Supporting Online Material for

Transition-Metal-Free Oxidative Aliphatic C-H Azidation

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Materials and Methods

CH_3CN, Toluene, DCE, DMSO and DCM etc. used in reactions were dried according to the purification handbook *Purification of Laboratory Chemicals* before using. $K_2S_2O_8$ (99.99%) was purchased from Aladdin. Compounds **1a**[1],**1b**[1], **1c**[1], **1d**[1], **1e**[1], **1f**[1], **1j**[1], **1k**[2], **1l**[1], **1m**[1], **1o**[2], **1q**[2], **1r**[1], **1s**[1] and 2-azidosulfonyl-benzoic acid methyl ester[3] were prepared and characterized as corresponding reference reported. Deuterated solvents were purchased from Sigma-Aldrich. TLC was performed on silica gel Huanghai $HSGF_{254}$ plates and visualized by quenching of UV fluorescence (λ_{max}= 254 nm). 200-300 mesh silica gel was purchased from Qingdao Haiyang Chemical Co., China. Unless otherwise noted, all other reagents and starting materials were purchased from commercial sources and used without further purification. The data for NMR spectra (^{1}H NMR, ^{13}C NMR and ^{19}F NMR) were recorded at 293 K on a Bruker AVANCE AV 400 (400MHz, 101MHz and 376MHz) and chemical shifts were recorded relative to the solvent resonance. Signal positions were recorded in ppm and the following abbreviations are used singularly or in combination to indicate the multiplicity of signals: s singlet, d doublet, t triplet, q quartet, m multiplet, Hz Hertz. For ^{1}H NMR: $CDCl_3$ = δ 7.26 ppm, CD_3CN = δ 1.94 ppm. For ^{13}C NMR: $CDCl_3$ = δ 77.16 ppm, CD_3CN = δ 118.26 ppm. Mass spectra were obtained on Agilent 6520 Q-TOF LC/MS and Aligent 7890/5975C-GS/MSD. HRMS were obtained on Varian 7.0T FTMS. IR spectra were obtained on Bruker Alpha FT-IR Spectrometer.

Caution: Azides are potentially hazardous compounds and adequate safety measures should be taken. Reaction, especially when involving bigger quantities or heating, should be conducted behind safety shields.

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[1] Guo, S.; Zhang, X.; Tang, P. *Angew. Chem. Int. Ed*. **2015**, 54, 4065.

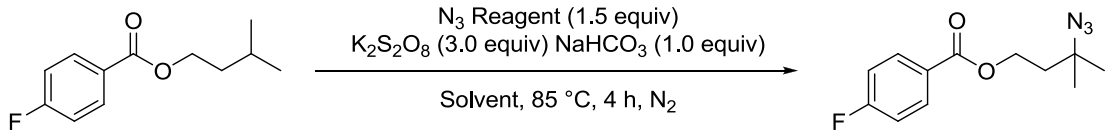
[2] Zhang, X.; Guo, S.; Tang, P. *Org. Chem. Front.*, **2015**, 2, 806.

[3] Waser, J.; Gaspar, B.; Nambu, H.; Carreira, E. M. *J. Am. Chem. Soc.* **2006**, *128*, 11693.

Experimental Data

Experimental Procedures and Compound Characterization

Effect of solvents on the reaction



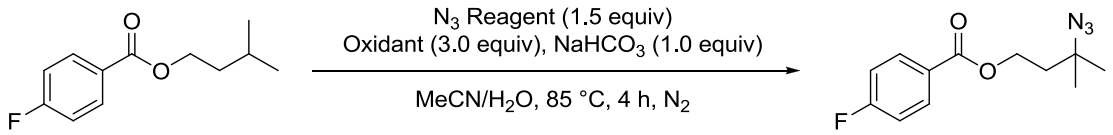
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

Yields are reported in Table S1.

Table S1: Effect of solvents on the reaction

Solvent	Yield [%] (^{19}FNMR)	Solvent	Yield [%] (^{19}FNMR)
MeCN	0	MeCN/H_2O 3:2 (v/v)	64
H_2O	12	DCE/H_2O 3:2 (v/v)	0
DCE	0	DMSO/H_2O 3:2 (v/v)	13
DMSO	3	Acetone/H_2O 3:2 (v/v)	9
Acetone	0	Toluene/H_2O 3:2 (v/v)	0
Toluene	0		

Effect of oxidant on the reaction



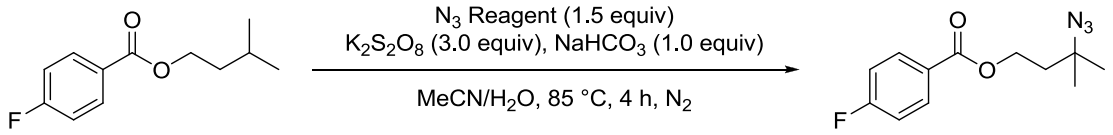
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.5 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and oxidant (0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$ = 3:2) and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

Yields are reported in Table S2.

Table S2: Effect of oxidant on the reaction

Oxidant	Yield [%] (^{19}FNMR)
-	0
$Na_2S_2O_8$	46
$K_2S_2O_8$	65
$(NH_4)_2S_2O_8$	64
Benzoyl peroxide	4
m-CPBA	0
H_2O_2	0

Effect of different N_3 Reagents on the reaction

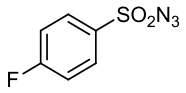
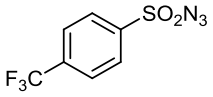
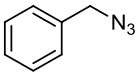
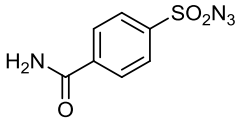
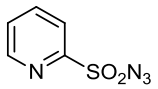
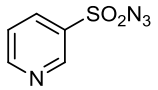
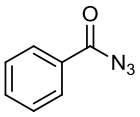
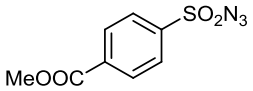
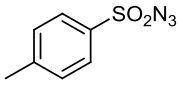
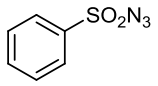
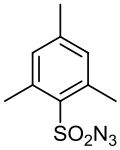
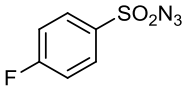
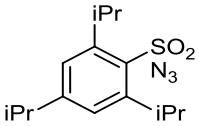
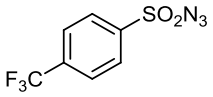


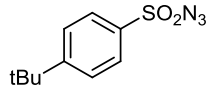
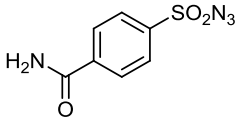
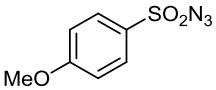
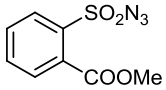
A 10 mL Schlenk tube was charged with azide (0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent

($MeCN/H_2O$=3:2) and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

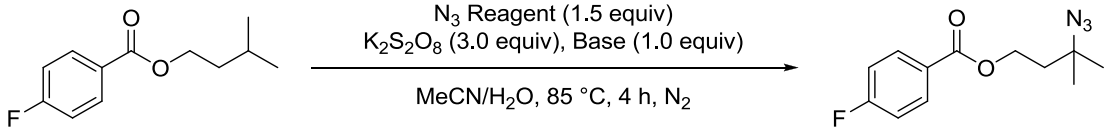
Yields are reported in Table S3.

Table S3: Effect of different N_3 Reagents on the reaction

N_3 Reagent	Yield [%] (^{19}FNMR)	N_3 Reagent	Yield [%] (^{19}FNMR)
NaN_3	4		57
$TMSN_3$	7		60
	0		9
$Ph_3C\text{-}N_3$	0		52
$(n\text{Bu})_3SnN_3$	0		46
	0		65
	56		60
	40		57
	50		60

	55		9
	49		65

Effect of base on the reaction



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.500 equiv), Base (0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

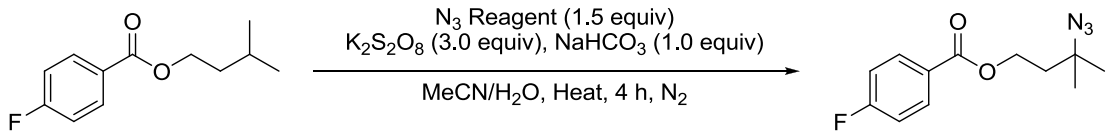
Yields are reported in Table S4.

Table S4: Effect of base on the reaction

Base	Yield [%] (^{19}FNMR)
-	61
NaOH	58
NaOAc	60
Na_2HPO_4	57
Na_2CO_3	57
K_2CO_3	60
Cs_2CO_3	57

$NaHCO_3$	65
$KHCO_3$	60
Pyridine	58
DBU	37
Triethylamine	20
DABCO	27

Effect of temperature on the reaction



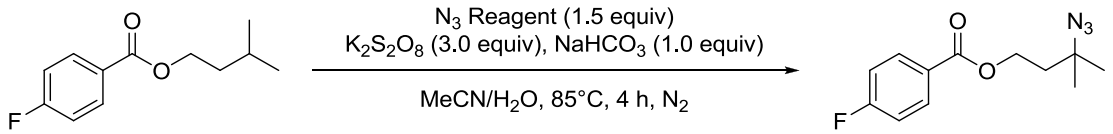
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred and heated for 4 hr. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

Yields are reported in Table S5.

Table S5: Effect of temperature on the reaction

Temperature	Yield [%] (^{19}FNMR)
35 ^{o}C	0
60 ^{o}C	8
85 ^{o}C	65
100 ^{o}C	51

Effect of concentration on the reaction



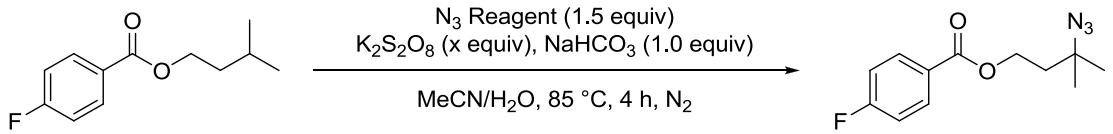
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of solvent and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

Yields are reported in Table S6.

Table S6: Effect of concentration on the reaction

Concentartion	Yield [%] (^{19}FNMR)
0.3 M	7%
0.15 M	39%
0.08 M	67%
0.04 M	62%

Effect of $K_2S_2O_8$ amount on the reaction



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$. The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and 3-methylbutyl 4-fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, 1-fluoro-3-nitrobenzene (18.0 μL, 0.169 mmol) was added to the reaction mixture. The yield of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) was determined by comparing the integration of the ^{19}F NMR resonance of 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) (-105.50 ppm) with that of 1-fluoro-3-nitrobenzene (-109.00 ppm).

Yields are reported in Table S7.

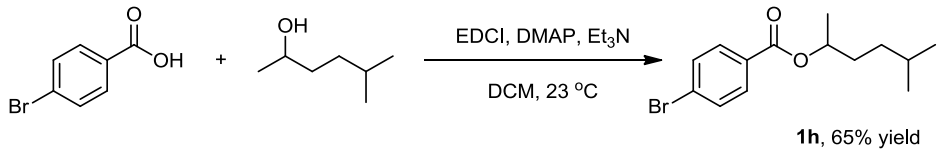
Table S7: Effect of $K_2S_2O_8$ amount on the reaction

Amount of $K_2S_2O_8$ (equiv)	Yield [%] (^{19}FNMR)
0	5
0.5	13
1.0	24
2.0	55
3.0	65
3.5	57

1,4-Dimethylpentyl 4-chlorobenzoate (1g)

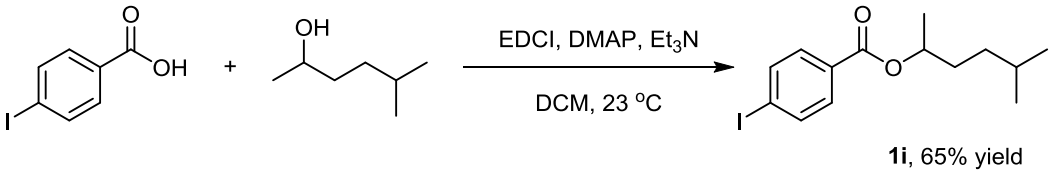
To a solution of 4-chlorobenzoic acid (1.10 g, 7.00 mmol, 1.00 equiv), DMAP (4-dimethylaminepyridine) (0.170 g, 0.140 mmol, 0.200 equiv) and Et_3N (2.0 mL, 15 mmol, 2.1 equiv) in CH_2Cl_2 (50.0 mL) at 23 ^oC were added EDCI (1-ethyl-(3-(3-dimethylamino)propyl)-carbodiimide hydrochloride) (2.60 g, 14.0 mmol, 2.00 equiv) and 5-methylhexan-2-ol (0.810 g, 7.00 mmol, 1.00 equiv). The reaction mixture was warmed to 23 ^oC and stirred for 6 hr before quenched with H_2O (10.0 mL) and extracted 3 times with CH_2Cl_2 (20.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v) to afford 1.54 g 1,4-dimethylpentyl 2-chlorobenzoate (**1g**) as a colourless liquid (87% yield). R_f = 0.3 (hexanes/EtOAc 50:1 (v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.08 – 7.85 (m, 2H), 7.52 – 7.31 (m, 2H), 5.21 – 5.00 (m, 1H), 1.79 – 1.67 (m, 1H), 1.66 – 1.48 (m, 2H), 1.33 (d, *J* = 6.3 Hz, 3H), 1.30 – 1.16 (m, 2H), 0.89 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 139.2, 131.0, 129.5, 128.7, 72.5, 34.6, 34.0, 28.1, 22.7, 22.6, 20.2. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{19}ClO_2Na$ $[M + Na]^+$, 277.0971. Found, 277.0969.

1,4-Dimethylpentyl 4-bromobenzoate (1h)



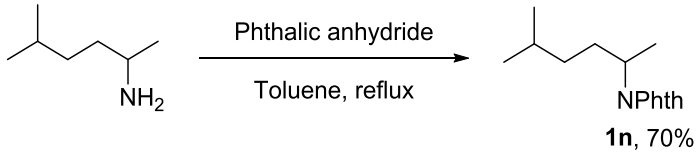
To a solution of 4-bromobenzoic acid (1.40 g, 7.00 mmol, 1.00 equiv), DMAP (4-dimethylaminepyridine) (0.170 g, 0.140 mmol, 0.200 equiv) and Et_3N (2.0 mL, 15 mmol, 2.1 equiv) in CH_2Cl_2 (50.0 mL) at 23 ^oC were added EDCI (1-ethyl-(3-(3-dimethylamino)propyl)-carbodiimide hydrochloride) (2.60 g, 14.0 mmol, 2.00 equiv) and 5-methylhexan-2-ol (0.810 g, 7.00 mmol, 1.00 equiv). The reaction mixture was warmed to 23 ^oC and stirred for 6 hr before quenched with H_2O (10 mL) and extracted 3 times with CH_2Cl_2 (20 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v) to afford 1.25 g 1,4-dimethylpentyl 4-bromobenzoate (**1h**) as a colourless liquid (60% yield). R_f = 0.5 (hexanes/EtOAc 20:1 (v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.6 Hz, 2H), 7.56 (d, *J* = 8.6 Hz, 2H), 5.18 – 5.05 (m, 1H), 1.78 – 1.66 (m, 1H), 1.66 – 1.49 (m, 2H), 1.33 (d, *J* = 6.3 Hz, 3H), 1.30 – 1.15 (m, 2H), 0.89 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.6, 131.7, 131.2, 129.9, 127.9, 72.5, 34.6, 34.0, 28.0, 22.7, 22.6, 20.2. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{19}BrO_2Na$ $[M + Na]^+$, 321.0466. Found, 321.0468.

1,4-Dimethylpentyl 4-bromobenzoate (1i)



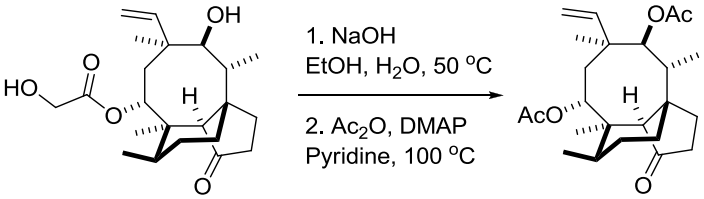
To a solution of 4-iodobenzoic acid (1.70 g, 7.00 mmol, 1.00 equiv), DMAP (4-dimethylaminepyridine) (0.170 g, 0.140 mmol, 0.200 equiv) and Et_3N (2.0 mL, 15 mmol, 2.1 equiv) in CH_2Cl_2 (50 mL) at 23 ^oC were added EDCI (1-ethyl-(3-(3-dimethylamino)propyl)-carbodiimide hydrochloride) (2.60 g, 14.0 mmol, 2.00 equiv) and 5-methylhexan-2-ol (0.810 g, 7.00 mmol, 1.00 equiv). The reaction mixture was warmed to 23 ^oC and stirred for 6 hr before quenched with H_2O (10 mL) and extracted 3 times with CH_2Cl_2 (20 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v) to afford 1.57 g 1,4-dimethylpentyl 4-iodobenzoate (**1i**) as a colourless liquid (65% yield). R_f = 0.5 (hexanes/EtOAc 20:1 (v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.6 Hz, 2H), 7.73 (d, *J* = 8.6 Hz, 2H), 5.01-5.21 (m, 1H), 1.80 – 1.66 (m, 1H), 1.66 – 1.47 (m, 2H), 1.32 (d, *J* = 6.3 Hz, 3H), 1.29 – 1.15 (m, 2H), 0.88 (d, *J* = 6.6 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 137.7, 137.7, 131.1, 130.5, 100.5, 72.4, 34.6, 33.9, 28.0, 22.7, 22.6, 20.1. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{19}IO_2Na$ $[M + Na]^+$, 369.0327. Found, 369.0325

_N_-Phthaloyl-5-methylhexan-2-amine (1n)



To a solution of 5-methylheptan-2-amine (345 mg, 3.00 mmol, 1.00 equiv) and phthalic anhydride (666 mg, 4.50 mmol, 1.50 equiv) in toluene (10.0 mL) were stirred and reflux for 5 hr before cooling down to 23 ^{o}C to afford the crude product. The crude product was quenched with H_2O (20.0 mL) and extracted 3 times with EtOAc (30.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated in vacuo and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 514 mg *N*-Phthaloyl-5-methylheptan-2-amine (**1n**) as a colourless liquid (70% yield). R_f= 0.3 (hexanes/EtOAc 20:1 (v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.70 (dd, *J* = 5.4, 3.0 Hz, 2H), 4.46 – 4.18 (m, 1H), 2.13 – 1.96 (m, 1H), 1.80 – 1.67 (m, 1H), 1.56 – 1.50 (m, 1H), 1.47 (d, *J* = 6.9 Hz, 3H), 1.27 – 1.13 (m, 1H), 1.13 – 0.99 (m, 1H), 0.85 (dd, *J* = 6.5, 4.4 Hz, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.7, 133.9, 132.2, 123.2, 48.0, 36.1, 31.8, 27.9, 22.8, 22.6, 18.9. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{15}H_{19}NO_2Na[M + Na]^+$, 268.1313. Found, 268.1312.

5,8-Diacetate-19,20-dihydromutilin (1x)[4]

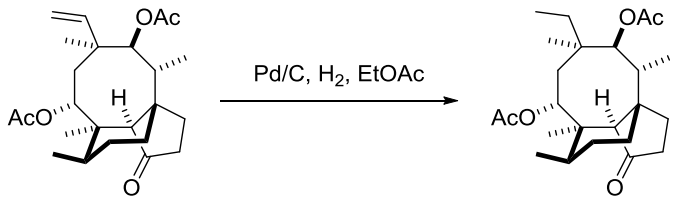


A solution of pleuromutilin (2.40 g, 6.34 mmol, 1.00 equiv) in water (9.0 mL) and ethanol (15.0 mL) was added 1.26 mL NaOH (50% aq.). The mixture was heated at 50 ^{o}C for 3 hr. After cooling to room temperature, the reaction was diluted with water and concentrated to precipitate the crude product. The solid was filtered, washed with water and hexanes, and then dried under vacuum to afford a white solid. The white solid dissolved with pyridine (90 mL) was added DMAP (1.05 g, 8.60 mmol, 0.500 equiv) and acetic anhydride (45 mL, 482 mmol, 28 equiv). The mixture was heated at 100 ^{o}C for 6h. After cooling to room temperature, the reaction was quenched with EtOAc 100 mL and washed with 2M HCl (20 mL) 3 times. The aqueous layer was extracted once with EtOAc. The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 5:1 (v/v) to afford 4.46 g 5,8-diacetatemutilin[5] (59% yield). R_f = 0.2 (hexanes/EtOAc 5:1 (v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.35 (dd, *J* = 17.5, 11.2 Hz, 1H), 5.64 (d, *J* = 8.1 Hz, 1H), 5.25 (dd, *J* = 11.2, 1.1 Hz, 1H), 5.17 (dd, *J* = 17.5, 1.2 Hz, 1H), 4.88 (d, *J* = 6.7 Hz, 1H), 2.50 (p, *J* = 7.0 Hz, 1H), 2.31 (dd, *J* = 19.5, 10.5 Hz, 1H), 2.23 – 2.10 (m, 3H), 2.08 (s, 3H), 1.97 (s,

[4] Duquenne, C.; Gallagher, T. F.; Axten, J. M. *Tetrahedron Lett.* **2010**, *51*, 1937.

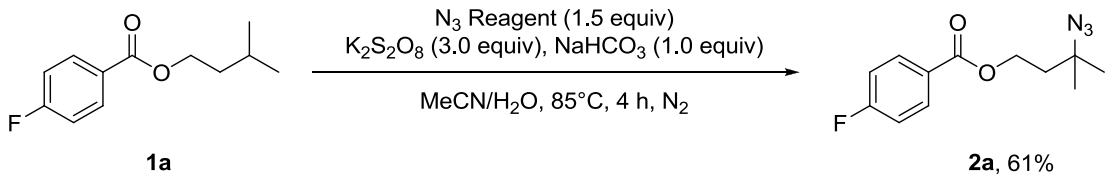
[5] Hicklin, R. W.; López Silva, T. L.; Hergenrother, P. J. *Angew. Chem. Int. Ed.* **2014**, *53*, 9880.

3H), 1.95 – 1.82 (m, 1H), 1.77 – 1.53 (m, 3H), 1.45 (s, 3H), 1.35 (dd, *J* = 14.5, 9.0 Hz, 3H), 1.12 (td, *J* = 14.0, 4.4 Hz, 1H), 1.00 (s, 3H), 0.79 (d, *J* = 7.1 Hz, 3H), 0.71 (d, *J* = 6.8 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 217.6, 170.7, 169.8, 139.7, 116.3, 68.3, 58.8, 45.4, 45.3, 43.0, 42.0, 36.9, 36.2, 34.7, 30.4, 27.4, 27.0, 25.2, 22.1, 20.9, 16.4, 15.0, 11.9.



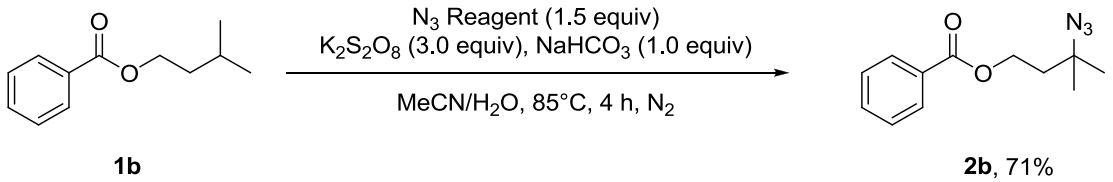
To a solution of 5, 8-diacetatemutilin (404 mg, 1.00 mmol, 1.0 equiv) in EtOAc (15 mL) was added 10 percent palladium on activated carbon (40 mg, 10%). The reaction mixture was stirred at 23 ^{o}C for 5 hr under H_2, before filtered on Celite and concentrated *in vacuo* to afford 288 mg 5, 8-diacetate-19, 20-dihydromutilin (**1x**)[4] (71% yield). R_f = 0.2 (hexanes/EtOAc 5:1 (v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.62 (d, *J* = 7.9 Hz, 1H), 4.83 (d, *J* = 6.8 Hz, 1H), 2.55 (p, *J* = 7.0 Hz, 1H), 2.30 (dd, *J* = 19.8, 10.9 Hz, 1H), 2.21 – 2.11 (m, 3H), 2.07 (s, 3H), 1.98 (s, 3H), 1.93 – 1.51 (m, 6H), 1.44 (s, 3H), 1.38 – 1.29 (m, 3H), 1.11 (td, *J* = 13.9, 4.5 Hz, 1H), 0.83 – 0.72 (m, 9H), 0.70 (d, *J* = 6.7 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 217.8, 170.7, 170.1, 78.1, 67.9, 58.9, 45.5, 41.9, 41.0, 40.1, 36.9, 34.7, 34.6, 30.5, 27.0, 25.7, 25.1, 22.1, 22.0, 21.0, 16.4, 15.0, 11.9, 8.2.

3-Azido-3-methylbutyl 4-fluorobenzoate (2a)



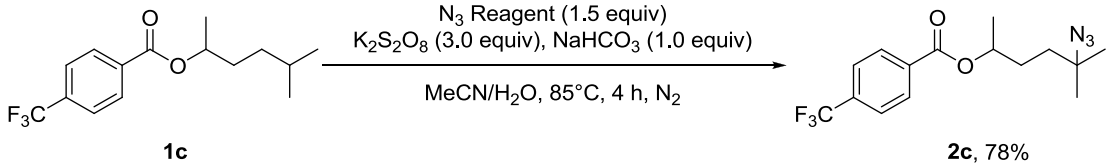
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 3-methylbutyl fluorobenzoate (**1a**) (63.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 49.1 mg 3-azido-3-methylbutyl 4-fluorobenzoate (**2a**) as a colorless liquid (61% yield). R_f= 0.20 (hexanes/EtOAc 50:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (dd, *J* = 8.7, 5.5 Hz, 2H), 7.10 (t, *J* = 8.6 Hz, 2H), 4.43 (t, *J* = 6.8 Hz, 2H), 1.97 (t, *J* = 6.8 Hz, 2H), 1.37 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9 (d, *J* = 254.0 Hz), 165.6, 132.2 (d, *J* = 9.2 Hz), 126.5, 115.7 (d, *J* = 21.9 Hz), 61.5, 60.3, 39.8, 26.5. IR(neat): υ(cm^{-1}) 2973, 2934, 2876, 2101, 1721, 1604, 1462, 1276, 1091, 854, 767. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{12}H_{14}FN_3O_2Na$ $[M + Na]^+$, 274.0968. Found, 274.0965.

3-Azido-3-methylbutyl benzoate (2b)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 3-methylbutyl benzoate (**1b**) (57.6 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated in vacuo and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 49.8 mg 3-azido-3-methylbutyl benzoate (**2b**) as a colorless liquid (71% yield). R_f= 0.20 (hexanes/EtOAc 50:1 (v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, CDCl3) δ 8.18 – 7.90 (m, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.7 Hz, 2H), 4.44 (t, *J* = 6.8 Hz, 2H), 1.98 (t, *J* = 6.8 Hz, 2H), 1.38 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.6, 133.1, 130.3, 129.7, 128.5, 61.4, 60.4, 39.9, 26.5. IR(neat): υ(cm^{-1}) 2971, 2933, 2875, 2101, 1720, 1316, 1114, 712. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{12}H_{15}N_3O_2Na$ $[M + Na]^+$, 256.1062. Found, 256.1058.

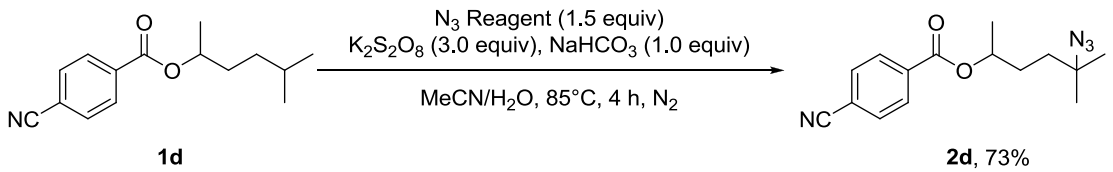
4-Azido-1,4-dimethylpentyl 4-(trifluoromethyl) benzoate (2c)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl 4-(trifluoromethyl) benzoate (**1c**) (86.4 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 77.0 mg 4-azido-1,4-dimethylpentyl 4-(trifluoromethyl) benzoate (**2c**) as a colorless liquid (78% yield). R_f= 0.30 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.15 (d, *J* = 8.1 Hz, 2H), 7.70 (d, *J* = 8.2 Hz, 2H), 5.06 – 5.16 (m, 1H), 1.97 – 1.68 (m, 2H), 1.68 – 1.45 (m, 2H), 1.38 (d, *J* = 6.2 Hz, 3H), 1.28 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.0, 134.5 (q, *J* = 32.7 Hz), 134.0, 125.5 (q, *J* = 3.7 Hz), 123.8 (q, *J* = 272.7 Hz),

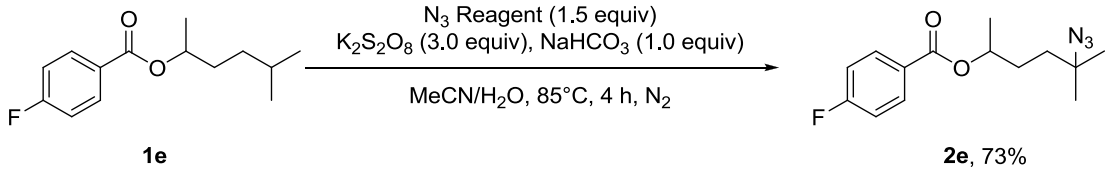
72.4, 61.3, 37.2, 30.8, 26.2, 26.1, 20.2. IR(neat): υ(cm^{-1}) 2978, 2934, 2875, 2096, 1722, 1462, 1279, 1169, 1132, 1018, 863, 776, 705. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{15}H_{18}F_3N_3O_2Na$ $[M + Na]^+$, 352.1249. Found, 352.1247.

4-Azido-1,4-dimethylpentyl 4-cyanobenzoate (2d)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl 4-cyanobenzoate (**1d**) (85.8 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 71.6 mg 4-azido-1,4-dimethylpentyl 4-cyanobenzoate (**2d**) as a colorless liquid (73% yield). R_f= 0.30 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 8.12 (d, *J* = 7.8 Hz, 2H), 7.73 (d, *J* = 7.9 Hz, 2H), 5.04 – 5.24 (m, 1H), 1.92 – 1.65 (m, 2H), 1.65 – 1.45 (m, 2H), 1.36 (d, *J* = 6.1 Hz, 3H), 1.26 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.5, 134.5, 132.3, 130.1, 118.1, 116.3, 72.7, 61.2, 37.0, 30.7, 26.1, 26.1, 20.1. IR(neat): υ(cm^{-1}) 2979, 2930, 2861, 2230, 2108, 1715, 1344, 1283, 1149, 858, 765, 688. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{15}H_{18}N_4O_2Na$ $[M + Na]^+$, 309.1327. Found, 309.1328.

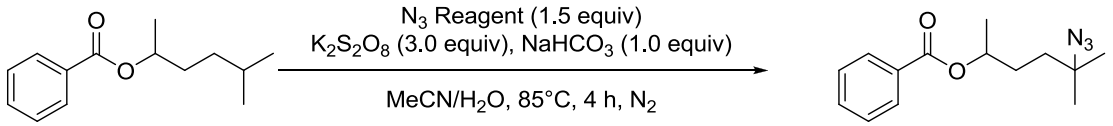
4-Azido-1,4-dimethylpentyl 4-fluorobenzoate (2e)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl 4-fluorobenzoate (**1e**) (71.4 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 61.1 mg 4-azido-1,4-dimethylpentyl 4-fluorobenzoate (**2e**) as a colorless liquid (73% yield). R_f= 0.30

(hexanes/EtOAc 50:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (t, *J* = 6.4 Hz, 2H), 7.10 (t, *J* = 8.1 Hz, 2H), 5.02 – 5.22 (m, 1H), 1.88 – 1.65 (m, 2H), 1.66 – 1.46 (m, 2H), 1.35 (d, *J* = 6.1 Hz, 3H), 1.27 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.8 (d, *J* = 253.7 Hz), 165.3, 132.2 (d, *J* = 9.3 Hz), 126.9 (d, *J* = 2.9 Hz), 115.6 (d, *J* = 22.0 Hz), 71.8, 61.3, 37.1, 30.9, 26.1 (d, *J* = 7.3 Hz), 20.2. IR(neat): υ(cm^{-1}) 2962, 2932, 2887, 2097, 1732, 1461, 1368, 1247, 1026, 974. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{18}FN_3O_2Na$ [M + Na]$^+$, 302.1281. Found, 302.1278.

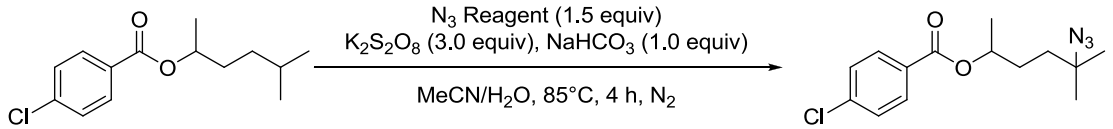
4-Azido-1,4-dimethylpentyl benzoate (2f)



1f **2f**, 67%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl benzoate (**1f**) (66.0 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 52.5 mg 4-azido-1,4-dimethylpentyl benzoate (**2f**) as a colorless liquid (67% yield). R_f= 0.30 (hexanes/EtOAc 50:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (d, *J* = 7.2 Hz, 2H), 7.56 (t, *J* = 7.4 Hz, 1H), 7.44 (t, *J* = 7.6 Hz, 2H), 5.05 – 5.25 (m, 1H), 1.88 – 1.67 (m, 2H), 1.67 – 1.49 (m, 2H), 1.37 (d, *J* = 6.3 Hz, 3H), 1.28 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.2, 132.9, 130.7, 129.6, 128.4, 71.6, 61.3, 37.2, 30.9, 26.2, 26.1, 20.3. IR(neat): υ(cm^{-1}) 2975, 2933, 29872, 2095, 1717, 1276, 1112, 1067, 804, 713. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{19}N_3O_2Na$ [M + Na]$^+$, 284.1375. Found, 284.1372.

4-Azido-1,4-dimethylpentyl 4-chlorobenzoate (2g)

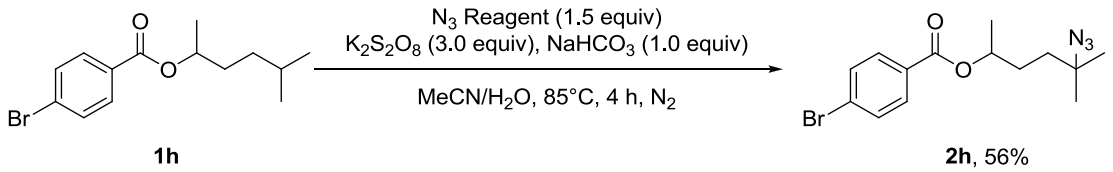


1g **2g**, 65%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl 4-chlorobenzoate (**1g**) (76.4 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0

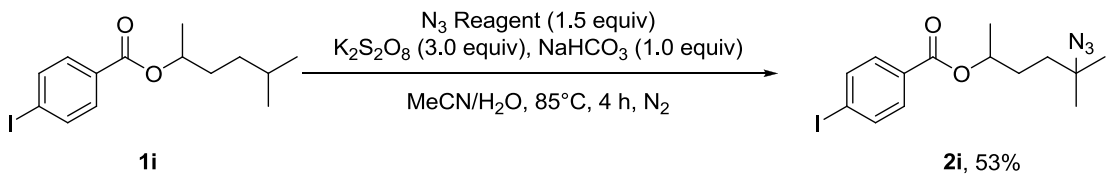
mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 57.7 mg 4-azido-1,4-dimethylpentyl 4-chlorobenzoate (**2g**) as a colorless liquid (65% yield). R_f= 0.30 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 8.5 Hz, 2H), 7.41 (d, *J* = 8.5 Hz, 2H), 5.05 – 5.25 (m, 1H), 1.88 – 1.66 (m, 2H), 1.65 – 1.47 (m, 2H), 1.36 (d, *J* = 6.2 Hz, 3H), 1.27 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.4, 139.4, 131.1, 129.2, 128.8, 72.0, 61.3, 37.2, 30.9, 26.2, 26.1, 20.2. IR(neat): υ(cm^{-1}) 2976, 2931, 2855, 2095, 1719 1591, 1272, 1115, 851, 760. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{18}ClN_3O_2Na$ [M + Na]$^+$, 318.0985. Found, 318.0982.

4-Azido-1,4-dimethylpentyl 2-bromobenzoate (2h)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl 2-bromobenzoate (**1h**) (89.8 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 57.1 mg 4-azido-1,4-dimethylpentyl 2-bromobenzoate (**2h**) as a colorless liquid (56 % yield). R_f= 0.30 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 7.8 Hz, 2H), 7.57 (d, *J* = 7.9 Hz, 2H), 5.05 – 5.25 (m, 1H), 1.89 – 1.65 (m, 2H), 1.64 – 1.46 (m, 2H), 1.35 (d, *J* = 6.2 Hz, 3H), 1.27 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.5, 131.8, 131.2, 129.6, 128.0, 72.0, 61.3, 37.1, 30.8, 26.2, 26.1, 20.2. IR(neat): υ(cm^{-1}) : 2976, 2932, 2871, 2095, 1718, 1590, 1270, 1114, 849, 757. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{18}BrN_3O_2Na$ [M + Na]$^+$, 362.0480. Found, 362.0478.

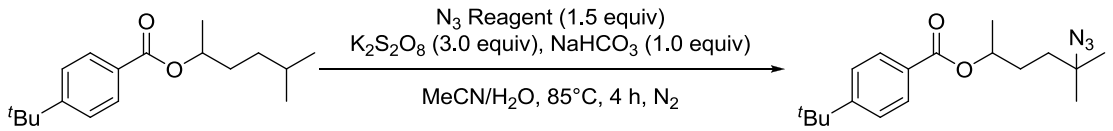
4-Azido-1,4-dimethylpentyl 2-iodobenzoate (2i)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed

by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and 4-azido-1,4-dimethylpentyl 2-iodobenzoate (**1i**) (103.9 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 61.6 mg 1,4-dimethylpentyl 2-iodobenzoate (**2i**) as a colorless liquid (53% yield). R_f= 0.30 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 7.80 (d, *J* = 8.3 Hz, 2H), 7.73 (d, *J* = 8.3 Hz, 2H), 5.12 (m, 1H), 1.89 – 1.65 (m, 2H), 1.64 – 1.46 (m, 2H), 1.35 (d, *J* = 6.2 Hz, 3H), 1.27 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 165.7, 137.8, 131.1, 130.2, 100.7, 72.0, 61.3, 37.2, 30.9, 26.2, 26.1, 20.2. IR(neat): υ(cm-1) : 2974, 2930, 2855, 2095, 1718, 1586, 1114, 1103, 1008, 847, 754. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{18}IN_3O_2Na$ $[M + Na]^+$, 410.0341. Found, 410.0340.

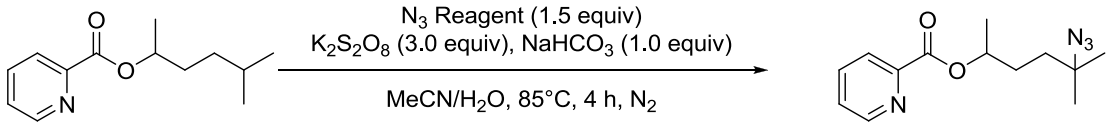
4-Azido-1,4-dimethylpentyl 4-(*tert*-butyl) benzoate (2j)



1j **2j**, 54%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and 1,4-dimethylpentyl 4-(*tert*-butyl) benzoate (**1j**) (82.9 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 51.6 mg 4-azido-1,4-dimethylpentyl 4-(*tert*-butyl) benzoate (**2j**) as a colorless liquid (54% yield). R_f= 0.30 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 7.98 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 5.05 – 5.25 (m, 1H), 1.89 – 1.64 (m, 2H), 1.65 – 1.47 (m, 2H), 1.45 – 1.30 (m, 12H), 1.28 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.3, 156.6, 129.5, 128.0, 125.4, 71.3, 61.3, 37.2, 35.2, 31.2, 30.9, 26.2, 26.1, 20.3. IR(neat): $\upsilon(cm^{-1})$: 2967, 2870, 2095, 1717, 1188, 1063, 855, 775, 708. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{18}H_{27}N_3O_2Na$ $[M + Na]^+$, 340.2001. Found, 340.2000.

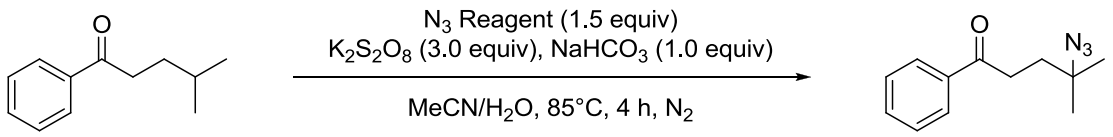
4-Azido-1,4-dimethylpentyl picolinate (2k)



1k **2k**, 50%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 1,4-dimethylpentyl picolinate (**1k**) (66.4 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 10:1 (v/v), to afford 39.3 mg 4-azido-1,4-dimethylpentyl picolinate (**2k**) as a colorless liquid (50% yield). R_f= 0.40 (hexanes/EtOAc 2:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, *J* = 4.4 Hz, 1H), 8.12 (d, *J* = 7.8 Hz, 1H), 7.84 (t, *J* = 7.7 Hz, 1H), 7.47 (dd, *J* = 7.4, 4.8 Hz, 1H), 5.36 – 5.14 (m, 1H), 2.00 – 1.83 (m, 1H), 1.82 – 1.69 (m, 1H), 1.69 – 1.48 (m, 2H), 1.42 (d, *J* = 6.3 Hz, 3H), 1.28 (s, 3H), 1.27 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 164.8, 150.0, 148.4, 137.1, 126.9, 125.2, 72.8, 61.3, 37.3, 30.8, 26.2, 25.9, 20.2. IR(neat): υ(cm^{-1}) : 2976, 2932, 2872, 2095, 1738, 1716 1305, 1246, 1125, 748, 708, 619. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{13}H_{18}N_4O_2Na$ $[M + Na]^+$, 285.1328. Found, 285.1327.

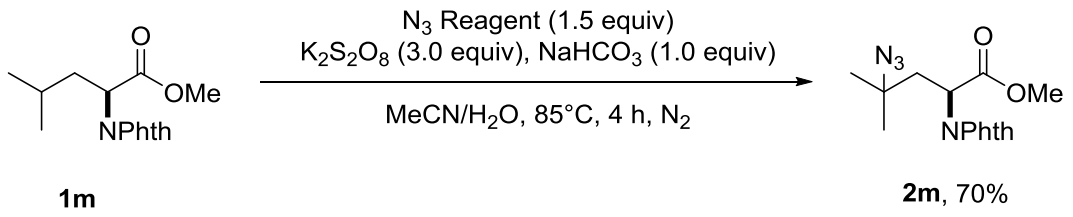
4-Azido-4-methyl-1-phenyl-1-pentanone (2l)



1l **2l**, 56%

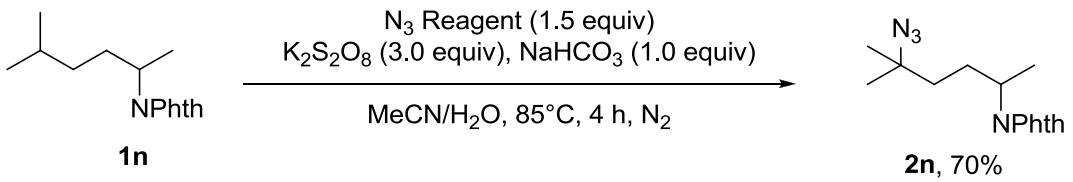
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 4-methyl-1-phenyl-1-pentanone (**1l**) (52.9 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 36.5 mg 4-azido-4-methyl-1-phenyl-1-pentanone (**2l**) as a colorless liquid (56% yield). R_f= 0.30 (hexanes/EtOAc 10:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.97 (d, *J* = 7.4 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.47 (t, *J* = 7.6 Hz, 2H), 3.07 (t, *J* = 7.7 Hz, 2H), 1.94 (t, *J* = 7.7 Hz, 2H), 1.34 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 199.5, 136.8, 133.2, 128.7, 128.1, 61.2, 35.4, 33.7, 26.2. IR(neat): υ(cm^{-1}) : 2970, 2929, 2855, 2100, 1687, 1258, 743, 690. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{12}H_{15}N_3ONa$ $[M + Na]^+$, 240.1113. Found, 240.1110.

_N_-Phthaloyl-4-azido-_L_-leucine methyl ester (2m)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and *N*-phthaloyl-L-leucine methyl ester (**1m**) (82.5 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 2:1 (v/v), to afford 66.4 mg *N*-Phthaloyl-4-azido-*L*-leucine methyl ester (**2m**) as a colorless liquid (70% yield). R_f= 0.20 (hexanes/EtOAc 5:1 ((v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 7.87 (dd, *J* = 4.7, 2.2 Hz, 2H), 7.74 (dd, *J* = 4.7, 2.2 Hz, 2H), 5.05 (d, *J* = 10.0 Hz, 1H), 3.72 (s, 3H), 2.62 – 2.31 (m, 2H), 1.37 (s, 3H), 1.30 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.8, 167.7, 134.4, 131.9, 123.7, 60.3, 53.2, 48.6, 39.0, 26.9, 25.3. IR(neat): $\upsilon(cm^{-1})$: 2971, 2957, 2930,2852,098, 1775, 1748, 1717, 1390, 1267, 758. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{15}H_{16}N_4O_4Na$ $[M + Na]^+$, 339.1068. Found, 339.1069

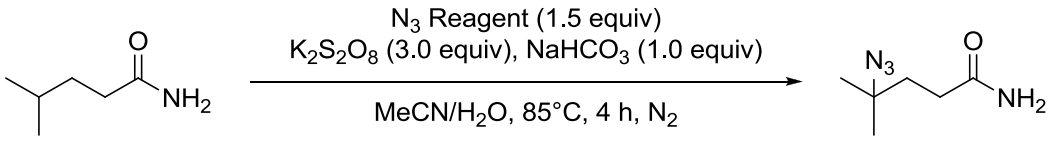
_N_-Phthaloyl-5-azido-5-methylhexan-2-amine (2n)



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and *N*-phthaloyl-6-methylheptan-2-amine (**1n**) (73.6 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 60.1 mg *N*-Phthaloyl-5-azido-5-methylhexan-2-amine (**2n**) as a colorless liquid (70 % yield). R_f= 0.40 (hexanes/EtOAc 10:1 ((v/v)). NMR Spectroscopy: ^1H NMR (400 MHz, $CDCl_3$) δ 7.82 (dd, *J* = 5.4, 3.1 Hz, 2H), 7.71 (dd, *J* = 5.5, 3.0 Hz, 2H), 4.38 – 4.23 (m, 1H), 2.28 – 2.05 (m, 1H),

1.90 – 1.73 (m, 1H), 1.48 (d, *J* = 6.9 Hz, 3H), 1.33 (td, *J* = 13.5, 13.0, 4.5 Hz, 2H), 1.23 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 168.6, 134.0, 132.0, 123.3, 61.3, 47.7, 38.7, 28.6, 26.2, 25.9, 19.0. IR(neat): υ(cm^{-1}) : 2956, 2925, 2854, 2094, 1709, 1465, 1369, 1259, 877, 798, 721. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{18}BrN_3O_2Na$ [M + Na]$^+$, 309.1327. Found, 309.1328.

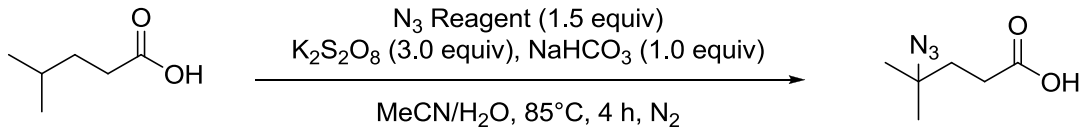
4-Azido-4-methylpentanamide (2o)



1o **2o**, 69%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv), $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv) and 4-methylpentanamide (**1o**) (34.6 mg, 0.300 mmol, 1.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 1:1 (v/v), to afford 32.3 mg 4-azido-4-methylpentanamide (**2o**) as a white solid (69% yield). R_f= 0.30 (hexanes/EtOAc 1:2 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.12 – 5.52 (br, 2H), 2.29 (t, *J* = 8.0 Hz, 2H), 1.82 (t, *J* = 8.0 Hz, 2H), 1.28 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 175.2, 61.1, 36.7, 30.8, 26.0. IR(neat): υ(cm^{-1}) :3195, 2933, 2864, 2102,1611, 1643, 1470, 1262. Mass Spectrometry: MS-EI (m/z): Calcd for $C_6H_{12}N_4O$ [M], 156.1. Found, 156.1.

