Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Supporting Information

Employing Thiocyanate Salts as Nitrogen Source via C≡N Bond Cleavage: Divergent Synthesis of α-Ketoamides and 2-Acyloxazoles

*Can Wang,[+a] Xiao Geng,[+a] Peng Zhao,[a] Zhou You,[a] Yan-Dong Wu *,[a] and An-Xin Wu*,[a]*

[a]*Key Laboratory of Pesticide & Chemical Biology, Ministry of Education, College of Chemistry, Central China Normal University, Wuhan 430079, P. R. China*

[+] These authors contributed equally to this work.

E-mail: chwuyd@mail.ccnu.edu.cn, chwuax@mail.ccnu.edu.cn

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1. General

All substrates and reagents were commercially available and used without further purification. TLC analysis was performed using pre-coated glass plates. Column chromatography was performed using silica gel (200–300 mesh). IR spectra were recorded on a Perkin-Elmer PE-983 infrared spectrometer as KBr pellets with absorption in cm^{-1}. ^1H spectra were recorded in $CDCl_3$ or DMSO-d_6 on 400/600 MHz NMR spectrometers and resonances (δ) are given in parts per million relative to tetramethylsilane. Data are reported as follows: chemical shift, multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet), coupling constants (Hz) and integration. ^{13}C spectra were recorded in $CDCl_3$ or DMSO-d6 on 100/150 MHz NMR spectrometers and resonances (δ) are given in ppm. HRMS were obtained on a Bruker 7-tesla FT-ICR MS equipped with an electrospray source. Melting points were determined using XT-4 apparatus and not corrected.

2. Experimental procedures and characterizations of substrates

2.1. General procedure for the synthesis of 3 (3a as an example)

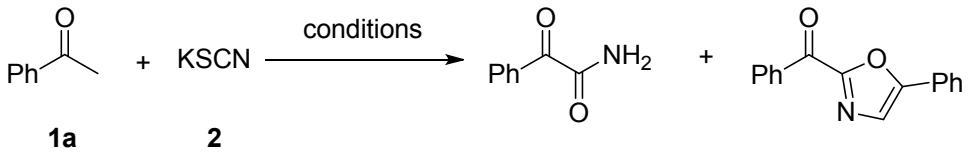
General procedure: A sealed tube was charged with acetophenone (**1a**) (60 mg, 0.5 mmol), potassium thiocyanate (**2**) (48.6 mg, 0.5 mmol), iodine (203 mg, 0.8 mmol) at room temperature, and DMSO (2 mL) was added. The resulting mixture was stirred at 120 °C for 2 h. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 5:1) to yield the desired product **3a** as a yellow solid.

2.2. General procedure for the synthesis of 4 (4a as an example)

General procedure: A sealed tube was charged with acetophenone (**1a**) (60 mg, 0.5 mmol), potassium thiocyanate (**2**) (48.6 mg, 0.5 mmol), iodine (203 mg, 0.8 mmol) and oxone (922.1 mg, 1.5 mmol) at room temperature, and DMSO (2 mL) was added. The resulting mixture was stirred at 140 °C for 2 h. After the reaction completed, the mixture was quenched with saturation $Na_2S_2O_3$ solution (50 mL), extracted with EtOAc (3 × 50 mL). The combined organic layers were washed with brine, dried over anhydrous Na_2SO_4 and concentrated under reduced pressure. The residue was purified by column chromatography on silica gel (petroleum ether/EtOAc = 50:1) to yield the desired product **4a** as a yellow solid.

3. Optimization of the Reaction Conditions

Table S1. Optimization of the Standard Conditions [a]

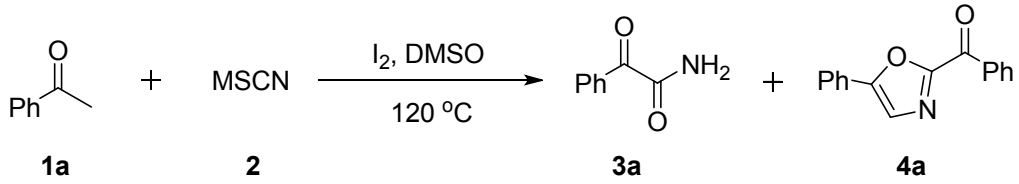


1a **2** **3a** **4a**

entry	I_2 (eq.)	temp (°C)	Additive (1.0 eq.)	3a[b] (%)	4a[b] (%)
1	1.6	100	-	60	<10
2	1.6	110	-	65	12
3	**1.6**	**120**	**-**	**73**	**trace**
4	1.6	130	-	71	trace
5	0.8	120	-	32	trace
6	1.2	120	-	68	trace
7	2.0	120	-	38	33
8	1.6	120	TFA	72	trace
9	1.6	120	HCl	36	0
10	1.6	120	$Cu(OAc)_2 \cdot H_2O$	55	trace
11	1.6	120	$FeCl_3$	23	0
12	1.6	120	TBHP	45	trace
13	1.6	120	H_2O_2	39	trace
14	1.6	120	oxone	22	40
15	1.6	120	PIDA	trace	trace
16	1.6	130	oxone	15	44
17	1.6	140	oxone	trace	37
18	1.6	150	oxone	trace	21
19[c]	1.6	140	oxone	trace	48
20[d]	**1.6**	**140**	**oxone**	**trace**	**61**
21[e]	1.6	140	oxone	0	50

[a)] Reaction conditions: **1a** (0.5 mmol), **2** (0.5 mmol), additive (x mmol), I_2 were heated in 2 mL of DMSO within 2 h. [b)] Isolated yields. [c)] oxone (1.0 mmol). [d)] oxone (1.5 mmol). [e)] oxone (2.0 mmol).

Table S2. Optimization of the Reaction Conditions 3a [a]

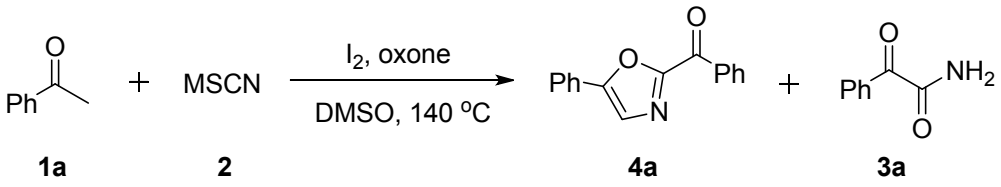


1a **2** **3a** **4a**

2	Yields of 3a[b]	Yields of 4a[b]
CuSCN	**57%**	**trace**
NaSCN	**71 %**	**trace**
$PhCH_2SCN$	**<10 %**	**45 %**

[a)]Reaction conditions: **1a** (0.5 mmol), **2** (0.5 mmol), I_2 (0.8 mmol) were heated in 2 mL of DMSO within 2 h. [b)] Isolated yields.

Table S3. Optimization of the Reaction Conditions 4a[a]

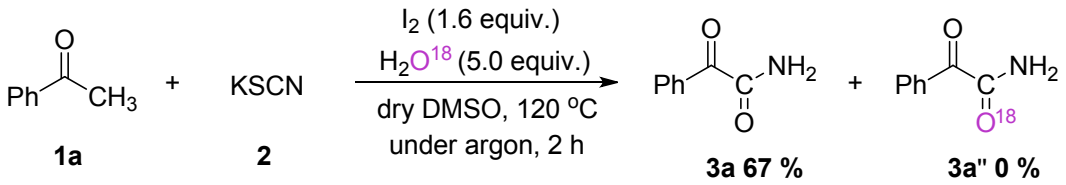


1a **2** **4a** **3a**

2	Yields of 4a[b]	Yields of 3a[b]
CuSCN	**34 %**	**trace**
NaSCN	**41 %**	**trace**
$PhCH_2SCN$	**49 %**	**trace**

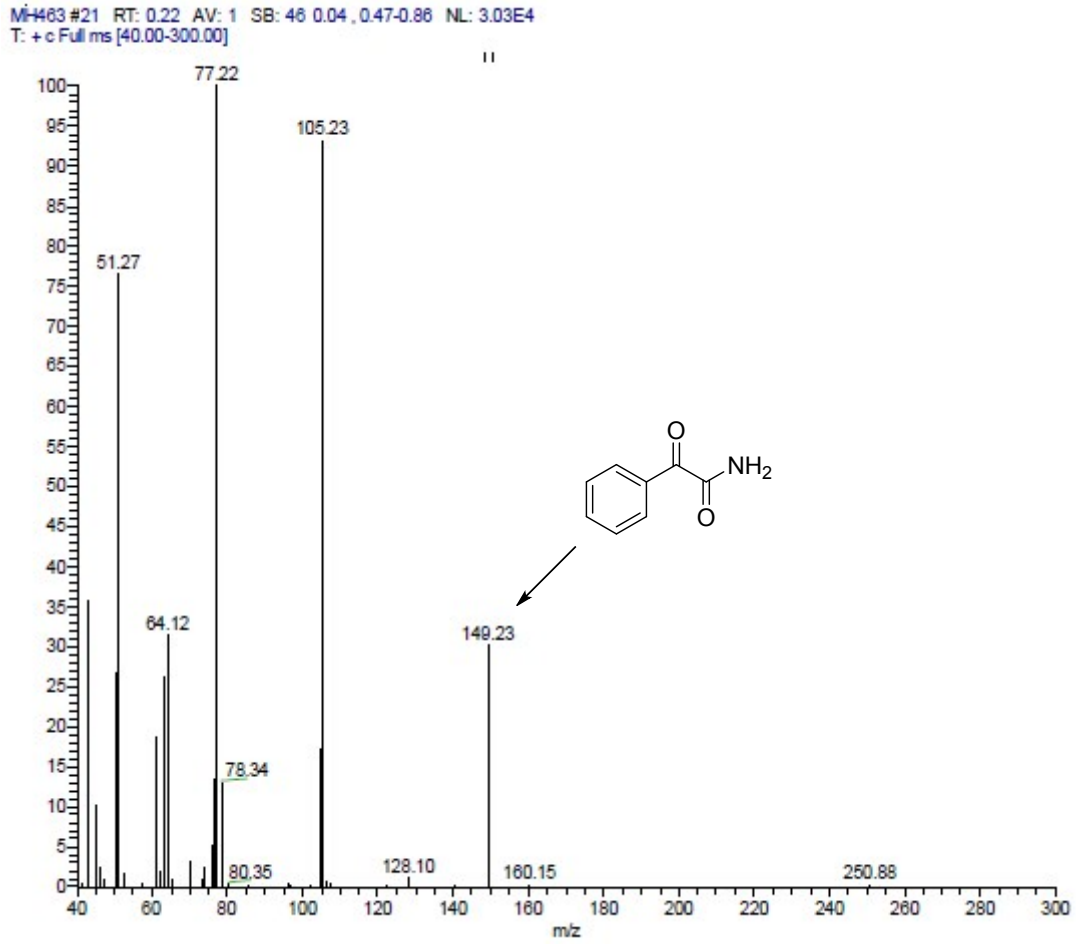
[a)]Reaction conditions: **1a** (0.5 mmol), **2** (0.5 mmol), oxone (1.5 mmol) and I_2 (0.8 mmol) were heated in 2 mL of DMSO within 2 h. [b)]Isolated yields.

4. Mechanistic studies

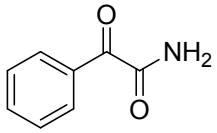


1a **2** **3a 67 %** **3a" 0 %**

Acetophenone (**1a**) (60 mg, 0.5 mmol), potassium thiocyanate (**2**) (48.6 mg, 0.5 mmol), iodine (203 mg, 0.8 mmol) in dry DMSO (2 mL) was added H_2O^{18} (50 mg, 2.5 mmol) at room temperature. The resulting mixture was stirred under argon at 120 °C for 2 h.



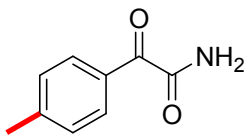
5. Characterization data for target compound



3a

2-oxo-2-phenylacetamide (3a)[1]

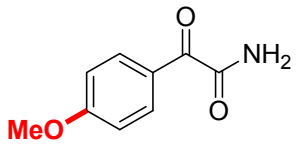
Yield 73%; 108.88 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.27 (d, J = 7.8 Hz, 2H), 7.62 (t, J = 7.2 Hz, 1H), 7.48 (t, J = 7.8 Hz, 2H), 7.14 (s, 1H), 6.70 (s, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 187.6, 164.4, 134.5, 132.9, 131.0, 128.5. The spectroscopic data match a literature report.



3b

2-oxo-2-(p-tolyl)acetamide (3b)[1]

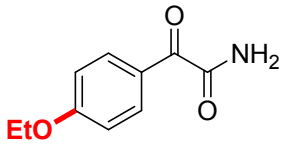
Yield 72%; 117.48 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.23 (d, *J* = 7.8 Hz, 2H), 7.34 - 7.23 (m, 2H), 7.04 (s, 1H), 6.28 (s, 1H), 2.43 (s, 3H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 186.8, 164.3, 145.8, 131.3, 130.4, 129.3, 21.9. The spectroscopic data match a literature report.



3c

2-(4-methoxyphenyl)-2-oxoacetamide (3c)[1]

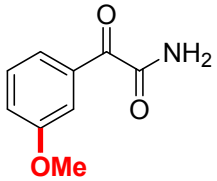
Yield 60%; 107.50 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.28 (s, 1H), 7.97 (d, *J* = 8.4 Hz, 2H), 7.94 (s, 1H), 7.10 (d, *J* = 7.8 Hz, 2H), 3.86 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.4, 167.6, 164.2, 132.3, 125.6, 114.4, 55.8. The spectroscopic data match a literature report.



3d

2-(4-ethoxyphenyl)-2-oxoacetamide (3d)[1]

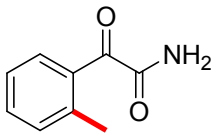
Yield 65%; 125.58 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.27 (s, 1H), 7.96 (d, *J* = 9.0 Hz, 2H), 7.93 (s, 1H), 7.08 (d, *J* = 9.0 Hz, 2H), 4.16 - 4.10 (m, 2H), 1.35 (t, *J* = 7.2 Hz, 4H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.3, 167.6, 163.5, 132.3, 125.5, 114.7, 63.8, 14.5. The spectroscopic data match a literature report.



3e

2-(3-methoxyphenyl)-2-oxoacetamide (3e)[1]

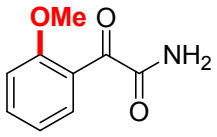
Yield 78%; 139.75 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.85 (d, *J* = 7.2 Hz, 1H), 7.67 (s, 1H), 7.31 (t, *J* = 8.4 Hz, 1H), 7.13 - 7.07 (m, 1H), 7.03 (s, 1H), 6.64 (s, 1H), 3.77 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 187.3, 164.4, 159.4, 134.0, 129.6, 124.0, 121.4, 114.4, 55.4. The spectroscopic data match a literature report.



3f

2-oxo-2-(o-tolyl)acetamide (3f)

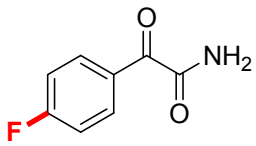
Yield 75%; 122.38 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.10 (s, 1H), 7.75 (s, 1H), 7.49 (d, J = 7.2 Hz, 1H), 7.32 (t, J = 6.6 Hz, 1H), 7.16 (t, J = 8.4 Hz, 2H), 2.28 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 193.6, 167.6, 139.5, 133.0, 132.3, 131.9, 131.8, 126.0, 20.8; HRMS (ESI) m/z calcd for $C_9H_{10}NO_2^+$ $(M+H)^+$ 164.07060, found 164.07008.



3g

2-(2-methoxyphenyl)-2-oxoacetamide (3g)[1]

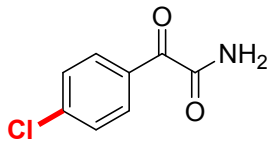
Yield 40%; 71.67 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.03 (s, 1H), 7.67–7.58 (m, 3H), 7.17 (d, J = 8.4 Hz, 1H), 7.08 (t, J = 7.8 Hz, 1H), 3.80 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 191.8, 167.9, 159.5, 135.2, 130.3, 124.1, 120.8, 112.8, 56.1. The spectroscopic data match a literature report.



3h

2-(4-fluorophenyl)-2-oxoacetamide (3h)[1]

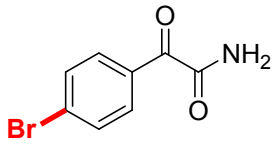
Yield 54%; 90.26 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.38 (s, 1H), 8.14–8.02 (m, 3H), 7.39 (t, J = 7.8 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.1, 166.8, 165.8 (d, $J_{C\text{-}F}$ = 252.0 Hz), 133.0 (d, $J_{C\text{-}F}$ = 9.3Hz), 129.6, 116.2 (d, $J_{C\text{-}F}$ = 22.5 Hz). The spectroscopic data match a literature report.



3i

2-(4-chlorophenyl)-2-oxoacetamide (3i)[1]

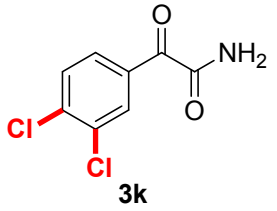
Yield 78%; 143.20 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.36 (s, 1H), 8.05 (s, 1H), 8.01 (t, J = 2.4 Hz, 1H), 8.00 (t, J = 1.8 Hz, 1H), 7.65 (t, J = 2.4 Hz, 1H), 7.63 (t, J = 1.8 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.4, 166.5, 139.5, 131.61, 131.55, 129.2. The spectroscopic data match a literature report.



3j

2-(4-bromophenyl)-2-oxoacetamide (3j)[1]

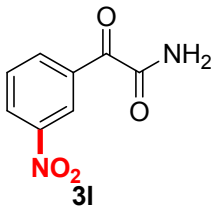
Yield 80%; 182.42 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.36 (s, 1H), 8.05 (s, 1H), 7.93 (d, J = 8.4 Hz, 2H), 7.77 (d, J = 8.4 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.6, 166.5, 132.1, 131.9, 131.7, 128.9. The spectroscopic data match a literature report.



3k

2-(3,4-dichlorophenyl)-2-oxoacetamide (3k)[1]

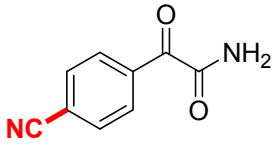
Yield 60%; 130.82 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.37 (s, 1H), 8.15 (d, J = 1.8 Hz, 1H), 8.09 (s, 1H), 7.98 - 7.92 (m, 1H), 7.77 (d, J = 8.4 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 187.6, 165.4, 137.4, 133.1, 131.9, 131.4, 131.3, 129.9. The spectroscopic data match a literature report.



3l

2-(3-nitrophenyl)-2-oxoacetamide (3l)[2]

Yield 45%; 87.36 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.75 (s, 1H), 8.52 (d, J = 7.8 Hz, 1H), 8.45 (d, J = 9.6 Hz, 1H), 8.41 (d, J = 6.6 Hz, 1H), 8.18 (s, 1H), 7.86 (t, J = 7.8 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 188.0, 165.4, 147.9, 135.9, 134.2, 130.8, 128.6, 124.4. The spectroscopic data match a literature report.

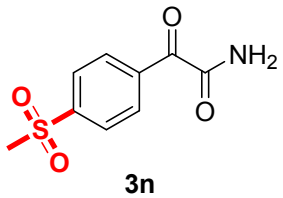


3m

2-(4-cyanophenyl)-2-oxoacetamide (3m)

Yield 51%; 88.82 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.43 (s, 1H), 8.15 (s, 1H), 8.12 (d, J = 7.8 Hz, 2H), 8.05 (d, J = 8.4 Hz, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ

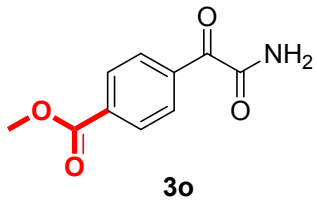
189.3, 165.8, 136.2, 132.9, 130.3, 118.1, 116.1. This product could't be detected by HRMS (ESI), so we used GC-MS (EI) to detect it (see below).



3n

2-(4-(methylsulfonyl)phenyl)-2-oxoacetamide (3n)

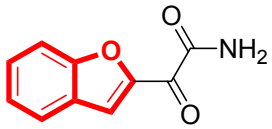
Yield 42%; 95.44 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.44 (d, J = 7.2 Hz, 1H), 8.21 (d, J = 7.8 Hz, 2H), 8.16 (s, 1H), 8.13 (d, J = 7.8 Hz, 2H), 3.31 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 189.5, 166.0, 145.1, 136.7, 130.7, 127.6, 43.2. This product could't be detected by HRMS (ESI), so we used GC-MS (EI) to detect it (see below).



3o

Methyl 4-(2-amino-2-oxoacetyl)benzoate (3o)

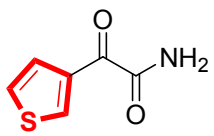
Yield 40%; 82.87 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.42 (s, 1H), 8.14 - 8.07 (m, 4H), 8.05 (s, 1H), 3.89 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 190.1, 166.5, 165.5, 136.2, 134.2, 130.1, 129.7, 52.7; HRMS (ESI) m/z calcd for $C_{10}H_{10}NO_4^+$ $(M+H)^+$ 208.06043, found 208.06111.



3p

2-(benzofuran-2-yl)-2-oxoacetamide (3p)

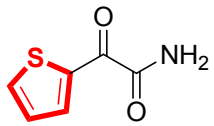
Yield 43%; 81.34 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.38 (s, 1H), 8.28 (s, 1H), 8.07 (s, 1H), 7.88 (d, J = 7.8 Hz, 1H), 7.71 (d, J = 8.4 Hz, 1H), 7.56 (t, J = 7.2 Hz, 1H), 7.36 (t, J = 7.2 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 178.0, 163.6, 155.5, 149.2, 129.6, 126.8, 124.5, 124.3, 120.6, 112.3; HRMS (ESI) m/z calcd for $C_{10}H_8NO_3^+$ $(M+H)^+$ 190.04987, found 190.04965.



3q

2-oxo-2-(thiophen-3-yl)acetamide (3q)

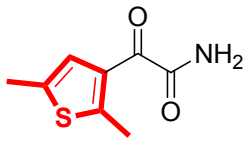
Yield 85%; 131.89 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 9.07 (s, 1H), 7.77 (d, J = 5.4 Hz, 1H), 7.36 - 7.30(m, 1H), 7.19 (s, 1H), 6.16 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 179.7, 163.4, 139.6, 136.7, 128.5, 125.9; HRMS (ESI) m/z calcd for $C_6H_6NO_2S^+$ $(M+H)^+$ 156.01138, found 156.01146.



3r

2-oxo-2-(thiophen-2-yl)acetamide (3r)[1]

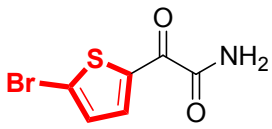
Yield 83%; 128.79 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (s, 1H), 7.83 (s, 1H), 7.36 (s, 1H), 7.19 (s, 1H), 6.74 (s, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.1, 163.3, 138.6, 138.2, 136.6, 128.3. The spectroscopic data match a literature report.



3s

2-(2,5-dimethylthiophen-3-yl)-2-oxoacetamide (3s)

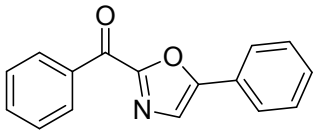
Yield 76%; 139.25 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.18 (s, 1H), 7.84 (s, 1H), 7.16 (s, 1H), 2.62 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 185.7, 167.5, 150.0, 135.4, 131.8, 127.4, 15.4, 14.5; HRMS (ESI) m/z calcd for $C_8H_{10}NO_2S^+$ $(M+H)^+$ 184.04268, found 184.04228.



3t

2-(5-bromothiophen-2-yl)-2-oxoacetamide (3t)

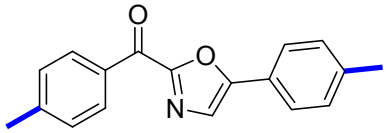
Yield 74%; 173.21 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.40 (s, 1H), 8.12 (s, 1H), 7.90 (d, J = 4.2 Hz, 1H), 7.41 (d, J = 3.6 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 178.2, 163.3, 137.3, 137.0, 131.7, 126.5. This product could't be detected by HRMS (ESI), so we used GC-MS (EI) to detect it (see below).



4a

phenyl(5-phenyloxazol-2-yl)methanone(4a)[3]

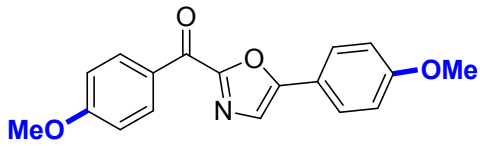
Yield 61%; 152.05 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.48 (d, *J* = 7.2 Hz, 2H), 7.83 (d, *J* = 7.2 Hz, 2H), 7.65 (t, *J* = 7.2 Hz, 1H), 7.62 (s, 1H), 7.54 (t, *J* = 7.2 Hz, 2H), 7.48 (t, *J* = 7.2 Hz, 2H), 7.43 (d, *J* = 7.8 Hz, 1H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.7, 156.9, 154.1, 135.3, 133.7, 130.7, 130.0, 129.1, 128.4, 126.6, 125.4, 123.9. The spectroscopic data match a literature report.



4b

(5-phenyloxazol-2-yl)(p-tolyl)methanone(4b)[3]

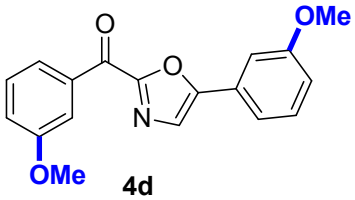
Yield 51%; 141.43 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.39 (d, *J* = 7.8 Hz, 2H), 7.72 (d, *J* = 7.8 Hz, 2H), 7.55 (s, 1H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 7.8 Hz, 2H), 2.45 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.3, 156.8, 154.2, 144.7, 140.2, 132.8, 130.8, 129.7, 129.2, 125.3, 123.9, 123.2, 21.8, 21.5. The spectroscopic data match a literature report.



4c

(4-methoxyphenyl)(5-(4-methoxyphenyl)oxazol-2-yl)methanone(4c)[3]

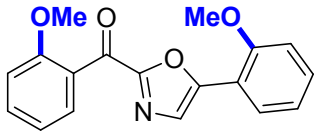
Yield 57%; 176.31 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.53 (d, *J* = 7.8 Hz, 2H), 7.76 (d, *J* = 7.8 Hz, 2H), 7.47 (s, 1H), 7.03-6.95 (m, 4H), 3.90 (s, 3H), 3.86 (s, 3H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 176.2, 164.0, 160.7, 156.4, 153.5, 133.1, 127.8, 127.0, 123.4, 119.1, 115.0, 114.1, 55.8, 55.5. The spectroscopic data match a literature report.



4d

(3-methoxyphenyl)(5-(3-methoxyphenyl)oxazol-2-yl)methanone(4d)[4]

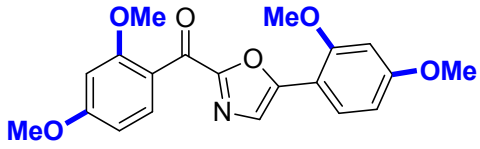
Yield 49%; 151.57 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.14 (d, *J* = 7.2 Hz, 1H), 7.96 (s, 1H), 7.60 (s, 1H), 7.45 (t, *J* = 7.8 Hz, 1H), 7.42-7.36 (m, 2H), 7.34 (s, 1H), 7.20 (d, *J* = 7.8 Hz, 1H), 6.97 (d, *J* = 7.8 Hz, 1H), 3.90 (s, 3H), 3.88 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 178.3, 160.0, 159.5, 156.9, 154.0, 136.4, 130.2, 129.4, 127.8, 124.2, 123.6, 120.5, 117.8, 115.9, 114.6, 110.4, 55.4. The spectroscopic data match a literature report.



4e

(2-methoxyphenyl)(5-(2-methoxyphenyl)oxazol-2-yl)methanone(4e)[3]

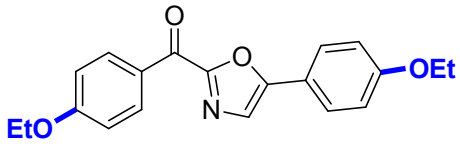
Yield 55%; 170.13 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.96 (d, *J* = 7.8 Hz, 1H), 7.76 (s, 1H), 7.68 (d, *J* = 7.2 Hz, 1H), 7.53 (t, *J* = 7.2 Hz, 1H), 7.38 (t, *J* = 7.2 Hz, 1H), 7.08 (t, *J* = 7.2 Hz, 2H), 7.05-7.00 (m, 2H), 3.99 (s, 3H), 3.82 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 181.1, 158.5, 156.7, 156.4, 150.6, 133.4, 130.60, 130.55, 128.2, 127.1, 126.7, 121.0, 120.3, 115.9, 111.8, 110.9, 55.8, 55.5. The spectroscopic data match a literature report.



4f

(2,4-dimethoxyphenyl)(5-(2,4-dimethoxyphenyl)oxazol-2-yl)methanone(4f)[3]

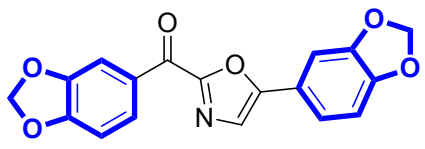
Yield 60%; 221.62 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 7.83 (d, *J* = 9.0 Hz, 1H), 7.79 (d, *J* = 8.4 Hz, 1H), 7.58 (s, 1H), 6.58-6.53 (m, 2H), 6.50 (s, 2H), 3.91 (s, 3H), 3.84 (s, 3H), 3.82 (s, 3H), 3.78 (s, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 179.2, 164.2, 161.7, 160.8, 157.7, 156.5, 150.5, 133.3, 128.0, 126.1, 119.5, 109.2, 105.1, 104.4, 98.8, 98.3, 55.7, 55.42, 55.37. The spectroscopic data match a literature report.



4g

(3-ethoxyphenyl)(5-(4-ethoxyphenyl)oxazol-2-yl)methanone(4g)[3]

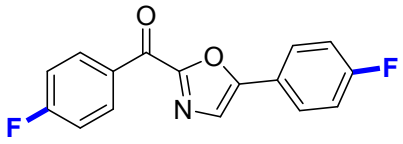
Yield 53%; 178.81 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.52 (d, *J* = 8.4 Hz, 2H), 7.74 (d, *J* = 8.4 Hz, 2H), 7.46 (s, 1H), 7.01-6.94 (m, 4H), 4.16-4.11 (m, 2H), 4.10-4.05 (m, 2H), 1.48–1.41 (m, 6H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.9, 163.5, 160.2, 156.7, 154.0, 133.2, 128.1, 126.9, 122.2, 119.2, 114.9, 114.1, 63.8, 63.6, 14.7, 14.6. The spectroscopic data match a literature report.



