Electronic Supplementary Material (ESI) for Organic Chemistry Frontiers.

Catalytic one-pot synthesis of 4-(hetero)aryl substituted 5-(2-oxoethyl) oxazol-2(3H)-ones by coupling-isomerization-elimination (CIE) sequence

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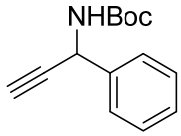
1 Analytical data of the *N*-Boc protected propargyl carbamates 2

The *N*-boc protected propargyl carbamates **2** were prepared accordingly to literature procedures.[1,2]

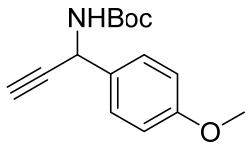
1.1 *tert*-Butyl (1-phenylprop-2-yn-1-yl)carbamate (2a)



$C_{14}H_{17}NO_2$ (MW 231.29)

Colorless solid; Mp 87-88 °C; R_f (petroleum ether/ethyl acetate 20:1) = 0.23. ^{1}H NMR ($CDCl_3$, 500 MHz), δ = 1.46 (s, 9 H), 2.49 (d, *J* = 2.5 Hz, 1 H), 5.1 (br, 1 H), 5.7 (br, 1 H), 7.28-7.33 (m, 1 H), 7.34-7.39 (m, 2 H), 7.50 (d, *J* = 7.6 Hz, 2 H). ^{13}C NMR ($CDCl_3$, 125 MHz), δ = 28.3 (CH_3), 46.1 (CH), 72.9 (C_{quat}), 80.2 (C_{quat}), 82.1 (CH), 126.8 (CH), 128.1 (CH), 128.7 (CH), 138.7 (C_{quat}), 154.7 (C_{quat}). MS (EI), *m/z*: 175 ((M-C_4H_9+H)$^+$, 30), 146 (10), 131 ((M-$C_5H_9O_2$+2H)$^+$, 4), 130 (17), 115 (52), 103 ($C_5H_{11}O_2^+$, 9), 102 ($C_5H_{10}O_2^+$, 2), 57 ($C_4H_9^+$, 100), 41 (27). IR (KBr), $\tilde{\nu}$ [cm^{-1}]: 3357 (s), 3274 (s), 3012 (w), 2980 (w), 2938 (w), 1683 (s), 1515 (s), 1392 (w), 700 (m), 683 (m), 661 (m), 619 (w). Anal. calcd. for $C_{14}H_{17}NO_2$ (231.3): C 72.70, H 7.41, N 6.06; Found: C 72.68, H 7.50, N 5.97.

1.2 *t*ert-Butyl (1-(4-methoxyphenyl)prop-2-yn-1-yl)carbamate (2b)



$C_{15}H_{19}NO_3$ (MW 261.32)

Colorless solid; Mp 91-96 °C; R_f (petroleum ether/ethyl acetate 10:1) = 0.24. ^{1}H NMR ($CDCl_3$, 500 MHz), δ = 1.46 (s, 9 H), 2.48 (d, *J* = 2.5 Hz, 1 H), 3.80 (s, 3 H), 5.0 (br, 1 H), 5.6 (br, 1 H), 6.88 (d, *J* = 8.8 Hz, 2 H), 7.42 (d, *J* = 8.5 Hz, 2 H). ^{13}C NMR ($CDCl_3$, 125 MHz), δ = 28.4 (CH_3), 45.6 (CH), 55.3 (CH_3), 72.7 (C_{quat}), 80.2 (C_{quat}), 82.4 (CH), 114.0 (CH), 128.1 (CH), 130.9 (C_{quat}), 154.7 (C_{quat}), 159.4 (C_{quat}). MS (EI), *m/z*: 261 (M$^+$, 1), 206 (16), 205.6 (11), 205.3 ((M-C_4H_9+H)$^+$, 100), 204 (17), 176 (12), 162 ((M-$C_5H_9O_2$+2H)$^+$, 12), 160 (23), 149 (13), 147 (11), 146 (41), 145.6 (11), 145.3 (63), 134 (12), 133 (25), 109 (15), 102 ($C_5H_{10}O_2^+$, 12), 57 ($C_4H_9^+$, 74), 41 (26). IR (KBr), $\tilde{\nu}$ [cm^{-1}]: 3364 (s), 3273 (s), 2971 (w), 2936 (w), 1684 (s), 1613 (w), 1511 (s), 1391 (w), 653 (w). Anal. calcd. for $C_{15}H_{19}NO_3$ (261.3): C 68.94, H 7.33, N 5.63; Found: C 68.96, H 7.60, N 5.26.

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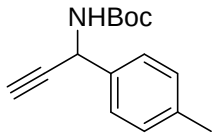
[1] E.-S. Lee, H.-S. Yeom, J.-H. Hwang and S. Shin, *Eur. J. Org. Chem.*, **2007**, 3503.
[2] T. Mecozzi and M. Petrini, *J. Org. Chem.*, 1999, **64**, 8970.

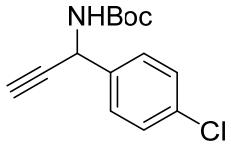
1.3 *tert*-Butyl (1-(*p*-tolyl)prop-2-yn-1-yl)carbamate (2c)



$C_{15}H_{19}NO_2$ (MW 245.32)

Pale brown solid; Mp 91 °C; R_f (petroleum ether/ethyl acetate 20:1) = 0.22. ^{1}H NMR ($CDCl_3$, 300 MHz), δ = 1.46 (s, 9 H), 2.35 (s, 3 H), 2.47 (d, *J* = 2.4 Hz, 1 H), 5.0 (br, 1 H), 5.45-5.75 (m, 1 H), 7.17 (d, *J* = 7.9 Hz, 2 H), 7.39 (d, *J* = 8.0 Hz, 2 H). ^{13}C NMR ($CDCl_3$, 75MHz), δ = 21.5 (CH_3), 28.7 (CH_3), 46.3 (CH), 73.1 (C_{quat}), 80.6 (C_{quat}), 82.7 (CH), 127.1 (CH), 129.7 (CH), 136.2 (C_{quat}), 138.3 (C_{quat}), 155.0 (C_{quat}). MS (EI), *m/z*: 190 (13), 189 ($(M\text{-}C_4H_9+H)^+$, 100), 188 ($(M\text{-}C_4H_9)^+$, 11), 174 ($(M\text{-}C_4H_9\text{-}CH_3+H)^+$, 47), 146 (40), 144 ($(M\text{-}C_5H_9O_2)^+$, 24), 143 (12), 130 (23), 129 ($(M\text{-}C_5H_9O_2\text{-}CH_3)^+$, 61), 128 (19), 118 (10), 117 (18), 57 ($C_4H_9^+$, 40), 41 (12). IR (ATR), $\tilde{\nu}$ [cm^{-1}]: 3354 (w), 3271 (w), 2970 (w), 1686 (s), 1508 (s), 1445 (w), 1389 (w), 675 (s), 654 (s), 613 (m). Anal. calcd. for $C_{15}H_{19}NO_2$ (245.3): C 73.44, H 7.81, N 5.71; Found: C 73.64, H 7.81, N 5.71.

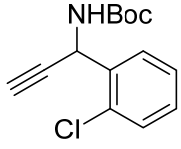
1.4 *tert*-Butyl (1-(4-chlorophenyl)prop-2-yn-1-yl)carbamate (2d)



$C_{14}H_{16}ClNO_2$ (MW 265.74)

Colorless solid; Mp 86 °C; R_f (petroleum ether/ethyl acetate 20:1) = 0.24. ^{1}H NMR ($CDCl_3$, 500 MHz), δ = 1.45 (s, 9 H), 2.50 (d, *J* = 2.5 Hz, 1 H), 5.1 (br, 1 H), 5.6 (br, 1 H), 7.33 (d, *J* = 8.5 Hz, 2 H), 7.44 (d, *J* = 8.2 Hz, 2 H). ^{13}C NMR ($CDCl_3$, 125 MHz), δ = 28.3 (CH_3), 45.6 (CH), 73.4 (C_{quat}), 80.5 (C_{quat}), 81.6 (CH), 128.3 (CH), 128.8 (CH), 134.0 (C_{quat}), 137.4 (C_{quat}), 154.7 (C_{quat}). MS (EI), *m/z*: 265 ($M(^{35}Cl)^+$), 211 ($(M\text{-}C_4H_9+H)^+$ (^{37}Cl), 10), 209 ($(M\text{-}C_4H_9+H)^+$ (^{35}Cl), 31), 174 (15), 167 ($(M\text{-}C_5H_9O_2+2H)^+$ (^{37}Cl), 1), 165 ($(M\text{-}C_5H_9O_2+2H)^+$ (^{35}Cl), 2), 151 (9), 149 (28), 146 (15), 102 ($C_5H_{10}O_2^+$, 1), 57 ($C_4H_9^+$, 100), 41 (26). IR (KBr), $\tilde{\nu}$ [cm^{-1}]: 3352 (m), 3281 (m), 3008 (w), 2990 (w), 2974 (w), 2936 (w), 1687 (s), 1515 (s), 1445 (m), 1390 (m), 671 (m), 647 (m). Anal. calcd. for $C_{14}H_{16}ClNO_2$ (265.7): C 63.28, H 6.07, N 5.27; Found: C 63.43, H 6.10, N 5.15.

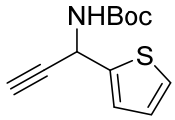
1.5 *tert*-Butyl (1-(2-chlorophenyl)prop-2-yn-1-yl)carbamate (2e)



$C_{14}H_{16}ClNO_2$ (MW 265.74)

Colorless solid; Mp 90-93 °C; R_f (petroleum ether/ethyl acetate 20:1) = 0.24. ^{1}H NMR ($CDCl_3$, 300 MHz), δ = 1.40 (s, 9 H), 2.43 (d, *J* = 2.4 Hz, 1 H), 5.1 (br, 1 H), 5.8 (d, *J* = 7.4 Hz, 1 H), 7.18-7.30 (m, 2 H), 7.31-7.40 (m, 1 H), 7.54-7.62 (m, 1 H). ^{13}C NMR ($CDCl_3$, 75MHz), δ = 28.4 (CH_3), 44.7 (CH), 73.0 (C_{quat}), 80.5 (C_{quat}), 81.4 (CH), 127.3 (CH), 128.7 (CH), 129.7 (CH), 130.2 (CH), 133.3 (C_{quat}), 136.3 (C_{quat}), 154.4 (C_{quat}). MS (EI), *m/z*: 230 ((M-Cl)$^+$, 5), 210 ((M(^{37}Cl)-C_4H_9)$^+$, 2), 208 ((M(^{35}Cl)-C_4H_9)$^+$, 6), 174 ((M-Cl-C_4H_9+H)$^+$, 100), 151 ((M(^{37}Cl)-$C_5H_{10}NO_2$)$^+$, 10), 149 ((M(^{35}Cl)-$C_5H_{10}NO_2$)$^+$, 30), 57 ($C_4H_9^+$, 23). IR (ATR), $\tilde{\nu}$ [cm^{-1}]: 3328 (w), 3308 (w), 2986 (w), 2968 (w), 2930 (w), 1674 (s), 1645 (w), 1439 (w), 1391 (w), 665 (s), 637 (s), 608 (m). Anal. calcd. for $C_{14}H_{16}ClNO_2$ (265.7): C 63.28, H 6.07, N 5.27; Found: C 63.54, H 6.06, N 5.21.

1.6 *tert*-Butyl (1-(thiophen-2-yl)prop-2-yn-1-yl)carbamate (2f)

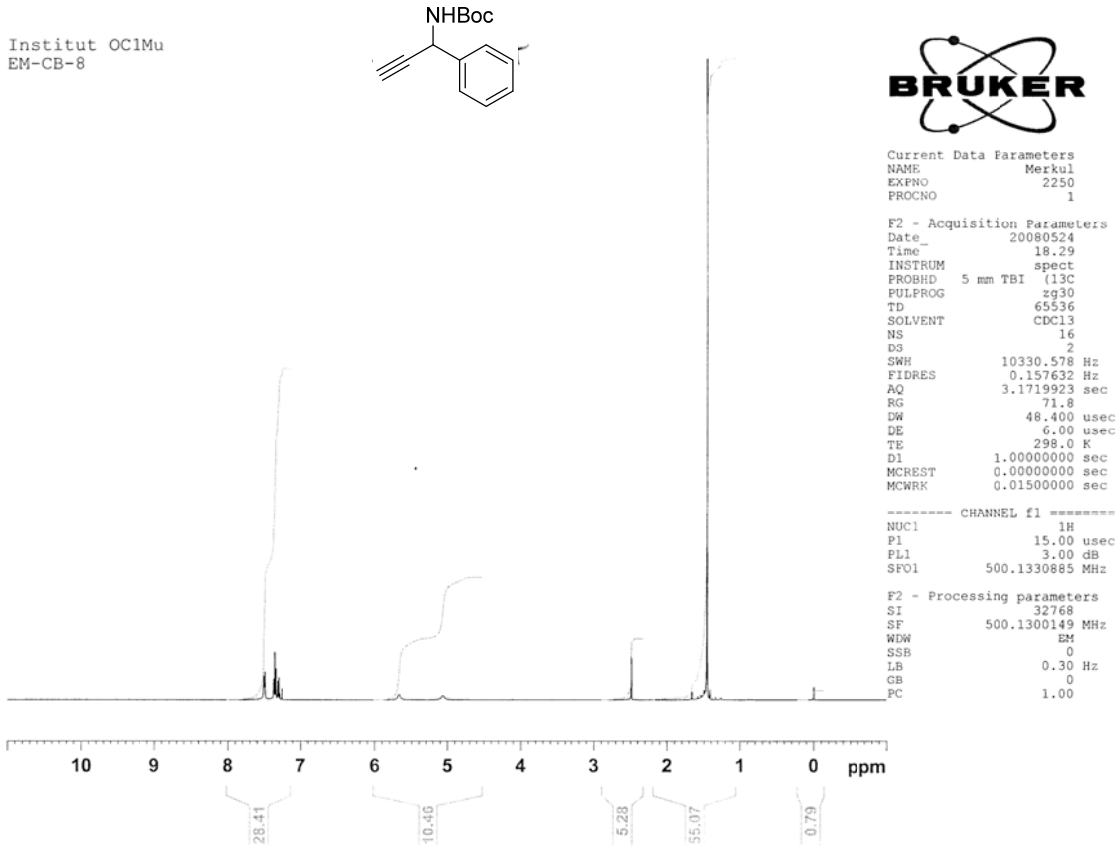


$C_{12}H_{15}NO_2S$ (MW 237.32)

Colorless solid; Mp 62 °C; R_f (petroleum ether/ethyl acetate 20:1) = 0.18. ^{1}H NMR ($CDCl_3$, 300 MHz), δ = 1.47 (s, 9 H), 2.50 (d, *J* = 2.4 Hz, 1 H), 5.1 (s, 1 H), 5.9 (br, 1 H), 6.95 (dd, *J* = 5.1 Hz, *J* = 3.5 Hz, 1 H), 7.17 (dd, *J* = 3.5 Hz, *J* = 1.2 Hz, 1 H), 7.25 (dd, *J* = 5.1 Hz, *J* = 1.2 Hz, 1 H). ^{13}C NMR ($CDCl_3$, 75MHz), δ = 28.5 (CH_3), 42.3 (CH), 72.5 (C_{quat}), 80.7 (C_{quat}), 81.6 (CH), 125.8 (CH), 125.9 (CH), 126.9 (CH), 142.7 (C_{quat}), 154.5 (C_{quat}). MS (EI), *m/z*: 237 (M$^+$, 0.36), 182 (11), 181 ((M-C_4H_9+H)$^+$, 100), 180 (13), 136 ((M-$C_5H_9O_2$)$^+$, 37), 135 (13), 125 (17), 121 ((M-$C_5H_{10}NO_2$)$^+$, 75), 111 (25), 110 (18), 109 (19), 57 ($C_4H_9^+$, 51), 41 (17). IR (ATR), $\tilde{\nu}$ [cm^{-1}]: 3292 (m), 2982 (w), 1678 (s), 1516 (s), 1433 (w), 1393 (w), 706 (s), 679 (s), 648 (s), 606 (m). Anal. calcd. for $C_{12}H_{15}NO_2S$ (237.3): C 60.73, H 6.37, N 5.90; Found: C 61.00, H 6.39, N 5.93.

2 ^{1}H NMR and ^{13}C NMR spectra of *N*-Boc protected propargyl carbamates 2

2.1 *tert*-Butyl (1-phenylprop-2-yn-1-yl)carbamate (2a)



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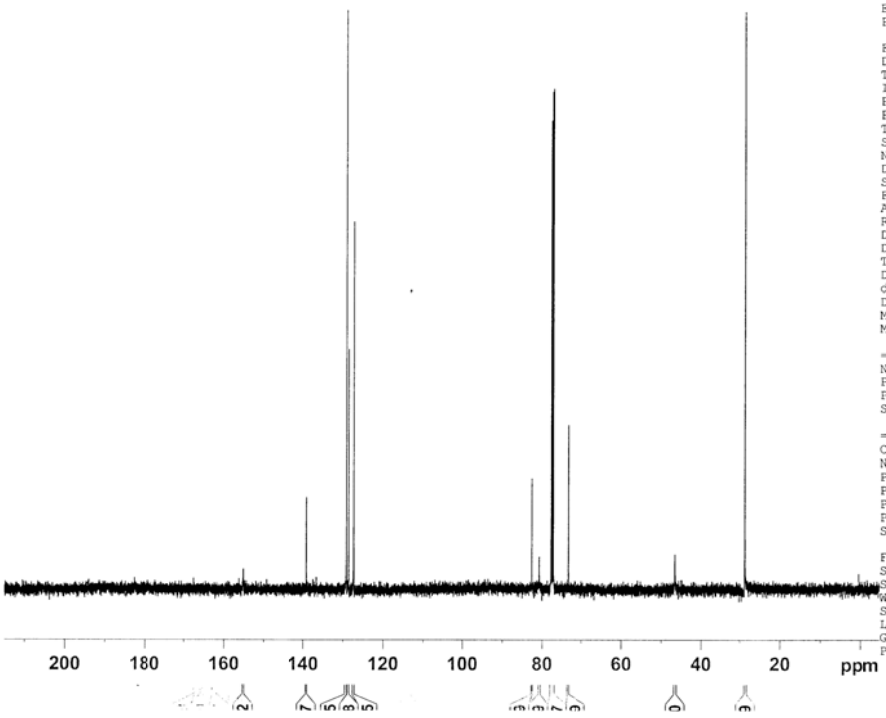


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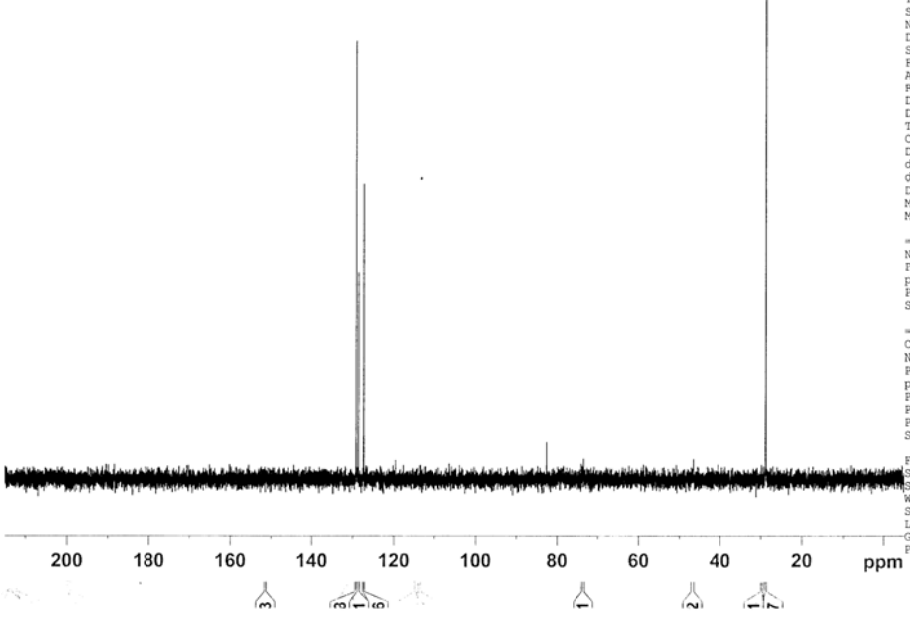