4-Azido-4-methylpentanoic acid (2p)

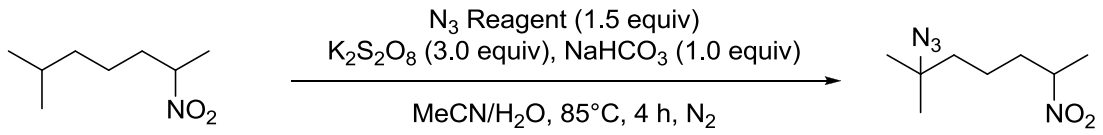


1p **2p**, 78%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 4-methylpentanoic acid (**1p**) (34.9 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 2:1 (v/v), to afford 36.8 mg 4-azido-4-methylpentanoic acid (**2p**) as a colorless liquid (78% yield). R_f= 0.10 (hexanes/EtOAc 1:1 ((v/v)). NMR

Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.45 (d, *J* = 8.1 Hz, 2H), 1.83 (t, *J* = 8.1 Hz, 2H), 1.29 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 179.8, 60.6, 35.8, 29.3, 25.8. IR(neat): υ(cm^{-1}) : 2972, 2932, 2099, 1714, 1391, 1372, 1260, 1129, 869, 799, 611. Mass Spectrometry: MS-EI (m/z): Calcd for $C_6H_{11}N_3O_2$ [M],157.1 . Found, 157.1.

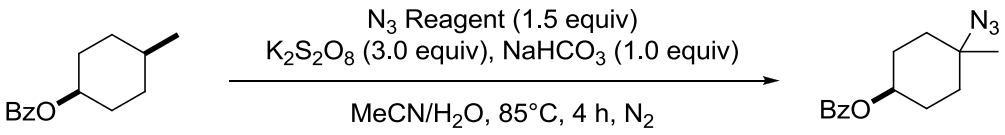
2-Azido-2-methyl-6-nitroheptane (2q)



1q **2q**, 69%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and 2-azido-2-methyl-6-nitroheptane (**1q**) (47.8 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 41.4 mg 2-azido-2-methyl-6-nitroheptane (**2q**) as a colorless liquid (69% yield). R_f= 0.20 (hexanes/EtOAc 50:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ4.66 – 4.49 (m, 1H), 2.11 – 1.97 (m, 1H), 1.81 – 1.67 (m, 1H). 1.54 (d, *J* = 6.6 Hz, 3H), 1.52 – 1.33 (m, 4H), 1.25 (s, 6H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 83.4, 61.3, 60.9, 40.9, 35.4, 26.1, 26.0, 20.7, 19.4. IR(neat): υ(cm^{-1}) : 2962, 2926, 2855, 2097, 1720, 1553, 1459, 1261, 1096, 1021, 802.

4-Azido-4-methylcyclohexyl benzoate (2r)



1r **2r**, 63%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and *cis*-4-methylcyclohexyl benzoate (**1r**) (65.5 mg, 0.300 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 50.6 mg 4-methylcyclohexyl benzoate (**2r**) as a colorless liquid (63% yield, d.r.=1:0.75).

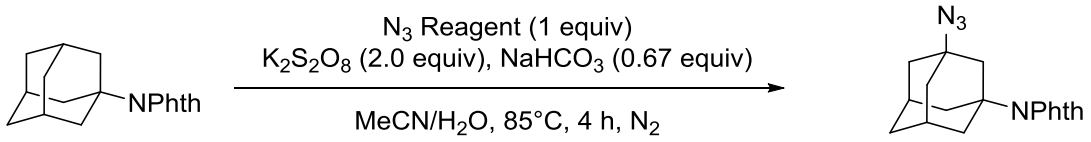
2r isomer 1

R_f= 0.40 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (d, *J* = 7.3 Hz, 2H), 7.57 (t, *J* = 7.4 Hz, 1H), 7.45 (t, *J* = 7.7 Hz, 2H), 5.33 – 5.10 (m, 1H), 1.99 – 1.83 (m, 4H), 1.77 (td, *J* = 12.7, 11.5, 4.2 Hz, 2H), 1.72 – 1.64 (m, 2H), 1.39 (s, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 166.1, 133.0, 130.7, 129.7, 128.4, 72.1, 60.5, 34.4, 27.4, 26.1. IR(neat): υ(cm-1) : 2957, 2928, 2854, 2110, 2089, 1717, 1273, 1069, 713. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{17}N_3O_2Na$ [M +Na]$^+$, 282.1218. Found, 282.1218.

2r isomer 2

R_f= 0.40 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.03 (dd, *J* = 8.3, 1.3 Hz, 2H), 7.57 (tt, *J* = 6.9, 1.3 Hz, 1H), 7.45 (t, *J* = 7.6 Hz, 2H), 5.29 – 5.19 (m, 1H), 1.99 – 1.83 (m, 4H), 1.77 (td, *J* = 12.7, 11.4, 4.3 Hz, 2H), 1.68 (dt, *J* = 14.0, 3.8 Hz, 2H), 1.39 (s, 3H).^{13}C NMR (101 MHz, $CDCl_3$) δ 165.9, 133.0, 130.9, 129.7, 128.5, 69.6, 61.1, 31.9, 26.6, 26.4. IR(neat): υ(cm^{-1}) : 2927, 2853, 2855, 2097, 1717, 1276, 1070, 712. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{14}H_{17}N_3O_2Na$ [M +Na]$^+$, 282.1218. Found, 282.1216.

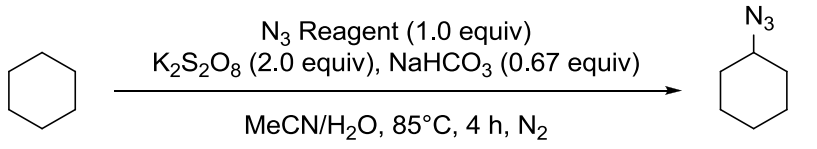
3-Azido-adamantan-1-ylisoindoline-1,3-dione (2s)



1s **2s**, 75%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv), $K_2S_2O_8$ (245 mg, 0.900 mmol, 200 equiv) and adamantan-1-ylisoindoline-1,3-dione (**1s**) (379 mg, 1.35 mmol, 3.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 109 mg 3-azido-adamantan-1-ylisoindoline-1,3-dione (**2s**) as a white solid (75% yield). R_f= 0.20 (hexanes/EtOAc 20:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.77 (dd, *J* = 5.5, 3.1 Hz, 2H), 7.68 (dd, *J* = 5.5, 3.0 Hz, 2H), 2.58 (s, 2H), 2.52 – 2.44 (m, 4H), 2.38 (s, 2H), 1.84 (dd, *J* = 34.4, 12.5 Hz, 4H), 1.67 (dd, *J* = 49.6, 12.7 Hz, 2H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 169.5, 133.9, 131.8, 122.8, 60.9, 59.8, 44.0, 40.4, 38.8, 34.6, 30.3. IR(neat): υ(cm^{-1}) : 2912, 2896, 2855, 2103, 1768, 1699, 1363, 1325, 1256, 1081, 713. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{18}H_{18}N_4O_2Na$ [M +Na]$^+$, 345.1327. Found, 345.1325.

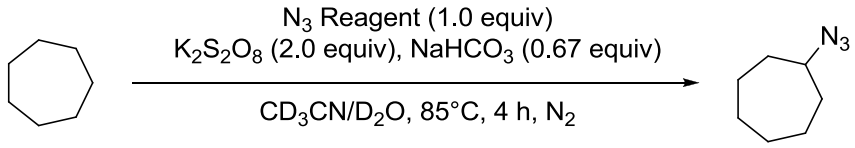
Azidocyclohexane (2t)



1t **2t**, 24%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 2.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and cyclohexane (**1t**) (189.5 mg, 2.25 mmol, 5.0 equiv). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (10.0 mL) and H_2O (1.0 mL). The yield of azidocyclohexane (**2t**) was determined by GC (24% yield) with acetophenone as a standard.

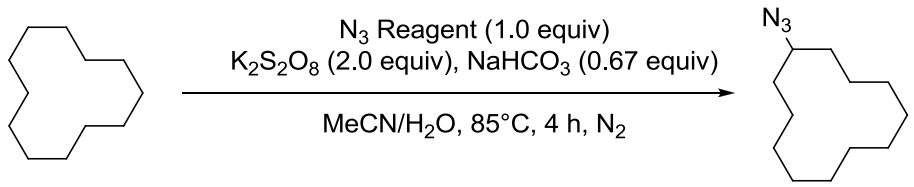
Azidocycloheptane(2u)



1u **2u**, 50%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 2.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and Cycloheptane (**1u**) (220.7 mg, 2.25 mmol, 5.00 eq.). The system was stirred for 4 hr at 85 ^oC. The yield of azidocycloheptane (**2u**) was determined by ^1H NMR (50% yield) with acetophenone as a standard.

Azidocyclododecane (2v)

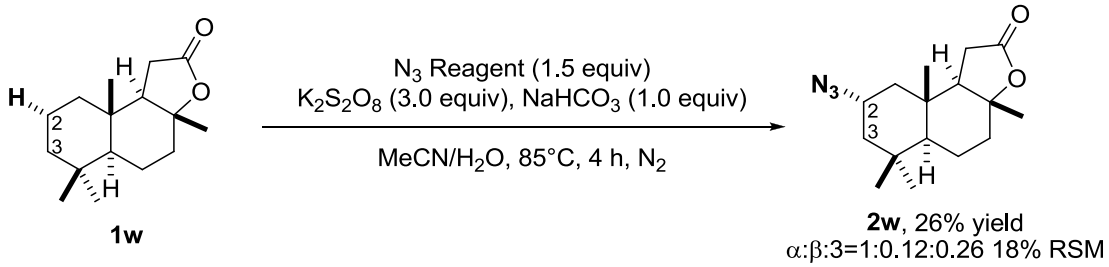


1v **2v**, 54%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv), $K_2S_2O_8$ (245 mg, 0.900 mmol, 2.00 equiv) and dodecane (**1v**) (379 mg, 2.25 mmol, 5.00 eq.). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes to afford 50.9 mg azidocyclododecane (**2v**) as a colorless liquid

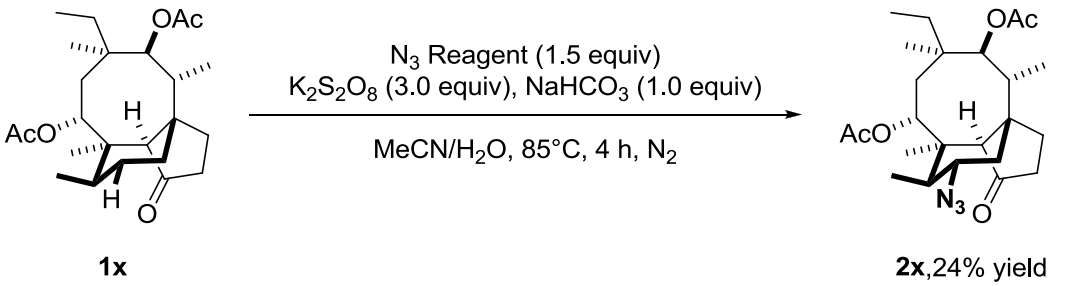
(54% yield). R_f= 0.50 (hexanes). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.57 – 3.40 (m, 1H),1.78 – 1.60 (m, 2H), 1.60 – 1.43 (m, 4H), 1.42 – 1.26 (m, 16H).^{13}C NMR (101 MHz, $CDCl_3$) δ 59.3, 29.1, 24.0, 23.8, 23.5, 23.3, 21.4. IR(neat): υ(cm^{-1}) : 2934, 2864, 2092, 1470, 1445, 1250, 719. Mass Spectrometry: MS-EI (m/z): Calcd for $C_{12}H_{23}N_3$ [M], 209.2 . Found, 209.1.

2*α*-Azidosclareolide (2w)[6]



A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv), $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv) and sclareolide (**1w**) (75.0 mg, 0.300 mmol, 1.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2). The system was stirred for 4 hr at 85 ^{o}C. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated in *vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 20:1 (v/v), to afford 22.7 mg 2*α*-azidosclareolide (**2w**) as a colorless liquid (26% yield). R_f= 0.20 (hexanes/EtOAc 10:1 (v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 3.61 (tt, *J* = 12.1, 4.2 Hz, 1H), 2.53 – 2.37 (m, 1H), 2.27 (dd, *J* = 16.2, 6.5 Hz, 1H), 2.16 – 1.97 (m, 2H), 1.95 – 1.64 (m, 4H), 1.45 – 1.16 (m, 6H), 1.14 – 1.01 (m, 2H), 1.01 – 0.94 (m, 5H), 0.94 – 0.87 (m, 3H). IR(KBr): υ(cm^{-1}) : 2955, 2928, 2971, 2853, 2144, 1738, 1434, 1296, 1174, 743, 655, 610, 568.

11-Azido-19, 20-dihydromutilin-5, 8-diacetate (2x)

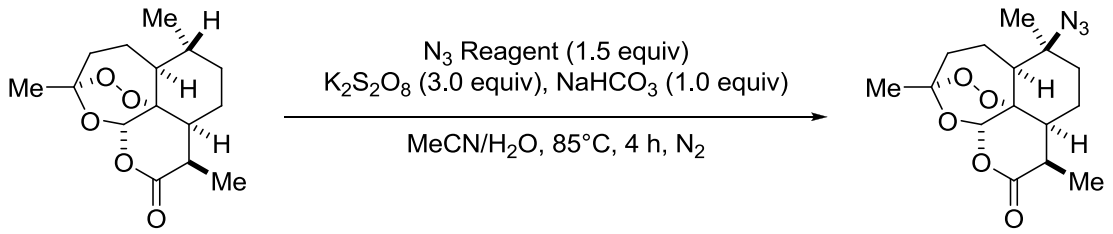


A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv), $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv) and 19, 20-dihydromutilin-5, 8-diacetate (**1x**) (122 mg, 0.300 mmol,

[6] Huang, X.; Bergsten, T. M.; Groves, J. T. *J. Am. Chem. Soc.* **2015**, *137*, 5300.

1.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 20:1 (v/v), to afford 32.2 mg 11-azido-19, 20-dihydromutilin-5, 8-diacetate (**2x**) as a colorless liquid (24% yield). R_f= 0.10 (hexanes/EtOAc 10:1 (v/v)). NMR Spectroscopy:^{1}H NMR (400 MHz, $CDCl_3$) δ 5.51 (d, *J* = 7.7 Hz, 1H), 4.83 (d, *J* = 6.8 Hz, 1H), 3.50 (td, *J* = 11.6, 3.9 Hz, 1H), 2.50 (p, *J* = 7.0 Hz, 1H), 2.36 (dd, *J* = 19.8, 11.0 Hz, 1H), 2.29 – 2.11 (m, 2H), 2.09 (s, 3H), 2.02 (s, 3H), 2.01 – 1.92 (m, 2H), 1.80 (dd, *J* = 15.0, 7.4 Hz, 3H), 1.69 – 1.60 (m, 2H), 1.49 (s, 2H), 1.46 – 1.31 (m, 3H), 1.19 – 1.06 (m, 1H), 0.87 (t, *J* = 8.5 Hz, 5H), 0.80 (s, 3H), 0.74 (t, *J* = 7.3 Hz, 3H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 216.5, 170.8, 170.3, 77.8, 68.3, 61.2, 58.2, 45.7, 42.9, 42.2, 41.0, 40.0, 36.5, 35.9, 34.4, 25.7, 25.2, 22.2, 22.1, 21.0, 15.2, 12.8, 12.2, 8.2. IR(KBr): υ(cm^{-1}) : 2962, 2932, 2887, 2097, 1732, 1461, 1368, 1247, 1162, 1026, 974. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{24}H_{37}N_3O_5Na$ $[M+Na]^+$, 470.2631. Found, 470.2628.

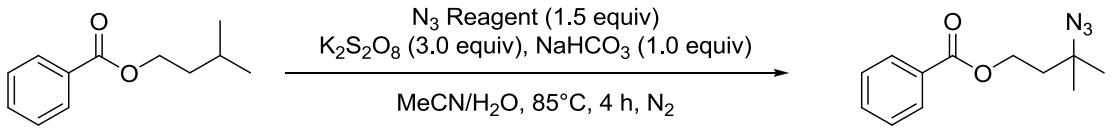
6*β*-Azidoartemisinin (2y)



1y **2y**, 33%

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.50 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 1.00 equiv), $K_2S_2O_8$ (245 mg, 0.900 mmol, 3.00 equiv) and artemisinin (**1y**) (84.6 mg, 0.300 mmol, 1.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2). The system was stirred for 4 hr at 85 ^oC. After cooling to room temperature, the reaction was diluted with EtOAc (5.0 mL) and H_2O (1.0 mL), then extracted 3 times with EtOAc (5.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated *in vacuo* and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 32.0 mg 6-azidoartemisinin (**2y**) as a withe solid (33% yield). R_f= 0.20 (hexanes/EtOAc 5:1 ((v/v)). NMR Spectroscopy: ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.38 (s, 1H), 3.40 – 3.21 (m, 1H), 2.39 (td, *J* = 13.8, 3.8 Hz, 1H), 2.19 – 1.88 (m, 3H), 1.87 – 1.72 (m, 3H), 1.68 (dd, *J* = 11.6, 6.8 Hz, 1H), 1.56 – 1.31 (m, 7H), 1.29 – 1.14 (m, 4H). ^{13}C NMR (101 MHz, $CDCl_3$) δ 172.0, 105.3, 93.8, 79.3, 64.1, 51.8, 45.2, 37.1, 35.5, 32.8, 25.3, 25.0, 19.9, 19.8, 12.7. IR(KBr): υ(cm^{-1}) : 2927, 2854, 2106, 1739, 1125, 1026, 994. Mass Spectrometry: HRMS-ESI (m/z): Calcd for $C_{15}H_{21}N_3O_5Na$ $[M+Na]^+$, 346.1379. Found, 346.1379.

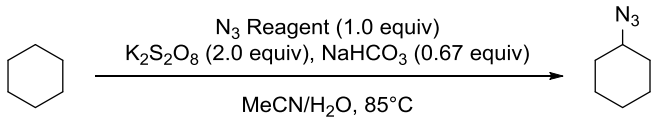
Gram-scale synthesis of 3-azido-3-methylbutyl benzoate (2b)



1b **2b**, 71%

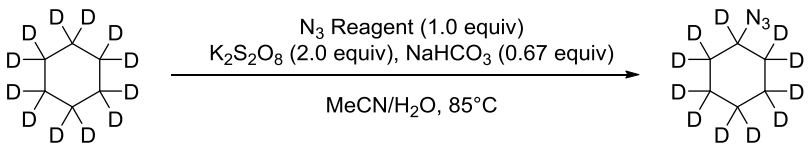
A 250 mL round-bottom flask was charged with 2-azidosulfonyl-benzoic acid methyl ester (1.88 g, 7.82 mmol, 1.50 equiv), $NaHCO_3$ (437 mg, 5.21 mmol, 1.00 equiv) and $K_2S_2O_8$ (4.22 g, 15.6 mmol, 3.00 equiv). The flask was evacuated and filled with N_2 twice, followed by addition of 65 mL of solvent and 3-methylbutyl benzoate (**1b**) (1.00 g, 5.21 mmol, 1.00 equiv). The system was stirred for 4 hr at 85 ^oC under N_2. After cooling to room temperature, the reaction was diluted with EtOAc (15.0 mL) and H_2O (5.0 mL), then extracted 3 times with EtOAc (15.0 mL). The combined organic layer was dried over $MgSO_4$. The filtrate was concentrated in vacuo and the residue was purified by chromatography on silica gel, eluting with hexanes/EtOAc 50:1 (v/v), to afford 0.887 g 3-azido-3-methylbutyl benzoate (**2b**) as a colorless liquid (73% yield).

The intermolecular kinetic isotope effect study



1t **2t**

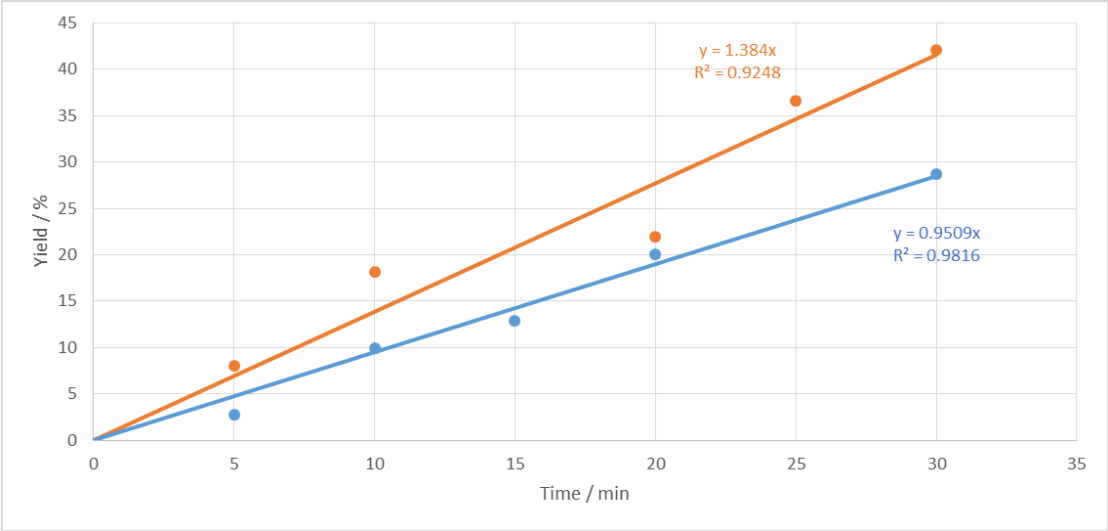
A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 2.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and cyclohexane (**1t**) (114 mg, 1.35 mmol, 3.00 equiv). The system was stirred at 85 ^oC. The reaction was cooled down to 0 ^oC immediately and quenched with EtOAc (10.0 mL) and H_2O (1.0 mL) after different periods of time. The yield of azidocyclohexane (**2t**) was determined by GC.

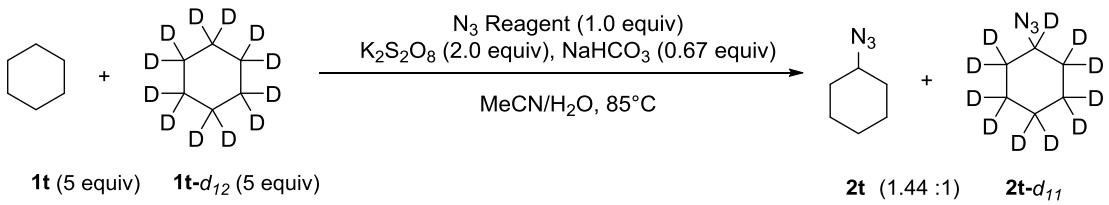


1t-d_{12} **2t-d_{11}**

A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 2.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent ($MeCN/H_2O$=3:2) and cyclohexane-d_{12} (**1t**-d_{12}) (129 mg, 1.35 mmol, 3.00 equiv). The system was stirred at 85 ^oC. The reaction was cooled down to 0 ^oC immediately and quenched with EtOAc (10.0 mL) and H_2O (1.0 mL) after different periods of time. The yield of azidocyclohexane-d_{11} (**2t**-d_{11}) was determined by GC.

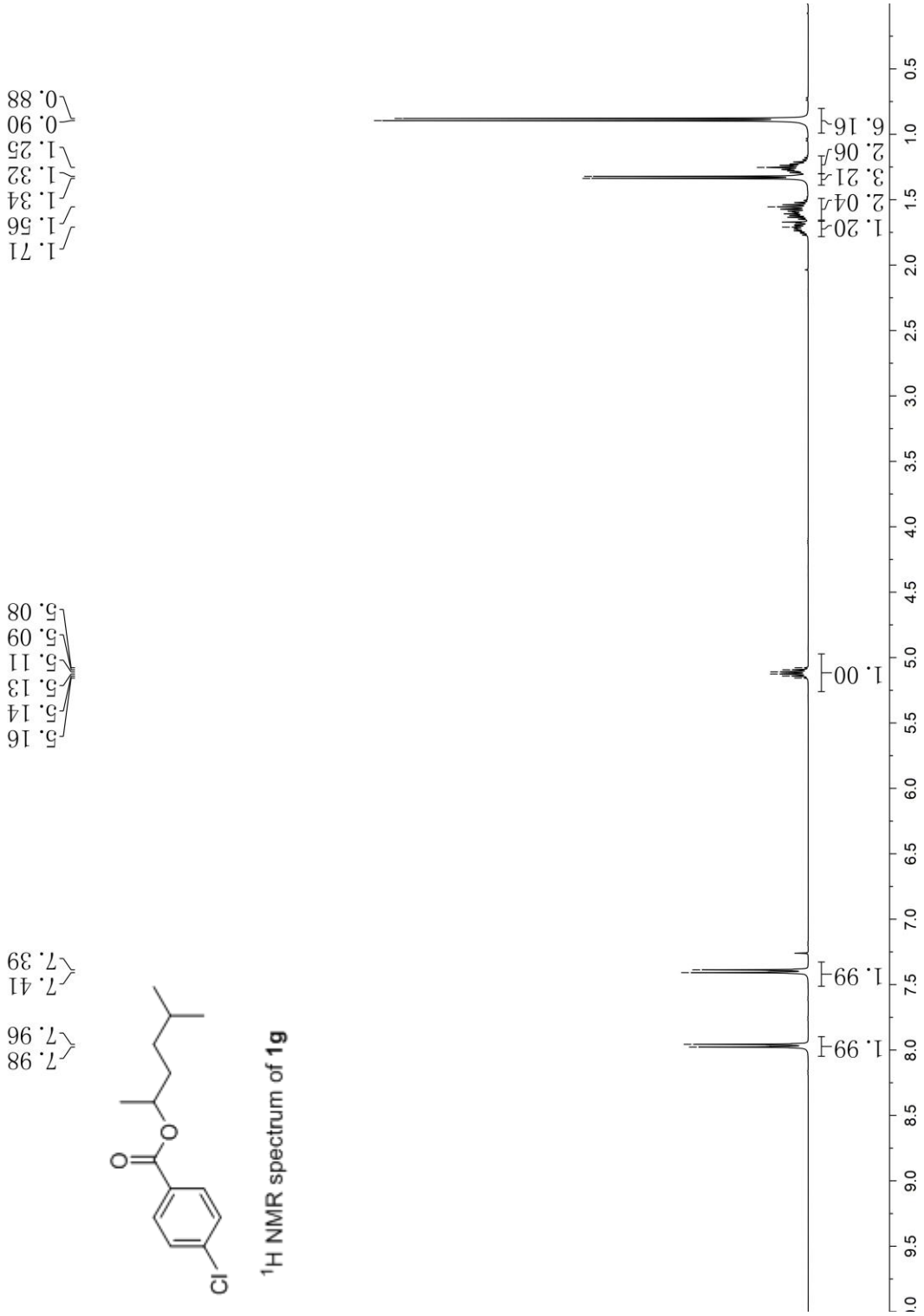
$$k_H / k_D = 1.384 / 0.9509 = 1.45$$



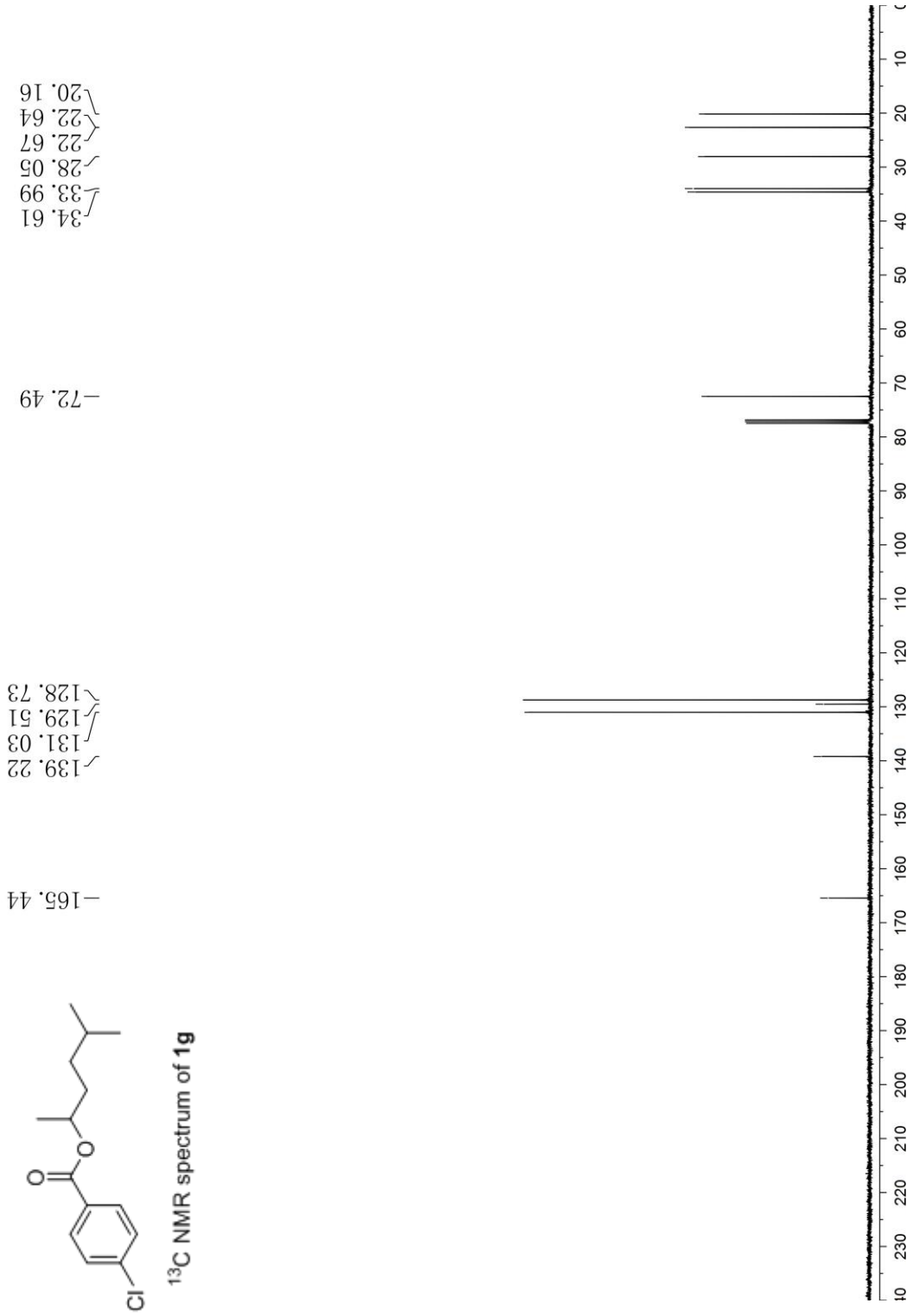


A 10 mL Schlenk tube was charged with 2-azidosulfonyl-benzoic acid methyl ester (109 mg, 0.450 mmol, 1.00 equiv), $NaHCO_3$ (25.2 mg, 0.300 mmol, 0.670 equiv) and $K_2S_2O_8$ (245 mg, 0.900 mmol, 2.00 equiv). The Schlenk tube was evacuated and filled with N_2 twice, followed by addition of 3.8 mL of solvent (MeCN/H_2O=3:2) and cyclohexane (**1t**) (189 mg, 2.25 mmol, 5.00 equiv), cyclohexane-d_{12} (**1t**-d_{12}) (216 mg, 2.25 mmol, 5.0 equiv). The system was stirred at 85 ^{o}C for 4 hr. After cooling to room temperature, the reaction was diluted with EtOAc (10.0 mL) and H_2O (1.0 mL). The ratio of azidocyclohexane (**2t**) and azidocyclohexane-d_{11} (**2t**-d_{11}) was determined by GC to be 1.44 to 1.00.

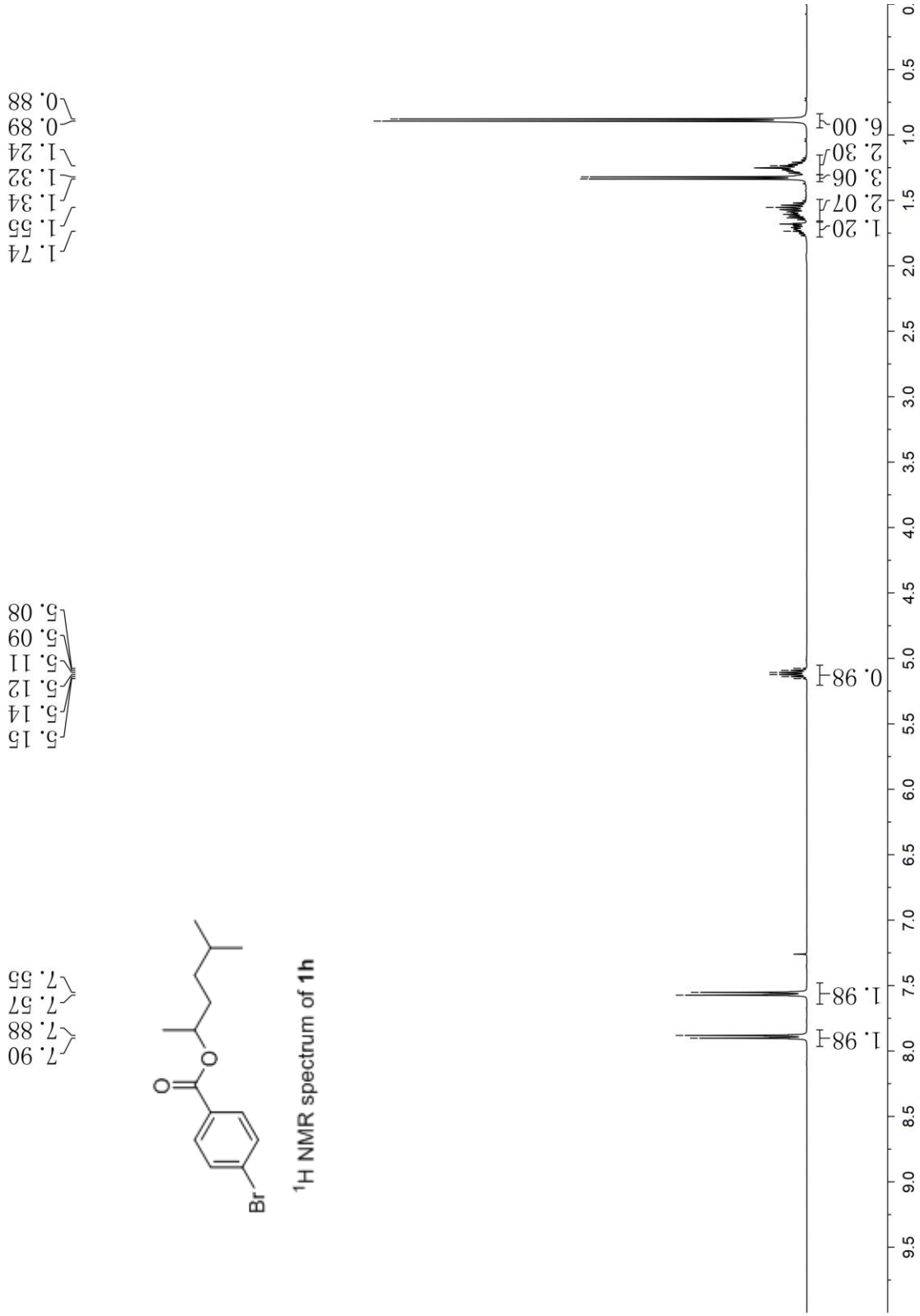
Spectroscopic Date



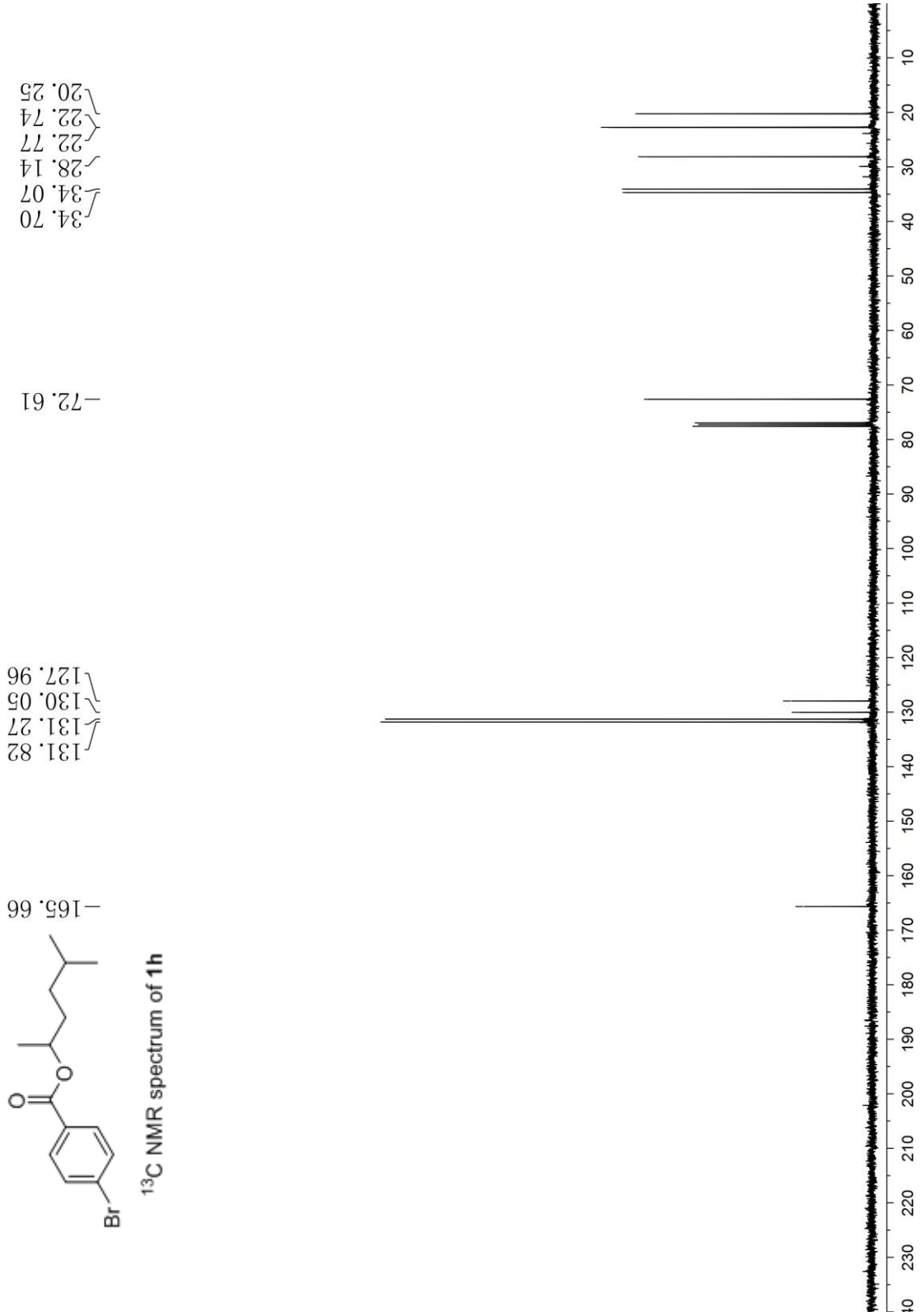
^{1}H NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **1g**



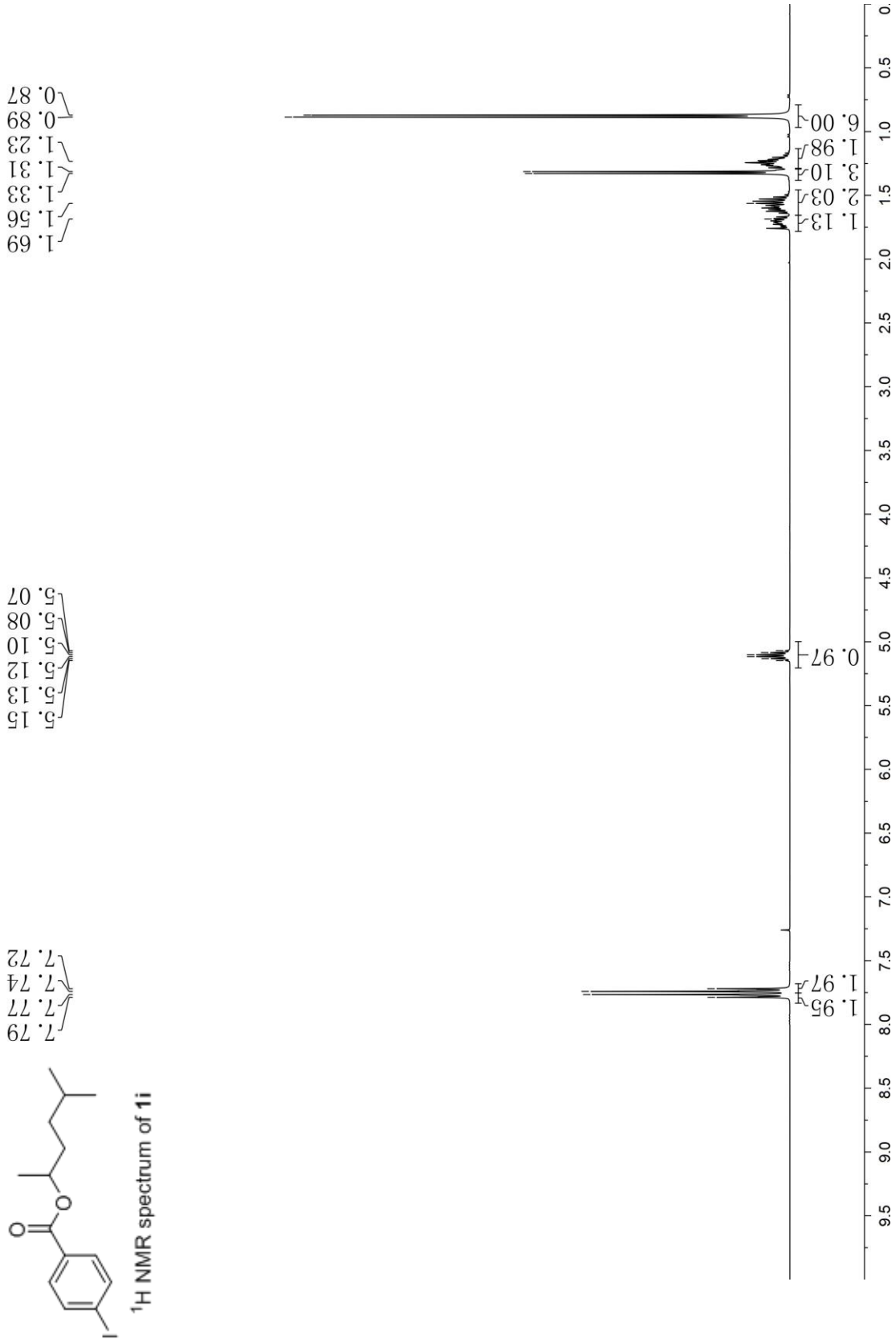
^{13}C NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **1g**



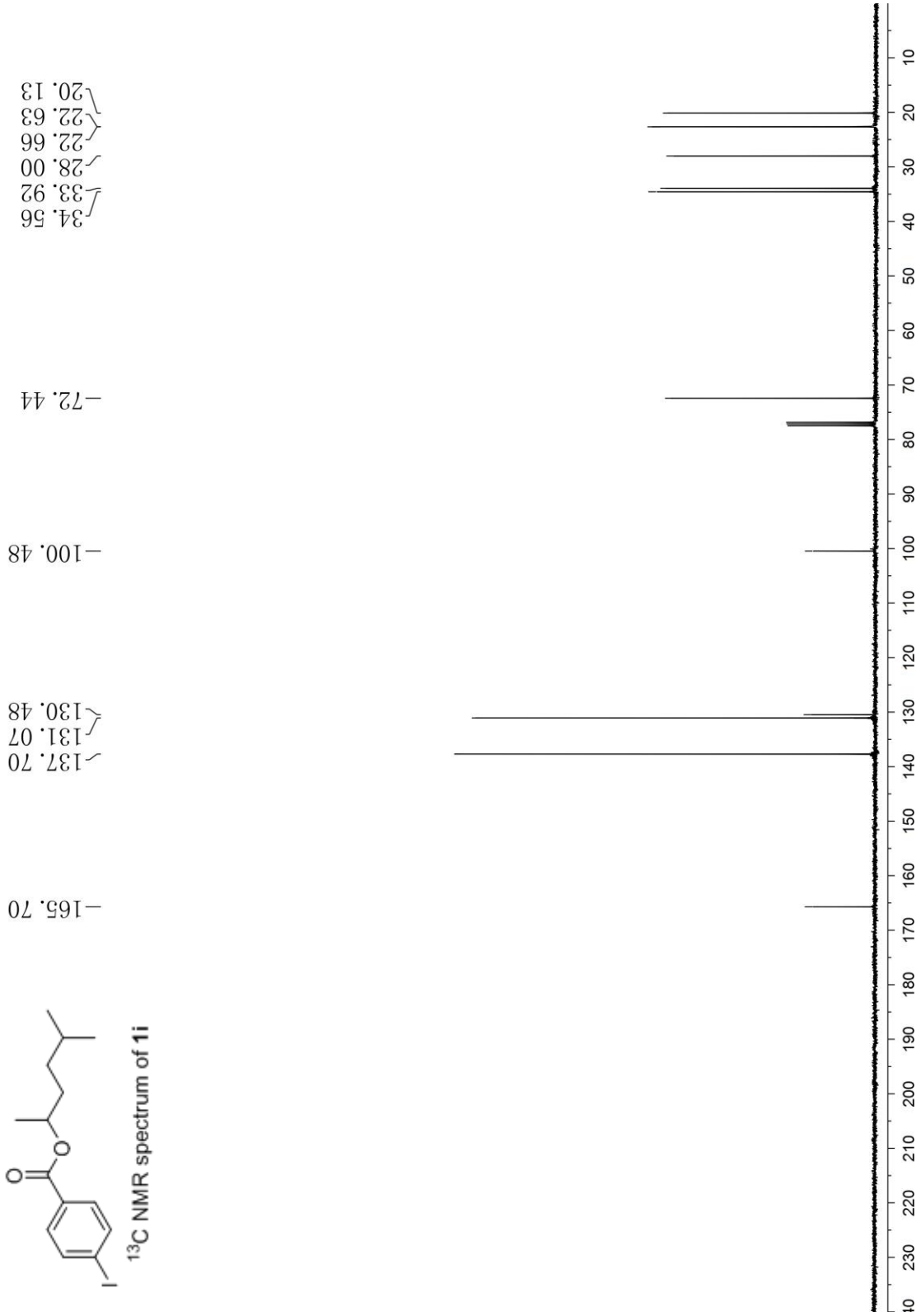
^{1}H NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **1h**



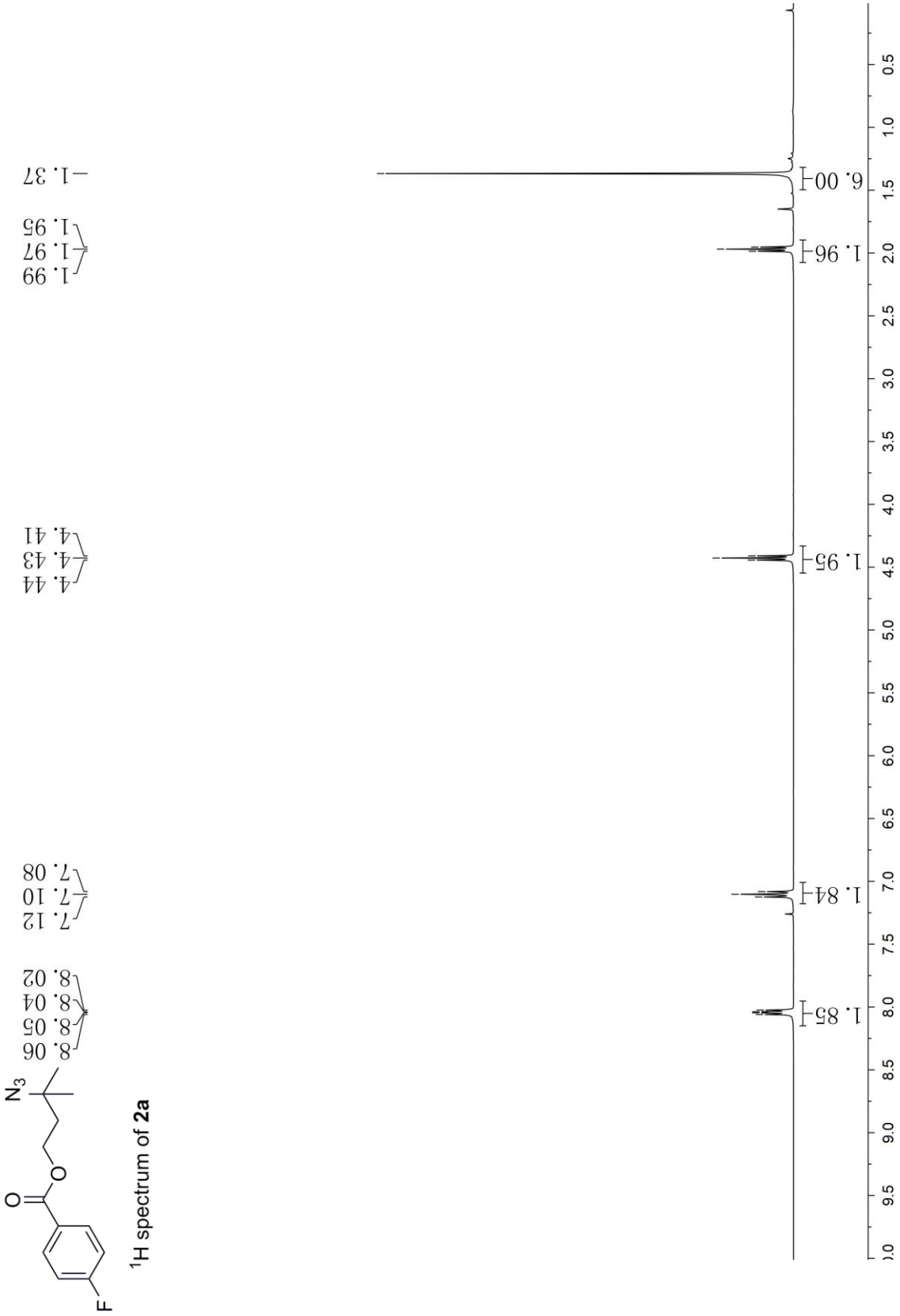
^{13}C NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **1h**



