**Supporting Information**

# Efficient visible light mediated synthesis of Quinolin-2(1H)-ones from Quinoline *N*-oxides

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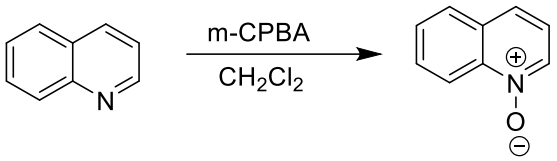
## General experimental details:

All commercially available compounds were purchased from Sigma-aldrich, TCI and other commercial suppliers and used as received. NMR spectra were recorded on BRUKER AVANCE III 400 (400 MHz for $^{1}H$; 100 MHz for $^{13}C$) spectrometer. The chemical shifts are given in parts per million (ppm) relative to $CDCl_3$ (7.28 ppm for $^{1}H$ and 77.00 for $^{13}C$) and DMSO-$d_6$ (2.49 for $^{1}H$ and 40.09 for $^{13}C$). High resolution mass spectra were recorded on Agilent Technologies, Accurate Mass Q-TOF LC/MS G65208. Normal column chromatography was performed on silica gel (60-120 mesh) purchased from SRL and eluted with petroleum ether and ethyl acetate mixture.

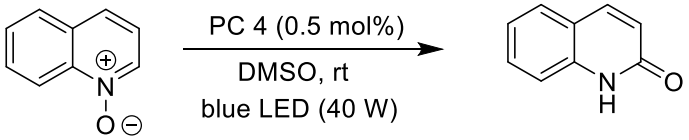
## Experimental Section:

(a) **General procedure for the synthesis of substituted quinoline N-oxides**.




To a 100 mL round bottom flask, corresponding quinoline substrates (5 mmol) and m-chloroperbenzoic acid (7.5 mmol, 1.5 equiv.) were added in 50 mL $CH_2Cl_2$. The reaction mixture was stirred at room temperature for 10 hours. Upon completion the reaction, the mixture was extracted with $CH_2Cl_2$ (30 mL x 3), dried over $Na_2SO_4$ and concentrated under reduced pressure. The crude product was purified by column chromatography (eluted with methanol/chloroform: 0 to 10 % methanol in chloroform) on silica gel to obtained quinoline N-oxides.

**(b) General procedure for the synthesis of quinoline-2(1H)-one:**




**1a** **2a**

A 4 mL screw cap vial with a small magnetic bar was charged with quinoline N-oxide (0.4 mmol, 58 mg), 1,8-dimethoxy-10-phenyl-9-(o-tolyl)acridin-10-ium chloride (PC 4, 0.002 mmol, 0.9 mg)

and DMSO (3 mL). The vial was then sealed with plastic screw cap and placed on stirring plate and irradiated for 8 hours with a 40 W blue LED at room temperature. Upon completion of the reaction as monitored by TLC, the reaction mixture was concentrated under reduced pressure on speedvac. The reduced residue was purified by column chromatography (gradient eluent of EtOAc/petroleum ether: 1/2 to 3/1) on silica gel to afford quinolone as a white solid.

**(c) Kinetic studies of different concentrated solutions:**

Three different type of quinoline N-oxide solutions, 150 mM, 300 mM and 450 mM were taken in three different vials, V1, V2 and V3 respectively and 1 mg of **PC5** is added to each solution. Then all three solution mixtures were irradiated with blue LED with stirring at room temperature. With different time interval 400 µL of solution is taken in an NMR tube and 200 µL $CDCl_3$ is added to it and checked the NMR spectra. The stack plots for the progress of the reaction with respect to concentration are as follows:

