Supporting Information
For

Nickel-Catalysed Direct Alkylation of Thiophenes via Double C(sp3)-H/C(sp2)-H Bond Cleavage: The Importance of KH_2PO_4

Xie Wang,[a,†] Peipei Xie,[b,†] Renhua Qiu,[*,a,c] Longzhi Zhu,[a,c] Ting Liu,[a] You Li,[a] Takanori Iwasaki,[c] Chak-Tong Au,[d] Xinhua Xu,[a] Yuanzhi Xia,[*,b] Shuang-Feng Yin[*,a] Nobuaki Kambe[c]

[a]State Key Laboratory of Chemo/Biosensing and Chemometrics, College of Chemistry and Chemical Engineering, Hunan University, Changsha, 410082, P.R. China

[b]College of Chemistry and Chemical Engineering, Wenzhou University, Wenzhou, 325035, P.R. China

[c]Graduate School of Engineering, Osaka University, Suita, Osaka, 565-0871, Japan

[d]College of Chemistry and Chemical Engineering, Hunan Institute of Engineering, Xiangtan, 411114, P.R. China

[†] Xie Wang and Peipei Xie contribute equally to this work.

Tel/Fax: +86-731-88821171
renhuaqiu@hnu.edu.cn (Dr. Qiu)
xyz@wzu.edun.cn (Dr. Xia)
sf_yin@hnu.edu.cn (Dr. Yin)

1. General

Instrumentation

All the reactions were carried out under an N_2 atmosphere using standard Schlenk techniques. Glassware was dried in an oven (150 °C) and heated under reduced pressure before use. Flash column chromatography was performed using Qingdao Haiyang silica gel (300-400) with distilled solvents. ^1H NMR (400MHz) spectra were recorded on Bruker Avance 400 spectrometers in $CDCl_3$ [using $(CH_3)_4Si$ (for ^1H, δ = 0.00) as internal standard]. ^{13}C NMR (100 MHz) spectra on Bruker Avance 400 spectrometers in $CDCl_3$ [using $CDCl_3$ (for ^{13}C, δ = 77.00) as an internal standard]. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiple. Chemical shifts (*δ*) are in parts per million relatives to $CDCl_3$ at 7.26 ppm for ^1H and at 77.16 ppm for $^{13}C\{^1H\}$, respectively. The NMR yields were determined by ^1H NMR spectra with dibromomethane as an internal standard.

Chemicals

Unless otherwise noted, all the solvents and commercially available reagents were purchased from commercial sources and used directly without further purification. Starting materials were prepared according to literature procedures.[1]

2. Functionalized thiophenes and related compounds

Drugs such as duloxetine and tiaprofenic acid contain thiophene units (Figure S1).[1] Moreover, an alkyl-substituted derivative of shikonin containing the thiophenyl functionality exhibits *in vitro* antitumor activity. The prominence of thiophenes in the biological area is also known, with some being used as mAChR agonists and gelatinase inhibitors. Likewise, in the material sciences, thiophenes are a privileged motif. These sulfur-based aromatic species are key scaffolds of organic solar cell polymers and related functional materials such as JK-225 and JK-188.[2]

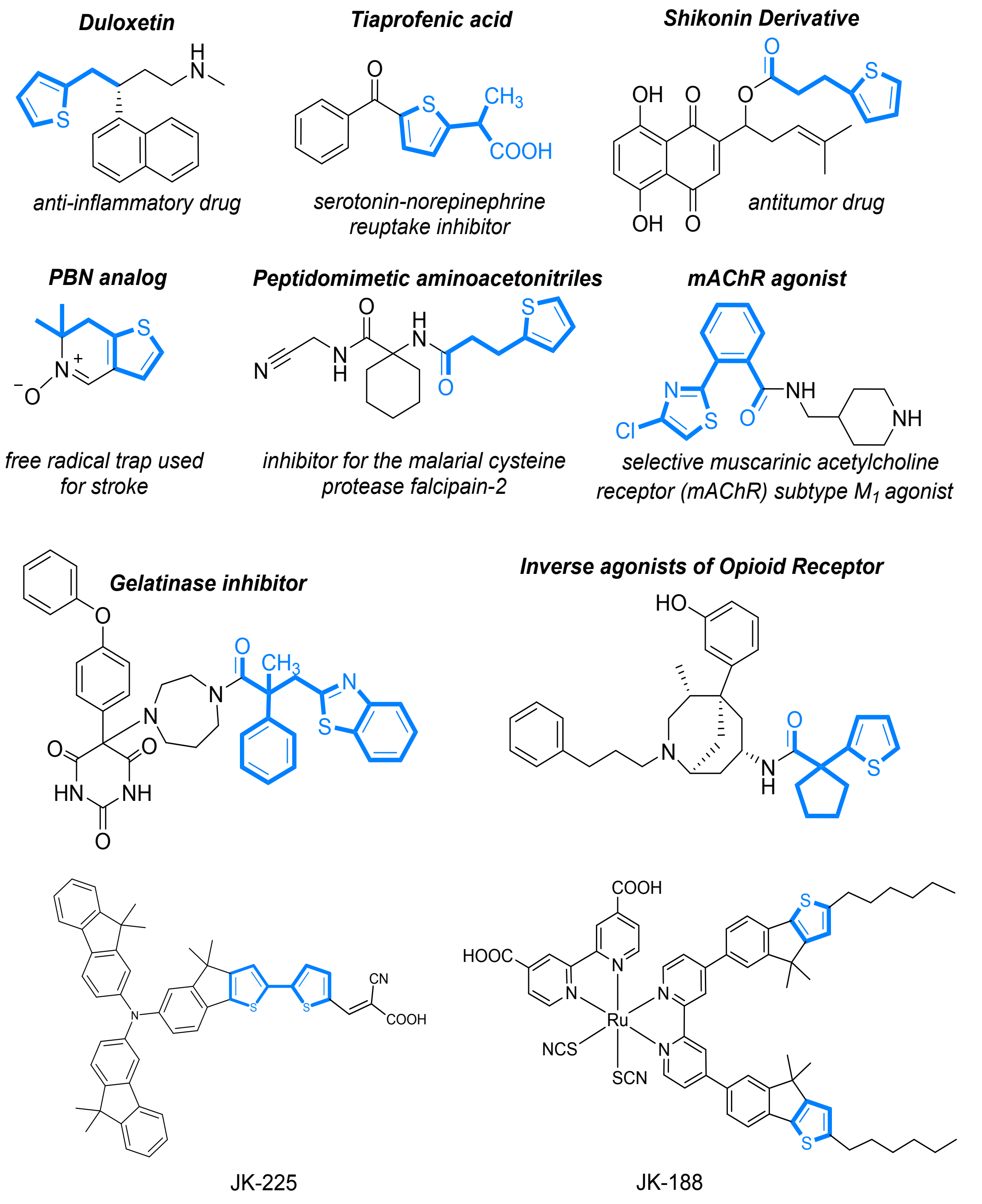
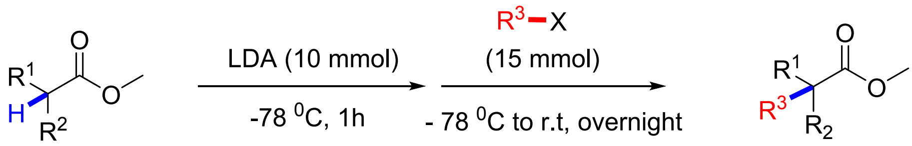


Figure S1. Functional compounds containing thiophene and thiazole units (ref 1-2 see in main text)

3. Structures of Starting Materials

General Procedure for the Preparation of Starting Materials

A solution of LDA (10 mmol) in THF was prepared from diisopropylamine (1.5 mL, 10.7 mmol) and 2.5 M *n*-BuLi in hexane (4.0 mL, 10 mmol) at -78 ˚C. To this LDA solution, a carboxylic acid ester (10 mmol) was added dropwise at -78 ˚C and the mixture was stirred at this temperature for 1 h. An alkyl halide (15 mmol) was then added dropwise to the solution at -78 ˚C [Eq.(1)]. After the addition, the mixture was warmed to room temperature and stirred overnight. Then the mixture was quenched with water at 0 ˚C, extracted with Et_2O (15 mL x 3). The combined organic layers were washed with brine, dried over $MgSO_4$, and then evaporated in vacuo to give the crude ester.



[Eq. (1)]

10 mmol

1b, R^1 = Me, R^2 = Ph, R^3 = Me, X = I;
1c, R^1 = Me, R^2 = Bn, R^3 = Me, X= I;
1d, R^1-R^2=-$(CH_2)_5$-; R^3 = Me, X = I;
1e, R^1 = Et, R^2 =Me, R^3 = Naphthalen-2-yl-methyl, X = Br;
1f, R^1 = R^2 = Ph, R^3 = Me, X =I;
1g, R^1 = Et, R^2 = Ph, R^3 = Me, X = I;
1g[CD_3], R^1 = Et, R^2 = Ph, R^3 = CD_3, X = I.

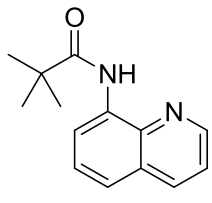
To the ester obtained as above was added a solution of NaOH (2 M, 8.0 mL) and methanol (10 mL).The mixture was stirred overnight at 60 ˚C. After removal of methanol in vacuo, the pH of the mixture was adjusted to 2 with 3.0 M HCl. The mixture was then saturated with NaCl and extracted with Et_2O (15 mL x 3). The combined organic layers were washed with brine, dried over $MgSO_4$, and then evaporated in vacuo to give the crude carboxylic acid, which was used directly for the next step without further purification.

Oxalyl chloride (1.75 mL, 20 mmol) was added slowly to a stirred solution of thus formed carboxylic acid in CH_2Cl_2 (20 mL) and DMF (0.1 mL) at 0 ˚C. The mixture was stirred for 1 h at 0 ˚C and another 16 h at room temperature, and evaporated in vacuo. The residue was then dissolved in toluene (5.0 mL), evaporated in vacuo twice, to give the crude acid chloride, which was used directly for the next step without further purification.

The acid chloride obtained as above was added dropwise to a solution of 8-aminoquinoline (1.01 g, 7.0 mmol) and Et_3N (1.7 mL, 12 mmol) in CH_2Cl_2 (12 mL). The mixture was stirred overnight at room temperature. Then the mixture was diluted with CH_2Cl_2 (10 mL), washed successively with water, saturated aqueous $NaHCO_3$, and brine. The organic layer was dried over $MgSO_4$ and concentrated under reduced pressure. The residue was purified by flash column chromatography on silica gel, eluting with EtOAc/Hexane (1:60, v/v), to afford the corresponding 8-aminoquinolinyl amides.

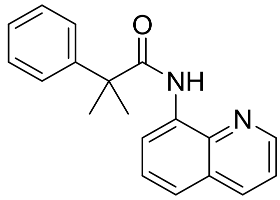
Analytical Data for Starting Materials

N-(quinolin-8-yl)pivalamide **(1a)**



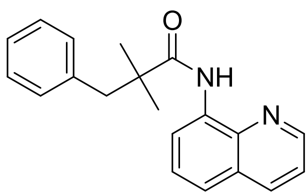
This amide was obtained as yellow oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.43 (s, 9H), 7.43 – 7.55 (m, 3 H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.79 – 8.82 (m, 2 H), 10.28 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 27.76, 40.37, 116.22, 121.23, 121.53, 127.46, 127.94, 134.73, 136.32, 138.83, 148.22, 177.28.

2-methyl-2-phenyl-*N*-(quinolin-8-yl)propanamide **(1b)**



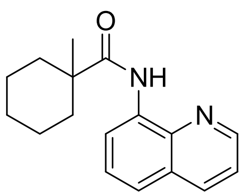
This amide was obtained as white solid. Melting point: 100-101 ˚C. δ_H (400 MHz; $CDCl_3$; Me_4Si) δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.78 (s, 6H), 7.25 – 7.35 (m, 2 H), 7.38 – 7.44 (m, 3 H), 7.48 – 7.55 (m, 3 H), 8.06 (d, *J* = 8.0 Hz, 1H), 8.59 (d, *J* = 3.2 Hz, 1H), 8.76 (d, *J* = 7.2 Hz, 1H), 9.87 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 27.02, 48.41, 115.98, 121.26, 121.43, 126.37, 127.02, 127.33, 127.84, 128.79, 134.72, 136.09, 138.69, 144.91, 148.12, 175.82.

2,2-dimethyl-3-phenyl-*N*-(quinolin-8-yl)propanamide **(1c)**



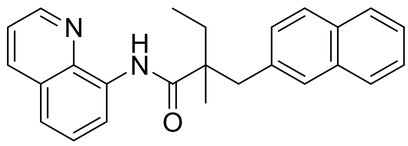
This amide was obtained as pale yellow solid. Melting point: 60 ˚C. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.29 (s, 6 H), 2.92 (s, 2H), 7.00 – 7.11 (m, 5H), 7.23 (dd, *J* = 8.4, 4.0 Hz, 1H), 7.31 – 7.33 (m, 1 H), 7.40 (t, *J* = 8.0 Hz, 1H), 7.94 (d, *J* = 8.4 Hz, 1H), 8.58 (d, *J* = 4.0 Hz, 1H), 8.73 (d, *J* = 7.6 Hz, 1H), 10.05 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.32, 45.01, 46.93, 116.31, 121.42, 121.55, 126.42, 127.43, 127.92, 128.04, 130.32, 134.54, 136.24, 137.98, 138.80, 148.21, 176.08;

1-methyl-*N*-(quinolin-8-yl)cyclohexanecarboxamide (**1d**)



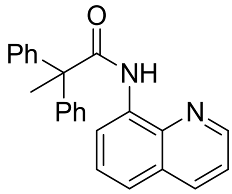
This amide was obtained as yellow oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.36 (s, 3H). 1.51 – 1.66 (m, 8H), 2.18 – 2.22 (m, 2H), 7.40 – 7.54 (m, 3H), 8.12 (d, *J* = 8.4 Hz, 1H), 8.80 – 8.83 (m, 2H), 10.29 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 23.00, 25.87, 26.60, 35.80, 44.38, 116.24, 121.12, 121.50, 127.45, 127.95, 134.82, 136.28, 138.84, 148.22, 176.62;

2-methyl-2-(naphthalen-2-ylmethyl)-*N*-(quinolin-8-yl)butanamide (**1e**)



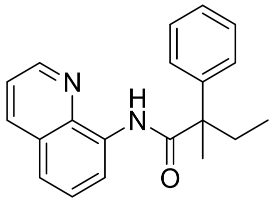
This amide was obtained as brown oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.03 (t, J = 7.6 Hz, 3H), 1.40 (s, 3H), 1.62 – 1.70 (m, 1 H), 2.07 – 2.16 (m, 1 H), 2.99, 3.42 (AB, J_{AB} = 13.2 Hz, 2 H), 7.31 – 7.37 (m, 4H), 7.47 – 7.49 (m, 1 H), 7.56 (t, J = 8.0 Hz, 1H), 7.64 – 7.71 (m, 4 H), 8.10 (d, J = 8.4 Hz, 1H), 8.59 (d, J = 4.0 Hz, 1H), 8.87 (d, J = 7.6 Hz, 1H), 10.10 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 9.22, 20.36, 32.88, 46.22, 49.21, 116.31, 121.34, 121.45, 125.23, 125.69, 127.40, 127.44, 127.56, 127.88, 128.80, 128.85, 132.21, 133.32, 134.43, 135.56, 136.12, 138.74, 148.10, 175.31.

2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (**1f**)



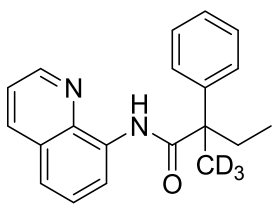
This amide was obtained as white solid. Melting point: 153 ˚C. δ_H (400 MHz; $CDCl_3$; Me_4Si) 2.18 (s, 3H), 7.30 – 7.42 (m, 11H), 7.46 – 7.55 (m, 2H), 8.08 (d, J = 7.2 Hz, 1H), 8.51 (d, J = 2.8 Hz, H), 8.87 (d, J = 7.2 Hz, 1H), 10.13 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 27.17, 58.45, 116.02, 121.45, 121.58, 126.99, 127.34, 127.82, 128.35, 128.57, 134.51, 136.01, 138.80, 144.95, 148.05, 173.73.

2-methyl-2-phenyl-*N*-(quinolin-8-yl)butanamide (**1g**)



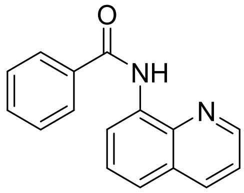
This amide was obtained as yellow oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 0.80 (t, J = 7.2 Hz, 3H)**, 1.63 (s, 3H),** 2.04 – 2.24 (m, 2 H), 7.14 – 7.20 (m, 3 H), 7.24 – 7.29 (m, 2 H), 7.35 – 7.40 (m, 3 H), 7.90 (d, J = 8.4 Hz, 1H), 8.46 (d, J = 4.4 Hz, 1H), 8.68 (d, J = 7.6 Hz, 1H), 9.76 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 9.09, **23.02**, 31.76, 52.29, 115.99, 121.24, 121.45, 126.06, 126.85, 126.94, 127.33, 127.86, 128.40, 128.75, 134.75, 136.09, 138.67, 143.91, 148.13, 175.44.

[D_3]-2-methyl-2-phenyl-*N*-(quinolin-8-yl)butanamide ([D_3]-**1g**)



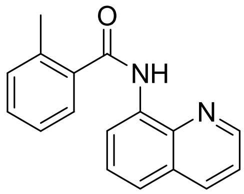
This amide was obtained as yellow oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 0.81 (t, J = 7.2 Hz, 3H). 2.05 – 2.25 (m, 2 H),7.14 – 7.21 (m, 2 H), 7.26 – 7.31 (m, 3 H), 7.36 – 7.41 (m, 3 H), 7.92 (d, J = 8.4 Hz, 1H), 8.48 (d, J = 4.4 Hz, 1H), 8.68 (d, J = 7.6 Hz, 1H), 9.77 (s, 1H), δ_C (100 MHz; $CDCl_3$; Me_4Si) 9.06, 31.67, 52.07, 115.99, 121.20, 121.42, 126.83, 126.90, 127.32, 127.85, 128.72, 134.74, 136.07, 138.68, 143.87, 148.11, 175.43.

N-(quinolin-8-yl)benzamide (**1h**)



This amide was obtained as white solid. Melting point: 89-90 ˚C. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.46-7.50 (m, 1H), 7.54-7.63 (m, 5H), 8.08-8.10 (m, 2H), 8.19 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.86 (q, *J* = 2.0 Hz, 1H), 8.95 (dd, *J* = 7.6, 1.1 Hz, 1H), 10.76 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 116.54, 121.67, 127.29, 127.47, 127.99, 128.78, 131.82, 134.60, 135.17, 136.38, 138.78, 148.28, 165.46.

2-methyl-*N*-(quinolin-8-yl)benzamide (**1i**)



This amide was obtained as white solid. Melting point: 98 ˚C. δ_H (400 MHz; $CDCl_3$; Me_4Si) 2.62 (s, 3H), 7.30 – 7.34 (m, 2H), 7.38 – 7.45 (m, 2H), 7.53 – 7.60 (m, 2H), 7.70 (d, *J* = 7.6 Hz, 1H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.77 (d, *J* = 4.4 Hz, 1H), 8.96 (d, *J* = 7.6 Hz, 1H), 10.22 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 20.23, 116.53, 121.69, 121.80, 126.04, 127.28, 127.43, 128.03, 130.35, 131.41, 134.77, 136.37, 136.67, 136.70, 138.64, 148.29, 168.22.

4. Optimization of reaction conditions

Optimization of reaction conditions

As a model reaction, the cross-coupling between an aliphatic amide **1a** and thiophene (**2a**) was examined. After extensive screening of reaction conditions, it was realized that the coupling of **1a** and **2a** could take place in the presence of an oxidant using a nickel salt as catalyst and tetrabutylammonium bromide (TBAB). Previously, we highlighted the role of TBAB to improve the reactivity of a Ni catalytic system, presumably because of the increased solubility of reagents and intermediates [Ref. 14 in main text]. As shown in Table 1, no product was observed in the absence of a base. However, when KH_2PO_4 was used as a base and Ag_2CO_3 as an oxidant, the desired product **3a** was obtained in 57% isolated yield (Entry 2). Further studies showed that the use of alternate silver salts resulted in lower yields of **3a** (Table 1 entry 5 and Table S1). Other oxidants such as DTBP (di-*tert*-butyl peroxide) and $Cu(OAc)_2$ were also assessed (Entries 3-4); However, none of the desired product was obtained. Among the nickel catalysts screened, $Ni(OTf)_2$ showed the highest catalytic activity, giving **3a** in 64% yield (Table 1 Entries 6-7 and Table S2). The efficiency of the reaction was also significantly affected by the solvent, and DMSO was found to be the best (Table S3).

Table 1. Optimization for alkylation of thiophene[a]

Entry	Catalyst	Oxidant (3.0 equiv)	Additive (3.0 equiv)	Yield (%)[b]
1	$NiBr_2$	Ag_2CO_3	[Base][c]	0-7
2	$NiBr_2$	Ag_2CO_3	KH_2PO_4	57
3	$NiBr_2$	DTBP	KH_2PO_4	0
4	$NiBr_2$	$Cu(OAc)_2$	KH_2PO_4	0
5	$NiBr_2$	[Ag salts]	KH_2PO_4	12-42
6	[Ni]	Ag_2CO_3	KH_2PO_4	40-60
7	$Ni(OTf)_2$	Ag_2CO_3	KH_2PO_4	64

[a]Reaction conditions: **1a** (0.2 mmol), **2a** (0.6 mmol), nickel (0.04 mmol), MesCOOH (0.08 mmol), base (0.4 mmol), TBAB (0.6 mmol), oxidant (0.6 mmol) in solvent (0.5 mL) at 160 °C for 24 h in 10 mL screw-capped vials. [b]Isolated yields. [c]Na_2CO_3, $NaHCO_3$, K_2CO_3, and K_2HPO_4.

Table S1: Silver salts

entry	Silver salts	Yield
1	$AgNO_3$	12%
2	AgCl	trace
3	AgBr	trace
4	AgF	6%

5	Ag_2O	23%
6	Ag(OAc)	42%
7	Ag(OTf)	18%

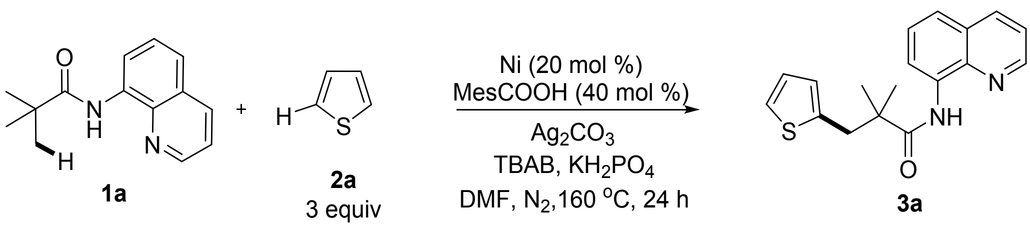
Table S2: Nickel salts

entry	Nickel salts	Yield
1	NiF_2	48%
2	$NiBr_2$	58%
3	$NiCl_2$	trace
4	$Ni(acac)_2$	trace
5	$Ni(OAc)_2$	52%
6	$Ni(PPh_3)_2Cl_2$	40%

Table S3: Solvents

entry	Solvents	Yield
1	DMSO	64%
2	DMF	41%
3	Dioxane	trace
4	Toluene	trace

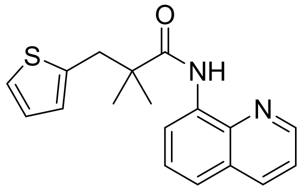
General Procedure for Nickel-Catalyzed heteroarylation of amide with thiophene



A 10-mL Schlenk tube was charged with amide **1a** (0.2 mmol, 1.0 equiv, 45.6 mg), thiophene **2a** (0.6 mmol, 3 equiv, 50.5 mg), $Ni(OTf)_2$ (0.04 mmol, 20 mol%, 14.3 mg), MesCOOH (0.08 mmol, 40 mol%, 13.1 mg), KH_2PO_4 (0.4 mmol, 2.0 equiv, 54.4 mg), Ag_2CO_3 (0.6 mmol, 3 .0 equiv, 165.4 mg), TBAB (0.6 mmol, 3.0 equiv, 193.4 mg) and DMSO (0.5 mL). The vial was evacuated and filled with N_2, and stirred at 160 °C for 24 h. The mixture was then cooled to room temperature, diluted with CH_2Cl_2 (2.0 mL), filtered through a celite pad, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel, eluting with EtOAc/Hexane (1:100 ~ 1:60, v/v), to afford the desired product **3a**.

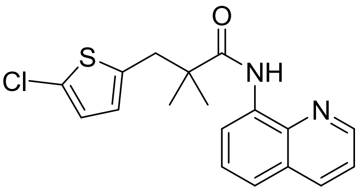
5. Analytical Data for the Products

2,2-dimethyl-N-(quinolin-8-yl)-3-(thiophen-2-yl) propanamide (**3a**)



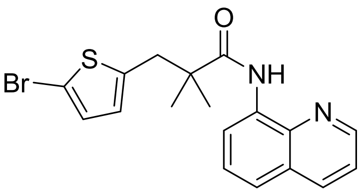
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), thiophene (50.5 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 39.7 mg (64%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.46 (s, 6H), 3.26 (s, 2H), 6.84 – 6.87 (m, 2 H), 7.07 (d, J = 5.2 Hz, 1H), 7.44 (dd, J = 8.4, 4.4 Hz, 1H), 7.49 – 7.55 (m, 2 H), 8.15 (d, J = 8.4 Hz, 1H), 8.77 (d, J = 4.0 Hz, 1H), 8.84 (d, J = 8.0 Hz, 1H), 10.23 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.38, 40.85, 45.08, 116.40, 121.43, 121.54, 124.08, 126.60, 126.96, 127.46, 127.93, 134.49, 136.28, 138.81, 139.86, 148.23, 175.68; HRMS (ESI): M+H$^+$ found 310.1147; $C_{18}H_{18}N_2S_1O_1$ requires 310.1140.

3-(5-chlorothiophen-2-yl)-2,2-dimethyl-N-(quinolin-8-yl) propanamide (**3b**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-chlorothiophene (71.1 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 43.3 mg (63%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.46 (s, 6H), 3.14 (s, 2H), 6.60 (d, J = 3.6 Hz, 1H), 6.66 (d, J = 3.6 Hz, 1H), 7.44 (dd, J = 8.0, 4.0 Hz, 1H), 7.42 – 7.50 (m, 2H), 8.15 (d, J = 8.4 Hz, 1H), 8.71 (d, J = 8.0 Hz, 1H), 8.82 (d, J = 7.6 Hz, 1H), 10.23 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.46, 41.32, 45.00, 116.44, 121.55, 121.58, 125.61, 126.33, 127.44, 127.88, 127.94, 134.37, 136.31, 138.79, 138.94, 148.27, 175.33; HRMS (ESI): M+H$^+$ found 344.0758; $C_{18}H_{17}N_2S_1O_1Cl_1$ requires 344.0750.

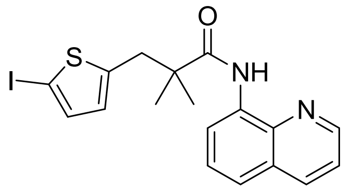
3-(5-bromothiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl) propanamide (**3c**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-bromothiophene (97.8 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 47.3 mg (61%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.46 (s, 6H), 3.17 (s, 2H), 6.59 (d, J = 3.6 Hz, 1H), 6.80 (d, J = 3.6 Hz, 1H), 7.44 (dd, J = 8.4, 4.4

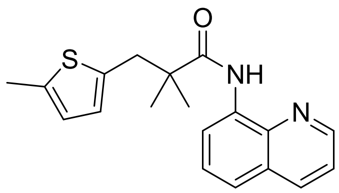
Hz, 1H), 7.50 – 7.57 (m, 2 H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.78 (d, *J* = 4.4 Hz, 1H), 8.82 (d, *J* = 7.2 Hz, 1H), 10.22 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.46, 41.25, 44.97, 110.09, 116.45, 121.55, 121.58, 127.39, 127.44, 127.94, 129.40, 134.37, 136.31, 138.78, 141.87, 148.28, 175.33; HRMS (ESI): M+H$^+$ found 388.0241; $C_{18}H_{17}N_2S_1O_1Br_1$ requires 388.0245.

3-(5-iodothiophen-2-yl)-2,2-dimethyl-N-(quinolin-8-yl) propanamide (**3d**)



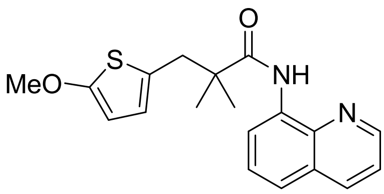
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-iodothiophene (126.0 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 57.6 mg (66%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.45 (s, 6H), 3.22 (s, 2H), 6.53 (d, *J* = 3.2 Hz, 1H), 6.99 (d, *J* = 3.6 Hz, 1H), 7.44 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.50 – 7.57 (m, 2 H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.78 (d, *J* = 4.0 Hz, 1H), 8.81 (d, *J* = 7.2 Hz, 1H), 10.21 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.45, 41.06, 45.02, 71.15, 116.45, 121.54, 121.58, 127.44, 127.93, 128.78, 134.38, 136.31, 136.56, 138.78, 146.39, 148.28, 175.34; HRMS (ESI): M+H$^+$ found 436.0097; $C_{18}H_{17}N_2S_1O_1I_1$ requires 436.0106.

2,2-dimethyl-3-(5-methylthiophen-2-yl)-N-(quinolin-8-yl)propanamide **(3e)**



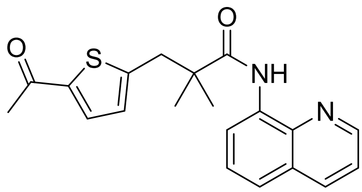
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-methylthiophene (58.9 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 45.4 mg (70%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.45 (s, 6H). 2.34 (s, 3H), 3.16 (s, 2H), 6.50 (s, 1H), 6.60 (d, *J* = 3.2 Hz, 1H), 7.44 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.49 – 7.57 (m, 2H), 8.15 (d, *J* = 8.4 Hz, 1H), 8.78 (d, *J* = 4.0 Hz, 1H), 8.84 (d, *J* = 7.2 Hz, 1H), 10.23 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 15.16, 25.36, 41.07, 44.98, 116.41, 121.34, 121.50, 124.63, 126.77, 127.47, 127.93, 134.58, 136.26, 137.52, 138.39, 138.85, 148.18, 175.81; HRMS (ESI): M+H$^+$ found 324.1300; $C_{19}H_{20}N_2S_1O_1$ requires 324.1296.

3-(5-methoxythiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3f**)



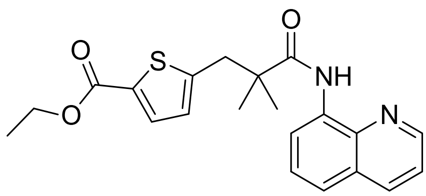
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-methoxythiophene (68.5 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 32.0 mg (47%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.45 (s, 6H), 3.07 (s, 2H), 3.75 (s, 3H), 5.94 (d, J = 3.6 Hz, 1H), 6.43 (d, J = 3.2 Hz, 1H), 7.44 (dd, J = 8.0, 4.0 Hz, 1H), 7.49 – 7.57 (m, 2H), 8.15 (d, J = 8.4 Hz, 1H), 8.79 (d, J = 4.0 Hz, 1H), 8.83 (d, J = 7.2 Hz, 1H), 10.23 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.34, 41.51, 45.01, 60.05, 103.15, 116.40, 121.35, 121.50, 124.14, 126.01,127.46, 127.92, 134.54, 136.25, 138.83, 148.19, 164.88, 175.75; HRMS (ESI): M+H$^+$ found 340.1237; $C_{19}H_{20}N_2S_1O_2$ requires 340.1245.

3-(5-acetylthiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3g**)



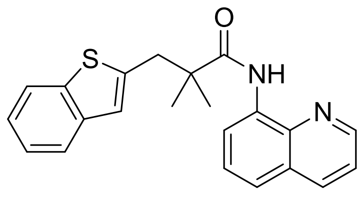
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 1-(thiophen-2-yl)ethan-1-one (75.7 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 28.9 mg (41%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.48 (s, 6H), 2.43 (s, 3H), 3.26 (s, 2H), 6.86 (d, J = 3.6 Hz, 1H), 7.43 – 7.46 (m, 2H), 7.52 – 7.55 (m, 2H), 8.15 (d, J = 8.0 Hz, 1H), 8.77 (d, J = 4.0 Hz, 1H), 8.81 (d, J = 7.2 Hz, 1H),10.22 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.51, 26.54, 41.37, 45.14, 116.46, 121.61, 121.64, 127.44, 127.92, 128.32, 132.67, 134.27, 136.33, 138.76, 142.98, 148.29, 149.87, 175.00, 190.51; HRMS (ESI): M+H$^+$ found 352.1242; $C_{20}H_{20}N_2S_1O_2$ requires 352.1245.

Ethyl 5-(2,2-dimethyl-3-oxo-3-(quinolin-8-ylamino)propyl)thiophene-2-carboxylate (**3h**)



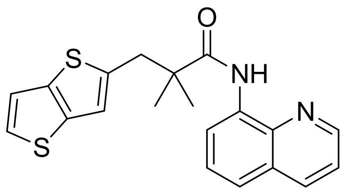
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), ethyl thiophene-2-carboxylate (93.7 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 48.9 mg (64%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.30 (t, J = 7.2 Hz, 3H), 1.48 (s, 6H), 3.25 (s, 2H), 4.26 (q, J = 7.2 Hz, 2H), 6.83 (d, J = 3.6 Hz, 1H), 7.44 (dd, J = 8.4, 4.4 Hz, 1H), 7.50 – 7.58 (m, 3H), 8.15 (d, J = 8.4 Hz, 1H), 8.77 (d, J = 4.0 Hz, 1H), 8.82 (d, J = 7.6 Hz, 1H), 10.22 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 14.32. 25.48, 41.14, 45.08, 60.91, 116.46, 121.60, 127.42, 127.91, 132.30, 133.32, 134.30, 136.31, 138.77, 147.89, 148.28, 162.25, 175.12; HRMS (ESI): M+H$^+$ found 382.1355; $C_{21}H_{22}N_2S_1O_3$ requires 382.1351.

3-(benzo[b]thiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3k**)



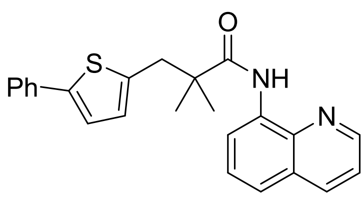
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), benzo[b]thiophene (80.5 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 52.6 mg (73%) as pale viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.52 (s, 6H), 3.34 (s, 2H), 7.07 (s, 1H), 7.17 – 7.24 (m, 2H), 7.40 (dd, *J* = 8.4, 4.0 Hz, 1H), 7.50 – 7.61 (m, 3H), 7.67 (d, *J* = 7.6 Hz, 1H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.69 (d, *J* = 4.0 Hz, 1H), 8.86 (d, *J* = 7.6 Hz, 1H), 10.26 (s, 1H), δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.67, 41.69, 45.07, 116.50, 121.47, 121.51, 121.95, 122.83, 123.53, 123.63, 123.93, 127.45, 127.95, 134.54, 136.22, 138.85, 139.93, 140.04, 141.28, 148.21, 175.51; HRMS (ESI): $M+H^+$ found 360.1299; $C_{22}H_{20}N_2S_1O_1$ requires 360.1296.

2,2-dimethyl-*N*-(quinolin-8-yl)-3-(thieno[3,2-b]thiophen-2-yl)propanamide (**3l**)



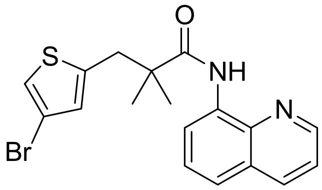
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), thieno[3,2-b]thiophene (84.1 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 36.6 mg (50%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.51 (s, 6H), 3.30 (s, 2H), 7.02 (s, 1H), 7.09 (d, *J* = 5.2 Hz, 1H), 7.23 (d, *J* = 5.2 Hz, 1H), 7.41 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.49 – 7.58 (m, 2H), 8.14 (d, *J* = 8.0 Hz, 1H), 8.72 (d, *J* = 4.0 Hz, 1H), 8.85 (d, *J* = 7.6 Hz, 1H), 10.25 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.57, 42.11, 45.20, 116.45, 119.14, 119.32, 121.51, 121.55, 125.72, 127.44, 134.46, 127.92, 136.26, 138.51, 138.65, 138.78, 142.70, 148.23, 175.54; HRMS (ESI): $M+H^+$ found 366.0859; $C_{20}H_{18}N_2S_2O_1$ requires 366.0861.

2,2-dimethyl-3-(5-phenylthiophen-2-yl)-*N*-(quinolin-8-yl)propanamide (**3m**)



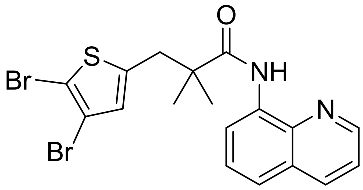
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-phenylthiophene (96.1 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 47.9 mg (62%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.50 (s, 6H), 3.24 (s, 2H), 6.80 (d, *J* = 3.2 Hz, 1H), 7.06 (d, *J* = 3.2 Hz, 1H), 7.17 – 7.21 (m, 1H), 7.26 – 7.29 (m, 2H), 7.41 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.46 – 7.55 (m, 4H), 8.13 (d, *J* = 8.4 Hz, 1H), 8.75 (d, *J* = 4.0 Hz, 1H), 8.85 (d, *J* = 7.2 Hz, 1H), 10.25 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.44, 41.16, 45.10, 116.43, 121.44, 121.52, 122.69, 125.53, 127.03, 127.44, 127.93, 128.04, 128.72, 134.50, 134.54, 136.25, 138.82, 139.67, 142.92, 148.23, 175.62; HRMS (ESI): M+H$^+$ found 386.1449; $C_{24}H_{22}N_2S_1O_1$ requires 386.1453.

3-(4-bromothiophen-2-yl)-2,2-dimethyl-N-(quinolin-8-yl)propanamide (**3n**)



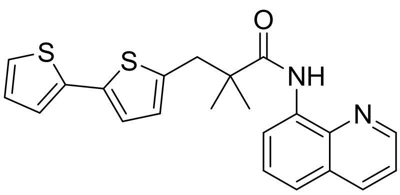
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 3-bromothiophene (97.8 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 55.1 mg (71%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.46 (s, 6H). 3.20 (s, 2H), 6.77 (s, 1H), 6.96 (s, 1H), 7.44 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.50-7.57 (m, 2H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.78 (d, *J* = 4.0 Hz, 1H), 8.81 (d, *J* = 7.6 Hz, 1H), 10.22 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.44, 40.90, 45.06, 108.87, 116.45, 121.59, 121.71, 127.43, 127.93, 129.51, 134.33, 136.31, 138.78, 141.58, 148.29, 175.22; HRMS (ESI): M+H$^+$ found 388.0244; $C_{18}H_{17}N_2S_1O_1Br_1$ requires 388.0245

3-(4,5-dibromothiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3o**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2,3-dibromothiophene (145.1 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 56.7 mg (61%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.47 (s, 6H). 3.13 (s, 2H), 6.67 (s, 1H), 7.45 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.51 – 7.58 (m, 2H), 8.16 (d, *J* = 8.4 Hz, 1H), 8.79 – 8.81 (m, 2H), 10.21 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.55, 41.31, 44.99, 112.86, 116.52, 121.63, 121.70, 127.42, 127.94, 128.85, 129.68, 134.23, 136.34, 138.76, 141.97, 148.34, 175.01; HRMS (ESI): M+H$^+$ found 465.9355; $C_{18}H_{16}N_2S_1O_1Br_2$ requires 465.9350.

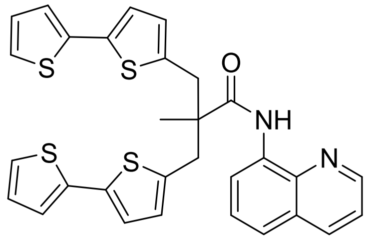
3-([2,2'-bithiophen]-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3p**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2,2'-bithiophene (99.7 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 37.6 mg (48%) as yellow solid. δ_H (400 MHz; $CDCl_3$;

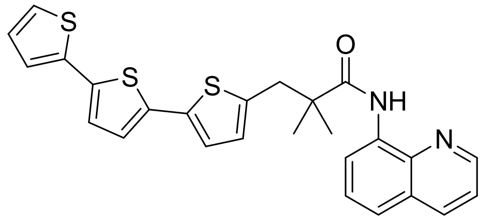
Me4Si) 1.49 (s, 6H)，3.21 (s, 2H), 6.73 (d, J = 3.2 Hz, 1H), 6.92 – 6.94 (m, 2H), 7.01 (d, J = 3.2 Hz, 1H), 7.12 (d, J = 5.2 Hz, 1H), 7.42 (dd, J = 8.0, 4.0 Hz, 1H), 7.49 – 7.58 (m, 2H), 8.14 (d, J = 8.4 Hz, 1H), 8.76 (d, J = 4.0 Hz, 1H), 8.84 (d, J = 7.2 Hz, 1H), 10.24 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.45, 41.03, 45.09, 116.43, 121.49, 121.55, 123.18, 123.39, 123.81, 127.43, 127.62, 127.76, 127.93, 134.44, 136.04, 136.27, 137.67, 138.80, 139.29, 148.25, 175.55; HRMS (ESI): M+H$^+$ found 392.1019; $C_{22}H_{20}N_2S_2O_1$ requires 392.1017.

3-([2,2'-bithiophen]-5-yl)-2-([2,2'-bithiophen]-5-ylmethyl)-2-methyl-*N*-(quinolin-8-yl)propanamide (**3p'**)



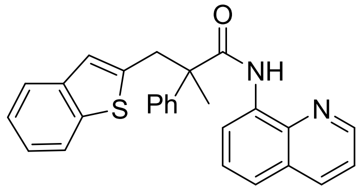
This amide was obtained 17.8 mg (16%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.55 (s, 3H), 3.05, 3.55 (AB, J_{AB} = 14.4 Hz, 4H), 6.76 (d, J = 3.6 Hz, 2H), 6.91 – 6.94 (m, 4H), 7.00 (d, J = 3.6 Hz, 2H), 7.12 (d, J = 5.2 Hz, 2H), 7.37 (dd, J = 8.0, 4.0 Hz, 1H), 7.50 – 7.59 (m, 2H), 8.11 (d, J = 8.0 Hz, 1H), 8.67 (d, J = 4.0 Hz, 1H), 8.87 (d, J = 7.6 Hz, 1H), 10.15 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 22.63, 40.11, 49.84, 116.62, 121.52, 121.69, 123.27, 123.46, 123.90, 127.36, 127.63, 127.88, 128.14, 134.15, 136.14, 136.31, 137.54, 138.32, 138.75, 148.25, 173.84; HRMS (ESI): M+H$^+$ found 556.0778; $C_{30}H_{24}N_2S_4O_1$ requires 556.0771.

3-([2,2':5',2''-terthiophen]-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3q**)



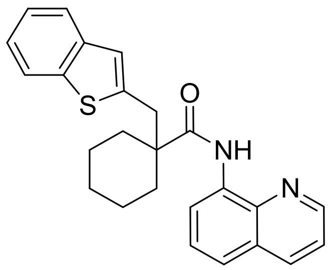
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2,2':5',2''-terthiophene (149.0 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 50.2 mg (53%) as white solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.50 (s, 6H), 3.22 (s, 2H), 6.74 (d, J = 3.6 Hz, 1H), 6.91– 6.92 (m, 2H), 6.98 –7.00 (m, 2H), 7.12 (d, J = 3.2 Hz, 1H), 7.18 (d, J = 5.2 Hz, 1H), 7.42 (dd, J = 8.4, 4.4 Hz, 1H), 7.50 – 7.56 (m, 2H), 8.14 (d, J = 8.0 Hz, 1H), 8.76 (d, J = 4.4 Hz, 1H), 8.84 (d, J = 7.6 Hz, 1H), 10.25 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 24.44, 40.07, 44.09, 115.43, 120.47, 120.53, 122.34, 122.49, 122.70, 123.19, 123.27, 126.41, 126.79, 126.86, 126.92, 133.44, 134.61, 134.75, 135.24, 135.51, 136.23, 137.80, 138.53, 147.23, 161.69, 174.47; HRMS (ESI): M+H$^+$ found 474.0897; $C_{26}H_{22}N_2S_3O_1$ requires 474.0894.

3-(benzo[b]thiophen-2-yl)-2-methyl-2-phenyl-*N*-(quinolin-8-yl)propanamide (**4a**)



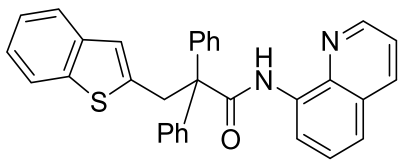
Following the general procedure, reaction was conducted using 2-methyl-2-phenyl-N-(quinolin-8-yl)propanamide (58.1 mg, 0.2 mmol), benzo[b]thiophene (80.5 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 56.5 mg (67%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.83 (s, 3H), 3.66, 3.95 (AB, J_{AB} = 14.4 Hz, 2H), 6.91 (s, 1H), 7.17 – 7.26 (m, 2H), 7.32 – 7.47 (m, 5H), 7.52 – 7.65 (m, 5H), 8.07 (d, *J* = 8.0 Hz, 1H), 8.56 (d, *J* = 4.4 Hz, 1H), 8.81 (d, *J* = 7.6 Hz, 1H), 9.92 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 22.85, 40.89, 52.57, 116.15, 121.47, 121.91, 122.75, 123.50, 123.86, 124.20, 127.21, 127.32, 127.58, 127.85, 128.90, 134.57, 136.09, 138.66, 139.52, 140.13, 141.03, 142.35, 148.16, 174.53; HRMS (ESI): M+H$^+$ found 422.1454; $C_{27}H_{22}N_2S_1O_1$ requires 422.1453.

1-(benzo[b]thiophen-2-ylmethyl)-*N*-(quinolin-8-yl)cyclohexanecarboxamide (**4b**)



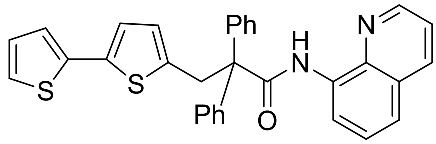
Following the general procedure, reaction was conducted using 1-methyl-N-(quinolin-8-yl)cyclohexane-1-carboxamide (53.7 mg, 0.2 mmol), benzo[b]thiophene (80.5 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 45.6 mg (57%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.59 – 1.74 (m, 8H), 2.27 – 2.30 (m, 2H), 3.30 (s, 2H), 6.99 (s, 1H), 7.14 – 7.21 (m, 2H), 7.34 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.48 – 7.57 (m, 3H), 7.62 (d, *J* = 7.6 Hz, 1H), 8.10 (d, *J* = 8.0 Hz, 1H), 8.53 (d, *J* = 4.0 Hz, 1H), 8.84 (d, *J* = 7.6 Hz, 1H), 10.18 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 22.96, 25.84, 34.05, 40.68, 49.33, 116.54, 121.34, 121.41, 121.82, 122.74, 123.41, 123.60, 123.82, 127.39, 127.86, 134.46, 136.05, 138.77, 139.91, 139.97, 140.28, 148.10, 174.46; HRMS (ESI): M+H$^+$ found 400.1611; $C_{25}H_{24}N_2S_1O_1$ requires 400.1609.

3-(benzo[b]thiophen-2-yl)-2,2-diphenyl-N-(quinolin-8-yl)propanamide (**4c**)



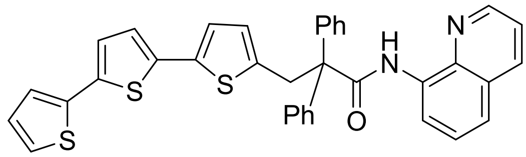
Following the general procedure, reaction was conducted using 2,2-diphenyl-N-(quinolin-8-yl)propanamide (70.5 mg, 0.2 mmol), benzo[b]thiophene (80.5 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 68.7 mg (71%) as white solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 4.12 (s, 2H), 6.58 (s, 1H), 7.07 – 7.14 (m, 2H), 7.18 (s, 1H), 7.22 – 7.24 (m, 6H), 7.37 – 7.45 (m, 7H), 7.55 (d, *J* = 7.6 Hz, 1H), 7.98 (d, *J* = 8.4 Hz, 1H), 8.40 (d, *J* = 4.4 Hz, 1H), 8.77 (d, *J* = 7.6 Hz, 1H), 10.12 (s, 1H), δ_C (100 MHz; $CDCl_3$; Me_4Si) 40.58, 64.01, 116.15, 121.46, 121.55, 121.83, 122.72, 123.37, 123.65, 125.03, 127.30, 127.39, 127.84, 128.40, 129.34, 134.56, 135.99, 138.73, 139.34, 140.33, 141.24, 141.86, 148.12, 172.13; HRMS (ESI): M+H$^+$ found 484.1611; $C_{32}H_{24}N_2S_1O_1$ requires 484.1609.

3-([2,2'-bithiophen]-5-yl)-2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (**4d**)



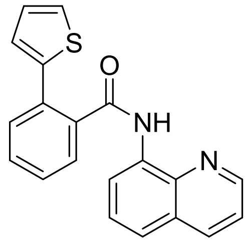
Following the general procedure, reaction was conducted using 2,2-diphenyl-N-(quinolin-8-yl)propanamide (70.5 mg, 0.2 mmol), 2,2'-bithiophene (99.7 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 60.9 mg (59%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 3.99 (s, 2H). 6.19 (d, *J* = 3.2 Hz, 1H), 6.69 (d, *J* = 3.2 Hz, 1H), 6.82 – 6.84 (m, 1H), 6.91 (d, *J* = 2.4 Hz, 1H), 7.01 (d, *J* = 4.4 Hz, 1H), 7.17 – 7.27 (m, 7H), 7.36 (d, *J* = 7.2 Hz, 5H), 7.44 (t, *J* = 8.0 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 8.43 (d, *J* = 2.4 Hz, 1H), 8.74 (d, *J* = 7.6 Hz, 1H), 10.10 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 39.96, 64.18, 116.15, 121.47, 121.52, 122.66, 123.03, 123.60, 127.28, 127.35, 127.58, 127.85, 128.40, 129.05, 129.39, 134.56, 136.00, 136.43, 137.99, 138.73, 139.33, 141.93, 148.14, 172.11; HRMS (ESI): $M+H^+$ found 516.1322; $C_{32}H_{24}N_2S_2O_1$ requires 516.1330.

3-([2,2':5',2''-terthiophen]-5-yl)-2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (**4e**)



Following the general procedure, reaction was conducted using 2,2-diphenyl-N-(quinolin-8-yl)propanamide (70.5 mg, 0.2 mmol), 2,2':5',2''-terthiophene (149.0 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 49.0 mg (41%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 4.07 (s, 2H), 6.27 (d, *J* = 3.6 Hz, 1H), 6.76 (d, *J* = 3.2 Hz, 1H), 6.89 (d, *J* = 3.6 Hz, 1H), 6.97 (d, *J* = 4.0 Hz, 2H), 7.10 (d, *J* = 3.6 Hz, 1H), 7.16 (d, *J* = 4.8 Hz, 1H), 7.38 – 7.25 (m, 7H), 7.44 (d, *J* = 7.6 Hz, 5H), 7.52 (t, *J* = 8.0 Hz, 1H), 8.05 (d, *J* = 8.0 Hz, 1H), 8.52 (d, *J* = 4.0 Hz, 1H), 8.82 (d, *J* = 7.6 Hz, 1H), 10.19 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 40.02, 64.19, 116.15, 121.48, 121.54, 122.63, 123.46, 123.58, 124.21, 124.23, 127.29, 127.39, 127.83, 128.42, 129.18, 129.38, 134.55, 135.40, 136.01, 136.14, 136.88, 137.33, 138.72, 139.63, 141.92, 148.15, 172.08; HRMS (ESI): $M+H^+$ found 598.1211; $C_{36}H_{26}N_2S_3O_1$ requires 598.1207.

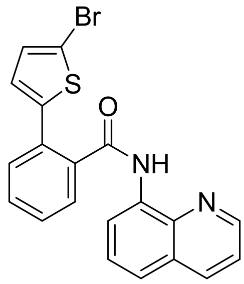
N-(quinolin-8-yl)-2-(thiophen-2-yl)benzamide (**5a**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)benzamide (49.6 mg, 0.2 mmol), thiophene (50.5 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 56.8 mg (86%) as white solid. δ_H (400 MHz; $CDCl_3$; Me_4Si)

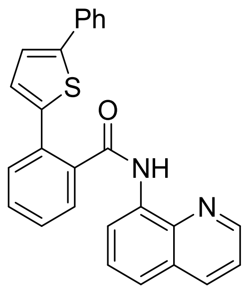
6.89 (t, J = 4.2 Hz, 1H). 7.22 – 7.23 (m, 2H), 7.38 (dd, J = 8.4, 4.0 Hz, 1H), 7.45 – 7.60 (m, 5H), 7.81 (d, J = 7.2 Hz, 1H), 8.11 (d, J = 8.4 Hz, 1H), 8.62 (d, J = 4.0 Hz, 1H), 8.87 (d, J = 7.2 Hz, 1H), 9.98 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 116.54, 121.54, 121.74, 126.33, 127.14, 127.35, 127.61, 127.85, 128.06, 128.88, 130.35, 130.90, 132.43, 134.62, 136.12, 136.50, 138.49, 141.07, 147.98, 167.80; HRMS (ESI): M+H$^+$ found 330.0826; $C_{20}H_{14}N_2S_1O_1$ requires 330.0827.

2-(5-bromothiophen-2-yl)-*N*-(quinolin-8-yl)benzamide (**5b**)



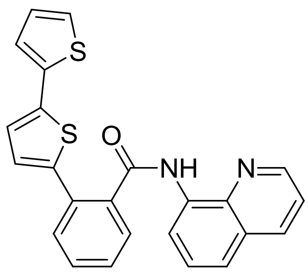
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)benzamide (49.6 mg, 0.2 mmol), 2-bromothiophene (97.8 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired 64.3 mg (79%) as white solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 6.83 (d, J = 3.6 Hz, 1H), 6.95 (d, J = 4.0 Hz, 1H), 7.41 (dd, J = 8.4, 4.4 Hz, 1H), 7.47 – 7.59 (m, 5H), 7.82 (d, J = 6.8 Hz, 1H), 8.13 (d, J = 8.4 Hz, 1H), 8.67 (d, J = 4.0 Hz, 1H), 8.85 (d, J = 7.2 Hz, 1H), 10.04 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 112.90, 116.67, 121.63, 121.95, 127.33, 127.53, 127.88, 128.53, 129.06, 130.51, 130.56, 130.74, 131.57, 134.47, 136.18, 136.31, 138.49, 142.59, 148.14, 167.33; HRMS (ESI): M+H$^+$ found 407.9928; $C_{20}H_{13}N_2S_1O_1Br_1$ requires 407.9932.