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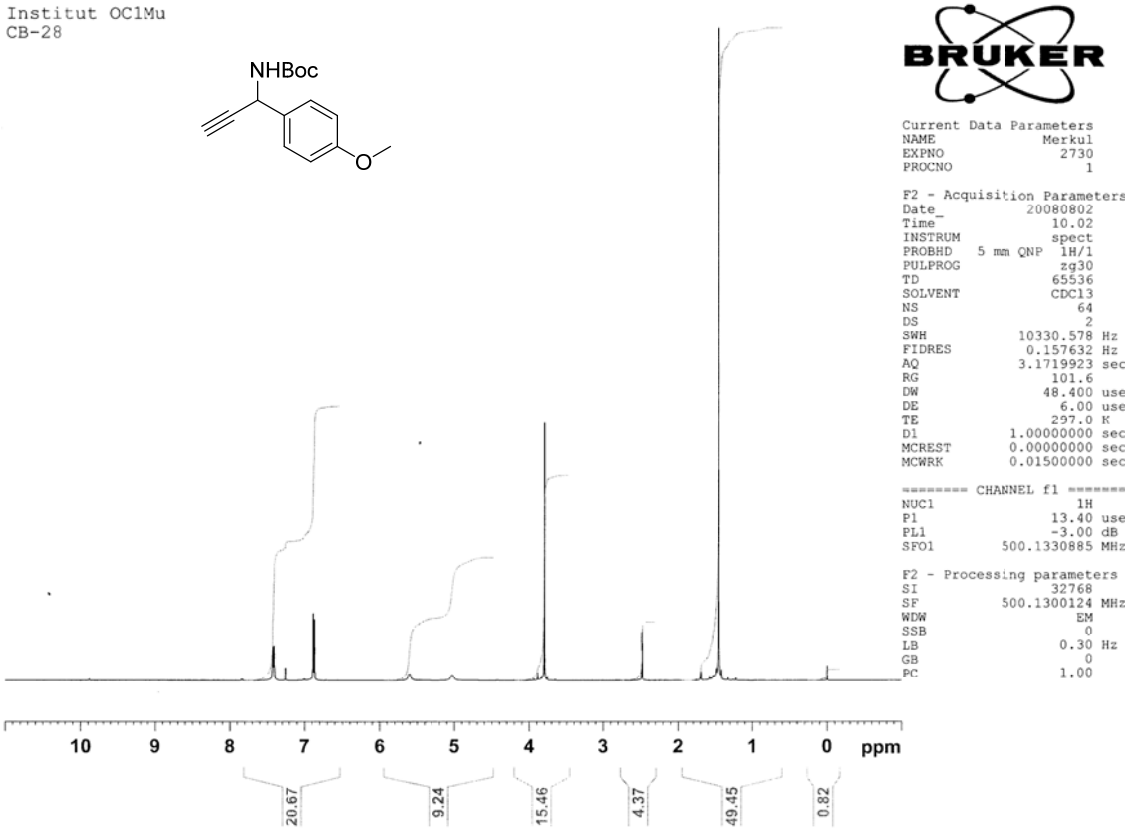
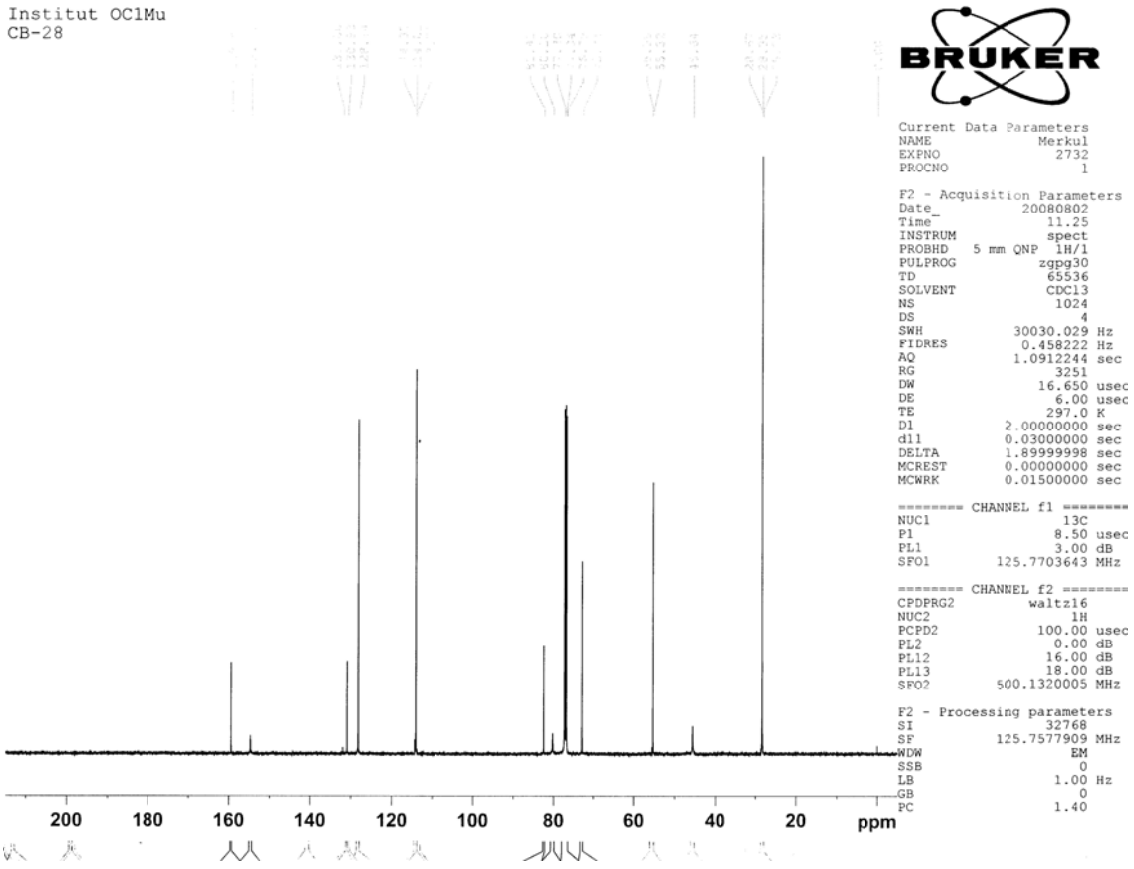
2.2 *tert*-Butyl (1-(4-methoxyphenyl)prop-2-yn-1-yl)carbamate (2b)





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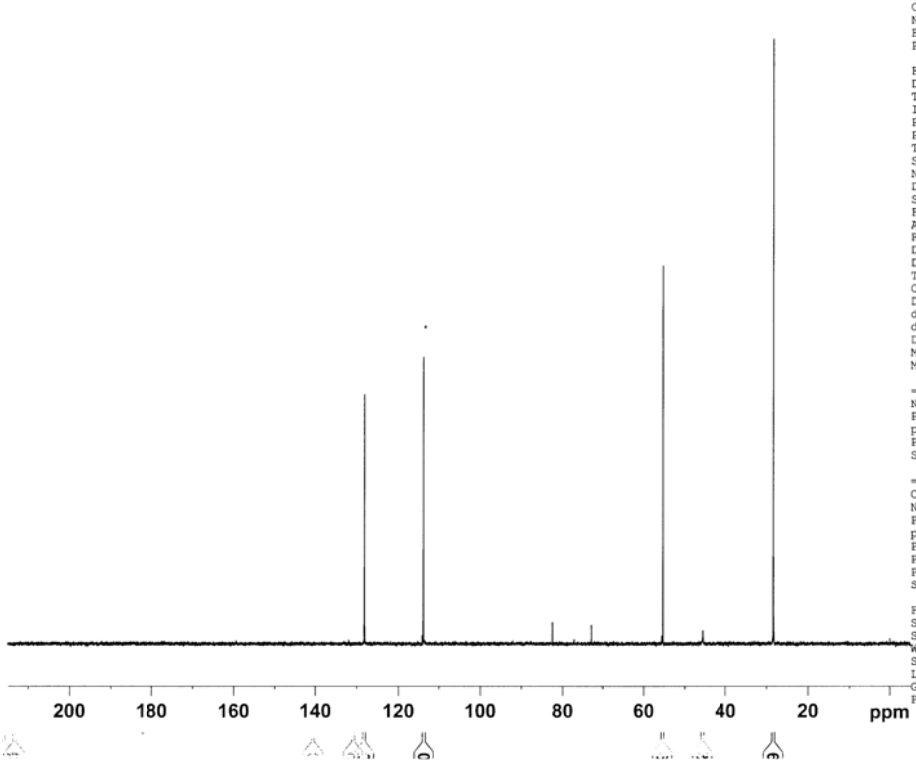


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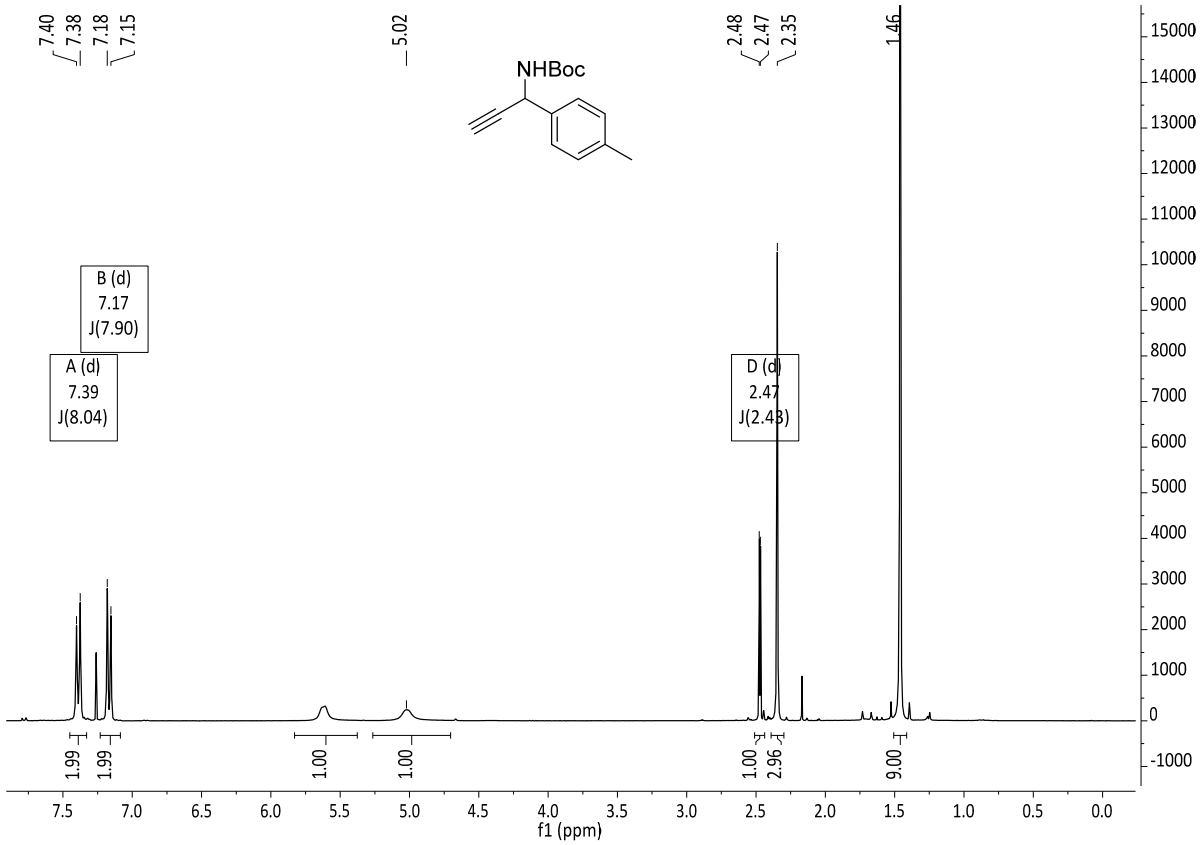

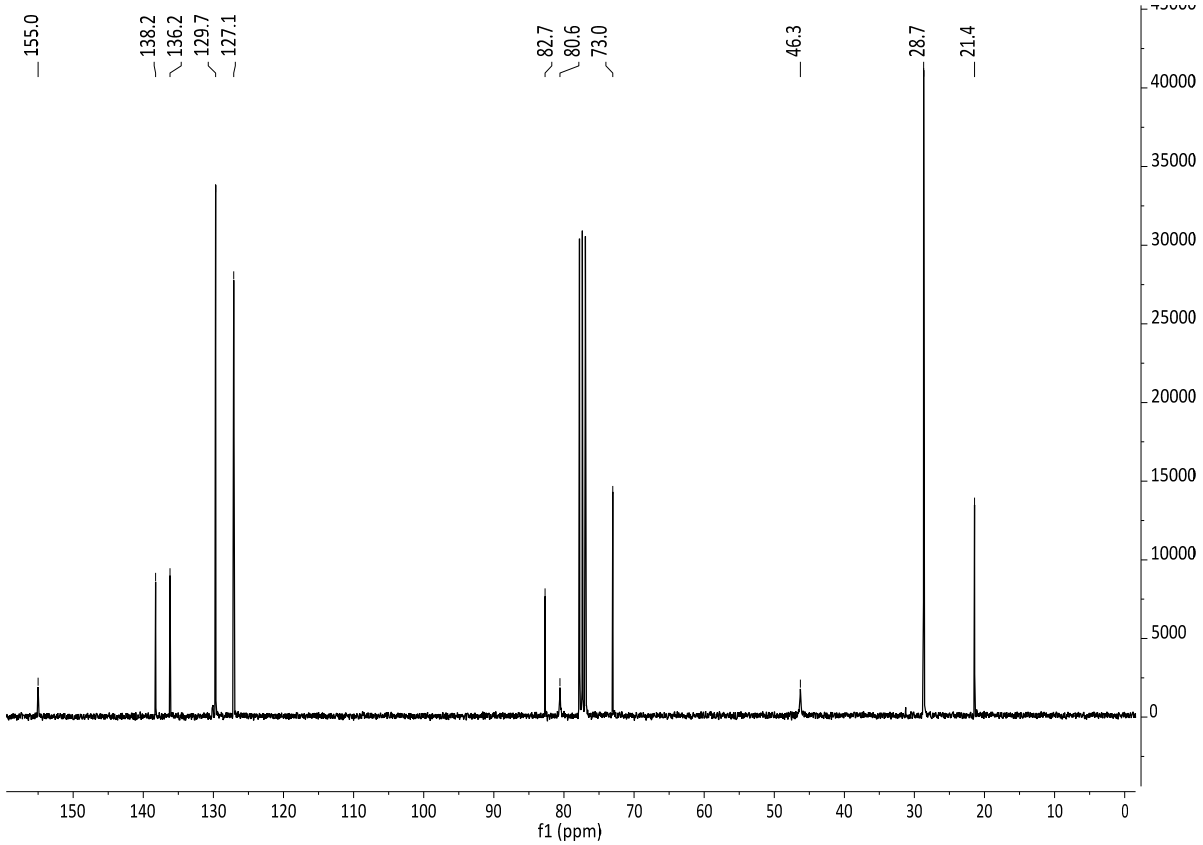

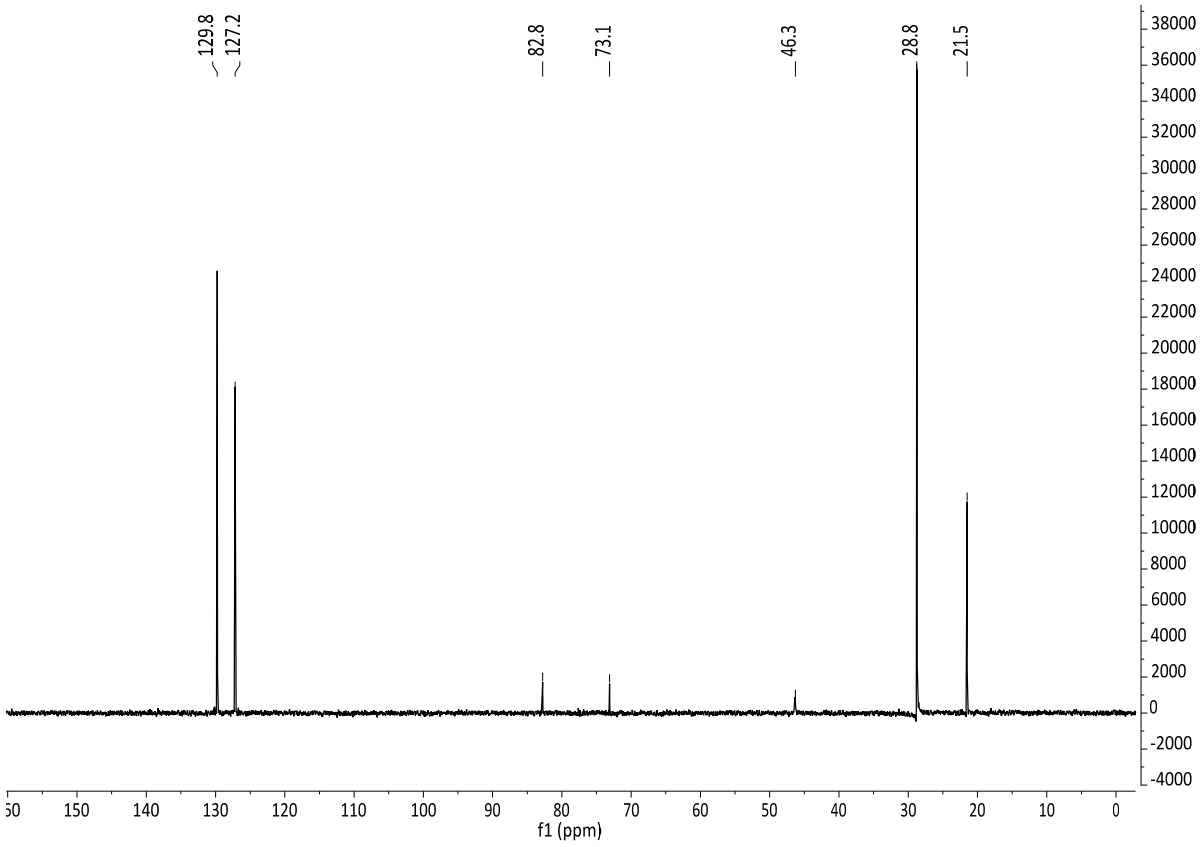
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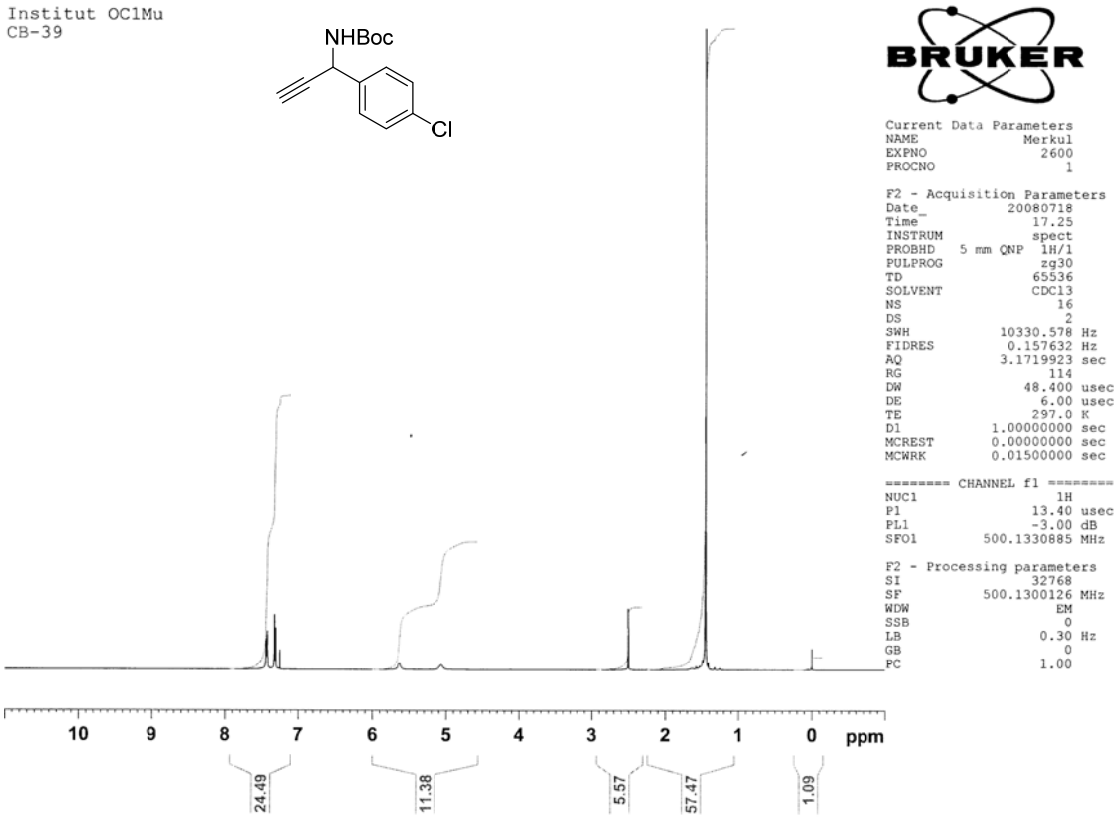

