

Supporting information.

Synthesis of New Quinolinequinone Derivatives and Preliminary Exploration of their Cytotoxic Properties

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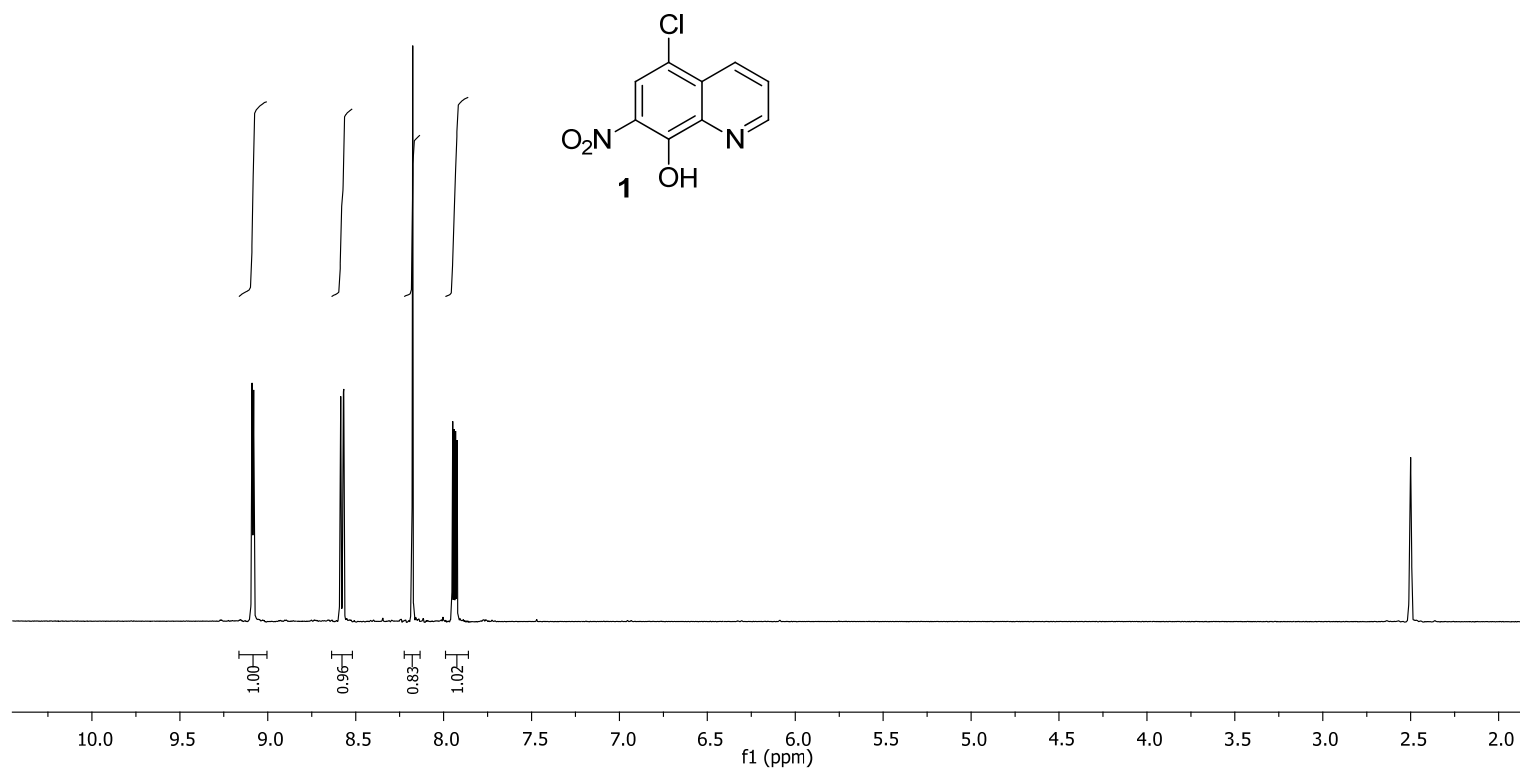
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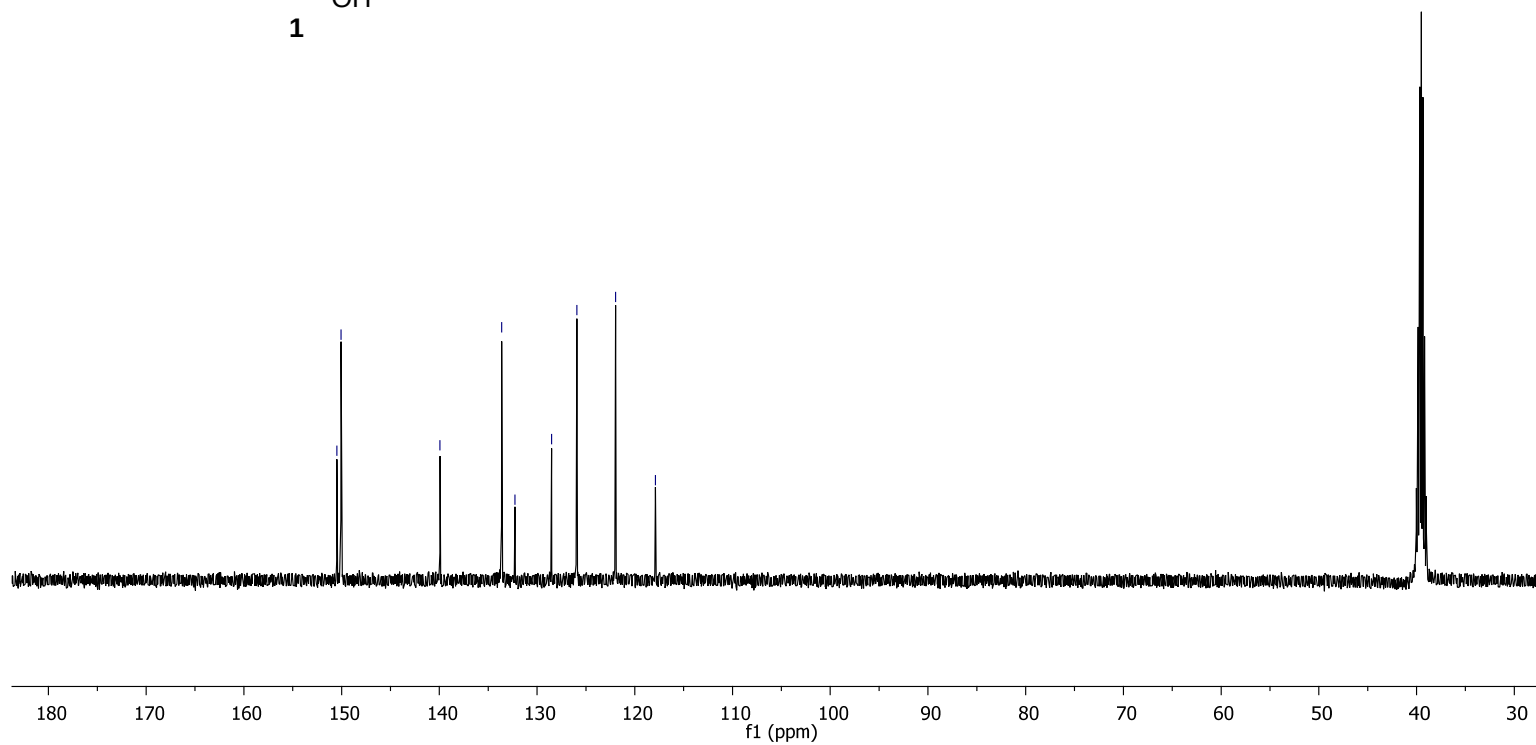
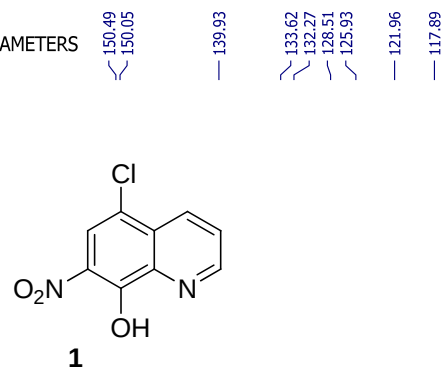
500 MHz ^1H -NMR of 5-chloro-8-hydroxy-7-nitroquinoline (**1**) in DMSO

CMK-01-121a-proton
STANDARD PROTON PARAMETERS



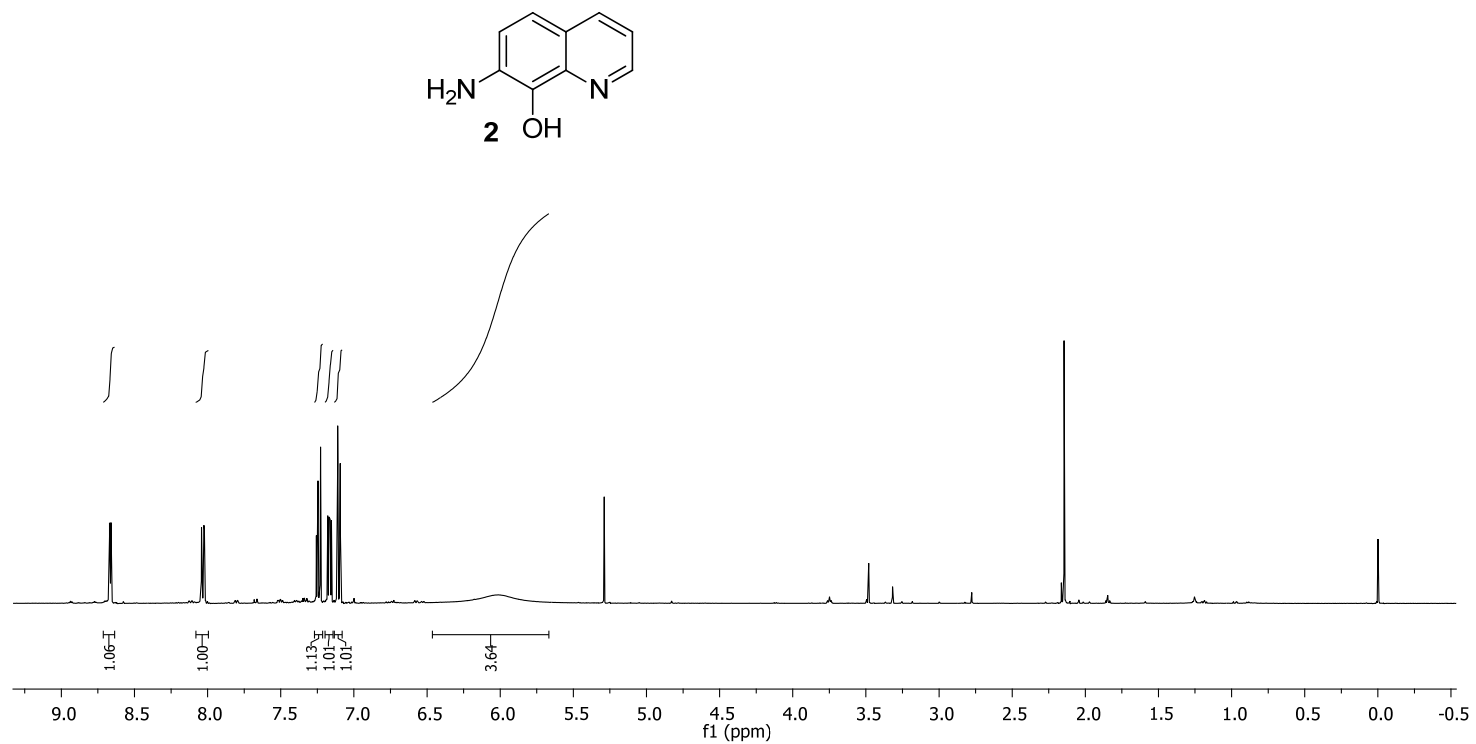
125 MHz ^{13}C -NMR of 5-chloro-8-hydroxy-7-nitroquinoline (**1**) in DMSO

CMK-01-121a-C13
STANDARD CARBON PARAMETERS



500 MHz ^1H -NMR of 7-amino-8-hydroxyquinoline (**2**) in CDCl_3

CMK-01-95-proton-1
Std proton



125 MHz ^{13}C -NMR of 7-amino-8-hydroxyquinoline (**2**) in CDCl_3

CMK-01-95-C13
Std carbon

147.95

137.89

136.61

136.06

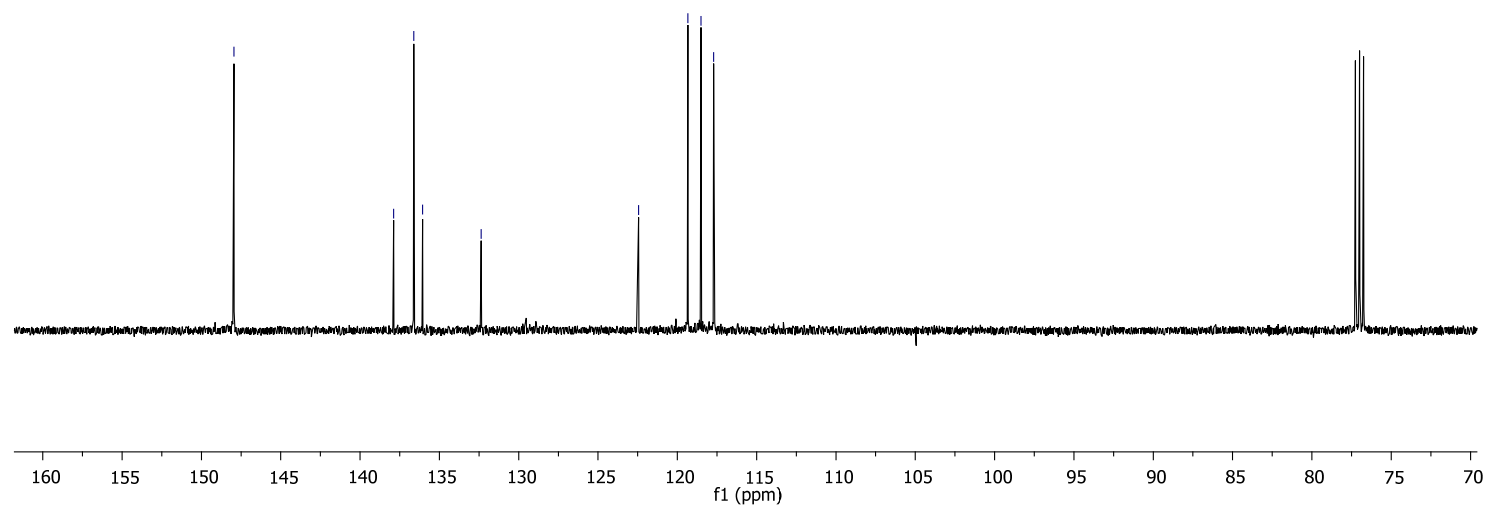
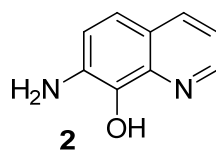
132.36

122.44

119.33

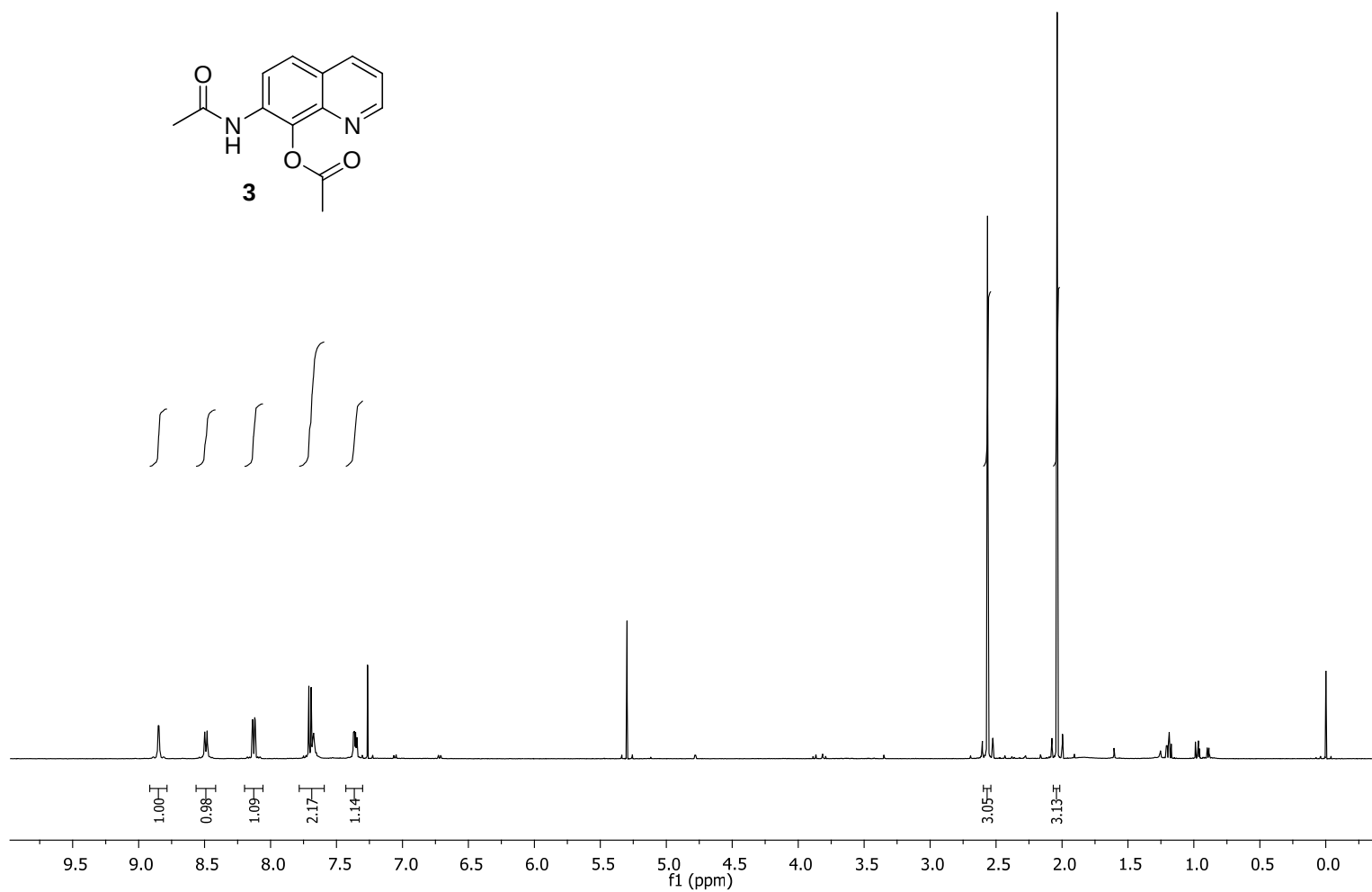
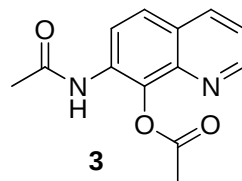
118.51

117.71



500 MHz ^1H -NMR of 7-acetamido-8-acetyloxyquinoline (**3**) in CDCl_3

CMK-01-98p-proton
Std proton



125 MHz ^{13}C -NMR of 7-acetamido-8-acetyloxyquinoline (**3**) in CDCl_3

CMK-01-98p-C13
Std carbon

169.66
168.48

150.64

140.66

136.81

134.87

130.83

125.80

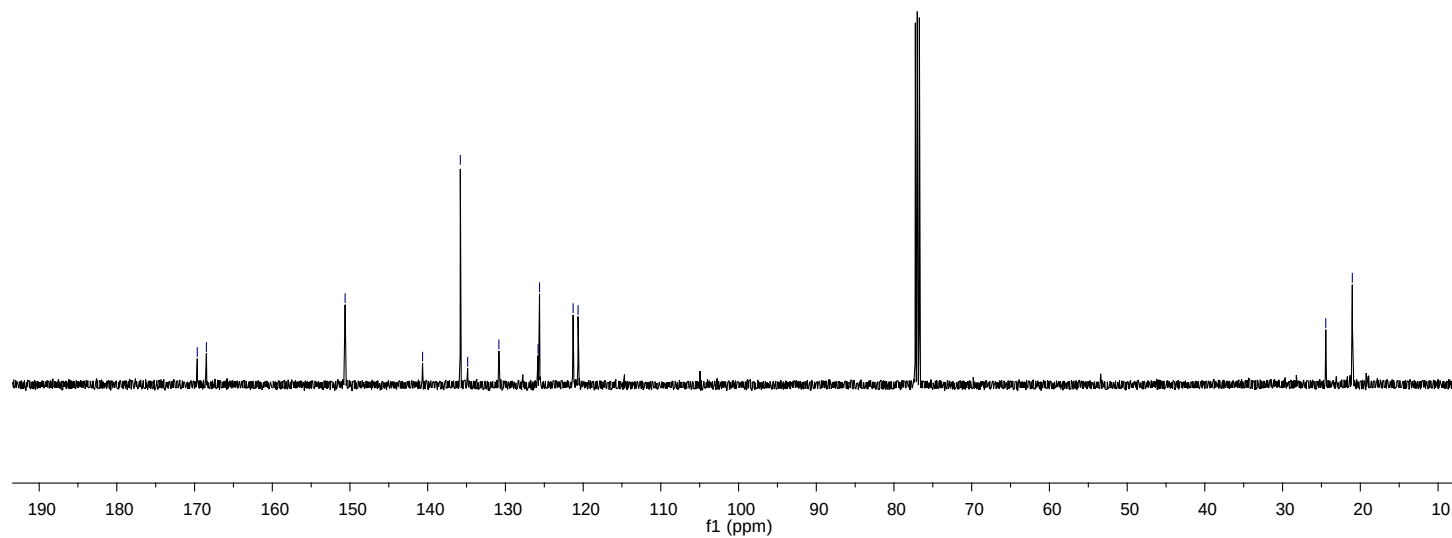
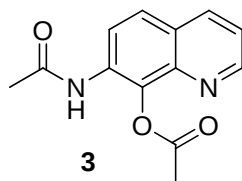
125.61