2-(5-phenylthiophen-2-yl)-N-(quinolin-8-yl)benzamide (**5c**)



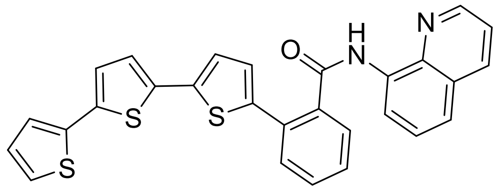
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)benzamide (49.6 mg, 0.2 mmol), 2-phenylthiophene (96.1 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 68.2 mg (84%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 7.07 (d, J = 3.6 Hz, 1H), 7.17 (d, J = 3.6 Hz, 1H), 7.22 – 7.26 (m, 1H), 7.30 – 7.33 (m, 3H), 7.47 – 7.56 (m, 6H), 7.63 (d, J = 7.6 Hz, 1H), 7.83 (d, J = 7.2 Hz, 1H), 8.09 (d, J = 8.2 Hz, 1H), 8.55 (d, J = 4.1 Hz, 1H), 8.88 (d, J = 7.5 Hz, 1H), 10.08 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 116.63, 121.51, 121.81, 123.86, 125.69, 127.32, 127.51, 127.86, 128.10, 128.17, 128.82, 129.06, 130.44, 130.66, 132.33, 134.19, 134.63, 136.08, 136.21, 138.51, 140.38, 145.27, 148.05, 167.81; HRMS (ESI): M+H$^+$ found 406.1143; $C_{26}H_{18}N_2S_1O_1$ requires 406.1140.

2-([2,2'-bithiophen]-5-yl)-*N*-(quinolin-8-yl)benzamide (**5d**)



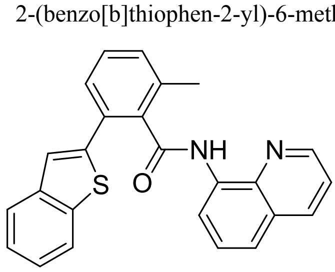
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)benzamide (49.6 mg, 0.2 mmol), 2,2'-bithiophene (99.7 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 65.1 mg (79%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 6.93 – 6.97 (m, 2H), 7.07 (d, J = 3.6 Hz, 1H), 7.11 (d, J = 3.6 Hz, 1H), 7.16 (d, J = 4.8 Hz, 1H), 7.32 (dd, J = 8.4, 4.4 Hz, 1H), 7.45 – 7.61 (m, 5H), 7.84 (d, J = 7.6 Hz, 1H), 8.08 (d, J = 8.4 Hz, 1H), 8.58 (d, J = 4.4 Hz, 1H), 8.89 (d, J = 7.6 Hz, 1H), 10.09 (s, 1H), δ_C (100 MHz; $CDCl_3$; Me_4Si) 116.65, 121.55, 121.86, 123.75, 124.45, 124.49, 127.30, 127.77, 127.87, 127.94, 128.17, 129.09, 130.46, 130.63, 132.02, 134.61, 136.08, 136.22, 137.17, 138.33, 138.51, 139.90, 148.08, 167.68, HRMS (ESI): $M+H^+$ found 412.0709; $C_{24}H_{16}N_2S_2O_1$ requires 412.0704.

2-([2,2':5',2''-terthiophen]-5-yl)-*N*-(quinolin-8-yl)benzamide (**5e**)



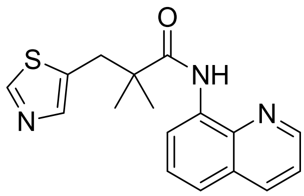
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)benzamide (49.6 mg, 0.2 mmol), 2,2':5',2''-terthiophene (149.0 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 78.1 mg (79%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 6.92 – 6.93 (m, 1H), 6.97 – 7.03 (m, 3H), 7.10 – 7.14 (m, 2H), 7.20 – 7.21 (m, 1H), 7.34 – 7.36 (m, 1H), 7.48 – 7.61 (m, 5H), 7.83 – 7.84 (m, 1H), 8.09 – 8.11 (m, 1H), 8.59 – 8.60 (m, 1H), 8.86 – 8.88 (m, 1H), 10.08 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 115.64, 123.39, 123.26, 122.67, 120.84, 120.55, 123.49, 126.29, 126.86, 127.01, 127.19, 128.10, 129.46, 129.59, 130.93, 133.55, 134.92, 135.08, 135.17, 135.25, 136.05, 136.97, 137.49, 138.98, 147.06, 166.62. HRMS (ESI): $M+H^+$ found 494.0586; $C_{28}H_{18}N_2S_3O_1$ requires 494.0581.

2-(benzo[b]thiophen-2-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (**5f**)



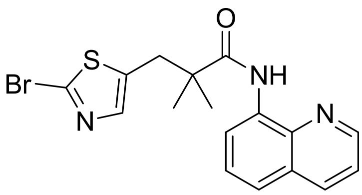
Following the general procedure, reaction was conducted using 2-methyl-N-(quinolin-8-yl)benzamide (52.7 mg, 0.2 mmol), benzo[b]thiophene (80.5 mg, 0.6 mmol),$Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 53.6 mg (68%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 2.53 (s, 3H), 7.16 – 7.22 (m, 2H), 7.31 – 7.33 (m, 2H), 7.40 – 7.56 (m, 5H), 7.60 (d, *J* = 7.6 Hz, 1H), 7.69 (d, *J* = 7.2 Hz, 1H), 8.06 (d, *J* = 8.0 Hz, 1H), 8.61 (d, *J* = 4.4 Hz, 1H), 8.88 (d, *J* = 7.6 Hz, 1H), 9.89 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 19.66, 116.91, 121.52, 121.88, 122.03, 123.28, 123.76, 124.12, 124.16, 127.26, 127.90, 128.09, 129.32, 130.44, 131.92, 134.38, 136.00, 136.14, 136.91, 138.49, 140.22, 140.34, 141.69, 148.14, 168.10; HRMS (ESI): M+H$^+$ found 394.1143; $C_{25}H_{18}N_2S_1O_1$ requires 394.1140.

2,2-dimethyl-*N*-(quinolin-8-yl)-3-(thiazol-5-yl)propanamide (**6a**)



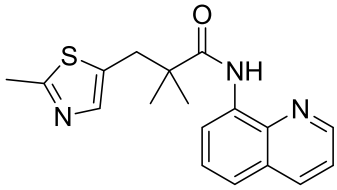
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), thiazole (51.1 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 29.2 mg (47%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.47 (s, 6 H), 3.27 (s, 2 H), 7.44 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.50 – 7.57 (m, 2H), 7.65 (s, 1H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.58 (s, 1H), 8.76 (d, *J* = 4.0 Hz, 1H), 8.81 (d, *J* = 7.2 Hz, 1H), 10.22 (s, 1H). δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.48, 37.73, 44.93, 116.45, 121.63, 121.68, 127.41, 127.93, 134.13, 134.24, 136.33, 138.74, 142.81, 148.32, 152.71, 175.09; HRMS (ESI): M+H$^+$ found 311.1097; $C_{17}H_{17}N_3S_1O_1$ requires 311.1092.

3-(2-bromothiazol-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6b**)



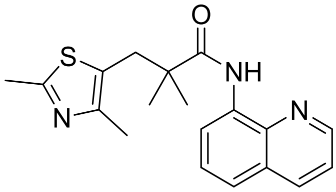
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-bromothiazole (98.4 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 24.1 mg (31%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.47 (s, 6H), 3.19 (s, 2H), 7.32 (s, 1H), 7.45 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.52 – 7.58 (m, 2H), 8.17 (d, *J* = 8.4 Hz, 1H), 8.78 – 8.80 (m, 2H), 10.23 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.65, 38.20, 44.78, 116.54, 121.65, 121.78, 127.40, 127.96, 134.16, 135.42, 136.36, 138.75, 141.84, 148.36, 174.91; HRMS (ESI): M+H$^+$ found 389.0199; $C_{17}H_{16}N_3S_1O_1Br_1$ requires 389.0197.

2,2-dimethyl-3-(2-methylthiazol-5-yl)-*N*-(quinolin-8-yl)propanamide (**6c**)



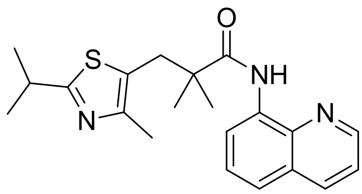
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-methylthiazole (59.5 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 35.1 mg (54%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.46 (s, 6H), 2.55 (s, 3H), 3.18 (s, 2H), 7.35 (s, 1H), 7.43–7.57 (m, 3H), 8.14–8.16 (m, 1H), 8.77–8.82 (m, 2H), 10.22 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 19.08, 25.48, 38.06, 44.81, 116.46, 121.60, 127.44, 127.93, 133.67, 134.32, 136.33, 138.77, 141.44, 148.29, 165.65, 175.26; HRMS (ESI): M+H$^+$ found 325.1253; $C_{18}H_{19}N_3S_1O_1$ requires 325.1249.

3-(2,4-dimethylthiazol-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6d**)



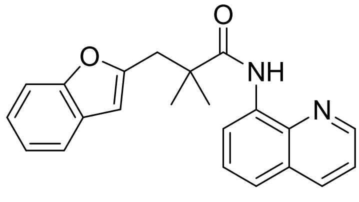
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2,4-dimethylthiazole (67.9 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 41.4 mg (61%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.46 (s, 6H), 2.32 (s, 3H), 2.51 (s, 3H), 3.13 (s, 2H), 7.45 (dd, *J* = 8.4, 4.4 Hz, 1H), 7.50 – 7.58 (m, 2H), 8.16 (d, *J* = 8.0 Hz, 1H), 8.78 (d, *J* = 4.0 Hz, 1H), 8.82 (d, *J* = 7.2 Hz, 1H), 10.23 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 15.30, 18.92, 25.35, 37.42, 45.53, 116.43, 121.56, 121.59, 126.49, 127.46, 127.93, 134.39, 136.32, 138.78, 148.27, 149.33, 163.14, 175.37; HRMS (ESI): M+H$^+$ found 339.1407; $C_{19}H_{21}N_3S_1O_1$ requires 339.1405.

3-(2-isopropyl-4-methylthiazol-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6e**)



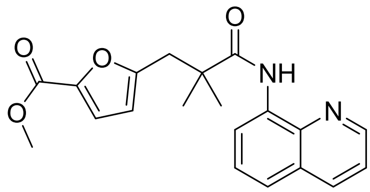
Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), 2-isopropyl-4-methylthiazole (84.7 mg, 0.6 mmol), Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 51.4 mg (70%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.22 (d, *J* = 6.8 Hz, 6H), 1.47 (s, 6H), 2.32 (s, 2H), 3.07 – 3.12 (m, 1H), 3.12 (s, 2H), 7.43 (dd, *J* = 8.0, 4.0 Hz, 1H), 7.49– 7.55 (m, 2H), 8.15 (d, *J* = 8.0 Hz, 1H), 8.76 (d, *J* = 4.0 Hz, 1H), 8.81 (d, *J* = 7.2 Hz, 1H), 10.20 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 15.38, 23.06, 25.29, 33.07, 37.43, 45.51, 116.44, 121.53, 121.56, 125.48, 127.44, 127.92, 130.93, 134.39, 136.30, 138.78, 148.25, 149.10, 175.12, 175.45; HRMS (ESI): M+H$^+$ found 367.1719; $C_{21}H_{25}N_3S_1O_1$ requires 367.1718.

3-(benzofuran-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6f**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), benzofuran (70.9 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 44.7 mg (65%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.52 (s, 6 H), 3.22 (s, 2H), 6.49 (s, 1H), 7.10 – 7.16 (m, 2H), 7.30 (d, J = 7.6 Hz, 1H), 7.39 – 7.43 (m, 2H), 7.49 – 7.57 (m, 2H), 8.14 (d, J = 8.0 Hz, 1H), 8.69 (d, J = 4.0 Hz, 1H), 8.83 (d, J = 7.6 Hz, 1H), 10.26 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.50, 39.22, 44.49, 104.93, 110.84, 116.38, 120.38, 121.47, 121.53, 122.37, 123.27, 127.40, 127.91, 128.80, 134.51, 136.23, 138.78, 148.22, 154.74, 155.98, 175.54; HRMS (ESI): M+H$^+$ found 344.1528; $C_{22}H_{20}N_2O_2$ requires 344.1525.

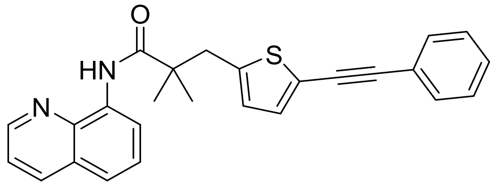
Methyl 5-(2,2-dimethyl-3-oxo-3-(quinolin-8-ylamino)propyl)furan-2-carboxylate (**6g**)



Following the general procedure, reaction was conducted using N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), methyl furan-2-carboxylate (75.7 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 35.9 mg (51%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.48 (s, 6H), 3.14 (s, 2H), 3.78 (s, 3H), 6.22 (d, J = 3.2 Hz, 1H), 7.03 (d, J = 3.2 Hz, 1H), 7.45 (dd, J = 8.0, 4.4 Hz, 1H), 7.50– 7.55 (m, 2 H), 8.16 (d, J = 8.0 Hz, 1H), 7.78 – 8.81 (m, 2H), 10.24 (s, 1H), δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.40, 39.00, 44.65, 51.62, 110.34, 116.38, 119.28, 121.54, 121.60, 127.39, 127.92, 128.85, 130.91, 134.37, 136.29, 138.79, 143.31, 148.30, 157.85, 159.15, 175.16; HRMS (ESI): M+H$^+$ found 352.1427; $C_{20}H_{20}N_2O_4$ requires 352.1423.

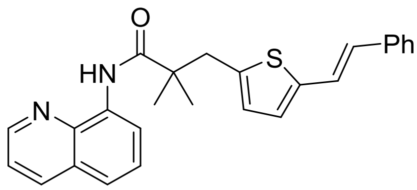
Further applications of alkyl-substituted iodothiophene

2,2-dimethyl-3-(5-(phenylethynyl)thiophen-2-yl)-*N*-(quinolin-8-yl)propanamide (**7**)



A 10-mL Schlenk tube was charged with 3-(5-iodothiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (131.2 mg, 0.3 mmol), ethynylbenzene (61.3 mg, 0.6 mmol), $Pd(PPh_3)_2Cl_2$ (10.5 mg, 0.015 mmol), CuI (2.8 mg, 0.015 mmol), Et_3N (151.8 mg, 1.5 mmol) in DMF 1 ml. The vial was evacuated and filled with N_2, and stirred at 110 °C for 6 h. Purification by flash column chromatography gave the desired product 60.7 mg (74%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.48 (s, 6H), 3.23 (s, 2H), 6.74 (d, J = 3.6 Hz, 1H), 7.04 (d, J = 3.6 Hz, 1H), 7.29 – 7.30 (m, 3H), 7.42 – 7.45 (m, 3H), 7.52 – 7.56 (m, 2H), 8.15 (d, J = 8.0 Hz, 1H), 8.79 (d, J = 4.4 Hz, 1H), 8.84 (d, J = 7.2 Hz, 1H), 10.25 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.48, 41.08, 45.14, 82.97, 92.53, 116.44, 121.54, 121.59, 121.86, 123.08, 127.17, 127.45, 127.94, 128.20, 128.30, 131.32, 131.85, 134.41, 136.30, 138.80, 142.42, 148.29, 175.36; HRMS (ESI): M+H+ found 410.1461; $C_{26}H_{22}N_2O_1S_1$ requires 410.1453.

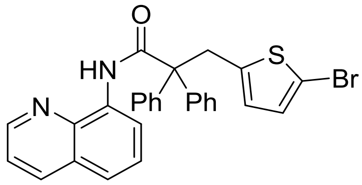
2,2-dimethyl-*N*-(quinolin-8-yl)-3-(5-styrylthiophen-2-yl)propanamide (**8**)



A 10-mL Schlenk tube was charged with 3-(5-iodothiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (131.2 mg, 0.3 mmol), styrene (62.5 mg, 0.6 mmol), $Pd(PPh_3)_2Cl_2$ (21.0 mg, 0.03 mmol), Na_2CO_3 (63.6 mg, 0.6 mmol) in DMF 1 ml. The vial was evacuated and filled with N_2, and stirred at 150 °C for 12 h. Purification by flash column chromatography gave the desired product 51.1 mg (62%) as yellow viscous oil. δ_H (400 MHz; $CDCl_3$; Me_4Si) 1.41 (s, 6H), 3.14 (s, 2H), 6.64 – 6.74 (m, 3H), 6.99 (d, J =8.0 Hz, 1H), 7.10 – 7.14 (m, 1H), 7.17 – 7.23 (m, 2H), 7.29 – 7.35 (m, 3H), 7.41 – 7.50 (m, 2H), 8.05 (d, J = 8.0 Hz, 1H), 8.69 (d, J = 2.8 Hz, 1H), 8.78 (d, J = 7.2 Hz, 1H), 10.18 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 25.49, 41.25, 45.13, 99.98, 116.42, 121.51, 121.58, 121.98, 126.12, 126.16, 127.35, 127.42, 127.46, 127.68, 127.93, 128.64, 134.48, 136.29, 138.81, 139.44, 141.69, 148.28, 175.61; HRMS (ESI): M+H+ found 412.1613; $C_{26}H_{24}N_2O_1S_1$ requires 412.1609.

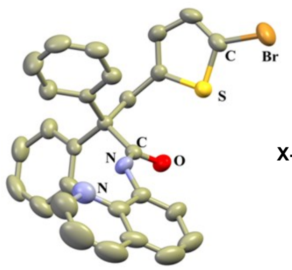
Product Distribution

3-(5-bromothiophen-2-yl)-2,2-diphenyl-*N*-(quinolin-8-yl) propanamide (**9**)



Following the general procedure, reaction was conducted using 2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (70.5 mg, 0.2 mmol), 2-bromothiophene (97.8 mg, 0.6 mmol), $Ni(OTf)_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO, Purification by flash column chromatography gave the desired product 68.6 mg (67%) as yellow solid. δ_H (400 MHz; $CDCl_3$; Me_4Si) 4.07 (s, 2H), 6.05 (d, J = 3.2 Hz, 1H), 6.82 (d, J = 3.6 Hz, 1H), 7.26 – 7.35 (m, 7H), 7.39 – 7.47 (m, 5H), 7.52 (t, J = 8.0 Hz, 1H), 8.07 (d, J = 8.0 Hz, 1H), 8.53 (d, J = 4.4 Hz, 1H), 8.80 (d, J = 7.6 Hz, 1H), 10.15 (s, 1H); δ_C (100 MHz; $CDCl_3$; Me_4Si) 40.22, 64.02, 116.12, 121.49, 121.55, 127.28, 127.41, 127.83, 128.43, 129.27, 130.00, 134.47, 135.68, 136.02, 141.79, 146.34, 148.15, 172.01; HRMS (ESI): $M+H^+$ found 512.0549; $C_{28}H_{21}N_2O_1S_1Br_1$ requires 512.0558.

The structure of compound **9** was confirmed by single crystal X–ray diffraction (CCDC 1529734). CCDC 1529734 (**9**) contains the supplementary crystallographic data for this paper. These data are provided free of charge by The Cambridge Crystallographic Data Centre.



X-ray Structure of 9

Selected data of Single Crystal X-ray Diffractions of 9

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R-factor (gt) are based on F. The threshold expression of
F^2^ > 2.0 sigma(F^2^) is used only for calculating R-factor (gt).
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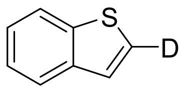
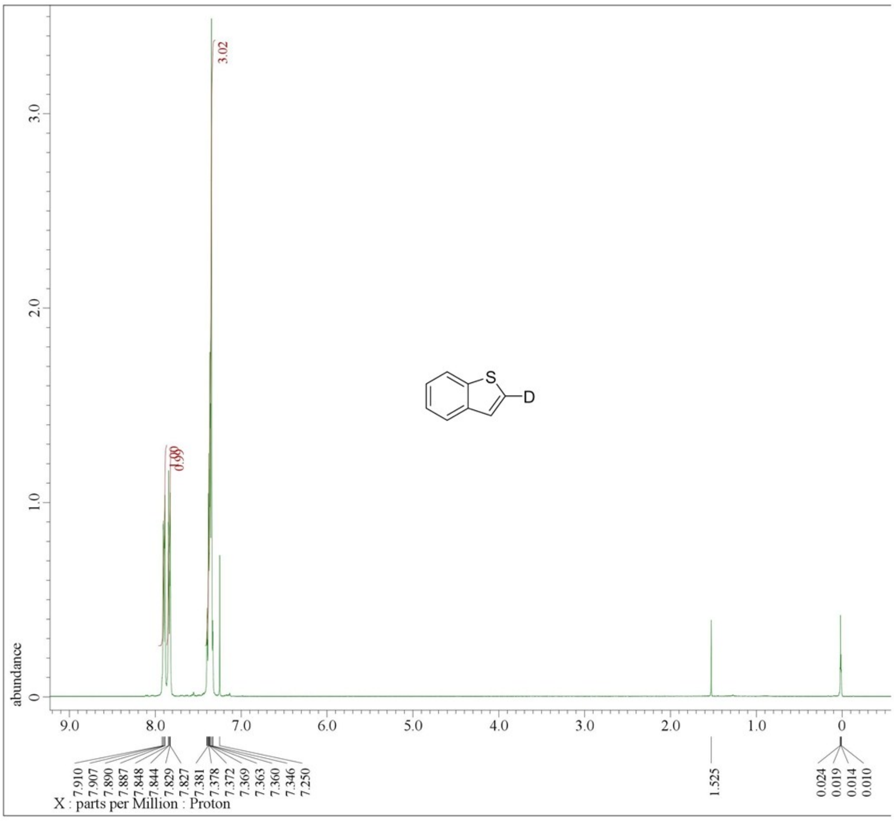
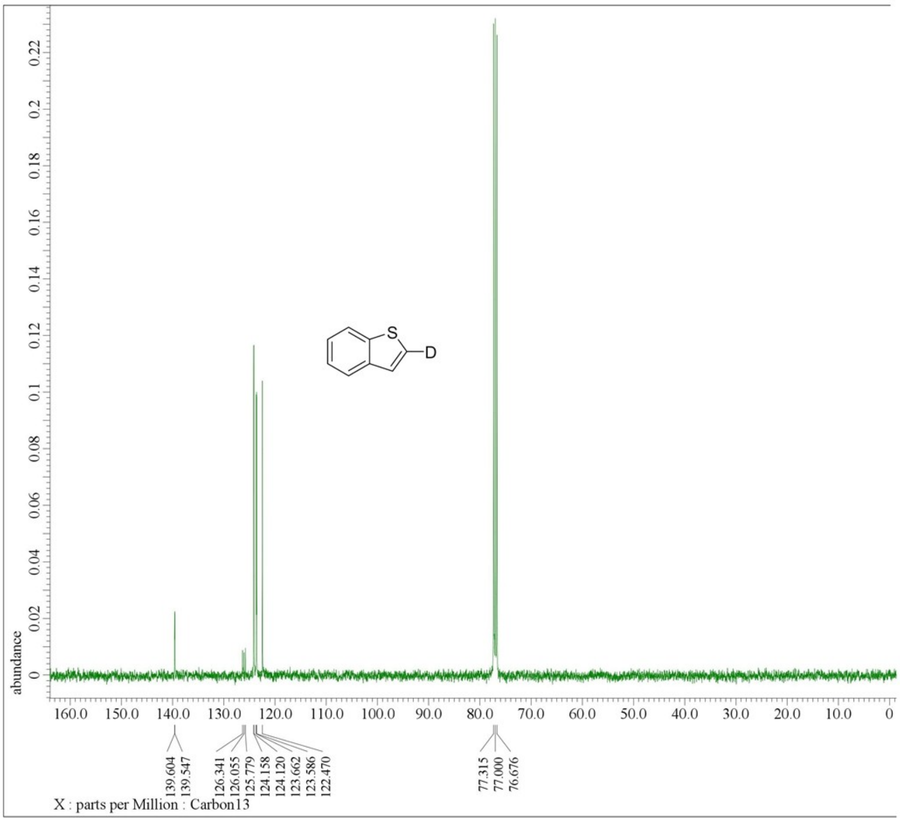
6. Deuterium Labeling Experiment

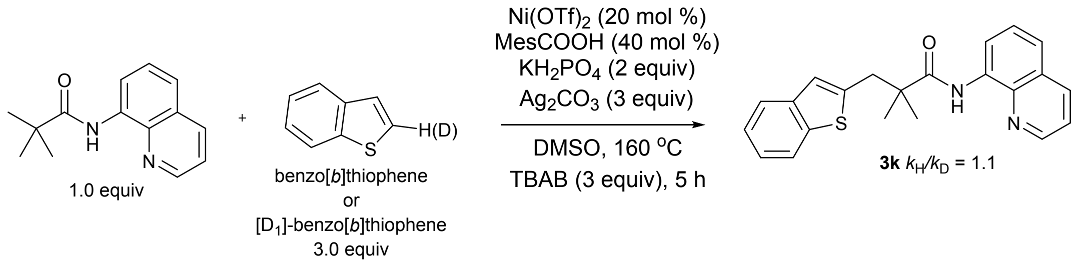
Synthesis of [D_1]-benzo[*b*]thiophene



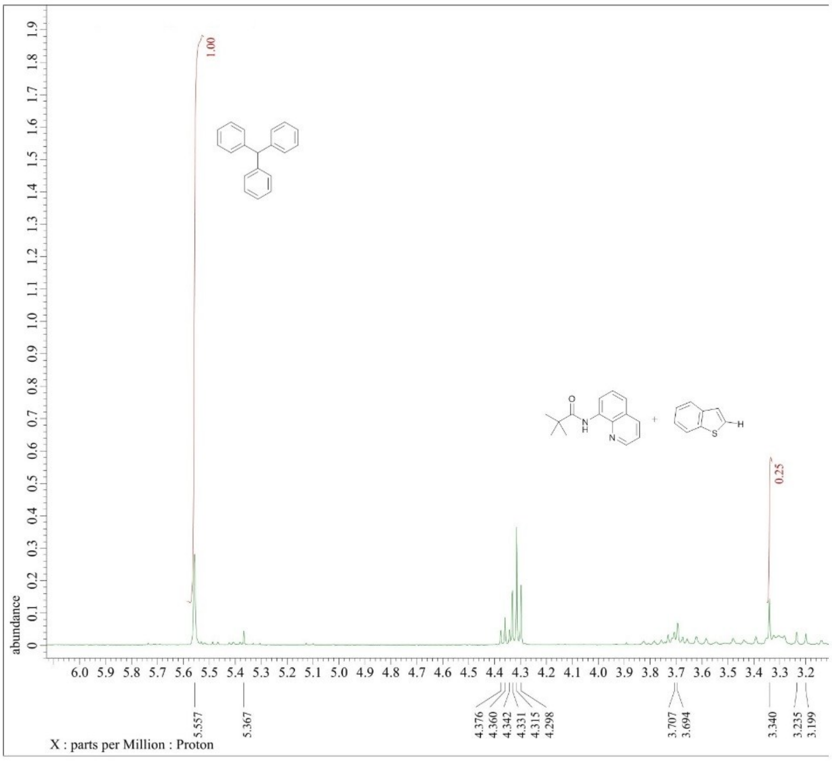
[D_1]-benzo[*b*]thiophene was synthesized according to reported procedure.[J] *n*-BuLi (1.55 M solution in hexane, 24 mL, 37.2 mmol, 1.5 equiv) was added dropwise to a solution of benzo[*b*]thiophene (3.3 g, 24.8 mmol, 1.0 equiv) in dry THF (67 mL) at -78 °C. The resulting mixture was stirred for 2 h at -78 °C and D_2O (10 mL) was added. The white suspension was warmed to room temperature and stirred for an additional hour. H_2O was added (20 mL) and the product was extracted with Et_2O (3 x 30 mL). The combined organic phases were washed with brine, dried over $MgSO_4$ and the solvent was removed under reduced pressure. Flash column chromatography on silica gel (eluent: pentane) gave the **[D_1]-benzo[*b*]thiophene** as a white crystalline solid in 84% yield (2.8 g, >99% deuteration). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89-7.92 (m, 1H), 7.83-7.85 (m, 1H), 7.33-7.40 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 139.60, 139.55, 126.06 (t, 28.1 Hz), 124.16, 124.12, 123.66, 123.59, 122.47. HRMS(DART) *m*/*z* [M+H]$^+$, calcd for $C_8H_5D_1S_1$ 135.02530; Found 135.02449.

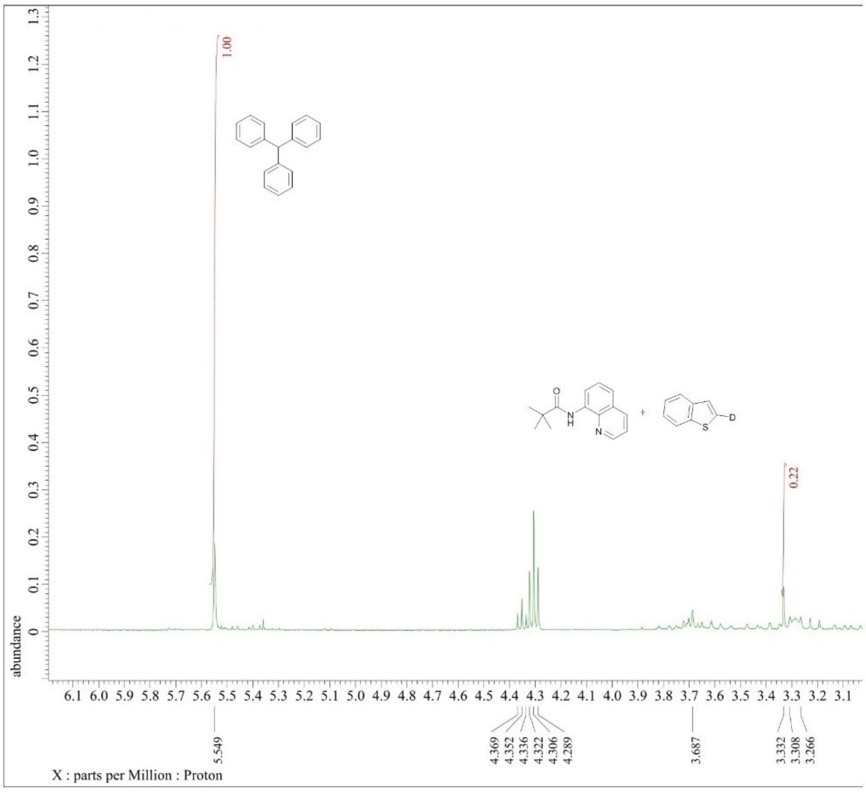


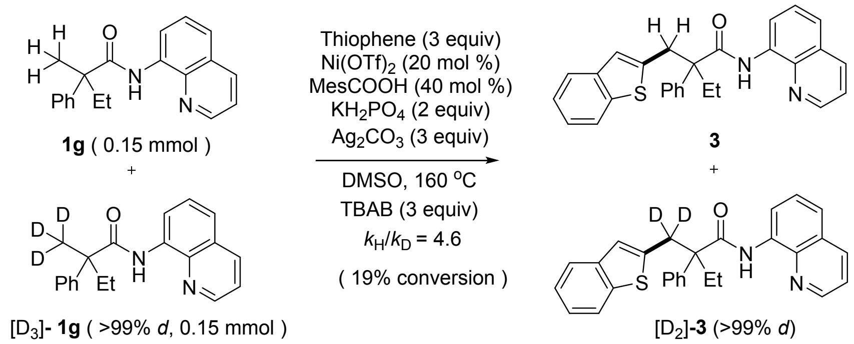


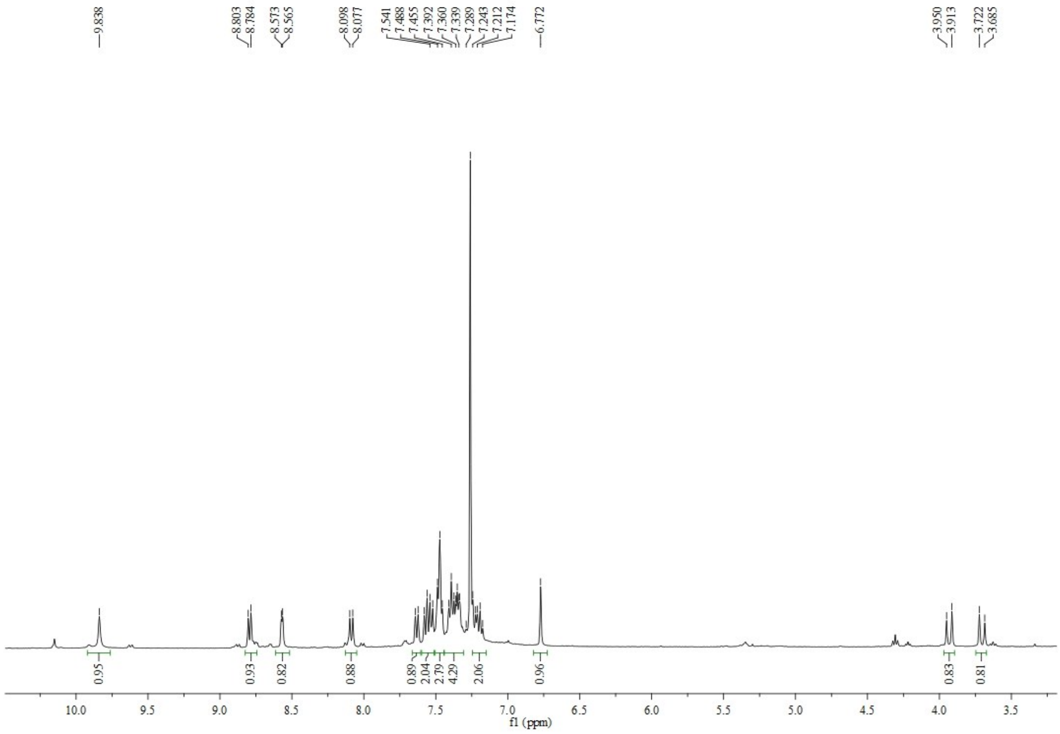


Two sets of reactions were carried out in a parallel manner. In each case, 10-mL Schlenk tube was charged with **1a** (45.6 mg, 0.2 mmol), **benzo[*b*]thiophene** or **[D$_1$]-benzo[*b*]thiophene** (0.6 mmol), respectively. Ni(OTf)$_2$ (14.3 mg, 0.04 mmol), MesCOOH (13.1 mg, 0.08 mmol), KH_2PO_4 (54.4 mg, 0.4 mmol), Ag_2CO_3(165.4 mg, 0.6 mmol), TBAB (193.4 mg, 0.6 mmol) in 0.5 mL DMSO. The vial was evacuated and filled with N_2, and stirred at 160 °C for 5 h. The mixture was then cooled to room temperature, diluted with CH_2Cl_2 (2 mL), filtered through a celite pad, and concentrated in vacuo. The yield of **3k** was determined by ^{1}H NMR of the crude product using Triphenylmethane as internal standard.





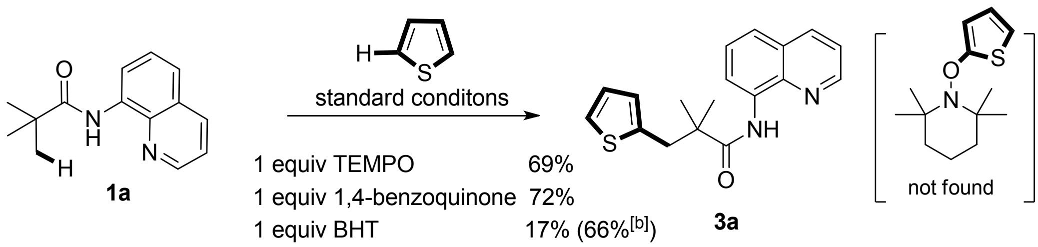




A 10-mL Schlenk tube was charged with **1g** (45.6 mg, 0.15 mmol), **[D$_3$]-1g** (46.1 mg, 0.15 mmol), benzothiophene (120.8 mg, 0.9 mmol), Ni(OTf)$_2$ (21.4 mg, 0.06 mmol), MesCOOH (19.7 mg, 0.12 mmol), KH_2PO_4 (81.6 mg, 0.6 mmol), TBAB (290.1 mg, 0.9 mmol), Ag_2CO_3 (248.1 mg, 0.9 mmol) and DMSO (0.7 mL). The vial was evacuated and filled with N_2, and stirred at 160 °C for 1 h. The mixture was then cooled to room temperature, diluted with CH_2Cl_2 (2 mL), filtered through a celite pad, analyzed by GC-MS, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel, eluting with EtOAc/Hexane (1:100 ~ 1:20, v/v), to afford the heteroarylated product. The ratio of **3** and **[D$_2$]-3** was determined by ^{1}H NMR.

The mixture of **9** and **[D$_2$]-9**: δ_H (400 MHz; $CDCl_3$; Me_4Si) **3.69–3.95 (m, 1.64 H),** 6.77 (s, 1H), 7.17 – 7.24 (m, 2 H), 7.33 – 7.41 (m, 4 H), 7.45 – 7.49 (m, 3 H), 7.52 – 7.58 (m, 2 H), 7.63 (d, J =8.0 Hz, 1H), 8.09 (d, J = 8.4 Hz, 1H), 8.57 (d, J = 3.2 Hz, 1H), 8.79 (d, J = 7.6 Hz, 1H), 9.84 (s, 1H);

Radical Trapping Experiment



A 10-mL Schlenk tube was charged with N-(quinolin-8-yl)pivalamide (45.6 mg, 0.2 mmol), TEMPO (31.2 mg, 0.2 mmol, 1.0 equiv) or BHT (44.1 mg, 0.2 mmol, 1.0 equiv) or 1,4-benzoquinone (21.6 mg, 0.2 mmol, 1.0 equiv) under standard reaction conditions. The vial was evacuated and filled with N_2, and stirred at 160 °C for 24 h. The mixture was then cooled to room temperature, diluted with CH_2Cl_2 (2 mL), filtered through a celite pad, analyzed by GC-MS, and concentrated in vacuo. The residue was purified by flash column chromatography on silica gel, eluting with EtOAc/hexane (1:100 ~ 1:20, v/v), to afford the heteroarylated product **3a** (yield = 17% to 69%).

7 Computational Details and Results

7.1 Computational Details

All calculations were carried out by using the Gaussian 09 suite of computational programs.[d] All stationary points along the reaction coordinate were fully optimized at the DFT level using the B3LYP hybrid functional.[e-g] The 6-31G(d) basis set was applied for all atoms except Ni, which was described by the Lanl2dz basis set and effective core potential implemented. Frequencies were analytically computed at the same level of theory to get the thermodynamic corrections and to confirm whether the structures are minima (no imaginary frequency) or transition states (only one imaginary frequency). Intrinsic reaction coordinate (IRC) calculations were carried out to confirm that all transition state structures connect the proposed reactants and products. The solvation effect was examined by performing single-point self-consistent reaction field (SCRF) calculations at the M06/6-311+G(d,p)/SDD(Ni) level[h-i] based on the SMD solvation model for gas-phase optimized structures. DMSO was used as the solvent, corresponding to the original experimental conditions. The relative free energies corrected by solvation effects calculations are used for discussion. For species that has more than one conformer, only the one having the lowest energy value is used for discussion.

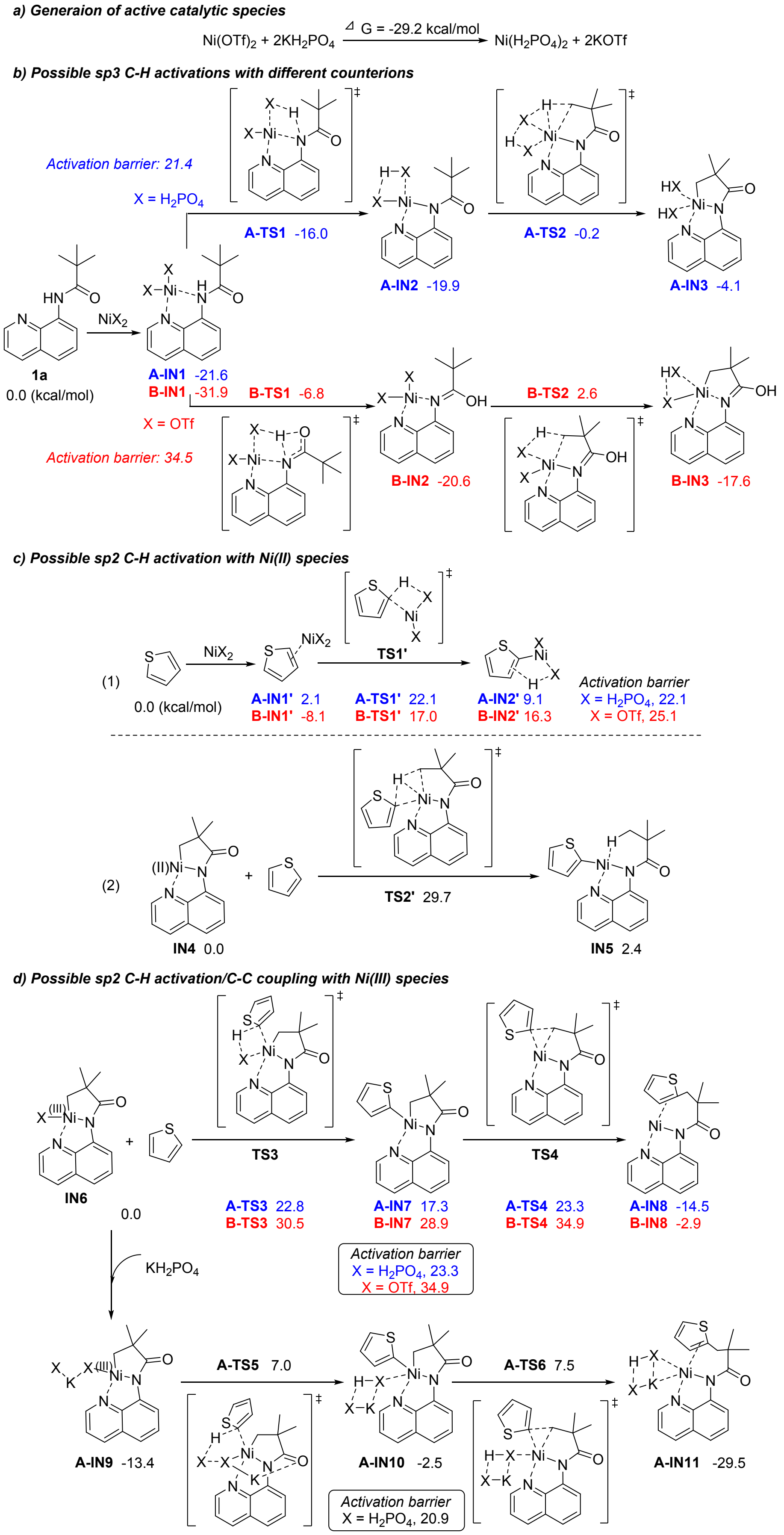
7.2 Calculated Energies

Table S4. Energies (in Hartree) calculated at SMD-B3LYP/BSII//B3LYP/BS1 level

Species	E_0[a]	H_{298}[b]	G_{298}[c]	E[d]	G_{Sol}[e]
$Ni(OTf)_2$	-2092.110893	-2092.09307	-2092.158818	-2092.1698056	-2093.76205760
K_2HPO_4	-671.695459	-671.686967	-671.728652	-671.7335791	-671.924173088
$Ni(H_2PO_4)_2$	-1456.354307	-1456.340154	-1456.394304	-1456.4331242	-1458.08383046
KOTf	-989.596166	-989.585759	-989.634065	-989.6242858	-989.785776271
1a	-727.619214	-727.602959	-727.662278	-727.8957368	-727.565927809
A-IN1	-2184.001702	-2183.971880	-2184.061640	-2184.360296	-2185.71054678
A-TS1	-2183.996522	-2183.967114	-2184.055606	-2184.3486933	-2185.69601244
A-IN2	-2184.007046	-2183.977311	-2184.065586	-2184.36368	-2185.70733779
A-TS2	-2183.962495	-2183.933554	-2184.019491	-2184.3138823	-2185.67213098
A-IN3	-2183.967344	-2183.937662	-2184.025477	-2184.3228397	-2185.68134469
B-IN1	-2819.741629	-2819.707118	-2819.809804	-2820.0792855	-2821.40377708
B-TS1	-2819.716514	-2819.682169	-2819.784365	-2820.0509918	-2821.36104719
B-IN2	-2819.712081	-2819.677360	-2819.780448	-2820.0492372	-2821.38509182
B-TS2	-2819.671826	-2819.637791	-2819.739730	-2820.0034767	-2821.34316210
B-IN3	-2819.719330	-2819.684494	-2819.790282	-2820.0549795	-2821.37630760
A-IN1'	-2009.286932	-2009.267214	-2009.335032	-2009.4344019	-2011.01528206
A-TS1'	-2009.262854	-2009.243883	-2009.309602	-2009.4052425	-2010.97969967
A-IN2'	-2009.278526	-2009.258960	-2009.326234	-2009.4254368	-2011.00408305
B-IN1'	-2645.046859	-2645.023128	-2645.103246	-2645.1738781	-2646.70889488
B-TS1'	-2645.014552	-2644.991363	-2645.070851	-2645.1364579	-2646.66395999
B-IN2'	-2645.013082	-2644.989292	-2645.070056	-2645.1387915	-2646.66818553
IN4	-895.733293	-895.716880	-895.775734	-895.98703	-897.336543828
TS2'	-1448.630499	-1448.608832	-1448.679774	-1448.9481982	-1450.22055708
IN5	-1448.681914	-1448.659839	-1448.733113	-1449.0048248	-1450.27509246
IN6	-1539.262089	-1539.238567	-1539.315507	-1539.315507	-1540.90208916
A-TS3	-2092.166077	-2092.137422	-2092.225256	-2092.5219694	-2093.79657501
A/B-IN7	-1448.070685	-1448.048954	-1448.121746	-1448.3819703	-1449.64997761
A/B-TS4	-1448.053639	-1448.032431	-1448.103566	-1448.3640661	-1449.64068335
A/B-IN8	-1448.112484	-1448.091363	-1448.161738	-1448.4257466	-1449.70444600
A-IN9	-2211.021502	-2210.990440	-2211.085016	-2211.3554856	-2212.87332659
A-TS5	-2763.928567	-2763.891974	-2763.997984	-2764.3236999	-2765.77031863
A-IN10	-2763.950234	-2763.912806	-2764.020335	-2764.3521061	-2765.79148832
A-TS6	-2763.927166	-2763.890228	-2763.997081	-2764.3277737	-2765.77453615
A-IN11	-2763.986921	-2763.950344	-2764.054397	-2764.3899526	-2765.83831506

[a] Sum of electronic and zero-point energies
[b] Sum of electronic and thermal enthalpies
[c] Sum of electronic and thermal free energies
[d] Electronic energies
[e] Single point energies in solution

Scheme 4. Computational Results in large scale figures as shown in main text



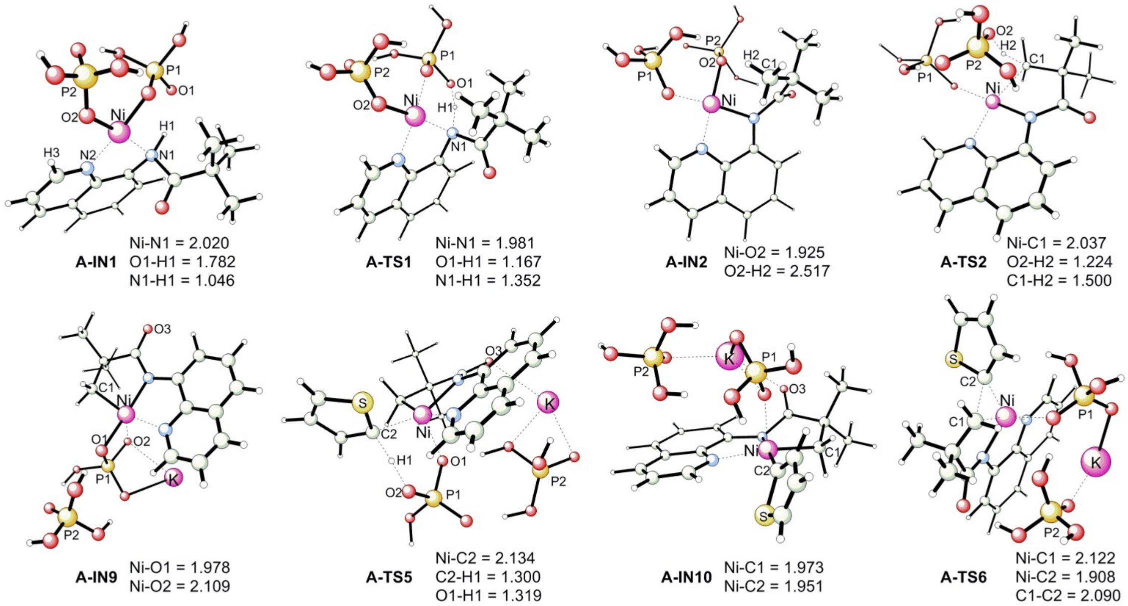


Figure 3. Geometric Structures for Key Intermediates and Transition States (Distances are in Angstrom)

7.3 Cartesian Coordinates for All Species

$Ni(OTf)_2$

S	1.93343000	1.94986800	-2.21213700
O	2.58373100	1.46729600	-0.91007300
O	0.48492100	2.11031000	-1.73543000
C	-0.13278300	2.27245100	3.28997500
F	-1.38358400	2.59437800	3.59844200
F	0.44812300	3.27788000	2.63691000
F	0.55398600	1.98887000	4.39045600
S	-0.15687400	0.76198700	2.18659400
O	1.29181200	0.60462300	1.70907000
O	-0.77375900	-0.31792800	2.92262700
O	-0.80892200	1.24456000	0.88576000
Ni	0.88740100	1.35753600	-0.01273400
O	2.55312400	3.02791000	-2.94852300
C	1.90745100	0.43849000	-3.31448900
F	3.15785800	0.11384700	-3.62156000
F	1.22228200	0.72301000	-4.41574300
F	1.32387300	-0.56526200	-2.66136200

K_2HPO_4

P	-0.38840200	0.40348700	0.23463800
O	1.06529500	0.73767600	0.28586400
O	-0.71023100	-0.35432100	-1.26201300
H	-0.04709800	-0.03480900	-1.89346800
O	-1.26297100	1.79341500	0.06593000
H	-0.62396500	2.52319600	0.09381000
O	-1.12622800	-0.50317500	1.19062800
K	-2.20182300	-2.24974500	-0.21361200

$Ni(H_2PO_4)_2$

Ni	1.06143400	1.51026400	0.06663900
P	1.58526800	1.65744500	-2.34334800
O	2.45097800	1.07293300	-1.20682400
O	2.40924300	2.74568800	-3.20580400
H	2.97756900	3.29033600	-2.63472600
O	0.34199900	2.17182700	-1.60070200
O	1.15462700	0.64655300	-3.50495200
H	1.82152500	0.56806900	-4.20733700
P	0.50389900	1.31440100	2.46553300
O	-0.32787200	1.95808000	1.33611600
O	1.78714100	0.87555300	1.74206800
O	-0.15623500	0.06770200	3.21835700
H	-0.73471700	0.32992300	3.95376100
O	0.68882200	2.32972200	3.70723600
H	0.82081800	3.24259600	3.39904500

KOTf

C	2.65048100	3.24877900	-2.21805500
F	2.53738100	3.98188100	-1.10497500
F	2.14437100	3.94110600	-3.24476200
F	3.94679400	3.01592700	-2.45203200
S	1.74188800	1.64852700	-2.01989500
O	1.91725700	0.91343600	-3.30148400
O	2.37892400	0.95397100	-0.86877900
O	0.32300100	2.01103000	-1.75670600
K	0.30784700	-0.86564400	-1.70797700

1a

C	-1.41120000	-0.80751400	-2.13781300
C	-2.66109100	-1.15788800	-2.97750300
H	-3.57537500	-1.07139700	-2.37965000
H	-2.77234300	-0.51352500	-3.85697900
H	-2.58957700	-2.19156900	-3.33589600
C	-0.14306700	-0.89754100	-3.01718300
H	-0.19436200	-0.24361000	-3.89499000
H	0.75250500	-0.62576600	-2.44727800
H	-0.01377300	-1.92439300	-3.37889700
C	-1.29131200	-1.79109200	-0.96275500
H	-0.41905200	-1.56234500	-0.34407900
H	-2.17208200	-1.74381500	-0.31595500
H	-1.19191200	-2.81425000	-1.34337200
C	-1.54561700	0.62345400	-1.56055800
O	-1.52786500	0.85253300	-0.35745700
N	-1.68291000	1.61300200	-2.50896100
H	-1.69225600	1.36082100	-3.49259100
C	-1.82361500	2.99015300	-2.32533400
C	-1.94955900	3.75532500	-3.53633200
C	-1.84905800	3.64203500	-1.10267900
C	-2.09833700	5.17346900	-3.46227500
C	-1.99737900	5.04779500	-1.05295900
H	-1.75491800	3.06355300	-0.19462900
C	-2.03572600	3.76767700	-5.83775200
C	-2.21762500	5.86936400	-4.69191700
C	-2.11980900	5.80836400	-2.19388600
H	-2.01344900	5.52941500	-0.07896200
C	-2.18726300	5.17358900	-5.87879800
H	-2.33245600	6.95079000	-4.68005900
H	-2.23281300	6.88791300	-2.14004100
H	-2.27675500	5.68055900	-6.83467500
H	-2.00902500	3.19585600	-6.76435000
N	-1.92091000	3.07889100	-4.71837100