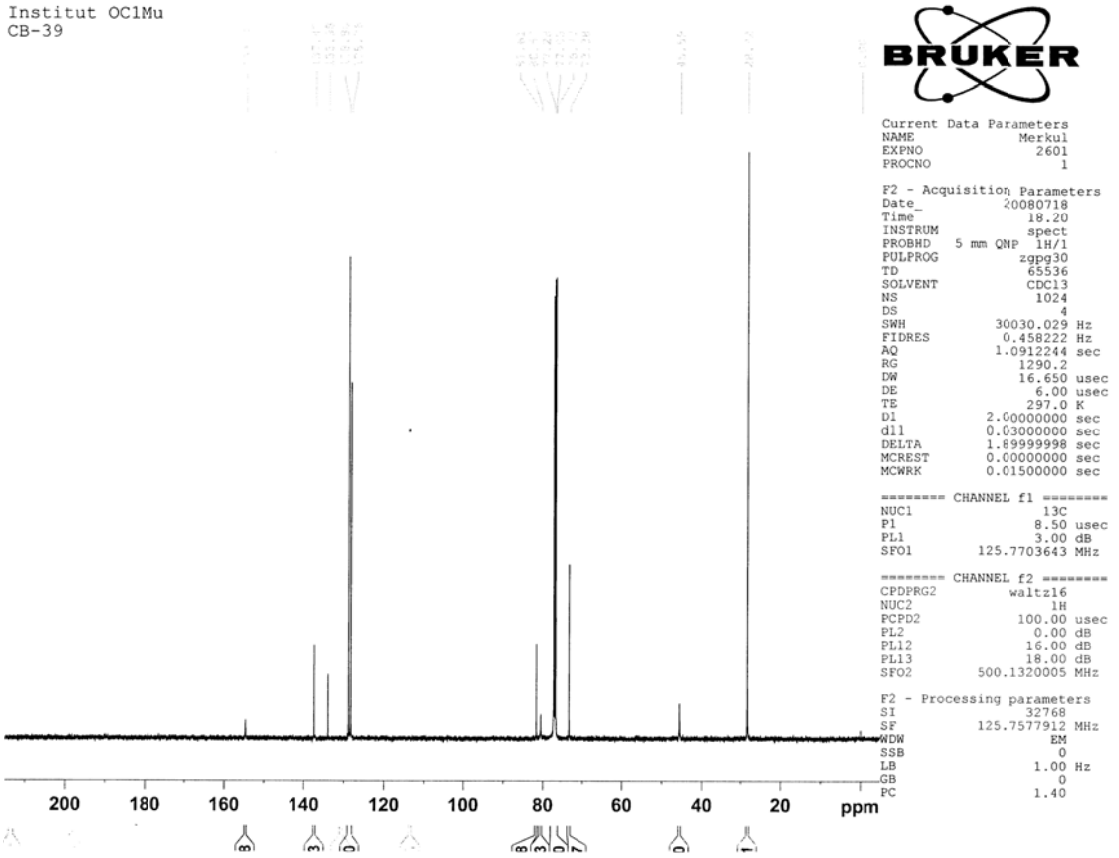

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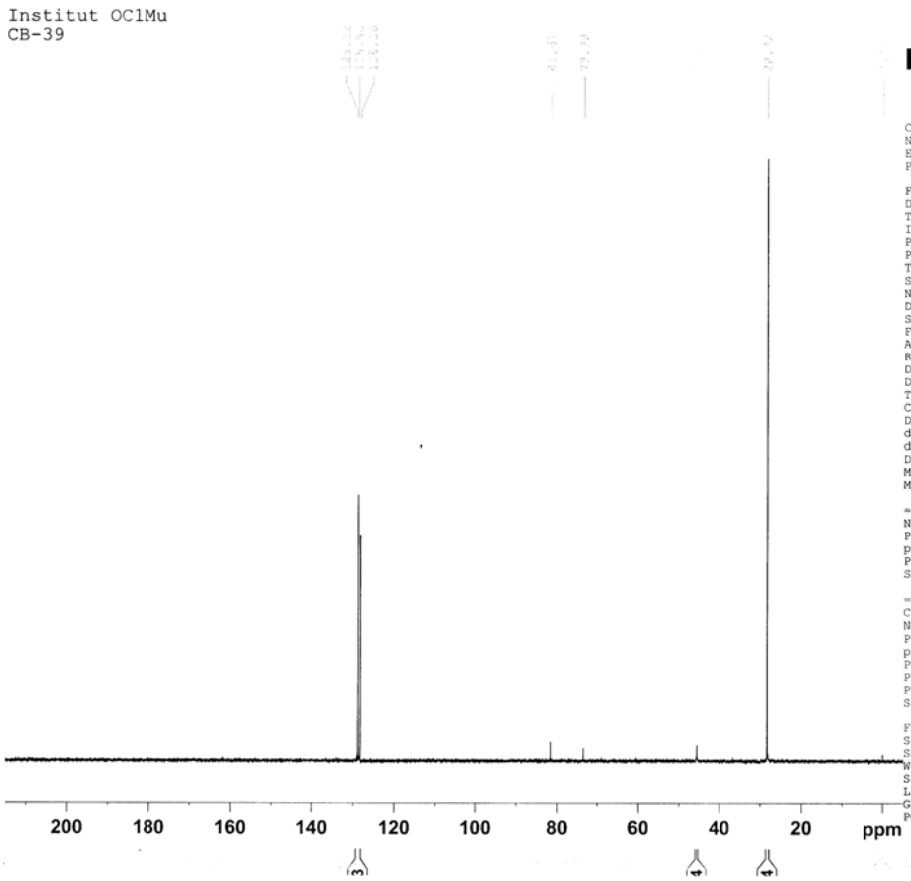

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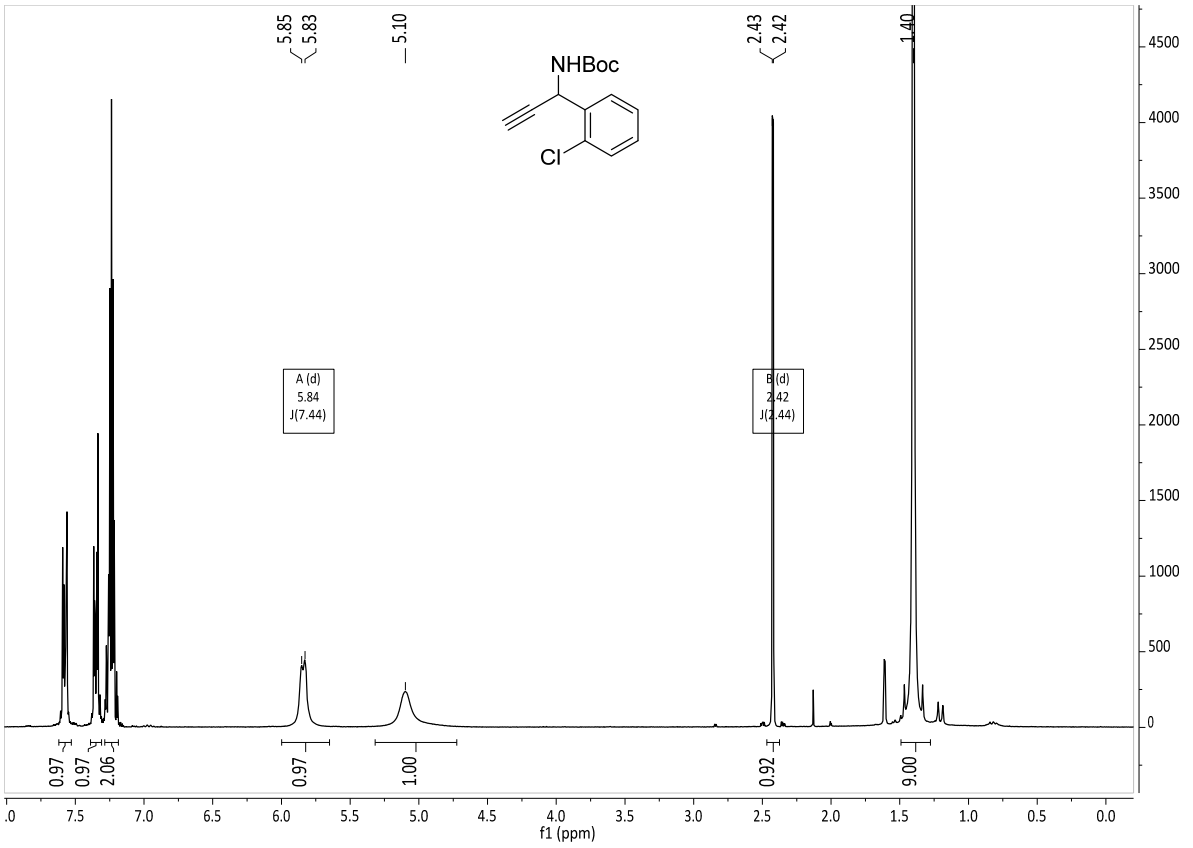
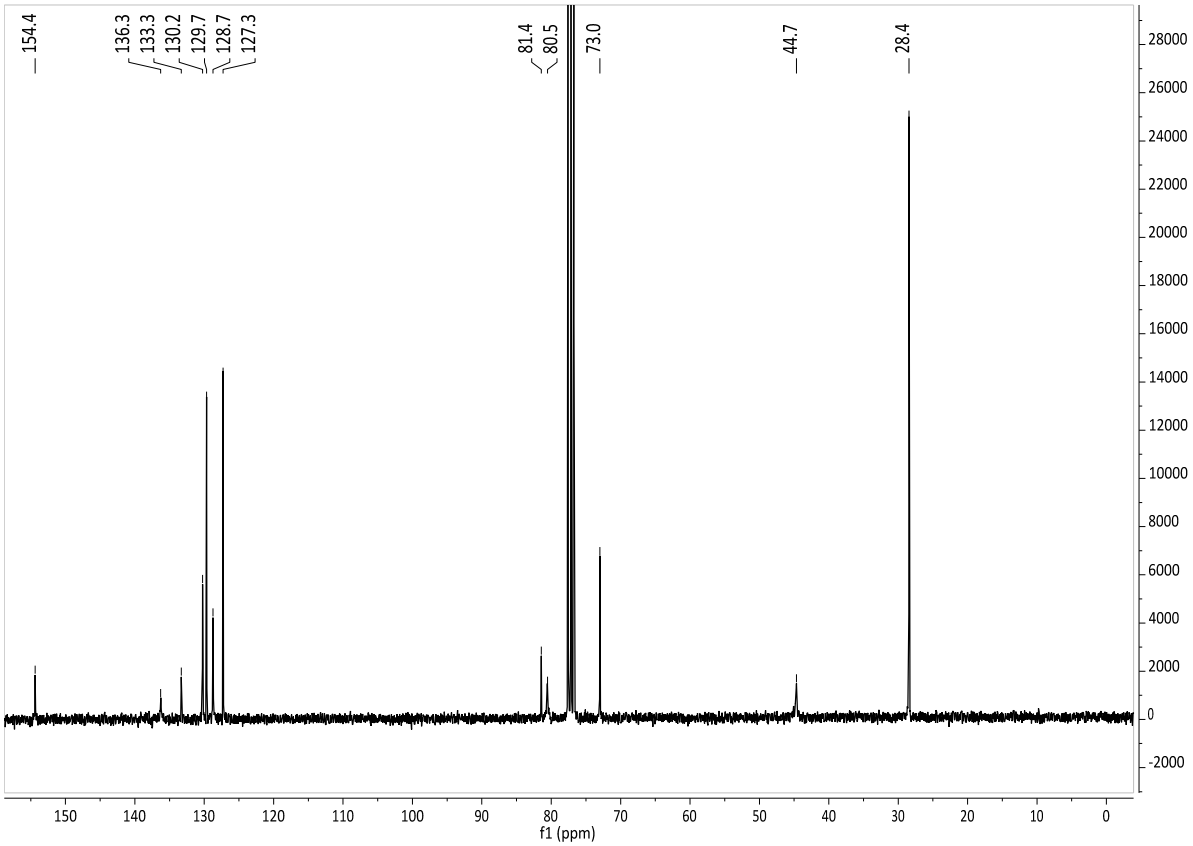
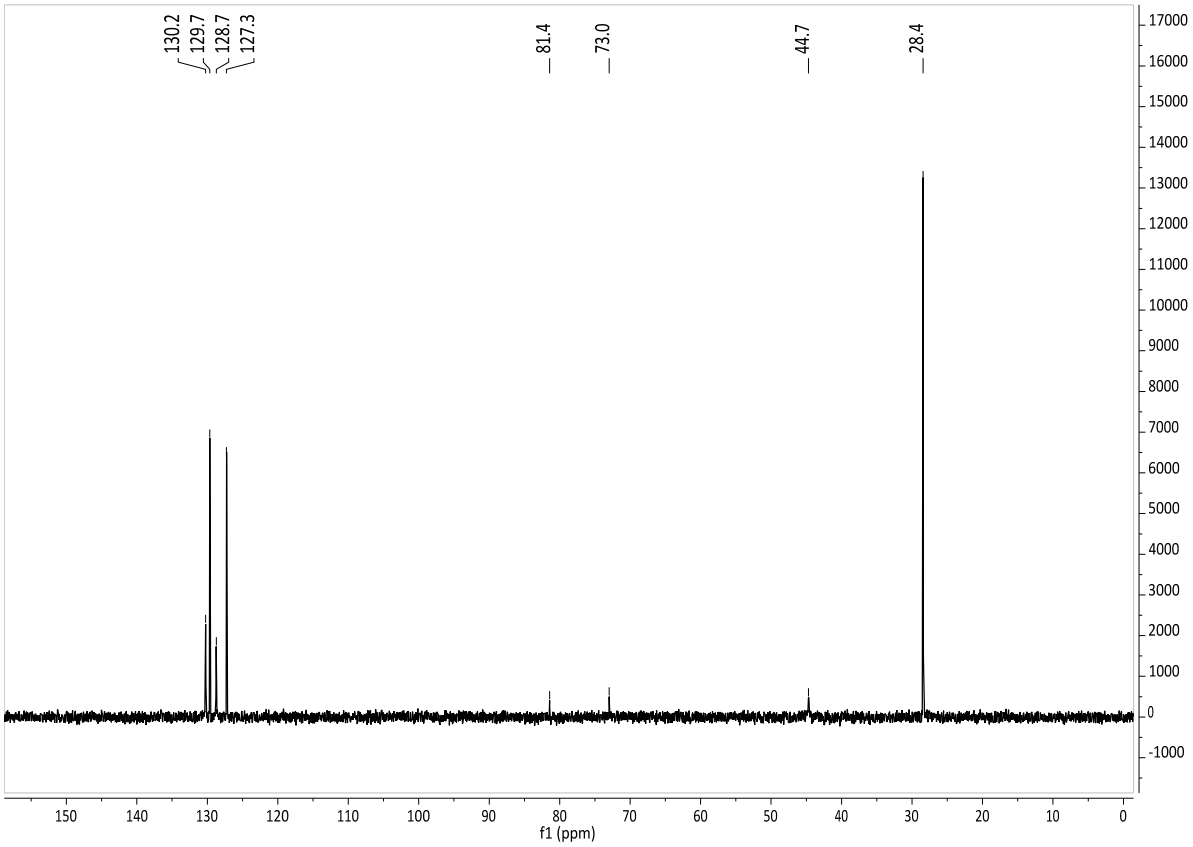
P3 16.00 usec
p4 32.00 usec
PCPD2 100.00 usec
PL2 0.00 dB
PL12 16.00 dB
SFO2 500.1320005 MHz

F2 - Processing parameters
SI 32768
SF 125.7577914 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

2.5 *tert*-Butyl (1-(2-chlorophenyl)prop-2-yn-1-yl)carbamate (2e)



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129.7
128.7
127.3
81.4
73.0
44.7
28.4
17000
16000
15000
14000
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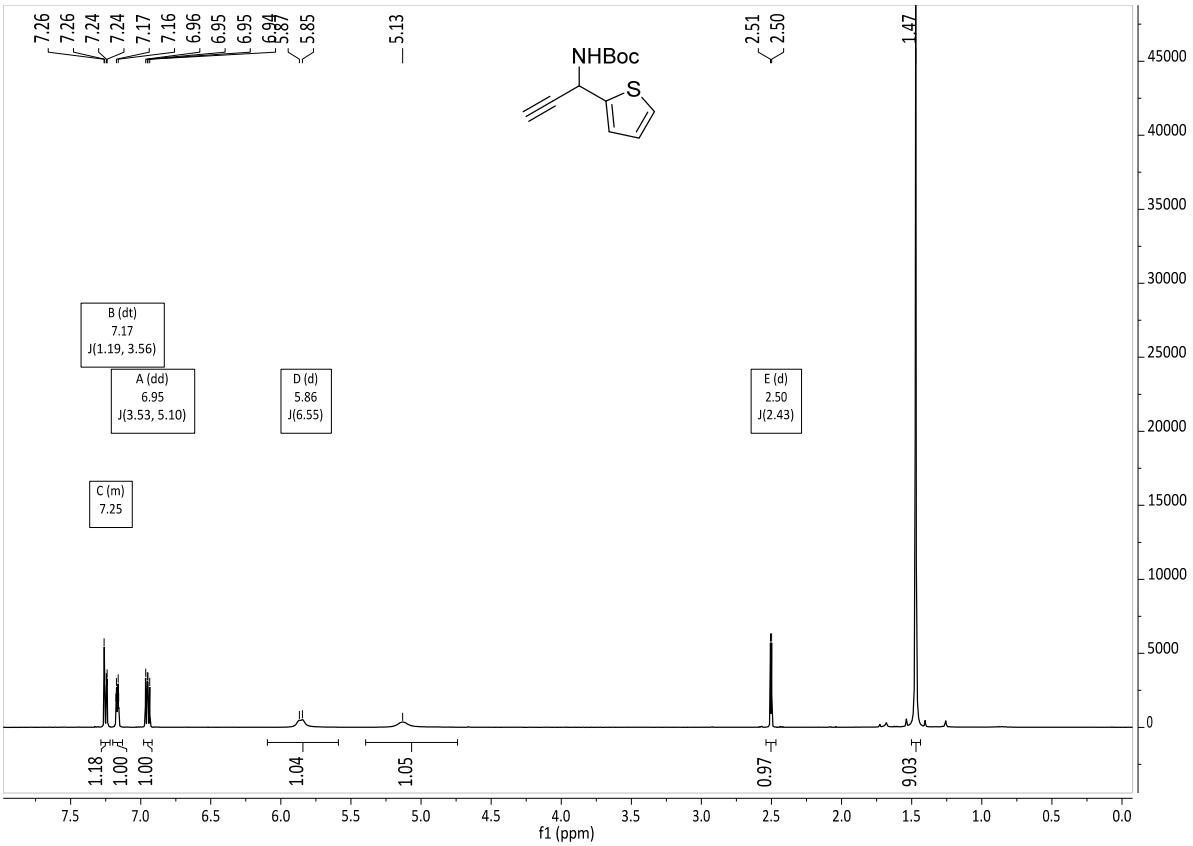
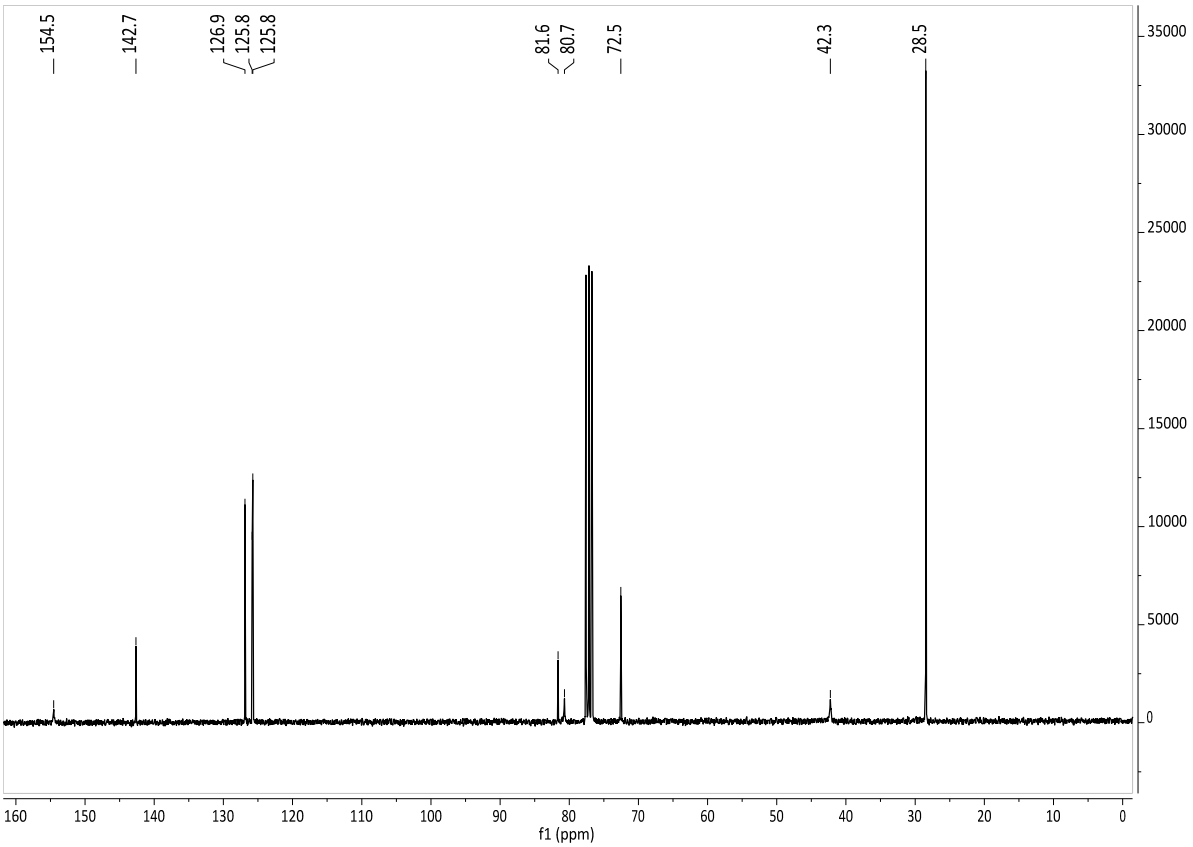
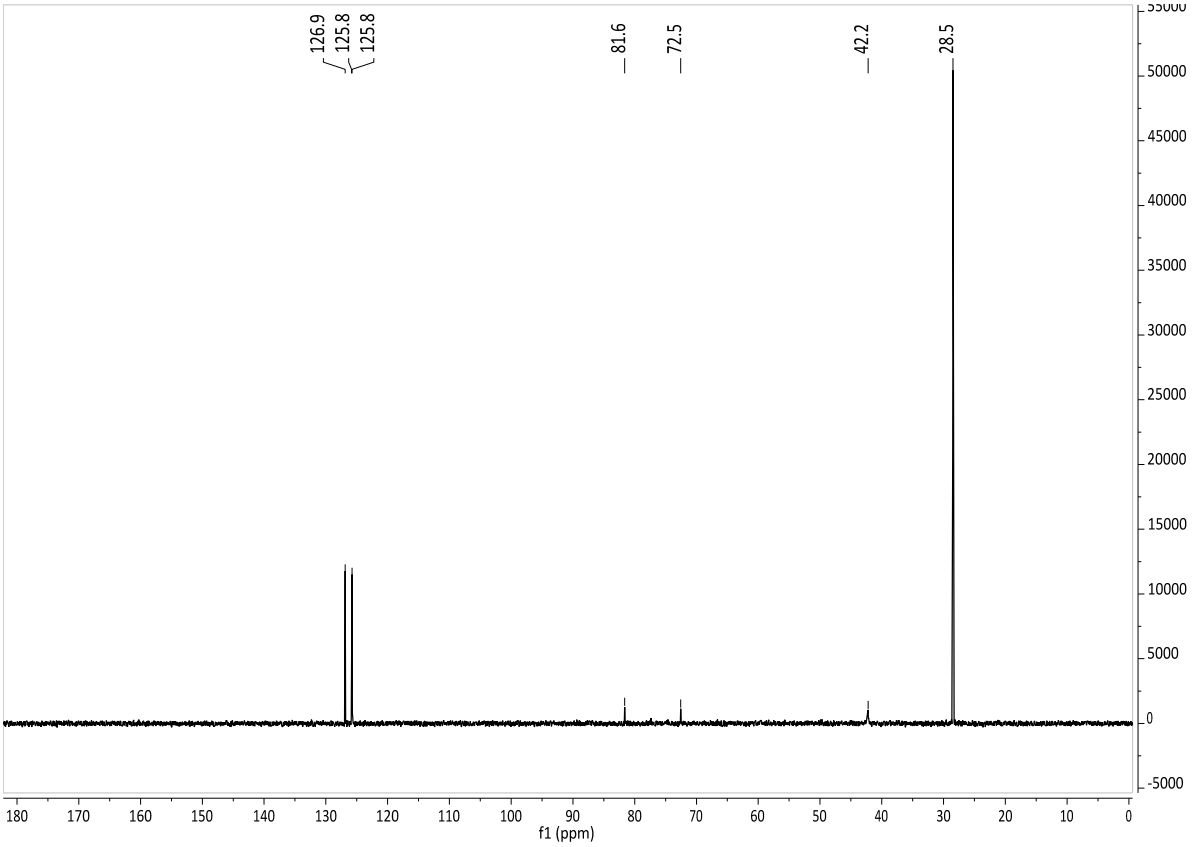
12000
11000
10000
9000
8000
7000
6000
5000
4000
3000
2000
1000
0
-1000
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

