
C	-1.086133	4.245998	-0.903578	C	2.832066	0.096976	-1.604487
C	-1.682615	4.049246	1.438894	C	3.988704	-0.383221	-2.231052
C	-0.902271	5.617297	-0.742731	C	1.613980	-0.615149	-1.668729
H	-0.913038	3.787330	-1.873701	C	3.941803	-1.585772	-2.948456
C	-1.490665	5.424476	1.595869	H	4.914853	0.186177	-2.192518
H	-1.984469	3.448374	2.291074	C	1.588238	-1.817994	-2.395792
C	-1.104275	6.208759	0.508332	H	0.808857	-1.434388	0.404382
H	-0.592689	6.222254	-1.589940	C	2.740040	-2.301619	-3.033563
H	-1.645202	5.880139	2.569807	H	4.829223	-1.943237	-3.465361
H	-0.955461	7.277350	0.634097	H	0.657662	-2.377250	-2.467402
P	-1.648740	1.654996	-0.098533	H	2.696344	-3.220285	-3.615374
Cs	-3.654429	-2.465572	0.225130	C	5.920213	3.443316	-0.610434
Cs	2.268470	-4.602158	0.286835	H	5.919515	4.229751	0.153537
				H	6.866825	2.893768	-0.553535
INT6A				H	5.820020	3.895822	-1.598434
C	4.768300	1.009073	2.975883	Pd	0.017711	0.261464	-0.759720
C	5.282931	1.751632	1.902257	C	1.287170	1.870778	-0.867490
C	4.521009	1.829614	0.738727	H	1.078827	2.611451	-0.089271
C	3.284945	1.167527	0.614228	H	1.126823	2.329832	-1.850339
C	2.769512	0.474641	1.699750	C	-0.699356	-2.558907	0.234954
C	3.519480	0.387606	2.888322	O	-1.273808	-3.597115	0.565449
H	5.338793	0.948040	3.898628	O	-1.136473	-1.655185	-0.572692
H	6.234887	2.266160	1.987005	O	0.542537	-2.298009	0.805497
H	1.777501	0.035230	1.637906	C	-4.596072	-0.008183	2.920758

C	-4.022601	0.724796	1.877807	H	-0.687850	6.152520	-0.644996
C	-2.661779	0.568708	1.558086	H	-1.887982	5.231042	3.384310
C	-1.887338	-0.321959	2.319679	H	-1.109376	6.881157	1.697046
C	-2.461348	-1.059457	3.358271	P	-1.856062	1.431317	0.132816
C	-3.817789	-0.908076	3.658439	Cs	-4.060045	-2.575099	-0.224042
H	-5.646578	0.130804	3.163408	Cs	3.582014	-2.979828	0.702351
H	-4.640275	1.412284	1.308498				
H	-0.839214	-0.463541	2.078006	**INT7A**			
H	-1.849490	-1.756381	3.923573	C	1.033152	5.495131	-0.932222
H	-4.264912	-1.478094	4.468405	C	0.736355	4.455851	-0.049093
C	-3.206518	1.507569	-1.124288	C	0.294887	3.218434	-0.538381
C	-4.237473	2.459389	-1.073506	C	0.162576	3.038155	-1.924947
C	-3.201253	0.563173	-2.166524	C	0.449229	4.082306	-2.804668
C	-5.263513	2.442011	-2.020520	C	0.886813	5.312471	-2.309157
H	-4.228176	3.226744	-0.304422	H	1.381398	6.448079	-0.542869
C	-4.230484	0.546869	-3.111912	H	0.858954	4.607780	1.018574
H	-2.375129	-0.139032	-2.248659	H	-0.147992	2.071940	-2.313373
C	-5.267375	1.481233	-3.035734	H	0.347536	3.927839	-3.875236
H	-6.053059	3.186737	-1.973170	H	1.122103	6.122619	-2.993975
H	-4.203429	-0.172042	-3.927255	C	0.710288	2.128984	2.145986
H	-6.059804	1.478615	-3.778919	C	0.241895	3.052815	3.095464
C	-1.678455	3.170205	0.679294	C	1.895793	1.423548	2.403294
C	-1.230280	4.106825	-0.268957	C	0.953504	3.266454	4.276594
C	-1.911050	3.584845	1.997807	H	-0.683259	3.592912	2.915515
C	-1.032575	5.436997	0.095922	C	2.607402	1.641752	3.583704
H	-1.033236	3.793838	-1.290954	H	2.262432	0.698822	1.685208
C	-1.704005	4.918386	2.360254	C	2.137329	2.563255	4.521383
H	-2.256303	2.874481	2.742516	H	0.582629	3.980448	5.007163
C	-1.268055	5.844966	1.412395	H	3.521078	1.080936	3.760549

H	2.686790	2.731593	5.443801	H	1.889649	0.702893	-2.289732
C	-1.932163	2.053334	0.913010	C	2.381029	-1.977219	-1.847299
C	-2.498379	1.501470	2.074174	C	2.940492	-3.019078	-2.590391
C	-2.785129	2.598990	-0.059298	C	1.013319	-1.981826	-1.495887
C	-3.882718	1.473038	2.246098	C	2.138209	-4.080739	-3.014053
H	-1.858338	1.094514	2.851719	H	3.993234	-2.990392	-2.861654
C	-4.168518	2.574564	0.118616	C	0.222862	-3.050076	-1.944325
H	-2.370058	3.035979	-0.962352	C	0.778688	-4.091950	-2.696182
C	-4.722789	2.001316	1.264673	H	2.570155	-4.887424	-3.600998
H	-4.302934	1.026667	3.142784	H	-0.841538	-3.073120	-1.721071
H	-4.816912	2.987001	-0.649007	H	0.146381	-4.909033	-3.037339
H	-5.801082	1.959443	1.386576	C	6.707813	0.331117	-1.954253
P	-0.142482	1.805652	0.553869	H	7.008331	1.244613	-1.426340
C	5.596423	-1.087588	2.154725	H	7.493414	-0.423927	-1.825794
C	6.075930	-0.596077	0.931140	H	6.581246	0.547595	-3.016714
C	5.194390	-0.570337	-0.145292	C	-1.681635	-1.116206	-0.010189
C	3.862632	-1.001619	-0.026207	C	-2.723876	-0.929939	-0.804791
C	3.410105	-1.508019	1.180757	H	-2.592570	-0.487133	-1.785362
C	4.283414	-1.546339	2.281550	C	-0.613053	-2.914036	1.431400
H	6.265620	-1.121842	3.010518	C	-1.607090	-3.512417	2.445382
H	7.101423	-0.254375	0.828692	H	0.399023	-2.909331	1.855358
H	2.387623	-1.864199	1.265319	H	-0.576818	-3.523747	0.526724
H	3.935642	-1.940741	3.232431	C	-1.258430	-4.958975	2.815596
N	5.440051	-0.154969	-1.458924	H	-1.619222	-2.894884	3.356236
C	4.311708	-0.315227	-2.258448	H	-2.616574	-3.456084	2.021183
O	4.266504	-0.071281	-3.451354	C	-2.245746	-5.561722	3.820339
C	3.151009	-0.777205	-1.349577	H	-1.241482	-5.570329	1.902483
C	2.124758	0.385652	-1.268253	H	-0.239980	-4.996301	3.228233
H	2.541545	1.247370	-0.732850	H	-1.983776	-6.596717	4.068577

H	-2.258494	-4.985704	4.754130	H	0.462981	3.510503	3.976154
H	-3.265520	-5.559639	3.416706	H	2.405165	5.065327	4.064417
C	-4.090306	-1.279819	-0.316234	C	3.042970	1.502838	-1.396928
C	-5.275699	-0.759456	-1.077301	C	4.448313	1.532888	-1.418414
C	-6.545357	-1.221973	-0.694188	C	2.339054	1.888776	-2.549293
C	-5.181213	0.182801	-2.113532	C	5.130855	1.953697	-2.559774
C	-7.691652	-0.761580	-1.335442	H	5.010854	1.206383	-0.549026
H	-6.604447	-1.942997	0.114291	C	3.025180	2.307519	-3.691316
C	-6.330409	0.647639	-2.753631	H	1.253202	1.863877	-2.545902
H	-4.217937	0.581412	-2.410892	C	4.420377	2.343179	-3.698593
C	-7.586922	0.175775	-2.368159	H	6.217527	1.972330	-2.561046
H	-8.667595	-1.130992	-1.032311	H	2.464664	2.605126	-4.573295
H	-6.243963	1.379594	-3.552084	H	4.953622	2.668091	-4.588104
H	-8.480933	0.536934	-2.869602	C	3.194000	-0.337459	0.802347
O	-4.256643	-1.961729	0.690623	C	3.794322	-1.297219	-0.029011
C	-1.018855	-1.497099	1.094732	C	3.412185	-0.416066	2.185757
H	-0.971176	-0.792563	1.925218	C	4.597276	-2.303203	0.507479
Pd	0.359391	-0.346988	-0.433292	H	3.650274	-1.253874	-1.101814
				C	4.216938	-1.422545	2.720120
INT7B				H	2.956428	0.310011	2.850230
C	3.382443	4.177587	2.358324	C	4.814517	-2.367472	1.884831
C	3.324778	3.188455	1.375270	H	5.053226	-3.033469	-0.155910
C	2.235342	2.308861	1.320901	H	4.370331	-1.468986	3.794583
C	1.206738	2.438153	2.265486	H	5.441131	-3.149987	2.304555
C	1.271399	3.417891	3.256046	P	2.079762	0.952663	0.080123
C	2.359307	4.292000	3.302350	Pd	-0.211617	0.485150	-0.554266
H	4.226762	4.861422	2.384225	C	-4.785696	-0.146491	2.882520
H	4.121614	3.117557	0.642357	C	-5.492195	-0.017609	1.676695
H	0.343616	1.783588	2.204071	C	-4.824094	0.541822	0.591178

C	-3.483969	0.952476	0.676222	C	1.375457	-3.385688	1.730604
C	-2.810829	0.851182	1.880596	C	0.527438	-2.310138	1.439800
C	-3.463910	0.291587	2.991958	C	0.076659	-1.500886	2.497164
H	-5.284397	-0.579646	3.745776	C	0.428176	-1.786985	3.815687
H	-6.525930	-0.340271	1.596726	C	1.255515	-2.875733	4.097007
H	-1.789410	1.212105	1.949555	H	2.404669	-4.494735	3.256760
H	-2.940742	0.204716	3.940718	H	1.782741	-3.995546	0.933276
N	-5.313484	0.802270	-0.692094	H	-0.555953	-0.645720	2.283447
C	-4.348253	1.425556	-1.484254	H	0.060829	-1.154031	4.619338
O	-4.539938	1.823487	-2.619535	H	1.536834	-3.098935	5.122693
C	-3.021911	1.411209	-0.694883	C	0.929373	-2.791370	-1.468330
C	-2.128475	0.331163	-1.353919	C	1.039259	-4.192592	-1.482715
H	-2.583958	-0.655487	-1.256980	C	1.589263	-2.051360	-2.461121
H	-2.022106	0.570889	-2.418839	C	1.833019	-4.830647	-2.435902
C	-2.209177	2.680048	-0.710401	H	0.485880	-4.785469	-0.760380
C	-2.780484	3.954374	-0.739047	C	2.379326	-2.690484	-3.419072
C	-0.804739	2.489115	-0.682459	H	1.486179	-0.969991	-2.481219
C	-1.964032	5.085889	-0.753652	C	2.511272	-4.079878	-3.400881
H	-3.862241	4.061511	-0.774503	H	1.914811	-5.914262	-2.431566
C	-0.012819	3.649419	-0.704441	H	2.886955	-2.099948	-4.176881
C	-0.577750	4.929003	-0.740017	H	3.127186	-4.579283	-4.143979
H	-2.406362	6.078663	-0.785577	C	-1.716838	-2.749687	-0.310068
H	1.070175	3.579285	-0.693905	C	-2.150662	-3.381560	-1.485880
H	0.071168	5.802440	-0.757915	C	-2.616775	-2.621247	0.759713
C	-6.654455	0.514211	-1.144531	C	-3.447954	-3.889566	-1.580397
H	-6.855509	-0.563504	-1.098731	H	-1.482800	-3.470501	-2.336580
H	-7.398141	1.038098	-0.530789	C	-3.913197	-3.124307	0.659919
H	-6.729989	0.857060	-2.178287	H	-2.327522	-2.102820	1.666453
C	1.735783	-3.663622	3.050349	C	-4.333426	-3.762025	-0.509258

H	-3.766253	-4.376717	-2.498309	C	-1.866772	-2.109227	0.248295
H	-4.596401	-2.993395	1.493330	C	-1.130302	-1.197306	-0.744966
H	-5.345815	-4.149290	-0.588050	H	-0.411083	-1.783429	-1.333786
P	-0.090852	-1.872141	-0.245891	H	-1.834369	-0.724439	-1.433862
				C	-0.999394	-2.511920	1.431739
$Cs_2CO_3H^+$				C	-1.500699	-3.516946	2.275859
H	0.828606	2.864926	-0.000362	C	-0.952342	-3.774668	3.526778
C	-0.099675	1.195555	0.000338	H	-2.370153	-4.079234	1.944198
O	0.069750	-0.053877	0.001470	C	0.631744	-1.993958	3.146886
O	-1.152485	1.860446	-0.001441	C	0.104136	-2.983799	3.973833
O	1.103585	1.932703	0.001087	H	-1.361514	-4.563354	4.152287
Cs	-3.072561	-0.358218	-0.000028	H	1.487668	-1.438841	3.511371
Cs	3.065336	-0.368190	-0.000165	H	0.540793	-3.144250	4.956038
				C	-5.540594	-1.241085	0.451254
TS8A-E				H	-5.424495	-0.367537	1.094341
Pd	0.107223	-0.000283	0.408821	H	-5.971169	-0.931423	-0.508084
C	-4.342343	-4.927892	-1.804272	H	-6.211023	-1.964600	0.929882
C	-4.860168	-3.805155	-1.141964	C	-0.663309	5.347689	1.970091
C	-3.958882	-2.975375	-0.484699	C	-0.497727	4.522415	0.856097
C	-2.578718	-3.229569	-0.480700	C	-0.891788	3.178706	0.909536
C	-2.080484	-4.344930	-1.135678	C	-1.450290	2.669576	2.096016
C	-2.972382	-5.200978	-1.800075	C	-1.627812	3.504659	3.199140
H	-5.023149	-5.595745	-2.325057	C	-1.230868	4.843168	3.141201
H	-5.925713	-3.596884	-1.141821	H	-0.340652	6.384214	1.921043
H	-1.013588	-4.552812	-1.124667	H	-0.038453	4.925933	-0.039529
H	-2.595114	-6.080845	-2.313193	H	-1.741661	1.623817	2.153028
N	-4.226521	-1.813600	0.256011	H	-2.064815	3.102188	4.109001
C	-3.069232	-1.265798	0.774867	H	-1.355978	5.487351	4.007435
O	-3.025523	-0.267507	1.477768	C	-2.269737	1.929171	-1.344148

C	-3.472500	2.050151	-0.634271	C	4.164865	-3.098326	-1.737542
C	-2.313548	1.605048	-2.710517	C	6.040366	-3.123957	-0.213190
C	-4.693867	1.863450	-1.283818	C	4.904190	-3.843338	-2.657629
H	-3.460940	2.273697	0.425785	H	3.159346	-2.780208	-1.996153
C	-3.536269	1.417043	-3.355065	C	6.775499	-3.874980	-1.126582
H	-1.390174	1.500091	-3.273174	H	6.464404	-2.820256	0.738443
C	-4.731179	1.545658	-2.642715	C	6.208326	-4.238356	-2.352310
H	-5.618334	1.966110	-0.721806	H	4.463080	-4.111615	-3.614151
H	-3.553866	1.168321	-4.412696	H	7.791711	-4.177143	-0.886680
H	-5.684038	1.400029	-3.144587	H	6.782051	-4.822345	-3.067462
C	0.451767	2.825411	-1.692476	C	1.960821	0.348688	1.692490
C	0.036941	3.956751	-2.416292	H	1.521867	0.557148	2.666850
C	1.748418	2.328153	-1.884652	C	3.119130	1.244505	1.306700
C	0.918153	4.595294	-3.288424	C	2.766852	2.731659	1.409485
H	-0.975830	4.332700	-2.300791	H	3.441121	1.006431	0.285025
C	2.628507	2.968261	-2.759561	H	3.986270	1.010044	1.939336
H	2.066148	1.442742	-1.344219	C	3.881195	3.664486	0.925418
C	2.217139	4.105746	-3.456020	H	1.865705	2.925873	0.820516
H	0.590774	5.473039	-3.838973	H	2.499720	2.979173	2.447738
H	3.632694	2.576180	-2.893552	C	3.438643	5.131345	0.894578
H	2.902583	4.606401	-4.134380	H	4.768097	3.549412	1.563801
P	-0.643832	1.992592	-0.479102	H	4.187732	3.360060	-0.085647
C	0.134732	-1.757221	1.848733	H	4.249950	5.794483	0.571941
C	1.804733	-0.936319	1.152170	H	2.598789	5.264620	0.200835
C	2.533545	-1.825692	0.417949	H	3.103275	5.464234	1.884865
H	2.008402	-2.548255	-0.196264				
C	3.991617	-1.910168	0.526319	**INT8A-E**			
O	4.631282	-1.357495	1.427402	Pd	0.796248	0.297106	-0.844214
C	4.723005	-2.735356	-0.502184	C	-2.531624	6.460450	-0.993577

C	-1.135553	6.325884	-1.029541	C	4.364470	-1.456393	3.603574
C	-0.611478	5.061506	-0.793488	C	4.056325	-1.633970	2.256451
C	-1.425324	3.950616	-0.530404	C	3.030974	-0.883124	1.657382
C	-2.802253	4.095863	-0.494903	C	2.325854	0.052253	2.427724
C	-3.355937	5.363399	-0.731040	C	2.637511	0.228479	3.778831
H	-2.974099	7.435877	-1.175752	C	3.653510	-0.523873	4.367375
H	-0.495100	7.177854	-1.236636	H	5.159158	-2.042002	4.058430
H	-3.434253	3.234280	-0.295552	H	4.614175	-2.356168	1.666672
H	-4.434318	5.492234	-0.712008	H	1.536101	0.643154	1.975476
N	0.745928	4.664885	-0.789875	H	2.077509	0.954679	4.360030
C	0.857171	3.316499	-0.579261	H	3.895719	-0.386315	5.418093
O	1.900969	2.663448	-0.675871	C	4.206720	-0.815789	-0.977537
C	-0.547281	2.728002	-0.323241	C	5.160329	-1.827049	-1.171595
C	-0.674462	1.635733	-1.409302	C	4.489720	0.488493	-1.416696
H	-1.693663	1.280074	-1.541675	C	6.374768	-1.540004	-1.796188
H	-0.321125	2.033639	-2.373307	H	4.949911	-2.842387	-0.848513
C	-0.657729	2.232396	1.137951	C	5.709166	0.771403	-2.034605
C	-0.191383	3.082728	2.152334	H	3.761396	1.281491	-1.268627
C	-0.254556	2.727421	3.498802	C	6.651951	-0.240532	-2.227684
H	0.230056	4.047204	1.880503	H	7.104328	-2.331816	-1.945175
C	-1.294900	0.651346	2.869534	H	5.918616	1.783441	-2.370840
C	-0.811940	1.501683	3.863149	H	7.597806	-0.019319	-2.715110
H	0.124628	3.408764	4.255803	C	2.255319	-2.878622	-0.297836
H	-1.733893	-0.306494	3.136629	C	2.318579	-3.470314	-1.571642
H	-0.872474	1.209693	4.908083	C	1.723314	-3.619795	0.767571
C	1.853222	5.519941	-1.166612	C	1.866502	-4.773621	-1.770523
H	1.707951	5.912194	-2.180113	H	2.712820	-2.904149	-2.411221
H	1.941328	6.360896	-0.469875	C	1.262796	-4.922647	0.562993
H	2.764037	4.920188	-1.134833	H	1.662596	-3.178798	1.757711

C	1.330553	-5.502338	-0.704416	H	-1.391996	-3.648381	0.533661
H	1.921823	-5.216986	-2.761046	H	-2.819816	-2.647733	0.342905
H	0.846096	-5.481381	1.396689	C	-3.518296	-5.168239	-0.479757
H	0.966538	-6.513614	-0.862948	H	-3.197553	-3.605832	-1.940197
P	2.598734	-1.082863	-0.122750	H	-1.807040	-4.666607	-1.717855
C	-1.225157	0.994221	1.511961	H	-3.939209	-5.892922	-1.187220
C	-1.763245	0.014954	0.505344	H	-2.962625	-5.729048	0.283299
C	-3.104373	0.092630	0.291806	H	-4.355090	-4.664811	0.020735
H	-3.661318	0.783382	0.924455				
C	-3.928909	-0.605471	-0.718649	**TS8A-Z**			
O	-3.602934	-0.670803	-1.904170	Pd	-0.196652	0.268682	0.492019
C	-5.224294	-1.217171	-0.267064	C	5.115310	-3.742658	-1.647651
C	-5.531900	-1.394133	1.090231	C	4.024406	-4.387306	-1.045487
C	-6.122423	-1.683172	-1.239644	C	3.086079	-3.587740	-0.403098
C	-6.720173	-2.020457	1.468298	C	3.207184	-2.191372	-0.354853
H	-4.829170	-1.061184	1.848220	C	4.287096	-1.561563	-0.955206
C	-7.309435	-2.305041	-0.862691	C	5.248956	-2.352253	-1.603141
H	-5.860874	-1.551067	-2.284567	H	5.867010	-4.340354	-2.156570
C	-7.611182	-2.474388	0.493082	H	3.921139	-5.467673	-1.081032
H	-6.947637	-2.159539	2.521823	H	4.363941	-0.479069	-0.918007
H	-8.000313	-2.661940	-1.621925	H	6.104197	-1.878577	-2.077095
H	-8.536264	-2.963270	0.787525	N	1.920308	-3.984310	0.275791
C	-0.739838	-0.915074	-0.035514	C	1.239432	-2.898273	0.788050
H	-0.174589	-1.289584	0.830226	O	0.193325	-2.964853	1.419380
C	-1.139332	-2.076307	-0.934110	C	2.005020	-1.611225	0.358037
C	-2.008092	-3.129837	-0.215053	C	1.081099	-0.893351	-0.631646
H	-0.232104	-2.574565	-1.286742	H	1.625519	-0.090514	-1.140742
H	-1.660766	-1.700149	-1.815894	H	0.669486	-1.596840	-1.359101
C	-2.616264	-4.148923	-1.182617	C	2.294027	-0.788474	1.601844

C	3.269165	-1.271038	2.485499	H	-1.547502	-1.072065	-3.395390
C	3.423608	-0.752357	3.767404	C	-1.300806	-4.433529	-2.952898
H	3.900974	-2.092774	2.157075	H	-1.639280	-5.460939	-1.085943
C	1.583945	0.747788	3.333905	H	-1.025168	-3.129246	-4.650665
C	2.554458	0.245140	4.201379	H	-1.064954	-5.339122	-3.505342
H	4.196145	-1.141702	4.425218	C	-2.933066	0.599826	-1.728653
H	0.954575	1.550540	3.697574	C	-4.033399	0.193385	-2.503129
H	2.633542	0.652429	5.206039	C	-2.465954	1.916671	-1.842596
C	1.453236	-5.348128	0.388326	C	-4.673880	1.101173	-3.346077
H	0.535387	-5.333265	0.978275	H	-4.382947	-0.833940	-2.450223
H	1.243007	-5.766305	-0.603443	C	-3.106887	2.823180	-2.689557
H	2.201375	-5.974574	0.888399	H	-1.600760	2.226222	-1.265197
C	-5.522544	-0.818964	1.772516	C	-4.215360	2.419072	-3.435353
C	-4.668007	-0.556681	0.699920	H	-5.527837	0.779634	-3.936026
C	-3.316642	-0.922133	0.767887	H	-2.737140	3.841838	-2.765995
C	-2.830072	-1.551852	1.928724	H	-4.716421	3.124768	-4.092308
C	-3.694179	-1.824983	2.989259	P	-2.094866	-0.536502	-0.556653
C	-5.039859	-1.455826	2.916803	C	1.454995	0.283438	2.010965
H	-6.565145	-0.518375	1.712055	C	0.589457	1.998605	1.309868
H	-5.056654	-0.046062	-0.174110	C	1.441534	2.889406	0.715730
H	-1.779756	-1.823002	2.002752	H	1.266189	3.932253	0.969685
H	-3.308271	-2.316214	3.878386	C	2.618596	2.577914	-0.074067
H	-5.706821	-1.657244	3.750861	O	3.023476	1.424444	-0.287810
C	-1.909276	-2.094017	-1.522696	C	3.418191	3.734989	-0.617732
C	-1.922959	-3.341076	-0.881584	C	2.861262	4.995463	-0.881631
C	-1.577990	-2.030845	-2.886172	C	4.773295	3.519600	-0.911293
C	-1.623445	-4.501631	-1.596234	C	3.643840	6.019015	-1.418002
H	-2.140671	-3.410207	0.177185	H	1.806432	5.173586	-0.694390
C	-1.279549	-3.194116	-3.596252	C	5.559337	4.544672	-1.431865

H	5.189425	2.535882	-0.719756	H	5.357711	-5.659850	-1.084873
C	4.996286	5.798914	-1.687324	H	2.933009	-6.207598	-1.300110
H	3.196672	6.987234	-1.627995	H	4.396515	-1.567933	-0.106013
H	6.610956	4.367486	-1.642296	H	6.082057	-3.366422	-0.499071
H	5.607244	6.598248	-2.098804	N	0.929611	-4.241291	-0.920889
C	-0.717241	2.065724	1.808968	C	0.380105	-3.013787	-0.710016
H	-0.957041	1.548543	2.736312	O	-0.816682	-2.727918	-0.879053
C	-1.646817	3.208866	1.451468	C	1.494470	-1.996407	-0.388279
C	-3.121518	2.788516	1.455459	C	1.244307	-0.905543	-1.453197
H	-1.376742	3.604160	0.463368	H	2.060836	-0.189266	-1.508895
H	-1.507716	4.045571	2.157320	H	1.110056	-1.364384	-2.443647
C	-4.080701	3.875835	0.962297	C	1.387870	-1.479692	1.064960
H	-3.234664	1.904606	0.821318	C	1.273736	-2.442161	2.079482
H	-3.410223	2.466297	2.466692	C	1.189601	-2.091571	3.424235
C	-5.524636	3.372720	0.860642	H	1.252691	-3.493765	1.804153
H	-4.031602	4.749381	1.627826	C	1.371064	0.223220	2.793620
H	-3.749353	4.220836	-0.027769	C	1.237431	-0.744380	3.785210
H	-6.207409	4.162464	0.526148	H	1.094291	-2.865168	4.181521
H	-5.593364	2.543289	0.145669	H	1.428598	1.274092	3.063779
H	-5.883508	3.003248	1.829363	H	1.178126	-0.448358	4.829048
				C	0.182265	-5.406171	-1.350505
INT8A-Z				H	0.501631	-5.717215	-2.352012
Pd	-0.663833	-0.302724	-0.873517	H	0.339062	-6.237133	-0.654108
C	4.615355	-4.880894	-0.933920	H	-0.875130	-5.138777	-1.370280
C	3.255211	-5.198907	-1.059719	C	-4.835065	-1.134174	3.278980
C	2.343479	-4.171208	-0.859188	C	-4.582902	-0.633402	2.002935
C	2.737041	-2.860605	-0.552166	C	-3.265206	-0.540136	1.525478
C	4.083897	-2.563208	-0.403765	C	-2.206875	-0.960825	2.344094
C	5.023559	-3.585520	-0.606665	C	-2.463325	-1.459111	3.624077

C	-3.774334	-1.546232	4.092668	C	1.444963	-0.117397	1.433964
H	-5.858287	-1.205562	3.638568	C	1.490514	1.038451	0.472896
H	-5.411747	-0.322292	1.373363	C	2.661910	1.664225	0.157681
H	-1.184654	-0.905976	1.985831	H	2.606661	2.546307	-0.466212
H	-1.629850	-1.778967	4.241863	C	3.998365	1.224897	0.560059
H	-3.973510	-1.937042	5.087224	O	4.205617	0.264632	1.311952
C	-4.217312	-0.529029	-1.204807	C	5.185749	1.988372	0.023545
C	-5.462510	0.091746	-1.387898	C	5.133750	2.827308	-1.100865
C	-3.964477	-1.758858	-1.836519	C	6.416603	1.811477	0.676094
C	-6.437347	-0.505590	-2.189192	C	6.281736	3.479165	-1.553955
H	-5.669746	1.045913	-0.912678	H	4.205119	2.957751	-1.646905
C	-4.945141	-2.354392	-2.630949	C	7.559558	2.471295	0.232872
H	-3.005768	-2.251655	-1.699542	H	6.448015	1.145541	1.532271
C	-6.181286	-1.729423	-2.811265	C	7.495275	3.309136	-0.884975
H	-7.397050	-0.013988	-2.325836	H	6.227744	4.117586	-2.431893
H	-4.739458	-3.305523	-3.114937	H	8.502602	2.332156	0.755208
H	-6.940849	-2.192254	-3.435691	H	8.387216	3.822340	-1.235113
C	-3.291817	1.940382	0.040356	C	0.172260	1.456882	-0.058774
C	-3.449962	2.724700	-1.115704	H	-0.521277	1.575370	0.783170
C	-3.302419	2.571303	1.292827	C	0.101130	2.673108	-0.975800
C	-3.628060	4.103824	-1.018874	C	0.150382	4.012603	-0.218546
H	-3.431454	2.252517	-2.094726	H	-0.842329	2.640845	-1.529163
C	-3.471011	3.955431	1.386705	H	0.895038	2.624668	-1.733036
H	-3.181517	1.982526	2.196780	C	0.023274	5.227520	-1.143909
C	-3.634472	4.724662	0.234145	H	-0.675449	4.028119	0.505595
H	-3.752504	4.695614	-1.921608	H	1.077432	4.086636	0.366271
H	-3.473619	4.430258	2.364166	C	-0.050260	6.551841	-0.377614
H	-3.762762	5.800964	0.308236	H	0.871986	5.246942	-1.842846
P	-2.883014	0.154739	-0.137284	H	-0.880421	5.111706	-1.758750

H	-0.137254	7.409178	-1.055678	C	-4.254114	-1.073279	-0.863467
H	-0.919702	6.562085	0.291968	C	-3.275680	0.401955	-3.024058
H	0.844236	6.702017	0.239748	H	-1.316862	-0.065678	-2.254526
				C	-5.140476	-0.479210	-1.764278
TS8B-E				H	-4.647038	-1.631042	-0.020313
C	-4.060452	-2.739327	3.278407	C	-4.653408	0.258314	-2.845995
C	-3.458365	-2.719550	2.020536	H	-2.889472	0.983707	-3.856097
C	-2.422664	-1.811055	1.738562	H	-6.211428	-0.588122	-1.615129
C	-1.986136	-0.946397	2.753328	H	-5.344250	0.728021	-3.540567
C	-2.589957	-0.969058	4.012096	P	-1.630919	-1.743612	0.069493
C	-3.630442	-1.860625	4.276014	Pd	0.366947	-0.628765	0.114344
H	-4.860042	-3.446799	3.480971	C	7.137956	0.427636	2.103169
H	-3.781037	-3.428218	1.263784	C	6.777996	1.143793	0.952327
H	-1.172037	-0.257162	2.554505	C	5.549677	0.848758	0.371146
H	-2.240698	-0.291199	4.786097	C	4.690533	-0.124052	0.902614
H	-4.098303	-1.878979	5.256614	C	5.060521	-0.830199	2.035860
C	-1.703017	-3.508657	-0.439587	C	6.295656	-0.548795	2.640115
C	-2.211875	-3.908925	-1.681821	H	8.092431	0.636251	2.578762
C	-1.140494	-4.471695	0.414790	H	7.436553	1.897343	0.531537
C	-2.159821	-5.252545	-2.062514	H	4.405952	-1.599726	2.436330
H	-2.645272	-3.176409	-2.355283	H	6.600070	-1.096908	3.527008
C	-1.096278	-5.810676	0.034978	N	4.972729	1.410547	-0.777777
H	-0.723810	-4.167013	1.370801	C	3.744272	0.837328	-1.060549
C	-1.604128	-6.204262	-1.207045	O	3.053959	1.122261	-2.025826
H	-2.554823	-5.551776	-3.029554	C	3.423732	-0.189046	0.067804
H	-0.655051	-6.545615	0.702448	C	3.118985	-1.555506	-0.539870
H	-1.562624	-7.248034	-1.506147	C	4.176947	-2.305292	-1.072455
C	-2.868875	-0.936738	-1.037107	C	1.777872	-2.005936	-0.616830
C	-2.388438	-0.190203	-2.124290	C	3.934021	-3.520781	-1.708191

H	5.196665	-1.934228	-0.987295	H	-5.483771	6.281265	0.616904
C	1.570349	-3.227214	-1.282387	H	-7.070509	4.624564	-0.342874
C	2.620388	-3.977410	-1.819304	C	1.585837	2.978071	0.354028
H	4.759865	-4.099062	-2.115292	C	1.376469	4.022987	-0.755946
H	0.565467	-3.613132	-1.399417	H	2.665756	2.824571	0.458959
H	2.408656	-4.918448	-2.323372	H	1.192994	3.342640	1.306429
C	5.592992	2.420459	-1.608394	C	1.850586	5.415361	-0.327753
H	5.777337	3.334013	-1.030926	H	1.923375	3.691166	-1.649847
H	6.545434	2.058745	-2.014038	H	0.316623	4.078743	-1.022129
H	4.906832	2.638521	-2.428295	C	1.693783	6.455702	-1.441240
C	2.244426	0.312811	0.910990	H	1.271672	5.724426	0.551706
H	1.949816	-0.461260	1.638166	H	2.903867	5.365520	-0.012756
H	2.495212	1.179494	1.511211	H	2.033996	7.446431	-1.117402
C	0.877249	1.682220	-0.032978	H	2.273094	6.175421	-2.330212
H	1.045225	1.471848	-1.091662	H	0.643428	6.544489	-1.744343
C	-0.411375	1.263129	0.435095				
C	-1.596353	1.818700	0.743472	**INT8B-E**			
H	-2.407793	1.164225	1.051398	C	-3.919281	1.938281	3.326535
C	-1.953478	3.257219	0.669883	C	-3.746610	1.410177	2.044960
O	-1.137160	4.162039	0.844595	C	-2.632175	1.771776	1.277277
C	-3.392427	3.595429	0.398672	C	-1.697749	2.673395	1.811448
C	-4.291639	2.668103	-0.148933	C	-1.874395	3.206212	3.087527
C	-3.831801	4.902791	0.661198	C	-2.985866	2.834666	3.850397
C	-5.608822	3.039929	-0.419095	H	-4.782824	1.643984	3.916984
H	-3.963540	1.664026	-0.389293	H	-4.467594	0.700756	1.651301
C	-5.149446	5.269594	0.402256	H	-0.818497	2.949569	1.232425
H	-3.118406	5.613219	1.066659	H	-1.140027	3.898005	3.490784
C	-6.042314	4.337080	-0.137966	H	-3.119267	3.238707	4.850144
H	-6.290666	2.313690	-0.853154	C	-3.429467	-0.345176	-0.557614

C	-4.461817	-0.395589	-1.502633	H	-2.389093	-1.459494	4.584109
C	-3.172192	-1.469656	0.245305	H	-1.917302	-3.792007	3.820507
C	-5.225406	-1.557467	-1.643819	H	0.510924	0.068964	1.800217
H	-4.668910	0.462411	-2.134490	H	-1.131820	0.444167	3.614896
C	-3.940893	-2.621653	0.105054	N	0.002025	-4.335943	1.840356
H	-2.364535	-1.449502	0.967150	C	1.042181	-4.104612	0.958356
C	-4.966157	-2.670997	-0.844007	O	1.818192	-4.955710	0.560119
H	-6.021045	-1.589822	-2.383450	C	0.989432	-2.602455	0.541373
H	-3.723962	-3.483817	0.729448	C	0.193845	-2.550009	-0.808491
H	-5.557319	-3.575236	-0.961773	C	-0.116008	-3.746628	-1.483027
C	-2.955620	2.361012	-1.536105	C	-0.236726	-1.339839	-1.398497
C	-2.278329	2.589938	-2.743510	C	-0.825107	-3.764935	-2.683101
C	-4.116408	3.096022	-1.248860	H	0.220516	-4.695778	-1.086035
C	-2.760204	3.531866	-3.654992	C	-0.937075	-1.368455	-2.613882
H	-1.370150	2.032875	-2.962191	C	-1.241575	-2.568342	-3.256464
C	-4.593603	4.038871	-2.159001	H	-1.040997	-4.715811	-3.162997
H	-4.640249	2.933472	-0.310940	H	-1.271740	-0.438539	-3.064796
C	-3.917526	4.256314	-3.363503	H	-1.795660	-2.558885	-4.191987
H	-2.228353	3.702654	-4.586964	C	-0.281701	-5.634318	2.411988
H	-5.491459	4.605929	-1.928330	H	-0.062385	-5.645330	3.487144
H	-4.290580	4.992857	-4.070003	H	-1.335513	-5.896636	2.263501
P	-2.292209	1.083654	-0.394850	H	0.352717	-6.363564	1.905567
Pd	0.027086	0.506101	-0.644545	C	2.451107	-2.075450	0.420706
C	-1.666546	-1.633576	3.791534	H	2.760296	-1.644658	1.379485
C	-1.423134	-2.944707	3.355135	H	3.077628	-2.953965	0.239155
C	-0.498576	-3.123220	2.332171	C	2.769814	-1.056096	-0.702423
C	0.143786	-2.046627	1.689819	H	2.370564	-1.479133	-1.633018
C	-0.048067	-0.769046	2.198002	C	2.005504	0.211064	-0.471897
C	-0.964961	-0.561648	3.244051	C	2.381018	1.408037	0.027535

H	1.629664	2.220507	0.002273	C	5.705732	-1.719877	-0.403884
C	3.616267	1.795343	0.757785	C	4.657223	-1.166045	0.329968
O	4.272566	0.984667	1.407114	C	3.345105	-1.196044	-0.173573
C	4.007008	3.246615	0.748756	C	3.107399	-1.771864	-1.428935
C	3.528184	4.150984	-0.211447	C	4.157378	-2.337090	-2.153913
C	4.910376	3.698420	1.723287	C	5.455535	-2.314799	-1.643795
C	3.936775	5.485183	-0.189493	H	6.716917	-1.687717	-0.007134
H	2.857388	3.807241	-0.993603	H	4.859246	-0.699855	1.289663
C	5.311223	5.031424	1.750373	H	2.105026	-1.757504	-1.844867
H	5.284265	2.982043	2.447804	H	3.959779	-2.776357	-3.127387
C	4.823167	5.928724	0.794454	H	6.273065	-2.748942	-2.213278
H	3.567871	6.176169	-0.942786	C	1.587951	-1.821604	2.087032
H	6.005398	5.373855	2.513258	C	0.307098	-1.866968	2.662645
H	5.137771	6.968955	0.813751	C	2.576393	-2.705094	2.541584
C	4.297466	-0.917169	-0.899751	C	0.031765	-2.772139	3.687471
C	4.892780	-2.063899	-1.727572	H	-0.486313	-1.222888	2.295068
H	4.795410	-0.852192	0.071543	C	2.289982	-3.619009	3.557405
H	4.504862	0.032427	-1.411463	H	3.566549	-2.697100	2.098025
C	6.413987	-1.954438	-1.887481	C	1.019459	-3.651971	4.135163
H	4.651406	-3.031488	-1.265129	H	-0.964934	-2.798343	4.119184
H	4.423085	-2.078958	-2.722795	H	3.061508	-4.306765	3.893741
C	7.008787	-3.088378	-2.729063	H	0.798187	-4.366309	4.923920
H	6.661223	-0.985768	-2.345292	C	2.553435	0.871035	1.737121
H	6.881392	-1.948709	-0.892752	C	1.998627	1.176901	2.990124
H	8.096369	-2.990104	-2.827440	C	3.477997	1.756856	1.168229
H	6.800020	-4.065449	-2.275680	C	2.363218	2.348556	3.652998
H	6.580246	-3.095876	-3.739254	H	1.283141	0.502597	3.450287
				C	3.834861	2.931734	1.829442

TS8B-Z

H	3.907098	1.542492	0.196372

C	3.278311	3.231303	3.073139	H	-0.120462	-5.425240	-0.400953
H	1.928933	2.571871	4.624059	C	-5.496396	-0.004826	2.153435
H	4.523718	3.621197	1.351609	H	-4.786488	0.124869	2.971772
H	3.551417	4.149389	3.586331	H	-6.072049	0.918175	2.016429
P	1.911425	-0.560961	0.777703	H	-6.188355	-0.820683	2.393825
Pd	0.003404	-0.085945	-0.398295	C	-2.098725	0.317450	-1.137665
C	-6.950909	-0.860327	-2.000716	H	-1.567185	-0.049594	-2.031236
C	-6.640309	-0.551324	-0.668461	H	-2.719923	1.129953	-1.495601
C	-5.299971	-0.578308	-0.300087	C	-1.281182	1.873758	0.134913
C	-4.283309	-0.899172	-1.210130	H	-1.415877	1.435950	1.123862
C	-4.603582	-1.207965	-2.522746	C	0.070138	1.981079	-0.323878
C	-5.949862	-1.186556	-2.918726	C	0.818997	3.052690	-0.637413
H	-7.989955	-0.848250	-2.318204	H	0.532918	4.053239	-0.307000
H	-7.419475	-0.303604	0.045781	C	2.127495	3.054026	-1.327170
H	-3.820162	-1.476278	-3.226376	O	2.926648	3.969442	-1.128874
H	-6.214696	-1.429626	-3.943593	C	2.475625	1.983150	-2.325253
N	-4.738235	-0.314602	0.959847	C	1.507278	1.298935	-3.075747
C	-3.362630	-0.444402	0.937263	C	3.833019	1.743996	-2.590055
O	-2.637530	-0.283958	1.908989	C	1.890052	0.384094	-4.058462
C	-2.937061	-0.815159	-0.515264	H	0.456856	1.510380	-2.914159
C	-2.138960	-2.120805	-0.494266	C	4.215902	0.821059	-3.558893
C	-2.809925	-3.350904	-0.484363	H	4.573878	2.307586	-2.031594
C	-0.728191	-2.047844	-0.442535	C	3.243354	0.140257	-4.297908
C	-2.090066	-4.544767	-0.451661	H	1.129829	-0.132550	-4.638475
H	-3.896901	-3.377537	-0.515336	H	5.269811	0.629214	-3.739245
C	-0.035392	-3.270163	-0.412958	H	3.541093	-0.576423	-5.058928
C	-0.695610	-4.501814	-0.423762	C	-2.325089	2.938134	-0.157260
H	-2.614786	-5.496947	-0.451832	C	-2.221126	4.074874	0.877787
H	1.050012	-3.276074	-0.357341	H	-3.335745	2.513126	-0.099683

H	-2.185488	3.337063	-1.169674	H	-0.522335	-2.667571	0.820354
C	-3.266356	5.172319	0.638873	C	-1.615655	-5.252333	-1.095486
H	-2.352883	3.655276	1.885355	H	-3.106818	-5.101194	-2.646161
H	-1.217499	4.516003	0.856592	H	-0.162876	-5.079294	0.497088
C	-3.183312	6.301047	1.671612	H	-1.445094	-6.314361	-1.250822
H	-3.132424	5.584552	-0.370959	C	-3.452430	-0.122974	-1.644000
H	-4.270856	4.725859	0.657641	C	-3.053785	0.626371	-2.760934
H	-3.936532	7.074070	1.481187	C	-4.813811	-0.413691	-1.461774
H	-3.344125	5.918466	2.687155	C	-4.000179	1.066247	-3.688982
H	-2.197323	6.781036	1.650852	H	-2.003709	0.876308	-2.891761
				C	-5.757048	0.027358	-2.389498
INT8B-Z				H	-5.132925	-0.979431	-0.590678
C	-4.103141	-1.402230	3.133757	C	-5.350989	0.765864	-3.505289
C	-3.525847	-1.596542	1.876762	H	-3.681663	1.649091	-4.548969
C	-2.981431	-0.512856	1.174487	H	-6.809003	-0.201575	-2.240847
C	-3.029442	0.770880	1.744833	H	-6.088158	1.111276	-4.225254
C	-3.611391	0.959653	2.998379	P	-2.164541	-0.694716	-0.465675
C	-4.145841	-0.126323	3.698342	Pd	-0.099452	0.538581	-0.621057
H	-4.515514	-2.251557	3.672170	C	-0.070807	-2.296641	3.796818
H	-3.483421	-2.594917	1.453762	C	1.037711	-3.066273	3.412956
H	-2.592927	1.613578	1.217774	C	1.864697	-2.555523	2.419239
H	-3.636957	1.955386	3.433403	C	1.599983	-1.339899	1.759166
H	-4.590503	0.021593	4.678936	C	0.541731	-0.562932	2.208499
C	-2.040719	-2.507594	-0.712605	C	-0.301167	-1.047597	3.224262
C	-2.761525	-3.203403	-1.690335	H	-0.741772	-2.671591	4.564807
C	-1.102910	-3.198714	0.074420	H	1.255671	-4.015845	3.892117
C	-2.546596	-4.571410	-1.880127	H	0.353265	0.411569	1.770814
H	-3.483715	-2.683063	-2.311600	H	-1.145523	-0.448187	3.547588
C	-0.897472	-4.562387	-0.114089	N	3.083212	-3.083704	1.970620

C	3.696307	-2.206338	1.096427	C	-1.866050	5.014103	0.492487
O	4.857362	-2.285307	0.731436	C	-0.051044	6.842892	1.566912
C	2.634056	-1.158360	0.645747	H	1.442021	5.335191	1.254030
C	2.060226	-1.653802	-0.721156	C	-2.306753	6.266854	0.908878
C	2.671991	-2.731952	-1.386695	H	-2.558147	4.291766	0.072864
C	0.940305	-1.032650	-1.322310	C	-1.400117	7.184894	1.448088
C	2.206997	-3.202851	-2.613689	H	0.655352	7.550057	1.992673
H	3.547232	-3.210330	-0.964731	H	-3.356757	6.529868	0.813937
C	0.502698	-1.512139	-2.570644	H	-1.744252	8.162177	1.775986
C	1.114930	-2.585974	-3.215669	C	4.057835	2.278025	-0.775327
H	2.706205	-4.041817	-3.091599	C	5.388881	1.780507	-1.355630
H	-0.357183	-1.049291	-3.049223	H	4.237567	2.752255	0.201066
H	0.735853	-2.933884	-4.173819	H	3.670663	3.066191	-1.435286
C	3.759503	-4.214266	2.568009	C	6.426741	2.899341	-1.510040
H	3.890814	-4.065999	3.647403	H	5.812063	0.987440	-0.725389
H	3.186848	-5.134669	2.405610	H	5.201689	1.319767	-2.336762
H	4.737775	-4.302198	2.092573	C	7.752118	2.404110	-2.098434
C	3.337662	0.229385	0.546240	H	6.013114	3.693293	-2.148479
H	3.190929	0.771710	1.488217	H	6.609392	3.360759	-0.528764
H	4.405839	0.012885	0.461498	H	8.477949	3.219484	-2.199340
C	2.982028	1.176407	-0.636097	H	8.200567	1.631942	-1.461220
H	3.008785	0.569109	-1.549479	H	7.601027	1.964320	-3.092085
C	1.572998	1.672452	-0.469527				
C	1.292493	2.955626	-0.067373	**TS9A**			
H	2.064347	3.705759	0.081202	Pd	1.074036	0.526217	-0.771246
C	-0.086242	3.310632	0.146062	C	-4.131371	5.431388	-1.143570
O	-0.996822	2.451010	-0.054728	C	-2.777770	5.797654	-1.146702
C	-0.508642	4.662383	0.598506	C	-1.845311	4.806609	-0.864941
C	0.394209	5.592052	1.141785	C	-2.220626	3.486253	-0.576787

C	-3.560972	3.132172	-0.593155	C	2.474052	0.214222	2.481741
C	-4.519689	4.117186	-0.877829	C	2.757381	0.369364	3.839987
H	-4.884304	6.183736	-1.362158	C	3.949924	-0.128092	4.368149
H	-2.471964	6.815212	-1.369496	H	5.795339	-1.163217	3.939025
H	-3.858353	2.104584	-0.412592	H	5.296536	-1.441985	1.532576
H	-5.572256	3.849977	-0.896402	H	1.552083	0.619967	2.073190
N	-0.444301	4.918688	-0.845270	H	2.044178	0.887563	4.474698
C	0.154934	3.703559	-0.591917	H	4.173704	-0.002801	5.424515
O	1.360206	3.502052	-0.590203	C	4.537314	-0.500172	-1.012115
C	-0.964821	2.662653	-0.309989	C	5.413460	-1.574381	-1.228447
C	-0.799521	1.471685	-1.292182	C	4.894569	0.778439	-1.468736
H	-1.741939	1.209922	-1.768052	C	6.630418	-1.370165	-1.882174
H	-0.098644	1.720543	-2.122121	H	5.140087	-2.571653	-0.894929
C	-0.893230	2.243512	1.172730	C	6.115546	0.981562	-2.112425
C	-0.353192	3.094858	2.143375	H	4.205333	1.607842	-1.323513
C	-0.339719	2.734165	3.491884	C	6.984962	-0.092428	-2.321153
H	0.075982	4.047182	1.849191	H	7.300651	-2.209574	-2.048960
C	-1.437798	0.662766	2.938025	H	6.382847	1.975541	-2.461401
C	-0.884943	1.514935	3.894507	H	7.931712	0.064343	-2.831414
H	0.098132	3.407874	4.223312	C	2.524000	-2.455743	-0.289352
H	-1.854900	-0.297252	3.230299	C	2.178940	-2.934904	-1.566403
H	-0.875532	1.225409	4.941779	C	2.421256	-3.321799	0.807191
C	0.291945	6.118862	-1.182147	C	1.753533	-4.249228	-1.742856
H	0.055923	6.444137	-2.202488	H	2.227833	-2.262522	-2.419605
H	0.043823	6.928911	-0.486692	C	1.979191	-4.637443	0.630461
H	1.355493	5.886072	-1.110133	H	2.680391	-2.971576	1.801457
C	4.861943	-0.781154	3.533546	C	1.646558	-5.105306	-0.640756
C	4.579365	-0.940771	2.176580	H	1.486765	-4.601932	-2.735465
C	3.379599	-0.449347	1.638150	H	1.896393	-5.295233	1.491855