4h

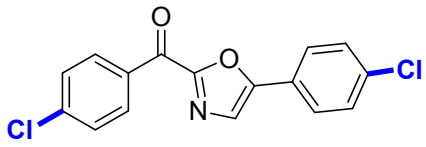
benzo[d][1,3]dioxol-5-yl(5-(benzo[d][1,3]dioxol-5-yl)oxazol-2-yl)methanone(4h)[3]

Yield 52%; 175.39 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.28 (d, J = 7.8 Hz, 1H), 7.95 (s, 1H), 7.45 (s, 1H), 7.35 (d, J = 8.4 Hz, 1H), 7.26 (s, 1H), 6.94 (d, J = 8.4 Hz, 1H), 6.90 (d, J = 8.4 Hz, 1H), 6.09 (s, 2H), 6.04 (s, 2H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.4, 156.6, 153.9, 152.5, 149.1, 148.3, 147.9, 129.7, 128.0, 122.7, 120.7, 120.0, 110.2, 109.0, 108.0, 105.6, 102.0, 101.6. The spectroscopic data match a literature report.



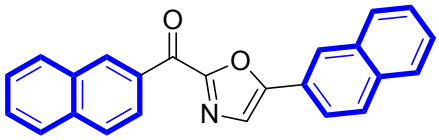
4i

(4-fluorophenyl)(5-(4-fluorophenyl)oxazol-2-yl)methanone(4i)[3]
Yield 34%; 96.64 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62–8.50 (m, 2H), 7.84-7.75 (m, 2H), 7.54 (s, 1H), 7.23–7.12 (m, 4H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 176.7, 166.2 (d, $J_{C\text{-}F}$ = 255.0 Hz), 163.5 (d, $J_{C\text{-}F}$ = 250.5 Hz), 156.7, 153.4, 133.6 (d, $J_{C\text{-}F}$ = 9.0 Hz), 131.4, 127.4 (d, $J_{C\text{-}F}$ = 7.5 Hz), 123.5, 122.8, 116.4 (d, $J_{C\text{-}F}$ = 21.0 Hz), 115.7 (d, $J_{C\text{-}F}$ = 21.0 Hz). The spectroscopic data match a literature report.



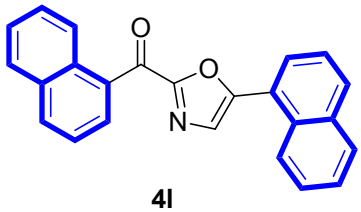
4j

(5-chlorophenyl)(5-(4-chlorophenyl)oxazol-2-yl)methanone(4j)[3]
Yield 42%; 143.17 mg; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.48 (d, J = 8.4 Hz, 2H), 7.76 (d, J = 8.4 Hz, 2H), 7.60 (s, 1H), 7.51 (d, J = 8.4 Hz, 2H), 7.46 (d, J = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 177.1, 156.8, 153.3, 140.6, 136.1, 133.4, 132.2, 129.5, 128.8, 126.6, 125.0, 124.2. The spectroscopic data match a literature report.



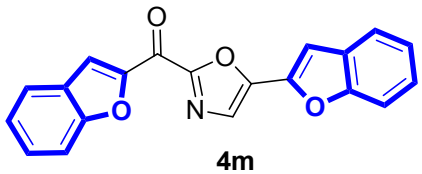
4k

naphthalen-2-yl(5-(naphthalen-2-yl)oxazol-2-yl)methanone(4k)[3]
Yield 51%; 178.18 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.18 (s, 1H), 8.43 (s, 1H), 8.31 (d, J = 8.4 Hz, 1H), 8.25 (s, 1H), 8.16 (d, J = 7.8 Hz, 1H), 8.09-8.00 (m, 5H), 7.98 (d, J = 8.4 Hz, 1H), 7.96-7.93 (m, 1H), 7.72–7.68 (m, 1H), 7.66–7.62 (m, 1H), 7.60-7.56 (m, 2H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 177.7, 156.8, 153.5, 135.3, 133.3, 133.2, 132.8, 132.3, 131.8, 130.0, 129.3, 129.1, 128.6, 128.2, 127.9, 127.8, 127.4, 127.2, 125.6, 125.3, 124.4, 123.7, 122.4. The spectroscopic data match a literature report.



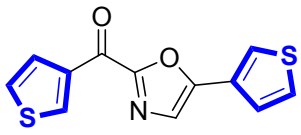
4l

naphthalen-1-yl(5-(naphthalen-1-yl)oxazol-2-yl)methanone(4l)[3]
Yield 45%; 157.22 mg; ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.57 (d, J = 8.4 Hz, 1H), 8.39 (d, J = 8.4 Hz, 1H), 8.36 (d, J = 7.2 Hz, 1H), 8.10 (d, J = 8.4 Hz, 1H), 7.97-7.91 (m, 4H), 7.73 (s, 1H), 7.66-7.60 (m, 3H), 7.59-7.55 (m, 3H); ^{13}C NMR (150 MHz, $CDCl_3$) δ 181.3, 158.2, 154.0, 133.78, 133.76, 133.6, 132.5, 131.3, 131.0, 130.9, 129.9, 128.9, 128.7, 128.6, 128.1, 127.7, 127.6, 127.5, 126.6, 126.5, 125.2, 124.5, 124.2, 123.8. The spectroscopic data match a literature report.



4m

benzofuran-2-yl(5-(benzofuran-2-yl)oxazol-2-yl)methanone(4m)[3]
Yield 41%; 135.02 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 8.92 (s, 1H), 8.65 (s, 1H), 7.93 (d, J = 7.8 Hz, 1H), 7.70 (d, J = 8.4 Hz, 1H), 7.67 (d, J = 7.2 Hz, 1H), 7.57 (t, J = 7.2 Hz, 2H), 7.41 (s, 1H), 7.38 (t, J = 7.2 Hz, 1H), 7.33 (t, J = 7.2 Hz, 1H), 7.26 (t, J = 7.2 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 166.2, 156.5, 155.7, 154.3, 149.5, 147.2, 139.3, 133.8, 129.5, 127.9, 126.8, 125.2, 124.4, 124.3, 123.4, 121.5, 120.3, 112.2, 111.1, 104.6. The spectroscopic data match a literature report.



4n

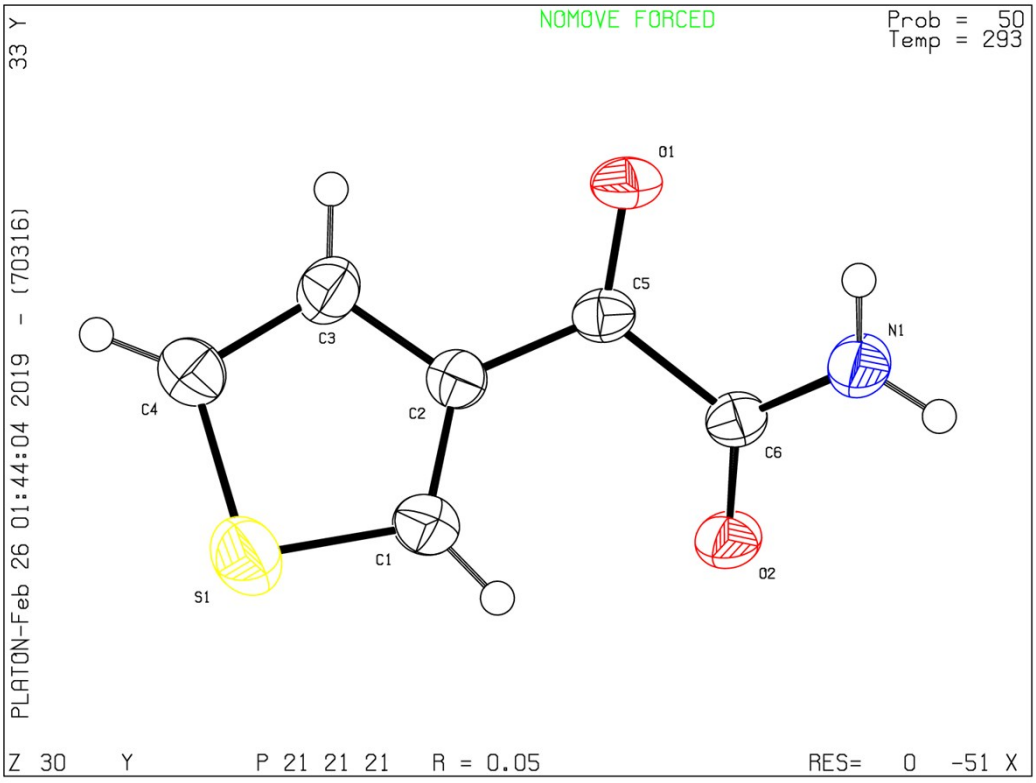
thiophen-3-yl(5-(thiophen-3-yl)oxazol-2-yl)methanone(4n)
Yield 62%; 162.02 mg; ^{1}H NMR (600 MHz, DMSO-d_6) δ 9.08 (d, J = 1.8 Hz, 1H), 8.12 (d, J = 1.8 Hz, 1H), 7.92 (s, 1H), 7.83 (d, J = 4.8 Hz, 1H), 7.78-7.75 (m, 1H), 7.72-7.69 (m, 1H), 7.60 (d, J = 4.2 Hz, 1H); ^{13}C NMR (150 MHz, DMSO-d_6) δ 171.3, 156.0, 150.4, 138.4, 137.9, 137.8, 128.7, 128.0, 127.6, 125.2, 124.6, 124.5; HRMS (ESI) m/z calcd for $C_{12}H_8NO_2S_2^+$ $(M+H)^+$ 261.99910, found 261.99902.

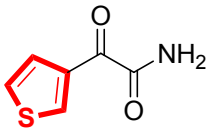
6. Reference

[1] S. Liu, Q. Gao, X. Wu, J. Zhang, K. Ding and A. Wu, *Org. Biomol. Chem.*, **2015**, *13*, 2239-2242.

[2] A. Nagaki, Y. Takahashi and J.-I. Yoshida, *Angew. Chem. Int. Ed.*, **2016**, *55*, 5327-5331.
[3] W.-J. Xue, W. Zhang, K.-L. Zheng, Y. Dai, Y.-Q. Guo, H.-Z. Li, F.-F. Gao and A.-X. Wu, *Asian J. Org. Chem.*, **2013**, *2*, 638-641.
[4] N. Pogaku, P. R. Krishna and Y. L. Prapurna, *Synth. Commun.*, **2018**, *48*, 1986-1993.

7. Crystallographic data and molecular structure of 3q and 4i





3q

Figure S1. X-ray crystal structure of **3q**

Crystal Data for Compound **3q**: CCDC 1899222 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Bond precision: C-C = 0.0038 A Wavelength=0.71073

Cell: a=6.1602(12) b=7.5933(16) c=14.282(3)
alpha=90 beta=90 gamma=90
Temperature: 293 K

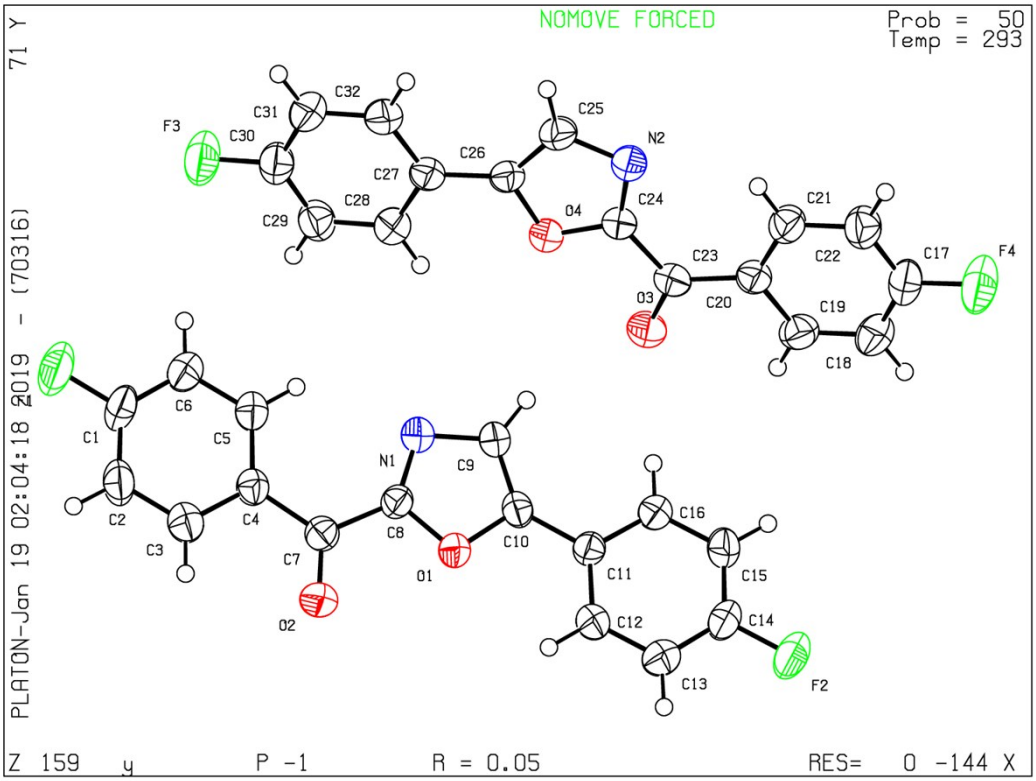
	Calculated	Reported
Volume	668.1(2)	668.0(2)
Space group	P 21 21 21	P 21 21 21
Hall group	P 2ac 2ab	P 2ac 2ab
Moiety formula	C6 H5 N O2 S	?
Sum formula	C6 H5 N O2 S	C6 H5 N O2 S
Mr	155.17	155.17
Dx,g cm-3	1.543	1.543
Z	4	4
Mu (mm-1)	0.412	0.412
F000	320.0	320.0
F000'	320.64	
h,k,lmax	9,11,21	9,11,20
Nref	2352[1381]	2193
Tmin,Tmax	0.952,0.960	
Tmin'	0.952	

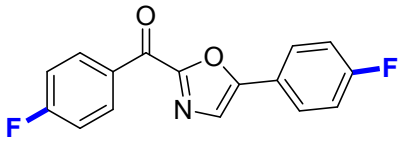
Correction method= Not given

Data completeness= 1.59/0.93 Theta(max)= 32.125

R(reflections)= 0.0459(2038) wR2(reflections)= 0.1505(2193)

S = 1.118 Npar= 92





4i

Figure S2. X-ray crystal structure of **4i**

Crystal Data for Compound **4i**: CCDC 1891920 contains the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic.

Bond precision: C-C = 0.0034 A Wavelength=0.71073

Cell: a=7.5984(15) b=11.344(2) c=14.767(3)
alpha=91.674(3) beta=98.949(3) gamma=90.820(3)
Temperature: 293 K

	Calculated	Reported
Volume	1256.6(4)	1256.6(4)
Space group	P -1	P -1
Hall group	-P 1	-P 1
Moiety formula	C16 H9 F2 N O2	C16 H9 F2 N O2
Sum formula	C16 H9 F2 N O2	C16 H9 F2 N O2
Mr	285.24	285.24
Dx,g cm-3	1.508	1.508
Z	4	4
Mu (mm-1)	0.120	0.120
F000	584.0	584.0
F000'	584.37	
h,k,lmax	8,12,16	8,12,16
Nref	3640	3599
Tmin,Tmax	0.983,0.988	0.657,0.745
Tmin'	0.982	

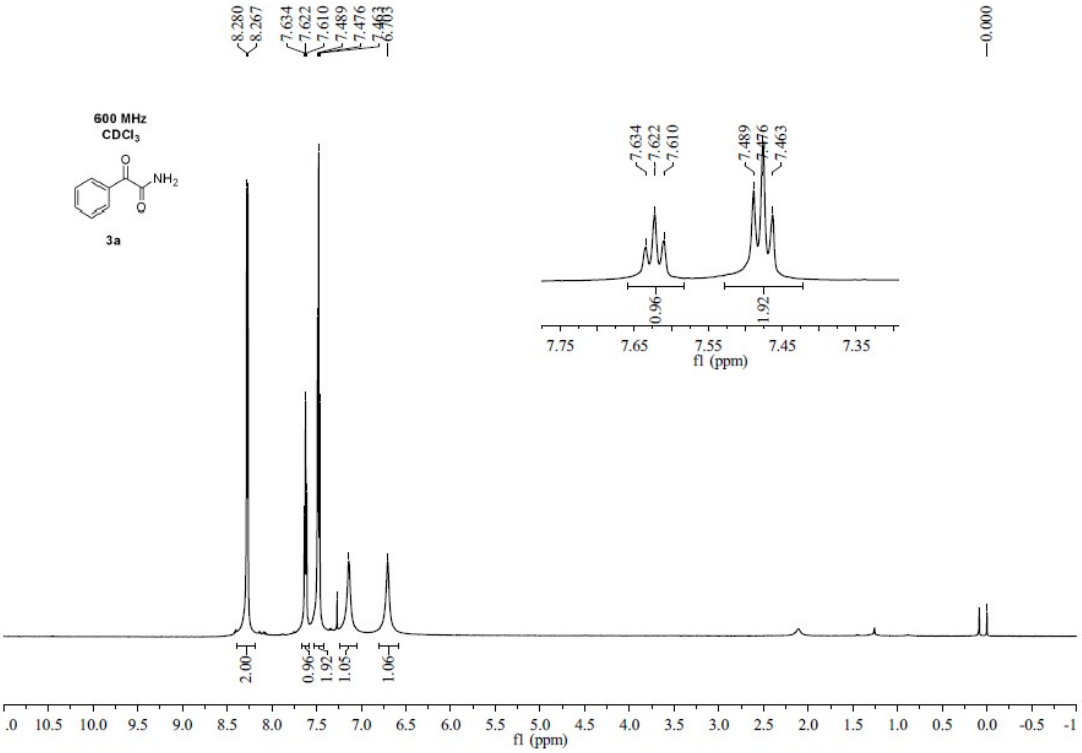
Correction method= # Reported T Limits: Tmin=0.657 Tmax=0.745
AbsCorr = MULTI-SCAN

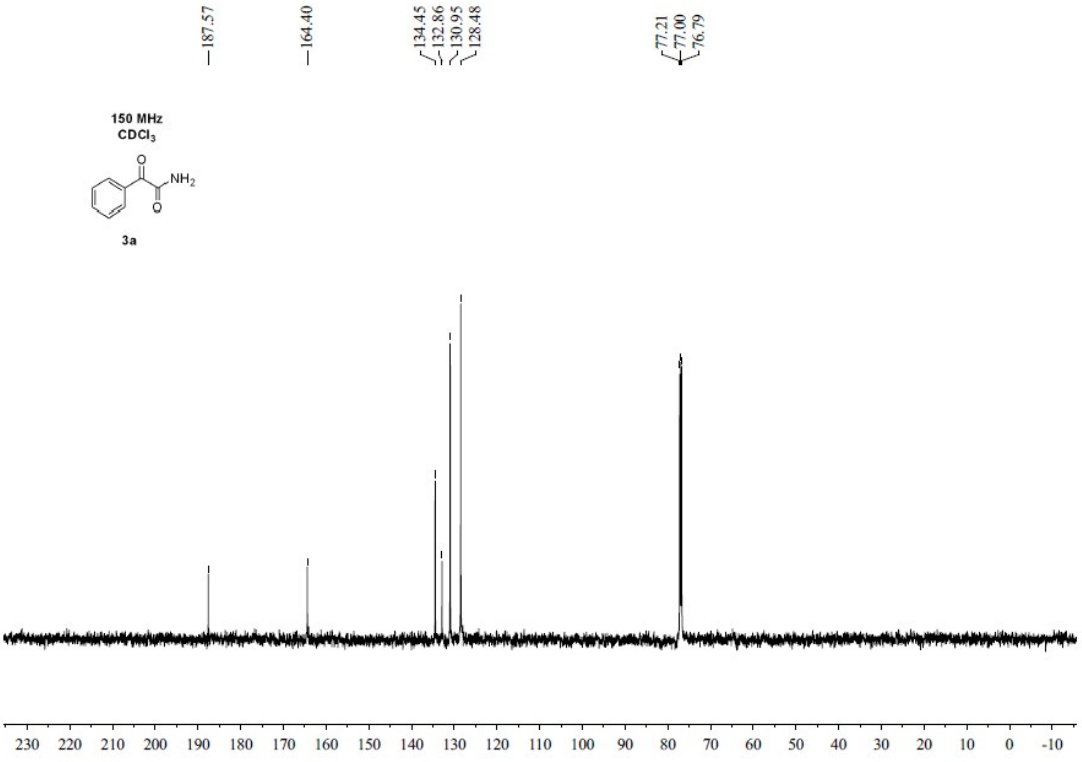
Data completeness= 0.989 Theta(max)= 23.314

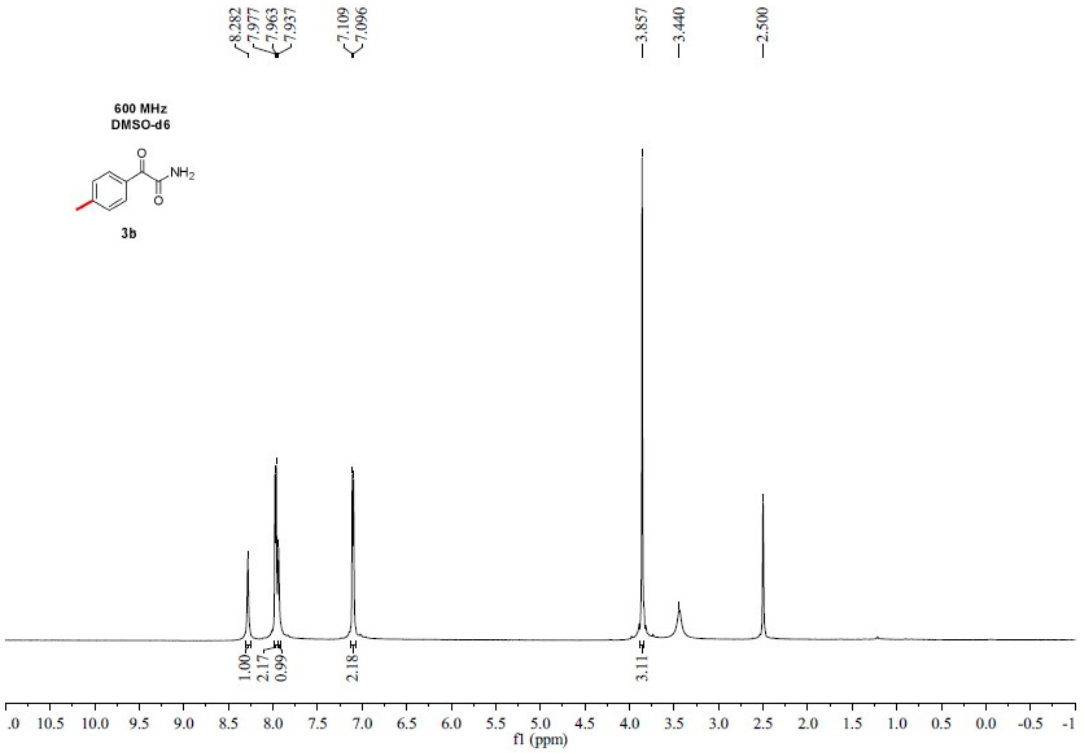
R(reflections)= 0.0456(2848) wR2(reflections)= 0.1743(3599)

S = 1.091 Npar= 380

8. Copies of 1H and 13C NMR spectra



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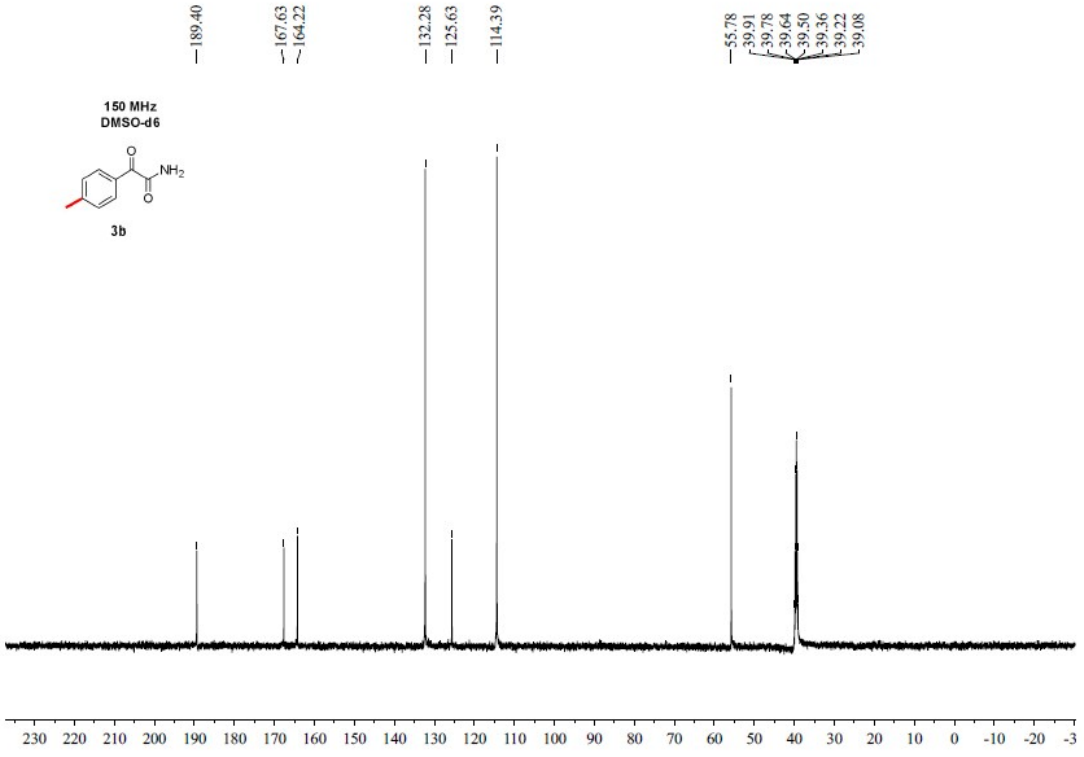
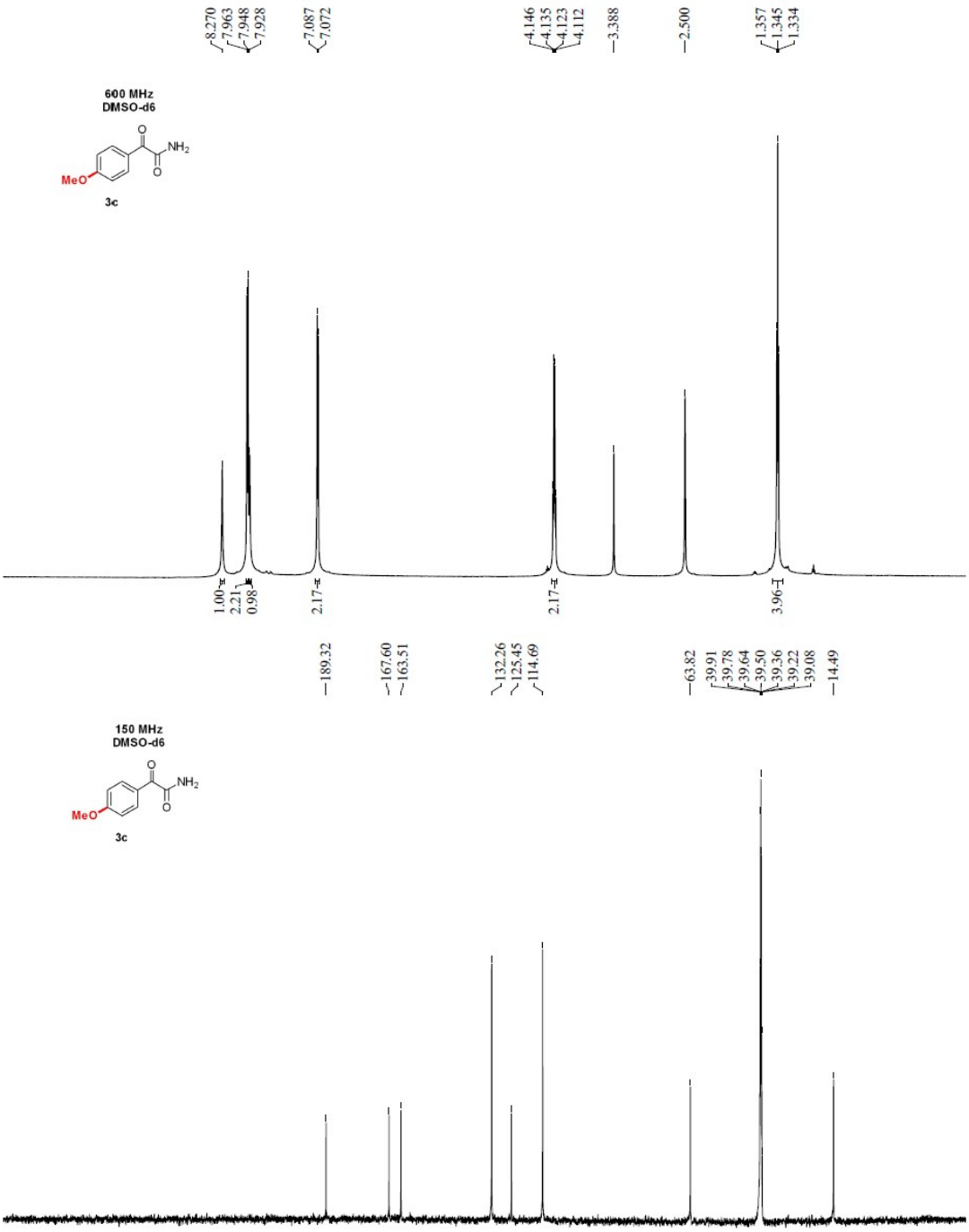
7.977
7.963
7.937
7.109
7.096
3.857
3.440
2.500
600 MHz
DMSO-d6
NH2
3b
1.00
2.17
0.99
2.18
3.11
f1 (ppm)