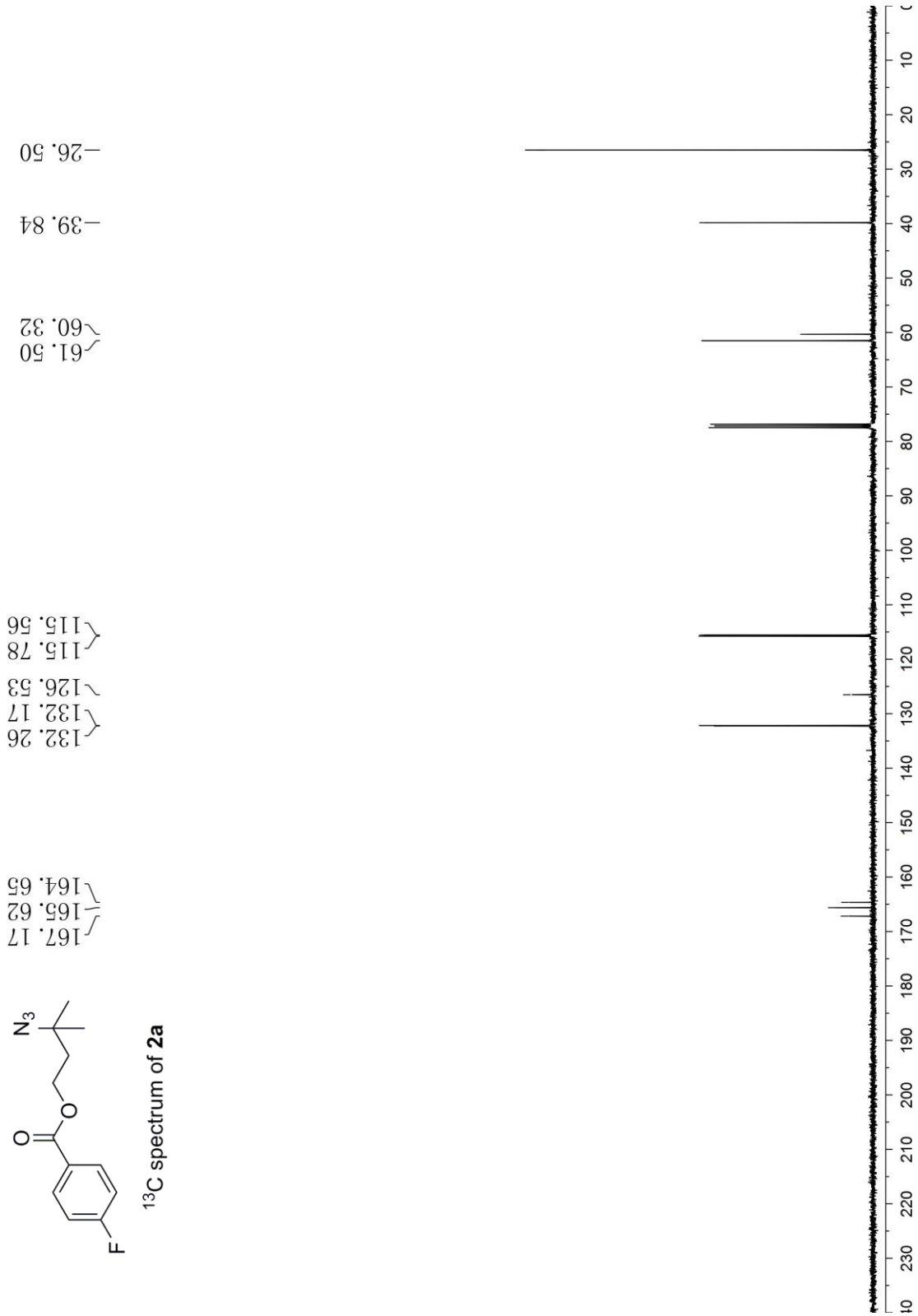
^{1}H NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **1i**



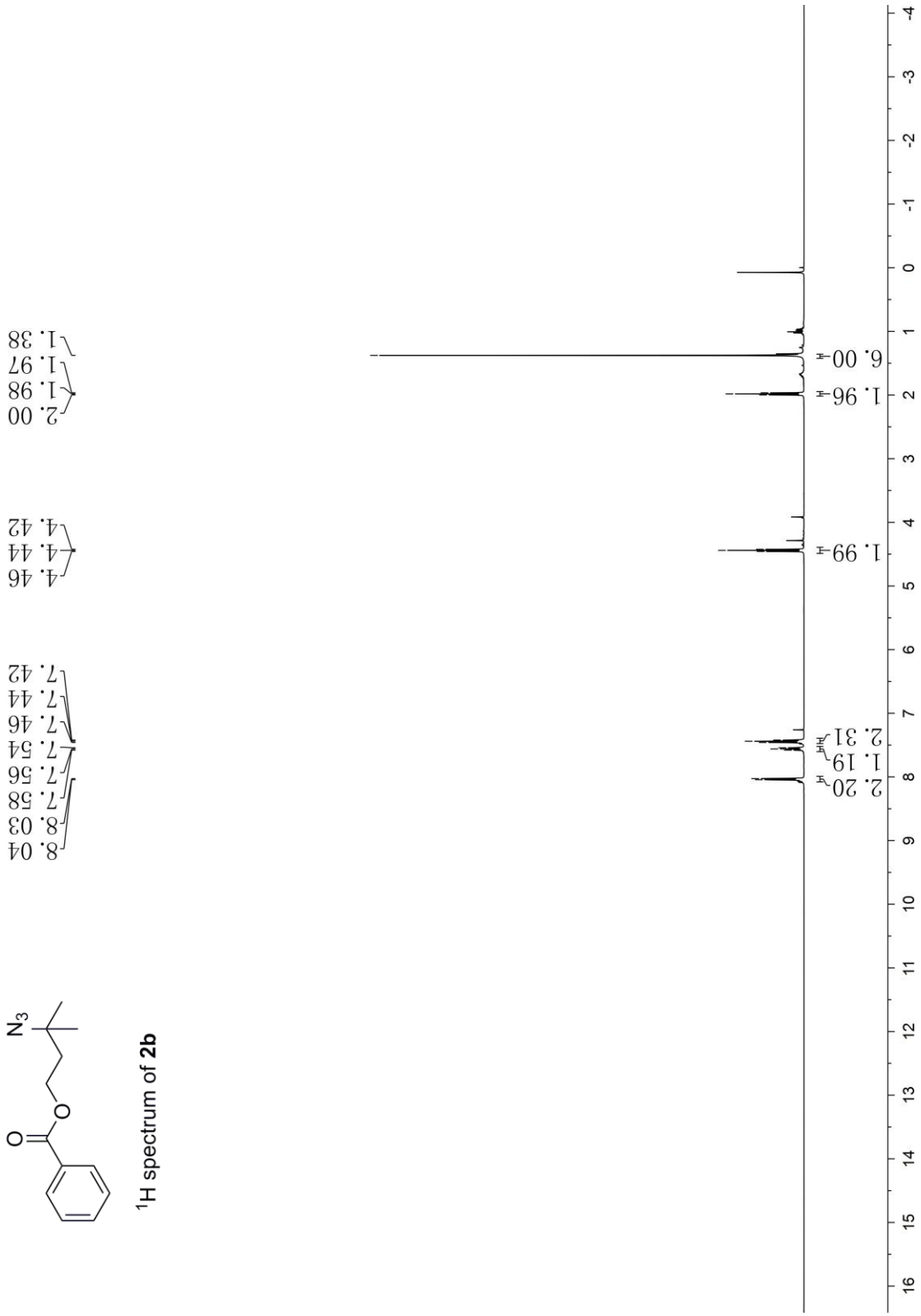
^{13}C NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **1i**



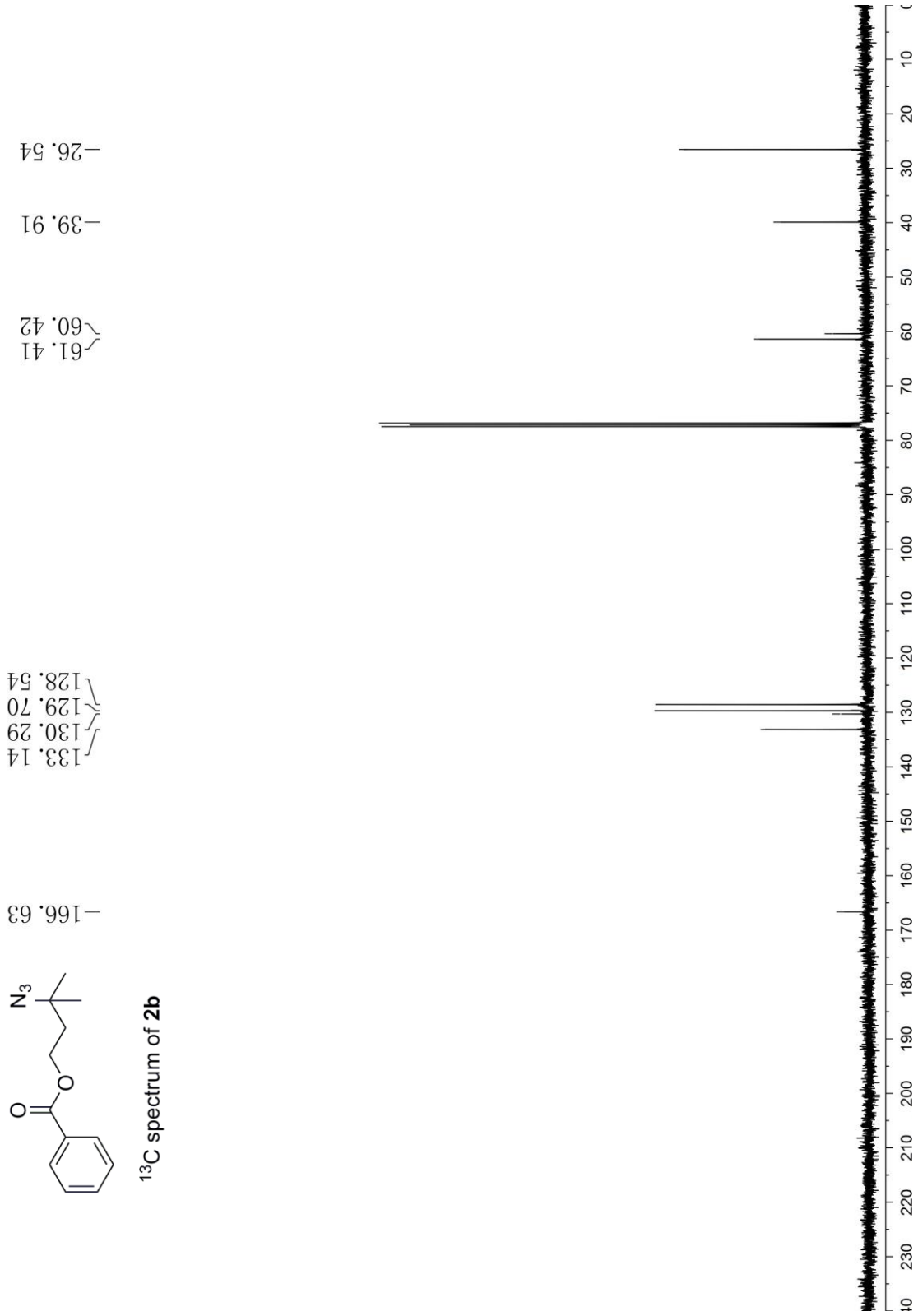
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2a**



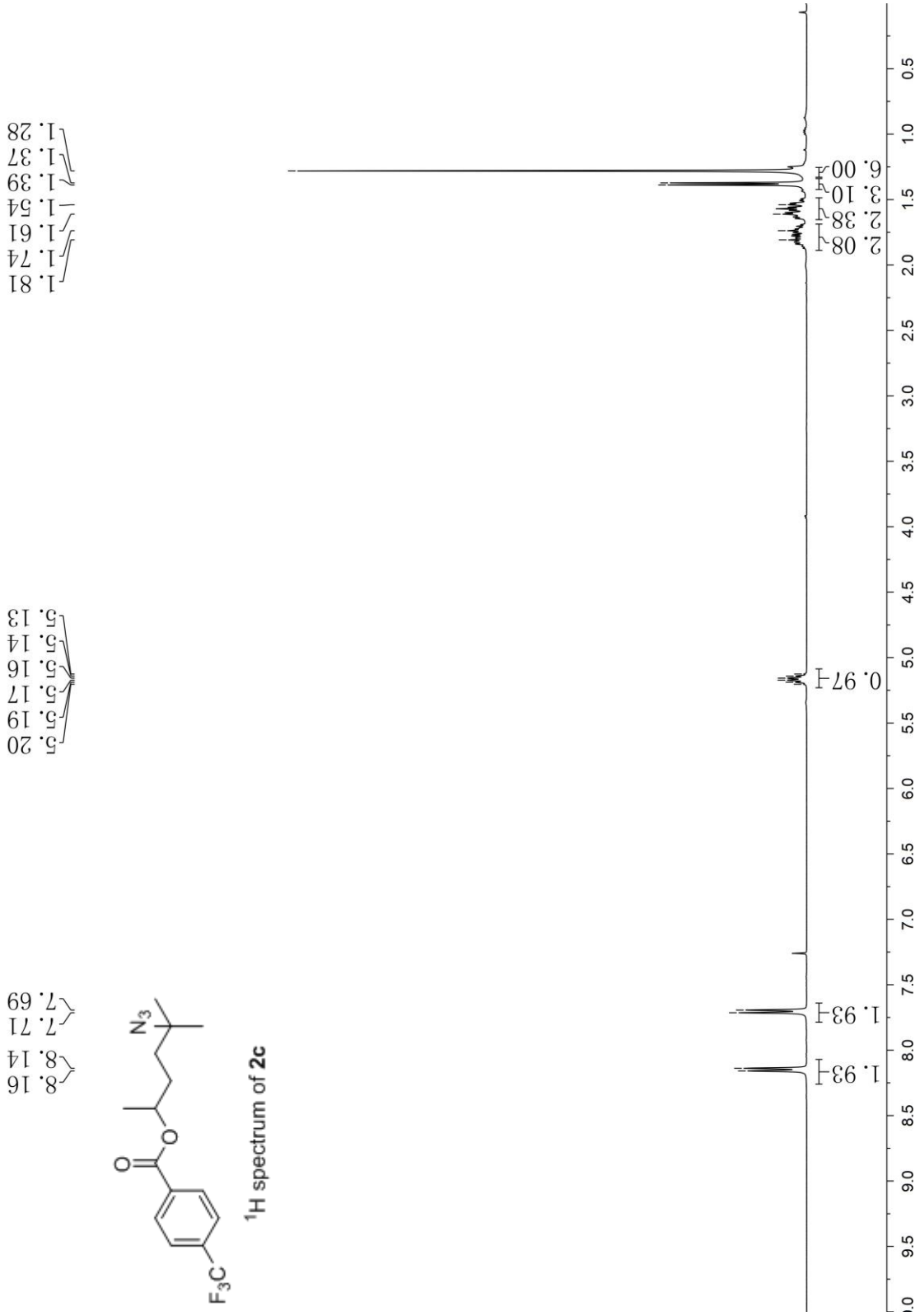
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2a**



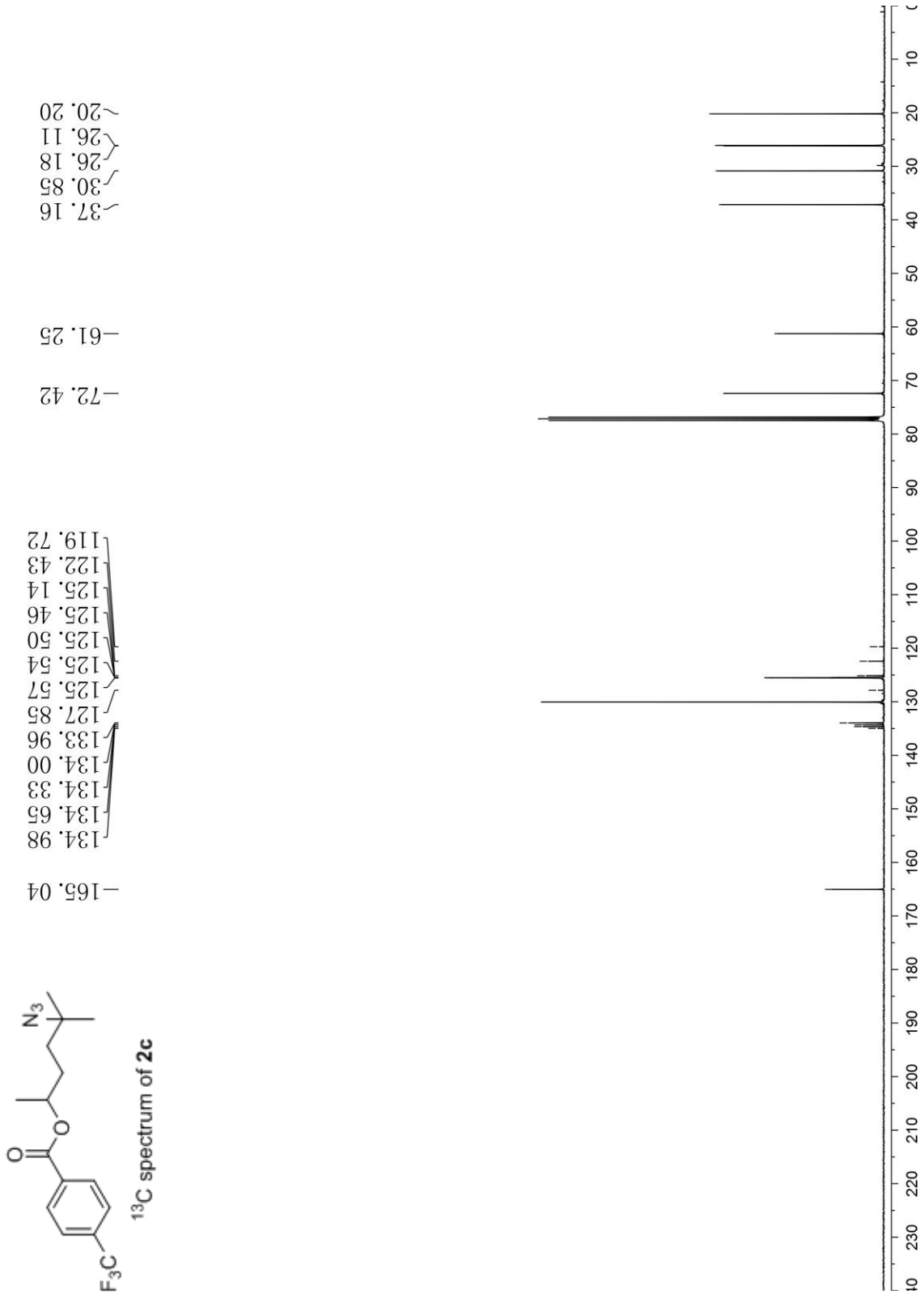
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2b**



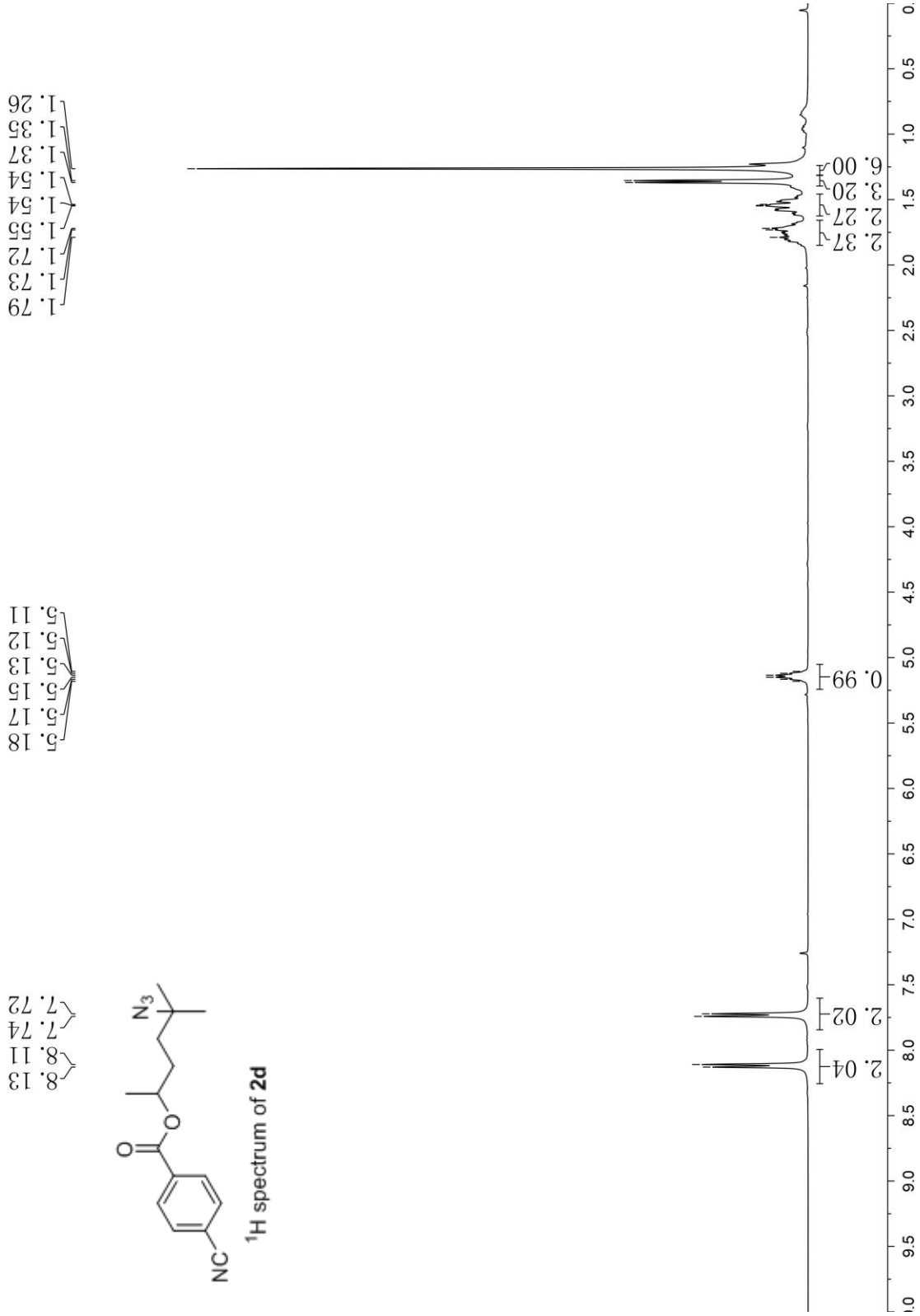
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2b**



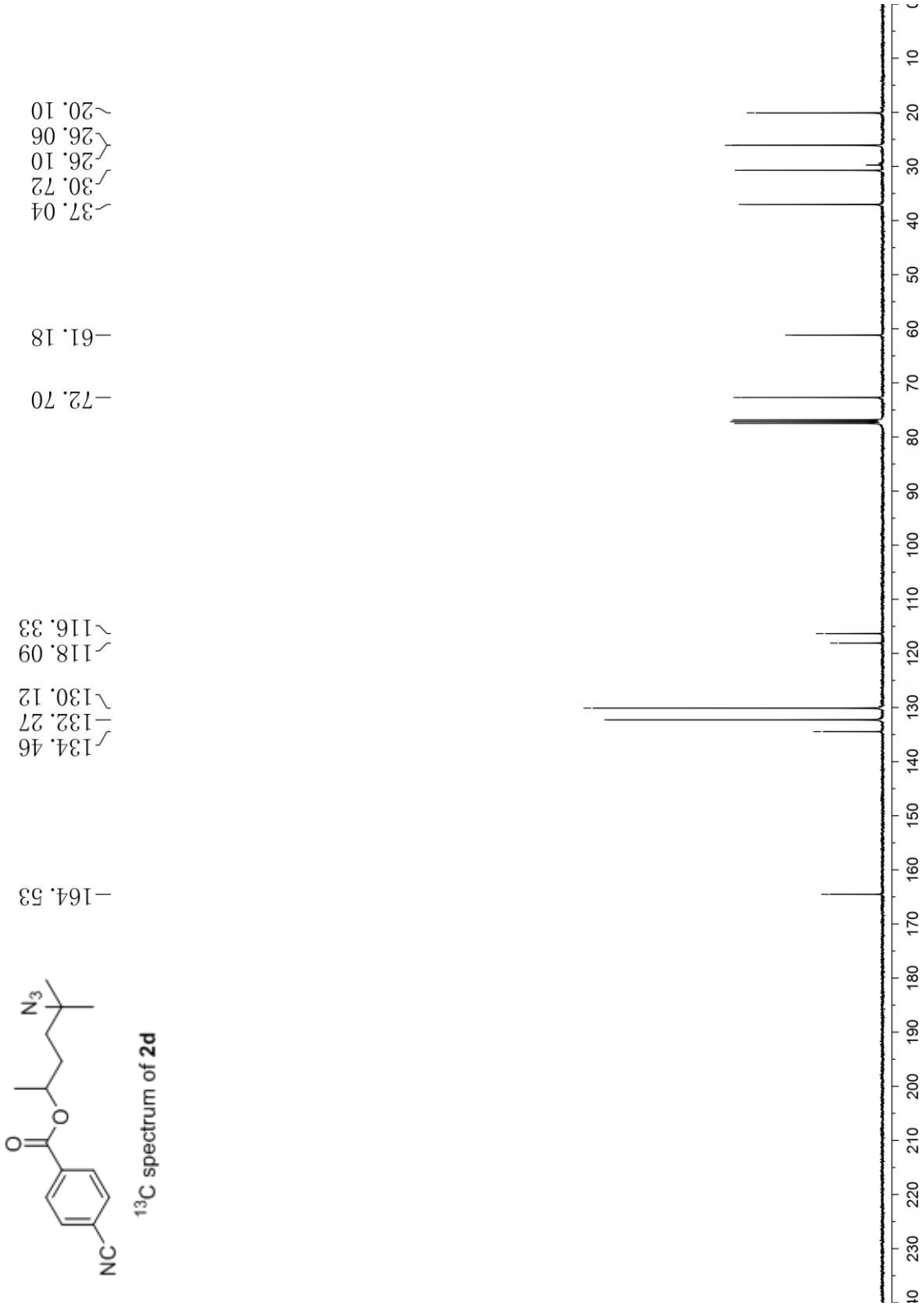
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2c**



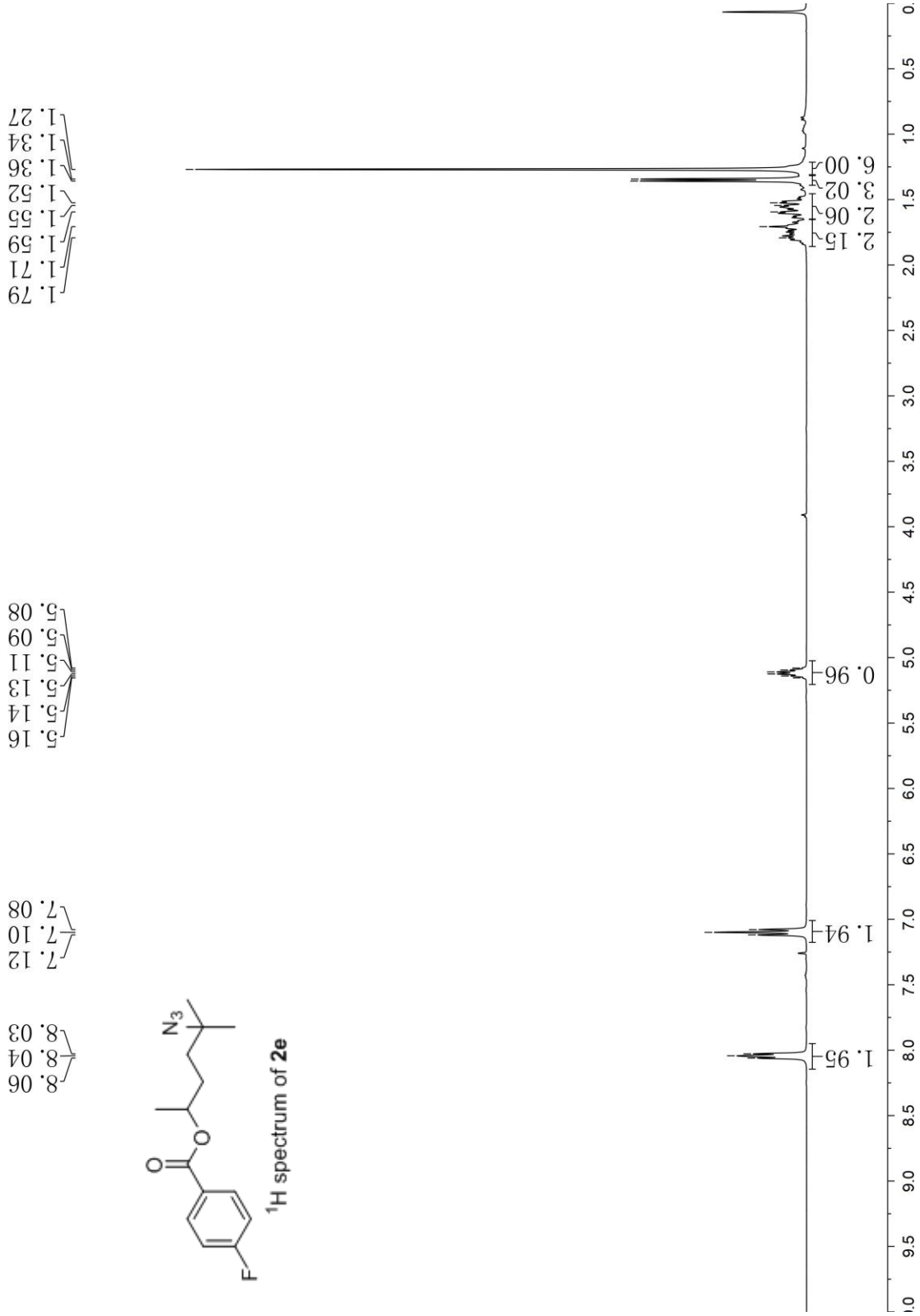
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2c**



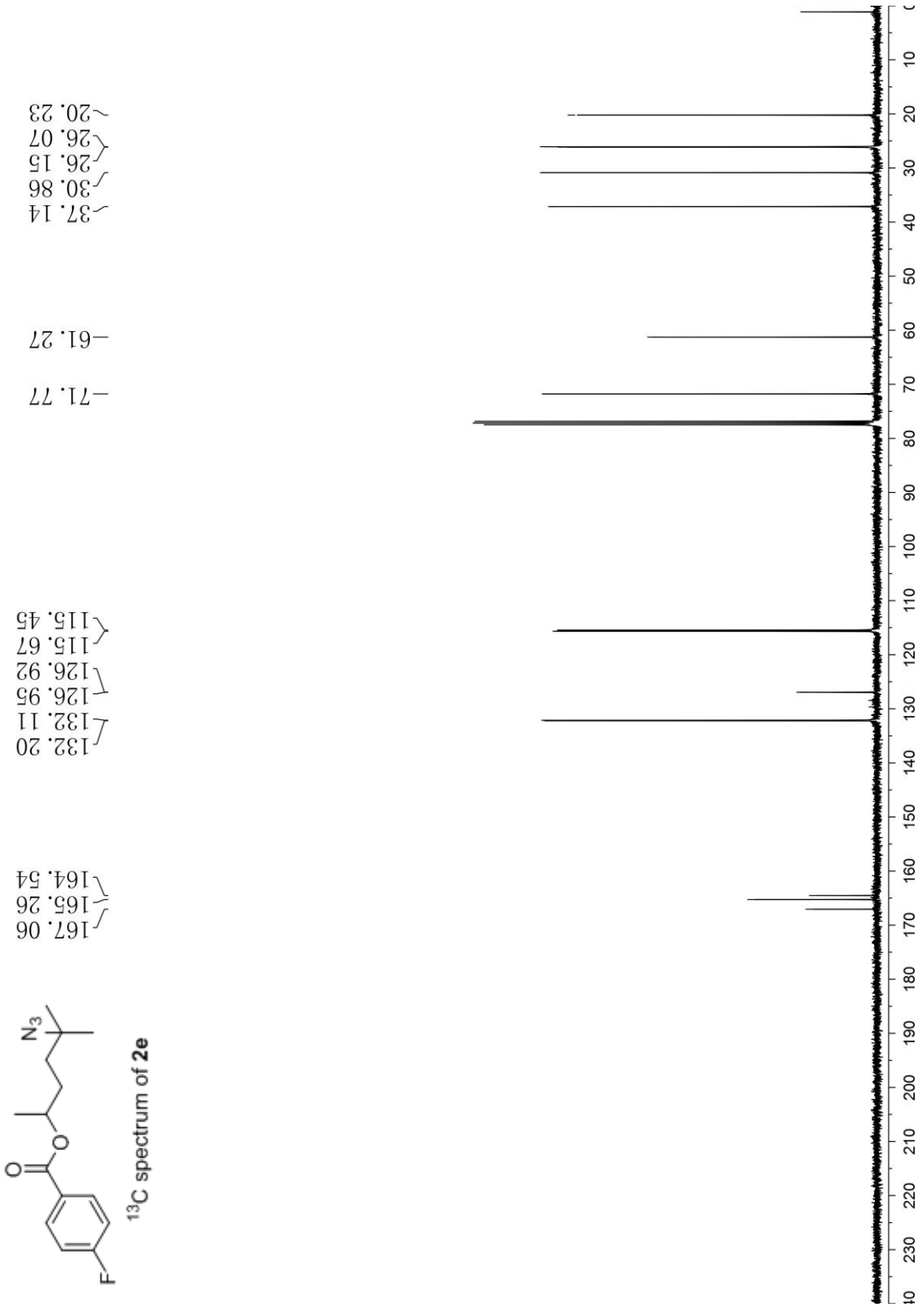
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2d**



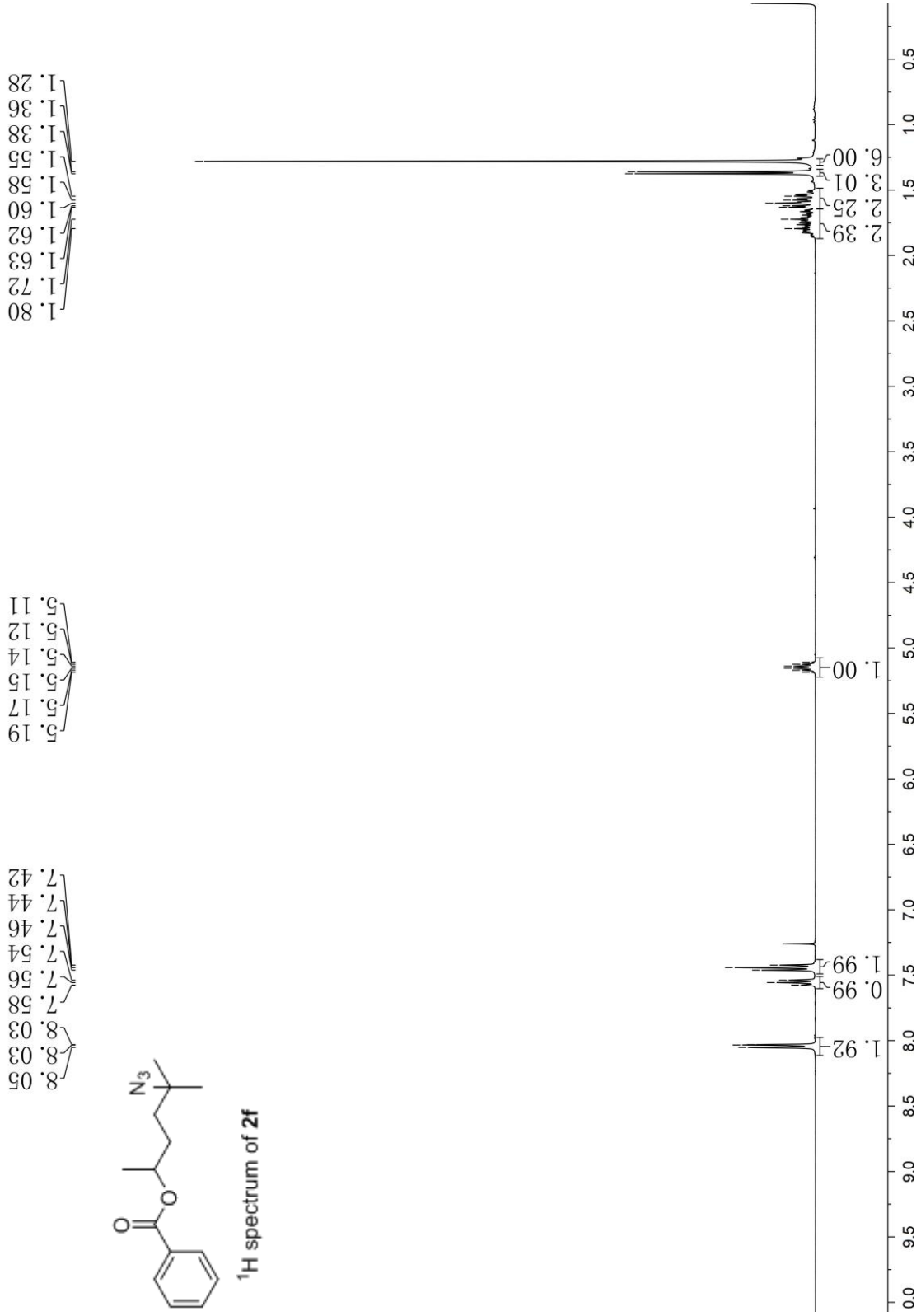
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2d**



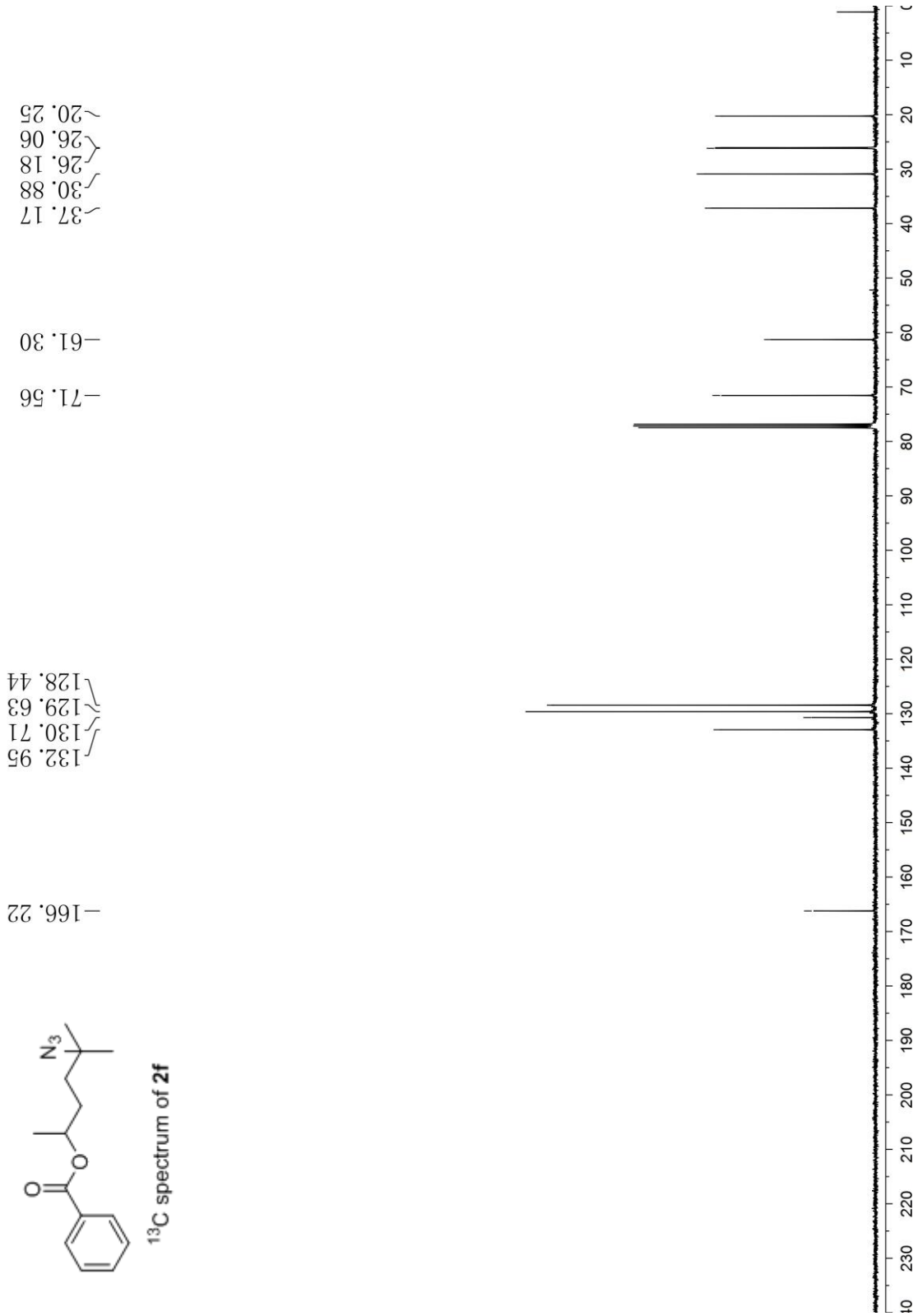
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2e**



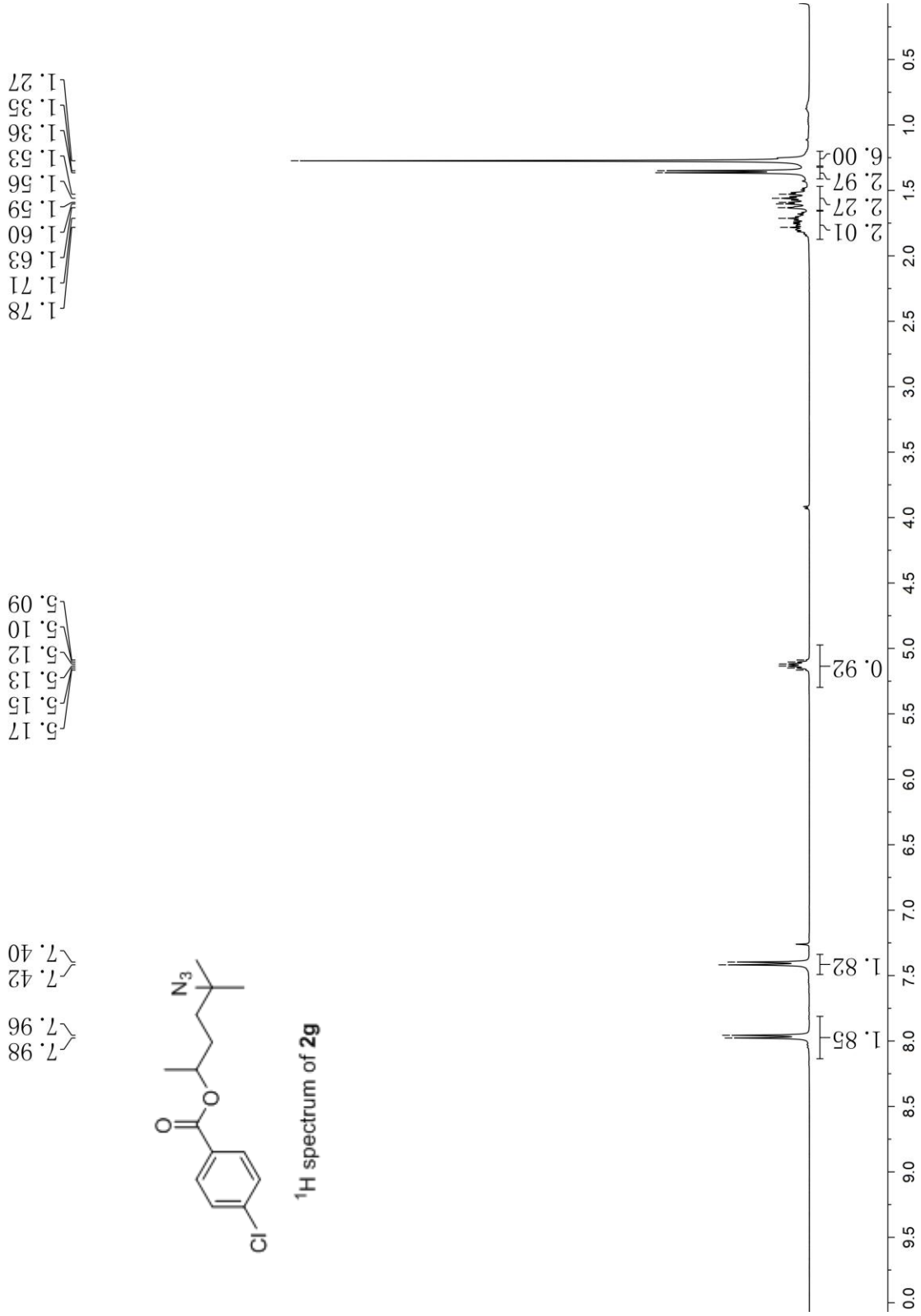
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2e**



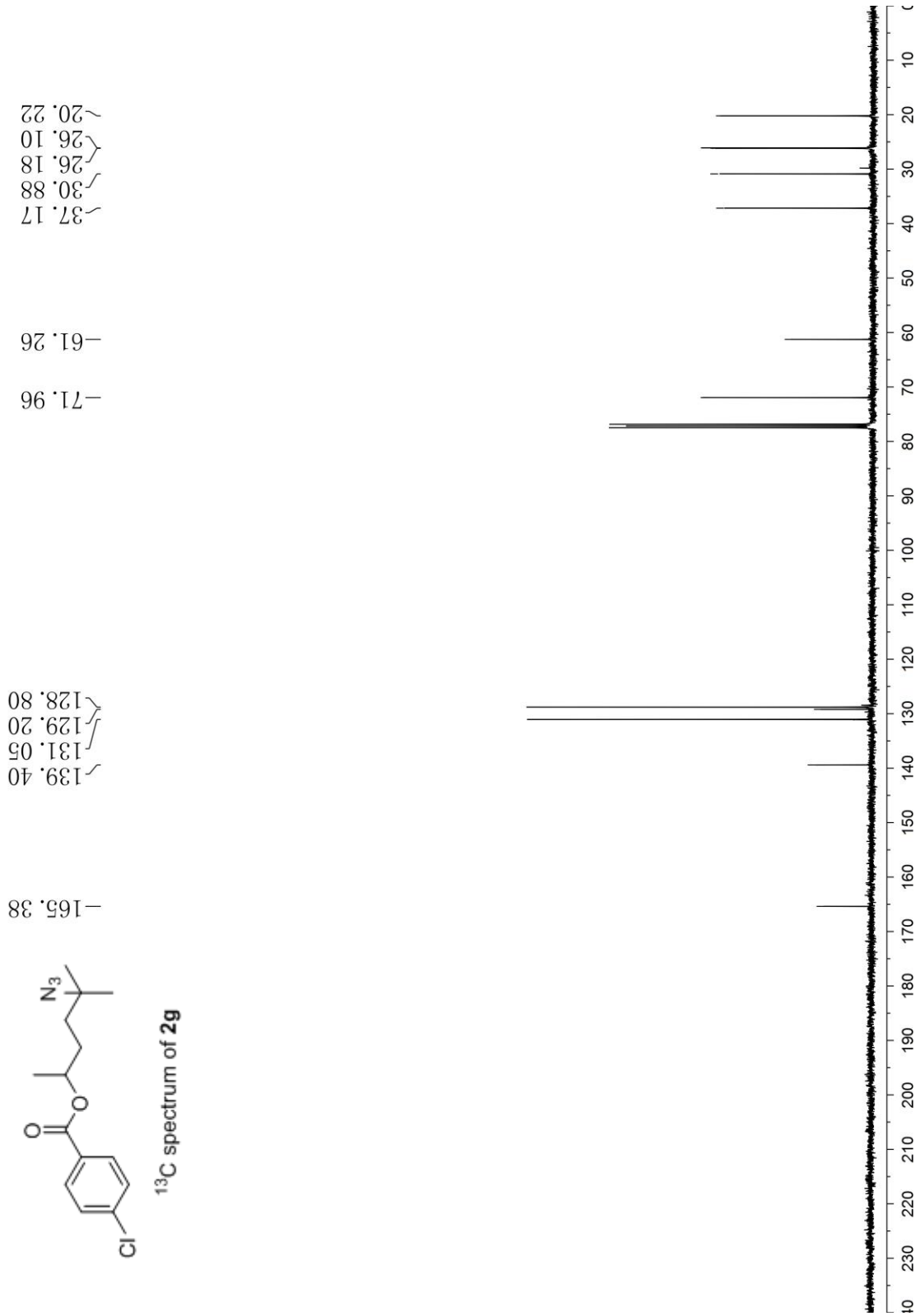
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2f**