2.6 *tert*-Butyl (1-(thiophen-2-yl)prop-2-yn-1-yl)carbamate (2f)






126.9
125.8
125.8
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72.5
42.2
28.5
50000
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40000
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25000
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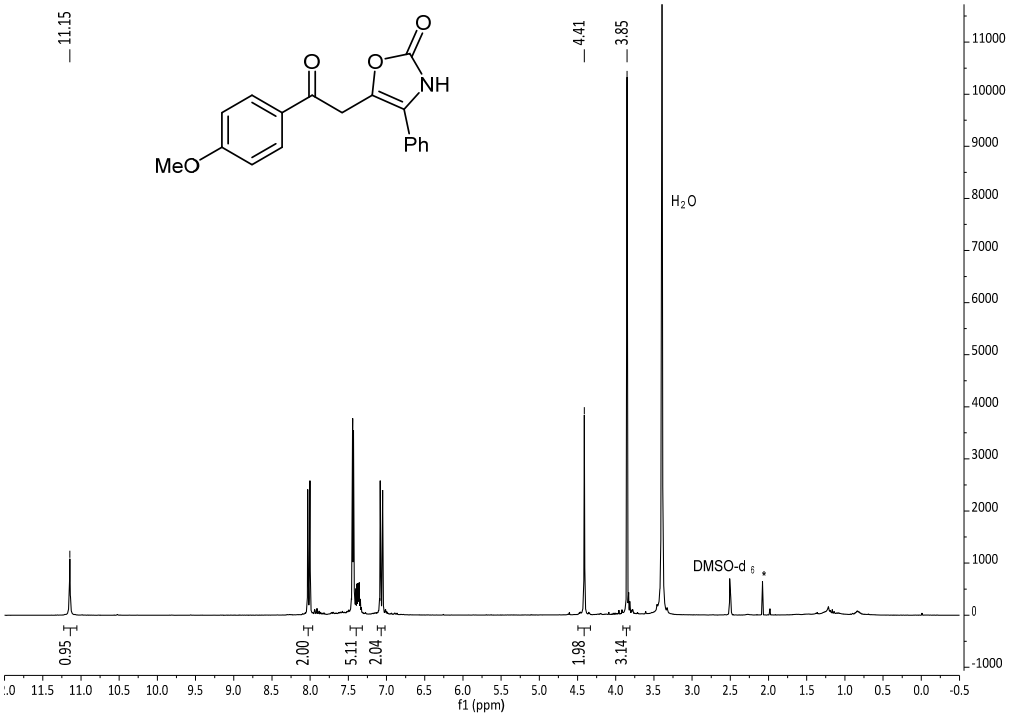
15000
10000
5000
0
-5000
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

3 ^{1}H NMR and ^{13}C NMR Spectra of 5-Substituted 2-Oxoethyl Oxazol-2(3*H*)-ones 3

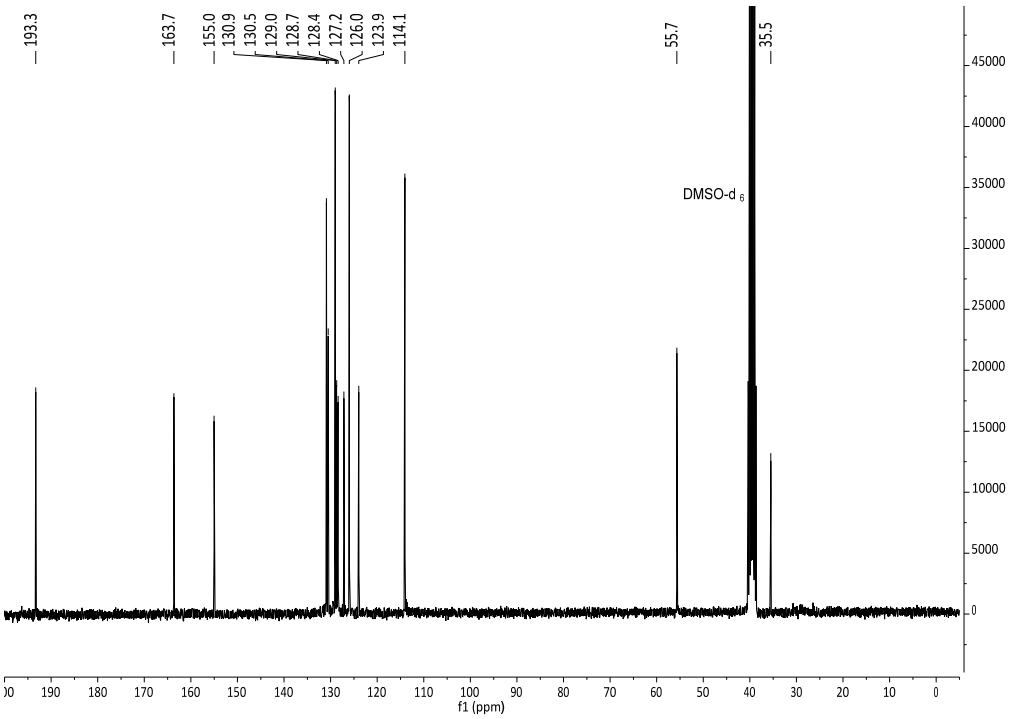
3.1 5-(2-(4-Methoxyphenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3a)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



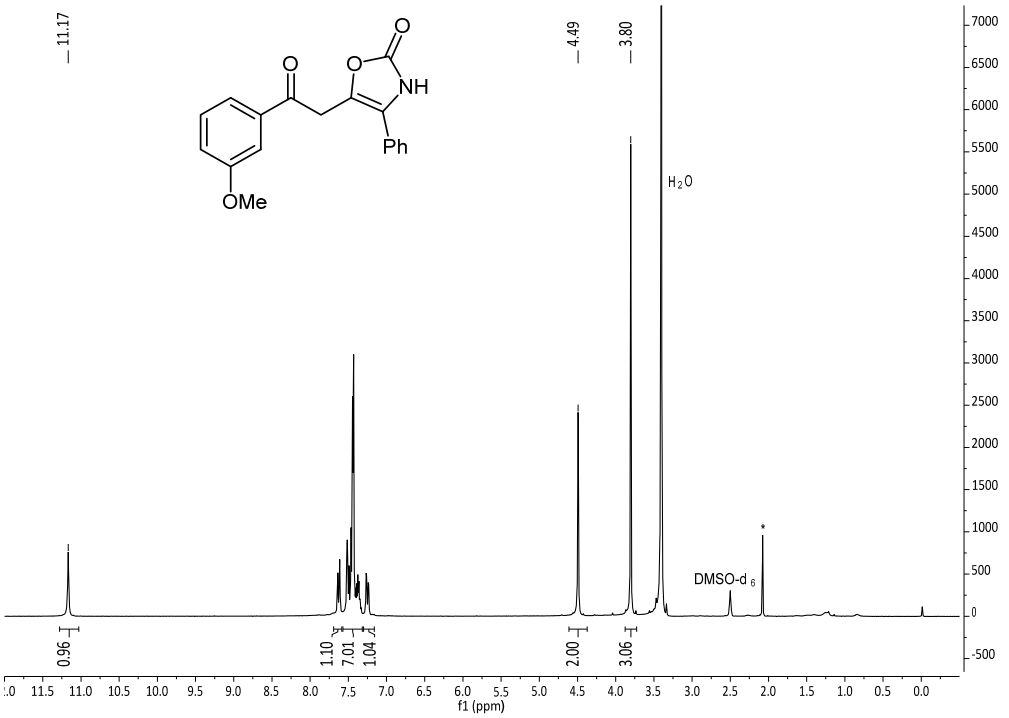
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



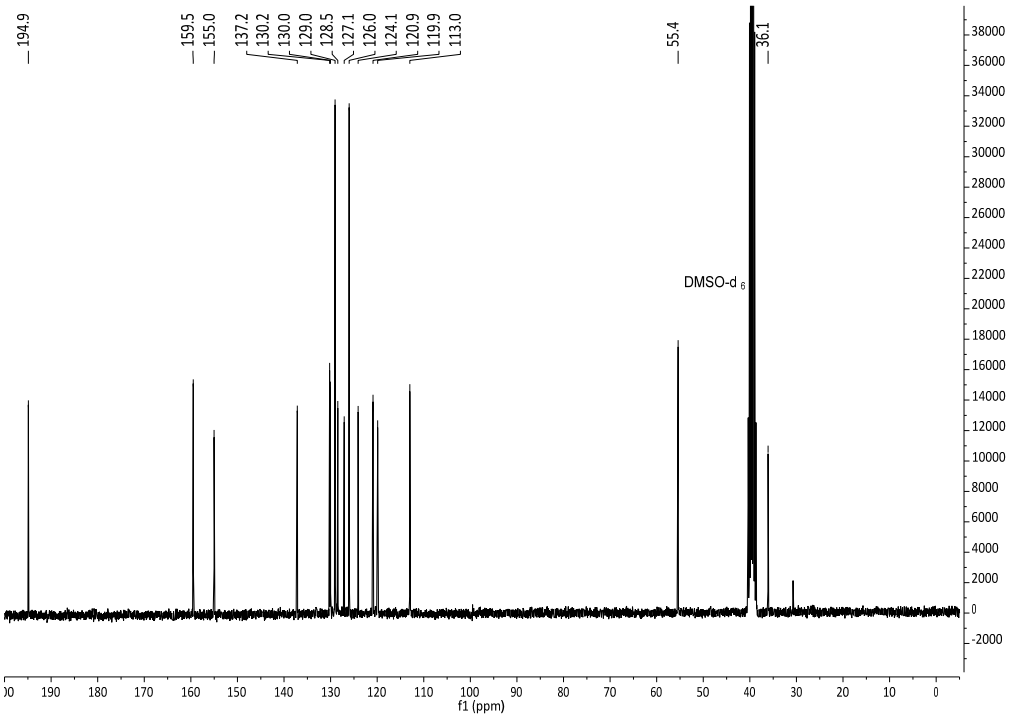
3.2 5-(2-(3-Methoxyphenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3b)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



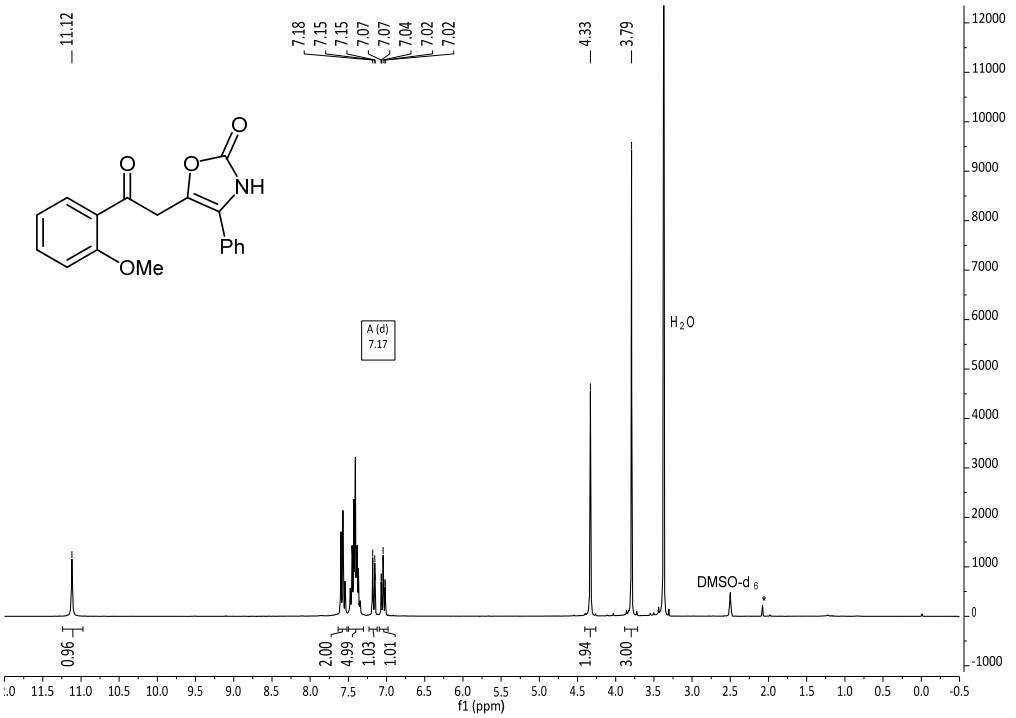
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



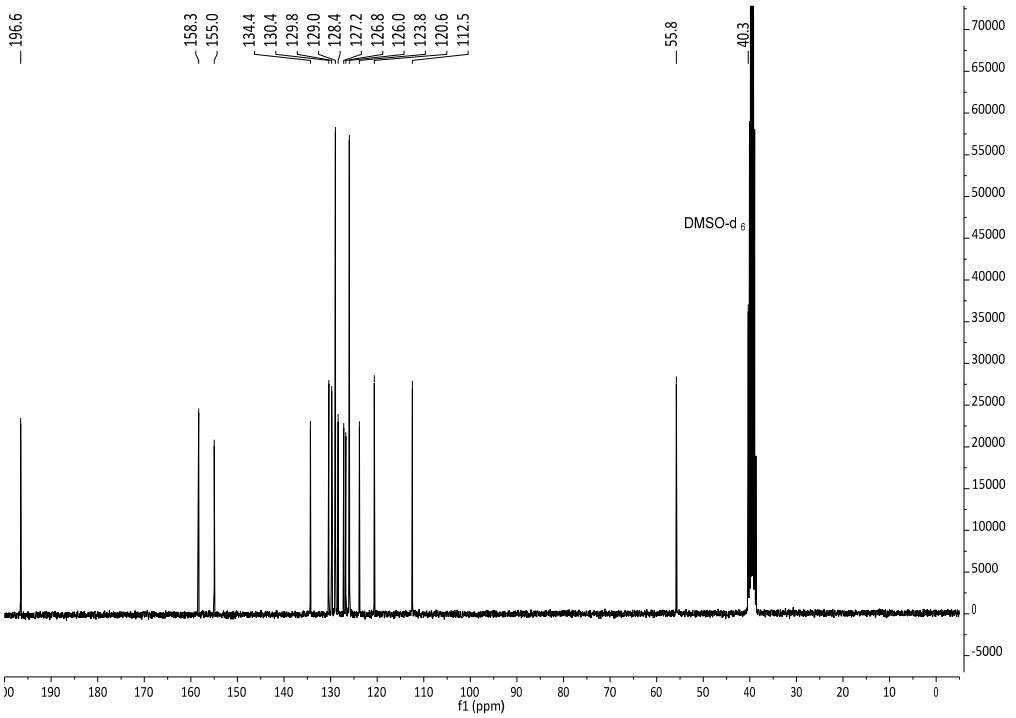
3.3 5-(2-(2-Methoxyphenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3c)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



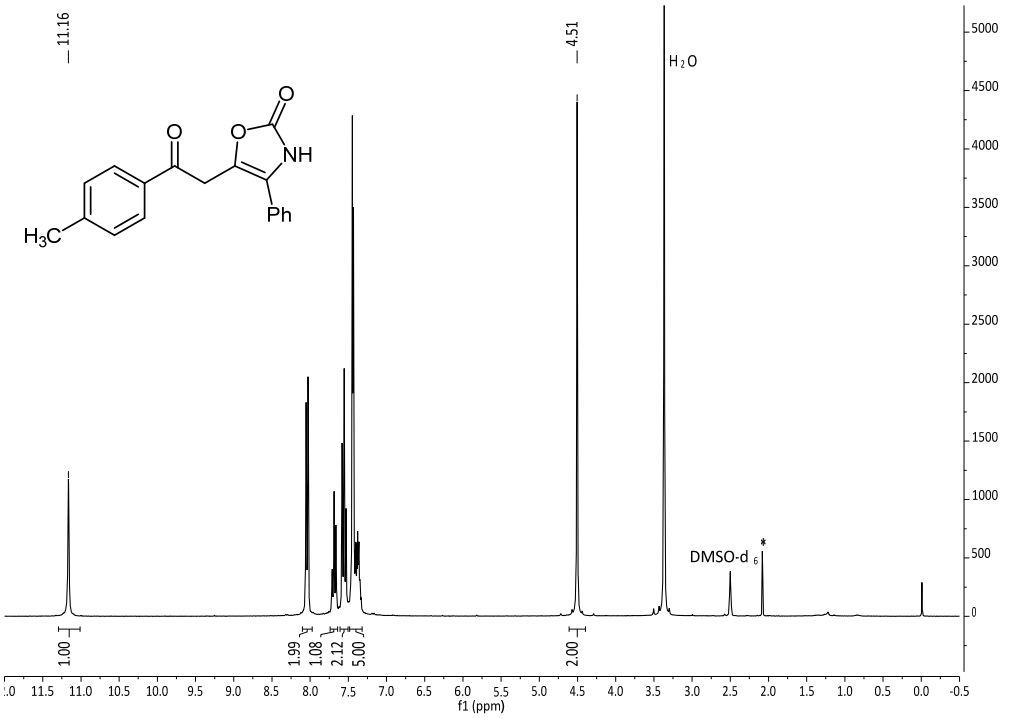
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



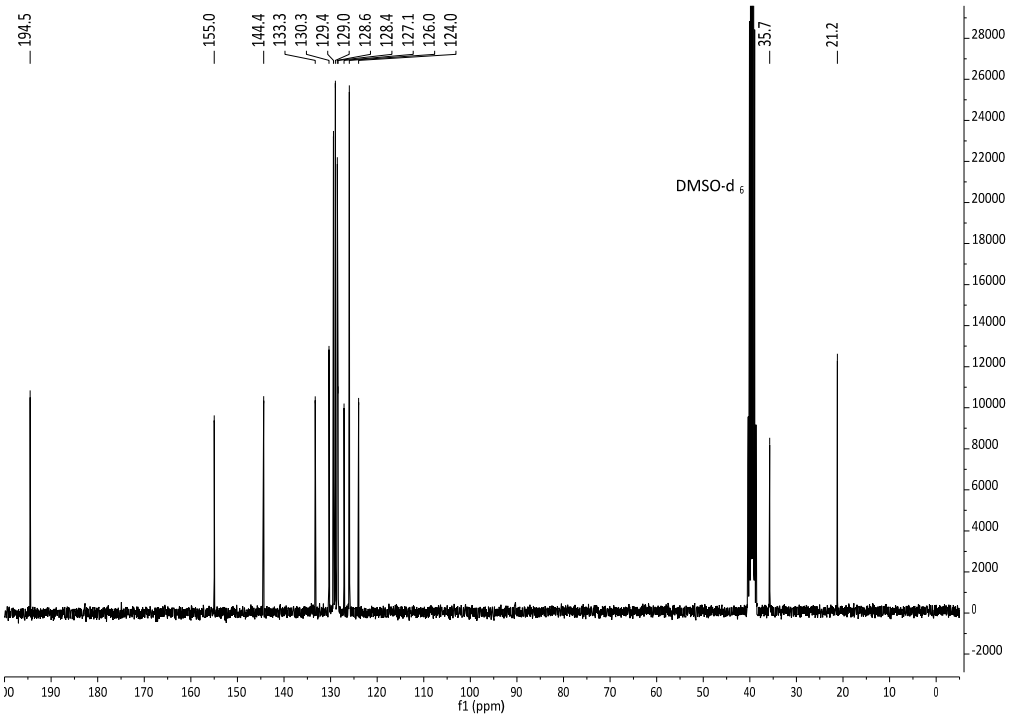
3.4 5-(2-Oxo-2-(4-tolyl)ethyl)-4-phenyloxazol-2(3*H*)-one (3d)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



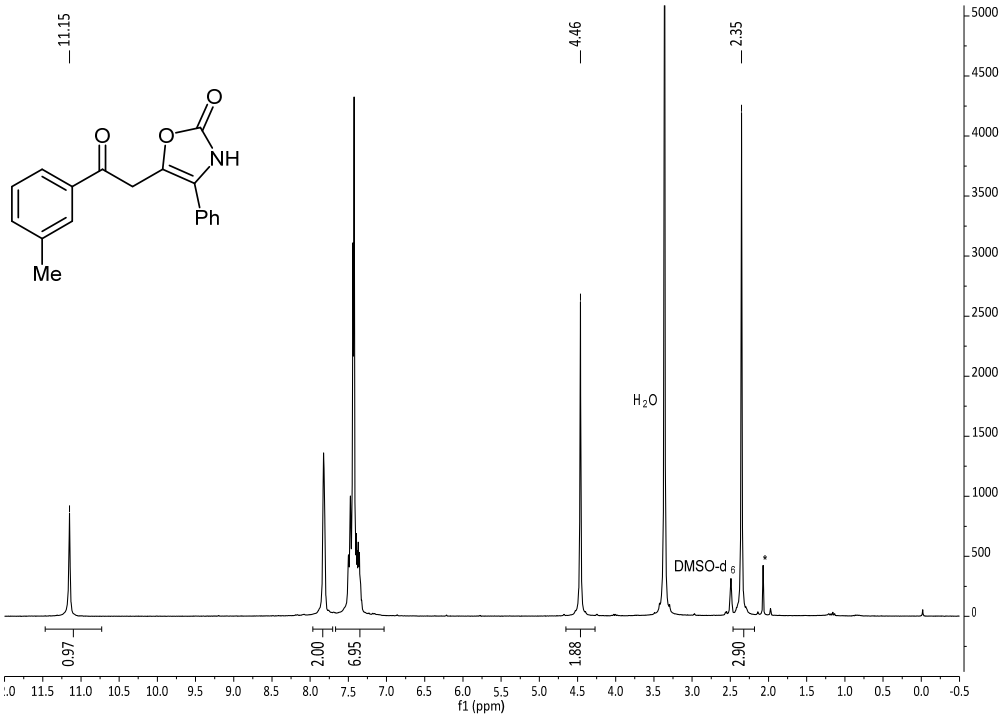
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



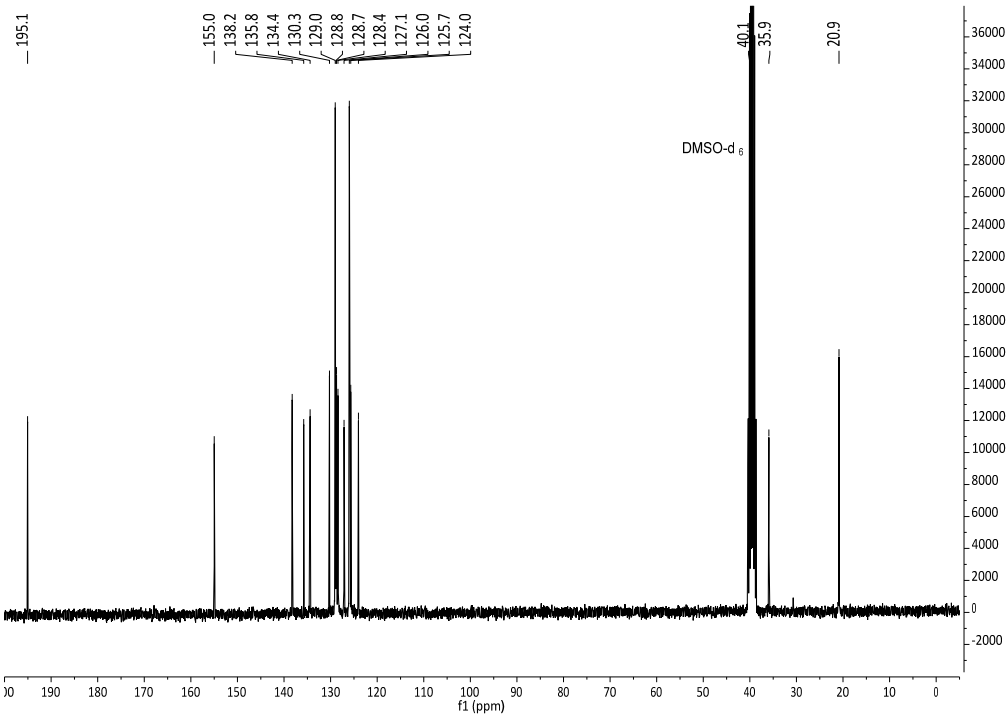
3.5 5-(2-Oxo-2-(3-tolyl)ethyl)-4-phenyloxazol-2(3*H*)-one (3e)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



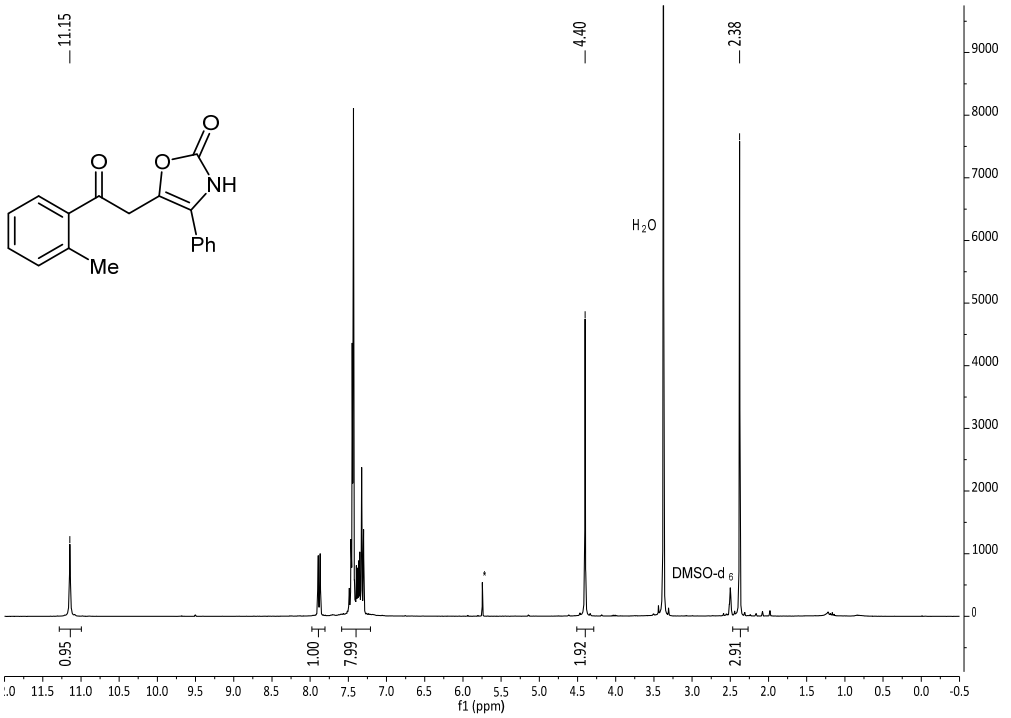
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



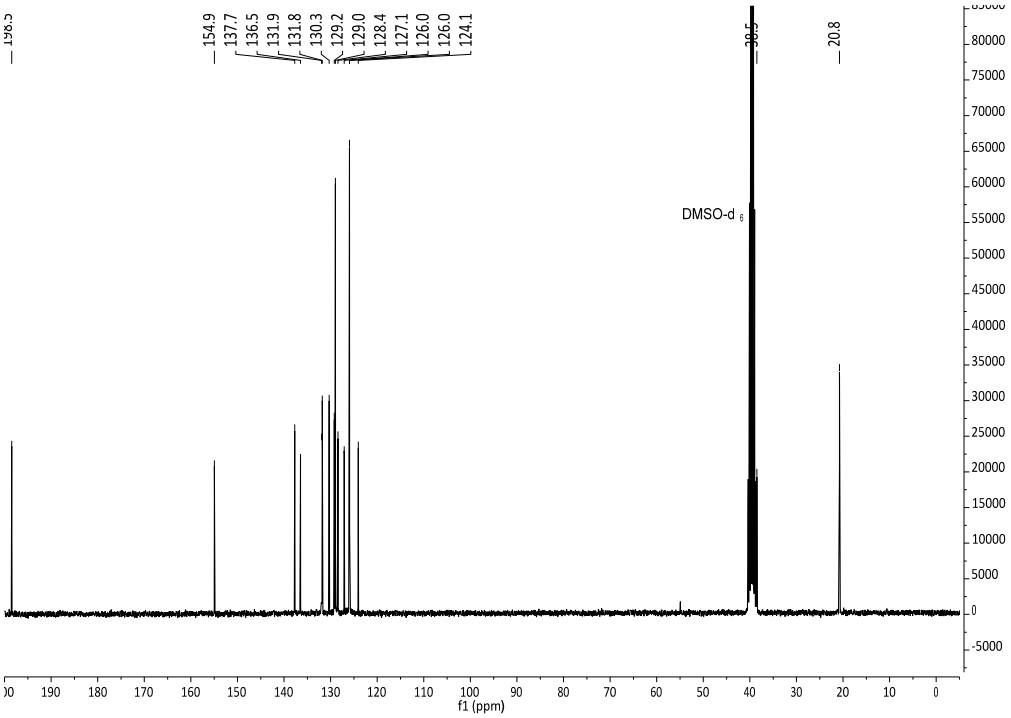
3.6 5-(2-Oxo-2-(2-tolyl)ethyl)-4-phenyloxazol-2(3*H*)-one (3f)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



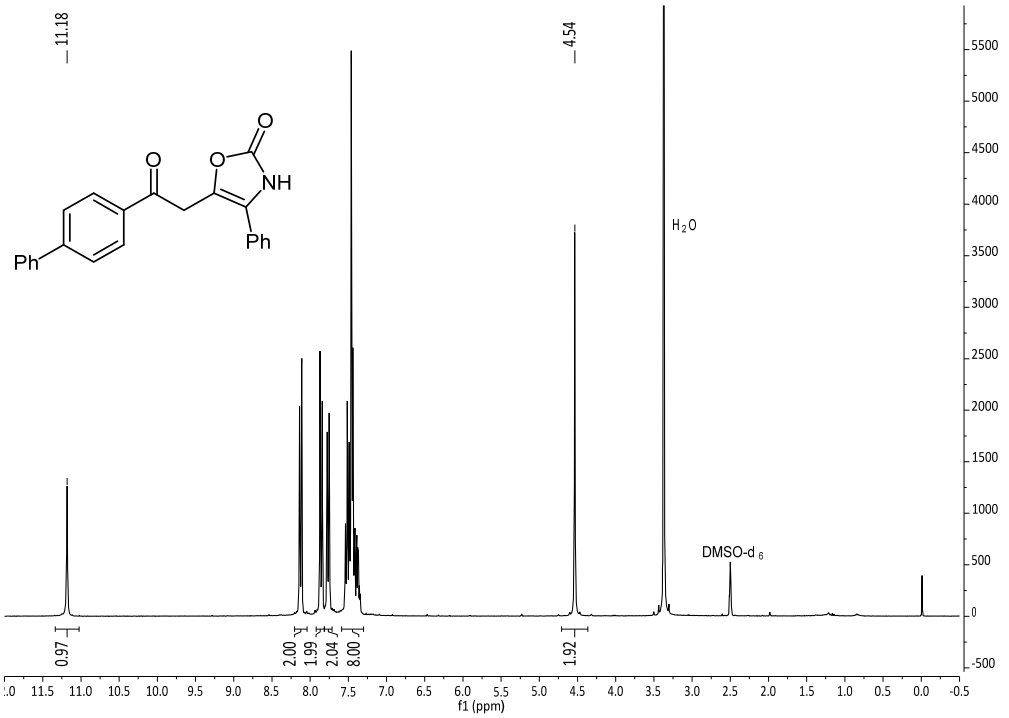
*Minor impuritiy.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)

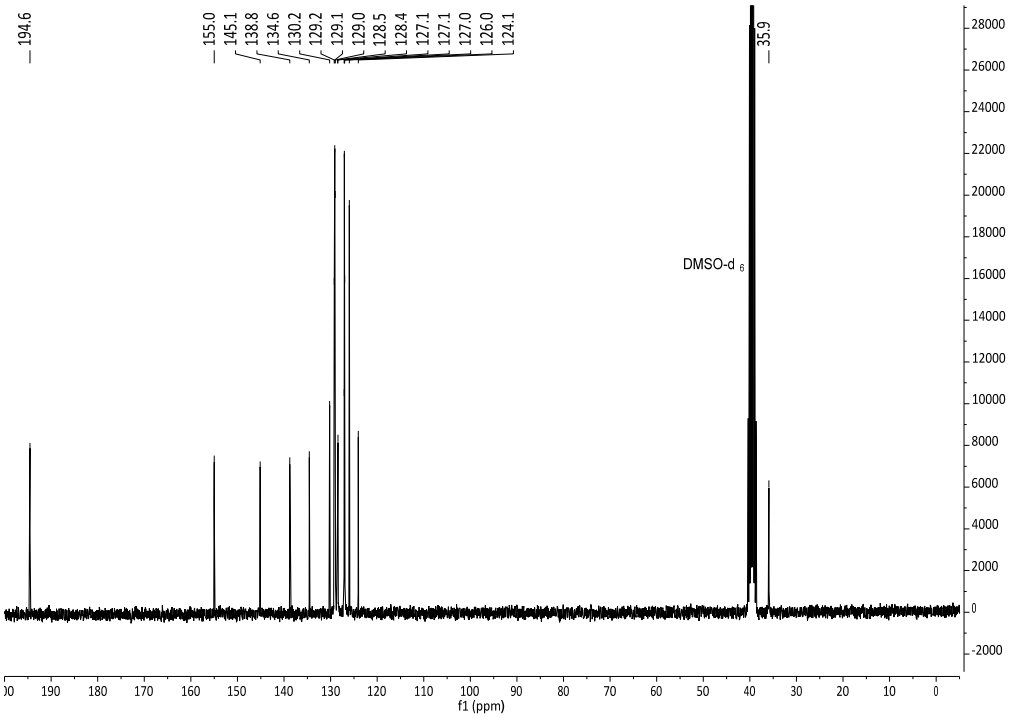


3.7 5-(2-([1,1'-Biphenyl]-4-yl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3g)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)

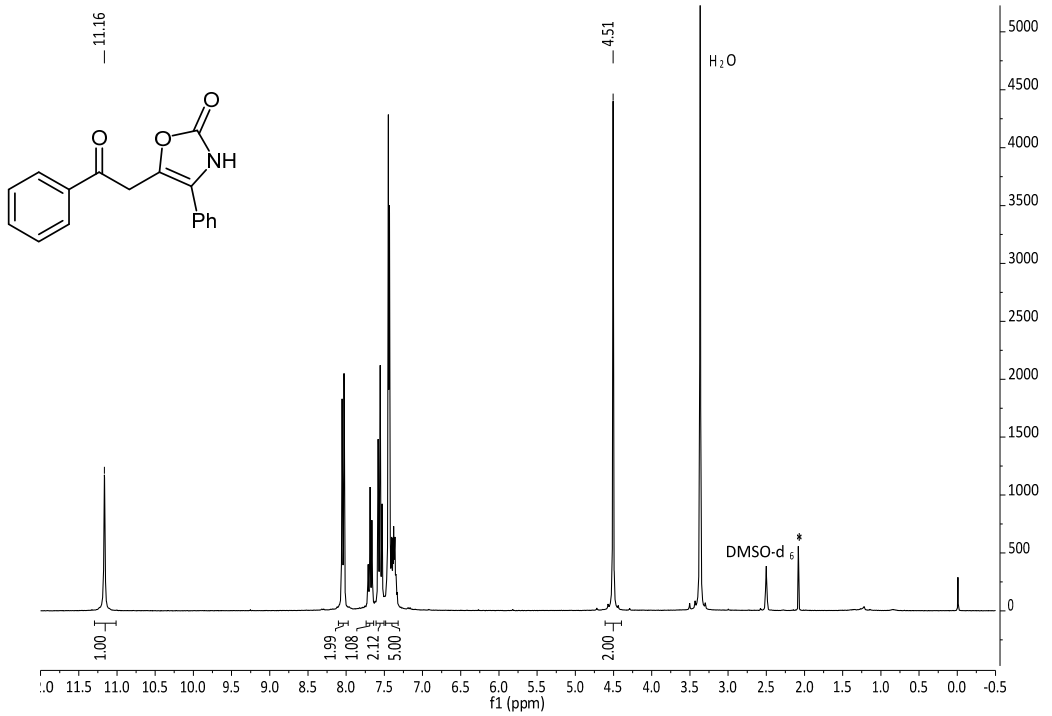


^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



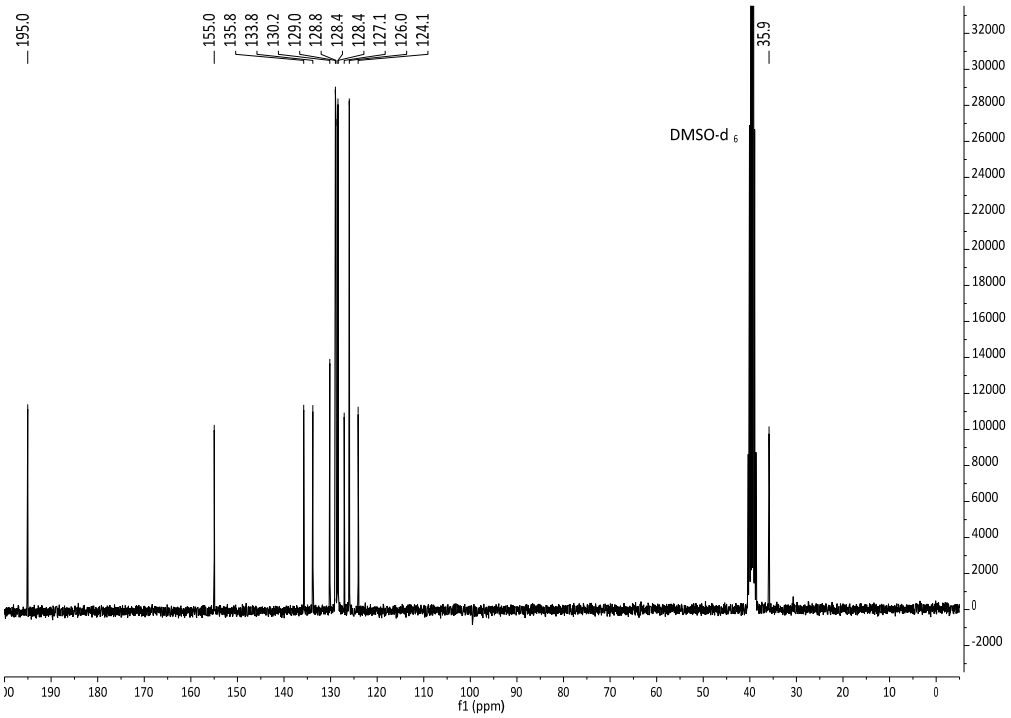
3.8 5-(2-Oxo-2-phenylethyl)-4-phenyloxazol-2(3*H*)-one (3h)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



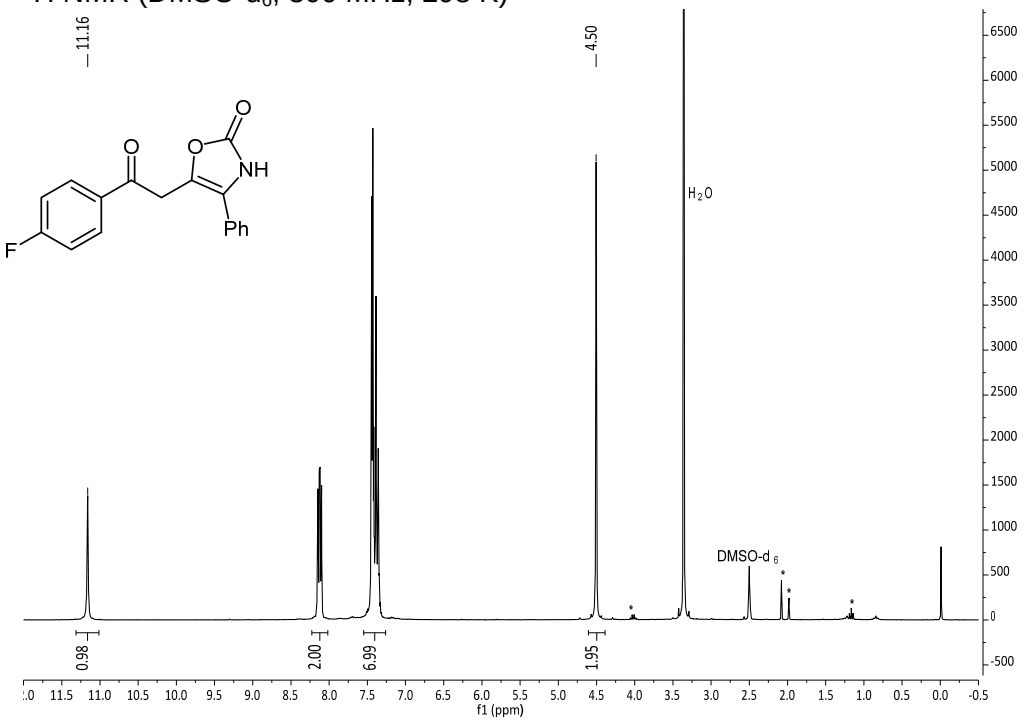
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



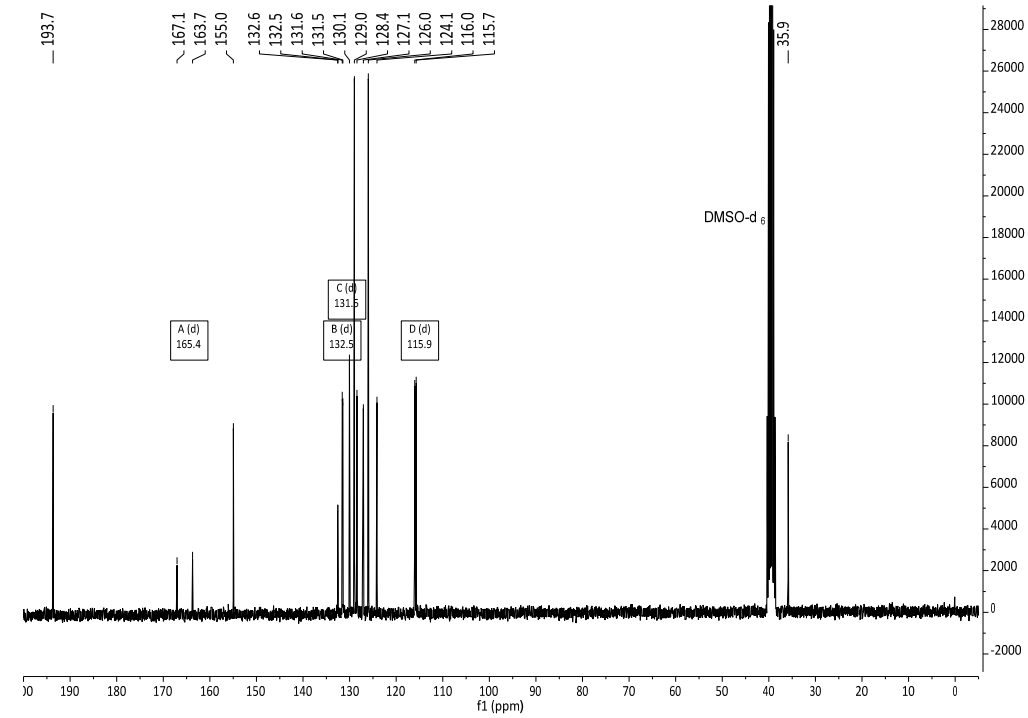
3.9 5-(2-(4-Fluorophenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3i)

^{1}H NMR (DMSO-d$_6$, 300 MHz, 298 K)



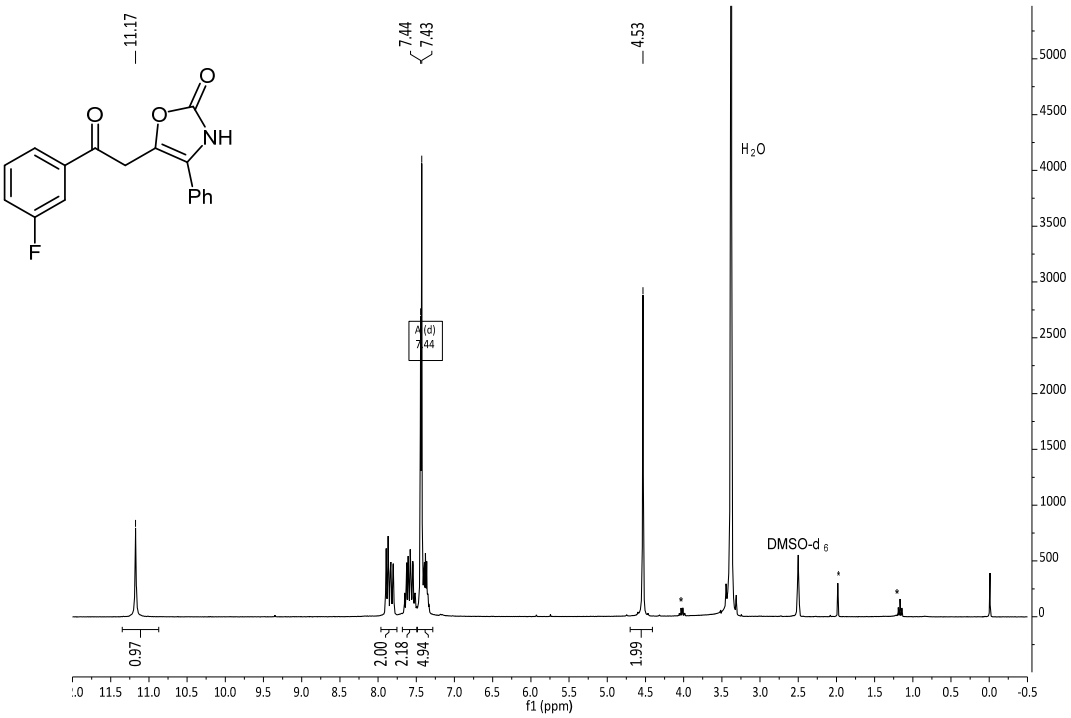
*Impuritiy from residual ethyl acetate and acetone.