189.40
167.63
164.22
132.28
125.63
114.39
55.78
39.91
39.78
39.64
39.50
39.36
39.22
39.08
150 MHz
DMSO-d6
NH2
3b


600 MHz
DMSO-d6
MeO
NH2
3c
8.270
7.963
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7.087
7.072
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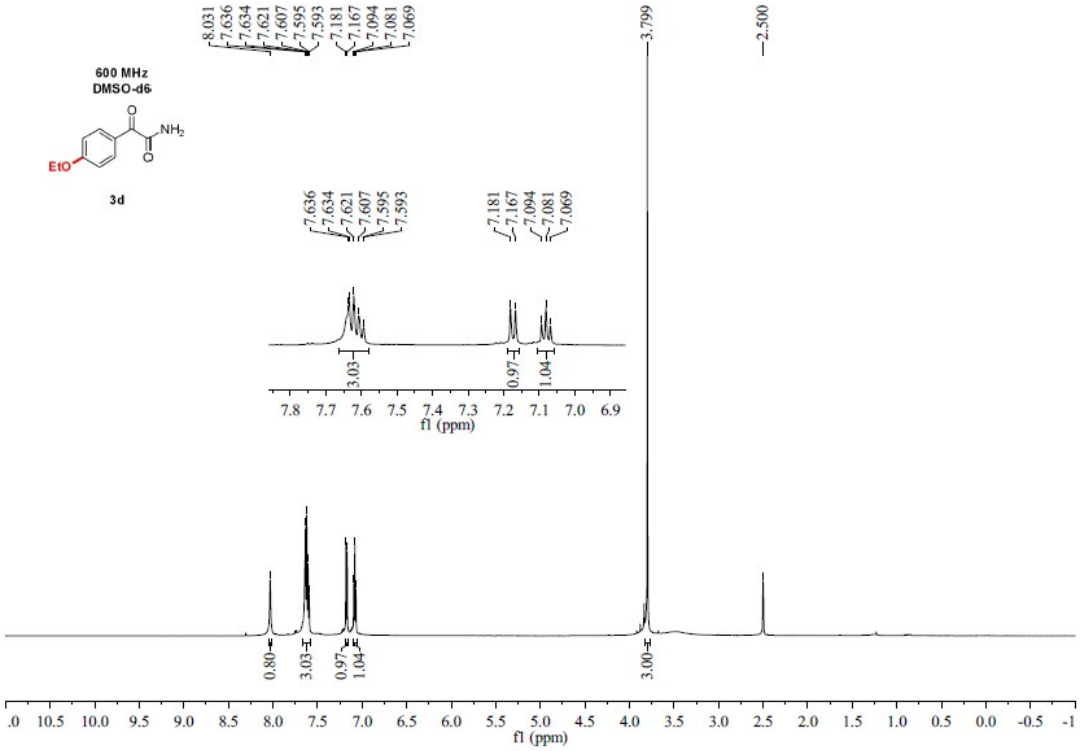
4.135
4.123
4.112
3.388
2.500
1.357
1.345
1.334
1.00
2.21
0.98
2.17
2.17
3.96
189.32
167.60
163.51
132.26
125.45
114.69
63.82
39.91
39.78
39.64
39.50
39.36
39.22
39.08
14.49
150 MHz
DMSO-d6
MeO
NH2
3c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DMSO-d6
3d
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7.636
7.634
7.621
7.607
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7.593
7.181
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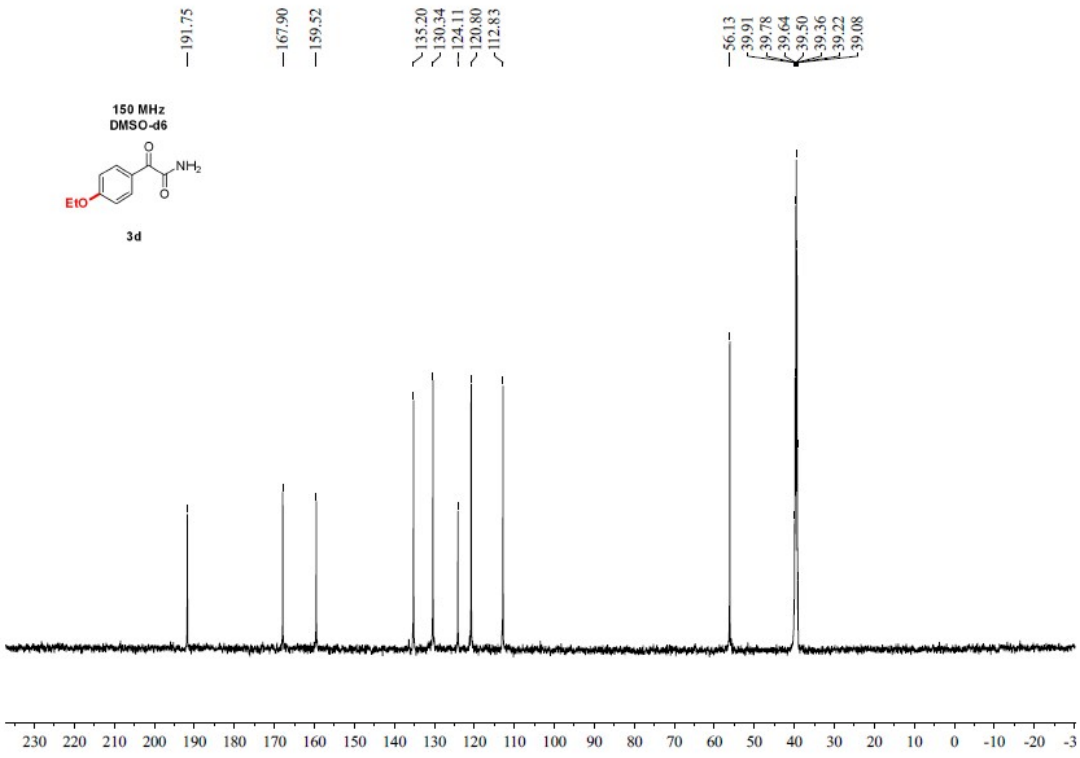
7.094
7.081
7.069
3.799
2.500
0.80
3.03
0.97
1.04
3.00
f1 (ppm)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DMSO-d6
3d
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159.52
135.20
130.34
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120.80
112.83
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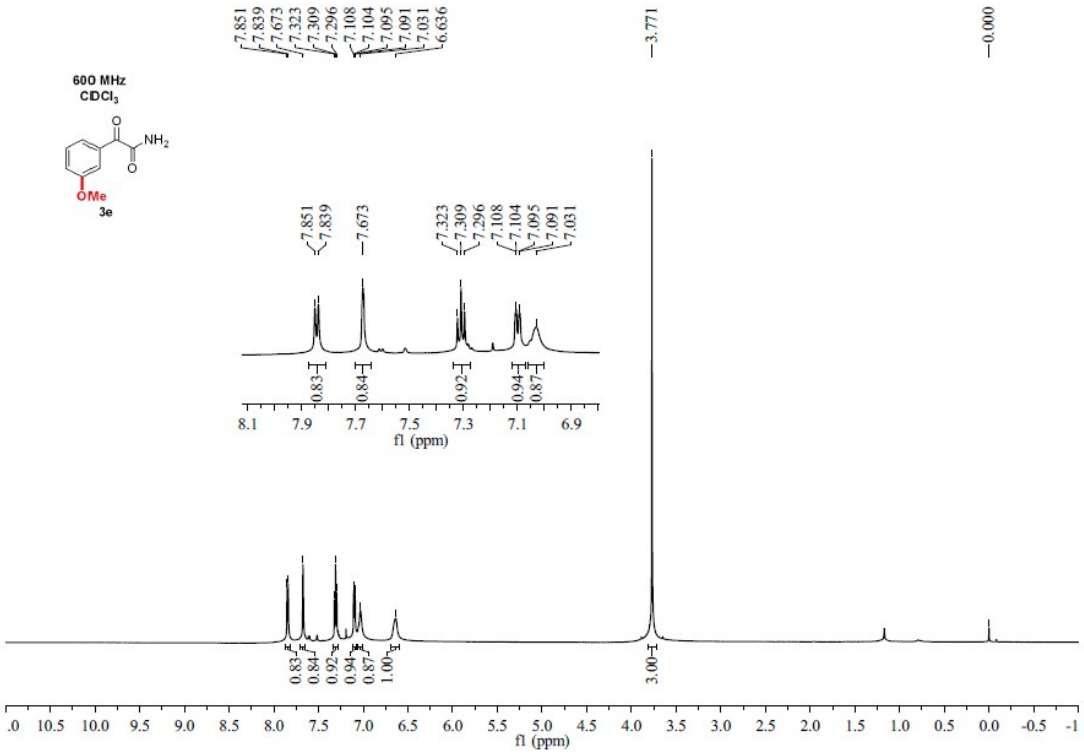
39.78
39.64
39.50
39.36
39.22
39.08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7.839
7.673
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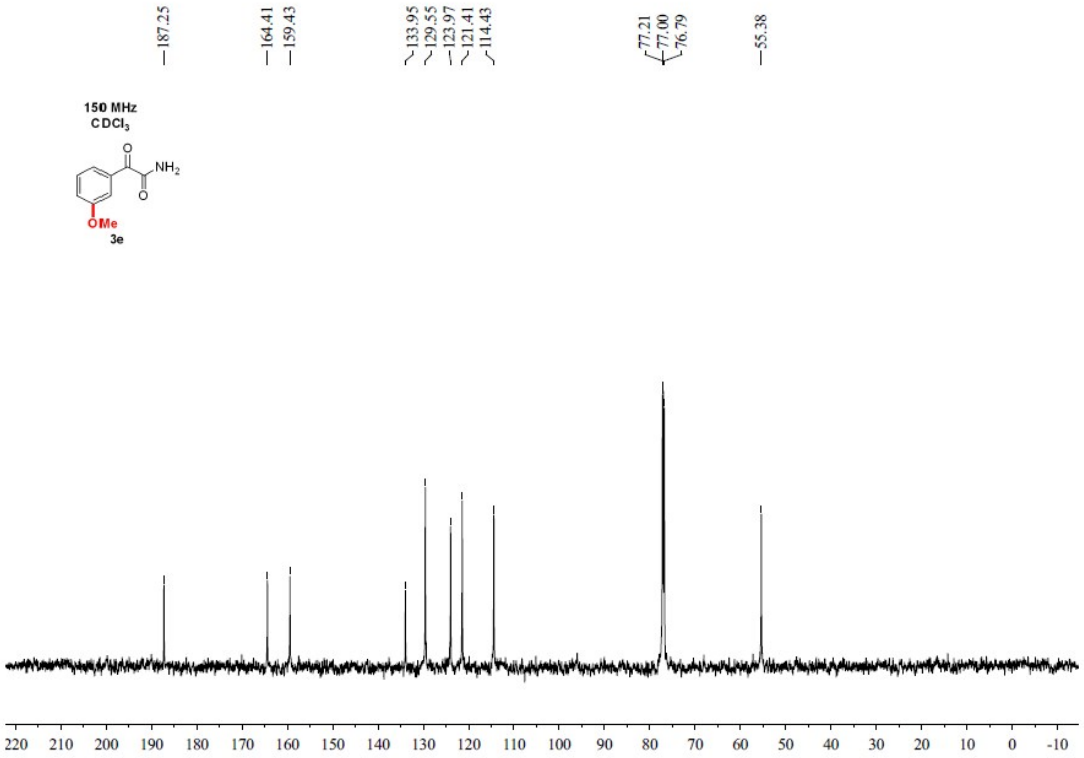
7.309
7.296
7.108
7.104
7.095
7.091
7.031
6.636
3.771
0.000
600 MHz
CDCl3
NH2
OMe
3e
0.83
0.84
0.92
0.94
0.87
1.00
3.00
f1 (ppm)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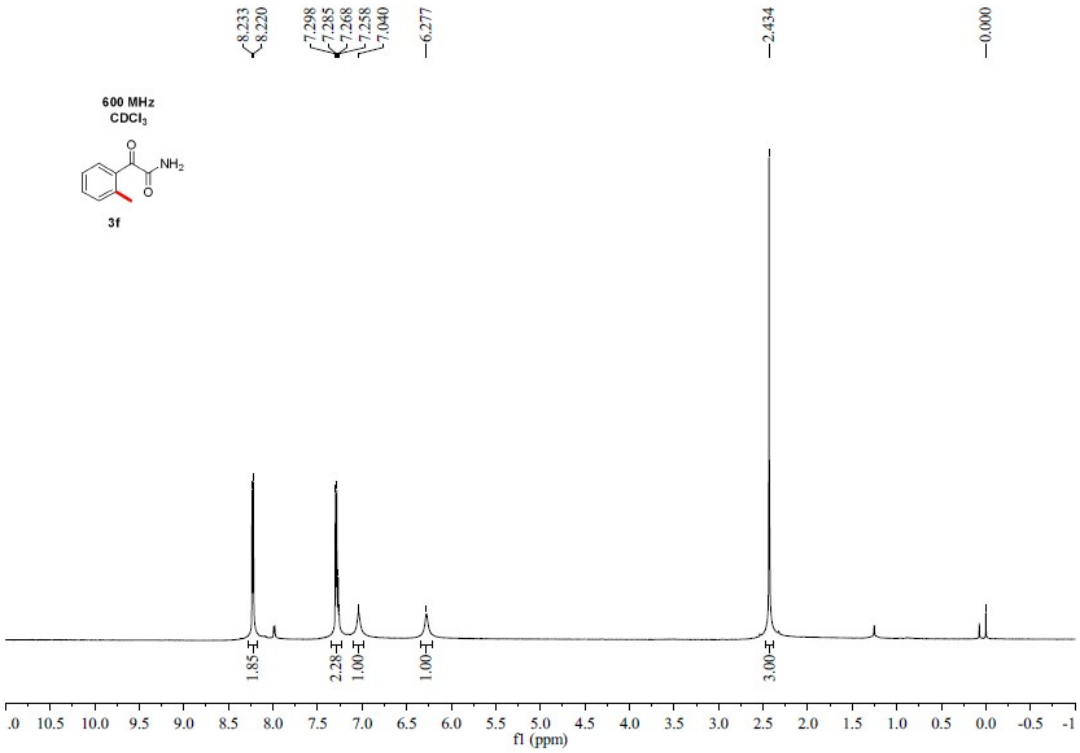
164.41
159.43
133.95
129.55
123.97
121.41
114.43
77.21
77.00
76.79
55.38
150 MHz
CDCl3
NH2
OMe
3e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8.220
7.298
7.285
7.268
7.258
7.040
6.277
2.434
0.000
600 MHz
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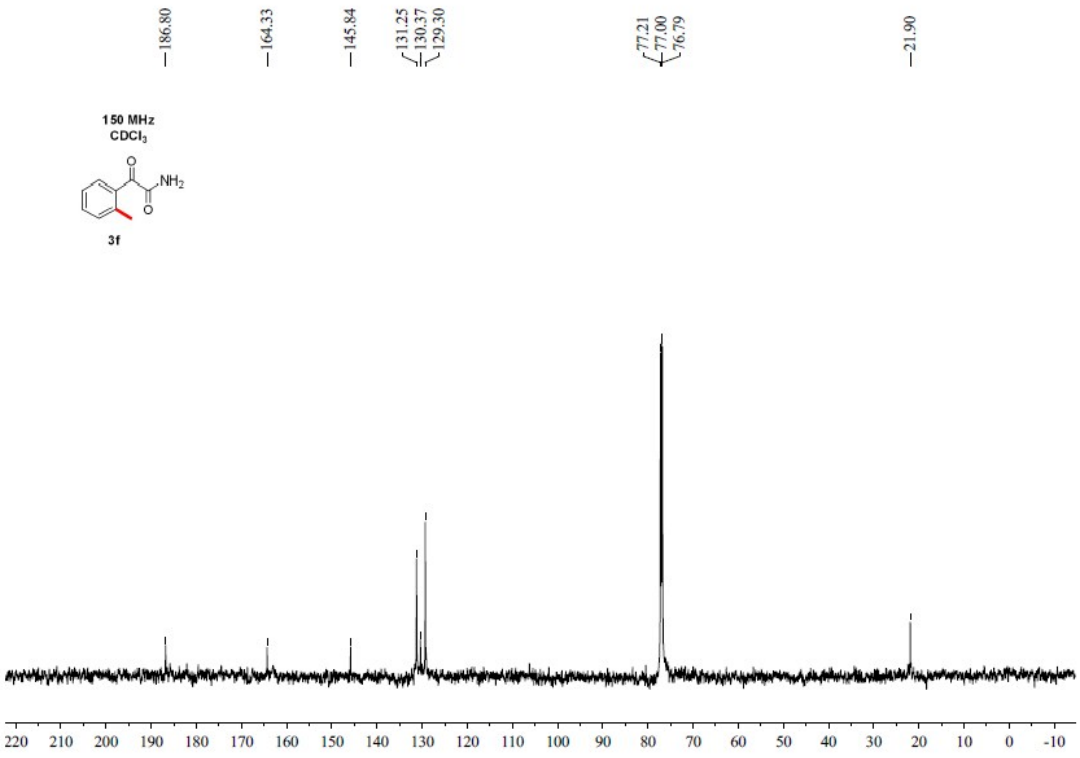
NH2
O
O
3f
1.85
2.28
1.00
1.00
3.00
f1 (ppm)


186.80
164.33
145.84
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130.37
129.30
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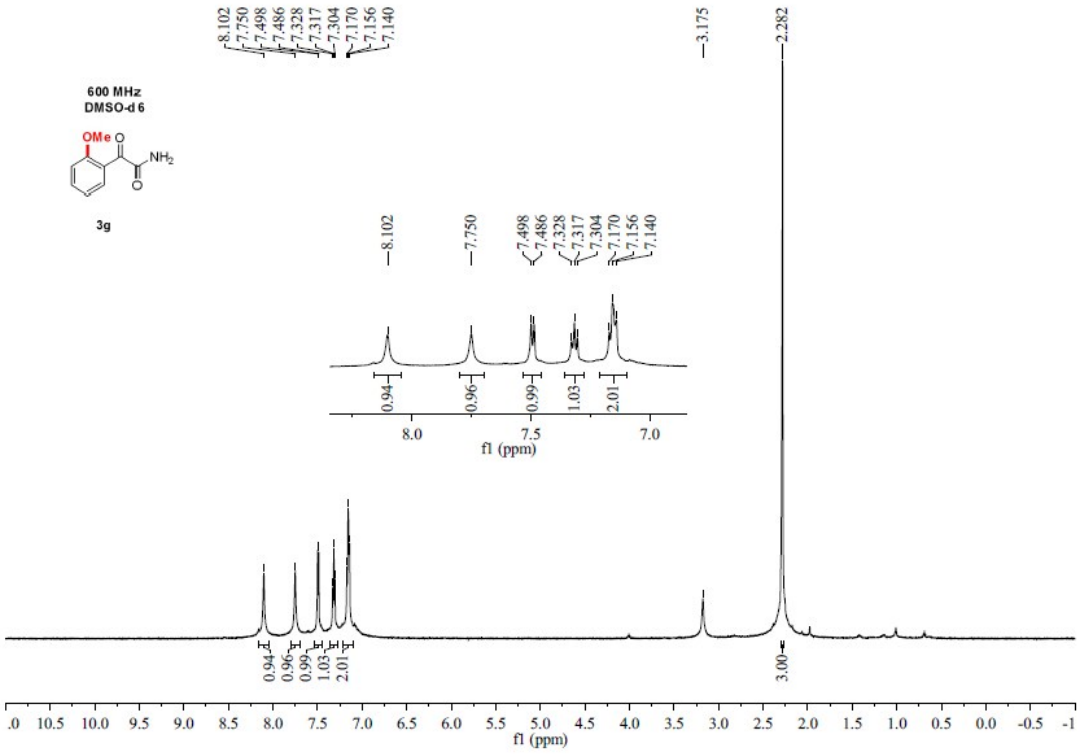
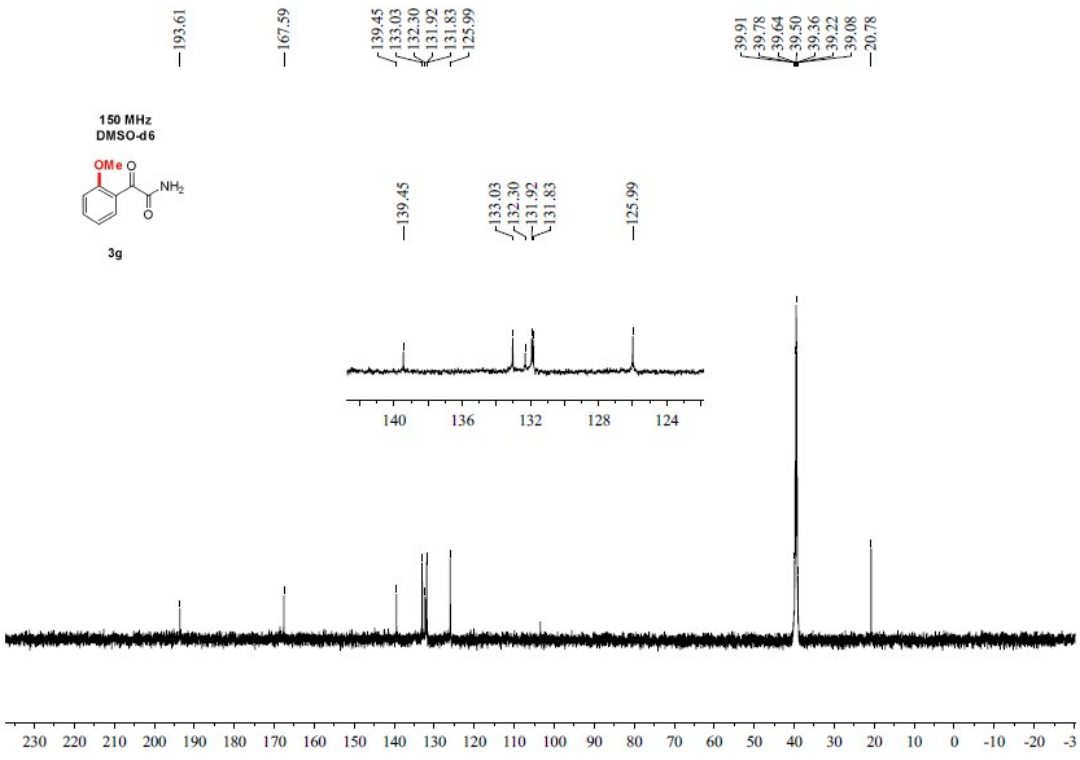
77.00
76.79
21.90
150 MHz
CDCl3
NH2
O
O
3f


600 MHz
DMSO-d 6
OMe
NH2
3g
8.102
7.750
7.498
7.486
7.328
7.317
7.304
7.170
7.156
7.140
3.175
2.282
0.94
0.96
0.99
1.03
2.01
3.00
f1 (ppm)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DMSO-d6
OMe
NH2
3g
193.61
167.59
139.45
133.03
132.30
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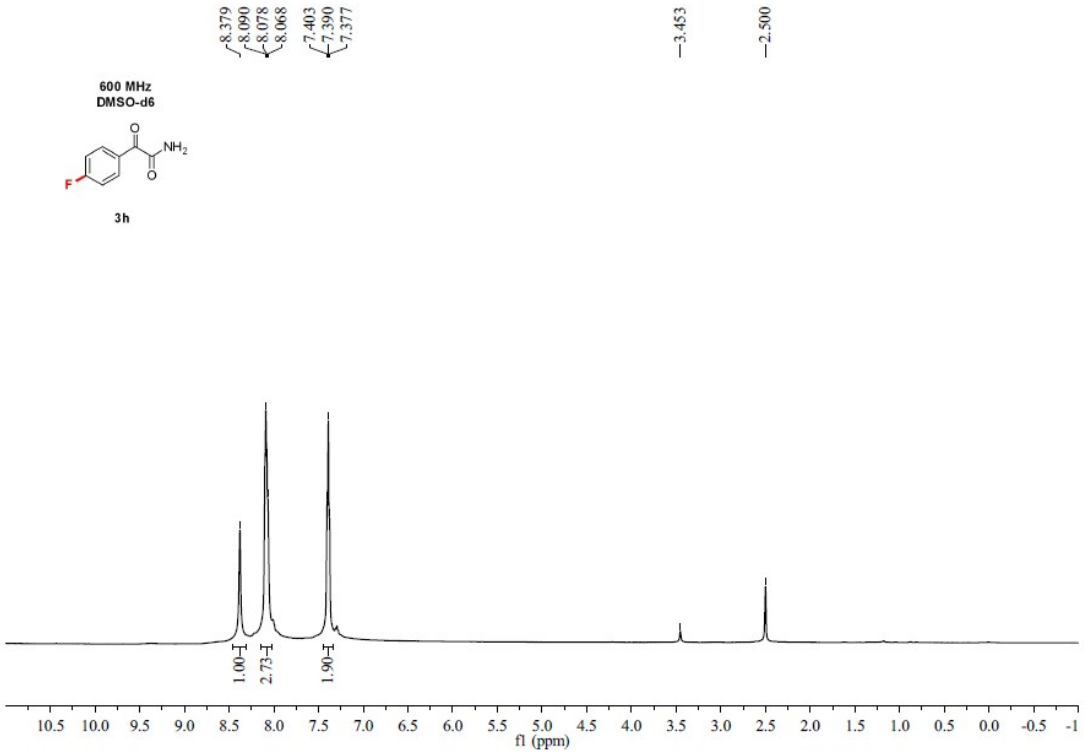
39.36
39.22
39.08
20.78
f1 (ppm)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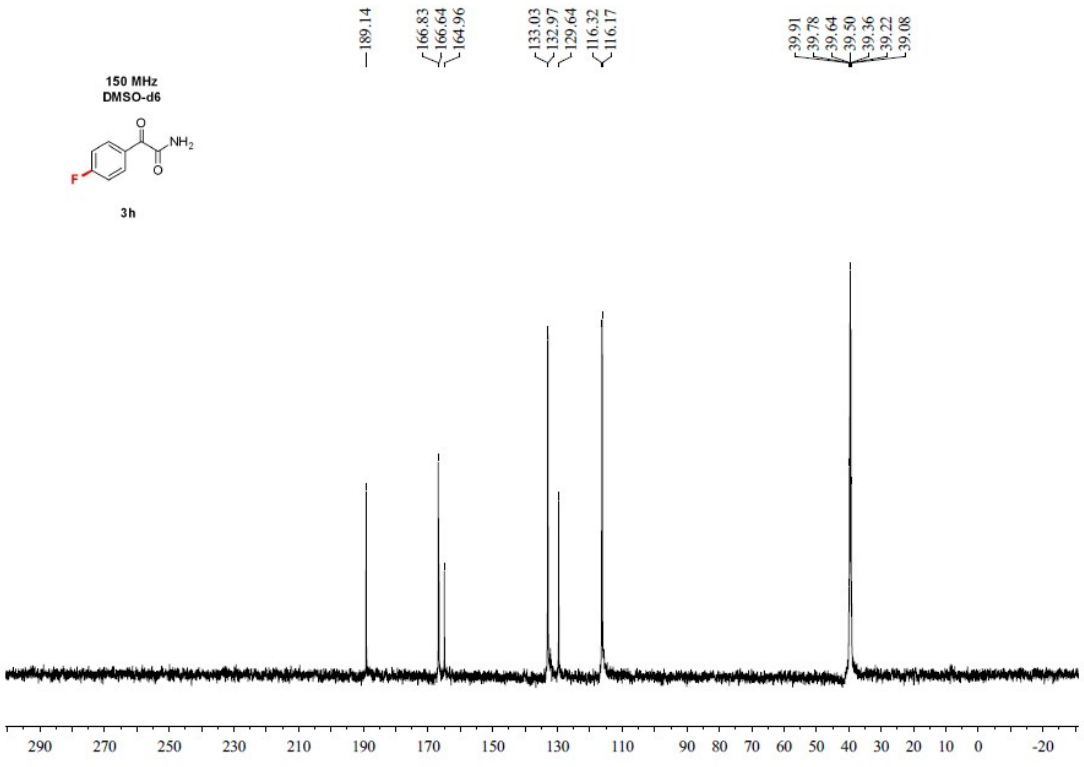
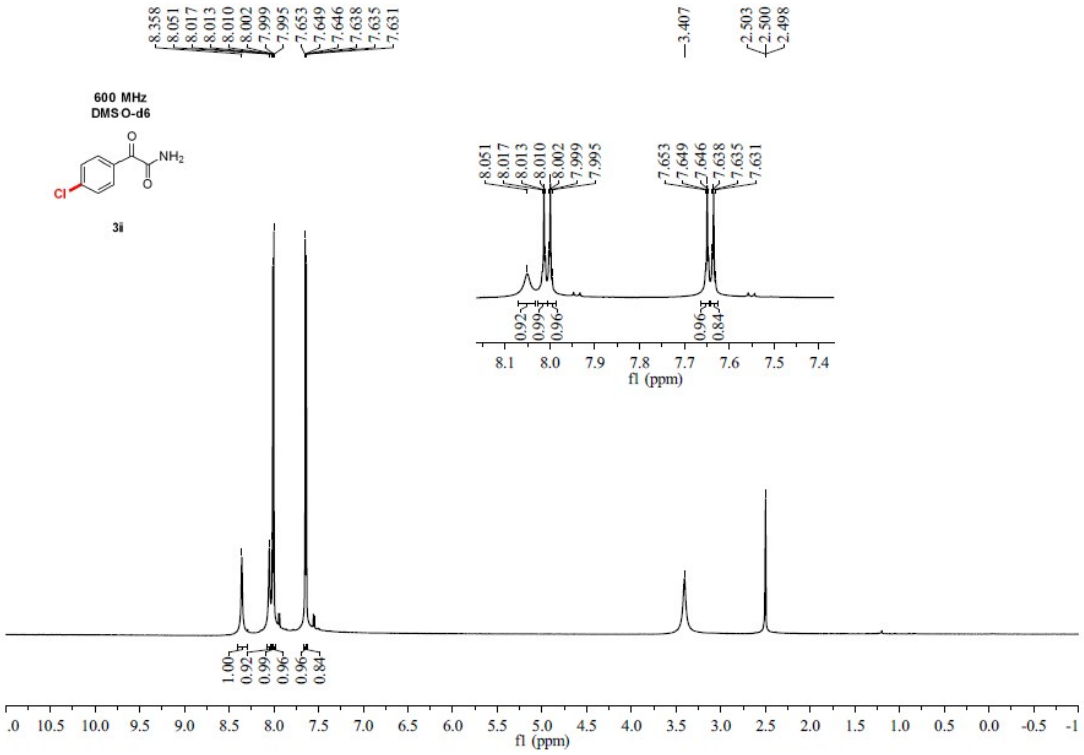
8.078
8.068
7.403
7.390
7.377
3.453
2.500
600 MHz
DMSO-d6
NH2
F
O
O
3h
1.00
2.73
1.90
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)


