Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Remote Arylalkylation of Unactivated Alkenes via 6- or 7-Membered Nickelacycles with Excellent Diastereofidelity

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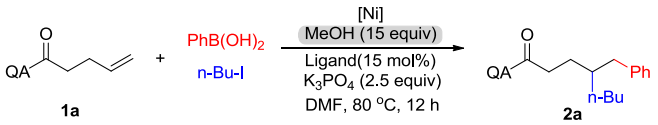
1. General Remarks

All the manipulations were performed in an argon-filled glovebox, unless mentioned otherwise. Anhydrous solvent was purchased from commercial sources and transferred under argon atmosphere. Alkene substrates and Amine benzoate substrates were prepared according to previously reported procedures, all arylboronic acids were purchased from commercial sources and used without further purification. All reagents were purchased from Energy Chemicals and used as received.

^{1}H NMR, ^{13}C NMR spectra were recorded using Bruker 400 MHz NMR spectrometer. ^{1}H NMR and ^{13}C NMR spectra were referenced to resonances of the residual protons in the deuterated solvents. Multiplicities are recorded as: s = singlet, d = doublet, t = triplet, dd = doublet of doublets, and m = multiplet. GC-MS analysis was performed on Shimadzu GC-2010 gas chromatography coupled to a Shimadzu QP2010 mass selective detector. Analytical HPLC/MS was performed with an Agilent 6520 Series HPLC. X-Band EPR spectra were recorded on a Bruker ELEXSYS E580-10/12 EPR spectrometer.

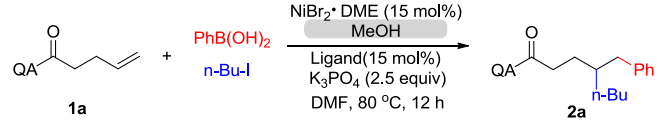
2. Optimization of Reaction Conditions

Table S1. Screening of nickel catalysts



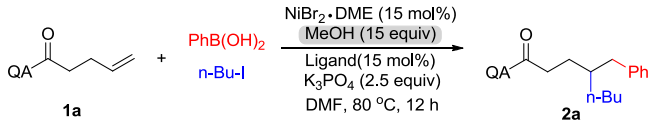
entry	Cat.(15 mol%)	yield **2a** (%)
1	$NiBr_2$•DME	90
2	$Ni(COD)_2$	69
3	$NiCl_2$	29
4	$NiBr_2$	30
5	NiI_2	85
6	$NiBr_2$•DME (10 mol%)	79

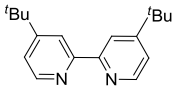
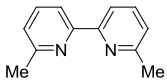
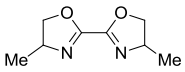
Table S2. Screening of the amount of methanol



entry	deviation from standard conditions	yield **2a** (%)
1	MeOH omitted	3
2	0.5 eq MeOH	60
3	1 eq MeOH	64
4	2 eq MeOH	69
5	15 eq MeOH	90

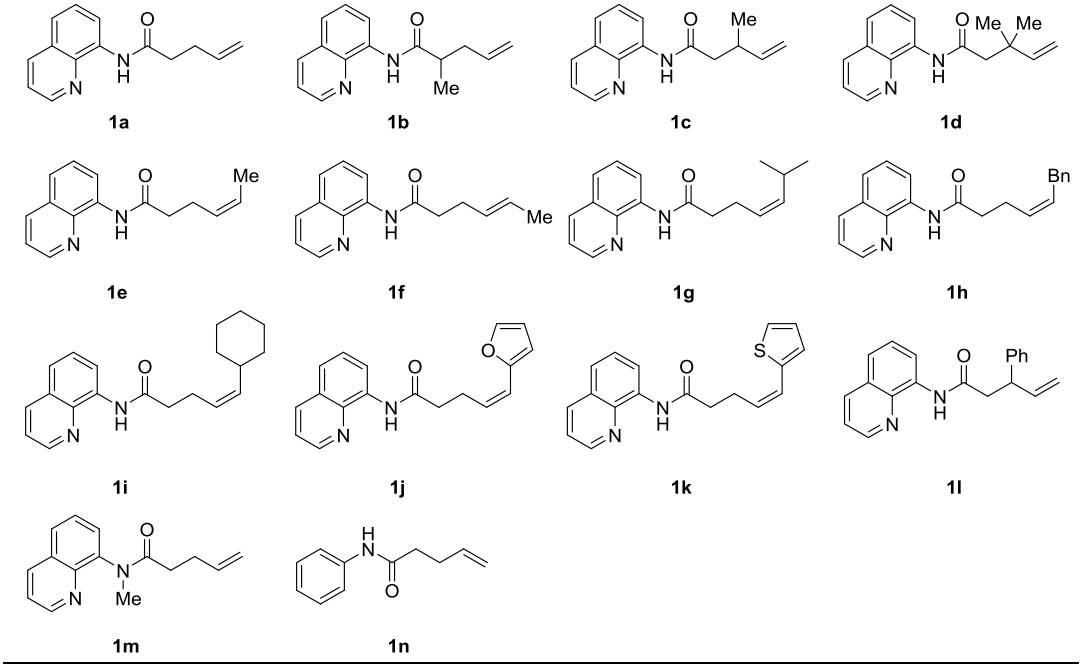
Table S3. Screening of ligands



entry	deviation from standard conditions	yield **2a** (%)
1	xantphos	<2
2	dppf	<2
3		76
4		83
5		86

3. Alkenes Substrate Synthesis

Table S4. Substrate synthesis of olefins containing guiding groups



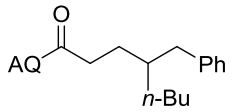
Alkene substrates **1a–1n** were prepared according to literature methods.[1, 2, 3]

4. General Procedure for the Ni-Catalyzed Arylalkylation of Alkenes

In an argon-filled glovebox, $NiBr_2$•DME (0.03 mmol, 15 mol%), alkene substrate (0.2 mmol, 1.0 eq), appropriate aryl boric acid nucleophile (0.40 mmol, 2 eq), K_3PO_4 (0.5 mmol, 2.5 eq), appropriate alkyl iodide electrophile (0.4 mmol, 2 eq), MeOH (3 mmol, 15 eq), DMF (1 mL) were added to a 12 mL tube. The reaction mixture was stirred at 80 ˚C for 12 h. The crude product was purified by column chromatography on silica gel with a mixture of ethyl acetate and hexane as eluent. The conditions for flash chromatography and data for characterization of the products are listed below.

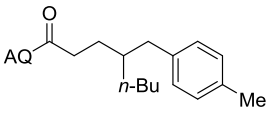
5. Product Derivatization

4-benzyl-N-(quinolin-8-yl)octanamide **(2a)**



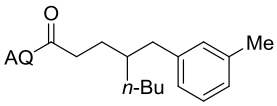
The title compound was isolated as a yellow oil (90% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (m, 1H), 8.21 (m, 1H), 8.14 (m, 1H), 7.85 (m, 1H), 7.43 (m, 1H), 6.03–5.87 (m, 1H), 5.31–5.15 (m, 2H), 4.13–4.04 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.0, 141.1, 138.3, 136.4, 134.5, 129.2, 128.2, 127.9, 127.4, 125.7, 121.5, 121.3, 116.4, 40.4, 39.3, 35.6, 32.7, 29.1, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{24}H_{39}N_2O^+$ $[M+H]^+$ 371.2274, found 371.2276.

4-(4-methylbenzyl)-N-(quinolin-8-yl)octanamide **(2b)**



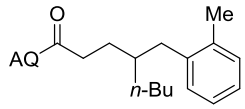
The title compound was isolated as a black oil (78% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.55 (dd, *J* = 4.8, 0.7 Hz, 1H), 8.44 (m, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 7.83 (m, 1H), 7.46–7.29 (m, 5H), 7.25 (m, 1H), 5.77 (m, 1H), 5.27 (dd, *J* = 15.4, 7.0 Hz, 1H), 5.22–5.04 (m, 2H), 2.77–2.65 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.0, 138.3, 137.9, 136.3, 135.1, 134.6, 129.1, 128.9, 127.9, 127.4, 121.5, 121.3, 116.4, 39.9, 39.3, 35.6, 32.7, 29.1, 28.7, 23.0, 21.0, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375.2436.

4-(3-methylbenzyl)-N-(quinolin-8-yl)octanamide **(2c)**



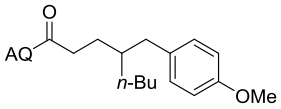
The title compound was isolated as a black oil (60% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.57–8.51 (m, 1H), 8.19 (d, *J* = 7.8 Hz, 1H), 8.08 (m, 1H), 7.84 (m, 1H), 7.41 (m, 1H), 4.88–4.77 (m, 2H), 3.61 (dd, *J* = 12.9, 6.9 Hz, 2H), 2.35 (t, *J* = 6.9 Hz, 2H), 1.79 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 147.8, 141.0, 138.0, 137.7, 136.7, 134.4, 129.9, 128.1, 128.0, 127.6, 126.5, 126.2, 121.5, 121.3, 116.8, 40.3, 39.3, 35.6, 32.7, 29.1, 28.6, 23.0, 21.3, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375.2432.

***4-(2-methylbenzyl)-N-(quinolin-8-yl)octanamide* (2d)**



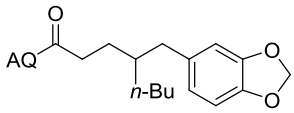
The title compound was isolated as a black oil (60% yield) after chromatography on silica with ethyl acetate:hexane (1:20).[1]H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81–8.75 (m, 2H), 8.15 (dd, *J* = 8.2, 1.1 Hz, 1H), 7.54–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.15–7.06 (m, 4H), 2.67–2.49 (m, 4H), 2.31 (s, 3H), 1.92–1.74 (m, 3H), 1.36 (d, *J* = 4.5 Hz, 4H), 1.32–1.24 (m, 3H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.0, 139.3, 138.3, 136.3, 136.2, 134.5, 130.3, 130.0, 127.9, 127.4, 125.9, 125.7, 121.5, 121.3, 116.4, 38.1, 38.0, 35.7, 33.0, 29.3, 28.7, 23.0, 19.6, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375.2438.

***4-(4-methoxybenzyl)-N-(quinolin-8-yl)octanamide* (2e)**



The title compound was isolated as a fulvous oil (62% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81–8.77 (m, 2H), 8.15 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.51–7.43 (m, 3H), 7.09 (d, *J* = 8.5 Hz, 2H), 6.81 (d, *J* = 8.6 Hz, 2H), 3.76 (s, 3H), 2.56 (dd, *J* = 13.5, 6.4 Hz, 4H), 1.83–1.72 (m, 3H), 1.35–1.24 (m, 6H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 157.7, 148.1, 138.3, 136.3, 134.5, 133.1, 130.0, 127.9, 127.4, 121.5, 121.3, 116.4, 113.7, 55.2, 39.4, 35.6, 32.7, 29.7, 29.1, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O_2^+$ $[M+H]^+$ 391.2380, found 390.2384.

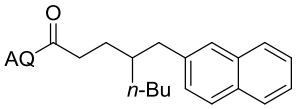
***4-(benzo[d][1,3]dioxol-5-ylmethyl)-N-(quinolin-8-yl)octanamide* (2f)**



The title compound was isolated as a brown oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.75 (m, 3H), 8.17–8.14 (m, 1H), 7.55–7.44 (m, 4H), 6.69 (dd, *J* = 12.7, 4.6 Hz, 2H), 6.63 (dd, *J* = 7.9, 1.4 Hz, 1H), 5.89 (dd, *J* = 4.1, 1.3 Hz, 2H), 2.61–2.47 (m, 5H), 1.80

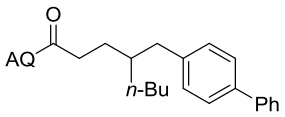
(dd, *J* = 14.9, 7.2 Hz, 2H), 1.71 (dd, *J* = 7.8, 3.7 Hz, 1H), 1.30 (dd, *J* = 20.8, 7.3 Hz, 7H), 0.88 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.1, 147.5, 145.5, 138.3, 136.3, 134.9, 134.5, 127.9, 127.4, 121.9, 121.5, 121.3, 116.4, 109.4, 108.0, 100.7, 40.2, 39.4, 35.6, 32.7, 29.0, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{29}N_2O_3^+$ $[M+H]^+$ 405.2173, found 405.2176.

4-(naphthalen-2-ylmethyl)-N-(quinolin-8-yl)octanamide **(2g)**



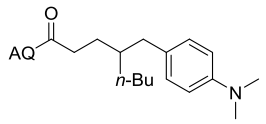
The title compound was isolated as a yellow oil (85% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.79–8.73 (m, 2H), 8.10 (d, *J* = 7.2 Hz, 1H), 7.56–7.39 (m, 9H), 7.32–7.23 (m, 3H), 2.66 (t, *J* = 7.0 Hz, 2H), 2.63–2.49 (m, 3H), 1.88–1.78 (m, 3H), 1.39–1.25 (m, 7H), 0.89 (t, J = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.0, 138.7, 138.3, 136.3, 134.5, 133.5, 132.0, 127.9, 127.8, 127.8, 127.5, 127.4, 127.4, 127.4, 125.8, 125.0, 121.5, 121.3, 116.4, 40.6, 39.2, 35.7, 32.8, 29.2, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{28}H_{31}N_2O^+$ $[M+H]^+$ 411.2431, found 411.2431.

4-([1,1'-biphenyl]-4-ylmethyl)-N-(quinolin-8-yl)octanamide **(2h)**



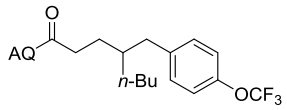
The title compound was isolated as a black oil (83% yield) after chromatography on silica with ethyl acetate:hexane (1:25). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.79–8.73 (m, 2H), 8.10 (d, *J* = 7.2 Hz, 1H), 7.56–7.39 (m, 9H), 7.32–7.23 (m, 3H), 2.66 (t, *J* = 7.0 Hz, 2H), 2.63–2.49 (m, 3H), 1.88–1.78 (m, 3H), 1.39–1.25 (m, 7H), 0.89 (t, *J* = 6.6 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.1, 141.1, 140.2, 138.6, 138.3, 136.3, 134.5, 129.6, 128.7, 127.9, 127.4, 126.9, 121.5, 121.4, 121.3, 116.4, 116.4, 40.0, 39.3, 35.6, 32.8, 29.1, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{30}H_{33}N_2O^+$$[M+H]^+$ 437.2587, found 437.2601.

***4-(4-(dimethylamino)benzyl)-N-(quinolin-8-yl)octanamide* (2i)**



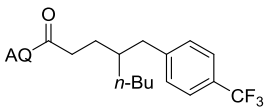
The title compound was isolated as a brown oil (52% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.71 (m, 2H), 8.08 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.48–7.35 (m, 3H), 6.97 (t, *J* = 8.8 Hz, 2H), 6.58 (dd, *J* = 14.6, 7.7 Hz, 2H), 2.84–2.78 (m, 6H), 2.45 (m, 4H), 1.74 (m, 2H), 1.65 (d, *J* = 5.5 Hz, 1H), 1.29–1.20 (m, 6H), 0.81 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.1, 148.9, 148.0, 138.3, 136.3, 134.6, 129.7, 129.2, 127.9, 127.4, 121.5, 121.2, 116.4, 112.9, 40.9, 39.5, 35.7, 32.7, 29.7, 29.1, 28.7, 23.0, 14.1.HRMS (ESI) m/z calculated for $C_{26}H_{34}N_3O^+$ $[M+H]^+$ 403.2696, found 403.2702.

***N-(quinolin-8-yl)-4-(4-(trifluoromethoxy)benzyl)octanamide* (2j)**



The title compound was isolated as a fulvous oil (92% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.78 (dd, *J* = 9.4, 5.1 Hz, 2H), 8.14 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.55–7.42 (m, 3H), 7.18 (d, *J* = 8.5 Hz, 2H), 7.10 (d, *J* = 8.1 Hz, 2H), 2.62 (d, *J* = 6.4 Hz, 2H), 2.54 (m, 2H), 1.85–1.73 (m, 3H), 1.36–1.23 (m, 6H), 0.87 (t, *J* = 6.9 Hz, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 148.1, 147.4, 139.8, 138.3, 136.3, 134.5, 130.3, 127.9, 127.4, 124.3, 121.8, 121.5, 121.3, 120.7, 119.2, 116.7, 116.4, 77.3, 77.0, 76.7, 39.7, 39.2, 35.5, 32.6, 29.0, 28.6, 22.9, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$) δ -62.21. HRMS (ESI) m/z calculated for $C_{25}H_{28}F_3N_2O_2^+$ $[M+H]^+$ 445.2097, found 445.2098.

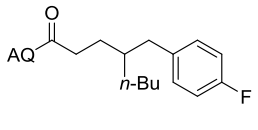
***N-(quinolin-8-yl)-4-(4-(trifluoromethyl)benzyl)octanamide* (2k)**



The title compound was isolated as a brown oil (93% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (s, 1H), 8.72–8.63 (m, 2H), 8.05 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.38 (m, 5H), 7.21–7.16 (m, 2H), 2.56 (t, *J* = 9.7 Hz,

2H), 2.45 (m, 2H), 1.76–1.66 (m, 3H), 1.27–1.15 (m, 6H), 0.79 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 148.1, 145.3, 138.3, 136.3, 134.5, 129.4, 128.6, 128.4, 128.3, 127.9, 127.9, 127.6, 127.4, 125.7, 125.2, 125.1, 125.1, 125.1, 123.0, 121.6, 121.4, 120.3, 116.4, 40.2, 39.1, 35.4, 32.6, 29.0, 28.6, 22.9, 14.0; ^{19}F NMR (376 MHz, $CDCl_3$)δ -62.21. HRMS (ESI) m/z calculated for $C_{25}H_{28}F_3N_2O^+$ $[M+H]^+$ 429.2148, found 429.2150.

4-(4-fluorobenzyl)-N-(quinolin-8-yl)octanamide **(2l)**



The title compound was isolated as a fulvous oil (95% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 4.7 Hz, 1H), 8.20 (d, *J* = 7.8 Hz, 1H), 8.16 (br, 1H), 7.85 (m, 1H), 7.44–7.41 (m, 1H), 7.22 (dd, *J* = 8.6, 6.1 Hz, 2H), 7.18–7.13 (m, 3H), 5.73 (m, 1H), 5.61–5.54 (m, 1H), 3.57 (dd, *J* = 13.2, 6.8 Hz, 2H), 3.43 (d, *J* = 7.3 Hz, 2H), 2.52 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 162.4, 160.0, 148.1, 138.3, 136.6, 136.6, 136.3, 134.5, 130.4, 130.4, 127.9, 127.4, 121.6, 121.3, 116.3, 115.1, 114.8, 39.5, 39.3, 35.5, 32.6, 29.0, 28.6, 23.0, 14.1; ^{19}F NMR (376 MHz, $CDCl_3$) δ -117.80. HRMS (ESI) m/z calculated for $C_{24}H_{28}FN_2O^+$ $[M+H]^+$ 379.2180, found 378.2183.

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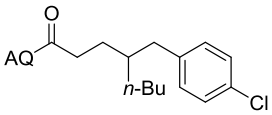
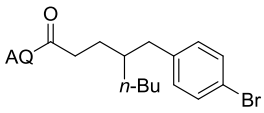
4-(4-chlorobenzyl)-N-(quinolin-8-yl)octanamide **(2m)**



The title compound was isolated as a brown oil (93% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.71–8.65 (m, 2H), 8.04 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.44–7.36 (m, 2H), 7.33 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.00 (d, *J* = 8.4 Hz, 2H), 2.46 (m, 4H), 1.74–1.59 (m, 3H), 1.26–1.15 (m, 6H), 0.78 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 148.1, 139.5, 138.3, 136.3, 134.5, 131.5, 130.5, 128.3, 127.9, 127.4, 121.6,

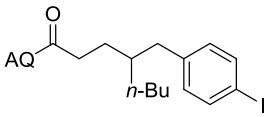
121.3, 116.3, 39.7, 39.2, 35.5, 32.6, 29.0, 28.6, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{24}H_{28}ClN_2O^+$ $[M+H]^+$ 395.1885, found 395.1885.

***4-(4-bromobenzyl)-N-(quinolin-8-yl)octanamide* (2n)**



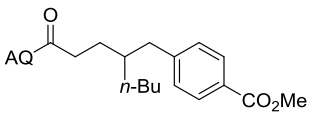
The title compound was isolated as a brown oil (87% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.78 (m, 2H), 8.13 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.54–7.46 (m, 2H), 7.43 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.35 (dd, *J* = 6.1, 4.5 Hz, 2H), 7.04 (d, *J* = 8.3 Hz, 2H), 2.61–2.46 (m, 4H), 1.84–1.67 (m, 3H), 1.28 (m, 6H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 148.1, 140.0, 138.3, 136.3, 134.5, 131.3, 130.9, 127.9, 127.4, 121.6, 121.3, 119.5, 116.3, 39.8, 39.2, 35.5, 32.6, 29.0, 28.6, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{24}H_{28}BrN_2O^+$ $[M+H]^+$ 439.1380, found 439.1380.

***4-(4-iodobenzyl)-N-(quinolin-8-yl)octanamide* (2o)**



The title compound was isolated as a black oil (75% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.81–8.79 (m, 1H), 8.76 (dd, *J* = 7.3, 1.5 Hz, 1H), 8.16 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.57–7.50 (m, 4H), 7.46–7.44 (m, 1H), 6.93 (d, *J* = 8.2 Hz, 2H), 2.59–2.52 (m, 4H), 1.83–1.73 (m, 3H), 1.34–1.26 (m, 6H), 0.87 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 148.1, 140.7, 138.3, 137.2, 136.4, 134.5, 131.2, 127.9, 127.4, 121.6, 121.3, 116.4, 90.9, 39.9, 39.1, 35.5, 32.6, 29.0, 28.6, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{24}H_{28}IN_2O$ $[M+H]^+$ 487.1241, found 487.1241.

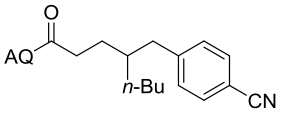
***methyl 4-(2-(3-oxo-3-(quinolin-8-ylamino)propyl)hexyl)benzoate* (2p)**



The title compound was isolated as a black oil (76% yield) after chromatography on silica with ethyl acetate:hexane

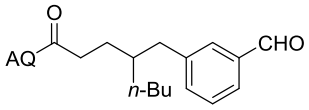
(1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.69 (m, 2H), 8.05 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.85 (d, *J* = 8.2 Hz, 2H), 7.46–7.33 (m, 3H), 7.17 (t, *J* = 5.3 Hz, 2H), 3.79 (s, 3H), 2.67–2.37 (m, 4H), 1.81–1.65 (m, 3H), 1.21 (m, 6H), 0.78 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 167.1, 148.1, 146.8, 138.3, 136.3, 134.5, 129.6, 129.2, 127.9, 127.8, 127.4, 121.5, 121.3, 116.3, 51.9, 40.5, 39.1, 35.5, 32.7, 29.1, 28.6, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{26}H_{31}N_2O_3$ $[M+H]^+$ 419.2329, found 419.2331.

4-(4-cyanobenzyl)-N-(quinolin-8-yl)octanamide **(2q)**



The title compound was isolated as a brown oil (98% yield) after chromatography on silica with ethyl acetate:hexane (1:6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.65 (s, 1H), 8.71–8.63 (m, 2H), 8.05 (d, *J* = 8.2 Hz, 1H), 7.44–7.33 (m, 5H), 7.17 (d, *J* = 8.0 Hz, 2H), 2.61–2.51 (m, 2H), 2.51–2.37 (m, 2H), 1.75–1.64 (m, 3H), 1.25–1.15 (m, 6H), 0.78 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.4, 148.1, 147.0, 138.2, 136.4, 134.4, 132.0, 129.9, 127.9, 127.4, 121.6, 121.4, 119.1, 116.3, 109.6, 40.6, 39.0, 35.4, 32.7, 29.0, 28.5, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{25}H_{28}N_3O^+$ $[M+H]^+$ 386.2227, found 386.2228.

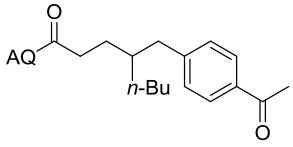
4-(3-formylbenzyl)-N-(quinolin-8-yl)octanamide **(2r)**



The title compound was isolated as a brown oil (94% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.95 (s, 1H), 9.76 (s, 1H), 8.79–8.74 (m, 2H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.68–7.76 (m, 2H), 7.53–7.41 (m, 5H), 2.75–2.67 (m, 2H), 2.62–2.50 (m, 2H), 1.85–1.78 (m, 3H), 1.38–1.27 (m, 6H), 0.88 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.5, 171.6, 148.1, 142.2, 138.2, 136.4, 136.3, 135.4, 134.4, 130.1, 128.9, 127.9, 127.5, 127.4, 121.6,

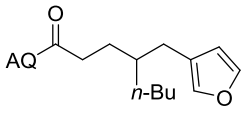
121.4, 116.3, 40.1, 39.2, 35.5, 32.6, 29.0, 28.6, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{25}H_{29}N_2O_2^+$ $[M+H]^+$ 389.2224, found 368.2223.

***N-(3-(piperidin-1-yl)-4-(o-tolyl)butyl)picolinamide* (2s)**



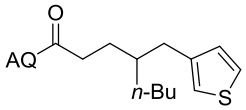
The title compound was isolated as a brown oil (90% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.68 (dd, *J* = 8.3, 5.5 Hz, 2H), 8.07–8.01 (m, 1H), 7.76 (d, *J* = 8.1 Hz, 2H), 7.39 (m, 3H), 7.17 (d, *J* = 7.9 Hz, 2H), 2.58 (s, 2H), 2.50–2.39 (m, 5H), 1.71 (dd, *J* = 13.8, 6.8 Hz, 3H), 1.27–1.16 (m, 6H), 0.79 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 197.7, 171.6, 148.1, 147.1, 138.2, 136.3, 135.0, 134.4, 129.3, 128.4, 127.9, 127.4, 121.6, 121.4, 116.3, 40.4, 39.1, 35.5, 32.7, 29.1, 28.6, 26.5, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{26}H_{31}N_2O_2^+$ $[M+H]^+$ 403.2380, found 403.2380.

***4-(furan-3-ylmethyl)-N-(quinolin-8-yl)octanamide* (2t)**



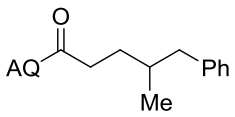
The title compound was isolated as a fulvous oil (70% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.79 (s, 1H), 8.82–8.75 (m, 2H), 8.16 (d, *J* = 8.2 Hz, 1H), 7.56–7.48 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.34 (s, 1H), 7.26 (d, *J* = 2.7 Hz, 1H), 6.27 (s, 1H), 2.57 (dd, *J* = 8.9, 6.5 Hz, 2H), 2.45 (d, *J* = 6.5 Hz, 2H), 1.81 (dd, *J* = 15.0, 7.2 Hz, 2H), 1.72–1.64 (m, 1H), 1.41–1.18 (m, 6H), 0.89 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.1, 142.7, 139.7, 138.3, 136.3, 134.5, 127.9, 127.4, 123.0, 121.5, 121.3, 116.4, 111.5, 37.9, 35.6, 32.8, 29.1, 28.8, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{22}H_{27}N_2O_2^+$ $[M+H]^+$ 351.2067, found 351.2061.

***N-(quinolin-8-yl)-4-(thiophen-3-ylmethyl)octanamide* (2u)**



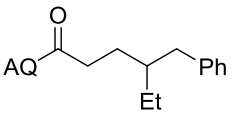
The title compound was isolated as a yellow oil (86% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.78 (dd, *J* = 8.4, 5.1 Hz, 2H), 8.12 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.52–7.42 (m, 3H), 7.22 (dd, *J* = 4.8, 3.0 Hz, 1H), 6.94 (dd, *J* = 8.6, 3.7 Hz, 2H), 2.67–2.63 (m, 2H), 2.56–2.51 (m, 2H), 1.81 (dd, *J* = 14.4, 6.6 Hz, 3H), 1.35–1.27 (m, 6H), 0.88 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.1, 141.1, 138.3, 136.3, 134.5, 128.7, 127.9, 127.4, 125.1, 121.5, 121.3, 121.0, 116.4, 38.6, 35.6, 34.6, 32.9, 29.2, 28.7, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{22}H_{27}N_2OS^+$ $[M+H]^+$ 367.1839, found 367.1833.

4-methyl-5-phenyl-N-(quinolin-8-yl)pentanamide **(2v)**



The title compound was isolated as a black oil (65% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.78 (dd, *J* = 4.5, 2.8 Hz, 2H), 8.14 (s, 1H), 7.52–7.47 (m, 2H), 7.43 (d, *J* = 4.1 Hz, 1H), 7.27–7.23 (m, 2H), 7.18–7.14 (m, 3H), 2.73 (dd, *J* = 13.3, 5.8 Hz, 1H), 2.66–2.52 (m, 3H), 2.45 (dd, *J* = 13.4, 8.0 Hz, 1H), 1.91 (dd, *J* = 7.1, 4.1 Hz, 1H), 1.74–1.66 (m, 1H), 0.94 (d, *J* = 6.5 Hz, 3H);^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.1, 140.9, 138.3, 136.4, 134.5, 129.2, 128.2, 127.9, 127.4, 125.8, 121.5, 121.3, 116.4, 43.5, 36.0, 34.7, 32.3, 19.2. HRMS (ESI) m/z calculated for $C_{21}H_{23}N_2O^+$ $[M+H]^+$ 319.1805, found 319.1808.

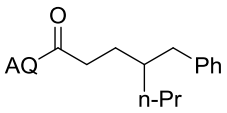
4-benzyl-N-(quinolin-8-yl)hexanamide **(2w)**



The title compound was isolated as a black oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.79 (m, 2H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.55–7.50 (m, 2H), 7.48–7.43 (m, 2H), 7.28–7.24 (m, 2H), 7.20–7.15 (m, 2H), 2.65–2.53 (m, 3H), 1.85–1.72 (m, 2H), 1.61–1.16 (m, 4H), 0.97–0.91 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.0, 141.1, 136.4, 134.5, 129.2,

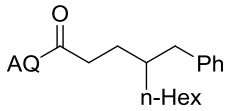
128.2, 127.9, 127.4, 125.7, 121.5, 121.3, 116.4, 40.77, 39.97, 35.67, 28.65, 25.35, 10.69. HRMS (ESI) m/z calculated for $C_{22}H_{24}N_2O^+[M+H]^+$ 333.1961, found 333.1966.

4-benzyl-N-(quinolin-8-yl)octanamide **(2x)**



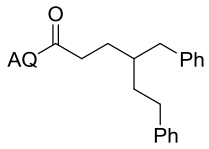
The title compound was isolated as a yellow oil (86% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.78 (m, 2H), 8.14 (d, *J* = 8.3 Hz, 1H), 7.52–7.42 (m, 3H), 7.26 (t, *J* = 7.2 Hz, 2H), 7.17 (dd, *J* = 11.4, 7.3 Hz, 3H), 2.67–2.44 (m, 4H), 1.90–1.69 (m, 3H), 1.29 (dd, *J* = 20.7, 9.8 Hz, 6H), 0.87 (dd, *J* = 7.1, 5.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 148.0, 141.1, 138.3, 136.4, 134.5, 129.2, 128.2, 127.9, 127.4, 125.7, 121.5, 121.3, 116.4, 40.45, 39.18, 35.62, 35.39, 29.12, 19.67, 14.42. HRMS (ESI) m/z calculated for $C_{23}H_{27}N_2O^+$ $[M+H]^+$ 347.2118, found 347.2121.

4-benzyl-N-(quinolin-8-yl)nonanamide **(2y)**



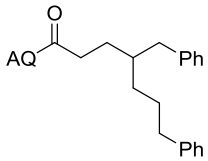
The title compound was isolated as a yellow oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.76 (dd, *J* = 7.3, 1.5 Hz, 1H), 8.15 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.53–7.49 (m, 2H), 7.47–7.42 (m, 2H), 7.25 (dd, *J* = 4.9, 2.3 Hz, 2H), 7.19–7.15 (m, 2H), 2.64–2.59 (m, 2H), 2.55 (m, 2H), 1.85–1.76 (m, 3H), 1.33 (s, 4H), 1.25 (t, *J* = 7.2 Hz, 6H), 0.86 (t, *J* = 6.8 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.3, 147.3, 141.1, 134.7, 134.1, 131.0, 129.2, 128.2, 127.9, 125.7, 121.5, 121.4, 40.4, 39.3, 35.5, 33.0, 31.8, 29.6, 29.1, 26.4, 22.6, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375,2431.

4-benzyl-6-phenyl-N-(quinolin-8-yl)hexanamide **(2z)**



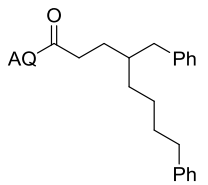
The title compound was isolated as a yellow oil (75% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.77 (s, 1H), 8.81–8.75 (m, 2H), 8.14 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.56–7.39 (m, 4H), 7.27–7.12 (m, 9H), 2.75–2.58 (m, 4H), 2.58–2.44 (m, 2H), 1.88 (m, 3H), 1.66 (dd, *J* = 13.8, 8.1 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 148.1, 142.5, 140.7, 138.3, 136.4, 134.8, 134.5, 130.9, 129.2, 128.3, 127.9, 127.4, 125.9, 125.7, 121.6, 121.4, 116.4, 40.3, 38.9, 35.5, 34.9, 32.9, 29.1. HRMS (ESI) m/z calculated for $C_{28}H_{29}N_2O^+$ $[M+H]^+$ 409.2274, found 409.2275.

4-benzyl-7-phenyl-N-(quinolin-8-yl)heptanamide **(2aa)**



The title compound was isolated as a brown oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.17 (s, 1H), 8.52 (m, 1H), 8.16 (d, *J* = 7.8 Hz, 1H), 7.81 (m, 1H), 7.39 (m, 1H), 7.31 (d, *J* = 8.7 Hz, 2H), 7.13 (t, *J* = 7.7 Hz, 1H), 7.06 (d, *J* = 7.6 Hz, 1H), 3.69 (m, 1H), 3.24 (m, 1H), 3.02 (d, *J* = 12.5 Hz, 1H), 2.88–2.66 (m, 3H), 2.50 (s, 2H), 2.35–2.22 (m, 1H), 1.73 (s, 6H), 1.54–1.48 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.1, 142.5, 140.9, 138.3, 136.9, 136.3, 134.5, 129.2, 128.4, 128.2, 127.9, 127.4, 125.8, 125.6, 121.5, 121.3, 116.4, 40.3, 39.2, 36.1, 35.5, 32.5, 29.1, 28.3. HRMS (ESI) m/z calculated for $C_{29}H_{31}N_2O^+$ $[M+H]^+$ 423.2431, found 423.2436.

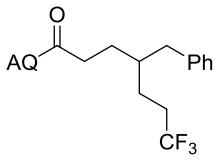
4-benzyl-8-phenyl-N-(quinolin-8-yl)octanamide **(2ab)**



The title compound was isolated as a brown oil (85% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.80–8.75 (m, 2H), 8.15 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.85–7.77 (m, 1H), 7.55–7.42 (m, 5H), 7.25 (d, *J* = 3.0 Hz, 2H), 7.18–7.11 (m, 5H), 2.63–2.51 (m, 5H), 1.86–1.74 (m, 2H), 1.60 (m, 3H), 1.44–1.33 (m, 4H), 0.94 (d, *J* = 6.5 Hz, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9,

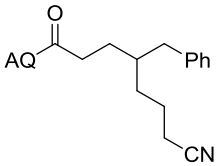
148.0, 142.7, 141.0, 138.2, 136.5, 134.7, 134.5, 129.2, 128.4, 128.2, 127.9, 127.5, 125.8, 125.5, 121.5, 121.4, 116.6, 40.4, 39.3, 35.6, 32.8, 32.5, 31.7, 29.1, 26.1. HRMS (ESI) m/z calculated for $C_{30}H_{33}N_2O^+$ $[M+H]^+$ 437.2587, found 437.2594.

4-benzyl-7,7,7-trifluoro-N-(quinolin-8-yl)heptanamide **(2ac)**



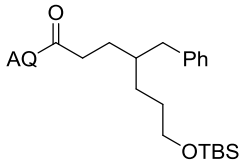
The title compound was isolated as a black oil (70% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.33 (s, 1H), 8.66–8.62 (m, 1H), 8.18 (d, *J* = 7.8 Hz, 1H), 8.15–8.05 (m, 1H), 7.83 (m, 1H), 7.42 (m, 1H), 7.28 (s, 1H), 7.20 (t, *J* = 7.4 Hz, 1H), 7.14 (d, *J* = 7.0 Hz, 2H), 3.76–3.67 (m, 1H), 3.18 (m, 3H), 3.06 (dd, *J* = 13.1, 3.6 Hz, 1H), 2.88 (s, 7H), 2.35 (dd, *J* = 13.1, 10.3 Hz, 1H), 1.77 (m, 1H), 1.59 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 150.2, 148.1, 137.4, 130.2, 129.3, 128.6, 128.5, 126.1, 122.3, 69.5, 51.6, 39.6, 35.1, 35.1, 27.9; ^{19}F NMR (376 MHz, $CDCl_3$) δ -66.35. HRMS (ESI) m/z calculated for $C_{23}H_{24}F_3N_2O^+$ $[M+H]^+$ 401.1835, found 401.1838.

4-benzyl-7-cyano-N-(quinolin-8-yl)heptanamide **(2ad)**



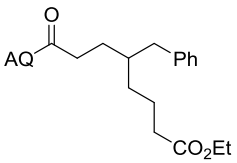
The title compound was isolated as a brown oil (75% yield) after chromatography on silica with ethyl acetate:hexane (1:6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (s, 1H), 8.68 (dd, *J* = 16.5, 4.6 Hz, 2H), 8.13 (d, *J* = 7.1 Hz, 1H), 8.06–8.01 (m, 1H), 7.41–7.38 (m, 2H), 7.34 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 2H), 7.07 (d, *J* = 7.7 Hz, 2H), 2.63–2.54 (m, 1H), 2.47 (dd, *J* = 13.8, 6.7 Hz, 3H), 2.16 (m, 2H), 1.77–1.64 (m, 3H), 1.63–1.51 (m, 2H), 1.34 (dd, *J* = 10.1, 5.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.3, 147.1, 139.1, 137.2, 135.3, 134.5, 133.3, 128.0, 127.3, 126.8, 126.3, 125.0, 120.6, 120.4, 118.6, 115.3, 39.2, 37.6, 34.2, 31.2, 27.8, 21.5, 16.3. HRMS (ESI) m/z calculated for $C_{24}H_{26}N_3O^+$ $[M+H]^+$ 372.2070, found 372.2081.

***4-benzyl-7-((tert-butyldimethylsilyl)oxy)-N-(quinolin-8-yl)heptanamide* (2ae)**



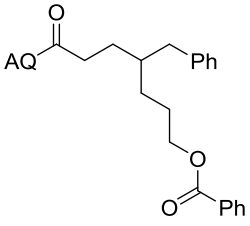
The title compound was isolated as a brown oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:20). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.78–8.72 (m, 2H), 8.10 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.51–7.43 (m, 2H), 7.40 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.22 (dd, *J* = 9.5, 5.2 Hz, 2H), 7.17–7.12 (m, 2H), 3.54 (d, *J* = 6.5 Hz, 1H), 2.62–2.49 (m, 3H), 1.80 (t, *J* = 7.1 Hz, 2H), 1.63–1.49 (m, 2H), 1.48–1.28 (m, 2H), 0.88–0.80 (m, 9H), -0.00 (s, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.0, 140.9, 138.3, 136.3, 134.5, 129.2, 128.3, 127.9, 127.4, 125.8, 121.5, 121.3, 116.4, 63.4, 40.4, 39.2, 35.5, 29.7, 29.1, 26.0, 26.0, 18.3, -5.2. HRMS (ESI) m/z calculated for $C_{29}H_{41}N_2O_2Si^+$ $[M+H]^+$ 477.2932, found 477.2937.

***ethyl 5-benzyl-8-oxo-8-(quinolin-8-ylamino)octanoate* (2af)**



The title compound was isolated as a brown oil (65% yield) after chromatography on silica with ethyl acetate:hexane (1:12). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.69 (s, 1H), 8.70 (m, 2H), 8.07 (dd, *J* = 8.2, 1.2 Hz, 1H), 7.46–7.34 (m, 3H), 7.18 (t, *J* = 7.5 Hz, 2H), 7.09 (d, *J* = 7.5 Hz, 2H), 4.02 (q, *J* = 7.2 Hz, 2H), 2.56 (d, *J* = 5.8 Hz, 1H), 2.48 (dd, *J* = 14.6, 7.7 Hz, 2H), 2.19 (t, *J* = 7.4 Hz, 2H), 1.80–1.51 (m, 5H), 1.32–1.19 (m, 2H), 1.15 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 173.5, 171.6, 148.1, 140.7, 138.3, 136.3, 134.5, 129.1, 128.3, 127.9, 127.4, 125.8, 121.5, 121.3, 116.4, 60.2, 40.2, 39.1, 35.5, 34.5, 32.4, 28.9, 21.9, 14.2. HRMS (ESI) m/z calculated for $C_{26}H_{31}N_2O_3^+$ $[M+H]^+$ 419.2329, found 419.2329.

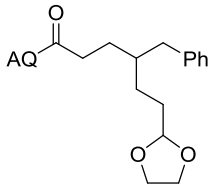
4-*benzyl-7-oxo-7-(quinolin-8-ylamino)heptyl benzoate* (2ag)



The title compound was isolated as a yellow oil (85% yield) after chromatography on silica with ethyl acetate:hexane (1:12). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.79 (s, 1H), 8.77 (t, *J* = 4.2 Hz, 2H),

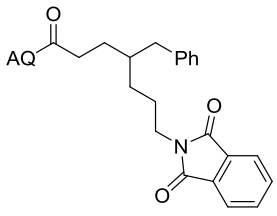
8.13 (dd, *J* = 8.2, 1.3 Hz, 1H), 8.00 (t, *J* = 8.2 Hz, 2H), 7.50 (m, 3H), 7.42 (m, 3H), 7.24 (t, *J* = 7.3 Hz, 2H), 7.17 (dd, *J* = 12.8, 7.0 Hz, 3H), 4.32–4.24 (m, 2H), 2.71 (dd, *J* = 13.6, 5.5 Hz, 1H), 2.60 (m, 3H), 1.93–1.78 (m, 5H), 1.56–1.42 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 166.6, 148.1, 140.6, 138.3, 136.3, 134.5, 132.8, 130.4, 129.5, 129.1, 128.3, 128.3, 127.9, 127.4, 125.9, 121.6, 121.4, 116.4, 65.1, 40.2, 39.0, 35.5, 29.2, 29.1, 25.7. HRMS (ESI) m/z calculated for $C_{30}H_{31}N_2O_3^+$ $[M+H]^+$ 467.2329, found 467.2328.

4-benzyl-6-(1,3-dioxolan-2-yl)-N-(quinolin-8-yl)hexanamide **(2ah)**



The title compound was isolated as a black oil (85% yield) after chromatography on silica with ethyl acetate:hexane (1:12). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.67 (s, 1H), 8.69 (m, 2H), 8.05 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.44–7.37 (m, 2H), 7.34 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.17 (t, *J* = 7.4 Hz, 2H), 7.08 (dd, *J* = 13.0, 7.0 Hz, 3H), 4.75 (t, *J* = 4.7 Hz, 1H), 3.89–3.81 (m, 2H), 3.76–3.70 (m, 2H), 2.61–2.36 (m, 4H), 1.80–1.59 (m, 5H), 1.40 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 148.1, 140.7, 138.3, 136.3, 134.5, 129.2, 128.3, 127.9, 127.4, 125.9, 121.5, 121.3, 116.4, 104.7, 64.8, 40.3, 39.2, 35.4, 30.8, 28.9, 27.1. HRMS (ESI) m/z calculated for $C_{25}H_{28}N_2O_3^+$ $[M+H]^+$ 405.2173, found 405.2178.

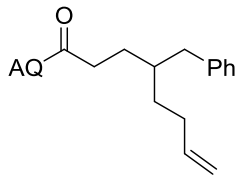
4-benzyl-7-(1,3-dioxoisoindolin-2-yl)-N-(quinolin-8-yl)heptanamide **(2ai)**



The title compound was isolated as a brown oil (65% yield) after chromatography on silica with ethyl acetate:hexane (1:6). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.79 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.74 (dd, *J* = 7.2, 1.6 Hz, 1H), 8.14 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.81 (m, 2H), 7.68 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.54–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.25–7.04 (m, 5H), 3.66 (t, *J* = 7.2 Hz, 2H), 2.57 (m, 4H), 1.86–1.70 (m, 5H), 1.39 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 168.4, 148.1, 140.5,

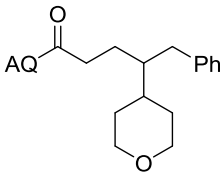
138.3, 136.3, 134.5, 133.8, 132.1, 129.1, 128.2, 127.9, 127.4, 125.8, 123.1, 121.5, 121.3, 116.4, 40.1, 38.9, 38.1, 35.5, 29.9, 29.0, 25.4. HRMS (ESI) m/z calculated for $C_{31}H_{30}N_3O_3^+$ $[M+H]^+$ 492.2282, found 492.2286.

4-benzyl-N-(quinolin-8-yl)oct-7-enamide **(2aj)**



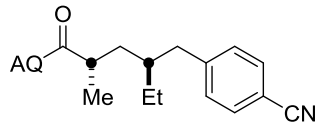
The title compound was isolated as a brown oil (62% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.80–8.75 (m, 2H), 8.14 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.84–7.77 (m, 1H), 7.54–7.45 (m, 3H), 7.45–7.41 (m, 2H), 7.26 (s, 1H), 7.18 (d, *J* = 7.4 Hz, 3H), 5.77 (m, 1H), 5.03–4.89 (m, 2H), 2.63 (t, *J* = 6.0 Hz, 2H), 2.54 (m, 2H), 2.19–2.08 (m, 2H), 1.86–1.78 (m, 3H), 1.43 (dd, *J* = 13.4, 7.7 Hz, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 147.5, 140.8, 138.8, 137.4, 134.1, 129.5, 129.2, 128.2, 128.1, 127.8, 125.8, 121.5, 121.4, 117.5, 114.5, 40.2, 38.8, 35.4, 32.2, 30.8, 29.0. HRMS (ESI) m/z calculated for $C_{24}H_{27}N_2O^+$ $[M+H]^+$ 359.2118, found 359.2121.

5-phenyl-N-(quinolin-8-yl)-4-(tetrahydro-2H-pyran-4-yl)pentanamide **(2ak)**



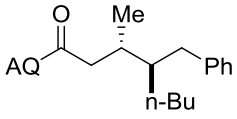
The title compound was isolated as a brown oil (40% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.16 (s, 1H), 8.50–8.43 (m, 1H), 8.15 (d, *J* = 7.8 Hz, 1H), 7.80 (m, 1H), 7.42–7.34 (m, 2H), 7.24 (d, *J* = 1.5 Hz, 1H), 7.20–7.14 (m, 1H), 7.14–7.08 (m, 2H), 3.75–3.50 (m, 5H), 3.24 (m, 1H), 3.00 (dd, *J* = 13.1, 3.5 Hz, 1H), 2.94–2.66 (m, 3H), 2.62–2.43 (m, 2H), 2.31 (dd, *J* = 13.0, 10.2 Hz, 1H), 1.76 (dd, *J* = 10.0, 4.9 Hz, 1H), 1.61 (m, 1H), 1.47 (s, 9H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 148.0, 141.1, 138.3, 136.3, 134.4, 129.0, 128.4, 127.9, 127.4, 125.9, 121.5, 121.4, 116.4, 68.4, 44.5, 37.4, 37.0, 36.1, 29.7, 29.5, 26.0. HRMS (ESI) m/z calculated for $C_{25}H_{29}N_2O_2^+$ $[M+H]^+$ 389.2224, found 389.2225.

***(2S,4S)-4-(4-cyanobenzyl)-2-methyl-N-(quinolin-8-yl)hexanamide* (2al)**



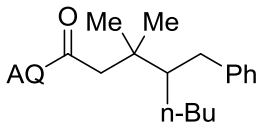
The title compound was isolated as a yellow oil (54% yield) afterchromatography on silica with ethyl acetate:hexane (1:6). This product was isolated as a single diastereomer. The reported dr was determined by ^{1}H NMR analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.81 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.78 (dd, *J* = 6.9, 2.0 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.53 (dd, *J* = 12.0, 5.1 Hz, 2H), 7.47 (dd, *J* = 8.3, 2.8 Hz, 3H), 7.25 (d, *J* = 8.2 Hz, 2H), 2.74 (dd, *J* = 13.6, 6.5 Hz, 1H), 2.63 (dd, *J* = 13.7, 7.5 Hz, 2H), 1.95 (m, 1H), 1.73 (dd, *J* = 13.0, 6.6 Hz, 1H), 1.43–1.38 (m, 1H), 1.34–1.29 (m, 2H), 1.28 (d, *J* = 6.8 Hz, 3H), 0.91 (dd, *J* = 9.3, 5.5 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.9, 148.2, 147.1, 138.4, 136.4, 134.4, 132.0, 129.9, 127.9, 127.4, 121.6, 121.5, 119.0, 116.5, 109.6, 40.6, 40.4, 39.0, 38.2, 26.0, 18.5, 10.4. HRMS (ESI) m/z calculated for $C_{24}H_{26}N_3O^+$ $[M+H]^+$ 372.2070, found 372.2070.

***(3S,4R)-4-benzyl-3-methyl-N-(quinolin-8-yl)octanamide* (2am)**



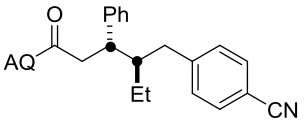
The title compound was isolated as a yellow oil (70% yield) after chromatography on silica with ethyl acetate:hexane (1:15). This product was isolated as a single diastereomer. The reported dr was determined by GC-MS analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.80 (s, 1H), 8.81–8.77 (m, 2H), 8.18–8.13 (m, 1H), 7.54–7.44 (m, 3H), 7.26–7.15 (m, 5H), 2.74–2.57 (m, 2H), 2.49–2.38 (m, 2H), 1.72 (s, 1H), 1.36–1.20 (m, 6H), 1.04 (dd, *J* = 16.2, 6.3 Hz, 3H), 0.87–0.79 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.5, 148.1, 141.7, 138.3, 136.3, 134.5, 129.2, 128.2, 127.9, 127.4, 125.6, 121.5, 121.3, 116.4, 44.5, 43.0, 36.8, 31.9, 30.2, 29.7, 22.9, 15.7, 14.0. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375.2432.

***(R)-4-benzyl-3,3-dimethyl-N-(quinolin-8-yl)octanamide* (2an)**



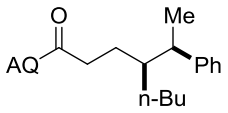
The title compound was isolated as an orange oil (30% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.82–8.78 (m, 2H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.55–7.49 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.25–7.21 (m, 4H), 7.16–7.12 (m, 1H), 3.02 (dd, *J* = 13.7, 3.9 Hz, 1H), 2.54 (s, 2H), 2.38 (dd, *J* = 13.7, 9.1 Hz, 1H), 1.75–1.70 (m, 1H), 1.56–1.50 (m, 1H), 1.26 (d, *J* = 5.2 Hz, 1H), 1.21 (s, 3H), 1.19 (s, 3H), 1.14–1.06 (m, 3H), 0.92–0.87 (m, 1H), 0.71 (t, *J* = 7.1 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.8, 148.1, 142.6, 138.4, 136.3, 134.5, 129.1, 128.1, 127.9, 127.4, 125.5, 121.5, 121.3, 116.3, 49.6, 48.6, 37.7, 37.5, 31.9, 30.4, 25.5, 23.0, 13.8. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 389.2587, found 375.2592.

(3S,4R)-4-(4-cyanobenzyl)-3-phenyl-N-(quinolin-8-yl)hexanamide **(2ao)**



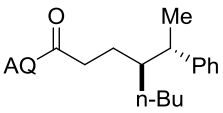
The title compound was isolated as a white solid (70% yield) after chromatography on silica with ethyl acetate:hexane (1:6). This product was isolated as a single diastereomer. The reported dr was determined by ^{1}H NMR analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.75 (m, 1H), 8.67 (dd, *J* = 6.2, 2.7 Hz, 1H), 8.14 (dd, *J* = 8.2, 1.5 Hz, 1H), 7.49 (dd, *J* = 8.9, 5.3 Hz, 4H), 7.44 (dd, *J* = 8.3, 4.3 Hz, 1H), 7.29 (dd, *J* = 7.7, 5.7 Hz, 4H), 7.22–7.14 (m, 3H), 3.48 (m, 1H), 3.12–2.99 (m, 1H), 2.92 (dd, *J* = 14.7, 9.0 Hz, 1H), 2.73 (dd, *J* = 13.7, 4.8 Hz, 1H), 2.37 (dd, *J* = 13.7, 9.4 Hz, 1H), 2.05–2.00 (m, 1H), 1.42–1.30 (m, 2H), 0.93 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.1, 148.0, 147.5, 142.0, 138.2, 136.3, 134.2, 132.0, 129.8, 128.5, 128.4, 127.8, 127.3, 126.7, 121.5, 121.4, 119.1, 116.4, 109.6, 46.2, 43.7, 41.5, 37.2, 22.3, 10.5. HRMS (ESI) m/z calculated for $C_{29}H_{28}N_3O^+$ $[M+H]^+$ 434.2227, found 434.2227.

(S)-4-((R)-1-phenylethyl)-N-(quinolin-8-yl)octanamide **(2ap)**



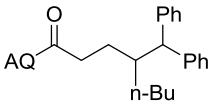
The title compound was isolated as a yellow oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:15). This product was isolated as a single diastereomer. The reported dr was determined by GC-MS analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.71 (s, 1H), 8.76 (m, 2H), 8.12 (d, *J* = 8.3 Hz, 1H), 7.52–7.40 (m, 3H), 7.30–7.10 (m, 5H), 2.80 (m, 1H), 2.57–2.36 (m, 2H), 1.83–1.74 (m, 1H), 1.73–1.60 (m, 2H), 1.35 (m, 3H), 1.28 (dd, *J* = 12.3, 5.0 Hz, 6H), 0.87 (dd, *J* = 9.4, 4.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 48.0, 146.3, 138.3, 136.3, 134.5, 128.2, 127.9, 127.7, 127.4, 125.8, 121.5, 121.3, 116.3, 43.6, 41.9, 35.9, 29.4, 28.7, 27.2, 23.1, 17.91, 14.11. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375.2430.

(S)-4-((S)-1-phenylethyl)-N-(quinolin-8-yl)octanamide **(2aq)**



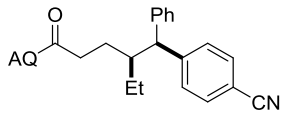
The title compound was isolated as a fulvous oil (75% yield) after chromatography on silica with ethyl acetate:hexane (1:20). This product was isolated as a single diastereomer. The reported dr was determined by GC-MS analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.78 (dd, *J* = 13.7, 5.2 Hz, 2H), 8.15 (d, *J* = 8.1 Hz, 1H), 7.52 (dd, *J* = 14.8, 7.2 Hz, 2H), 7.46–7.43 (m, 1H), 7.26 (d, *J* = 7.7 Hz, 2H), 7.22–7.13 (m, 3H), 2.82 (p, *J* = 7.0 Hz, 1H), 2.58–2.50 (m, 1H), 2.46–2.37 (m, 1H), 1.97–1.84 (m, 1H), 1.83–1.74 (m, 1H), 1.67 (dd, *J* = 10.1, 5.4 Hz, 1H), 1.34–1.18 (m, 9H), 0.87–0.81 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 148.0, 146.5, 138.3, 136.4, 134.5, 128.1, 127.9, 127.7, 127.4, 125.8, 121.5, 121.3, 116.4, 43.6, 41.6, 35.6, 30.6, 29.0, 25.6, 22.9, 17.3, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{31}N_2O^+$ $[M+H]^+$ 375.2431, found 375.2430.

(S)-4-benzhydryl-N-(quinolin-8-yl)octanamide **(2ar)**



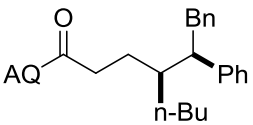
The title compound was isolated as a yellow oil (62% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.76 (m, 2H), 8.13 (dd, *J* = 8.3, 1.4 Hz, 1H), 7.53–7.40 (m, 4H), 7.35–7.10 (m, 10H), 3.75 (d, *J* = 11.0 Hz, 1H), 2.58–2.32 (m, 3H), 1.96–1.71 (m, 2H), 1.46–1.03 (m, 7H), 0.82 (m, 3H); ^{3}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.0, 144.3, 144.1, 138.3, 136.3, 134.7, 134.5, 130.9, 128.6, 128.5, 128.1, 127.9, 127.4, 126.2, 121.5, 121.3, 116.3, 56.4, 40.1, 34.9, 30.1, 27.8, 26.7, 23.0, 14.0. HRMS (ESI) m/z calculated for $C_{30}H_{33}N_2O^+$ $[M+H]^+$ 437.2587, found 437.2587.

(S)-4-((S)-(4-cyanophenyl)(phenyl)methyl)-N-(quinolin-8-yl)hexanamide **(2as)**



The title compound was isolated as a white solid (75% yield) after chromatography on silica with ethyl acetate:hexane (1:6). This product was isolated as a single diastereomer. The reported dr was determined by ^{1}H NMR analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.58 (s, 1H), 8.71 (dd, *J* = 4.2, 1.6 Hz, 1H), 8.65 (dd, *J* = 7.1, 1.8 Hz, 1H), 8.08 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.41 (m, 7H), 7.19 (t, *J* = 3.7 Hz, 4H), 7.12–7.07 (m, 1H), 3.74 (d, *J* = 11.2 Hz, 1H), 2.46–2.29 (m, 3H), 1.79–1.70 (m, 1H), 1.69–1.62 (m, 1H), 1.43 (m, 1H), 1.29–1.23 (m, 1H), 0.80 (d, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.2, 149.8, 148.1, 142.7, 138.2, 136.4, 134.4, 132.5, 128.8, 128.8, 128.0, 127.9, 127.4, 126.7, 121.7, 121.5, 118.8, 116.3, 110.0, 56.1, 40.6, 34.9, 26.0, 22.2, 9.2. HRMS (ESI) m/z calculated for $C_{29}H_{28}N_3O^+$ $[M+H]^+$ 434.2232, found 434.2232.

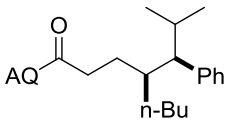
4-(1,2-diphenylethyl)-N-(quinolin-8-yl)octanamide **(2at)**



The title compound was isolated as a yellow oil (80% yield) after chromatography on silica with ethyl acetate:hexane (1:12). This product was isolated as a 2:1 mixture of diastereomers.

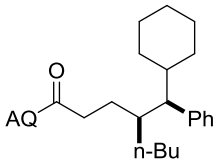
The reported dr was determined by ^{1}H NMR analysis. The following analytical data correspond to the mixture.^{1}H NMR (400 MHz, $CDCl_3$) δ 9.64 (s, 1H), 9.59 (s, 1H), 8.72–8.66 (m, 2H), 8.65 (m, 1H), 8.07–8.02 (m, 1H), 7.73 (m, 1H), 7.47–7.37 (m, 4H), 7.36–7.31 (m, 2H), 7.16–7.08 (m, 3H), 7.05–6.96 (m, 8H), 6.92 (m, 3H), 3.06 (m, 1H), 2.95–2.82 (m, 2H), 2.81–2.72 (m, 1H), 2.49–2.20 (m, 3H), 1.98–1.87 (m, 1H), 1.75 (m, 1H), 1.68–1.59 (m, 2H), 1.46–1.05 (m, 11H), 0.80 (t, *J* = 7.1 Hz, 3H), 0.74 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.9, 171.3, 148.1, 148.0, 144.6, 142.8, 141.0, 141.0, 140.5, 138.3, 136.3, 136.3, 134.5, 129.9, 129.1, 129.0, 128.8, 128.5, 128.4, 128.3, 128.2, 128.0, 127.9, 127.9, 127.7, 127.4, 126.0, 126.0, 125.7, 125.5, 121.5, 121.5, 121.3, 121.2, 116.4, 116.3, 50.0, 45.6, 44.4, 43.6, 41.7, 39.1, 35.7, 33.2, 32.7, 30.2, 28.8, 28.0, 26.7, 26.5, 23.0, 22.9, 14.1, 14.0. HRMS (ESI) m/z calculated for $C_{27}H_{31}N_3O^+$ $[M+H]^+$ 451.2744, found 451.2744.

***N-(2-(2-phenyl-1-(piperidin-1-yl)ethyl)hexyl)picolinamide* (2au)**



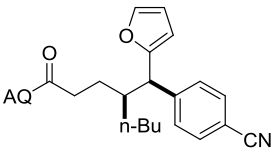
The title compound was isolated as a fulvous oil (82% yield) after chromatography on silica with ethyl acetate:hexane (1:15). This product was isolated as a single diastereomer. The reported dr was determined by GC-MS analysis. The following analytical data correspond to the mixture. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.65 (s, 1H), 8.73–8.66 (m, 2H), 8.08 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.45–7.36 (m, 3H), 7.19–7.14 (m, 2H), 7.12–7.03 (m, 3H), 2.49 (m, 1H), 2.39–2.28 (m, 2H), 2.13 (dd, *J* = 14.5, 6.7 Hz, 1H), 1.95 (m, 1H), 1.90–1.80 (m, 1H), 1.36–1.15 (m, 9H), 0.84 (dd, *J* = 12.4, 6.8 Hz, 6H), 0.64 (dd, *J* = 11.8, 7.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 147.9, 141.6, 138.2, 136.4, 134.5, 129.7, 127.9, 127.6, 127.4, 125.8, 121.5, 121.2, 116.4, 54.8, 38.2, 36.1, 30.2, 28.9, 28.5, 26.1, 23.1, 21.7, 20.2, 14.1. HRMS (ESI) m/z calculated for $C_{27}H_{35}N_2O^+$ $[M+H]^+$ 403.2744, found 403.2744.

***(S)-4-((R)-cyclohexyl(phenyl)methyl)-N-(quinolin-8-yl)octanamide* (2av)**



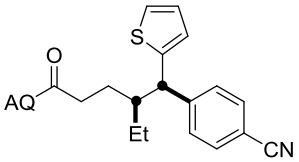
The title compound was isolated as a brown oil (85% yield) after chromatography on silica with ethyl acetate:hexane (1:15). This product was isolated as a single diastereomer. The reported dr was determined by GC-MS analysis. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.65 (s, 1H), 8.72–8.65 (m, 2H), 8.04 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.45–7.38 (m, 2H), 7.34 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.16 (m, 2H), 7.12–6.99 (m, 3H), 2.51–2.44 (m, 1H), 2.43–2.21 (m, 2H), 2.01–1.78 (m, 2H), 1.77–1.65 (m, 2H), 1.61–1.48 (m, 3H), 1.40–0.94 (m, 11H), 0.87–0.77 (m, 3H), 0.76–0.62 (m, 2H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 13C NMR (101 MHz, CDCl3) δ 172.0, 148.0, 141.8, 138.3, 136.3, 134.5, 129.7, 127.9, 127.7, 127.4, 125.8, 121.5, 121.2, 116.3, 53.9, 38.5, 37.3, 36.2, 32.0, 30.8, 30.2, 29.0, 26.6, 26.2, 23.0, 14.2. HRMS (ESI) m/z calculated for $C_{30}H_{39}N_2O$ $[M+H]^+$ 443.3057, found 443.3058.

(S)-4-((R)-(4-cyanophenyl)(furan-2-yl)methyl)-N-(quinolin-8-yl)octanamide **(2aw)**



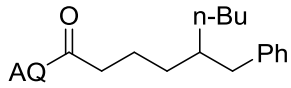
The title compound was isolated as a white solid (75% yield) after chromatography on silica with ethyl acetate:hexane (1:6). This product was isolated as a single diastereomer. The reported dr was determined by ^{1}H NMR analysis. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.80 (dd, *J* = 4.2, 1.4 Hz, 1H), 8.72 (dd, *J* = 6.8, 2.0 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.3 Hz, 1H), 7.53 (t, *J* = 7.5 Hz, 4H), 7.46 (t, *J* = 7.3 Hz, 3H), 7.33 (d, *J* = 1.5 Hz, 1H), 6.30–6.27 (m, 1H), 6.15 (d, *J* = 3.2 Hz, 1H), 3.98 (d, *J* = 9.7 Hz, 1H), 2.52–2.37 (m, 2H), 1.74–1.65 (m, 2H), 1.52–1.44 (m, 1H), 1.39–1.30 (m, 2H), 0.90 (t, *J* = 7.4 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 154.9, 148.1, 147.0, 141.7, 138.2, 136.4, 134.3, 132.3, 129.2, 127.9, 127.4, 121.7, 121.5, 118.8, 116.3, 110.4, 110.2, 106.9, 48.9, 41.9, 35.1, 26.2, 23.0, 10.0. HRMS (ESI) m/z calculated for $C_{29}H_{30}N_3O_2^+$ $[M+H]^+$ 452.2338, found 452.2339.

(S)-4-((R)-(4-cyanophenyl)(thiophen-2-yl)methyl)-N-(quinolin-8-yl)hexanamide **(2ax)**



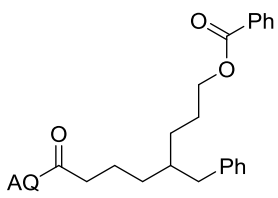
The title compound was isolated as a white solid (70% yield) after chromatography on silica with ethyl acetate:hexane (1:6). This product was isolated as a 20:1 mixture of diastereomers. The reported dr was determined by ^{1}H NMR analysis. ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.66 (s, 1H), 8.80 (dd, *J* = 4.2, 1.7 Hz, 1H), 8.72 (dd, *J* = 6.9, 2.1 Hz, 1H), 8.17 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.55–7.44 (m, 7H), 7.18–7.13 (m, 1H), 6.93–6.88 (m, 2H), 4.17 (d, *J* = 10.2 Hz, 1H), 2.55–2.41 (m, 2H), 2.33 (m, 1H), 1.85–1.77 (m, 1H), 1.71–1.65 (m, 1H), 1.56 (m, 1H), 1.44 (dd, *J* = 12.0, 4.6 Hz, 1H), 0.96–0.90 (m, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.1, 148.9, 148.1, 146.1, 138.2, 136.4, 134.3, 132.5, 128.9, 127.9, 127.4, 126.7, 124.8, 124.1, 121.7, 121.5, 118.8, 116.3, 110.4, 50.8, 43.4, 34.9, 26.1, 22.7, 9.9. HRMS (ESI) m/z calculated for $C_{27}H_{25}N_3OS^+$ $[M+H]^+$ 440.1791, found 440.1791.

5-benzyl-N-(quinolin-8-yl)nonanamide **(2ay)**



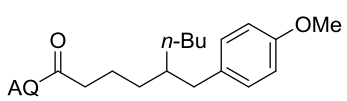
The title compound was isolated as a colorless oil (60% yield) after chromatography on silica with ethyl acetate:hexane (1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.74 (s, 1H), 8.78–8.74 (m, 2H), 8.10 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.47 (dd, *J* = 12.2, 4.5 Hz, 2H), 7.39 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.24 (t, *J* = 7.4 Hz, 2H), 7.17–7.10 (m, 3H), 2.53–2.43 (m, 3H), 1.81–1.48 (m, 6H), 1.34–1.08 (m, 6H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 148.1, 146.1, 138.4, 136.4, 134.6, 128.25, 128.0, 127.7, 127.4, 125.8, 121.6, 121.3, 116.4, 45.9, 38.2, 36.7, 29.9, 27.4, 25.8, 22.8, 14.1. HRMS (ESI) m/z calculated for $C_{25}H_{30}N_2O^+$$[M+H]^+$ 374.2358, found 374.2358.