H	1.299186	-6.126105	-0.774994	H	-2.984660	-3.422526	-2.365705
P	2.923602	-0.656420	-0.139538	H	-1.327213	-3.925160	-2.692972
C	-1.446354	1.014350	1.583583	H	-2.715592	-5.908746	-2.023200
C	-2.009993	0.095430	0.554238	H	-1.470291	-5.600750	-0.796959
C	-3.328627	-0.211914	0.637622	H	-3.147432	-5.106541	-0.502672
H	-3.867076	0.156085	1.510898				
C	-4.167324	-0.938025	-0.346282	**3aa**			
O	-4.184597	-0.615864	-1.534769	C	-6.196288	-0.024642	0.820545
C	-5.030521	-2.059549	0.144050	C	-5.267840	-0.515654	1.748796
C	-4.897580	-2.588924	1.436584	C	-3.932446	-0.557771	1.363111
C	-5.949069	-2.639533	-0.744996	C	-3.511674	-0.129668	0.094949
C	-5.673321	-3.677791	1.835080	C	-4.439759	0.358390	-0.811239
H	-4.170169	-2.161755	2.120407	C	-5.793556	0.408112	-0.444159
C	-6.723894	-3.725015	-0.346882	H	-7.246721	0.018031	1.095098
H	-6.028490	-2.224702	-1.744592	H	-5.581734	-0.849601	2.732772
C	-6.587392	-4.246182	0.944614	H	-4.121331	0.687681	-1.796744
H	-5.560136	-4.086535	2.835457	H	-6.529972	0.785044	-1.147710
H	-7.432287	-4.170050	-1.040371	N	-2.829034	-0.994006	2.107030
H	-7.189464	-5.096535	1.253915	C	-1.651190	-0.868506	1.388281
C	-0.974100	-0.398805	-0.383868	O	-0.544485	-1.170999	1.794042
H	-0.192903	-0.814931	0.280448	C	-2.007087	-0.262155	0.000694
C	-1.278067	-1.423841	-1.467431	C	-1.492985	-1.150657	-1.122804
C	-1.569588	-2.809789	-0.860944	C	-2.322196	-2.046987	-1.802465
H	-0.397816	-1.514969	-2.112265	C	-0.127578	-1.058791	-1.475461
H	-2.108174	-1.097241	-2.097005	C	-1.829955	-2.823321	-2.851186
C	-2.075417	-3.819738	-1.893968	H	-3.365257	-2.128776	-1.515045
H	-0.651631	-3.191056	-0.393669	C	0.345483	-1.829743	-2.552026
H	-2.310323	-2.728143	-0.056714	C	-0.493635	-2.703234	-3.236597
C	-2.369561	-5.188485	-1.272331	H	-2.492698	-3.507923	-3.373451

H	1.379465	-1.719274	-2.864600	H	4.340259	-1.798506	-1.292276
H	-0.108071	-3.283269	-4.070547	C	6.983302	-1.642050	0.832334
C	-2.887032	-1.511221	3.457540	H	7.098377	-0.385465	2.583287
H	-3.295082	-0.759240	4.143165	H	6.582353	-2.758741	-0.968905
H	-3.514838	-2.409030	3.501390	H	7.973166	-2.068479	0.972632
H	-1.868095	-1.762885	3.756312	O	2.856758	1.163912	0.930892
C	0.774842	-0.184087	-0.696081	C	0.198749	1.111365	-0.151758
C	2.058032	-0.582183	-0.485005	H	0.556637	1.205629	0.875842
H	2.336678	-1.560656	-0.858753	C	-1.343720	1.130745	-0.156765
C	0.752300	2.317734	-0.950250	H	-1.712847	1.538562	-1.106738
C	0.383674	3.673506	-0.338614	H	-1.706609	1.796917	0.632428
H	0.382783	2.259920	-1.985204				
H	1.841590	2.239693	-0.991190	**4aa**			
C	1.002788	4.852420	-1.098827	C	5.762893	-0.999415	0.161001
H	-0.707999	3.800782	-0.311439	C	4.920567	-1.364608	-0.898203
H	0.727083	3.692366	0.705523	C	3.574807	-1.030659	-0.793432
C	0.644389	6.210470	-0.487371	C	3.061612	-0.354225	0.321700
H	2.094931	4.732967	-1.118399	C	3.903965	-0.003086	1.364189
H	0.672537	4.821873	-2.147350	C	5.266597	-0.327339	1.279685
H	1.099355	7.036681	-1.045946	H	6.819258	-1.247753	0.106503
H	-0.441720	6.367310	-0.483577	H	5.307089	-1.888308	-1.766885
H	0.991208	6.277408	0.551216	H	3.508972	0.505416	2.239578
C	3.069297	0.104468	0.334326	H	5.936765	-0.057174	2.090368
C	4.421285	-0.547233	0.473659	N	2.544701	-1.276773	-1.711263
C	5.225967	-0.147507	1.552603	C	1.337784	-0.759118	-1.272056
C	4.925943	-1.494386	-0.430598	O	0.303141	-0.777818	-1.915985
C	6.491611	-0.695905	1.736726	C	1.574400	-0.130780	0.133380
H	4.832816	0.598194	2.235697	C	0.711299	-0.802998	1.202664
C	6.200744	-2.033588	-0.255054	C	1.157443	-1.954249	1.852214

C	-0.548660	-0.248696	1.531087	C	-2.682754	-0.867963	-1.295975
C	0.398871	-2.554857	2.858284	C	-4.709394	-2.792194	-1.290449
H	2.120659	-2.375962	1.581599	H	-5.374199	-1.840751	0.533813
C	-1.281370	-0.846610	2.571316	C	-2.736240	-1.826225	-2.308123
C	-0.816808	-1.985420	3.227970	H	-1.874009	-0.151576	-1.302811
H	0.764787	-3.450430	3.352738	C	-3.749416	-2.785004	-2.310200
H	-2.230958	-0.423972	2.877298	H	-5.497851	-3.540334	-1.290076
H	-1.411828	-2.424674	4.023906	H	-1.968429	-1.822260	-3.075372
C	2.714246	-1.927921	-2.992500	H	-3.791353	-3.532086	-3.099121
H	3.417598	-1.369613	-3.621895	O	-4.454824	0.054355	1.747232
H	3.091153	-2.948578	-2.859246	C	-0.242053	1.671385	0.041335
H	1.737175	-1.959121	-3.477058	C	1.243401	1.375752	0.085202
C	-1.084339	0.912085	0.777468	H	1.680056	1.838478	0.982990
C	-0.618982	2.876561	-0.782591	H	1.755105	1.831703	-0.770167
C	-0.219979	4.206198	-0.109890	C	-2.564992	1.231981	0.915352
H	-1.690597	2.901899	-1.004757	H	-2.861247	1.946736	0.140703
H	-0.111006	2.805115	-1.755488	H	-2.750468	1.729894	1.874586
C	-0.558346	5.433285	-0.963191				
H	-0.727585	4.278765	0.862134	**INT5C**			
H	0.857703	4.199957	0.107273	C	-0.954332	2.271577	4.687437
C	-0.163834	6.751765	-0.290610	C	-0.287827	2.401646	3.468159
H	-0.052620	5.347921	-1.935580	C	-0.174594	1.298989	2.608859
H	-1.636142	5.437040	-1.179289	C	-0.735444	0.066395	2.983248
H	-0.415808	7.613936	-0.918431	C	-1.393499	-0.058642	4.206601
H	-0.680353	6.874200	0.669369	C	-1.505919	1.042918	5.058493
H	0.914673	6.785741	-0.092302	H	-1.039405	3.129676	5.347913
C	-3.608522	0.100692	0.862691	H	0.140932	3.358549	3.186632
C	-3.632844	-0.874265	-0.266249	H	-0.663033	-0.798199	2.328792
C	-4.648686	-1.847254	-0.272985	H	-1.822102	-1.016451	4.484396

H	-2.022554	0.944819	6.009043	C	-4.564870	-3.147799	-1.808448
C	0.742197	3.194946	0.588186	C	-5.920090	-3.384716	-2.081430
C	1.869967	4.014988	0.733344	H	-7.943140	-2.670023	-1.904902
C	-0.453863	3.743651	0.090062	H	-7.318450	-0.576429	-0.705464
C	1.805144	5.363038	0.370694	H	-3.805386	-3.866539	-2.102608
H	2.796111	3.608953	1.126828	H	-6.212114	-4.292168	-2.600572
C	-0.515329	5.092070	-0.255802	N	-4.610759	0.045467	-0.107349
H	-1.335554	3.116688	-0.016198	C	-3.275727	-0.092853	-0.103999
C	0.616454	5.902682	-0.123601	O	-2.433531	0.775930	0.231769
H	2.684574	5.990763	0.481181	C	-2.870890	-1.448844	-0.678121
H	-1.442522	5.509435	-0.637412	C	-1.836501	-1.074374	-1.761262
H	0.570081	6.950713	-0.404569	H	-1.373092	-1.944393	-2.232910
C	2.447546	0.925389	1.400596	H	-2.292058	-0.445574	-2.533161
C	3.453702	1.082156	0.429556	C	-2.291160	-2.315620	0.458005
C	2.772775	0.314534	2.621512	C	-3.029734	-2.473881	1.640823
C	4.754526	0.650753	0.679364	C	-1.040999	-2.940009	0.359098
H	3.226611	1.542149	-0.526086	C	-2.521642	-3.213325	2.706411
C	4.077270	-0.123942	2.864733	H	-4.010737	-2.015202	1.729140
H	2.015106	0.186844	3.387212	C	-0.529329	-3.681011	1.430605
C	5.069366	0.043183	1.897946	H	-0.452411	-2.862020	-0.546440
H	5.518004	0.775819	-0.082490	C	-1.261701	-3.813359	2.609107
H	4.315411	-0.589770	3.816753	H	-3.110441	-3.324498	3.612569
H	6.080687	-0.304348	2.085944	H	0.441135	-4.159773	1.332343
P	0.722279	1.415184	1.017143	H	-0.864535	-4.388751	3.440052
Pd	-0.521433	0.115007	-0.643559	C	-5.328569	1.232488	0.332678
C	-6.898688	-2.467734	-1.688621	H	-5.835097	1.701083	-0.517166
C	-6.557738	-1.286433	-1.013526	H	-6.070628	0.957900	1.088147
C	-5.211431	-1.072068	-0.761310	H	-4.607641	1.928774	0.762459
C	-4.214136	-1.978027	-1.152726	C	1.177883	-0.652248	-1.477653

C	2.090053	-1.489182	-1.006667	H	-1.155561	4.998343	-3.215875
H	1.996280	-1.913253	-0.014968				
C	3.281209	-1.788076	-1.870003	**TS6C**			
O	3.322535	-1.370167	-3.022798	C	-0.572379	4.578951	2.229874
C	4.397797	-2.586097	-1.287531	C	-0.758051	3.837166	1.064057
C	5.381507	-3.070563	-2.167785	C	-0.105423	2.601255	0.901108
C	4.522358	-2.842712	0.088329	C	0.723196	2.120168	1.925326
C	6.456422	-3.809723	-1.684931	C	0.903786	2.866307	3.090873
H	5.278687	-2.855573	-3.226208	C	0.258893	4.094342	3.244594
C	5.607354	-3.573277	0.570875	H	-1.081130	5.531065	2.348434
H	3.803922	-2.445453	0.796685	H	-1.417815	4.212725	0.287625
C	6.571158	-4.063118	-0.313585	H	1.218906	1.161750	1.820558
H	7.206739	-4.187856	-2.373089	H	1.544964	2.476861	3.874791
H	5.701493	-3.757835	1.637214	H	0.394796	4.670690	4.155104
H	7.411801	-4.638519	0.063922	C	-2.108994	1.796357	-1.043993
C	0.751634	0.163257	-2.500710	C	-2.535443	1.804101	-2.381101
C	1.254799	1.555550	-2.782642	C	-3.072507	1.818149	-0.021267
H	0.171408	-0.294399	-3.302639	C	-3.898130	1.829219	-2.686734
C	0.169533	2.526660	-3.266924	H	-1.813159	1.805406	-3.189837
H	1.755053	1.968648	-1.903160	C	-4.431197	1.846011	-0.331147
H	2.026057	1.433755	-3.559149	H	-2.768701	1.812920	1.018809
C	0.721203	3.935305	-3.512543	C	-4.848607	1.847656	-1.664090
H	-0.290520	2.135773	-4.185617	H	-4.212830	1.843733	-3.726321
H	-0.626570	2.576959	-2.511878	H	-5.163723	1.860998	0.470381
H	1.181746	4.303785	-2.586094	H	-5.907912	1.862254	-1.902578
H	1.521159	3.887541	-4.264173	C	0.552393	2.513019	-1.974078
C	-0.361611	4.916763	-3.968543	C	0.759305	1.843068	-3.193009
H	0.051378	5.918522	-4.127937	C	1.018003	3.826781	-1.827415
H	-0.823210	4.591221	-4.908385	C	1.394882	2.486689	-4.253533

H	0.434235	0.811626	-3.307038	H	2.230169	-2.423187	1.971476
C	1.666388	4.462771	-2.888830	C	3.892428	0.873616	3.131864
H	0.886004	4.356704	-0.890349	H	4.304957	1.236253	1.060421
C	1.851107	3.799007	-4.102316	C	3.315040	0.015780	4.071940
H	1.543929	1.960556	-5.192014	H	2.277413	-1.852231	4.360355
H	2.026446	5.479790	-2.763258	H	4.363577	1.798467	3.452231
H	2.354275	4.298169	-4.925203	H	3.337242	0.264932	5.128881
P	-0.324495	1.622183	-0.628548	C	3.327833	-4.544019	-1.264141
C	7.062380	-2.113296	-1.743211	H	3.542962	-4.678193	-2.329131
C	5.991563	-3.002368	-1.575047	H	3.965107	-5.214872	-0.680406
C	4.808092	-2.479432	-1.077275	H	2.278888	-4.770883	-1.071228
C	4.655088	-1.126594	-0.734964	Pd	0.393420	-0.530025	-0.411597
C	5.721035	-0.257612	-0.918421	C	-1.581040	-1.427169	0.046542
C	6.928029	-0.759874	-1.427432	C	-2.764669	-1.400801	-0.566550
H	8.005438	-2.486121	-2.130821	H	-2.979714	-0.813478	-1.447313
H	6.088697	-4.052681	-1.829962	C	-3.804672	-2.237805	0.109429
H	5.629397	0.798216	-0.684873	O	-3.490362	-2.877342	1.120552
H	7.766212	-0.086635	-1.577918	C	-5.193459	-2.280564	-0.414118
N	3.576702	-3.163894	-0.876596	C	-6.146854	-3.031528	0.298146
C	2.636143	-2.298504	-0.462986	C	-5.587948	-1.602190	-1.580613
O	1.406450	-2.533384	-0.371976	C	-7.463566	-3.099780	-0.143977
C	3.245091	-0.931093	-0.184187	H	-5.831087	-3.553465	1.194975
C	2.334606	0.085298	-0.920649	C	-6.908157	-1.674062	-2.021411
H	2.604051	1.111630	-0.662731	H	-4.878021	-1.014357	-2.149628
H	2.414920	-0.030827	-2.006797	C	-7.847172	-2.420391	-1.305336
C	3.270654	-0.639100	1.330129	H	-8.192348	-3.681850	0.412301
C	2.703491	-1.497760	2.280908	H	-7.203931	-1.150242	-2.925883
C	3.864991	0.549860	1.776044	H	-8.875387	-2.474705	-1.651805
C	2.721606	-1.170455	3.640382	C	-1.194401	-2.132405	1.156746

C	-1.117390	-1.611976	2.558133	C	-3.066753	1.918861	0.121598
H	-0.726934	-3.103158	0.979927	C	-3.769518	2.487535	-2.518809
C	-1.846645	-0.293214	2.799420	H	-1.660412	2.556958	-2.916385
H	-1.505955	-2.409195	3.206784	C	-4.410580	2.019216	-0.236761
H	-0.050912	-1.514516	2.815066	H	-2.808135	1.691388	1.149690
C	-1.660825	0.251693	4.218005	C	-4.766545	2.300561	-1.558489
H	-1.465509	0.447683	2.089310	H	-4.036292	2.718378	-3.546195
H	-2.912705	-0.428479	2.578115	H	-5.179468	1.875575	0.516996
H	-2.011323	-0.489329	4.949324	H	-5.813902	2.381895	-1.835516
H	-0.587311	0.395057	4.407195	C	0.649621	2.962576	-1.469356
C	-2.400004	1.577290	4.424686	C	0.954978	2.555313	-2.779686
H	-2.256256	1.962041	5.440041	C	1.063656	4.228277	-1.031850
H	-2.038133	2.340504	3.725480	C	1.639561	3.409349	-3.643205
H	-3.478229	1.454510	4.264524	H	0.668552	1.562988	-3.118908
				C	1.760871	5.075029	-1.896446
INT6C				H	0.855616	4.556511	-0.019226
C	-0.659511	4.061008	3.035564	C	2.045075	4.671655	-3.201939
C	-0.805619	3.592332	1.730529	H	1.866553	3.084559	-4.654586
C	-0.142798	2.420635	1.320600	H	2.082028	6.051491	-1.545394
C	0.657376	1.725774	2.239380	H	2.586815	5.333887	-3.870959
C	0.800228	2.200531	3.544479	P	-0.293023	1.806185	-0.397922
C	0.144679	3.365738	3.943868	C	7.070519	-1.995402	-1.811112
H	-1.175785	4.965513	3.343673	C	5.948444	-2.831870	-1.892480
H	-1.441887	4.131455	1.034798	C	4.759768	-2.347592	-1.368196
H	1.167076	0.816771	1.939778	C	4.646613	-1.085361	-0.765624
H	1.421068	1.648943	4.242646	C	5.764069	-0.265545	-0.704448
H	0.251749	3.729373	4.961770	C	6.978890	-0.728014	-1.232574
C	-2.057365	2.107270	-0.837384	H	8.019455	-2.339705	-2.210764
C	-2.422193	2.394928	-2.161050	H	6.012078	-3.813390	-2.351231

H	5.705933	0.725677	-0.266417	O	-3.053546	-2.816613	0.388437
H	7.856865	-0.090672	-1.191866	C	-5.041040	-2.194460	-0.758595
N	3.485789	-2.981074	-1.385152	C	-5.754603	-3.246746	-0.149767
C	2.560070	-2.162111	-0.855787	C	-5.711414	-1.303954	-1.621790
O	1.318320	-2.350603	-0.881334	C	-7.111501	-3.405503	-0.406409
C	3.211949	-0.913273	-0.273755	H	-5.235182	-3.928021	0.515265
C	2.389358	0.282688	-0.825875	C	-7.069425	-1.469124	-1.870406
H	2.688261	1.211627	-0.332435	H	-5.175873	-0.480457	-2.080894
H	2.576096	0.403671	-1.900488	C	-7.769610	-2.518612	-1.266004
C	3.154789	-0.940286	1.266914	H	-7.659154	-4.218058	0.060792
C	2.506159	-1.950560	1.987977	H	-7.584941	-0.782063	-2.534431
C	3.758505	0.104312	1.982353	H	-8.830030	-2.645276	-1.464122
C	2.448825	-1.910803	3.384741	C	-1.634024	-2.399723	0.497017
H	2.027499	-2.772787	1.467355	C	-1.312036	-2.145814	1.974056
C	3.713437	0.140074	3.375160	H	-1.054101	-3.253044	0.122967
H	4.259825	0.905178	1.449256	C	-1.999503	-0.908104	2.554920
C	3.051733	-0.866192	4.084746	H	-1.580240	-3.043780	2.543650
H	1.937020	-2.704614	3.921740	H	-0.225338	-2.028962	2.042468
H	4.193539	0.957579	3.905686	C	-1.636000	-0.655559	4.021388
H	3.015773	-0.840024	5.170043	H	-1.699739	-0.033082	1.967211
C	3.199723	-4.235126	-2.062524	H	-3.089376	-1.004058	2.452262
H	3.481337	-4.163565	-3.118234	H	-1.902401	-1.534048	4.625274
H	3.762563	-5.048616	-1.594761	H	-0.546061	-0.540084	4.101200
H	2.130318	-4.431874	-1.981489	C	-2.328842	0.590700	4.580560
Pd	0.370730	-0.343066	-0.627473	H	-2.046166	0.772012	5.623216
C	-1.484528	-1.238855	-0.430378	H	-2.055713	1.481859	4.003641
C	-2.720715	-1.069877	-1.018984	H	-3.420042	0.484073	4.544642
H	-2.984967	-0.317990	-1.748517				
C	-3.627740	-2.015847	-0.488068	**TS6D**			

C	-4.092911	-3.685565	1.893030	C	1.701760	-5.038754	-2.206712
C	-2.738872	-3.345768	1.890034	H	3.524764	-4.232943	-1.373999
C	-2.198390	-2.627649	0.812726	H	-0.269147	-5.668448	-2.814178
C	-3.031070	-2.248644	-0.253605	H	2.213855	-5.679165	-2.918754
C	-4.378820	-2.605963	-0.251878	P	-0.424920	-2.177337	0.746036
C	-4.912925	-3.321937	0.822749	Pd	-0.086500	0.082084	0.216437
H	-4.504684	-4.240251	2.731148	C	-2.078786	6.695590	1.136830
H	-2.108279	-3.640027	2.722597	C	-2.296147	5.612869	1.999669
H	-2.627795	-1.679965	-1.084377	C	-1.956776	4.352605	1.530817
H	-5.010538	-2.324403	-1.089535	C	-1.425843	4.135283	0.251515
H	-5.964237	-3.594860	0.825988	C	-1.211135	5.217704	-0.590203
C	0.253476	-2.555381	2.404878	C	-1.539841	6.503443	-0.137474
C	0.726767	-3.840514	2.717931	H	-2.332203	7.697418	1.469361
C	0.254583	-1.557888	3.394536	H	-2.709474	5.759772	2.992112
C	1.199615	-4.119428	4.000581	H	-0.794428	5.082806	-1.583060
H	0.729820	-4.620492	1.963215	H	-1.374081	7.357595	-0.786307
C	0.727859	-1.845422	4.675290	N	-2.048333	3.117312	2.223911
H	-0.121955	-0.564950	3.170697	C	-1.561884	2.117679	1.466263
C	1.203008	-3.123048	4.979602	O	-1.378249	0.940122	1.844652
H	1.565623	-5.115170	4.233319	C	-1.207297	2.634408	0.066696
H	0.728531	-1.069113	5.435225	C	0.308024	2.320416	-0.217324
H	1.574960	-3.342285	5.976266	H	0.553235	2.774983	-1.176022
C	0.376321	-3.378732	-0.378157	H	0.911143	2.786226	0.562392
C	1.782046	-3.399871	-0.430751	C	-2.161950	2.067290	-1.001041
C	-0.357537	-4.204809	-1.240316	C	-3.242552	1.236039	-0.676558
C	2.439422	-4.226580	-1.340047	C	-1.986201	2.442455	-2.341765
H	2.362819	-2.778762	0.247144	C	-4.121504	0.792344	-1.668478
C	0.307106	-5.029970	-2.150783	H	-3.400607	0.907840	0.344908
H	-1.441936	-4.206861	-1.206257	C	-2.860809	1.997428	-3.330640

H	-1.165156	3.093347	-2.624272	H	0.221392	1.067544	-2.935814
C	-3.935644	1.168651	-2.997571	H	1.346121	-0.149686	-3.534057
H	-4.951570	0.150472	-1.390087	C	-1.080816	-0.901788	-4.565355
H	-2.705308	2.302645	-4.361052	H	-0.383965	-1.929428	-2.797167
H	-4.620262	0.825903	-3.767368	H	-1.487800	-0.592084	-2.472473
C	-2.472061	2.975131	3.608602	H	-1.295531	0.129431	-4.876695
H	-1.820337	3.562894	4.263085	H	-0.250829	-1.249843	-5.195081
H	-3.503022	3.324338	3.718080	C	-2.315439	-1.778098	-4.797090
H	-2.410440	1.920556	3.878438	H	-2.618266	-1.779785	-5.849639
C	1.658477	0.881703	-0.650183	H	-2.120444	-2.816910	-4.502732
C	2.868741	1.319366	-0.271121	H	-3.164120	-1.416904	-4.202519
H	2.984943	2.048219	0.521438				
C	4.069464	0.803525	-0.993779	**INT6D**			
O	3.942039	0.069881	-1.973637	C	4.429254	-3.604441	0.501947
C	5.423688	1.202047	-0.506234	C	3.883138	-2.424528	1.003277
C	6.516552	0.952807	-1.355346	C	2.737991	-1.867874	0.406930
C	5.654943	1.786706	0.750496	C	2.125870	-2.527866	-0.664914
C	7.806570	1.296081	-0.964532	C	2.682300	-3.705110	-1.169260
H	6.326924	0.492214	-2.319026	C	3.836127	-4.238863	-0.594296
C	6.950200	2.119655	1.145072	H	5.315477	-4.028601	0.964843
H	4.836256	1.963765	1.440801	H	4.345403	-1.933083	1.854888
C	8.026145	1.881100	0.287081	H	1.206779	-2.138770	-1.090494
H	8.642662	1.108682	-1.631990	H	2.204704	-4.207117	-2.004212
H	7.120012	2.563508	2.121706	H	4.266921	-5.154725	-0.988761
H	9.033701	2.147857	0.593432	C	2.111502	-0.382984	2.820285
C	1.170940	-0.178428	-1.449729	C	3.153170	0.140779	3.601186
C	0.537847	0.027911	-2.809698	C	1.038671	-1.043655	3.445999
H	1.728584	-1.108063	-1.358223	C	3.124721	-0.005369	4.989208
C	-0.643032	-0.906771	-3.098495	H	3.981123	0.660505	3.129108

C	1.018082	-1.186684	4.832720	C	-2.958575	-0.537029	0.909485
H	0.220003	-1.440854	2.850140	O	-1.996162	-0.243844	1.635477
C	2.060567	-0.667863	5.605559	C	-2.938414	-0.830107	-0.617992
H	3.935423	0.398763	5.588607	C	-1.994646	-1.986659	-0.964581
H	0.187052	-1.697992	5.310094	C	-1.627618	-2.927339	0.010528
H	2.042056	-0.776923	6.686060	C	-1.622159	-2.233838	-2.294818
C	3.362978	0.989744	0.576173	C	-0.942525	-4.091431	-0.337279
C	3.069792	2.330750	0.882042	H	-1.885495	-2.761247	1.051160
C	4.583790	0.675376	-0.035049	C	-0.934911	-3.398755	-2.644781
C	3.990756	3.336230	0.597126	H	-1.893532	-1.538288	-3.082602
H	2.118822	2.588698	1.342236	C	-0.608156	-4.340874	-1.668959
C	5.501334	1.687754	-0.321823	H	-0.675370	-4.806470	0.435099
H	4.817788	-0.348864	-0.301686	H	-0.674716	-3.573919	-3.684904
C	5.210910	3.014762	-0.003693	H	-0.093117	-5.257133	-1.940782
H	3.752623	4.368454	0.836024	C	-4.643330	-0.419900	2.734066
H	6.441265	1.435480	-0.803576	H	-5.415578	0.354855	2.772963
H	5.927652	3.798566	-0.231128	H	-5.040194	-1.343786	3.167426
P	2.091922	-0.263289	0.988943	H	-3.767903	-0.096577	3.297493
C	-7.114232	-1.771926	-0.750976	C	-0.121553	0.964765	-1.603149
C	-6.470583	-1.338799	0.416484	H	-0.107265	0.054389	-2.195840
C	-5.109424	-1.079330	0.330805	C	0.949144	1.966426	-1.958209
C	-4.388877	-1.235173	-0.857437	O	0.813286	3.161441	-1.709891
C	-5.033833	-1.668632	-2.005592	C	2.192772	1.460688	-2.614009
C	-6.409023	-1.937234	-1.945734	C	3.176674	2.407849	-2.945102
H	-8.178088	-1.986395	-0.720055	C	2.429934	0.105952	-2.901381
H	-7.017297	-1.217431	1.345943	C	4.365370	2.010003	-3.547497
H	-4.483027	-1.813035	-2.930456	H	2.989478	3.449867	-2.712310
H	-6.928143	-2.281408	-2.834672	C	3.628379	-0.293984	-3.488970
N	-4.238167	-0.646622	1.356600	H	1.696881	-0.652275	-2.659052

C	4.596674	0.657395	-3.817424	C	-0.769026	4.412685	0.179284
H	5.117149	2.751729	-3.800677	C	-0.874534	5.804489	0.223170
H	3.803719	-1.347334	-3.687235	C	-2.128058	6.409291	0.332928
H	5.528071	0.346648	-4.282511	H	-4.257092	6.091646	0.488704
C	-2.705130	2.787674	0.622145	H	-4.084488	3.626709	0.404758
C	-3.340473	4.030427	-0.048640	H	0.210824	3.948655	0.104615
H	-3.457530	1.999660	0.710806	H	0.023439	6.414171	0.179099
H	-2.396810	3.050282	1.642062	H	-2.207524	7.491879	0.372769
C	-4.551907	4.556038	0.732558	C	-3.135336	1.096895	1.085854
H	-2.585034	4.821628	-0.142024	C	-4.402028	0.832417	0.543130
H	-3.643485	3.770750	-1.072408	C	-2.902722	0.833834	2.446989
H	-5.296067	3.752344	0.829298	C	-5.414349	0.306997	1.349120
H	-4.238464	4.812274	1.754063	H	-4.597508	1.029850	-0.506386
C	-5.192769	5.776397	0.064591	C	-3.918442	0.315036	3.250385
H	-6.053024	6.135063	0.639574	H	-1.922624	1.038681	2.872545
H	-4.476471	6.602287	-0.017651	C	-5.174699	0.046424	2.700168
H	-5.541940	5.535619	-0.946623	H	-6.391352	0.103700	0.920174
C	-1.436965	1.322469	-1.081912	H	-3.728773	0.118247	4.301800
C	-2.673219	0.500481	-1.417376	H	-5.964454	-0.363776	3.322795
H	-2.653520	0.247343	-2.480132	C	-2.107966	1.399635	-1.648258
H	-3.556285	1.130536	-1.287854	C	-2.448937	0.083864	-2.008027
C	-1.499031	2.349518	-0.145431	C	-1.887325	2.348648	-2.657941
H	-0.645349	3.019460	-0.091469	C	-2.561331	-0.275387	-3.350853
Pd	-0.023883	0.489143	0.439679	H	-2.633634	-0.659721	-1.240614
				C	-2.004211	1.985289	-4.001331
TS7C				H	-1.629148	3.370699	-2.397936
C	-3.281689	5.622394	0.398000	C	-2.334482	0.673697	-4.351014
C	-3.184915	4.232471	0.348572	H	-2.824379	-1.297036	-3.610898
C	-1.926861	3.619653	0.236531	H	-1.842600	2.731401	-4.774407

H	-2.424447	0.395551	-5.397259	H	5.589523	3.659397	-0.114332
P	-1.755447	1.801262	0.108445	H	3.971664	4.037409	0.542308
C	7.189184	-0.411432	0.893105	C	-0.097954	-1.695672	-0.670440
C	6.590098	0.846923	0.742540	H	0.217637	-1.357887	-1.643194
C	5.227426	0.876247	0.483620	C	-0.815202	-2.848587	-0.422463
C	4.456074	-0.286927	0.349794	O	-1.095716	-3.021581	0.878845
C	5.057551	-1.524171	0.536039	C	-1.320786	-3.836523	-1.363273
C	6.433436	-1.581636	0.804825	C	-2.103948	-4.913947	-0.910572
H	8.253692	-0.470833	1.097947	C	-1.044337	-3.707341	-2.739580
H	7.169684	1.758963	0.840030	C	-2.602685	-5.843579	-1.818984
H	4.477335	-2.441597	0.493797	H	-2.316602	-5.009706	0.148605
H	6.911250	-2.545343	0.950194	C	-1.548625	-4.639808	-3.640062
N	4.391943	2.014388	0.385832	H	-0.433915	-2.885099	-3.099483
C	3.094009	1.643978	0.277719	C	-2.328215	-5.708293	-3.182918
O	2.123042	2.412991	0.397478	H	-3.206777	-6.673389	-1.464876
C	3.020833	0.116108	0.024899	H	-1.332397	-4.538418	-4.699462
C	2.652039	-0.168577	-1.455683	H	-2.719284	-6.434599	-3.889462
C	1.892470	0.733752	-2.216254	C	0.080940	-2.236430	2.872161
C	2.967137	-1.411347	-2.019749	C	-0.837668	-2.987579	3.843040
C	1.423729	0.382332	-3.484129	H	0.953568	-2.851858	2.619917
H	1.632481	1.708394	-1.820046	H	0.455239	-1.320079	3.345721
C	2.507490	-1.761023	-3.290863	C	-0.133373	-3.366979	5.150884
H	3.568329	-2.124134	-1.468980	H	-1.714178	-2.360573	4.065345
C	1.721290	-0.869976	-4.024510	H	-1.220332	-3.891452	3.352463
H	0.809759	1.086554	-4.036528	H	0.742338	-3.990615	4.922253
H	2.763293	-2.733313	-3.702367	H	0.254510	-2.457105	5.631039
H	1.355334	-1.142638	-5.010305	C	-1.055213	-4.110244	6.122545
C	4.835632	3.378113	0.626865	H	-0.530120	-4.373084	7.046852
H	5.266124	3.464541	1.630353	H	-1.921960	-3.495014	6.393535

H	-1.432679	-5.038100	5.676148	H	6.762535	-0.168640	-0.588670
C	1.985412	-0.548384	0.979590	H	4.632231	2.971732	1.439286
H	2.144302	-1.626188	0.943298	H	6.722612	2.110994	0.402654
H	2.141193	-0.242921	2.019677	C	2.204891	-2.444948	-0.632606
C	-0.633013	-1.826923	1.591363	C	2.459518	-2.104985	-1.971702
H	-1.552586	-1.282749	1.846944	C	2.072781	-3.797349	-0.288036
Pd	0.300582	0.926949	0.645750	C	2.604962	-3.096080	-2.940297
C	0.096522	-1.000369	0.547164	H	2.569631	-1.061406	-2.251383
				C	2.204345	-4.789619	-1.263931
INT7C				H	1.880879	-4.079709	0.742252
C	3.509696	-3.041324	3.924292	C	2.476232	-4.443352	-2.589028
C	3.413528	-2.346394	2.719369	H	2.817030	-2.818336	-3.969069
C	2.157172	-1.962429	2.222831	H	2.106717	-5.834455	-0.982779
C	1.001221	-2.283899	2.951567	H	2.589883	-5.216945	-3.343033
C	1.103885	-2.984206	4.156028	P	1.985336	-1.100120	0.607332
C	2.355369	-3.362760	4.644110	C	-7.219056	-1.785412	-0.157475
H	4.486046	-3.330779	4.302485	C	-6.272936	-2.007833	0.852428
H	4.316194	-2.097961	2.169623	C	-4.984667	-1.543661	0.626402
H	0.024971	-1.987546	2.582848	C	-4.617306	-0.879224	-0.548924
H	0.204939	-3.227690	4.715998	C	-5.560827	-0.670333	-1.543525
H	2.433765	-3.902884	5.583379	C	-6.871144	-1.126383	-1.339110
C	3.524459	-0.105445	0.475328	H	-8.236897	-2.135626	-0.015847
C	4.707653	-0.586294	-0.106414	H	-6.541311	-2.522934	1.768959
C	3.510338	1.184167	1.029320	H	-5.291744	-0.174060	-2.470921
C	5.852172	0.212691	-0.134566	H	-7.620094	-0.969309	-2.108921
H	4.738248	-1.581164	-0.539143	N	-3.862391	-1.639584	1.483627
C	4.658226	1.974234	1.011491	C	-2.771105	-1.063493	0.925380
H	2.593217	1.572084	1.466039	O	-1.666251	-0.969790	1.489229
C	5.830301	1.491845	0.424696	C	-3.141718	-0.511475	-0.468405

C	-2.331767	-1.165838	-1.591126	H	5.277804	3.713978	-2.709639
C	-1.564628	-2.318547	-1.374185	C	-2.248914	3.955213	0.475245
C	-2.382783	-0.630409	-2.886879	C	-1.890436	5.153516	1.362771
C	-0.849676	-2.907343	-2.418182	H	-2.226635	4.242206	-0.584806
H	-1.500629	-2.757647	-0.383982	H	-3.272274	3.626550	0.696825
C	-1.669548	-1.218831	-3.931956	C	-2.849551	6.335773	1.175401
H	-2.976970	0.255442	-3.091101	H	-1.897370	4.839610	2.416907
C	-0.894705	-2.357432	-3.698447	H	-0.864515	5.473285	1.141131
H	-0.241822	-3.783375	-2.220428	H	-2.847854	6.638566	0.118884
H	-1.725297	-0.789101	-4.928339	H	-3.875175	6.010603	1.400076
H	-0.331095	-2.813136	-4.506958	C	-2.483708	7.534949	2.055729
C	-3.890691	-2.241023	2.806862	H	-3.181363	8.365463	1.905169
H	-4.608887	-1.714441	3.443696	H	-2.507003	7.266433	3.118802
H	-4.181530	-3.293590	2.732091	H	-1.474951	7.899241	1.826489
H	-2.893061	-2.164528	3.239640	C	-2.963141	1.041901	-0.413045
C	-0.500438	1.596771	-1.212043	H	-3.418176	1.464282	-1.316124
H	-0.474514	1.119167	-2.181954	H	-3.575153	1.402143	0.420694
C	0.487944	2.483073	-0.716944	C	-1.307335	2.763036	0.670229
O	0.050737	3.197373	0.330321	H	-1.271808	2.475654	1.728275
C	1.786102	2.826780	-1.269927	Pd	-0.013220	0.131586	0.311046
C	2.433300	4.009071	-0.870626	C	-1.550876	1.570407	-0.252506
C	2.406969	1.971681	-2.198698				
C	3.680854	4.328937	-1.398658	**TS8C**			
H	1.951079	4.666533	-0.155632	C	5.201529	-2.169704	1.813361
C	3.657506	2.290689	-2.711494	C	4.461708	-1.708148	0.721245
H	1.917375	1.046511	-2.485177	C	3.070027	-1.873049	0.694769
C	4.297622	3.469375	-2.311328	C	2.431621	-2.507172	1.774252
H	4.176311	5.245564	-1.093328	C	3.173509	-2.974009	2.858300
H	4.143073	1.617763	-3.411322	C	4.561370	-2.802460	2.880458

H	6.278984	-2.032925	1.828396	C	-5.754475	-2.961806	0.403628
H	4.967776	-1.213970	-0.102533	C	-4.704333	-2.081440	0.186706
H	1.350231	-2.625960	1.766107	C	-4.667080	-0.792766	0.732660
H	2.670596	-3.461122	3.688910	C	-5.707853	-0.370701	1.548112
H	5.139321	-3.158635	3.728334	C	-6.778755	-1.243592	1.790549
C	3.066512	-0.073595	-1.613776	H	-7.642206	-3.179222	1.412833
C	3.942805	-0.483889	-2.630344	H	-5.765443	-3.954771	-0.033583
C	2.987808	1.289393	-1.280687	H	-5.705019	0.616523	1.998817
C	4.730404	0.457652	-3.295678	H	-7.596910	-0.922378	2.427404
H	4.005306	-1.532720	-2.905809	N	-3.520035	-2.313039	-0.552081
C	3.776557	2.226680	-1.946537	C	-2.692538	-1.247330	-0.492796
H	2.302869	1.622915	-0.506347	O	-1.553681	-1.237749	-0.999683
C	4.648607	1.810573	-2.955943	C	-3.397105	-0.092253	0.257048
H	5.404666	0.133700	-4.083356	C	-3.731007	1.052971	-0.719875
H	3.696572	3.277240	-1.681085	C	-3.342395	1.037151	-2.064870
H	5.259402	2.538974	-3.481742	C	-4.411269	2.180260	-0.233589
C	1.809308	-2.706931	-1.798526	C	-3.607383	2.130444	-2.895599
C	0.771607	-2.660919	-2.744737	H	-2.800742	0.192404	-2.473475
C	2.644051	-3.832798	-1.740703	C	-4.672384	3.271510	-1.059421
C	0.581522	-3.724309	-3.626866	H	-4.724262	2.224262	0.804231
H	0.109926	-1.801216	-2.780436	C	-4.265241	3.253934	-2.396521
C	2.445125	-4.896875	-2.623231	H	-3.291804	2.098592	-3.934518
H	3.445165	-3.880528	-1.009071	H	-5.192127	4.136350	-0.657452
C	1.416845	-4.843749	-3.566511	H	-4.466502	4.104238	-3.041355
H	-0.218406	-3.680418	-4.361036	C	-3.186671	-3.572340	-1.200955
H	3.095243	-5.765679	-2.573477	H	-3.195270	-4.383099	-0.465424
H	1.265529	-5.672789	-4.251951	H	-3.917906	-3.791152	-1.985261
P	2.024820	-1.267224	-0.688386	H	-2.191015	-3.482839	-1.636836
C	-6.803304	-2.517728	1.219863	C	-1.092779	2.308555	0.288780

H	-1.712546	2.571619	-0.551337	H	-2.316562	-0.452395	2.101119
C	0.021533	2.995425	0.696726	C	-0.092753	1.205756	2.029286
O	0.557580	2.414821	1.816599	H	0.895747	0.378420	1.358226
C	0.745189	4.115581	0.114038	Pd	0.091547	-0.242109	0.101650
C	1.975922	4.529412	0.654860	C	-1.250036	1.148157	1.135483
C	0.243756	4.762721	-1.031124				
C	2.690296	5.566037	0.056815	**INT8C**			
H	2.368782	4.031122	1.534523	C	-4.682966	-3.171668	1.531912
C	0.962177	5.797403	-1.621266	C	-4.143562	-1.905875	1.286678
H	-0.705235	4.453869	-1.459643	C	-3.047454	-1.758557	0.425337
C	2.188296	6.201409	-1.082083	C	-2.504377	-2.899128	-0.188418
H	3.639671	5.878477	0.481832	C	-3.053289	-4.158344	0.046975
H	0.567546	6.290183	-2.504835	C	-4.142977	-4.298445	0.911643
H	2.746829	7.008851	-1.546314	H	-5.527406	-3.272634	2.208491
C	0.022323	0.671758	3.436288	H	-4.577208	-1.036355	1.769507
C	1.476356	0.534500	3.911185	H	-1.646673	-2.797893	-0.847376
H	-0.541118	1.338139	4.103843	H	-2.624629	-5.031493	-0.437658
H	-0.472666	-0.305797	3.462263	H	-4.564659	-5.281624	1.102752
C	1.596296	-0.137679	5.282692	C	-3.078010	0.297733	-1.610074
H	2.036647	-0.058106	3.174380	C	-4.135484	-0.443822	-2.157513
H	1.942959	1.526976	3.936601	C	-2.576481	1.409693	-2.308810
H	1.029228	0.436710	6.028057	C	-4.683518	-0.079084	-3.389620
H	1.127829	-1.131719	5.236377	H	-4.531964	-1.304638	-1.628404
C	3.054421	-0.277617	5.731703	C	-3.133361	1.769603	-3.535765
H	3.124826	-0.771281	6.706740	H	-1.760853	1.989555	-1.885253
H	3.629241	-0.869078	5.008943	C	-4.184119	1.026234	-4.080352
H	3.535477	0.703952	5.817840	H	-5.501158	-0.660867	-3.807092
C	-2.537072	0.407589	1.459774	H	-2.741426	2.632198	-4.068042
H	-3.173344	1.072272	2.058611	H	-4.611427	1.307131	-5.039442

C	-3.121359	1.043261	1.197991	C	4.681932	-3.171802	-1.533252
C	-4.397758	1.575726	0.965716	H	4.576102	-1.036490	-1.770945
C	-2.435800	1.378509	2.374263	C	3.053293	-4.158255	-0.047026
C	-4.984721	2.423536	1.906490	H	1.647386	-2.797663	0.848218
H	-4.928523	1.334203	0.049292	C	4.142346	-4.298489	-0.912486
C	-3.028303	2.220685	3.314511	H	5.525874	-3.272864	-2.210438
H	-1.431539	0.999264	2.537598	H	2.624960	-5.031345	0.438003
C	-4.302335	2.744254	3.082254	H	4.563837	-5.281709	-1.103803
H	-5.971916	2.836817	1.717655	C	3.078089	0.297400	1.610113
H	-2.487390	2.481477	4.219965	C	4.136147	-0.443828	2.156880
H	-4.758665	3.408696	3.811233	C	2.576138	1.408725	2.309541
P	-2.324888	-0.112933	0.018838	C	4.684344	-0.079388	3.389000
Cl	-0.000010	2.482322	0.000400	H	4.532931	-1.304192	1.627262
Pd	0.000000	0.030872	-0.000007	C	3.133165	1.768331	3.536525
H	0.000068	-1.521178	-0.000269	H	1.760125	1.988389	1.886467
C	4.985211	2.423219	-1.906320	C	4.184506	1.025299	4.080431
C	4.398189	1.575226	-0.965759	H	5.502437	-0.660910	3.805946
C	3.121454	1.043463	-1.197831	H	2.740888	2.630434	4.069348
C	2.435641	1.379587	-2.373705	H	4.611930	1.305965	5.039537
C	3.028205	2.221953	-3.313753	P	2.324890	-0.112883	-0.018874
C	4.302550	2.744832	-3.081685				
H	5.972664	2.835953	-1.717637	**INT8D**			
H	4.929168	1.332986	-0.049649	C	4.416324	3.471508	1.740937
H	1.431158	1.000877	-2.536899	C	3.968653	2.187438	1.415632
H	2.487090	2.483424	-4.218890	C	2.930532	2.013112	0.490641
H	4.758931	3.409427	-3.810492	C	2.355593	3.145457	-0.109671
C	3.047296	-1.758512	-0.425619	C	2.813337	4.423009	0.205555
C	4.142762	-1.905953	-1.287738	C	3.843348	4.590051	1.136732
C	2.504608	-2.899002	0.188645	H	5.215957	3.592056	2.466916

H	4.429384	1.324988	1.885444	C	-5.207119	-2.078209	-1.698122
H	1.544582	3.024503	-0.822484	C	-4.528026	-1.251045	-0.801692
H	2.360673	5.289186	-0.269704	C	-3.235608	-0.799363	-1.103140
H	4.193295	5.587208	1.389960	C	-2.629897	-1.188599	-2.306629
C	3.075745	0.097998	-1.665743	C	-3.315112	-2.006935	-3.203579
C	4.161092	0.871287	-2.106306	C	-4.603484	-2.454142	-2.899945
C	2.565304	-0.910925	-2.498874	H	-6.205451	-2.431448	-1.454359
C	4.727682	0.637221	-3.360775	H	-5.001308	-0.963252	0.132200
H	4.563465	1.656398	-1.473905	H	-1.614609	-0.871683	-2.525941
C	3.138321	-1.141431	-3.749774	H	-2.835329	-2.310332	-4.129848
H	1.731558	-1.519710	-2.162708	H	-5.132093	-3.101615	-3.594455
C	4.217853	-0.368416	-4.184264	C	-2.930511	2.013126	-0.490739
H	5.567014	1.242571	-3.692787	C	-3.969263	2.187227	-1.415068
H	2.736796	-1.926272	-4.385029	C	-2.355161	3.145623	0.108894
H	4.658999	-0.547749	-5.161202	C	-4.417140	3.471217	-1.740401
C	3.235780	-0.799302	1.103318	H	-4.430334	1.324671	-1.884349
C	4.528284	-1.250823	0.801984	C	-2.813101	4.423099	-0.206353
C	2.629980	-1.188690	2.306705	H	-1.543681	3.024833	0.821197
C	5.207372	-2.077953	1.698440	C	-3.843740	4.589911	-1.136877
H	5.001656	-0.962943	-0.131837	H	-5.217267	3.591585	-2.465867
C	3.315194	-2.007003	3.203688	H	-2.360105	5.289398	0.268366
H	1.614638	-0.871891	2.525934	H	-4.193845	5.587006	-1.390131
C	4.603649	-2.454035	2.900177	C	-3.075728	0.098097	1.665789
H	6.205776	-2.431051	1.454765	C	-4.160596	0.871860	2.106671
H	2.835335	-2.310505	4.129885	C	-2.565799	-0.911394	2.498566
H	5.132249	-3.101492	3.594709	C	-4.727223	0.637713	3.361117
P	2.321422	0.341269	-0.003825	H	-4.562608	1.657359	1.474526
Pd	0.000025	0.093735	0.000081	C	-3.138863	-1.141984	3.749419
H	0.000122	1.645122	0.000350	H	-1.732387	-1.520509	2.162161