189.14
166.83
166.64
164.96
133.03
132.97
129.64
116.32
116.17
39.91
39.78
39.64
39.50
39.36
39.22
39.08
150 MHz
DMSO-d6
NH2
F
O
O
3h
290 270 250 230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0 -20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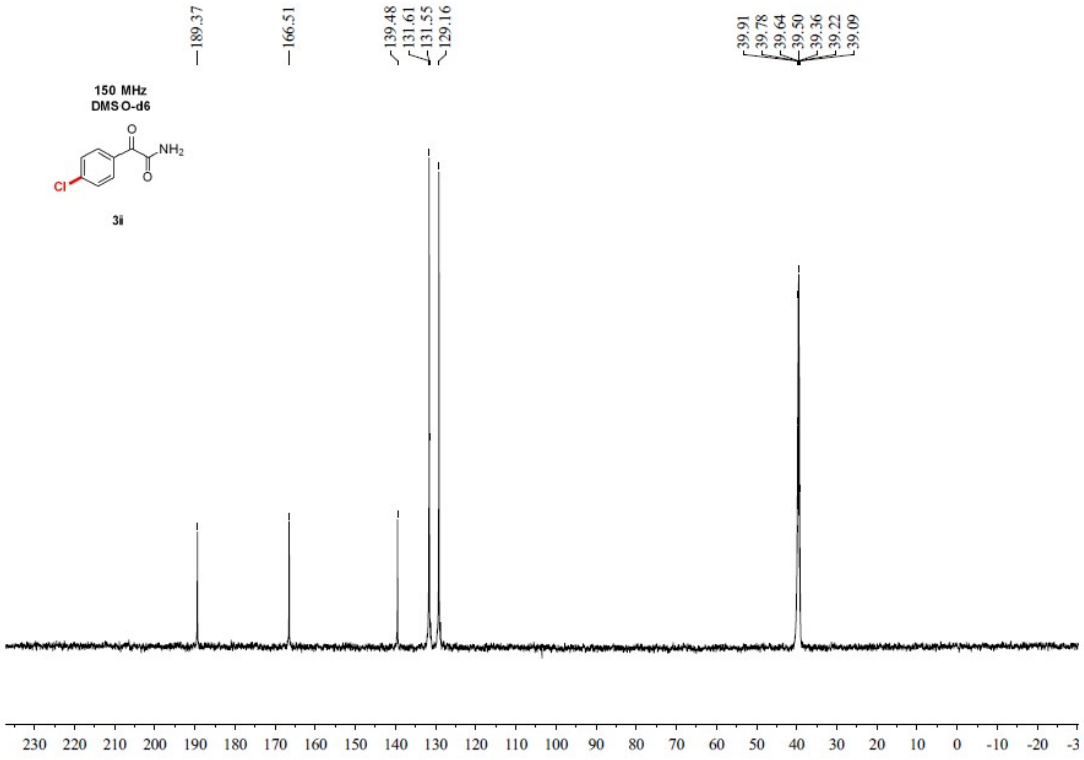
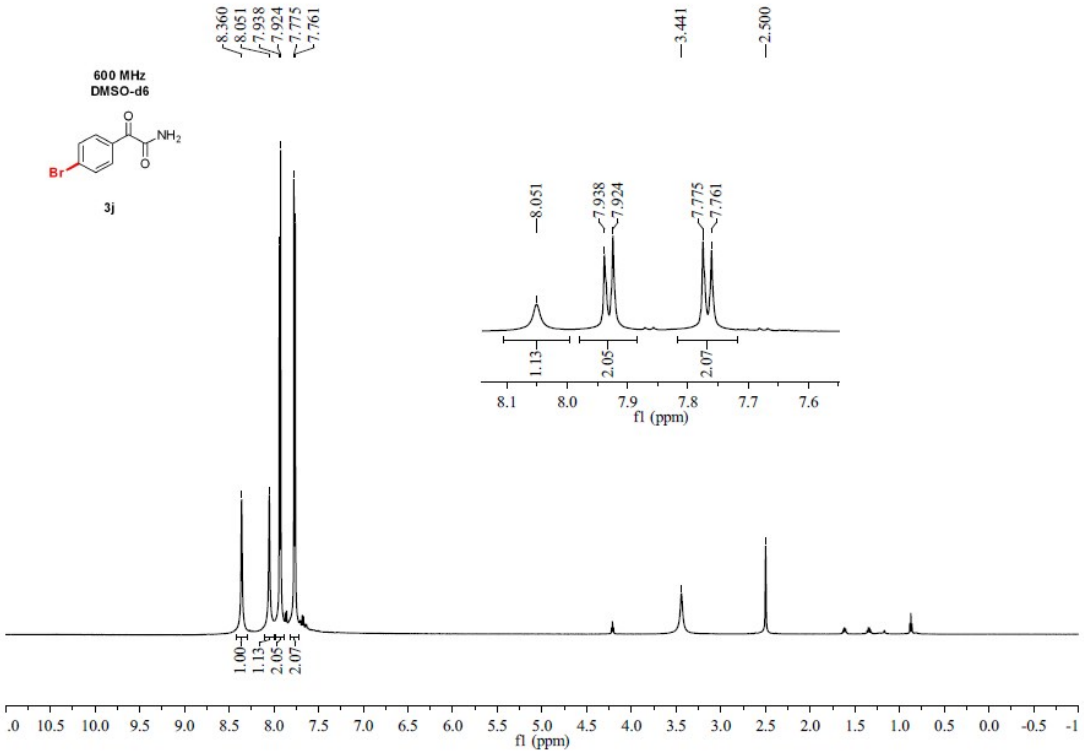
8.051
8.017
8.013
8.010
8.002
7.999
7.995
7.653
7.649
7.646
7.638
7.635
7.631
3.407
2.503
2.500
2.498
600 MHz
DMSO-d6
NH2
Cl
O
3i
1.00
0.92
0.99
0.96
0.96
0.84
f1 (ppm)


189.37
166.51
139.48
131.61
131.55
129.16
39.91
39.78
39.64
39.50
39.36
39.22
39.09
150 MHz
DMSO-d6
NH2
Cl
O
3i


600 MHz
DMSO-d6
3j
8.360
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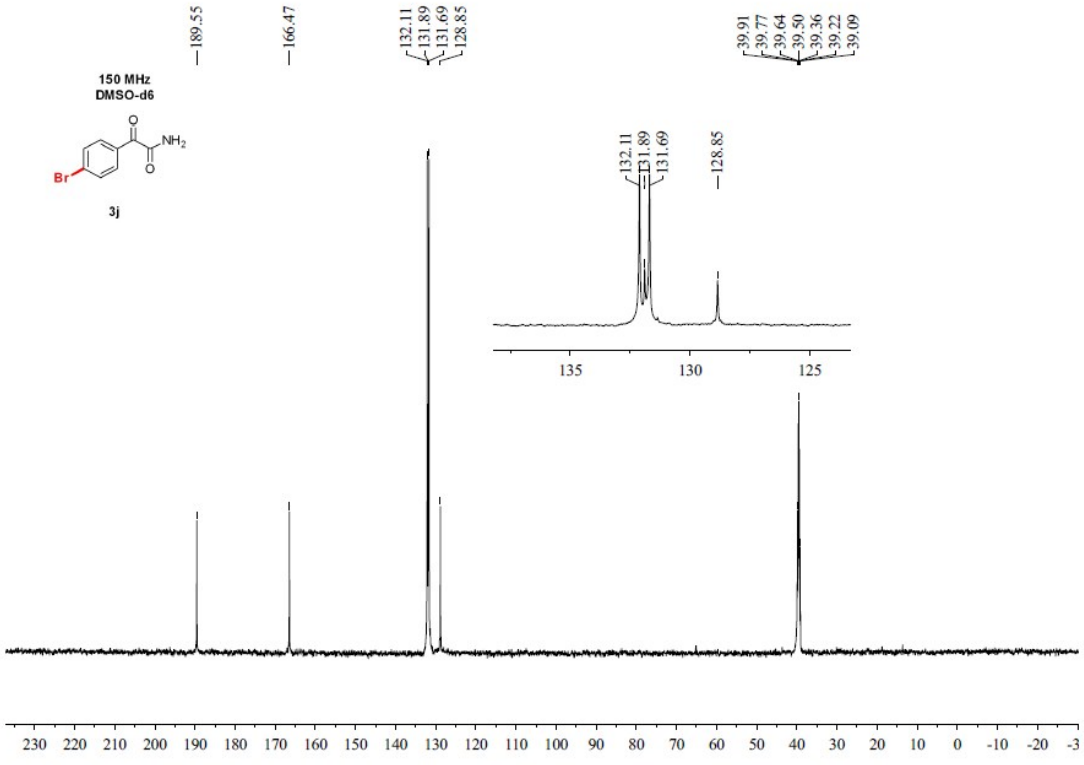
7.775
7.761
3.441
2.500
1.00
1.13
2.05
2.07
f1 (ppm)


150 MHz
DMSO-d6
3j
189.55
166.47
132.11
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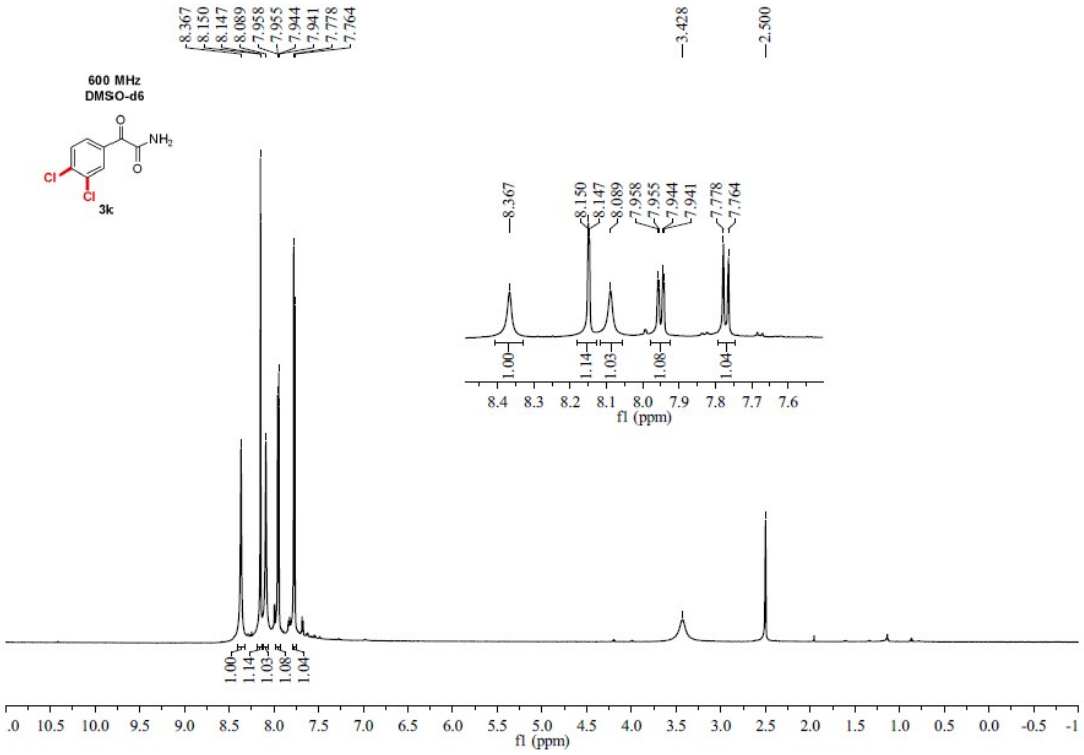
39.77
39.64
39.50
39.36
39.22
39.09
f1 (ppm)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8.150
8.147
8.089
7.958
7.955
7.944
7.941
7.778
7.764
3.428
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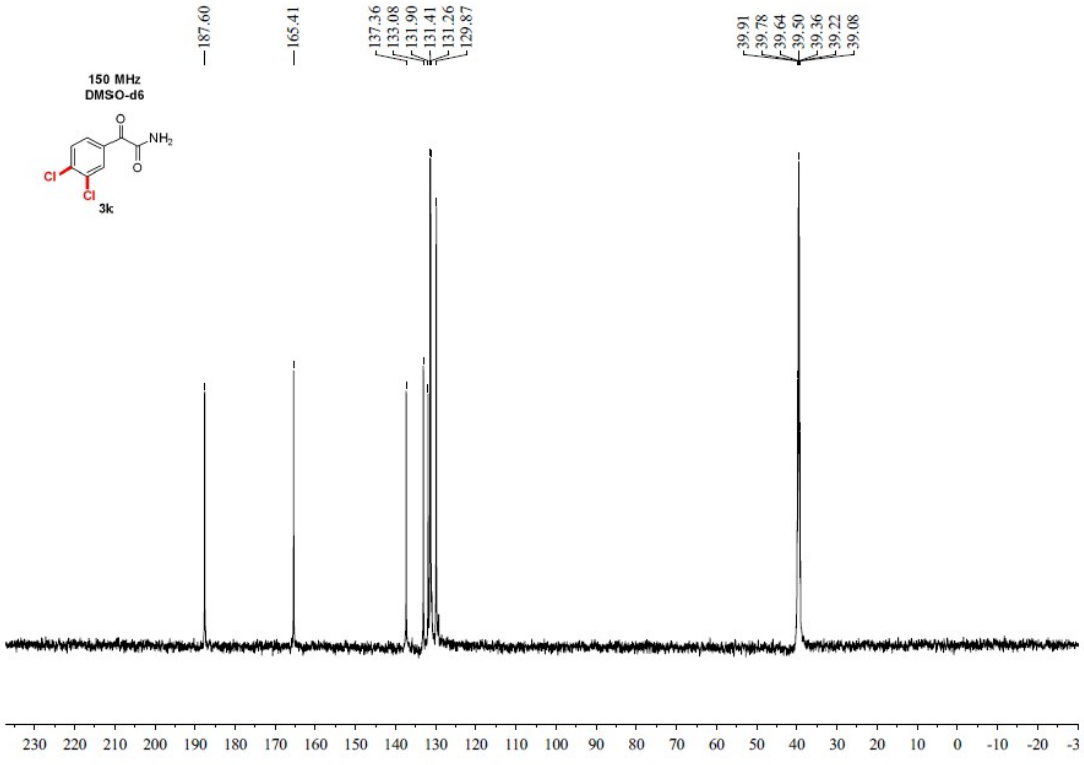
600 MHz
DMSO-d6
NH2
Cl
Cl
3k
1.00
1.14
1.03
1.08
1.04
f1 (ppm)


187.60
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137.36
133.08
131.90
131.41
131.26
129.87
39.91
39.78
39.64
39.50
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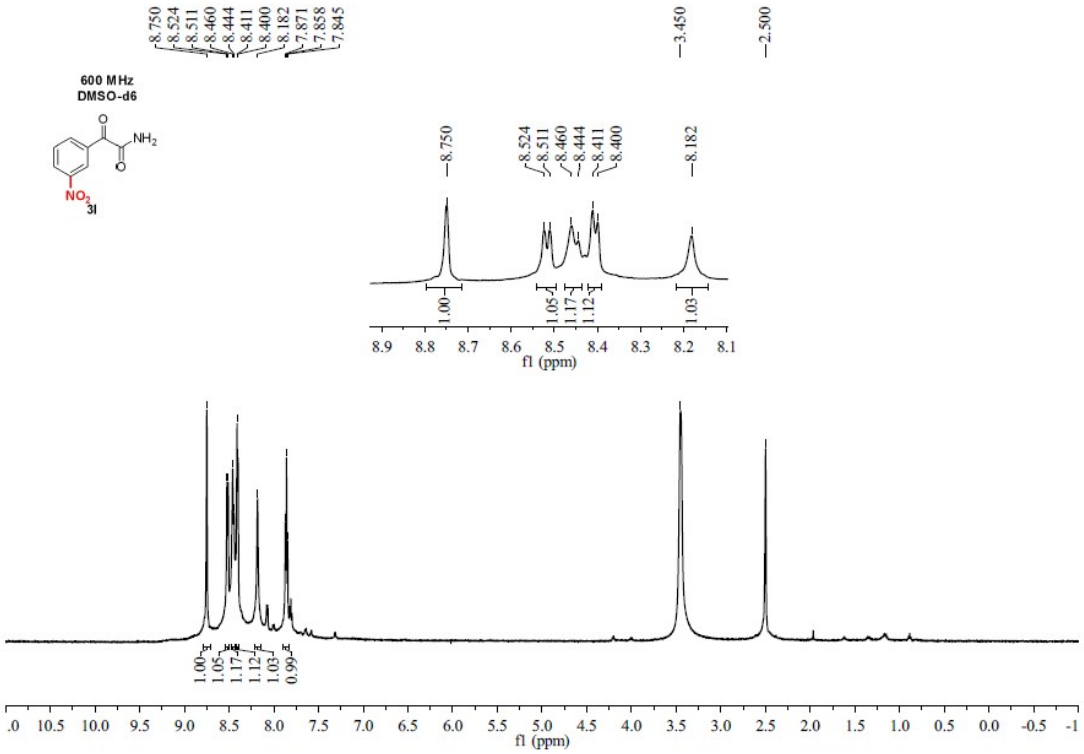
39.22
39.08
150 MHz
DMSO-d6
NH2
Cl
Cl
3k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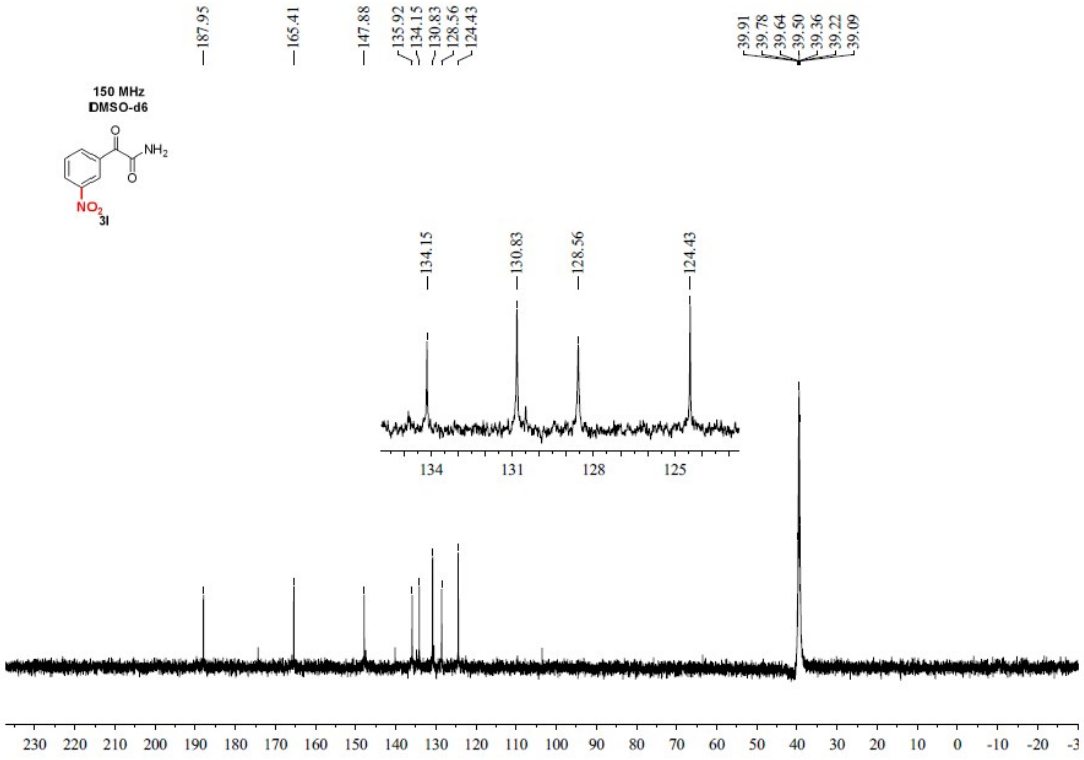
8.524
8.511
8.460
8.444
8.411
8.400
8.182
7.871
7.858
7.845
3.450
2.500
600 MHz
DMSO-d6
NH2
NO2
3l
fl (ppm)
1.00
1.05
1.17
1.12
1.03
0.99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128.56
124.43
39.91
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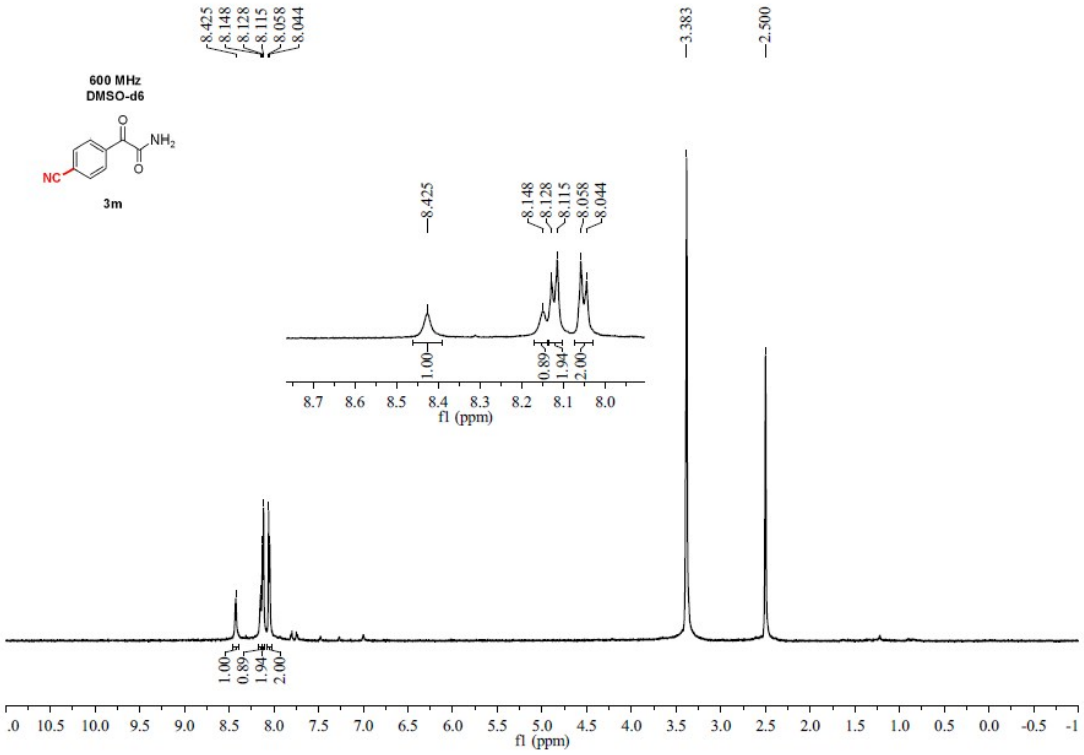
39.36
39.22
39.09
150 MHz
DMSO-d6
NH2
NO2
3l
fl (ppm)


600 MHz
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3m
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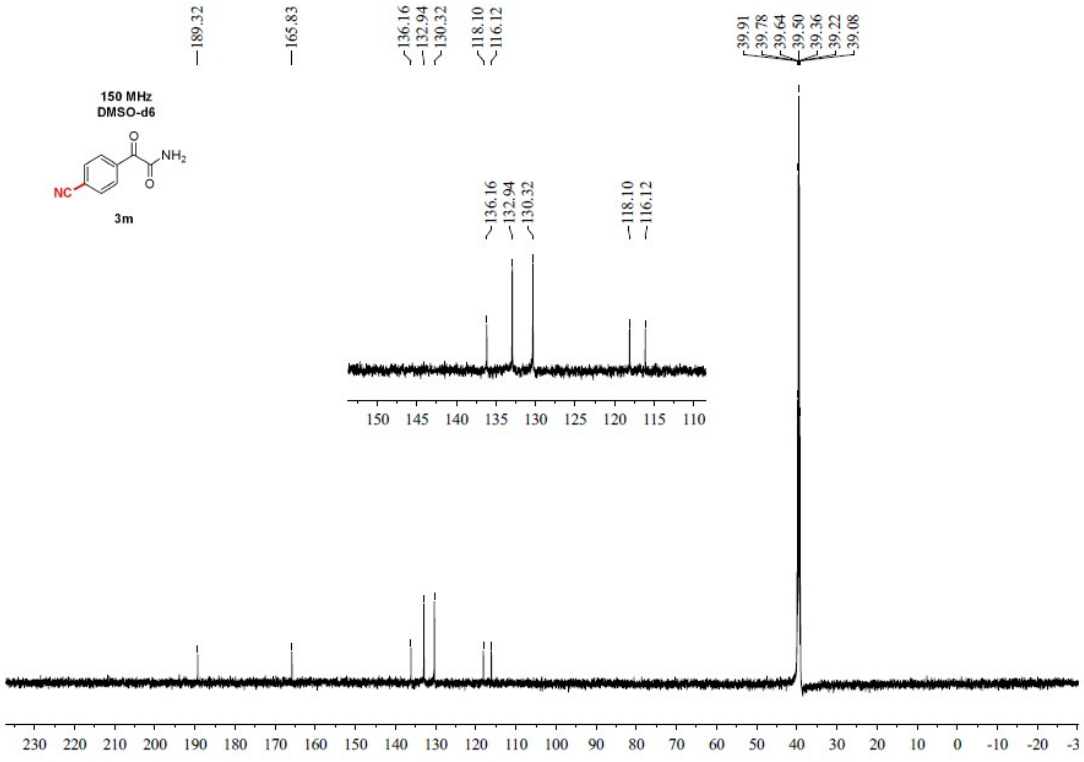
2.00
f1 (ppm)


150 MHz
DMSO-d6
3m
189.32
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136.16
132.94
130.32
118.10
116.12
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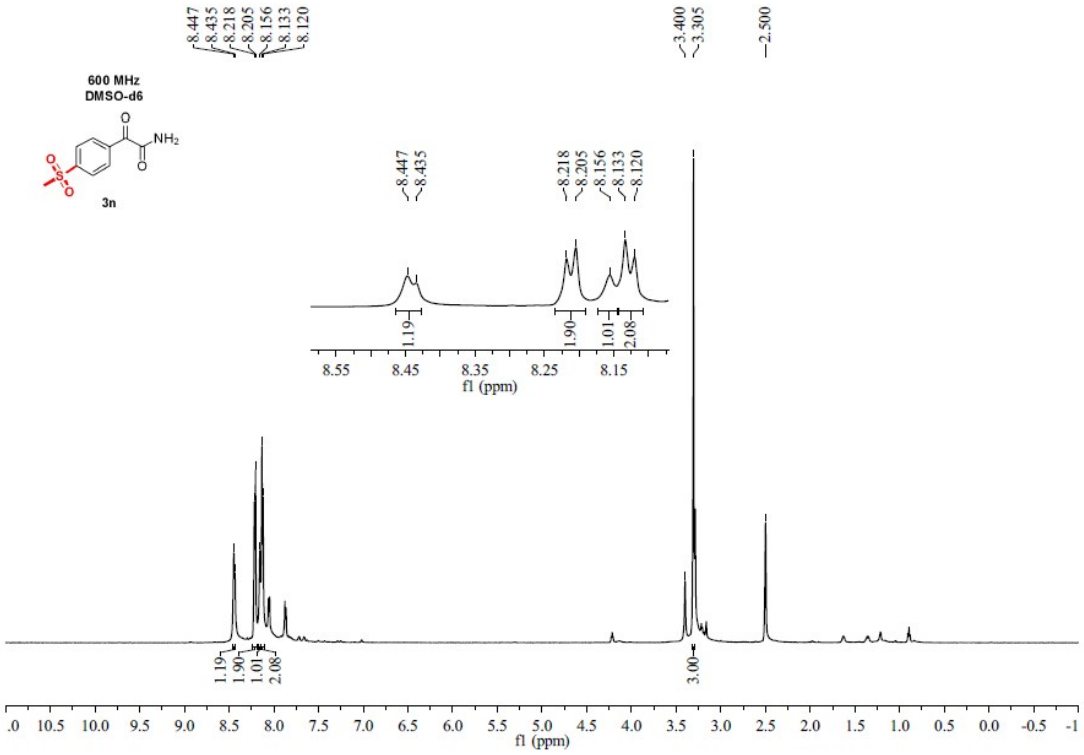
39.50
39.36
39.22
39.08
f1 (ppm)