4-benzyl-8-oxo-8-(quinolin-8-ylamino)octyl benzoate **(2az)**



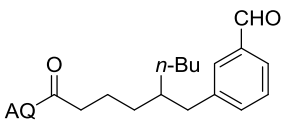
The title compound was isolated as a colorless oil (59% yield) after chromatography on silica with ethyl acetate:hexane (1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.81–8.73 (m, 2H), 8.15 (dd, *J* = 8.2, 1.4 Hz, 1H), 8.06–7.96 (m, 2H), 7.56–7.40 (m, 6H), 7.26 (t, *J* = 3.7 Hz, 2H), 7.23–7.13 (m, 3H), 4.23 (t, *J* = 6.3 Hz, 2H), 2.64–2.55 (m, 1H), 2.55–2.42 (m, 2H), 1.82–1.60 (m, 6H), 1.36–1.32 (m, 1H), 1.31–1.20 (m, 2H), 0.90–0.83 (m, 1H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.7, 166.6, 148.0, 145.1, 138.3, 136.3, 134.5, 132.7, 130.4, 129.5, 128.4, 128.3, 127.9, 127.6, 127.4, 126.1, 121.5, 121.3, 116.4, 65.0, 45.6, 38.1, 36.7, 33.1, 27.2, 26.8, 25.6. HRMS (ESI) m/z calculated for $C_{31}H_{33}N_2O_3^+[M+H]^+$ 481.2486, found 481.2486.

5-(4-methoxybenzyl)-N-(quinolin-8-yl)nonanamide **(2ba)**



The title compound was isolated as a colorless oil (50% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.75 (s, 1H), 8.79–8.75 (m, 2H), 8.14 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.53–7.47 (m, 2H), 7.44 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.04 (d, *J* = 8.6 Hz, 2H), 6.79 (d, *J* = 8.6 Hz, 2H), 3.76 (s, 3H), 2.51–2.41 (m, 3H), 1.94–1.62 (m, 4H), 1.61–1.44 (m, 2H), 1.31–1.18 (m, 4H), 1.17–1.05 (m, 2H), 0.81 (t, *J* = 7.2 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.8, 157.6, 148.0, 138.3, 138.0, 136.3, 134.5, 128.4, 127.9, 127.4, 121.5, 121.3, 116.4, 113.6, 55.1, 44.9, 38.2, 36.8, 33.1, 29.8, 27.3, 25.7, 22.7, 14.0. HRMS (ESI) m/z calculated for $C_{26}H_{33}N_2O_2^+[M+H]^+$ 405.2537, found 405.2536.

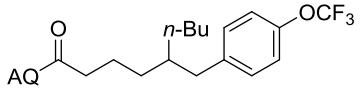
5-(3-formylbenzyl)-N-(quinolin-8-yl)nonanamide **(2bb)**



The title compound was isolated as a colorless oil (73% yield) after chromatography on silica with ethyl acetate:hexane (1:12). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.97 (s, 1H), 9.74 (s, 1H), 8.81–8.73 (m, 2H), 8.14 (d, *J* = 8.1 Hz, 1H), 7.70–7.63 (m, 2H), 7.51 (dd, *J* =

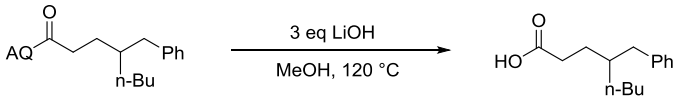
12.9, 5.7 Hz, 2H), 7.47–7.39 (m, 3H), 2.63–2.57 (m, 1H), 2.49 (dd, *J* = 9.1, 5.8 Hz, 1H), 1.77 (dd, *J* = 16.5, 8.4 Hz, 2H), 1.69–1.52 (m, 3H), 1.47–0.93 (m, 8H), 0.86–0.74 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 192.6, 171.6, 148.1, 147.2, 138.3, 136.5, 136.3, 134.5, 134.0, 128.9, 128.6, 127.9, 127.7, 127.4, 121.5, 121.3, 116.4, 45.7, 38.0, 36.5, 36.4, 29.7, 27.2, 25.6, 22.6, 13.9. HRMS (ESI) m/z calculated for $C_{26}H_{31}N_2O_2^+[M+H]^+$ 403.2308, found 403.2308.

N-(quinolin-8-yl)-5-(4-(trifluoromethoxy)benzyl)nonanamide **(2bc)**



The title compound was isolated as a fulvous oil (65% yield) after chromatography on silica with ethyl acetate:hexane (1:15). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.76 (s, 1H), 8.82–8.74 (m, 2H), 8.16 (dd, *J* = 8.3, 1.6 Hz, 1H), 7.56–7.48 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.14–7.06 (m, 3H), 2.54–2.45 (m, 2H), 1.87–1.45 (m, 6H), 1.42–0.94 (m, 7H), 0.89–0.74 (m, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.6, 148.0, 147.2, 144.7, 138.3, 137.8, 137.7, 136.3, 134.5, 128.7, 127.9, 127.4, 121.5, 121.3, 120.7, 119.2, 116.4, 45.3, 38.0, 36.6, 36.6, 29.7, 27.2, 25.6, 22.6, 13.9. ^{19}F NMR (376 MHz, $CDCl_3$) δ -57.83. HRMS (ESI) m/z calculated for $C_{25}H_{30}N_2O^+[M+H]^+$ 374.2358, found 374.2358.

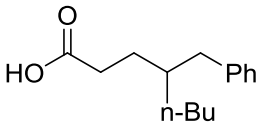
6. Derivatization of 2a



2a
0.2 mmol

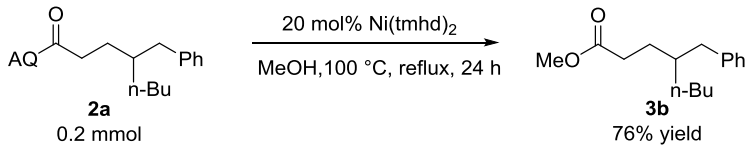
3a
94% yield

4-benzyloctanoic acid **(3a)**

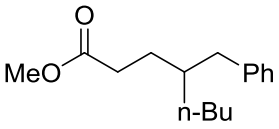


To a 10 mL schlenk tube equipped with a magnetic stir bar were added LiOH (3 eq), 8-aminoquinoline amide **2a** (0.2 mmol, 75.0 mg) and methanol (1 mL). The resulting mixture was stirred at 120 ℃ for 16 h. At this time, the reaction mixture was allowed to cool

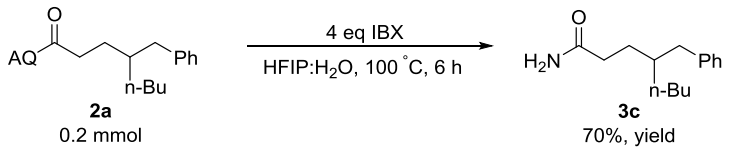
to room temperature, diluted with 50 mL of EtOAc and washed with HCl (1 M, 3 × 2 mL). The organic layers were combined, dried over Na_2SO_4, and concentrated in vacuo to give pure hydrolysis free acid product. The title compound was isolated as a yellow oil (44.2 mg, 94% yield) ^{1}H NMR (400 MHz, $CDCl_3$) δ 10.60 (s, 1H), 7.29–7.24 (m, 2H), 7.21–7.09 (m, 3H), 2.53 (m, 2H), 2.34 (dd, *J* = 16.9, 7.9 Hz, 2H), 1.64 (m, 3H), 1.27 (dd, *J* = 9.9, 6.9 Hz, 6H), 0.87 (dd, *J* = 8.0, 4.0 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 180.4, 140.9, 129.1, 128.2, 125.8, 40.2, 39.1, 32.2, 31.5, 28.5, 28.0, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{15}H_{23}O_2^+[M+H]^+$ 235.1693, found 235.1693.



methyl 4-benzyloctanoate **(3b)**



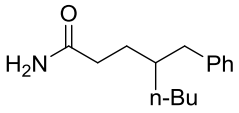
To a 10 mL schlenk tube equipped with a magnetic stir bar were added Ni(tmhd)$_2$ (20 mol%, 18.0 mg), **2a** (0.2 mmol, 75.0 mg) and methanol (1 mL) under an argon atmosphere. After the tube was tightly sealed, the mixture was allowed to stir at 100 ˚C for 24 h. After cooling to room temperature, methanol was removed and the crude mixture was directly purified by flash silica gel column chromatography (eluent: 7:1 ethyl acetate:hexane) to give **3b** as a black oil (38 mg, 76% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 (t, *J* = 7.3 Hz, 2H), 7.20–7.11 (m, 3H), 3.64 (s, 3H), 2.54 (m, 2H), 2.36–2.23 (m, 2H), 1.66–1.57 (m, 3H), 1.26 (d, *J* = 4.2 Hz, 6H), 0.87 (t, *J* = 5.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 174.3, 141.0, 129.1, 128.2, 125.7, 51.4, 40.2, 39.1, 32.5, 31.5, 28.6, 28.3, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{16}H_{25}O_2^+[M+H]^+$ 249.1849, found 249.1849.



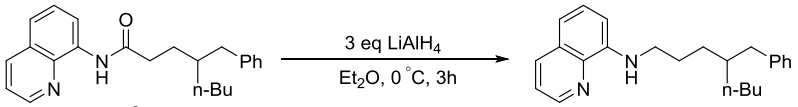
2a
0.2 mmol

3c
70%, yield

4-benzyloctanamide **(3c)**



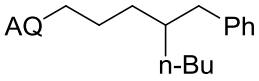
To a 10 mL schlenk tube equipped with a magnetic stir bar were added 2a (0.2 mmol, 1 eq), IBX (2-iodoxybenzoic acid, 0.8 mmol, 4 eq), and HFIP:H_2O (1:1) 3 mL under an argon atmosphere. After the tube was tightly sealed, the mixture was allowed to stir at 100 ˚C for 6 h.[4] After cooling to room temperature, and the crude mixture was directly purified by flash silica gel column chromatography (eluent: 1:1 ethyl acetate : hexane) to give amide **3c** as a brown oil (33 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (dd, *J* = 8.3, 6.6 Hz, 2H), 7.10 (dd, *J* = 17.6, 7.2 Hz, 3H), 5.39 (d, *J* = 63.8 Hz, 2H), 2.54 (dd, *J* = 13.6, 6.5 Hz, 1H), 2.43 (dd, *J* = 13.6, 7.1 Hz, 1H), 2.18–2.05 (m, 2H), 1.58–1.51 (m, 2H), 1.32–1.25 (m, 1H), 1.24–1.16 (m, 6H), 0.80 (t, *J* = 6.7 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.7, 141.1, 129.1, 128.2, 125.8, 40.4, 39.2, 33.3, 32.8, 29.0, 28.6, 22.9, 14.0. HRMS (ESI) m/z calculated for $C_{15}H_{24}NO^+[M+H]^+$ 234.1852, found 234.1852.



2a
0.2 mmol

3d
84%, yield

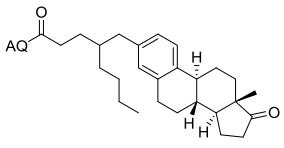
4-benzyloctanamide (3d)



To a 10 mL schlenk tube equipped with a magnetic stir bar were added $LiAlH_4$ (0.6 mmol, 3 eq), **2a** (0.2 mmol, 1 eq) and diethyl ether (1 mL). After the tube was tightly sealed, the mixture was allowed to stir at 0 ˚C for 3 h. And the crude mixture was directly purified by flash silica gel column chromatography (eluent: 1:15 ethyl acetate:hexane) to give amide **3d** as a black oil (48.6 mg, 70% yield). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.60 (dd, *J* = 4.2, 1.6 Hz, 1H), 7.93 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.29–7.21 (m, 2H), 7.15 (t, *J* = 7.3 Hz,

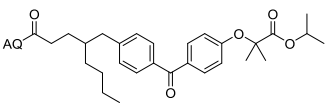
2H), 7.09–7.02 (m, 3H), 6.92 (d, *J* = 7.6 Hz, 1H), 6.53 (d, *J* = 7.5 Hz, 1H), 6.02 (s, 1H), 3.15 (d, *J* = 4.3 Hz, 2H), 2.53–2.42 (m, 2H), 1.70 (m, 3H), 1.33 (dd, *J* = 14.5, 7.7 Hz, 2H), 1.18 (d, *J* = 11.7 Hz, 6H), 0.78 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.7, 141.4, 135.9, 129.1, 128.7, 128.1, 127.8, 125.6, 121.3, 113.4, 104.4, 43.8, 40.4, 39.5, 32.8, 30.6, 28.8, 26.2, 23.0, 14.1. HRMS (ESI) m/z calculated for $C_{24}H_{30}N_2^+[M+H]^+$ 347.2482, found 347.2482.

***4-(((8R,9S,13S,14S)-13-methyl-17-oxo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-3-yl)methyl)-N-(quinolin-8-yl)octanamide (*4a)**



The title compound was isolated as a white solid (67% yield) after chromatography on silica with ethyl acetate:hexane (1:8). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.68 (d, *J* = 4.3 Hz, 1H), 8.76–8.67 (m, 2H), 8.09 (dd, *J* = 8.3, 1.5 Hz, 1H), 7.48–7.36 (m, 3H), 7.09 (dd, *J* = 7.9, 2.9 Hz, 1H), 6.89 (d, *J* = 7.9 Hz, 1H), 6.83 (s, 1H), 2.82–2.73 (m, 2H), 2.47 (m, 5H), 2.34–2.27 (m, 1H), 2.17–1.85 (m, 5H), 1.74 (dd, *J* = 14.4, 6.9 Hz, 3H), 1.59–1.38 (m, 6H), 1.30–1.20 (m, 6H), 0.84–0.79 (m, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 170.9, 147.0, 137.4, 137.3, 136.0, 135.3, 135.1, 133.5, 128.7, 128.7, 126.9, 126.4, 125.6, 124.1, 120.5, 120.2, 115.3, 49.5, 46.9, 43.2, 38.8, 38.2, 37.1, 34.8, 34.6, 31.8, 30.6, 28.3, 28.0, 27.6, 25.5, 24.6, 22.0, 20.5, 13.1, 12.8. HRMS (ESI) m/z calculated for $C_{36}H_{45}N_2O_2^+[M+H]^+$537.3476, found 537.3476.

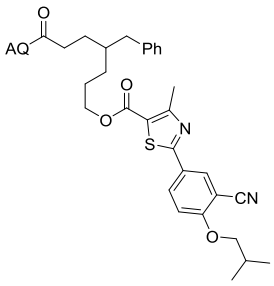
Isopropyl 2-methyl-2-(4-(4-(2-(3-oxo-3-(quinolin-8-ylamino)propyl)hexyl)benzoyl)phenoxy)propanoate (4b)



The title compound was isolated as a colorless oil (87% yield) after chromatography on silica with ethyl acetate:hexane (1:12). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.68 (d, *J* = 6.5 Hz, 2H), 8.05 (d, *J* = 7.5 Hz, 1H), 7.66 (d, *J* = 8.6 Hz, 2H), 7.60 (d, *J* = 7.9 Hz, 2H), 7.46–7.38 (m, 2H), 7.34 (dd, *J* = 8.2, 4.2 Hz, 1H), 7.19 (d, *J*

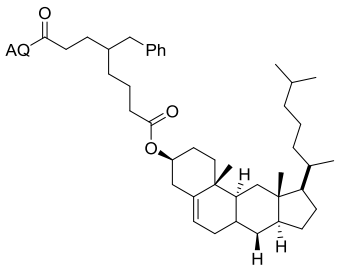
= 8.0 Hz, 2H), 6.76 (d, *J* = 8.7 Hz, 2H), 4.99 (m, 1H), 2.61 (d, *J* = 2.9 Hz, 2H), 2.49 (m, 2H), 1.75 (s, 3H), 1.57 (s, 6H), 1.30–1.20 (m, 6H), 1.11 (d, *J* = 6.3 Hz, 6H), 0.80 (t, *J* = 6.9 Hz, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 195.2, 173.1, 171.6, 159.3, 148.1, 145.9, 138.3, 136.3, 135.7, 134.5, 131.9, 130.9, 130.0, 129.0, 127.9, 127.4, 121.6, 121.4, 117.2, 116.3, 79.3, 69.3, 40.4, 39.2, 35.5, 32.7, 29.1, 28.6, 25.4, 22.9, 21.5, 14.0. HRMS (ESI) m/z calculated for $C_{36}H_{45}N_2O_2^+$[M+H]$^+$ 609.3323, found 609.3323.

4-benzyl-7-oxo-7-(quinolin-8-ylamino)heptyl 2-(3-cyano-4-isobutoxyphenyl)-4-methylthiazole-5-carboxylate (4c)



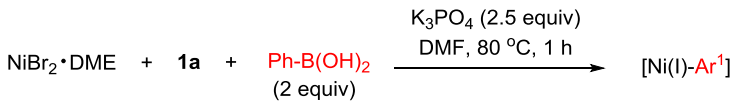
The title compound was isolated as a colorless oil (45% yield) after chromatography on silica with ethyl acetate:hexane (1:8). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.78 (s, 1H), 8.79–8.74 (m, 2H), 8.17–8.12 (m, 2H), 8.04 (dd, *J* = 8.8, 2.3 Hz, 1H), 7.55–7.48 (m, 2H), 7.45 (dd, *J* = 8.3, 4.2 Hz, 1H), 7.24 (d, *J* = 7.4 Hz, 2H), 7.17 (dd, *J* = 16.0, 7.3 Hz, 3H), 6.94 (d, *J* = 8.9 Hz, 1H), 4.26 (t, *J* = 6.4 Hz, 2H), 3.88 (d, *J* = 6.5 Hz, 2H), 2.72 (s, 3H), 2.61 (t, *J* = 6.3 Hz, 2H), 2.23–2.18 (m, 1H), 1.87 (dd, *J* = 6.1, 3.3 Hz, 2H), 1.57 (d, *J* = 13.0 Hz, 2H), 1.52–1.44 (m, 2H), 1.25 (s, 2H), 1.09 (d, *J* = 6.7 Hz, 6H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 171.3, 167.0, 162.3, 161.8, 160.9, 147.9, 140.4, 138.1, 136.2, 134.3, 132.4, 131.9, 129.0, 128.2, 127.8, 127.3, 125.9, 125.8, 121.7, 121.4, 121.2, 116.3, 115.2, 112.4, 102.8, 75.5, 65.2, 40.2, 38.8, 35.3, 29.0, 28.8, 28.0, 25.5, 18.9, 17.3. HRMS (ESI) m/z calculated for $C_{39}H_{41}N_4O_4S^+$[M+H]$^+$ 661.2843, found 661.2448.

(3S,7aS,10S,10aR,11aS,11bR)-10a,11b-dimethyl-10-(5-methylhexyl)-2,3,4,6,6a,7,7a,8,9,10,10a,11,11a,11b-tetradecahydro-1H-cyclopenta[b]phenanthren-3-yl 5-benzyl-8-oxo-8-(quinolin-8-ylamino)octanoate (4d)



The title compound was isolated as a colorless oil (47% yield) after chromatography on silica with ethyl acetate:hexane (1:3). ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.70 (s, 1H), 8.71 (m, 2H), 8.09 (dd, *J*= 8.3, 1.6 Hz, 1H), 7.47–7.36 (m, 3H), 7.19–7.16 (m, 2H), 7.16–7.04 (m, 3H), 5.28 (d, *J*= 4.3 Hz, 1H), 4.52 (m, 1H), 2.58–2.46 (m, 3H), 2.26–2.15 (m, 4H), 1.90 (t, *J* = 18.5 Hz, 2H), 1.82–1.69 (m, 6H), 1.68–1.58 (m, 2H), 1.54 (s, 2H), 1.51–1.34 (m, 8H), 1.33–1.24 (m, 5H), 1.23–1.13 (m, 3H), 1.03 (m, 7H), 0.92 (s, 3H), 0.84 (d, *J* = 6.5 Hz, 4H), 0.79 (dd, *J* = 6.6, 1.7 Hz, 6H), 0.60 (s, 3H); ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.9, 171.6, 148.1, 140.7, 139.7, 138.3, 136.3, 134.5, 129.1, 128.3, 127.9, 127.4, 125.8, 122.6, 121.5, 121.3, 116.4, 73.8, 56.7, 56.1, 50.0, 42.3, 40.3, 39.7, 39.5, 39.1, 38.1, 37.0, 36.5, 36.2, 35.7, 35.5, 34.8, 32.4, 31.9, 29.0, 28.2, 28.0, 27.8, 24.2, 23.8, 22.7, 22.5, 22.0, 21.0, 19.3, 18.7, 11.8. HRMS (ESI) m/z calculated for $C_{50}H_{69}N_2O_3^+$[M+H]$^+$ 745.5303, found 745.5303.

7. EPR Experiment



Procedure: To a 25 mL schlenk tube were added $NiBr_2$•DME (0.03 mmol, 15 mol%), K_3PO_4 (0.50 mmol, 2.5 eq), alkene substrate (0.20 mmol, 1.0 eq), phenylboronic acid (0.40 mmol, 2 eq), and DMF (1 mL). The resulting mixture was stired for 1h at 80 ℃. A small portion of this solution (300 μL) was taken into a capillary tube and sealed tight with wax for EPR experiment (Figure S1). The tube was sealed in the glovebox and immediately frozen in liquid nitrogen.

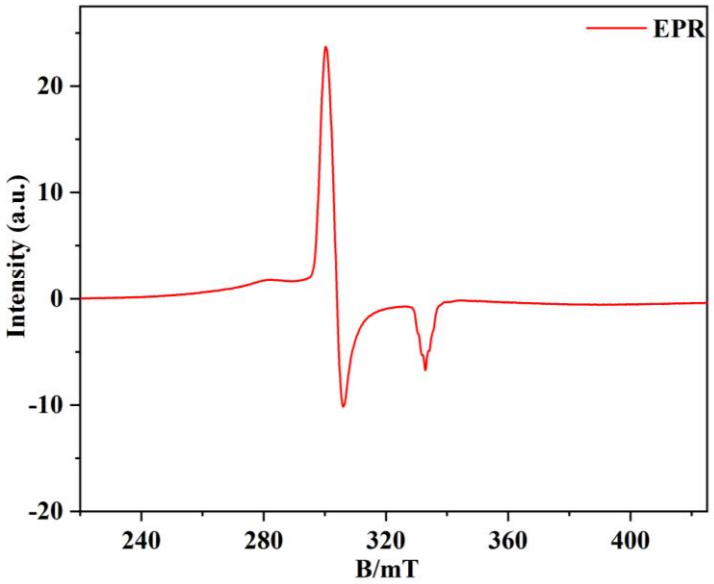


Figure S1. EPR Spectrum of complex Ni(I)-Ar^1. Temperature = 95 K, solvent = DMF. Spectroscopic parameters: g = [2.00 2.19 2.22]. Microwave frequency = 9.3714 GHz, power = 0.4743 mW, modulation amplitude = 5.00 G

8. X-ray Crystallographic Data

Single crystals for X-ray studies were grown by slow evaporation of a solution of compound **2ao** in a mixture of petroleum ether and ethyl acetate at room temperature. X-Ray structural analysis of single crystal **2ao** was obtained to confirm the absolute configuration. The X-ray data of **2ao** is deposited in the Cambridge Crystallographic Data Centre with a number of CCDC 2129040.

Crystal Data for $C_{29}H_{27}N_3O$ (M =433.53 g/mol): triclinic, space group P-1 (no. 2), a = 10.0837(10) Å, b = 11.1991(10) Å, c = 11.8993(11) Å, α = 105.919(8) °, β = 108.497(9) °, γ = 96.764(8) °, V = 1194.2(2) Å^3, Z = 2, T = 293(2) K, μ(MoKα) = 0.074 mm^{-1}, *Dcalc* = 1.206 g/cm^3, 8547 reflections measured (4.372° ≤ 2Θ ≤ 50.012°), 4198 unique (R_{int} = 0.0257, R_{sigma} = 0.0554) which were used in all calculations. The final R_1 was 0.0599 (I > 2σ(I)) and wR_2 was 0.1931 (all data).

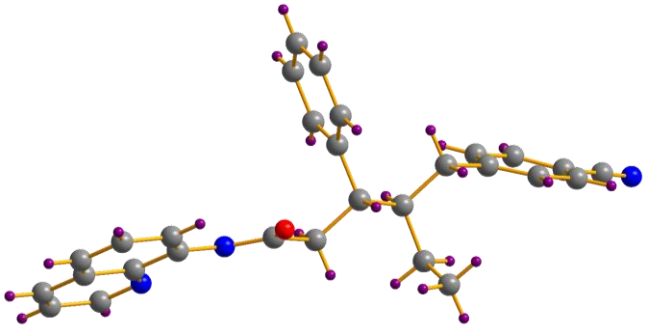


Figure S2. X-ray structure of compound **2ao (** CCDC 2129040).

Table S5. Crystal data and structure refinement for 2ao.

Identification code	A210509C
Empirical formula	$C_{29}H_{27}N_3O$
Formula weight	433.53
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1

a/Å	10.0837(10)
b/Å	11.1991(10)
c/Å	11.8993(11)
α/°	105.919(8)
β/°	108.497(9)
γ/°	96.764(8)
Volume/Å^3	1194.2(2)
Z	2
ρ_{calc}g/cm^3	1.206
μ/mm^{-1}	0.074
F(000)	460.0
Crystal size/mm^3	0.25 × 0.22 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.372 to 50.012
Index ranges	-11 ≤ h ≤ 11, -13 ≤ k ≤ 13, -12 ≤ l ≤ 14
Reflections collected	8547
Independent reflections	4198 [R_{int} = 0.0257, R_{sigma} = 0.0554]
Data/restraints/parameters	4198/21/300
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0599, wR_2 = 0.1564
Final R indexes [all data]	R_1 = 0.1113, wR_2 = 0.1931
Largest diff. peak/hole / e Å^{-3}	0.23/-0.18

Single crystals for X-ray studies were grown by slow evaporation of a solution of compound **2as** in a mixture of petroleum ether and ethyl acetate at room temperature. X-Ray structural analysis of single crystal **2as** was obtained to confirm the absolute configuration. The X-ray data of **2as** is deposited in the Cambridge Crystallographic Data Centre with a number of CCDC 2129080.

Crystal Data for $C_{29}H_{26}N_3O$ (*M* =432.53 g/mol): triclinic, space group P-1 (no. 2), *a* = 10.2156(16) Å, *b* = 10.6541(17) Å, *c* = 12.2607(19) Å, *α* = 75.489(14) °, *β* = 86.653(13) °, *γ* = 68.487(15) °, *V* = 1201.0(4) Å^3, *Z* = 2, *T* = 293(2) K, μ(MoKα) = 0.073 mm^{-1}, *Dcalc* = 1.196 g/cm^3, 8562 reflections measured (4.288° ≤ 2Θ ≤ 50.012°), 4226 unique (R_{int} = 0.0648, R_{sigma} = 0.1460) which were used in all calculations. The final R_1 was 0.0829 (I > 2σ(I)) and wR_2 was 0.2746 (all data).

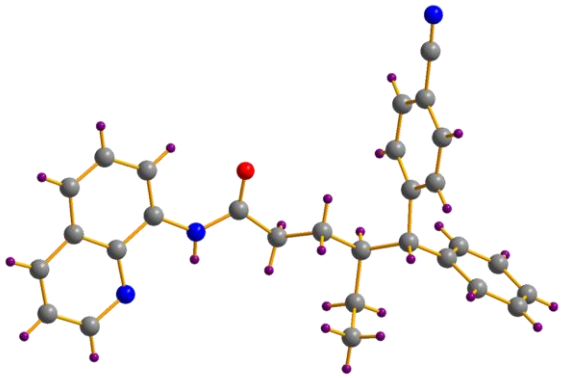


Figure S3. X-ray structure of compound **2as (**CCDC 2129080).

Table S6. Crystal data and structure refinement for 2ao.

Identification code	A210509C
Empirical formula	$C_{29}H_{27}N_3O$
Formula weight	433.53
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	10.0837(10)
b/Å	11.1991(10)
c/Å	11.8993(11)
α/°	105.919(8)
β/°	108.497(9)
γ/°	96.764(8)

Volume/$Å^3$	1194.2(2)
Z	2
$\rho_{calc}g/cm^3$	1.206
μ/mm^{-1}	0.074
F(000)	460.0
Crystal size/mm^3	0.25 × 0.22 × 0.18
Radiation	MoKα (λ = 0.71073)
2Θ range for data collection/°	4.372 to 50.012
Index ranges	$-11 \leq h \leq 11$, $-13 \leq k \leq 13$, $-12 \leq l \leq 14$
Reflections collected	8547
Independent reflections	4198 [R_{int} = 0.0257, R_{sigma} = 0.0554]
Data/restraints/parameters	4198/21/300
Goodness-of-fit on F^2	1.054
Final R indexes [I>=2σ (I)]	R_1 = 0.0599, wR_2 = 0.1564
Final R indexes [all data]	R_1 = 0.1113, wR_2 = 0.1931
Largest diff. peak/hole / e $Å^{-3}$	0.23/-0.18

9. Kinetic Studies

Reaction set up & analysis (Standard condition)

In an argon-filled glovebox, $NiBr_2$•DME (0.03 mmol, 15 mol%), N-(quinolin-8-yl)pent-4-enamide (**1a**) (0.20 mmol, 1 eq), phenylboronic acid (0.40 mmol, 2 eq), dimethyl terephthalate (0.05 mmol, 25 mol%) as internal standard, n-butyl iodide (0.4 mmol, 2 eq), MeOH (3 mmol, 15 eq) and DMF (1 mL), were added to a 12 mL tube, The test tube was sealed with a PTFE/silicon septa cap. The reaction mixture was stirred at 80 ˚C. 2.0 μL of the reaction mixture was taken out at 30, 50, 70, 90, 110, 130, 150, 170, 190, 210 minutes and quenched with 0.6 mL ethyl acetate immediately. The yield was monitored by GC-MS.[5]

Table S7. Experimental data of standard condition.

Time	Yield of **2a**	Time	Yield of **2a**
3	6.1%	25	50.7%
6	15.1%	30	56.1%
9	19.9%	35	61.1%
12	25.4%	45	67.8%
15	30.4%	60	72.9%
18	33.4%	120	78.0%
21	41.5%		

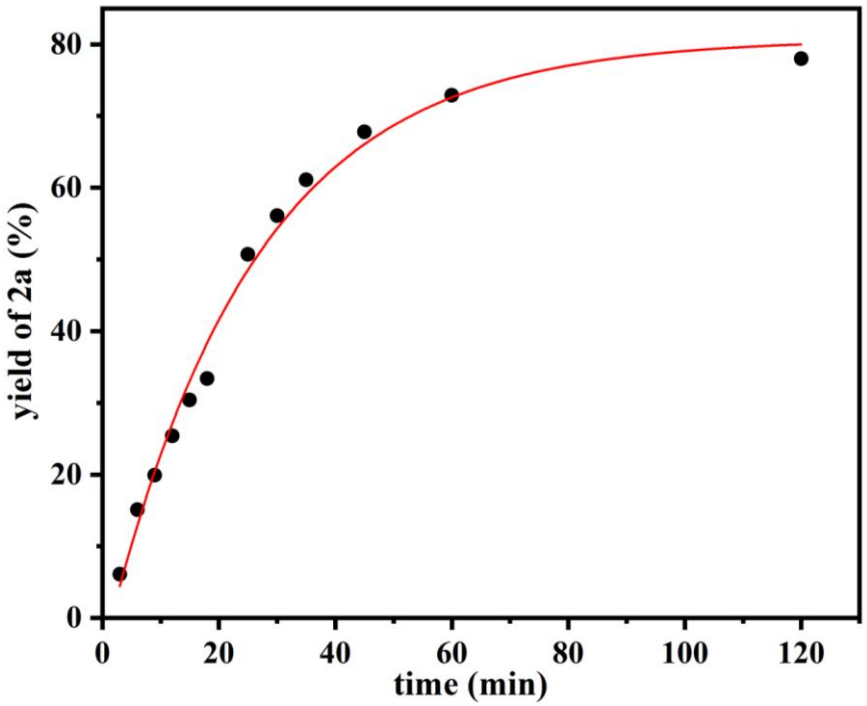


Figure S4. Plot of the formation of product **2a** from the reaction of **1a** (0.20 mmol), phenylboronic acid (0.40 mmol) and ^{n}BuI (0.40 mmol) in 1 mL dry DMF at different time intervals at 80 ˚C.

Table S8. The molar concentration ($\times 10^{-3}$ M) of product **2a** in different concentrations of $NiBr_2$•DME at different time.

	[Ni] 7.5 mol% (0.015 M)	[Ni] 15 mo% (0.030 M)	[Ni] 30 mo% (0.045 M)	[Ni] 60 mol% (0.060 M)
Time (min)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3}M)
3	1.231	1.606	2.231	2.849
6	1.925	2.746	3.768	4.773
9	2.423	3.970	5.287	6.616
12	3.532	4.891	6.821	8.730
15	3.860	6.086	8.270	10.650
18	4.622	6.995	9.895	12.450

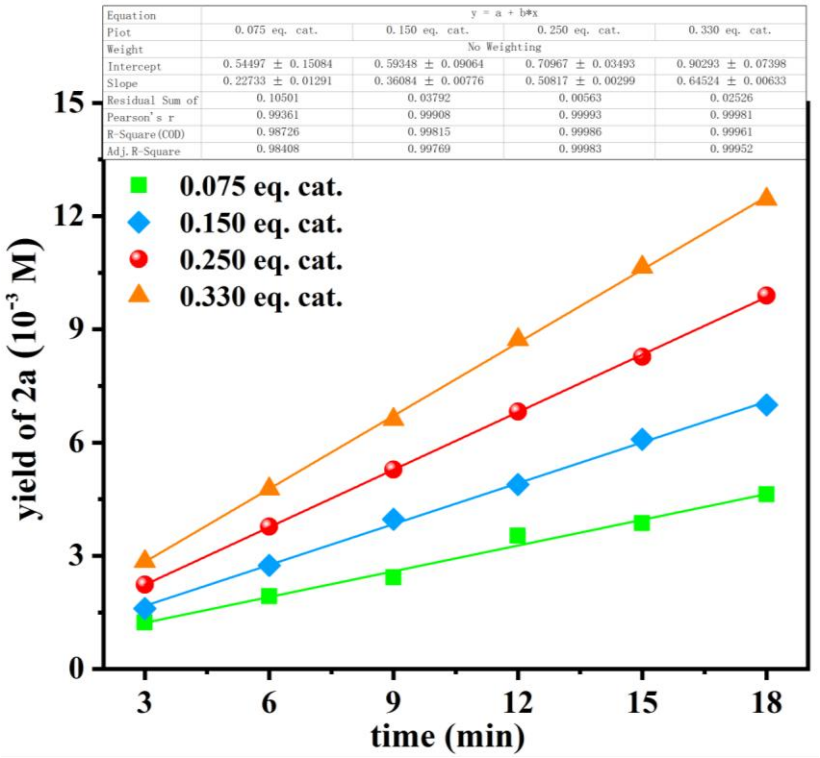


Figure S5. Plot of the formation of product **2a** from the reaction of **1a** (0.2 mmol), phenylboronic acid (0.40 mmol); 1-iodobutane (0.40 mmol);with 0.015 M, 0.030 M, 0.045 M, 0.060 M $NiBr_2$•DME at different time at 80 ˚C.

Table S9. The K_{in} value of product **2a** in different concentrations of $NiBr_2$•DME.

[Ni] (M)	K_{in} (M min^{-1})
0.015	0.2273×10^{-3}
0.030	0.3608×10^{-3}
0.050	0.5082×10^{-3}
0.066	0.6452×10^{-3}

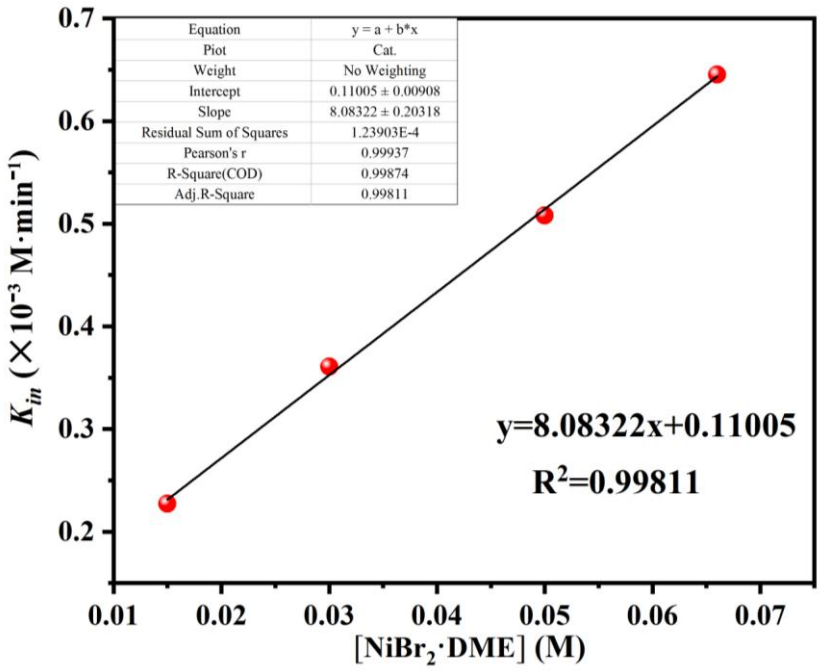


Figure S6. Plot of K_{in} versus of $NiBr_2$•DME from the reaction of **1a** (0.20 mmol), phenylboronic acid (0.40 mmol); 1-iodobutane (0.40 mmol); with 0.015 M, 0.030 M, 0.045 M, 0.060 M $NiBr_2$•DME.

Table S10. The molar concentration ($\times 10^{-3}$ M) of product **2a** in different concentrations of **1a** at different time.

	[**1a**] 0.5 mmol (0.05 M)	[**1a**] 1.0 mmol (0.10 M)	[**1a**] 2.0mmol (0.20 M)	[**1a**] 4.0 mmol (0.40 M)
Time (min)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3}M)
3	3.159	2.296	1.210	1.156
6	4.439	4.811	3.026	2.211
9	4.482	6.610	3.970	3.456
12	4.657	7.361	5.074	4.020
15	4.573	8.139	6.086	5.848
18	4.532	8.706	6.674	6.708
21	4.512	8.820	8.296	7.760
25	4.519	8.930	10.132	9.100

30	4.523	9.090	11.212	10.468

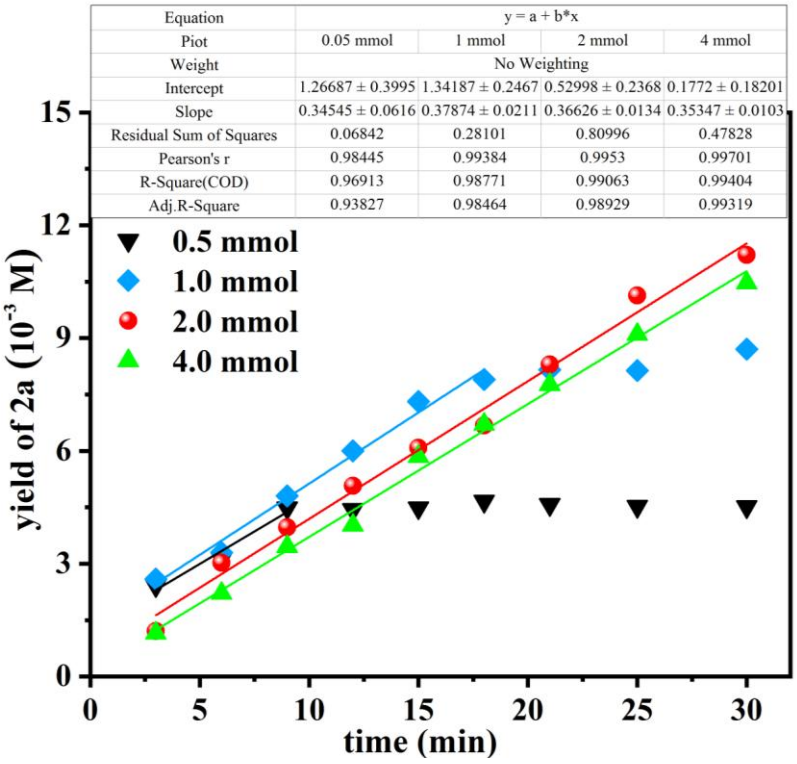


Figure S7. Plot of the formation of product **2a** from the reaction of phenylboronic acid (0.40 mmol), 1-iodobutane (0.40 mmol), with 0.05 M, 0.10 M, 0.20 M, 0.40 M and 0.80 M of **1a** at different time at 80 ˚C.

Table S11. The K_{in} value of product **2a** in different concentrations of **1a**.

[1a] (M)	K_{in} (M min^{-1})
0.050	0.3455×10^{-3}
0.10	0.3787×10^{-3}
0.20	0.3663×10^{-3}
0.40	0.3535×10^{-3}

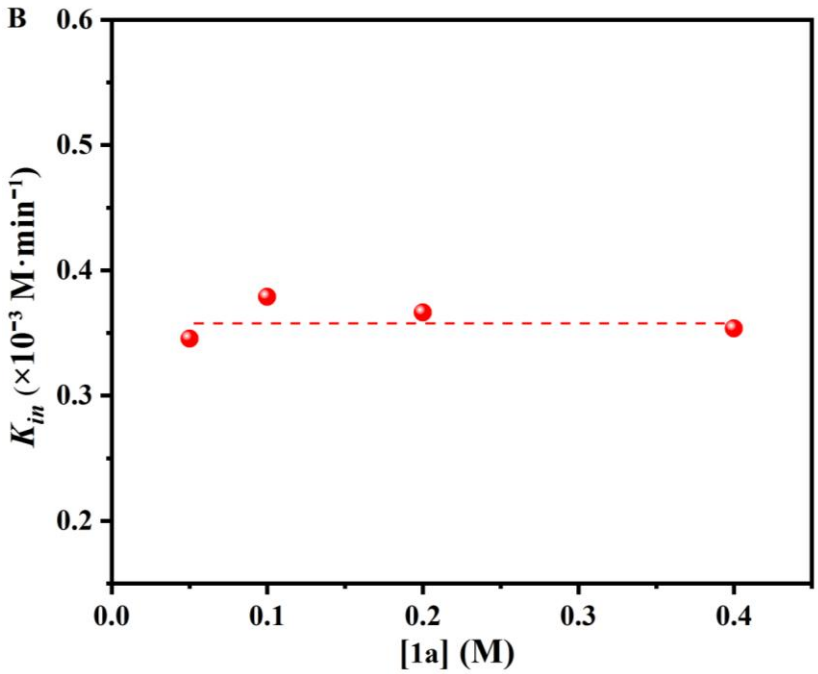


Figure S8. Plot of K_{in} versus of **1a** from the reaction of phenylboronic acid (0.40 mmol), 1-iodobutane (0.40 mmol), with 0.05 M, 0.10 M, 0.20 M, 0.40 M and 0.80 M of **1a.**

Table S12. The molar concentration ($\times 10^{-3}$ M) of product **2a** in different concentrations of phenylboronic acid at different time.

	$PhB(OH)_2$ 0.25 eq (0.05 M)	**$PhB(OH)_2$** 0.5 eq (0.10 M)	**$PhB(OH)_2$** 1.0 eq (0.20 M)	**$PhB(OH)_2$** 2.0 eq (0.40 M)	**$PhB(OH)_2$** 4.0 eq (0.80 M)
Time (min)	**[2a] (10^{-3} M)**	**[2a] (10^{-3} M)**	**[2a] (10^{-3} M)**	**[2a] (10^{-3}M)**	**[2a] (10^{-3}M)**
3	0.690	1.064	3.708	1.210	0.906
6	1.804	2.086	5.328	3.026	1.046
9	2.600	3.136	6.825	3.970	1.232
12	3.010	4.592	8.193	5.074	1.414
15	3.372	5.488	9.625	6.086	2.064
18	3.668	5.901	11.302	6.674	2.264
21	3.894	6.676	12.510	8.296	2.420

25	4.266	7.316	14.162	10.132	2.968
30	4.768	8.362	16.210	11.212	3.336

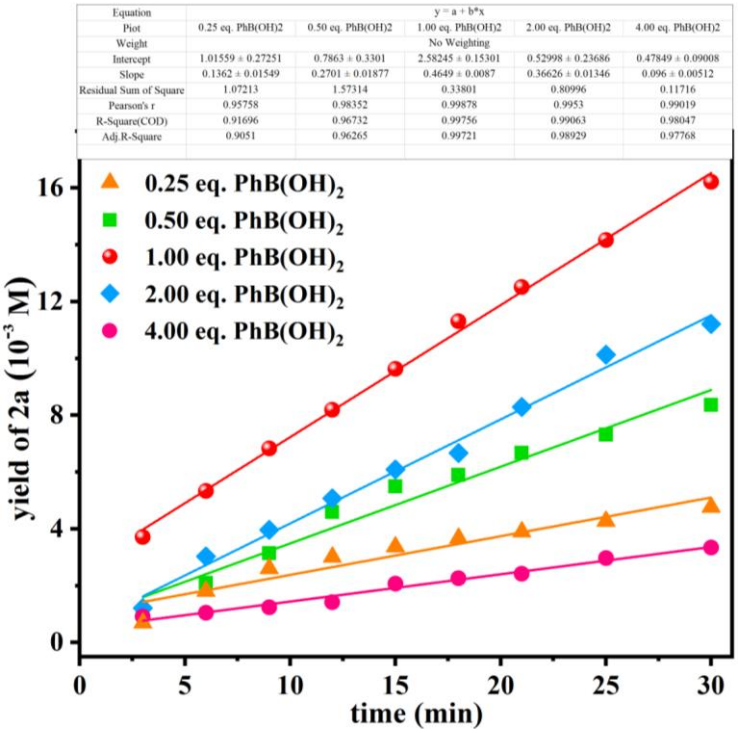


Figure S9. Plot of the formation of product **2a** from the reaction of **1a** (0.2 mmol), 1-iodobutane (0.40 mmol) with 0.05 M, 0.10 M, 0.20 M, 0.40 M and 0.80 M of phenylboronic acid at different time at 80 ˚C.

Table S13. The K_{in} value of product **2a** in different concentrations of phenylboronic acid.

$PhB(OH)_2$ (M)	K_{in} (M min^{-1})
0.050	0.1362×10^{-3}
0.10	0.2701×10^{-3}
0.20	0.4649×10^{-3}
0.40	0.3663×10^{-3}
0.80	0.0960×10^{-3}

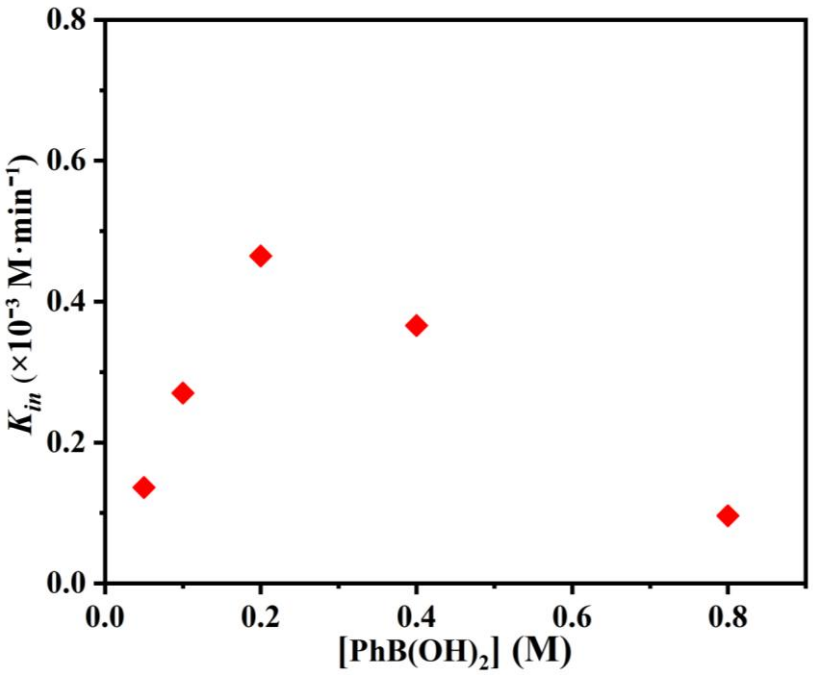


Figure S10. Plot of K_{in} versus phenylboronic acid from the reaction of **1a** (0.2 mmol), iodobutane (0.4 mmol) with 0.05 M, 0.10 M, 0.20 M, 0.40 M and 0.80 M of phenylboronic acid.

Table S14. The molar concentration ($\times 10^{-3}$ M) of product **2a** in different concentrations of 1-iodobutane at different time.

	^{n}BuI 1.0 eq (0.2 M)	^{n}BuI 2.0 eq (0.4 M)	^{n}BuI 3.0 eq (0.6 M)	^{n}BuI 4.0 eq (0.8 M)
Time (min)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3} M)	[**2a**] (10^{-3}M)
3	0.280	1.210	1.350	1.586
6	1.244	3.026	3.100	3.726
9	2.250	3.970	4.452	5.250
12	3.130	5.074	5.628	6.460
15	4.080	6.086	7.120	8.580
18	5.128	6.674	8.480	9.962
21	5.880	8.296	9.520	11.890
25	7.314	10.132	11.200	12.870
30	8.650	11.212	12.012	13.924

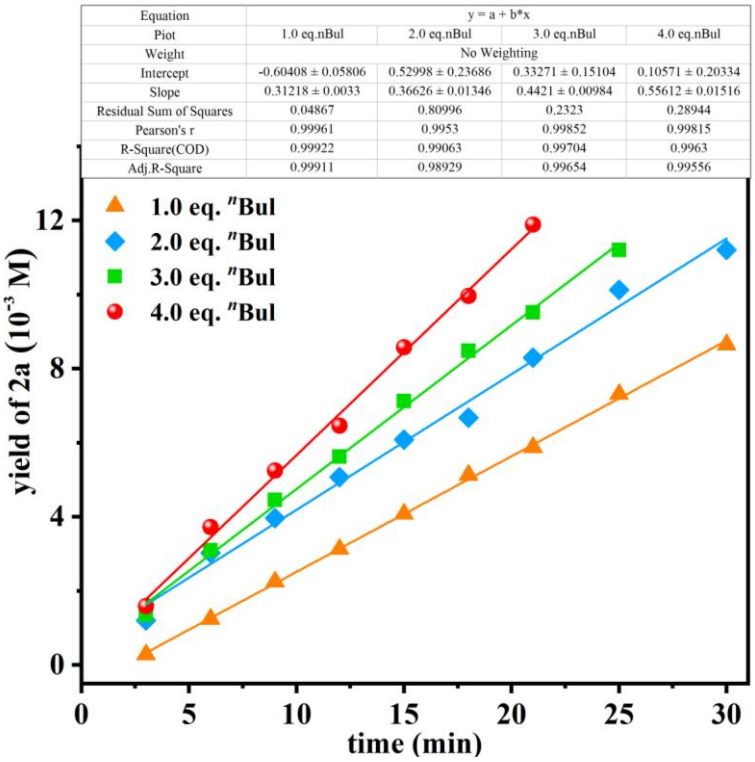


Figure S11. Plot of the formation of product **2a** from the reaction of **1a** (0.20 mmol), phenylboronic acid (0.40 mmol) with 0.20 M, 0.40 M, 0.60 M and 0.80 M of 1-iodobutane at different time at 80 ˚C.

Table S15. The K_{in} value of product **2a** in different concentrations of 1-iodobutane.

[^{n}BuI] **(M)**	K_{in} (M min^{-1})
0.20	0.3121×10^{-3}
0.40	0.3662×10^{-3}
0.60	0.4421×10^{-3}
0.80	0.5561×10^{-3}

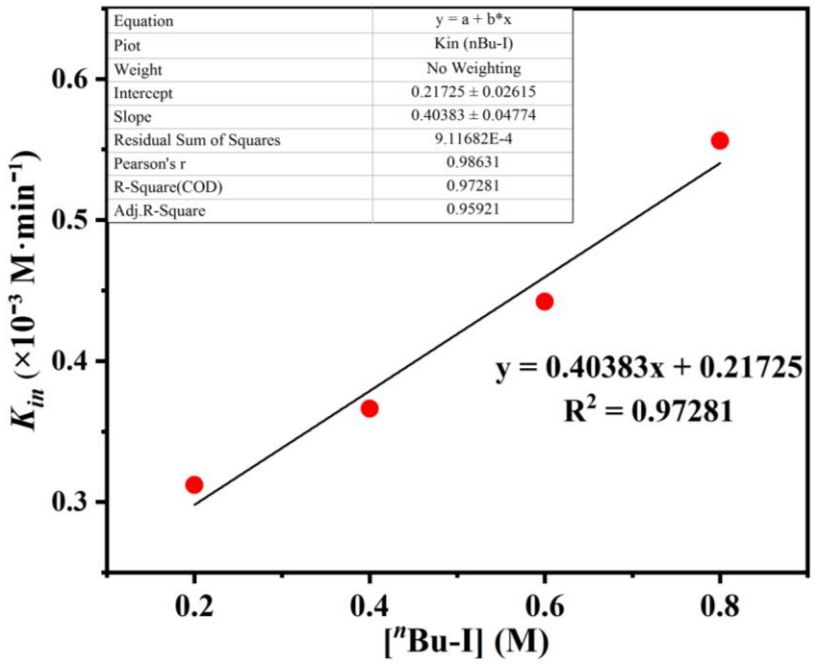


Figure S12. Plot of K_{in} versus [^{n}Bu-I] from the reaction of **1a** (0.2 mmol), phenylboronic acid (0.4mmol) with 0.20 M, 0.40 M, 0.60 M and 0.8 M of 1-iodobutane.

10. DFT Calculations

All the DFT calculations were performed by the Gaussian 16 package.[6,7] Molecular structures were optimized under (U)M06[8] hybrid functional with all-electron base set def2-SVP. A self-consistent response field (SCRF) model in the SMD solvation model[9] was used to consider the solvent effect of DMF, and the solvent entropy correction[10] was carried out. And the all-electron basis set def2-TZVP was used for single point correction. The Gibbs free energy of all the structures was conducted in solution at 373.15 K and at 1atm. The frequency analysis was performed to ensure that the optimized structure was the minimum energy point. Combined with the intrinsic reaction coordinate (IRC) calculation,[11] each transition state was determined to connect the intermediates. The non-covalent interaction was reached by NCI

analysis[12] using Multiwfn program[13] and plotted by VMD.[14] The 3D structures of the transition states and intermediates were drawn by CYLview software.[15]

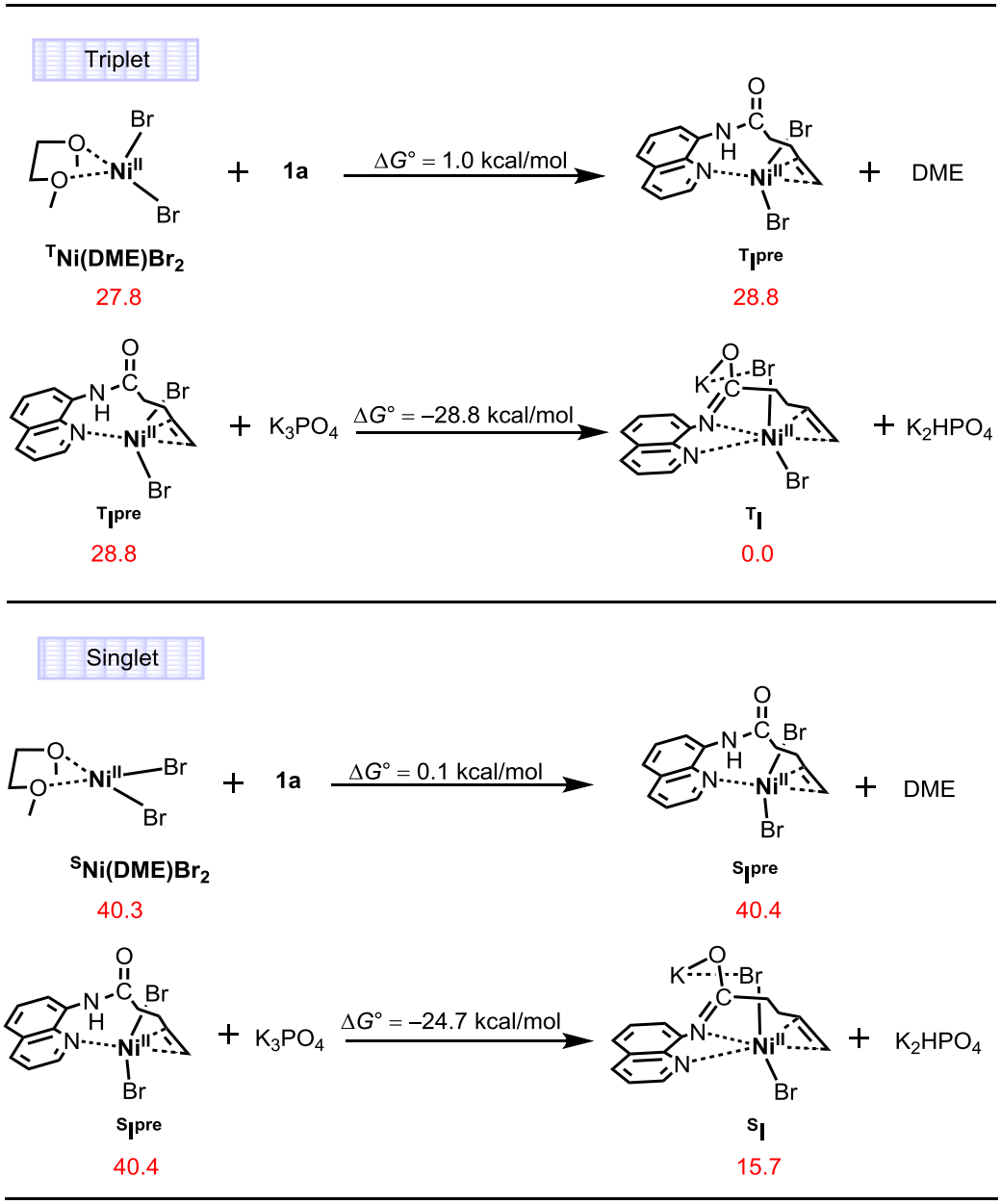


Figure S13. The relative stability of Ni(II) complexes.

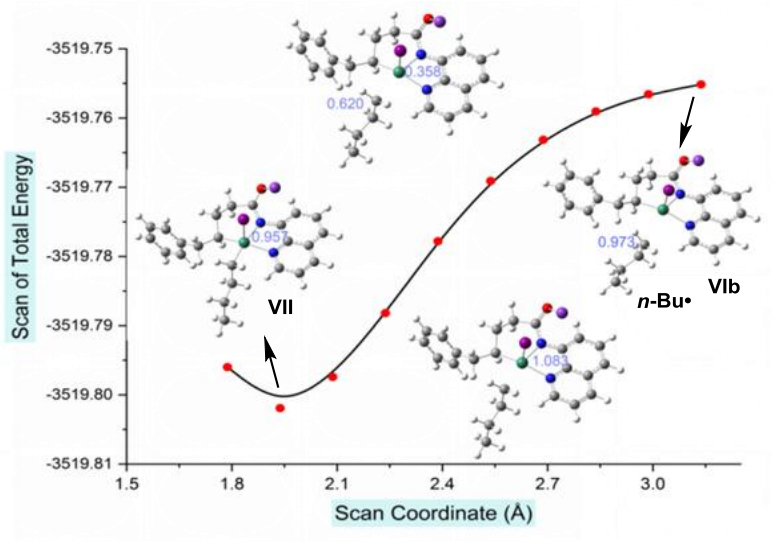


Figure S14. The barrier-free radical addition of *n*-Bu$^{\bullet}$ to **VIb**.

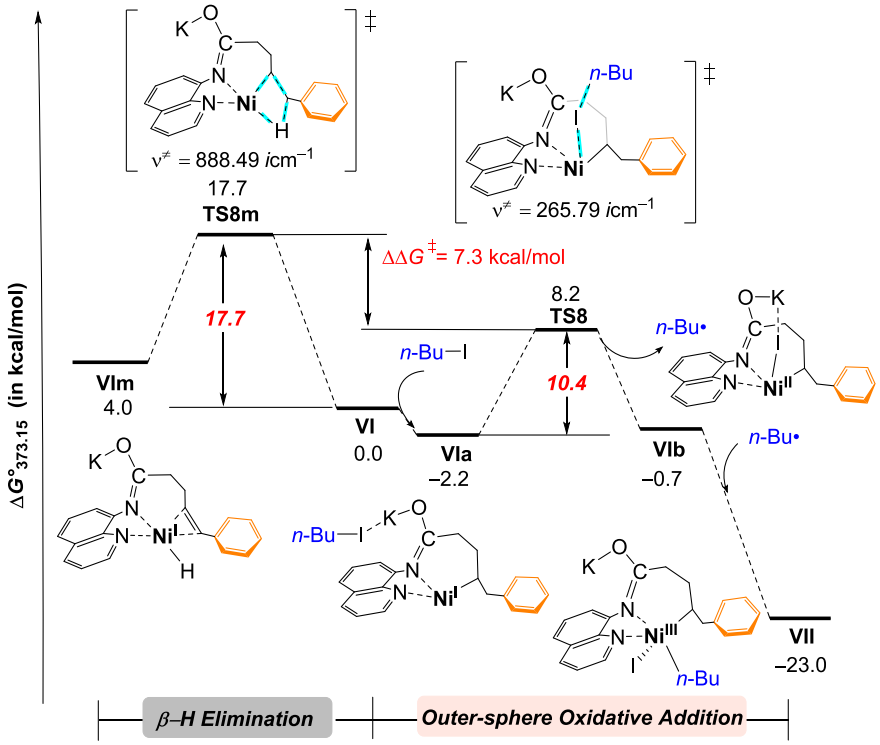


Figure S15. Two possible competing paths from intermediate **VI**.

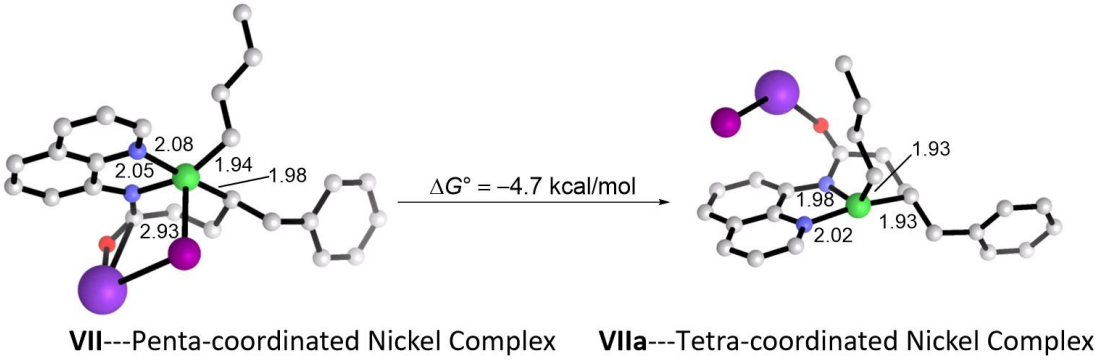


Figure S16. Two different coordination forms of trivalent nickel intermediates.

Nickel(III) complexes prefer a tetra-coordinated structure and thus a penta-coordinated **VII** is a thermodynamically unfavorable configuration. We also tried to find the reductive elimination transition state of **VII**. Unfortunately, iodine anion tends to be far away from the nickel center and interact with K cation, eventually forming the tetra-coordinated nickel(III) complex **VIIa**.

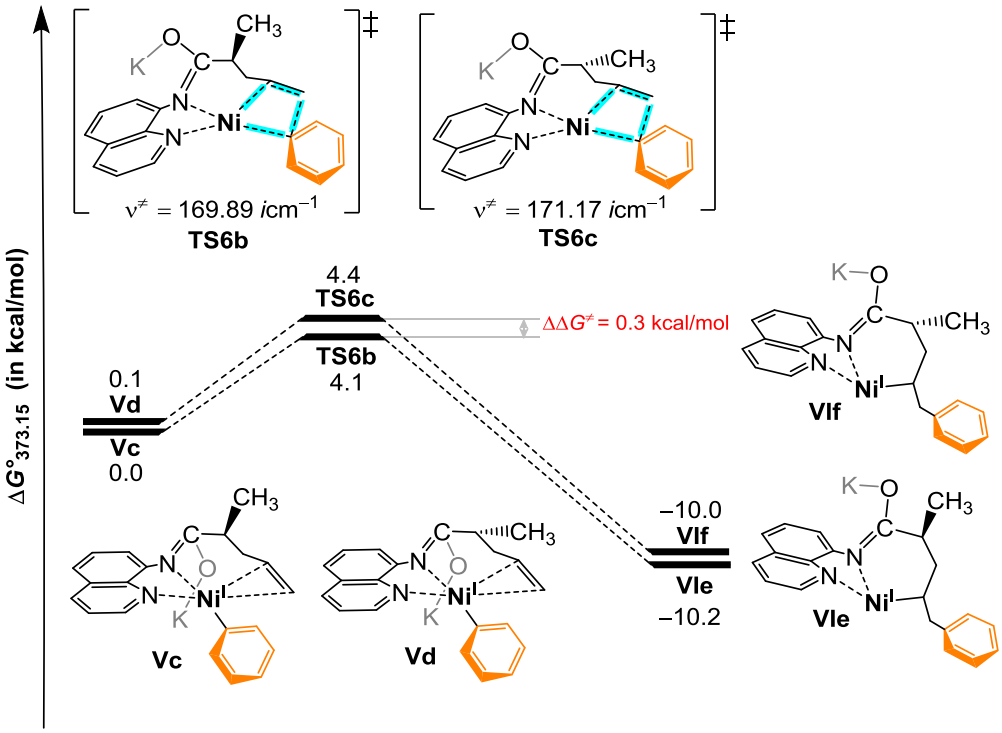


Figure S17. Migration insertion of the different methyl α-substitution intermediates **Vc** and **Vd**.