C	-4.217922	-0.368482	4.184239	H	-6.482094	-3.598987	0.877092
H	-5.566187	1.243437	3.693376	C	-2.575758	1.001785	-1.410727
H	-2.737752	-1.927265	4.384392	C	-3.927537	1.208504	-1.722466
H	-4.659100	-0.547880	5.161151	C	-1.595719	1.748626	-2.086856
P	-2.321310	0.341351	0.003921	C	-4.291593	2.150335	-2.687874
I	-0.000014	-2.700814	-0.000174	H	-4.696947	0.634089	-1.215669
				C	-1.964085	2.697708	-3.039436
TS9C				H	-0.545458	1.592545	-1.863194
C	-2.061922	2.967041	2.581362	C	-3.312682	2.899470	-3.344164
C	-2.323816	2.183783	1.453511	H	-5.341958	2.297966	-2.925404
C	-1.839070	0.871022	1.377034	H	-1.192870	3.273392	-3.543739
C	-1.104045	0.352980	2.456411	H	-3.599393	3.632822	-4.093389
C	-0.841646	1.134311	3.580357	P	-1.993030	-0.186510	-0.129073
C	-1.315176	2.448823	3.641633	Cl	0.122111	-3.924949	-1.441803
H	-2.435242	3.987121	2.625477	Pd	0.080093	-1.301662	-0.577073
H	-2.883263	2.604490	0.623615	H	0.932060	-2.705685	-0.973236
H	-0.696893	-0.651745	2.395374	C	0.718023	3.733872	-0.082071
H	-0.242429	0.725280	4.389051	C	1.022738	2.435741	0.324615
H	-1.098450	3.066848	4.508912	C	1.805512	1.597885	-0.488230
C	-3.452650	-1.243884	0.235054	C	2.274106	2.090631	-1.716314
C	-4.512403	-0.828358	1.057137	C	1.960750	3.389447	-2.123203
C	-3.490357	-2.523175	-0.342016	C	1.181086	4.214530	-1.309268
C	-5.599134	-1.673533	1.284461	H	0.102548	4.359126	0.558385
H	-4.482474	0.152793	1.523373	H	0.637050	2.070893	1.269401
C	-4.581714	-3.364063	-0.115621	H	2.878601	1.458340	-2.359955
H	-2.657758	-2.865925	-0.952311	H	2.328973	3.755353	-3.078165
C	-5.636565	-2.940661	0.695594	H	0.934436	5.222979	-1.630145
H	-6.414464	-1.344938	1.923792	C	3.601323	-0.622498	-0.862898
H	-4.599751	-4.353600	-0.564050	C	4.823409	-0.090350	-0.421247

C	3.591231	-1.482861	-1.969123	C	2.112574	-1.043203	1.347839
C	6.011115	-0.417664	-1.073268	C	1.298822	-0.589952	2.400923
H	4.848510	0.573521	0.437838	C	1.094796	-1.377782	3.532000
C	4.781694	-1.804445	-2.626556	C	1.704695	-2.632919	3.628271
H	2.650182	-1.903653	-2.312698	H	3.008472	-4.056888	2.666246
C	5.991983	-1.274309	-2.178589	H	3.354642	-2.667892	0.651213
H	6.952530	-0.005554	-0.719402	H	0.787754	0.364751	2.314958
H	4.759960	-2.474282	-3.481767	H	0.435757	-1.022622	4.319261
H	6.919400	-1.529115	-2.684625	H	1.533836	-3.256774	4.501520
C	2.375601	-0.196572	1.740848	C	3.438867	1.272529	0.211218
C	2.954052	0.888427	2.416813	C	4.582163	0.993879	0.978165
C	2.043485	-1.350756	2.468587	C	3.226759	2.574940	-0.264205
C	3.186418	0.823059	3.791885	C	5.507970	2.001415	1.247492
H	3.201368	1.796832	1.876189	H	4.739834	-0.007632	1.369640
C	2.283284	-1.418054	3.841431	C	4.157031	3.580805	0.006296
H	1.577860	-2.189094	1.955845	H	2.323782	2.806358	-0.823630
C	2.850851	-0.328452	4.507393	C	5.297441	3.294761	0.758920
H	3.626880	1.674549	4.303917	H	6.389923	1.780248	1.842878
H	2.017743	-2.317011	4.391173	H	3.981031	4.587891	-0.361109
H	3.029115	-0.376189	5.578383	H	6.017527	4.079577	0.974957
P	1.994853	-0.189000	-0.064877	C	2.962962	-1.132335	-1.409269
				C	4.312154	-1.072152	-1.783002
HCl				C	2.134298	-2.111763	-1.986568
Cl	0.000000	0.000000	0.071667	C	4.825069	-1.979923	-2.713916
H	0.000000	0.000000	-1.218333	H	4.963528	-0.318635	-1.351251
				C	2.653941	-3.025395	-2.901436
TS9D				H	1.083864	-2.164428	-1.713110
C	2.528128	-3.084267	2.595110	C	4.001001	-2.959685	-3.270043
C	2.732459	-2.295075	1.459002	H	5.871590	-1.920257	-3.001189

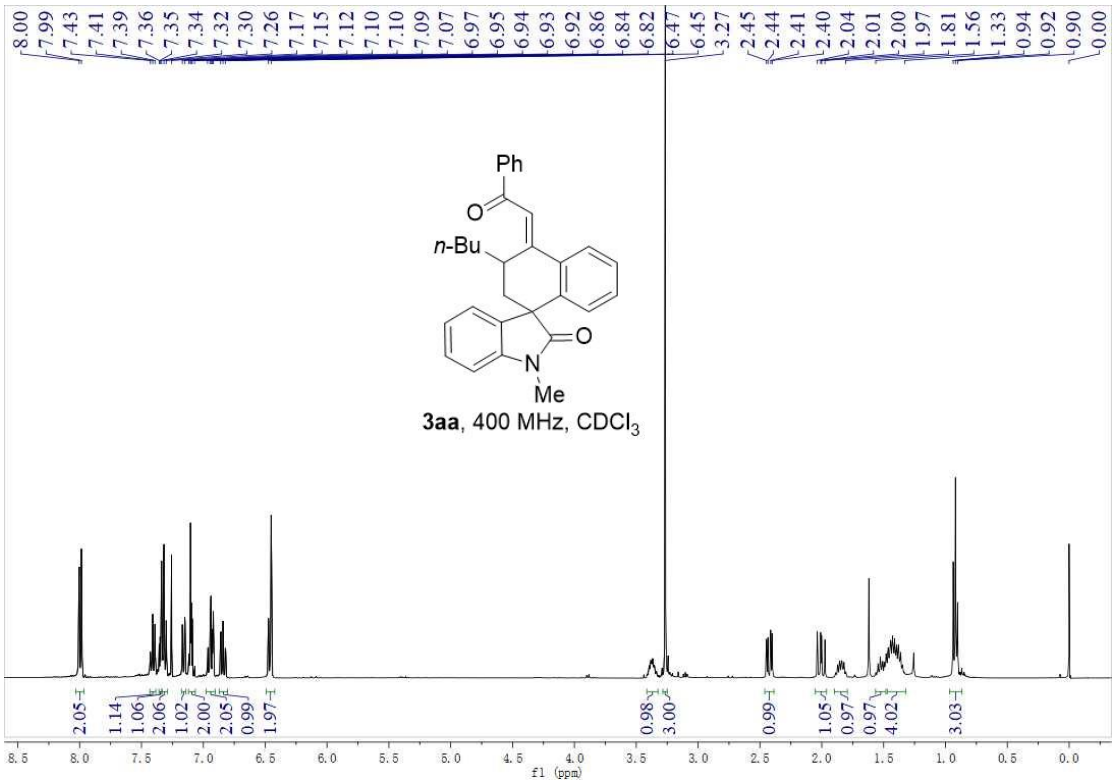
H	2.002154	-3.782175	-3.329606	C	-2.105421	0.700900	2.401560
H	4.404350	-3.665447	-3.991371	C	-3.003384	-1.541240	3.803589
P	2.183408	-0.005127	-0.181113	H	-2.942150	-2.567280	1.914955
Pd	-0.087235	0.601296	-0.629892	C	-2.335517	0.782262	3.775361
H	-0.930439	2.023228	-0.454551	H	-1.743286	1.571830	1.861809
C	-0.254973	-4.274645	-0.040835	C	-2.779539	-0.339937	4.480212
C	-0.684169	-3.000635	0.326248	H	-3.348551	-2.417212	4.346545
C	-1.616826	-2.306743	-0.467024	H	-2.160016	1.720716	4.294130
C	-2.104785	-2.915224	-1.633180	H	-2.950075	-0.278488	5.551783
C	-1.666336	-4.189900	-1.999990	P	-1.973268	-0.538900	-0.092821
C	-0.740273	-4.872180	-1.207789	I	-0.908623	3.934802	-0.471988
H	0.471483	-4.789560	0.581401				
H	-0.283044	-2.541023	1.223295	HI			
H	-2.823686	-2.392729	-2.257336	I	0.000000	0.000000	0.030366
H	-2.051411	-4.648854	-2.906795	H	0.000000	0.000000	-1.609410
H	-0.398856	-5.862411	-1.497212				
C	-3.597502	-0.210451	-0.883288	**5aa**			
C	-4.753869	-0.928808	-0.538475	C	-1.628654	0.578214	0.855503
C	-3.673282	0.792621	-1.859006	C	-1.953561	-0.472549	-0.241451
C	-5.965478	-0.650414	-1.167865	C	-1.304720	-1.720145	0.321454
H	-4.705774	-1.701094	0.224398	C	-1.166047	-2.994916	-0.206810
C	-4.890083	1.070729	-2.487525	C	-0.395907	-3.944684	0.482636
H	-2.782771	1.360404	-2.114180	C	0.232794	-3.603610	1.681876
C	-6.034107	0.349696	-2.144067	C	0.109449	-2.317039	2.223051
H	-6.857247	-1.209132	-0.896350	C	-0.662469	-1.395266	1.525162
H	-4.940946	1.854079	-3.238501	H	-1.639286	-3.251670	-1.150893
H	-6.981067	0.567575	-2.630749	H	-0.286261	-4.946777	0.078632
C	-2.325617	-0.504634	1.715428	H	0.831802	-4.343125	2.206049
C	-2.782047	-1.623581	2.427734	H	0.613787	-2.047320	3.145342

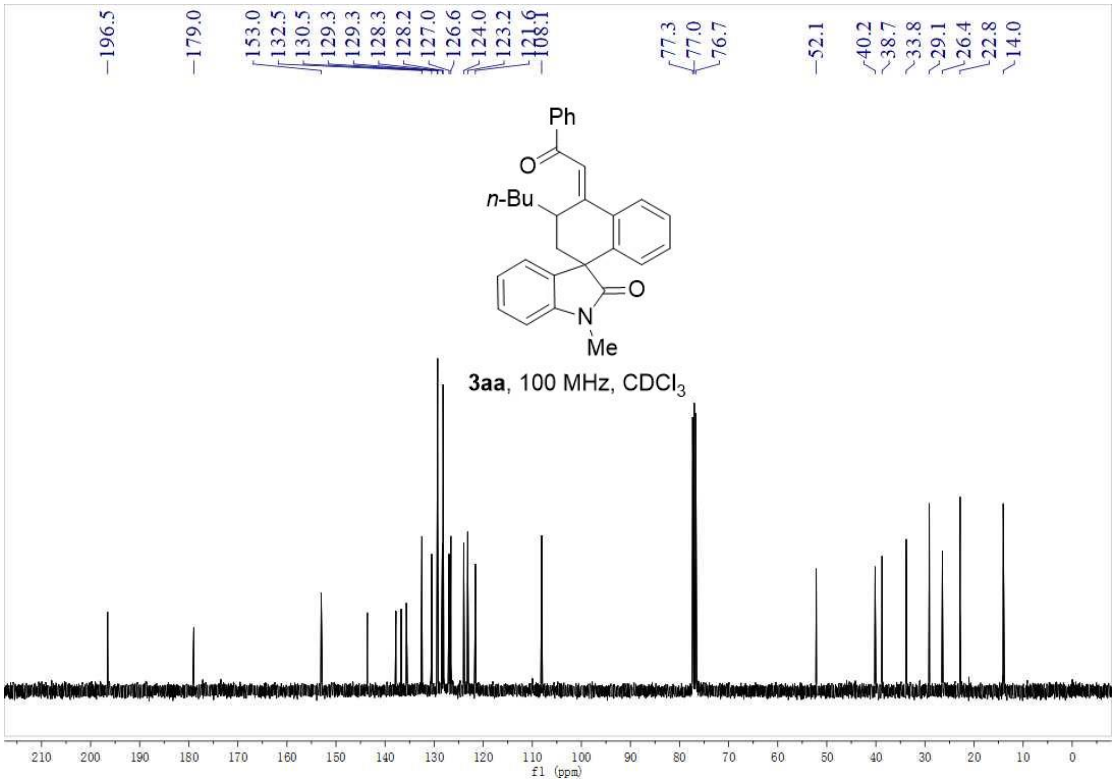
N	-0.894462	-0.050253	1.840829	H	0.869197	3.399889	-1.990449
C	-0.330171	0.640804	2.981124	C	0.206671	4.984718	0.214559
H	0.764076	0.665158	2.916277	H	0.306181	2.976201	0.990196
H	-0.717766	1.660541	2.974142	H	1.834644	3.554627	0.320875
H	-0.623020	0.144031	3.912687	C	0.527064	5.692193	1.534695
O	-1.924970	1.762506	0.844221	H	0.621156	5.561887	-0.624811
C	-3.464433	-0.541859	-0.481890	H	-0.881702	4.958344	0.066570
C	-4.149273	0.613527	-0.894359	H	0.129905	6.713638	1.551248
C	-4.198538	-1.720169	-0.300128	H	0.091921	5.150369	2.383589
C	-5.521125	0.581766	-1.136644	H	1.610370	5.750852	1.698767
H	-3.608689	1.548375	-0.989369	C	3.829941	-0.572029	-0.712460
C	-5.573275	-1.752268	-0.546748	C	4.902640	0.336883	-0.697130
H	-3.703113	-2.620094	0.045815	C	4.093571	-1.932766	-0.467461
C	-6.240018	-0.604159	-0.971060	C	6.200797	-0.106393	-0.452832
H	-6.030142	1.489115	-1.451226	H	4.707347	1.388352	-0.880694
H	-6.120629	-2.679975	-0.400772	C	5.393375	-2.369636	-0.229868
H	-7.309244	-0.629338	-1.163856	H	3.271568	-2.643025	-0.446595
C	-1.199336	-0.023842	-1.546449	C	6.455024	-1.460015	-0.221520
H	-1.364254	-0.804677	-2.297928	H	7.018534	0.609702	-0.446007
H	-1.678905	0.884285	-1.919372	H	5.578676	-3.424158	-0.042173
C	0.269529	0.215165	-1.342593	H	7.468507	-1.803138	-0.032510
C	1.293904	-0.780309	-1.204608				
C	0.894066	1.426253	-1.183557				
C	2.469209	-0.123888	-0.965851				
H	1.157364	-1.849834	-1.264528				
O	2.231552	1.230602	-0.962822				
C	0.422025	2.838978	-1.156320				
C	0.747200	3.552795	0.169611				
H	-0.661847	2.840162	-1.305590				

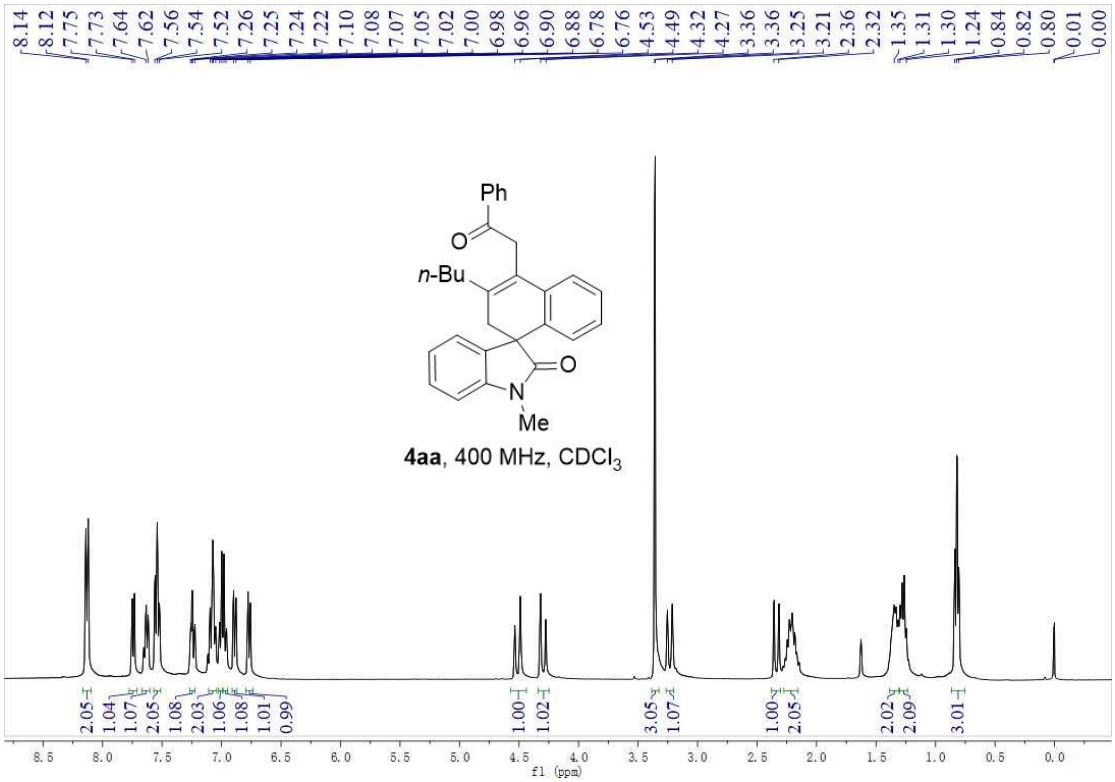
12) References

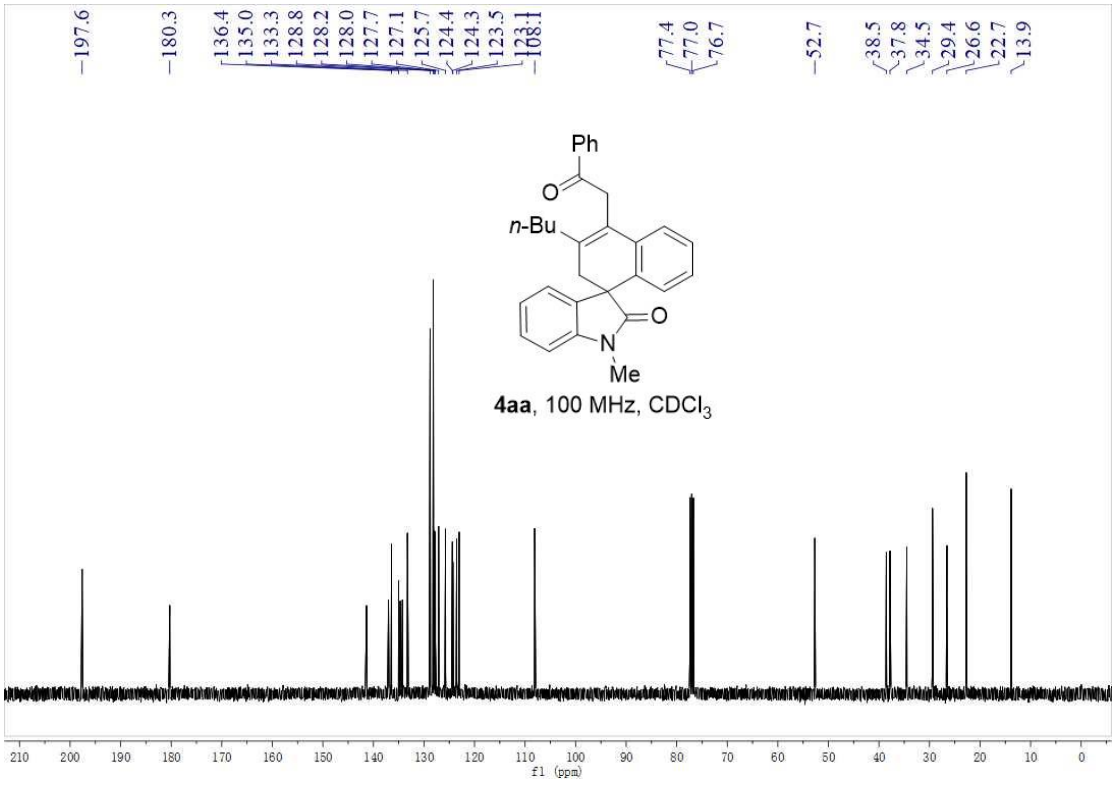
1. H. Y. Kim, J.-Y. Li, K. Oh, *J. Org. Chem.* **2012**, *77*, 11132-11145.
2. (a) H. Yoon, A. Lossouarn, F. Landau, M. Lautens, *Org. Lett.* **2016**, 18, 6324-6327; (b) C. Shao, Z. Wu, X. Ji, B. Zhou, Y. Zhang, *Chem. Commun*. **2017**, 53, 10429-10432; (c) G. Xiao, L. Chen, G. Deng, J. Liu, Y. Liang, *Tetrahedron Lett*. **2018**, 59, 1836-1840.
3. (a) T. Kashiwabara, M. Tanaka, *Adv. Synth. Catal.* **2011**, *353*, 1485-1490; (b) Y. Zhang, J. Zhang, Y. Yuan, L. Liu, B. Chen, T. Sun, *Eur. J. Org. Chem*. **2020**, 1976-1986; (c) R. Hou, Z. Wang, J. Peng, Y. Yuan, J. Zhang, D. Wang, T. Sun, *Asian J. Org. Chem.* **2021**, 10, 3334-3342.
4. Gaussian 09, Revision E.01, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A.; Peralta, Jr., J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Keith, T.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, O.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; and Fox, D. J. Gaussian, Inc., Wallingford CT, **2013**.
5. (a) A. D. Becke, *J. Chem. Phys.* **1993**, 98, 5648-5456; (b) C. Lee, W. Yang, R. G. Parr, *Phys. Rev. B*, **1988**, *37*, 785-789.
6. S. Grimme, J. Antony, S. Ehrlich, H. Krieg, *J. Chem. Phys.* **2010**, *132*, 154104-154123.
7. (a) M. Dolg, U. Wedig, H. Stoll, H. Preuss, *J. Chem. Phys.* **1987**, *86*, 866-872; (b) A. Nicklass, M. Dolg, H. Stoll, H. Preuss, *J. Chem. Phys.* **1995**, *102*, 8942-8952.
8. (a) R. Ditchfield, W. J. Hehre, J. A. Pople, *J. Chem. Phys.* **1971**, *54*, 724-728; (b) W. J. Hehre, R. Ditchfield, J. A. Pople, *J. Chem. Phys.* **1972**, *56*, 2257-2261; (c) P. C. Hariharan, J. A. Pople, *Theor. Chem. Acc.* **1973**, *28*, 213-217.
9. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc.* **2008**, *120*, 215-241.
10. (a) T. Clark, J. Chandrasekhar, G. W. Spitznagel, P. Von R. Schleyer, *J. Comput. Chem.* **1983**, *4*, 294-301; (b) R. Krishnan, J. S. Binkley, R. Seeger, J. A. Pople, *J. Chem. Phys.* **1980**, *72*, 650-654.
11. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*. **2009**, *113*, 6378-6396.
12. C. Y. Legault, CYL View, version 1.0 b; Universite de Sherbrooke, Sherbrooke, Quebec, Canada, **2009**; http://www.cylview.org.

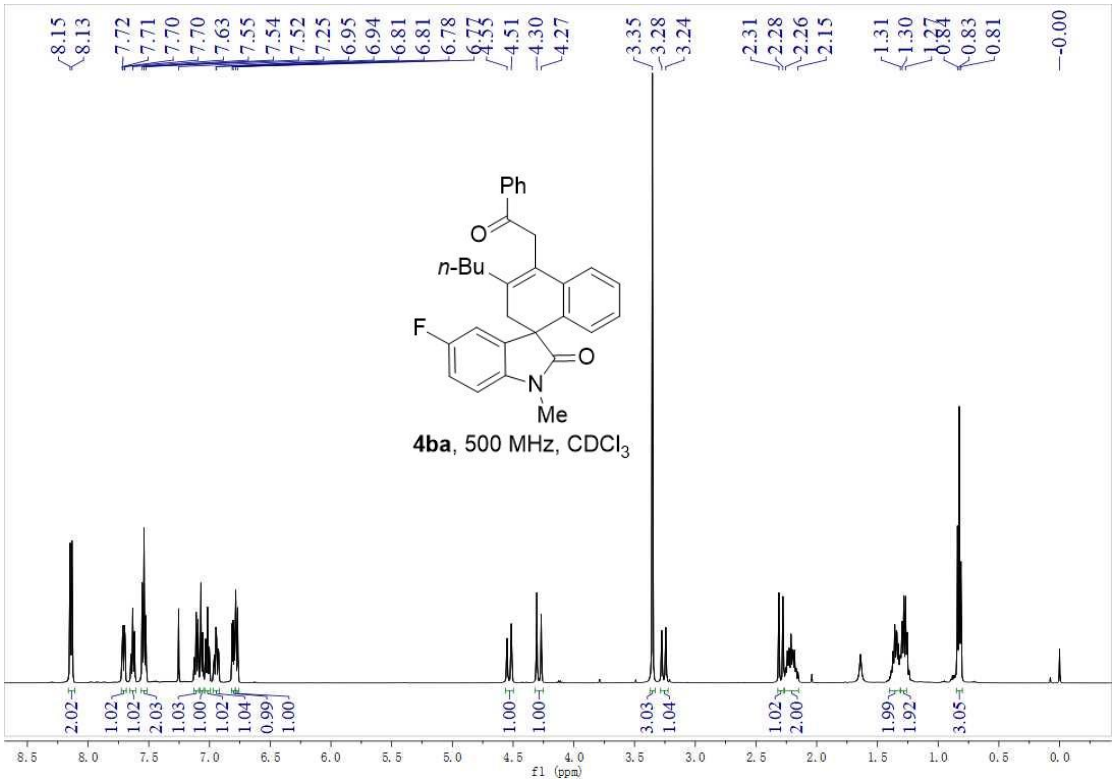
13) NMR Spectra

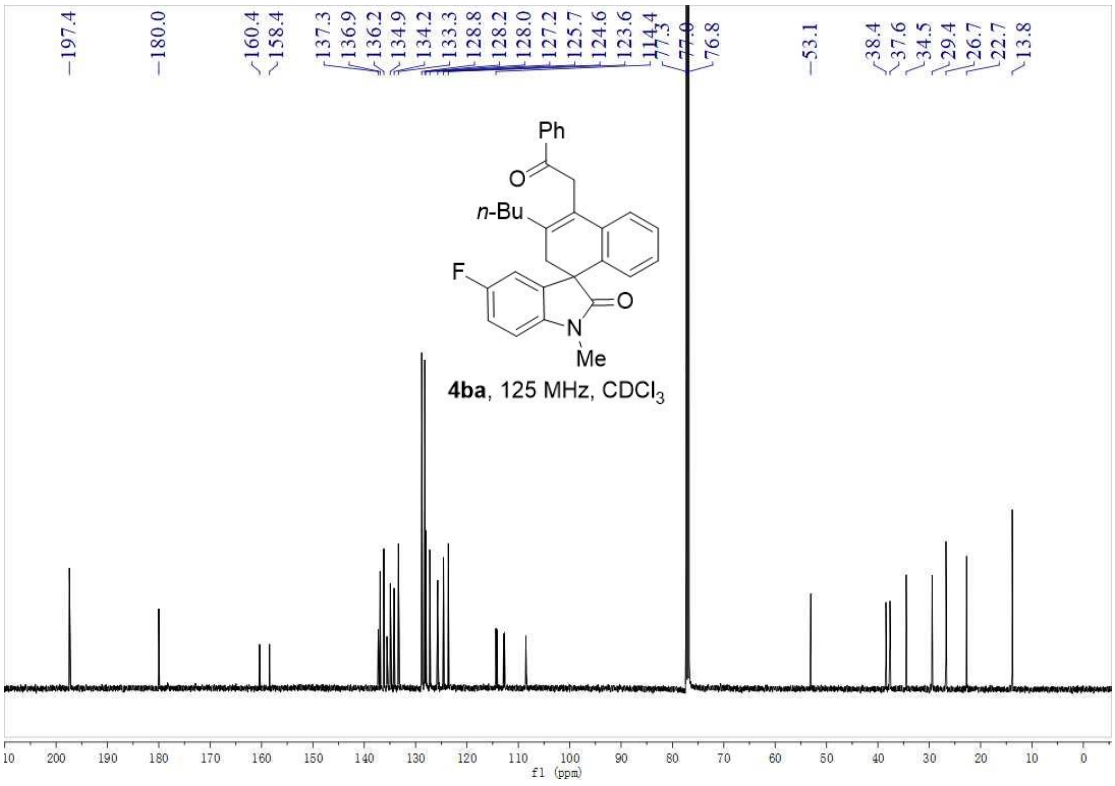


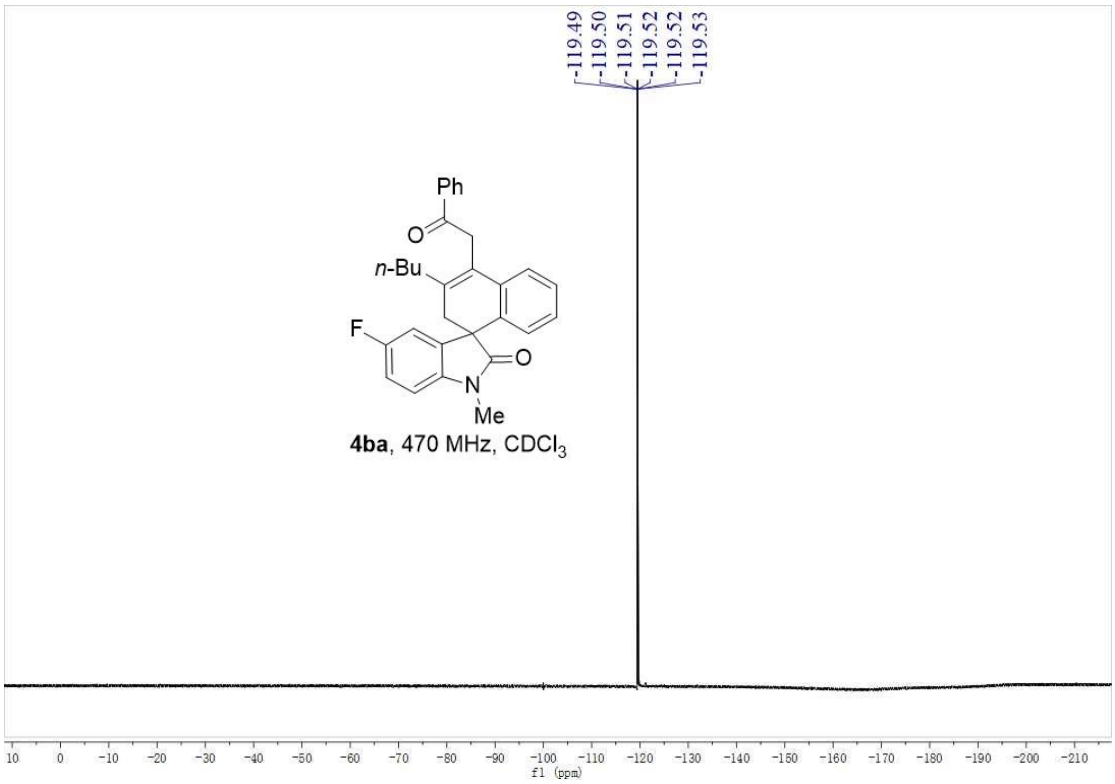


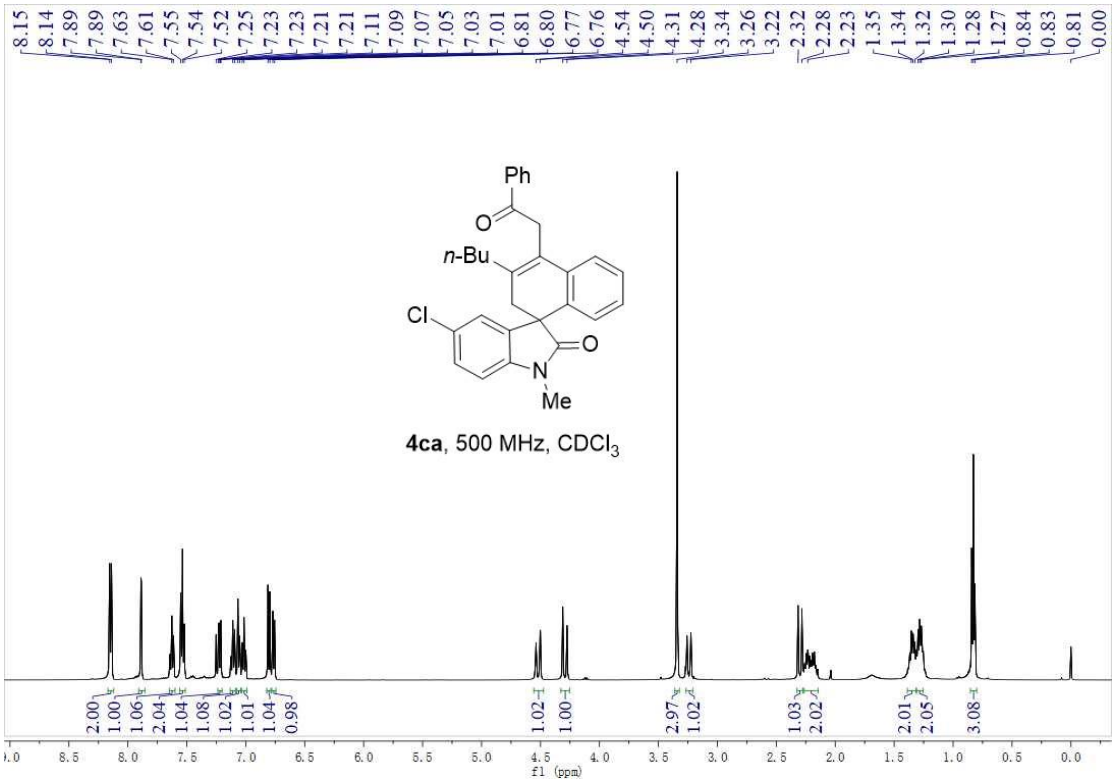

Ph
O
n-Bu
O
N
Me
4aa, 400 MHz, CDCl3
f1 (ppm)

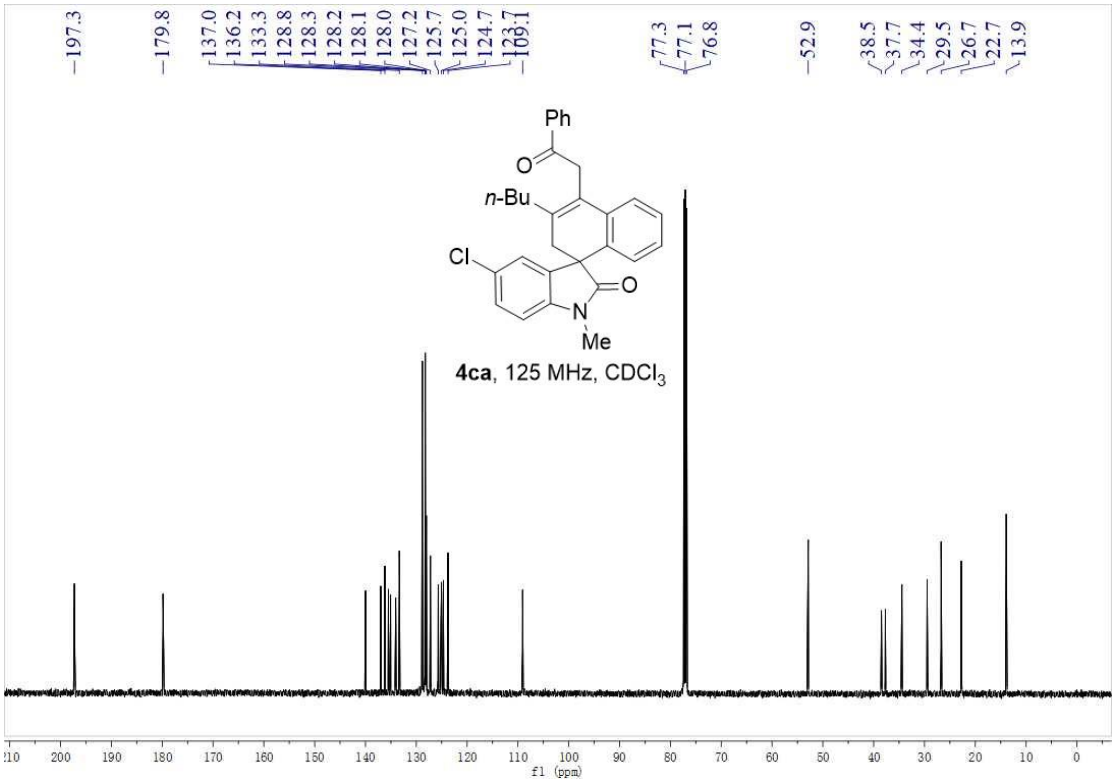

Ph
O
n-Bu
O
N
Me
4aa, 100 MHz, CDCl3
f1 (ppm)

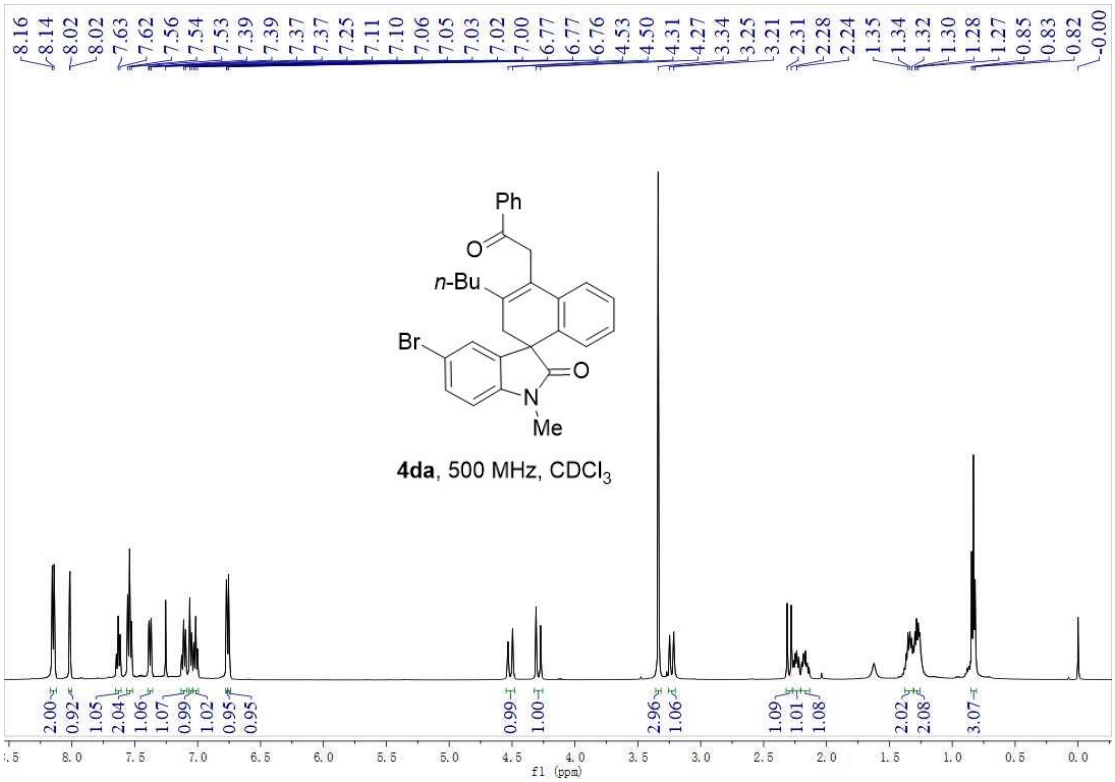

8.15
8.13
7.72
7.71
7.70
7.70
7.63
7.55
7.54
7.52
7.25
6.95
6.94
6.81
6.81
6.78
4.51
4.30
4.27
3.35
3.28
3.24
2.31
2.28
2.26
2.15
1.31
1.30
0.84
0.83
0.81
-0.00
Ph
O
n-Bu
F
O
N
Me
4ba, 500 MHz, CDCl3
2.02
1.02
1.02
2.03
1.03
1.00
1.02
1.04
0.99
1.00
1.00
1.00
3.03
1.04
1.02
2.00
1.99
1.92
3.05
f1 (ppm)

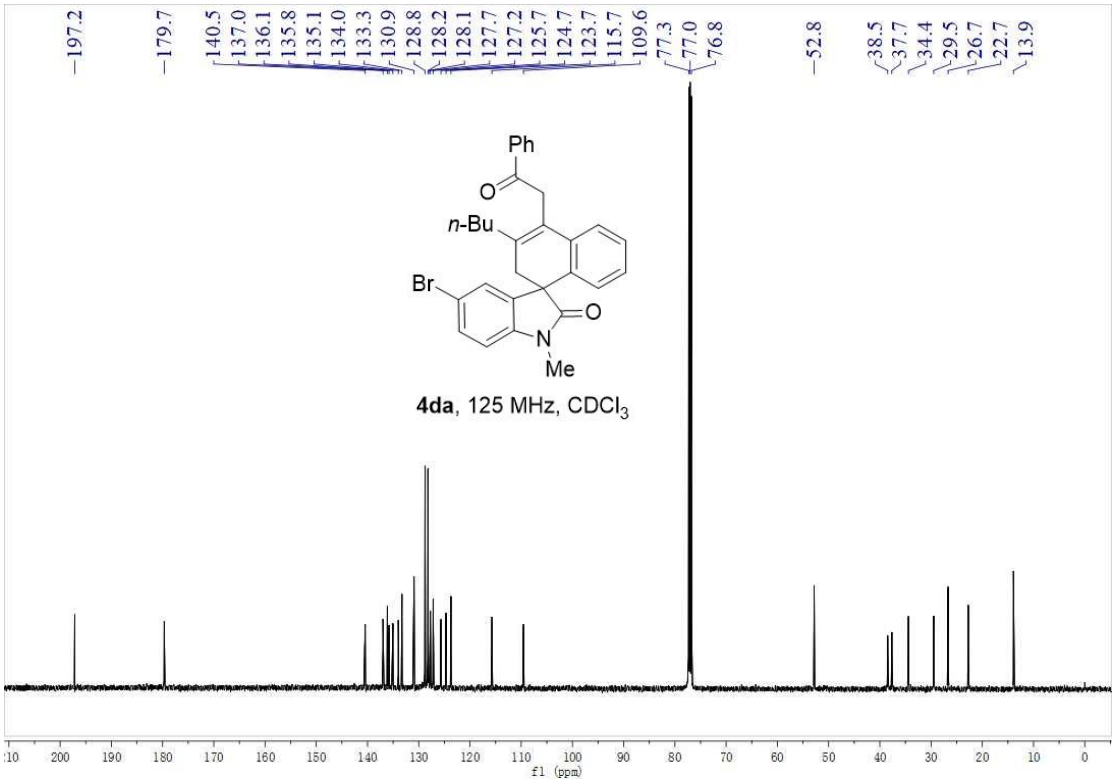

197.4
180.0
160.4
158.4
137.3
136.9
136.2
134.9
134.2
133.3
128.8
128.2
128.0
127.2
125.7
124.6
123.6
114.4
77.3
77.0
76.8
53.1
38.4
37.6
34.5
29.4
26.7
22.7
13.8
Ph
O
n-Bu
F
O
N
Me
4ba, 125 MHz, CDCl3
f1 (ppm)

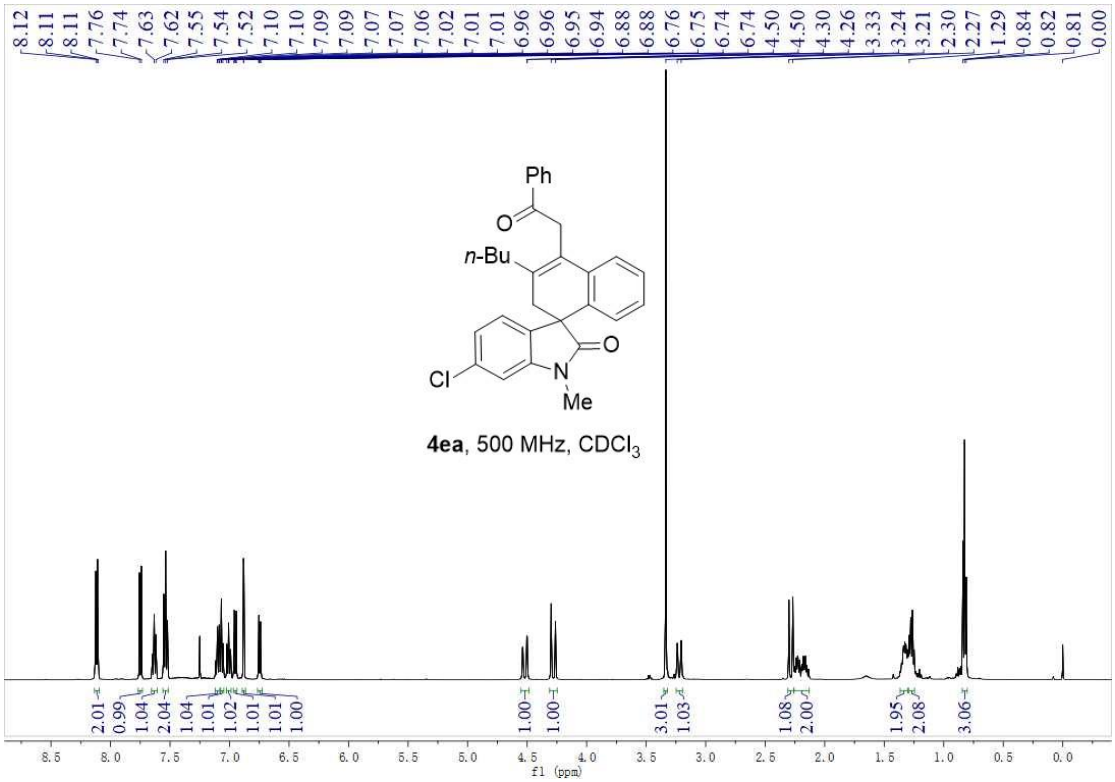

-119.49
-119.50
-119.51
-119.52
-119.52
-119.53
Ph
O
n-Bu
F
O
N
Me
4ba, 470 MHz, CDCl3
10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210
f1 (ppm)

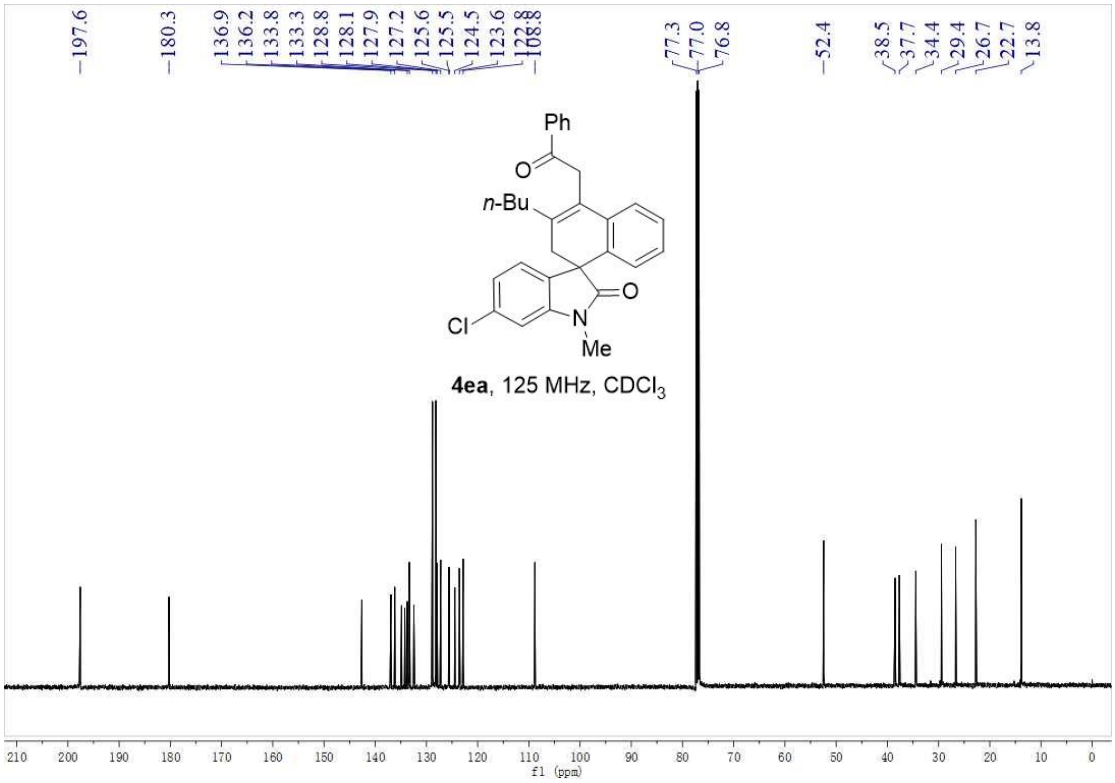

Ph
O
n-Bu
Cl
O
N
Me
4ca, 500 MHz, CDCl3
f1 (ppm)