8.447
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8.205
8.156
8.133
8.120
3.400
3.305
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600 MHz
DMSO-d6
NH2
3n
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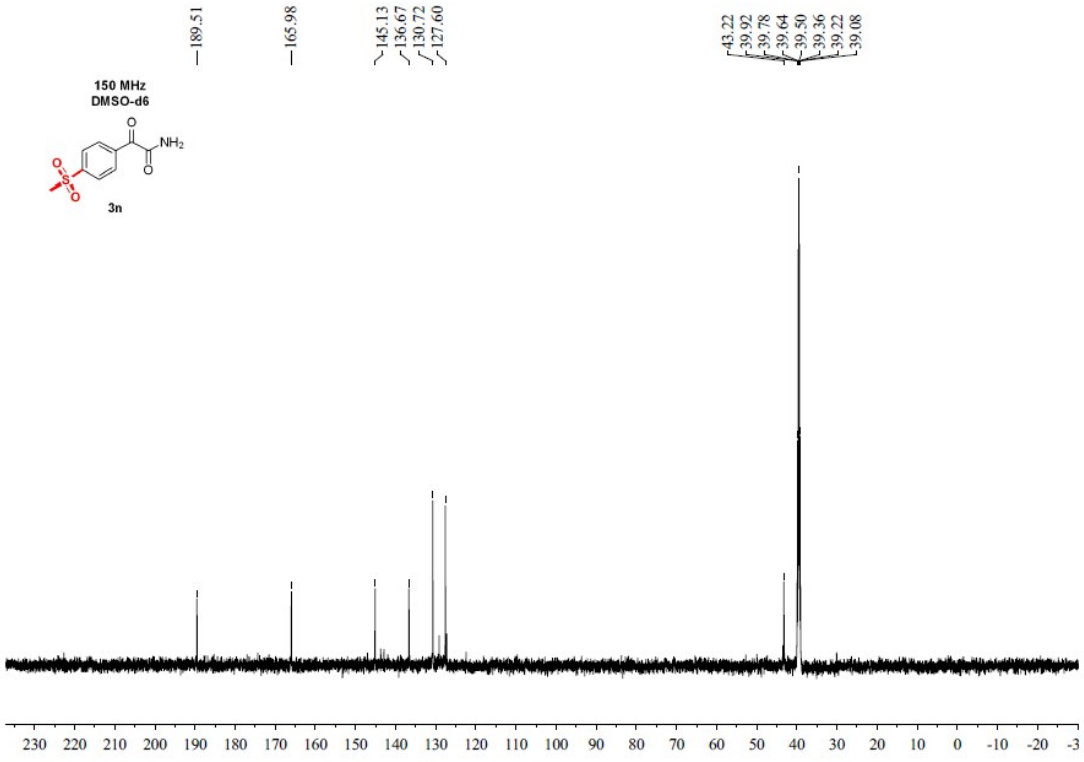
1.90
1.01
2.08
3.00
f1 (ppm)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127.60
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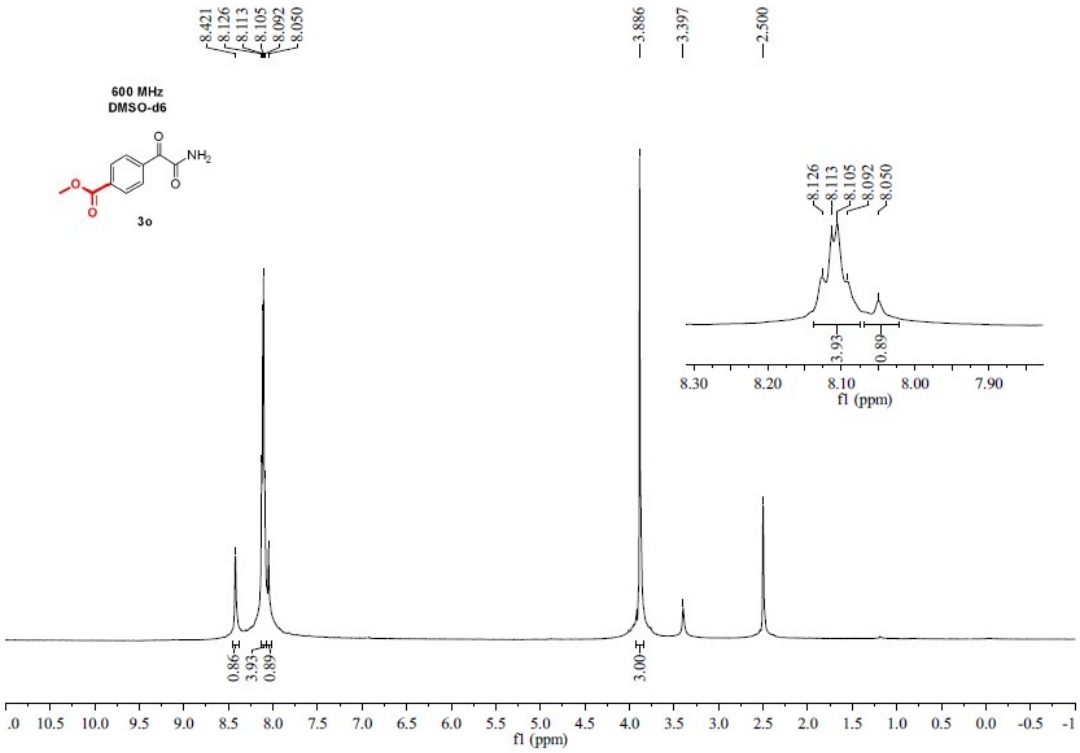
39.22
39.08
150 MHz
DMSO-d6
NH2
3n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8.113
8.105
8.092
8.050
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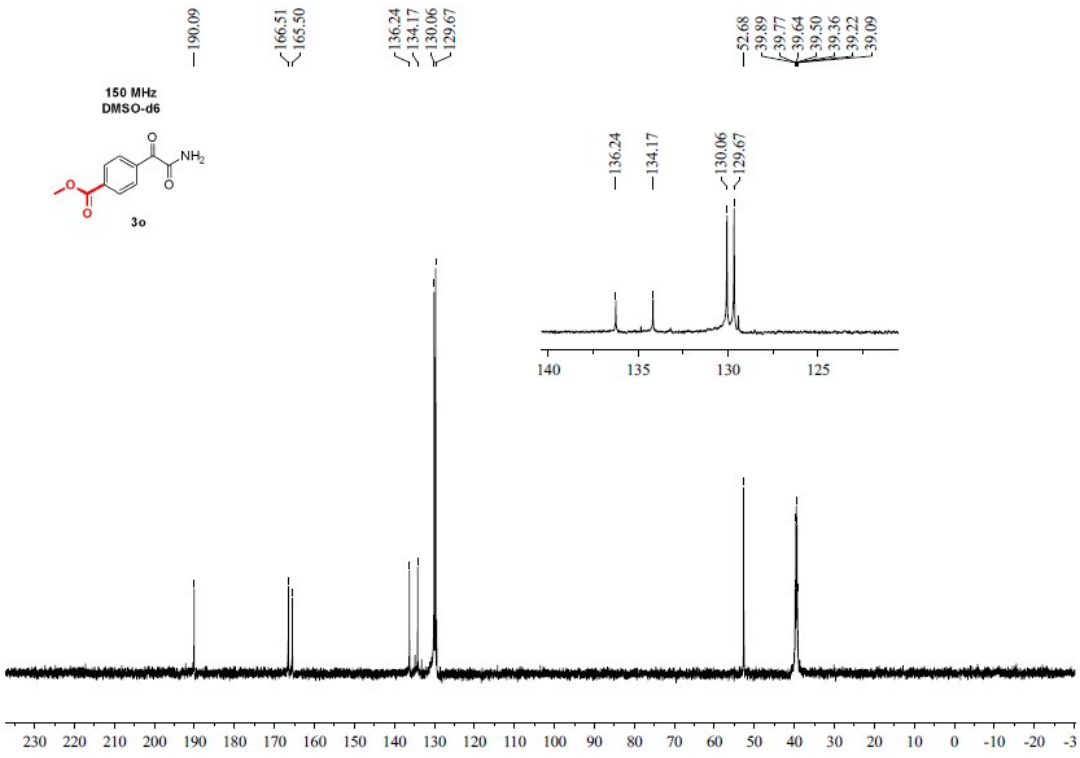
3.397
2.500
600 MHz
DMSO-d6
NH2
3o
0.86
3.93
0.89
3.00
f1 (ppm)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166.51
165.50
136.24
134.17
130.06
129.67
52.68
39.89
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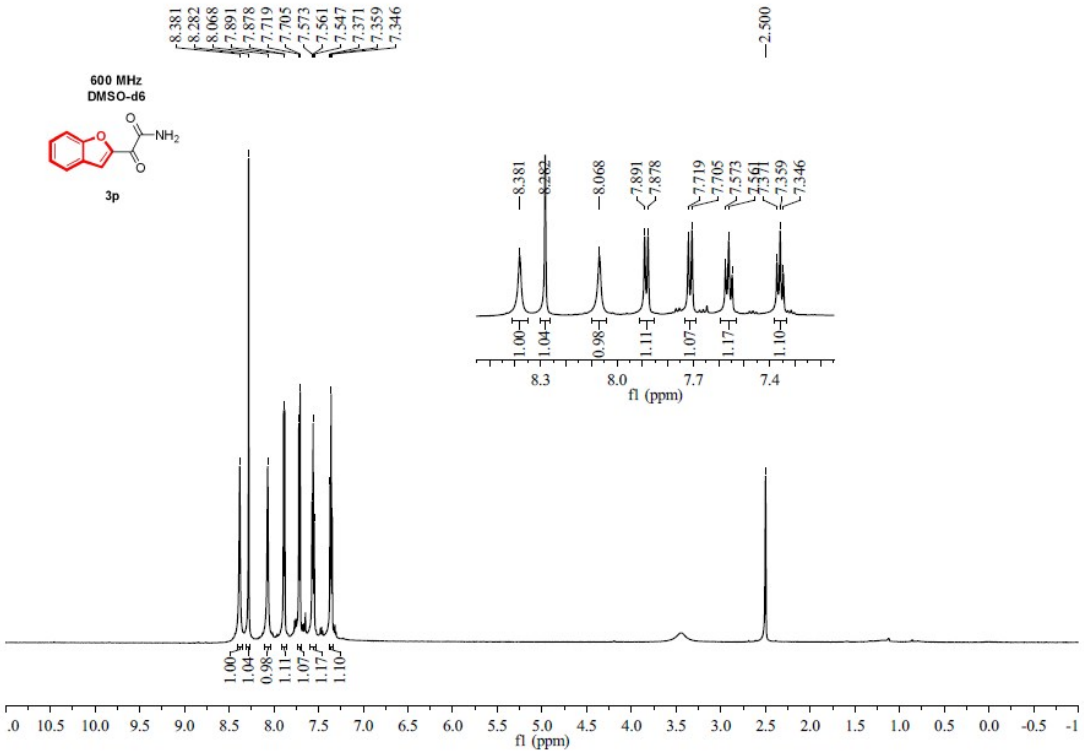
39.50
39.36
39.22
39.09
150 MHz
DMSO-d6
NH2
3o
f1 (ppm)


600 MHz
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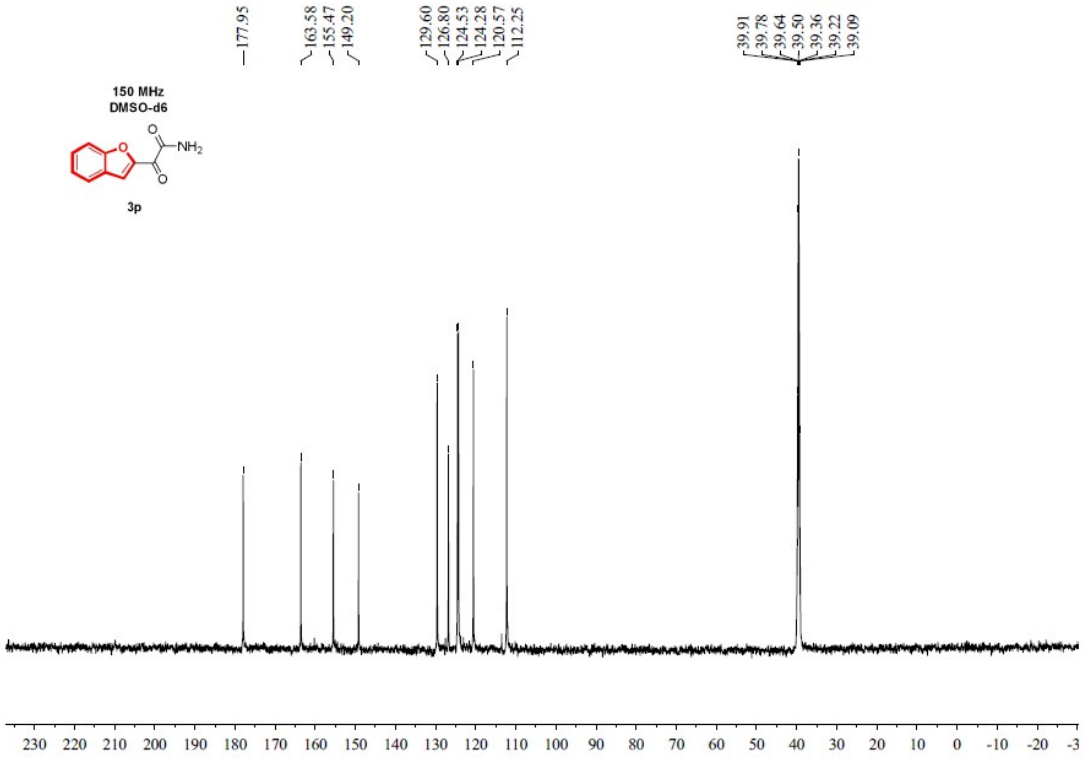
7.878
7.719
7.705
7.573
7.561
7.547
7.371
7.359
7.346
2.500
1.00
1.04
0.98
1.11
1.07
1.17
1.10
f1 (ppm)


150 MHz
DMSO-d6
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39.64
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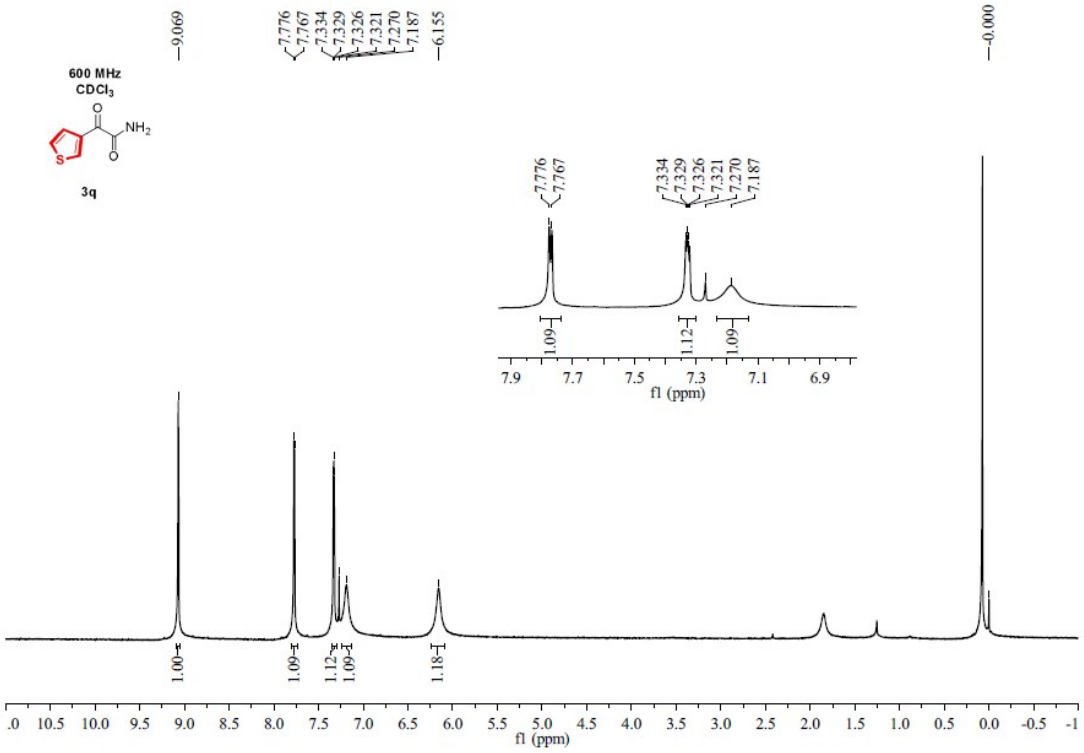
39.36
39.22
39.09


600 MHz
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1.09
1.12
1.09
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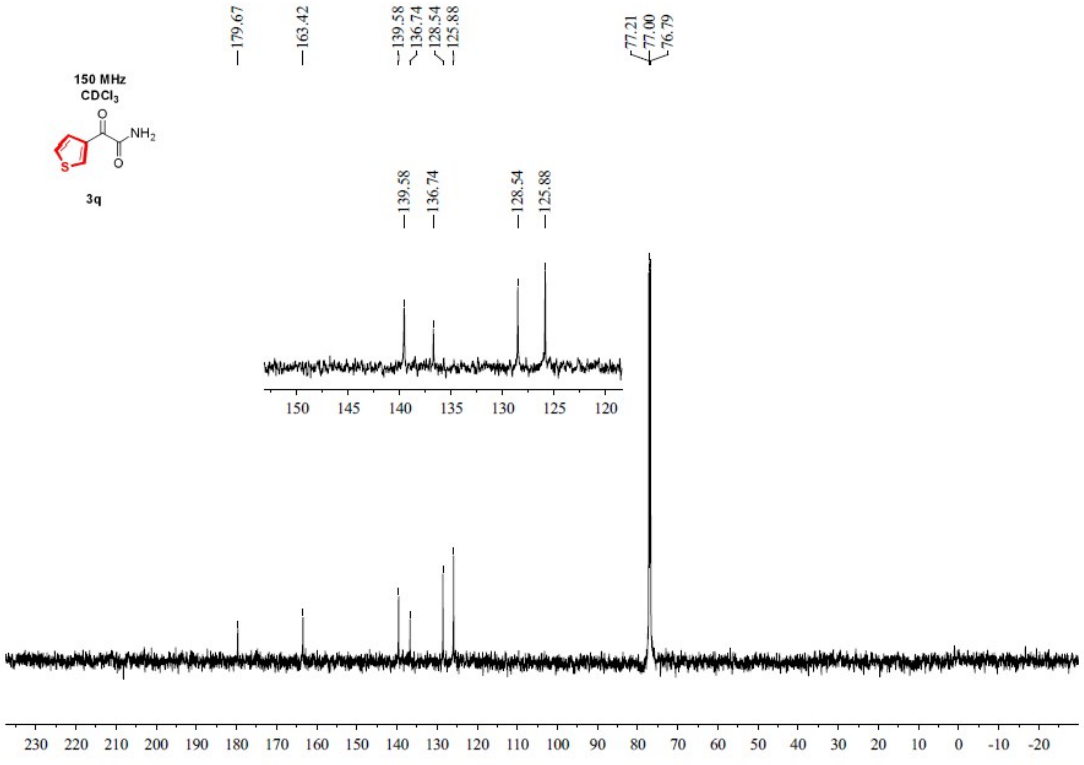
fl (ppm)


150 MHz
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3q
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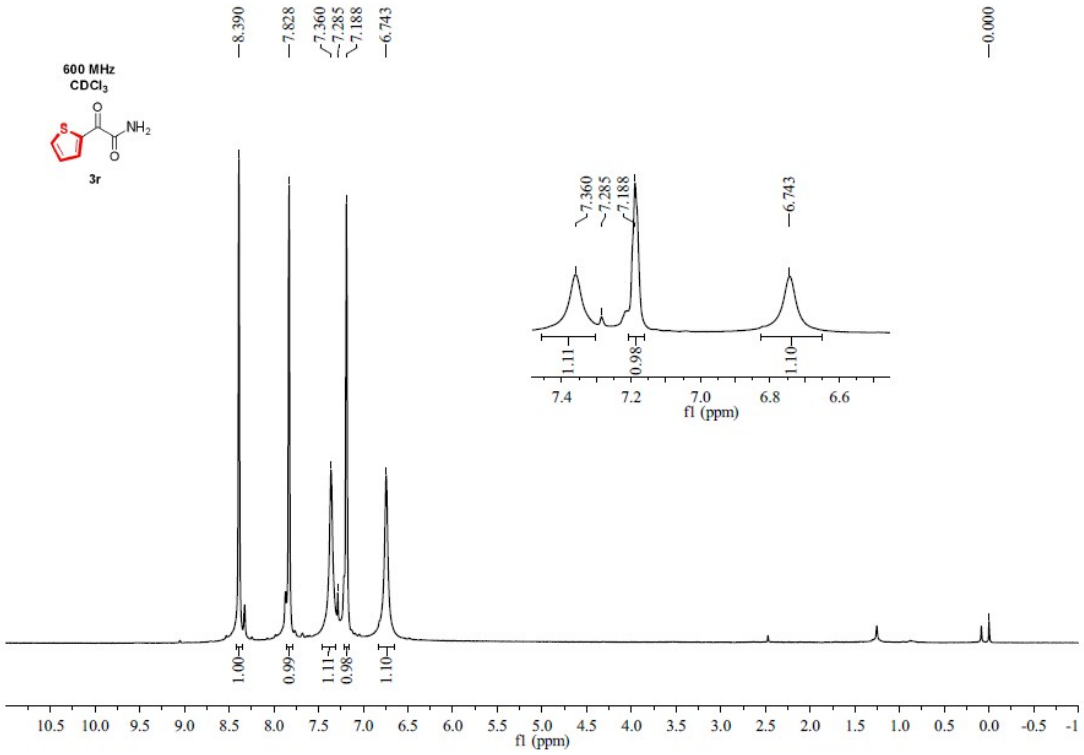
77.00
76.79
fl (ppm)


600 MHz
CDCl3
3r
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7.828
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7.188
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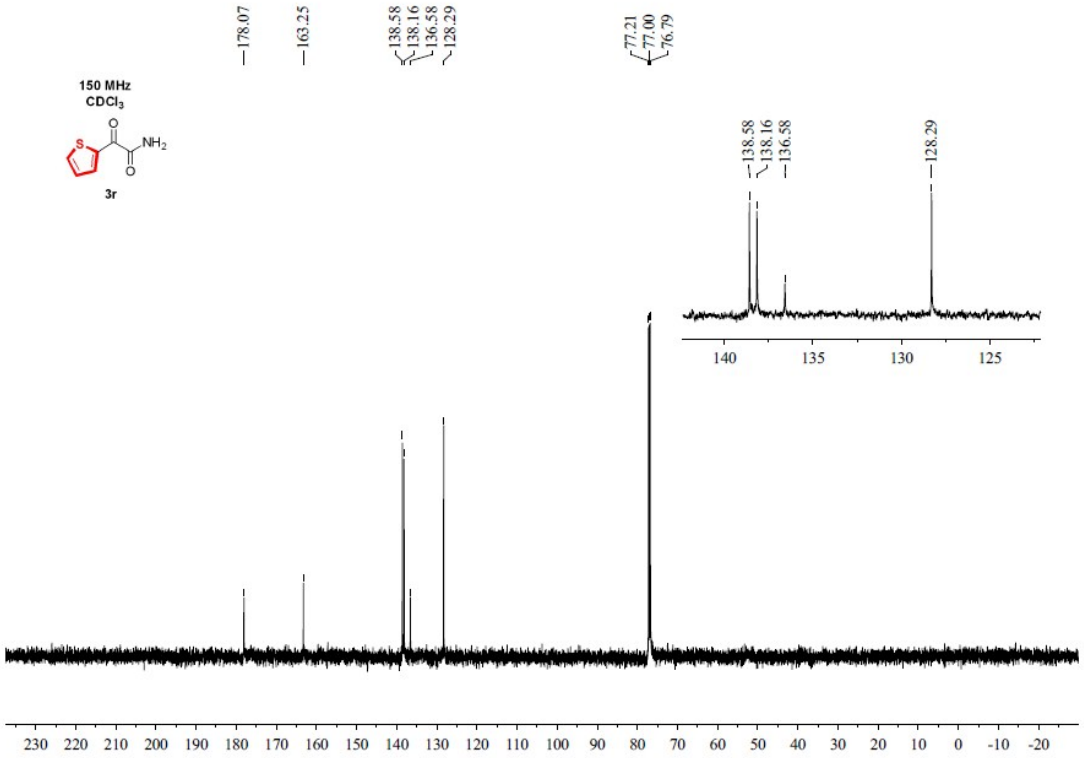
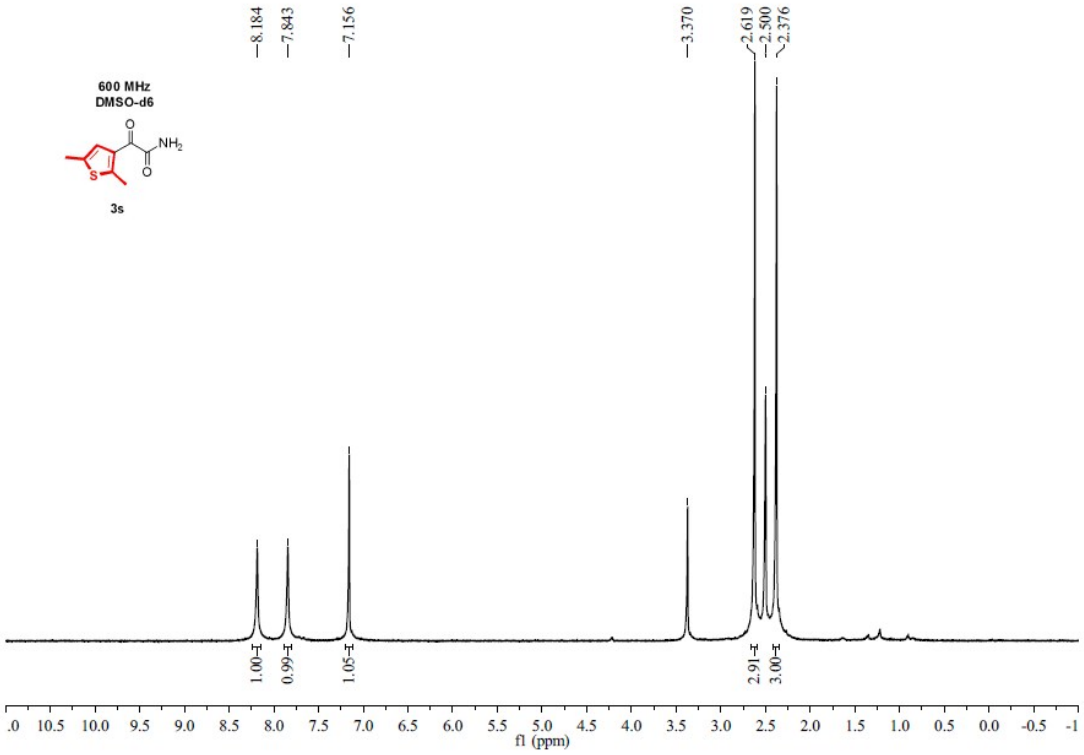
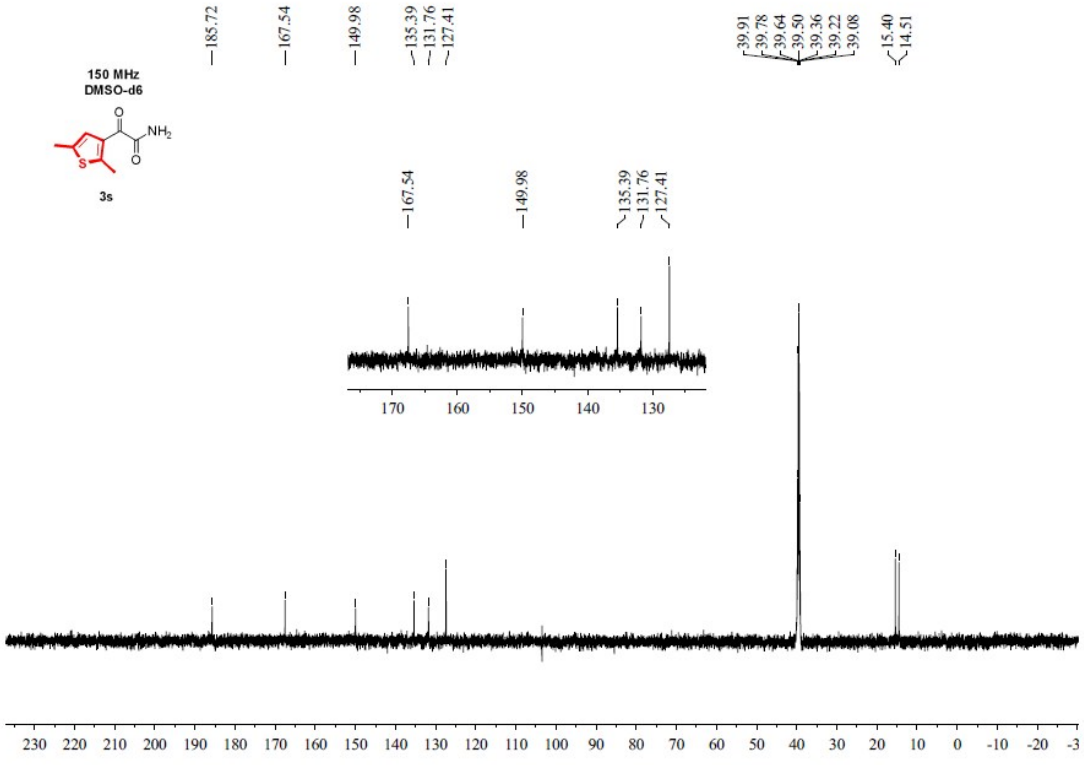
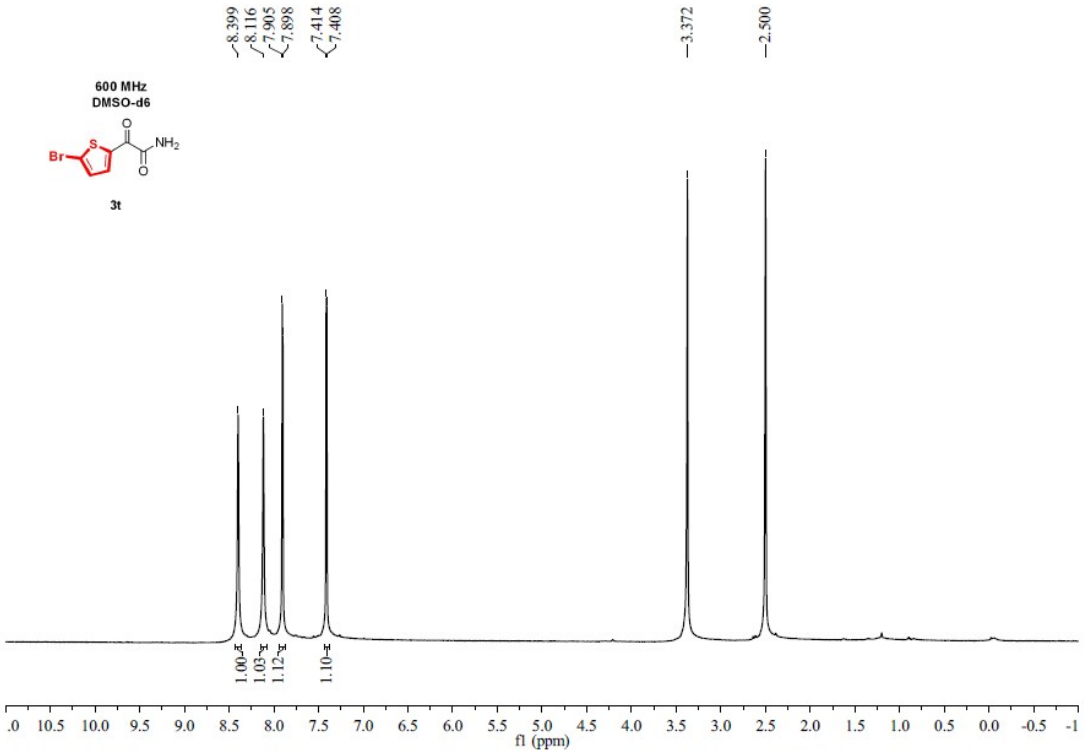
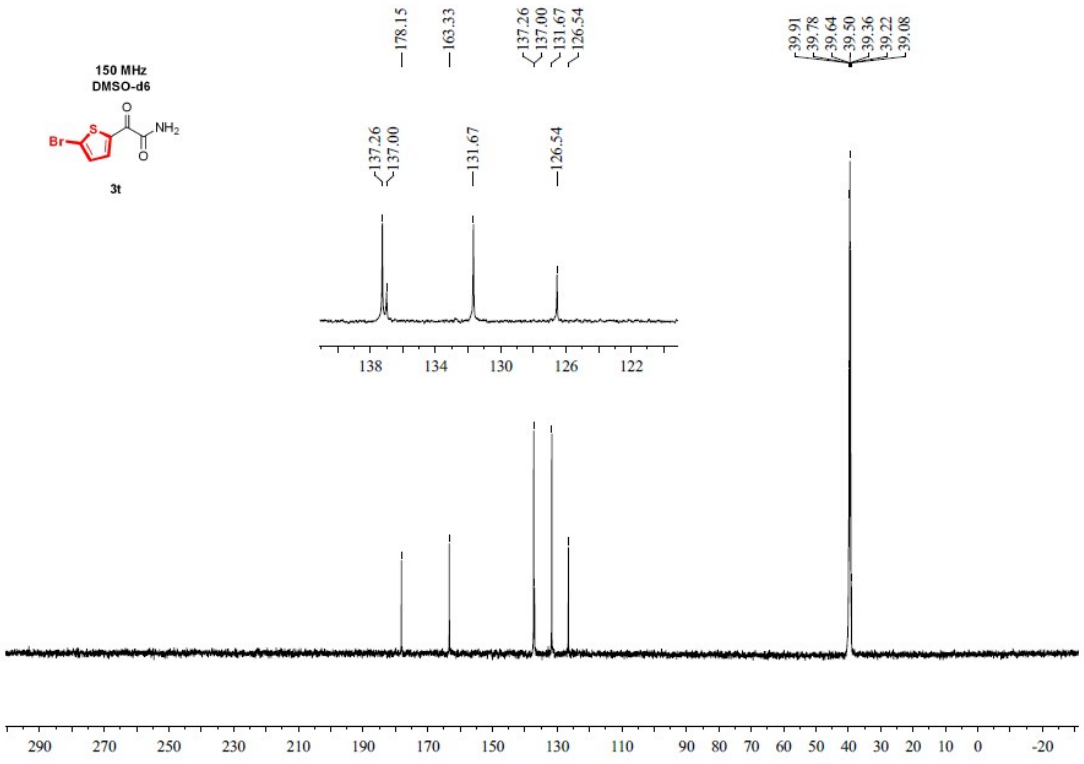
0.000
1.00
0.99
1.11
0.98
1.10
f1 (ppm)