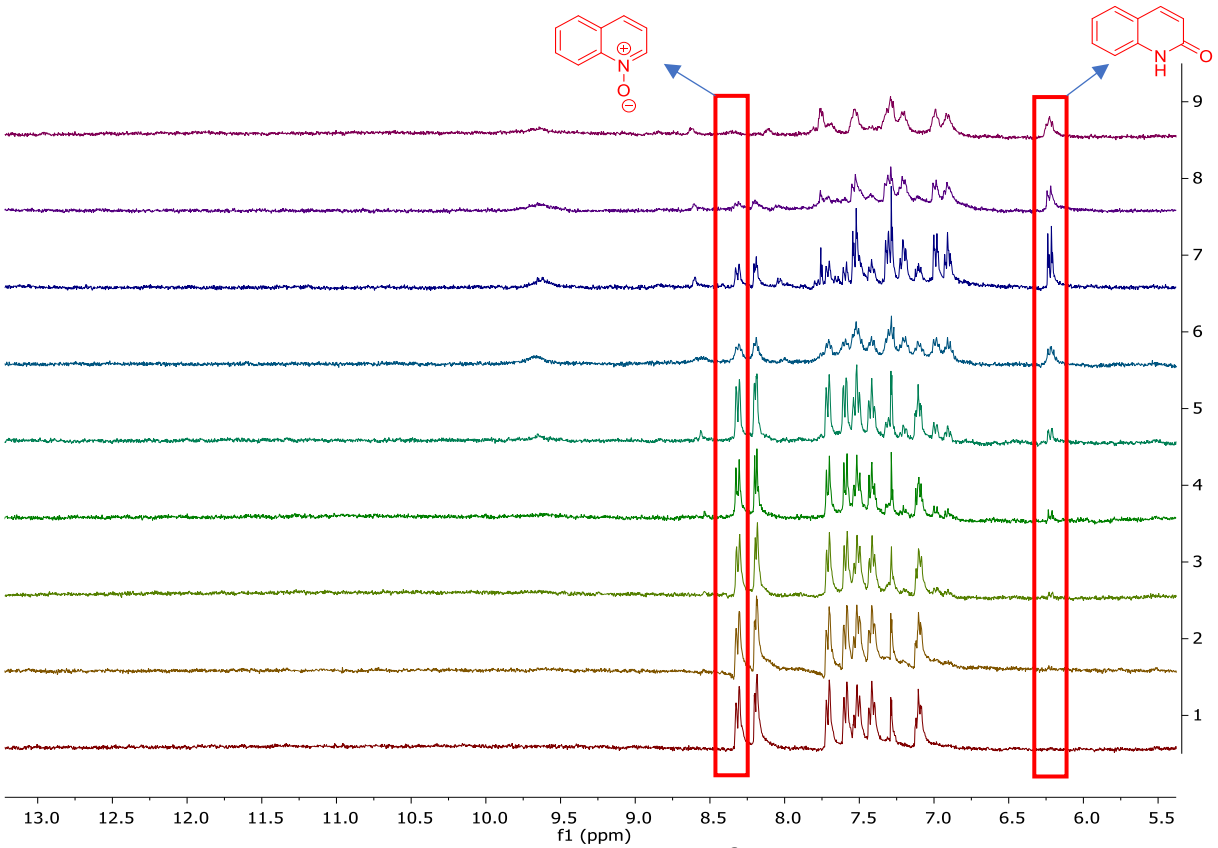



**Figure S1 A: Stack plot of 150 mM solution**

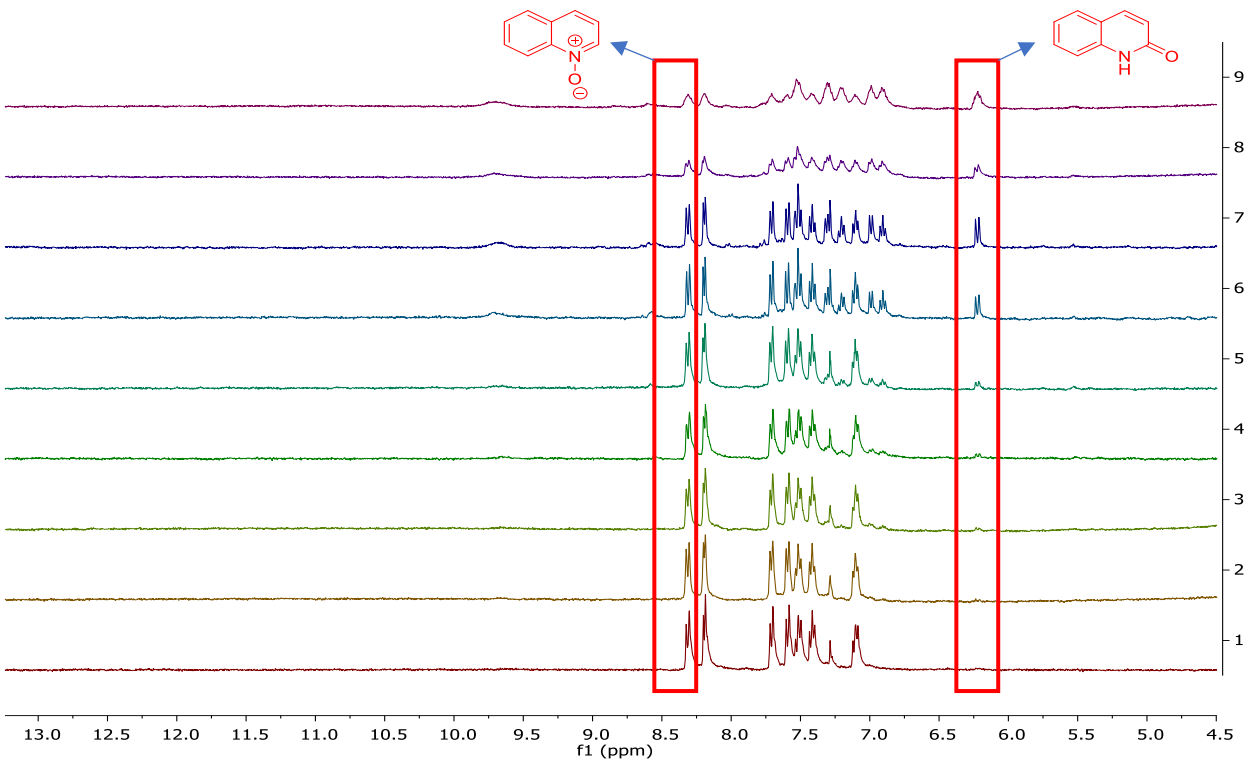



**Figure S1 B: Stack plot of 300 mM solution**

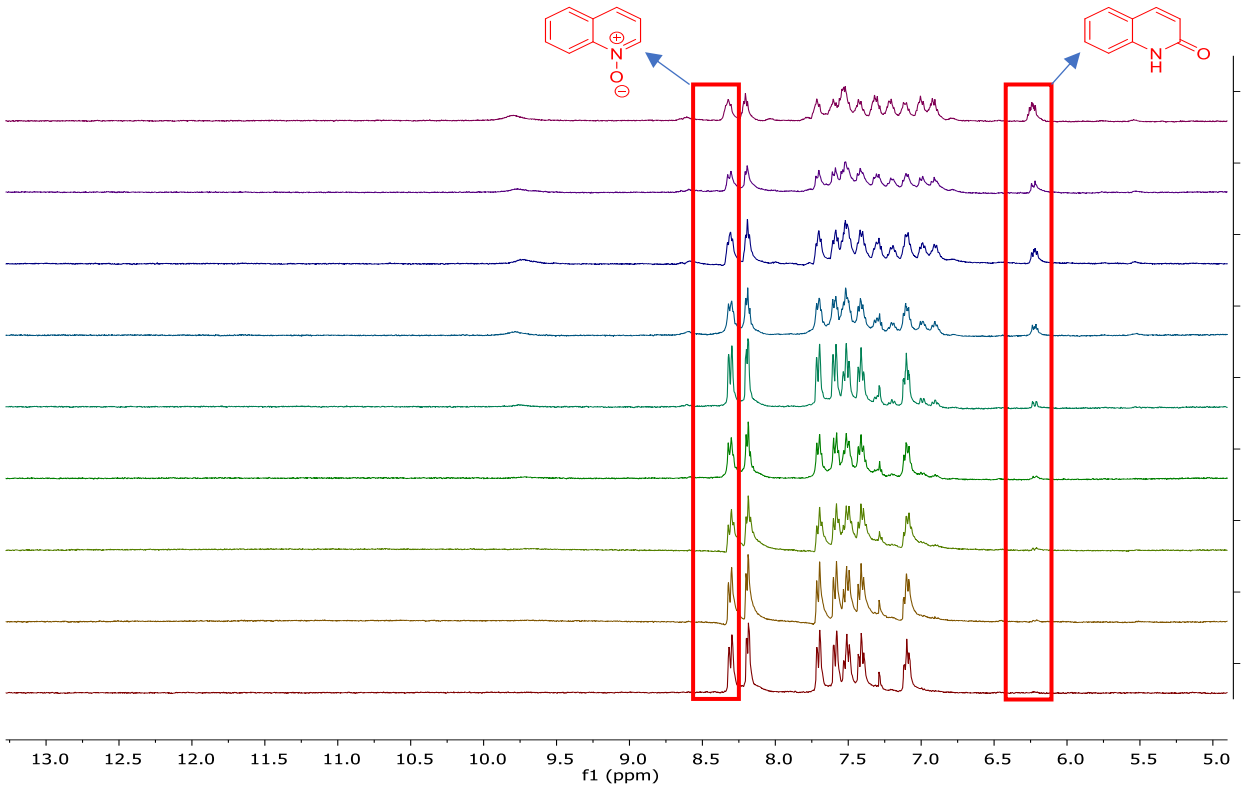



**Figure S1 C: Stack plot of 450 mM solution**

## DFT calculations of reaction pathways:

### Computational Details:

We have used M06-2X functional and 6-311G(d,p) basis set for all calculations.[1] Solvation Model based on Density (SMD) is considered to create an implicit solvation model taking acetonitrile as solvent implemented in Gaussian 16 software.[2-3] All the geometries were fully optimized and confirmed the stationary points by computing no imaginary mode of vibration for substrate, product and intermediates. The transition state geometries having one imaginary mode of vibration associated with the reaction coordinate. The excited state reduction potential of the photocatalyst computed using TD-DFT formalism.

References


1. Y. Zhao, D. G. Truhlar, *Theor. Chem. Acc*. **2008**, *120*, 215−241.
2. A. V. Marenich, C. J. Cramer, D. G. Truhlar, *J. Phys. Chem. B*. **2009**, *113*, 6378-6396.
3. M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox, Gaussian 16, Revision A.03, Gaussian, Inc., Wallingford CT, **2016**.


Cartesian Coordinate

**PC**
55

| | | | |
|---|---|---|---|
| C | -2.802254 | -0.000020 | -1.563098 |
| C | -2.333317 | 0.000010 | -0.257575 |
| C | -3.211285 | -0.000006 | 0.832036 |
| C | -4.574410 | -0.000021 | 0.568547 |
| C | -5.058799 | -0.000035 | -0.739516 |
| C | -4.173373 | -0.000039 | -1.806818 |
| C | -0.851593 | 0.000035 | -0.053074 |
| C | -0.142505 | -1.223194 | 0.000239 |
| C | 1.288397 | -1.206393 | -0.000322 |
| N | 1.937784 | -0.000060 | -0.014669 |
| C | 1.288478 | 1.206317 | -0.000468 |
| C | -0.142429 | 1.223239 | 0.000173 |
| C | -0.783234 | -2.527354 | 0.038049 |
| C | -0.026645 | -3.677940 | 0.014536 |
| C | 1.372314 | -3.598678 | -0.014726 |
| C | 2.036452 | -2.400192 | -0.012964 |
| C | 2.036645 | 2.400041 | -0.013315 |
| C | 1.372625 | 3.598590 | -0.015143 |
| C | -0.026320 | 3.677989 | 0.014310 |
| C | -0.783020 | 2.527483 | 0.038027 |
| C | 3.388933 | -0.000096 | -0.043380 |