11. References

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12. Cartesian Coordinates of Optimized Structures

1a

Gibbs free energy before correction = -725.47113800

Gibbs free energy after correction = -725.45667162

C	-1.69942100	0.60887200	-0.12054500
O	-1.87217500	1.81465600	-0.09627300
N	-0.46465400	0.01478700	-0.07615700
H	-0.41779500	-1.00670100	-0.10043500
C	-2.83237100	-0.38679500	-0.21364000
C	-4.20650200	0.25421700	-0.12610900
H	-2.70113800	-1.14869400	0.57745300
H	-2.71832900	-0.93859000	-1.16701600
H	-4.31709200	0.78594900	0.83599600
H	-4.28310000	1.02579900	-0.91513200
C	-5.30191600	-0.74843300	-0.28990400
H	-5.28801000	-1.32447900	-1.22890800
C	-6.25906000	-0.99377200	0.60665700
H	-6.30364800	-0.44477500	1.55737200
H	-7.03716800	-1.74562400	0.43036800
C	2.63999100	-2.47621500	-0.02447000
C	1.90082200	-0.30112900	0.00145500
C	3.22681300	0.21276500	0.06143300
C	4.28252700	-0.73224000	0.07629400
C	3.99529200	-2.07542700	0.03361500
H	2.39422200	-3.54676500	-0.05928200
C	0.78958600	0.61022700	-0.01655900
C	3.43949900	1.61400200	0.10309600
H	5.31651900	-0.37200400	0.12201400
H	4.78720900	-2.82974100	0.04358900
C	2.35711700	2.46209600	0.08486600
C	1.03179600	1.97346400	0.02545800
H	4.46529700	1.99510200	0.14939600
H	2.51193200	3.54575600	0.11683000
H	0.18680700	2.66287300	0.01217000
N	1.63560600	-1.62980600	-0.04014500

K_3PO_4

Gibbs free energy before correction = -2441.64779000

Gibbs free energy after correction = -2441.63332405

O	0.89017900	-0.00231900	-1.25097700
O	-0.95700900	-1.29076700	0.00322400
O	0.88896100	0.00194600	1.25511000
P	-0.06258600	0.00019700	0.00176600
O	-0.95609300	1.29180300	-0.00156300
K	1.62198000	2.25389600	-0.00120100
K	1.62032700	-2.25495200	-0.00135700
K	-3.13649300	0.00062100	-0.00127500

1a'

Gibbs free energy before correction = -1324.76701600

Gibbs free energy after correction = -1324.75254997

C	-2.93371900	-1.03917600	0.38354900
C	-3.52659300	0.19813000	-0.29074800
H	-3.16820900	-1.03218300	1.46200700
H	-3.38227900	-1.94827700	-0.05949600
H	-3.03275600	1.10499200	0.10920500
H	-3.27410300	0.14979800	-1.36753000
C	-5.00580700	0.30066200	-0.12098800
H	-5.58955000	-0.55657900	-0.49369700
C	-5.64761300	1.32069100	0.45254000
H	-5.10027700	2.19007000	0.84253400
H	-6.73915600	1.33455300	0.55462900
C	0.83441300	2.67026100	-0.26020100
C	1.20363500	0.55581400	0.57404000
C	2.61991500	0.69535100	0.42244000
C	3.10410100	1.92148700	-0.10576800
C	2.21804300	2.91141400	-0.44855000
H	0.11384800	3.45635500	-0.52972100
C	0.65389400	-0.68356300	1.08380900
C	3.48716000	-0.37308500	0.76850800
H	4.18508400	2.05360500	-0.23162900
H	2.55717100	3.86728300	-0.85835600
C	2.95111500	-1.54363600	1.26332900
C	1.55685400	-1.69401600	1.41857600
H	4.56729900	-0.24595200	0.63694800
H	3.61013300	-2.37610800	1.53390700
H	1.14721600	-2.63415800	1.80569800
N	0.34659700	1.55219600	0.22244500
N	-0.69985600	-0.83786300	1.24770600
C	-1.43390600	-1.06923100	0.17718900
O	-1.00996300	-1.27691000	-0.99558500

K	1.27206000	-1.32500300	-1.98090700

K_2HPO_4

Gibbs free energy before correction = -1842.35072200

Gibbs free energy after correction = -1842.33625572

O	1.29418700	0.96605500	0.90857100
O	0.01351000	-0.52067000	-0.70365800
P	-0.00187000	0.81433500	0.10967300
O	-1.33829200	0.98047700	0.84937500
K	-2.37527900	-1.15628900	-0.01503500
K	2.42914700	-1.07822300	-0.03687000
O	0.01674500	2.05459800	-1.00610700
H	-0.88462400	2.39701400	-1.04434100

DME

Gibbs free energy before correction = -308.34613200

Gibbs free energy after correction = -308.33166569

C	-2.72923000	-0.41887700	-0.05619700
H	-2.82347300	-0.55789700	-1.15411900
H	-3.21130300	-1.27566800	0.44082000
C	2.72923000	-0.41887600	0.05619700
H	3.29510800	0.49919800	-0.21062800
H	3.21130300	-1.27566700	-0.44082100
O	1.39953500	-0.35440900	-0.35332100
O	-1.39953500	-0.35440900	0.35332100
C	-0.71652000	0.72127100	-0.22211500
H	-1.18510200	1.68858000	0.06572700
H	-0.75725500	0.66669200	-1.33330300
C	0.71652000	0.72127100	0.22211500
H	0.75725600	0.66669200	1.33330300
H	1.18510200	1.68858000	-0.06572700
H	-3.29510800	0.49919800	0.21062800
H	2.82347300	-0.55789700	1.15411900

$^{T}Ni(DME)Br_2$

Gibbs free energy before correction = -6964.08487700

Gibbs free energy after correction = -6964.07041085

Ni	0.18044100	-0.24542000	-0.06782000
Br	-1.81363700	-1.46351500	-0.07981900
C	-0.75744800	0.74337600	2.61315500
H	-0.22906500	-0.15482300	2.96592700
H	-0.65490900	1.54534300	3.36424500

C	-1.26236400	1.37385900	-2.19125500
H	-1.14096200	2.19733600	-2.91508700
H	-2.21474400	1.49840800	-1.64658600
O	-0.14712400	1.35422500	-1.30645800
O	-0.15279700	1.14613700	1.39487400
C	-0.73062800	2.30938000	0.81079000
H	-0.59784700	3.17498800	1.48462500
H	-1.81840400	2.14939200	0.66191600
C	-0.01446000	2.52354200	-0.49241900
H	1.06572100	2.66234200	-0.31603300
H	-0.40302800	3.40570900	-1.02690100
H	-1.82638400	0.50724500	2.46491300
H	-1.27927400	0.41614600	-2.72945000
Br	2.47178900	-0.60031900	-0.07896900

^{S}Ni(DME)Br$_2$

Gibbs free energy before correction = -6964.06053300

Gibbs free energy after correction = -6964.04606685

Ni	-0.10893400	0.00001400	0.00000900
Br	1.48568800	1.61871800	0.21093400
C	-1.56379400	-2.65920600	0.40006200
H	-0.68004200	-3.14052400	-0.03367400
H	-1.49768500	-2.68471900	1.50267300
C	-1.56316200	2.65956700	-0.39993100
H	-2.47671800	3.18548100	-0.07586000
H	-1.49632000	2.68518400	-1.50249400
O	-1.61484900	1.31471800	0.06833200
O	-1.61514600	-1.31439600	-0.06834800
C	-2.82597200	-0.67090100	0.32197300
H	-2.86564300	-0.59173600	1.42618200
H	-3.69218600	-1.26556300	-0.01703200
C	-2.82580200	0.67151200	-0.32208900
H	-3.69189700	1.26635000	0.01689800
H	-2.86543200	0.59239700	-1.42630200
H	-2.47715100	-3.18513500	0.07545200
H	-0.67968800	3.14084000	0.03441400
Br	1.48531900	-1.61904300	-0.21094700

^{T}I^{pre}

Gibbs free energy before correction = -7381.20428800

Gibbs free energy after correction = -7381.18982182

O	-0.83705700	2.52894200	-1.85686700

N	-0.57558500	1.67035000	0.24583700
C	2.18414400	2.84145900	-1.17627900
C	2.75755600	1.65370500	-0.47174600
C	2.64172800	1.35418300	0.83707900
H	-0.31310300	2.00937100	1.17599400
H	1.96814900	2.57880500	-2.22704900
H	3.38201600	0.99418400	-1.08952000
H	3.19891100	0.51332200	1.26399700
H	2.10114900	1.99174200	1.54727000
H	2.98063400	3.60770800	-1.23379600
C	-0.98894900	-2.13286200	-1.16082900
C	-2.00334000	-0.23262400	-0.31811400
C	-3.29748700	-0.80522200	-0.45417000
C	-3.38212300	-2.10805200	-1.00267900
C	-2.23215000	-2.76547400	-1.36694200
H	-0.04786800	-2.64264600	-1.40335100
C	-1.88036000	1.07933400	0.20150000
C	-4.43201300	-0.06643200	-0.03553500
H	-4.36726800	-2.57100500	-1.12481800
H	-2.25741000	-3.77082700	-1.79455100
C	-4.28231100	1.19416900	0.49418600
C	-2.99873600	1.77467200	0.60046600
H	-5.42168600	-0.52303300	-0.14154600
H	-5.15678800	1.76317400	0.82319000
H	-2.88194900	2.78999100	0.99399200
N	-0.87557200	-0.91791200	-0.65942500
C	-0.25014500	2.56213900	-0.80132900
C	0.93628300	3.45299200	-0.54614000
H	0.71825700	4.41311600	-1.03860600
H	1.08033700	3.65137700	0.52839700
Br	0.47167700	-0.67354800	2.36296900
Ni	0.88405000	-0.11201900	0.04339400
Br	2.39932900	-1.72586000	-0.89272400

S_I^{pre}

Gibbs free energy before correction = -7381.18495900

Gibbs free energy after correction = -7381.17049282

O	0.41160400	-3.31350300	-0.22205300
N	-0.06025300	-1.33524900	-1.24810000
C	3.02611800	-1.78206800	0.07653300
C	2.99445500	-0.36955100	0.57129700
C	3.02777300	0.76192300	-0.18641100

H	0.32741500	-0.55941400	-1.79089100
H	2.70057400	-2.45914300	0.88426100
H	3.15527300	-0.26200700	1.64821400
H	3.27340100	1.72510900	0.27880200
H	3.12337000	0.71112800	-1.27481100
H	4.09773400	-2.00972300	-0.08526000
C	-1.43343000	1.97395700	0.85118200
C	-1.86396000	-0.07307800	-0.17471300
C	-3.25999500	0.07098300	0.08512100
C	-3.70650700	1.25324100	0.72126500
C	-2.79781500	2.21578000	1.08598800
H	-0.68241900	2.70124400	1.18011100
C	-1.41583300	-1.23146300	-0.88008900
C	-4.15596000	-0.96360900	-0.28084900
H	-4.77744600	1.37791800	0.91393300
H	-3.10212200	3.14445600	1.57430800
C	-3.68810700	-2.09960000	-0.89598100
C	-2.31890700	-2.22128900	-1.21021600
H	-5.22002500	-0.83303900	-0.05791900
H	-4.37577000	-2.90427200	-1.17243200
H	-1.95439800	-3.10304700	-1.74441400
N	-0.98584000	0.88228700	0.25753400
C	0.78393000	-2.34342400	-0.85059400
C	2.24037100	-2.11048900	-1.19114700
H	2.62293700	-3.05573100	-1.60801900
H	2.37094700	-1.33717800	-1.96764000
Br	0.80491300	1.88588200	-1.83915800
Ni	0.93219300	0.65801500	0.21205000
Br	0.67440600	-0.18216300	2.40105600

^{S}1

Gibbs free energy before correction = -7980.52405400

Gibbs free energy after correction = -7980.50958821

C	1.25583800	-2.61227300	-1.80268500
C	2.28331300	-2.42260600	-0.69356000
H	1.62354900	-2.11460200	-2.71959000
H	1.13762500	-3.68372900	-2.02723000
H	1.91515700	-2.83367300	0.26303800
H	3.18843500	-3.00675300	-0.95323700
C	2.73337900	-1.00825200	-0.52203000
H	2.97805000	-0.48277600	-1.45665200
C	3.13985600	-0.43949800	0.66124500

H	3.10812400	-1.01426000	1.59373700
H	3.74091000	0.47549200	0.66206100
C	-0.38947900	2.31721300	1.34665600
C	-1.45555100	1.02701400	-0.27566800
C	-2.66555100	1.76352500	-0.11446700
C	-2.67407000	2.81789600	0.83277100
C	-1.54391400	3.09462300	1.56280200
H	0.53116000	2.51327800	1.90776800
C	-1.36989900	-0.07481800	-1.19875000
C	-3.80317800	1.41507700	-0.88169100
H	-3.59340700	3.39799800	0.96933500
H	-1.51912200	3.89943600	2.30189000
C	-3.71654300	0.36668600	-1.77410600
C	-2.52574400	-0.36939600	-1.93174700
H	-4.72819600	1.98586100	-0.75042100
H	-4.58875400	0.09147000	-2.37719200
H	-2.49783800	-1.19702100	-2.64594200
N	-0.35634500	1.33319000	0.47035700
N	-0.16730100	-0.72755500	-1.30580300
C	-0.11581300	-2.05894100	-1.46804700
O	-1.06452600	-2.85648400	-1.31205100
K	-2.40252200	-2.27601200	0.79965300
Ni	1.22246700	0.24967800	0.21615300
Br	0.36875800	-1.12919600	2.04427200
Br	2.12807100	2.09883800	-0.96178800

^{T}I

Gibbs free energy before correction = -7980.54857700

Gibbs free energy after correction = -7980.53411121

C	-1.60803700	2.28157000	-1.97810900
C	-2.70944700	2.11059200	-0.93976900
H	-1.82833000	1.63105500	-2.84524200
H	-1.59441300	3.32158200	-2.33723100
H	-2.45945900	2.63665400	-0.00017900
H	-3.62291500	2.59645700	-1.33306000
C	-3.04668400	0.68659500	-0.66272600
H	-3.12677800	0.02445900	-1.53822400
C	-3.34682100	0.18748200	0.55341200
H	-3.34213600	0.82796000	1.44276900
H	-3.69069000	-0.84648400	0.66844700
C	0.94750700	-2.27604900	1.38857300
C	1.71756300	-0.82001900	-0.24655600

C	3.03676500	-1.34900900	-0.16461400
C	3.25936400	-2.39477700	0.76650500
C	2.22397700	-2.85606900	1.54441000
H	0.09348600	-2.62820000	1.98119600
C	1.39209000	0.25406100	-1.14208700
C	4.05168600	-0.81479300	-0.99330900
H	4.26513800	-2.82110700	0.85133500
H	2.36817700	-3.65975000	2.27119400
C	3.73443200	0.20753800	-1.86217200
C	2.43099700	0.74126100	-1.93859700
H	5.06582600	-1.22233600	-0.92877300
H	4.50734200	0.62616600	-2.51574300
H	2.23297800	1.55326400	-2.64199700
N	0.71862100	-1.30479700	0.53291600
N	0.07060700	0.68485800	-1.17290900
C	-0.20401300	1.97533400	-1.50483200
O	0.61733500	2.90433500	-1.44473300
K	1.83547000	2.68206200	0.84083300
Ni	-1.06684600	-0.40399200	0.14621000
Br	-0.59186300	1.12878300	2.15749900
Br	-1.85413800	-2.50548500	-0.84398900

B

Gibbs free energy before correction = -523.20493800

Gibbs free energy after correction = -523.19047200

B	0.58190500	0.00157200	-0.28371900
C	-0.97923700	0.00055600	-0.09826300
C	-1.69844700	-1.20232100	-0.01392300
C	-1.70010600	1.20234800	-0.01238800
C	-3.08329300	-1.20908600	0.15004200
H	-1.15529900	-2.15266600	-0.07897800
C	-3.08496300	1.20697800	0.15158900
H	-1.15827700	2.15352900	-0.07626000
C	-3.77927200	-0.00158900	0.23308200
H	-3.62556700	-2.15896000	0.21360000
H	-3.62854800	2.15602100	0.21636400
H	-4.86719600	-0.00241400	0.36219700
O	1.22940200	1.19805100	-0.36024100
H	2.18848700	1.07183000	-0.47435500
O	1.23083800	-1.19403500	-0.36162900
H	2.18967900	-1.06569200	-0.47613900
C	4.28885300	-0.00258500	0.91050200

H	4.90244900	-0.90009900	1.10044800
H	3.44510200	-0.00561500	1.61862300
H	4.90002500	0.89558500	1.10508600
O	3.74618700	0.00006200	-0.39920000
H	4.46698400	0.00219200	-1.04727300

KBr

Gibbs free energy before correction = -3173.71411800

Gibbs free energy after correction = -3173.69965183

K	0.00000000	0.00000000	-1.90882200
Br	0.00000000	0.00000000	1.03621800

^{T}Ia

Gibbs free energy before correction = -5929.35901300

Gibbs free energy after correction = -5929.34454683

C	0.67861700	-2.65520100	0.30735400
C	1.48943400	-2.61077200	-0.98913400
H	0.68429900	-3.66953600	0.73964400
H	1.13716900	-1.97514300	1.05158800
H	1.60836600	-1.56006200	-1.30506900
H	2.50565800	-2.99608600	-0.78205500
C	0.84606600	-3.39714100	-2.08563000
H	0.78936600	-4.48678800	-1.93569700
C	0.30711700	-2.85890700	-3.18179000
H	0.33739200	-1.77249500	-3.35267800
H	-0.17649200	-3.47029000	-3.95273000
C	-1.68870800	2.92300400	-0.14972100
C	-2.42553300	0.83270200	-0.84970100
C	-3.61673600	1.38394100	-1.39716800
C	-3.79615600	2.78564900	-1.28305300
C	-2.84195600	3.55434400	-0.66005000
H	-0.91035800	3.51235200	0.35129500
C	-2.16278400	-0.58020500	-0.90274500
C	-4.55752300	0.52653700	-2.01665300
H	-4.70440200	3.23769300	-1.69664600
H	-2.95623400	4.63619100	-0.55521300
C	-4.29740400	-0.82569300	-2.07360200
C	-3.12341600	-1.38163900	-1.52211700
H	-5.47312400	0.95433100	-2.43768400
H	-5.01540800	-1.49752100	-2.55599600
H	-2.95667500	-2.45911500	-1.58845900
N	-1.49632200	1.62479400	-0.24570500

N	-0.95664500	-0.99993700	-0.36646900
C	-0.76580400	-2.26354000	0.08663100
O	-1.67261100	-3.07244700	0.33790100
K	-3.08806900	-1.58160300	1.96720300
Ni	0.10227900	0.56024000	0.36825600
Br	-0.56831300	0.20234400	2.74332900
B	2.32608700	1.63585400	-0.51552200
C	3.46677900	0.51754700	-0.23504100
C	3.52013500	-0.21988400	0.95855700
C	4.39008600	0.17590500	-1.23865600
C	4.44174700	-1.25479300	1.14334700
H	2.81731900	0.02450000	1.76765200
C	5.31886800	-0.85157800	-1.06654000
C	5.34546500	-1.57439900	0.12902500
H	4.45794500	-1.81460200	2.08597100
H	6.02831100	-1.09229800	-1.86686000
H	6.07240500	-2.38205100	0.26987900
O	1.22390100	1.02807700	-1.33577600
H	1.53879100	0.35335100	-1.95074800
O	1.59357200	1.92362800	0.77171800
H	1.31190900	2.84812800	0.78545100
O	2.77246900	2.83991300	-1.15371500
H	4.37989500	0.73696900	-2.18421500
C	3.81345300	3.53744600	-0.56055000
H	4.76393800	2.96184800	-0.53148000
H	4.01533900	4.46741100	-1.12317600
H	3.59627300	3.83833300	0.48794700

^{S}Ia

Gibbs free energy before correction = -5929.32489500

Gibbs free energy after correction = -5929.31042883

C	0.65002700	-2.76411500	0.40241000
C	1.52119300	-2.64663300	-0.84904100
H	0.58657400	-3.81548400	0.72941700
H	1.10183000	-2.18493600	1.22633200
H	1.69613200	-1.58105000	-1.08271600
H	2.51280200	-3.08182100	-0.62262000
C	0.91489500	-3.33426700	-2.02929500
H	0.76465400	-4.42101900	-1.92996200
C	0.51828500	-2.72023400	-3.14586900
H	0.64485600	-1.63520600	-3.27455000
H	0.06096800	-3.26741100	-3.97861900

C	-2.16330800	2.86475600	0.27377500
C	-2.46250800	0.82329300	-0.76456600
C	-3.56106200	1.31990500	-1.52846900
C	-3.91990500	2.67995600	-1.34227300
C	-3.22645200	3.45691200	-0.44737200
H	-1.59914200	3.46235000	1.00485900
C	-2.03835200	-0.54631900	-0.90902300
C	-4.24612000	0.46483900	-2.42316600
H	-4.75496500	3.08866000	-1.92254300
H	-3.48073200	4.50779400	-0.28335900
C	-3.83668000	-0.84482800	-2.54426600
C	-2.75065100	-1.34794100	-1.80085900
H	-5.08842100	0.85989800	-3.00094000
H	-4.35425100	-1.51898900	-3.23500000
H	-2.45423400	-2.39111400	-1.93480900
N	-1.80227800	1.61241700	0.12244500
N	-0.92292300	-0.98166400	-0.19063800
C	-0.76774700	-2.29338400	0.16379200
O	-1.71409400	-3.07834400	0.29721000
K	-3.08122000	-1.35782500	1.82335900
Ni	0.16647400	0.37166700	0.57012900
Br	-0.27839300	-0.20805500	2.82863600
B	2.03964500	1.69243200	-0.38770800
C	3.34507600	0.74652800	-0.36336300
C	3.74280000	0.02352700	0.77159700
C	4.08256000	0.55026700	-1.54353500
C	4.82455800	-0.86026600	0.73347600
H	3.18029800	0.15065300	1.70606400
C	5.16289600	-0.33176600	-1.59592900
C	5.53658600	-1.04271100	-0.45311600
H	5.11398500	-1.41337800	1.63458900
H	5.71924200	-0.46656100	-2.53063700
H	6.38427800	-1.73606200	-0.48765900
O	0.91011900	0.99240300	-1.11766400
H	1.22202500	0.29477800	-1.71092900
O	1.42751500	1.74967500	1.00514000
H	0.96214100	2.59334300	1.11256900
O	2.19227400	2.99568500	-0.94061300
H	3.79940700	1.10666500	-2.44876600
C	3.23200800	3.78379700	-0.46190200
H	4.23393700	3.37817700	-0.71663900
H	3.16826300	4.79562700	-0.90063100

H	3.20909800	3.90832500	0.64210700

^{S}TS1

Gibbs free energy before correction = -5929.30771300

Gibbs free energy after correction = -5929.29324683

C	-0.41342800	2.25468500	1.55838000
C	-0.81421900	3.53458300	0.81780300
H	-0.18885400	2.47809800	2.61461600
H	-1.23204000	1.52256100	1.53110500
H	-1.05474700	3.29551700	-0.23478500
H	-1.74791300	3.91567700	1.27508000
C	0.23451600	4.59816000	0.86302400
H	0.56875600	4.90466800	1.86683400
C	0.78099300	5.17367700	-0.21024000
H	0.47643200	4.88592700	-1.22650400
H	1.54507100	5.95514300	-0.12285600
C	1.30720800	-2.84973500	-1.00053600
C	2.09242300	-0.67925100	-1.24703900
C	3.26890500	-1.10775200	-1.91307100
C	3.42068900	-2.50458100	-2.10267800
C	2.45612400	-3.36857800	-1.63486100
H	0.51390400	-3.50796100	-0.62832000
C	1.85250700	0.68159200	-0.92716300
C	4.20319600	-0.12423300	-2.31862700
H	4.31335800	-2.88046800	-2.61439300
H	2.55651100	-4.45037400	-1.75340300
C	3.95242700	1.20385900	-2.03532100
C	2.79574600	1.61343400	-1.33577800
H	5.11007700	-0.43358700	-2.84815300
H	4.67113700	1.96770600	-2.34999000
H	2.64408000	2.67196400	-1.10303500
N	1.13225100	-1.55312800	-0.83172500
N	0.68219000	0.93740200	-0.19871900
C	0.82904400	1.68156500	0.94041500
O	1.93152500	1.94970300	1.43878400
K	2.90062300	-0.34991600	2.16072500
Ni	-0.48113300	-0.60794800	-0.32785800
Br	0.02120000	-1.30572700	2.71481400
B	-2.77229400	-1.41262100	-0.09408900
C	-2.35195900	0.24436800	-0.67818200
C	-3.09945100	1.20888200	0.02459400
C	-2.15506100	0.47044600	-2.05885600

C	-3.62619600	2.33225200	-0.60584700
H	-3.31386100	1.03136600	1.08569300
C	-2.63321500	1.61584500	-2.69397500
C	-3.37945700	2.54344900	-1.96509700
H	-4.23187900	3.04984700	-0.04126300
H	-2.45004500	1.77430200	-3.76212200
H	-3.78326200	3.43200700	-2.46279100
O	-1.52057800	-2.17379500	-0.47024300
H	-1.60383600	-2.44378800	-1.39972000
O	-3.02791800	-1.46066300	1.27806500
H	-2.21140300	-1.43179400	1.80835300
O	-3.86057000	-1.78089700	-0.93339500
H	-1.62716200	-0.27977000	-2.66526400
C	-4.45975900	-3.00514800	-0.64116700
H	-4.92528000	-3.02356000	0.36394100
H	-5.25272800	-3.21466200	-1.38095400
H	-3.74392300	-3.85414400	-0.68110800

^{T}TS1

Gibbs free energy before correction = -5929.33138700

Gibbs free energy after correction = -5929.31692083

C	-0.29557800	2.52831700	1.38550700
C	-0.61933100	3.59862200	0.33970300
H	-0.14814300	2.99138000	2.37568000
H	-1.13252300	1.81577800	1.45559300
H	-0.83999300	3.11718100	-0.63103300
H	-1.54402400	4.12007600	0.65295500
C	0.48604700	4.59020800	0.16985800
H	0.76584800	5.16144400	1.06940300
C	1.15440800	4.79649500	-0.96712400
H	0.90935200	4.23382900	-1.87937000
H	1.96568300	5.53063400	-1.03870100
C	1.36678600	-2.91549300	-1.05602200
C	2.25118800	-0.76962300	-1.07890700
C	3.42736800	-1.20694100	-1.75226700
C	3.51409500	-2.58507100	-2.07228400
C	2.49686900	-3.43944700	-1.71738900
H	0.53608700	-3.56712200	-0.75994200
C	2.08851400	0.59228400	-0.66588500
C	4.44693300	-0.27113300	-2.04444700
H	4.40497900	-2.95225100	-2.59388600
H	2.54392900	-4.50850400	-1.93994300

C	4.28262600	1.04158200	-1.65266000
C	3.12887800	1.47120000	-0.96709800
H	5.34824100	-0.60764400	-2.56699400
H	5.06511700	1.77605000	-1.87128800
H	3.04273500	2.51930900	-0.66551900
N	1.24834000	-1.63523700	-0.76223700
N	0.90621900	0.93474500	-0.02127300
C	0.97488500	1.80246800	1.02724500
O	2.00811000	2.02792200	1.67813300
K	2.79105500	-0.36367800	2.29502800
Ni	-0.44285300	-0.67673300	-0.03178500
Br	-0.29710500	-1.16636800	2.42262100
B	-2.82491300	-1.77858200	-0.18155200
C	-2.32793600	0.17905600	-0.49121700
C	-3.16183400	1.04503900	0.23485600
C	-2.11042600	0.51415600	-1.84451600
C	-3.74991800	2.17433700	-0.34246200
H	-3.37343000	0.81178000	1.28825300
C	-2.67831600	1.64078100	-2.44085800
C	-3.50778100	2.47390200	-1.68432600
H	-4.40391700	2.82274400	0.25283300
H	-2.48589500	1.86827800	-3.49584700
H	-3.96800300	3.35582500	-2.14405300
O	-1.56148500	-2.42179100	-0.48814700
H	-1.54034700	-2.61539400	-1.43749700
O	-3.28219200	-1.86378700	1.12354100
H	-2.55233500	-1.76775500	1.75416900
O	-3.75330000	-1.98353100	-1.20703800
H	-1.47913900	-0.14449300	-2.46784900
C	-5.05124500	-1.50362400	-1.07595800
H	-5.66460400	-1.86580100	-1.91917800
H	-5.53578300	-1.83670200	-0.13806900
H	-5.08913300	-0.39420300	-1.08907200

BH

Gibbs free energy before correction = -291.40914900

Gibbs free energy after correction = -291.39468271

O	0.57099700	1.38770400	-0.00004100
H	-0.30255400	1.79636700	0.00016100
O	-0.59445700	-0.72551200	0.00005300
B	0.54826300	0.02592500	-0.00007200
O	1.75073600	-0.61632100	-0.00030800

H	1.62932500	-1.57404600	-0.00036800
C	-1.86439400	-0.13087100	0.00030100
H	-2.03426400	0.49381000	-0.89821600
H	-2.63182000	-0.92146200	0.00055100
H	-2.03384200	0.49396900	0.89878900

^{S}Ib

Gibbs free energy before correction = -5637.95173800

Gibbs free energy after correction = -5637.93727179

C	0.46782000	-2.66530200	2.01013700
C	-0.09587700	-3.31733900	0.74833400
H	-0.36625700	-2.46683500	2.71104600
H	1.16318900	-3.35592100	2.51265000
H	0.68420300	-3.40610600	-0.02791400
H	-0.40689800	-4.34973000	1.00431800
C	-1.30184300	-2.60728100	0.21113500
H	-2.09193300	-2.46092800	0.96454200
C	-1.66201900	-2.46805700	-1.12353700
H	-1.02376900	-2.87070700	-1.91903600
H	-2.70903600	-2.28356900	-1.39184500
C	-0.79538200	1.82658100	-1.84409800
C	0.51362700	1.71919000	0.07346200
C	0.96418600	3.05798700	-0.11212300
C	0.47288500	3.76602500	-1.23810700
C	-0.39973300	3.15488200	-2.10495000
H	-1.49719300	1.31439600	-2.51373400
C	0.98620400	0.92231700	1.17927300
C	1.88124800	3.62302900	0.80734900
H	0.80357500	4.79815800	-1.39912000
H	-0.79379600	3.67240000	-2.98343000
C	2.32210900	2.86248200	1.86964000
C	1.88948500	1.53363300	2.05587400
H	2.22192900	4.65249900	0.65529600
H	3.02709800	3.29080400	2.59069700
H	2.26494800	0.96249300	2.90892800
N	-0.35663500	1.14685100	-0.80517400
N	0.48245100	-0.35122900	1.29176700
C	1.21988900	-1.36612700	1.77702900
O	2.44657700	-1.33501500	2.00196000
K	3.67071500	-0.29887500	-0.01822600
Ni	-0.79800600	-0.76193900	-0.42317100
Br	1.28458800	-1.30025800	-1.83790900

C	-4.88641100	1.01556600	1.12142700
C	-3.84843600	0.75312300	2.01666200
C	-2.64496800	0.20335600	1.56379000
C	-2.45740700	-0.09881300	0.20866300
C	-3.50620200	0.16823000	-0.68079500
C	-4.70947500	0.72197700	-0.23102400
H	-5.82902500	1.44633000	1.47641800
H	-3.97327200	0.97902600	3.08243900
H	-1.83568100	0.00616600	2.27842800
H	-3.39461000	-0.05148200	-1.75122800
H	-5.51499500	0.92297100	-0.94723400

^{T}Ib

Gibbs free energy before correction = -5637.94895000

Gibbs free energy after correction = -5637.93448379

C	0.43260900	-2.45317600	2.37977400
C	-0.15079100	-3.37072200	1.30925700
H	-0.38906400	-2.08557800	3.02342000
H	1.12306600	-3.02526600	3.01794800
H	0.60039700	-3.61012600	0.53390700
H	-0.40898100	-4.33021300	1.79742000
C	-1.39180100	-2.83586700	0.68068900
H	-2.11567400	-2.37548700	1.37087100
C	-1.71199000	-2.93473300	-0.62059100
H	-1.04272100	-3.42687500	-1.33534000
H	-2.68424300	-2.58967300	-0.99227800
C	-0.38269300	1.91031400	-2.00653700
C	0.71734900	1.80746200	0.03354100
C	1.18588500	3.14657600	-0.09725800
C	0.80770200	3.85489000	-1.26645500
C	0.03090400	3.24276700	-2.22090600
H	-1.00134900	1.38884300	-2.74952900
C	1.05934400	1.00144800	1.17238400
C	2.00037600	3.70062400	0.91787300
H	1.14874100	4.88866400	-1.39156600
H	-0.27031800	3.76373000	-3.13363200
C	2.32444900	2.92565800	2.01180500
C	1.86998700	1.59792000	2.14170000
H	2.35836000	4.73031000	0.81524400
H	2.95091400	3.34289500	2.80767100
H	2.15584600	1.02447800	3.02692300
N	-0.05323300	1.23554600	-0.92740900

N	0.52085700	-0.27725100	1.24729400
C	1.21659500	-1.25768300	1.88048500
O	2.44448200	-1.23588100	2.06891700
K	3.45599300	-0.52669200	-0.22223600
Ni	-0.71525900	-0.64597700	-0.37819700
Br	1.08609300	-1.63643700	-1.97423700
C	-5.01758900	1.25601500	0.82276800
C	-4.00803800	1.13512200	1.77987900
C	-2.77830800	0.56446400	1.43408900
C	-2.50559200	0.08840200	0.13866600
C	-3.54590300	0.22585700	-0.80039700
C	-4.78117400	0.79759600	-0.47451100
H	-5.98273200	1.70352500	1.08644200
H	-4.18058100	1.49037800	2.80365900
H	-2.00315200	0.48492100	2.21266100
H	-3.40052800	-0.12823900	-1.83420600
H	-5.56499300	0.88488000	-1.23739300

^{T}Ic

Gibbs free energy before correction = -3586.76811700

Gibbs free energy after correction = -3586.75365076

C	-1.64078000	-1.03556300	2.60134100
C	-1.55869600	-2.38661300	3.30086700
H	-2.05430500	-1.13719300	1.58248300
H	-2.34894600	-0.37182500	3.13466900
H	-1.05228400	-2.27409600	4.27427900
H	-2.58714200	-2.73737600	3.50323500
C	-0.85655600	-3.41524000	2.47309700
H	-1.34304600	-3.66776000	1.51689800
C	0.28662000	-4.02988600	2.79356100
H	0.80058200	-3.81663200	3.74187700
H	0.73305400	-4.79161300	2.14154500
C	-0.28050800	2.99067500	-1.62821700
C	0.73450300	2.48345100	0.40184500
C	1.62749600	3.58180500	0.28085800
C	1.50479700	4.39575300	-0.87169600
C	0.54878000	4.11316600	-1.82047200
H	-1.03637700	2.71288700	-2.37416100
C	0.77276200	1.60289500	1.54386800
C	2.59138500	3.81094000	1.29439700
H	2.18175300	5.24931700	-0.98950100
H	0.43041500	4.72983300	-2.71510600

C	2.63389400	2.96227900	2.37610100
C	1.74559500	1.87013100	2.50911400
H	3.28153300	4.65520400	1.19529300
H	3.37397100	3.12681200	3.16690100
H	1.80981000	1.22804300	3.38783700
N	-0.18204200	2.21551100	-0.56663000
N	-0.20278700	0.61181600	1.54982300
C	-0.31845500	-0.29372000	2.55228600
O	0.55990300	-0.55617700	3.38882100
K	1.88353800	-1.69732000	1.24946400
Ni	-0.94279400	0.33675700	-0.34343600
C	-5.75225000	0.68702200	-0.50894200
C	-4.98546900	1.62909300	0.18158000
C	-3.59284100	1.51022600	0.21105400
C	-2.91311400	0.46333300	-0.43953100
C	-3.71579900	-0.46850600	-1.12290300
C	-5.11140100	-0.36663800	-1.16216700
H	-6.84443600	0.77370400	-0.53598800
H	-5.47881800	2.46019900	0.70068500
H	-3.01511700	2.26474200	0.76890000
H	-3.24917200	-1.31842400	-1.64754100
H	-5.70248000	-1.11451900	-1.70517600
B	0.13867000	-1.53604800	-1.92423700
C	1.74432000	-1.30621700	-1.82408300
C	2.32161900	-0.03780700	-1.64957100
C	2.60078800	-2.41710600	-1.71592900
C	3.67617900	0.11929100	-1.33483100
H	1.69276500	0.85631300	-1.75232300
C	3.95909600	-2.27591600	-1.41982100
C	4.49901200	-1.00228300	-1.21206000
H	4.09215700	1.12311700	-1.18698000
H	4.60118400	-3.16067600	-1.34168100
H	5.55975900	-0.88579400	-0.96533300
O	-0.51544000	-0.25673900	-2.34279000
H	-1.36634500	-0.45772400	-2.75716500
O	-0.29722500	-2.65660400	-2.70628300
O	-0.31976000	-1.78186200	-0.50162000
H	-1.06423700	-2.40143100	-0.51660100
H	2.18003900	-3.42397200	-1.84780600
C	0.02202500	-2.66394600	-4.05721200
H	-0.34778300	-3.59237100	-4.52818500
H	-0.42991300	-1.81593000	-4.61470500

H	1.11701300	-2.61663800	-4.24137100

^{S}Ic

Gibbs free energy before correction = -3547.53424100

Gibbs free energy after correction = -3547.51977496

C	1.99865900	-0.42620600	2.06932800
C	3.36034300	-1.02711700	1.70114700
H	1.87461400	-0.41162900	3.16513700
H	1.95326500	0.61036700	1.70008800
H	3.55955600	-0.85563000	0.62964200
H	4.13780100	-0.47638700	2.26353600
C	3.45579500	-2.49009100	1.99228700
H	3.36750700	-2.79066400	3.04814800
C	3.59735000	-3.42955900	1.05409500
H	3.67223700	-3.15925800	-0.00978900
H	3.64867200	-4.49671000	1.30097500
C	-2.34934000	0.23582300	-2.06274600
C	-1.30027500	-1.64269300	-1.21041800
C	-2.22209200	-2.52100400	-1.83849300
C	-3.24368000	-1.92585200	-2.62216500
C	-3.30574300	-0.55630400	-2.73452600
H	-2.36696500	1.32843700	-2.13906100
C	-0.24375000	-2.12874600	-0.38593000
C	-2.07148400	-3.91551100	-1.64355200
H	-3.97093100	-2.56950900	-3.12890900
H	-4.07996200	-0.06861200	-3.33228800
C	-1.04318300	-4.38095800	-0.84905300
C	-0.13422600	-3.50342400	-0.21878900
H	-2.77256700	-4.60139500	-2.13002700
H	-0.92079400	-5.45854700	-0.69808300
H	0.66534000	-3.90664900	0.41007900
N	-1.38941000	-0.28465700	-1.32340400
N	0.58365400	-1.15389400	0.18254900
C	0.86066000	-1.24956900	1.51553200
O	0.22911700	-1.99140200	2.28639700
K	-2.23239300	-1.28555300	1.77036400
Ni	0.36059100	0.52104700	-0.73946000
B	-0.79291200	3.27810100	-0.45171400
C	-1.49772900	2.47584700	0.78916800
C	-2.88819000	2.30721800	0.88283200
C	-0.73892400	2.05066700	1.89523200
C	-3.49988500	1.76367500	2.01880400

H	-3.52308100	2.64584600	0.05310400
C	-1.32881600	1.51206400	3.04198900
C	-2.72068400	1.37565900	3.11301300
H	-4.59121800	1.66683100	2.06288900
H	-0.70671800	1.21709000	3.89614300
H	-3.19434400	0.98002300	4.01988900
O	-0.14476700	2.21921300	-1.41139800
H	0.61855400	2.66687200	-1.80316900
O	-1.70032300	4.07389100	-1.24434400
H	-2.26821700	3.51742600	-1.78574000
O	0.25080500	4.12223700	0.07595900
H	0.33141200	4.88998700	-0.50088500
H	0.35019300	2.18876000	1.87219500
C	2.95346900	0.02904800	-1.66529800
C	4.30626600	0.25570000	-1.93539900
C	4.94184800	1.38668000	-1.41939000
C	4.20309500	2.29555100	-0.65933200
C	2.84207500	2.07713400	-0.41765300
C	2.19125900	0.92751900	-0.89563500
H	2.48714700	-0.88741800	-2.05532800
H	4.87083600	-0.46248100	-2.54244100
H	6.00577900	1.56245400	-1.61420200
H	4.68982100	3.19302100	-0.25795900
H	2.27027300	2.82851100	0.14536900

^{S}TS2

Gibbs free energy before correction = -3586.71644400

Gibbs free energy after correction = -3586.70197776

C	-0.18924200	-1.50118900	2.40638800
C	-1.57845900	-2.14130000	2.52486300
H	0.34267800	-1.57077800	3.37116800
H	0.39717200	-2.04280800	1.64403500
H	-2.04968500	-2.19174000	1.52729000
H	-1.44361100	-3.18492000	2.86761500
C	-2.48557900	-1.41206600	3.46225300
H	-2.14720900	-1.32826600	4.50710900
C	-3.63917800	-0.84556900	3.10128400
H	-3.99748600	-0.90128600	2.06272900
H	-4.27373200	-0.31064300	3.81792100
C	-0.32469000	1.53891300	-3.09300000
C	-1.14339300	1.89414900	-0.96366500
C	-1.84278100	3.06829400	-1.38228100

C	-1.73213500	3.44168300	-2.74720100
C	-0.98075000	2.68138000	-3.60841000
H	0.29075300	0.91323800	-3.75734500
C	-1.23477000	1.43855800	0.40678300
C	-2.61530900	3.80824700	-0.45670900
H	-2.26145000	4.33744900	-3.09192100
H	-0.88291300	2.94065300	-4.66651900
C	-2.69975400	3.36400600	0.84481200
C	-2.02879700	2.20181000	1.27279300
H	-3.13664100	4.71058400	-0.79362800
H	-3.30505500	3.91426100	1.57351500
H	-2.13862800	1.88267100	2.31168800
N	-0.39998300	1.17186200	-1.83619100
N	-0.59389000	0.26134900	0.76257000
C	-0.31161600	-0.03376800	2.06125600
O	-0.18312400	0.81059400	2.96267500
K	1.13030600	2.73713100	1.78651200
Ni	0.28366900	-0.76996400	-0.61899500
B	2.48578100	-1.75704100	-1.17325500
C	2.18175700	0.03886000	-0.12077000
C	2.60575100	1.18112100	-0.83618900
C	2.73649700	-0.09969200	1.16768100
C	3.51296200	2.11053900	-0.32092800
H	2.22871900	1.33980100	-1.85694200
C	3.65484400	0.81141200	1.70528500
C	4.05149000	1.92400600	0.95826600
H	3.81448900	2.97804200	-0.92018100
H	4.06899900	0.64894800	2.70768300
H	4.77707100	2.63735200	1.36530600
O	1.27302700	-1.73519600	-1.95893100
H	0.90042800	-2.62643900	-2.06103000
O	3.67264700	-1.45188000	-1.82200500
H	3.52434200	-0.83169000	-2.54539800
O	2.52161200	-2.77246100	-0.22649200
H	2.46139100	-0.97168600	1.77717400
C	-2.58042200	-1.33752000	-1.15203300
C	-3.67663800	-2.18401400	-1.34139200
C	-3.51253600	-3.57128500	-1.30685000
C	-2.23778900	-4.09444000	-1.09137200
C	-1.14912300	-3.23348100	-0.91015100
C	-1.28239100	-1.83078100	-0.92631600
H	-2.75870800	-0.25266900	-1.17358400

H	-4.67182900	-1.75667100	-1.51671100
H	-4.37144400	-4.23686300	-1.44811800
H	-2.08795500	-5.18059500	-1.05700500
H	-0.16570100	-3.69194200	-0.71304000
C	3.74440500	-3.18432900	0.30962800
H	3.55787100	-3.92589500	1.10436100
H	4.39689100	-3.65572000	-0.44956700
H	4.31347800	-2.34587000	0.75701100

^{T}TS2

Gibbs free energy before correction = -3586.73071900

Gibbs free energy after correction = -3586.71625276

C	0.71747400	-1.72050000	2.23433600
C	1.88852200	-2.49511800	2.82908100
H	0.45630400	-2.10549500	1.22932500
H	-0.19069800	-1.87886900	2.84732200
H	2.16906700	-2.05432700	3.80037200
H	1.55690900	-3.53190000	3.02143700
C	3.07759300	-2.53410300	1.92247300
H	2.92489400	-3.05040900	0.96122000
C	4.27592600	-1.99937000	2.18017500
H	4.47677500	-1.48274500	3.12965700
H	5.11103600	-2.08941900	1.47322300
C	-2.14258600	1.93350800	-1.57698700
C	-0.67745100	2.37432800	0.17350700
C	-0.82726200	3.77826400	-0.00161600
C	-1.68588200	4.22154400	-1.03787400
C	-2.34645300	3.30638800	-1.82249300
H	-2.63783500	1.16660000	-2.18525700
C	0.17417000	1.83418100	1.20748600
C	-0.13244700	4.66954200	0.85293300
H	-1.81248900	5.29874100	-1.19407000
H	-3.01827100	3.61934600	-2.62605600
C	0.66689700	4.15347000	1.84581900
C	0.82542600	2.76164700	2.02982200
H	-0.25219000	5.74851300	0.70925600
H	1.20057100	4.83002300	2.52240200
H	1.45198700	2.39706000	2.84428700
N	-1.34103200	1.49639000	-0.62550700
N	0.21987800	0.45044500	1.27245700
C	0.95917400	-0.22136500	2.17725700
O	1.82322200	0.27796500	2.92282000

K	3.32147600	0.76225700	0.75872700
Ni	-0.87615600	-0.44573200	-0.25791400
C	-4.69582500	-1.91206400	2.40689300
C	-4.11451500	-0.65876200	2.61577600
C	-3.01631300	-0.25939100	1.84846800
C	-2.44961100	-1.06858700	0.84340500
C	-3.06622700	-2.32451800	0.66405700
C	-4.16312400	-2.74803900	1.42563000
H	-5.55549200	-2.23363400	3.00604900
H	-4.52158600	0.01038700	3.38443300
H	-2.58218500	0.73153400	2.05429400
H	-2.66946300	-3.02366600	-0.09067900
H	-4.60322300	-3.73820800	1.25194700
B	-0.70047500	-1.86750500	-2.41140500
C	0.86327900	-0.63194100	-1.57891300
C	1.24640100	0.58370400	-2.19032200
C	1.92944500	-1.52254800	-1.32491300
C	2.57076300	0.88527100	-2.53390700
H	0.48049800	1.33680500	-2.43013400
C	3.25796600	-1.25438900	-1.66824000
C	3.58753400	-0.04061700	-2.28170900
H	2.80932800	1.84170500	-3.01479300
H	4.04114200	-1.99601500	-1.46422100
H	4.62365400	0.17837900	-2.56499400
O	-1.87579500	-1.10914500	-2.13985700
H	-2.55834900	-1.68464000	-1.76354900
O	-0.20581700	-1.90979300	-3.70845400
O	-0.62107500	-3.05953700	-1.69048400
H	0.03717200	-3.64810700	-2.07955100
H	1.70775100	-2.49483600	-0.86111100
C	-0.34142600	-0.84451600	-4.59372100
H	-0.48563900	-1.22882200	-5.61905900
H	-1.20379800	-0.19421500	-4.35270300
H	0.56594400	-0.20852400	-4.60563600

^{S}II

Gibbs free energy before correction = -3295.36256100

Gibbs free energy after correction = -3295.34809494

C	0.34023500	-2.13426800	2.40712700
C	-0.28650500	-0.91969500	3.07670000
H	0.92497900	-2.72003900	3.13954200
H	-0.45117700	-2.82537400	2.05951700

H	-0.88457900	-0.34253100	2.34427400
H	-0.99633000	-1.29007100	3.84182000
C	0.71017100	-0.02035300	3.73556100
H	1.38229600	-0.50204300	4.46423000
C	0.82999100	1.28935500	3.50775900
H	0.18036700	1.79707500	2.77943400
H	1.57037300	1.90485200	4.03235300
C	0.67400900	3.07050000	-0.19663800
C	2.04677400	1.21420900	-0.41448900
C	3.08451400	1.98729500	-0.99764600
C	2.85286500	3.37595500	-1.15461100
C	1.65960700	3.91906700	-0.73881300
H	-0.29727900	3.47383300	0.11582700
C	2.21972200	-0.19017900	-0.14786700
C	4.29148900	1.34802300	-1.38125700
H	3.63631200	3.99918100	-1.59991900
H	1.45558100	4.98921000	-0.83049000
C	4.43909200	-0.00079500	-1.15425500
C	3.42700300	-0.77180600	-0.53647300
H	5.08304000	1.94261400	-1.84936700
H	5.36873800	-0.50178200	-1.44595700
H	3.60350100	-1.82883100	-0.33099900
N	0.85091900	1.76860600	-0.05136500
N	1.16119400	-0.74630900	0.55801400
C	1.28212500	-1.90417800	1.24109800
O	2.08736500	-2.81517500	0.96469300
K	0.83996700	-3.33375200	-1.28383800
Ni	-0.47345600	0.31862900	0.15596800
C	-2.78881000	-3.43714400	-1.55473300
C	-2.92251100	-3.16211700	-0.19120500
C	-2.31845400	-2.03086800	0.36924100
C	-1.53592700	-1.14003400	-0.39052800
C	-1.45145900	-1.42748200	-1.77362500
C	-2.06088900	-2.54839200	-2.35123600
H	-3.26361300	-4.32072800	-1.99481500
H	-3.50968700	-3.83545500	0.44493500
H	-2.46551600	-1.84677000	1.44329900
H	-0.88526100	-0.75102500	-2.43440000
H	-1.96541200	-2.72872400	-3.42963700
C	-1.98720000	1.39813700	-0.10763300
C	-2.82289500	1.71710500	0.98123400
C	-3.89516900	2.60794400	0.86038200

C	-4.18119000	3.20257500	-0.36959900
C	-3.38169100	2.89137400	-1.47237800
C	-2.30936000	2.00581300	-1.33714700
H	-2.63780200	1.25981500	1.96523000
H	-4.51539800	2.83658700	1.73596000
H	-5.02198300	3.89815600	-0.46995000
H	-3.59518600	3.34592200	-2.44785900
H	-1.69550200	1.79087000	-2.22508400

^{T}II

Gibbs free energy before correction = -3295.35068300

Gibbs free energy after correction = -3295.33621694

C	-0.12443400	2.52304400	1.82018800
C	-0.52995800	3.59903200	0.81183600
H	0.13854700	2.97238500	2.79266700
H	-0.98038000	1.84022200	1.99317700
H	-0.87015300	3.11562900	-0.12332900
H	-1.39286200	4.15785200	1.21928500
C	0.60007600	4.53507600	0.52415900
H	0.94131400	5.15146400	1.37114400
C	1.23515400	4.63063300	-0.64604300
H	0.92882600	4.02545400	-1.51106700
H	2.07558400	5.31907100	-0.79367800
C	-0.33922300	-1.38177500	-2.68422900
C	1.44914300	-0.30157500	-1.67387700
C	2.37601200	-0.87451200	-2.58572600
C	1.85662400	-1.74372500	-3.57813400
C	0.50578900	-1.99626400	-3.63179300
H	-1.42182100	-1.56430000	-2.69610200
C	1.88415800	0.59050500	-0.62907500
C	3.75317700	-0.56070600	-2.46711100
H	2.54710900	-2.20251000	-4.29460800
H	0.07774900	-2.65888600	-4.38858600
C	4.16349600	0.29813200	-1.47083700
C	3.25142900	0.86932100	-0.55575700
H	4.46436400	-1.00594000	-3.17064000
H	5.22487900	0.55226200	-1.37610200
H	3.61598800	1.55421700	0.21419300
N	0.11673700	-0.57449700	-1.74696900
N	0.87396900	1.11537800	0.14664000
C	1.06755200	1.71714000	1.34124300
O	2.08912600	1.62871000	2.04262800

K	2.40889400	-0.97208000	2.11777300
Ni	-0.91073100	0.14128800	-0.12651900
C	0.18516300	-3.37147000	3.07232700
C	-0.42472200	-2.18016400	3.47809000
C	-0.78811700	-1.21930600	2.52582600
C	-0.55749000	-1.38597100	1.14294400
C	0.04808300	-2.60620200	0.77408500
C	0.41044900	-3.58562100	1.70955200
H	0.47211800	-4.12918600	3.80970500
H	-0.61783200	-1.99995300	4.54270100
H	-1.27024900	-0.29779900	2.88964500
H	0.25995500	-2.81471600	-0.28702100
H	0.87783000	-4.51939600	1.37328100
C	-2.87293100	0.13345900	-0.45154200
C	-3.65360100	1.30851300	-0.40700900
C	-5.04013000	1.30509900	-0.59927100
C	-5.70748000	0.10614800	-0.85272900
C	-4.97279000	-1.08105800	-0.90238500
C	-3.59031500	-1.05614200	-0.69822900
H	-3.16931100	2.27874800	-0.21455000
H	-5.60350500	2.24549700	-0.55251300
H	-6.79255400	0.09546000	-1.00723300
H	-5.48407300	-2.03231700	-1.09634700
H	-3.04869300	-2.01532100	-0.72694500

^{S}TS3

Gibbs free energy before correction = -3295.33762200

Gibbs free energy after correction = -3295.32315594

C	-0.20154900	2.82206900	-1.45181300
C	-0.50947800	1.91971600	-2.63796400
H	0.10696600	3.82951600	-1.78393700
H	-1.11994000	2.97721500	-0.85215800
H	-0.83676300	0.93277100	-2.26173500
H	-1.36318400	2.35660000	-3.19103700
C	0.65133500	1.75349100	-3.56542000
H	1.03205100	2.67741200	-4.03027900
C	1.24725000	0.59274900	-3.84743700
H	0.89999100	-0.34678200	-3.39203700
H	2.09672000	0.52798700	-4.53766800
C	0.94675300	-2.89101100	0.31882300
C	2.24348300	-0.97378000	0.18325100
C	3.43470100	-1.69571800	0.46608400

C	3.31222800	-3.09256500	0.67632100
C	2.07434800	-3.68818000	0.60209100
H	-0.05478300	-3.33883400	0.25684300
C	2.26609500	0.44630900	-0.05594200
C	4.66888200	-1.00259100	0.52720300
H	4.21212700	-3.67809300	0.89563300
H	1.94901300	-4.76361700	0.75559300
C	4.68459000	0.35868100	0.30799000
C	3.50818700	1.08491500	0.02708700
H	5.58457800	-1.55942300	0.75247800
H	5.63393000	0.90403600	0.35353600
H	3.56861700	2.16297500	-0.13901400
N	1.02553100	-1.58625600	0.11956300
N	1.05270400	1.00011500	-0.41229400
C	0.87356700	2.34071700	-0.50392800
O	1.47526000	3.18414500	0.18757500
K	0.96742100	1.90088000	2.40257700
Ni	-0.45464200	-0.31154500	-0.09868200
C	-3.44490600	2.70450200	1.54342400
C	-3.66764400	2.33801500	0.20892300
C	-3.02777400	1.23569600	-0.34508200
C	-2.11337400	0.44092300	0.39830300
C	-1.99181100	0.77761400	1.78207200
C	-2.60756700	1.90365700	2.32785900
H	-3.94703000	3.57655500	1.97488700
H	-4.35102700	2.93121400	-0.41074100
H	-3.22739600	0.97748400	-1.39360100
H	-1.42066800	0.10985200	2.44471200
H	-2.45988700	2.14268800	3.38942100
C	-2.06642000	-1.27014200	0.01148100
C	-2.36085300	-1.64910300	-1.32880100
C	-2.94601200	-2.87650600	-1.63074600
C	-3.32217800	-3.75574300	-0.61031200
C	-3.09227500	-3.38483000	0.72083300
C	-2.48283600	-2.17237800	1.02473600
H	-2.12118900	-0.95964100	-2.14963500
H	-3.12500300	-3.14676800	-2.67839200
H	-3.80428900	-4.71026000	-0.84673000
H	-3.39356200	-4.05625600	1.53397100
H	-2.32046300	-1.90932000	2.07834600

^{S}III

Gibbs free energy before correction = -2832.90360100

Gibbs free energy after correction = -2832.88913515

C	2.97714600	-1.26681000	-0.79216100
C	3.53695300	-0.04735200	-0.04531500
H	3.03515200	-1.06645500	-1.87875000
H	3.57724300	-2.16828000	-0.58340500
H	3.35038100	-0.16714600	1.04290400
H	4.64343600	-0.04891900	-0.15214600
C	2.90482100	1.22813600	-0.55307600
H	3.21893600	1.46514000	-1.58935500
C	2.43668600	2.32650600	0.26355000
H	2.64052100	2.30029100	1.35169000
H	2.53282500	3.35432300	-0.13101900
C	-1.52735400	2.42157900	0.31305500
C	-1.54126600	0.19097900	-0.32392600
C	-2.95686100	0.11860700	-0.24236400
C	-3.64829100	1.30670600	0.11006400
C	-2.93656000	2.45278100	0.37757100
H	-0.93711000	3.31260500	0.55689800
C	-0.75560900	-0.95151800	-0.69663900
C	-3.59702300	-1.11786500	-0.50413400
H	-4.74227800	1.29040000	0.16800700
H	-3.43967100	3.38371500	0.65338600
C	-2.83370100	-2.22342400	-0.82062000
C	-1.42722300	-2.15316200	-0.91263800
H	-4.68896200	-1.17597200	-0.44388200
H	-3.32507100	-3.18298600	-1.01521600
H	-0.85527700	-3.04616500	-1.17948100
N	-0.84724200	1.33680200	-0.02433900
N	0.60207400	-0.71025900	-0.83790700
C	1.53985400	-1.59825500	-0.42841600
O	1.30694000	-2.59173700	0.28887800
K	0.19339900	-1.24818900	2.21162500
Ni	1.05523300	1.13184600	-0.34162500

Ph_2

Gibbs free energy before correction = -462.49850200

Gibbs free energy after correction = -462.48403598

C	-0.74067700	-0.00000100	0.00000000
C	-1.46260700	-1.15384400	-0.34616000
C	-2.85595100	-1.15385500	-0.34689500
C	-3.55945600	0.00000100	0.00000000

C	-2.85595000	1.15385600	0.34689500
C	-1.46260600	1.15384300	0.34616100
C	0.74067700	-0.00000100	0.00000000
C	1.46260700	-1.15384400	0.34616000
C	2.85595100	-1.15385500	0.34689500
C	3.55945600	0.00000100	0.00000000
C	2.85595000	1.15385600	-0.34689500
C	1.46260600	1.15384300	-0.34616000
H	-0.92434500	-2.06107900	-0.64222800
H	-3.39737300	-2.06330200	-0.62840100
H	-4.65445500	0.00000100	0.00000000
H	-3.39737100	2.06330300	0.62840000
H	-0.92434300	2.06107800	0.64222800
H	0.92434500	-2.06107900	0.64222800
H	3.39737300	-2.06330200	0.62840000
H	4.65445500	0.00000100	0.00000000
H	3.39737100	2.06330300	-0.62840100
H	0.92434300	2.06107800	-0.64222800

^{T}IVa

Gibbs free energy before correction = -10813.46077900

Gibbs free energy after correction = -10813.44631298

C	-4.50459100	-1.31056300	2.82211100
C	-4.45158600	-2.57406000	1.95181800
H	-5.54046700	-0.92307100	2.81484800
H	-4.23370000	-1.53930100	3.86691600
H	-3.39374100	-2.89453300	1.83829200
H	-4.94744300	-3.40494800	2.49889200
C	-5.07323400	-2.31436000	0.59790200
H	-6.17421200	-2.20034300	0.65817600
C	-4.51936800	-2.71726000	-0.67591500
H	-3.60921400	-3.34967700	-0.67822400
H	-5.21090600	-3.01487000	-1.48496500
C	-3.07984900	0.38927600	-2.65191300
C	-2.96043400	1.55661900	-0.65189100
C	-2.34362200	2.67351000	-1.27493400
C	-2.12456600	2.59573400	-2.67571500
C	-2.49370800	1.46116300	-3.35888700
H	-3.35521900	-0.53630600	-3.17114900
C	-3.22689700	1.54128600	0.75768400
C	-1.98465700	3.79005300	-0.48083800
H	-1.66437100	3.44607400	-3.19216200

H	-2.33368500	1.36766000	-4.43661400
C	-2.20683800	3.75295000	0.88186200
C	-2.80353000	2.63765500	1.50552500
H	-1.53115000	4.66336300	-0.96251900
H	-1.92018600	4.61055700	1.50101800
H	-2.97165300	2.64359200	2.58682400
N	-3.31535000	0.42991800	-1.35097400
N	-3.93096100	0.44085400	1.22046100
C	-3.55470200	-0.22399300	2.34228800
O	-2.46420800	-0.07439100	2.92306400
K	-1.13013300	-0.79722600	0.70123600
Ni	-4.22225100	-0.87035100	-0.22282000
Br	0.00063900	-1.44354100	-2.21077500
Br	4.51036800	-0.30438400	-0.79182800
C	2.08697100	-2.86167900	1.96528600
C	2.86667200	-3.55085300	0.84990800
H	1.00856700	-3.07744700	1.84236200
H	2.39847600	-3.26578900	2.94002600
H	3.92479800	-3.23113400	0.85158900
H	2.86879600	-4.63849900	1.05214600
C	2.25661700	-3.34834900	-0.49336500
H	1.17070200	-3.51853300	-0.55794000
C	2.93878400	-3.07756900	-1.62431200
H	4.03006600	-2.97909300	-1.61359600
H	2.43668700	-3.06016400	-2.59850200
C	1.61175300	1.77237200	-2.14455800
C	1.51753700	1.62423300	0.16988900
C	1.37092500	3.03220400	0.30303000
C	1.35708300	3.79944700	-0.88901100
C	1.47244500	3.17617100	-2.10855900
H	1.70390100	1.24292000	-3.10147100
C	1.54983200	0.76705700	1.31719500
C	1.23431400	3.59723600	1.59246600
H	1.25050000	4.88756900	-0.81548300
H	1.46090300	3.74114400	-3.04422400
C	1.21763200	2.76600700	2.69192200
C	1.36559900	1.36772100	2.56283400
H	1.12450100	4.68233100	1.69087000
H	1.08740700	3.18702600	3.69420400
H	1.34596800	0.74754300	3.46277200
N	1.64204400	1.04011900	-1.05179300
N	1.66507400	-0.60942100	1.09155600

C	2.31215800	-1.36803700	2.02828700
O	3.07054100	-0.91418100	2.89306600
K	4.66238600	0.98899100	2.12146200
Ni	2.07281900	-0.95028500	-0.91777600

^{T}IVb

Gibbs free energy before correction = -10813.49219100

Gibbs free energy after correction = -10813.47772498

C	-4.93885500	-2.03792800	1.43512600
C	-4.87675900	-2.56554000	0.00320100
H	-5.91005400	-1.53051200	1.59518800
H	-4.88687400	-2.87045400	2.15395100
H	-3.84467500	-2.88694400	-0.23531600
H	-5.51159100	-3.47037400	-0.05768400
C	-5.34789700	-1.57791300	-1.02249400
H	-6.41401700	-1.29877300	-0.95800200
C	-4.64515700	-1.28075200	-2.18457000
H	-3.68420500	-1.77094700	-2.40110000
H	-5.14961500	-0.78903900	-3.02987300
C	-3.30834500	2.74203500	-1.85110200
C	-2.73598600	2.08216500	0.30569100
C	-1.97871600	3.26587700	0.51151700
C	-1.92102100	4.19889800	-0.55261900
C	-2.58599000	3.94460700	-1.72940700
H	-3.84775000	2.50475700	-2.77583100
C	-2.89428500	1.09872400	1.34798000
C	-1.33034900	3.47362500	1.75399500
H	-1.34385500	5.12091500	-0.41454700
H	-2.56215600	4.64829200	-2.56565400
C	-1.47403600	2.53127900	2.74597200
C	-2.25162100	1.36472600	2.55990700
H	-0.74125600	4.38450500	1.90335900
H	-0.99085700	2.68414200	3.71753100
H	-2.37962700	0.67223100	3.39418200
N	-3.38047600	1.85442600	-0.87505900
N	-3.72667500	0.03269800	1.03416500
C	-3.82992300	-1.07411200	1.80900500
O	-3.09647400	-1.34584500	2.77375600
K	-0.58513900	-1.28810100	2.05173400
Ni	-4.36750900	0.15113600	-0.82780300
C	3.16904100	-2.84911700	1.74622100
C	3.50523900	-3.34801700	0.33590800
H	2.19180200	-3.26414800	2.06051200
H	3.92616100	-3.19056400	2.46981600
H	4.29786800	-2.70697000	-0.09805000
H	3.93184800	-4.36685200	0.40941100
C	2.31544900	-3.37101300	-0.58285600

H	1.55372500	-4.13172600	-0.34324600
C	2.29900800	-2.78231100	-1.84362500
H	3.18185700	-2.23105100	-2.20498500
H	1.56777500	-3.09986100	-2.59964600
C	0.50203600	0.76782000	-2.14923700
C	1.48034400	1.19477100	-0.09360200
C	1.47045100	2.59701100	-0.32332200
C	0.96994600	3.04671100	-1.56975400
C	0.48813300	2.13752800	-2.48283200
H	0.09790000	0.01543600	-2.83897200
C	2.03367000	0.64737400	1.11403400
C	1.95445200	3.47085200	0.68235300
H	0.96912100	4.12156100	-1.78537000
H	0.08815800	2.45632600	-3.44960800
C	2.39876000	2.94477700	1.87633900
C	2.43567500	1.54809900	2.09809700
H	1.94421500	4.55134500	0.50000900
H	2.74175200	3.61307500	2.67407600
H	2.81466400	1.16706600	3.05016300
N	0.98886900	0.31902800	-1.01049300
N	2.09374900	-0.74399900	1.19272000
C	3.15936400	-1.33528600	1.78969900
O	4.13894700	-0.74633400	2.27389200
K	5.38030200	1.12441500	0.98183100
Ni	1.33823700	-1.60224400	-0.52922600
Br	4.70465300	0.29584800	-1.83925400
Br	-1.07244300	-2.38434300	-0.87387500

^{T}TS4

Gibbs free energy before correction = -10813.44728300

Gibbs free energy after correction = -10813.43281698

C	-5.34676700	-1.47358000	1.59257400
C	-5.34047500	-2.14508100	0.22356500
H	-6.23067400	-0.81114900	1.66819400
H	-5.42985300	-2.22380200	2.39371700
H	-4.39355700	-2.69733900	0.07232900
H	-6.14495800	-2.90602300	0.20229500
C	-5.54904700	-1.19470800	-0.91705900
H	-6.47241000	-0.59323500	-0.87519900
C	-4.84754800	-1.27992000	-2.10828700
H	-4.09096000	-2.05907300	-2.27077000
H	-5.21477900	-0.75827400	-3.00394500

C	-2.33149200	2.27680200	-2.12314300
C	-2.37872600	2.05383300	0.18753800
C	-1.42422300	3.09336600	0.35575200
C	-0.92560200	3.71031800	-0.81752200
C	-1.36710600	3.30133000	-2.05383400
H	-2.71295000	1.93238500	-3.09232300
C	-2.91734000	1.34002300	1.31366000
C	-1.01309100	3.45721700	1.66002000
H	-0.18447000	4.51183300	-0.71787800
H	-0.98986800	3.75538500	-2.97391300
C	-1.55633100	2.79513700	2.73862700
C	-2.49026700	1.74901600	2.58020100
H	-0.26694500	4.24862700	1.78558100
H	-1.25584100	3.07522600	3.75403400
H	-2.88851400	1.24287700	3.46187600
N	-2.82318600	1.69252000	-1.04886400
N	-3.82949000	0.34193700	1.01620800
C	-4.11733200	-0.64377400	1.90431200
O	-3.44483500	-0.91465600	2.90929500
K	-1.00445800	-1.02595200	1.89185000
Ni	-4.04973000	0.15119100	-0.95582400
C	2.28361200	-2.79916500	2.07181500
C	2.62047400	-3.51013300	0.75398700
H	1.22561800	-3.00802900	2.33094100
H	2.90205900	-3.18818200	2.89596500
H	3.55821900	-3.09254800	0.33860000
H	2.82024500	-4.57793200	0.96902900
C	1.52106000	-3.39962000	-0.26853700
H	0.56389400	-3.86832900	0.02146500
C	1.72557100	-3.10502300	-1.61474500
H	2.74259100	-2.90771300	-1.98478600
H	0.96243300	-3.36576200	-2.35831200
C	1.34711100	0.81964600	-2.51102300
C	1.82506400	1.27730800	-0.29235600
C	2.21726100	2.60866500	-0.59932600
C	2.20425100	2.98952900	-1.96405600
C	1.77821200	2.10080100	-2.92014700
H	0.96787500	0.08903100	-3.23697400
C	1.93321400	0.77011000	1.04953400
C	2.62469400	3.47502400	0.44632700
H	2.53859800	3.99797500	-2.23611900
H	1.76737300	2.36396800	-3.98130500

C	2.63142600	3.01064500	1.74468400
C	2.29840000	1.67108400	2.04670600
H	2.92188400	4.50210300	0.20545000
H	2.91703300	3.68221400	2.56249700
H	2.35723500	1.31846000	3.08008300
N	1.38299400	0.42962700	-1.25715400
N	1.68106600	-0.58621100	1.23987500
C	2.54099900	-1.30324700	2.00779000
O	3.53996100	-0.85094400	2.59003600
K	5.33550900	0.41617500	1.31105200
Ni	1.14541300	-1.46296200	-0.60251700
Br	4.60771100	-0.71243100	-1.31469800
Br	-1.35785600	-1.55160500	-1.16529000

^{T}IVc

Gibbs free energy before correction = -10813.49521400

Gibbs free energy after correction = -10813.48074798

C	-4.36643200	-1.75329400	2.59568700
C	-4.71352700	-2.61294200	1.38537700
H	-5.26923400	-1.18904300	2.90220400
H	-4.08310300	-2.39127400	3.44759100
H	-3.81890300	-3.17146400	1.04588200
H	-5.44039500	-3.38270500	1.71436900
C	-5.29343100	-1.84538300	0.23124100
H	-6.11666200	-1.15683700	0.48060200
C	-5.06362700	-2.16493100	-1.09702000
H	-4.45770000	-3.03936400	-1.36904700
H	-5.71717200	-1.76507500	-1.88424900
C	-3.36312300	1.70556800	-2.26577800
C	-2.77773900	1.93167000	-0.03466700
C	-2.27629700	3.24462500	-0.24492000
C	-2.38311100	3.77616100	-1.55487300
C	-2.92772000	3.01389700	-2.56212600
H	-3.76737200	1.05626800	-3.05273100
C	-2.75352200	1.31787600	1.26845900
C	-1.68766300	3.94345700	0.83809700
H	-2.01842700	4.79210200	-1.74682200
H	-3.01683400	3.39557200	-3.58294100
C	-1.61522600	3.33110600	2.07136700
C	-2.13218600	2.03636700	2.29533300
H	-1.28895000	4.95068800	0.67220400
H	-1.14626800	3.85695200	2.91096600