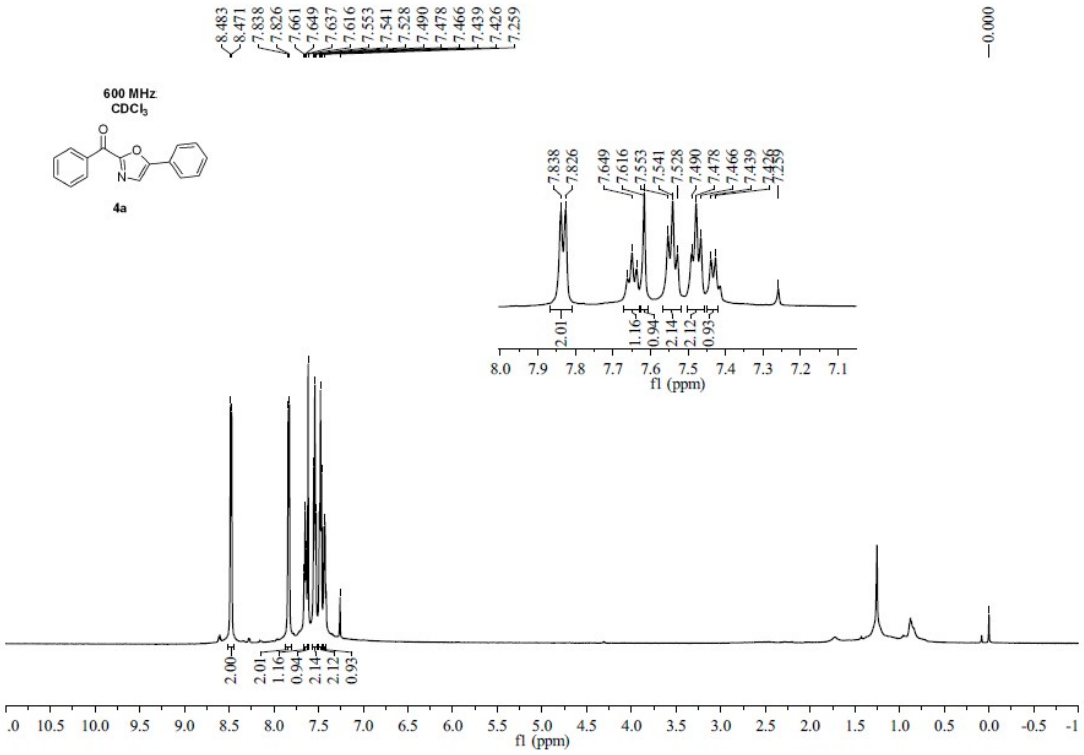

150 MHz
CDCl3
3r
178.07
163.25
138.58
138.16
136.58
128.29
77.21
77.00
76.79
f1 (ppm)

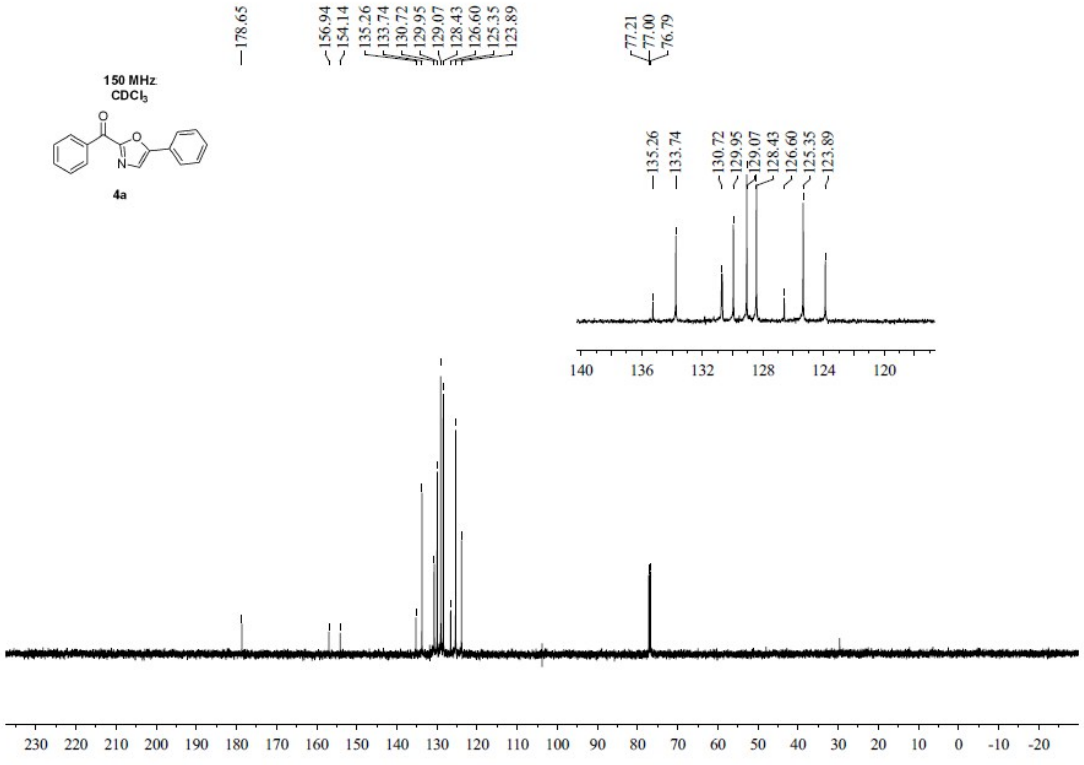

600 MHz
DMSO-d6
3s
8.184
7.843
7.156
3.370
2.619
2.500
2.376
1.00
0.99
1.05
2.91
3.00
f1 (ppm)

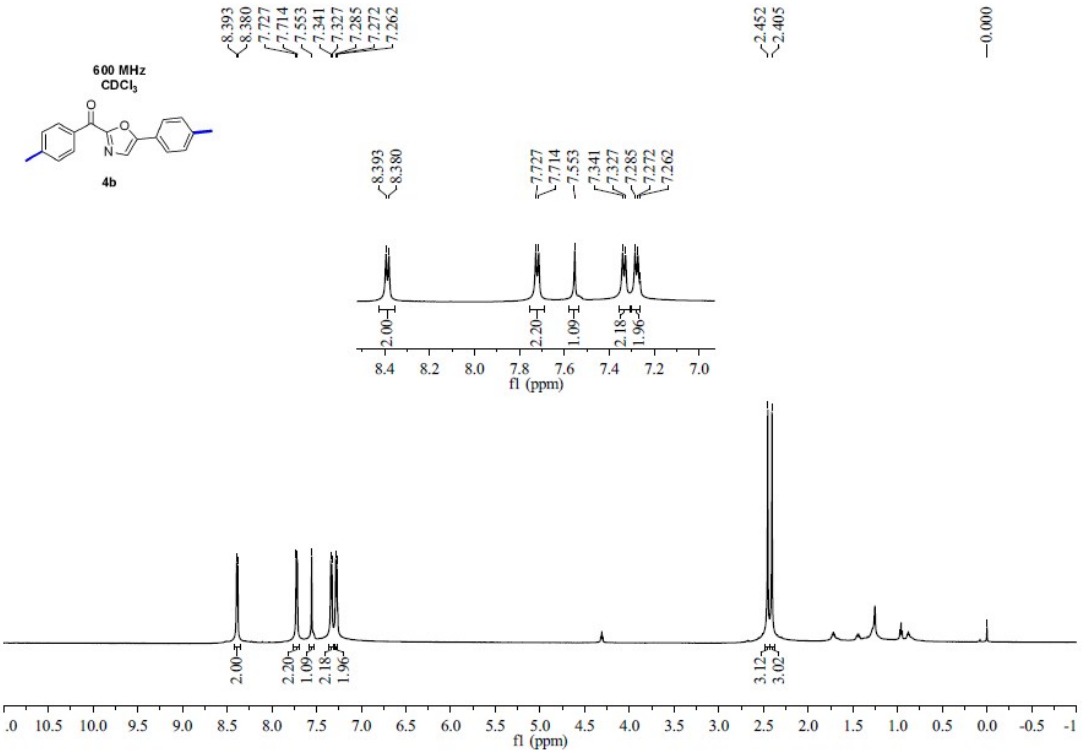

150 MHz
DMSO-d6
3s
185.72
167.54
149.98
135.39
131.76
127.41
39.91
39.78
39.64
39.50
39.36
39.22
39.08
15.40
14.51

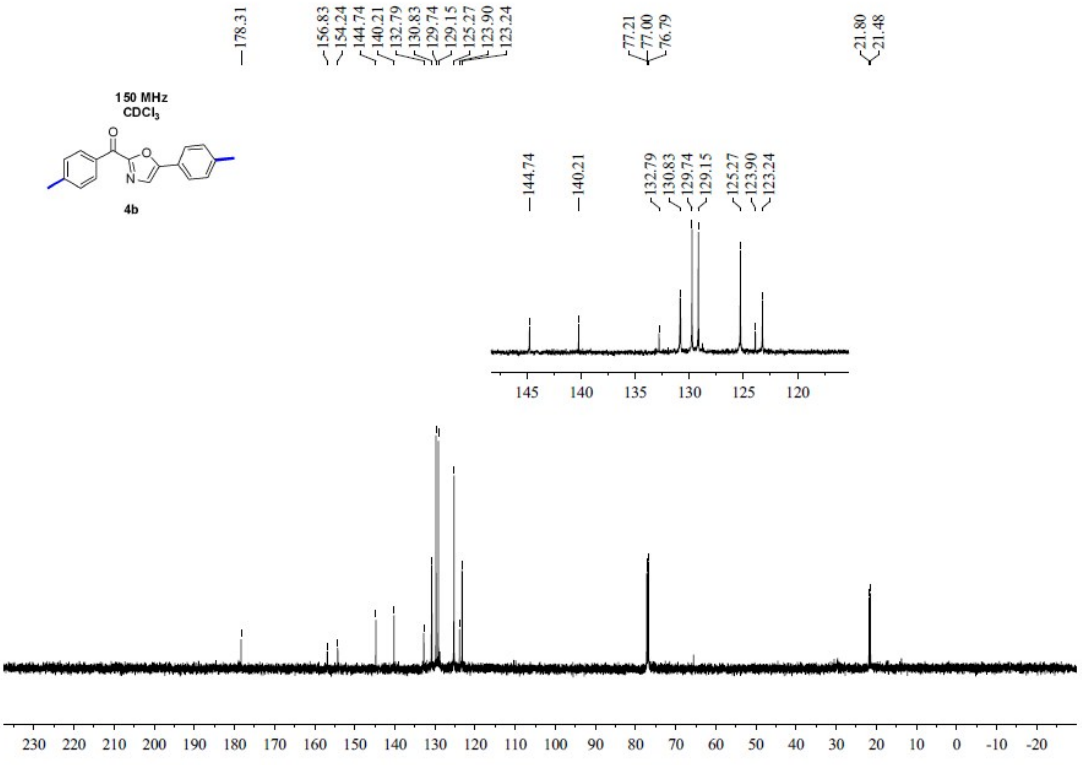

600 MHz
DMSO-d6
3t
8.399
8.116
7.905
7.898
7.414
7.408
3.372
2.500
1.00
1.03
1.12
1.10
f1 (ppm)

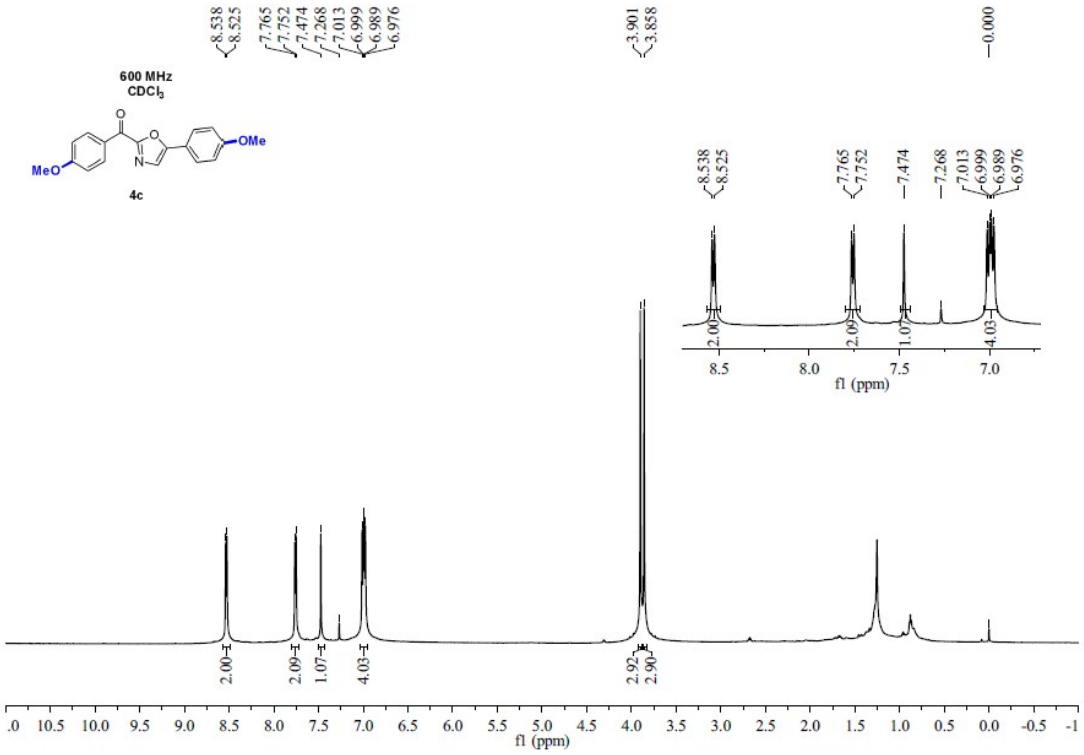

150 MHz
DMSO-d6
3t
178.15
163.33
137.26
137.00
131.67
126.54
39.91
39.78
39.64
39.50
39.36
39.22
39.08

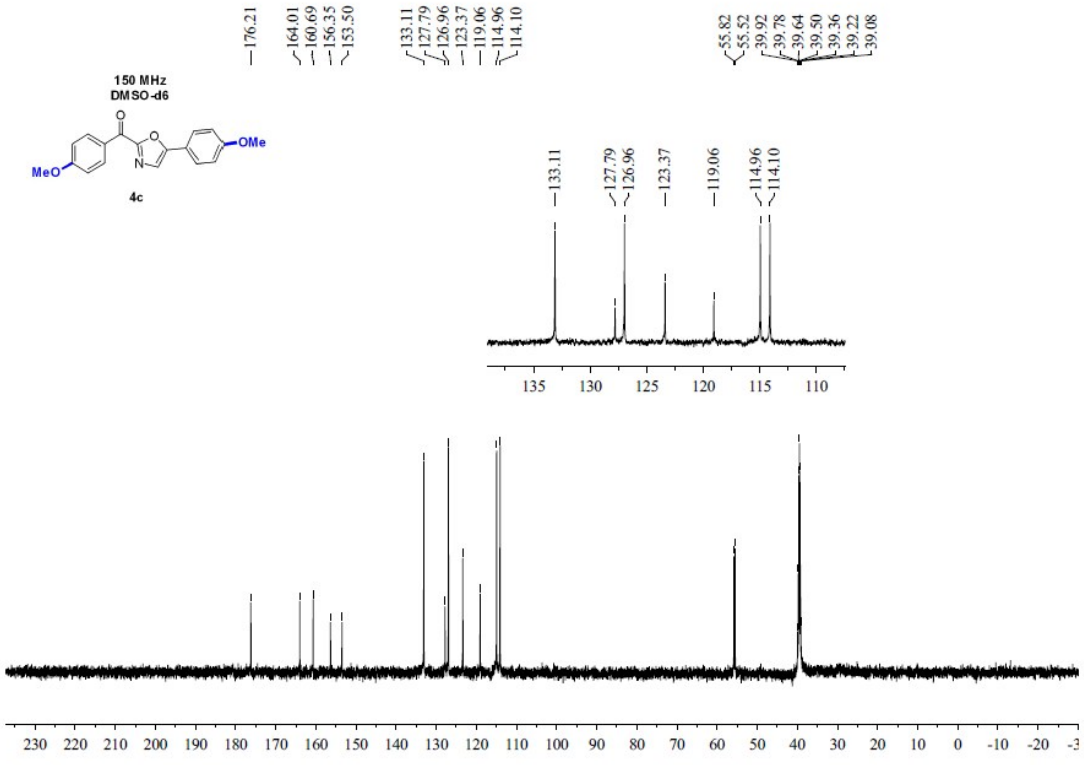

600 MHz
CDCl3
4a
fl (ppm)

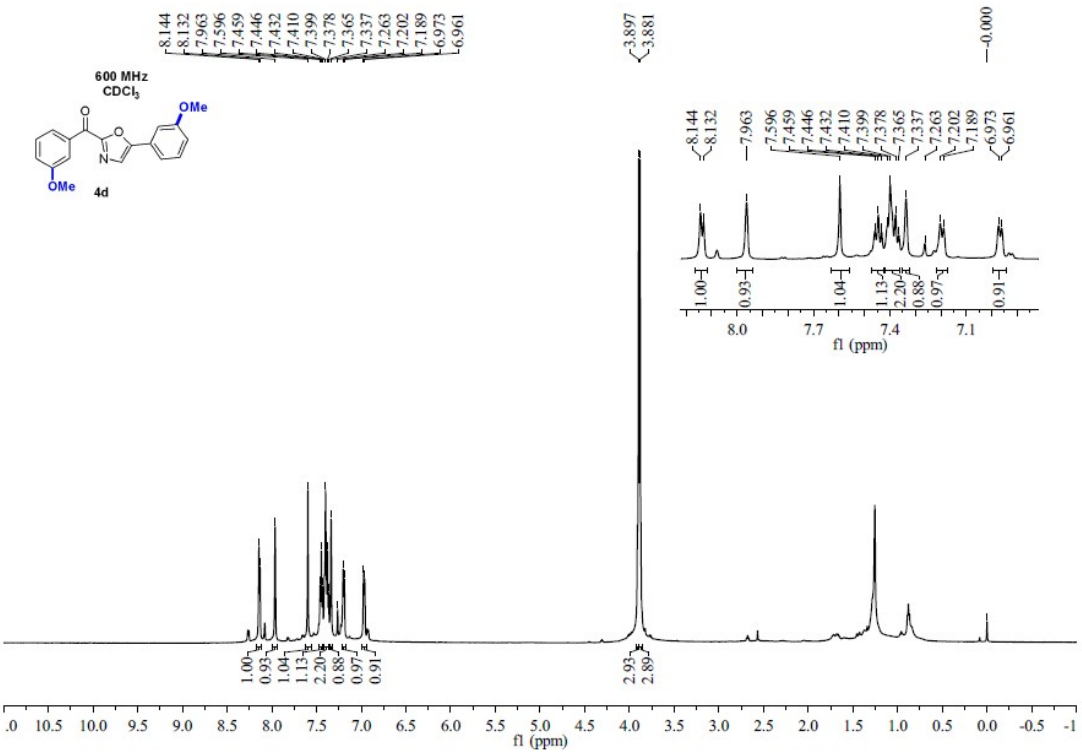

150 MHz
CDCl3
4a
fl (ppm)

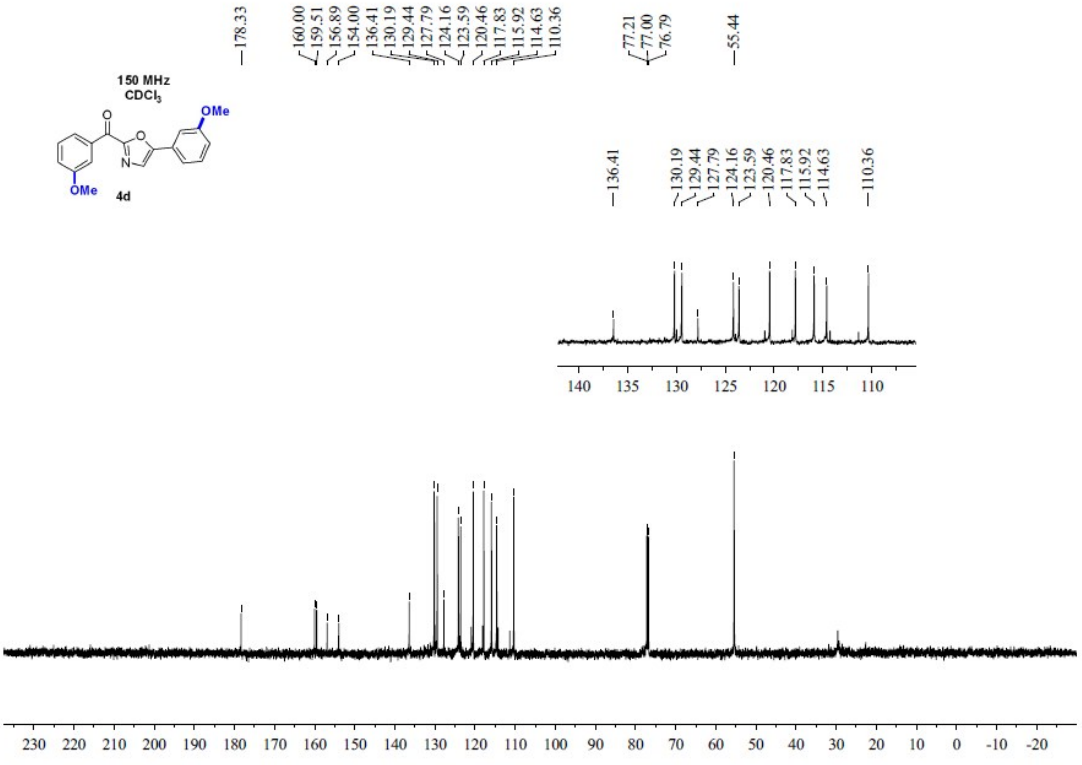

600 MHz
CDCl3
4b
8.393
8.380
7.727
7.714
7.553
7.341
7.327
7.285
7.272
7.262
2.452
2.405
0.000
2.00
2.20
1.09
2.18
1.96
3.12
3.02
fl (ppm)

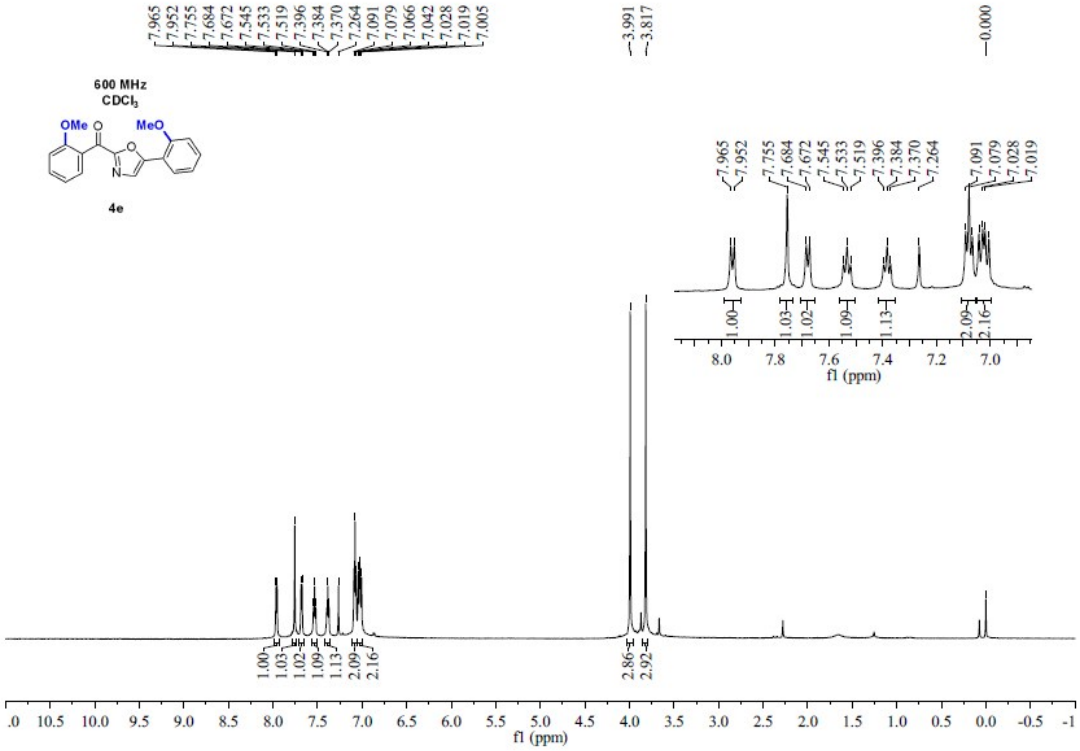

150 MHz
CDCl3
4b
178.31
156.83
154.24
144.74
140.21
132.79
130.83
129.74
129.15
125.27
123.90
123.24
77.21
77.00
76.79
21.80
21.48
fl (ppm)

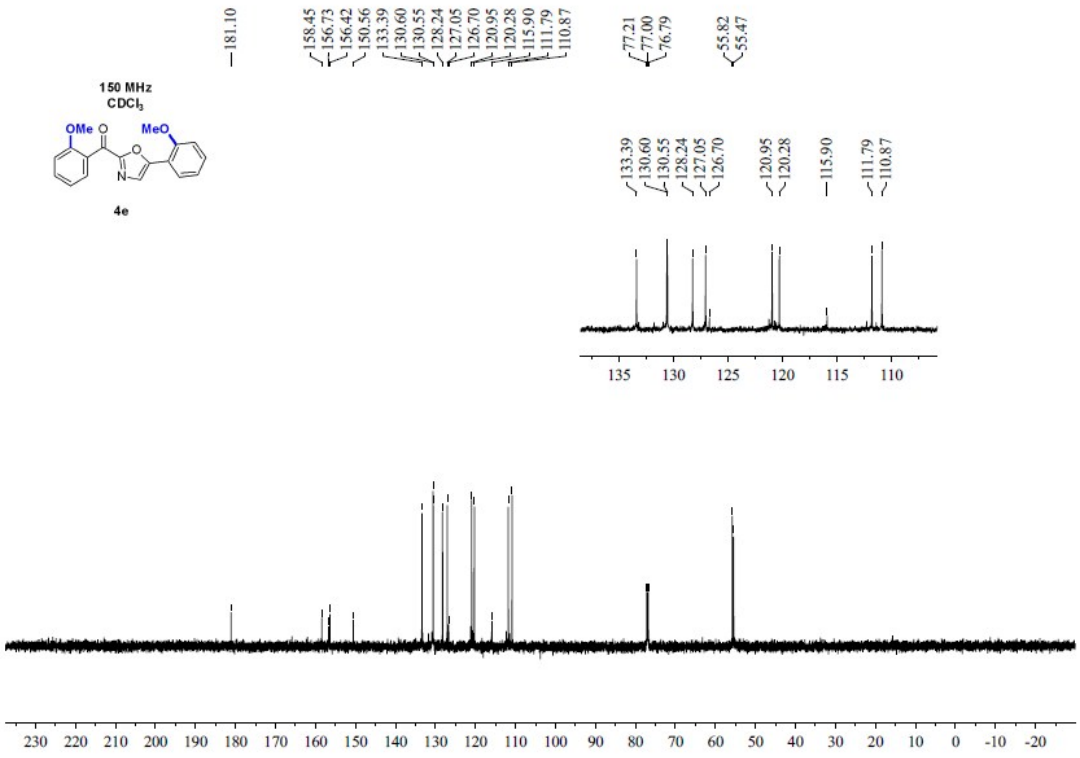

600 MHz
CDCl3
MeO
OMe
4c
8.538
8.525
7.765
7.752
7.474
7.268
7.013
6.999
6.989
6.976
3.901
3.858
0.000
2.00
2.09
1.07
4.03
2.92
2.90
fl (ppm)