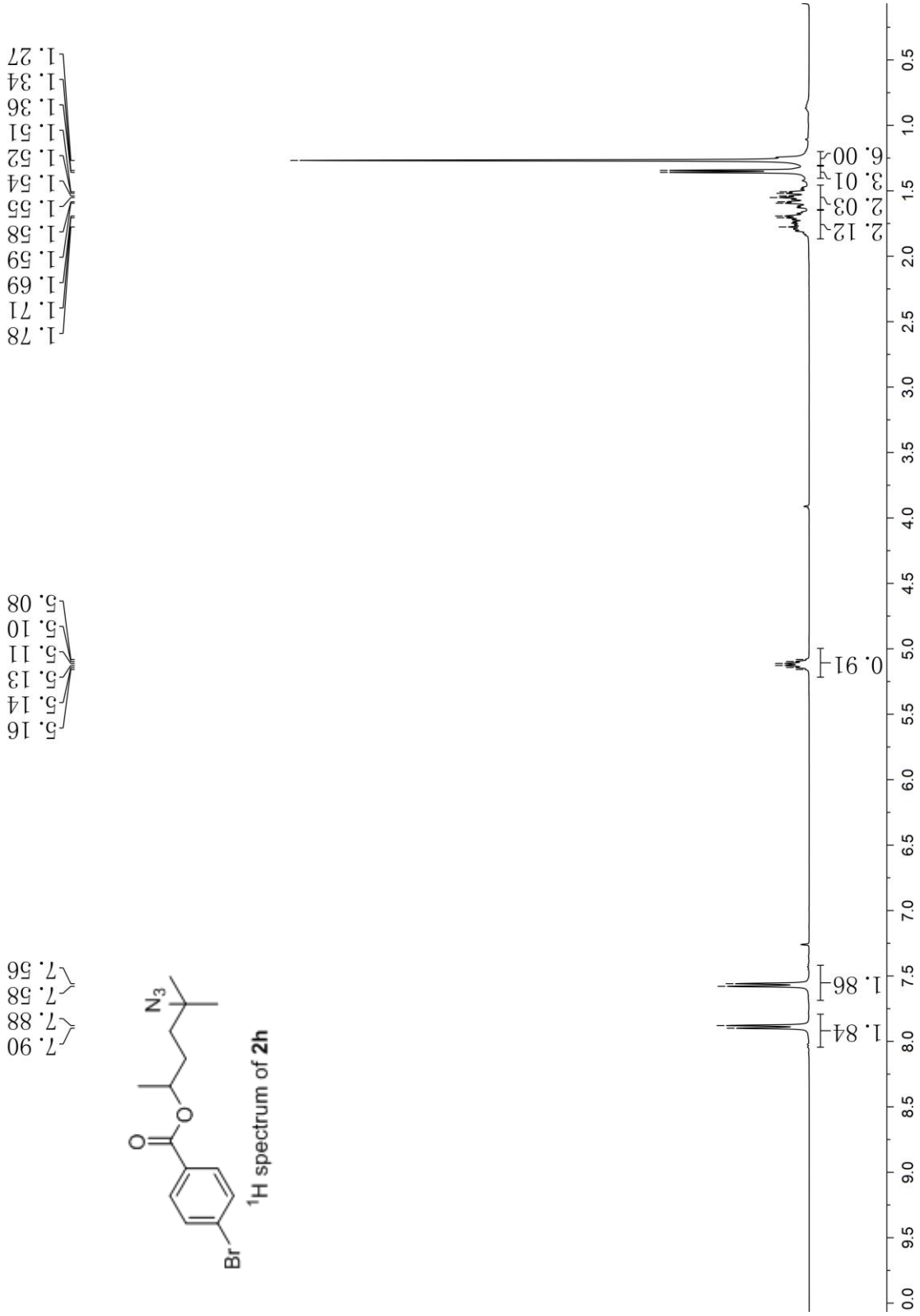
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2f**



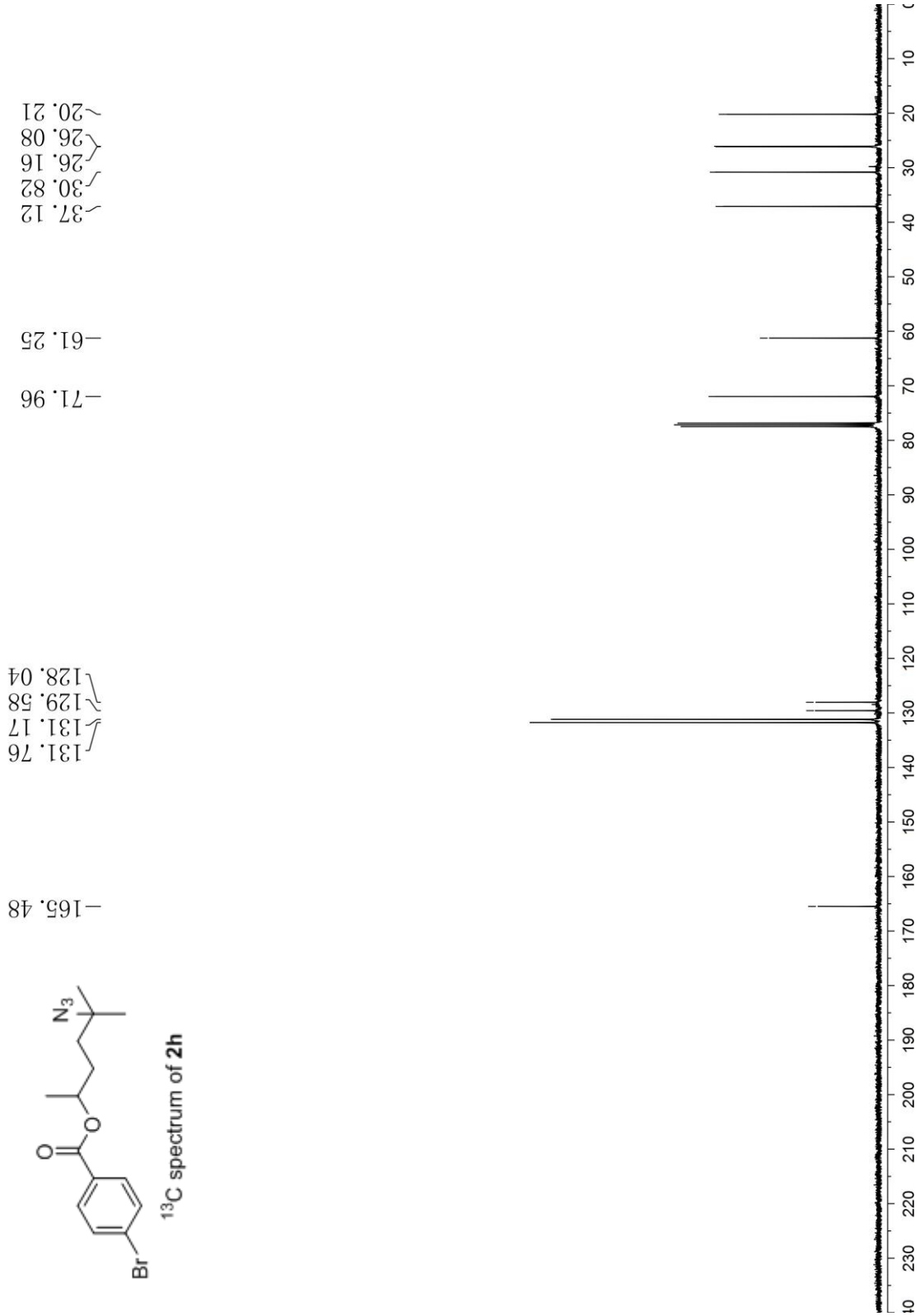
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2g**



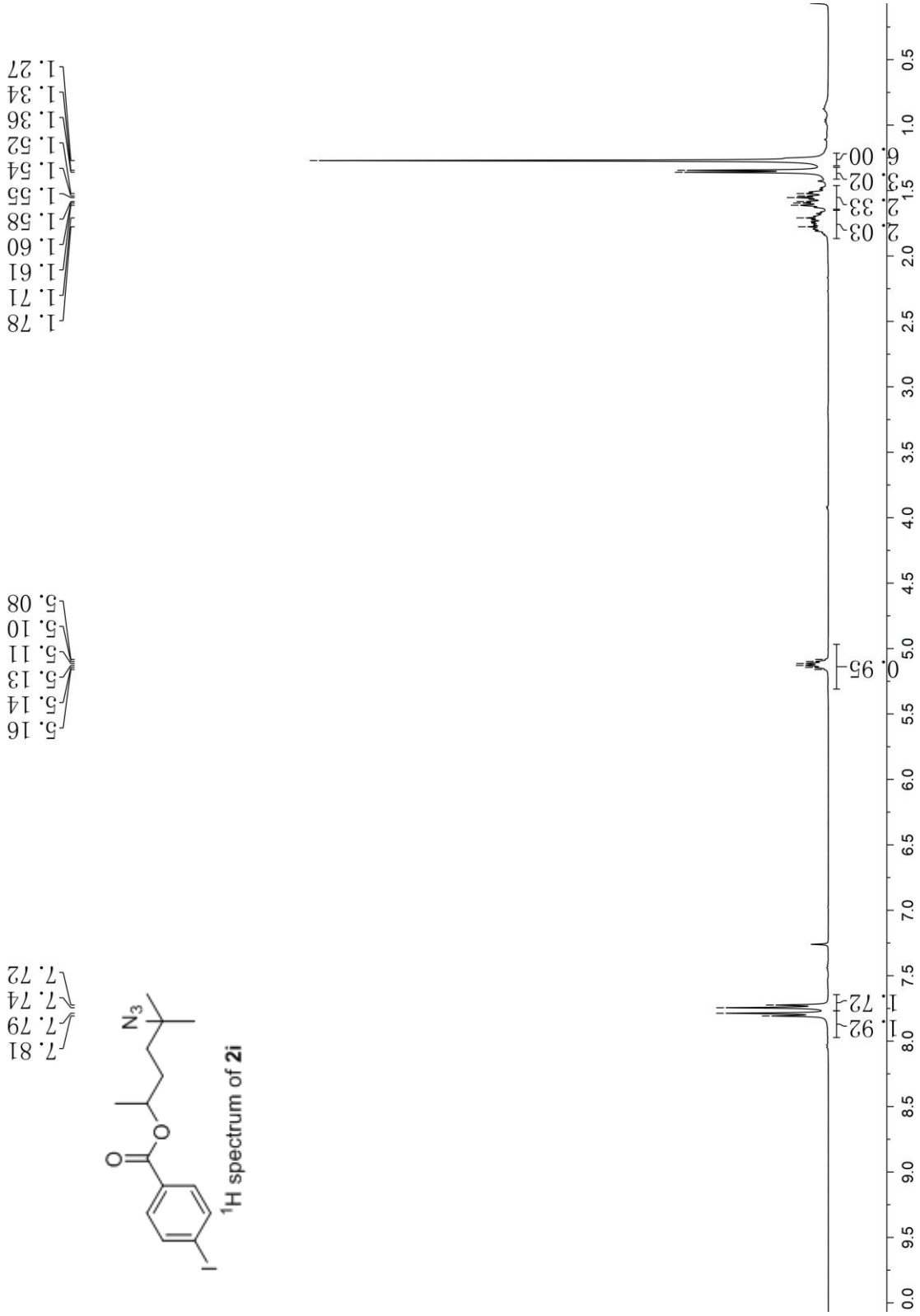
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2g**



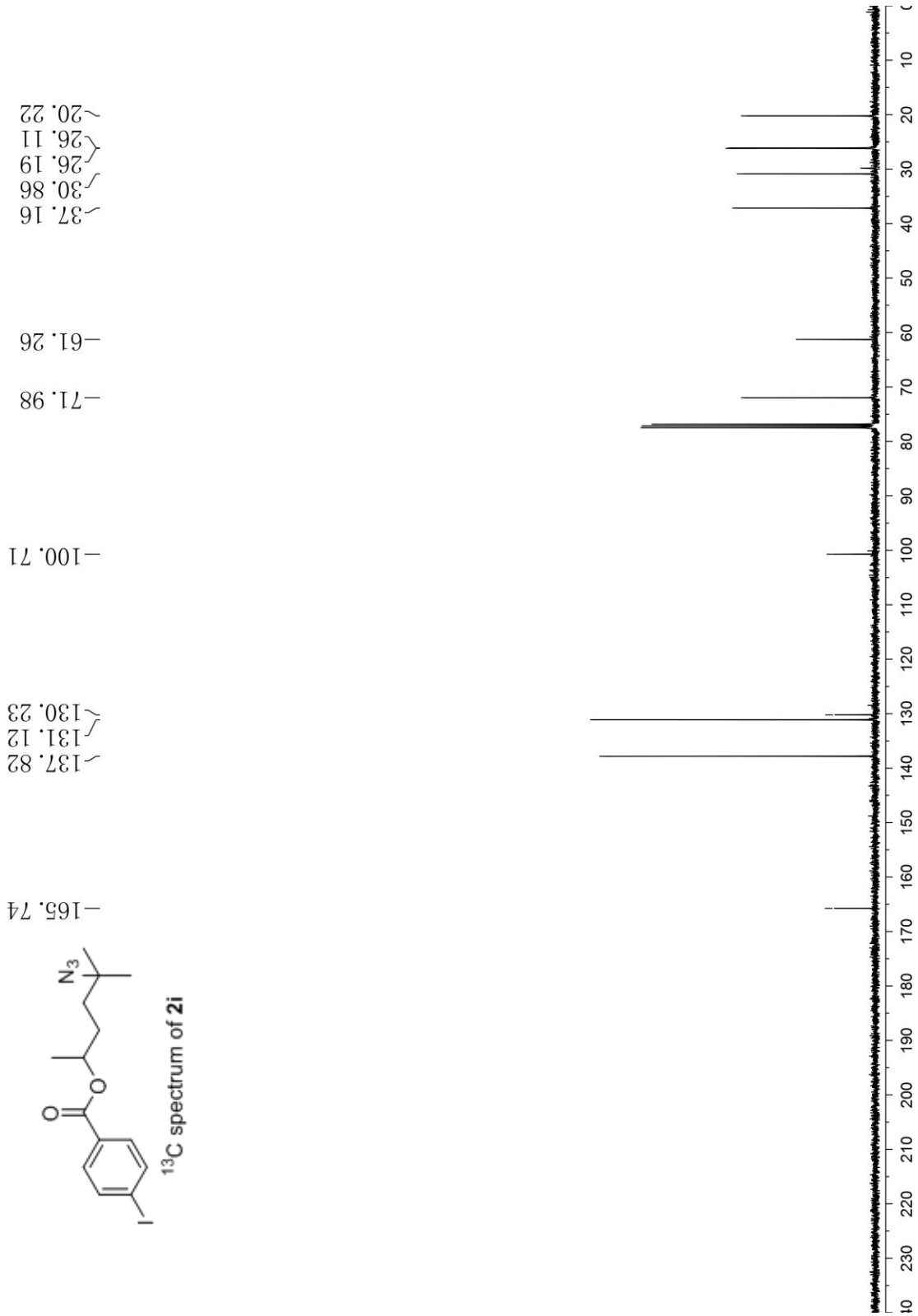
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2h**



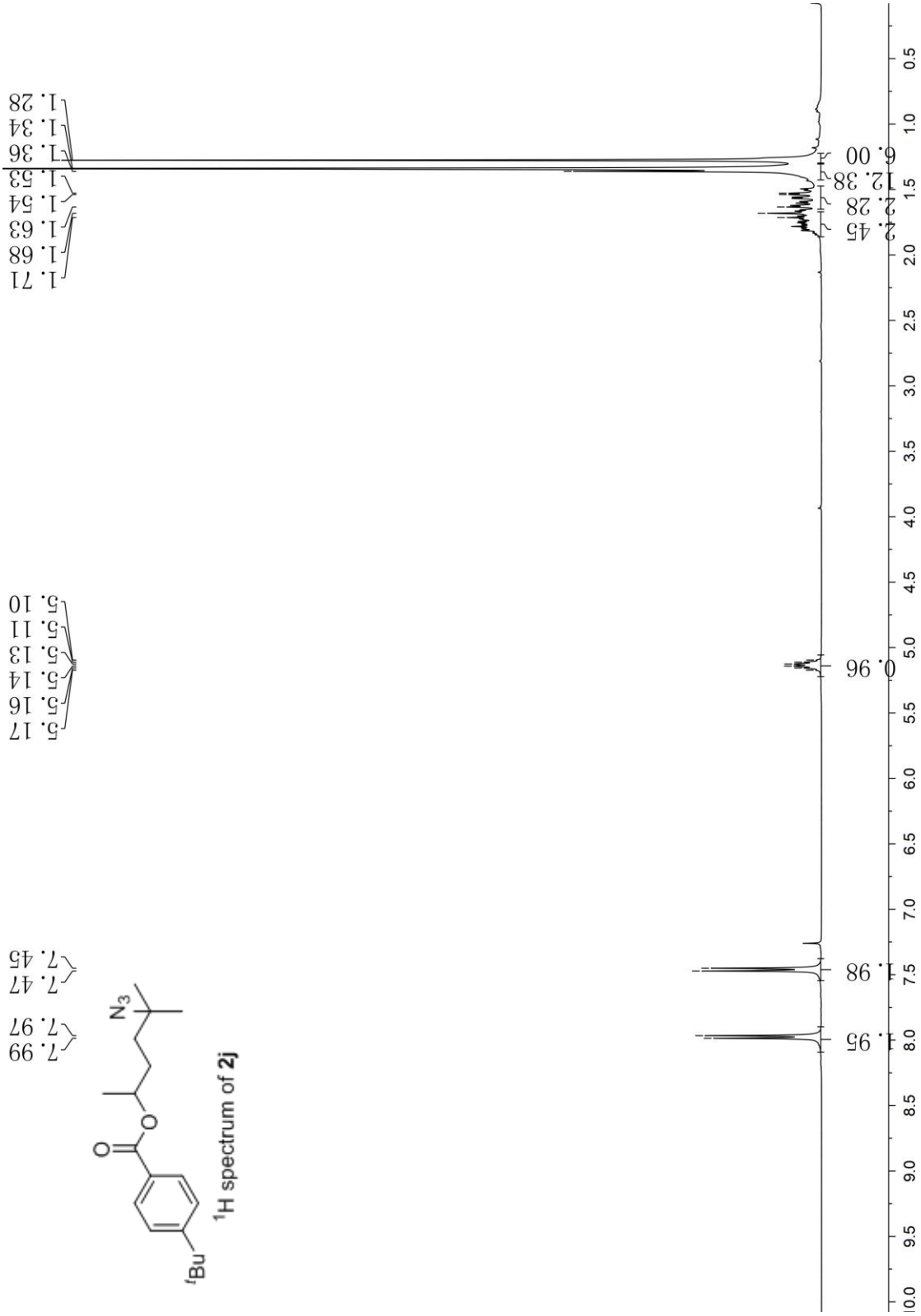
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2h**



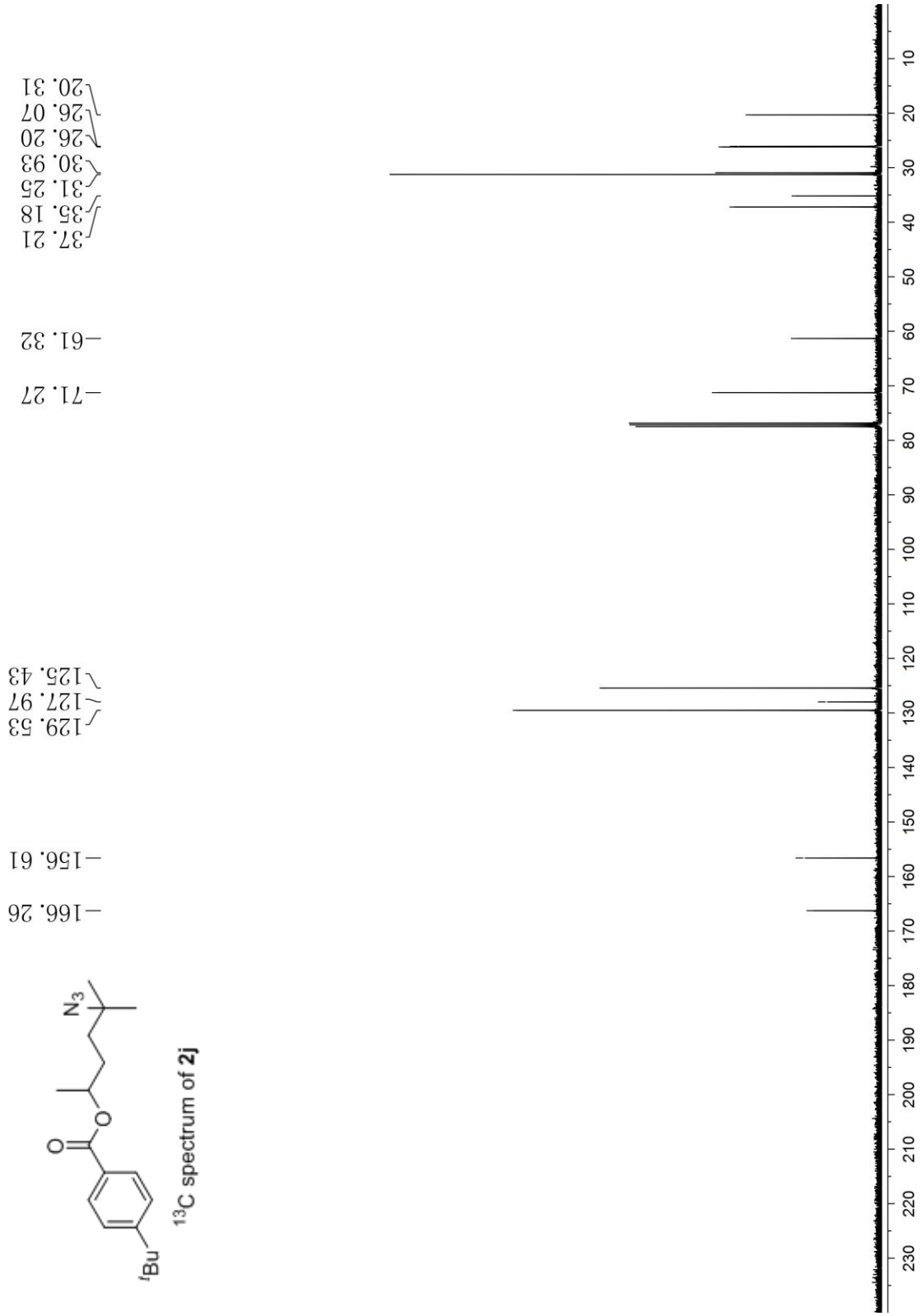
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2i**



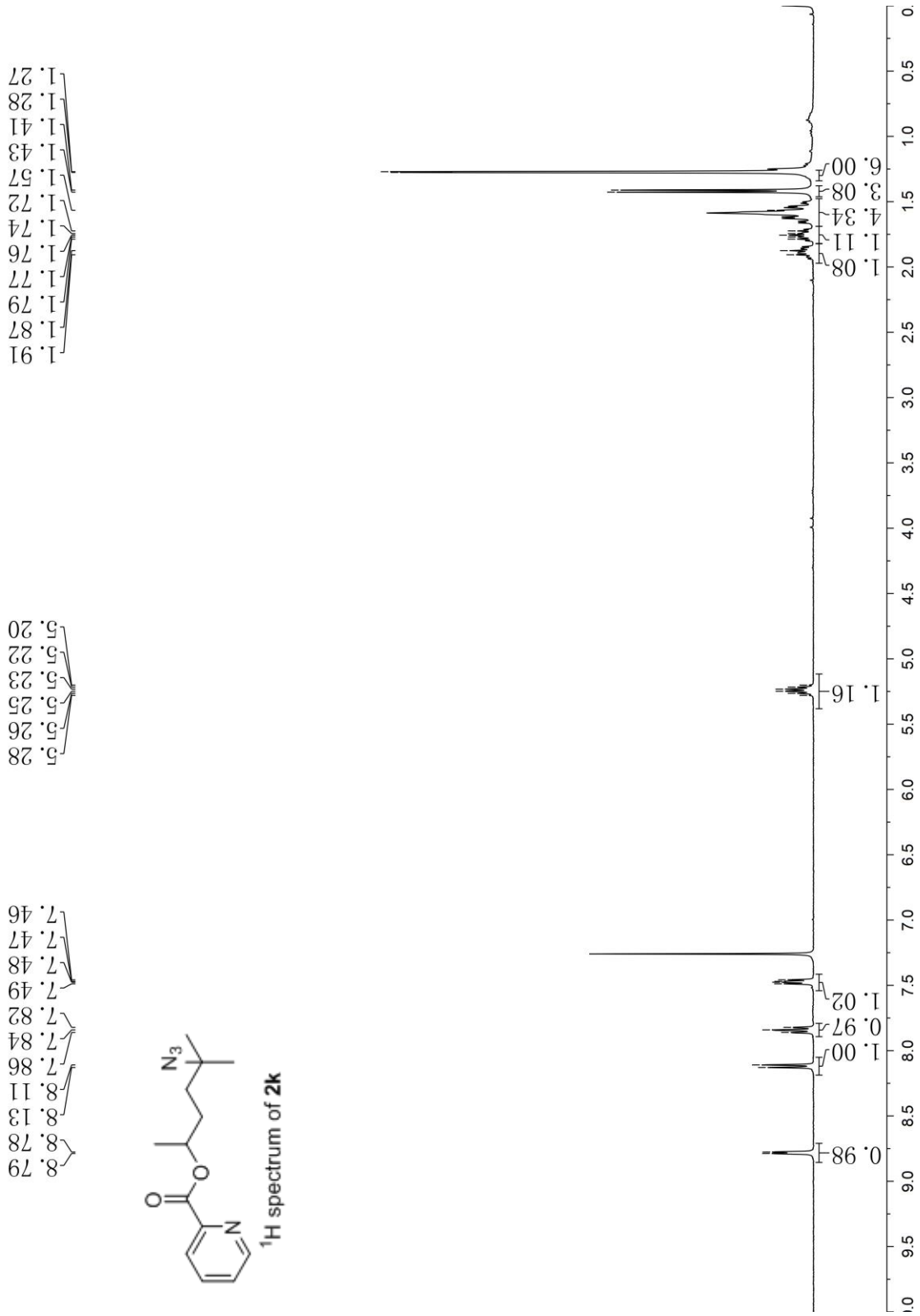
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2i**



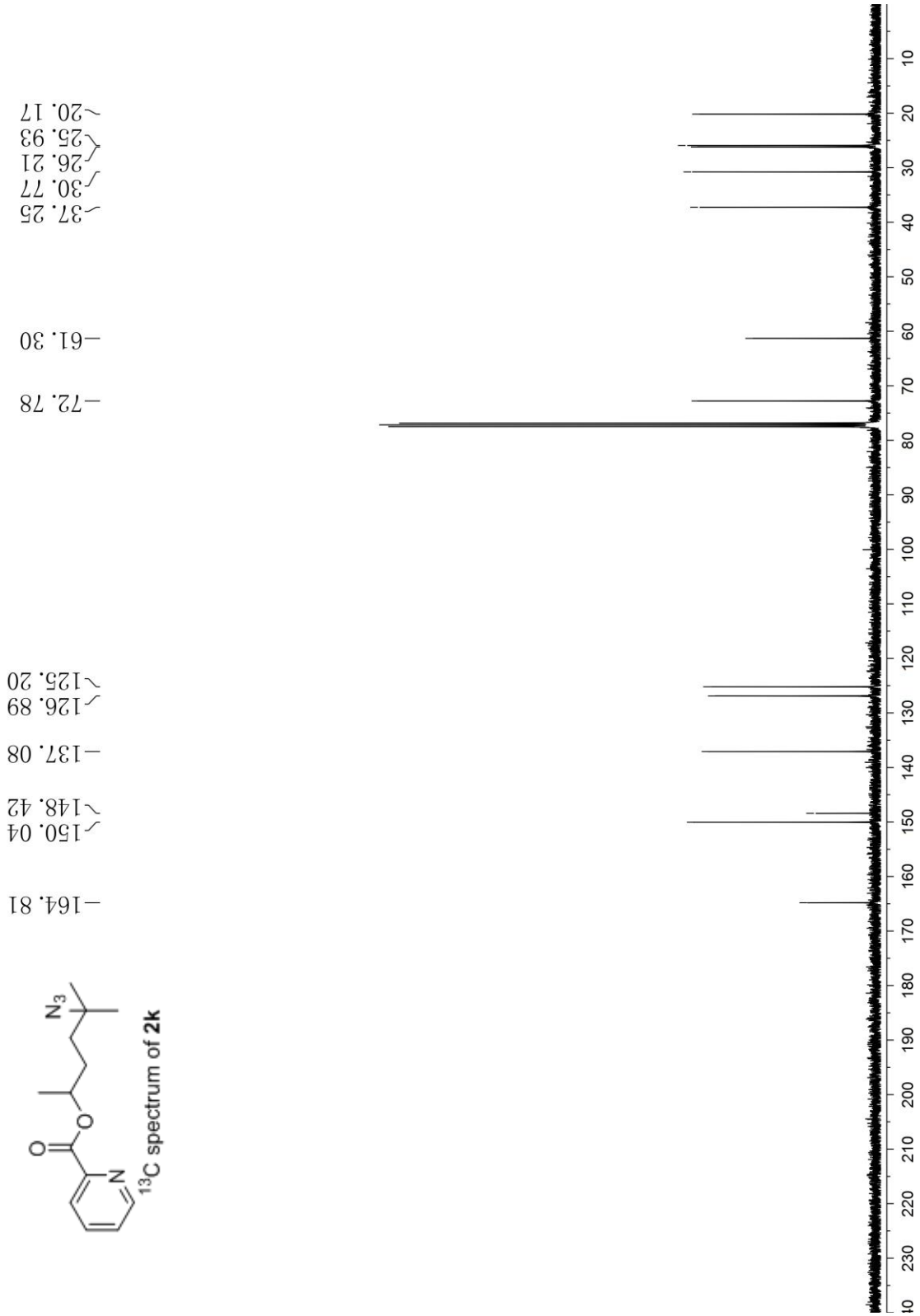
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2j**



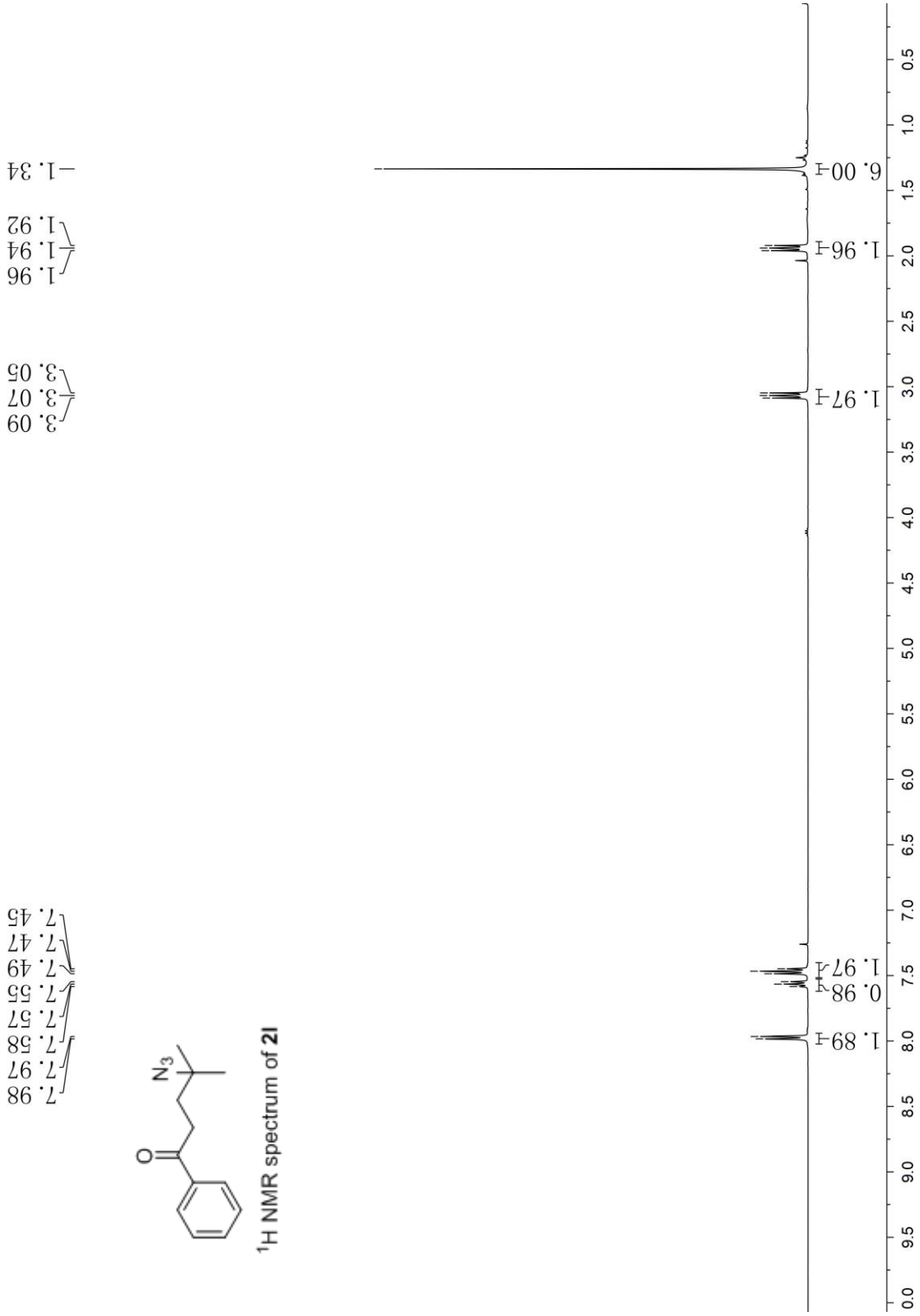
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2j**



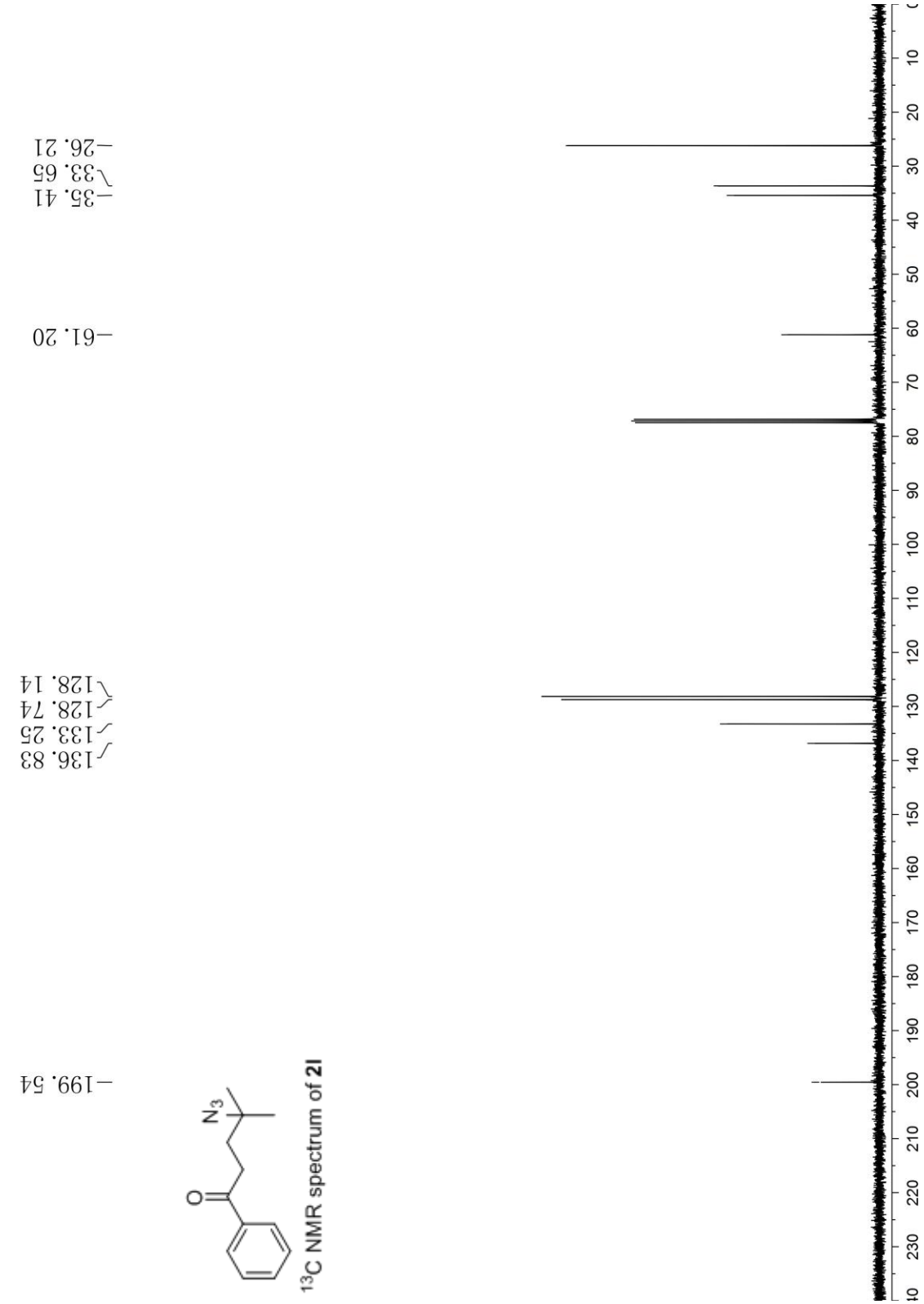
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2k**



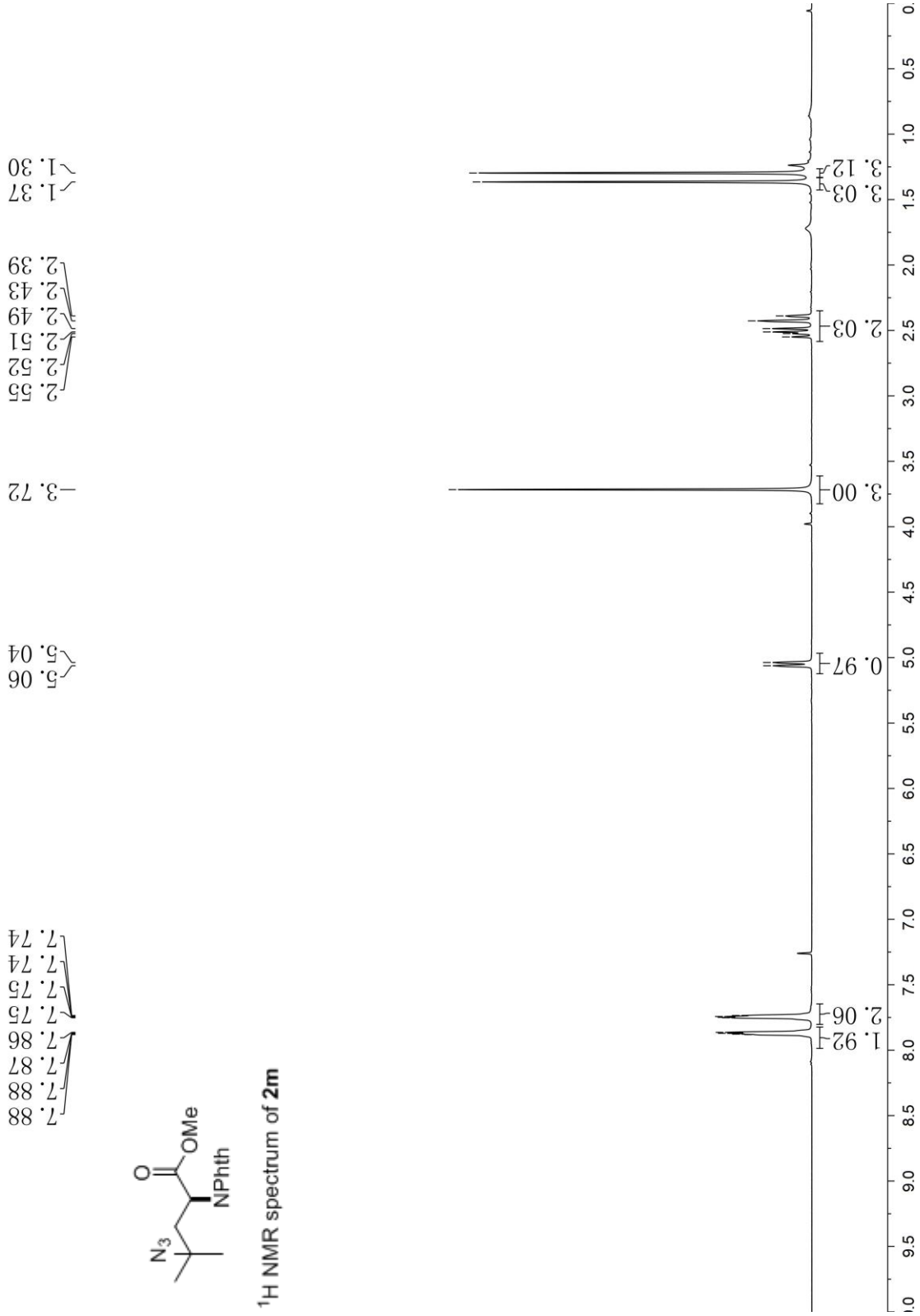
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2k**



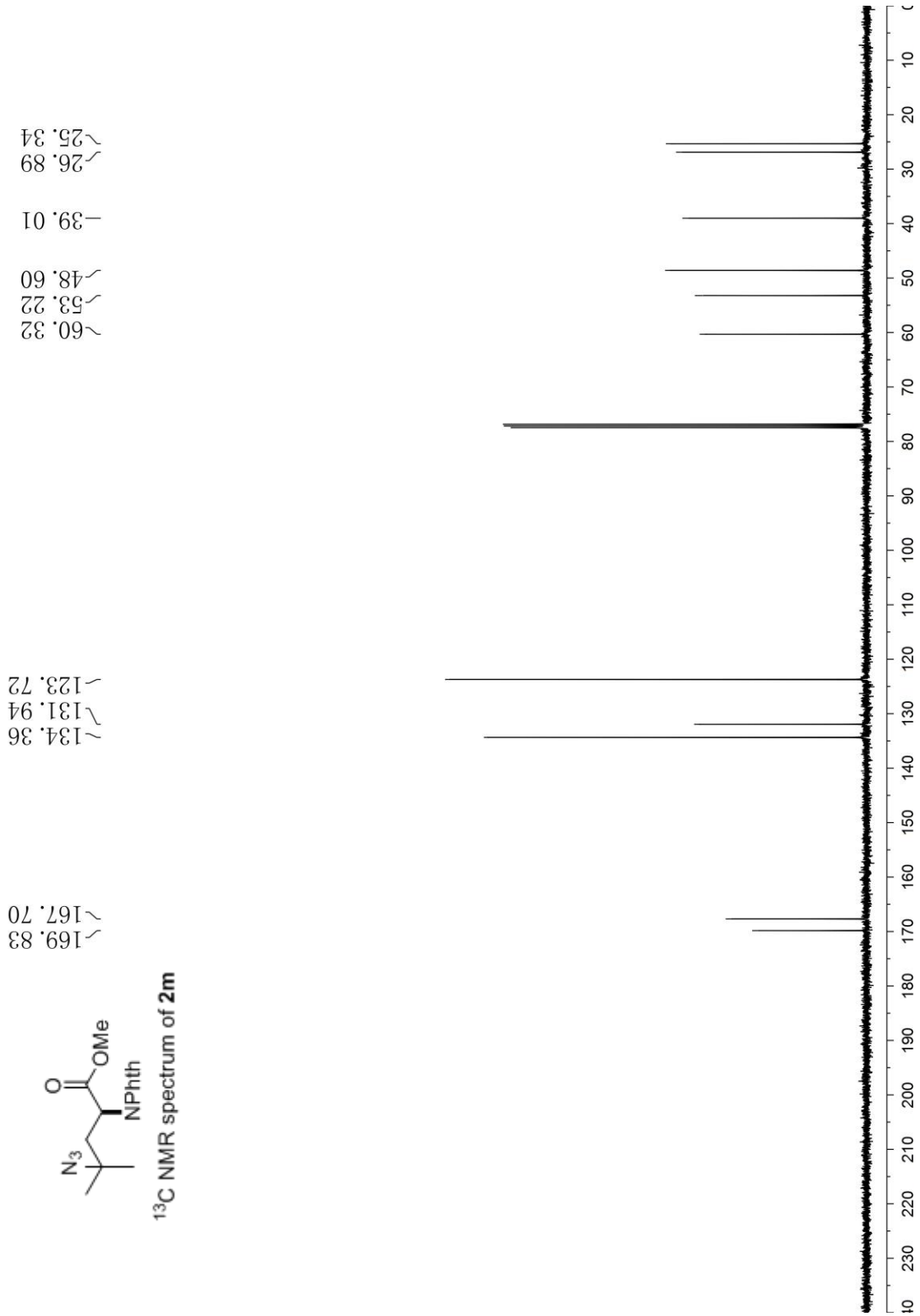
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2l**



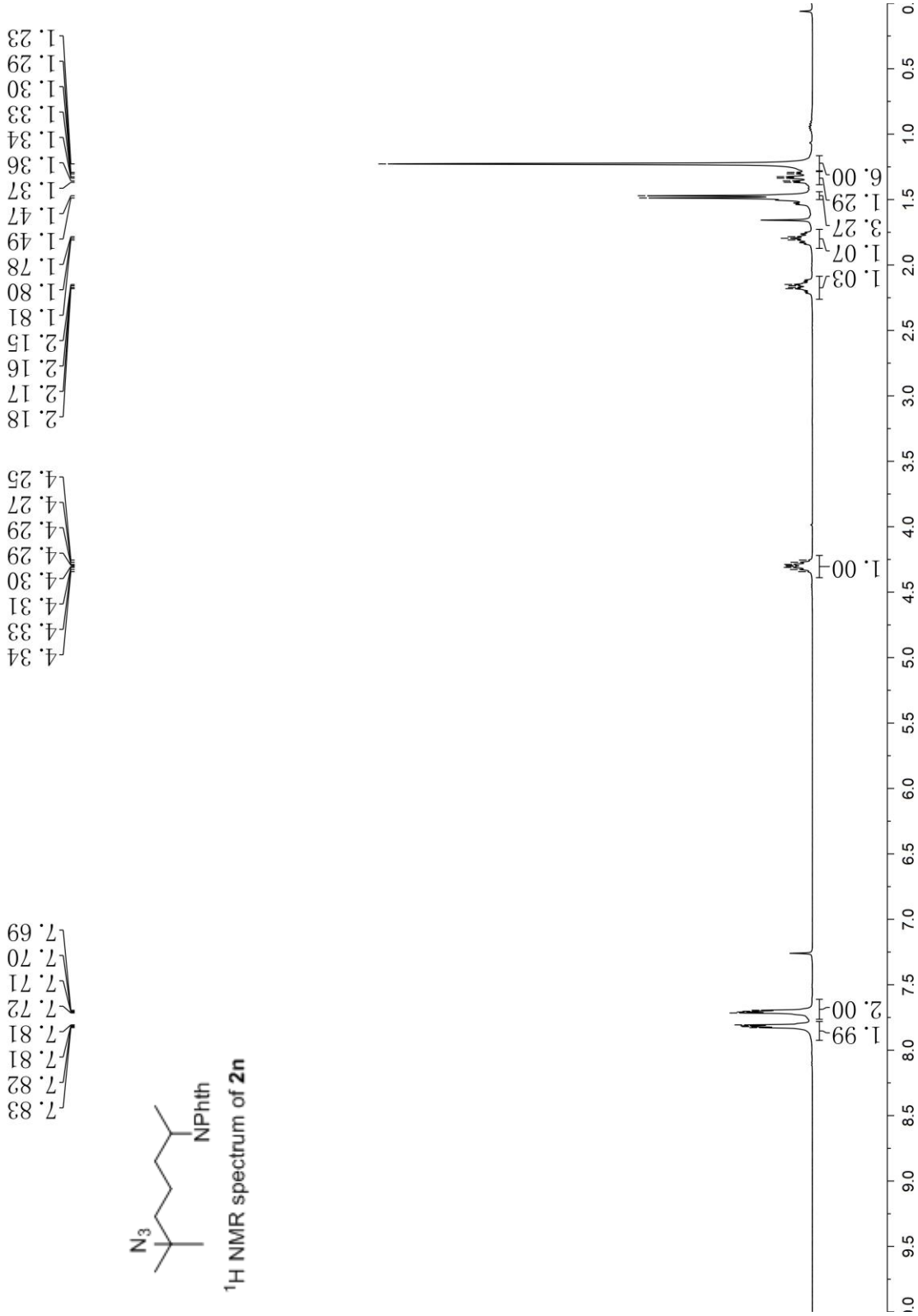
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2l**