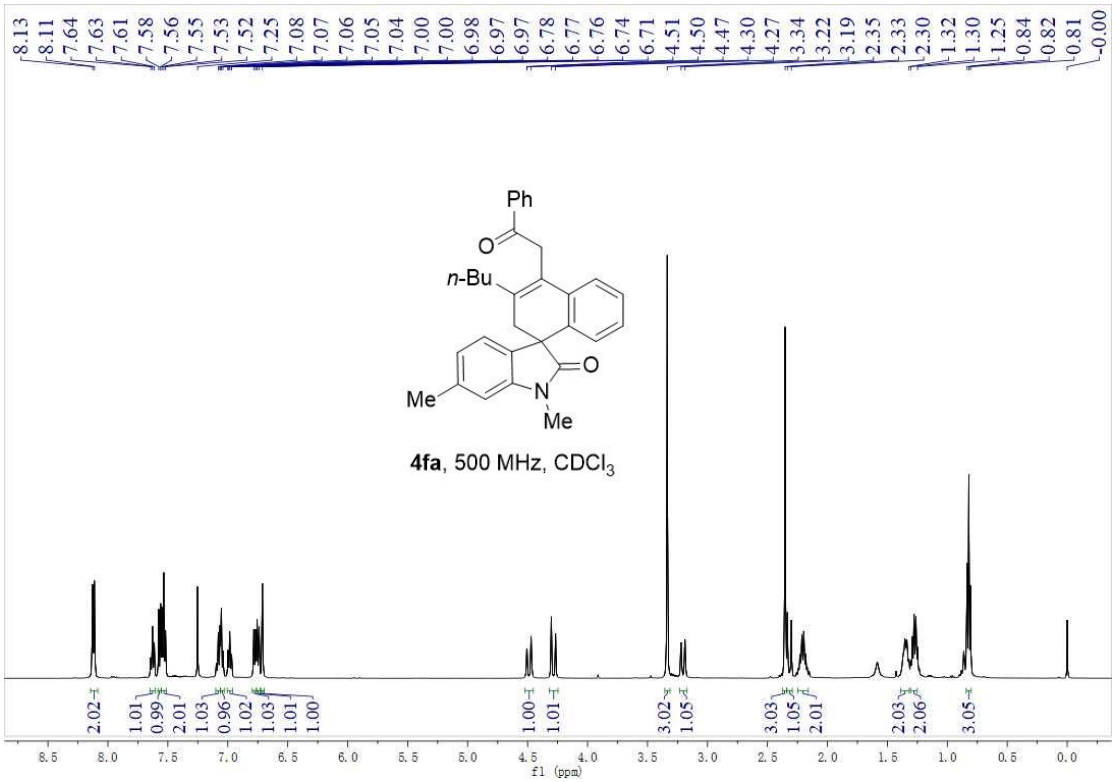

Ph
O
n-Bu
Cl
O
N
Me
4ca, 125 MHz, CDCl3
f1 (ppm)

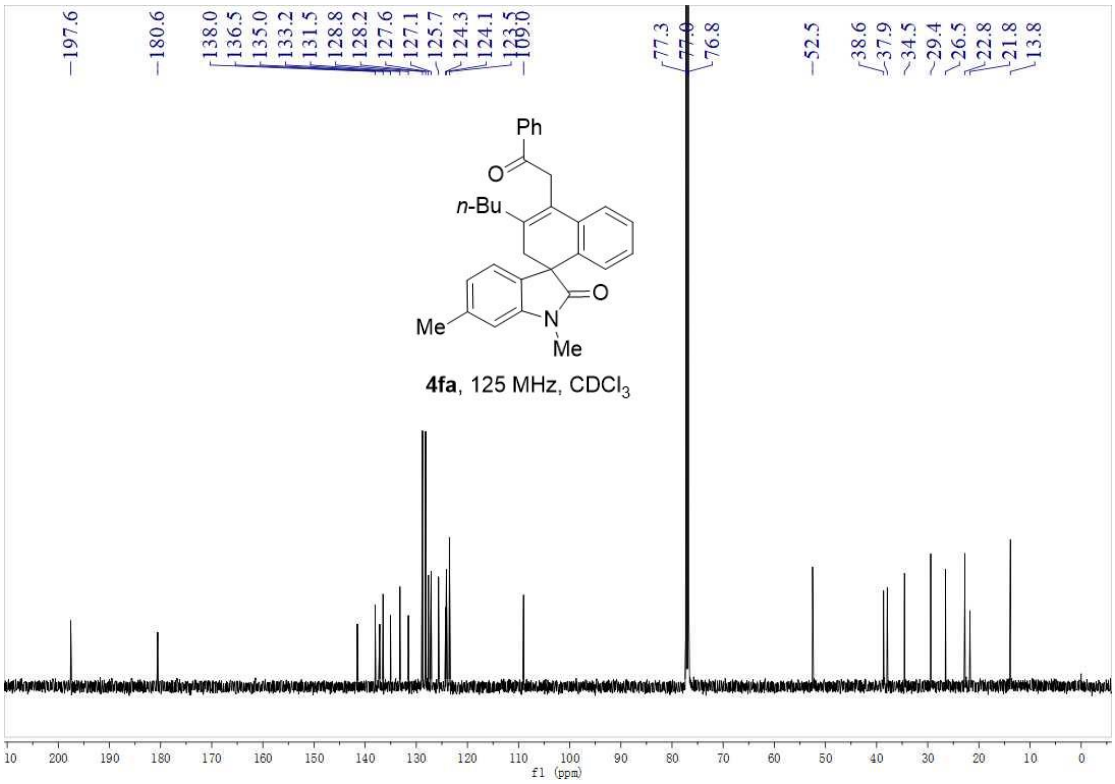

Ph
O
n-Bu
Br
O
N
Me
4da, 500 MHz, CDCl3
f1 (ppm)

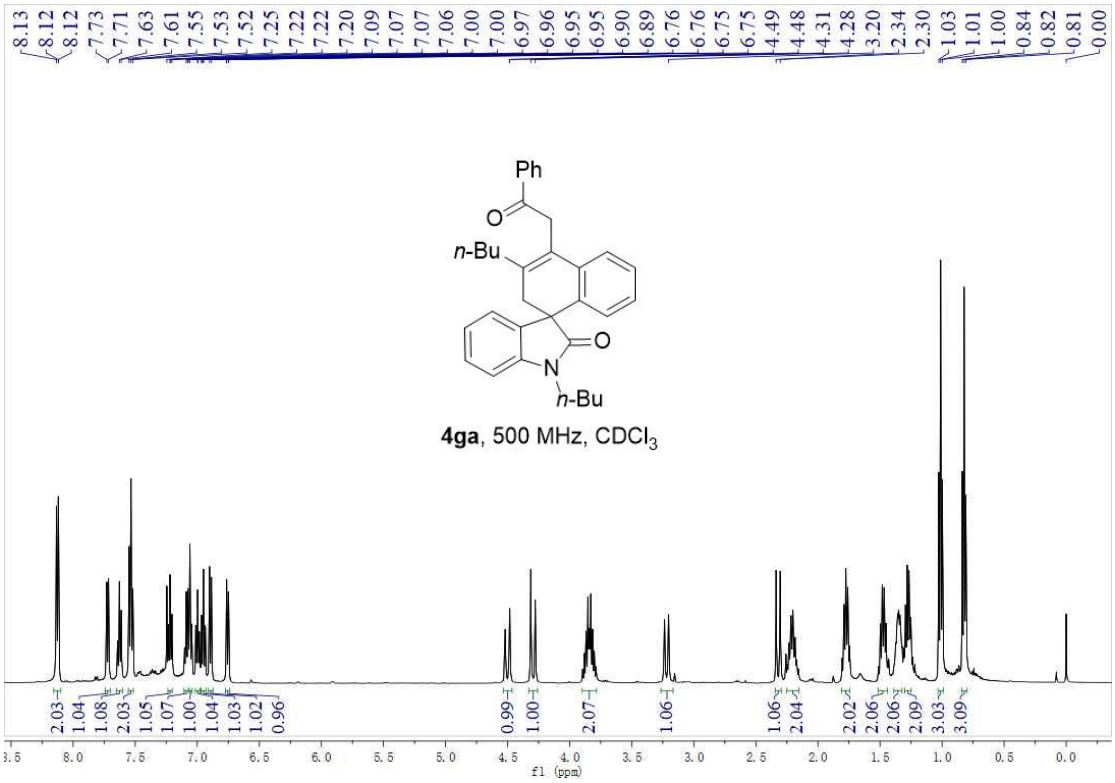

Ph
O
n-Bu
Br
O
N
Me
4da, 125 MHz, CDCl3
f1 (ppm)

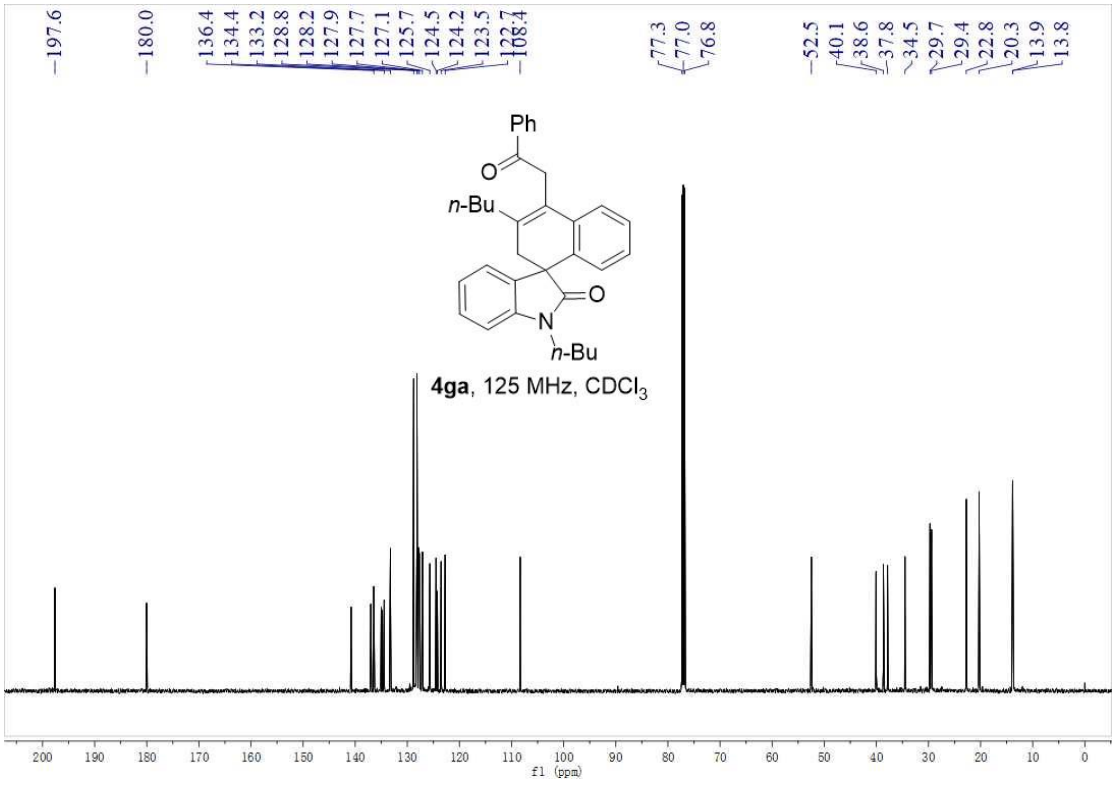

Ph
O
n-Bu
O
Cl
N
Me
4ea, 500 MHz, CDCl3
f1 (ppm)

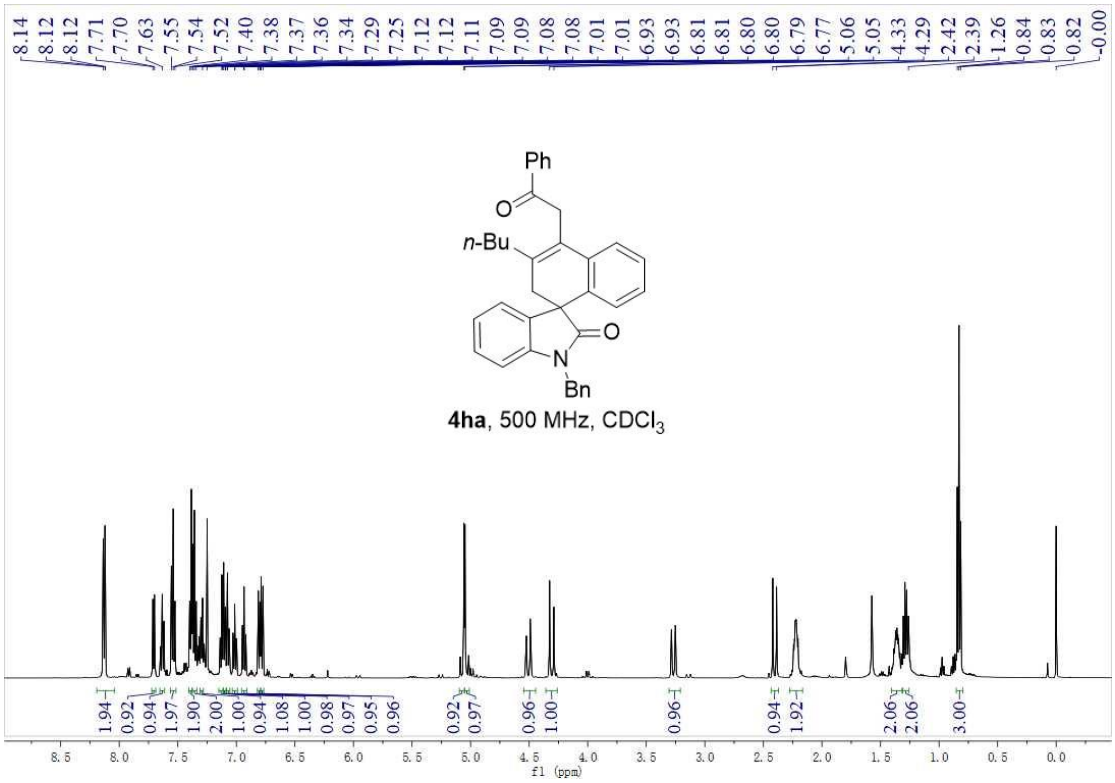

Ph
O
n-Bu
O
Cl
N
Me
4ea, 125 MHz, CDCl3
f1 (ppm)

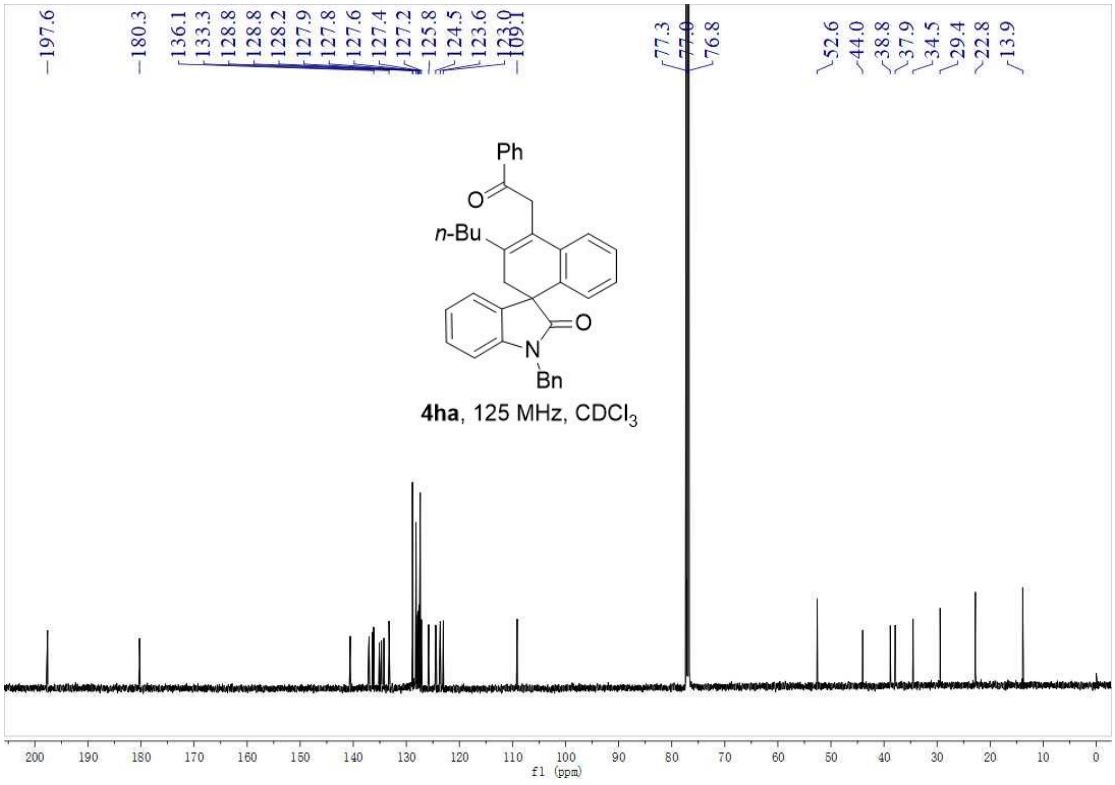

Ph
O
n-Bu
O
N
Me
Me
4fa, 500 MHz, CDCl3
f1 (ppm)

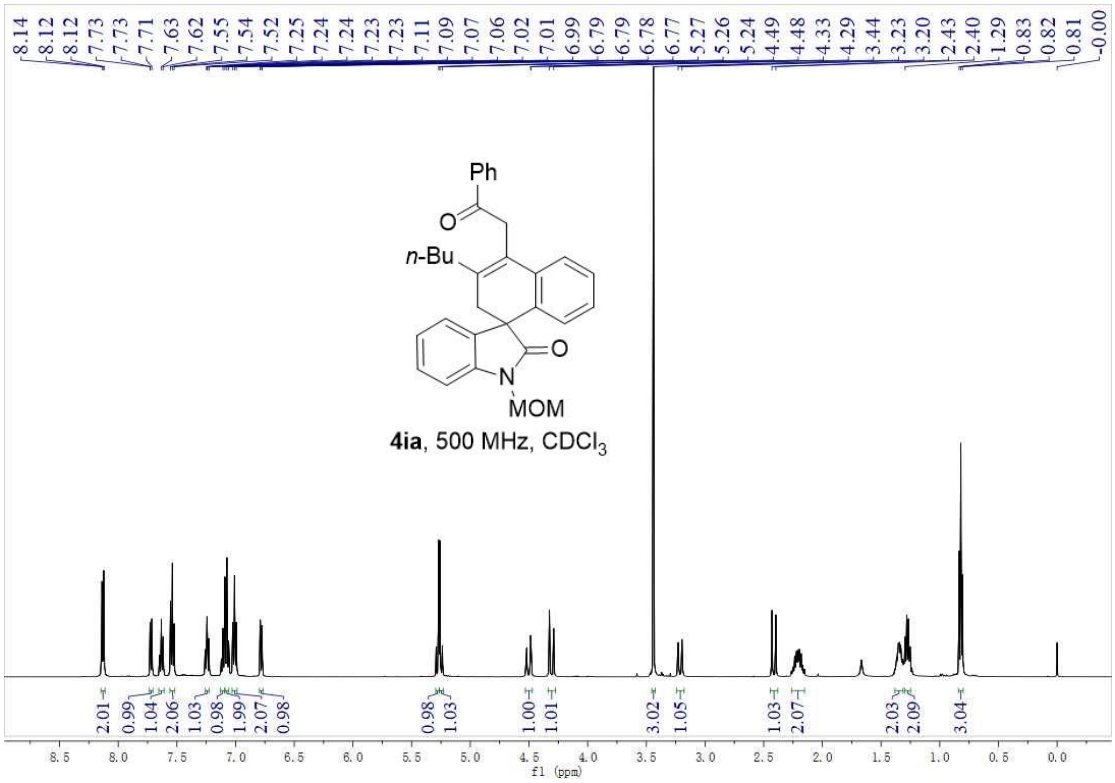

Ph
O
n-Bu
O
N
Me
Me
4fa, 125 MHz, CDCl3
f1 (ppm)

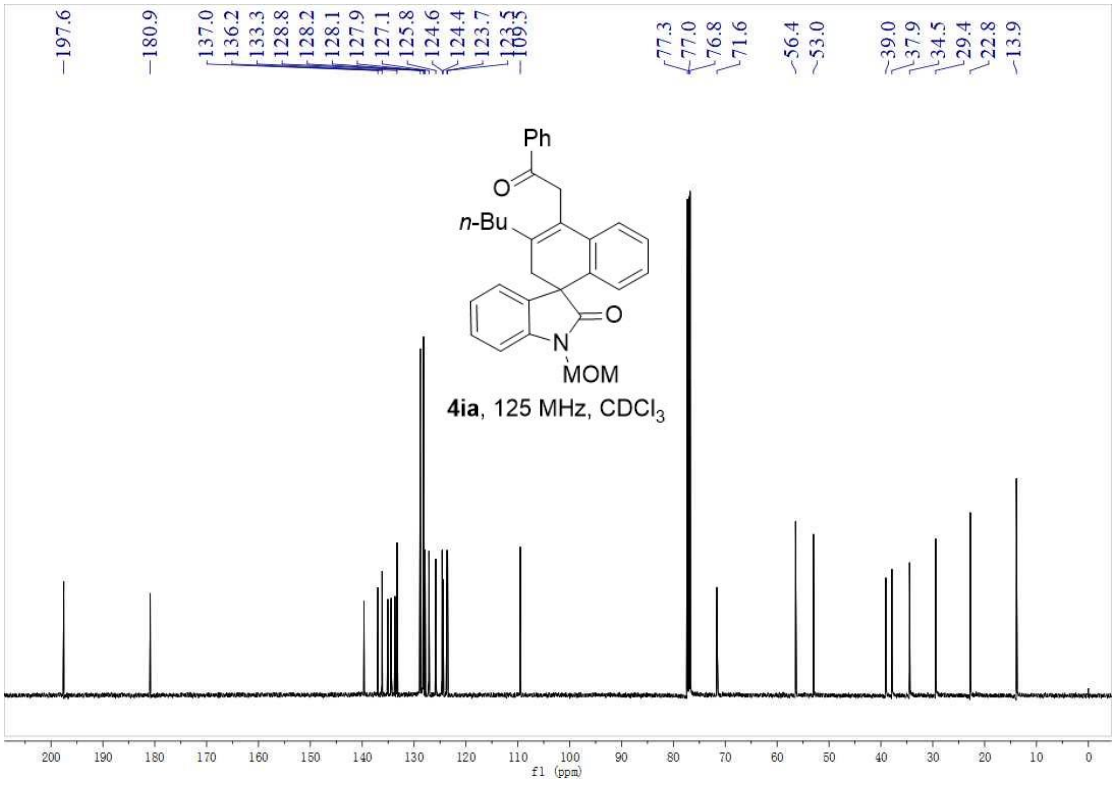

Ph
O
n-Bu
O
N
n-Bu
4ga, 500 MHz, CDCl3
f1 (ppm)

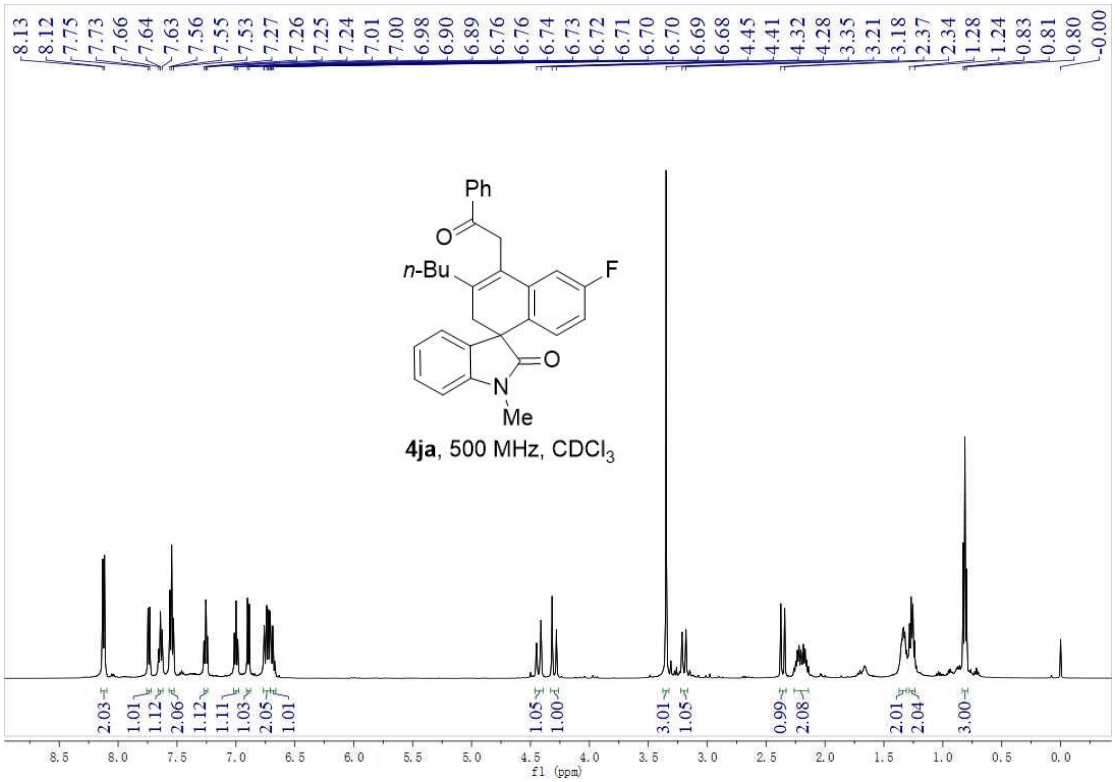

Ph
O
n-Bu
O
N
n-Bu
4ga, 125 MHz, CDCl3
f1 (ppm)

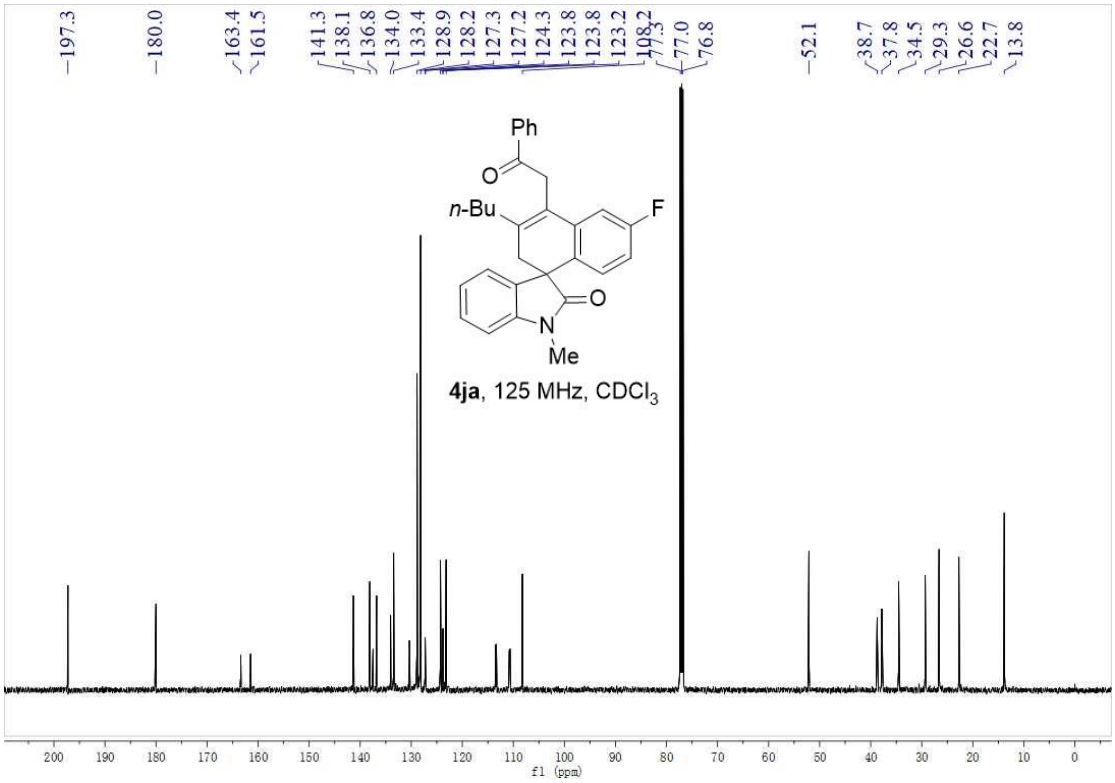

Ph
O
n-Bu
O
N
Bn
4ha, 500 MHz, CDCl3
f1 (ppm)

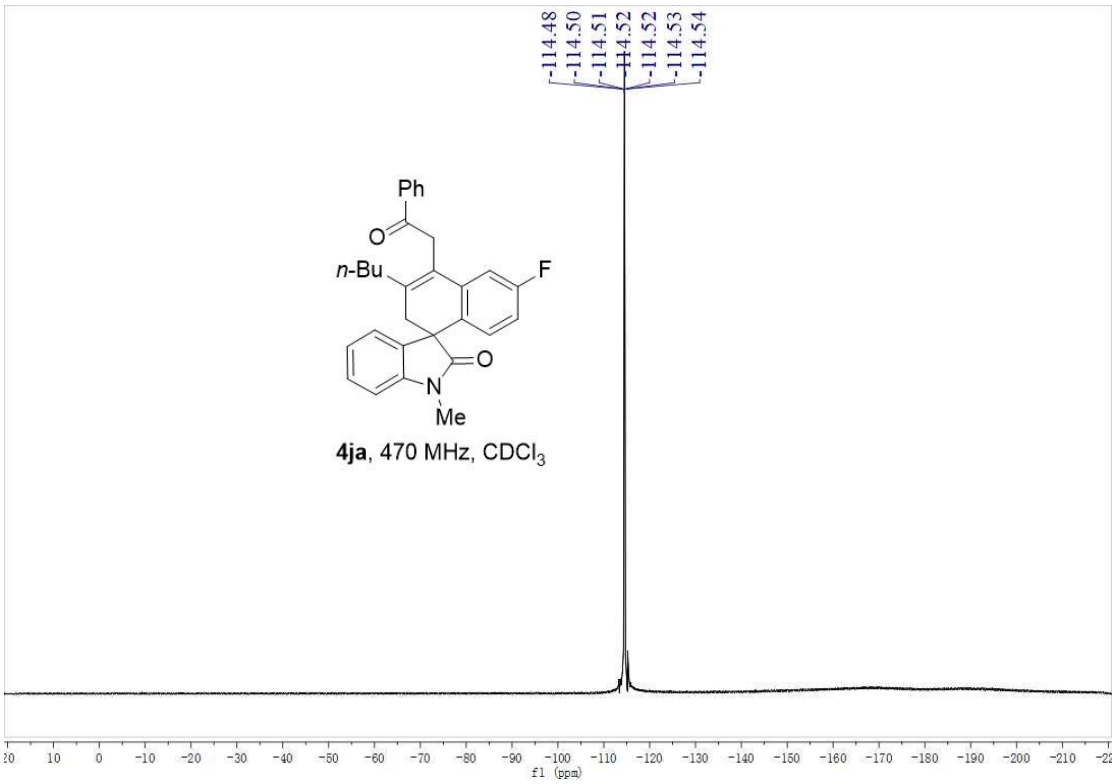

Ph
O
n-Bu
O
N
Bn
4ha, 125 MHz, CDCl3
f1 (ppm)

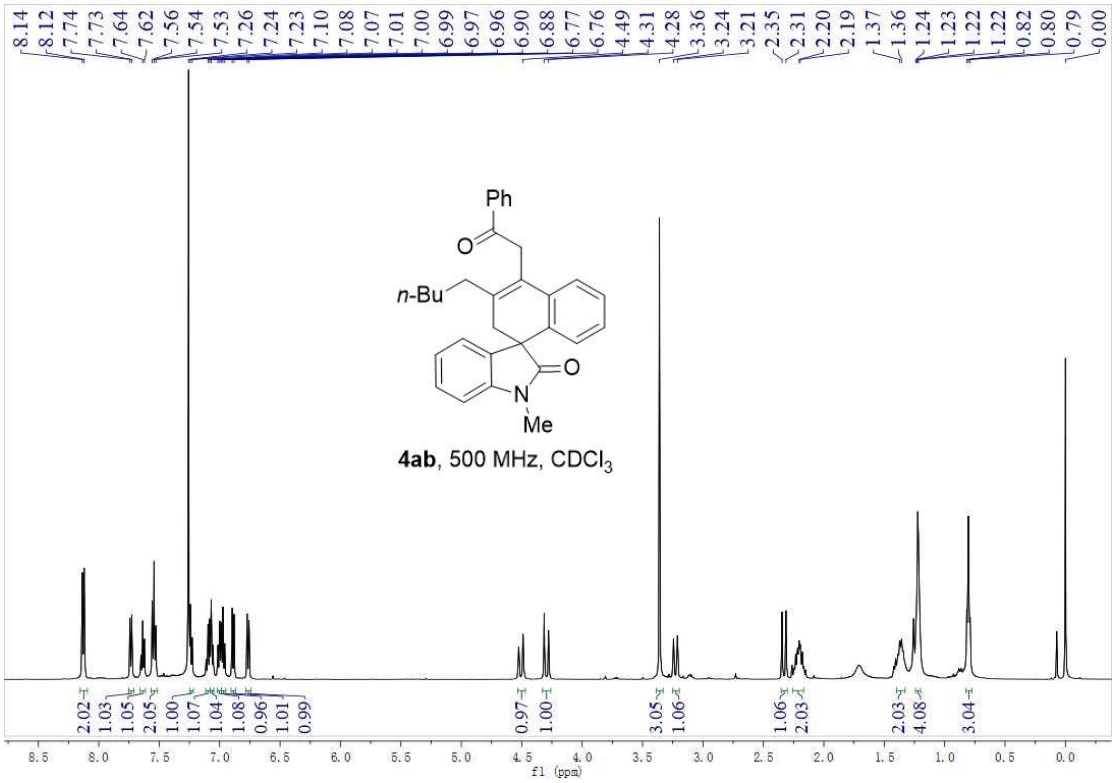

Ph
O
n-Bu
O
N
MOM
4ia, 500 MHz, CDCl3
f1 (ppm)

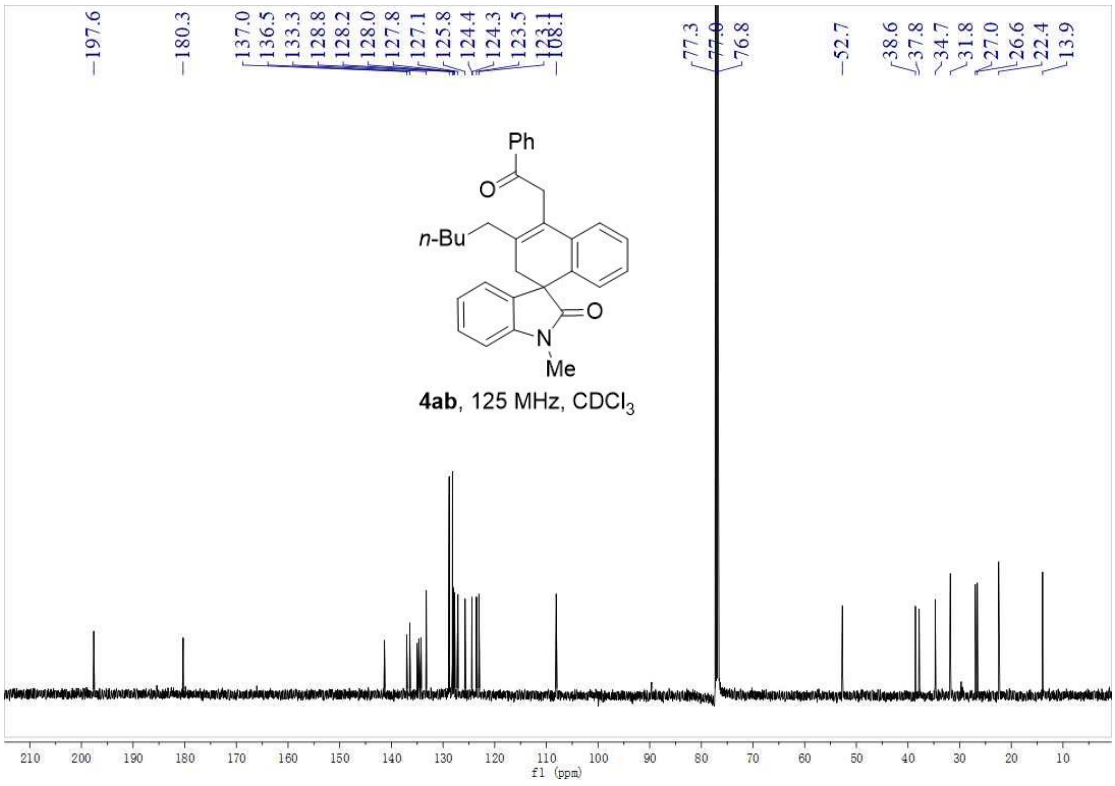

Ph
O
n-Bu
O
N
MOM
4ia, 125 MHz, CDCl3
f1 (ppm)

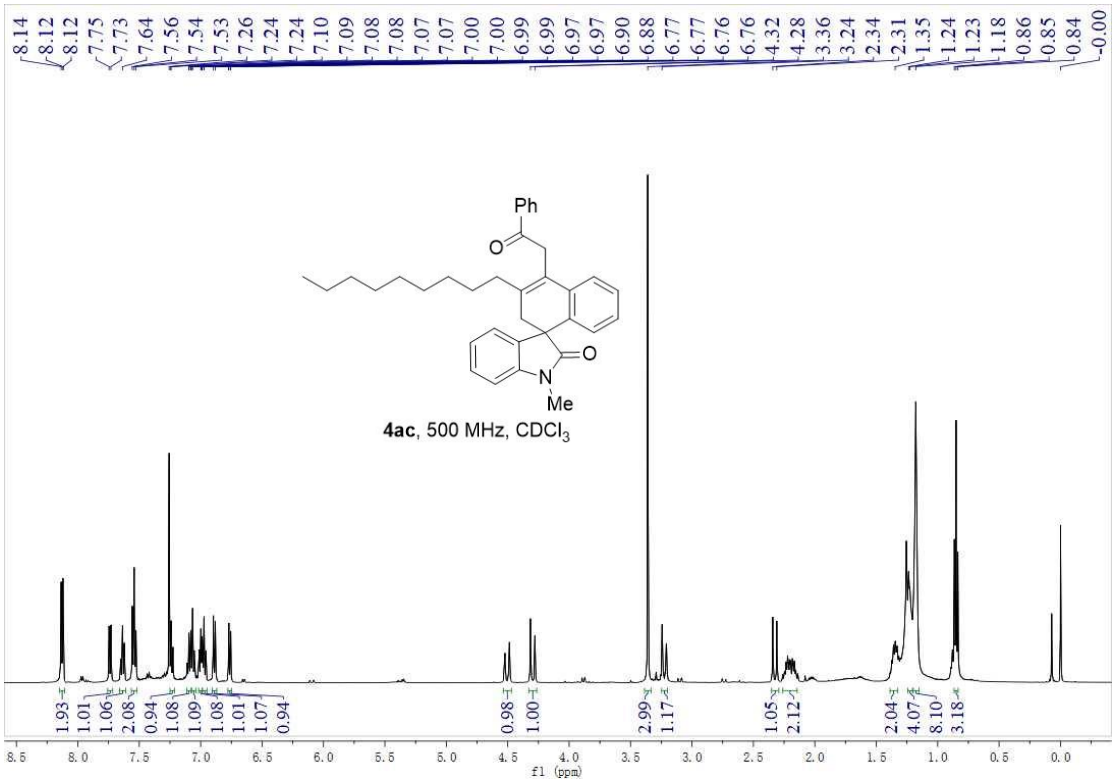

Ph
O
n-Bu
F
O
N
Me
4ja, 500 MHz, CDCl3
f1 (ppm)

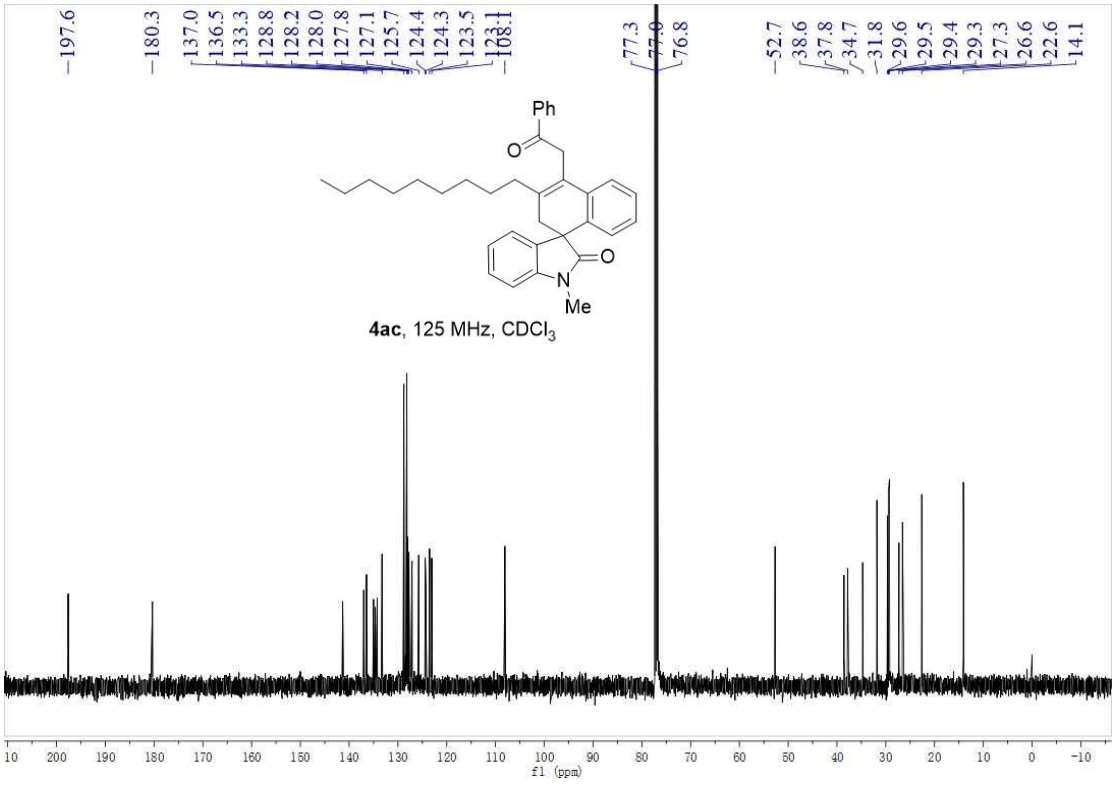

Ph
O
n-Bu
F
O
N
Me
4ja, 125 MHz, CDCl3
f1 (ppm)

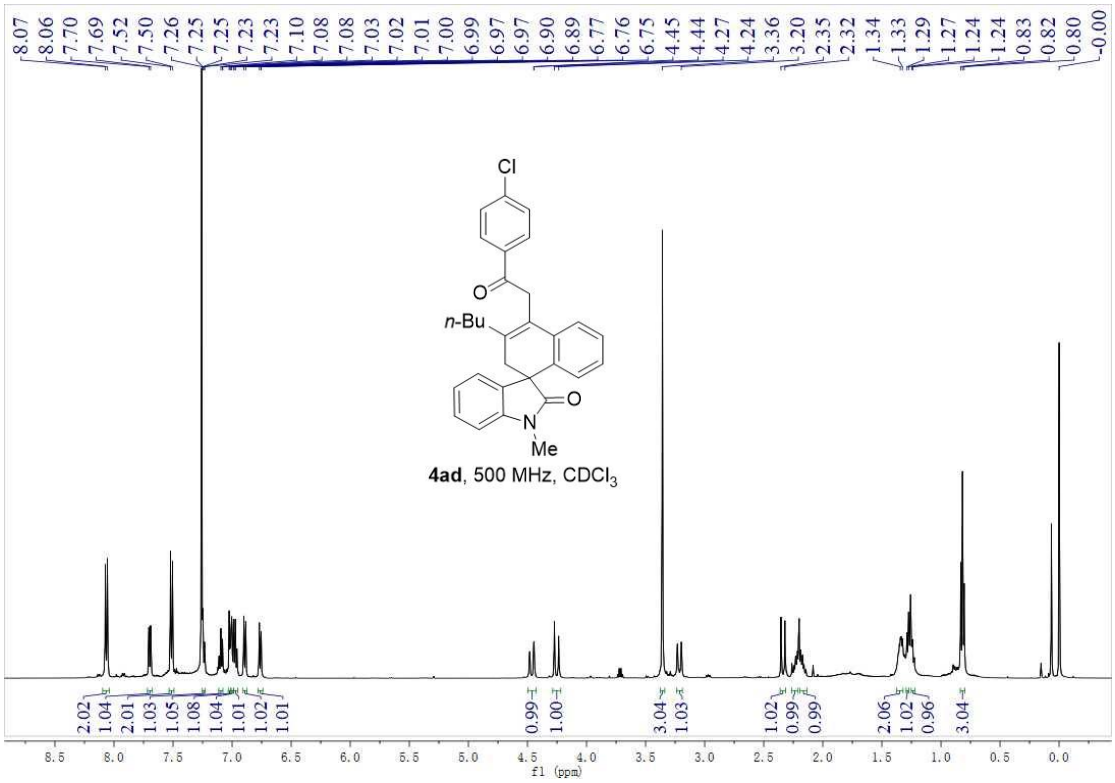

-114.48
-114.50
-114.51
-114.52
-114.52
-114.53
-114.54
Ph
O
n-Bu
F
O
N
Me
4ja, 470 MHz, CDCl3
f1 (ppm)

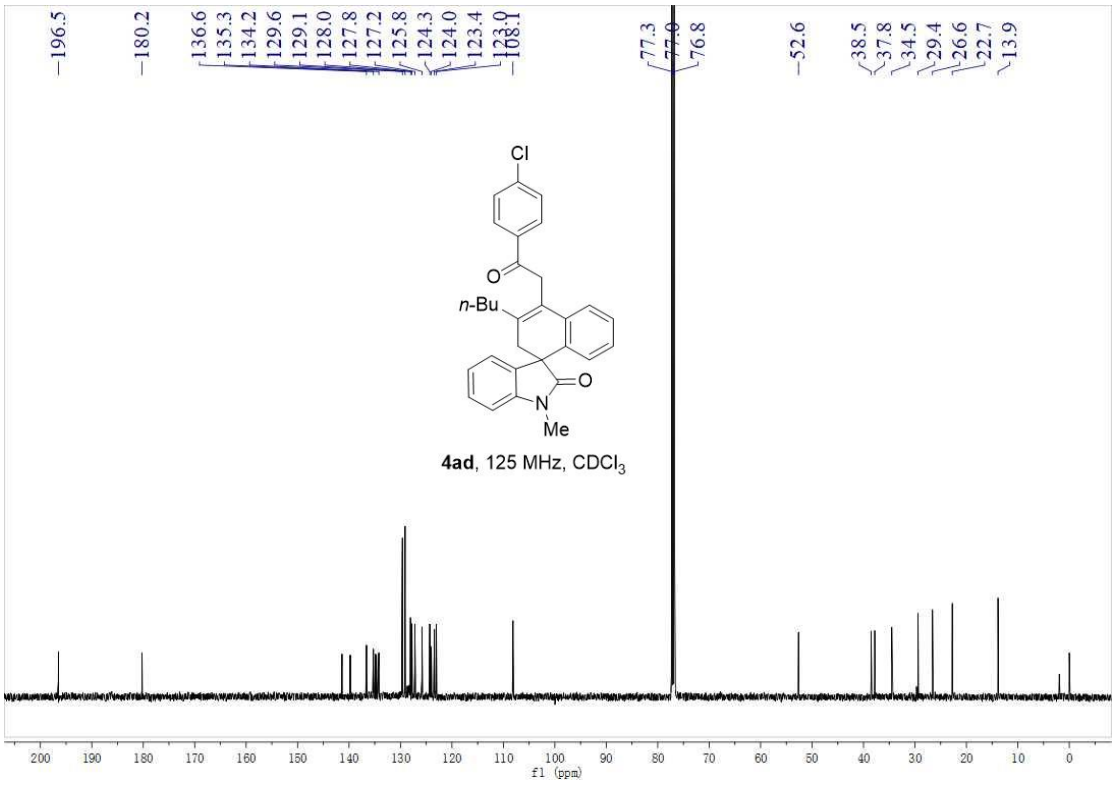

Ph
O
n-Bu
O
N
Me
4ab, 500 MHz, CDCl3
f1 (ppm)