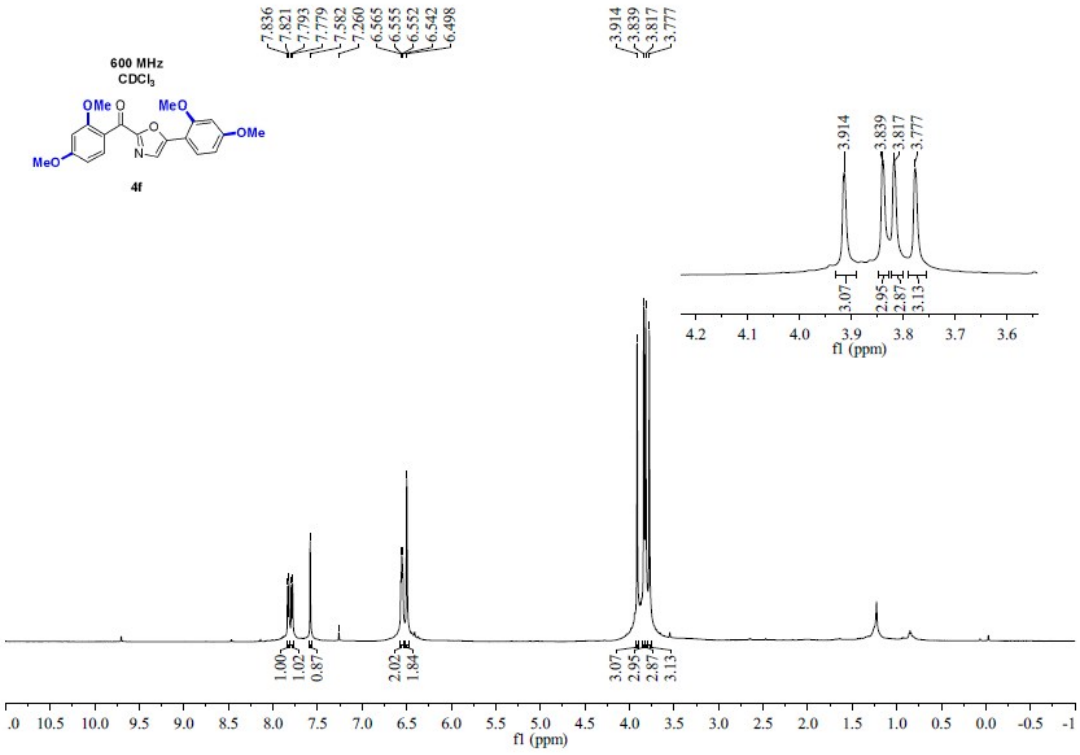

150 MHz
DMSO-d6
MeO
OMe
4c
176.21
164.01
160.69
156.35
153.50
133.11
127.79
126.96
123.37
119.06
114.96
114.10
55.82
55.52
39.92
39.78
39.64
39.50
39.36
39.22
39.08
fl (ppm)

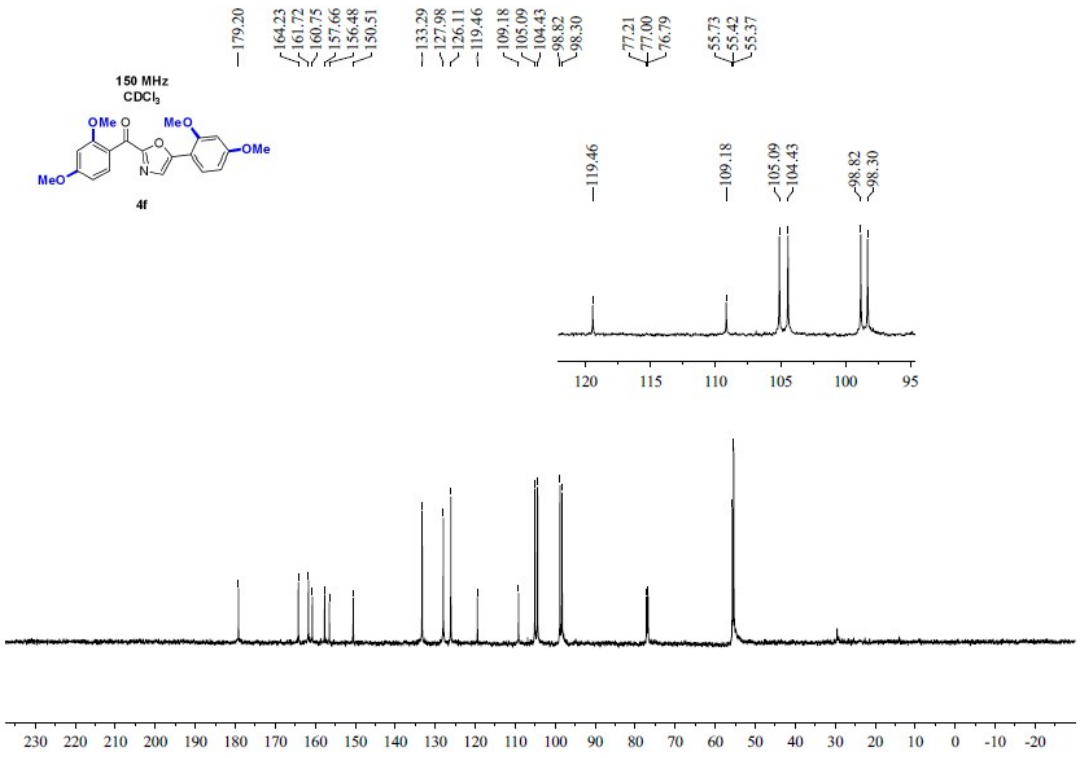

8.144
8.132
7.963
7.596
7.459
7.446
7.432
7.410
7.399
7.378
7.365
7.337
7.263
7.202
7.189
6.973
6.961
3.897
3.881
-0.000
600 MHz
CDCl3
OMe
OMe
4d
1.00
0.93
1.04
1.13
2.20
0.88
0.97
0.91
2.93
2.89
f1 (ppm)

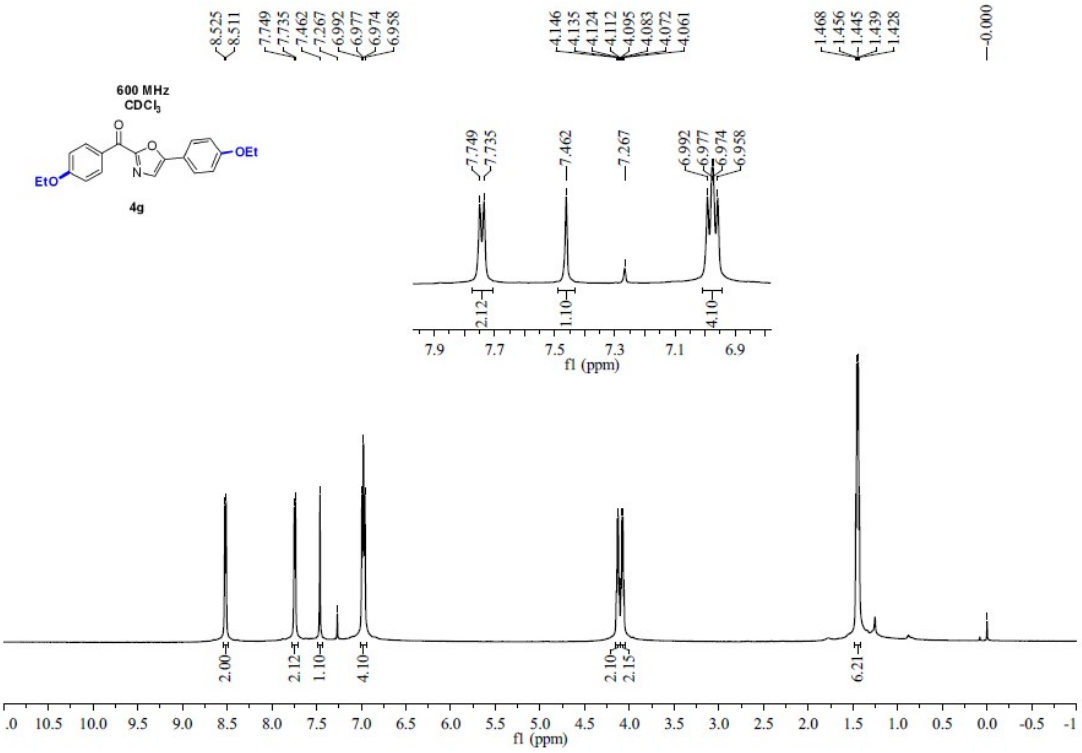

178.33
160.00
159.51
156.89
154.00
136.41
130.19
129.44
127.79
124.16
123.59
120.46
117.83
115.92
114.63
110.36
77.21
77.00
76.79
55.44
150 MHz
CDCl3
OMe
OMe
4d
f1 (ppm)

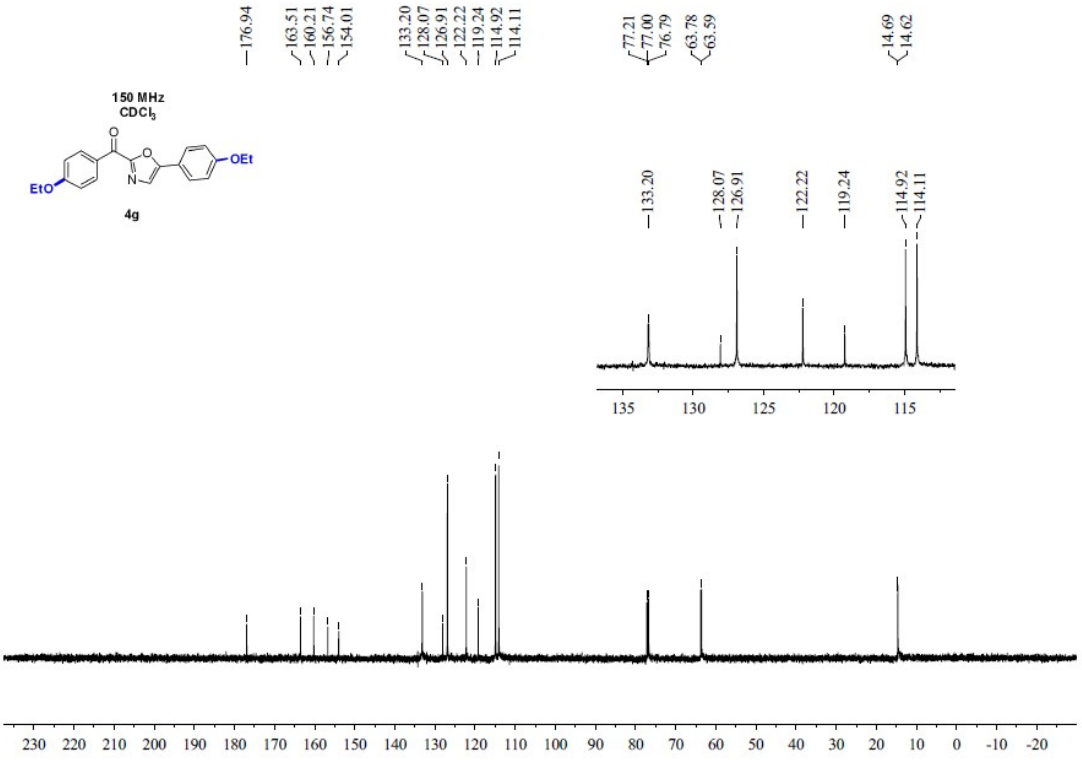

600 MHz
CDCl3
4e
fl (ppm)

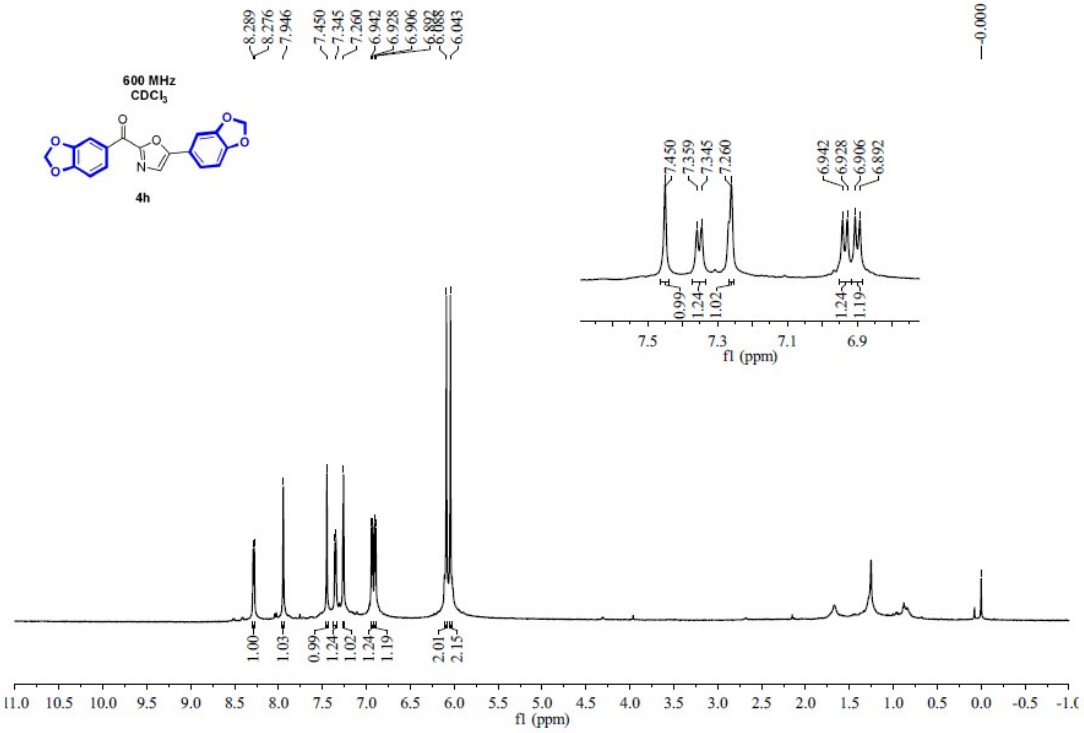

150 MHz
CDCl3
4e

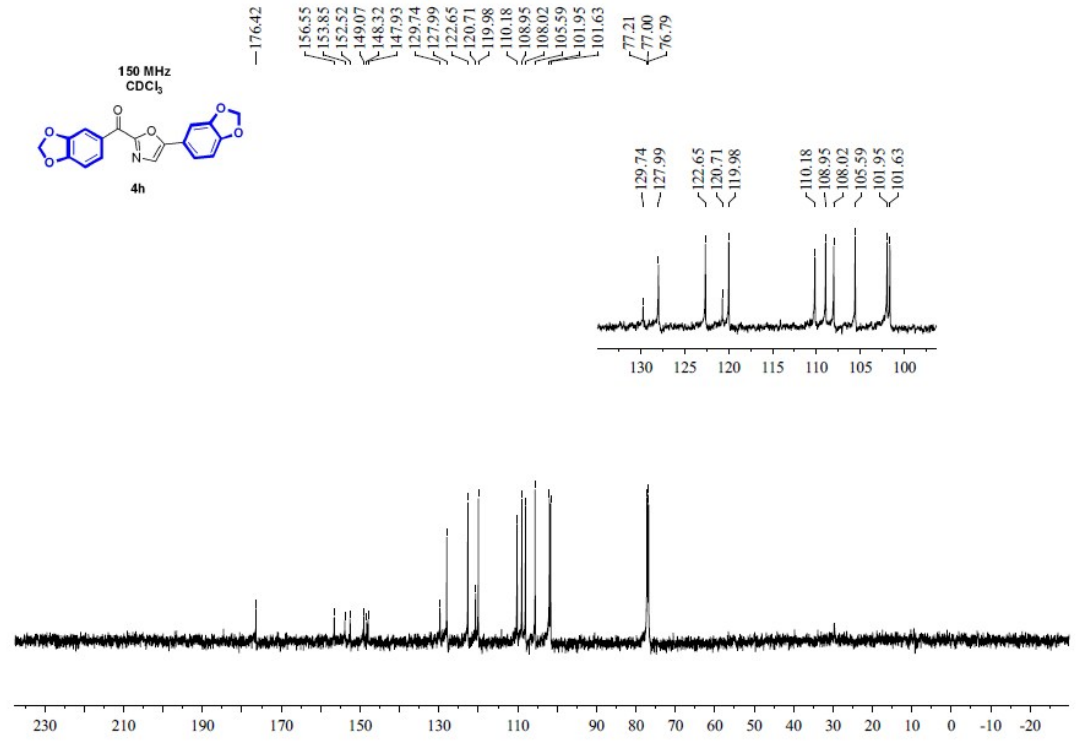

600 MHz
CDCl3
4f
7.836
7.821
7.793
7.779
7.582
7.260
6.565
6.555
6.552
6.542
6.498
3.914
3.839
3.817
3.777
1.00
1.02
0.87
2.02
1.84
3.07
2.95
2.87
3.13
f1 (ppm)

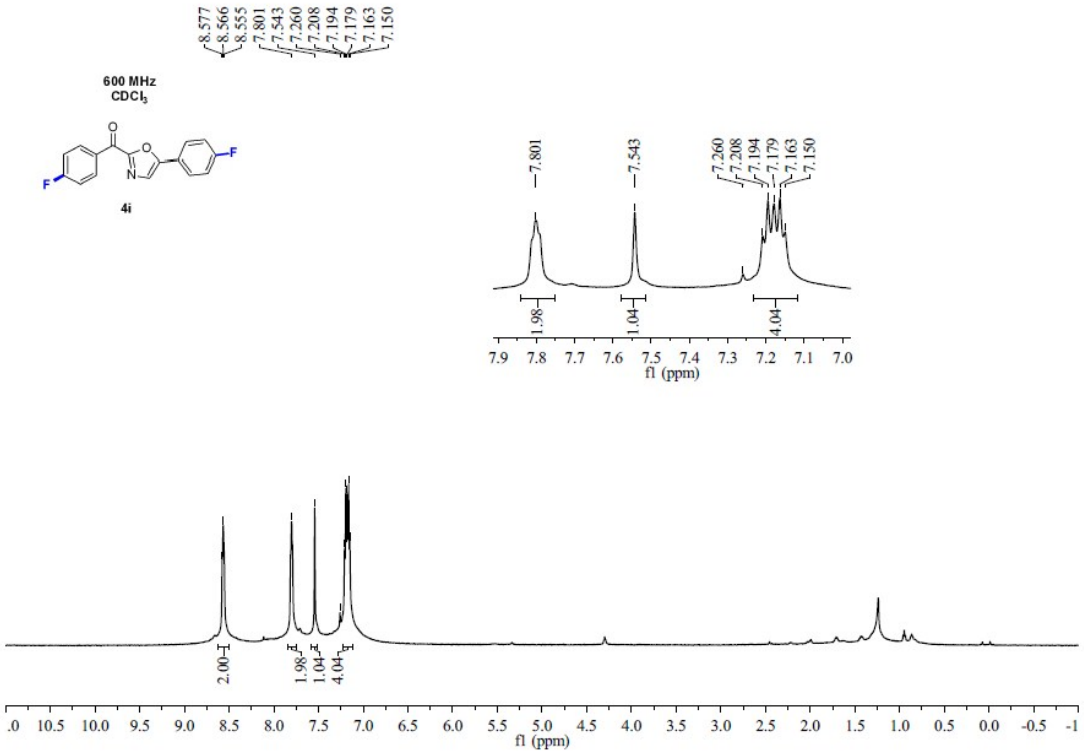

150 MHz
CDCl3
4f
179.20
164.23
161.72
160.75
157.66
156.48
150.51
133.29
127.98
126.11
119.46
109.18
105.09
104.43
98.82
98.30
77.21
77.00
76.79
55.73
55.42
55.37
f1 (ppm)

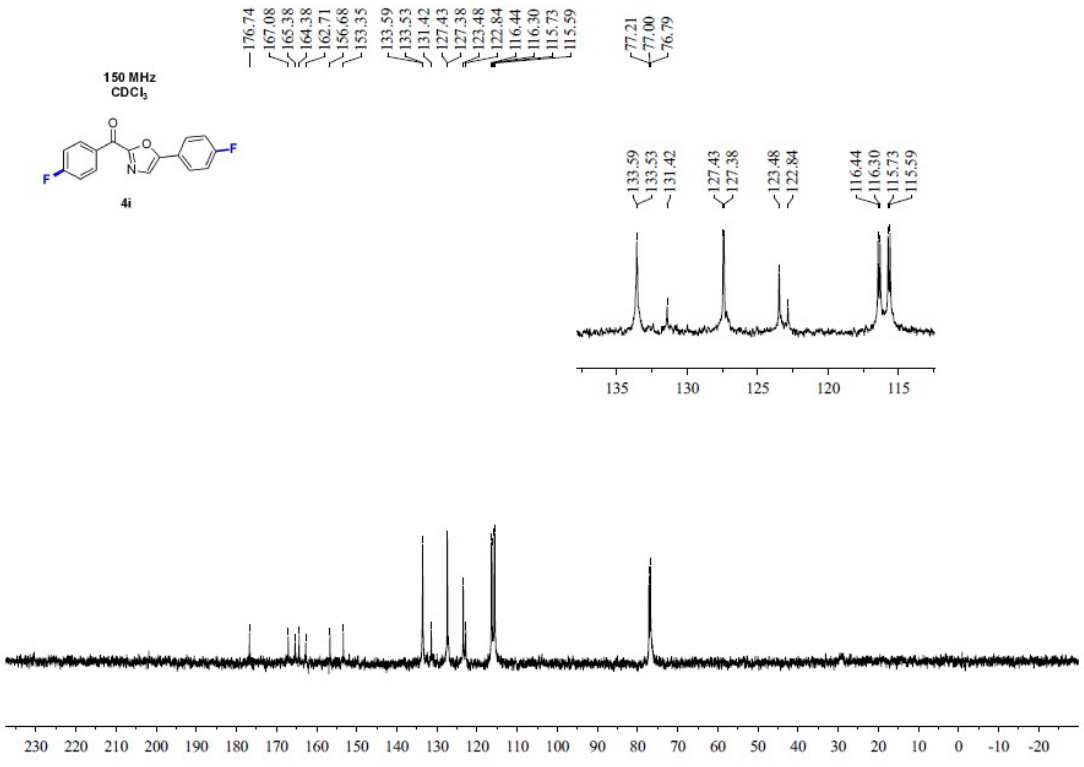

600 MHz
CDCl3
EtO
OEt
4g
f1 (ppm)

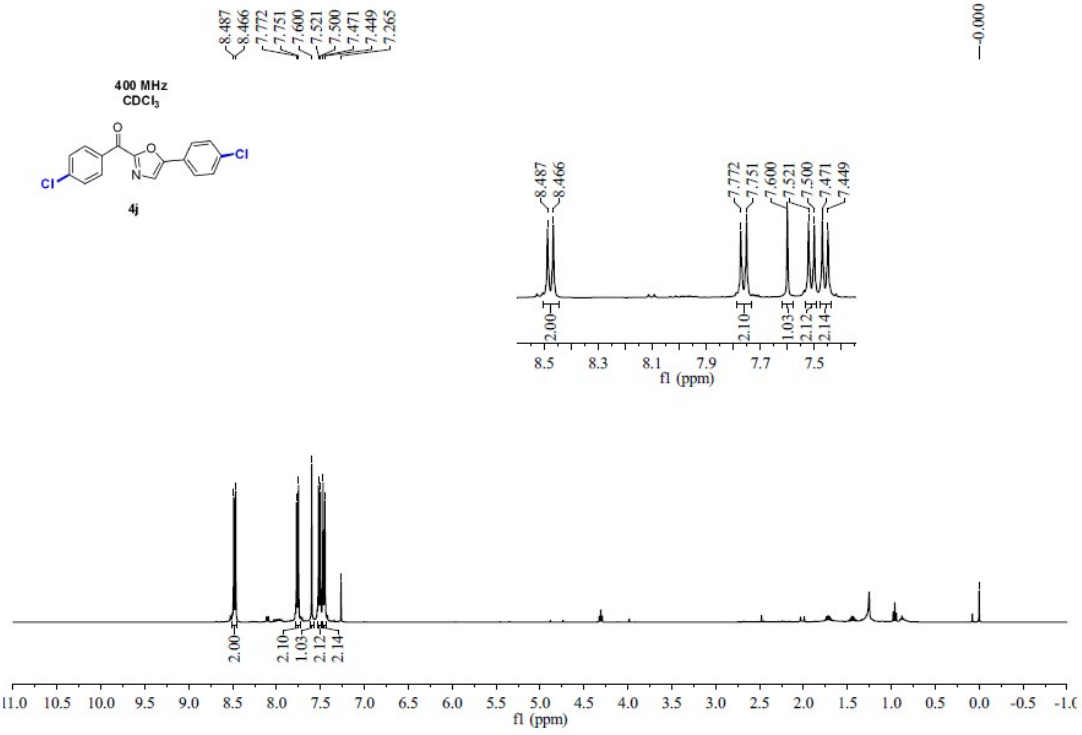

150 MHz
CDCl3
EtO
OEt
4g

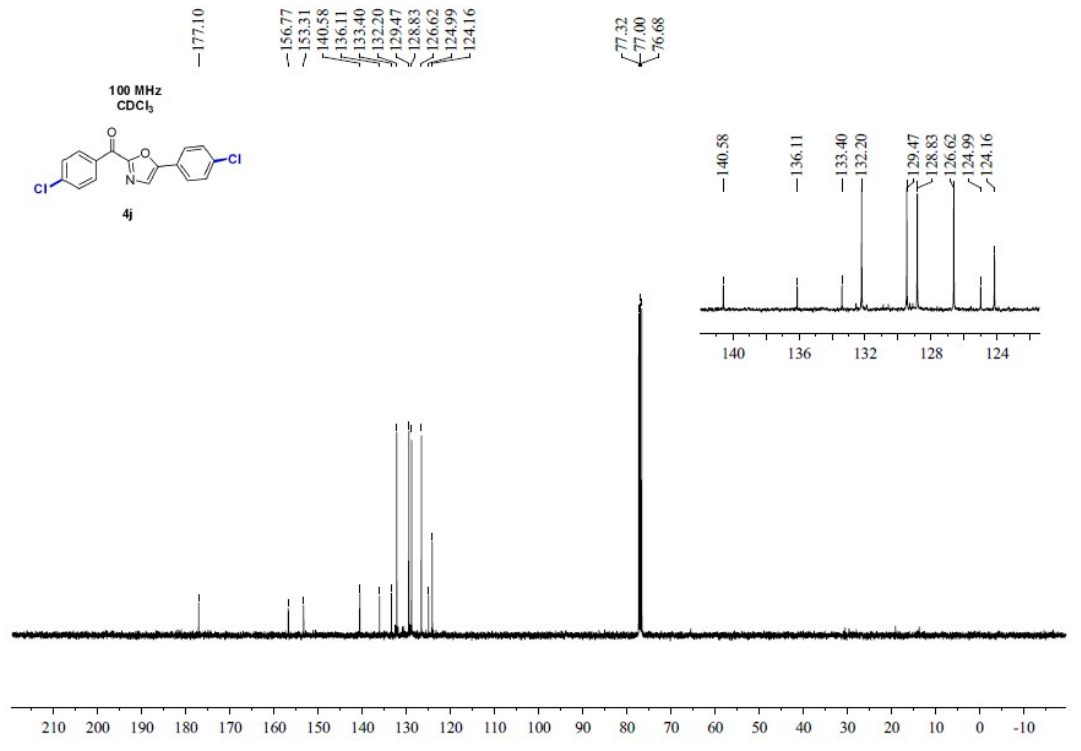

600 MHz
CDCl3
4h
8.289
8.276
7.946
7.450
7.345
7.260
6.942
6.928
6.906
6.892
6.888
6.043
-0.000
1.00
1.03
0.99
1.24
1.02
1.24
1.19
2.01
2.15
f1 (ppm)

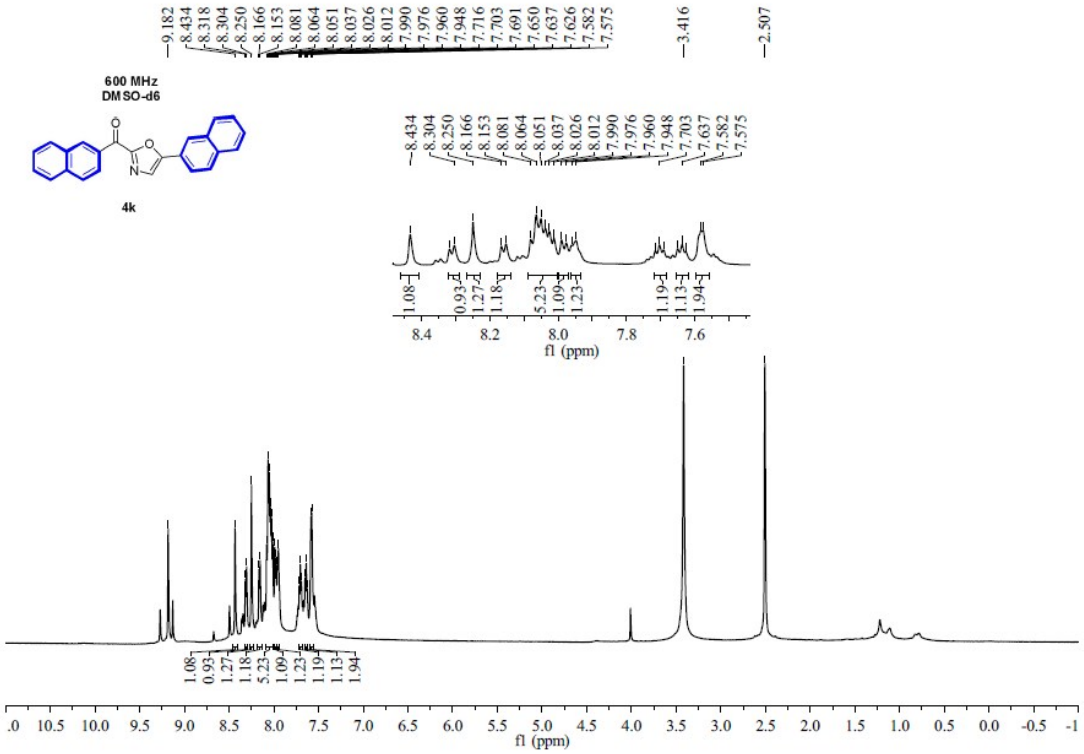

150 MHz
CDCl3
4h
176.42
156.55
153.85
152.52
149.07
148.32
147.93
129.74
127.99
122.65
120.71
119.98
110.18
108.95
108.02
105.59
101.95
101.63
77.21
77.00
76.79