^{13}C NMR (DMSO-d$_6$, 75 MHz, 298 K)



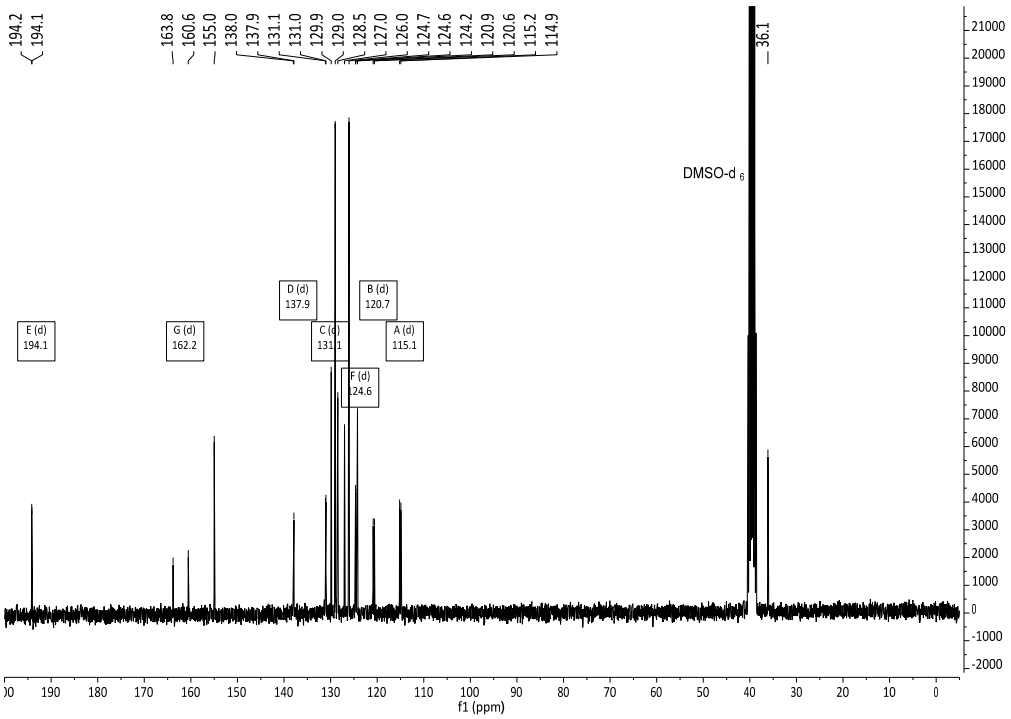
3.10 5-(2-(3-Fluorophenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3j)

^{1}H NMR (DMSO-d$_6$, 300 MHz, 298 K)



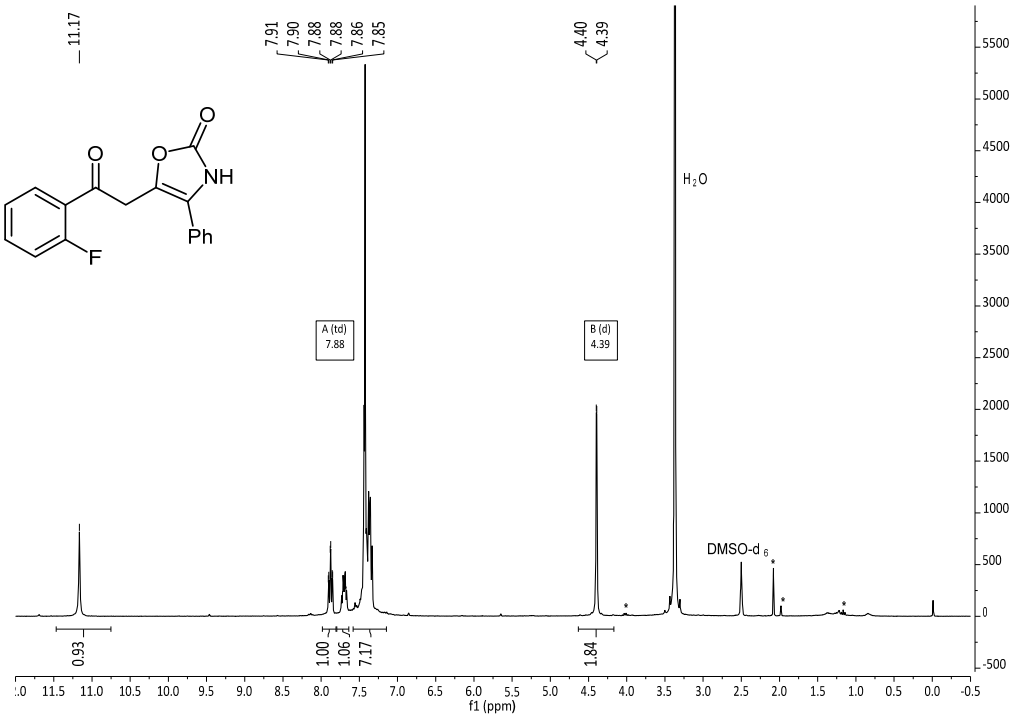
*Impuritiy from residual ethyl acetate.

^{13}C NMR (DMSO-d$_6$, 75 MHz, 298 K)



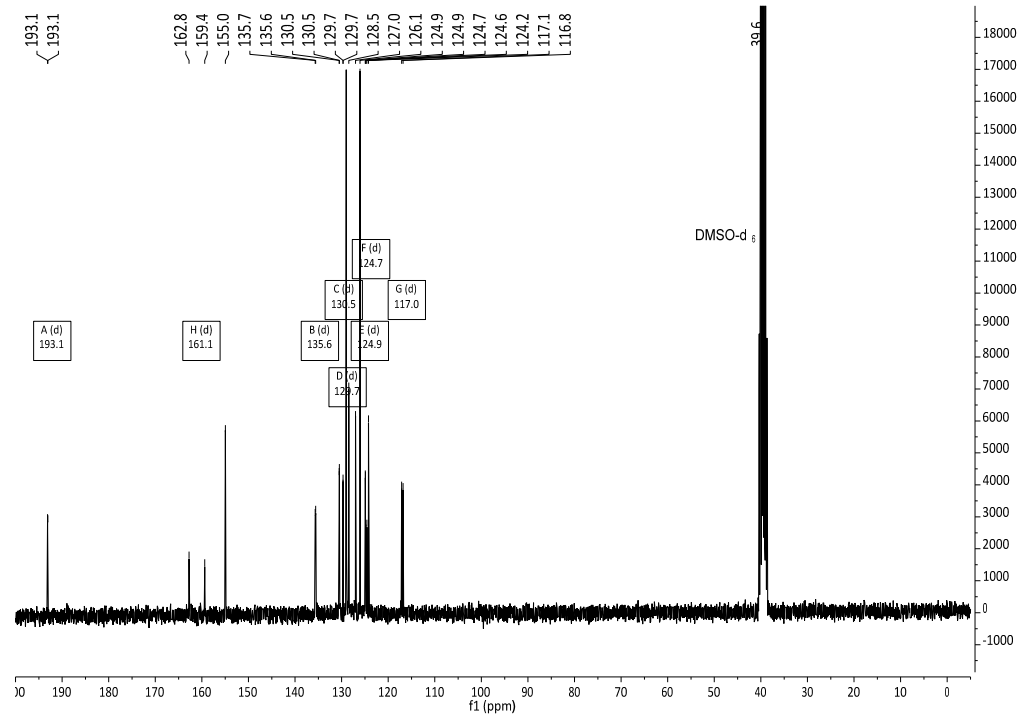
3.11 5-(2-(2-Fluorophenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3k)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



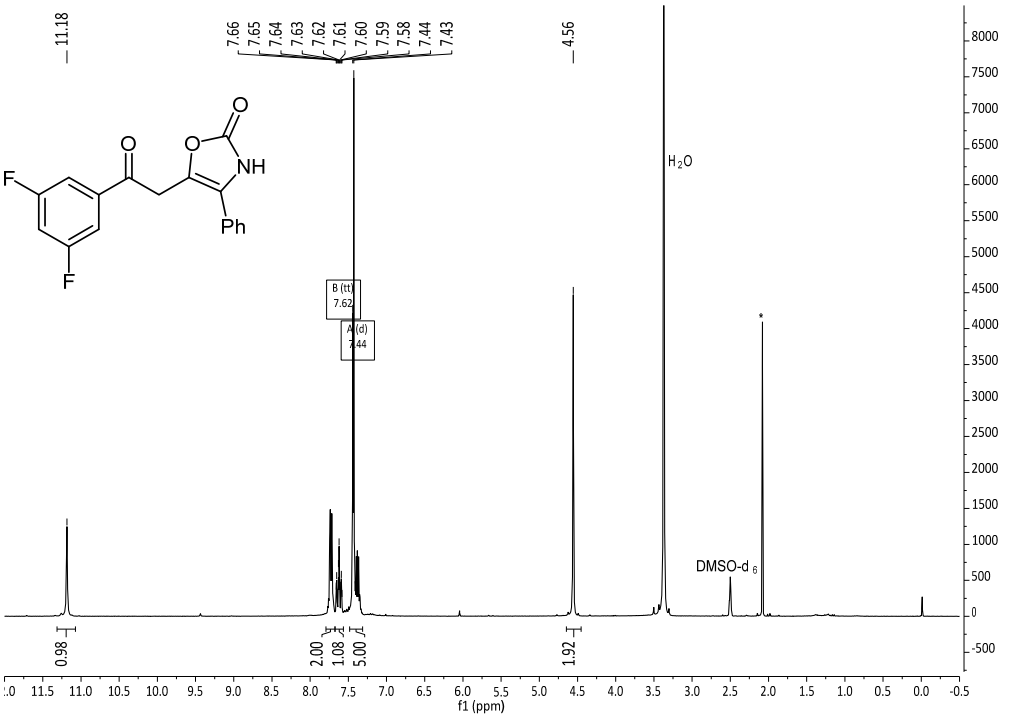
*Impurities from residual ethyl acetate and acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



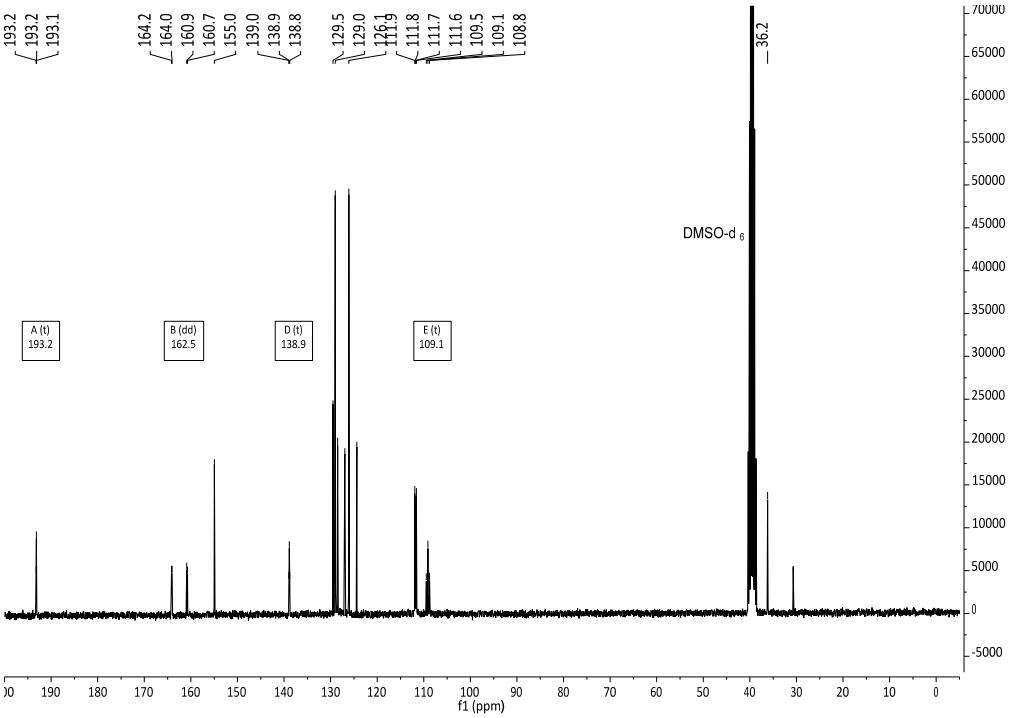
3.12 5-(2-(3,5-Difluorophenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3l)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



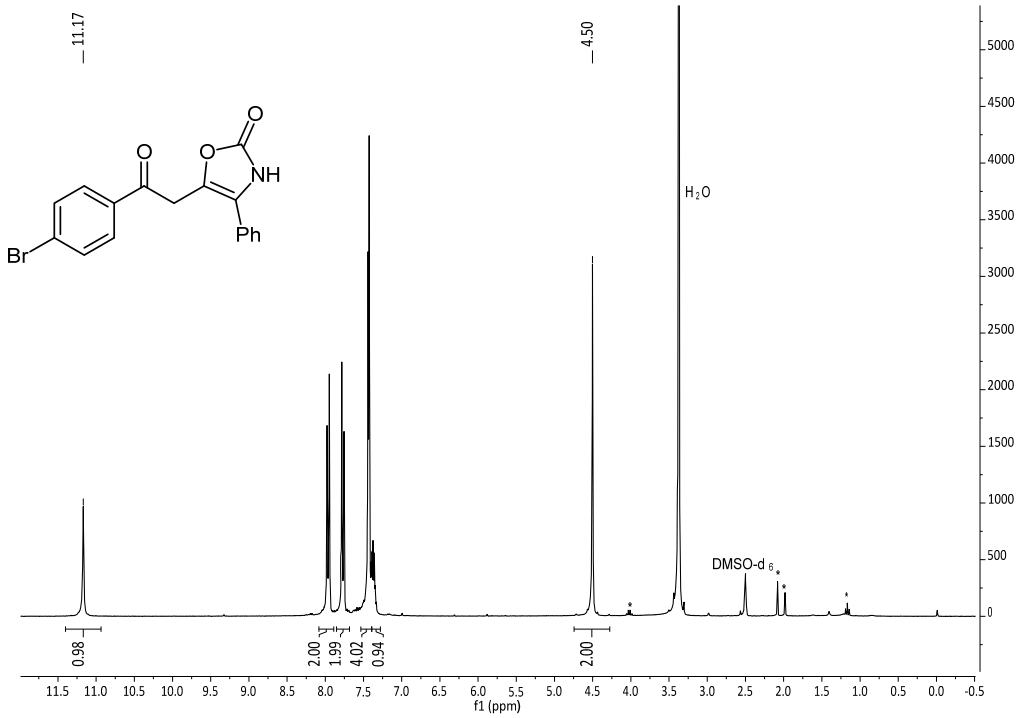
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



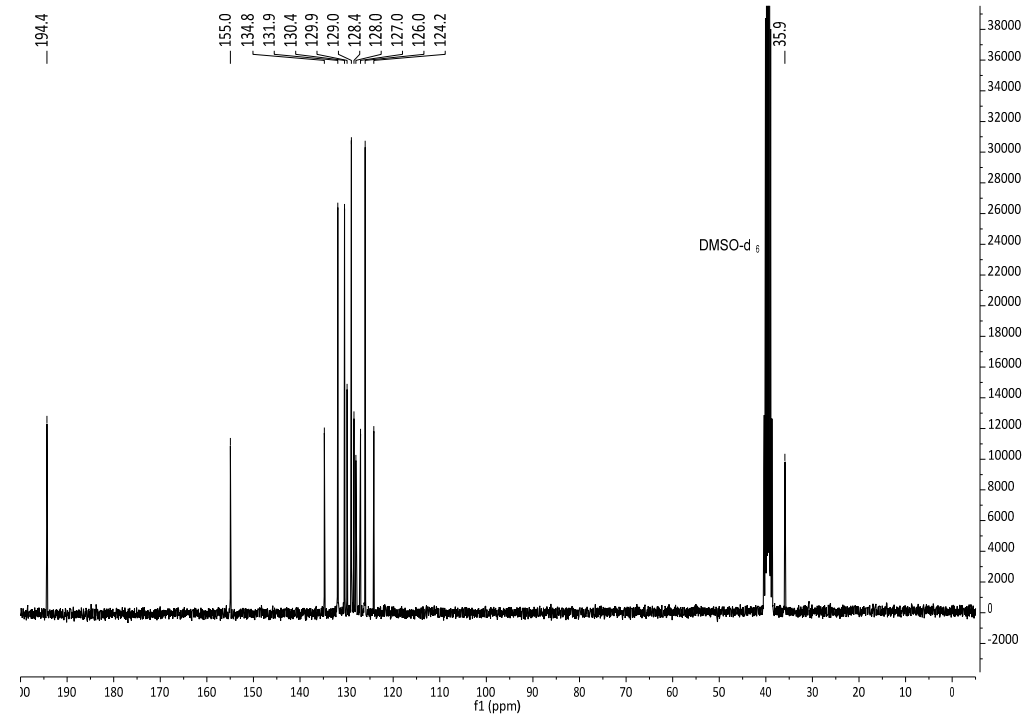
3.13 5-(2-(4-Bromophenyl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3m)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



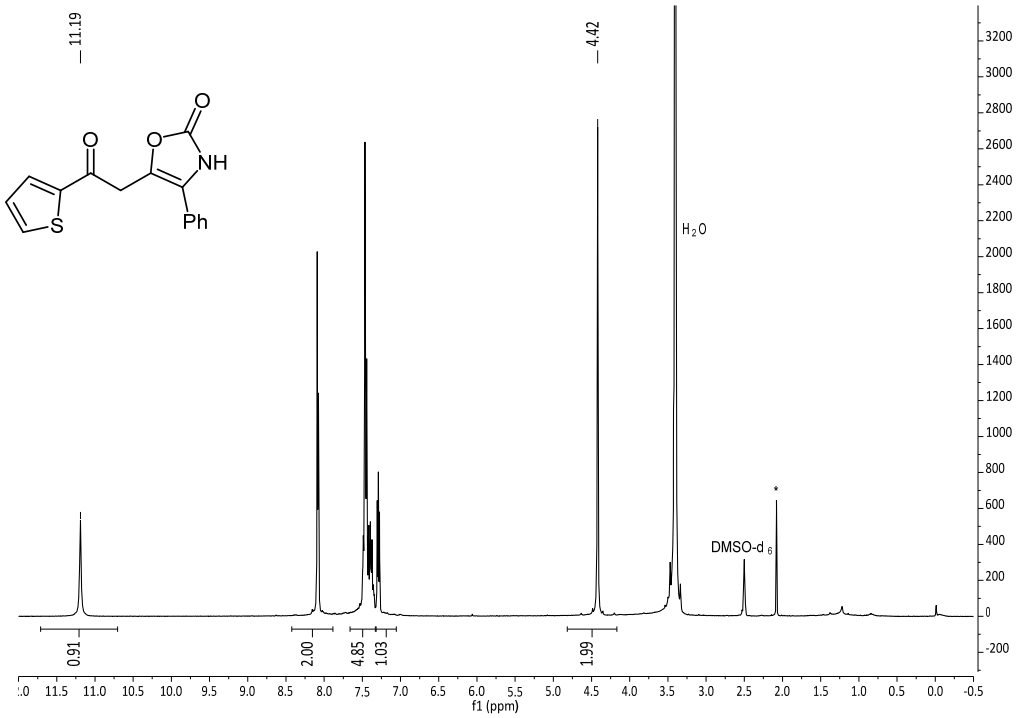
*Impurities from residual ethyl acetate and acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