| C | 4.083830 | 0.000030 | 1.157257 |
| C | 5.473990 | -0.000003 | 1.125002 |

| | | | |
|---|---|---|---|
| C | 6.143184 | -0.000157 | -0.095096 |
| C | 5.428465 | -0.000278 | -1.289141 |
| C | 4.038064 | -0.000246 | -1.269366 |
| H | 1.945932 | -4.517580 | -0.028487 |
| O | -2.108793 | -2.535103 | 0.124379 |
| C | -2.809935 | -3.772766 | 0.130880 |
| O | -2.108553 | 2.535440 | 0.124676 |
| C | -2.809484 | 3.773222 | 0.131187 |
| H | 1.946331 | 4.517435 | -0.029056 |
| H | -0.501902 | -4.647024 | 0.035580 |
| H | -0.501481 | 4.647121 | 0.035379 |
| H | 3.114657 | -2.371087 | -0.023472 |
| H | 3.114847 | 2.370828 | -0.023912 |
| H | 3.461366 | -0.000340 | -2.187055 |
| H | 5.951524 | -0.000396 | -2.237025 |
| H | 7.225775 | -0.000182 | -0.115448 |
| H | 6.032322 | 0.000092 | 2.052548 |
| H | 3.541907 | 0.000150 | 2.095929 |
| H | -2.100452 | -0.000021 | -2.389982 |
| H | -4.540694 | -0.000058 | -2.825509 |
| H | -5.271169 | -0.000020 | 1.399894 |
| H | -3.860588 | 3.503021 | 0.181051 |
| H | -2.534073 | 4.368503 | 1.005089 |
| H | -2.611532 | 4.332109 | -0.786262 |
| H | -3.861003 | -3.502381 | 0.180506 |
| H | -2.611898 | -4.331785 | -0.786470 |
| H | -2.534799 | -4.368001 | 1.004900 |
| H | -6.127129 | -0.000048 | -0.918507 |
| C | -2.674637 | 0.000016 | 2.236021 |
| H | -3.482616 | 0.000047 | 2.966897 |
| H | -2.054945 | -0.884065 | 2.415061 |
| H | -2.054912 | 0.884081 | 2.415025 |

**1a**

18

| | | | |
|---|---|---|---|
| C | -0.022490 | 0.000000 | -0.037100 |
| C | -0.039972 | 0.000000 | 1.370872 |
| C | 1.150466 | -0.000000 | 2.052655 |
| C | 2.380873 | -0.000000 | 1.355584 |
| C | 2.401591 | -0.000000 | -0.014571 |
| C | 1.192744 | -0.000000 | -0.756923 |
| H | -0.996114 | 0.000000 | 1.874222 |
| H | 1.149005 | -0.000000 | 3.136092 |
| H | 3.310190 | -0.000000 | 1.912543 |
| H | 3.339071 | -0.000000 | -0.559201 |
| C | 1.165080 | -0.000000 | -2.174106 |
| C | -0.047088 | 0.000000 | -2.805292 |
| C | -1.237956 | 0.000000 | -2.062515 |
| N | -1.241646 | 0.000000 | -0.726459 |
| H | 2.096212 | -0.000000 | -2.727532 |
| H | -0.126211 | 0.000000 | -3.884654 |
| H | -2.221109 | 0.000000 | -2.511189 |
| O | -2.337522 | 0.000000 | -0.066925 |