H	-2.06598300	1.59363300	3.29161500
N	-3.30558400	1.19652300	-1.05102600
N	-3.39632500	0.09844300	1.35196800
C	-3.25647600	-0.73452200	2.41337000
O	-2.30467700	-0.71925100	3.21068200
K	-0.55775500	-0.73482000	1.13781700
Ni	-3.79885300	-0.68381600	-0.50836400
Br	-1.73543500	-1.64437500	-1.65703800
Br	4.20484500	-0.56322000	-1.91225300
C	2.74693100	-2.66039800	2.23930700
C	2.83210400	-3.47899900	0.95277300
H	1.72120400	-2.73856200	2.65057900
H	3.43152800	-3.07578900	2.99509600
H	3.82906100	-3.34700500	0.48929000
H	2.75883400	-4.55138700	1.22036200
C	1.76606900	-3.14984800	-0.05414200
H	0.72584100	-3.22889300	0.30477500
C	1.98300800	-3.09991300	-1.41953200
H	2.96718200	-3.33448000	-1.84519300
H	1.12583800	-3.11570400	-2.10740700
C	0.84374700	1.16010800	-2.03527600
C	1.72916100	1.51097300	0.08032400
C	1.62490500	2.92165400	-0.05113500
C	1.10152300	3.42057200	-1.27027700
C	0.70714700	2.54628700	-2.25639300
H	0.53743100	0.43432700	-2.79921200
C	2.25342200	0.90813400	1.27721200
C	2.04135700	3.75105200	1.01931800
H	1.01317900	4.50511500	-1.40536900
H	0.29528400	2.90347900	-3.20416700
C	2.52694700	3.17006700	2.17099100
C	2.63523000	1.76794800	2.30866800
H	1.96229500	4.83844800	0.91377900
H	2.84146400	3.80233400	3.00833500
H	3.02410700	1.34844700	3.23992300
N	1.34428300	0.66679000	-0.91822200
N	2.24540700	-0.47954400	1.29919000
C	3.09434500	-1.19135800	2.08125900
O	4.11866600	-0.74272200	2.62158300
K	5.37480700	0.58138600	0.74795200
Ni	2.07168000	-1.21204200	-0.66742800

IV

Gibbs free energy before correction = -5406.74718000

Gibbs free energy after correction = -5406.73271382

Br	-1.26931400	-1.56602400	1.58736500
C	-2.29983100	2.32337600	-1.12550000
C	-3.16402000	1.06635100	-1.15595600
H	-2.05692000	2.61323800	-2.16660000
H	-2.86124000	3.15998200	-0.68056600
H	-3.41510000	0.75260400	-0.12403100
H	-4.12874800	1.32902100	-1.63505700
C	-2.54026800	-0.08651800	-1.89097400
H	-2.14223200	0.14510100	-2.89206800
C	-2.69250900	-1.41455300	-1.52289300
H	-3.33112800	-1.69254700	-0.67379200
H	-2.46563600	-2.21546900	-2.23983300
C	1.53099000	-2.36909400	-0.79702900
C	1.82322200	-0.08308100	-0.55488800
C	3.22776100	-0.22607100	-0.38788300
C	3.75719900	-1.53962000	-0.45984800
C	2.91507700	-2.60749800	-0.66585900
H	0.82876500	-3.20170900	-0.92974400
C	1.19007300	1.20894600	-0.50665700
C	4.01847000	0.92583200	-0.15280700
H	4.83717900	-1.68416200	-0.34338100
H	3.29476200	-3.63133600	-0.72095300
C	3.40518700	2.15925000	-0.08680100
C	2.01164000	2.31001000	-0.25106800
H	5.09996500	0.81416900	-0.02200700
H	4.00801600	3.05511700	0.09889600
H	1.56791800	3.30671800	-0.19105900
N	1.01212900	-1.15819800	-0.75417600
N	-0.16366200	1.21769800	-0.77666900
C	-0.98190500	2.22095800	-0.37931100
O	-0.73305200	3.02297600	0.53801500
K	-0.07852600	1.21855900	2.36431000
Ni	-0.94996300	-0.67937700	-0.78295900

Va

Gibbs free energy before correction = -3355.53121800

Gibbs free energy after correction = -3355.51675176

C	0.31611500	3.11894600	0.72333400
C	0.71874700	3.63207700	-0.65314000

H	0.51973800	3.87347500	1.50360400
H	-0.77495500	2.94015700	0.77595700
H	0.52725400	2.84641600	-1.40409300
H	0.07435100	4.49409800	-0.90979200
C	2.15376300	4.05082700	-0.69391700
H	2.42889400	4.88380500	-0.02694600
C	3.10042900	3.48222100	-1.44365700
H	2.86582000	2.64327400	-2.11429700
H	4.14031100	3.82943300	-1.42564800
C	0.82189000	-2.43236500	-1.80764200
C	2.17387900	-1.19141700	-0.38811000
C	3.16582700	-2.20769000	-0.35096700
C	2.92109800	-3.37709900	-1.11604700
C	1.75427900	-3.49032600	-1.83655600
H	-0.12387200	-2.48905000	-2.36000300
C	2.31504700	0.02268900	0.36535100
C	4.32223300	-2.01358400	0.44287500
H	3.66755000	-4.17933400	-1.11554100
H	1.53668100	-4.38285500	-2.42982300
C	4.45117100	-0.84723300	1.17045800
C	3.46429900	0.15886600	1.14643700
H	5.08899300	-2.79496300	0.47152300
H	5.34216600	-0.69056500	1.78857700
H	3.60516000	1.06715600	1.73942700
N	1.02658900	-1.32348300	-1.11612200
N	1.32182000	0.96498100	0.18877000
C	1.00435500	1.84485500	1.16660400
O	1.15793000	1.63757800	2.38414400
K	-0.10239300	-0.68374400	2.25601900
Ni	-0.13214600	0.25939800	-1.05009600
B	-2.64112600	0.31173800	-1.24633000
C	-2.81750200	-0.29167200	0.26166500
C	-2.71678100	-1.66614400	0.54489400
C	-3.10068400	0.55654500	1.34816300
C	-2.88962000	-2.17086200	1.83765800
H	-2.49117400	-2.35930900	-0.27600500
C	-3.27222400	0.06951900	2.64769600
C	-3.16559100	-1.30223200	2.89911600
H	-2.80843100	-3.24853900	2.02229600
H	-3.49298400	0.76060300	3.46920400
H	-3.30331600	-1.69205000	3.91365500
O	-1.74364200	1.50842100	-1.24239500

H	-2.03523700	2.20638700	-0.64383400
O	-1.85585500	-0.66661400	-2.03955900
H	-1.91479300	-0.39729800	-2.96626900
O	-3.88833800	0.68588700	-1.86951900
H	-3.20287600	1.63878600	1.17969000
C	-4.88836700	-0.26916500	-1.92308500
H	-5.73832700	0.10275600	-2.52546700
H	-4.55639300	-1.22233900	-2.39082400
H	-5.29718300	-0.53393200	-0.92210000

TS5

Gibbs free energy before correction = -3355.50806200

Gibbs free energy after correction = -3355.49359576

C	0.62980800	3.10787800	0.58133900
C	1.18102200	3.65024500	-0.73323400
H	0.77362300	3.83431300	1.39971300
H	-0.46192600	2.94905200	0.49784600
H	0.98509600	2.92601500	-1.54273500
H	0.63181400	4.57621500	-0.98773700
C	2.64442100	3.94252400	-0.63788700
H	2.92991400	4.72641900	0.08196200
C	3.60204200	3.30920800	-1.31886300
H	3.35809900	2.51662300	-2.04026500
H	4.66257900	3.55756100	-1.19303100
C	0.21023700	-2.55165800	-1.59149000
C	1.87477700	-1.41881500	-0.44603000
C	2.75271200	-2.53584500	-0.50388000
C	2.28410100	-3.69164400	-1.17982800
C	1.02374000	-3.69605500	-1.73035400
H	-0.80888800	-2.53868100	-1.99975700
C	2.27290100	-0.19002900	0.18269000
C	4.02544600	-2.44650800	0.11018000
H	2.93855200	-4.56743200	-1.25320800
H	0.63658700	-4.56952300	-2.26215600
C	4.38502700	-1.27706200	0.75038900
C	3.52785000	-0.15938500	0.79383100
H	4.69913900	-3.30902700	0.07133100
H	5.36616400	-1.20329800	1.23243700
H	3.85693600	0.75677000	1.29316600
N	0.61389700	-1.45685100	-0.96999500
N	1.39787900	0.86788200	0.05537200
C	1.25939000	1.80236300	1.02647800

O	1.52934800	1.62669700	2.22745800
K	0.09609100	-0.57737600	2.55362400
Ni	-0.40828100	0.25300400	-0.62108700
B	-2.49104000	0.61712100	-1.74318200
C	-2.10178500	-0.20617900	0.30324200
C	-2.40650300	-1.55233500	0.60716000
C	-2.52363500	0.73104800	1.28049400
C	-3.02885300	-1.94581600	1.79882000
H	-2.13516700	-2.33944700	-0.11204300
C	-3.14261200	0.36271700	2.47784600
C	-3.39065600	-0.98855100	2.75096300
H	-3.23324500	-3.00706900	1.98707100
H	-3.43490700	1.13003100	3.20541000
H	-3.87439300	-1.28792700	3.68732700
O	-1.56106400	1.69638700	-1.85347900
H	-1.92317700	2.49072500	-1.43646100
O	-2.34275800	-0.44405900	-2.64057600
H	-1.43742600	-0.48426000	-2.97211700
O	-3.78607500	1.02924800	-1.44216200
H	-2.36669400	1.80548200	1.09531600
C	-4.82752800	0.11001700	-1.36683300
H	-5.79109300	0.64809800	-1.35094700
H	-4.84475100	-0.58566900	-2.22728000
H	-4.77495700	-0.50466200	-0.44410300

V

Gibbs free energy before correction = -3064.13487900

Gibbs free energy after correction = -3064.12041282

C	2.04722100	-2.88112100	0.53992600
C	2.87945400	-2.22199300	-0.55818900
H	1.56067800	-3.78414000	0.12210000
H	2.70124800	-3.21525700	1.36124400
H	3.38905400	-1.32723600	-0.15214100
H	3.69061600	-2.92706400	-0.83310800
C	2.09655600	-1.84160700	-1.78687700
H	1.51583300	-2.65655800	-2.24916200
C	2.31364400	-0.67707300	-2.52114300
H	3.13464200	0.00479700	-2.25554800
H	1.96594000	-0.60931300	-3.56140800
C	-1.88005400	0.63104100	-2.40101900
C	-1.96425600	-0.42087700	-0.34048000
C	-3.31886500	-0.03779200	-0.14028100

C	-3.94079300	0.70681100	-1.17496200
C	-3.22877600	1.03468100	-2.30517000
H	-1.27522900	0.90996800	-3.27423200
C	-1.25345300	-1.19587400	0.64712200
C	-3.97569800	-0.40319100	1.06146300
H	-4.98634800	1.01220400	-1.05480400
H	-3.68239500	1.60622800	-3.11960000
C	-3.28421200	-1.12307800	2.01276200
C	-1.94113400	-1.51353700	1.82378600
H	-5.01765800	-0.10253800	1.21406900
H	-3.78322200	-1.40672200	2.94622700
H	-1.43295000	-2.09088700	2.60060200
N	-1.27603100	-0.06854800	-1.46041200
N	0.01285100	-1.58830400	0.28227000
C	0.94547500	-2.03496700	1.15500600
O	0.95974300	-1.79572300	2.37619300
K	0.49493000	0.78984600	2.36826500
Ni	0.75693100	-0.42098800	-1.24666500
C	1.13937600	1.44067700	-0.58328300
C	2.41145700	1.66800900	-0.00047000
C	2.71469000	2.77597500	0.80147900
C	1.73898400	3.74497000	1.05339500
C	0.47465300	3.58440000	0.47909300
C	0.19484700	2.45957900	-0.30837300
H	3.22026000	0.93893500	-0.16993200
H	3.71781300	2.88456300	1.23288000
H	1.96350800	4.61663100	1.67816200
H	-0.30321200	4.33861200	0.65361200
H	-0.82670200	2.38191200	-0.71461700

TS6

Gibbs free energy before correction = -3064.10554800

Gibbs free energy after correction = -3064.09108182

C	-0.92942200	-3.49967100	0.15700900
C	0.58481900	-3.47572900	0.16651400
H	-1.27970600	-4.02373700	-0.75520200
H	-1.33232300	-4.07643400	1.00502600
H	0.96019500	-3.13084400	1.14978200
H	0.96125200	-4.51229000	0.05079800
C	0.92619900	2.21802100	0.35465400
C	-1.06550300	1.23656800	-0.38843600
C	-1.73582900	2.50215900	-0.42830500

C	-0.99401900	3.64680900	-0.02858600
C	0.34124100	3.46856400	0.38753900
H	1.96536200	2.08360400	0.66858600
C	-1.76535100	0.05014600	-0.68631400
C	-3.08359600	2.52720500	-0.86449700
H	-1.46970400	4.63390000	-0.03091900
H	0.93710400	4.32033400	0.73303300
C	-3.72514000	1.35401300	-1.28098400
C	-3.07980200	0.11839600	-1.19618200
H	-3.60087500	3.49301200	-0.91473800
H	-4.74787800	1.40399300	-1.67334300
H	-3.59104500	-0.80034600	-1.50101700
N	0.26353800	1.09698500	-0.06068300
N	-1.03190200	-1.13189500	-0.47660500
C	-1.64189800	-2.16438400	0.13935200
O	-2.78119200	-2.10827500	0.64791700
K	-3.85077700	-0.01070300	1.64854600
Ni	0.86484000	-0.75140400	-0.39181600
C	2.70817200	-0.23409200	-0.07442700
C	3.40161700	0.58657800	-0.97790400
C	4.43935800	1.41431900	-0.54874600
C	4.81401900	1.43458100	0.79659000
C	4.14308300	0.61197300	1.70588000
C	3.11182200	-0.22099000	1.27249900
H	3.12253300	0.57605300	-2.03995000
H	4.96235800	2.04911400	-1.27329400
H	5.63200000	2.08004300	1.13398700
H	4.43327200	0.61188800	2.76288700
H	2.61331600	-0.88387400	1.99319400
C	1.14471200	-2.59625800	-0.91164300
H	0.70229800	-2.71855700	-1.91206500
C	2.44468900	-2.05430000	-0.82321600
H	2.97519600	-1.84713700	-1.75994900
H	3.09893200	-2.44894100	-0.03541700

VI

Gibbs free energy before correction = -3064.14016700

Gibbs free energy after correction = -3064.12570082

C	-0.40156300	-3.11644900	-0.93076600
C	0.82725900	-3.06009500	-0.01712800
H	-0.07443800	-2.93016300	-1.97223400
H	-0.85963200	-4.11921500	-0.90135800

H	0.48144800	-3.05954700	1.03978300
H	1.37287500	-4.02797500	-0.12956300
C	0.33065000	2.66363400	0.32722800
C	-1.55713500	1.46099100	-0.28092100
C	-2.38257800	2.61310500	-0.18872500
C	-1.76423400	3.83033000	0.19630700
C	-0.41311000	3.85405000	0.45215100
H	1.41108900	2.66147800	0.51731500
C	-2.09650200	0.18351700	-0.66527400
C	-3.76427900	2.50463300	-0.48754000
H	-2.37517700	4.73612800	0.27824500
H	0.09616300	4.77647100	0.74486000
C	-4.27453600	1.28582600	-0.88319000
C	-3.46047200	0.13527800	-0.97272100
H	-4.39756500	3.39505400	-0.41416100
H	-5.33578600	1.19938500	-1.14318700
H	-3.89422400	-0.80276200	-1.33462400
N	-0.21395800	1.50675800	-0.01965700
N	-1.17577300	-0.83288200	-0.76538100
C	-1.49363000	-2.12715500	-0.58449900
O	-2.57777800	-2.54875100	-0.12614900
K	-4.25807400	-1.66810300	1.49529100
Ni	0.67330200	-0.21086300	-0.20753100
C	3.84280500	-0.70903600	0.46329800
C	5.06539100	-0.84572100	-0.20172900
C	5.87464100	0.26505100	-0.46210600
C	5.47238400	1.53550600	-0.05351900
C	4.25309000	1.68883900	0.61377100
C	3.44613400	0.57951200	0.85858500
H	5.38884900	-1.84449200	-0.52211900
H	6.82785100	0.13337700	-0.98628700
H	6.10674900	2.40655800	-0.25051100
H	3.93322500	2.68309700	0.94728600
H	2.48101100	0.69690500	1.37397100
C	1.73349600	-1.86106100	-0.26866500
H	2.15300800	-1.98690700	-1.29781000
C	2.92923700	-1.87755300	0.68722800
H	3.52548700	-2.81743000	0.61112300
H	2.55808200	-1.84814400	1.73336500

_n_-BuI

Gibbs free energy before correction = -455.29395900

Gibbs free energy after correction = -455.27949273

C	-0.48337300	0.82158100	0.00010300
C	-1.60213500	-0.19268000	0.00034000
H	-0.50239600	1.46551900	-0.89335600
H	-0.50215100	1.46564300	0.89347600
C	-2.96616700	0.48558500	-0.00012700
H	-1.51441200	-0.85259300	-0.88403500
H	-1.51457300	-0.85188800	0.88525500
C	-4.10892000	-0.51142500	-0.00010500
H	-3.04164900	1.15036900	0.88158700
H	-3.04120700	1.14985500	-0.88226800
H	-5.09149200	-0.01144600	-0.00029600
H	-4.07004800	-1.16579200	-0.88872000
H	-4.07026000	-1.16551000	0.88872700
I	1.47758000	-0.09061400	-0.00003100

VIa

Gibbs free energy before correction = -3519.42530600

Gibbs free energy after correction = -3519.41083995

C	1.36487400	-0.87340700	2.60536600
C	2.24097900	-0.28076700	1.49556400
H	1.62719700	-1.94171900	2.72692800
H	1.57080000	-0.36552200	3.56253500
H	1.89230200	0.75490300	1.28309100
H	3.26019400	-0.14805100	1.92685800
C	-1.59799700	-2.24288800	-2.36048400
C	-2.32249800	-2.04938400	-0.16704400
C	-3.67079500	-2.30484600	-0.53310600
C	-3.93631100	-2.54708900	-1.90536400
C	-2.90443000	-2.51824500	-2.81420300
H	-0.75995200	-2.19657600	-3.06721600
C	-1.95474300	-1.78404000	1.19816000
C	-4.67420000	-2.29359600	0.46850800
H	-4.96554900	-2.75111600	-2.22076800
H	-3.07710900	-2.69850500	-3.87871900
C	-4.31819000	-2.04171800	1.77771000
C	-2.97942900	-1.78703900	2.14849000
H	-5.71389000	-2.48709900	0.18448700
H	-5.08739300	-2.03859300	2.55796400
H	-2.73644600	-1.60096800	3.19908000
N	-1.31332900	-2.02094500	-1.08809900
N	-0.60943200	-1.60132100	1.41996500

C	-0.12477700	-0.76509100	2.36261300
O	-0.79114600	0.09271900	2.97659300
K	-2.56034200	1.30093800	1.56792400
Ni	0.42234600	-1.51762300	-0.32626900
C	4.63181200	-0.36011400	-0.41899700
C	5.16062300	0.85062500	0.04882800
C	6.48115400	0.93947900	0.49397900
C	7.30392500	-0.18712800	0.47836500
C	6.79334900	-1.40148900	0.01374200
C	5.47293000	-1.48306900	-0.42623700
H	4.51916400	1.74183000	0.06038900
H	6.87111500	1.89792700	0.85484400
H	8.34101900	-0.11947900	0.82423200
H	7.43230400	-2.29152200	-0.00885500
H	5.07730500	-2.44006300	-0.79179300
C	2.25918900	-1.10171100	0.20878000
H	2.69454700	-2.09689900	0.47672700
C	3.19250300	-0.48629400	-0.84684600
H	2.82160300	0.51894800	-1.13274500
H	3.15473100	-1.10024400	-1.76778000
I	-0.29022500	1.33057400	-1.29017500
C	-0.81392400	3.40674600	-1.84560800
C	-1.82871500	4.03656500	-0.92145900
H	0.14352200	3.95329500	-1.84941500
H	-1.18136200	3.32759500	-2.87970400
C	-1.31869400	4.33804000	0.47992700
H	-2.16652200	4.98682400	-1.38238900
H	-2.74277800	3.40734900	-0.87907900
C	-2.38882800	4.91363800	1.38909700
H	-0.86639100	3.42794000	0.92850600
H	-0.46923900	5.04261900	0.40773600
H	-2.01470000	5.09518100	2.40960800
H	-2.76541500	5.87410700	0.99737800
H	-3.27467900	4.25408100	1.46786300

TS7

Gibbs free energy before correction = -3519.40070500

Gibbs free energy after correction = -3519.38623895

C	-0.51504200	-2.45228900	1.50174500
C	-1.53381900	-2.25080500	0.39350400
H	-0.77105400	-1.82339200	2.37871400
H	-0.53318400	-3.48915500	1.88947900

H	-1.21065300	-2.83181600	-0.49723500
H	-2.48117000	-2.74167500	0.72030100
C	2.02725600	1.57756800	-2.20422900
C	2.78239100	-0.42095600	-1.31922300
C	4.06548700	-0.25631700	-1.91473100
C	4.28045000	0.91136700	-2.69098300
C	3.26249000	1.82135100	-2.84034100
H	1.20662900	2.29618800	-2.32130700
C	2.48113300	-1.58511100	-0.52993300
C	5.06304000	-1.24099300	-1.70855600
H	5.25698600	1.06480600	-3.16348100
H	3.38854900	2.72767200	-3.43887000
C	4.76631500	-2.35620700	-0.95065700
C	3.49568000	-2.53428300	-0.36759800
H	6.05063800	-1.10070500	-2.16030300
H	5.53007100	-3.12576800	-0.79356400
H	3.29288900	-3.43184200	0.22387000
N	1.78866900	0.50861700	-1.46452700
N	1.20242000	-1.67223200	-0.03712500
C	0.93665000	-2.16914300	1.18547900
O	1.78535200	-2.36203400	2.08253400
K	3.51001500	-0.46474900	2.06469100
Ni	0.07798500	0.03073200	-0.41314300
C	-4.10377100	-1.16203900	-0.86388000
C	-4.52287100	-2.42991800	-1.28999100
C	-5.78749100	-2.92280200	-0.96190000
C	-6.66489100	-2.15185000	-0.19887000
C	-6.26394000	-0.88521900	0.23355200
C	-4.99815200	-0.40150500	-0.09444800
H	-3.83996300	-3.03974900	-1.89614100
H	-6.09124200	-3.91729900	-1.30802200
H	-7.65886500	-2.53443000	0.05692100
H	-6.94653900	-0.26812900	0.82874600
H	-4.68551100	0.59502300	0.24869800
C	-1.72299600	-0.78773300	0.00852700
H	-2.18552200	-0.27904400	0.89092000
C	-2.71953600	-0.64361900	-1.15288900
H	-2.32468100	-1.17102500	-2.04588800
H	-2.80537100	0.42394900	-1.43980100
C	-0.61542300	2.23534200	-0.28044800
C	-1.98453300	2.72864800	0.10666800
H	-0.70116800	1.51619600	-1.14075700

H	0.05924500	3.04895300	-0.59029400
C	-2.70244300	3.35802400	-1.08371800
H	-2.59123700	1.89095900	0.50180000
H	-1.91043600	3.47216300	0.92295400
C	-4.10206200	3.82193600	-0.72942000
H	-2.10167100	4.20633500	-1.46360300
H	-2.74446200	2.62659600	-1.91415200
H	-4.61009700	4.29127800	-1.58791000
H	-4.72922900	2.97595400	-0.39561200
H	-4.08511100	4.56050100	0.09124800
I	0.50159100	1.70279400	1.70014200

TS8

Gibbs free energy before correction = -3519.41749100

Gibbs free energy after correction = -3519.40302495

C	1.39783700	-0.75005000	2.59714500
C	2.25719100	-0.15273800	1.47900600
H	1.67777000	-1.81374700	2.72375400
H	1.60612800	-0.23614200	3.54982700
H	1.91479600	0.88568300	1.27489200
H	3.28228600	-0.03357300	1.89607000
C	-1.61171600	-2.39753500	-2.33380100
C	-2.28996200	-2.11630800	-0.13356500
C	-3.62082400	-2.50855600	-0.44008500
C	-3.89860000	-2.86465400	-1.78393700
C	-2.90003700	-2.81303900	-2.72814600
H	-0.79924900	-2.32559400	-3.06783100
C	-1.91035200	-1.73874000	1.20366700
C	-4.59734600	-2.51841000	0.58718000
H	-4.91503400	-3.17484500	-2.05080200
H	-3.08589300	-3.07938600	-3.77192200
C	-4.23218900	-2.14993800	1.86399800
C	-2.91107400	-1.76047600	2.17853800
H	-5.62278100	-2.81725700	0.34634500
H	-4.97836500	-2.15759600	2.66607800
H	-2.66188200	-1.48914600	3.20787000
N	-1.31992900	-2.07019600	-1.08967500
N	-0.57375900	-1.45017500	1.37803700
C	-0.09915800	-0.68112500	2.38637100
O	-0.79170700	0.07051500	3.09676800
K	-2.41415400	1.38689000	1.57489800
Ni	0.42016900	-1.31946700	-0.38117400

C	4.65815100	-0.30918600	-0.42461300
C	5.22571000	0.88037500	0.05146800
C	6.54525900	0.92035500	0.50547600
C	7.32701300	-0.23511100	0.49041500
C	6.77693500	-1.42874600	0.01751200
C	5.45744400	-1.46194700	-0.43168300
H	4.61576100	1.79323200	0.06298400
H	6.96682600	1.86272900	0.87283200
H	8.36341800	-0.20608200	0.84354500
H	7.38384900	-2.34087800	-0.00379200
H	5.03000200	-2.40267300	-0.80338500
C	2.26352000	-0.95942900	0.18803400
H	2.62888700	-1.98543700	0.44073700
C	3.21741900	-0.37615800	-0.86103000
H	2.88425800	0.64432100	-1.13686400
H	3.15673700	-0.98109400	-1.78662100
I	-0.26758700	1.21250400	-1.26027000
C	-1.07358200	3.58930800	-2.01332700
C	-2.10758300	4.09303300	-1.05852500
H	-0.11967900	4.13907100	-2.02186300
H	-1.42606200	3.33769100	-3.02329500
C	-1.56011400	4.48564300	0.30670700
H	-2.62220000	4.98084200	-1.49049600
H	-2.92252000	3.34422400	-0.94637900
C	-2.63174400	4.96253100	1.26980700
H	-0.98148000	3.63998100	0.73565800
H	-0.80143100	5.27948100	0.17245200
H	-2.22321900	5.20167600	2.26520300
H	-3.12818500	5.87162700	0.88875100
H	-3.44013400	4.21824800	1.40801000

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Gibbs free energy before correction = -157.45783300

Gibbs free energy after correction = -157.44336659

C	-1.99100000	-0.08440200	-0.00000300
C	-0.63327600	0.51308300	-0.00001700
H	-2.45307800	-0.42399000	-0.93509800
H	-2.45317200	-0.42375800	0.93512900
C	0.49414100	-0.52851800	0.00002100
H	-0.49884400	1.16499100	-0.88572900
H	-0.49885400	1.16505900	0.88564400
C	1.87070300	0.10721000	-0.00000200

H	0.37635400	-1.18654400	0.88199000
H	0.37635200	-1.18660600	-0.88190200
H	2.67522900	-0.64691500	0.00001200
H	2.01629800	0.74674000	-0.88862600
H	2.01630900	0.74678500	0.88858700

VIb

Gibbs free energy before correction = -3361.98343200

Gibbs free energy after correction = -3361.96896589

C	-1.03990500	2.19961100	1.70892500
C	-1.90163700	0.98268200	1.40370600
H	-1.32698800	3.01764700	1.02065500
H	-1.20310700	2.55858600	2.73737800
H	-1.70462800	0.18620700	2.15351700
H	-2.96381800	1.26886400	1.55984500
C	2.36610200	-1.38819000	-1.85878700
C	2.72428600	0.68571000	-0.89444900
C	4.02209200	0.79330800	-1.46071100
C	4.45318000	-0.27488400	-2.28672900
C	3.62564700	-1.35395300	-2.49325400
H	1.70289300	-2.25340100	-1.97930000
C	2.17556100	1.72007200	-0.08036300
C	4.79871400	1.94159400	-1.17569000
H	5.44418200	-0.22373200	-2.75107200
H	3.92801900	-2.19109200	-3.12786700
C	4.27547100	2.92358100	-0.35872200
C	2.97948600	2.82406100	0.18852900
H	5.80072100	2.03014800	-1.60801300
H	4.87174400	3.81368300	-0.13115100
H	2.59666600	3.63133100	0.81871700
N	1.93073300	-0.40879300	-1.08638500
N	0.85406400	1.54044000	0.31432900
C	0.44319500	1.97977800	1.54020700
O	1.21513900	2.15858500	2.49509500
K	1.98467500	-0.40362600	2.48385600
Ni	0.11804000	-0.14831700	-0.28333700
C	-4.09271400	0.17413200	-0.69310500
C	-5.13091200	0.12382900	0.24616900
C	-6.33357300	0.79870100	0.02720200
C	-6.51962700	1.53838400	-1.14059100
C	-5.49404800	1.59730100	-2.08686600
C	-4.29523200	0.92271100	-1.86195200

H	-4.99222400	-0.46279600	1.16333100
H	-7.13278000	0.74317100	0.77462500
H	-7.46315600	2.06628400	-1.31568700
H	-5.63251200	2.17081200	-3.01009700
H	-3.49302100	0.96841700	-2.61002400
C	-1.67773600	0.44510900	0.00718600
H	-1.67270100	1.30318800	-0.70347400
C	-2.77615400	-0.51658700	-0.45082600
H	-2.91697800	-1.31400300	0.30232700
H	-2.46067800	-1.01724000	-1.38587000
I	-0.13629200	-2.61068400	0.46408800

VII

Gibbs free energy before correction = -3519.47299400

Gibbs free energy after correction = -3519.45852795

C	0.86630300	-1.43029700	-2.54725900
C	1.72274000	-1.49166400	-1.29307600
H	1.04055200	-0.47369600	-3.07419400
H	1.11867400	-2.25297700	-3.23406800
H	1.36138700	-2.31552500	-0.64057100
H	2.74994700	-1.79659800	-1.58252600
C	-2.15181200	2.35655000	1.03779200
C	-2.84223100	0.71621100	-0.43969800
C	-4.21012900	1.04981500	-0.23756100
C	-4.50289000	2.09667000	0.66856300
C	-3.47681300	2.75076400	1.30586900
H	-1.32367600	2.86974700	1.54101800
C	-2.46287400	-0.34136600	-1.33475000
C	-5.21736800	0.33882500	-0.93569900
H	-5.54931000	2.36897700	0.84479800
H	-3.66303400	3.56405500	2.01179000
C	-4.84829000	-0.66173000	-1.80338700
C	-3.49334600	-1.00809600	-2.00356800
H	-6.26695100	0.60289900	-0.77047800
H	-5.61386700	-1.21527100	-2.35760000
H	-3.24663600	-1.80555900	-2.70659100
N	-1.84208000	1.38432700	0.20146200
N	-1.09565900	-0.54042800	-1.47006700
C	-0.58936000	-1.56845200	-2.19414100
O	-1.20366600	-2.60609500	-2.49422900
K	-2.04027600	-3.23259000	-0.07212900
Ni	0.02255300	0.53394200	-0.12854900

C	4.21543800	-0.48923100	0.28918600
C	4.91557300	-1.69835300	0.19256900
C	6.25393700	-1.72558300	-0.20471400
C	6.91780600	-0.53824200	-0.51180100
C	6.23313500	0.67575200	-0.41875800
C	4.89660900	0.69637300	-0.02442900
H	4.39887100	-2.63488800	0.43840500
H	6.78218500	-2.68300600	-0.27246100
H	7.96812000	-0.55695900	-0.82157600
H	6.74722100	1.61445000	-0.65289700
H	4.36265700	1.65355500	0.04846800
C	1.82439300	-0.20228300	-0.49406900
H	2.26168600	0.57615100	-1.15397700
C	2.76414800	-0.44281200	0.69503700
H	2.49523700	-1.40103800	1.17625400
H	2.64750000	0.32893300	1.47413500
C	0.96966800	2.10028900	0.52027400
C	0.81602800	3.15607700	-0.55483200
H	2.03693700	1.95000700	0.73960600
H	0.48151500	2.38612300	1.47204700
C	1.49565400	4.47735400	-0.20182500
H	1.24717500	2.78240200	-1.50842300
H	-0.25129700	3.35719500	-0.77541800
C	1.34351800	5.52794700	-1.28468000
H	1.07676500	4.85094300	0.75319500
H	2.56854200	4.28859900	-0.00194900
H	1.84081900	6.47542800	-1.01758700
H	1.77869700	5.18397900	-2.23981900
H	0.27975800	5.75545300	-1.47593300
I	-0.55926900	-1.09679600	2.23094300

VIIa

Gibbs free energy before correction = -3519.48210500

Gibbs free energy after correction = -3519.46763895

C	-2.11375300	-0.22911700	2.49408800
C	-3.06216500	-0.70846900	1.41562500
H	-2.20003300	0.86679100	2.62724400
H	-2.37459400	-0.65607300	3.47923300
H	-2.96653200	-1.80366900	1.27564200
H	-4.10193600	-0.54747600	1.76979900
C	0.87536900	-1.35860900	-2.64047200
C	1.36346800	-1.83094800	-0.42202700

C	2.58161800	-2.46956200	-0.77125100
C	2.91123500	-2.52667100	-2.14715300
C	2.06543200	-1.97202000	-3.07992700
H	0.18126800	-0.90718400	-3.36034200
C	0.94626800	-1.71130200	0.94232800
C	3.40556600	-2.99380000	0.25504300
H	3.84634100	-3.01126300	-2.44894600
H	2.29573300	-1.99770600	-4.14790100
C	3.00155100	-2.87588900	1.56610800
C	1.78707500	-2.24234300	1.91745300
H	4.34866600	-3.48036600	-0.01393900
H	3.62771100	-3.28219300	2.36747200
H	1.49769100	-2.18600000	2.96963400
N	0.53863900	-1.29718700	-1.36592200
N	-0.30198200	-1.12717400	1.13313000
C	-0.64688800	-0.53282500	2.30152300
O	0.15093700	-0.21081200	3.19638300
K	2.25830300	1.05925300	2.37336300
Ni	-1.12911400	-0.50972900	-0.55223200
C	-5.26159600	-0.11381400	-0.71058400
C	-6.14558800	-1.08921900	-0.23431800
C	-7.46725400	-0.76633700	0.07728800
C	-7.92537600	0.54162800	-0.08227100
C	-7.05295100	1.52403800	-0.55529600
C	-5.73358900	1.19697000	-0.86418100
H	-5.78824000	-2.11926800	-0.10923100
H	-8.14512700	-1.54369300	0.44643200
H	-8.96271500	0.79602100	0.15975600
H	-7.40535200	2.55284900	-0.68758400
H	-5.04899800	1.96940500	-1.23896800
C	-2.86930500	0.01431100	0.09919200
H	-2.95854000	1.10436700	0.26439900
C	-3.81917300	-0.43445100	-1.00883400
H	-3.71428600	-1.52528700	-1.16710300
H	-3.53568300	0.05511300	-1.95941300
C	-0.97290300	1.26460200	-1.30805600
C	-0.05270000	2.02456300	-0.38152400
H	-1.93070700	1.79059300	-1.46271000
H	-0.50525100	1.08233900	-2.29582500
C	0.29775700	3.42971900	-0.86371000
H	-0.51491800	2.10183400	0.62617400
H	0.89193200	1.45168900	-0.25629500

C	1.17022200	4.18443100	0.12181700
H	0.80638400	3.35819700	-1.84467800
H	-0.63928500	3.98902600	-1.04837000
H	1.37333400	5.21646500	-0.20916200
H	0.69041900	4.24851900	1.11583300
H	2.15215700	3.69101300	0.24828000
I	4.17415100	1.12528800	-0.47919900

TS9

Gibbs free energy before correction = -3519.46142400

Gibbs free energy after correction = -3519.44695795

C	1.68997400	0.25885700	-2.47717300
C	2.62536900	-0.35475500	-1.45127600
H	1.73689800	1.36450000	-2.44769700
H	2.01156600	-0.01018000	-3.49944600
H	2.45689500	-1.44619100	-1.39526300
H	3.66428900	-0.23428400	-1.82139400
C	-0.84560700	-2.07330600	2.35854500
C	-1.55034900	-2.03380900	0.14883400
C	-2.71797900	-2.78033100	0.45313300
C	-2.90601100	-3.16718400	1.80261800
C	-1.97635800	-2.81482200	2.75401500
H	-0.08857200	-1.77204800	3.09319200
C	-1.27856500	-1.57898400	-1.18874900
C	-3.63658900	-3.08355600	-0.58366100
H	-3.79998500	-3.74105100	2.07089500
H	-2.09802500	-3.09571100	3.80332900
C	-3.36530900	-2.66082400	-1.86619900
C	-2.20267600	-1.91845500	-2.17793300
H	-4.54270100	-3.65000500	-0.34516900
H	-4.06226200	-2.90158100	-2.67639700
H	-2.01366100	-1.62427100	-3.21407500
N	-0.64008400	-1.70461500	1.10722400
N	-0.08720800	-0.90094600	-1.33119200
C	0.23185600	-0.14189300	-2.39452500
O	-0.55377700	0.26100200	-3.27259200
K	-2.75252000	1.23575900	-2.33314800
Ni	0.75882100	-0.44628500	0.42933100
C	4.93276400	-0.41186200	0.63751700
C	5.61013800	-1.49638700	0.06857100
C	6.96593100	-1.40538900	-0.25081900
C	7.66518000	-0.22355300	-0.00608500

C	7.00044300	0.86585200	0.56087100
C	5.64651700	0.77016700	0.87815000
H	5.06217300	-2.42719800	-0.12460200
H	7.47978300	-2.26549100	-0.69367500
H	8.72940600	-0.15111500	-0.25419500
H	7.54343800	1.79583000	0.76155800
H	5.12641400	1.62531400	1.32987800
C	2.60101200	0.28109500	-0.05470300
H	3.02658300	1.28834600	-0.19698700
C	3.46219800	-0.47972100	0.95556000
H	3.14399500	-1.53884300	0.99217900
H	3.29627600	-0.06234700	1.96575300
C	1.23199500	1.35927600	0.97459400
C	0.58115300	2.43030400	0.13306800
H	2.08728000	1.75490600	1.54457100
H	0.51234100	0.98619400	1.76151900
C	0.17624700	3.65598700	0.94177600
H	1.26537700	2.73986000	-0.68130200
H	-0.32383500	2.01912900	-0.35856300
C	-0.54184600	4.68940100	0.09609400
H	-0.47355400	3.33837500	1.78077000
H	1.07753700	4.09763800	1.40868900
H	-0.81573600	5.58505300	0.67780200
H	0.08417700	5.02181400	-0.75100300
H	-1.47533400	4.27457900	-0.32767100
I	-3.29123700	1.28452100	1.05247200

VIIb

Gibbs free energy before correction = -3519.49845200

Gibbs free energy after correction = -3519.48398595

C	-1.84113300	0.59549800	2.06617100
C	-2.72719300	0.13365400	0.91335200
H	-1.89043000	1.69122600	2.19254800
H	-2.24432200	0.19543500	3.01599500
H	-2.38622100	-0.86400500	0.51936900
H	-3.71028500	-0.13821900	1.33739300
C	1.17339800	-2.45220400	-2.15772100
C	1.64816900	-2.03126400	0.07867700
C	2.88590200	-2.72120800	-0.00808000
C	3.23785600	-3.28049700	-1.26196300
C	2.38969200	-3.14102400	-2.33499200
H	0.47368100	-2.33627200	-2.99333900
C	1.23466200	-1.40112700	1.30681400

C	3.71735800	-2.80936900	1.13640000
H	4.19014200	-3.81381700	-1.35676600
H	2.63566100	-3.55569500	-3.31612000
C	3.30240300	-2.23434900	2.31715200
C	2.07718000	-1.53717500	2.41042200
H	4.67233300	-3.33966000	1.06046400
H	3.92924800	-2.31355200	3.21213300
H	1.77209500	-1.11117600	3.37038100
N	0.81208100	-1.92545300	-1.00042500
N	0.00473000	-0.77166300	1.26387600
C	-0.37500500	0.19865700	2.11208400
O	0.35619500	0.77421100	2.94040100
K	2.69060200	1.57806700	2.23337500
Ni	-0.79645300	-0.97290000	-0.50454000
C	-5.25603500	-0.06456300	-0.70135200
C	-5.51214900	-1.42120700	-0.46706600
C	-6.73175600	-1.83953300	0.06736900
C	-7.71822700	-0.90350800	0.37768800
C	-7.47685000	0.45243300	0.14778500
C	-6.25743500	0.86503000	-0.38711700
H	-4.73801500	-2.16041500	-0.70900600
H	-6.91267400	-2.90574900	0.24182800
H	-8.67654600	-1.22979300	0.79546600
H	-8.24801500	1.19415500	0.38269300
H	-6.07485700	1.93097600	-0.57424500
C	-3.00740200	1.09369600	-0.24485900
H	-3.54040500	1.97341300	0.17605200
C	-3.94082900	0.40374900	-1.25371000
H	-3.38372100	-0.45415100	-1.68118700
H	-4.12945300	1.10554800	-2.08679300
C	-1.79490800	1.62066000	-1.01126200
C	-0.86789900	2.59523500	-0.30309300
H	-2.18031400	2.12688000	-1.91807200
H	-1.19893500	0.76433300	-1.42746400
C	0.04110500	3.33424700	-1.27219600
H	-1.47238500	3.32978300	0.26638900
H	-0.24463400	2.07188700	0.44907300
C	0.95520900	4.33416800	-0.59386900
H	0.64239700	2.59448200	-1.83753100
H	-0.58219600	3.85087400	-2.02765600
H	1.61478400	4.84835000	-1.31281300
H	0.37884800	5.10811900	-0.05638600

H	1.61208300	3.84491800	0.14854200
I	3.53523500	1.10936200	-1.04085100

IVd

Gibbs free energy before correction = -3130.75812700

Gibbs free energy after correction = -3130.74366081

C	-1.65778700	3.00089400	-0.96889300
C	-2.69113500	1.94462600	-1.34117600
H	-1.23787800	3.43340000	-1.89855400
H	-2.13907400	3.82703900	-0.42240800
H	-3.12525900	1.49743200	-0.42606100
H	-3.52958000	2.45753500	-1.85312700
C	-2.17188100	0.85293600	-2.23142800
H	-1.63565300	1.18188600	-3.13595300
C	-2.57729200	-0.46859300	-2.12992200
H	-3.35878600	-0.75972600	-1.41419300
H	-2.39507800	-1.16800500	-2.95761600
C	1.38064100	-2.22204600	-1.42381300
C	1.95537300	-0.13934200	-0.57773300
C	3.29844200	-0.54437300	-0.35293800
C	3.64411700	-1.87094100	-0.71339600
C	2.69243600	-2.70703600	-1.24952900
H	0.59080200	-2.86888400	-1.82653100
C	1.50596400	1.19055900	-0.25866800
C	4.21427400	0.37692900	0.21285500
H	4.67344500	-2.21206400	-0.55632500
H	2.93088400	-3.73494400	-1.53510800
C	3.77881400	1.64534800	0.52948200
C	2.44578100	2.05646600	0.30807300
H	5.24840600	0.06327300	0.38918300
H	4.47880200	2.36592300	0.96650900
H	2.14841000	3.07458400	0.56996300
N	1.03254400	-0.98942900	-1.10620900
N	0.19856000	1.46894300	-0.61162000
C	-0.47419700	2.54460100	-0.13759600
O	-0.18419300	3.16452100	0.90100300
K	0.09109900	1.14204900	2.54275300
Ni	-0.80572900	-0.20801600	-1.17584500
I	-1.52878100	-1.61631800	1.23653700

P^{pre}

Gibbs free energy before correction = -1713.54322000

Gibbs free energy after correction = -1713.52875413

C	0.94414600	1.49679400	1.19550900
C	2.03948900	1.06295500	0.23055900
H	1.02520500	0.96636800	2.16176800
H	1.08213300	2.57101500	1.42584600
H	1.72941200	1.33615100	-0.79799500
H	2.95290100	1.64941400	0.43706400
C	-3.15082300	-2.16287900	-0.54056100
C	-3.33571600	-0.09908400	0.46711900
C	-4.72510800	-0.01407400	0.12614800
C	-5.29644500	-1.10383500	-0.58265900
C	-4.51618300	-2.18053100	-0.91771500
H	-2.51389400	-3.02036400	-0.80382300
C	-2.70400500	0.99428500	1.17280100
C	-5.48159800	1.13617000	0.46563800
H	-6.35843400	-1.06118900	-0.85099300
H	-4.92262700	-3.03734500	-1.46282400
C	-4.86753800	2.17187700	1.13837100
C	-3.50283800	2.09779900	1.48373000
H	-6.54026400	1.17819400	0.18720600
H	-5.43846600	3.06798500	1.40582500
H	-3.02831400	2.93074700	2.01564200
N	-2.58323600	-1.17699800	0.11319800
N	-1.37951300	0.96287200	1.54119900
C	-0.47985000	1.38825500	0.67429900
O	-0.70766000	1.77516300	-0.50777500
K	-2.79998900	2.04625200	-1.82861800
C	4.81246200	0.03071000	-0.44464600
C	5.20413000	1.10496800	-1.25331700
C	6.37215800	1.81974400	-0.98338500
C	7.17116100	1.47119000	0.10572300
C	6.79432300	0.40104200	0.91959100
C	5.62741900	-0.31041200	0.64425300
H	4.57723100	1.38440900	-2.10959100
H	6.66010900	2.65621900	-1.62960900
H	8.08848100	2.03022900	0.31905100
H	7.41800100	0.11583100	1.77394900
H	5.33932500	-1.15605500	1.28208000
C	2.40157500	-0.41988800	0.27533300
H	2.76976700	-0.64419100	1.30168400
C	3.54349900	-0.73034100	-0.70399700
H	3.18636200	-0.52366000	-1.73202000

H	3.77135700	-1.81052600	-0.66005900
C	1.19399200	-1.31853400	0.02029300
C	1.45102000	-2.80988200	0.17083700
H	0.79243600	-1.10716500	-0.99429500
H	0.38239200	-1.03540500	0.71768000
C	0.18688000	-3.64923500	0.08626400
H	2.16053800	-3.16586200	-0.60152200
H	1.95280000	-2.99771200	1.14289600
C	0.44814500	-5.13567100	0.23301500
H	-0.52929800	-3.31095500	0.86090900
H	-0.31111800	-3.44772100	-0.88324900
H	-0.47856100	-5.72995500	0.16709700
H	1.13255800	-5.50281100	-0.55250600
H	0.91849500	-5.36539000	1.20575800

P

Gibbs free energy before correction = -1114.23927400

Gibbs free energy after correction = -1114.22480776

C	0.70250900	-1.82580600	-0.64059400
C	1.82892900	-1.19106300	0.16036000
H	0.73863400	-1.51019600	-1.69951600
H	0.82869100	-2.92508200	-0.64839200
H	1.58391100	-1.26930100	1.23793700
H	2.74722400	-1.78554800	0.01169000
C	-3.33322900	1.73936100	0.94656400
C	-3.59881600	-0.33599800	0.00463600
C	-4.99008100	-0.35542200	0.32973000
C	-5.51420500	0.75699600	1.03514400
C	-4.68738200	1.80391500	1.35617200
H	-2.66912800	2.58868400	1.16601800
C	-3.04827100	-1.46386900	-0.68226600
C	-5.80315100	-1.44536600	-0.07029900
H	-6.57610600	0.76094400	1.30621500
H	-5.05318300	2.67997800	1.89925300
C	-5.25433900	-2.49181200	-0.77308300
C	-3.87337900	-2.50182700	-1.06728100
H	-6.86854200	-1.42809600	0.18479300
H	-5.87772500	-3.33214100	-1.09439200
H	-3.43257300	-3.34952700	-1.60309500
N	-2.80626100	0.72494500	0.30284200
N	-1.67455600	-1.50414400	-1.00088300
C	-0.67714800	-1.59489100	-0.05917400

O	-0.89145600	-1.55113300	1.13702900
C	4.59306900	0.05408900	0.44377600
C	5.08582400	-0.85994900	1.38348400
C	6.27798000	-1.55015000	1.15767500
C	6.99925600	-1.33772100	-0.01723600
C	6.52026400	-0.42880900	-0.96279800
C	5.32993500	0.25888700	-0.73140600
H	4.52085200	-1.03138600	2.30851200
H	6.64645800	-2.25935900	1.90695100
H	7.93552300	-1.87729500	-0.19538900
H	7.08220900	-0.25078100	-1.88622200
H	4.96121400	0.97893600	-1.47339700
C	2.12773700	0.26632700	-0.18766000
H	2.44072600	0.29850700	-1.25518900
C	3.29950800	0.78802000	0.65646800
H	3.00913300	0.73766600	1.72394900
H	3.46333200	1.85539600	0.42364900
C	0.89940000	1.16227500	-0.04714700
C	1.07374200	2.59043500	-0.53877200
H	0.56629600	1.16263500	1.01216300
H	0.05918200	0.71702400	-0.61375800
C	-0.21998500	3.38895700	-0.52374400
H	1.82660800	3.12862100	0.06935500
H	1.48305600	2.57281200	-1.57020600
C	-0.05183200	4.80028900	-1.05231100
H	-0.98937200	2.85092500	-1.11260700
H	-0.61071200	3.41866600	0.51282200
H	-0.99617100	5.36932300	-1.03038000
H	0.68818200	5.36560500	-0.45821100
H	0.30668000	4.79636300	-2.09716100
H	-1.43503000	-1.76112300	-1.95676800

TS8m

Gibbs free energy before correction = -3064.11963200

Gibbs free energy after correction = -3064.10516582

C	-0.61283300	-3.42429100	-0.72574900
C	0.73865400	-3.33788300	-0.03284400
H	-0.45029600	-3.44655600	-1.82113200
H	-1.13058800	-4.35835000	-0.45783900
H	0.60829000	-3.37533400	1.06548300
H	1.32814400	-4.23704200	-0.30174600
C	0.26235100	2.41458100	0.78372600

C	-1.49550800	1.27971300	-0.28178800
C	-2.30071700	2.45852100	-0.31127100
C	-1.74905000	3.64374700	0.24844700
C	-0.45807200	3.59990600	0.78449800
H	1.27820400	2.36324700	1.19318100
C	-1.96919500	0.04906100	-0.80749500
C	-3.58671800	2.37273800	-0.89426500
H	-2.33588800	4.56870300	0.24304500
H	0.00721500	4.50055000	1.19826900
C	-4.03135000	1.17094100	-1.44059400
C	-3.24282000	0.01555600	-1.40994100
H	-4.22010700	3.26706700	-0.91235400
H	-5.02568900	1.12219500	-1.89906100
H	-3.62171400	-0.92142900	-1.82637200
N	-0.23137800	1.25935800	0.26287300
N	-1.09843200	-1.02787300	-0.65267200
C	-1.57150600	-2.28411900	-0.45041200
O	-2.72849400	-2.54172800	-0.06782900
K	-3.02685700	-0.72889000	1.78713400
Ni	0.53301200	-0.48734600	0.33526200
C	3.35756000	-0.43351700	0.06397400
C	4.30738100	-0.01650400	1.00922600
C	5.26587700	0.94399700	0.69203600
C	5.29260100	1.51293300	-0.58163200
C	4.35202200	1.10890300	-1.53183600
C	3.39495500	0.14790500	-1.21451000
H	4.28284800	-0.45543400	2.01423100
H	5.99707200	1.25238100	1.44704300
H	6.04228900	2.27011400	-0.83384300
H	4.36244000	1.54964500	-2.53454600
H	2.66047900	-0.14770600	-1.97230300
C	1.49173600	-2.10030500	-0.40968800
H	1.56456800	-1.90083700	-1.48990400
C	2.34413800	-1.43339500	0.46183100
H	2.49925400	-1.86403400	1.46075500
H	1.13901500	-0.11008200	1.64516400

VIm

Gibbs free energy before correction = -3064.13964300

Gibbs free energy after correction = -3064.12517682

C	0.95021700	-3.22451700	1.23106300
C	-0.44910900	-3.37306900	0.63383100

H	0.85279800	-2.98978600	2.30860800
H	1.49891700	-4.17633600	1.15145700
H	-0.37207100	-3.62490000	-0.44221200
H	-0.93143500	-4.24878000	1.11337900
C	-0.57269300	2.38501200	-0.50575600
C	1.41627000	1.45004700	0.23007600
C	2.06805800	2.71310600	0.24593800
C	1.29404800	3.84347300	-0.12028400
C	-0.02253400	3.68376400	-0.48584300
H	-1.60939100	2.21975200	-0.83052700
C	2.10708000	0.24697200	0.61678400
C	3.43516200	2.78208900	0.61169800
H	1.76211100	4.83419300	-0.10871500
H	-0.64241900	4.53771800	-0.77228600
C	4.10359700	1.62023900	0.93807900
C	3.46209400	0.36382800	0.93692800
H	3.93838200	3.75466700	0.61875300
H	5.16368300	1.66446200	1.21156800
H	4.02628800	-0.53159700	1.21066600
N	0.11758300	1.31586800	-0.15949800
N	1.32665300	-0.88595900	0.68782800
C	1.82599800	-2.14492200	0.61783200
O	2.89814800	-2.45042500	0.06938000
K	2.25686000	-1.13672900	-2.17005700
Ni	-0.46164800	-0.65469800	-0.28568400
C	-3.17680000	-0.61608300	0.03934000
C	-4.10432700	-0.32248400	-0.97717700
C	-5.00366400	0.73401700	-0.85259900
C	-5.00207800	1.52897300	0.29506700
C	-4.08993500	1.24865100	1.31571800
C	-3.19032100	0.19338600	1.19222200
H	-4.10617500	-0.93891500	-1.88470200
H	-5.71389500	0.93888800	-1.66126000
H	-5.70717500	2.36077400	0.39474700
H	-4.07805100	1.86332500	2.22259100
H	-2.47676300	0.00433100	2.00220300
C	-1.30183600	-2.14808600	0.80315200
H	-1.35997000	-1.74845000	1.82741900
C	-2.20592200	-1.70335000	-0.15901900
H	-2.35430400	-2.30462300	-1.06723200
H	-0.39939900	-0.65756300	-1.95986300

VIIc

Gibbs free energy before correction = -3558.70766000

Gibbs free energy after correction = -3558.69319384

C	1.22673900	-2.14431600	-1.51919800
C	2.39496700	-1.73150100	-0.62968100
H	1.10866000	-1.37412600	-2.31196800
H	2.35821800	-2.32176800	0.30854400
H	3.33614100	-2.03316700	-1.13494500
C	-1.05270500	2.08978400	2.04314100
C	-1.62978600	-0.14087900	1.77424900
C	-2.76189000	-0.00468900	2.61896900
C	-3.00615500	1.27590100	3.17218300
C	-2.16124300	2.32248800	2.88198600
H	-0.35861200	2.90278000	1.79458400
C	-1.32000700	-1.38336900	1.13410300
C	-3.58827200	-1.13179500	2.85318800
H	-3.87511900	1.41515200	3.82462500
H	-2.32860100	3.32279300	3.28907700
C	-3.26287300	-2.33671900	2.26954900
C	-2.14194000	-2.47007000	1.41658200
H	-4.46251400	-1.02701600	3.50374000
H	-3.88018400	-3.22047400	2.46427400
H	-1.91078100	-3.44825100	0.98525000
N	-0.79651900	0.90588500	1.52099400
N	-0.18984100	-1.37546600	0.32388300
C	-0.10681400	-2.15966700	-0.77874700
O	-1.04246400	-2.84023900	-1.22608200
K	-3.54686300	-2.37178700	-1.45338300
Ni	0.76520600	0.34108900	0.37774800
I	-3.58343900	1.02458000	-1.30556500
C	1.47739300	-3.48550100	-2.19088300
H	2.39070100	-3.44685500	-2.80675900
H	1.61628400	-4.28091400	-1.43633300
H	0.63850500	-3.78124300	-2.83770200
C	4.79233500	-0.27594800	0.65628100
C	5.35633200	-1.41495200	1.24286300
C	6.68500500	-1.76405500	0.99520600
C	7.47101400	-0.97760300	0.15320600
C	6.91939500	0.16092300	-0.43829200
C	5.59202500	0.50560800	-0.18888800
H	4.74258700	-2.03409500	1.90898700
H	7.10964000	-2.65726100	1.46632400

H	8.51411500	-1.24910300	-0.04065900
H	7.53052400	0.78752800	-1.09704200
H	5.16188800	1.40329200	-0.65170800
C	2.46026300	-0.25200000	-0.31695600
H	2.79192400	0.30795200	-1.20987100
C	3.34581800	0.08864200	0.87944100
H	2.97541800	-0.44382500	1.77778300
H	3.28067400	1.17287300	1.09578500
C	0.77546400	1.77061700	-0.92869100
C	1.70833500	2.90060800	-0.55991100
H	-0.28634500	2.08577300	-0.88115900
H	0.97832500	1.38732000	-1.94441100
C	1.52210600	4.13335900	-1.44184100
H	1.56378400	3.19898900	0.50032800
H	2.76404900	2.57033600	-0.63387700
C	2.47754700	5.25778900	-1.09185900
H	1.65270500	3.83758000	-2.50083000
H	0.47509700	4.48310000	-1.35836700
H	2.33226600	6.14092700	-1.73619900
H	2.34410100	5.58660500	-0.04590300
H	3.52939100	4.93884800	-1.20078000

VIId

Gibbs free energy before correction = -3558.70559300

Gibbs free energy after correction = -3558.69112684

C	1.75875200	-2.41546000	-1.44255400
C	2.70599400	-1.82063300	-0.40998400
H	2.59724400	-2.36717500	0.54736300
H	3.74372300	-2.02790300	-0.75059500
C	-1.16171700	1.13899800	2.49444900
C	-1.70411800	-0.92421200	1.57843600
C	-2.93801600	-0.96535600	2.27911800
C	-3.24302900	0.12952800	3.12323600
C	-2.36176300	1.18042200	3.23144300
H	-0.44076100	1.96404700	2.55478400
C	-1.31181000	-1.98293000	0.69318500
C	-3.80314900	-2.07160800	2.09287400
H	-4.18839400	0.12503300	3.67672000
H	-2.57268200	2.04098300	3.87114600
C	-3.42267600	-3.08591400	1.24347600
C	-2.19226500	-3.05276000	0.54699200
H	-4.75809900	-2.09777000	2.62755100

H	-4.08081200	-3.94869800	1.09635700
H	-1.92570200	-3.88341100	-0.10981000
N	-0.84735400	0.12640800	1.70803500
N	-0.05581700	-1.83304800	0.10783900
C	0.29636100	-2.48146700	-1.02815800
O	-0.49630900	-3.08080400	-1.77401400
K	-2.28277200	-1.25060200	-2.29847400
Ni	0.78884300	-0.09279300	0.55077000
I	-3.85857200	1.39182000	-0.86920500
C	4.87303600	0.14979200	0.71613100
C	5.68948000	-0.89441700	1.16649800
C	7.04800400	-0.92807800	0.84738800
C	7.61089400	0.08419800	0.06979200
C	6.80652400	1.13075500	-0.38547600
C	5.45020500	1.16005700	-0.06515000
H	5.25001700	-1.69032900	1.78078200
H	7.67220300	-1.75143500	1.21144500
H	8.67705200	0.05977700	-0.17933500
H	7.24092300	1.93263600	-0.99233800
H	4.81950100	1.98522900	-0.42063600
C	2.55637000	-0.33405900	-0.16353000
H	2.78773800	0.25004300	-1.07158000
C	3.39407800	0.17602500	1.00937700
H	3.19027000	-0.43687000	1.90878600
H	3.10213700	1.21617400	1.25276000
C	0.54071000	1.38973000	-0.66515300
C	1.15126400	2.67873000	-0.16899600
H	-0.56790600	1.43705500	-0.63888600
H	0.86106500	1.15546500	-1.69562200
C	0.63698000	3.89863200	-0.93041300
H	0.94093100	2.82228200	0.91177300
H	2.25569400	2.64131200	-0.25674500
C	1.26416600	5.19599000	-0.45855900
H	0.82848800	3.75264600	-2.01118900
H	-0.46469400	3.94697000	-0.82802900
H	0.88060500	6.06755500	-1.01473900
H	1.06177200	5.37259100	0.61271100
H	2.36132800	5.18034800	-0.58433800
H	2.03588700	-3.48003200	-1.57492200
C	1.86817000	-1.74866400	-2.81118400
H	2.92193700	-1.68452800	-3.13172800
H	1.31610100	-2.31859000	-3.57472900

H	1.46178800	-0.72110400	-2.79810400

TS9b

Gibbs free energy before correction = -3558.69130600

Gibbs free energy after correction = -3558.67683984

C	1.41087100	-1.62482900	-2.18575300
C	2.47772800	-1.26369400	-1.15216000
H	1.30593800	-0.79966900	-2.91877200
H	2.44152600	-2.02842800	-0.35200500
H	3.46637100	-1.38888100	-1.63710500
C	-0.78315000	0.61465600	2.91183000
C	-1.50545000	-1.15662500	1.59294500
C	-2.61093200	-1.40738900	2.44745800
C	-2.75798400	-0.56945600	3.58086300
C	-1.84946100	0.43689400	3.81536000
H	-0.04332400	1.41032600	3.06617200
C	-1.28119300	-1.94061100	0.40665000
C	-3.51476700	-2.45030300	2.12331600
H	-3.60358800	-0.73642800	4.25723100
H	-1.93971500	1.09799700	4.68103200
C	-3.29016700	-3.20805700	0.99455900
C	-2.18887600	-2.96637100	0.14168700
H	-4.37247000	-2.63603700	2.77796400
H	-3.97563400	-4.02495200	0.74345300
H	-2.03471600	-3.60671800	-0.73190200
N	-0.62037800	-0.15045400	1.84769700
N	-0.14472000	-1.61630500	-0.30482000
C	0.00643100	-1.85180400	-1.62120500
O	-0.89517900	-2.20917900	-2.40204500
K	-3.26351800	-1.20090200	-2.27465600
Ni	0.62970800	0.11660900	0.34447800
I	-3.30031100	1.65638400	-0.39613700
C	1.82844800	-2.87505400	-2.95396800
H	2.78525000	-2.71605300	-3.47794000
H	1.96326000	-3.72826200	-2.26416200
H	1.06986300	-3.15841000	-3.69888300
C	4.57836600	-0.01937900	0.79074900
C	5.14807000	-1.25672700	1.11339000
C	6.52257100	-1.46512300	0.99131700
C	7.35015400	-0.43550700	0.54333700
C	6.79404700	0.80376500	0.21999600
C	5.42029300	1.00721700	0.34179600

H	4.50020800	-2.06693800	1.47020700
H	6.95029100	-2.43965600	1.25070400
H	8.42925600	-0.59676600	0.44911100
H	7.43715600	1.62022200	-0.12605900
H	4.98704200	1.98427400	0.09151800
C	2.43508500	0.13003200	-0.52159200
H	3.02923600	0.81685300	-1.14289200
C	3.08908600	0.19616800	0.87542500
H	2.66128200	-0.56347400	1.55636000
H	2.89092600	1.18817100	1.32586500
C	0.97139700	1.38712700	-1.10776100
C	1.23617000	2.73369800	-0.47226200
H	-0.13491400	1.21730100	-1.19041700
H	1.34805200	1.32983300	-2.13873000
C	0.63927100	3.88402000	-1.27350000
H	0.81039600	2.75382200	0.55552400
H	2.32523600	2.89856900	-0.34926700
C	0.88198800	5.23466300	-0.62919200
H	1.06413100	3.86516100	-2.29569300
H	-0.44735500	3.71004300	-1.39855000
H	0.44919100	6.05889900	-1.21990000
H	0.43592000	5.28169800	0.37997200
H	1.96181600	5.43811500	-0.51796400

TS9c

Gibbs free energy before correction = -3558.68832000

Gibbs free energy after correction = -3558.67385384

C	1.64277100	-1.47740800	-2.32721500
C	2.50330000	-1.27313000	-1.08071000
H	2.30712800	-2.10028900	-0.37421000
H	3.56073700	-1.40139100	-1.39342900
C	-0.95989400	-0.60780300	2.98480100
C	-1.72254300	-1.66266400	1.06070600
C	-2.91785200	-2.07757600	1.70385800
C	-3.08732000	-1.71014600	3.06149200
C	-2.11391700	-0.97919100	3.70219200
H	-0.16746200	-0.02181600	3.46607600
C	-1.46684000	-1.98853800	-0.32056400
C	-3.88345600	-2.81318200	0.97083000
H	-4.00150800	-2.01449500	3.58311800
H	-2.21835000	-0.68130600	4.74864600
C	-3.63410800	-3.12393100	-0.34720400

C	-2.44307000	-2.72366100	-0.99505400
H	-4.80930900	-3.11987500	1.46839600
H	-4.37083200	-3.69856900	-0.91906300
H	-2.27327300	-3.00999900	-2.03660600
N	-0.77177900	-0.93773700	1.71950800
N	-0.23898400	-1.57236100	-0.78976400
C	0.13766400	-1.56777600	-2.08319800
O	-0.62776600	-1.64410400	-3.06186000
K	-2.54999400	0.05428100	-2.60509600
Ni	0.61192800	-0.26157500	0.46653700
I	-3.39645800	1.77677100	0.21522900
C	4.58834100	-0.16655200	0.91387500
C	5.17051600	-1.40941300	1.18770600
C	6.54379500	-1.60492000	1.03428200
C	7.35651800	-0.55693700	0.60185000
C	6.78707300	0.68767400	0.32564500
C	5.41477100	0.87866000	0.47998900
H	4.53306600	-2.23511400	1.52769300
H	6.98220800	-2.58415900	1.25520100
H	8.43448700	-0.70841100	0.48197100
H	7.41852500	1.51788400	-0.00892600
H	4.96971300	1.85934700	0.26711900
C	2.41241300	0.06538000	-0.34285900
H	2.92855400	0.82595500	-0.94915900
C	3.10110900	0.04383200	1.03128600
H	2.67842600	-0.75543300	1.67150900
H	2.91367700	1.00377700	1.54599600
C	0.89303000	1.38959700	-0.57153200
C	1.38911700	2.65173700	0.09546900
H	-0.21583600	1.32233800	-0.39954800
H	1.02444400	1.42026100	-1.66441600
C	0.70081200	3.89849700	-0.44824400
H	1.21084500	2.59068000	1.18850700
H	2.48447000	2.76543800	-0.02852200
C	1.18493700	5.17050400	0.22019100
H	0.86924700	3.95435100	-1.54119600
H	-0.39429200	3.79461700	-0.32056000
H	0.68156800	6.06600500	-0.18025100
H	0.99914100	5.14603800	1.30852600
H	2.27130400	5.31024800	0.07848700
H	1.87808000	-2.50364800	-2.68041200
C	1.98534200	-0.54203700	-3.47906100