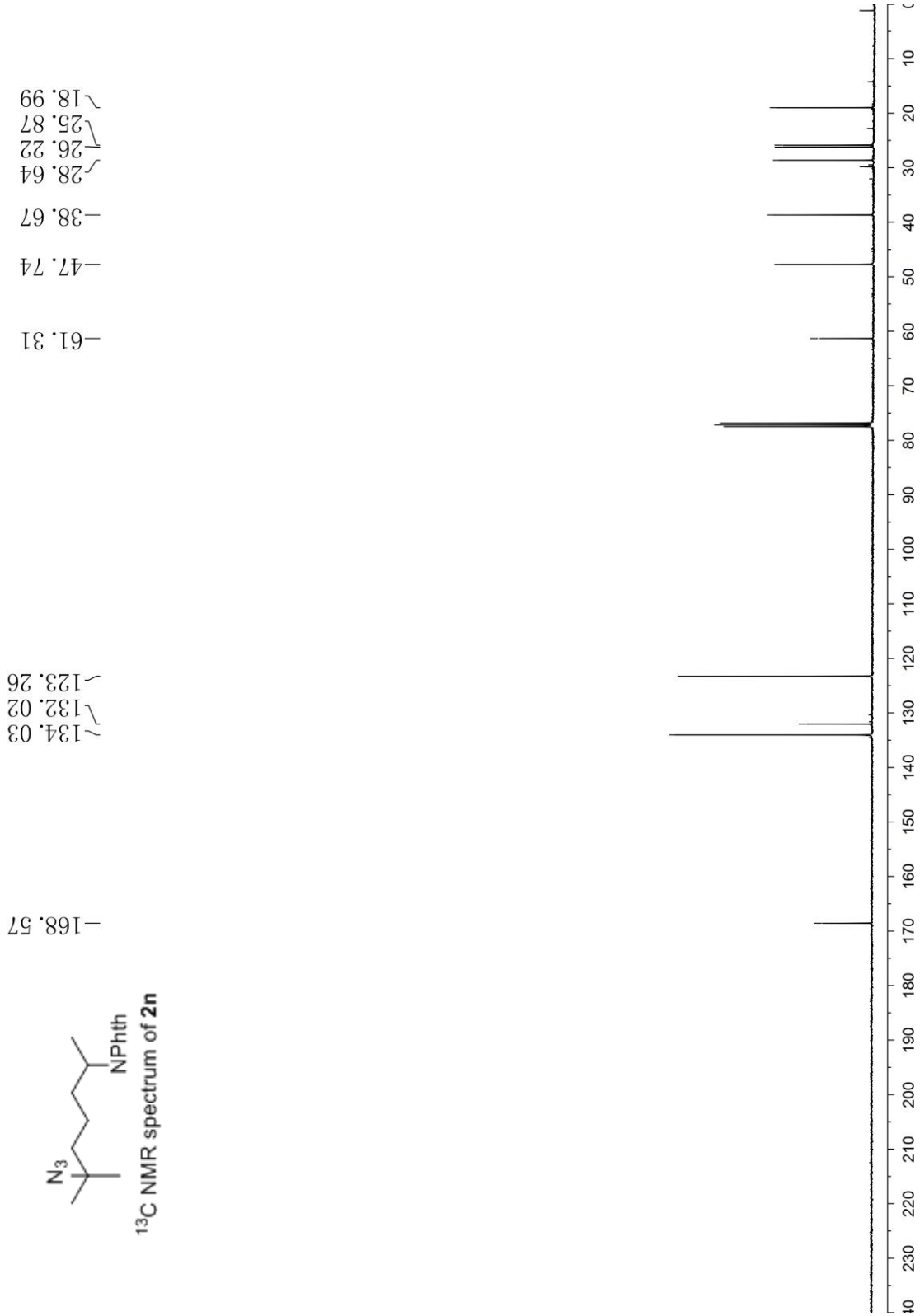
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2m**



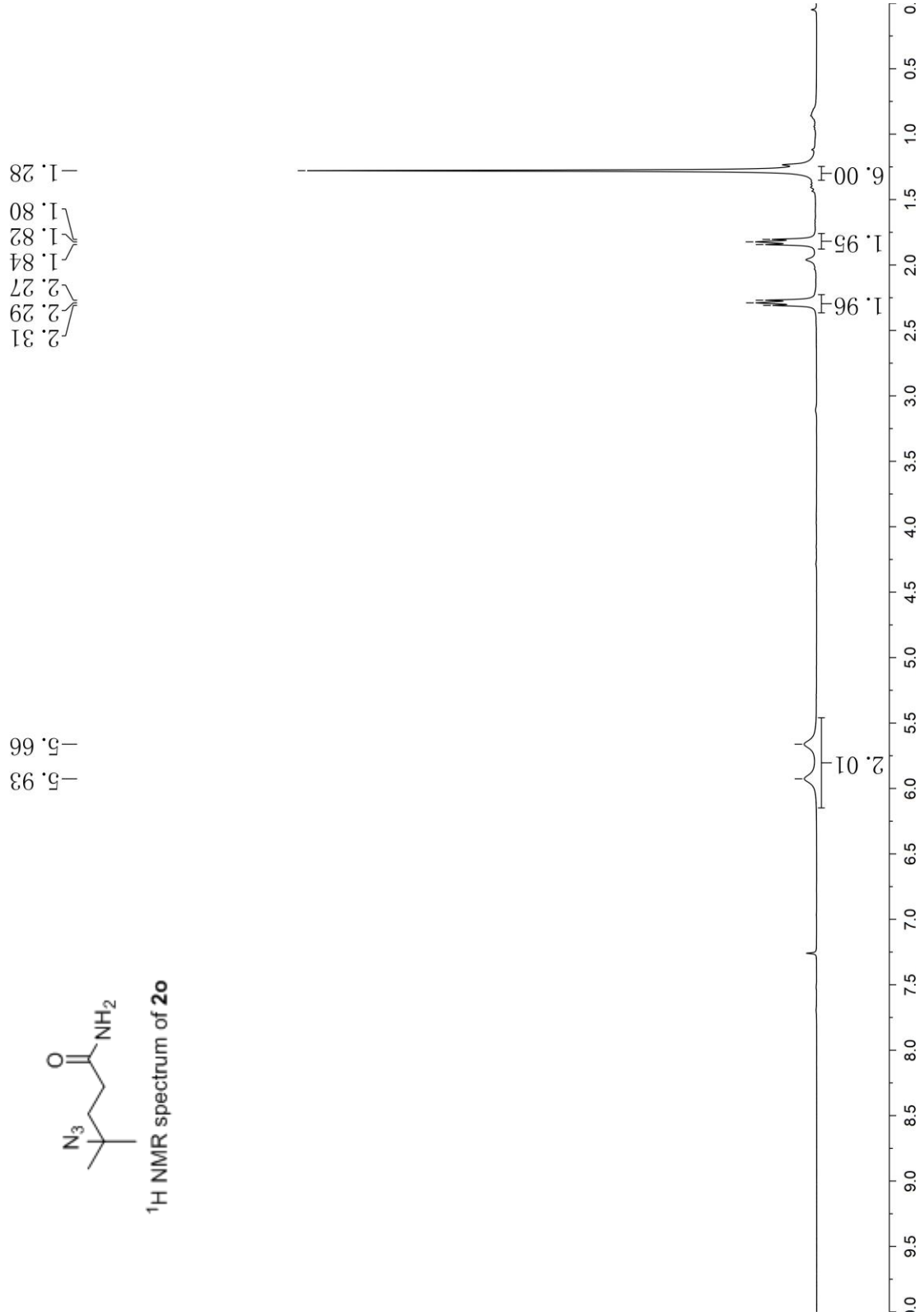
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2m**



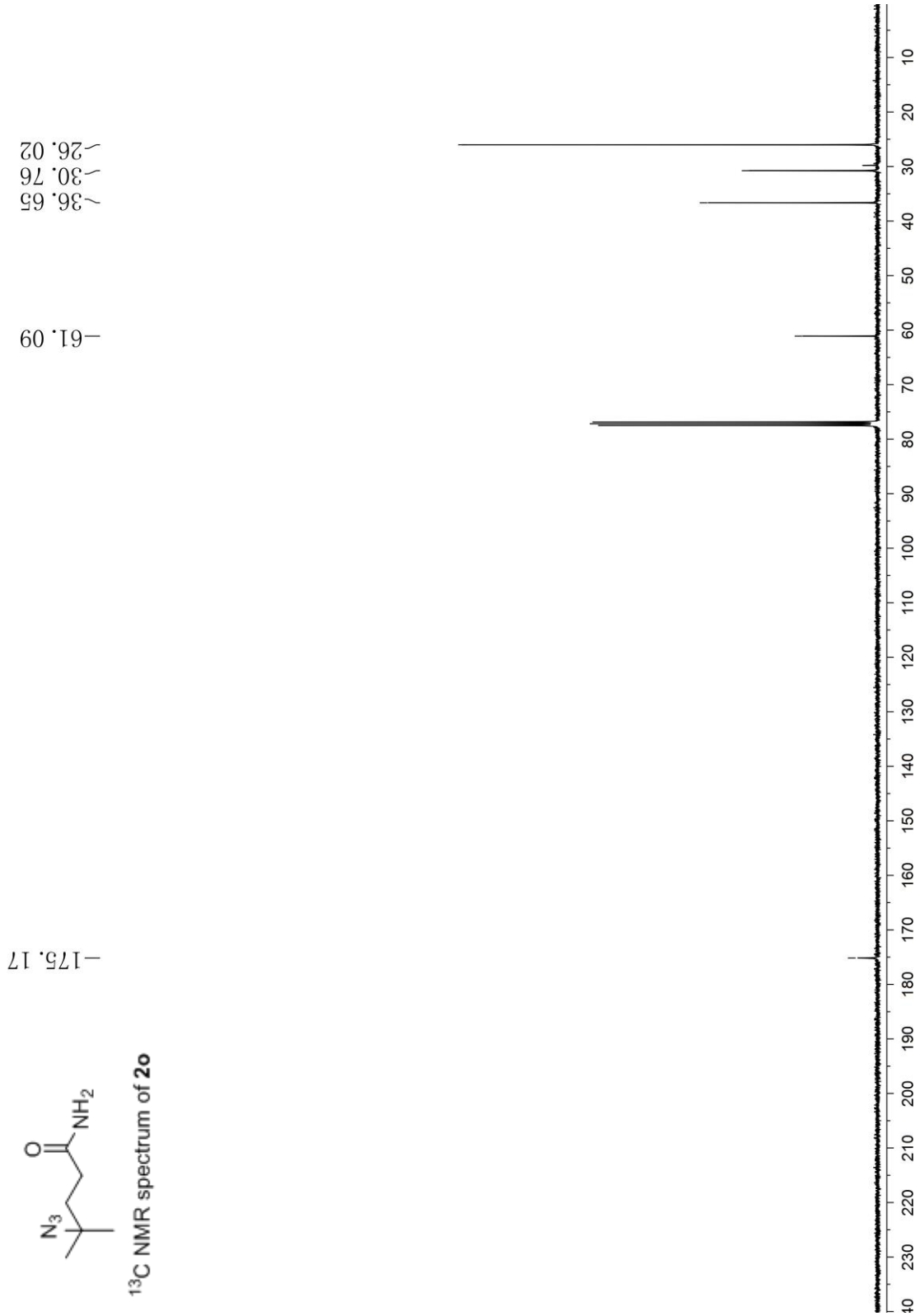
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2n**



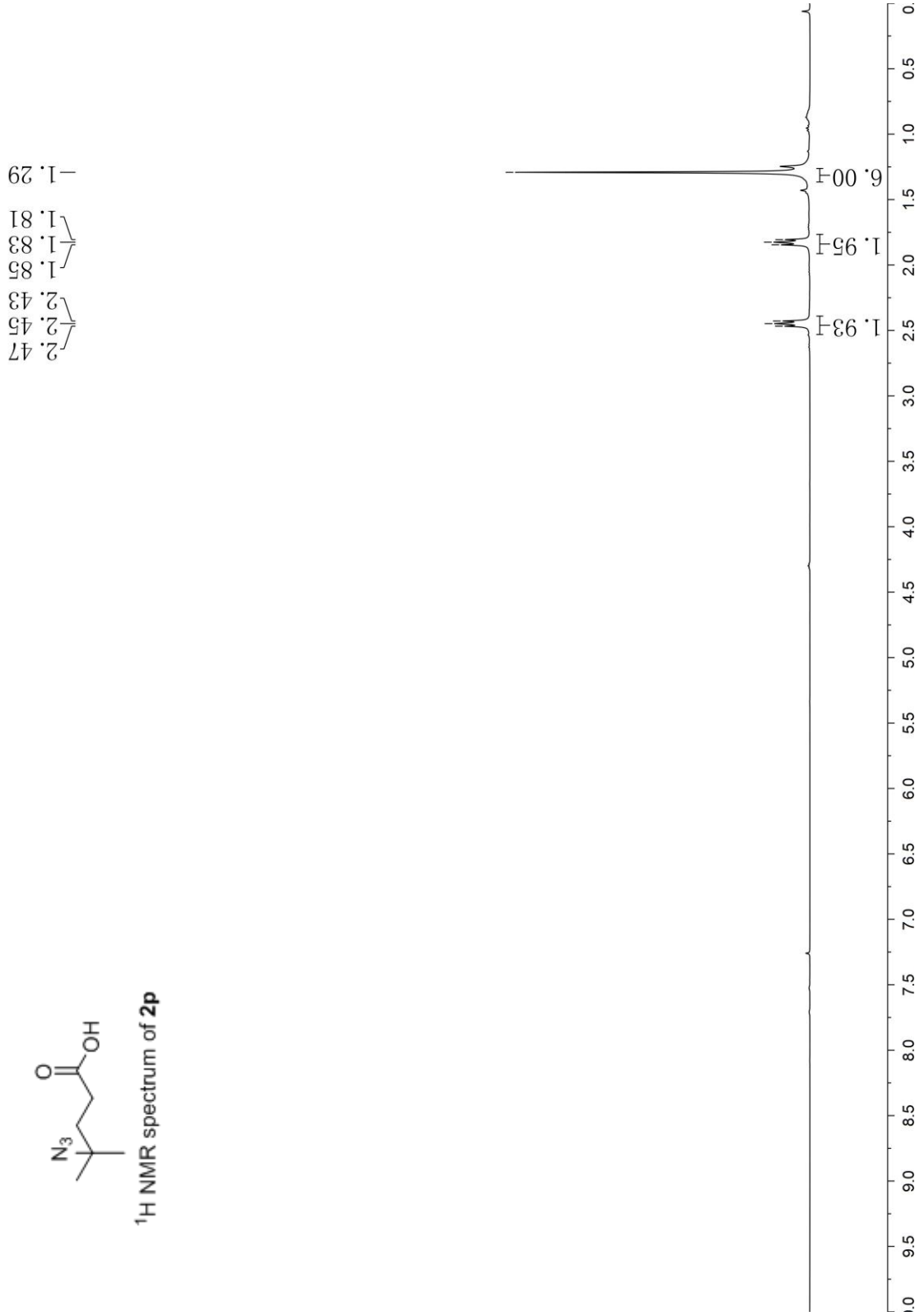
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2n**



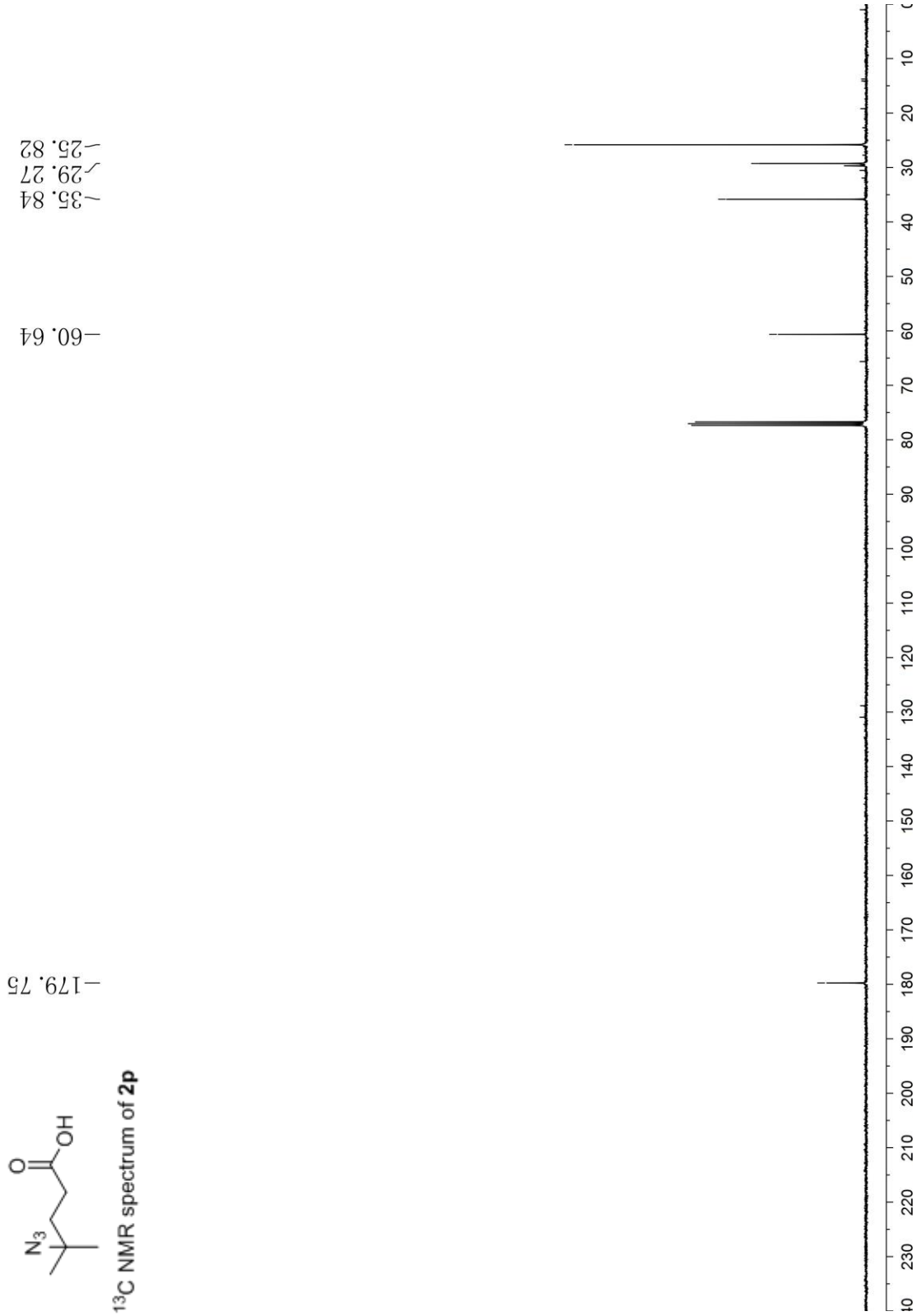
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2o**



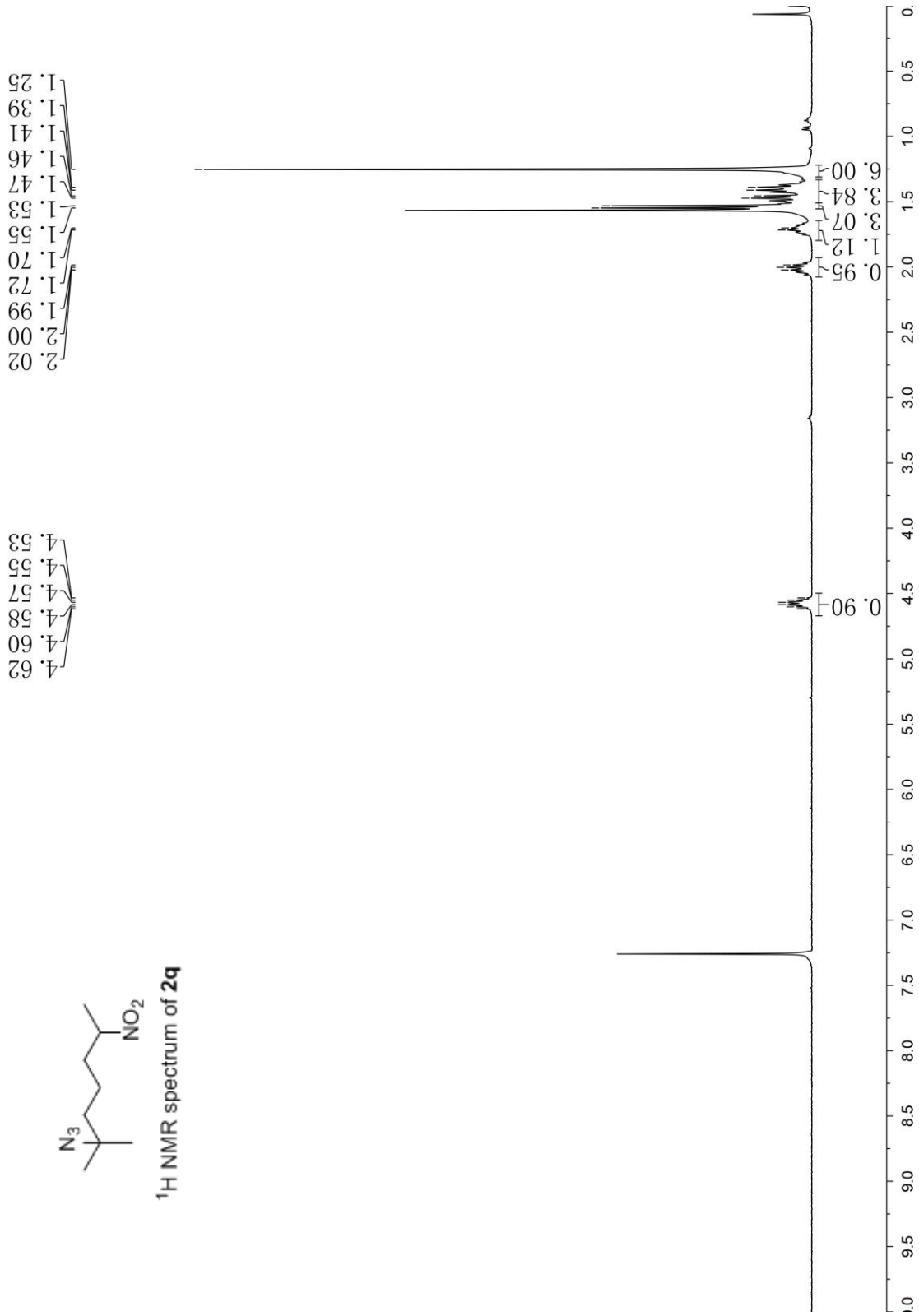
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2o**



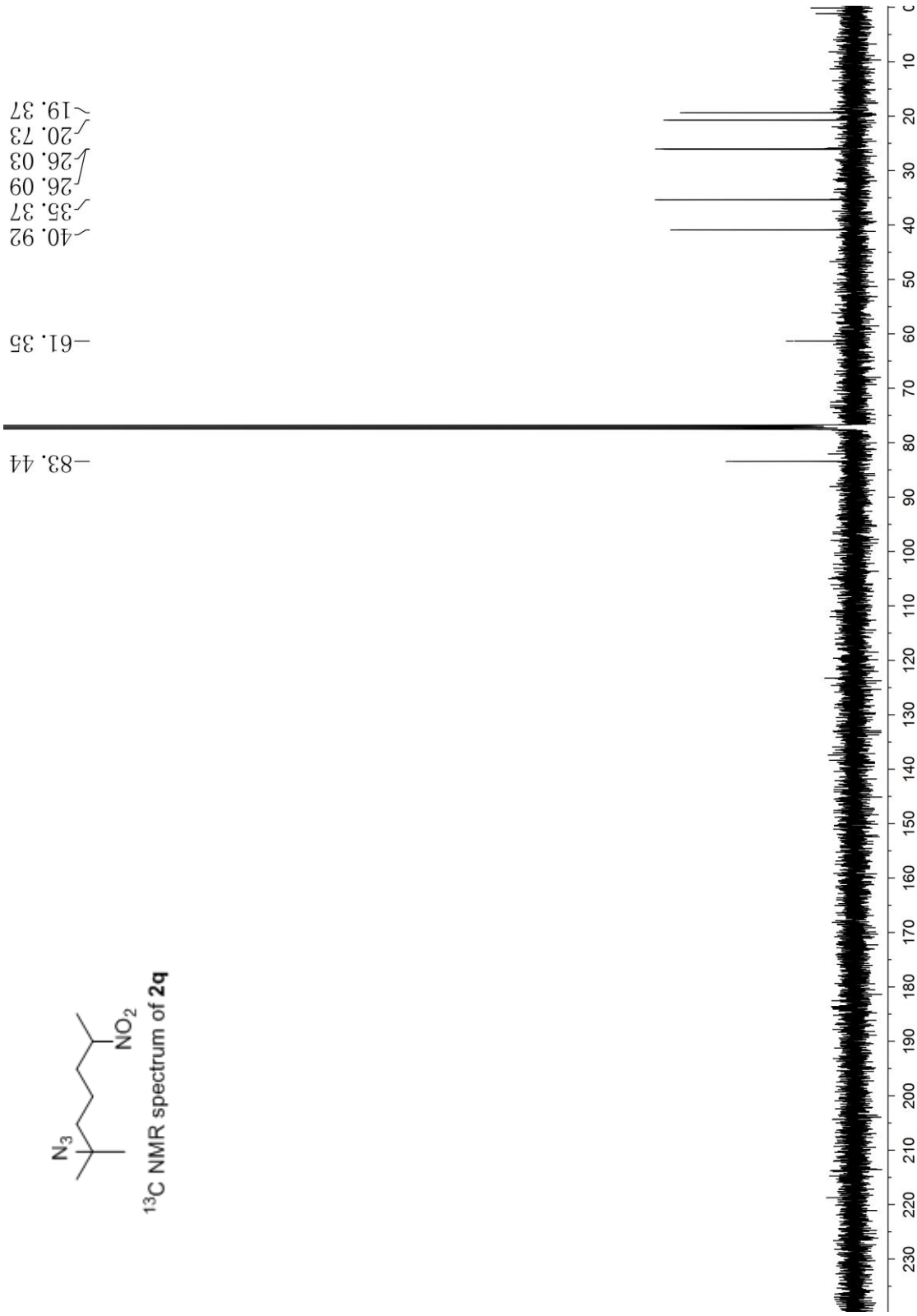
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2p**



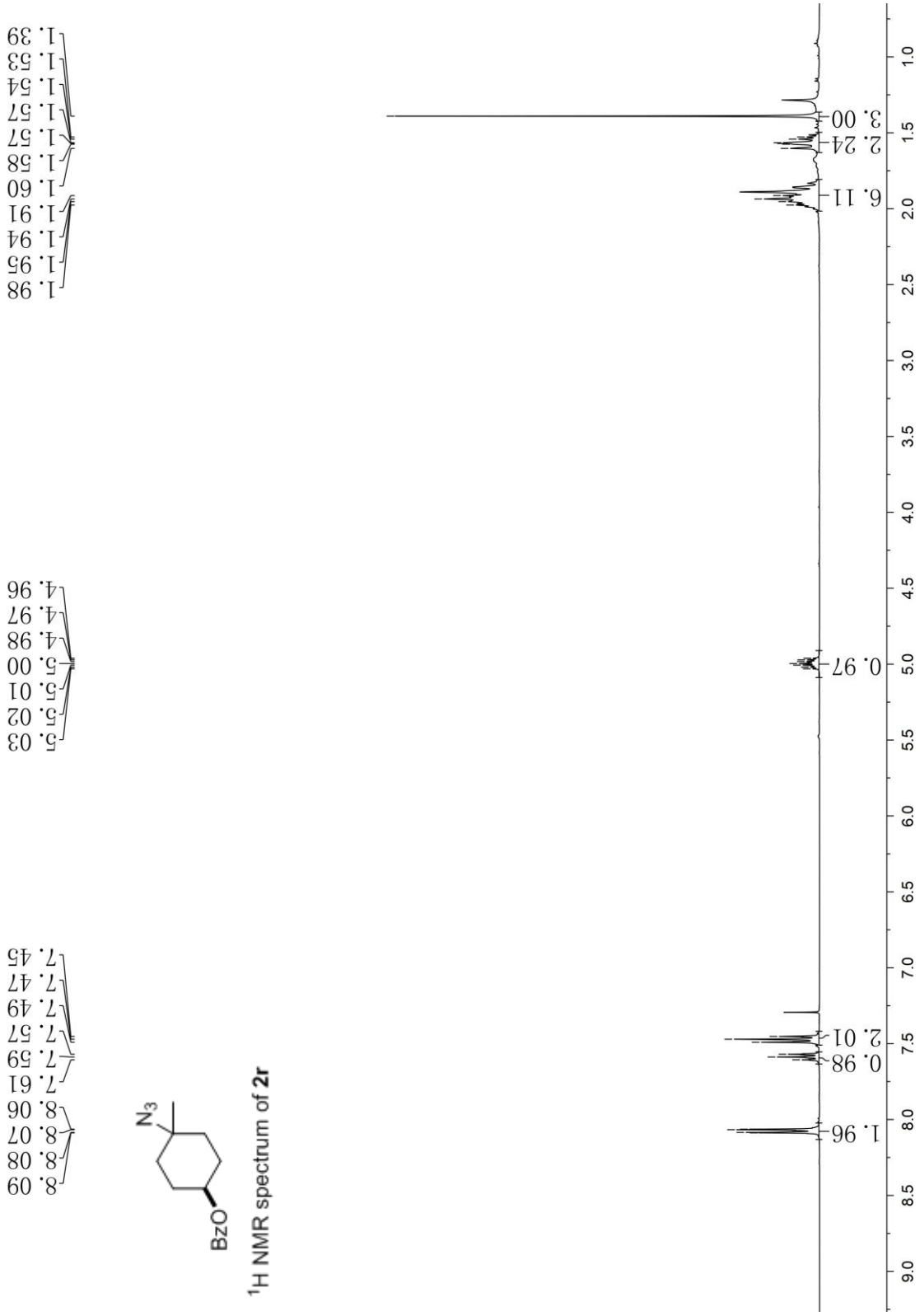
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2p**



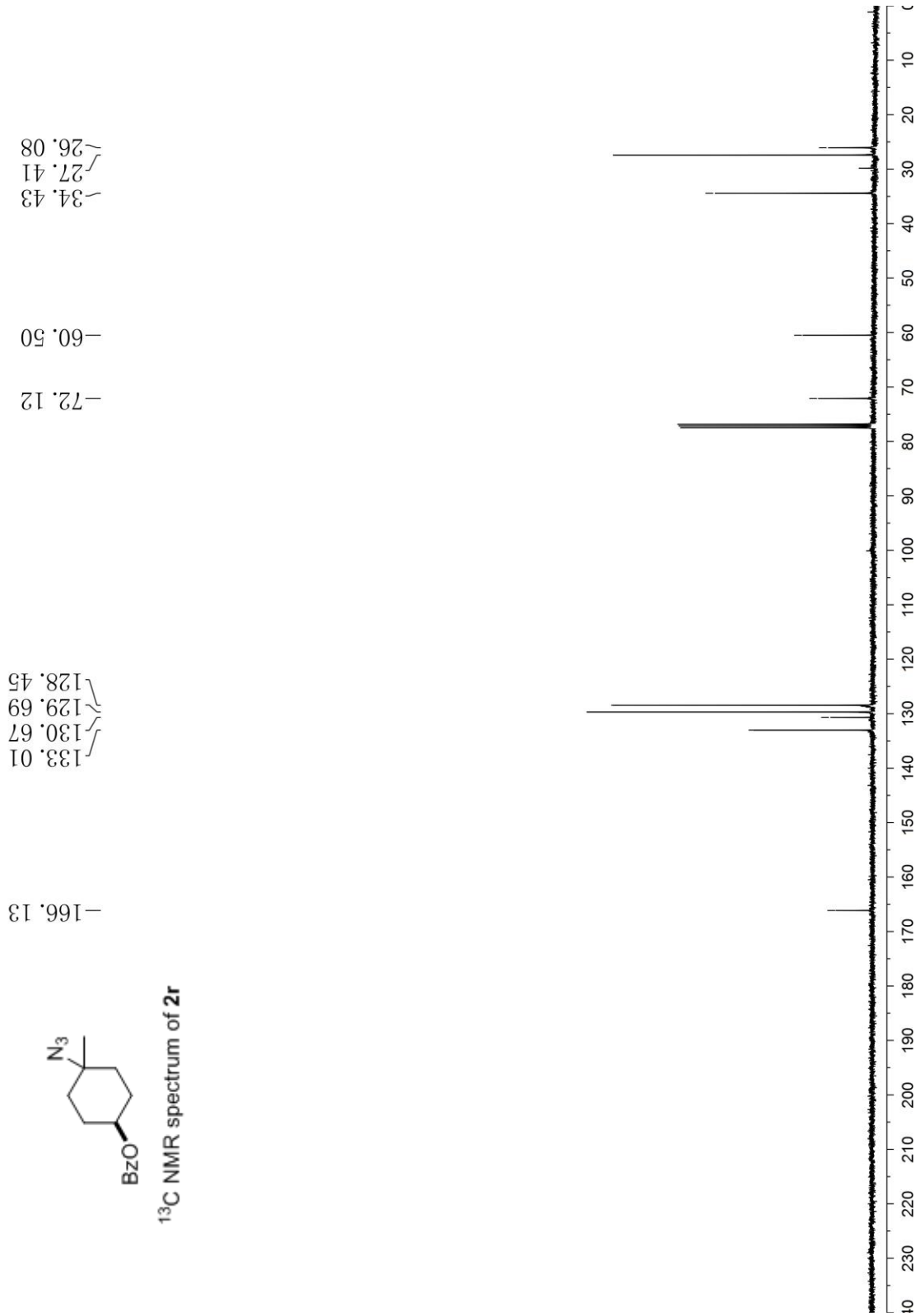
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2q**



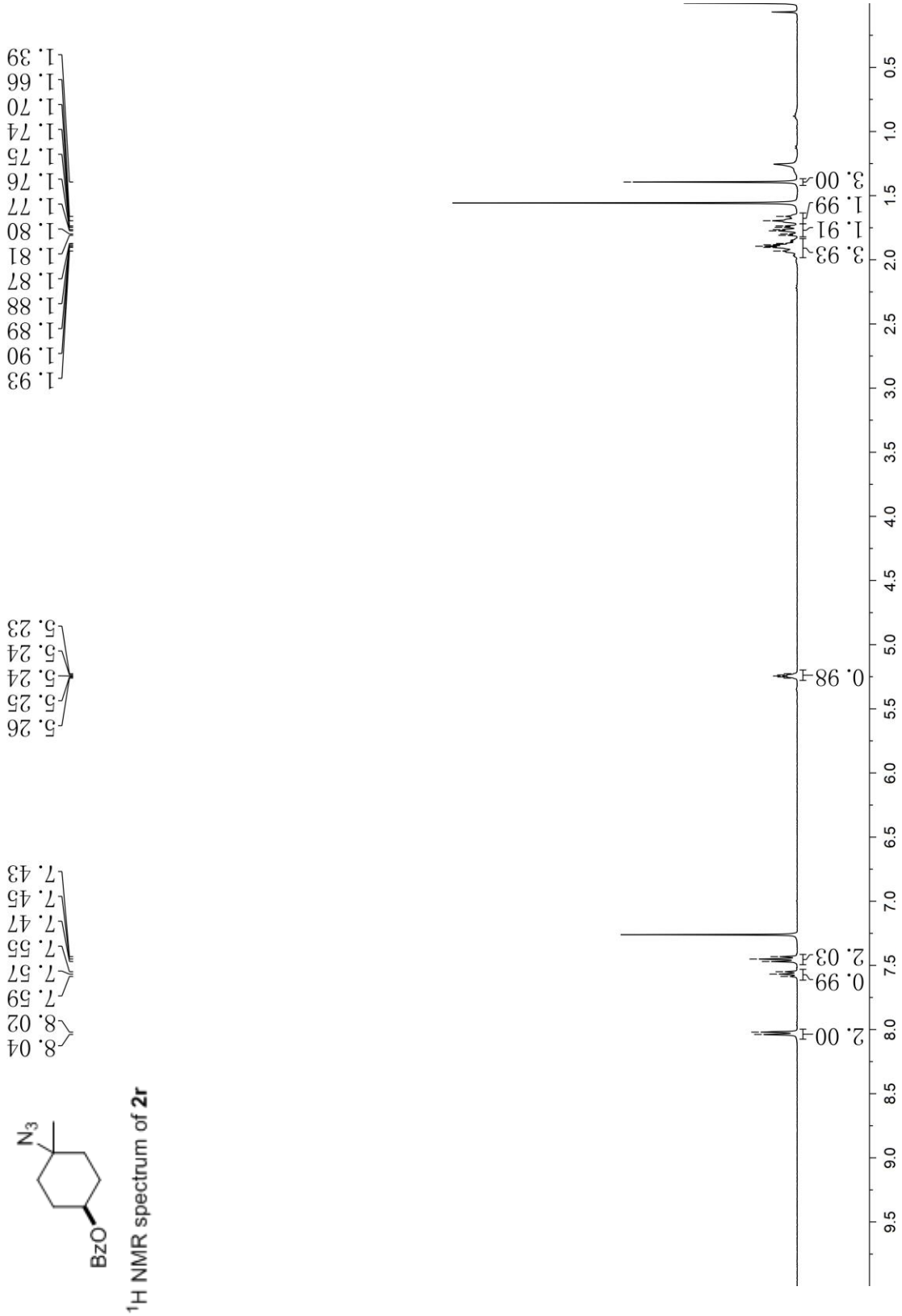
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2q**



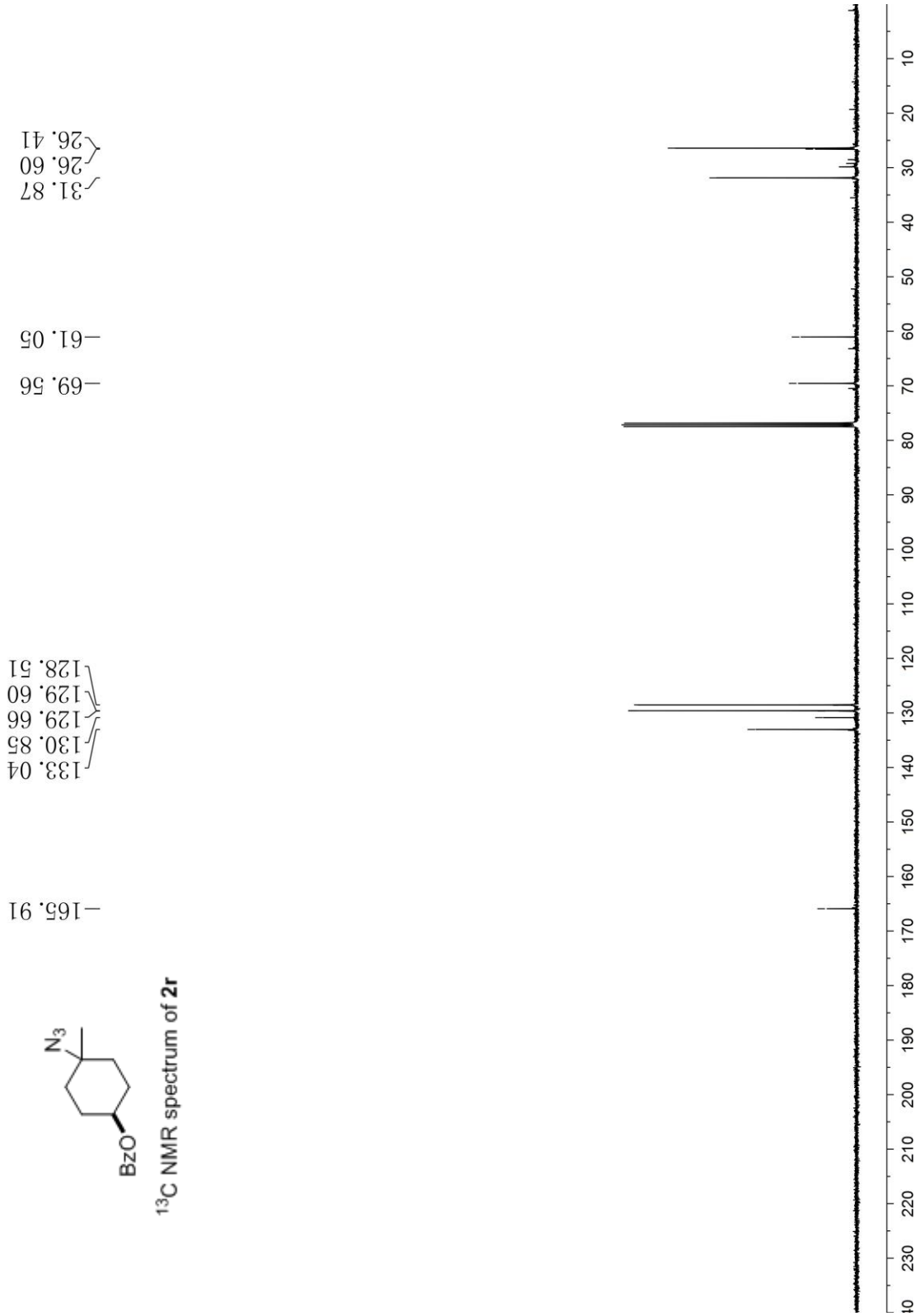
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2r isomer 1**



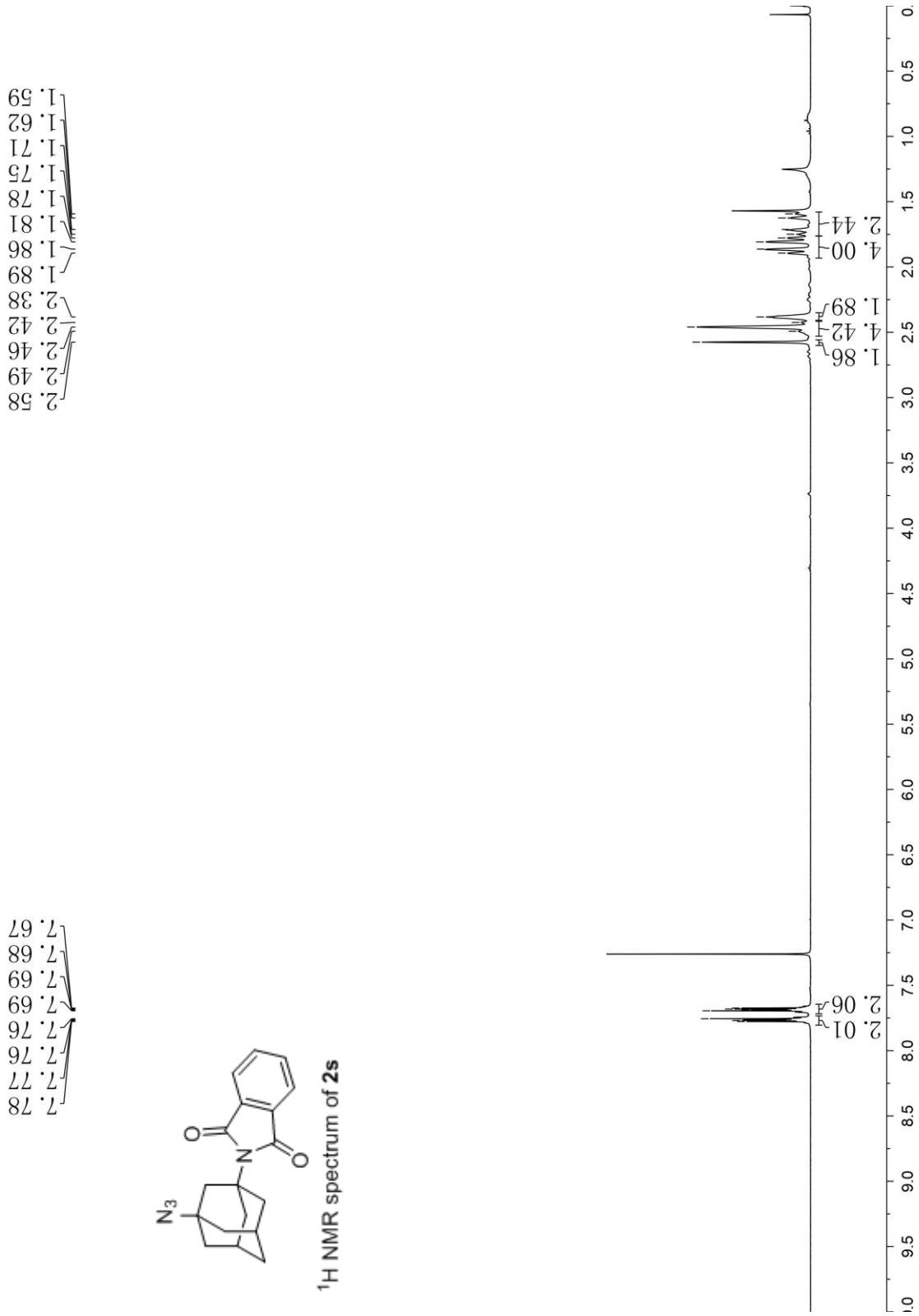
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2r isomer 1**



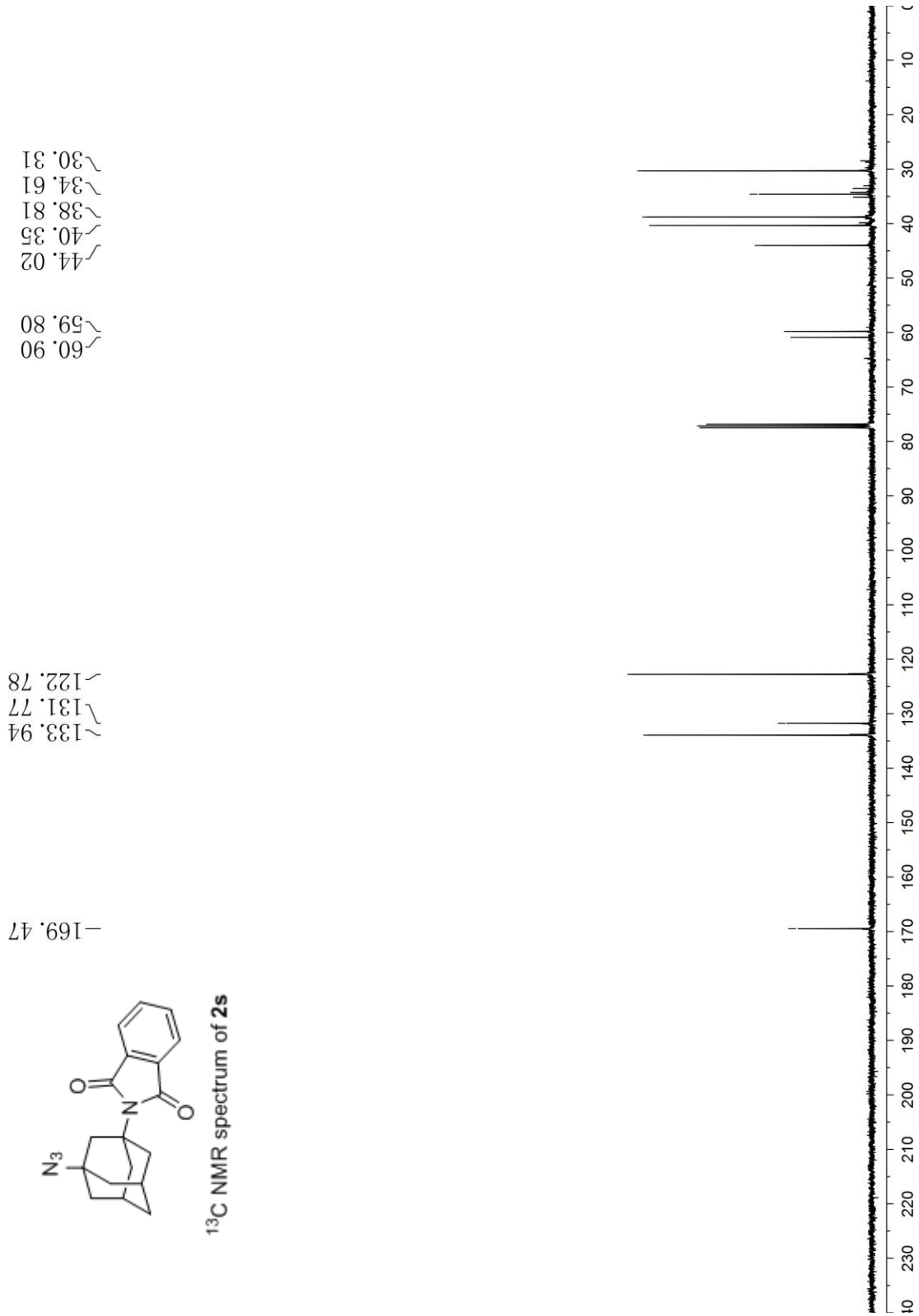
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2r isomer 2**