121.30

120.64

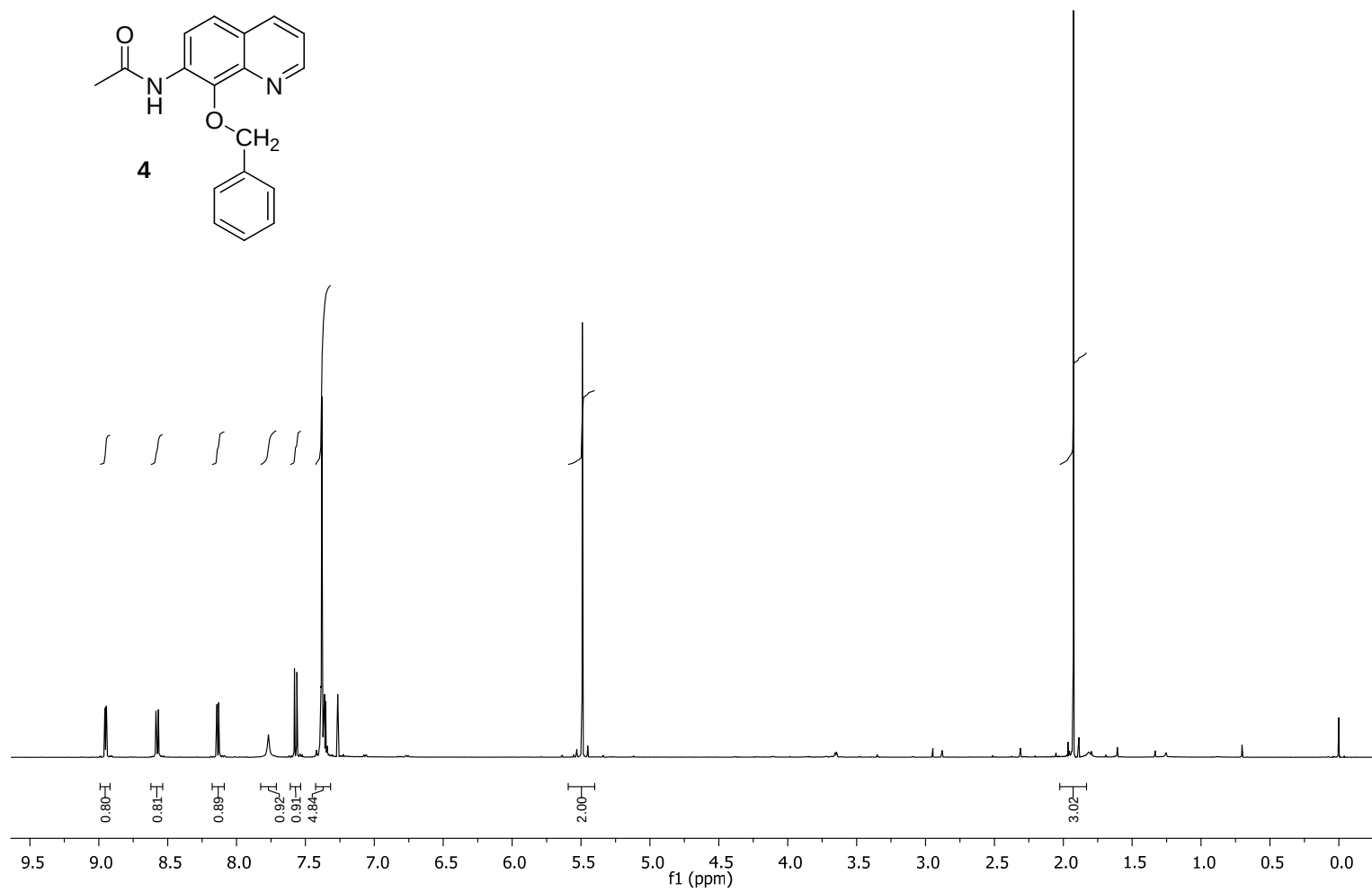
24.45

21.02

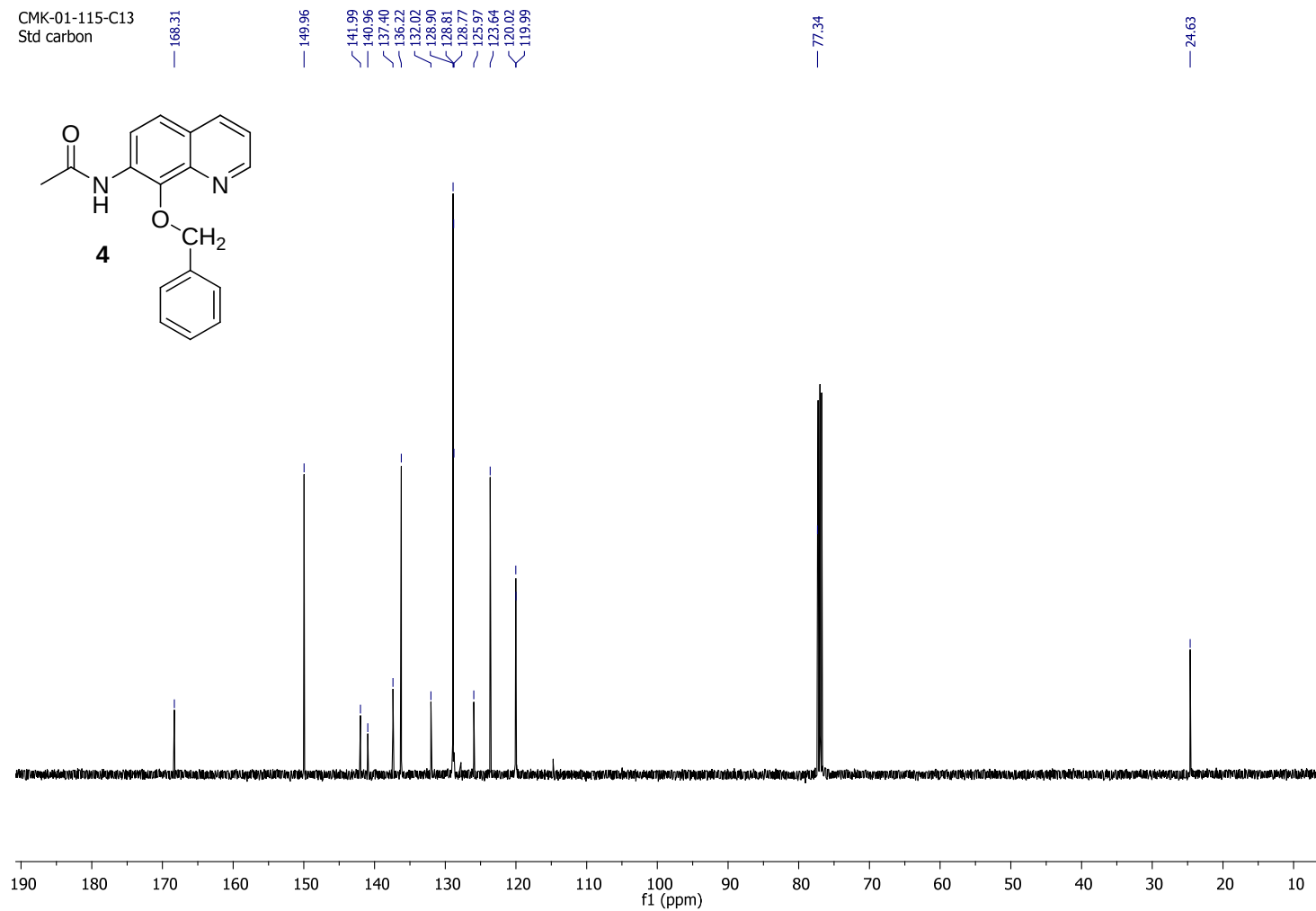


500 MHz ^1H -NMR of 7-acetamido-8-benzyloxyquinoline (**4**) in CDCl_3

CMK-01-115-proton
Std proton

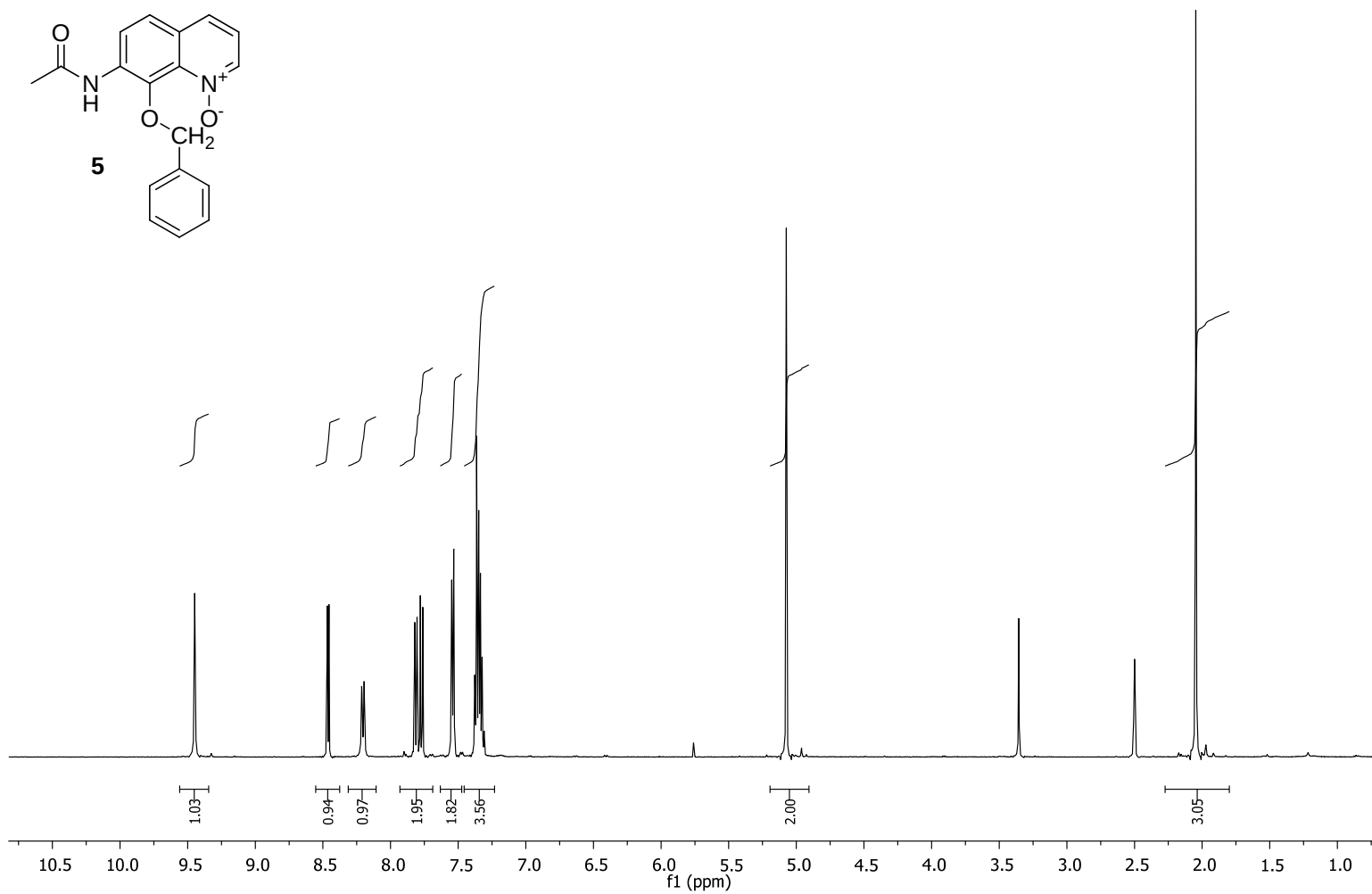


125 MHz ^{13}C -NMR of 7-acetamido-8-benzyloxyquinoline (**4**) in CDCl_3



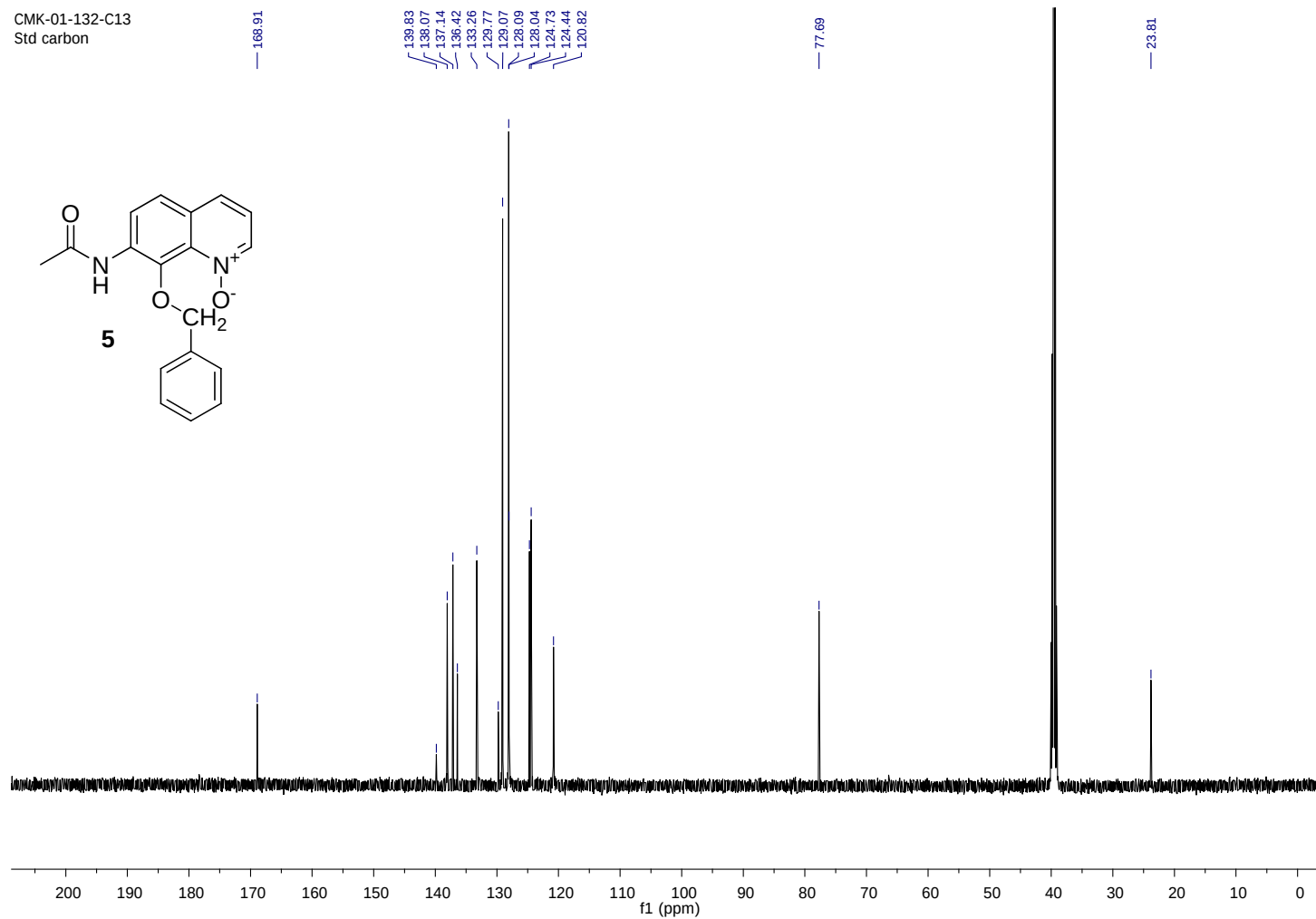
500 MHz ^1H -NMR of 7-acetamido-8-benzyloxyquinoline-1-oxide (**5**) in DMSO

CMK-01-132-proton
Std proton



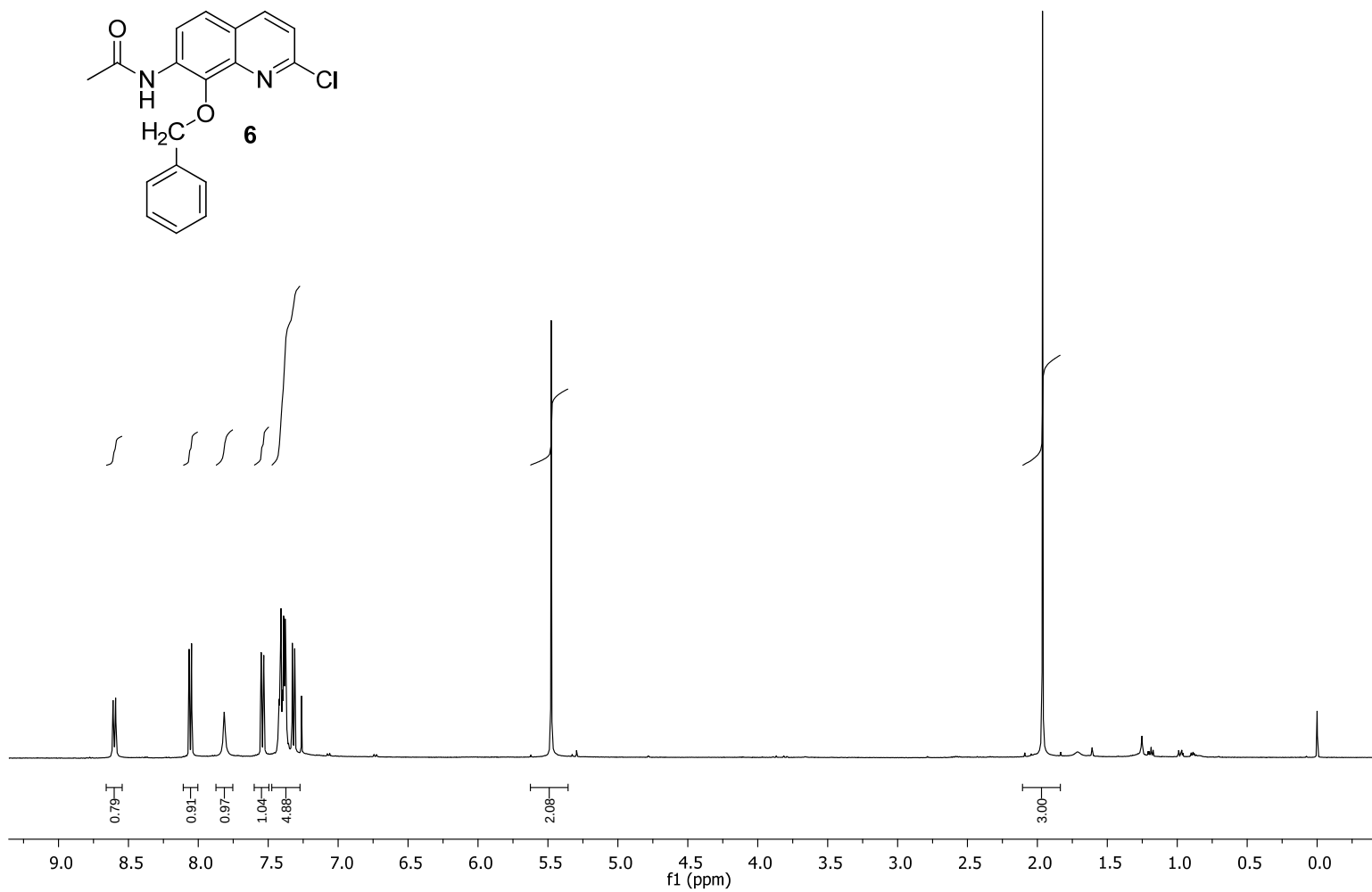
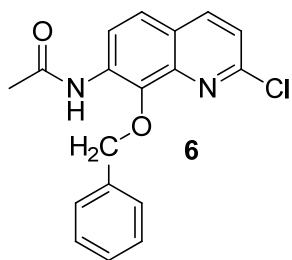
125 MHz ^{13}C -NMR of 7-acetamido-8-benzyloxyquinoline-1-oxide (**5**) in DMSO

CMK-01-132-C13
Std carbon

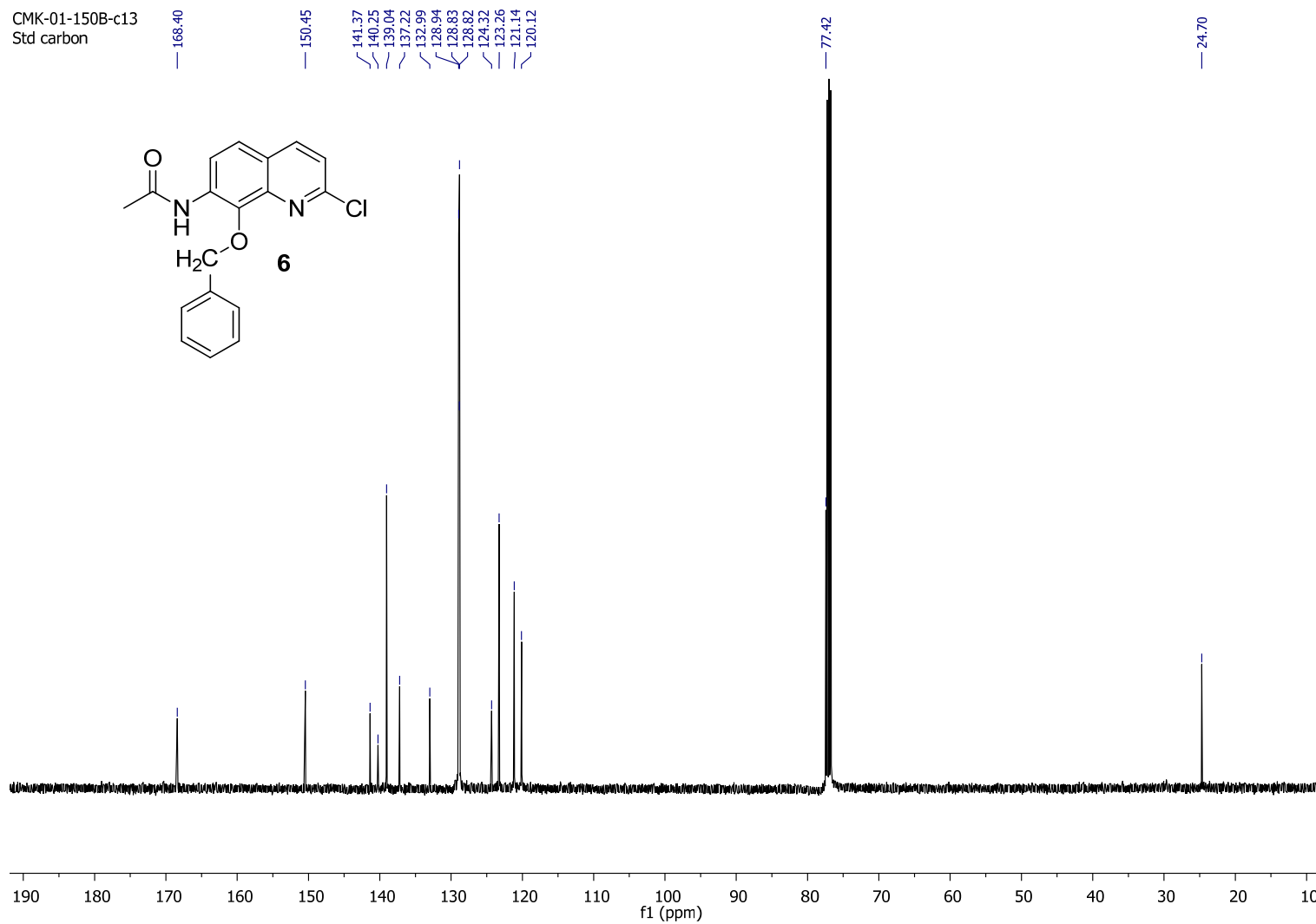


500 MHz ^1H -NMR of 7-acetamido-8-benzyloxy-2-chloroquinoline (**6**) in CDCl_3

CMK-01-150B-proton
Std proton



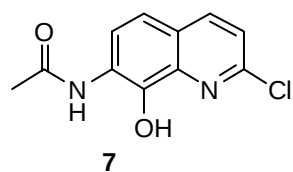
125 MHz ^{13}C -NMR of 7-acetamido-8-benzyloxy-2-chloroquinoline (**6**) in CDCl_3



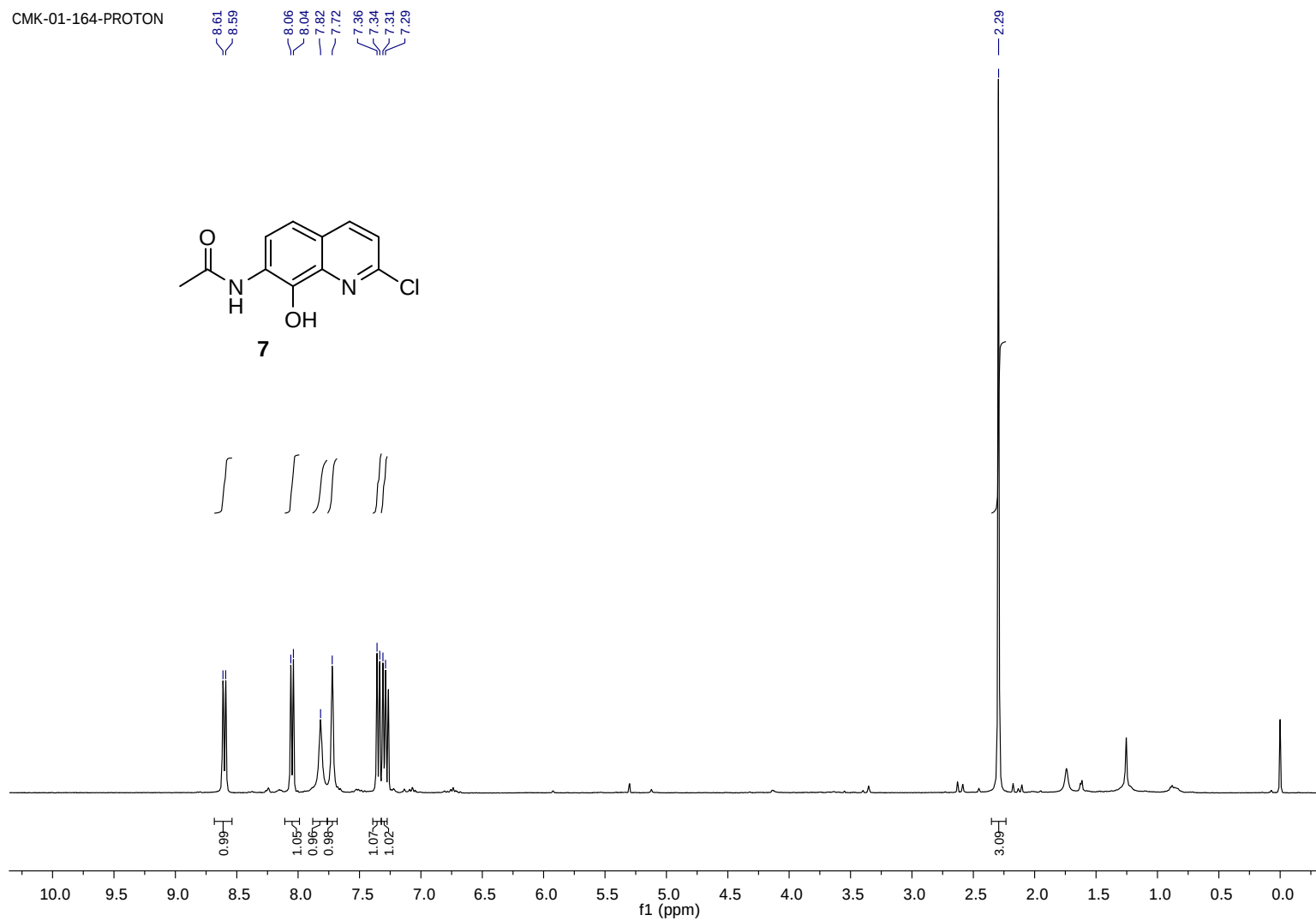
400 MHz ^1H -NMR of 7-acetamido-2-chloro-8-hydroxyquinoline (**7**) in CDCl_3

CMK-01-164-PROTON

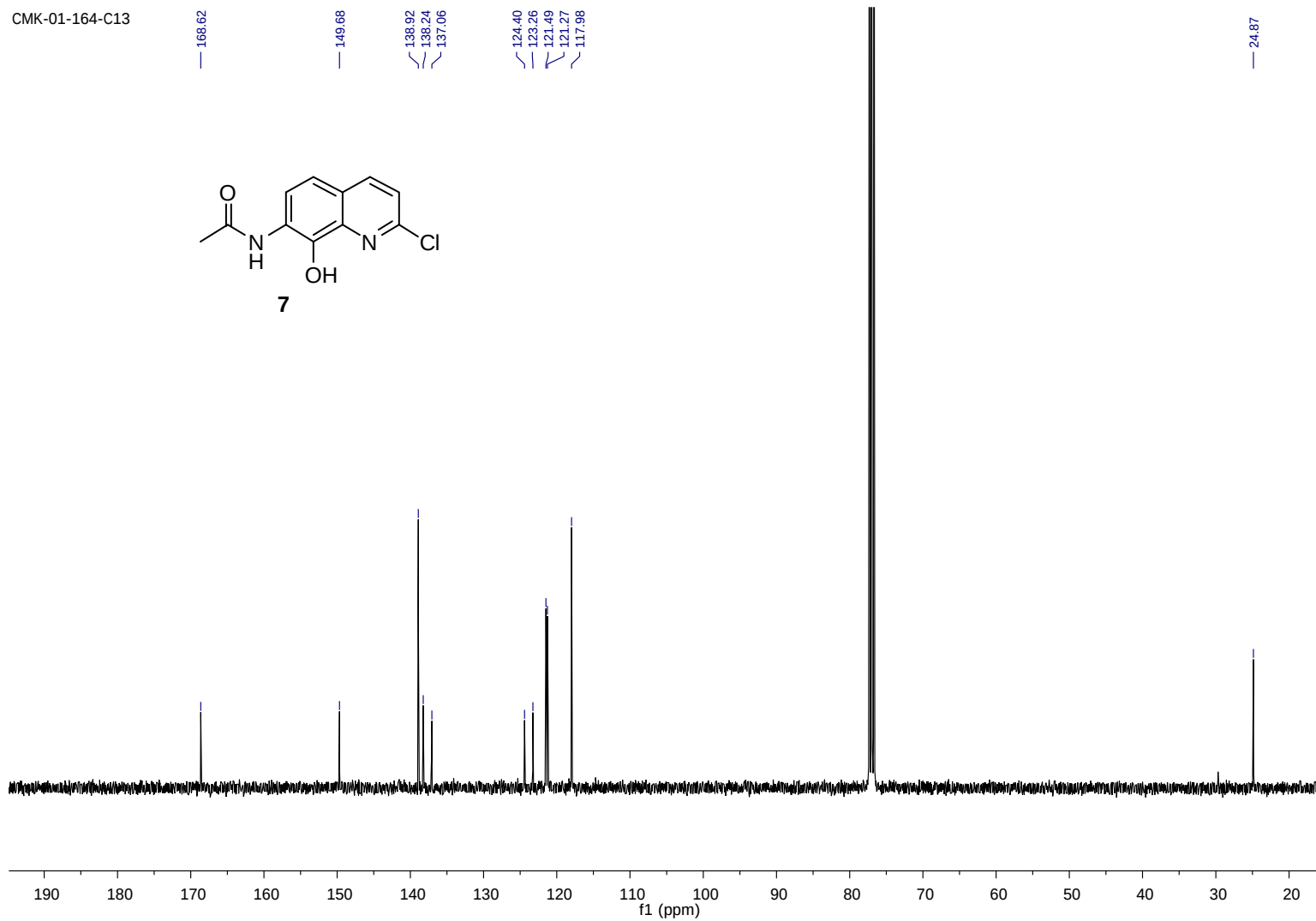
8.61
8.59
8.06
8.04
7.82
7.72
7.36
7.34
7.31
7.29