A-IN1

C	-1.07065200	3.01101000	-1.32495500
C	0.34909600	2.99045900	-1.94513900
H	1.08636400	2.54312100	-1.27629800
H	0.35296100	2.43349400	-2.88918900
H	0.65182900	4.02167300	-2.15993300
C	-2.05131600	3.64101900	-2.33499000
H	-2.08033300	3.07578800	-3.26960700
H	-3.07009900	3.68005700	-1.93437100
H	-1.72996700	4.66474700	-2.55471300
C	-1.07246900	3.83549800	-0.01932600
H	-2.06475800	3.83801900	0.45017800
H	-0.33878700	3.48224600	0.71041400
H	-0.82666200	4.87508700	-0.26249400
C	-1.53507800	1.56504000	-1.08721300
O	-2.28817400	0.97625800	-1.82521600
N	-1.05376100	0.83529700	0.11632700
C	-2.10658600	0.00207600	0.67204600
C	-2.11776900	-1.33592200	0.22583800
C	-3.09029300	0.45056700	1.52210200
C	-3.17174200	-2.21711800	0.58153600
C	-4.12627700	-0.43276600	1.92088300
H	-3.08098000	1.47646500	1.87757000
C	-1.00743700	-2.97831300	-0.99689800
C	-3.11238800	-3.53103200	0.04941100
C	-4.18356000	-1.72692800	1.44892000
H	-4.89363800	-0.06909800	2.59714600
C	-2.04865600	-3.90024600	-0.74553100
H	-3.90402900	-4.23845000	0.28188900
H	-4.99404800	-2.38745400	1.74358500
H	-1.97786200	-4.89902400	-1.16215900
H	-0.11144700	-3.23980500	-1.54895000
N	-1.04963700	-1.74259000	-0.52514900
Ni	0.38634500	-0.46475300	-0.44444700
P	1.90100400	1.17018300	1.44768700
O	1.77346400	0.74233900	-0.06503800
O	3.20629500	2.13629800	1.36213000
H	3.41337500	2.51189500	2.23357900
O	2.29707000	-0.09862500	2.31856500
H	2.80292100	-0.79934900	1.78070700
O	0.68865200	1.86317700	2.01139200
H	-0.58065300	1.42062700	0.84222800
P	3.07925500	-1.75351500	-0.70904300
O	1.55464500	-1.76516600	-1.06738400
O	3.68363800	-3.01396200	-1.52217700
H	4.29037200	-3.49254200	-0.93413300
O	3.43538200	-1.84835900	0.75334100
O	3.76491700	-0.50983900	-1.47112600
H	3.31149400	0.29712700	-1.14232100

A-TS1

C	-1.02721000	2.92558300	-1.43975500
C	-0.06084600	2.30601200	-2.47710500
H	0.74235900	1.73366700	-2.00622400
H	-0.59459100	1.65600400	-3.18026100
H	0.40835600	3.11044800	-3.05582300
C	-2.03958400	3.81770800	-2.18785700
H	-2.60887200	3.24822600	-2.92687500
H	-2.75685900	4.27246500	-1.49757700
H	-1.50075900	4.62059700	-2.70354500
C	-0.24380100	3.79733100	-0.43696500
H	-0.89554800	4.18892200	0.35243900
H	0.57783500	3.25640900	0.02865600
H	0.18471600	4.65434800	-0.96910400
C	-1.83341500	1.80977500	-0.73607000
O	-3.01744000	1.66012400	-0.97565400
N	-1.18748600	0.93095100	0.22262700
C	-2.14565800	-0.01633400	0.74441600
C	-2.09651900	-1.30704000	0.17642600
C	-3.10066800	0.25411600	1.69923400
C	-3.04729200	-2.30931300	0.50570800
C	-4.03259100	-0.74715800	2.07269400
H	-3.15489300	1.24118800	2.14694400
C	-0.95823800	-2.71704100	-1.29493300
C	-2.92404500	-3.55063800	-0.16770400
C	-4.02711300	-1.99396400	1.48294800
H	-4.77689000	-0.51252000	2.82777700
C	-1.90118800	-3.74428400	-1.07312000
H	-3.63591800	-4.34503900	0.04129000
H	-4.76052000	-2.74478700	1.76285700
H	-1.78639100	-4.68565700	-1.59934600
H	-0.08984000	-2.84914800	-1.92982300
N	-1.06141200	-1.54366300	-0.68858000
Ni	0.28529400	-0.19960700	-0.46907500
P	1.66145700	1.26897100	1.69084200
O	1.67266800	0.98356400	0.15925700
O	2.64181000	2.51096500	1.99003500
H	3.45687600	2.20804500	2.42305600
O	2.25811400	0.06669400	2.50730300
H	2.55368000	-0.74242800	1.90672800
O	0.24081400	1.68327700	2.13511700

H	-0.49347100	1.45522000	1.25731700
P	2.95170600	-1.53223600	-0.53568200
O	1.55979300	-1.37057200	-1.20546600
O	3.67426600	-2.75443600	-1.30212300
H	4.10217500	-3.32645400	-0.64428500
O	2.96557500	-1.79405700	0.95844100
O	3.86448500	-0.27197500	-0.96659300
H	3.33350100	0.53025500	-0.77589300

A-IN2

C	-0.80673700	2.93856300	-1.19842600
C	-0.17710400	2.18414200	-2.38022400
H	0.79956400	1.76805600	-2.11793900
H	-0.81922600	1.37098600	-2.73206300
H	-0.02683800	2.88103900	-3.21362200
C	-2.17401500	3.52092200	-1.65427000
H	-2.86208900	2.72676400	-1.96840200
H	-2.64500500	4.09074700	-0.84745500
H	-2.01991000	4.18997500	-2.50879400
C	0.11124900	4.08858800	-0.74364300
H	-0.33437000	4.63348900	0.09254500
H	1.08519800	3.70844900	-0.42145600
H	0.26967800	4.78858600	-1.57244300
C	-1.16729800	2.04872700	0.00525800
O	-1.44611900	2.57500500	1.09210700
N	-1.29157100	0.68084200	-0.19923100
C	-2.35601900	-0.04634300	0.31672900
C	-2.26087300	-1.44058200	0.02613100
C	-3.51867300	0.39980000	0.94140700
C	-3.31829100	-2.35162300	0.28874400
C	-4.56709400	-0.50769600	1.21783900
H	-3.62114700	1.44272500	1.21358200
C	-0.88921400	-3.11509200	-0.85711300
C	-3.09541600	-3.70270700	-0.07801800
C	-4.49558000	-1.85029900	0.90070500
H	-5.46101200	-0.12288300	1.70165400
C	-1.89757400	-4.07891300	-0.65117300
H	-3.87614700	-4.43771700	0.10120600
H	-5.31424200	-2.52670100	1.12692400
H	-1.70928400	-5.10828300	-0.93703500
H	0.08106000	-3.36609600	-1.26892000
N	-1.07561800	-1.84396400	-0.52616100
Ni	0.22331500	-0.43889900	-0.41066600
P	1.73617600	1.09715800	1.70448900
O	1.43294100	0.94064400	0.17274400
O	2.33268200	2.60633200	1.75648500
H	2.86580800	2.72795100	2.55992000
O	2.69761900	0.10656800	2.30758100
H	3.36973500	-0.96546500	1.47723500
O	0.37898300	1.08391800	2.54532200
H	-0.34924200	1.64457600	2.16901700
P	3.13951900	-1.41497000	-0.65394200
O	1.64646200	-1.68595200	-0.77873500
O	3.93250200	-2.44931400	-1.57566100
H	4.78699900	-2.69490100	-1.18343100
O	3.75125700	-1.63026900	0.77722600
O	3.52649500	0.02743600	-1.21210200
H	2.87128900	0.67699600	-0.84025300

A-TS2

C	-0.32409000	2.73704000	1.60381400
C	0.71521400	1.61991800	1.79545800
H	1.45383500	1.40401600	0.50777300
H	1.70000400	2.01856700	2.07583900
H	0.44760300	0.98156200	2.65148500
C	0.26907800	3.96074700	0.86725200
H	0.66868600	3.69689500	-0.11606800
H	-0.50329500	4.72332200	0.72784800
H	1.08447400	4.39408600	1.45850200
C	-0.88710400	3.20075200	2.96387800
H	-1.67650400	3.94358500	2.81469400
H	-1.31352900	2.36005500	3.52449300
H	-0.09037400	3.64533700	3.57156800
C	-1.50025800	2.21298500	0.76127300
O	-2.53847800	2.84578100	0.61448300
N	-1.25143400	0.97404000	0.17178700
C	-2.25134600	0.23292400	-0.48595400
C	-1.93059700	-1.14792100	-0.61700000
C	-3.45523500	0.68013600	-1.01760100
C	-2.79408300	-2.06087100	-1.28246900
C	-4.31671300	-0.22949400	-1.67768900
H	-3.72790300	1.72051400	-0.91602900
C	-0.38373900	-2.82184900	-0.12143500
C	-2.37182200	-3.41182500	-1.34623200
C	-4.00967600	-1.56609100	-1.82050400
H	-5.24928600	0.15197100	-2.08438300
C	-1.17727600	-3.78980100	-0.77009700
H	-3.00058400	-4.14222600	-1.84927200
H	-4.68346200	-2.24646900	-2.33319600
H	-0.83422800	-4.81828500	-0.80401600
H	0.55742900	-3.07799300	0.34843600
N	-0.74838100	-1.54884000	-0.05131500

Ni	0.18705700	-0.06269400	0.77664900
O	3.04275100	-1.98836600	-0.60352800
O	1.65386200	-1.14981400	1.43600100
O	3.77232900	-2.46132400	1.76032200
P	1.93375500	1.22301100	-1.85495400
O	2.16932500	-0.21213900	-2.25522600
O	0.44610200	1.75123800	-2.10210400
H	-0.18211300	1.48169100	-1.38624800
O	2.81249900	2.22699400	-2.75371800
H	3.20428800	1.74135300	-3.49820200
O	2.30571100	1.55649500	-0.35714400
P	3.03251900	-1.37758800	0.85253800
O	3.98277400	-0.10120300	0.89266600
H	3.55221800	0.66737600	0.42211600
H	4.65161400	-2.69388200	1.41806000
H	2.70731300	-1.33506700	-1.31944100

A-IN3

C	-0.38639200	2.73518800	1.69525700
C	0.60299800	1.57917500	1.93409300
H	1.78731400	1.55838800	0.17012800
H	1.64679700	1.92393800	1.99224600
H	0.41226000	1.08278000	2.89674500
C	0.26947500	3.92633200	0.95817200
H	0.69317900	3.63572200	-0.00930500
H	-0.46995300	4.71202900	0.77278600
H	1.07775200	4.34635100	1.56875500
C	-0.98473400	3.24734400	3.02195600
H	-1.74989000	4.00596400	2.82999700
H	-1.45162900	2.42990600	3.58404300
H	-0.19770700	3.68373200	3.64806500
C	-1.54425900	2.23151600	0.81462900
O	-2.59024700	2.84990600	0.66738000
N	-1.24952500	1.01326500	0.19514000
C	-2.22695900	0.25779700	-0.48526200
C	-1.88410700	-1.11940600	-0.63753600
C	-3.43021500	0.69927700	-1.02341300
C	-2.73872600	-2.02642400	-1.32596700
C	-4.27691300	-0.20564000	-1.70743000
H	-3.71475900	1.73484700	-0.90597200
C	-0.34240700	-2.79351700	-0.15513500
C	-2.31299100	-3.37564600	-1.40661800
C	-3.95396100	-1.53592100	-1.86829100
H	-5.20966300	0.17333200	-2.11638900
C	-1.12446900	-3.75856100	-0.82344600
H	-2.93651200	-4.09936100	-1.92587800

H	-4.61602600	-2.21604000	-2.39678600
H	-0.77882800	-4.78612400	-0.86612000
H	0.59535300	-3.06071700	0.31705000
N	-0.70373100	-1.52153000	-0.06885800
Ni	0.18092400	0.00789700	0.86762800
O	2.98387900	-2.06804500	-0.52023800
O	1.72219000	-1.01811100	1.51247200
O	3.78133000	-2.43718800	1.83520000
P	1.85565600	1.14600200	-1.98367700
O	2.06666200	-0.31154100	-2.25676600
O	0.37719300	1.69970100	-2.02835900
H	-0.20407700	1.43932200	-1.24917100
O	2.64194300	2.08240900	-3.01601100
H	3.01954100	1.54754800	-3.73400200
O	2.47165200	1.61736700	-0.55488100
P	3.05083800	-1.37078000	0.90289700
O	4.09649800	-0.16264600	0.81781300
H	3.73917700	0.59894800	0.30259600
H	4.64757200	-2.70922000	1.48881400
H	2.61722700	-1.46651300	-1.24324100

B-IN1

C	-2.12974100	-0.91724900	2.52351400
C	-2.05894000	0.60228900	2.30761000
H	-1.09604000	0.91793300	1.89626300
H	-2.86967300	0.97479000	1.67213600
H	-2.15680000	1.09453800	3.28114800
C	-3.47002800	-1.28904900	3.20127100
H	-4.32805600	-0.96249600	2.60075400
H	-3.54525100	-2.36848700	3.35417000
H	-3.53268700	-0.79256700	4.17513500
C	-0.95051600	-1.36458100	3.43154400
H	-0.98573000	-2.44368900	3.60524000
H	0.01685600	-1.10763400	2.99233300
H	-1.03663200	-0.84977100	4.39486000
C	-2.02250000	-1.77187400	1.25431500
O	-2.20334300	-2.96161500	1.24205400
N	-1.65301200	-1.15167400	-0.06616000
H	-1.39238700	-1.96699700	-0.65647200
C	-2.72192200	-0.38855600	-0.69242900
C	-2.33602200	0.86204900	-1.21933700
C	-4.02215900	-0.82464100	-0.82420700
C	-3.27546900	1.68469300	-1.89605100
C	-4.97136100	-0.00315800	-1.48349500
H	-4.31470900	-1.79469100	-0.43420800
C	-0.60010500	2.37521600	-1.56846100

C	-2.79510000	2.91354700	-2.41733500
C	-4.61280800	1.22014200	-2.00870100
H	-5.99320800	-0.35617200	-1.57997600
C	-1.46865500	3.24971200	-2.25842100
H	-3.47793000	3.57529200	-2.94332800
H	-5.34543400	1.83853700	-2.51921500
H	-1.07092000	4.17819000	-2.65281700
H	0.44964000	2.59963000	-1.42911800
N	-1.02453600	1.22676100	-1.05945800
C	2.04383100	3.16923600	0.97380700
F	0.73281400	3.46072700	1.09460600
F	2.46966500	3.66741500	-0.19838000
F	2.70632100	3.75984100	1.96578200
S	2.29086500	1.32299600	1.03428500
O	3.73093400	1.11776900	0.96574800
O	1.52376500	0.88540900	2.20622400
O	1.58080500	0.93761900	-0.29302000
S	1.18165200	-2.82416600	-0.44639800
O	0.03392000	-2.96181600	-1.37568600
O	0.97975000	-1.61266800	0.49587200
Ni	0.02712600	-0.12444500	-0.17634500
O	1.65318700	-3.98952200	0.28584800
C	2.59170900	-2.26923200	-1.53290800
F	2.19327600	-1.24037700	-2.29688300
F	2.95249300	-3.28045300	-2.32716000
F	3.62725700	-1.89320400	-0.79065900

B-TS1

C	-2.26092200	-0.98193800	2.57539000
C	-2.46657500	0.53757300	2.46474300
H	-1.55732800	1.04220700	2.12122800
H	-3.29201600	0.80436700	1.79868800
H	-2.70339000	0.93629400	3.45775000
C	-3.55906500	-1.66840200	3.05751000
H	-4.40215700	-1.45322900	2.39026500
H	-3.42700400	-2.75282700	3.11221300
H	-3.82177100	-1.30035300	4.05580600
C	-1.13017000	-1.25397200	3.60374400
H	-0.95788800	-2.32732300	3.71532000
H	-0.19150700	-0.77874200	3.29941200
H	-1.42102800	-0.83904300	4.57563900
C	-1.80176700	-1.67395000	1.26909900
O	-1.51935300	-2.86355300	1.28165200
N	-1.58505200	-0.95627100	0.05114000
H	-0.80957900	-2.61207900	-0.67187000
C	-2.63412500	-0.24665200	-0.53175300
C	-2.26068800	0.95574000	-1.18812700
C	-3.97016500	-0.62870600	-0.59226100
C	-3.19287500	1.75477200	-1.90177400
C	-4.91054300	0.17125100	-1.28253600
H	-4.29092300	-1.55393900	-0.12340400
C	-0.48451000	2.39260700	-1.67888600
C	-2.68329300	2.92231000	-2.52388300
C	-4.54775400	1.33481200	-1.93208100
H	-5.94648100	-0.15492700	-1.30816600
C	-1.34392900	3.23370900	-2.41562500
H	-3.35652300	3.56457600	-3.08576300
H	-5.28156600	1.93059500	-2.46613000
H	-0.93186200	4.11984300	-2.88596600
H	0.57199200	2.59946200	-1.57052000
N	-0.93830800	1.29590500	-1.08336700
C	2.15293500	3.23741000	0.88022900
F	0.84949000	3.55905900	0.96060700
F	2.62417400	3.69599500	-0.28975500
F	2.80550100	3.83081000	1.87781500
S	2.36028100	1.38909500	0.98361000
O	3.79870000	1.15313800	0.96878900
O	1.54626300	0.97576600	2.13478500
O	1.68866000	0.96776200	-0.35005500
S	1.28820000	-2.79919500	-0.32545700
O	-0.04498300	-3.08149200	-1.14056000
O	1.10418900	-1.57584100	0.51172300
Ni	0.07694100	-0.01459400	-0.14625900
O	1.84793400	-3.97092100	0.30693900
C	2.38965800	-2.32218400	-1.76474700
F	1.83024400	-1.31744100	-2.43678000
F	2.52662000	-3.37659000	-2.56213700
F	3.56441100	-1.95374900	-1.27914200

B-IN2

C	-5.07327100	-1.58771600	5.01695600
F	-6.38555400	-1.34233500	5.12130300
F	-4.43934600	-0.95490200	6.01564500
F	-4.87253600	-2.90559100	5.15426900
S	-4.43360400	-1.00821600	3.37243900
O	-2.97931200	-1.31499000	3.41962500
O	-5.21484900	-1.75580200	2.37103900
O	-4.72240800	0.46392100	3.40792800
C	-6.10321200	4.96906300	0.22439900
F	-5.99041500	6.21963400	-0.21772200
F	-7.35418300	4.76438800	0.65927500
F	-5.86483300	4.12333800	-0.79237000

S	-4.88480600	4.67265700	1.60203100
O	-5.27135800	3.24014300	2.05497900
O	-3.56423900	4.67449500	0.94956500
O	-5.19829300	5.66018800	2.62538500
Ni	-4.16052000	1.83271100	1.49000600
C	-1.16460500	1.29513300	2.24420500
C	-0.12897000	2.08012100	1.39280400
H	0.62800000	1.41596500	0.96157500
H	-0.61395100	2.62698400	0.57727400
H	0.38244300	2.80669300	2.03257100
C	-2.21564200	2.26518700	2.80009600
H	-2.62582000	2.91153300	1.99025800
H	-2.97574500	1.74996000	3.40082500
H	-1.75339100	3.01444200	3.45205300
C	-0.45414500	0.57828200	3.41517100
H	-1.14925700	-0.07305700	3.95027400
H	-0.05418700	1.33074300	4.10205700
C	-1.81718900	0.28654900	1.30612800
O	-1.09409900	-0.76302500	0.92419600
N	-2.98337200	0.49468900	0.77106500
C	-3.63706400	-0.34250400	-0.17233300
C	-5.00831500	-0.01239700	-0.33286900
C	-3.11627300	-1.39151100	-0.91130600
C	-5.86012200	-0.76673600	-1.18062200
C	-3.95455300	-2.12620800	-1.78450300
H	-2.07766500	-1.67029300	-0.82091000
C	-6.77035100	1.36502800	0.35193800
C	-7.22764800	-0.39988800	-1.21952200
C	-5.29396900	-1.83878200	-1.91664700
H	-3.51947200	-2.94626500	-2.34737000
C	-7.68106900	0.64915800	-0.45012600
H	-7.91082700	-0.96147600	-1.85087100
H	-5.92919900	-2.42567000	-2.57347300
H	-8.72539700	0.94050900	-0.44660400
H	-7.07755600	2.19960000	0.96857000
N	-5.48380400	1.04993400	0.38361300
H	0.41310300	-0.01226800	3.08274600
H	-0.36873400	-0.90398100	1.55759100

B-TS2

C	-5.06897700	-2.64698400	3.01448400
F	-5.04716600	-2.49022400	1.67012500
F	-6.35229000	-2.66272600	3.40139200
F	-4.52525500	-3.83870900	3.29434700
S	-4.13577800	-1.27303100	3.85081100
O	-4.23248300	-1.58046400	5.28198100
O	-2.77582400	-1.38362700	3.24927700
O	-4.87821900	-0.05589100	3.40014300
C	-5.50328900	4.89009900	0.39232000
F	-5.16960400	6.13801900	0.08725800
F	-6.83046600	4.76315400	0.41046200
F	-4.99089900	4.05126700	-0.51068800
S	-4.85238500	4.46176900	2.09122900
O	-5.31768200	3.05595400	2.34830500
O	-3.31998000	4.39980300	1.84485000
O	-5.29353600	5.50025600	2.99829900
Ni	-4.11435600	1.61944400	1.68101100
C	-1.26665000	1.29398200	2.23918500
C	-0.41579700	2.27166800	1.38199400
H	0.42336500	1.75939900	0.89772500
H	-1.01958500	2.75158400	0.60457200
H	-0.00456300	3.05345500	2.02994500
C	-2.48056000	2.01752100	2.84338200
H	-3.00393300	3.31988000	2.08667100
H	-2.98544900	1.38726900	3.58237700
H	-2.12718100	2.88535000	3.41931500
C	-0.38194600	0.67184700	3.34192100
H	-0.93205200	-0.09782500	3.88863900
H	-0.07423200	1.45682300	4.04010300
C	-1.79134000	0.24350800	1.28470200
O	-1.00725200	-0.74821000	0.87374300
N	-2.96742200	0.42123400	0.76435500
C	-3.62151600	-0.39398600	-0.18427300
C	-5.01565600	-0.12526800	-0.26672600
C	-3.07730000	-1.36549000	-1.00702100
C	-5.85672600	-0.85676000	-1.14608400
C	-3.91174900	-2.08254700	-1.89878400
H	-2.02142600	-1.59161800	-0.96768000
C	-6.80273000	1.11256800	0.56555900
C	-7.23924600	-0.54539600	-1.12453400
C	-5.26680500	-1.84759400	-1.97298800
H	-3.46058900	-2.84270500	-2.52942200
C	-7.70994100	0.42735100	-0.26958700
H	-7.91757100	-1.08665700	-1.77876000
H	-5.89505000	-2.41580300	-2.65277100
H	-8.76450000	0.67599600	-0.22178200
H	-7.13278900	1.88332800	1.25270600
N	-5.50447100	0.85197600	0.55497600
H	0.55005400	0.24171500	2.93996300
H	-0.28729600	-0.87093400	1.51792200

B-IN3

C	-5.14203600	0.50455100	5.91181300
F	-5.79682800	1.66772300	5.97007700
F	-3.82730900	0.73756500	6.00285000
F	-5.51742300	-0.26562900	6.93511700
S	-5.53215600	-0.36178800	4.31042700
O	-4.59234500	-1.47796000	4.19753600
O	-6.97380400	-0.61653600	4.32791500
O	-5.19069700	0.77587400	3.30469000
C	-5.75890100	4.21004700	0.86157600
F	-5.09669400	3.10536600	0.47990900
F	-5.07685200	5.28246100	0.45684500
F	-6.96339300	4.20866200	0.29302000
S	-5.91030200	4.25033800	2.71730900
O	-6.78569100	5.36390200	3.03009200
O	-6.71644400	2.89422100	2.94549200
O	-4.55277700	4.14899200	3.23877600
Ni	-3.99773400	0.43540100	1.82667400
C	-1.18347300	0.67496200	2.01935300
C	-0.06205000	1.73690400	2.04083000
H	0.88682100	1.38346700	1.60340600
H	-0.36419400	2.65226800	1.52058500
H	0.15748200	1.99983000	3.07998900
C	-2.46856600	1.16525000	2.71777000
H	-6.10341900	2.11848100	3.16358400
H	-2.47832800	0.90595200	3.77875300
H	-2.59733300	2.25031300	2.61618900
C	-0.67958600	-0.63609100	2.67989100
H	-1.48844300	-1.37005300	2.74413000
H	-0.34158900	-0.41428500	3.69735200
C	-1.58328300	0.33028000	0.60042500
O	-0.66378300	0.17032500	-0.36126600
N	-2.84324500	0.13799100	0.36334300
C	-3.46954700	-0.28801700	-0.82956300
C	-4.87478700	-0.49863200	-0.67224200
C	-2.88903500	-0.51284500	-2.06804400
C	-5.66715400	-0.94157700	-1.76589500
C	-3.68389200	-0.94845100	-3.15511300
H	-1.82923400	-0.35732300	-2.21280500
C	-6.70827100	-0.45146700	0.75593100
C	-7.05281600	-1.13423800	-1.52664300
C	-5.03772000	-1.16201800	-3.01853700
H	-3.20372500	-1.11591600	-4.11465100
C	-7.56918800	-0.89335900	-0.27407600
H	-7.69091800	-1.47253300	-2.33893500
H	-5.63583000	-1.49798000	-3.86099100
H	-8.62278100	-1.03473300	-0.05862200
H	-7.08409700	-0.26151900	1.75655000
N	-5.41153800	-0.25855700	0.56485500
H	0.16116700	-1.08268700	2.13308500
H	0.21410100	0.37827900	0.00368300

A-IN1'

Ni	1.67859400	1.38229000	0.70644000
P	1.53991700	1.54273700	-1.79339700
O	2.56675800	0.79292500	-0.91941800
O	2.26104400	2.50681400	-2.86427000
H	2.99955400	3.00195700	-2.47022400
O	0.64344200	2.24546100	-0.76054500
O	0.65663100	0.64115000	-2.77051200
H	1.05848100	0.50789400	-3.64515600
P	-0.71229700	1.73824800	2.30339200
O	0.77556100	2.21663400	2.06429300
O	-0.86757600	0.27770000	2.58486500
O	-1.57392000	2.31456800	1.06767400
H	-1.00867000	2.41903600	0.27620200
O	-1.25748000	2.65856300	3.52189400
H	-1.47765300	2.07379900	4.26517100
C	4.41827500	-0.89910500	1.15237200
C	4.43372500	0.34351200	1.71800300
C	3.15705200	0.71637000	2.25323300
C	2.18260000	-0.27454500	2.05610000
S	2.85951500	-1.65640500	1.24895800
H	5.23443300	-1.40969200	0.65729700
H	5.31209100	0.97727300	1.75834200
H	2.97676800	1.58612900	2.87447400
H	1.18136200	-0.32572900	2.48545100

A-TS1'

Ni	1.17477300	0.72888100	0.07370400
P	1.11886900	1.85727000	-2.16974200
O	2.28102300	1.11122100	-1.47903900
O	1.58058800	3.34117200	-2.61261800
H	2.17287300	3.73781100	-1.95092800
O	-0.04689200	1.78750900	-1.17429900
O	0.64886600	1.26471400	-3.57961700
H	1.23497500	1.51737400	-4.31239300
P	-0.02199100	1.86988900	2.23176700
O	-0.13214400	0.55292200	1.42911000
O	1.43586400	2.15042100	2.64017900
O	-0.90812700	1.85264000	3.56578000
H	-1.85551400	1.94709000	3.36977100

O	-0.69759700	3.04805900	1.36334300
H	-0.65495300	2.81466400	0.40653400
C	3.92833700	-1.76822400	2.20012200
C	4.71101700	-0.85704300	1.51462600
C	3.94848800	0.21170400	1.00316100
C	2.58302200	0.16651100	1.31519900
S	2.27508900	-1.32033400	2.22369000
H	4.26620500	-2.66892400	2.69905300
H	5.78427100	-0.95935900	1.39531500
H	4.36924400	1.02275600	0.41782200
H	2.10752900	1.24813000	2.04432500

A-IN2'

Ni	1.78400200	1.75570700	0.23566300
P	1.00779700	1.75733100	-2.17708600
O	2.29021900	1.18050900	-1.54275500
O	1.38289700	2.66722600	-3.45487400
H	2.20972700	3.15686000	-3.30362900
O	0.26308000	2.47774300	-1.04609600
O	0.02101000	0.68696800	-2.84536800
H	0.35709300	0.32899900	-3.68413700
P	-0.27972900	1.76375900	2.15834000
O	0.99120700	2.51924300	1.79265000
O	0.06608500	0.31523700	2.74181300
O	-1.32048200	1.66700700	0.97921700
H	-0.91838800	1.96239300	0.11074600
O	-1.13850700	2.44766000	3.31429700
H	-0.79260700	2.25044700	4.20085600
C	4.59191100	-1.13056500	1.86569200
C	4.24319900	-0.32501000	2.91464200
C	3.32089300	0.70369800	2.53571700
C	2.97332600	0.67705700	1.19818100
S	3.80069200	-0.64037900	0.39916100
H	5.26341000	-1.97981000	1.87122400
H	4.62880200	-0.44825100	3.92188800
H	2.96601700	1.46985000	3.21735200
H	0.99895100	0.07880500	2.51924400

B-IN1'

Ni	1.59643200	1.38260300	0.66582200
O	2.50244500	0.56498400	-0.82184800
O	2.49912200	1.92421400	-2.98583100
O	0.95935500	2.33552300	-0.97816500
O	0.67066900	2.39549300	1.92199000
O	-1.21602300	1.01256400	1.10207900
O	-1.58914300	3.45950900	1.69764800
C	4.45757600	-0.65735200	1.33056400
C	4.48318800	0.66118600	1.70763300
C	3.24059200	1.08844300	2.25371600
C	2.26224800	0.07658300	2.23243300
S	2.93287700	-1.41574200	1.62039100
H	5.25492600	-1.21951800	0.86078700
H	5.34763300	1.30384200	1.59191300
H	3.06980100	2.05168700	2.72211200
H	1.35199900	0.05389700	2.81716400
S	1.74039300	1.39214300	-1.87361500
C	0.47911500	0.19881100	-2.56701100
F	1.11957400	-0.72704900	-3.27932400
F	-0.36315800	0.86861300	-3.34511500
F	-0.17987500	-0.37731600	-1.56702300
S	-0.88042500	2.20356300	1.89235900
C	-1.16623600	1.73808100	3.67429500
F	-0.70704900	2.68892600	4.48741200
F	-0.52736000	0.58370000	3.95937900
F	-2.46911100	1.56161000	3.88356000

B-TS1'

Ni	1.29811300	1.49272400	-0.08872600
O	2.46156400	1.53941100	-1.62267800
O	1.73403300	3.08559800	-3.52321000
O	0.23371800	2.33666500	-1.58495500
O	-0.11166800	1.58296500	1.21634600
O	1.52696000	2.09238700	3.00202300
O	-0.46830100	3.59961300	2.72795300
C	4.66186500	-0.70583000	1.51635900
C	3.53123800	-1.43140200	1.82505800
C	2.34692600	-0.70602500	1.55731600
C	2.55245600	0.59228500	1.07588800
S	4.28522600	0.85195500	0.89689600
H	5.69289000	-1.00866400	1.65336900
H	3.55490700	-2.43488900	2.23551400
H	1.35186600	-1.09992900	1.74012500
H	2.06262600	1.44350100	2.22313000
S	1.36456800	2.07220000	-2.55724900
C	0.82999300	0.56151200	-3.51376200
F	1.83747400	0.14389200	-4.27596600
F	-0.21512400	0.87370400	-4.27544000
F	0.48660900	-0.40518700	-2.65766800
S	0.05489000	2.26164500	2.55417700
C	-0.87276200	1.11384300	3.69686300
F	-0.73621100	1.54388800	4.94564100
F	-2.15460300	1.10733900	3.35091400
F	-0.36651000	-0.11555500	3.58502100

B-IN2'

Ni	1.37044800	1.31459400	-0.20707500
O	2.43100700	1.47339700	-1.80593900
O	1.65144200	3.21544300	-3.50297900
O	0.23762000	2.33828600	-1.55469400
O	0.05623000	1.32695300	1.22023600
O	1.56243600	1.75499400	3.18046400
O	-0.12458200	3.49198400	2.57209700
C	4.78644900	-0.64296600	1.66284600
C	3.68228100	-1.24834700	2.19447900
C	2.45870200	-0.69134800	1.69312300
C	2.64466300	0.33565400	0.77894700
S	4.35010200	0.60713400	0.53918300
H	5.82780400	-0.85528700	1.86850600
H	3.72555300	-2.06180000	2.91095900
H	1.47797900	-1.07791500	1.95722500
H	2.04834400	1.04864300	2.62955300
S	1.29900400	2.12910900	-2.61217500
C	0.64845700	0.73550700	-3.66829500
F	1.58224700	0.36825900	-4.54180800
F	-0.43798800	1.15068500	-4.31580700
F	0.33296000	-0.30178500	-2.88752300
S	0.16660100	2.07927900	2.50736600
C	-1.01746000	1.15017900	3.61712000
F	-0.96759800	1.68221900	4.83045500
F	-2.23754100	1.26183200	3.11078700
F	-0.65201600	-0.12865900	3.66088700

IN4

C	0.10663200	3.01070400	-0.18617000
C	-0.73891100	1.83715300	-0.71742000
H	-0.89674300	1.91295000	-1.80446300
H	-1.71926500	1.76564100	-0.21850200
C	-0.31081700	3.37318200	1.25789300
H	-0.27955400	2.49137400	1.90895600
H	0.35790000	4.13308100	1.67589000
H	-1.33408700	3.76805000	1.26656700
C	0.01848700	4.26240300	-1.07657100
H	0.69912400	5.04007600	-0.71496000
H	0.29422800	4.02929900	-2.11193800
H	-1.00391200	4.65868200	-1.07852200
C	1.57210500	2.54179000	-0.11053800
O	2.53028500	3.29544600	0.02440400
N	1.66126700	1.16387300	-0.15864600
C	2.81386700	0.40585900	-0.01928000
C	2.59602600	-1.01048000	-0.08053000
C	4.11784400	0.85877500	0.17791000
C	3.67326900	-1.93334600	0.05892700
C	5.17825000	-0.06447400	0.31442300
H	4.29772000	1.92359000	0.22561700
C	1.04490100	-2.72985900	-0.33880000
C	3.35301800	-3.31186100	-0.01431700
C	4.98305000	-1.42972000	0.25931200
H	6.18097700	0.32616500	0.46718800
C	2.04802700	-3.71143700	-0.21107000
H	4.14805100	-4.04658800	0.08703600
H	5.81246400	-2.12298500	0.36535300
H	1.78000600	-4.76123000	-0.26889600
H	0.00684600	-3.01411000	-0.49319000
N	1.30420600	-1.42962900	-0.27841700
Ni	0.15374500	0.18719300	-0.47286900

TS2'

C	0.32900100	3.08497200	0.09890800
C	1.39906000	2.02104300	-0.12587200
H	2.31993000	2.18799500	0.43294400
H	1.64210100	1.87165400	-1.18672100
C	0.55871600	4.29087900	-0.83416700
H	0.59550500	3.97949200	-1.88433300
H	-0.26724500	5.00071800	-0.72419000
H	1.50050700	4.79727700	-0.59296600
C	0.32277800	3.56318500	1.56804900
H	-0.48455700	4.28438400	1.73037700
H	0.17774400	2.72322500	2.25712700
H	1.27530500	4.04809800	1.81442600
C	-1.05237600	2.47119900	-0.19017500
O	-2.04978800	3.15291300	-0.40881300
N	-1.00481700	1.09563200	-0.12290900
C	-2.12446400	0.27186600	-0.18431600
C	-1.83894900	-1.10865900	0.05505600
C	-3.44766500	0.63342200	-0.42960200
C	-2.87390100	-2.08798500	0.07562100
C	-4.46666400	-0.34690900	-0.43095000
H	-3.68073800	1.67315900	-0.61004900
C	-0.21325800	-2.69048400	0.57871100
C	-2.49467400	-3.41962100	0.37166700
C	-4.20713400	-1.67835100	-0.18349400
H	-5.48666900	-0.02745300	-0.62785000
C	-1.17455000	-3.71954400	0.63320300
H	-3.25660400	-4.19494400	0.39865200
H	-5.00364700	-2.41700800	-0.17716000
H	-0.86020100	-4.72941000	0.87508200

H	0.83486700	-2.89392200	0.76785800
N	-0.52723000	-1.43520600	0.28464500
Ni	0.65664400	0.25167500	0.17182600
C	2.38001100	-0.54530900	0.18491600
C	3.57261800	-0.33698300	0.83947000
C	4.66772900	-1.10178800	0.33096800
C	4.31547400	-1.89888100	-0.72295300
S	2.62703000	-1.73445800	-1.09564400
H	1.19384100	0.39655800	1.48292700
H	3.67574600	0.35965700	1.66547500
H	5.67518500	-1.05244000	0.73159000
H	4.94255200	-2.56121100	-1.30589000

IN5

C	0.29849700	3.24344800	0.04902300
C	1.48258100	2.27288500	-0.00645800
H	2.45770700	2.77284600	-0.00417600
H	1.48819500	1.68160100	-0.94360500
C	0.32505700	4.16808800	-1.18451500
H	0.30455300	3.58950800	-2.11637900
H	-0.55004300	4.82304700	-1.17371700
H	1.23094600	4.78634200	-1.18680300
C	0.37231600	4.09079600	1.33589700
H	-0.49818700	4.74952800	1.39576800
H	0.38042000	3.45638300	2.23105500
H	1.28118000	4.70465800	1.34453700
C	-1.05950700	2.49760700	0.05425900
O	-2.10343900	3.15329400	0.05043200
N	-0.97653500	1.12985200	0.06788600
C	-2.09536800	0.30397100	0.06902600
C	-1.76754500	-1.08583800	0.08151100
C	-3.44674600	0.64920500	0.05692600
C	-2.77076300	-2.09685300	0.07751500
C	-4.44052200	-0.35600100	0.05481100
H	-3.71849200	1.69455100	0.04861800
C	-0.05114100	-2.67941500	0.10764300
C	-2.33406300	-3.44322100	0.08695600
C	-4.13189900	-1.70021500	0.06395400
H	-5.48244100	-0.04674700	0.04480300
C	-0.98631200	-3.73196300	0.10155900
H	-3.07303100	-4.24069400	0.08262600
H	-4.90881100	-2.45923800	0.06082000
H	-0.62570100	-4.75500000	0.10877700
H	1.01498100	-2.86299100	0.12817300
N	-0.42895200	-1.40389600	0.09769100
Ni	0.66555900	0.14709900	0.09849100
C	2.33879700	-0.76684700	0.15835200
C	3.05078700	-1.26767700	1.22500800
C	4.31599000	-1.84700200	0.87619500
C	4.57150100	-1.79647600	-0.46546400
S	3.25571500	-1.03267200	-1.31232700
H	1.53897300	1.63750700	0.90982700
H	2.68526300	-1.23029700	2.24799900
H	5.00111500	-2.27963000	1.59898400
H	5.44297900	-2.15250600	-0.99943200

IN6

C	1.02178200	2.45526600	-1.70201900
C	-0.19174000	1.53549900	-1.69458200
H	-0.61571000	1.29548000	-2.67033000
H	-0.97761000	1.82041900	-0.98861300
C	0.63060400	3.90522200	-1.35762300
H	0.10113500	3.95588900	-0.39953600
H	1.53025400	4.52417600	-1.27995200
H	-0.02251100	4.32145100	-2.13254500
C	1.73414800	2.41481500	-3.07495600
H	2.64459800	3.02223000	-3.05429400
H	2.01002800	1.39011500	-3.35058500
H	1.07003000	2.80875900	-3.85271500
C	2.03143900	1.94166100	-0.66490700
O	2.95433000	2.61055100	-0.22840000
N	1.78739300	0.60571900	-0.33442100
C	2.63467900	-0.17330600	0.47062200
C	2.19401100	-1.52282000	0.64194800
C	3.81896000	0.21743100	1.08675100
C	2.94363600	-2.45228900	1.41256400
C	4.56188900	-0.71253800	1.85248800
H	4.16399600	1.23488500	0.97526800
C	0.54368700	-3.10012000	0.16277000
C	2.41894900	-3.76456900	1.52383900
C	4.15039400	-2.01677100	2.02025300
H	5.48306800	-0.37450100	2.31880900
C	1.22957900	-4.08541700	0.90671800
H	2.96332800	-4.50597000	2.10380100
H	4.73185200	-2.71728300	2.61312400
H	0.80278700	-5.07975800	0.98434600
H	-0.41671400	-3.30631100	-0.30380700
N	1.01730600	-1.86670800	0.03537200
Ni	0.27484900	-0.22003500	-0.96934400
P	-2.54218100	-1.53085300	-1.04793000
O	-2.53936100	-2.93133300	-0.52893000
O	-2.89535100	-0.41617700	0.09259400

H	-3.55857900	-0.77117500	0.70702900
O	-3.71843500	-1.32667500	-2.15833500
H	-4.08518400	-2.20054000	-2.36921600
O	-1.26722500	-0.94145700	-1.69891300

A-TS3

Ni	1.29811300	1.49272400	-0.08872600
O	2.46156400	1.53941100	-1.62267800
O	1.73403300	3.08559800	-3.52321000
O	0.23371800	2.33666500	-1.58495500
O	-0.11166800	1.58296500	1.21634600
O	1.52696000	2.09238700	3.00202300
O	-0.46830100	3.59961300	2.72795300
C	4.66186500	-0.70583000	1.51635900
C	3.53123800	-1.43140200	1.82505800
C	2.34692600	-0.70602500	1.55731600
C	2.55245600	0.59228500	1.07588800
S	4.28522600	0.85195500	0.89689600
H	5.69289000	-1.00866400	1.65336900
H	3.55490700	-2.43488900	2.23551400
H	1.35186600	-1.09992900	1.74012500
H	2.06262600	1.44350100	2.22313000
S	1.36456800	2.07220000	-2.55724900
C	0.82999300	0.56151200	-3.51376200
F	1.83747400	0.14389200	-4.27596600
F	-0.21512400	0.87370400	-4.27544000
F	0.48660900	-0.40518700	-2.65766800
S	0.05489000	2.26164500	2.55417700
C	-0.87276200	1.11384300	3.69686300
F	-0.73621100	1.54388800	4.94564100
F	-2.15460300	1.10733900	3.35091400
F	-0.36651000	-0.11555500	3.58502100

A/B-IN7

C	-2.72108000	-2.36546500	-1.53171700
C	-1.33363900	-2.33581500	-0.88412000
H	-0.53038700	-2.15590500	-1.60971800
H	-1.11299900	-3.22972100	-0.30331000
C	-3.72774700	-3.11045100	-0.62293100
H	-3.77618000	-2.65552100	0.37318300
H	-4.73088900	-3.08874200	-1.06121400
H	-3.42324900	-4.15698500	-0.50372200
C	-2.67179600	-3.04644500	-2.91253800
H	-3.65523700	-2.99005300	-3.39021700
H	-1.94881700	-2.55300500	-3.57219400
H	-2.38261100	-4.09893600	-2.81380200
C	-3.24407600	-0.92946600	-1.68497000
O	-4.14371500	-0.62001600	-2.45726200
N	-2.60429500	-0.07051800	-0.80313200
C	-2.96930500	1.26090300	-0.60695300
C	-2.16194200	1.94348400	0.35831300
C	-3.99071300	1.97499000	-1.22822800
C	-2.37982000	3.31533400	0.67081800
C	-4.21051700	3.33449600	-0.90399700
H	-4.60536300	1.47824500	-1.96527100
C	-0.36212100	1.80292600	1.82690700
C	-1.50840400	3.90636300	1.61801800
C	-3.43494300	4.00460800	0.01749600
H	-5.01710200	3.85931300	-1.40887700
C	-0.50085300	3.15838700	2.18957400
H	-1.64190500	4.95275400	1.88171800
H	-3.61252300	5.05118200	0.24842800
H	0.18396200	3.59015200	2.91199500
H	0.41225100	1.17714700	2.25881300
N	-1.16620200	1.21473200	0.95235700
Ni	-1.17188800	-0.72216000	0.21265700
C	0.07782000	-1.55106800	1.40582100
C	0.10995900	-1.40688900	2.78551000
C	1.15853700	-2.12001500	3.43851800
C	1.94545200	-2.81767400	2.55812500
S	1.38256200	-2.61881300	0.93181000
H	-0.62329500	-0.81766100	3.32893800
H	1.32195100	-2.11202600	4.51165400
H	2.82585900	-3.40936400	2.77443900

A/B-TS4

C	-2.67179900	-2.30508700	-1.29961700
C	-1.26835200	-2.31551300	-0.66629900
H	-0.49887600	-1.88025500	-1.31774900
H	-0.97414300	-3.33675000	-0.43667500
C	-3.69052600	-3.06312200	-0.42085800
H	-3.82786200	-2.57175600	0.54808700
H	-4.66121700	-3.09294100	-0.92516500
H	-3.35960200	-4.09277400	-0.23823200
C	-2.55942300	-3.01355700	-2.66841800
H	-3.52193300	-2.93886300	-3.18251700
H	-1.80325100	-2.53944500	-3.30498400
H	-2.29558700	-4.07056000	-2.54595800
C	-3.23671500	-0.87889700	-1.52313600
O	-4.16006500	-0.68031100	-2.31574000
N	-2.62919700	0.03557300	-0.71957700
C	-2.96218800	1.37239600	-0.62569700
C	-2.15282600	2.10654400	0.30869500

C	-3.95886600	2.06802200	-1.30945700
C	-2.36279500	3.49831500	0.53793800
C	-4.15660600	3.44768000	-1.07720300
H	-4.57409900	1.52902100	-2.01721900
C	-0.40147200	2.03469800	1.84561500
C	-1.51731500	4.13047200	1.48251300
C	-3.38990700	4.16293500	-0.17969300
H	-4.94437600	3.95463200	-1.62885100
C	-0.54217900	3.40626500	2.13623800
H	-1.64874100	5.19088700	1.68455400
H	-3.55860200	5.22306100	-0.01278900
H	0.11451800	3.87004600	2.86502100
H	0.35441100	1.43200700	2.34217700
N	-1.17299300	1.40867900	0.96632100
Ni	-1.19178600	-0.54841300	0.42348700
C	-0.71670700	-2.08529700	1.37789000
C	0.61118400	-2.40209900	1.61536700
C	0.82696700	-3.04424200	2.87221200
C	-0.33381600	-3.26307900	3.56448700
S	-1.71490100	-2.65604000	2.69960700
H	1.40489500	-2.20367700	0.90188500
H	1.80523600	-3.34242700	3.23505300
H	-0.45807300	-3.73607300	4.53006500

A/B-IN8

C	-2.54232800	-2.42454200	-1.03657300
C	-1.03370800	-2.73193400	-0.79676700
H	-0.46405000	-2.32164300	-1.64001100
H	-0.91235200	-3.82268600	-0.85391700
C	-3.41282900	-2.82478400	0.17520900
H	-3.18976300	-2.22024900	1.05890200
H	-4.47170800	-2.68116200	-0.06669700
H	-3.26930400	-3.88365600	0.42897300
C	-2.97121300	-3.27350200	-2.24992600
H	-4.01000900	-3.06917400	-2.51263200
H	-2.36208300	-3.04484100	-3.13165100
H	-2.86216900	-4.34119100	-2.02248900
C	-2.84094600	-0.92660900	-1.35832100
O	-3.61710500	-0.68081000	-2.28828100
N	-2.27315400	0.00354400	-0.52739000
C	-2.63790600	1.34682000	-0.58053600
C	-2.04724000	2.19505000	0.42796700
C	-3.51828000	1.96658000	-1.47577500
C	-2.36426200	3.58712800	0.51686500
C	-3.81741100	3.34256100	-1.38277200
H	-3.97310000	1.36430700	-2.24672000
C	-0.60867700	2.35215200	2.26531100
C	-1.74692000	4.33373600	1.54980100
C	-3.26700200	4.15427600	-0.41472700
H	-4.50976800	3.76511400	-2.10693100
C	-0.87477100	3.72441100	2.42619800
H	-1.97309700	5.39365700	1.63929600
H	-3.50786000	5.21183500	-0.35275700
H	-0.39260100	4.27713600	3.22590300
H	0.07934200	1.83597000	2.92967200
N	-1.16854700	1.62086300	1.30820600
Ni	-0.84549600	-0.26996700	0.81696200
C	-0.35172400	-2.25333000	0.46485200
C	0.83715200	-1.49223800	0.51926000
C	1.48123400	-1.53457300	1.80962200
C	0.83199300	-2.33350700	2.70567300
S	-0.59311500	-3.07151900	2.02985800
H	1.32235000	-1.10555200	-0.37219000
H	2.39280800	-0.99271500	2.03797700
H	1.08660000	-2.50803500	3.74334000

A-IN9

C	0.50324300	2.64406300	0.36510800
C	1.29796400	1.35624200	0.51657500
H	1.98771900	1.31293400	1.35911500
H	1.76340100	0.99785500	-0.40944300
C	1.21512000	3.62069400	-0.59259500
H	1.40202900	3.15744900	-1.56837200
H	0.58206000	4.49962300	-0.75249200
H	2.17558300	3.94211900	-0.17456000
C	0.28909300	3.31661100	1.74125000
H	-0.37295100	4.18314700	1.64215900
H	-0.14255000	2.61057800	2.45745700
H	1.25034500	3.65752300	2.14339500
C	-0.88985100	2.30768200	-0.20570100
O	-1.62771500	3.14589800	-0.71172100
N	-1.19660200	0.97306200	-0.02697600
C	-2.41396900	0.38362700	-0.35548200
C	-2.51094300	-1.01352200	-0.03572700
C	-3.52230400	0.98532300	-0.95140500
C	-3.68437500	-1.76986000	-0.32972500
C	-4.68677600	0.23153700	-1.22588700
H	-3.47295300	2.03495400	-1.20402600
C	-1.41334800	-2.88283300	0.83638000
C	-3.65632500	-3.14831200	0.00300800
C	-4.78684700	-1.11312200	-0.93281100
H	-5.52607700	0.74009700	-1.69315400

C	-2.53051600	-3.70690800	0.57564000
H	-4.52888900	-3.76103300	-0.21171200
H	-5.68665400	-1.67591300	-1.16464000
H	-2.48433600	-4.76436700	0.81592000
H	-0.50138800	-3.26730000	1.28598300
N	-1.41882100	-1.58822600	0.55056700
Ni	0.07285800	-0.14656700	0.82593700
P	1.15447600	-1.12156600	3.00252900
O	0.03607500	-0.03213600	2.93145900
O	0.67249000	-2.37755600	3.75267500
O	2.45630600	-0.49018200	3.69089800
H	3.19249100	-1.16757700	3.67784800
O	1.45464500	-1.40524200	1.47200100
P	3.52992300	-3.79451700	2.66917100
O	4.12200700	-2.59956400	3.35816700
O	3.09365100	-3.52756400	1.15360900
H	2.51405700	-2.71413200	1.10640200
O	2.29266400	-4.45617800	3.42392200
H	1.62311500	-3.73409900	3.64582300
O	4.55344900	-5.02778300	2.53507600
H	5.43417000	-4.72800000	2.81236200
K	-1.72435700	-1.42815400	4.26649800

A-TS5

C	0.50274400	3.14355700	0.60157400
C	1.35653100	2.36053300	-0.39573800
H	2.41355300	2.30573900	-0.14447300
H	1.19656600	2.63752400	-1.44113700
C	0.18274100	4.54721300	0.03586900
H	-0.33279100	4.47954500	-0.92938900
H	-0.46513600	5.09037000	0.73219000
H	1.10485500	5.12178700	-0.10806600
C	1.23022800	3.28573600	1.95648300
H	0.58690900	3.80300600	2.67757500
H	1.51496600	2.30702000	2.35266000
H	2.14263000	3.88009500	1.83154100
C	-0.82950200	2.41123900	0.83368600
O	-1.70196200	2.86861400	1.59511700
N	-0.90286500	1.23464300	0.15861500
C	-1.99617600	0.36979300	0.20106200
C	-1.70814200	-0.98888400	-0.15529500
C	-3.31199900	0.69785100	0.52305900
C	-2.72893900	-1.98224800	-0.13930000
C	-4.32497800	-0.29018700	0.51702400
H	-3.55567200	1.72454900	0.76245300
C	-0.08241300	-2.54872300	-0.74103300
C	-2.34611200	-3.31065700	-0.46152700
C	-4.05418200	-1.60554700	0.20483900
H	-5.34146800	0.00628000	0.76347800
C	-1.03180100	-3.59474200	-0.74857700
H	-3.10009600	-4.09416100	-0.46281000
H	-4.83860600	-2.35724200	0.20844300
H	-0.70510800	-4.60488600	-0.97075400
H	0.97148600	-2.74231200	-0.91264100
N	-0.41327100	-1.29218500	-0.48133600
Ni	0.77831800	0.44885000	-0.41832300
C	2.27375700	-0.10664300	-1.83560000
C	3.36901500	0.66926200	-2.20980600
C	3.50843200	0.89718000	-3.60001500
C	2.51040500	0.28895800	-4.32902200
S	1.41847700	-0.56984400	-3.31178500
H	2.52062600	-0.97812900	-0.90255700
H	4.07397500	1.04098700	-1.47148900
H	4.31124600	1.47216200	-4.04969100
H	2.37673700	0.30068200	-5.40383100
P	2.72525300	-1.17436200	1.44029200
O	1.67508600	0.00616200	1.33140800
O	2.44010100	-2.13660500	2.57719100
O	4.11190600	-0.35377000	1.76757200
H	4.72689000	-0.95227300	2.22177100
O	2.86470700	-1.83403700	0.04017000
P	-0.59701600	-1.34636900	3.90408300
O	-1.63441200	-0.88139800	4.87726300
O	-0.27276500	-0.09146100	2.95361800
H	0.54095300	-0.13085700	2.32521600
O	-1.13242800	-2.54008400	2.93505800
H	-2.06118200	-2.39131700	2.69452500
O	0.74785400	-1.91239800	4.46875500
H	1.47865400	-2.03287900	3.74031500
K	-2.07203500	1.59561300	3.91297000

A-IN10

C	0.10672300	2.90669500	0.75350700
C	0.97575100	2.57789300	-0.47727100
H	2.04366400	2.55824900	-0.26799300
H	0.77053000	3.20831900	-1.34810300
C	-0.53535700	4.30707400	0.59332500
H	-1.15108200	4.35881600	-0.31227700
H	-1.17063800	4.53598900	1.45634200
H	0.24305700	5.07573200	0.52162600
C	0.94549100	2.87317000	2.04490400
H	0.29969300	3.00944800	2.91814400