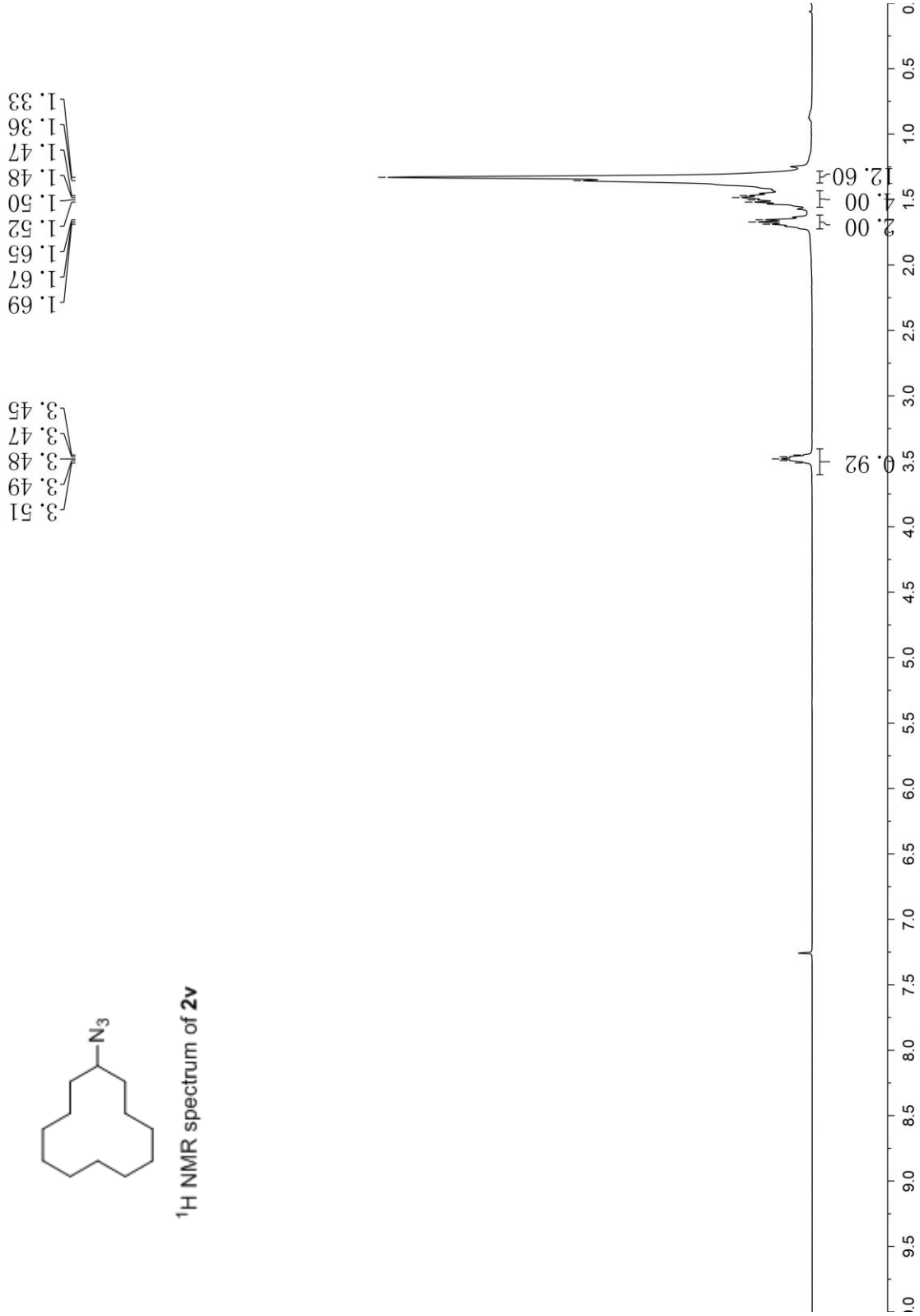
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2r isomer 2**



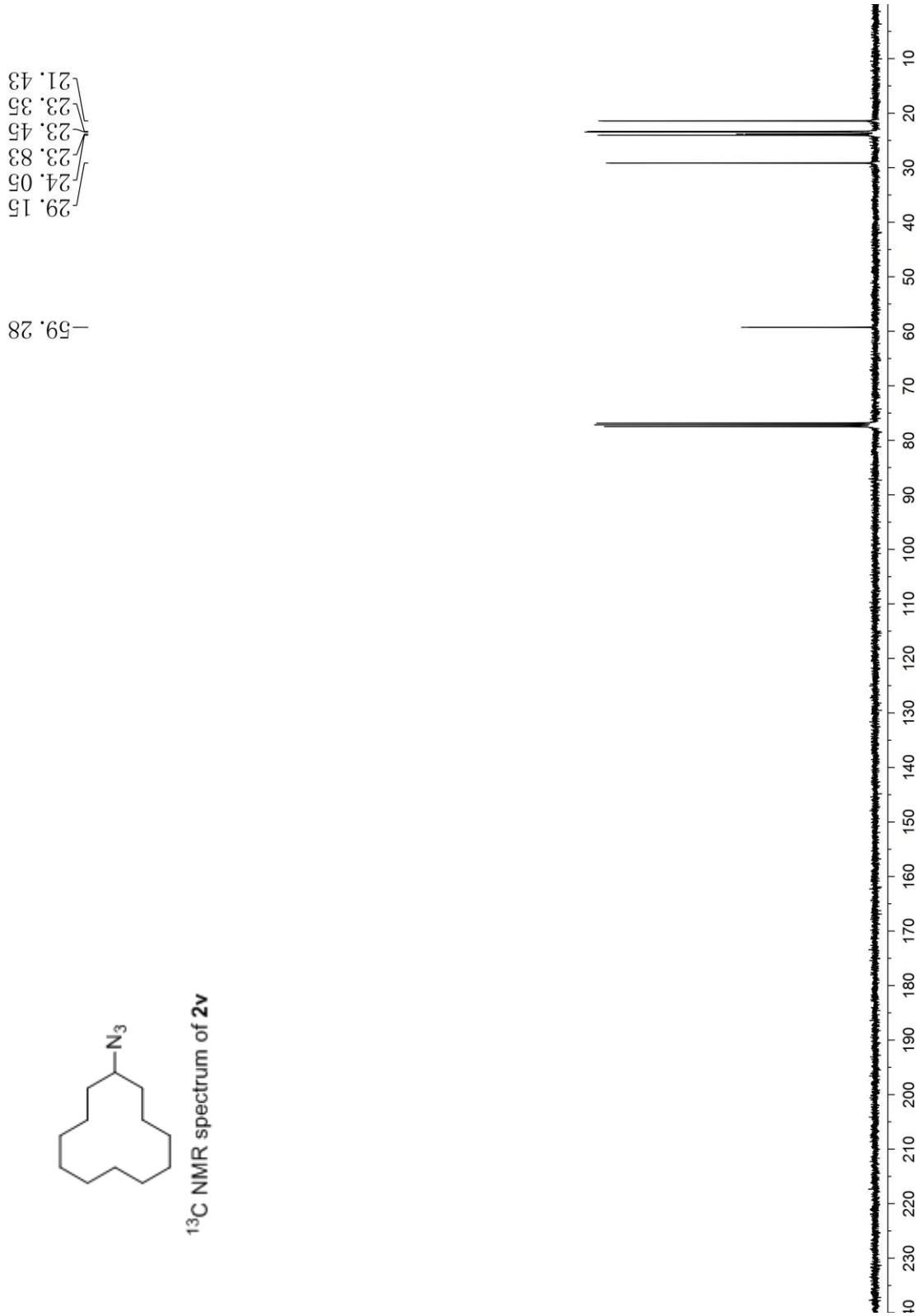
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2s**



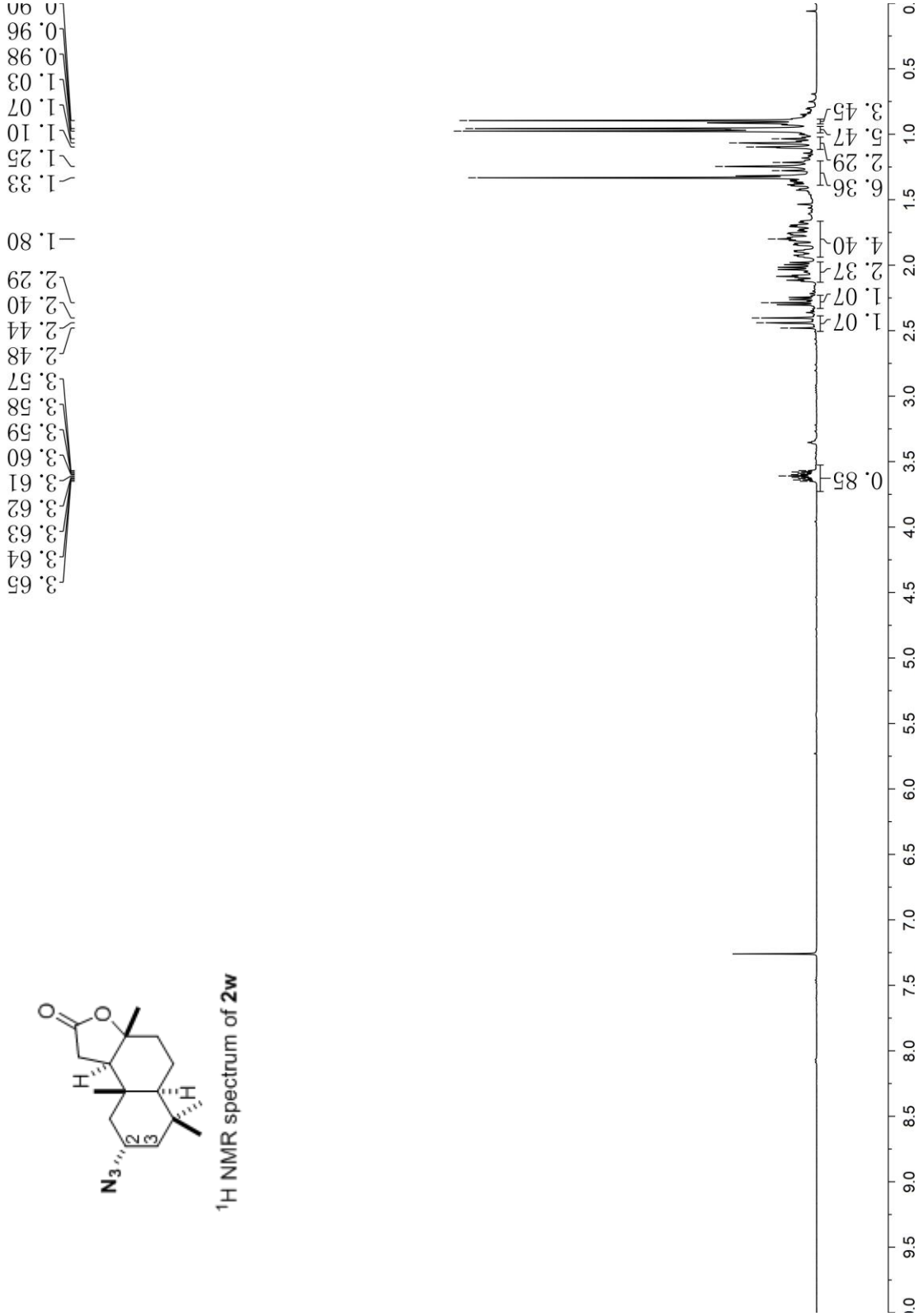
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2s**



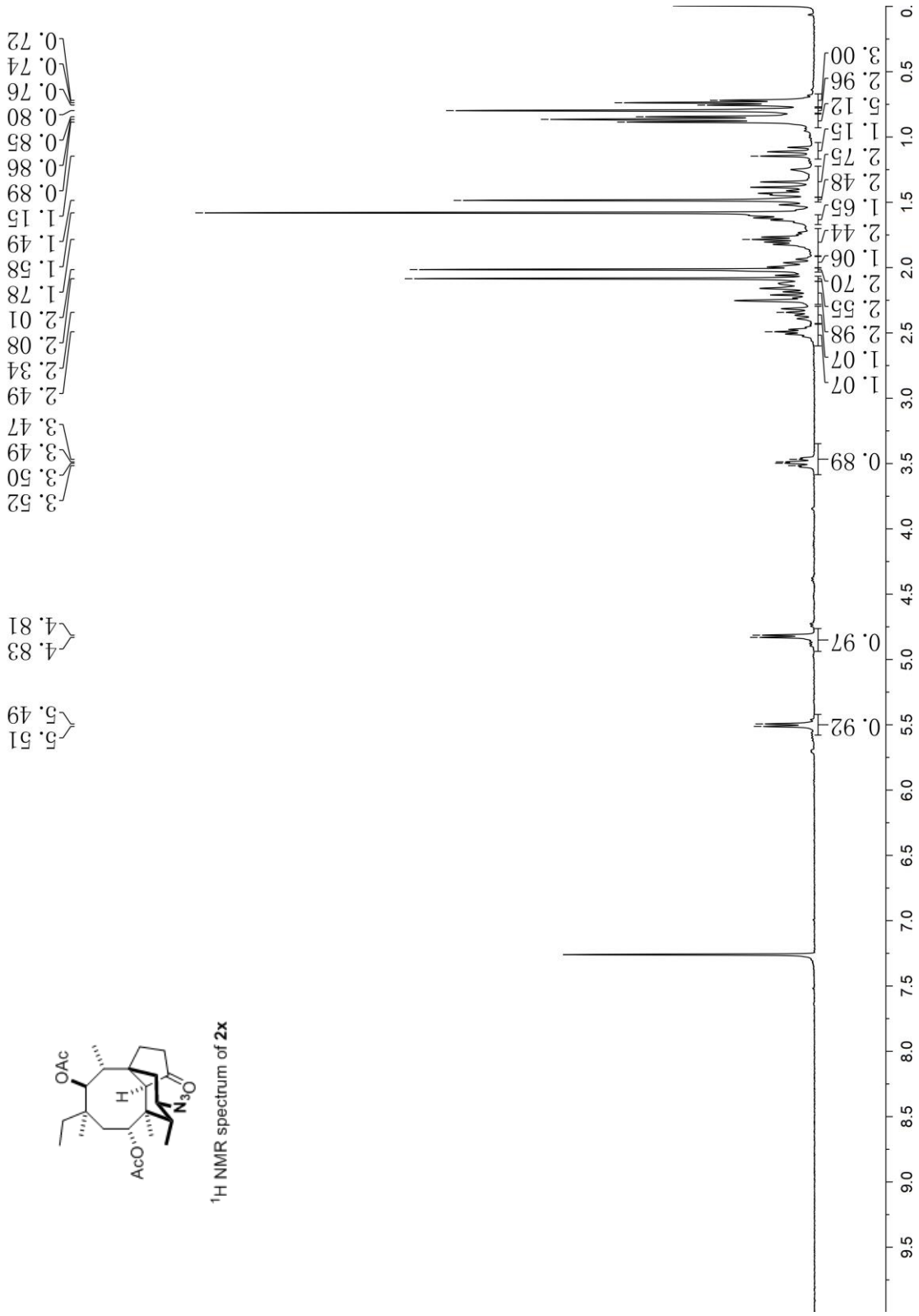
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2v**



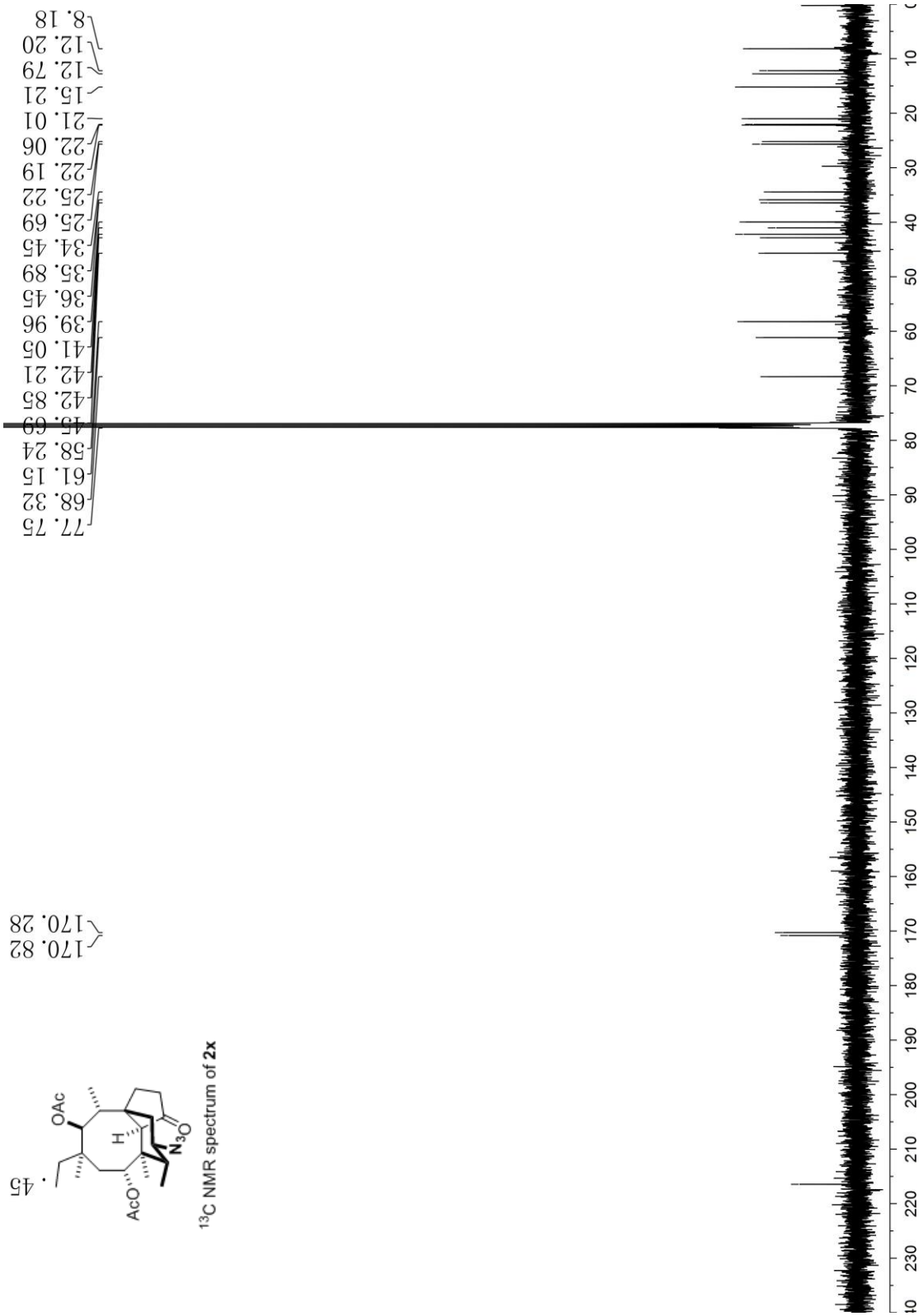
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2v**



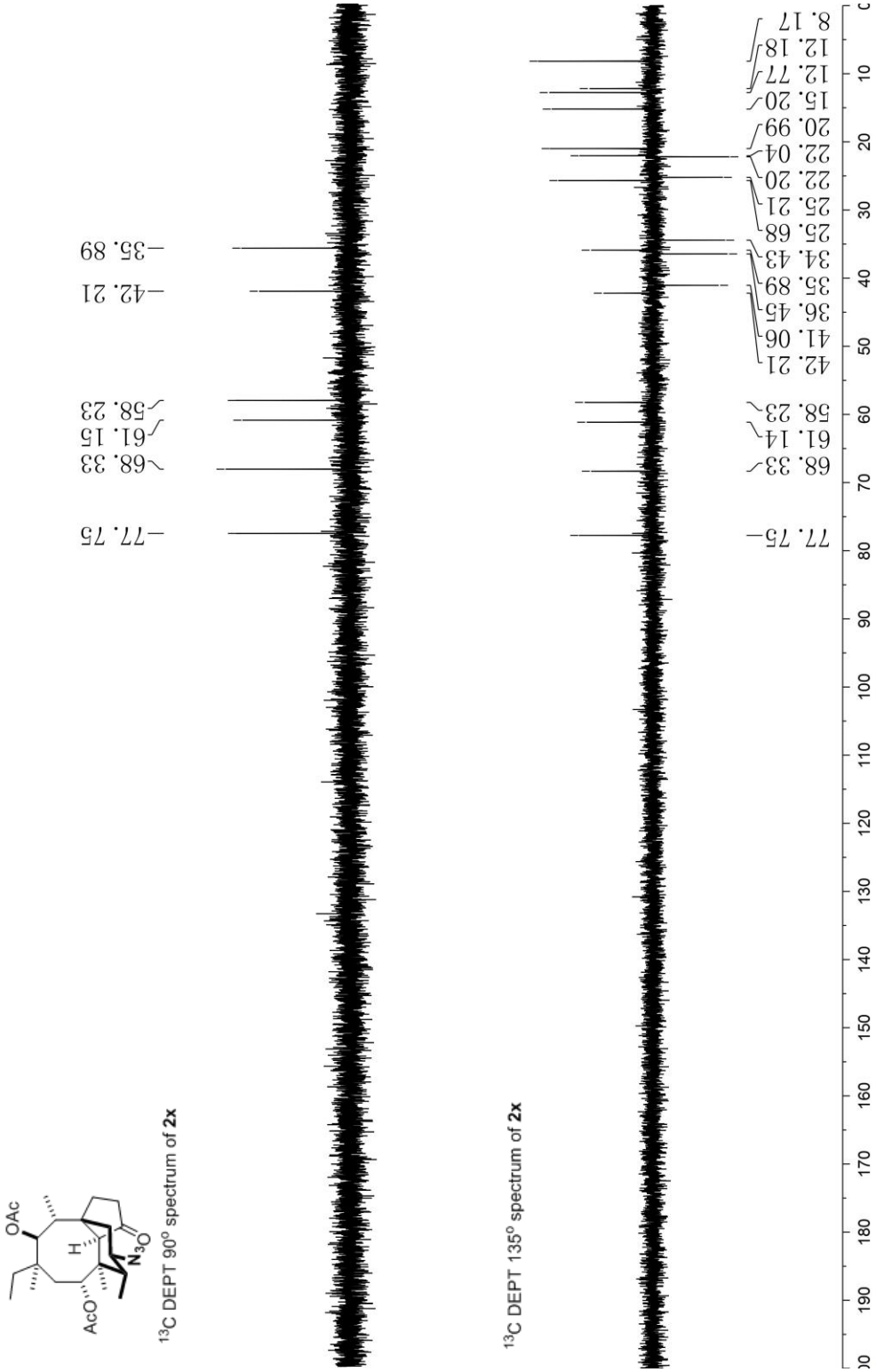
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2w**



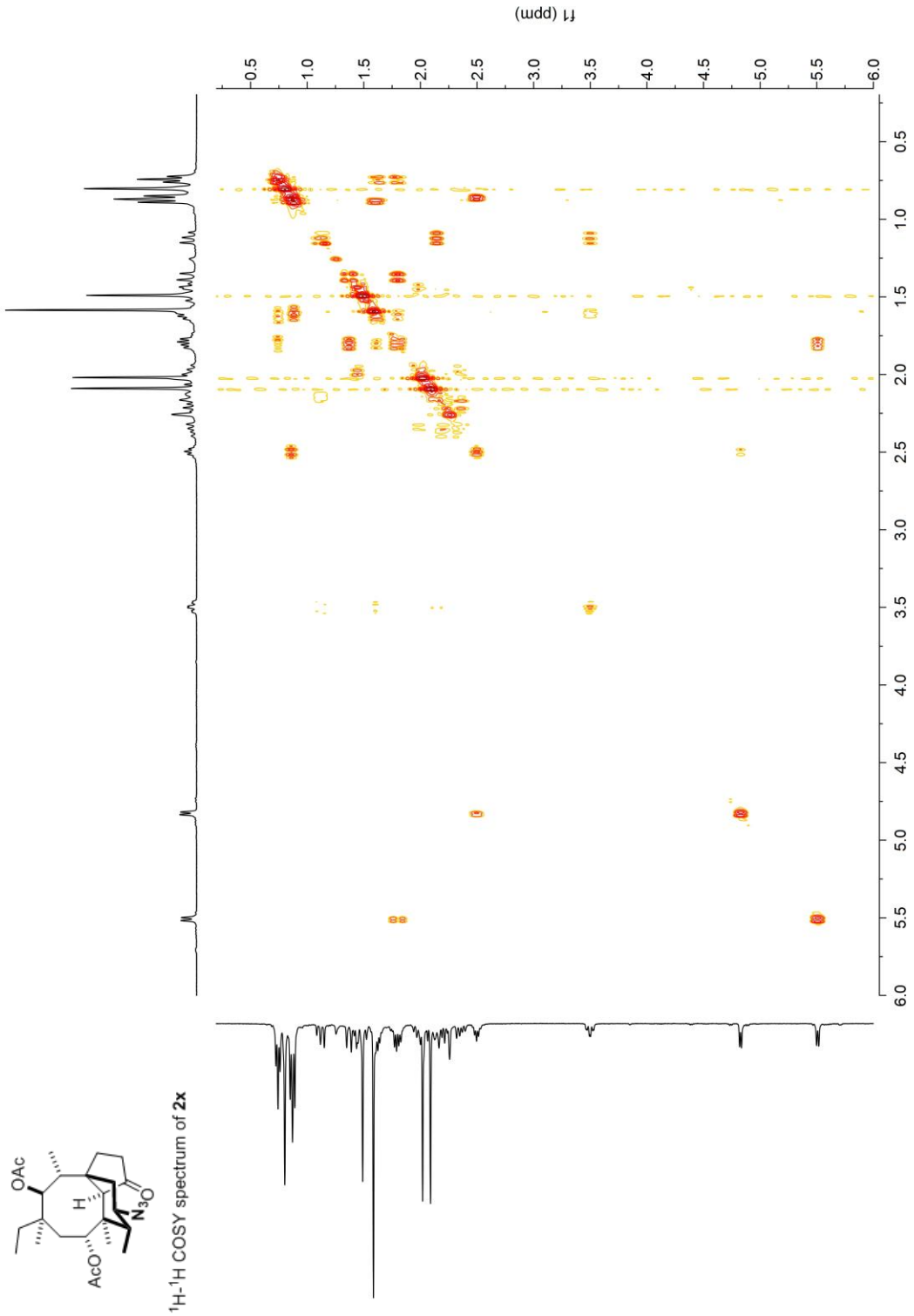
^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2x**



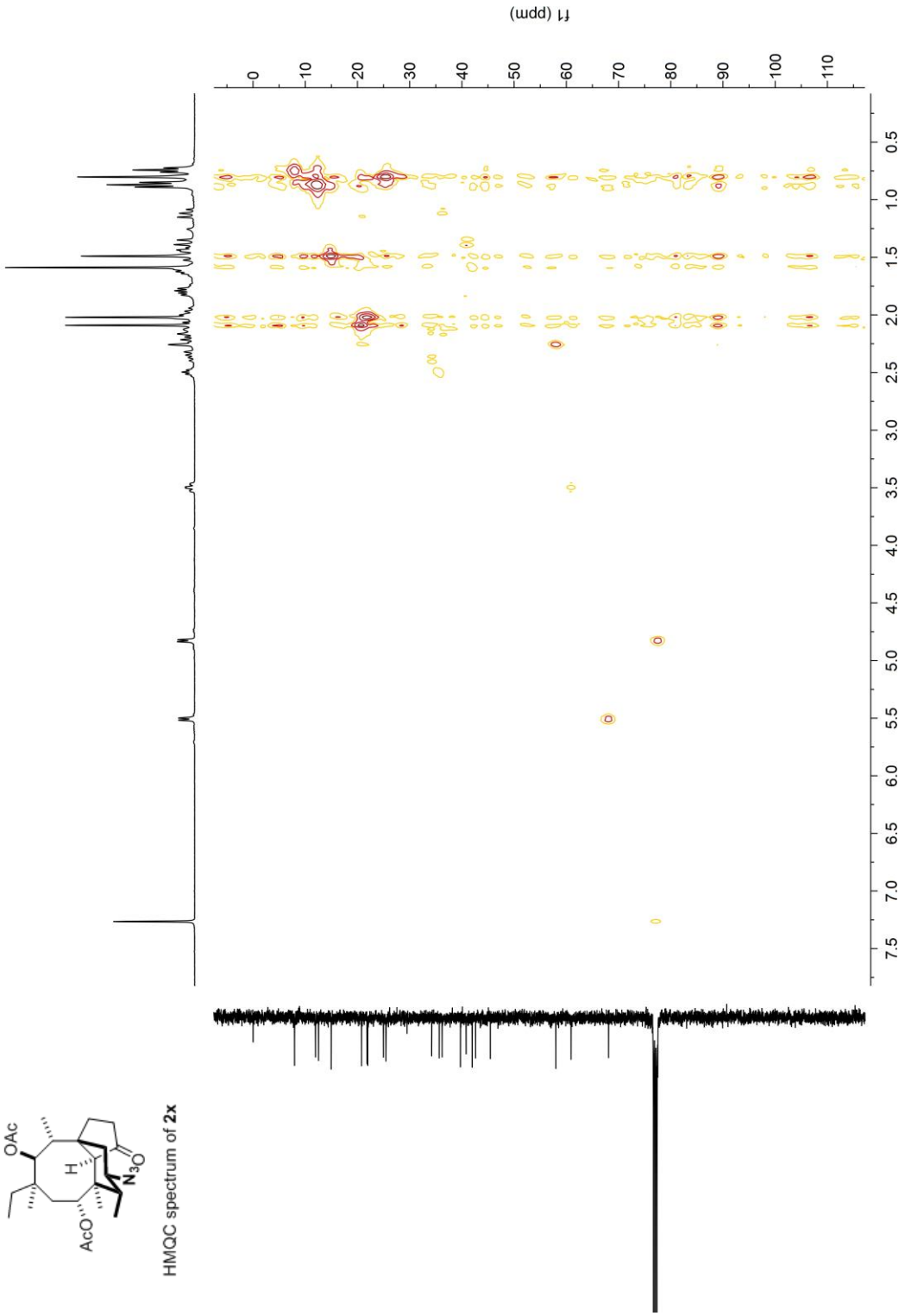
^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2x**



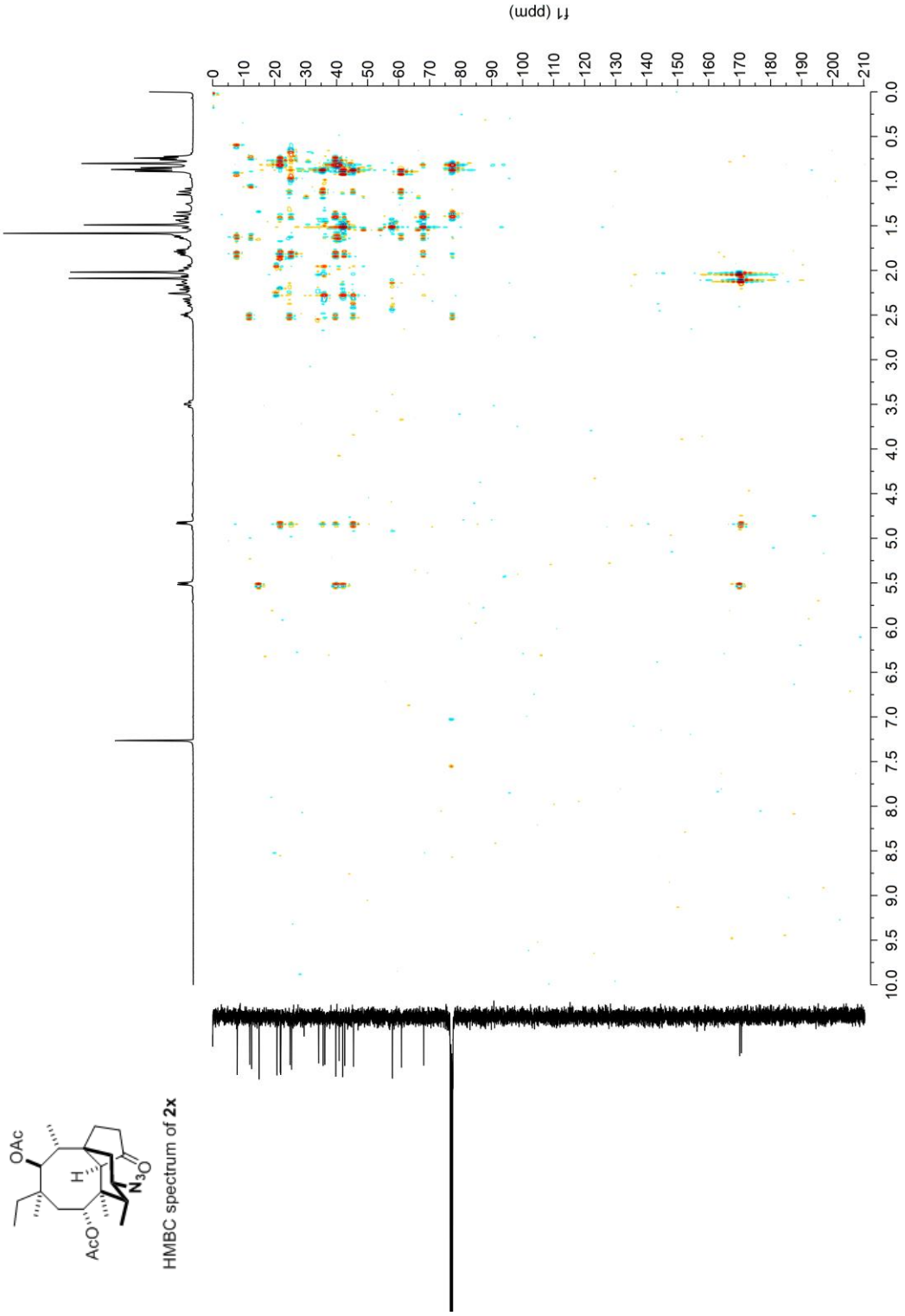
^{13}C DEPT spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2x**



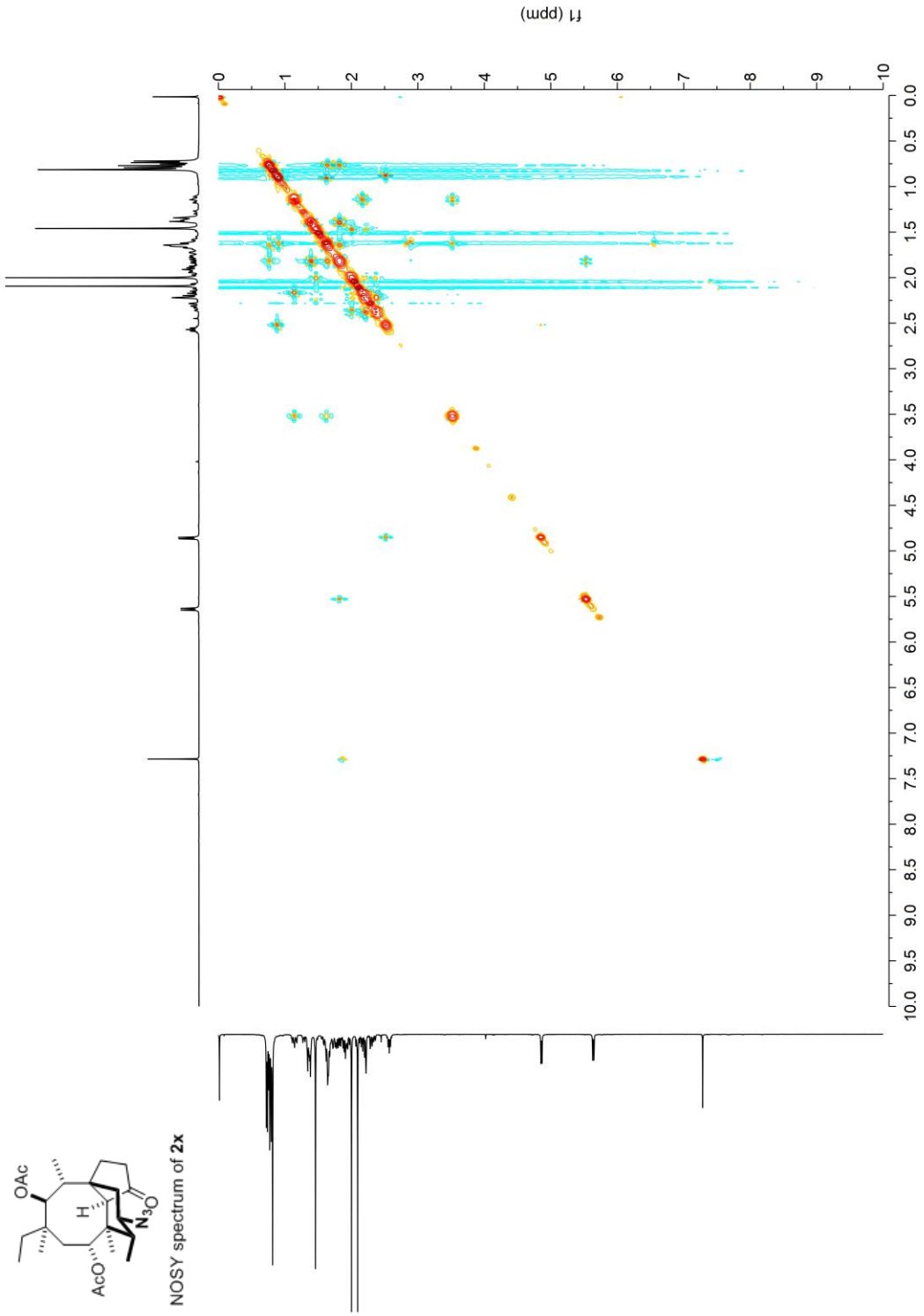
^{1}H-^{1}H COSY spectrum (400 MHz, $CDCl_3$, 23 ^{o}C) of **2x**



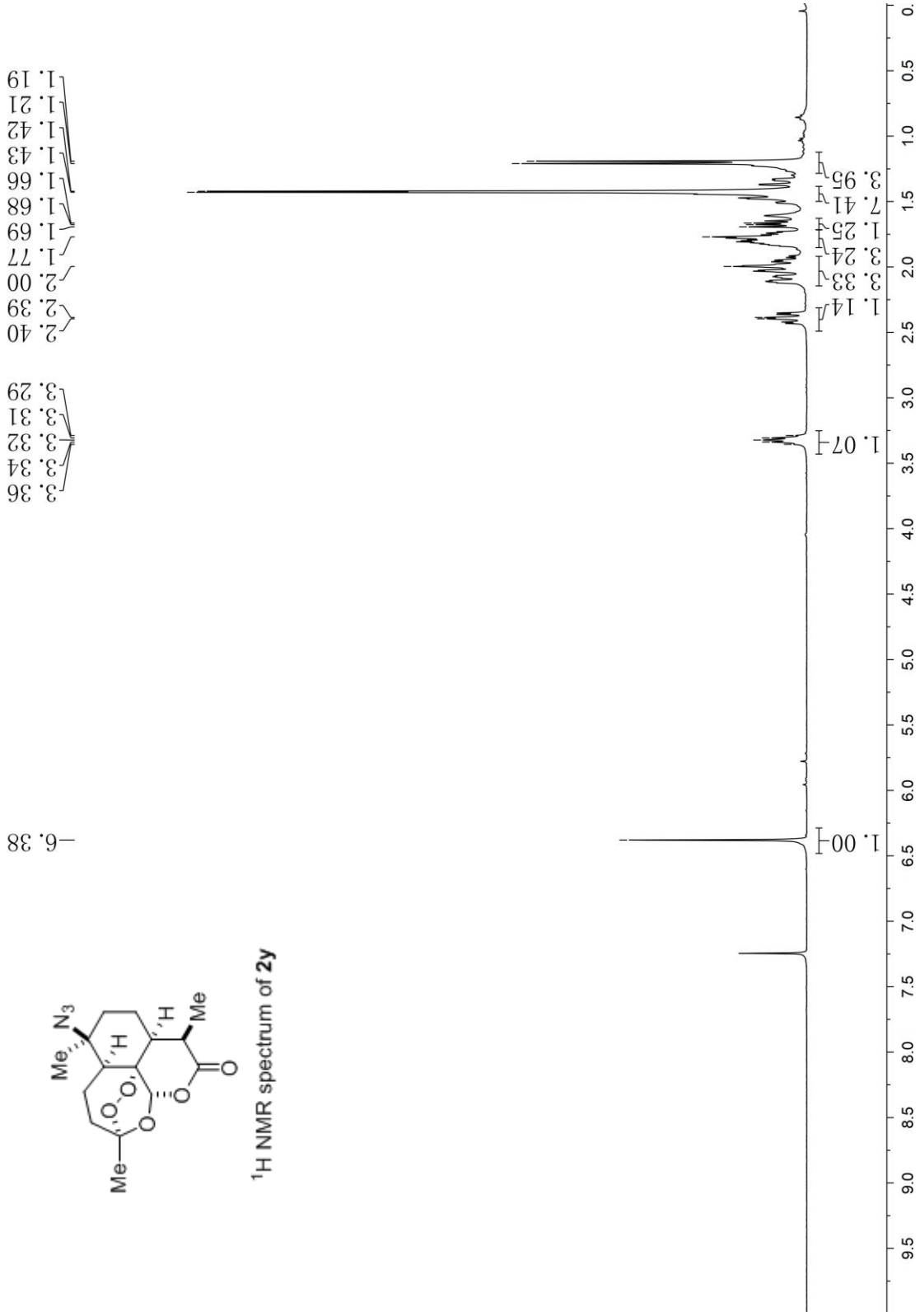
HMQC spectrum ($CDCl_3$, 23 ^oC) of **2x**



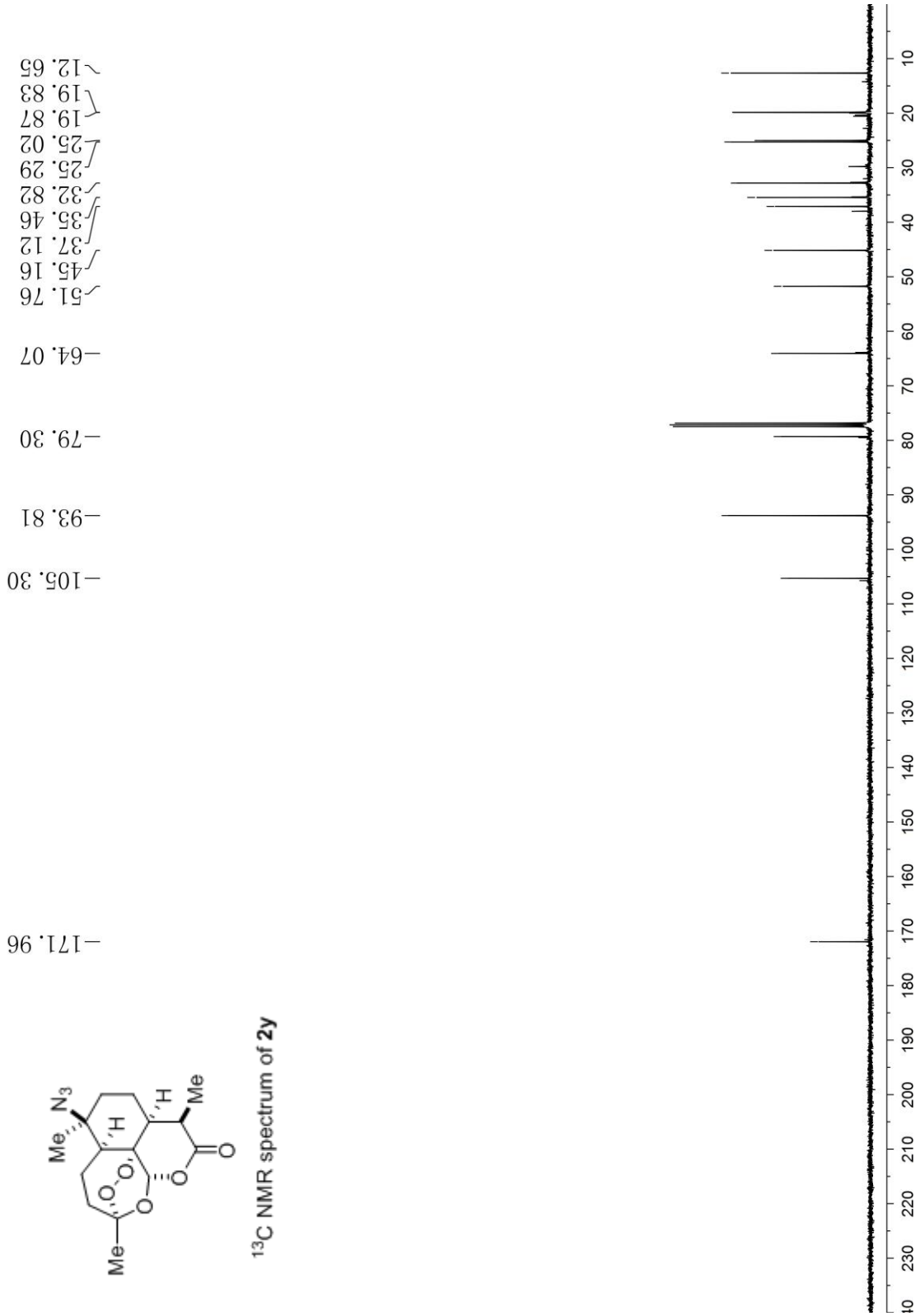
HMBC spectrum ($CDCl_3$, 23 ^oC) of **2x**



NOESY spectrum ($CDCl_3$, 23 ^oC) of **2x**



^{1}H NMR spectrum (400 MHz, $CDCl_3$, 23 ^oC) of **2y**



^{13}C NMR spectrum (101 MHz, $CDCl_3$, 23 ^{o}C) of **2y**

X-ray Crystal Structure Data for 6β-azidoartemisinin (2y)

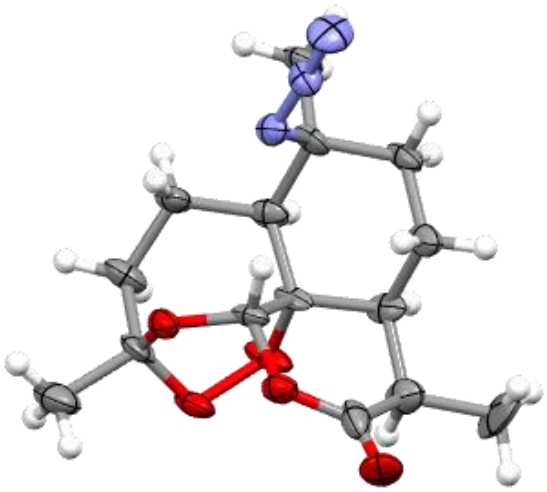


Table 8. Crystal data and structure refinement for shelxl.