H	3.06748100	-0.56926800	-3.69114900
H	1.45297300	-0.83848700	-4.39564300
H	1.71541500	0.50669400	-3.26603500

VIIe

Gibbs free energy before correction = -3558.73348000

Gibbs free energy after correction = -3558.71901384

C	-1.52477900	0.10993400	2.83495200
C	-2.40570600	0.12910400	1.58533900
H	-1.58908200	1.09617200	3.32938900
H	-2.41775400	-0.90421000	1.10872800
H	-3.45538300	0.09999700	1.93542600
C	0.52453900	-2.60284600	-1.98870600
C	1.57750300	-2.14221200	0.03304800
C	2.80546900	-2.67954400	-0.43284100
C	2.83614400	-3.19481100	-1.75260100
C	1.70262200	-3.15496400	-2.52988600
H	-0.39294200	-2.55627300	-2.58753000
C	1.47103300	-1.57306600	1.35376200
C	3.94102900	-2.65958100	0.41598200
H	3.77252100	-3.61388000	-2.13697900
H	1.69634000	-3.53898100	-3.55323000
C	3.83043500	-2.12703700	1.68116400
C	2.61222000	-1.58734300	2.15430200
H	4.88665600	-3.07056300	0.04757800
H	4.70084700	-2.11752000	2.34611100
H	2.55598800	-1.18705500	3.17053700
N	0.46112100	-2.12169800	-0.75935600
N	0.21804000	-1.09014400	1.67960500
C	-0.03439800	-0.14700900	2.60259500
O	0.81064800	0.48325200	3.26371500
K	2.54833100	1.57483200	1.67324500
Ni	-1.01007000	-1.29151600	0.18066500
I	2.48425100	1.17772500	-1.73930900
C	-2.02261200	-0.95103400	3.81329600
H	-3.05596600	-0.74092200	4.13619900
H	-2.00963500	-1.94870600	3.33989000
H	-1.38725300	-0.99463500	4.71361100
C	-3.92186300	0.11556300	-0.98462600
C	-3.91191300	-1.23535400	-1.35286200
C	-5.09960200	-1.95839100	-1.47356800
C	-6.32214500	-1.33497400	-1.22705000

C	-6.34761900	0.01320100	-0.86252600
C	-5.15837800	0.73054500	-0.74437800
H	-2.94619600	-1.72704200	-1.55015500
H	-5.06821800	-3.01401300	-1.76351200
H	-7.25679900	-1.89776800	-1.32134500
H	-7.30463800	0.51079300	-0.67169600
H	-5.18427900	1.79108700	-0.46378800
C	-2.29432100	1.31391700	0.60048300
H	-3.06393600	2.04931000	0.91470600
C	-2.64062600	0.88617800	-0.83492000
H	-1.79912500	0.27313400	-1.23637600
H	-2.68815300	1.78778400	-1.47202000
C	-0.96050900	2.06231000	0.63711900
C	-0.91897000	3.32502100	-0.21140100
H	-0.14824800	1.37994800	0.30609700
H	-0.74027200	2.34408200	1.68499800
C	0.27342200	4.21570800	0.09961700
H	-0.89234200	3.06399700	-1.28787500
H	-1.85432700	3.90293000	-0.06316200
C	0.33829100	5.44645500	-0.78326200
H	0.24686300	4.50835000	1.16807100
H	1.20459900	3.62960000	-0.04091400
H	1.19526500	6.09326900	-0.53284600
H	0.43644900	5.16398300	-1.84681200
H	-0.57753200	6.05662000	-0.68966300

VIIf

Gibbs free energy before correction = -3558.73077300

Gibbs free energy after correction = -3558.71630684

C	-1.65619900	0.33954000	2.75855900
C	-2.47074800	0.15124600	1.47069000
H	-2.43753100	-0.93465100	1.13287800
H	-3.53505900	0.12975600	1.77528800
C	0.67772800	-2.88491400	-1.58409500
C	1.64346200	-2.09214100	0.37792200
C	2.90629600	-2.63794000	0.03047400
C	3.00123100	-3.33672000	-1.19880700
C	1.89428500	-3.45756800	-2.00553100
H	-0.22122800	-2.96458500	-2.20718400
C	1.46817600	-1.34808700	1.60050500
C	4.01040200	-2.44841900	0.89945000
H	3.96536900	-3.76700000	-1.49135700

H	1.93797100	-3.98578000	-2.96150000
C	3.83553200	-1.74604500	2.07133000
C	2.58150600	-1.19866200	2.42708200
H	4.98315400	-2.86715500	0.62141600
H	4.68115400	-1.60470800	2.75313700
H	2.47354000	-0.66440400	3.37528700
N	0.55424500	-2.23480200	-0.44004100
N	0.18516600	-0.89150900	1.82486800
C	-0.14191800	0.15848000	2.60075800
O	0.65449900	0.93230200	3.15982900
K	2.41655400	1.84822700	1.47138900
Ni	-0.98451500	-1.35725700	0.33401500
I	2.69726700	0.90339400	-1.83157100
C	-4.05678800	-0.19563300	-1.00908600
C	-4.07263500	-1.59285500	-1.09938900
C	-5.27386500	-2.30243000	-1.07602400
C	-6.48419200	-1.61935500	-0.96044500
C	-6.48361200	-0.22549600	-0.87193900
C	-5.28066500	0.47850700	-0.89819100
H	-3.11449000	-2.12706800	-1.18699400
H	-5.26333100	-3.39517900	-1.14959800
H	-7.42932000	-2.17220900	-0.94230200
H	-7.43081300	0.31788800	-0.78568800
H	-5.28602200	1.57415300	-0.83607800
C	-2.36182100	1.18975300	0.33527900
H	-3.10490800	1.98192100	0.56697000
C	-2.76079700	0.56353900	-1.01090500
H	-1.94042700	-0.12115000	-1.33109100
H	-2.80948800	1.36087100	-1.77426100
C	-1.01241000	1.90017700	0.20448500
C	-1.01881600	3.07440600	-0.76557000
H	-0.23792700	1.16670500	-0.10602300
H	-0.71218300	2.27973900	1.19951000
C	0.16437000	4.01311400	-0.58619100
H	-1.02742700	2.71014700	-1.81178300
H	-1.95830000	3.65080300	-0.63969800
C	0.15822600	5.16459200	-1.57248800
H	0.16892400	4.40178100	0.45227100
H	1.10419000	3.43714000	-0.71273000
H	1.01120200	5.84644400	-1.42120900
H	0.20989400	4.79553900	-2.61218500
H	-0.76576700	5.76300000	-1.48351500

H	-1.94506100	-0.51803500	3.40076700
C	-2.03529600	1.60686500	3.50410200
H	-3.12392000	1.63574300	3.67965900
H	-1.53307400	1.65624400	4.48251400
H	-1.76294500	2.52309000	2.95367700

TS6b

Gibbs free energy before correction = -3103.33482600

Gibbs free energy after correction = -3103.32035976

C	1.21623500	3.23154800	0.38303300
C	-0.29968500	3.35365800	0.35178800
H	1.58645000	3.64930000	1.33624200
H	-0.72811900	3.01106100	1.31357600
H	-0.56026400	4.43028000	0.27609100
C	-1.21907600	-2.28833300	0.23510600
C	0.87151800	-1.46688100	-0.42389700
C	1.41680000	-2.78804300	-0.52727000
C	0.56009300	-3.87510200	-0.20434300
C	-0.75942200	-3.59019400	0.20300100
H	-2.24606000	-2.07058900	0.54213300
C	1.68862600	-0.34077600	-0.64579300
C	2.76440700	-2.92036900	-0.94453500
H	0.93748100	-4.90241000	-0.25734100
H	-1.44193700	-4.39745300	0.49005700
C	3.52559900	-1.79403900	-1.28249800
C	3.00090100	-0.50805500	-1.13671800
H	3.18646100	-3.92785800	-1.04300900
H	4.54671500	-1.92194000	-1.66111800
H	3.60351200	0.37295900	-1.38126900
N	-0.44327300	-1.21590400	-0.10559500
N	1.07138400	0.89637000	-0.38434300
C	1.75830300	1.81164600	0.32796400
O	2.85587800	1.59405600	0.88331900
K	3.69709000	-0.66258800	1.73575300
Ni	-0.85583900	0.69919800	-0.33629300
C	-2.74301800	0.35248900	-0.04709200
C	-3.51291400	-0.33957100	-0.99528000
C	-4.63022900	-1.08185700	-0.61233200
C	-5.00917200	-1.14294700	0.73062800
C	-4.26148200	-0.44695400	1.68468300
C	-3.14999300	0.30144400	1.29781300

H	-3.23122700	-0.29443900	-2.05574200
H	-5.21245000	-1.61703300	-1.37132800
H	-5.88928400	-1.72108900	1.03179400
H	-4.55361400	-0.47938400	2.74065800
H	-2.58900700	0.86777500	2.05416500
C	-0.94546000	2.58624400	-0.76421100
H	-0.51058300	2.70830100	-1.76693900
C	-2.29460800	2.17833700	-0.68432400
H	-2.85344100	2.08079800	-1.62232900
H	-2.89587300	2.59398400	0.13438300
C	1.88186500	4.01235300	-0.75039200
H	1.60136100	5.07870800	-0.71202200
H	2.98021300	3.94779300	-0.68026700
H	1.58891100	3.61957400	-1.73982800

TS6c

Gibbs free energy before correction = -3103.33550200

Gibbs free energy after correction = -3103.32103576

C	1.22130700	3.25161100	-0.12935900
C	-0.29577900	3.35413000	-0.11945300
H	1.56022300	3.58752300	-1.13418400
H	-0.67929300	3.12740100	0.89652600
H	-0.57078700	4.41249700	-0.30989400
C	-1.20552000	-2.25716700	0.44146300
C	0.86229100	-1.51763700	-0.37166300
C	1.40602500	-2.84317600	-0.34514500
C	0.56141900	-3.88582400	0.12418200
C	-0.74470200	-3.55521000	0.54000400
H	-2.22277400	-2.00397000	0.75410800
C	1.66913500	-0.42318700	-0.74265800
C	2.73947600	-3.02396900	-0.78858100
H	0.93858600	-4.91340500	0.17366100
H	-1.41595300	-4.32429500	0.93732600
C	3.48725500	-1.94308000	-1.27301300
C	2.96551600	-0.64782500	-1.25367100
H	3.15965400	-4.03704900	-0.78869000
H	4.49609600	-2.11361900	-1.66744500
H	3.56035500	0.19894500	-1.61142400
N	-0.44238200	-1.23152900	-0.04156000
N	1.05764100	0.83618300	-0.60156300
C	1.77251000	1.83156000	-0.03583500
O	2.88671700	1.66715400	0.50220200

K	3.73964700	-0.49060000	1.59396300
Ni	-0.86343800	0.64285500	-0.47758300
C	-2.74342400	0.33996100	-0.10073500
C	-3.54024600	-0.46118300	-0.93385300
C	-4.64492800	-1.14822500	-0.43000600
C	-4.98320700	-1.04451100	0.92110600
C	-4.20776600	-0.23949800	1.76051500
C	-3.11002200	0.45415300	1.25211000
H	-3.29018700	-0.54706500	-1.99969400
H	-5.24914600	-1.77027800	-1.10039900
H	-5.85329700	-1.57921100	1.31678800
H	-4.46779000	-0.14243900	2.82092200
H	-2.52791300	1.10750600	1.91667100
C	-0.96404700	2.46200900	-1.11967400
H	-0.53769000	2.47197000	-2.13428500
C	-2.31174600	2.06637000	-0.97117600
H	-2.88329600	1.85705500	-1.88294800
H	-2.90168800	2.58096200	-0.20200900
C	1.83815800	4.16723700	0.91206900
H	2.93593000	4.18038900	0.84794700
H	1.47189700	5.20002200	0.78627900
H	1.56925200	3.83947000	1.93225800

Vc

Gibbs free energy before correction = -3103.33926000

Gibbs free energy after correction = -3103.32479376

C	1.13915400	3.23111700	0.48296500
C	-0.35955300	3.36733800	0.26809700
H	1.38676400	3.58312100	1.50004700
H	-0.91618700	3.03153300	1.16321300
H	-0.60085200	4.44318200	0.15065600
C	-1.12355000	-2.33774500	0.27786000
C	0.91919700	-1.43732400	-0.43356700
C	1.51493700	-2.73626000	-0.53403700
C	0.71119400	-3.85552200	-0.18532600
C	-0.60680800	-3.61760400	0.25206200
H	-2.15171600	-2.16616800	0.60664400
C	1.69097400	-0.28488400	-0.66279900
C	2.86083300	-2.81742700	-0.96946400
H	1.12958900	-4.86675900	-0.23527000
H	-1.24885100	-4.44688100	0.56811600
C	3.57721900	-1.66419000	-1.31325200

C	3.00542300	-0.39950500	-1.15938500
H	3.31895600	-3.80865300	-1.07075000
H	4.59913600	-1.75416100	-1.70022400
H	3.57155000	0.50656800	-1.40095600
N	-0.40398700	-1.23445100	-0.10197700
N	1.03624600	0.92776200	-0.38428500
C	1.68485300	1.81486800	0.39545900
O	2.75698100	1.57982000	0.99154400
K	3.71136100	-0.67030800	1.71610300
Ni	-0.91615600	0.63188300	-0.37604400
C	-2.71390600	0.11160300	-0.01586000
C	-3.54108500	-0.54676300	-0.93602800
C	-4.76459100	-1.09558000	-0.54433500
C	-5.19193500	-0.99040000	0.78136400
C	-4.38782100	-0.31932200	1.70515100
C	-3.16711700	0.23332400	1.30619200
H	-3.21975000	-0.64974900	-1.98187000
H	-5.39018000	-1.61304200	-1.28155400
H	-6.15019700	-1.42168200	1.09110300
H	-4.71510900	-0.22175500	2.74727900
H	-2.55521200	0.76449500	2.04959200
C	-0.86736500	2.61905500	-0.92456400
H	-0.24838200	2.63385600	-1.83075300
C	-2.16749300	2.18833400	-1.02408400
H	-2.58631500	1.88774300	-1.99143700
H	-2.89843900	2.47720600	-0.26069900
C	1.93686900	4.08128900	-0.50641800
H	1.66153800	5.14597600	-0.42086900
H	3.01913500	3.99323900	-0.31861600
H	1.75279500	3.76692700	-1.54909700

Vd

Gibbs free energy before correction = -3103.34012800

Gibbs free energy after correction = -3103.32566176

C	1.14729300	3.28059800	-0.00660100
C	-0.35953000	3.36735800	-0.17379900
H	1.60153400	3.70881000	-0.92696500
H	-0.86654300	3.12861600	0.78273000
H	-0.62341600	4.42121900	-0.39480700
C	-1.06665900	-2.25822300	0.60366400
C	0.92054700	-1.46278600	-0.35016800
C	1.51621000	-2.76501900	-0.32198300

C	0.74328300	-3.82759600	0.22089400
C	-0.54412900	-3.53126800	0.71197500
H	-2.07178700	-2.04052800	0.97464500
C	1.66928200	-0.34836600	-0.76829800
C	2.83147900	-2.90338600	-0.83062300
H	1.16366400	-4.83775200	0.27593200
H	-1.15713500	-4.31025700	1.17804600
C	3.51641900	-1.80406400	-1.36326600
C	2.94918500	-0.52798700	-1.33105800
H	3.28846800	-3.90030400	-0.83582700
H	4.51153800	-1.94395100	-1.80179100
H	3.49555200	0.33848200	-1.71825700
N	-0.37983600	-1.21699700	0.03540700
N	1.02445400	0.88985900	-0.59386500
C	1.71862600	1.86817800	0.02110500
O	2.83576700	1.70333100	0.55375800
K	3.82129800	-0.45579200	1.50375100
Ni	-0.92104900	0.58747200	-0.47835200
C	-2.70999800	0.07993500	-0.05632400
C	-3.49517200	-0.72345000	-0.89466600
C	-4.70703900	-1.26018300	-0.45381600
C	-5.16535600	-0.99697800	0.83926100
C	-4.40465600	-0.18009600	1.67860200
C	-3.19570300	0.35977100	1.22957700
H	-3.14812900	-0.95214700	-1.91201200
H	-5.29909800	-1.89293500	-1.12592700
H	-6.11437100	-1.41885200	1.18797200
H	-4.75728500	0.04291400	2.69278900
H	-2.61864900	1.00919900	1.90383500
C	-0.90000100	2.49136300	-1.25726300
H	-0.30113000	2.41402600	-2.17443100
C	-2.20025100	2.04937700	-1.27111600
H	-2.64549000	1.64615900	-2.18789000
H	-2.91009200	2.41896500	-0.52288600
C	1.61267500	4.10607600	1.17913200
H	2.70967800	4.14343400	1.24409400
H	1.23455600	5.13959900	1.10502700
H	1.23535800	3.67993800	2.12605900

VIe

Gibbs free energy before correction = -3103.36020700

Gibbs free energy after correction = -3103.34574076

C	0.26176200	3.37393500	0.10011100
C	-1.24300700	3.13859100	0.15448200
H	0.54724300	4.04245000	0.93194900
H	-1.53437900	2.90765000	1.19874300
H	-1.75326300	4.10153400	-0.07642300
C	-0.62181300	-2.71583000	-0.30492900
C	1.23416200	-1.31184500	-0.53211100
C	2.12430000	-2.42763600	-0.66250100
C	1.56001100	-3.72895700	-0.56541700
C	0.17008500	-3.84688700	-0.39080600
H	-1.70676900	-2.80316100	-0.20515400
C	1.73114900	0.01003500	-0.60745900
C	3.49688200	-2.16886700	-0.89749600
H	2.20637100	-4.60979800	-0.65023800
H	-0.30644300	-4.83192400	-0.33978300
C	3.95543000	-0.85821700	-1.06991700
C	3.08754300	0.22779300	-0.93895200
H	4.18325400	-3.01851300	-0.99543600
H	5.01007700	-0.67886900	-1.31069100
H	3.45394400	1.25134700	-1.07107100
N	-0.12375800	-1.44887300	-0.36130400
N	0.78241300	1.02215900	-0.41401700
C	1.12628900	2.13347900	0.27766300
O	2.15852000	2.23154100	0.97219600
K	3.37677600	0.21756700	2.00259100
Ni	-0.99218800	0.33466400	-0.29957200
C	-3.20182900	0.28165700	-0.06100700
C	-3.90053000	-0.79893800	-0.64925500
C	-4.07827800	-1.98839200	0.03596400
C	-3.53230700	-2.15380700	1.32290500
C	-2.79643900	-1.13185800	1.89712400
C	-2.61575100	0.08628200	1.21120500
H	-4.35008200	-0.65946100	-1.63971700
H	-4.65045500	-2.80221900	-0.42192200
H	-3.68961200	-3.09178200	1.86567000
H	-2.37796900	-1.25146000	2.90214300
H	-2.20442500	0.94148300	1.76136000
C	-1.71939900	2.03893700	-0.75796200
H	-1.40697600	2.22265900	-1.80295700
C	-3.18602700	1.66852900	-0.66865600
H	-3.67963600	1.63930400	-1.65491600
H	-3.77282700	2.36550800	-0.03543900

C	0.70116600	4.04499900	-1.20131400
H	0.18932000	5.01350100	-1.33631200
H	1.78807300	4.23728100	-1.20093400
H	0.47793900	3.41676000	-2.08044100

VIf

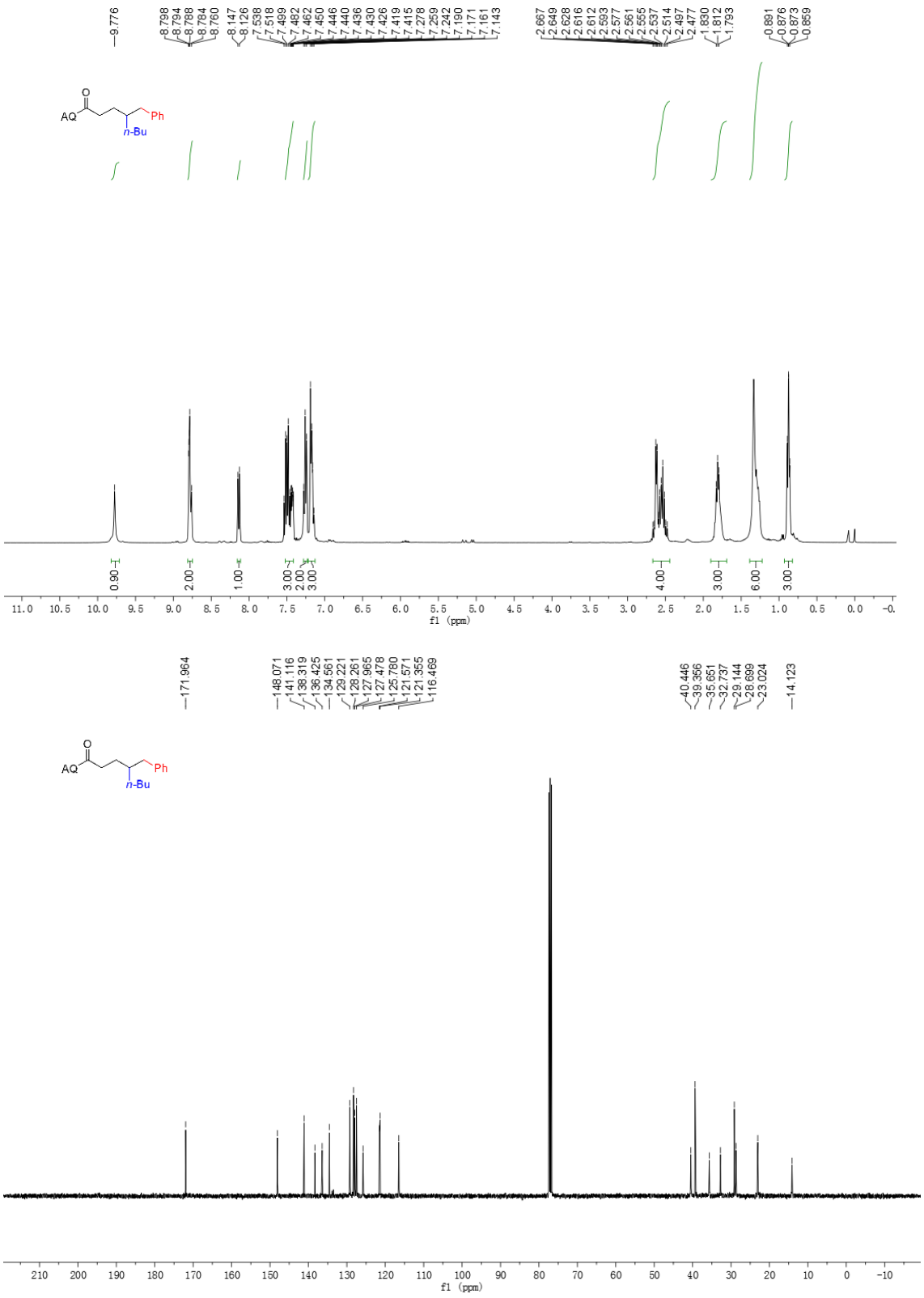
Gibbs free energy before correction = -3103.36104700

Gibbs free energy after correction = -3103.34658076

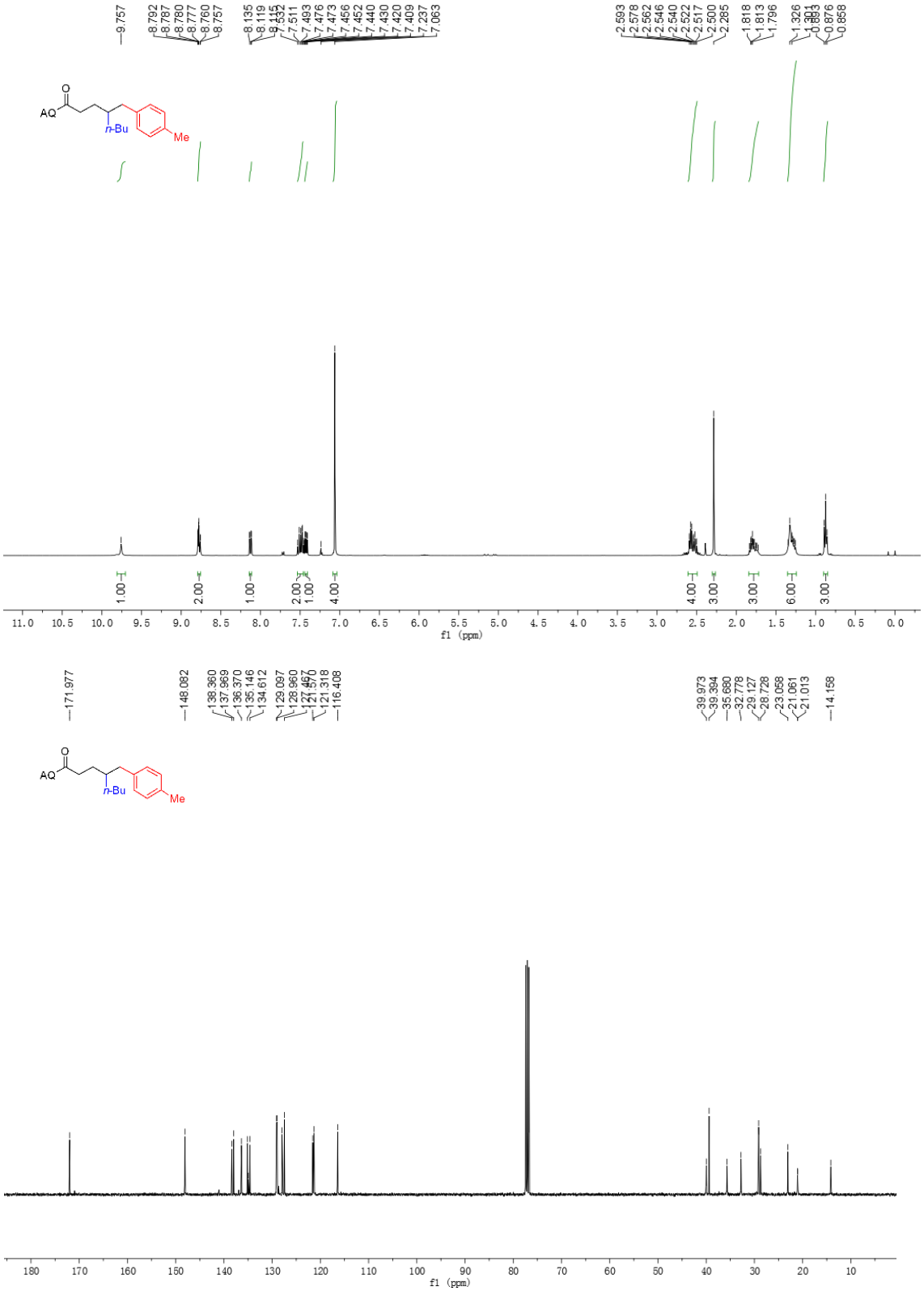
C	0.24989500	3.35716800	-0.39927900
C	-1.24629500	3.10375300	-0.25227900
H	0.43594400	3.53843600	-1.48032400
H	-1.48403800	2.98617200	0.82630900
H	-1.78481600	4.02788200	-0.56122300
C	-0.59648700	-2.75729300	-0.13818000
C	1.25361000	-1.37290300	-0.50511400
C	2.14926500	-2.49187100	-0.51594500
C	1.59060800	-3.77994600	-0.29098000
C	0.20070600	-3.88760400	-0.11106600
H	-1.68138100	-2.83902600	-0.03216900
C	1.74256600	-0.06162100	-0.71521900
C	3.52259100	-2.25159400	-0.76354400
H	2.24202600	-4.66113300	-0.28401500
H	-0.27130500	-4.86525700	0.03513200
C	3.97672100	-0.96208800	-1.05966200
C	3.10301300	0.12692400	-1.05050300
H	4.21387700	-3.10287300	-0.76727200
H	5.03383500	-0.80095800	-1.30216900
H	3.47052900	1.13288500	-1.27607200
N	-0.10343900	-1.50006800	-0.31953200
N	0.78644400	0.95973500	-0.63381100
C	1.12976300	2.14995500	-0.08018900
O	2.15334200	2.31563100	0.61183700
K	3.20832000	0.34429300	1.90025100
Ni	-0.97963000	0.27139000	-0.42410200
C	-3.18320700	0.22432500	-0.13810300
C	-3.88689700	-0.91702200	-0.59008500
C	-4.03933600	-2.02702800	0.22289700
C	-3.46240600	-2.05054200	1.50675700
C	-2.72418200	-0.96769800	1.95150800
C	-2.57017400	0.17137500	1.13526400
H	-4.35897900	-0.88778900	-1.57945300
H	-4.61490300	-2.88868800	-0.13163100

H	-3.59869100	-2.92612000	2.15010400
H	-2.28352900	-0.97565700	2.95415100
H	-2.15574000	1.08321200	1.58220500
C	-1.72728900	1.91351200	-1.03506700
H	-1.42151200	2.00559700	-2.09550800
C	-3.18806100	1.53788000	-0.89200300
H	-3.68758100	1.39628500	-1.86546700
H	-3.77890400	2.29349500	-0.33392500
C	0.67839500	4.58728000	0.37875000
H	1.74025100	4.82914000	0.22054500
H	0.07798600	5.46254700	0.07834700
H	0.53390300	4.43887400	1.46347800

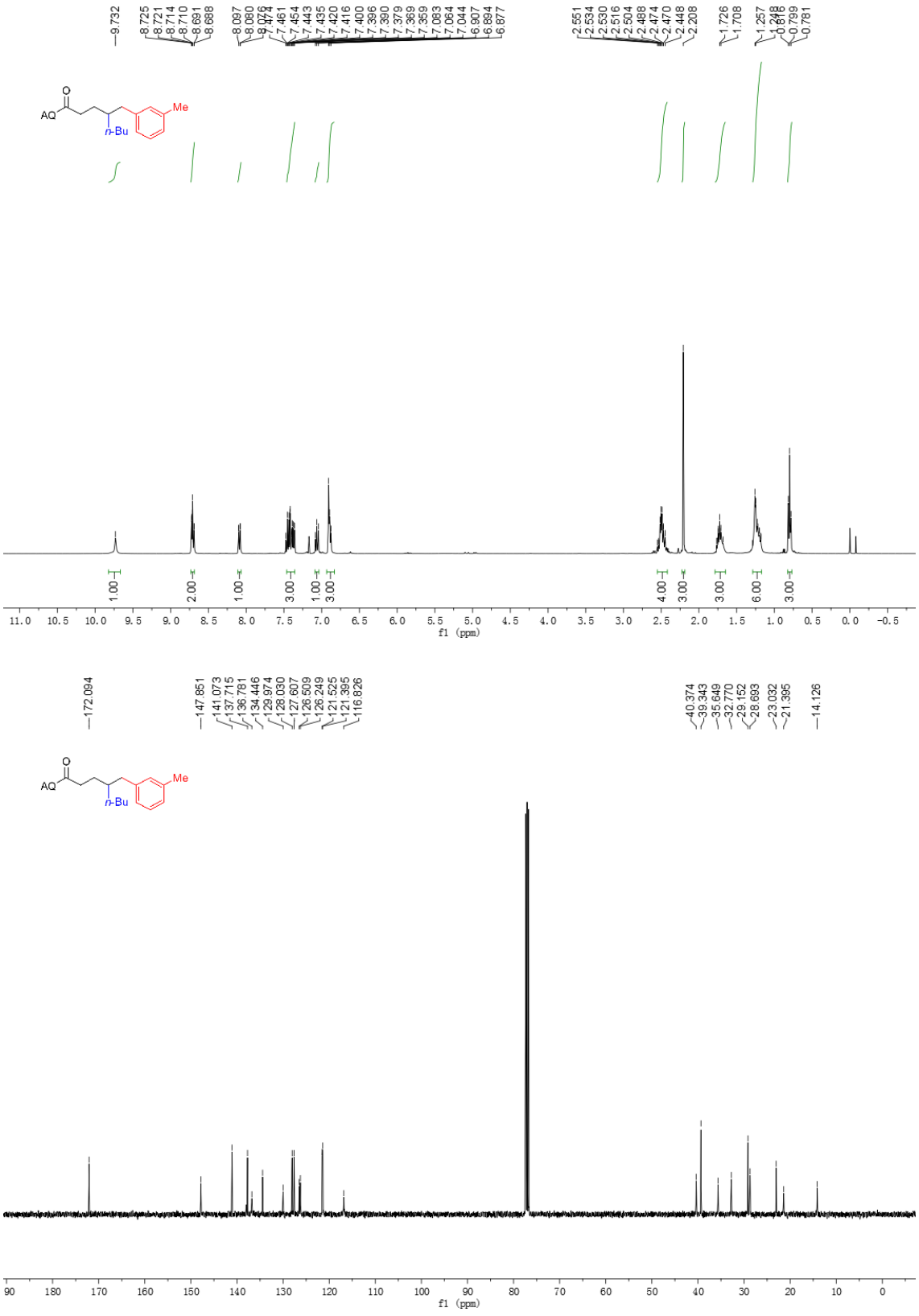
13. NMR Spectra



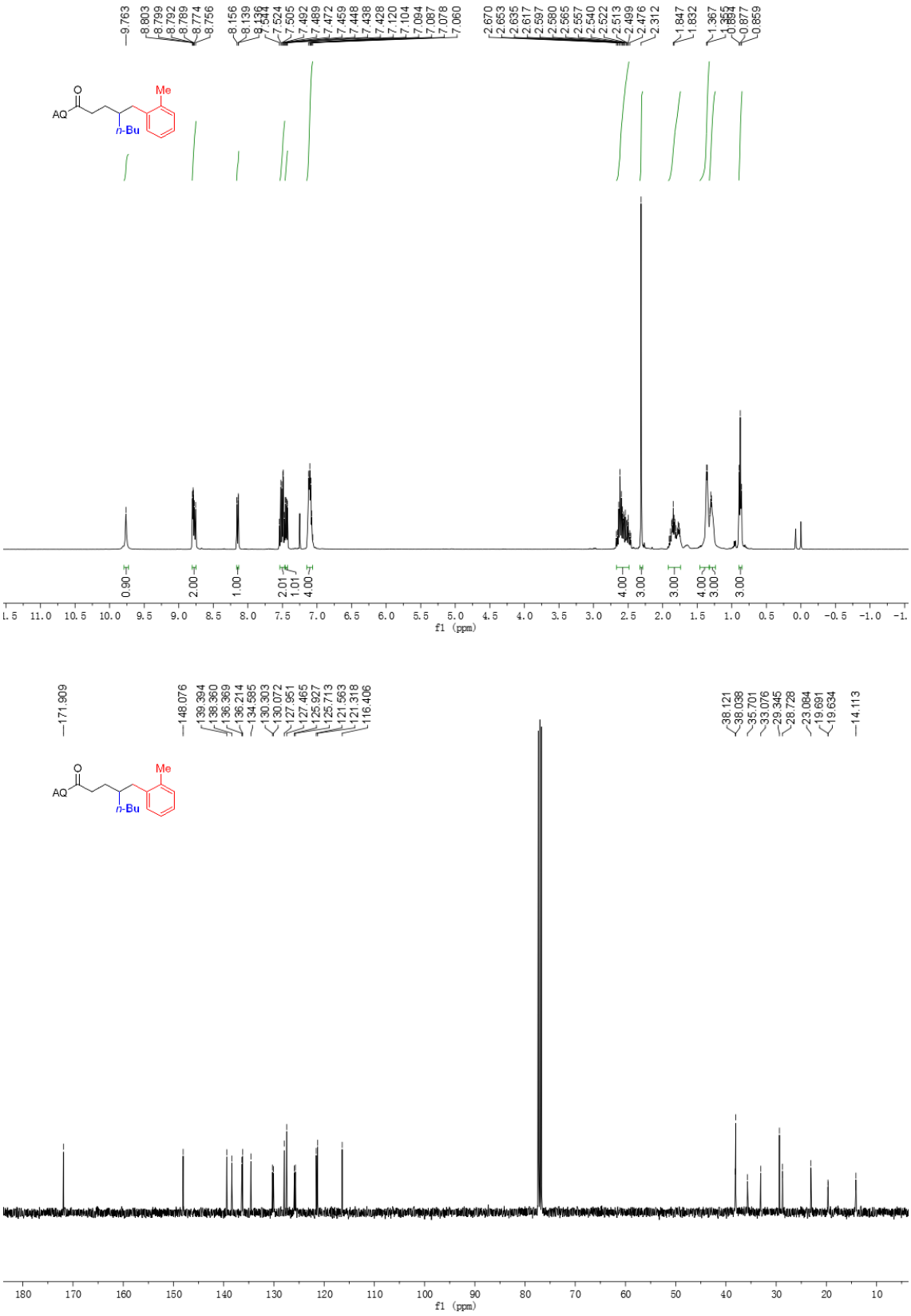
Scheme 1. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2a**



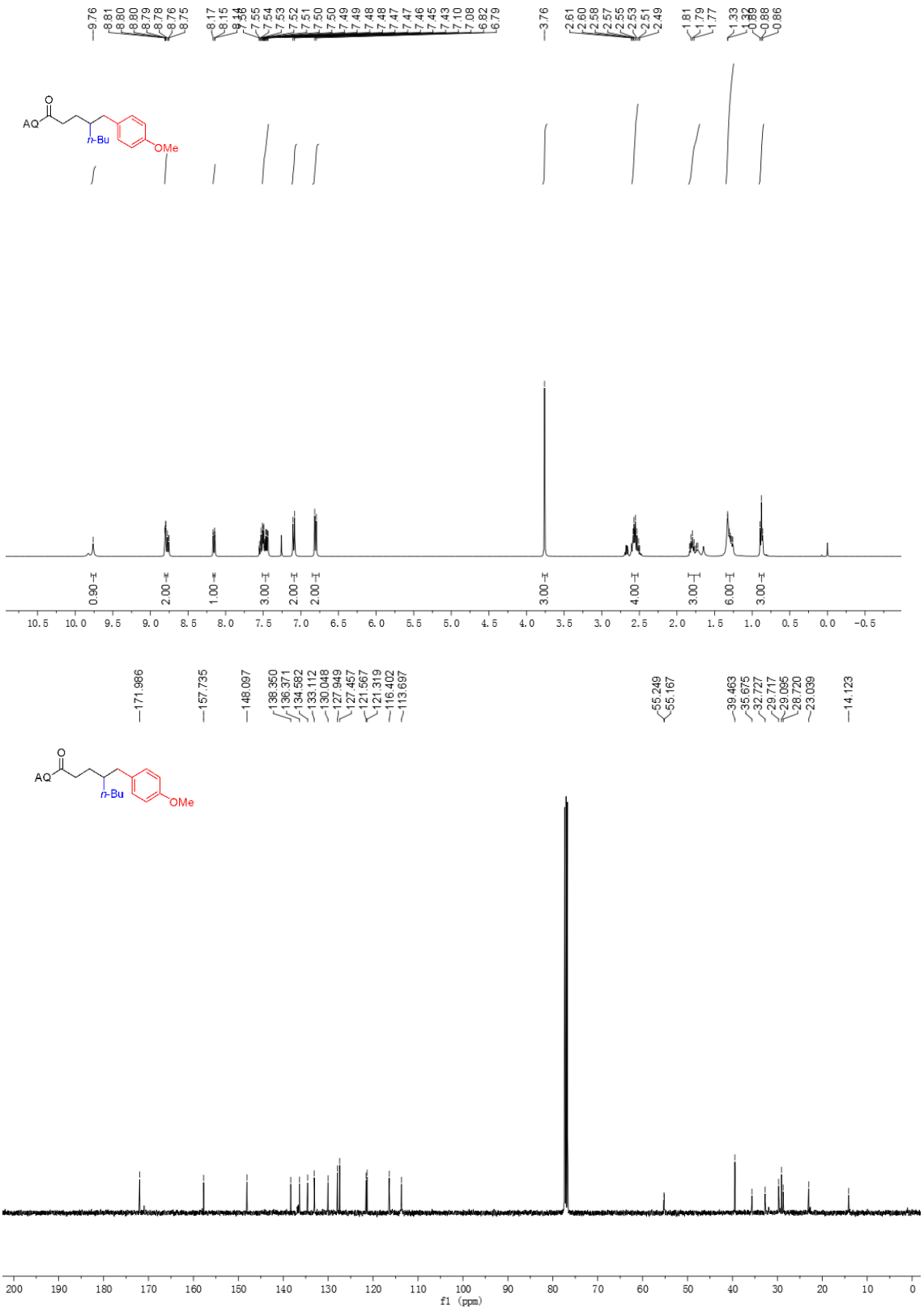
Scheme 2. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2b**.



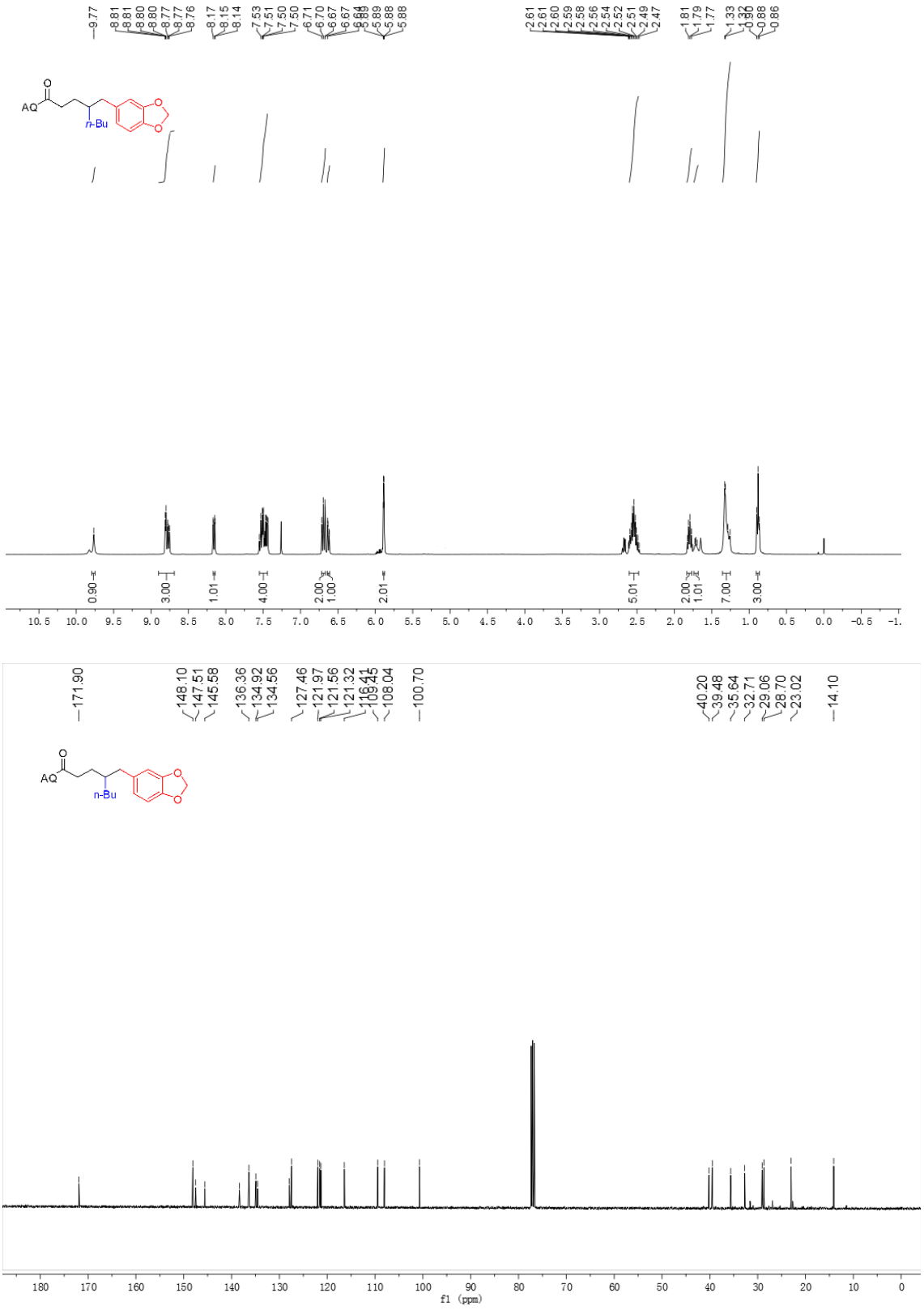
Scheme 3. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2c**.



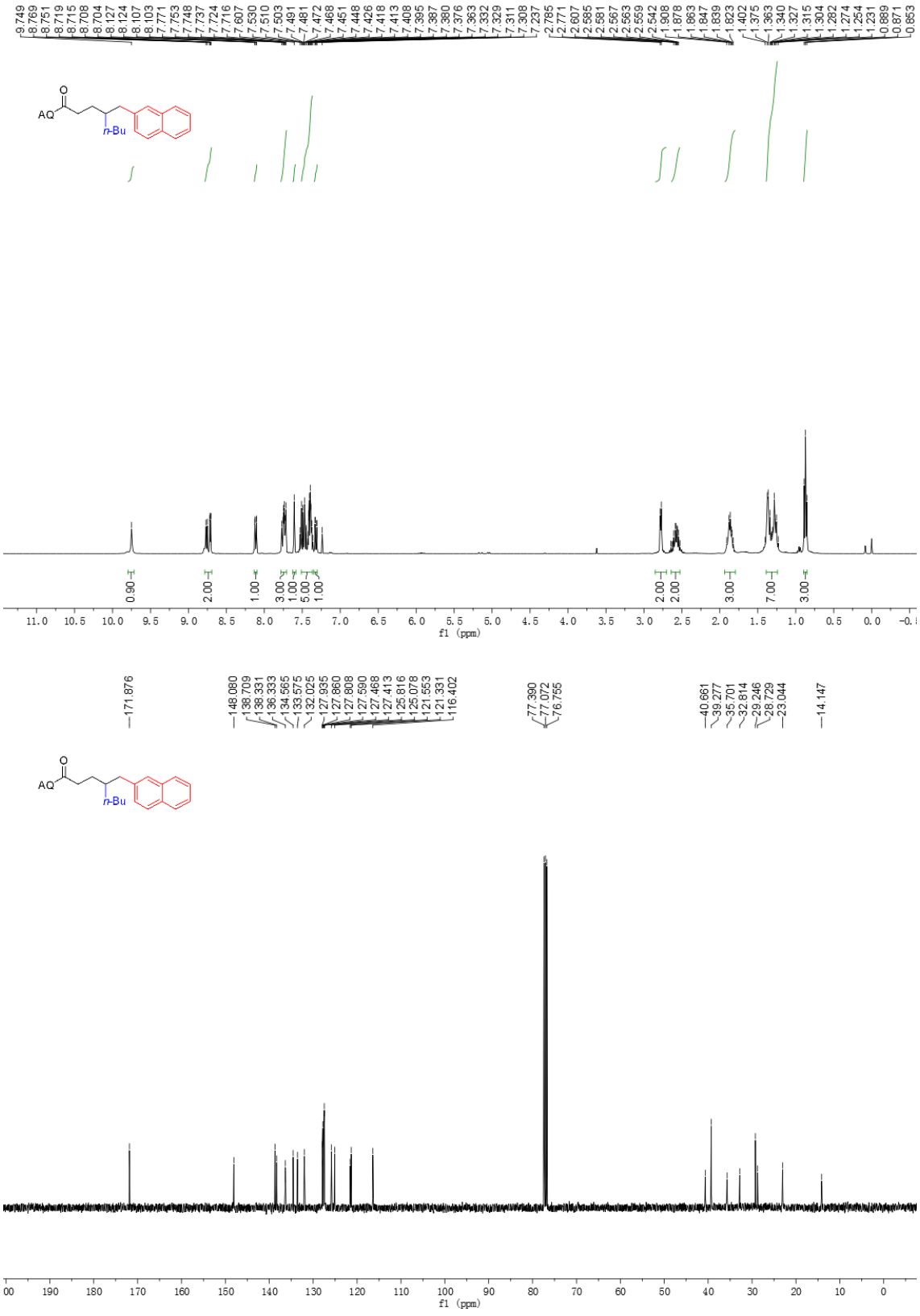
Scheme 4. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2d**.



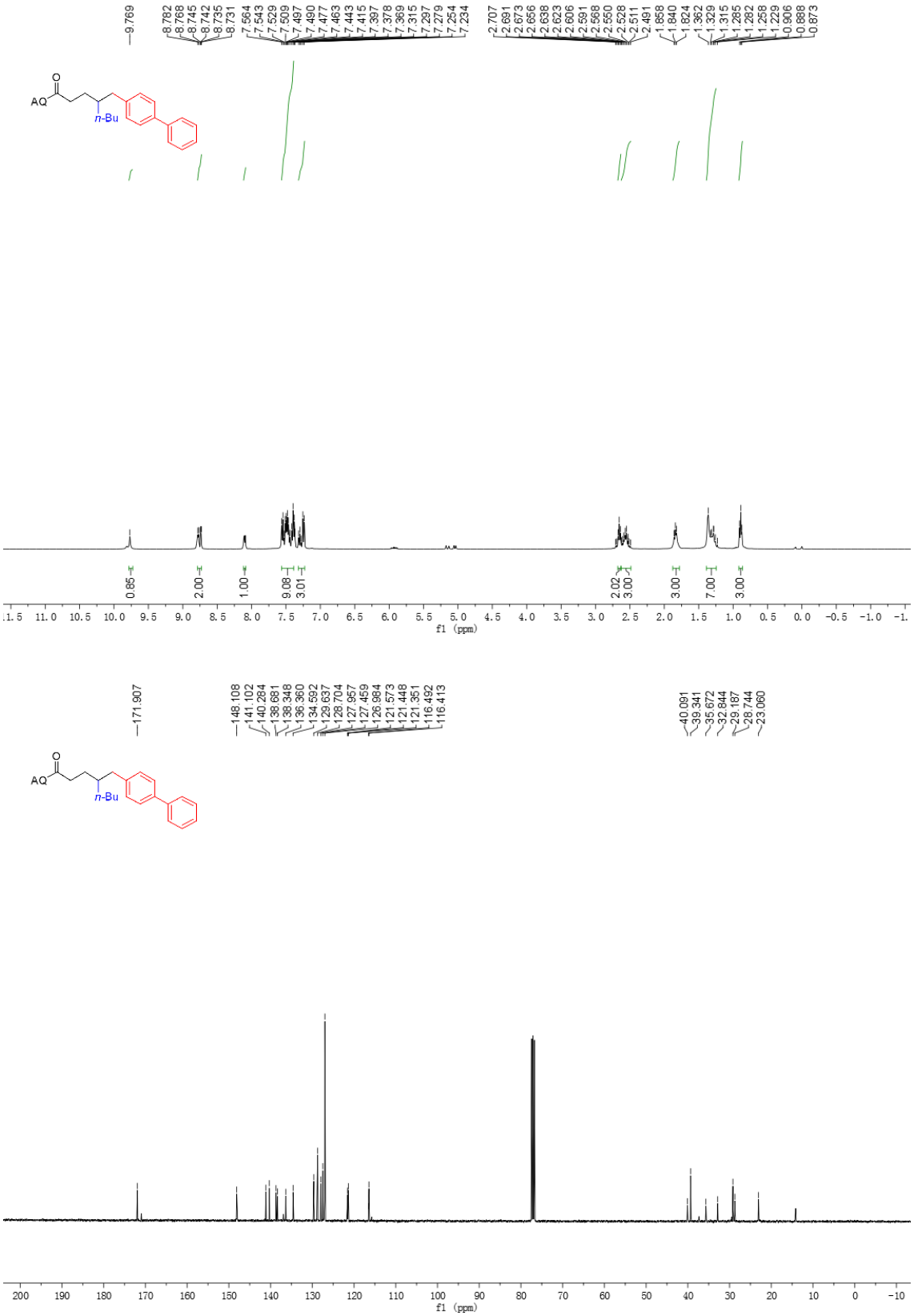
Scheme 5. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2e**



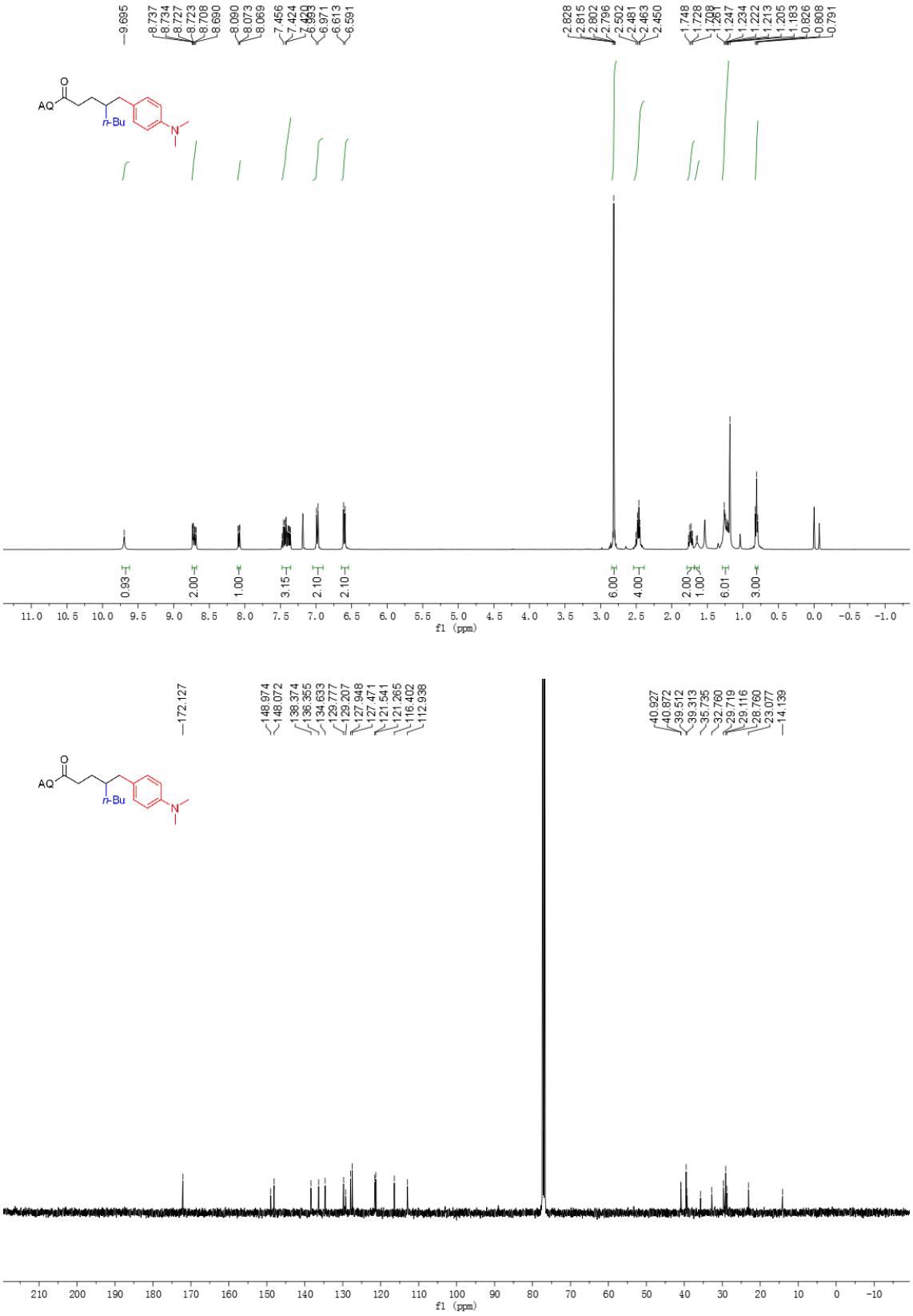
Scheme 6. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2f**



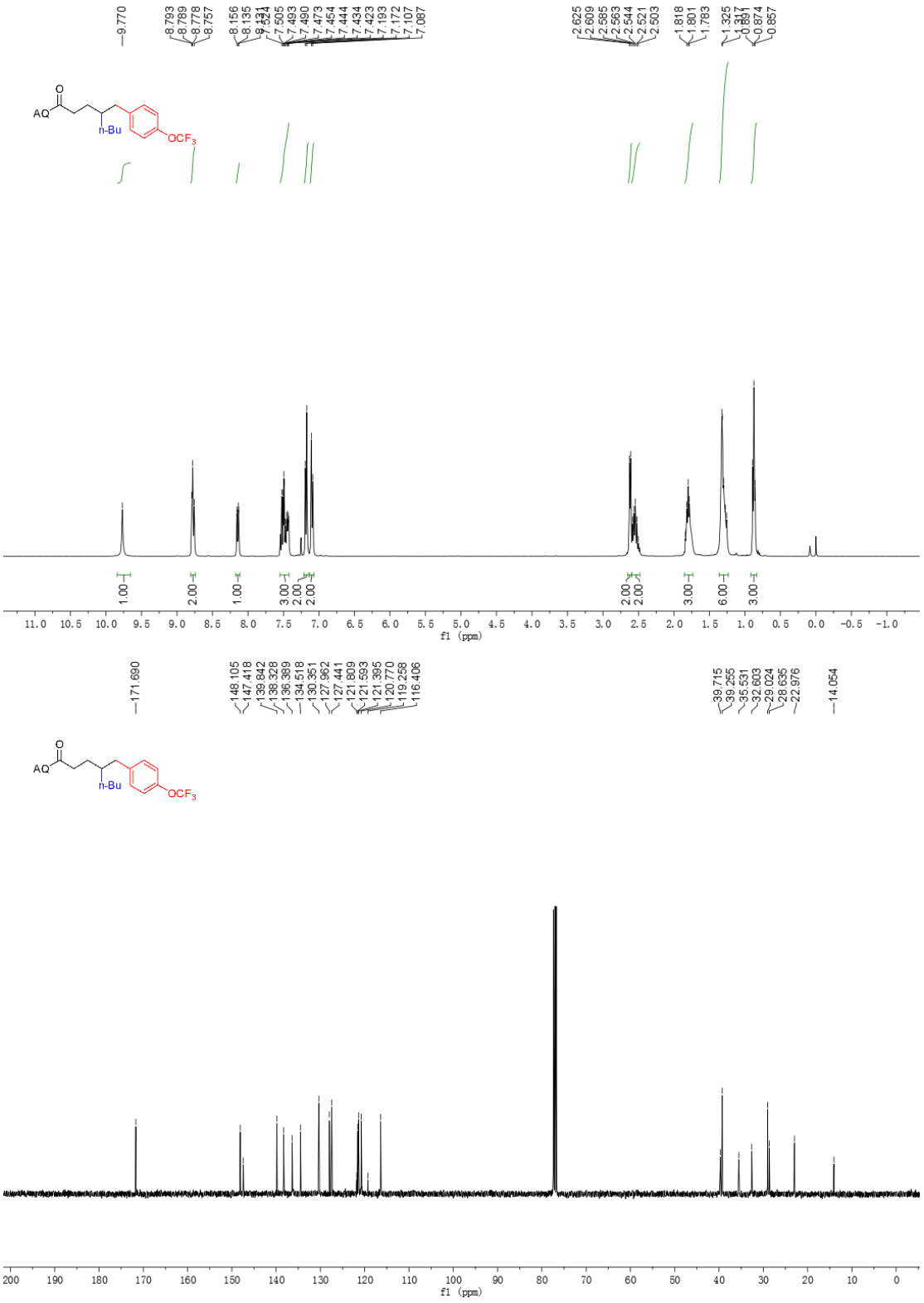
Scheme 7. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2g**



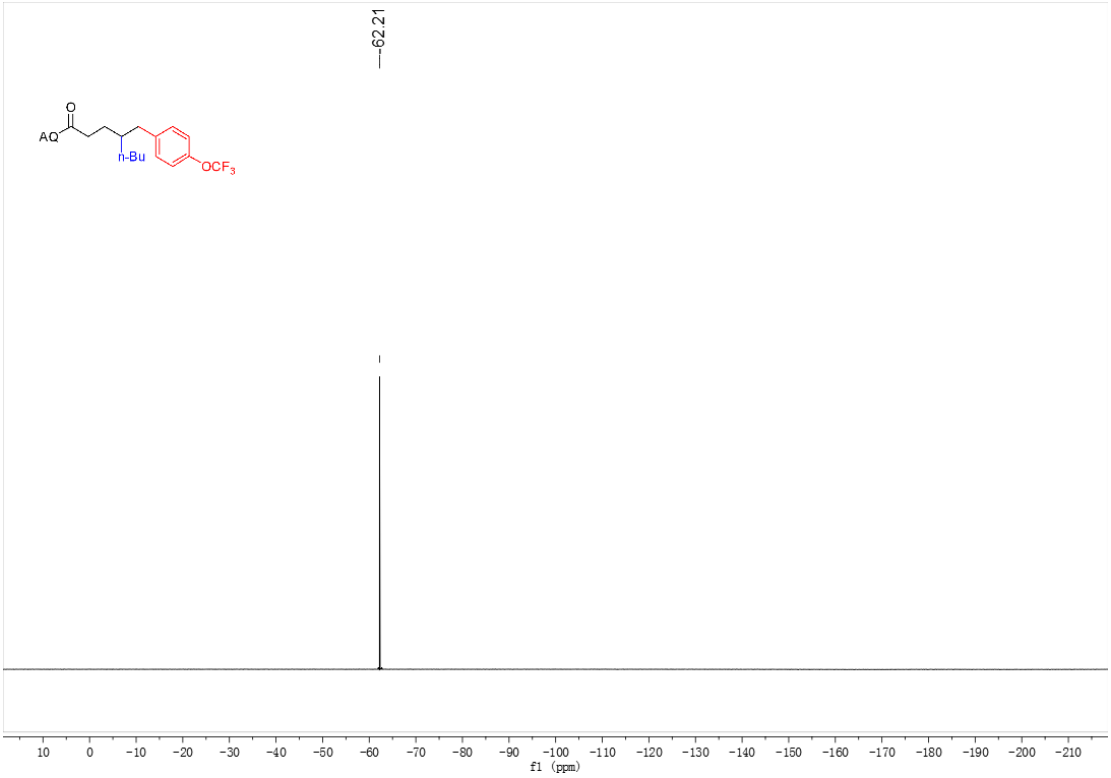
Scheme 8. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2h**



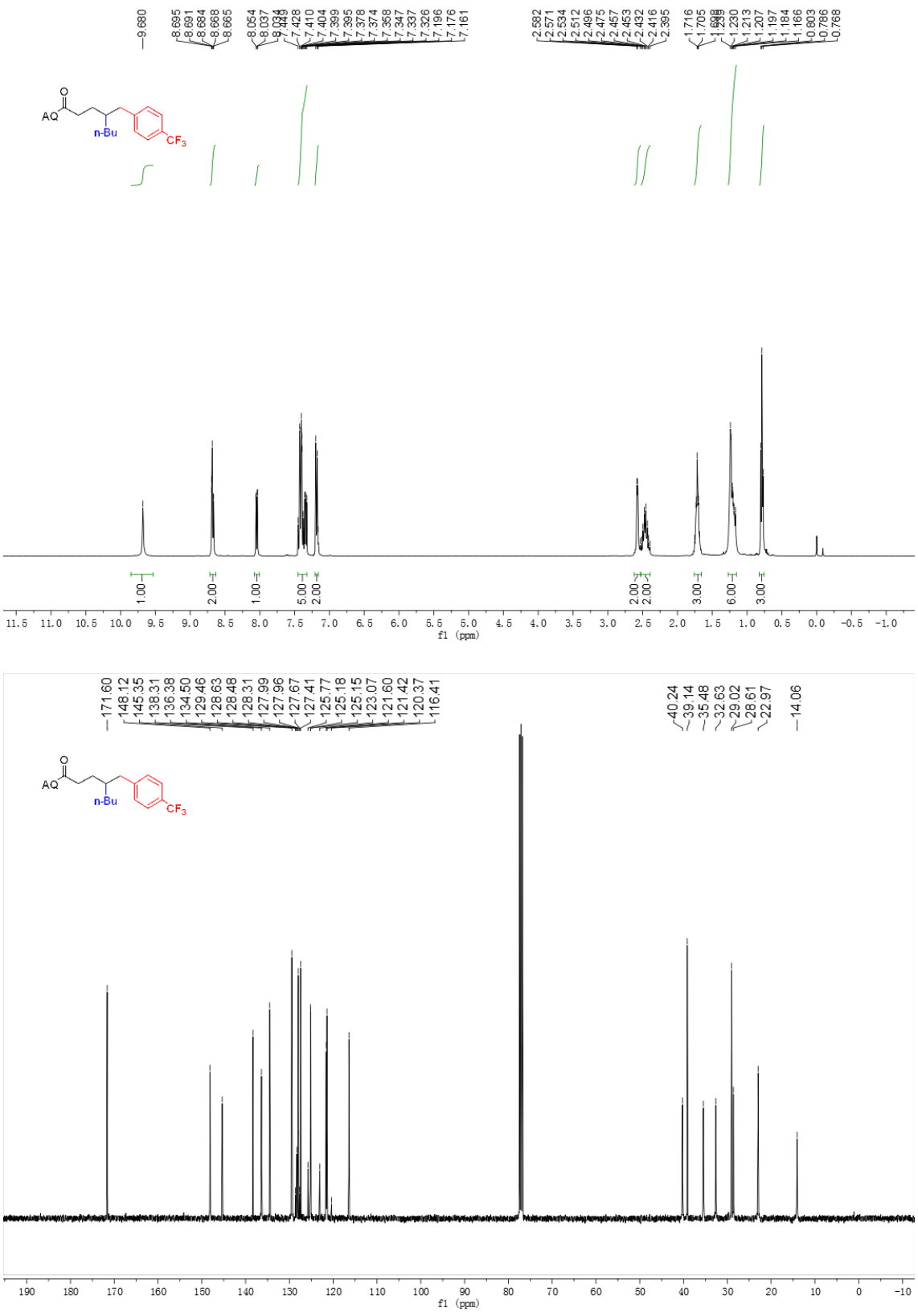
Scheme 9. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2i**



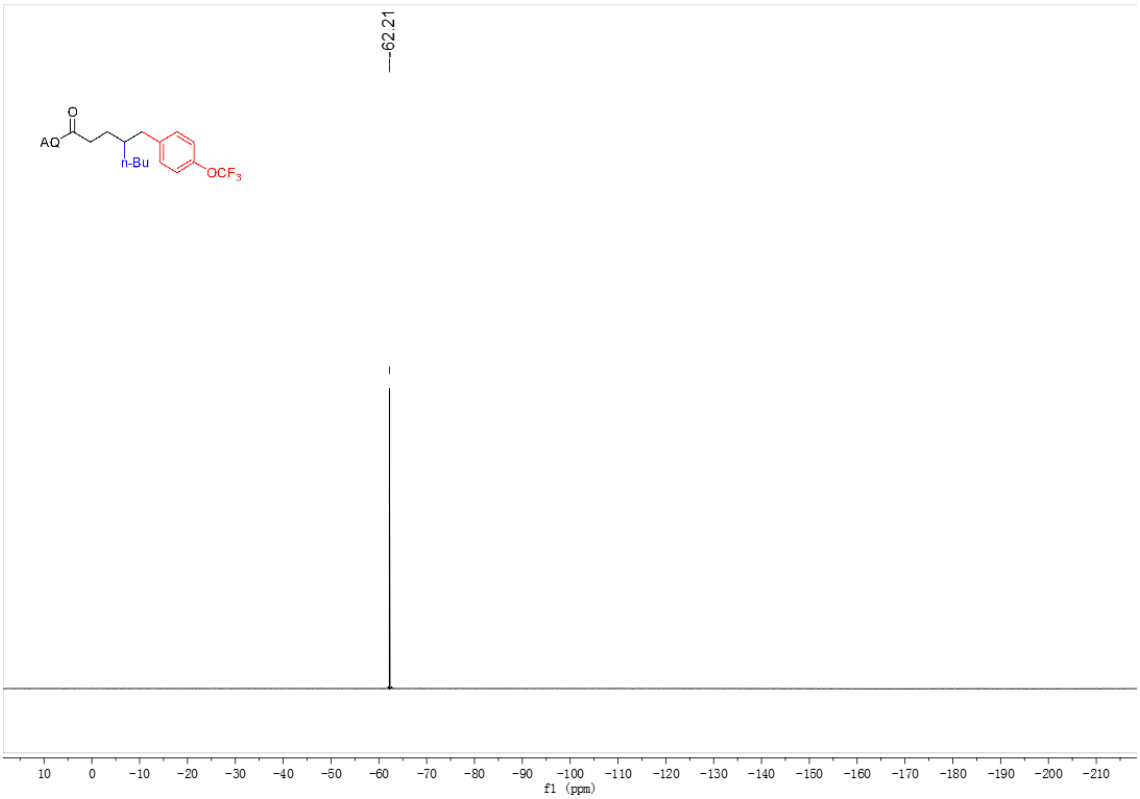
Scheme 10. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2j**