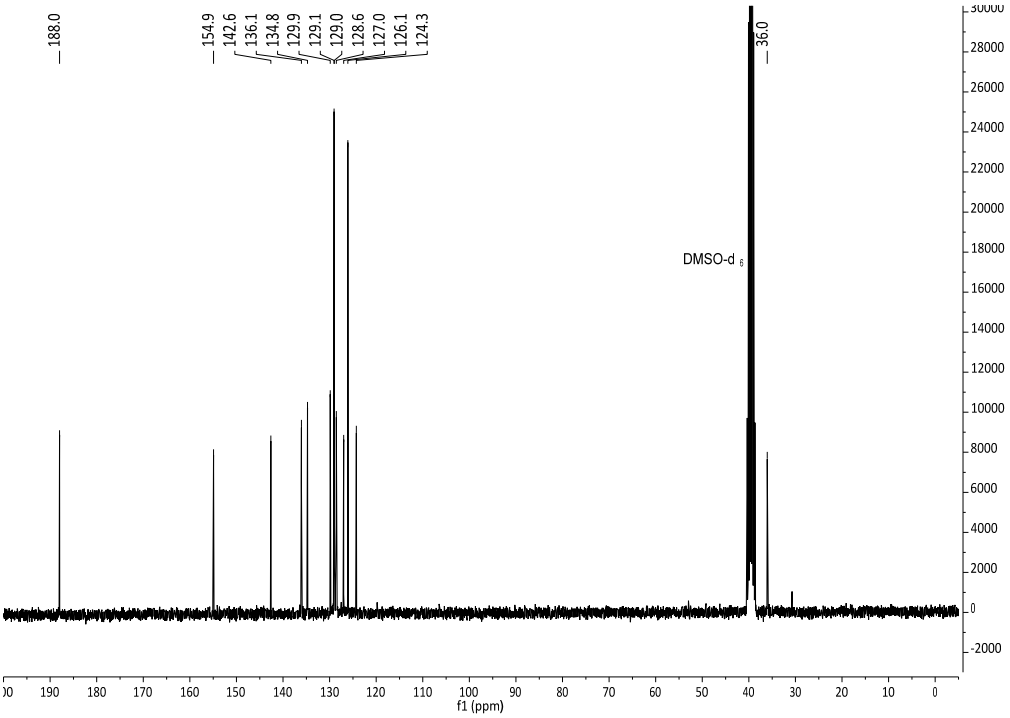
3.14 5-(2-Oxo-2-(thiophen-2-yl)ethyl)-4-phenyloxazol-2(3*H*)-one (3n)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



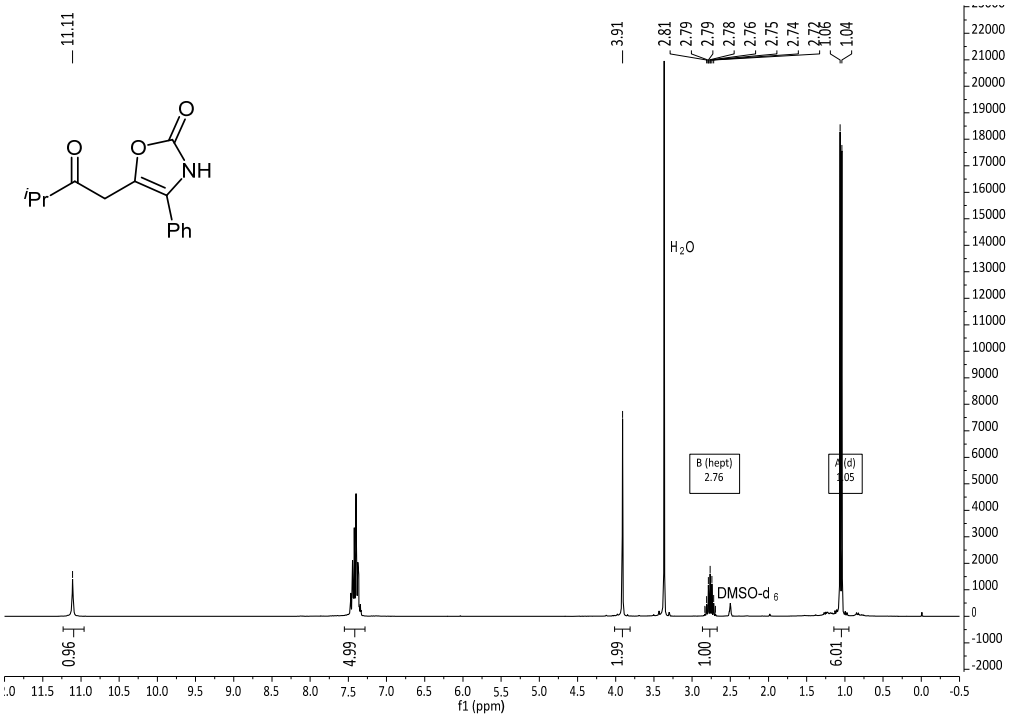
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)

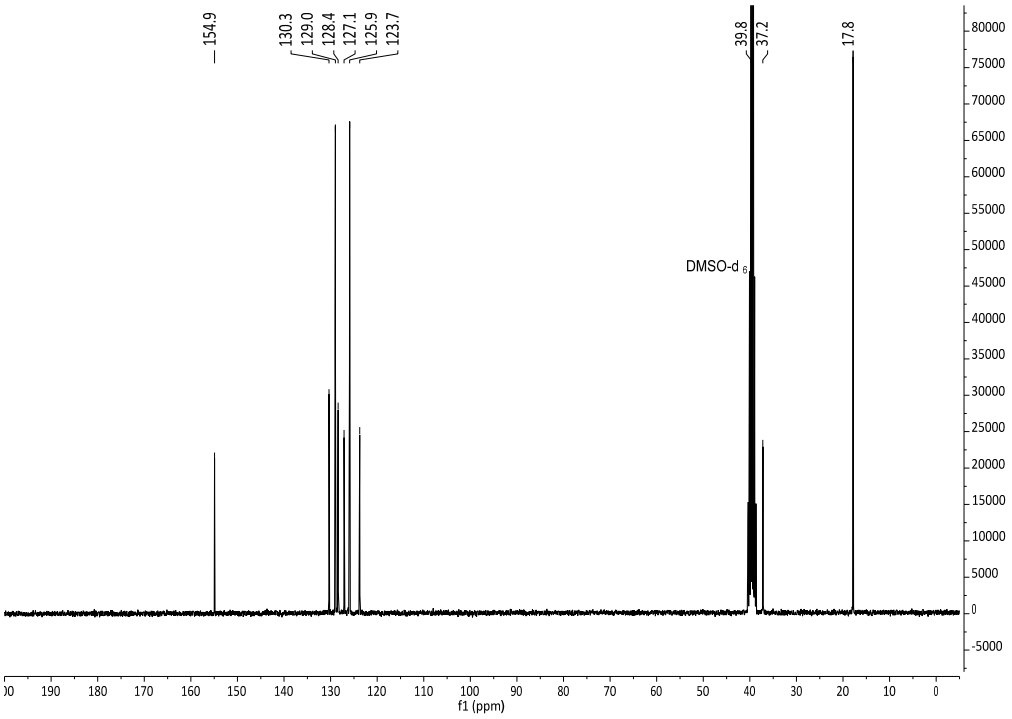


3.15 5-(3-Methyl-2-oxobutyl)-4-phenyloxazol-2(3*H*)-one (3o)

^{1}H NMR (DMSO-d$_6$, 300 MHz, 298 K)

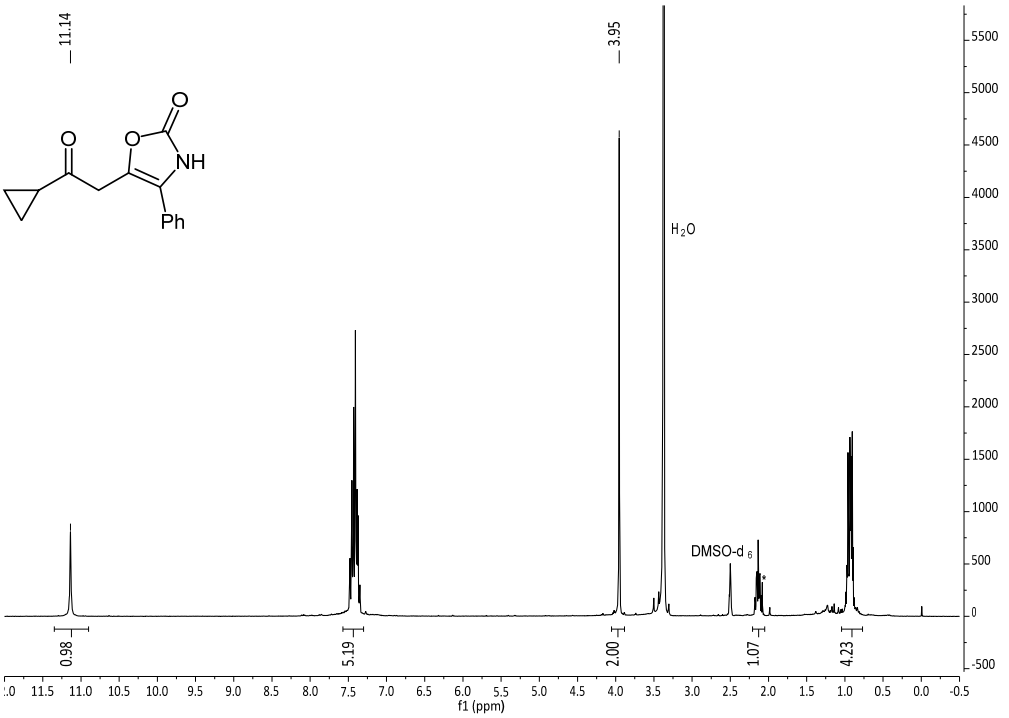


^{13}C NMR (DMSO-d$_6$, 75 MHz, 298 K)



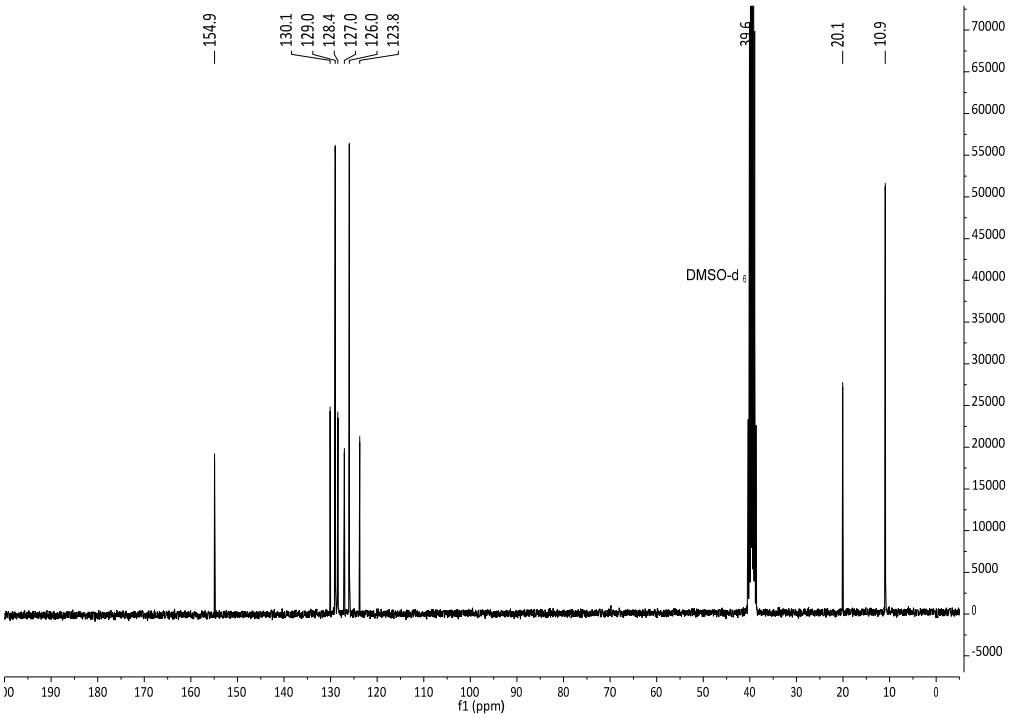
3.16 5-(2-Cyclopropyl-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3p)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



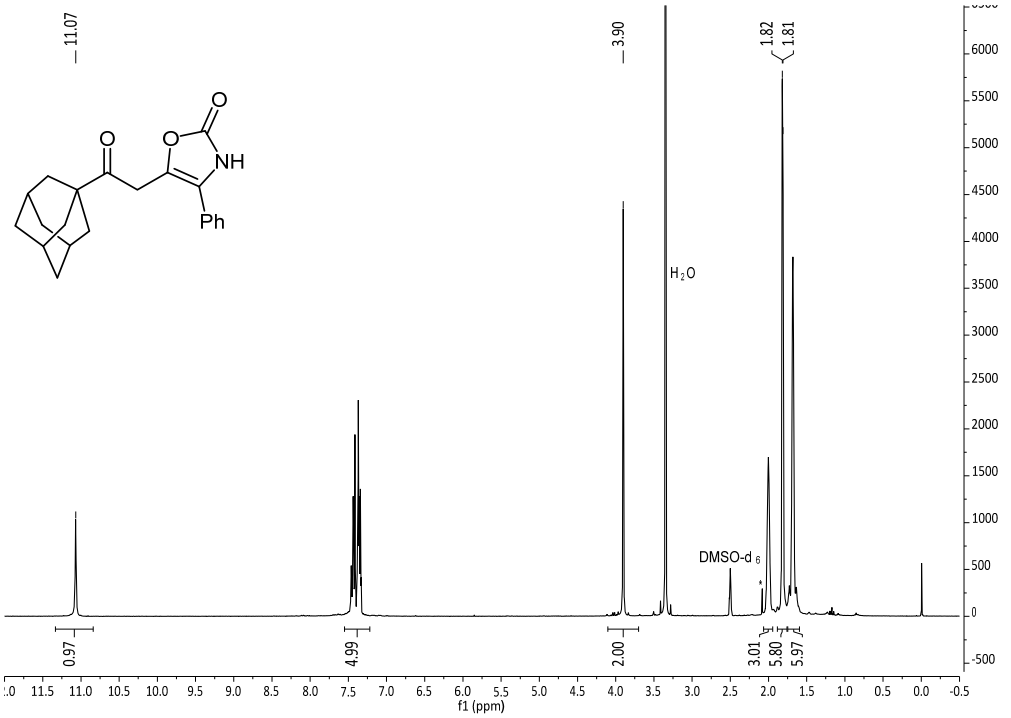
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



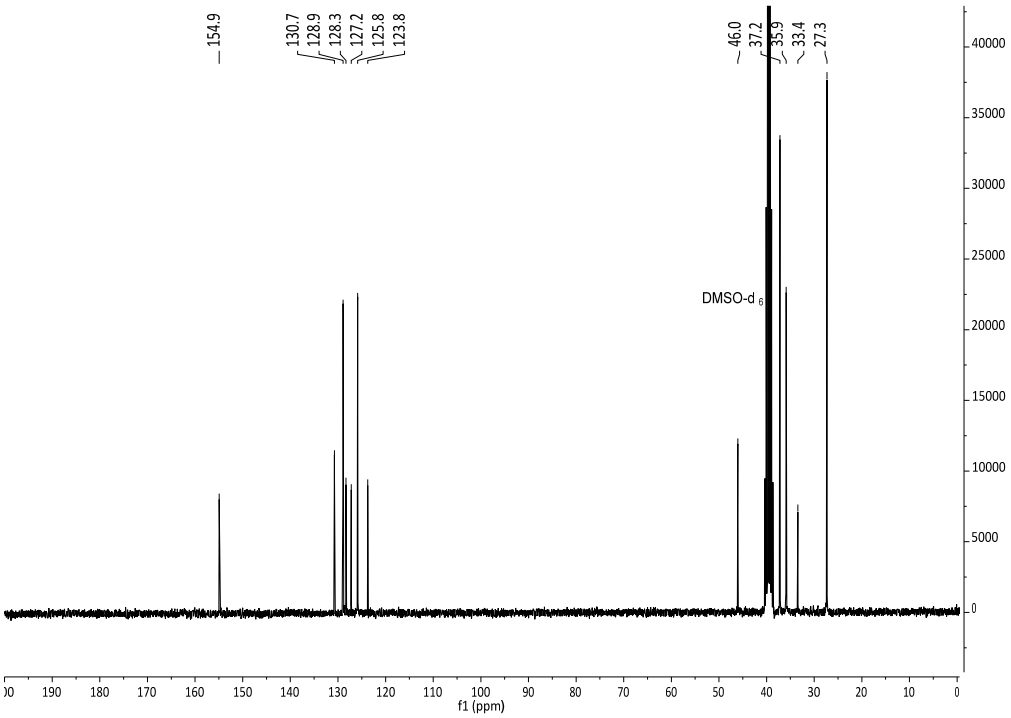
3.17 5-(2-(Adamantan-1-yl)-2-oxoethyl)-4-phenyloxazol-2(3*H*)-one (3q)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



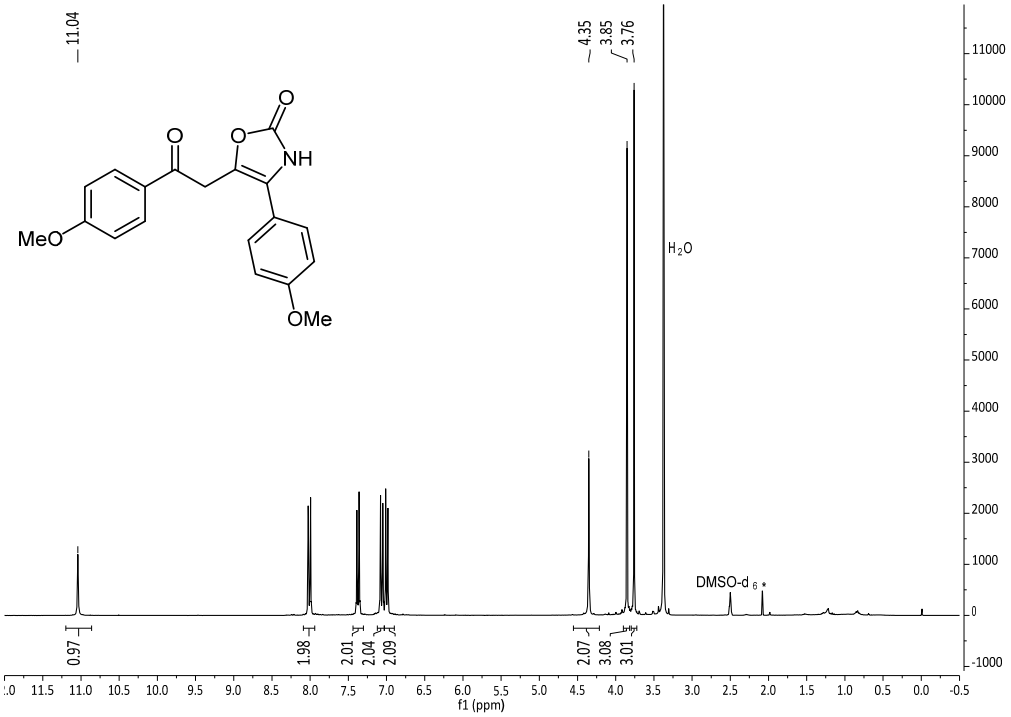
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



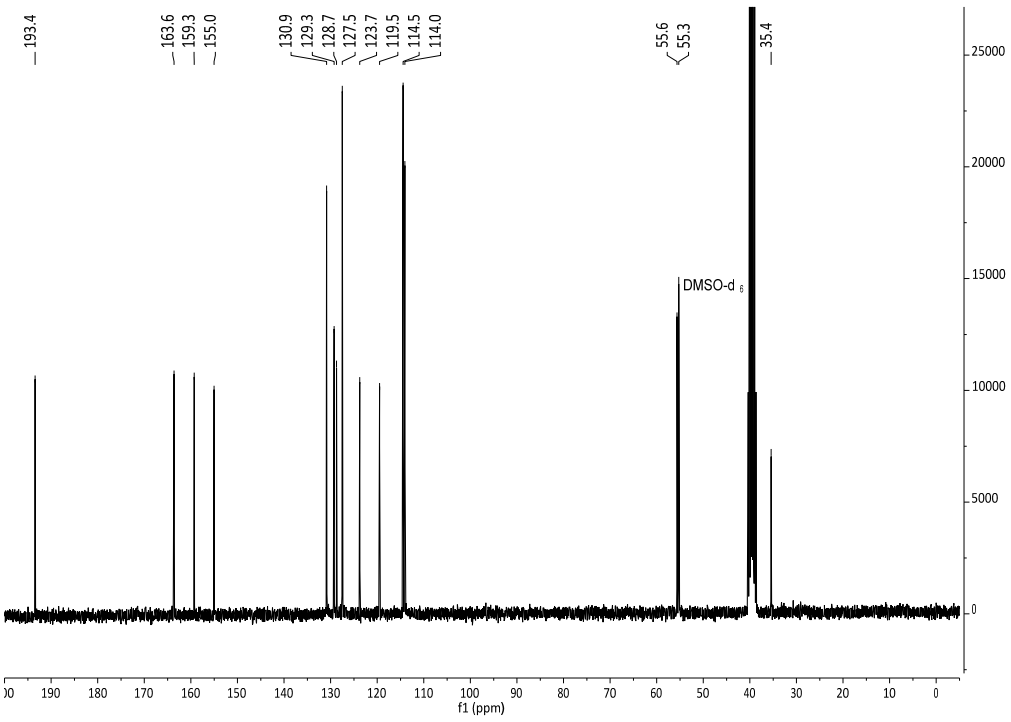
3.18 4-(4-Methoxyphenyl)-5-(2-(4-methoxyphenyl)-2-oxoethyl)oxazol-2(3*H*)-one (3r)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