**II**

18

| | | | |
|---|---|---|---|
| C | -0.026091 | 0.000000 | -0.005265 |
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| C | 1.168121 | -0.000000 | 2.052955 |
| C | 2.389158 | -0.000000 | 1.358574 |
| C | 2.403758 | -0.000000 | -0.017091 |
| C | 1.186160 | -0.000000 | -0.735002 |
| H | -0.984594 | 0.000000 | 1.919909 |
| H | 1.170100 | -0.000000 | 3.136157 |
| H | 3.319212 | -0.000000 | 1.912326 |
| H | 3.333117 | -0.000000 | -0.573705 |
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| C | -1.242194 | 0.000000 | -2.106636 |
| N | -1.229153 | 0.000000 | -0.734708 |
| H | 2.078577 | -0.000000 | -2.694531 |
| H | -0.116473 | 0.000000 | -3.899057 |
| H | -2.233559 | 0.000000 | -2.540181 |
| O | -2.329346 | 0.000000 | -0.123522 |

**$TS_{II\_III}$**

18

| | | | |
|---|---|---|---|
| C | -0.027935 | 0.087482 | 0.093121 |
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| C | 1.206963 | 0.065640 | 2.114194 |
| C | 2.391943 | 0.017028 | 1.377637 |
| C | 2.366646 | -0.010598 | -0.009719 |
| C | 1.142878 | 0.022593 | -0.683648 |
| H | -0.960651 | 0.147429 | 2.020945 |
| H | 1.244339 | 0.076380 | 3.196303 |

| | | | |
|---|---|---|---|
| H | 3.342097 | -0.006995 | 1.896317 |
| H | 3.284166 | -0.059629 | -0.584415 |
| C | 1.041157 | -0.080554 | -2.122275 |
| C | -0.143535 | -0.020440 | -2.789168 |
| C | -1.328858 | 0.189194 | -2.036887 |
| N | -1.235449 | 0.100302 | -0.646169 |
| H | 1.966915 | -0.185508 | -2.678316 |
| H | -0.205507 | -0.037156 | -3.867856 |
| H | -2.250324 | 0.597272 | -2.429962 |
| O | -1.892261 | -1.005340 | -0.948146 |

**III**

18

| | | | |
|---|---|---|---|
| N | -1.342314 | -0.276644 | -0.651114 |
| C | -0.076032 | -0.164957 | -0.001504 |
| C | 1.144819 | 0.007805 | -0.732314 |
| C | 1.128573 | -0.013897 | -2.136565 |
| C | -0.059201 | -0.202366 | -2.811596 |
| C | -1.338892 | -0.226690 | -2.086851 |
| C | 2.366288 | 0.157293 | -0.016287 |
| C | 2.366381 | 0.123921 | 1.354602 |
| C | 1.156883 | -0.067584 | 2.045918 |
| C | -0.064087 | -0.212312 | 1.367355 |
| O | -1.641522 | 0.953207 | -1.380954 |
| H | -0.991338 | -0.349967 | 1.908912 |
| H | 1.162590 | -0.102161 | 3.128790 |
| H | 3.288683 | 0.235538 | 1.909260 |
| H | 3.282775 | 0.280745 | -0.581304 |
| H | 2.060371 | 0.079105 | -2.682436 |
| H | -0.077422 | -0.328341 | -3.886919 |
| H | -2.176390 | -0.716000 | -2.570172 |

**IV**

18

| | | | |
|---|---|---|---|
| N | -1.331247 | -0.265725 | -0.641995 |
| C | -0.053034 | -0.134039 | -0.004276 |
| C | 1.139113 | 0.043978 | -0.725064 |
| C | 1.110595 | -0.025594 | -2.183612 |
| C | -0.042365 | -0.206085 | -2.831970 |
| C | -1.320166 | -0.204959 | -2.086943 |
| C | 2.335036 | 0.179366 | -0.016647 |
| C | 2.345328 | 0.127401 | 1.372547 |
| C | 1.159785 | -0.081624 | 2.072943 |
| C | -0.039775 | -0.220198 | 1.380910 |
| O | -1.650850 | 0.966312 | -1.385735 |
| H | -0.976419 | -0.379252 | 1.902633 |
| H | 1.167041 | -0.131019 | 3.155191 |
| H | 3.279899 | 0.239484 | 1.909368 |
| H | 3.259330 | 0.316849 | -0.567679 |
| H | 2.057940 | 0.003470 | -2.711147 |
| H | -0.086254 | -0.351911 | -3.904098 |
| H | -2.163792 | -0.699757 | -2.557605 |

**$TS_{IV\_2a}$**

18

| | | | |
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| N | -1.231759 | -0.311192 | -0.539602 |
| C | -0.059918 | -0.153727 | 0.022597 |
| C | 1.171494 | -0.023844 | -0.739202 |
| C | 1.104715 | 0.008944 | -2.171110 |
| C | -0.103783 | -0.025677 | -2.760013 |
| C | -1.385787 | -0.147588 | -1.985258 |
| C | 2.375570 | 0.080973 | -0.041329 |
| C | 2.380820 | 0.062854 | 1.342020 |
| C | 1.192449 | -0.059328 | 2.106361 |
| C | -0.003467 | -0.155688 | 1.463327 |
| O | -2.221238 | 0.885604 | -2.108021 |
| H | -0.944349 | -0.248900 | 1.992724 |
| H | 1.250546 | -0.072055 | 3.186922 |
| H | 3.327860 | 0.146721 | 1.863882 |
| H | 3.303945 | 0.179381 | -0.591246 |
| H | 2.027241 | 0.118371 | -2.730445 |
| H | -0.210290 | 0.049503 | -3.837213 |
| H | -1.783884 | -1.157657 | -2.297574 |

**2a**

18

| | | | |
|---|---|---|---|
| N | -1.211201 | 0.000000 | -0.730267 |
| C | -0.029978 | 0.000000 | -0.018411 |
| C | 1.186053 | -0.000000 | -0.724954 |
| C | 1.128433 | -0.000000 | -2.165687 |
| C | -0.048870 | 0.000000 | -2.820528 |
| C | -1.325853 | 0.000000 | -2.105701 |
| C | 2.392762 | -0.000000 | -0.006039 |
| C | 2.389135 | -0.000000 | 1.374556 |

| | | | |
|---|---|---|---|
| C | 1.167893 | -0.000000 | 2.065673 |
| C | -0.033847 | 0.000000 | 1.384050 |
| H | -2.084709 | 0.000000 | -0.213056 |
| H | -0.980383 | 0.000000 | 1.913160 |
| H | 1.163614 | -0.000000 | 3.149446 |
| H | 3.322239 | -0.000000 | 1.924263 |
| H | 3.325824 | -0.000000 | -0.559385 |
| H | 2.065003 | -0.000000 | -2.714417 |
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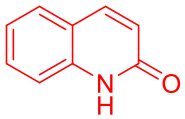
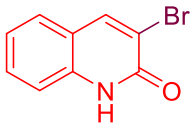
| O | -2.421472 | 0.000000 | -2.646658 |

## Characterization Data of Compounds:



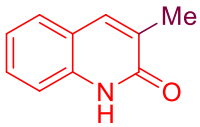
2a

***quinolin-2(1H)-one(2a):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 11.87 (s, 1H), 7.89 (d, $J$ = 9.5 Hz, 1H), 7.63 (d, $J$ = 7.7 Hz, 1H), 7.48 (t, $J$ = 7.7 Hz, 1H), 7.34 (d, $J$ = 8.2 Hz, 1H), 7.15 (t, $J$ = 7.5 Hz, 1H), 6.52 (d, $J$ = 9.5 Hz, 1H). $^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.45, 140.87, 139.25, 130.85, 128.32, 122.31, 122.09, 119.65, 115.70. HRMS: m/z (ESI) calculated for ($C_9H_7NO$) $[M+H]^+$ : 146.0600, measured: 146.0623.



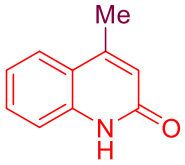
3

***3-bromoquinolin-2(1H)-one (3):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 12.06 (s, 1H), 8.51 (s, 1H), 7.68 (d, $J$ = 7.7 Hz, 1H), 7.55 (t, $J$ = 8.2 Hz, 1H), 7.34 (d, $J$ = 8.2 Hz, 1H), 7.22 (t, $J$ = 7.5 Hz, 1H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 158.15, 142.18, 138.65, 131.21, 127.80, 122.79, 119.87, 117.55, 115.70. HRMS: m/z (ESI) calculated for ($C_9H_6BrNO$) $[M+H]^+$: 223.9705 and 225.9685, measured: 223.9682 and 225.9705.



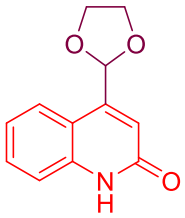
4

***3-methylquinolin-2(1H)-one (4):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 10.95 (s, 1H), 7.67 (s, 1H), 7.53 (d, *J* = 7.7 Hz, 1H), 7.47 (t, *J* = 6.9 Hz, 1H), 7.33 (d, *J* = 7.4 Hz, 1H), 7.22 (t, *J* = 7.4 Hz, 1H), 2.31 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.14, 137.42, 137.34, 130.21, 129.32, 126.97, 122.49, 120.36, 115.30, 16.80. HRMS: m/z (ESI) calculated for ($C_{10}H_9NO$) $[M+H]^+$: 160.0757, measured: 106.0783.




5

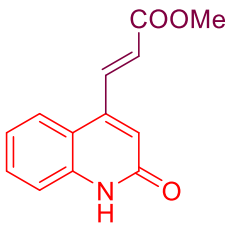
***4-methylquinolin-2(1H)-one (5):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 12.88 (s, 1H), 7.68 (d, *J* = 8.0 Hz, 1H), 7.50 (d, *J* = 6.0 Hz, 2H), 7.31 – 7.15 (m, 1H), 6.61 (s, 1H), 2.52 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.56, 149.34, 138.29, 130.50, 124.35, 122.49, 120.43, 116.74, 19.19. HRMS: m/z (ESI) calculated for ($C_{10}H_9NO$) $[M+H]^+$: 160.0757, measured: 160.0793.




6

***4-(1,3-dioxolan-2-yl)quinolin-2(1H)-one:*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 12.45 (s, 1H), 7.94 (d, *J* = 7.7 Hz, 1H), 7.55 (t, *J* = 7.6 Hz, 1H), 7.48 (d, *J* = 7.6 Hz, 1H), 7.31 – 7.24 (m, 1H), 7.00 (s, 1H), 6.30 (s, 1H), 4.15 (s, 4H).

$^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.32, 147.57, 138.89, 130.63, 125.03, 122.73, 117.96, 117.88, 116.61, 100.25, 65.39. HRMS: m/z (ESI) calculated for ($C_{12}H_{11}NO$) $[M+H]^+$: 218.2315, measured: 218.2297.



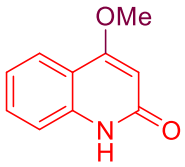

7

***methyl (E)-3-(2-oxo-1,2-dihydroquinolin-4-yl)acrylate (7):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^1$H NMR (400 MHz, Chloroform-*d*) δ 11.54 (s, 1H), 7.59 – 7.51 (m, 2H), 7.40 (d, *J* = 8.1 Hz, 1H), 7.26 – 7.17 (m, 2H), 6.61 (s, 1H), 6.35 (d, *J* = 12.1 Hz, 1H), 3.63 (s, 3H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 165.10, 147.62, 138.33, 138.18, 130.82, 125.16, 125.10, 122.73, 119.53, 118.60, 116.48, 51.68. HRMS: m/z (ESI) calculated for ($C_{13}H_{11}NO_3$) $[M+H]^+$: 230.0812, measured: 230.0823.


8

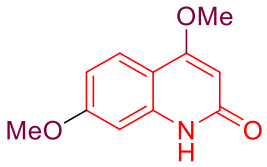
***4-(hydroxymethyl)quinolin-2(1H)-one (8):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 11.63 (s, 1H), 7.65 (d, *J* = 8.1 Hz, 1H), 7.49 (t, *J* = 7.7 Hz, 1H), 7.32 (d, *J* = 8.1 Hz, 1H), 7.17 (t, *J* = 7.6 Hz, 1H), 6.55 (s, 1H), 5.50 (t, *J* = 5.6 Hz, 1H), 4.76 (d, *J* = 5.5 Hz, 2H).

$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.35, 151.75, 139.16, 130.60, 124.15, 122.04, 117.77, 115.96, 60.02. HRMS: m/z (ESI) calculated for ($C_{10}H_9NO_2$) $[M+H]^+$: 176.0706, measured: 176.0719.



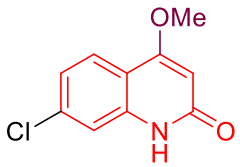

9

***4-methoxyquinolin-2(1H)-one (9):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^1$H NMR (400 MHz, Chloroform-*d*) δ 12.17 (s, 1H), 7.88 (d, *J* = 7.7 Hz, 1H), 7.51 (t, *J* = 7.1 Hz, 1H), 7.40 (d, *J* = 8.2 Hz, 1H), 7.20 (t, *J* = 7.6 Hz, 1H), 6.04 (s, 1H), 3.97 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 166.27, 165.03, 138.26, 131.18, 122.71, 122.21, 116.12, 115.52, 95.87, 55.98. HRMS: m/z (ESI) calculated for ($C_{10}H_9NO_2$) $[M+H]^+$: 176.0706, measured: 176.0693.




10

***4,7-dimethoxyquinolin-2(1H)-one (10):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 11.33 (s, 1H), 7.65 (d, *J* = 8.8 Hz, 1H), 6.87 (s, 1H), 6.76 (d, *J* = 7.7 Hz, 1H), 5.73 (s, 1H), 3.89 (s, 3H), 3.79 (s, 3H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 164.18, 163.89, 161.87, 140.89, 124.17, 110.59, 108.79, 98.59, 94.67, 56.44, 55.80. HRMS: m/z (ESI) calculated for ($C_{11}H_{11}NO_3$) $[M+H]^+$: 206.0812, measured: 206.0817.

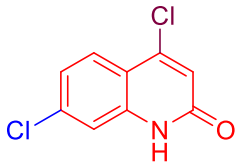



11

***7-chloro-4-methoxyquinolin-2(1H)-one (11):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 11.57 (s, 1H), 7.75 (d, $J$ = 8.4 Hz, 1H), 7.40 (s, 1H), 7.19 (d, $J$ = 8.1 Hz, 1H), 5.90 (s, 1H), 3.92 (s, 3H).

$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 163.69, 163.16, 139.78, 135.82, 124.69, 122.01, 114.96, 113.86, 97.40, 56.77.

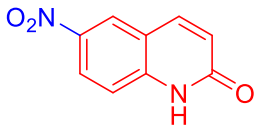
HRMS: m/z (ESI) calculated for ($C_{10}H_8ClNO_2$) $[M+H]^+$: 210.0316, measured: 210.0351.




12

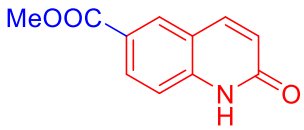
***4,7-dichloroquinolin-2(1H)-one (12):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 12.07 (s, 1H), 7.81 (d, $J$ = 8.6 Hz, 1H), 7.37 (s, 1H), 7.30 (d, $J$ = 8.6 Hz, 1H), 6.82 (s, 1H).

$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 160.82, 143.97, 139.86, 136.83, 127.04, 123.15, 122.01, 116.58, 115.39. HRMS: m/z (ESI) calculated for ($C_9H_5Cl_2NO$) $[M+H]^+$: 213.9821, measured: 213.9836.



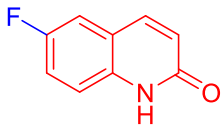

13

***6-nitroquinolin-2(1H)-one (13):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 12.32 (s, 1H), 8.63 (s, 1H), 8.27 (d, $J$ = 9.1 Hz, 1H), 8.08 (d, $J$ = 9.6 Hz, 1H), 7.42 (d, $J$ = 9.1 Hz, 1H), 6.64 (d, $J$ = 9.6 Hz, 1H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.40, 143.72, 141.85, 140.53, 125.42, 124.70, 124.26, 118.95, 116.52. HRMS: m/z (ESI) calculated for ($C_9H_6N_2O_3$) $[M+H]^+$: 191.0451, measured: 191.0472.




14

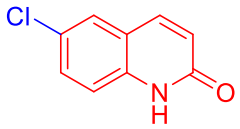
***methyl 2-oxo-1,2-dihydroquinoline-6-carboxylate (14):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 12.04 (s, 1H), 8.31 (s, 1H), 8.03 (t, $J$ = 8.6 Hz, 2H), 7.37 (d, $J$ = 8.6 Hz, 1H), 6.57 (d, $J$ = 9.6 Hz, 1H), 3.86 (s, 3H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 166.17, 162.52, 142.59, 140.87, 131.05, 130.37, 123.35, 123.23, 119.14, 115.88, 52.51. HRMS: m/z (ESI) calculated for ($C_{11}H_9NO_3$) $[M+H]^+$: 204.0655, measured: 204.0643.




15

***6-fluoroquinolin-2(1H)-one (15):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 11.84 (s, 1H), 7.89 (d, $J$ = 9.6 Hz, 1H), 7.55 (dd, $J$ = 9.2, 2.8 Hz, 1H), 7.41 (td, $J$ = 8.8, 2.8 Hz, 1H), 7.32 (dd, $J$ = 9.0, 4.9 Hz, 1H), 6.57 (d, $J$ = 9.6 Hz, 1H).

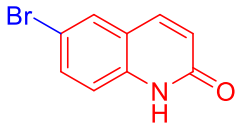
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.11, 158.52, 156.16, 139.90, 136.04, 123.66, 120.16, 118.95, 118.71, 117.39, 113.22, 112.99. HRMS: m/z (ESI) calculated for ($C_9H_6FNO$) $[M+H]^+$: 164.0506, measured: 164.0492.




16

***6-chloroquinolin-2(1H)-one (16):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 11.90 (s, 1H), 7.87 (d, $J$ = 9.6 Hz, 1H), 7.77 (s, 1H), 7.52 (d, $J$ = 8.8 Hz, 1H), 7.30 (d, $J$ = 8.8 Hz, 1H), 6.56 (d, $J$ = 9.6 Hz, 1H).

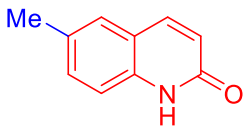
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.17, 139.66, 138.04, 130.66, 127.33, 126.01, 123.63, 120.71, 117.43. HRMS: m/z (ESI) calculated for ($C_9H_6ClNO$) $[M+H]^+$: 180.0211, measured: 180.0219.




17

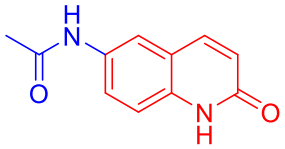
***6-bromoquinolin-2(1H)-one (17):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^1$H NMR (400 MHz, DMSO-$d_6$) δ 11.85 (s, 1H), 7.92 (s, 1H), 7.88 (d, $J$ = 9.6 Hz, 1H), 7.64 (d, $J$ = 10.9 Hz, 1H), 7.26 (d, $J$ = 8.8 Hz, 1H), 6.55 (d, $J$ = 9.6 Hz, 1H).

$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.07, 139.58, 138.42, 133.31, 130.35, 123.61, 121.28, 117.73, 113.76. HRMS: m/z (ESI) calculated for ($C_9H_6BrNO$) $[M+H]^+$: 223.9705 and 225.9685, measured: 223.9718 and 225.9691



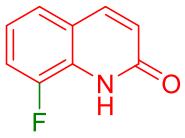

18

***6-methylquinolin-2(1H)-one (18):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 12.26 (s, 1H), 7.79 (d, *J* = 9.5 Hz, 1H), 7.37 (d, *J* = 8.7 Hz, 3H), 6.72 (d, *J* = 9.5 Hz, 1H), 2.44 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.39, 140.87, 136.40, 132.31, 132.10, 127.39, 121.24, 119.92, 115.99, 20.91. HRMS: m/z (ESI) calculated for ($C_{10}H_9NO$) $[M+H]^+$: 160.0757, measured: 160.0762.



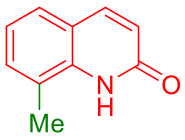

19

***N-(2-oxo-1,2-dihydroquinolin-6-yl)acetamide (19):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 11.66 (s, 1H), 9.99 (s, 1H), 7.97 (s, 1H), 7.86 (d, *J* = 9.6 Hz, 1H), 7.56 (d, *J* = 8.8 Hz, 1H), 7.24 (d, *J* = 8.8 Hz, 1H), 6.48 (s, 1H), 2.05 (s, 3H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 168.62, 162.09, 140.56, 135.38, 134.01, 123.23, 122.72, 119.48, 117.61, 115.84, 24.31. HRMS: m/z (ESI) calculated for ($C_{11}H_{10}N_2O_2$) $[M+H]^+$: 203.0815, measured: 203.0821.



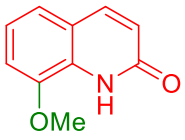

20

***8-fluoroquinolin-2(1H)-one (20):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 10.56 (s, 1H), 7.79 (d, *J* = 10.7 Hz, 1H), 7.37 (d, *J* = 7.9 Hz, 1H), 7.33 – 7.25 (m, 1H), 7.21 – 7.12 (m, 1H), 6.76 (d, *J* = 9.6 Hz, 1H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.62, 150.59, 148.14, 140.11, 127.32, 123.29, 123.20, 122.15, 121.51, 115.65, 115.48. HRMS: m/z (ESI) calculated for ($C_9H_6FNO$) $[M+H]^+$: 164.0506, measured: 164.0513.



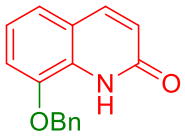

21

***8-methylquinolin-2(1H)-one (21):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 10.02 (s, 1H), 7.79 (d, *J* = 9.5 Hz, 1H), 7.44 (d, *J* = 7.8 Hz, 1H), 7.37 (d, *J* = 7.3 Hz, 1H), 7.14 (t, *J* = 7.6 Hz, 1H), 6.69 (d, *J* = 9.5 Hz, 1H), 2.54 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 163.45, 141.35, 136.88, 131.84, 126.09, 123.23, 122.29, 121.40, 119.70, 16.86.
HRMS: m/z (ESI) calculated for ($C_{10}H_9NO$) $[M+H]^+$: 160.0757, measured: 160.0781.



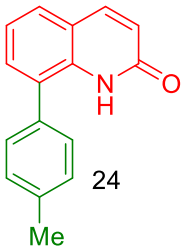

22

***8-methoxyquinolin-2(1H)-one (22):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 9.43 (s, 1H), 7.74 (d, *J* = 9.5 Hz, 1H), 7.22 – 7.08 (m, 2H), 6.99 (d, *J* = 9.1 Hz, 1H), 6.68 (d, *J* = 9.5 Hz, 1H), 3.99 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.15, 145.56, 140.46, 128.54, 122.53, 122.21, 120.01, 119.58, 110.16, 56.02.
HRMS: m/z (ESI) calculated for ($C_{10}H_9NO_2$) $[M+H]^+$: 176.0706, measured: 176.0716.




23

***8-(benzyloxy)quinolin-2(1H)-one (23):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 9.28 (s, 1H), 7.76 (d, *J* = 9.6 Hz, 1H), 7.51 – 7.36 (m, 5H), 7.19 (d, *J* = 6.7 Hz, 1H), 7.14 (t, *J* = 7.8 Hz, 1H), 7.08 (d, *J* = 9.0 Hz, 1H), 6.69 (d, *J* = 9.6 Hz, 1H), 5.21 (s, 2H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.03, 144.61, 140.46, 135.61, 128.85, 127.89, 122.60, 122.20, 120.19, 119.87, 111.45, 71.06. HRMS: m/z (ESI) calculated for ($C_{16}H_{13}NO_2$) $[M+H]^+$: 252.1019, measured: 252.1030.

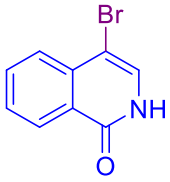



24

***8-(p-tolyl)quinolin-2(1H)-one (24):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 8.85 (s, 1H), 7.83 (d, *J* = 9.6 Hz, 1H), 7.57 (d, *J* = 6.8 Hz, 1H), 7.44 (d, *J* = 7.4 Hz, 1H), 7.39 – 7.24 (m, 5H), 6.67 (d, *J* = 9.6 Hz, 1H), 2.47 (s, 3H).
$^{13}$C NMR (100 MHz, $CDCl_3$) δ 162.45, 141.00, 138.66, 135.43, 132.82, 131.40, 130.28, 129.07, 128.73, 127.26, 122.41, 121.81, 120.00, 21.21. HRMS: m/z (ESI) calculated for ($C_{16}H_{13}NO$) $[M+H]^+$: 236.1070, measured: 236.1052.