Identification code	shelxl
Empirical formula	C15 H21 N3 O5
Formula weight	323.35
Temperature	173(2) K
Wavelength	1.54187 A
Crystal system, space group	Monoclinic, P2(1)
Unit cell dimensions	a = 6.359(2) A alpha = 90 deg. b = 22.998(5) A beta = 90.0100(10) deg. c = 32.023(7) A gamma = 90 deg.
Volume	4683(2) A^3
Z, Calculated density	12, 1.376 Mg/m^3
Absorption coefficient	0.872 mm^-1
F(000)	2064
Crystal size	0.320 x 0.180 x 0.160 mm
Theta range for data collection	6.402 to 77.739 deg.
Limiting indices	-7<=h<=5, -27<=k<=29, -40<=l<=40
Reflections collected / unique	41927 / 17889 [R(int) = 0.0428]
Completeness to theta = 67.687	99.4 %
Absorption correction	Semi-empirical from eq.alents
Max. and min. transmission	0.889 and 0.767

Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	17889 / 1 / 1263
Goodness-of-fit on F^2	1.099
Final R indices [I>2sigma(I)]	R1 = 0.0682, wR2 = 0.1499
R indices (all data)	R1 = 0.0806, wR2 = 0.1575
Absolute structure parameter	-0.04(8)
Extinction coefficient	0.00052(4)
Largest diff. peak and hole	0.283 and -0.357 e.A^-3

Table 9. Atomic coordinates (x 10^4) and eq.alent isotropic displacement parameters (A^2 x 10^3) for shelxl. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U(eq)
O(1)	6652(11)	9828(3)	984(2)	45(2)
O(2)	4611(11)	10154(3)	976(2)	39(2)
O(3)	2994(10)	8979(3)	848(2)	35(1)
O(4)	2896(12)	8534(3)	240(2)	49(2)
O(5)	2847(10)	9563(3)	1427(2)	32(1)
N(1)	5879(12)	8477(3)	1985(2)	31(2)
N(2)	5964(12)	7979(3)	2128(2)	31(2)
N(3)	5865(17)	7533(3)	2264(2)	49(2)
C(1)	6371(12)	9264(4)	1184(2)	27(2)
C(2)	4057(14)	9124(4)	1235(2)	29(2)
C(3)	3946(19)	8755(4)	512(3)	46(3)
C(4)	6306(16)	8830(5)	471(3)	44(2)
C(5)	7466(14)	8838(5)	898(2)	37(2)
C(6)	7672(16)	8239(4)	1100(3)	44(2)
C(7)	8900(14)	8300(4)	1505(3)	35(2)
C(8)	7925(14)	8721(4)	1822(3)	32(2)
C(9)	7452(14)	9314(4)	1607(2)	32(2)
C(10)	6277(16)	9724(4)	1918(2)	35(2)
C(11)	5322(15)	10257(4)	1715(3)	41(2)
C(12)	3764(15)	10126(3)	1372(3)	35(2)
C(13)	7240(20)	8388(8)	149(3)	89(5)

C(14)	9440(15)	8788(4)	2182(3)	43(2)
C(15)	1844(19)	10548(5)	1371(3)	54(3)
O(1A)	1326(11)	5556(3)	628(2)	41(2)
O(2A)	-707(12)	5250(3)	683(2)	55(2)
O(3A)	-2173(11)	6437(3)	839(2)	47(2)
O(4A)	-1941(12)	6871(3)	1436(2)	50(2)
O(5A)	-2604(12)	5866(3)	254(2)	62(2)
N(1A)	310(20)	6919(5)	-343(3)	77(4)
N(2A)	450(30)	7403(6)	-530(4)	110(6)
N(3A)	380(30)	7837(8)	-686(4)	140(8)
C(1A)	991(17)	6118(5)	433(3)	46(2)
C(2A)	-1283(15)	6291(5)	434(3)	43(2)
C(3A)	-975(15)	6647(3)	1156(2)	32(2)
C(4A)	1355(17)	6551(4)	1149(2)	39(2)
C(5A)	2307(16)	6540(5)	703(3)	42(2)
C(6A)	2511(18)	7116(5)	491(3)	47(2)
C(7A)	3584(19)	7060(5)	59(3)	58(3)
C(8A)	2480(20)	6646(5)	-229(3)	64(4)
C(9A)	1936(19)	6076(5)	-19(3)	56(3)
C(10A)	640(20)	5670(6)	-289(3)	74(4)
C(11A)	-420(20)	5140(6)	-72(4)	87(6)
C(12A)	-1794(18)	5279(5)	309(4)	68(4)
C(13A)	2464(15)	6969(4)	1441(3)	39(2)
C(14A)	3750(30)	6566(6)	-628(3)	95(6)
C(15A)	-3640(20)	4880(6)	358(5)	90(5)
O(1B)	1418(11)	5517(3)	4280(2)	53(2)
O(2B)	-544(12)	5190(3)	4319(2)	56(2)
O(3B)	-2323(11)	6361(3)	4417(2)	46(2)
O(4B)	-2375(12)	6856(4)	5006(3)	64(2)
O(5B)	-2440(12)	5750(3)	3858(2)	52(2)
N(1B)	587(16)	6841(4)	3279(3)	59(2)
N(2B)	659(16)	7111(3)	2959(3)	54(2)
N(3B)	550(20)	7375(5)	2642(3)	79(4)
C(1B)	1099(15)	6085(4)	4078(3)	43(2)
C(2B)	-1318(15)	6198(4)	4021(3)	43(2)

C(3B)	-1296(18)	6615(4)	4751(3)	49(3)
C(4B)	1019(16)	6528(5)	4778(3)	52(3)
C(5B)	2142(14)	6519(4)	4359(3)	41(2)
C(6B)	2324(17)	7111(4)	4149(3)	49(2)
C(7B)	3581(15)	7039(4)	3735(3)	46(2)
C(8B)	2641(19)	6604(5)	3429(3)	55(3)
C(9B)	2163(16)	6018(4)	3639(3)	46(2)
C(10B)	1040(20)	5590(5)	3372(4)	61(3)
C(11B)	-20(20)	5054(6)	3556(3)	64(3)
C(12B)	-1552(18)	5193(5)	3900(3)	56(3)
C(13B)	1948(17)	6947(5)	5088(4)	59(3)
C(14B)	4110(20)	6511(6)	3060(4)	72(4)
C(15B)	-3390(20)	4774(6)	3953(5)	76(4)
O(1C)	8519(10)	759(3)	2503(2)	43(2)
O(2C)	10506(11)	412(3)	2480(2)	40(2)
O(3C)	12329(11)	1564(4)	2401(2)	57(2)
O(4C)	12584(13)	2052(4)	1824(3)	74(2)
O(5C)	12273(12)	969(3)	2971(2)	49(2)
N(1C)	9248(17)	2050(4)	3523(3)	65(3)
N(2C)	9145(18)	2492(4)	3720(3)	55(2)
N(3C)	9230(20)	2874(6)	3955(4)	86(4)
C(1C)	8842(16)	1307(4)	2719(4)	48(3)
C(2C)	11143(16)	1422(4)	2790(3)	43(2)
C(3C)	11317(17)	1827(4)	2082(3)	47(2)
C(4C)	8973(18)	1780(4)	2029(4)	59(3)
C(5C)	7871(15)	1746(4)	2445(4)	50(3)
C(6C)	7611(18)	2324(4)	2668(5)	72(4)
C(7C)	6250(20)	2269(4)	3075(5)	76(4)
C(8C)	7140(20)	1821(4)	3370(4)	62(3)
C(9C)	7669(17)	1244(4)	3145(3)	48(2)
C(10C)	8707(18)	823(5)	3424(3)	49(2)
C(11C)	9645(19)	273(4)	3224(3)	47(3)
C(12C)	11383(16)	391(4)	2897(3)	38(2)
C(13C)	8210(20)	2219(6)	1719(5)	88(5)
C(14C)	5590(20)	1731(5)	3720(5)	84(5)

C(15C)	13153(18)	-26(5)	2889(3)	48(3)
O(1D)	3823(12)	5080(3)	2449(3)	71(2)
O(2D)	5829(12)	5385(3)	2513(3)	56(2)
O(3D)	7408(11)	4203(3)	2603(3)	57(2)
O(4D)	7291(15)	3704(3)	3183(3)	74(3)
O(5D)	7791(10)	4820(3)	2050(2)	50(2)
N(1D)	4892(16)	3804(5)	1397(4)	77(3)
N(2D)	4800(20)	3390(6)	1174(5)	84(4)
N(3D)	4920(20)	3020(8)	929(4)	108(5)
C(1D)	4153(18)	4537(3)	2229(4)	60(3)
C(2D)	6470(19)	4387(4)	2213(4)	66(4)
C(3D)	6322(16)	3949(4)	2941(4)	58(3)
C(4D)	3910(20)	4035(5)	2894(6)	98(6)
C(5D)	2999(16)	4088(4)	2484(5)	79(5)
C(6D)	2782(19)	3499(4)	2240(5)	82(5)
C(7D)	1723(18)	3607(4)	1800(6)	92(6)
C(8D)	2773(19)	4031(4)	1555(6)	87(5)
C(9D)	3267(18)	4609(4)	1771(4)	64(4)
C(10D)	4540(20)	5034(5)	1534(5)	80(4)
C(11D)	5420(19)	5559(4)	1755(4)	69(4)
C(12D)	6897(17)	5397(4)	2125(4)	54(3)
C(13D)	2860(20)	3609(6)	3238(6)	126(9)
C(14D)	1450(20)	4157(6)	1142(6)	128(8)
C(15D)	8770(20)	5815(5)	2182(4)	64(3)
O(1E)	3640(10)	4810(3)	5973(2)	35(1)
O(2E)	5569(12)	5145(3)	5978(2)	48(2)
O(3E)	7350(10)	3980(3)	6088(2)	34(1)
O(4E)	7572(12)	3504(3)	6681(2)	50(2)
O(5E)	7327(10)	4561(3)	5511(2)	41(2)
N(1E)	4272(14)	3448(4)	4996(2)	53(2)
N(2E)	4257(18)	3193(4)	4645(2)	60(3)
N(3E)	4420(30)	2963(10)	4353(4)	156(9)
C(1E)	3922(14)	4248(3)	5757(2)	24(2)
C(2E)	6195(14)	4108(4)	5702(2)	32(2)
C(3E)	6457(12)	3733(4)	6423(2)	32(2)

C(4E)	4139(14)	3807(3)	6478(2)	29(2)
C(5E)	2863(13)	3804(3)	6064(2)	25(2)
C(6E)	2644(15)	3219(4)	5850(2)	34(2)
C(7E)	1364(13)	3270(4)	5455(2)	35(2)
C(8E)	2201(15)	3699(4)	5129(2)	35(2)
C(9E)	2718(13)	4303(4)	5345(2)	31(2)
C(10E)	3849(16)	4724(4)	5040(2)	42(2)
C(11E)	4790(17)	5274(4)	5238(3)	42(2)
C(12E)	6425(19)	5125(5)	5583(3)	52(3)
C(13E)	3219(17)	3372(4)	6801(3)	42(2)
C(14E)	646(16)	3788(5)	4775(3)	50(3)
C(15E)	8230(20)	5561(6)	5585(4)	70(4)

Table 10. Bond lengths [A] and angles [deg] for shelxl.

O(1)-C(1)	1.458(9)
O(1)-O(2)	1.499(9)
O(2)-C(12)	1.377(11)
O(3)-C(3)	1.337(11)
O(3)-C(2)	1.451(9)
O(4)-C(3)	1.208(13)
O(5)-C(2)	1.410(11)
O(5)-C(12)	1.431(11)
N(1)-N(2)	1.234(10)
N(1)-C(8)	1.509(12)
N(2)-N(3)	1.116(10)
C(1)-C(5)	1.511(13)
C(1)-C(2)	1.515(12)
C(1)-C(9)	1.523(11)
C(2)-H(2)	1.0000
C(3)-C(4)	1.516(16)
C(4)-C(5)	1.556(12)
C(4)-C(13)	1.565(16)
C(4)-H(4)	1.0000
C(5)-C(6)	1.527(13)
C(5)-H(5)	1.0000

C(6)-C(7)	1.519(13)
C(6)-H(6A)	0.9900
C(6)-H(6B)	0.9900
C(7)-C(8)	1.533(13)
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-C(14)	1.510(12)
C(8)-C(9)	1.557(11)
C(9)-C(10)	1.561(12)
C(9)-H(9)	1.0000
C(10)-C(11)	1.516(11)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-C(12)	1.510(12)
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(15)	1.560(14)
C(13)-H(13A)	0.9800
C(13)-H(13B)	0.9800
C(13)-H(13C)	0.9800
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
O(1A)-C(1A)	1.449(12)
O(1A)-O(2A)	1.482(10)
O(2A)-C(12A)	1.384(12)
O(3A)-C(3A)	1.358(11)
O(3A)-C(2A)	1.454(11)
O(4A)-C(3A)	1.203(11)
O(5A)-C(2A)	1.411(12)
O(5A)-C(12A)	1.456(14)
N(1A)-N(2A)	1.266(16)

N(1A)-C(8A)	1.559(16)
N(2A)-N(3A)	1.118(18)
C(1A)-C(2A)	1.500(14)
C(1A)-C(5A)	1.545(14)
C(1A)-C(9A)	1.571(14)
C(2A)-H(2A)	1.0000
C(3A)-C(4A)	1.498(14)
C(4A)-C(13A)	1.517(13)
C(4A)-C(5A)	1.551(12)
C(4A)-H(4A)	1.0000
C(5A)-C(6A)	1.493(14)
C(5A)-H(5A)	1.0000
C(6A)-C(7A)	1.547(12)
C(6A)-H(6A1)	0.9900
C(6A)-H(6A2)	0.9900
C(7A)-C(8A)	1.503(18)
C(7A)-H(7A1)	0.9900
C(7A)-H(7A2)	0.9900
C(8A)-C(9A)	1.515(17)
C(8A)-C(14A)	1.521(14)
C(9A)-C(10A)	1.518(16)
C(9A)-H(9A)	1.0000
C(10A)-C(11A)	1.56(2)
C(10A)-H(10C)	0.9900
C(10A)-H(10D)	0.9900
C(11A)-C(12A)	1.536(19)
C(11A)-H(11C)	0.9900
C(11A)-H(11D)	0.9900
C(12A)-C(15A)	1.498(19)
C(13A)-H(13D)	0.9800
C(13A)-H(13E)	0.9800
C(13A)-H(13F)	0.9800
C(14A)-H(14D)	0.9800
C(14A)-H(14E)	0.9800
C(14A)-H(14F)	0.9800

C(15A)-H(15D)	0.9800
C(15A)-H(15E)	0.9800
C(15A)-H(15F)	0.9800
O(1B)-O(2B)	1.463(11)
O(1B)-C(1B)	1.470(10)
O(2B)-C(12B)	1.489(13)
O(3B)-C(3B)	1.382(14)
O(3B)-C(2B)	1.469(11)
O(4B)-C(3B)	1.203(12)
O(5B)-C(2B)	1.356(13)
O(5B)-C(12B)	1.408(14)
N(1B)-N(2B)	1.201(12)
N(1B)-C(8B)	1.494(15)
N(2B)-N(3B)	1.183(12)
C(1B)-C(5B)	1.498(15)
C(1B)-C(9B)	1.569(12)
C(1B)-C(2B)	1.569(13)
C(2B)-H(2B)	1.0000
C(3B)-C(4B)	1.488(15)
C(4B)-C(13B)	1.506(16)
C(4B)-C(5B)	1.522(13)
C(4B)-H(4B)	1.0000
C(5B)-C(6B)	1.522(13)
C(5B)-H(5B)	1.0000
C(6B)-C(7B)	1.556(13)
C(6B)-H(6B1)	0.9900
C(6B)-H(6B2)	0.9900
C(7B)-C(8B)	1.524(16)
C(7B)-H(7B1)	0.9900
C(7B)-H(7B2)	0.9900
C(8B)-C(14B)	1.519(15)
C(8B)-C(9B)	1.538(13)
C(9B)-C(10B)	1.487(17)
C(9B)-H(9B)	1.0000
C(10B)-C(11B)	1.521(17)

C(10B)-H(10E)	0.9900
C(10B)-H(10F)	0.9900
C(11B)-C(12B)	1.507(16)
C(11B)-H(11E)	0.9900
C(11B)-H(11F)	0.9900
C(12B)-C(15B)	1.524(16)
C(13B)-H(13G)	0.9800
C(13B)-H(13H)	0.9800
C(13B)-H(13I)	0.9800
C(14B)-H(14G)	0.9800
C(14B)-H(14H)	0.9800
C(14B)-H(14I)	0.9800
C(15B)-H(15G)	0.9800
C(15B)-H(15H)	0.9800
C(15B)-H(15I)	0.9800
O(1C)-C(1C)	1.453(11)
O(1C)-O(2C)	1.497(9)
O(2C)-C(12C)	1.447(9)
O(3C)-C(3C)	1.350(12)
O(3C)-C(2C)	1.492(13)
O(4C)-C(3C)	1.264(13)
O(5C)-C(2C)	1.392(12)
O(5C)-C(12C)	1.464(11)
N(1C)-N(2C)	1.198(12)
N(1C)-C(8C)	1.524(14)
N(2C)-N(3C)	1.158(15)
C(1C)-C(5C)	1.474(13)
C(1C)-C(2C)	1.504(14)
C(1C)-C(9C)	1.562(15)
C(2C)-H(2C)	1.0000
C(3C)-C(4C)	1.504(15)
C(4C)-C(13C)	1.496(15)
C(4C)-C(5C)	1.507(17)
C(4C)-H(4C)	1.0000
C(5C)-C(6C)	1.517(16)

C(5C)-H(5C)	1.0000
C(6C)-C(7C)	1.571(19)
C(6C)-H(6C1)	0.9900
C(6C)-H(6C2)	0.9900
C(7C)-C(8C)	1.506(17)
C(7C)-H(7C1)	0.9900
C(7C)-H(7C2)	0.9900
C(8C)-C(14C)	1.504(19)
C(8C)-C(9C)	1.547(14)
C(9C)-C(10C)	1.472(14)
C(9C)-H(9C)	1.0000
C(10C)-C(11C)	1.539(14)
C(10C)-H(10G)	0.9900
C(10C)-H(10H)	0.9900
C(11C)-C(12C)	1.546(14)
C(11C)-H(11G)	0.9900
C(11C)-H(11H)	0.9900
C(12C)-C(15C)	1.479(14)
C(13C)-H(13J)	0.9800
C(13C)-H(13K)	0.9800
C(13C)-H(13L)	0.9800
C(14C)-H(14J)	0.9800
C(14C)-H(14K)	0.9800
C(14C)-H(14L)	0.9800
C(15C)-H(15J)	0.9800
C(15C)-H(15K)	0.9800
C(15C)-H(15L)	0.9800
O(1D)-C(1D)	1.449(12)
O(1D)-O(2D)	1.470(10)
O(2D)-C(12D)	1.415(15)
O(3D)-C(3D)	1.411(13)
O(3D)-C(2D)	1.448(14)
O(4D)-C(3D)	1.140(15)
O(5D)-C(2D)	1.404(14)
O(5D)-C(12D)	1.464(12)

N(1D)-N(2D)	1.192(16)
N(1D)-C(8D)	1.530(17)
N(2D)-N(3D)	1.161(18)
C(1D)-C(5D)	1.508(16)
C(1D)-C(2D)	1.514(17)
C(1D)-C(9D)	1.579(17)
C(2D)-H(2D)	1.0000
C(3D)-C(4D)	1.553(17)
C(4D)-C(5D)	1.44(2)
C(4D)-C(13D)	1.619(17)
C(4D)-H(4D)	1.0000
C(5D)-C(6D)	1.569(17)
C(5D)-H(5D)	1.0000
C(6D)-C(7D)	1.58(2)
C(6D)-H(6D1)	0.9900
C(6D)-H(6D2)	0.9900
C(7D)-C(8D)	1.42(2)
C(7D)-H(7D1)	0.9900
C(7D)-H(7D2)	0.9900
C(8D)-C(9D)	1.531(14)
C(8D)-C(14D)	1.59(2)
C(9D)-C(10D)	1.479(18)
C(9D)-H(9D)	1.0000
C(10D)-C(11D)	1.507(15)
C(10D)-H(10I)	0.9900
C(10D)-H(10J)	0.9900
C(11D)-C(12D)	1.558(15)
C(11D)-H(11I)	0.9900
C(11D)-H(11J)	0.9900
C(12D)-C(15D)	1.543(13)
C(13D)-H(13M)	0.9800
C(13D)-H(13N)	0.9800
C(13D)-H(13O)	0.9800
C(14D)-H(14M)	0.9800
C(14D)-H(14N)	0.9800

C(14D)-H(14O)	0.9800
C(15D)-H(15M)	0.9800
C(15D)-H(15N)	0.9800
C(15D)-H(15O)	0.9800
O(1E)-O(2E)	1.448(9)
O(1E)-C(1E)	1.477(10)
O(2E)-C(12E)	1.378(12)
O(3E)-C(3E)	1.342(10)
O(3E)-C(2E)	1.468(9)
O(4E)-C(3E)	1.208(10)
O(5E)-C(2E)	1.406(10)
O(5E)-C(12E)	1.437(14)
N(1E)-N(2E)	1.267(11)
N(1E)-C(8E)	1.500(12)
N(2E)-N(3E)	1.080(14)
C(1E)-C(2E)	1.492(12)
C(1E)-C(9E)	1.530(10)
C(1E)-C(5E)	1.571(10)
C(2E)-H(2E)	1.0000
C(3E)-C(4E)	1.494(12)
C(4E)-C(13E)	1.553(11)
C(4E)-C(5E)	1.555(10)
C(4E)-H(4E)	1.0000
C(5E)-C(6E)	1.516(12)
C(5E)-H(5E)	1.0000
C(6E)-C(7E)	1.510(11)
C(6E)-H(6E1)	0.9900
C(6E)-H(6E2)	0.9900
C(7E)-C(8E)	1.531(12)
C(7E)-H(7E1)	0.9900
C(7E)-H(7E2)	0.9900
C(8E)-C(14E)	1.518(11)
C(8E)-C(9E)	1.588(13)
C(9E)-C(10E)	1.553(13)
C(9E)-H(9E)	1.0000

C(10E)-C(11E)	1.536(14)
C(10E)-H(10K)	0.9900
C(10E)-H(10L)	0.9900
C(11E)-C(12E)	1.556(14)
C(11E)-H(11K)	0.9900
C(11E)-H(11L)	0.9900
C(12E)-C(15E)	1.524(17)
C(13E)-H(13P)	0.9800
C(13E)-H(13Q)	0.9800
C(13E)-H(13R)	0.9800
C(14E)-H(14P)	0.9800
C(14E)-H(14Q)	0.9800
C(14E)-H(14R)	0.9800
C(15E)-H(15P)	0.9800
C(15E)-H(15Q)	0.9800
C(15E)-H(15R)	0.9800
C(1)-O(1)-O(2)	110.2(6)
C(12)-O(2)-O(1)	107.5(5)
C(3)-O(3)-C(2)	124.4(8)
C(2)-O(5)-C(12)	111.8(7)
N(2)-N(1)-C(8)	115.7(7)
N(3)-N(2)-N(1)	174.1(10)
O(1)-C(1)-C(5)	104.7(6)
O(1)-C(1)-C(2)	110.8(6)
C(5)-C(1)-C(2)	112.0(7)
O(1)-C(1)-C(9)	105.6(7)
C(5)-C(1)-C(9)	112.3(7)
C(2)-C(1)-C(9)	111.1(6)
O(5)-C(2)-O(3)	106.4(6)
O(5)-C(2)-C(1)	115.1(7)
O(3)-C(2)-C(1)	114.2(7)
O(5)-C(2)-H(2)	106.9
O(3)-C(2)-H(2)	106.9
C(1)-C(2)-H(2)	106.9
O(4)-C(3)-O(3)	119.4(11)

O(4)-C(3)-C(4)	122.1(9)
O(3)-C(3)-C(4)	118.3(10)
C(3)-C(4)-C(5)	113.2(8)
C(3)-C(4)-C(13)	111.1(10)
C(5)-C(4)-C(13)	114.0(9)
C(3)-C(4)-H(4)	105.9
C(5)-C(4)-H(4)	105.9
C(13)-C(4)-H(4)	105.9
C(1)-C(5)-C(6)	111.5(6)
C(1)-C(5)-C(4)	108.8(7)
C(6)-C(5)-C(4)	113.8(9)
C(1)-C(5)-H(5)	107.5
C(6)-C(5)-H(5)	107.5
C(4)-C(5)-H(5)	107.5
C(7)-C(6)-C(5)	108.8(8)
C(7)-C(6)-H(6A)	109.9
C(5)-C(6)-H(6A)	109.9
C(7)-C(6)-H(6B)	109.9
C(5)-C(6)-H(6B)	109.9
H(6A)-C(6)-H(6B)	108.3
C(6)-C(7)-C(8)	114.5(7)
C(6)-C(7)-H(7A)	108.6
C(8)-C(7)-H(7A)	108.6
C(6)-C(7)-H(7B)	108.6
C(8)-C(7)-H(7B)	108.6
H(7A)-C(7)-H(7B)	107.6
N(1)-C(8)-C(14)	108.9(7)
N(1)-C(8)-C(7)	110.2(7)
C(14)-C(8)-C(7)	108.2(7)
N(1)-C(8)-C(9)	108.1(7)
C(14)-C(8)-C(9)	111.8(7)
C(7)-C(8)-C(9)	109.7(7)
C(1)-C(9)-C(8)	114.5(7)
C(1)-C(9)-C(10)	113.3(7)
C(8)-C(9)-C(10)	109.9(7)

C(1)-C(9)-H(9)	106.2
C(8)-C(9)-H(9)	106.2
C(10)-C(9)-H(9)	106.2
C(11)-C(10)-C(9)	114.1(7)
C(11)-C(10)-H(10A)	108.7
C(9)-C(10)-H(10A)	108.7
C(11)-C(10)-H(10B)	108.7
C(9)-C(10)-H(10B)	108.7
H(10A)-C(10)-H(10B)	107.6
C(12)-C(11)-C(10)	114.4(7)
C(12)-C(11)-H(11A)	108.7
C(10)-C(11)-H(11A)	108.7
C(12)-C(11)-H(11B)	108.7
C(10)-C(11)-H(11B)	108.7
H(11A)-C(11)-H(11B)	107.6
O(2)-C(12)-O(5)	108.3(7)
O(2)-C(12)-C(11)	113.8(8)
O(5)-C(12)-C(11)	111.0(6)
O(2)-C(12)-C(15)	106.1(7)
O(5)-C(12)-C(15)	104.1(8)
C(11)-C(12)-C(15)	112.9(8)
C(4)-C(13)-H(13A)	109.5
C(4)-C(13)-H(13B)	109.5
H(13A)-C(13)-H(13B)	109.5
C(4)-C(13)-H(13C)	109.5
H(13A)-C(13)-H(13C)	109.5
H(13B)-C(13)-H(13C)	109.5
C(8)-C(14)-H(14A)	109.5
C(8)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(8)-C(14)-H(14C)	109.5
H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(12)-C(15)-H(15A)	109.5
C(12)-C(15)-H(15B)	109.5

H(15A)-C(15)-H(15B)	109.5
C(12)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(1A)-O(1A)-O(2A)	110.3(7)
C(12A)-O(2A)-O(1A)	108.0(8)
C(3A)-O(3A)-C(2A)	122.0(7)
C(2A)-O(5A)-C(12A)	112.4(7)
N(2A)-N(1A)-C(8A)	113.6(14)
N(3A)-N(2A)-N(1A)	173(2)
O(1A)-C(1A)-C(2A)	112.1(9)
O(1A)-C(1A)-C(5A)	103.9(7)
C(2A)-C(1A)-C(5A)	110.8(8)
O(1A)-C(1A)-C(9A)	106.5(8)
C(2A)-C(1A)-C(9A)	112.8(8)
C(5A)-C(1A)-C(9A)	110.3(9)
O(5A)-C(2A)-O(3A)	107.1(9)
O(5A)-C(2A)-C(1A)	113.0(8)
O(3A)-C(2A)-C(1A)	116.0(7)
O(5A)-C(2A)-H(2A)	106.8
O(3A)-C(2A)-H(2A)	106.8
C(1A)-C(2A)-H(2A)	106.8
O(4A)-C(3A)-O(3A)	115.0(8)
O(4A)-C(3A)-C(4A)	125.5(8)
O(3A)-C(3A)-C(4A)	119.4(7)
C(3A)-C(4A)-C(13A)	110.9(8)
C(3A)-C(4A)-C(5A)	113.8(7)
C(13A)-C(4A)-C(5A)	113.4(9)
C(3A)-C(4A)-H(4A)	106.0
C(13A)-C(4A)-H(4A)	106.0
C(5A)-C(4A)-H(4A)	106.0
C(6A)-C(5A)-C(1A)	110.5(8)
C(6A)-C(5A)-C(4A)	116.0(8)
C(1A)-C(5A)-C(4A)	108.2(8)
C(6A)-C(5A)-H(5A)	107.3

C(1A)-C(5A)-H(5A)	107.3
C(4A)-C(5A)-H(5A)	107.3
C(5A)-C(6A)-C(7A)	111.8(9)
C(5A)-C(6A)-H(6A1)	109.3
C(7A)-C(6A)-H(6A1)	109.3
C(5A)-C(6A)-H(6A2)	109.3
C(7A)-C(6A)-H(6A2)	109.3
H(6A1)-C(6A)-H(6A2)	107.9
C(8A)-C(7A)-C(6A)	113.3(10)
C(8A)-C(7A)-H(7A1)	108.9
C(6A)-C(7A)-H(7A1)	108.9
C(8A)-C(7A)-H(7A2)	108.9
C(6A)-C(7A)-H(7A2)	108.9
H(7A1)-C(7A)-H(7A2)	107.7
C(7A)-C(8A)-C(9A)	112.4(8)
C(7A)-C(8A)-C(14A)	110.1(12)
C(9A)-C(8A)-C(14A)	112.9(10)
C(7A)-C(8A)-N(1A)	107.7(9)
C(9A)-C(8A)-N(1A)	104.6(11)
C(14A)-C(8A)-N(1A)	108.8(9)
C(8A)-C(9A)-C(10A)	113.7(9)
C(8A)-C(9A)-C(1A)	116.4(9)
C(10A)-C(9A)-C(1A)	110.8(11)
C(8A)-C(9A)-H(9A)	104.9
C(10A)-C(9A)-H(9A)	104.9
C(1A)-C(9A)-H(9A)	104.9
C(9A)-C(10A)-C(11A)	117.5(9)
C(9A)-C(10A)-H(10C)	107.9
C(11A)-C(10A)-H(10C)	107.9
C(9A)-C(10A)-H(10D)	107.9
C(11A)-C(10A)-H(10D)	107.9
H(10C)-C(10A)-H(10D)	107.2
C(12A)-C(11A)-C(10A)	115.9(10)
C(12A)-C(11A)-H(11C)	108.3
C(10A)-C(11A)-H(11C)	108.3

C(12A)-C(11A)-H(11D)	108.3
C(10A)-C(11A)-H(11D)	108.3
H(11C)-C(11A)-H(11D)	107.4
O(2A)-C(12A)-O(5A)	109.1(7)
O(2A)-C(12A)-C(15A)	105.7(12)
O(5A)-C(12A)-C(15A)	107.7(9)
O(2A)-C(12A)-C(11A)	113.1(9)
O(5A)-C(12A)-C(11A)	107.4(11)
C(15A)-C(12A)-C(11A)	113.7(10)
C(4A)-C(13A)-H(13D)	109.5
C(4A)-C(13A)-H(13E)	109.5
H(13D)-C(13A)-H(13E)	109.5
C(4A)-C(13A)-H(13F)	109.5
H(13D)-C(13A)-H(13F)	109.5
H(13E)-C(13A)-H(13F)	109.5
C(8A)-C(14A)-H(14D)	109.5
C(8A)-C(14A)-H(14E)	109.5
H(14D)-C(14A)-H(14E)	109.5
C(8A)-C(14A)-H(14F)	109.5
H(14D)-C(14A)-H(14F)	109.5
H(14E)-C(14A)-H(14F)	109.5
C(12A)-C(15A)-H(15D)	109.5
C(12A)-C(15A)-H(15E)	109.5
H(15D)-C(15A)-H(15E)	109.5
C(12A)-C(15A)-H(15F)	109.5
H(15D)-C(15A)-H(15F)	109.5
H(15E)-C(15A)-H(15F)	109.5
O(2B)-O(1B)-C(1B)	112.2(7)
O(1B)-O(2B)-C(12B)	106.6(7)
C(3B)-O(3B)-C(2B)	124.7(8)
C(2B)-O(5B)-C(12B)	116.4(8)
N(2B)-N(1B)-C(8B)	115.4(9)
N(3B)-N(2B)-N(1B)	174.4(13)
O(1B)-C(1B)-C(5B)	105.6(8)
O(1B)-C(1B)-C(9B)	104.2(7)

C(5B)-C(1B)-C(9B)	114.3(8)
O(1B)-C(1B)-C(2B)	109.5(8)
C(5B)-C(1B)-C(2B)	113.2(8)
C(9B)-C(1B)-C(2B)	109.5(8)
O(5B)-C(2B)-O(3B)	107.2(8)
O(5B)-C(2B)-C(1B)	115.8(8)
O(3B)-C(2B)-C(1B)	111.5(8)
O(5B)-C(2B)-H(2B)	107.3
O(3B)-C(2B)-H(2B)	107.3
C(1B)-C(2B)-H(2B)	107.3
O(4B)-C(3B)-O(3B)	116.8(10)
O(4B)-C(3B)-C(4B)	125.9(12)
O(3B)-C(3B)-C(4B)	117.2(9)
C(3B)-C(4B)-C(13B)	109.9(9)
C(3B)-C(4B)-C(5B)	114.4(9)
C(13B)-C(4B)-C(5B)	114.0(9)
C(3B)-C(4B)-H(4B)	105.9
C(13B)-C(4B)-H(4B)	105.9
C(5B)-C(4B)-H(4B)	105.9
C(1B)-C(5B)-C(6B)	111.4(8)
C(1B)-C(5B)-C(4B)	109.3(8)
C(6B)-C(5B)-C(4B)	114.5(8)
C(1B)-C(5B)-H(5B)	107.1
C(6B)-C(5B)-H(5B)	107.1
C(4B)-C(5B)-H(5B)	107.1
C(5B)-C(6B)-C(7B)	108.7(8)
C(5B)-C(6B)-H(6B1)	109.9
C(7B)-C(6B)-H(6B1)	109.9
C(5B)-C(6B)-H(6B2)	109.9
C(7B)-C(6B)-H(6B2)	109.9
H(6B1)-C(6B)-H(6B2)	108.3
C(8B)-C(7B)-C(6B)	114.6(9)
C(8B)-C(7B)-H(7B1)	108.6
C(6B)-C(7B)-H(7B1)	108.6
C(8B)-C(7B)-H(7B2)	108.6

C(6B)-C(7B)-H(7B2)	108.6
H(7B1)-C(7B)-H(7B2)	107.6
N(1B)-C(8B)-C(14B)	109.8(9)
N(1B)-C(8B)-C(7B)	108.0(9)
C(14B)-C(8B)-C(7B)	110.6(10)
N(1B)-C(8B)-C(9B)	106.7(9)
C(14B)-C(8B)-C(9B)	109.8(9)
C(7B)-C(8B)-C(9B)	111.8(8)
C(10B)-C(9B)-C(8B)	115.1(9)
C(10B)-C(9B)-C(1B)	112.0(9)
C(8B)-C(9B)-C(1B)	113.0(8)
C(10B)-C(9B)-H(9B)	105.2
C(8B)-C(9B)-H(9B)	105.2
C(1B)-C(9B)-H(9B)	105.2
C(9B)-C(10B)-C(11B)	121.6(10)
C(9B)-C(10B)-H(10E)	106.9
C(11B)-C(10B)-H(10E)	106.9
C(9B)-C(10B)-H(10F)	106.9
C(11B)-C(10B)-H(10F)	106.9
H(10E)-C(10B)-H(10F)	106.7
C(12B)-C(11B)-C(10B)	113.5(10)
C(12B)-C(11B)-H(11E)	108.9
C(10B)-C(11B)-H(11E)	108.9
C(12B)-C(11B)-H(11F)	108.9
C(10B)-C(11B)-H(11F)	108.9
H(11E)-C(11B)-H(11F)	107.7
O(5B)-C(12B)-O(2B)	105.2(9)
O(5B)-C(12B)-C(11B)	112.5(9)
O(2B)-C(12B)-C(11B)	112.4(9)
O(5B)-C(12B)-C(15B)	106.2(10)
O(2B)-C(12B)-C(15B)	103.0(9)
C(11B)-C(12B)-C(15B)	116.5(11)
C(4B)-C(13B)-H(13G)	109.5
C(4B)-C(13B)-H(13H)	109.5
H(13G)-C(13B)-H(13H)	109.5

C(4B)-C(13B)-H(13I)	109.5
H(13G)-C(13B)-H(13I)	109.5
H(13H)-C(13B)-H(13I)	109.5
C(8B)-C(14B)-H(14G)	109.5
C(8B)-C(14B)-H(14H)	109.5
H(14G)-C(14B)-H(14H)	109.5
C(8B)-C(14B)-H(14I)	109.5
H(14G)-C(14B)-H(14I)	109.5
H(14H)-C(14B)-H(14I)	109.5
C(12B)-C(15B)-H(15G)	109.5
C(12B)-C(15B)-H(15H)	109.5
H(15G)-C(15B)-H(15H)	109.5
C(12B)-C(15B)-H(15I)	109.5
H(15G)-C(15B)-H(15I)	109.5
H(15H)-C(15B)-H(15I)	109.5
C(1C)-O(1C)-O(2C)	111.5(6)
C(12C)-O(2C)-O(1C)	107.3(6)
C(3C)-O(3C)-C(2C)	119.2(8)
C(2C)-O(5C)-C(12C)	114.4(7)
N(2C)-N(1C)-C(8C)	114.5(10)
N(3C)-N(2C)-N(1C)	169.5(12)
O(1C)-C(1C)-C(5C)	104.5(8)
O(1C)-C(1C)-C(2C)	111.2(8)
C(5C)-C(1C)-C(2C)	112.1(9)
O(1C)-C(1C)-C(9C)	105.5(8)
C(5C)-C(1C)-C(9C)	112.7(9)
C(2C)-C(1C)-C(9C)	110.5(9)
O(5C)-C(2C)-O(3C)	104.5(8)
O(5C)-C(2C)-C(1C)	115.7(8)
O(3C)-C(2C)-C(1C)	114.0(8)
O(5C)-C(2C)-H(2C)	107.4
O(3C)-C(2C)-H(2C)	107.4
C(1C)-C(2C)-H(2C)	107.4
O(4C)-C(3C)-O(3C)	111.9(10)
O(4C)-C(3C)-C(4C)	126.0(10)

O(3C)-C(3C)-C(4C)	121.7(9)
C(13C)-C(4C)-C(3C)	110.3(10)
C(13C)-C(4C)-C(5C)	118.0(11)
C(3C)-C(4C)-C(5C)	111.4(9)
C(13C)-C(4C)-H(4C)	105.3
C(3C)-C(4C)-H(4C)	105.3
C(5C)-C(4C)-H(4C)	105.3
C(1C)-C(5C)-C(4C)	111.6(9)
C(1C)-C(5C)-C(6C)	111.4(10)
C(4C)-C(5C)-C(6C)	114.9(9)
C(1C)-C(5C)-H(5C)	106.1
C(4C)-C(5C)-H(5C)	106.1
C(6C)-C(5C)-H(5C)	106.1
C(5C)-C(6C)-C(7C)	112.3(8)
C(5C)-C(6C)-H(6C1)	109.1
C(7C)-C(6C)-H(6C1)	109.1
C(5C)-C(6C)-H(6C2)	109.1
C(7C)-C(6C)-H(6C2)	109.1
H(6C1)-C(6C)-H(6C2)	107.9
C(8C)-C(7C)-C(6C)	111.6(10)
C(8C)-C(7C)-H(7C1)	109.3
C(6C)-C(7C)-H(7C1)	109.3
C(8C)-C(7C)-H(7C2)	109.3
C(6C)-C(7C)-H(7C2)	109.3
H(7C1)-C(7C)-H(7C2)	108.0
C(14C)-C(8C)-C(7C)	108.5(12)
C(14C)-C(8C)-N(1C)	112.4(11)
C(7C)-C(8C)-N(1C)	107.2(10)
C(14C)-C(8C)-C(9C)	111.8(9)
C(7C)-C(8C)-C(9C)	112.2(10)
N(1C)-C(8C)-C(9C)	104.6(9)
C(10C)-C(9C)-C(8C)	112.3(9)
C(10C)-C(9C)-C(1C)	112.1(9)
C(8C)-C(9C)-C(1C)	115.5(9)
C(10C)-C(9C)-H(9C)	105.3

C(8C)-C(9C)-H(9C)	105.3
C(1C)-C(9C)-H(9C)	105.3
C(9C)-C(10C)-C(11C)	117.4(9)
C(9C)-C(10C)-H(10G)	108.0
C(11C)-C(10C)-H(10G)	108.0
C(9C)-C(10C)-H(10H)	108.0
C(11C)-C(10C)-H(10H)	108.0
H(10G)-C(10C)-H(10H)	107.2
C(10C)-C(11C)-C(12C)	114.6(8)
C(10C)-C(11C)-H(11G)	108.6
C(12C)-C(11C)-H(11G)	108.6
C(10C)-C(11C)-H(11H)	108.6
C(12C)-C(11C)-H(11H)	108.6
H(11G)-C(11C)-H(11H)	107.6
O(2C)-C(12C)-O(5C)	105.5(7)
O(2C)-C(12C)-C(15C)	107.4(8)
O(5C)-C(12C)-C(15C)	107.3(8)
O(2C)-C(12C)-C(11C)	110.8(8)
O(5C)-C(12C)-C(11C)	109.0(7)
C(15C)-C(12C)-C(11C)	116.2(8)
C(4C)-C(13C)-H(13J)	109.5
C(4C)-C(13C)-H(13K)	109.5
H(13J)-C(13C)-H(13K)	109.5
C(4C)-C(13C)-H(13L)	109.5
H(13J)-C(13C)-H(13L)	109.5
H(13K)-C(13C)-H(13L)	109.5
C(8C)-C(14C)-H(14J)	109.5
C(8C)-C(14C)-H(14K)	109.5
H(14J)-C(14C)-H(14K)	109.5
C(8C)-C(14C)-H(14L)	109.5
H(14J)-C(14C)-H(14L)	109.5
H(14K)-C(14C)-H(14L)	109.5
C(12C)-C(15C)-H(15J)	109.5
C(12C)-C(15C)-H(15K)	109.5
H(15J)-C(15C)-H(15K)	109.5

C(12C)-C(15C)-H(15L)	109.5
H(15J)-C(15C)-H(15L)	109.5
H(15K)-C(15C)-H(15L)	109.5
C(1D)-O(1D)-O(2D)	110.7(7)
C(12D)-O(2D)-O(1D)	107.7(7)
C(3D)-O(3D)-C(2D)	125.5(9)
C(2D)-O(5D)-C(12D)	110.5(8)
N(2D)-N(1D)-C(8D)	115.2(10)
N(3D)-N(2D)-N(1D)	171.2(18)
O(1D)-C(1D)-C(5D)	104.8(10)
O(1D)-C(1D)-C(2D)	110.8(9)
C(5D)-C(1D)-C(2D)	109.6(8)
O(1D)-C(1D)-C(9D)	108.0(7)
C(5D)-C(1D)-C(9D)	113.6(10)
C(2D)-C(1D)-C(9D)	109.9(11)
O(5D)-C(2D)-O(3D)	106.3(8)
O(5D)-C(2D)-C(1D)	115.6(8)
O(3D)-C(2D)-C(1D)	116.0(12)
O(5D)-C(2D)-H(2D)	106.1
O(3D)-C(2D)-H(2D)	106.1
C(1D)-C(2D)-H(2D)	106.1
O(4D)-C(3D)-O(3D)	117.5(10)
O(4D)-C(3D)-C(4D)	131.5(11)
O(3D)-C(3D)-C(4D)	110.9(11)
C(5D)-C(4D)-C(3D)	119.7(13)
C(5D)-C(4D)-C(13D)	120.2(13)
C(3D)-C(4D)-C(13D)	105.4(11)
C(5D)-C(4D)-H(4D)	102.9
C(3D)-C(4D)-H(4D)	102.9
C(13D)-C(4D)-H(4D)	102.9
C(4D)-C(5D)-C(1D)	110.8(10)
C(4D)-C(5D)-C(6D)	114.6(10)
C(1D)-C(5D)-C(6D)	111.4(12)
C(4D)-C(5D)-H(5D)	106.5
C(1D)-C(5D)-H(5D)	106.5

C(6D)-C(5D)-H(5D)	106.5
C(5D)-C(6D)-C(7D)	110.2(9)
C(5D)-C(6D)-H(6D1)	109.6
C(7D)-C(6D)-H(6D1)	109.6
C(5D)-C(6D)-H(6D2)	109.6
C(7D)-C(6D)-H(6D2)	109.6
H(6D1)-C(6D)-H(6D2)	108.1
C(8D)-C(7D)-C(6D)	113.6(10)
C(8D)-C(7D)-H(7D1)	108.8
C(6D)-C(7D)-H(7D1)	108.9
C(8D)-C(7D)-H(7D2)	108.9
C(6D)-C(7D)-H(7D2)	108.9
H(7D1)-C(7D)-H(7D2)	107.7
C(7D)-C(8D)-N(1D)	111.2(9)
C(7D)-C(8D)-C(9D)	116.3(14)
N(1D)-C(8D)-C(9D)	105.3(9)
C(7D)-C(8D)-C(14D)	109.6(11)
N(1D)-C(8D)-C(14D)	104.7(14)
C(9D)-C(8D)-C(14D)	109.0(9)
C(10D)-C(9D)-C(8D)	117.0(13)
C(10D)-C(9D)-C(1D)	110.6(9)
C(8D)-C(9D)-C(1D)	113.7(9)
C(10D)-C(9D)-H(9D)	104.8
C(8D)-C(9D)-H(9D)	104.8
C(1D)-C(9D)-H(9D)	104.8
C(9D)-C(10D)-C(11D)	119.4(12)
C(9D)-C(10D)-H(10I)	107.5
C(11D)-C(10D)-H(10I)	107.5
C(9D)-C(10D)-H(10J)	107.5
C(11D)-C(10D)-H(10J)	107.5
H(10I)-C(10D)-H(10J)	107.0
C(10D)-C(11D)-C(12D)	113.0(8)
C(10D)-C(11D)-H(11I)	109.0
C(12D)-C(11D)-H(11I)	109.0
C(10D)-C(11D)-H(11J)	109.0

C(12D)-C(11D)-H(11J)	109.0
H(11I)-C(11D)-H(11J)	107.8
O(2D)-C(12D)-O(5D)	108.3(8)
O(2D)-C(12D)-C(15D)	106.2(9)
O(5D)-C(12D)-C(15D)	106.5(9)
O(2D)-C(12D)-C(11D)	112.5(9)
O(5D)-C(12D)-C(11D)	109.0(9)
C(15D)-C(12D)-C(11D)	114.0(8)
C(4D)-C(13D)-H(13M)	109.5
C(4D)-C(13D)-H(13N)	109.5
H(13M)-C(13D)-H(13N)	109.5
C(4D)-C(13D)-H(13O)	109.5
H(13M)-C(13D)-H(13O)	109.5
H(13N)-C(13D)-H(13O)	109.5
C(8D)-C(14D)-H(14M)	109.5
C(8D)-C(14D)-H(14N)	109.5
H(14M)-C(14D)-H(14N)	109.5
C(8D)-C(14D)-H(14O)	109.5
H(14M)-C(14D)-H(14O)	109.5
H(14N)-C(14D)-H(14O)	109.5
C(12D)-C(15D)-H(15M)	109.5
C(12D)-C(15D)-H(15N)	109.5
H(15M)-C(15D)-H(15N)	109.5
C(12D)-C(15D)-H(15O)	109.5
H(15M)-C(15D)-H(15O)	109.5
H(15N)-C(15D)-H(15O)	109.5
O(2E)-O(1E)-C(1E)	111.6(6)
C(12E)-O(2E)-O(1E)	107.9(7)
C(3E)-O(3E)-C(2E)	123.3(6)
C(2E)-O(5E)-C(12E)	113.2(7)
N(2E)-N(1E)-C(8E)	115.1(9)
N(3E)-N(2E)-N(1E)	173.9(15)
O(1E)-C(1E)-C(2E)	111.2(7)
O(1E)-C(1E)-C(9E)	105.7(6)
C(2E)-C(1E)-C(9E)	113.6(7)

O(1E)-C(1E)-C(5E)	103.0(6)
C(2E)-C(1E)-C(5E)	110.5(6)
C(9E)-C(1E)-C(5E)	112.3(7)
O(5E)-C(2E)-O(3E)	105.0(7)
O(5E)-C(2E)-C(1E)	112.8(7)
O(3E)-C(2E)-C(1E)	115.3(6)
O(5E)-C(2E)-H(2E)	107.8
O(3E)-C(2E)-H(2E)	107.8
C(1E)-C(2E)-H(2E)	107.8
O(4E)-C(3E)-O(3E)	118.9(8)
O(4E)-C(3E)-C(4E)	123.2(8)
O(3E)-C(3E)-C(4E)	117.6(7)
C(3E)-C(4E)-C(13E)	112.1(7)
C(3E)-C(4E)-C(5E)	114.4(7)
C(13E)-C(4E)-C(5E)	111.6(7)
C(3E)-C(4E)-H(4E)	106.0
C(13E)-C(4E)-H(4E)	106.0
C(5E)-C(4E)-H(4E)	106.0
C(6E)-C(5E)-C(4E)	115.9(6)
C(6E)-C(5E)-C(1E)	109.6(6)
C(4E)-C(5E)-C(1E)	107.9(6)
C(6E)-C(5E)-H(5E)	107.7
C(4E)-C(5E)-H(5E)	107.7
C(1E)-C(5E)-H(5E)	107.7
C(7E)-C(6E)-C(5E)	111.1(7)
C(7E)-C(6E)-H(6E1)	109.4
C(5E)-C(6E)-H(6E1)	109.4
C(7E)-C(6E)-H(6E2)	109.4
C(5E)-C(6E)-H(6E2)	109.4
H(6E1)-C(6E)-H(6E2)	108.0
C(6E)-C(7E)-C(8E)	115.7(7)
C(6E)-C(7E)-H(7E1)	108.3
C(8E)-C(7E)-H(7E1)	108.3
C(6E)-C(7E)-H(7E2)	108.3
C(8E)-C(7E)-H(7E2)	108.3