H	1.47332400	1.91944600	2.13930400
H	1.69070300	3.67710900	2.03274400
C	-1.05237100	1.89749600	0.87056200
O	-1.72015100	1.75924300	1.90759300
N	-1.21434300	1.17057700	-0.27251100
C	-2.24609300	0.26320700	-0.48315300
C	-1.95293300	-0.77109800	-1.43308400
C	-3.51669200	0.28300800	0.09260200
C	-2.93746300	-1.73378900	-1.79704200
C	-4.48863600	-0.67681900	-0.27510300
H	-3.75691600	1.05214500	0.81568500
C	-0.37032400	-1.73466600	-2.83465100
C	-2.55920700	-2.71967700	-2.74355900
C	-4.22219700	-1.66495100	-1.19916700
H	-5.47159200	-0.62141200	0.18559900
C	-1.28429500	-2.72205000	-3.26054100
H	-3.28472000	-3.47080800	-3.04589400
H	-4.97713700	-2.39657800	-1.47273200
H	-0.96335500	-3.47173300	-3.97558300
H	0.64161200	-1.70767400	-3.22556900
N	-0.68747000	-0.79228200	-1.96097900
Ni	0.47947500	0.78884600	-1.14370700
C	2.09837100	0.69411400	-2.22837400
C	3.44273300	0.64151400	-1.91227000
C	4.32612500	0.60750700	-3.04210800
C	3.66374800	0.65434400	-4.23608600
S	1.94510300	0.72992000	-3.97819400
H	2.70820600	-1.46949000	-1.08071800
H	3.80678000	0.67063400	-0.88918300
H	5.40746200	0.55525900	-2.95987100
H	4.07635700	0.64304000	-5.23673700
P	2.18605200	-1.20404600	1.01775800
O	1.11999100	-0.18878800	0.64578400
O	1.84594200	-2.18102200	2.11779400
O	3.53766400	-0.37370100	1.37734400
H	4.15911700	-0.93646200	1.86896600
O	2.57902600	-2.07966600	-0.31851600
P	-0.07511500	-4.44802700	0.78460900
O	-1.13811700	-3.49628300	1.24101000
O	1.10157200	-4.69087500	1.83005200
H	1.50299100	-3.80464600	2.07421900
O	0.60977900	-4.10292300	-0.62279900
H	1.35549500	-3.46164200	-0.55008100
O	-0.64431200	-5.92149800	0.48012000
H	-1.51842500	-6.01423700	0.89180000
K	-1.02110400	-1.02850800	2.15980400

A-TS6

C	0.95907000	3.26564700	-0.95554500
C	-0.35282000	2.46617100	-0.79820200
H	-0.71052900	2.04488900	-1.74126100
H	-1.12161500	3.12941100	-0.41037400
C	1.28079100	4.06822200	0.32703500
H	1.44137100	3.40760300	1.18373500
H	2.18521400	4.66902400	0.18099700
H	0.45412900	4.74774500	0.56731600
C	0.74408400	4.24572000	-2.12932900
H	1.64986900	4.83775800	-2.28822300
H	0.52492600	3.70782300	-3.05666000
H	-0.08884800	4.92481000	-1.91400900
C	2.19025700	2.37523700	-1.23936300
O	3.10120200	2.76209400	-2.00750000
N	2.15691600	1.21461500	-0.55910900
C	3.19863100	0.31382000	-0.45380000
C	2.81847200	-0.97604700	0.06295400
C	4.54854400	0.53119600	-0.73042700
C	3.80367000	-1.97929000	0.32652500
C	5.50895200	-0.47191400	-0.47989700
H	4.84899000	1.48497600	-1.14305200
C	1.08865500	-2.36859100	0.77416400
C	3.34282200	-3.21267900	0.85818600
C	5.16530100	-1.70348800	0.04080100
H	6.55085700	-0.25735800	-0.70305000
C	1.99674900	-3.40611700	1.09016100
H	4.06479300	-3.99428400	1.08501300
H	5.91782800	-2.46164100	0.23977300
H	1.62088100	-4.33647500	1.50421900
H	0.01842900	-2.50397300	0.89820400
N	1.48223200	-1.20496200	0.27195000
Ni	0.31986400	0.50610900	-0.34134900
C	-1.04662500	1.25630500	0.75803700
C	-2.41628800	1.03987700	0.67075900
C	-3.09376400	1.10313000	1.92826600
C	-2.25842500	1.39489000	2.97237400
S	-0.61717200	1.59132100	2.42489100
H	-2.92607700	0.92046600	-0.28159100
H	-4.16059700	0.93998000	2.04444400
H	-2.50219100	1.48644600	4.02283000
P	-1.52878600	-1.83966300	-1.79308000
O	-0.74851000	-0.51551900	-1.89816000
O	-0.85111100	-3.11670800	-2.20137100

O	-2.89250800	-1.58019700	-2.64852200
H	-3.30665900	-2.43060900	-2.86927900
O	-2.01935100	-1.99976100	-0.24622200
P	1.84315300	0.39185600	-4.45984600
O	2.33103900	-0.90611200	-3.90910600
O	2.81594900	1.64577700	-4.43102300
H	2.97036800	2.05661700	-3.52935100
O	0.48859400	0.91477500	-3.78657100
H	0.00825600	0.25628900	-3.20198200
O	1.56226400	0.24710000	-6.04206500
H	1.42366300	1.11361100	-6.45873800
K	1.70802500	-2.91654200	-2.50824500
H	-2.20055500	-1.12807200	0.16356400

A-IN11

C	1.20607100	3.27976200	-1.00376700
C	-0.33285100	3.11085900	-0.78904700
H	-0.75934300	2.69725000	-1.70923700
H	-0.74713700	4.12496600	-0.68453200
C	1.87979800	3.93512000	0.22387100
H	1.85294300	3.28230000	1.09803400
H	2.93242100	4.15493500	0.00747900
H	1.38675600	4.88441800	0.46750500
C	1.38184400	4.22631700	-2.20732300
H	2.43868100	4.33764800	-2.46739700
H	0.85188300	3.87269400	-3.09551900
H	0.98713300	5.21767500	-1.95569400
C	1.92476100	1.92424100	-1.26518000
O	2.44320200	1.67906600	-2.40096600
N	1.97002900	1.09277900	-0.21593100
C	2.92307700	0.09950300	-0.07585500
C	2.51688400	-1.11900000	0.57647600
C	4.27221700	0.22416500	-0.42355100
C	3.46986300	-2.12992900	0.89693500
C	5.20688100	-0.79012000	-0.11833300
H	4.60713500	1.13419900	-0.91077000
C	0.77056900	-2.37858000	1.44487200
C	2.98790900	-3.29086000	1.55627900
C	4.82952100	-1.94719100	0.53461100
H	6.24869800	-0.63977300	-0.39190900
C	1.64772600	-3.41279200	1.83695500
H	3.68886500	-4.07755000	1.82461700
H	5.55525200	-2.71854200	0.77672200
H	1.24937400	-4.29315600	2.33039300
H	-0.29895800	-2.46967400	1.60513000
N	1.18529400	-1.27470300	0.84453300
Ni	0.04882700	0.24006200	0.07696300
C	-0.85569200	2.26563100	0.35520300
C	-1.86448000	1.29620500	0.27310600
C	-2.43734100	0.94935800	1.54822500
C	-1.90659400	1.66170800	2.58002300
S	-0.68207200	2.77813600	2.04551500
H	-2.28357400	0.97126400	-0.67335600
H	-3.21506300	0.20251800	1.66678000
H	-2.13235400	1.57674700	3.63532300
P	-0.38616900	-2.25088000	-2.06812900
O	-0.75785500	-0.79506700	-1.63665300
O	1.05650800	-2.64025000	-1.95383000
O	-0.99484300	-2.46657900	-3.55278800
H	-0.45008500	-1.94574800	-4.19254700
O	-1.30613600	-3.26991700	-1.19434500
P	0.11434300	0.74076700	-4.69791600
O	0.71719400	-0.63679400	-4.72426500
O	1.16783000	1.93567900	-4.68813500
H	1.67206100	1.99167700	-3.81273400
O	-0.87467600	0.98264100	-3.48170500
H	-0.86991300	0.22674100	-2.77292700
O	-0.71843300	1.01486600	-6.04476400
H	-1.08798700	1.91270800	-6.07290800
K	2.80041600	-1.06093700	-3.05108000
H	-2.24564700	-3.05661200	-1.31581900

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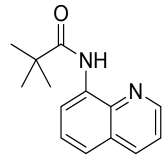
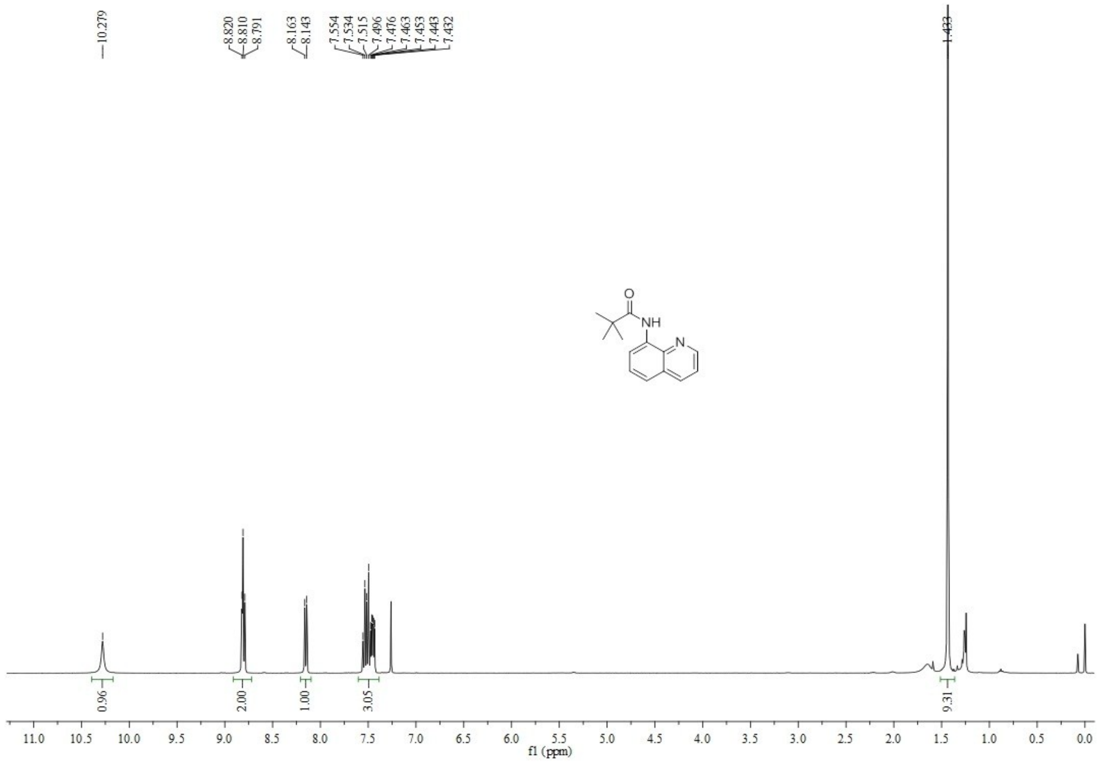
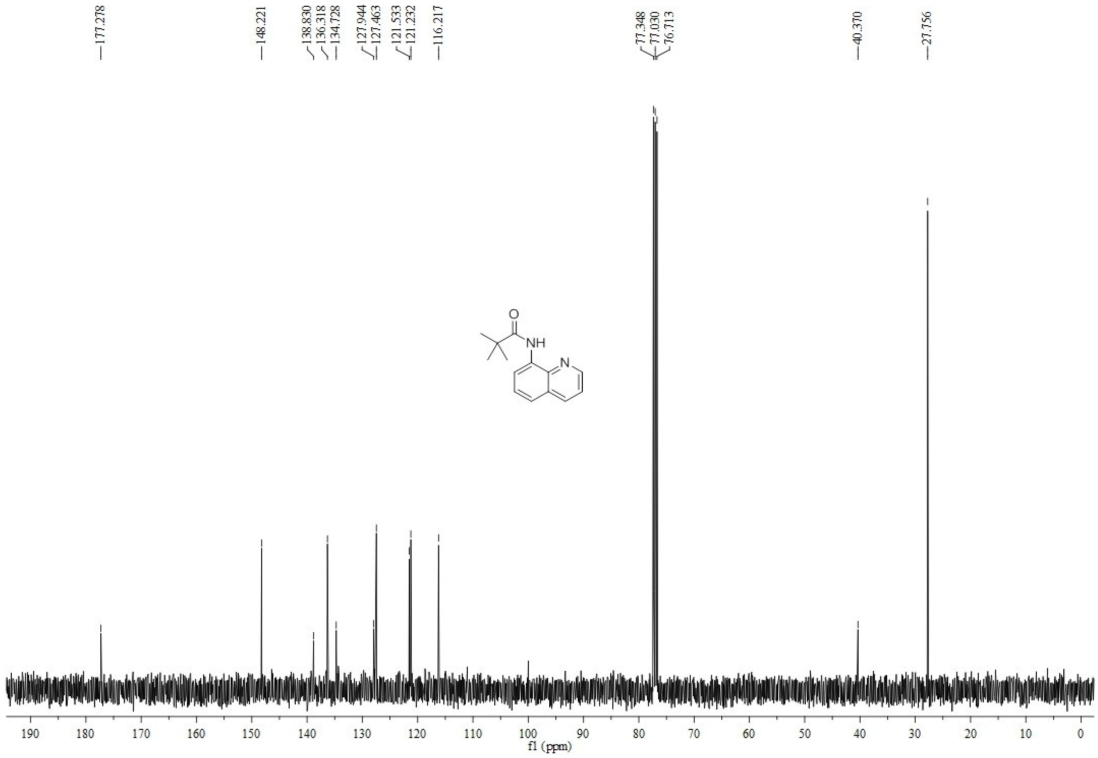
9. Copies of [1]H, [13]C NMR Charts for the Compounds

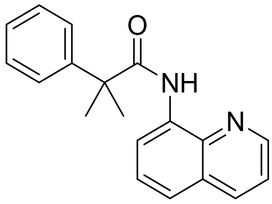
N-(quinolin-8-yl)pivalamide **(1a)**

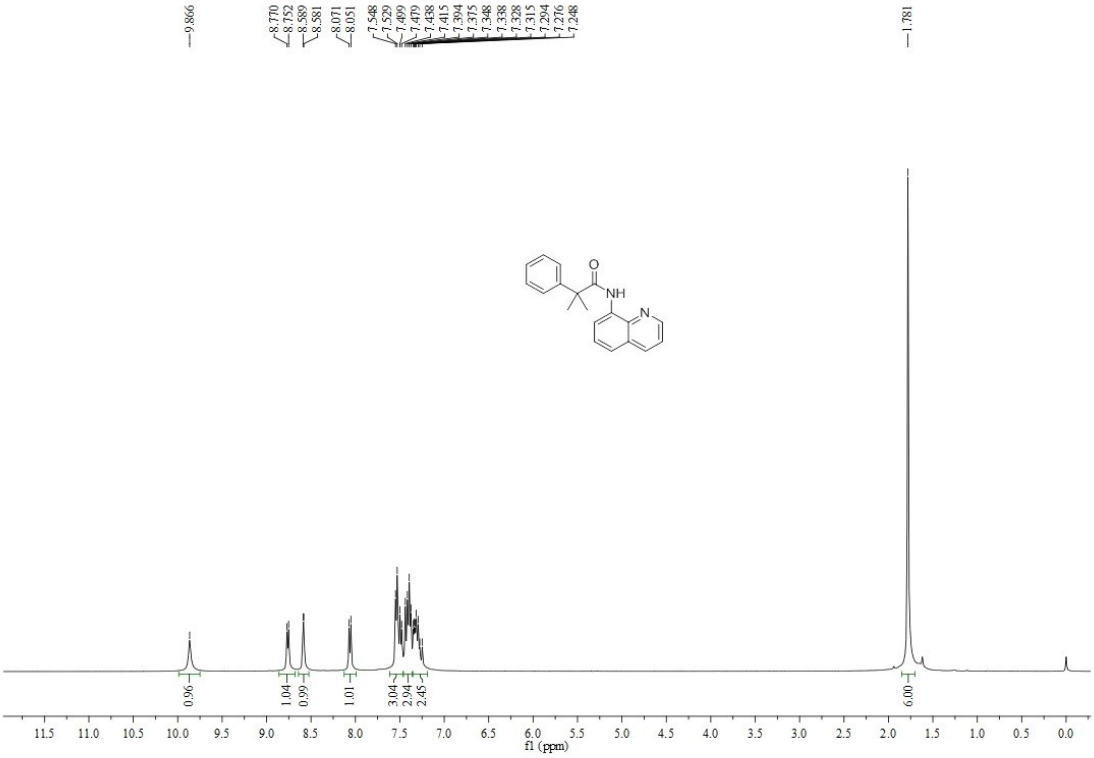


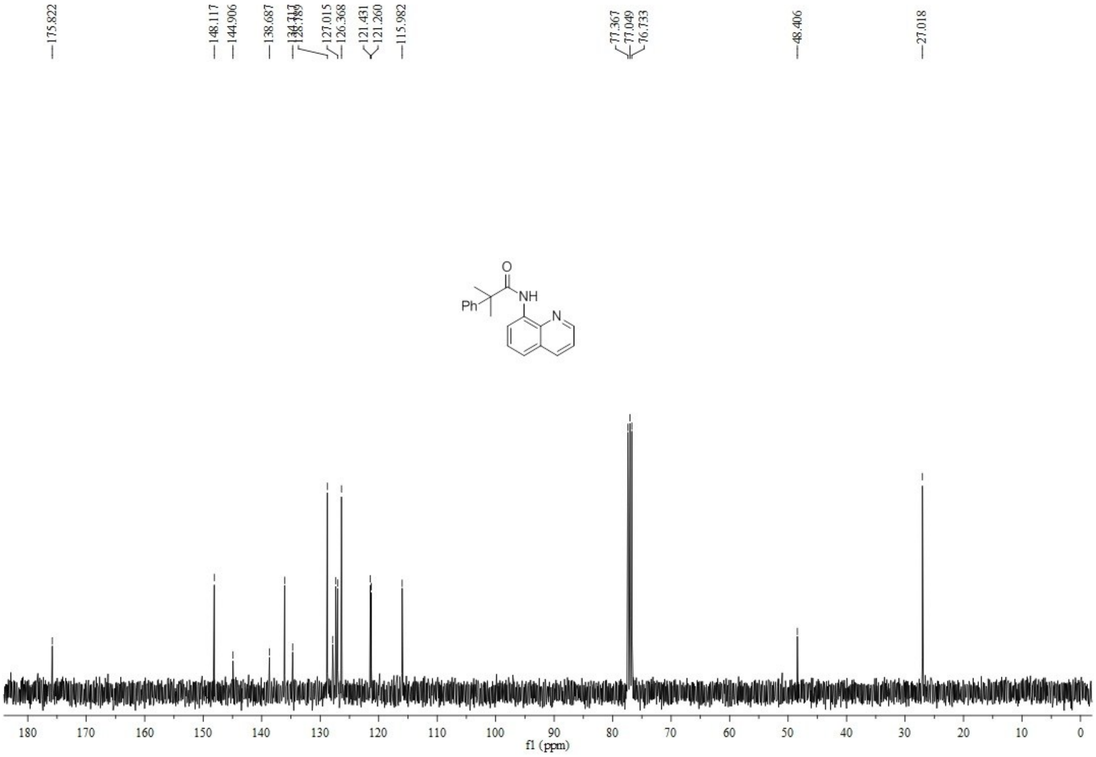




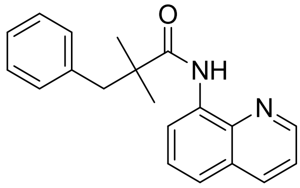
2-methyl-2-phenyl-*N*-(quinolin-8-yl)propanamide **(1b)**

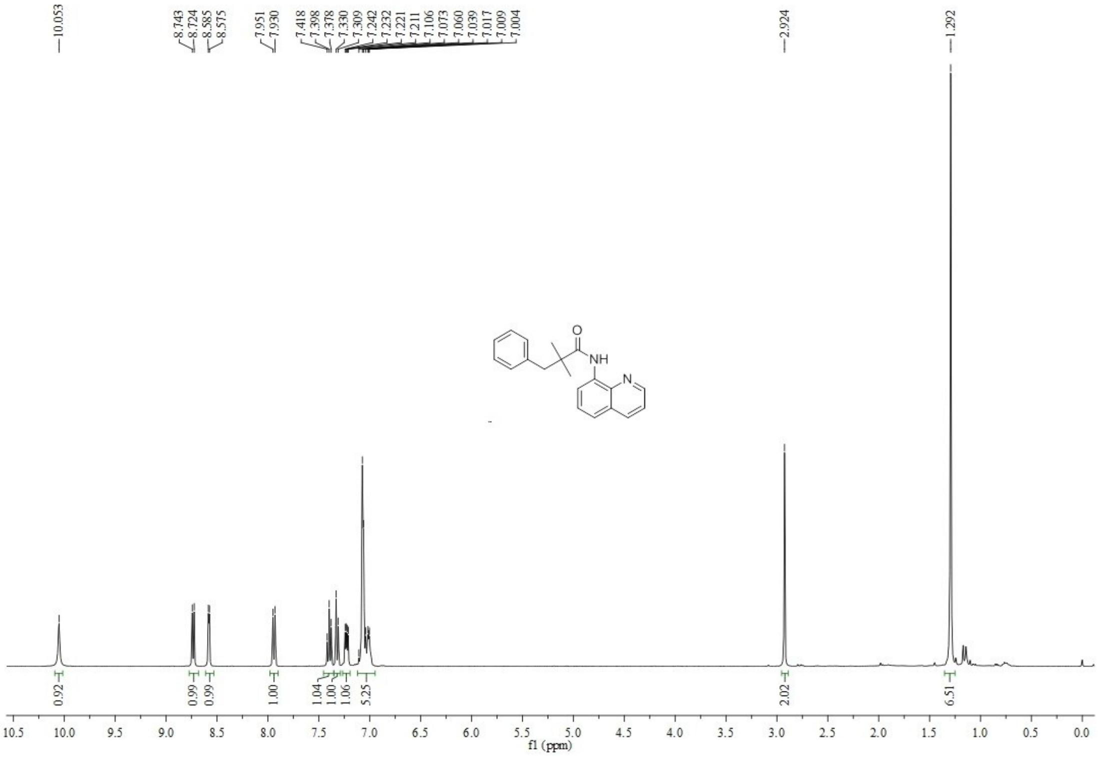


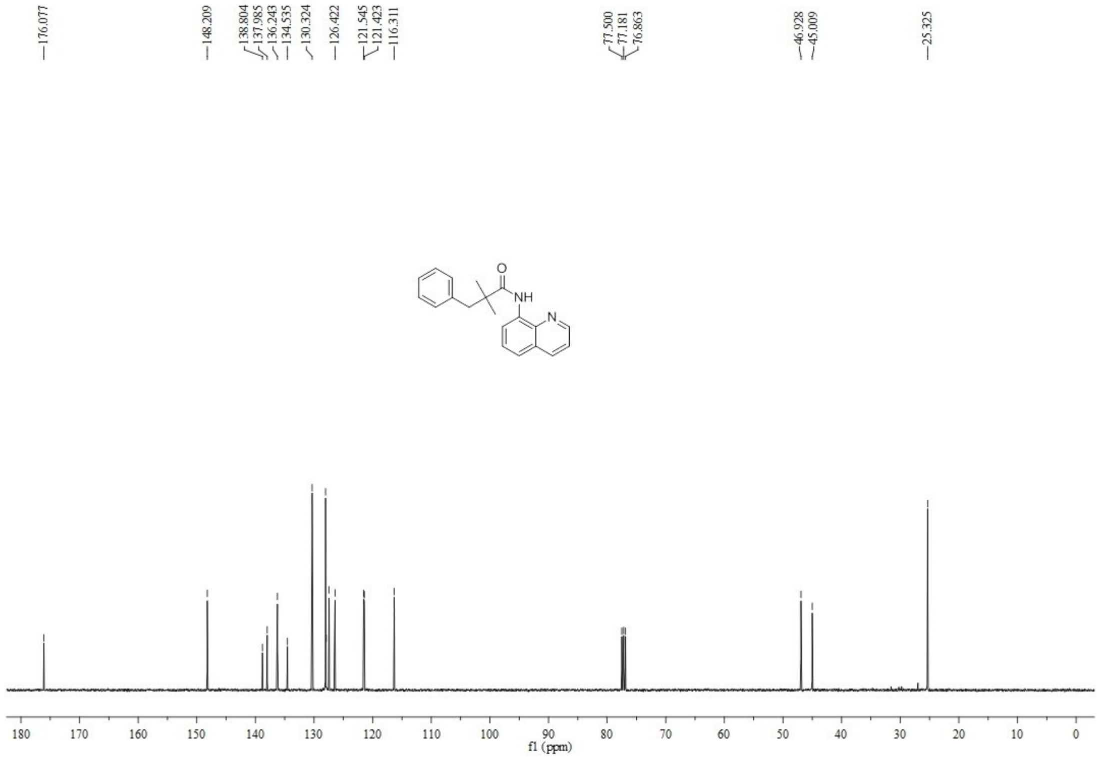




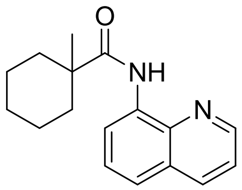
2,2-dimethyl-3-phenyl-*N*-(quinolin-8-yl)propanamide **(1c)**

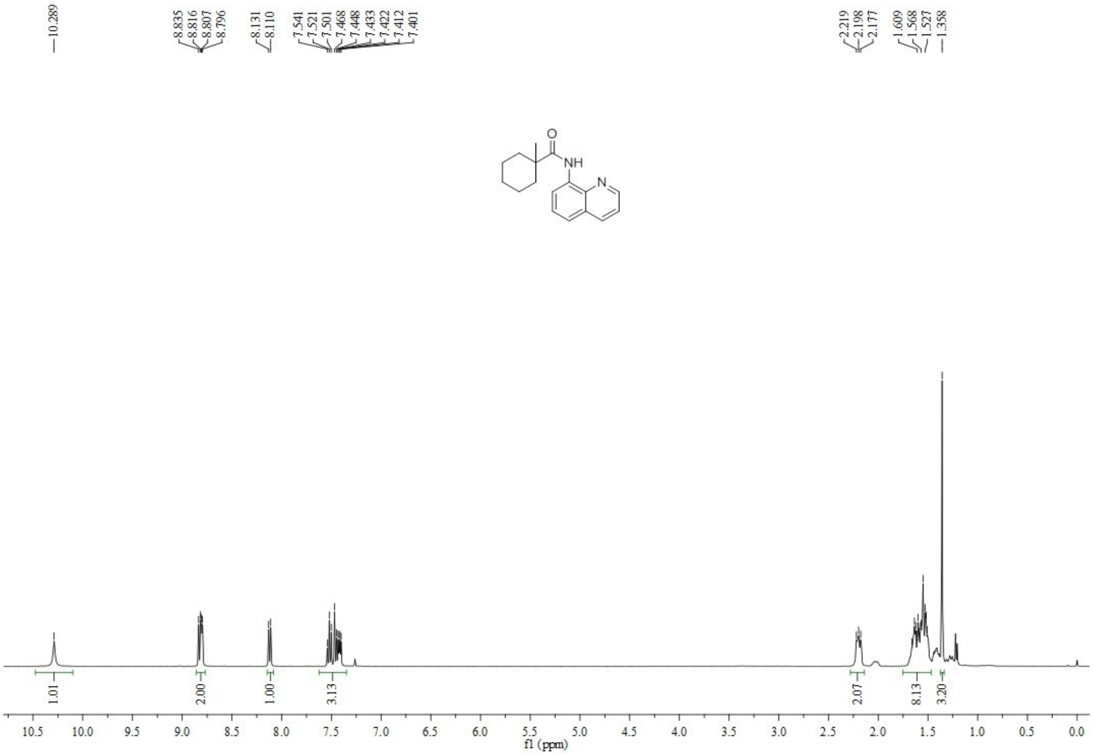


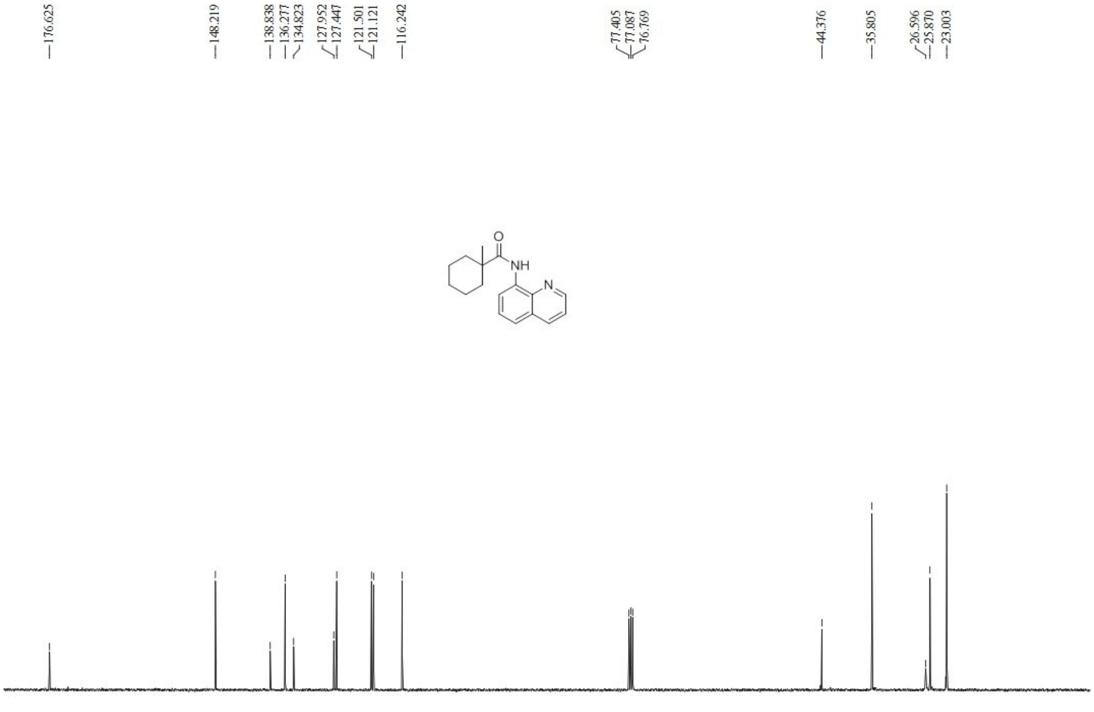




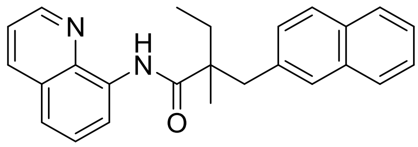
1-methyl-*N*-(quinolin-8-yl)cyclohexanecarboxamide (**1d**)

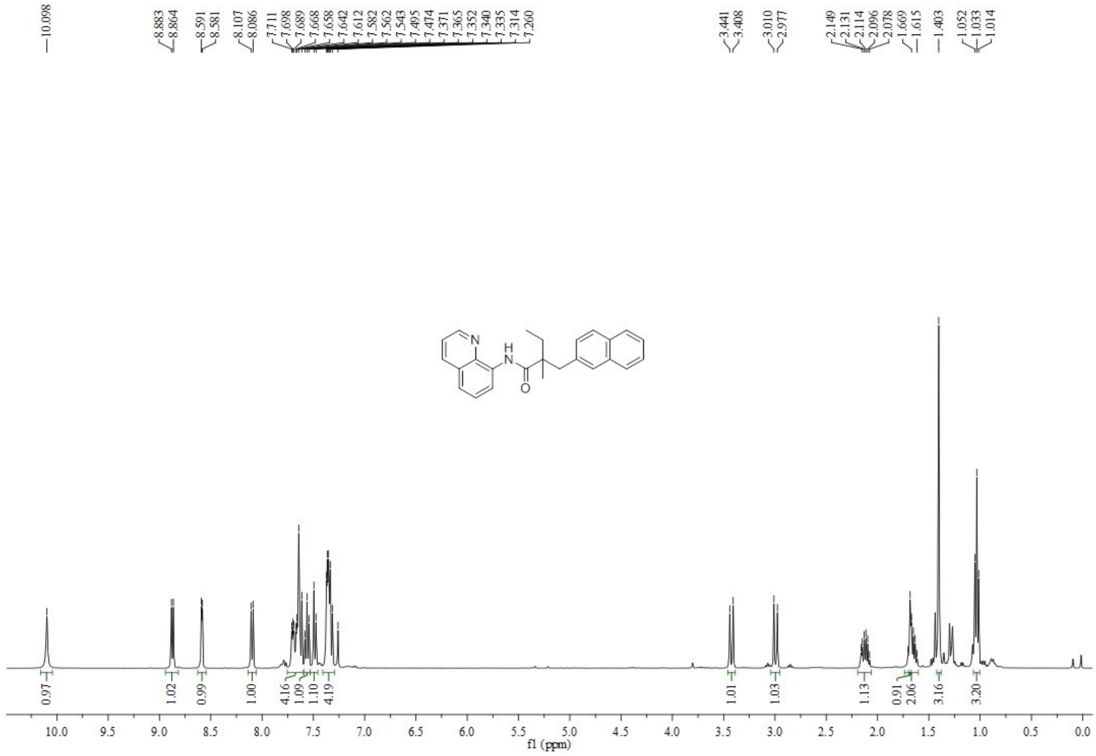


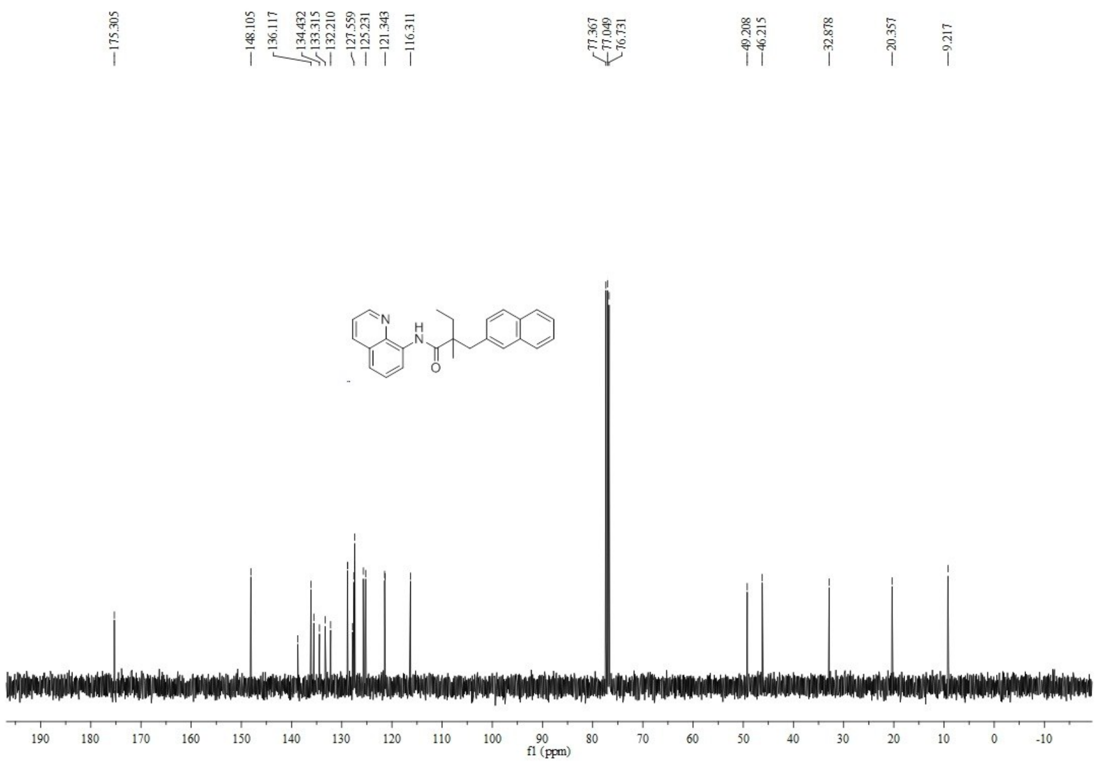




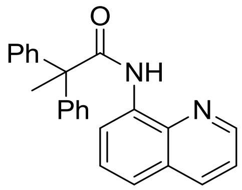
2-methyl-2-(naphthalen-2-ylmethyl)-*N*-(quinolin-8-yl)butanamide (**1e**)

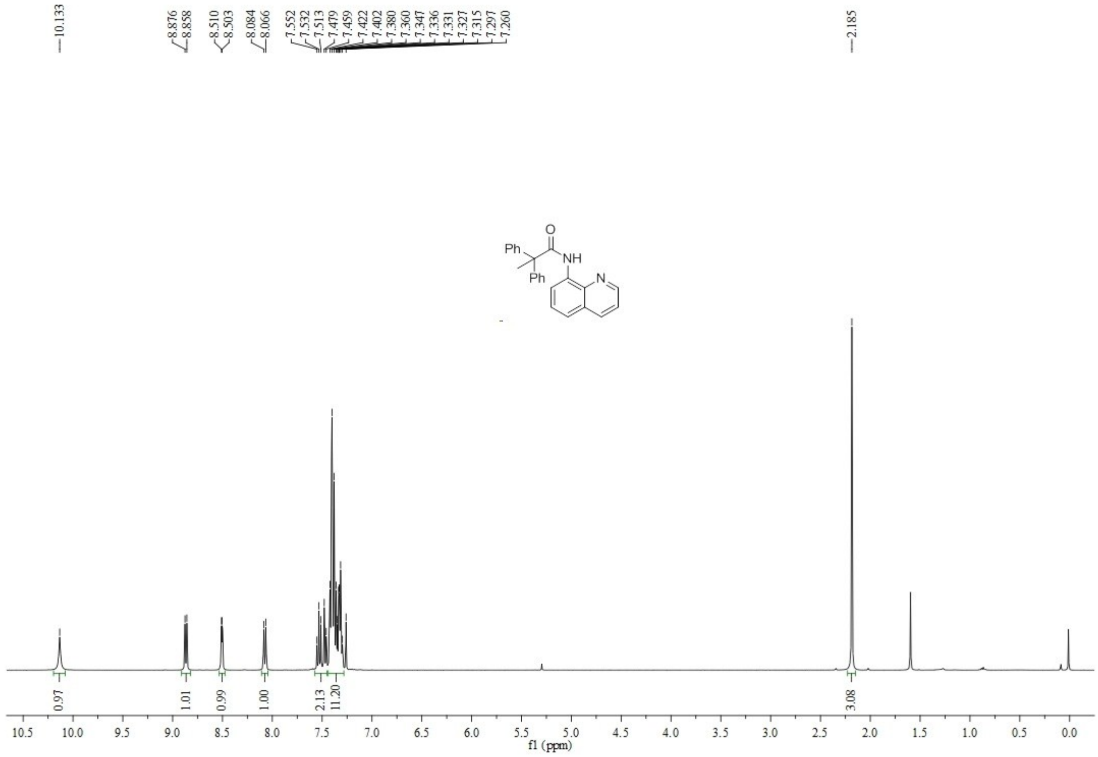


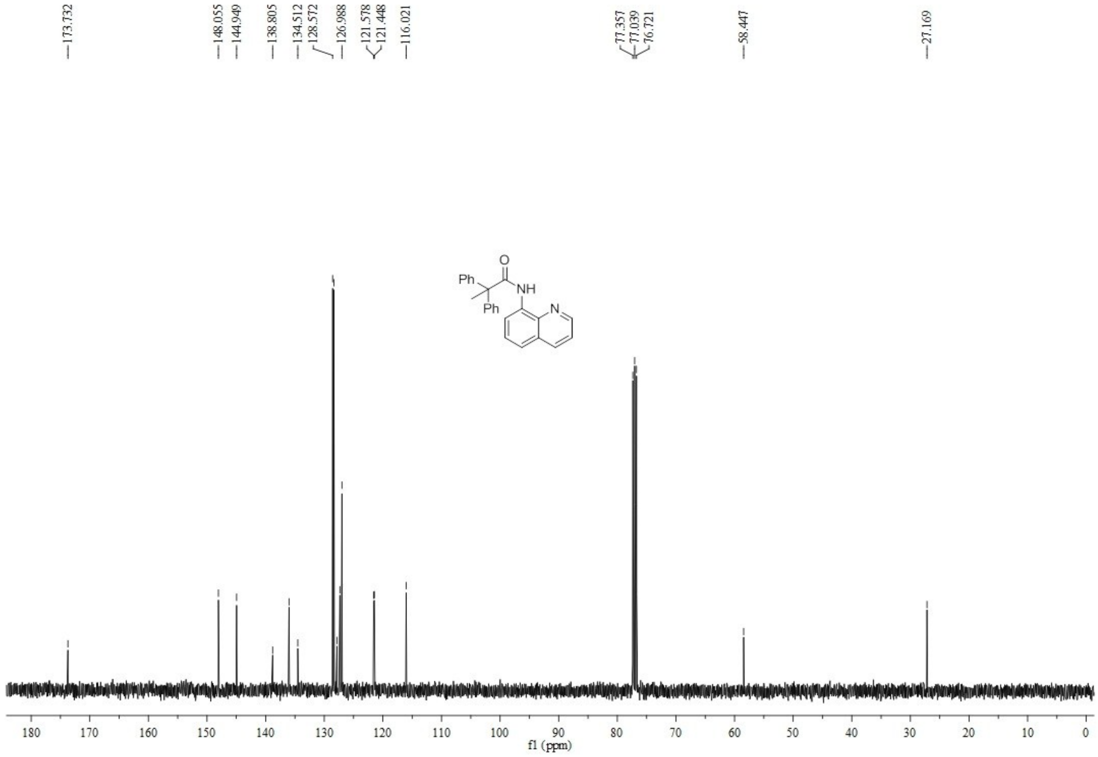




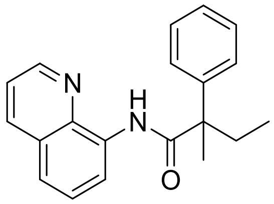
2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (**1f**)

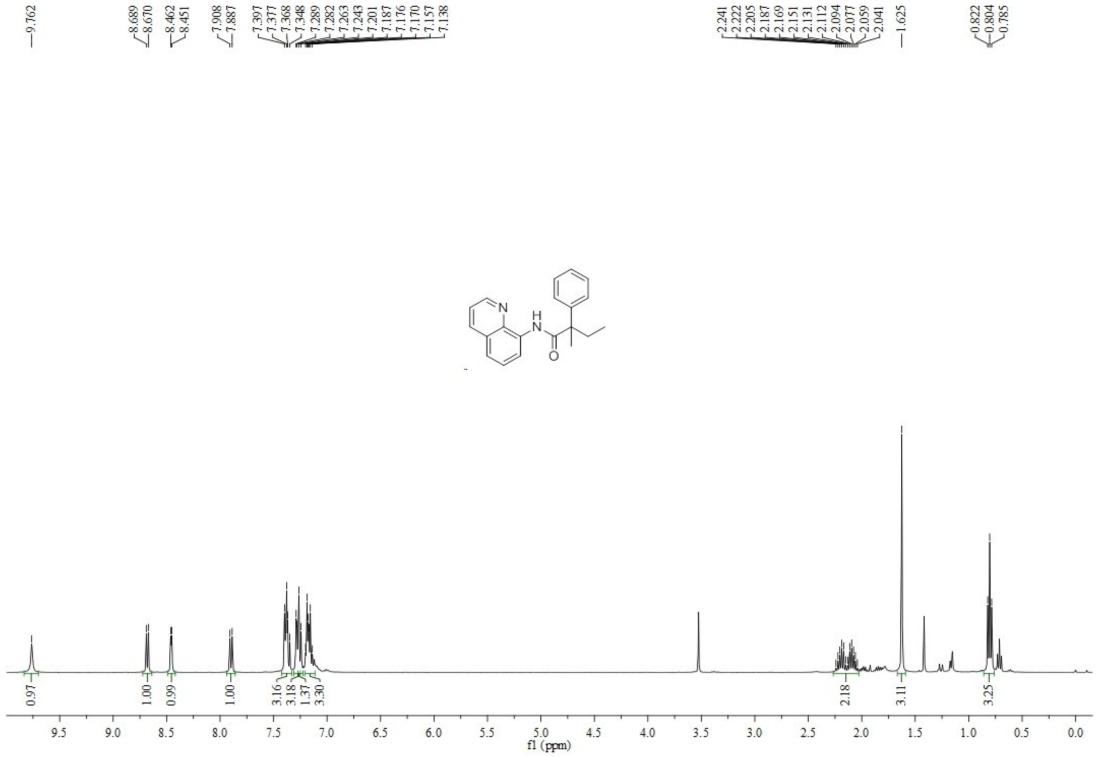


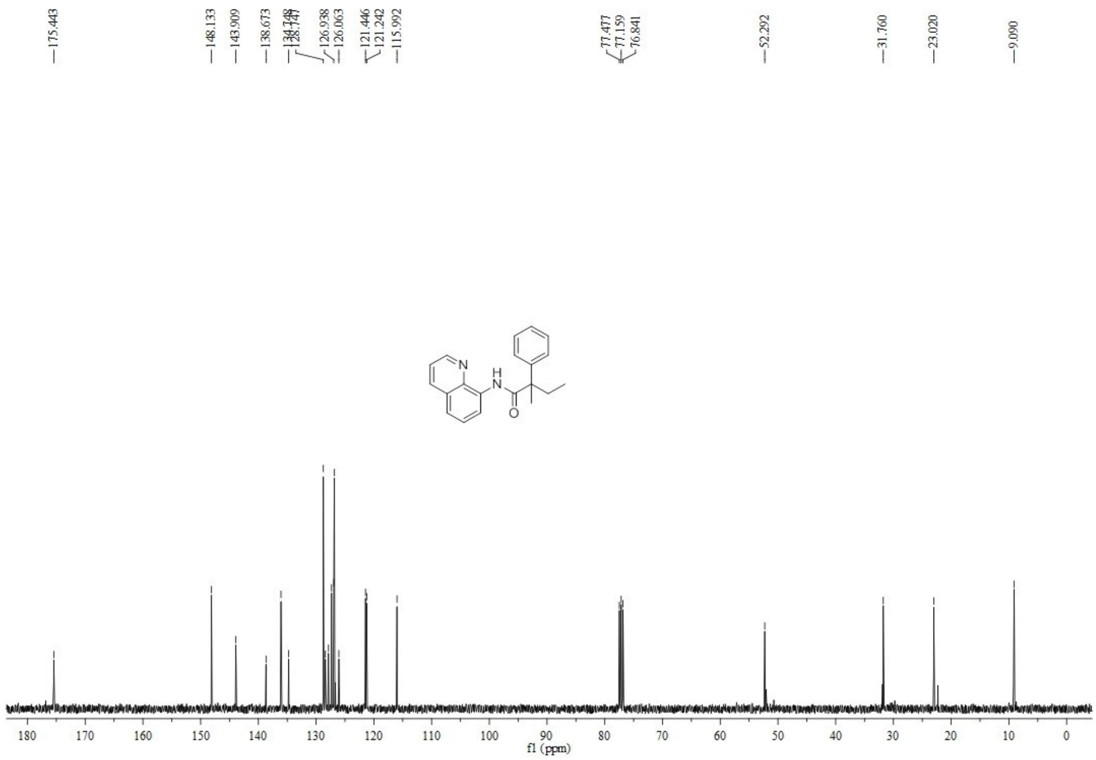




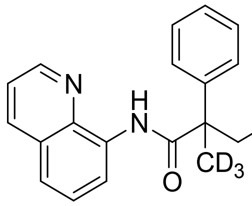
2-methyl-2-phenyl-*N*-(quinolin-8-yl)butanamide (**1g**)

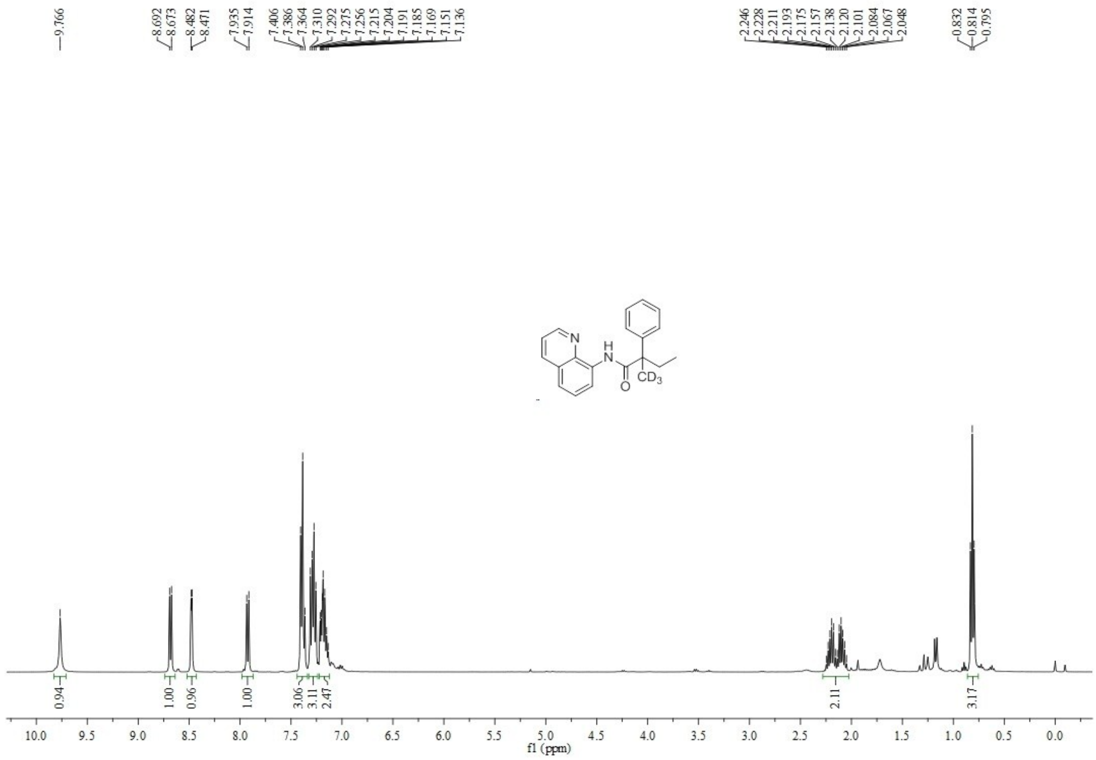


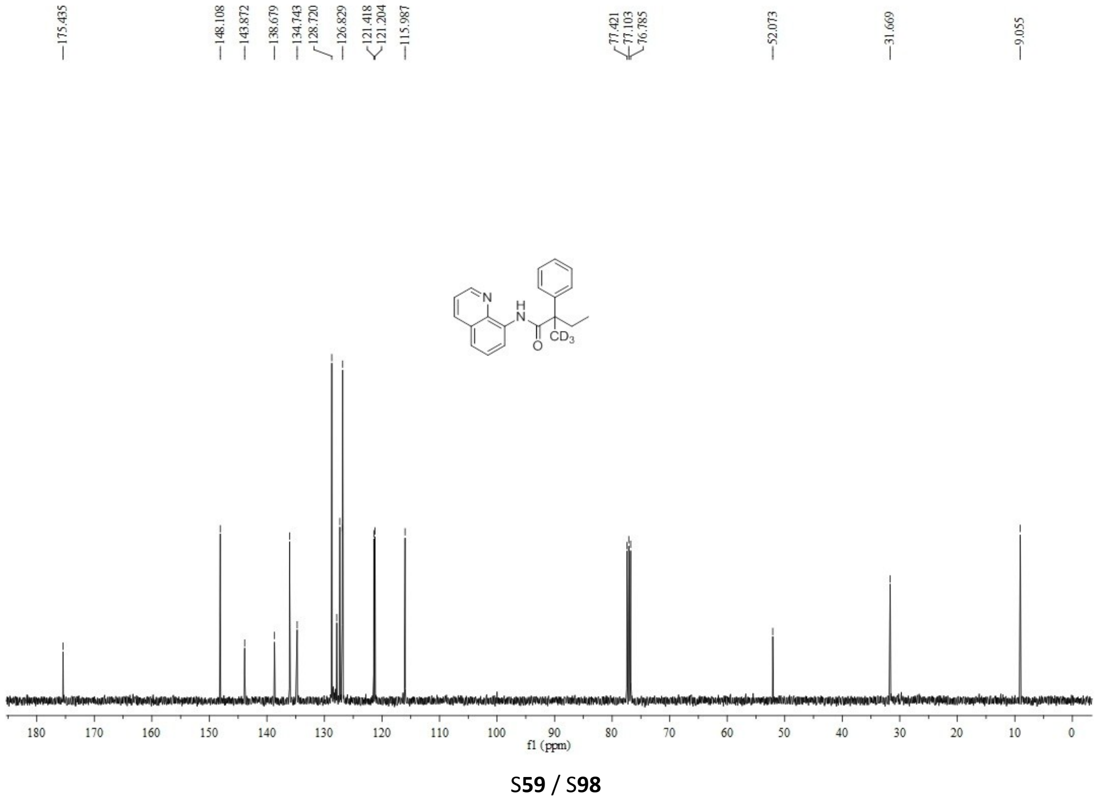




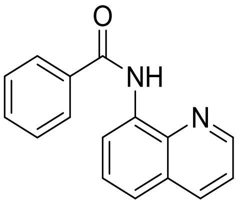
[D_3]-2-methyl-2-phenyl-*N*-(quinolin-8-yl)butanamide ([D_3]-**1g**)