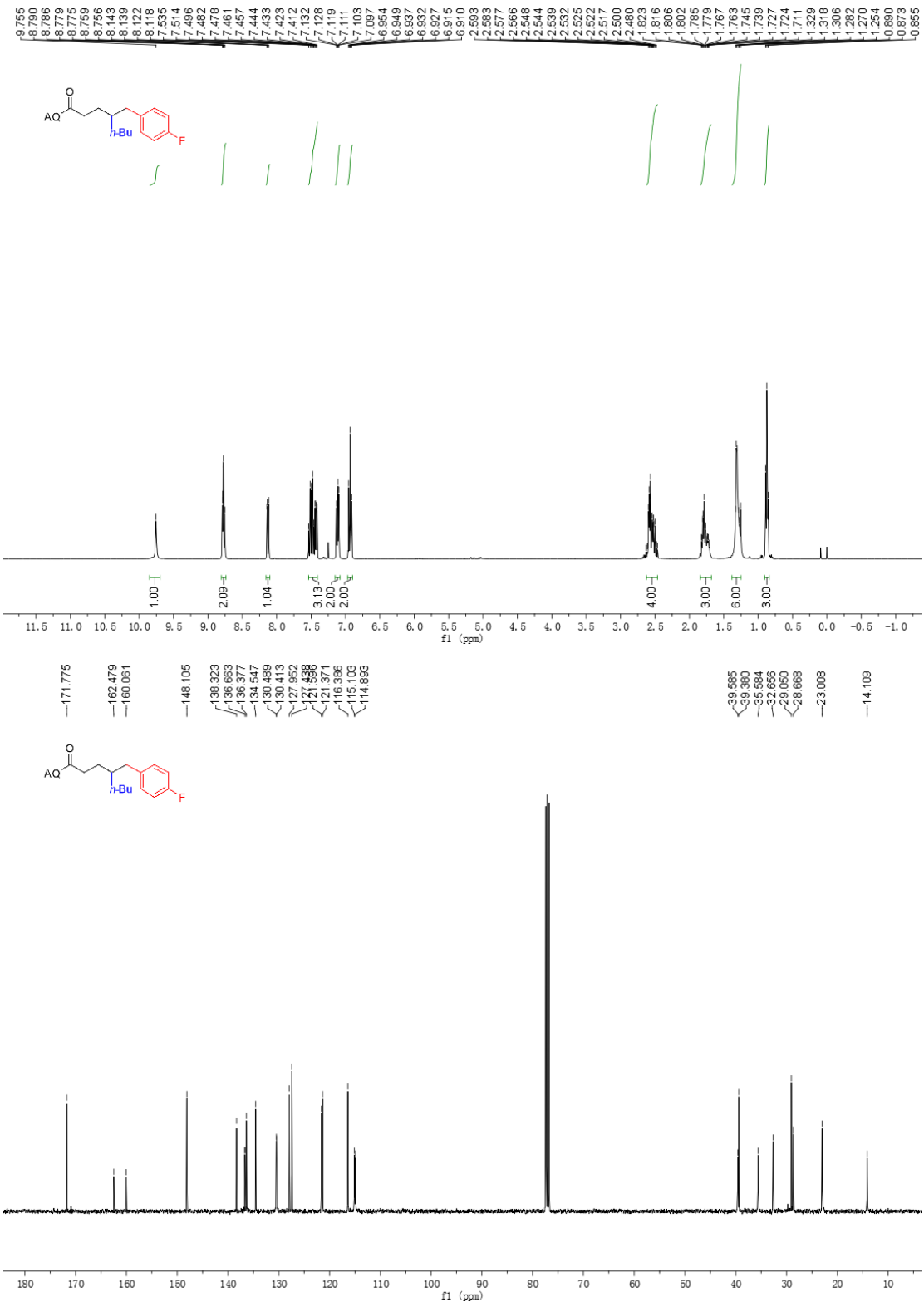
Scheme 11. ^{19}F NMR (376 MHz, $CDCl_3$) spectra of **2j**



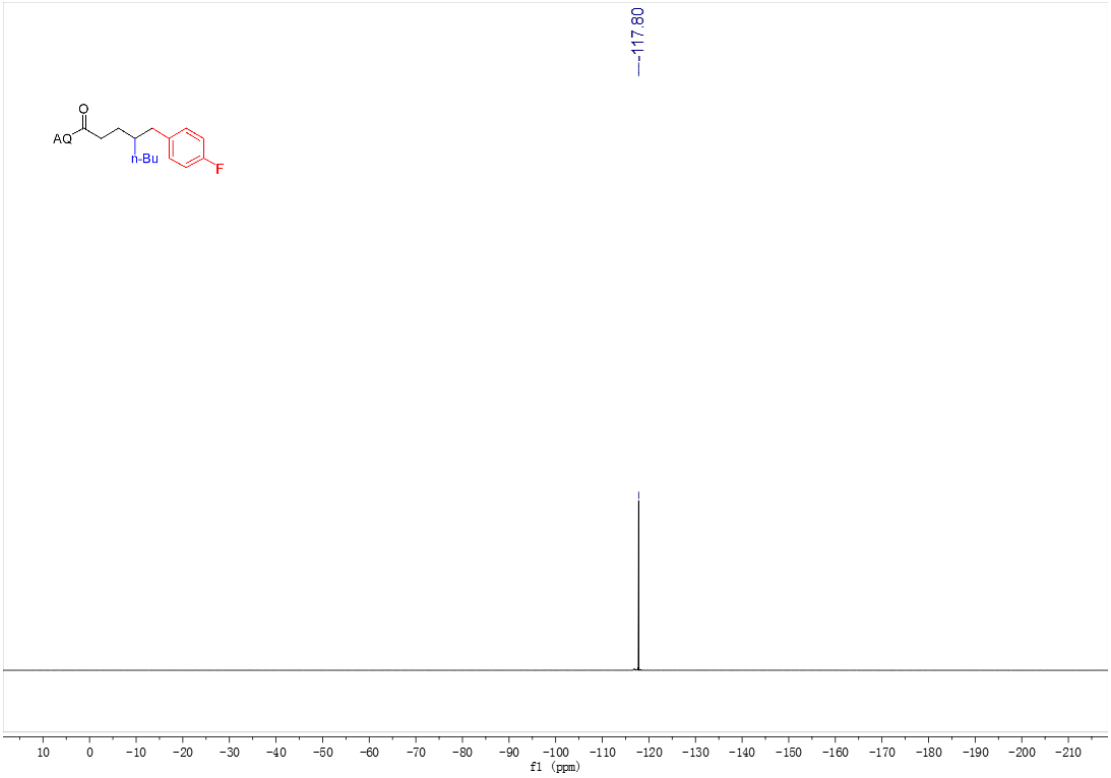
Scheme 12. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2k**



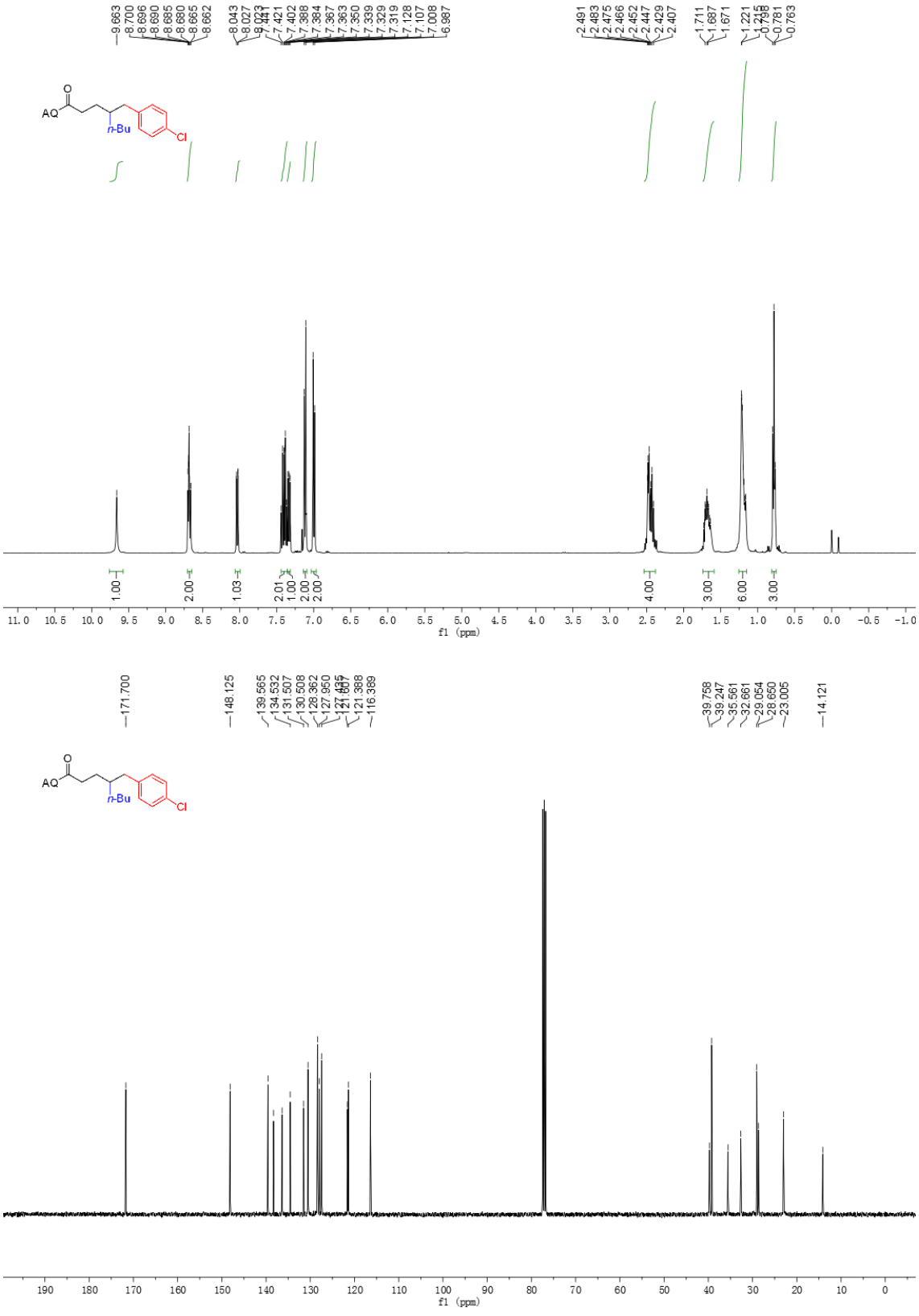
Scheme 13. ^{19}F NMR (376 MHz, $CDCl_3$) spectra of **2k**



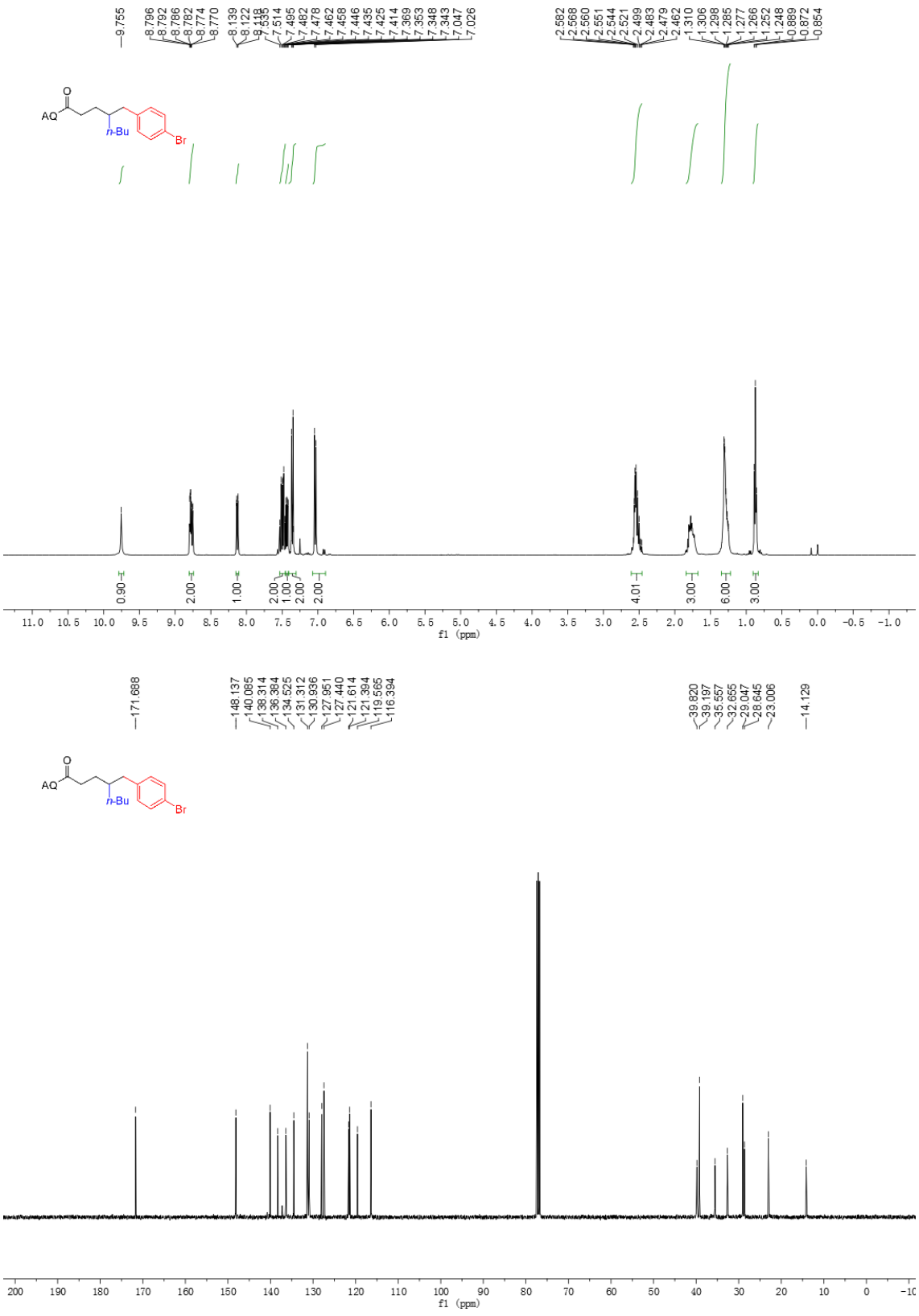
Scheme 14. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2l**



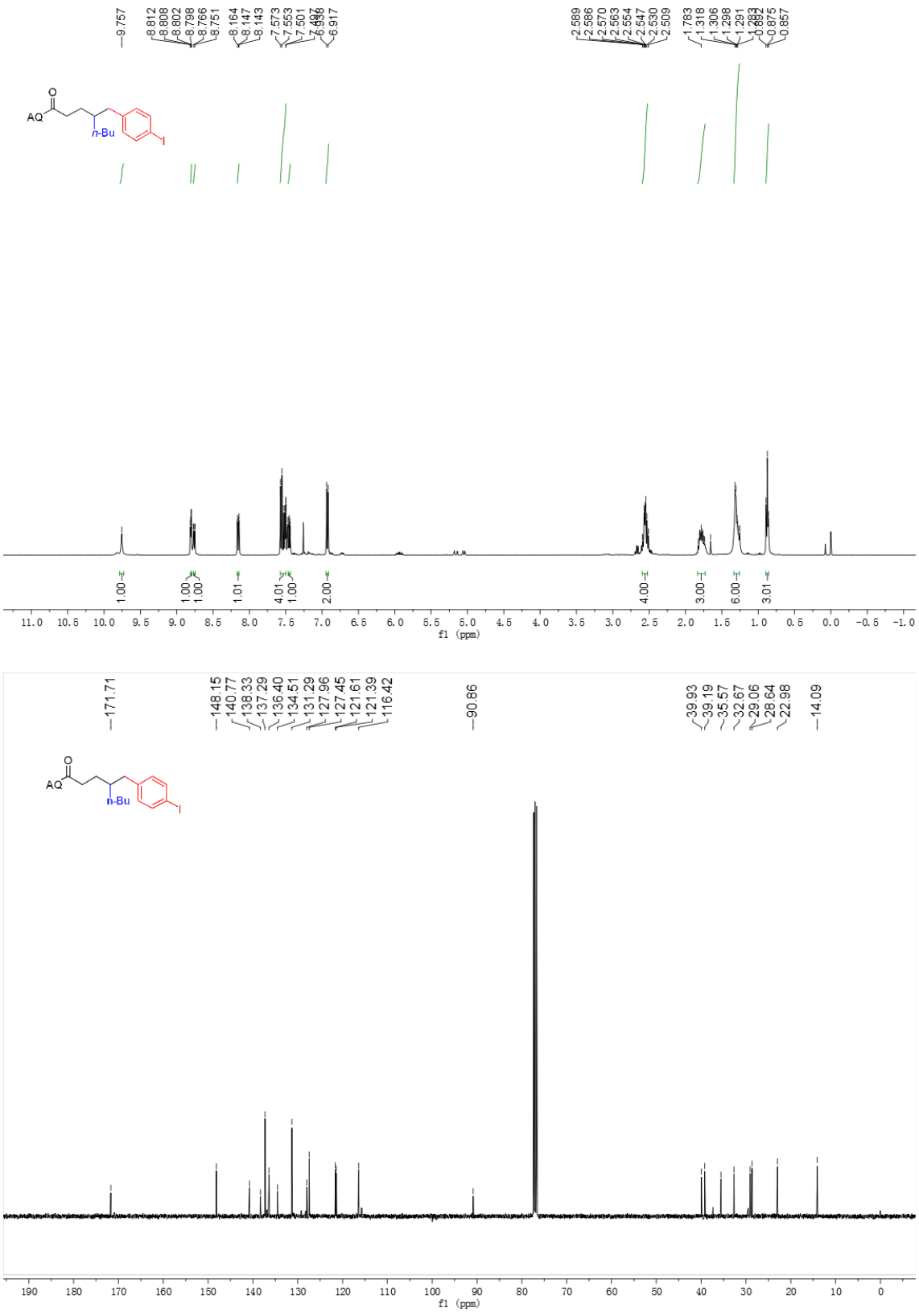
Scheme 15. ^{19}F NMR (376 MHz, $CDCl_3$) spectra of **2l**



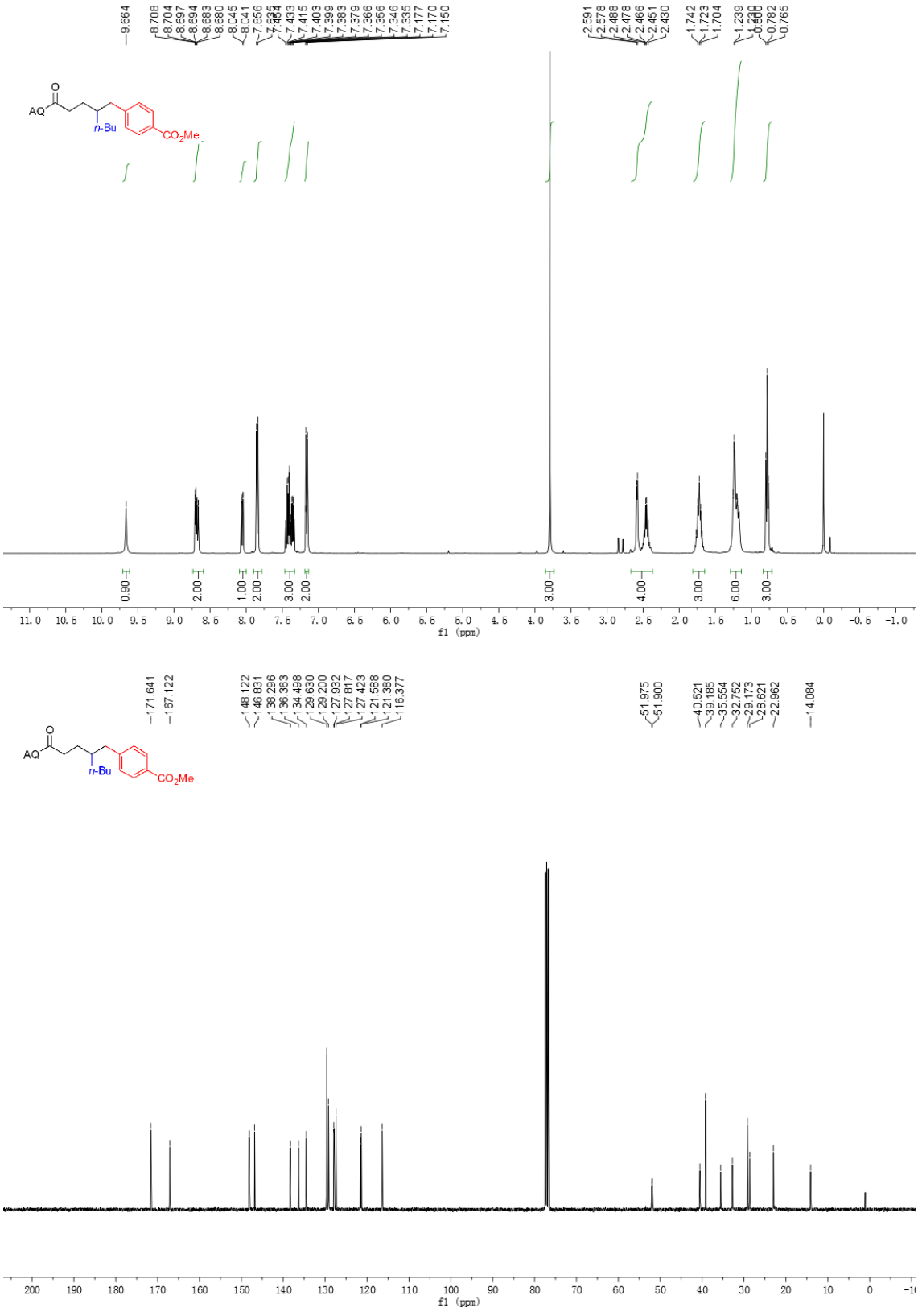
Scheme 16. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2m**



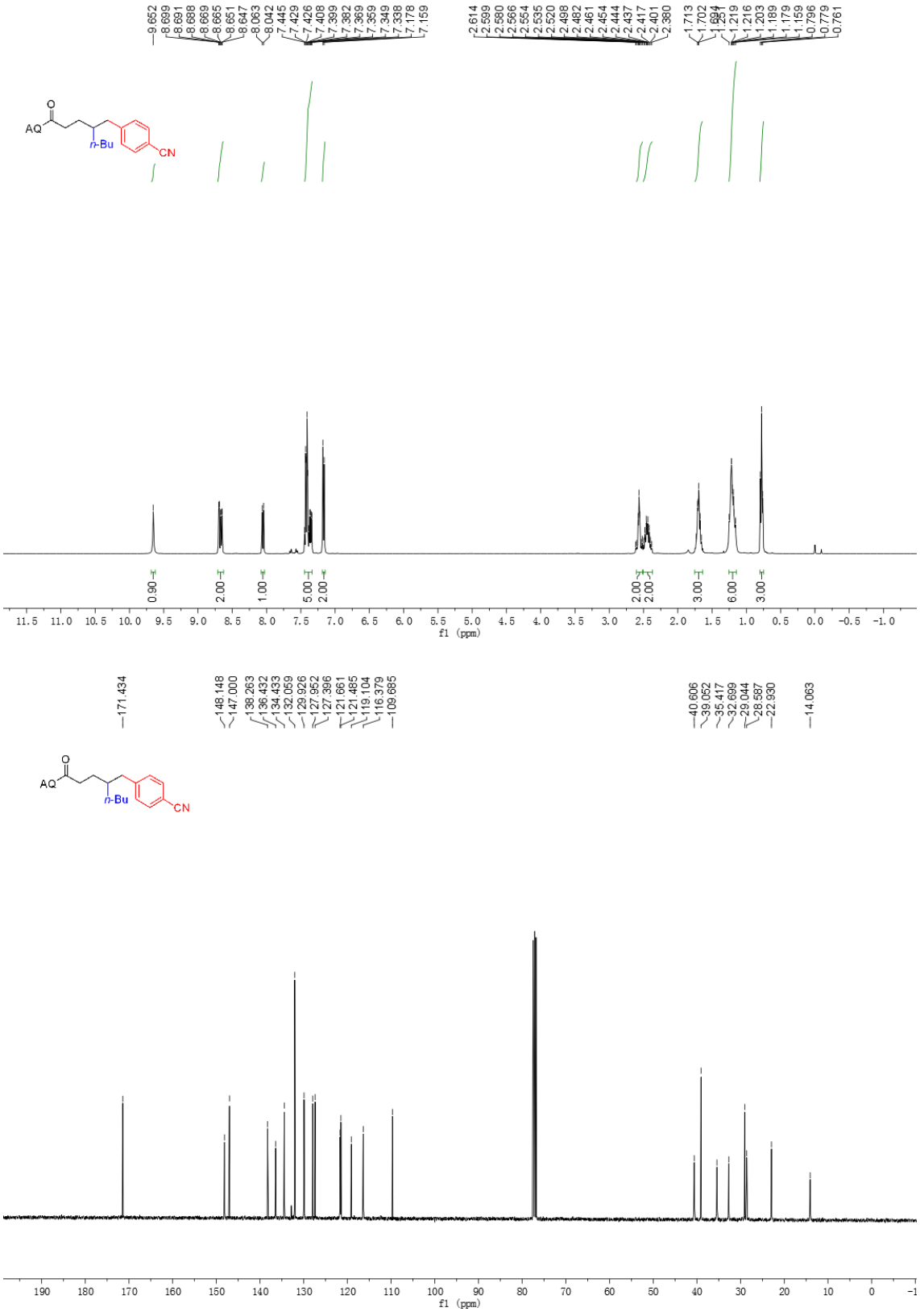
Scheme 17. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2n**



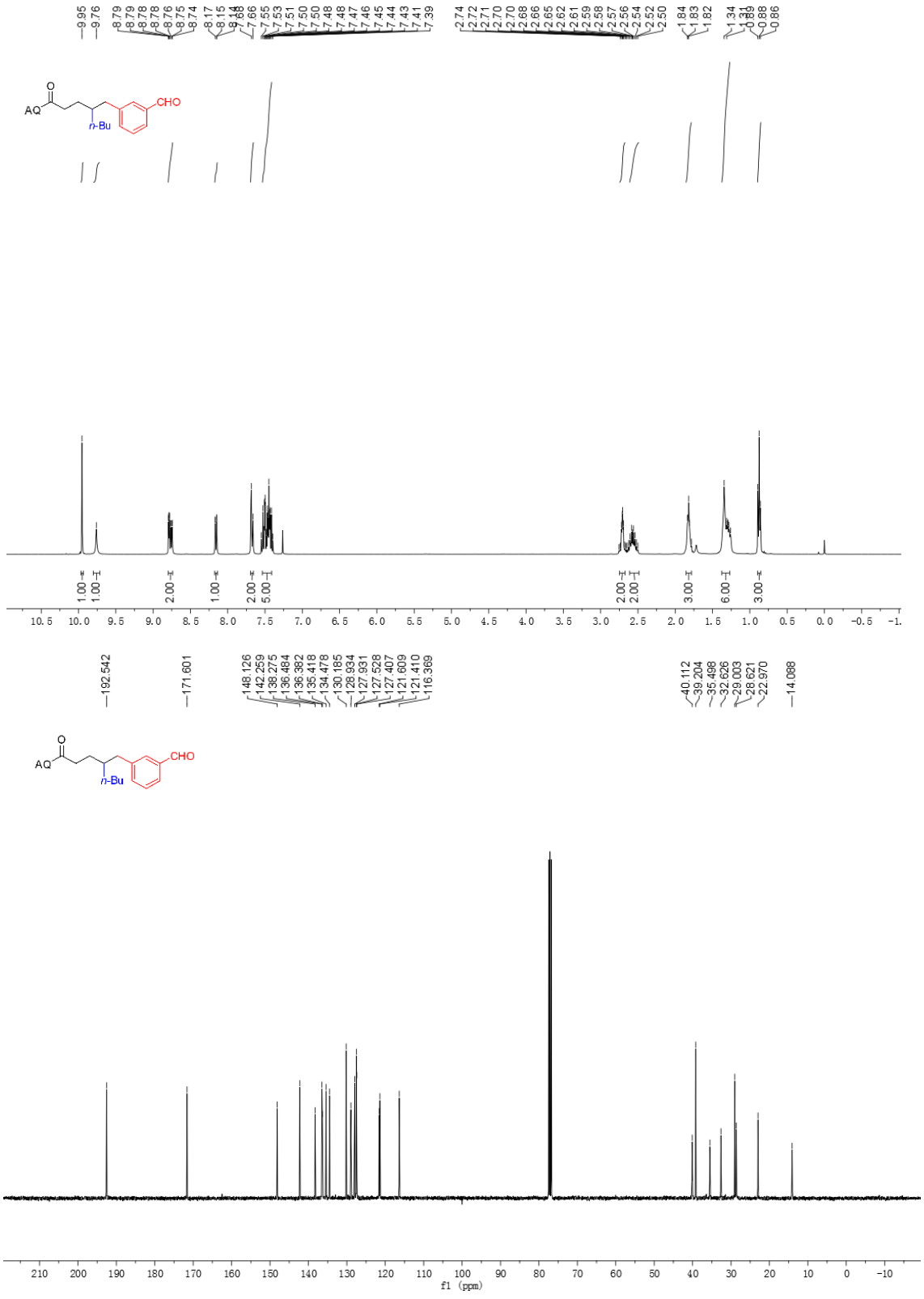
Scheme 18. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2o**



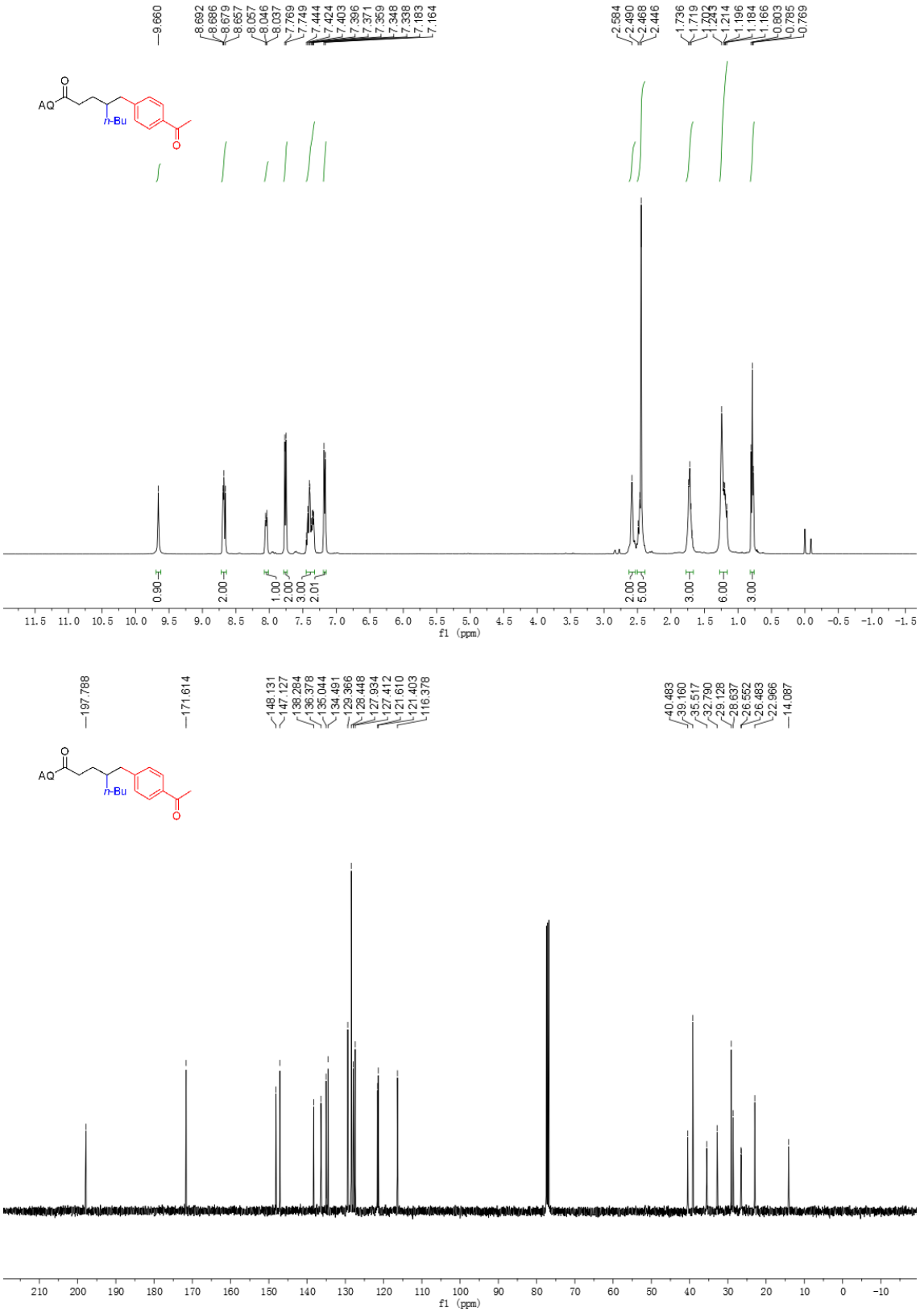
Scheme 19. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2p**



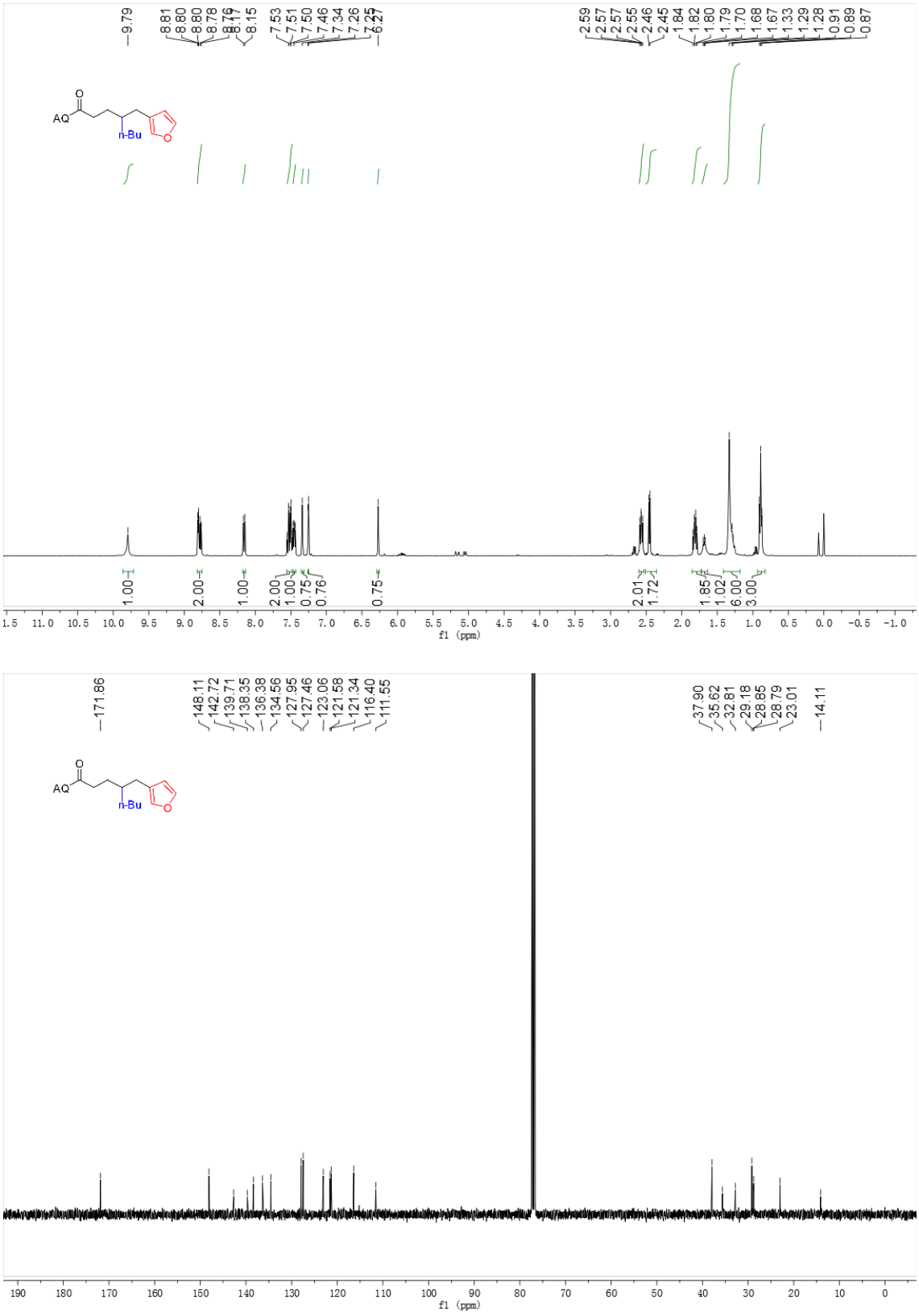
Scheme 20. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2q**



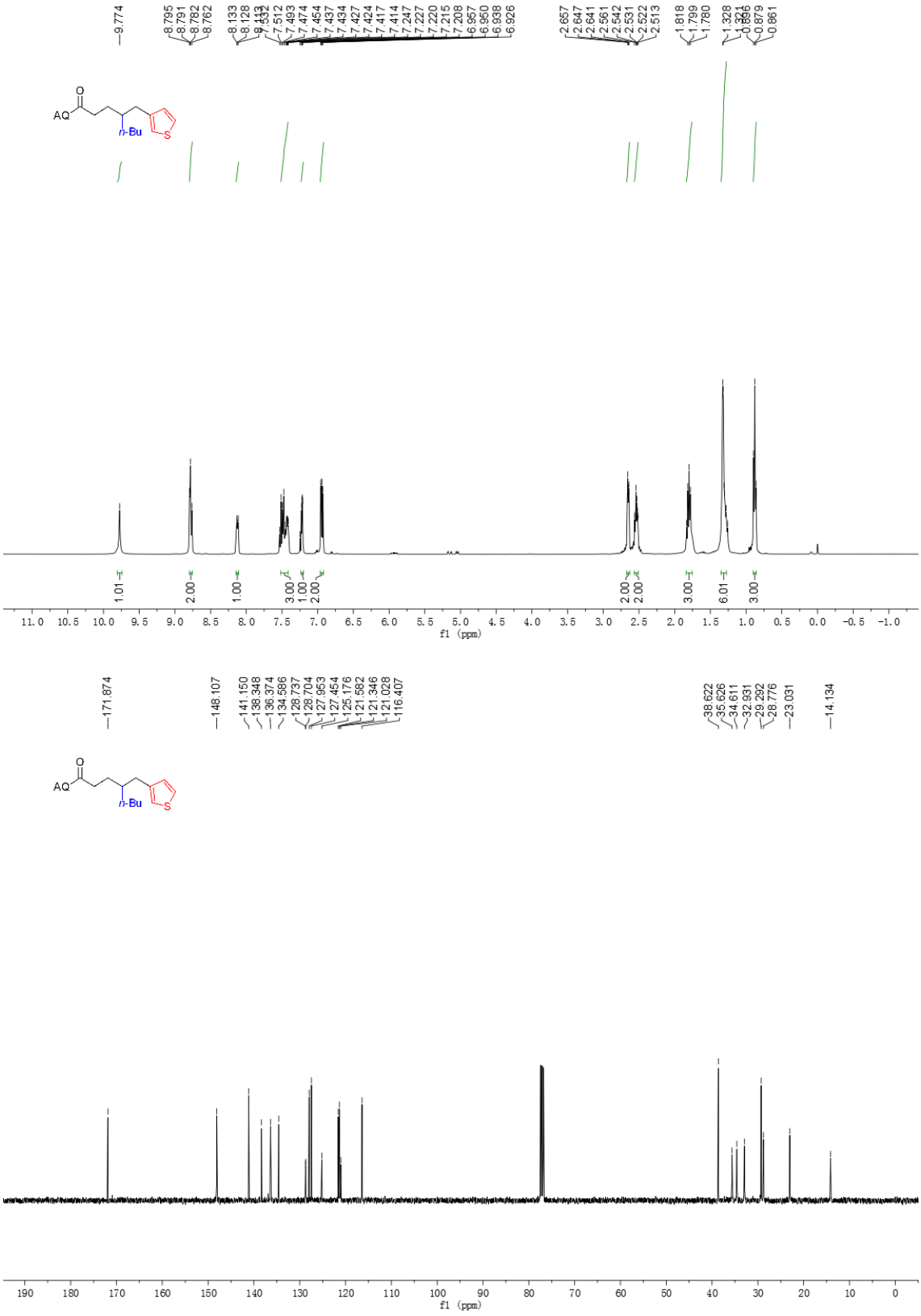
Scheme 21. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2r**



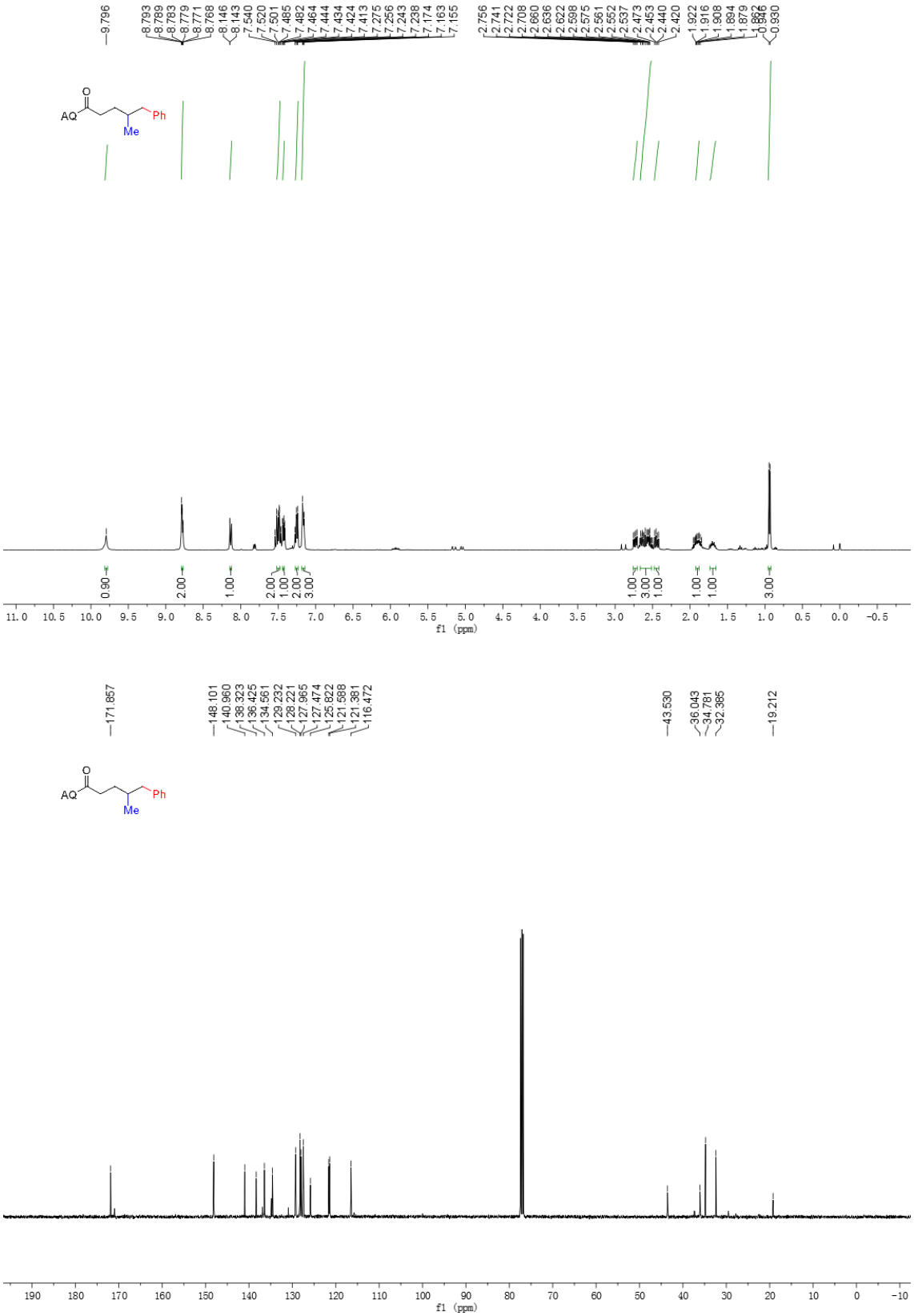
Scheme 22. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2s**



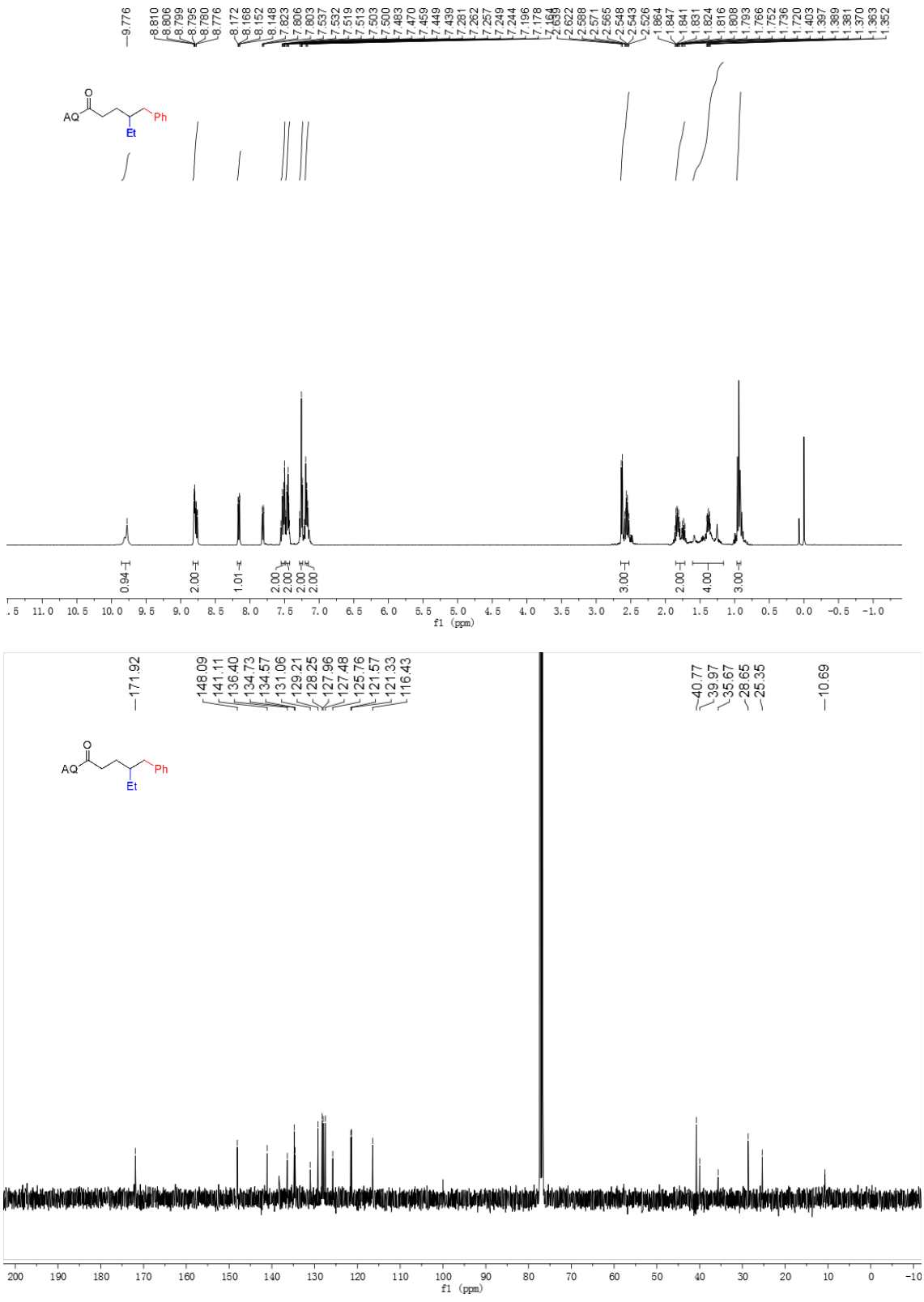
Scheme 23. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2t**



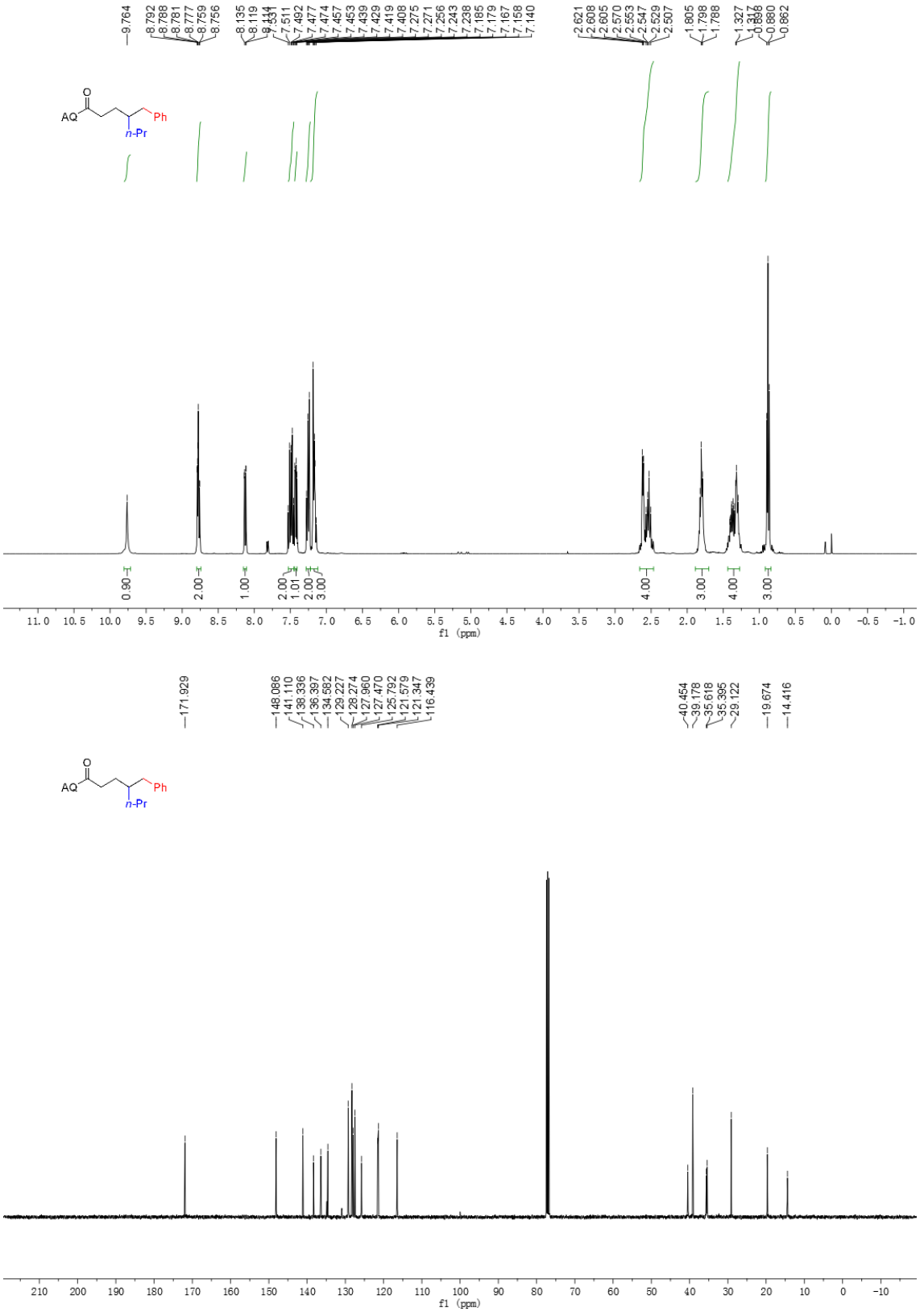
Scheme 24. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2u**



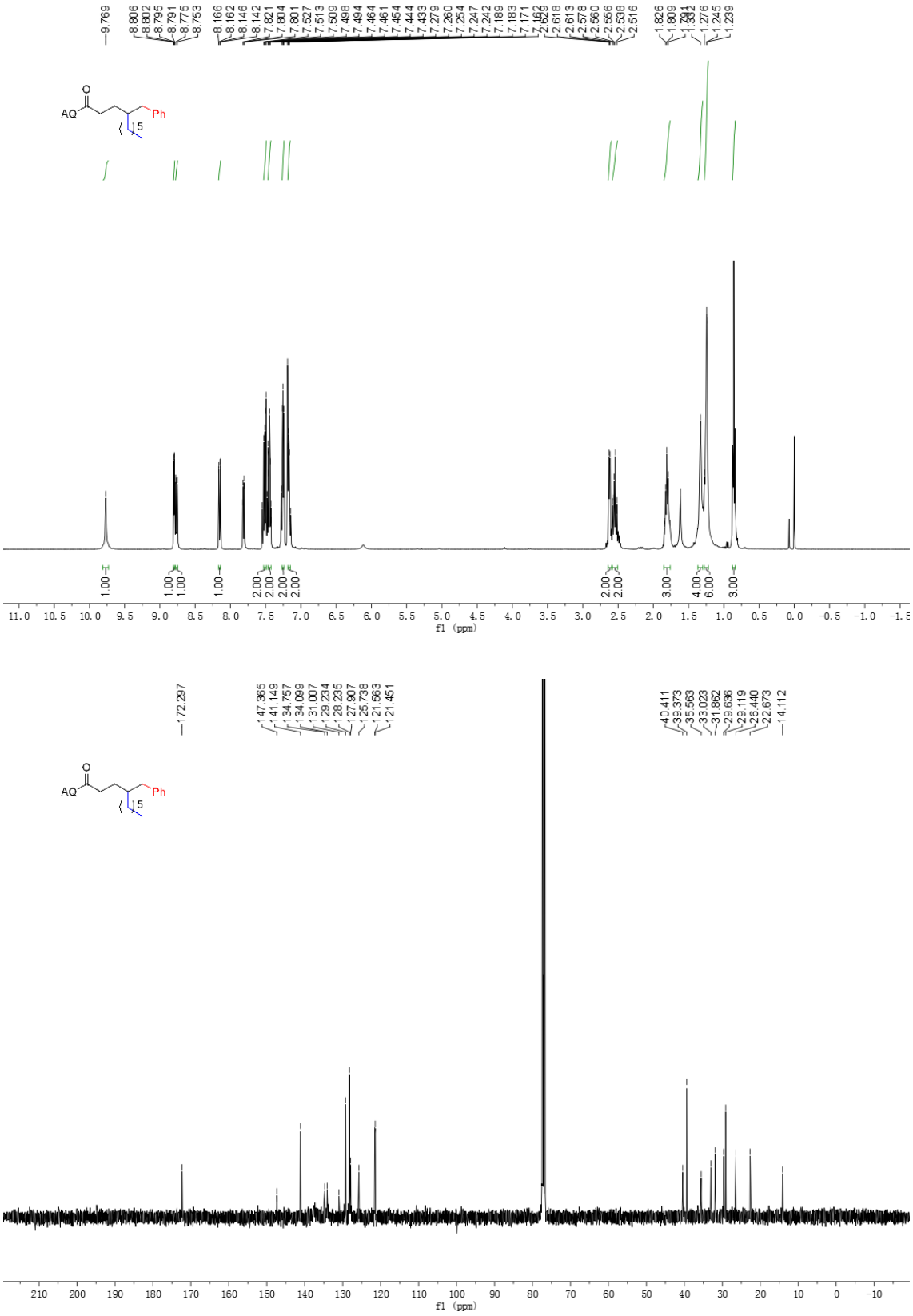
Scheme 25. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2v**



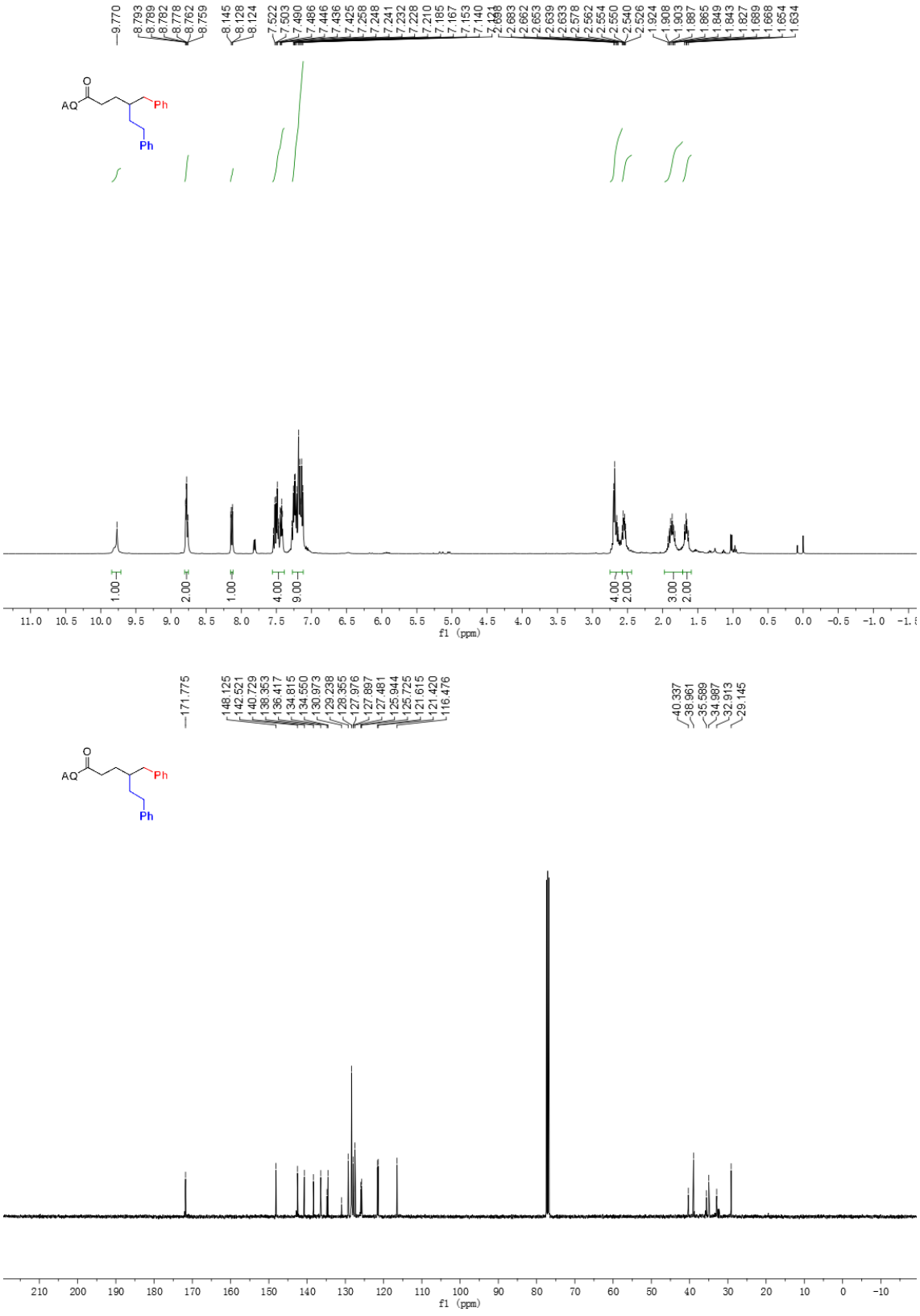
Scheme 26. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2w**



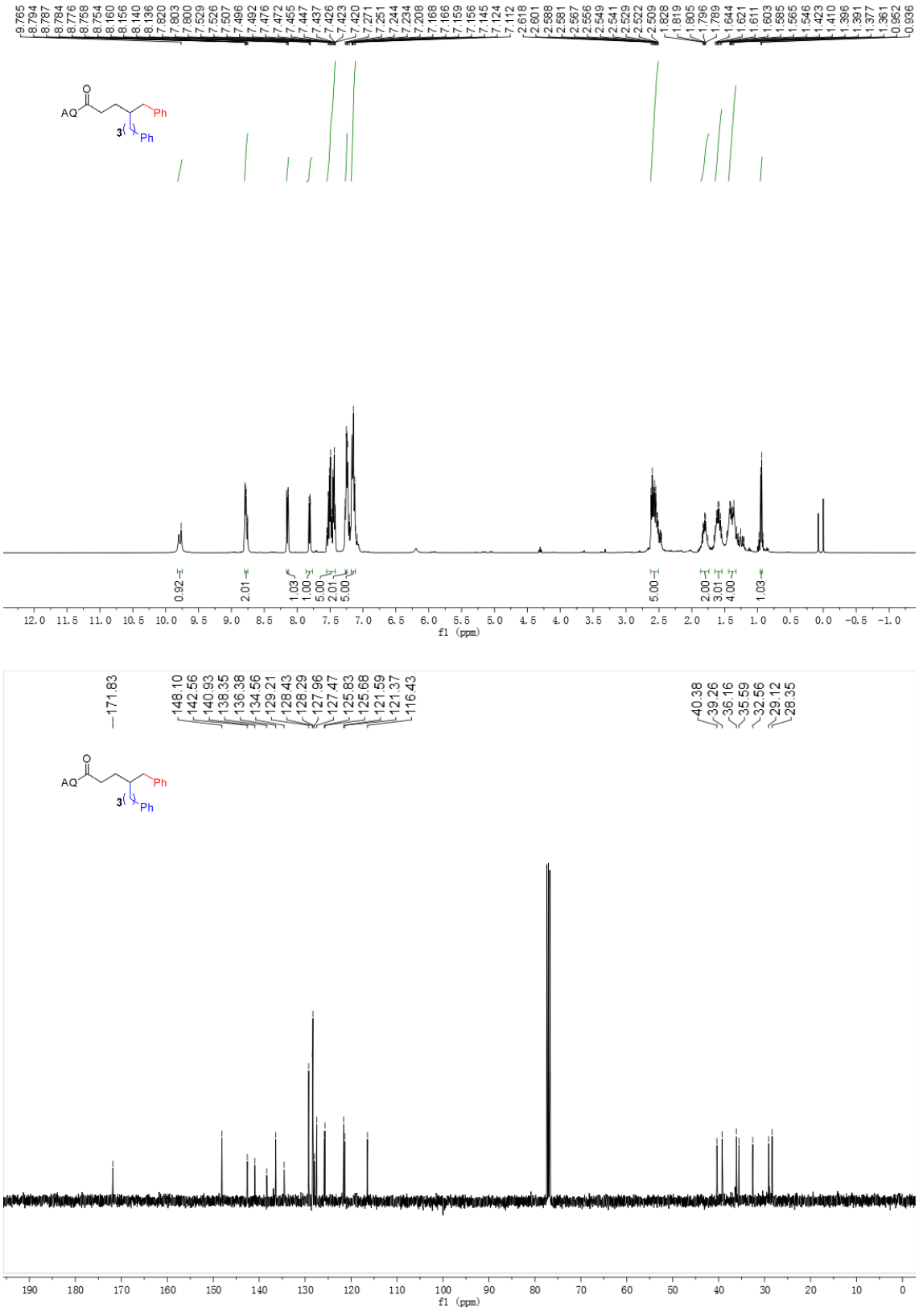
Scheme 27. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2x**



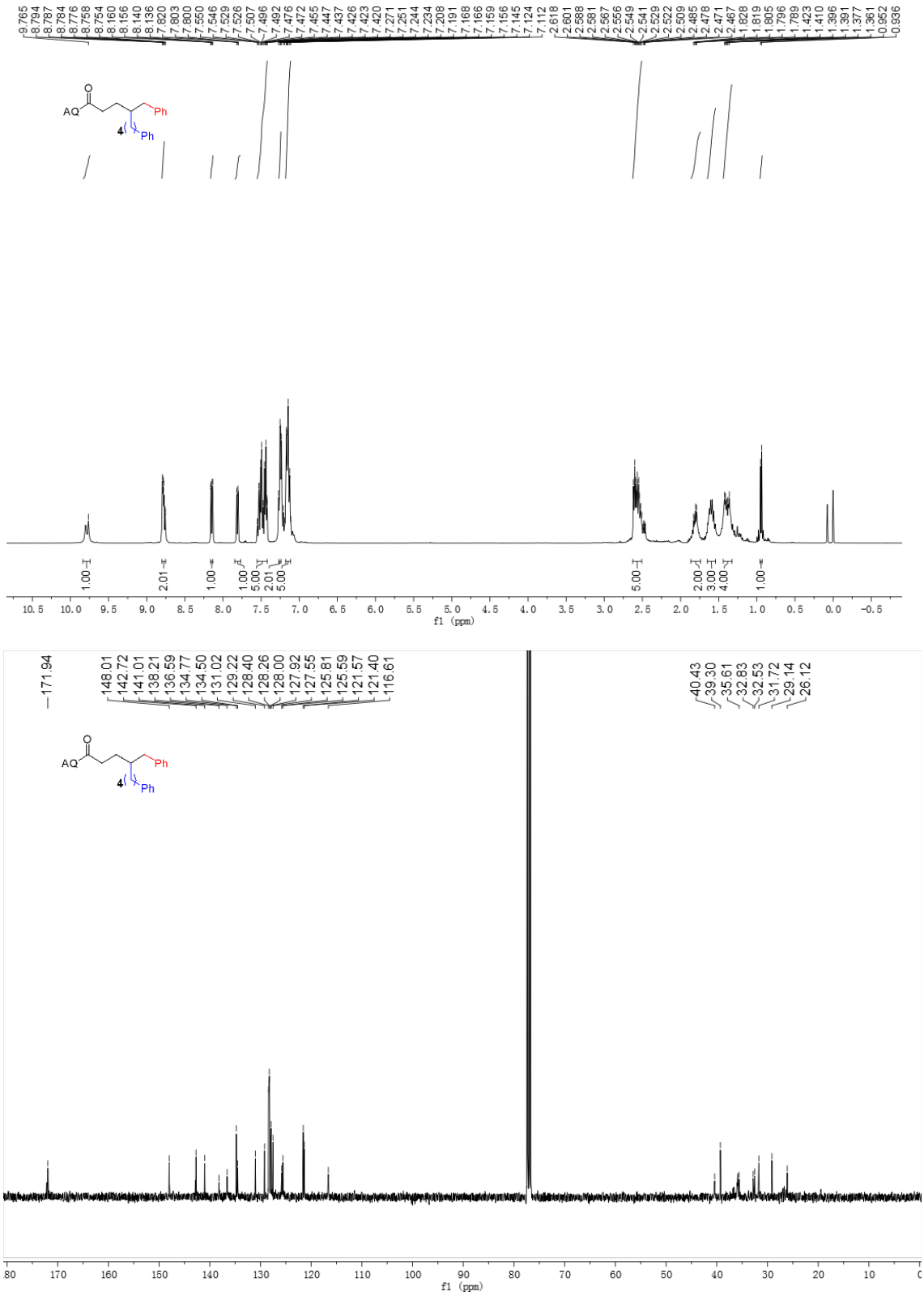
Scheme 28. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2y**