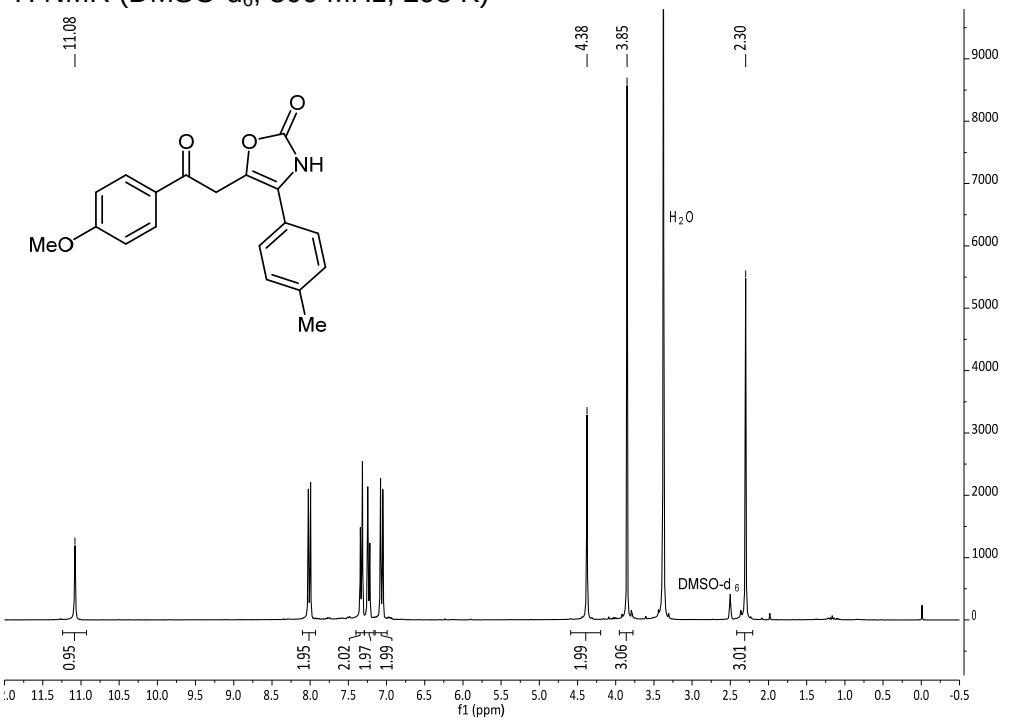
*Impuritiy from residual acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)

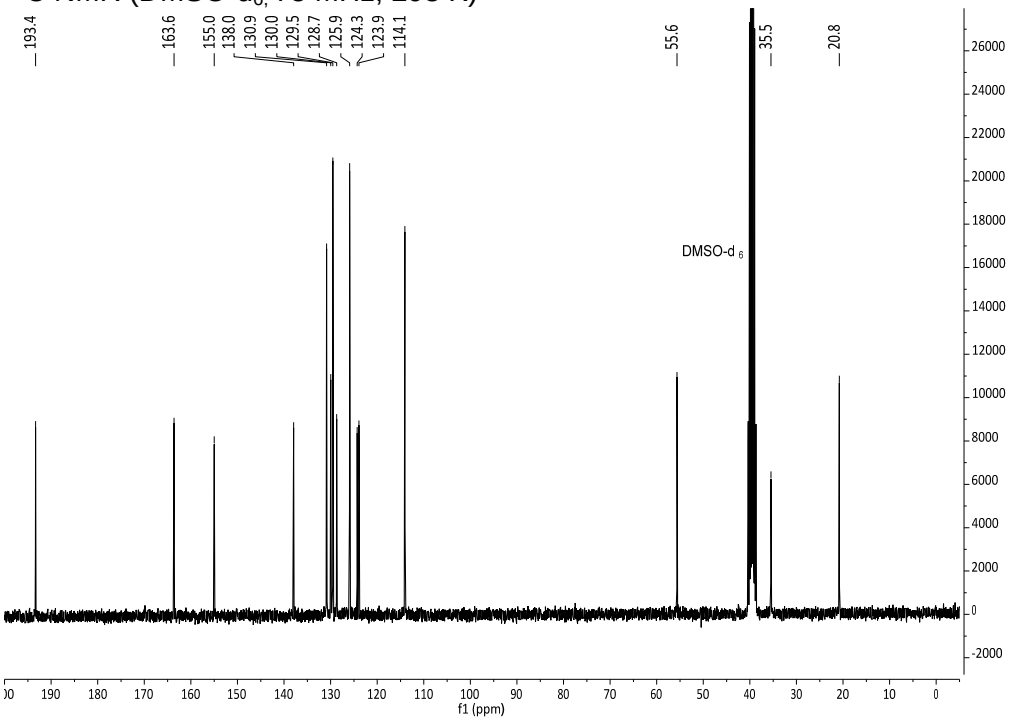


3.19 5-(2-(4-Methoxyphenyl)-2-oxoethyl)-4-(4-tolyl)oxazol-2(3*H*)-one (3s)

^{1}H NMR (DMSO-d$_6$, 300 MHz, 298 K)

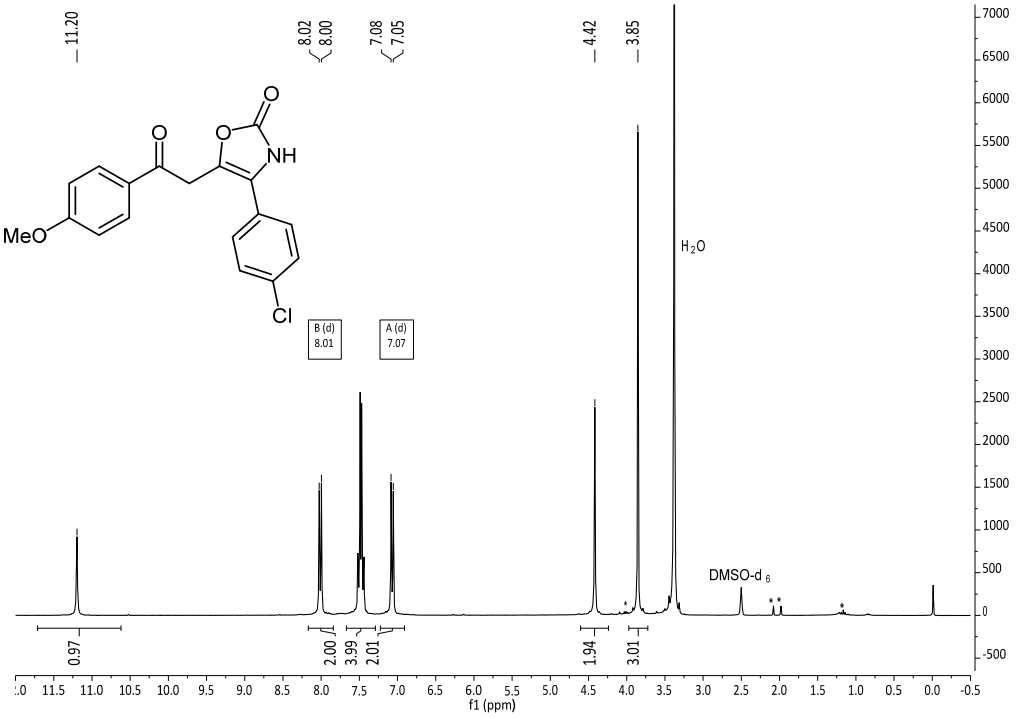


^{13}C NMR (DMSO-d$_6$, 75 MHz, 298 K)



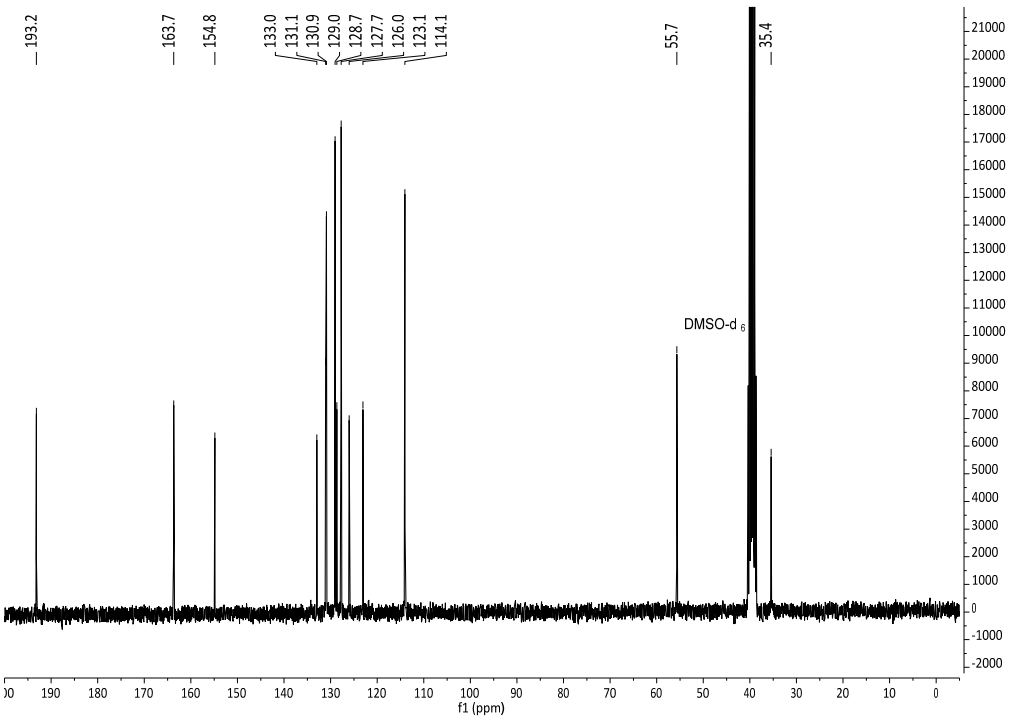
3.20 4-(4-Chlorophenyl)-5-(2-(4-methoxyphenyl)-2-oxoethyl)oxazol-2(3*H*)-one (3t)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



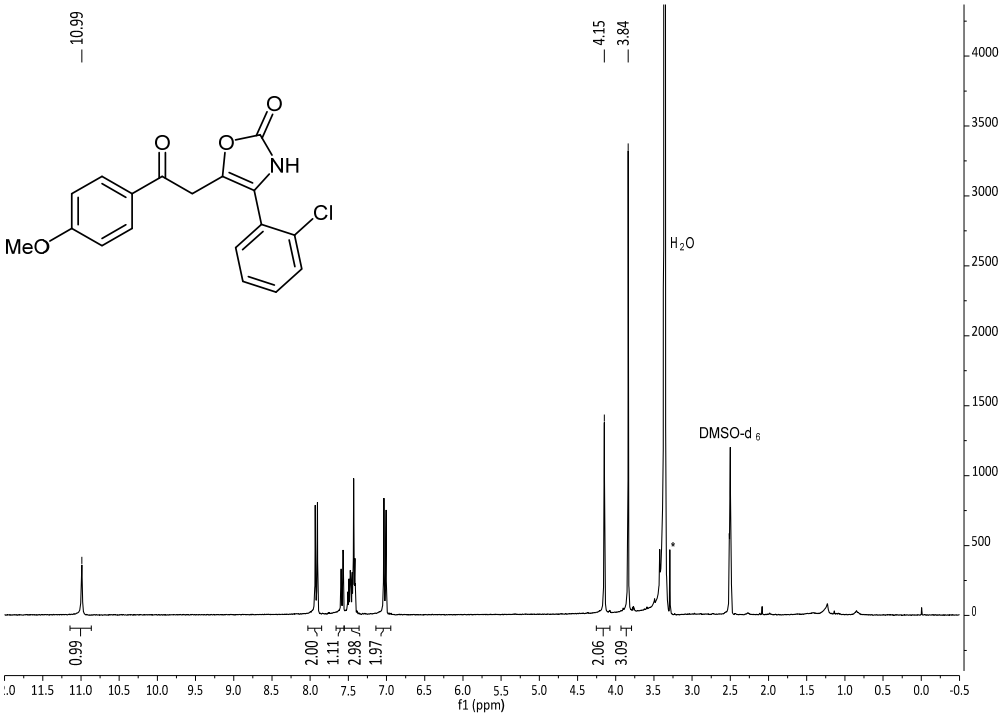
*Impurities from residual ethyl acetate and acetone.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



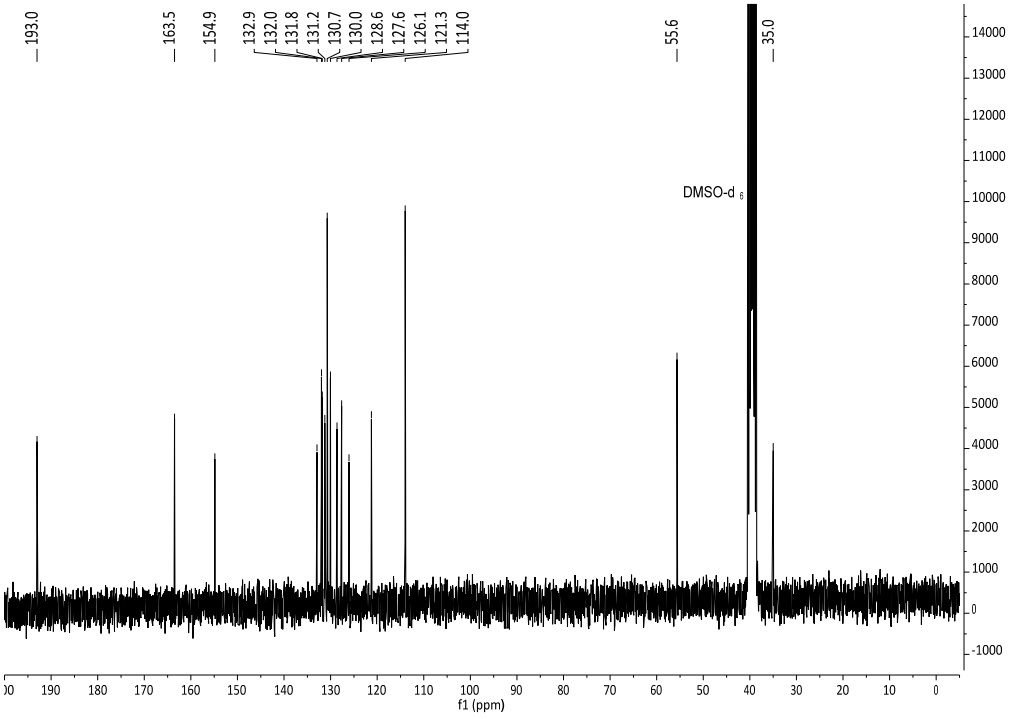
3.21 4-(2-Chlorophenyl)-5-(2-(4-methoxyphenyl)-2-oxoethyl)oxazol-2(3*H*)-one (3u)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



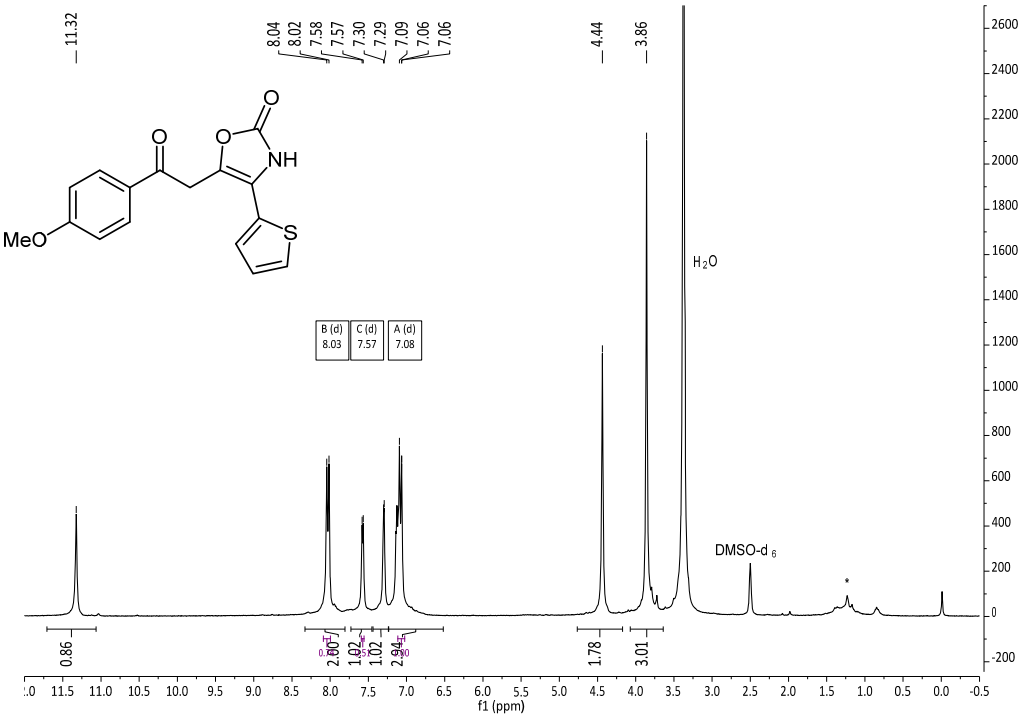
*Minor impurity.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



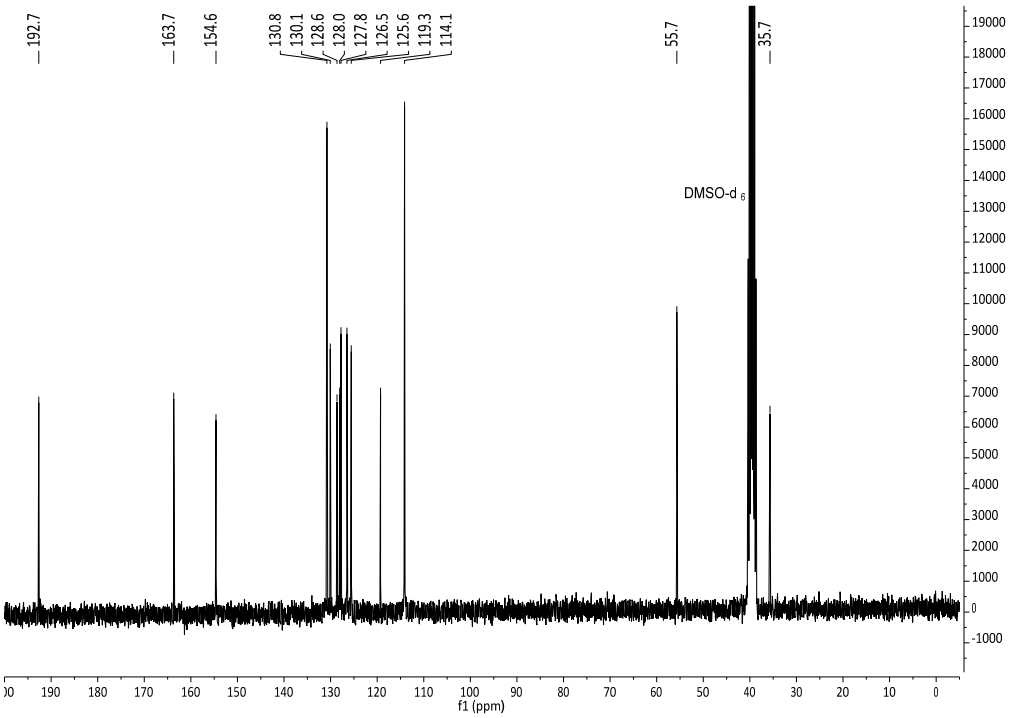
3.22 5-(2-(4-Methoxyphenyl)-2-oxoethyl)-4-(thiophen-2-yl)oxazol-2(3*H*)-one (3v)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



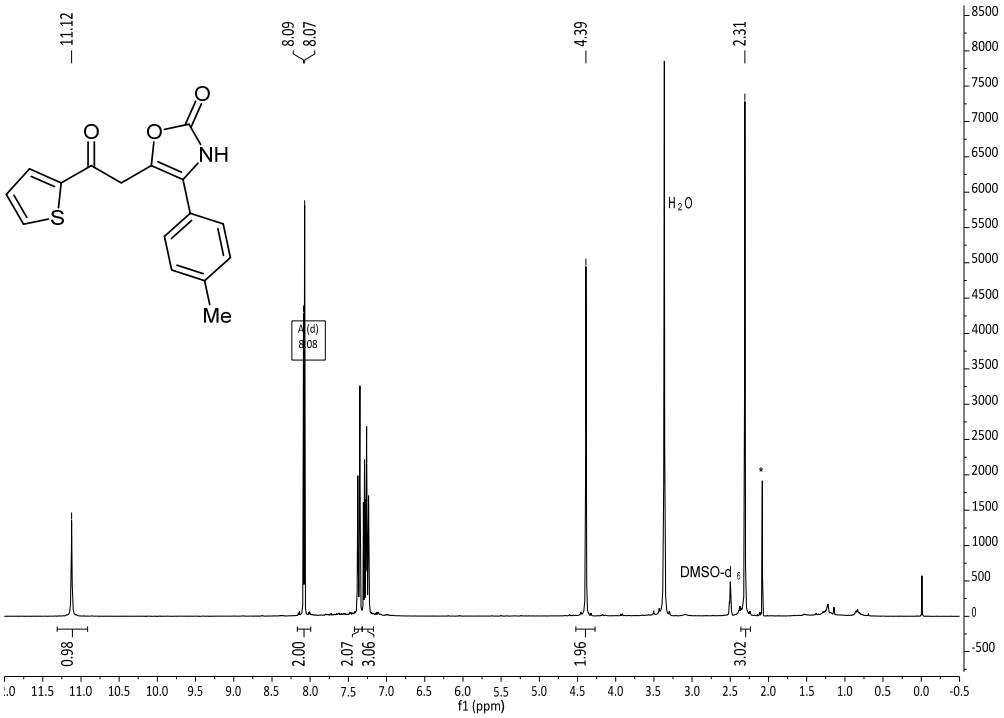
*Minor impurity.

^{13}C NMR (DMSO-d_6, 75 MHz, 298 K)



3.23 5-(2-Oxo-2-(thiophen-2-yl)ethyl)-4-(4-tolyl)oxazol-2(3*H*)-one (3w)

^{1}H NMR (DMSO-d_6, 300 MHz, 298 K)



*Impuritiy from residual acetone.