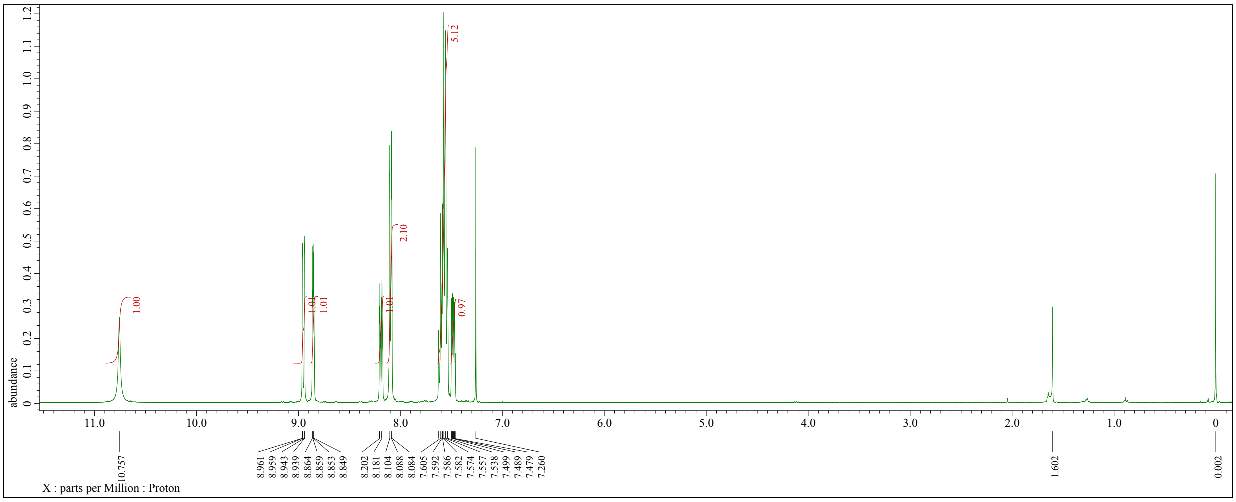


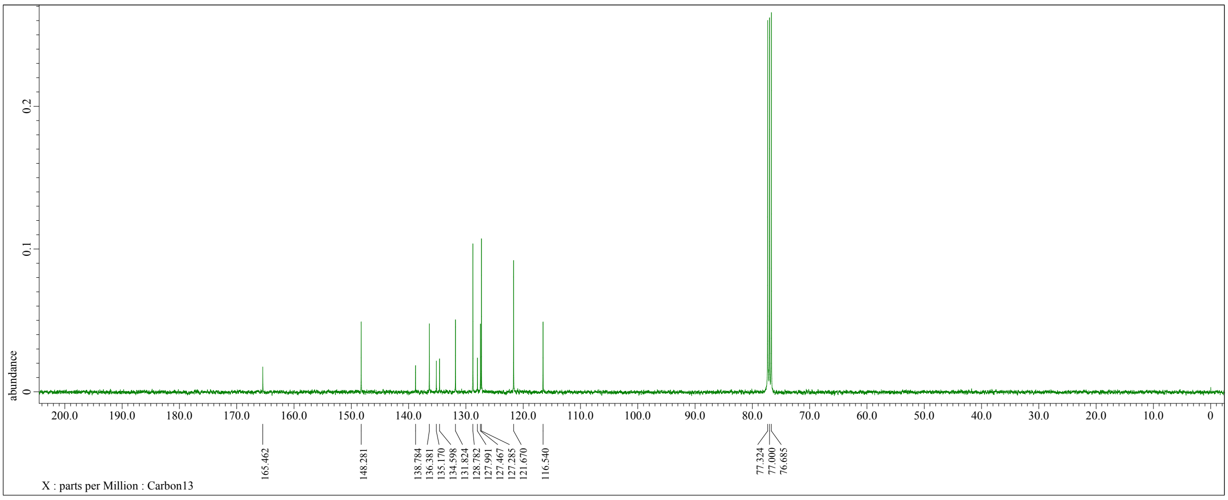




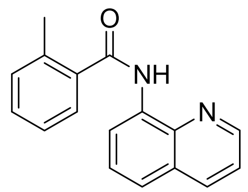
N-(quinolin-8-yl)benzamide (**1h**)

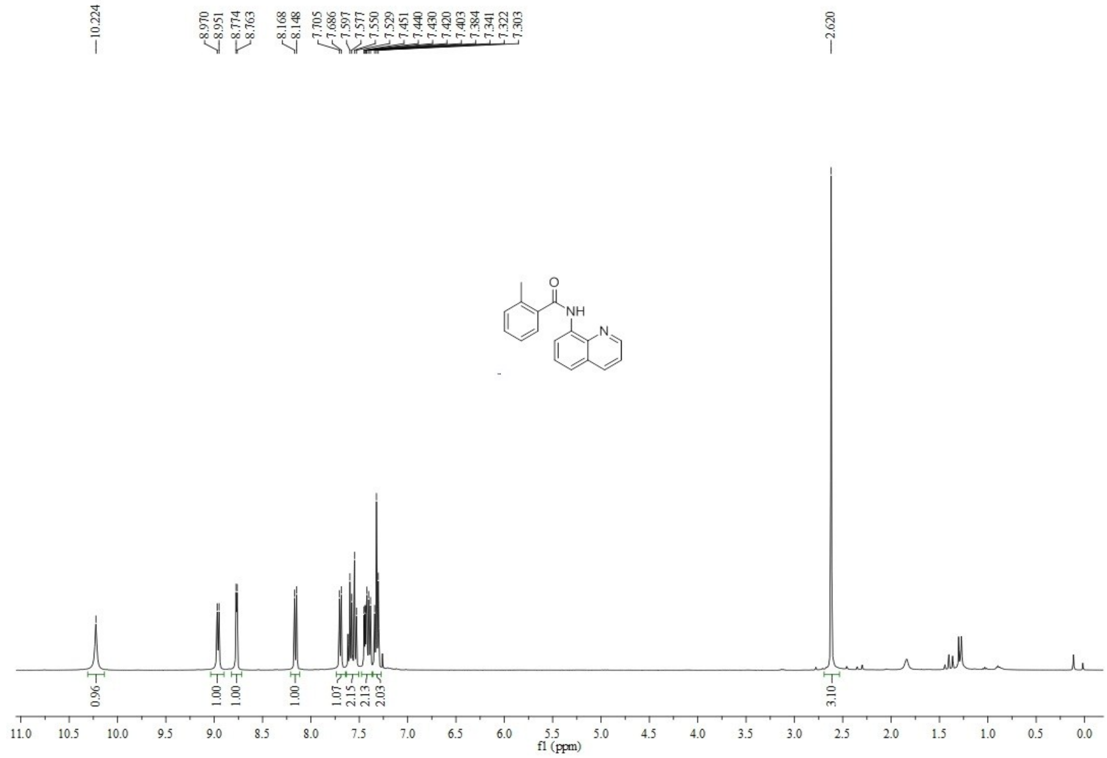


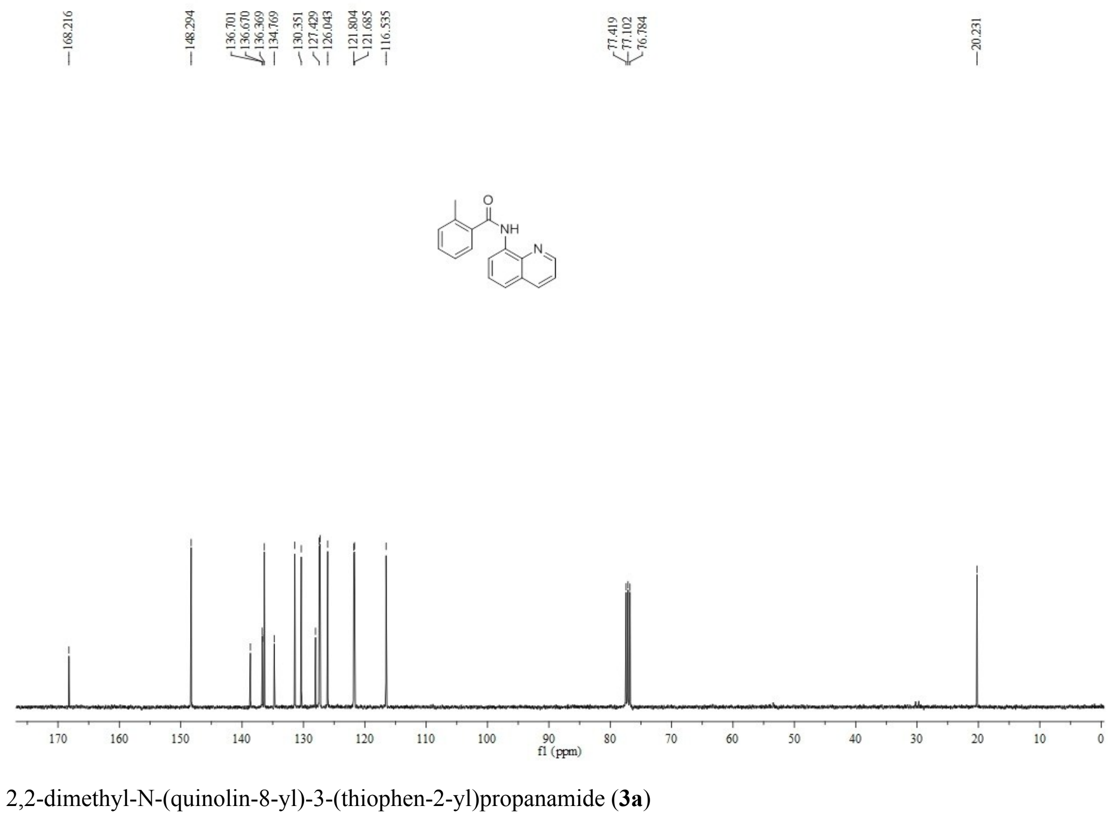




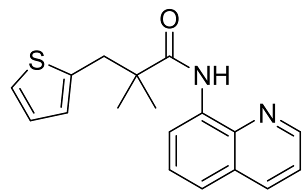
2-methyl-*N*-(quinolin-8-yl)benzamide (**1i**)

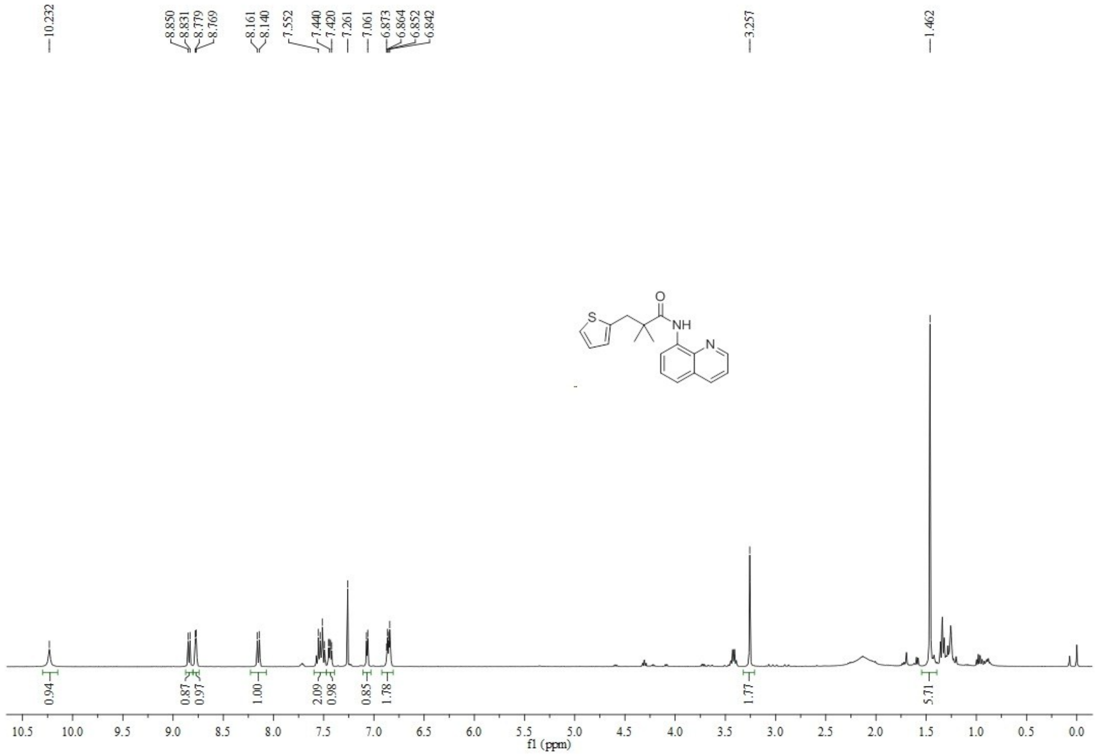


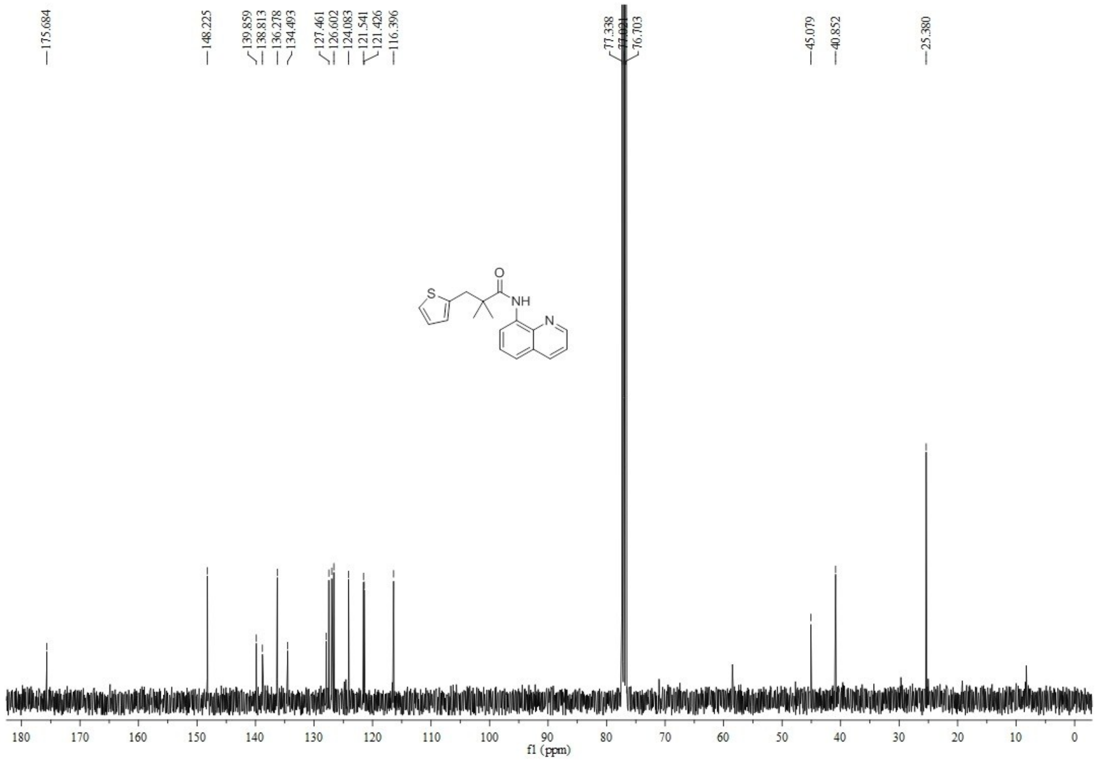




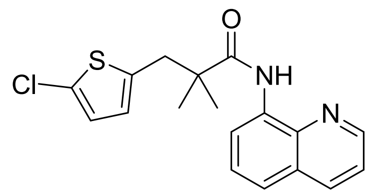
2,2-dimethyl-N-(quinolin-8-yl)-3-(thiophen-2-yl)propanamide (**3a**)

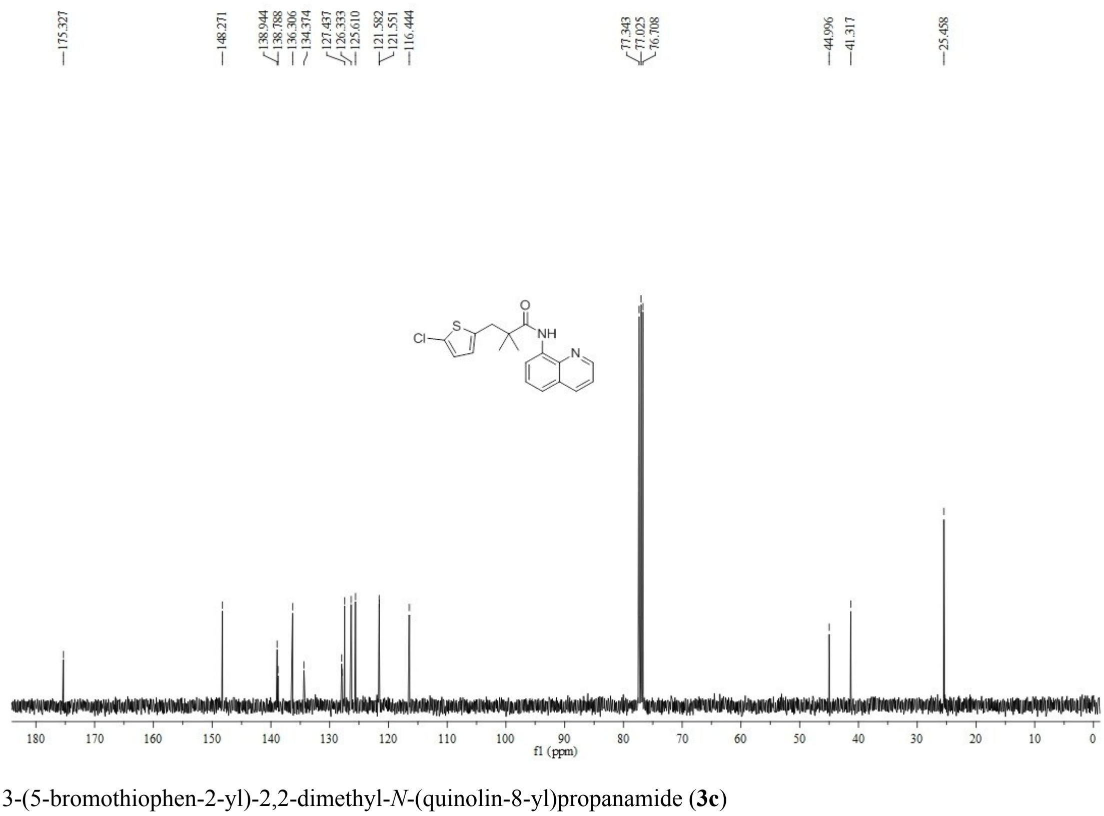




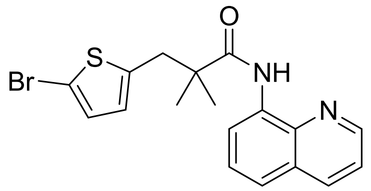


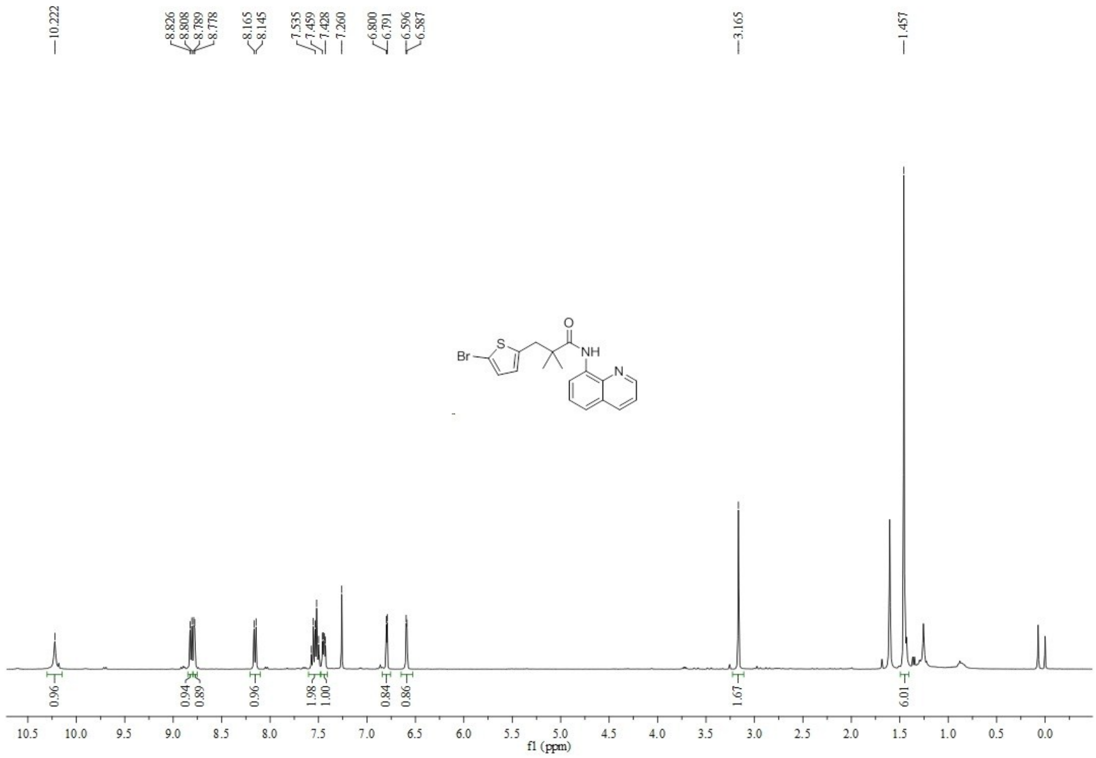
3-(5-chlorothiophen-2-yl)-2,2-dimethyl-N-(quinolin-8-yl)propanamide (**3b**)

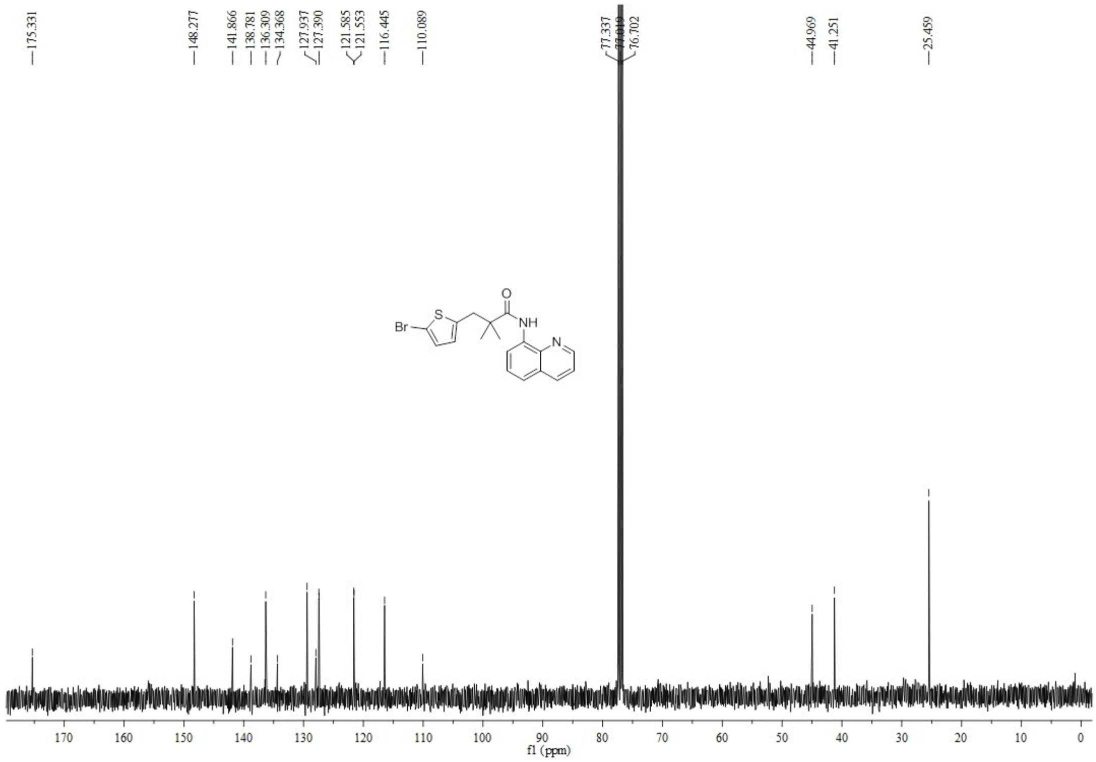




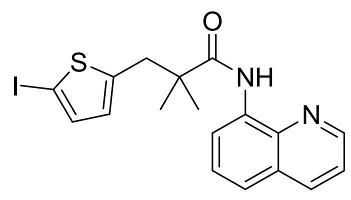
3-(5-bromothiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3c**)

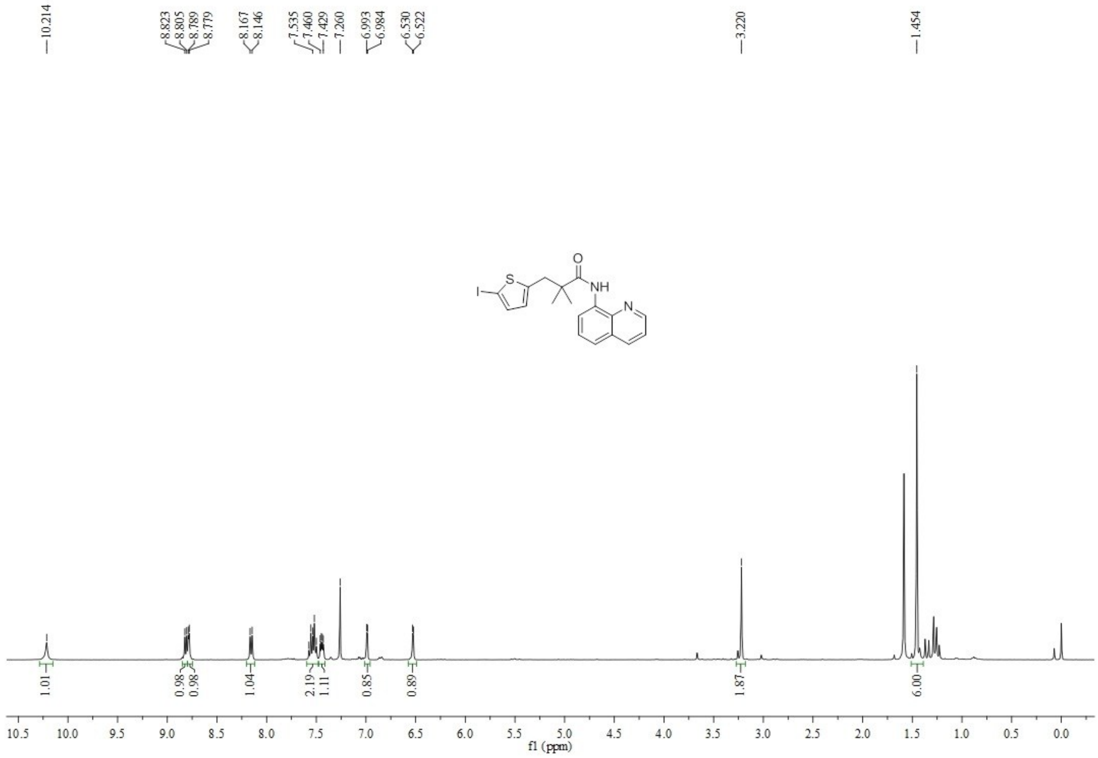


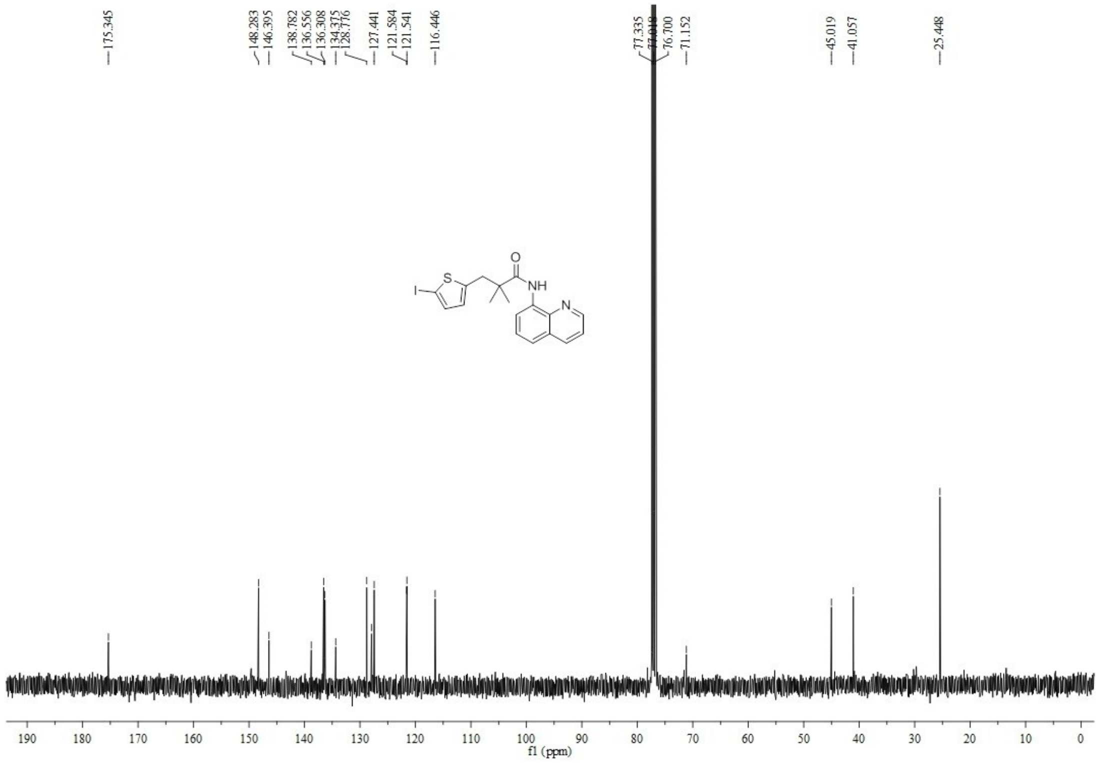




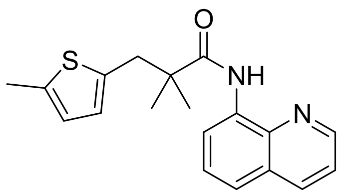
3-(5-iodothiophen-2-yl)-2,2-dimethyl-N-(quinolin-8-yl)propanamide (**3d**)

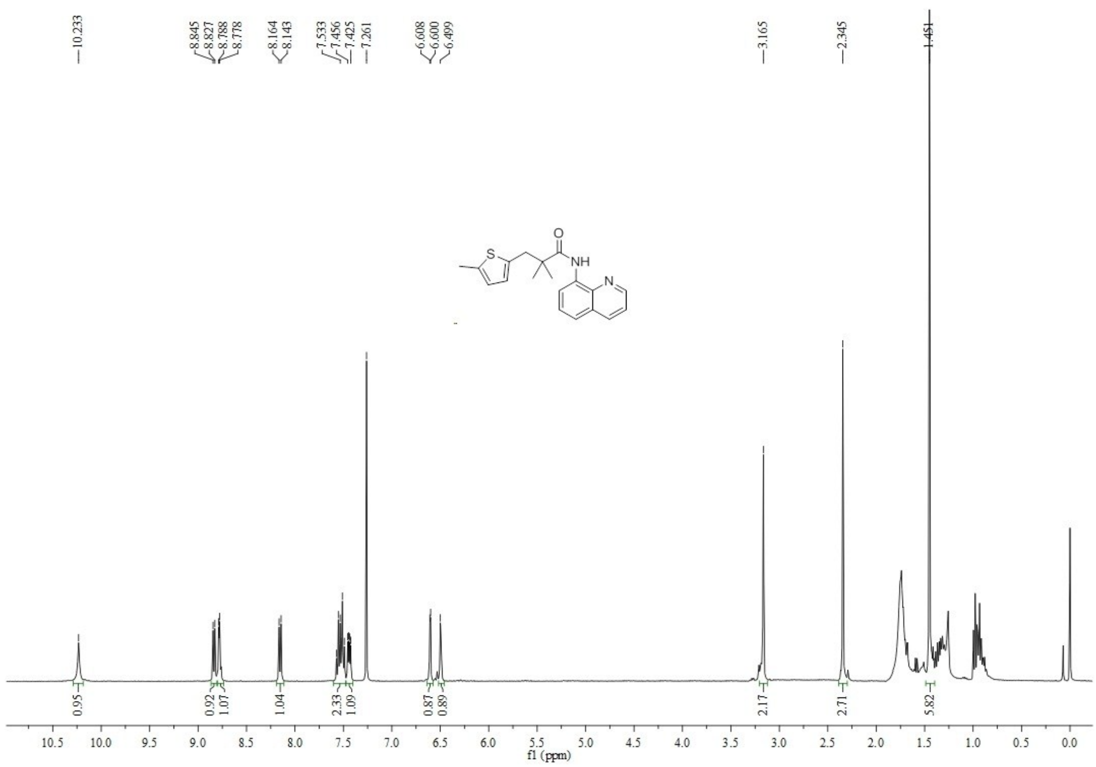


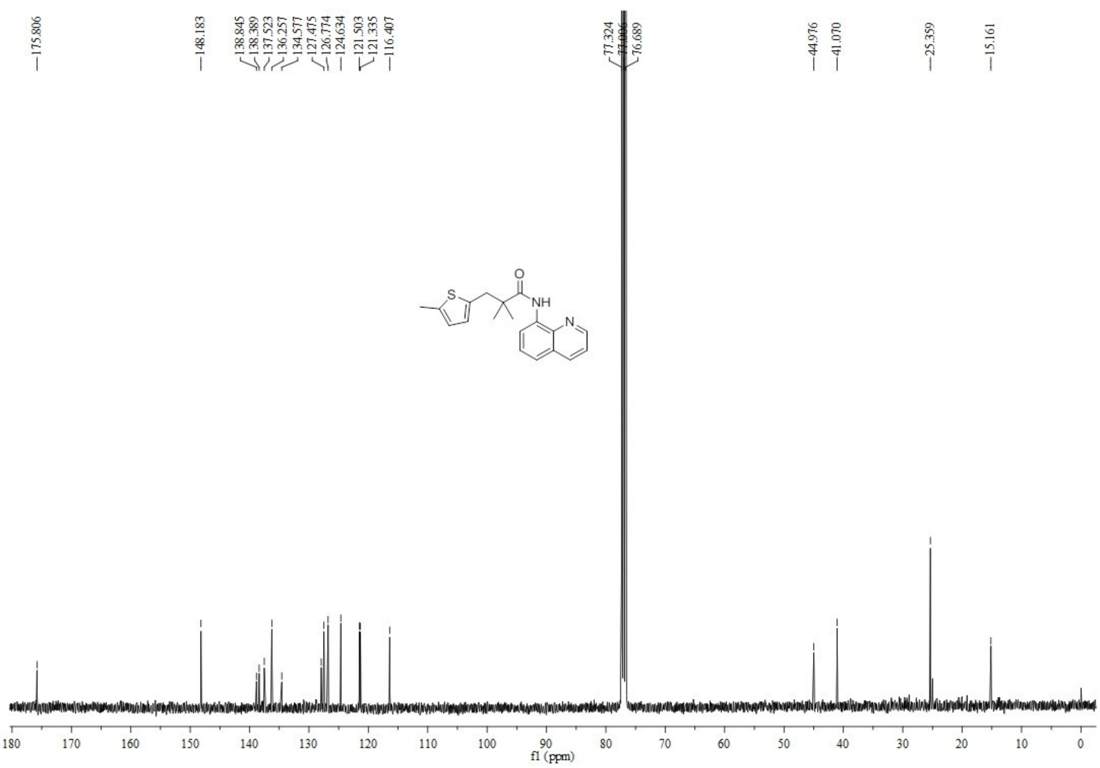




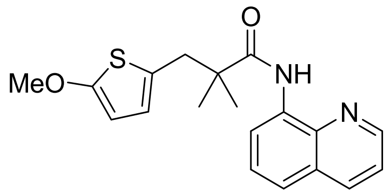
2,2-dimethyl-3-(5-methylthiophen-2-yl)-N-(quinolin-8-yl)propanamide **(3e)**

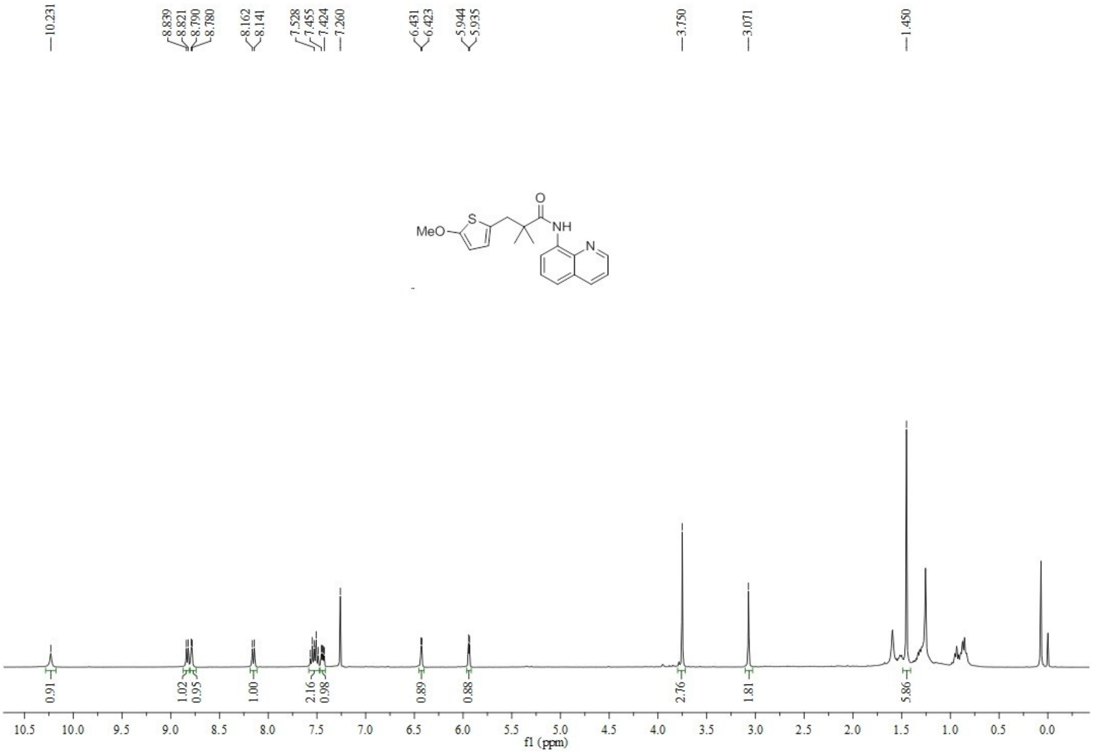


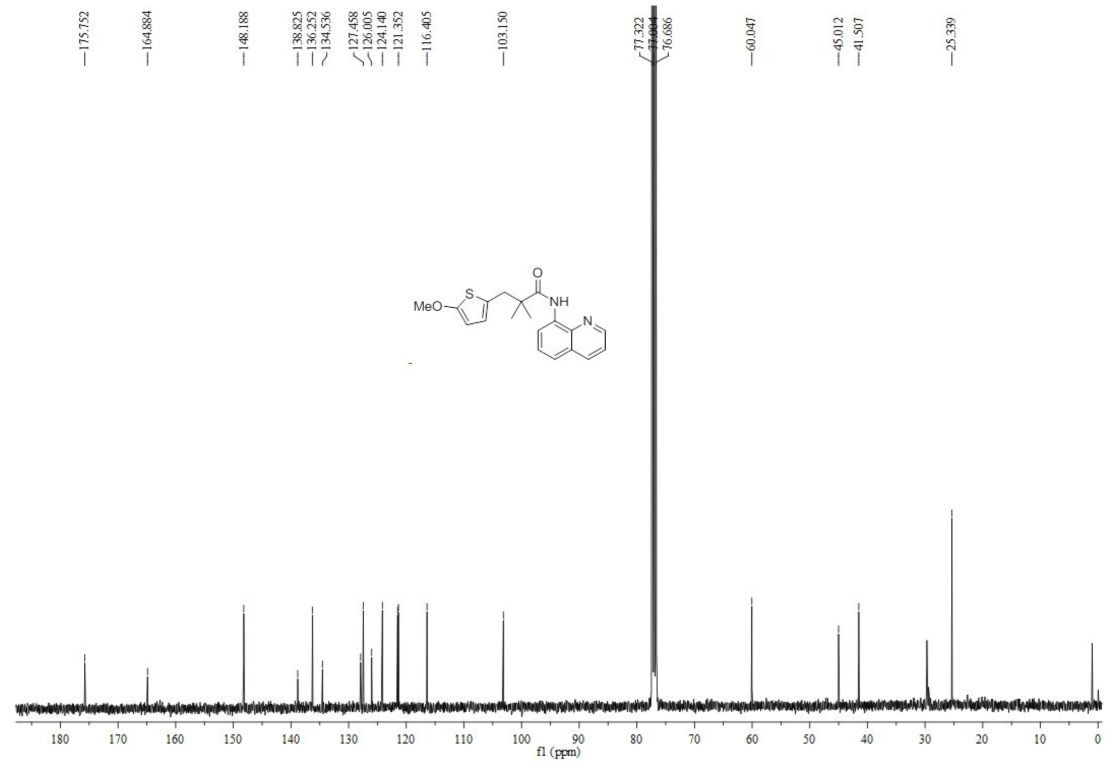




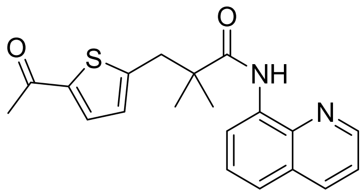
3-(5-methoxythiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3f**)

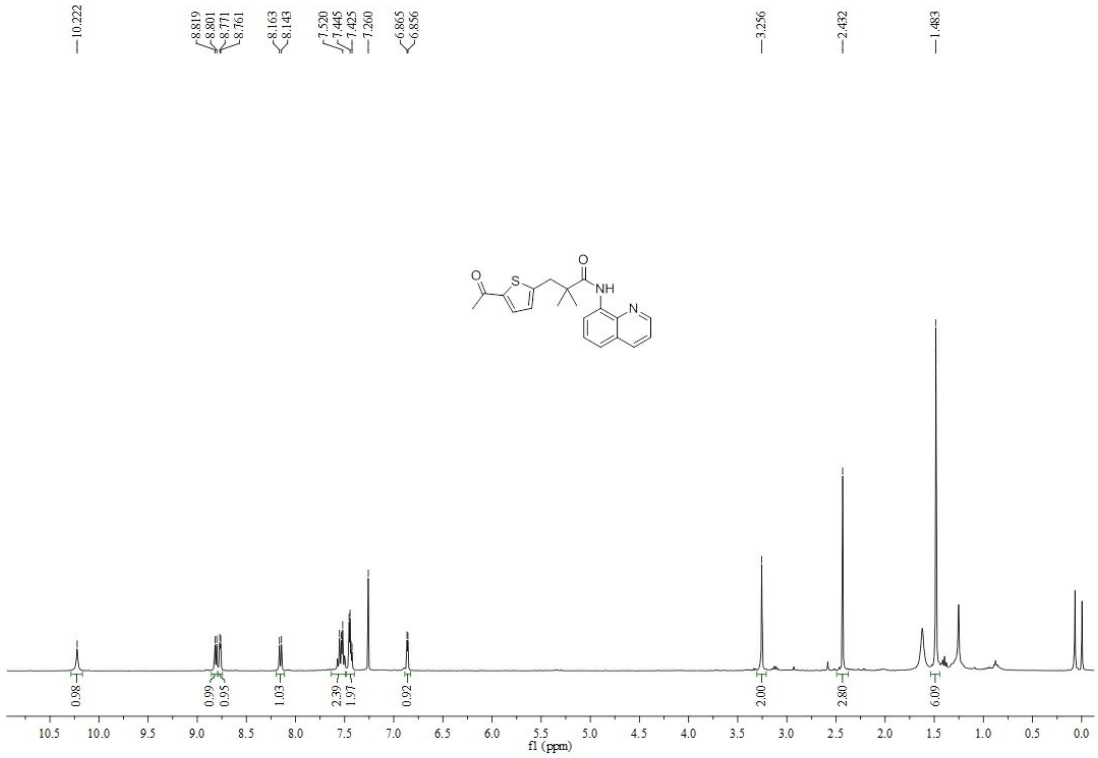


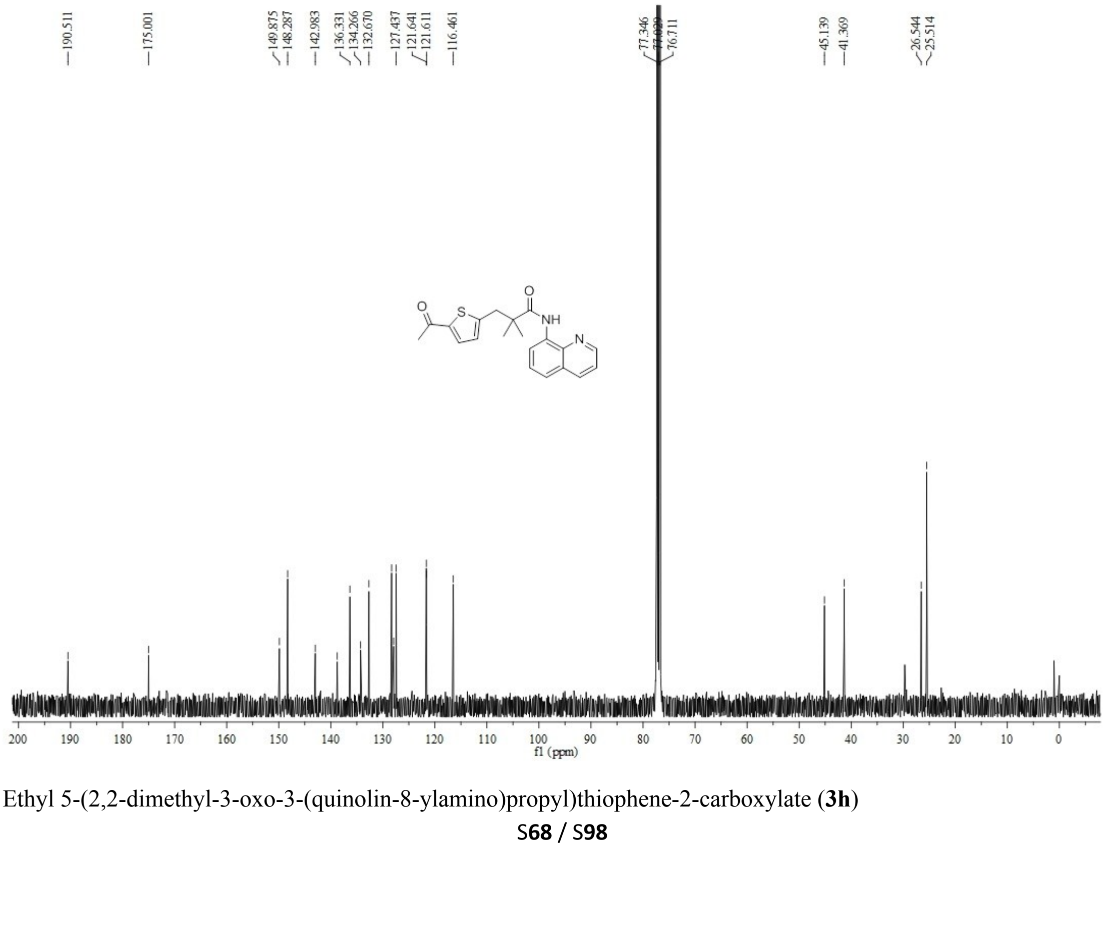




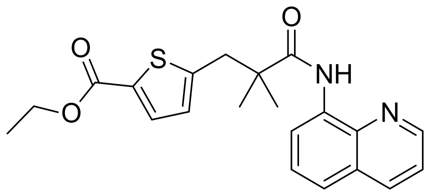
3-(5-acetylthiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3g**)

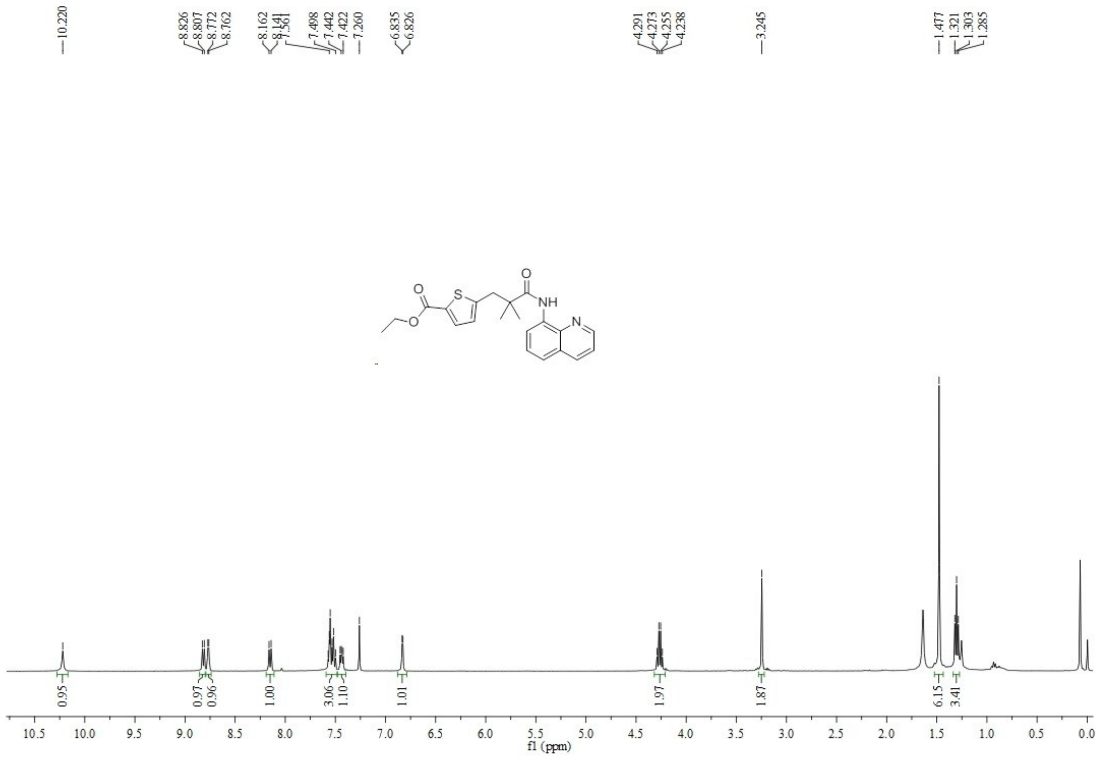


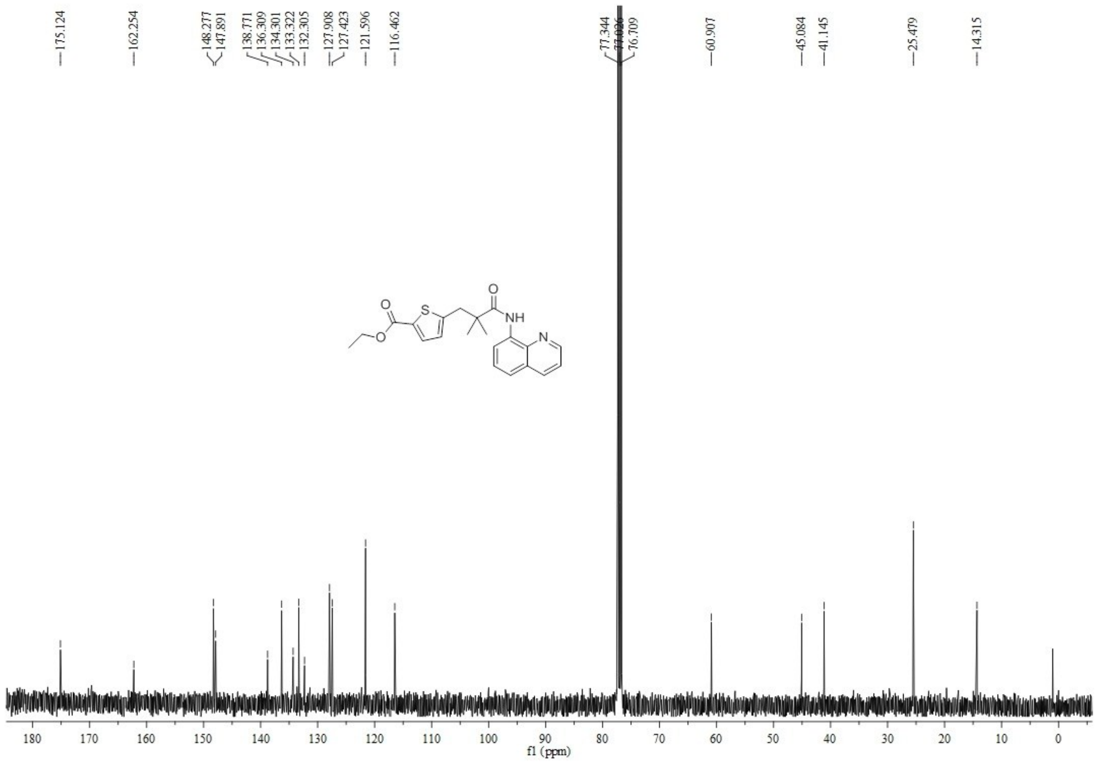




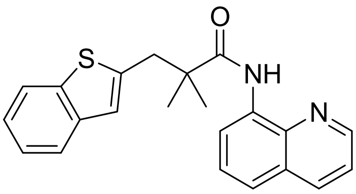
Ethyl 5-(2,2-dimethyl-3-oxo-3-(quinolin-8-ylamino)propyl)thiophene-2-carboxylate (**3h**)

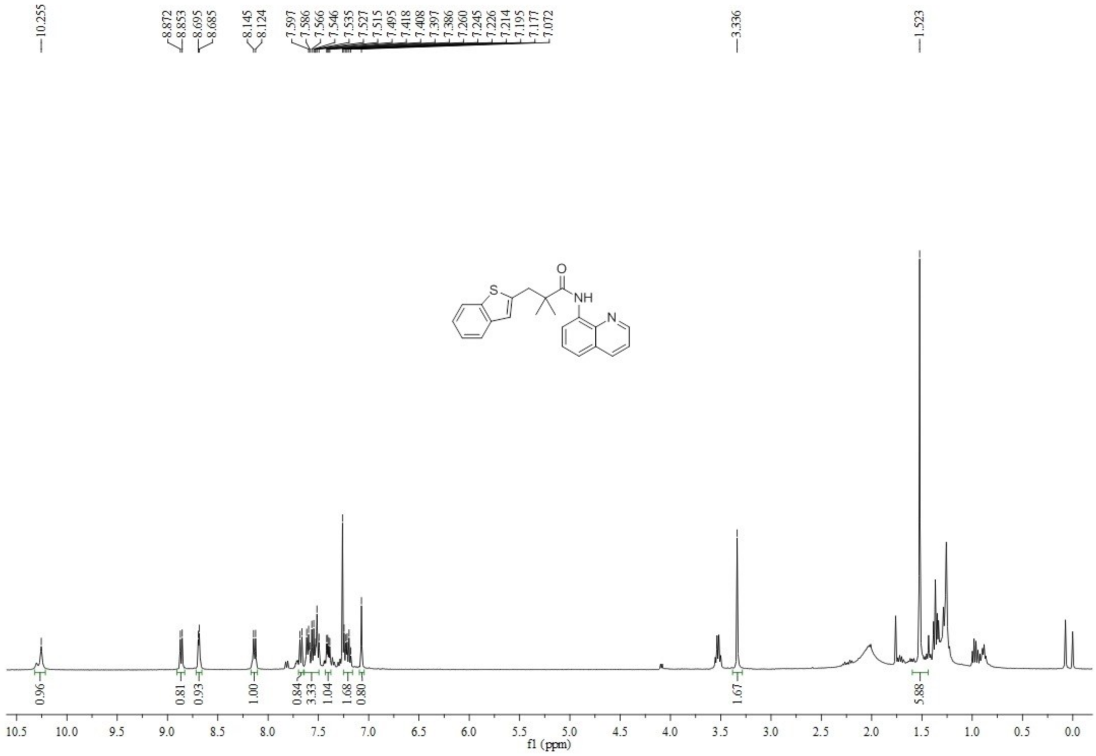


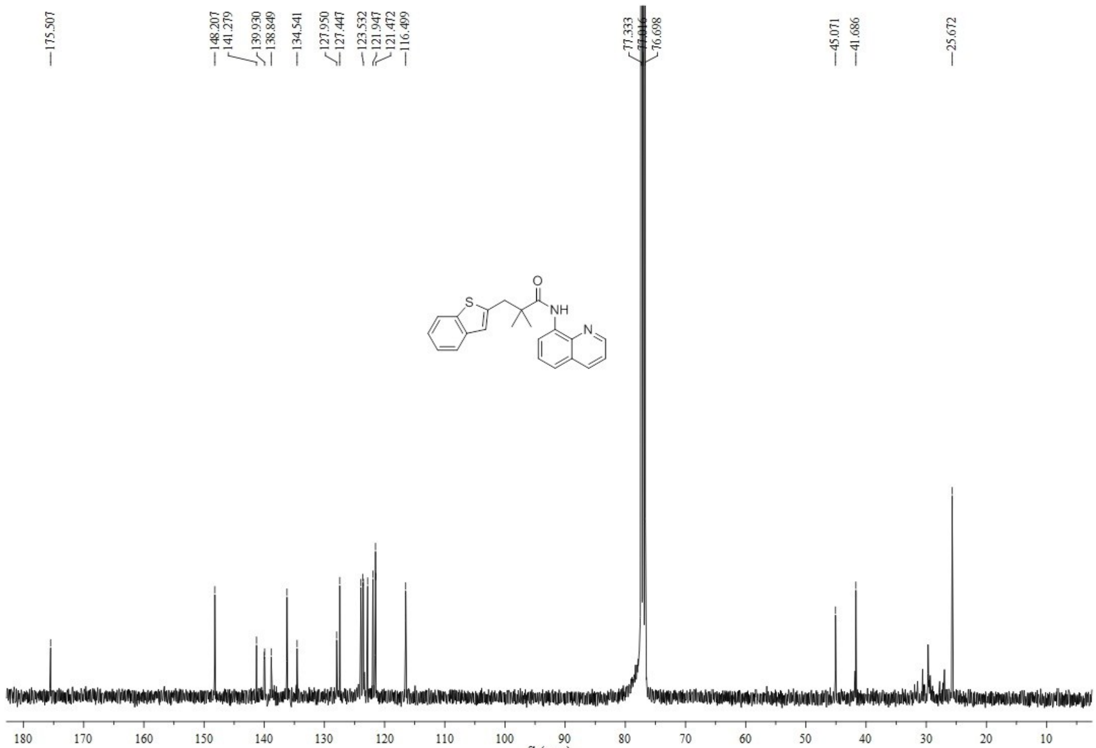




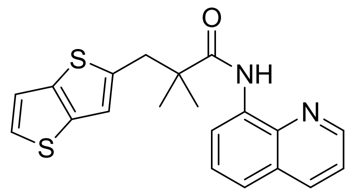
3-(benzo[b]thiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3k**)