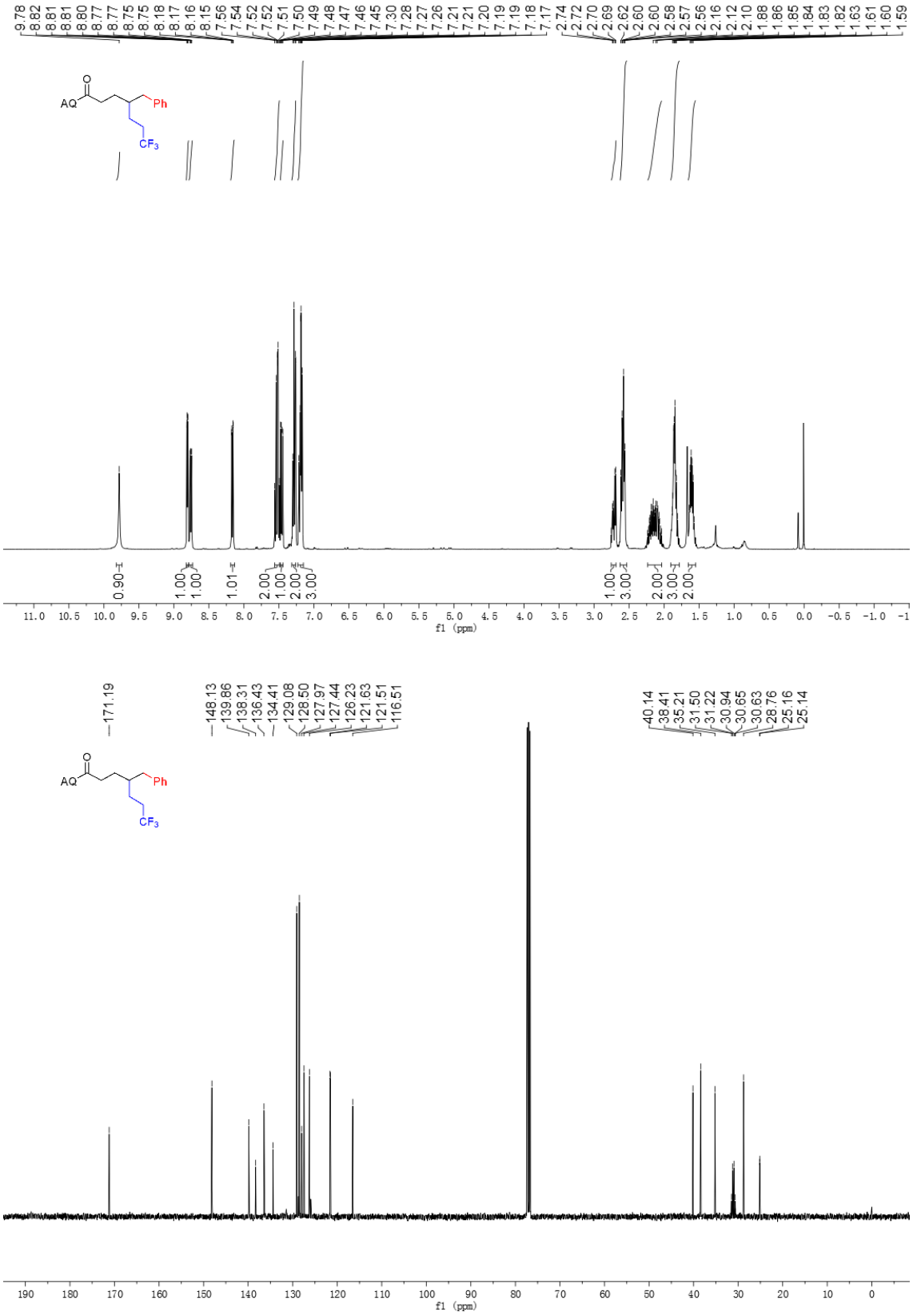
Scheme 29. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2z**



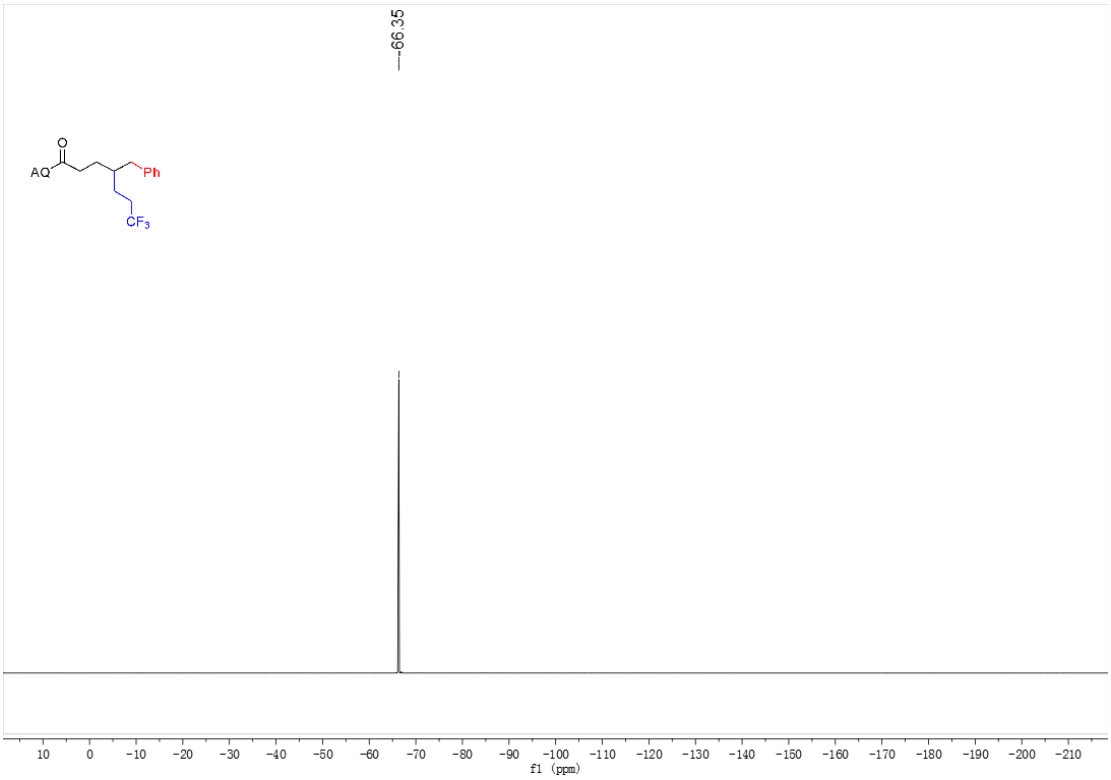
Scheme 30. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2aa**



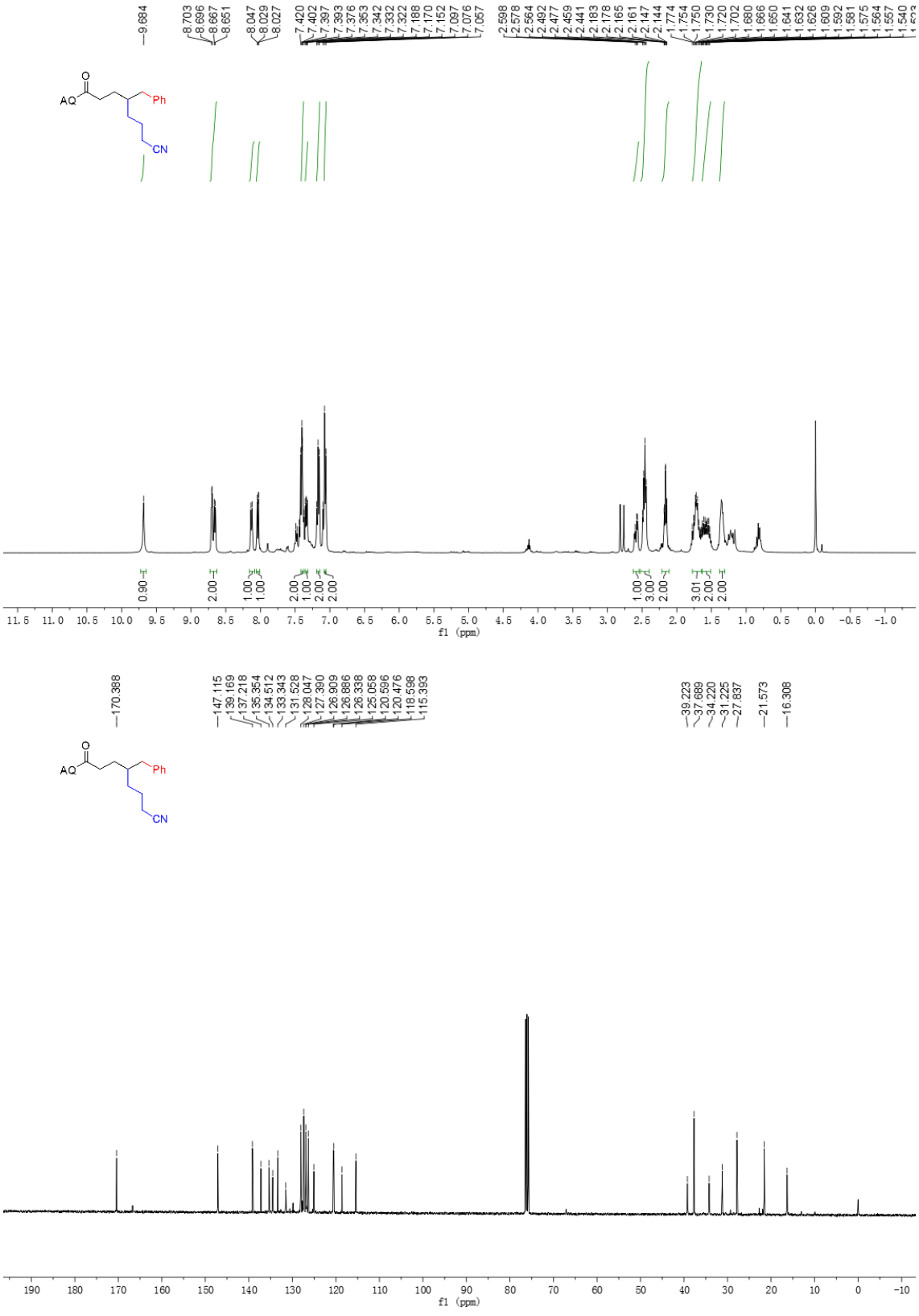
Scheme 31. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ab**



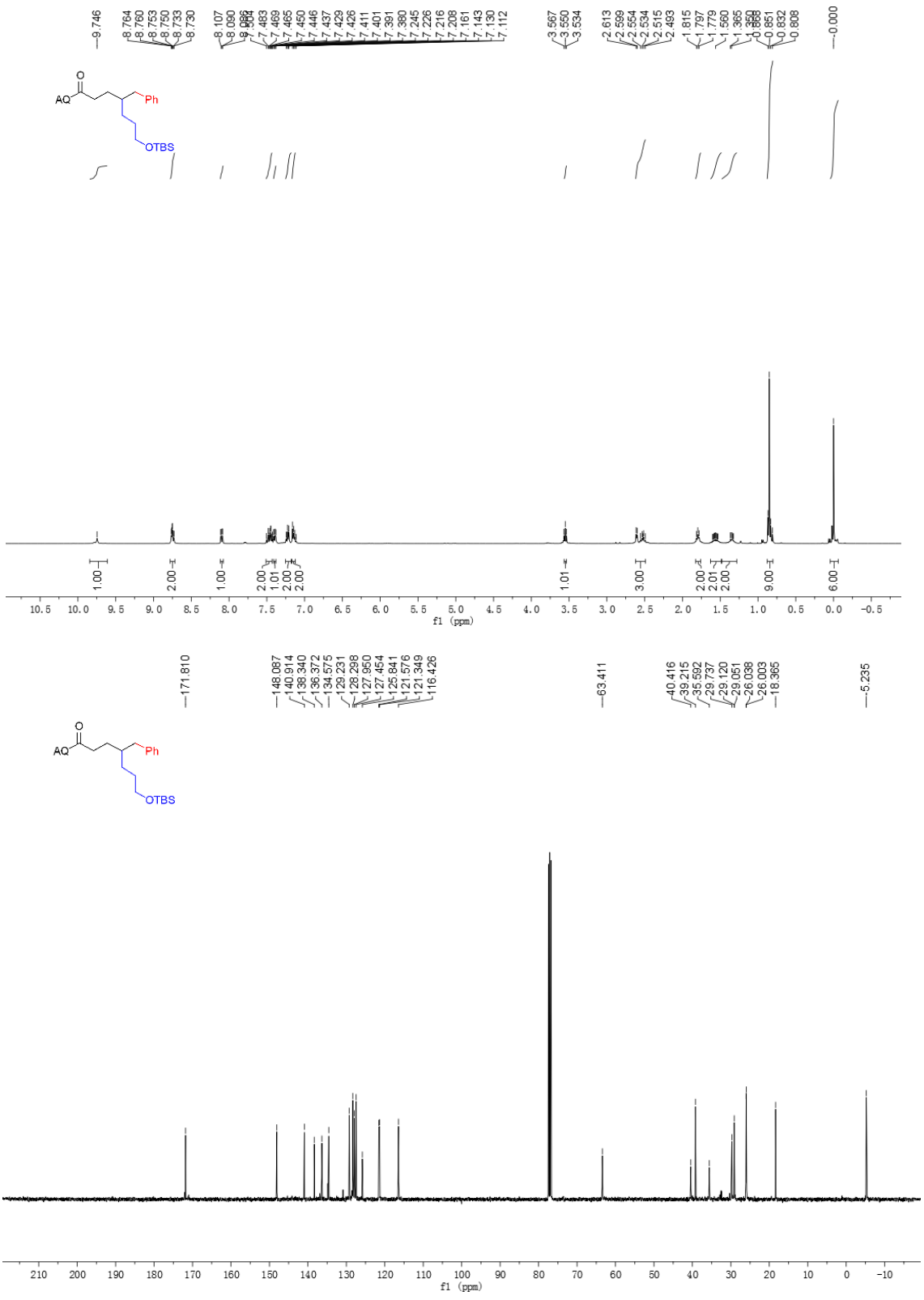
Scheme 32. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ac**



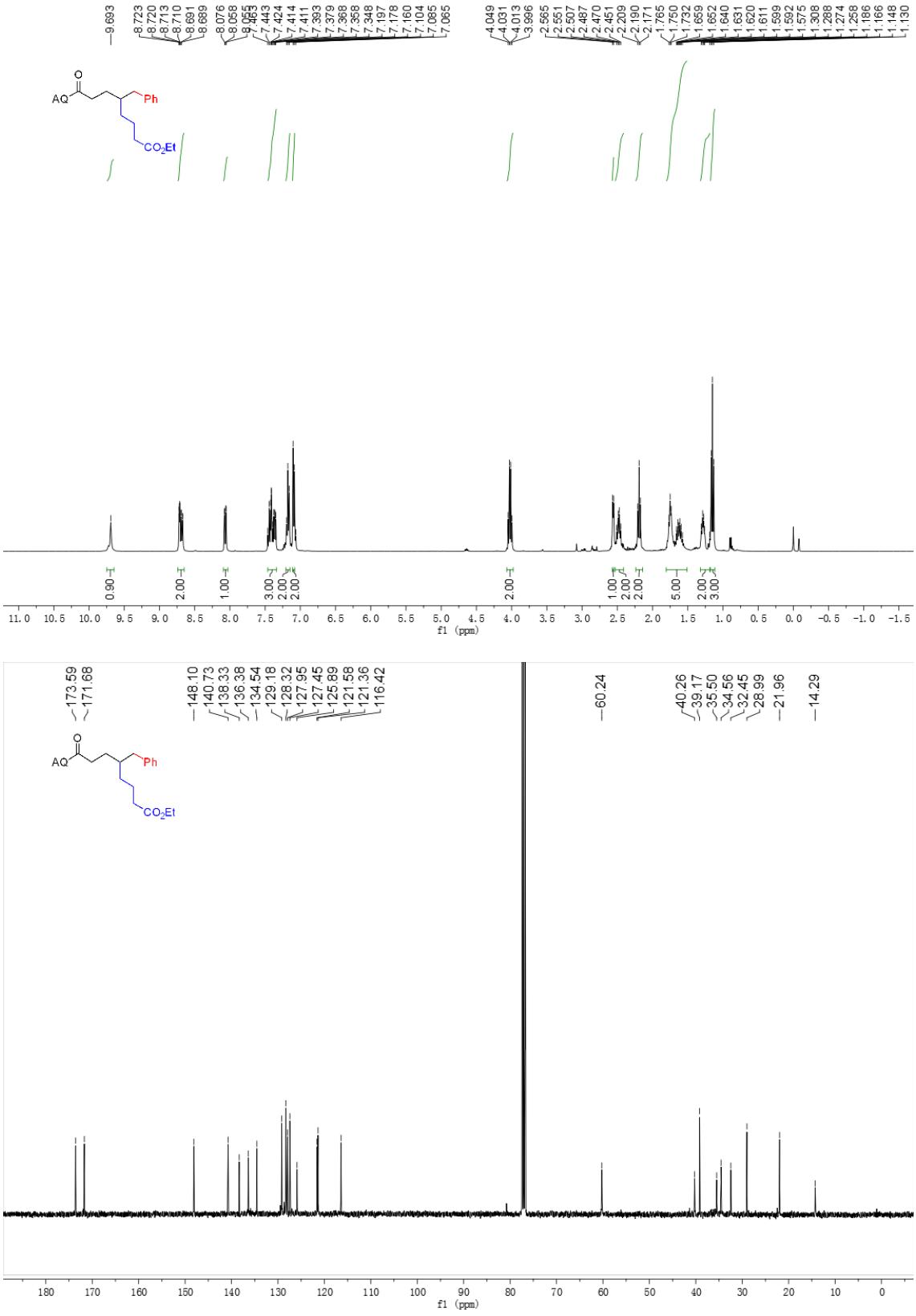
Scheme 33. ^{19}F NMR (376 MHz, $CDCl_3$) spectra of **2ac**



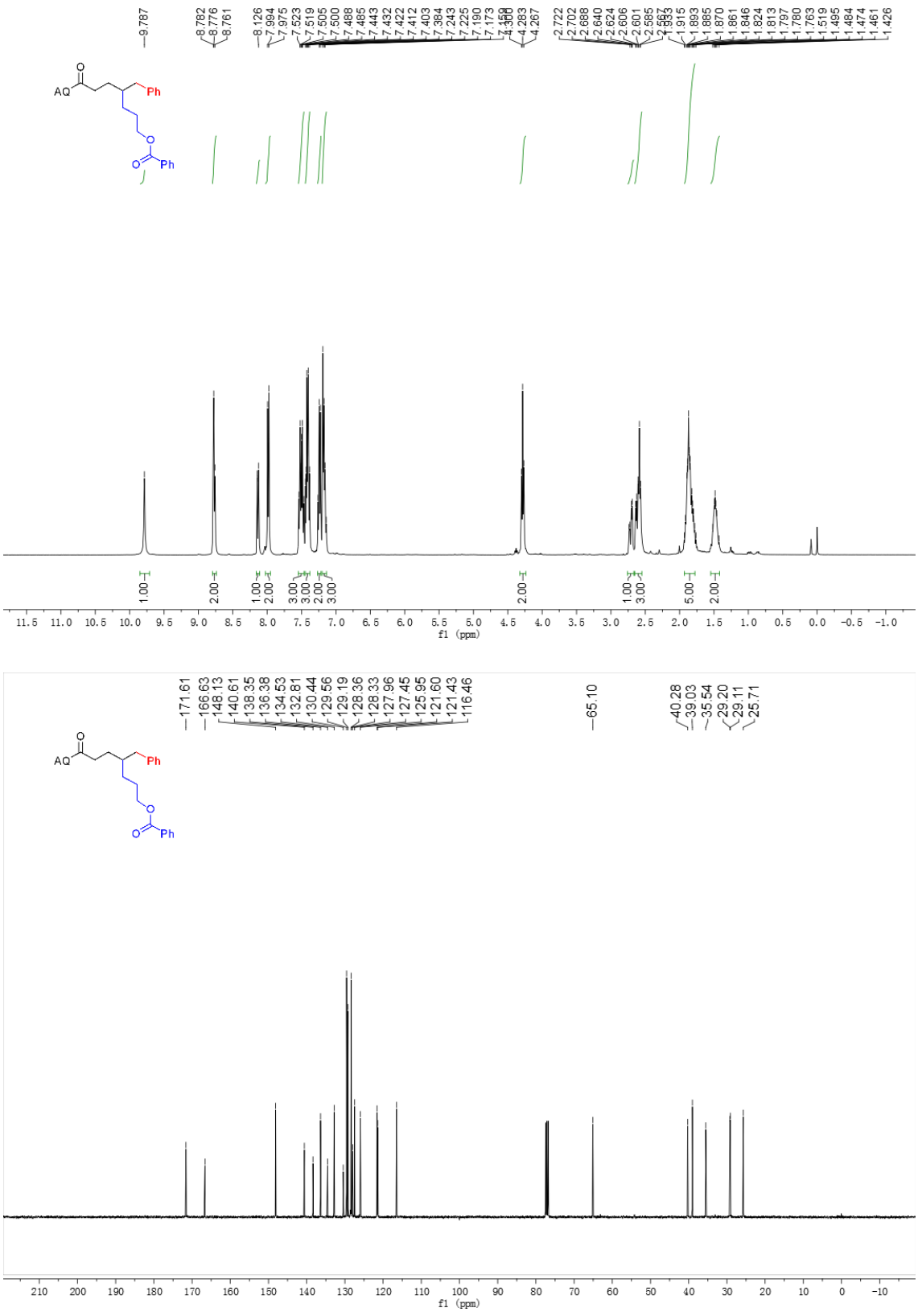
Scheme 34. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR(101 MHz, $CDCl_3$) spectra of **2ad**



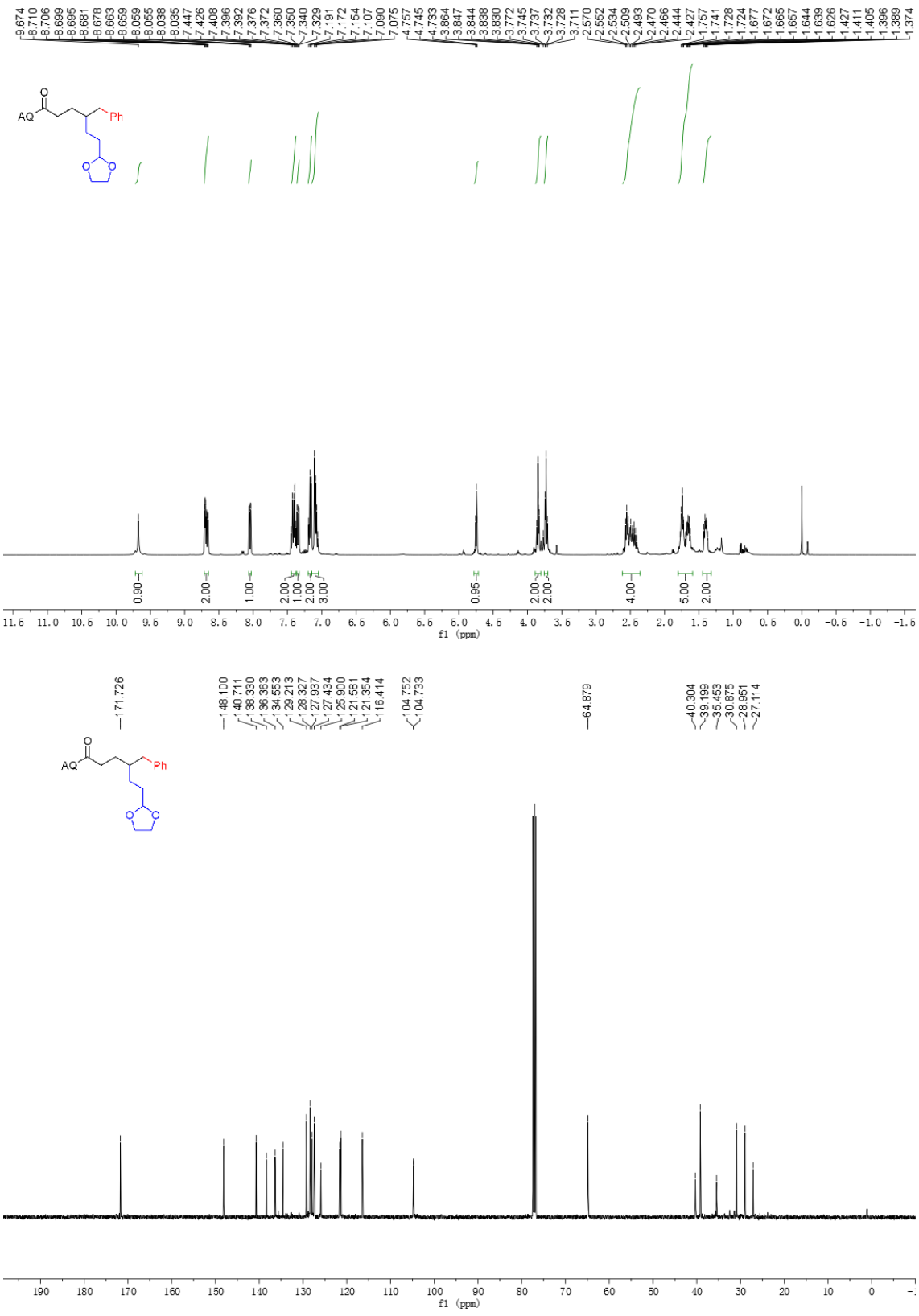
Scheme 35. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ae**



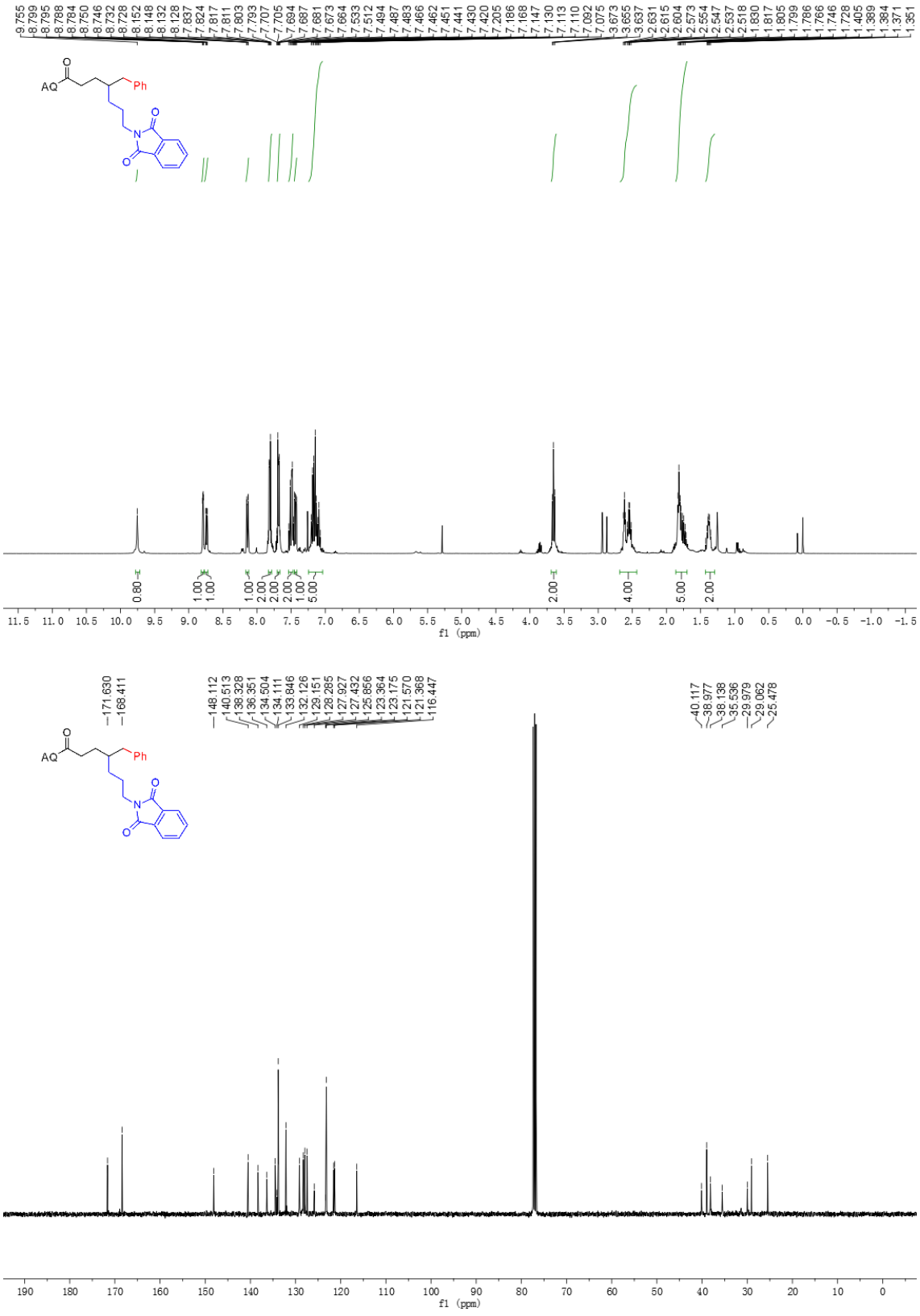
Scheme 36. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2af**



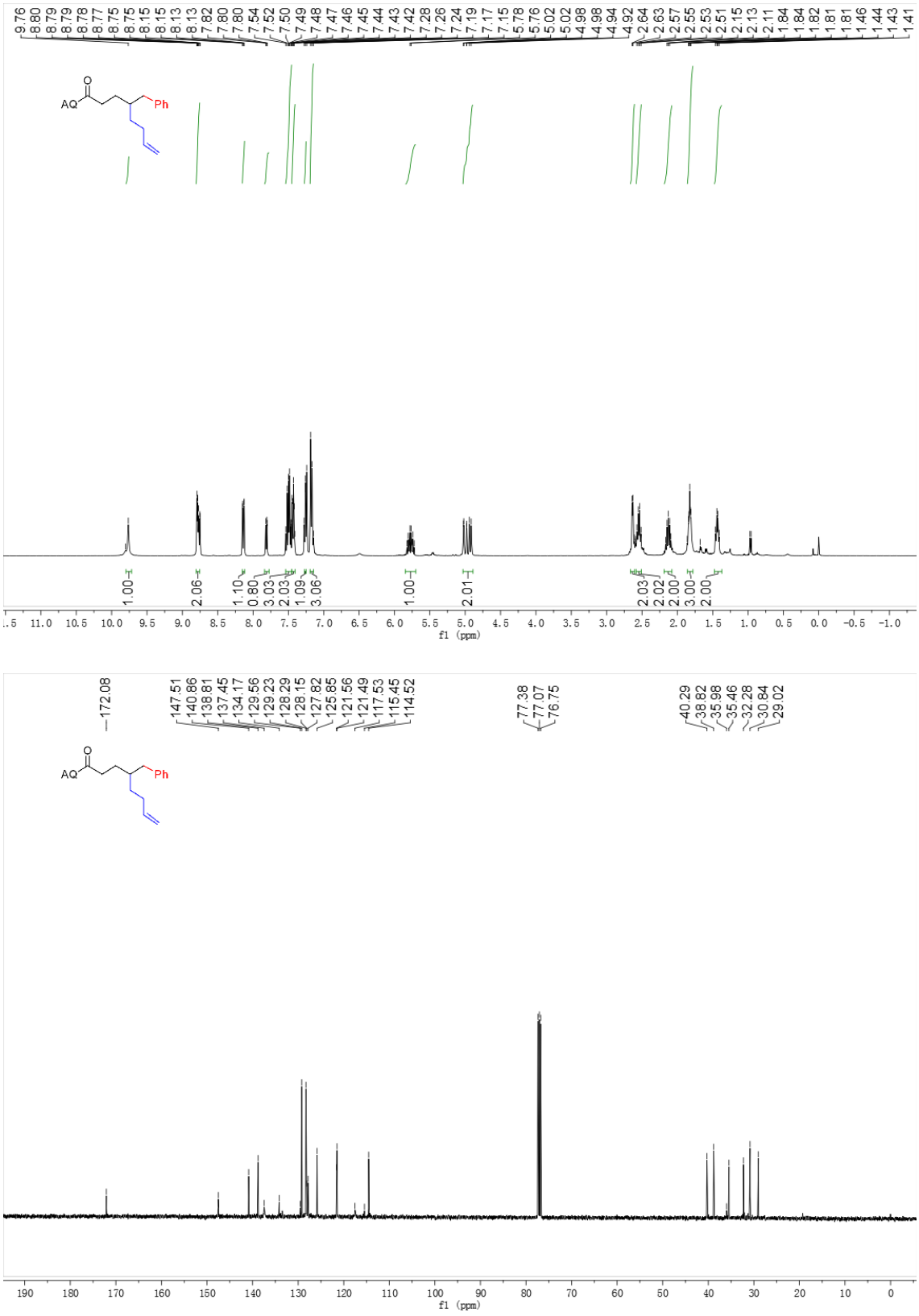
Scheme 37. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ag**



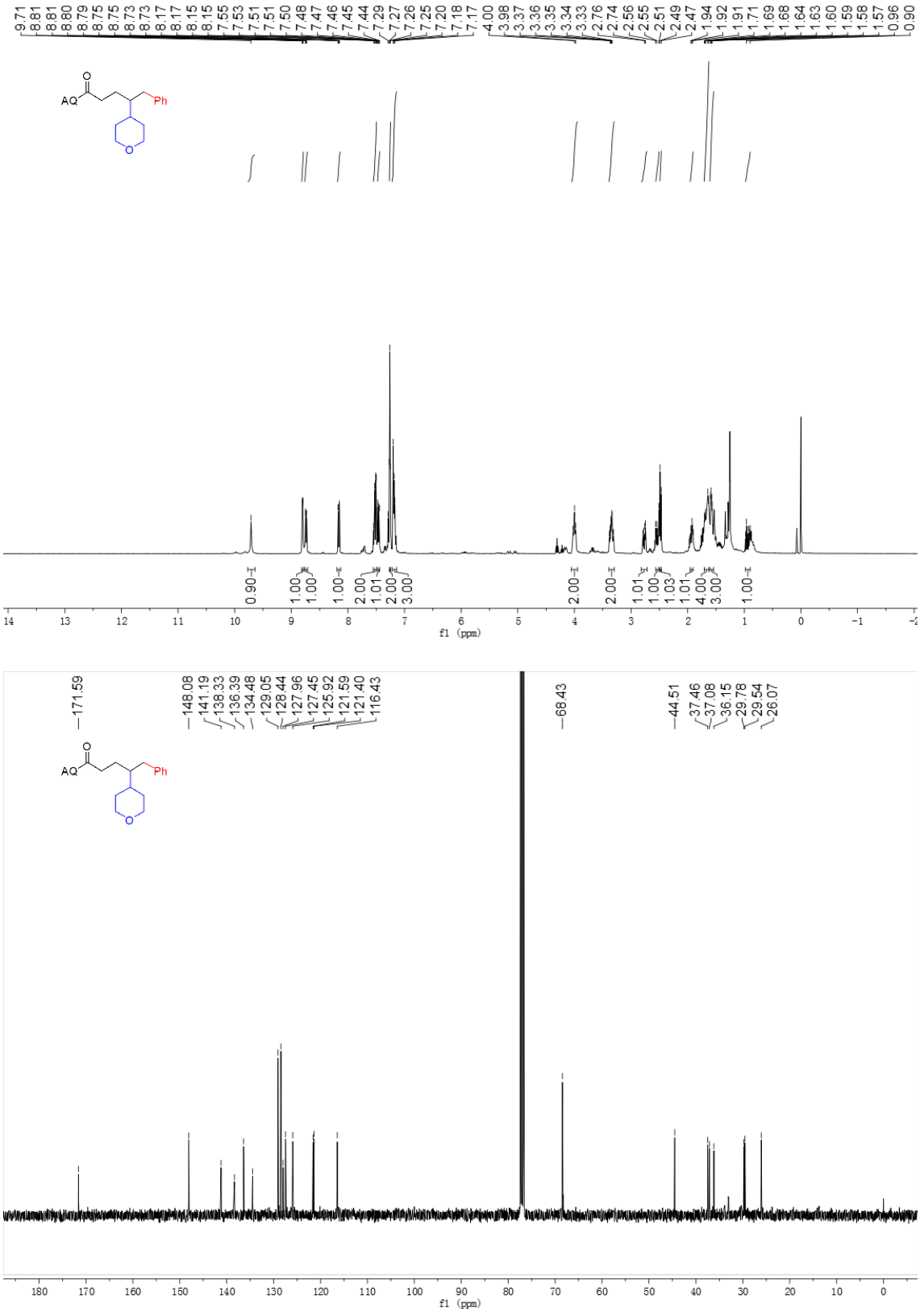
Scheme 38. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ah**



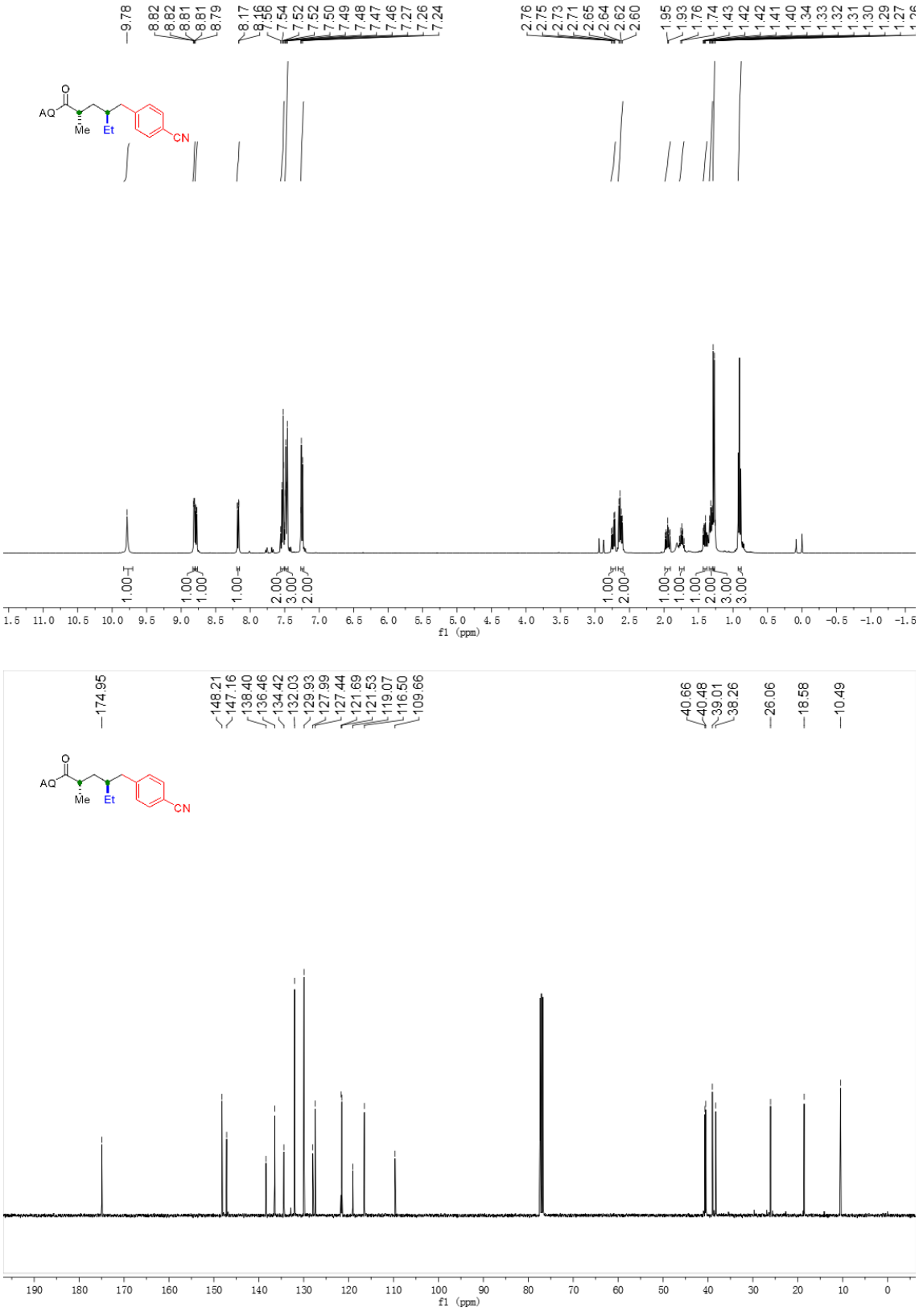
Scheme 39. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ai**



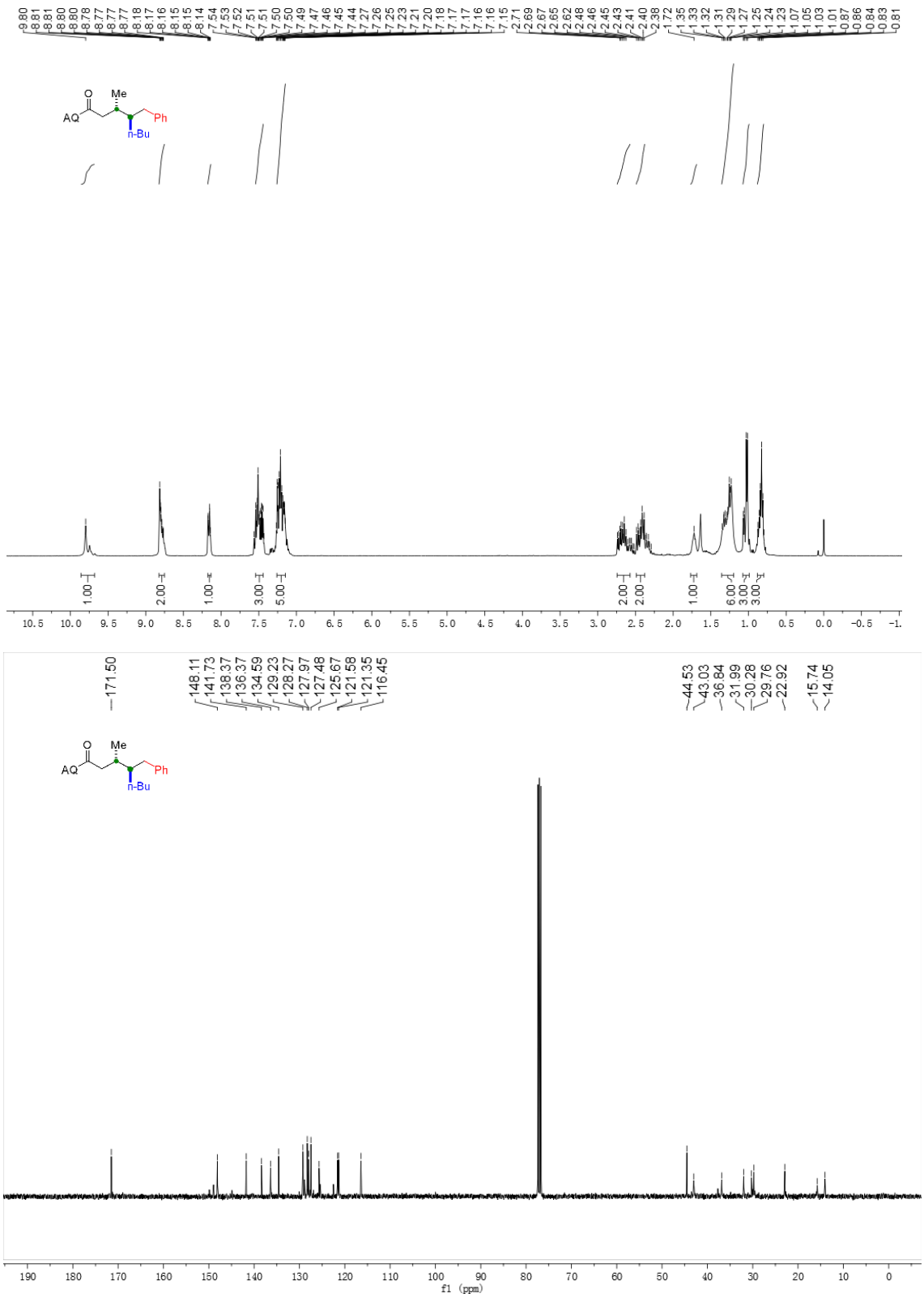
Scheme 40. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2aj**



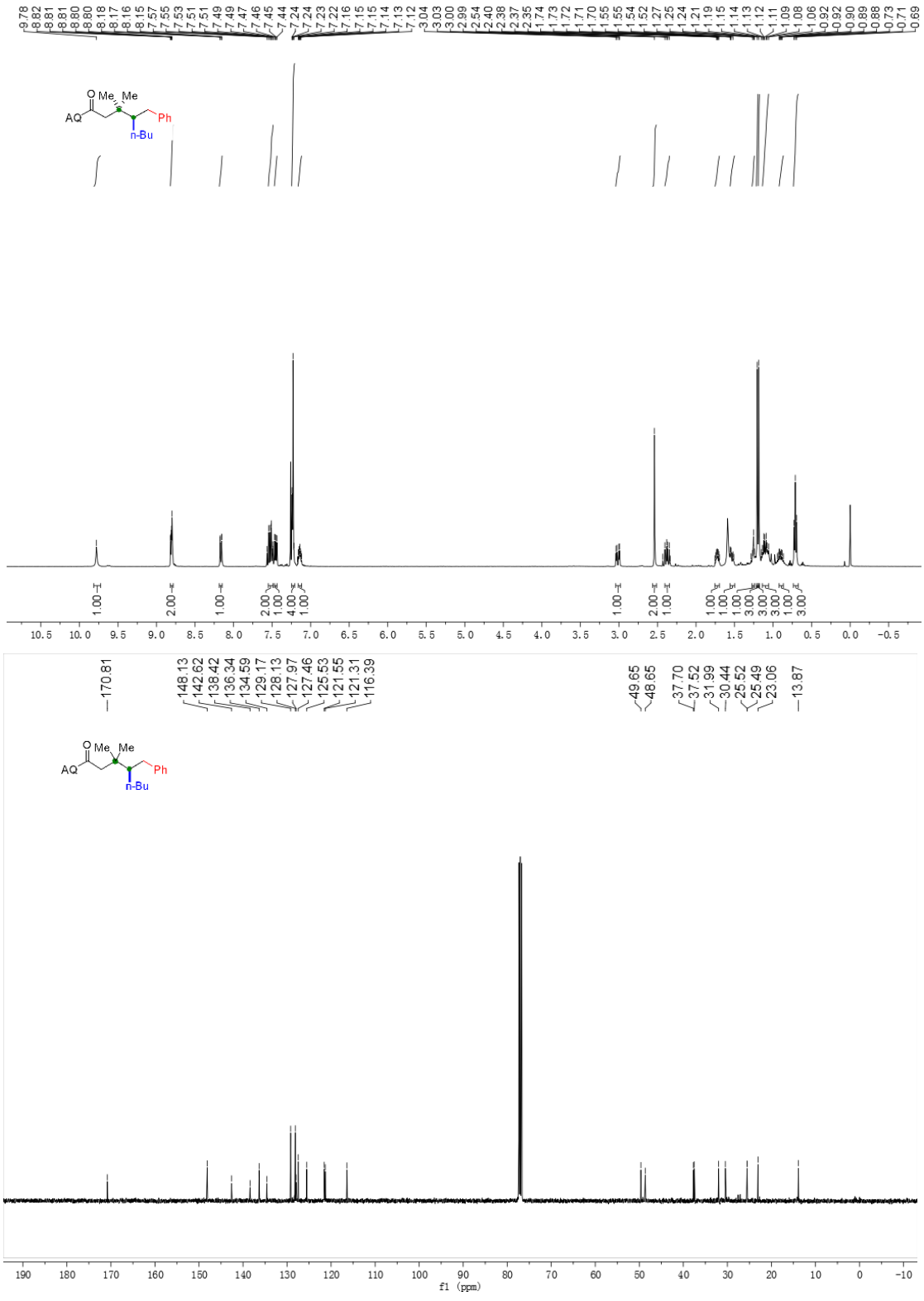
Scheme 41. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ak**



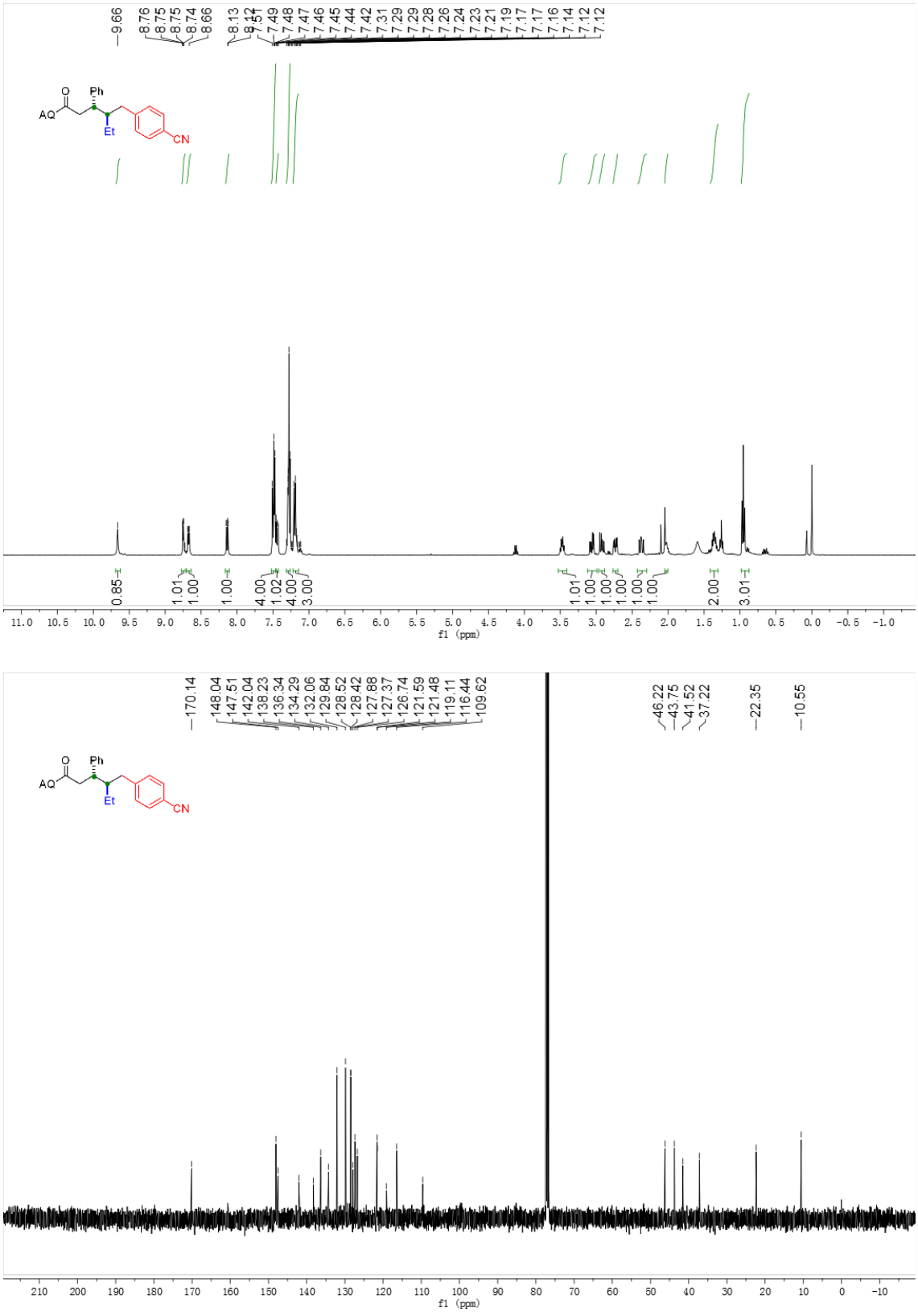
Scheme 42. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2al**



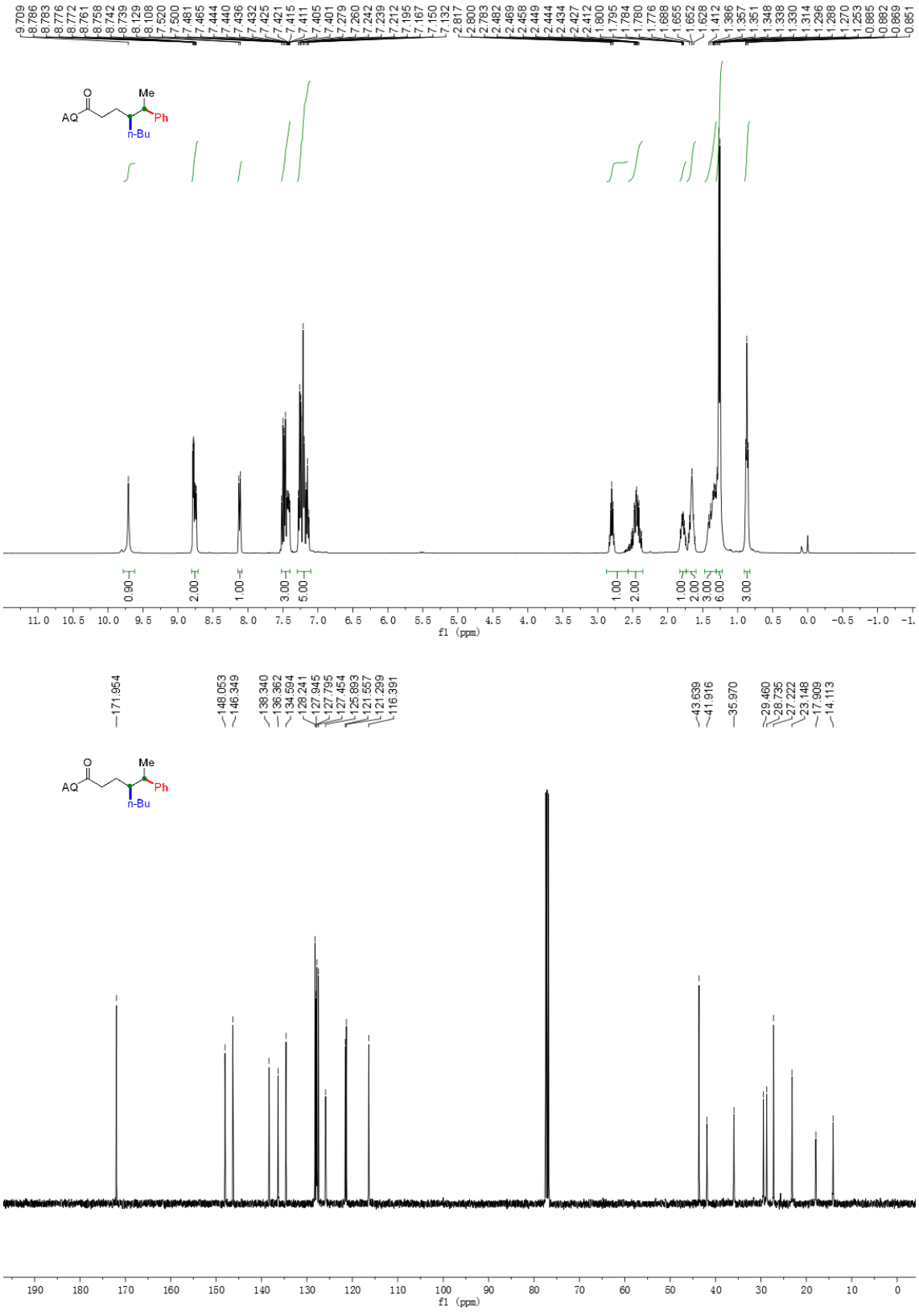
Scheme 43. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2am**



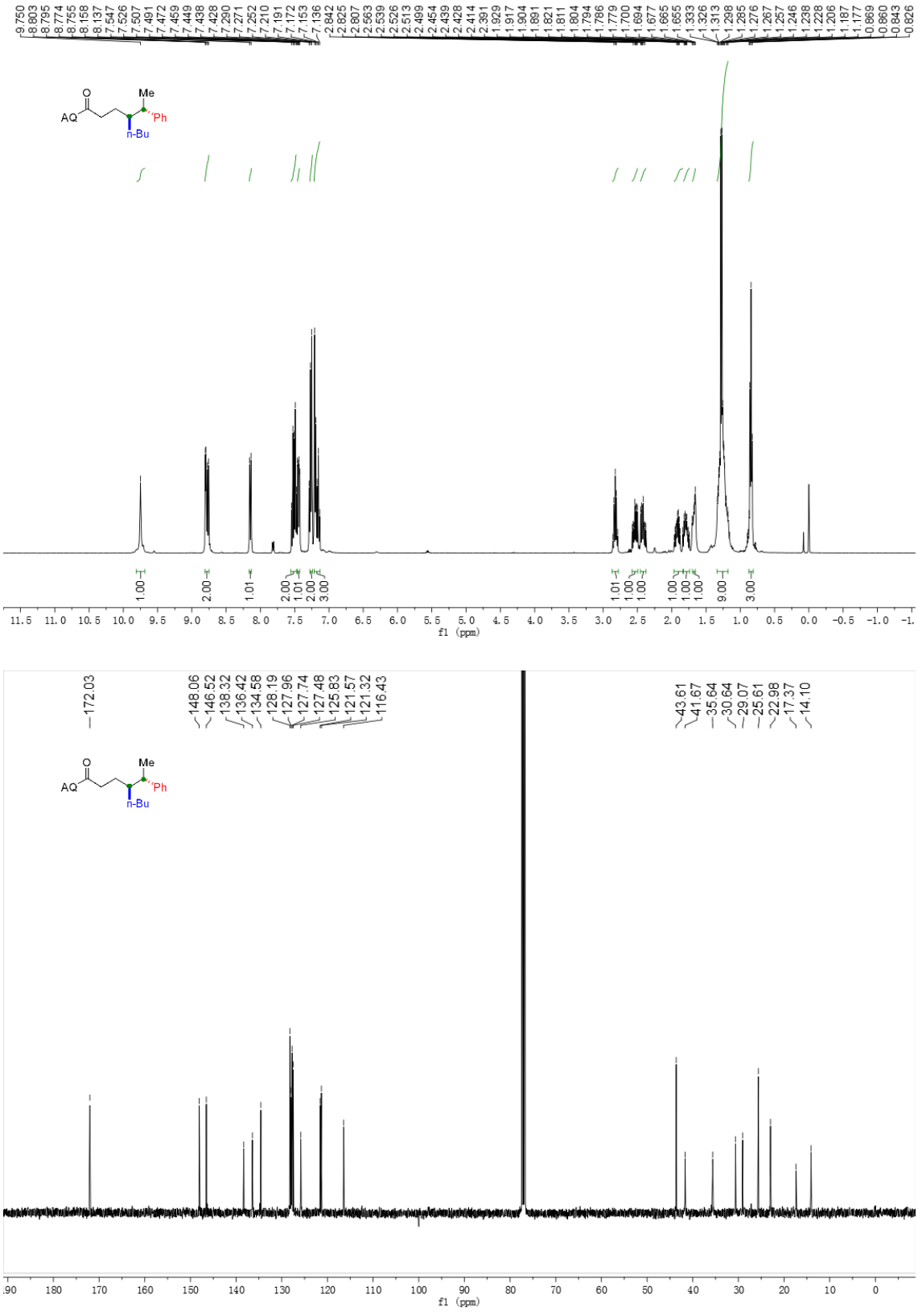
Scheme 44. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2an**



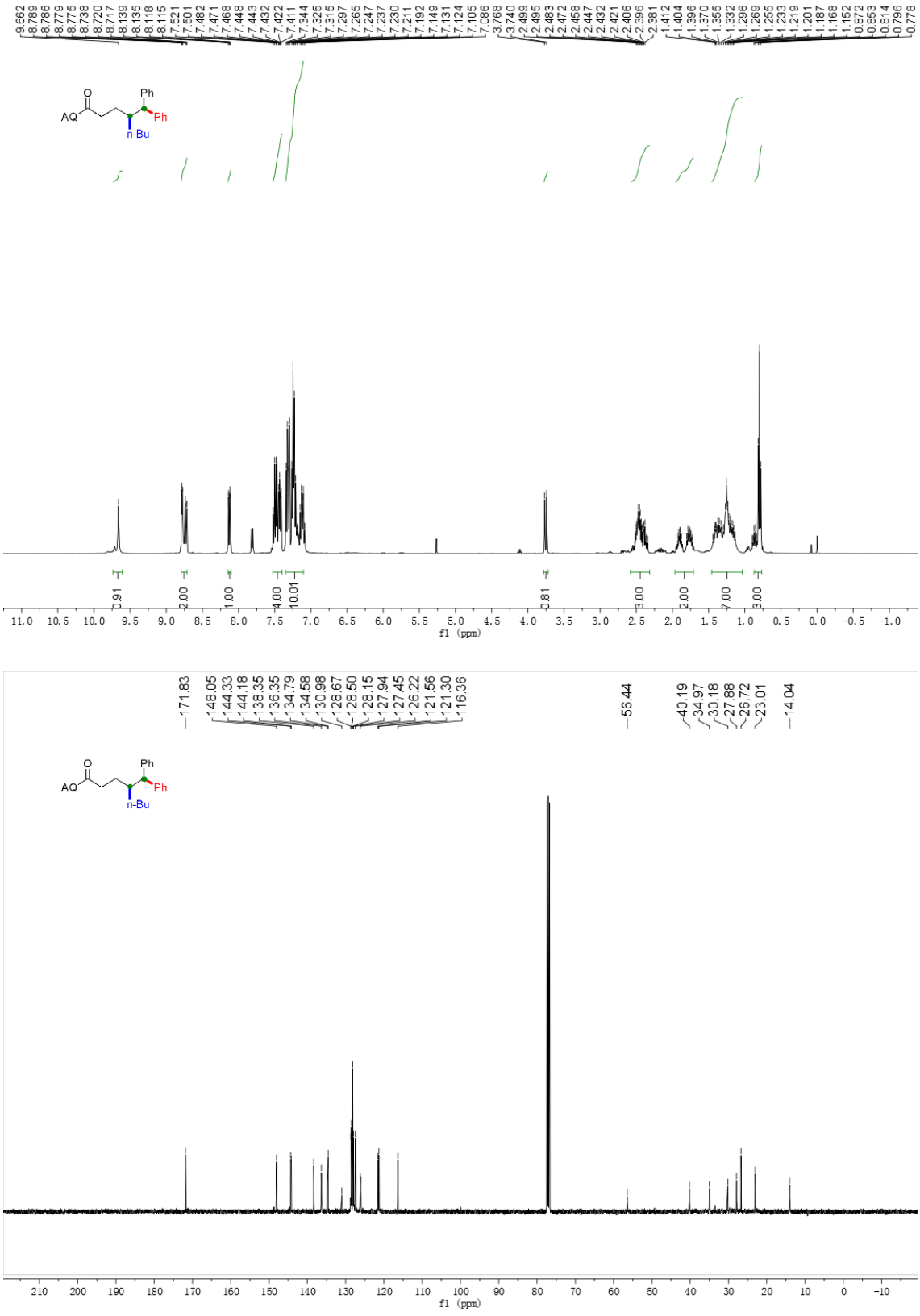
Scheme 45. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ao**



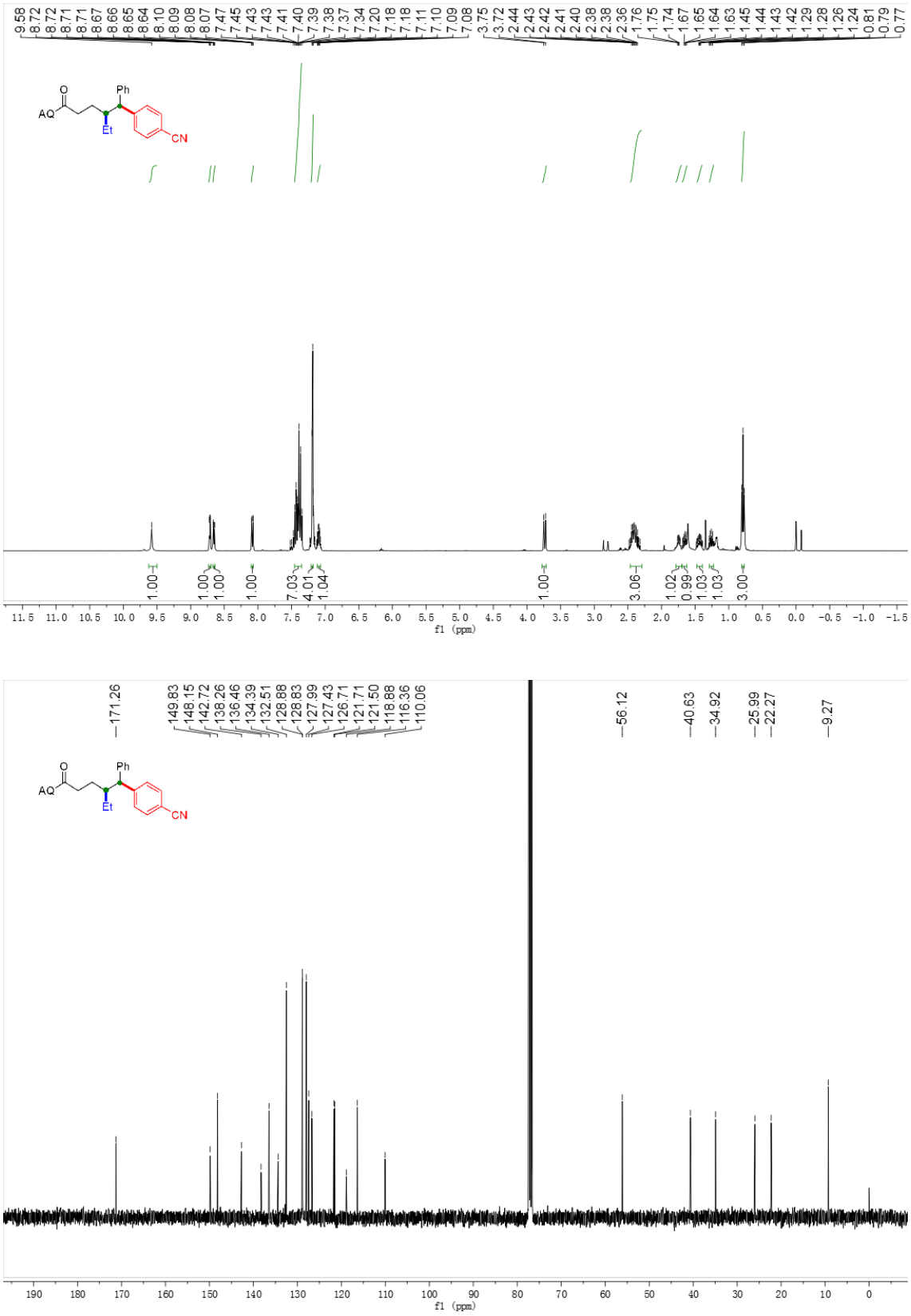
Scheme 46. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ap**



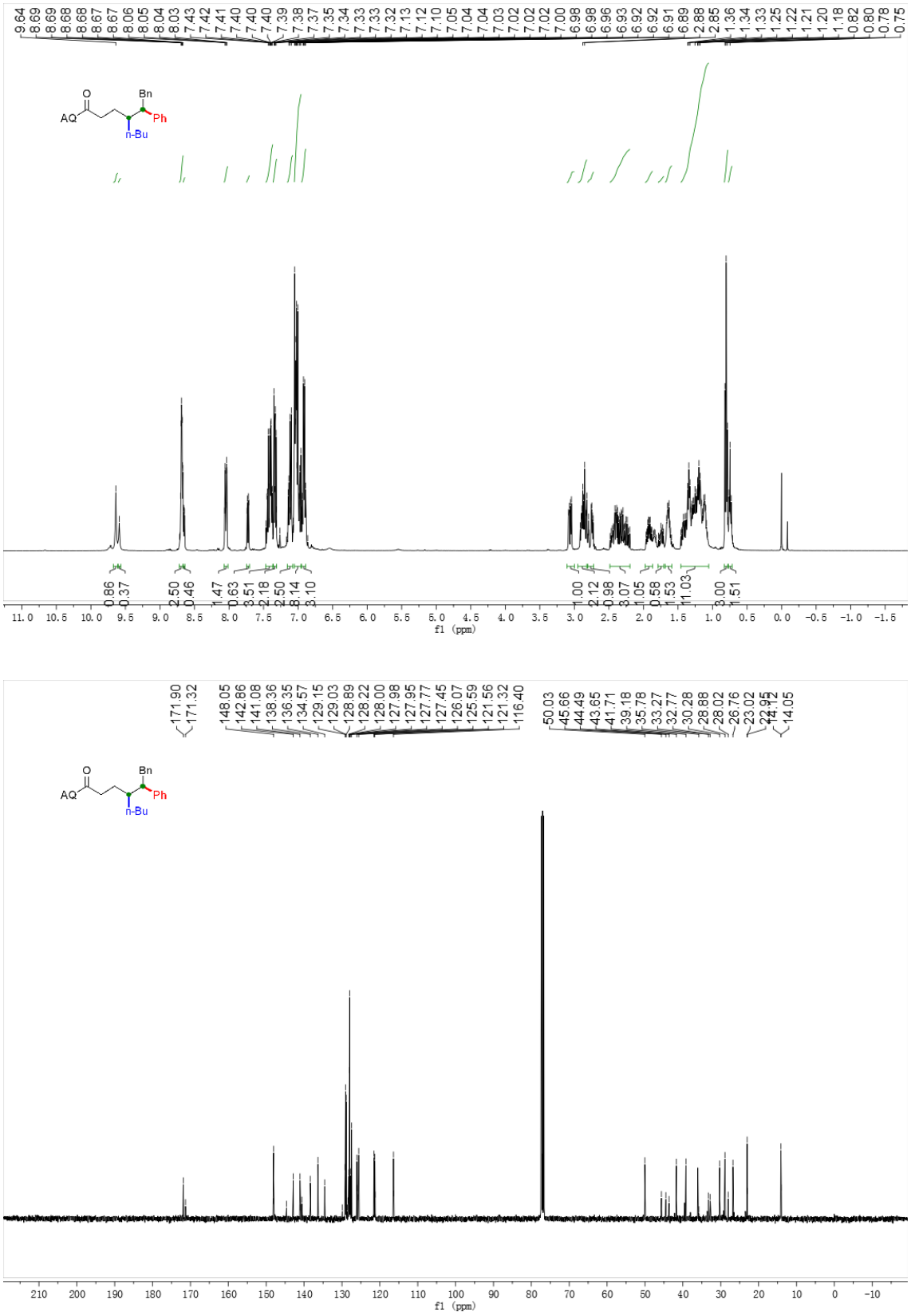
Scheme 47. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2aq**