Integration values: 0.99, 1.06, 0.96, 0.98, 1.07, 1.02

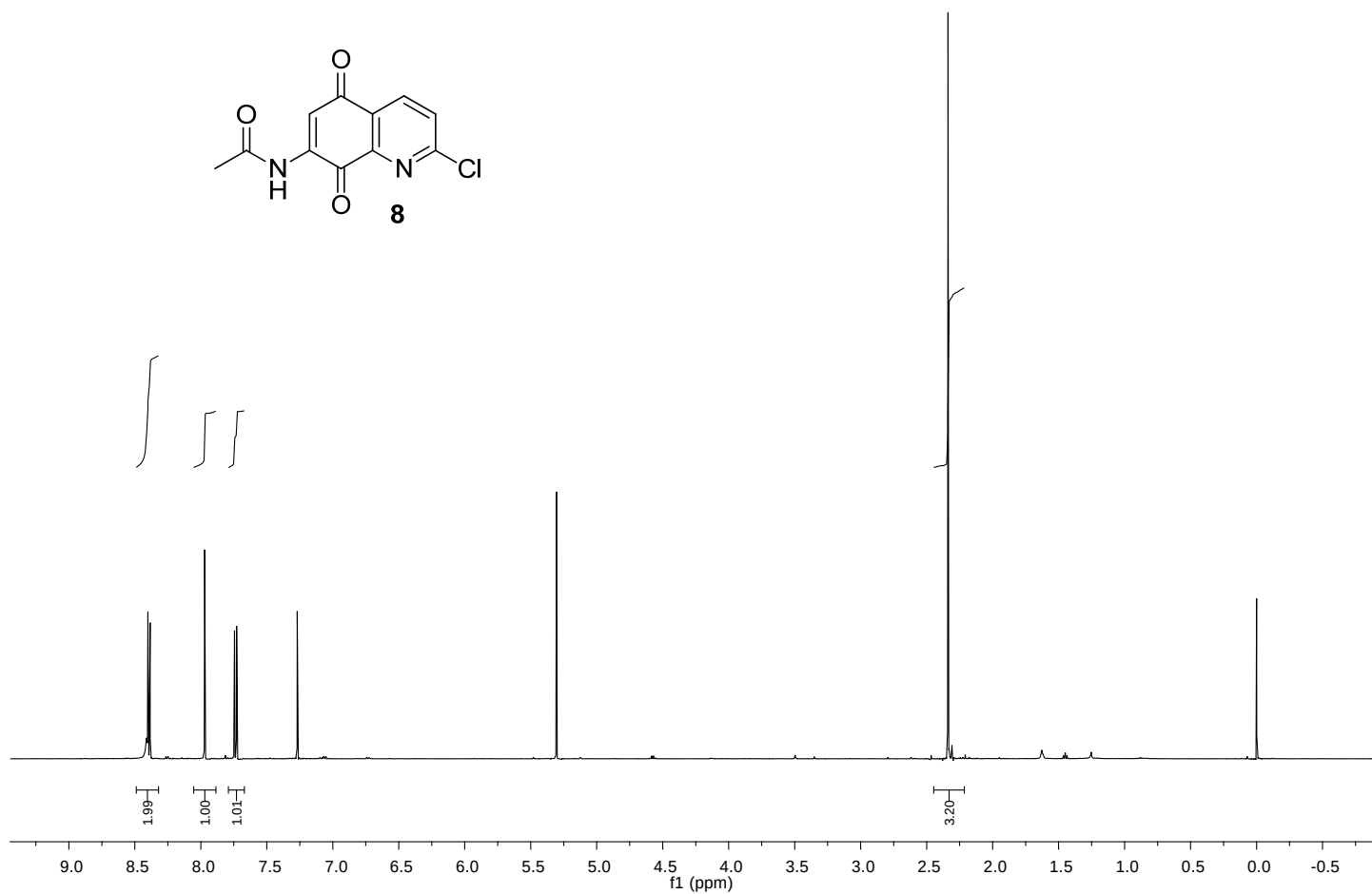


100 MHz ^{13}C -NMR of 7-acetamido-2-chloro-8-hydroxyquinoline (**7**) in CDCl_3



500 MHz ^1H -NMR of 7-acetamido-2-chloroquinoline-5,8-dione (**8**) in CDCl_3

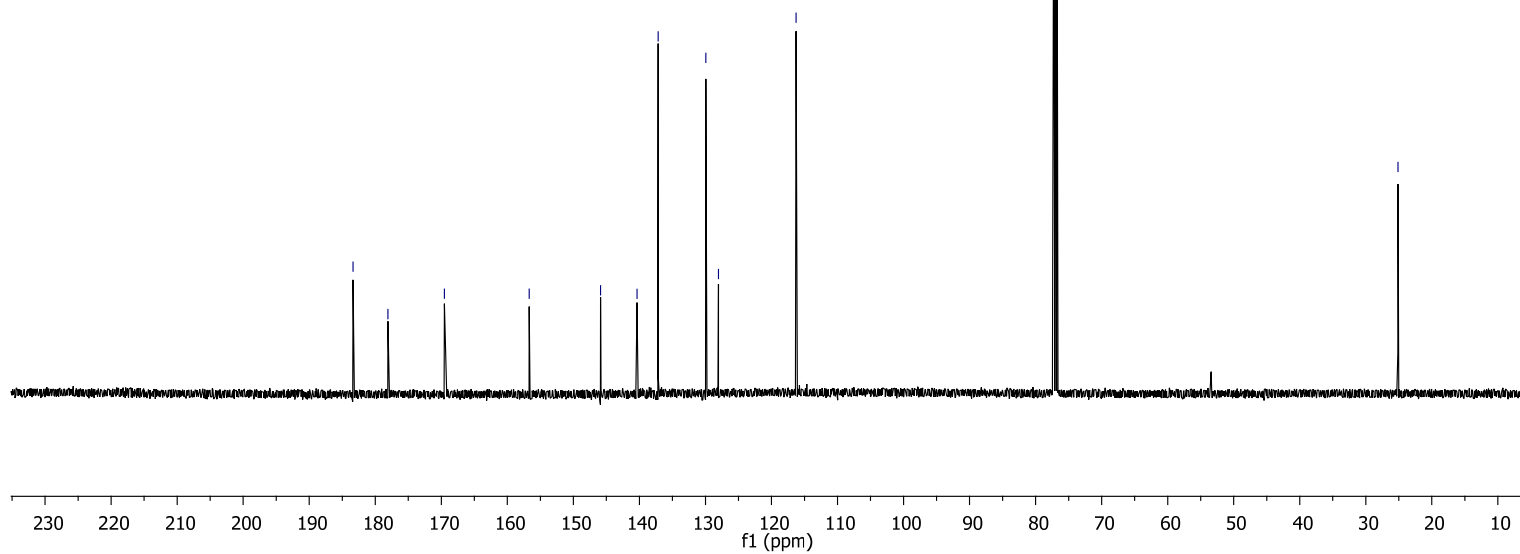
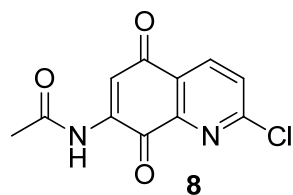
CMK-01-165-proton
STANDARD PROTON PARAMETERS



125 MHz ^{13}C -NMR of 7-acetamido-2-chloroquinoline-5,8-dione (**8**) in CDCl_3

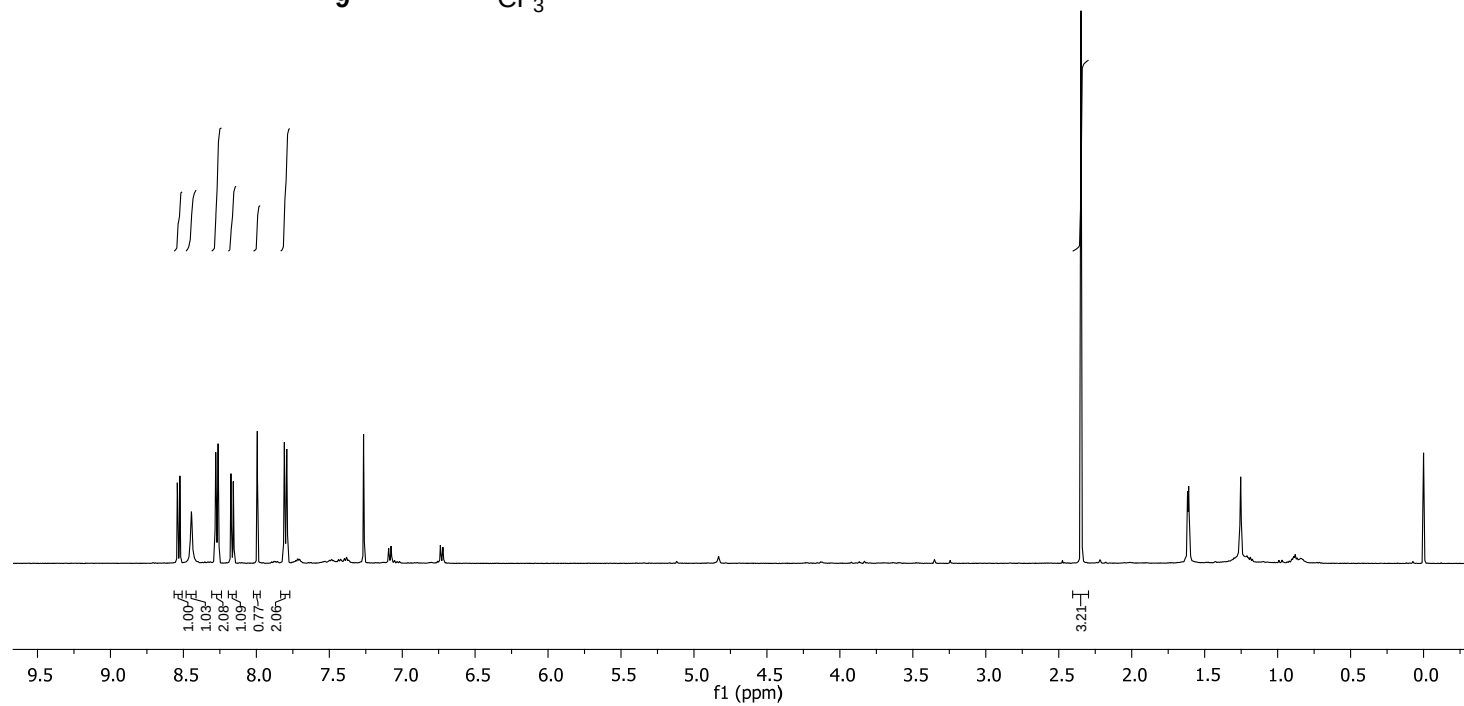
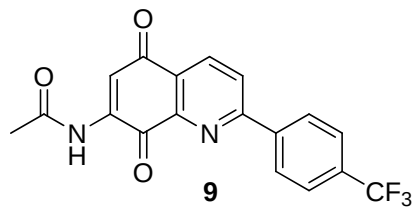
CMK-01-165a-C13
STANDARD CARBON PARAMETERS

183.37 178.08 169.53 156.69 145.88 140.36 137.17 129.94 128.03 116.27 25.13

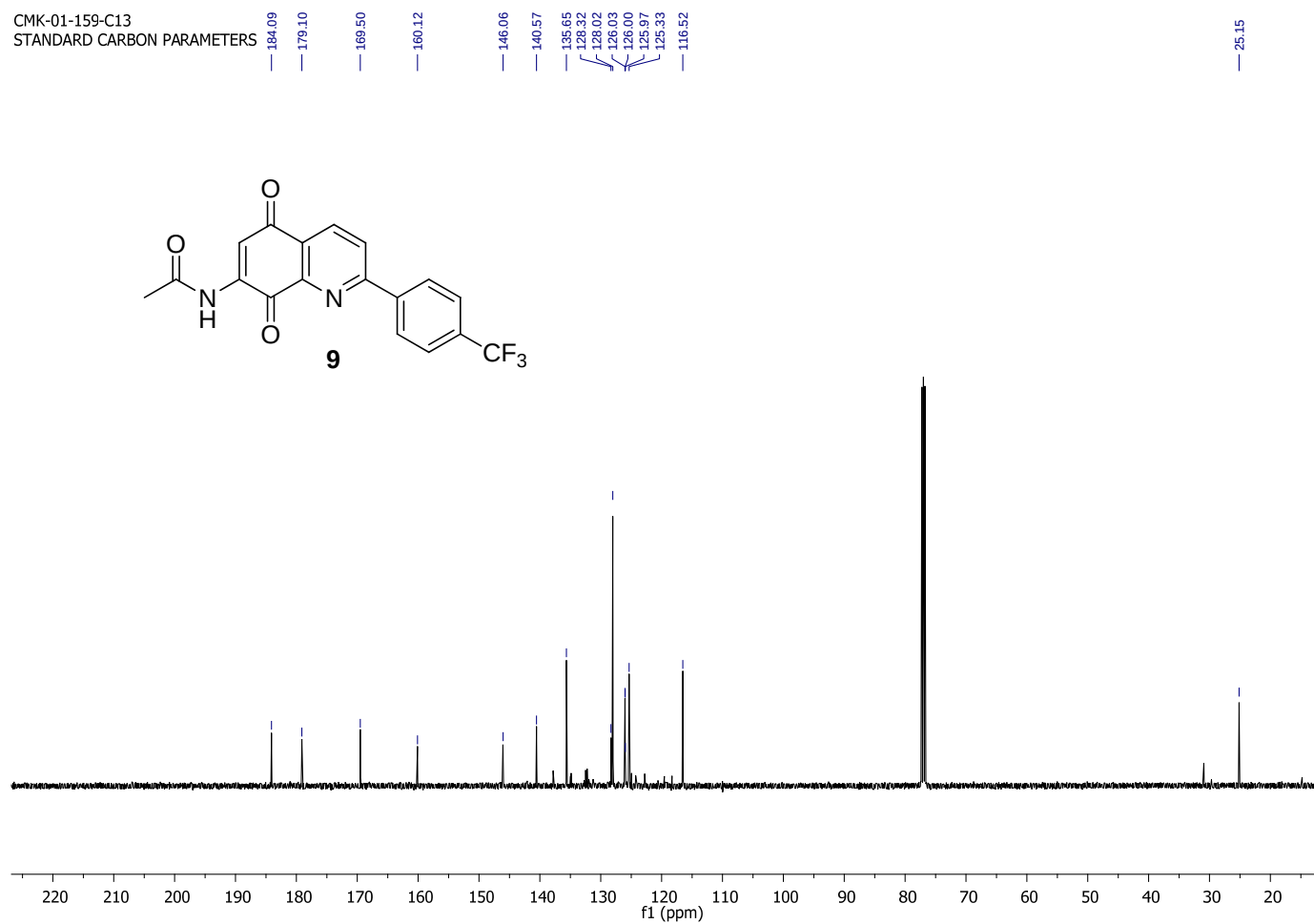


500 MHz ^1H -NMR of 7-acetamido-2-(4-trifluoromethylphenyl)quinoline-5,8-dione (**9**) in CDCl_3

CMK-01-158p-proton
Std proton

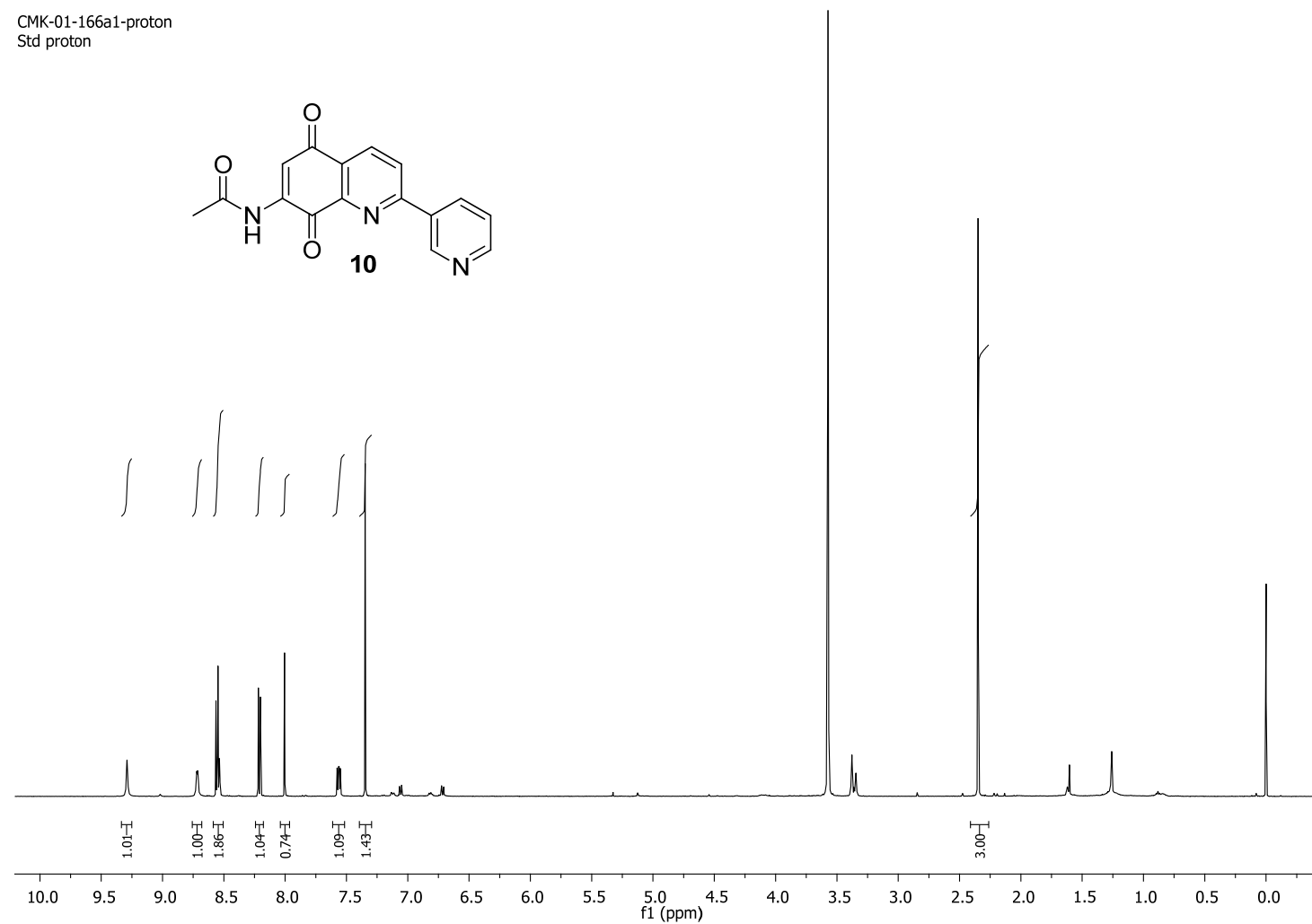


125 MHz ^{13}C -H-NMR of 7-acetamido-2-(4-trifluoromethylphenyl)quinoline-5,8-dione (**9**) in CDCl_3

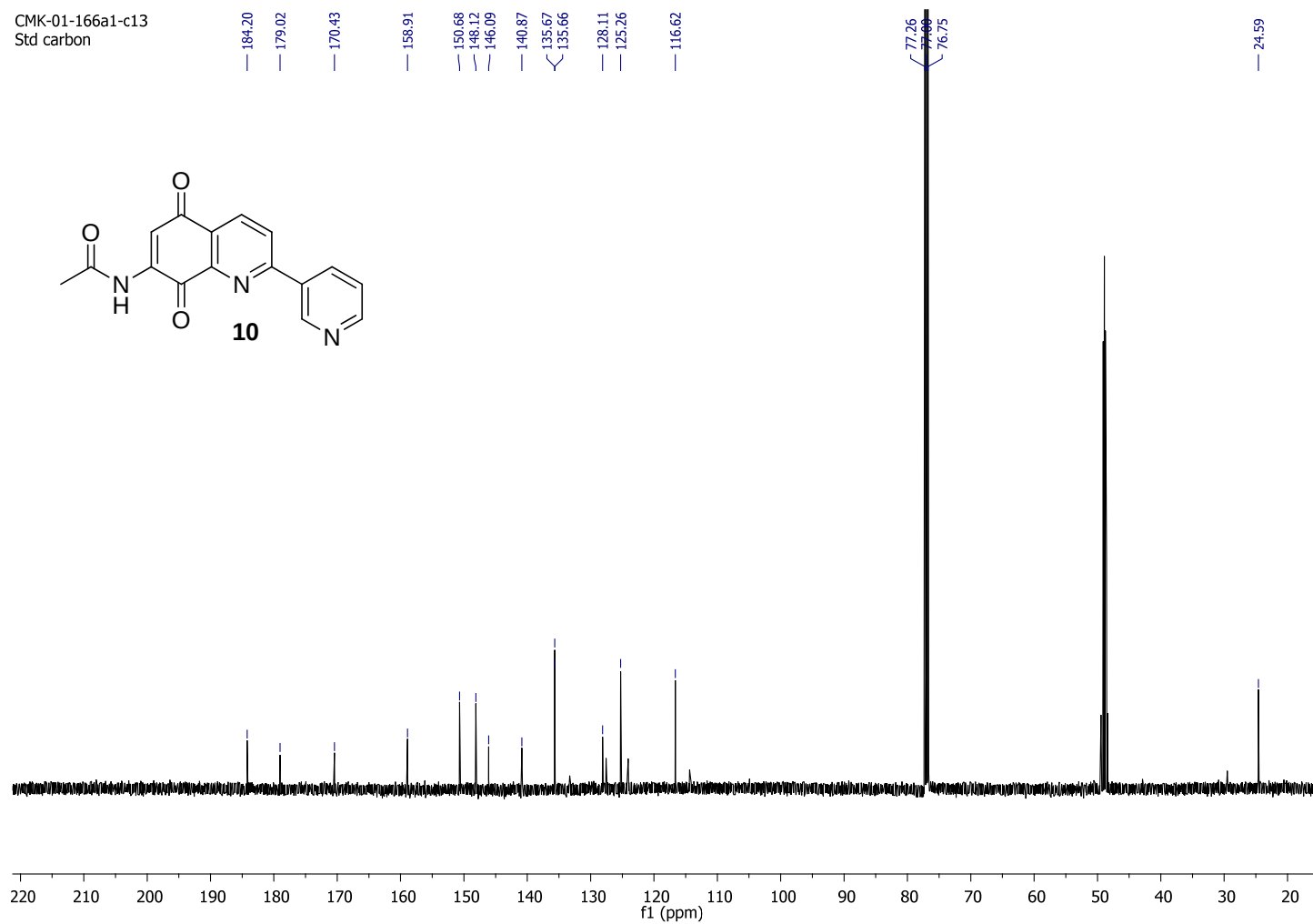


500 MHz ^1H -NMR of 7-acetamido-2-(3-pyridinyl)quinoline-5,8-dione (**10**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-166a1-proton
Std proton

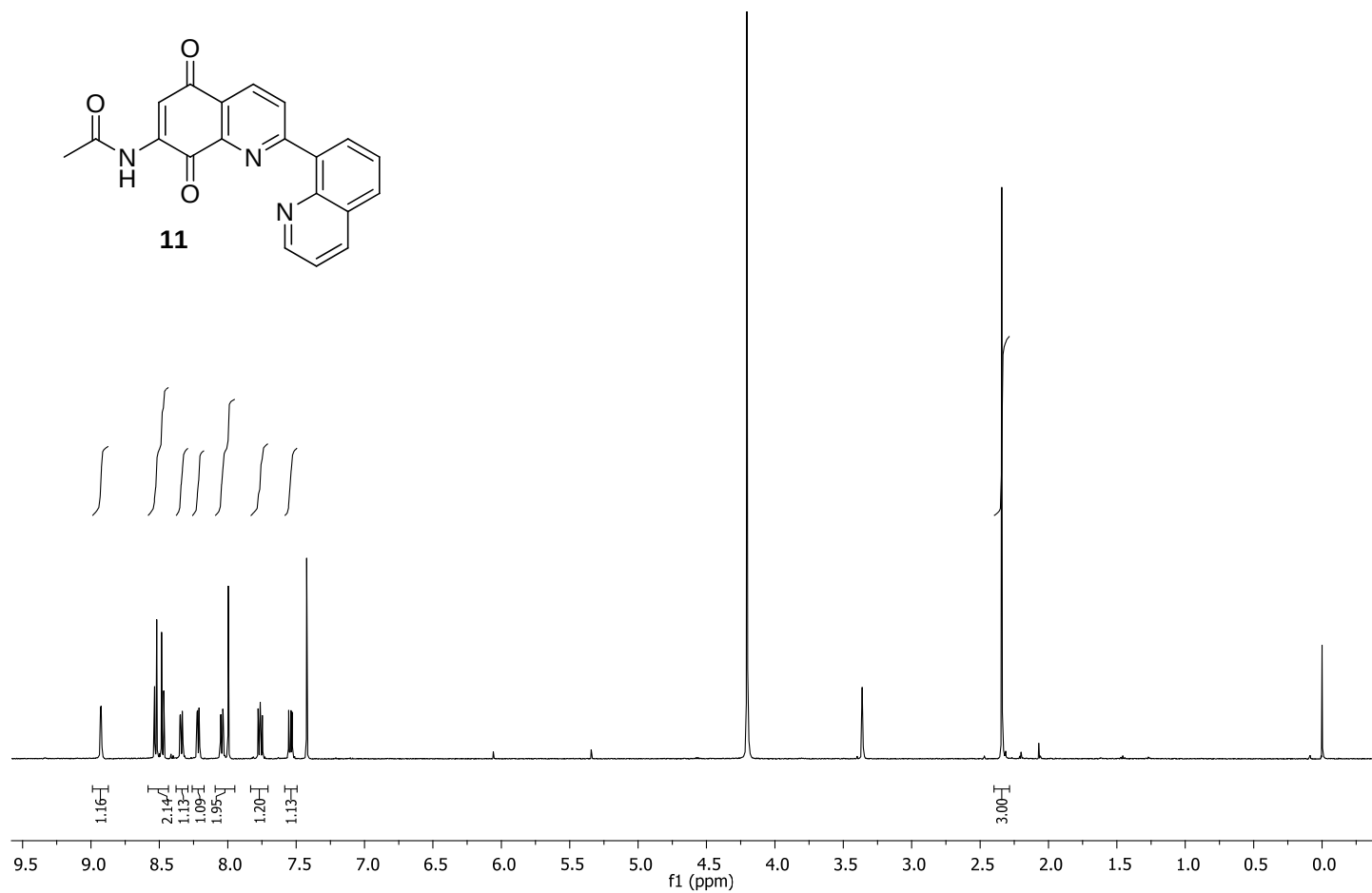


125 MHz ^{13}C -H-NMR of 7-acetamido-2-(3-pyridinyl)quinoline-5,8-dione (**10**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

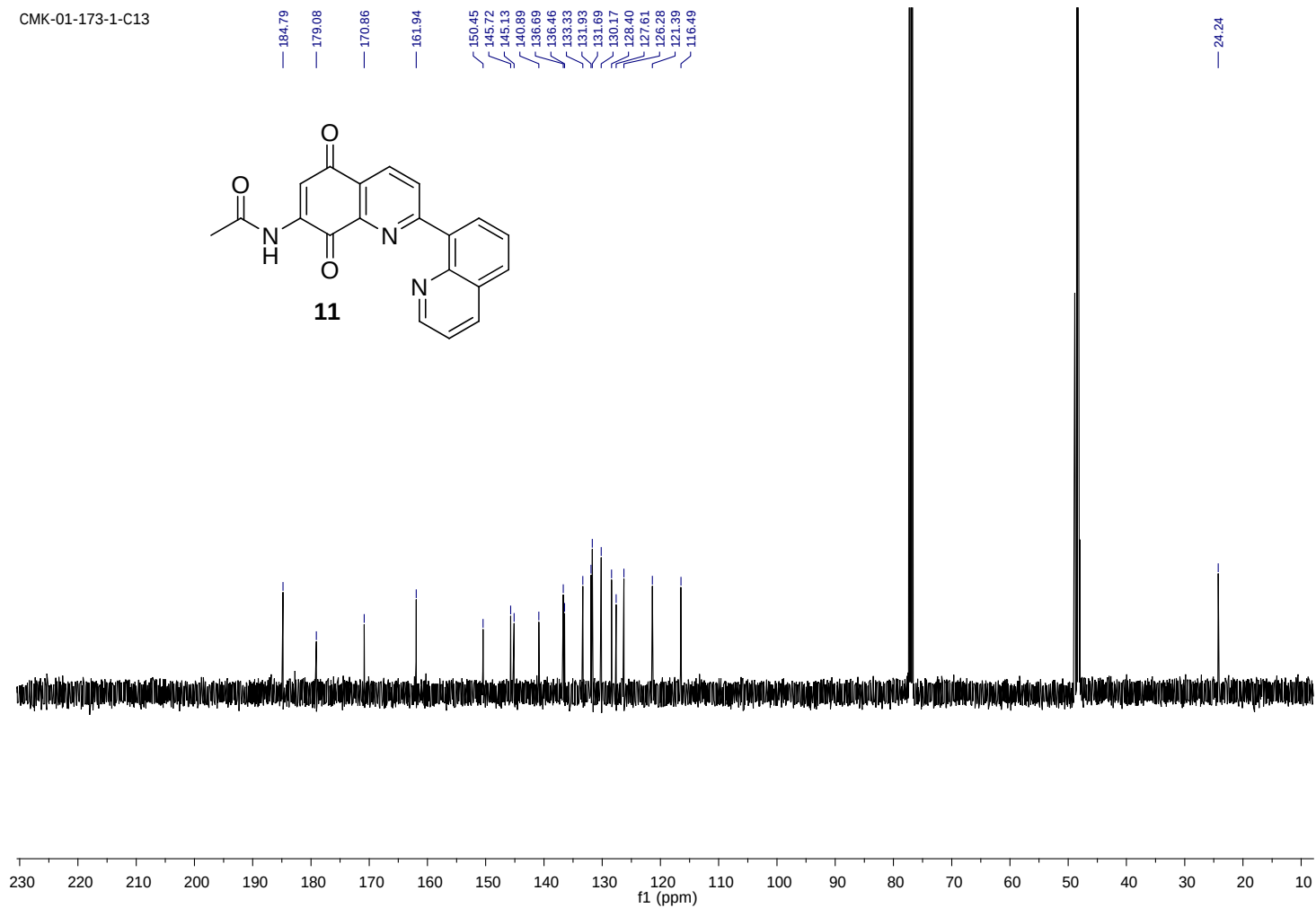


500 MHz ^1H -NMR of 7-acetamido-2-(8'-(quinolyl))quinoline-5,8-dione (**11**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-173-1-proton
STANDARD PROTON PARAMETERS

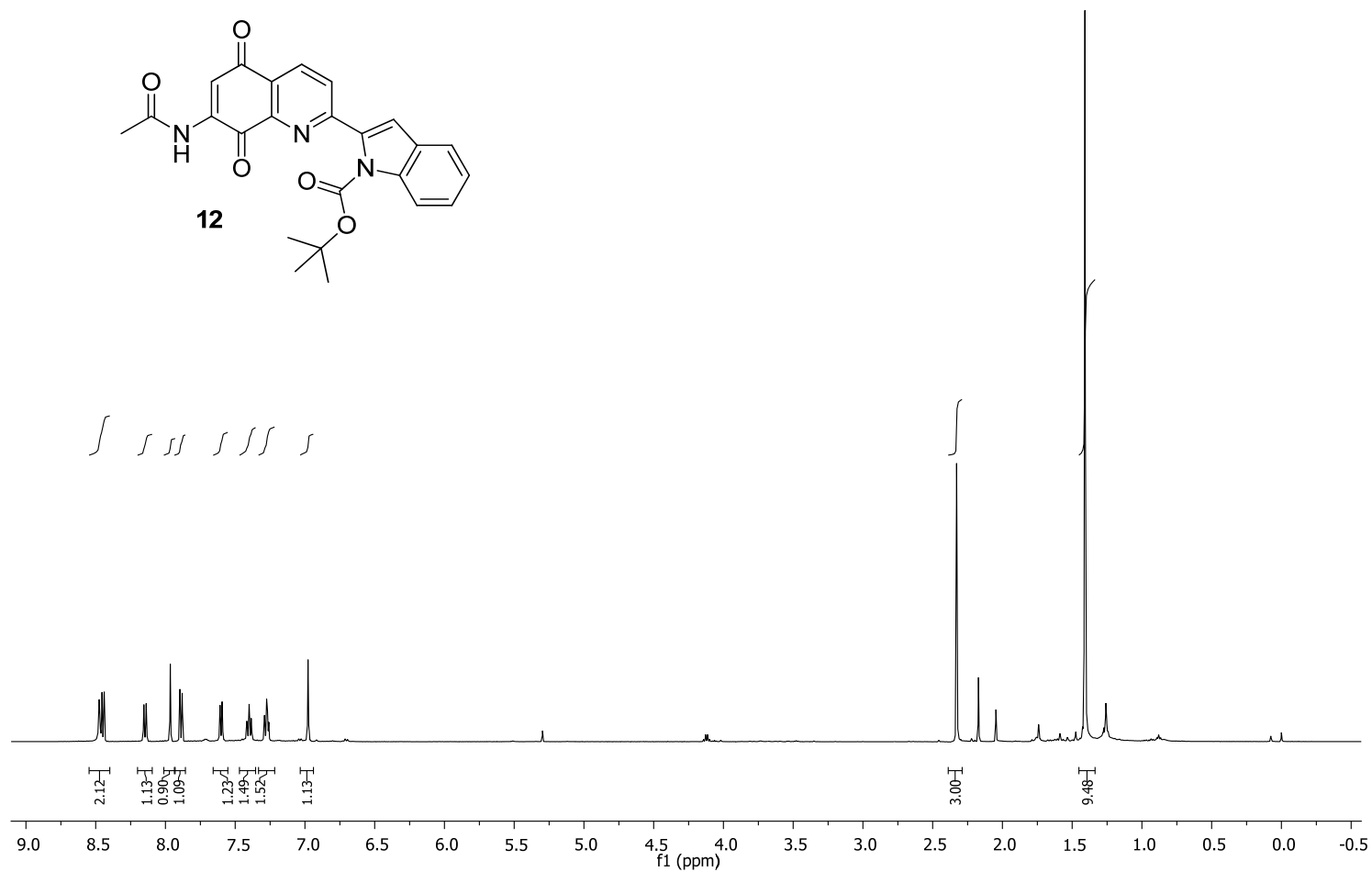


125 MHz ^{13}C -NMR of 7-acetamido-2-(8'-(quinolyl))quinoline-5,8-dione (**11**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

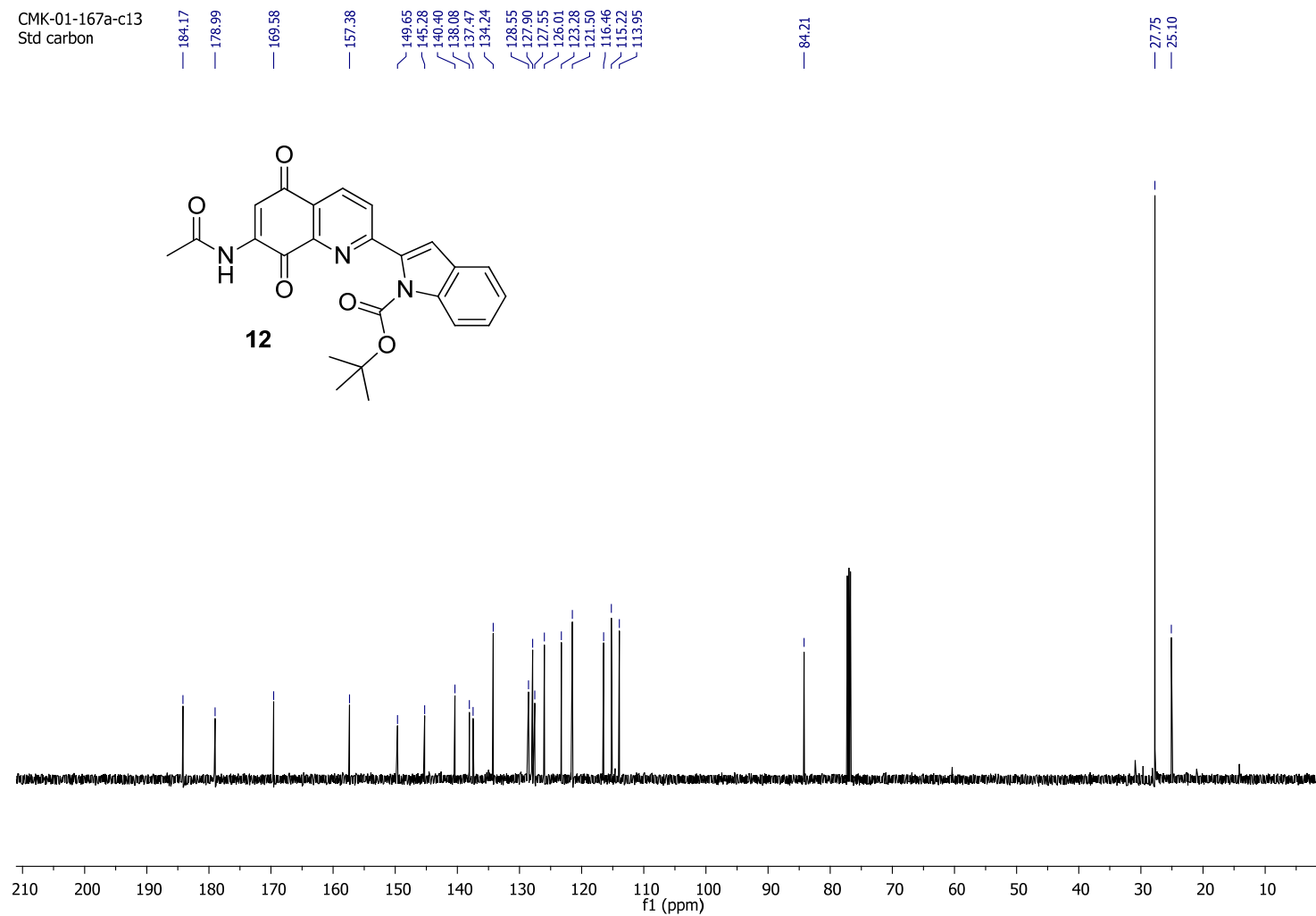


500 MHz ^1H -NMR of 7-acetamido-2-(2-(1-*tert*butoxycarbonylindolyl)quinoline-5,8-dione (**12**)
in CDCl_3

CMK-01-167A-proton
Std proton

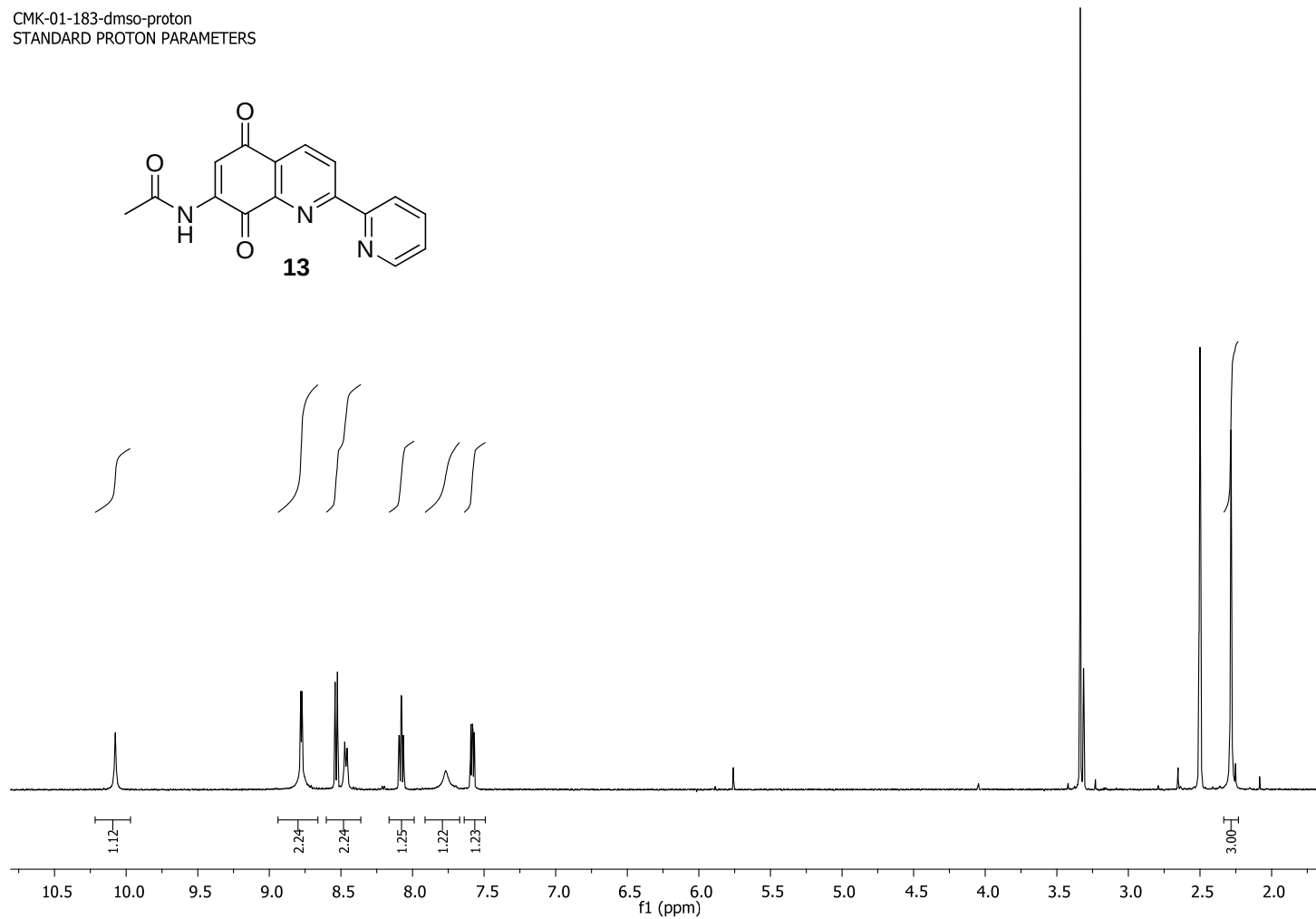


125 MHz ^{13}C -NMR of 7-acetamido-2-(2-(1-*tert*butoxycarbonylindolyl)quinoline-5,8-dione (**12**)
in CDCl_3



500 MHz ^1H -NMR of 7-acetamido-2-(2-(pyridinyl))quinoline-5,8-dione (**13**) in DMSO

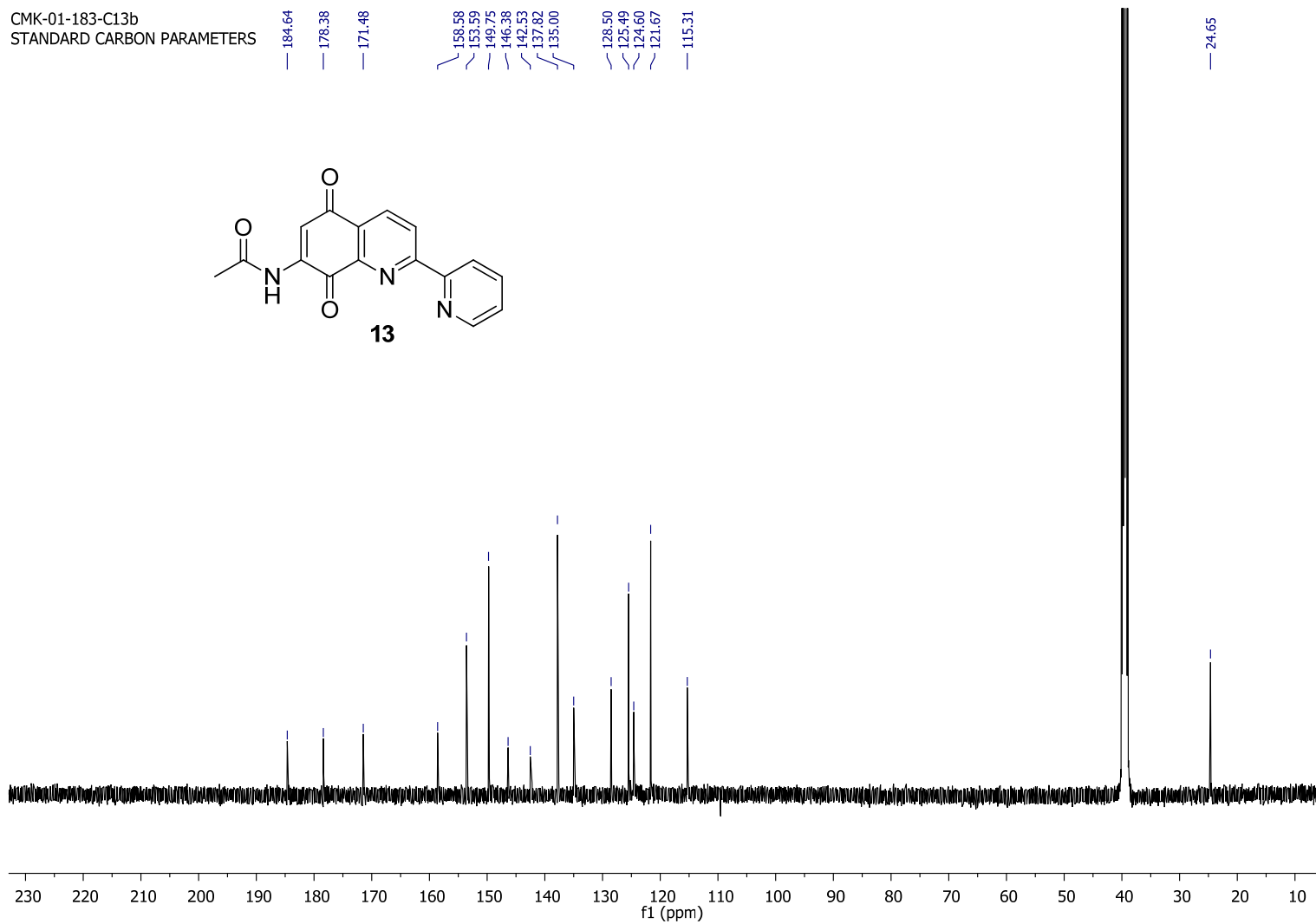
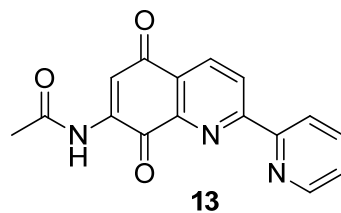
CMK-01-183-dms0-proton
STANDARD PROTON PARAMETERS



125 MHz ^{13}C -NMR of 7-acetamido-2-(2-(pyridinyl))quinoline-5,8-dione (**13**) in DMSO

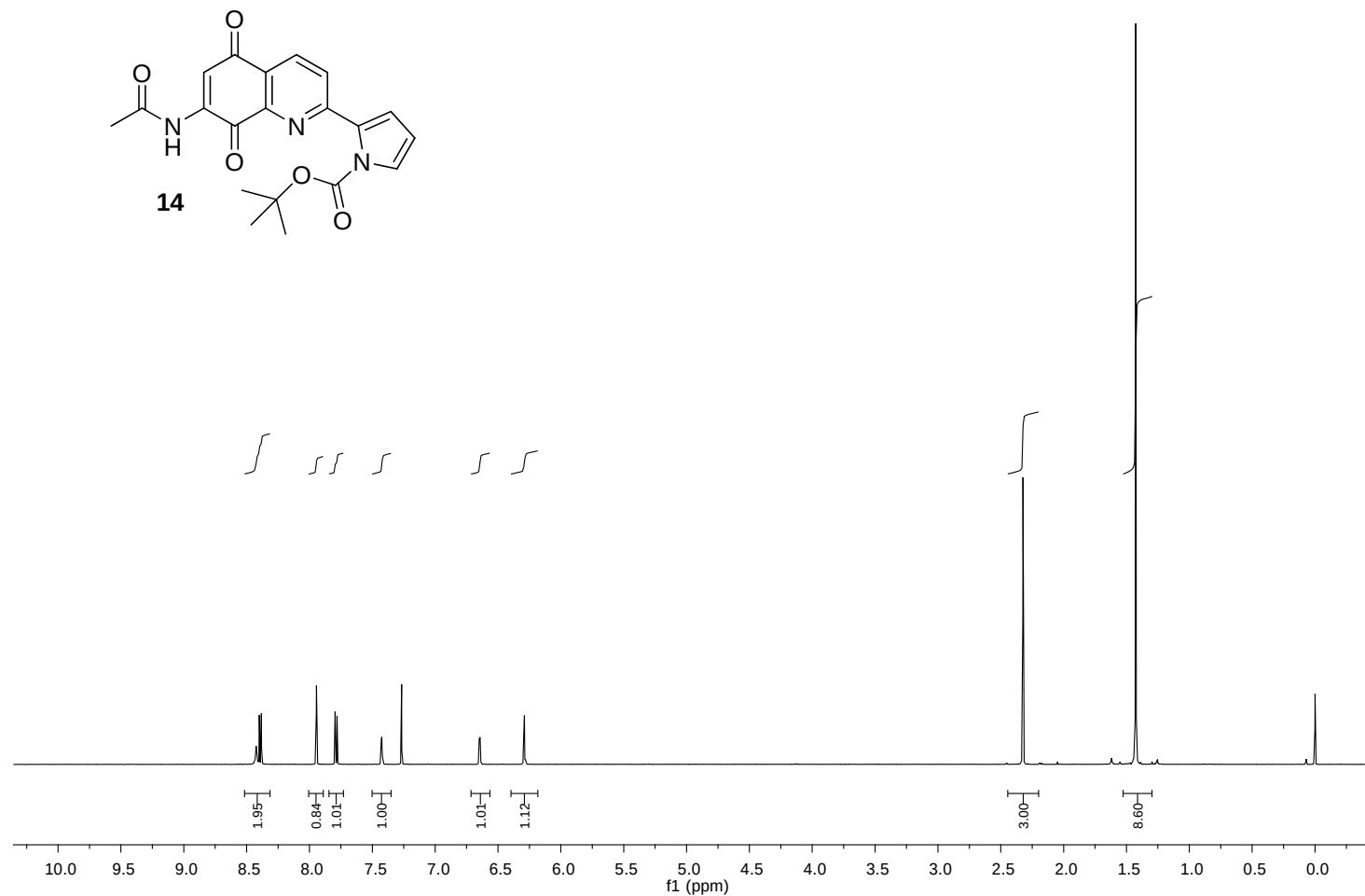
CMK-01-183-C13b
STANDARD CARBON PARAMETERS

184.64
178.38
171.48
158.58
153.59
149.75
146.38
142.53
137.82
135.00
128.50
125.49
124.60
121.67
115.31
24.65



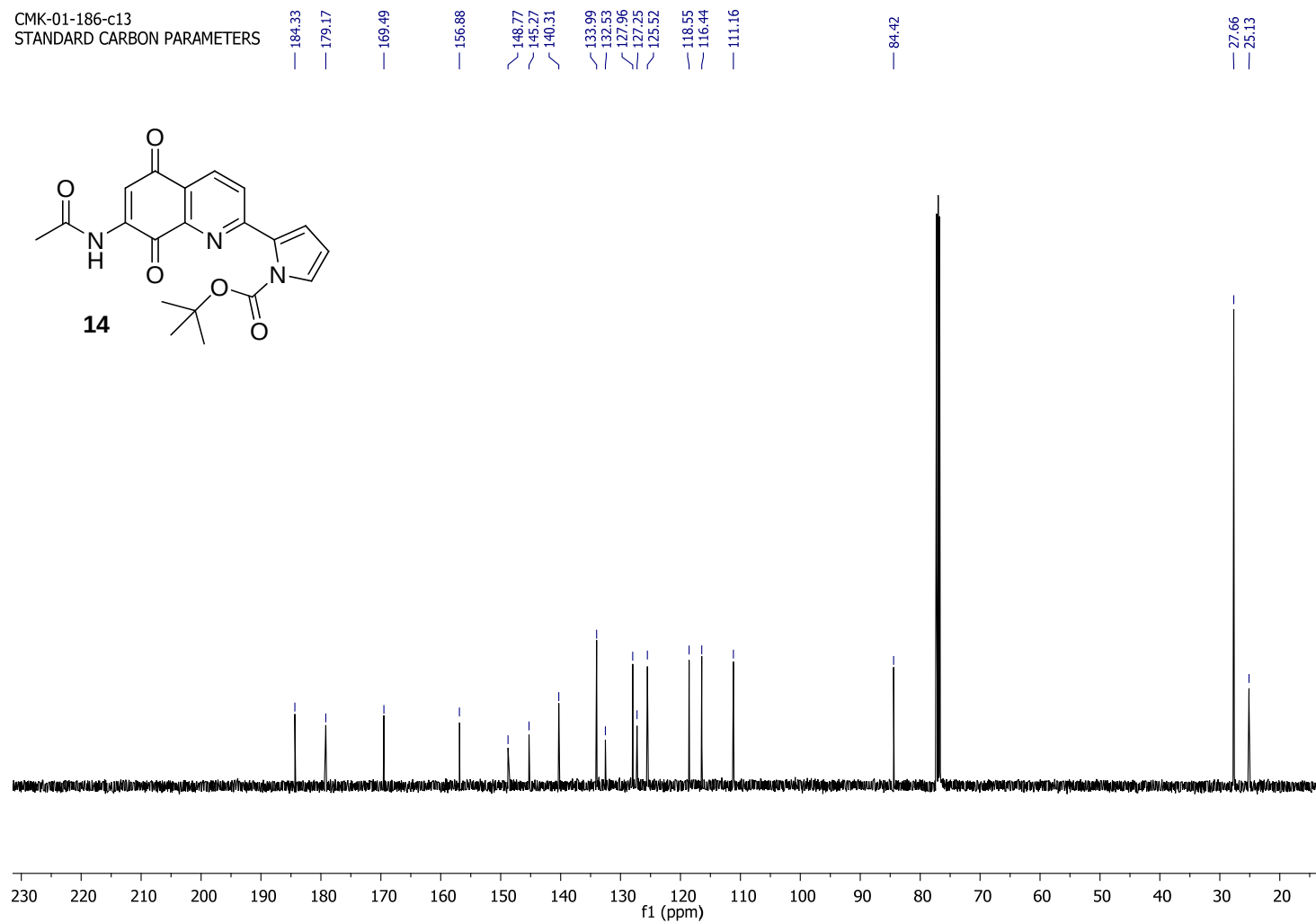
500 MHz ^1H -NMR of 7-acetamido-2-(2-(1-*tert*-butoxypyrrolyl))quinoline-5,8-dione (**14**) in CDCl_3

CMK-01-186-proton
STANDARD PROTON PARAMETERS



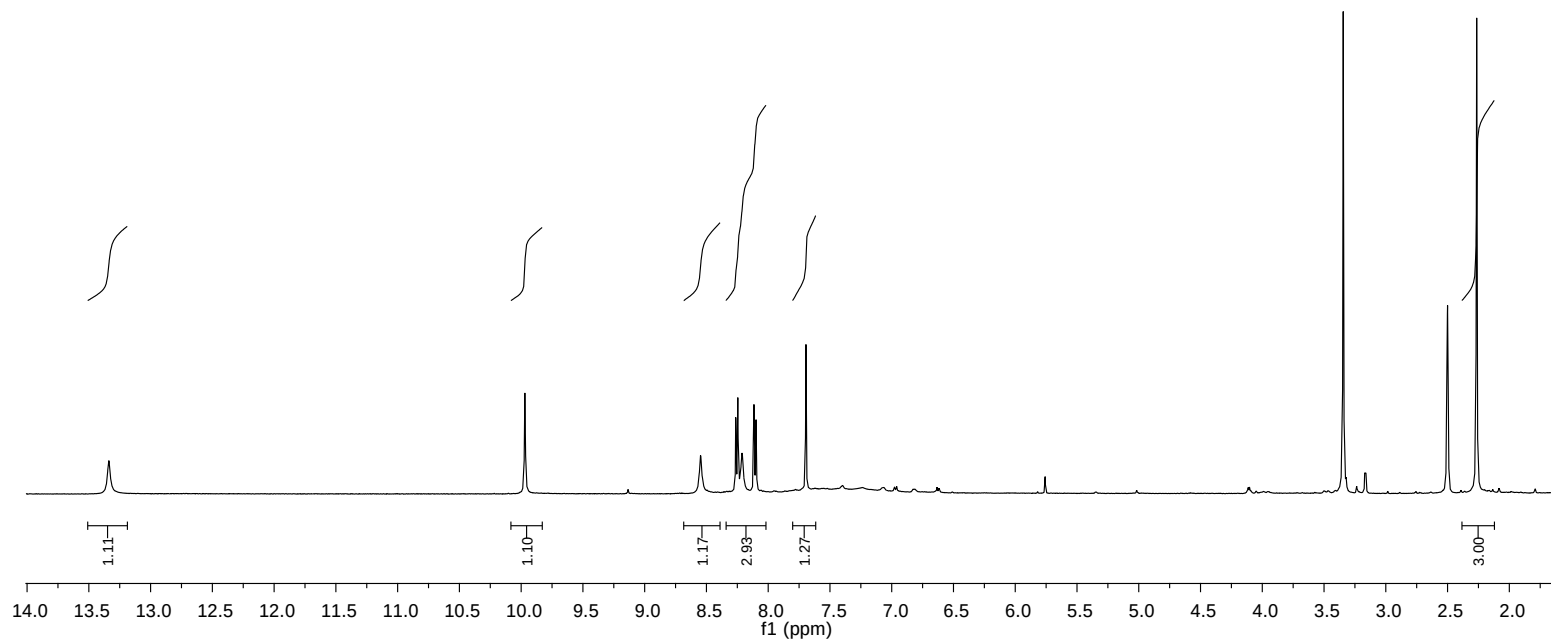
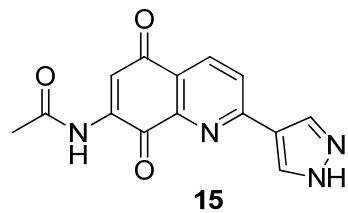
125 MHz ^{13}C -NMR of 7-acetamido-2-(2-(1-*tert*-butoxypyrrolyl))quinoline-5,8-dione (**14**) in CDCl_3

CMK-01-186-c13
STANDARD CARBON PARAMETERS



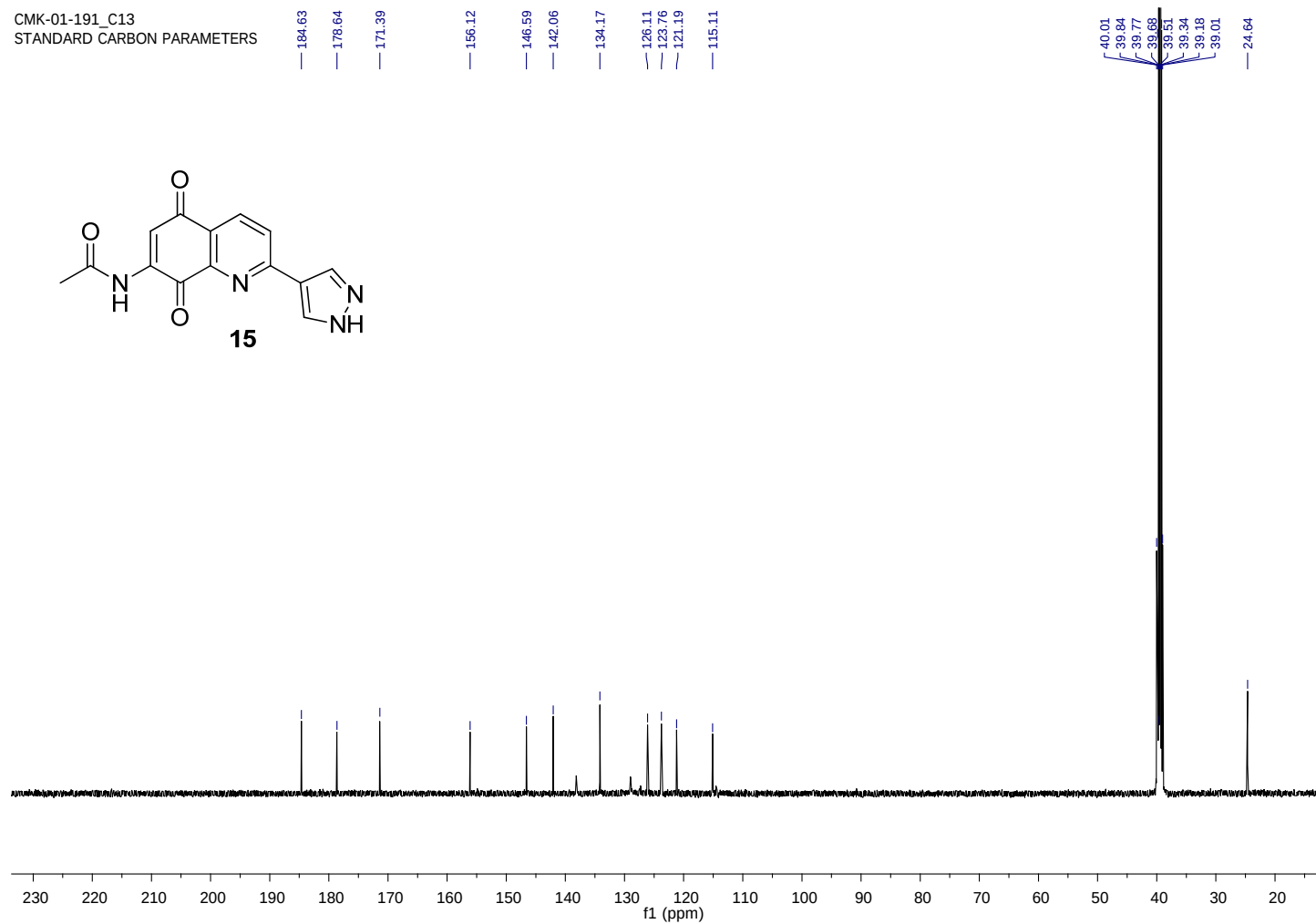
500 MHz ^1H -NMR of 7-acetamido-2-(4-pyrazolyl)quinoline-5,8-dione (**15**) in DMSO

CMK-01-191-proton2
STANDARD PROTON PARAMETERS



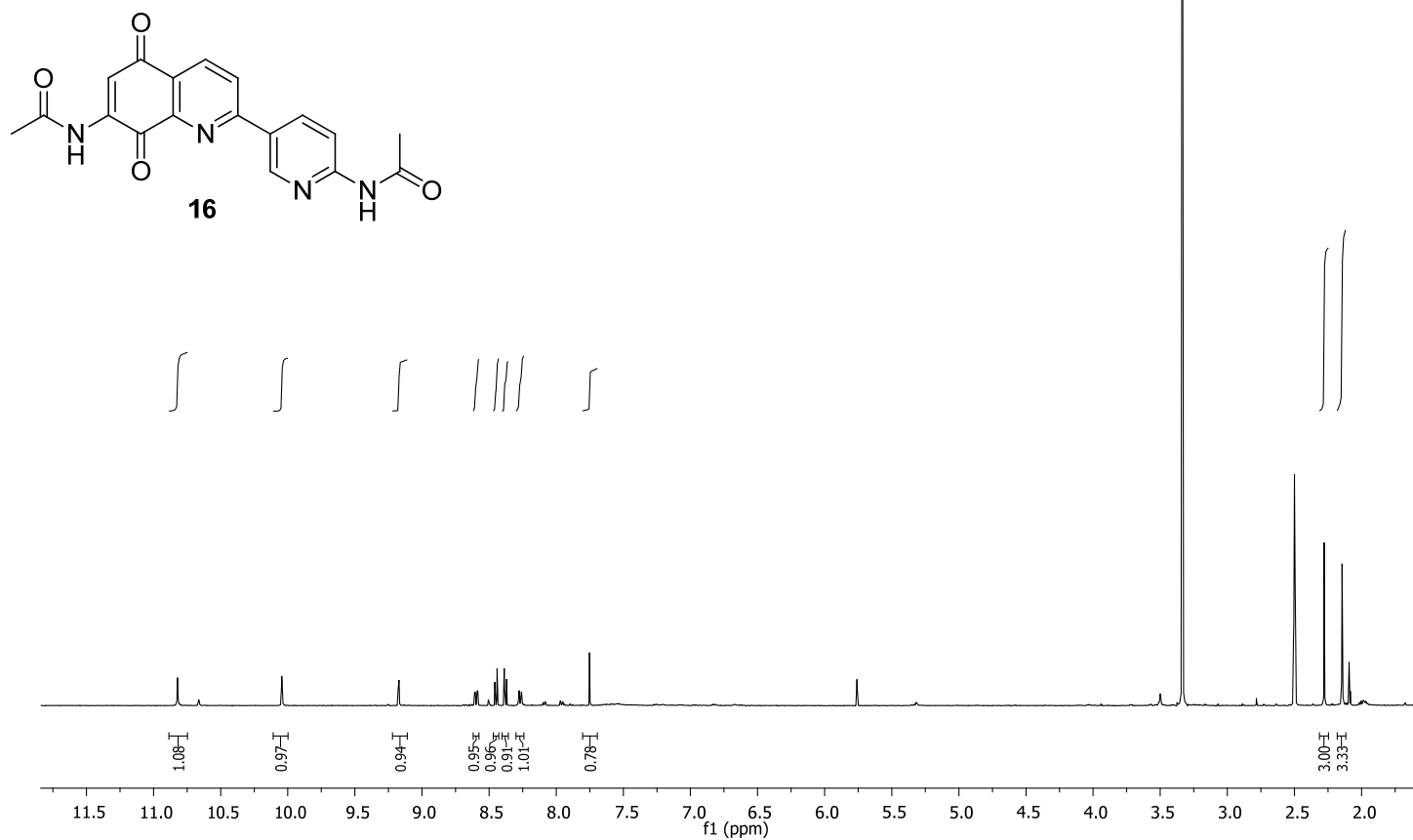
125 MHz ^{13}C -NMR of 7-acetamido-2-(4-pyrazolyl)quinoline-5,8-dione (**15**) in DMSO

CMK-01-191_C13
STANDARD CARBON PARAMETERS



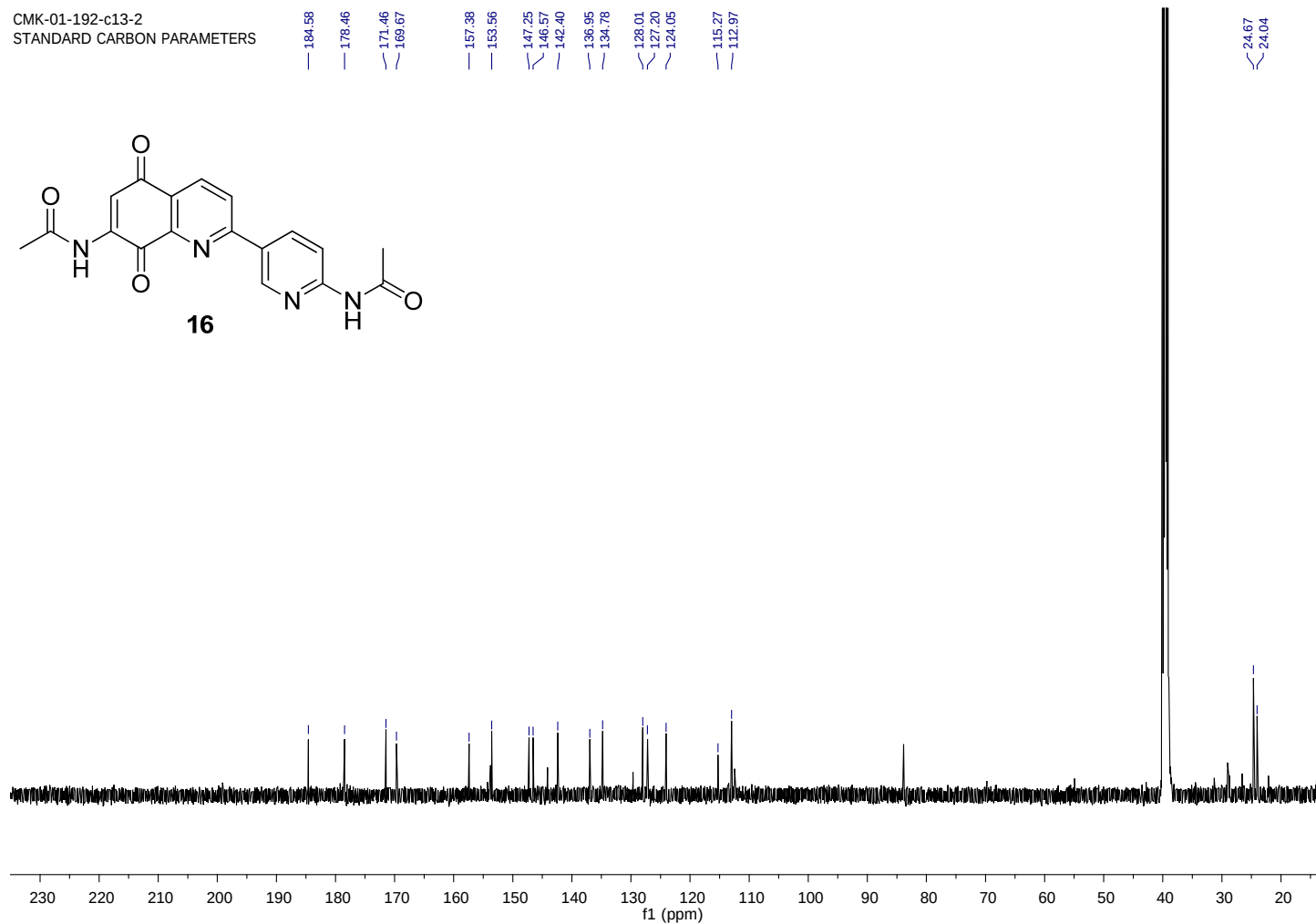
500 MHz ^1H -NMR of 7-acetamido-2-(3-(2-acetamidopyridinyl))quinoline-5,8-dione (**16**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-192-proton
STANDARD PROTON PARAMETERS



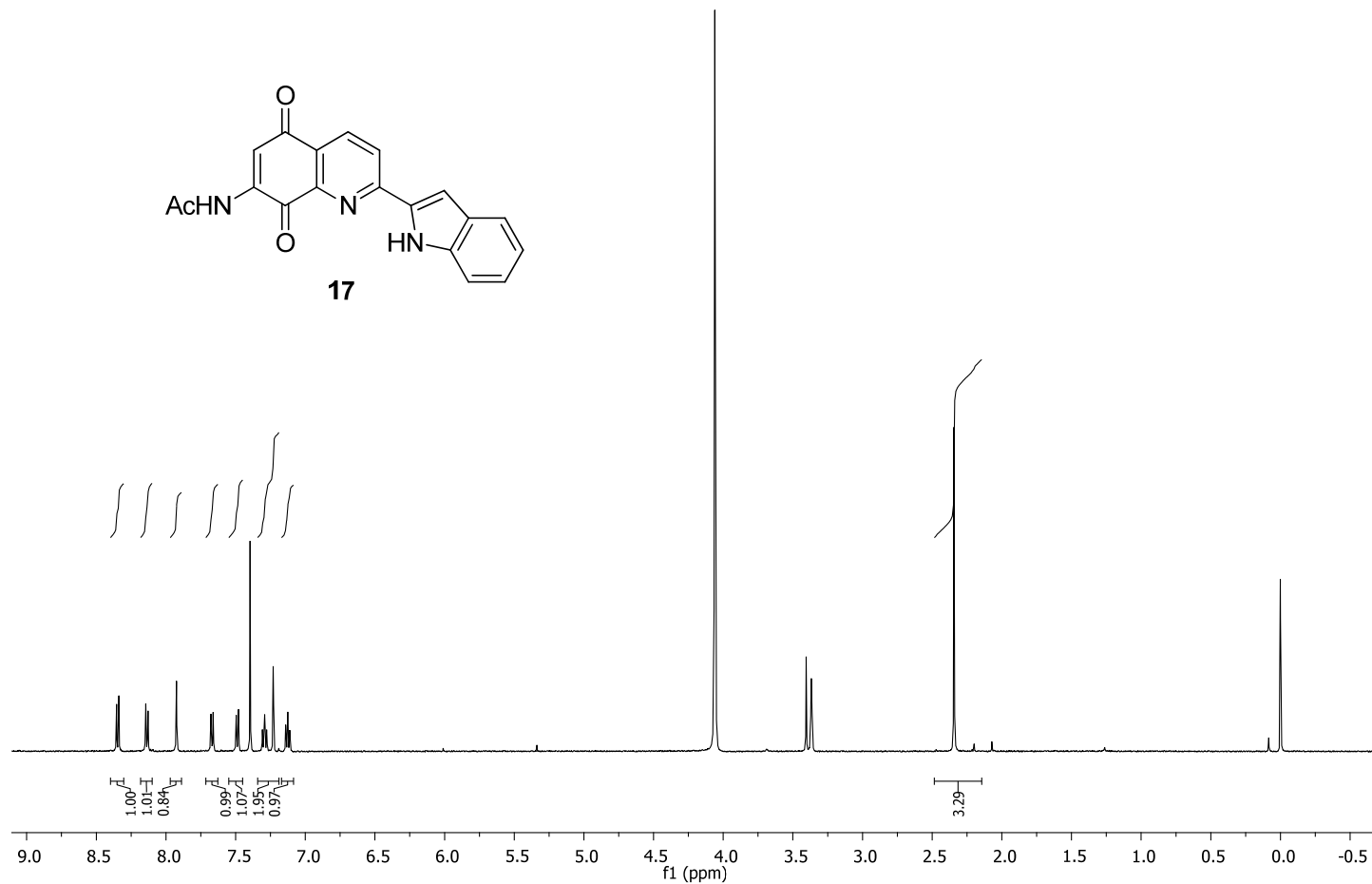
125 MHz ^{13}C -NMR of 7-acetamido-2-(3-(2-acetamidopyridinyl))quinoline-5,8-dione (**16**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-192-c13-2
STANDARD CARBON PARAMETERS

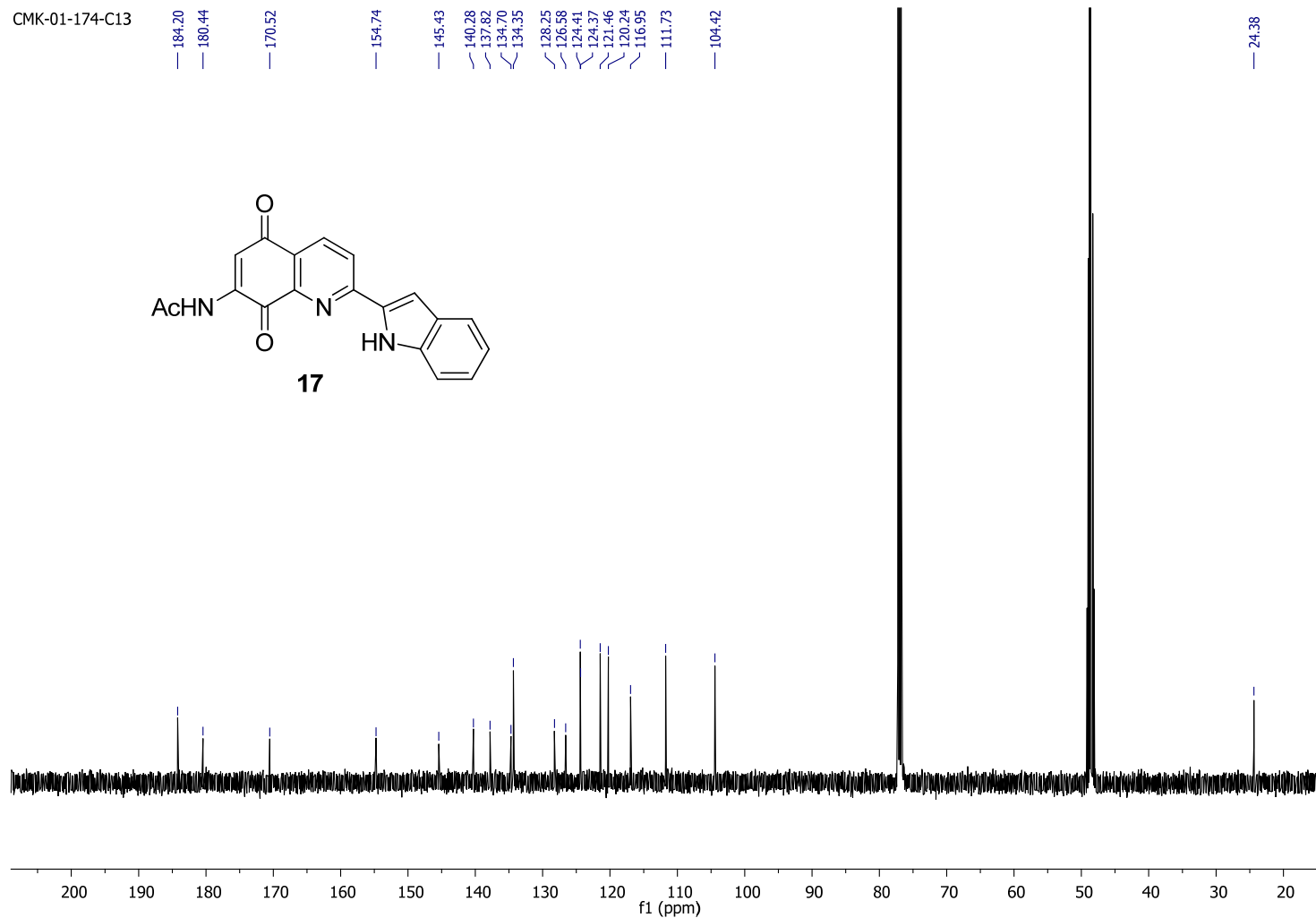


500 MHz ^1H -NMR of 7-acetamido-2-(2-(indolyl))quinoline-5,8-dione (**17**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-174-proton
STANDARD PROTON PARAMETERS

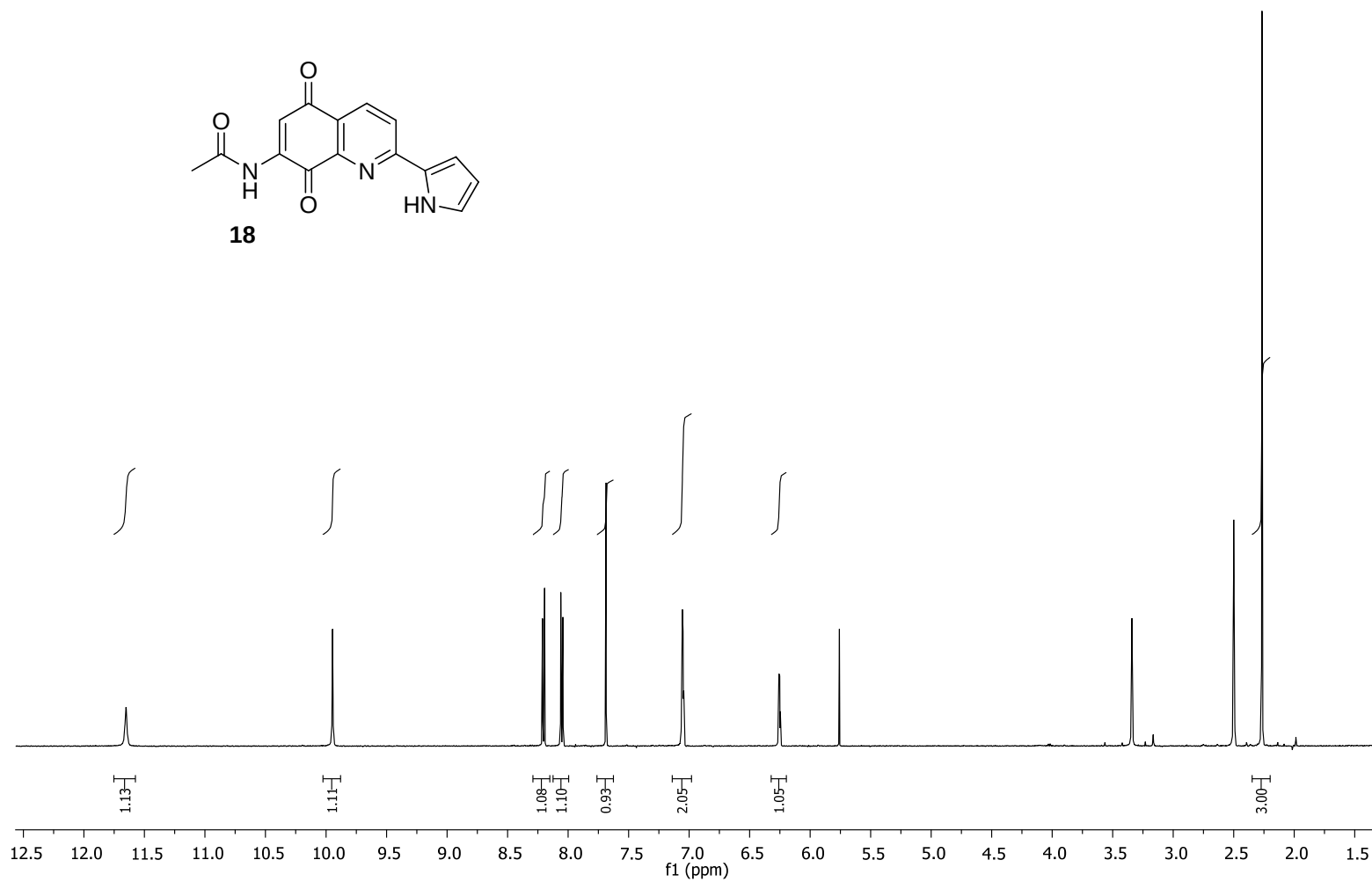
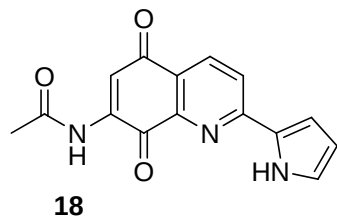


125 MHz ^{13}C -NMR of 7-acetamido-2-(2-(indolyl))quinoline-5,8-dione (**17**) in CDCl_3



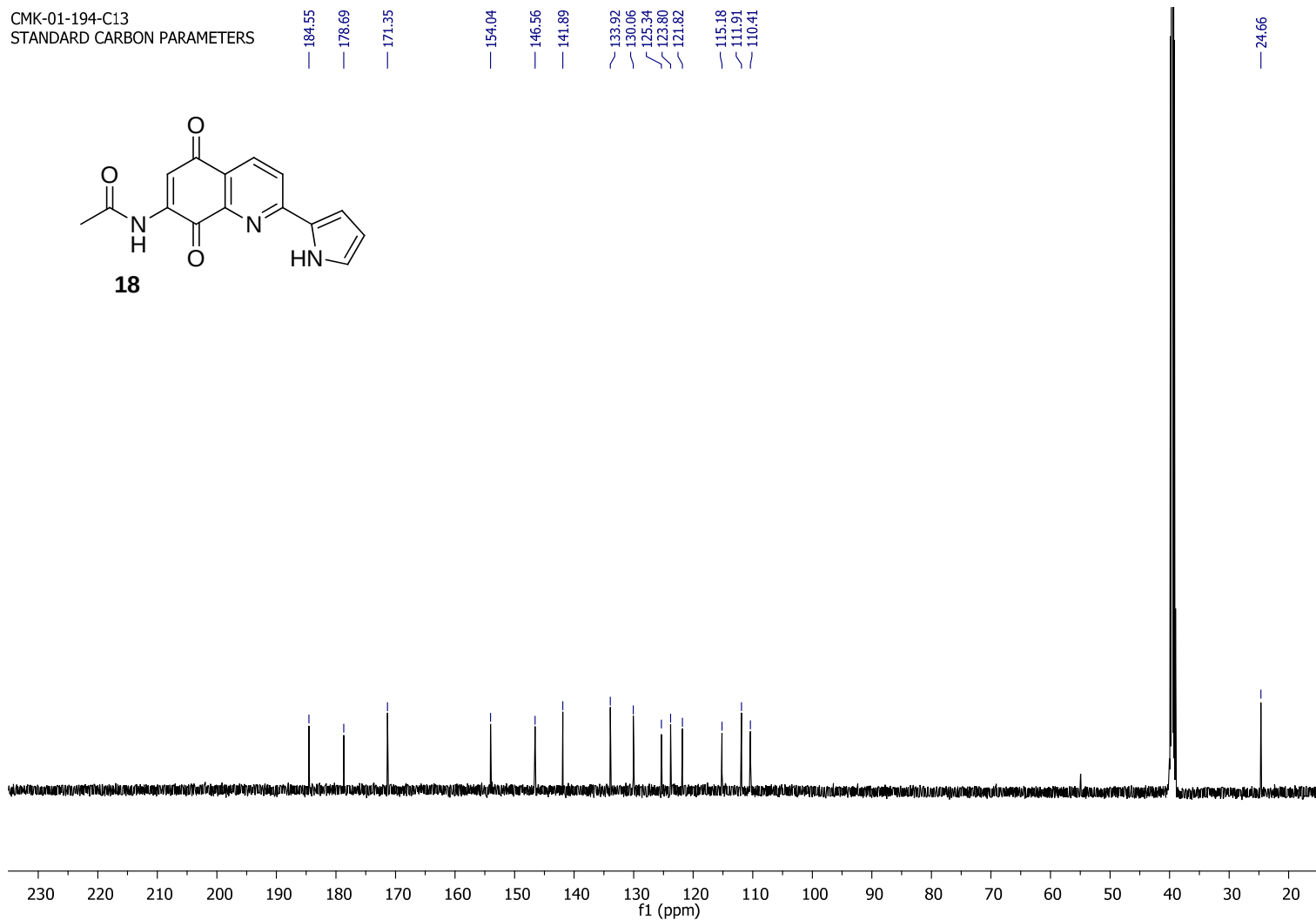
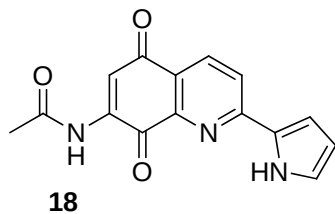
500 MHz ^1H -NMR of 7-acetamido-2-(2-(pyrrolyl))quinoline-5,8-dione (**18**) in DMSO

CMK-01-194-dms0-proton
STANDARD PROTON PARAMETERS



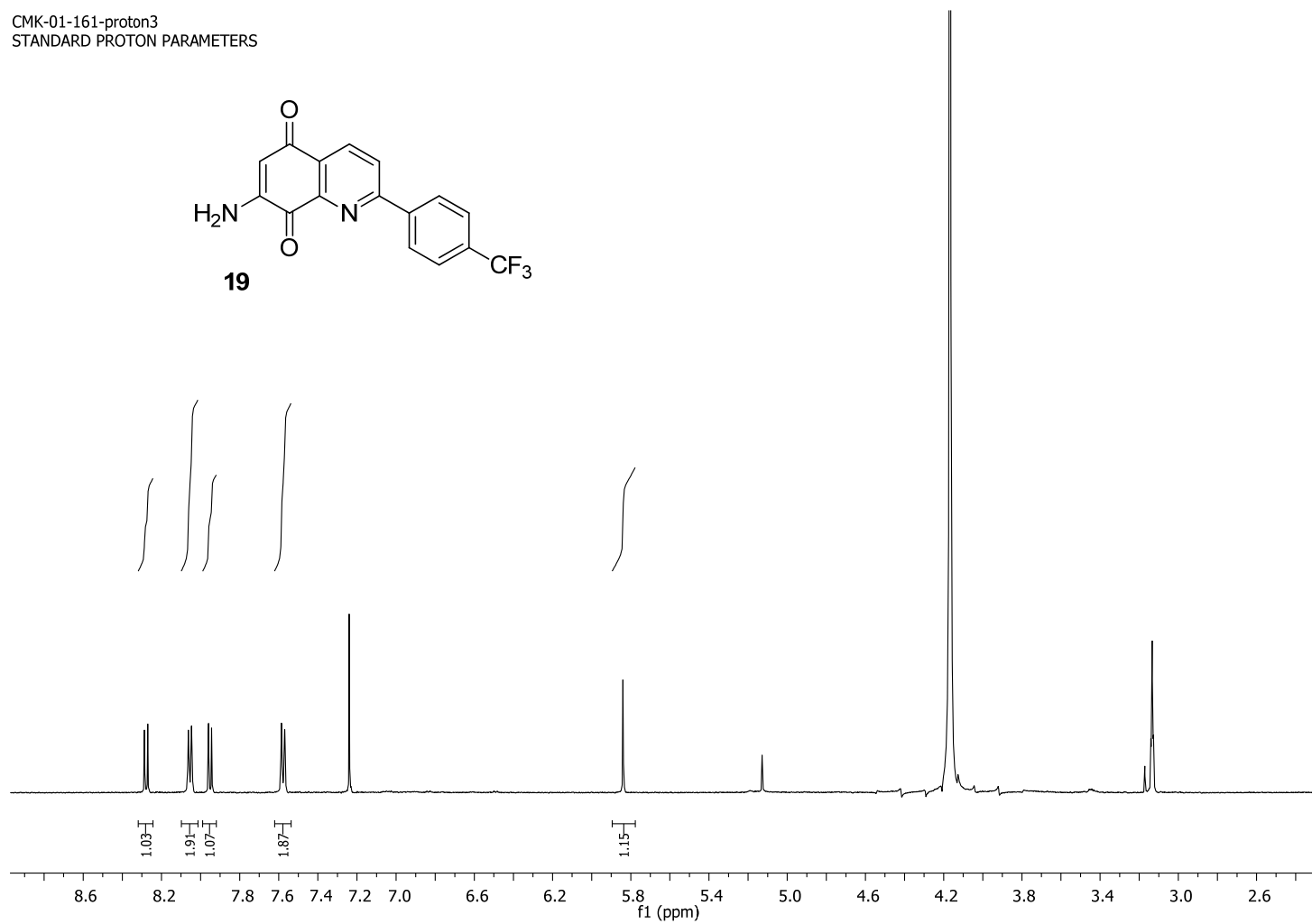
125 MHz ^{13}C -NMR of 7-acetamido-2-(2-(pyrrolyl))quinoline-5,8-dione (**18**) in DMSO

CMK-01-194-C13
STANDARD CARBON PARAMETERS



500 MHz ^1H -NMR of 7-amino-2-(4-trifluorophenyl)quinoline-5,8-dione (**19**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-161-proton3
STANDARD PROTON PARAMETERS



125 MHz ^{13}C -NMR of 7-amino-2-(4-trifluorophenyl)quinoline-5,8-dione (**19**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-161-C13-2
STANDARD CARBON PARAMETERS

— 182.23
— 180.05

— 158.69

— 150.33

— 146.32

— 140.61

— 135.08

— 129.44

— 127.65

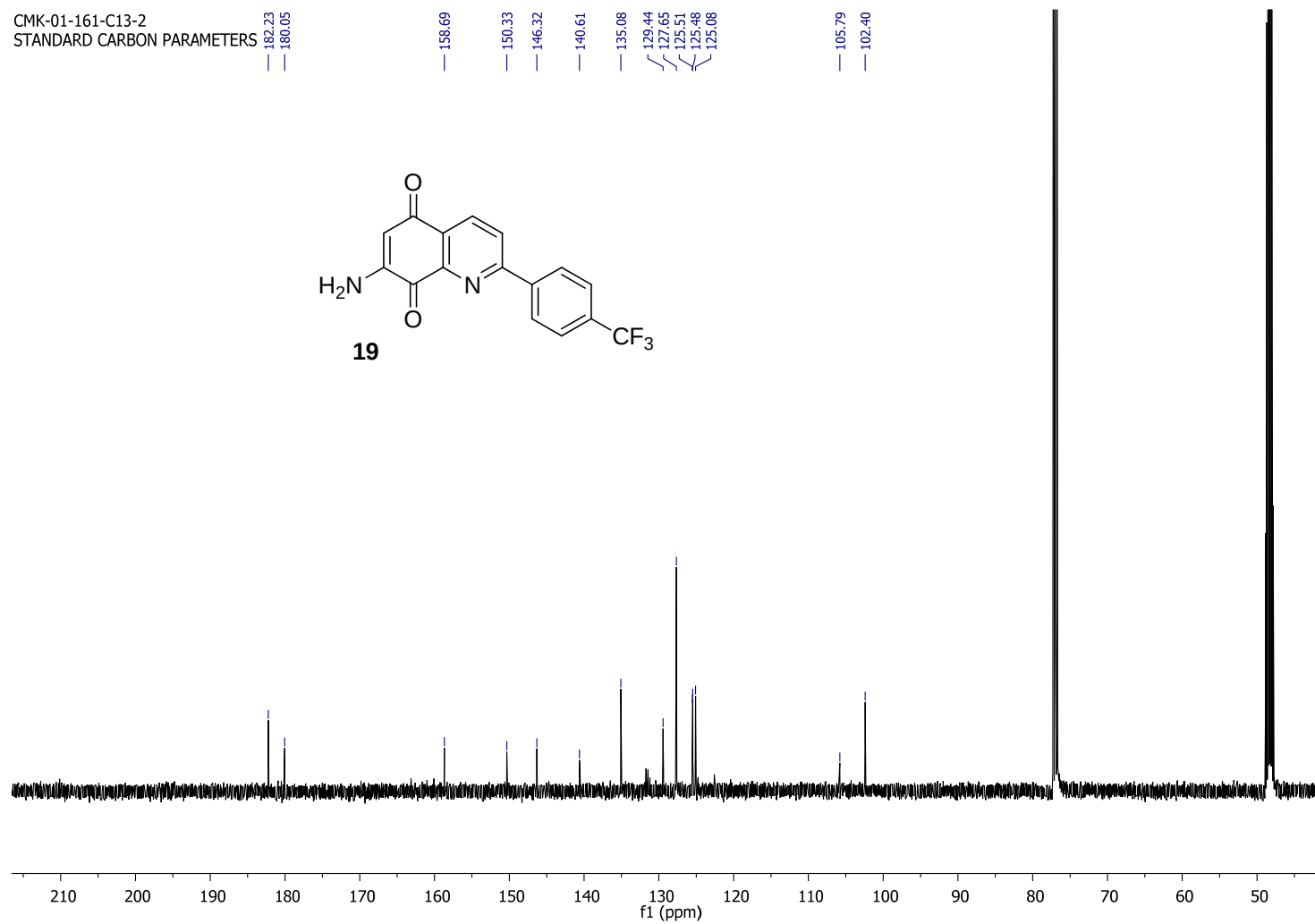
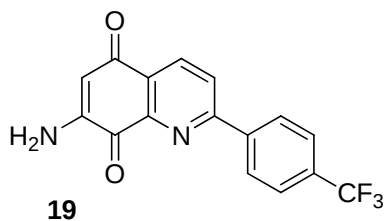
— 125.51

— 125.48

— 125.08

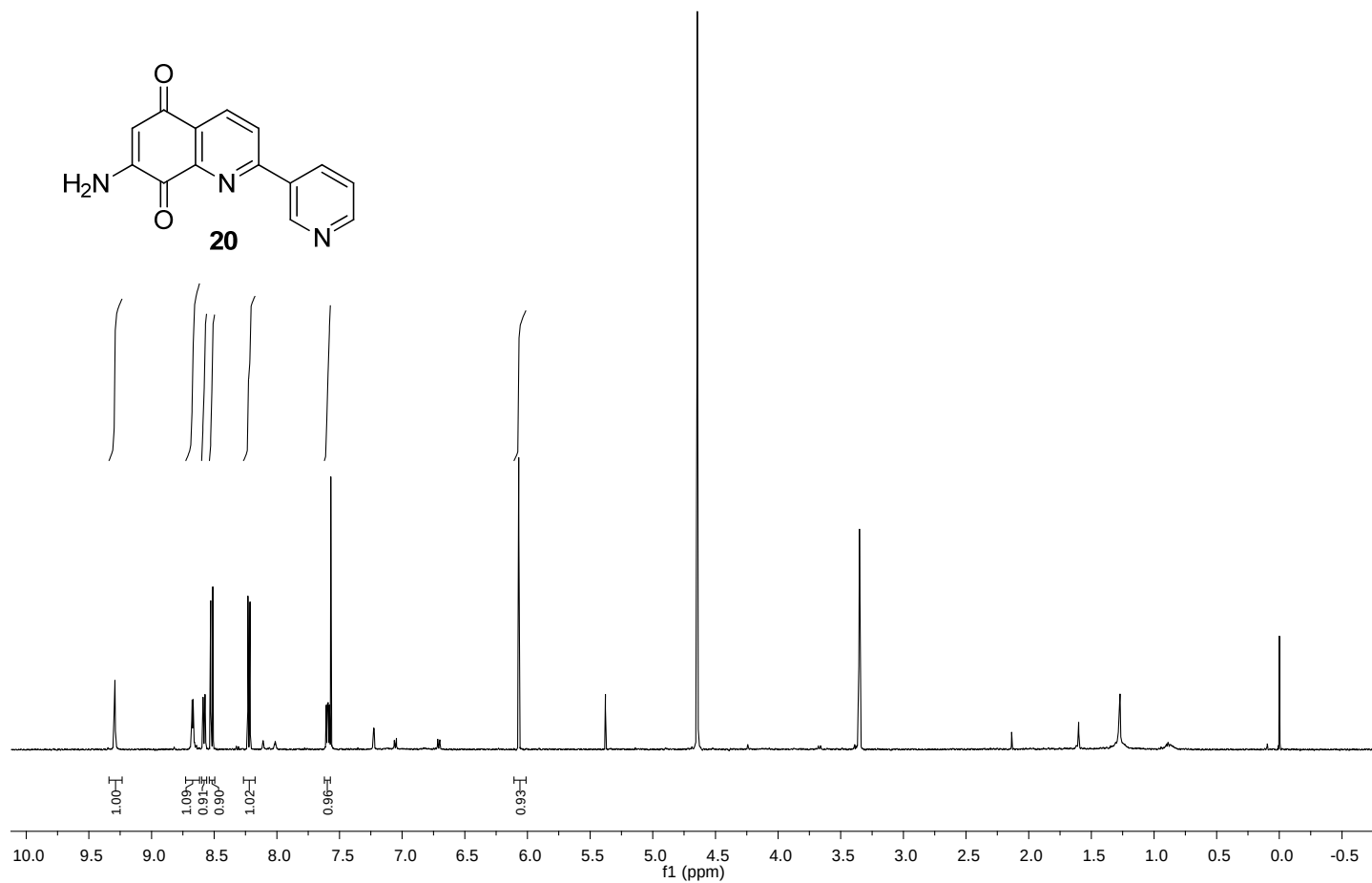
— 105.79

— 102.40



500 MHz ^1H -NMR of 7-amino-2-(3-pyridinyl)quinoline-5,8-dione (**20**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-168-a2-proton
STANDARD PROTON PARAMETERS



125 MHz ^{13}C -NMR of 7-amino-2-(3-pyridinyl)quinoline-5,8-dione (**20**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-168-a2-c13
STANDARD CARBON PARAMETERS

181.91
179.84

157.04

150.44

149.62

147.58

146.34

135.44

135.00

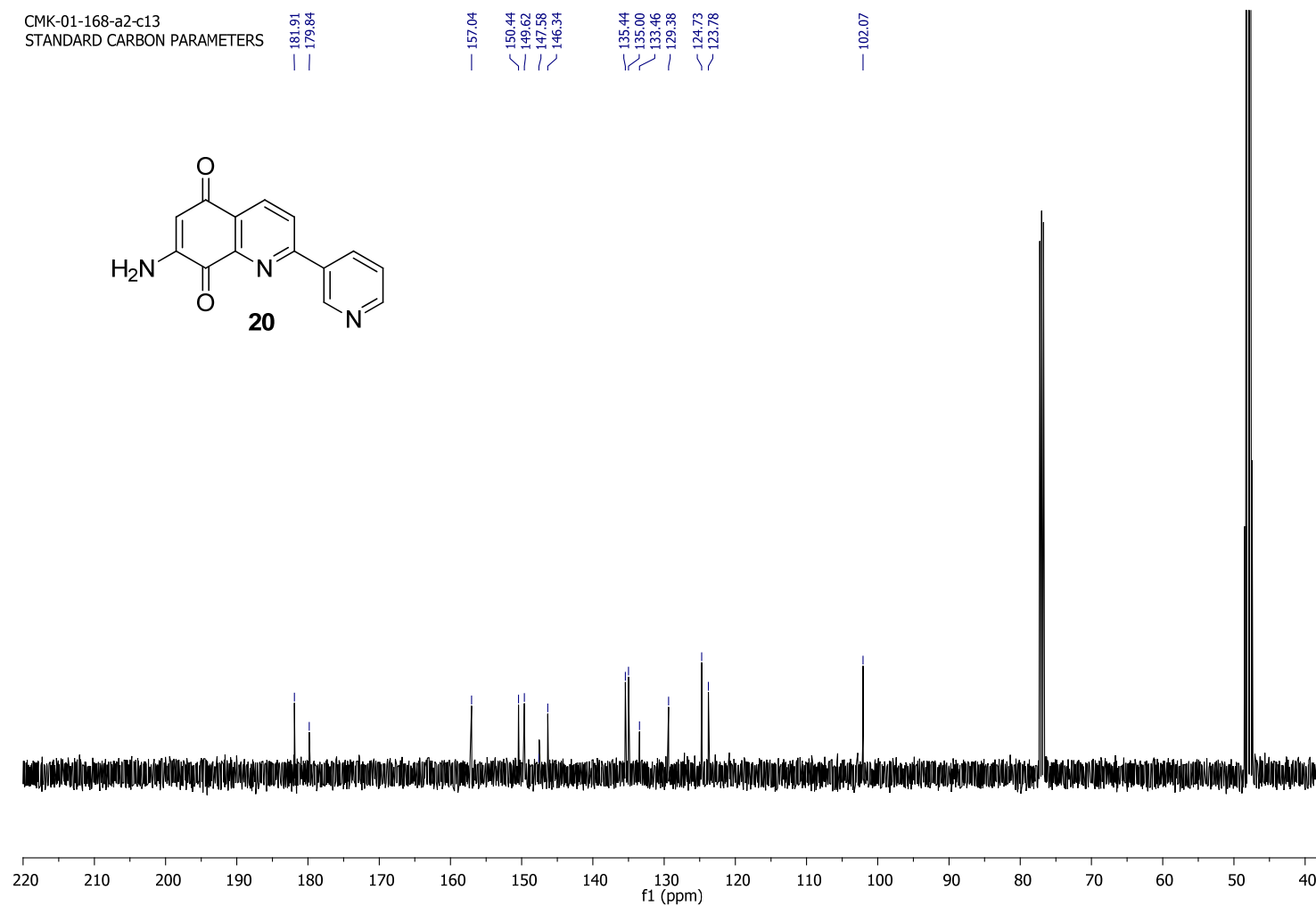
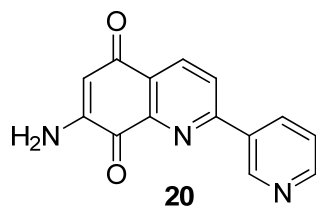
133.46

129.38

124.73

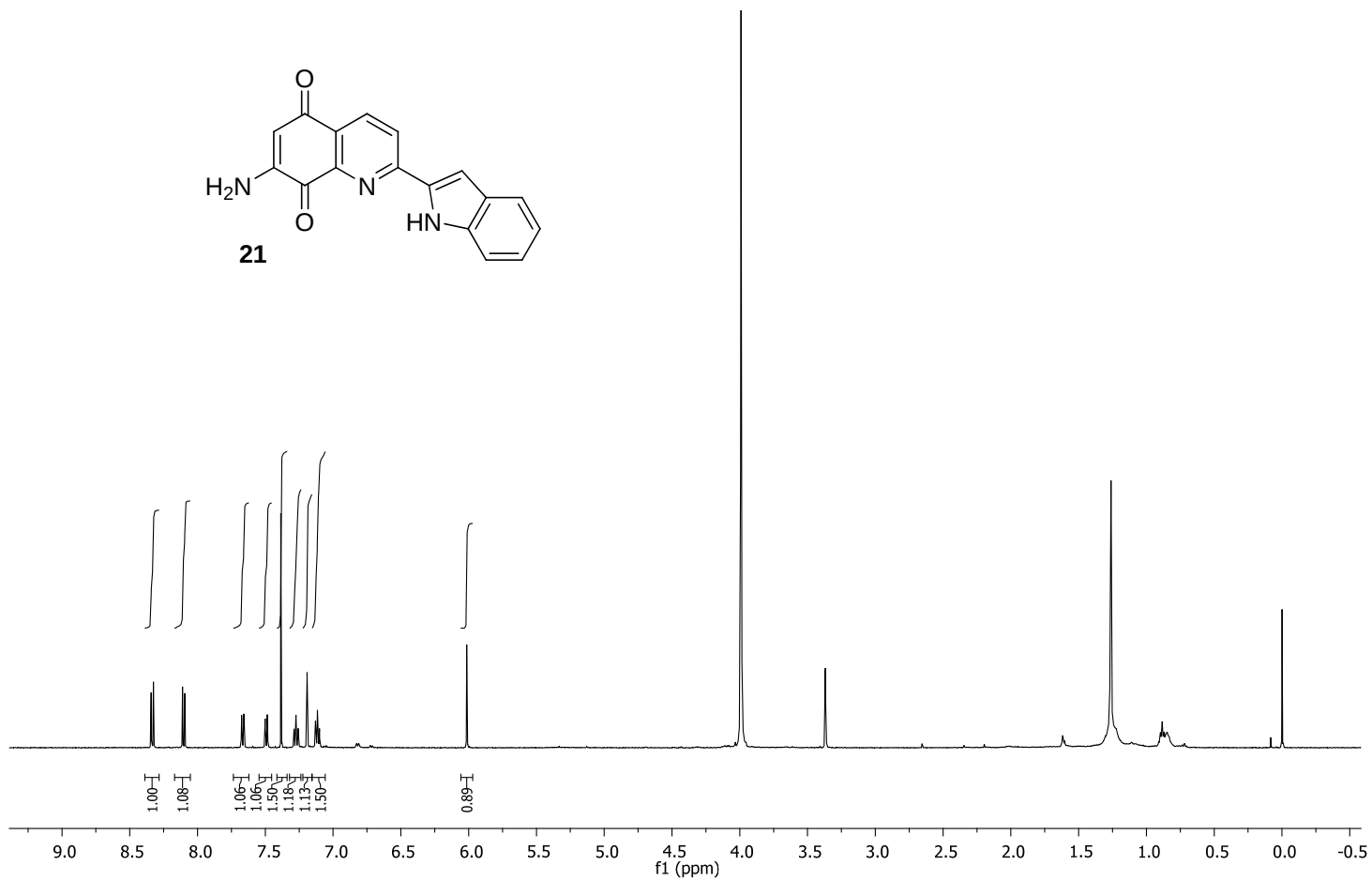
123.78

102.07



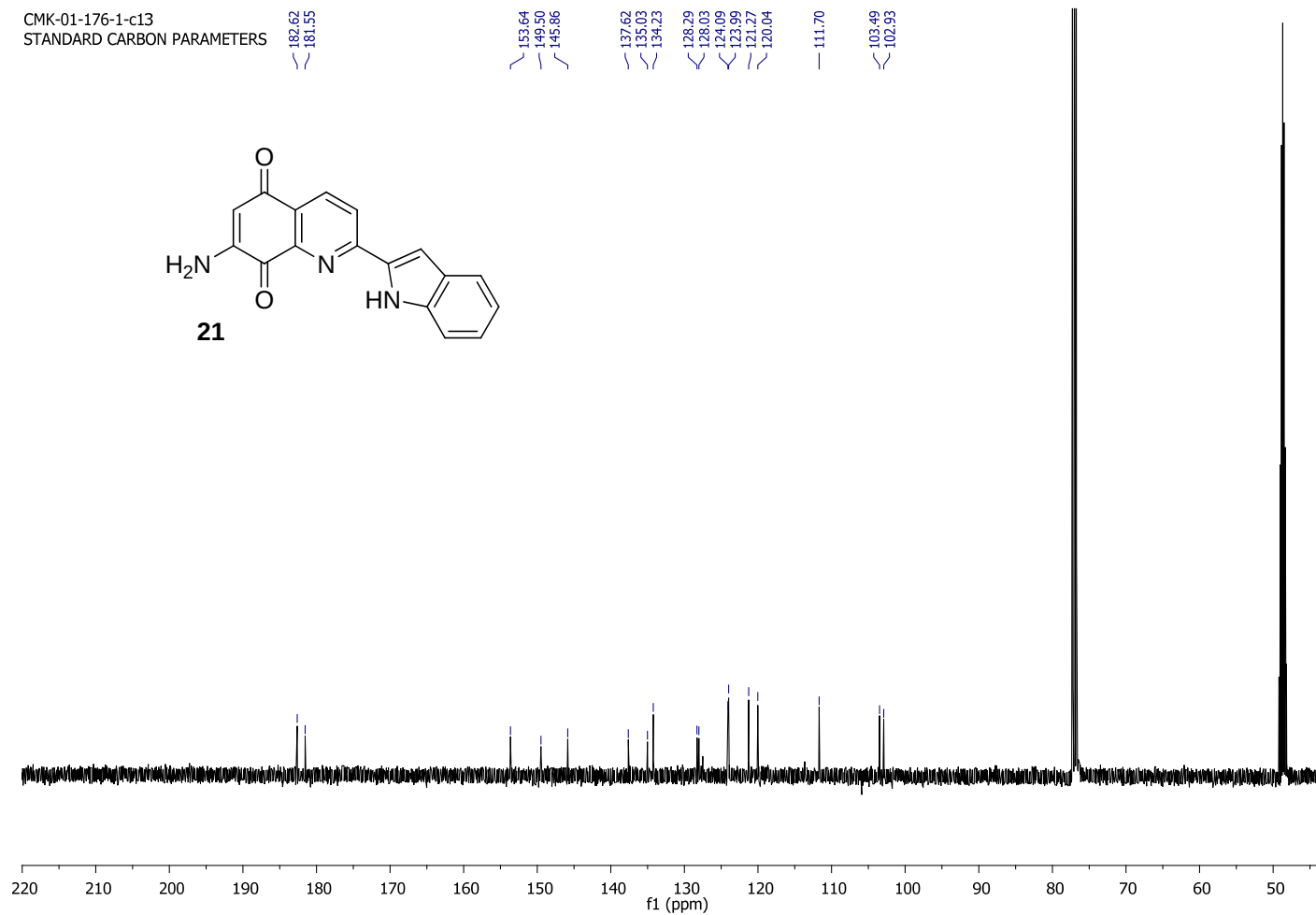
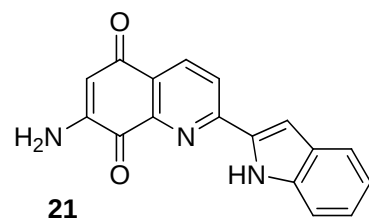
500 MHz ^1H -NMR of 7-amino-2-(2-indolyl)quinoline-5,8-dione (**21**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-176-1-proton1
STANDARD PROTON PARAMETERS



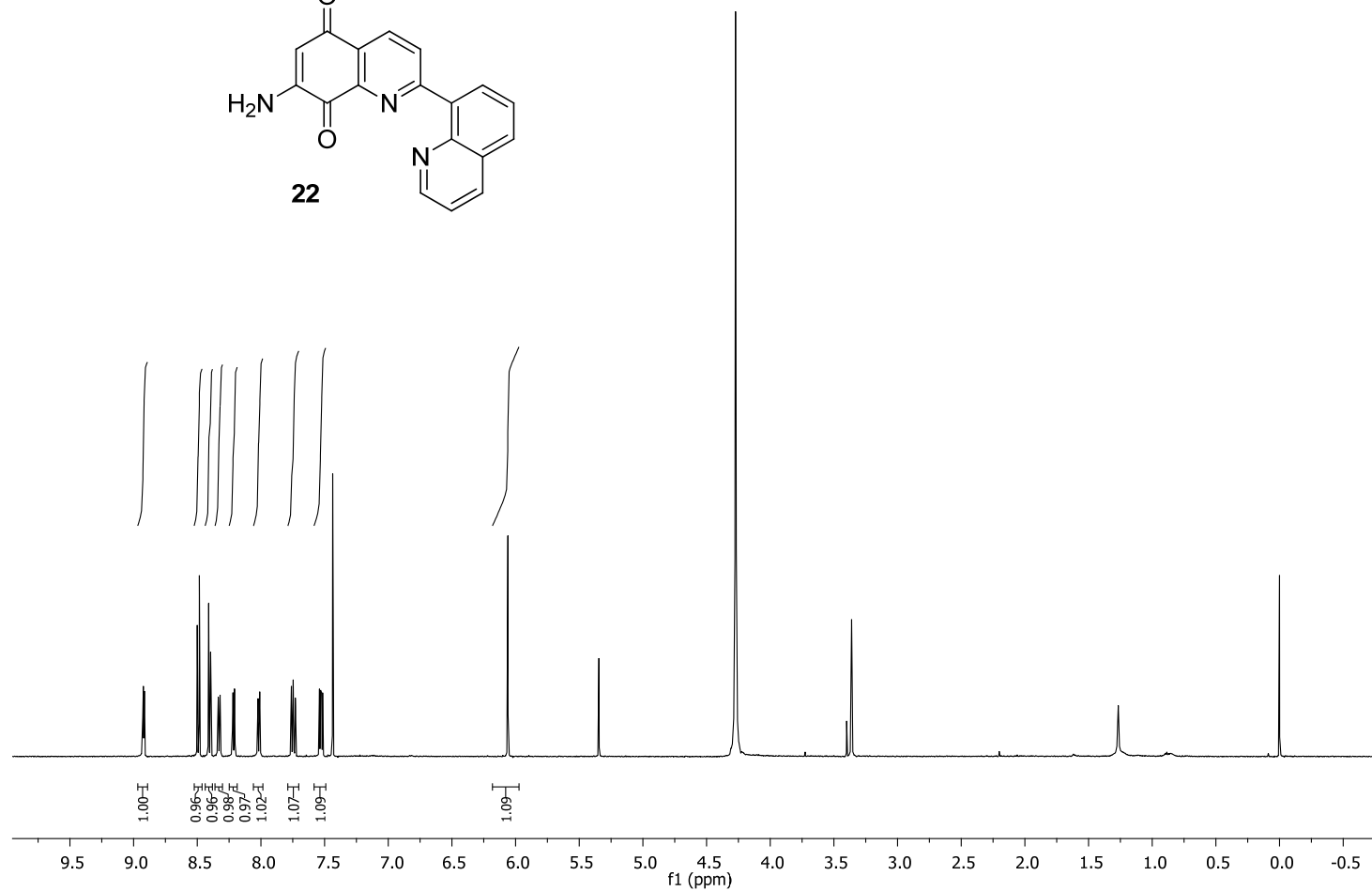
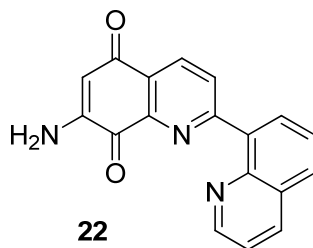
125 MHz ^{13}C -NMR of 7-amino-2-(2-indolyl)quinoline-5,8-dione (**21**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-176-1-c13
STANDARD CARBON PARAMETERS



500 MHz ^1H -NMR of 7-amino-2-(8'-quinolyl)quinoline-5,8-dione (**22**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-187-meoh-proton
STANDARD PROTON PARAMETERS



125 MHz ^{13}C -NMR of 7-amino-2-(8'-quinolyl)quinoline-5,8-dione (**22**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-187-c13
STANDARD CARBON PARAMETERS

— 182.79
— 180.13

— 160.45

— 150.27

— 150.21

— 146.23

— 145.17

— 136.70

— 136.65

— 133.15

— 131.64

— 131.47

— 129.79

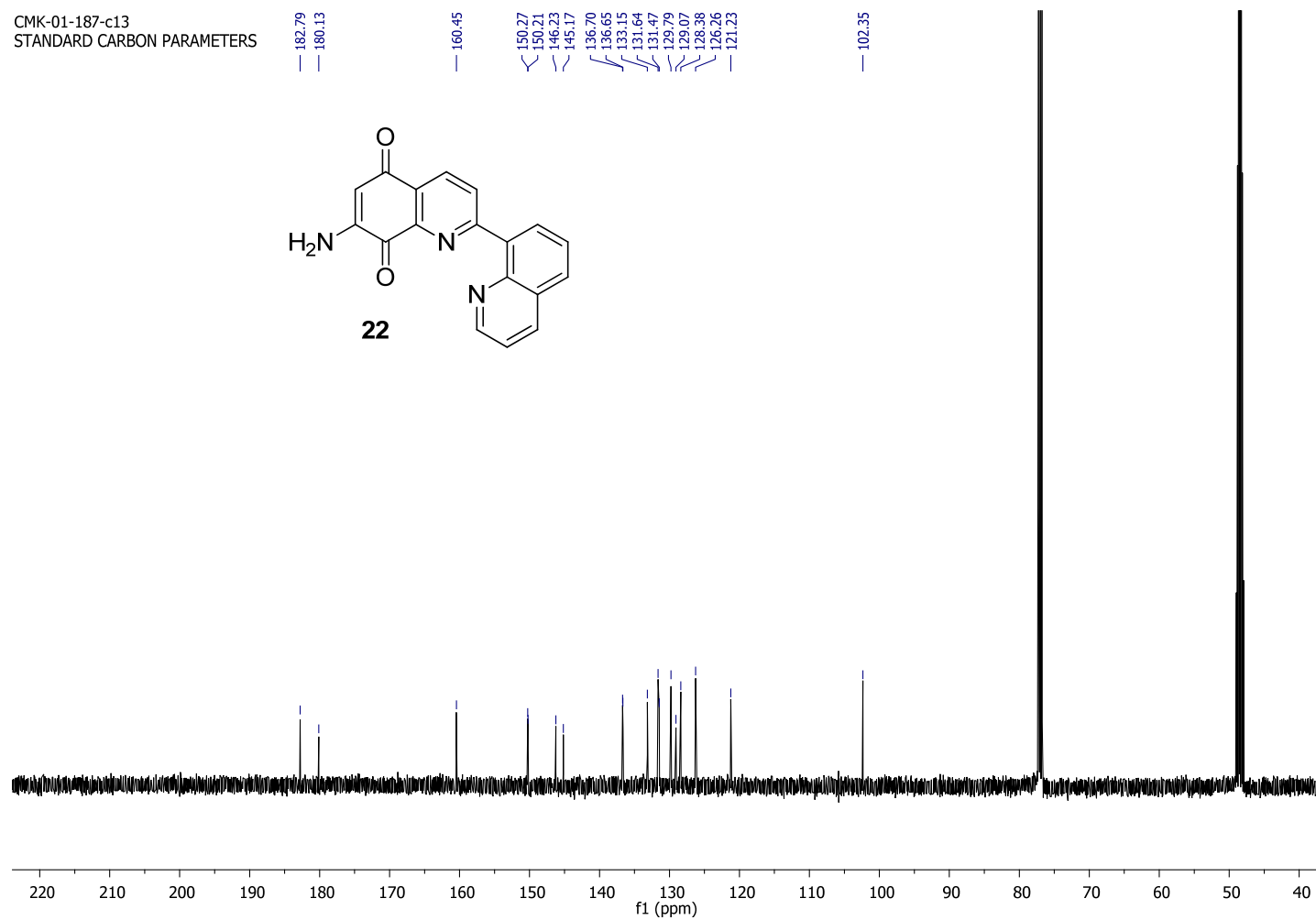
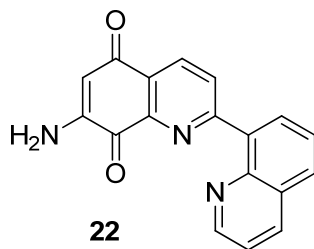
— 129.07

— 128.38

— 126.26

— 121.23

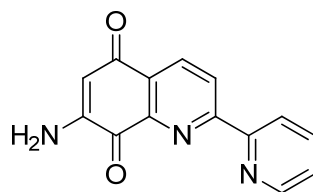
— 102.35



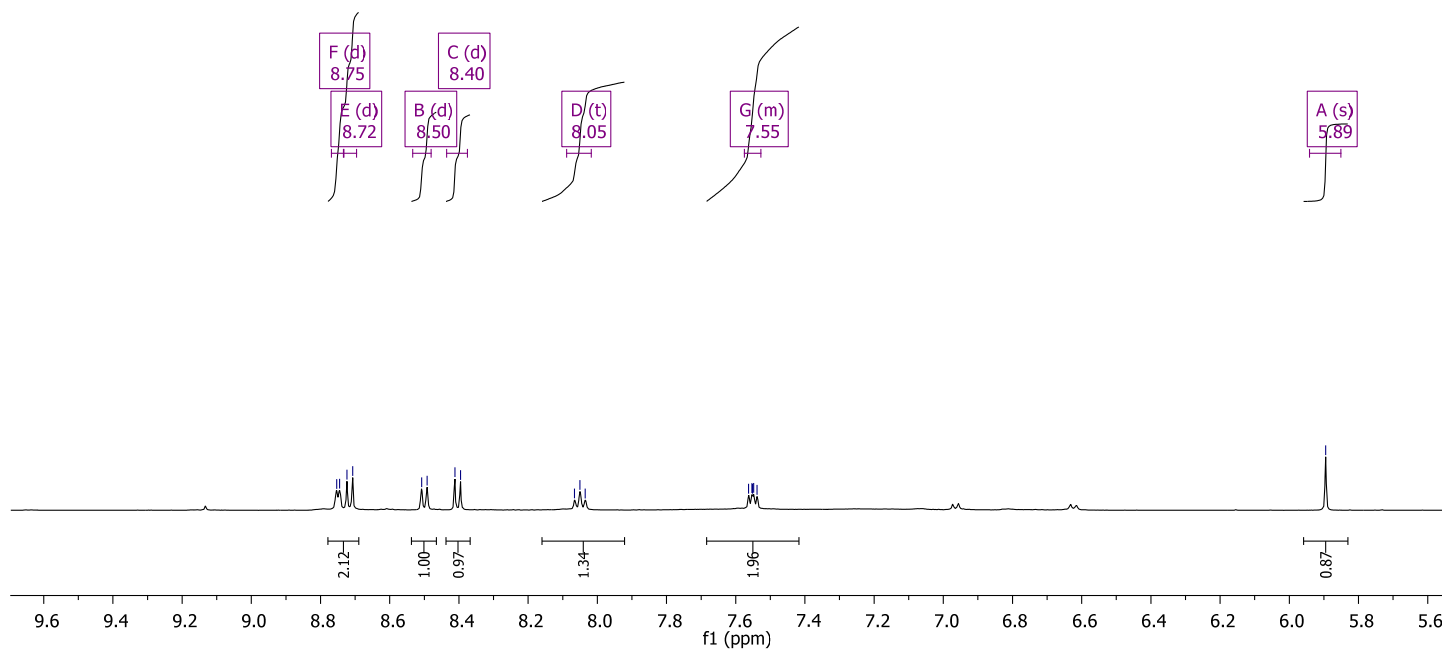
500 MHz ^1H -NMR of 7-amino-2-(2-pyridyl)quinoline-5,8-dione (**23**) in DMSO

CMK-01-193-proton
STANDARD PROTON PARAMETERS

8.75 8.74 8.72 8.71 8.51 8.49 8.41 8.40 8.07 8.05 8.04 7.56 7.55 7.55 7.54 5.89

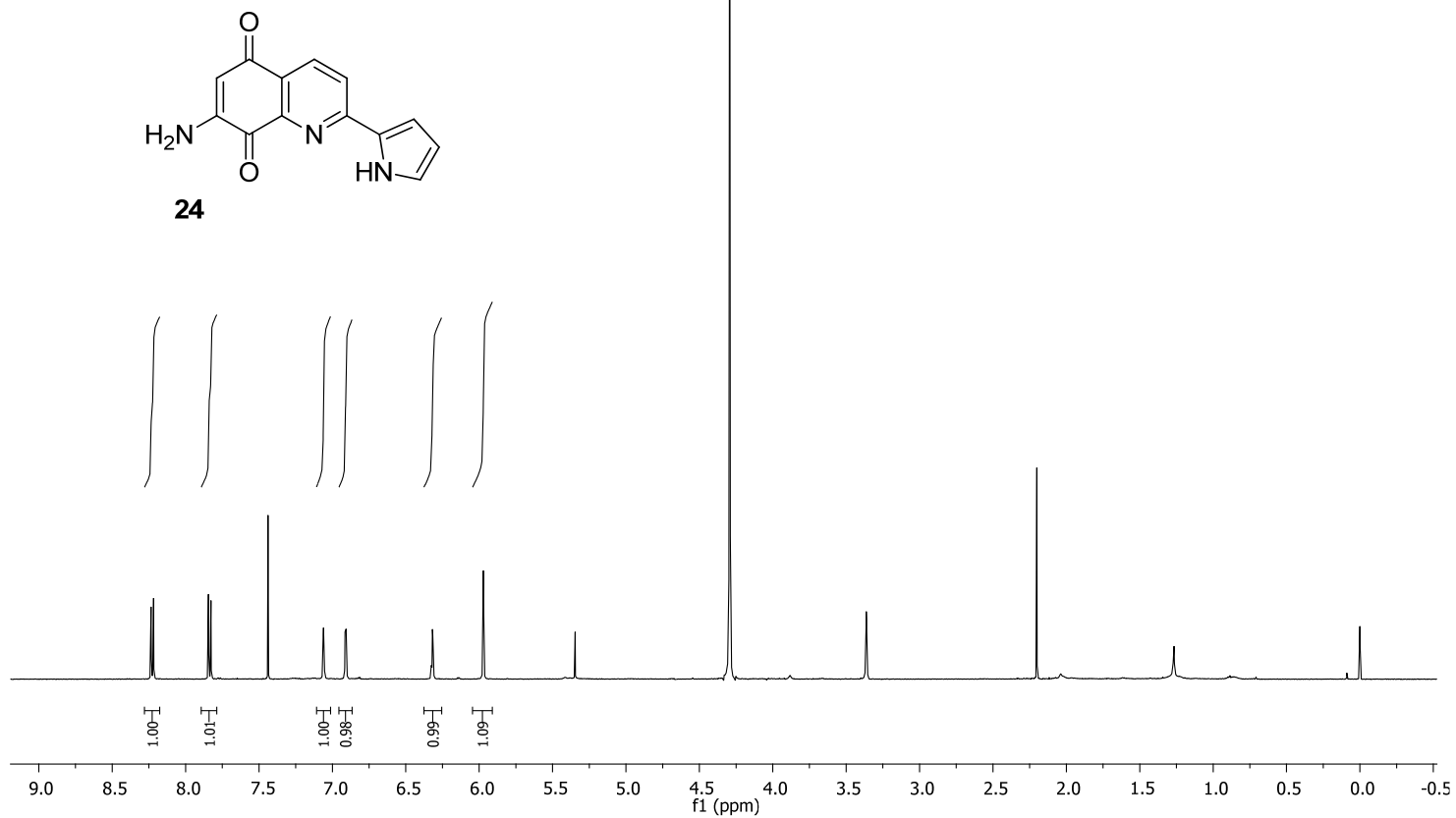


23



500 MHz ^1H -NMR of 7-amino-2-(2-pyrrolyl)quinoline-5,8-dione (**24**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

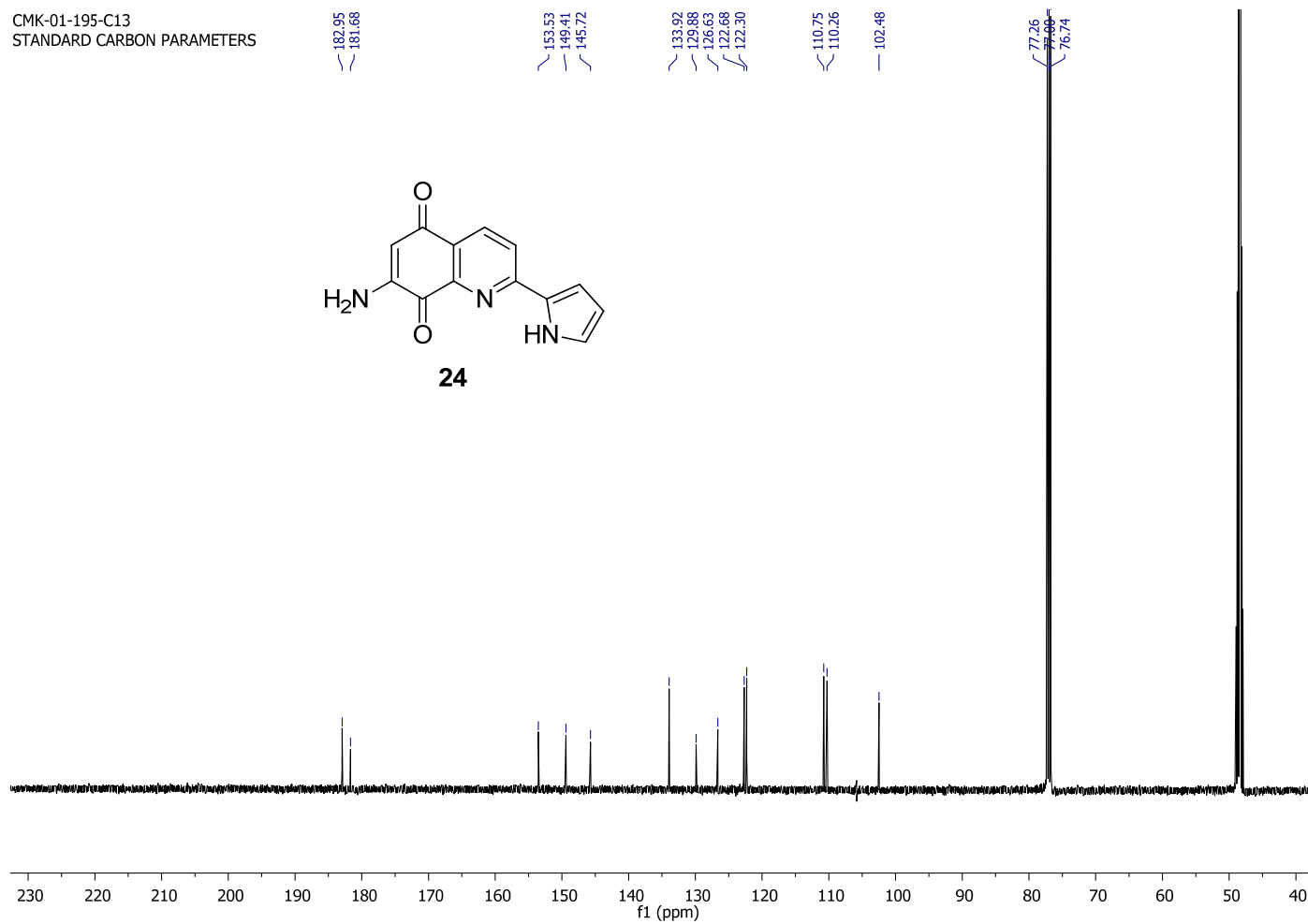
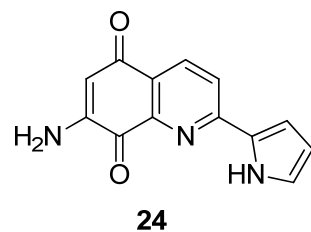
CMK-01-195-proton1
STANDARD PROTON PARAMETERS



125 MHz ^{13}C -NMR of 7-amino-2-(2-pyrrolyl)quinoline-5,8-dione (**24**) in $\text{CDCl}_3/\text{CD}_3\text{OD}$ mixture

CMK-01-195-C13
STANDARD CARBON PARAMETERS

182.95
181.68
153.53
149.41
145.72
133.92
129.88
126.63
122.68
122.30
110.75
110.26
102.48
77.26
77.09
76.74



400 MHz ^1H -NMR of the aromatic region of 7-amino-2-(4-trifluorophenyl)quinoline-5,8-dione **(19)** in $[\text{}^2\text{H}_8]\text{THF}$

CMK-01-161THF-proton

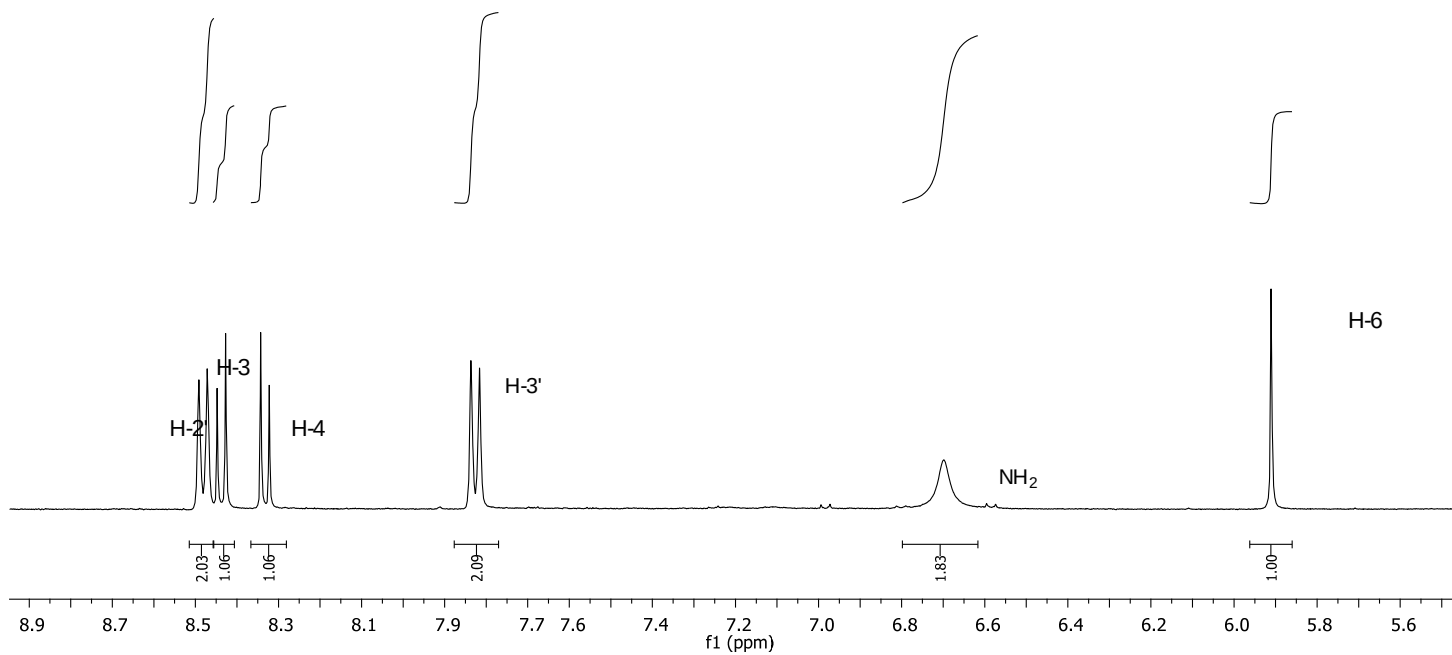
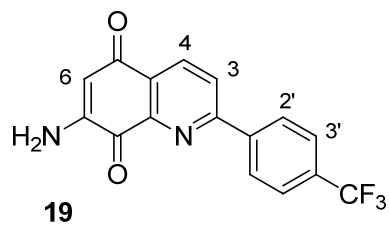


Table S1. Chemical shifts (δ) of protons upon addition of Zinc(II) triflate to **(19)** (^1H NMR (400 MHz, THF)).

Zn^{2+} equiv.	H-2'	H-3	H-4	H-7'	H-4'	H-5'	H-6'	H-3'	NH_2	H-6
0	8.85 (dd, $J = 4.1, 1.8$)	8.54 (d, $J = 8.2$)	8.36 (d, $J = 8.2$)	8.30 (dd, $J = 7.2, 1.3$)	8.20 (dd, $J = 8.3, 1.7$)	7.88 (dd, $J = 8.2, 1.2$)	7.65 – 7.59 (m)	7.39 (dd, $J = 8.3, 4.1$)	6.44 (s)	5.90 (s)
1	9.12 (dd, $J = 4.6, 1.2$)	8.62 (d, $J = 8.6$)	8.45 (d, $J = 8.5$)	8.46 (m)	8.64 (dd, $J = 8.8, 1.4$)	8.19 (d, 8.3)	7.82 (t, $J = 7.8$)	7.79 (dd, $J = 8.1, 4.5$)	6.86 (s)	6.05 (s)
2	9.11 (dd, $J = 4.8, 1.6$)	8.62 (d, $J = 8.4$)	8.46 (d, $J = 8.5$)	8.46 (dd, $J = 7.8, 0.8$)	8.64 (dd, $J = 8.4, 1.6$)	8.20 (dd, $J = 8.1, 0.9$)	7.83 (t, $J = 7.8$)	7.79 (dd, $J = 8.2, 4.8$)	6.88 (s)	6.07 (s)
3	9.11 (dd, $J = 4.8, 1.7$)	8.62 (d, $J = 8.4$)	8.46 (d, $J = 8.6$)	8.46 (dd, $J = 6.8, 1.1$)	8.64 (d, $J = 8.2, 1.7$)	8.20 (d, $J = 8.1, 0.9$)	7.82 (t, $J = 7.8$)	7.79 (dd, $J = 8.2, 4.8$)	6.88 (s)	6.07 (s)
4	9.10 (dd, $J = 4.8, 1.6$)	8.62 (d, $J = 8.3$)	8.46 (d, $J = 8.5$)	8.46 (m)	8.65 (d, $J = 9.3, 1.6$)	8.19 (m)	7.83 (d, $J = 7.8$)	7.79 (dd, $J = 8.3, 4.8$)	6.89 (s)	6.07 (s)
5	9.10 (dd, $J = 4.8, 1.6$)	8.62 (d, $J = 8.4$)	8.46 (d, $J = 8.2$)	8.46 (d, $J = 8.2$)	8.64 (d, $J = 8.2, 1.4$)	8.19 (d, $J = 8.1$)	7.82 (d, $J = 7.8$)	7.79 (dd, $J = 8.3, 4.8$)	6.87 (s)	6.08(s)
10	9.09 (dd, $J = 4.8, 1.7$)	8.62 (d, $J = 8.3$)	8.46 (d, $J = 8.4$)	8.46 (d, $J = 8.4$)	8.64 (dd, $J = 8.1, 1.7$)	8.19 (dd, $J = 8.1, 0.7$)	7.81 (d, $J = 7.8$)	7.78(dd, $J = 8.3, 4.8$)	6.89 (s)	6.09(s)

400 MHz ^1H -NMR of the aromatic region of 7-amino-2-(8'-quinolyl)quinoline-5,8-dione (**22**) in $[\text{2H}_8]\text{THF}/\text{CDCl}_3$ mixture

CMK-01-187-PROTON-thfcdcl3

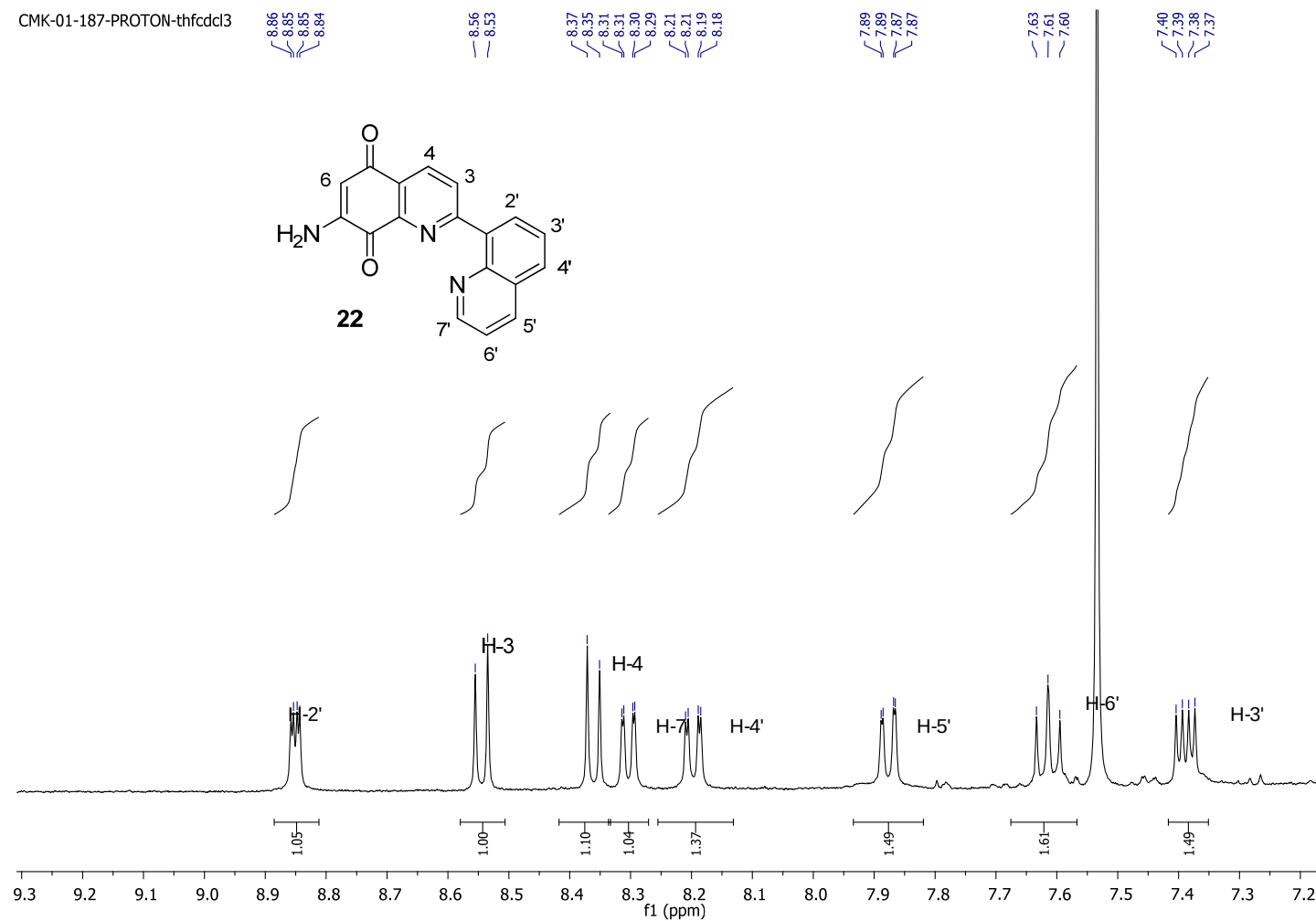


Table S2. Chemical shifts (δ , ppm), multiplicity and coupling constant (J , Hz) of **(22)** protons upon addition of Zinc(II) triflate (^1H NMR (400 MHz, THF/ CDCl_3)

Zn^{2+} equiv.	$H\text{-}2'$	$H\text{-}3$	$H\text{-}4$	$H\text{-}7'$	$H\text{-}4'$	$H\text{-}5'$	$H\text{-}6'$	$H\text{-}3'$	NH_2	$H\text{-}6$
0	8.85 (dd, J = 4.1, 1.8)	8.54 (d, J = 8.2)	8.36 (d, J = 8.2)	8.30 (dd, J = 7.2, 1.3)	8.20 (dd, J = 8.3, 1.7)	7.88 (dd, J = 8.2, 1.2)	7.65 – 7.59 (m)	7.39 (dd, J = 8.3, 4.1)	6.44 (s)	5.90 (s)
1	9.12 (dd, J = 4.6, 1.2)	8.62 (d, J = 8.6)	8.45 (d, J = 8.5)	8.46 (m)	8.64 (dd, J = 8.8, 1.4)	8.19 (d, 8.3)	7.82 (t, J = 7.8)	7.79 (dd, J = 8.1, 4.5)	6.86 (s)	6.05 (s)
2	9.11 (dd, J = 4.8, 1.6)	8.62 (d, J = 8.4)	8.46 (d, J = 8.5)	8.46 (dd, J = 7.8, 0.8)	8.64 (dd, J = 8.4, 1.6)	8.20 (dd, J = 8.1, 0.9)	7.83 (t, J = 7.8)	7.79 (dd, J = 8.2, 4.8)	6.88 (s)	6.07 (s)
3	9.11 (dd, J = 4.8, 1.7)	8.62 (d, J = 8.4)	8.46 (d, J = 8.6)	8.46 (dd, J = 6.8, 1.1)	8.64 (d, J = 8.2, 1.7)	8.20 (d, J = 8.1, 0.9)	7.82 (t, J = 7.8)	7.79 (dd, J = 8.2, 4.8)	6.88 (s)	6.07 (s)
4	9.10 (dd, J = 4.8, 1.6)	8.62 (d, J = 8.3)	8.46 (d, J = 8.5)	8.46 (m)	8.65 (d, J = 9.3, 1.6)	8.19 (m)	7.83 (d, J = 7.8)	7.79 (dd, J = 8.3, 4.8)	6.89 (s)	6.07 (s)
5	9.10 (dd, J = 4.8, 1.6)	8.62 (d, J = 8.4)	8.46 (d, J = 8.2)	8.46 (d, J = 8.2)	8.64 (d, J = 8.2, 1.4)	8.19 (d, J = 8.1)	7.82 (d, J = 7.8)	7.79 (dd, J = 8.3, 4.8)	6.87 (s)	6.08(s)
10	9.09 (dd, J = 4.8, 1.7)	8.62 (d, J = 8.3)	8.46 (d, J = 8.4)	8.46 (d, J = 8.4)	8.64 (dd, J = 8.1, 1.7)	8.19 (dd, J = 8.1, 0.7)	7.81 (d, J = 7.8)	7.78(dd, J = 8.3, 4.8)	6.89 (s)	6.09(s)

400 MHz ^1H -NMR of the aromatic region of 7-amino-2-(2-pyridyl)quinoline-5,8-dione (**23**) in $[\text{D}_8]\text{THF}$.

CMK-01-193-thf

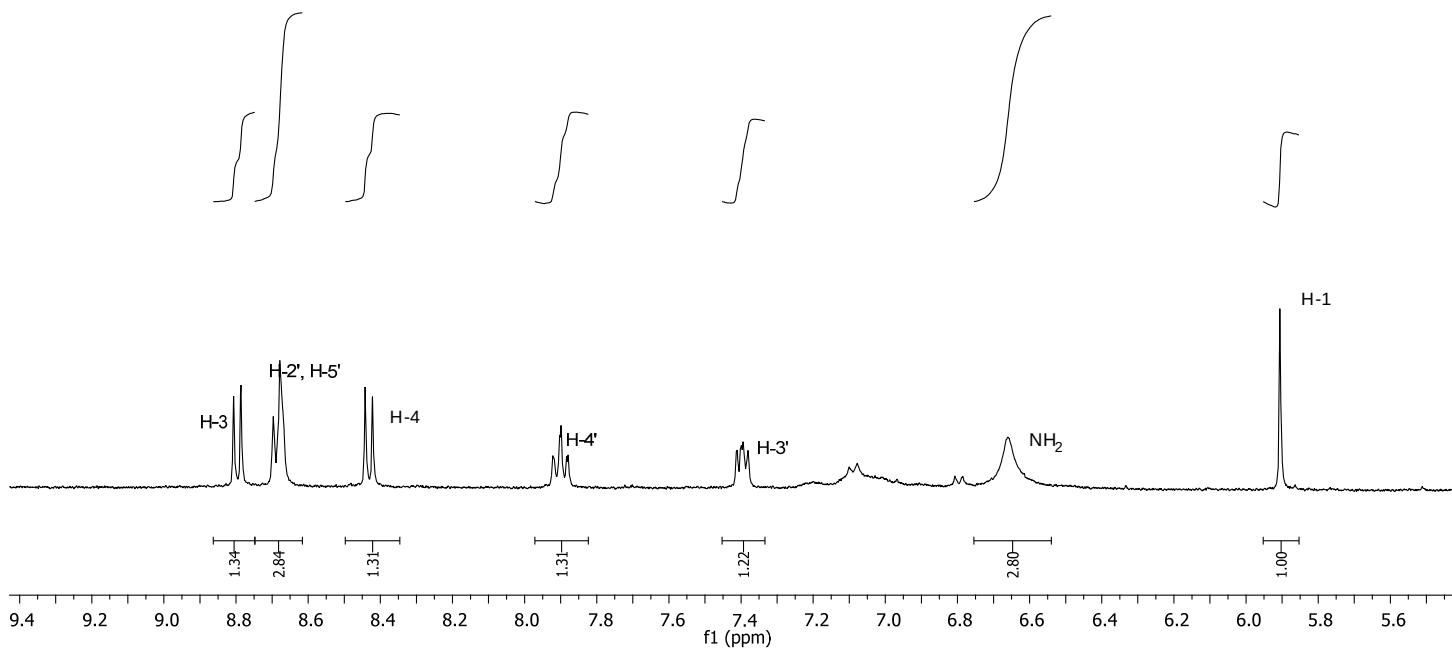
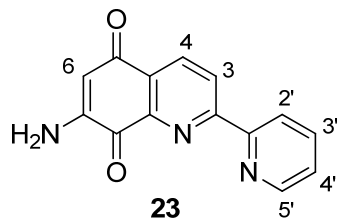
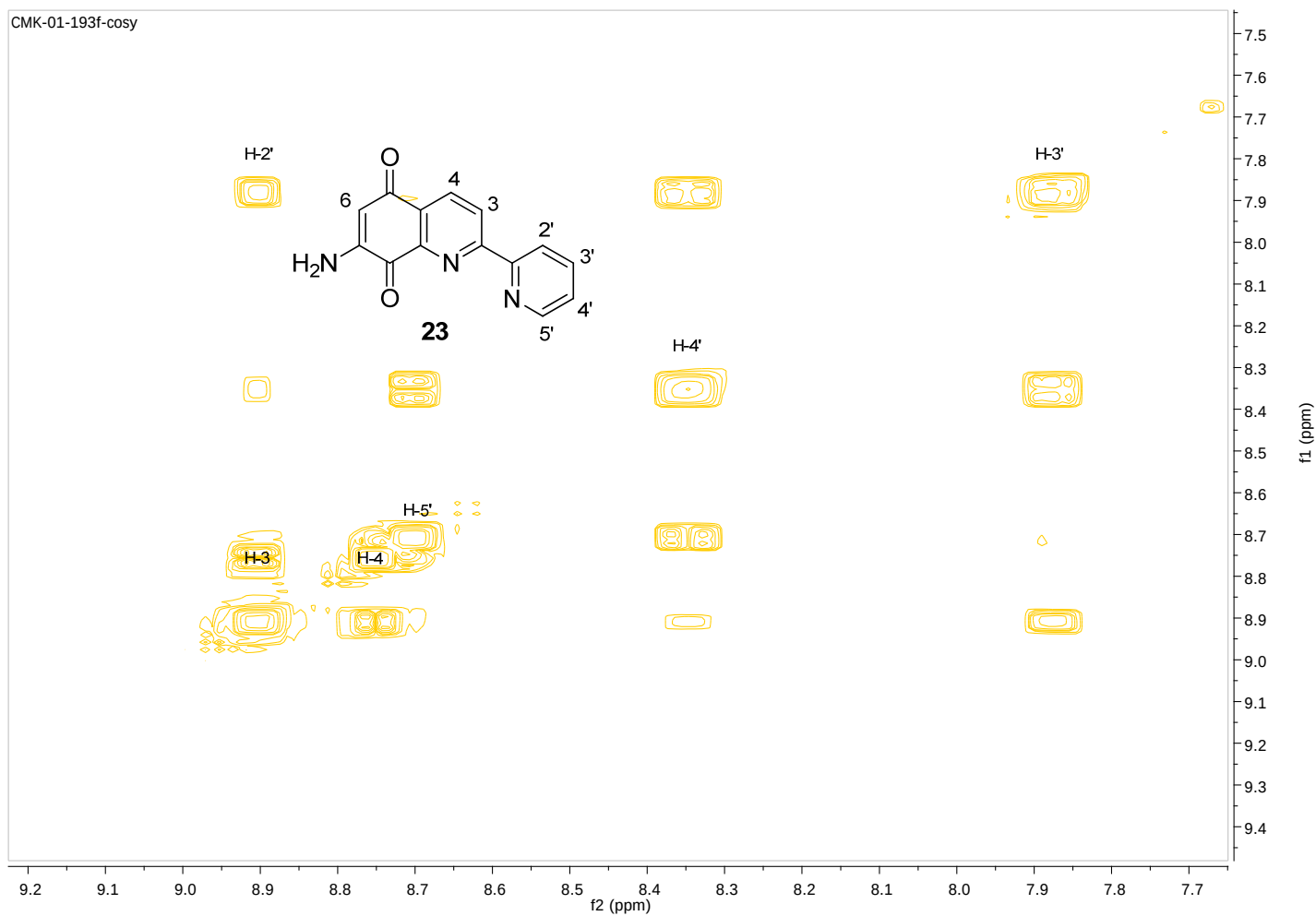


Table S3. Chemical shifts (δ , ppm) and coupling constants (J , Hz) of **(23)** protons upon addition of Zinc(II) triflate (^1H NMR (400 MHz, [$^2\text{H}_8$]THF))

Zn^{2+} equiv.	H-2'	H-3	H-4	H-3'	H-5'	H-4'	NH_2	H-6
0	8.69 (d, J = 7.3)	8.80 (d, J = 8.2)	8.43 (d, J = 8.2)	7.40 (dd, 7.2, 5.2)	8.68(m)	7.90 (td, J = 7.8, 1.5)	6.66 (s)	5.91 (s)
1	8.91 (d, J = 4.7)	8.89 (d, J = 8.4)	8.75 (d, J = 8.1)	7.88 (dd, J = 7.4, 5.4)	8.69 (d, J = 8.1)	8.35 (td, J = 7.8, 1.3)	7.20 (s)	6.08 (s)
2	8.91 (d, J = 5.5)	8.89 (d, J = 8.4)	8.75 (d, J = 8.2)	7.88 (m)	8.69 (d, J = 8.1)	8.35 (td, J = 7.9, 1.5)	7.20 (s)	6.09 (s)
3	8.91 (d, J = 6.4)	8.89 (d, J = 8.5)	8.75 (d, J = 8.2)	7.88 (dd, J = 7.4, 5.2)	8.70 (d, J = 8.1)	8.35 (td, J = 8.0, 1.2)	7.20 (s)	6.09 (s)
4	8.91 (d, J = 5.4)	8.89 (d, J = 8.3)	8.75 (d, J = 8.2)	7.87 (dd, J = 7.4, 5.3)	8.70 (d, J = 8.0)	8.35 (td, J = 7.8, 1.3)	7.20(s)	6.09(s)
5	8.91 (d, J = 3.9)	8.89 (d, J = 8.2)	8.75 (d, J = 8.2)	7.87 (dd, J = 7.2, 5.5)	8.70 (d, J = 8.0)	8.35 (td, J = 7.9, 1.4)	7.21 (s)	6.10(s)
10	8.90 (m)	8.89 (d, J = 8.2)	8.75 (d, J = 8.2)	7.87 (dd, J = 7.6, 5.2)	8.70 (d, J = 8.1)	8.35 (td, J = 7.9, 1.4)	7.21 (s)	6.10(s)

400 MHz COSY-NMR spectrum of the aromatic region of 7-amino-2-(2-pyridyl)quinoline-5,8-dione (**23**) + 10 equiv. $\text{Zn}(\text{SO}_3\text{CF}_3)_2$ in $[\text{}^2\text{H}_8]\text{THF}$



CMK-01-183-thf-cdcl3

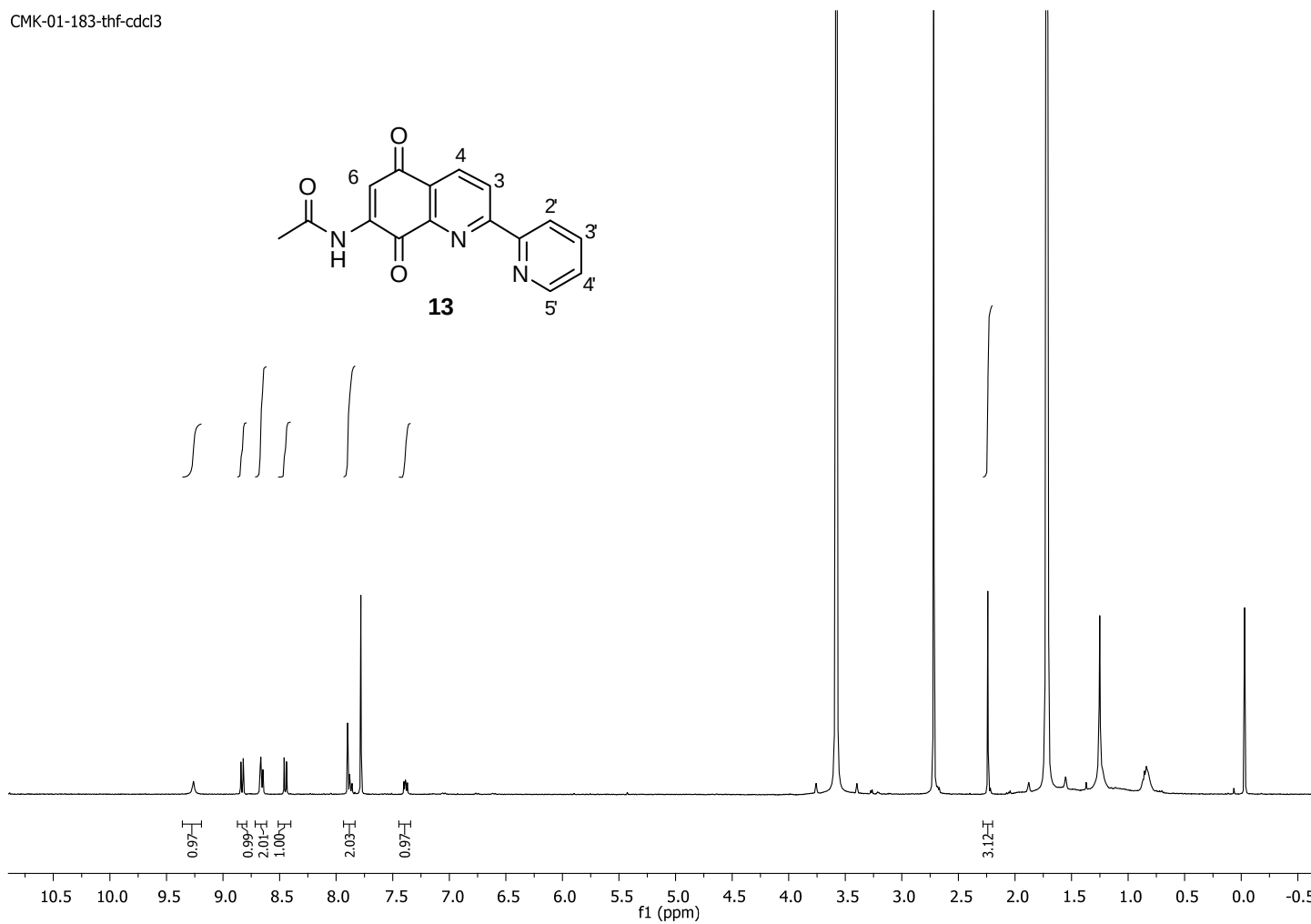
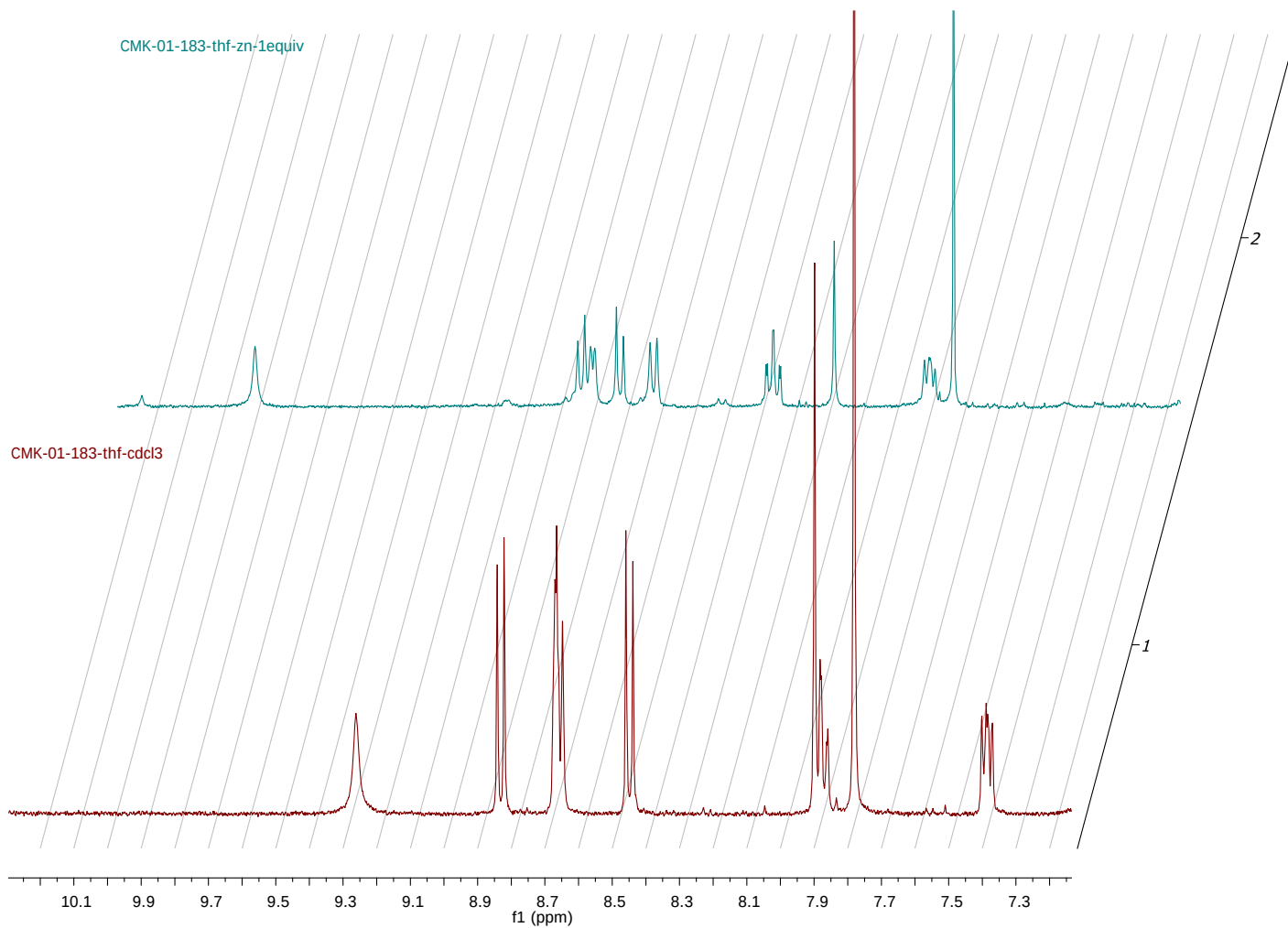


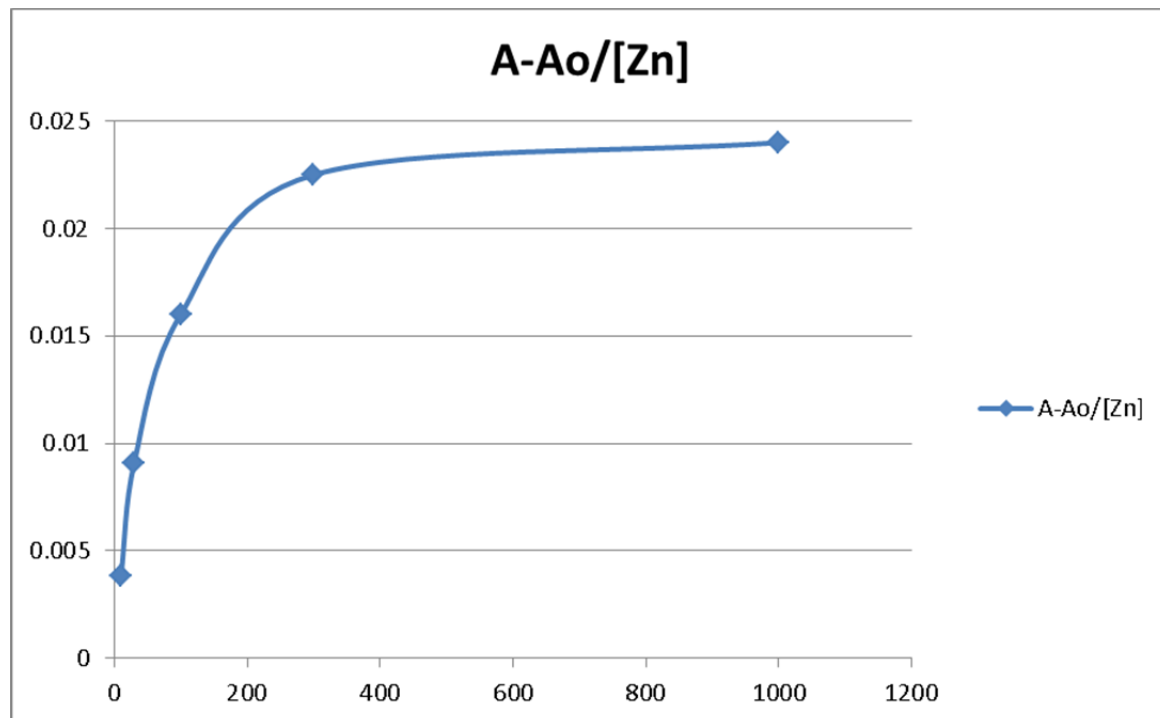
Table S4. Chemical shifts (δ , ppm) and coupling constants (J , Hz) of **(13)** protons upon addition of Zinc(II) triflate (^1H NMR (400 MHz, [$^2\text{H}_8$]THF))

Zn^{2+} equiv.	H-2'	H-3	H-4	H-3'	H-5'	H-4'	NH	H-6	$-\text{CH}_3$
0	8.67 (m)	8.83 (d, $J = 8.2$)	8.45 (d, $J = 8.2$)	7.39 (m)	8.66(m)	7.87 (dd, $J = 7.8, 1.6$)	9.26 (s)	7.90 (s)	2.24 (s)
1	8.88 (d, $J = 4.8$)	8.92 (d, $J = 8.3$)	8.80 (d, $J = 8.2$)	7.88 (m)	8.70 (d, $J = 8.1$)	8.35 (td, $J = 7.9, 1.6$)	9.89 (s)	8.16 (s)	2.33 (s)
2	8.88 (d, $J = 4.7$)	8.92 (d, $J = 8.4$)	8.80 (d, $J = 8.3$)	7.88 (m)	8.70 (d, $J = 8.1$)	8.35 (td, $J = 7.9, 1.6$)	9.89 (s)	8.16 (s)	2.28 (s)
3	8.88 (d, $J = 4.7$)	8.92 (d, $J = 8.4$)	8.79 (d, $J = 8.3$)	7.88 (dd, $J = 7.0, 5.5$)	8.70 (d, $J = 8.0$)	8.34 (td, $J = 7.8, 1.4$)	9.88 (s)	8.16 (s)	2.28 (s)
4	8.88 (d, $J = 4.8$)	8.92 (d, $J = 8.3$)	8.79 (d, $J = 8.3$)	7.88 (dd, $J = 7.1, 5.4$)	8.70 (d, $J = 8.0$)	8.34 (td, $J = 7.9, 1.6$)	9.87 (s)	8.16 (s)	2.27 (s)
5	8.88 (d, $J = 4.7$)	8.92 (d, $J = 8.2$)	8.79 (d, $J = 8.3$)	7.88 (dd, $J = 7.2, 5.4$)	8.70 (d, $J = 8.0$)	8.34 (td, $J = 7.8, 1.4$)	9.87 (s)	8.16 (s)	2.27 (s)
10	8.88 (d, $J = 4.6$)	8.92 (d, $J = 8.3$)	8.79 (d, $J = 8.3$) H-3 8.3, H-2', H-5'	7.88 (dd, $J = 7.1, 5.4$)	8.70 (d, $J = 8.0$)	8.34 (td, $J = 7.8, 1.5$)	9.88 (s)	8.15 (s)	2.27 (s)

400 MHz ^1H -NMR spectrum of the aromatic region of 7-acetamido-2-(2-pyridyl)quinoline-5,8-dione (**13**) in $[\text{D}_8]\text{THF}$ and addition of 1 equiv. of $\text{Zn}(\text{SO}_3\text{CF}_3)_2$.



Affinity constant for compound **(23)** binding with Zn^{2+}



LC/MS analyses

LC/MS analyses were obtained on a Waters ACQUITY UPLC-series liquid chromatography system equipped with a diode array detector and a Waters Quattro Premier Tandem Quadrupole mass spectrometer (ionization type electrospray). The liquid chromatography conditions were as follows: a Waters ACQUITY UPLC column (BEH, C18, 1.7 μ m, 1.0x100 mm) was used, and it was eluted with a gradient made up of two solvent mixtures. Solvent A consisted of water and 0.2% formic acid. Solvent B consisted of methanol. The gradient was processed as follows:

<u>Time (min)</u>	<u>Flow (ml/min)</u>	<u>%A</u>	<u>%B</u>
Initial	0.200	90.0	10.0
1.00	0.200	90.0	10.0
8.00	0.200	5.0	95.0
12.00	0.200	5.0	95.0
12.10	0.200	90.0	10.0
15.00	0.200	90.0	10.0

Compound purity was assigned on the basis of 254-nM detection data assessed by comparing relative peak areas of the signals.

Compound	Retention Time (min)	Purity (%)
9	7.60	95
10	3.99	94.6
11	4.59	100
13	4.70	96
15	4.89	100
17	7.22	100
18	6.35	97.9
19	7.18	97.1
20	3.70	96
21	6.87	97.5
22	4.29	96
23	4.07	89.7
24	5.84	100