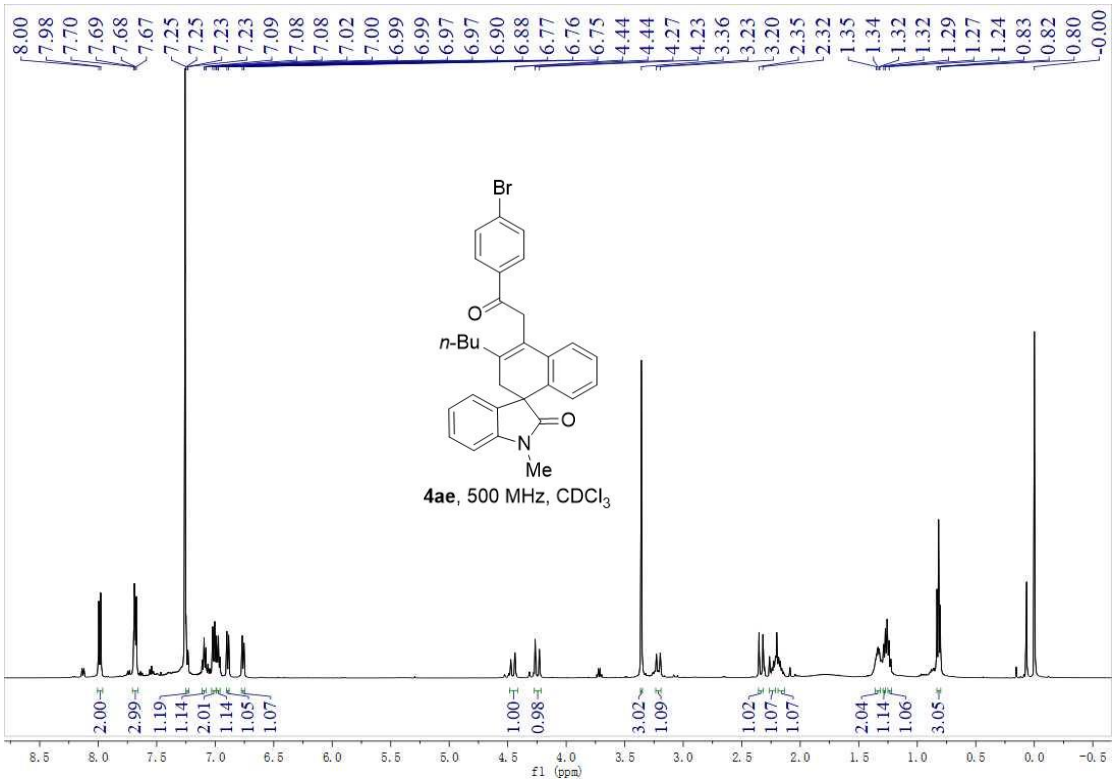

Ph
O
n-Bu
O
N
Me
4ab, 125 MHz, CDCl3
f1 (ppm)

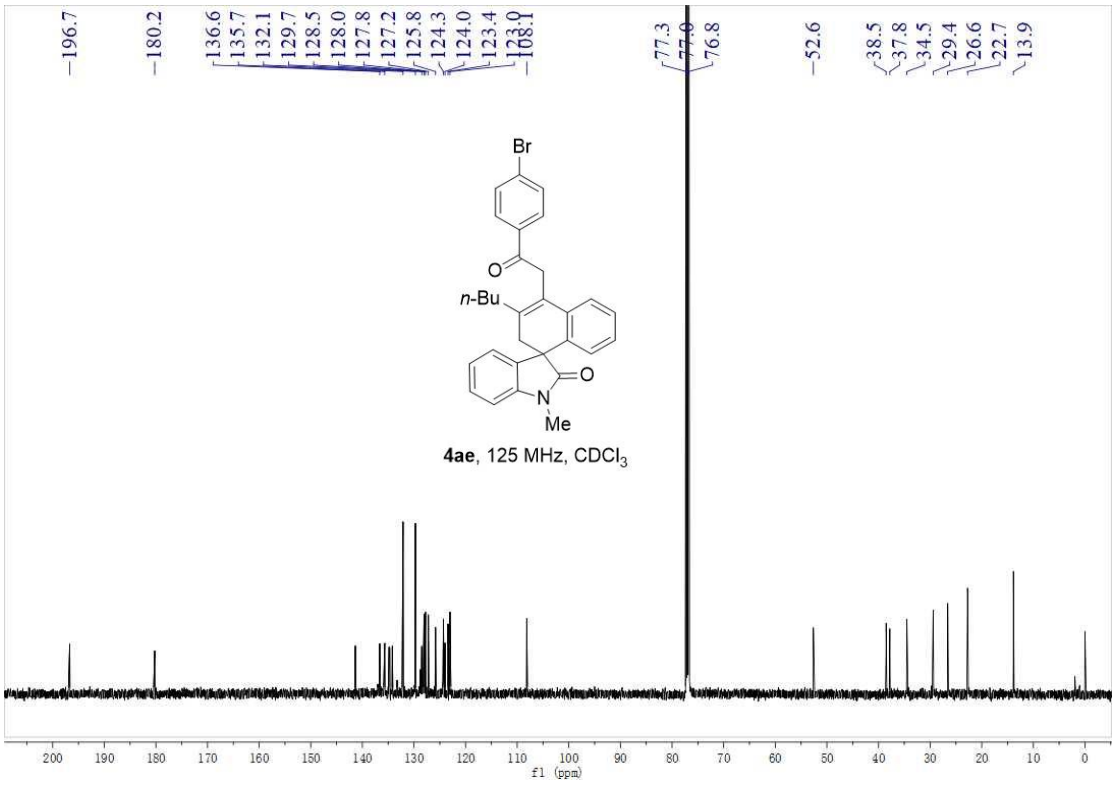

Ph
O
O
N
Me
4ac, 500 MHz, CDCl3
f1 (ppm)

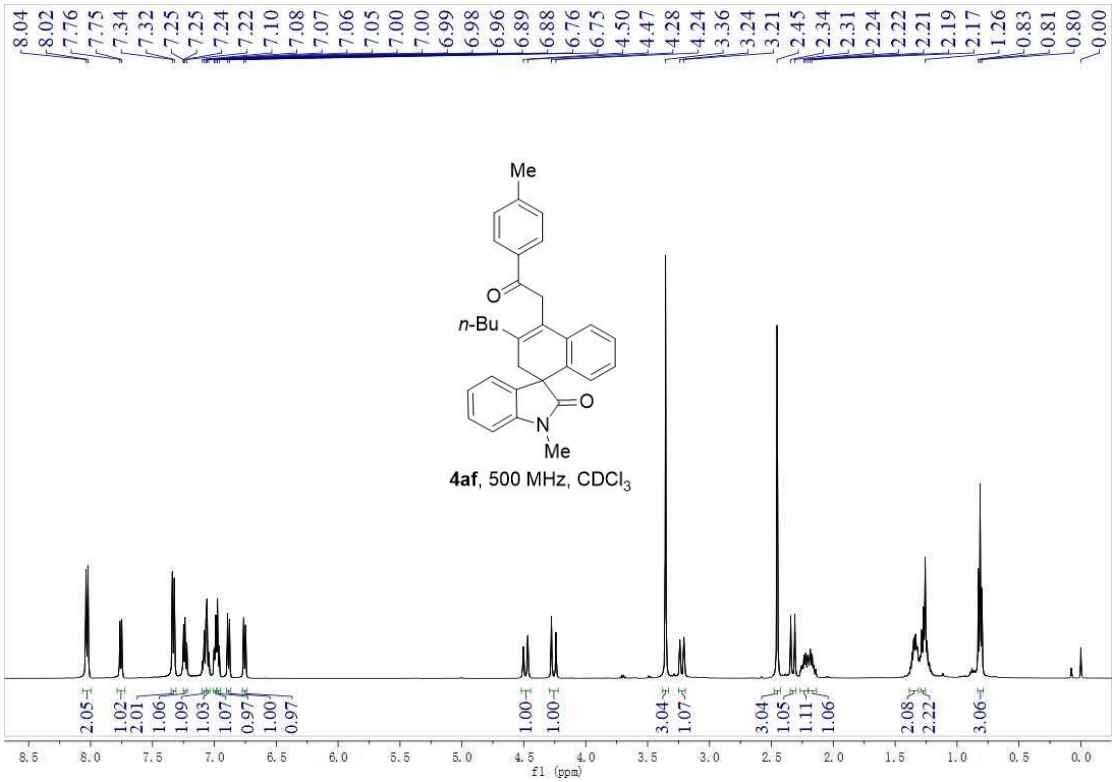

Ph
O
O
N
Me
4ac, 125 MHz, CDCl3
f1 (ppm)

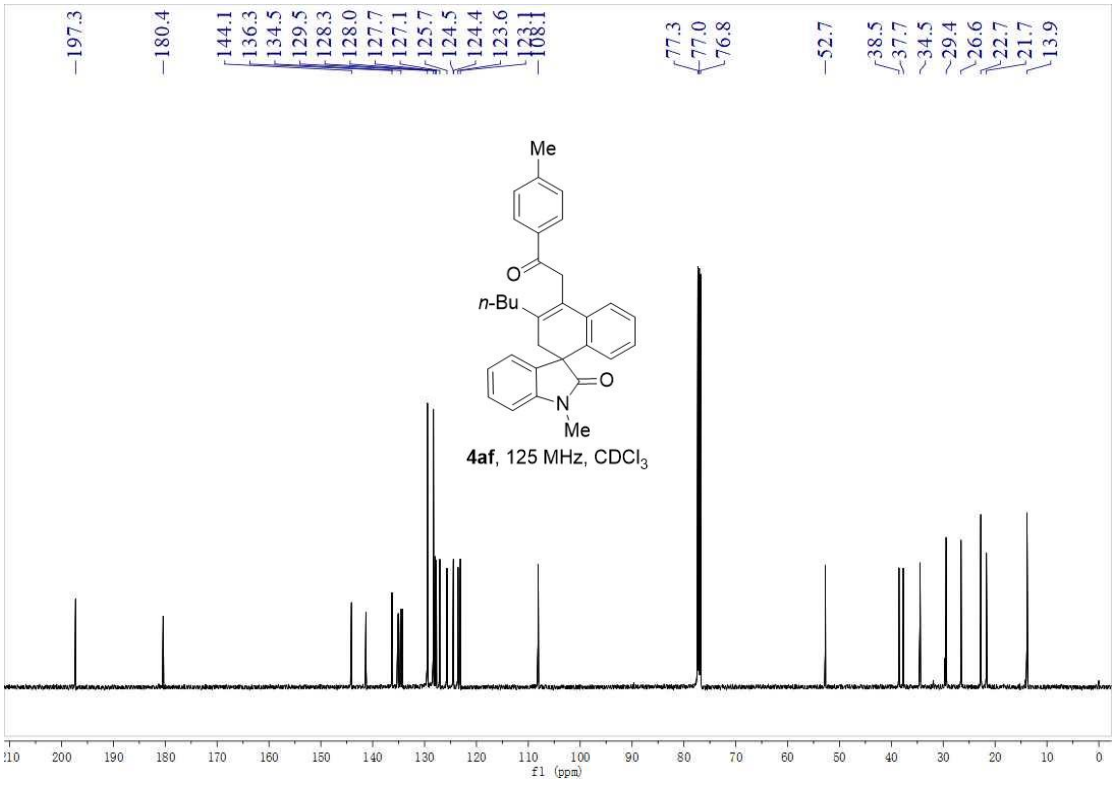

8.07
8.06
7.70
7.69
7.52
7.50
7.26
7.25
7.25
7.23
7.23
7.10
7.08
7.08
7.03
7.02
7.01
7.00
6.99
6.97
6.97
6.90
6.89
6.77
6.76
6.75
4.45
4.44
4.27
4.24
3.36
3.20
2.35
2.32
1.34
1.33
1.29
1.27
1.24
1.24
0.83
0.82
0.80
0.00
Cl
O
n-Bu
O
N
Me
4ad, 500 MHz, CDCl3
2.02
1.04
2.01
1.03
1.05
1.08
1.04
1.01
1.02
1.01
0.99
1.00
3.04
1.03
1.02
0.99
0.99
2.06
1.02
0.96
3.04
f1 (ppm)

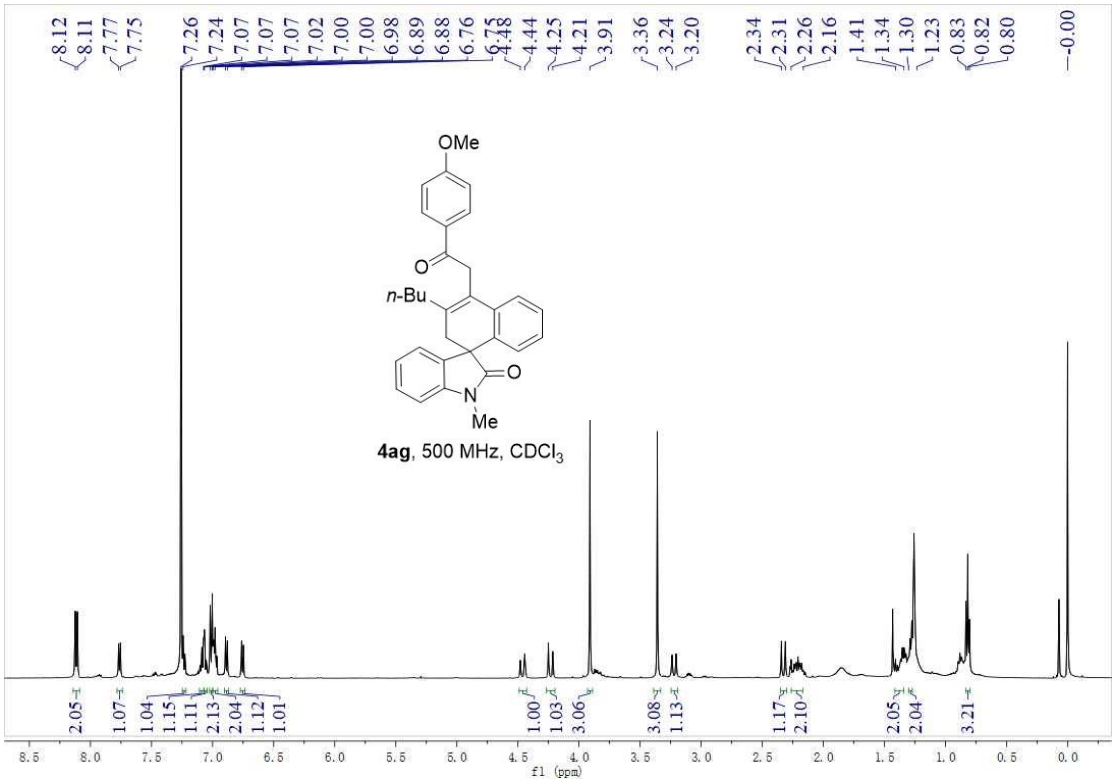

196.5
180.2
136.6
135.3
134.2
129.6
129.1
128.0
127.8
127.2
125.8
124.3
124.0
123.4
123.0
108.1
77.3
77.0
76.8
52.6
38.5
37.8
34.5
29.4
26.6
22.7
13.9
Cl
O
n-Bu
O
N
Me
4ad, 125 MHz, CDCl3
f1 (ppm)

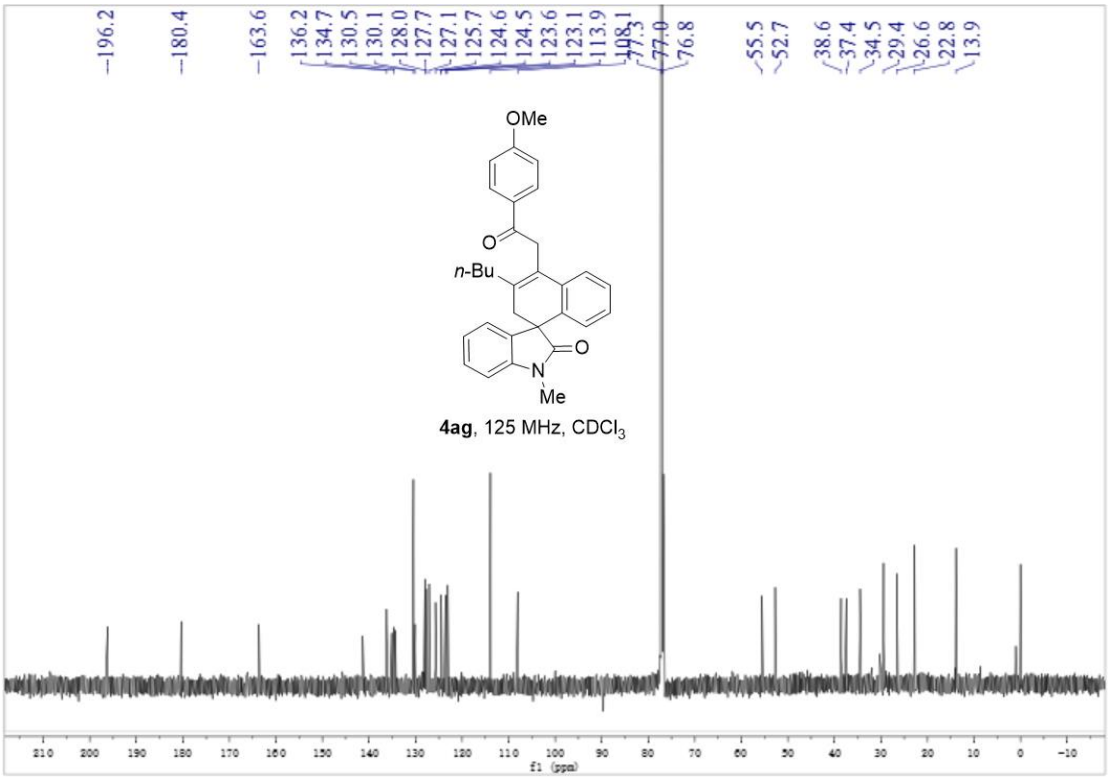

8.00
7.98
7.70
7.69
7.68
7.67
7.25
7.25
7.23
7.23
7.09
7.08
7.08
7.02
7.00
6.99
6.99
6.97
6.97
6.90
6.88
6.77
6.76
6.75
4.44
4.44
4.27
4.23
3.36
3.23
3.20
2.35
2.32
1.35
1.34
1.32
1.32
1.29
1.27
1.24
0.83
0.82
0.80
-0.00
Br
O
n-Bu
O
N
Me
4ae, 500 MHz, CDCl3
2.00
2.99
1.19
1.14
2.01
1.14
1.05
1.07
1.00
0.98
3.02
1.09
1.02
1.07
1.07
2.04
1.14
1.06
3.05
f1 (ppm)

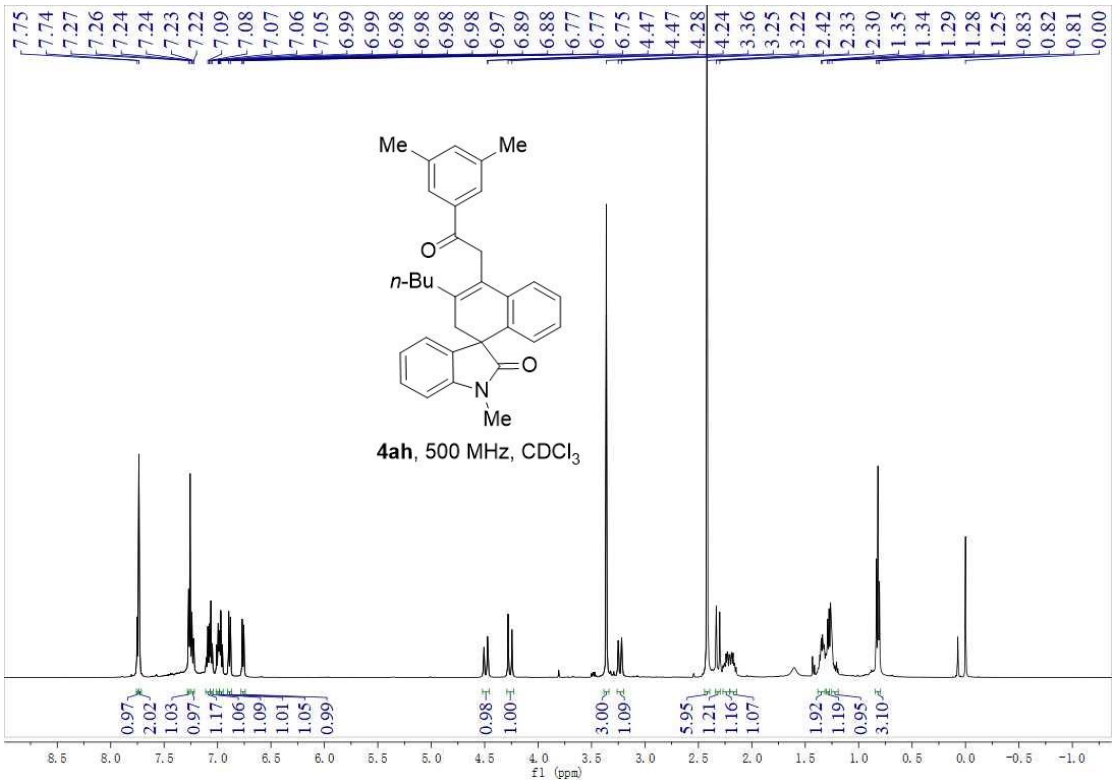

196.7
180.2
136.6
135.7
132.1
129.7
128.5
128.0
127.8
127.2
125.8
124.3
124.0
123.4
123.0
108.1
77.3
77.0
76.8
52.6
38.5
37.8
34.5
29.4
26.6
22.7
13.9
Br
O
n-Bu
O
N
Me
4ae, 125 MHz, CDCl3
f1 (ppm)

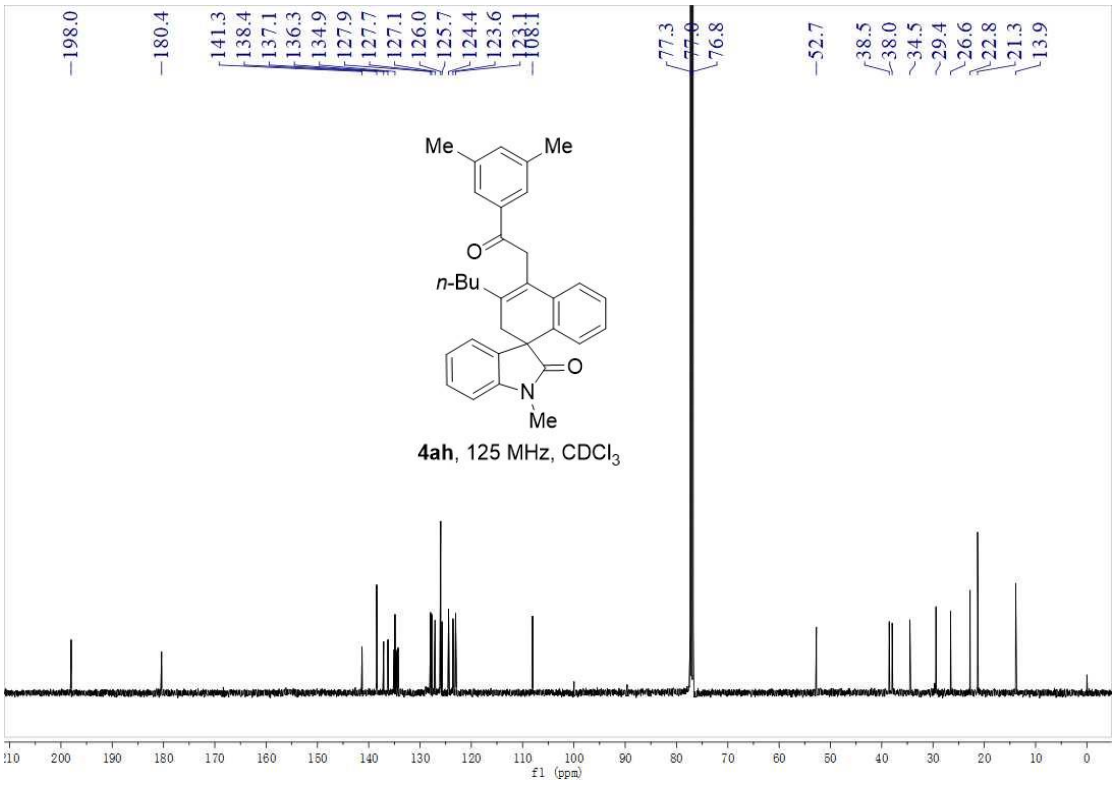

8.04
8.02
7.76
7.75
7.34
7.32
7.25
7.25
7.24
7.22
7.10
7.08
7.07
7.06
7.05
7.00
7.00
6.99
6.98
6.96
6.89
6.88
6.76
6.75
4.50
4.47
4.28
4.24
3.36
3.24
3.21
2.45
2.34
2.31
2.24
2.22
2.21
2.19
2.17
1.26
0.83
0.81
0.80
0.00
Me
O
n-Bu
O
N
Me
4af, 500 MHz, CDCl3
2.05
1.02
2.01
1.06
1.09
1.03
1.07
0.97
1.00
0.97
1.00
1.00
3.04
1.07
3.04
1.05
1.11
1.06
2.08
2.22
3.06
f1 (ppm)

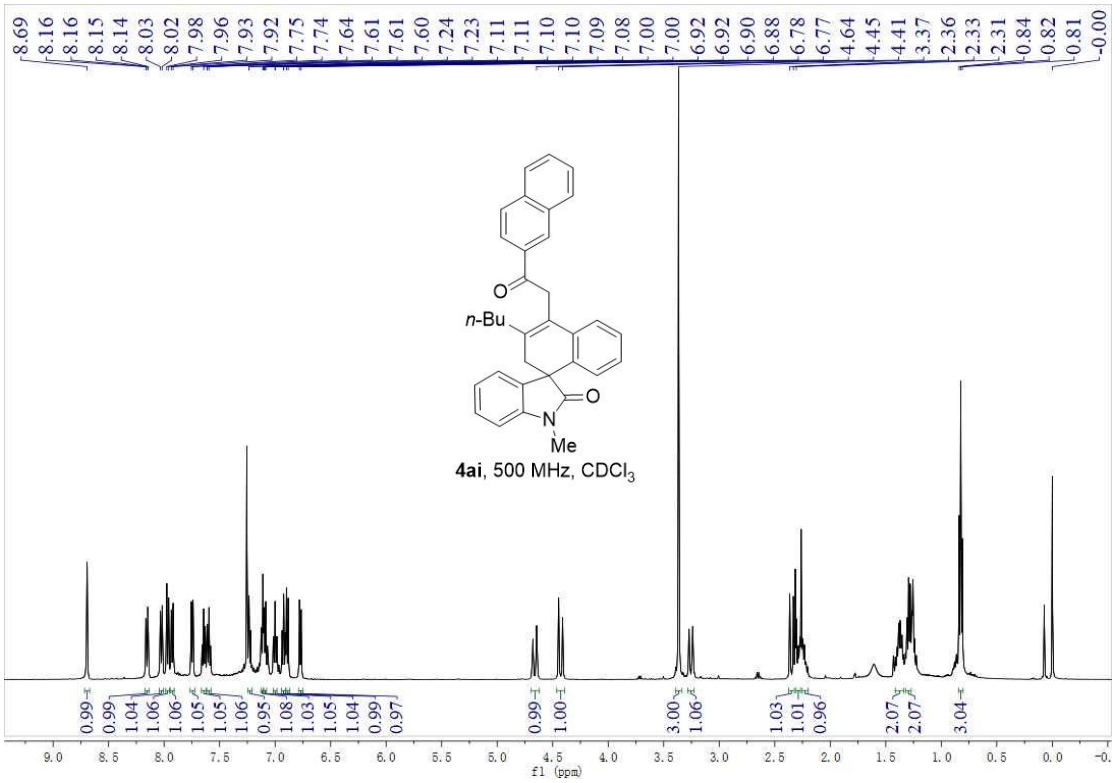

197.3
180.4
144.1
136.3
134.5
129.5
128.3
128.0
127.7
127.1
125.7
124.5
124.4
123.6
77.3
77.0
76.8
52.7
38.5
37.7
34.5
29.4
26.6
22.7
21.7
13.9
Me
O
n-Bu
O
N
Me
4af, 125 MHz, CDCl3
f1 (ppm)

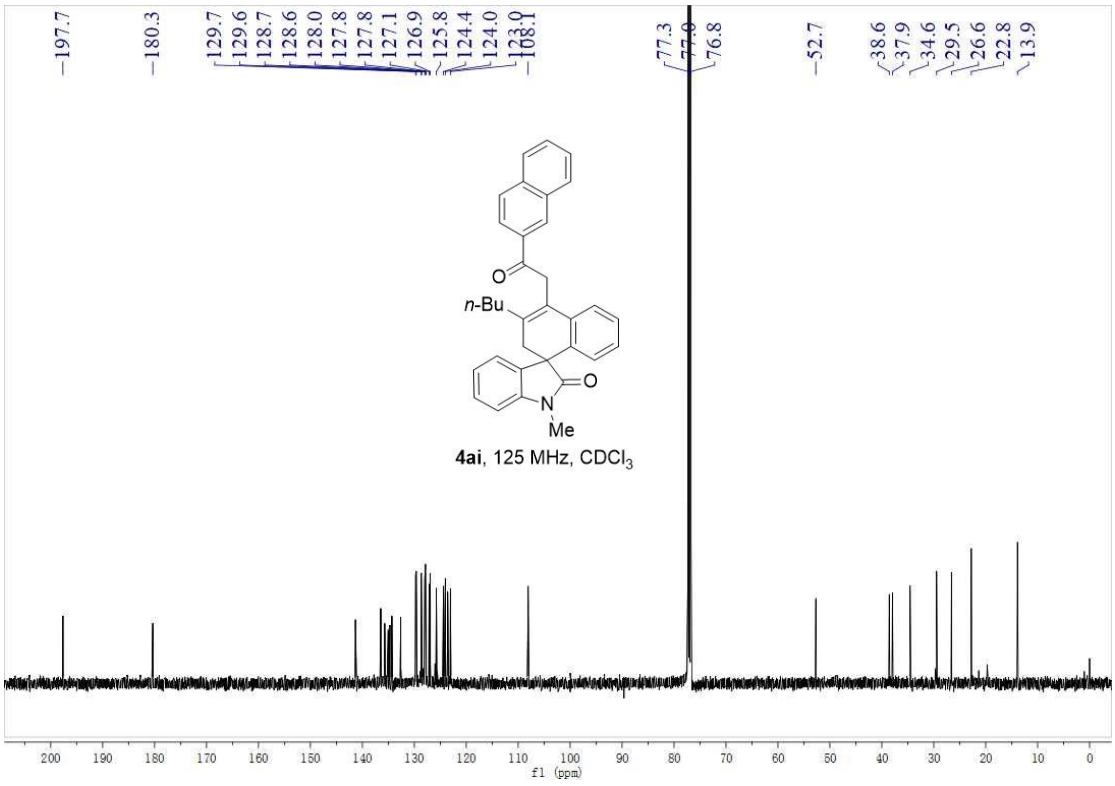

8.12
8.11
7.77
7.75
7.26
7.24
7.07
7.07
7.07
7.02
7.00
7.00
6.98
6.89
6.88
6.76
6.75
4.48
4.44
4.25
4.21
3.91
3.36
3.24
3.20
2.34
2.31
2.26
2.16
1.41
1.34
1.30
1.23
0.83
0.82
0.80
-0.00
OMe
O
n-Bu
O
N
Me
4ag, 500 MHz, CDCl3
2.05
1.07
1.04
1.15
1.11
2.13
2.04
1.12
1.01
1.00
1.03
3.06
3.08
1.13
1.17
2.10
2.05
2.04
3.21
f1 (ppm)

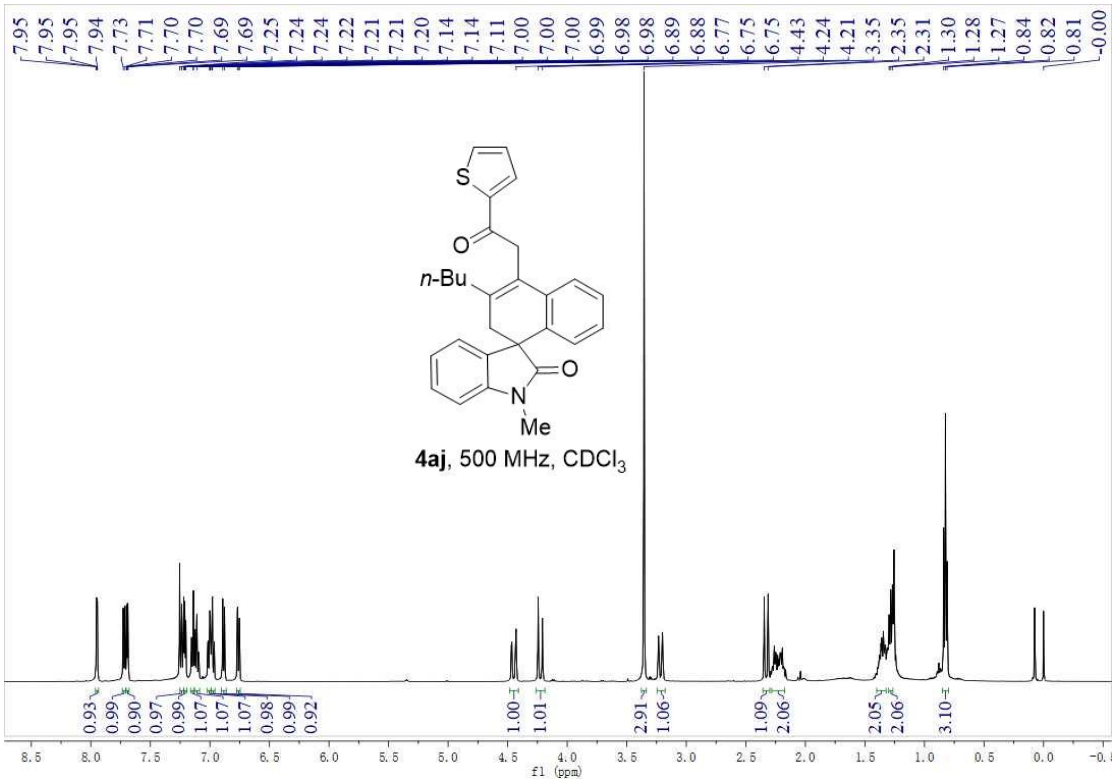

196.2
180.4
163.6
136.2
134.7
130.5
130.1
128.0
127.7
127.1
125.7
124.6
124.5
123.6
123.1
113.9
108.1
77.3
77.0
76.8
55.5
52.7
38.6
37.4
34.5
29.4
26.6
22.8
13.9
OMe
O
n-Bu
O
N
Me
4ag, 125 MHz, CDCl3
f1 (ppm)

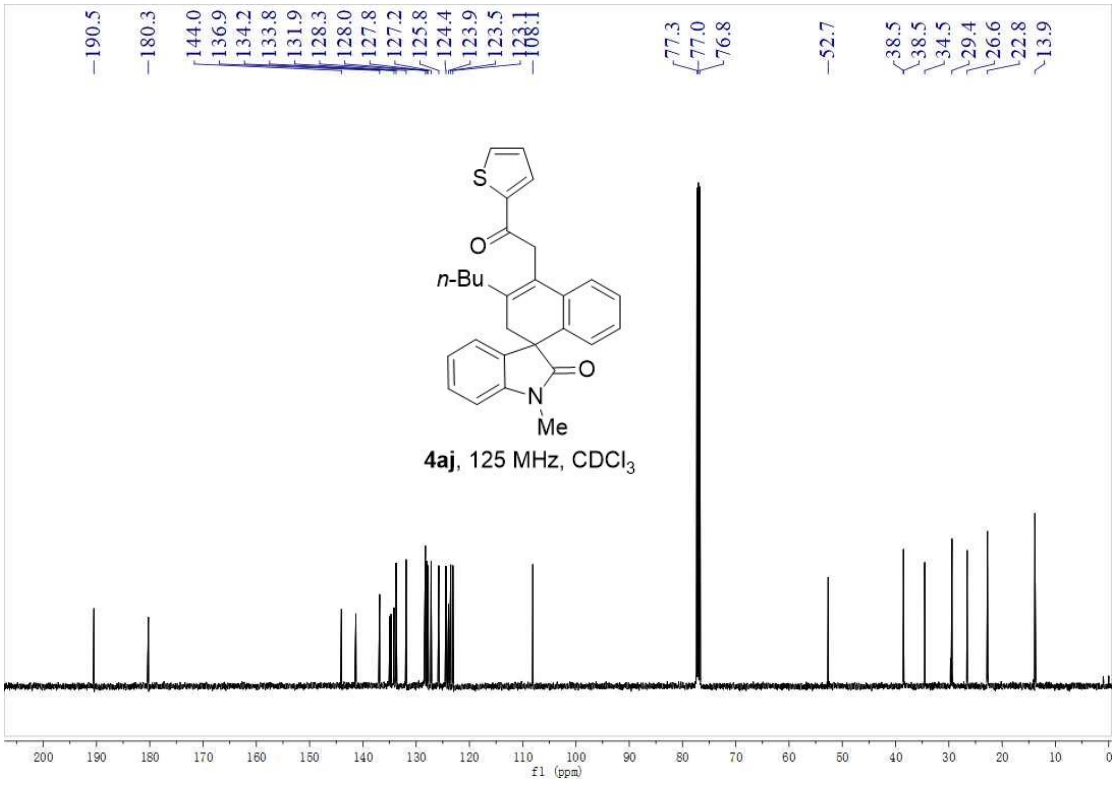

Me
Me
O
n-Bu
O
N
Me
4ah, 500 MHz, CDCl3
f1 (ppm)

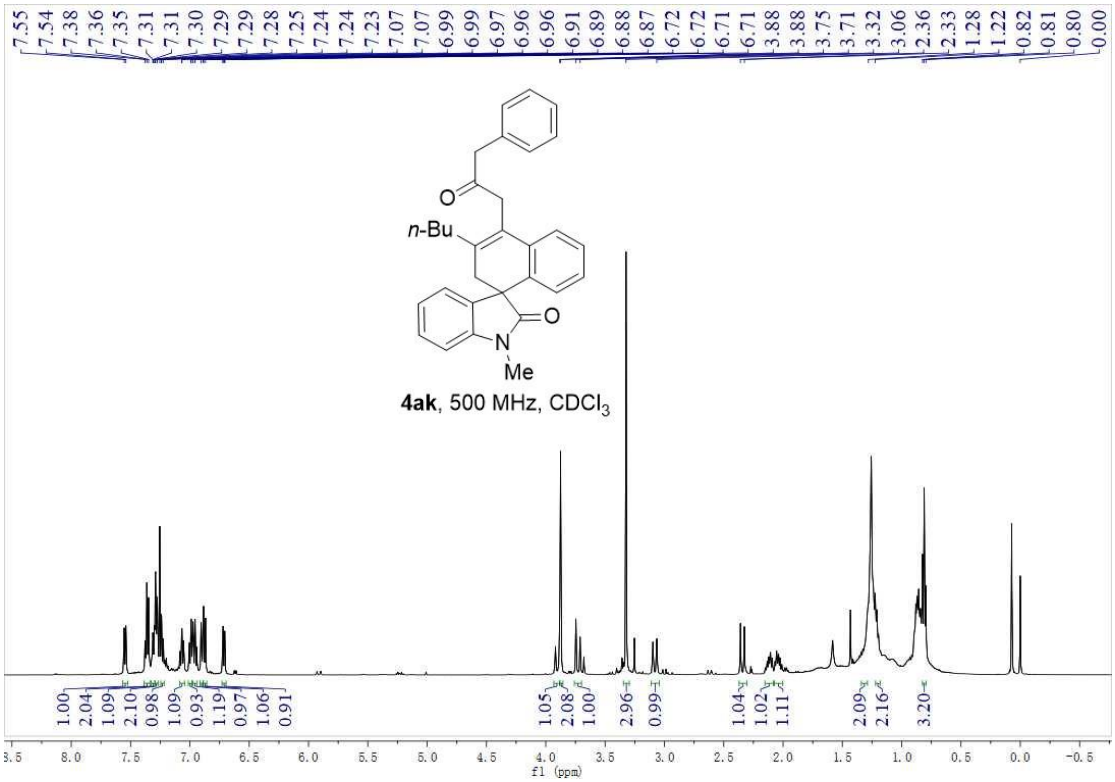

Me
Me
O
n-Bu
O
N
Me
4ah, 125 MHz, CDCl3
f1 (ppm)

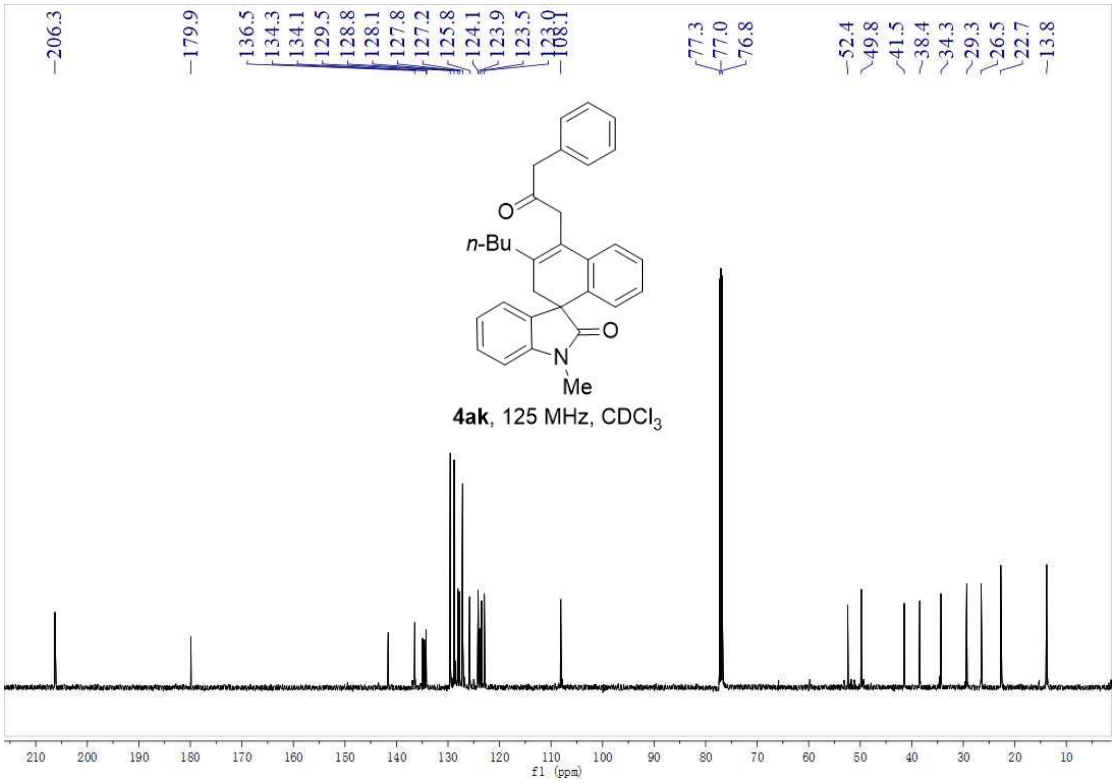

8.69
8.16
8.16
8.15
8.14
8.03
8.02
7.98
7.96
7.93
7.92
7.75
7.74
7.64
7.61
7.61
7.60
7.24
7.23
7.11
7.11
7.10
7.10
7.09
7.08
7.00
7.00
6.92
6.90
6.88
6.78
6.77
4.64
4.45
4.41
3.37
2.36
2.33
2.31
0.84
0.82
0.81
-0.00
O
n-Bu
O
N
Me
4ai, 500 MHz, CDCl3
0.99
0.99
1.04
1.06
1.06
1.05
1.05
1.06
0.95
1.08
1.03
1.05
1.04
0.99
0.97
0.99
1.00
3.00
1.06
1.03
1.01
0.96
2.07
2.07
3.04
f1 (ppm)

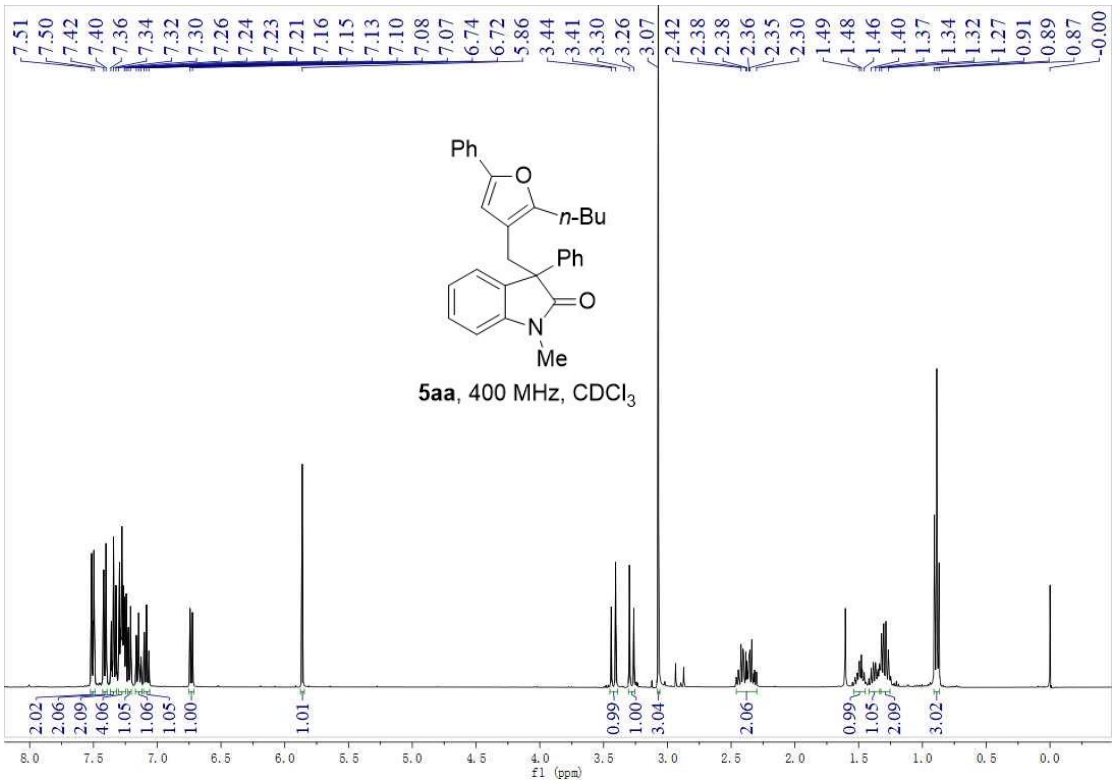

197.7
180.3
129.7
129.6
128.7
128.6
128.0
127.8
127.8
127.1
126.9
125.8
124.4
124.0
123.0
108.1
77.3
77.0
76.8
52.7
38.6
37.9
34.6
29.5
26.6
22.8
13.9
O
n-Bu
O
N
Me
4ai, 125 MHz, CDCl3
f1 (ppm)

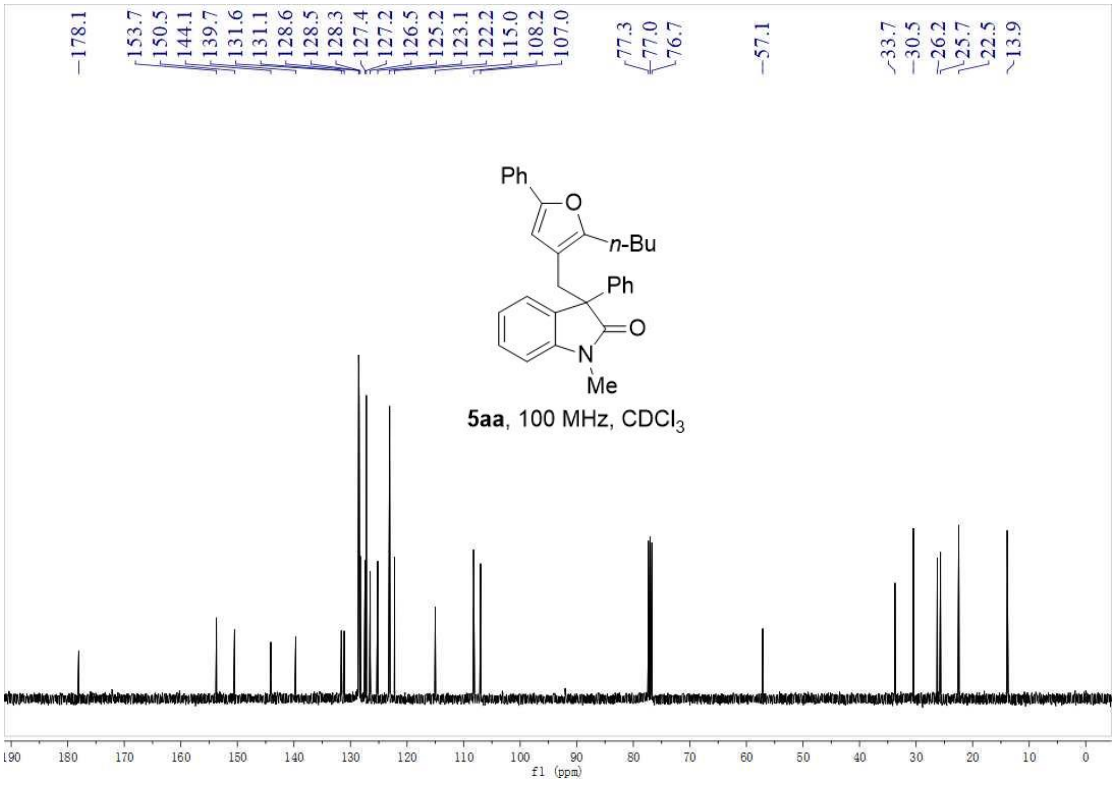

7.95
7.95
7.95
7.94
7.73
7.71
7.70
7.70
7.69
7.69
7.25
7.24
7.24
7.22
7.21
7.21
7.20
7.14
7.14
7.11
7.00
7.00
7.00
6.99
6.98
6.98
6.89
6.88
6.77
6.75
6.75
4.43
4.24
4.21
3.35
2.35
2.31
1.30
1.28
1.27
0.84
0.82
0.81
-0.00
S
O
n-Bu
O
N
Me
4aj, 500 MHz, CDCl3
0.93
0.99
0.90
0.97
0.99
1.07
1.07
1.07
0.98
0.99
0.92
1.00
1.01
2.91
1.06
1.09
2.06
2.05
2.06
3.10
f1 (ppm)

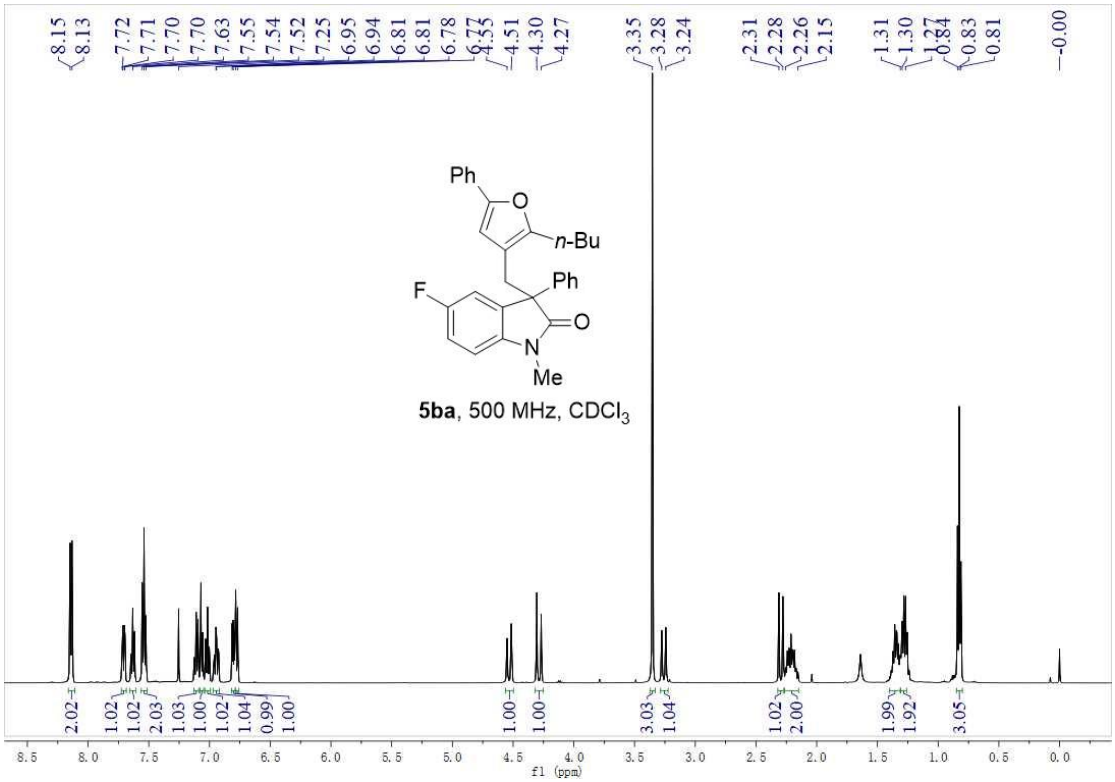

190.5
180.3
144.0
136.9
134.2
133.8
131.9
128.3
128.0
127.8
127.2
125.8
124.4
123.9
123.5
123.1
108.1
77.3
77.0
76.8
52.7
38.5
38.5
34.5
29.4
26.6
22.8
13.9
S
O
n-Bu
O
N
Me
4aj, 125 MHz, CDCl3
f1 (ppm)

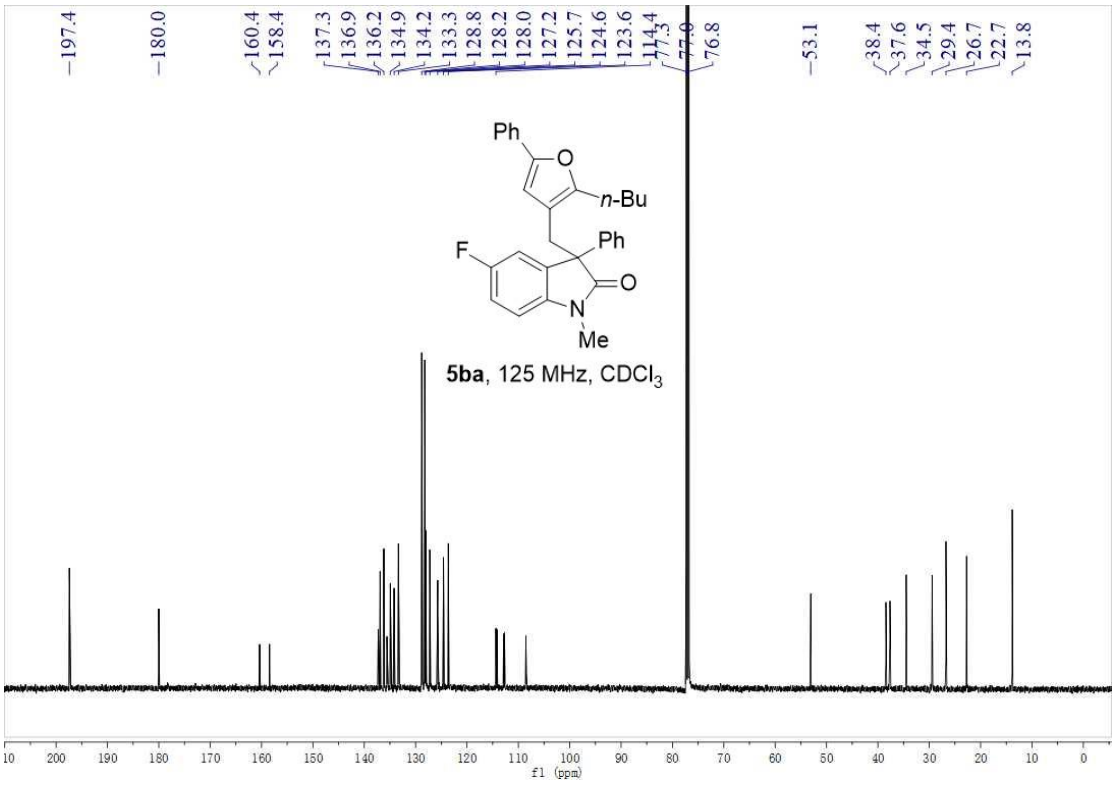

7.55 7.54 7.38 7.36 7.35 7.31 7.31 7.30 7.29 7.29 7.28 7.25 7.24 7.24 7.23 7.07 7.07 6.99 6.99 6.97 6.96 6.96 6.91 6.89 6.88 6.87 6.72 6.72 6.71 6.71 3.88 3.88 3.75 3.71 3.32 3.06 2.36 2.33 1.28 1.22 0.82 0.81 0.80 0.00
O
n-Bu
O
N
Me
4ak, 500 MHz, CDCl3
1.00 2.04 1.09 2.10 0.98 1.09 0.93 1.19 0.97 1.06 0.91
1.05 2.08 1.00 2.96 0.99 1.04 1.02 1.11 2.09 2.16 3.20
f1 (ppm)

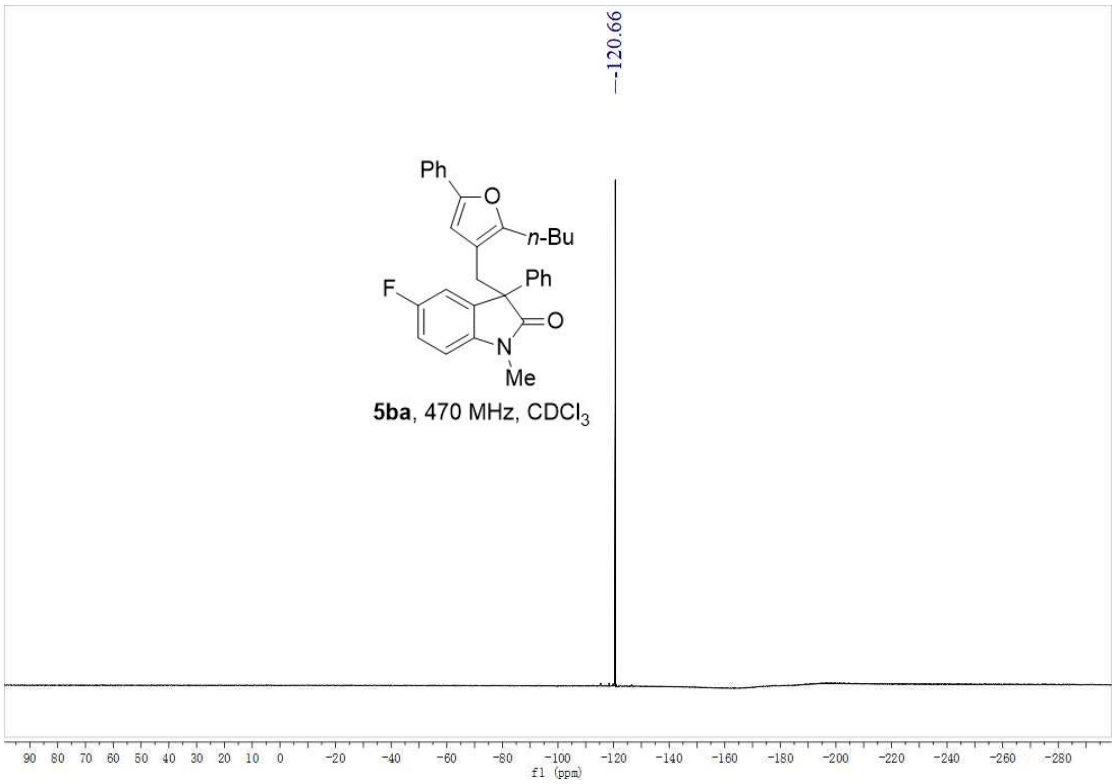

206.3 179.9 136.5 134.3 134.1 129.5 128.8 128.1 127.8 127.2 125.8 124.1 123.9 123.5 123.0 108.1 77.3 77.0 76.8 52.4 49.8 41.5 38.4 34.3 29.3 26.5 22.7 13.8
O
n-Bu
O
N
Me
4ak, 125 MHz, CDCl3
f1 (ppm)

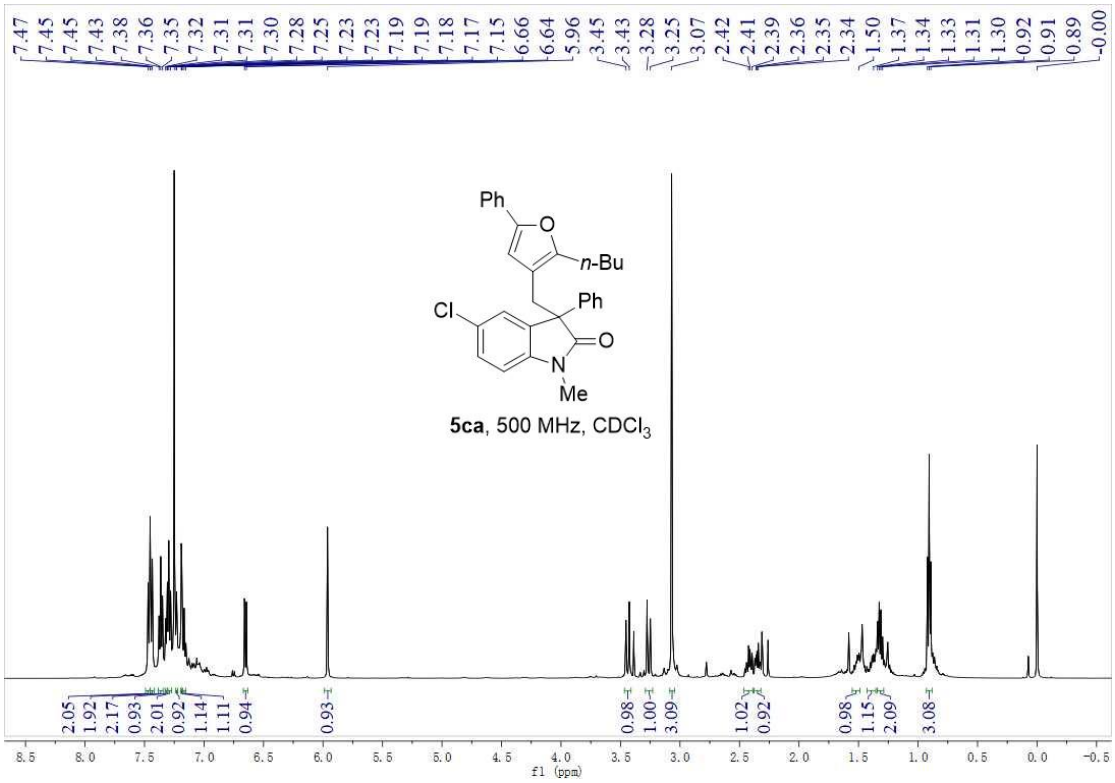

Ph
O
n-Bu
Ph
O
N
Me
5aa, 400 MHz, CDCl3
f1 (ppm)

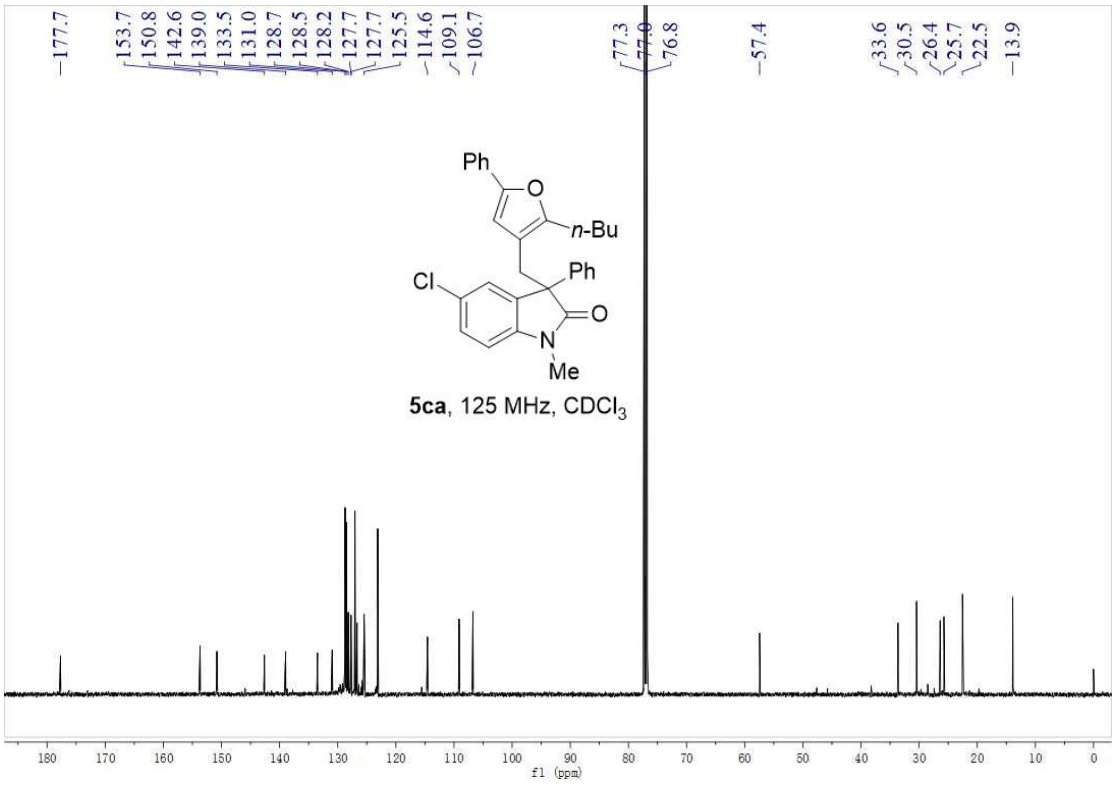

Ph
O
n-Bu
Ph
O
N
Me
5aa, 100 MHz, CDCl3
f1 (ppm)

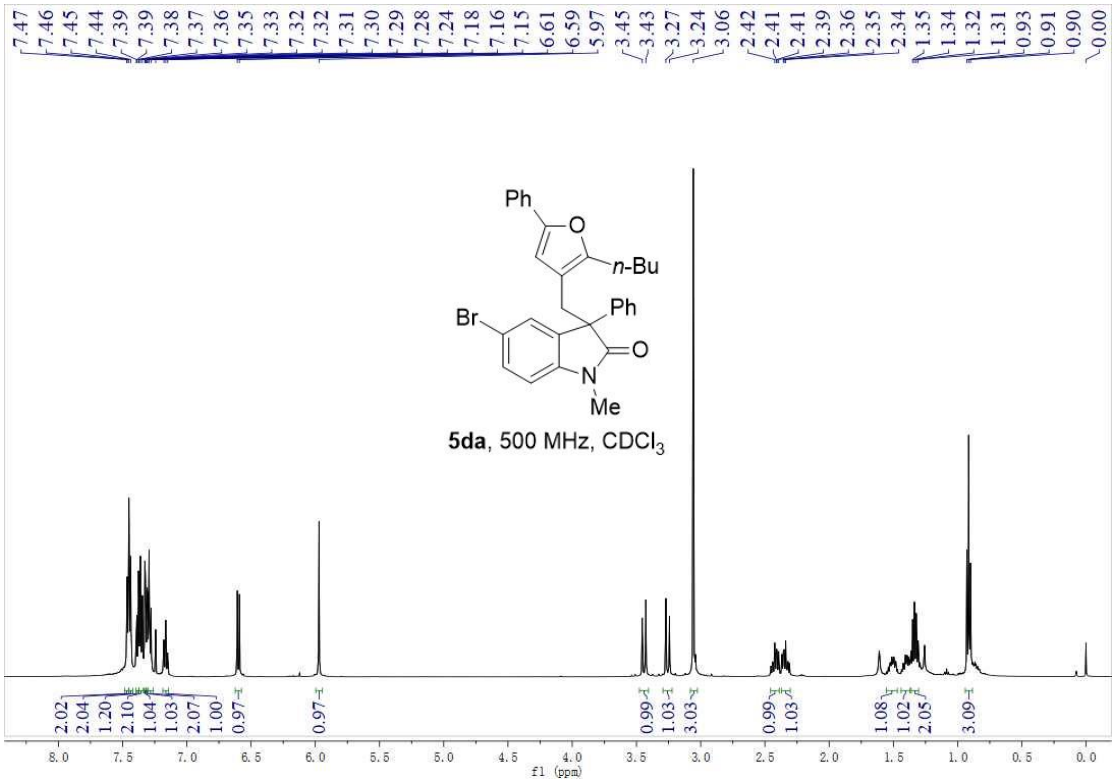

8.15
8.13
7.72
7.71
7.70
7.70
7.63
7.55
7.54
7.52
7.25
6.95
6.94
6.81
6.81
6.78
4.55
4.51
4.30
4.27
3.35
3.28
3.24
2.31
2.28
2.26
2.15
1.31
1.30
0.84
0.83
0.81
-0.00
Ph
O
n-Bu
F
Ph
O
N
Me
5ba, 500 MHz, CDCl3
2.02
1.02
1.02
2.03
1.03
1.00
1.02
1.04
0.99
1.00
1.00
1.00
3.03
1.04
1.02
2.00
1.99
1.92
3.05
f1 (ppm)

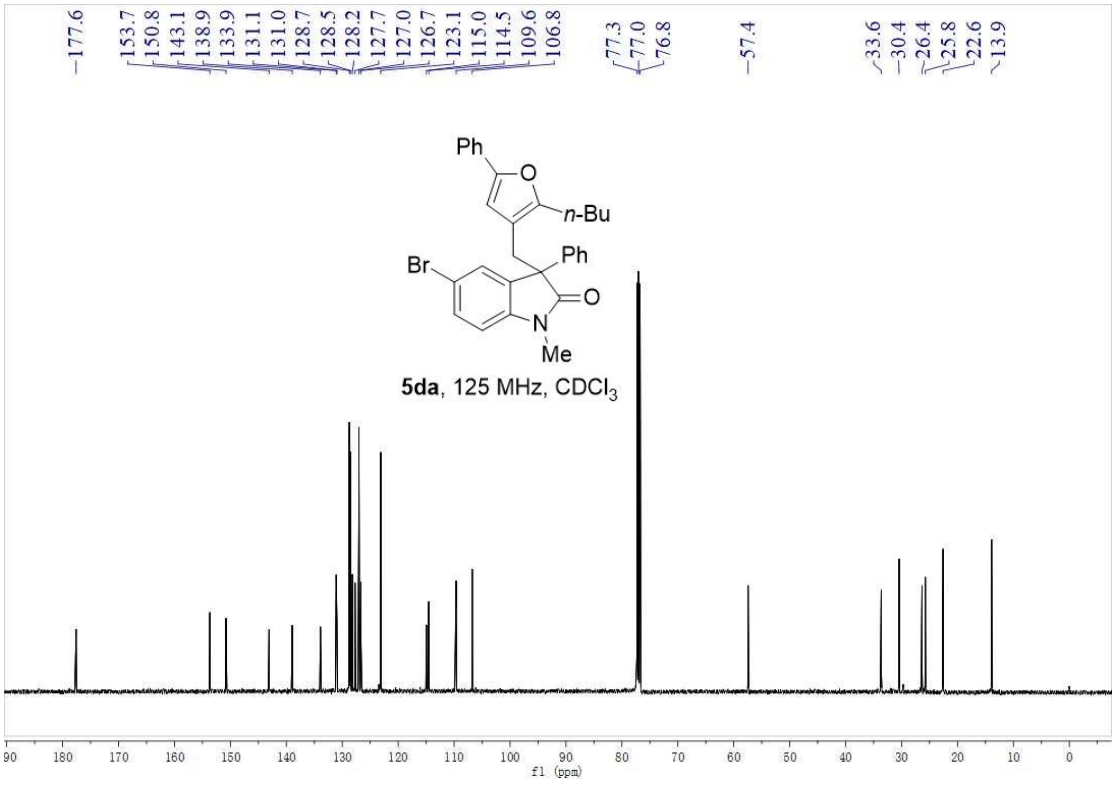

197.4
180.0
160.4
158.4
137.3
136.9
136.2
134.9
134.2
133.3
128.8
128.2
128.0
127.2
125.7
124.6
123.6
114.4
77.3
77.0
76.8
53.1
38.4
37.6
34.5
29.4
26.7
22.7
13.8
Ph
O
n-Bu
F
Ph
O
N
Me
5ba, 125 MHz, CDCl3
f1 (ppm)

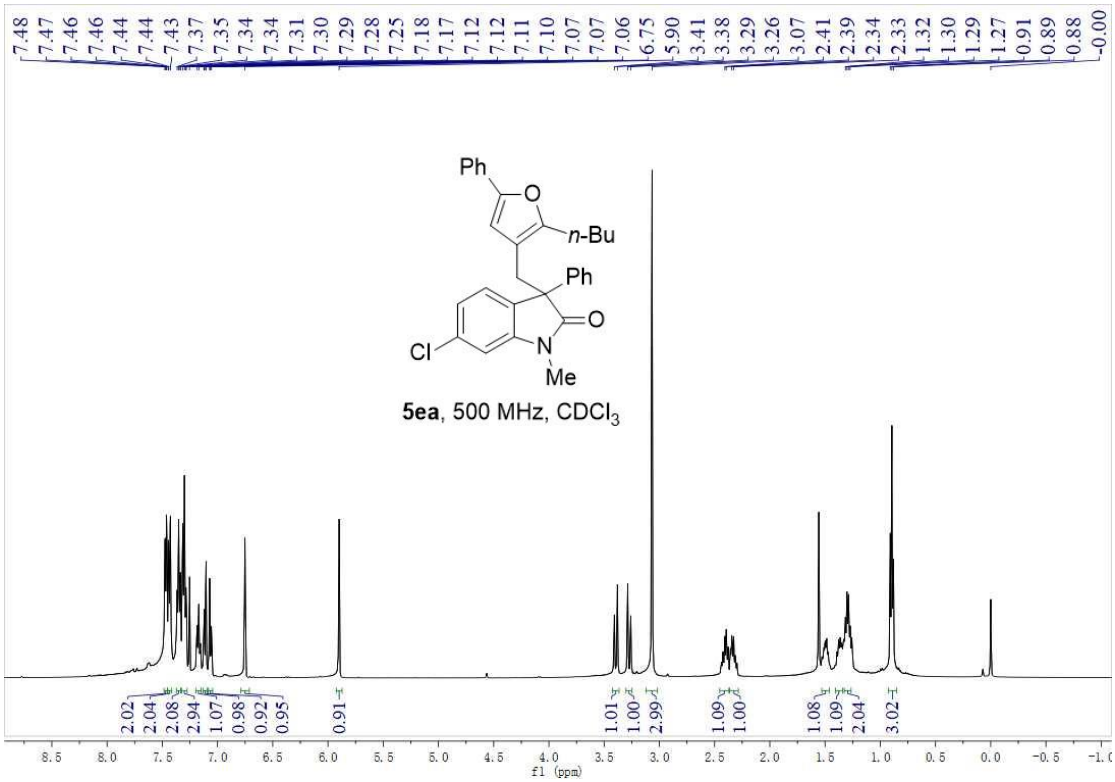

-120.66
Ph
O
n-Bu
Ph
F
O
N
Me
5ba, 470 MHz, CDCl3
90 80 70 60 50 40 30 20 10 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280
f1 (ppm)

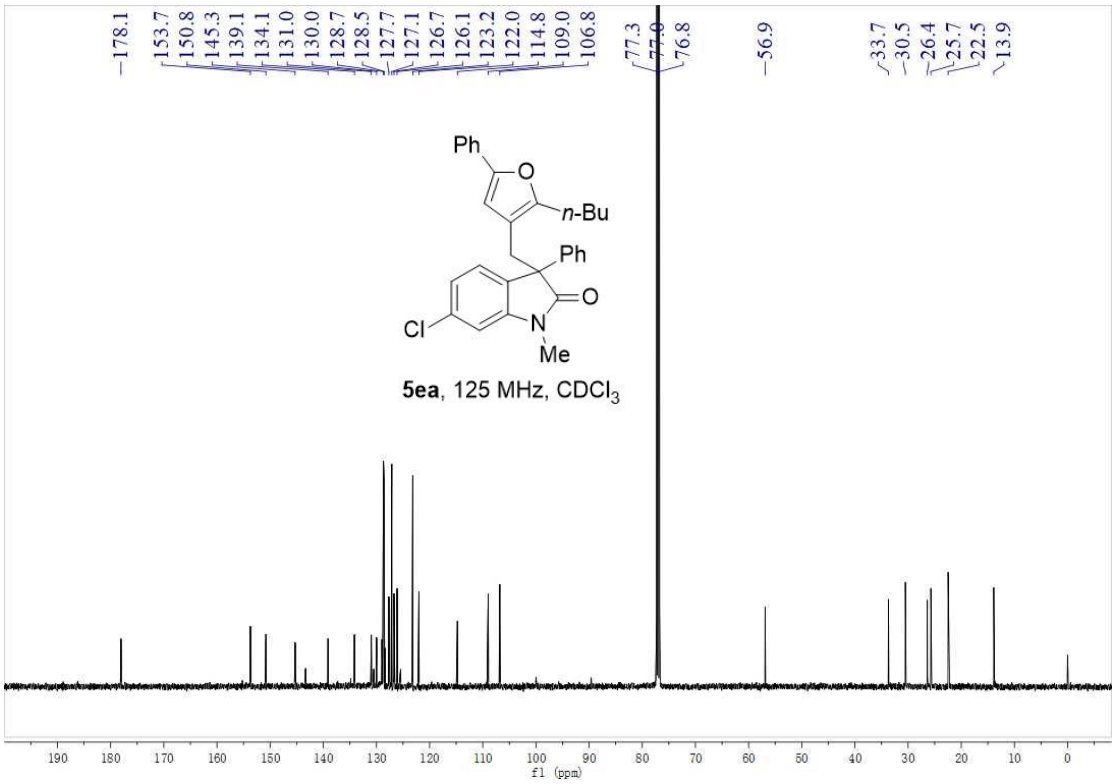

7.47 7.45 7.45 7.43 7.38 7.36 7.35 7.32 7.31 7.31 7.30 7.28 7.25 7.23 7.23 7.19 7.19 7.18 7.17 7.15 6.66 6.64 5.96 3.45 3.43 3.28 3.25 3.07 2.42 2.41 2.39 2.36 2.35 2.34 1.50 1.37 1.34 1.33 1.31 1.30 0.92 0.91 0.89 -0.00
Ph
O
n-Bu
Cl
Ph
O
N
Me
5ca, 500 MHz, CDCl3
2.05 1.92 2.17 0.93 2.01 0.92 1.14 1.11 0.94 0.93 0.98 1.00 3.09 1.02 0.92 0.98 1.15 2.09 3.08
f1 (ppm)

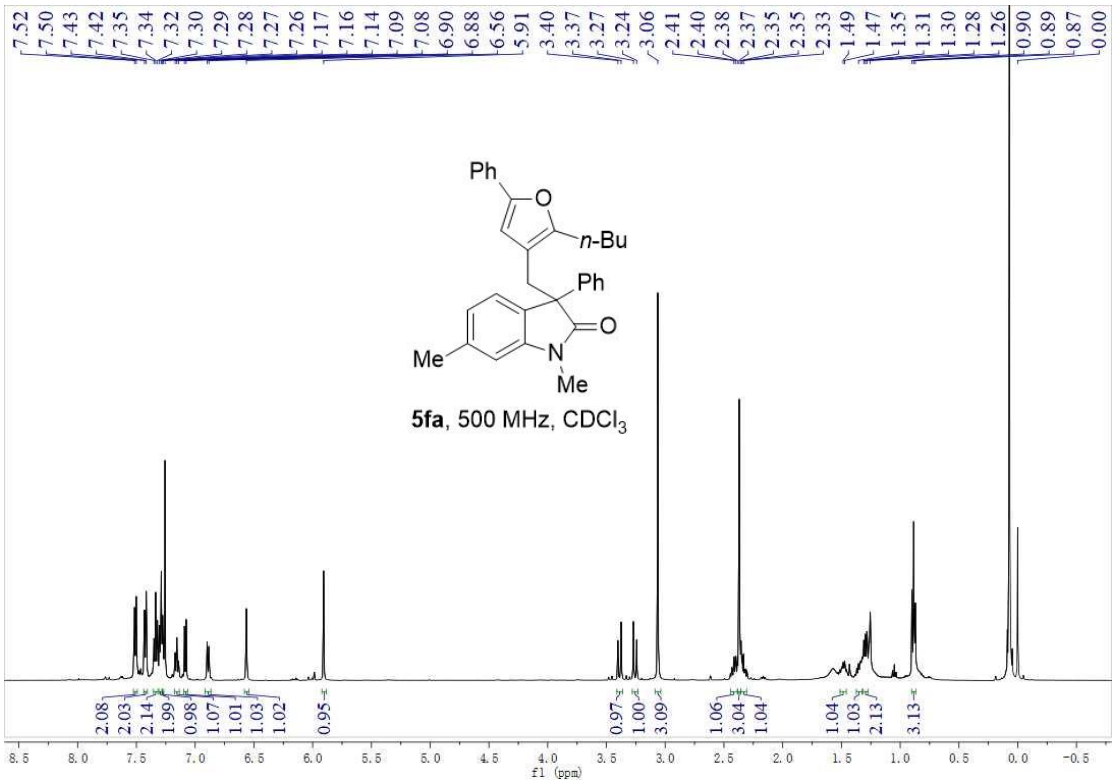

177.7 153.7 150.8 142.6 139.0 133.5 131.0 128.7 128.5 128.2 127.7 127.7 125.5 114.6 109.1 106.7 77.3 77.0 76.8 57.4 33.6 30.5 26.4 25.7 22.5 13.9
Ph
O
n-Bu
Cl
Ph
O
N
Me
5ca, 125 MHz, CDCl3
f1 (ppm)


7.47
7.46
7.45
7.44
7.39
7.39
7.38
7.37
7.36
7.35
7.33
7.32
7.32
7.31
7.30
7.29
7.28
7.24
7.18
7.16
7.15
6.61
6.59
5.97
3.45
3.43
3.27
3.24
3.06
2.42
2.41
2.41
2.39
2.36
2.35
2.34
1.35
1.34
1.32
1.31
0.93
0.91
0.90
0.00
Ph
O
n-Bu
Br
Ph
O
N
Me
5da, 500 MHz, CDCl3
2.02
2.04
1.20
2.10
1.04
1.03
2.07
1.00
0.97
0.97
0.99
1.03
3.03
0.99
1.03
1.08
1.02
2.05
3.09
f1 (ppm)

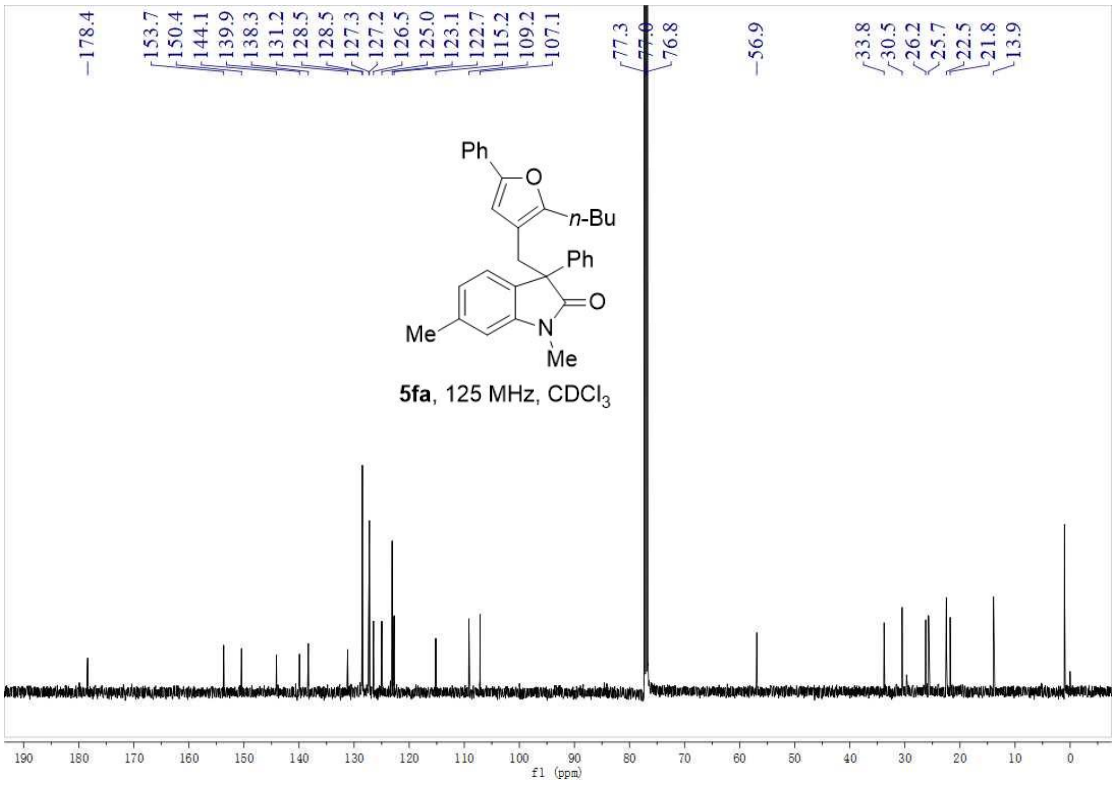

177.6
153.7
150.8
143.1
138.9
133.9
131.1
131.0
128.7
128.5
128.2
127.7
127.0
126.7
123.1
115.0
114.5
109.6
106.8
77.3
77.0
76.8
57.4
33.6
30.4
26.4
25.8
22.6
13.9
Ph
O
n-Bu
Br
Ph
O
N
Me
5da, 125 MHz, CDCl3
f1 (ppm)


Ph
O
n-Bu
Ph
O
Cl
N
Me
5ea, 500 MHz, CDCl3
f1 (ppm)

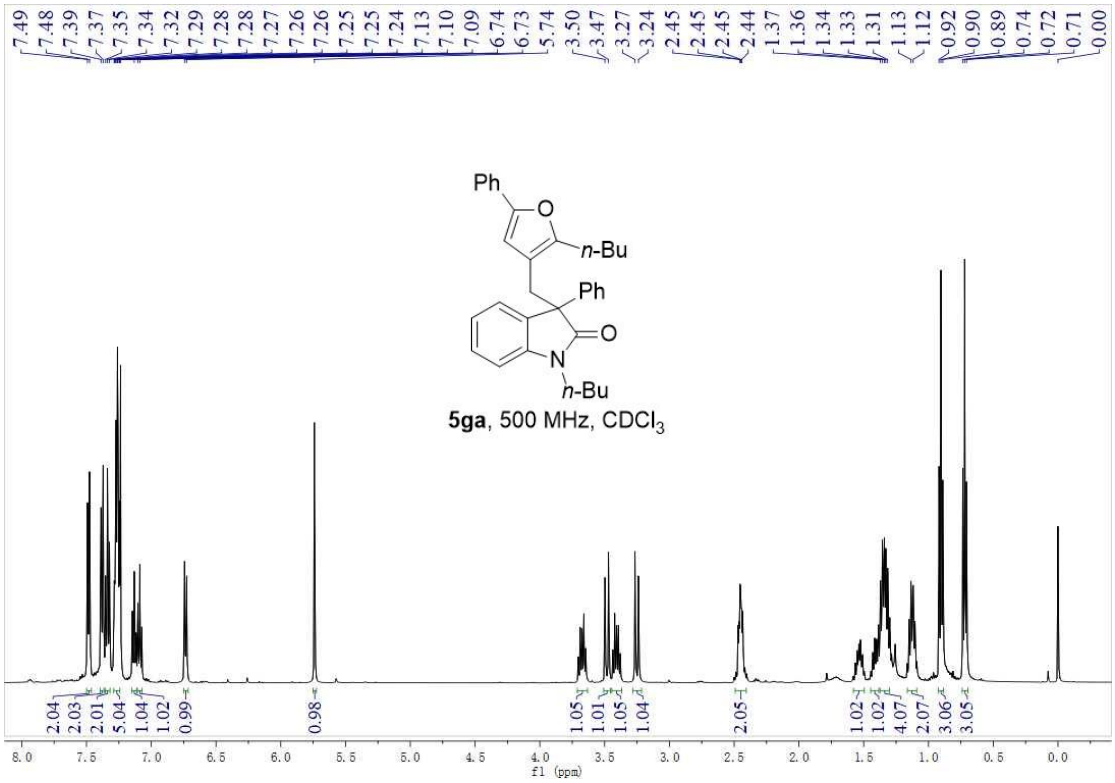

Ph
O
n-Bu
Ph
O
Cl
N
Me
5ea, 125 MHz, CDCl3
f1 (ppm)

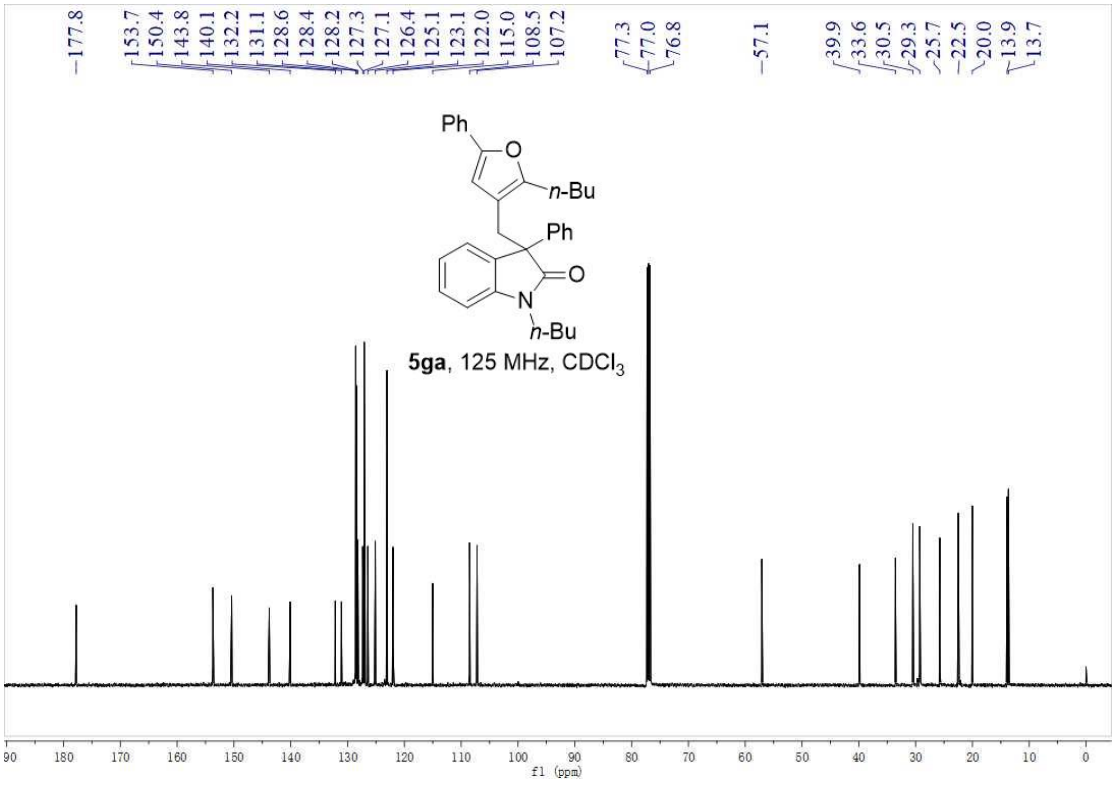


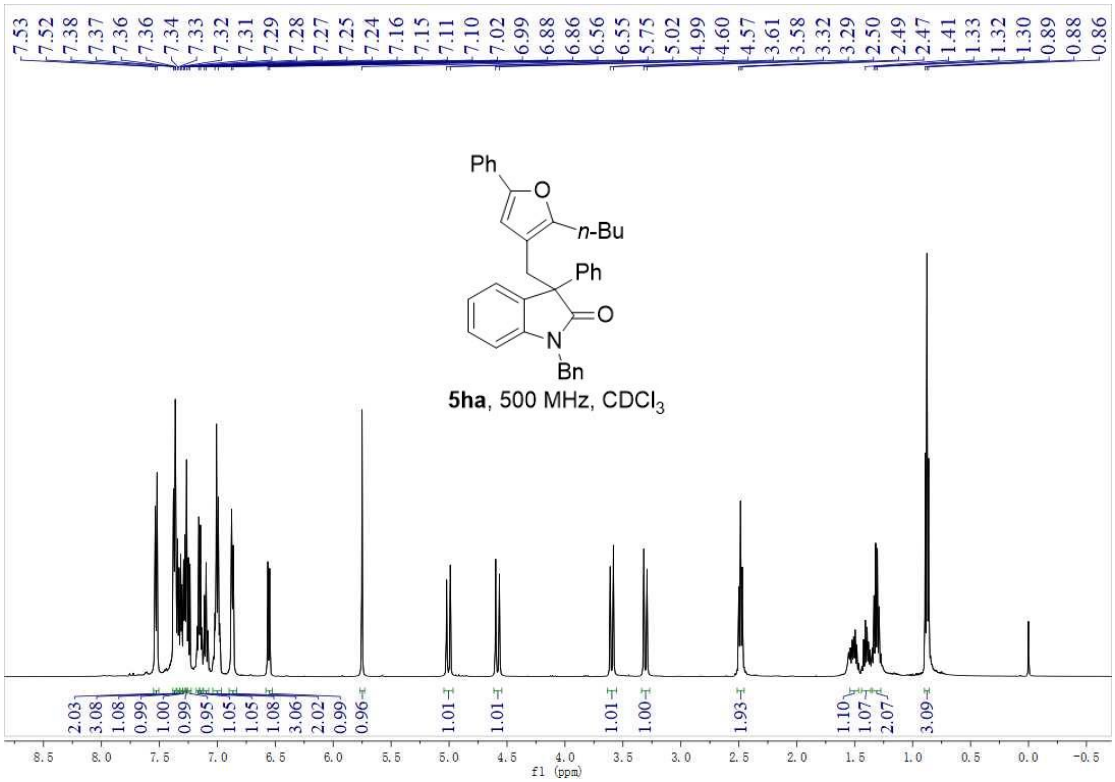
5fa, 500 MHz, $CDCl_3$

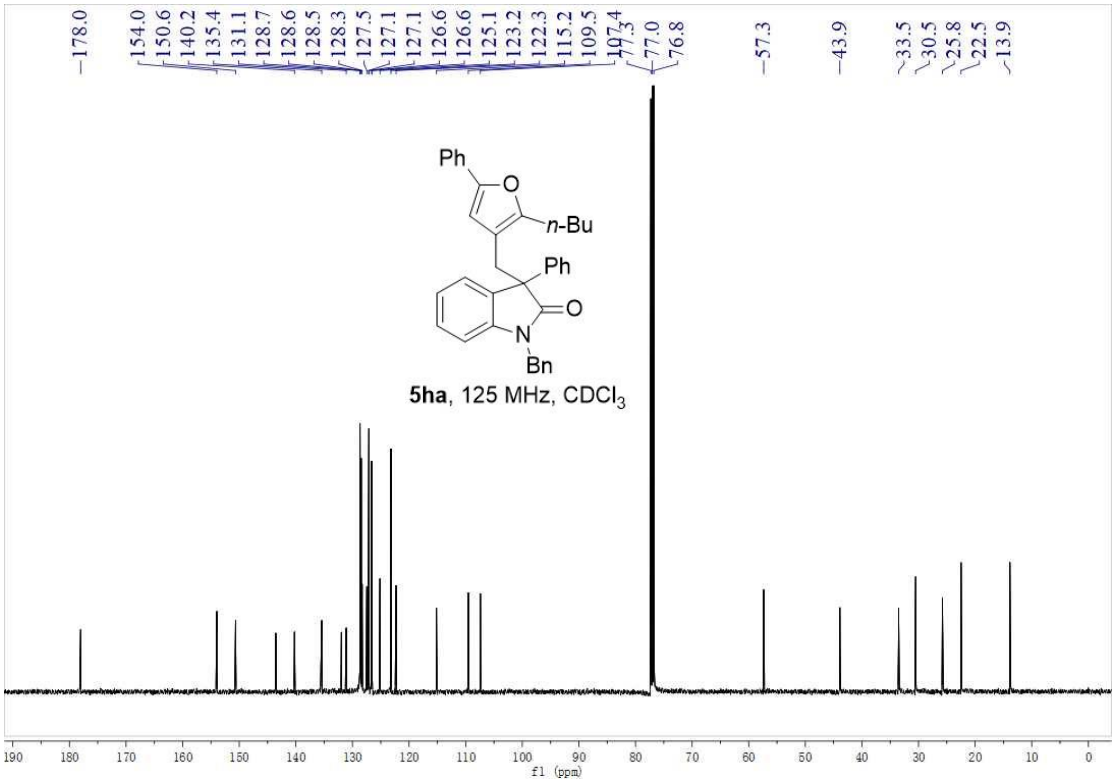


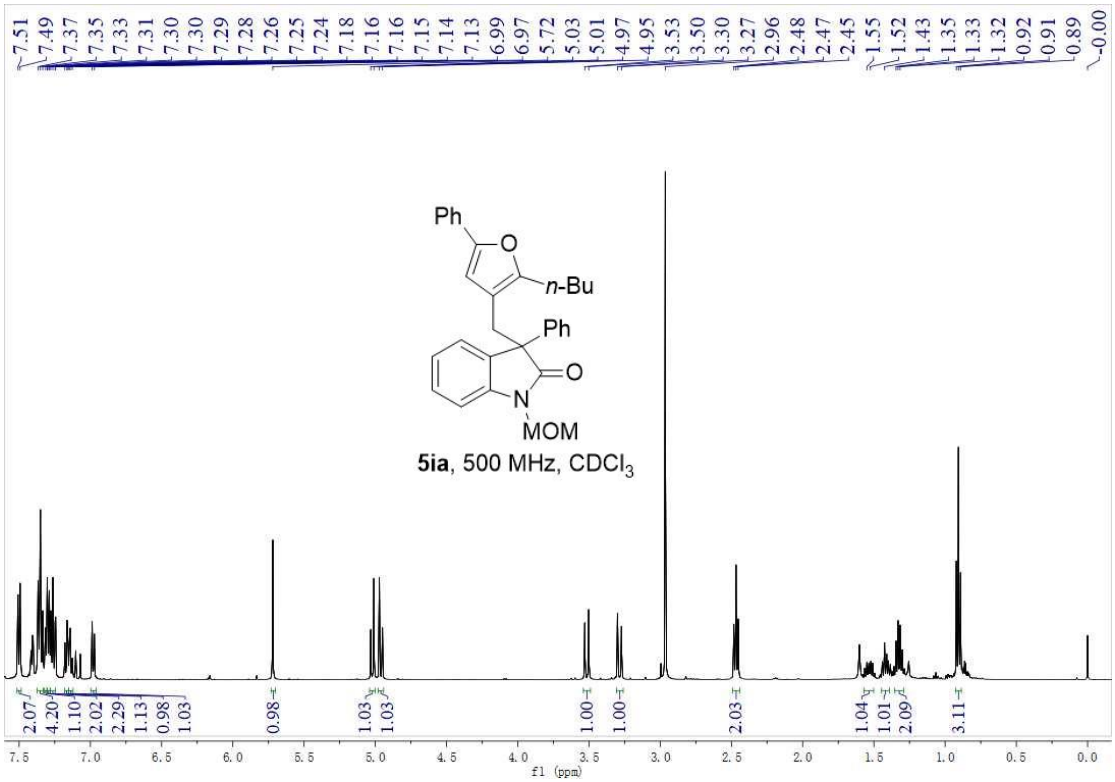
5fa, 125 MHz, $CDCl_3$

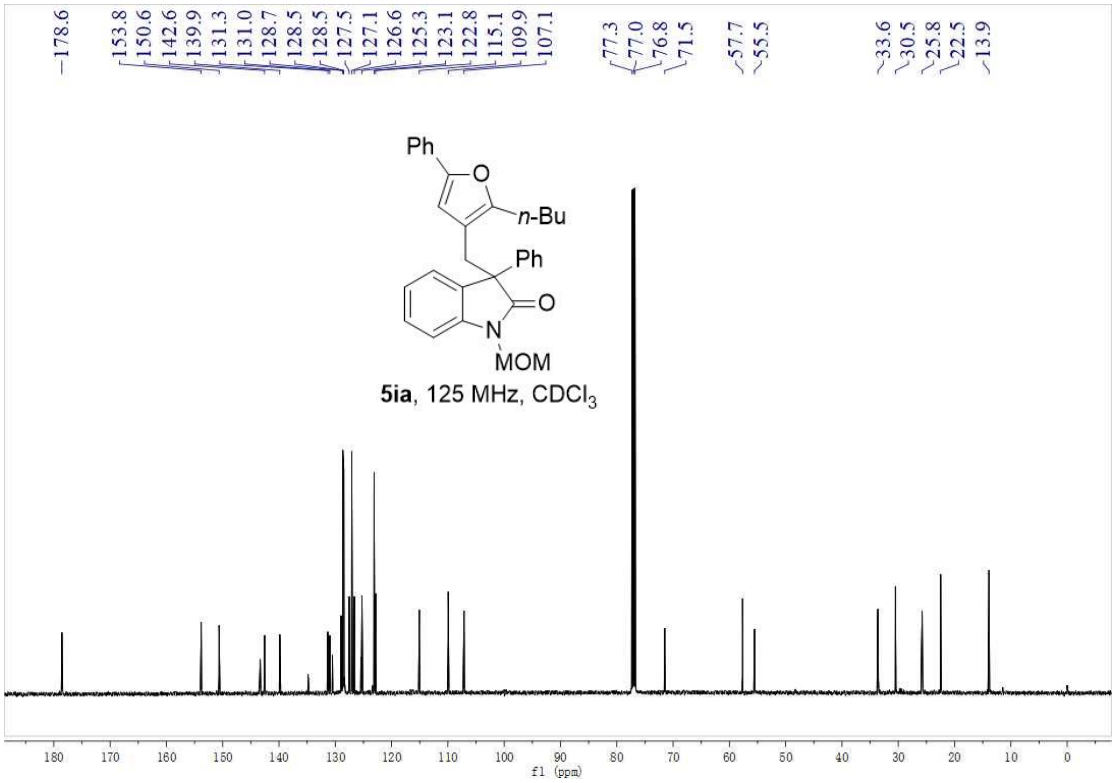

7.49 7.48 7.39 7.37 7.35 7.34 7.32 7.29 7.28 7.28 7.27 7.26 7.26 7.25 7.25 7.24 7.13 7.10 7.09 6.74 6.73 5.74 3.50 3.47 3.27 3.24 2.45 2.45 2.45 2.44 1.37 1.36 1.34 1.33 1.31 1.13 1.12 0.92 0.90 0.89 0.74 0.72 0.71 0.00
Ph
O
n-Bu
Ph
O
N
n-Bu
5ga, 500 MHz, CDCl3
2.04 2.03 2.01 5.04 1.04 1.02 0.99 0.98 1.05 1.01 1.05 1.04 2.05 1.02 1.02 4.07 2.07 3.06 3.05
f1 (ppm)