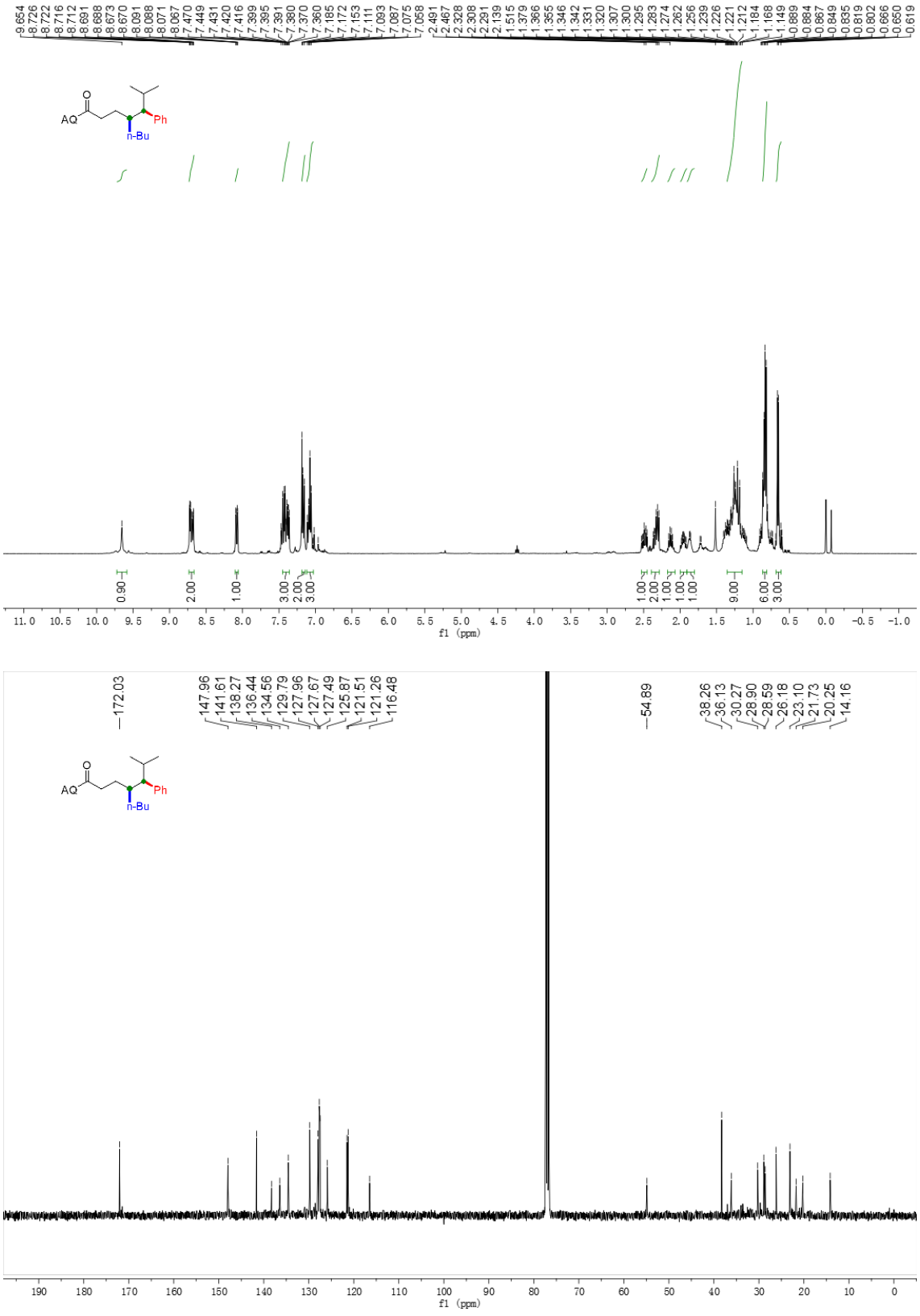
Scheme 48. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ar**



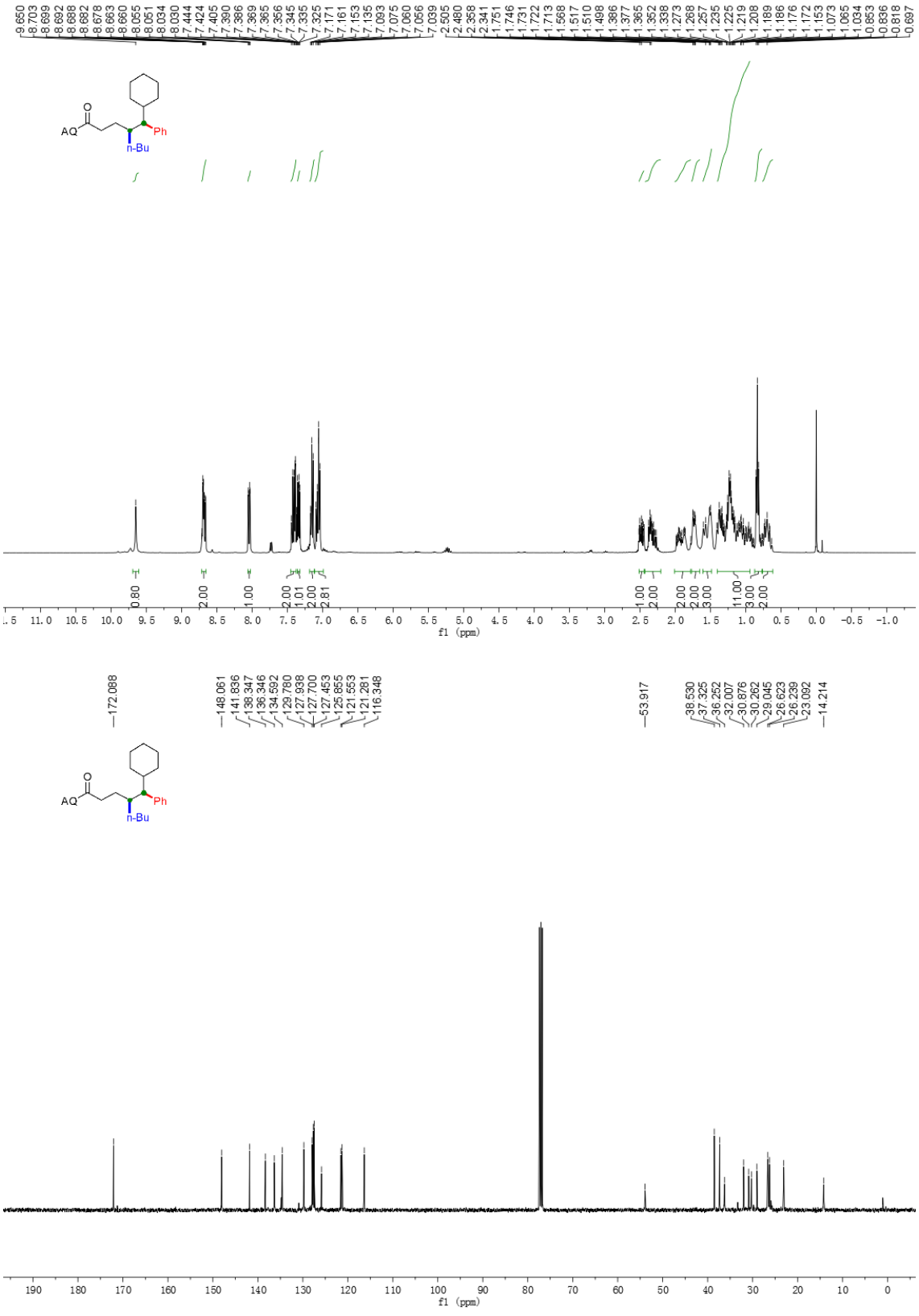
Scheme 49. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2as**



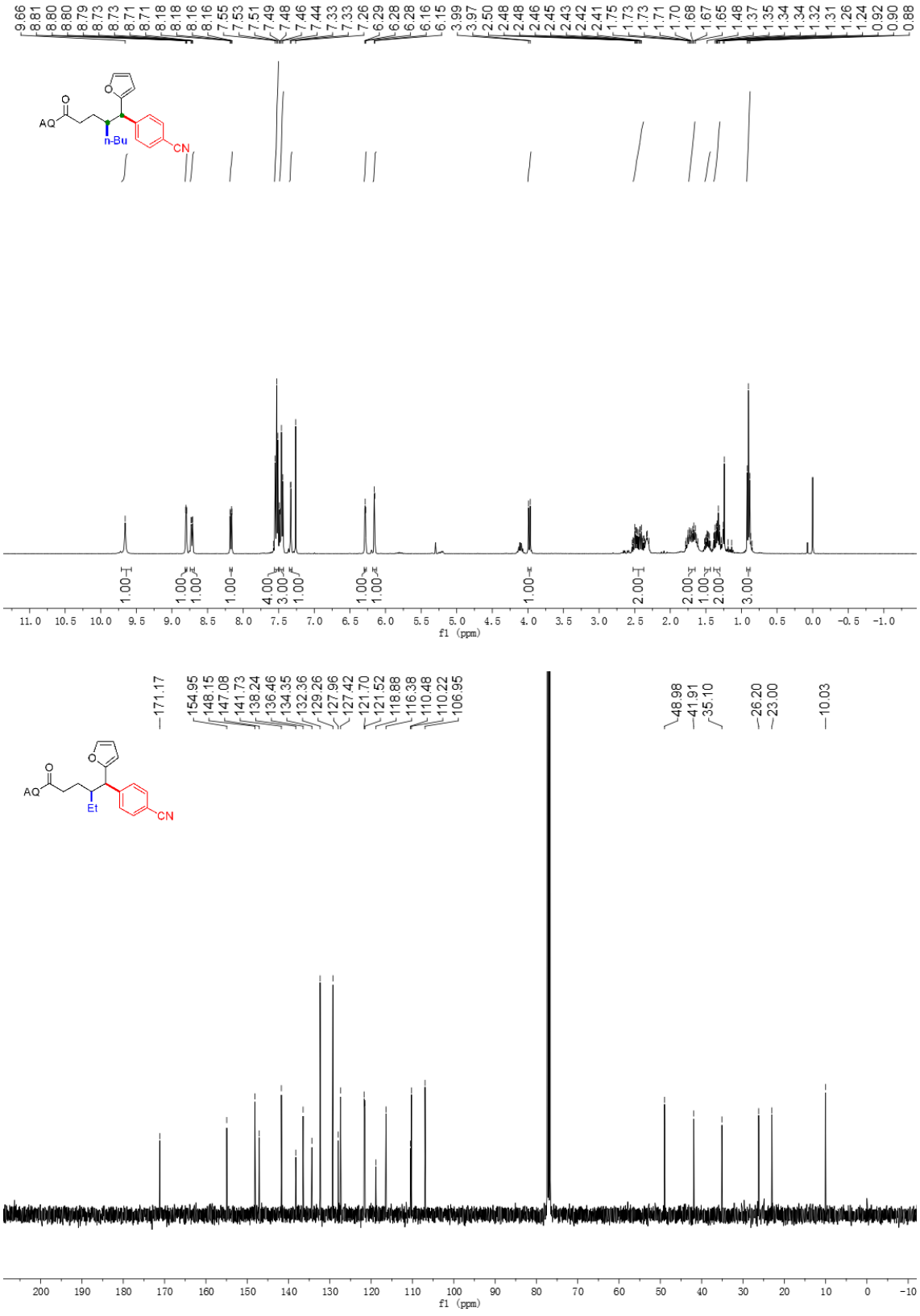
Scheme 50. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra off **2at**



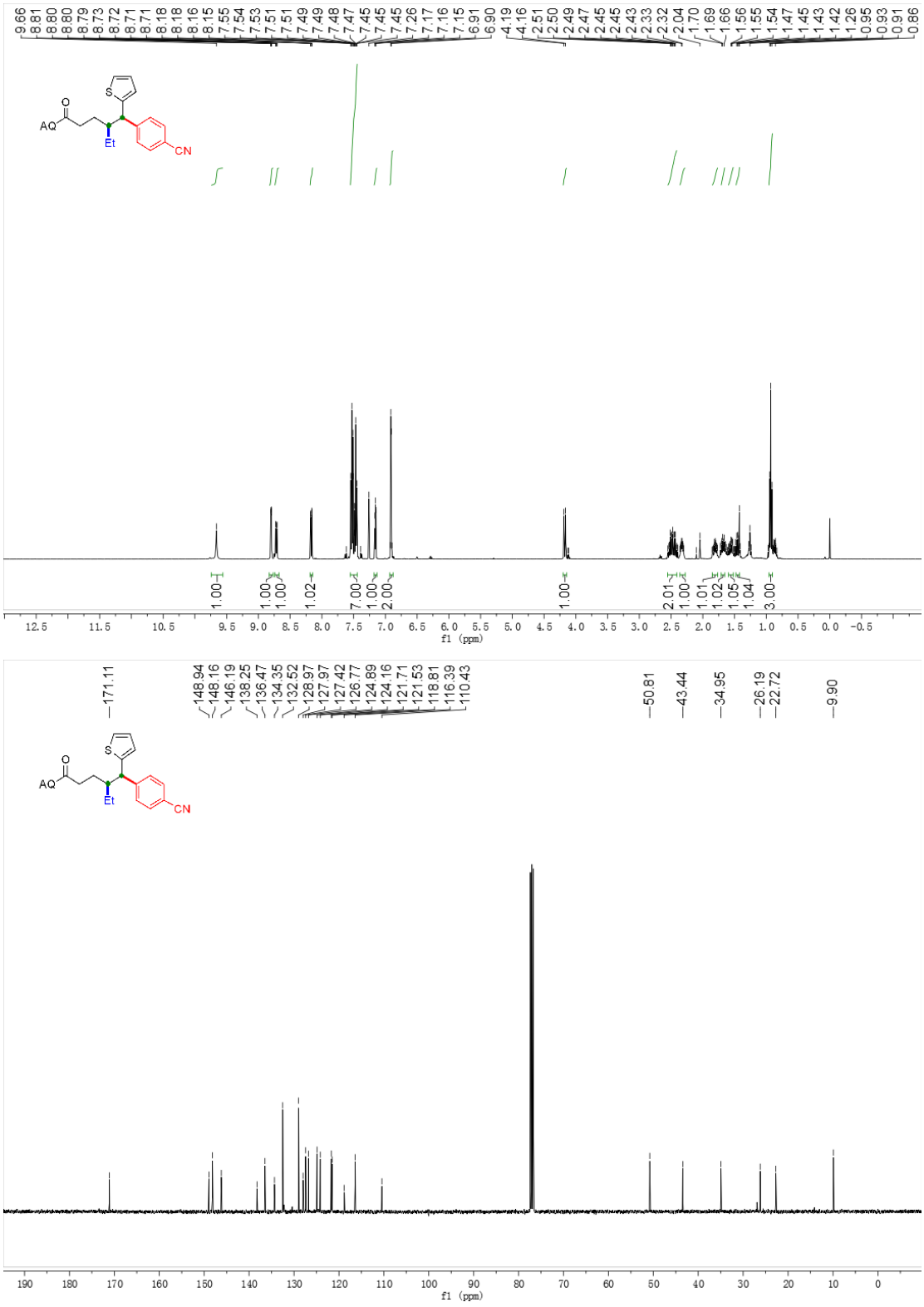
Scheme 51. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2au**



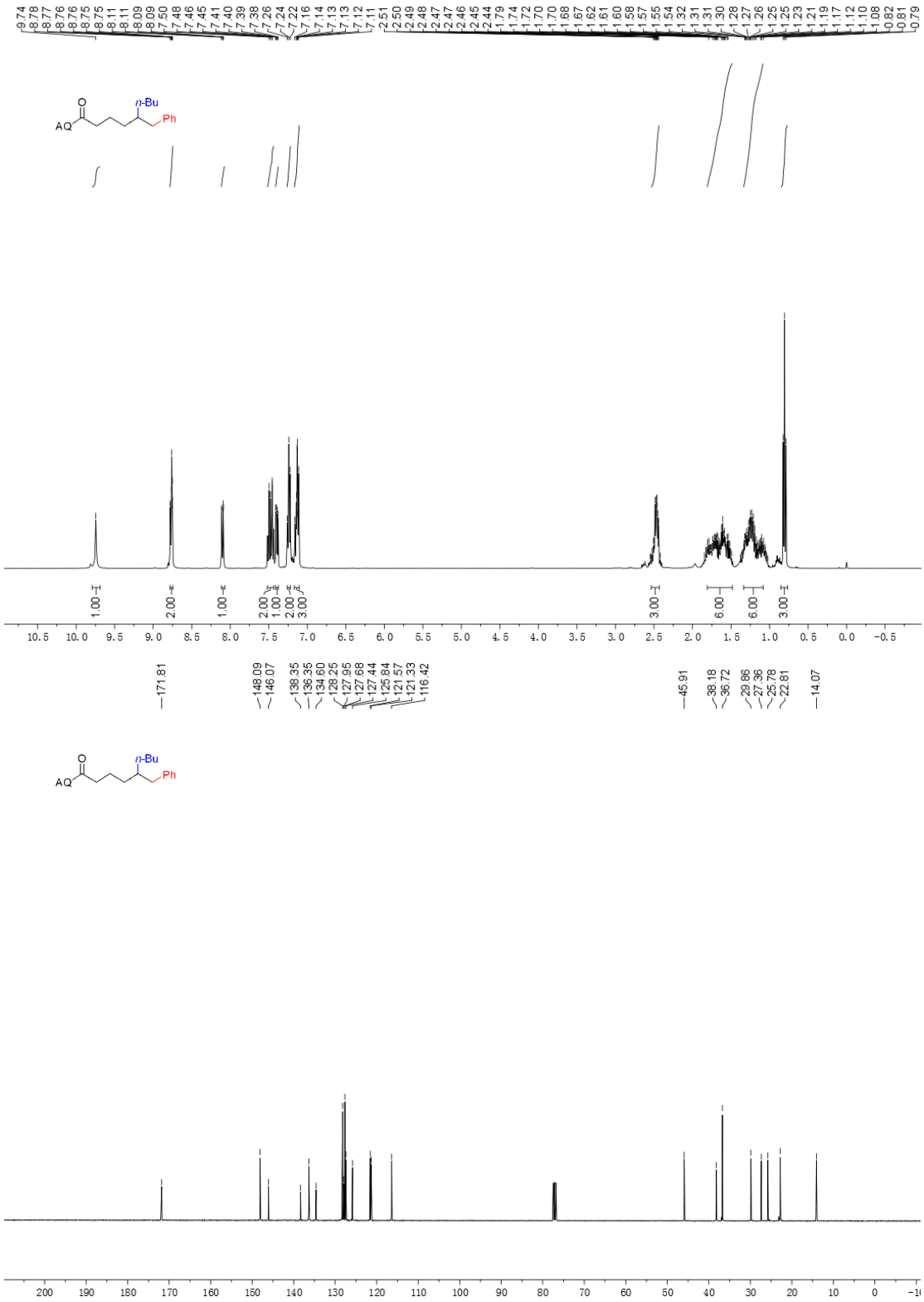
Scheme 52. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2av**



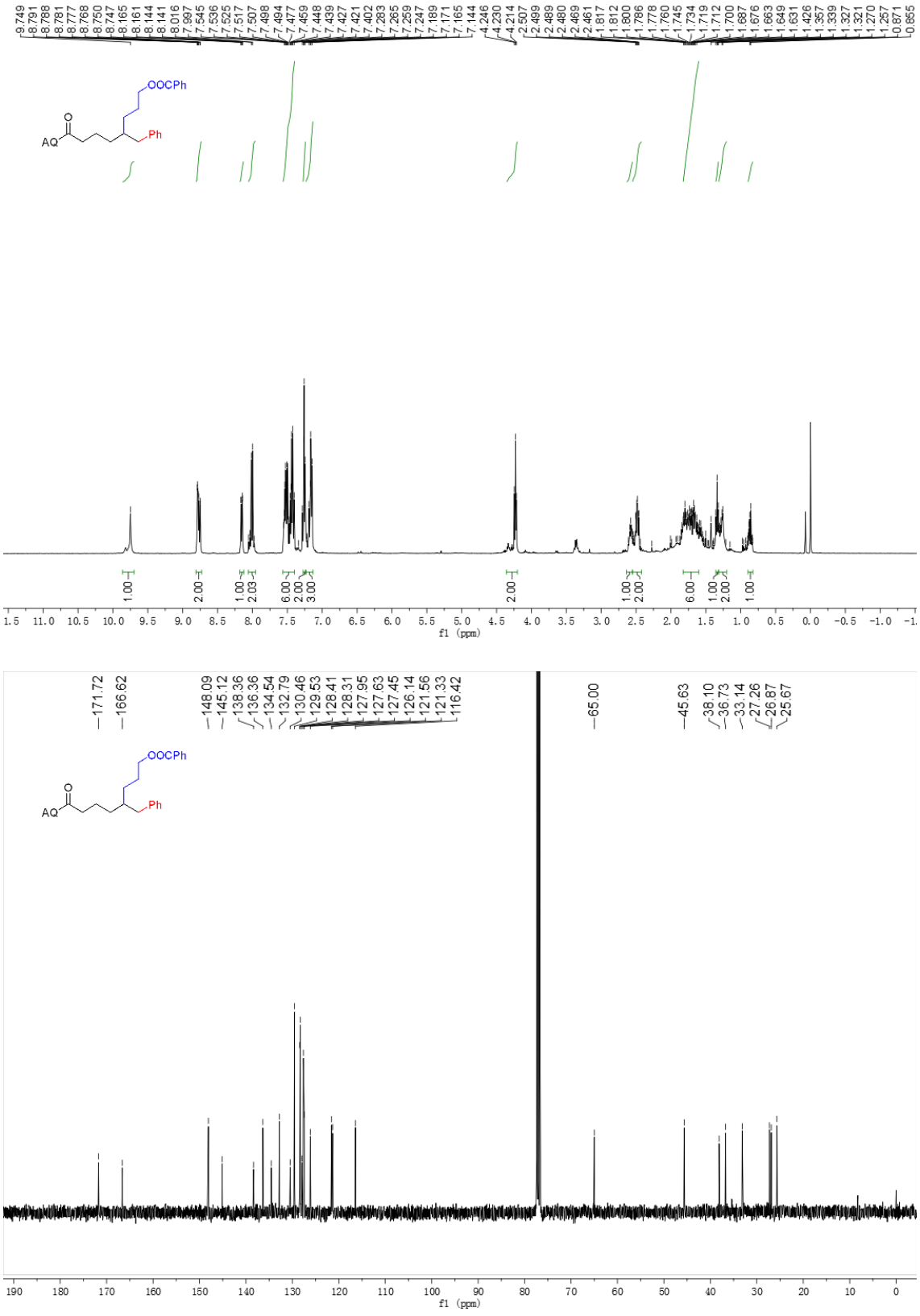
Scheme 53. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2aw**



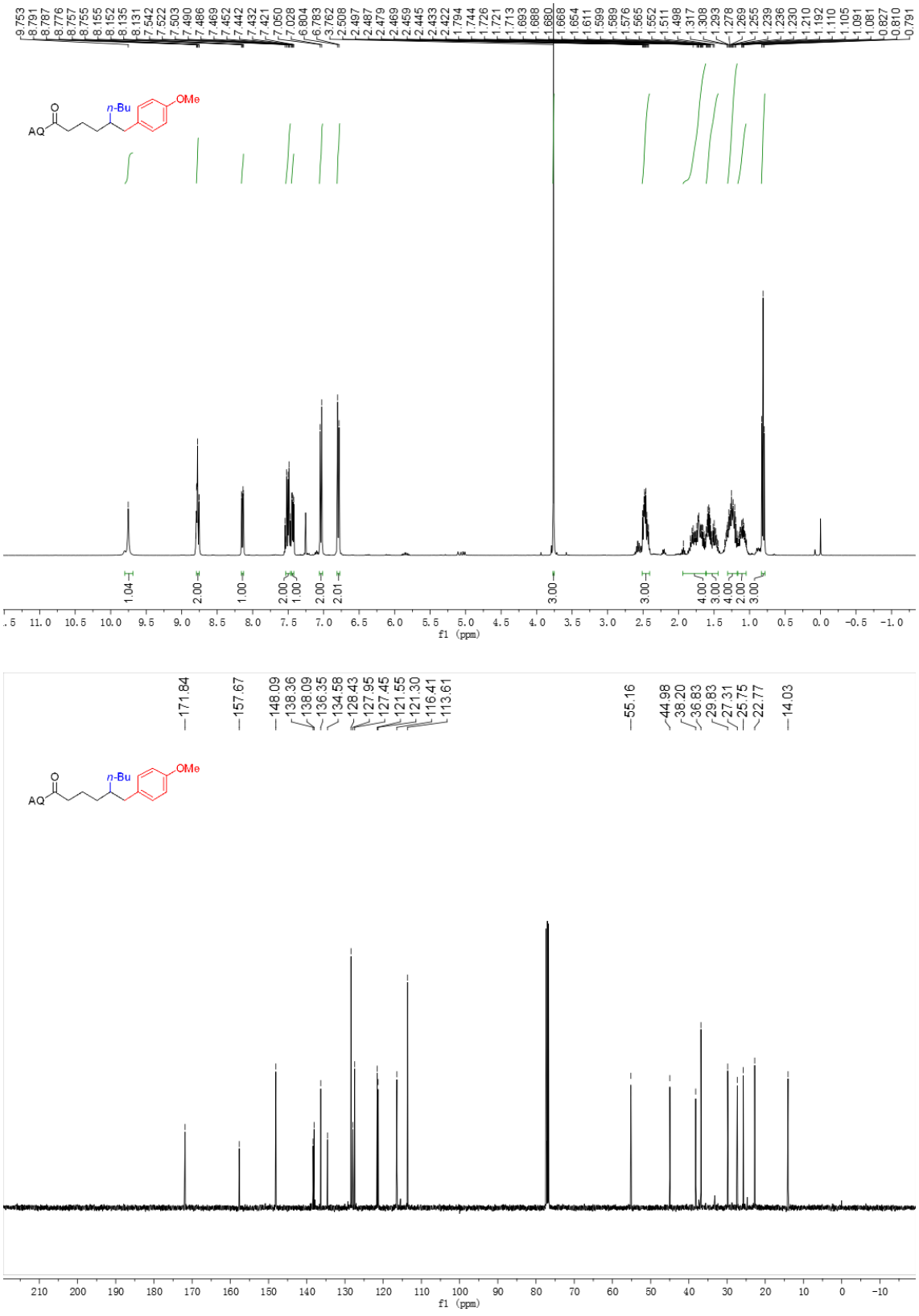
Scheme 54. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ax**



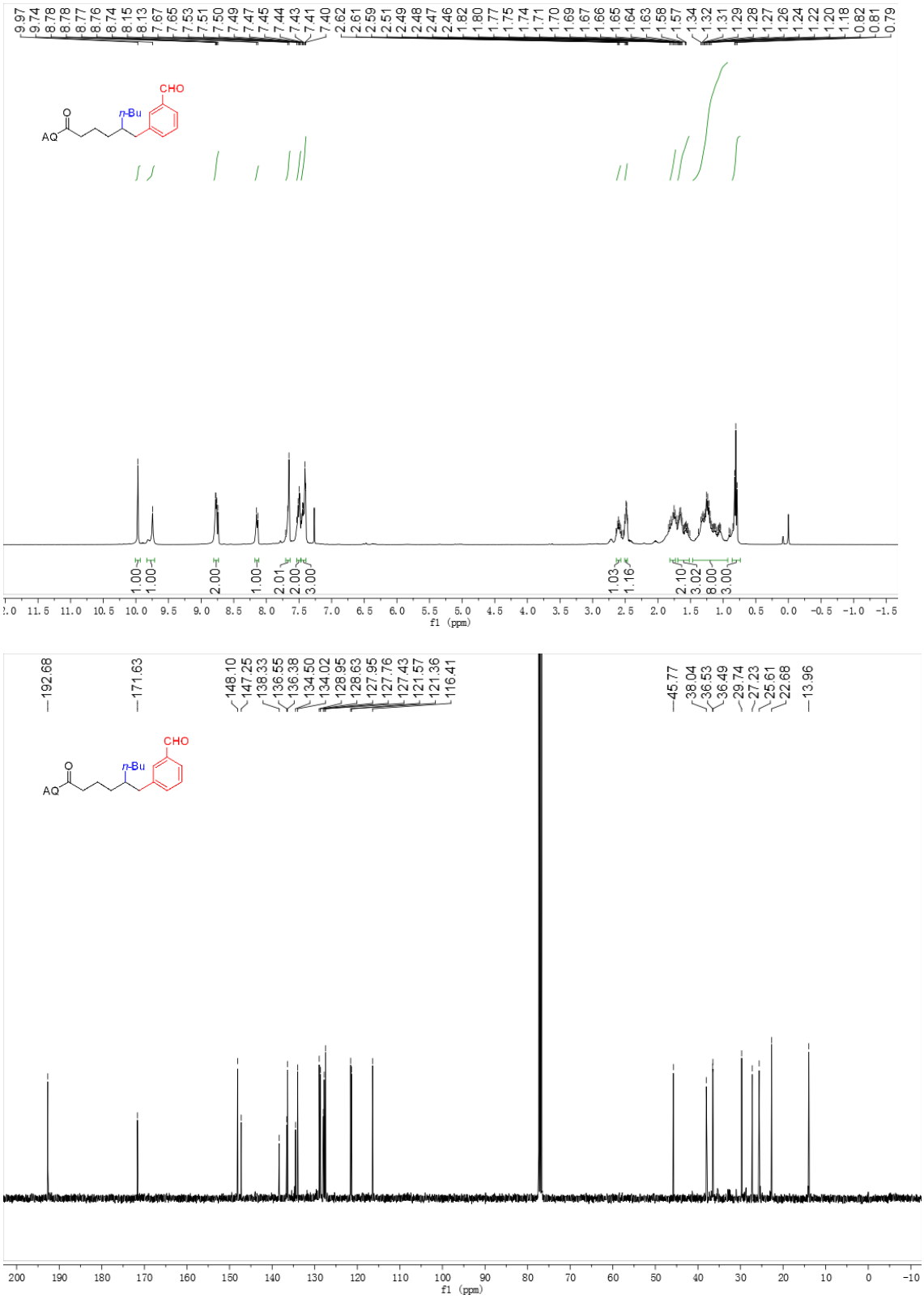
Scheme 55. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ay**



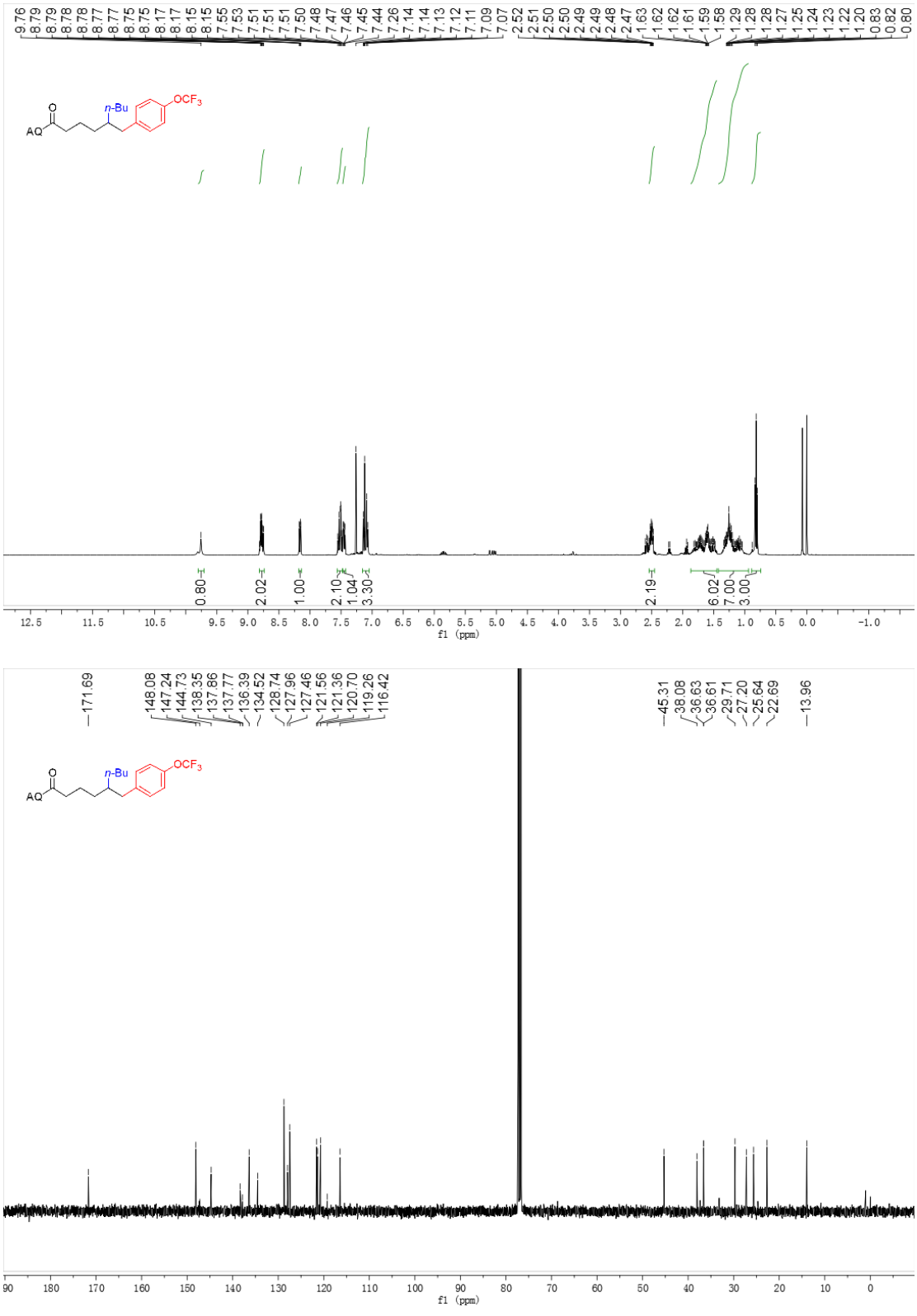
Scheme 56. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2az**



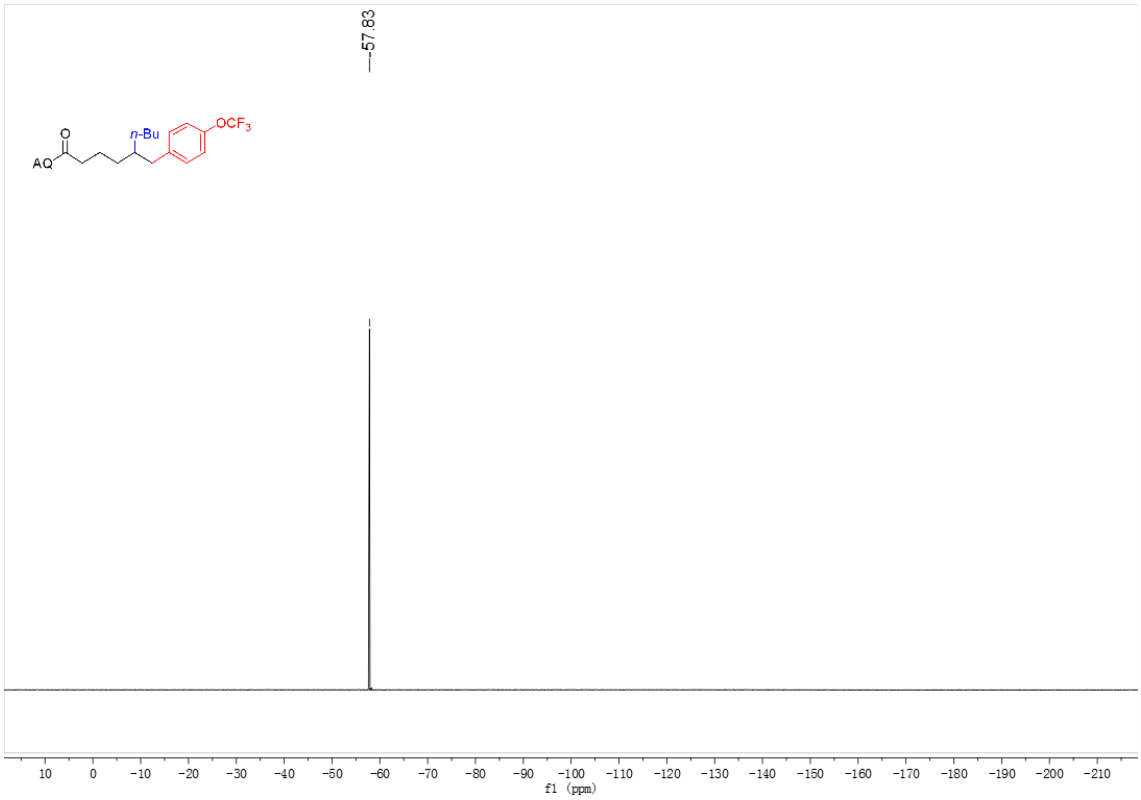
Scheme 57. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2ba**



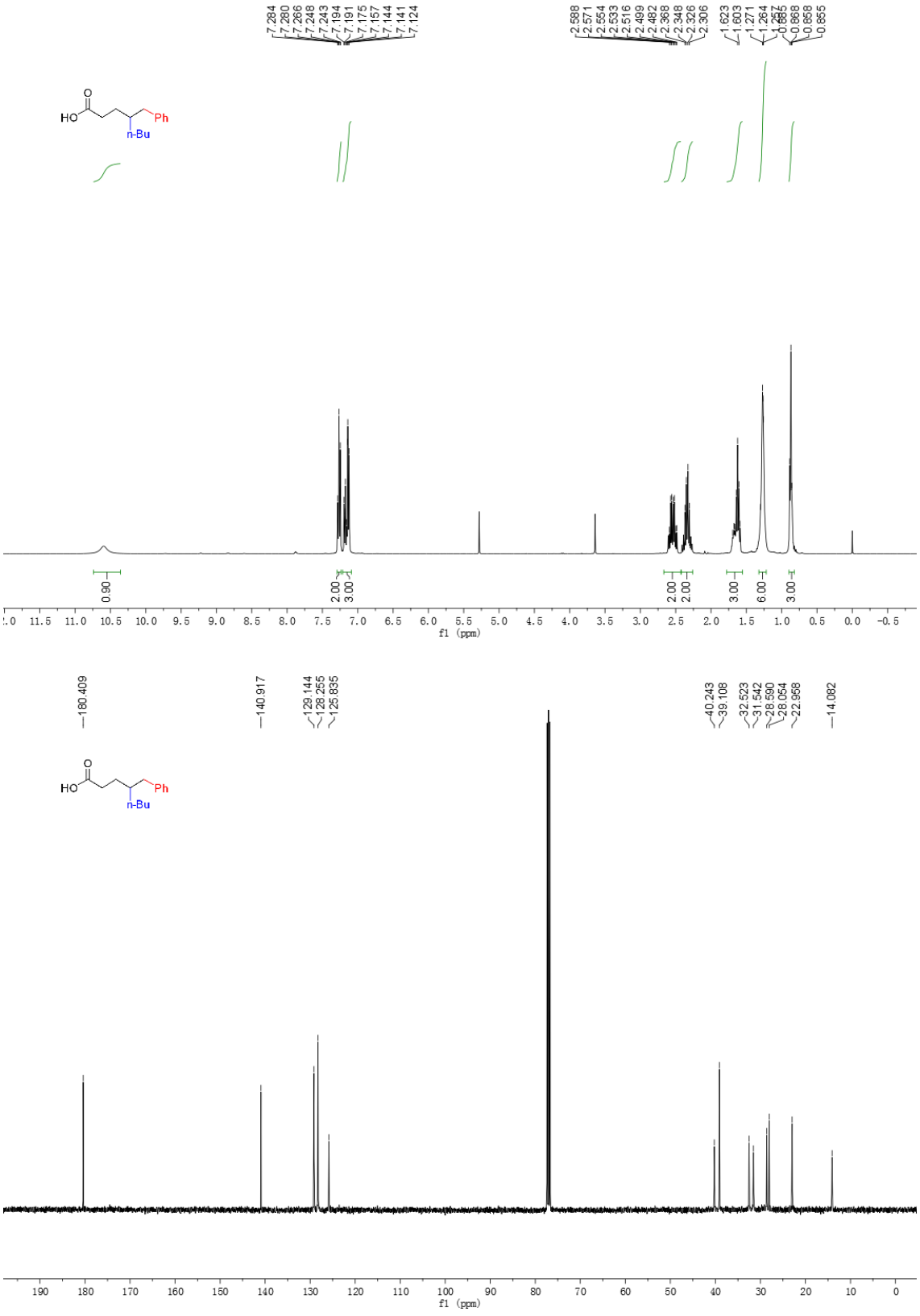
Scheme 58. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2bb**



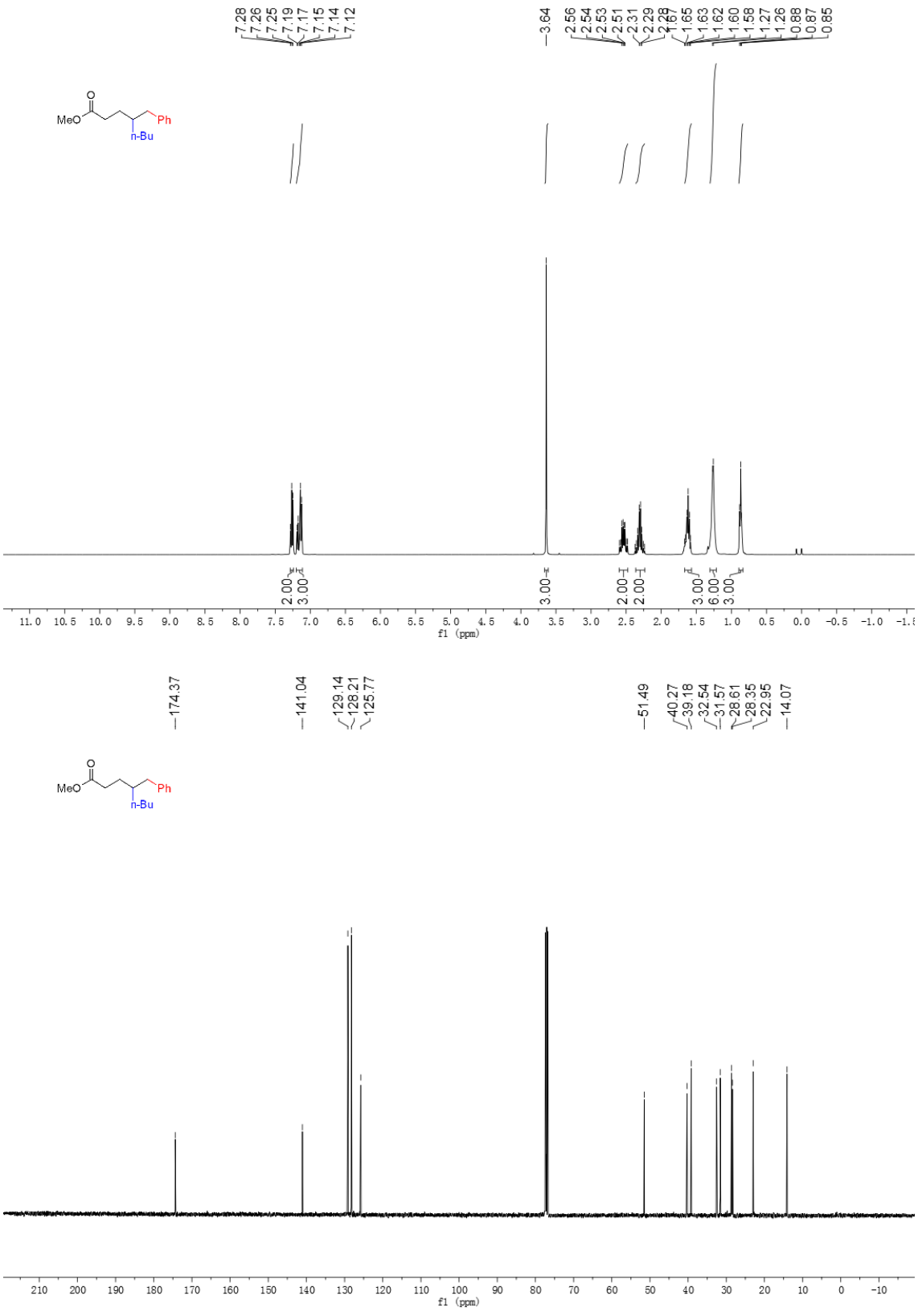
Scheme 59. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **2bc**



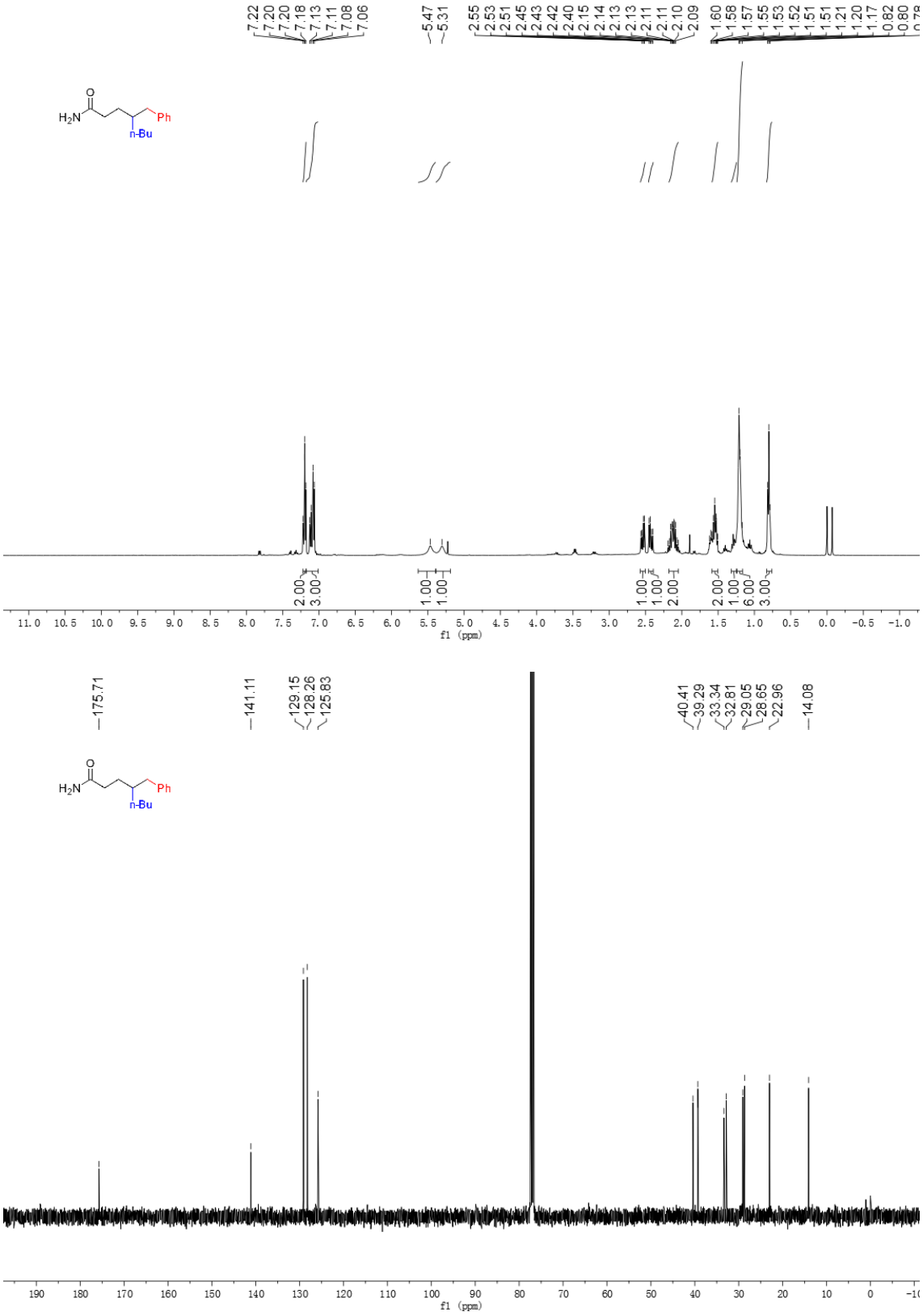
Scheme 60. ^{19}F NMR (376 MHz, $CDCl_3$) spectra of **2bc**



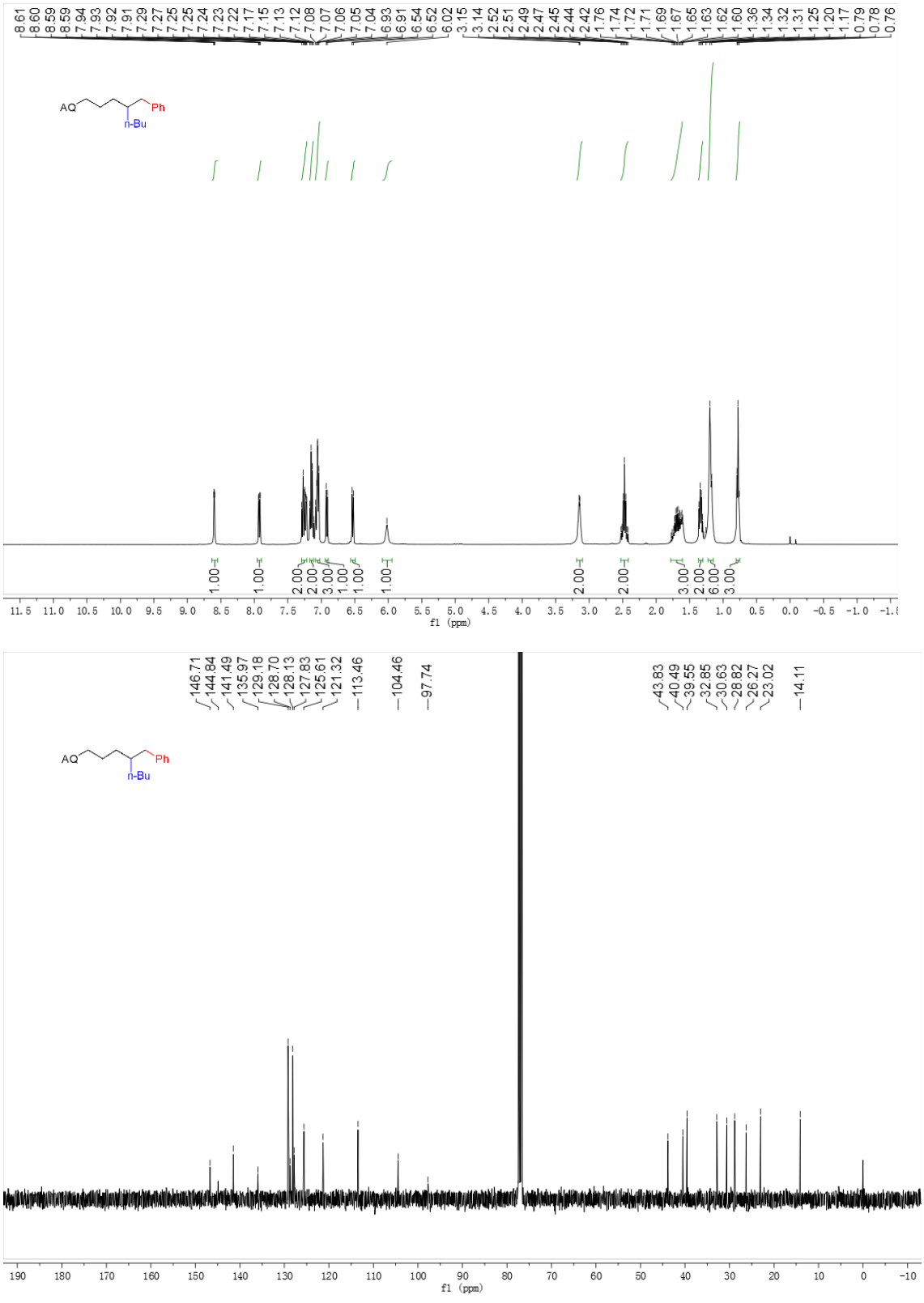
Scheme 61. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **3a**



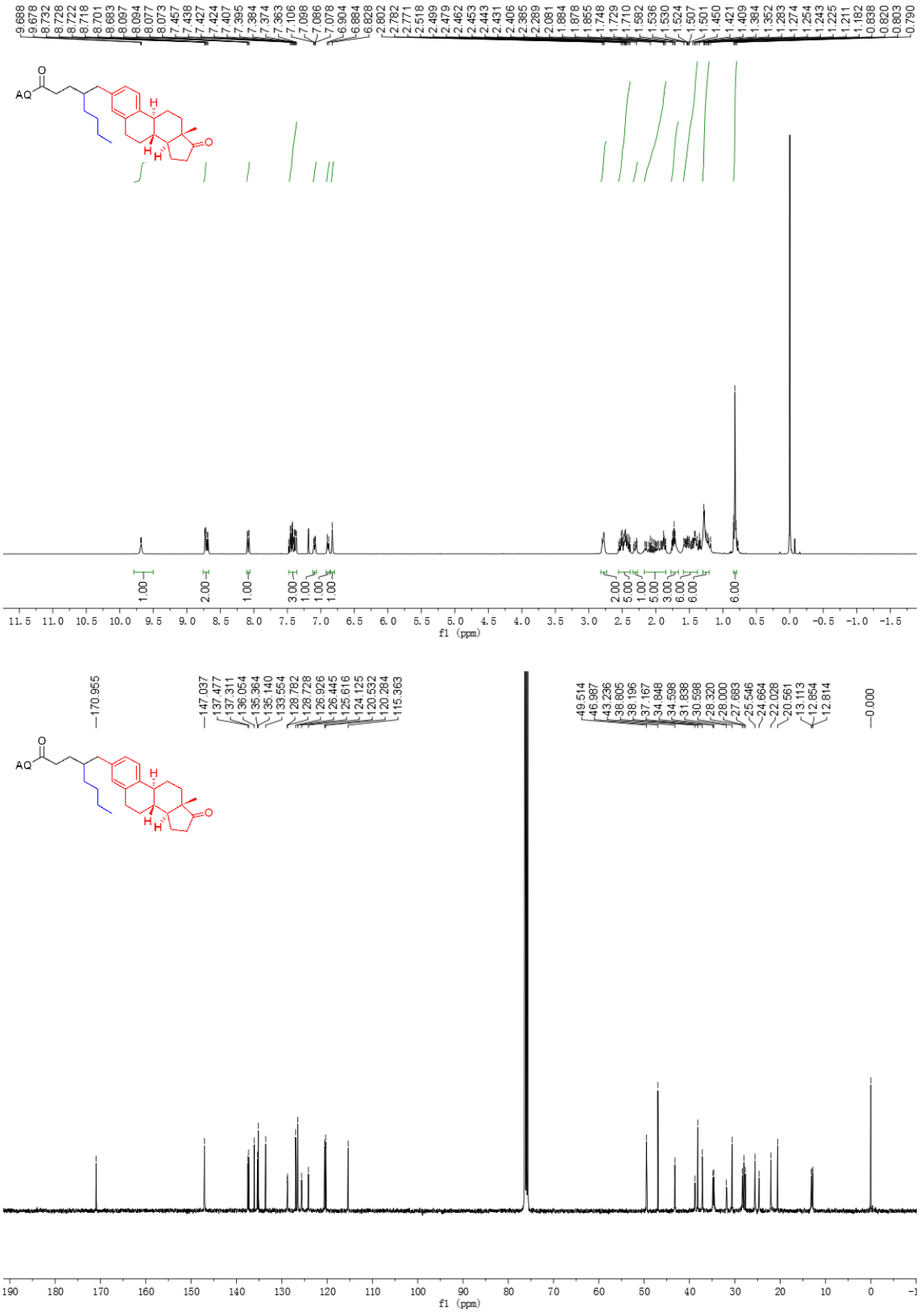
Scheme 62. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **3b**



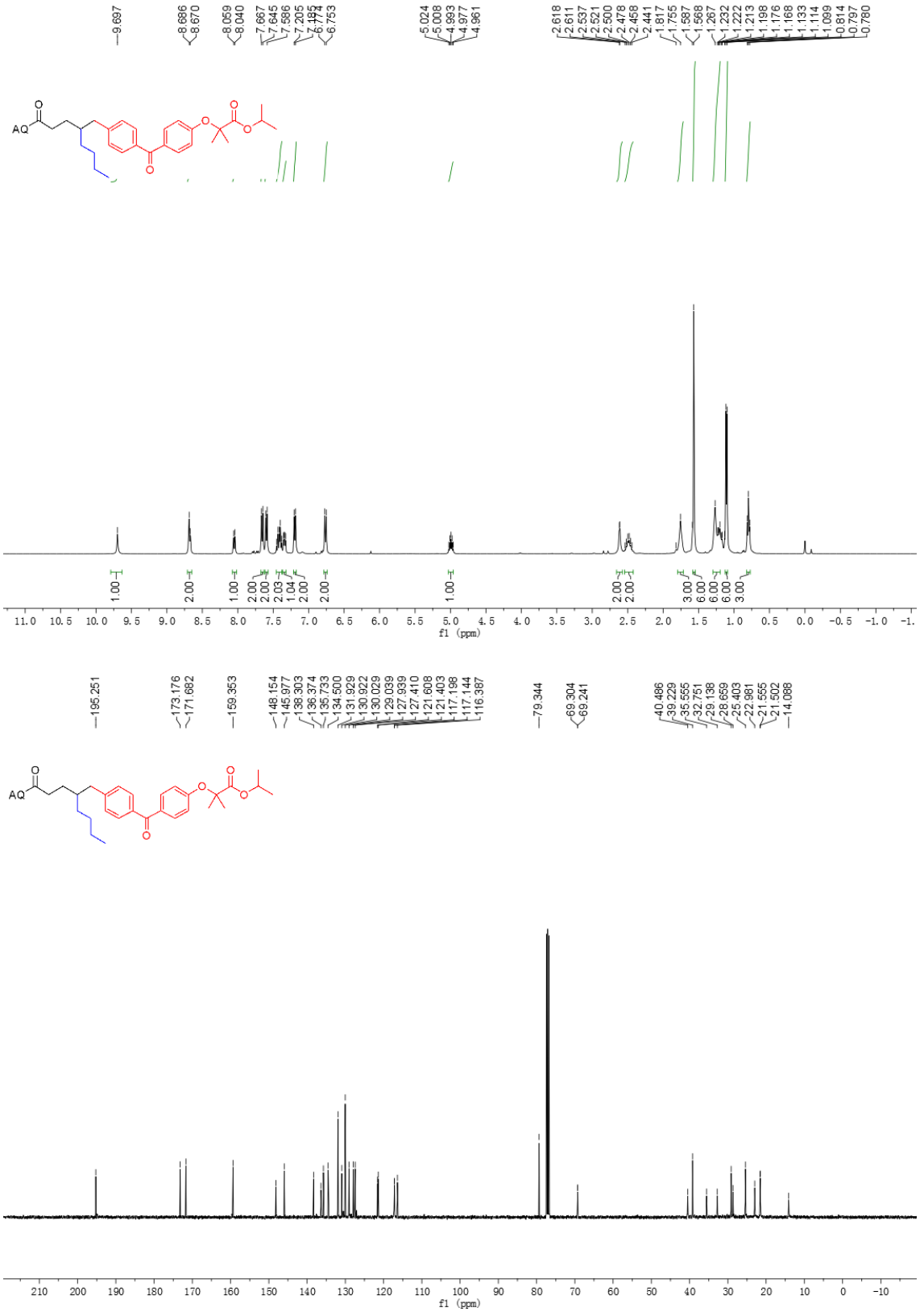
Scheme 63. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR(101 MHz, $CDCl_3$) spectra of **3c**



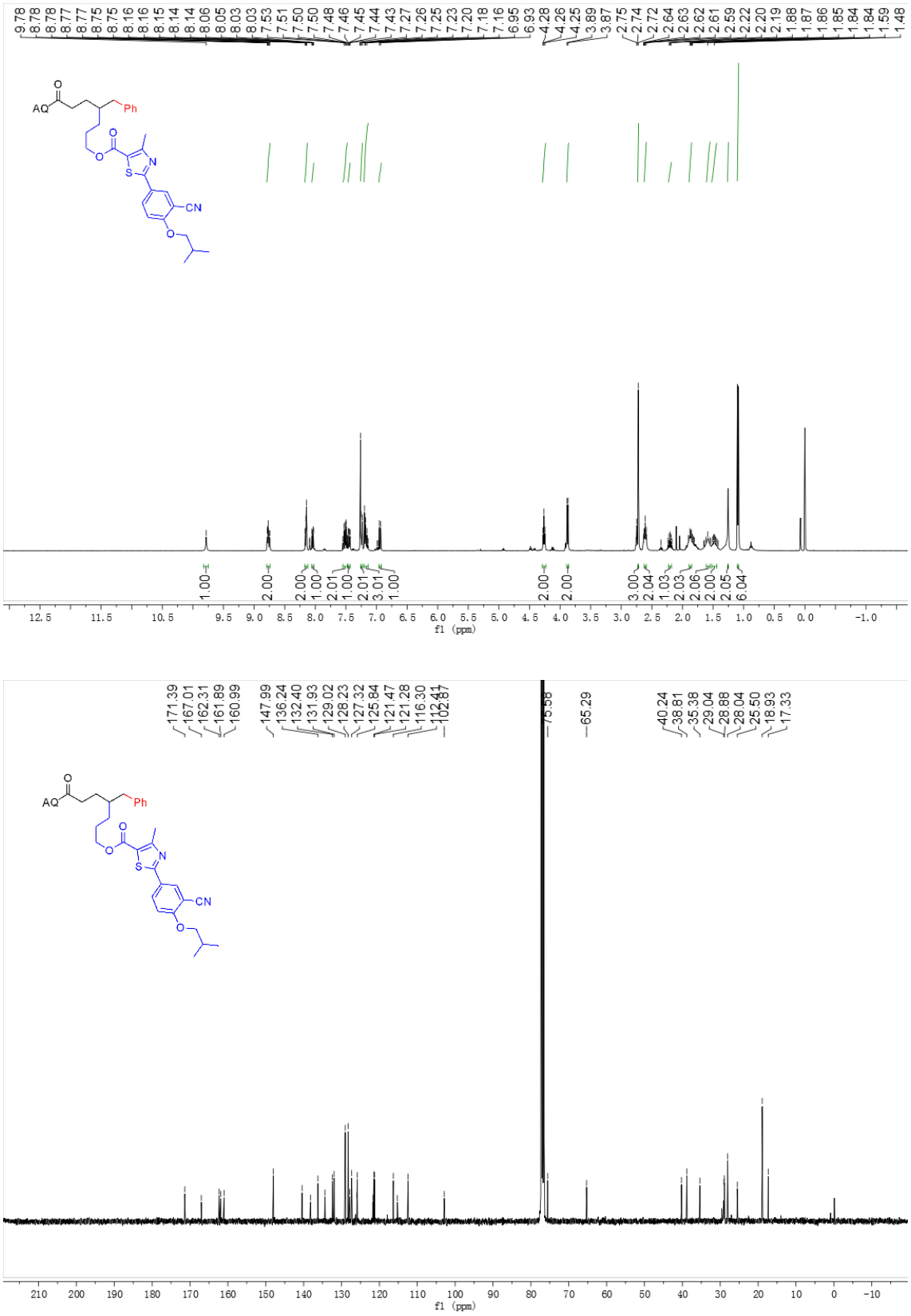
Scheme 64. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **3d**



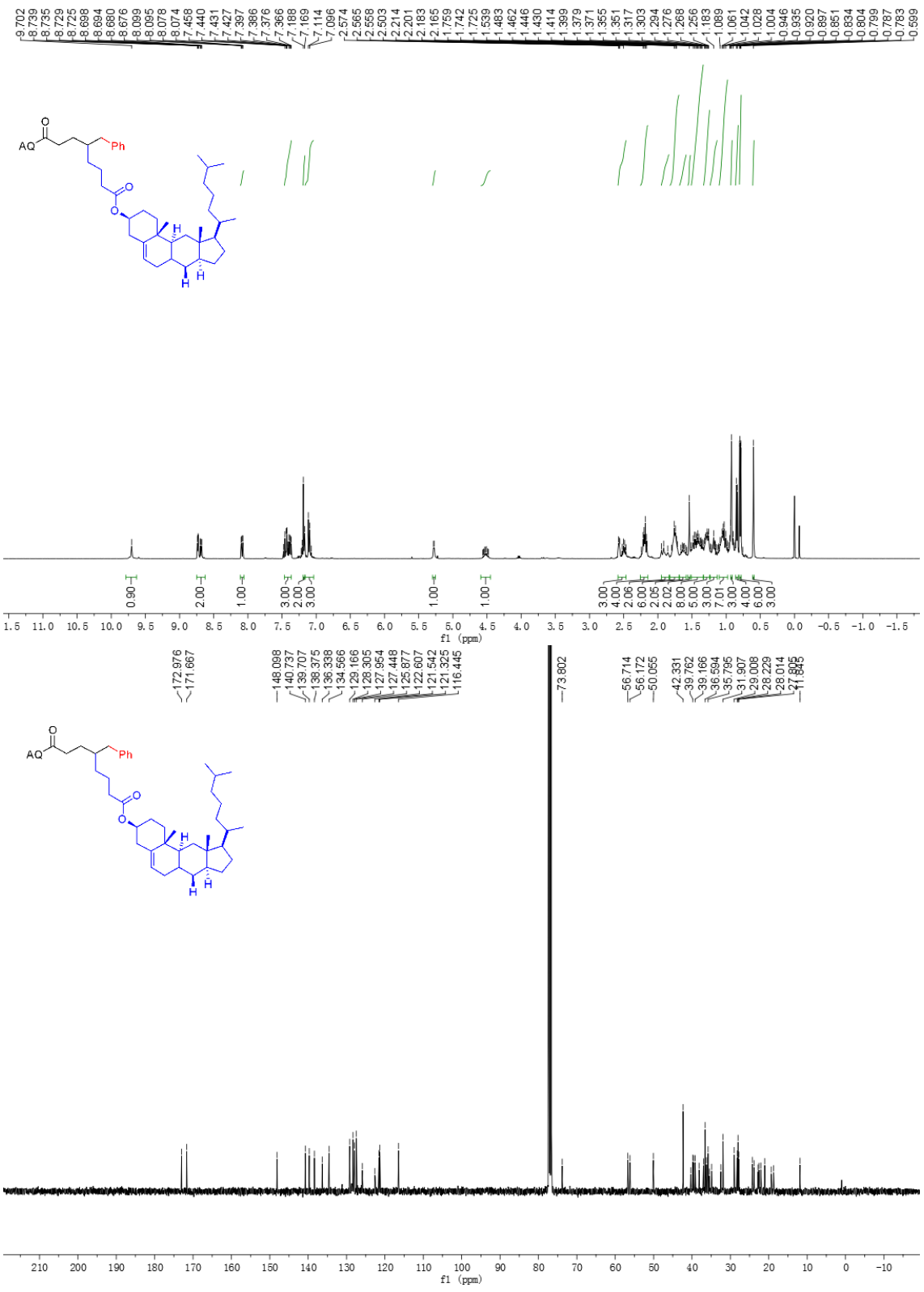
Scheme 65. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **4a**



Scheme 66. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **4b**



Scheme 67. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **4c**



Scheme 68. ^{1}H NMR (400 MHz, $CDCl_3$) and ^{13}C NMR (101 MHz, $CDCl_3$) spectra of **4d**