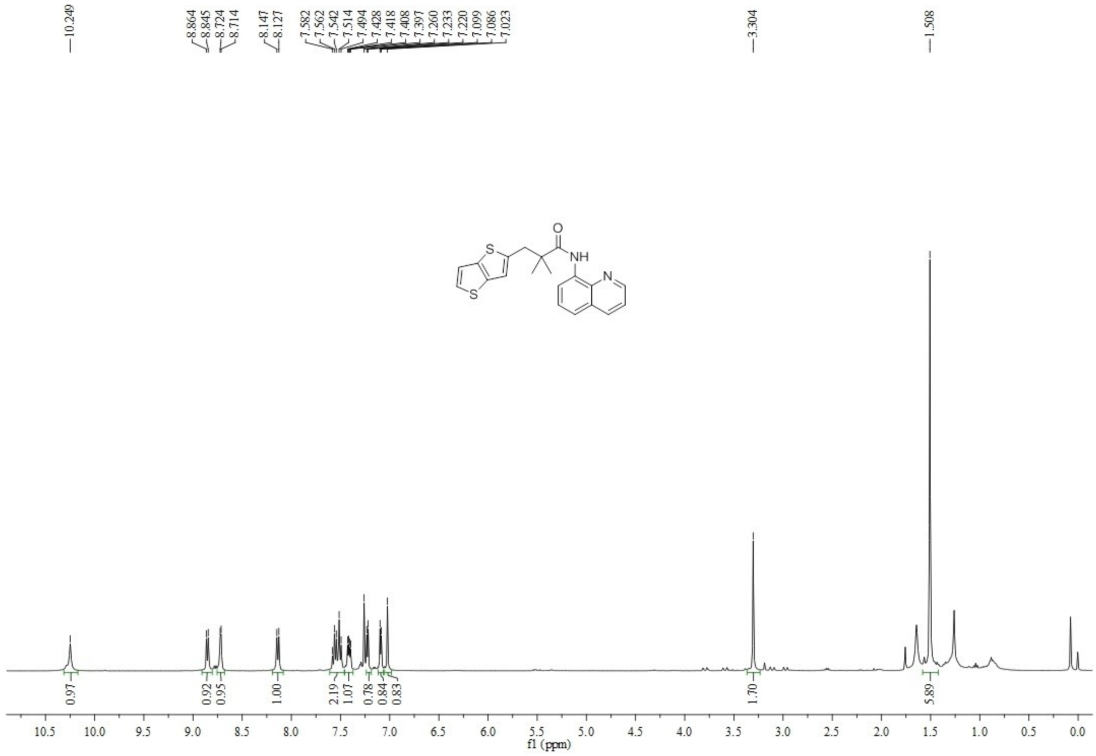


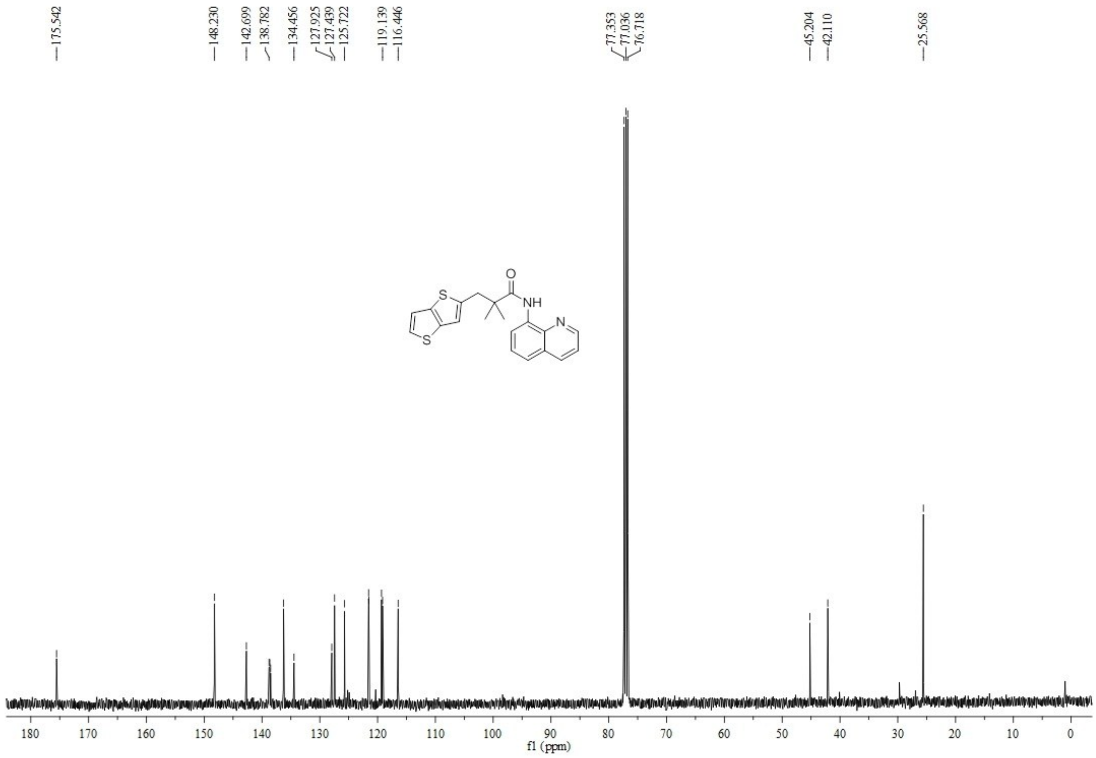




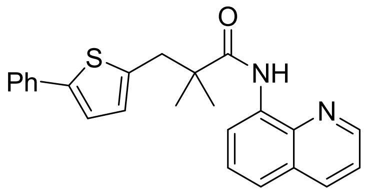
2,2-dimethyl-*N*-(quinolin-8-yl)-3-(thieno[3,2-b]thiophen-2-yl)propanamide (**3l**)

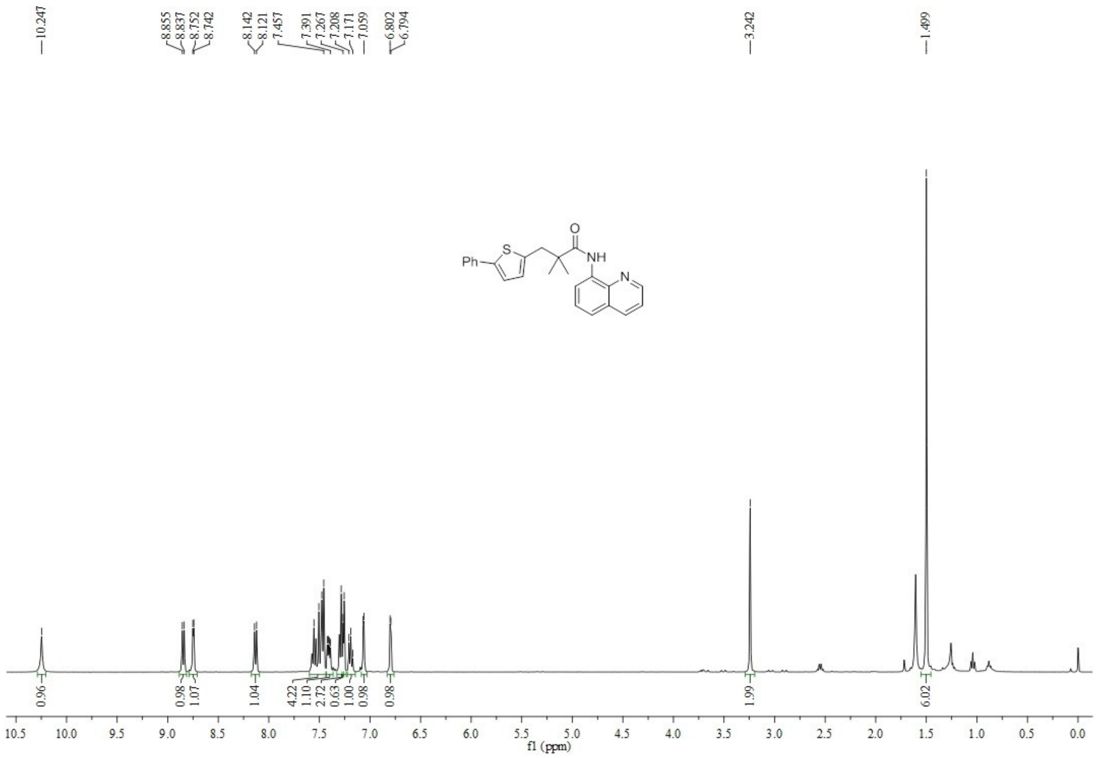


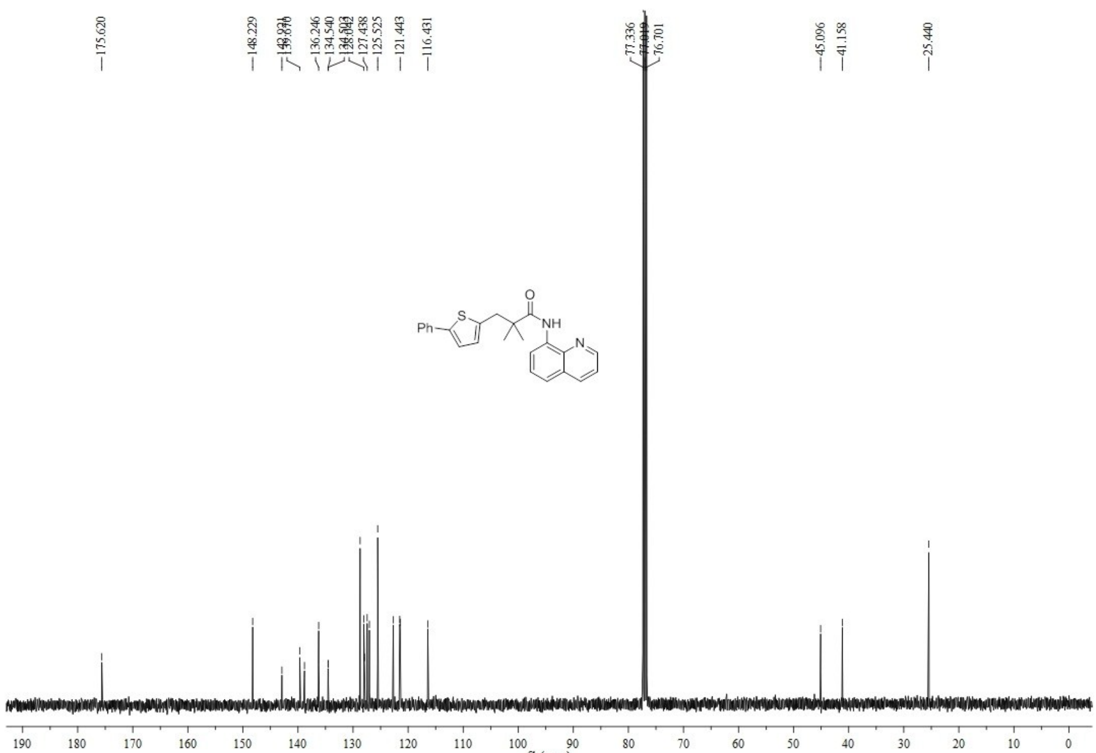




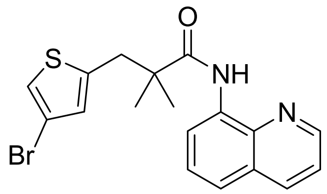
2,2-dimethyl-3-(5-phenylthiophen-2-yl)-*N*-(quinolin-8-yl)propanamide (**3m**)

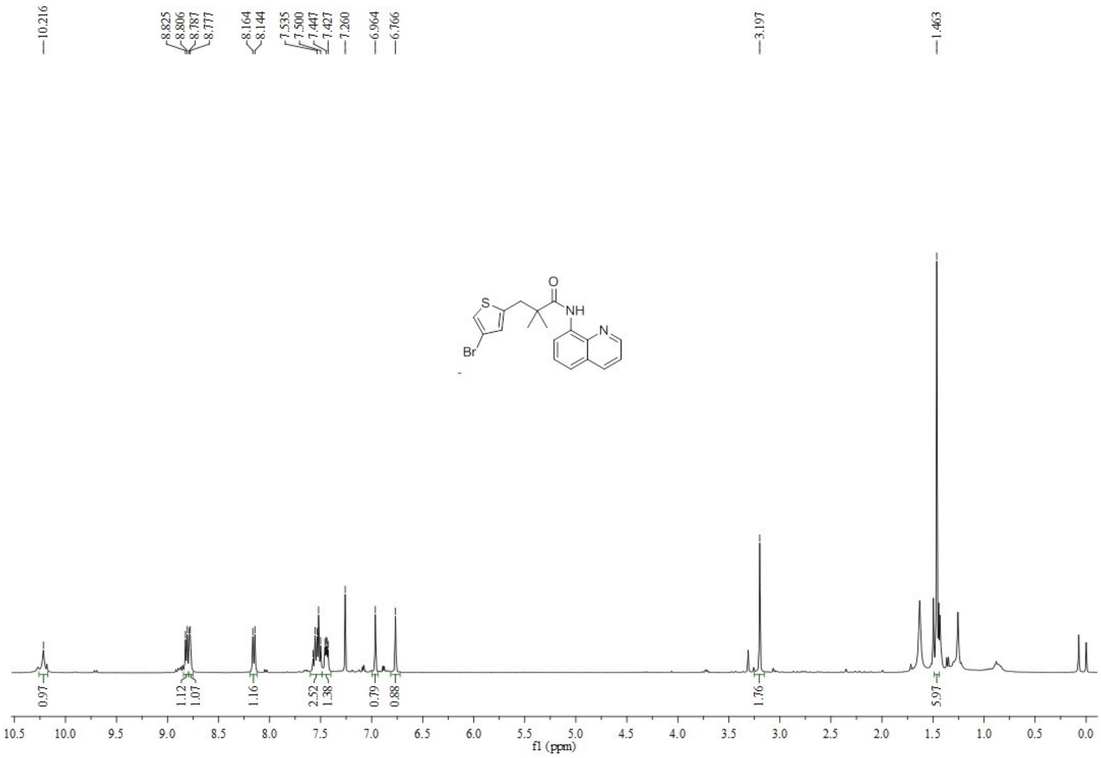


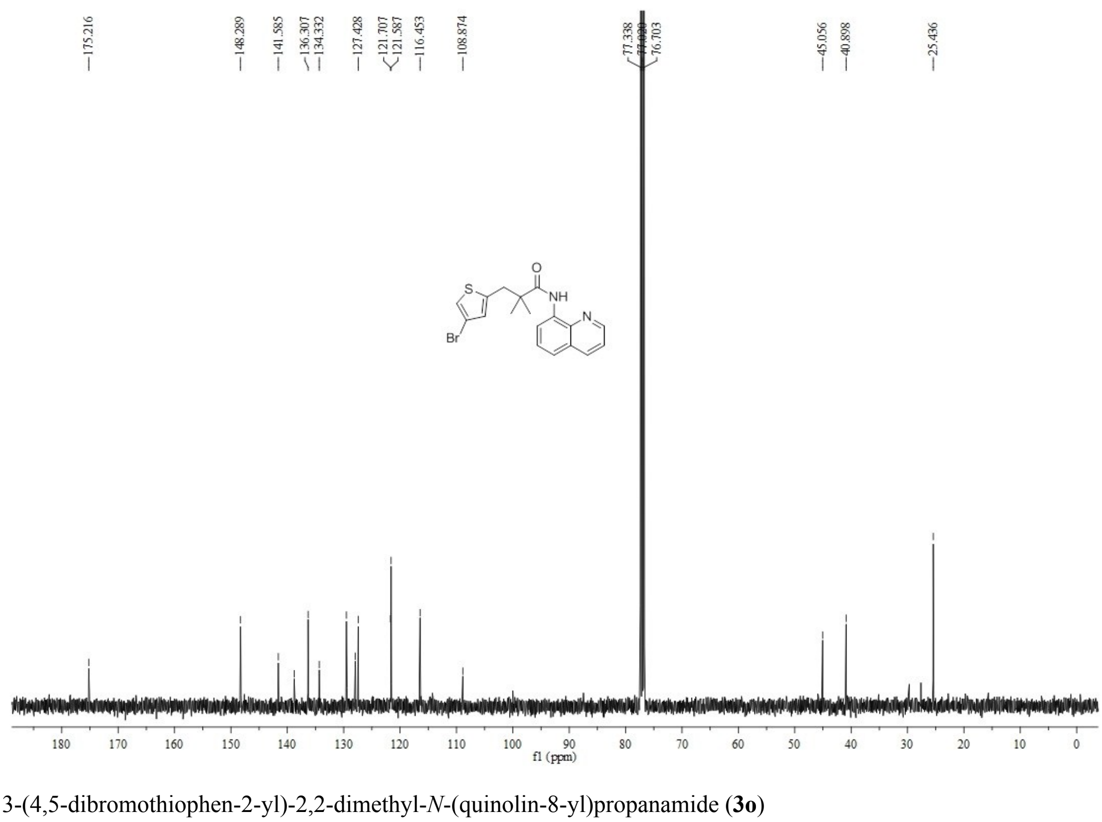




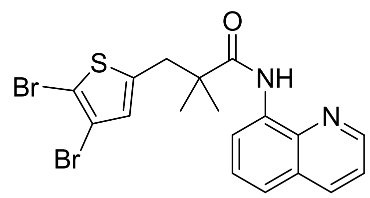
3-(4-bromothiophen-2-yl)-2,2-dimethyl-N-(quinolin-8-yl)propanamide (**3n**)

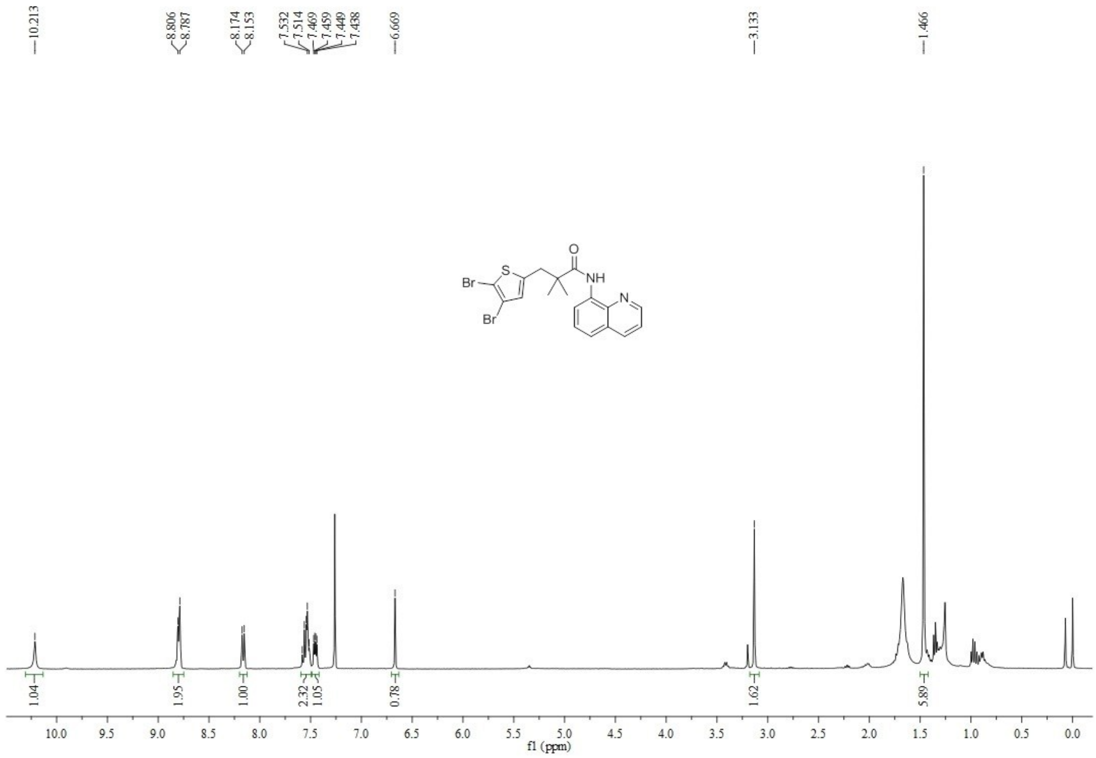


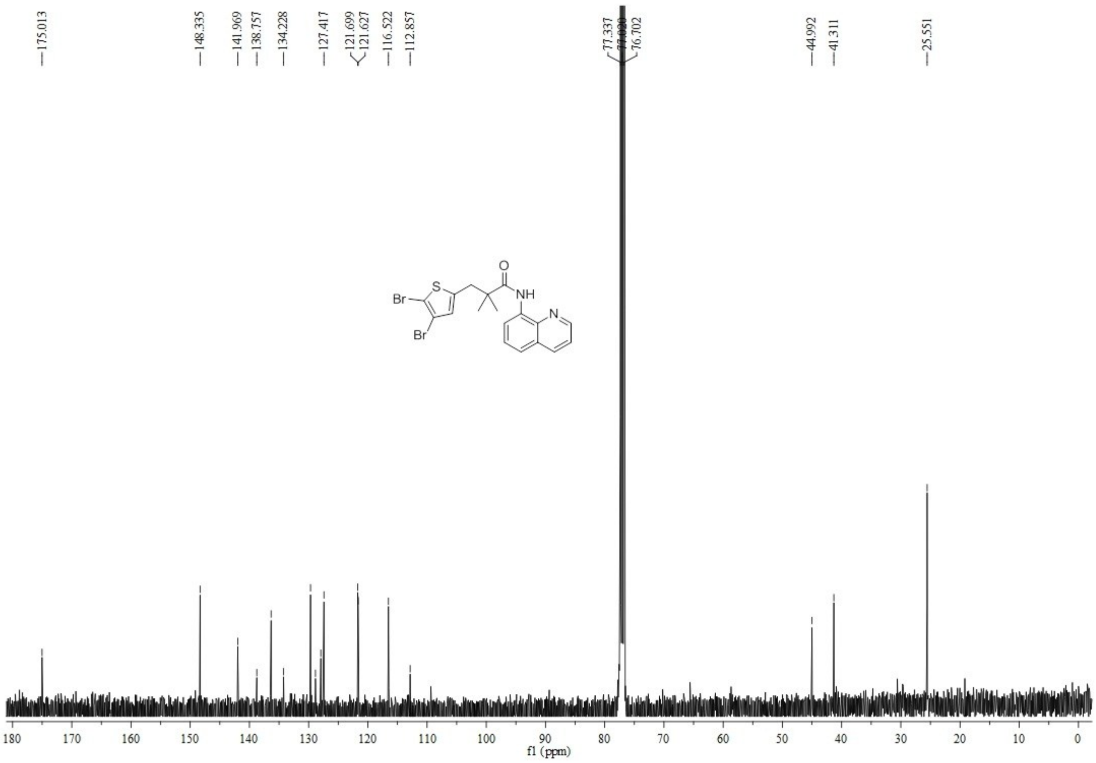




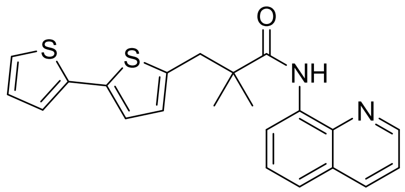
3-(4,5-dibromothiophen-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3o**)

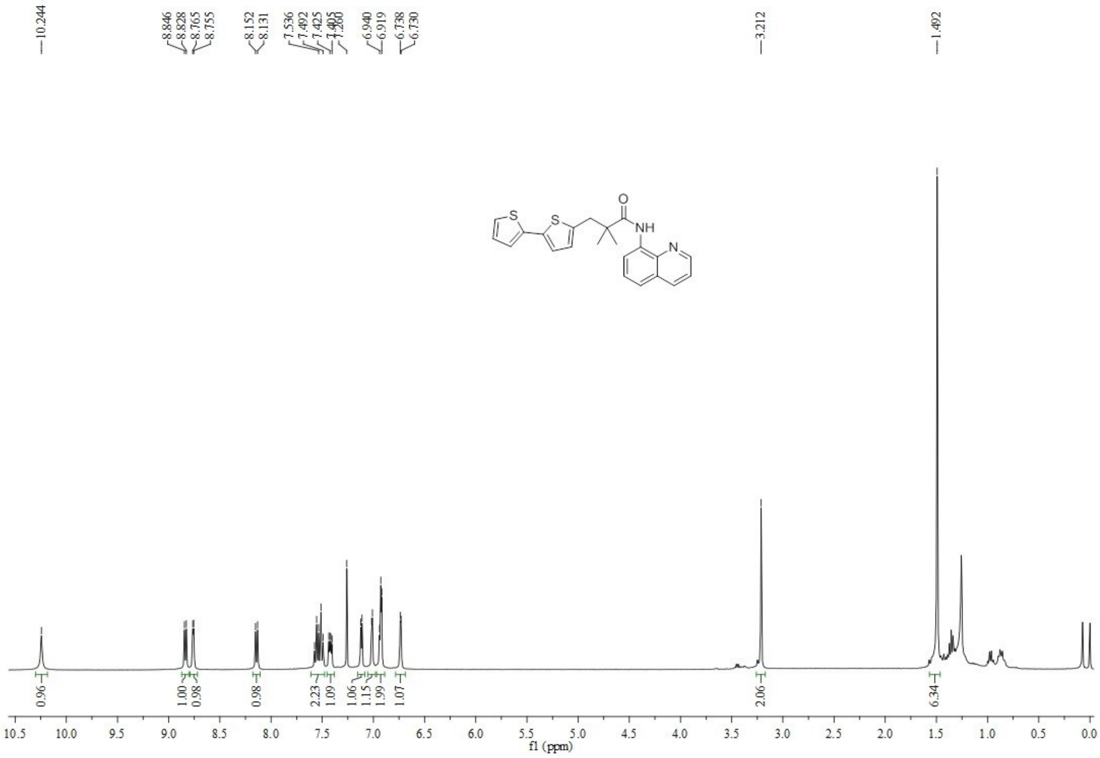


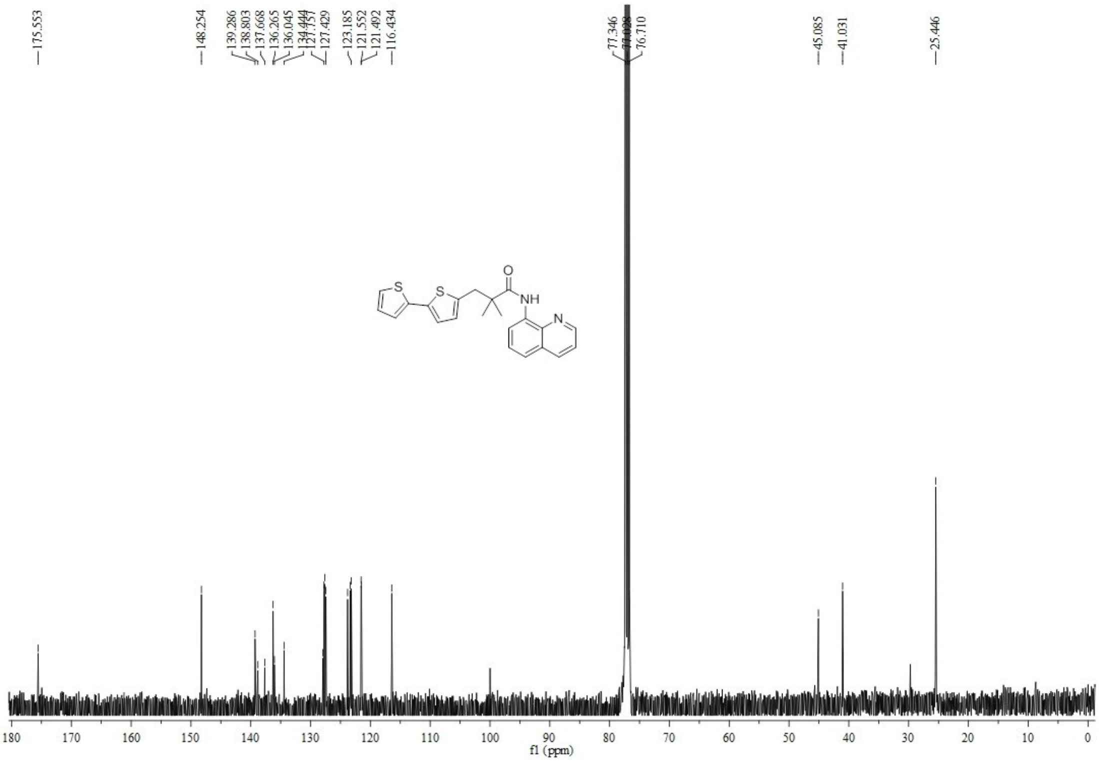




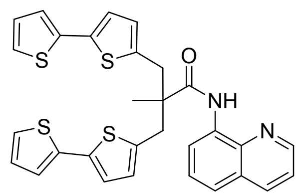
3-([2,2'-bithiophen]-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**3p**)

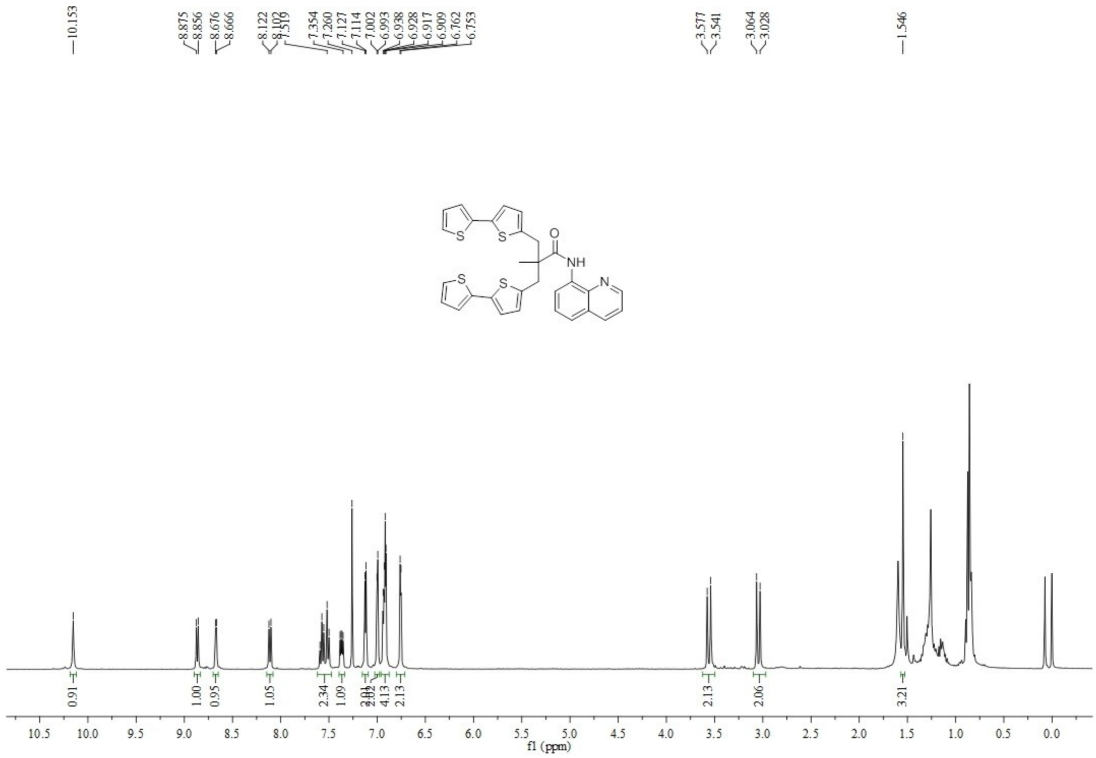


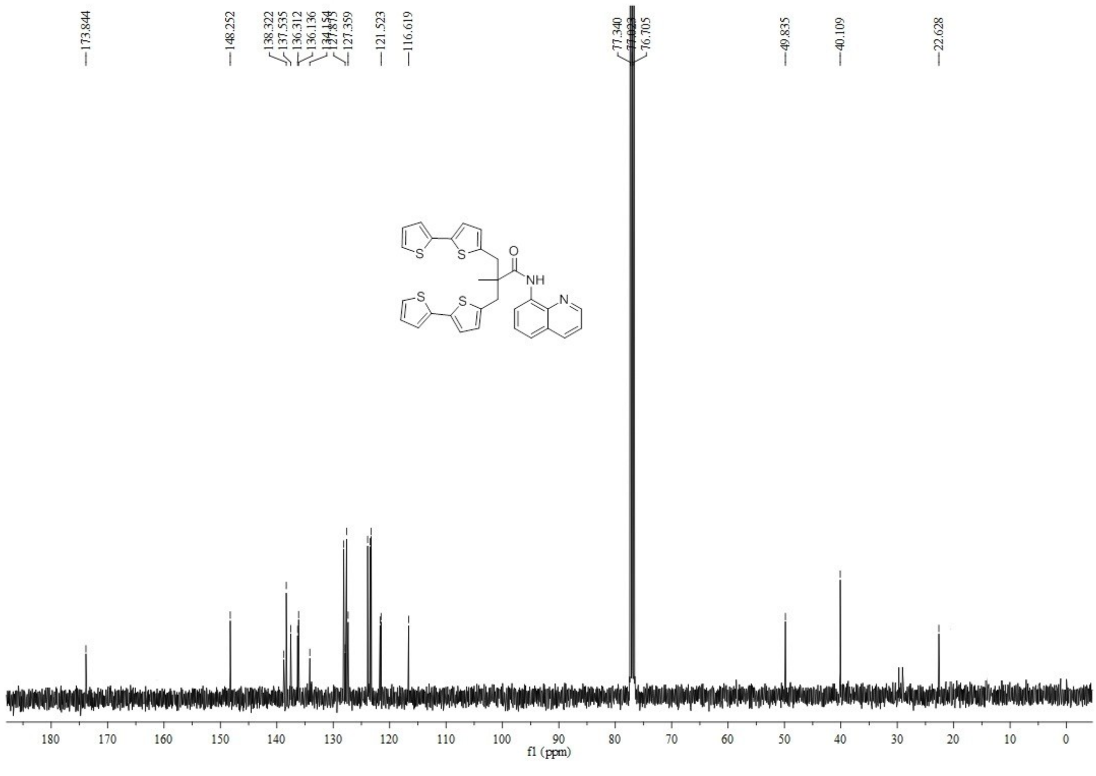




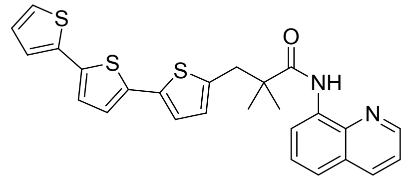
3-([2,2'-bithiophen]-5-yl)-2-([2,2'-bithiophen]-5-ylmethyl)-2-methyl-*N*-(quinolin-8-yl)propanamide (**3p’**)

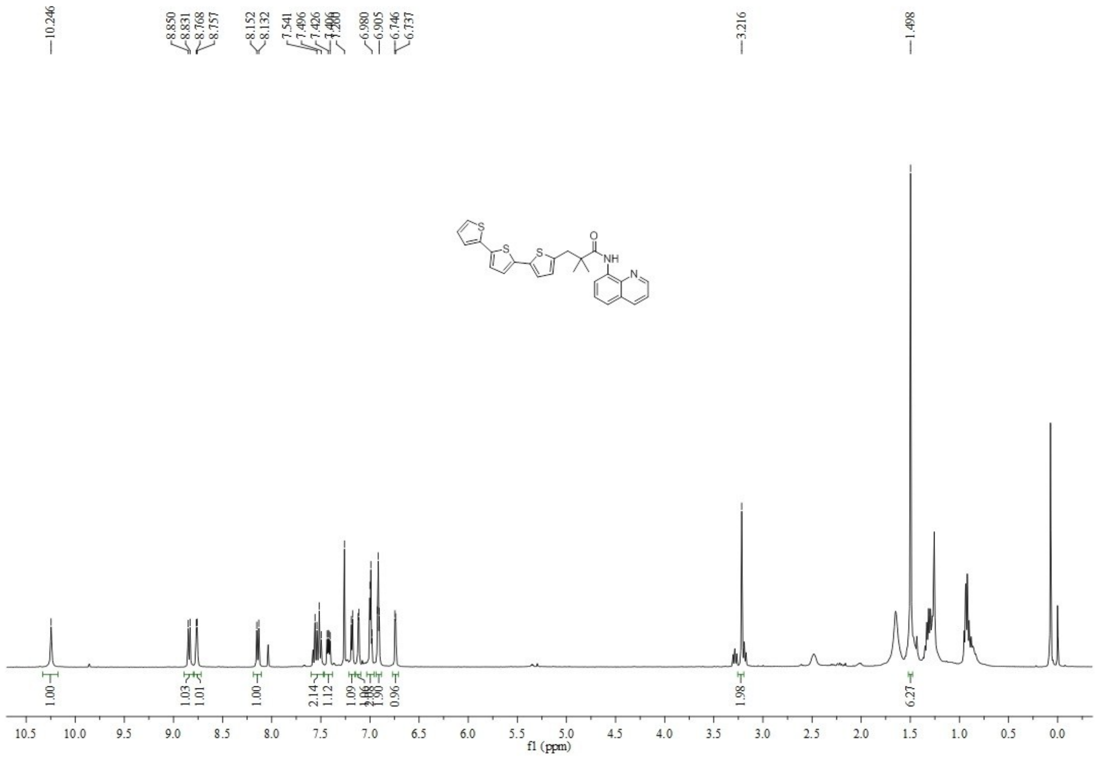


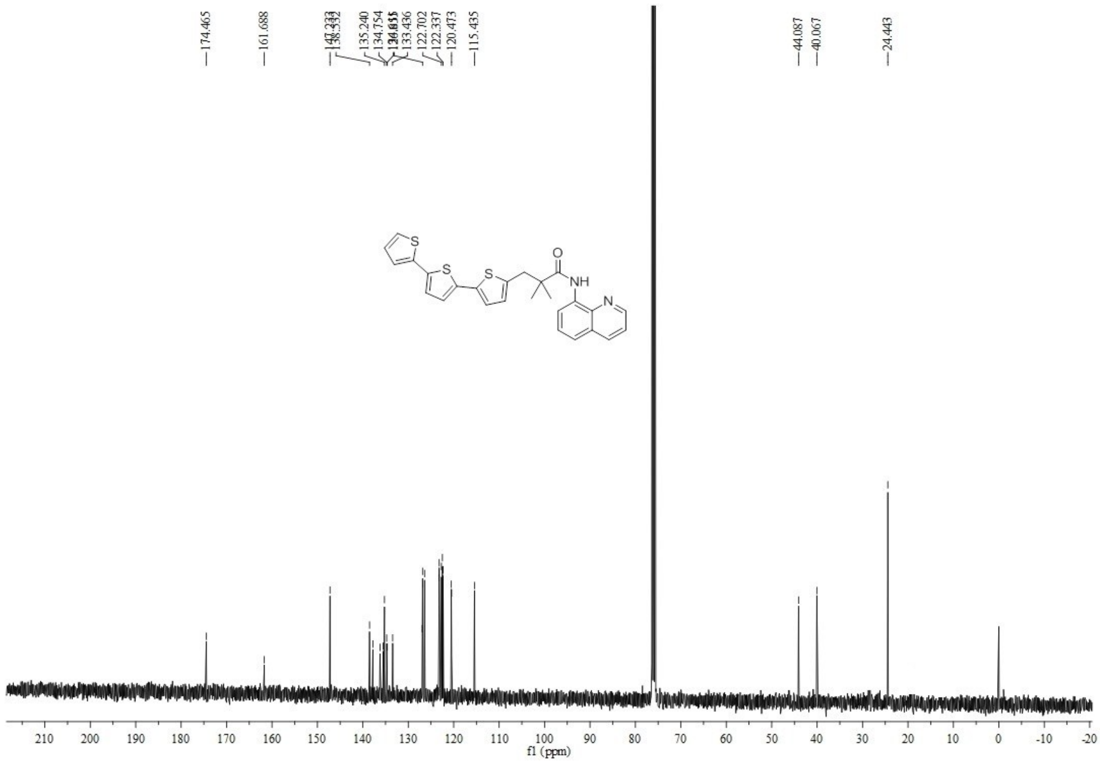




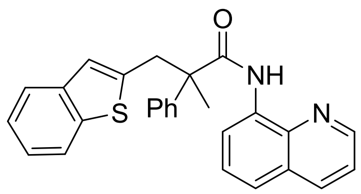
3-([2,2':5',2''-terthiophen]-5-yl)-2,2-dimethyl-N-(quinolin-8-yl)propanamide (**3q**)

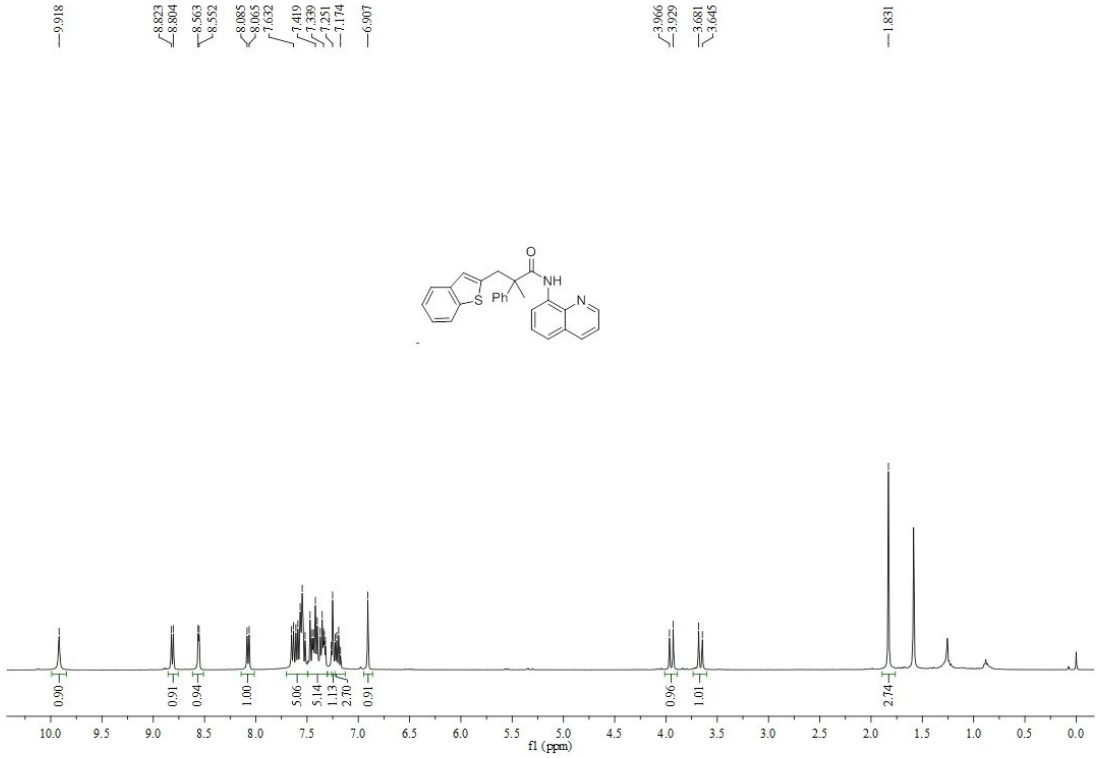


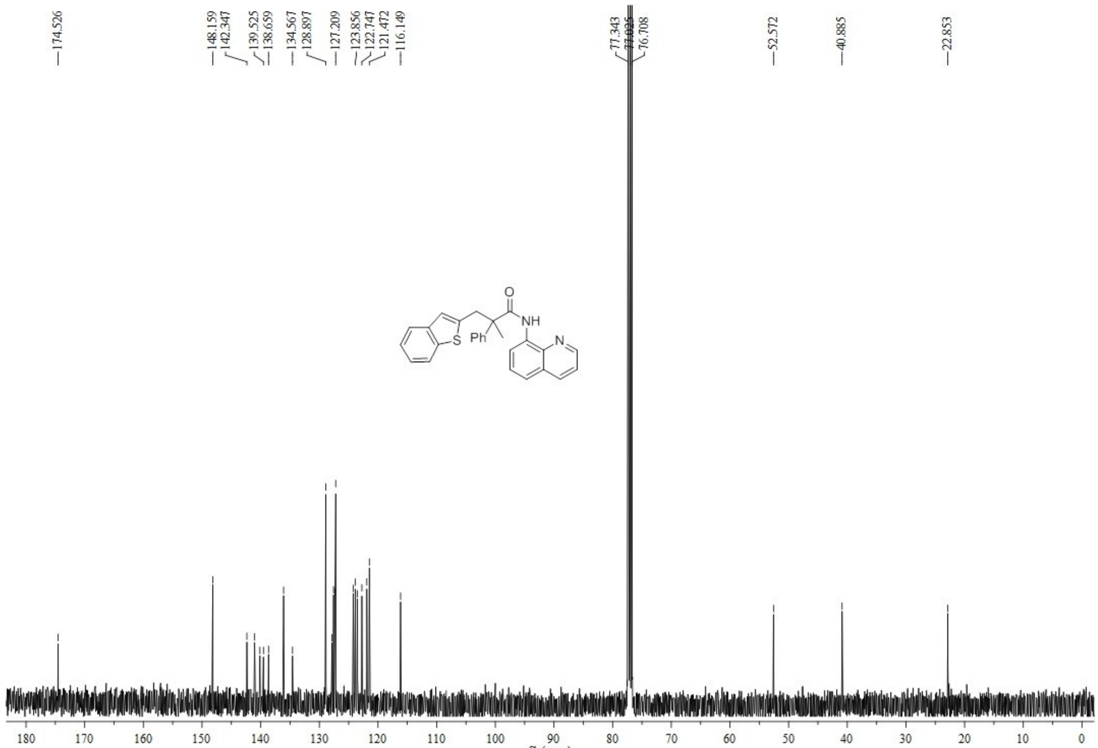




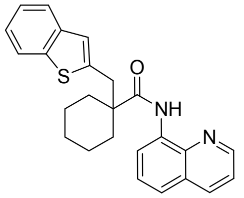
3-(benzo[b]thiophen-2-yl)-2-methyl-2-phenyl-*N*-(quinolin-8-yl)propanamide (**4a**)

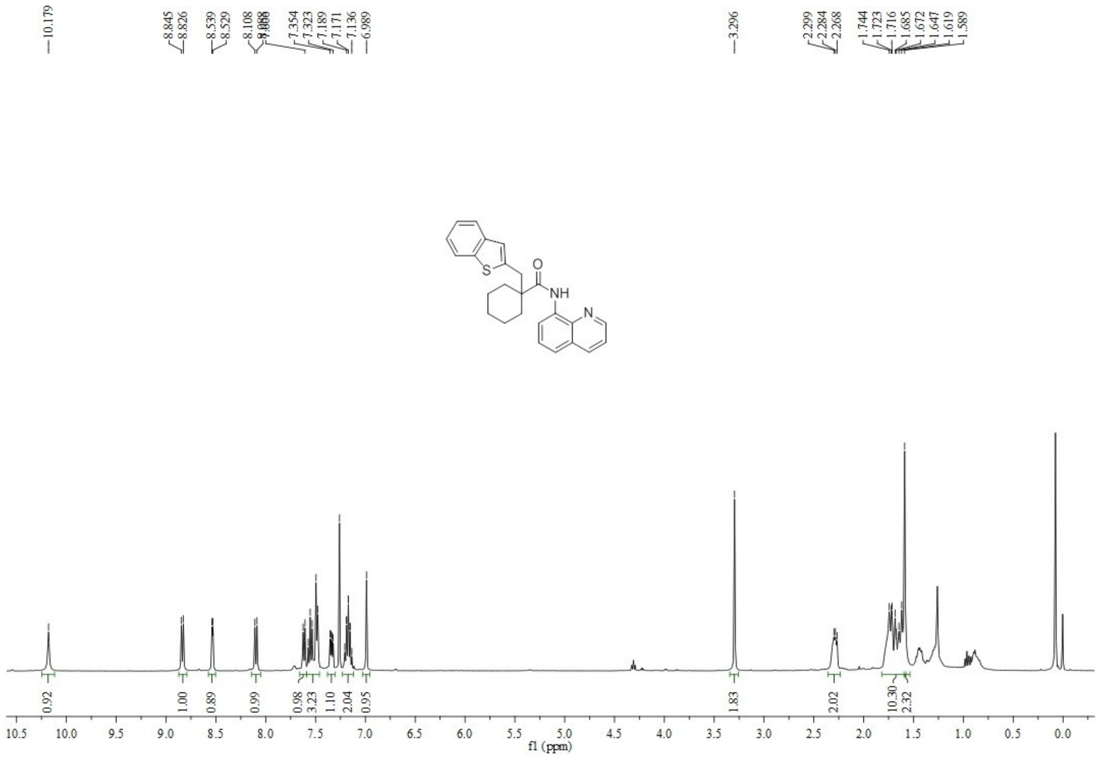


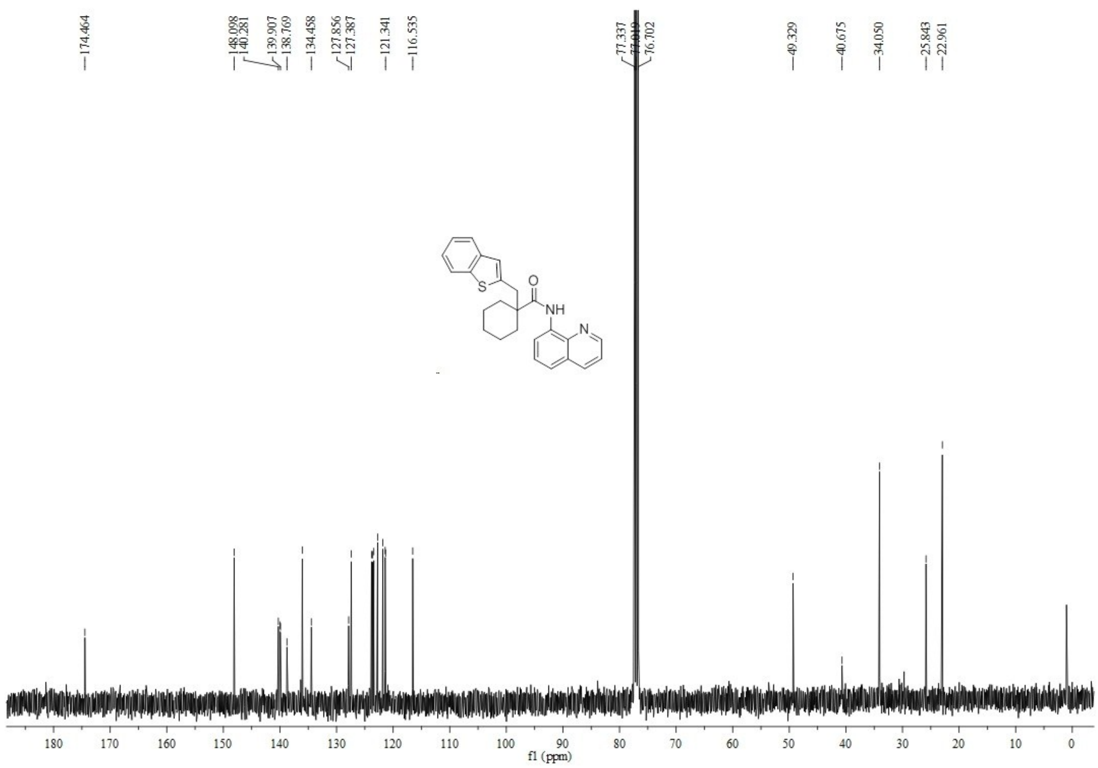




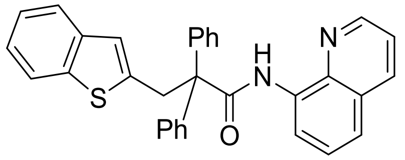
1-(benzo[b]thiophen-2-ylmethyl)-*N*-(quinolin-8-yl)cyclohexanecarboxamide (**4b**)

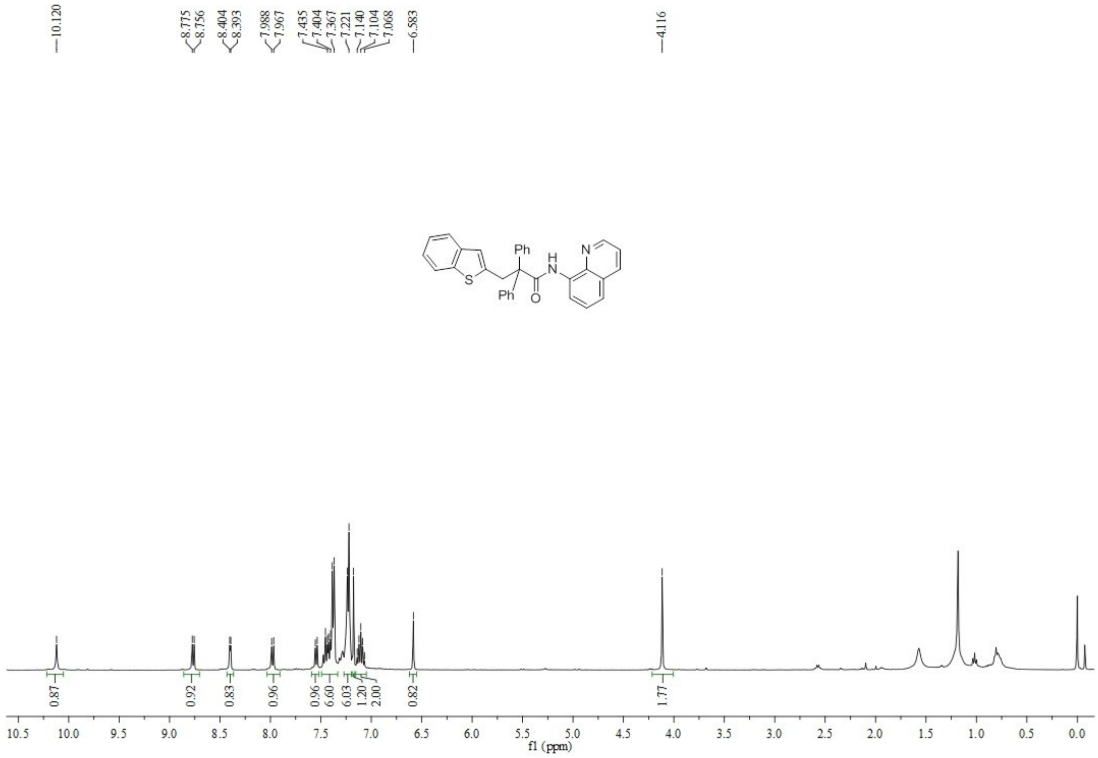


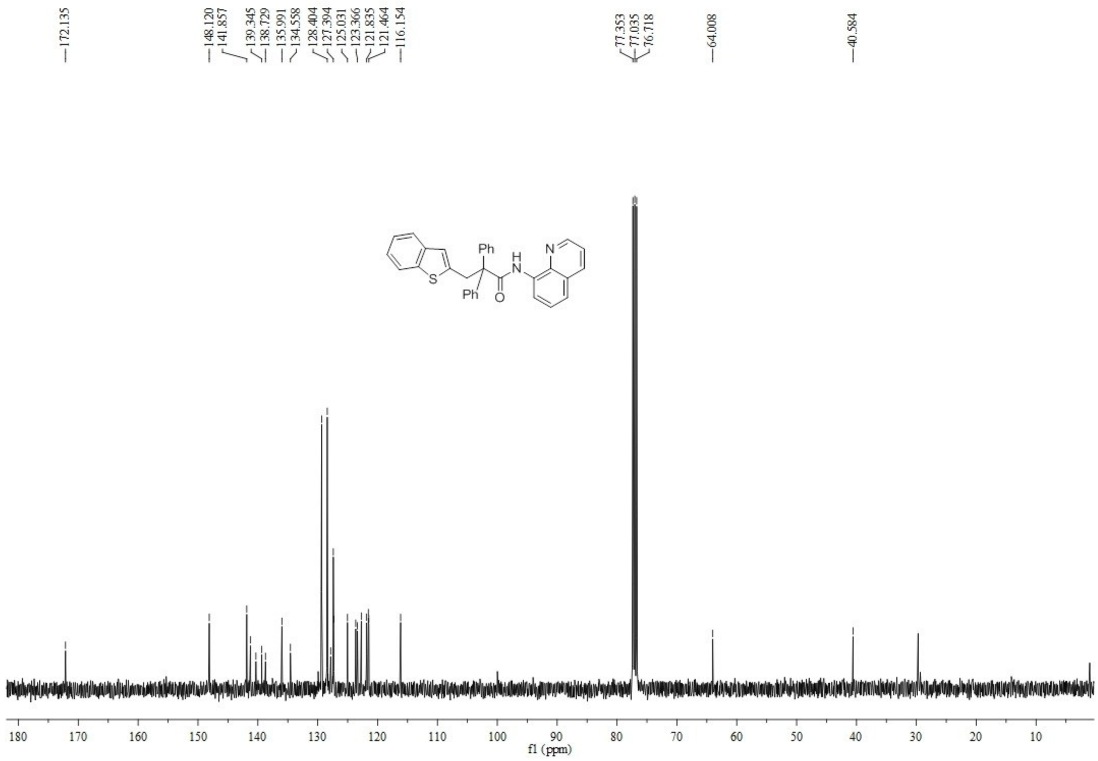




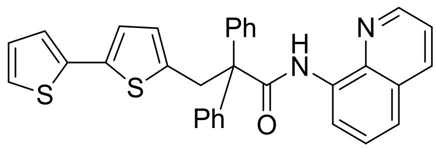
3-(benzo[b]thiophen-2-yl)-2,2-diphenyl-N-(quinolin-8-yl)propanamide (**4c**)

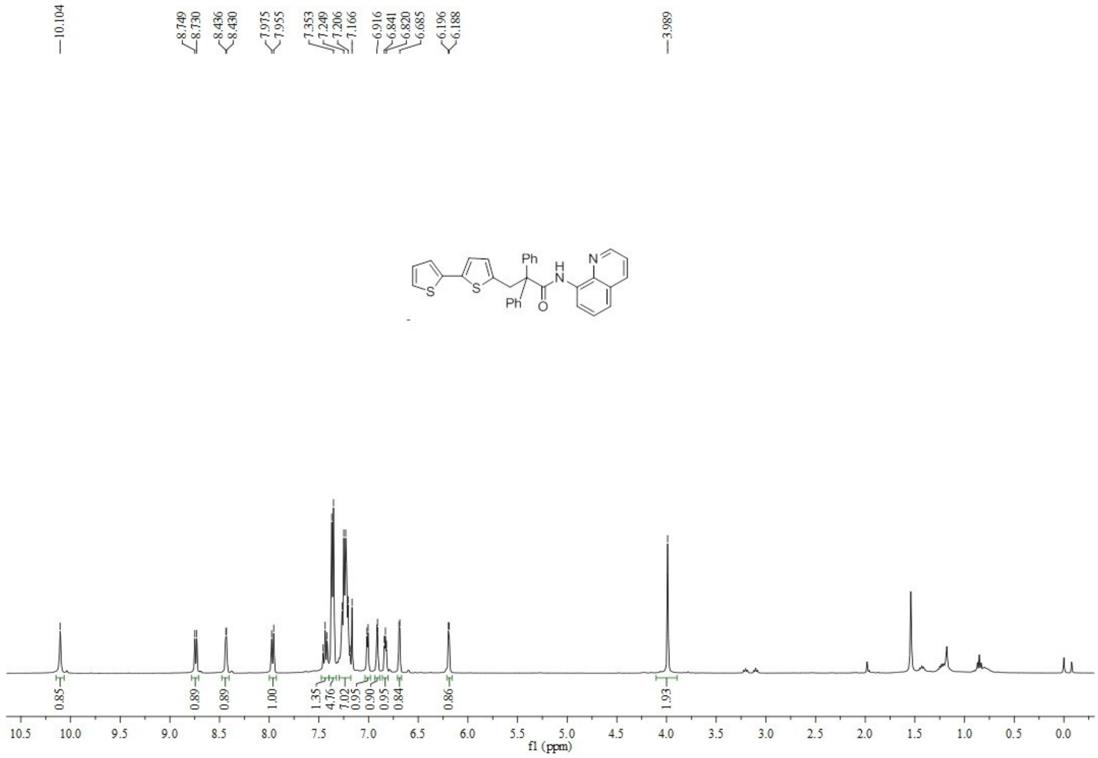


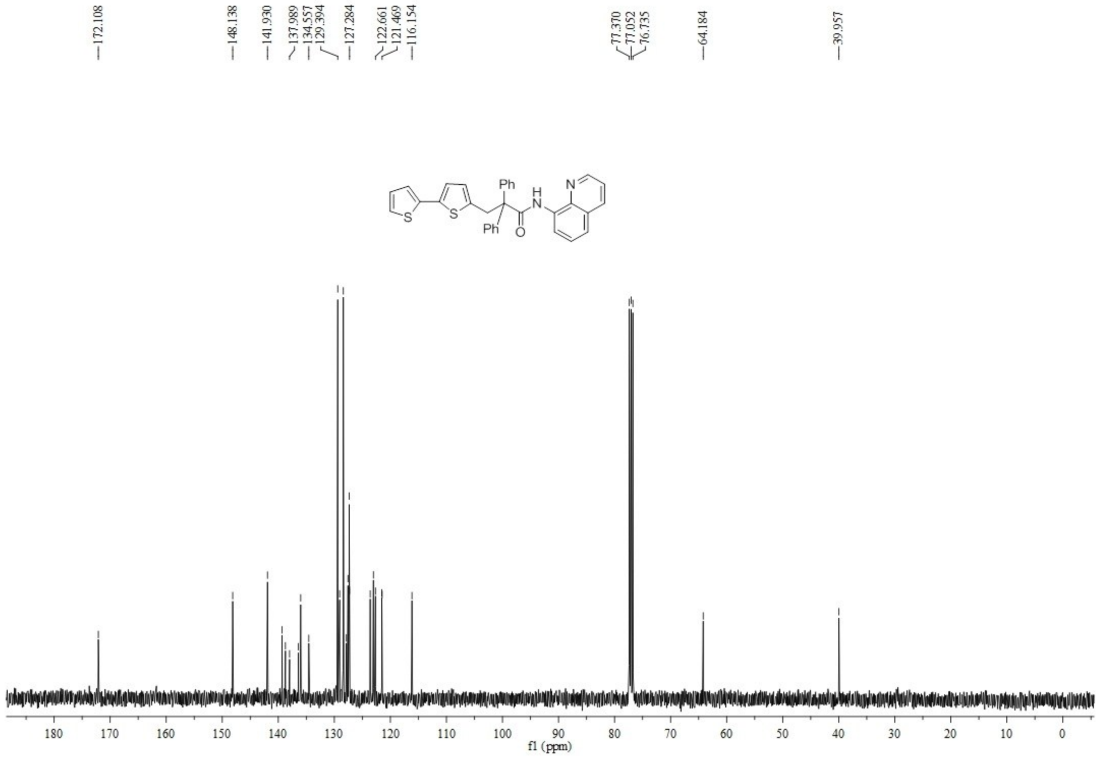




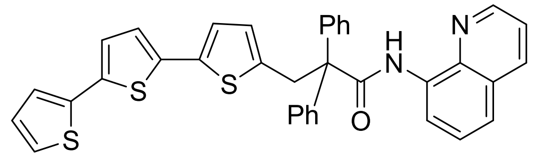
3-([2,2'-bithiophen]-5-yl)-2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (**4d**)

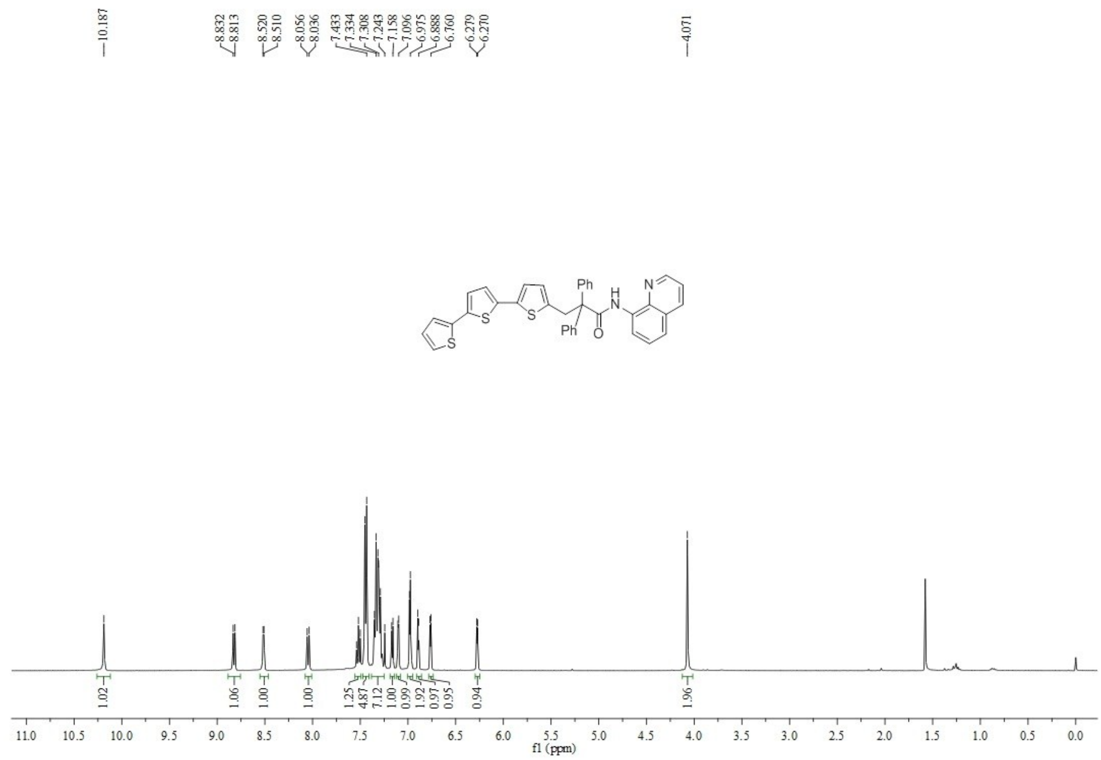


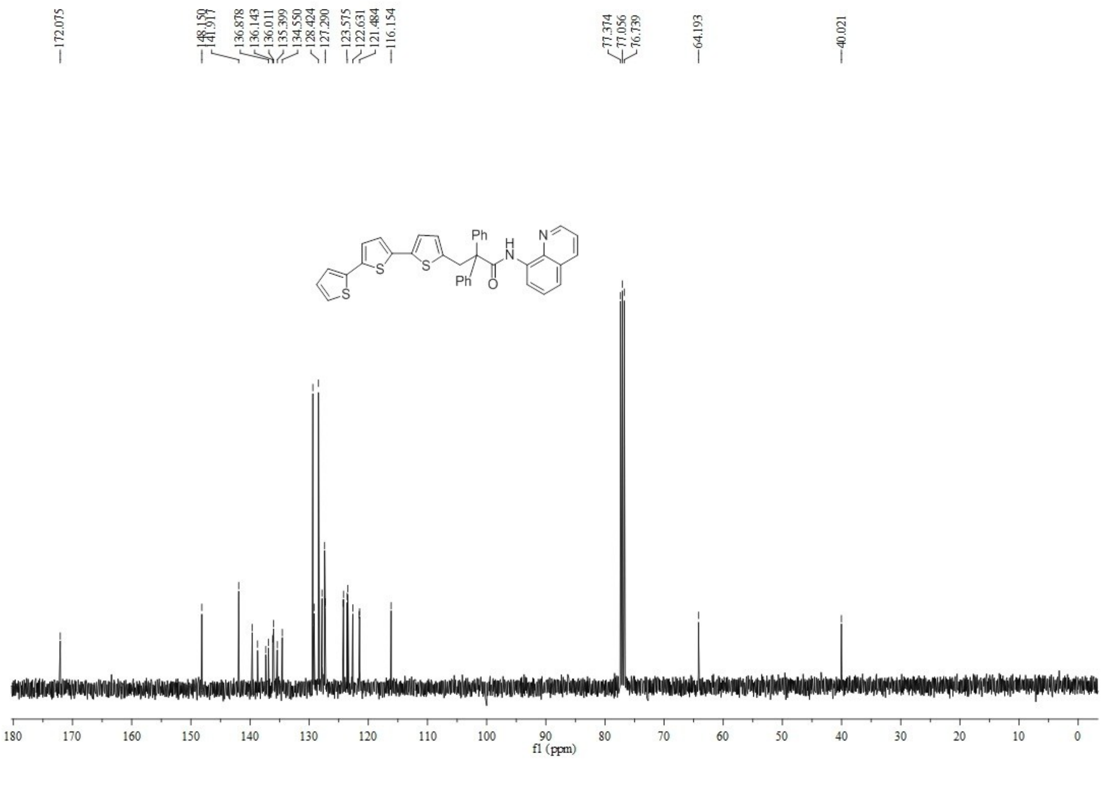




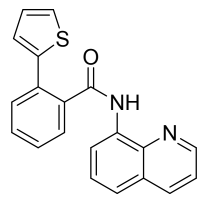
3-([2,2':5',2''-terthiophen]-5-yl)-2,2-diphenyl-*N*-(quinolin-8-yl)propanamide (**4e**)

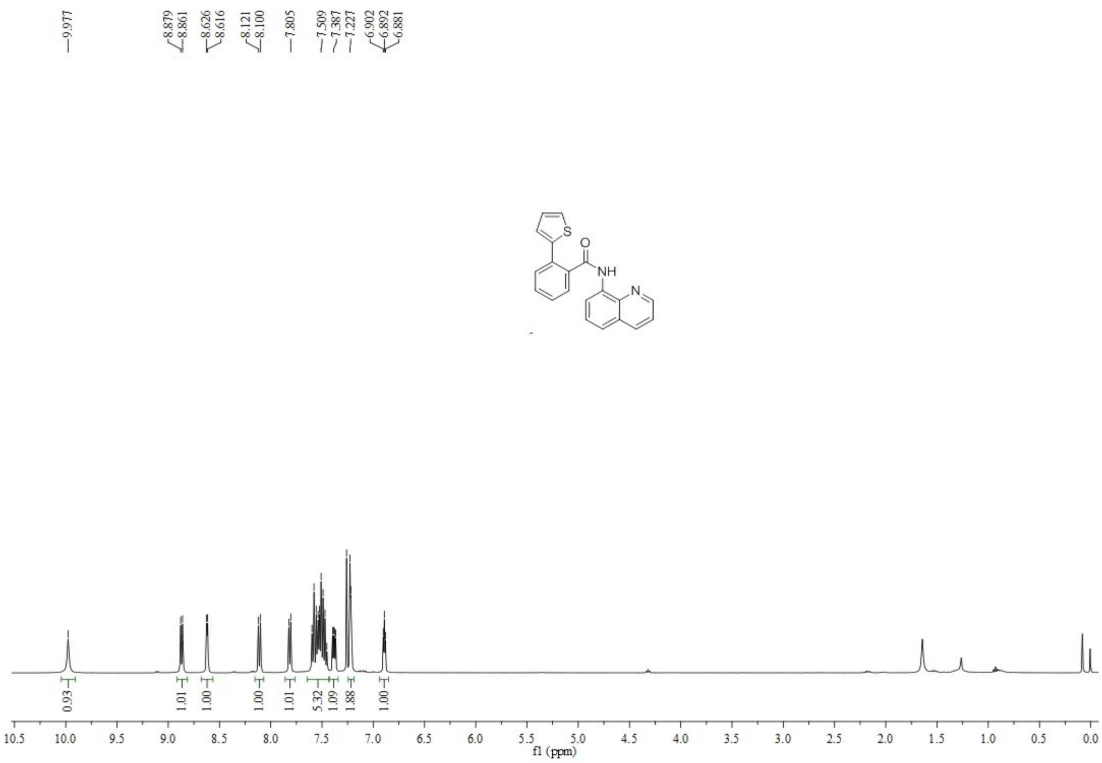


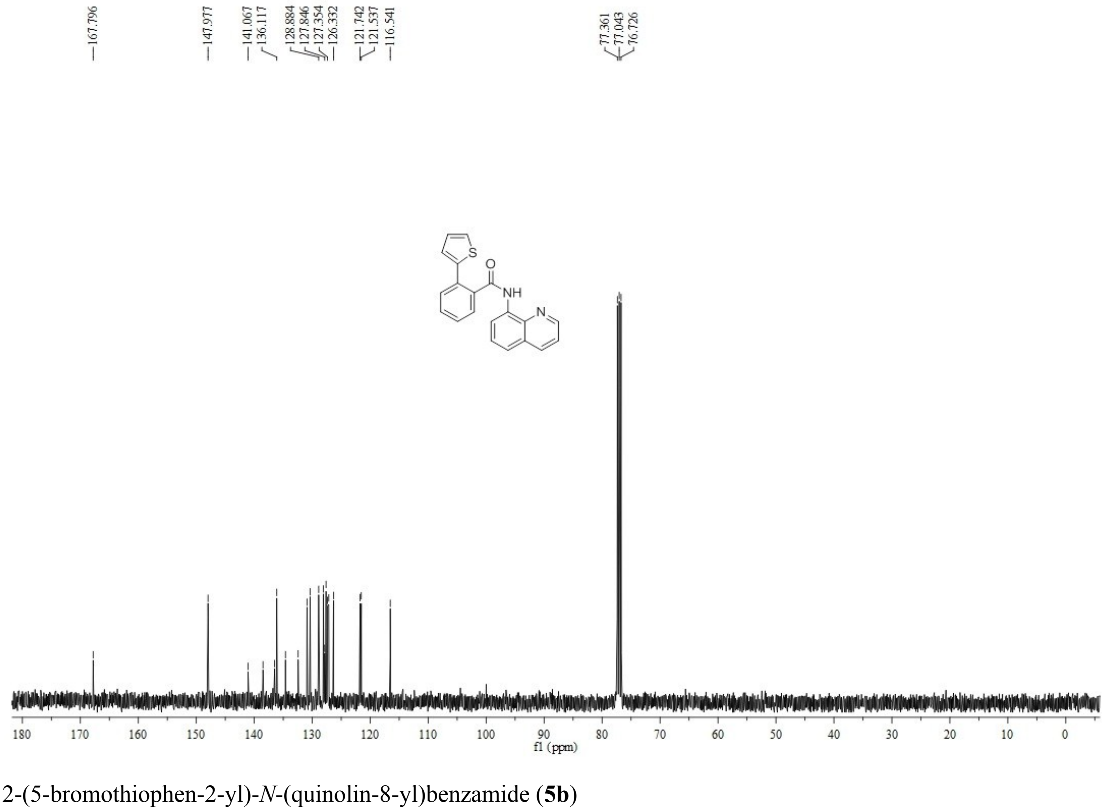




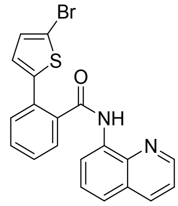
N-(quinolin-8-yl)-2-(thiophen-2-yl)benzamide (**5a**)

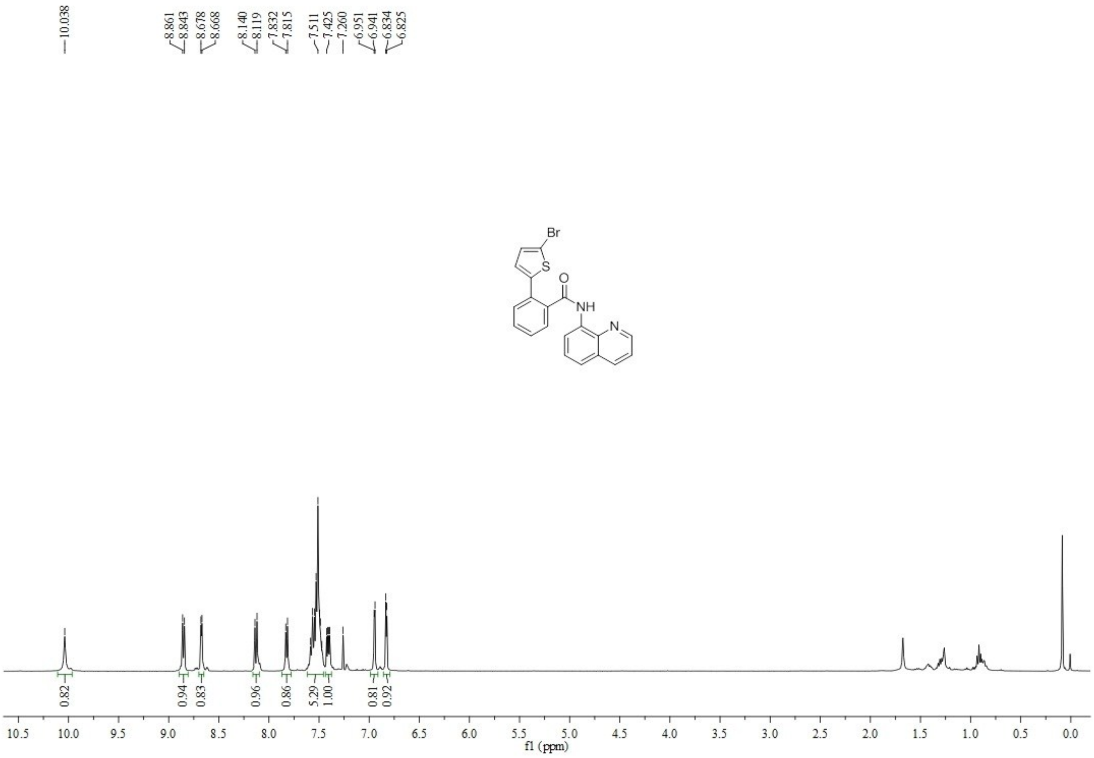


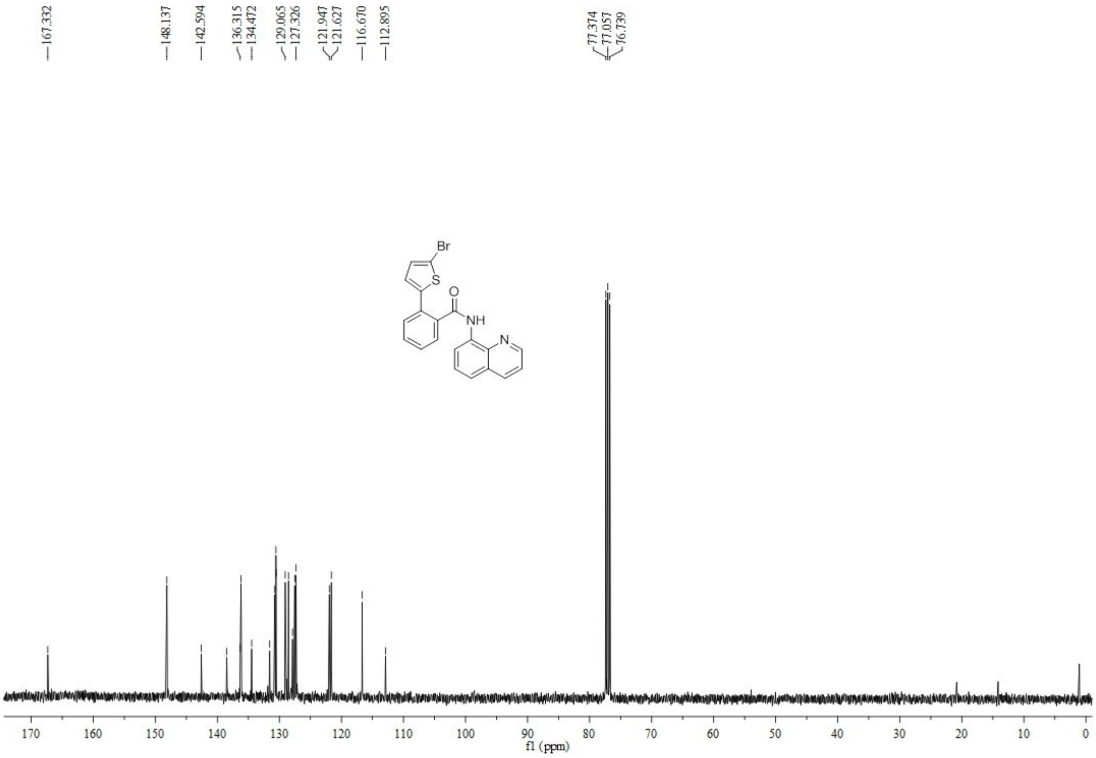




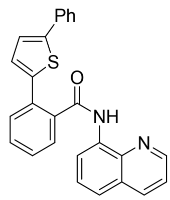
2-(5-bromothiophen-2-yl)-*N*-(quinolin-8-yl)benzamide (**5b**)

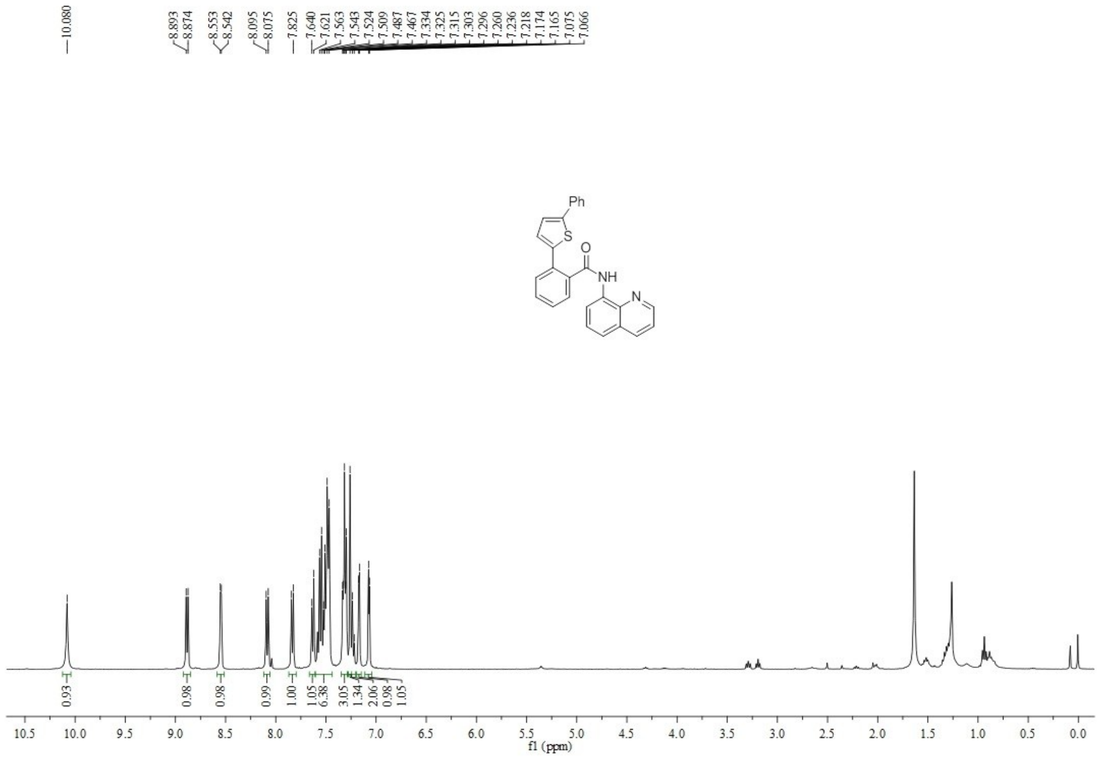


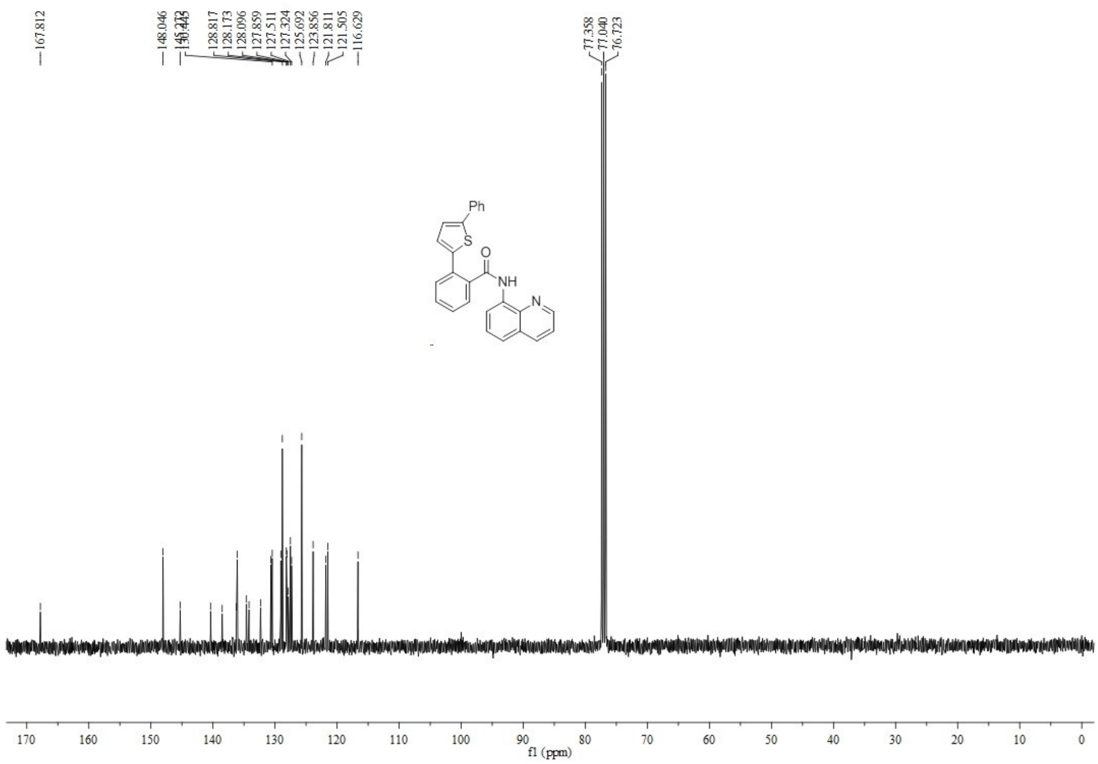




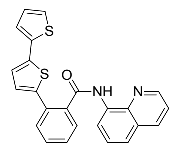
2-(5-phenylthiophen-2-yl)-N-(quinolin-8-yl)benzamide (**5c**)

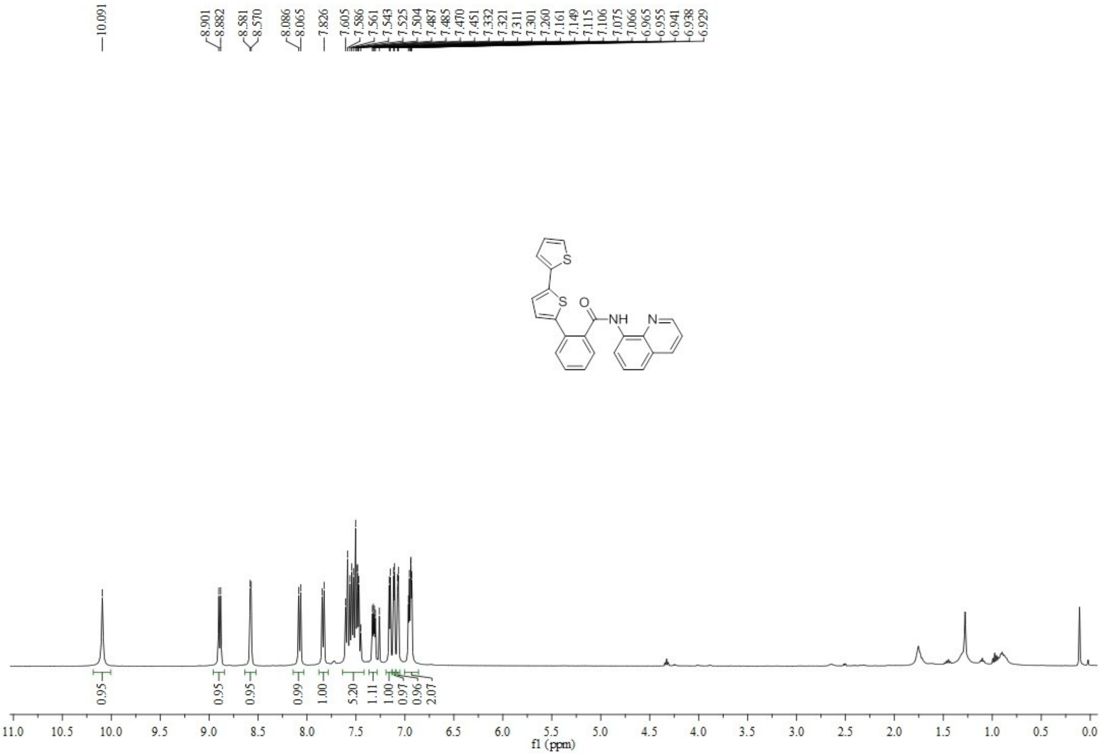


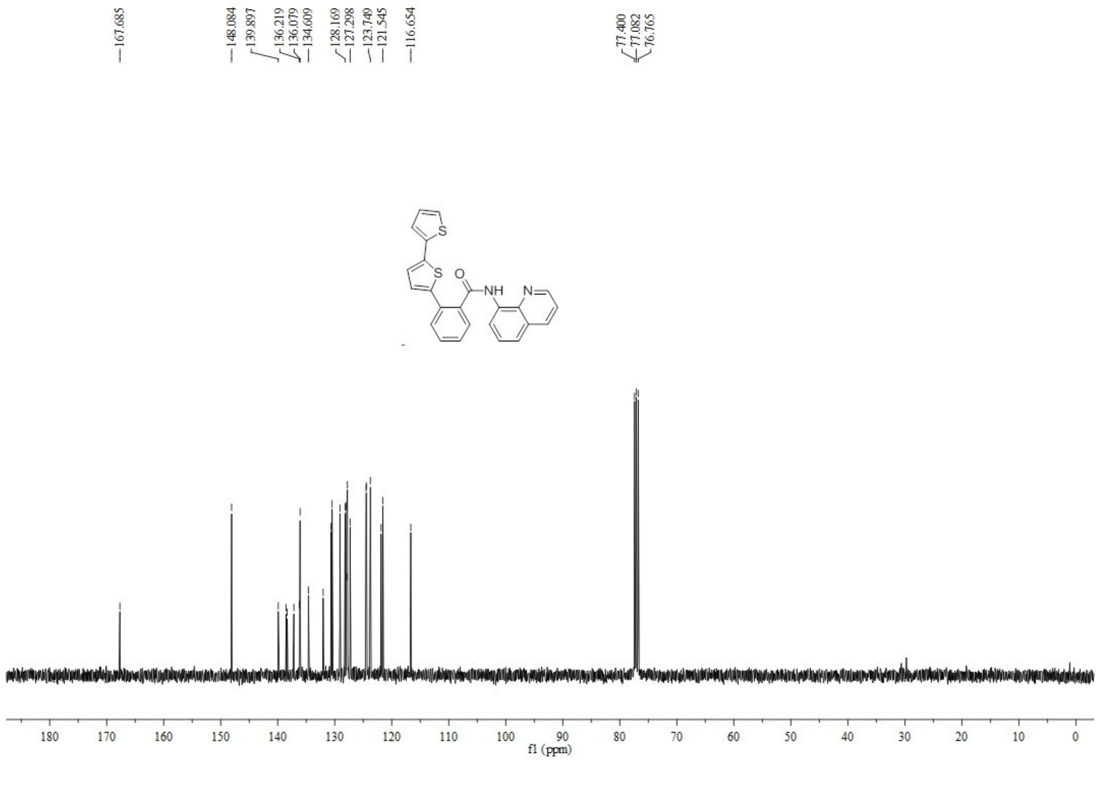




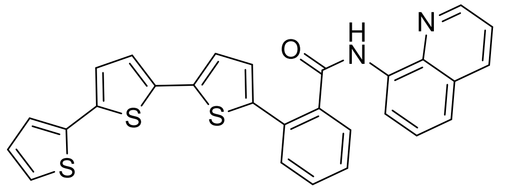
2-([2,2'-bithiophen]-5-yl)-*N*-(quinolin-8-yl)benzamide (**5d**)

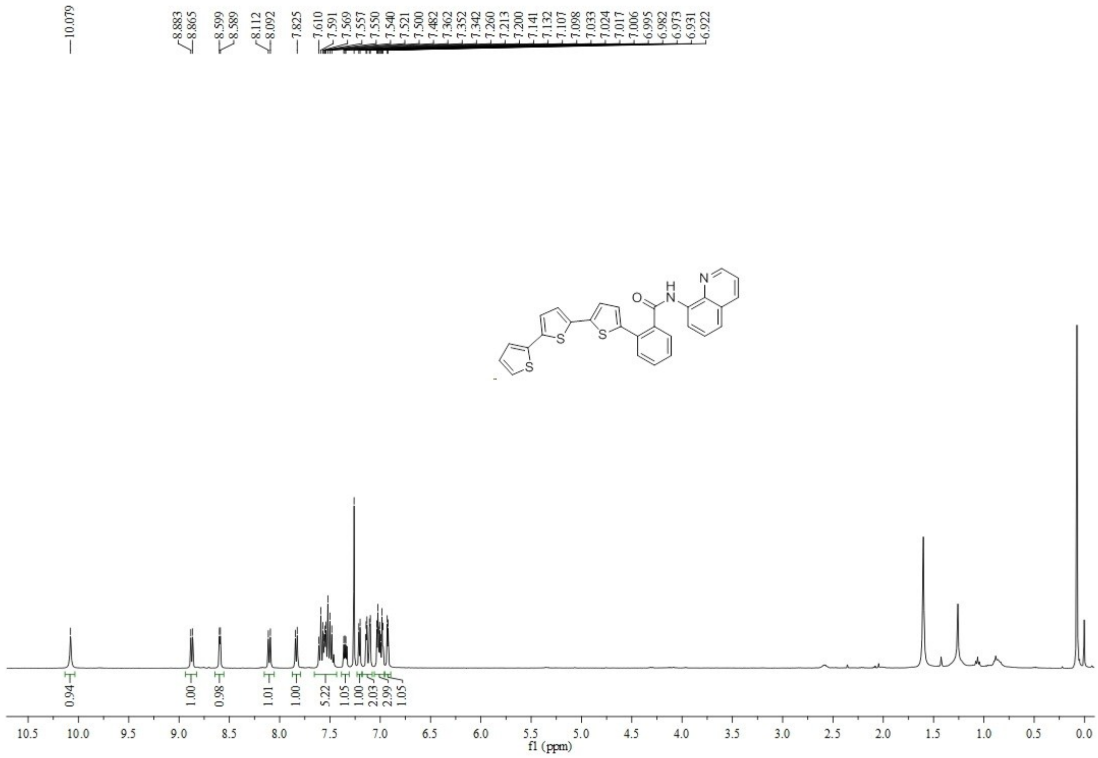


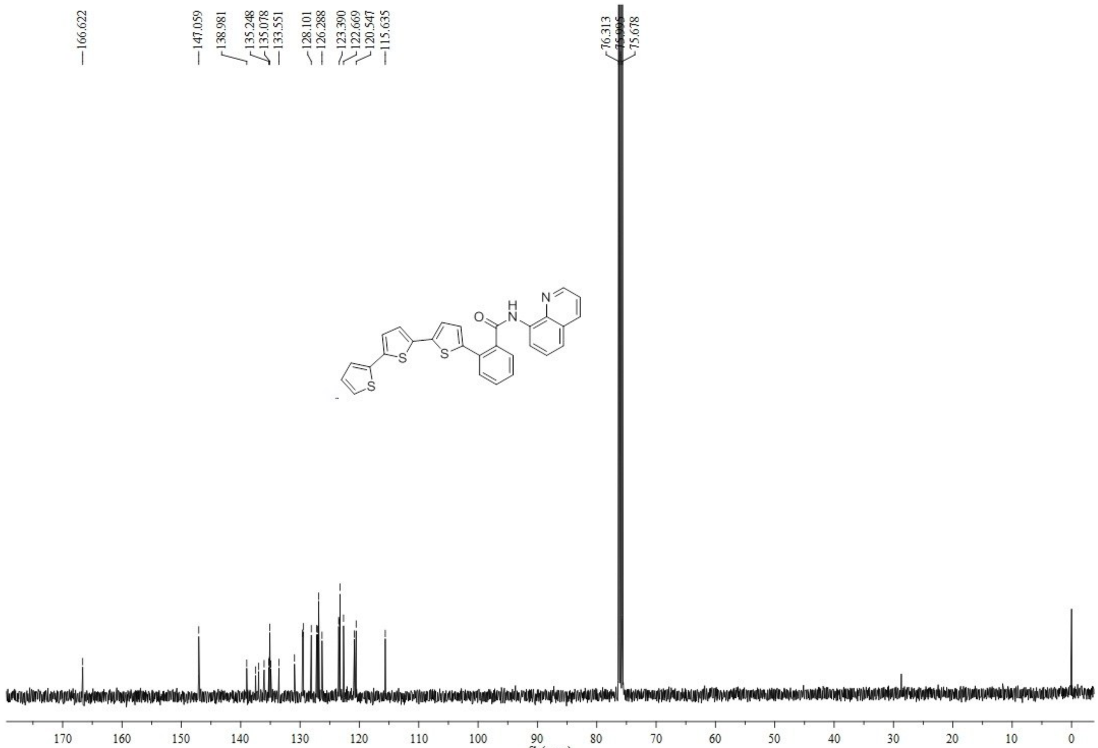




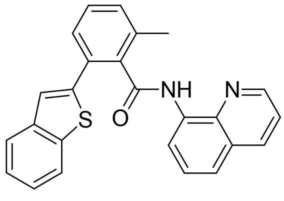
2-([2,2':5',2''-terthiophen]-5-yl)-*N*-(quinolin-8-yl)benzamide (**5e**)

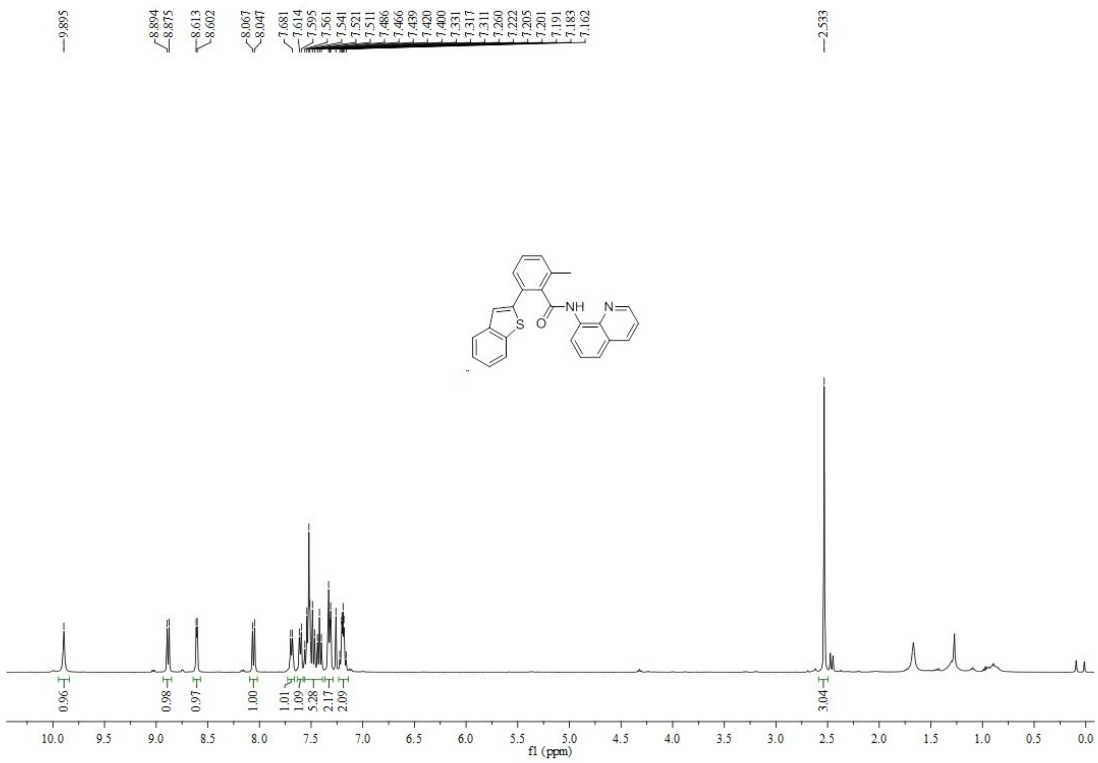


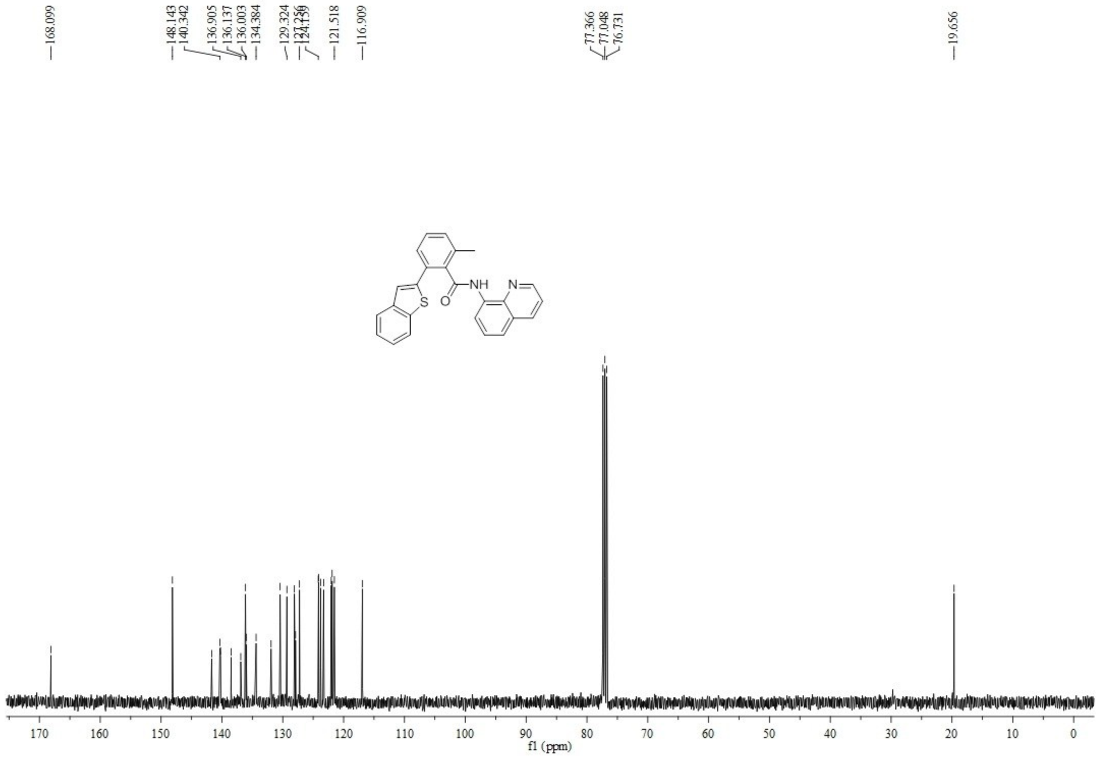




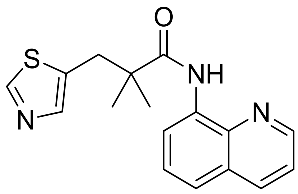
2-(benzo[b]thiophen-2-yl)-6-methyl-*N*-(quinolin-8-yl)benzamide (**5f**)

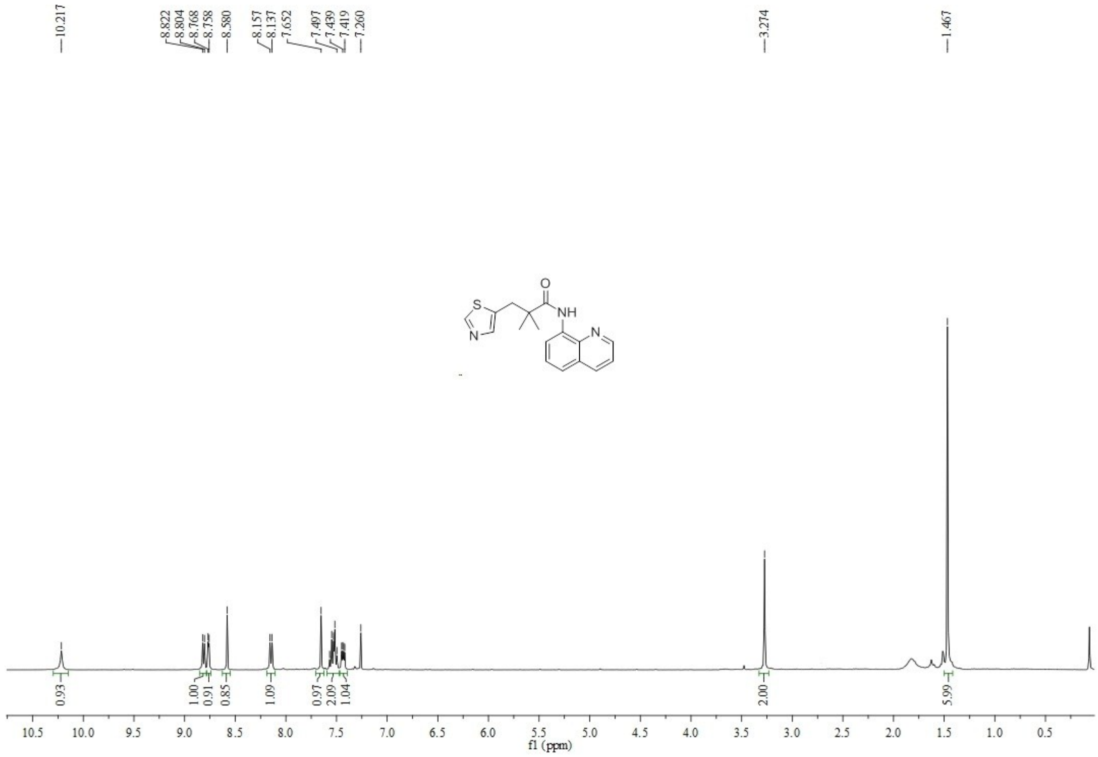






2,2-dimethyl-*N*-(quinolin-8-yl)-3-(thiazol-5-yl)propanamide (**6a**)

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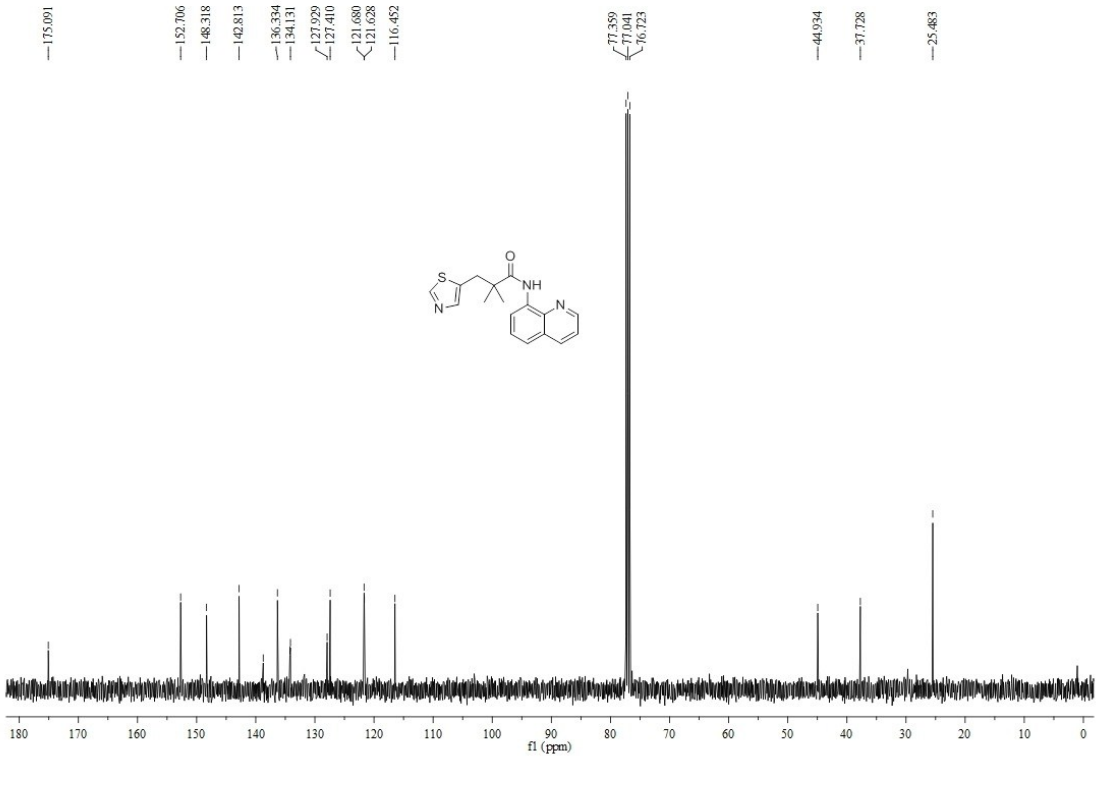
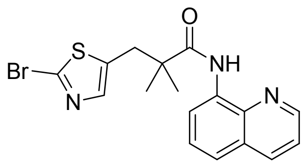
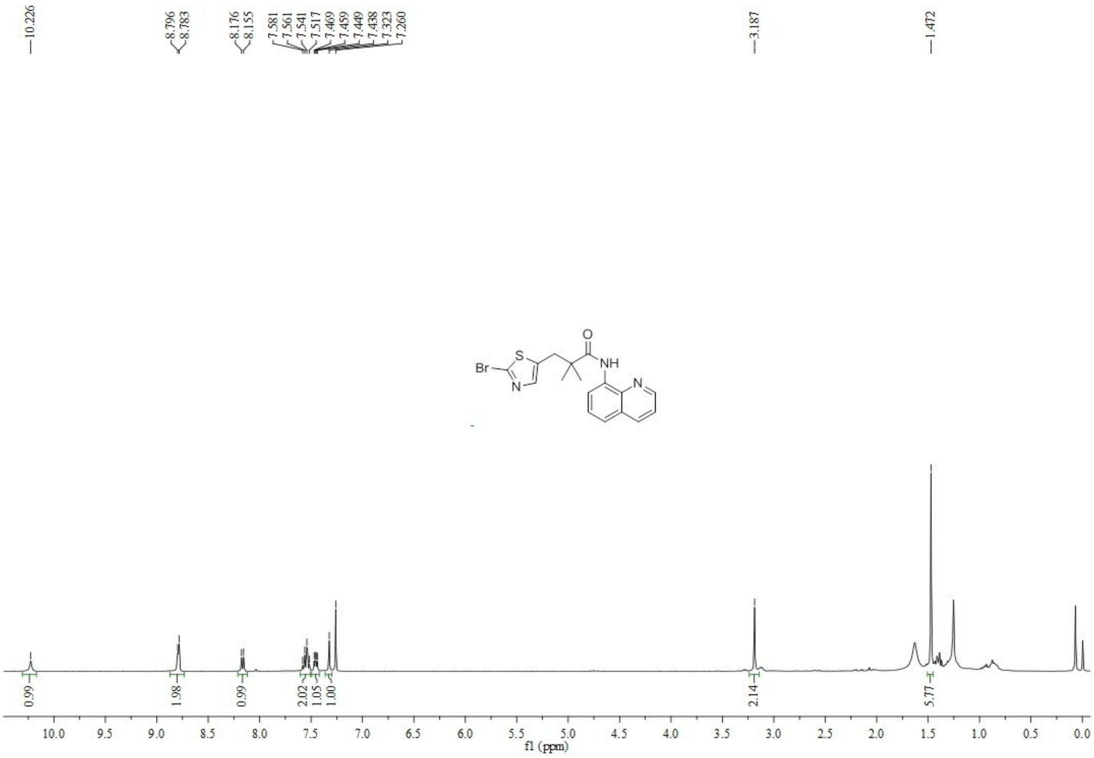
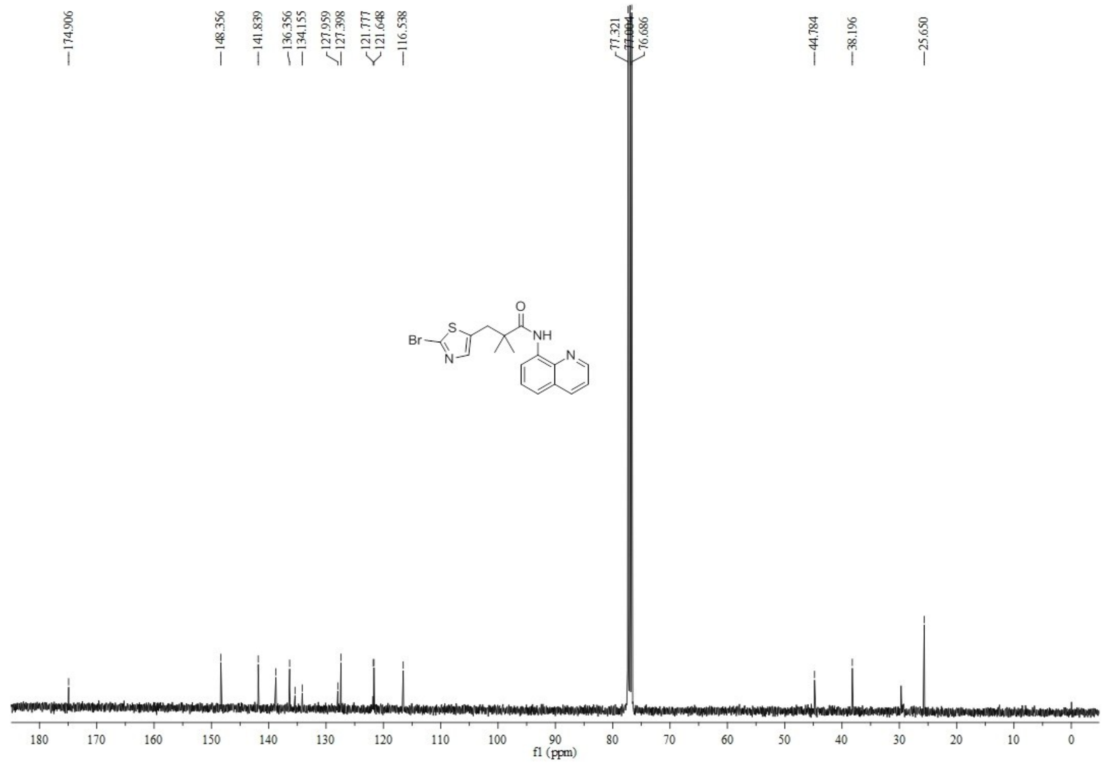
8.822
8.804
8.768
8.758
8.580
8.157
8.137
7.652
7.497
7.439
7.419
7.260
3.274
1.467
0.93
1.00
0.91
0.85
1.09
0.97
2.09
1.04
2.00
5.99
f1 (ppm)


175.091
152.706
148.318
142.813
136.334
134.131
127.929
127.410
121.680
121.628
116.452
77.359
77.041
76.723
44.934
37.728
25.483
f1 (ppm)

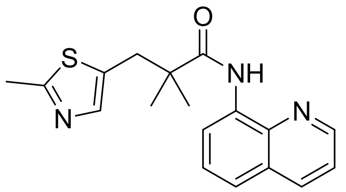
3-(2-bromothiazol-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6b**)

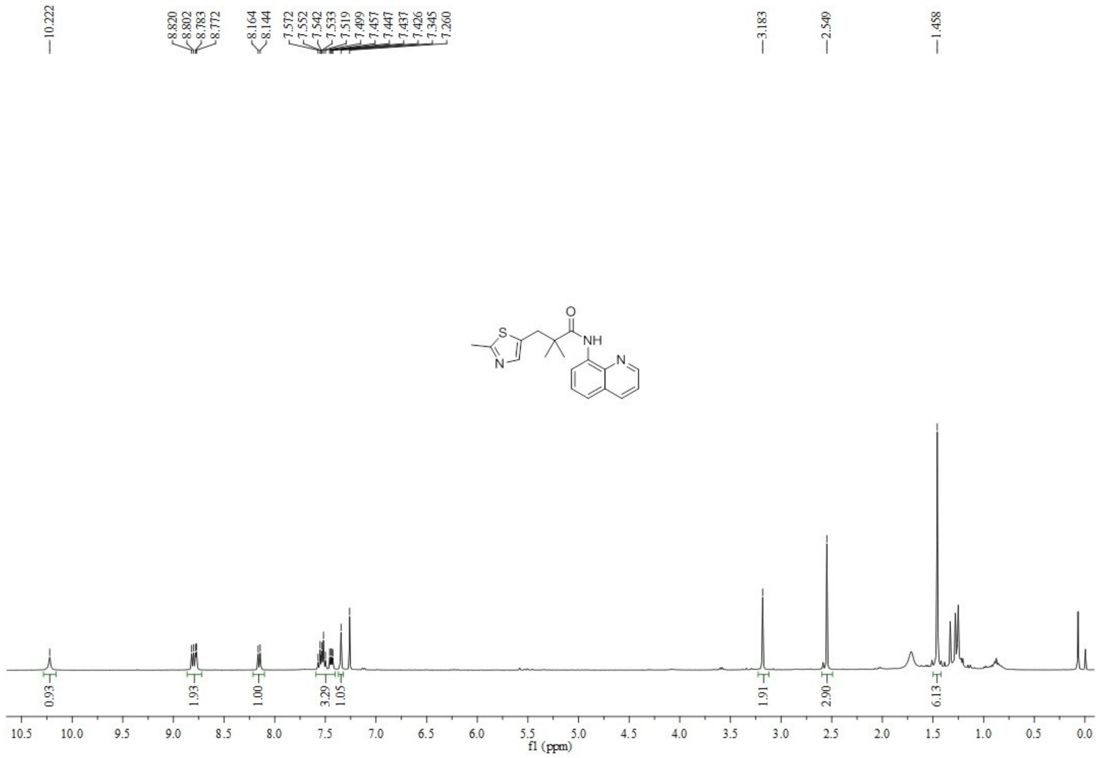


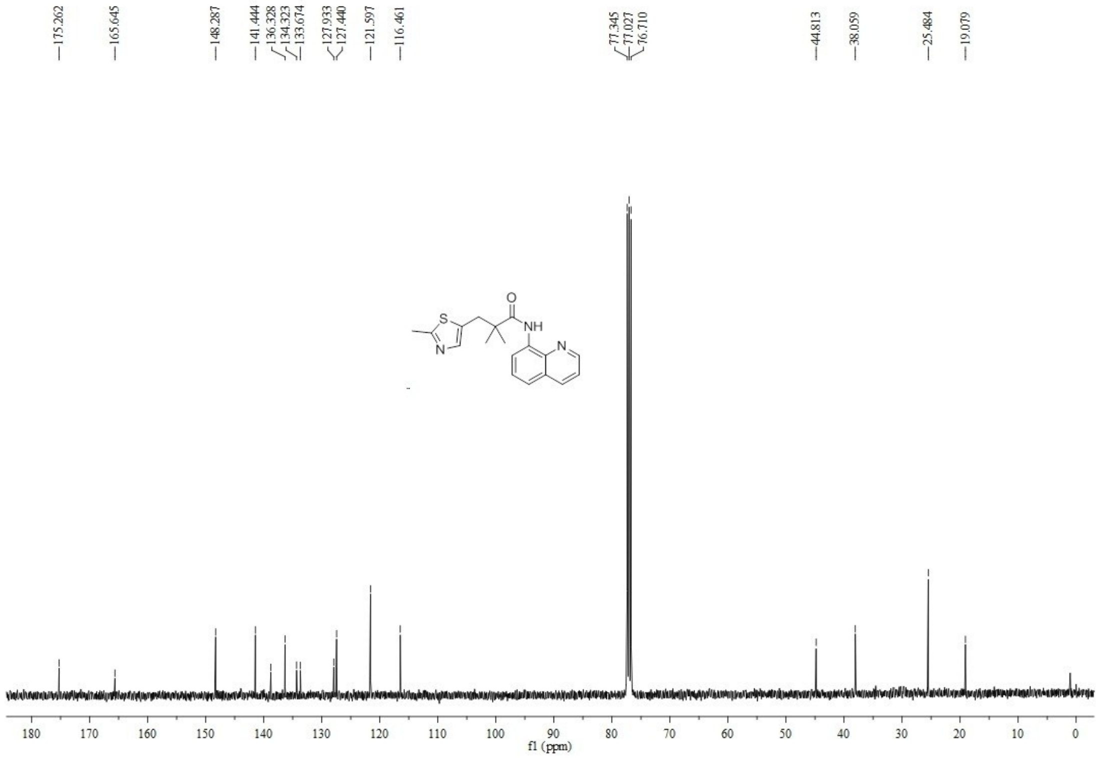




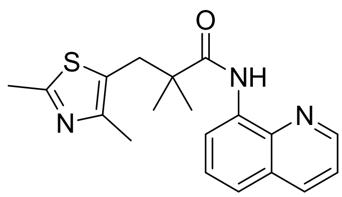
2,2-dimethyl-3-(2-methylthiazol-5-yl)-*N*-(quinolin-8-yl)propanamide (**6c**)

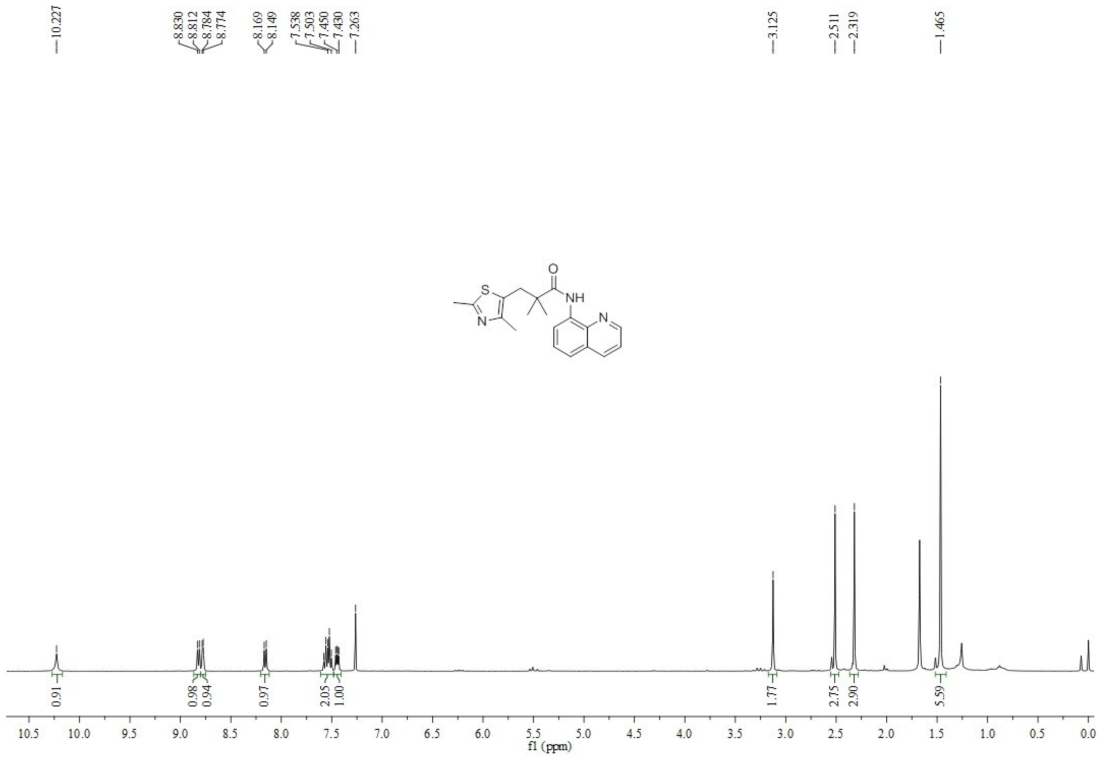


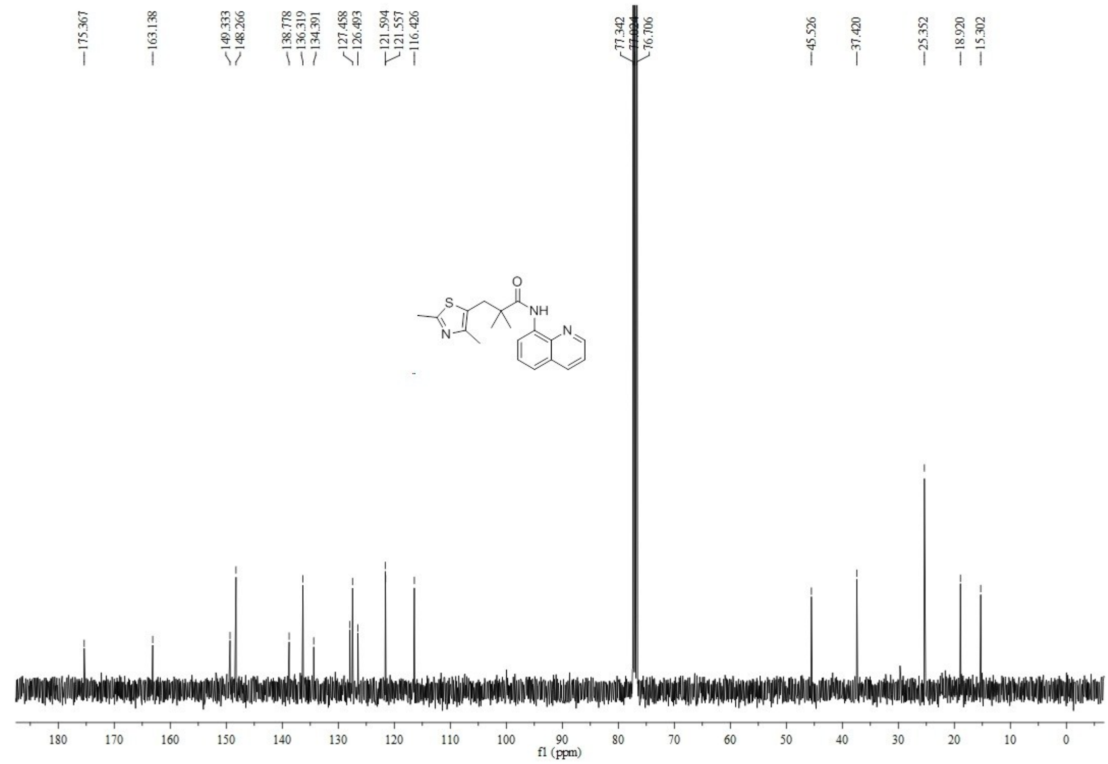




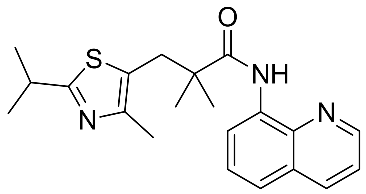
3-(2,4-dimethylthiazol-5-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6d**)

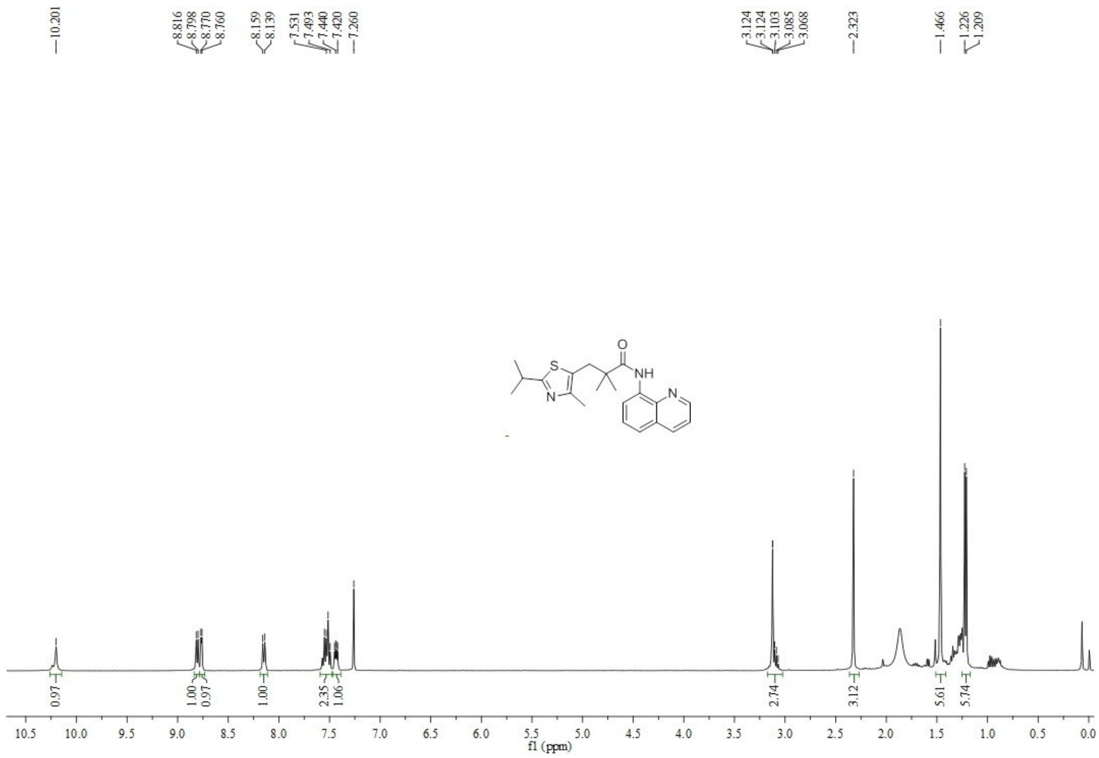


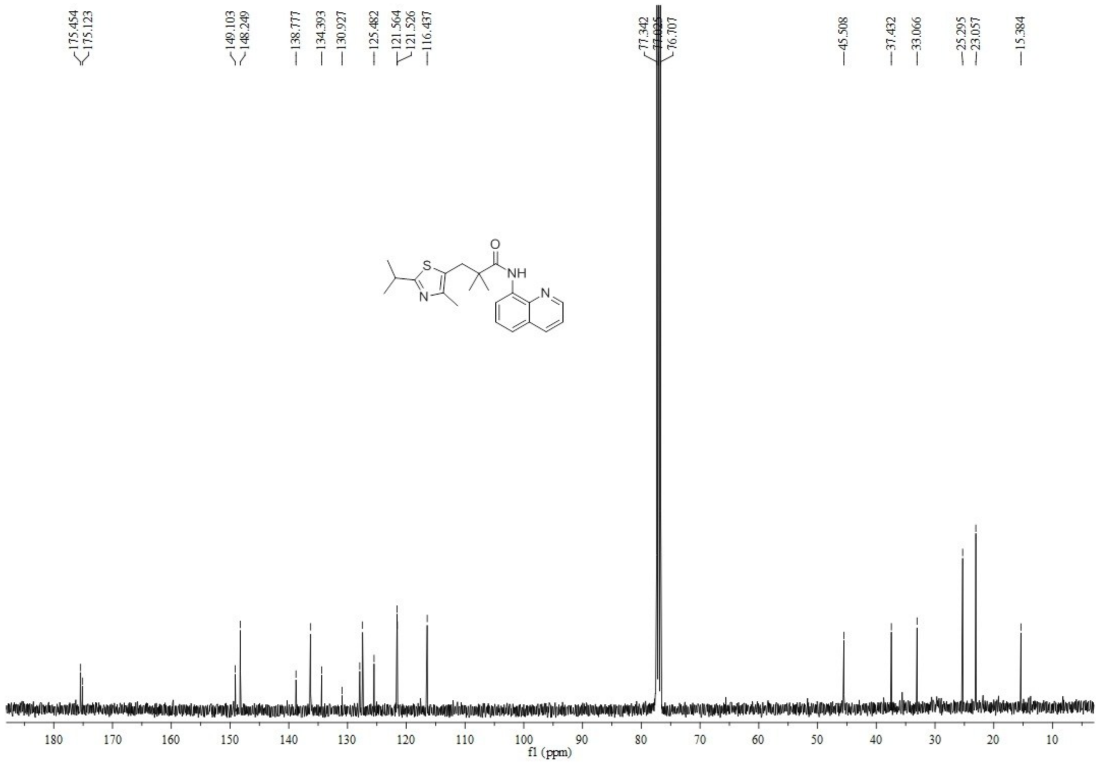




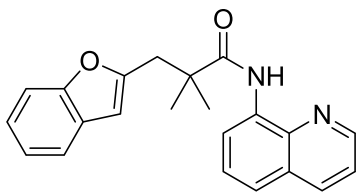
3-(2-isopropyl-4-methylthiazol-5-yl)-2,2-dimethyl-N-(quinolin-8-yl)propanamide (**6e**)

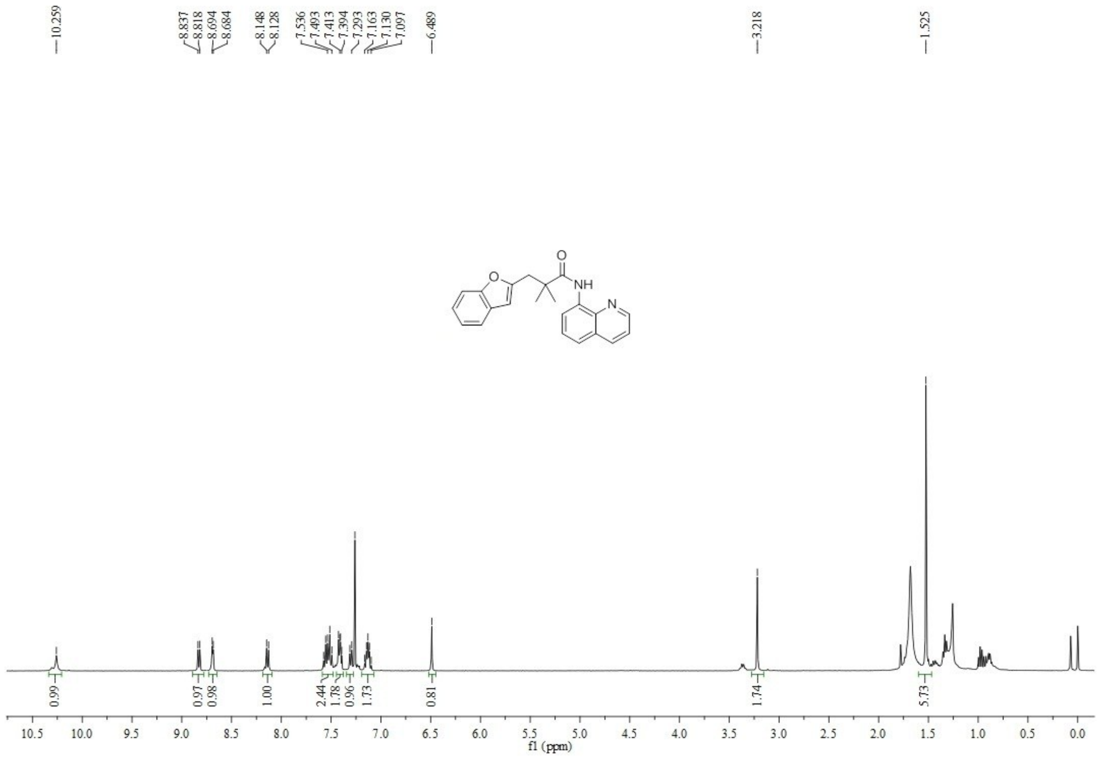


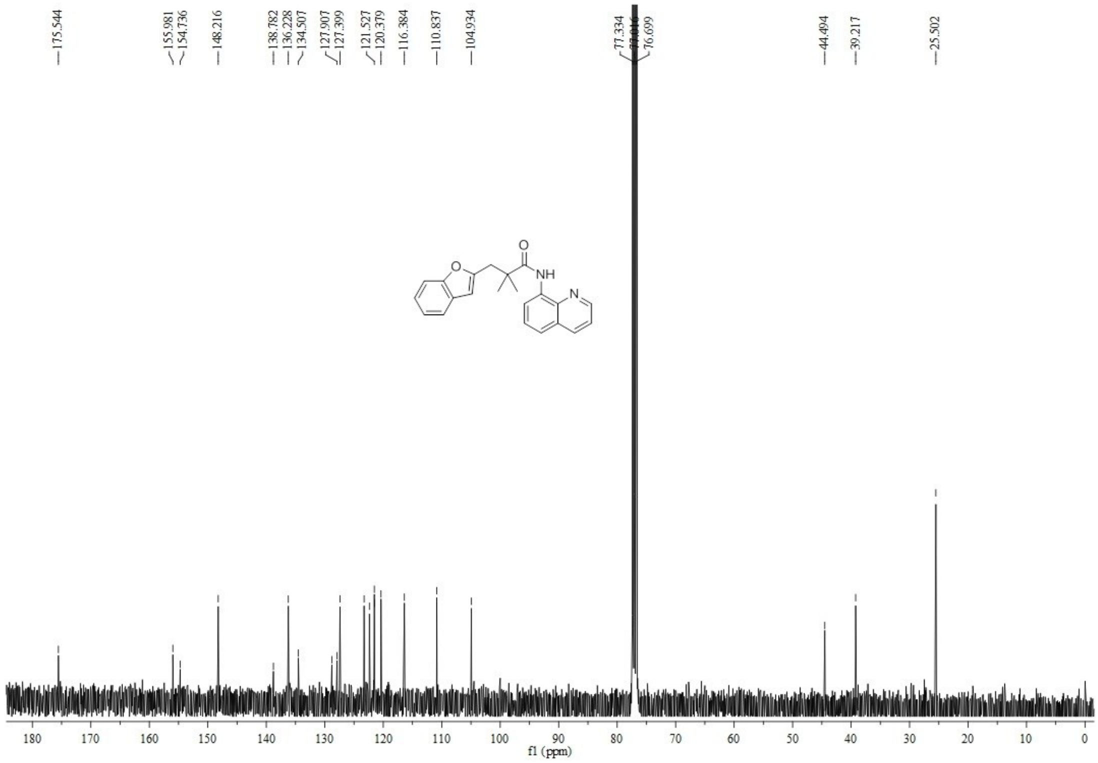




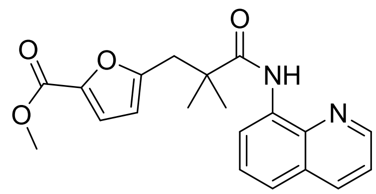
3-(benzofuran-2-yl)-2,2-dimethyl-*N*-(quinolin-8-yl)propanamide (**6f**)

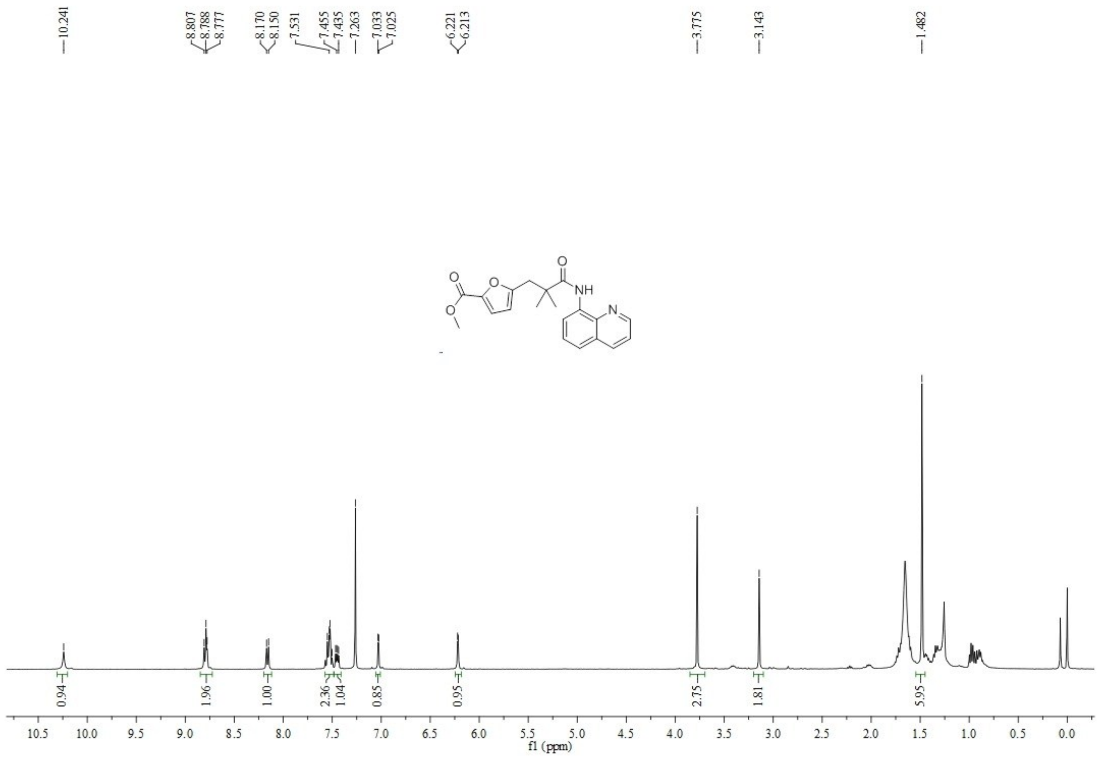


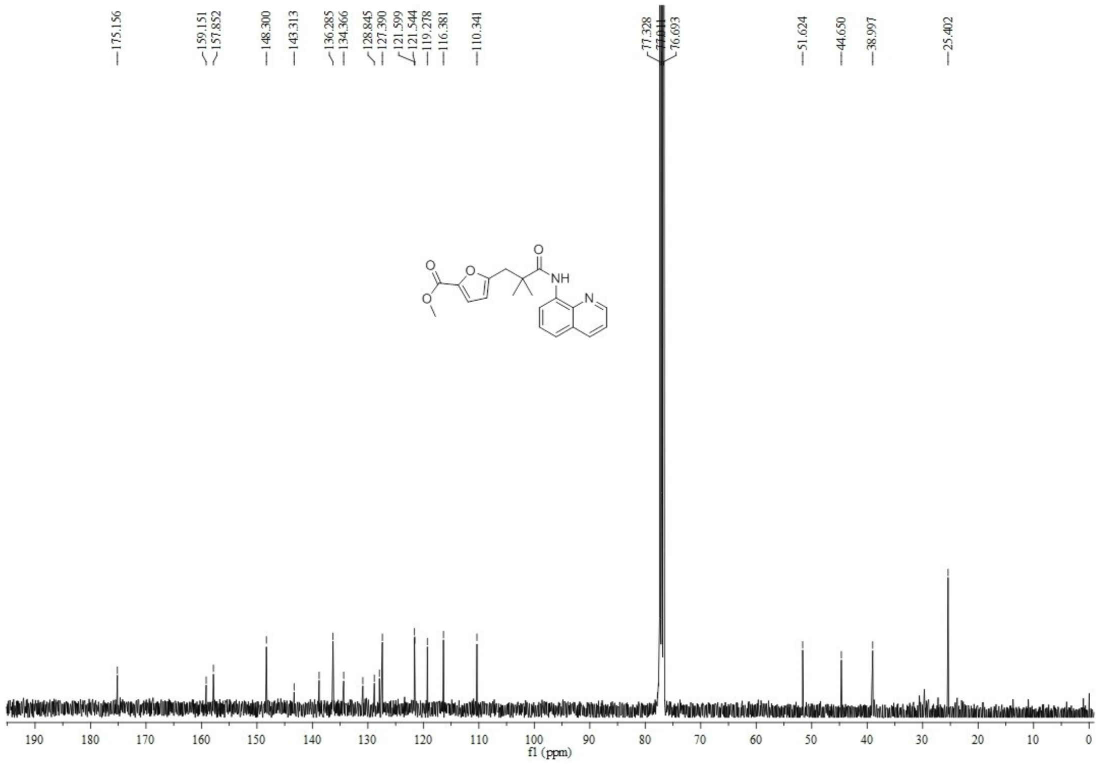




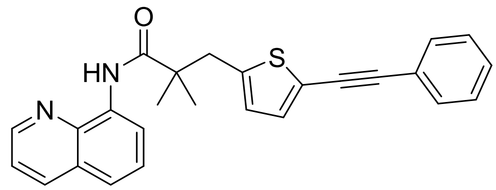
Methyl 5-(2,2-dimethyl-3-oxo-3-(quinolin-8-ylamino)propyl)furan-2-carboxylate (**6g**)

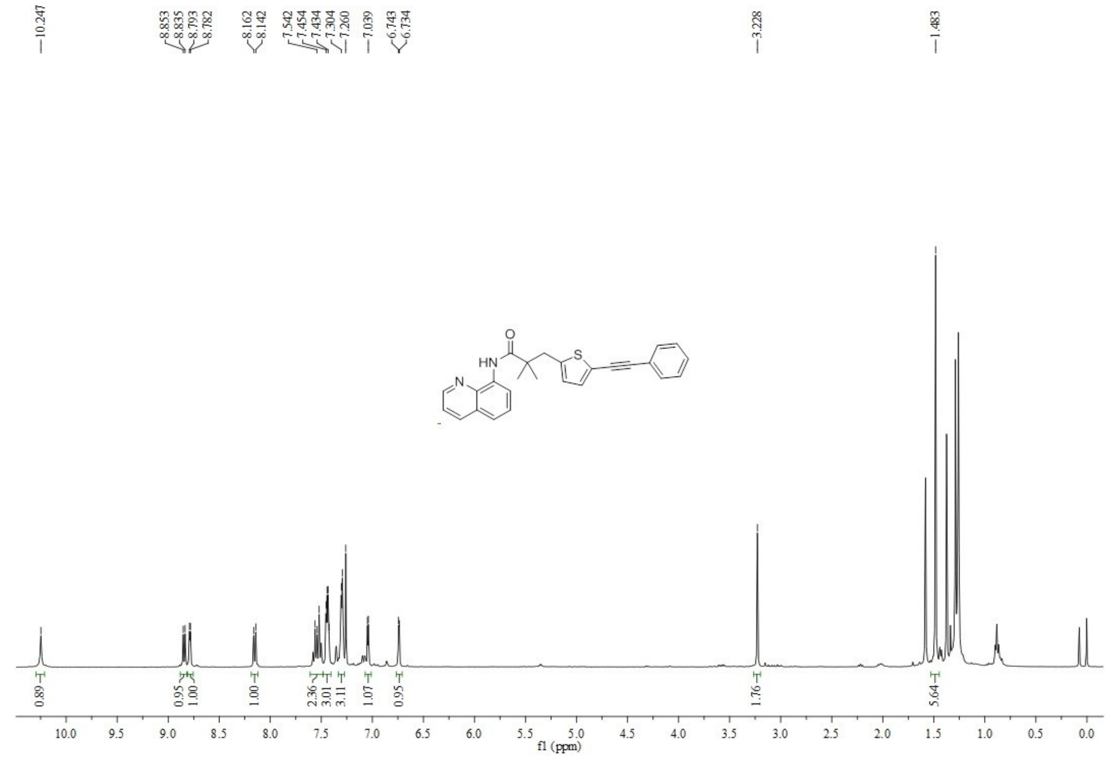


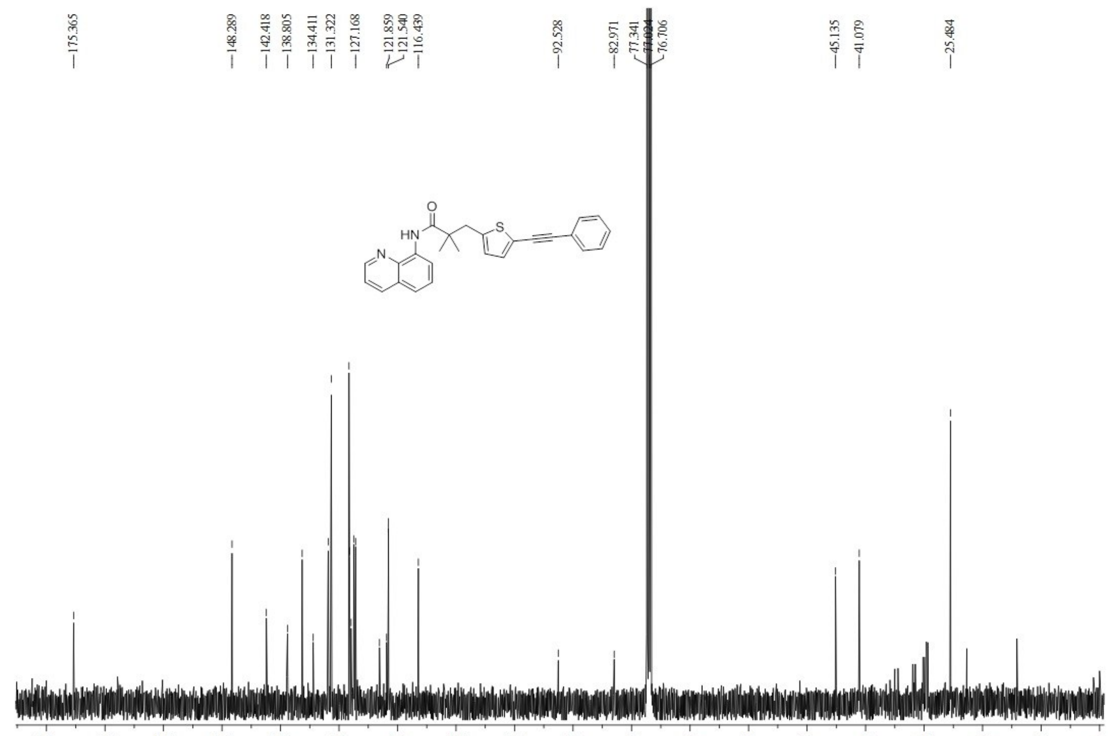




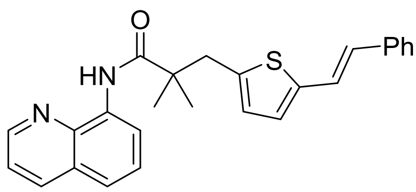
2,2-dimethyl-3-(5-(phenylethynyl)thiophen-2-yl)-*N*-(quinolin-8-yl)propanamide (**7**)

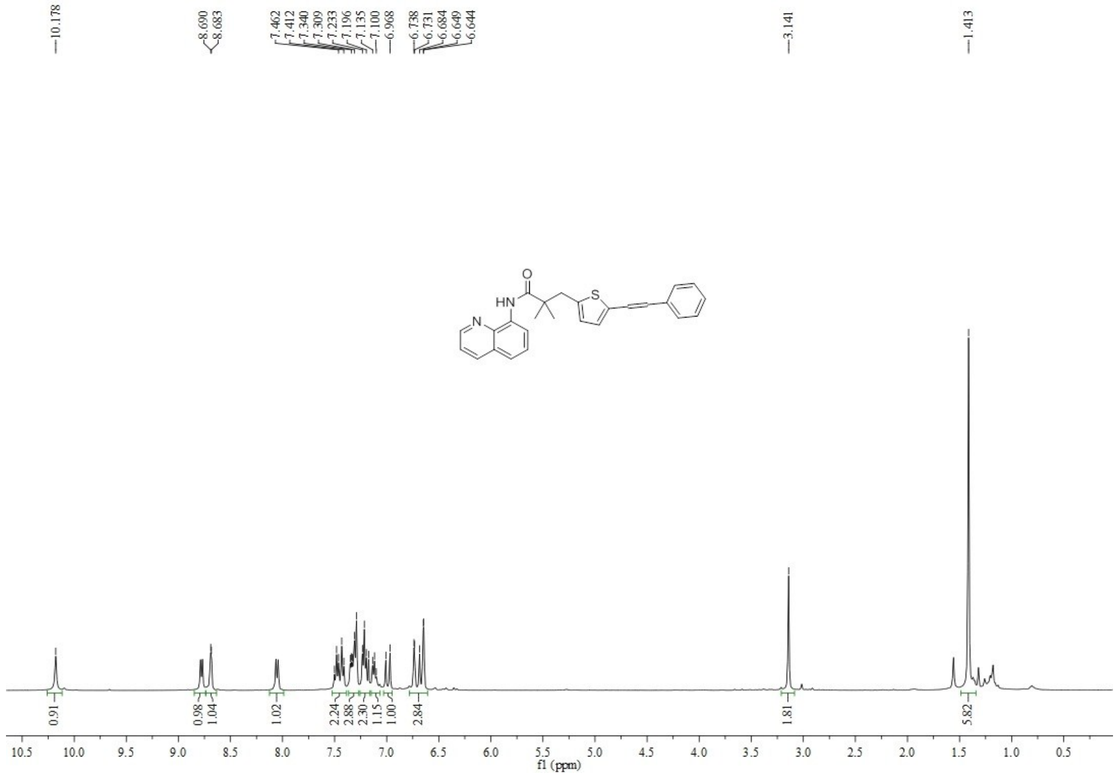


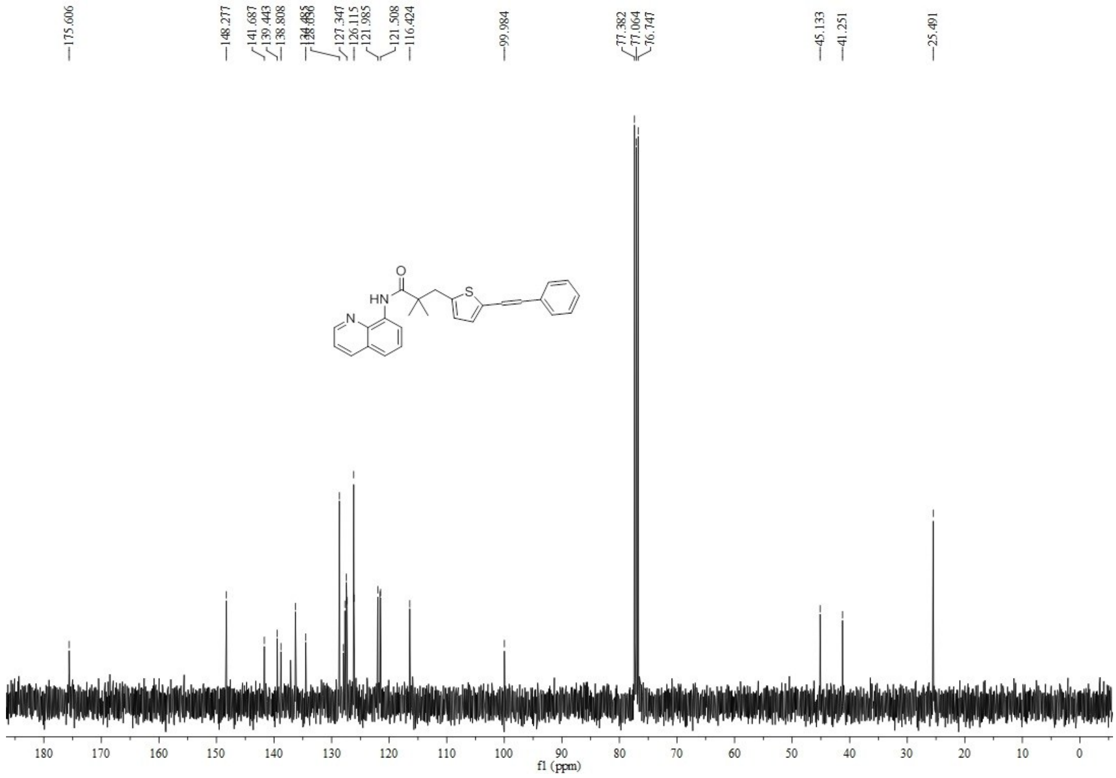




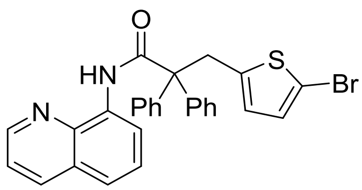
2,2-dimethyl-*N*-(quinolin-8-yl)-3-(5-styrylthiophen-2-yl)propanamide (**8**)

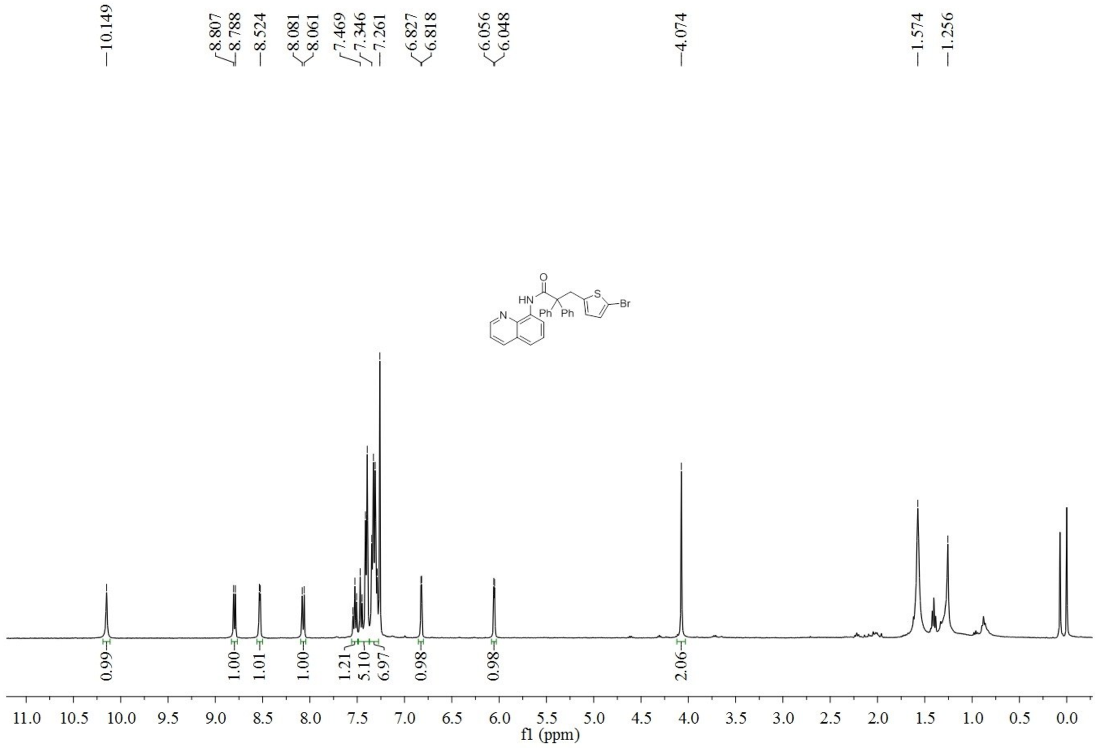


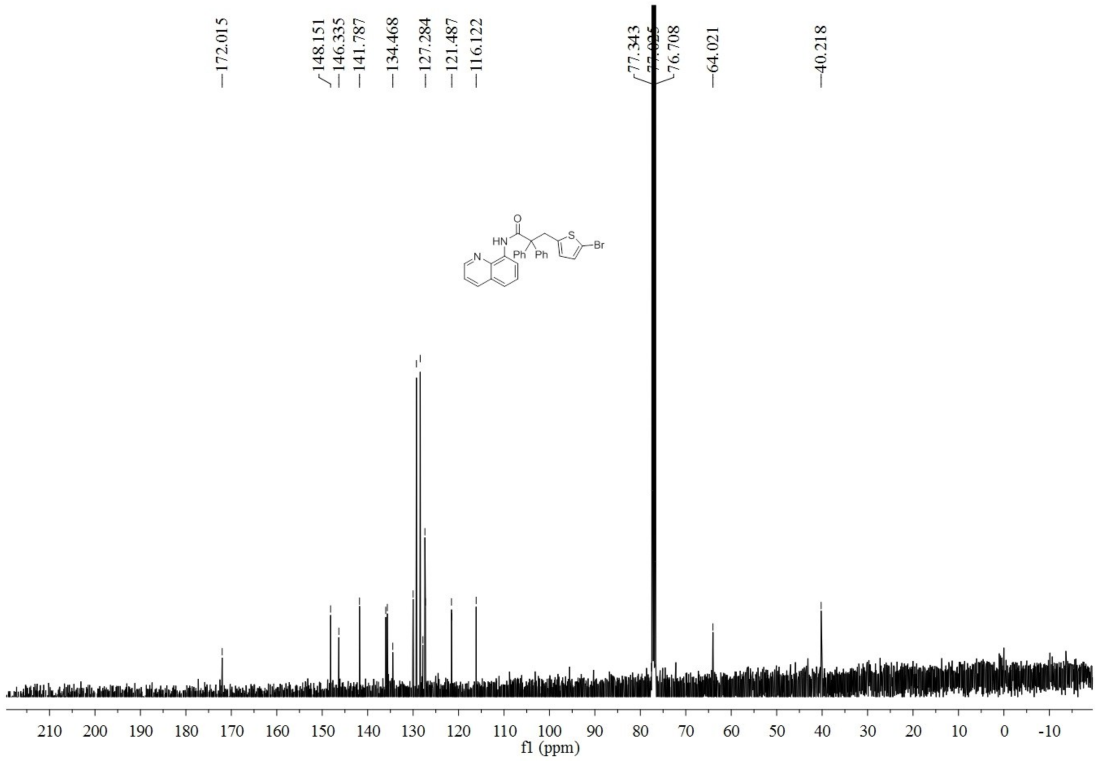




3-(5-bromothiophen-2-yl)-2,2-diphenyl-*N*-(quinolin-8-yl) propanamide (**9**)


O
HN
S
Br
N
Ph
Ph


10.149
8.807
8.788
8.524
8.081
8.061
7.469
7.346
7.261
6.827
6.818
6.056
6.048
4.074
1.574
1.256
0.99
1.00
1.01
1.00
1.21
5.10
6.97
0.98
0.98
2.06
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


172.015
148.151
146.335
141.787
134.468
127.284
121.487
116.122
77.343
76.708
64.021
40.218
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10
f1 (ppm)