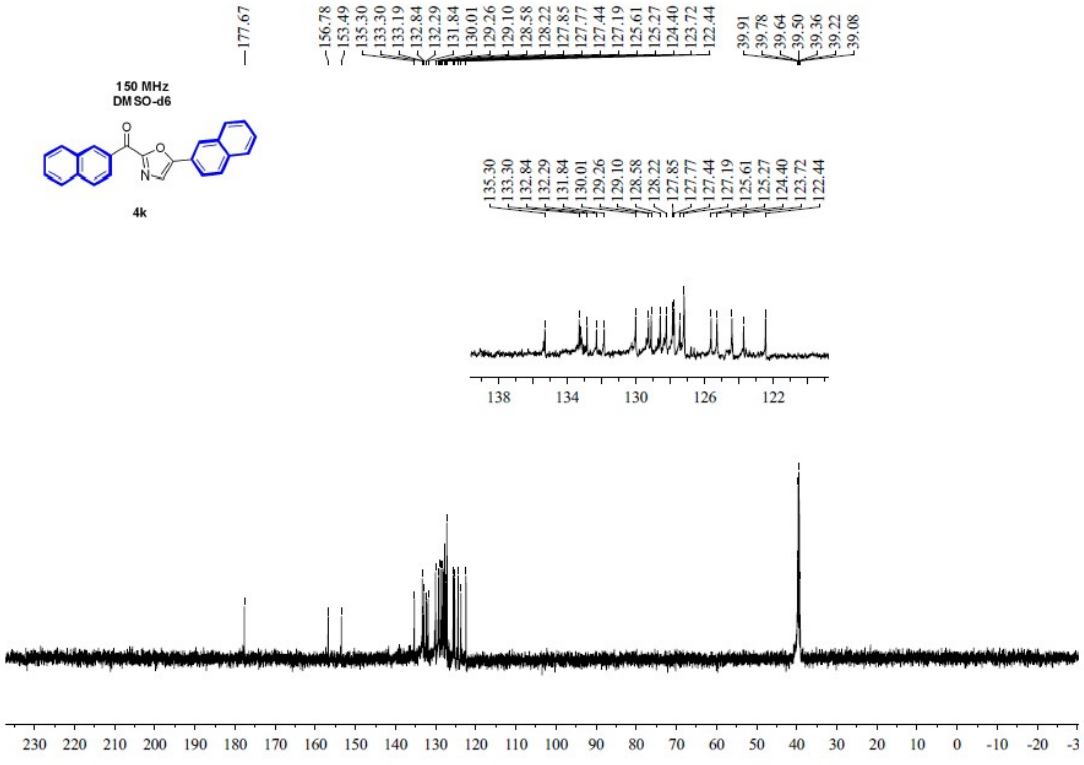

8.577
8.566
8.555
7.801
7.543
7.260
7.208
7.194
7.179
7.163
7.150
600 MHz
CDCl3
4i
F
F
O
N
7.801
7.543
7.260
7.208
7.194
7.179
7.163
7.150
1.98
1.04
4.04
7.9 7.8 7.7 7.6 7.5 7.4 7.3 7.2 7.1 7.0
f1 (ppm)
2.00
1.98
1.04
4.04
.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 -0.5 -1
f1 (ppm)

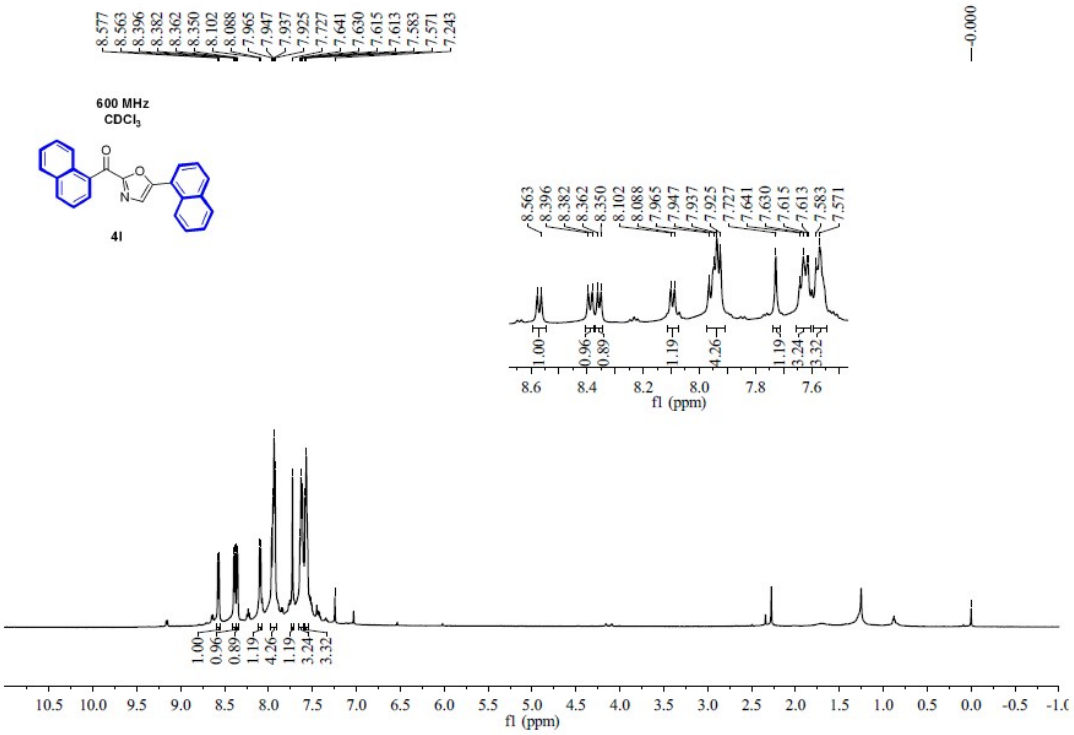

176.74
167.08
165.38
164.38
162.71
156.68
153.35
133.59
133.53
131.42
127.43
127.38
123.48
122.84
116.44
116.30
115.73
115.59
77.21
77.00
76.79
150 MHz
CDCl3
4i
F
F
O
N
133.59
133.53
131.42
127.43
127.38
123.48
122.84
116.44
116.30
115.73
115.59
135 130 125 120 115
230 220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 -10 -20

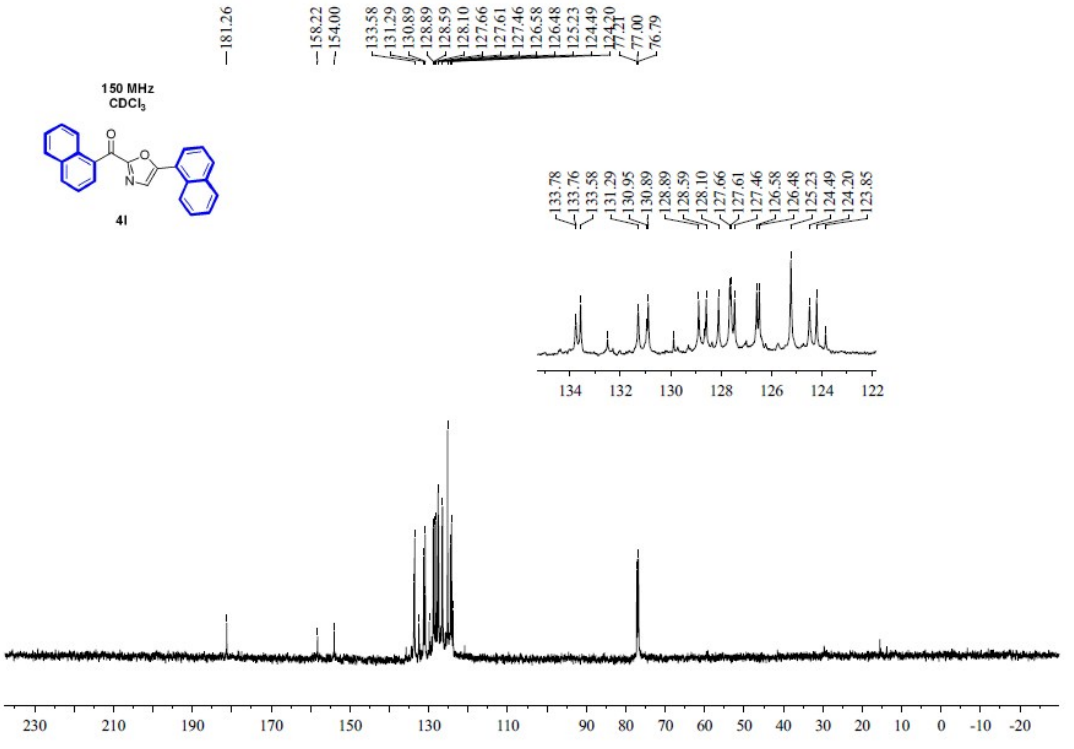

8.487
8.466
7.772
7.751
7.600
7.521
7.500
7.471
7.449
7.265
-0.000
400 MHz
CDCl3
Cl
O
N
O
Cl
4j
2.00
2.10
1.03
2.12
2.14
fl (ppm)

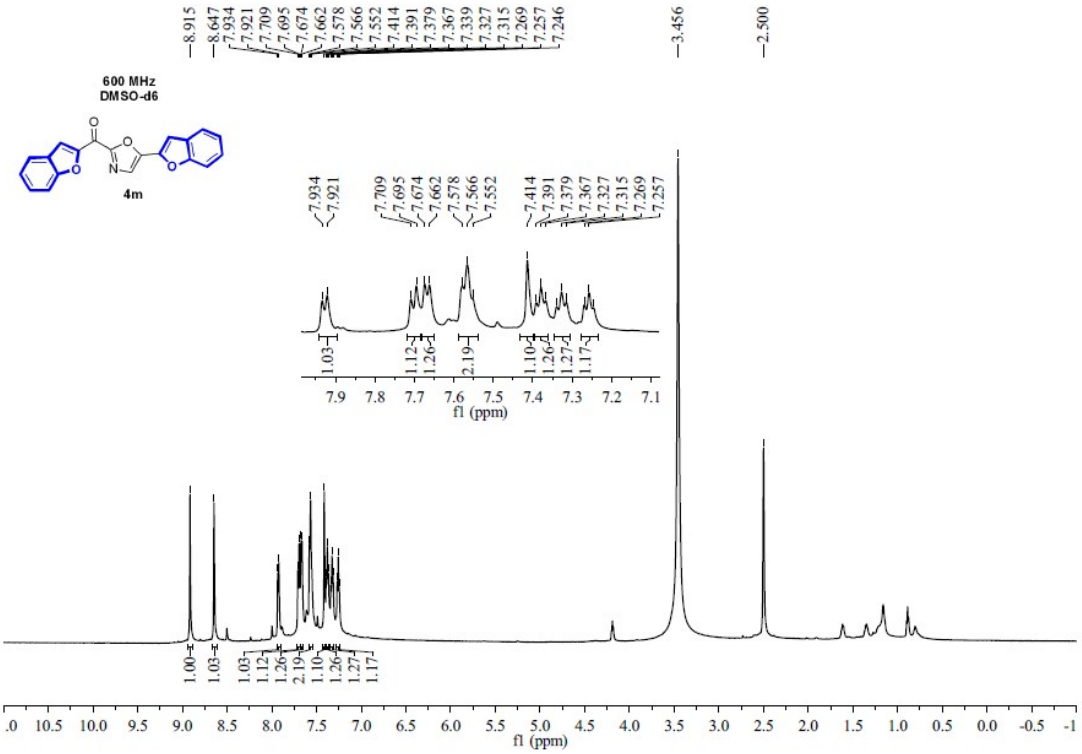

177.10
156.77
153.31
140.58
136.11
133.40
132.20
129.47
128.83
126.62
124.99
124.16
77.32
77.00
76.68
100 MHz
CDCl3
Cl
O
N
O
Cl
4j
fl (ppm)

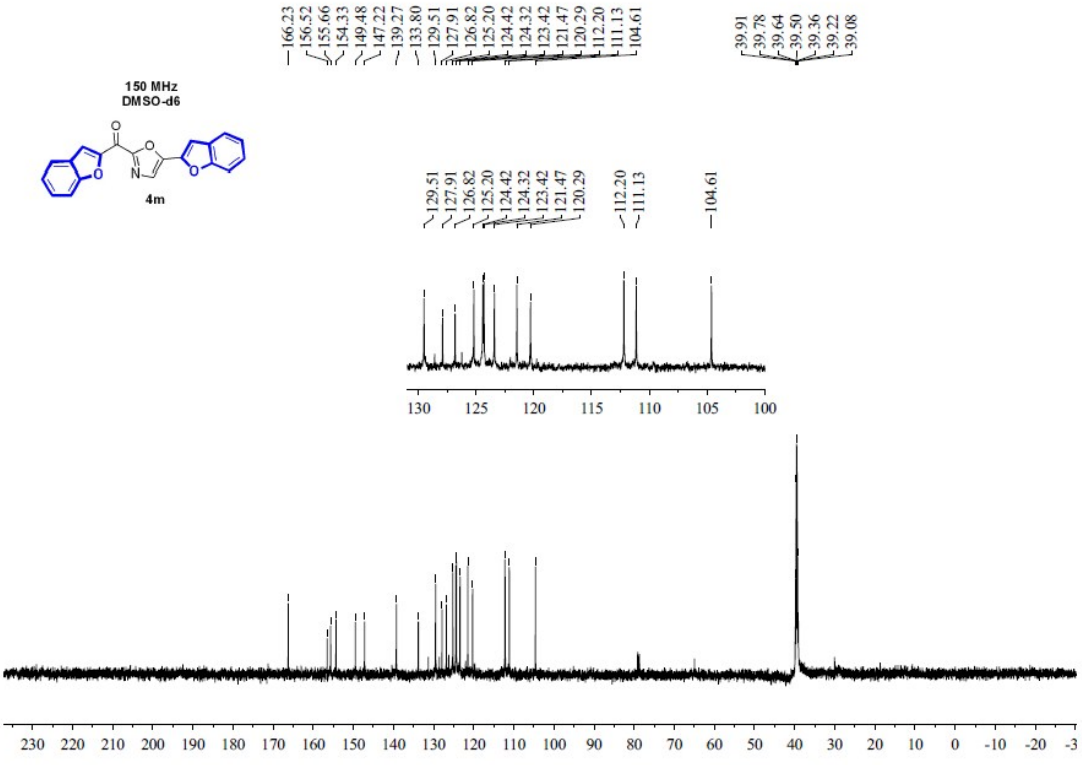

600 MHz
DMSO-d6
4k
fl (ppm)

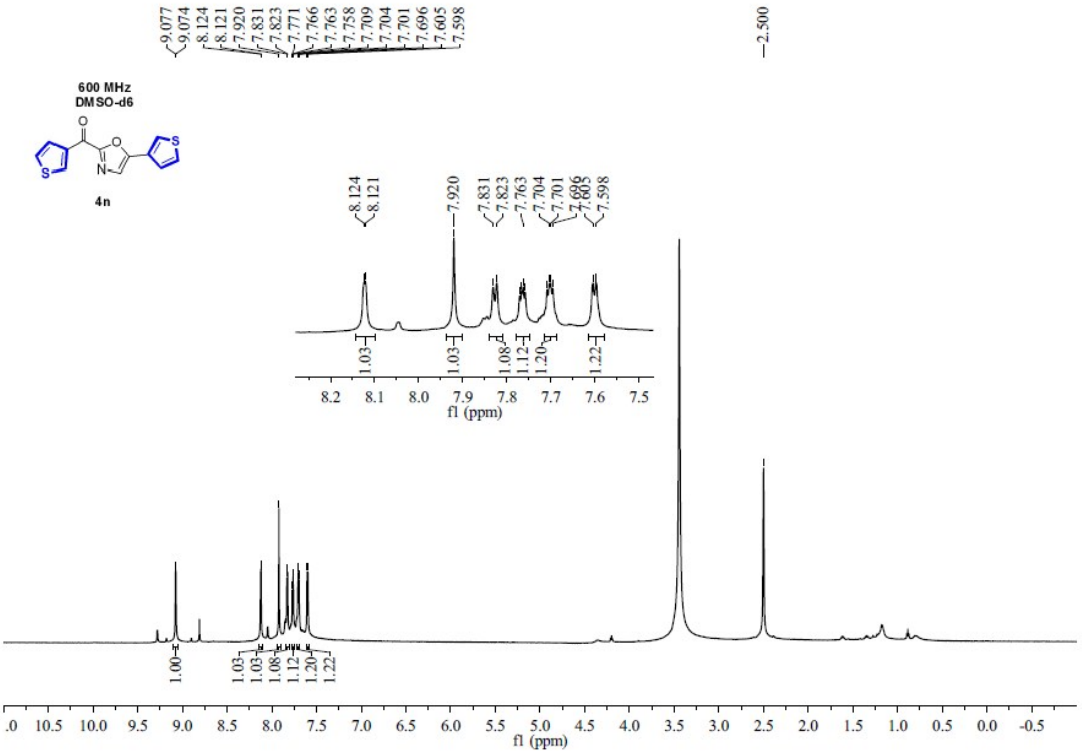

150 MHz
DMSO-d6
4k

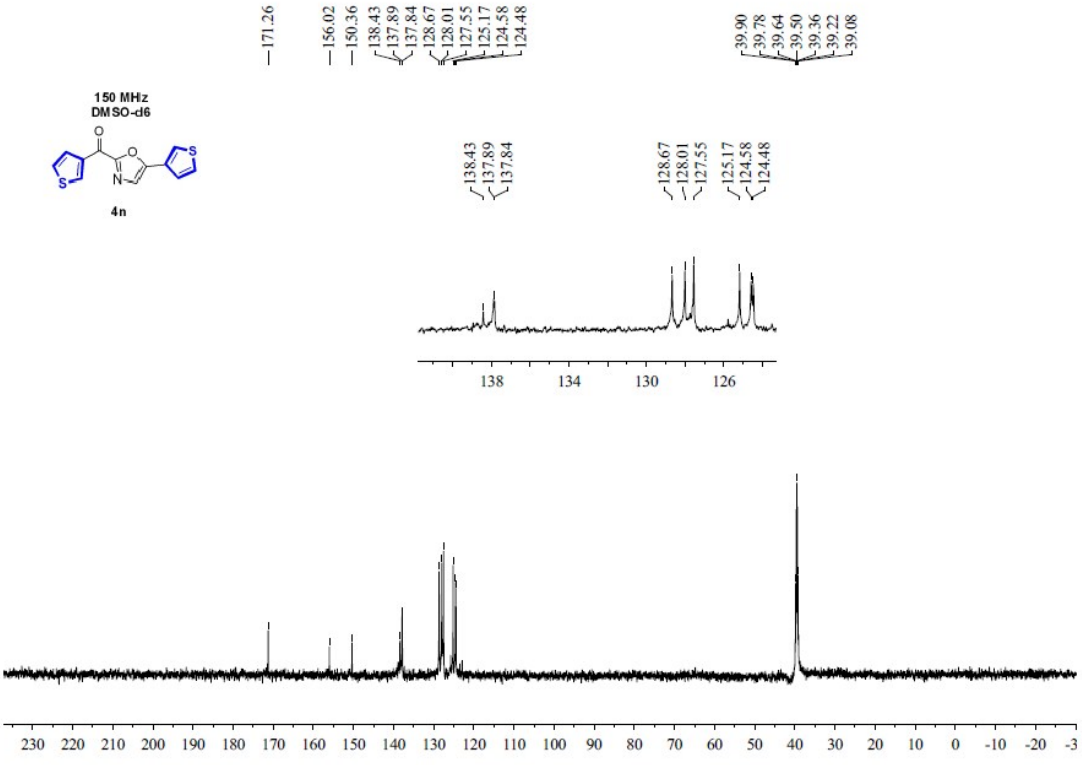

600 MHz
CDCl3
4l
fl (ppm)

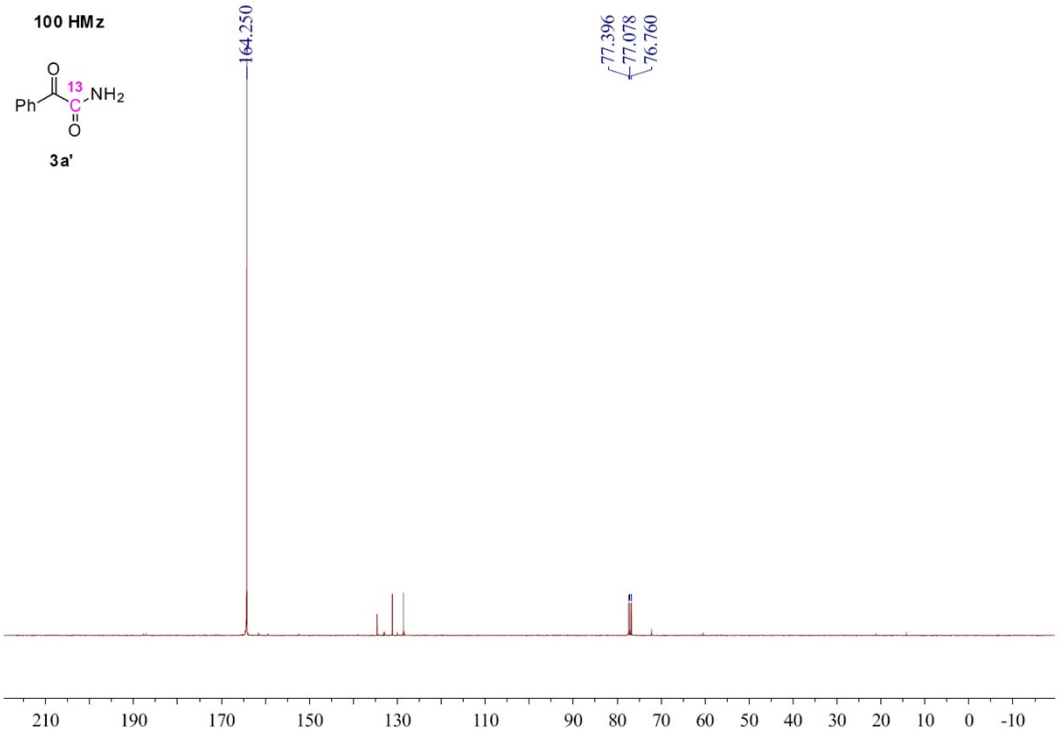

150 MHz
CDCl3
4l


600 MHz
DMSO-d6
4m
fl (ppm)

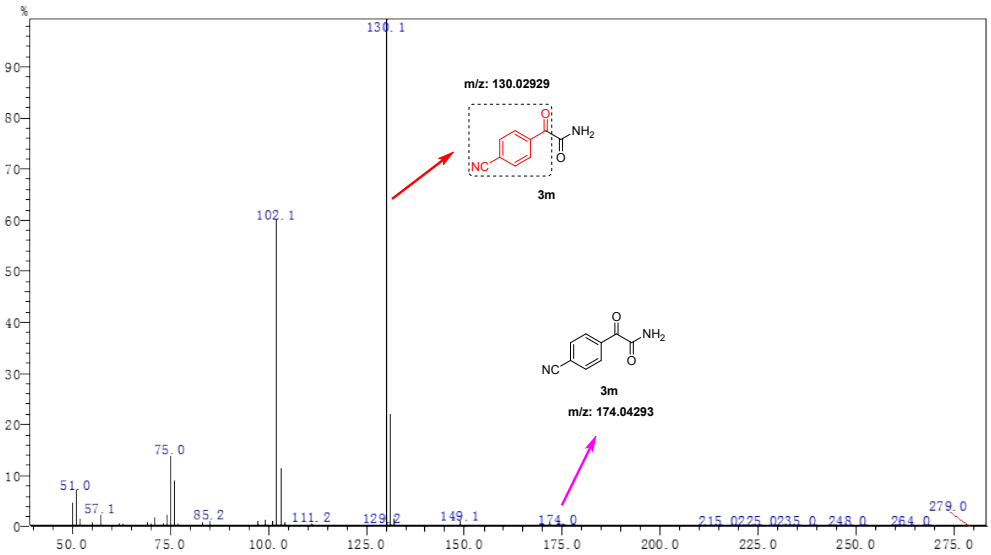

150 MHz
DMSO-d6
4m
fl (ppm)

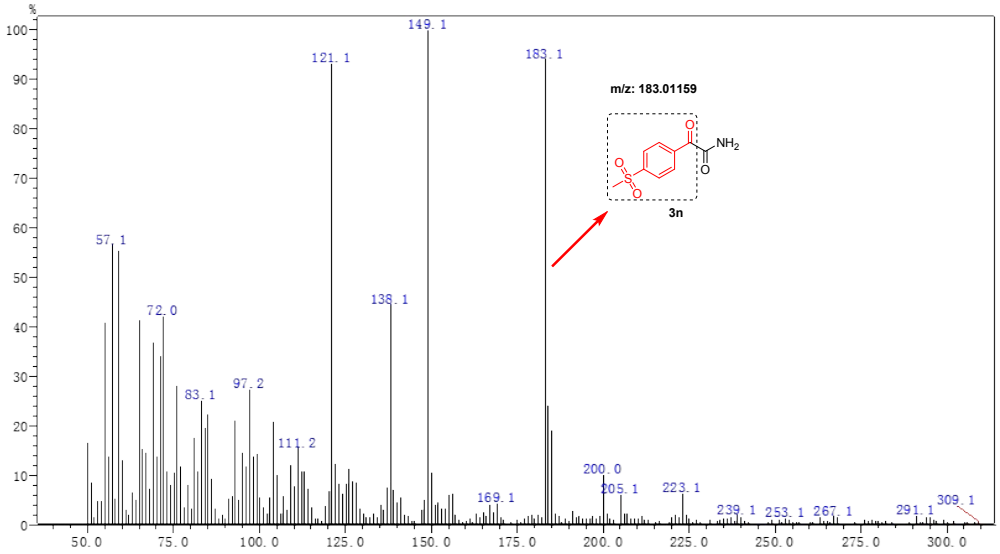

600 MHz
DMSO-d6
4n
9.077
9.074
8.124
8.121
7.920
7.831
7.823
7.771
7.766
7.763
7.758
7.709
7.704
7.701
7.696
7.605
7.598
2.500
1.00
1.03
1.03
1.08
1.12
1.20
1.22
f1 (ppm)

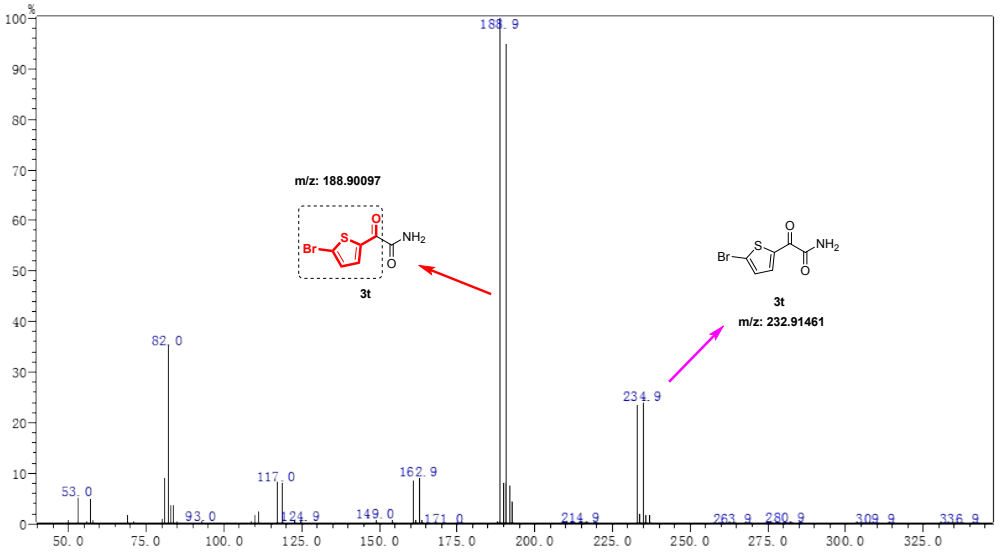

150 MHz
DMSO-d6
4n
171.26
156.02
150.36
138.43
137.89
137.84
128.67
128.01
127.55
125.17
124.58
124.48
39.90
39.78
39.64
39.50
39.36
39.22
39.08
f1 (ppm)



9. The products of 3m, 3n, 3t were detected by GC-MS




%
100
90
80
70
60
50
40
30
20
10
0
149. 1
121. 1
183. 1
57. 1
72. 0
138. 1
83. 1
97. 2
111. 2
200. 0
205. 1
223. 1
169. 1
239. 1
253. 1
267. 1
291. 1
309. 1
50. 0
75. 0
100. 0
125. 0
150. 0
175. 0
200. 0
225. 0
250. 0
275. 0
300. 0
m/z: 183.01159
O
NH2
O
O
S
O
3n


%
100
90
80
70
60
50
40
30
20
10
0
188. 9
m/z: 188.90097
Br
S
O
NH2
O
3t
82. 0
53. 0
93. 0
117. 0
124. 9
162. 9
149. 0
171. 0
214. 9
234. 9
263. 9
280. 9
309. 9
336. 9
50. 0
75. 0
100. 0
125. 0
150. 0
175. 0
200. 0
225. 0
250. 0
275. 0
300. 0
325. 0
Br
S
O
NH2
O
3t
m/z: 232.91461