H(7E1)-C(7E)-H(7E2)	107.4
N(1E)-C(8E)-C(14E)	114.3(7)
N(1E)-C(8E)-C(7E)	104.6(8)
C(14E)-C(8E)-C(7E)	111.7(8)
N(1E)-C(8E)-C(9E)	106.2(8)
C(14E)-C(8E)-C(9E)	110.0(8)
C(7E)-C(8E)-C(9E)	109.8(6)
C(1E)-C(9E)-C(10E)	111.3(7)
C(1E)-C(9E)-C(8E)	114.0(7)
C(10E)-C(9E)-C(8E)	111.6(6)
C(1E)-C(9E)-H(9E)	106.5
C(10E)-C(9E)-H(9E)	106.5
C(8E)-C(9E)-H(9E)	106.5
C(11E)-C(10E)-C(9E)	115.7(7)
C(11E)-C(10E)-H(10K)	108.3
C(9E)-C(10E)-H(10K)	108.3
C(11E)-C(10E)-H(10L)	108.3
C(9E)-C(10E)-H(10L)	108.3
H(10K)-C(10E)-H(10L)	107.4
C(10E)-C(11E)-C(12E)	111.8(8)
C(10E)-C(11E)-H(11K)	109.3
C(12E)-C(11E)-H(11K)	109.3
C(10E)-C(11E)-H(11L)	109.3
C(12E)-C(11E)-H(11L)	109.3
H(11K)-C(11E)-H(11L)	107.9
O(2E)-C(12E)-O(5E)	109.6(8)
O(2E)-C(12E)-C(15E)	105.8(9)
O(5E)-C(12E)-C(15E)	107.1(10)
O(2E)-C(12E)-C(11E)	112.4(10)
O(5E)-C(12E)-C(11E)	110.6(8)
C(15E)-C(12E)-C(11E)	111.1(8)
C(4E)-C(13E)-H(13P)	109.5
C(4E)-C(13E)-H(13Q)	109.5
H(13P)-C(13E)-H(13Q)	109.5
C(4E)-C(13E)-H(13R)	109.5

H(13P)-C(13E)-H(13R)	109.5
H(13Q)-C(13E)-H(13R)	109.5
C(8E)-C(14E)-H(14P)	109.5
C(8E)-C(14E)-H(14Q)	109.5
H(14P)-C(14E)-H(14Q)	109.5
C(8E)-C(14E)-H(14R)	109.5
H(14P)-C(14E)-H(14R)	109.5
H(14Q)-C(14E)-H(14R)	109.5
C(12E)-C(15E)-H(15P)	109.5
C(12E)-C(15E)-H(15Q)	109.5
H(15P)-C(15E)-H(15Q)	109.5
C(12E)-C(15E)-H(15R)	109.5
H(15P)-C(15E)-H(15R)	109.5
H(15Q)-C(15E)-H(15R)	109.5

Symmetry transformations used to generate eq.alent atoms:

Table 11. Anisotropic displacement parameters (A^2 x 10^3) for shelxl. The anisotropic displacement factor exponent takes the form:

-2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
O(1)	31(4)	49(4)	56(4)	36(3)	0(3)	5(3)
O(2)	33(4)	45(3)	40(3)	19(3)	-6(3)	12(3)
O(3)	21(3)	52(4)	30(3)	7(3)	-2(2)	5(3)
O(4)	45(4)	63(4)	39(3)	-11(3)	-25(3)	8(4)
O(5)	22(3)	45(3)	29(3)	7(2)	3(2)	10(3)
N(1)	25(4)	39(4)	29(3)	4(3)	3(3)	2(3)
N(2)	27(4)	28(3)	37(3)	6(3)	7(3)	-2(3)
N(3)	75(6)	27(4)	45(4)	13(3)	3(4)	-9(4)
C(1)	13(4)	38(4)	31(4)	25(3)	6(3)	1(3)
C(2)	24(4)	36(4)	28(3)	14(3)	-7(3)	3(3)
C(3)	55(6)	34(5)	49(5)	13(4)	21(5)	20(5)
C(4)	29(5)	67(7)	34(4)	5(4)	2(4)	5(5)
C(5)	17(4)	65(6)	28(4)	18(4)	9(3)	2(4)
C(6)	34(5)	64(6)	34(4)	16(4)	11(4)	20(5)
C(7)	20(4)	47(5)	39(4)	21(4)	7(3)	13(4)
C(8)	22(4)	33(4)	42(4)	8(3)	-6(3)	8(3)
C(9)	20(4)	41(5)	34(4)	7(3)	-5(3)	-1(4)
C(10)	42(5)	35(4)	30(4)	3(3)	-15(4)	8(4)
C(11)	35(5)	36(5)	54(5)	13(4)	-13(4)	8(4)
C(12)	40(5)	23(4)	44(4)	7(3)	-11(4)	14(4)
C(13)	56(8)	181(16)	29(5)	-19(7)	18(5)	35(9)
C(14)	29(5)	54(6)	44(5)	17(4)	-9(4)	13(4)
C(15)	54(7)	55(6)	54(6)	22(5)	-9(5)	14(5)
O(1A)	29(3)	42(3)	53(3)	-18(3)	-12(3)	10(3)
O(2A)	39(4)	48(4)	77(5)	-27(3)	-28(4)	10(3)
O(3A)	29(4)	59(4)	53(4)	-25(3)	0(3)	15(3)
O(4A)	37(4)	60(4)	53(4)	-16(3)	3(3)	2(3)
O(5A)	52(5)	63(4)	71(4)	-40(4)	-43(4)	32(4)
N(1A)	92(9)	94(8)	46(5)	7(5)	-5(5)	58(7)
N(2A)	162(15)	97(9)	70(7)	50(7)	15(8)	71(10)
N(3A)	164(17)	175(15)	82(8)	55(9)	37(10)	110(14)

C(1A)	38(6)	61(6)	40(5)	-17(4)	1(4)	17(5)
C(2A)	29(5)	57(6)	44(5)	-26(4)	-15(4)	17(4)
C(3A)	32(5)	30(4)	33(4)	-7(3)	5(3)	1(3)
C(4A)	50(6)	43(5)	25(4)	0(3)	-6(4)	12(5)
C(5A)	27(5)	60(6)	40(4)	4(4)	-4(4)	4(5)
C(6A)	52(6)	59(6)	30(4)	8(4)	21(4)	10(5)
C(7A)	52(7)	77(8)	43(5)	10(5)	13(5)	21(6)
C(8A)	80(9)	81(8)	31(4)	14(5)	18(5)	52(7)
C(9A)	54(7)	76(7)	40(5)	-14(5)	-14(4)	37(6)
C(10A)	80(9)	104(10)	38(5)	-34(6)	-28(6)	47(8)
C(11A)	74(10)	95(10)	94(9)	-67(8)	-51(8)	56(8)
C(12A)	43(7)	75(8)	86(8)	-49(6)	-34(6)	8(6)
C(13A)	26(5)	47(5)	44(4)	-4(4)	-5(4)	13(4)
C(14A)	140(15)	113(11)	32(5)	-2(6)	20(7)	82(11)
C(15A)	55(8)	73(8)	141(13)	-58(9)	-26(8)	11(7)
O(1B)	32(4)	54(4)	72(4)	38(3)	14(3)	19(3)
O(2B)	42(4)	61(5)	65(4)	19(4)	12(3)	4(4)
O(3B)	22(3)	62(4)	55(4)	13(3)	11(3)	7(3)
O(4B)	32(4)	80(5)	80(5)	-5(4)	26(4)	13(4)
O(5B)	34(4)	67(5)	54(4)	17(3)	5(3)	10(4)
N(1B)	51(5)	69(6)	58(5)	31(5)	16(4)	23(5)
N(2B)	54(5)	32(4)	76(6)	16(4)	9(5)	16(4)
N(3B)	111(10)	81(7)	47(5)	47(5)	11(5)	53(7)
C(1B)	22(5)	49(5)	60(5)	28(4)	16(4)	23(4)
C(2B)	26(5)	54(6)	49(5)	20(4)	21(4)	24(4)
C(3B)	44(6)	35(5)	68(6)	10(4)	15(5)	15(4)
C(4B)	27(5)	63(6)	65(6)	28(5)	17(4)	13(5)
C(5B)	15(4)	39(5)	69(6)	15(4)	7(4)	13(4)
C(6B)	32(5)	48(5)	68(6)	20(5)	6(5)	10(5)
C(7B)	34(5)	43(5)	60(6)	34(4)	22(4)	18(4)
C(8B)	49(6)	52(6)	65(6)	32(5)	25(5)	3(5)
C(9B)	27(5)	56(6)	55(5)	17(4)	23(4)	19(4)
C(10B)	67(8)	42(6)	74(7)	15(5)	23(6)	20(6)
C(11B)	51(7)	77(8)	65(6)	7(6)	11(5)	14(6)
C(12B)	43(6)	69(7)	57(6)	19(5)	-4(5)	-8(6)

C(13B)	27(5)	63(7)	88(8)	16(6)	11(5)	3(5)
C(14B)	51(7)	92(9)	71(7)	43(7)	25(6)	25(7)
C(15B)	46(7)	79(9)	102(10)	-3(7)	3(7)	-20(7)
O(1C)	31(3)	36(3)	63(4)	-12(3)	-11(3)	1(3)
O(2C)	45(4)	38(3)	39(3)	-2(3)	-16(3)	11(3)
O(3C)	22(3)	72(5)	77(5)	16(4)	-14(3)	1(3)
O(4C)	35(4)	92(6)	94(6)	28(5)	-7(4)	-8(4)
O(5C)	43(4)	38(3)	65(4)	-4(3)	-27(4)	-2(3)
N(1C)	58(6)	39(5)	98(7)	-37(5)	-15(6)	6(4)
N(2C)	75(7)	47(5)	43(4)	11(4)	-7(4)	-19(5)
N(3C)	79(8)	111(9)	66(6)	-28(6)	-20(6)	-8(7)
C(1C)	27(5)	32(5)	85(7)	3(5)	-11(5)	-2(4)
C(2C)	31(5)	39(5)	58(5)	-2(4)	-7(4)	-10(4)
C(3C)	45(6)	33(4)	63(6)	20(4)	-4(5)	-3(4)
C(4C)	44(6)	38(5)	96(8)	15(5)	-35(6)	-5(5)
C(5C)	22(5)	45(5)	84(7)	26(5)	-3(5)	-10(4)
C(6C)	37(6)	21(4)	159(13)	12(6)	-39(8)	-5(4)
C(7C)	55(7)	15(4)	158(13)	-1(6)	2(8)	-3(5)
C(8C)	49(7)	30(5)	108(9)	-12(5)	-30(7)	-8(5)
C(9C)	33(5)	29(4)	82(7)	-8(4)	5(5)	0(4)
C(10C)	39(6)	49(6)	59(6)	-6(5)	-2(5)	1(5)
C(11C)	62(7)	39(5)	41(4)	-16(4)	9(5)	-13(5)
C(12C)	39(5)	42(5)	33(4)	3(4)	-16(4)	-4(4)
C(13C)	51(8)	59(7)	154(14)	45(8)	-38(9)	-2(6)
C(14C)	53(8)	47(7)	153(14)	-41(8)	4(9)	-12(6)
C(15C)	53(7)	50(6)	42(5)	-4(4)	-11(4)	20(5)
O(1D)	35(4)	24(3)	153(8)	-10(4)	2(5)	-1(3)
O(2D)	39(4)	31(3)	98(5)	0(3)	3(4)	-14(3)
O(3D)	24(4)	42(4)	106(6)	15(4)	12(4)	2(3)
O(4D)	66(6)	35(4)	121(7)	20(4)	47(6)	10(4)
O(5D)	22(3)	41(3)	87(5)	10(3)	-7(3)	-9(3)
N(1D)	50(6)	54(6)	126(9)	-5(6)	-31(6)	0(5)
N(2D)	56(7)	84(9)	111(10)	-20(7)	-20(7)	5(6)
N(3D)	80(10)	158(15)	85(9)	6(10)	-18(7)	-1(10)
C(1D)	45(6)	6(4)	128(10)	14(4)	-10(6)	5(4)

C(2D)	48(7)	28(5)	122(10)	6(5)	-34(7)	-2(4)
C(3D)	26(5)	32(5)	117(9)	22(6)	27(6)	-3(4)
C(4D)	32(6)	42(6)	218(18)	55(9)	44(9)	19(5)
C(5D)	14(5)	29(5)	194(15)	24(7)	-9(7)	5(4)
C(6D)	43(6)	17(5)	187(15)	7(6)	27(8)	9(4)
C(7D)	33(6)	23(5)	219(17)	-8(7)	-47(9)	-1(4)
C(8D)	37(6)	22(5)	201(16)	-15(7)	-43(8)	10(4)
C(9D)	50(7)	21(4)	121(10)	-4(5)	-37(7)	2(4)
C(10D)	71(9)	36(6)	133(11)	18(6)	-40(8)	-5(6)
C(11D)	53(7)	30(5)	125(10)	15(6)	-40(7)	-11(5)
C(12D)	34(6)	24(4)	105(8)	7(5)	-16(5)	-8(4)
C(13D)	55(9)	67(9)	260(20)	71(12)	83(12)	9(7)
C(14D)	75(11)	68(9)	240(20)	-14(11)	-104(13)	-14(8)
C(15D)	71(8)	47(6)	74(7)	18(5)	-32(6)	-32(6)
O(1E)	35(3)	40(3)	30(3)	16(2)	-11(2)	-6(3)
O(2E)	41(4)	56(4)	48(3)	8(3)	-11(3)	-19(3)
O(3E)	25(3)	43(3)	33(3)	27(2)	-5(2)	-6(3)
O(4E)	47(4)	58(4)	46(3)	32(3)	-13(3)	4(3)
O(5E)	24(3)	50(4)	48(3)	26(3)	12(3)	-9(3)
N(1E)	31(4)	83(6)	45(4)	-9(4)	3(4)	8(4)
N(2E)	69(7)	84(7)	28(4)	-9(4)	-4(4)	30(6)
N(3E)	118(14)	290(20)	61(7)	-84(11)	-10(8)	38(16)
C(1E)	31(4)	18(3)	23(3)	3(3)	-4(3)	0(3)
C(2E)	23(4)	48(5)	27(4)	22(3)	-3(3)	3(4)
C(3E)	13(4)	51(5)	31(4)	3(4)	-12(3)	1(4)
C(4E)	30(4)	26(4)	29(4)	11(3)	-4(3)	-9(3)
C(5E)	21(4)	29(4)	26(3)	8(3)	0(3)	1(3)
C(6E)	29(4)	37(4)	37(4)	14(3)	-7(3)	-4(4)
C(7E)	15(4)	57(5)	35(4)	4(4)	-6(3)	-1(4)
C(8E)	31(5)	52(5)	23(3)	2(3)	5(3)	7(4)
C(9E)	17(4)	60(5)	17(3)	6(3)	0(3)	12(4)
C(10E)	38(5)	64(6)	22(4)	16(4)	-9(3)	3(5)
C(11E)	46(6)	45(5)	35(4)	29(4)	-1(4)	-8(4)
C(12E)	52(7)	66(7)	39(5)	20(5)	7(4)	-18(6)
C(13E)	43(6)	53(5)	30(4)	10(4)	1(4)	-3(4)

C(14E)	32(5)	87(7)	30(4)	5(4)	-14(4)	11(5)
C(15E)	67(9)	71(8)	71(7)	39(6)	4(6)	-18(7)

Table 12. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (A^2 x 10^3) for shelxl.

	x	y	z	U(eq)
H(2)	3967	8773	1419	35
H(4)	6522	9224	346	52
H(5)	8920	8988	848	44
H(6A)	6259	8078	1159	53
H(6B)	8414	7971	909	53
H(7A)	10339	8436	1438	43
H(7B)	9023	7912	1636	43
H(9)	8849	9499	1553	38
H(10A)	5145	9501	2057	43
H(10B)	7278	9851	2136	43
H(11A)	4607	10490	1933	50
H(11B)	6469	10498	1598	50
H(13A)	6792	7993	222	133
H(13B)	8780	8410	155	133
H(13C)	6736	8484	-132	133
H(14A)	8765	9009	2407	64
H(14B)	10698	8995	2087	64
H(14C)	9842	8403	2286	64
H(15A)	2341	10950	1343	81
H(15B)	1069	10507	1634	81
H(15C)	914	10453	1137	81
H(2A)	-1402	6647	257	52
H(4A)	1588	6153	1267	47
H(5A)	3753	6372	726	51
H(6A1)	3347	7381	670	56
H(6A2)	1097	7289	455	56
H(7A1)	3637	7449	-73	69
H(7A2)	5049	6926	100	69

H(9A)	3315	5873	18	68
H(10C)	1556	5520	-514	89
H(10D)	-484	5902	-424	89
H(11C)	-1297	4935	-281	105
H(11D)	702	4867	17	105
H(13D)	2360	7365	1330	59
H(13E)	3949	6859	1466	59
H(13F)	1802	6953	1718	59
H(14D)	3910	6942	-768	143
H(14E)	3011	6295	-814	143
H(14F)	5135	6409	-558	143
H(15D)	-3151	4476	360	134
H(15E)	-4617	4938	125	134
H(15F)	-4358	4966	622	134
H(2B)	-1473	6535	3826	52
H(4B)	1223	6132	4901	62
H(5B)	3605	6378	4411	49
H(6B1)	3059	7387	4336	59
H(6B2)	906	7267	4089	59
H(7B1)	3674	7423	3596	55
H(7B2)	5031	6915	3804	55
H(9B)	3569	5839	3696	55
H(10E)	2065	5450	3161	74
H(10F)	-55	5807	3217	74
H(11E)	-766	4845	3330	77
H(11F)	1082	4791	3667	77
H(13G)	3427	6848	5138	89
H(13H)	1170	6923	5352	89
H(13I)	1853	7344	4978	89
H(14G)	3437	6251	2858	107
H(14H)	5424	6337	3158	107
H(14I)	4407	6886	2927	107
H(15G)	-3918	4798	4240	114
H(15H)	-2915	4376	3896	114
H(15I)	-4514	4878	3758	114

H(2C)	11256	1765	2980	51
H(4C)	8732	1393	1894	71
H(5C)	6416	1604	2385	60
H(6C1)	6935	2605	2476	87
H(6C2)	9016	2478	2742	87
H(7C1)	6192	2650	3218	91
H(7C2)	4793	2158	2998	91
H(9C)	6279	1065	3075	57
H(10G)	7671	699	3637	59
H(10H)	9852	1029	3573	59
H(11G)	8497	53	3088	57
H(11H)	10236	25	3447	57
H(13J)	6765	2126	1638	132
H(13K)	9119	2212	1472	132
H(13L)	8253	2607	1846	132
H(14J)	6302	1537	3954	127
H(14K)	4427	1489	3622	127
H(14L)	5052	2108	3813	127
H(15J)	12605	-422	2858	73
H(15K)	13946	3	3151	73
H(15L)	14081	65	2654	73
H(2D)	6595	4047	2019	79
H(4D)	3681	4430	3017	117
H(5D)	1539	4240	2524	95
H(6D1)	1913	3225	2404	99
H(6D2)	4189	3324	2201	99
H(7D1)	1693	3236	1643	110
H(7D2)	249	3733	1843	110
H(9D)	1868	4801	1808	77
H(10I)	3662	5177	1300	96
H(10J)	5736	4821	1409	96
H(11I)	4243	5798	1862	83
H(11J)	6215	5798	1552	83
H(13M)	1417	3737	3296	190
H(13N)	3685	3620	3495	190

H(13O)	2830	3210	3129	190
H(14M)	615	3814	1070	192
H(14N)	2414	4247	912	192
H(14O)	513	4489	1189	192
H(15M)	8257	6217	2194	96
H(15N)	9743	5773	1947	96
H(15O)	9506	5723	2443	96
H(2E)	6295	3759	5517	39
H(4E)	3939	4202	6602	34
H(5E)	1417	3949	6128	30
H(6E1)	4057	3065	5782	41
H(6E2)	1953	2941	6043	41
H(7E1)	-83	3388	5531	42
H(7E2)	1275	2880	5324	42
H(9E)	1336	4487	5414	37
H(10K)	4994	4508	4899	50
H(10L)	2832	4844	4822	50
H(11K)	3645	5511	5360	50
H(11L)	5479	5510	5018	50
H(13P)	3415	2973	6699	63
H(13Q)	1716	3449	6839	63
H(13R)	3948	3418	7069	63
H(14P)	1307	4018	4554	75
H(14Q)	-596	3993	4880	75
H(14R)	222	3409	4663	75
H(15P)	7715	5938	5685	105
H(15Q)	8781	5604	5301	105
H(15R)	9347	5422	5770	105

Table 13. Torsion angles [deg] for shelxl.

C(1)-O(1)-O(2)-C(12)	48.2(8)
O(2)-O(1)-C(1)-C(5)	133.5(7)
O(2)-O(1)-C(1)-C(2)	12.6(9)
O(2)-O(1)-C(1)-C(9)	-107.8(7)
C(12)-O(5)-C(2)-O(3)	-102.1(7)
C(12)-O(5)-C(2)-C(1)	25.5(8)
C(3)-O(3)-C(2)-O(5)	154.3(8)
C(3)-O(3)-C(2)-C(1)	26.1(11)
O(1)-C(1)-C(2)-O(5)	-51.3(9)
C(5)-C(1)-C(2)-O(5)	-167.8(6)
C(9)-C(1)-C(2)-O(5)	65.7(8)
O(1)-C(1)-C(2)-O(3)	72.3(9)
C(5)-C(1)-C(2)-O(3)	-44.2(8)
C(9)-C(1)-C(2)-O(3)	-170.7(7)
C(2)-O(3)-C(3)-O(4)	164.3(8)
C(2)-O(3)-C(3)-C(4)	-20.4(12)
O(4)-C(3)-C(4)-C(5)	-152.7(9)
O(3)-C(3)-C(4)-C(5)	32.2(13)
O(4)-C(3)-C(4)-C(13)	-22.9(14)
O(3)-C(3)-C(4)-C(13)	162.0(9)
O(1)-C(1)-C(5)-C(6)	169.6(7)
C(2)-C(1)-C(5)-C(6)	-70.3(9)
C(9)-C(1)-C(5)-C(6)	55.5(10)
O(1)-C(1)-C(5)-C(4)	-64.1(9)
C(2)-C(1)-C(5)-C(4)	56.1(9)
C(9)-C(1)-C(5)-C(4)	-178.1(7)
C(3)-C(4)-C(5)-C(1)	-49.7(11)
C(13)-C(4)-C(5)-C(1)	-178.0(10)
C(3)-C(4)-C(5)-C(6)	75.3(11)
C(13)-C(4)-C(5)-C(6)	-53.0(12)
C(1)-C(5)-C(6)-C(7)	-58.6(10)
C(4)-C(5)-C(6)-C(7)	177.8(7)

C(5)-C(6)-C(7)-C(8)	58.0(10)
N(2)-N(1)-C(8)-C(14)	-65.3(10)
N(2)-N(1)-C(8)-C(7)	53.1(9)
N(2)-N(1)-C(8)-C(9)	173.0(7)
C(6)-C(7)-C(8)-N(1)	67.6(9)
C(6)-C(7)-C(8)-C(14)	-173.5(8)
C(6)-C(7)-C(8)-C(9)	-51.3(10)
O(1)-C(1)-C(9)-C(8)	-163.1(7)
C(5)-C(1)-C(9)-C(8)	-49.6(10)
C(2)-C(1)-C(9)-C(8)	76.7(9)
O(1)-C(1)-C(9)-C(10)	69.8(9)
C(5)-C(1)-C(9)-C(10)	-176.7(7)
C(2)-C(1)-C(9)-C(10)	-50.3(10)
N(1)-C(8)-C(9)-C(1)	-74.0(9)
C(14)-C(8)-C(9)-C(1)	166.1(7)
C(7)-C(8)-C(9)-C(1)	46.2(10)
N(1)-C(8)-C(9)-C(10)	54.8(9)
C(14)-C(8)-C(9)-C(10)	-65.1(10)
C(7)-C(8)-C(9)-C(10)	175.0(7)
C(1)-C(9)-C(10)-C(11)	-37.8(11)
C(8)-C(9)-C(10)-C(11)	-167.2(7)
C(9)-C(10)-C(11)-C(12)	58.1(11)
O(1)-O(2)-C(12)-O(5)	-77.5(8)
O(1)-O(2)-C(12)-C(11)	46.4(8)
O(1)-O(2)-C(12)-C(15)	171.2(7)
C(2)-O(5)-C(12)-O(2)	37.6(8)
C(2)-O(5)-C(12)-C(11)	-88.0(8)
C(2)-O(5)-C(12)-C(15)	150.3(7)
C(10)-C(11)-C(12)-O(2)	-97.4(9)
C(10)-C(11)-C(12)-O(5)	25.1(11)
C(10)-C(11)-C(12)-C(15)	141.5(9)
C(1A)-O(1A)-O(2A)-C(12A)	48.2(9)
O(2A)-O(1A)-C(1A)-C(2A)	13.3(9)
O(2A)-O(1A)-C(1A)-C(5A)	133.0(7)
O(2A)-O(1A)-C(1A)-C(9A)	-110.5(8)

C(12A)-O(5A)-C(2A)-O(3A)	-98.6(10)
C(12A)-O(5A)-C(2A)-C(1A)	30.3(13)
C(3A)-O(3A)-C(2A)-O(5A)	154.4(8)
C(3A)-O(3A)-C(2A)-C(1A)	27.3(13)
O(1A)-C(1A)-C(2A)-O(5A)	-54.1(11)
C(5A)-C(1A)-C(2A)-O(5A)	-169.7(8)
C(9A)-C(1A)-C(2A)-O(5A)	66.1(12)
O(1A)-C(1A)-C(2A)-O(3A)	70.0(11)
C(5A)-C(1A)-C(2A)-O(3A)	-45.6(12)
C(9A)-C(1A)-C(2A)-O(3A)	-169.8(9)
C(2A)-O(3A)-C(3A)-O(4A)	163.9(9)
C(2A)-O(3A)-C(3A)-C(4A)	-20.3(12)
O(4A)-C(3A)-C(4A)-C(13A)	-22.8(13)
O(3A)-C(3A)-C(4A)-C(13A)	161.9(8)
O(4A)-C(3A)-C(4A)-C(5A)	-152.0(9)
O(3A)-C(3A)-C(4A)-C(5A)	32.6(12)
O(1A)-C(1A)-C(5A)-C(6A)	167.7(8)
C(2A)-C(1A)-C(5A)-C(6A)	-71.7(11)
C(9A)-C(1A)-C(5A)-C(6A)	53.8(11)
O(1A)-C(1A)-C(5A)-C(4A)	-64.4(9)
C(2A)-C(1A)-C(5A)-C(4A)	56.3(11)
C(9A)-C(1A)-C(5A)-C(4A)	-178.2(8)
C(3A)-C(4A)-C(5A)-C(6A)	74.9(12)
C(13A)-C(4A)-C(5A)-C(6A)	-53.1(12)
C(3A)-C(4A)-C(5A)-C(1A)	-49.9(11)
C(13A)-C(4A)-C(5A)-C(1A)	-177.9(8)
C(1A)-C(5A)-C(6A)-C(7A)	-59.4(12)
C(4A)-C(5A)-C(6A)-C(7A)	177.0(9)
C(5A)-C(6A)-C(7A)-C(8A)	56.6(13)
C(6A)-C(7A)-C(8A)-C(9A)	-47.2(13)
C(6A)-C(7A)-C(8A)-C(14A)	-174.0(9)
C(6A)-C(7A)-C(8A)-N(1A)	67.5(11)
N(2A)-N(1A)-C(8A)-C(7A)	61.1(12)
N(2A)-N(1A)-C(8A)-C(9A)	-179.2(10)
N(2A)-N(1A)-C(8A)-C(14A)	-58.3(16)

C(7A)-C(8A)-C(9A)-C(10A)	174.6(9)
C(14A)-C(8A)-C(9A)-C(10A)	-60.1(15)
N(1A)-C(8A)-C(9A)-C(10A)	58.0(11)
C(7A)-C(8A)-C(9A)-C(1A)	44.0(14)
C(14A)-C(8A)-C(9A)-C(1A)	169.3(11)
N(1A)-C(8A)-C(9A)-C(1A)	-72.6(12)
O(1A)-C(1A)-C(9A)-C(8A)	-159.3(9)
C(2A)-C(1A)-C(9A)-C(8A)	77.3(13)
C(5A)-C(1A)-C(9A)-C(8A)	-47.1(12)
O(1A)-C(1A)-C(9A)-C(10A)	68.8(10)
C(2A)-C(1A)-C(9A)-C(10A)	-54.6(12)
C(5A)-C(1A)-C(9A)-C(10A)	-179.1(8)
C(8A)-C(9A)-C(10A)-C(11A)	-166.6(10)
C(1A)-C(9A)-C(10A)-C(11A)	-33.3(13)
C(9A)-C(10A)-C(11A)-C(12A)	53.6(14)
O(1A)-O(2A)-C(12A)-O(5A)	-74.0(10)
O(1A)-O(2A)-C(12A)-C(15A)	170.5(8)
O(1A)-O(2A)-C(12A)-C(11A)	45.4(12)
C(2A)-O(5A)-C(12A)-O(2A)	31.8(14)
C(2A)-O(5A)-C(12A)-C(15A)	146.1(10)
C(2A)-O(5A)-C(12A)-C(11A)	-91.1(10)
C(10A)-C(11A)-C(12A)-O(2A)	-92.6(13)
C(10A)-C(11A)-C(12A)-O(5A)	27.8(12)
C(10A)-C(11A)-C(12A)-C(15A)	146.8(11)
C(1B)-O(1B)-O(2B)-C(12B)	50.3(10)
O(2B)-O(1B)-C(1B)-C(5B)	129.5(8)
O(2B)-O(1B)-C(1B)-C(9B)	-109.7(8)
O(2B)-O(1B)-C(1B)-C(2B)	7.3(11)
C(12B)-O(5B)-C(2B)-O(3B)	-103.1(9)
C(12B)-O(5B)-C(2B)-C(1B)	22.1(11)
C(3B)-O(3B)-C(2B)-O(5B)	152.7(8)
C(3B)-O(3B)-C(2B)-C(1B)	25.0(12)
O(1B)-C(1B)-C(2B)-O(5B)	-47.1(11)
C(5B)-C(1B)-C(2B)-O(5B)	-164.5(7)
C(9B)-C(1B)-C(2B)-O(5B)	66.6(10)

O(1B)-C(1B)-C(2B)-O(3B)	75.9(11)
C(5B)-C(1B)-C(2B)-O(3B)	-41.6(11)
C(9B)-C(1B)-C(2B)-O(3B)	-170.4(8)
C(2B)-O(3B)-C(3B)-O(4B)	161.6(9)
C(2B)-O(3B)-C(3B)-C(4B)	-22.9(13)
O(4B)-C(3B)-C(4B)-C(13B)	-19.2(15)
O(3B)-C(3B)-C(4B)-C(13B)	165.8(8)
O(4B)-C(3B)-C(4B)-C(5B)	-148.9(11)
O(3B)-C(3B)-C(4B)-C(5B)	36.1(13)
O(1B)-C(1B)-C(5B)-C(6B)	168.6(7)
C(9B)-C(1B)-C(5B)-C(6B)	54.6(10)
C(2B)-C(1B)-C(5B)-C(6B)	-71.7(10)
O(1B)-C(1B)-C(5B)-C(4B)	-63.9(9)
C(9B)-C(1B)-C(5B)-C(4B)	-177.9(7)
C(2B)-C(1B)-C(5B)-C(4B)	55.8(10)
C(3B)-C(4B)-C(5B)-C(1B)	-52.8(11)
C(13B)-C(4B)-C(5B)-C(1B)	179.5(8)
C(3B)-C(4B)-C(5B)-C(6B)	73.0(13)
C(13B)-C(4B)-C(5B)-C(6B)	-54.7(12)
C(1B)-C(5B)-C(6B)-C(7B)	-57.7(10)
C(4B)-C(5B)-C(6B)-C(7B)	177.6(9)
C(5B)-C(6B)-C(7B)-C(8B)	57.2(11)
N(2B)-N(1B)-C(8B)-C(14B)	-26.5(15)
N(2B)-N(1B)-C(8B)-C(7B)	94.2(11)
N(2B)-N(1B)-C(8B)-C(9B)	-145.4(10)
C(6B)-C(7B)-C(8B)-N(1B)	66.6(9)
C(6B)-C(7B)-C(8B)-C(14B)	-173.2(8)
C(6B)-C(7B)-C(8B)-C(9B)	-50.6(11)
N(1B)-C(8B)-C(9B)-C(10B)	56.1(11)
C(14B)-C(8B)-C(9B)-C(10B)	-62.9(13)
C(7B)-C(8B)-C(9B)-C(10B)	174.0(9)
N(1B)-C(8B)-C(9B)-C(1B)	-74.3(12)
C(14B)-C(8B)-C(9B)-C(1B)	166.7(10)
C(7B)-C(8B)-C(9B)-C(1B)	43.6(12)
O(1B)-C(1B)-C(9B)-C(10B)	66.3(10)

C(5B)-C(1B)-C(9B)-C(10B)	-179.0(8)
C(2B)-C(1B)-C(9B)-C(10B)	-50.8(11)
O(1B)-C(1B)-C(9B)-C(8B)	-161.8(9)
C(5B)-C(1B)-C(9B)-C(8B)	-47.0(11)
C(2B)-C(1B)-C(9B)-C(8B)	81.2(12)
C(8B)-C(9B)-C(10B)-C(11B)	-164.9(10)
C(1B)-C(9B)-C(10B)-C(11B)	-34.0(14)
C(9B)-C(10B)-C(11B)-C(12B)	54.0(15)
C(2B)-O(5B)-C(12B)-O(2B)	37.5(11)
C(2B)-O(5B)-C(12B)-C(11B)	-85.1(11)
C(2B)-O(5B)-C(12B)-C(15B)	146.3(9)
O(1B)-O(2B)-C(12B)-O(5B)	-76.9(9)
O(1B)-O(2B)-C(12B)-C(11B)	45.8(11)
O(1B)-O(2B)-C(12B)-C(15B)	172.0(9)
C(10B)-C(11B)-C(12B)-O(5B)	27.7(14)
C(10B)-C(11B)-C(12B)-O(2B)	-90.8(12)
C(10B)-C(11B)-C(12B)-C(15B)	150.7(12)
C(1C)-O(1C)-O(2C)-C(12C)	49.7(9)
C(8C)-N(1C)-N(2C)-N(3C)	130(7)
O(2C)-O(1C)-C(1C)-C(5C)	131.6(8)
O(2C)-O(1C)-C(1C)-C(2C)	10.5(11)
O(2C)-O(1C)-C(1C)-C(9C)	-109.4(8)
C(12C)-O(5C)-C(2C)-O(3C)	-100.2(9)
C(12C)-O(5C)-C(2C)-C(1C)	25.9(13)
C(3C)-O(3C)-C(2C)-O(5C)	156.4(8)
C(3C)-O(3C)-C(2C)-C(1C)	29.2(13)
O(1C)-C(1C)-C(2C)-O(5C)	-50.5(12)
C(5C)-C(1C)-C(2C)-O(5C)	-167.1(9)
C(9C)-C(1C)-C(2C)-O(5C)	66.3(11)
O(1C)-C(1C)-C(2C)-O(3C)	70.6(11)
C(5C)-C(1C)-C(2C)-O(3C)	-46.0(12)
C(9C)-C(1C)-C(2C)-O(3C)	-172.6(8)
C(2C)-O(3C)-C(3C)-O(4C)	163.1(9)
C(2C)-O(3C)-C(3C)-C(4C)	-23.9(15)
O(4C)-C(3C)-C(4C)-C(13C)	-21.5(18)

O(3C)-C(3C)-C(4C)-C(13C)	166.5(11)
O(4C)-C(3C)-C(4C)-C(5C)	-154.6(11)
O(3C)-C(3C)-C(4C)-C(5C)	33.4(14)
O(1C)-C(1C)-C(5C)-C(4C)	-63.4(10)
C(2C)-C(1C)-C(5C)-C(4C)	57.1(12)
C(9C)-C(1C)-C(5C)-C(4C)	-177.5(8)
O(1C)-C(1C)-C(5C)-C(6C)	166.7(9)
C(2C)-C(1C)-C(5C)-C(6C)	-72.8(12)
C(9C)-C(1C)-C(5C)-C(6C)	52.6(11)
C(13C)-C(4C)-C(5C)-C(1C)	-178.2(10)
C(3C)-C(4C)-C(5C)-C(1C)	-49.1(12)
C(13C)-C(4C)-C(5C)-C(6C)	-50.2(13)
C(3C)-C(4C)-C(5C)-C(6C)	78.9(11)
C(1C)-C(5C)-C(6C)-C(7C)	-57.9(12)
C(4C)-C(5C)-C(6C)-C(7C)	174.0(9)
C(5C)-C(6C)-C(7C)-C(8C)	55.7(12)
C(6C)-C(7C)-C(8C)-C(14C)	-172.0(9)
C(6C)-C(7C)-C(8C)-N(1C)	66.4(12)
C(6C)-C(7C)-C(8C)-C(9C)	-48.0(13)
N(2C)-N(1C)-C(8C)-C(14C)	-56.1(14)
N(2C)-N(1C)-C(8C)-C(7C)	63.1(15)
N(2C)-N(1C)-C(8C)-C(9C)	-177.6(10)
C(14C)-C(8C)-C(9C)-C(10C)	-62.9(13)
C(7C)-C(8C)-C(9C)-C(10C)	175.0(10)
N(1C)-C(8C)-C(9C)-C(10C)	59.1(13)
C(14C)-C(8C)-C(9C)-C(1C)	166.8(10)
C(7C)-C(8C)-C(9C)-C(1C)	44.6(14)
N(1C)-C(8C)-C(9C)-C(1C)	-71.3(12)
O(1C)-C(1C)-C(9C)-C(10C)	69.1(10)
C(5C)-C(1C)-C(9C)-C(10C)	-177.4(8)
C(2C)-C(1C)-C(9C)-C(10C)	-51.2(11)
O(1C)-C(1C)-C(9C)-C(8C)	-160.5(8)
C(5C)-C(1C)-C(9C)-C(8C)	-47.0(12)
C(2C)-C(1C)-C(9C)-C(8C)	79.3(11)
C(8C)-C(9C)-C(10C)-C(11C)	-170.2(10)

C(1C)-C(9C)-C(10C)-C(11C)	-38.2(13)
C(9C)-C(10C)-C(11C)-C(12C)	60.6(13)
O(1C)-O(2C)-C(12C)-O(5C)	-74.5(8)
O(1C)-O(2C)-C(12C)-C(15C)	171.3(7)
O(1C)-O(2C)-C(12C)-C(11C)	43.4(9)
C(2C)-O(5C)-C(12C)-O(2C)	35.1(11)
C(2C)-O(5C)-C(12C)-C(15C)	149.4(8)
C(2C)-O(5C)-C(12C)-C(11C)	-83.9(10)
C(10C)-C(11C)-C(12C)-O(2C)	-94.1(10)
C(10C)-C(11C)-C(12C)-O(5C)	21.6(11)
C(10C)-C(11C)-C(12C)-C(15C)	142.9(9)
C(1D)-O(1D)-O(2D)-C(12D)	48.8(10)
O(2D)-O(1D)-C(1D)-C(5D)	130.2(9)
O(2D)-O(1D)-C(1D)-C(2D)	12.1(13)
O(2D)-O(1D)-C(1D)-C(9D)	-108.3(10)
C(12D)-O(5D)-C(2D)-O(3D)	-101.7(10)
C(12D)-O(5D)-C(2D)-C(1D)	28.5(14)
C(3D)-O(3D)-C(2D)-O(5D)	155.2(9)
C(3D)-O(3D)-C(2D)-C(1D)	25.2(13)
O(1D)-C(1D)-C(2D)-O(5D)	-53.8(15)
C(5D)-C(1D)-C(2D)-O(5D)	-169.0(11)
C(9D)-C(1D)-C(2D)-O(5D)	65.5(12)
O(1D)-C(1D)-C(2D)-O(3D)	71.6(11)
C(5D)-C(1D)-C(2D)-O(3D)	-43.6(13)
C(9D)-C(1D)-C(2D)-O(3D)	-169.1(8)
C(2D)-O(3D)-C(3D)-O(4D)	161.8(11)
C(2D)-O(3D)-C(3D)-C(4D)	-15.2(15)
O(4D)-C(3D)-C(4D)-C(5D)	-147.9(14)
O(3D)-C(3D)-C(4D)-C(5D)	28.5(15)
O(4D)-C(3D)-C(4D)-C(13D)	-9(2)
O(3D)-C(3D)-C(4D)-C(13D)	167.8(11)
C(3D)-C(4D)-C(5D)-C(1D)	-50.5(14)
C(13D)-C(4D)-C(5D)-C(1D)	176.2(11)
C(3D)-C(4D)-C(5D)-C(6D)	76.6(14)
C(13D)-C(4D)-C(5D)-C(6D)	-56.7(15)

O(1D)-C(1D)-C(5D)-C(4D)	-63.4(11)
C(2D)-C(1D)-C(5D)-C(4D)	55.5(14)
C(9D)-C(1D)-C(5D)-C(4D)	178.8(9)
O(1D)-C(1D)-C(5D)-C(6D)	167.7(9)
C(2D)-C(1D)-C(5D)-C(6D)	-73.4(13)
C(9D)-C(1D)-C(5D)-C(6D)	50.0(12)
C(4D)-C(5D)-C(6D)-C(7D)	178.8(10)
C(1D)-C(5D)-C(6D)-C(7D)	-54.4(12)
C(5D)-C(6D)-C(7D)-C(8D)	54.6(14)
C(6D)-C(7D)-C(8D)-N(1D)	70.9(14)
C(6D)-C(7D)-C(8D)-C(9D)	-49.7(13)
C(6D)-C(7D)-C(8D)-C(14D)	-173.8(11)
N(2D)-N(1D)-C(8D)-C(7D)	62.0(18)
N(2D)-N(1D)-C(8D)-C(9D)	-171.1(12)
N(2D)-N(1D)-C(8D)-C(14D)	-56.2(15)
C(7D)-C(8D)-C(9D)-C(10D)	174.3(10)
N(1D)-C(8D)-C(9D)-C(10D)	50.6(14)
C(14D)-C(8D)-C(9D)-C(10D)	-61.2(15)
C(7D)-C(8D)-C(9D)-C(1D)	43.5(14)
N(1D)-C(8D)-C(9D)-C(1D)	-80.2(15)
C(14D)-C(8D)-C(9D)-C(1D)	168.0(12)
O(1D)-C(1D)-C(9D)-C(10D)	66.9(12)
C(5D)-C(1D)-C(9D)-C(10D)	-177.2(10)
C(2D)-C(1D)-C(9D)-C(10D)	-54.0(11)
O(1D)-C(1D)-C(9D)-C(8D)	-159.1(10)
C(5D)-C(1D)-C(9D)-C(8D)	-43.3(14)
C(2D)-C(1D)-C(9D)-C(8D)	79.9(12)
C(8D)-C(9D)-C(10D)-C(11D)	-168.5(10)
C(1D)-C(9D)-C(10D)-C(11D)	-36.3(15)
C(9D)-C(10D)-C(11D)-C(12D)	59.1(16)
O(1D)-O(2D)-C(12D)-O(5D)	-76.3(8)
O(1D)-O(2D)-C(12D)-C(15D)	169.6(7)
O(1D)-O(2D)-C(12D)-C(11D)	44.2(9)
C(2D)-O(5D)-C(12D)-O(2D)	34.1(10)
C(2D)-O(5D)-C(12D)-C(15D)	148.0(9)

C(2D)-O(5D)-C(12D)-C(11D)	-88.6(11)
C(10D)-C(11D)-C(12D)-O(2D)	-94.6(13)
C(10D)-C(11D)-C(12D)-O(5D)	25.5(15)
C(10D)-C(11D)-C(12D)-C(15D)	144.4(12)
C(1E)-O(1E)-O(2E)-C(12E)	45.5(9)
O(2E)-O(1E)-C(1E)-C(2E)	14.9(7)
O(2E)-O(1E)-C(1E)-C(9E)	-108.9(7)
O(2E)-O(1E)-C(1E)-C(5E)	133.2(6)
C(12E)-O(5E)-C(2E)-O(3E)	-99.3(8)
C(12E)-O(5E)-C(2E)-C(1E)	27.1(10)
C(3E)-O(3E)-C(2E)-O(5E)	155.8(8)
C(3E)-O(3E)-C(2E)-C(1E)	31.0(11)
O(1E)-C(1E)-C(2E)-O(5E)	-52.5(8)
C(9E)-C(1E)-C(2E)-O(5E)	66.6(9)
C(5E)-C(1E)-C(2E)-O(5E)	-166.2(6)
O(1E)-C(1E)-C(2E)-O(3E)	68.1(9)
C(9E)-C(1E)-C(2E)-O(3E)	-172.7(7)
C(5E)-C(1E)-C(2E)-O(3E)	-45.5(9)
C(2E)-O(3E)-C(3E)-O(4E)	160.7(8)
C(2E)-O(3E)-C(3E)-C(4E)	-25.1(12)
O(4E)-C(3E)-C(4E)-C(13E)	-21.6(13)
O(3E)-C(3E)-C(4E)-C(13E)	164.4(7)
O(4E)-C(3E)-C(4E)-C(5E)	-150.0(9)
O(3E)-C(3E)-C(4E)-C(5E)	36.0(11)
C(3E)-C(4E)-C(5E)-C(6E)	72.7(9)
C(13E)-C(4E)-C(5E)-C(6E)	-56.0(10)
C(3E)-C(4E)-C(5E)-C(1E)	-50.6(9)
C(13E)-C(4E)-C(5E)-C(1E)	-179.3(7)
O(1E)-C(1E)-C(5E)-C(6E)	169.2(6)
C(2E)-C(1E)-C(5E)-C(6E)	-72.0(8)
C(9E)-C(1E)-C(5E)-C(6E)	55.9(9)
O(1E)-C(1E)-C(5E)-C(4E)	-63.8(8)
C(2E)-C(1E)-C(5E)-C(4E)	55.1(8)
C(9E)-C(1E)-C(5E)-C(4E)	-177.0(7)
C(4E)-C(5E)-C(6E)-C(7E)	179.5(7)

C(1E)-C(5E)-C(6E)-C(7E)	-58.1(9)
C(5E)-C(6E)-C(7E)-C(8E)	57.5(10)
N(2E)-N(1E)-C(8E)-C(14E)	-19.5(14)
N(2E)-N(1E)-C(8E)-C(7E)	102.9(10)
N(2E)-N(1E)-C(8E)-C(9E)	-140.9(9)
C(6E)-C(7E)-C(8E)-N(1E)	64.6(10)
C(6E)-C(7E)-C(8E)-C(14E)	-171.3(8)
C(6E)-C(7E)-C(8E)-C(9E)	-48.9(11)
O(1E)-C(1E)-C(9E)-C(10E)	71.0(9)
C(2E)-C(1E)-C(9E)-C(10E)	-51.3(10)
C(5E)-C(1E)-C(9E)-C(10E)	-177.5(7)
O(1E)-C(1E)-C(9E)-C(8E)	-161.8(7)
C(2E)-C(1E)-C(9E)-C(8E)	76.0(9)
C(5E)-C(1E)-C(9E)-C(8E)	-50.2(9)
N(1E)-C(8E)-C(9E)-C(1E)	-67.3(9)
C(14E)-C(8E)-C(9E)-C(1E)	168.6(8)
C(7E)-C(8E)-C(9E)-C(1E)	45.3(10)
N(1E)-C(8E)-C(9E)-C(10E)	59.8(9)
C(14E)-C(8E)-C(9E)-C(10E)	-64.3(9)
C(7E)-C(8E)-C(9E)-C(10E)	172.4(7)
C(1E)-C(9E)-C(10E)-C(11E)	-40.4(11)
C(8E)-C(9E)-C(10E)-C(11E)	-168.9(8)
C(9E)-C(10E)-C(11E)-C(12E)	58.5(11)
O(1E)-O(2E)-C(12E)-O(5E)	-74.1(10)
O(1E)-O(2E)-C(12E)-C(15E)	170.8(8)
O(1E)-O(2E)-C(12E)-C(11E)	49.3(10)
C(2E)-O(5E)-C(12E)-O(2E)	35.0(11)
C(2E)-O(5E)-C(12E)-C(15E)	149.3(8)
C(2E)-O(5E)-C(12E)-C(11E)	-89.4(8)
C(10E)-C(11E)-C(12E)-O(2E)	-97.4(11)
C(10E)-C(11E)-C(12E)-O(5E)	25.5(11)
C(10E)-C(11E)-C(12E)-C(15E)	144.3(10)

Symmetry transformations used to generate eq.alent atoms: