Atroposelective synthesis of N−N axially chiral pyrrolyl(aza)quinolinone by de novo ring formation

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Electronic Supplementary Information

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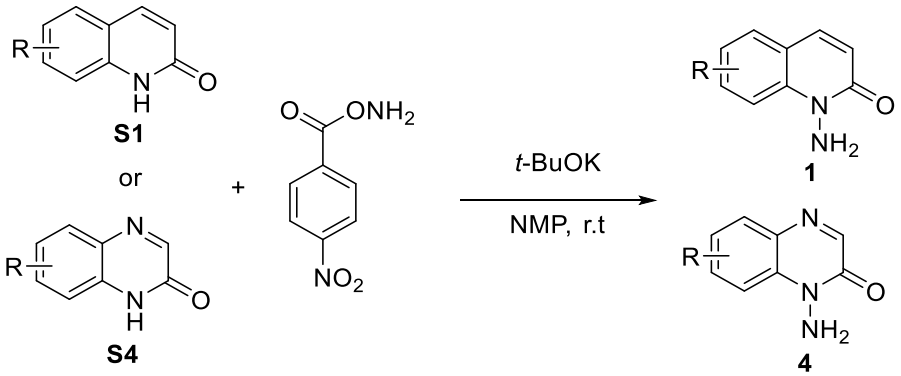
(1) General Information

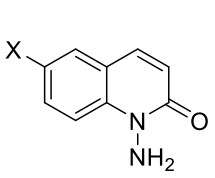
All reactions sensitive to air or moisture were carried out in flame-dried glassware under nitrogen pressure using standard Schlenk techniques. All reagents and solvents were purchased from commercial sources (Xi'an Yizhichen Biotechnology Co., Ltd) without further purification unless specially noted. Melting points were taken on a WRS-1B digital melting point apparatus without correction. Flash chromatography was performed on silica (300-400 mesh) with EtOAc–PE. Infrared spectra were obtained using a Nicolet AVATAR 370 FT-IR spectrometer. ^{1}H, ^{13}C, and ^{19}F-NMR spectra were recorded on a Bruker AV-500 or Varian 400 MHz spectrometer. NMR spectra were calibrated to the respective residual solvent signals of $CDCl_3$ [δ (^{1}H) = 7.26 ppm, δ (^{13}C) = 77.16 ppm] and DMSO [δ (^{1}H) = 2.50 ppm, δ (^{13}C) = 39.52 ppm]. The following abbreviations for single multiplicities were used: s-singlet, d-doublet, t-triplet, q-quartet. High resolution mass spectroscopy (HR-MS) was performed on a Thermo Fisher Scientific LTQ FTICR-MS (DART) or Thermo Scientific Q Exactive HF Orbitrap-FTMS (ESI). The enantiomeric excess (ee) of products were determined by chiral phase HPLC analysis on Agress 1100 or Agilent HPLC units, chiral column: FLM-MD(2), FLM-ND(2), FLM-NQ(2) and FLM-MJ(2).

(2) Preparation of Substrates

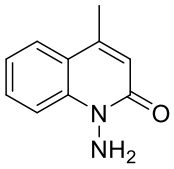
Typical procedure for synthesis substrate **1**[1] and **4** [1]



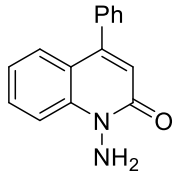
To a solution of **S1** or **S4** (2 mmol) in 15 mL *N*-methylpyrrolidone (NMP) was added 2.4 mL *t*-BuOK (1 M in THF) and the reaction mixture was stirred at room temperature for 0.5 h. Then a solution of *O*-(4-nitrobenzoyl)hydroxylamine (2.4 mmol) was added to the mixture, which was stirred at room temperature for 2 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with H_2O and the aqueous layer was extracted with EtOAc (3×10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure. The residue was purified through flash column chromatography on silica gel.



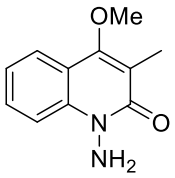
1r (X = F)
1s (X = Cl)
1t (X = Br)



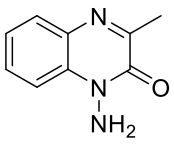
1u



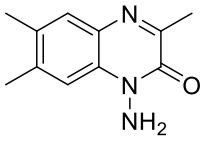
1v



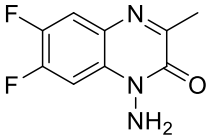
1w



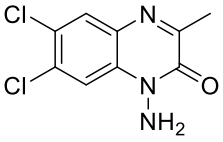
4a



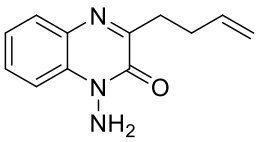
4i



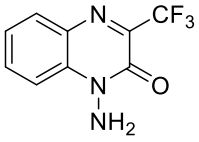
4j



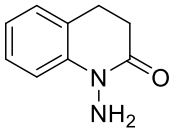
4k



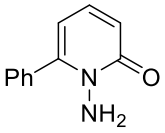
4l



4m



6



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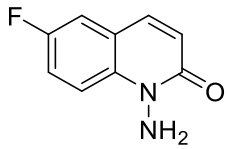
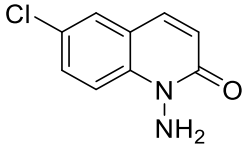
Characterization of the new substrates is shown below:

1-amino-6-fluoroquinolin-2(1*H*)-one (1r):



White solid (62% yield).
M.p.: 202-204 ℃.
^{1}H NMR (400 MHz, DMSO-d_6): δ 7.88 (dd, *J* = 9.5, 3.6 Hz, 2H), 7.59 (dd, *J* = 9.0, 2.9 Hz, 1H), 7.51 (td, *J* = 8.9, 3.0 Hz, 1H), 6.77 (d, *J* = 9.5 Hz, 1H), 5.90 (s, 2H).
^{13}C NMR (101 MHz, DMSO-d_6): δ 159.7, 157.5 (d, *J* = 238.4 Hz), 137.7 (d, *J* = 3.0 Hz), 136.9, 121.9, 120.7 (d, *J* = 9.1 Hz), 119.0 (d, *J* = 24.2 Hz), 117.2 (d, *J* = 8.1 Hz), 113.4 (d, *J* = 23.2 Hz).
^{19}F NMR (376 MHz, DMSO-d_6): δ -121.8.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 179.0615; found: 179.0611.

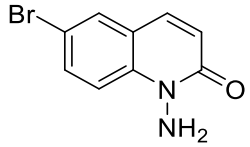
1-amino-6-chloroquinolin-2(1*H*)-one (1s):



White solid (52% yield).
M.p.: 196-198 ℃.

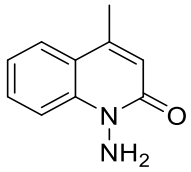
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.91 (d, *J* = 8.7 Hz, 2H), 7.44 (d, *J* = 8.6 Hz, 2H), 4.22 (dd, *J* = 8.2, 5.5 Hz, 1H), 3.77 (s, 3H), 3.68 (dd, *J* = 18.4, 8.2 Hz, 1H), 3.47 (dd, *J* = 18.4, 5.6 Hz, 1H), 2.43 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 160.9, 138.7, 137.7, 131.1, 128.0, 127.4, 121.6, 121.1, 116.4.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 195.0320; found: 195.0315.

1-amino-6-bromoquinolin-2(1*H*)-one (1t):



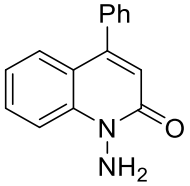
White solid (68% yield).
M.p.: 176-178 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 8.9 Hz, 1H), 7.69 (d, *J* = 2.1 Hz, 1H), 7.66 (dd, *J* = 8.9, 2.2 Hz, 1H), 7.62 (d, *J* = 9.5 Hz, 1H), 6.78 (d, *J* = 9.5 Hz, 1H), 4.97 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 160.9, 137.6, 133.8, 130.4, 121.6, 121.6, 116.7, 115.4
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.:238.9815; found: 238.9813.

1-amino-4-methylquinolin-2(1*H*)-one (1u):



White solid (55% yield).
M.p.: 136-138 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.98 (d, *J* = 8.5 Hz, 1H), 7.67 (dd, *J* = 8.0, 1.4 Hz, 1H), 7.61 - 7.55 (m, 1H), 7.28 - 7.22 (m, 1H), 6.60 (d, *J* = 1.2 Hz, 1H), 4.99 (s, 2H), 2.46 (d, *J* = 1.1 Hz, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 160.8, 146.6, 139.5, 130.8, 124.9, 122.3, 120.7, 119.6, 114.9, 19.1.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 175.0866; found: 175.0862.

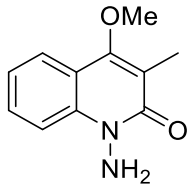
1-amino-4-phenylquinolin-2(1*H*)-one (1v):



White solid (43% yield).
M.p.: 143-145 ℃.

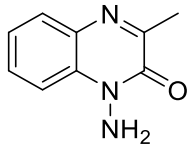
^{1}H NMR (400 MHz, $CDCl_3$): δ 8.05 (d, *J* = 8.5 Hz, 1H), 7.60 (t, *J* = 7.8 Hz, 1H), 7.53 (d, *J* = 8.1 Hz, 1H), 7.50 - 7.45 (m, 3H), 7.42 - 7.36 (m, 2H), 7.16 (t, *J* = 7.6 Hz, 1H), 6.70 (s, 1H), 5.13 (s, 2H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 160.5, 150.9, 140.0, 137.0, 131.0, 129.0, 128.8, 128.7, 127.4, 122.3, 119.8, 119.7, 114.9.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.:237.1023; found: 237.1017.

1-amino-4-methoxy-3-methylquinolin-2(1*H*)-one (1w):



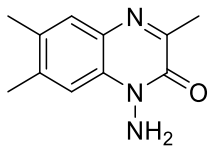
White solid (65% yield).
M.p.: 134-136 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.97 (d, *J* = 8.6 Hz, 1H), 7.82 (d, *J* = 8.0 Hz, 1H), 7.57 (t, *J* = 7.8 Hz, 1H), 7.28−7.23 (m, 1H), 5.00 (s, 2H), 3.91 (s, 3H), 2.24 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 163.3, 160.4, 138.6, 130.4, 122.9, 122.4, 118.0, 117.0, 114.6, 61.4, 10.7.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 205.0972; found: 205.0967.

1-Amino-3-methylquinoxalin-2(1*H*)-one (4a):



White solid (49% yield).
M.p.: 170-172 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, *J* = 9.7 Hz, 2H), 7.56 (t, *J* = 8.5 Hz, 1H), 7.38−7.32 (m, 1H), 5.11 (s, 2H), 2.63 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 157.3, 154.0, 132.9, 132.5, 130.0, 129.1, 124.2, 113.9, 21.6.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.:176.0819; found: 176.0813.

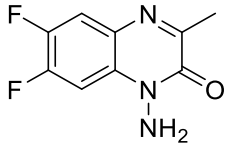
1-Amino-3,6,7-trimethylquinoxalin-2(1*H*)-one (4i):



Light yellow solid (65% yield).
M.p.: 179-181 ℃.
^{1}H NMR (400 MHz, DMSO-d_6): δ 7.53 (s, 1H), 7.49 (s, 1H), 6.07 (s, 2H), 2.43 (s, 3H), 2.35 (s, 3H), 2.28 (s, 3H).

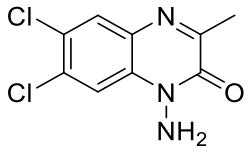
^{13}C NMR (101 MHz, DMSO-d6): δ 155.2, 152.4, 138.9, 132.0, 130.6, 130.2, 128.2, 114.4, 21.1, 20.0, 18.9.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.:204.1132; found: 204.1128.

1-Amino-6,7-difluoro-3-methylquinoxalin-2(1*H*)-one (4j):



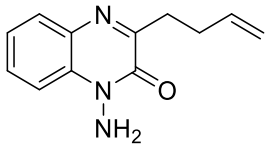
White solid (47% yield).
M.p.: 166-168 ℃.
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.82 (dd, *J* = 10.9, 8.2 Hz, 1H), 7.70 (dd, *J* = 12.0, 7.8 Hz, 1H), 6.06 (s, 2H), 2.44 (s, 3H).
^{19}F NMR (376 MHz, DMSO-*d*$_6$): δ -133.8, -143.8.
^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ 158.2, 153.0, 150.3 (dd, *J* = 252.5, 14.1 Hz), 147.2 (d, *J* = 248.0, 14.1 Hz), 130.9 (d, *J* = 10.1 Hz), 128.2 (d, *J* = 8.1 Hz), 116.2 (d, *J* = 18.2 Hz), 103.1 (d, *J* = 23.2 Hz), 21.4.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 212.0630; found: 212.0628.

1-Amino-6,7-dichloro-3-methylquinoxalin-2(1*H*)-one (4k):



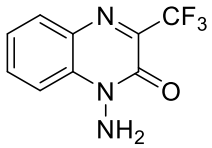
Red solid (56% yield).
M.p.: 239-241 ℃.
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.99 (s, 1H), 7.93 (s, 1H), 6.11 (s, 2H), 2.47 (s, 3H).
^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ 159.2, 152.6, 132.9, 131.8, 131.0, 129.2, 125.2, 115.8, 21.3.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 244.0039; found: 244.0041.

1-Amino-3-(but-3-en-1-yl)quinoxalin-2(1*H*)-one (4l):



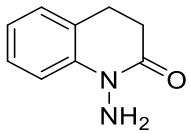
White solid (70% yield).
M.p.: 84-86 ℃.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.82 (d, *J* = 7.9 Hz, 1H), 7.78 (d, *J* = 8.6 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 5.93 (ddt, *J* = 16.9, 10.1, 6.5 Hz, 1H), 5.15−5.06 (m, 3H), 4.99 (d, *J* = 10.2 Hz, 1H), 3.08−3.02 (m, 2H), 2.60 - 2.52 (m, 2H).
^{13}C NMR (101 MHz, CDCl$_3$): δ 159.2, 153.6, 137.6, 132.7, 132.5, 130.0, 129.3, 124.0, 115.4, 113.9, 33.4, 30.7.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 216.1132; found: 216.1126.

1-Amino-3-(trifluoromethyl)-8,8a-dihydroquinoxalin-2(1*H*)-one (4m):



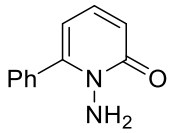
White solid (61% yield).
M.p.: 157-159 ℃.
^{1}H NMR (400 MHz, DMSO-*d*$_6$): δ 7.87 (t, *J* = 8.0 Hz, 2H), 7.76 (t, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 7.6 Hz, 1H), 6.34 (s, 2H).
^{13}C NMR (101 MHz, DMSO-*d*$_6$): δ 149.7, 141.8 (q, *J* = 32.3 Hz), 134.3, 133.6, 130.3, 130.0, 124.4, 121.6 (q, *J* = 277.8 Hz), 114.9.
^{19}F NMR (376 MHz, DMSO-*d*$_6$): δ -68.6.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 230.0536; found: 230.0533.

1-Amino-3,4-dihydroquinolin-2(1*H*)-one (6):



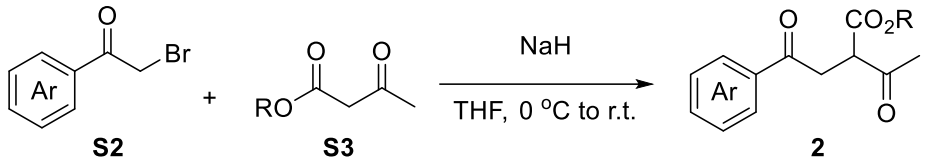
White solid (29% yield).
M.p.: 139-141 ℃.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.56 (d, *J* = 8.4 Hz, 1H), 7.29−7.24 (m, 1H), 7.00 (t, *J* = 7.5 Hz, 1H), 4.50 (s, 2H), 2.91 (dd, *J* = 8.7, 6.2 Hz, 2H), 2.71 (dd, *J* = 8.6, 6.3 Hz, 2H).
^{13}C NMR (101 MHz, CDCl$_3$): δ 169.2, 140.2, 127.6, 127.6, 124.7, 123.2, 115.0, 31.1, 25.1.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 163.0866; found: 163.0865.

1-Amino-6-phenylpyridin-2(1*H*)-one (8):



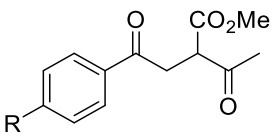
White solid (47% yield).
M.p.: 137-139 ℃.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.53−7.44 (m, 5H), 7.35 (dd, *J* = 9.1, 7.0 Hz, 1H), 6.64 (d, *J* = 8.6 Hz, 1H), 6.18 (d, *J* = 7.0 Hz, 1H), 5.29 (s, 2H).
^{13}C NMR (101 MHz, CDCl$_3$): δ 161.0, 148.0, 137.8, 133.8, 129.6, 129.0, 128.5, 117.2, 107.6.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 187.0866; found: 187.0859.

Typical procedure for synthesis substrate **2**[1]

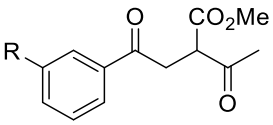


S2 **S3** **2**

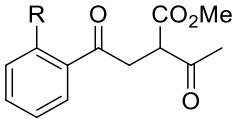
To a solution of sodium hydride (60% dispersion in mineral oil, 25.1 mmol) in 20 mL anhydrous tetrahydrofuran (THF) was slowly added the solution of methyl acetoacetate **S3** (25 mmol) in 20 mL THF at 0 ℃. The reaction mixture was stirred at 0 ℃ for 0.5 h. Then a solution of **S2** (25.1 mmol) in 10 mL THF was added to the mixture, which was stirred at room temperature for another 12 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with H_2O and the aqueous layer was extracted with EtOAc (3×50 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure. The residue was purified through flash column chromatography on silica gel to afford pure product **2**.



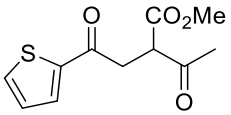
2a (R = H)
2b (R = OMe)
2c (R = Me)
2d (R = F)
2e (R = Cl)
2f (R = Br)
2g (R = CN)



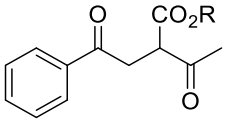
2h (R = OMe)
2i (R = F)
2j (R = Cl)



2k (R = OMe)
2l (R = F)



2m

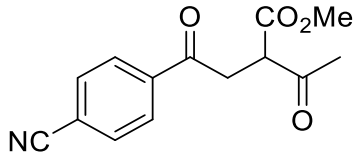


2n (R = Et)
2o (R = *i*Pr)
2p (R = Bn)
2q (R = *t*Bu)

The 1,4-diketone substrates were prepared according to the procedure in the reported literature. Substrates **2a**[1], **2b**[2], **2c-2f**[1], **2h**[3], **2i-2j**[1], **2l**[4], **2m**[1], **2n**[5], **2o**[4], **2p**[5] and **2q**[6] were known compounds.

Characterization of the new compounds is shown below:

Methyl 2-acetyl-4-(4-cyanophenyl)-4-oxobutanoate (2g):



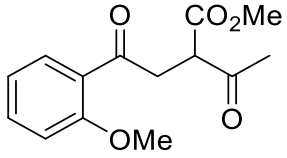
White solid (44% yield).

M.p.: 106-108 ℃.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.04 (d, *J* = 8.4 Hz, 2H), 7.76 (d, *J* = 8.4 Hz, 2H), 4.21 (dd, *J* = 8.2, 5.5 Hz, 1H), 3.76 (s, 3H), 3.69 (dd, *J* = 18.5, 8.2 Hz, 1H), 3.47 (dd, *J* = 18.5, 5.5 Hz, 1H), 2.42 (s, 3H).

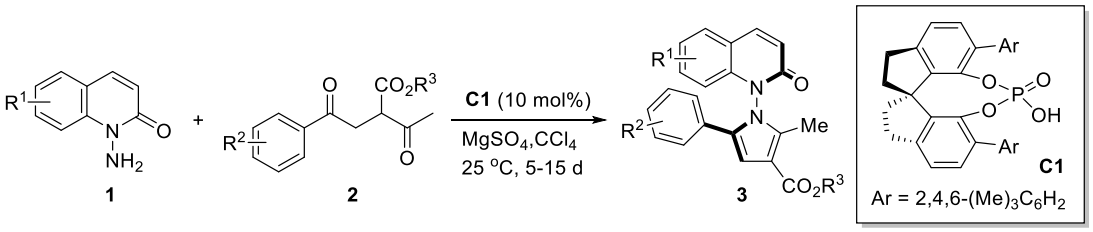
^{13}C NMR (101 MHz, $CDCl_3$): δ 201.9, 196.0, 169.1, 139.0, 132.6, 128.6, 117.9, 116.8, 53.6, 53.0, 37.6, 30.3.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 260.0918; found: 260.0920.

Methyl 2-acetyl-4-(2-methoxyphenyl)-4-oxobutanoate (2k):

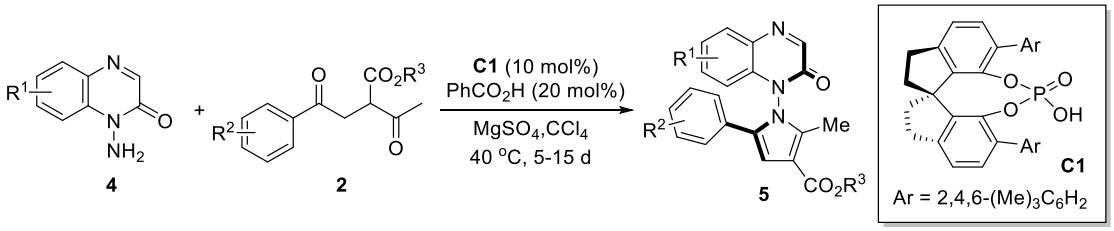


White solid (68% yield).
M.p.: 62-64 ℃.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (dd, *J* = 7.8, 1.7 Hz, 1H), 7.45 (ddd, *J* = 8.4, 7.4, 1.9 Hz, 1H), 6.99–6.92 (m, 2H), 4.17 (dd, *J* = 8.0, 5.8 Hz, 1H), 3.89 (s, 3H), 3.73 (s, 3H), 3.69 (dd, *J* = 19.0, 8.1 Hz, 1H), 3.54 (dd, *J* = 19.0, 5.8 Hz, 1H), 2.38 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 202.9, 198.3, 169.8, 159.2, 134.3, 130.7, 126.5, 120.6, 111.7, 55.6, 54.1, 52.6, 42.8, 30.2.
HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 265.1071; found: 265.1065.

(3) Synthesis and Characterization of Products 3 and 5



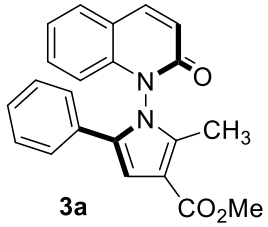
General Procedure A:
To a flame dried Schlenk tube were added **1** (0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2** (0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 5-15 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography to afford the pure product **3**.



General Procedure B:
To a flame dried Schlenk tube were added **4** (0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), $PhCO_2H$ (0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2** (0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 5-15 d. Then the solution was concentrated under vacuum and the mixture was purified through column

chromatography to afford the pure product **5**.

Methyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (**3a**):



3a

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ^oC for 5 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3a** in 98% yield (36.4 mg) as a white solid.

M.p.: 76-78 ℃

IR (film) υ_{max}/cm^{-1}: 2947, 1705, 1680, 1597, 1496, 1446, 1251, 1208, 835.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 9.7 Hz, 1H), 7.55 (d, *J* = 6.4 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.25–7.19 (m, 3H), 7.18–7.11 (m, 3H), 6.89 (s, 1H), 6.76 (d, *J* = 9.7 Hz, 1H), 6.36 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).

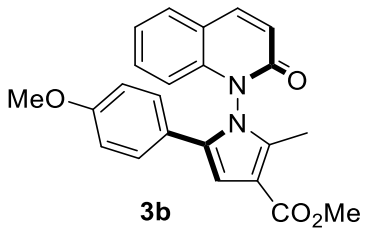
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.4, 160.3, 141.0, 140.6, 137.0, 133.2, 131.9, 130.1, 128.8, 128.6, 127.9, 127.7, 124.0, 121.4, 120.0, 113.0, 112.3, 108.9, 51.3, 10.4.

HRMS (ESI) m/z: $[C_{22}H_{18}N_2O_3+H]^+$ calcd.: 359.1390; found: 359.1381.

Optical Rotation: $[\alpha]_D^{28}$ = +3.9 (*c* = 0.1, $CHCl_3$) [91% *ee*].

Chiral HPLC: 91% *ee* [Chiral MD (2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/min, 254 nm, t_R = 10.12 min (major), 17.15 min (minor)].

Methyl (*S*)-5-(4-methoxyphenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3b):



3b

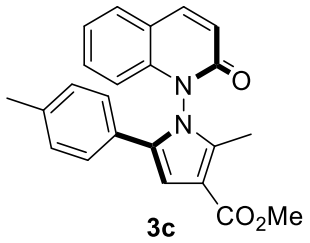
To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2b** (26.4 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ^oC for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3b** in 98% yield (38.0 mg) as a faint yellow solid.

M.p.: 132-134 ℃

IR (film) υ_{max}/cm^{-1}**:** 2974, 1708, 1681, 1598, 1448, 1243, 1219, 1071, 828, 753, 698.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 9.7 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.9 Hz, 1H), 7.22 (t, *J* = 7.6 Hz, 1H), 7.14 (d, *J* = 8.7 Hz, 2H), 6.80 (s, 1H), 6.76 (d, *J* = 9.7 Hz, 1H), 6.67 (d, *J* = 8.7 Hz, 2H), 6.34 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H), 3.68 (s, 3H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.5, 160.4, 159.3, 141.0, 140.6, 136.5, 133.0, 131.9, 129.2, 128.8, 123.9, 122.6, 121.4, 120.0, 114.0, 113.0, 112.1, 108.2, 55.2, 51.3, 10.4.
HRMS (ESI) m/z: $[C_{23}H_{20}N_2O_4+H]^+$ calcd.: 389.1496; found: 389.1489.
Optical Rotation: $[\alpha]_D^{28}$ = +7.9 (*c* = 0.1, $CHCl_3$) [85% *ee*].
Chiral HPLC: 87% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 20.43 min (major), 33.24 min (minor)].

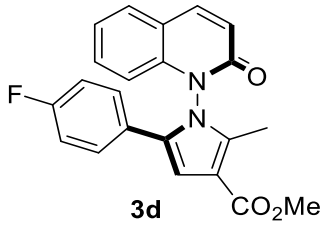
Methyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-(p-tolyl)-1*H*-pyrrole-3-carboxylate (3c):



3c

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2c** (30.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3c** in 97% yield (35.9 mg) as a faint yellow solid.
M.p.: 131-133 ℃.
IR (film) υ_{max}/cm^{-1}**:** 2948, 1708, 1683, 1598, 1448, 1243, 1219, 828.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 9.7 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.44–7.37 (m, 1H), 7.25–7.19 (m, 1H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.95 (d, *J* = 7.9 Hz, 2H), 6.85 (s, 1H), 6.77 (d, *J* = 9.6 Hz, 1H), 6.36 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.25 (s, 3H), 2.20 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.5, 160.4, 141.0, 140.7, 137.8, 136.7, 133.3, 131. 9, 129.3, 128.8, 127.6, 127.2, 124.0, 121.4, 120.0, 113.0, 112.2, 108.5, 51.3, 21.2, 10.4.
HRMS (ESI) m/z: $[C_{23}H_{20}N2O_3+H]^+$ calcd.: 373.1547; found: 373.1542.
Optical Rotation: $[\alpha]_D^{28}$= +7.7 (*c* = 0.1, $CHCl_3$) [82% *ee*].
Chiral HPLC: 82% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 11.62 min (major), 19.53 min (minor)].

Methyl (*S*)-5-(4-fluorophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3d):



3d

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2d** (30.3 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 6 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3d** in 85% yield (32.0 mg) as a faint yellow solid.

M.p.: 121-123 ℃.

IR (film) υ_{max}/cm^{-1}**:** 2948, 1708, 1685, 1599, 1439, 1401, 1220, 829, 752.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 9.6 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 8.6 Hz, 1H), 7.25–7.15 (m, 3H), 6.87–6.80 (m, 3H), 6.75 (d, *J* = 9.7 Hz, 1H), 6.33 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$):** δ 165.3, 162.5 (d, *J* = 249.5 Hz), 160.3, 141.1, 140.5, 136.9, 132.2, 131.9, 129.8 (d, *J* = 10.1 Hz), 128.9, 126.2 (d, *J* = 3.0 Hz), 124.1, 121.2, 120.0, 115.6 (d, *J* = 21.2 Hz), 112.8, 112.2, 108.9, 51.3, 10.4.

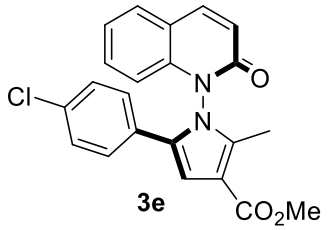
^{19}F NMR (**376 MHz, $CDCl_3$):** δ -113.4.

HRMS (ESI) m/z: $[C_{22}H_{17}FN_2O_3+H]^+$ calcd.: 377.1296; found: 377.1288.

Optical Rotation: $[\alpha]_D^{28}$ = +9.6 (*c* = 0.1, $CHCl_3$) [92% *ee*].

Chiral HPLC: 92% *ee* [Chiral ND(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 11.46 min (major), 14.41 min (minor)].

Methyl (*S*)-5-(4-chlorophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3e):



3e

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2e** (32.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 12 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3e** in 94% yield (36.4 mg) as a faint yellow solid.

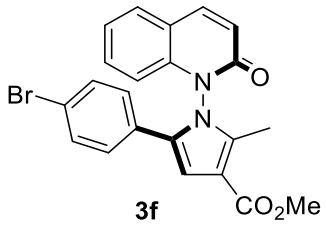
M.p.: 135-137 ℃.

IR (film) υ_{max}/cm^{-1}: 3017, 2949, 1703, 1677, 1599, 1448, 1249, 1212, 843, 752.

^{1}H NMR (400 MHz, $CDCl_3$):δ 7.78 (d, *J* = 9.7 Hz, 1H), 7.57 (d, *J* = 6.4 Hz, 1H), 7.41 (t, *J* = 7.2 Hz, 1H), 7.26–7.22 (m, 1H), 7.17–7.10 (m, 4H), 6.88 (s, 1H), 6.77 (d, *J* = 9.7

Hz, 1H), 6.32 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.2, 160.3, 141.2, 140.5, 137.3, 133.9, 132.0, 128.98, 128.96, 128.90, 128.6, 124.2, 121.3, 120.1, 112.8, 112.5, 109.2, 51.4, 10.4.
HRMS (ESI) m/z: $[C_{22}H_{17}ClN_2O_3+H]^+$ calcd.: 393.1001; found: 393.0997.
Optical Rotation: $[\alpha]_D^{28}$ = +7.9 (*c* = 0.1, $CHCl_3$) [88% *ee*].
Chiral HPLC: 89% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 12.83 min (major), 23.70 min (minor)].

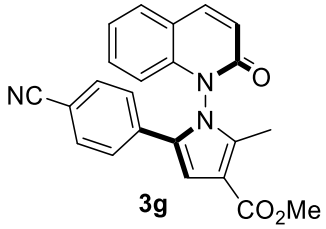
Methyl (*S*)-5-(4-bromophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3f):



3f

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2f** (37.6 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 16 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3f** in 90% yield (39.2 mg) as a white solid.
M.p.: 118-120 ℃.
IR (film) υ_{max}/cm^{-1}**:** 2944, 1712, 1681, 1598, 1440, 1245, 1217, 1067, 825, 775, 749.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.78 (d, *J* = 9.7 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.41 (t, *J* = 8.6 Hz, 1H), 7.30–7.22 (m, 4H), 7.11–7.06 (m, 2H), 6.89 (s, 1H), 6.76 (d, *J* = 9.7 Hz, 1H), 6.31 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.2, 160.3, 141.2, 140.5, 137.4, 132.0, 131.8, 129.2, 129.1, 129.0, 124.2, 122.2, 121.3, 120.1, 112.8, 112.5, 109.2, 51.4, 10.4.
HRMS (ESI) m/z: $[C_{22}H_{17}BrN_2O_3+H]^+$ calcd.: 437.0496; found: 437.0495.
Optical Rotation: $[\alpha]_D^{28}$ = +5.6 (*c* = 0.1, $CHCl_3$) [89% *ee*].
Chiral HPLC: 89% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 12.83 min (major), 25.52 min (minor)].

Methyl (*S*)-5-(4-cyanophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3g):



3g

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2g** (31.0 mg, 0.12 mmol). The

resulting reaction mixture was stirred at 25 ºC for 23 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3g** in 98% yield (34.4 mg) as a yellow solid.

M.p.: 150-152 ℃.

IR (film) υ_{max}/cm^{-1}: 2942, 2222, 1712, 1678, 1601, 1521, 1439, 1221, 824, 770, 756.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.82 (d, *J* = 9.7 Hz, 1H), 7.61 (d, *J* = 7.8 Hz, 1H), 7.47–7.40 (m, 3H), 7.32–7.23 (m, 4H), 7.02 (s, 1H), 6.78 (d, *J* = 9.7 Hz, 1H), 6.33 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).

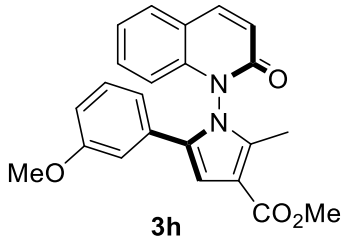
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 164.9, 160.1, 141.4, 140.3, 138.6, 134.5, 132.6, 132.2, 131.1, 129.2, 127.4, 124.4, 121.2, 120.0, 118.6, 113.0, 112.5, 111.1, 110.8, 51.5, 10.4.

HRMS (ESI) m/z: $[C_{23}H_{17}N_3O_2+H]^+$ calcd.: 384.1343; found: 384.1334.

Optical Rotation: $[\alpha]_D^{28}$ = +7.1 (*c* = 0.1, $CHCl_3$) [94% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 35/65, 0.8 mL/min, 254 nm, t_R = 12.66min (major), 30.74 min (minor)].

Methyl (*S*)-5-(3-methoxyphenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3h):



3h

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2h** (31.7 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ºC for 13 d. Then the solution was concentrated under vacuum. Finally, the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3h** in 93% yield (36.1 mg) as a white solid.

M.p.: 54-56 ℃.

IR (film) υ_{max}/cm^{-1}:1708, 1680, 1598, 1448, 1223, 1075, 773, 753.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.77 (d, *J* = 9.9 Hz, 1H), 7.57 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 8.6 Hz, 1H), 7.26–7.21 (m, 1H), 7.06 (t, *J* = 8.0 Hz, 1H), 6.90 (s, 1H), 6.81 (dt, *J* = 7.7, 1.3 Hz, 1H), 6.78–6.75 (m, 2H), 6.68 (dd, *J* = 8.3, 2.6 Hz, 1H), 6.38 (d, *J* = 8.3 Hz, 1H), 3.87 (s, 3H), 3.58 (s, 3H), 2.27 (s, 3H).

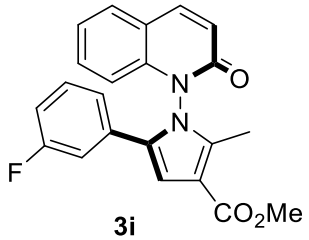
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 165.4, 160.3, 159.5, 141.1, 140.7, 137.2, 133.1, 132.0, 131.3, 129.7, 128.9, 124.0, 121.4, 120.1, 120.0, 114.4, 113.0, 112.3, 112.2, 109.0, 55.1, 51.3, 10.4.

HRMS (ESI) m/z: $[C_{23}H_{20}N_2O_4+H]^+$ calcd.: 389.1496; found: 389.1488.

Optical Rotation: $[\alpha]_D^{28}$ = +1.0 (*c* = 1.0, $CHCl_3$) [84% *ee*].

Chiral HPLC: 84% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 16.52 min (major), 27.38 min (minor)].

Methyl (*S*)-5-(3-fluorophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3i):



3i

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2i** (30.3 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 5 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3i** in 98% yield (36.8 mg) as a white solid.

M.p.: 53-55 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3066, 2948, 1709, 1681, 1598, 1448, 1222, 1075, 773, 752.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 9.7 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 8.6 Hz, 1H), 7.27–7.22 (m, 1H), 7.11 (td, *J* = 8.0, 6.1 Hz, 1H), 6.99 (d, *J* = 7.8 Hz, 1H), 6.93–6.89 (m, 2H), 6.82 (td, *J* = 8.2, 1.6 Hz, 1H), 6.77 (d, *J* = 9.7 Hz, 1H), 6.35 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$**)**:**δ 165.2, 163.7(d, *J* = 247.4 Hz), 160.2, 141.2, 140.4, 137.5, 132.1, 132.0, 131.8 (d, *J* = 2.0 Hz), 130.2(d, *J* = 10.1 Hz), 128.0, 124.2, 123.1(d, *J* = 3.0 Hz), 121.3, 120.0, 114.8(d, *J* = 20.2 Hz), 114.4(d, *J* = 30.3 Hz), 112.8, 112.5, 109.5, 51.4, 10.4.

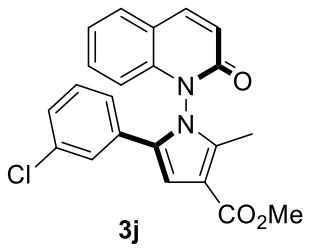
^{19}F NMR (**376 MHz, $CDCl_3$**)**:** -112.4.

HRMS (ESI) m/z: $[C_{22}H_{17}FN_2O_3+H]^+$ calcd: 377.1296; found: 377.1286

Optical Rotation: $[\alpha]_D^{28}$ = +4.8 (*c* = 1.0, $CHCl_3$) [90% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 12.44 min (major), 18.87 min (minor)].

Methyl (*S*)-5-(3-chlorophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3j):



3j

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2j** (32.3 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 13 d. Then the solution was

concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3j** in 80% yield (36.4 mg) as a white solid.

M.p.: 60-62 ℃.

IR (film) υ_{max}/cm^{-1}: 3063, 2947, 1709, 1681, 1599, 1439, 1244, 1219, 1074, 774, 752.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.79 (d, *J* = 9.3 Hz, 1H), 7.58 (d, *J* = 7.8 Hz, 1H), 7.43 (t, *J* = 8.6 Hz, 1H), 7.27–7.24 (m, 1H), 7.23–7.21 (m, 1H), 7.12–7.05 (m, 3H), 6.92 (s, 1H), 6.78 (d, *J* = 9.7 Hz, 1H), 6.34 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).

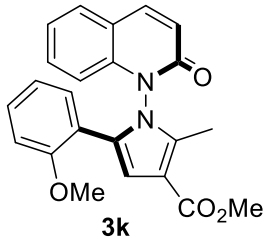
^{13}C NMR (101 MHz, CDCl$_3$): δ 165.2, 160.2, 141.2, 140.5, 137.6, 134.5, 132.1, 131.8, 131.6, 129.9, 129.0, 128.0, 127.6, 125.4, 124.2, 121.3, 120.0, 112.8, 112.5, 109.6, 51.4, 10.4.

HRMS (ESI) m/z: $[C_{22}H_{17}ClN_2O_3+H]^+$ calcd: 393.1001; found: 393.0995.

Optical Rotation: $[\alpha]_D^{28}$ = +2.6 (*c* = 1.0, $CHCl_3$) [92% *ee*].

Chiral HPLC: 92 % *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 13.27 min (major), 21.30 min (minor)].

Methyl (*S*)-5-(2-methoxyphenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3k):



3k

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2k** (32.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ºC for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3k** in 80% yield (30.2 mg) as a white solid.

M.p.: 134-136 ℃.

IR (film) υ_{max}/cm^{-1}: 3000, 2946, 2830, 1707, 1677, 1598, 1447, 1256, 1218, 1072, 766.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.67 (d, *J* = 9.7 Hz, 1H), 7.49 (d, *J* = 9.2 Hz, 1H), 7.43–7.37 (m, 1H), 7.21–7.15 (m, 2H), 7.15–7.10 (m, 1H), 6.85 (s, 1H), 6.74 (t, *J* = 7.5 Hz, 1H), 6.65–7.70 (m, 2H), 6.59 (d, *J* = 8.5 Hz, 1H), 3.86 (s, 3H), 3.50 (s, 3H), 2.28 (s, 3H).

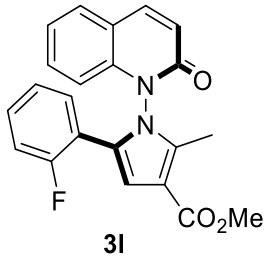
^{13}C NMR (101 MHz, CDCl$_3$): δ 165.6, 160.0, 157.4, 140.6, 140.5, 136.5, 131.9, 131.1, 129.9, 129.0, 128.4, 123.6, 121.3, 120.3, 119.8, 118.9, 113.9, 111.9, 110.6, 110.5, 55.0, 51.2, 10.7.

HRMS (ESI) m/z: $[C_{23}H_{20}N_2O_4+H]^+$ calcd.: 389.1496; found: 389.1493.

Optical Rotation: $[\alpha]_D^{28}$ = +2.4 (*c* = 1.0, $CHCl_3$) [90% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R =17.72min (minor), 20.66 min (major)].

Methyl (*S*)-5-(2-fluorophenyl)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (3l):



3l

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2l** (30.3 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ^oC for 16 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3l** in 94% yield (35.4 mg) as a white solid.

M.p.: 150-152 ℃.

IR (film) υ_{max}/cm^{-1}: 2924, 1709, 1685, 1599, 1485, 1449, 1246, 1221, 753.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.73 (d, *J* = 9.7 Hz, 1H), 7.52 (d, *J* = 7.7 Hz, 1H), 7.44–7.38 (m, 1H), 7.24–7.16 (m, 2H), 7.15–7.09 (m, 1H), 6.96 (s, 1H), 6.94–6.88 (m, 2H), 6.73 (d, *J* = 9.7 Hz, 1H), 6.41 (d, *J* = 8.4 Hz, 1H), 3.86 (s, 3H), 2.28 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$**)**:** δ 165.3, 160.3, 160.0 (d, *J* = 250.5 Hz), 141.0, 140.4, 137.2, 131.8, 130.7, 130.0 (d, *J* = 8.1 Hz), 128.7, 125.5, 124.0, 124.0, 121.2, 119.9, 117.8 (d, *J* = 14.1 Hz), 115.9 (d, *J* = 23.2 Hz), 113.0, 112.3, 111.5 (d, *J* = 3.0 Hz), 51.3, 10.5.

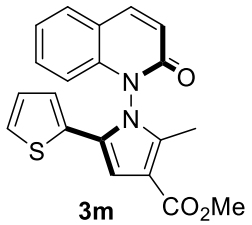
^{19}F NMR (**376 MHz, $CDCl_3$**)**:** δ -113.8.

HRMS (ESI) m/z: $[C_{22}H_{17}FN_2O_3+H]^+$ calcd.: 377.1296; found: 377.1289.

Optical Rotation: $[\alpha]_D^{28}$ = +3.4 (*c* = 1.0, $CHCl_3$) [71% *ee*].

Chiral HPLC: 71% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 10/90, 0.8 mL/min, 254 nm, t_R = 22.11 min (major), 26.44 min (minor)].

Methyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-(thiophen-2-yl)-1*H*-pyrrole-3-carboxylate (3m):

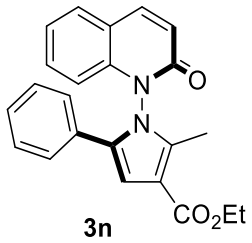


3m

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2m** (28.8 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ^oC for 9 d. Then the solution was concentrated under vacuum. Finally, the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3m** in 91% yield (33.0 mg) as a

white solid.
M.p.: 78-80 ℃.
IR (film) υ_{max}/cm^{-1}: 2946, 1707, 1682, 1598, 1447, 1244, 1222, 1076, 828, 772, 753.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.84 (d, *J* = 9.7 Hz, 1H), 7.64 (d, *J* = 9.2 Hz, 1H), 7.44 (t, *J* = 8.6 Hz, 1H), 7.29 (d, *J* = 8.5 Hz, 1H), 7.04–6.99 (m, 2H), 6.82–6.77 (m, 3H), 6.47 (d, *J* = 7.5 Hz, 1H), 3.87 (s, 3H), 2.27 (s, 3H).
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 165.2, 160.0, 141.2, 140.5, 137.1, 132.0, 130.9, 129.0, 127.4, 126.1, 125.1, 124.6, 124.1, 121.5, 120.2, 112.9, 112.3, 109.0, 51.4, 10.4.
HRMS (ESI) m/z: $[C_{20}H_{16}N_2O_3S+H]^+$ calcd.: 365.0955; found: 365.0945.
Optical Rotation: $[\alpha]_D^{28}$ = +4.8 (*c* = 1.0, $CHCl_3$) [88% *ee*].
Chiral HPLC: 88% *ee* [Chiral ND(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 19.07min (major), 48.76 min (minor)].

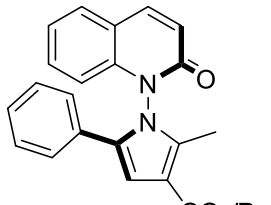
Ethyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-(o-tolyl)-1*H*-pyrrole-3-carboxylate (3n):



3n

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), C1 (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2n** (30.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3n** in 89% yield (33.0 mg) as a white solid.
M.p.: 138-140 ℃.
IR (film) υ_{max}/cm^{-1}: 3068, 2977, 1679, 1598, 1451, 1245, 1219, 1070, 829, 755, 697.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.76 (d, *J* = 9.6 Hz, 1H), 7.55 (d, *J* = 9.2 Hz, 1H), 7.44–7.38 (m, 1H), 7.25–7.19 (m, 3H), 7.18–7.11 (m, 3H), 6.90 (s, 1H), 6.77 (d, *J* = 9.7 Hz, 1H), 6.38 (d, *J* = 8.3 Hz, 1H), 4.38–4.31 (m, 2H), 2.26 (s, 3H), 1.38 (t, *J* = 7.1 Hz, 3H).
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 165.0, 160.4, 141.0, 140.6, 136.8, 133.1, 131.9, 130.2, 128.8, 128.6, 127.9, 127.7, 124.0, 121.4, 120.0, 113.0, 112.6, 109.0, 60.0, 14.6, 10.4.
HRMS (ESI) m/z: $[C_{23}H_{20}N_2O_3+H]^+$ calcd.: 373.1547; found: 373.1539.
Optical Rotation: $[\alpha]_D^{28}$ = +10.8 (*c* = 1.0, $CHCl_3$) [88% *ee*].
Chiral HPLC: 88% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 11.49 min (major), 15.72 min (minor)].

Isopropyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3o):



3o

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (1.2 mg, 0.01 mmol) anhydrous CCl_4 (1.0 mL) and **2o** (31.5 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ºC for 13 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3o** in 97% yield (37.5 mg) as a white solid.

M.p.: 118-120 ℃.

IR (film) υ_{max}/cm^{-1}: 2977, 2930, 1705, 1672, 1599, 1447, 1246, 1220, 1063, 755.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 9.7 Hz, 1H), 7.55 (d, *J* = 9.1 Hz, 1H), 7.41 (t, *J* = 8.6 Hz, 1H), 7.25–7.20 (m, 3H), 7.18–7.11 (m, 3H), 6.90 (s, 1H), 6.77 (d, *J* = 9.7 Hz, 1H), 6.39 (d, *J* = 8.4 Hz, 1H), 5.23 (hept, *J* = 6.3 Hz, 1H), 2.26 (s, 3H), 1.36 (t, *J* = 6.4 Hz, 6H).

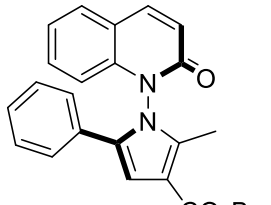
^{13}C NMR (101 MHz, $CDCl_3$): δ 164.6, 160.4, 141.0, 140.6, 136.6, 133.0, 131.9, 130.2, 128.8, 128.6, 127.8, 127.7, 124.0, 121.4, 120.0, 113.1, 113.0, 109.1, 67.2, 22.3, 10.5.

HRMS (ESI) m/z: $[C_{24}H_{22}N_2O_3+H]^+$ calcd.: 387.1703; found: 387.1698.

Optical Rotation: $[\alpha]_D^{28}$ = +5.8 (*c* = 1.0, $CHCl_3$) [88% *ee*].

Chiral HPLC: 88% *ee* [Chiral NQ(2), 250×4.6, *i*-PrOH/*n*-heptane = 40/60, 0.8 mL/min, 254 nm, t_R = 14.97 min (major), 27.96min (minor)].

Benzyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3p):



3p

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2p** (37.2 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ºC for 13 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3p** in 86% yield (37.3 mg) as a white solid.

M.p.: 60-62 ℃.

IR (film) υ_{max}/cm^{-1}**:** 2921, 1683, 1598, 1448, 1213, 1119, 1061, 828, 752, 696.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 9.7 Hz, 1H), 7.55 (d, *J* = 9.2 Hz, 1H), 7.47

(d, *J* = 6.7 Hz, 2H), 7.44–7.37 (m, 3H), 7.36–7.30 (m, 1H), 7.25–7.20 (m, 3H), 7.16–7.12 (m, 3H), 6.93 (s, 1H), 6.77 (d, *J* = 9.7 Hz, 1H), 6.38 (d, *J* = 8.4 Hz, 1H), 5.35 (s, 2H), 2.27 (s, 3H).

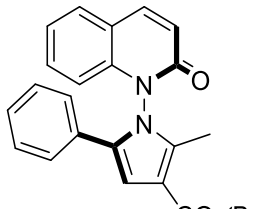
^{13}C NMR (101 MHz, $CDCl_3$): δ 164.7, 160.3, 141.0, 140.6, 137.2, 136.7, 133.2, 131.9, 130.1, 128.8, 128.7, 128.6, 128.3, 128.2, 127.9, 127.7, 124.0, 121.4, 120.0, 113.0, 112.2, 109.0, 65.8, 10.5.

HRMS (ESI) m/z: $[C_{28}H_{22}N_2O_3+H]^+$ calcd.: 435.1703; found: 435.1699.

Optical Rotation: $[\alpha]_D^{28}$ = +3.3 (*c* = 1.0, $CHCl_3$) [84% *ee*].

Chiral HPLC: 84% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 16.96 min (major), 25.06 min (minor)].

***tert*-Butyl (*S*)-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3q):**



3q

To a flame dried Schlenk tube were added **1a** (16.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (1.2 mg, 0.01 mmol), anhydrous CCl_4 (1.0 mL) and **2q** (33.2 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ºC for 13 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3q** in 97% yield (38.7 mg) as a white solid.

M.p.:145-147 ℃.

IR (film) υ_{max}/cm^{-1}: 3068, 2971, 1706, 1678, 1599, 1450, 1246, 1156, 1065, 834, 751, 699.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.75 (d, *J* = 9.5 Hz, 1H), 7.54 (d, *J* = 9.2 Hz, 1H), 7.41 (t, *J* = 8.6 Hz, 1H), 7.24–7.19 (m, 3H), 7.17–7.11 (m, 3H), 6.85 (s, 1H), 6.77 (d, *J* = 9.7 Hz, 1H), 6.39 (d, *J* = 8.5 Hz, 1H), 2.24 (s, 3H), 1.59 (s, 9H).

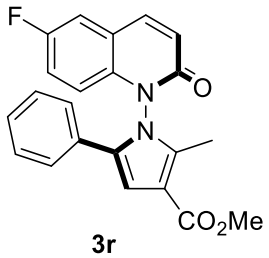
^{13}C NMR (101 MHz, $CDCl_3$): δ 164.4, 160.4, 141.0, 140.6, 136.1, 132.7, 131.9, 130.3, 128.8, 128.6, 127.8, 127.6, 123.9, 121.4, 120.0, 114.1, 113.1, 109.2, 80.2, 28.5, 10.4.

HRMS (ESI) m/z: $[C_{25}H_{24}N_2O_3+H]^+$ calcd.: 401.1860; found: 401.1862.

Optical Rotation: $[\alpha]_D^{28}$ = +5.0 (*c* = 1.0, $CHCl_3$) [86% *ee*].

Chiral HPLC: 86% *ee* [Chiral NQ (2), 250×4.6, *i*-PrOH/*n*-heptane = 35/65, 0.8 mL/min, 254 nm, t_R = 12.28 min (major), 43,68 min (minor)].

Methyl (*S*)-1-(6-fluoro-2-oxoquinolin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3r):



3r

To a flame dried Schlenk tube were added **1r** (17.8 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 7 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3r** in 60% yield (22.6 mg) as a white solid.

M.p.: 100-102 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3064, 2949, 2923, 1708, 1672, 1570, 1438, 1220, 1070, 886, 811, 759.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.70 (d, *J* = 9.7 Hz, 1H), 7.25–7.19 (m, 3H), 7.18 – 7.09 (m, 4H), 6.88 (s, 1H), 6.82 (d, *J* = 9.7 Hz, 1H), 6.30 (dd, *J* = 9.2, 4.3 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$):** δ 165.3, 160.0, 158.9 (d, *J* = 245.4 Hz), 140.0 (d, *J* = 3.0 Hz), 137.0, 136.9, 133.2, 129.9, 128.7, 128.1, 127.6, 122.8, 120.8 (d, *J* = 9.1 Hz), 119.6 (d, *J* = 24.2 Hz), 114.8 (d, *J* = 8.1 Hz), 114.1 (d, *J* = 23.2 Hz), 112.5, 109.0, 51.4, 10.4.

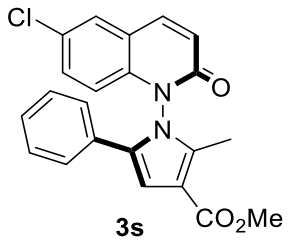
^{19}F NMR (**376 MHz, $CDCl_3$):** δ -118.26.

HRMS (ESI) m/z: $[C_{22}H_{17}FN_2O_3+H]^+$ calcd.: 377.1296; found:377.1286.

Optical Rotation: $[\alpha]_D^{28}$ = +6.0 (*c* = 1.0, $CHCl_3$) [94% *ee*].

Chiral HPLC: 90%*ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane=35/65, 0.8 mL/min, 254 nm, t_R = 15.03min (major), 26.99min (minor)].

Methyl (*S*)-1-(6-chloro-2-oxoquinolin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3s):

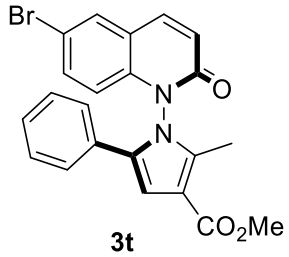


3s

To a flame dried Schlenk tube were added **1s** (19.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 23 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3s** in 92% yield (36.2 mg) as a white solid.

M.p.: 76-78 ℃.
IR (film) υ_{max}/cm^{-1}: 3062, 2947, 1683, 1558, 1428, 1242, 1210, 1071, 811, 758, 697.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.68 (d, *J* = 9.8 Hz, 1H), 7.53 (d, *J* = 2.3 Hz, 1H), 7.34 (dd, *J* = 8.9, 2.3 Hz, 1H), 7.23–7.14 (m, 5H), 6.88 (s, 1H), 6.80 (d, *J* = 9.7 Hz, 1H), 6.28 (d, *J* = 8.9 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$): δ 165.2, 159.8, 139.8, 139.1, 136.8, 133.1, 131.9, 129.9, 129.5, 128.7, 128.1, 128.0, 127.6, 122.7, 121.0, 114.5, 112.5, 109.0, 51.4, 10.4.
HRMS (ESI) m/z: $[C_{22}H_{17}ClN_2O_3+H]^+$ calcd.: 393.1001; found: 393.0994.
Optical Rotation: $[\alpha]_D^{28}$ = +3.0(*c* = 1.0, $CHCl_3$) [94% *ee*].
Chiral HPLC: 88% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/min, 254 nm, t_R = 11.63min (major), 18.48min (minor)].

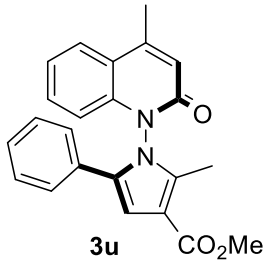
Methyl (*S*)-1-(6-bromo-2-oxoquinolin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3t):



3t

To a flame dried Schlenk tube were added **1t** (23.9 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 13 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3t** in 97% yield (42.4 mg) as a white solid.
M.p.: 151-153 ℃.
IR (film) υ_{max}/cm^{-1}: 3113, 2944, 1706, 1682, 1585, 1425, 1245, 1216, 1081, 929, 820, 778, 761, 696.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.69–7.65 (m, 2H), 7.47 (dd, *J* = 8.9, 2.1 Hz, 1H), 7.23–7.14 (m, 5H), 6.88 (s, 1H), 6.80 (d, *J* = 9.8 Hz, 1H), 6.22 (d, *J* = 8.9 Hz, 1H), 3.87 (s, 3H), 2.26 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$): δ 165.3, 159.8, 139.7, 139.6, 136.8, 134.6, 133.2, 131.1, 129.9, 128.7, 128.1, 127.7, 122.7, 121.4, 116.9, 114.8, 112.5, 109.0, 51.4, 10.4.
HRMS (ESI) m/z: $[C_{22}H_{17}BrN_2O_3+H]^+$ calcd.: 437.0496; found: 437.0488.
Optical Rotation: $[\alpha]_D^{28}$= -1.1 (*c* = 1.0, $CHCl_3$) [84% *ee*].
Chiral HPLC: 84% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 15.47min (major), 26.67min (minor)].

Methyl (*S*)-2-methyl-1-(4-methyl-2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3u):



3u

To a flame dried Schlenk tube were added **1u** (17.4 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3u** in 86% yield (32.2 mg) as a white solid.

M.p.: 145-147 ℃.

IR (film) υ_{max}/cm^{-1}: 2923, 2854, 1704, 1683, 1539, 1437, 1246, 1203, 1070, 765, 750.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.66 (d, *J* = 8.0 Hz, 1H), 7.43–7.37 (m, 1H), 7.26–7.22 (m, 3H), 7.18–7.12 (m, 3H), 6.88 (s, 1H), 6.65 (s, 1H), 6.33 (d, *J* = 8.4 Hz, 1H), 3.87 (s, 3H), 2.50 (s, 3H), 2.24 (s, 3H).

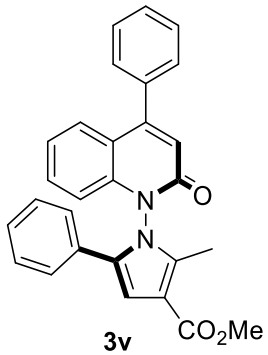
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.4, 160.1, 149.2, 140.1, 137.2, 133.3, 131.7, 130.2, 128.6, 127.8, 127.7, 125.6, 123.8, 120.8, 120.5, 113.2, 112.2, 108.8, 51.3, 19.5, 10.4.

HRMS (ESI) m/z: $[C_{22}H_{17}BrN_2O_3+H]^+$ calcd.: 373.1547; found: 373.1545.

Optical Rotation: $[\alpha]_D^{28}$= +2.8 (*c* = 1.0, $CHCl_3$) [84% *ee*].

Chiral HPLC: 84% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 13.31min (major), 22.43min (minor)].

Methyl (*S*)-2-methyl-1-(2-oxo-4-phenylquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (3v):



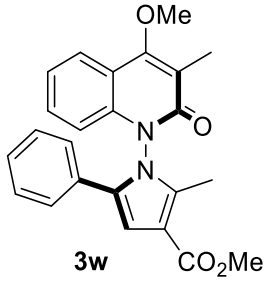
3v

To a flame dried Schlenk tube were added **1v** (23.6 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 23 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3v** in 97% yield (42.0 mg) as a white solid.

M.p.: 184-186 ℃.

IR (film) υ_{max}/cm^{-1}: 2947, 1697, 1675, 1444, 1249, 1207, 1079, 866, 752, 698.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.55–7.49 (m, 4H), 7.46–7.39 (m, 3H), 7.31–7.27 (m, 2H), 7.22–7.13 (m, 4H), 6.92 (s, 1H), 6.73 (s, 1H), 6.40 (d, *J* = 8.4 Hz, 1H), 3.89 (s, 3H), 2.33 (s, 3H).
^{13}C NMR (**101 MHz, CDCl$_3$**)**:** δ 165.4, 160.0, 153.2, 140.7, 137.2, 136.3, 133.3, 131.9, 130.2, 129.4, 128.9, 128.9, 128.7, 128.0, 127.9, 127.8, 123.8, 120.7, 119.9, 113.3, 112.3, 109.0, 51.3, 10.6.
HRMS (ESI) m/z: $[C_{28}H_{22}N_2O_3+H]^+$ calcd.: 435.1703; found: 435.1691.
Optical Rotation: $[\alpha]_D^{28}$ = +11.6(*c* = 1.0, $CHCl_3$) [84% *ee*].
Chiral HPLC: 86% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/Fmin, 254 nm, t_R = 9.79min (major), 13.64min (minor)].

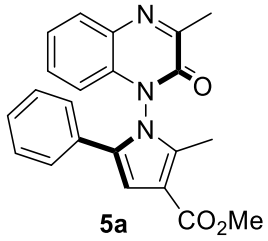
Methyl (*S*)-1-(4-methoxy-3-methyl-2-oxoquinolin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (3w):



3w

To a flame dried Schlenk tube were added **1w** (20.4 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 °C for 7 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **3w** in 97% yield (39.0 mg) as a white solid.
M.p.: 126-128 ℃.
IR (film) υ_{max}/cm^{-1}**:** 2949, 2846, 1714, 1661, 1601, 1455, 1242, 1127, 1066, 768, 750.
^{1}H NMR (400 MHz, CDCl$_3$):δ 7.80 (d, *J* = 7.9 Hz, 1H), 7.37 (t, *J* = 7.1 Hz, 1H), 7.26–7.21 (m, 1H), 7.20–7.16 (m, 2H), 7.16–7.11 (m, 3H), 6.87 (s, 1H), 6.37 (d, *J* = 8.2 Hz, 1H), 3.96 (s, 3H), 3.87 (s, 3H), 2.25 (s, 3H), 2.23 (s, 3H).
^{13}C NMR (**101 MHz, CDCl$_3$**)**:** δ 165.5, 162.6, 161.8, 138.9, 137.3, 133.3, 131.2, 130.3, 128.6, 127.8, 127.6, 123.7, 123.6, 118.5, 117.3, 112.9, 112.1, 108.8, 61.5, 51.3, 10.8, 10.5.
HRMS (ESI) m/z: $[C_{22}H_{17}BrN_2O_3+H]^+$ calcd.: 403.1653; found: 403.1650.
Optical Rotation: $[\alpha]_D^{28}$ = +3.0 (*c* = 1.0, $CHCl_3$) [87% *ee*].
Chiral HPLC: 87% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 10.91 min (major), 37.63 min (minor)].

Methyl (*S*)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (5a):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5a** in 80% yield (29.8 mg) as a white solid.

M.p.:131-133 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3084, 2945, 1705, 1677, 1603, 1438, 1243, 1212, 1141, 1069, 775, 762, 695.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.9 Hz, 1H), 7.42–7.36 (m, 1H), 7.35–7.30 (m, 1H), 7.15 (s, 5H), 6.87 (s, 1H), 6.42 (d, *J* = 8.2 Hz, 1H), 3.87 (s, 3H), 2.62 (s, 3H), 2.26 (s, 3H).

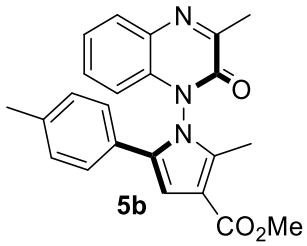
^{13}C NMR (**101 MHz, $CDCl_3$**)**:** δ 165.2, 159.1, 153.2, 136.7, 133.7, 133.3, 132.1, 130.8, 129.8, 129.5, 128.7, 128.2, 127.7, 125.3, 112.7, 112.5, 109.1, 51.4, 21.6, 10.5.

HRMS (ESI) m/z: $[C_{22}H_{17}BrN_2O_3+H]^+$ calcd.: 374.1499; found: 374.1491.

Optical Rotation: $[\alpha]_D^{28}$ = +6.7 (*c* = 1.0, $CHCl_3$) [90% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 8.66 min (major), 16.16 min (minor)].

Methyl (*S*)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-5-(p-tolyl)-1*H*-pyrrole-3-carboxylate (5b):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2b** (29.8 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 10 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5b** in 82% yield (31.6 mg) as a white solid.

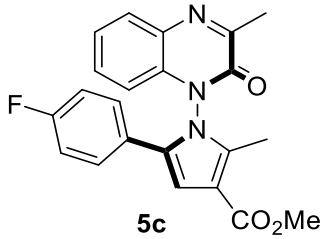
M.p.: 121-123 ℃.

IR (film) υ_{max}/cm^{-1}**:** 2945, 1714, 1673, 1604, 1437, 1238, 1212, 1144, 1070, 771, 758.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.79 (d, *J* = 7.9 Hz, 1H), 7.38 (t, *J* = 7.8 Hz, 1H), 7.32

(t, *J* = 7.6 Hz, 1H), 7.04 (d, *J* = 8.1 Hz, 2H), 6.96 (d, *J* = 8.5 Hz, 2H), 6.83 (s, 1H), 6.40 (d, *J* = 9.5 Hz, 1H), 3.87 (s, 3H), 2.63 (s, 3H), 2.25 (s, 3H), 2.21 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.3, 159.1, 153.2, 138.1, 136.4, 133.7, 133.4, 132.1, 130.7, 129.5, 127.6, 126.9, 125.3, 112.6, 108.8, 51.4, 21.6, 21.2, 10.5.
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 388.1656; found: 388.1651.
Optical Rotation: $[\alpha]_D^{28}$ = +5.0 (*c* = 1.0, $CHCl_3$) [94% *ee*].
Chiral HPLC: 86% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 6.95 min (major), 16.48 min (minor)].

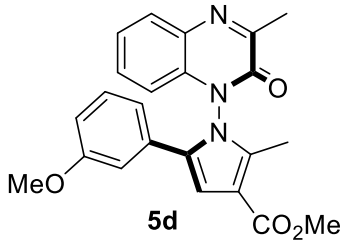
Methyl (*S*)-5-(4-fluorophenyl)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (5c):



5c

To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2c** (30.2 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40°C for 10 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5c** in 81% yield (31.7 mg) as a white solid.
M.p.: 152-154 ℃.
IR (film) υ_{max}/cm^{-1}**:** 2924, 1709, 1690, 1608, 1582, 1441, 1239, 1222, 1139, 1065, 840, 775, 756.
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.80 (dd, *J* = 7.8, 1.6 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.15–7.09 (m, 2H), 6.89–6.81 (m, 3H), 6.39 (dd, *J* = 8.1, 1.4 Hz, 1H), 3.87 (s, 3H), 2.62 (s, 3H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.1, 162.6 (d, *J* = 252.5 Hz), 159.0, 153.1, 136.6, 133.6, 132.2 (d, *J* = 10.1 Hz), 130.8, 129.8 (d, *J* = 8.1 Hz), 129.6, 125.9 (d, *J* = 3.0 Hz), 125.4, 115.9, 115.7, 112.7, 112.4, 109.2, 51.4, 21.6, 10.5.
^{19}F NMR (376 MHz, $CDCl_3$): δ -112.8.
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 392.1405; found: 392.1399.
Optical Rotation: $[\alpha]_D^{28}$ = +3.0 (*c* = 1.0, $CHCl_3$) [94% *ee*].
Chiral HPLC: 94% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/Fmin, 254 nm, t_R = 7.12 min (major), 15.64 min (minor)].

Methyl (*S*)-5-(3-methoxyphenyl)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (5d):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), C1 (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl4 (1.0 mL) and **2d** (31.7 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 12 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 10/1) to afford the product **5d** in 96% yield (38.7 mg) as a white solid.

M.p.: 88-90 ℃.

IR (film) υ_{max}/cm^{-1}: 2950, 2835, 1715, 1683, 1606, 1540, 1456, 1261, 1221, 1145, 1077, 800, 774, 753.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.81 (d, *J* = 7.7 Hz, 1H), 7.40 (t, *J* = 7.7 Hz, 1H), 7.34 (t, *J* = 7.6 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.88 (d, *J* = 0.9 Hz, 1H), 6.77 – 6.67 (m, 3H), 6.44 (d, *J* = 8.2 Hz, 1H), 3.88 (s, 3H), 3.56 (s, 3H), 2.62 (s, 3H), 2.26 (s, 3H).

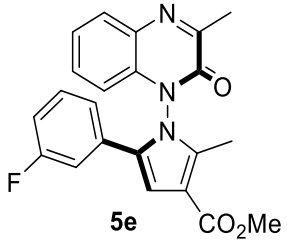
^{13}C NMR (**101 MHz, $CDCl_3$):** δ 165.2, 159.6, 159.1, 153.2, 136.8, 133.8, 133.2, 132.2, 131.0, 130.8, 129.9, 129.6, 125.3, 112.0, 114.6, 112.7, 112.6, 112.3, 109.3, 55.1, 51.4, 21.6, 10.5.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 404.1605; found: 404.1598.

Optical Rotation: $[\alpha]_D^{28}$ = +5.7 (*c* = 1.0, $CHCl_3$) [88% *ee*].

Chiral HPLC: 88% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/min, 254 nm, t_R = 8.31min (major), 15.02min (minor)].

Methyl (*S*)-5-(3-fluorophenyl)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (5e):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2e** (30.3 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 12 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 10/1) to afford the product **5e** in 97% yield (38.1 mg) as a white solid.

M.p.: 143-145 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3062, 2946, 1713, 1681, 1607, 1539, 1439, 1257, 1213, 1142, 1075,

864, 773, 758

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 9.3 Hz, 1H), 7.40 (t, *J* = 8.6 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.12 (q, *J* = 7.2 Hz, 1H), 6.93–6.82 (m, 4H), 6.39 (d, *J* = 8.0 Hz, 1H), 3.87 (s, 3H), 2.64 (s, 3H), 2.25 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$**)**:**δ 165.0, 162.7(d, *J* = 247.4 Hz), 159.1, 153.1, 137.2, 133.6, 132.2, 131.9(d, *J* = 3.0 Hz) , 131.7(d, *J* = 9.09 Hz), 130.9, 130.4(d, *J* = 8.08 Hz), 129.7, 125.5, 123.0(d, *J* = 2.0 Hz), 115.2(d, *J* = 20.2 Hz), 114.6(d, *J* = 23.23 Hz), 112.9, 112.3, 109.8, 51.5, 21.6, 10.5.

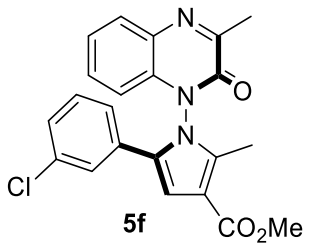
^{19}F NMR (**376 MHz, $CDCl_3$**)**:** δ -111.92.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 393.1405; found:393.1400.

Optical Rotation: $[\alpha]_D^{28}$ = +3.6 (*c* = 1.0, $CHCl_3$) [94% *ee*].

Chiral HPLC: 94% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/Fmin, 254 nm, t_R = 6.90 min (major), 12.37 min (minor)].

Methyl (*S*)-5-(3-chlorophenyl)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (5f):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2f** (32.2 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 12 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5f** in 70% yield (28.6 mg) as a white solid.

M.p.: 105-107 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3065, 2945, 1711, 1674, 1604, 1569, 1438, 1238, 1211, 1144, 1070, 772, 756, 690.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.82 (d, *J* = 7.9 Hz, 1H), 7.41 (t, *J* = 7.7 Hz, 1H), 7.35 (t, *J* = 7.5 Hz, 1H), 7.20 (s, 1H), 7.13 (d, *J* = 8.0 Hz, 1H), 7.07 (t, *J* = 7.8 Hz, 1H), 6.98 (d, *J* = 7.2 Hz, 1H), 6.90 (s, 1H), 6.37 (d, *J* = 8.0 Hz, 1H), 3.88 (s, 3H), 2.64 (s, 3H), 2.26 (s, 3H).

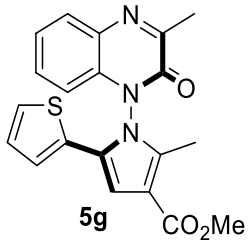
^{13}C NMR (**101 MHz, $CDCl_3$**)**:** δ 165.0, 159.1, 153.2, 137.3, 134.6, 133.6, 132.2, 131.8, 131.4, 130.9, 130.1, 129.7, 128.3, 127.8, 125.5, 125.3, 112.9, 112.3, 109.9, 51.5, 21.6, 10.5.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 408.1110; found: 408.1103.

Optical Rotation: $[\alpha]_D^{28}$ = +7.7 (*c* = 1.0, $CHCl_3$) [94% *ee*].

Chiral HPLC: 94% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/Fmin, 254 nm, t_R = 7.04 min (major), 12.48 min (minor)].

Methyl (*S*)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-5-(thiophen-2-yl)-1*H*-pyrrole-3-carboxylate (5g):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2g** (28.8 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 20 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5g** in 98% yield (37.0 mg) as a white solid.

M.p.: 139-141 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3127, 2939, 1708, 1688, 1602, 1437, 1244, 1224, 1146, 1076, 773, 750, 716.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.87 (d, *J* = 7.6 Hz, 1H), 7.43–7.34 (m, 2H), 7.05 (d, *J* = 5.0 Hz, 1H), 6.98 (s, 1H), 6.83–6.80 (m, 1H), 6.77 (d, *J* = 3.7 Hz, 1H), 6.49 (d, *J* = 9.6 Hz, 1H), 3.87 (s, 3H), 2.65 (s, 3H), 2.27 (s, 3H).

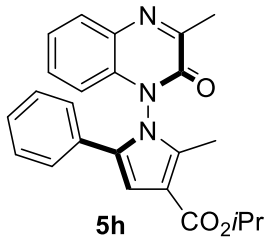
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.0, 159.2, 153.0, 136.7, 133.6, 132.3, 130.8, 130.4, 129.6, 127.5, 126.0, 125.4, 125.4, 125.1, 112.7, 112.4, 109.4, 51.4, 21.6, 10.5.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 380.1064; found: 380.1056.

Optical Rotation: $[\alpha]_D^{28}$ = +11.3 (*c* = 1.0, $CHCl_3$) [90% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/Fmin, 254 nm, t_R = 8.98min (major), 24.08min (minor)].

Isopropyl (*S*)-2-methyl-1-(3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (5h):



To a flame dried Schlenk tube were added **4a** (17.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2h** (28.1 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 12 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the pure product **5h** in 81% yield (32.5mg) as a white solid.

M.p.: 144-146 ℃.

IR (film) υ_{max}/cm^{-1}**:** 2976, 2929, 1704, 1681, 1604, 1538, 1414,1372, 1242, 1143, 1059, 777, 755, 699

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.79 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.8 Hz, 1H), 7.33 (t, *J* = 7.5 Hz, 1H), 7.16 (s, 5H), 6.88 (s, 1H), 6.45 (d, *J* = 8.1 Hz, 1H), 5.24 (hept, *J* = 6.2 Hz, 1H), 2.63 (s, 3H), 2.25 (s, 3H), 1.37 (d, *J* = 4.0 Hz, 6H).

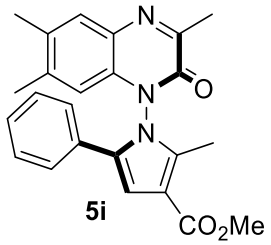
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 164.4, 159.1, 153.2, 136.3, 133.7, 133.1, 132.2, 130.8, 129.9, 129.5, 128.7, 128.2, 127.6, 125.3, 113.4, 112.6, 109.3, 67.4, 22.2, 21.6, 10.5.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 402.1812; found: 402.1809.

Optical Rotation: $[\alpha]_D^{28}$ = +8.9 (*c* = 1.0, $CHCl_3$) [92% *ee*].

Chiral HPLC: 92% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/Fmin, 254 nm, t_R = 10.96min (major), 30.92min (minor)].

Methyl (*S*)-2-methyl-5-phenyl-1-(3,6,7-trimethyl-2-oxoquinoxalin-1(2*H*)-yl)-1*H*-pyrrole-3-carboxylate (5i):



To a flame dried Schlenk tube were added **4i** (20.3 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 20 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5i** in 95% yield (38.2 mg) as a white solid.

M.p.: 100-102 ℃.

IR (film) υ_{max}/cm^{-1}**:** 2947, 2921, 1715, 1683, 1622, 1558, 1440, 1410, 1237, 1206, 1156, 1069, 756, 702.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.54 (s, 1H), 7.15 (m, 5H), 6.88 (s, 1H), 6.21 (s, 1H), 3.88 (s, 3H), 2.58 (s, 3H), 2.29 (s, 3H), 2.25 (s, 6H).

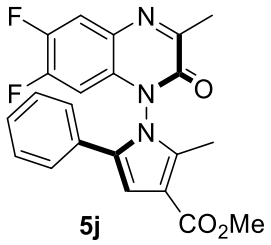
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 165.3, 157.6, 153.2, 140.9, 136.7, 134.3, 133.1, 131.7, 130.6, 129.9, 129.7, 128.7, 128.1, 127.5, 112.8, 112.5, 109.0, 51.4, 21.5, 20.5, 19.4, 10.5.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 402.1812; found: 402.1807.

Optical Rotation: $[\alpha]_D^{28}$ = +1.6 (*c* = 1.0, $CHCl_3$) [93% *ee*].

Chiral HPLC: 93% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/Fmin, 254 nm, t_R = 7.31min (major), 14.35min (minor)].

Methyl (*S*)-1-(6,7-difluoro-3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5j):



To a flame dried Schlenk tube were added **4j** (21.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (12.2 mg, 0.1 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 14 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5j** in 47% yield (19.0 mg) as a white solid.

M.p.: 93-95 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3135, 3069, 2948, 1708, 1697, 1593, 1501, 1437, 1243, 1197, 1158, 1085, 835, 801, 758, 686.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.58 (dd, *J* = 9.9, 7.7 Hz, 1H), 7.22–7.12 (m, 5H), 6.87 (s, 1H), 6.17 (dd, *J* = 10.3, 7.0 Hz, 1H), 3.88 (s, 3H), 2.61 (s, 3H), 2.27 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$**)**:** δ 164.98, 159.77, 159.73, 153.1 (d, *J* = 14.1 Hz), 152.79, 150.5 (d, *J* = 14.1 Hz), 148.9 (d, *J* = 14.1 Hz), 146.4 (d, *J* = 14.1 Hz), 136.30, 133.06, 130.8 (d, *J* = 8.1 Hz), 129.43, 128.90, 128.50, 127.67, 117.6 (d, *J* = 18.2 Hz), 113.13, 109.48, 101.4 (d, *J* = 23.2 Hz), 51.47, 21.57, 10.49.

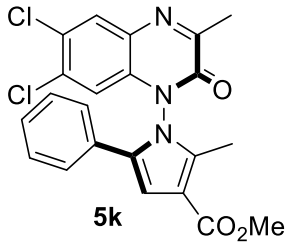
^{19}F NMR (**376 MHz, $CDCl_3$**)**:** δ -129.42, -139.25.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 410.1311; found: 410.1306.

Optical Rotation: $[\alpha]_D^{28}$ = +7.1 (*c* = 1.0, $CHCl_3$) [92% *ee*].

Chiral HPLC: 92% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 6.64min (major), 9.60min (minor)].

Methyl (*S*)-1-(6,7-dichloro-3-methyl-2-oxoquinoxalin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5k):

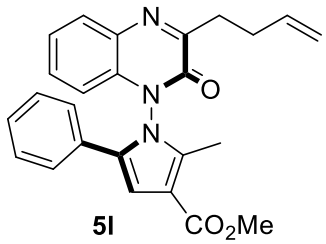


To a flame dried Schlenk tube were added **4k** (24.4 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 15 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 10/1) to afford the product **5k** in 54% yield (26.6 mg) as a white solid.

M.p.: 58-60 ℃.

IR (film) υ_{max}/cm^{-1}: 2923, 2853, 1716, 1698, 1652, 1558, 1456, 1240, 1144, 1070, 756, 697.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.86 (s, 1H), 7.21–7.18 (m, 3H), 7.15–7.11 (m, 2H), 6.88 (s, 1H), 6.49 (s, 1H), 3.88 (s, 3H), 2.61 (s, 3H), 2.27 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$): δ 165.0, 160.6, 152.5, 136.2, 135.1, 133.1, 133.0, 131.1, 130.7, 129.4, 129.3, 128.9, 128.5, 127.7, 113.9, 113.1, 109.5, 51.5, 21.7, 10.5.
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 442.0720; found: 442.0715.
Optical Rotation: $[\alpha]_D^{28}$ = -1.1 (*c* = 1.0, $CHCl_3$) [98% *ee*].
Chiral HPLC: 98% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/Fmin, 254 nm, t_R = 6.77min (minor),10.08 min (major)].

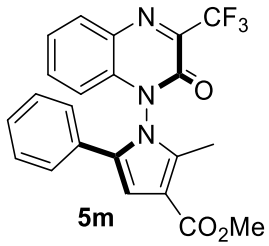
Methyl (*S*)-1-(3-(but-3-en-1-yl)-2-oxoquinoxalin-1(2*H*)-yl)-2-methyl-5-phenyl-1*H*-pyrrole-3-carboxylate (5l):



5l

To a flame dried Schlenk tube were added **4l** (21.5 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 9 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 10/1) to afford the product **5l** in 65% yield (26.9 mg) as a white solid.
M.p.: 108-110 ℃.
IR (film) υ_{max}/cm^{-1}**:** 3071, 2950, 1705, 1677, 1605, 1583, 1438, 1407, 1238, 1208, 1084, 904, 779, 756, 694.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.82 (d, *J* = 7.8 Hz, 1H), 7.39 (t, *J* = 7.7 Hz, 1H), 7.33 (t, *J* = 7.6 Hz, 1H), 7.15 (s, 5H), 6.87 (s, 1H), 6.43 (d, *J* = 8.2 Hz, 1H), 5.88 (ddt, *J* = 16.9, 10.1, 6.6 Hz, 1H), 5.03 (d, *J* = 17.1 Hz, 1H), 4.96 (d, *J* = 10.2 Hz, 1H), 3.88 (s, 3H), 3.16–3.00 (m, 2H), 2.61–2.49 (m, 2H), 2.25 (s, 3H).
^{13}C NMR (101 MHz, CDCl$_3$):δ 165.2, 161.2, 152.9, 137.2, 136.7, 133.5, 133.3, 132.2, 130.8, 129.80, 129.76, 128.7, 128.2, 127.7, 125.2, 115.7, 112.7, 112.5, 109.1, 51.4, 33.4, 30.7, 10.5.
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 414.1812; found: 414.1804.
Optical Rotation: $[\alpha]_D^{28}$ = +7.0 (*c* = 1.0, $CHCl_3$) [88% *ee*].
Chiral HPLC: 88% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/min, 254 nm, t_R = 7.03min (major), 9.25min (minor)].

Methyl (*S*)-2-methyl-1-(2-oxo-3-(trifluoromethyl)quinoxalin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (5m):



To a flame dried Schlenk tube were added **4m** (23.0 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (2.4 mg, 0.02 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 40 °C for 20 d. Then the solution was concentrated under vacuum and the mixture was purified through column chromatography (PE/EA = 8/1) to afford the product **5m** in 46% yield (20.0 mg) as a white solid.

M.p.: 117-119 ℃.

IR (film) υ_{max}/cm^{-1}**:** 1709, 1697, 1607, 1568, 1439, 1354, 1224, 1148, 1078, 796, 758, 694.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.96 (d, *J* = 6.8 Hz, 1H), 7.58 (t, *J* = 7.3 Hz, 1H), 7.43 (t, *J* = 8.3 Hz, 1H), 7.20 – 7.14 (m, 5H), 6.87 (s, 1H), 6.43 (d, *J* = 7.2 Hz, 1H), 3.89 (s, 3H), 2.30 (s, 3H).

^{13}C NMR (**101 MHz, $CDCl_3$):** δ 164.8, 159.3, 154.1, 152.8, 146.0, 138.1, 133.1 (d, *J* = 111.1 Hz), 131.0, 129.8, 128.3, 125.5, 124.6, 123.2, 122.6, 120.9, 113.2, 112.4, 110.9, 110.4, 101.1, 51.5, 21.6, 10.3.

^{19}F NMR (**376 MHz, $CDCl_3$):** δ -69.66.

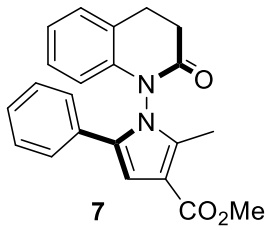
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 428.1217; found: 428.1211.

Optical Rotation: $[\alpha]_D^{28}$ = +16.8 (*c* = 1.0, $CHCl_3$) [87% *ee*].

Chiral HPLC: 87% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/min, 254 nm, t_R = 7.31min (major), 8.25min (minor)].

(4) Synthesis and Characterization of Products 7, 9-15

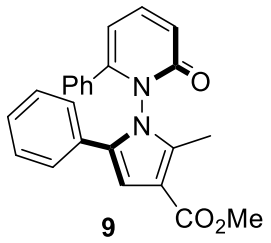
Methyl (*S*)-2-methyl-1-(2-oxo-3,4-dihydroquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (7):



To a flame dried Schlenk tube were added **6** (16.2 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (1.2 mg, 0.01 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25°C for 7 d. Then the solution was concentrated under vacuum. Finally, the mixture was purified through column chromatography (PE/EA = 5/1) to afford the pure product **7** in 97%

yield (35.0 mg) as a faint yellow solid.
M.p.: 53-55 ℃.
IR (film) υ_{max}/cm^{-1}**:** 3031, 2948, 1716, 1698, 1540, 1456, 1417, 1221, 1072, 755.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.25–7.18 (m, 5H), 7.17–7.09 (m, 2H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.81 (s, 1H), 6.15 (d, *J* = 8.1 Hz, 1H), 3.86 (s, 3H), 3.02–2.74 (m, 4H), 2.36 (s, 3H).
^{13}C NMR (**101 MHz, CDCl$_3$**)**:** δ 168.1, 165.5, 139.8, 137.2, 133.0, 130.5, 128.5, 128.3, 128.2, 127.9, 127.8, 124.5, 124.4, 113.7, 111.8, 108.6, 51.2, 31.8, 24.9, 10.5.
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 361.1547; found: 361.1539.
Optical Rotation: $[\alpha]_D^{28}$ = +1.5 (*c* = 1.0, $CHCl_3$) [85% *ee*].
Chiral HPLC: 85%*ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 20/80, 0.8 mL/min, 254 nm, t_R = 9.90min (major), 14.83min (minor)].

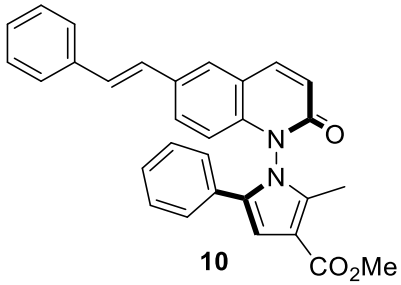
Methyl (*S*)-2-methyl-1-(2-oxo-6-phenyl-3,4-dihydropyridin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (9):



9

To a flame dried Schlenk tube were added **8** (18.6 mg, 0.1 mmol), **C1** (5.5 mg, 0.01 mmol), $MgSO_4$ (100 mg), PhCOOH (1.2 mg, 0.01 mmol), anhydrous CCl_4 (1.0 mL) and **2a** (28.0 mg, 0.12 mmol). The resulting reaction mixture was stirred at 25 ºC for 14 d. Then the solution was concentrated under vacuum. Finally, the mixture was purified through column chromatography (PE/EA = 5/1) to afford the product **9** in 42% yield (16.3 mg) as a faint yellow solid.
M.p.: 153-155 ℃.
IR (film) υ_{max}/cm^{-1}**:** 3050, 2944, 1704, 1677, 1605, 1544, 1439, 1244, 1086, 798, 760, 698.
^{1}H NMR (400 MHz, CDCl$_3$): δ 7.46 (d, *J* = 9.4 Hz, 1H), 7.30–7.25 (m, 2H), 7.23–7.17 (m, 3H), 7.12 (t, *J* = 7.8 Hz, 2H), 6.92–6.86 (m, 2H), 6.80 (d, *J* = 9.4 Hz, 1H), 6.62 (d, *J* = 7.3 Hz, 2H), 6.48 (s, 1H), 6.08 (d, *J* = 6.9 Hz, 1H), 3.80 (s, 3H), 2.51 (s, 3H).
^{13}C NMR (**101 MHz, CDCl$_3$**)**:** δ 165.5, 161.6, 150.8, 140.6, 137.4, 132.0, 131.9, 130.4, 129.7, 128.6, 128.2, 128.0, 127.7, 127.6, 120.3, 111.5, 108.3, 108.1, 51.2, 11.3.
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 385.1547; found: 385.1540.
Optical Rotation: $[\alpha]_D^{28}$ = -3.0 (*c* = 1.0, $CHCl_3$) [50% *ee*].
Chiral HPLC: 50% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/Fmin, 254 nm, t_R = 12.29min (minor), 18.33min (major)].

Methyl (*S, E*)-2-methyl-1-(2-oxo-6-styrylquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (10):



10

To an dry three-neck flask was added **3t** (50.0 mg, 0.11 mmol, 1.0 equiv., 90% ee), *E*-phenylethenylboronic acid (34.0 mg, 0.23 mmol, 2 equiv.), $PdCl_2(PPh_3)_2$ (0.4 mg, 0.00058 mmol, 0.5 mol%) and K_2CO_3 (39.7 mg, 0.29 mmol, 2.5 equiv.). The vial was capped and purged with N_2 before the addition of 1,4-dioxane (0.8 mL)/H_2O (0.2 mL). The reaction mixture was heated for 16 h at 89 ℃. The reaction mixture was then allowed to cool to room temperature and The reaction was quenched by the addition of water and the mixture was extracted with EtOAc. The organic phase was separated, washed with water and brine, dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by a silica gel chromatography with (PE/EA = 5/1) as the eluent to give compound **10** (75%, 87% ee, 34.7 mg) as a white solid

M.p.: 84-86 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3030, 2922, 1715, 1683, 1558, 1456, 1241, 1219, 1071, 812, 751, 695.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.76 (d, *J* = 9.7 Hz, 1H), 7.62 (s, 1H), 7.56 (d, *J* = 8.7 Hz, 1H), 7.49 (d, *J* = 7.1 Hz, 2H), 7.36 (t, *J* = 7.6 Hz, 2H), 7.29 (d, *J* = 7.4 Hz, 1H), 7.24 (d, *J* = 1.7 Hz, 2H), 7.18–7.14 (m, 3H), 7.06 (s, 2H), 6.91 (s, 1H), 6.78 (d, *J* = 9.6 Hz, 1H), 6.37 (d, *J* = 8.7 Hz, 1H), 3.88 (s, 3H), 2.30 (s, 3H).

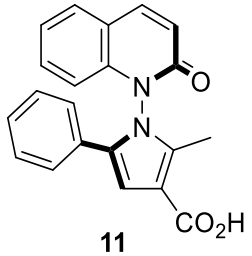
^{13}C NMR (101 MHz, $CDCl_3$): δ 165.4, 160.1, 140.9, 139.7, 137.0, 136.8, 133.5, 133.2, 130.0, 129.8, 128.9, 128.6, 128.2, 128.0, 127.6, 126.6, 126.5, 126.5, 121.7, 120.3, 113.4, 112.3, 108.9, 51.3, 10.4.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 461.1860; found: 451.1854.

Optical Rotation: $[\alpha]_D^{28}$ = -2.1 (*c* = 1.0, $CHCl_3$) [87% *ee*].

Chiral HPLC: 87% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 30/70, 0.8 mL/min, 254 nm, t_R = 40.13min (major), 55.03min (minor)].

(*S*)-2-Methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylic acid (11):



11

Compound **3a** (35.8 mg, 0.1 mmol, 1.0 equiv., 90% ee), KOH (40 mg, 1 mmol, 10 equiv.), 0.5 mL H_2O and 1.5 mL MeOH were added to a reaction tube. Then, the reaction mixture was stirred at 80 ℃ for 8 h. After the completion of the reaction which

was indicated by TLC, the reaction mixture was quenched with 0.5 mL 6 N HCl and the aqueous layer was extracted with DCM (3×5 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure to afford product **11** (95% yield, 93% ee, 32.7 mg) as a solid.

M.p.: 187-189 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3446, 1695, 1683, 1635, 1558, 1540, 1456, 1259, 1220, 1119, 827, 753, 696.

^{1}H NMR (400 MHz, DMSO-*d*$_6$**):**δ 12.38 (s, 1H), 8.14 (d, *J* = 9.7 Hz, 1H), 7.81 (d, *J* = 7.3 Hz, 1H), 7.52 (t, *J* = 7.5 Hz, 1H),, 7.30 (t, *J* = 7.5 Hz, 1H), 7.18 (q, *J* = 6.4, 5.5 Hz, 5H), 6.89 – 6.79 (m, 2H), 6.29 (d, *J* = 8.4 Hz, 1H), 2.12 (s, 3H).

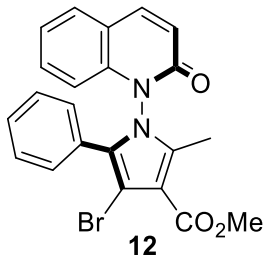
^{13}C NMR (**101 MHz,** DMSO-*d*$_6$)**:** δ 165.5, 159.5, 141.9, 139.8, 136.1, 132.3, 132.0, 129.7, 129.3, 128.7, 127.8, 126.7, 124.0, 120.7, 119.7, 112.5, 112.2, 108.5, 10.0.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 345,1234; found: 345.1227..

Optical Rotation: $[\alpha]_D^{28}$ = +3.8 (*c* = 1.0, $CHCl_3$) [93% *ee*].

Chiral HPLC: 93% *ee* [Chiral ND(2), 250×4.6, *i*-PrOH/*n*-heptane = 70/30, 0.8 mL/Fmin, 254 nm, t_R = 11.13min (major), 20.53min (minor)].

Methyl (*S*)-4-bromo-2-methyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (12):



12

To a stirring solution of **3a** (35.8 mg, 0.1 mmol, 1.0 equiv., 90% ee) in DMF (1 mL) was added NBS (27.0 mg, 0.15 mmol, 1.5 equiv.). The resulting mixture was allowed to stir at 25 ℃ for 2 d. The reaction was quenched by the addition of water and the mixture was extracted with EtOAc. The organic phase was separated, washed with water and brine, dried over anhydrous Na_2SO_4, filtered and concentrated. The residue was purified by a silica gel chromatography with (PE/EA = 4/1) as the eluent to give compound **12** (91%, 90% ee, 39.8 mg) as a white solid.

M.p.: 138-140 ℃.

IR (film) υ_{max}/cm^{-1}**:** 2951, 1706, 1683, 1599, 1558, 1436, 1239,1222, 1069, 825, 758, 706.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.68 (d, *J* = 9.7 Hz, 1H), 7.50 (d, *J* = 7.8 Hz, 1H), 7.45 (t, *J* = 8.6 Hz, 1H), 7.30–7.26 (m, 2H), 7.22 (t, *J* = 8.1 Hz, 1H), 7.20–7.16 (m, 3H), 6.68 (d, *J* = 9.7 Hz, 1H), 6.43 (d, *J* = 8.6 Hz, 1H), 3.90 (s, 3H), 2.26 (s, 3H).

^{13}C NMR (**101 MHz, CDCl$_3$**)**:** δ 164.3, 160.0, 141.1, 140.2, 137.0, 132.1, 131.8, 130.2, 128.9, 128.3, 128.2, 124.1, 121.1, 119.9, 112. 8, 111.7, 96.8, 51.4, 11.2.

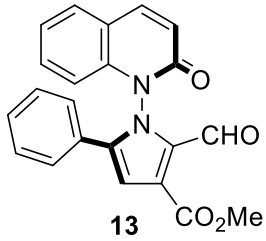
HRMS (ESI) m/z: $[C_{22}H_{17}BrN_2O_4+H]^+$ calcd.: 437.0496; found: 437.0487.

Optical Rotation: $[\alpha]_D^{28}$ = -1.2 (*c* = 1.0, $CHCl_3$) [90% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.7

mL/min, 254 nm, t_R = 10.90min (major), 15.75min (minor)].

Methyl (*R*)-2-formyl-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (13):



13

Compound **3a** (35.8 mg, 0.1 mmol, 1.0 equiv., 90% ee), CAN (530.0 mg, 1 mmol, 10 equiv.) and 3.2 mL THF were added to a reaction tube. Then, 3.2 mL HOAc and 3.2 mL H_2O were added to the reaction mixture, which was stirred at room temperature for 8 h. After that the reaction mixture was quenched with H_2O and the aqueous layer was extracted with EtOAc (3×10 mL). The combined organic layers were dried over anhydrous Na_2SO_4 and then concentrated under reduced pressure. The residue was purified through flash column chromatography on silica gel (PE/EA = 5/1) to afford the product **13** (97% yield, 90% ee, 36.1 mg) as a solid.

M.p.: 100-102 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3029, 2946, 1705, 1683, 1568, 1436, 1242, 1220, 1072, 826, 775, 696.

^{1}H NMR (400 MHz, $CDCl_3$): δ 10.31 (s, 1H), 7.76 (d, *J* = 9.7 Hz, 1H), 7.55 (d, *J* = 7.8 Hz, 1H), 7.41–7.31 (m, 3H), 7.27–7.17 (m, 5H), 7.06 (s, 1H), 6.72 (d, *J* = 9.7 Hz, 1H), 6.36 (d, *J* = 8.4 Hz, 1H), 3.96 (s, 3H).

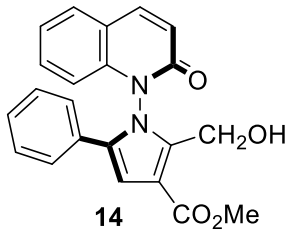
^{13}C NMR (101 MHz, $CDCl_3$): δ 180.4, 163.4, 160.5, 141.2, 140.6, 140.5, 131.6, 129.6, 129.5, 129.0, 128.9, 128.3, 128.0, 124.1, 123.8, 121.2, 120.2, 112.2, 111.3, 52.4.

HRMS (ESI) m/z: $[C_{22}H_{16}N_2O_4+H]^+$ calcd.: 373.1183; found:373.1171.

Optical Rotation: $[\alpha]_D^{28}$ = -7.6 (*c* = 1.0, $CHCl_3$) [90% *ee*].

Chiral HPLC: 90% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 50/50, 0.8 mL/min, 254 nm, t_R = 10.50min (major), 24.26min (minor)].

Methyl (*R*)-2-(hydroxymethyl)-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-1*H*-pyrrole-3-carboxylate (14):



14

Compound **13** (22.3 mg, 0.06 mmol, 1.0 equiv., 90% ee) and 1 mL MeOH were added to a reaction tube. Then, $NaBH_4$ (3.5 mg, 0.09 mmol, 1.5 equiv.) was added to the reaction mixture, which was stirred at 0 °C for 12 h. After the completion of the reaction which was indicated by TLC, the reaction mixture was quenched with acetone and then

concentrated under reduced pressure. The residue was purified through flash column chromatography on silica gel (PE/EA = 2/1) to afford product **14** (95% yield, 90% ee, 21.4 mg) as a solid.

M.p.: 84-86 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3446, 3055, 2947, 1716, 1683, 1597, 1449, 1244, 1201, 1086, 829, 749, 698.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.77 (d, *J* = 9.7 Hz, 1H), 7.54 (d, *J* = 7.8 Hz, 1H), 7.42 (t, *J* = 8.6 Hz, 1H), 7.25–7.14 (m, 6H), 6.92 (s, 1H), 6.74 (d, *J* = 9.6 Hz, 1H), 6.45 (d, *J* = 8.1 Hz, 1H), 4.57 (d, *J* = 13.9 Hz, 1H), 4.41 (d, *J* = 13.9 Hz, 1H), 3.92 (s, 3H).

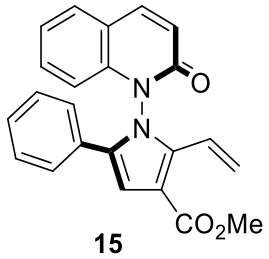
^{13}C NMR (**101 MHz, CDCl$_3$):** δ 165.7, 160.7, 141.4, 140.6, 139.2, 134.0, 131.9, 129.5, 128.8, 128.6, 128.3, 127.8, 124.2, 120.8, 119.8, 113.7, 113.0, 109.2, 54.2, 51.9.

HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 375.1340; found: 375.1337.

Optical Rotation: $[\alpha]_D^{28}$ = +4.8 (*c* = 1.0, $CHCl_3$) [89% *ee*].

Chiral HPLC: 89% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.8 mL/min, 254 nm, t_R = 16.66 min (major), 31.04 min (minor)].

Methyl (*R*)-1-(2-oxoquinolin-1(2*H*)-yl)-5-phenyl-2-vinyl-1*H*-pyrrole-3-carboxylate (15):



15

To a solution of Ph_3PCH_3Br (53.6 mg, 0.15 mmol, 1.5 equiv.) in dry THF (0.5 mL) was added KO*t*Bu (16.8 mg, 0.15 mmol, 1.5 equiv.) under nitrogen atmosphere. The mixture was allowed to stir for 1 h at 0 ℃. After that, **13** (37.2 mg, 0.1 mmol, 1.0 equiv., 90% ee) was added. The system was allowed to warm to room temperature slowly and stir for 12 h. The reaction mixture was concentrated under reduced pressure and directly purified by silica gel chromatography (PE/EA = 3/1) to afford compound **15** (82%, 89% ee, 30.5 mg).

M.p.: 122-124 ℃.

IR (film) υ_{max}/cm^{-1}**:** 3059, 2951, 1707, 1682, 1653, 1599, 1448, 1242, 1213, 1067, 1012, 906, 829, 763, 734, 698.

^{1}H NMR (400 MHz, CDCl$_3$): δ 7.74 (d, *J* = 9.6 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 1H), 7.42 (t, *J* = 8.5 Hz, 1H), 7.28–7.19 (m, 3H), 7.18–7.14 (m, 3H), 7.05–6.95 (m, 2H), 6.73 (d, *J* = 9.7 Hz, 1H), 6.42 (d, *J* = 8.4 Hz, 1H), 5.19–5.08 (m, 2H), 3.88 (s, 3H).

^{13}C NMR (**101 MHz, CDCl$_3$):** δ 164.8, 160.4, 141.1, 140.6, 135.4, 134.7, 131.9, 129.6, 128.8, 128.6, 128.4, 128.2, 124.0, 123.6, 121.4, 119.9, 118.0, 114.1, 113.2, 110.3, 51.6.

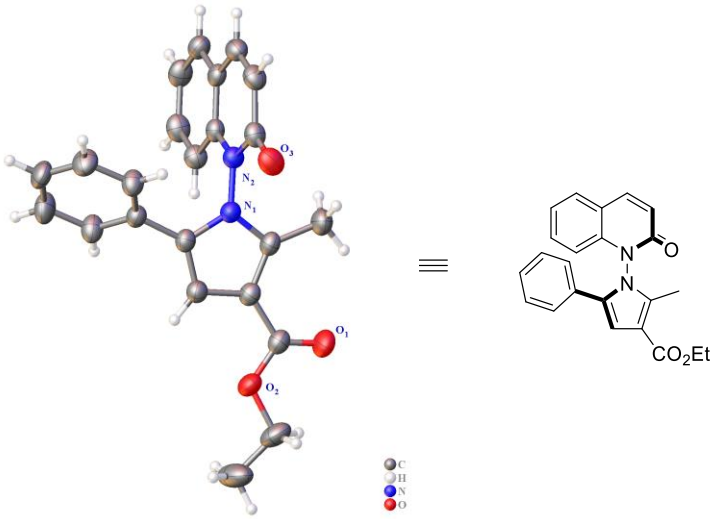
HRMS (ESI) m/z: $[C_{14}H_{12}NO_2+H]^+$ calcd.: 371.1390; found: 371.1383.

Optical Rotation: $[\alpha]_D^{28}$= -1.9 (*c* = 1.0, $CHCl_3$) [90% *ee*].

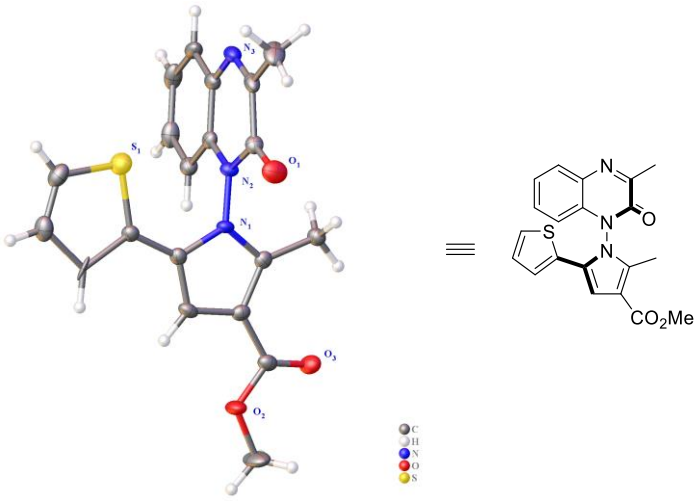
Chiral HPLC: 89% *ee* [Chiral MD(2), 250×4.6, *i*-PrOH/*n*-heptane = 25/75, 0.7 mL/min, 254 nm, t_R = 13.40 min (major), 16.06 min (minor)].

(5) X-ray Crystallographic Date for Compound 3n and 5g

Crystallographic data for **3n**: $C_{23}H_{20}N_2O_3$, M = 372.41, orthorhombic, P 21 (No. 19), a = 9.1943 (4) Å, b = 14.3898 (6) Å, c = 14.7328 (6) Å, V = 1949.21 (14) Å3, Z = 4, Crystal size: 0.07 × 0.05 × 0.02 mm, T = 256 K, ρcalcd = 1.269 g·cm-3, R1 = 0.0405 (I>4σ(I)), wR2 = 0.1125 (all data), GOF = 1.052, reflections collected/unique: 21328 / 3427 (Rint = 0.0708), Data: 3186, restraints: 0, parameters: 253. CCDC (2267510) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



Crystallographic data for **5g**: $C_{20}H_{17}N_3O_3S$, M = 379.42, monoclinic, P 21 (No. 4), a = 7.3762 (12) Å, b = 9.0242 (15) Å, c = 13.612 (2) Å, β = 102.049 (5)°, V = 886.1 (3) Å3, Z = 2, Crystal size: 0.35 × 0.28 × 0.25 mm, T = 211 K, ρcalcd = 1.422 g·cm^{-3}, R1 = 0.05 (I>4σ(I)), wR2 = 0.1412 (all data), GOF = 1.069, reflections collected/unique: 9166 / 2955 (Rint = 0.0401), Data: 2910, restraints: 0, parameters: 244. CCDC (2267692) contains the supplementary crystallographic data for this paper. The data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.



(6) Details of Calculation and Discussion

All of the DFT calculations were performed with the Gaussian 09 program package.[7] The geometry optimization of all the minima involved were performed at the M06-2X level of theory with Grimme's D3 empirical dispersion correction and def2-SVP basis set for all atoms (keyword 5D).[8] To obtain accurate energies, single-point energy calculations were performed at the M06-2X//def2-TZVP level[9], based on the optimized structures. The structures of the reactants, intermediates, transition states, and products were fully optimized without any restriction. The vibrational frequencies were computed at the same level to check whether each optimized structure is an energy minimum or a transition state and to evaluate its zero-point vibrational energy (ZPVE) and thermal corrections at 298 K. Solvent effects were computed using the SMD model[10] in CCl_4. The 3D structures of the optimized intermediates or transition states were demonstrated using CYLView software[11]. Noncovalent interaction (NCI) analyses were carried out using the Multiwfn 3.8 program.[12-13] Atoms-in-molecules (AIM) analyses[14] were used to explore the origin of stereoselectivity.

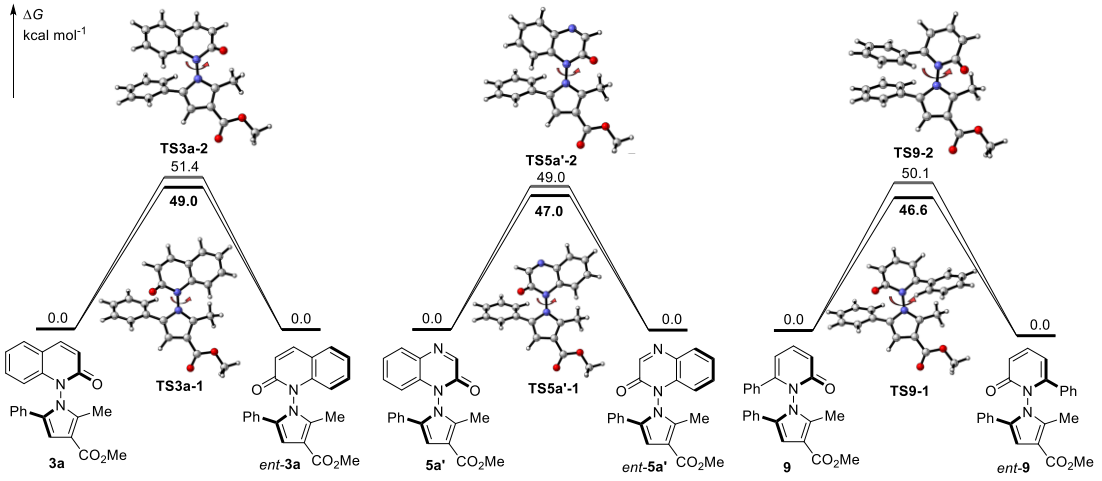


Fig. S1 DFT calculated prediction of rotational barriers of N–N axially chiral molecules.

DFT-Computed Energies of All Stationary Points

Table S1. Sum of electronic and zero-point energy (*E*, in Hartree), thermal enthalpy (*H*, in Hartree), thermal free energies (*G*, in Hartree), thermal correction to Gibbs free energy (CGFE, in Hartree), single-point energy (E_{sol}, in Hartree). For transition state structures, one imaginary frequency (Ifreq.) was observed and given below. For all minimum structures, no imaginary frequency was observed.

Structure	*E*	*H*	*G*	CGFE	E_{sol}	Ifreq
3a	-1182.696363	-1182.672916	-1182.749699	0.305239	-1184.363655	
TS3a-1	-1182.622405	-1182.600407	-1182.671365	0.309167	-1184.289443	-21.11
TS3a-2	-1182.617479	-1182.595287	-1182.667133	0.308023	-1184.284581	-33.87

5a'	-1198.721802	-1198.698467	-1198.775241	0.293357	-1200.397961	
TS5a'-1	-1198.65064	-1198.628738	-1198.699965	0.297074	-1200.326698	-22.76
TS5a'-2	-1198.646318	-1198.624234	-1198.696334	0.295756	-1200.322273	-33.07
9	-1259.97715	-1259.951668	-1260.033425	0.336111	-1261.762852	
TS9-1	-1259.907654	-1259.883487	-1259.959579	0.339492	-1261.692043	-28.65
TS9-2	-1259.901303	-1259.877326	-1259.953123	0.340364	-1261.687226	-13.87

Table S2. Sum of electronic and zero-point energy (*E*, in Hartree), thermal enthalpy (*H*, in Hartree), thermal free energies (*G*, in Hartree), thermal correction to Gibbs free energy (CGFE, in Hartree), single-point energy (E_{sol}, in Hartree). For transition state structures, one imaginary frequency (Ifreq.) was observed and given below. For all minimum structures, no imaginary frequency was observed**.**

Structure	*E*	*H*	*G*	CGFE	E_{sol}	Ifreq
C1	-1994.601113	-1994.564837	-1994.666832	0.554336	-1997.202061	
INT1	-1258.991259	-1258.966085	-1259.04765	0.328056	-1260.782123	
INT2	-1258.994075	-1258.969077	-1259.047709	0.332132	-1260.781603	
TS1-*Rs*	-3253.622843	-3253.562606	-3253.713852	0.915565	-3258.001114	-98.76
TS1-*Ss*	-3253.619948	-3253.55956	-3253.712223	0.912995	-3257.995827	-181.14
TS1-*Rr*	-3253.616472	-3253.556438	-3253.707155	0.915753	-3257.993230	-146.42
TS1-*Sr*	-3253.61801	-3253.558127	-3253.707513	0.918271	-3257.996840	-76.07
INT3-*Rs*	-3253.650143	-3253.588978	-3253.741389	0.917685	-3258.029152	
INT3-*Ss*	-3253.655765	-3253.595275	-3253.74754	0.917134	-3258.031024	
INT3-*Rr*	-3253.648688	-3253.587917	-3253.740759	0.916096	-3258.026305	
INT3-*Sr*	-3253.640912	-3253.57928	-3253.735988	0.912926	-3258.020073	
TS2-*Rs*	-3253.605635	-3253.544735	-3253.697964	0.914786	-3257.985245	-258.98
TS2-*Ss*	-3253.607942	-3253.546148	-3253.702591	0.910815	-3257.986306	-176.92
TS2-*Rr*	-3253.600029	-3253.538649	-3253.693298	0.912718	-3257.985024	-232.04
TS2-*Sr*	-3253.614081	-3253.552611	-3253.706714	0.913288	-3257.995706	-66.89
INT4-*Rs*	-3253.620438	-3253.557398	-3253.716998	0.90901	-3258.00333	
INT4-*Ss*	-3253.619437	-3253.557575	-3253.71351	0.909971	-3257.992404	
INT4-*Rr*	-3253.610393	-3253.54796	-3253.704459	0.911873	-3257.992407	
INT4-*Sr*	-3253.619546	-3253.55696	-3253.713223	0.912091	-3258.004606	
TS3-*Rs*	-3253.619437	-3253.557575	-3253.71351	0.909971	-3258.001108	-93.89
TS3-*Ss*	-3253.611016	-3253.548899	-3253.705727	0.907425	-3257.987256	-293.45
TS3-*Rr*	-3253.605506	-3253.543535	-3253.699624	0.908794	-3257.985424	-247.60
TS3-*Sr*	-3253.615337	-3253.553366	-3253.708994	0.909542	-3257.996484	-333.29
C1-H_2O	-2070.939223	-2070.900127	-2071.007102	0.57852	-2073.659075	

Cartesian coordinates of all the stationary point

3a

C	0.92549300	-1.13385200	-1.98518400	O	0.21467100	-0.72616700	-2.87675900
C	2.14558300	-1.91916000	-2.17307700	N	0.62018000	-0.85231700	-0.63949100
C	2.52991800	-2.03658300	0.23234700	C	3.29007300	-2.47296300	1.33095200
C	1.35914200	-1.28566200	0.46513500	H	4.19649100	-3.05083300	1.13965300
C	0.95743000	-0.98874700	1.77653900				

H	0.05010100	-0.41187000	1.95746200
C	2.89906000	-2.17694700	2.62579800
H	3.49533500	-2.51661900	3.47297800
C	1.72913100	-1.43624900	2.83981900
H	1.41303100	-1.20164100	3.85737300
C	-1.75408400	-0.60470300	-0.30635800
C	-0.46007400	1.26991200	-0.08563900
C	-2.56645600	0.44890500	0.08973800
C	-1.74843900	1.61310900	0.23416200
H	-2.10179400	2.60366100	0.50796700
N	-0.48918900	-0.08406600	-0.40700300
C	-1.99415900	-2.04142500	-0.61784900
H	-1.78180900	-2.23622800	-1.68070000
H	-1.33624100	-2.68698700	-0.01561400
H	-3.03533600	-2.30042100	-0.40972000
C	0.78217000	2.05984300	-0.10498500
C	1.65813300	2.00438500	-1.20004900
C	1.09530000	2.89354000	0.97743200
C	2.83244200	2.75335400	-1.19809400
H	1.39182400	1.40265900	-2.07150100
C	2.26339800	3.65247400	0.96816300
H	0.41967800	2.93134000	1.83422900
C	3.13890000	3.57748700	-0.11485100
H	3.50463200	2.70486100	-2.05638700
H	2.49674300	4.29764400	1.81683800
H	4.05749200	4.16663000	-0.11754100
C	-4.02009200	0.48224800	0.32076700
C	-6.03361200	-0.70710200	0.29290000
H	-6.36683100	-1.72339400	0.05724600
H	-6.28893300	-0.45634300	1.33194100
H	-6.52332000	0.01583900	-0.37383700
O	-4.62206300	1.46526700	0.67272200
O	-4.62684700	-0.69397600	0.10153500
C	2.89677600	-2.33431000	-1.13247600
H	3.80694100	-2.91306100	-1.30683000
H	2.40277300	-2.13686300	-3.20923600

TS3a-1

C	-0.05886400	-2.66474500	-0.25070200
C	-0.96538500	-3.55223800	0.50839200
C	-2.70196900	-1.89813100	0.26891100
C	-1.76370200	-1.01817300	-0.31727500
O	0.86988100	-3.03362800	-0.91786600
N	-0.39560500	-1.28994400	-0.05063500
C	-4.07222700	-1.63721500	0.12117200
H	-4.78618800	-2.31208600	0.59771200
C	-2.21454200	-0.04952100	-1.22038400
H	-1.50131100	0.52144900	-1.80833000
C	-4.51322800	-0.58256600	-0.66496600
H	-5.58010000	-0.38717700	-0.77675500
C	-3.57725500	0.17633000	-1.37424300
H	-3.90983400	0.94899900	-2.06906600
C	1.95063800	-0.58717100	0.11469600
C	0.42756500	1.07859100	-0.23376300
C	2.63409900	0.59935800	-0.13602500
C	1.68232400	1.62522200	-0.34345800
H	1.90036400	2.68711100	-0.42280500
N	0.60375700	-0.30802000	-0.05935000
C	2.51110100	-1.82170400	0.74820500
H	1.76380200	-2.29787800	1.39759100
H	2.85870100	-2.56587100	0.02238700
H	3.35899900	-1.51617100	1.36951500
C	-0.77044600	1.86882800	0.11906500
C	-1.50682400	1.56977600	1.27462600
C	-1.12868000	2.98664500	-0.64396900
C	-2.60750500	2.34312900	1.62950800
H	-1.21847400	0.71300600	1.88840800
C	-2.22541100	3.76630700	-0.28035300
H	-0.55555000	3.22742800	-1.54197300
C	-2.97622000	3.44023700	0.84873200
H	-3.17913900	2.09064500	2.52421900
H	-2.50001900	4.62953400	-0.88924400
H	-3.84183400	4.04421800	1.12543500
C	4.07963400	0.86947900	-0.10954900
C	6.23403000	-0.01938600	0.08877900
H	6.69076000	-1.00642100	0.21869200
H	6.57645400	0.43482500	-0.85117700
H	6.51649300	0.64087800	0.92062500
O	4.56048400	1.96703300	-0.24683400
O	4.83055200	-0.22899700	0.06391400
C	-2.21362500	-3.15236700	0.81428700
H	-2.90253500	-3.80264100	1.35742000
H	-0.57604400	-4.54347700	0.74341300

TS3a-2

C	-0.96483400	2.08484000	0.11344600
C	-2.20323300	2.61037000	-0.32646400
C	-2.00541800	0.09483600	0.89361500

N	-0.87974200	0.67533100	0.21988400
C	1.61142900	0.36320900	-0.08774900
C	0.28763800	-1.46589800	0.25336000
C	2.41869700	-0.75337200	0.11449700
C	1.59020300	-1.88360900	0.32219300
H	1.92478500	-2.91560000	0.38336100
N	0.30448200	-0.06955900	0.11258800
C	-2.33822300	3.99450300	-0.50219700
C	2.05076500	1.61257000	-0.80318000
H	1.23078800	2.06561200	-1.36743500
H	2.49555900	2.37383300	-0.14988000
H	2.82836600	1.31502700	-1.51488800
C	-0.87568400	-2.32929100	-0.03109700
C	-1.67858000	-2.05799900	-1.14795200
C	-1.13753200	-3.47007800	0.73561400
C	-2.73794900	-2.90077000	-1.47730600
H	-1.46584500	-1.18150800	-1.76493800
C	-2.18919100	-4.31782500	0.39528500
H	-0.52341300	-3.67578600	1.61401500
C	-2.99759500	-4.03323800	-0.70603300
H	-3.35499700	-2.67630900	-2.34929700
H	-2.38779900	-5.20244400	1.00288800
H	-3.82548500	-4.69530100	-0.96471400
C	3.88183800	-0.86867600	0.01147500
C	5.91707000	0.24542700	-0.28588600
H	6.25945300	1.27483900	-0.43685500
H	6.36126300	-0.17090000	0.62869300
H	6.21584100	-0.38138100	-1.13755900
O	4.48305900	-1.90980800	0.10123200
O	4.50322500	0.30706300	-0.17534300
C	0.00887500	2.96860300	0.58989100
H	-3.29203000	4.38292000	-0.86525400
H	0.88066100	2.57907700	1.10810500
C	-0.15359800	4.34066800	0.43221900
C	-1.30698500	4.85942700	-0.16183800
H	0.62254300	5.01275900	0.80146300
H	-1.42289900	5.93518300	-0.29686500
O	-1.90771000	-0.69823300	1.78827200
C	-3.35274200	1.72183900	-0.35588800
H	-4.28941500	2.07532600	-0.79203700
C	-3.27933300	0.54560700	0.29258600
H	-4.13284100	-0.11480000	0.44904800

5a'

C	0.95702600	-1.13261600	-1.96204600
C	2.19823400	-1.93795900	-2.07811600
C	2.51192300	-2.04307000	0.19860000
C	1.35226400	-1.28393100	0.45836800
O	0.30211200	-0.75285600	-2.90334700
N	0.61726900	-0.83648500	-0.64295400
C	3.28306500	-2.50531200	1.27584700
H	4.17447500	-3.08773100	1.03981900
C	0.96794800	-1.00086100	1.77520300
H	0.06863100	-0.41609300	1.97214800
C	2.90928500	-2.22352300	2.57911100
H	3.51187800	-2.58262100	3.41362900
C	1.75026000	-1.47350100	2.82075000
H	1.45133900	-1.25171600	3.84627700
N	2.90640200	-2.34841400	-1.09563100
C	-1.75941500	-0.59507700	-0.32278100
C	-0.46624100	1.28193800	-0.08311700
C	-2.57103100	0.45314500	0.08511700
C	-1.75497600	1.61769300	0.24080100
H	-2.11047600	2.60471400	0.52448900
N	-0.49445600	-0.06892200	-0.42328800
C	-1.99698000	-2.03058700	-0.64178000
H	-1.79036900	-2.22220600	-1.70629900
H	-1.33724500	-2.67848500	-0.04392500
H	-3.03702900	-2.29200000	-0.43106200
C	0.77557100	2.07234800	-0.09724600
C	1.64627100	2.03037600	-1.19701100
C	1.09401500	2.89128800	0.99479700
C	2.82161000	2.77772600	-1.19087100
H	1.37630400	1.44040400	-2.07560800
C	2.26313500	3.64866500	0.98991600
H	0.42237600	2.91878800	1.85510000
C	3.13359500	3.58687700	-0.09797800
H	3.48996800	2.73997300	-2.05262300
H	2.50145200	4.28214800	1.84593800
H	4.05298500	4.17465700	-0.09697000
C	-4.02512900	0.48122000	0.32068000
C	-6.03515600	-0.71424900	0.29051300
H	-6.36533000	-1.72961200	0.04703100
H	-6.28486400	-0.47451300	1.33344000
H	-6.53113300	0.01307700	-0.36663100
O	-4.62616700	1.45992100	0.68476500
O	-4.62899600	-0.69361500	0.09131200
H	2.49530500	-2.17316900	-3.10602600

TS5a'-1

C	-0.07040000	-2.61463800	-0.35407900
C	-0.98250700	-3.52275800	0.41585100
C	-2.65852400	-2.00270600	0.29751000
C	-1.79792400	-1.03282000	-0.26716000
O	0.86202600	-2.98980900	-1.00974100
N	-0.40759600	-1.26686800	-0.09512100
C	-4.04574900	-1.81912000	0.23833900
H	-4.67138300	-2.57544500	0.71381400
C	-2.35053600	-0.04083900	-1.08357400
H	-1.70551800	0.60153200	-1.67448400
C	-4.58473600	-0.75025700	-0.46177100
H	-5.66541100	-0.61582000	-0.51456400
C	-3.73044700	0.10635700	-1.16237800
H	-4.13916300	0.89536000	-1.79524800
N	-2.16496800	-3.21235200	0.78167400
C	1.91980400	-0.57940900	0.12680900
C	0.43385300	1.10494100	-0.31218200
C	2.63063600	0.58005200	-0.15783600
C	1.70277400	1.61706200	-0.42053100
H	1.94581800	2.67147100	-0.52537100
N	0.57994400	-0.27737900	-0.07350200
C	2.43431200	-1.81977700	0.78478800
H	1.65307300	-2.28883500	1.39882300
H	2.80627400	-2.56501100	0.07158300
H	3.25879600	-1.52705800	1.44309700
C	-0.73793900	1.93478200	0.04103700
C	-1.44515100	1.68379700	1.22560800
C	-1.09219500	3.04070800	-0.74124900
C	-2.51173200	2.49620100	1.59686300
H	-1.15869600	0.83704500	1.85398300
C	-2.15643300	3.85771400	-0.36256700
H	-0.54209600	3.24414500	-1.66253500
C	-2.87642600	3.58249500	0.79997000
H	-3.05953000	2.28146400	2.51586500
H	-2.42919200	4.71181100	-0.98494200
H	-3.71539600	4.21744600	1.08884000
C	4.08196500	0.81890300	-0.10977100
C	6.20623300	-0.11100700	0.19691300
H	6.63215000	-1.10045400	0.39459700
H	6.58761500	0.28116300	-0.75585700
H	6.48106300	0.58735900	0.99950400
O	4.59116400	1.89663800	-0.29001000
O	4.79840200	-0.28655800	0.14058200
H	-0.55607100	-4.50024000	0.67135100

TS5a'-2

C	1.04994300	2.04701100	-0.10119800
C	2.33405400	2.49046700	0.29772200
C	3.26649700	0.49323700	-0.21967100
C	1.98941000	0.04487600	-0.86716800
N	0.88617700	0.64296400	-0.20430800
N	3.41036000	1.60833500	0.38338500
C	-1.61491700	0.42707100	0.09933800
C	-0.35392900	-1.45353800	-0.22333600
C	-2.45807200	-0.66042300	-0.10405100
C	-1.67006300	-1.82187800	-0.30037300
H	-2.04243900	-2.84080300	-0.36233800
N	-0.32151900	-0.05637800	-0.08273000
C	2.57573000	3.85902500	0.46302600
C	-2.01716000	1.70063800	0.79288300
H	-1.18588700	2.14372000	1.34821100
H	-2.44507300	2.45780900	0.12354300
H	-2.80176000	1.43803200	1.51075400
C	0.77925400	-2.36107800	0.04194900
C	1.61714300	-2.13237400	1.14258200
C	0.97658400	-3.50375400	-0.74028800
C	2.64894600	-3.02084500	1.43884800
H	1.45295700	-1.25588500	1.77485300
C	1.99935600	-4.39756900	-0.43184800
H	0.33396900	-3.67508200	-1.60552900
C	2.84393900	-4.15583800	0.65187900
H	3.29520300	-2.83063200	2.29766700
H	2.14608000	-5.28403900	-1.05122700
H	3.65010500	-4.85311000	0.88518500
C	-3.92657100	-0.72307000	-0.01290600
C	-5.92335000	0.46586700	0.25158100
H	-6.22852500	1.50729600	0.39897100
H	-6.37250600	0.06554700	-0.66769300
H	-6.25239300	-0.14983000	1.10004700
O	-4.56104800	-1.74427800	-0.09711800
O	-4.50637200	0.47514600	0.15494900
C	0.12665900	2.99605800	-0.55036200
H	3.57042700	4.15429000	0.79908600
H	-0.78480400	2.66900700	-1.04170200
C	0.39477100	4.35369100	-0.41206200
C	1.60197900	4.79238900	0.13837400

H	-0.34237900	5.07623700	-0.76532100
H	1.80033600	5.85815600	0.25490400
O	1.92311100	-0.76371300	-1.74764100
H	4.09483300	-0.22218600	-0.28486600

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C	-0.53279900	2.82496000	-0.16946300
C	-1.61078500	3.62097400	0.38425400
C	-2.37929400	1.75797700	1.73642600
C	-1.36697600	0.96726700	1.27233500
O	0.26991100	3.18111500	-1.00461400
N	-0.47892800	1.49630100	0.34631900
C	1.79817000	0.74033000	0.05013200
C	0.16557900	-0.36521700	-1.11002800
C	2.38317200	-0.30387200	-0.65276100
C	1.35657900	-0.99572000	-1.36361500
H	1.50645800	-1.84387100	-2.02615400
N	0.45834700	0.67767900	-0.23406600
C	2.34631700	1.79917700	0.94322400
H	2.52863600	2.71891300	0.36639500
H	1.63139300	2.04650400	1.74184800
H	3.29008600	1.46930300	1.38727600
C	-1.19458800	-0.65865000	-1.58731400
C	-2.06655500	0.36039100	-1.99914500
C	-1.63159600	-1.99034400	-1.64056500
C	-3.35475900	0.05207300	-2.43151400
H	-1.72189700	1.39620800	-2.01560700
C	-2.91289000	-2.29575500	-2.09139800
H	-0.96195700	-2.78283100	-1.30037100
C	-3.78239300	-1.27494800	-2.47807900
H	-4.02225900	0.85478200	-2.74916800
H	-3.23966600	-3.33647300	-2.12751100
H	-4.79052900	-1.51384500	-2.82083200
C	3.79873100	-0.69410100	-0.72853600
C	5.99674500	-0.19419700	-0.10770700
H	6.51823800	0.57939800	0.46600500
H	6.17776400	-1.18273500	0.33711200
H	6.35966100	-0.20449500	-1.14460700
O	4.20238300	-1.65828200	-1.32852600
O	4.61692500	0.13512400	-0.06108300
C	-2.49311100	3.10249600	1.27872800
C	-1.20759600	-0.44238900	1.71363800
C	-2.31472800	-1.29668800	1.64435400
C	0.00763200	-0.92897300	2.21438700
C	-2.20717000	-2.62104200	2.06375800
H	-3.25355500	-0.92395500	1.22920300
C	0.11207800	-2.25409000	2.62656200
H	0.87315600	-0.26931100	2.29059000
C	-0.99292100	-3.10313300	2.54993000
H	-3.07287500	-3.28169500	1.99617100
H	1.06305500	-2.62483000	3.01183800
H	-0.90542100	-4.14265400	2.86997700
H	-3.06928600	1.35070800	2.47273300
H	-3.30308800	3.72639500	1.66187800
H	-1.67863700	4.64381700	0.01562100

TS9-1

C	0.77985600	2.69144600	0.41939300
C	0.42959800	3.92471600	-0.29363400
C	-1.61878400	2.90525400	-1.01877700
C	-1.25965700	1.71332000	-0.46587700
O	1.62885000	2.59653700	1.27084900
N	0.08099500	1.54877500	-0.08566700
C	2.15322100	0.32595700	-0.20314900
C	0.31722300	-0.95532300	0.27823800
C	2.58601100	-0.92255300	0.21499500
C	1.44010600	-1.71008600	0.50382300
H	1.44260500	-2.78216400	0.68641200
N	0.77084300	0.33177000	-0.08702700
C	2.95575400	1.42644900	-0.81545800
H	2.31726100	2.09882500	-1.40382100
H	3.48923300	2.01790200	-0.06087700
H	3.69556600	0.97571900	-1.48631800
C	-0.92953500	-1.59684200	-0.21302700
C	-1.21789900	-1.51687300	-1.58467900
C	-1.69773100	-2.44080400	0.59354200
C	-2.26688000	-2.24905300	-2.13131400
H	-0.59678900	-0.88405000	-2.22410200
C	-2.74795800	-3.17554200	0.04229300
H	-1.47222800	-2.51407100	1.65913000
C	-3.03807300	-3.08122500	-1.31790500
H	-2.47521700	-2.18096100	-3.20074800
H	-3.34568300	-3.82536100	0.68432800
H	-3.85825100	-3.66021400	-1.74570600
C	3.95447000	-1.45416200	0.28650100
C	6.23523500	-1.00916400	0.02024900
H	6.86360400	-0.15769800	-0.26228000
H	6.48374300	-1.34088700	1.03778100

H	6.39872900	-1.84669100	-0.67207600
O	4.22490100	-2.58122000	0.61804100
O	4.89261500	-0.55391600	-0.04600600
C	-0.69226400	4.00101100	-1.04705800
H	-0.95476600	4.92458500	-1.56618900
H	-2.67373400	3.08275800	-1.22817300
C	-2.32326400	0.88357300	0.16674800
C	-3.49006700	0.51509900	-0.50830800
C	-2.22508600	0.66611000	1.54829200
C	-4.54222800	-0.07380500	0.18894400
H	-3.56407600	0.67719800	-1.58542700
C	-3.28426800	0.08792400	2.24229000
H	-1.31682900	0.96254900	2.07859100
C	-4.44493300	-0.28491600	1.56514000
H	-5.44372900	-0.37251700	-0.34881100
H	-3.20105100	-0.06999400	3.31885100
H	-5.27322100	-0.74405800	2.10730800
H	1.11397200	4.76105300	-0.14965900

TS9-2

C	-0.45831600	-2.18098300	-0.45127500
C	0.00304600	-3.37944900	-0.90932500
C	2.21896000	-2.88028100	-0.14592200
C	1.66549800	-1.71584200	0.55698900
N	0.49564600	-1.20645000	-0.11114000
C	-0.91924900	0.84984300	-0.42303300
C	1.25258800	1.10825600	0.24096300
C	-0.71167900	2.17439400	-0.05480700
C	0.63808300	2.32653500	0.35067500
H	1.13476300	3.26782500	0.56998300
N	0.26435300	0.17897400	-0.13270500
C	-2.03811300	0.36738900	-1.30039200
H	-1.72575600	-0.48323200	-1.91541500
H	-2.94660300	0.09703200	-0.74774400
H	-2.29718600	1.19340000	-1.97198200
C	2.71206400	0.91590300	0.13018000
C	3.25412400	0.27628600	-0.99295400
C	3.57460800	1.46254000	1.08650800
C	4.63484500	0.16607500	-1.14246200
H	2.58595200	-0.13447700	-1.75433800
C	4.95438600	1.36325800	0.92672800
H	3.15238000	1.94658400	1.96872300
C	5.48972700	0.70901100	-0.18296500
H	5.04558300	-0.33459400	-2.02115000
H	5.61792500	1.78882600	1.68153000
H	6.57119900	0.62599300	-0.30216200
C	-1.63571600	3.31623000	-0.13535300
C	-3.81087000	4.04712200	-0.58473200
H	-4.75653200	3.60867400	-0.92100100
H	-3.93892000	4.51117700	0.40304100
H	-3.47676900	4.81784200	-1.29303300
O	-1.32829900	4.44970500	0.13835000
O	-2.87686000	2.98045000	-0.52043900
O	2.12185500	-1.20921000	1.54573900
C	-1.85362200	-2.07228900	0.04550800
C	-2.08899500	-1.45286100	1.27935500
C	-2.91913900	-2.66356600	-0.64321000
C	-3.37957300	-1.40415200	1.80164600
H	-1.25843800	-1.00311800	1.82851200
C	-4.20569400	-2.61638500	-0.11557800
H	-2.74263200	-3.13378800	-1.61309800
C	-4.44170900	-1.97885500	1.10418600
H	-3.55322000	-0.91381200	2.76069300
H	-5.03231500	-3.07035700	-0.66452400
H	-5.45290700	-1.93342500	1.51140800
H	-0.71431100	-4.17850200	-1.09280600
H	1.79210700	-4.57152200	-1.36950700
C	1.40987600	-3.66820300	-0.89092800
H	3.27134900	-3.09559300	0.04177200

C1

P	-0.02669900	-0.83926400	-0.13272200
O	0.68685500	-1.58356100	1.07411000
O	-0.60657400	-1.70358300	-1.15784400
H	-1.17638000	4.44417900	-2.83602700
H	-1.54807600	5.14052500	-1.25105000
H	-3.78483400	3.24495000	-2.56065300
C	-1.16014700	4.24079400	-1.75625700
C	-3.23128300	2.62844000	-1.84996800
H	0.86690100	4.73423300	-0.99147700
C	0.23926900	3.86630900	-1.23907800
C	-1.97960900	3.02480200	-1.38938800
H	0.76699600	3.26778000	-1.99771600
C	-3.77197600	1.42420400	-1.39742500
H	-4.76121700	1.11023800	-1.73608800
H	-0.96738600	4.71078200	0.99658000
H	1.44300500	5.13856800	1.28184800
C	-1.27880700	2.23335500	-0.47147600

C	-0.03411300	2.96442100	-0.00258500
C	-0.33085300	3.84906300	1.24194400
C	1.05534100	4.23504100	1.78043200
C	-3.06542600	0.57669800	-0.53409400
C	-1.80237800	1.00250100	-0.09576200
C	1.21940200	2.24718900	0.46822500
C	1.89013700	3.02967500	1.41687400
H	-0.86103400	3.23571900	1.98722400
O	1.05712800	0.19317400	-0.76060900
H	1.05785400	4.43577800	2.86084200
C	1.77152000	1.03001200	0.07828300
C	-3.86556100	-1.76506700	-1.00461900
C	-3.64243500	-0.72372400	-0.08068300
C	3.13332300	2.64076900	1.90767000
O	-1.02601600	0.14980400	0.67956900
C	4.01408100	-0.81828300	-1.25861500
C	3.02931900	0.61467900	0.54883500
H	3.65827100	3.25309100	2.64317500
C	3.69937700	1.45022200	1.45351900
C	-4.42062300	-2.96127400	-0.54701400
H	4.89984000	-2.11674100	-2.71973000
C	-3.97916700	-0.89446700	1.27472600
H	-4.58026100	-3.77346300	-1.26175000
C	4.60607400	-2.00917800	-1.67194700
C	3.63884500	-0.67207400	0.09718200
H	4.67817500	1.13407600	1.82049200
C	-4.76379800	-3.15476300	0.79406000
C	-4.53838400	-2.10812600	1.68804900
C	4.83488200	-3.06936000	-0.78637800
C	3.86677900	-1.72042600	1.00416400
H	-4.80448200	-2.23568500	2.74076900
C	4.45934900	-2.90349200	0.54299100
H	4.62191800	-3.71949500	1.25265000
C	5.46004700	-4.34821600	-1.27581500
H	5.61941000	-5.05800300	-0.45349800
H	4.81723500	-4.83496900	-2.02485800
H	6.43110200	-4.15542000	-1.75596700
C	3.48600400	-1.64859300	2.46364300
H	2.90258300	-2.53639600	2.74929000
H	4.38317300	-1.63265700	3.10198000
H	2.90722700	-0.74987800	2.71716200
C	3.79250800	0.29306400	-2.25152800
H	2.72082700	0.41085700	-2.47232200
H	4.15803600	1.25629800	-1.86571200
H	4.31240100	0.07959100	-3.19451300
C	-5.34597700	-4.46661700	1.24989400
H	-5.63964000	-4.43012300	2.30752100
H	-6.23309700	-4.73459000	0.65683700
H	-4.61556800	-5.28128000	1.12873000
C	-3.75141000	0.20567900	2.27966000
H	-2.67604800	0.34536700	2.47040400
H	-4.14689400	1.16738200	1.92035800
H	-4.23784800	-0.03211500	3.23492800
C	-3.49772800	-1.61505800	-2.45794100
H	-3.53797600	-2.58825600	-2.96529900
H	-4.18327200	-0.93414200	-2.98514100
H	-2.47797500	-1.21976300	-2.55441800
H	1.07688700	-1.00334900	1.74697700

INT1

C	-6.13273400	0.66428400	0.00152700
C	-5.74622400	-0.48532500	-0.66350900
C	-4.45221100	-1.01352400	-0.49946800
C	-3.54082100	-0.35133400	0.35311500
C	-3.93405500	0.82077700	1.02462200
C	-5.21742600	1.31119000	0.84613800
H	-7.13753800	1.06688700	-0.12979600
H	-6.44013600	-1.00553600	-1.32710800
H	-3.22479300	1.33249300	1.67177000
H	-5.51289600	2.22023200	1.37265900
C	-4.01391300	-2.21310600	-1.16462100
H	-4.71657800	-2.73055300	-1.82197600
C	-2.76658800	-2.69528400	-0.97802500
H	-2.40939600	-3.60476500	-1.46072100
N	-2.25620800	-0.85870800	0.49912600
C	-1.79600100	-2.03453800	-0.10631600
N	-1.49094200	-0.31598600	1.53429400
C	-0.36559200	0.21034300	1.23351500
C	0.46305100	0.69359700	2.38294100
C	0.16783200	0.39178000	-0.17440400
H	0.79391000	1.72520400	2.21142500
H	-0.12020900	0.61669500	3.30767900
H	1.36355900	0.06670200	2.47972900
H	-0.55751300	-0.03197800	-0.88171300
C	0.19852000	1.87392500	-0.51847600
O	-0.34229400	2.73988100	0.11400200
O	0.82813200	2.08093600	-1.67417300
C	1.50200400	-0.32170300	-0.42060600

H	1.44578300	-1.32743100	0.01927600
H	1.64303000	-0.47273400	-1.50316800
C	2.72125700	0.42762100	0.07643300
O	2.64261500	1.56766200	0.47921500
C	4.04746600	-0.27156400	0.02946800
C	4.19003600	-1.59393400	-0.40879800
C	5.17748100	0.44391400	0.44641100
C	5.44965900	-2.19003100	-0.42867200
H	3.32256000	-2.16942800	-0.73429300
C	6.43297800	-0.15254300	0.42607500
H	5.04403100	1.47214800	0.78530500
C	6.56963700	-1.47178800	-0.01183200
H	5.55584700	-3.22068000	-0.77014600
H	7.30977700	0.40958900	0.75148500
H	7.55446000	-1.94195700	-0.02775600
C	0.97104400	3.44026500	-2.06409400
H	1.52380300	3.43379400	-3.00913000
H	-0.01155300	3.91197000	-2.20100400
H	1.53243300	3.99531700	-1.29988500
O	-0.66357000	-2.44113600	0.08656300

INT2

C	3.71261600	-1.32619500	-1.37575900
C	3.46657000	-1.24935500	-0.01454800
C	2.17296800	-1.44388600	0.49757700
C	1.11187900	-1.71278900	-0.39472800
C	1.36397900	-1.80102700	-1.77305500
C	2.65370700	-1.60679800	-2.24891800
H	4.71982500	-1.17219800	-1.76401300
H	4.27554500	-1.03375100	0.68673900
H	0.54096300	-2.02032600	-2.45141300
H	2.83836400	-1.67793100	-3.32217900
C	1.88644700	-1.36884500	1.91218000
H	2.70842200	-1.13086100	2.59158700
C	0.64557000	-1.59041400	2.38904400
H	0.40464700	-1.55510000	3.45102500
N	-0.17429100	-1.85646000	0.12501100
C	-0.47111100	-1.92223400	1.50207000
N	-1.22574600	-2.13785400	-0.73363600
C	-2.36280200	-1.30736000	-0.67273000
C	-3.64624000	-2.07859600	-0.59998000
C	-2.24692400	0.04557100	-0.69126800
H	-4.47008600	-1.56126100	-1.09638500
H	-3.50773100	-3.07203000	-1.05314900
H	-3.91282000	-2.22046100	0.45797000
C	-3.42025100	0.89396200	-0.38876300
O	-4.53139900	0.52818300	-0.08854100
O	-3.10659600	2.20040500	-0.46502200
C	-0.94240900	0.74469600	-0.94750600
H	-0.27323600	0.11300200	-1.54592400
H	-1.12431600	1.65099200	-1.54585500
C	-0.22324100	1.19174700	0.31592700
O	-0.74705500	1.10760400	1.40214700
C	1.17391200	1.72839100	0.18009600
C	1.79703000	1.90062900	-1.06101000
C	1.87910100	2.02440200	1.35371000
C	3.11298200	2.35751400	-1.12607700
H	1.26237400	1.67630700	-1.98523600
C	3.19388700	2.47308600	1.28802500
H	1.37243500	1.88657900	2.31026900
C	3.81335800	2.63773000	0.04628300
H	3.59417500	2.48867200	-2.09665700
H	3.74041700	2.69980200	2.20518600
H	4.84520400	2.98990500	-0.00649200
C	-4.13974000	3.10604900	-0.11940200
H	-3.71234900	4.11069300	-0.20885000
H	-4.99801200	2.99907500	-0.79755600
H	-4.48161500	2.93111800	0.91010200
O	-1.58139500	-2.23595900	1.87053400
H	-1.47812300	-3.12154400	-0.65872900

TS1-*Sr*

C	2.93902000	-2.88727300	2.52492100
C	2.21773800	-1.76743200	2.04986000
C	4.37631400	-2.90560100	2.39602400
C	5.04564500	-1.82324600	1.95575700
N	2.94632000	-0.74014200	1.42181000
C	4.34853300	-0.60184100	1.55801200
N	2.27731800	0.28652500	0.74739200
C	2.50357700	1.65639200	1.18992700
C	2.77745100	1.94211600	2.62510400
C	2.35850900	2.48653500	0.14438400
H	2.89331500	1.01261000	3.19599200
H	1.94964200	2.52332200	3.05320100
H	3.69020500	2.54302700	2.72018000
C	2.63077900	3.93088800	0.28905400
O	2.77054200	4.50938000	1.33935800
C	2.00632800	1.81314400	-1.15439300

H	2.47108200	2.30131900	-2.02042000	H	-5.85682400	0.22637700	-1.18825400
H	0.91686500	1.81963800	-1.30891700	C	-3.14173200	-3.71114100	-2.37525500
C	2.47743100	0.36000700	-1.04792200	H	-2.76621700	-4.47825100	-3.05588300
O	1.73846100	-0.59879000	-1.54536600	H	-6.02832800	-2.39926600	1.49987900
C	3.93749300	0.10836800	-1.31591500	H	-6.79302100	-0.27300900	2.47342100
C	4.86349000	1.14403600	-1.46358600	C	-4.08010900	-1.79976900	-0.58605000
C	4.35702400	-1.22114400	-1.43077100	C	-4.84664000	-0.90092800	0.36721300
C	6.20348700	0.84952800	-1.70028800	C	-5.26311600	-1.62931600	1.67468600
H	4.55100600	2.18521600	-1.37472300	C	-5.72336200	-0.49993500	2.61431600
C	5.70117000	-1.51267900	-1.65017400	C	-2.23172300	-3.07541500	-1.52273300
H	3.61522700	-2.01672900	-1.33900400	C	-2.72151400	-2.08712700	-0.65106600
C	6.62629900	-0.47677400	-1.78316100	C	-4.26227000	0.37481400	0.94492400
H	6.92381300	1.66100500	-1.81268500	C	-4.86795200	0.66654100	2.17217300
H	6.02661100	-2.55208000	-1.72462200	H	-4.37304500	-2.12185500	2.09654100
H	7.67927200	-0.70287700	-1.96051800	O	-2.61875100	0.90529100	-0.70532800
H	1.22206100	0.15291900	0.75763700	H	-5.58330100	-0.74307500	3.67710800
H	0.72770000	-0.38437500	-1.70283400	C	-3.34492100	1.26893100	0.40738200
O	4.89571200	0.45490500	1.33887900	C	0.09959700	-3.22847900	-2.50675700
O	2.78468100	4.53012000	-0.89652900	C	-0.79865300	-3.49136500	-1.46106600
C	3.20048700	5.88872500	-0.84674500	C	-4.63470900	1.88672700	2.79988300
H	2.48713900	6.49628000	-0.27426300	O	-1.84635700	-1.36903400	0.13999300
H	3.25311900	6.23561000	-1.88364200	C	-2.77757900	4.02756800	-0.98038600
H	4.18776200	5.96773300	-0.36996000	C	-3.13480400	2.53141600	0.98347200
H	6.13261000	-1.77236700	1.90075900	H	-5.10964500	2.12198600	3.75435700
H	4.91442500	-3.80306700	2.70993300	C	-3.80066000	2.82147200	2.18108400
C	2.25496600	-3.92172100	3.18544200	C	1.43271000	-3.63862100	-2.36768800
H	2.83156100	-4.77952000	3.53780900	H	-2.40489300	5.37264100	-2.61493100
C	0.83603200	-1.68958600	2.28201700	C	-0.36984100	-4.20155900	-0.31856500
H	0.24099000	-0.83611100	1.96233700	H	2.13748000	-3.40948300	-3.17196500
C	0.89261400	-3.84135200	3.41407300	C	-2.03938700	5.00545400	-1.65207800
C	0.19644600	-2.71314100	2.96741500	C	-2.31361100	3.55028700	0.26318800
H	-0.87275100	-2.61579200	3.15958000	H	-3.65437600	3.80396700	2.63505000
H	0.37192700	-4.63846200	3.94596900	C	1.88681400	-4.30691300	-1.23282800
P	-1.26132400	0.03621500	-0.47493000	C	0.96414100	-4.59124200	-0.21896100
O	-0.37476600	0.61502800	0.59719400	C	-0.85906300	5.52924300	-1.12490500
O	-0.67702700	-0.16482900	-1.84844500	C	-1.12140500	4.05995200	0.81208200
H	-6.87015200	-1.70216700	-2.24807400	H	1.29082800	-5.14004900	0.66935500
H	-6.97845300	-2.59050200	-0.71894300	C	-0.42089500	5.04760400	0.11140700
H	-5.18202400	-3.86217800	-3.07807500	H	0.48916800	5.45641200	0.55906300
C	-6.35833700	-1.88120500	-1.29211400	C	-0.06290600	6.55727500	-1.88345600
C	-4.49810500	-3.37877800	-2.37782100	H	0.75554300	6.07524000	-2.44188900
H	-6.96086800	-0.27198400	0.11667000	H	-0.68954600	7.09148100	-2.61068900
C	-6.10529400	-0.59206000	-0.49509200	H	0.38454500	7.29869200	-1.20608500
C	-4.96107100	-2.42620500	-1.47623600	C	-0.57567800	3.54158000	2.11698800

H	0.42159300	3.96520000	2.30246700
H	-1.22085200	3.80589200	2.96825800
H	-0.50286900	2.44377000	2.07728400
C	-4.04673600	3.50490200	-1.60254800
H	-3.89186200	2.49011300	-2.00034000
H	-4.86553800	3.44987200	-0.87053600
H	-4.36538800	4.14964800	-2.43242300
C	3.32926700	-4.71591600	-1.08156100
H	3.41775500	-5.79279700	-0.87220000
H	3.90481600	-4.49942900	-1.99260100
H	3.80476700	-4.18272800	-0.24129700
C	-1.35470100	-4.57480200	0.75830800
H	-1.76210900	-3.68081300	1.25170000
H	-2.20874700	-5.12400100	0.33275600
H	-0.87989700	-5.20479100	1.52203400
C	-0.33909000	-2.53294300	-3.76912200
H	0.52468700	-2.08633900	-4.28139100
H	-0.80888900	-3.24367100	-4.46844200
H	-1.05849300	-1.73465300	-3.55137200

TS1-*Ss*

C	-4.91466100	-2.30634700	-1.25378200
C	-4.26693500	-1.34479900	-0.44192400
C	-4.12960800	-3.10109800	-2.16485300
C	-2.79412000	-2.94694700	-2.25876400
N	-2.87571200	-1.24965100	-0.52521000
C	-2.07636600	-1.97754800	-1.44115500
N	-2.14018900	-0.26387500	0.12985500
C	-2.33654400	0.05231900	1.51822800
C	-2.76166100	-0.99765200	2.48917500
C	-1.94176200	1.31996600	1.74296100
H	-3.14640900	-1.88231700	1.96815500
H	-1.88622900	-1.29288100	3.08707800
H	-3.51530400	-0.61236300	3.18653300
C	-1.92835100	1.90464400	3.10104000
O	-2.18888000	1.31878300	4.12159900
C	-1.41587800	2.07952300	0.55601300
H	-1.66420800	3.14557300	0.61364400
H	-0.31654400	2.01480400	0.51469800
C	-1.99795200	1.50059900	-0.72491500
O	-1.28148800	1.31354600	-1.76578300
C	-3.43217400	1.82125900	-1.02832500
C	-4.21637000	2.61352100	-0.18157800
C	-3.98584500	1.31511500	-2.21109000
C	-5.54713900	2.87367400	-0.50509500
H	-3.79568600	3.03001300	0.73523600
C	-5.31872200	1.56403100	-2.52368000
H	-3.35612200	0.72039500	-2.87519200
C	-6.10217100	2.34116100	-1.66854800
H	-6.15303100	3.49658900	0.15486700
H	-5.74782400	1.15361300	-3.43907100
H	-7.14701400	2.53962200	-1.91402600
H	-1.12561500	-0.54778500	0.05998400
H	-0.20661800	1.00835300	-1.62181700
O	-0.88567400	-1.76050600	-1.50530100
O	-1.60577900	3.20523300	3.06939000
C	-1.53709300	3.85859800	4.32921500
H	-1.29214700	4.90583700	4.12299800
H	-2.49911700	3.79061000	4.85514000
H	-0.75803600	3.40310900	4.95577800
P	1.46756500	-0.09366200	-0.25081100
O	0.99806400	0.60599100	-1.51271100
O	0.48926900	-0.40761200	0.83100600
H	6.76217300	-1.65338400	2.59058400
H	7.25068700	-2.32700900	1.02641900
H	5.16465000	-4.01319000	2.80524700
C	6.46695000	-1.74156700	1.53551900
C	4.57986800	-3.48170500	2.05204800
H	7.17714400	0.07564200	0.47392400
C	6.25313700	-0.38345600	0.85340900
C	5.11631800	-2.39639200	1.36759100
H	5.79047200	0.31845700	1.56465900
C	3.27241700	-3.87071100	1.77207400
H	2.83353200	-4.72217800	2.29696000
H	6.75004700	-1.95529500	-1.26585500
H	7.52433400	0.31770400	-1.81166600
C	4.36946600	-1.72977400	0.38895900
C	5.23146200	-0.67324000	-0.28359900
C	5.97982800	-1.21701100	-1.53137700
C	6.53759300	0.04112100	-2.21884500
C	2.47154700	-3.18183100	0.84838200
C	3.04724100	-2.10713300	0.15116600
C	4.67378200	0.62234700	-0.84511600
C	5.50193600	1.08682600	-1.87385000
H	5.24734500	-1.70730600	-2.19103000
O	2.65755900	0.82229000	0.41724000
H	6.65999600	-0.08204200	-3.30421300
C	3.56642500	1.37058200	-0.46094800

C	0.13239200	-3.53519200	1.69913400
C	1.06345700	-3.64347000	0.64296300
C	5.28339300	2.33567000	-2.44551500
O	2.30533300	-1.39515800	-0.76559200
C	2.05141000	3.91720600	0.73146900
C	3.32359400	2.63790000	-1.01866000
H	5.93018100	2.70516600	-3.24359800
C	4.21303900	3.10876700	-1.99310500
C	-1.13901200	-4.08919600	1.53808200
H	0.89117400	5.05921900	2.13451200
C	0.69747700	-4.28106000	-0.55402000
H	-1.85432600	-4.01451300	2.36263700
C	0.96134500	4.70755200	1.10115000
C	2.14539300	3.45465000	-0.59994100
H	4.03582100	4.09549000	-2.42604400
C	-1.51201200	-4.76319900	0.36950400
C	-0.58035500	-4.84349100	-0.66359100
C	-0.04180100	5.05253900	0.19208300
C	1.14509300	3.79111200	-1.53315200
H	-0.84909400	-5.36386600	-1.58720700
C	0.06673300	4.58177800	-1.11557200
H	-0.71999800	4.81890400	-1.83785900
H	-2.17588600	-3.51674900	-2.95088500
H	-4.64930400	-3.83039900	-2.79061900
C	-6.31265400	-2.44704300	-1.18325400
H	-6.78644000	-3.19648500	-1.82046300
C	-5.04662100	-0.53864600	0.40725700
H	-4.59321200	0.23677700	1.01723500
C	-7.06990400	-1.65662000	-0.33904100
C	-6.42255900	-0.69768900	0.45050900
H	-7.00339900	-0.05233200	1.11169800
H	-8.15281900	-1.77217900	-0.29301100
C	-1.23306000	5.85522800	0.64489000
H	-1.95098600	6.00777000	-0.17277400
H	-1.75306500	5.33747600	1.46773900
H	-0.93045700	6.84417100	1.02196800
C	1.19803200	3.32073800	-2.96453500
H	0.19044800	3.32528900	-3.40254300
H	1.83073100	3.98046500	-3.57942400
H	1.60065700	2.30259700	-3.03018200
C	3.10517600	3.57792200	1.75315700
H	3.05423000	2.51278200	2.02414000
H	4.11654900	3.76906300	1.36506000
H	2.96659000	4.17180400	2.66648900
C	-2.88087700	-5.38177900	0.25207100
H	-3.02269100	-5.86066500	-0.72655900
H	-3.03588500	-6.14579900	1.02954000
H	-3.67333000	-4.62641400	0.37779100
C	1.64778700	-4.34462900	-1.71834700
H	1.75985900	-3.34174800	-2.15877000
H	2.64792900	-4.68334600	-1.40978400
H	1.27470500	-5.02531900	-2.49544900
C	0.47377700	-2.80366400	2.97145700
H	-0.35209900	-2.87192700	3.69311800
H	1.37344900	-3.20660300	3.45549000
H	0.66762900	-1.74488200	2.73960500

TS1-*Rr*

C	4.66713600	-1.87702600	2.32276500
C	4.09347200	-0.74280000	1.70031200
C	3.81702900	-2.96965800	2.72407300
C	2.48651800	-2.92980700	2.51989900
N	2.71328500	-0.75417100	1.45810000
C	1.84850900	-1.80222900	1.85234500
N	2.05508200	0.24332100	0.72971200
C	2.21762200	1.62574800	1.12393300
C	2.36737800	1.93457600	2.57248200
C	2.08145900	2.42546700	0.04874400
H	2.60672800	2.99046600	2.72103600
H	3.12860900	1.30394600	3.05009900
H	1.40174200	1.71573000	3.05924300
C	2.33555700	3.88633900	0.10608000
O	2.47951900	4.54676900	1.10558900
C	1.69410500	1.72017000	-1.22526000
H	2.08945300	2.21567300	-2.12060800
H	0.59705300	1.69874000	-1.30664800
C	2.19894000	0.28087200	-1.16689600
O	1.47583500	-0.68792000	-1.60769600
C	3.66464700	0.06333300	-1.42234800
C	4.54279100	1.11857700	-1.68795000
C	4.13696800	-1.25446200	-1.43670000
C	5.88894400	0.85708300	-1.94064200
H	4.18577200	2.15034700	-1.69542800
C	5.48454100	-1.51054300	-1.67065400
H	3.42781500	-2.06665600	-1.26163700
C	6.36279600	-0.45415700	-1.92154500
H	6.56977700	1.68262000	-2.15421600
H	5.85146300	-2.53845500	-1.66486600

H	7.41851300	-0.65548400	-2.11183300	O	-2.00501400	-1.43858900	0.43220400
H	1.01124800	0.04466000	0.80438600	H	-7.12529000	-2.29166900	-1.60206200
H	0.39072500	-0.54442700	-1.65958700	C	-2.87205800	-2.27020100	-0.23823200
O	0.66289300	-1.71833500	1.62380400	C	-1.41058100	3.98001400	0.57883500
O	2.48147400	4.40188300	-1.11965400	C	-2.59242500	3.41057000	0.06449700
C	2.88156000	5.76596800	-1.16878800	C	-4.67580800	-3.84992800	-1.68293600
H	2.16911600	6.40157700	-0.62692000	O	-2.90244500	0.67796200	-0.63012000
H	2.91440700	6.04187000	-2.22741200	C	-0.26637400	-4.17302300	-0.00818600
H	3.87453000	5.88745600	-0.71307100	C	-2.37861100	-3.31132100	-1.04321300
H	1.81084000	-3.72330100	2.83558900	H	-5.37027200	-4.45501800	-2.26898400
H	4.27937200	-3.82785400	3.21689500	C	-3.30440000	-4.09575600	-1.74449000
C	6.05220600	-1.91242500	2.56520100	C	-0.70139200	4.89212400	-0.20979400
H	6.46827300	-2.80309300	3.04014200	H	1.57358600	-5.00136500	0.73757900
C	4.92510300	0.34486400	1.38370700	C	-3.03561100	3.75201800	-1.22923500
H	4.51961200	1.24278200	0.92863200	H	0.19561100	5.35536200	0.20994800
C	6.86686100	-0.85069200	2.21999100	C	1.07409200	-4.54725500	-0.12282500
C	6.28666700	0.28180800	1.63520100	C	-0.92071300	-3.62819700	-1.13137800
H	6.90677300	1.13871900	1.36671700	H	-2.92632300	-4.91167500	-2.36426700
H	7.93962300	-0.88795000	2.40952500	C	-1.11633500	5.23542600	-1.49910800
P	-1.48666600	-0.08127900	-0.31737700	C	-2.28563700	4.65410100	-1.98887600
O	-0.92841000	-0.40908800	-1.69021400	C	1.79188700	-4.37001400	-1.30890200
O	-0.61950900	0.67851500	0.63499200	C	-0.22354100	-3.45504000	-2.34097400
H	-5.56926000	-0.53878300	4.06371300	H	-2.63300400	4.91555900	-2.99211200
H	-6.86987100	-0.28877300	2.88971500	C	1.12747100	-3.81477900	-2.40194600
H	-5.26016600	2.32852900	3.76508200	H	1.67437800	-3.64811700	-3.33408400
C	-5.78237600	-0.44021200	2.98985100	C	3.23646200	-4.79179500	-1.39871100
C	-4.81856800	1.99838700	2.82267100	H	3.81003600	-4.44570400	-0.52447900
H	-6.03552900	-2.47644800	2.13490900	H	3.32551300	-5.88944500	-1.42722200
C	-5.30677800	-1.65391400	2.17119600	H	3.71304500	-4.39681400	-2.30696200
C	-5.02047000	0.70284500	2.35726900	C	-0.89795800	-2.88450900	-3.56194100
H	-4.36888500	-2.04547100	2.59496700	H	-1.54402900	-2.04029400	-3.29018000
C	-4.04433600	2.87896400	2.06401100	H	-0.14790800	-2.52874700	-4.28216500
H	-3.90895000	3.90979600	2.39767900	H	-1.51560400	-3.64111200	-4.07128200
H	-7.15922600	-0.58310500	0.57030000	C	-0.99356900	-4.34680100	1.29791400
H	-7.09639900	-2.98696600	0.02646700	H	-1.18133400	-3.36022400	1.74835400
C	-4.45981900	0.28974700	1.14277900	H	-1.96113300	-4.85170100	1.15861600
C	-5.00251000	-1.07521300	0.76234900	H	-0.39524700	-4.94187000	2.00259000
C	-6.32306100	-0.93647600	-0.04991800	C	-0.30849300	6.17653200	-2.35238600
C	-6.55012800	-2.32504700	-0.66604500	H	0.51264000	5.63630400	-2.85092500
C	-3.40963100	2.46854200	0.88509300	H	-0.92691300	6.63430800	-3.13673500
C	-3.60396400	1.14523500	0.45869600	H	0.13691500	6.98319600	-1.75314600
C	-4.24210200	-2.04852300	-0.12110000	C	-4.29754000	3.16792900	-1.81005700
C	-5.13769600	-2.81883900	-0.87175200	H	-4.14813100	2.11024400	-2.07420000
H	-6.15998800	-0.19987100	-0.85207600	H	-5.13129000	3.21374300	-1.09436100

H	-4.59134500	3.70894900	-2.71937500
C	-0.88949800	3.60454600	1.94223900
H	0.14082600	3.96727300	2.07004300
H	-1.49825200	4.04061600	2.74899000
H	-0.90541900	2.51063600	2.05428900

TS1-*Rs*

C	-3.77299300	-2.93367200	-1.67244100
C	-2.84508800	-2.01102300	-1.13710500
C	-5.11500000	-2.95131700	-1.14886300
C	-5.50097500	-2.06476000	-0.20999000
N	-3.24995600	-1.19367800	-0.07294600
C	-4.58914600	-1.05822600	0.33255500
N	-2.32838700	-0.24029000	0.37594400
C	-2.44882600	0.29952700	1.71144900
C	-2.81556800	-0.58153200	2.85876600
C	-2.01618200	1.57245900	1.74671800
H	-3.07891300	-1.58548700	2.50360200
H	-1.96588000	-0.64539800	3.55172700
H	-3.66434000	-0.15719500	3.40837300
C	-1.91756400	2.32090600	3.01678000
O	-2.08703700	1.86972900	4.12126000
C	-1.55905900	2.19351800	0.45779000
H	-1.82960200	3.25614100	0.40725000
H	-0.46076700	2.15067300	0.36621000
C	-2.18094500	1.49336100	-0.72830900
O	-1.48146400	1.20999300	-1.75901700
C	-3.63440200	1.68496100	-0.99671400
C	-4.43465100	2.49609800	-0.18501500
C	-4.20491000	0.99984100	-2.07734200
C	-5.79688900	2.60988200	-0.44599800
H	-4.00259700	3.03041500	0.66220900
C	-5.57107700	1.10155200	-2.32294000
H	-3.56557700	0.38157200	-2.71064300
C	-6.36732000	1.90556300	-1.50531900
H	-6.41856300	3.24163700	0.18977400
H	-6.01666500	0.55530200	-3.15583300
H	-7.43859000	1.98607300	-1.69781900
H	-1.35867500	-0.63047300	0.36216100
H	-0.42220000	0.96700200	-1.61091100
O	-4.93225500	-0.18694800	1.10534100
O	-1.62407200	3.61337200	2.79882300
C	-1.47131600	4.41961100	3.95668800
H	-1.28422600	5.43937300	3.60285000
H	-2.38062000	4.39480200	4.57253100
H	-0.62474000	4.06796400	4.56289200
P	1.32554400	-0.07657900	-0.19831100
O	0.80547000	0.47239900	-1.51624100
O	0.34445100	-0.35570000	0.89065500
H	6.64210400	-1.30236700	2.74283400
H	7.14359200	-2.09535300	1.23974500
H	5.08555200	-3.66269900	3.15944200
C	6.34914500	-1.48424300	1.69931900
C	4.49247900	-3.20760000	2.36389800
H	7.02374200	0.25335500	0.49033900
C	6.10906400	-0.19176500	0.90700700
C	5.01112600	-2.17598200	1.58885500
H	5.63124800	0.55649700	1.55832500
C	3.19072600	-3.64002500	2.12152600
H	2.76529900	-4.44734600	2.72153900
H	6.63341400	-1.92757400	-1.07795400
H	7.36283200	0.30470000	-1.81845200
C	4.25298200	-1.60751000	0.55827700
C	5.09421200	-0.59445100	-0.20047500
C	5.84899600	-1.22832700	-1.40112600
C	6.38021700	-0.02364100	-2.19586300
C	2.37944200	-3.04605400	1.14319400
C	2.93901400	-2.02672500	0.35532000
C	4.50980300	0.63860000	-0.86665000
C	5.32699000	1.02901900	-1.93490600
H	5.12320000	-1.78684600	-2.01229000
O	2.48504800	0.91889900	0.38095700
H	6.50094900	-0.23501900	-3.26767200
C	3.39218000	1.40134400	-0.54372000
C	0.03965000	-3.30392900	2.02349800
C	0.97201700	-3.52698200	0.98666600
C	5.08814400	2.22221800	-2.60835700
O	2.18494500	-1.40078500	-0.61787900
C	1.87140400	4.03898000	0.44169600
C	3.13102400	2.61477900	-1.20152700
H	5.72640100	2.53264900	-3.43783400
C	4.01008700	3.01601500	-2.21542200
C	-1.24049800	-3.84707400	1.90497600
H	0.73233900	5.31746200	1.73958200
C	0.60384400	-4.28109100	-0.14057400
H	-1.95946200	-3.68265700	2.71303800
C	0.79190200	4.87091300	0.74291700
C	1.95258300	3.45893900	-0.84378300

H	3.81796300	3.96251100	-2.72462000
C	-1.62093600	-4.62196700	0.80329900
C	-0.68506200	-4.82652800	-0.20814100
C	-0.21305000	5.14349800	-0.18910200
C	0.94887900	3.71661500	-1.79791200
H	-0.96127500	-5.42283800	-1.08202900
C	-0.11918100	4.55309300	-1.44869900
H	-0.90715700	4.73313900	-2.18580400
H	-6.51704800	-2.01668900	0.18009600
H	-5.82132600	-3.68150200	-1.55072500
C	-3.38236600	-3.77198400	-2.73146400
H	-4.11331900	-4.48259700	-3.12337100
C	-1.56632200	-1.92023200	-1.70965700
H	-0.83889600	-1.18915500	-1.37571800
C	-2.11633100	-3.68412900	-3.28357000
C	-1.21755800	-2.74079700	-2.77100500
H	-0.22088000	-2.63257600	-3.20203300
H	-1.82830700	-4.32767300	-4.11530800
C	-1.39237900	5.99631300	0.19734700
H	-1.06958800	6.98258400	0.56376900
H	-2.07383200	6.15225900	-0.64990600
H	-1.95963800	5.51577800	1.01157400
C	0.99184000	3.11613500	-3.18042000
H	-0.01853400	3.07588800	-3.61032700
H	1.61642000	3.71894200	-3.85862100
H	1.40108500	2.09872700	-3.15528900
C	2.92941700	3.78237600	1.48300900
H	2.86487200	2.74902000	1.85536600
H	3.93973400	3.91896300	1.06998900
H	2.80867300	4.46332500	2.33587700
C	-3.00106800	-5.22154800	0.74469400
H	-3.18890900	-5.70695600	-0.22285600
H	-3.13502000	-5.97649800	1.53534600
H	-3.77126100	-4.44989900	0.89865200
C	0.39274400	-2.48002000	3.23446600
H	-0.46132400	-2.42215300	3.92241300
H	1.24122500	-2.90468300	3.78879900
H	0.67077600	-1.46243400	2.92234700
C	1.58132200	-4.51188600	-1.26299000
H	1.85627700	-3.55898100	-1.74093700
H	2.51324900	-4.96673400	-0.89327000
H	1.15391200	-5.17473700	-2.02781100

INT3-*Sr*

C	2.71415800	-3.06771100	2.49102000
C	2.57296700	-1.74849500	2.01018900
C	3.90824100	-3.80322300	2.14802100
C	4.90382800	-3.23450000	1.43750100
N	3.59501500	-1.20756900	1.22021900
C	4.83467500	-1.84360100	0.98752600
N	3.43639600	0.05048500	0.70851600
C	4.09005700	1.15530400	1.22289400
C	4.73604800	1.05607900	2.55870400
C	4.00111700	2.19389500	0.35275200
H	4.03487900	0.62692200	3.29019100
H	5.06558500	2.04504300	2.88849300
H	5.60684500	0.38708900	2.48615100
C	4.52614300	3.53354200	0.58427400
O	5.06301600	3.95018100	1.58525800
C	3.27611200	1.75940100	-0.89824200
H	3.88188100	1.89322900	-1.80406700
H	2.33956100	2.31794900	-1.04888800
C	2.90788800	0.27261300	-0.64584700
O	1.50776700	0.10210100	-0.54620700
C	3.48337400	-0.73508700	-1.63474000
C	4.72453800	-0.51076900	-2.23898700
C	2.81611500	-1.94199100	-1.87089300
C	5.27952300	-1.46555400	-3.08605600
H	5.28227300	0.40117000	-2.02332400
C	3.37763900	-2.89899300	-2.71779000
H	1.85189500	-2.14556600	-1.39633700
C	4.60585700	-2.66202600	-3.33035100
H	6.24892900	-1.27768800	-3.55012100
H	2.84925100	-3.83694500	-2.89458300
H	5.04068800	-3.41084700	-3.99451300
H	0.25857800	0.68730200	0.34251200
H	1.07912300	-0.12658300	-1.39184700
O	5.74598700	-1.24446400	0.46010700
O	4.34603900	4.31603400	-0.50175200
C	4.81975000	5.64755800	-0.38791200
H	4.25180200	6.20112600	0.37422600
H	4.68466800	6.11232200	-1.37054100
H	5.88212500	5.66008900	-0.10832000
H	5.82405800	-3.76080000	1.18597800
H	3.99451800	-4.83687000	2.49223000
C	1.70346500	-3.61175400	3.30345800
H	1.82710800	-4.63201800	3.67368100
C	1.44013900	-0.99809900	2.35631600

H	1.34883500	0.02680800	2.00743900
C	0.58016800	-2.87261200	3.63340900
C	0.45506000	-1.56169800	3.15238700
H	-0.42314400	-0.96497600	3.40478300
H	-0.19699200	-3.30165200	4.26666300
P	-1.61801300	0.14244500	-0.46935700
O	-0.68903600	0.75073800	0.64769900
O	-0.95089000	-0.38126500	-1.67748100
H	-7.48452900	-0.49217300	-2.02643500
H	-7.80008000	-0.97813300	-0.35245100
H	-6.42223300	-3.15182000	-2.27941900
C	-7.02600000	-0.58504900	-1.03205600
C	-5.62061500	-2.70155500	-1.69090300
H	-7.18523500	1.38505000	-0.01672200
C	-6.44596400	0.74027700	-0.51257600
C	-5.81404400	-1.48782300	-1.03872100
H	-6.00712200	1.30531700	-1.34965900
C	-4.38190600	-3.33586400	-1.59246000
H	-4.22151300	-4.29669400	-2.08588800
H	-6.81561600	-0.60620800	1.77793800
H	-7.01218200	1.79370800	2.30055700
C	-4.78710500	-0.91934200	-0.27531200
C	-5.29852300	0.31413800	0.44692900
C	-5.88151900	-0.03082000	1.84626000
C	-6.04081000	1.33104100	2.54145100
C	-3.31315800	-2.76024900	-0.89266900
C	-3.54199500	-1.53642400	-0.24559500
C	-4.40758700	1.49011200	0.80784100
C	-4.90647900	2.13328700	1.94781400
H	-5.14402900	-0.64096800	2.39067900
O	-2.69211800	1.28779300	-0.85132400
H	-5.97797300	1.26438600	3.63665200
C	-3.28224500	2.00649900	0.17776900
C	-1.19401900	-3.59017100	-1.96996900
C	-1.98444500	-3.43684600	-0.81463300
C	-4.33916100	3.32198100	2.39458900
O	-2.49152800	-0.90181900	0.40236400
C	-1.68446000	4.17198600	-1.48678400
C	-2.69594800	3.21343400	0.59232600
H	-4.72961700	3.82587800	3.28078100
C	-3.25697000	3.86355200	1.69874100
C	0.03391500	-4.24867000	-1.86241200
H	-0.71523500	4.99824800	-3.21888200
C	-1.54012500	-3.94529300	0.42070300
H	0.63923900	-4.37027600	-2.76483100
C	-0.58623800	4.69179300	-2.17756700
C	-1.52489300	3.77708700	-0.14322800
H	-2.81414900	4.80571800	2.02784900
C	0.50427000	-4.74804300	-0.64468200
C	-0.30321500	-4.59301300	0.48279700
C	0.66541400	4.82731200	-1.57715100
C	-0.27275600	3.92055700	0.49077600
H	0.03544000	-4.99149700	1.44235000
C	0.80033900	4.43627400	-0.24166500
H	1.77860700	4.52781400	0.24084300
C	1.84186300	5.38130600	-2.33481500
H	2.70075100	4.69676300	-2.27509200
H	1.59427100	5.54766200	-3.39172400
H	2.16298000	6.34386500	-1.90632800
C	-0.06081500	3.53746300	1.93420200
H	0.99932600	3.30912300	2.11758900
H	-0.33497200	4.36413700	2.60887600
H	-0.66215800	2.66359400	2.21396900
C	-3.01108600	4.04851100	-2.19109900
H	-3.22755300	2.99755400	-2.43578900
H	-3.83648000	4.41750900	-1.56510200
H	-3.00621500	4.62061300	-3.12826100
C	1.85641200	-5.40273200	-0.54338700
H	1.90735600	-6.08063700	0.32067600
H	2.09353000	-5.98193500	-1.44769800
H	2.64847000	-4.64546600	-0.41885400
C	-2.38217600	-3.81404900	1.66297700
H	-2.43438800	-2.76508100	1.99334500
H	-3.41427200	-4.15144300	1.48474900
H	-1.96218900	-4.41166900	2.48288500
C	-1.63024400	-3.03206700	-3.29948500
H	-0.83043000	-3.14401200	-4.04398100
H	-2.52599100	-3.53872400	-3.68739400
H	-1.85928400	-1.96202300	-3.19896200

INT3-*Ss*

C	-5.10139100	-2.15046900	-1.33233400
C	-4.64786900	-1.16066300	-0.43366400
C	-4.13485900	-2.80606700	-2.18025400
C	-2.81853500	-2.53016000	-2.08372900
N	-3.28770300	-0.83284000	-0.42081100
C	-2.29985500	-1.54585200	-1.13279800
N	-2.89326400	0.28162400	0.27667500

C	-2.04458200	0.20982000	1.36020400	H	6.60327500	-0.14811000	-3.43863100
C	-1.87844800	-1.08577400	2.06720800	C	4.16558500	-2.02853200	-0.35723800
C	-1.52700100	1.44647900	1.61494000	C	4.87625400	-1.01149700	-1.23524000
H	-2.85575400	-1.57797000	2.18614200	C	5.07048900	-1.52780800	-2.68755700
H	-1.23523000	-1.73993900	1.45883800	C	5.50997500	-0.28441300	-3.47900100
H	-1.41002100	-0.94514300	3.04723800	C	2.37374900	-3.35292800	0.62339300
C	-0.63494500	1.76451700	2.69896400	C	2.80652100	-2.25710400	-0.14258400
O	0.12600300	0.96652600	3.25821900	C	4.33320200	0.37734800	-1.50984000
C	-2.02458900	2.44022300	0.59888400	C	4.80308700	0.83309300	-2.74692200
H	-2.71610100	3.17418000	1.03455500	H	4.09823700	-1.88312800	-3.06306300
H	-1.19586400	2.99084600	0.13384800	O	2.94407000	0.67529700	0.40959400
C	-2.69443800	1.56272500	-0.48773600	H	5.22947700	-0.33002400	-4.54075300
O	-1.87574900	1.34455500	-1.57374000	C	3.54133200	1.20691400	-0.72227100
C	-4.04852300	2.03876900	-0.99989300	C	0.45443300	-3.74839800	2.18912300
C	-4.96904600	2.67359500	-0.16013500	C	0.93941000	-3.69290900	0.86712400
C	-4.42203700	1.74302700	-2.31410500	C	4.56435300	2.14214000	-3.15097800
C	-6.23876600	3.00959800	-0.62469900	O	1.88296400	-1.36969500	-0.67287800
C	-5.69730800	2.06779100	-2.77567400	C	2.86605300	3.84935300	0.99314000
C	-6.60885100	2.70291000	-1.93420200	C	3.28038100	2.53133400	-1.10625200
H	-6.94483000	3.50764200	0.04212200	H	4.93400200	2.50775600	-4.11097300
H	-5.97775100	1.82428300	-3.80205100	C	3.82934500	2.98222600	-2.31516100
H	0.71224500	0.03080900	2.28042200	C	-0.84372900	-4.21582400	2.41933500
H	-0.98426900	1.06230000	-1.25995200	H	2.44163500	5.09267300	2.69691300
O	-1.12215300	-1.33225500	-0.94603500	C	0.11040700	-4.08484400	-0.20408200
O	-0.66992000	3.03507900	3.07803900	H	-1.21872000	-4.24569900	3.44642100
C	0.20845800	3.40494900	4.13555400	C	2.09551600	4.77113000	1.71049500
H	0.14091800	4.49398400	4.22379200	C	2.43710600	3.44994300	-0.28717900
H	-0.11025500	2.93016300	5.07434100	H	3.63853900	4.01474100	-2.61432800
H	1.23777700	3.09865700	3.91206100	C	-1.67503300	-4.62559400	1.37671900
P	1.49552100	-0.03858800	0.15728200	C	-1.17704200	-4.55071700	0.07315300
O	0.59348200	0.86174400	-0.58857400	C	0.90885600	5.29682700	1.19780000
O	1.12647300	-0.58607600	1.56732900	C	1.23965600	3.96517200	-0.82504800
H	7.15229200	-2.39351200	0.87473100	H	-1.80992400	-4.87756300	-0.75636300
H	6.99658900	-2.97322800	-0.79229400	C	0.50285600	4.88254600	-0.07244600
H	5.44980000	-4.60206700	1.49071400	H	-0.42929700	5.27631900	-0.48918100
C	6.51072200	-2.35775300	-0.01696500	H	-2.06547500	-3.02073000	-2.69994500
C	4.71302900	-3.94921300	1.01888800	H	-4.49562400	-3.54572300	-2.89898200
H	7.04125500	-0.53784500	-1.17400200	C	-6.47053900	-2.46967100	-1.36832500
C	6.25271200	-0.93028700	-0.51638100	H	-6.80870900	-3.23186900	-2.07328300
C	5.11274700	-2.85626400	0.25915000	C	-5.56015600	-0.53241900	0.42821600
H	6.15469800	-0.24903700	0.34302400	H	-5.20193700	0.22038800	1.12723200
C	3.35167500	-4.19509900	1.17361800	C	-7.37054600	-1.83545800	-0.53031900
H	3.01863400	-5.05709000	1.75498800	C	-6.90356900	-0.86999700	0.37297600
H	5.78306100	-2.36323900	-2.74104200	H	-7.60279000	-0.37171000	1.04651100

H	-8.43088300	-2.08665800	-0.56699300
C	0.05937200	6.25346800	1.99128600
H	-0.26332400	7.10546100	1.37524400
H	-0.85102200	5.74705700	2.35157100
H	0.60028900	6.64910500	2.86220400
C	0.72638300	3.54301300	-2.17851500
H	-0.37020500	3.60803800	-2.21041600
H	1.12284400	4.18889400	-2.97841000
H	1.00756000	2.50691000	-2.40250200
C	4.13933500	3.31140500	1.59345100
H	4.02943600	2.24707000	1.85197100
H	4.98052000	3.38962900	0.88876300
H	4.40296000	3.86173400	2.50676600
H	-7.60554200	2.96033000	-2.29674100
H	-4.70770700	2.89455500	0.87672100
H	-3.70098600	1.25133400	-2.96683700
C	-3.07951500	-5.10609500	1.63172800
H	-3.26777300	-6.06755500	1.13130100
H	-3.27079200	-5.23604000	2.70543100
H	-3.81923600	-4.38881300	1.24135500
C	0.58668400	-4.00906100	-1.62925700
H	0.57614500	-2.96009800	-1.96312100
H	1.61363300	-4.38855200	-1.73638300
H	-0.06450000	-4.59844900	-2.28994700
C	1.28936900	-3.29231700	3.35967200
H	0.64274300	-3.00189500	4.19973100
H	1.95785600	-4.08850300	3.72288300
H	1.91340600	-2.43151500	3.08704500

INT3-*Rr*

C	4.54676500	-1.94362900	2.38766700
C	4.15663500	-0.74854200	1.74878600
C	3.52705900	-2.88571200	2.76706800
C	2.22089800	-2.62185000	2.55188200
N	2.79818600	-0.55900500	1.43448100
C	1.79239100	-1.40001900	1.89136400
N	2.40238600	0.48475800	0.64400100
C	2.32553900	1.79041900	1.08039300
C	2.44901900	2.09604300	2.53323800
C	2.09771900	2.60885800	0.01598200
H	2.49323100	3.17824200	2.68346900
H	3.33662700	1.61870800	2.97256800
H	1.56390600	1.69712200	3.05494700
C	2.18388900	4.06086300	0.06876000
O	2.26465300	4.75163800	1.06418400
C	1.85009600	1.77176300	-1.22039100
H	2.29416400	2.17575000	-2.13719400
H	0.76447500	1.67192500	-1.38961600
C	2.41828800	0.37931800	-0.86900600
O	1.69113100	-0.70740600	-1.27706700
C	3.85809700	0.17058500	-1.33781000
C	4.71375800	1.24123400	-1.61440500
C	4.34502400	-1.13715200	-1.43966400
C	6.04597500	1.00667700	-1.95714800
H	4.34893500	2.26851100	-1.55252900
C	5.67672900	-1.37034100	-1.77438700
H	3.65784700	-1.96348600	-1.25137700
C	6.53303600	-0.29773000	-2.02890800
H	6.70448300	1.84972900	-2.17401200
H	6.04824800	-2.39490100	-1.84241800
H	7.57600700	-0.47944900	-2.29454700
H	-0.09946100	0.02153600	1.10983500
H	0.75725000	-0.49671400	-1.49952000
O	0.60283500	-1.11758800	1.75535800
O	2.24564200	4.60022200	-1.16519000
C	2.54468800	5.98557700	-1.20945000
H	1.79563700	6.57439900	-0.66318100
H	2.55330500	6.27005700	-2.26709300
H	3.52968800	6.17983000	-0.76029700
H	1.42047800	-3.29366500	2.85779500
H	3.83130000	-3.81191600	3.26030100
C	5.91047000	-2.16380500	2.66357700
H	6.19761600	-3.09866900	3.14895000
C	5.11792800	0.23268100	1.46191100
H	4.82154900	1.17361500	1.00340800
C	6.85986200	-1.21447600	2.33807700
C	6.45117400	-0.00728700	1.74999500
H	7.18830800	0.76147300	1.51305000
H	7.91427700	-1.39218600	2.55085000
P	-1.56321800	-0.12823400	-0.46661700
O	-0.92599300	-0.33168400	-1.78928400
O	-0.74934500	0.65114400	0.61460300
H	-5.50179100	-0.85252600	4.05419100
H	-6.82649800	-0.63296600	2.90128000
H	-5.31701800	2.01952300	3.83519600
C	-5.73228000	-0.73801100	2.98565300
C	-4.87894300	1.74136200	2.87469200
H	-5.90272600	-2.76260300	2.08683500

C	-5.21340200	-1.90741700	2.13211800
C	-5.03144000	0.45289100	2.37266700
H	-4.25184200	-2.26412500	2.53323500
C	-4.16251400	2.68201800	2.13165800
H	-4.06685800	3.70672400	2.49598100
H	-7.13751700	-0.89078000	0.57123600
H	-6.97382500	-3.28303600	0.00539600
C	-4.47471900	0.09873600	1.13656100
C	-4.95862000	-1.28344600	0.73181500
C	-6.29403000	-1.19869600	-0.06277900
C	-6.46476700	-2.59271400	-0.68747500
C	-3.53770800	2.33996900	0.92672600
C	-3.67789400	1.02101600	0.47018900
C	-4.16699200	-2.21091300	-0.17276300
C	-5.03452500	-3.02425400	-0.91062000
H	-6.17630600	-0.44801500	-0.85972900
O	-1.95069000	-1.48707400	0.32627800
H	-7.05021400	-2.57789600	-1.61734900
C	-2.79415700	-2.37783700	-0.31292900
C	-1.61338200	3.94327400	0.59863400
C	-2.78638300	3.33702100	0.10873000
C	-4.53215400	-4.03936700	-1.71902300
O	-2.97060000	0.63133400	-0.65635700
C	-0.09009600	-4.08598200	-0.04947500
C	-2.25452100	-3.39720800	-1.10939600
H	-5.20479000	-4.67885200	-2.29381100
C	-3.15179000	-4.22938000	-1.79263600
C	-0.95425400	4.88319100	-0.20036300
H	1.79573100	-4.78447100	0.71299800
C	-3.28156600	3.68167200	-1.16575400
H	-0.05403400	5.35969600	0.19604600
C	1.26768200	-4.39592700	-0.16206400
C	-0.78127200	-3.63059700	-1.19039200
H	-2.74565200	-5.03563100	-2.40689800
C	-1.41772400	5.22612200	-1.47215000
C	-2.58590500	4.61824700	-1.93289600
C	1.96419900	-4.23815800	-1.36257200
C	-0.09784300	-3.45235100	-2.40804600
H	-2.97194000	4.88223600	-2.92120200
C	1.26770800	-3.74759000	-2.46692400
H	1.80077100	-3.58444300	-3.40731500
C	3.41985600	-4.61633800	-1.45864200
H	3.98028400	-4.28694900	-0.57011600
H	3.53647900	-5.70978300	-1.52815700
H	3.88937800	-4.17592000	-2.34929900
C	-0.80604700	-2.92965200	-3.63098400
H	-1.39836100	-2.04042800	-3.37637700
H	-0.07870700	-2.65059700	-4.40519100
H	-1.48564600	-3.68045200	-4.06248000
C	-0.78548000	-4.23702200	1.27856000
H	-0.92225700	-3.24714800	1.74413800
H	-1.77890300	-4.69607200	1.17052000
H	-0.19418200	-4.86579300	1.95931200
C	-0.66054900	6.19288000	-2.34169600
H	0.17461900	5.67936100	-2.84426900
H	-1.30754600	6.61949100	-3.12053000
H	-0.23857600	7.01933000	-1.75317600
C	-4.54116500	3.06514300	-1.71889300
H	-4.35908500	2.02812900	-2.03948700
H	-5.34578700	3.04219200	-0.96966300
H	-4.89624100	3.63037200	-2.59076000
C	-1.04905200	3.59996200	1.95342600
H	0.00835000	3.89662200	2.00735000
H	-1.58443000	4.12676500	2.75949500
H	-1.12941300	2.52193400	2.14597400

INT3-*Rs*

C	-4.29571200	-2.79811600	-2.21408600
C	-3.44276400	-2.01374400	-1.40799600
C	-5.70068100	-2.84910200	-1.88387500
C	-6.18929700	-2.21799200	-0.79725300
N	-3.99656000	-1.30152800	-0.33674800
C	-5.32753100	-1.45520300	0.10912300
N	-3.18303100	-0.50302200	0.41214800
C	-2.49815400	-0.94435500	1.51262100
C	-2.69953700	-2.34401600	1.97543700
C	-1.73297900	0.06520100	2.01650700
H	-2.46256100	-3.05022300	1.16478800
H	-2.07045700	-2.54725300	2.84622600
H	-3.76016500	-2.47582500	2.24033800
C	-0.81832800	-0.04193600	3.13836400
O	-0.52107200	-1.05568400	3.74319600
C	-1.95053400	1.32431900	1.21508700
H	-2.39134300	2.12693300	1.82219700
H	-1.01697800	1.72801800	0.79520000
C	-2.90279800	0.91523500	0.05076000
O	-2.31712300	0.99052000	-1.20090300
C	-4.20394900	1.70792000	0.01434700

C	-4.92453400	1.91276900	1.19512300	C	2.29064300	-3.42168300	0.45731000
C	-4.69252400	2.23088500	-1.18381300	C	3.91959200	3.52636900	-2.75101900
C	-6.10357700	2.65167500	1.18313900	O	2.54249700	-0.91062600	-0.78861900
C	-5.87738400	2.97073200	-1.19710000	C	0.75736500	4.08275000	0.79803500
C	-6.58055100	3.18910000	-0.01429800	C	2.16715300	3.17740800	-1.08512800
H	-6.65578600	2.80531500	2.11170300	H	4.30050100	4.07923200	-3.61177400
H	-6.24933300	3.37928800	-2.13863500	C	2.71581400	3.89802000	-2.15540100
H	0.60987600	-1.26453100	1.52284200	C	0.27336700	-4.26355600	1.49687700
H	-1.36651300	0.78524500	-1.12436800	H	-0.54177400	4.92081700	2.28983900
O	-5.68845900	-0.98798500	1.16635400	C	1.84092100	-3.91237600	-0.78855300
O	-0.26506300	1.14542900	3.42953800	H	-0.33621400	-4.39483700	2.39497800
C	0.75628800	1.12997100	4.41005000	C	-0.47625400	4.53821100	1.26727200
H	1.07770200	2.16948200	4.53782000	C	0.84426700	3.57938500	-0.51803000
H	0.38233900	0.73021800	5.36276500	H	2.16068300	4.75724700	-2.53649700
H	1.60140100	0.51204800	4.07330900	C	-0.19863100	-4.73759600	0.27251500
P	1.49776800	0.02768700	0.00230600	C	0.61308700	-4.57064800	-0.85366700
O	0.30539500	0.24772300	-0.83853900	C	-1.62668400	4.51155300	0.47151600
O	1.30523400	-0.58535700	1.44655400	C	-0.30493400	3.52217500	-1.32870400
H	7.29104600	0.17801500	1.89538200	H	0.26840400	-4.95657200	-1.81709700
H	7.77391300	-0.22823700	0.24165800	C	-1.51915000	3.99464400	-0.81812800
H	6.62324200	-2.60889200	2.06370800	H	-2.41356800	3.92847100	-1.44188100
C	6.91062100	0.03633200	0.87419400	H	-7.23981700	-2.26474800	-0.51161300
C	5.79692200	-2.27266600	1.43467200	H	-6.36181800	-3.43186800	-2.52988300
H	6.83877200	2.02288200	-0.11757400	C	-3.75188900	-3.51423800	-3.29575200
C	6.17373700	1.27128700	0.33032200	H	-4.42410000	-4.11221500	-3.91463900
C	5.84726800	-1.03459400	0.80209900	C	-2.06420300	-1.98499000	-1.67266000
H	5.61028400	1.75541400	1.14301000	H	-1.39451600	-1.39097500	-1.05385200
C	4.66429300	-3.07346700	1.27825800	C	-2.39589400	-3.46499500	-3.57065300
H	4.60679100	-4.04226100	1.77820700	C	-1.55777600	-2.69788000	-2.74846400
H	6.87528900	-0.00617500	-1.91628800	H	-0.48587700	-2.64866500	-2.94751500
H	6.77076600	2.40311900	-2.44023900	H	-1.98336800	-4.01668100	-4.41603400
C	4.79069700	-0.60637100	-0.01255400	C	-2.94733100	5.00151800	1.00476500
C	5.16062700	0.69601000	-0.69914500	H	-3.13800000	4.60747600	2.01455900
C	5.87888300	0.43681500	-2.05334500	H	-2.95907000	6.10075400	1.07780400
C	5.89535400	1.80692000	-2.74632500	H	-3.77989700	4.69449100	0.35514900
C	3.56133600	-2.64132400	0.53215800	C	1.96853100	4.14021800	1.69286600
C	3.65240500	-1.39533500	-0.10743200	H	2.28345200	3.12884900	1.99121000
C	4.13594700	1.73399100	-1.13065700	H	2.82217000	4.61415400	1.18556200
C	4.61806700	2.43611200	-2.24306800	H	1.75001300	4.71249800	2.60429200
H	5.26959500	-0.26702300	-2.64128900	C	-0.26718800	2.92954500	-2.71456000
O	2.36077300	1.31245400	0.42853000	H	-1.28385600	2.68214600	-3.04640700
H	5.92095300	1.73414400	-3.84244800	H	0.17008400	3.62451100	-3.44799900
C	2.90187000	2.08919400	-0.59320500	H	0.33395600	2.00909200	-2.73012300
C	1.51526400	-3.62218500	1.61639800	C	2.65653800	-3.73060400	-2.04202200

H	2.58989700	-2.69326700	-2.40489800
H	3.72003100	-3.94778800	-1.86710100
H	2.29497800	-4.39364900	-2.83933900
C	-1.54565400	-5.39586100	0.13911800
H	-2.03567600	-5.51717100	1.11462100
H	-2.20516000	-4.79522100	-0.51005200
H	-1.45517800	-6.38939100	-0.32503900
C	1.96390400	-3.15982500	2.98223300
H	1.09759300	-2.88236000	3.59830700
H	2.50876100	-3.96303200	3.50403600
H	2.62960100	-2.28977900	2.92395800
H	-7.50293600	3.77264600	-0.02370700
H	-4.13269500	2.05956700	-2.10274600
H	-4.56830600	1.47171100	2.12864000

TS2-*Sr*

C	-4.71509000	2.40832000	-2.09967900
C	-3.65107000	1.79406000	-1.40565500
C	-5.97821300	2.58659200	-1.42253400
H	-6.79204400	3.06575400	-1.97185800
C	-6.16390800	2.18827100	-0.14726800
H	-7.10761900	2.32034300	0.38047200
N	-3.89346400	1.35911700	-0.09758500
C	-5.10531300	1.53150800	0.61548800
N	-2.92800600	0.67409700	0.59179100
C	-1.96815300	1.31087100	1.44866600
C	-1.49847200	0.37069900	2.28225700
C	-2.16298500	-0.94084400	2.00757900
C	-2.96746700	-0.65578800	0.77913700
O	-1.62768400	-1.19897100	-0.63113600
C	-4.12328000	-1.44756600	0.29645100
C	-4.43197900	-1.50879900	-1.06911100
C	-4.98089000	-2.03690100	1.23260200
C	-5.59249100	-2.15173600	-1.48821700
H	-3.74415700	-1.06957600	-1.79208900
C	-6.14384900	-2.67518000	0.80432000
H	-4.76512300	-1.97047800	2.29891700
C	-6.45195800	-2.73163400	-0.55336700
H	-5.82470800	-2.20199500	-2.55298500
H	-6.81329800	-3.12332800	1.53965000
H	-7.36335900	-3.23163400	-0.88545800
H	-1.21823500	-2.06902200	-0.48593800
H	-2.84595100	-1.22779000	2.82550000
H	-1.43363400	-1.75005700	1.86723100
O	-5.20222000	1.12885800	1.75220300
H	-0.87893200	-0.51574400	-0.63192200
C	-0.42671200	0.45033400	3.29355400
O	0.38150800	1.49324400	3.10580700
O	-0.31406000	-0.34564100	4.18867200
C	1.58687700	1.46860100	3.85470300
H	1.37983400	1.38104100	4.92993300
H	2.10089000	2.41146500	3.64132600
H	2.19461900	0.61241000	3.52712300
C	-1.60461500	2.72298900	1.19607100
H	-2.49221100	3.34105600	0.99593800
H	-0.93718300	2.74709500	0.31911300
H	-1.04795000	3.12813100	2.04659500
C	-4.50856100	2.83665500	-3.42188400
C	-2.40026500	1.63803500	-2.01762200
C	-3.28159600	2.66232200	-4.03997600
H	-3.13038500	2.99338400	-5.06762200
C	-2.23222800	2.06644400	-3.32827800
H	-1.25534900	1.93869300	-3.79771900
H	-5.33729600	3.31183600	-3.95059800
H	-1.55822600	1.20664900	-1.47527800
P	1.31425700	-0.22855700	0.26710000
O	0.96394200	-0.88549400	1.55428900
O	0.29722700	0.55886000	-0.52841900
H	5.73641300	-0.20590200	-4.07490100
H	6.89103300	-0.01528200	-2.74546600
H	5.27310900	2.58486800	-3.63078400
C	5.82761000	-0.19016200	-2.97957000
C	4.76525800	2.18867900	-2.74932400
H	6.05236300	-2.28362100	-2.27164900
C	5.31120900	-1.47278700	-2.31355900
C	4.96343000	0.87315800	-2.34399100
H	4.42991400	-1.84430900	-2.85956100
C	3.91569400	2.99997600	-2.00004800
H	3.77828600	4.04811700	-2.27487400
H	6.96344600	-0.54485700	-0.40579500
H	6.91861800	-2.99613900	-0.19834300
C	4.31874200	0.36565400	-1.20864200
C	4.85302200	-1.02362700	-0.89680200
C	6.07336100	-0.98616300	0.06542300
C	6.26448700	-2.45052200	0.50189900
C	3.21656900	2.50787000	-0.88936100
C	3.39970100	1.16349300	-0.52476600
C	4.02498900	-2.10749200	-0.23870000

C	4.85478100	-2.99604500	0.45281900	H	3.92875600	2.14429100	1.97129000
H	5.80802300	-0.37013600	0.93877500	H	4.91999500	3.34378300	1.12669900
O	1.84009800	-1.36997200	-0.81937600	H	4.30212400	3.70144300	2.75985000
H	6.71400100	-2.54413200	1.50072700	C	0.69909400	3.57422000	-1.97618000
C	2.65824100	-2.34359900	-0.30686700	H	-0.30606700	3.98166000	-2.15505700
C	1.22129600	4.02158200	-0.63554400	H	1.34715900	3.90079800	-2.80368200
C	2.37669100	3.44377800	-0.08432200	H	0.65098000	2.47460500	-2.00332700
C	4.33369300	-4.16995300	0.98802900				
O	2.68665300	0.63918000	0.52584700	**TS2-*Ss***			
C	0.16683600	-4.02747200	-1.30317000	C	7.04156600	-0.63843500	-0.63585600
C	2.11122300	-3.53591700	0.19561300	C	5.77175200	-0.06346700	-0.84564900
H	4.97318200	-4.87213200	1.52629600	C	7.12141700	-1.90507100	0.05375600
C	2.97359000	-4.44312700	0.82403400	H	8.11018100	-2.33629900	0.22610600
C	0.52614900	4.98765600	0.10146500	C	6.01482300	-2.55515200	0.46909200
H	-1.55494500	-4.51366600	-2.49905800	H	6.05220000	-3.51813200	0.97695500
C	2.81293200	3.82487600	1.20164000	N	4.64869700	-0.74245700	-0.34718900
H	-0.37814300	5.42789000	-0.32872900	C	4.67640300	-2.01979200	0.23930400
C	-1.17799000	-4.37259200	-1.48280400	N	3.41999400	-0.18089700	-0.58740700
C	0.66324200	-3.84794600	0.00638200	C	2.67926400	-0.47473300	-1.78495100
H	2.55873200	-5.37716700	1.20903800	C	1.56421000	0.27336400	-1.75040500
C	0.93619600	5.37906000	1.37501300	C	1.58107700	1.13304200	-0.52609500
C	2.08161800	4.78012600	1.91007500	C	2.67750800	0.52955800	0.27778700
C	-2.04652700	-4.54388500	-0.40336800	O	1.40006500	-1.02517800	0.97816000
C	-0.19942800	-4.00399100	1.11291500	C	3.08401400	1.04485300	1.59135800
H	2.42251300	5.07644700	2.90680600	C	2.04225300	1.35841100	2.48393600
C	-1.53991700	-4.33850200	0.88429600	C	4.41812000	1.27999500	1.95388300
H	-2.20830400	-4.44940500	1.74365100	C	2.35008300	1.89374900	3.72996700
C	-3.47279900	-4.97280600	-0.61560600	H	1.00310500	1.14244200	2.20913100
H	-4.15426800	-4.45996400	0.07760500	C	4.70840500	1.82835000	3.20068200
H	-3.80345400	-4.76784500	-1.64282600	H	5.23695600	1.07067200	1.26801100
H	-3.57894900	-6.05545500	-0.44017800	C	3.67799900	2.13164900	4.08908800
C	0.28763900	-3.78478400	2.52170200	H	1.54318300	2.11924900	4.42833200
H	0.96620800	-4.58843600	2.84435400	H	5.74661000	2.02020700	3.47439800
H	0.82863900	-2.83010800	2.58670300	H	3.91024400	2.55495700	5.06793900
H	-0.55668200	-3.76234900	3.22486000	H	1.89576800	-1.85390800	0.87997200
C	1.05255500	-3.85261400	-2.50864500	H	1.90410000	2.16471700	-0.77618200
H	1.28809900	-2.78847400	-2.66132100	H	0.63665300	1.23879200	0.02686500
H	2.00719700	-4.38424600	-2.38502100	O	3.64426200	-2.59721800	0.51666000
H	0.55705900	-4.22952400	-3.41303400	H	0.59475400	-1.09339700	0.39256100
C	0.16395000	6.39876200	2.17049300	C	0.41898900	0.32162500	-2.68667300
H	-0.20557700	5.96629700	3.11320800	O	0.22262500	-0.82581400	-3.33329000
H	0.79620900	7.25984600	2.43532300	O	-0.25545900	1.30418600	-2.83609700
H	-0.70155900	6.77313100	1.60735600	C	-1.02301600	-0.92290900	-4.01410600
C	4.05823600	3.22402600	1.80084800	H	-1.09138500	-0.17720500	-4.81822900

H	-1.07053000	-1.93543800	-4.42833100	C	-1.39993000	3.78745300	-1.18661200
H	-1.84205600	-0.76280800	-3.29738700	H	0.94836700	4.56532100	1.81055500
C	3.21718100	-1.48113700	-2.73504900	C	-0.45261500	-4.09054500	2.67167600
H	4.21698300	-1.19334100	-3.09506400	C	-1.66478100	-3.55919700	0.64418200
H	3.29427000	-2.46307500	-2.24313900	H	-3.16984800	-4.92627400	-1.15306600
H	2.53678400	-1.56936000	-3.58772400	C	0.75688900	4.55309700	-0.33718600
P	-1.64498300	0.00750400	0.38869500	C	-0.10192800	4.26871400	-1.39759200
O	-0.76391000	-0.80172800	-0.52841200	C	0.71247300	-4.34536400	1.95013500
O	-1.06775500	0.82672700	1.48862100	C	-0.50024800	-3.82596700	-0.10776800
H	-7.41006800	1.24895500	2.11666300	H	0.24455600	4.40744100	-2.42525100
H	-7.80511300	1.42880600	0.39984500	C	0.66530600	-4.21009100	0.55876300
H	-6.20996900	3.84182400	1.81543400	H	1.57446700	-4.38971600	-0.02282000
C	-7.00822900	1.12834400	1.10057400	C	1.98587800	-4.76723800	2.63446500
C	-5.46891900	3.24634900	1.27851900	H	2.14884400	-5.85183000	2.52813700
H	-7.31702900	-0.98662800	0.49024800	H	2.85112400	-4.25638000	2.18861800
C	-6.52036600	-0.30104700	0.81328700	H	1.95686300	-4.53754200	3.70835400
C	-5.75839800	1.94727200	0.87289200	C	-0.47398800	-3.64939700	-1.60413800
H	-6.05460700	-0.72089600	1.71824100	H	-1.01858800	-4.45186000	-2.12491600
C	-4.20725500	3.77548700	1.00264800	H	-0.92603200	-2.68489300	-1.86813000
H	-3.96920900	4.79703700	1.30678600	H	0.56219000	-3.65502000	-1.97143000
H	-6.97393700	0.60548800	-1.66971700	C	-2.86477400	-3.42687000	2.87990200
H	-7.30188000	-1.83883800	-1.71218700	H	-3.04942800	-2.34434900	2.94743500
C	-4.80920600	1.19229000	0.17489600	H	-3.76258600	-3.88626200	2.44112400
C	-5.41682500	-0.12825800	-0.26890900	H	-2.73685300	-3.81931500	3.89769800
C	-6.07131000	-0.02249200	-1.67496400	C	2.15813200	5.05683200	-0.57500800
C	-6.33022100	-1.47985400	-2.09075100	H	2.47378200	4.88680300	-1.61438900
C	-3.21341800	3.02065400	0.36612400	H	2.23180100	6.13869400	-0.38078600
C	-3.53555900	1.71286200	-0.04231400	H	2.87928800	4.56207200	0.09446400
C	-4.59977200	-1.39796900	-0.44821200	C	-2.29459500	3.49612500	-2.36091700
C	-5.18962800	-2.21289300	-1.42196300	H	-2.45158100	2.41274200	-2.45446700
H	-5.34221400	0.43400800	-2.36270000	H	-3.27664300	3.97785400	-2.23960700
O	-2.79866200	-0.96988500	1.05421600	H	-1.84032200	3.85226600	-3.29495000
H	-6.33748500	-1.62126200	-3.18096000	C	-1.44676800	3.64754100	2.63970100
C	-3.44697300	-1.82846100	0.20542800	H	-0.59731900	3.74681000	3.32980600
C	-1.00048800	3.87580900	1.21991700	H	-2.21364400	4.37324200	2.95051900
C	-1.84677300	3.57850000	0.13020700	H	-1.86454500	2.63692400	2.73892300
C	-4.68906800	-3.48606800	-1.67704900	C	8.17995000	0.03683200	-1.10848300
O	-2.58352300	0.91671100	-0.62365900	C	5.64903900	1.16338600	-1.51288600
C	-1.64110500	-3.69946300	2.04458800	C	8.06235700	1.24739800	-1.77059600
C	-2.91237400	-3.10688000	-0.04297400	H	8.95067600	1.76453900	-2.13356400
H	-5.15397000	-4.12945300	-2.42682400	C	6.79265100	1.80445600	-1.97011100
C	-3.56962500	-3.92678500	-0.96924100	H	6.69119000	2.75836400	-2.48945000
C	0.28651400	4.35391100	0.96526400	H	9.15991500	-0.41514100	-0.94328400
H	-0.44030000	-4.18999400	3.76047000	H	4.66848300	1.61265900	-1.67023600

TS2-*Rr*

C	6.61784400	-1.62969100	-0.57215700
C	5.53211400	-0.98523300	0.05404600
C	6.48761900	-2.02358400	-1.95596800
H	7.33718700	-2.51672300	-2.43340900
C	5.35446600	-1.79885600	-2.65027500
H	5.23079500	-2.09281900	-3.69182800
N	4.37749900	-0.74634700	-0.70918100
C	4.19014200	-1.15532600	-2.04696600
N	3.30632800	-0.17865500	-0.05878200
C	2.47580600	-0.94908300	0.83523400
C	1.65701000	-0.07774100	1.44591400
C	1.89340300	1.29624900	0.90900400
C	2.91130400	1.08019400	-0.15540500
O	1.17081200	0.78842000	-1.72049300
C	3.62835300	2.11965500	-0.91358400
C	2.91155200	3.01658700	-1.71742600
C	5.01592800	2.26637700	-0.76173400
C	3.58834100	4.03876000	-2.37673900
H	1.84084500	2.86494000	-1.84112200
C	5.67791200	3.30308900	-1.41405200
H	5.58018600	1.59802700	-0.11020600
C	4.96677200	4.18657500	-2.22562600
H	3.02990200	4.72559800	-3.01489300
H	6.75439900	3.41992600	-1.28314100
H	5.48981400	4.99351900	-2.74154500
H	1.66160900	0.20056800	-2.31233700
H	2.33926800	1.96256500	1.67316100
H	0.97767900	1.79914400	0.55581400
O	3.13733900	-0.96931700	-2.61442400
H	0.43451900	0.21220700	-1.36124400
C	0.77547700	-0.32001500	2.62080000
O	0.18355900	-1.50770100	2.58448300
O	0.71255300	0.45905500	3.53330500
C	-0.83430600	-1.70600100	3.55806600
H	-0.42270700	-1.63083800	4.57428200
H	-1.23578800	-2.70845200	3.37874300
H	-1.61247900	-0.94374600	3.41441600
C	2.64406400	-2.42145300	0.89497900
H	3.63486400	-2.71148700	1.27606500
H	2.51228300	-2.84429000	-0.11237800
H	1.85983600	-2.83611000	1.53751400
C	7.78825700	-1.86708400	0.16790600
C	5.62530200	-0.58809400	1.39616700
C	7.88298500	-1.47714200	1.49345300
H	8.79473500	-1.66797400	2.05951400
C	6.79570000	-0.83788800	2.10123600
H	6.85812900	-0.52778500	3.14519100
H	8.62278400	-2.36733900	-0.32711100
H	4.79057200	-0.09185300	1.89218000
P	-1.67199100	-0.03952400	0.16996400
O	-1.25179100	0.58351700	1.45466100
O	-0.71652600	-0.70498300	-0.77542000
H	-6.11455700	-0.67511200	-4.01018800
H	-7.21077200	-1.09730900	-2.68433000
H	-5.14349300	-3.34700500	-3.66873400
C	-6.19349300	-0.73952500	-2.91557600
C	-4.70864000	-2.89305800	-2.77607600
H	-6.76298500	1.26796900	-2.15158500
C	-5.89683400	0.59306800	-2.21081700
C	-5.15311200	-1.65751900	-2.31689400
H	-5.08812400	1.11968700	-2.74099100
C	-3.68672500	-3.54011600	-2.08215700
H	-3.33334200	-4.51644100	-2.42119400
H	-7.36463300	-0.69086500	-0.37238300
H	-7.73566300	1.72191800	-0.03570800
C	-4.60100900	-1.08111800	-1.16656600
C	-5.37043300	0.18118700	-0.80764100
C	-6.56834200	-0.12693900	0.13470200
C	-7.01591200	1.24939400	0.65348900
C	-3.06904400	-2.95838000	-0.96708400
C	-3.53362600	-1.70754300	-0.52296000
C	-4.74504600	1.35507400	-0.07481300
C	-5.71585300	2.01885700	0.68258900
H	-6.19984700	-0.73607000	0.97468400
O	-2.48066200	1.08675000	-0.74329300
H	-7.49745500	1.20084800	1.64049000
C	-3.43305500	1.82486400	-0.09446400
C	-0.74597600	-3.91745400	-0.96028100
C	-1.95270000	-3.67247100	-0.27869800
C	-5.40288400	3.19519200	1.35623200
O	-2.91275600	-1.07823000	0.52421800
C	-1.08569900	3.99717700	-0.56461800
C	-3.08632900	3.00072500	0.59547200
H	-6.15847800	3.72349900	1.94102600
C	-4.09722900	3.68066800	1.28975300
C	0.25456800	-4.65624300	-0.32001700

H	0.62802300	4.98102500	-1.41585200
C	-2.13093100	-4.15412700	1.03416400
H	1.18863200	-4.84911300	-0.85600000
C	0.17982200	4.59464600	-0.49596700
C	-1.69084800	3.53644900	0.61985000
H	-3.83469000	4.60139600	1.81505700
C	0.10159000	-5.14273100	0.97804300
C	-1.10039600	-4.87797600	1.63964000
C	0.87096900	4.72816000	0.70849600
C	-1.00334300	3.64654700	1.84936800
H	-1.24457200	-5.25471300	2.65710600
C	0.26268400	4.23648600	1.86716200
H	0.79069900	4.31247600	2.82267000
C	2.24328700	5.34823600	0.76325200
H	3.03139600	4.57628100	0.80378500
H	2.44108900	5.96658700	-0.12340200
H	2.35831900	5.97994800	1.65609500
C	-1.59357900	3.12004400	3.13136400
H	-2.35375100	3.80237500	3.54215900
H	-2.05678400	2.14193500	2.95045900
H	-0.80758600	2.99006200	3.88689300
C	-1.77347900	3.86964500	-1.89826500
H	-1.76727000	2.82006800	-2.22906700
H	-2.82460800	4.18874500	-1.84327500
H	-1.26532500	4.47649000	-2.65998300
C	1.19644500	-5.92379400	1.65782400
H	2.11574400	-5.93170400	1.05539300
H	1.43559300	-5.49755600	2.64420000
H	0.89558000	-6.97013800	1.82334800
C	-3.41205700	-3.90025100	1.78523700
H	-3.52758200	-2.82789600	2.00431100
H	-4.28844000	-4.20480700	1.19340400
H	-3.42727200	-4.45502800	2.73350500
C	-0.50823300	-3.38418600	-2.34909300
H	0.56438500	-3.40194500	-2.58929000
H	-1.03230100	-3.97856900	-3.11336600
H	-0.85912400	-2.34603200	-2.41406000

TS2-*Rs*

C	6.54609100	1.27482000	0.21926500
C	5.15368600	1.04466300	0.19687800
C	7.39481300	0.34728900	0.92927200
H	8.47084500	0.53636200	0.93444100
C	6.89067200	-0.72243600	1.57934600
H	7.51367600	-1.42747200	2.12849400
N	4.66845800	-0.09364900	0.85396800
C	5.45779200	-1.00674600	1.59611200
N	3.32550500	-0.35222300	0.90956300
C	2.56065800	-0.01100700	2.06776500
C	1.39800200	-0.68072800	2.00388800
C	1.43099600	-1.60968500	0.82268000
C	2.56908600	-1.05042900	0.01779000
O	1.60182500	0.37764100	-0.79694800
C	3.07980300	-1.74383800	-1.19409100
C	2.11135000	-2.17101700	-2.11922700
C	4.43200600	-2.01299200	-1.44760800
C	2.49419000	-2.83114800	-3.28184100
H	1.04896200	-1.97426100	-1.93846700
C	4.80349400	-2.69252200	-2.60657900
H	5.21451100	-1.71149400	-0.75762100
C	3.84104800	-3.09699800	-3.52763700
H	1.73272800	-3.13897400	-3.99960800
H	5.85894900	-2.90022200	-2.78662000
H	4.13883000	-3.62011700	-4.43778000
H	1.03137600	0.00936700	-1.50640200
H	1.75586800	-2.61746300	1.14699800
H	0.49134900	-1.73664400	0.26744300
O	4.93188200	-1.93526000	2.16653600
H	0.86062700	0.67017700	-0.14104500
C	0.18265900	-0.55340600	2.82950000
O	0.09533400	0.62143500	3.45818100
O	-0.65643300	-1.41156800	2.90088300
C	-1.17411700	0.90929700	4.02893900
H	-1.43143600	0.17714500	4.80681500
H	-1.09762900	1.91249300	4.46184900
H	-1.94489500	0.89087500	3.24418700
C	3.13483800	0.95268100	3.04026500
H	4.01809500	0.51557200	3.53123900
H	3.44674000	1.87772000	2.53194700
H	2.38570900	1.19229300	3.80059300
P	-1.45056600	0.10573900	-0.47007500
O	-0.52892200	0.78270800	0.52047200
O	-0.82909400	-0.62913100	-1.61770500
H	-7.15826300	-0.65497200	-2.50057500
H	-7.65846600	-0.95157400	-0.82821100
H	-6.16267000	-3.35774100	-2.31418900
C	-6.80754300	-0.64456100	-1.45883500
C	-5.40785400	-2.84964600	-1.71092700

H	-7.02583400	1.42310900	-0.67343200
C	-6.25473000	0.72342100	-1.02664600
C	-5.62333700	-1.55830000	-1.24095800
H	-5.72812100	1.19401100	-1.87145900
C	-4.20984700	-3.49205500	-1.39510300
H	-4.03906200	-4.51824500	-1.72771800
H	-6.86689900	-0.37189700	1.33980200
H	-7.05199200	2.06713400	1.62409300
C	-4.65734600	-0.91665800	-0.45754000
C	-5.21149300	0.39170700	0.07673000
C	-5.92862700	0.19189500	1.44179700
C	-6.11611800	1.61500800	1.99246400
C	-3.19821500	-2.84967400	-0.66900400
C	-3.43312700	-1.53738100	-0.22671100
C	-4.33585700	1.58723500	0.40274900
C	-4.91597300	2.34096200	1.43013800
H	-5.25954300	-0.37854900	2.10517100
O	-2.51305900	1.19599200	-1.08669400
H	-6.15172500	1.64969800	3.09049800
C	-3.14936300	2.01752000	-0.18392800
C	-1.01209000	-3.92782400	-1.32298600
C	-1.92932200	-3.55524600	-0.32034500
C	-4.36495700	3.56123800	1.80734900
O	-2.44099200	-0.84334000	0.42719400
C	-1.41326100	4.07324800	-1.89486300
C	-2.57849900	3.25270000	0.16757700
H	-4.81944400	4.15809000	2.60061500
C	-3.21854300	4.01531500	1.15394600
C	0.15693000	-4.59723200	-0.95262200
H	-0.33846800	4.85326300	-3.58470900
C	-1.67188100	-3.87047600	1.02754200
H	0.87444500	-4.87625800	-1.72963900
C	-0.28577900	4.61005200	-2.51969500
C	-1.35579600	3.76893000	-0.51799300
H	-2.79019000	4.98415000	1.41934700
C	0.44555600	-4.90024100	0.38174200
C	-0.48179700	-4.53005700	1.35538200
C	0.89857200	4.85531800	-1.82119000
C	-0.17019200	4.00090600	0.20491000
H	-0.27735100	-4.75148700	2.40626500
C	0.93574600	4.54087800	-0.46208800
H	1.85268100	4.72467400	0.10566100
C	2.09376900	5.43812400	-2.52967300
H	2.86282900	5.76607200	-1.81669200
H	2.54672000	4.70183300	-3.21266900
H	1.80696200	6.30699100	-3.14021200
C	-0.06302600	3.65929600	1.66910300
H	-0.64825600	4.34821500	2.29693000
H	-0.42718100	2.63726100	1.84192700
H	0.98366700	3.71682300	2.00015600
C	-2.66846200	3.84270900	-2.69575600
H	-2.84193400	2.76629600	-2.84400500
H	-3.55271400	4.24950800	-2.18337200
H	-2.59168200	4.31692200	-3.68332000
C	1.73170600	-5.59696400	0.74362800
H	1.91153200	-5.56982400	1.82698900
H	1.71204300	-6.65344200	0.43271600
H	2.59181400	-5.12845900	0.24050400
C	-2.65882500	-3.51399500	2.10622600
H	-2.68980600	-2.42498800	2.24636500
H	-3.67018400	-3.86299500	1.84827000
H	-2.36544200	-3.96316200	3.06427500
C	-1.25070700	-3.57091000	-2.76680100
H	-0.39471600	-3.87620000	-3.38484500
H	-2.14521400	-4.06524400	-3.17260300
H	-1.39440700	-2.48381800	-2.85967500
C	7.06220400	2.40409000	-0.43975200
C	4.30150900	1.93000000	-0.47522200
C	6.22241500	3.28273700	-1.10223800
H	6.63016500	4.15651600	-1.61091700
C	4.84318400	3.03713900	-1.11453600
H	4.17110700	3.71856200	-1.63774500
H	8.14047100	2.57328400	-0.41574200
H	3.23070000	1.73824300	-0.51679900

INT4-*Sr*

C	-4.64420200	2.50255200	-2.10908300
C	-3.63319300	1.84777500	-1.37551800
C	-5.92573600	2.72820500	-1.48287600
H	-6.69773300	3.23828900	-2.06374600
C	-6.18052400	2.33858700	-0.21661900
H	-7.13939200	2.50769800	0.27171200
N	-3.95301100	1.41689200	-0.08068200
C	-5.18803500	1.63227300	0.58665900
N	-3.04725900	0.68366800	0.64570900
C	-2.00001900	1.28173000	1.43695000
C	-1.55803100	0.31914200	2.26489600
C	-2.26633900	-0.95695900	1.98221100

C	-3.23734500	-0.58657200	0.93575900	C	4.85345600	2.18571500	-2.68623100
O	-1.55332900	-1.26030500	-0.99782800	H	6.09226000	-2.30273600	-2.20465000
C	-4.32088900	-1.39523300	0.38075000	C	5.35806600	-1.48604800	-2.25688500
C	-4.56614600	-1.42189200	-1.00062500	C	5.03474500	0.86544700	-2.28796200
C	-5.15494300	-2.09396700	1.26431700	H	4.48229800	-1.84982000	-2.81675600
C	-5.65808900	-2.13362300	-1.48530800	C	3.99798200	2.99788600	-1.94362500
H	-3.86569400	-0.92818400	-1.67546300	H	3.87196300	4.04838700	-2.21492600
C	-6.25402900	-2.79003500	0.76755400	H	6.98935000	-0.57086400	-0.32788900
H	-4.96798000	-2.05757700	2.33863000	H	6.91475600	-3.02074800	-0.10196800
C	-6.50728100	-2.80616100	-0.60375500	C	4.36880300	0.35977100	-1.16529300
H	-5.84429500	-2.16795500	-2.55949700	C	4.88207000	-1.03354200	-0.84743100
H	-6.91530300	-3.31846300	1.45519800	C	6.08800700	-1.00033200	0.13286600
H	-7.36791700	-3.35478600	-0.99021600	C	6.25774200	-2.46136900	0.58471100
H	-1.11526100	-2.12195200	-1.02225900	C	3.27642800	2.50450600	-0.84770200
H	-2.73650600	-1.44709300	2.84965400	C	3.44714200	1.15714200	-0.48671700
H	-1.54782800	-1.67345500	1.53303800	C	4.03092200	-2.10440700	-0.19517400
O	-5.35086300	1.21847100	1.71097200	C	4.84308400	-2.99099900	0.52060900
H	-0.82274100	-0.60969600	-1.03426500	H	5.81489900	-0.37460200	0.99690100
C	-0.46203500	0.36567700	3.25829200	O	1.85844500	-1.36759100	-0.83872700
O	0.32004400	1.42918700	3.09963400	H	6.69260200	-2.55137800	1.59039700
O	-0.33478000	-0.46110500	4.12195500	C	2.66175400	-2.33228300	-0.28626100
C	1.55576000	1.38651600	3.79908200	C	1.28716100	4.03312500	-0.62974300
H	1.39342800	1.20589900	4.87000800	C	2.42155600	3.43605100	-0.05416100
H	2.03048500	2.36049300	3.64289900	C	4.30830100	-4.15459800	1.06345400
H	2.17253800	0.58085400	3.37442700	O	2.71504000	0.61860600	0.54058400
C	-1.55459300	2.66895400	1.16728900	C	0.21548100	-4.09222800	-1.30945700
H	-2.36998700	3.29324000	0.77699300	C	2.10456900	-3.51821900	0.22306900
H	-0.73320800	2.62447400	0.43306200	H	4.93561500	-4.85295700	1.62076900
H	-1.15207300	3.11455000	2.08305800	C	2.95044700	-4.42108800	0.87938700
C	-4.36507000	2.92373400	-3.42032000	C	0.57002200	4.98256300	0.10795300
C	-2.36237500	1.64810600	-1.92629500	H	-1.46419500	-4.63886000	-2.54043900
C	-3.11950300	2.70232300	-3.98363200	C	2.81840200	3.78878500	1.25267200
H	-2.91142000	3.02494300	-5.00404700	H	-0.31813900	5.43633800	-0.34135300
C	-2.12363400	2.06955900	-3.22828700	C	-1.12095300	-4.45430900	-1.51910200
H	-1.13317700	1.90545900	-3.65557800	C	0.66522200	-3.84860400	0.00503200
H	-5.15230900	3.42888600	-3.98336900	H	2.52255900	-5.34820900	1.26698700
H	-1.56099500	1.18574900	-1.34869800	C	0.93999400	5.34350600	1.40278000
P	1.31102000	-0.18881200	0.20377200	C	2.06719100	4.73017200	1.95929000
O	0.88304700	-0.83136700	1.47703500	C	-2.02417500	-4.57389400	-0.46182300
O	0.40320200	0.65911300	-0.64478600	C	-0.22740000	-3.97403500	1.09042500
H	5.81769000	-0.22036300	-4.01103800	H	2.37830800	5.00413900	2.97211600
H	6.95819500	-0.04339700	-2.66794000	C	-1.55715600	-4.32390300	0.83201400
H	5.37684600	2.58504100	-3.55717300	H	-2.25215300	-4.40790200	1.67350700
C	5.89571200	-0.20649000	-2.91461200	C	-3.45294200	-4.98182700	-0.69900700

H	-4.13951600	-4.40276900	-0.06510600
H	-3.74239300	-4.83290600	-1.74815800
H	-3.60097400	-6.04679000	-0.45848500
C	0.21813700	-3.70615300	2.50412200
H	0.91516200	-4.47893700	2.86133100
H	0.72752400	-2.73338800	2.55990600
H	-0.64224600	-3.69652300	3.18788000
C	1.14128100	-3.95165600	-2.48952300
H	1.38554100	-2.89197600	-2.66113800
H	2.09010500	-4.48122100	-2.32036100
H	0.67576700	-4.35053300	-3.40045000
C	0.14840200	6.35143900	2.19443800
H	-0.21160500	5.91773400	3.14007500
H	0.76427800	7.22623800	2.45379500
H	-0.72407700	6.70695500	1.62962700
C	4.04552100	3.17574300	1.87645900
H	3.90817600	2.09448400	2.02884000
H	4.92443600	3.30102200	1.22597400
H	4.26606200	3.64007100	2.84759000
C	0.80867000	3.62317700	-1.99809300
H	-0.18906500	4.03914000	-2.19766200
H	1.48401100	3.97080400	-2.79455600
H	0.75909500	2.52491900	-2.05118000

INT4-*Ss*

C	-7.10013600	0.60601500	-0.50138300
C	-5.81796300	0.07851500	-0.75503900
C	-7.20444600	1.86216400	0.20619200
H	-8.20313800	2.25352600	0.41282200
C	-6.11218100	2.55054700	0.59573500
H	-6.17172100	3.50716700	1.11363600
N	-4.71011400	0.79290400	-0.27311400
C	-4.75912800	2.07223800	0.32045500
N	-3.46665200	0.26951600	-0.52743900
C	-2.73033100	0.61436100	-1.71174800
C	-1.60132900	-0.11607500	-1.68570000
C	-1.59606900	-0.97710600	-0.47435500
C	-2.78728600	-0.54264800	0.26961600
O	-1.23286500	1.39503800	1.00763200
C	-3.13892000	-0.98386500	1.61223700
C	-2.05806800	-1.17578200	2.49502300
C	-4.45706600	-1.21447800	2.04297300
C	-2.31243600	-1.58598900	3.80027200
H	-1.03550400	-0.95015200	2.17207400
C	-4.68930100	-1.64246300	3.34502100
H	-5.29934500	-1.09984600	1.36206300
C	-3.61991800	-1.82291100	4.22414800
H	-1.47868500	-1.71225500	4.49201800
H	-5.71068800	-1.83703500	3.67413000
H	-3.80911200	-2.14882800	5.24851300
H	-1.75379800	2.19755600	0.88462300
H	-1.71062900	-2.05286900	-0.72980100
H	-0.67793000	-0.94417600	0.14489100
O	-3.74093200	2.68167300	0.55934500
H	-0.47376800	1.47962900	0.39830700
C	-0.48249100	-0.17100900	-2.65767100
O	-0.31041300	0.96680200	-3.32377400
O	0.16939400	-1.16464500	-2.83066600
C	0.89055600	1.03418900	-4.08407000
H	0.88170800	0.29214300	-4.89467000
H	0.94021300	2.04743300	-4.49596200
H	1.74822600	0.84215500	-3.42342200
C	-3.28525900	1.63358500	-2.63771100
H	-4.30175100	1.36590000	-2.96420800
H	-3.32418400	2.61366800	-2.13788100
H	-2.63259100	1.71395200	-3.51258600
P	1.67205100	0.01518400	0.25484100
O	0.93363100	0.89560700	-0.70989400
O	0.96589500	-0.76501900	1.31309400
H	7.16351000	-1.74167800	2.39364100
H	7.66035300	-1.95342500	0.70636900
H	5.75594100	-4.20857100	2.01002000
C	6.84623600	-1.58509300	1.35291700
C	5.11249900	-3.55239700	1.42040900
H	7.38311900	0.49493800	0.78507700
C	6.50719300	-0.11850500	1.04163100
C	5.54772600	-2.28894500	1.03296400
H	6.01299900	0.33913300	1.91256500
C	3.82775700	-3.96244000	1.06304200
H	3.47345700	-4.95196500	1.36019700
H	7.06285900	-1.05954900	-1.40762800
H	7.60623300	1.34538300	-1.40657500
C	4.72298000	-1.45580600	0.26872800
C	5.47713000	-0.19259100	-0.12071900
C	6.22199200	-0.35427000	-1.47550100
C	6.63827800	1.07502200	-1.86072000
C	2.95269800	-3.12511100	0.35787400
C	3.42450700	-1.85948100	-0.03908100

C	4.79187100	1.14637100	-0.34931600
C	5.51994600	1.90515300	-1.27289600
H	5.50798900	-0.74448600	-2.21742500
O	2.86125000	0.87625100	1.01652000
H	6.74049200	1.21584100	-2.94622500
C	3.63817000	1.67759000	0.22365600
C	0.64523100	-3.80636700	1.10794400
C	1.55755600	-3.57067300	0.05397100
C	5.14942400	3.21554300	-1.55952600
O	2.59728000	-0.98347900	-0.68784900
C	1.86201800	3.70731600	1.92529500
C	3.23234000	2.99541300	-0.05981200
H	5.72074700	3.81378000	-2.27225600
C	4.02206500	3.75226400	-0.93542500
C	-0.64764900	-4.23319600	0.80248100
H	0.58258300	4.31278300	3.54511400
C	1.15810300	-3.77416200	-1.27797800
H	-1.35583100	-4.39928100	1.62037100
C	0.66775300	4.20477800	2.46046200
C	1.97836700	3.55386000	0.53170500
H	3.72191600	4.78019300	-1.15003400
C	-1.06511600	-4.44378000	-0.51751900
C	-0.14924900	-4.20701900	-1.54054200
C	-0.41195600	4.55556500	1.65323800
C	0.89987000	3.91388400	-0.30633900
H	-0.45302300	-4.35178500	-2.58073900
C	-0.27202900	4.40604600	0.26979600
H	-1.11253200	4.66490600	-0.38207000
C	-1.70272600	5.06522500	2.23849400
H	-1.92765900	6.08064700	1.87696300
H	-2.54557800	4.42041100	1.94615900
H	-1.65821500	5.09656200	3.33540300
C	0.97244200	3.72792900	-1.79971400
H	1.56342700	4.51983300	-2.28611800
H	1.42757200	2.75585100	-2.02523600
H	-0.03664800	3.74303000	-2.23566800
C	2.98973100	3.33370400	2.85143500
H	3.07022000	2.23942700	2.93304200
H	3.95583000	3.70763000	2.48169900
H	2.82076100	3.74337800	3.85642700
C	-2.47467900	-4.89403500	-0.80739300
H	-2.68098500	-4.89638500	-1.88667200
H	-2.65317200	-5.91228500	-0.42843500
H	-3.21284900	-4.23979100	-0.31489000
C	2.10519500	-3.52651600	-2.42037300
H	2.26083600	-2.44560900	-2.54568500
H	3.08274100	-3.99779000	-2.23968700
H	1.69376800	-3.92040500	-3.35961200
C	1.03039800	-3.57221000	2.54477700
H	0.14009200	-3.60727200	3.18860300
H	1.73686600	-4.33247300	2.91049300
H	1.50154800	-2.58529300	2.64487800
C	-8.22674300	-0.10507600	-0.94786200
C	-5.67049900	-1.13409300	-1.44270900
C	-8.08583500	-1.30404000	-1.62734700
H	-8.96581000	-1.84966200	-1.96831900
C	-6.80421700	-1.81143200	-1.87308800
H	-6.68390100	-2.75450100	-2.40795700
H	-9.21691400	0.30928600	-0.74852300
H	-4.68139700	-1.54759500	-1.64156500

INT4-*Rr*

C	-7.10022500	0.60604000	-0.50186600
C	-5.81799200	0.07846300	-0.75507700
C	-7.20472800	1.86212300	0.20579200
H	-8.20348300	2.25355800	0.41198200
C	-6.11257600	2.55034700	0.59592100
H	-6.17224500	3.50690800	1.11391800
N	-4.71026600	0.79277900	-0.27273600
C	-4.75942700	2.07193200	0.32124200
N	-3.46674100	0.26957300	-0.52708400
C	-2.73051900	0.61453500	-1.71140000
C	-1.60146900	-0.11583800	-1.68549900
C	-1.59607000	-0.97692600	-0.47420300
C	-2.78728600	-0.54261400	0.26985100
O	-1.23238200	1.39519100	1.00758400
C	-3.13883200	-0.98391300	1.61245700
C	-2.05795100	-1.17568500	2.49522900
C	-4.45695000	-1.21469400	2.04318000
C	-2.31226500	-1.58591400	3.80048400
H	-1.03542600	-0.94990200	2.17225400
C	-4.68912900	-1.64272500	3.34522500
H	-5.29923100	-1.10012300	1.36225800
C	-3.61971800	-1.82302800	4.22435000
H	-1.47850300	-1.71205800	4.49223800
H	-5.71048900	-1.83741000	3.67434800
H	-3.80887100	-2.14895900	5.24871900
H	-1.75266500	2.19828200	0.88557000

H	-1.71072200	-2.05264400	-0.72977400	C	1.55744400	-3.57074400	0.05395000
H	-0.67788200	-0.94405500	0.14497100	C	5.14956900	3.21552300	-1.55950000
O	-3.74130300	2.68115500	0.56091900	O	2.59735900	-0.98344300	-0.68800200
H	-0.47358300	1.47970200	0.39787000	C	1.86212700	3.70734600	1.92528500
C	-0.48269700	-0.17080200	-2.65754800	C	3.23247700	2.99541300	-0.05981000
O	-0.31068100	0.96691600	-3.32381600	H	5.72095600	3.81374900	-2.27218800
O	0.16913600	-1.16448300	-2.83050700	C	4.02225100	3.75228800	-0.93535700
C	0.89030700	1.03418900	-4.08414200	C	-0.64771200	-4.23319500	0.80268600
H	0.88142200	0.29203900	-4.89464100	H	0.58273900	4.31304200	3.54506300
H	0.93995800	2.04737800	-4.49617100	C	1.15781400	-3.77415800	-1.27796300
H	1.74795200	0.84223900	-3.42343900	H	-1.35580900	-4.39925400	1.62065400
C	-3.28535300	1.63396500	-2.63719800	C	0.66790700	4.20496500	2.46041800
H	-4.30206900	1.36673600	-2.96336500	C	1.97850600	3.55388000	0.53170200
H	-3.32369100	2.61407600	-2.13736900	H	3.72218300	4.78026200	-1.14986200
H	-2.63293100	1.71406200	-3.51228500	C	-1.06534700	-4.44370400	-0.51726900
P	1.67210000	0.01514900	0.25476500	C	-0.14958000	-4.20694200	-1.54039100
O	0.93358700	0.89548200	-0.71000000	C	-0.41171100	4.55593200	1.65316100
O	0.96609100	-0.76514600	1.31302900	C	0.90006000	3.91400200	-0.30637700
H	7.16360400	-1.74192000	2.39331600	H	-0.45350900	-4.35157400	-2.58056300
H	7.66037700	-1.95358700	0.70601300	C	-0.27177500	4.40636100	0.26971500
H	5.75594800	-4.20881700	2.00963900	H	-1.11219700	4.66540100	-0.38218400
C	6.84628800	-1.58528700	1.35261200	C	-1.70248800	5.06564500	2.23836400
C	5.11251000	-3.55257300	1.42010200	H	-1.92846200	6.08023800	1.87518800
H	7.38313000	0.49478500	0.78485800	H	-2.54505300	4.41969700	1.94767800
C	6.50722000	-0.11868200	1.04140800	H	-1.65732300	5.09890000	3.33519000
C	5.54776300	-2.28911700	1.03268800	C	0.97268700	3.72798000	-1.79973900
H	6.01305200	0.33890300	1.91238400	H	1.56417900	4.51950600	-2.28613100
C	3.82773400	-3.96254300	1.06278800	H	1.42732300	2.75563600	-2.02511700
H	3.47342200	-4.95207100	1.35992000	H	-0.03633800	3.74362800	-2.23582400
H	7.06280500	-1.05966100	-1.40788300	C	2.98976400	3.33361800	2.85146700
H	7.60624100	1.34526600	-1.40677600	H	3.06990400	2.23933100	2.93330400
C	4.72298800	-1.45594600	0.26852800	H	3.95597000	3.70714500	2.48161600
C	5.47712500	-0.19272300	-0.12091800	H	2.82096700	3.74357400	3.85637300
C	6.22195600	-0.35435800	-1.47572100	C	-2.47485800	-4.89423600	-0.80700400
C	6.63825800	1.07494400	-1.86088500	H	-2.68288300	-4.89176300	-1.88596600
C	2.95262800	-3.12517200	0.35770500	H	-2.65146100	-5.91456700	-0.43274300
C	3.42448300	-1.85956300	-0.03923800	H	-3.21302000	-4.24336400	-0.31011300
C	4.79187900	1.14626400	-0.34942800	C	2.10479500	-3.52647800	-2.42044200
C	5.51997000	1.90507700	-1.27298000	H	2.26075200	-2.44559100	-2.54549300
H	5.50792900	-0.74453400	-2.21764100	H	3.08222800	-3.99809300	-2.23999300
O	2.86122300	0.87628300	1.01642100	H	1.69312800	-3.92002200	-3.35971700
H	6.74042100	1.21581900	-2.94638700	C	1.03051600	-3.57229900	2.54482100
C	3.63822700	1.67754800	0.22357800	H	0.14025400	-3.60737500	3.18871000
C	0.64523300	-3.80645000	1.10801900	H	1.73703600	-4.33253600	2.91047900

H	1.50165500	-2.58537300	2.64488700
C	-8.22671700	-0.10491300	-0.94885000
C	-5.67036200	-1.13408900	-1.44279700
C	-8.08564100	-1.30380900	-1.62842200
H	-8.96553000	-1.84930600	-1.96981700
C	-6.80397100	-1.81128900	-1.87369400
H	-6.68351600	-2.75431000	-2.40861700
H	-9.21693500	0.30950700	-0.74986000
H	-4.68122200	-1.54765900	-1.64131700

INT4-*Rs*

C	-6.64981400	-1.48903800	0.14170900
C	-5.27006100	-1.19790300	0.11994800
C	-7.53739900	-0.61357000	0.86951200
H	-8.60332100	-0.85336600	0.87492100
C	-7.08559600	0.47288400	1.53158100
H	-7.74113100	1.14184300	2.08786800
N	-4.84402100	-0.05534200	0.81467200
C	-5.67079600	0.82732900	1.54838200
N	-3.50345700	0.22958700	0.90459000
C	-2.71167600	-0.24951800	2.00210100
C	-1.50116200	0.32605000	1.88143000
C	-1.50387500	1.23522000	0.70798100
C	-2.82726000	1.03442000	0.10692000
O	-1.39479200	-1.28189600	-0.83258200
C	-3.28899600	1.60286800	-1.15332800
C	-2.36204000	1.61915400	-2.21086100
C	-4.58391000	2.11527200	-1.33675500
C	-2.75837600	2.09375200	-3.45808600
H	-1.34132500	1.25183300	-2.05991600
C	-4.95250500	2.61762300	-2.57944200
H	-5.28183500	2.17253000	-0.50244900
C	-4.04830900	2.59108100	-3.64293100
H	-2.04984500	2.07996600	-4.28723200
H	-5.95121200	3.03335700	-2.71776100
H	-4.35019000	2.97065900	-4.62054600
H	-0.82680000	-0.80744800	-1.46133800
H	-1.43642300	2.29921200	1.02530300
H	-0.68052500	1.11269300	-0.02027900
O	-5.18347900	1.78542700	2.10628500
H	-0.74423900	-1.47377400	-0.12823600
C	-0.31194300	0.24089300	2.76469100
O	-0.20820000	-0.92116100	3.40078500
O	0.44656400	1.16189000	2.90154300
C	1.01971400	-1.10825600	4.09602300
H	1.12414600	-0.37355500	4.90646500
H	0.99304500	-2.12426100	4.50317000
H	1.85633500	-0.99430500	3.39170200
C	-3.32088100	-1.18793300	2.97689800
H	-4.16243000	-0.71172500	3.50258400
H	-3.69154500	-2.09001800	2.46686800
H	-2.56092500	-1.48238900	3.70757300
P	1.55559600	-0.13666000	-0.31242000
O	0.88041100	-0.96872100	0.73636800
O	0.75699000	0.49194800	-1.41899100
H	6.99696100	1.64994100	-2.57991500
H	7.47542600	2.01002200	-0.91287300
H	5.53113800	4.11450800	-2.35551300
C	6.67846700	1.56427900	-1.53130400
C	4.89895200	3.48103100	-1.73003800
H	7.27872100	-0.44446000	-0.79468100
C	6.38626500	0.11617100	-1.10820400
C	5.35691800	2.24987600	-1.27090800
H	5.91946600	-0.42586700	-1.94547200
C	3.61434400	3.89618800	-1.37924300
H	3.24963400	4.87089000	-1.71092000
H	6.87230000	1.26165800	1.27278500
H	7.50037200	-1.11341800	1.46809400
C	4.54733400	1.44588600	-0.46008900
C	5.33798000	0.24476700	0.03316500
C	6.05454000	0.53483400	1.38200200
C	6.51325000	-0.84632500	1.88088400
C	2.75761100	3.08580600	-0.62172300
C	3.24003100	1.84093600	-0.18176700
C	4.69912100	-1.09516900	0.35149900
C	5.43993800	-1.76070600	1.33507800
H	5.31553600	0.95450400	2.08232800
O	2.76898400	-0.98538600	-1.04066100
H	6.59566400	-0.90168600	2.97568300
C	3.58092200	-1.70907300	-0.20346900
C	0.41796700	3.77932100	-1.25405700
C	1.39046800	3.56897800	-0.25732700
C	5.11934000	-3.06541000	1.69719600
O	2.41974100	0.99553900	0.51643800
C	2.05685800	-3.93276500	-1.88710200
C	3.24091000	-3.03144200	0.13456200
H	5.69585600	-3.59133400	2.46088700
C	4.03970400	-3.69525700	1.07402400

C	-0.82707500	4.30579900	-0.88966200
H	0.95285400	-4.73705900	-3.54623400
C	1.10366000	3.88578800	1.08642900
H	-1.58126500	4.46178700	-1.66673000
C	0.95060600	-4.55611500	-2.46744600
C	2.06249700	-3.69930300	-0.49552900
H	3.78844700	-4.72556400	1.33490400
C	-1.13202800	4.63247200	0.43388200
C	-0.15140800	4.41255000	1.40743000
C	-0.15597600	-4.94987300	-1.71092600
C	0.96305400	-4.09966100	0.28781200
H	-0.36859800	4.65375200	2.45197600
C	-0.12832700	-4.71307200	-0.33718400
H	-0.98862400	-5.00256700	0.27313700
C	-1.34466300	-5.59281500	-2.37598100
H	-1.04217000	-6.46180600	-2.97946400
H	-2.08200300	-5.93344600	-1.63625000
H	-1.84150400	-4.88359500	-3.05620600
C	0.92467700	-3.85222300	1.77365000
H	1.53943500	-4.57985500	2.32657800
H	1.29223500	-2.84163300	1.98692900
H	-0.10569800	-3.93071700	2.14892600
C	3.21947400	-3.52236700	-2.75350500
H	3.25059700	-2.42809400	-2.86515700
H	4.17850700	-3.83494000	-2.31484700
H	3.13465000	-3.96752300	-3.75400200
C	-2.49525700	5.14851900	0.81574400
H	-3.08630300	4.37061000	1.32820800
H	-2.42175000	6.00075000	1.50667100
H	-3.06405900	5.46725100	-0.06849400
C	2.13164800	3.67121800	2.16403800
H	2.32807300	2.59668300	2.28486700
H	3.07959500	4.17108400	1.91323200
H	1.77339700	4.06008100	3.12650600
C	0.69158300	3.42562300	-2.69217200
H	-0.22134000	3.53332900	-3.29396800
H	1.46047500	4.07636800	-3.13401900
H	1.04939000	2.38744700	-2.75622200
C	-7.11266200	-2.62427800	-0.54600900
C	-4.37044100	-2.01408200	-0.57491700
C	-6.23024300	-3.44273400	-1.23028500
H	-6.59478300	-4.32248300	-1.76124700
C	-4.86448900	-3.12963000	-1.23986400
H	-4.16272500	-3.76390400	-1.78310600
H	-8.18173300	-2.84488900	-0.52758600
H	-3.30327800	-1.77641700	-0.61626200

TS3-*Sr*

C	4.83349100	-2.15348600	-1.46462900
C	3.78359000	-1.53836400	-0.75384100
C	6.15180900	-2.16393000	-0.87396500
H	6.95915700	-2.64594300	-1.43047400
C	6.40314000	-1.60172300	0.32801000
H	7.39315600	-1.60447100	0.78241400
N	4.09371500	-0.94246800	0.47556400
C	5.35911600	-0.93751900	1.10639800
N	3.09863600	-0.27834800	1.14232900
C	2.22478900	-0.93863900	2.04586200
C	1.43507400	0.02556500	2.57697800
C	1.76072500	1.30944500	1.93193400
C	2.91637100	1.04376100	1.11746500
O	1.58467400	1.34438300	-1.47690500
C	3.81743800	2.00070300	0.47533800
C	4.40540200	1.77399700	-0.77957700
C	4.13254900	3.16418300	1.19345600
C	5.31913400	2.69161700	-1.28529300
H	4.09784800	0.91824200	-1.37840000
C	5.05029100	4.07632700	0.67900600
H	3.68192700	3.33746800	2.17214600
C	5.64916200	3.83652500	-0.55642100
H	5.76653500	2.51985500	-2.26529500
H	5.30206100	4.97118400	1.24952300
H	6.36978400	4.54988900	-0.96016800
H	1.07489900	2.12049500	-1.20385700
H	1.66825900	2.25199800	2.47680700
H	0.85389500	1.30374200	1.13945200
O	5.49865000	-0.40805500	2.18425600
H	0.90165900	0.68542300	-1.70400500
C	0.28147900	-0.05648800	3.49899100
O	-0.09359000	-1.30354500	3.78427900
O	-0.25190600	0.92172200	3.95159500
C	-1.20716600	-1.41558100	4.66389100
H	-0.99502900	-0.91434600	5.61825000
H	-1.36768500	-2.48579800	4.82552900
H	-2.09756000	-0.95701700	4.21240400
C	2.33485600	-2.40852500	2.20906200
H	3.35321200	-2.68129000	2.52529900
H	2.11143300	-2.91620000	1.25835500

H	1.61524200	-2.74390200	2.96112800
C	4.55455700	-2.71744100	-2.72222000
C	2.48645000	-1.50182400	-1.27302100
C	3.27717400	-2.65644000	-3.25709000
H	3.07427900	-3.08247100	-4.24047100
C	2.24832000	-2.04605400	-2.52619800
H	1.23169900	-1.98065500	-2.91665500
H	5.36806800	-3.19497700	-3.27211200
H	1.65965300	-1.03783600	-0.73608300
P	-1.26196700	0.13197000	-0.40814900
O	-0.56640500	0.91668500	0.67326500
O	-0.50418500	-0.54742300	-1.50432700
H	-6.94055400	-1.03241900	-2.63494300
H	-7.42560100	-1.30305300	-0.95280800
H	-5.78726800	-3.63377300	-2.40716500
C	-6.59372000	-0.96665700	-1.59396800
C	-5.06628400	-3.07775400	-1.80487700
H	-6.93062000	1.11221900	-0.88789600
C	-6.12049600	0.43963600	-1.20345200
C	-5.35801000	-1.79817100	-1.34566800
H	-5.60243300	0.90597400	-2.05575800
C	-3.83119700	-3.63720500	-1.48718700
H	-3.58742000	-4.64742200	-1.82346400
H	-6.70432600	-0.62481500	1.19577000
H	-7.10424900	1.80343500	1.30975200
C	-4.44105400	-1.09057500	-0.55769400
C	-5.08051400	0.20030300	-0.07163400
C	-5.82030500	0.02293600	1.28318600
C	-6.14400000	1.45950700	1.72867500
C	-2.86444600	-2.92967700	-0.75915400
C	-3.18269200	-1.63916700	-0.30207700
C	-4.29885400	1.46815400	0.21418300
C	-4.99003700	2.24643100	1.15000000
H	-5.12539800	-0.44069700	2.00084000
O	-2.36948000	1.10912600	-1.13996100
H	-6.21291000	1.56490700	2.82071500
C	-3.11364500	1.94031600	-0.33964400
C	-0.67542200	-3.89845900	-1.52448900
C	-1.55406200	-3.58334000	-0.46783300
C	-4.56625000	3.53816100	1.44263800
O	-2.25221200	-0.90896100	0.39799700
C	-1.21468500	3.84560600	-2.01830000
C	-2.65315500	3.23644400	-0.04643200
H	-5.11306300	4.15819500	2.15562100
C	-3.41872000	4.02900000	0.81868300
C	0.50620600	-4.58507200	-1.23930400
H	0.13535600	4.32724700	-3.62177100
C	-1.23412700	-3.95555900	0.84970100
H	1.19454900	-4.81487000	-2.05753500
C	0.01915300	4.25133500	-2.53727200
C	-1.36715300	3.72741700	-0.62206700
H	-3.08349000	5.04662200	1.02751400
C	0.84221700	-4.97043300	0.06168600
C	-0.04283800	-4.64830900	1.09077100
C	1.10616700	4.54438900	-1.71315800
C	-0.29354900	4.05628000	0.23295900
H	0.19904300	-4.93949000	2.11710500
C	0.92375100	4.45390500	-0.32966300
H	1.76266200	4.68832300	0.33221700
C	2.45247700	4.86920600	-2.29836800
H	3.06421800	5.46197500	-1.60395700
H	2.99572600	3.93410000	-2.51063200
H	2.35866000	5.42256800	-3.24337100
C	-0.42003900	3.94977300	1.73077000
H	-1.13618200	4.67837700	2.13570800
H	-0.76837700	2.94698300	2.02122300
H	0.54727200	4.15184700	2.21226700
C	-2.34780300	3.53762300	-2.96162200
H	-2.47667800	2.45007400	-3.06554200
H	-3.29954200	3.94703600	-2.59322400
H	-2.14979700	3.95820300	-3.95656100
C	2.13555400	-5.69399500	0.33323300
H	2.33725900	-5.76590100	1.41111000
H	2.11230900	-6.71753200	-0.07243500
H	2.98296100	-5.17684900	-0.14366800
C	-2.15385500	-3.62005100	1.99358700
H	-2.15776900	-2.53427300	2.17114000
H	-3.19007600	-3.92075200	1.77791900
H	-1.83195000	-4.12751200	2.91310500
C	-0.97441900	-3.45866700	-2.93415500
H	-0.15161100	-3.73187300	-3.60963400
H	-1.89369200	-3.91616200	-3.32602600
H	-1.11250200	-2.36604000	-2.95114800

TS3-*Ss*

C	7.01216100	0.68027200	0.38298100
C	5.73502800	0.16130900	0.67623000
C	7.10336900	1.88774100	-0.40546800

H	8.09751800	2.27249100	-0.64393500	C	-6.69746400	-1.68030800	-1.57348000
C	6.00225300	2.53971700	-0.83043000	C	-4.92567400	-3.60818100	-1.54419900
H	6.04812400	3.46124400	-1.40961600	H	-7.30481900	0.38989300	-1.04217800
N	4.61655700	0.83221100	0.15715200	C	-6.40533000	-0.20978000	-1.24235600
C	4.65496100	2.06925600	-0.51497100	C	-5.40761000	-2.35701900	-1.17476900
N	3.38366300	0.30471700	0.45500300	H	-5.86377800	0.25657200	-2.07989800
C	2.68195200	0.64758400	1.64049000	C	-3.65565700	-3.99124600	-1.11729100
C	1.59197200	-0.15514700	1.67981800	H	-3.25951300	-4.96769100	-1.40443300
C	1.55673100	-0.98305100	0.46527500	H	-7.09625700	-1.14969600	1.17859800
C	2.73043800	-0.60486300	-0.27381000	H	-7.69836800	1.23913600	1.10393000
O	1.03628200	1.54540100	-0.94127200	C	-4.65026900	-1.51529600	-0.35234900
C	3.10034200	-1.06318300	-1.61373400	C	-5.45028800	-0.26557300	-0.01591800
C	2.05226600	-1.14535300	-2.54658700	C	-6.27800500	-0.42358800	1.28902500
C	4.40899500	-1.40585000	-1.98846900	C	-6.75174000	1.00233700	1.61757300
C	2.32640000	-1.56058800	-3.84720400	C	-2.84161100	-3.14432200	-0.35059300
H	1.04305100	-0.84263700	-2.25272800	C	-3.36793100	-1.89953700	0.04257700
C	4.66288500	-1.83435400	-3.28761500	C	-4.80691600	1.08822900	0.23425100
H	5.22456400	-1.37703600	-1.26577300	C	-5.62074400	1.85027100	1.08101000
C	3.62511000	-1.90765500	-4.21798300	H	-5.60614800	-0.78343300	2.08360200
H	1.51520000	-1.60726000	-4.57524400	O	-2.75247800	0.82286300	-0.94978400
H	5.67758200	-2.11483700	-3.57328400	H	-6.91969200	1.16205200	2.69212900
H	3.83157800	-2.23624100	-5.23802400	C	-3.62656200	1.63401300	-0.26356600
H	1.68357600	2.25827600	-0.88184800	C	-0.50902500	-3.77147200	-1.04170600
H	1.37645500	-2.06791700	0.57021200	C	-1.45286500	-3.57937800	-0.00567300
H	0.58566300	-0.76580100	-0.21843700	C	-5.30924400	3.17889100	1.35111400
O	3.63443400	2.66174900	-0.78728400	O	-2.61683800	-1.02259800	0.78484900
H	0.37572100	1.73682600	-0.25498000	C	-1.77417400	3.67710100	-1.88290400
C	0.52044200	-0.24047500	2.70126800	C	-3.27913300	2.97020500	0.00581500
O	0.40534500	0.86143300	3.43788400	H	-5.94583100	3.78110600	2.00259600
O	-0.15248700	-1.22540000	2.84958400	C	-4.15563300	3.73002400	0.79167200
C	-0.77521600	0.92888600	4.22795100	C	0.77011900	-4.22443800	-0.71893800
H	-0.77848600	0.14257100	4.99564900	H	-0.41175100	4.34163200	-3.40736900
H	-0.77704600	1.91785800	4.69827100	C	-1.09318200	-3.83428400	1.32749600
H	-1.65025800	0.80810600	3.57395700	H	1.50249700	-4.35796500	-1.52140400
C	3.20437900	1.73538200	2.50780200	C	-0.58094800	4.25270800	-2.33084500
H	4.25356700	1.55601300	2.78830800	C	-2.00176400	3.55868400	-0.49849000
H	3.14541600	2.69773800	1.97562600	H	-3.89962800	4.77212900	0.99397300
H	2.59267700	1.79986500	3.41226800	C	1.14759900	-4.49022100	0.60433500
P	-1.64741000	0.04305100	-0.01250400	C	0.20500500	-4.28439600	1.60934200
O	-1.06606000	0.96418900	1.00773500	C	0.39568600	4.70975000	-1.44806300
O	-0.74720100	-0.71326400	-0.96016100	C	-1.02648900	4.01508000	0.41511600
H	-6.94673200	-1.84276000	-2.63159900	H	0.47964600	-4.46827100	2.65131900
H	-7.54174300	-2.06571300	-0.97775500	C	0.15319000	4.57777800	-0.07781300
H	-5.52057200	-4.27257900	-2.17406000	H	0.91096700	4.92053900	0.63374600

C	1.69402000	5.28686600	-1.94685600
H	1.62623800	5.56343100	-3.00786800
H	1.97729600	6.18246200	-1.37429200
H	2.50924100	4.55455000	-1.83743400
C	-1.21638700	3.88676000	1.90542600
H	-1.83148000	4.70602900	2.31040600
H	-1.70101100	2.93279600	2.14544300
H	-0.24260600	3.91854200	2.41483300
C	-2.78690200	3.19696400	-2.88916800
H	-2.77945100	2.09819400	-2.94460100
H	-3.80666100	3.50541300	-2.61584300
H	-2.56053100	3.59320700	-3.88816400
C	2.54920700	-4.94789000	0.91494300
H	2.70012300	-5.07489000	1.99550800
H	2.77262500	-5.90758800	0.42440600
H	3.29230200	-4.22125600	0.54708600
C	-2.07069300	-3.61934900	2.45031700
H	-2.22479000	-2.54186700	2.60456600
H	-3.04491800	-4.07977200	2.22815000
H	-1.68744300	-4.04499800	3.38761000
C	-0.84752200	-3.45376800	-2.47488000
H	0.05880800	-3.47527700	-3.09601400
H	-1.56201500	-4.17410600	-2.89995900
H	-1.29815900	-2.45292900	-2.53767700
C	8.14674900	0.00963200	0.87028300
C	5.60137700	-1.00217300	1.44788100
C	8.01907200	-1.14126500	1.63015600
H	8.90490600	-1.65474500	2.00418800
C	6.74243400	-1.63961300	1.91748700
H	6.63269400	-2.54319200	2.51875000
H	9.13237100	0.41752400	0.63789700
H	4.61593700	-1.40592500	1.68240200

TS3-*Rr*

C	-7.10181500	0.48634200	-0.17140100
C	-5.84765100	-0.00544700	0.24294600
C	-7.15456800	1.75405600	-0.86320000
H	-8.12802000	2.11444800	-1.20314800
C	-6.04602300	2.49329500	-1.07218800
H	-6.06735000	3.46433000	-1.56540200
N	-4.70910600	0.74369600	-0.09063000
C	-4.73188000	2.05455400	-0.61106400
N	-3.48934100	0.27389500	0.33093100
C	-2.96701400	0.62666900	1.60855900
C	-1.78428600	-0.01087900	1.73019100
C	-1.48945300	-0.70163500	0.46674900
C	-2.65972300	-0.51735100	-0.35777300
O	-1.53288400	1.58112800	-1.95714900
C	-2.84782900	-1.09894200	-1.68617700
C	-1.67690200	-1.36519500	-2.41811900
C	-4.09552500	-1.43940300	-2.22874500
C	-1.75793900	-1.95573600	-3.67208200
H	-0.70766300	-1.06482400	-2.01442500
C	-4.16514000	-2.04070000	-3.48340000
H	-5.01733900	-1.27169200	-1.67516500
C	-3.00159000	-2.29743000	-4.20655100
H	-0.84340300	-2.14453800	-4.23605500
H	-5.13834600	-2.31175100	-3.89450900
H	-3.06458800	-2.76262900	-5.19174900
H	-1.98133000	2.17775300	-1.34346700
H	-1.00256100	-1.68754200	0.48013700
H	-0.63527000	-0.03671100	-0.07201000
O	-3.72231200	2.72448200	-0.64257400
H	-0.64061400	1.47490700	-1.58799000
C	-0.90354200	-0.05072500	2.93921200
O	-0.33258700	1.12303100	3.17103300
O	-0.78984700	-1.02443400	3.63026100
C	0.69153000	1.12106500	4.15829900
H	0.30609200	0.75956900	5.12143200
H	1.03209200	2.15772100	4.24906800
H	1.50968400	0.47272900	3.81610500
C	-3.72060500	1.54540100	2.50078500
H	-4.72515100	1.15726900	2.72829100
H	-3.82125000	2.53755100	2.03622200
H	-3.16658100	1.66438800	3.43964500
C	-8.25417900	-0.26555200	0.11411000
C	-5.75400900	-1.21699300	0.94198500
C	-8.16578400	-1.46633700	0.79889200
H	-9.06479900	-2.04236800	1.01860000
C	-6.91225100	-1.93320500	1.21417700
H	-6.83465500	-2.87394500	1.76095900
H	-9.22155800	0.11960900	-0.21388200
H	-4.78627300	-1.59634500	1.27111600
P	1.71906600	0.00041500	0.30199900
O	1.30927500	-0.63974600	1.57787600
O	0.66116200	0.59820600	-0.60999600
H	6.59811900	0.86795200	-3.50102100
H	7.52342300	1.21487800	-2.03132700

H	5.59174200	3.51934900	-3.14197400
C	6.54282500	0.87378400	-2.40325800
C	5.04679100	3.02105000	-2.33770800
H	7.01467300	-1.17519600	-1.68671200
C	6.16312200	-0.49157400	-1.81240800
C	5.43476600	1.76254800	-1.88899400
H	5.42466700	-0.98344700	-2.46449300
C	3.93259400	3.62845700	-1.76119000
H	3.60901200	4.61234400	-2.10672600
H	7.39690400	0.68523900	0.25984000
H	7.75569500	-1.74573700	0.44548400
C	4.75037200	1.13085200	-0.84248600
C	5.47299000	-0.15346400	-0.45998600
C	6.55563300	0.08226900	0.63039000
C	6.95709900	-1.33203700	1.08330500
C	3.17707100	2.98975600	-0.76956700
C	3.60912400	1.73199000	-0.31154800
C	4.77376900	-1.37234600	0.11869700
C	5.67032100	-2.10564100	0.90597600
H	6.09108600	0.62235600	1.46990700
O	2.54959200	-1.03410300	-0.67678600
H	7.32285300	-1.36333300	2.11941600
C	3.47332900	-1.83621500	-0.05140100
C	0.82943100	3.75227000	-1.16762400
C	1.90564200	3.59305700	-0.27102800
C	5.30264500	-3.33955100	1.43298300
O	2.89221700	1.08511400	0.66318600
C	1.15841800	-3.80574100	-0.98268800
C	3.07222400	-3.07702200	0.47552200
H	6.00124400	-3.91734300	2.04131800
C	4.01530200	-3.82343300	1.19226900
C	-0.37760800	4.27010300	-0.69064300
H	-0.56656000	-4.39528500	-2.12835400
C	1.76550600	3.97612700	1.07589400
H	-1.21828400	4.37165300	-1.38302500
C	-0.17640300	-4.20277000	-1.12527000
C	1.66489600	-3.54955500	0.30630600
H	3.71253200	-4.79025000	1.59946100
C	-0.54618000	4.63750600	0.64637300
C	0.54011200	4.49104100	1.51022500
C	-1.02236600	-4.34993400	-0.02582200
C	0.83322000	-3.71139800	1.43552600
H	0.43166000	4.78158800	2.55913600
C	-0.49476100	-4.10493100	1.24566300
H	-1.14338800	-4.19360300	2.12206900
C	-2.46287700	-4.75518500	-0.20066100
H	-3.12580100	-4.14704200	0.43385000
H	-2.78670500	-4.64110800	-1.24482900
H	-2.61788000	-5.80730600	0.08660200
C	1.32875400	-3.43579600	2.83043800
H	1.93410700	-4.27179000	3.21527900
H	1.93925300	-2.52472500	2.84033100
H	0.48140700	-3.27867800	3.50919800
C	2.01678400	-3.64604800	-2.21061300
H	2.17907200	-2.58034800	-2.43392600
H	3.00733400	-4.10315100	-2.07128600
H	1.53985200	-4.11405700	-3.08269000
C	-1.86008500	5.19628600	1.12622400
H	-2.69912600	4.72073300	0.59860200
H	-1.98904900	5.03944900	2.20654900
H	-1.92041000	6.28056400	0.93922900
C	2.90733000	3.83337400	2.04835000
H	3.07481800	2.77466100	2.29722700
H	3.84562400	4.21966600	1.62331500
H	2.70022500	4.38135600	2.97783800
C	0.93868600	3.33160900	-2.61211300
H	-0.05573700	3.27958100	-3.07077300
H	1.55958100	4.02708200	-3.19638900
H	1.39936400	2.33546000	-2.68983400

TS3-*Rs*

C	5.79516800	1.83656400	-0.74019700
C	4.56765500	1.25727000	-0.35998500
C	6.98979000	1.47811900	-0.01307400
H	7.93010800	1.94876600	-0.30964400
C	6.96935700	0.58437800	0.99821800
H	7.86357700	0.29447800	1.54884800
N	4.58947200	0.34569000	0.70972300
C	5.73764000	-0.08181300	1.40921900
N	3.42262600	-0.28856600	1.06422500
C	2.66095500	0.07251100	2.21349100
C	1.54613800	-0.69281000	2.17330500
C	1.56884800	-1.52613800	0.95502800
C	2.84592000	-1.24260600	0.34604800
O	1.33303600	2.18083100	1.01487900
C	3.39720700	-1.76943600	-0.90189200
C	2.57468700	-1.77177700	-2.03681200
C	4.71605700	-2.24088200	-0.96680800

C	3.09444000	-2.22175600	-3.24842300	C	-2.62027500	-3.10285100	-0.76088400
H	1.54944500	-1.39481400	-1.96325700	C	-3.13738600	-1.87052600	-0.32593300
C	5.21164200	-2.71231600	-2.17832500	C	-4.56446800	1.11414400	0.04765900
H	5.33071400	-2.27040200	-0.06425700	C	-5.47248800	1.79589500	0.86744300
C	4.40530000	-2.69312800	-3.31850300	H	-5.53112800	-0.93399200	1.60132600
H	2.46894900	-2.20527300	-4.14225100	O	-2.38033300	0.96679100	-0.91989500
H	6.23121600	-3.09567100	-2.23386400	H	-6.89565200	0.94925900	2.28432500
H	4.80278200	-3.05210600	-4.26931800	C	-3.34962100	1.70929900	-0.28445700
H	1.06267200	2.86671300	0.39310600	C	-0.26789400	-3.84911500	-1.20100200
H	1.26556400	-2.58256300	1.02599900	C	-1.31930800	-3.65909500	-0.28049700
H	0.78927000	-1.12132900	0.17436600	C	-5.22556000	3.10708800	1.25923600
O	5.64340900	-0.94097800	2.25836300	O	-2.45070700	-1.09804500	0.57532800
H	0.49098500	1.71568500	1.21486300	C	-1.56748000	3.96275300	-1.70117800
C	0.36090900	-0.70684100	3.06223800	C	-3.08860400	3.04264000	0.07637800
O	0.25390800	0.38200700	3.81663400	H	-5.93502600	3.64672200	1.88950000
O	-0.42042500	-1.62142500	3.07617900	C	-4.05219700	3.72640500	0.82970200
C	-0.99250500	0.53066300	4.48526900	C	0.90121200	-4.48746600	-0.77679100
H	-1.14139700	-0.27403900	5.21854000	H	-0.22377600	4.85188800	-3.12523400
H	-0.95570800	1.50169700	4.99020700	C	-1.17858800	-4.09091200	1.05175900
H	-1.80311100	0.51041000	3.74403000	H	1.71473600	-4.63115900	-1.49430500
C	3.16891200	1.13374600	3.11453100	C	-0.42757000	4.68757300	-2.06346500
H	3.26005800	2.06959200	2.54641400	C	-1.83691000	3.74501600	-0.33360200
H	2.44874200	1.28944800	3.92279100	H	-3.85400200	4.76522600	1.10195600
H	4.14312200	0.84518800	3.53559600	C	1.05803300	-4.93805300	0.53799100
P	-1.40432200	0.05735400	0.05054600	C	0.01034300	-4.72268000	1.43660100
O	-1.00900000	0.82795700	1.27263800	C	0.44645800	5.21629100	-1.11070200
O	-0.36271000	-0.55171900	-0.85373300	C	-0.95692300	4.25085000	0.64447900
H	-6.43516700	-1.44337400	-3.30910900	H	0.11622600	-5.05413300	2.47306100
H	-7.19539600	-1.83429900	-1.75783300	C	0.16045400	4.98914500	0.23746800
H	-5.12115500	-3.96719600	-2.94646100	H	0.84637000	5.36836700	1.00056100
C	-6.29147200	-1.40363900	-2.22010100	C	1.65612100	6.01780700	-1.51539800
C	-4.57514100	-3.38079200	-2.20502000	H	1.89969300	5.86730900	-2.57621600
H	-6.92788300	0.60439100	-1.51538600	H	1.48245900	7.09470400	-1.36286600
C	-6.01872700	0.01472400	-1.70038900	H	2.53591600	5.74070000	-0.91646500
C	-5.05662200	-2.14949600	-1.77351500	C	-1.15608900	3.96118400	2.11100300
H	-5.39965400	0.56278500	-2.42772900	H	-1.52973600	2.93690700	2.24587400
C	-3.37347700	-3.84956500	-1.67947000	H	-0.20070900	4.05389300	2.64498800
H	-2.98341300	-4.81830700	-1.99966600	H	-1.87516700	4.65582500	2.57262400
H	-6.92723200	-1.19484400	0.52547600	C	-2.48547700	3.43717300	-2.77339500
H	-7.53828900	1.18616800	0.65151600	H	-2.42191600	2.34065600	-2.83436700
C	-4.36474700	-1.41302400	-0.80614800	H	-3.53454200	3.69235900	-2.56185600
C	-5.18049100	-0.19671400	-0.40624800	H	-2.21849100	3.85443500	-3.75343400
C	-6.12688700	-0.48882700	0.78945700	C	2.34711000	-5.57399700	0.98778900
C	-6.63692500	0.89735400	1.21715600	H	2.17202000	-6.33631100	1.75968600

H	2.87502100	-6.04581200	0.14751700
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C	-2.28600700	-3.88971700	2.04935500
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H	-2.06180100	-4.40775700	2.99111700
C	-0.38330400	-3.35299800	-2.61906700
H	0.56415200	-3.49636600	-3.15502200
H	-1.16763600	-3.88166600	-3.17888100
H	-0.64355100	-2.28303300	-2.61617700
C	5.81654700	2.73935700	-1.81829900
C	3.38825400	1.56852600	-1.04893700
C	4.65507000	3.04673900	-2.50523500
H	4.67919400	3.74211000	-3.34473000
C	3.44545900	2.45665200	-2.11381500
H	2.52285200	2.69406300	-2.64622900
H	6.77030500	3.18694000	-2.10435600
H	2.43000600	1.16487600	-0.72607400

CPA-H_20

O	-1.40153800	-3.21834200	0.67195300
H	-1.52139800	-2.95709500	-0.25897900
H	-0.00755500	-2.36365500	0.96817600
H	-2.19879500	-2.87505200	1.10572100
P	-0.02798700	-0.67966900	-0.26846800
O	-0.73806800	-1.34269100	-1.37889700
O	0.62968000	-1.59908000	0.82491600
H	1.30331000	4.46523400	2.91768200
H	1.68514000	5.18434300	1.34470900
H	3.84688200	3.20317500	2.64105400
C	1.27548200	4.28523300	1.83400700
C	3.29276800	2.61887800	1.90408800
H	-0.74463100	4.84389500	1.10063300
C	-0.13152400	3.95716000	1.31505800
C	2.05888800	3.05735100	1.43474800
H	-0.66600300	3.34447500	2.05763600
C	3.81027100	1.41468100	1.42881700
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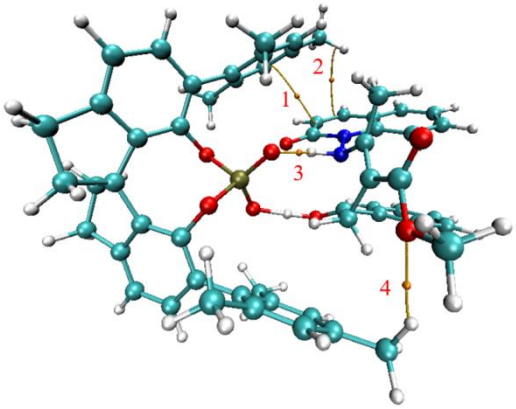
H	1.05690000	4.84587300	-0.92584300
H	-1.34400900	5.36291500	-1.09614300
C	1.34873900	2.31664300	0.48017400
C	0.11151100	3.09035600	0.04583400
C	0.38500900	4.01239700	-1.17506600
C	-1.01319500	4.46108500	-1.63683000
C	3.10112500	0.61803600	0.52108500
C	1.85921600	1.08933400	0.06690600
C	-1.17530500	2.42431600	-0.40733000
C	-1.87420600	3.27222800	-1.27492500
H	0.86260600	3.41285700	-1.96544900
O	-0.95880100	0.29319300	0.64545400
H	-1.05535000	4.69384500	-2.71001400
C	-1.73182100	1.20112100	-0.05870100
C	3.81938200	-1.74933500	0.96642600
C	3.65502100	-0.68768000	0.05400100
C	-3.15682000	2.94060400	-1.70097900
O	1.12506000	0.30067800	-0.80584300
C	-3.84326900	-0.75741800	1.28553800
C	-3.02183500	0.83469800	-0.47281600
H	-3.71090700	3.60222200	-2.36945500
C	-3.72826000	1.73987900	-1.27463200
C	4.35591500	-2.95467000	0.50929200
H	-4.55978000	-2.21104700	2.70357500
C	4.03568600	-0.84558700	-1.29173800
H	4.47288600	-3.78055200	1.21661600
C	-4.36389900	-2.00703700	1.64734900
C	-3.59796800	-0.48468700	-0.07484300
H	-4.73827300	1.47553900	-1.59395700
C	4.73827300	-3.13648000	-0.82238500
C	4.57390700	-2.06846400	-1.70494700
C	-4.64448800	-2.99212800	0.69623500
C	-3.88766400	-1.45893500	-1.05402300
H	4.87439800	-2.18592800	-2.74950400
C	-4.40097100	-2.69428200	-0.64793500
H	-4.60620200	-3.45335500	-1.40758400
C	-5.13525100	-4.35437100	1.10677500
H	-5.85136600	-4.75797200	0.37771400
H	-4.29193000	-5.06113200	1.16611900
H	-5.61931100	-4.32741500	2.09226600
C	-3.63271300	-1.20433300	-2.51654800
H	-3.69677600	-2.14187300	-3.08484000
H	-4.36975000	-0.50532700	-2.93934100
H	-2.63129900	-0.77849300	-2.66036400
C	-3.55996000	0.26785600	2.35245800
H	-2.47599800	0.39428400	2.49535800
H	-3.97073100	1.25108900	2.08054200
H	-3.99769700	-0.03789300	3.31183600
C	3.87857500	0.27705100	-2.28443700
H	2.81689800	0.44004400	-2.52450300

H	4.27448300	1.22358900	-1.88754300
H	4.40688500	0.04687100	-3.21899300
C	5.28697700	-4.45919200	-1.28836400
H	6.01608500	-4.86345200	-0.57146600
H	4.48080300	-5.20276800	-1.38893100
H	5.77926900	-4.36668300	-2.26580100
C	3.41717100	-1.61180800	2.41280800
H	3.35442500	-2.59938400	2.88973500
H	4.14513800	-1.01330000	2.98190900
H	2.43937400	-1.12066900	2.50471200

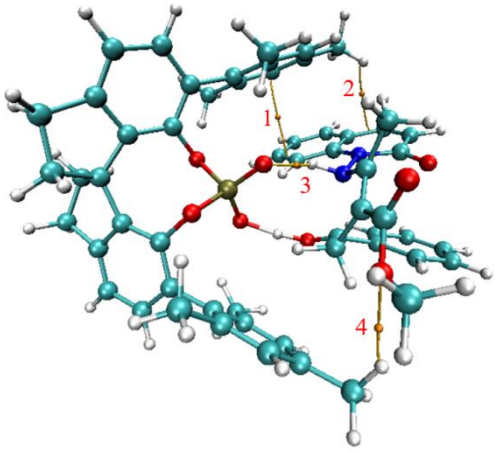
(7) NCI and topology analyses of TS1 and TS2

Summary of distances, types of interaction, electron densities (ρ_{bcp}), Lagrangian kinetic energies (G_b), potential energy densities (V_b), energy densities (H_b), and Laplacian of electron densities ($\nabla^2\rho$) at the bond critical points (BCPs) along the bond paths in TS1R (bond lengths in Å, other values in a.u.).



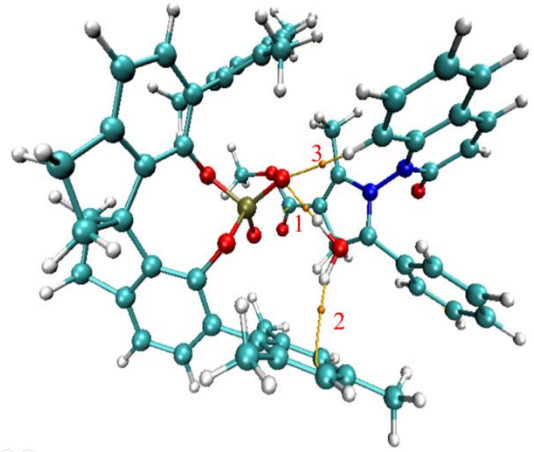
TS1-*Ss*

Entry	Type of interaction	Distance	$\rho_{bcp}\times10^{-2}$	$G_b\times10^{-2}$	$V_b\times10^{-2}$	$H_b\times10^{-3}$	$\nabla_{2\rho}\times10^{-1}$
1	C ··C	3.32	0.6975	0.4532	-0.3732	0.8001	0.2133
2	C-H ··C	3.00	0.5675	0.3731	-0.2840	0.8906	0.1848
3	N-H ··O	1.79	0.3674	0.3293	-0.3508	-0.2154	0.1231
4	C-H ··O	2.67	0.5962	0.4353	-0.3266	0.1086	0.2175



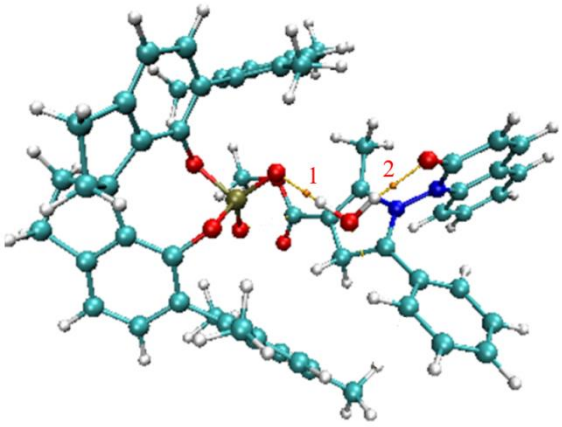
TS1-*Rs*

Entry	Type of interaction	Distance	$\rho_{bcp}\times10^{-2}$	$Gb\times10^{-2}$	$Vb\times10^{-2}$	$Hb\times10^{-3}$	$\nabla_{2\rho}\times10^{-1}$
1	π—π	3.39	0.7128	0.4326	-0.3504	0.8221	0.2059
2	C-H ··C	2.87	0.6136	0.4158	-0.3276	0.8822	0.2016
3	N-H ··O	1.80	0.3561	0.3250	-0.3373	-0.1229	0.1250
4	C-H ··O	2.63	0.6557	0.4865	-0.3679	0.1186	0.2420



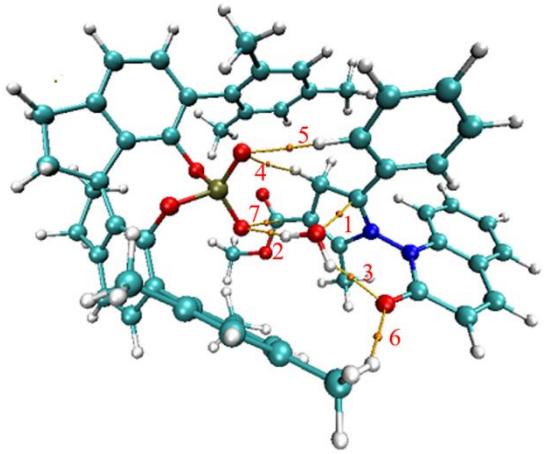
TS2-Sr

Entry	Type of interaction	Distance	$\rho_{bcp}\times10^{-2}$	$G_b\times10^{-2}$	$V_b\times10^{-2}$	$H_b\times10^{-3}$	$\nabla_{2\rho}\times10^{-1}$
1	O-H ··O	1.60	0.6071	0.4893	-0.6775	-0.1881	0.1204
2	O-H ··C	2.51	0.1029	0.7387	-0.5808	0.1579	0.3586
3	C-H ··O	2.18	0.1478	0.1262	-0.9814	0.2812	0.6175



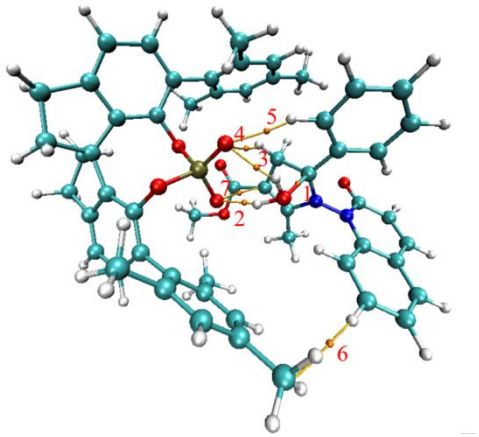
TS2-*Rr*

Entry	Type of interaction	Distance	$\rho_{bcp}\times10^{-2}$	$G_b\times10^{-2}$	$V_b\times10^{-2}$	$H_b\times10^{-3}$	$\nabla_{2\rho}\times10^{-1}$
1	O-H ··O	1.58	0.5910	0.5103	-0.6734	-0.163	0.1389
2	O-H ··O	1.91	0.2552	0.2481	-0.2264	0.2171	0.1079



TS2-*Ss*

Entry	Type of interaction	Distance	$\rho_{bcp}\times10^{-2}$	$G_b\times10^{-2}$	$V_b\times10^{-2}$	$H_b\times10^{-3}$	$\nabla_{2\rho}\times10^{-1}$
1	TS	2.13	0.5305	0.3609	-0.4471	-0.8613	0.1099
2	O-H ··O	1.67	0.4902	0.4234	-0.5255	-0.1021	0.1285
3	O-H ··O	1.93	0.2424	0.234	-0.2096	0.2437	0.1033
4	C-H ··O	2.28	0.2705	0.4043	-0.3067	-0.2662	-0.9034
5	C-H ··O	2.22	0.1376	0.1111	-0.8459	0.266	0.5511
6	C-H ··O	2.49	0.8302	0.6319	-0.4755	0.1564	0.3153
7	C ··O	2.71	0.1407	0.1237	-0.1039	0.1982	0.5743



TS2-*Rs*

Entry	Type of interaction	Distance	$\rho_{bcp}\times10^{-2}$	$G_b\times10^{-2}$	$V_b\times10^{-2}$	$H_b\times10^{-3}$	$\nabla_{2\rho}\times10^{-1}$
1	TS	1.91	0.8628	0.5238	-0.8238	-0.3000	0.8951
2	O-H ··O	1.54	0.6956	0.5501	-0.7967	-0.2466	0.1213
3	O-H ··O	1.97	0.2551	0.233	-0.2159	0.1719	0.1001
4	C-H ··O	2.55	0.9835	0.6966	-0.5565	0.1400	0.3346
5	C-H ··O	2.33	0.1186	0.9199	-0.7142	0.2057	0.4502
6	C-H ··C	2.84	0.5676	0.3827	-0.2962	0.8656	0.1877
7	C ··O	2.84	0.1362	0.1165	-0.9945	0.1706	0.5343

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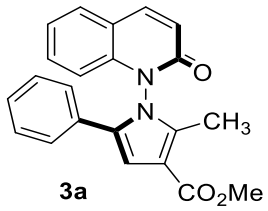
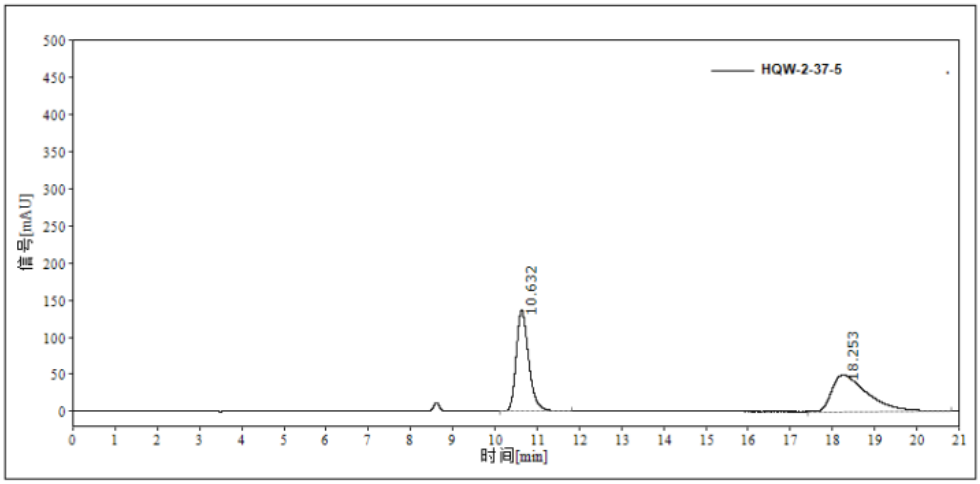
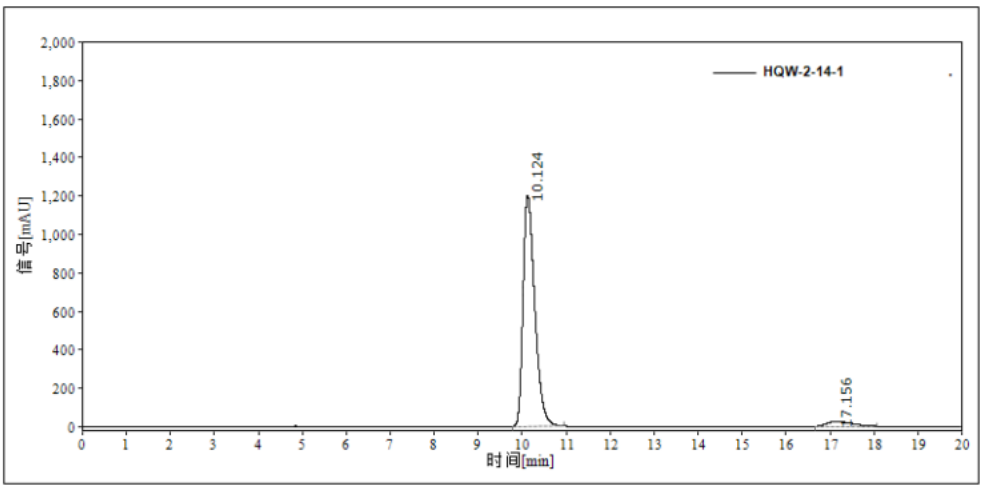
(9) HPLC Resolution Data



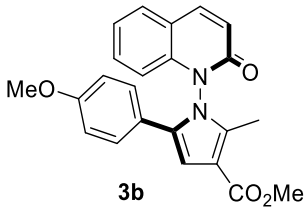
3a



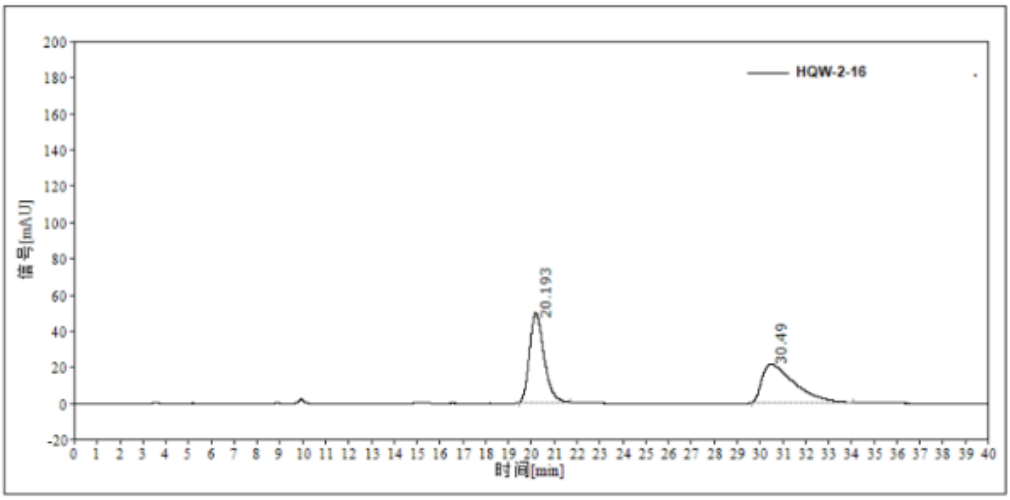
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.632	136.349	73.5	2832.712	49.8	n.a.
2	18.253	49.096	26.5	2858.217	50.2	n.a.
Total:		185.445	100.0	5690.929	100	



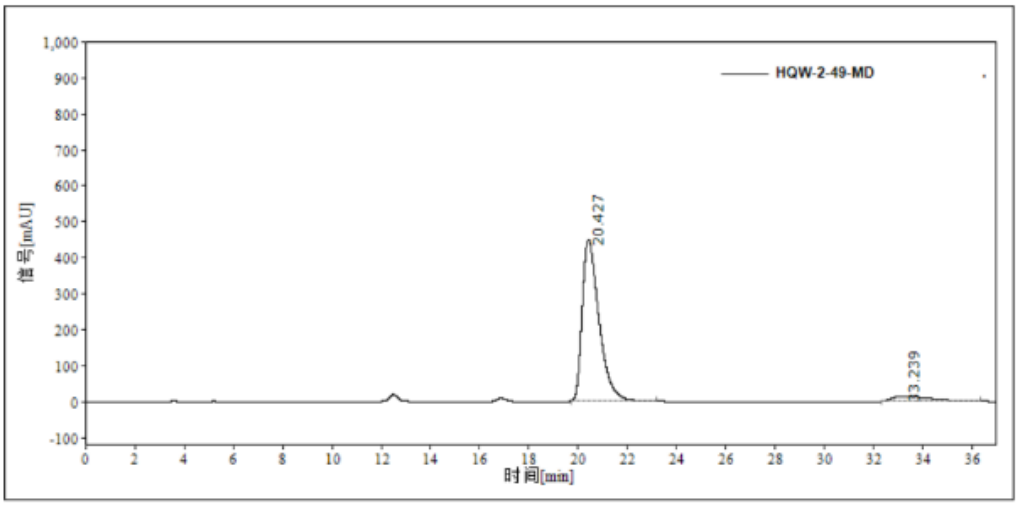
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.124	1201.289	97.9	22294.086	95.5	n.a.
2	17.156	25.734	2.1	1047.744	4.5	n.a.
Total:		1227.023	100	23341.830	100.0	



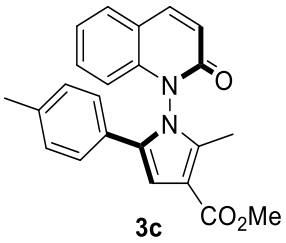
3b



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	20.193	49.293	69.9	2176.047	50.8	n.a.
2	30.490	21.264	30.1	2108.492	49.2	n.a.
Total:		70.557	100	4284.539	100.0	



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	20.427	449.015	96.9	21448.844	93.4	n.a.
2	33.239	14.237	3.1	1524.747	6.6	n.a.
Total:		463.252	100	22973.591	100.0	



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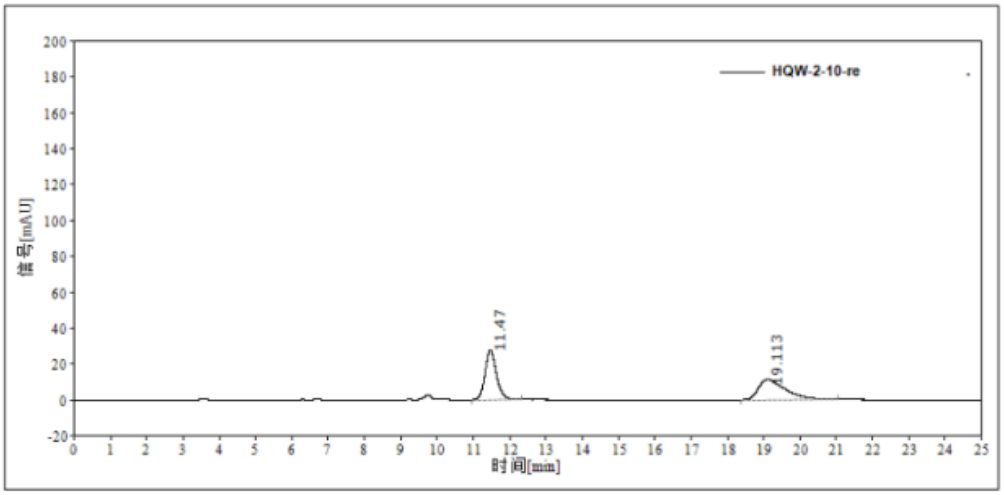
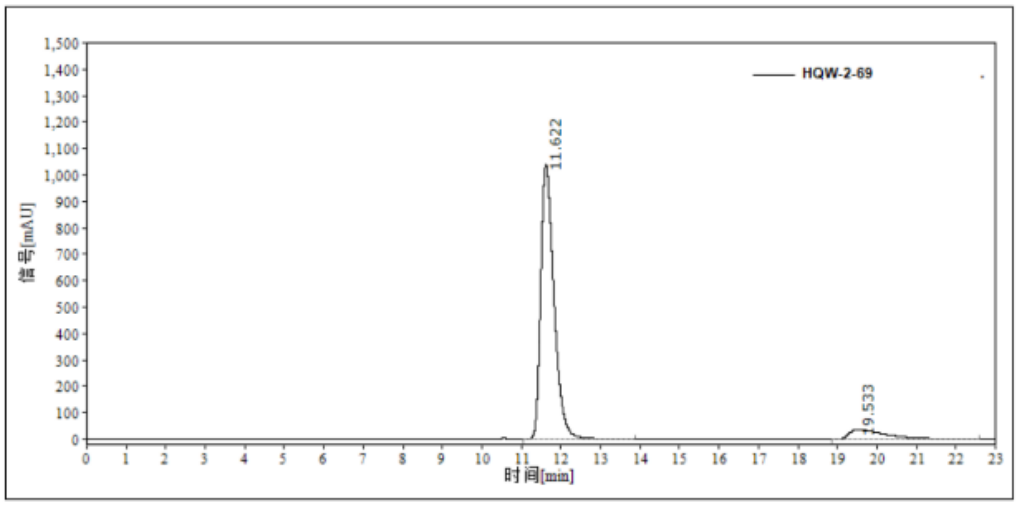
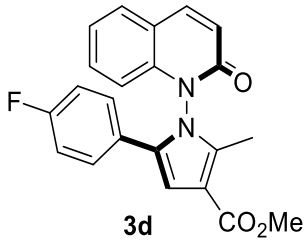


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.470	27.465	71.2	602.540	50.9	n.a.
2	19.113	11.113	28.8	581.549	49.1	n.a.
Total:		38.578	100	1184.089	100.0	

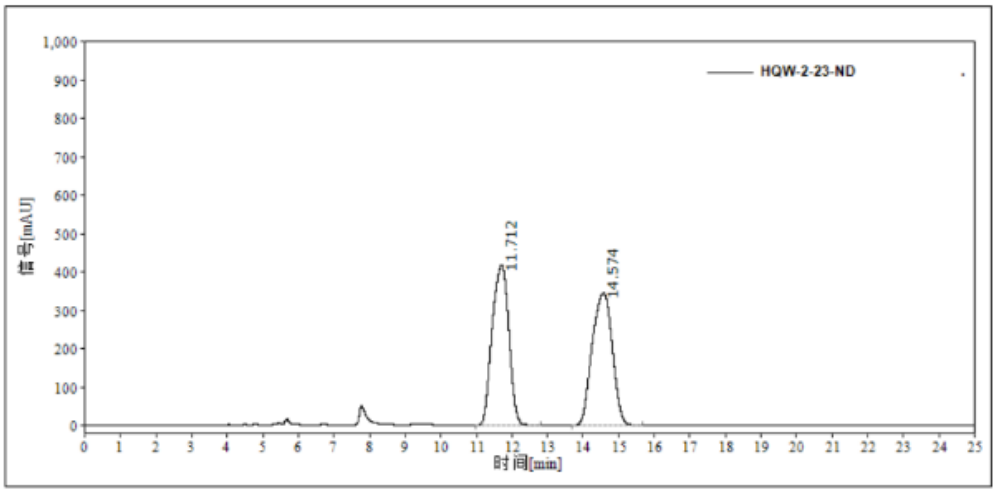


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.622	1039.543	96.6	24325.666	91.2	n.a.
2	19.533	36.445	3.4	2350.846	8.8	n.a.

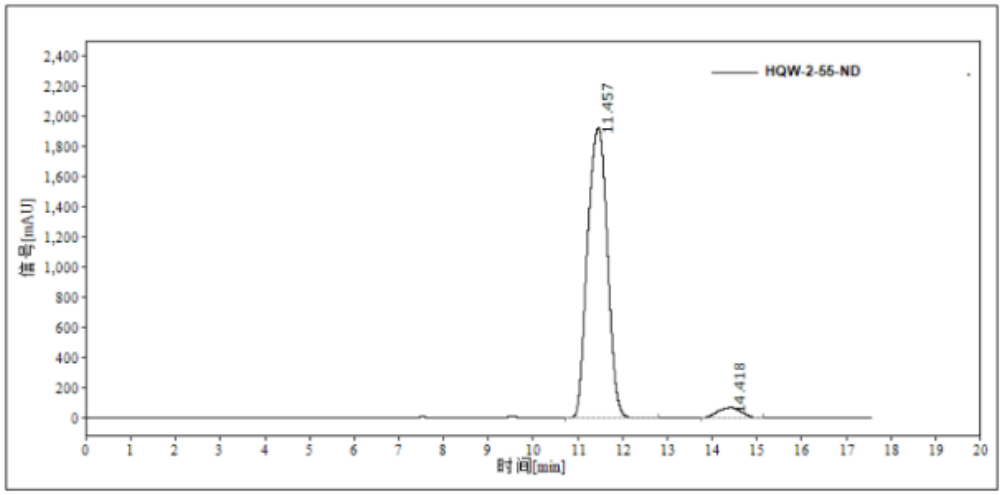
Total:		1075.988	100	26676.512	100.0	



3d

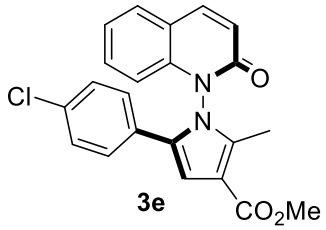


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.712	417.188	54.8	13600.258	50.0	n.a.
2	14.574	344.761	45.2	13588.861	50.0	n.a.
Total:		761.949	100	27189.119	100.0	



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.457	1925.644	96.6	59339.035	96.0	n.a.

2	14.418	66.938	3.4	2463.368	4.0	n.a.
Total:		1992.582	100	61802.403	100.0	



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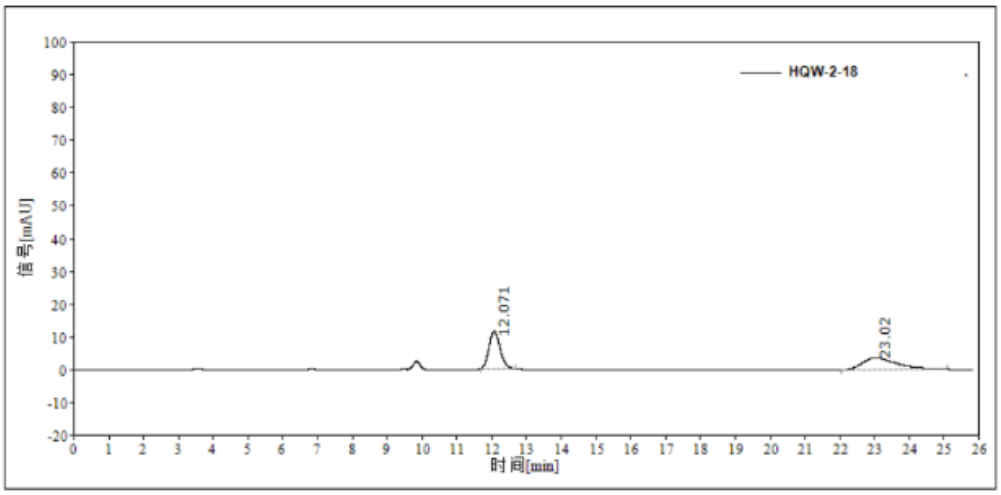
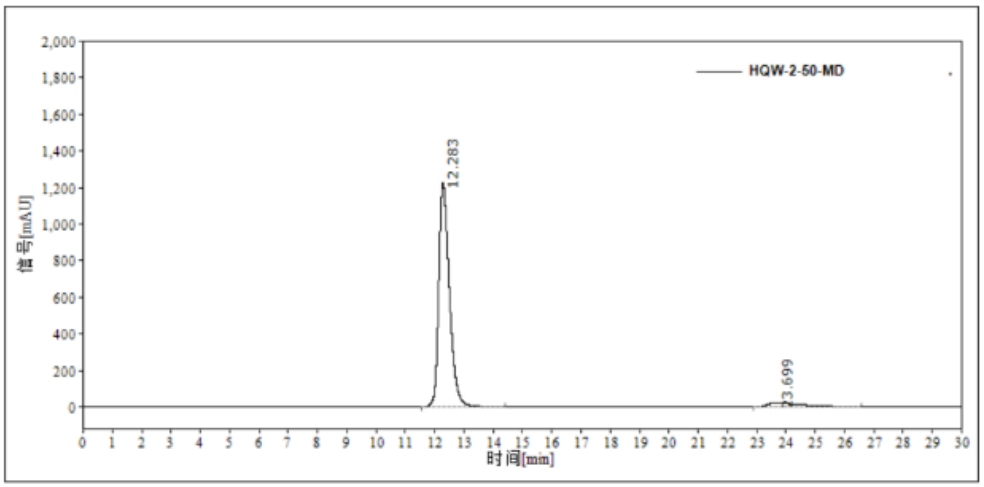
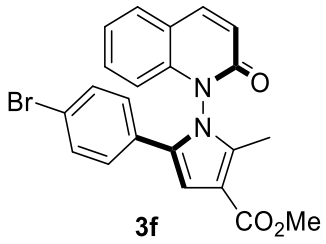


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.071	11.428	76.5	252.887	50.8	n.a.
2	23.020	3.517	23.5	245.125	49.2	n.a.
Total:		14.945	100	498.012	100.0	



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.283	1226.400	98.3	31009.774	94.4	n.a.

2	23.699	21.655	1.7	1822.181	5.6	n.a.
Total:		1248.055	100	32831.955	100.0	



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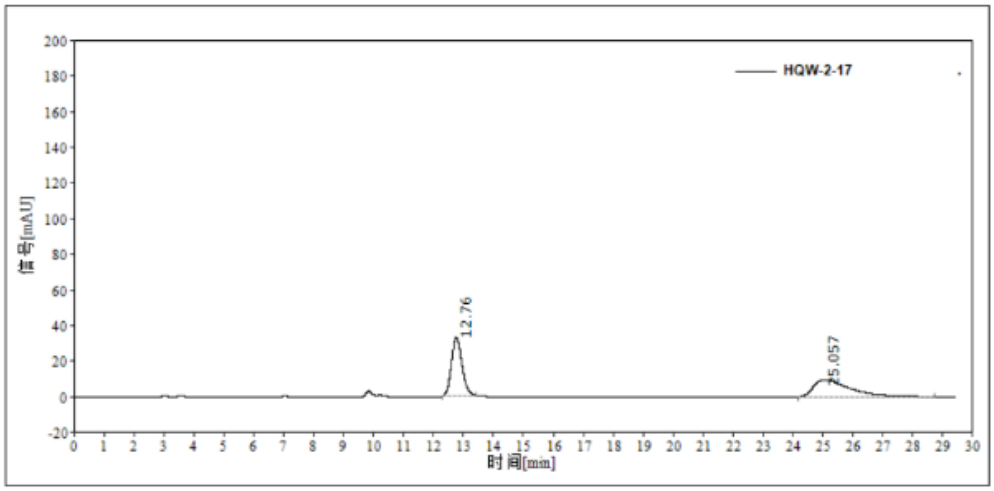
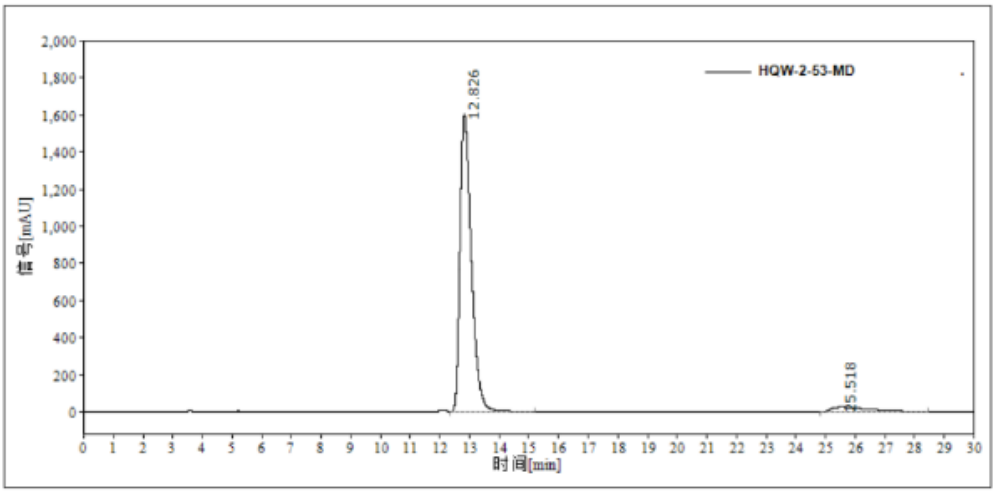
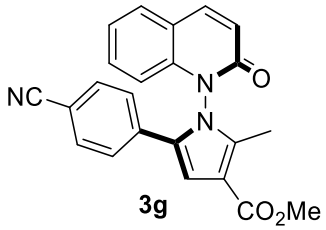


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.760	33.052	77.8	808.702	50.2	n.a.
2	25.057	9.410	22.2	801.436	49.8	n.a.
Total:		42.462	100	1610.138	100.0	



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

1	12.826	1605.033	98.4	42814.780	94.5	n.a.
2	25.518	26.723	1.6	2505.599	5.5	n.a.
Total:		1631.756	100	45320.379	100.0	



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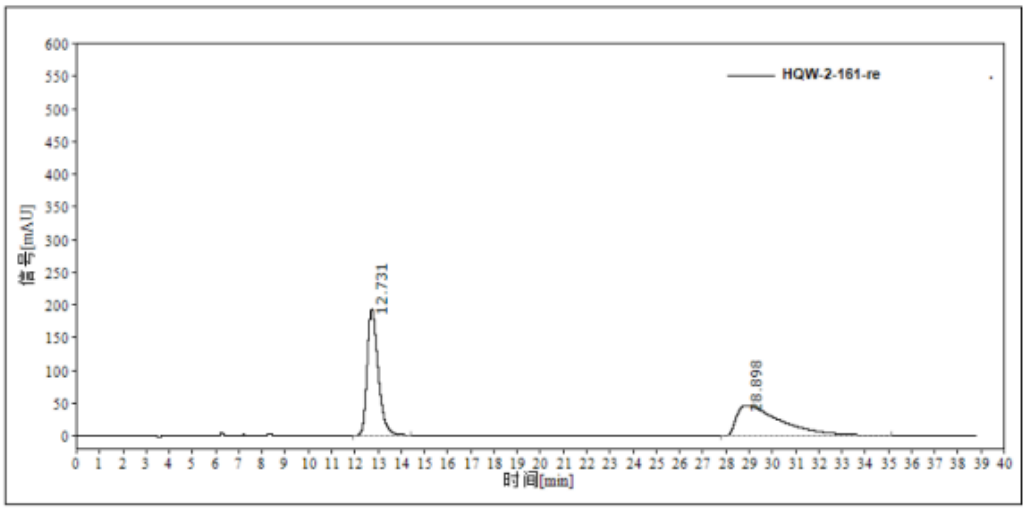
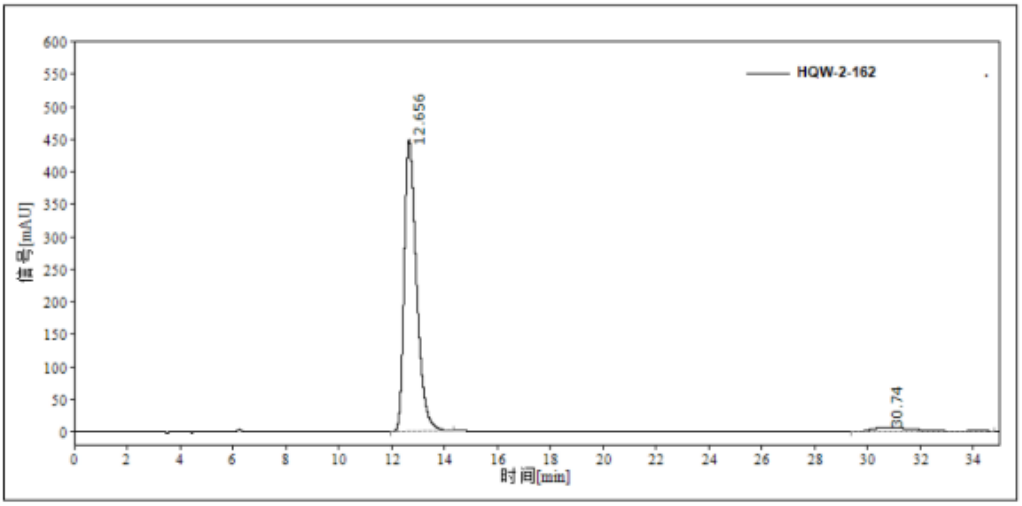
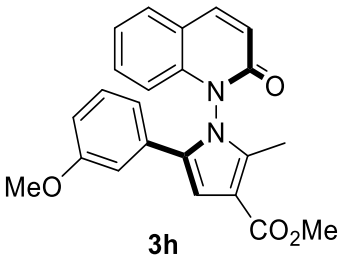


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.731	192.996	80.4	6392.628	50.4	n.a.
2	28.898	47.002	19.6	6288.735	49.6	n.a.
Total:		239.998	100	12681.363	100.0	

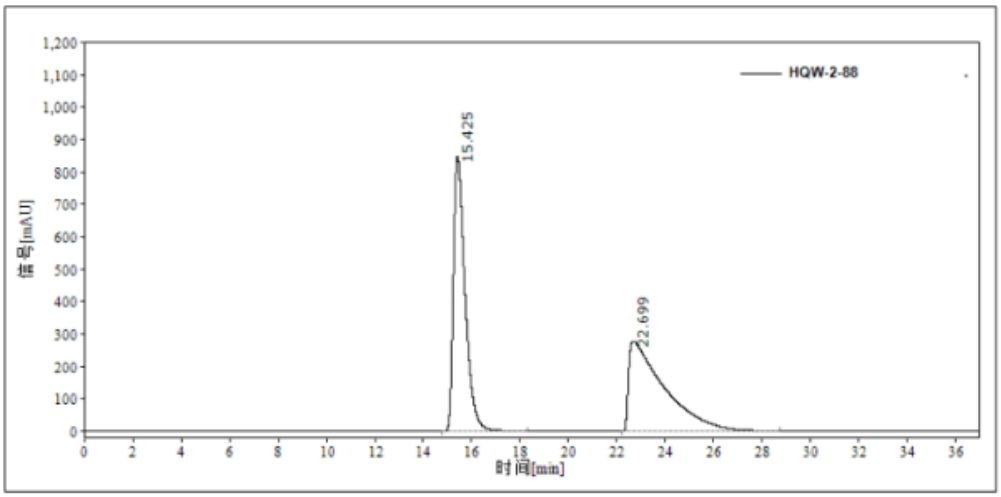


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

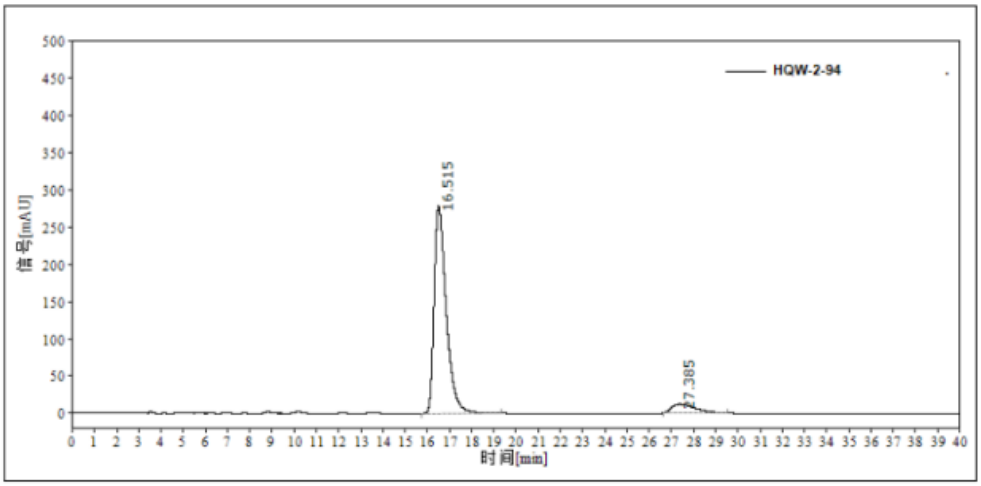
1	12.656	448.606	98.5	14612.750	94.8	n.a.
2	30.740	6.745	1.5	800.932	5.2	n.a.
Total:		455.351	100	15413.682	100.0	



3h

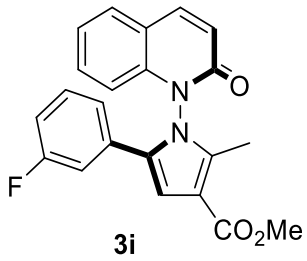


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	15.425	848.749	75.3	28484.700	50.0	n.a.
2	22.699	277.665	24.7	28473.799	50.0	n.a.
Total:		1126.414	100	56958.499	100.0	

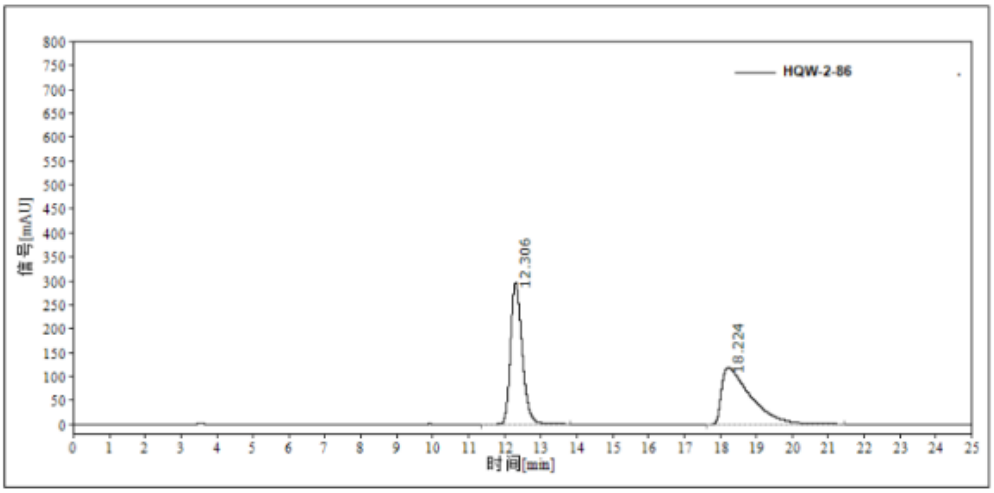


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

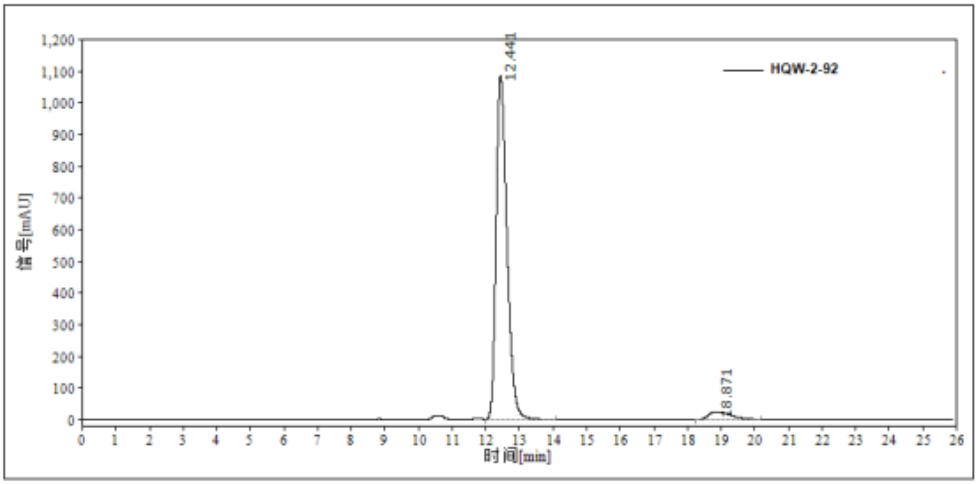
1	16.515	278.463	95.9	10601.021	92.1	n.a.
2	27.385	11.761	4.1	907.119	7.9	n.a.
Total:		290.224	100	11508.140	100.0	



3i

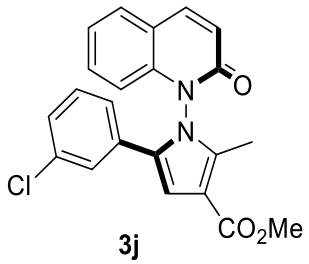


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.306	297.192	71.5	6682.103	50.1	n.a.
2	18.224	118.384	28.5	6653.987	49.9	n.a.
Total:		415.576	100	13336.090	100.0	



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

1	12.441	1085.337	97.7	24314.870	95.4	n.a.
2	18.871	25.772	2.3	1180.107	4.6	n.a.
Total:		11111.109	100	25494.977	100.0	



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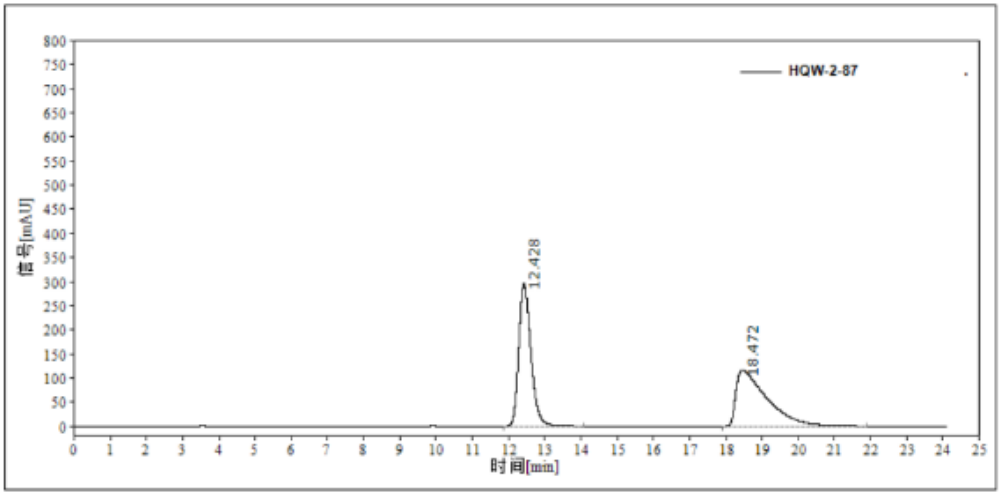
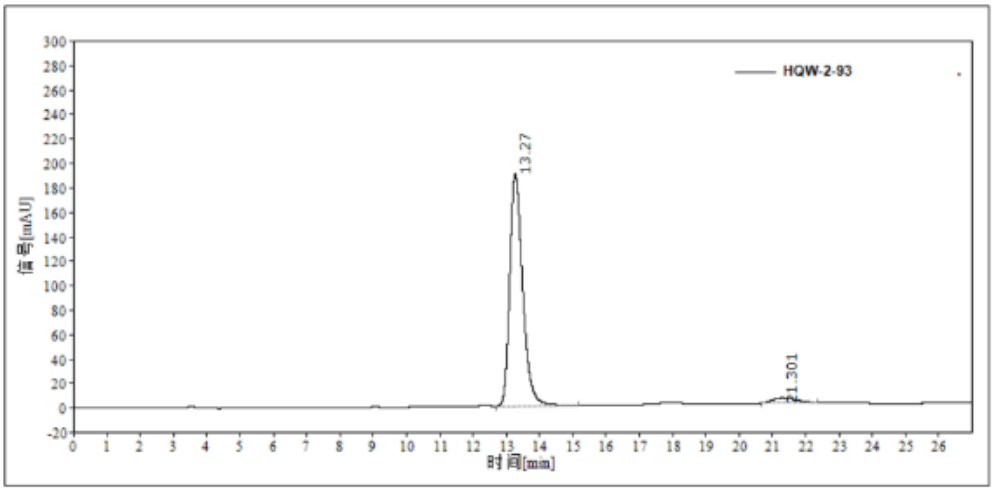
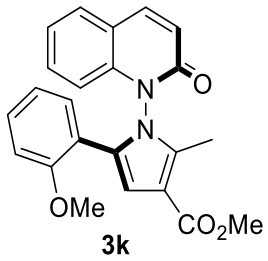


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.428	295.997	71.8	6905.642	50.0	n.a.
2	18.472	116.043	28.2	6894.641	50.0	n.a.
Total:		412.040	100	13800.283	100.0	

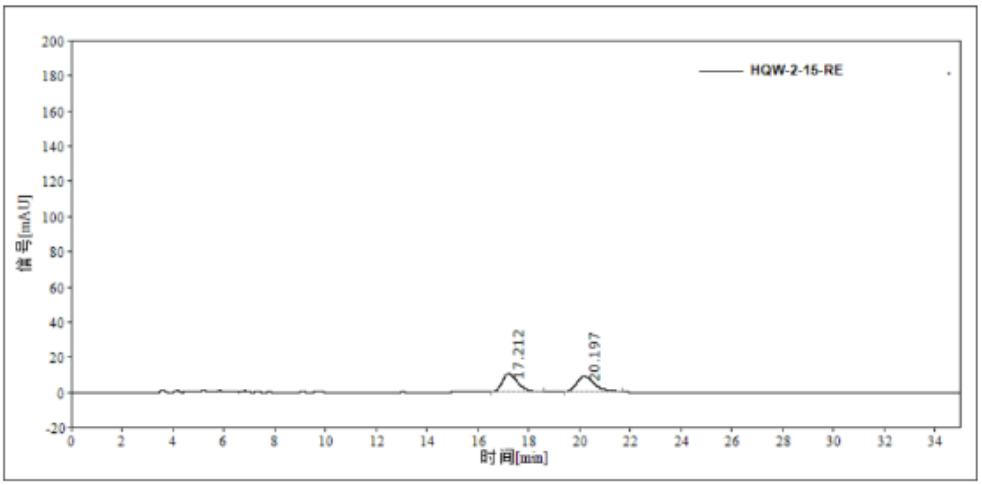


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

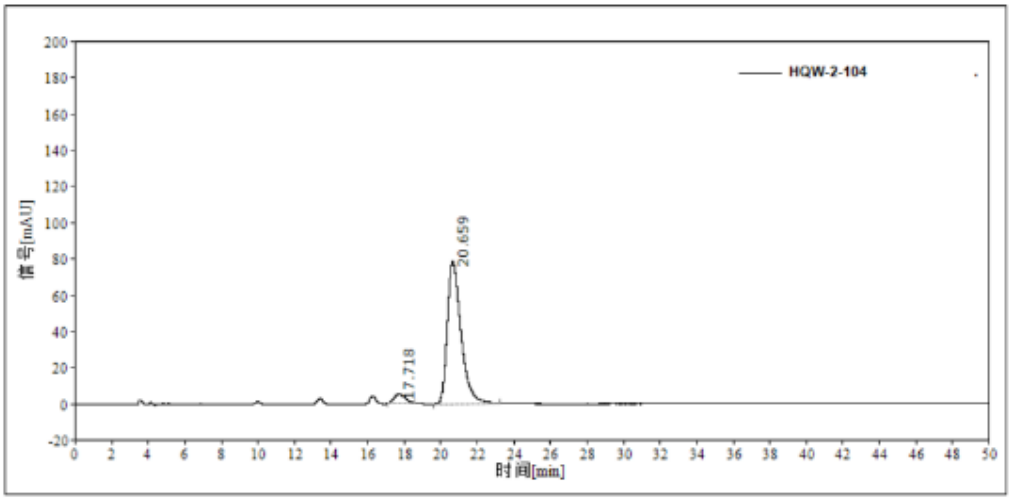
1	13.270	189.259	97.9	5117.954	96.1	n.a.
2	21.301	4.010	2.1	207.436	3.9	n.a.
Total:		193.269	100	5325.390	100.0	



3k

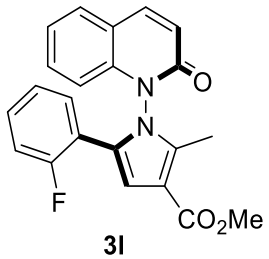


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	17.212	10.351	53.8	441.033	49.9	n.a.
2	20.197	8.904	46.2	442.452	50.1	n.a.
Total:		19.255	100	883.485	100.0	

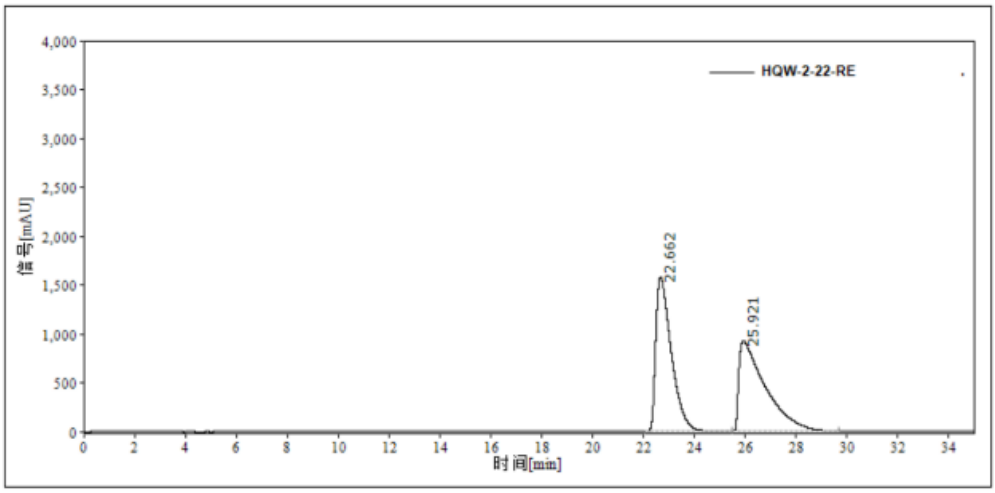


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

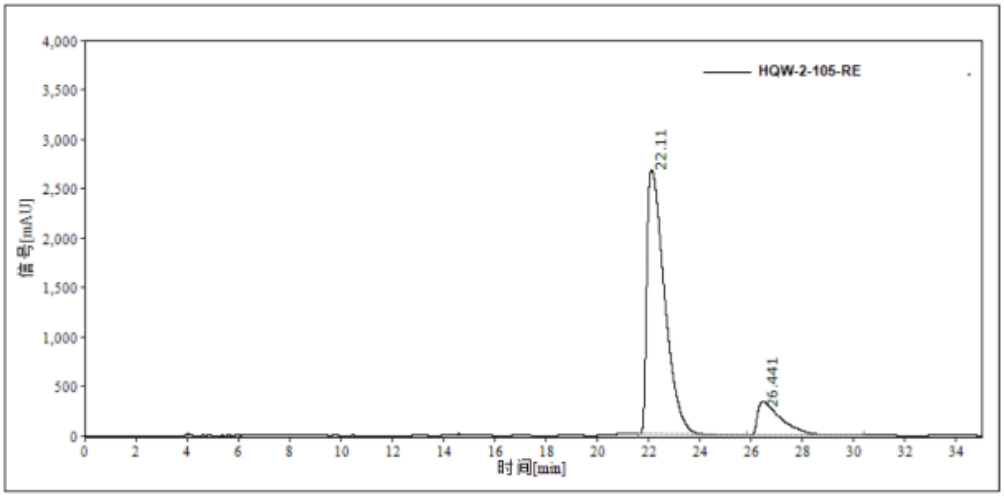
1	17.718	5111	6.1	214.327	5.0	n.a.
2	20.659	78.328	93.9	4078.902	95.0	n.a.
Total:		83.439	100	4293.229	100.0	



3l

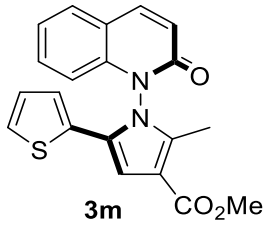


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	22.662	1586.410	63.2	67343.809	50.0	n.a.
2	25.921	925.281	36.8	67261.393	50.0	n.a.
Total:		2511.691	100	134605.202	100.0	

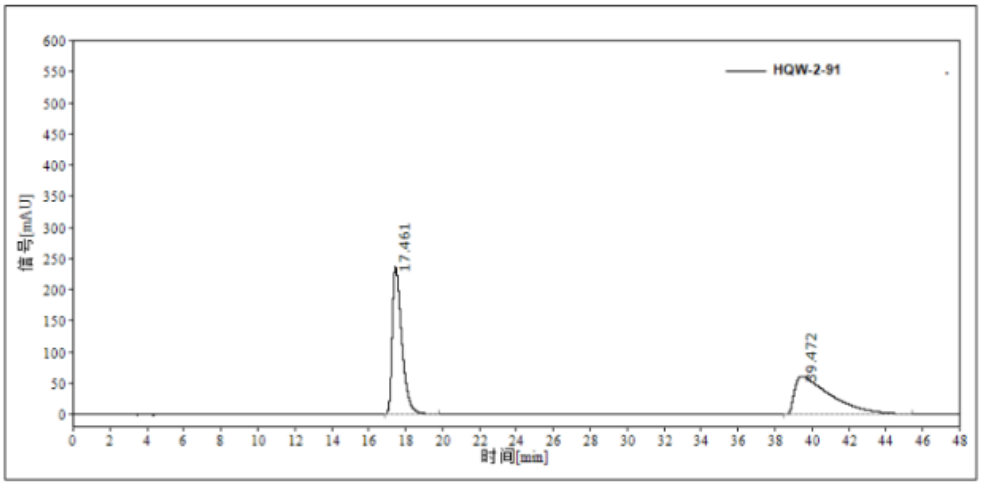


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

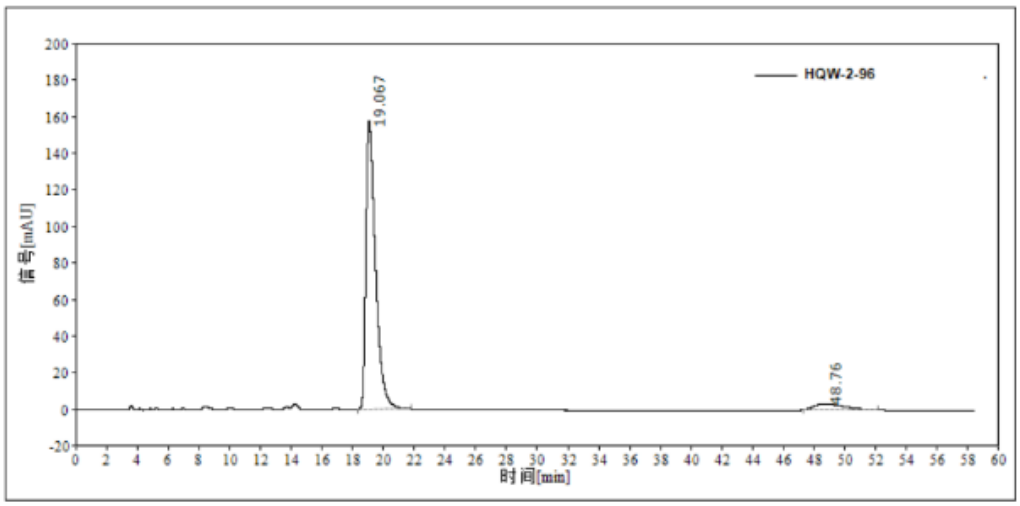
1	22.110	2679.687	88.7	129058.720	85.4	n.a.
2	26.441	341.326	11.3	22101.807	14.6	n.a.
Total:		3021.013	100	151160.527	100.0	



3m

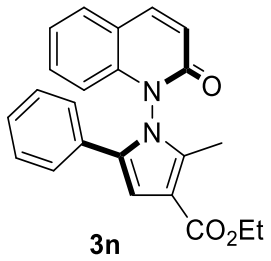


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	17.461	236.295	79.5	8546.690	50.5	n.a.
2	39.472	60.975	20.5	8365.900	49.5	n.a.
Total:		297.270	100	16912.590	100.0	



Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

1	19.067	157.896	98.0	6880.430	93.8	n.a.
2	48.760	3.283	2.0	451.268	6.2	n.a.
Total:		161.179	100	7331.698	100.0	



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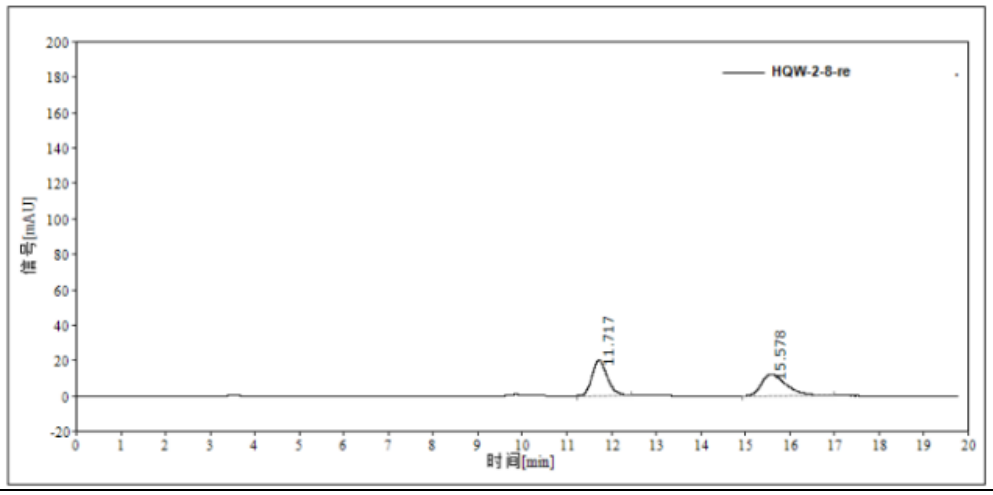
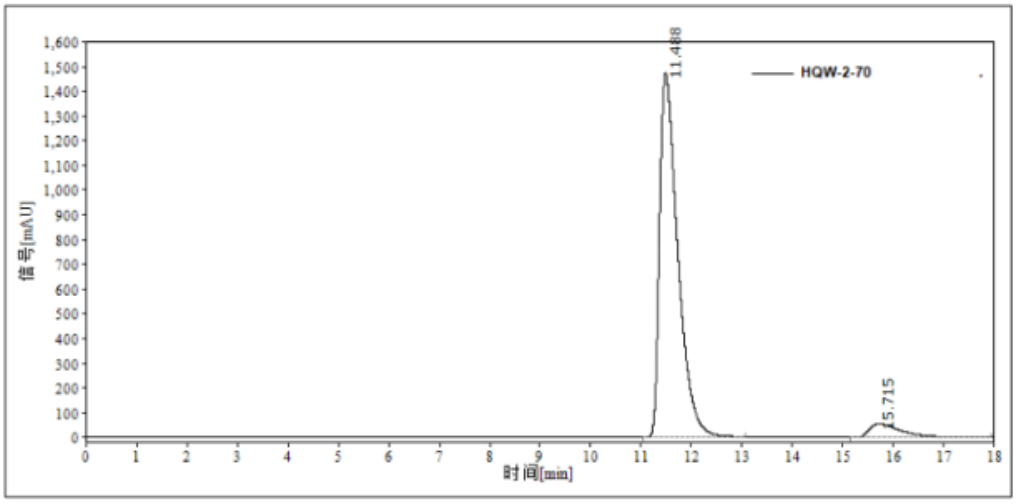
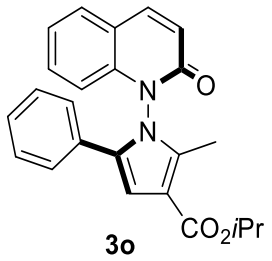


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.717	19.843	62.0	474.563	50.0	n.a.
2	15.578	12.165	38.0	473.768	50.0	n.a.
Total:		32.008	100	948.331	100.0	

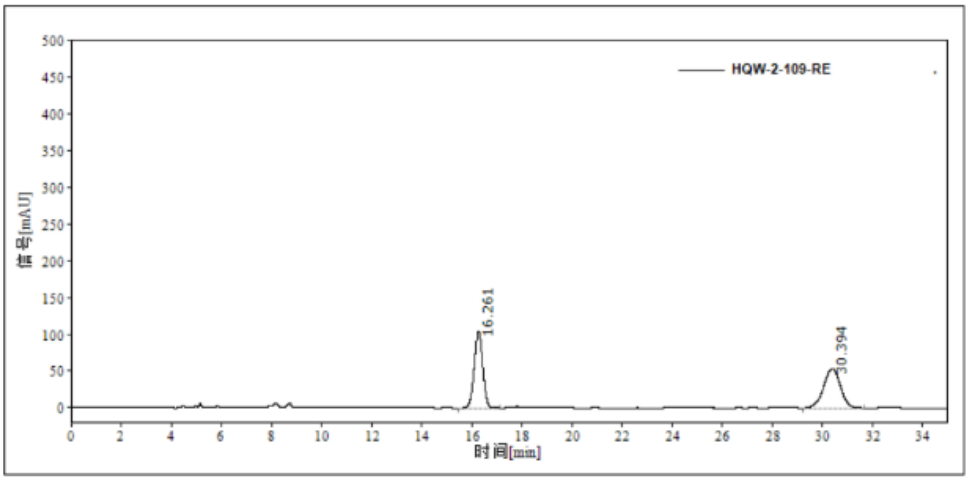


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

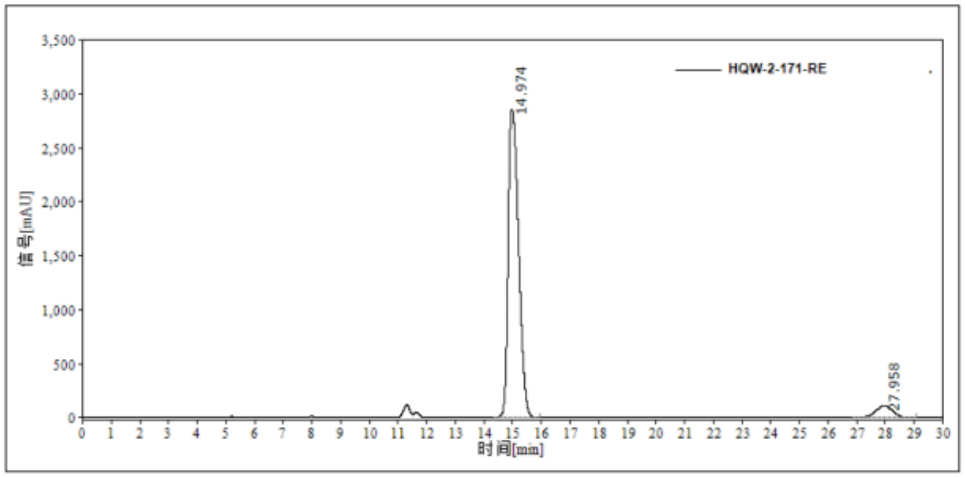
1	11.488	1473.234	96.4	36993.079	93.9	n.a.
2	15.715	54.867	3.6	2414.437	6.1	n.a.
Total:		1528.101	100	39407.516	100.0	



3o

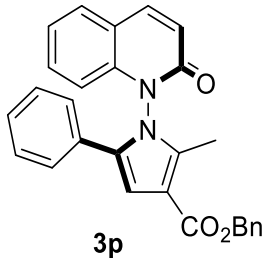


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	16.261	104.512	66.0	2483.586	49.7	n.a.
2	30.394	53.725	34.0	2513.712	50.3	n.a.
Total:		158.237	100	4997.298	100.0	

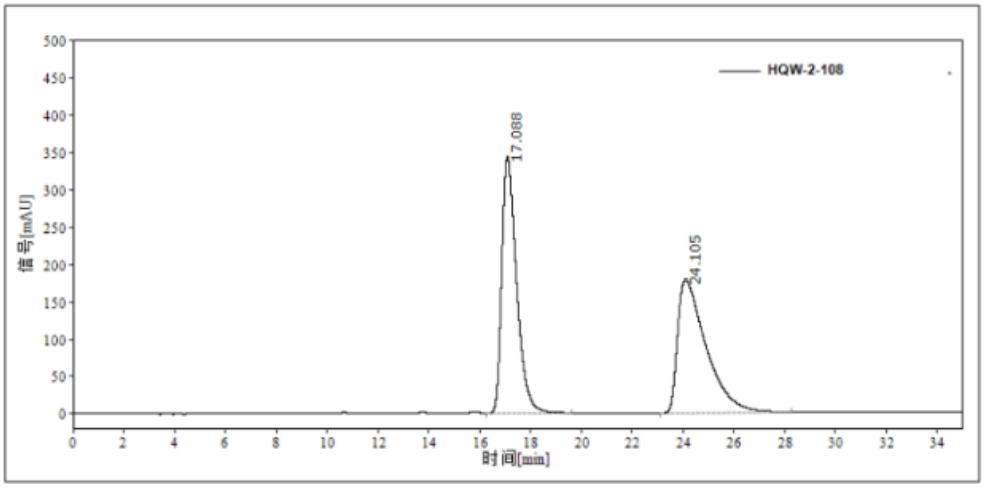


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	14.974	2856.815	96.3	72103.038	94.1	n.a.

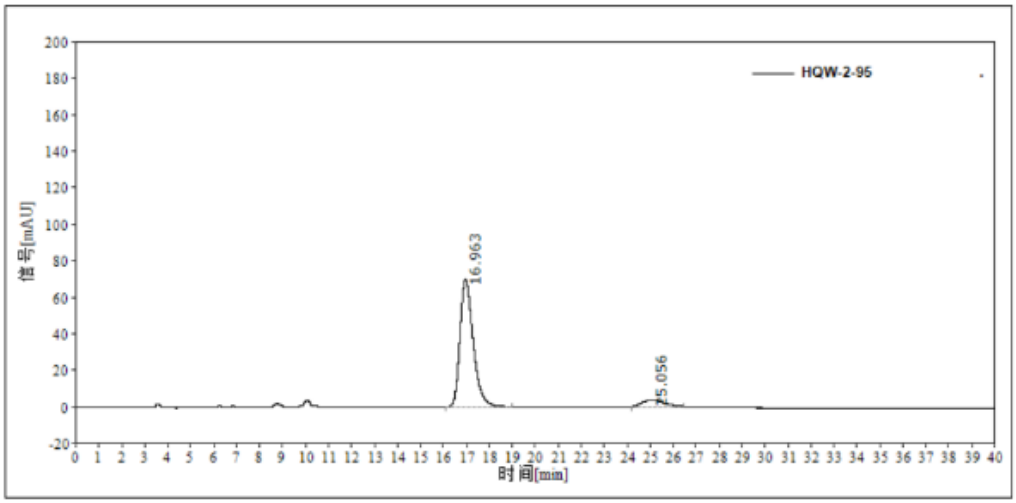
2	27.958	108.776	3.7	4516.421	5.9	n.a.
Total:		2965.591	100	76619.459	100.0	



3p

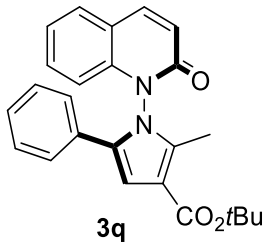


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	17.088	344.362	65.8	13927.176	50.1	n.a.
2	24.105	178.888	34.2	13898.869	49.9	n.a.
Total:		523.250	100	27826.045	100.0	

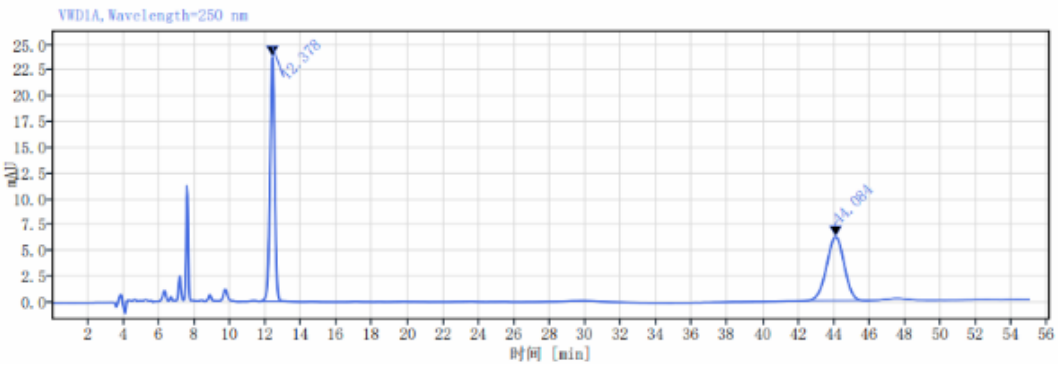


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.

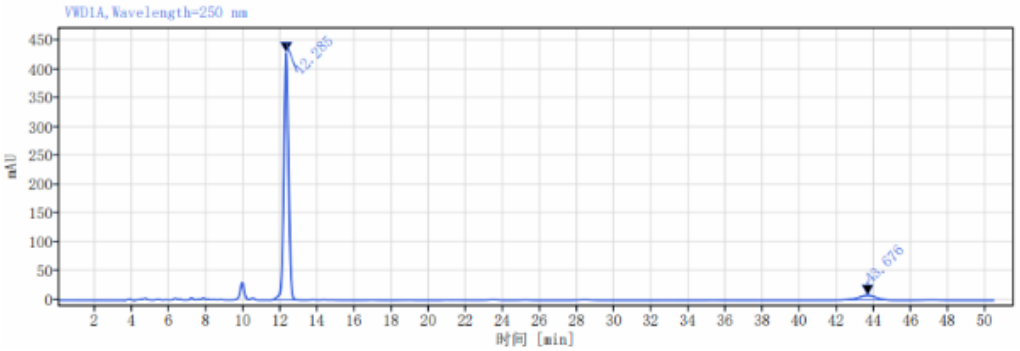
1	16.963	69.828	95.0	2813.132	92.0	n.a.
2	25.056	3.637	5.0	243.060	8.0	n.a.
Total:		73.465	100	3056.192	100.0	



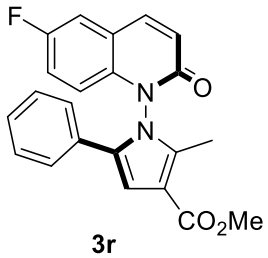
3q



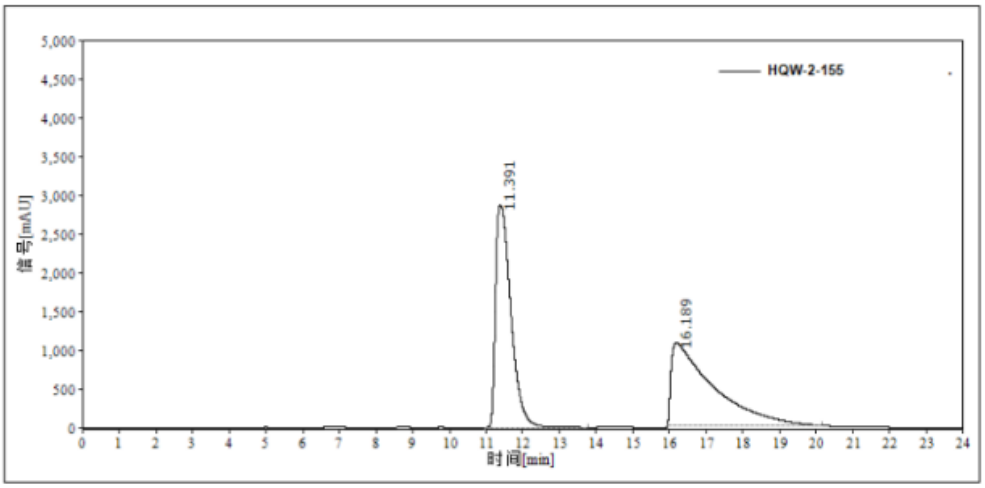
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.378	23.7621	427.5163	49.9685	n.a.
2	44.084	6.1996	428.0554	50.0315	n.a.
Total:			855.5717	100.0	



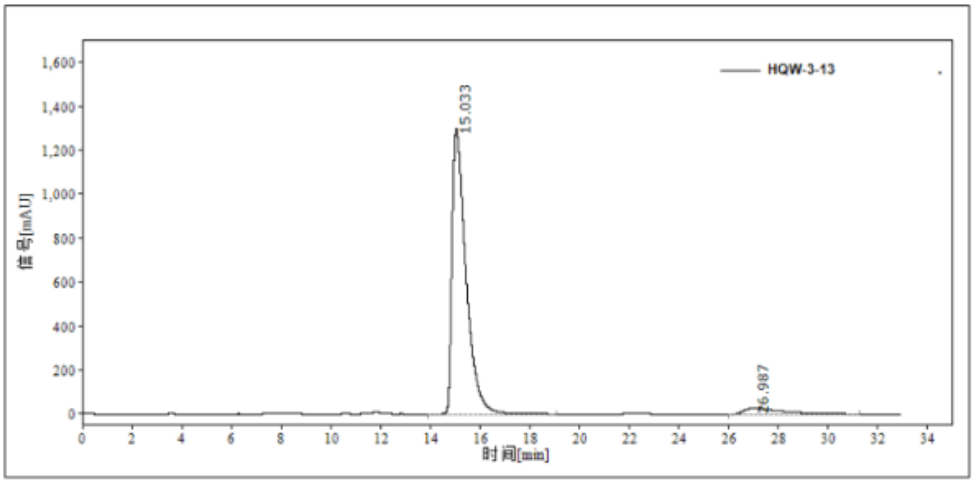
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.285	429.0025	7621.6976	93.2016	n.a.
2	43.676	8.1162	555.9513	6.7984	n.a.
Total:			8177.6489	100.0	



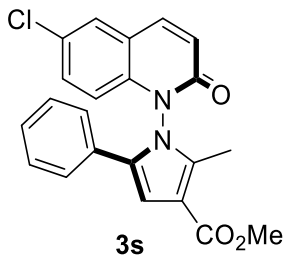
3r



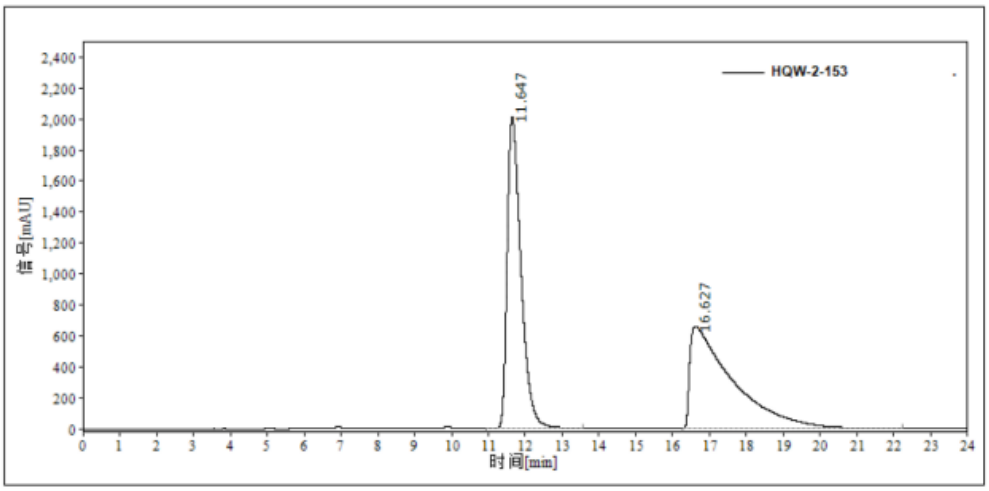
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.391	2872.453	72.9	83546.511	49.4	n.a.
2	16.189	1066.368	27.1	85535.165	50.6	n.a.
Total:		3938.821	100	169081.676	100.0	



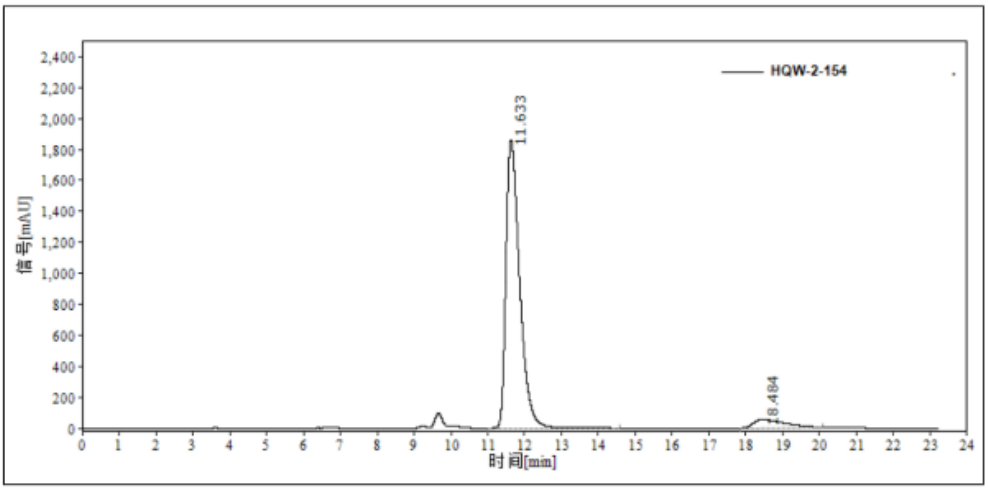
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	15.033	1298.979	98.0	50754.755	94.7	n.a.
2	26.987	25.900	2.0	2851.412	5.3	n.a.
Total:		1324.879	100	53606.167	100.0	



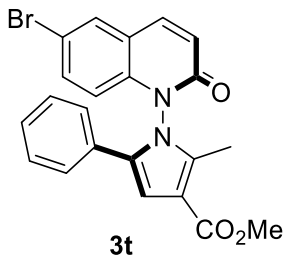
3s



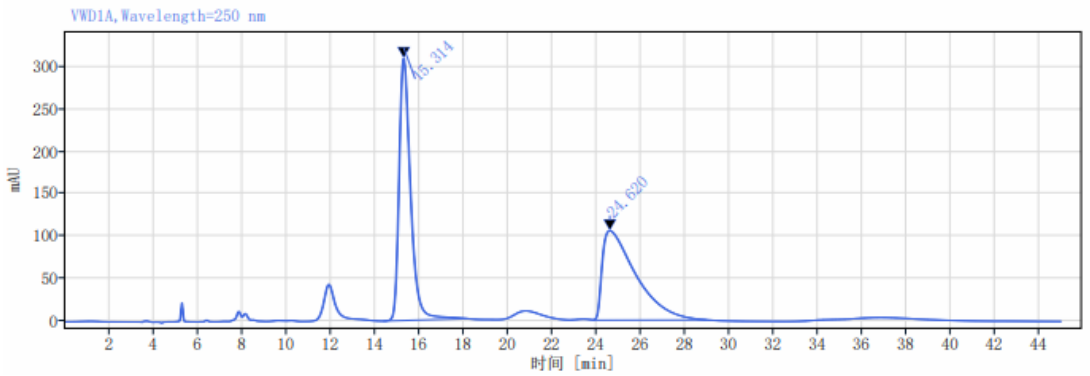
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.647	2009.881	75.3	52376.611	49.5	n.a.
2	16.627	658.206	24.7	53383.286	50.5	n.a.
Total:		2668.087	100	105759.897	100.0	



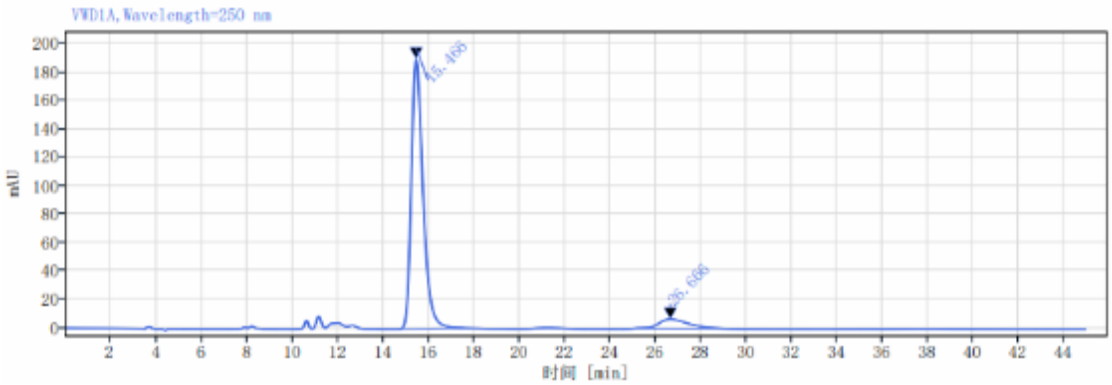
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.633	1866.528	97.2	48165.811	93.8	n.a.
2	18.484	54.353	2.8	3167.559	6.2	n.a.
Total:		1920.881	100	51333.370	100.0	



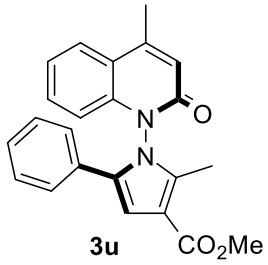
3t

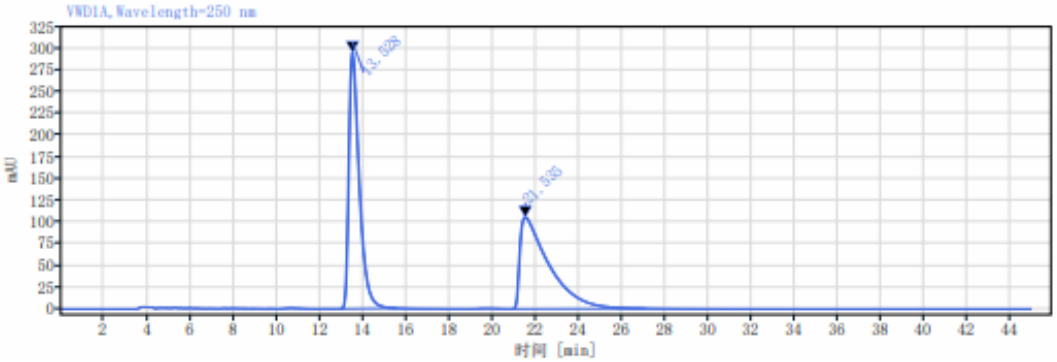


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	15.314	308.2540	11091.3310	49.9750	n.a.
2	24.620	105.1082	11102.4460	50.0250	n.a.
Total:			22193.7771	100.0	

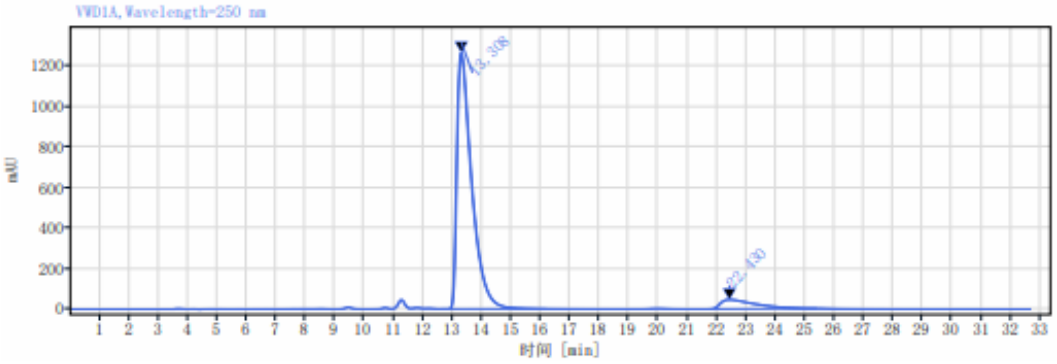


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	15.466	190.4433	6836.2637	92.0398	n.a.
2	26.666	6.5713	591.2485	7.9602j	n.a.
Total:			7427.5123	100.0	

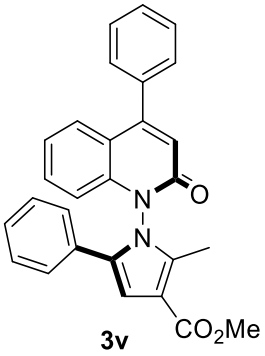




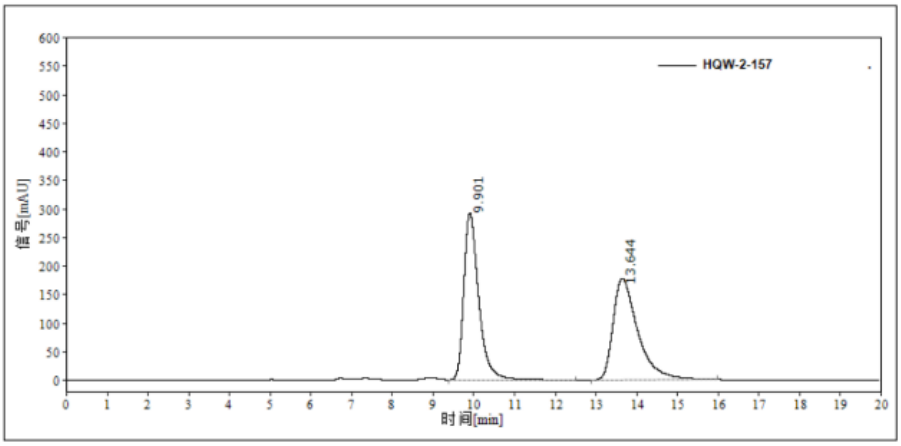
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	13.528	295.1258	9908.1450	50.1124	n.a.
2	21.535	105.6745	9863.6854	49.8878	n.a.
Total:			19771.8304	100.0	



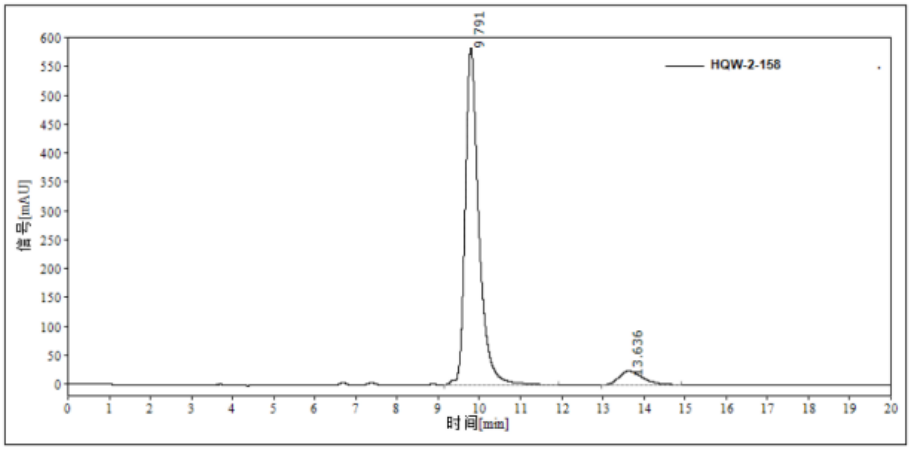
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	13.308	1266.4383	44296.0964	92.1585	n.a.
2	22.430	45.8941	3769.0477	7.8415	n.a.
Total:			8177.6489	100.0	



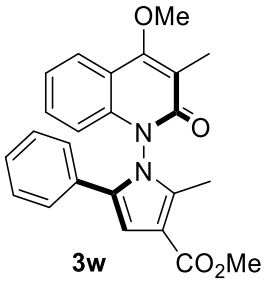
3v



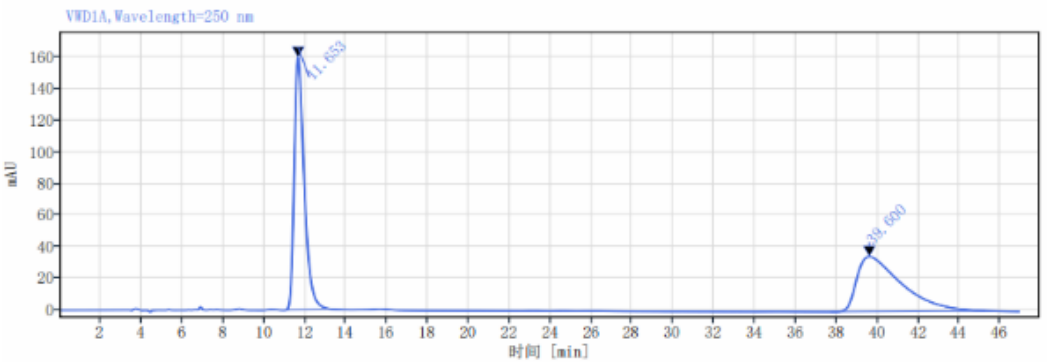
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	9.901	292.440	62.3	7442.900	49.8	n.a.
2	13.644	177.140	37.7	7505.731	50.2	n.a.
Total:		469.580	100	14948.631	100.0	



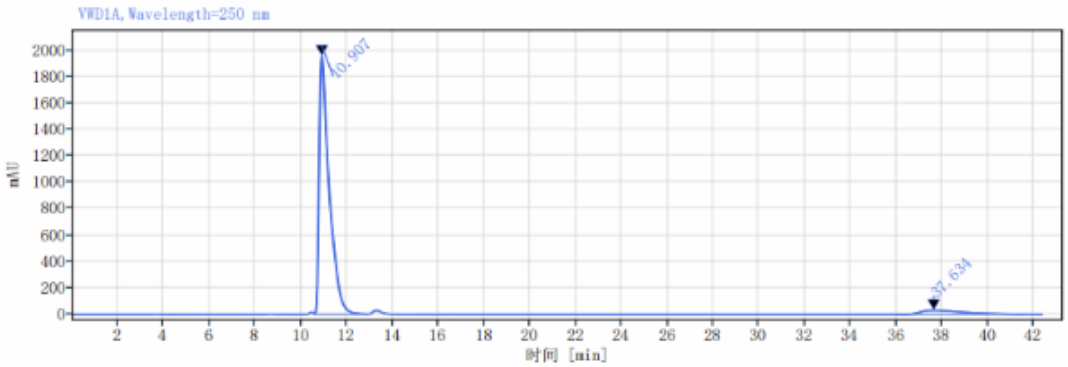
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	9.791	583.526	96.0	13444.933	93.2	n.a.
2	13.636	24.068	4.0	981.212	6.8	n.a.
Total:		607.594	100	14426.145	100.0	



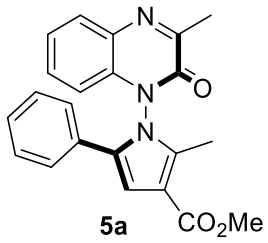
3w

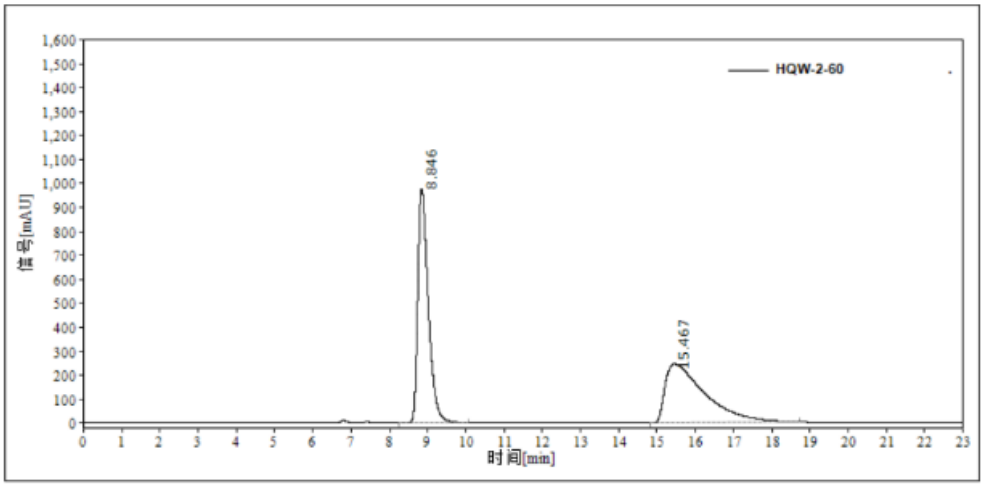


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.653	159.7510	5410.0696	50.7552	n.a.
2	39.600	34.7642	5249.0768	49.2448	n.a.
Total:		10659.1464		100.0	

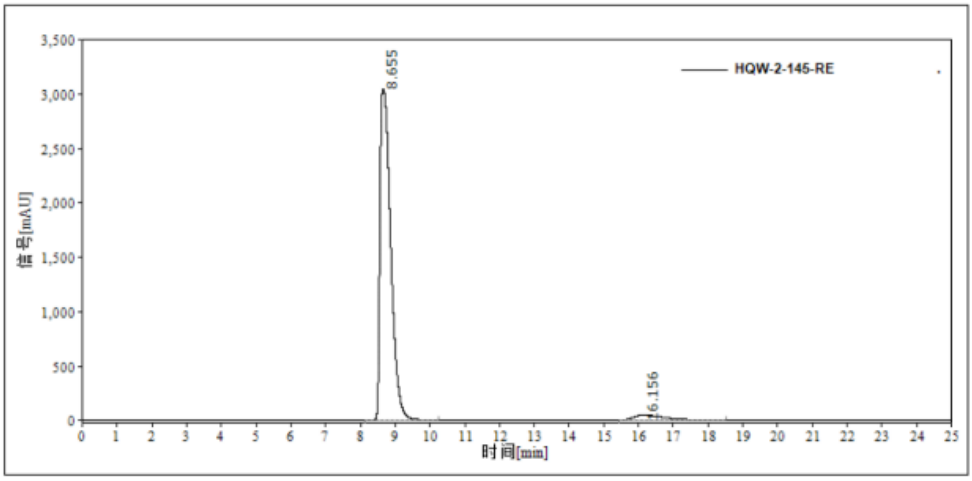


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.907	1956.6000	60201.6001	93.6625	n.a.
2	37.634	31.0814	4073.4583	6.3375	n.a.
Total:			64275.0581	100.0	

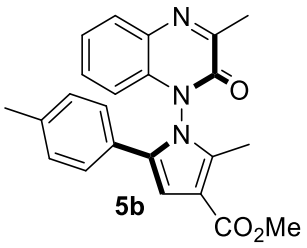


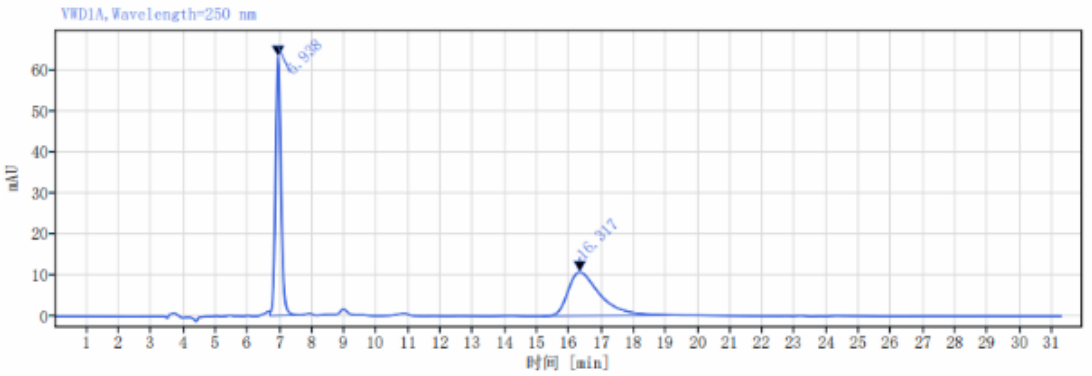


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	8.846	977.057	79.9	18653.071	50.9	n.a.
2	15.467	246.196	20.1	17967.676	49.1	n.a.
Total:		1223.253	100	36620.747	100.0	

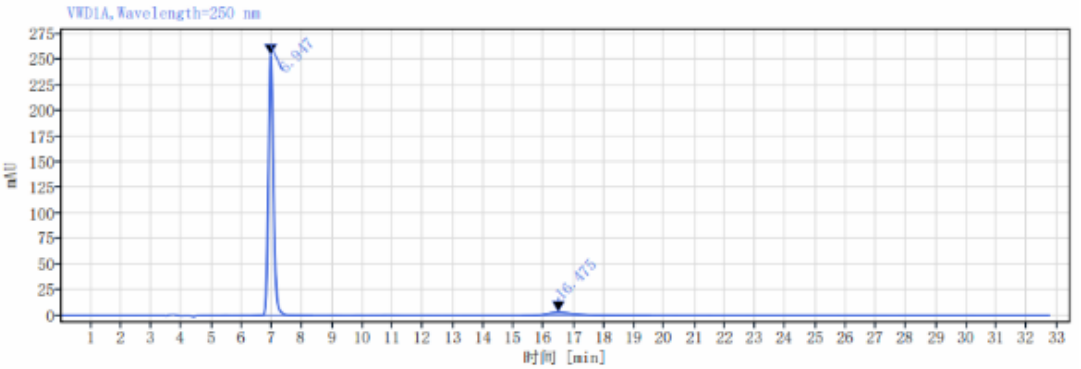


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	8.655	3048.798	98.4	65516.687	95.3	n.a.
2	16.156	49.670	1.6	3242.756	4.7	n.a.
Total:		3098.468	100	68759.443	100.0	

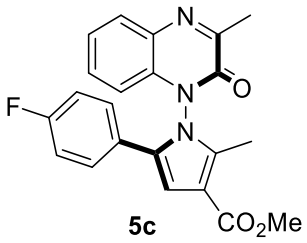




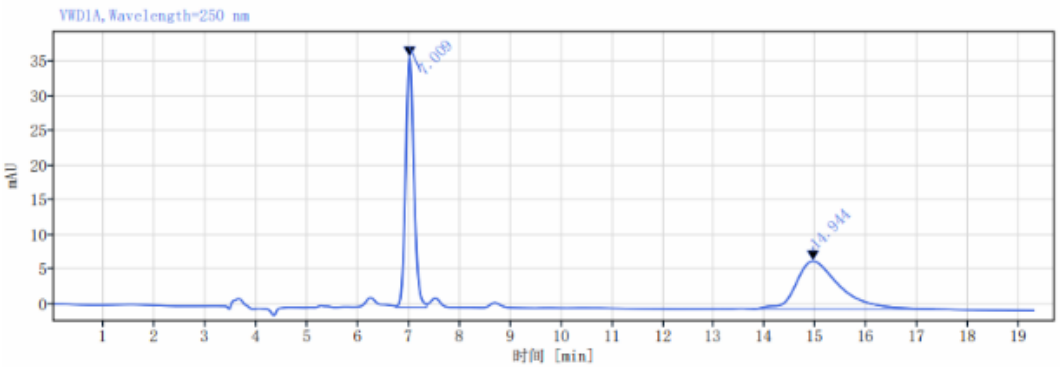
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.938	63.3407	746.7500	49.9631	n.a.
2	16.317	10.7054	747.8515	50.0369	n.a.
Total:			1494.6015	100.0	



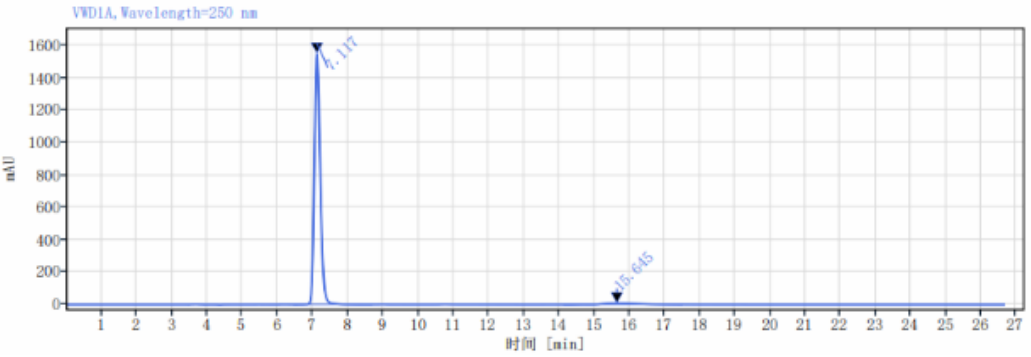
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.947	254.7298	2974.4030	93.0027	n.a.
2	16.475	3.0913	223.7874	6.9973	n.a.
Total:			3198.1904	100.0	



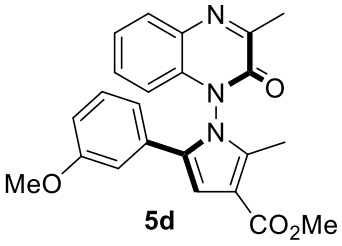
5c



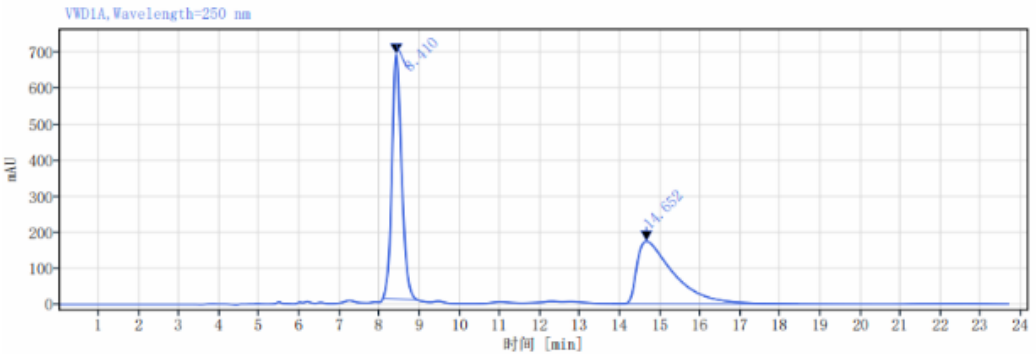
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.009	36.1059	409.5320	50.0420	n.a.
2	14.944	6.9037	408.8453	49.9580	n.a.
Total:			818.3772	100.0	



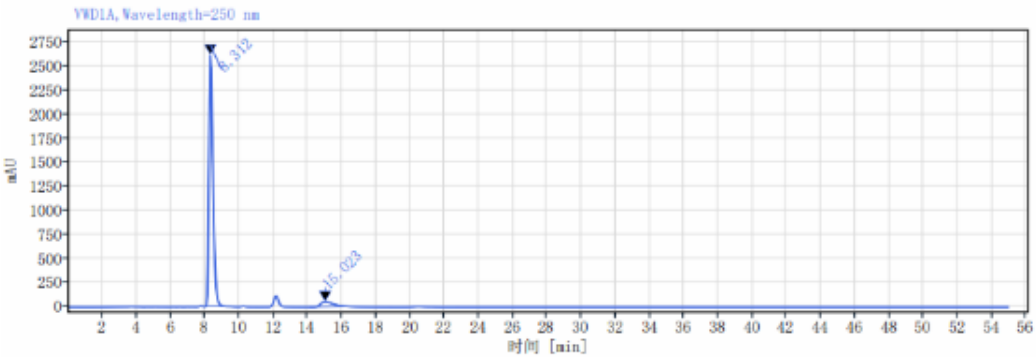
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.117	1552.4404	18094.8107	96.8600	n.a.
2	15.645	9.0979	586.5962	3.1400	n.a.
Total:			18681.4070	100.0	



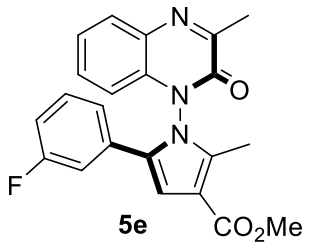
5d

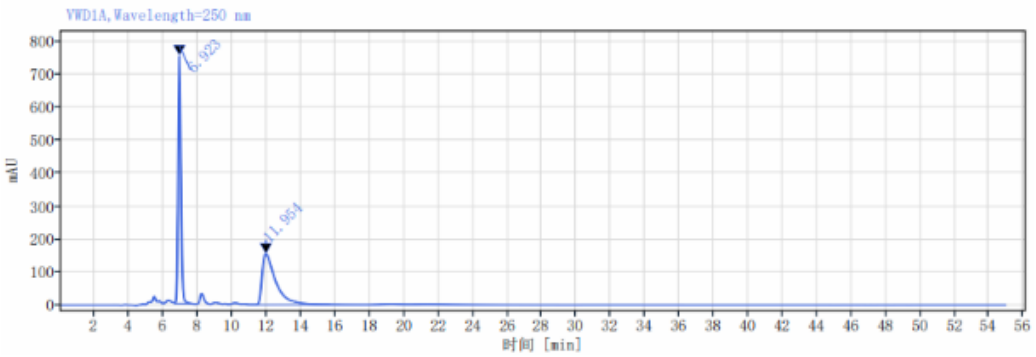


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	8.410	681.3107	11433.8246	50.9011	n.a.
2	14.652	173.7478	11029.0133	49.0989	n.a.
Total:			22462.8379	100.0	

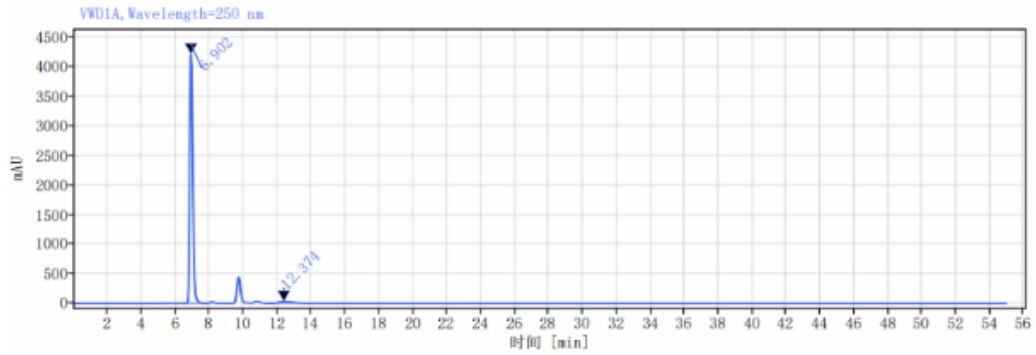


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	8.312	2616.3857	42794.0095	94.0126	n.a.
2	15.023	51.8281	2725.4348	5.9874	n.a.
Total:			45519.4443	100.0	

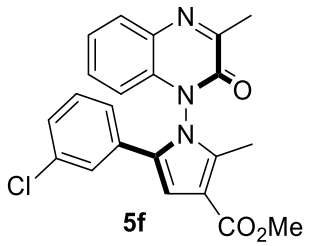


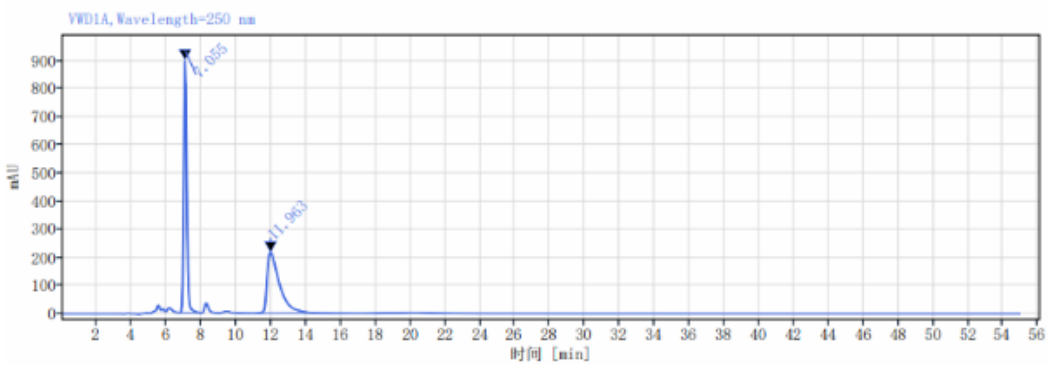


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.923	754.2580	8559.6870	50.3019	n.a.
2	11.954	154.4596	8456.9445	49.6981	n.a.
Total:			17016.6315	100.0	

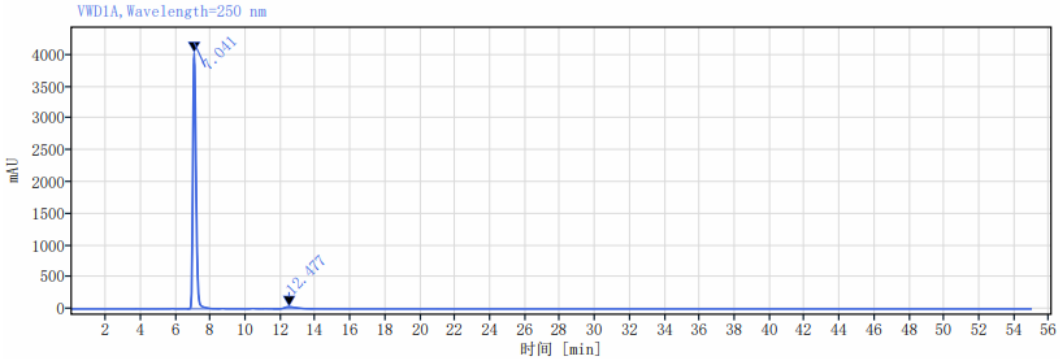


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.902	4223.8835	52666.5315	97.2154	n.a.
2	12.374	30.1210	1508.5644	2.7846	n.a.
Total:			54175.0959	100.0	

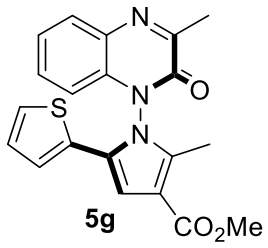




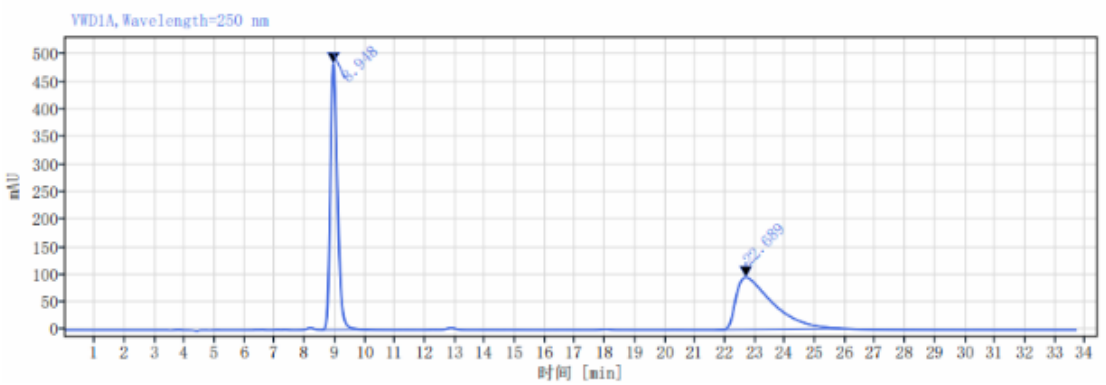
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.055	898.3779	10727.8356	49.9296	n.a.
2	11.963	216.7728	10758.0936	50.0704	n.a.
Total:			21485.9292	100.0	



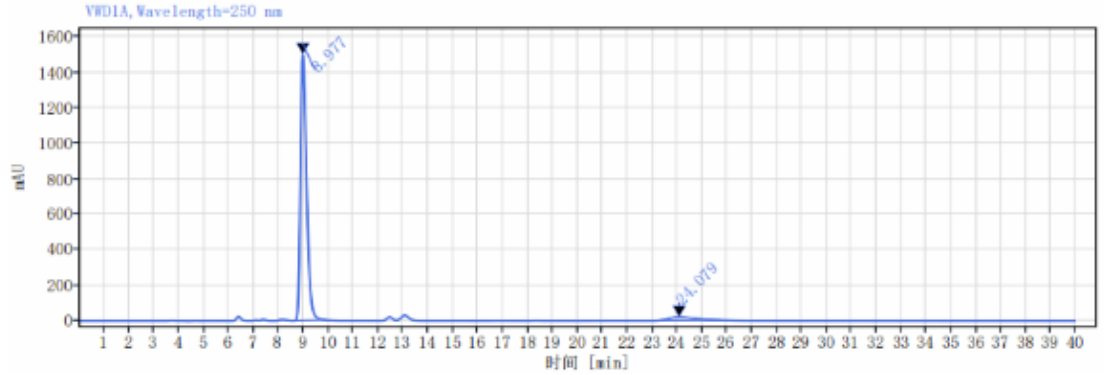
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.041	4039.0229	51083.4185	97.0692	n.a.
2	12.477	33.6634	1542.3607	2.9308	n.a.
Total:			52625.7792	100.0	



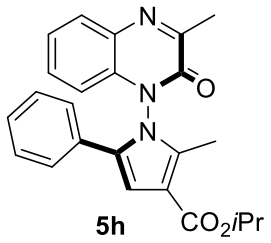
5g



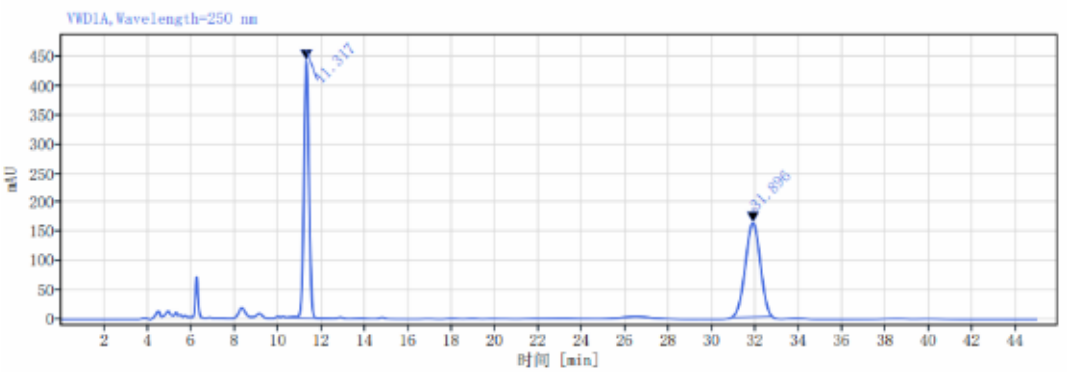
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	8.948	482.4462	7965.1127	49.9827	n.a.
2	22.689	94.3576	7970.6415	50.0173	n.a.
Total:			15935.7542	100.0	



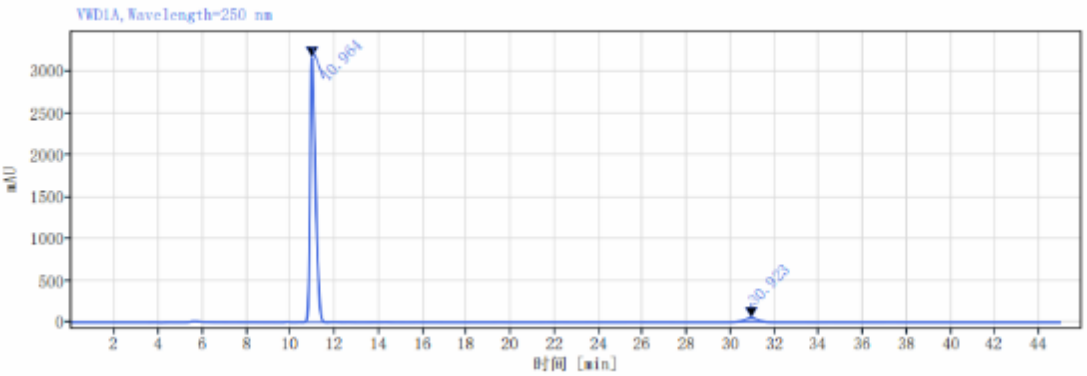
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	8.977	1499.9790	25478.5809	95.1783	n.a.
2	24.079	17.6977	1290.7278	4.8217	n.a.
Total:			26769.3086	100.0	



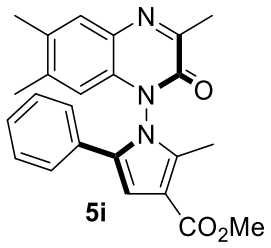
5h

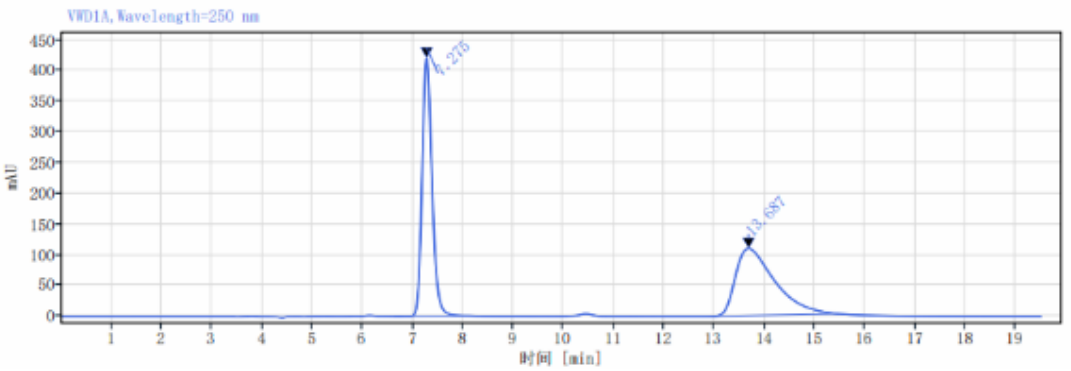


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.317	441.8860	7021.0275	47.5623	n.a.
2	31.896	161.6398	7740.7278	52.4377	n.a.
Total:			14761.7553	100.0	

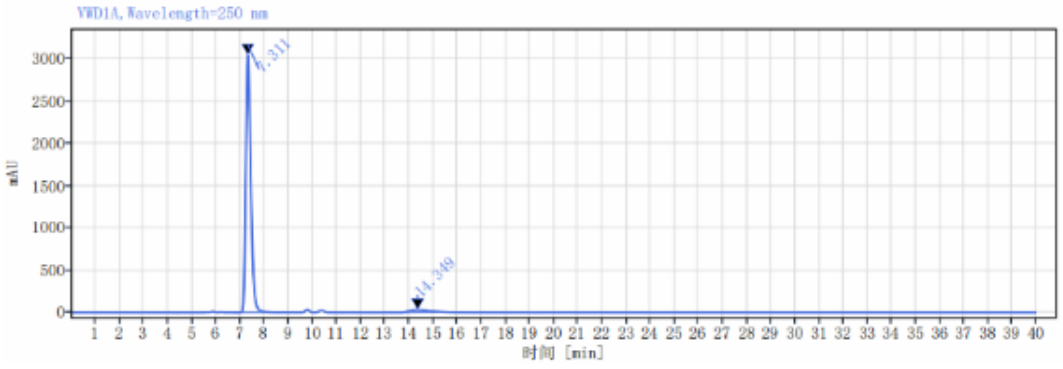


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.964	3169.4355	53028.4281	96.2500	n.a.
2	30.923	47.7779	2066.0272	3.7500	n.a.
Total:			55094.4553	100.0	

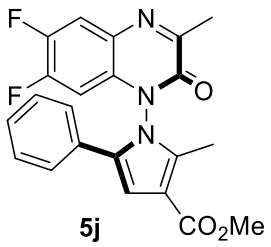




Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.275	419.8207	5768.3423	49.3694	n.a.
2	13.687	109.1021	5915.7048	50.6306	n.a.
Total:			11684.0472	100.0	



Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.311	3049.2228	44028.4355	96.5182	n.a.
2	14.349	30.5310	1588.3028	3.4818	n.a.
Total:			45616.7383	100.0	



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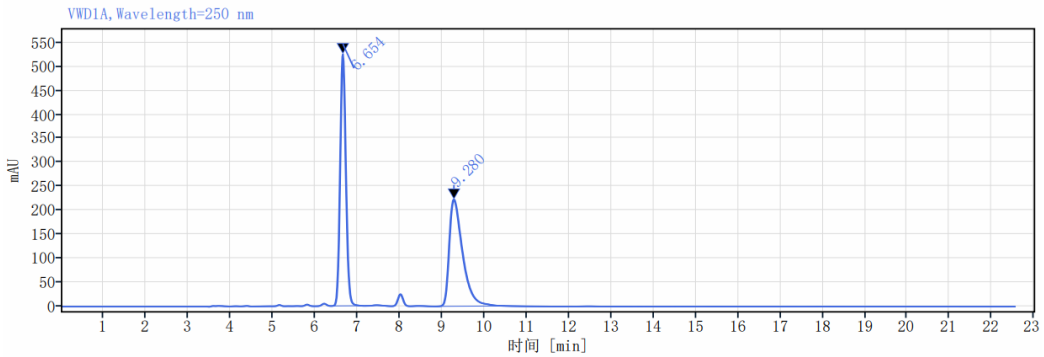
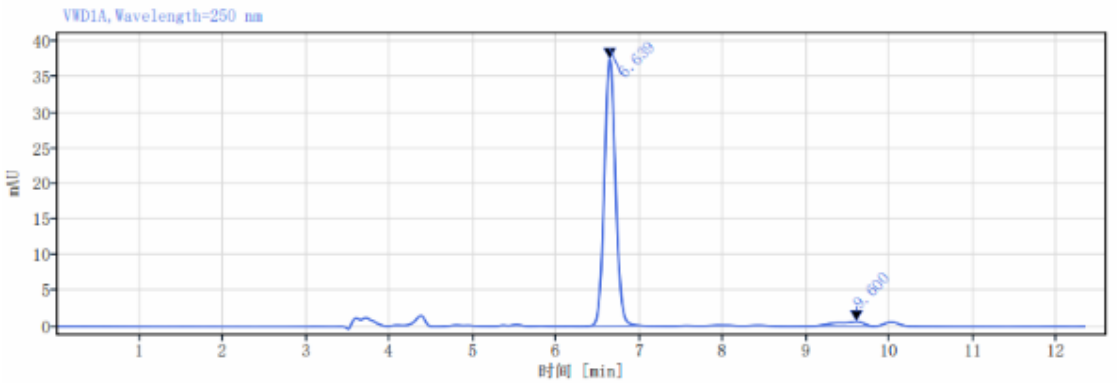
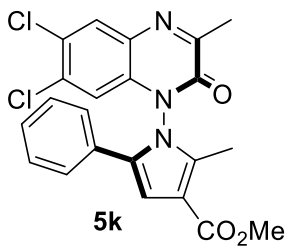
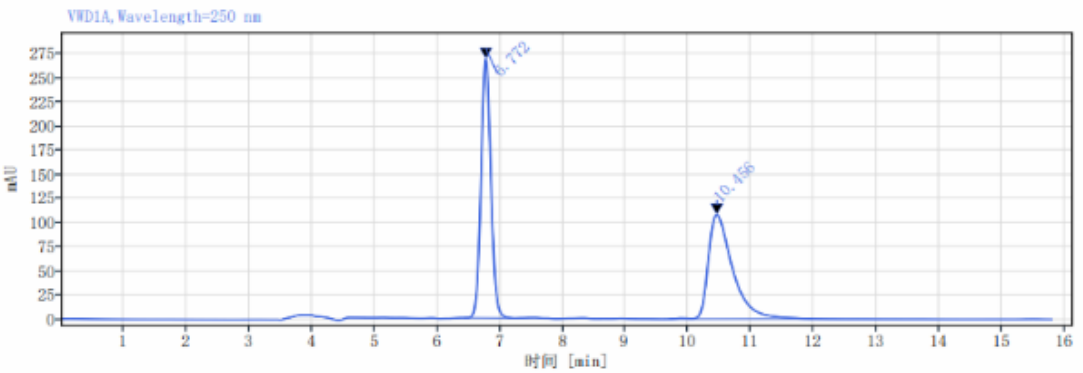


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.654	524.8013	4927.7546	50.2214	n.a.
2	9.280	222.5893	4884.3014v	49.7786	n.a.
Total:			9812.0561	100.0	

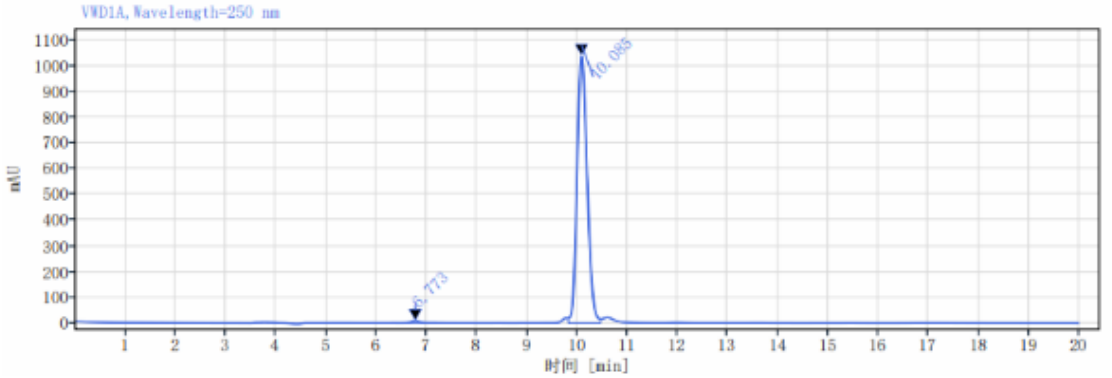


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.639	37.4358	349.3269	96.0039	n.a.
2	9.600	0.6323	14.5406	3.9961	n.a.
Total:			363.8675	100.0	

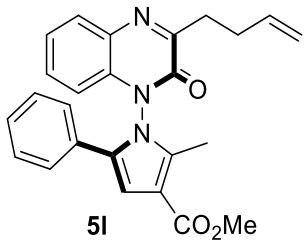




Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	0.7622	268.9715	2937.9258	50.2137	n.a.
2	2.2976	108.1154	2912.9140	49.7863	n.a.
Total:			5850.8398	100.0	



Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	6.773	9.3027	96.7654	0.6573	n.a.
2	10.085	1043.2557	14624.0630	99.3427	n.a.
Total:			14720.8284	100.0	



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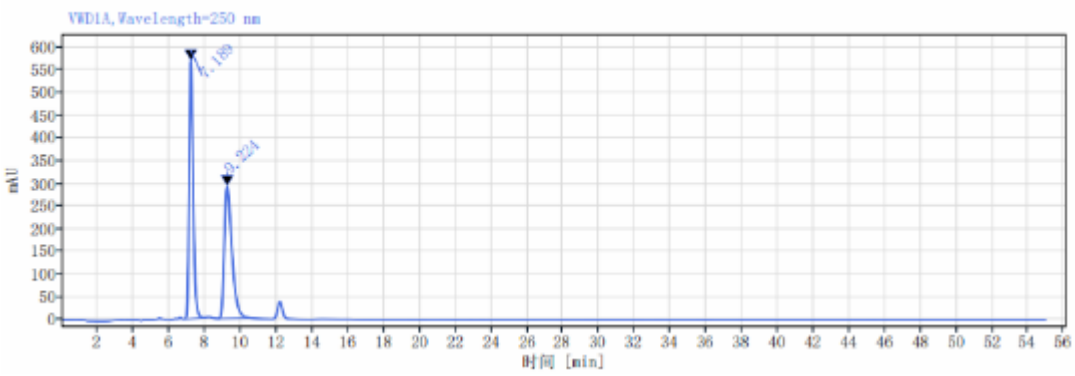
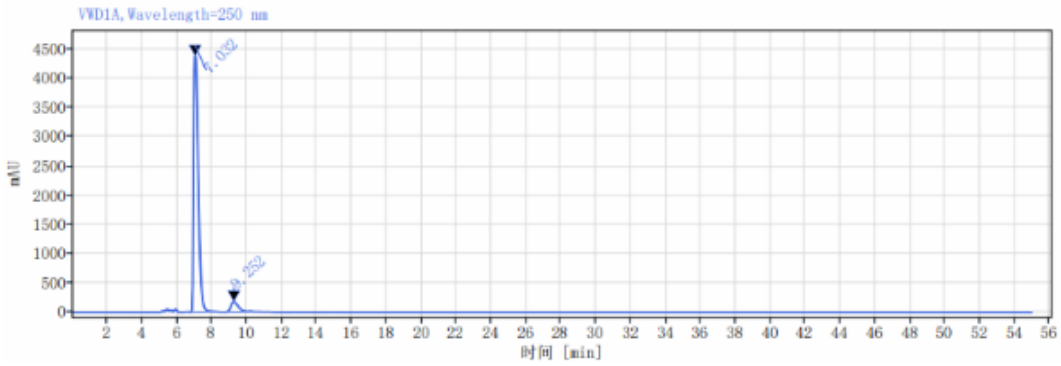
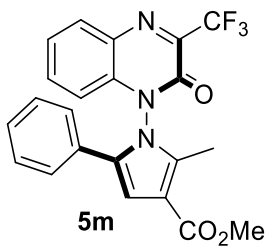
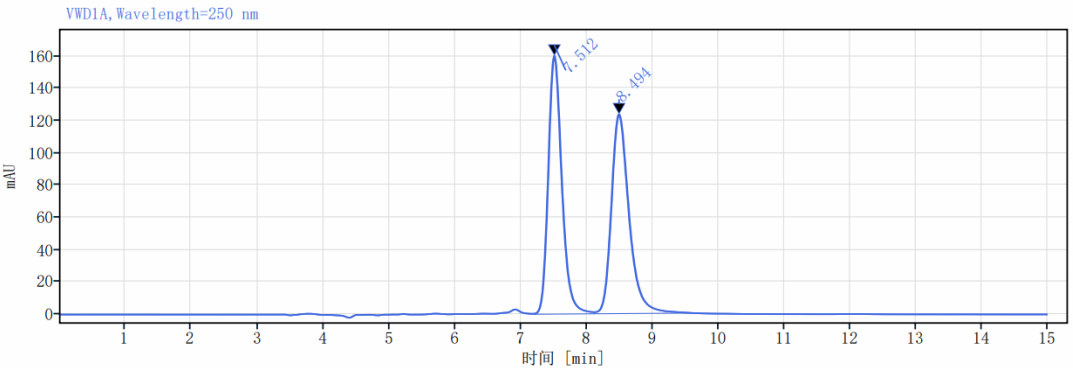


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.189	568.2935	8765.4597	50.3546	n.a.
2	9.224	291.0774	8641.9917	49.6454	n.a.
Total:			17407.4514	100.0	

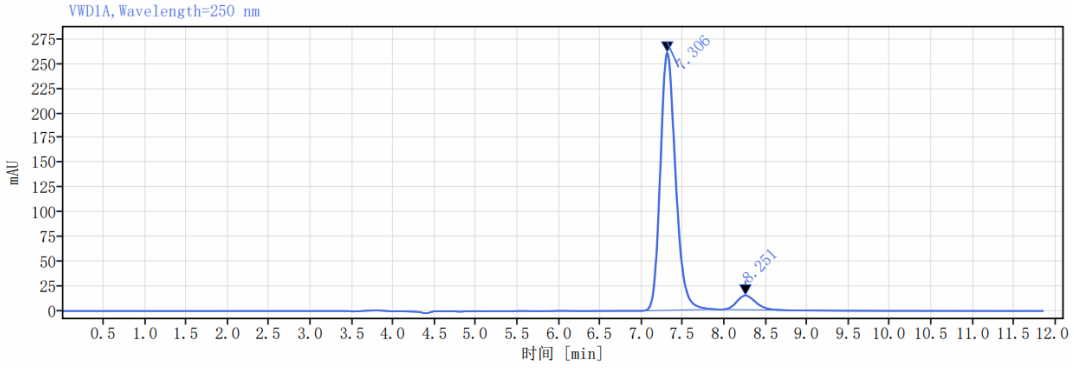


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.032	4387.0746	81538.3343	94.1835	n.a.
2	9.252	173.0436	5035.5593	5.8165	n.a.
Total:			86573.8936	100.0	

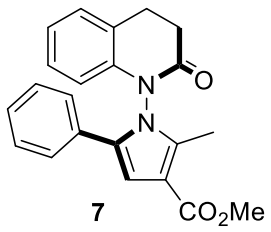




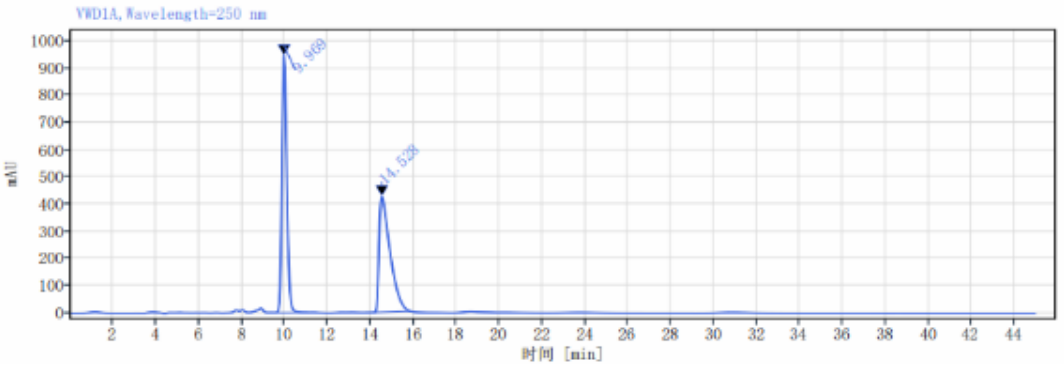
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.512	160.2102	2297.7527	49.8768	n.a.
2	8.494	123.5651	2309.1046	50.1232	n.a.
Total:			4606.8572	100.0	



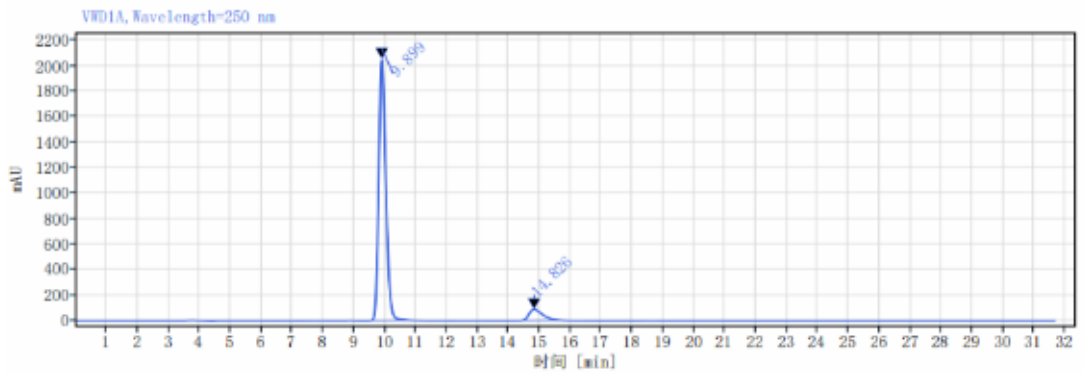
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	7.306	261.1420	3350.1005	93.5357	n.a.
2	8.251	14.3890	231.5267	6.4643	n.a.
Total:			3581.6272	100.0	



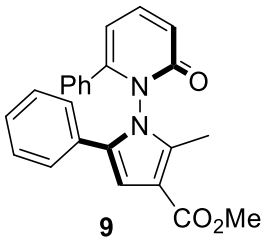
7



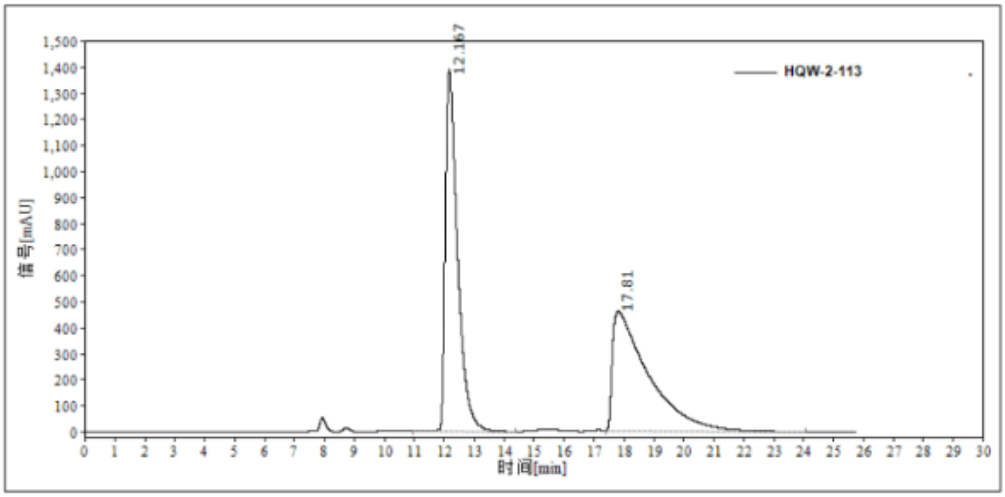
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	9.969	946.5972	14737.3247	49.1658	n.a.
2	14.528	426.1587	15237.4311	50.8342	n.a.
Total:			29974.7558	100.0	



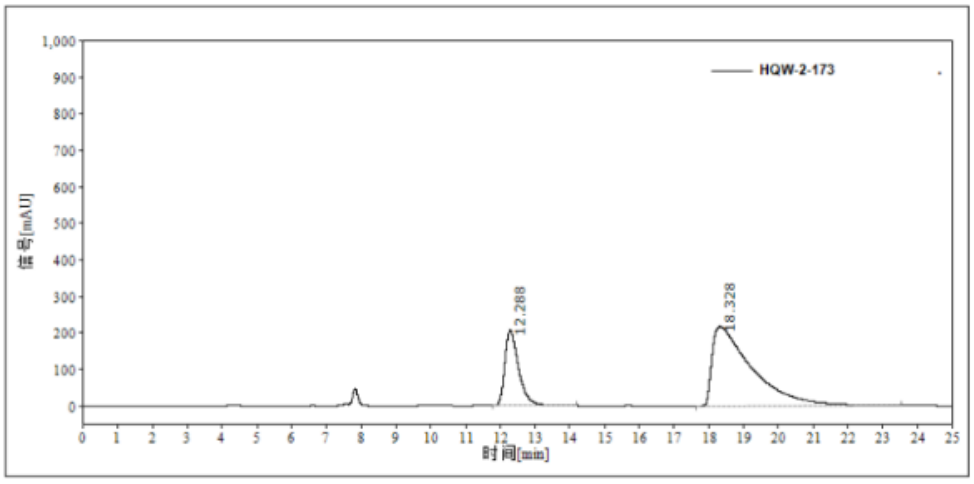
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	9.899	2051.1362	32575.1033	92.7547	n.a.
2	14.826	85.2594	2544.5102	7.2453	n.a.
Total:			35119.6134	100.0	



9

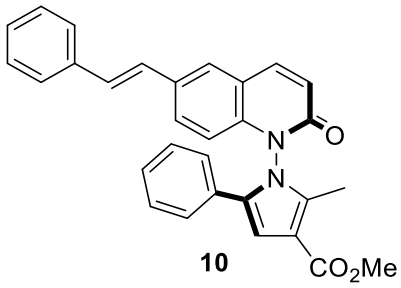


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12,167	1389.542	75.2	39428.910	50.8	n.a.
2	17.810	457.522	24.8	38208.609	49.2	n.a.
Total:		1847.064	100	77637.519	100.0	

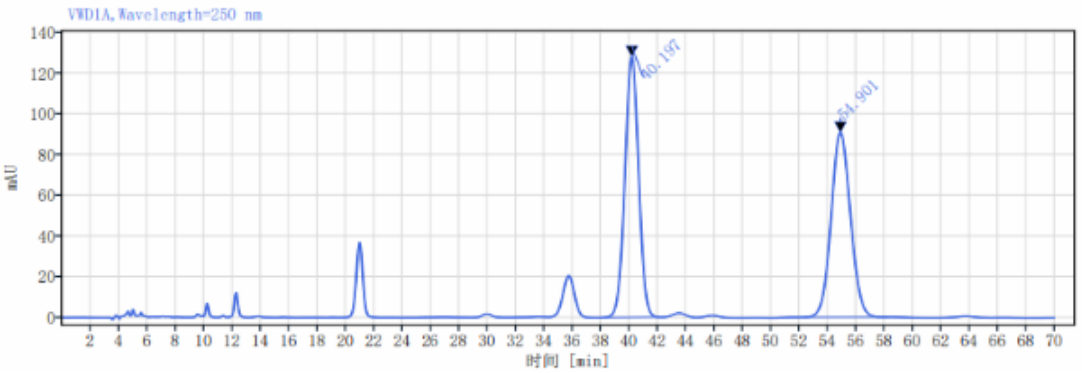


Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	12.288	205.783	48.7	5688.346	24.7	n.a.
2	18.328	217.087	51.3	17326.987	75.3	n.a.

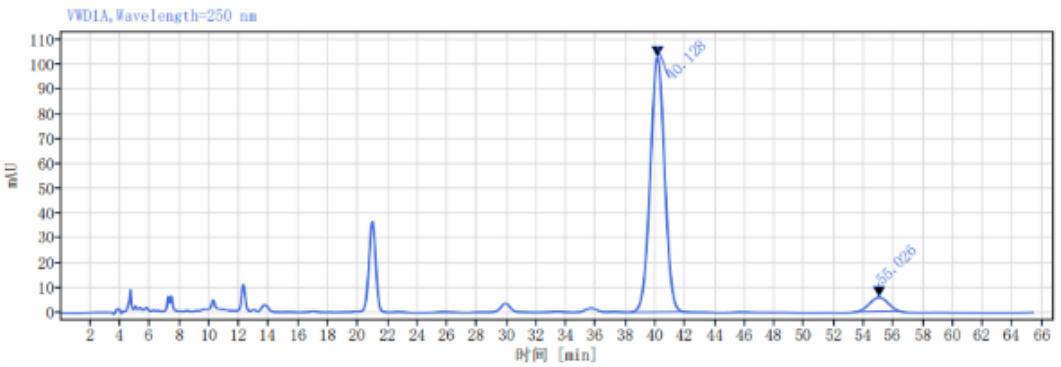
Total:		422.870	100	23015.333	100.0	



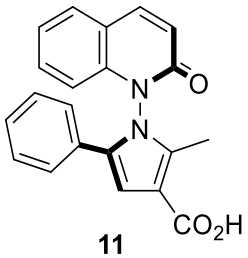
10



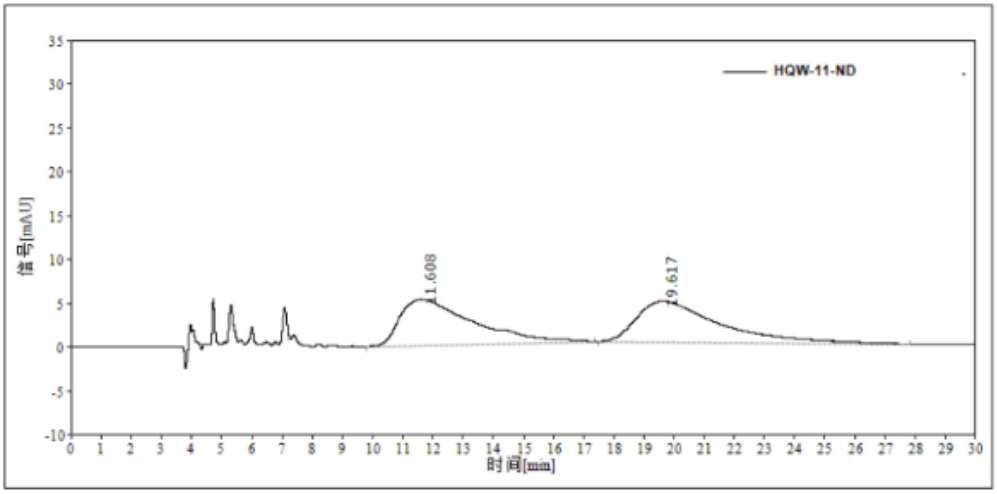
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	40.197	127.8267	8622.5235	50.0475	n.a.
2	54.901	90.5129	8606.1492	49.9525	n.a.
Total:			17228.6727	100.0	



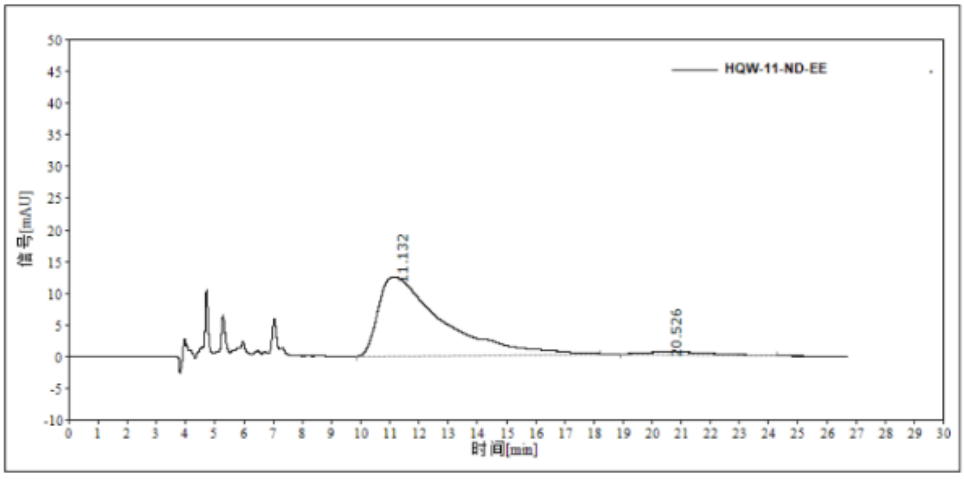
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	40.128	102.7744	6893.1299	93.4491	n.a.
2	55.026	5.6456	483.2165	6.5509	n.a.
Total:			7376.3464	100.0	



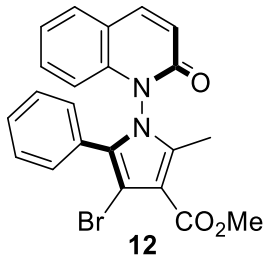
11



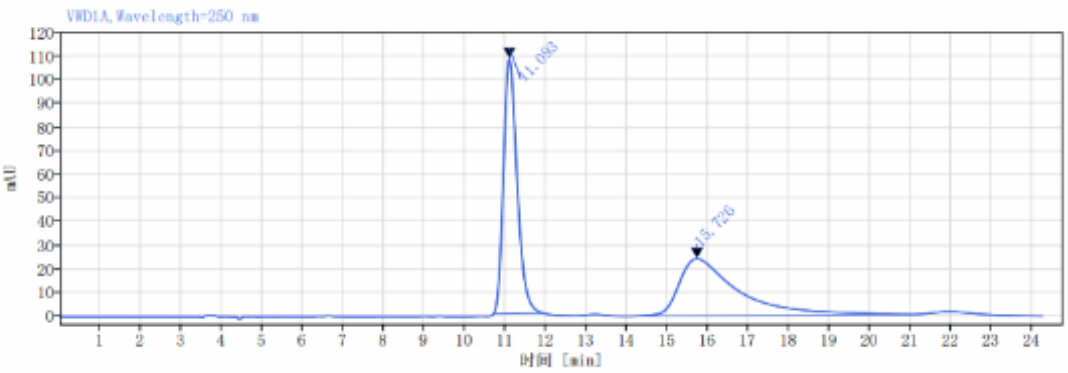
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.608	5.282	53.1	885.818	49.9	n.a.
2	19.617	4.663	46.9	889.026	50.1	n.a.
Total:		9.945	100	1774.844	100.0	



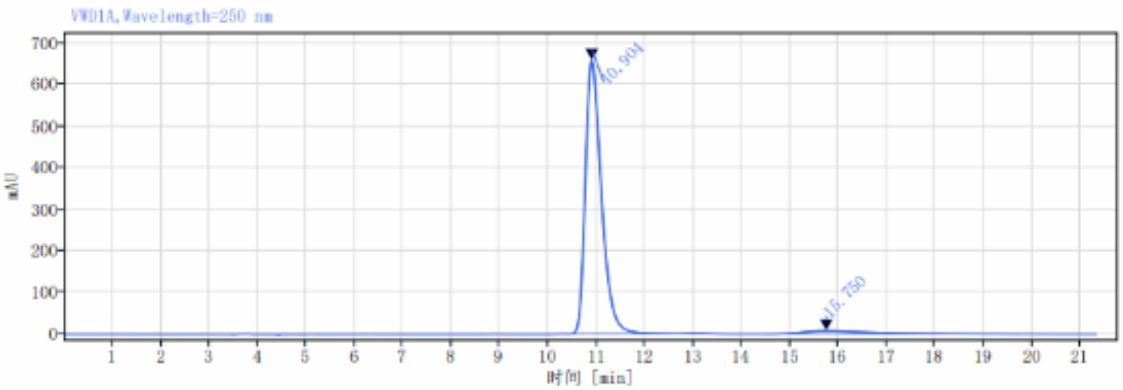
Integration Results						
#	Retention time [min]	Height [mAU]	Relative Height [%]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.132	12.563	96.8	1890.065	96.6	n.a.
2	20.526	0.420	3.2	66.975	3.4	n.a.
Total:		12.983	100	1957.040	100.0	



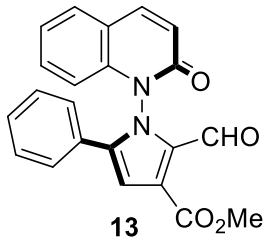
12



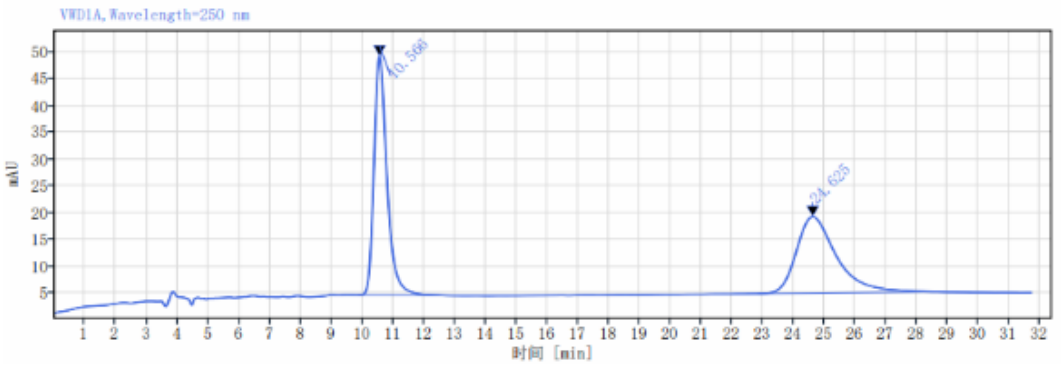
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	11.093	107.7274	2519.0494	50.8850	n.a.
2	15.726	24.0910	2431.4216	49.1150	n.a.
Total:			4950.4710	100.0	



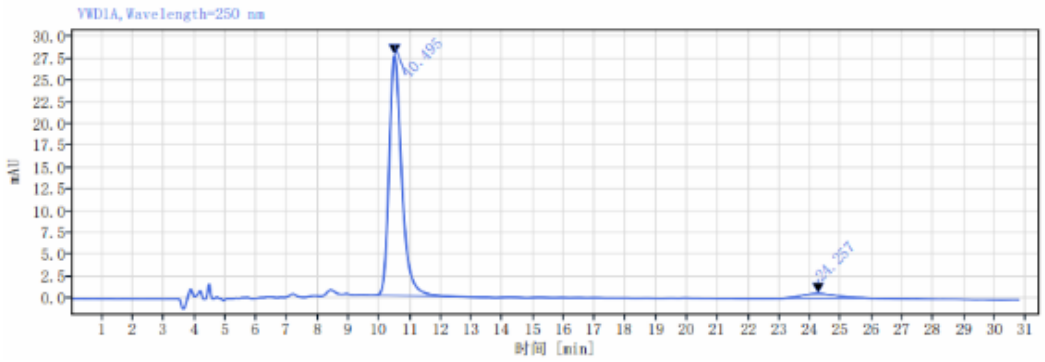
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.904	659.6101	15269.6064	95.1464	n.a.
2	15.750	7.5790	778.9350	4.8536	n.a.
Total:			16048.5414	100.0	



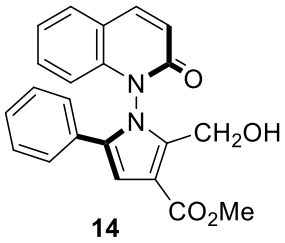
13



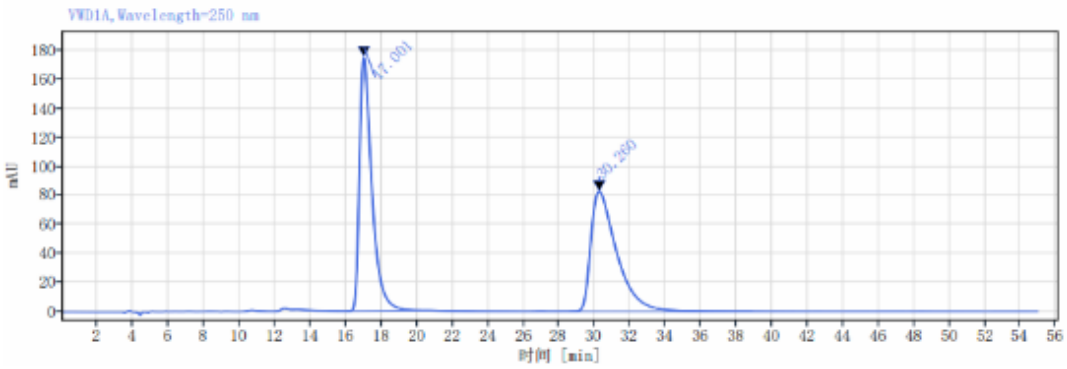
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.566	44.6343	1306.8471	50.3773	n.a.
2	24.625	14.2569	1287.2721	49.6227	n.a.
Total:			2594.1192	100.0	



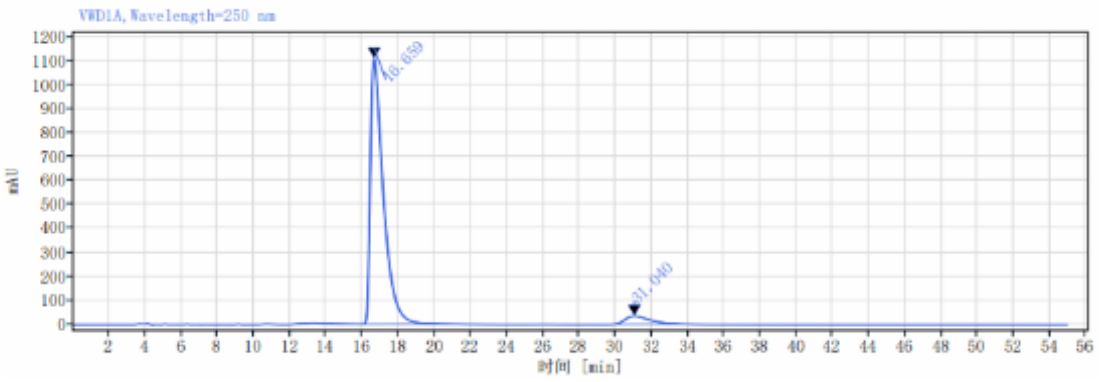
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	10.495	27.5807	788.3400	94.7843	n.a.
2	24.257	0.5401	43.3803	5.2157	n.a.
Total:			831.7203	100.0	



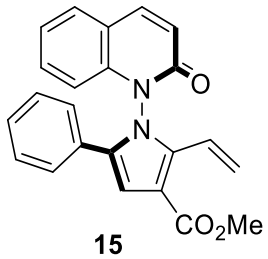
14



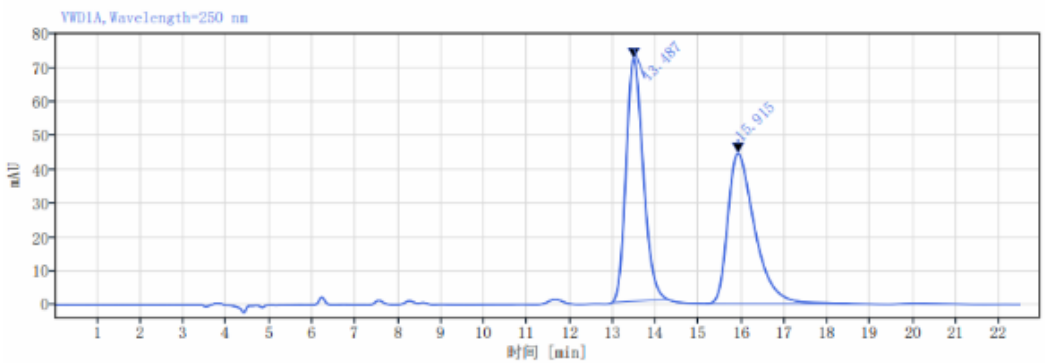
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	17.001	174.7254	8468.1850	50.2082	n.a.
2	30.260	82.5886	8397.9678	49.7918	n.a.
Total:			16866.1528	100.0	



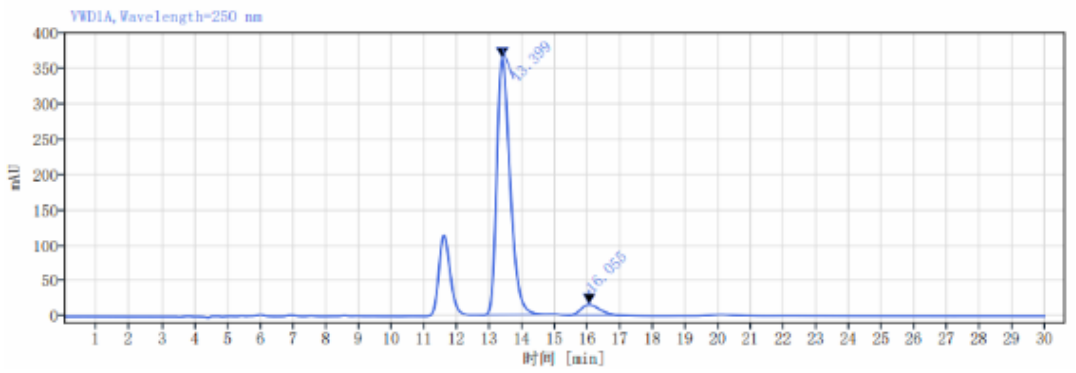
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	16.659	1107.6922	55331.3581	94.4839	n.a.
2	31.040	33.9138	3230.3397	5.5161	n.a.
Total:			58561.6977	100	



15

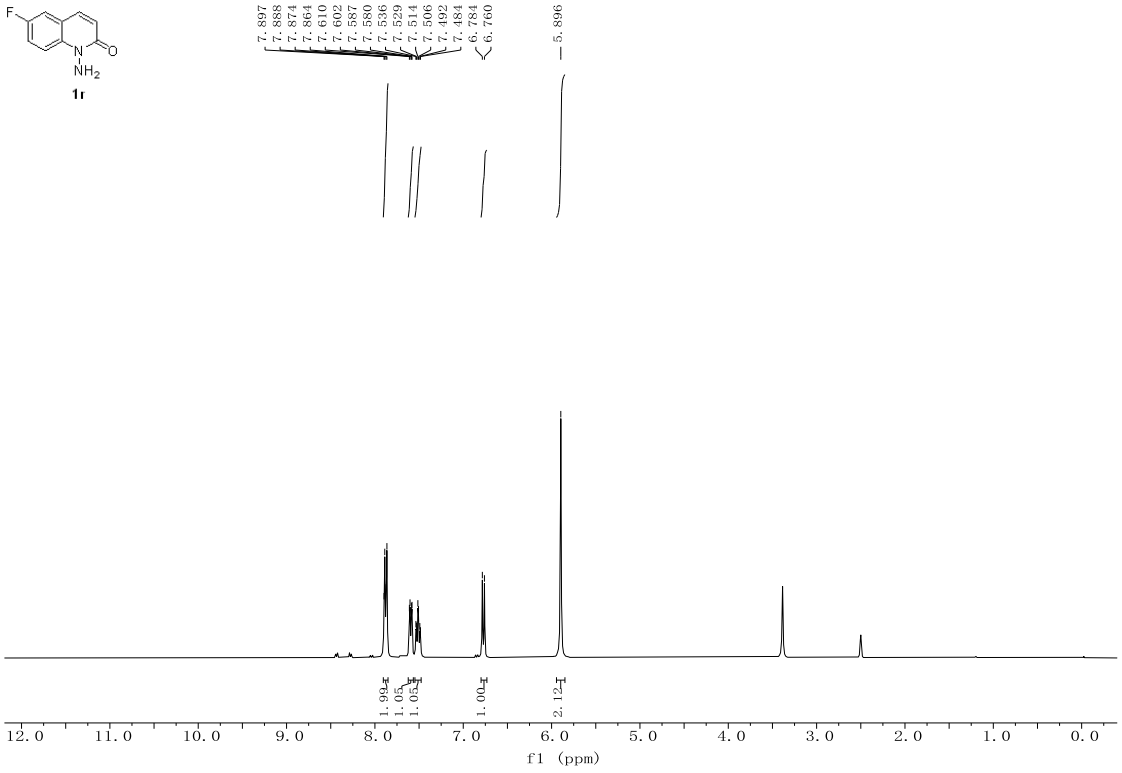


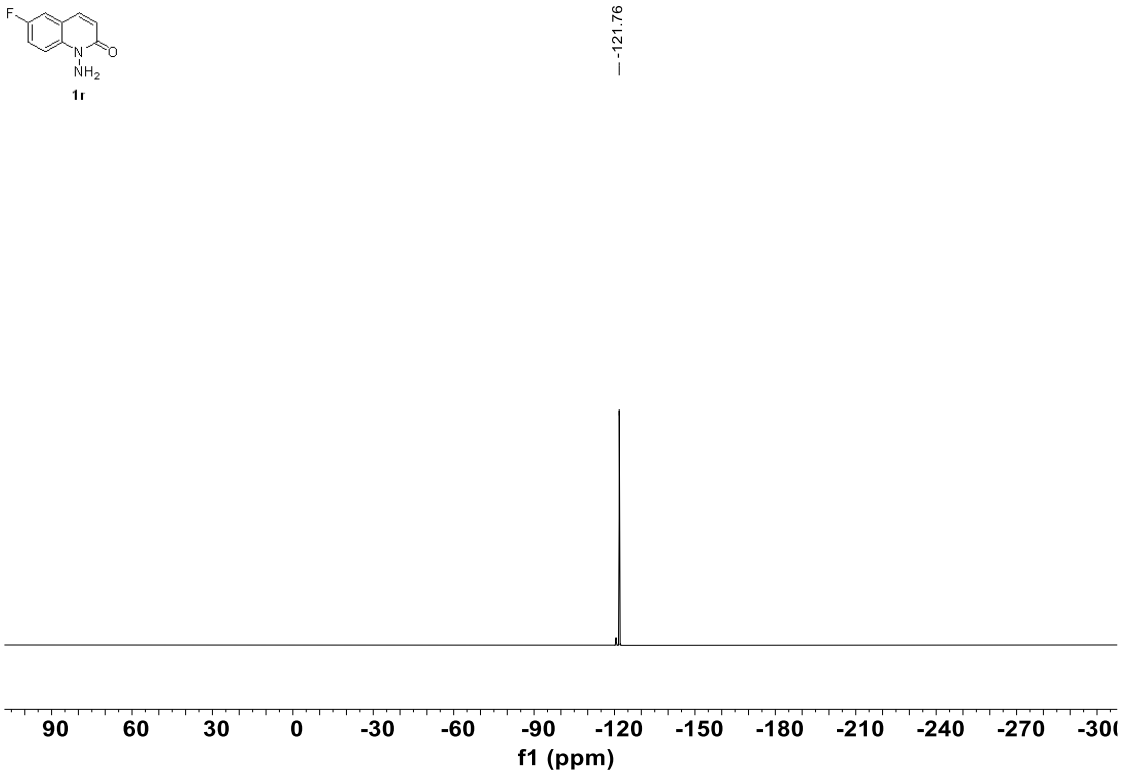
Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	13.487	71.6997	1992.2736	50.6756	n.a.
2	15.915	44.3822	1939.1521	49.3244	n.a.
Total:			3931.4258	100	

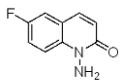


Integration Results					
#	Retention time [min]	Height [mAU]	Area [mAU*min]	Relative Area [%]	Amount n.a.
1	13.399	362.5703	10319.7334	94.6072	n.a.
2	16.055	14.6888	588.2424	5.3928	n.a.
Total:			10907.9758	100	

(10) Copies of ^{1}H, ^{13}C and ^{19}F NMR Spectra

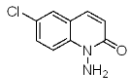






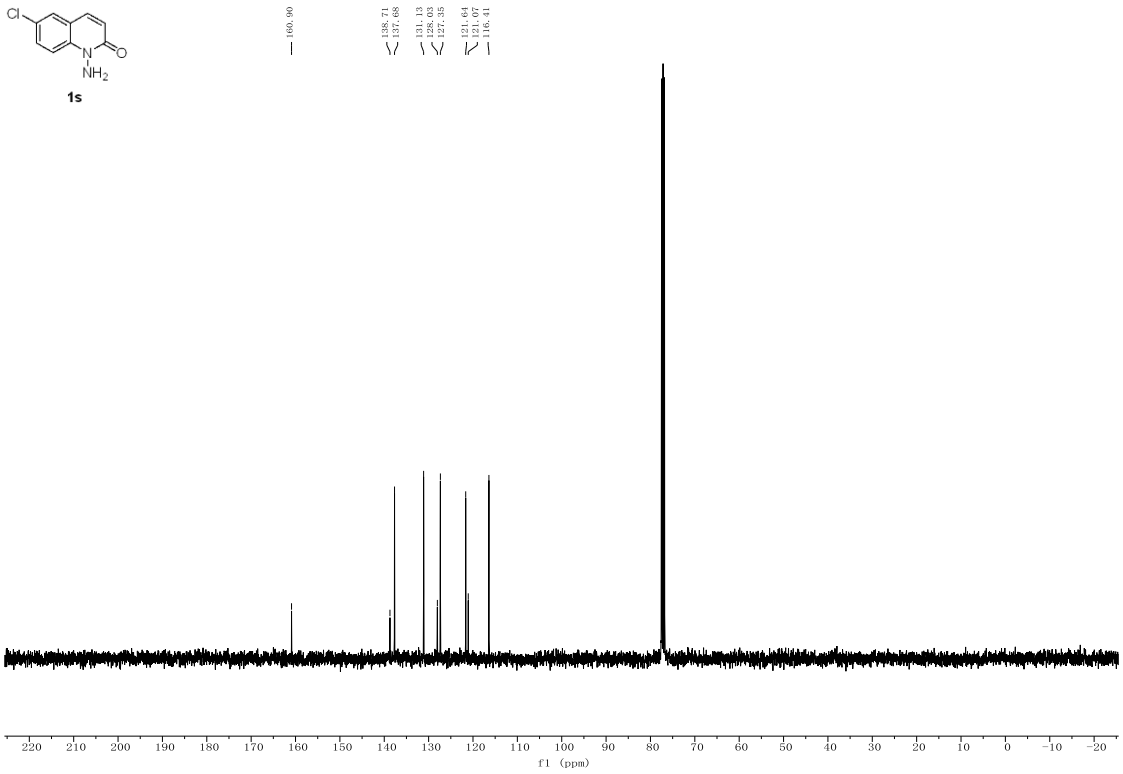
1r

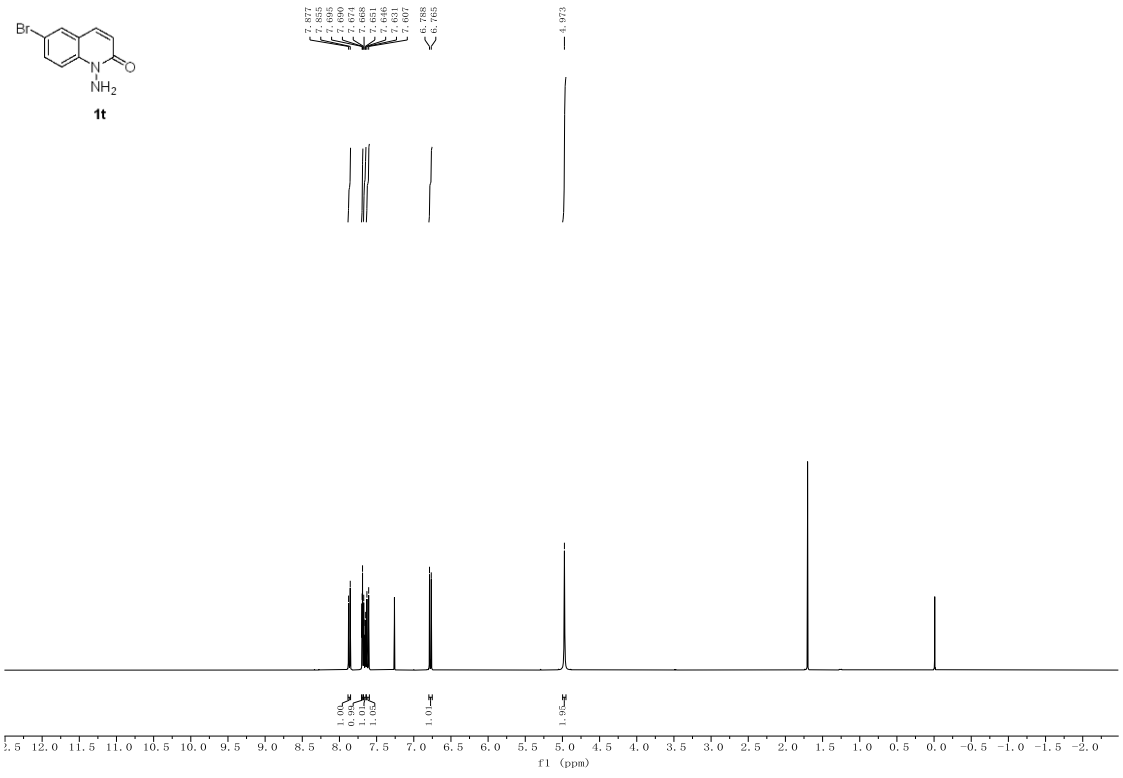
159.66
158.68
156.31
137.69
137.66
136.89
121.92
120.79
120.70
119.13
118.89
117.22
117.14
113.53
113.30
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)

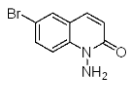


1s

7.92
7.90
7.45
7.42
4.23
4.22
4.21
4.20
3.77
3.71
3.69
3.67
3.55
3.50
3.48
3.46
3.44
2.43
2.00
2.04
0.93
2.91
1.09
1.03
2.92
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)

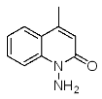

Cl
O
N
NH2
1s
160.90
138.71
137.68
131.13
128.03
127.35
121.64
121.07
116.41
f1 (ppm)


Br
O
N
NH2
1t
7.877
7.855
7.695
7.690
7.674
7.668
7.651
7.646
7.631
7.607
6.788
6.765
4.973
1.00
0.98
1.01
1.05
1.01
1.96
f1 (ppm)


Br
O
N
NH2

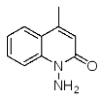
1t

160.89
139.11
137.62
133.84
130.42
121.60
121.56
116.67
116.41
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)


O
N
NH2

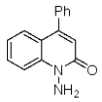
1u

7.987
7.966
7.682
7.678
7.662
7.658
7.605
7.602
7.584
7.566
7.562
7.270
7.267
7.252
7.250
7.232
7.229
6.606
6.603
4.986
2.460
2.458
1.00
1.00
1.03
1.16
0.95
2.02
3.17
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)



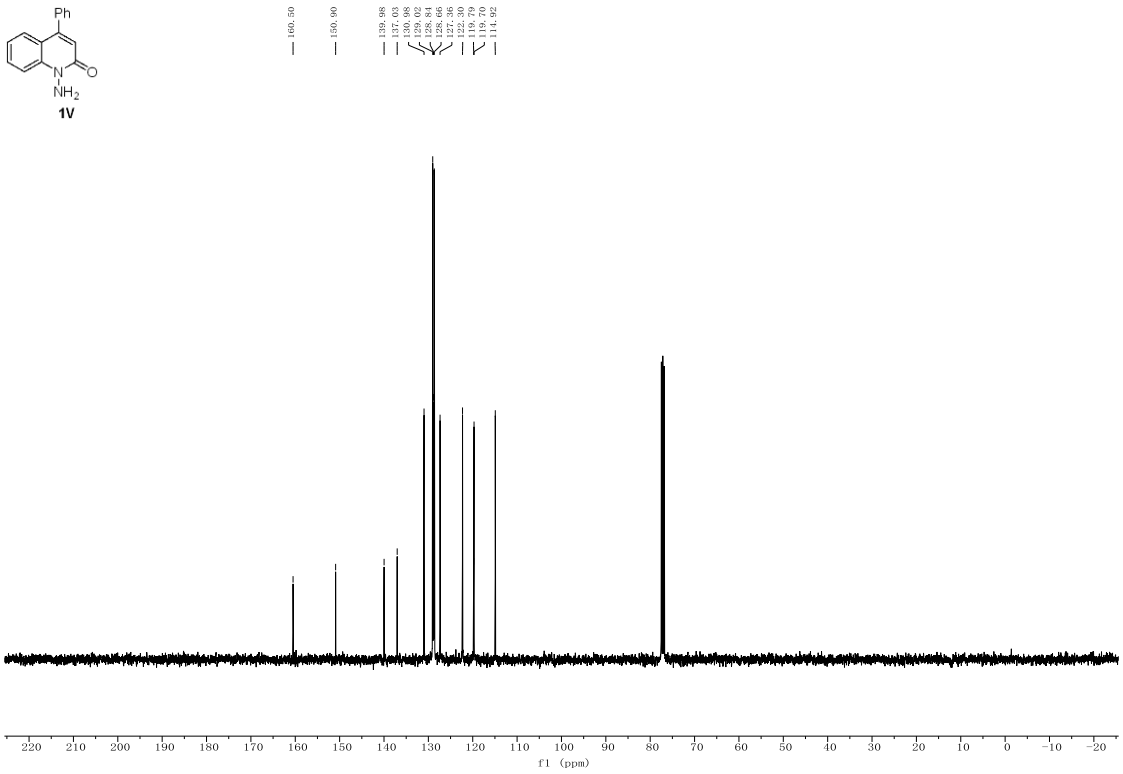
1u

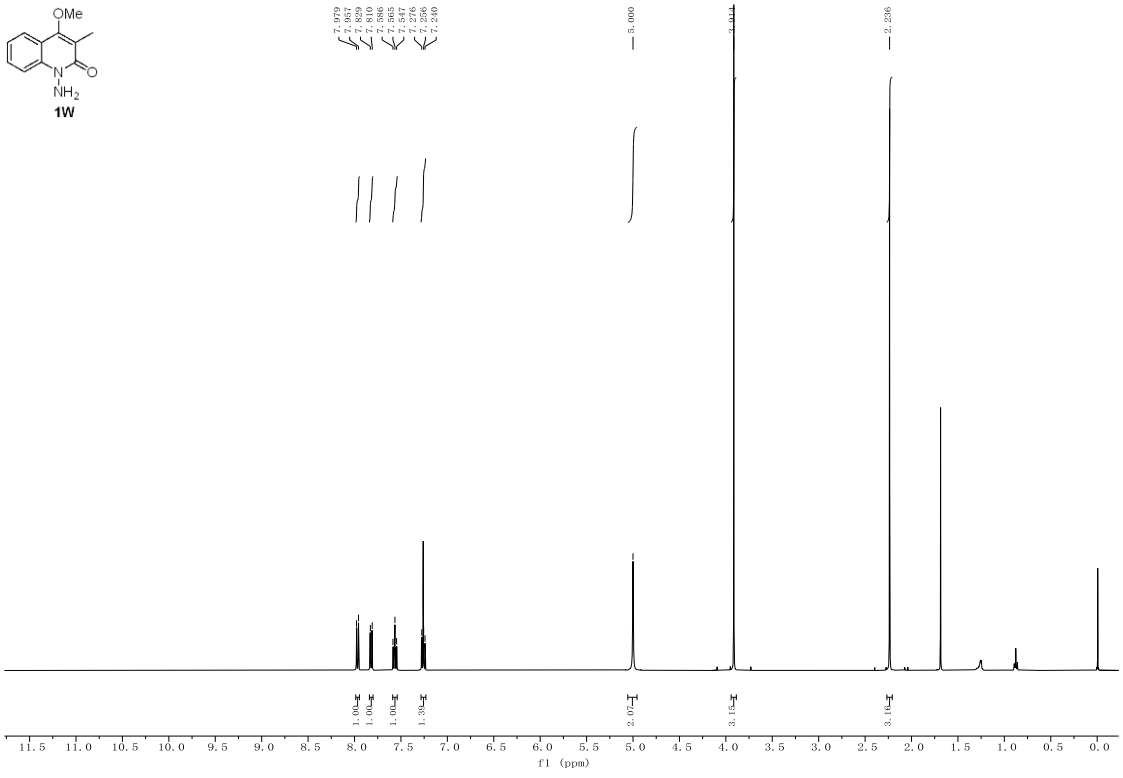
160.79
146.57
139.53
130.78
124.93
122.28
120.74
119.60
114.92
19.12
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)

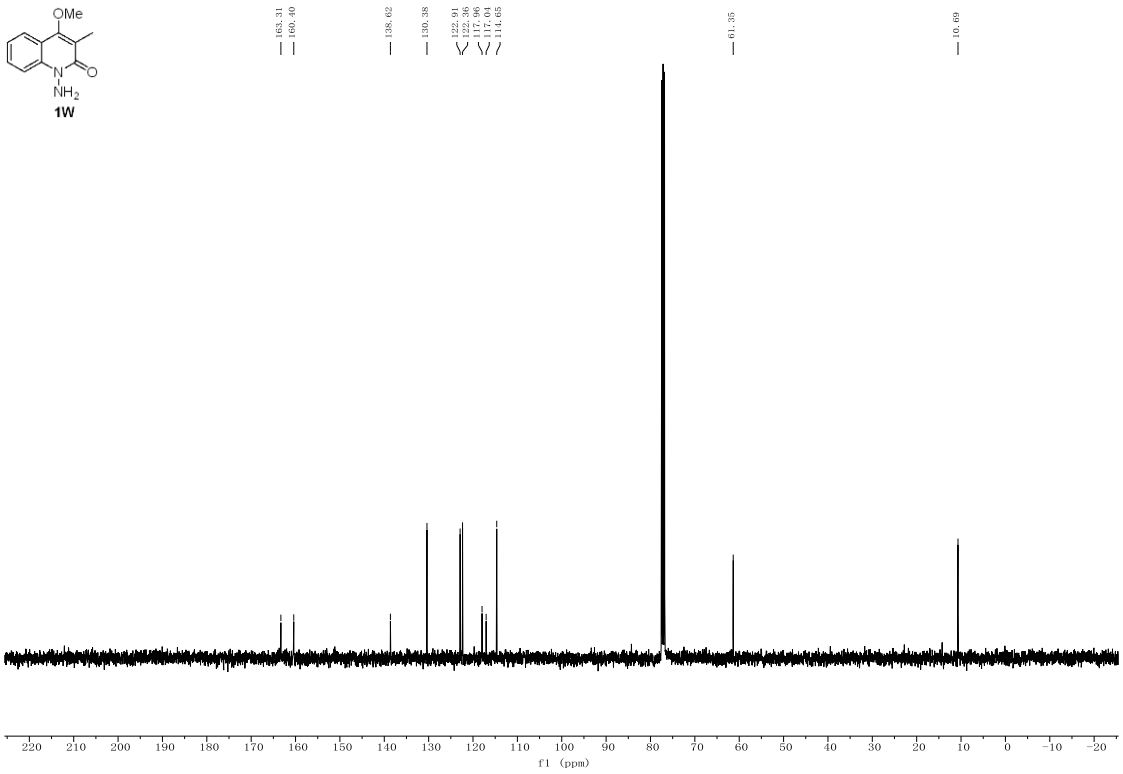


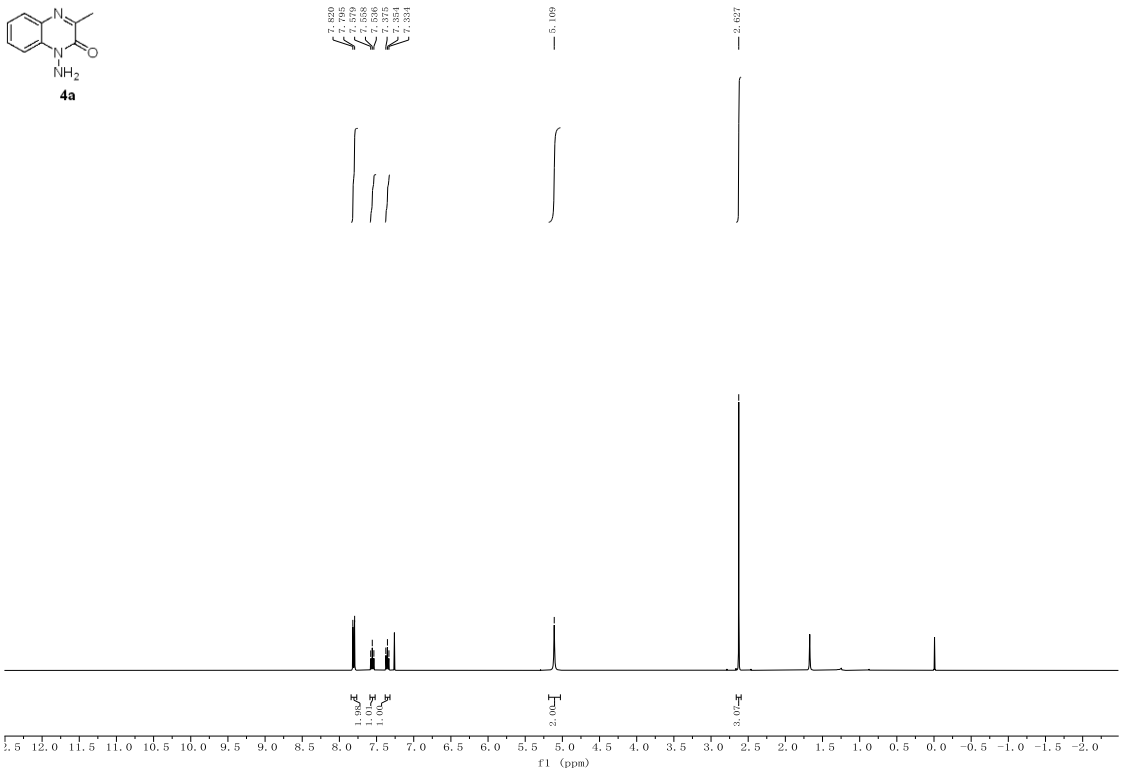
1V

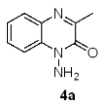
8.06
8.04
7.61
7.60
7.58
7.54
7.52
7.50
7.49
7.48
7.47
7.40
7.39
7.38
7.18
7.16
7.15
6.70
5.13
1.00
1.02
0.94
3.08
2.07
1.03
0.97
2.05
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)


Ph
N
O
NH2
1V
160.50
150.90
139.98
137.03
130.98
129.02
128.84
128.65
127.36
122.30
119.79
119.70
114.92
f1 (ppm)


OMe
N
O
NH2
1W
7.979
7.957
7.829
7.810
7.586
7.565
7.547
7.276
7.256
7.240
5.000
3.944
2.236
1.00
1.00
1.00
1.39
2.07
3.15
3.16
f1 (ppm)

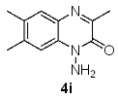

OMe
N
O
NH2
1W
163.31
160.40
138.62
130.38
122.91
122.36
117.96
117.04
114.65
61.35
10.69
f1 (ppm)


N
O
NH2
4a
7.820
7.795
7.579
7.558
7.536
7.375
7.354
7.344
5.109
2.627
1.98
1.01
1.04
2.01
3.07
f1 (ppm)



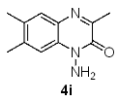
4a

157.30
153.99
132.93
132.52
130.01
129.12
124.16
113.94
21.55
f1 (ppm)



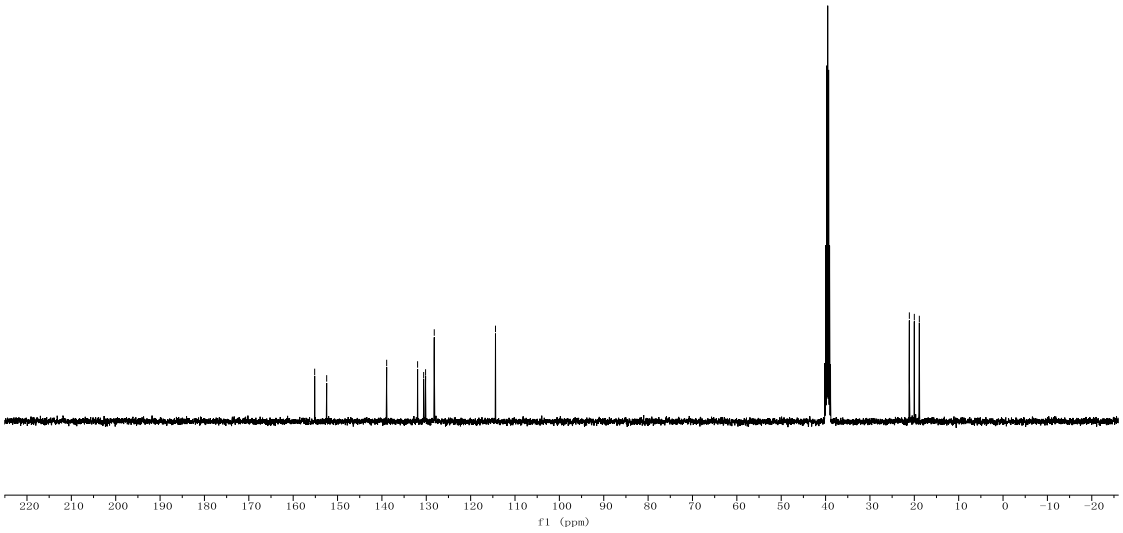
4i

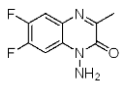
7.532
7.490
6.072
2.431
2.392
2.353
1.00
0.96
1.95
2.91
3.00
2.96
f1 (ppm)



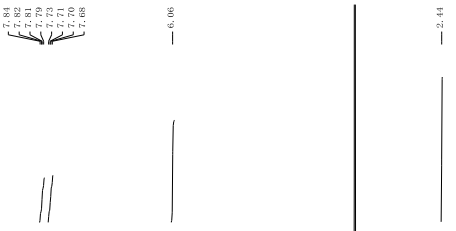
4i

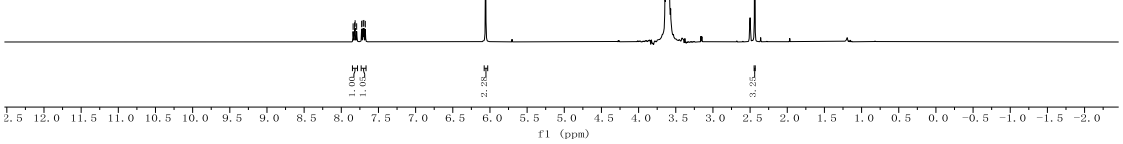

155.15
152.45
138.93
131.96
130.59
130.16
128.20
114.40
21.11
20.66
18.87

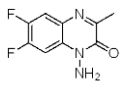

220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)



4j

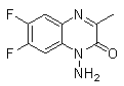

7.84
7.82
7.81
7.79
7.73
7.71
7.70
7.68
6.06
2.44


1.00
1.03
2.28
3.25
2.5 12.0 11.5 11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 −0.5 −1.0 −1.5 −2.0
f1 (ppm)



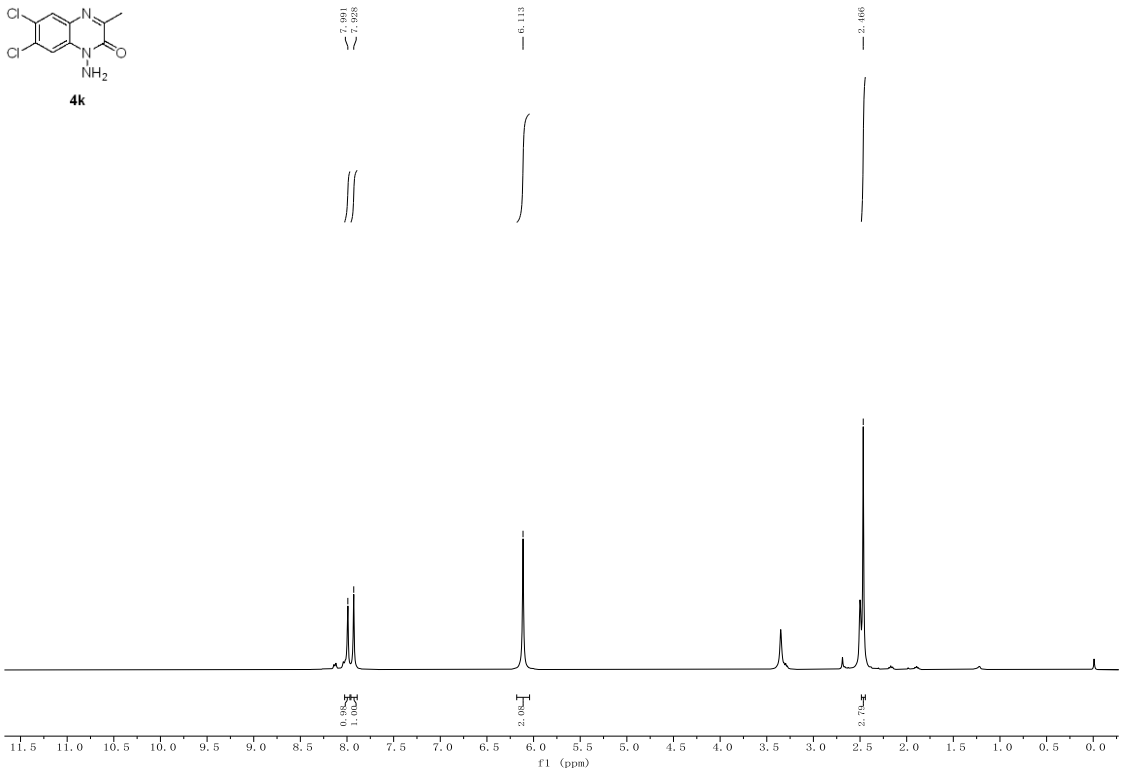
4j

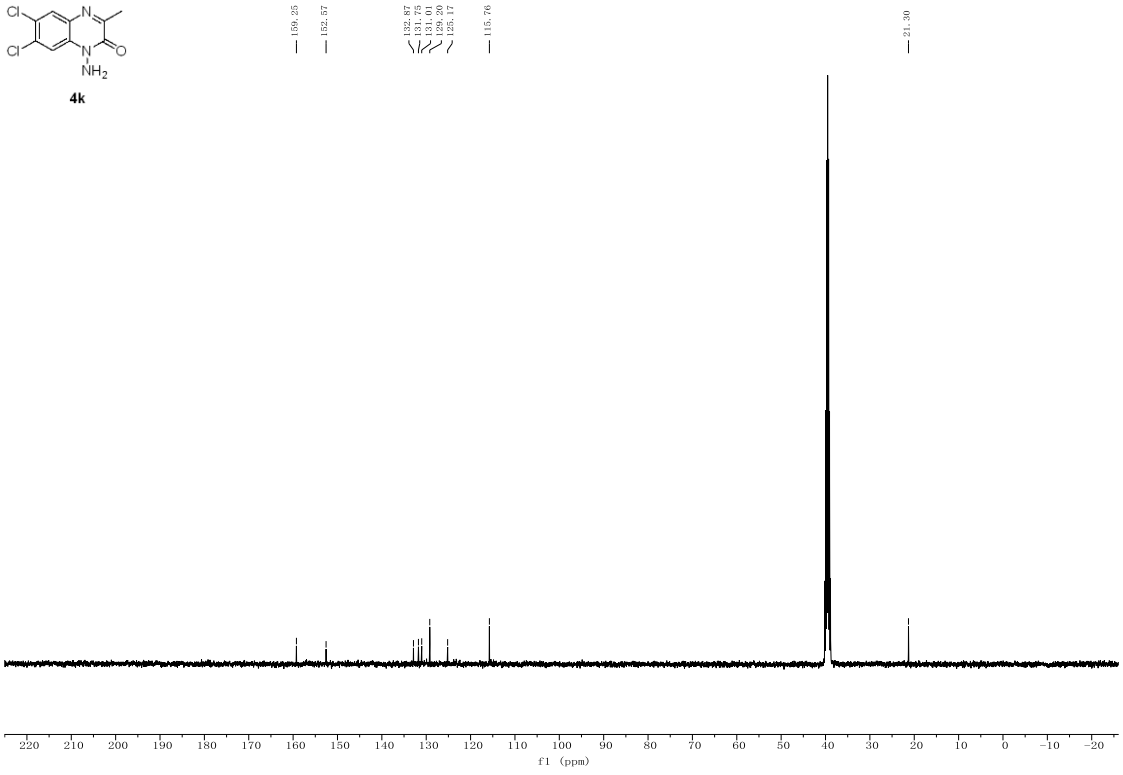
-133.75
-133.77
100 80 60 40 20 0 -20 -40 -60 -80 -100 -120 -140 -160 -180 -200 -220 -240 -260 -280 -300
f1 (ppm)

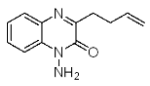


4j

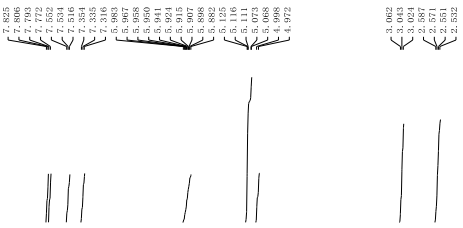
158.25
153.01
151.64
151.52
149.16
149.00
147.30
147.15
144.84
144.70
130.93
130.83
128.29
128.21
116.32
116.14
103.16
102.93
21.37
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)

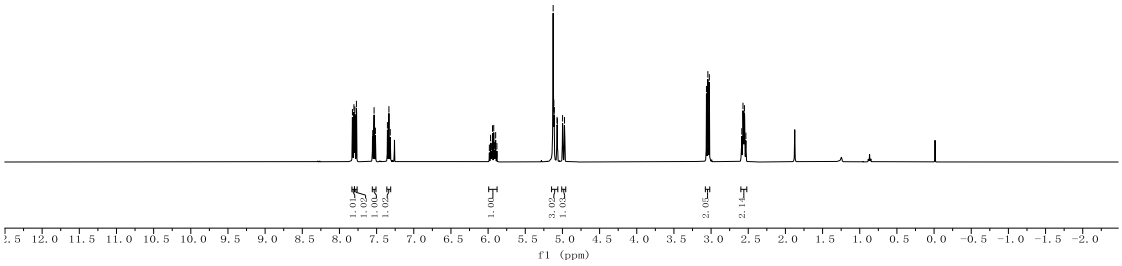

4k
7.991
7.928
6.113
2.466
0.98
1.00
2.00
2.70
f1 (ppm)

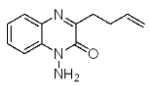

4k
159.25
152.57
132.87
131.75
131.01
129.20
125.17
115.76
21.30
f1 (ppm)



4l

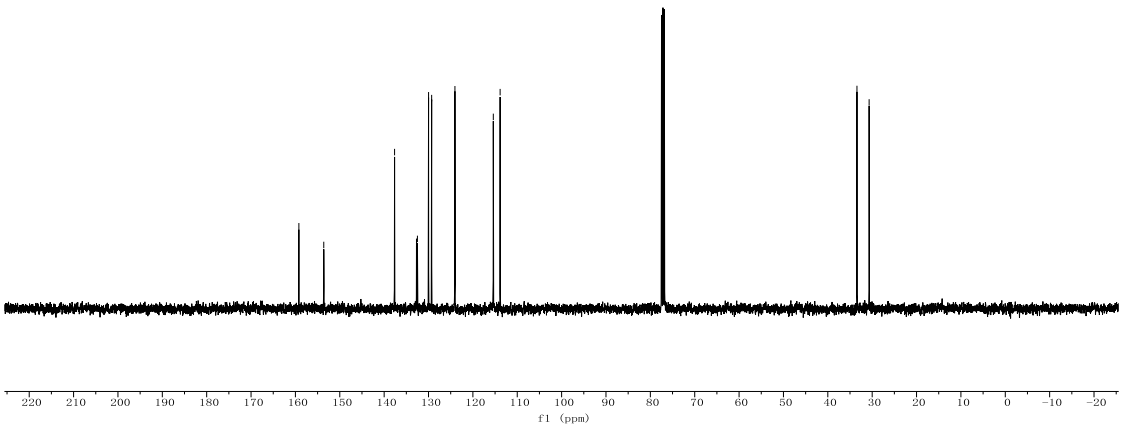

7.825
7.806
7.793
7.772
7.552
7.534
7.516
7.354
7.335
7.316
5.985
5.967
5.958
5.950
5.941
5.924
5.915
5.907
5.898
5.882
5.125
5.116
5.111
5.073
5.068
4.998
4.972
3.062
3.043
3.024
2.987
2.571
2.551
2.532

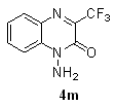

1.01
1.07
1.00
1.05
1.00
3.03
1.00
2.06
2.14
f1 (ppm)



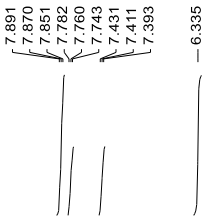
4l

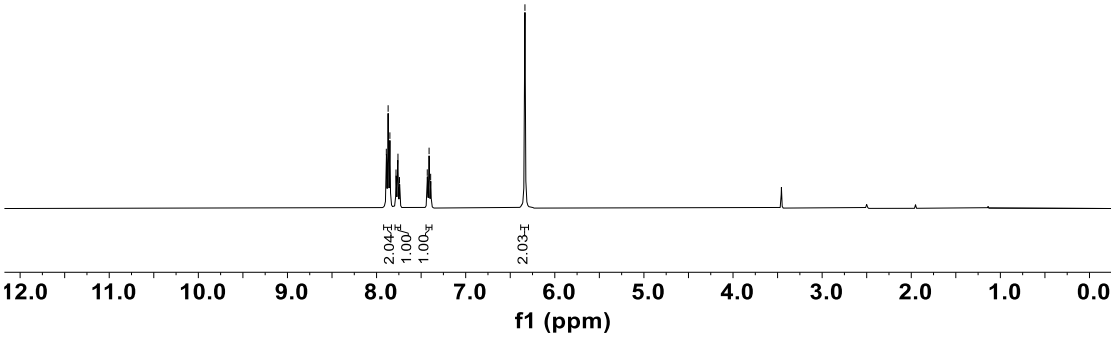

159.22
153.61
137.65
132.71
132.50
129.99
129.29
124.05
115.40
113.86
33.43
30.69

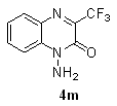

f1 (ppm)



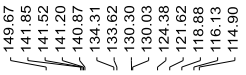
4m

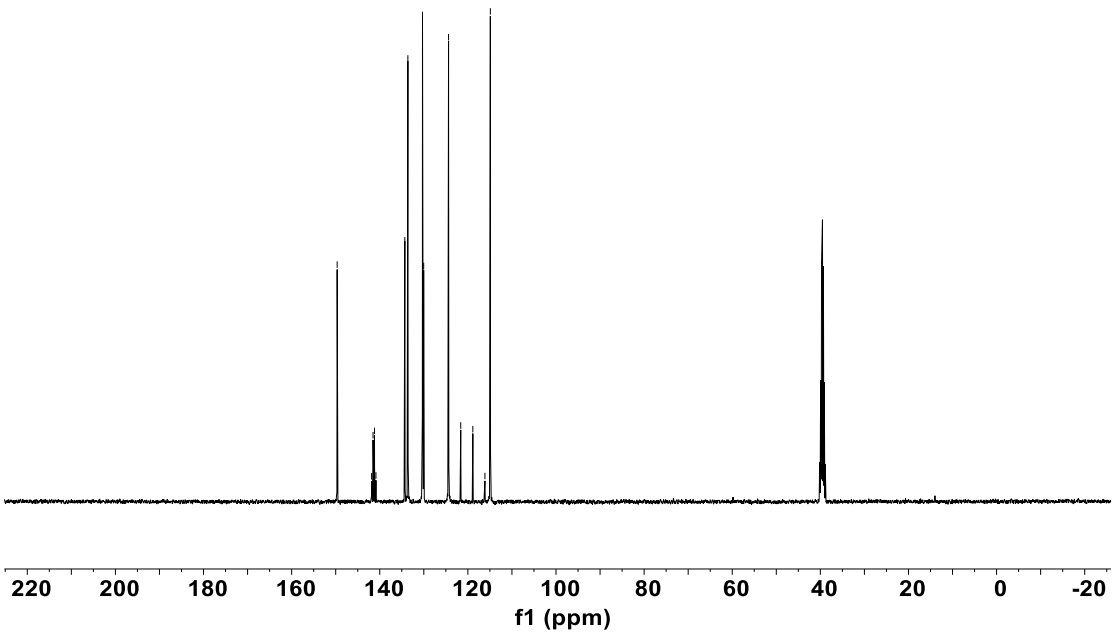

7.891
7.870
7.851
7.782
7.760
7.743
7.431
7.411
7.393
6.335

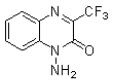

2.04
1.00
1.00
2.03
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
f1 (ppm)



4m

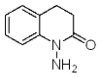

149.67
141.85
141.52
141.20
140.87
134.31
133.62
130.30
130.03
124.38
121.62
118.88
116.13
114.90


220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)



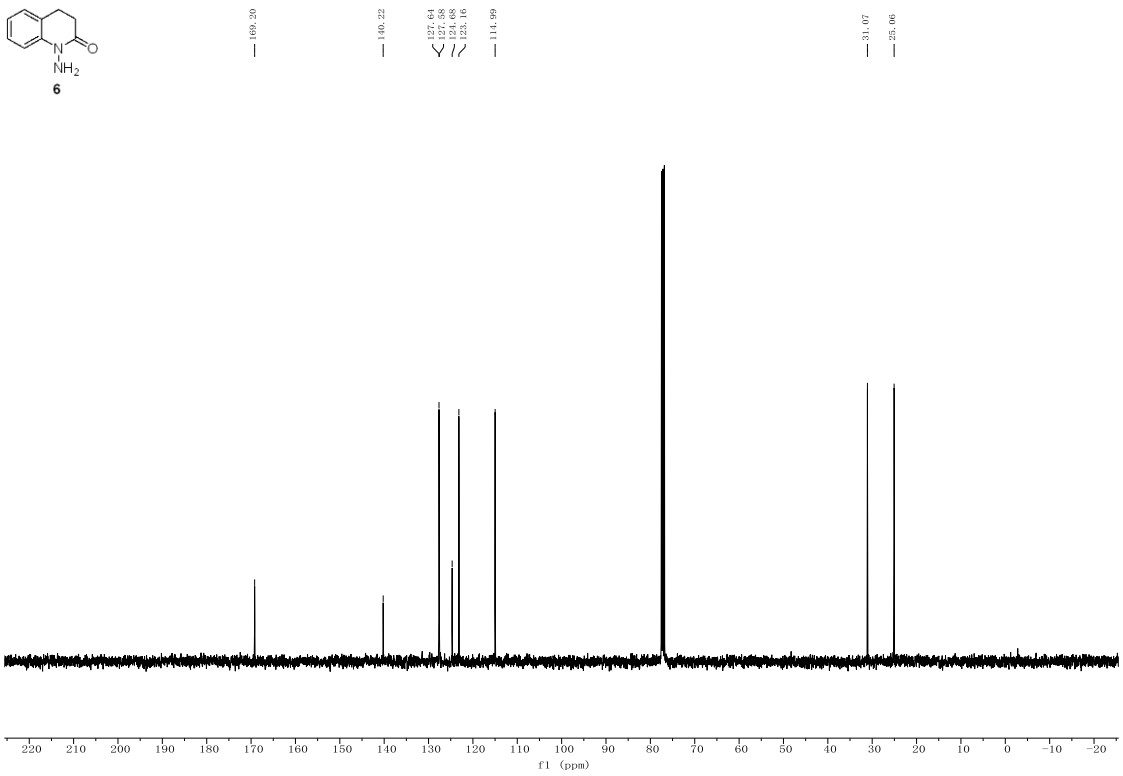
4m

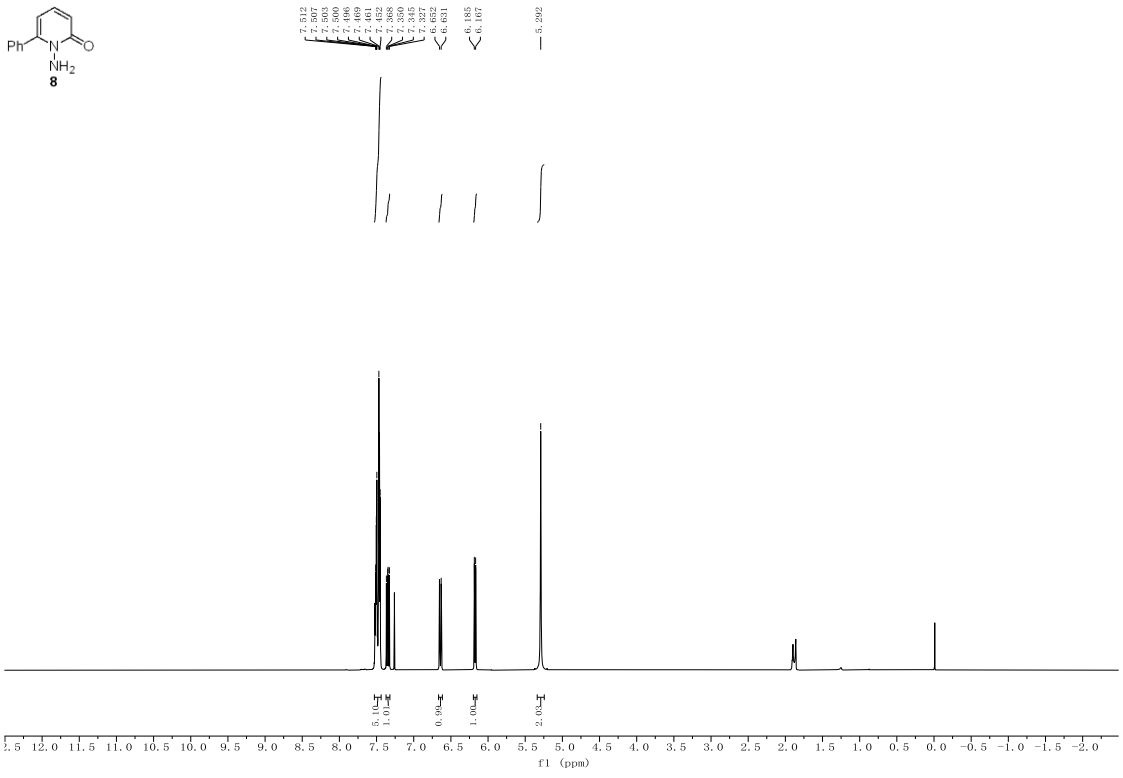
-68.58
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)



6

7.572
7.551
7.282
7.260
7.243
7.139
7.121
7.023
7.005
6.986
4.502
2.929
2.911
2.905
2.891
2.731
2.716
2.711
2.693
1.00
1.14
1.01
2.04
2.13
2.13
f1 (ppm)

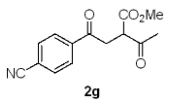

6
169.20
140.22
127.64
127.58
124.68
122.16
114.99
31.07
25.06
f1 (ppm)


Ph
8
7.512
7.507
7.503
7.500
7.496
7.469
7.461
7.452
7.388
7.350
7.345
7.337
6.652
6.631
6.185
6.167
5.292
5.10
1.01
0.99
1.00
2.03
f1 (ppm)


Ph
N
NH2
O

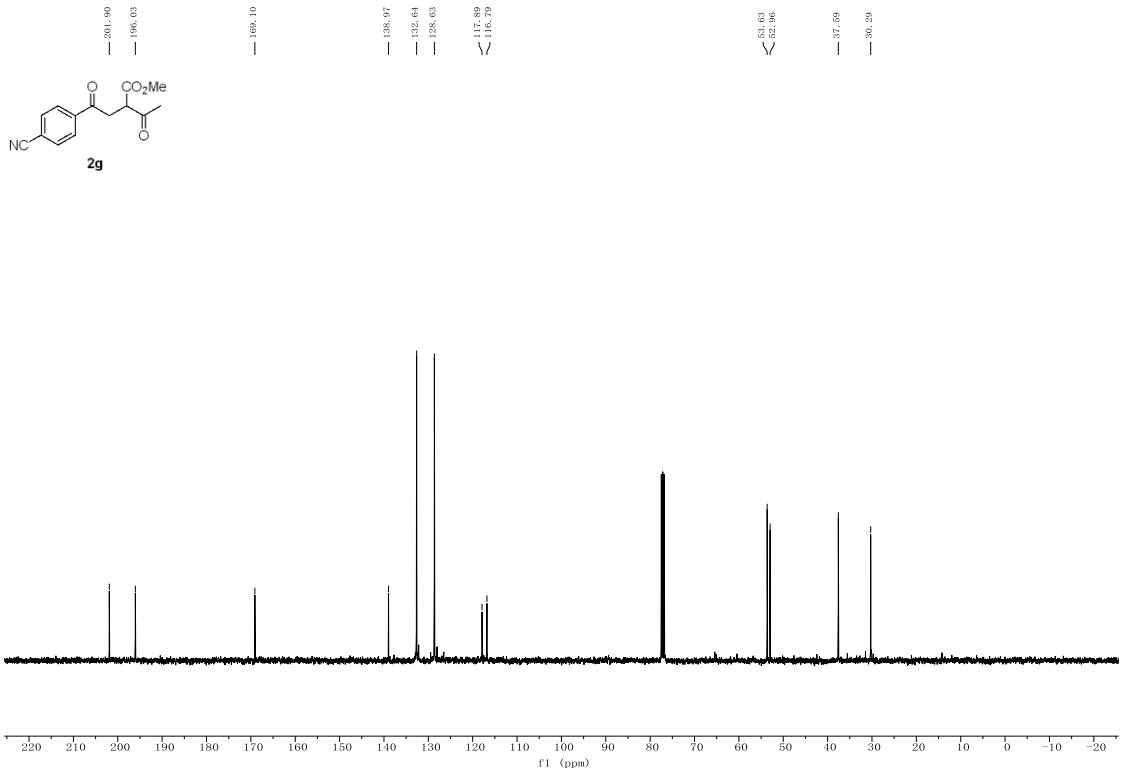
8

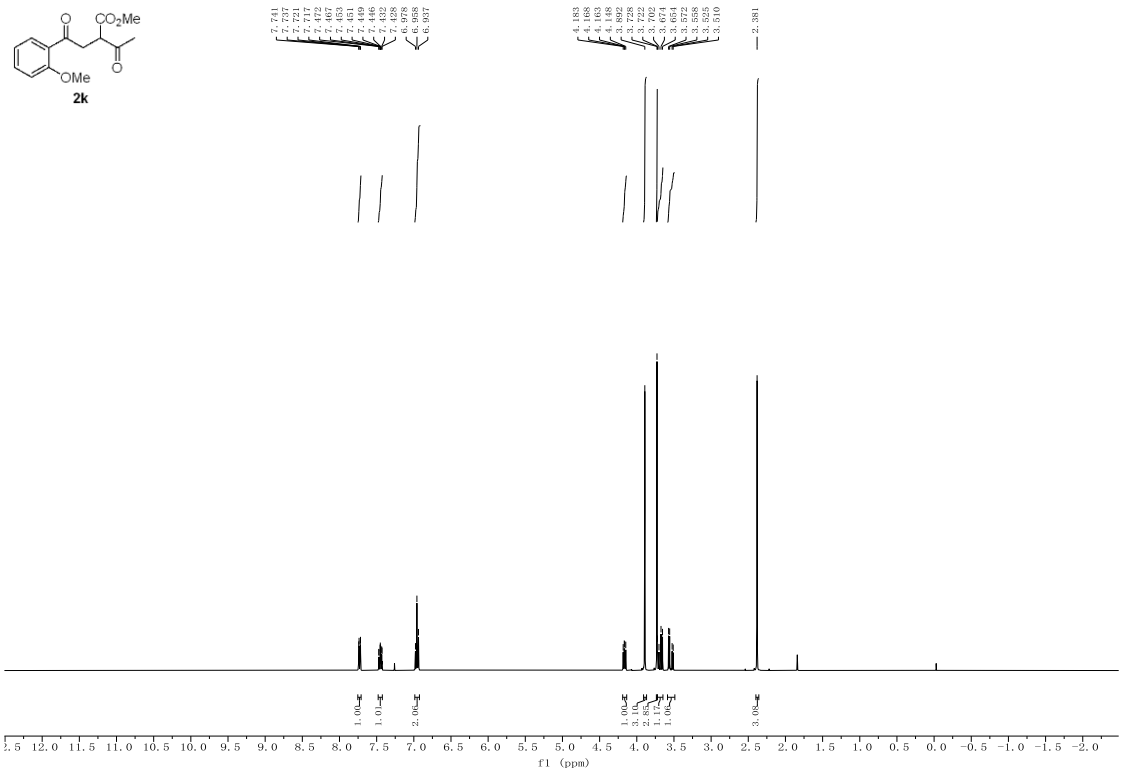
161.05
148.04
137.83
133.79
129.60
129.02
128.52
117.18
107.58
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 −10 −20
f1 (ppm)

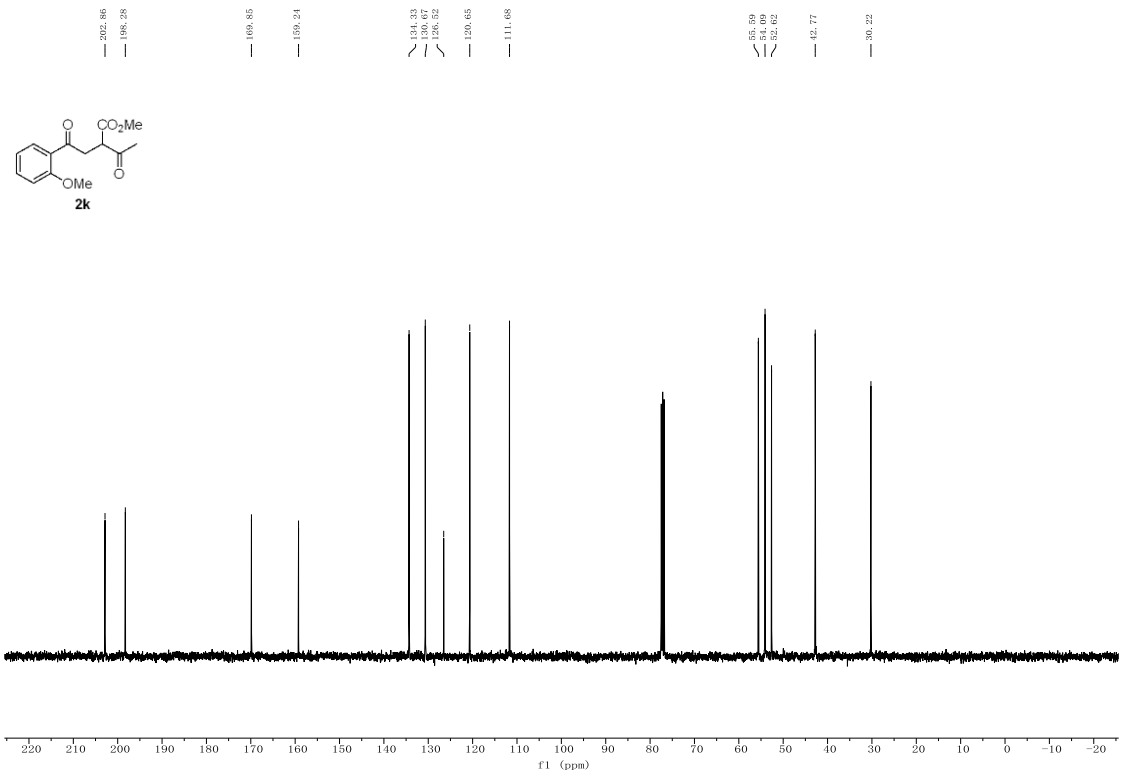

O
CO2Me
NC
O

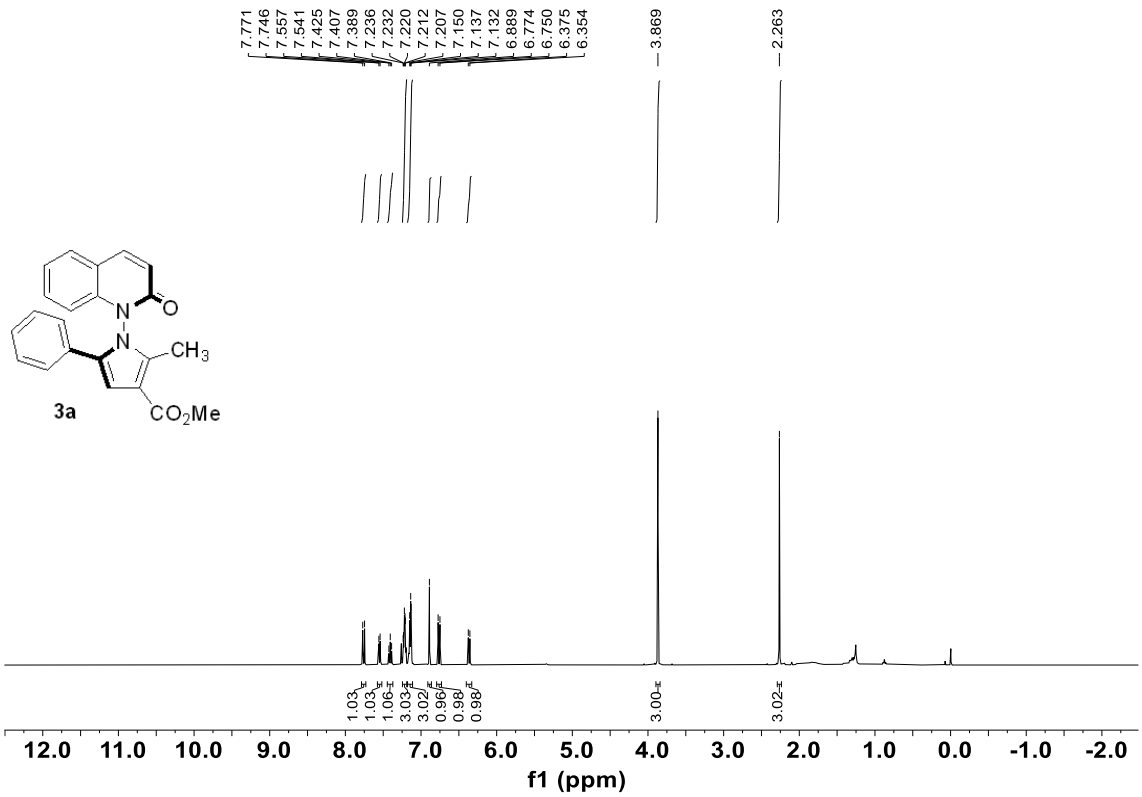
2g

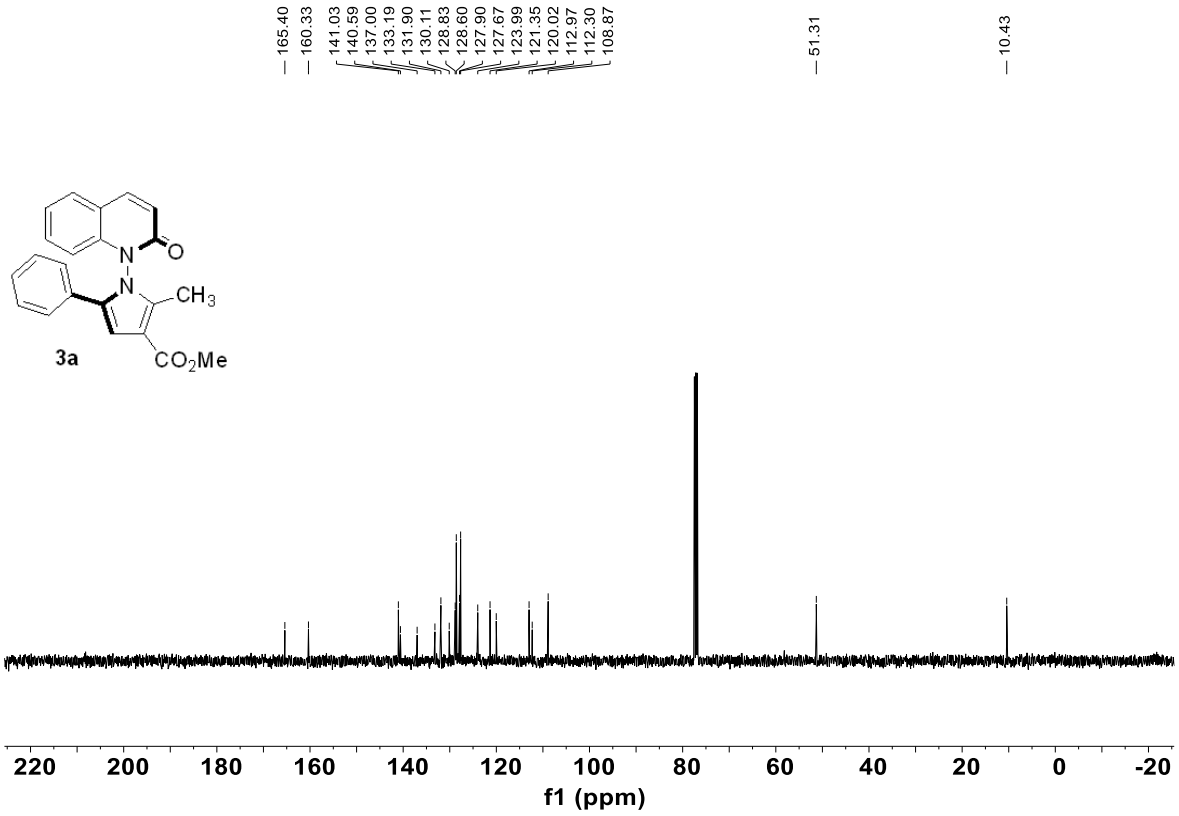
8.051
8.030
7.769
7.747
4.231
4.218
4.211
4.197
3.757
3.503
3.489
3.457
3.443
2.415
1.78
1.79
0.86
2.65
1.00
0.88
2.62
f1 (ppm)


201.90
196.03
169.10
138.97
132.64
128.63
117.89
116.79
53.63
52.96
37.59
30.29
CO2Me
NC
2g
f1 (ppm)


7.741
7.737
7.731
7.717
7.472
7.467
7.453
7.451
7.449
7.446
7.432
7.428
6.978
6.958
6.937
4.183
4.168
4.163
4.148
3.892
3.725
3.722
3.702
3.674
3.664
3.572
3.558
3.525
3.510
2.381
CO2Me
OMe
2k
1.00
1.01
2.06
1.00
3.04
1.00
3.08
f1 (ppm)


202.86
198.28
169.85
159.24
134.33
130.67
126.52
120.65
111.68
55.59
54.09
52.62
42.77
30.22
O
CO2Me
O
OMe
2k
f1 (ppm)


7.771
7.746
7.557
7.541
7.425
7.407
7.389
7.236
7.232
7.220
7.212
7.207
7.150
7.137
7.132
6.889
6.774
6.750
6.375
6.354
3.869
2.263
N
O
N
CH3
CO2Me
3a
1.03
1.03
1.06
3.03
3.02
0.96
0.98
0.98
3.00
3.02
f1 (ppm)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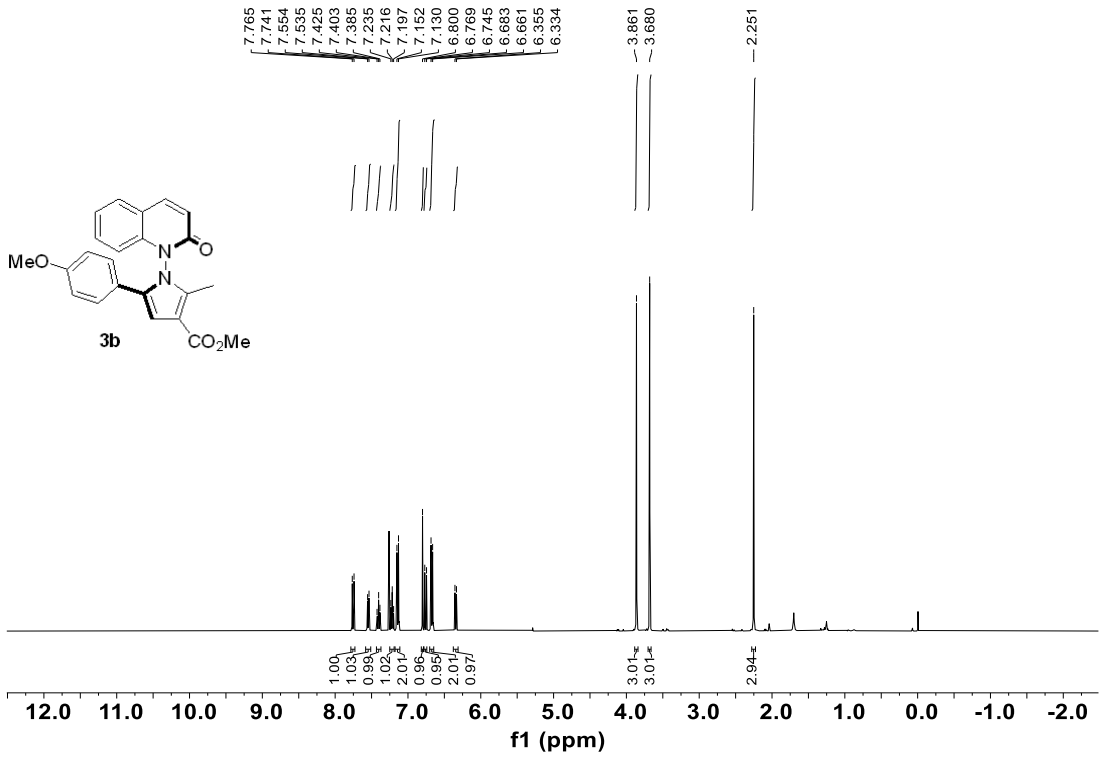
160.33
141.03
140.59
137.00
133.19
131.90
130.11
128.83
128.60
127.90
127.67
123.99
121.35
120.02
112.97
112.30
108.87
51.31
10.43
N
O
N
CH3
CO2Me
3a
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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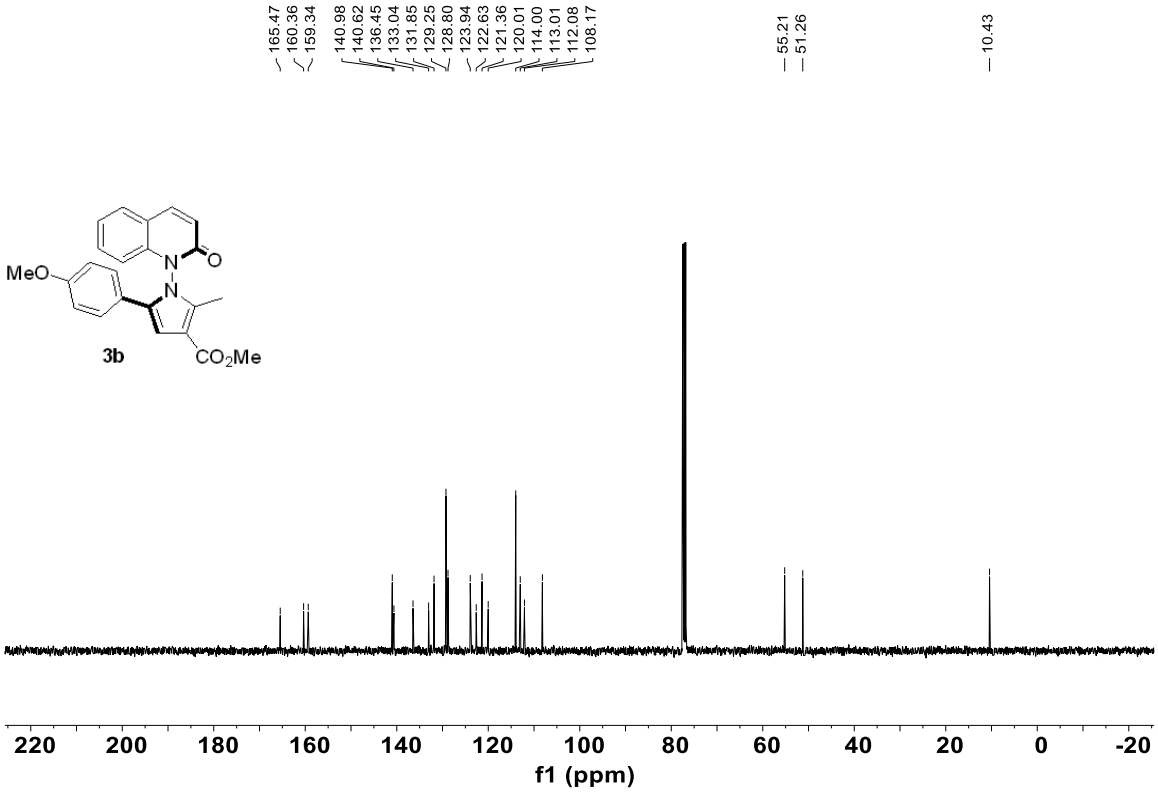
7.554
7.535
7.425
7.403
7.385
7.235
7.216
7.197
7.152
7.130
6.800
6.769
6.745
6.683
6.661
6.355
6.334
3.861
3.680
2.251
MeO
N
O
N
CO2Me
3b
1.00
1.03
0.99
1.02
2.01
0.96
0.95
2.01
0.97
3.01
3.01
2.94
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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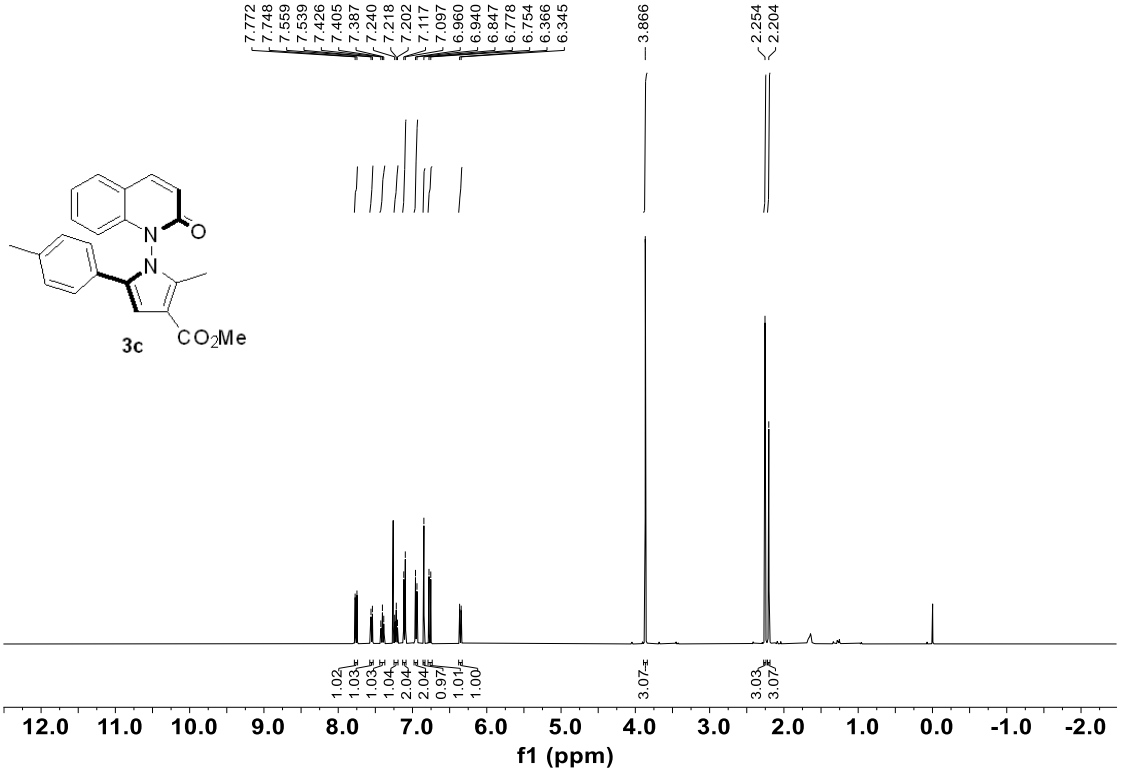
160.36
159.34
140.98
140.62
136.45
133.04
131.85
129.25
128.80
123.94
122.63
121.36
120.01
114.00
113.01
112.08
108.17
55.21
51.26
10.43
MeO
O
N
N
CO2Me
3b
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.539
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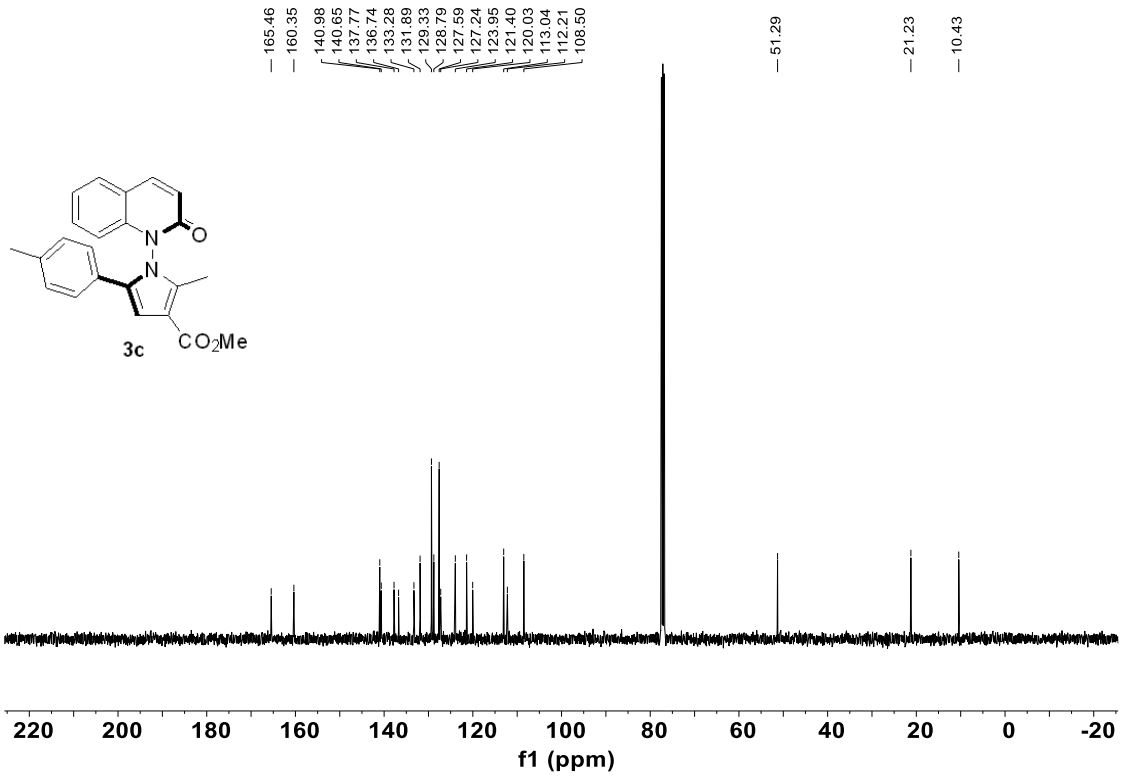
7.405
7.387
7.240
7.218
7.202
7.117
7.097
6.960
6.940
6.847
6.778
6.754
6.366
6.345
3.866
2.254
2.204
O
N
N
CO2Me
3c
1.02
1.03
1.03
1.04
2.04
2.04
0.97
1.01
1.00
3.07
3.03
3.07
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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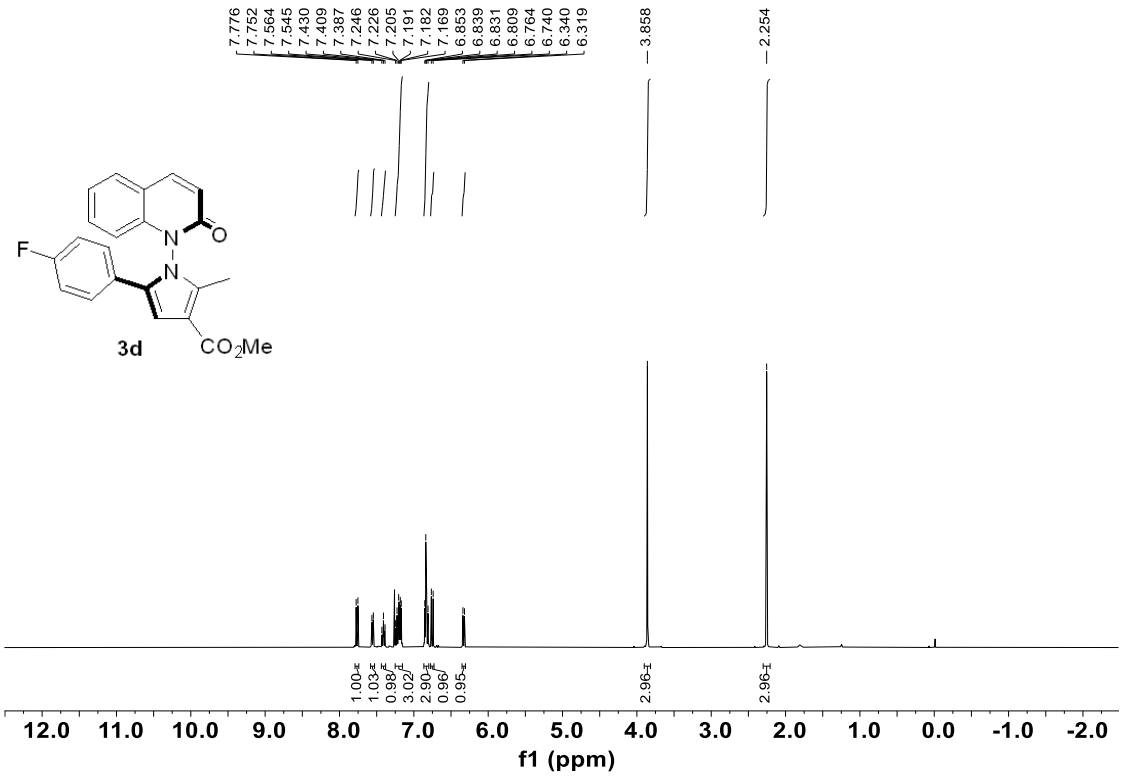
160.35
140.98
140.65
137.77
136.74
133.28
131.89
129.33
128.79
127.59
127.24
123.95
121.40
120.03
113.04
112.21
108.50
51.29
21.23
10.43
N
O
N
CO2Me
3c
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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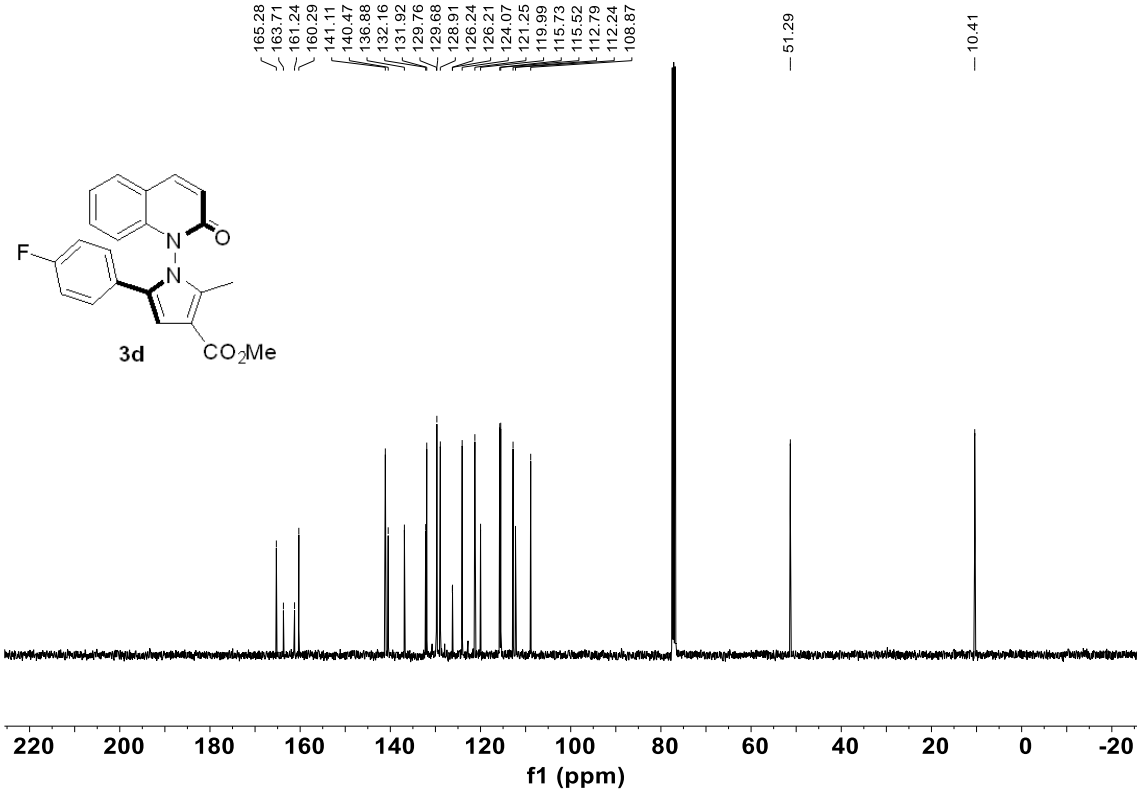
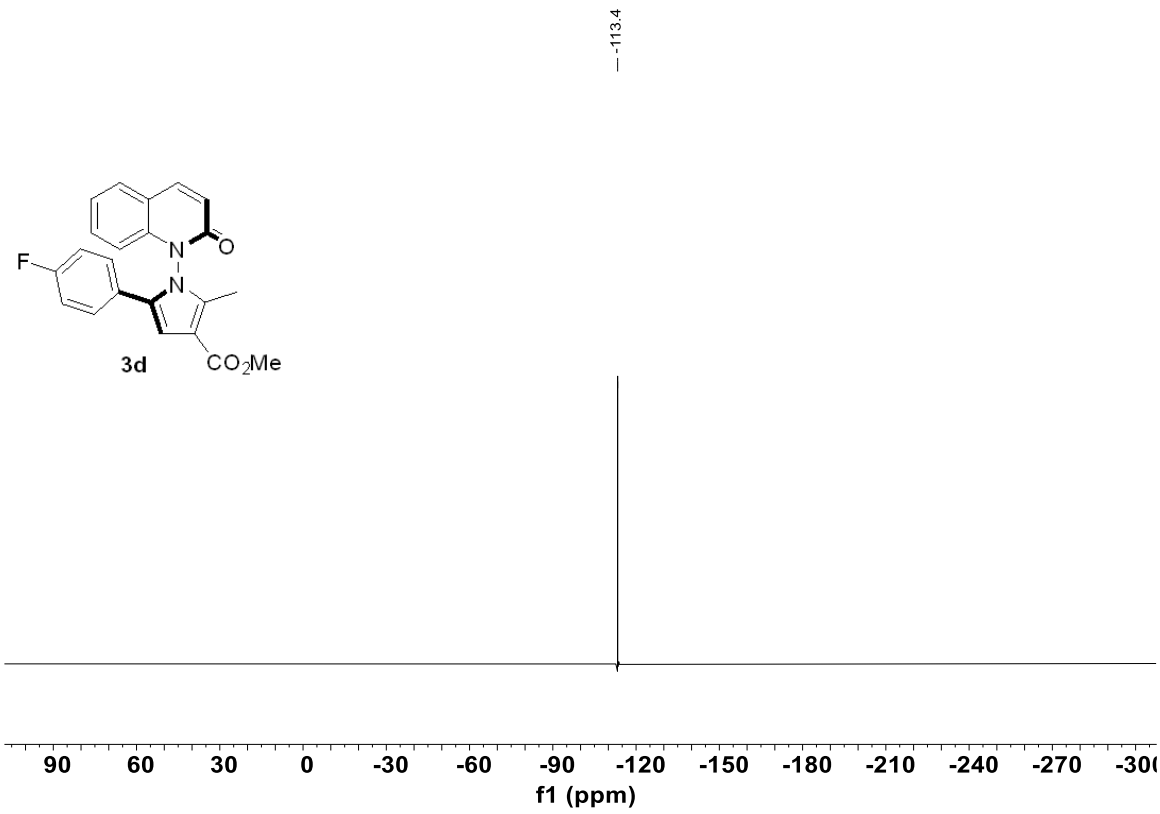
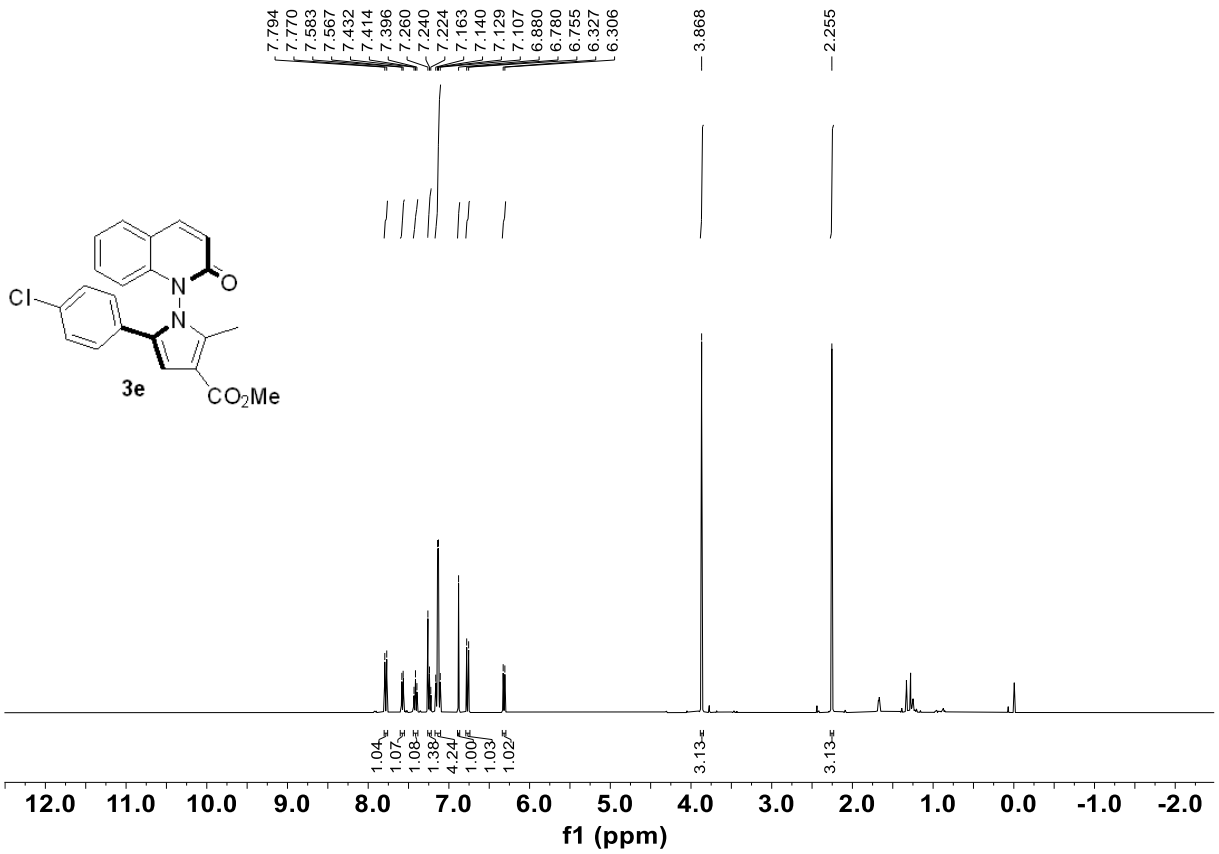
7.564
7.545
7.430
7.409
7.387
7.246
7.226
7.205
7.191
7.182
7.169
6.853
6.839
6.831
6.809
6.764
6.740
6.340
6.319
3.858
2.254
F
N
O
N
CO2Me
3d
1.00
1.03
0.98
3.02
2.90
0.96
0.95
2.96
2.96
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


165.28
163.71
161.24
160.29
141.11
140.47
136.88
132.16
131.92
129.76
129.68
128.91
126.24
126.21
124.07
121.25
119.99
115.73
115.52
112.79
112.24
108.87
51.29
10.41
F
N
N
O
3d
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


-113.4
F
N
N
O
3d
CO2Me
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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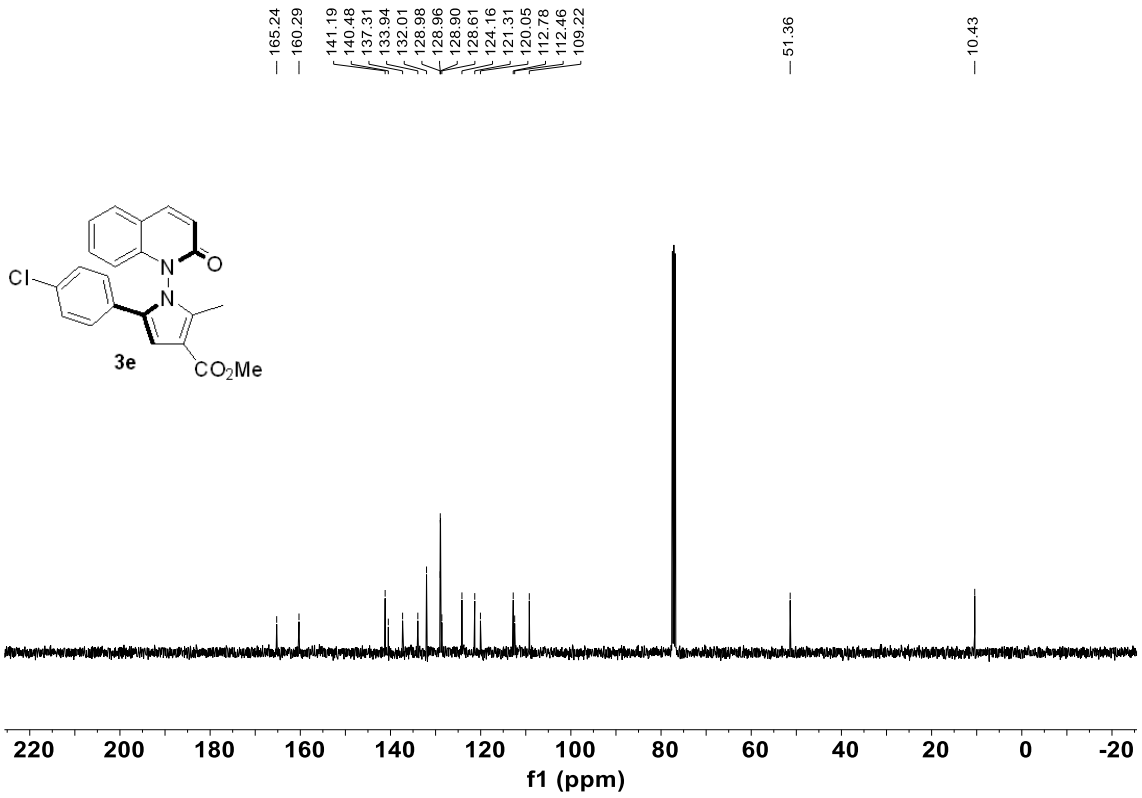
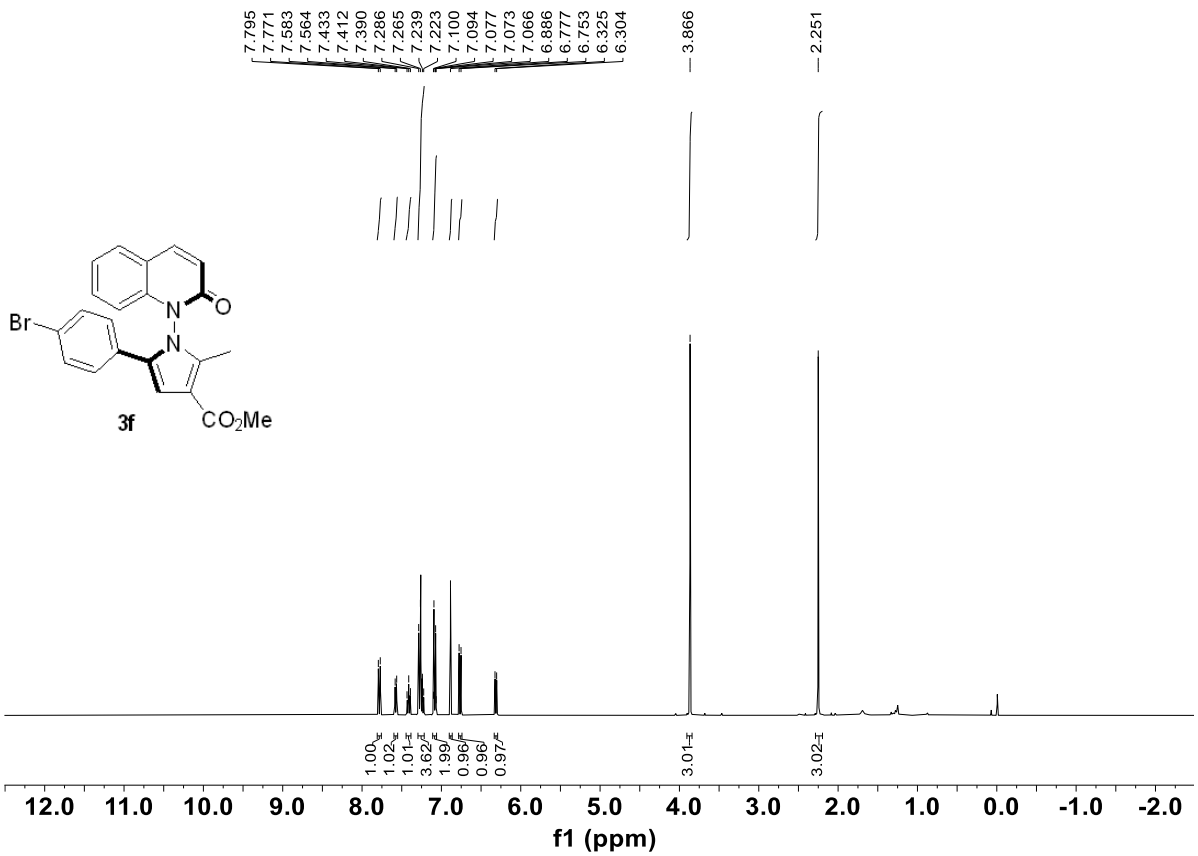
7.770
7.583
7.567
7.432
7.414
7.396
7.260
7.240
7.224
7.163
7.140
7.129
7.107
6.880
6.780
6.755
6.327
6.306
3.868
2.255
Cl
N
O
N
3e
CO2Me
1.04
1.07
1.08
1.38
4.24
1.00
1.03
1.02
3.13
3.13
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


165.24
160.29
141.19
140.48
137.31
133.94
132.01
128.98
128.96
128.90
128.61
124.16
121.31
120.05
112.78
112.46
109.22
51.36
10.43
Cl
N
O
N
3e
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.795
7.771
7.583
7.564
7.433
7.412
7.390
7.286
7.265
7.239
7.223
7.100
7.094
7.077
7.073
7.066
6.886
6.777
6.753
6.325
6.304
3.866
2.251
Br
N
N
O
CO2Me
3f
1.00
1.02
1.01
3.62
1.99
0.96
0.96
0.97
3.01
3.02
12.0
11.0
10.0
9.0
8.0
7.0
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5.0
4.0
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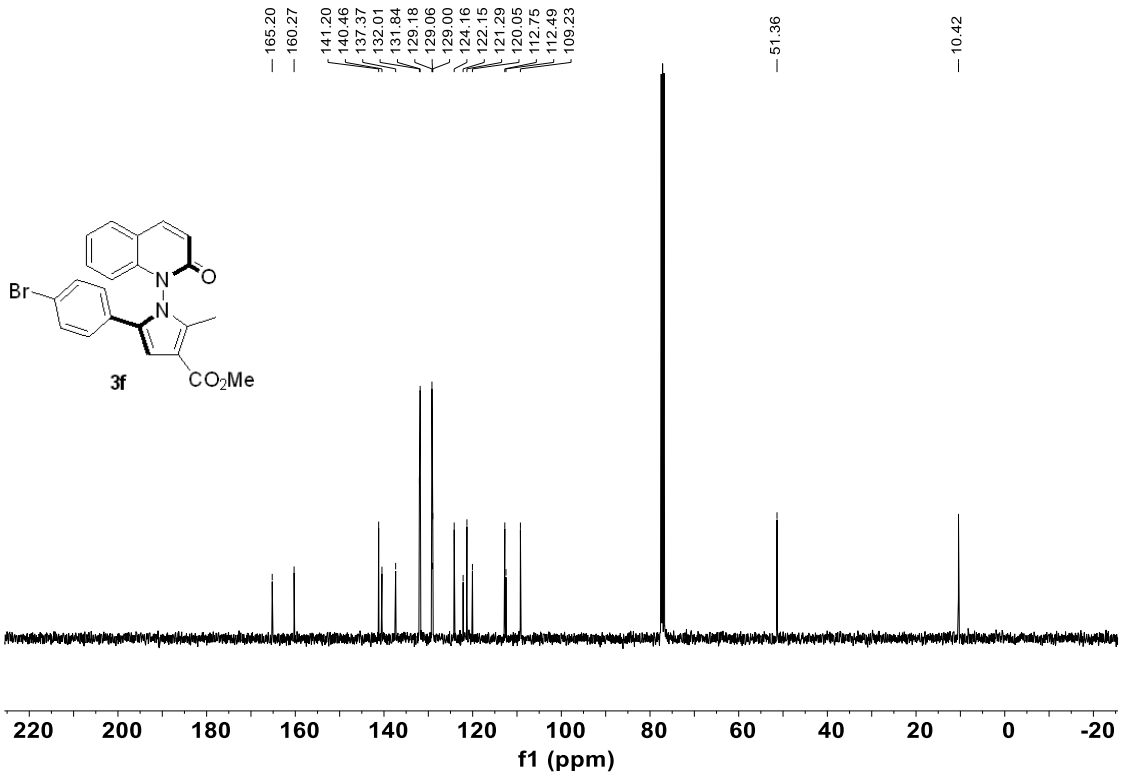
-2.0
f1 (ppm)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160.27
141.20
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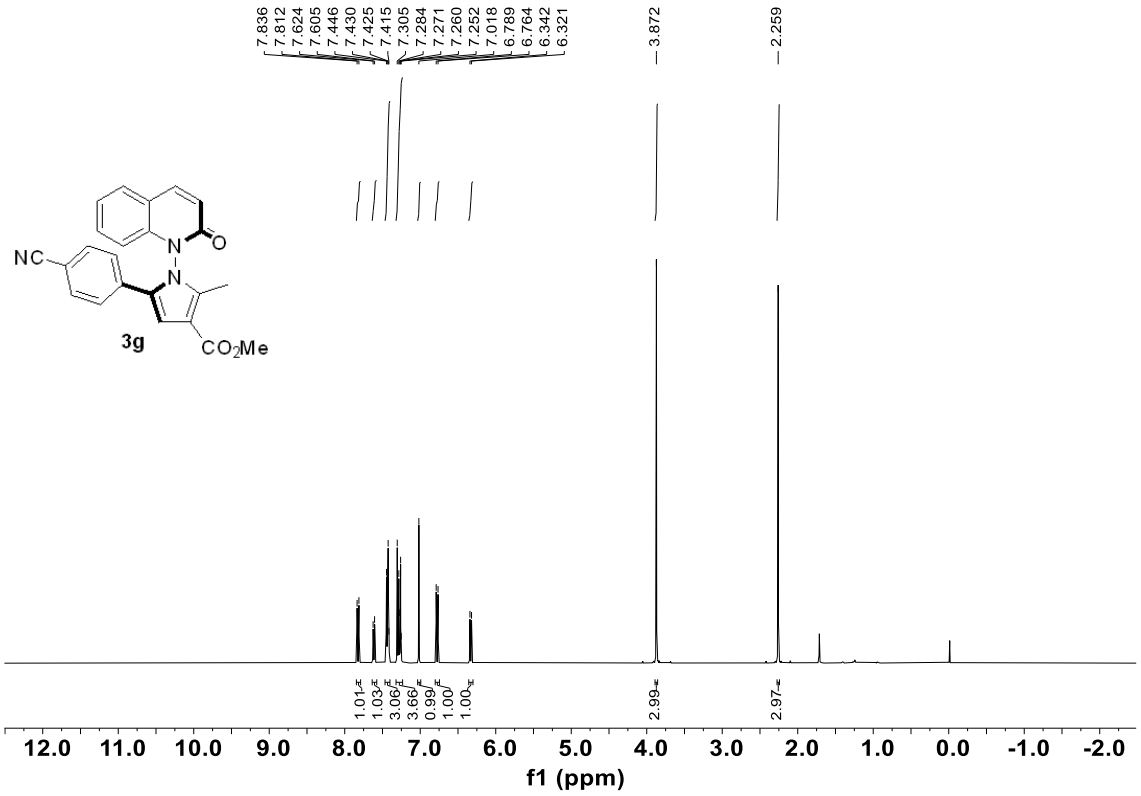
137.37
132.01
131.84
129.18
129.06
129.00
124.16
122.15
121.29
120.05
112.75
112.49
109.23
51.36
10.42
Br
N
N
O
CO2Me
3f
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.624
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7.425
7.415
7.305
7.284
7.271
7.260
7.252
7.018
6.789
6.764
6.342
6.321
3.872
2.259
NC
N
N
O
3g
CO2Me
1.01
1.03
3.06
0.99
1.00
1.00
2.99
2.97
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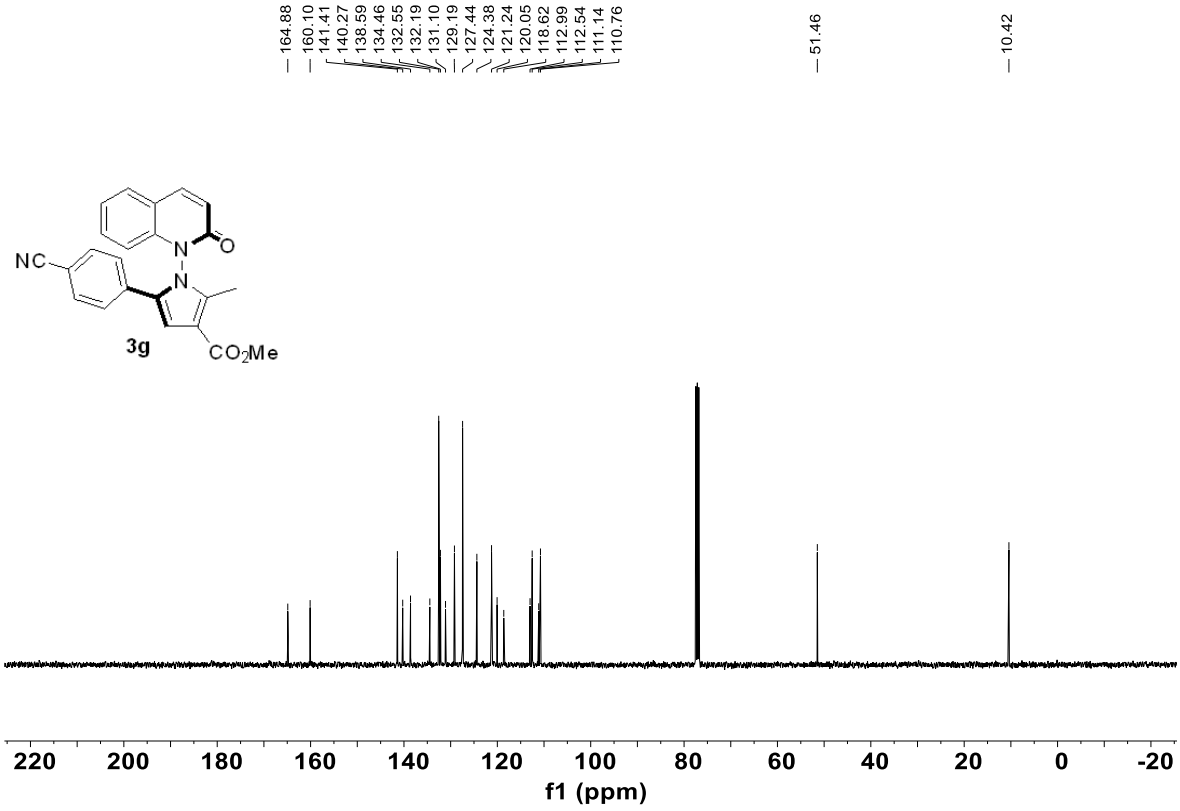
f1 (ppm)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132.19
131.10
129.19
127.44
124.38
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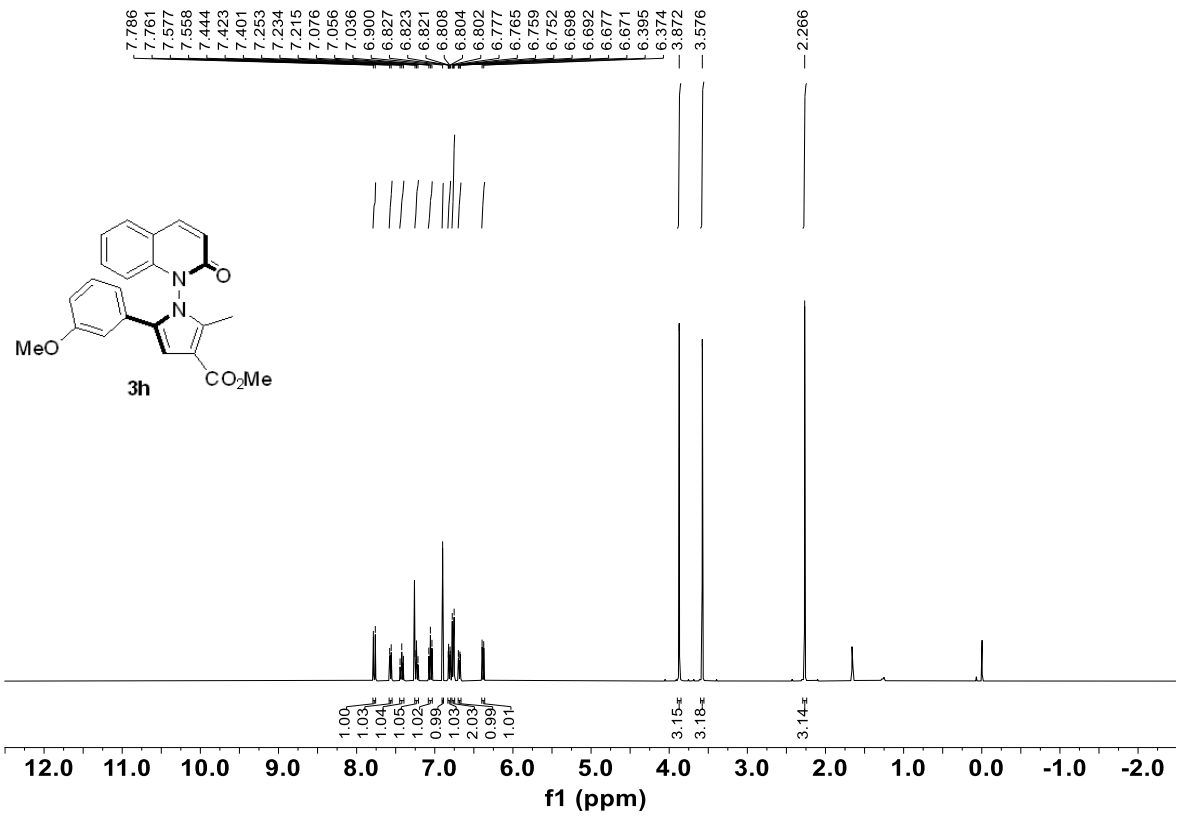
120.05
118.62
112.99
112.54
111.14
110.76
51.46
10.42
NC
N
N
O
3g
CO2Me
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)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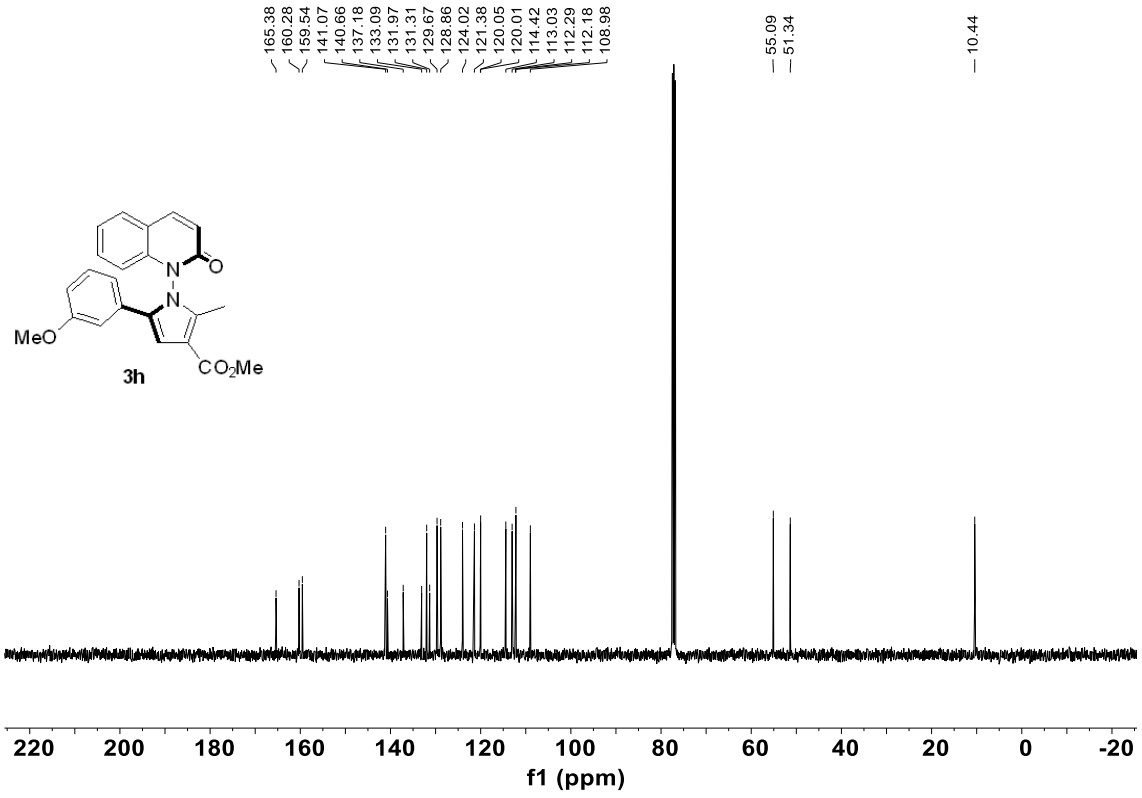
7.444
7.423
7.401
7.253
7.234
7.215
7.076
7.056
7.036
6.900
6.827
6.823
6.821
6.808
6.804
6.802
6.777
6.765
6.759
6.752
6.698
6.692
6.677
6.671
6.395
6.374
3.872
3.576
2.266
MeO
CO2Me
3h
1.00
1.03
1.04
1.05
1.02
0.99
1.03
2.03
0.99
1.01
3.15
3.18
3.14
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)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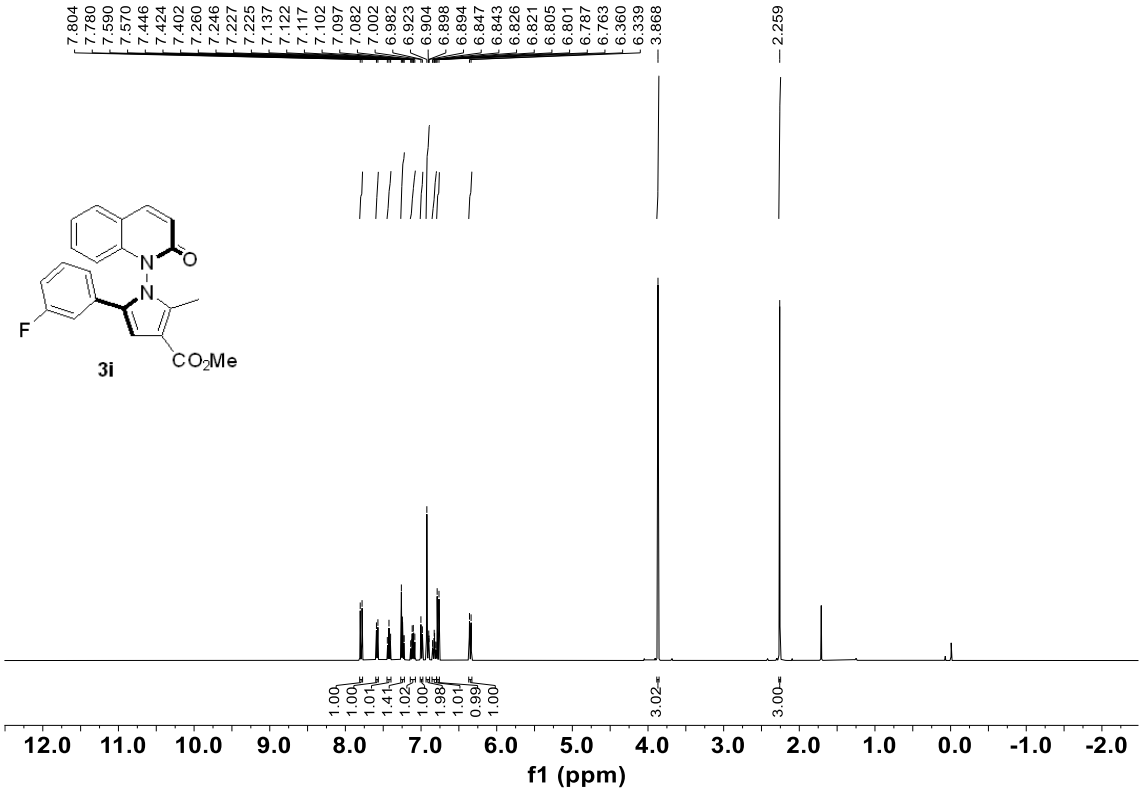
131.97
131.31
129.67
128.86
124.02
121.38
120.05
120.01
114.42
113.03
112.29
112.18
108.98
55.09
51.34
10.44
MeO
CO2Me
3h
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)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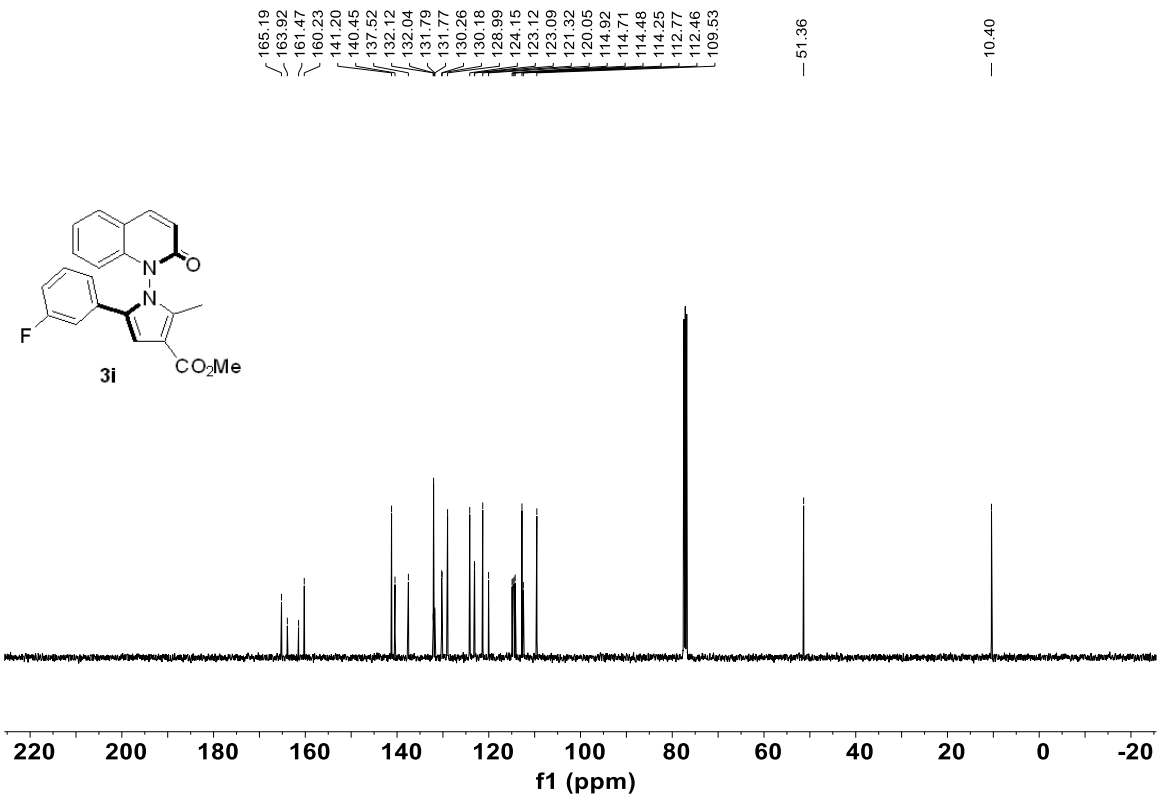
7.260
7.246
7.227
7.225
7.137
7.122
7.117
7.102
7.097
7.082
7.002
6.982
6.923
6.904
6.898
6.894
6.847
6.843
6.826
6.821
6.805
6.801
6.787
6.763
6.360
6.339
3.868
2.259
1.00
1.00
1.01
1.41
1.02
1.00
1.98
1.01
0.99
1.00
3.02
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)

O
N
N
F
CO2Me

3i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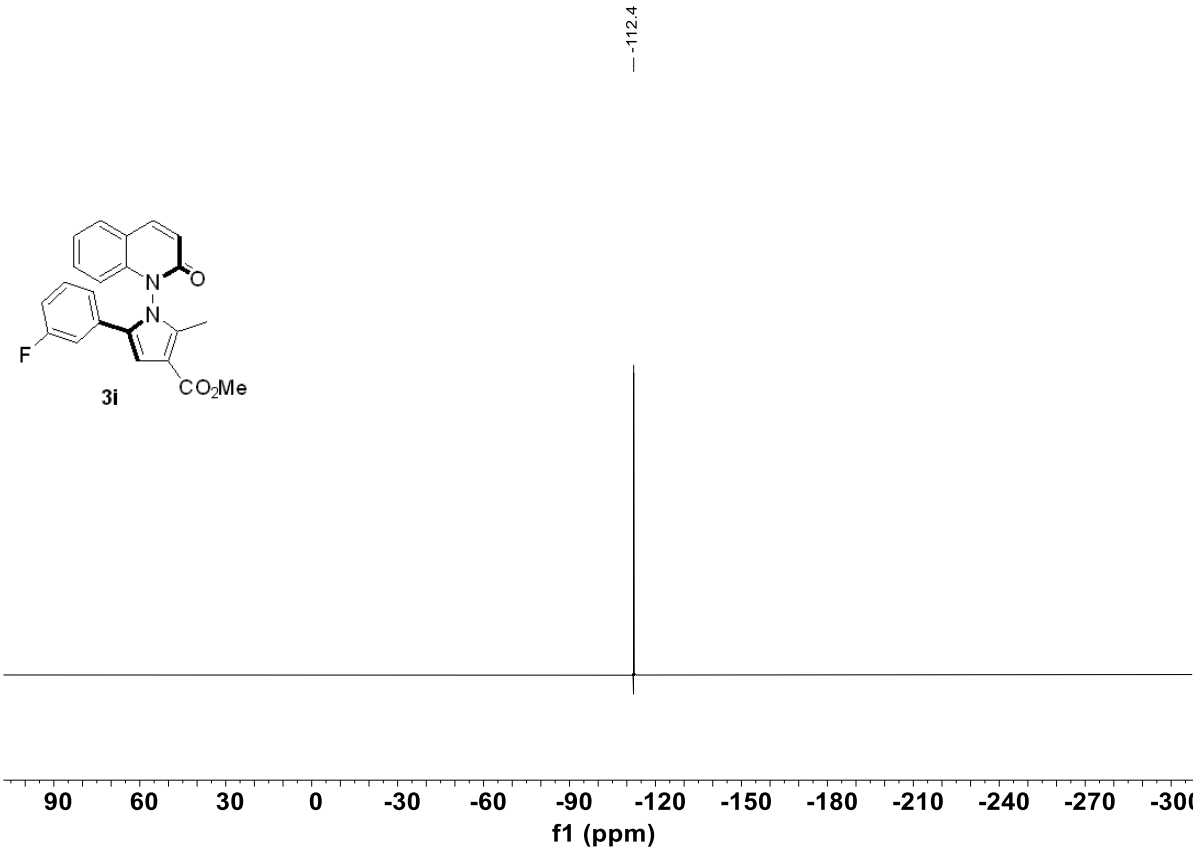
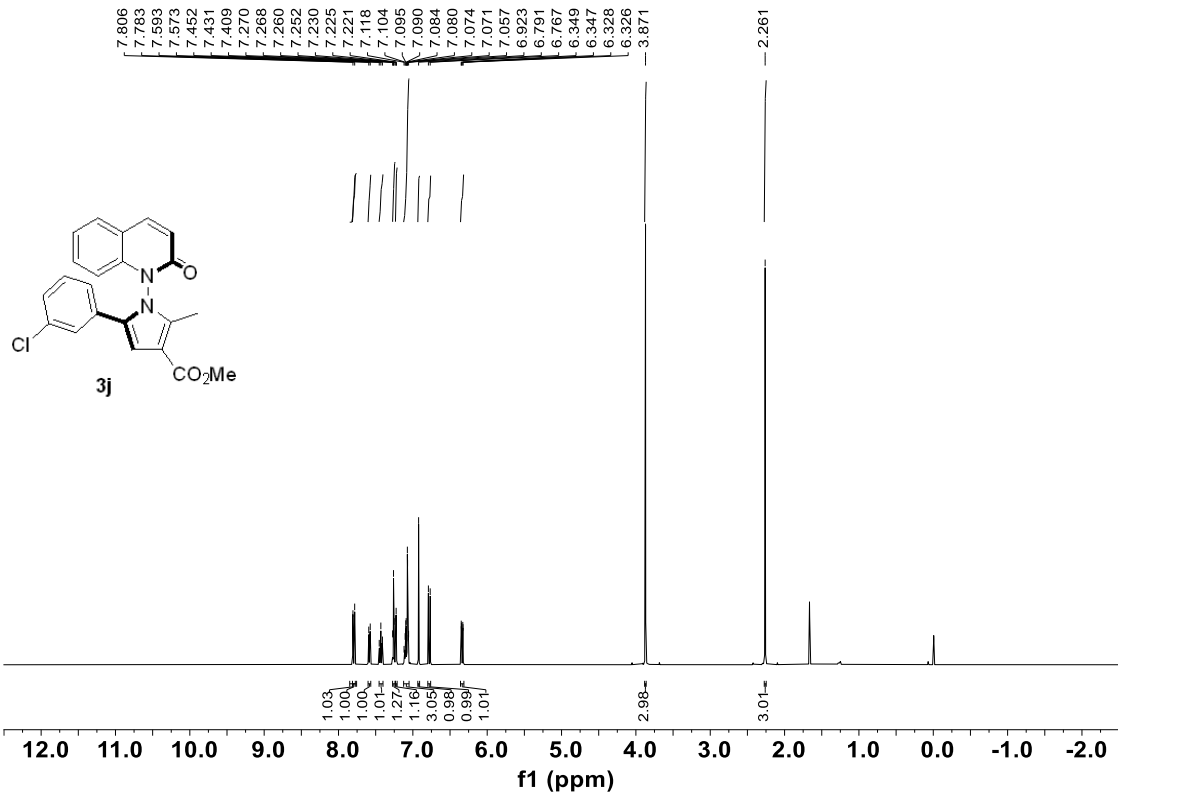
163.92
161.47
160.23
141.20
140.45
137.52
132.12
132.04
131.79
131.77
130.26
130.18
128.99
124.15
123.12
123.09
121.32
120.05
114.92
114.71
114.48
114.25
112.77
112.46
109.53
51.36
10.40
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)

O
N
N
F
CO2Me

3i


-112.4
F
O
N
N
CO2Me
3i
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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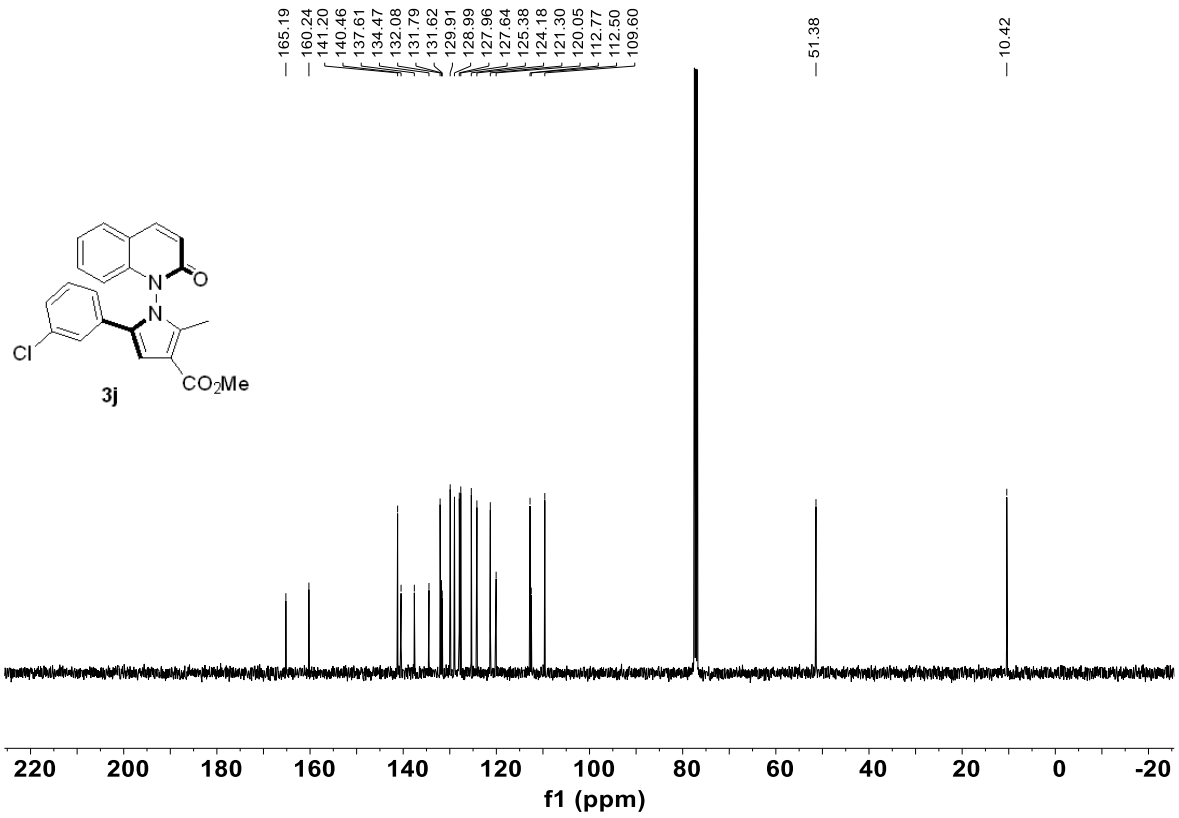
7.783
7.593
7.573
7.452
7.431
7.409
7.270
7.268
7.260
7.252
7.230
7.225
7.221
7.118
7.104
7.095
7.090
7.084
7.080
7.074
7.071
7.057
6.923
6.791
6.767
6.349
6.347
6.328
6.326
3.871
2.261
Cl
O
N
N
CO2Me
3j
1.03
1.00
1.00
1.01
1.27
1.16
3.05
0.98
0.99
1.01
2.98
3.01
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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137.61
134.47
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131.79
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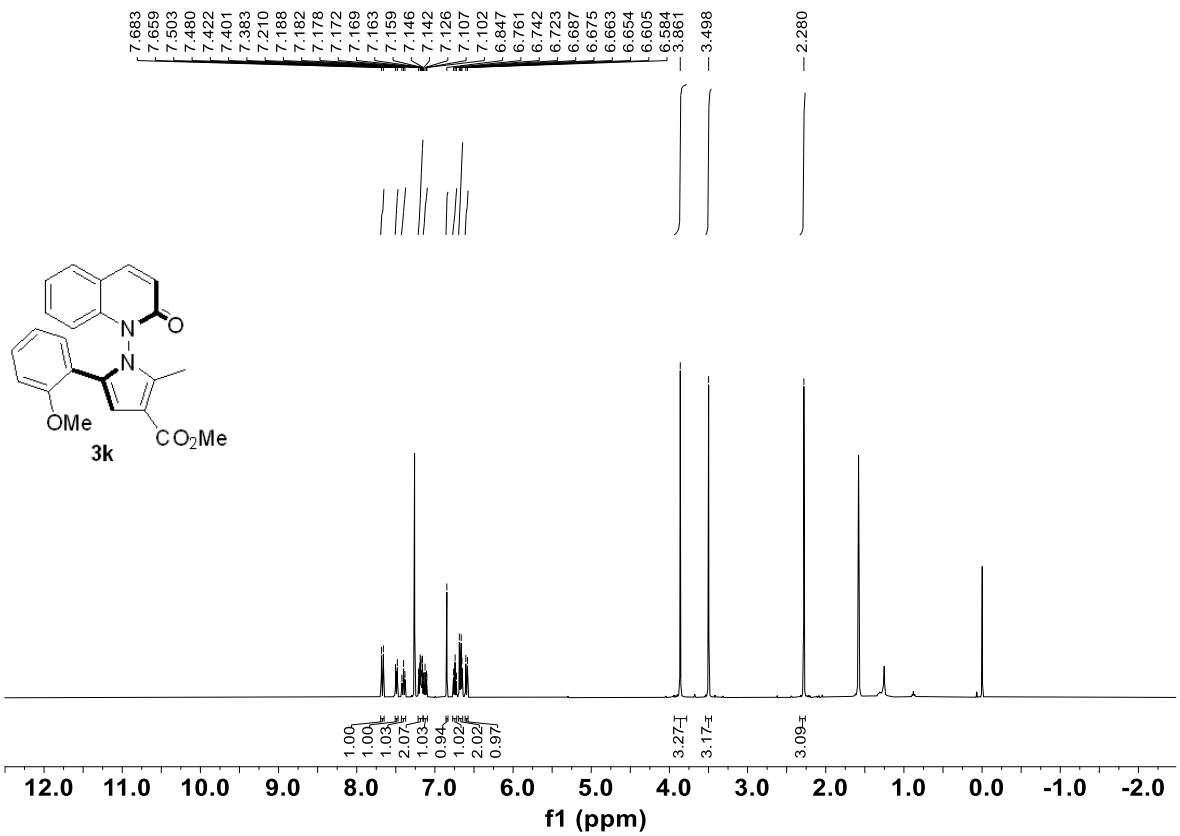
129.91
128.99
127.96
127.64
125.38
124.18
121.30
120.05
112.77
112.50
109.60
51.38
10.42
Cl
N
O
N
CO2Me
3j
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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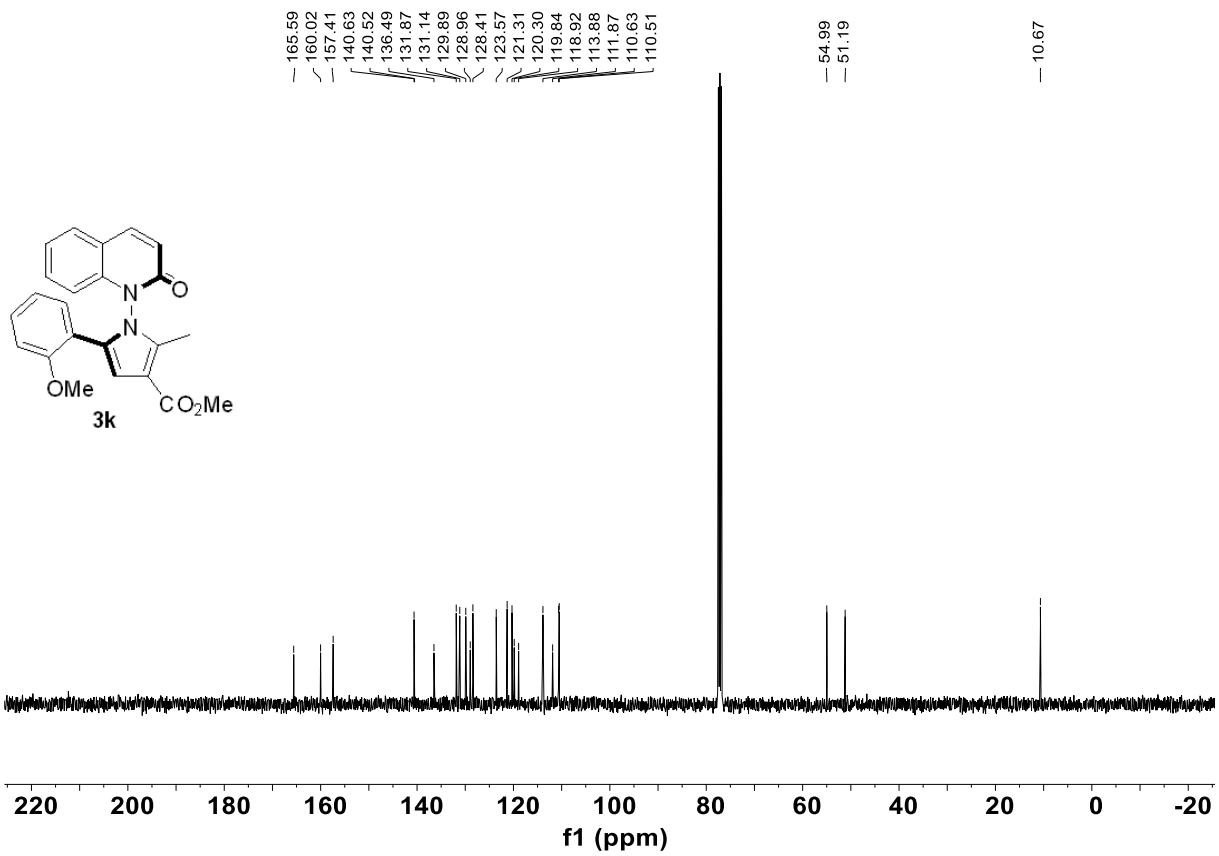
7.480
7.422
7.401
7.383
7.210
7.188
7.182
7.178
7.172
7.169
7.163
7.159
7.146
7.142
7.126
7.107
7.102
6.847
6.761
6.742
6.723
6.687
6.675
6.663
6.654
6.605
6.584
3.861
3.498
2.280
N
O
N
OMe
CO2Me
3k
1.00
1.00
1.03
2.07
1.03
0.94
1.02
2.02
0.97
3.27
3.17
3.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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157.41
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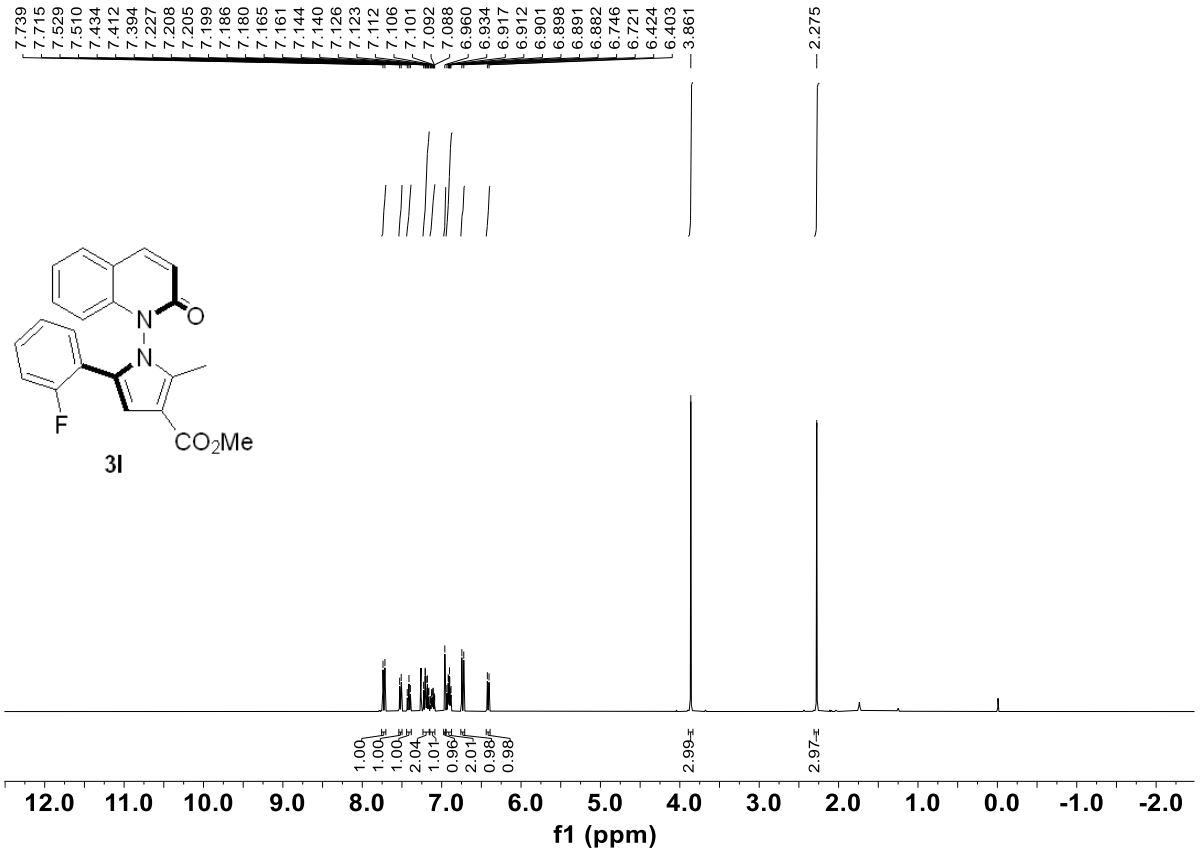
136.49
131.87
131.14
129.89
128.96
128.41
123.57
121.31
120.30
119.84
118.92
113.88
111.87
110.63
110.51
54.99
51.19
10.67
OMe
CO2Me
3k
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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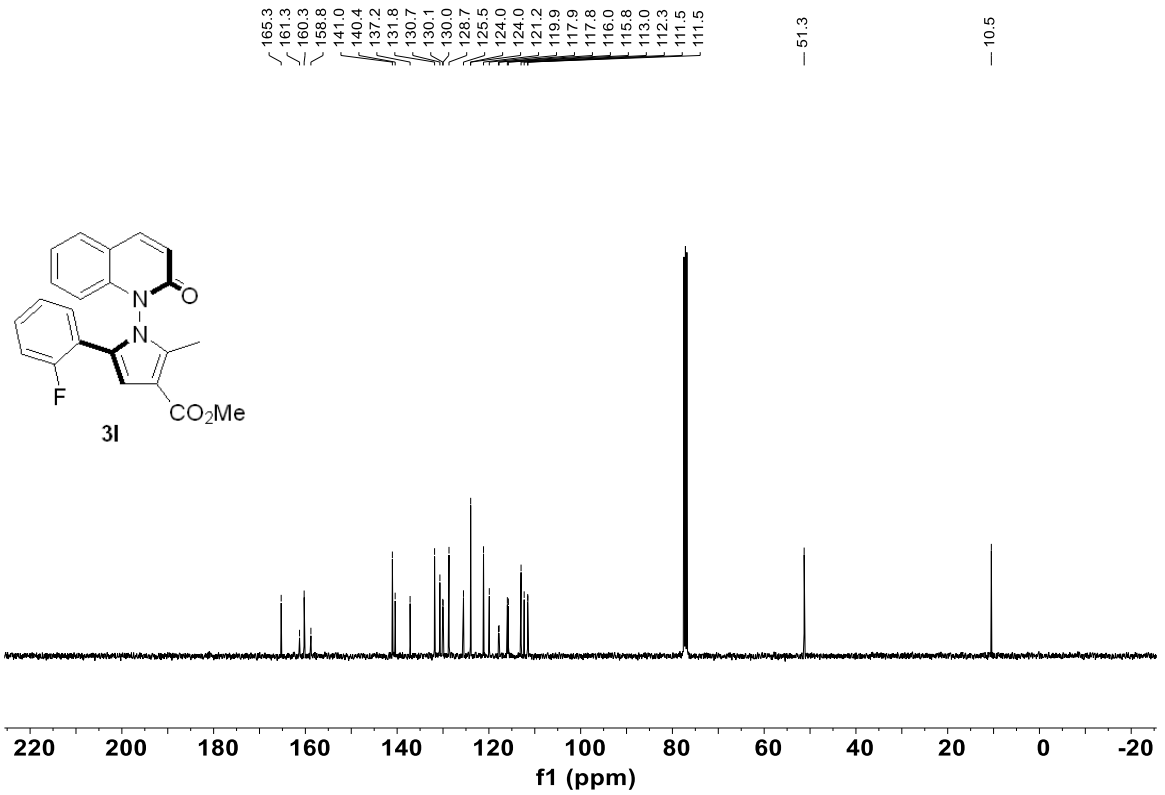
7.434
7.412
7.394
7.227
7.208
7.205
7.199
7.186
7.180
7.165
7.161
7.144
7.140
7.126
7.123
7.112
7.106
7.101
7.092
7.088
6.960
6.934
6.917
6.912
6.901
6.898
6.891
6.882
6.746
6.721
6.424
6.403
3.861
2.275
F
CO2Me
3l
1.00
1.00
1.00
2.04
1.01
0.96
2.01
0.98
0.98
2.99
2.97
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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160.3
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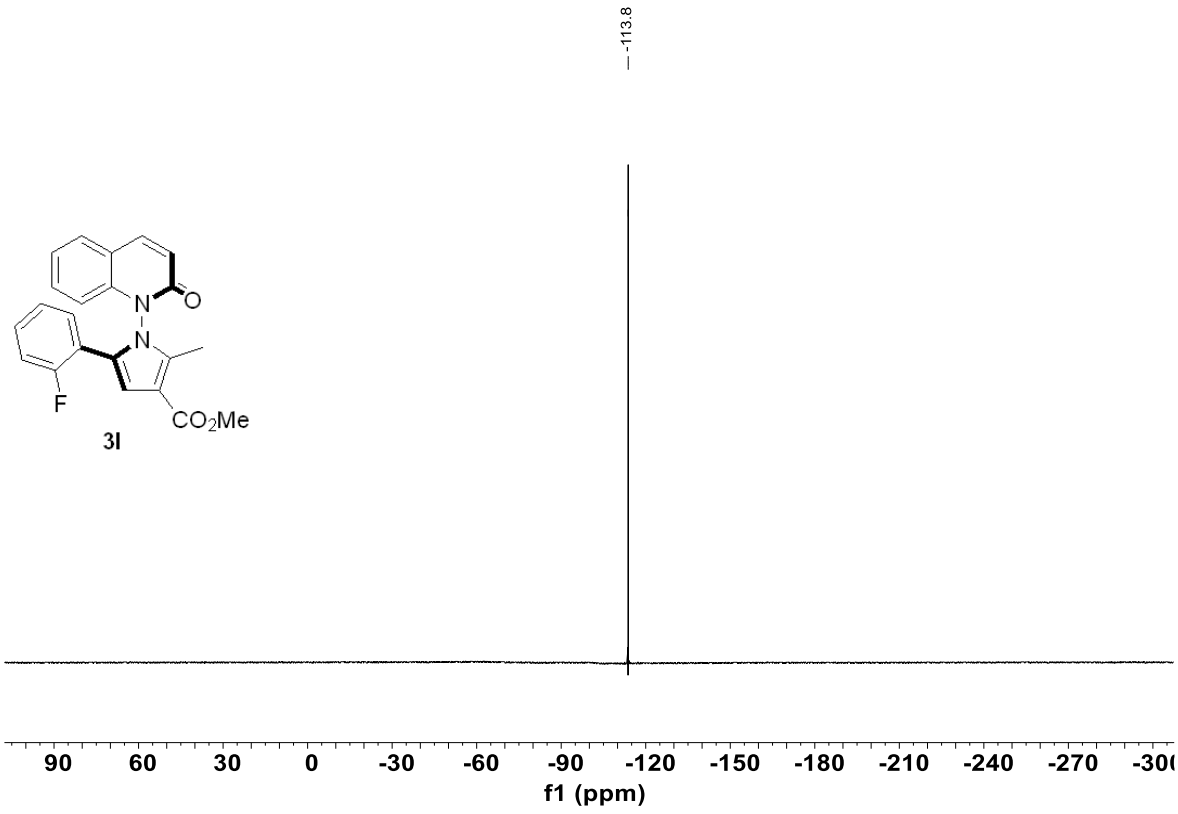
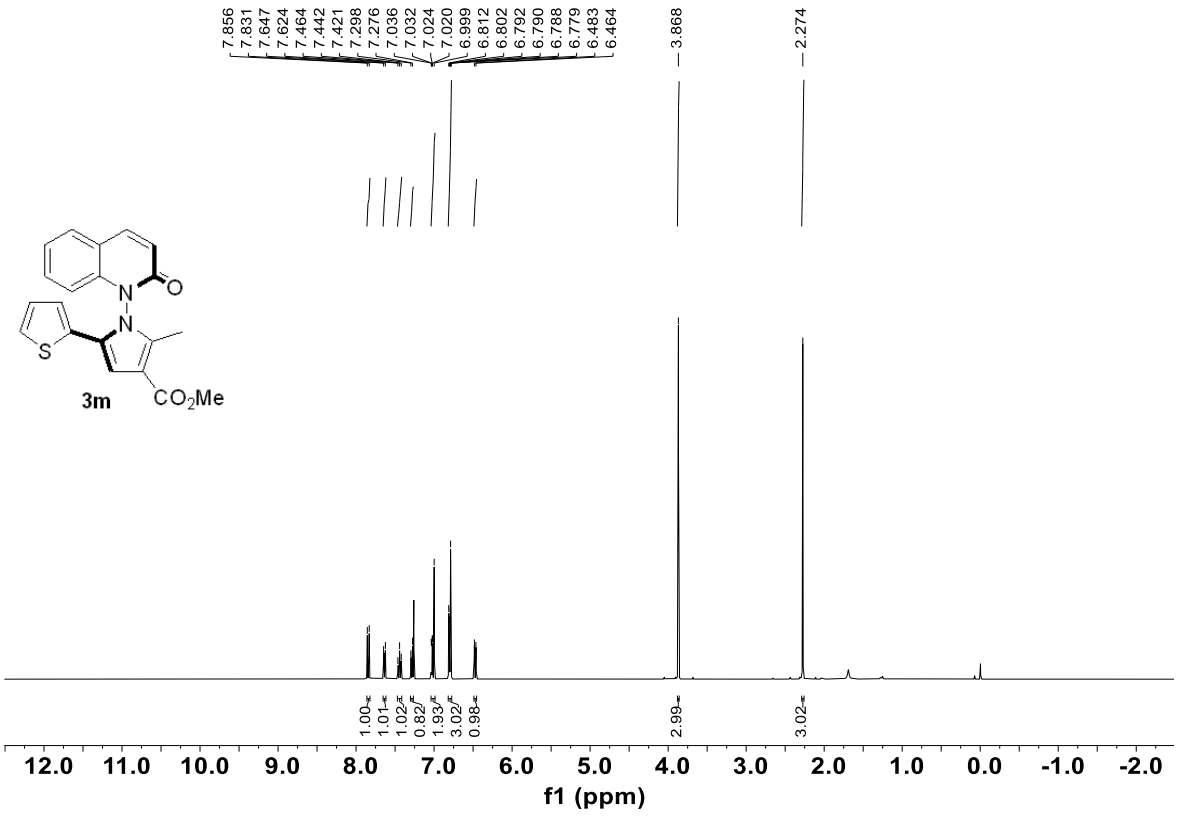
130.1
130.0
128.7
125.5
124.0
124.0
121.2
119.9
117.9
117.8
116.0
115.8
113.0
112.3
111.5
111.5
51.3
10.5
N
O
N
F
CO2Me
3l
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


-113.8
N
O
N
F
CO2Me
3l
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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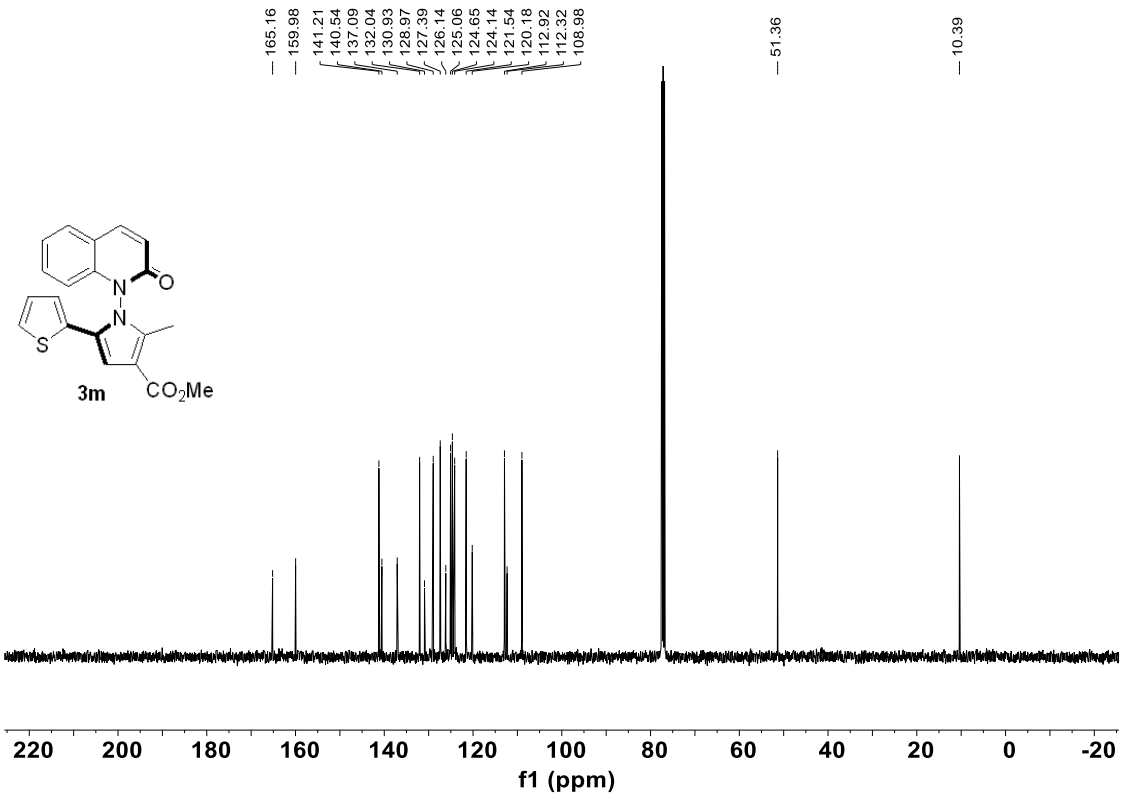
7.421
7.298
7.276
7.036
7.032
7.024
7.020
6.999
6.812
6.802
6.792
6.790
6.788
6.779
6.483
6.464
3.868
2.274
1.00
1.01
1.02
0.82
1.93
3.02
0.98
2.99
3.02
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)
3m
CO2Me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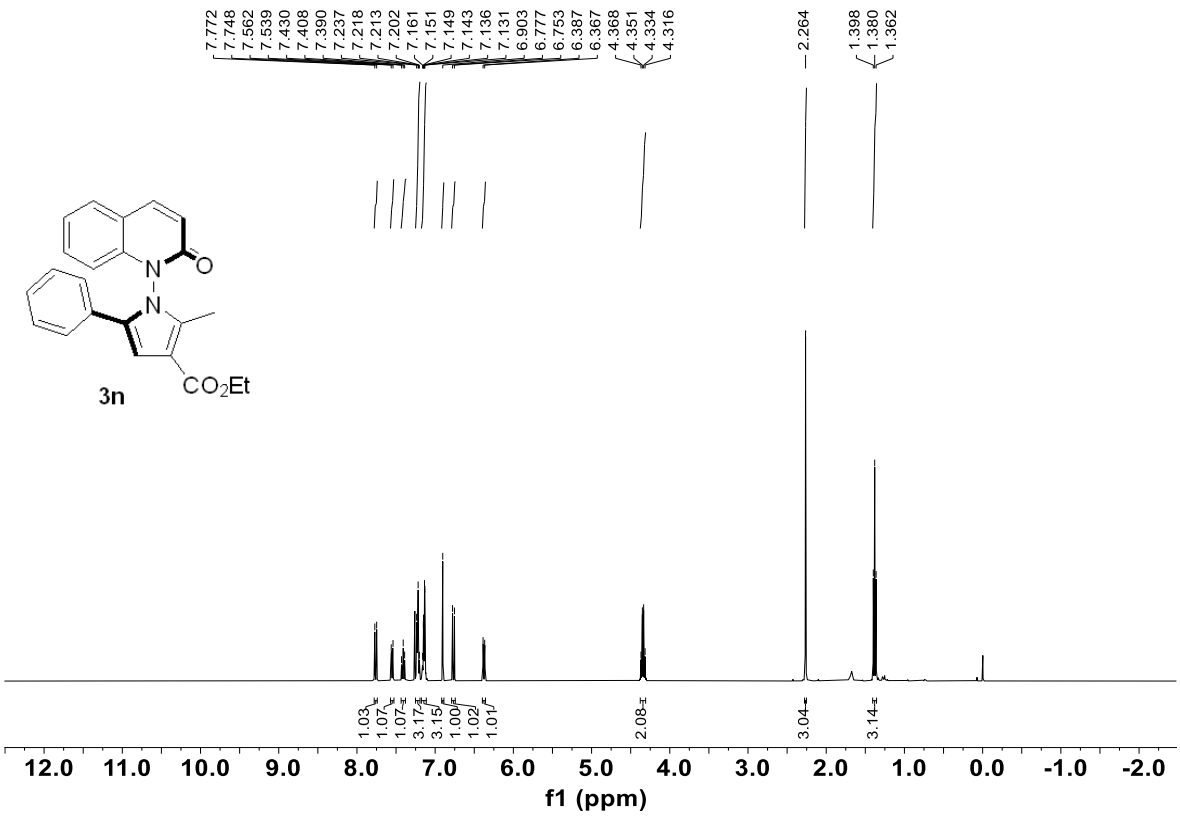
141.21
140.54
137.09
132.04
130.93
128.97
127.39
126.14
125.06
124.65
124.14
121.54
120.18
112.92
112.32
108.98
51.36
10.39
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)
3m
CO2Me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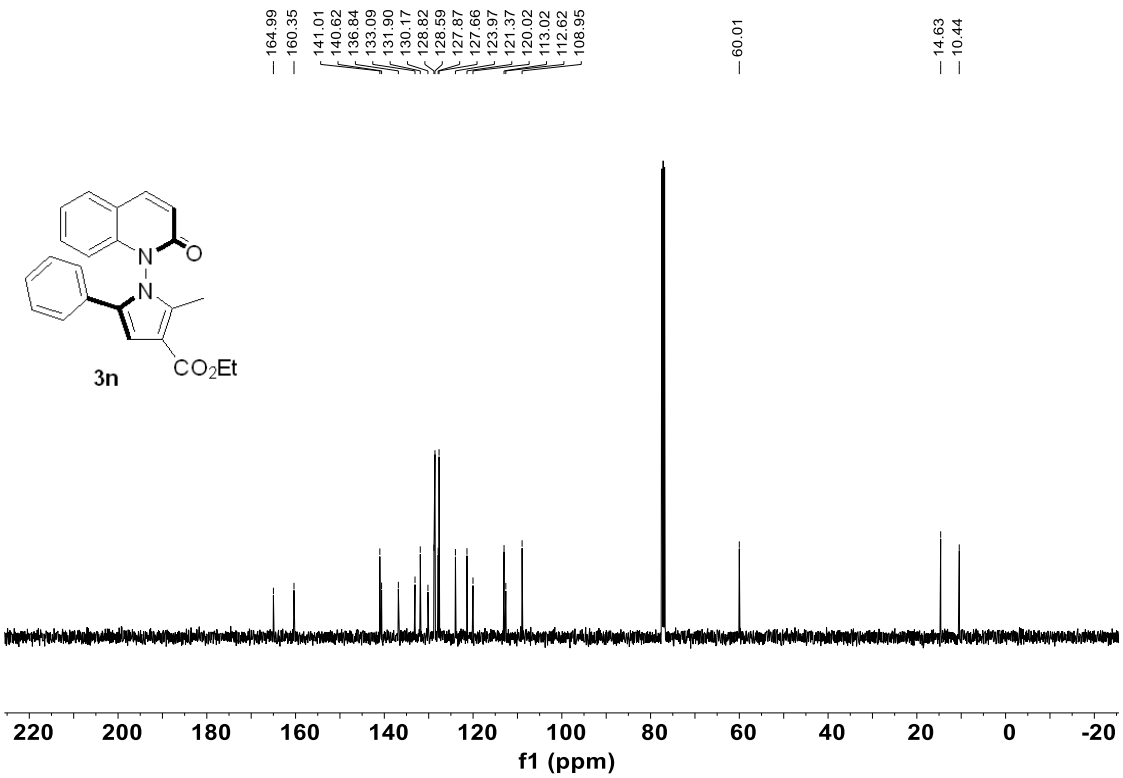
7.408
7.390
7.237
7.218
7.213
7.202
7.161
7.151
7.149
7.143
7.136
7.131
6.903
6.777
6.753
6.387
6.367
4.368
4.351
4.334
4.316
2.264
1.398
1.380
1.362
1.03
1.07
1.07
3.17
3.15
1.00
1.02
1.01
2.08
3.04
3.14
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)
3n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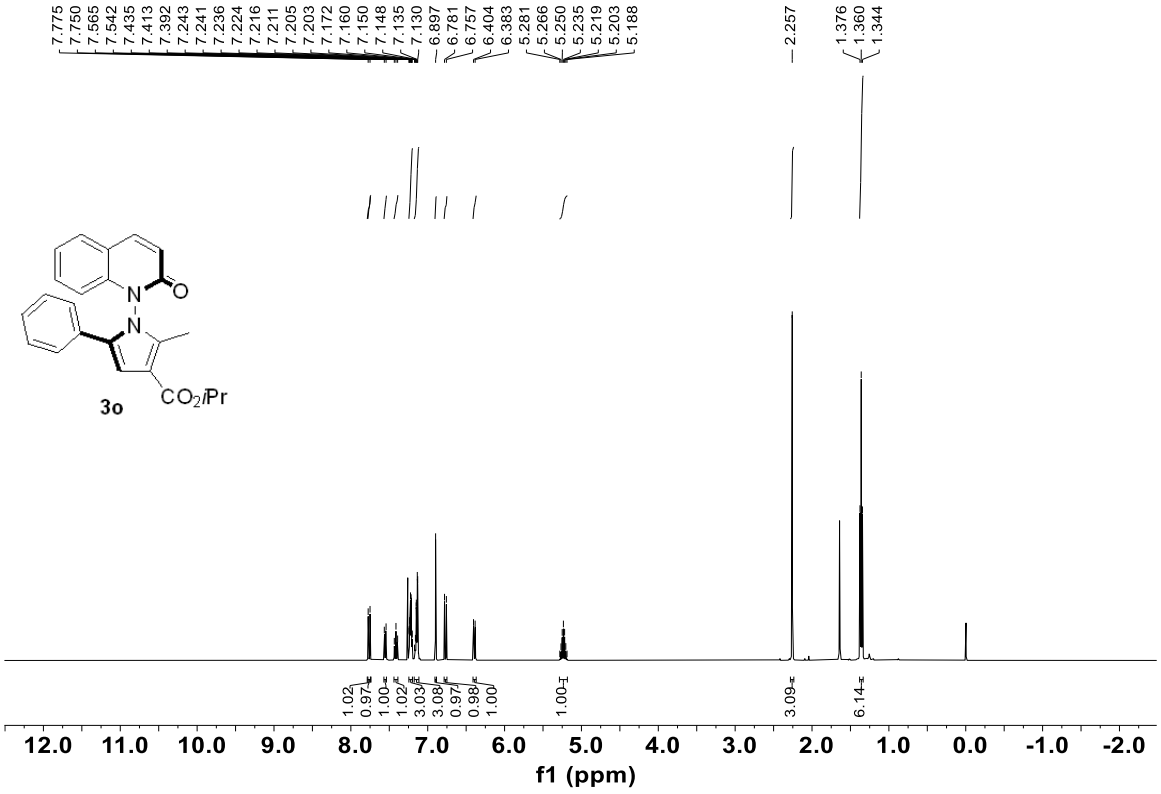
140.62
136.84
133.09
131.90
130.17
128.82
128.59
127.87
127.66
123.97
121.37
120.02
113.02
112.62
108.95
60.01
14.63
10.44
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)
3n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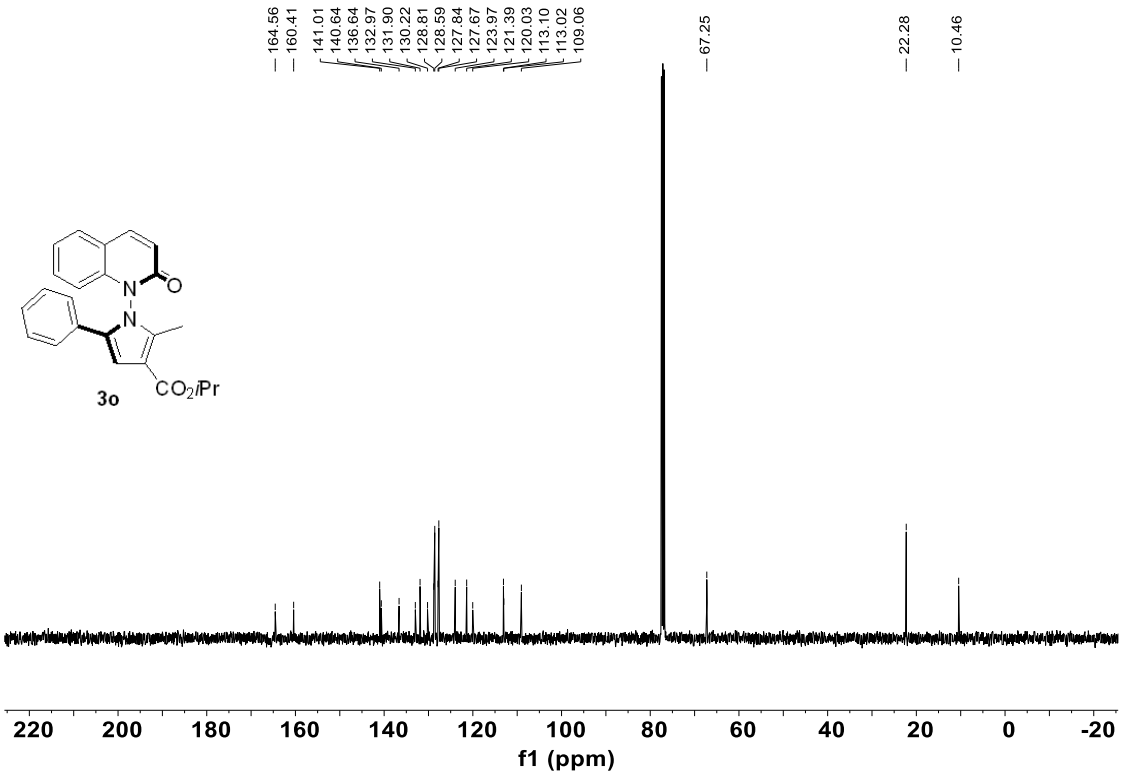
7.435
7.413
7.392
7.243
7.241
7.236
7.224
7.216
7.211
7.205
7.203
7.172
7.160
7.150
7.148
7.135
7.130
6.897
6.781
6.757
6.404
6.383
5.281
5.266
5.250
5.235
5.219
5.203
5.188
2.257
1.376
1.360
1.344
N
O
N
CO2iPr
3o
1.02
0.97
1.00
1.02
3.03
3.08
0.97
0.98
1.00
1.00
3.09
6.14
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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132.97
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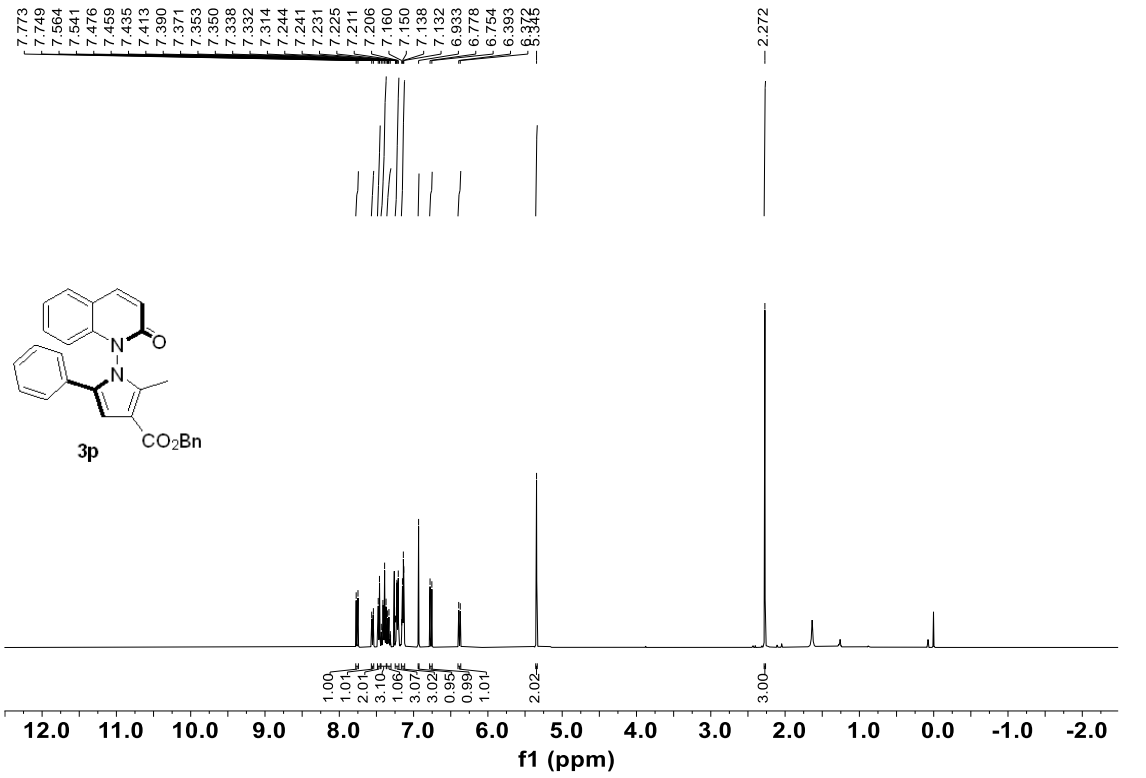
130.22
128.81
128.59
127.84
127.67
123.97
121.39
120.03
113.10
113.02
109.06
67.25
22.28
10.46
N
O
N
CO2iPr
3o
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.413
7.390
7.371
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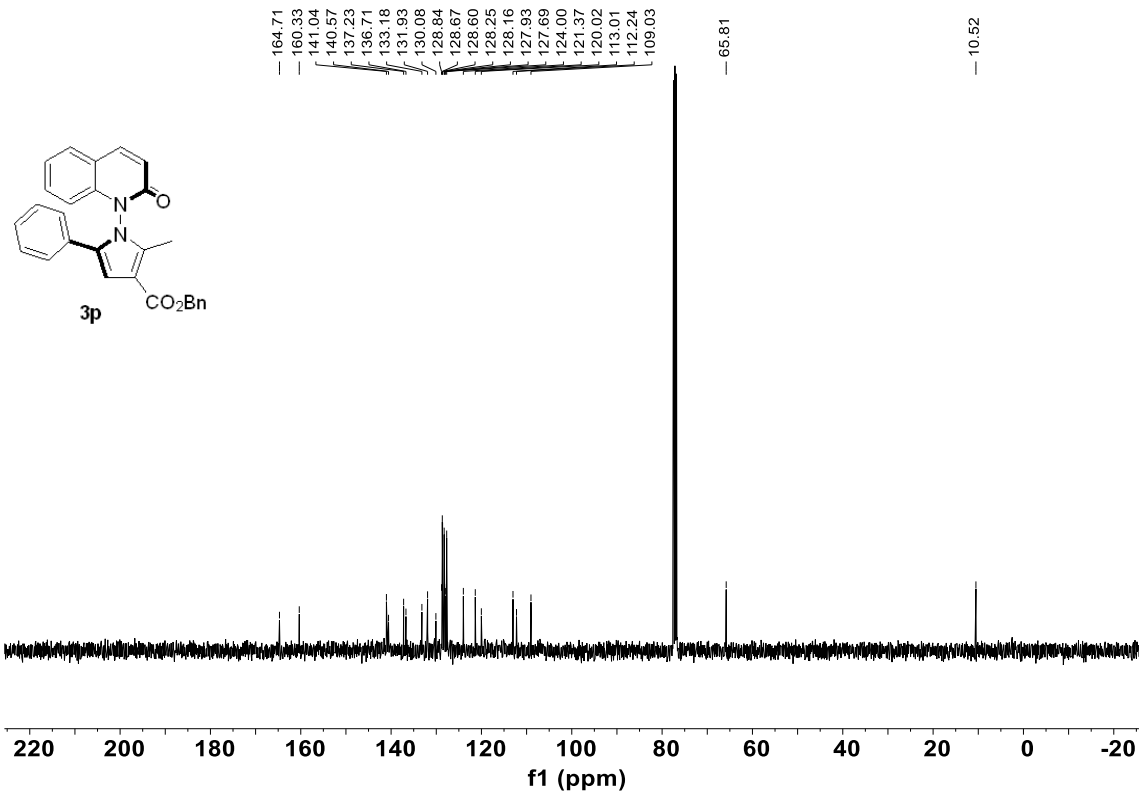
7.350
7.338
7.332
7.314
7.244
7.241
7.231
7.225
7.211
7.206
7.160
7.150
7.138
7.132
6.933
6.778
6.754
6.393
6.372
5.345
2.272
3p
CO2Bn
1.00
1.01
2.01
3.10
1.06
3.07
3.02
0.95
0.99
1.01
2.02
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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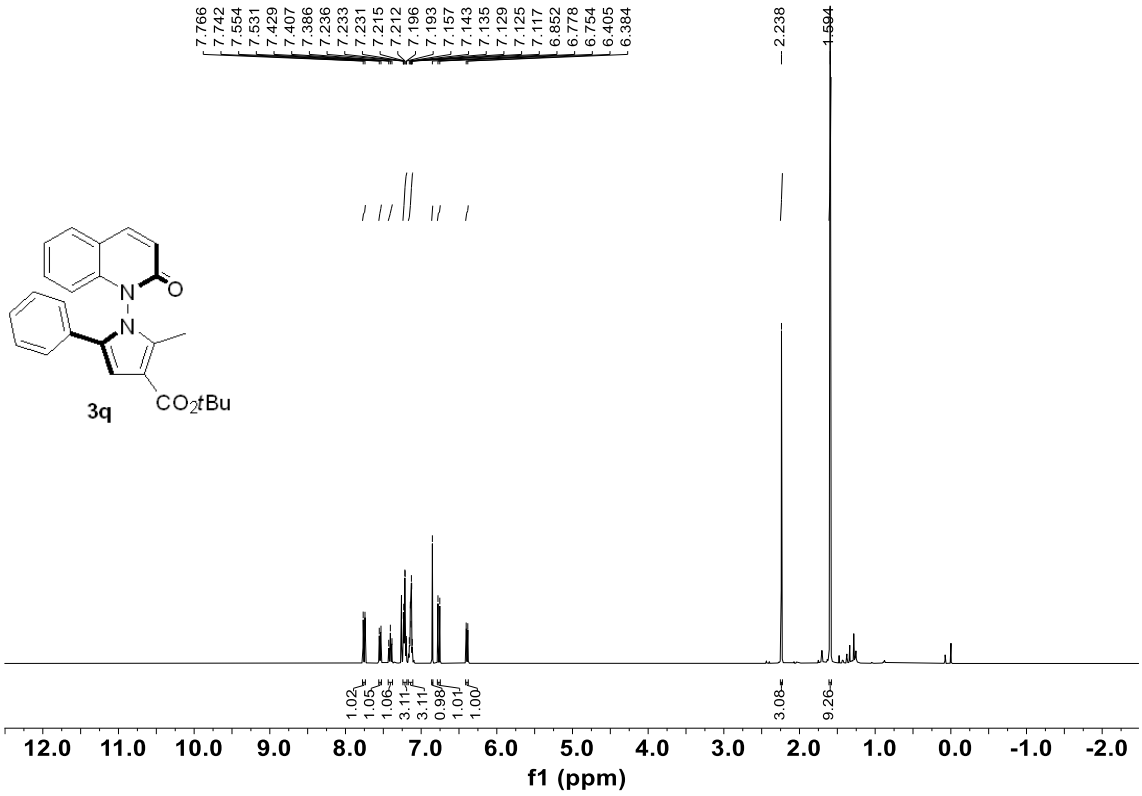
140.57
137.23
136.71
133.18
131.93
130.08
128.84
128.67
128.60
128.25
128.16
127.93
127.69
124.00
121.37
120.02
113.01
112.24
109.03
65.81
10.52
3p
CO2Bn
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.429
7.407
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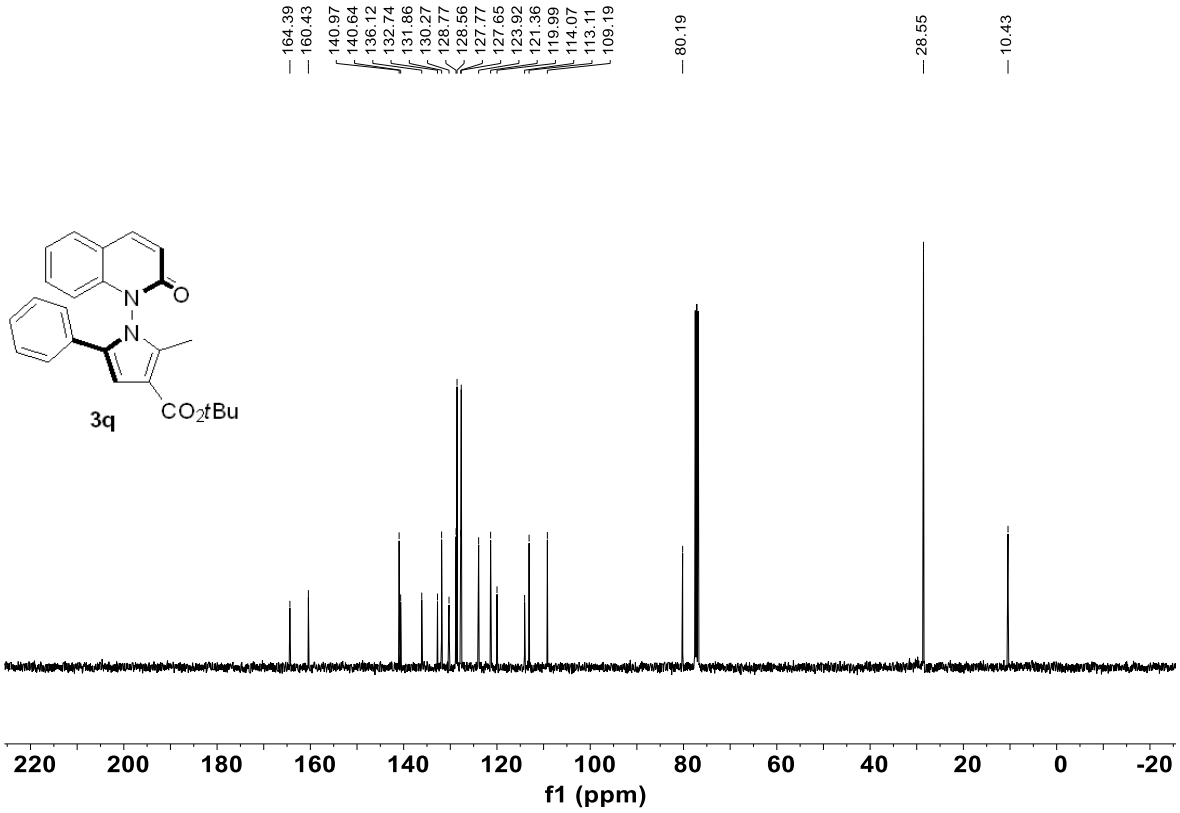
7.236
7.233
7.231
7.215
7.212
7.196
7.193
7.157
7.143
7.135
7.129
7.125
7.117
6.852
6.778
6.754
6.405
6.384
2.238
1.594
1.02
1.05
1.06
3.11
3.11
0.98
1.01
1.00
3.08
9.26
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)
3q
CO2tBu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130.27
128.77
128.56
127.77
127.65
123.92
121.36
119.99
114.07
113.11
109.19
80.19
28.55
10.43
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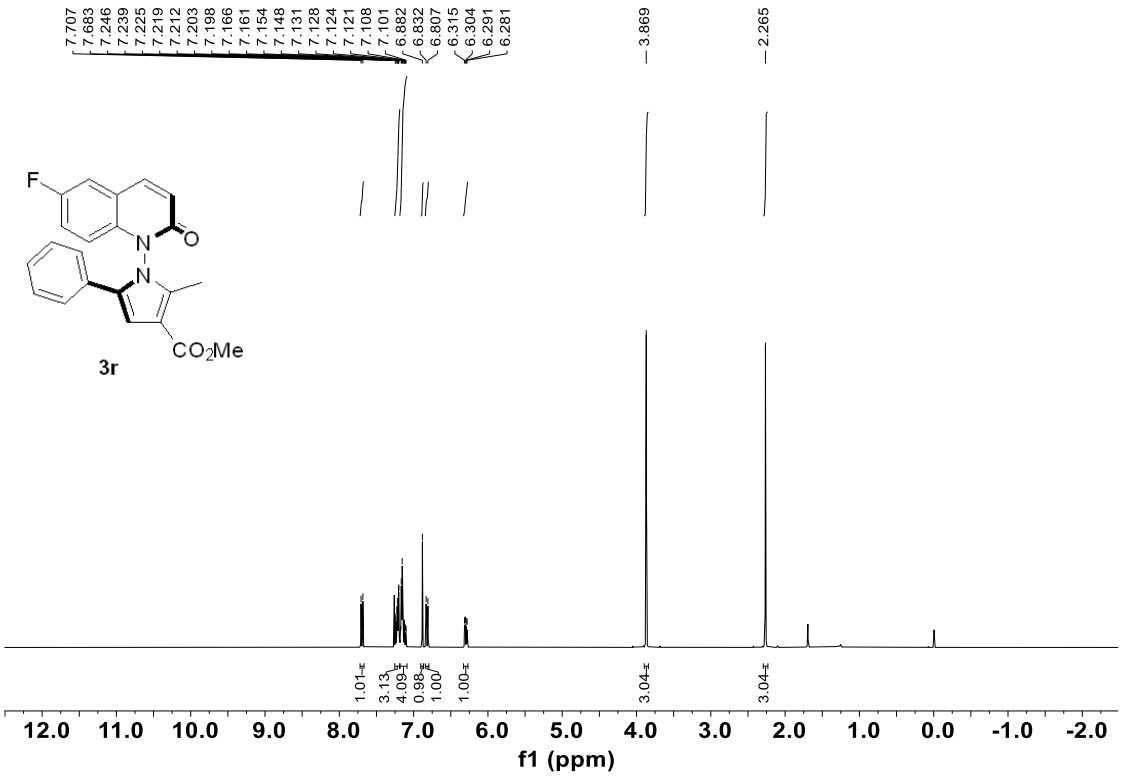
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)
3q
CO2tBu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7.246
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7.219
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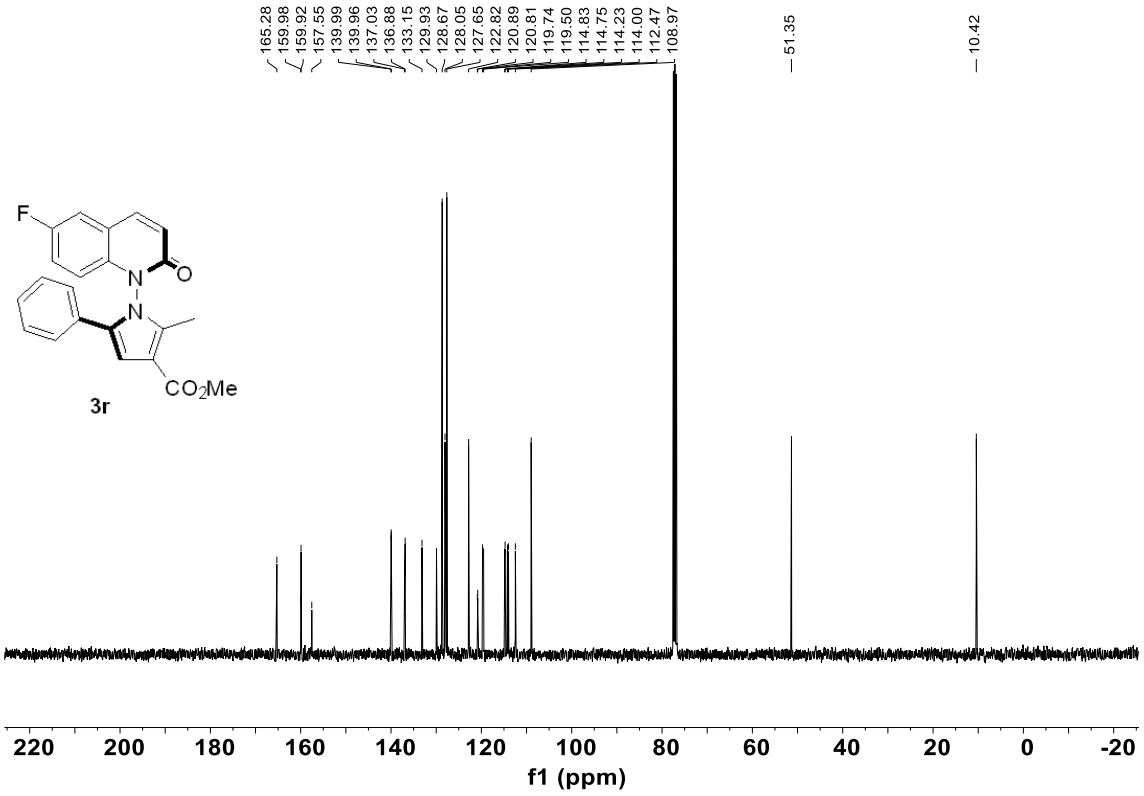
7.203
7.198
7.166
7.161
7.154
7.148
7.131
7.128
7.124
7.121
7.108
7.101
6.882
6.832
6.807
6.315
6.304
6.291
6.281
3.869
2.265
F
N
O
N
CO2Me
3r
1.01
3.13
4.09
0.98
1.00
1.00
3.04
3.04
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)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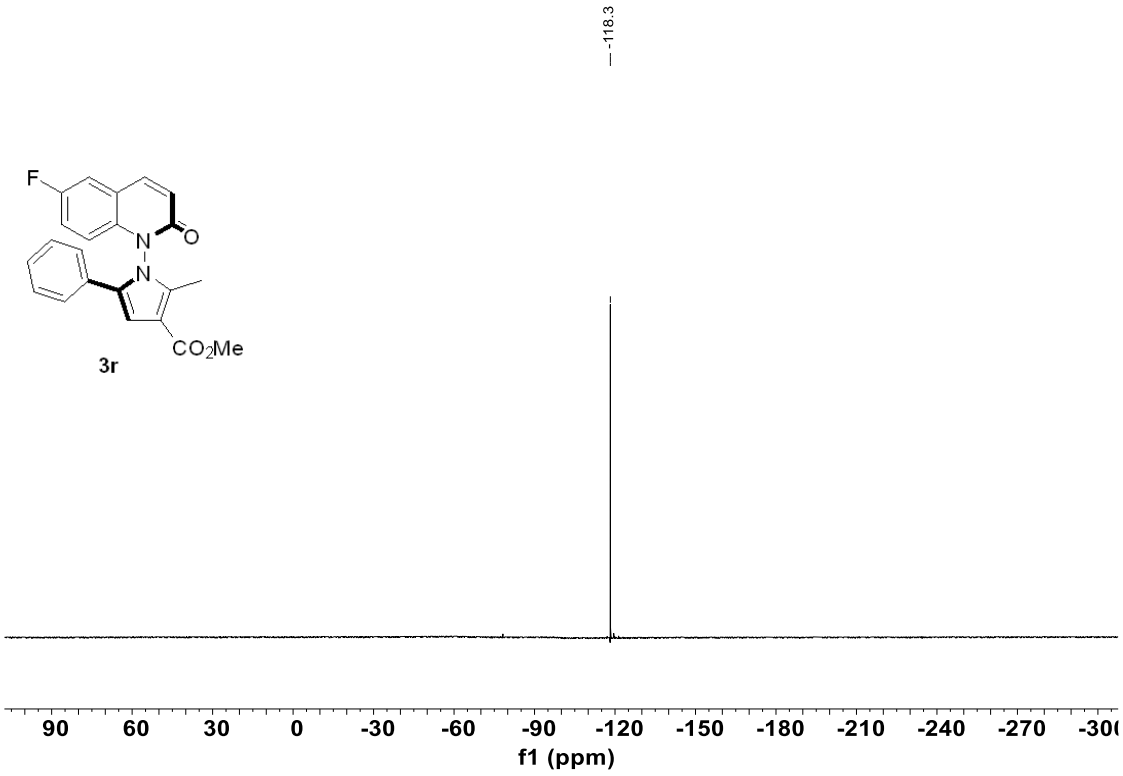
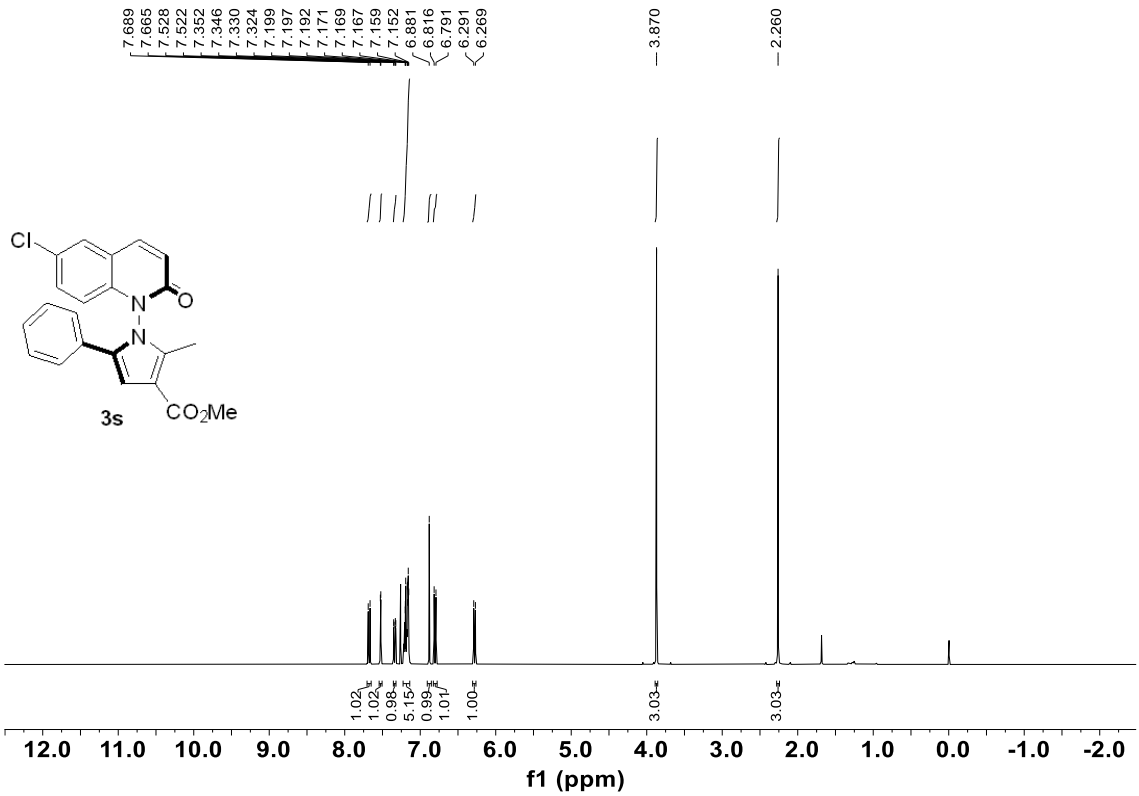
136.88
133.15
129.93
128.67
128.05
127.65
122.82
120.89
120.81
119.74
119.50
114.83
114.75
114.23
114.00
112.47
108.97
51.35
10.42
F
N
O
N
CO2Me
3r
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)


-118.3
F
N
O
N
CO2Me
3r
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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7.324
7.199
7.197
7.192
7.171
7.169
7.167
7.159
7.152
6.881
6.816
6.791
6.291
6.269
3.870
2.260
Cl
N
O
N
CO2Me
3s
1.02
1.02
0.98
5.15
0.99
1.01
1.00
3.03
3.03
12.0
11.0
10.0
9.0
8.0
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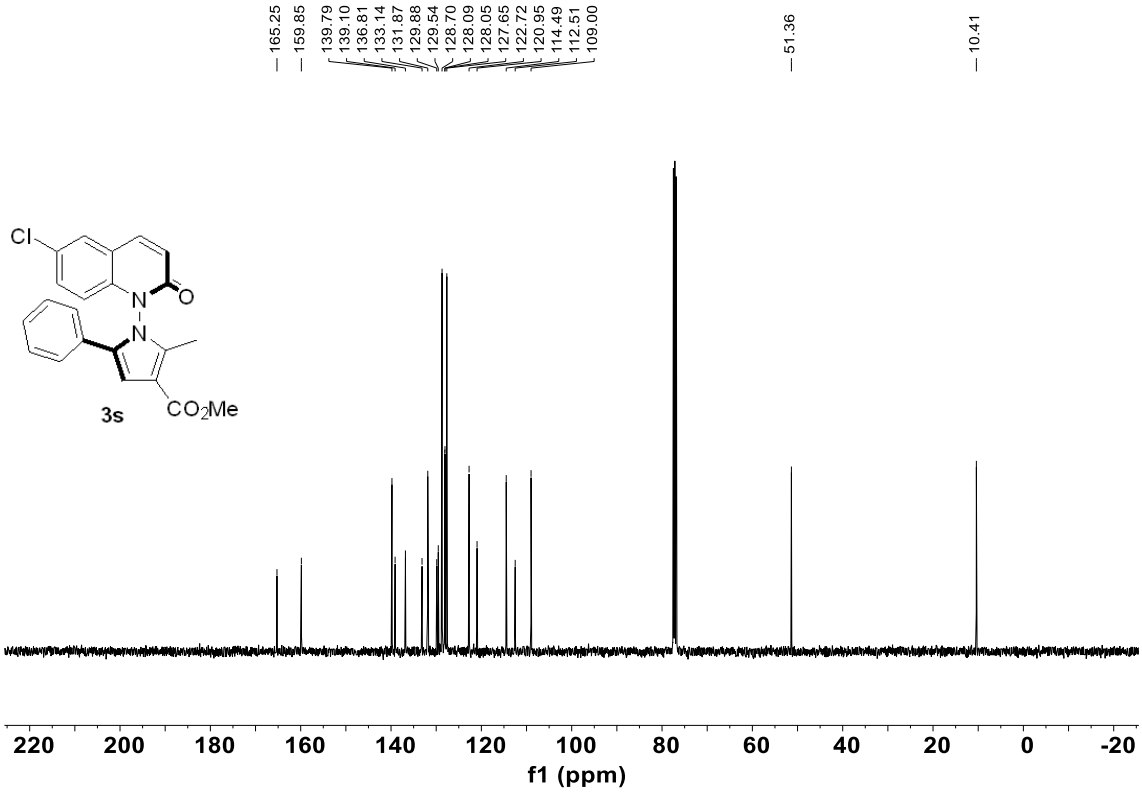
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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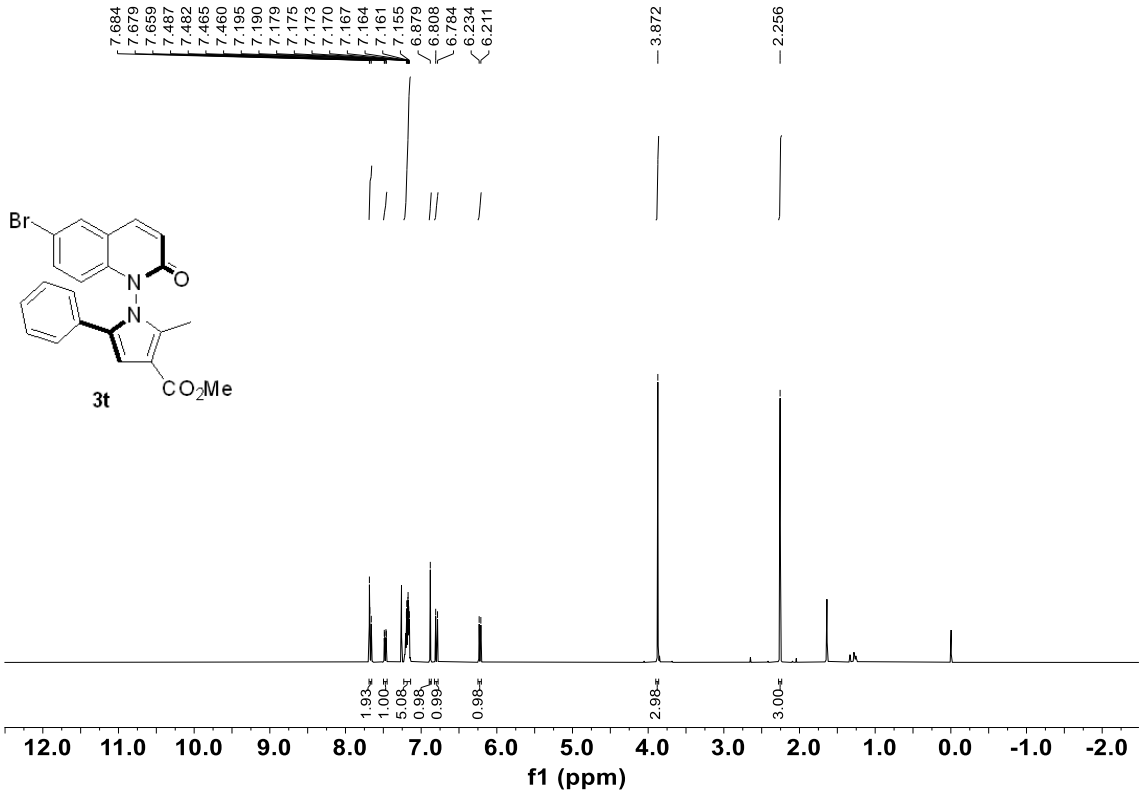
129.88
129.54
128.70
128.09
128.05
127.65
122.72
120.95
114.49
112.51
109.00
51.36
10.41
Cl
O
N
N
CO2Me
3s
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.482
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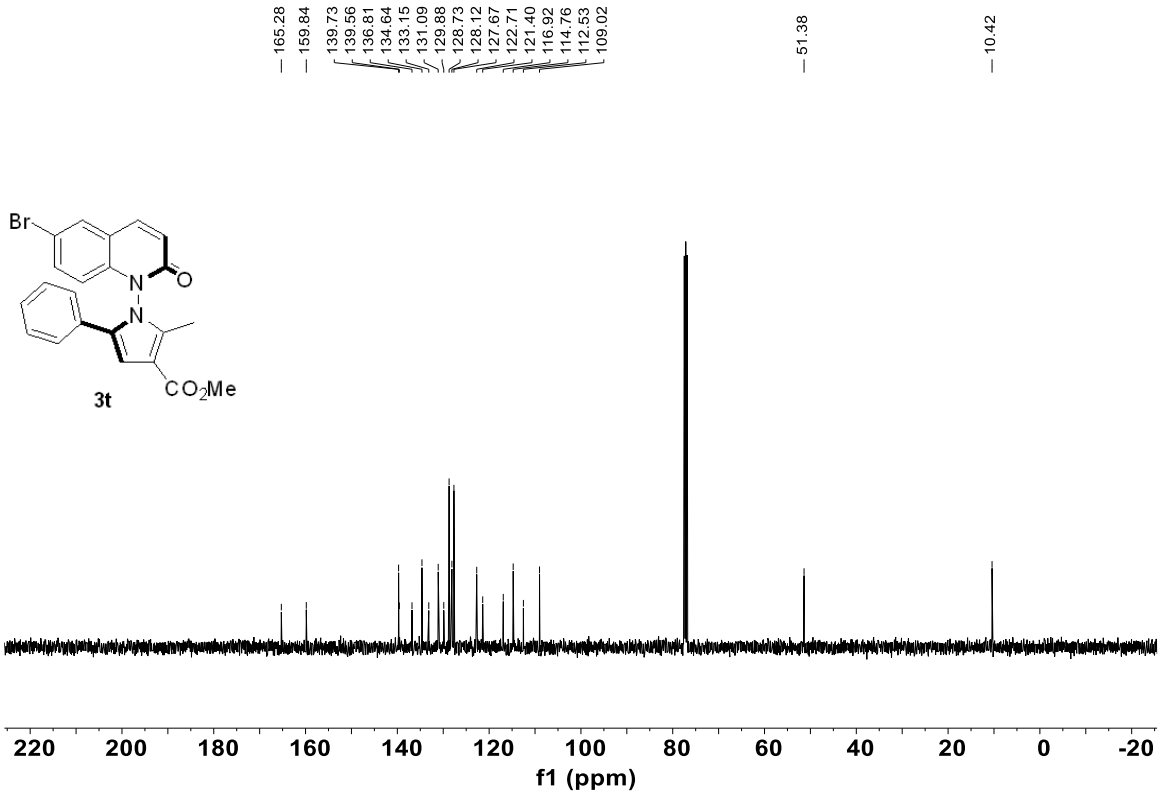
7.460
7.195
7.190
7.179
7.175
7.173
7.170
7.167
7.164
7.161
7.155
6.879
6.808
6.784
6.234
6.211
3.872
2.256
Br
O
N
N
CO2Me
3t
1.93
1.00
5.08
0.98
0.99
0.98
2.98
3.00
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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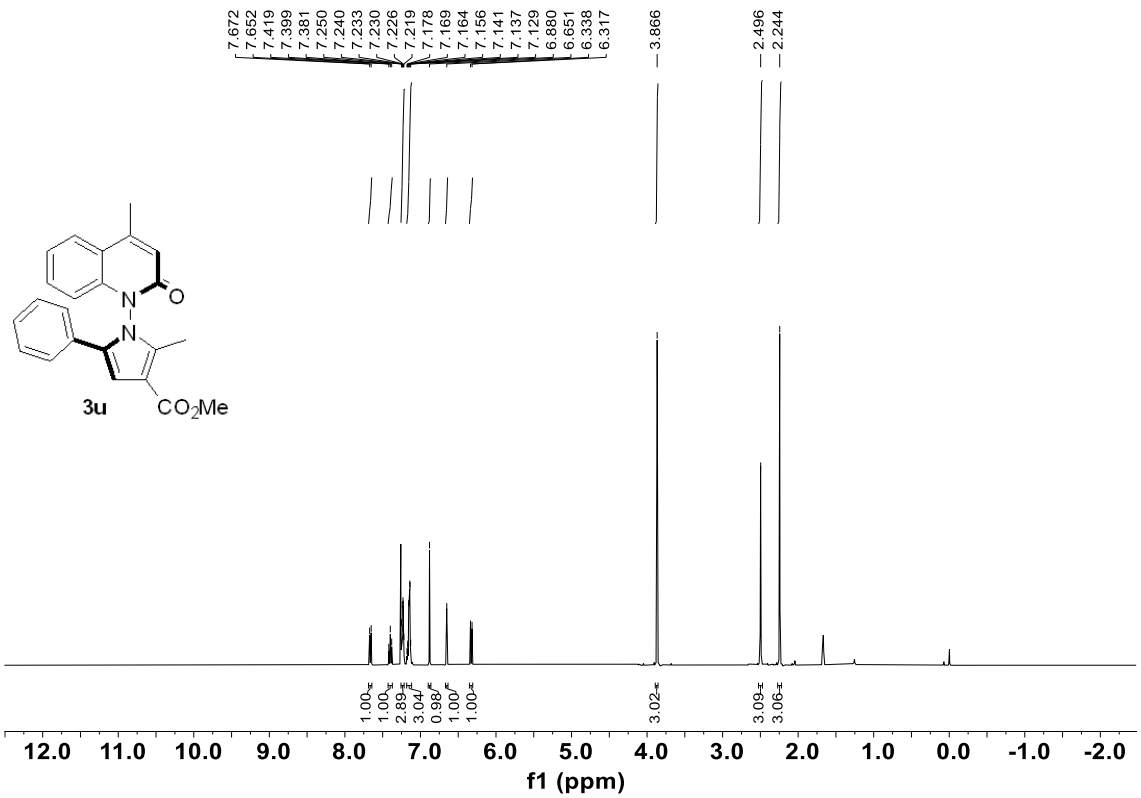
134.64
133.15
131.09
129.88
128.73
128.12
127.67
122.71
121.40
116.92
114.76
112.53
109.02
51.38
10.42
Br
O
N
N
CO2Me
3t
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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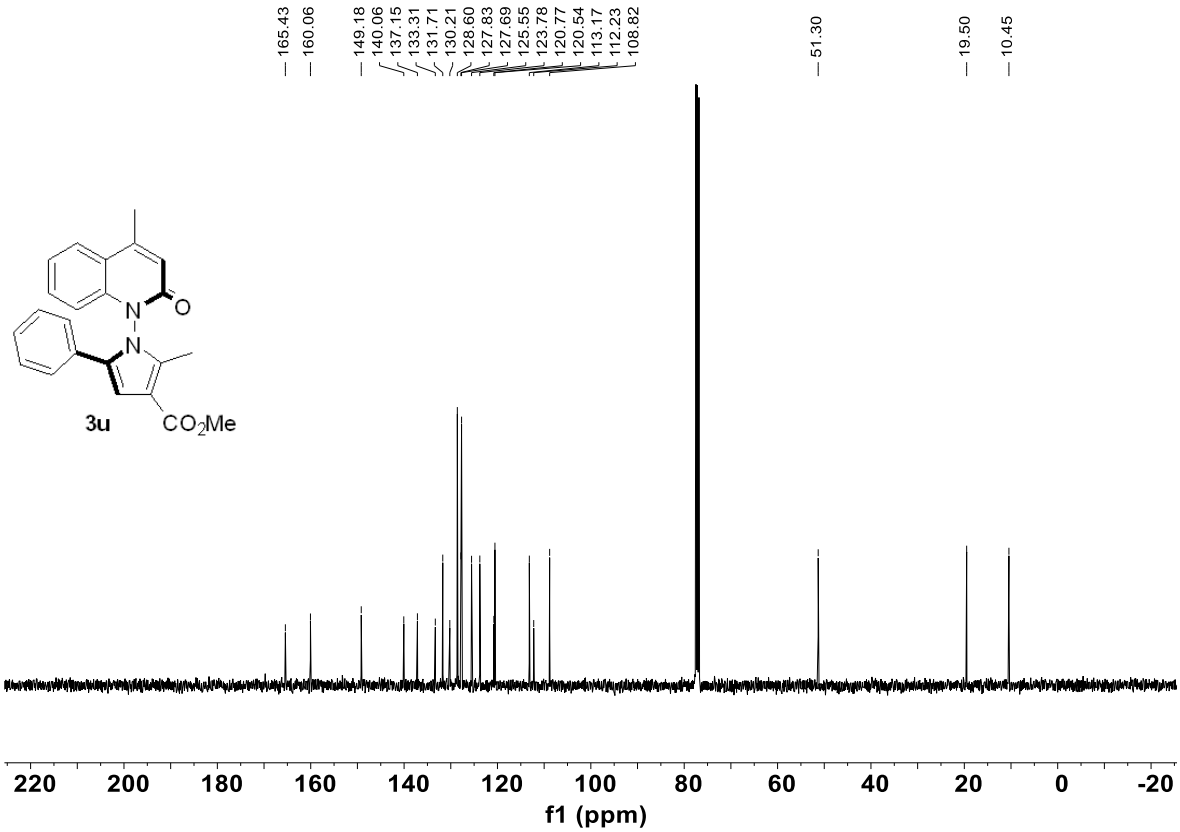
7.240
7.233
7.230
7.226
7.219
7.178
7.169
7.164
7.156
7.141
7.137
7.129
6.880
6.651
6.338
6.317
3.866
2.496
2.244
O
N
N
3u
CO2Me
1.00
1.00
2.89
3.04
0.98
1.00
1.00
3.02
3.09
3.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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160.06
149.18
140.06
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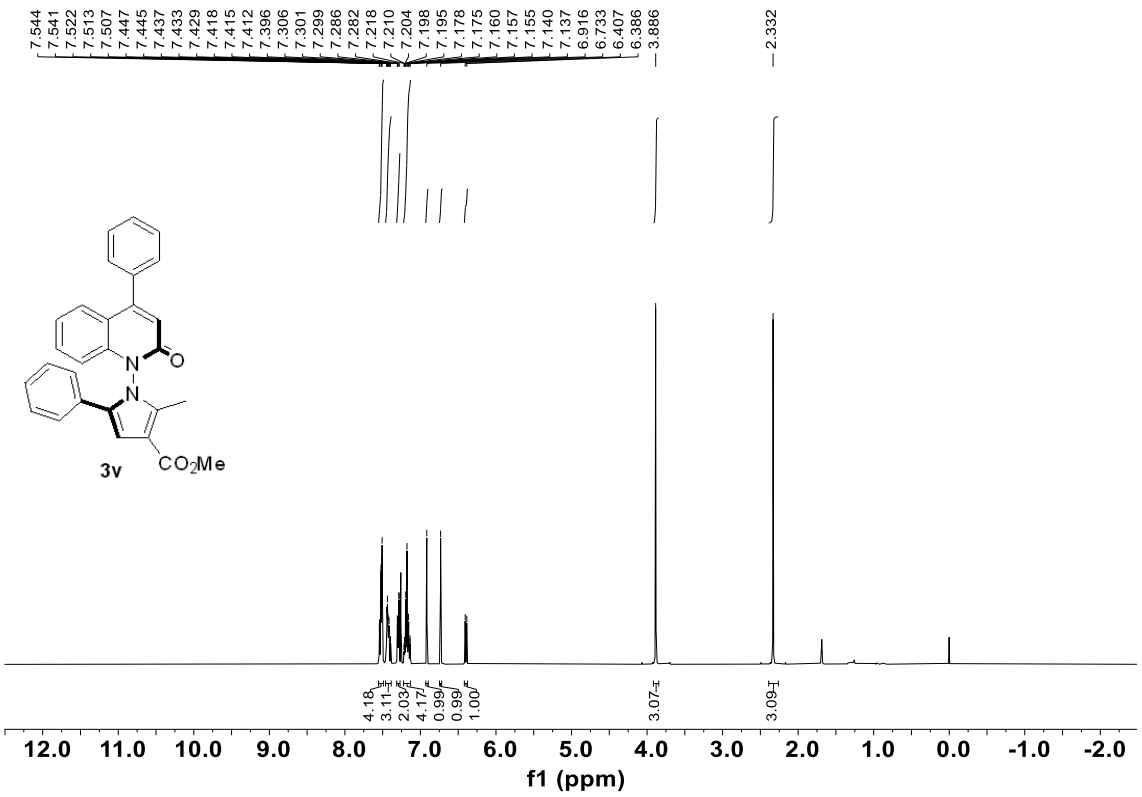
133.31
131.71
130.21
128.60
127.83
127.69
125.55
123.78
120.77
120.54
113.17
112.23
108.82
51.30
19.50
10.45
3u
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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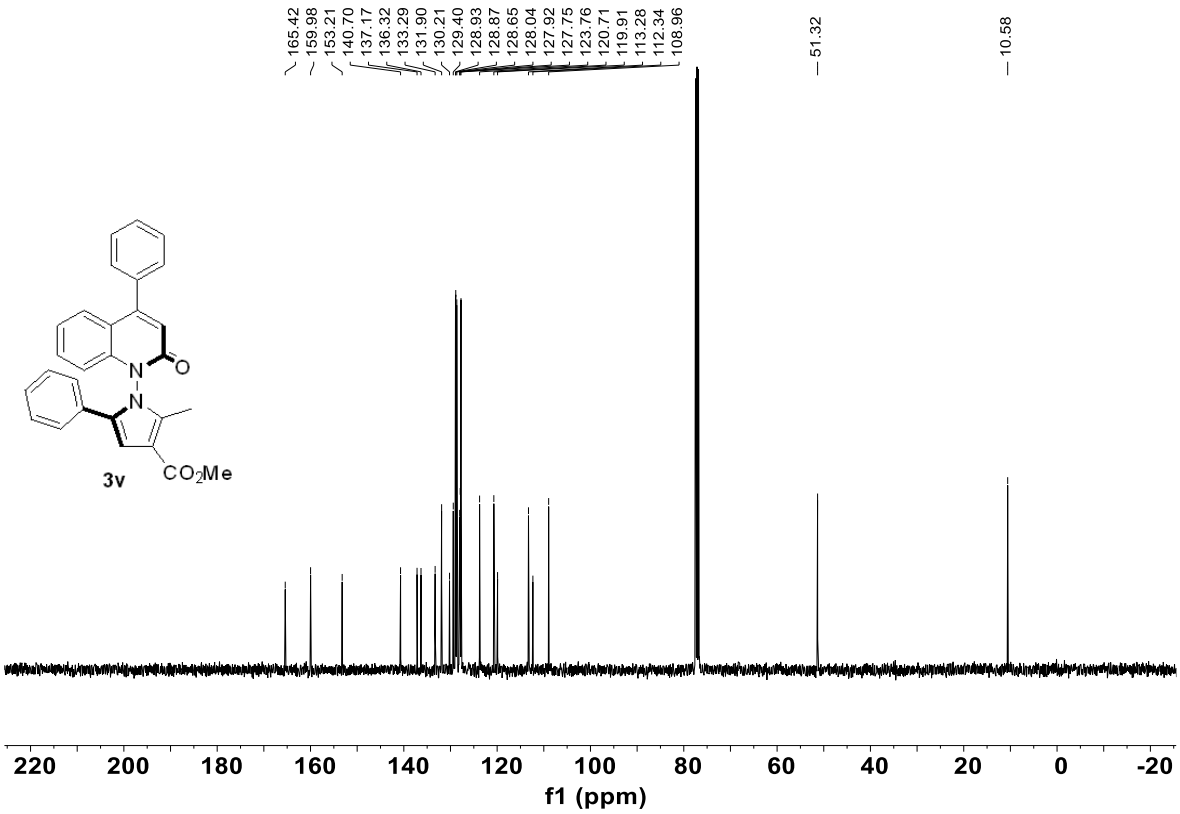
7.415
7.412
7.396
7.306
7.301
7.299
7.286
7.282
7.218
7.210
7.204
7.198
7.195
7.178
7.175
7.160
7.157
7.155
7.140
7.137
6.916
6.733
6.407
6.386
3.886
2.332
3v
CO2Me
4.18
3.11
2.03
4.17
0.99
0.99
1.00
3.07
3.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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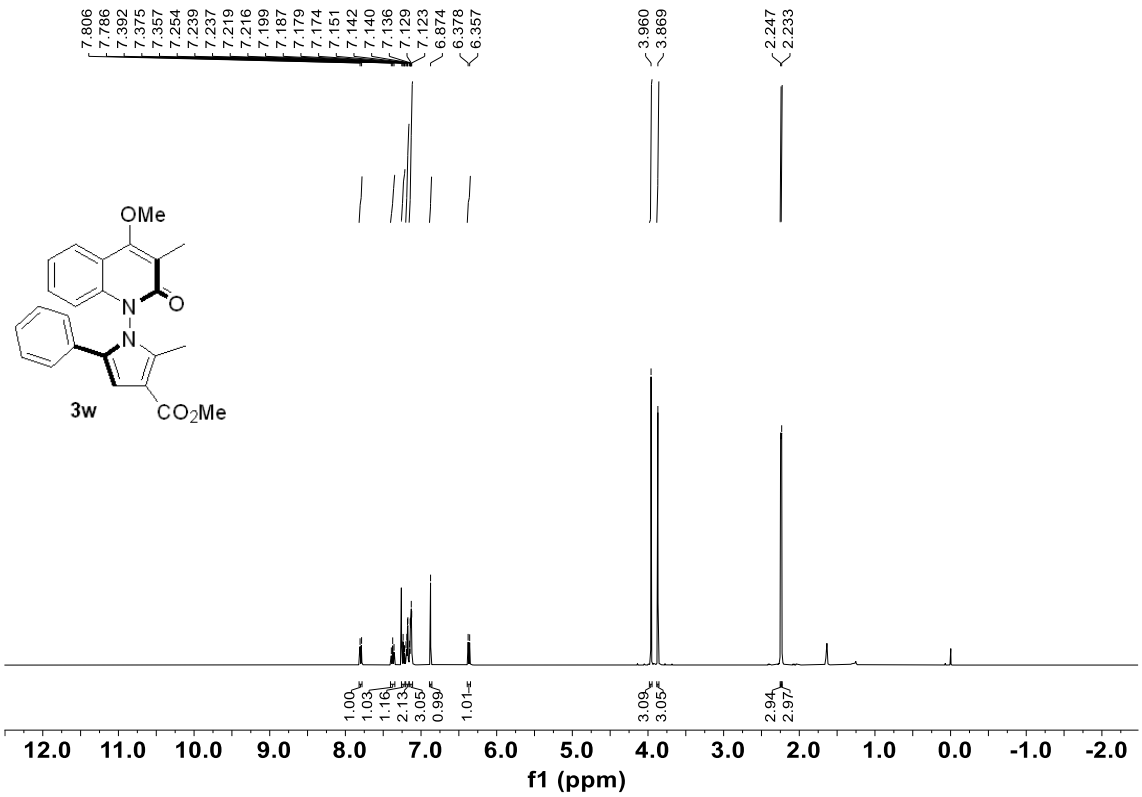
136.32
133.29
131.90
130.21
129.40
128.93
128.87
128.65
128.04
127.92
127.75
123.76
120.71
119.91
113.28
112.34
108.96
51.32
10.58
3v
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.239
7.237
7.219
7.216
7.199
7.187
7.179
7.174
7.151
7.142
7.140
7.136
7.129
7.123
6.874
6.378
6.357
3.960
3.869
2.247
2.233
OMe
3w
CO2Me
1.00
1.03
1.16
2.13
3.05
0.99
1.01
3.09
3.05
2.94
2.97
12.0
11.0
10.0
9.0
8.0
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5.0
4.0
3.0
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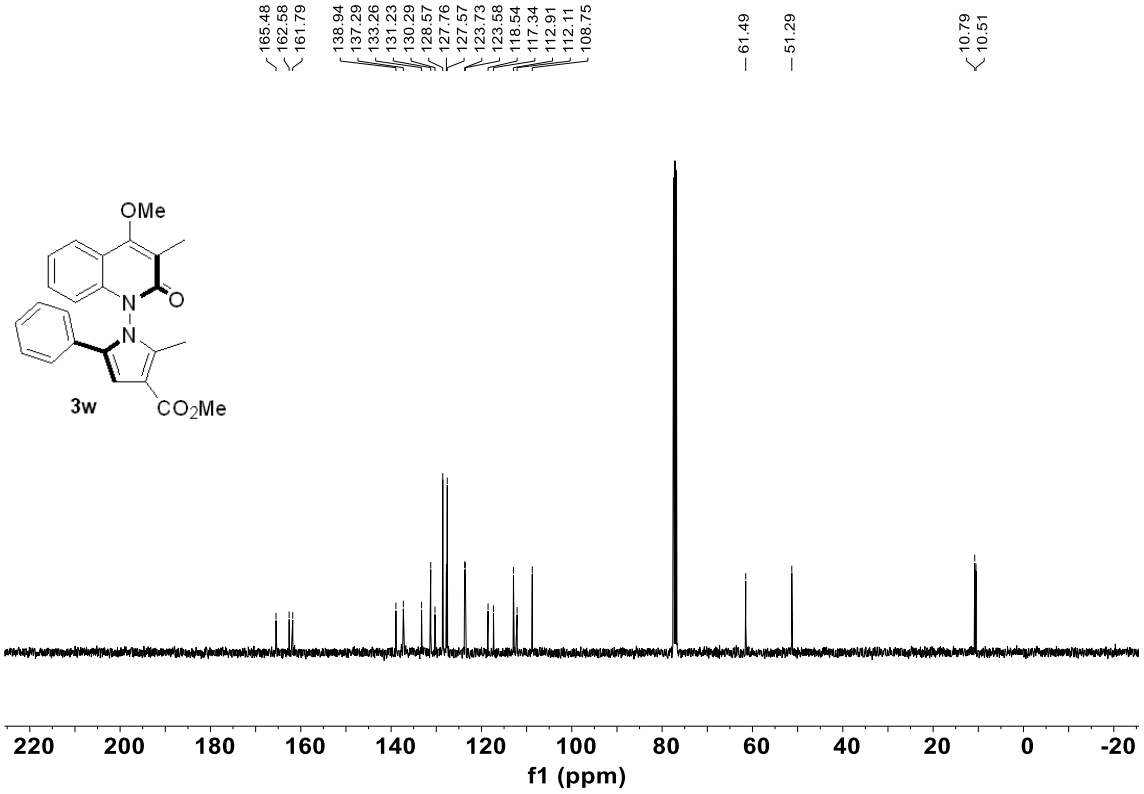
1.0
0.0
-1.0
-2.0
f1 (ppm)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137.29
133.26
131.23
130.29
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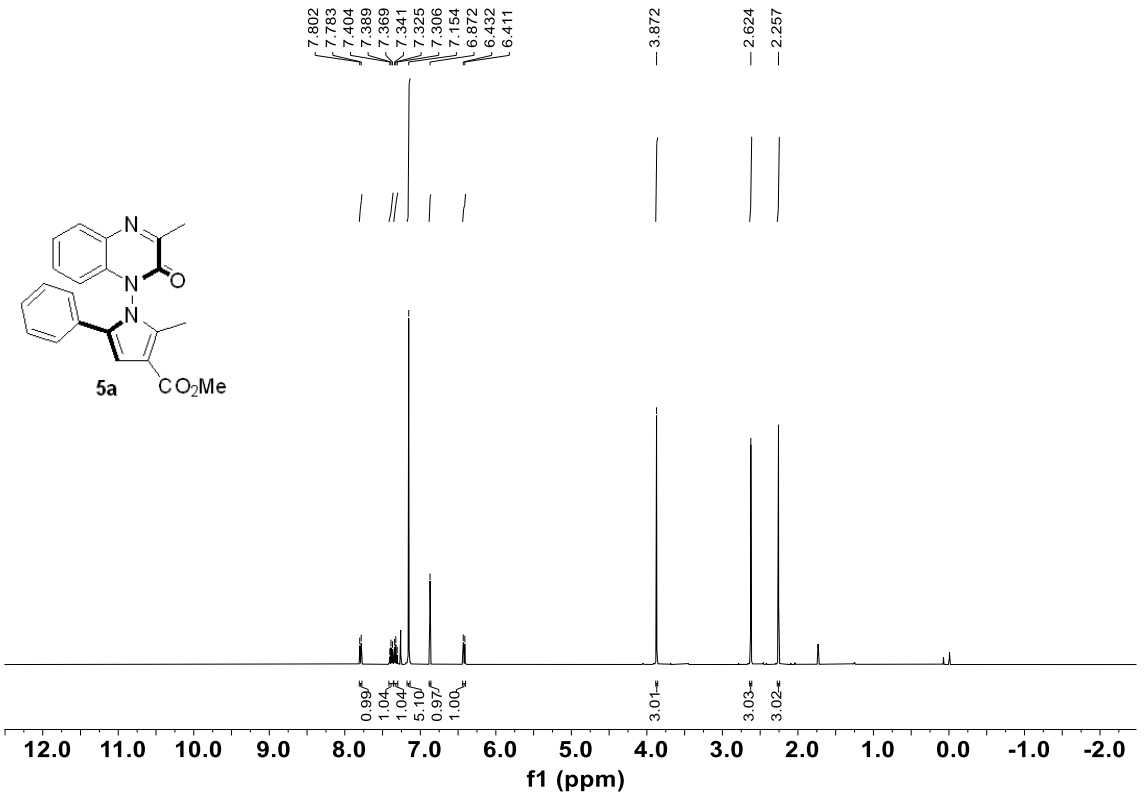
127.76
127.57
123.73
123.58
118.54
117.34
112.91
112.11
108.75
61.49
51.29
10.79
10.51
OMe
O
N
N
3w
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.306
7.154
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6.432
6.411
3.872
2.624
2.257
N
O
N
N
5a
CO2Me
0.99
1.04
1.04
5.10
0.97
1.00
3.01
3.03
3.02
12.0
11.0
10.0
9.0
8.0
7.0
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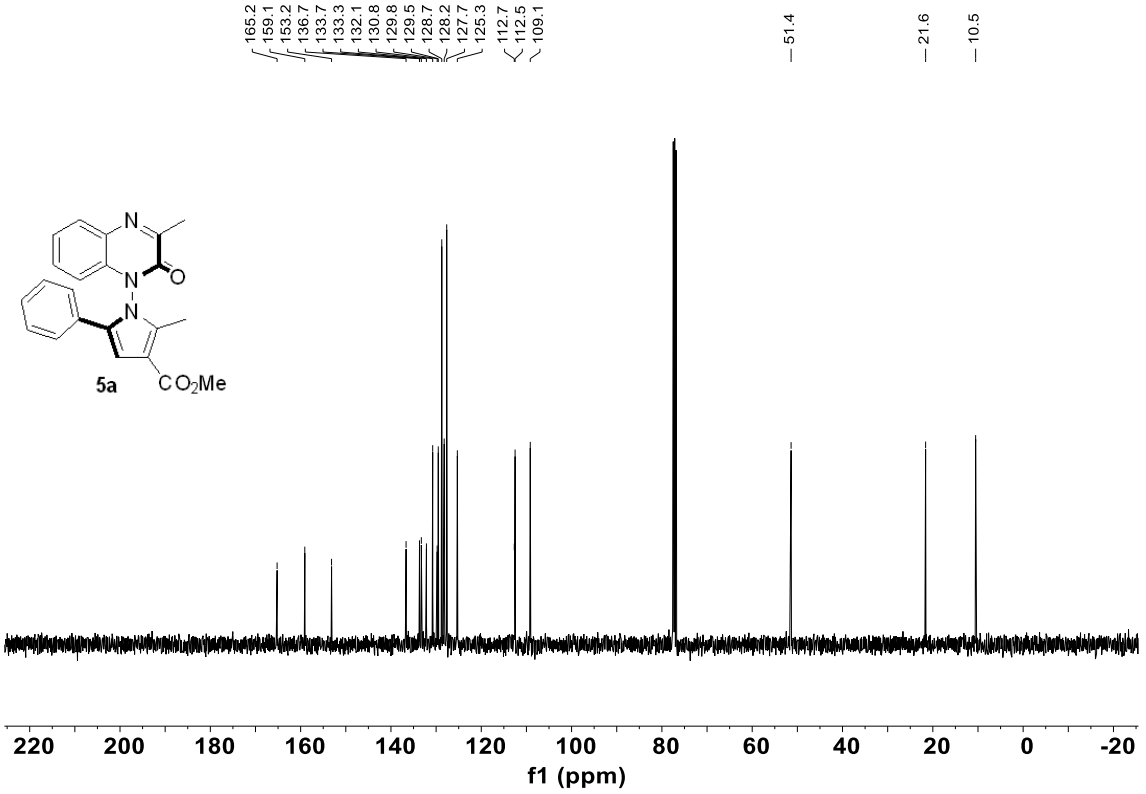
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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159.1
153.2
136.7
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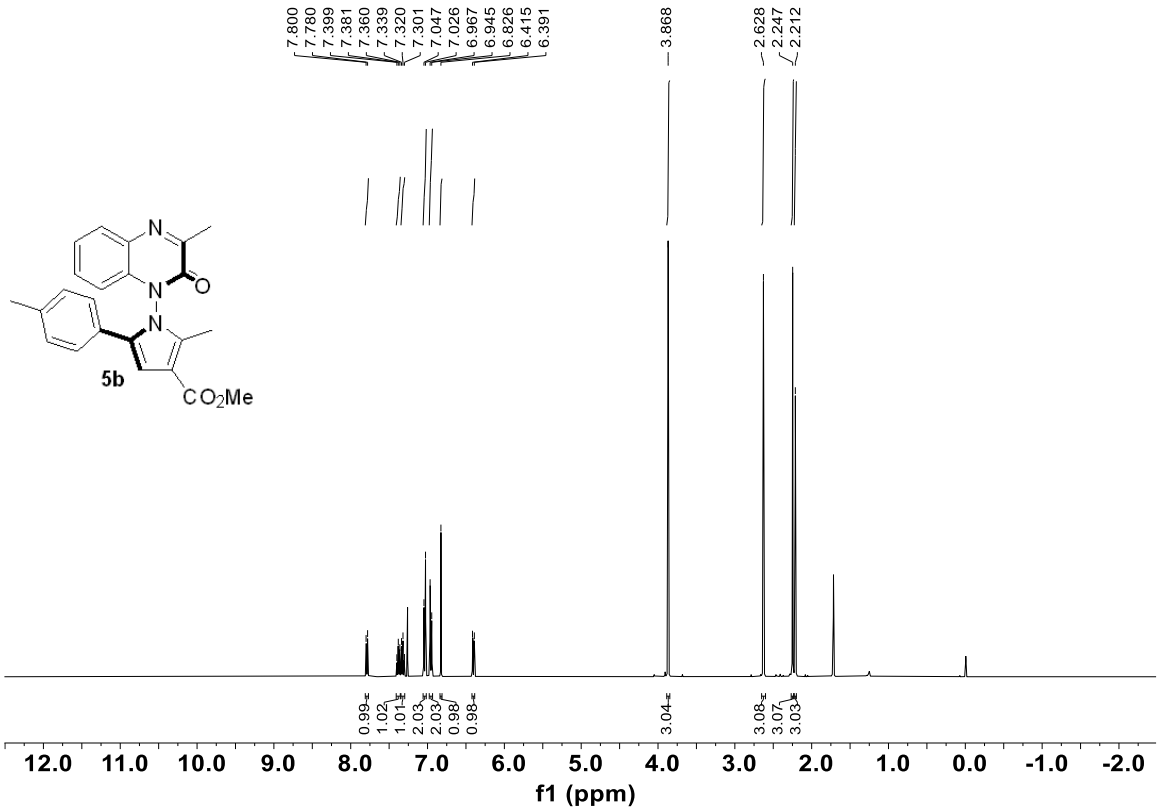
132.1
130.8
129.8
129.5
128.7
128.2
127.7
125.3
112.7
112.5
109.1
51.4
21.6
10.5
5a
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.301
7.047
7.026
6.967
6.945
6.826
6.415
6.391
3.868
2.628
2.247
2.212
5b
CO2Me
0.99
1.02
1.01
2.03
2.03
0.98
0.98
3.04
3.08
3.07
3.03
12.0
11.0
10.0
9.0
8.0
7.0
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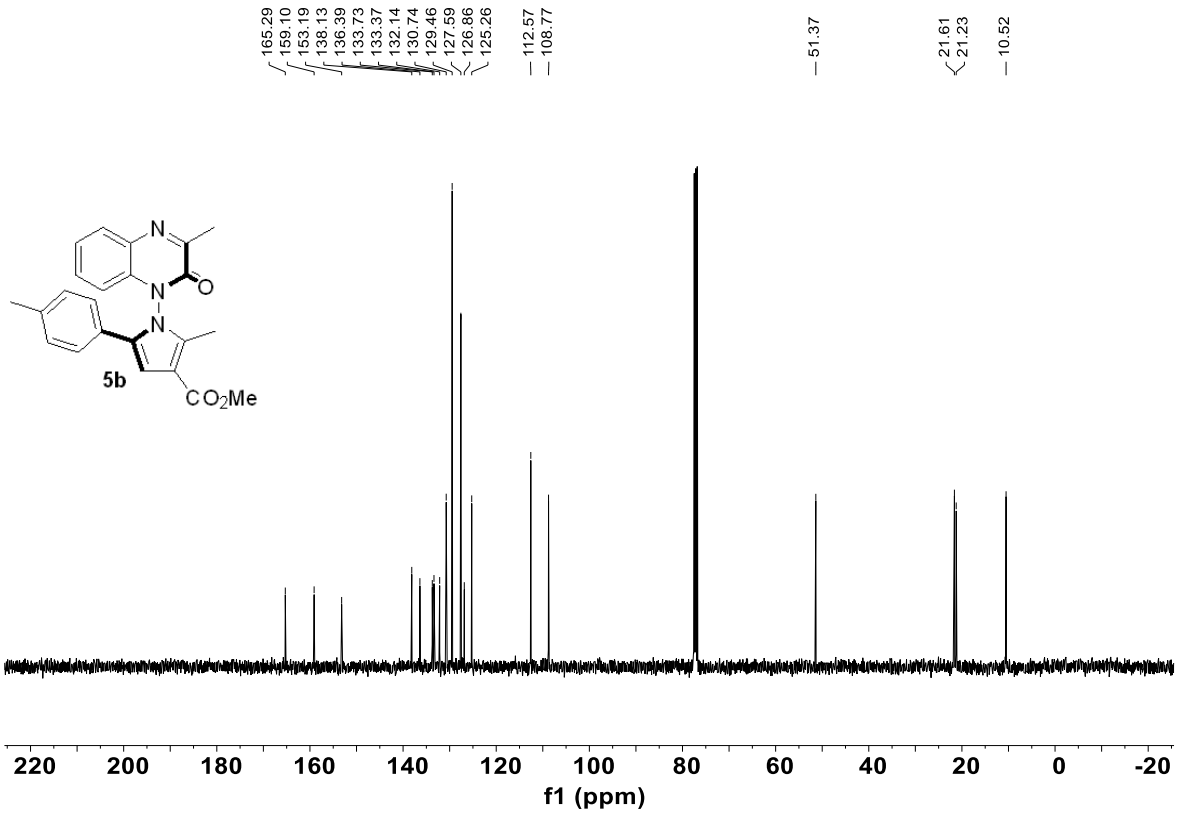
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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132.14
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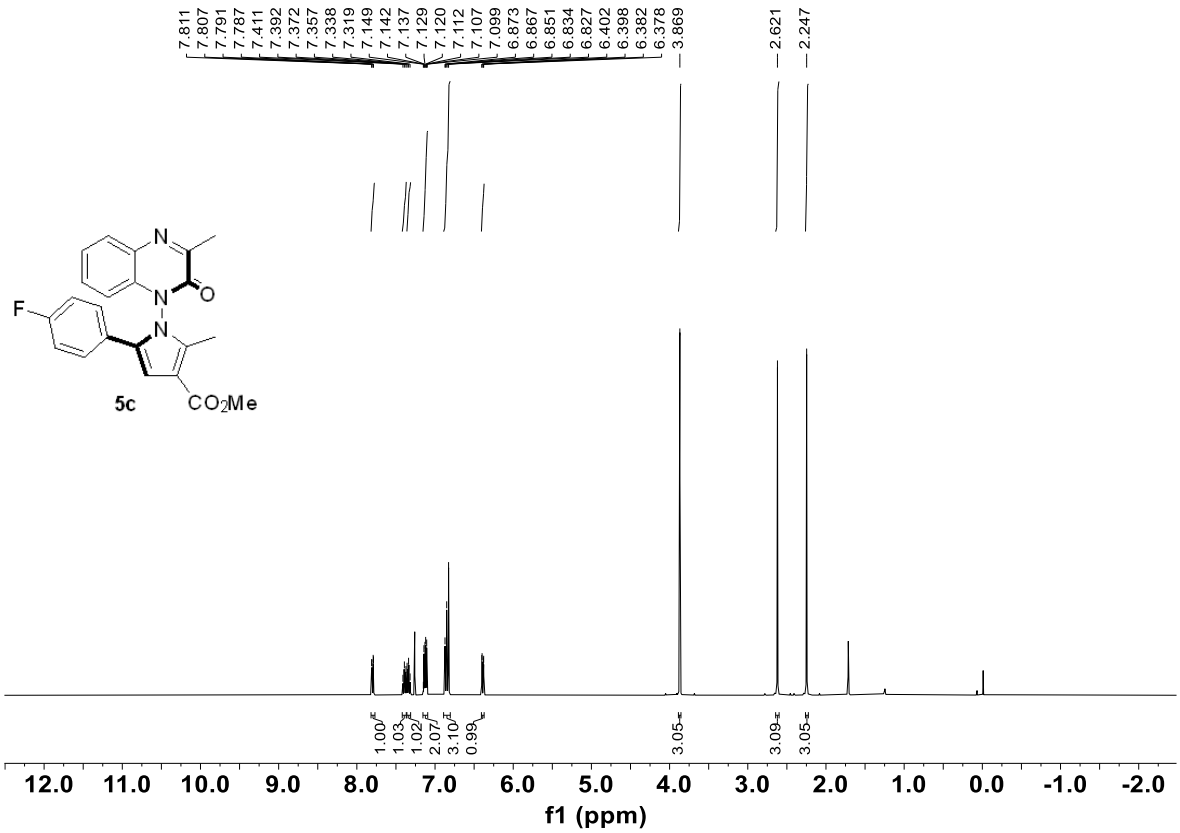
129.46
127.59
126.86
125.26
112.57
108.77
51.37
21.61
21.23
10.52
5b
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.357
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7.319
7.149
7.142
7.137
7.129
7.120
7.112
7.107
7.099
6.873
6.867
6.851
6.834
6.827
6.402
6.398
6.382
6.378
3.869
2.621
2.247
F
5c
CO2Me
1.00
1.03
1.02
2.07
3.10
0.99
3.05
3.09
3.05
12.0
11.0
10.0
9.0
8.0
7.0
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5.0
4.0
3.0
2.0
1.0
0.0
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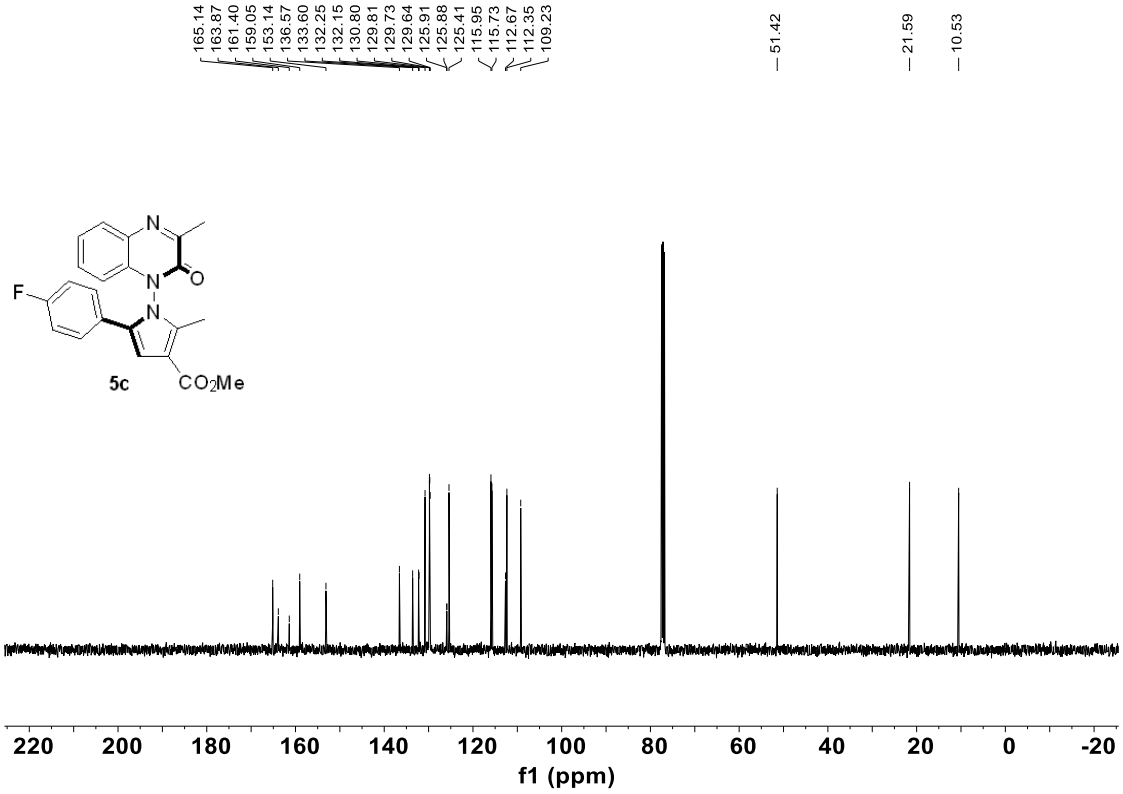
-2.0
f1 (ppm)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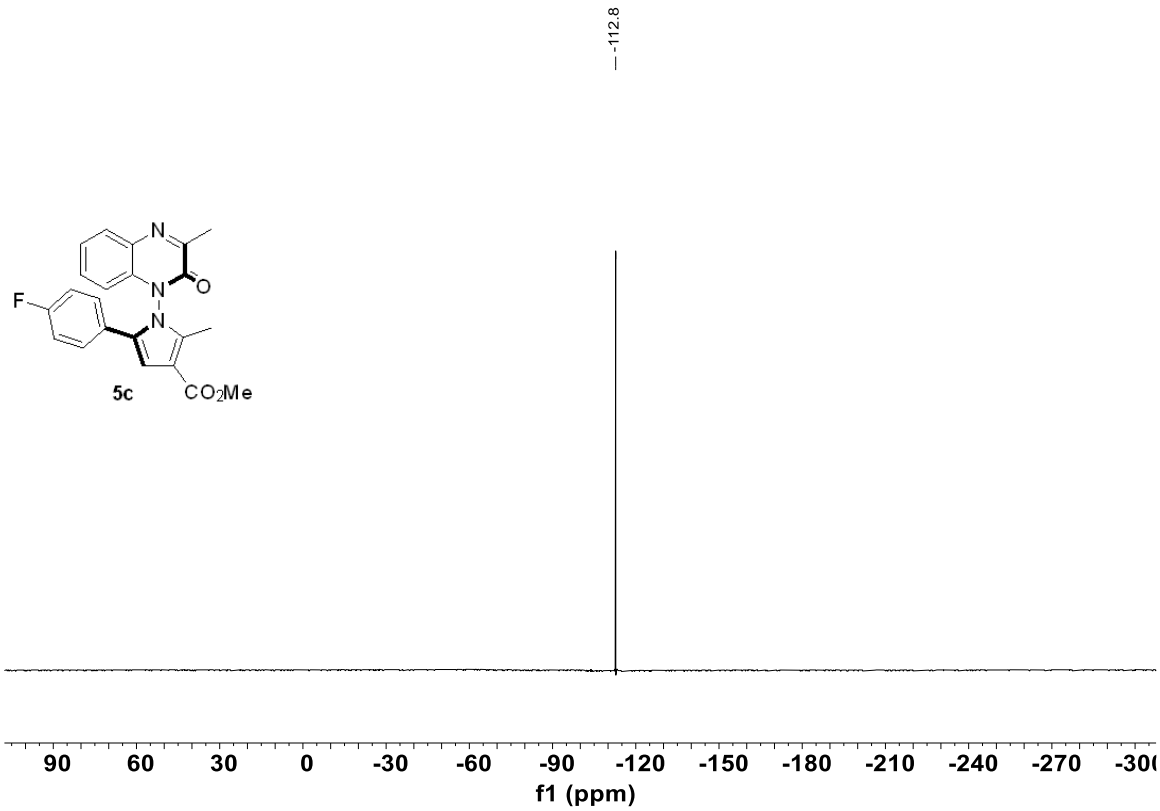
136.57
133.60
132.25
132.15
130.80
129.81
129.73
129.64
125.91
125.88
125.41
115.95
115.73
112.67
112.35
109.23
51.42
21.59
10.53
F
N
O
N
N
5c
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


-112.8
F
N
O
N
N
5c
CO2Me
90
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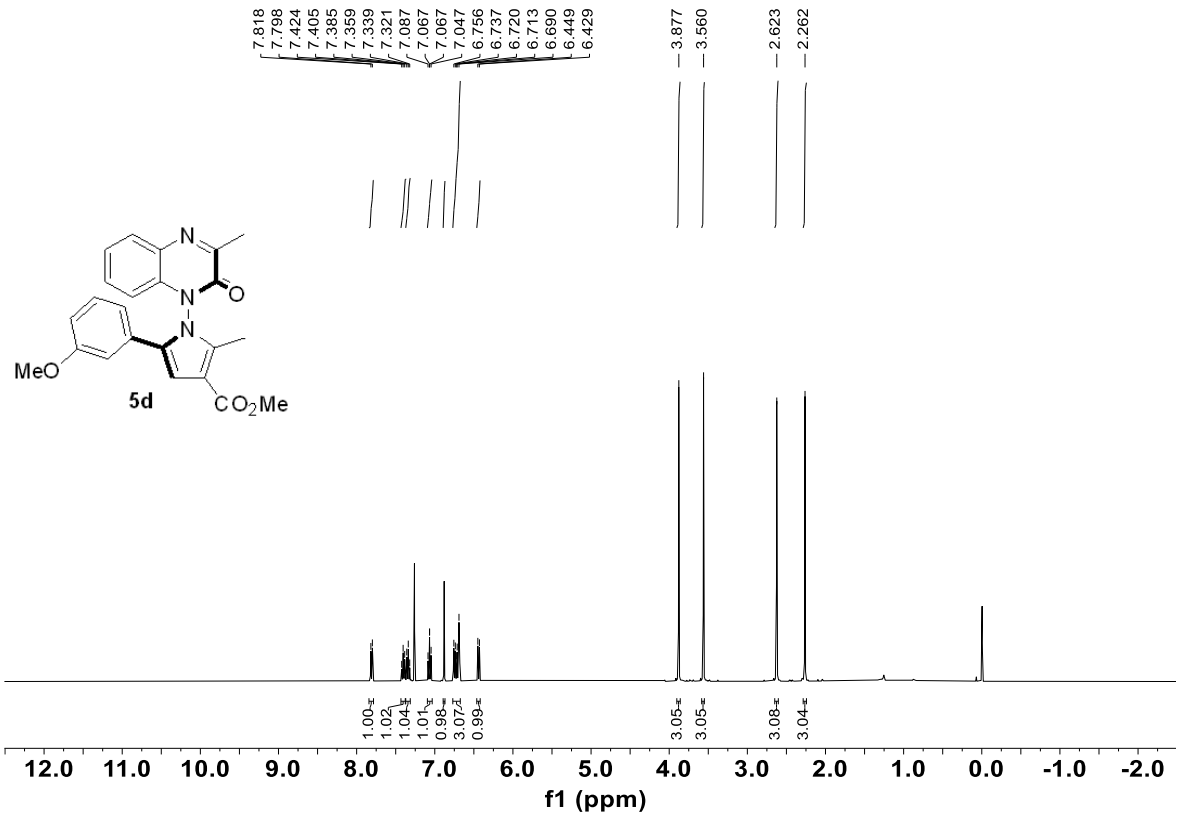
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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7.067
7.067
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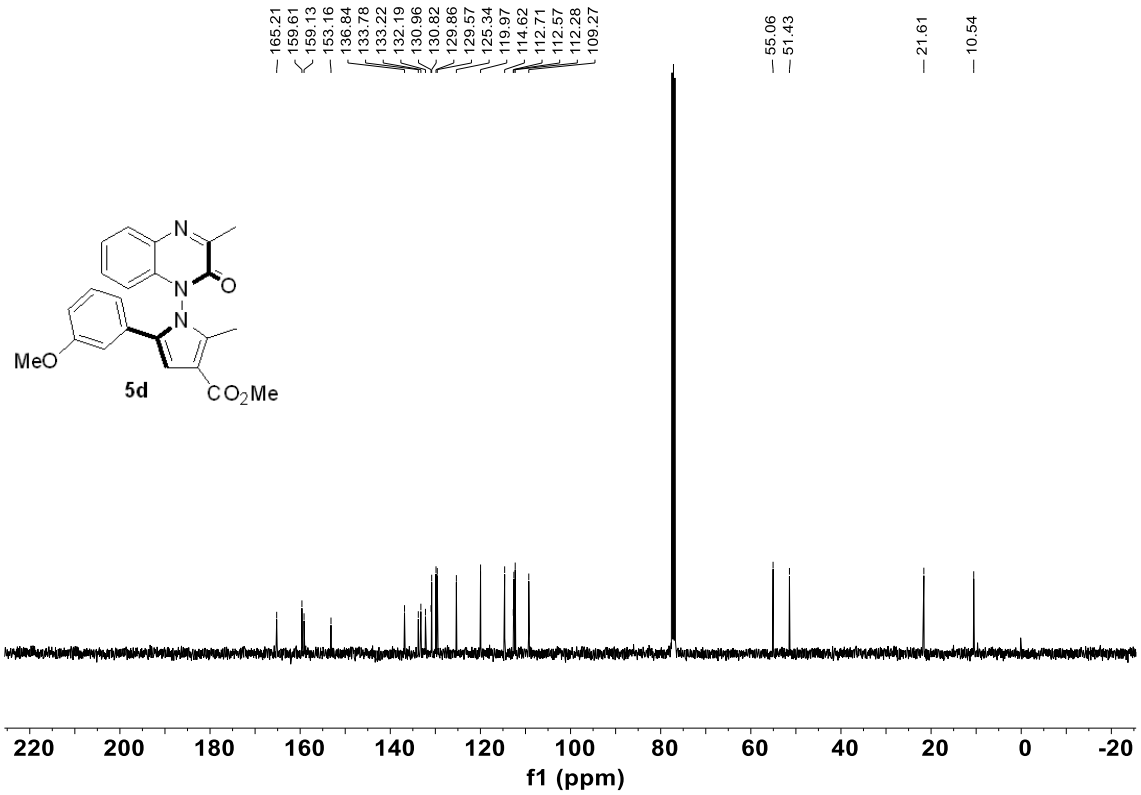
6.737
6.720
6.713
6.690
6.449
6.429
3.877
3.560
2.623
2.262
MeO
5d
CO2Me
1.00
1.02
1.04
1.01
0.98
3.07
0.99
3.05
3.05
3.08
3.04
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)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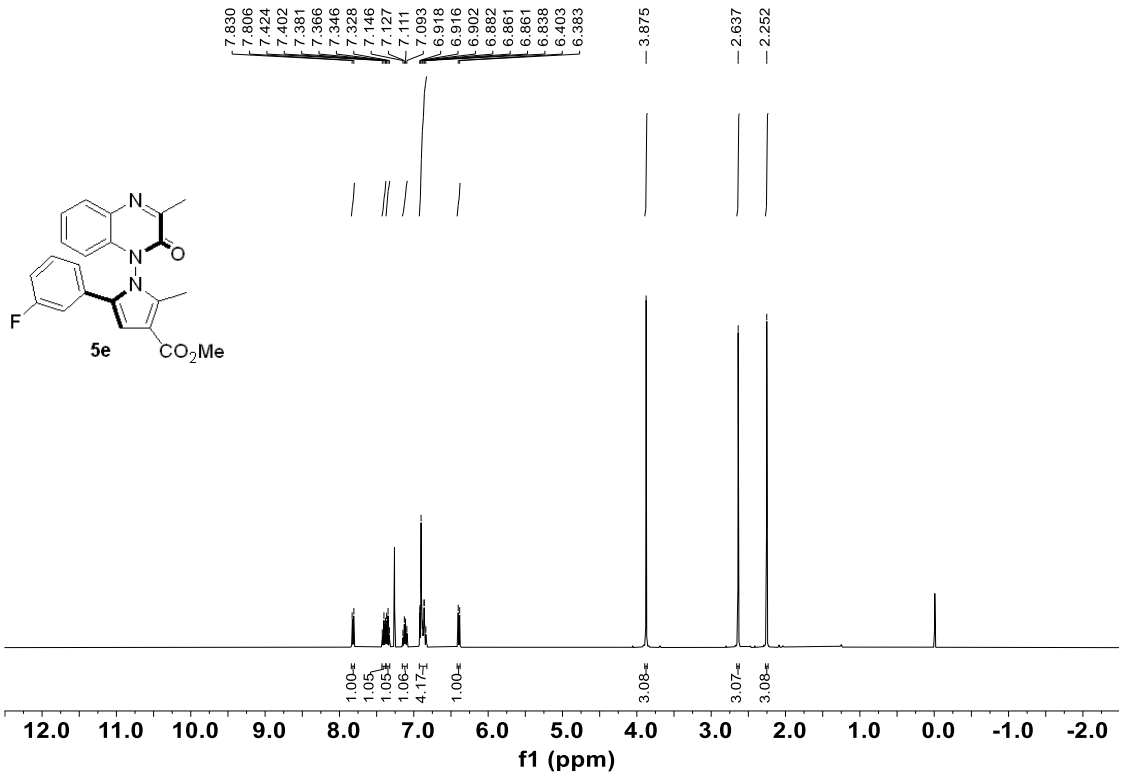
129.57
125.34
119.97
114.62
112.71
112.57
112.28
109.27
55.06
51.43
21.61
10.54
MeO
5d
CO2Me
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)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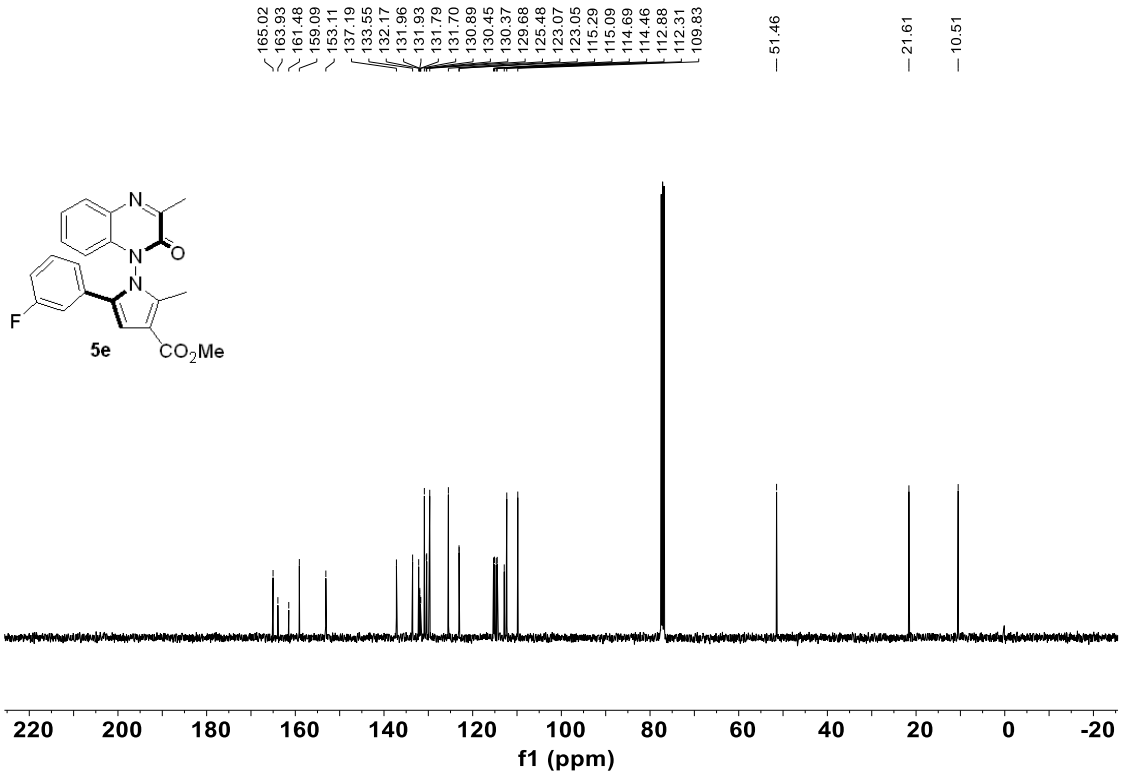
7.806
7.424
7.402
7.381
7.366
7.346
7.328
7.146
7.127
7.111
7.093
6.918
6.916
6.902
6.882
6.861
6.861
6.838
6.403
6.383
3.875
2.637
2.252
1.00
1.05
1.05
1.06
4.17
1.00
3.08
3.07
3.08
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)
5e
CO2Me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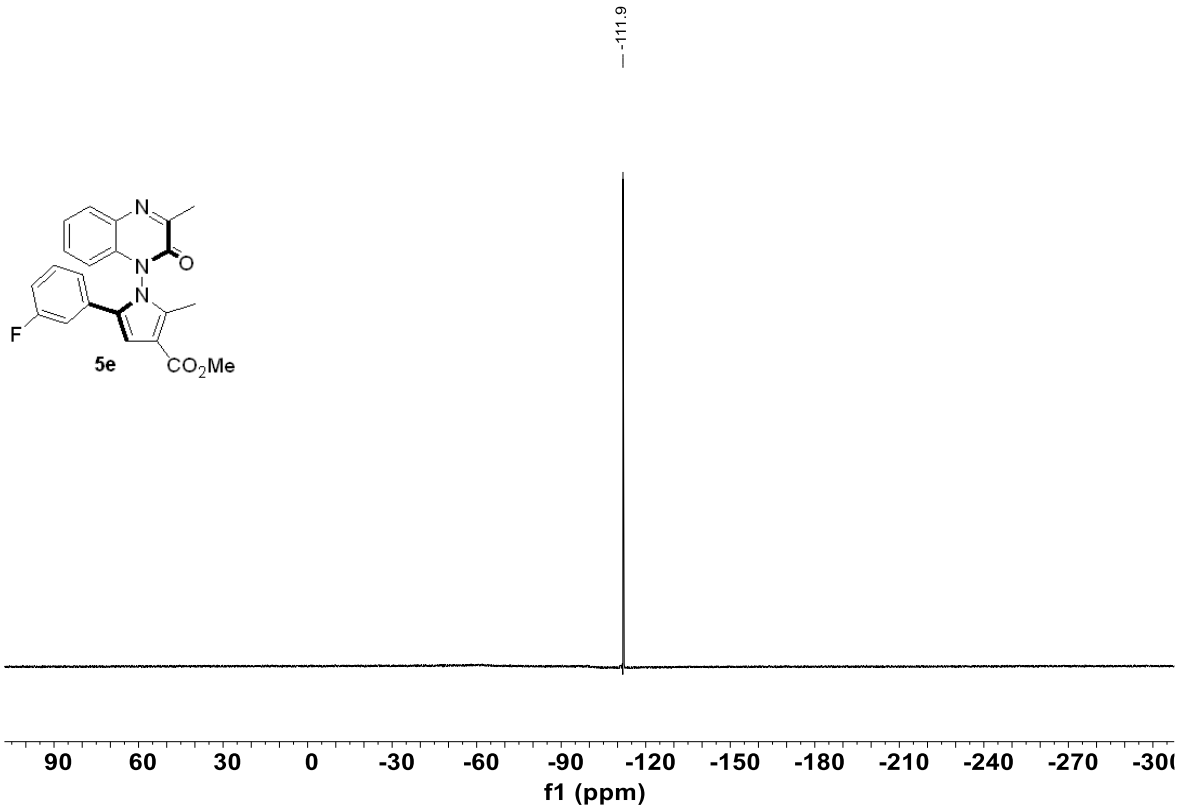
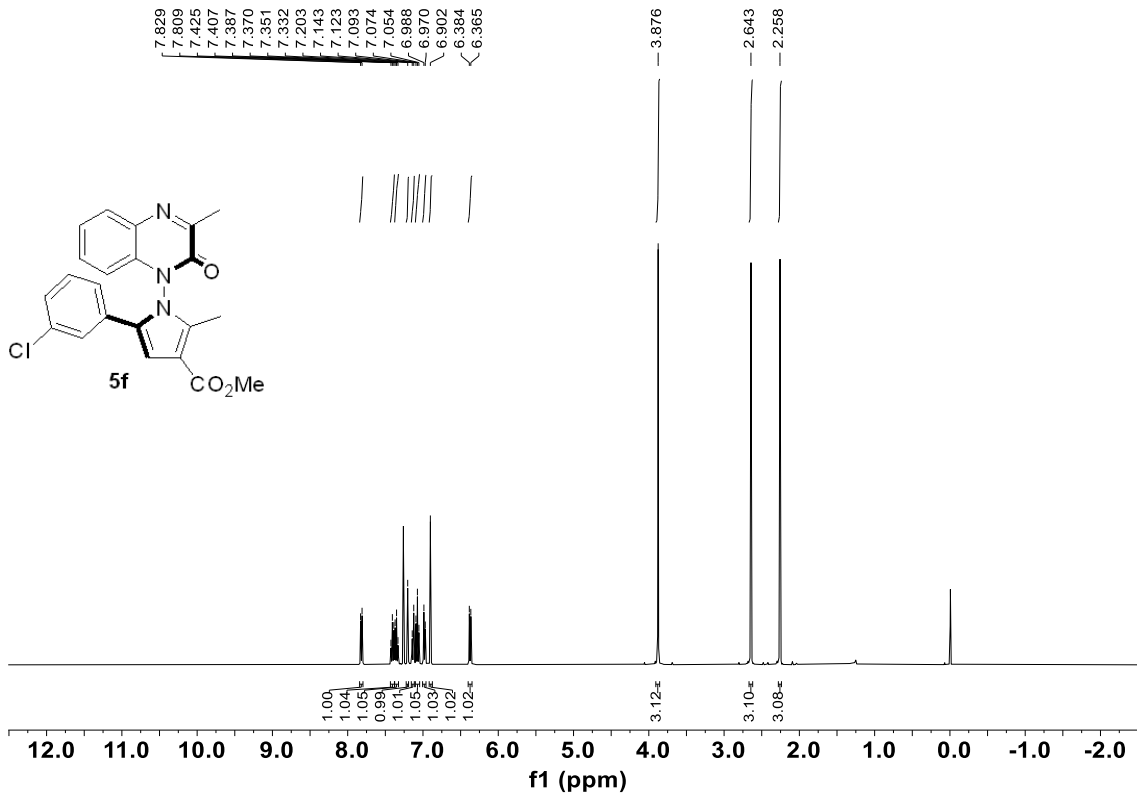
163.93
161.48
159.09
153.11
137.19
133.55
132.17
131.96
131.93
131.79
131.70
130.89
130.45
130.37
129.68
125.48
123.07
123.05
115.29
115.09
114.69
114.46
112.88
112.31
109.83
51.46
21.61
10.51
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)
5e
CO2Me


-111.9
F
5e
CO2Me
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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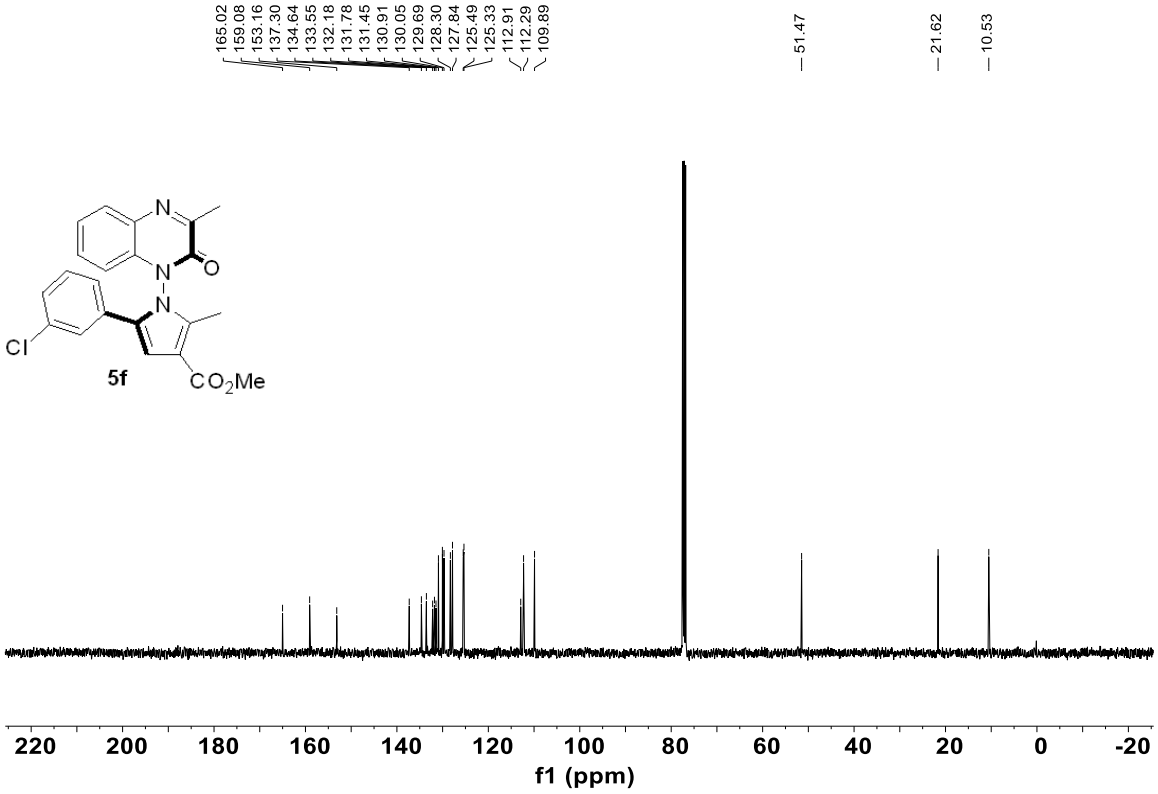
7.809
7.425
7.407
7.387
7.370
7.351
7.332
7.203
7.143
7.123
7.093
7.074
7.054
6.988
6.970
6.902
6.384
6.365
3.876
2.643
2.258
Cl
5f
CO2Me
1.00
1.04
1.05
0.99
1.01
1.05
1.03
1.02
1.02
3.12
3.10
3.08
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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159.08
153.16
137.30
134.64
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132.18
131.78
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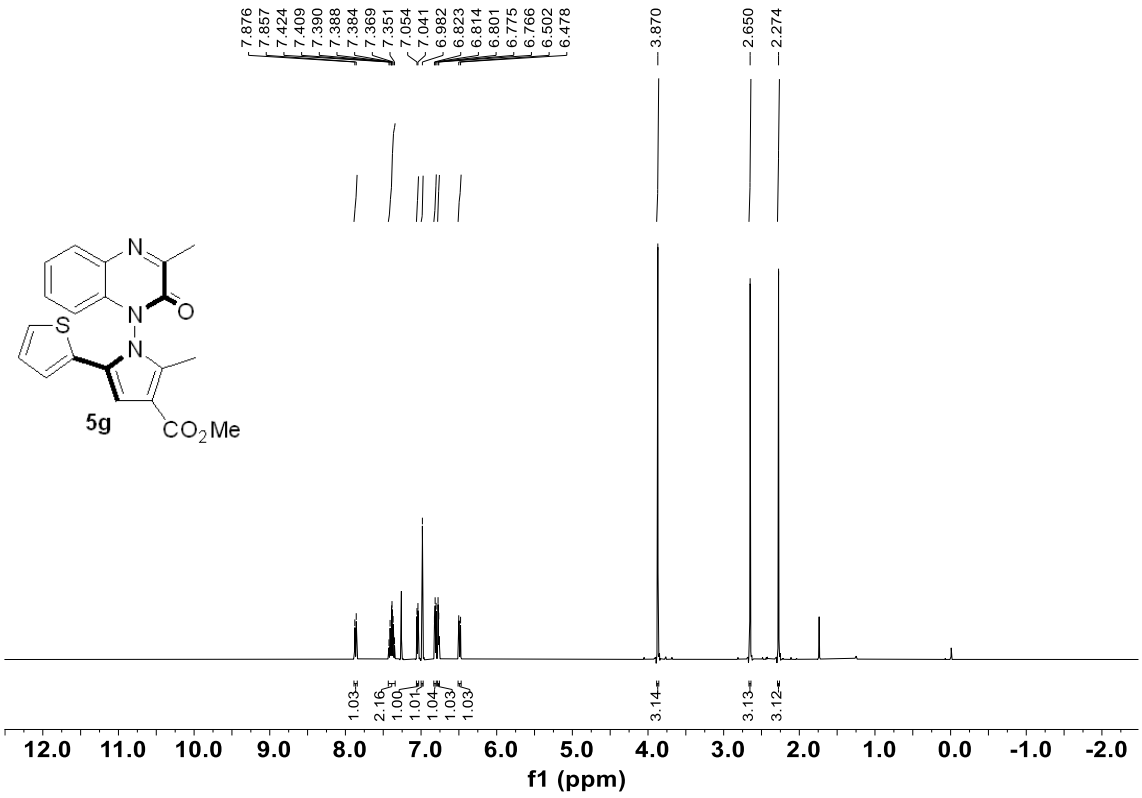
130.91
130.05
129.69
128.30
127.84
125.49
125.33
112.91
112.29
109.89
51.47
21.62
10.53
Cl
5f
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.857
7.424
7.409
7.390
7.388
7.384
7.369
7.351
7.054
7.041
6.982
6.823
6.814
6.801
6.775
6.766
6.502
6.478
3.870
2.650
2.274
5g
CO2Me
1.03
2.16
1.00
1.01
1.04
1.03
1.03
3.14
3.13
3.12
12.0
11.0
10.0
9.0
8.0
7.0
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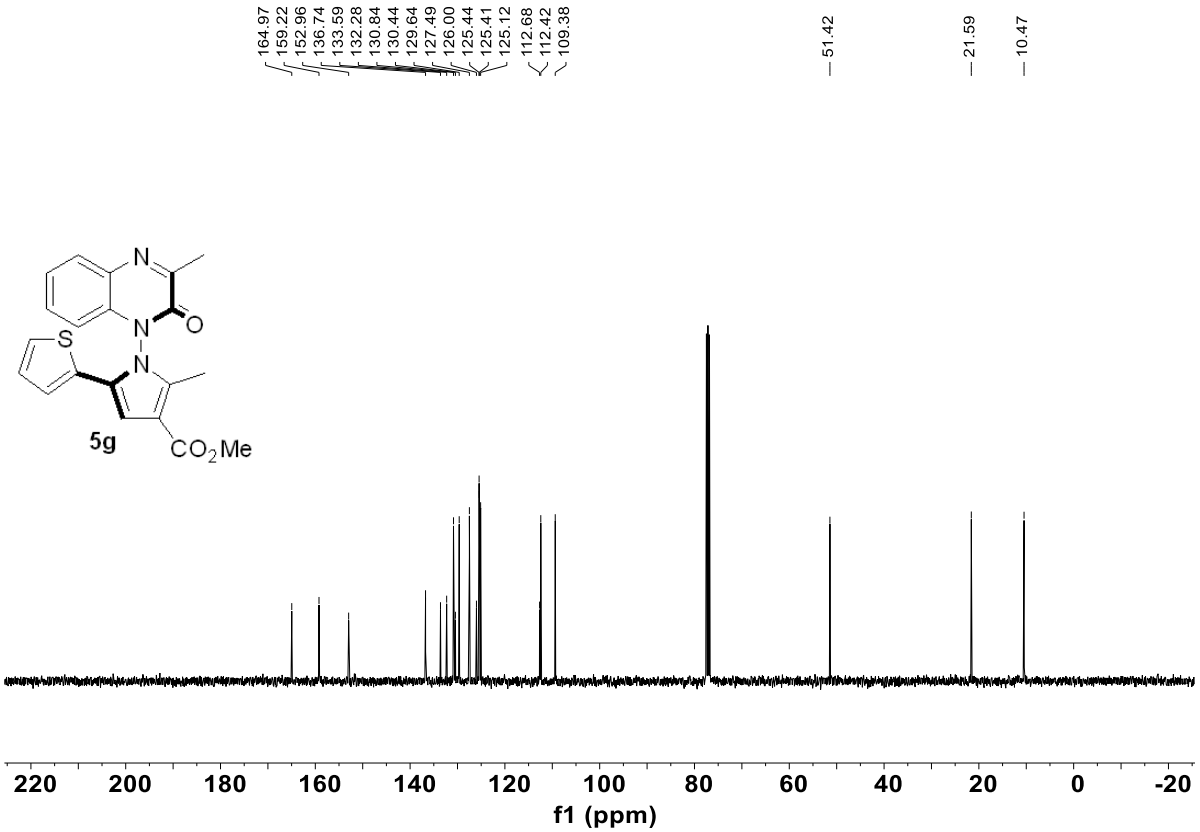
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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152.96
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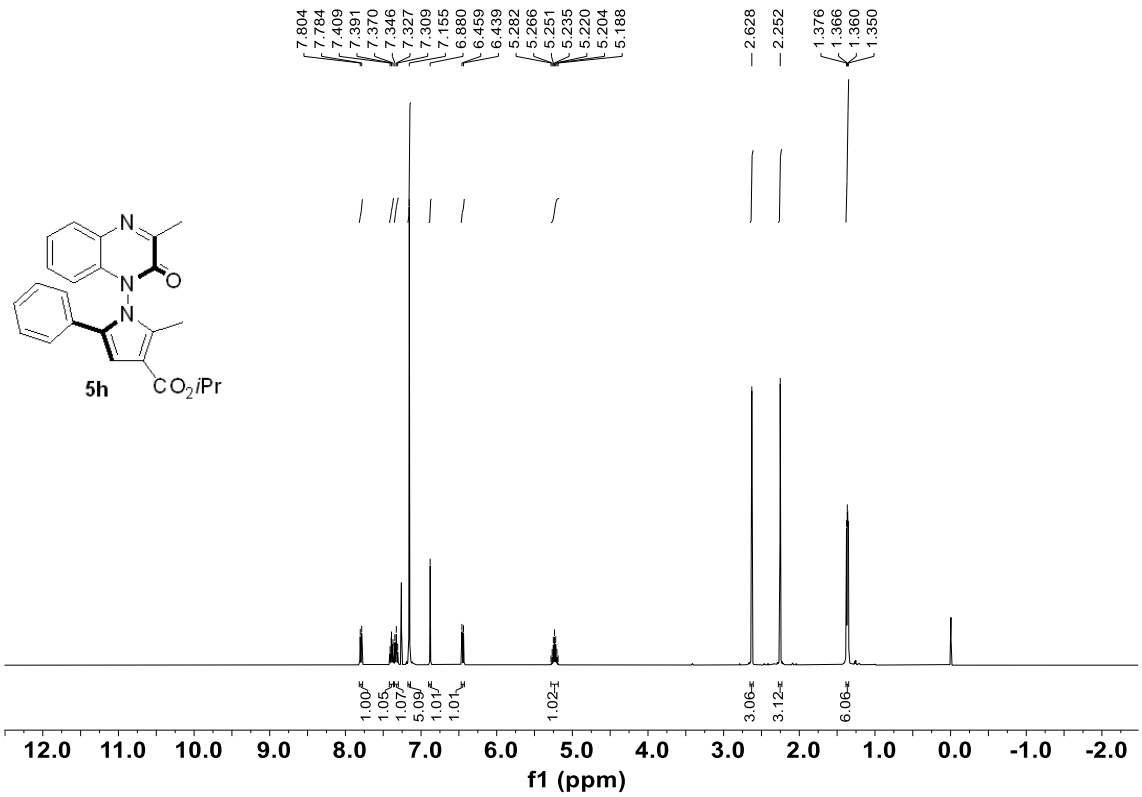
133.59
132.28
130.84
130.44
129.64
127.49
126.00
125.44
125.41
125.12
112.68
112.42
109.38
51.42
21.59
10.47
5g
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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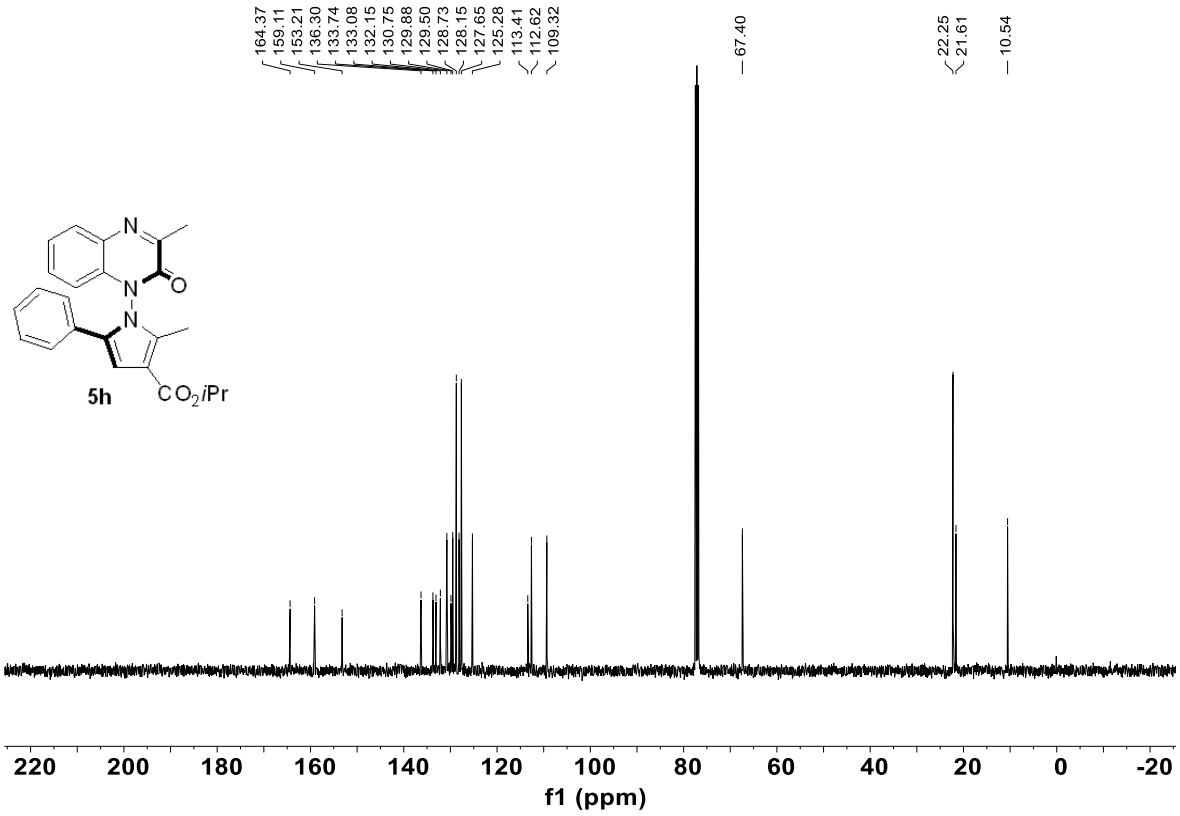
7.784
7.409
7.391
7.370
7.346
7.327
7.309
7.155
6.880
6.459
6.439
5.282
5.266
5.251
5.235
5.220
5.204
5.188
2.628
2.252
1.376
1.366
1.360
1.350
5h
CO2iPr
1.00
1.05
1.07
5.09
1.01
1.01
1.02
3.06
3.12
6.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


164.37
159.11
153.21
136.30
133.74
133.08
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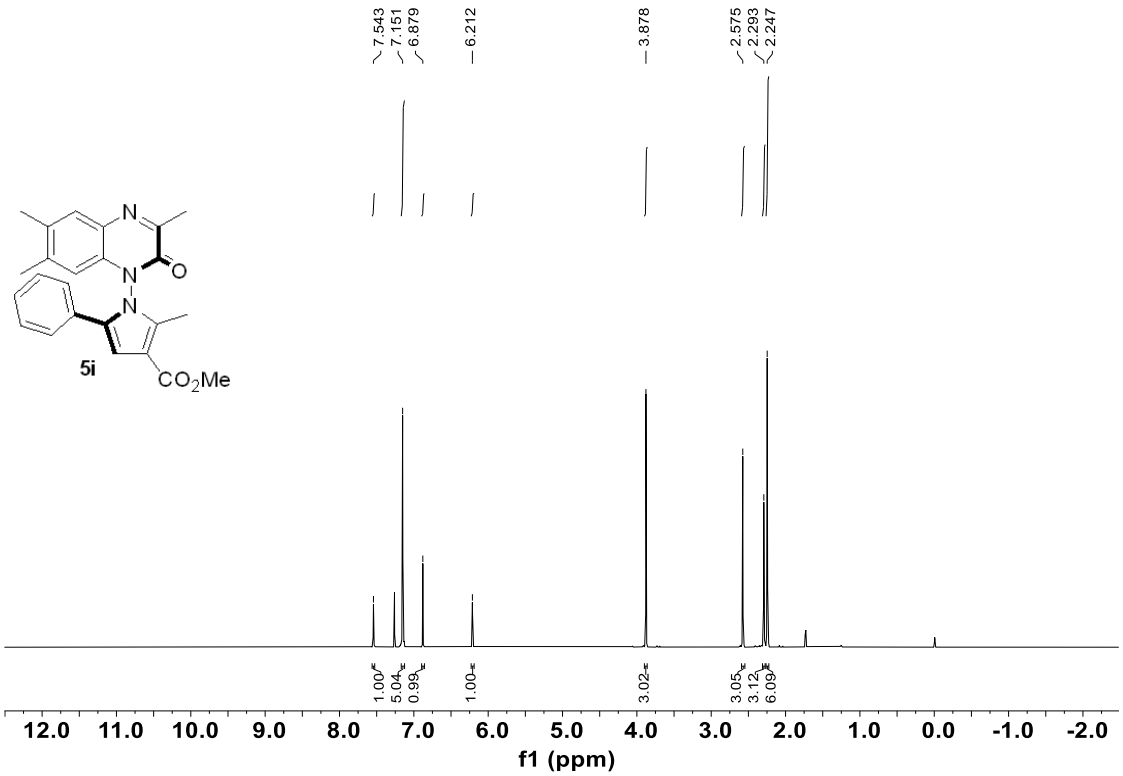
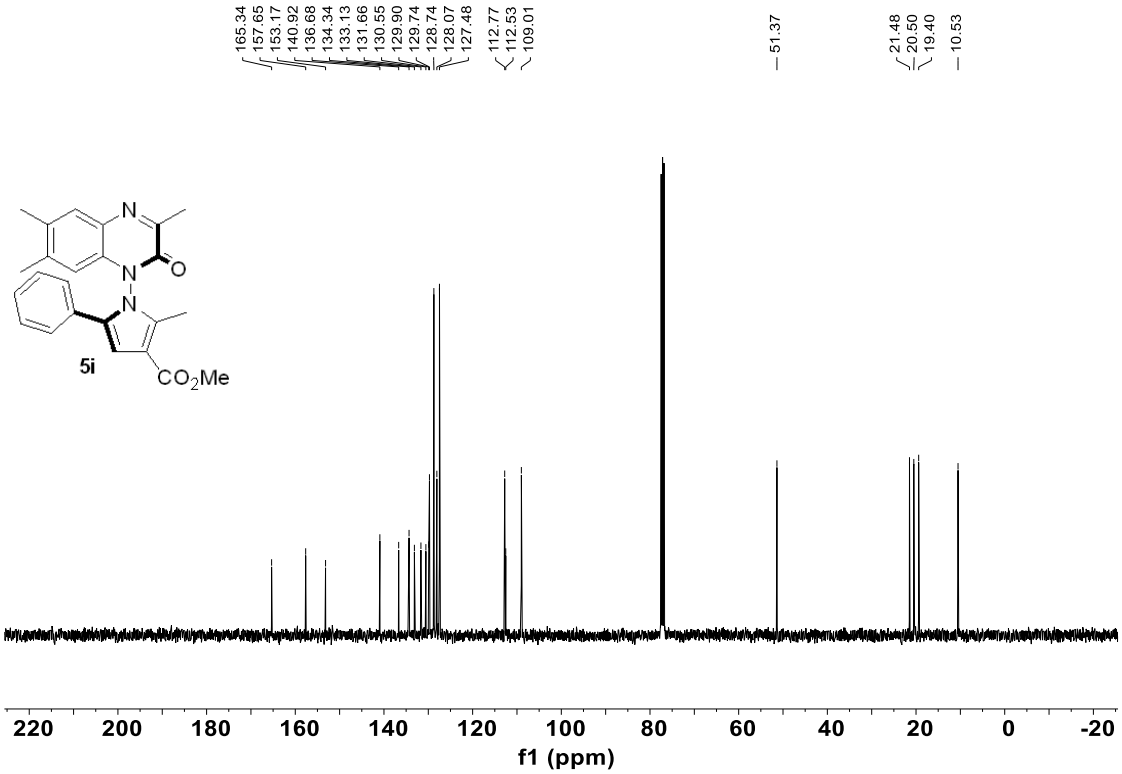
130.75
129.88
129.50
128.73
128.15
127.65
125.28
113.41
112.62
109.32
67.40
22.25
21.61
10.54
5h
CO2iPr
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


7.543
7.151
6.879
6.212
3.878
2.575
2.293
2.247
5i
CO2Me
1.00
5.04
0.99
1.00
3.02
3.05
3.12
6.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


165.34
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153.17
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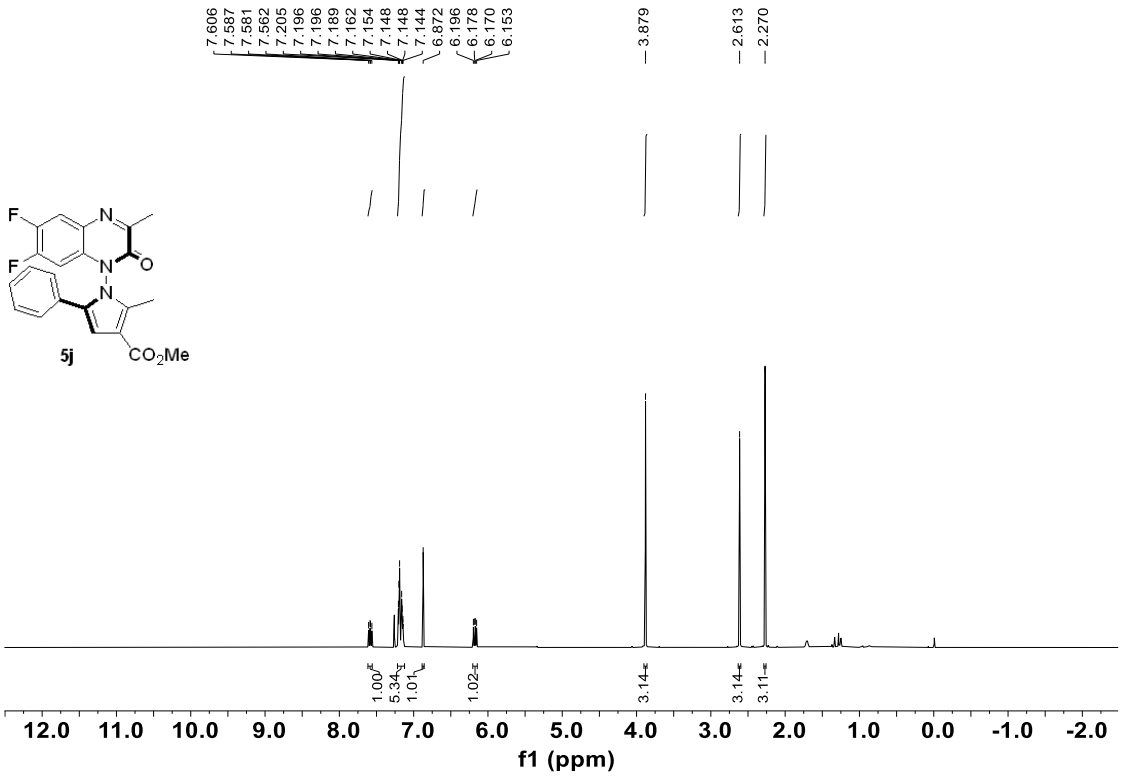
134.34
133.13
131.66
130.55
129.90
129.74
128.74
128.07
127.48
112.77
112.53
109.01
51.37
21.48
20.50
19.40
10.53
5i
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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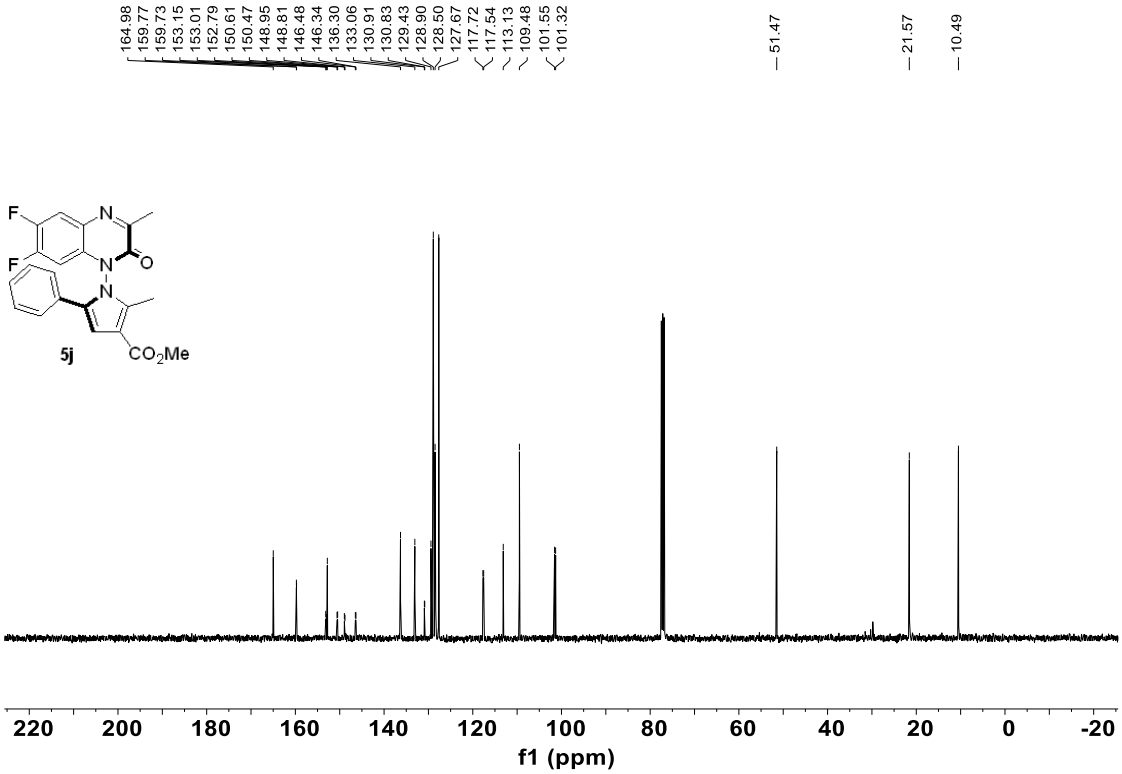
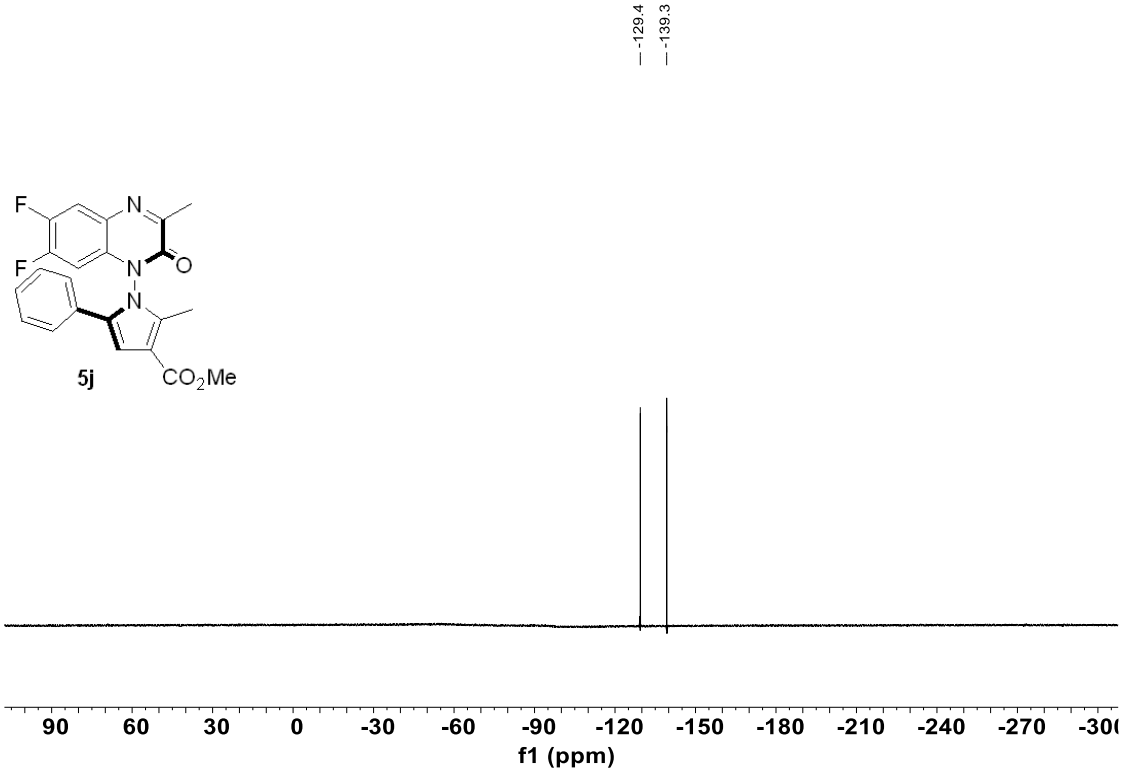
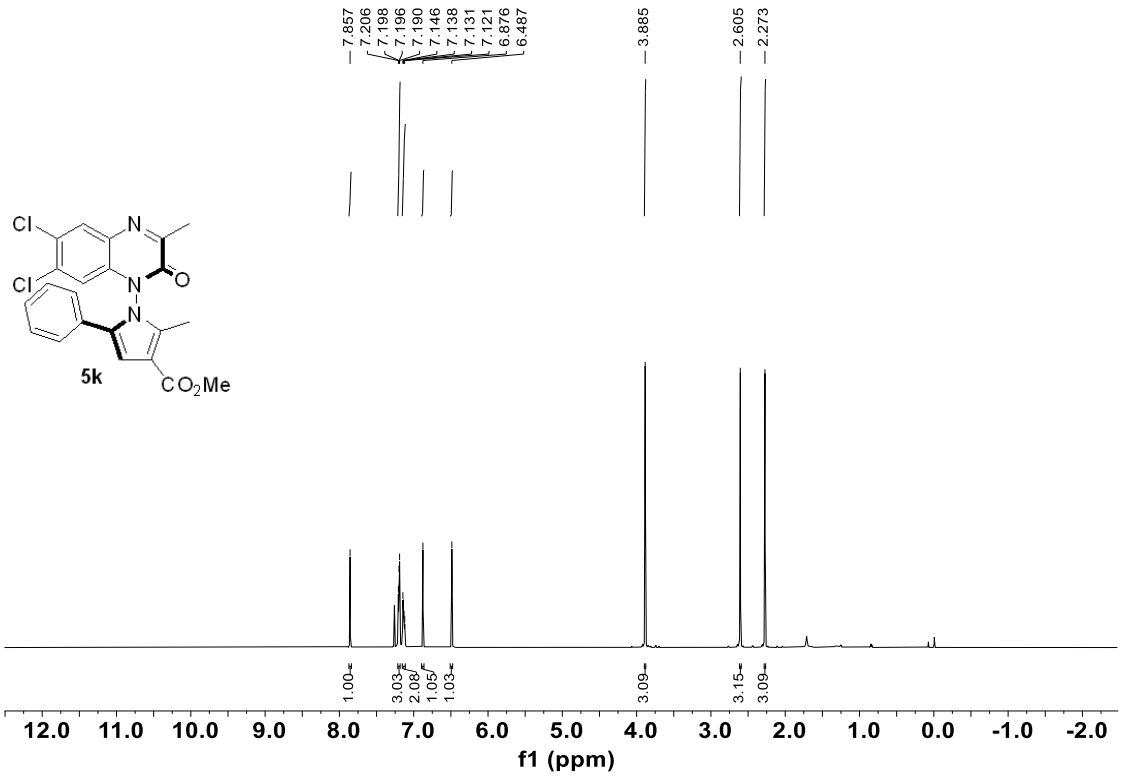
7.587
7.581
7.562
7.205
7.196
7.196
7.189
7.162
7.154
7.148
7.148
7.144
6.872
6.196
6.178
6.170
6.153
3.879
2.613
2.270
5j
CO2Me
1.00
5.34
1.01
1.02
3.14
3.14
3.11
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


164.98
159.77
159.73
153.15
153.01
152.79
150.61
150.47
148.95
148.81
146.48
146.34
136.30
133.06
130.91
130.83
129.43
128.90
128.50
127.67
117.72
117.54
113.13
109.48
101.55
101.32
51.47
21.57
10.49
F
F
N
O
N
N
5j
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)


-129.4
-139.3
F
F
N
O
N
N
5j
CO2Me
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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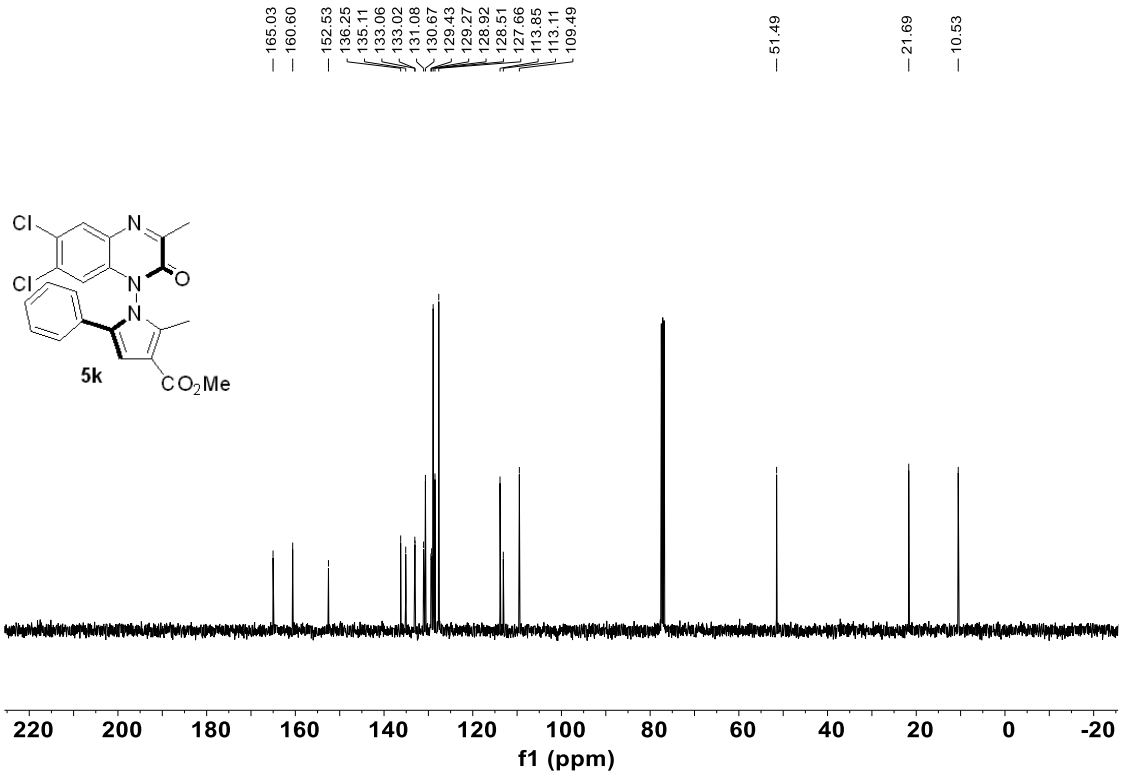
7.196
7.190
7.146
7.138
7.131
7.121
6.876
6.487
3.885
2.605
2.273
Cl
Cl
N
N
N
O
5k
CO2Me
1.00
3.03
2.08
1.05
1.03
3.09
3.15
3.09
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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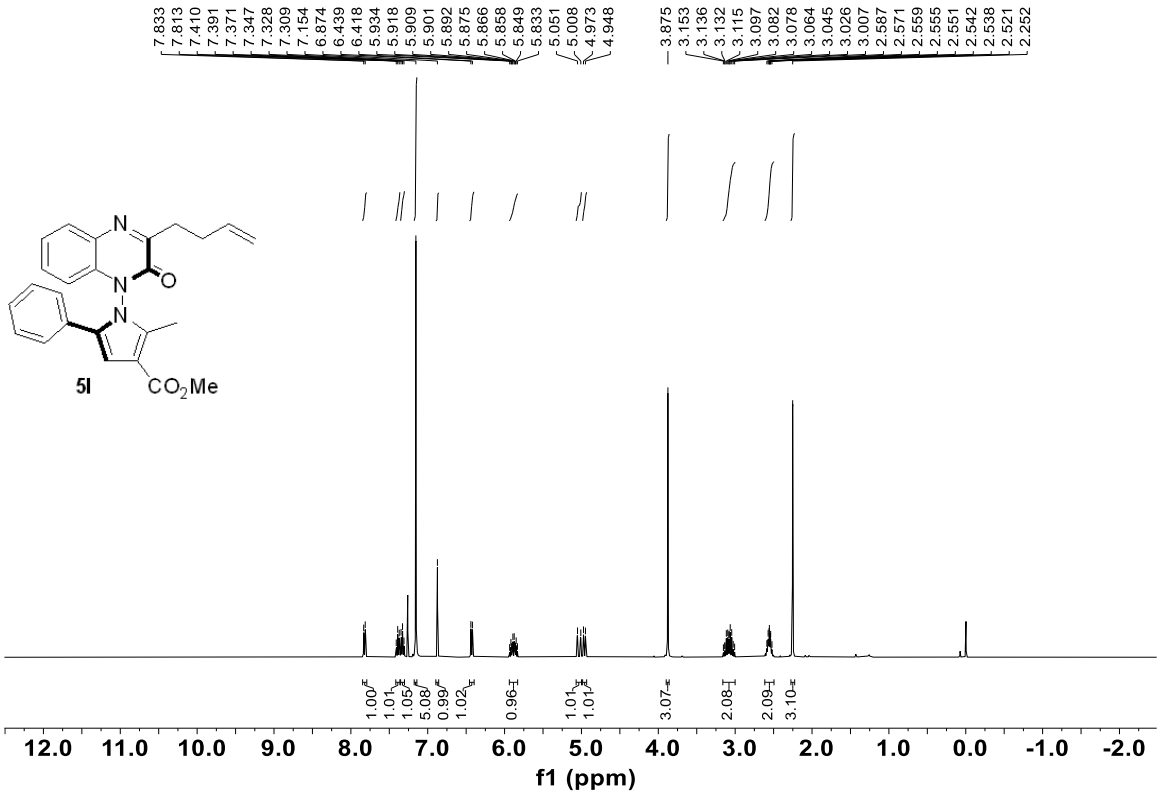
160.60
152.53
136.25
135.11
133.06
133.02
131.08
130.67
129.43
129.27
128.92
128.51
127.66
113.85
113.11
109.49
51.49
21.69
10.53
Cl
Cl
N
N
N
O
5k
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.813
7.410
7.391
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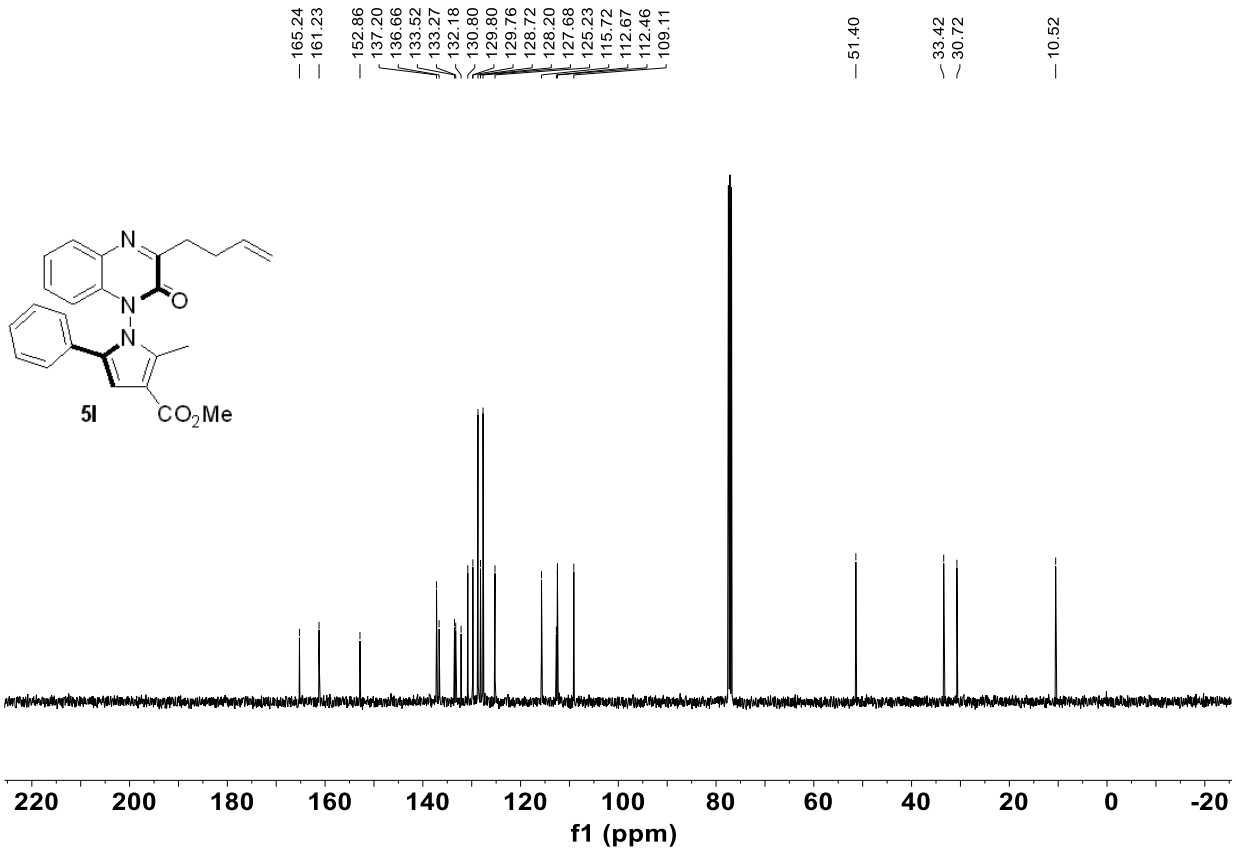
7.347
7.328
7.309
7.154
6.874
6.439
6.418
5.934
5.918
5.909
5.901
5.892
5.875
5.866
5.858
5.849
5.833
5.051
5.008
4.973
4.948
3.875
3.153
3.136
3.132
3.115
3.097
3.082
3.078
3.064
3.045
3.026
3.007
2.587
2.571
2.559
2.555
2.551
2.542
2.538
2.521
2.252
5l
CO2Me
1.00
1.01
1.05
5.08
0.99
1.02
0.96
1.01
1.01
3.07
2.08
2.09
3.10
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)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132.18
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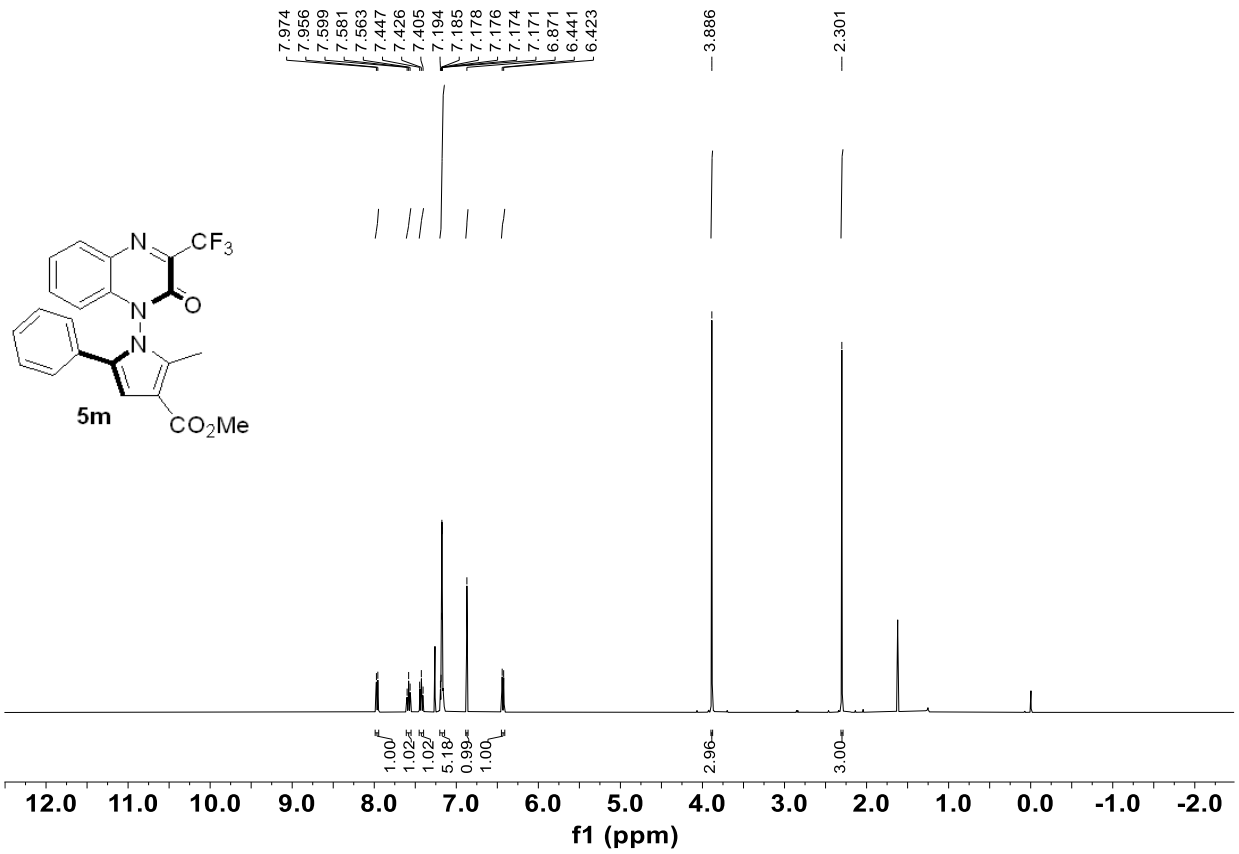
129.80
129.76
128.72
128.20
127.68
125.23
115.72
112.67
112.46
109.11
51.40
33.42
30.72
10.52
5l
CO2Me
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)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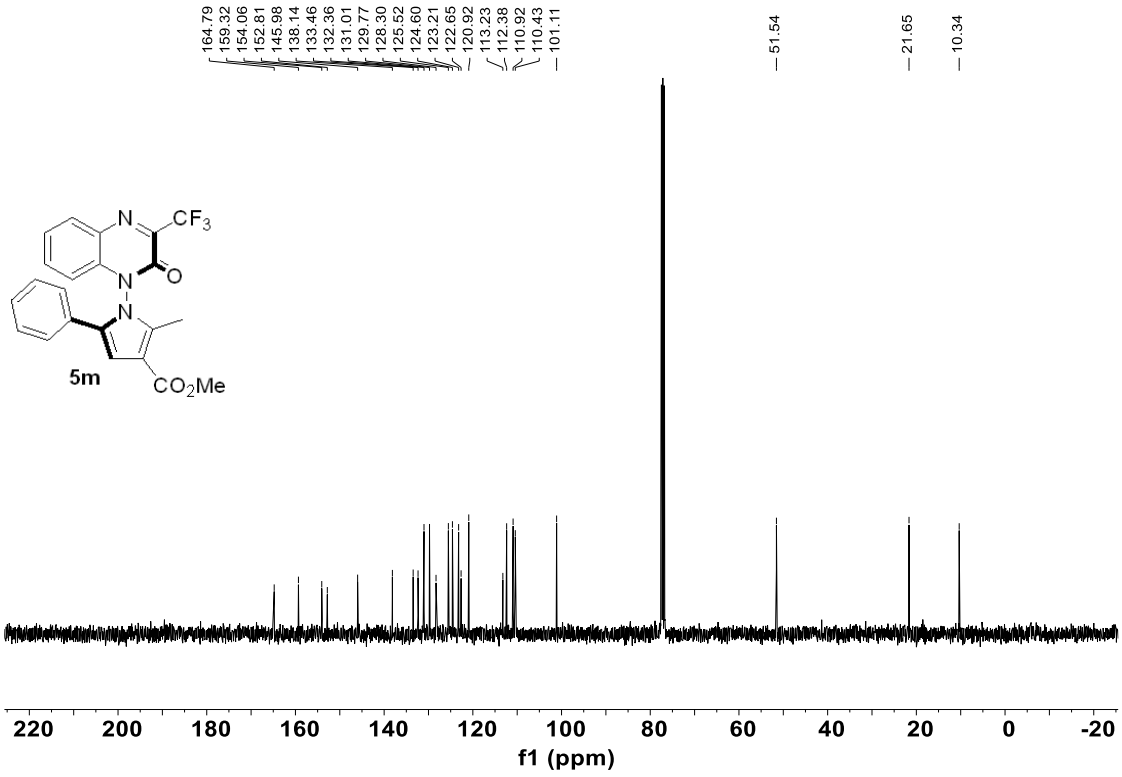
7.405
7.194
7.185
7.178
7.176
7.174
7.171
6.871
6.441
6.423
3.886
2.301
1.00
1.02
1.02
5.18
0.99
1.00
2.96
3.00
12.0 11.0 10.0 9.0 8.0 7.0 6.0 5.0 4.0 3.0 2.0 1.0 0.0 -1.0 -2.0
f1 (ppm)
N
CF3
O
N
N
5m
CO2Me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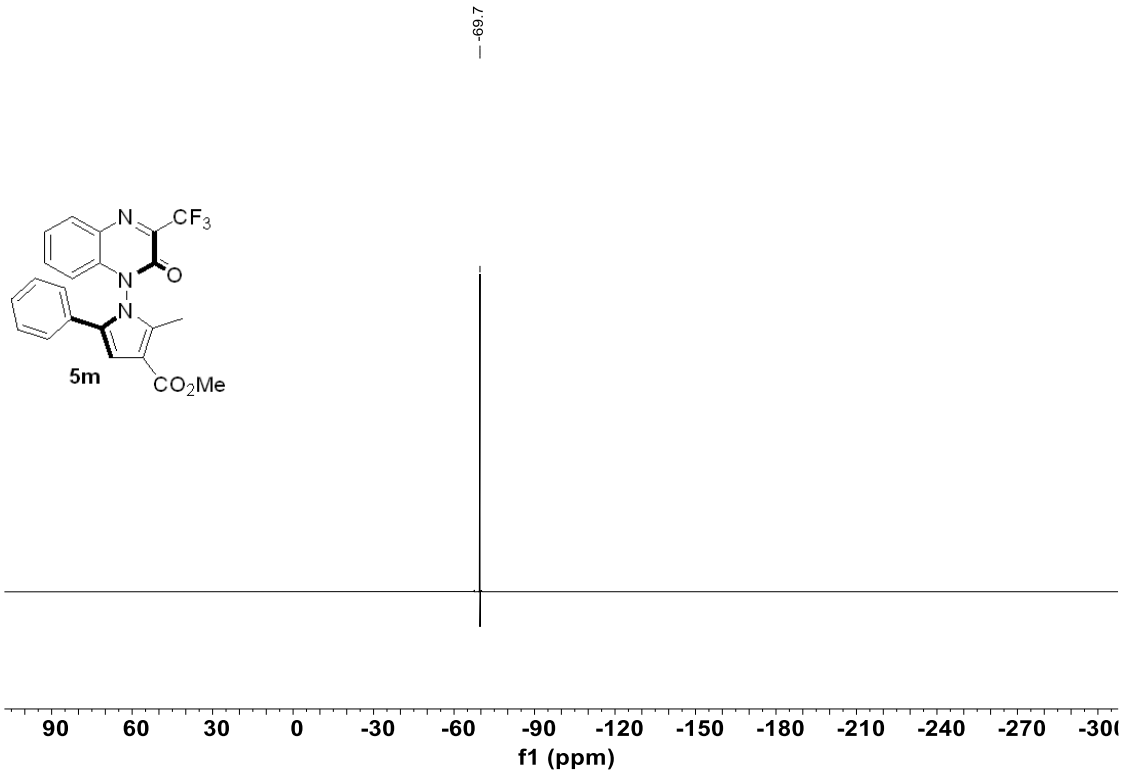
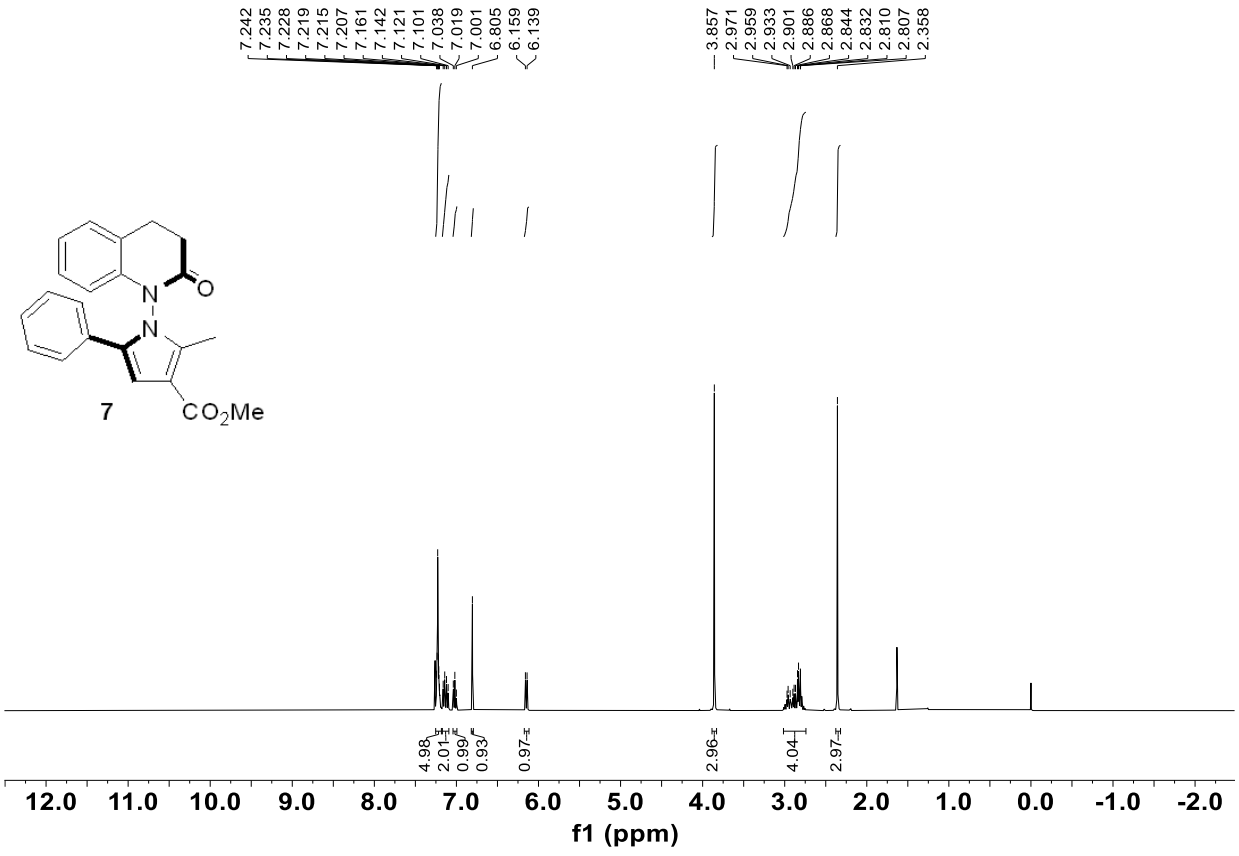
152.81
145.98
138.14
133.46
132.36
131.01
129.77
128.30
125.52
124.60
123.21
122.65
120.92
113.23
112.38
110.92
110.43
101.11
51.54
21.65
10.34
220 200 180 160 140 120 100 80 60 40 20 0 -20
f1 (ppm)
N
CF3
O
N
N
5m
CO2Me


-69.7
5m
CF3
CO2Me
90
60
30
0
-30
-60
-90
-120
-150
-180
-210
-240
-270
f1 (ppm)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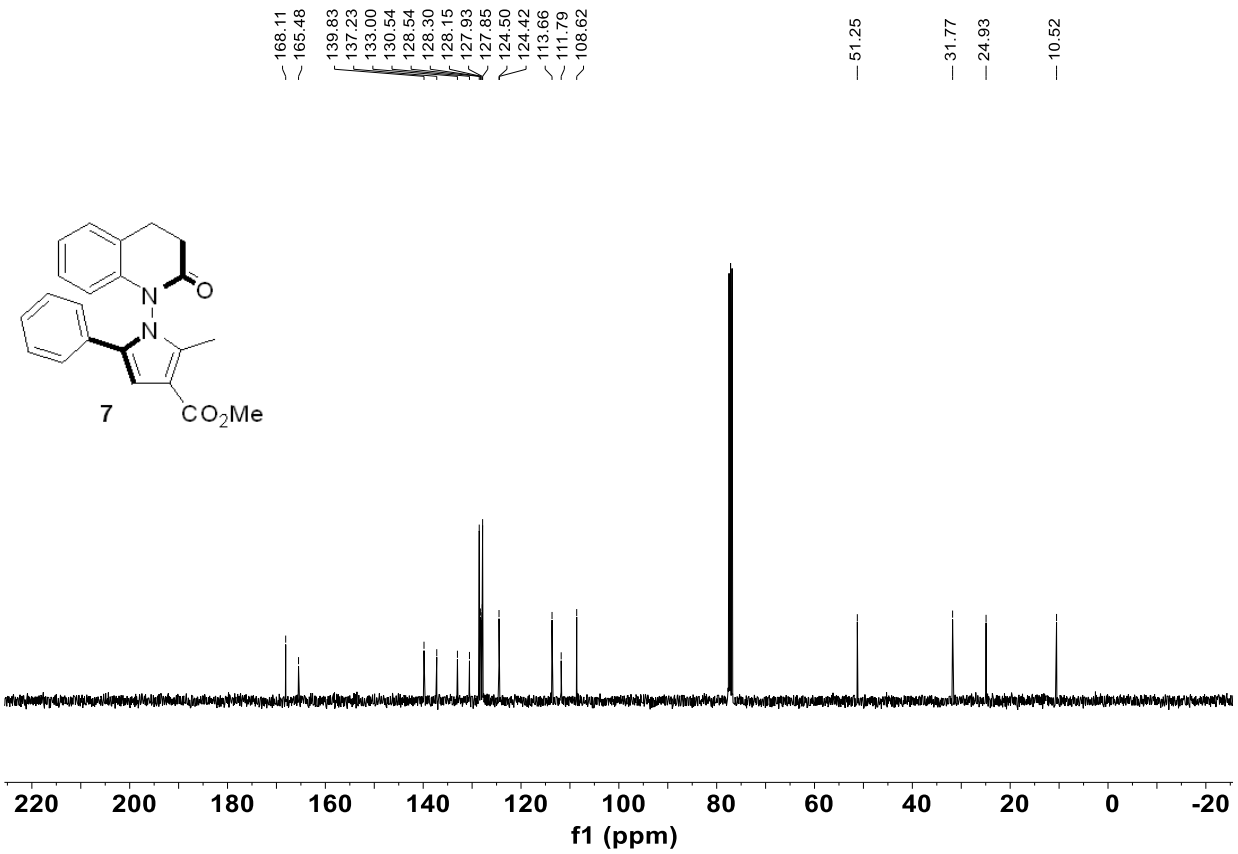
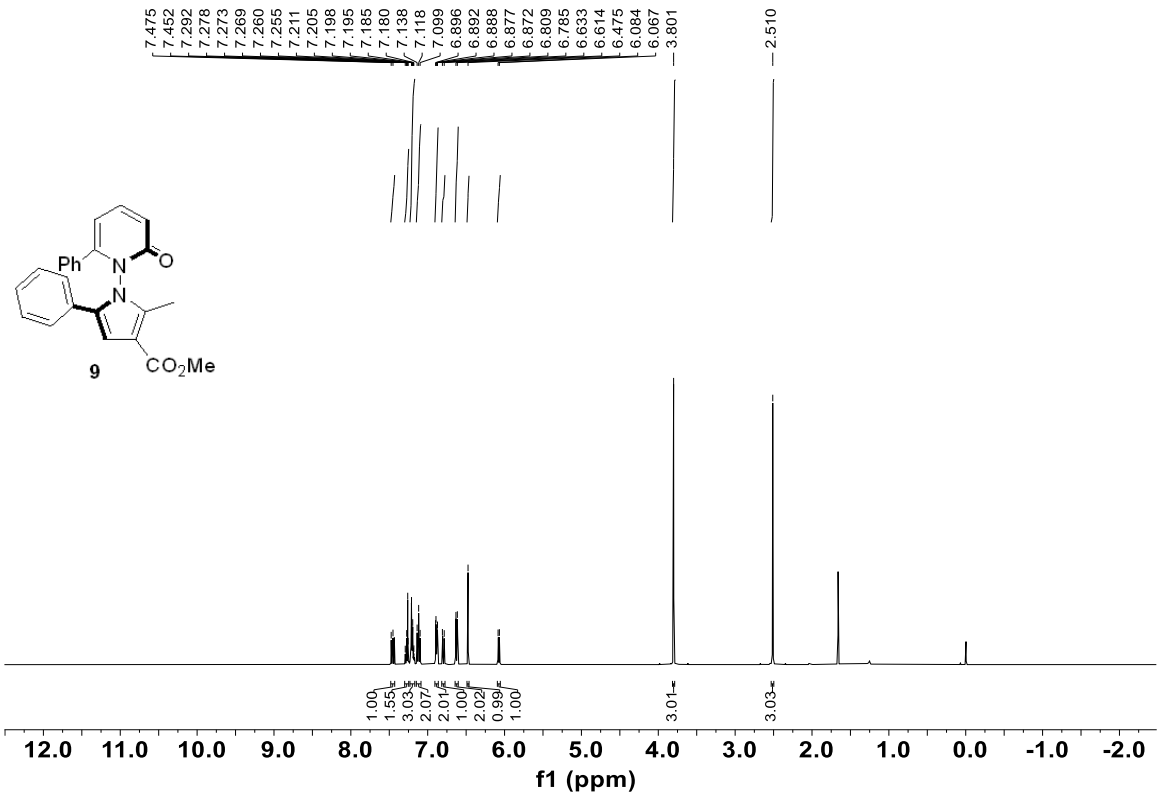
7.121
7.101
7.038
7.019
7.001
6.805
6.159
6.139
3.857
2.971
2.959
2.933
2.901
2.886
2.868
2.844
2.832
2.810
2.807
2.358
7
CO2Me
4.98
2.01
0.99
0.93
0.97
2.96
4.04
2.97
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


168.11
165.48
139.83
137.23
133.00
130.54
128.54
128.30
128.15
127.93
127.85
124.50
124.42
113.66
111.79
108.62
51.25
31.77
24.93
10.52
7
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.273
7.269
7.260
7.255
7.211
7.205
7.198
7.195
7.185
7.180
7.138
7.118
7.099
6.896
6.892
6.888
6.877
6.872
6.809
6.785
6.633
6.614
6.475
6.084
6.067
3.801
2.510
Ph
9
CO2Me
1.00
1.55
3.03
2.07
2.01
1.00
2.02
0.99
1.00
3.01
3.03
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
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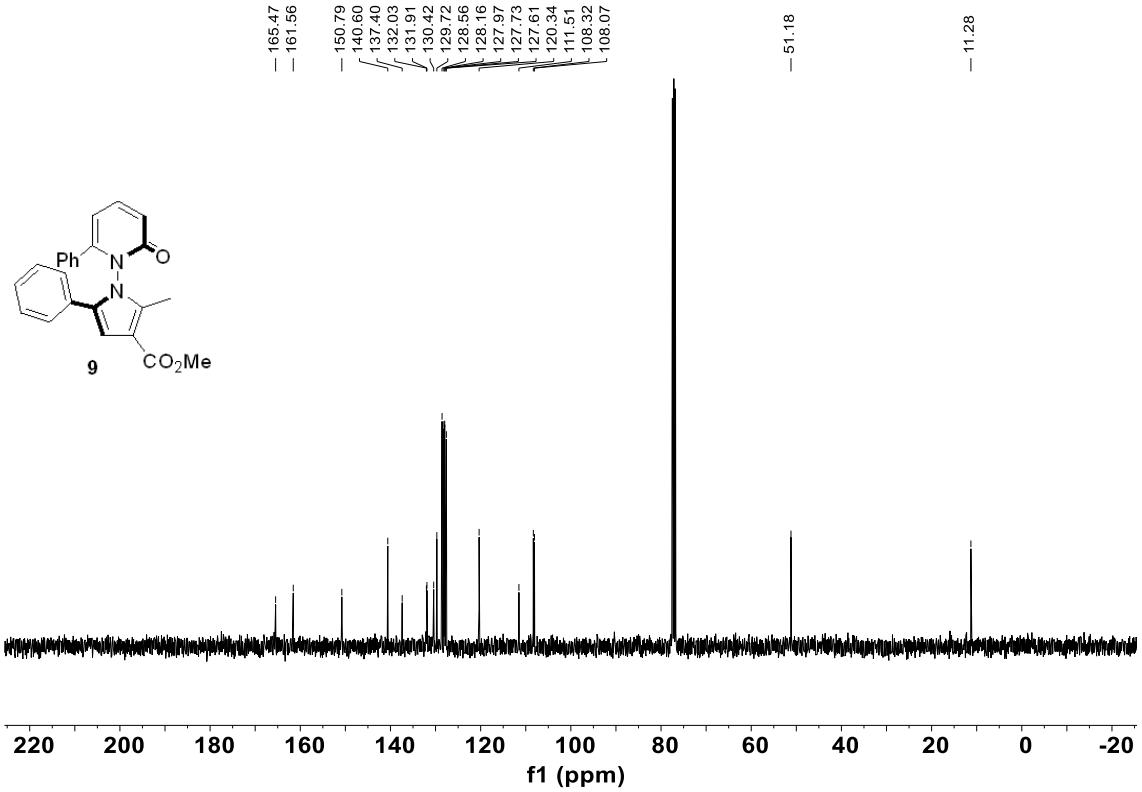
-2.0
f1 (ppm)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161.56
150.79
140.60
137.40
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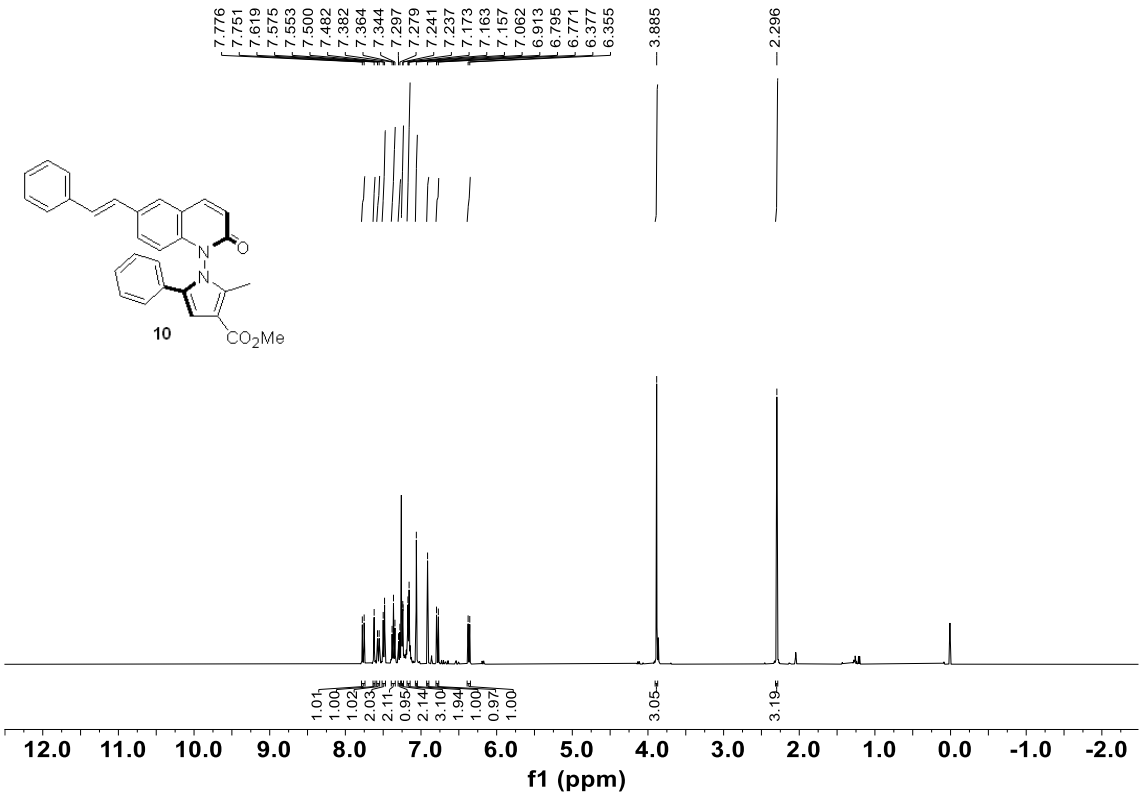
131.91
130.42
129.72
128.56
128.16
127.97
127.73
127.61
120.34
111.51
108.32
108.07
51.18
11.28
Ph
N
N
O
CO2Me
9
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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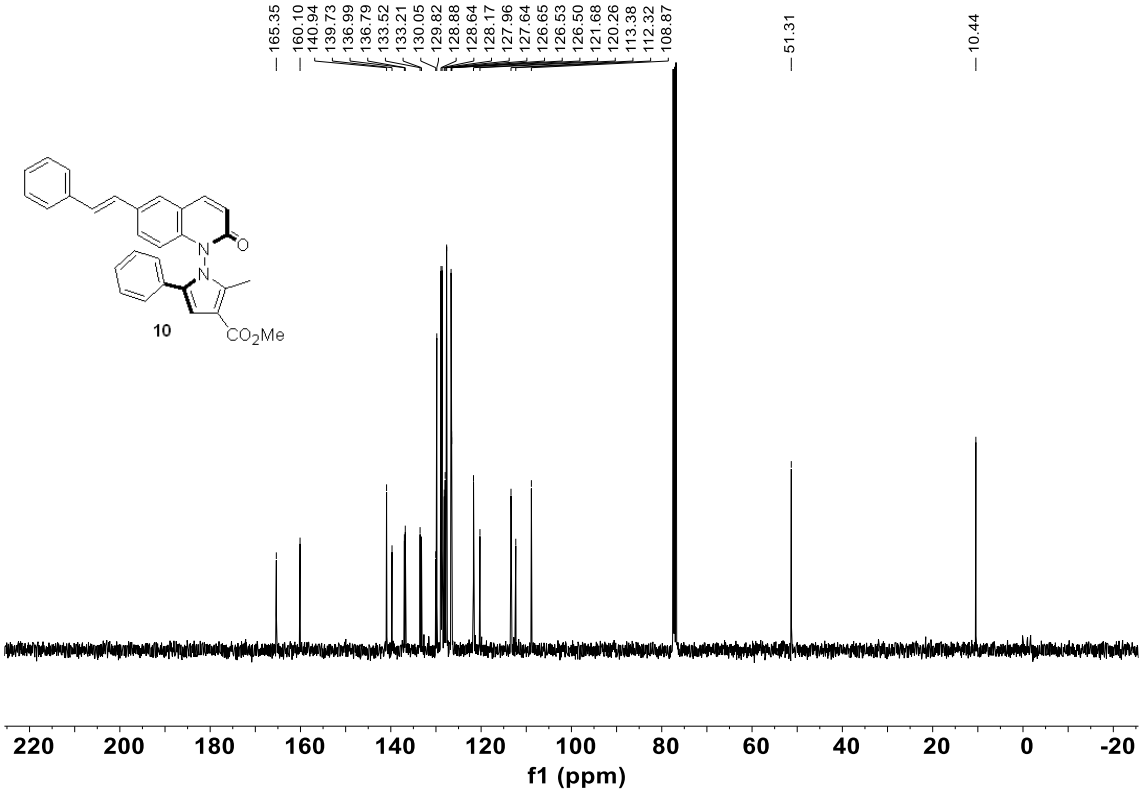
7.619
7.575
7.553
7.500
7.482
7.382
7.364
7.344
7.297
7.279
7.241
7.237
7.173
7.163
7.157
7.062
6.913
6.795
6.771
6.377
6.355
3.885
2.296
N
N
O
CO2Me
10
1.01
1.00
1.02
2.03
2.11
0.95
2.14
3.10
1.94
1.00
0.97
1.00
3.05
3.19
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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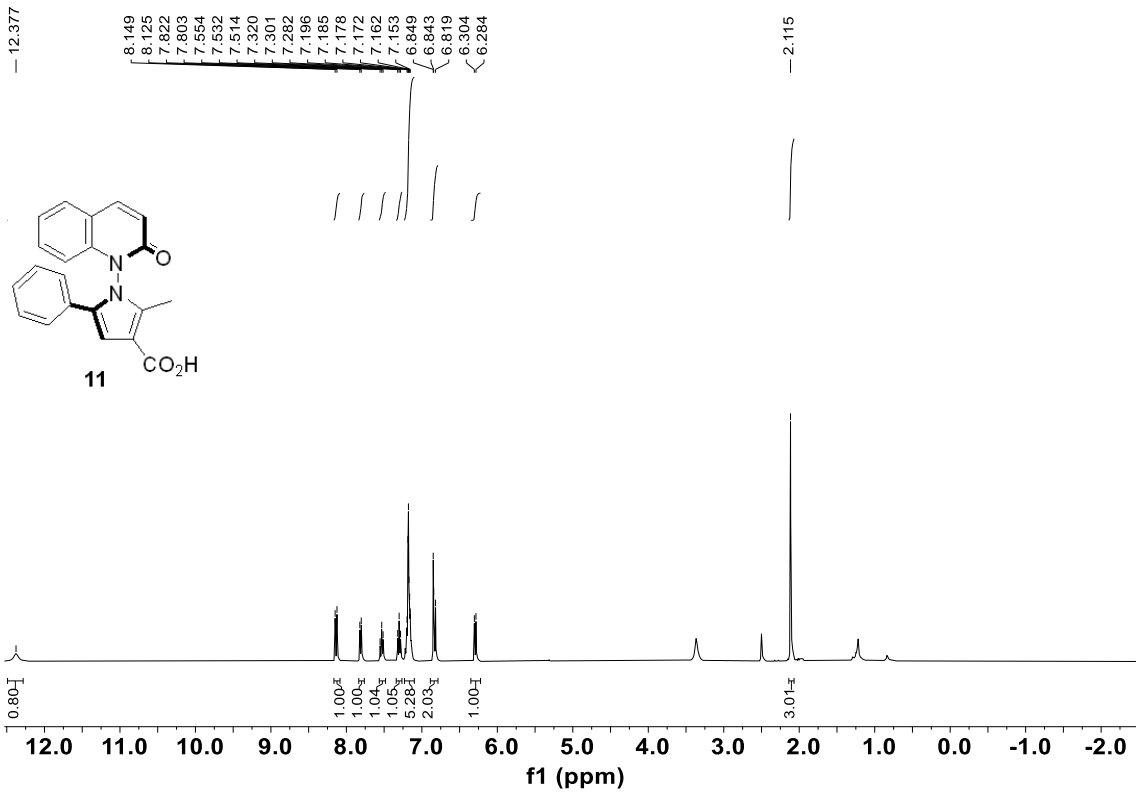
160.10
140.94
139.73
136.99
136.79
133.52
133.21
130.05
129.82
128.88
128.64
128.17
127.96
127.64
126.65
126.53
126.50
121.68
120.26
113.38
112.32
108.87
51.31
10.44
10
CO2Me
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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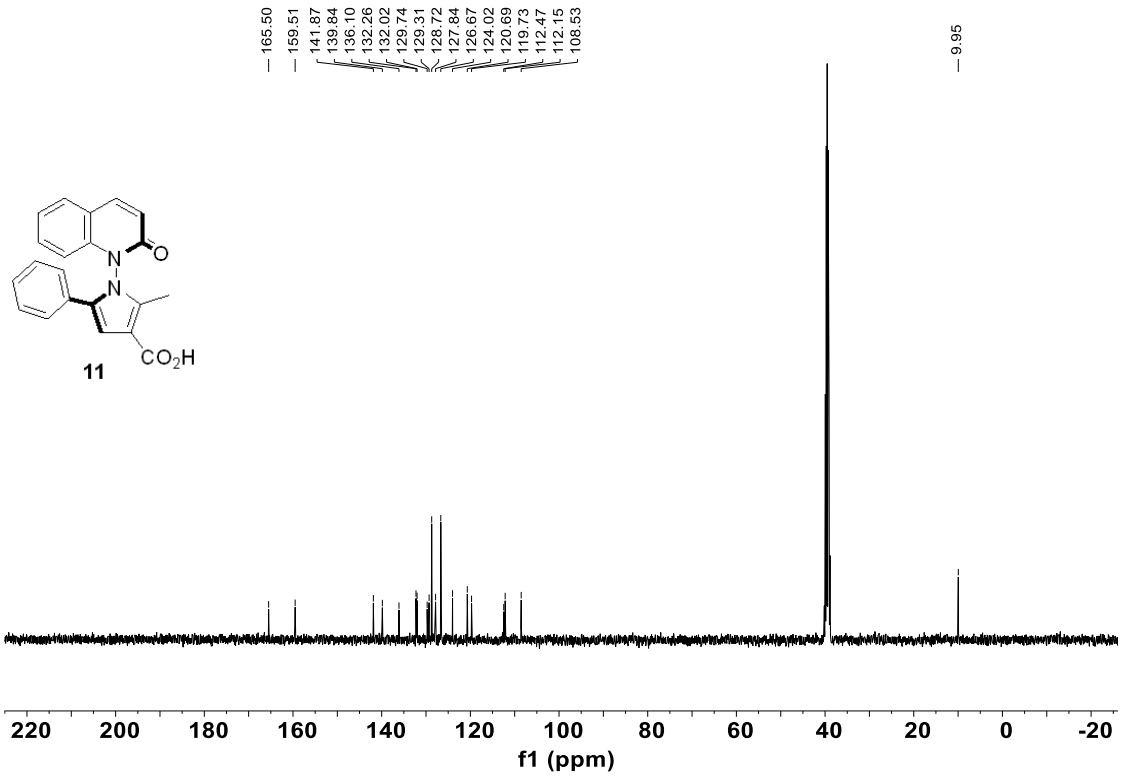
8.149
8.125
7.822
7.803
7.554
7.532
7.514
7.320
7.301
7.282
7.196
7.185
7.178
7.172
7.162
7.153
6.849
6.843
6.819
6.304
6.284
2.115
11
CO2H
0.80
1.00
1.00
1.04
1.05
5.28
2.03
1.00
3.01
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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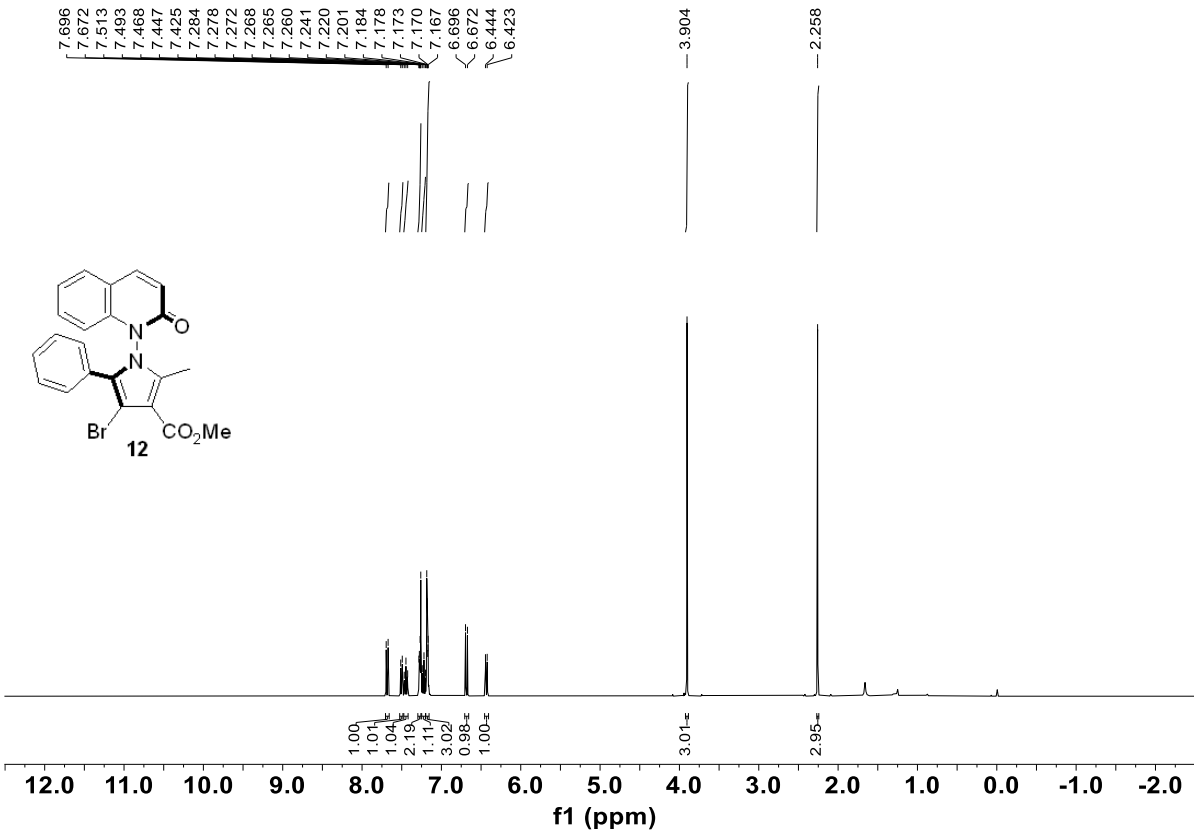
159.51
141.87
139.84
136.10
132.26
132.02
129.74
129.31
128.72
127.84
126.67
124.02
120.69
119.73
112.47
112.15
108.53
9.95
O
N
N
CO2H
11
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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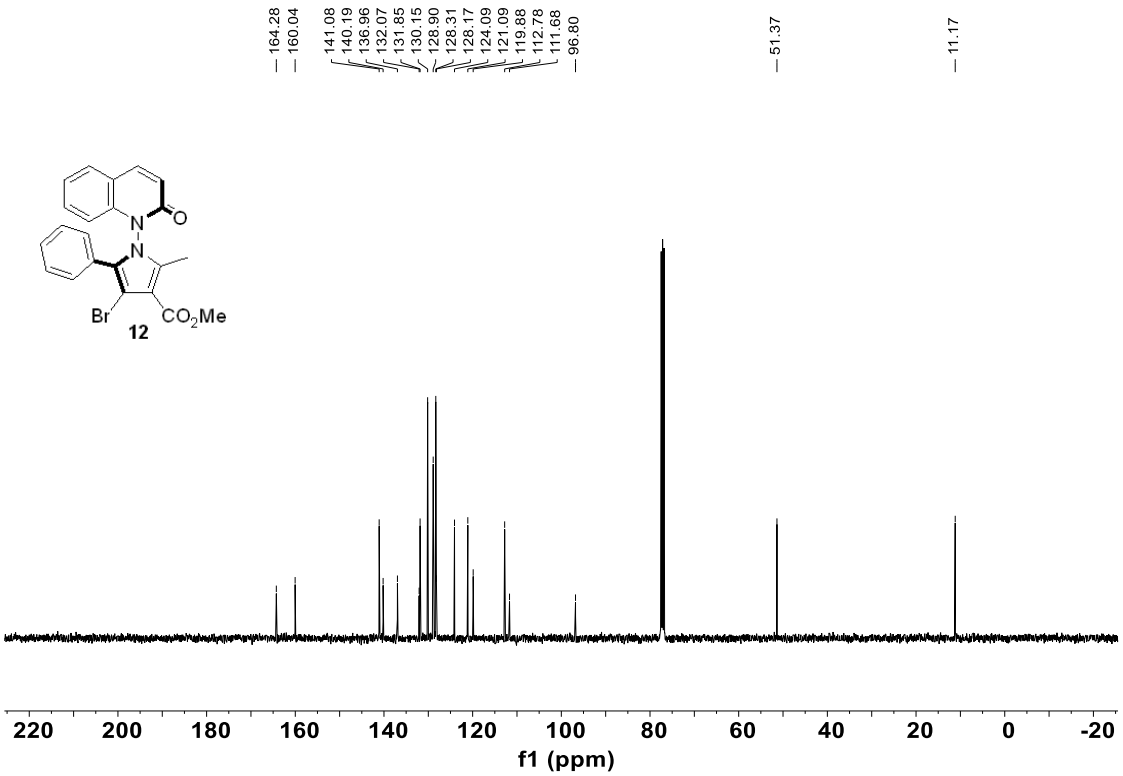
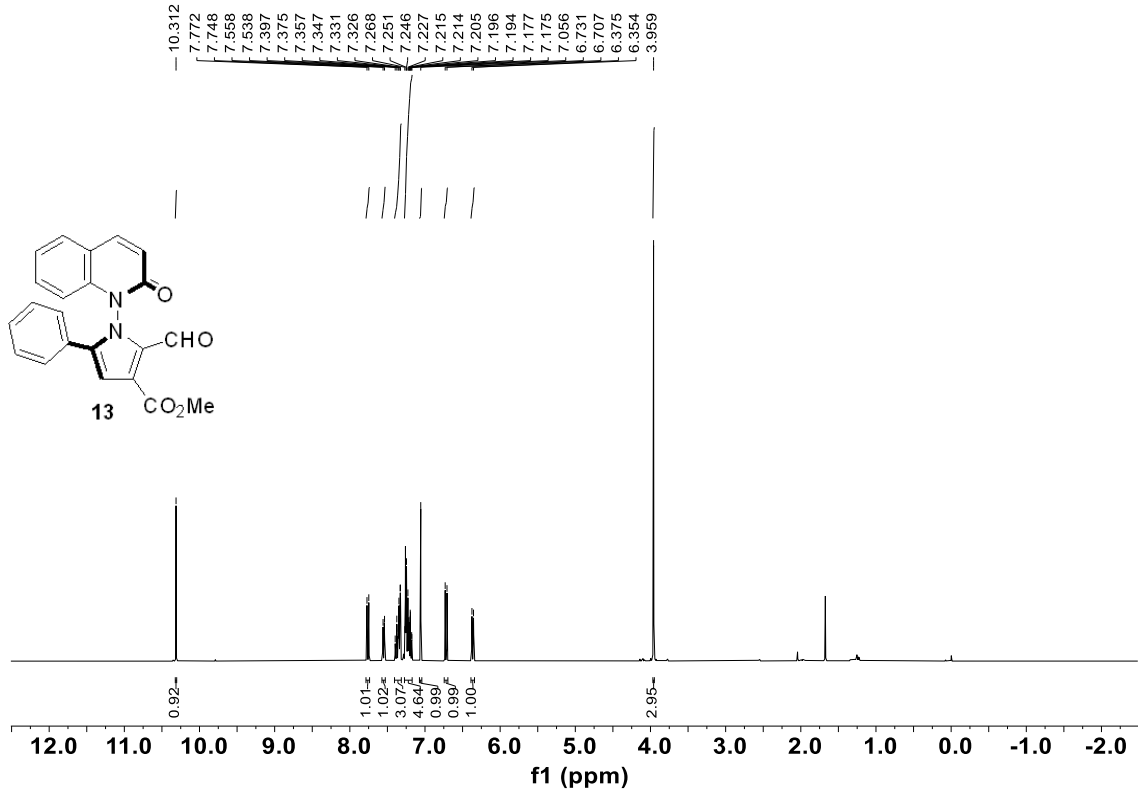
7.468
7.447
7.425
7.284
7.278
7.272
7.268
7.265
7.260
7.241
7.220
7.201
7.184
7.178
7.173
7.170
7.167
6.696
6.672
6.444
6.423
3.904
2.258
O
N
N
Br
CO2Me
12
1.00
1.01
1.04
2.19
1.11
3.02
0.98
1.00
3.01
2.95
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


164.28
160.04
141.08
140.19
136.96
132.07
131.85
130.15
128.90
128.31
128.17
124.09
121.09
119.88
112.78
111.68
96.80
51.37
11.17
Br
CO2Me
12
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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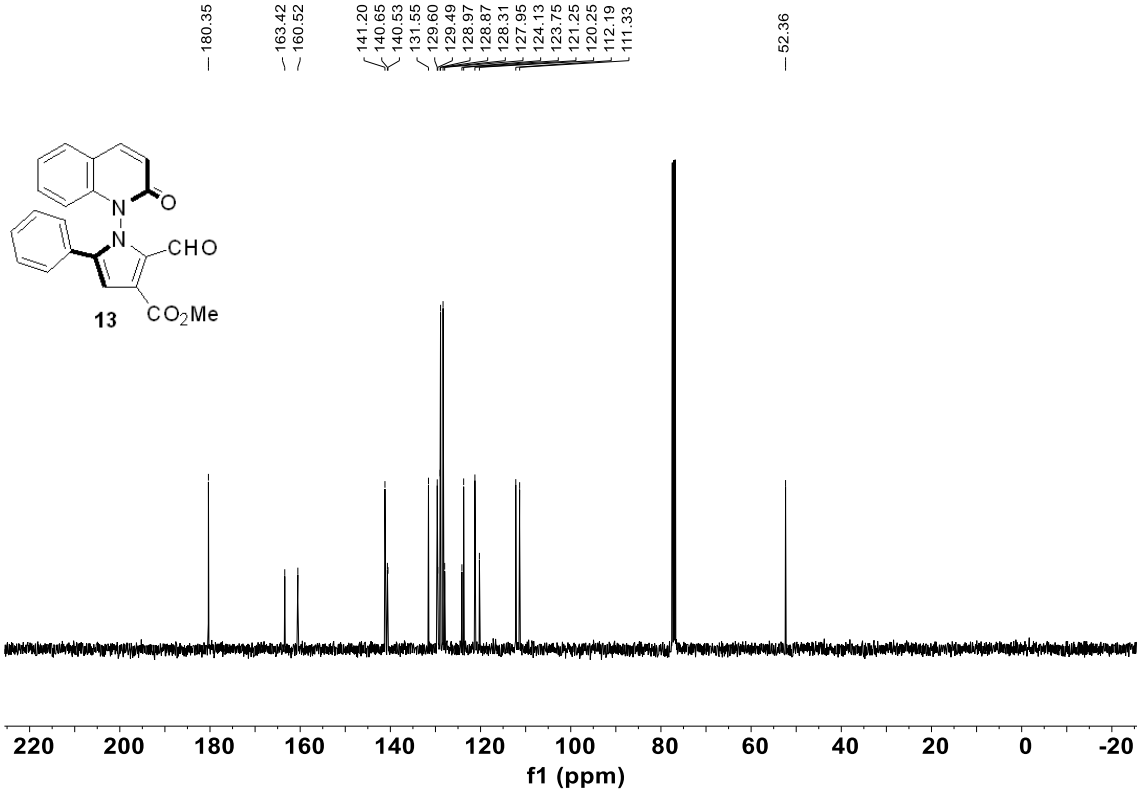
7.268
7.251
7.246
7.227
7.215
7.214
7.205
7.196
7.194
7.177
7.175
7.056
6.731
6.707
6.375
6.354
3.959
CHO
CO2Me
13
0.92
1.01
1.02
3.07
4.64
0.99
0.99
1.00
2.95
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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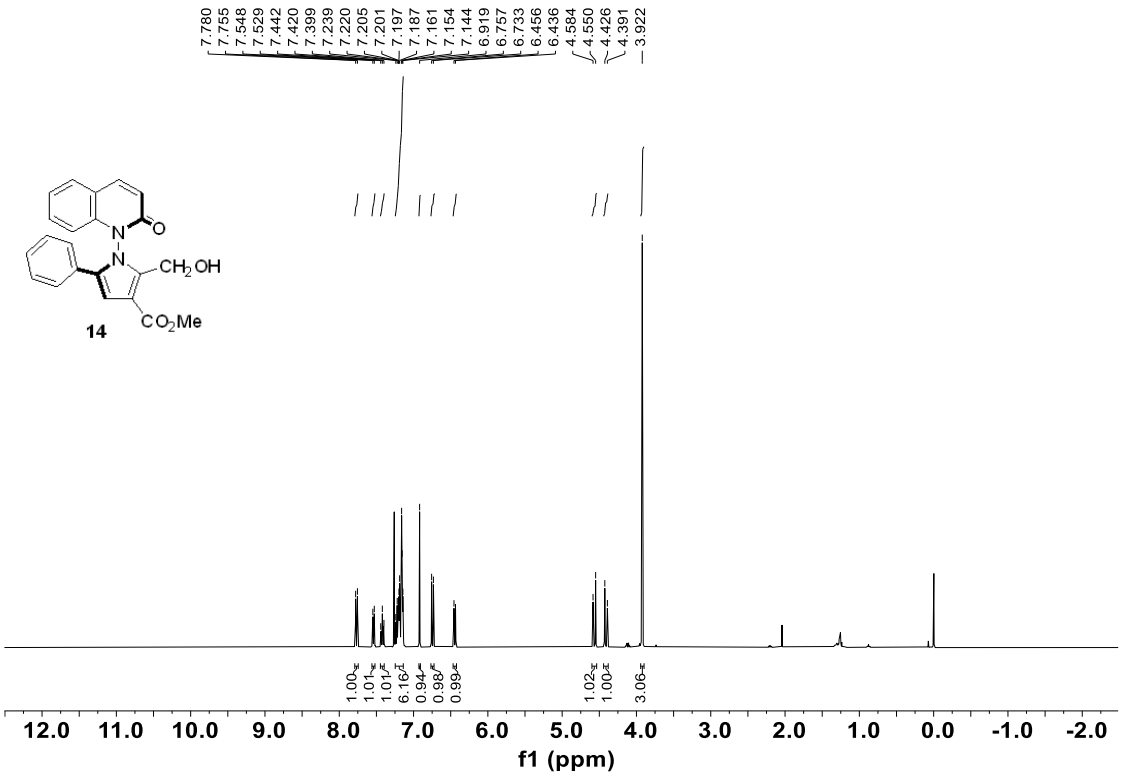
160.52
141.20
140.65
140.53
131.55
129.60
129.49
128.97
128.87
128.31
127.95
124.13
123.75
121.25
120.25
112.19
111.33
52.36
O
N
N
CHO
CO2Me
13
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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7.442
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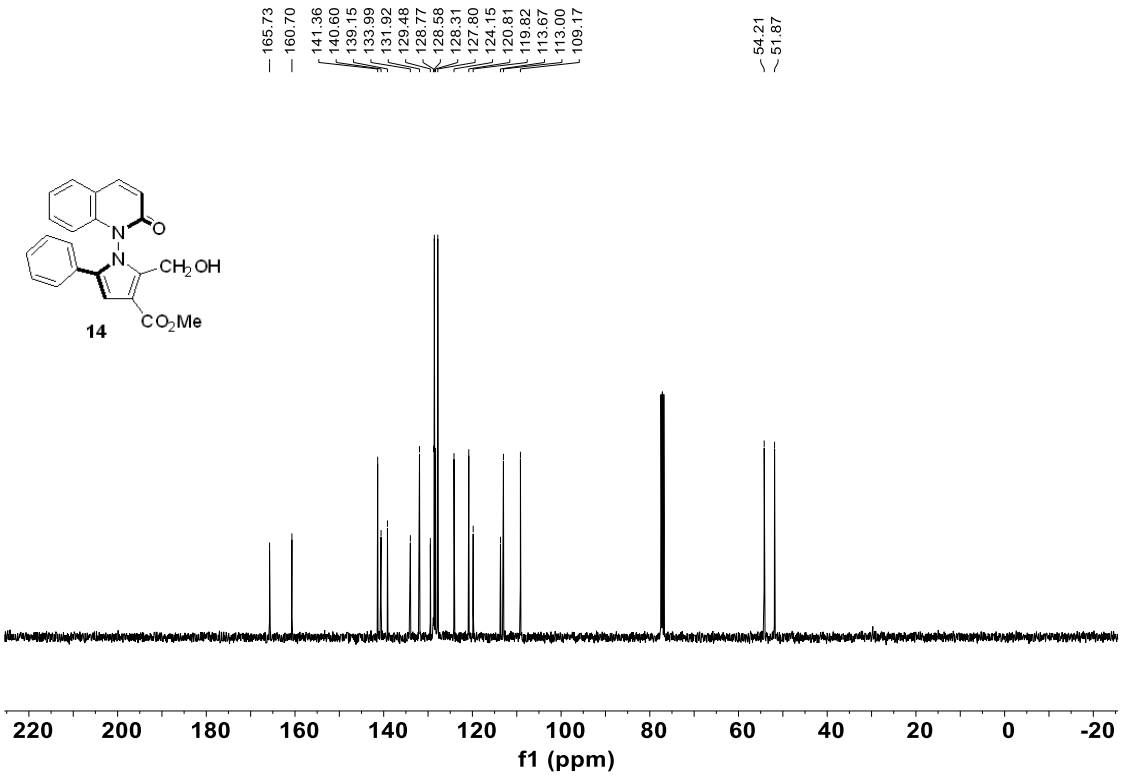
7.239
7.220
7.205
7.201
7.197
7.187
7.161
7.154
7.144
6.919
6.757
6.733
6.456
6.436
4.584
4.550
4.426
4.391
3.922
O
N
N
CH2OH
CO2Me
14
1.00
1.01
1.01
6.16
0.94
0.98
0.99
1.02
1.00
3.06
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)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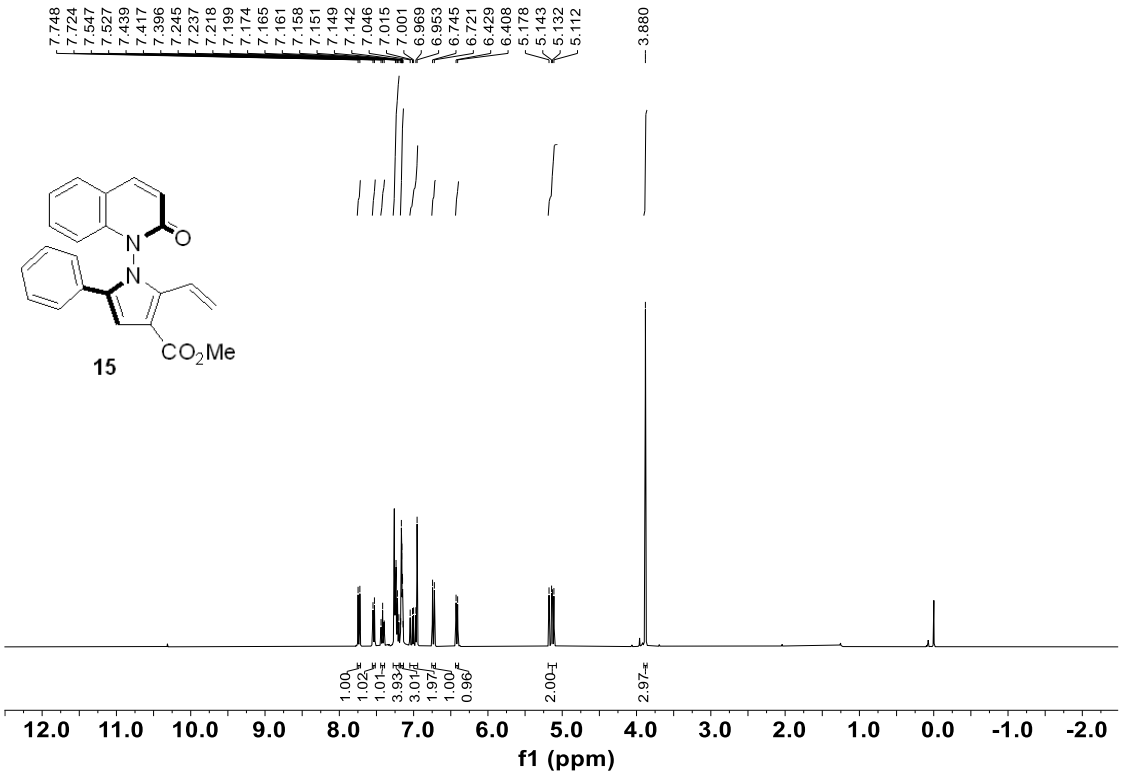
160.70
141.36
140.60
139.15
133.99
131.92
129.48
128.77
128.58
128.31
127.80
124.15
120.81
119.82
113.67
113.00
109.17
54.21
51.87
CH2OH
CO2Me
14
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)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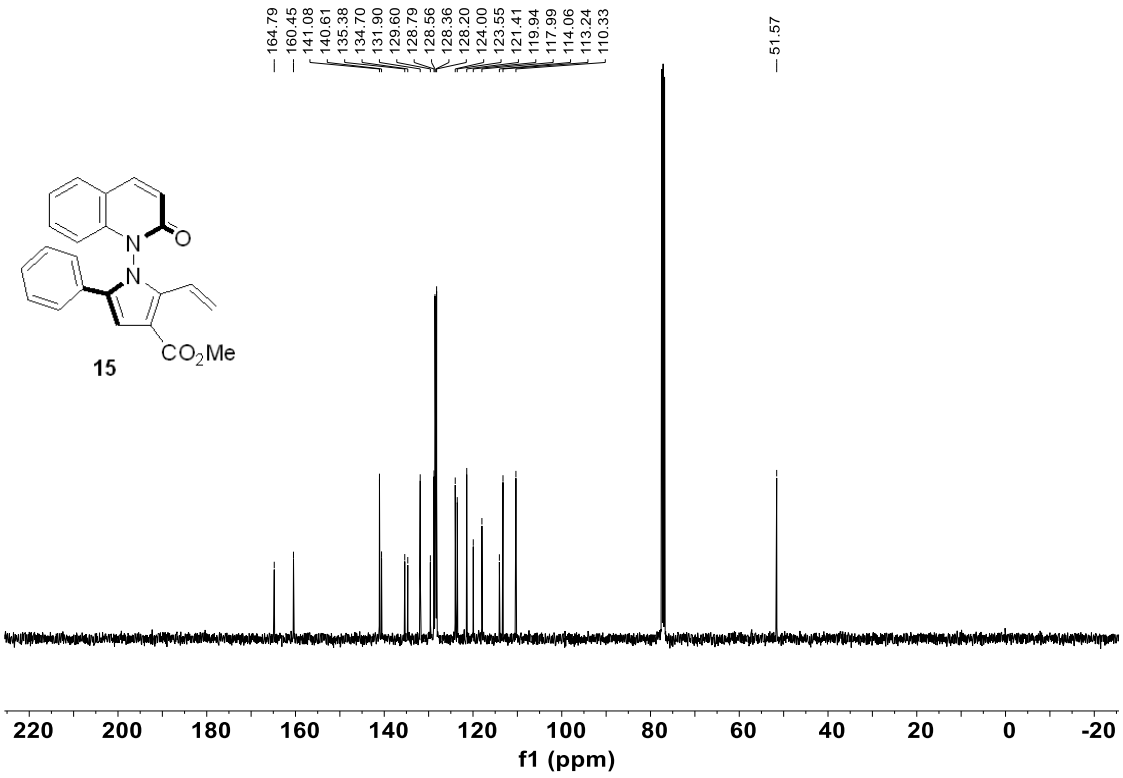
7.527
7.439
7.417
7.396
7.245
7.237
7.218
7.199
7.174
7.165
7.161
7.158
7.151
7.149
7.142
7.046
7.015
7.001
6.969
6.953
6.745
6.721
6.429
6.408
5.178
5.143
5.132
5.112
3.880
CO2Me
15
1.00
1.02
1.01
3.93
3.01
1.97
1.00
0.96
2.00
2.97
12.0
11.0
10.0
9.0
8.0
7.0
6.0
5.0
4.0
3.0
2.0
1.0
0.0
-1.0
-2.0
f1 (ppm)


164.79
160.45
141.08
140.61
135.38
134.70
131.90
129.60
128.79
128.56
128.36
128.20
124.00
123.55
121.41
119.94
117.99
114.06
113.24
110.33
51.57
N
N
O
CO2Me
15
220
200
180
160
140
120
100
80
60
40
20
0
-20
f1 (ppm)