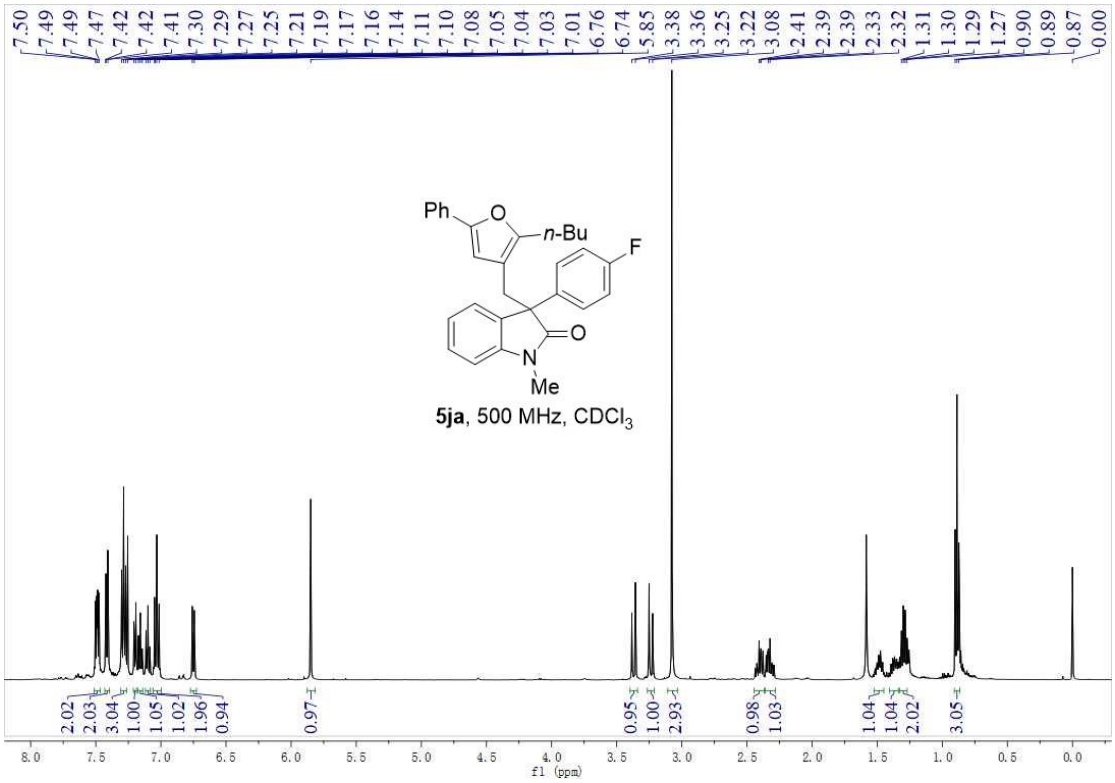

177.8 153.7 150.4 143.8 140.1 132.2 131.1 128.6 128.4 128.2 127.3 127.1 126.4 125.1 123.1 122.0 115.0 108.5 107.2 77.3 77.0 76.8 57.1 39.9 33.6 30.5 29.3 25.7 22.5 20.0 13.9 13.7
Ph
O
n-Bu
Ph
O
N
n-Bu
5ga, 125 MHz, CDCl3
f1 (ppm)

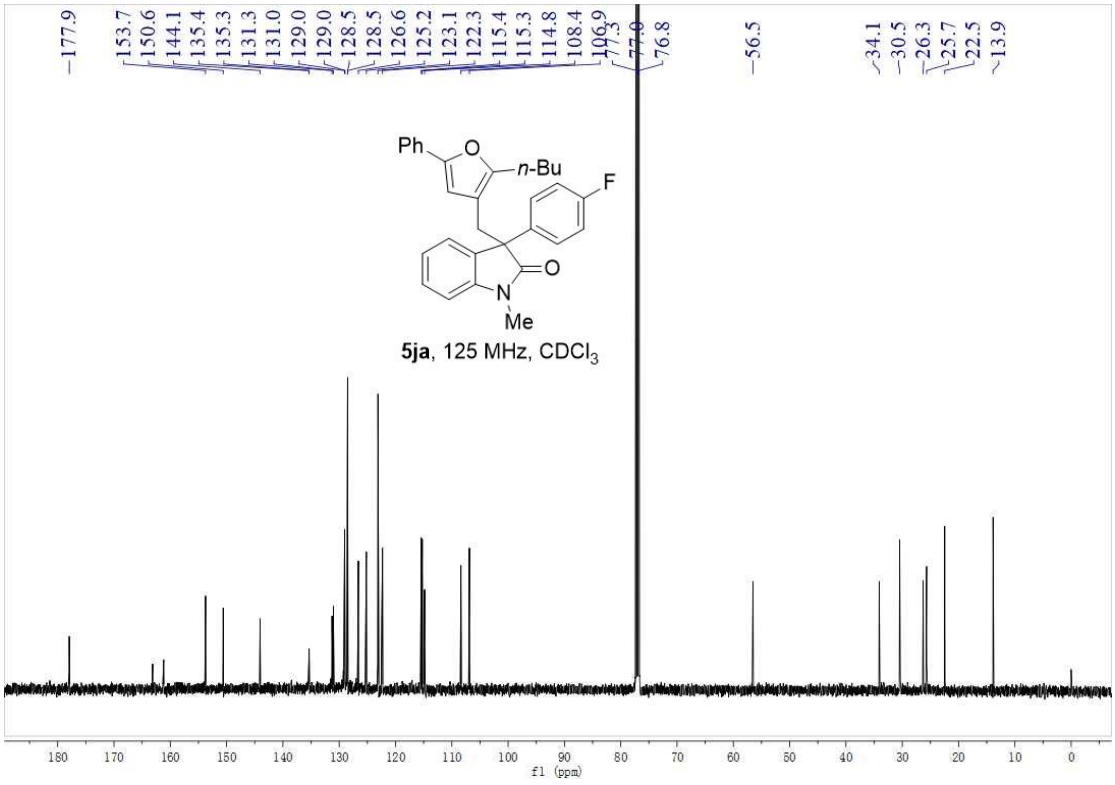

Ph
O
n-Bu
Ph
O
N
Bn
5ha, 500 MHz, CDCl3
f1 (ppm)

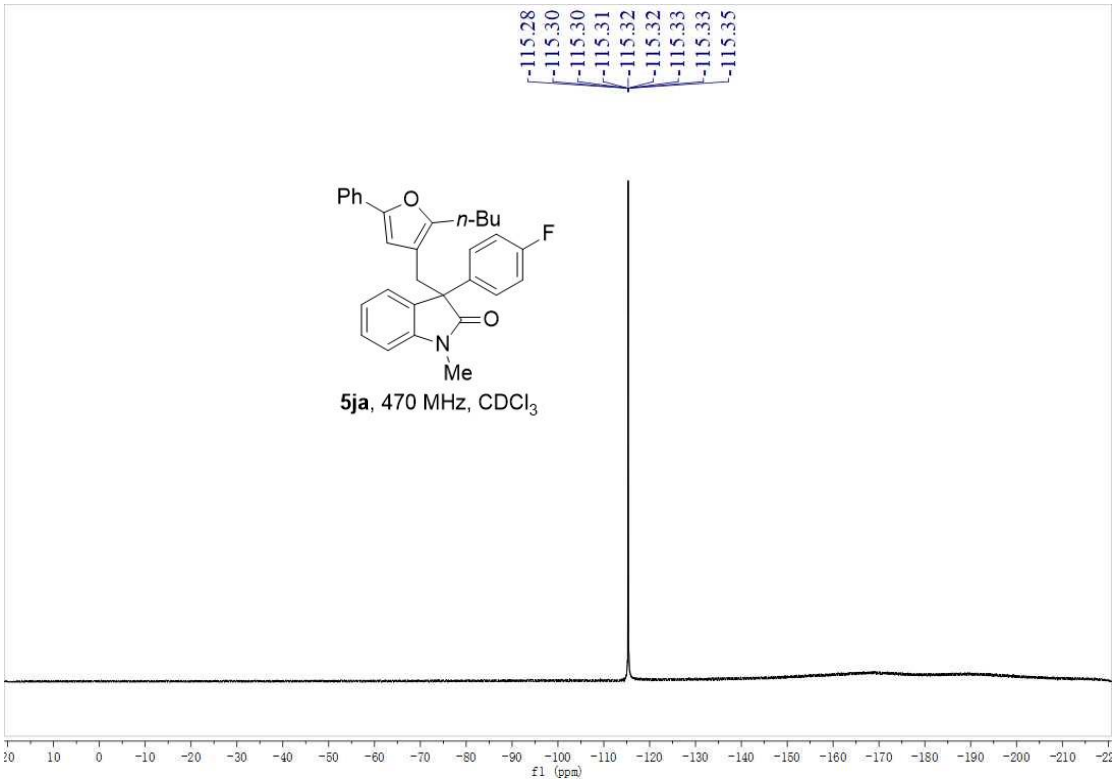

Ph
O
n-Bu
Ph
O
N
Bn
5ha, 125 MHz, CDCl3
f1 (ppm)

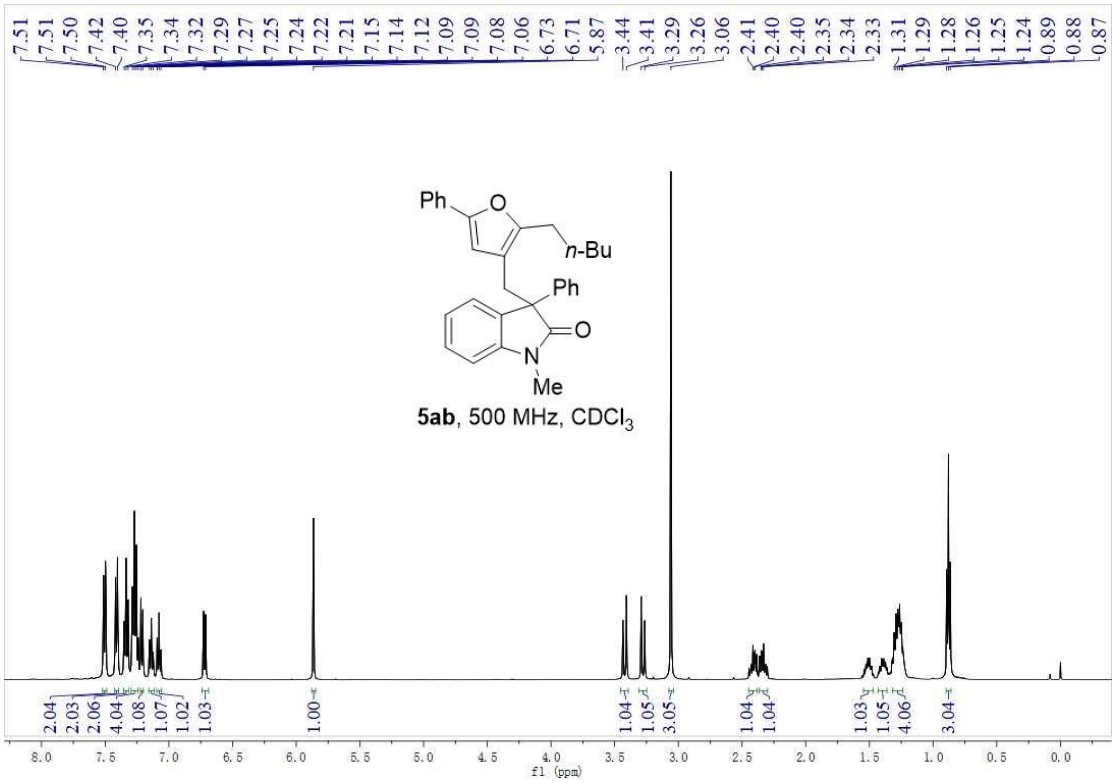

Ph
O
n-Bu
Ph
O
N
MOM
5ia, 500 MHz, CDCl3
f1 (ppm)

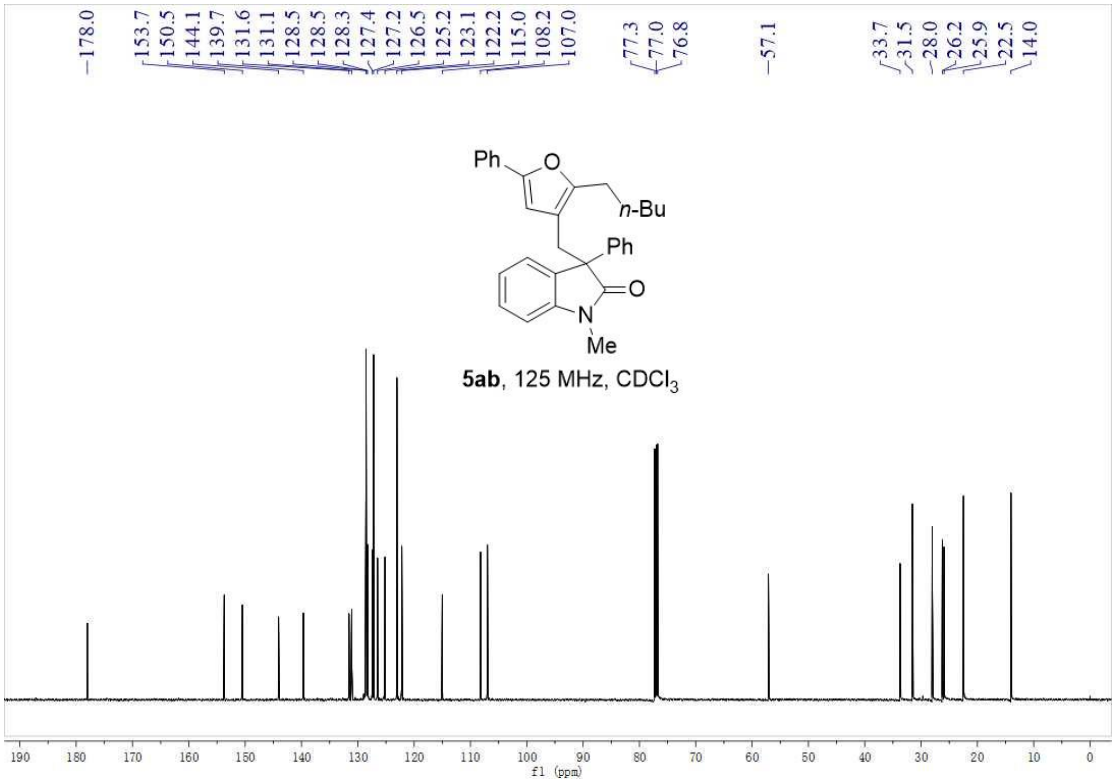

Ph
O
n-Bu
Ph
O
N
MOM
5ia, 125 MHz, CDCl3
f1 (ppm)

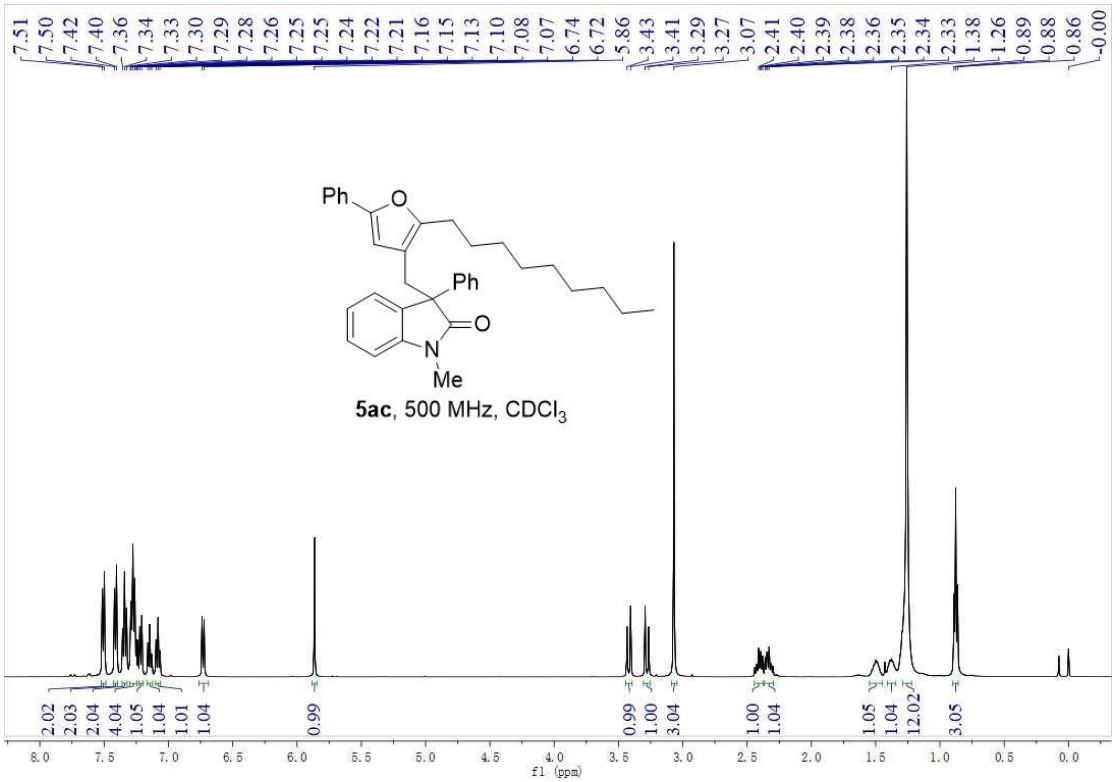

Ph
O
n-Bu
F
O
N
Me
5ja, 500 MHz, CDCl3
f1 (ppm)

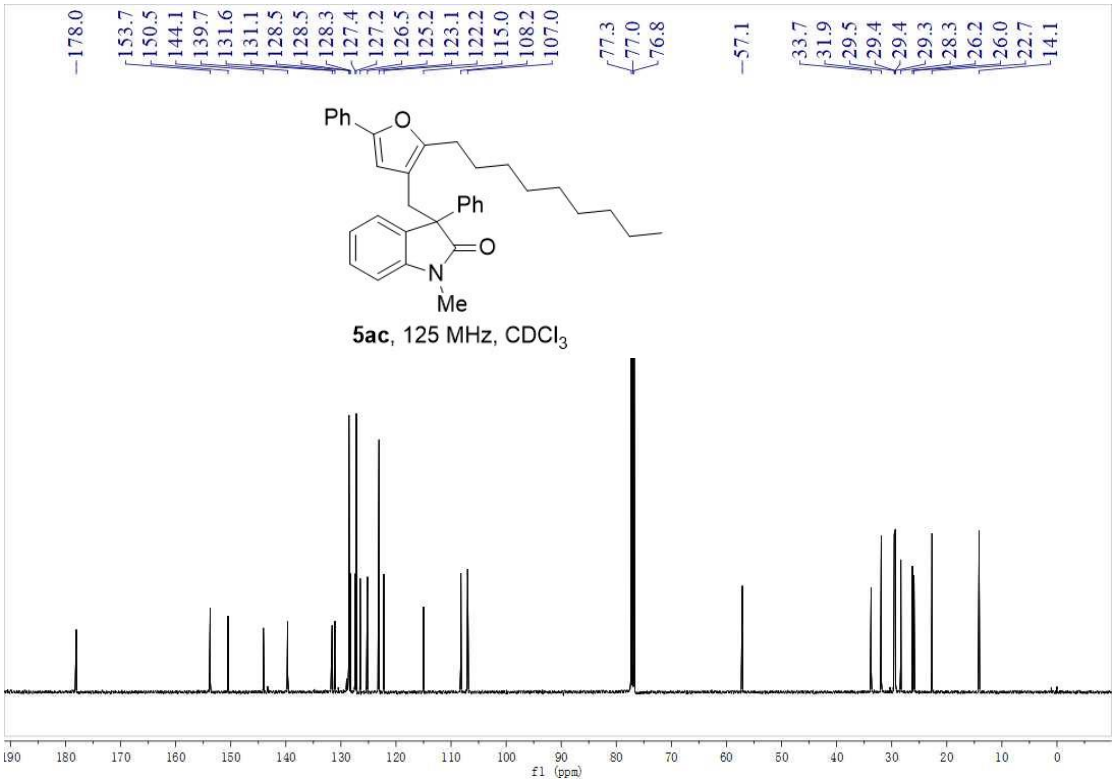

Ph
O
n-Bu
F
O
N
Me
5ja, 125 MHz, CDCl3
f1 (ppm)

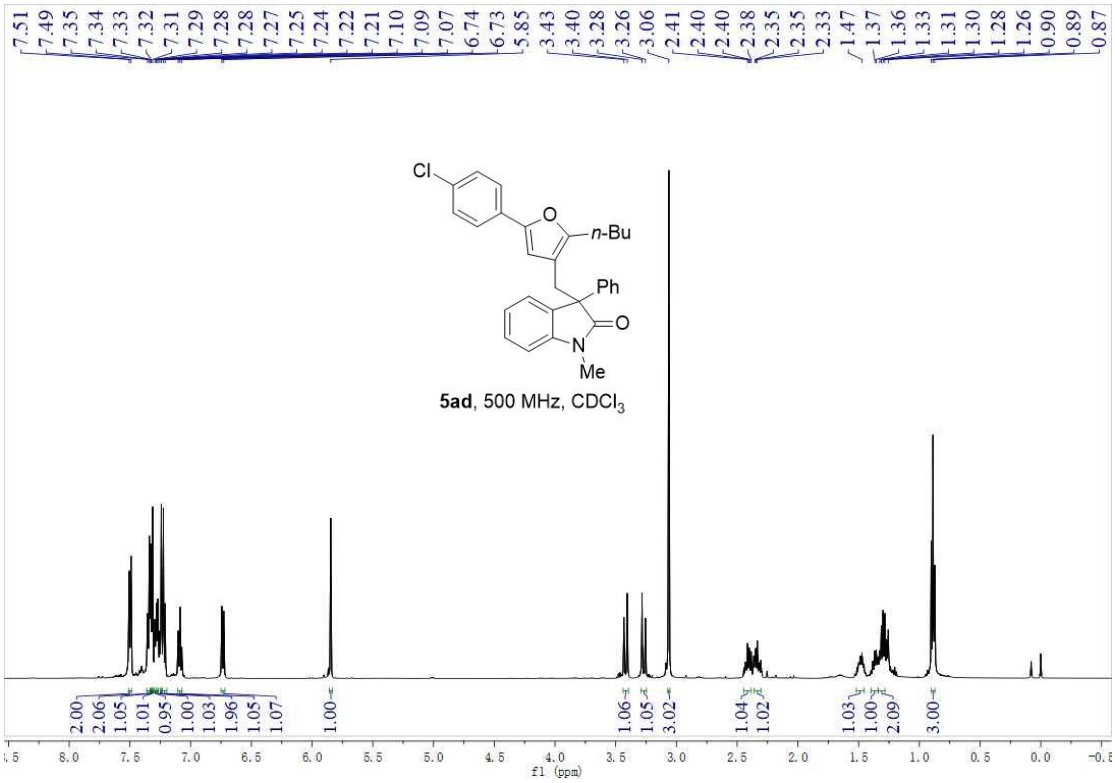

-115.28
-115.30
-115.30
-115.31
-115.32
-115.32
-115.33
-115.33
-115.35
Ph
O
n-Bu
F
O
N
Me
5ja, 470 MHz, CDCl3
f1 (ppm)

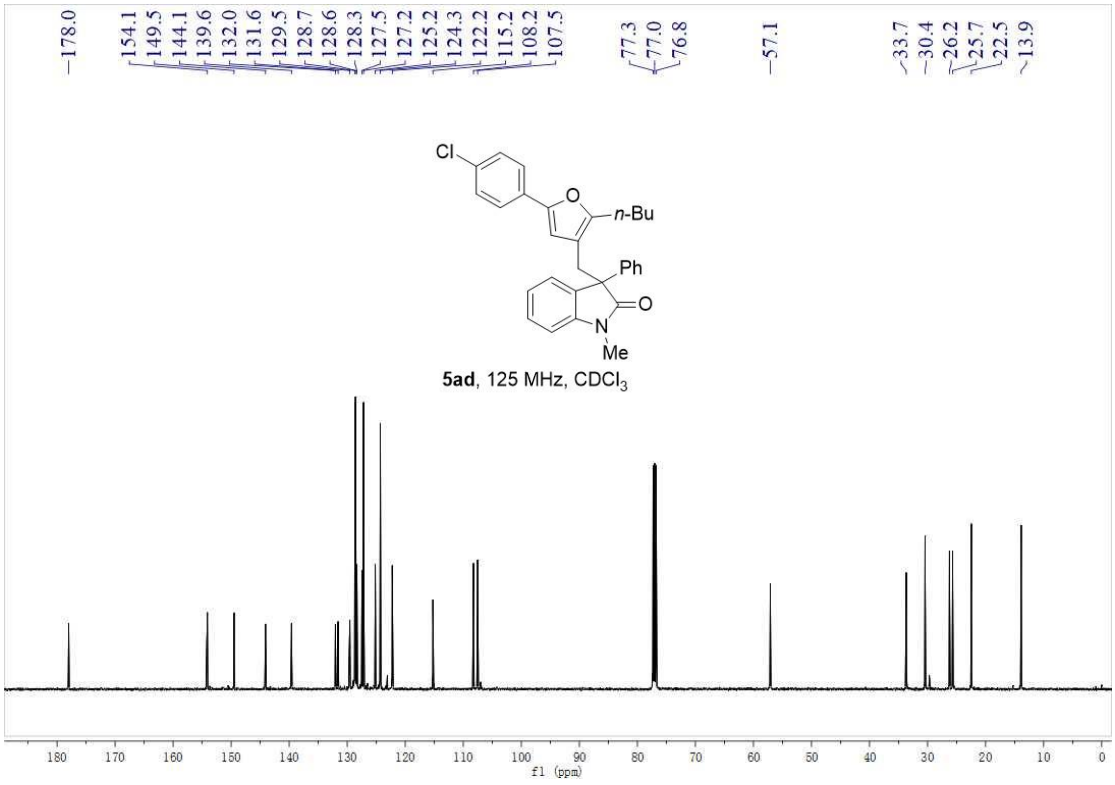

Ph
O
n-Bu
Ph
O
N
Me
5ab, 500 MHz, CDCl3
f1 (ppm)

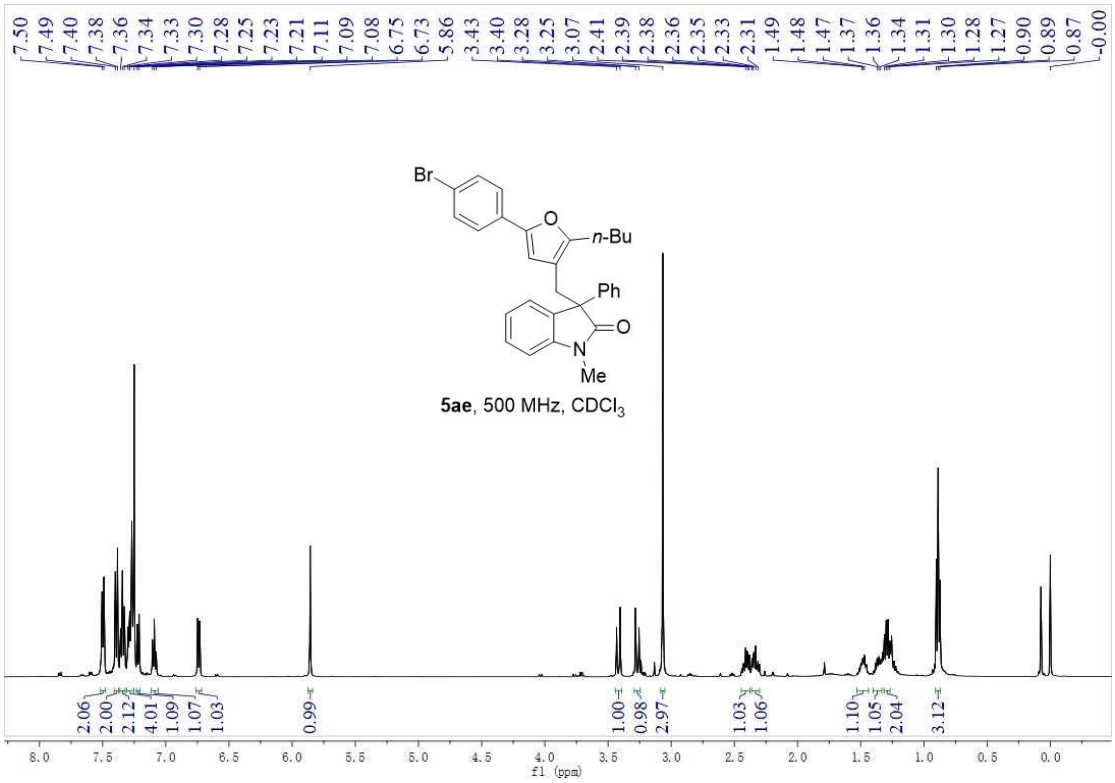

Ph
O
n-Bu
Ph
O
N
Me
5ab, 125 MHz, CDCl3
f1 (ppm)

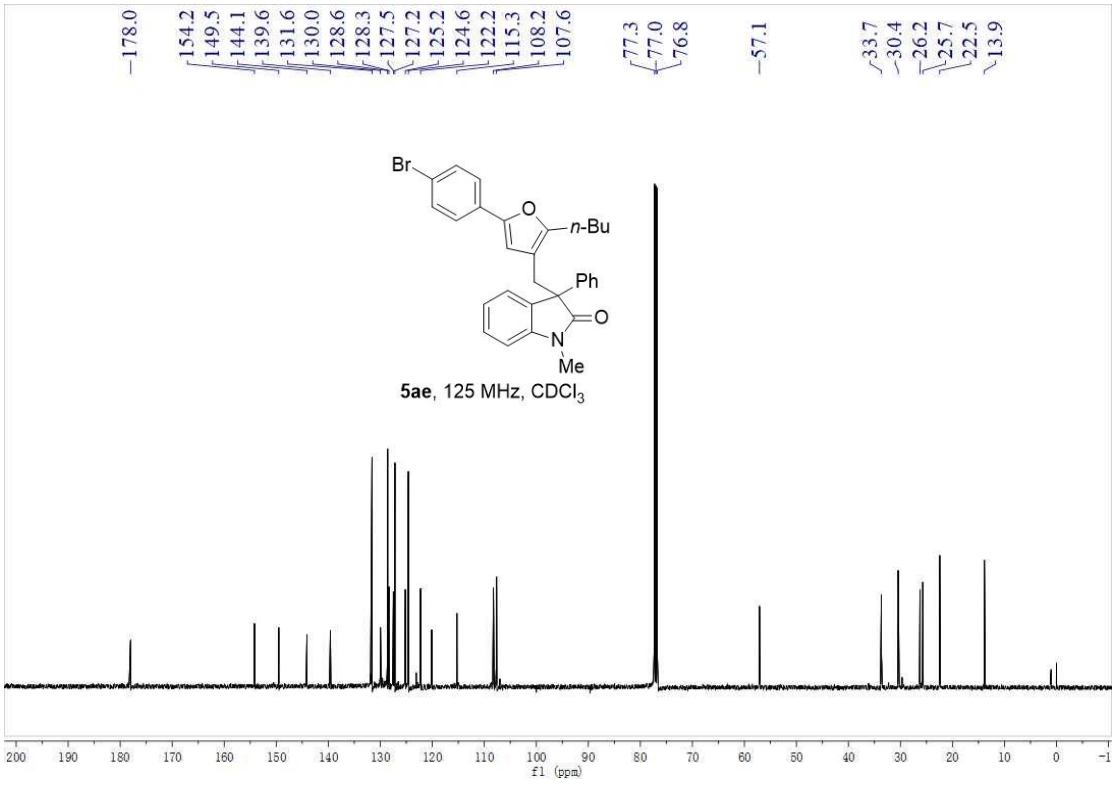

Ph
O
Ph
O
N
Me
5ac, 500 MHz, CDCl3
f1 (ppm)

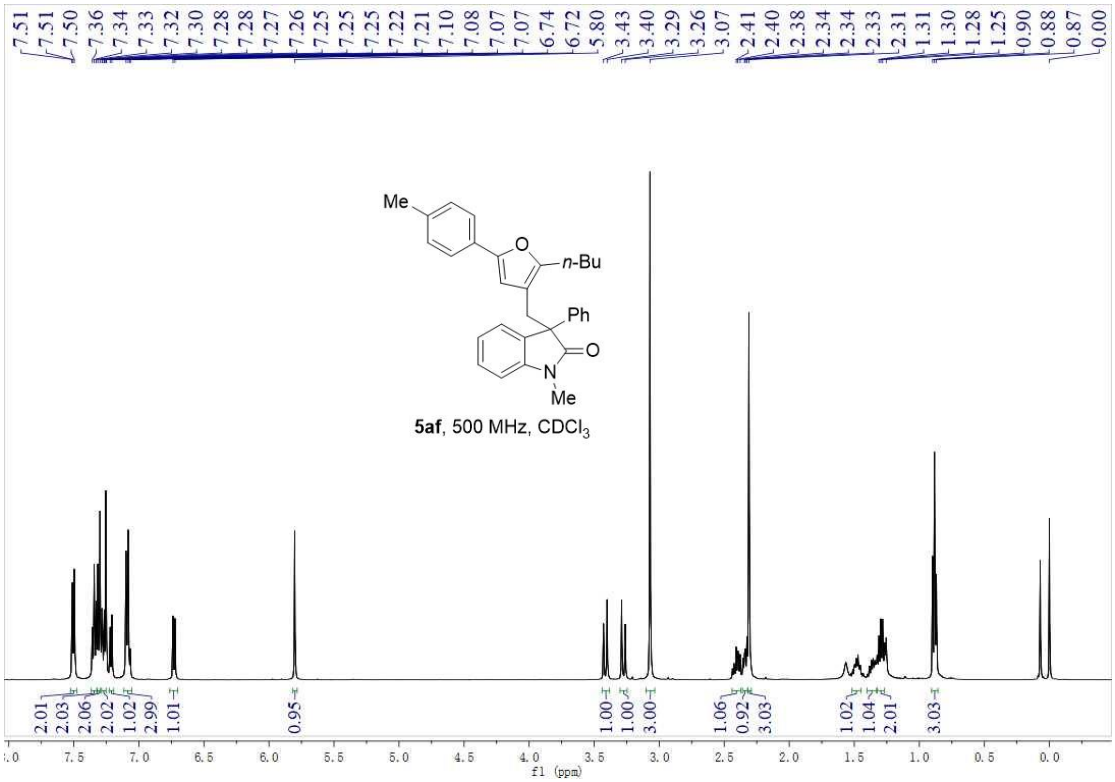

Ph
O
Ph
O
N
Me
5ac, 125 MHz, CDCl3
f1 (ppm)

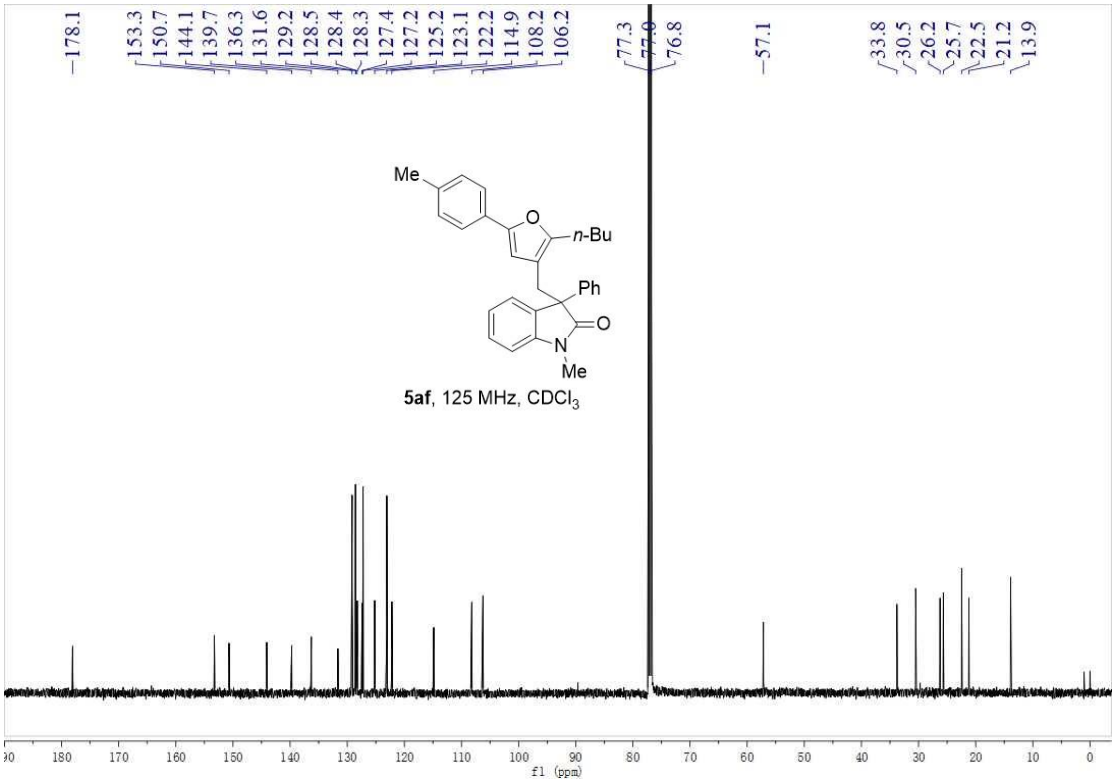

7.51
7.49
7.35
7.34
7.33
7.32
7.31
7.29
7.28
7.28
7.27
7.25
7.24
7.22
7.21
7.10
7.09
7.07
6.74
6.73
5.85
3.43
3.40
3.28
3.26
3.06
2.41
2.40
2.40
2.38
2.35
2.35
2.33
1.47
1.37
1.36
1.33
1.31
1.30
1.28
1.26
0.90
0.89
0.87
Cl
O
n-Bu
Ph
O
N
Me
5ad, 500 MHz, CDCl3
2.00
2.06
1.05
1.01
0.95
1.00
1.03
1.96
1.05
1.07
1.00
1.06
1.05
3.02
1.04
1.02
1.03
1.00
2.09
3.00
f1 (ppm)

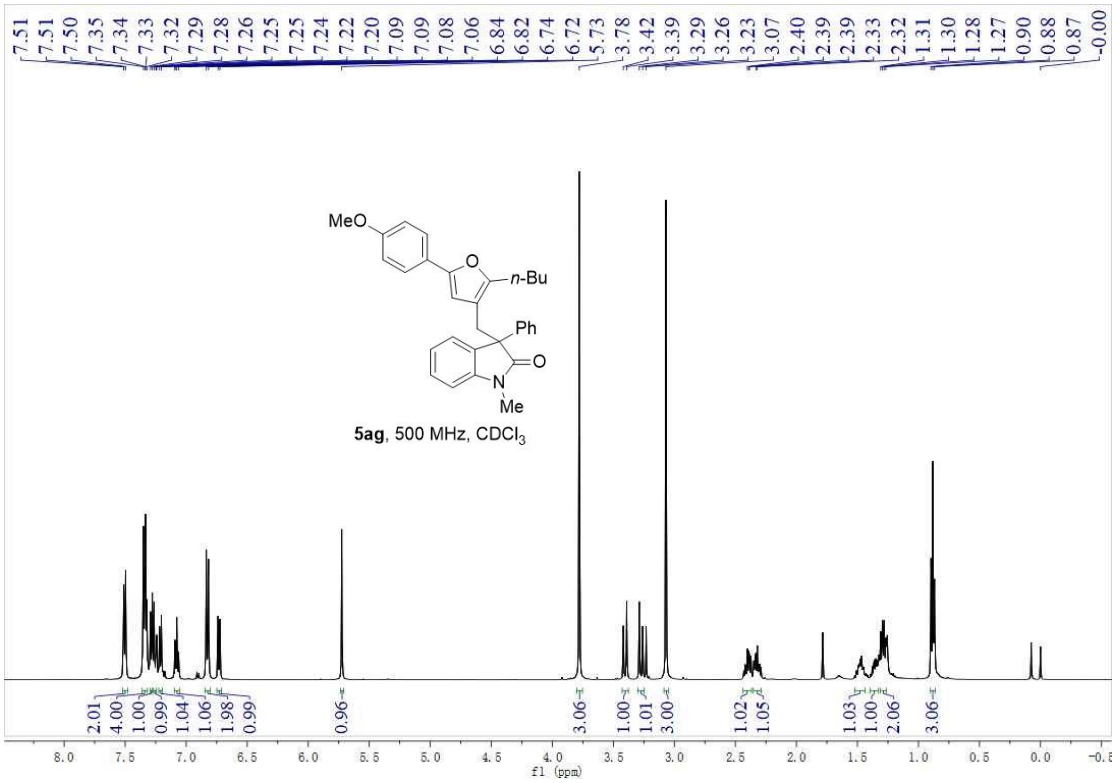

178.0
154.1
149.5
144.1
139.6
132.0
131.6
129.5
128.7
128.6
128.3
127.5
127.2
125.2
124.3
122.2
115.2
108.2
107.5
77.3
77.0
76.8
57.1
33.7
30.4
26.2
25.7
22.5
13.9
Cl
O
n-Bu
Ph
O
N
Me
5ad, 125 MHz, CDCl3
f1 (ppm)

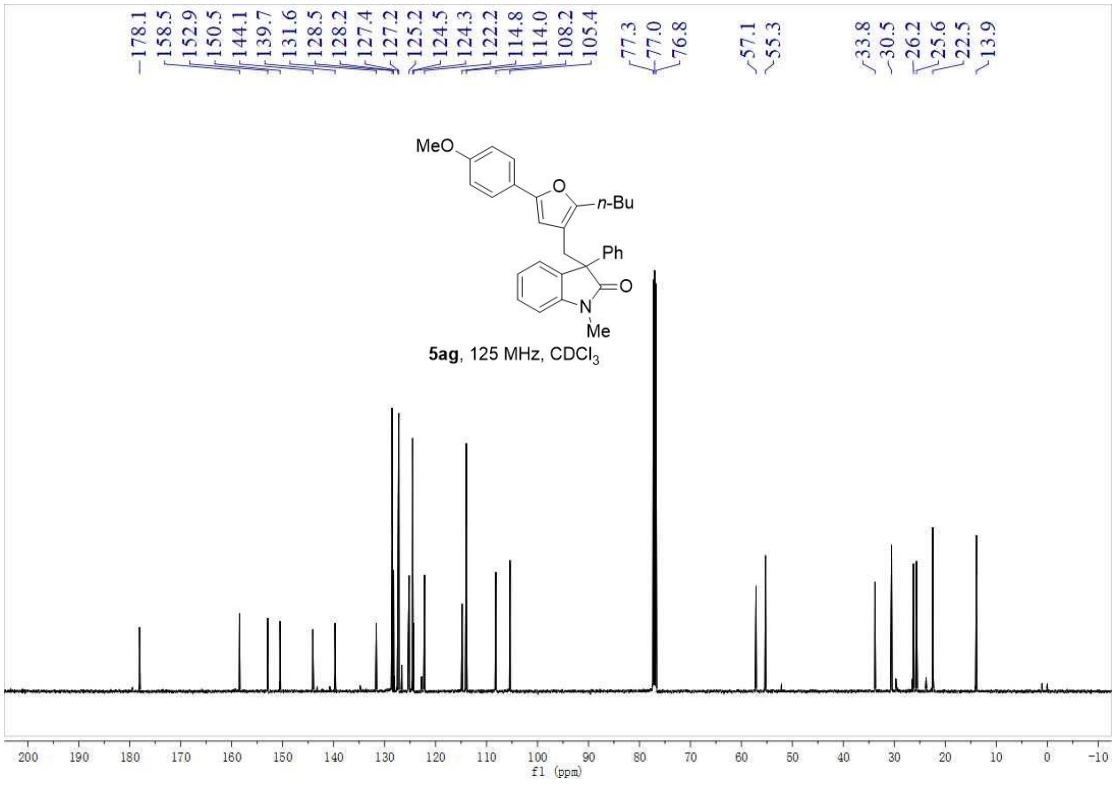

7.50
7.49
7.40
7.38
7.36
7.34
7.33
7.30
7.28
7.25
7.23
7.21
7.11
7.09
7.08
6.75
6.73
5.86
3.43
3.40
3.28
3.25
3.07
2.41
2.39
2.38
2.36
2.35
2.33
2.31
1.49
1.48
1.47
1.37
1.36
1.34
1.31
1.30
1.28
1.27
0.90
0.89
0.87
0.00
Br
O
n-Bu
Ph
O
N
Me
5ae, 500 MHz, CDCl3
2.06
2.00
2.12
4.01
1.09
1.07
1.03
0.99
1.00
0.98
2.97
1.03
1.06
1.10
1.05
2.04
3.12
f1 (ppm)

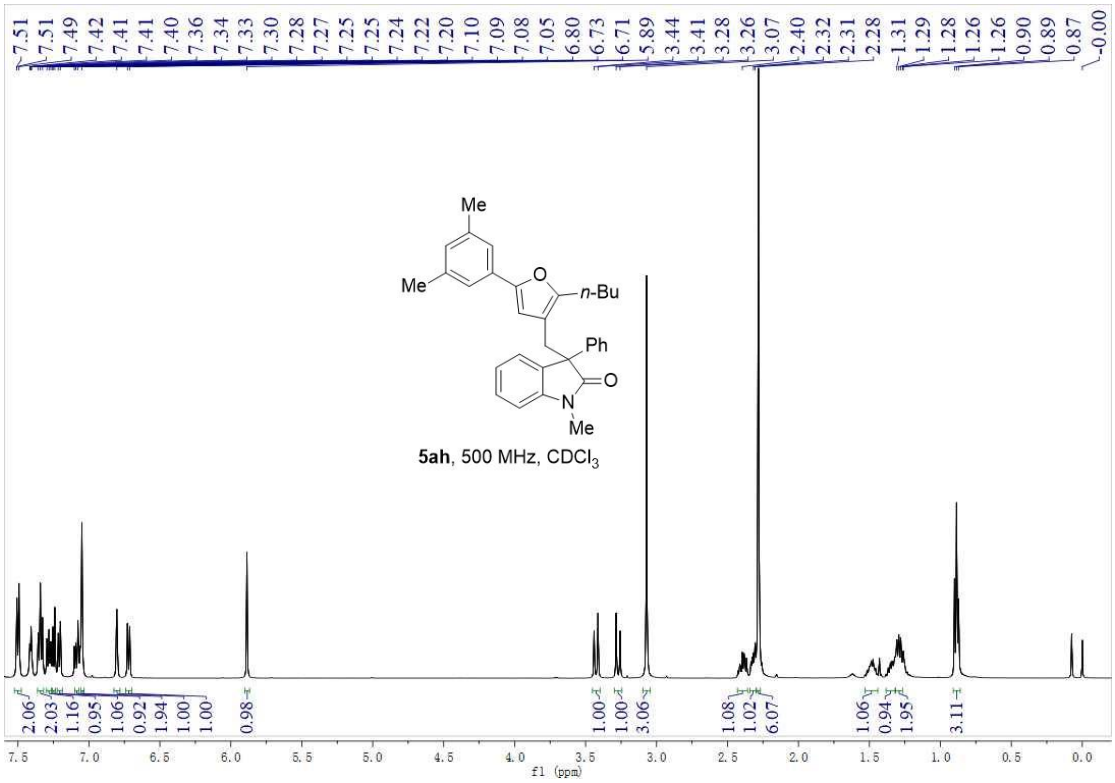

178.0
154.2
149.5
144.1
139.6
131.6
130.0
128.6
128.3
127.5
127.2
125.2
124.6
122.2
115.3
108.2
107.6
77.3
77.0
76.8
57.1
33.7
30.4
26.2
25.7
22.5
13.9
Br
O
n-Bu
Ph
O
N
Me
5ae, 125 MHz, CDCl3
f1 (ppm)

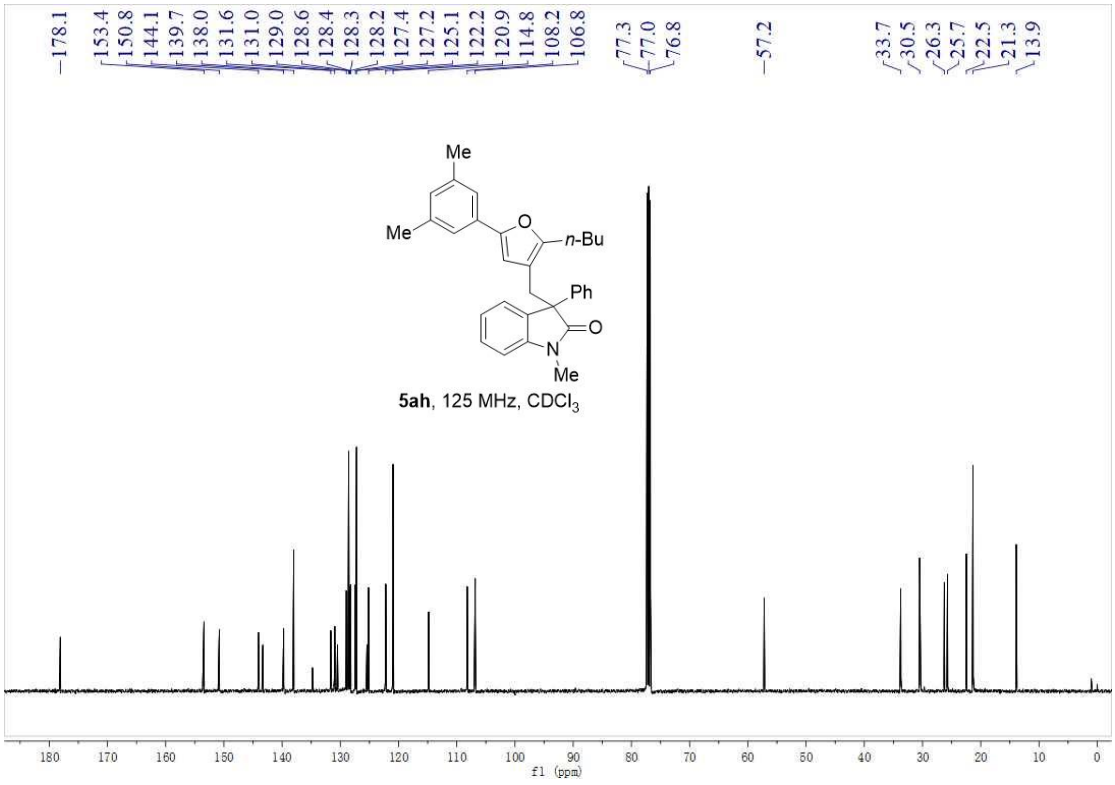

Me
O
n-Bu
Ph
O
N
Me
5af, 500 MHz, CDCl3
f1 (ppm)

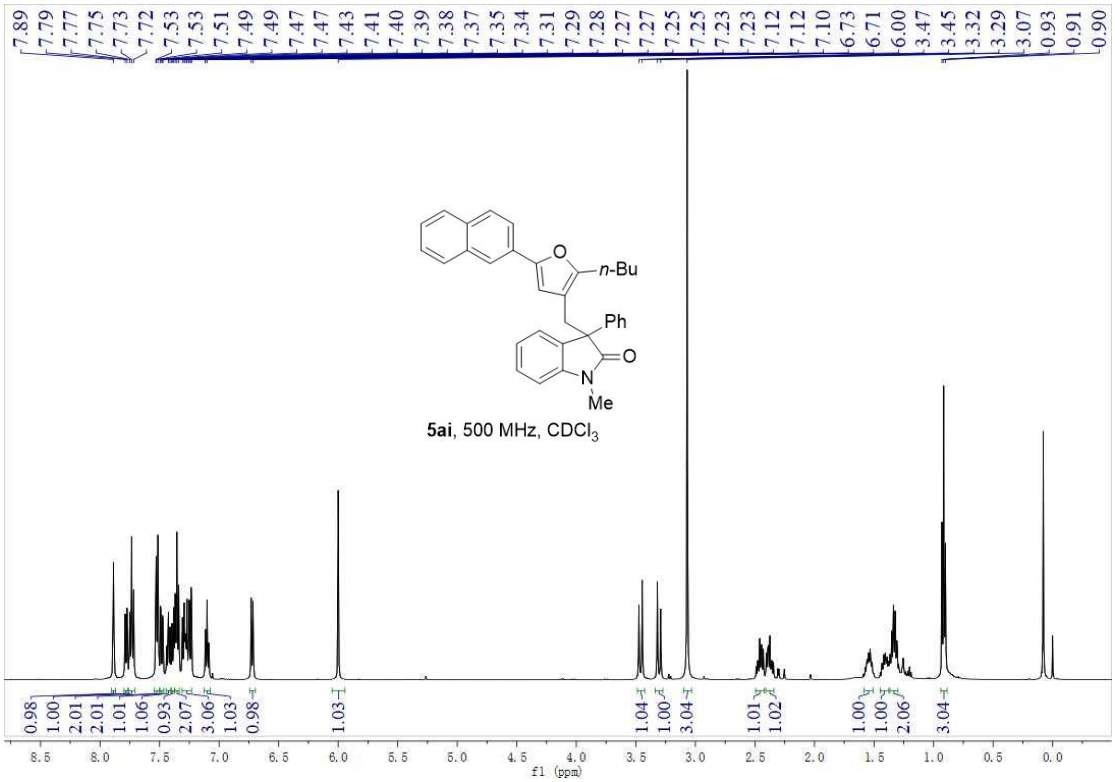

Me
O
n-Bu
Ph
O
N
Me
5af, 125 MHz, CDCl3
f1 (ppm)

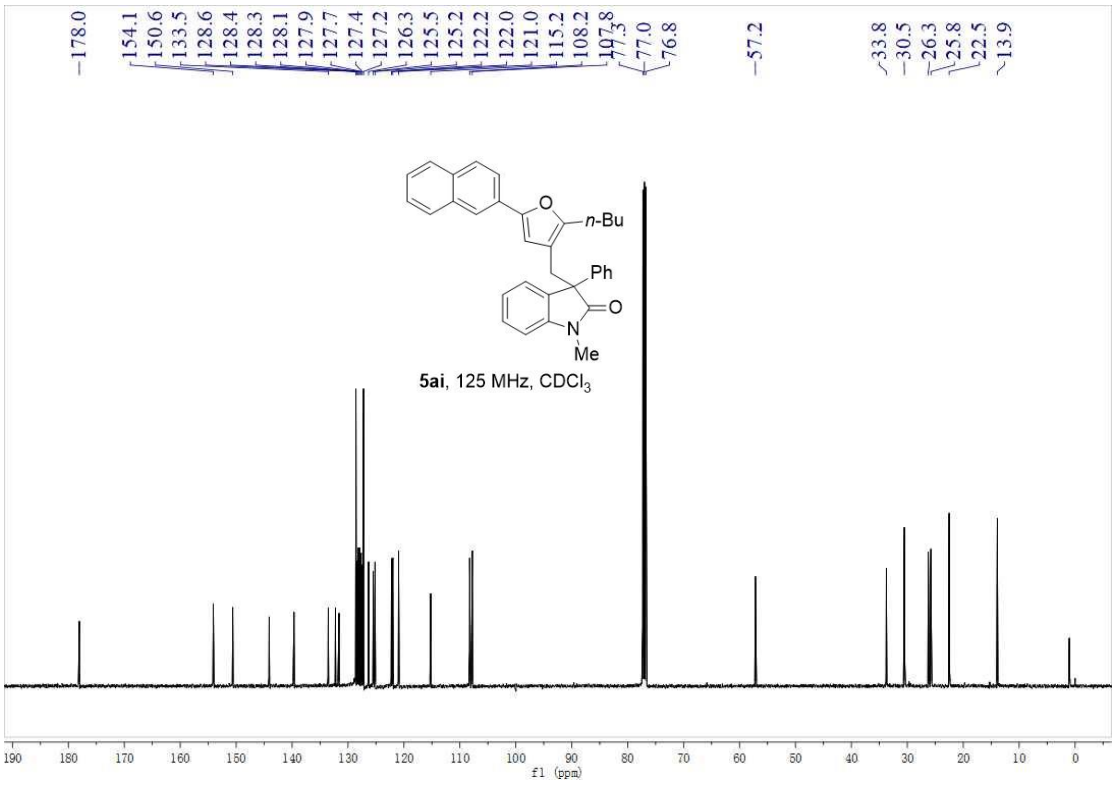

MeO
O
n-Bu
Ph
O
N
Me
5ag, 500 MHz, CDCl3
f1 (ppm)

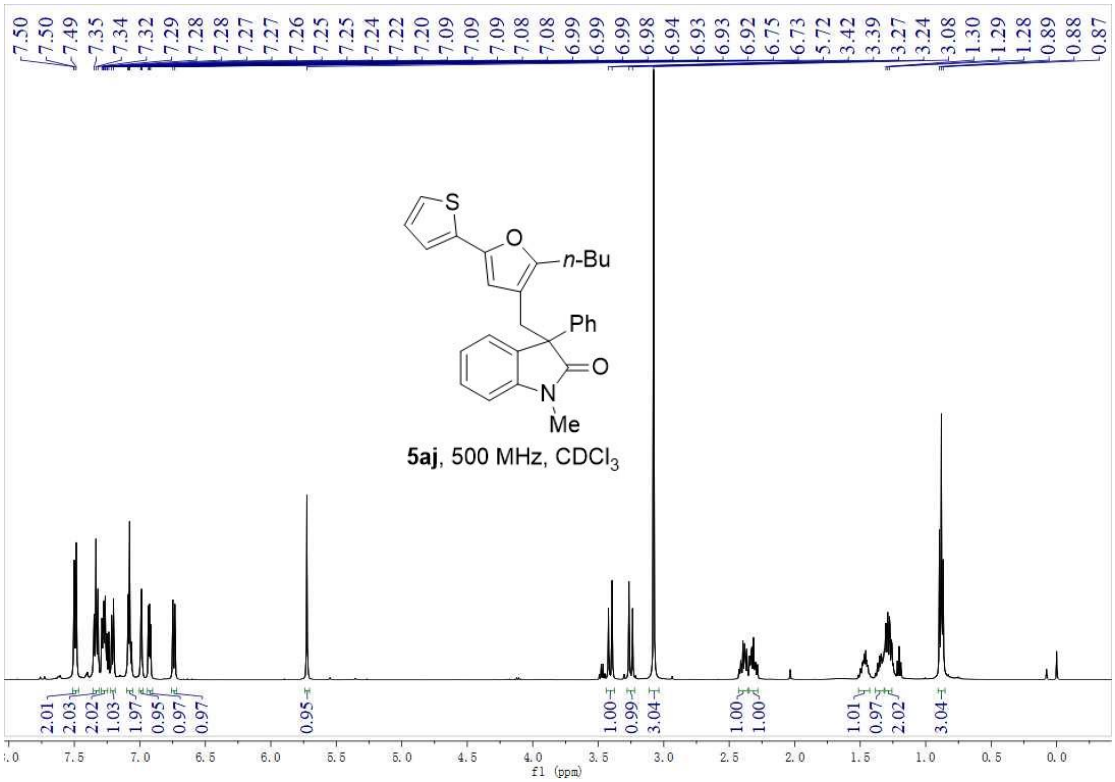

MeO
O
n-Bu
Ph
O
N
Me
5ag, 125 MHz, CDCl3
f1 (ppm)

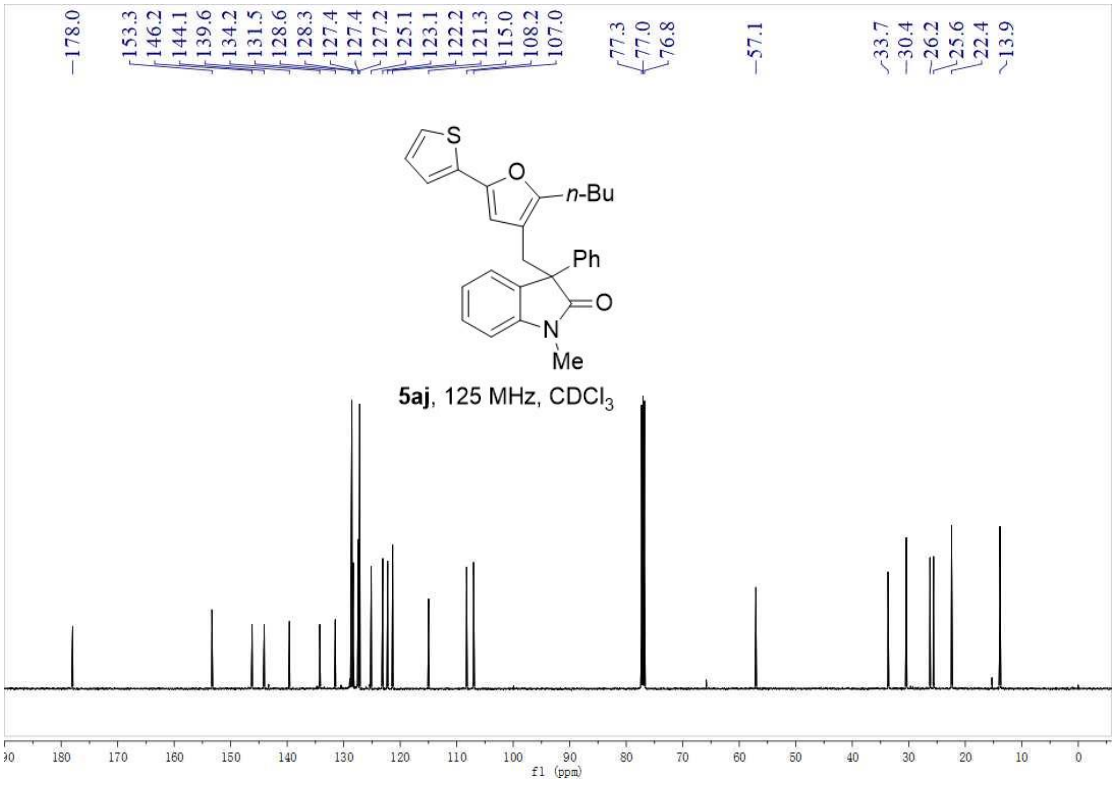

Me
Me
O
n-Bu
Ph
O
N
Me
5ah, 500 MHz, CDCl3
f1 (ppm)

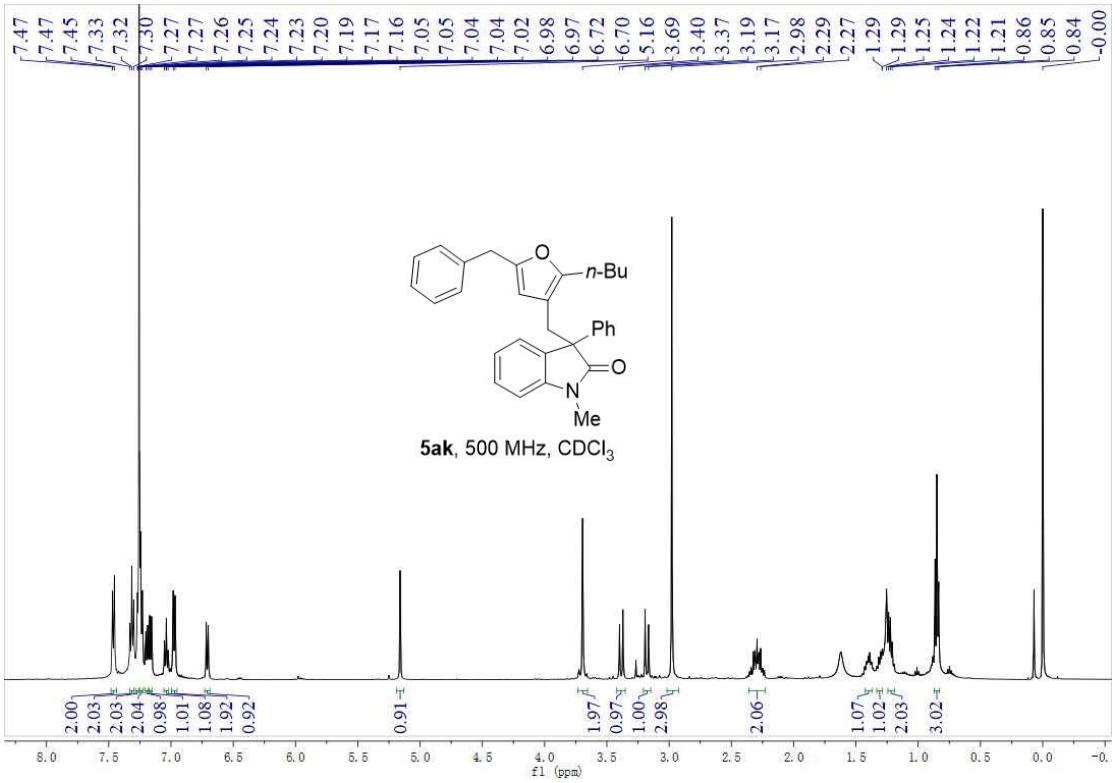

Me
Me
O
n-Bu
Ph
O
N
Me
5ah, 125 MHz, CDCl3
f1 (ppm)

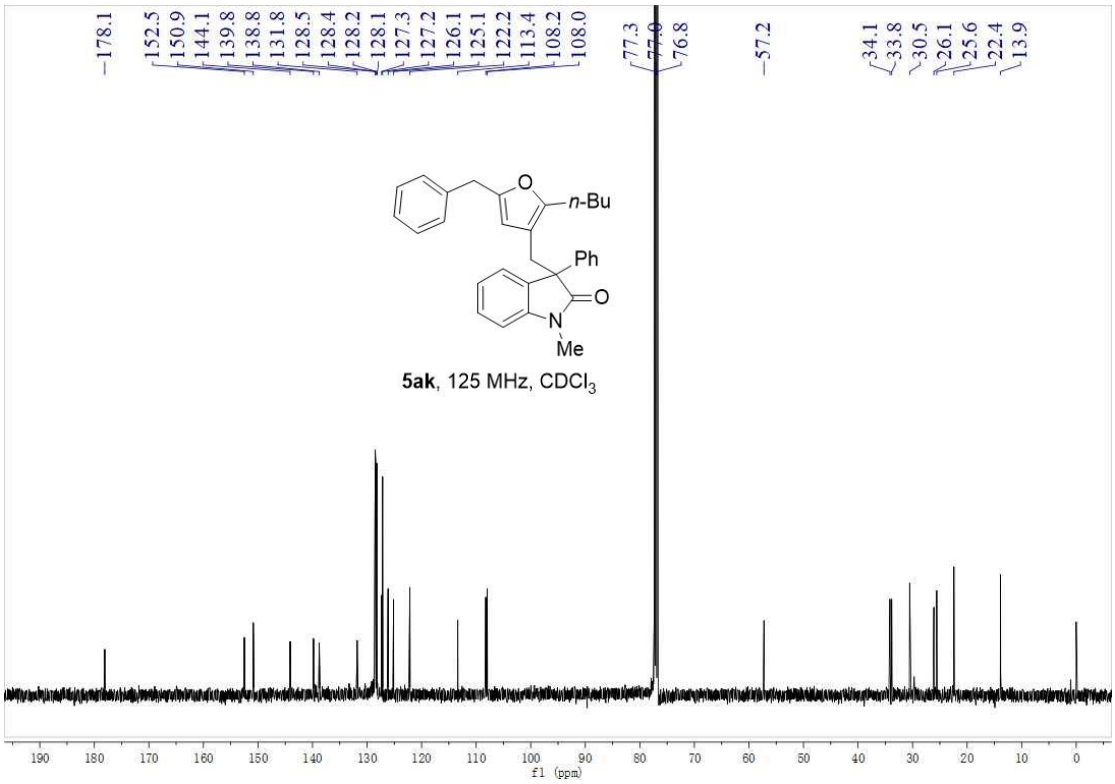

7.89
7.79
7.77
7.75
7.73
7.72
7.53
7.53
7.51
7.49
7.49
7.47
7.47
7.43
7.41
7.40
7.39
7.38
7.37
7.35
7.34
7.31
7.29
7.28
7.27
7.27
7.25
7.25
7.23
7.23
7.12
7.12
7.10
6.73
6.71
6.00
3.47
3.45
3.32
3.29
3.07
0.93
0.91
0.90
O
n-Bu
Ph
O
N
Me
5ai, 500 MHz, CDCl3
0.98
1.00
2.01
2.01
1.01
1.06
0.93
2.07
3.06
1.03
0.98
1.03
1.04
1.00
3.04
1.01
1.02
1.00
1.00
2.06
3.04
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)

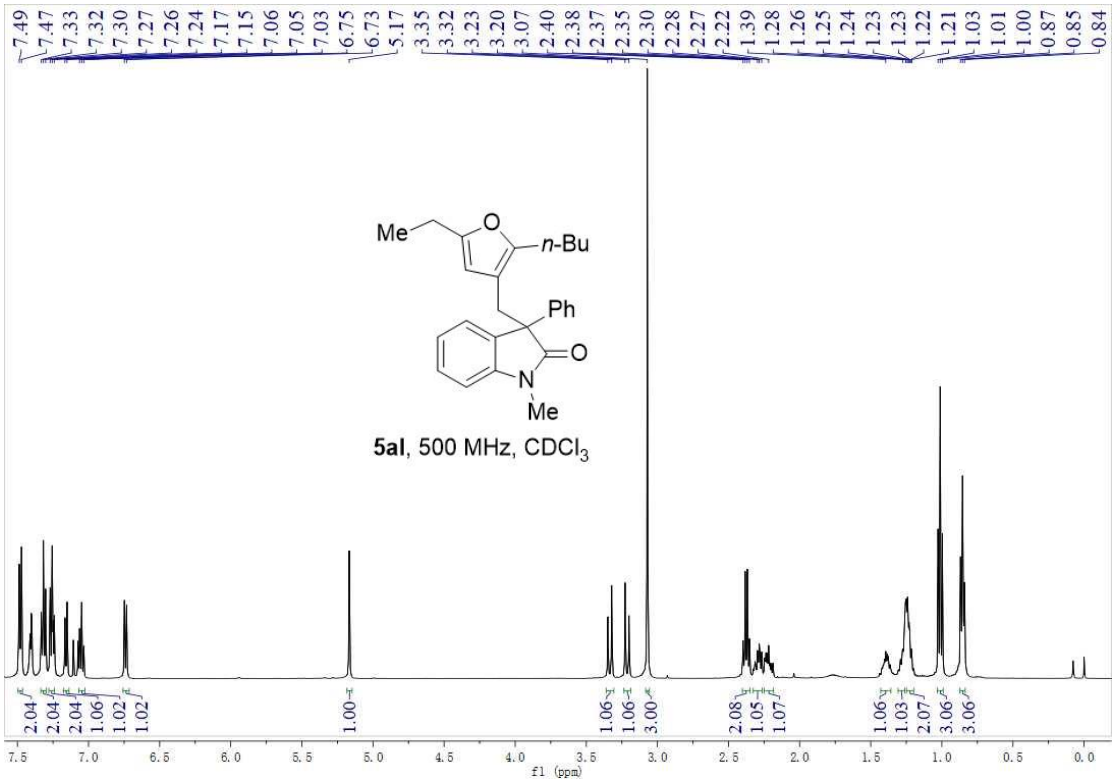

178.0
154.1
150.6
133.5
128.6
128.4
128.3
128.1
127.9
127.7
127.4
127.2
126.3
125.5
125.2
122.2
122.0
121.0
115.2
108.2
107.8
77.3
77.0
76.8
57.2
33.8
30.5
26.3
25.8
22.5
13.9
O
n-Bu
Ph
O
N
Me
5ai, 125 MHz, CDCl3
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

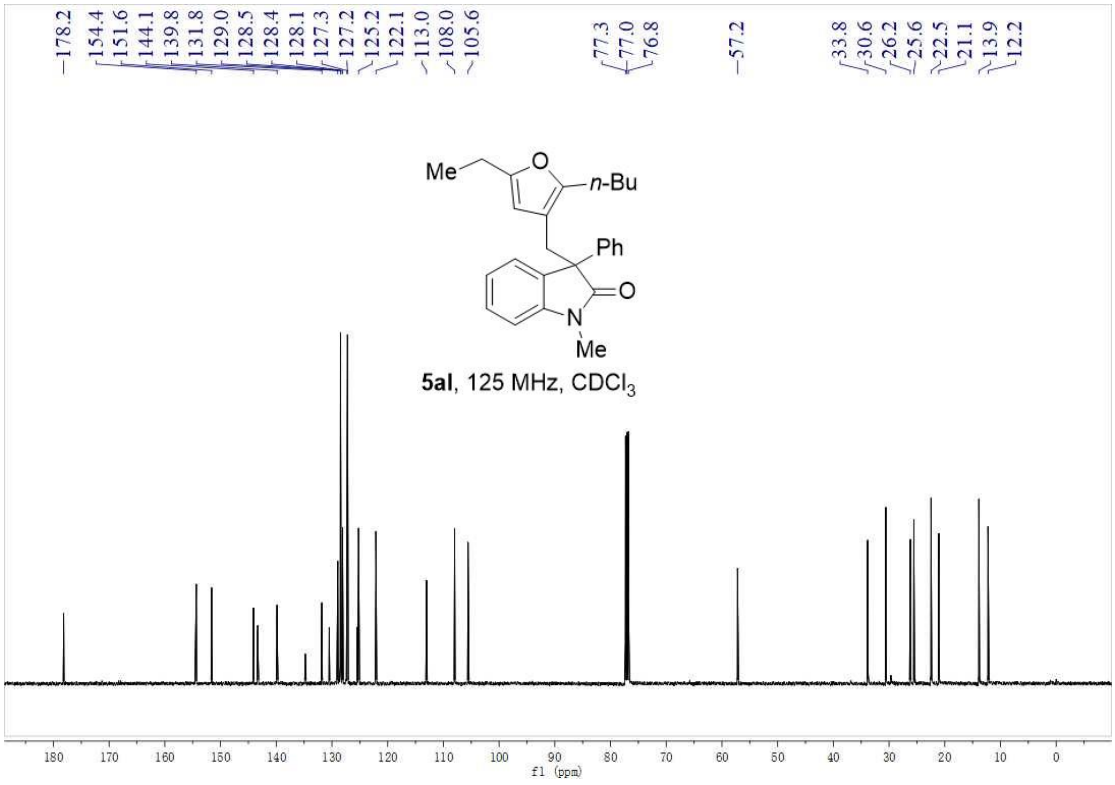

7.50
7.50
7.49
7.35
7.34
7.32
7.29
7.28
7.28
7.27
7.27
7.26
7.25
7.25
7.24
7.22
7.20
7.09
7.09
7.09
7.08
7.08
6.99
6.99
6.99
6.98
6.94
6.93
6.93
6.92
6.75
6.73
5.72
3.42
3.39
3.27
3.24
3.08
1.30
1.29
1.28
0.89
0.88
0.87
S
O
n-Bu
Ph
O
N
Me
5aj, 500 MHz, CDCl3
2.01
2.03
2.02
1.03
1.97
0.95
0.97
0.97
0.95
1.00
0.99
3.04
1.00
1.00
1.01
0.97
2.02
3.04
f1 (ppm)

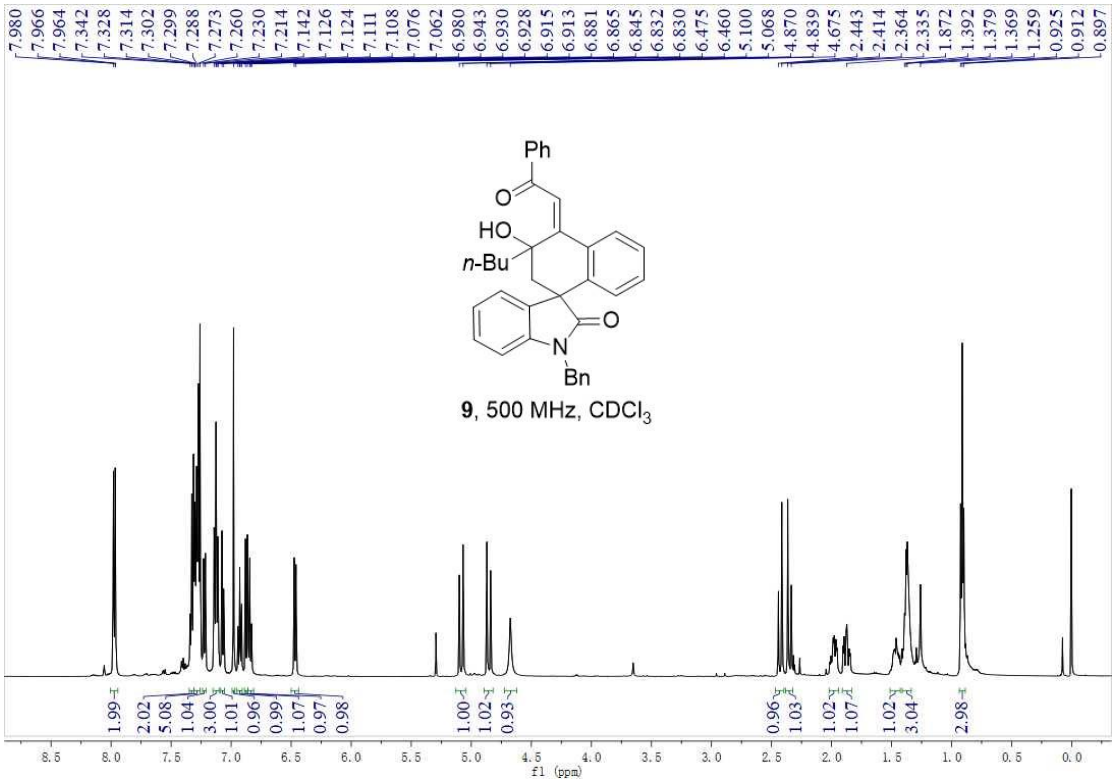

178.0
153.3
146.2
144.1
139.6
134.2
131.5
128.6
128.3
127.4
127.4
127.2
125.1
123.1
122.2
121.3
115.0
108.2
107.0
77.3
77.0
76.8
57.1
33.7
30.4
26.2
25.6
22.4
13.9
S
O
n-Bu
Ph
O
N
Me
5aj, 125 MHz, CDCl3
f1 (ppm)

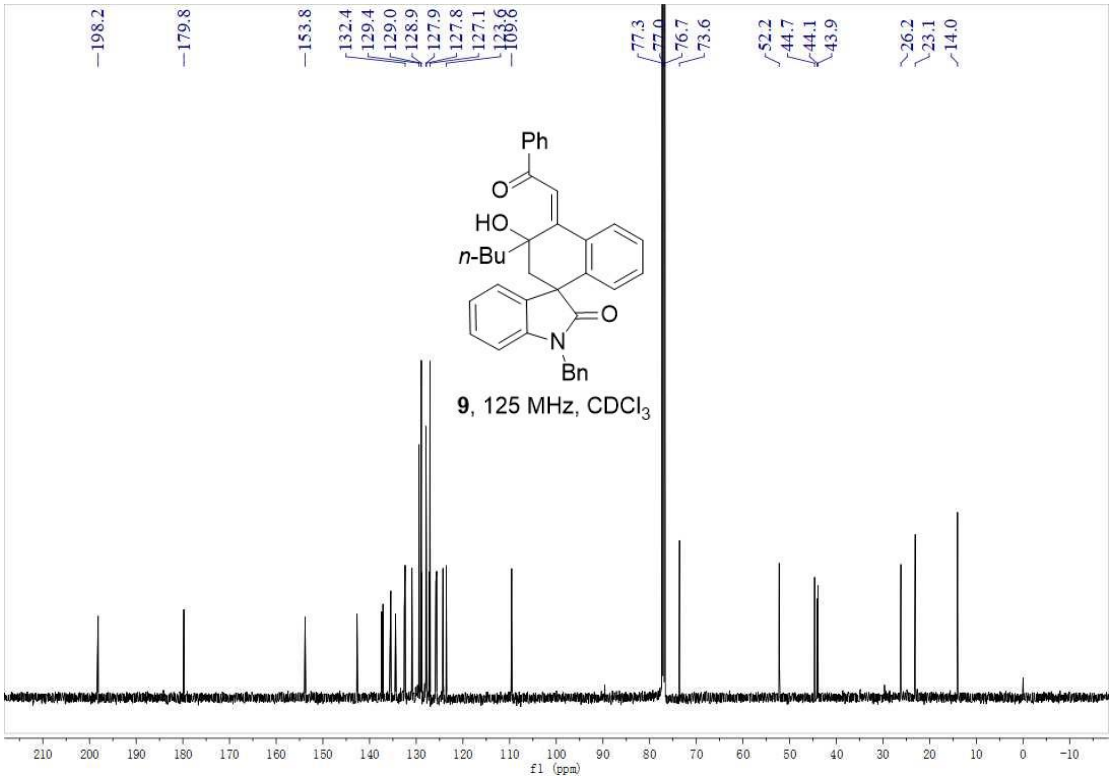

7.47 7.47 7.45 7.33 7.32 7.30 7.27 7.27 7.26 7.25 7.24 7.23 7.20 7.19 7.17 7.16 7.05 7.05 7.04 7.04 7.02 6.98 6.97 6.72 6.70 5.16 3.69 3.40 3.37 3.19 3.17 2.98 2.29 2.27 1.29 1.29 1.25 1.24 1.22 1.21 0.86 0.85 0.84 0.00
n-Bu
Ph
O
N
Me
5ak, 500 MHz, CDCl3
2.00 2.03 2.03 2.04 0.98 1.01 1.08 1.92 0.92 0.91 1.97 0.97 1.00 2.98 2.06 1.07 1.02 2.03 3.02
f1 (ppm)

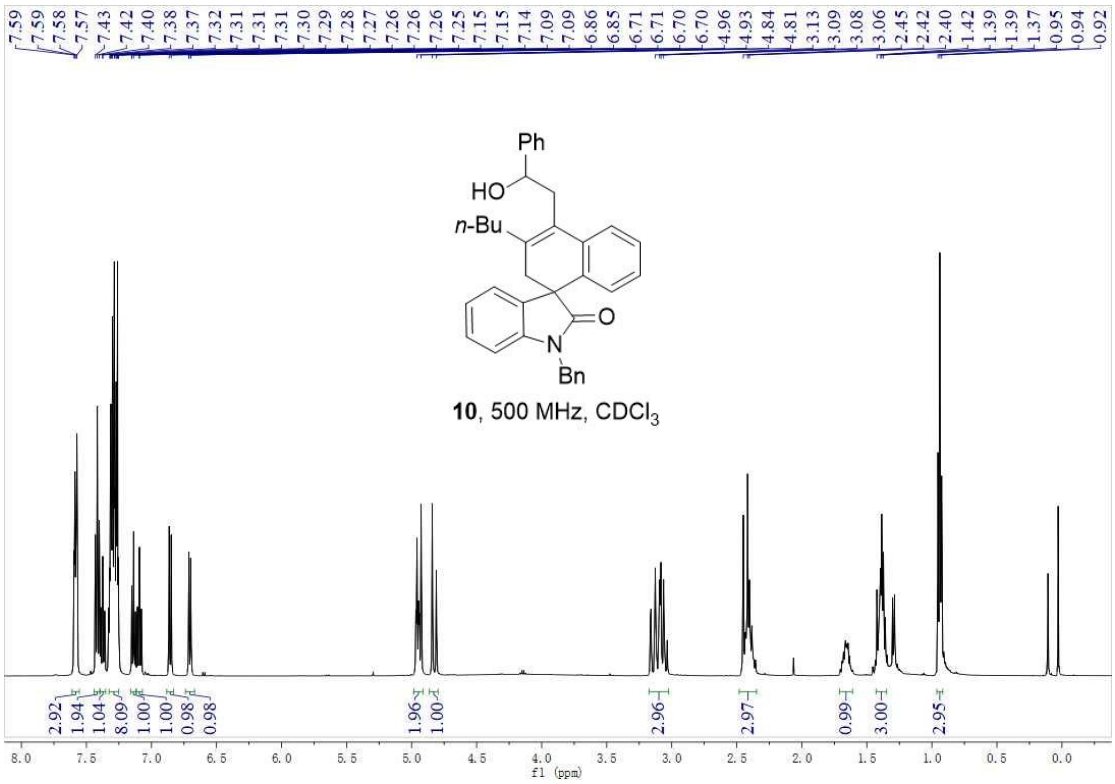

178.1 152.5 150.9 144.1 139.8 138.8 131.8 128.5 128.4 128.2 128.1 127.3 127.2 126.1 125.1 122.2 113.4 108.2 108.0 77.3 77.0 76.8 57.2 34.1 33.8 30.5 26.1 25.6 22.4 13.9
n-Bu
Ph
O
N
Me
5ak, 125 MHz, CDCl3
f1 (ppm)

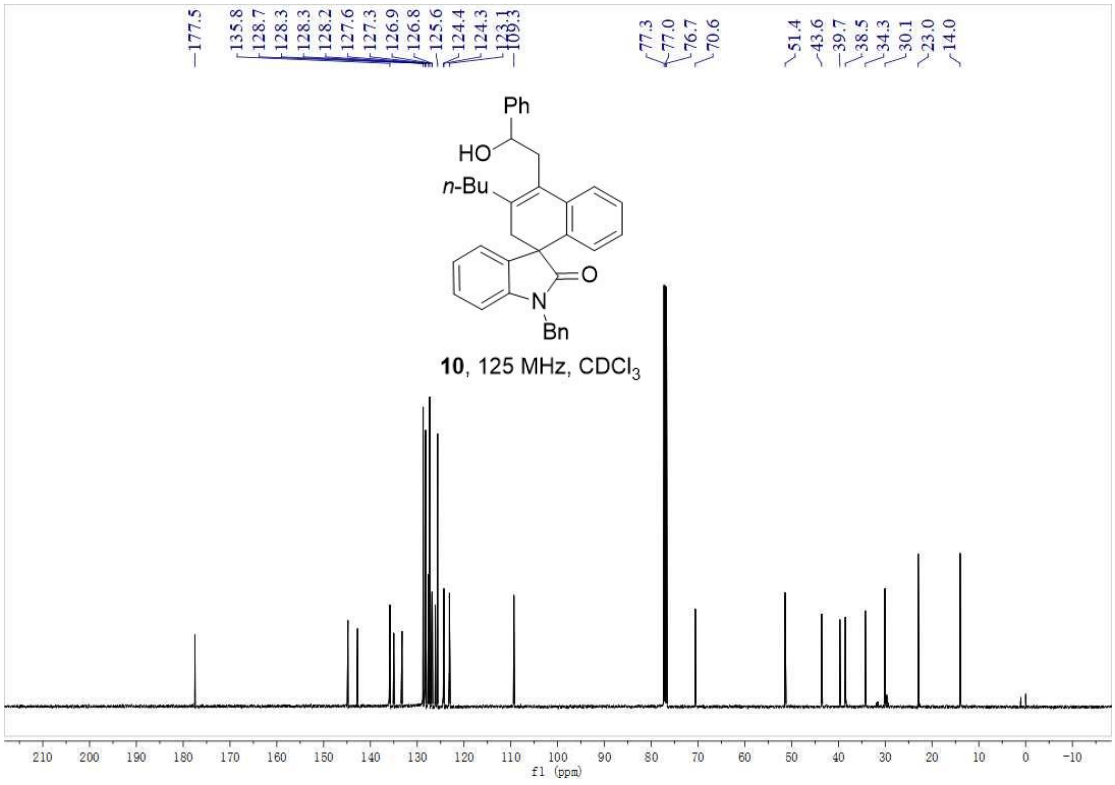

7.49
7.47
7.33
7.32
7.30
7.27
7.26
7.24
7.17
7.15
7.06
7.05
7.03
6.75
6.73
5.17
3.35
3.32
3.23
3.20
3.07
2.40
2.38
2.37
2.35
2.30
2.28
2.27
2.22
1.39
1.28
1.26
1.25
1.24
1.23
1.23
1.22
1.21
1.03
1.01
1.00
0.87
0.85
0.84
Me
O
n-Bu
Ph
O
N
Me
5al, 500 MHz, CDCl3
2.04
2.04
2.04
1.06
1.02
1.02
1.00
1.06
1.06
3.00
2.08
1.05
1.07
1.06
1.03
2.07
3.06
3.06
f1 (ppm)

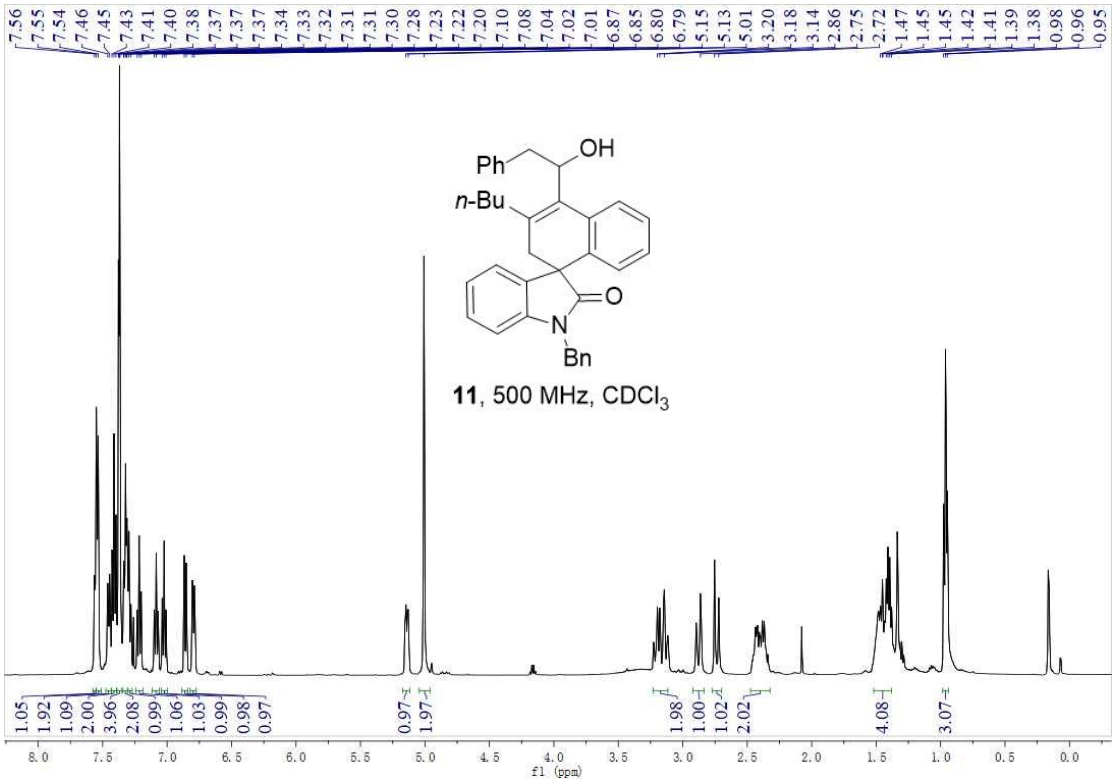

178.2
154.4
151.6
144.1
139.8
131.8
129.0
128.5
128.4
128.1
127.3
127.2
125.2
122.1
113.0
108.0
105.6
77.3
77.0
76.8
57.2
33.8
30.6
26.2
25.6
22.5
21.1
13.9
12.2
Me
O
n-Bu
Ph
O
N
Me
5al, 125 MHz, CDCl3
f1 (ppm)

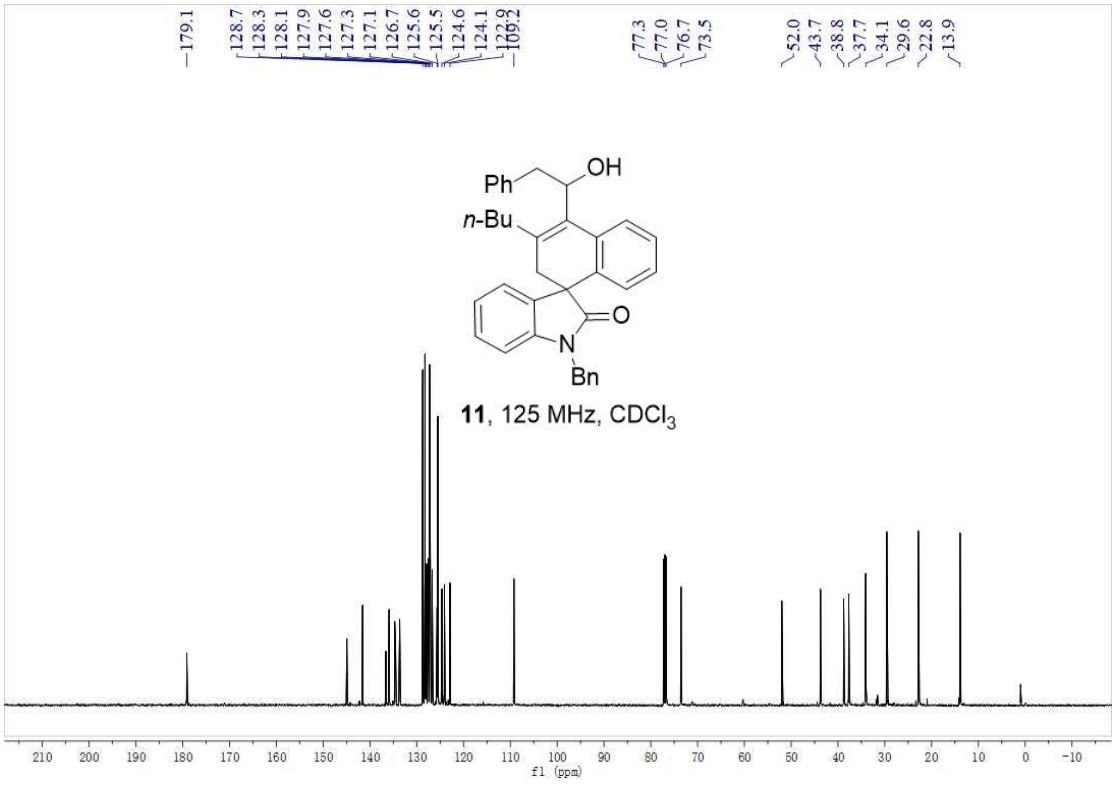

Ph
O
HO
n-Bu
O
N
Bn
9, 500 MHz, CDCl3
f1 (ppm)


Ph
O
HO
n-Bu
O
N
Bn
9, 125 MHz, CDCl3
f1 (ppm)


Ph
HO
n-Bu
O
N
Bn
10, 500 MHz, CDCl3
f1 (ppm)


Ph
HO
n-Bu
O
N
Bn
10, 125 MHz, CDCl3
f1 (ppm)


Ph
OH
n-Bu
O
N
Bn
11, 500 MHz, CDCl3
f1 (ppm)


Ph
OH
n-Bu
O
N
Bn
11, 125 MHz, CDCl3
f1 (ppm)