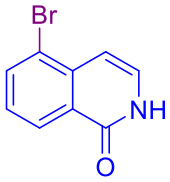

25

***isoquinolin-1(2H)-one (25):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 11.08 (s, 1H), 8.44 (d, *J* = 8.1 Hz, 1H), 7.71 (t, *J* = 7.5 Hz, 1H), 7.60 (d, *J* = 7.8 Hz, 1H), 7.54 (t, *J* = 7.6 Hz, 1H), 7.20 (d, *J* = 7.0 Hz, 1H), 6.61 (d, *J* = 7.1 Hz, 1H). $^{13}$C NMR (100 MHz, $CDCl_3$) δ 164.20, 138.11, 132.76, 127.49, 127.35, 126.91, 126.27, 126.03, 106.89. HRMS: m/z (ESI) calculated for ($C_9H_7NO$) $[M+H]^+$: 146.0600, measured: 146.0989.



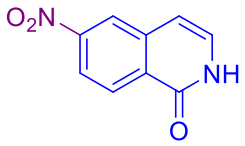
26

***4-bromoisoquinolin-1(2H)-one (26):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 11.56 (s, 1H), 8.24 (d, *J* = 7.7 Hz, 1H), 7.87 (t, *J* = 7.7 Hz, 1H), 7.77 (d, *J* = 8.0 Hz, 1H), 7.61 (t, *J* = 7.6 Hz, 1H), 7.55 (s, 1H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 161.45, 136.15, 133.95, 130.58, 128.09, 127.87, 126.93, 125.82, 98.02. HRMS: m/z (ESI) calculated for ($C_9H_6BrNO$) $[M+H]^+$: 223.9705 and 225.9685, measured: 223.9699 and 225.9707



27

***5-bromoisoquinolin-1(2H)-one (27):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, Chloroform-*d*) δ 11.32 (s, 1H), 8.48 – 8.37 (m, 1H), 7.96 (d, *J* = 7.8 Hz, 1H), 7.38 (t, *J* = 7.9 Hz, 1H), 7.31 – 7.24 (m, 1H), 6.97 (d, *J* = 7.4 Hz, 1H).
$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.65, 137.25, 137.09, 130.26, 128.21, 127.04, 126.92, 120.57, 104.98. HRMS: m/z (ESI) calculated for ($C_9H_6BrNO$) $[M+H]^+$: 223.9705 and 225.9685, measured: 223.9723 and 225.9689




28

***6-nitroisoquinolin-1(2H)-one (28):*** Gradient eluent: EtOAc/petroleum ether: 1/2 to 3/1; $^{1}$H NMR (400 MHz, DMSO-$d_6$) δ 12.32 (s, 1H), 8.63 (s, 1H), 8.27 (d, $J$ = 9.1 Hz, 1H), 8.08 (d, $J$ = 9.6 Hz, 1H), 7.42 (d, $J$ = 9.1 Hz, 1H), 6.64 (d, $J$ = 9.6 Hz, 1H).

$^{13}$C NMR (100 MHz, DMSO-$d_6$) δ 162.40, 143.72, 141.85, 140.53, 125.42, 124.70, 124.26, 118.95, 116.52. HRMS: m/z (ESI) calculated for ($C_9H_6N_2O_3$) $[M+H]^+$: 191.0451, measured: 191.0432.

## $^{1}$H and $^{13}$C NMR spectra of products:

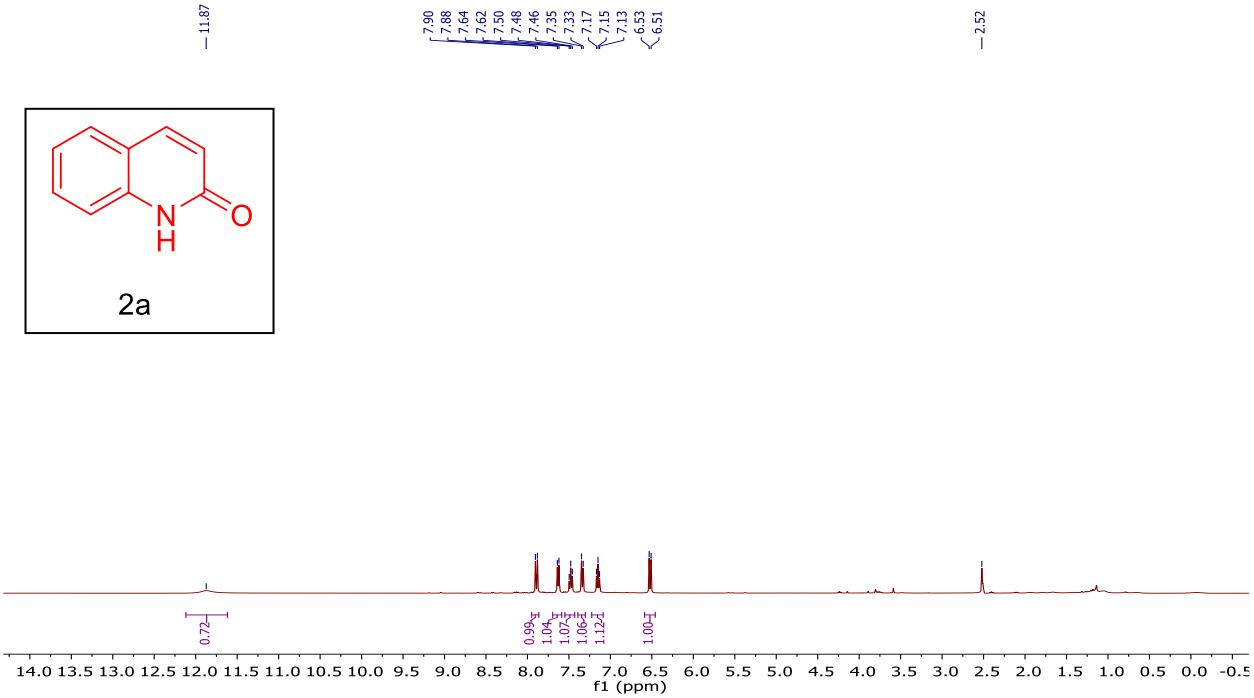



**Figure S1**. $^{1}$H NMR spectrum of **quinolin-2(1H)-one (2a).**

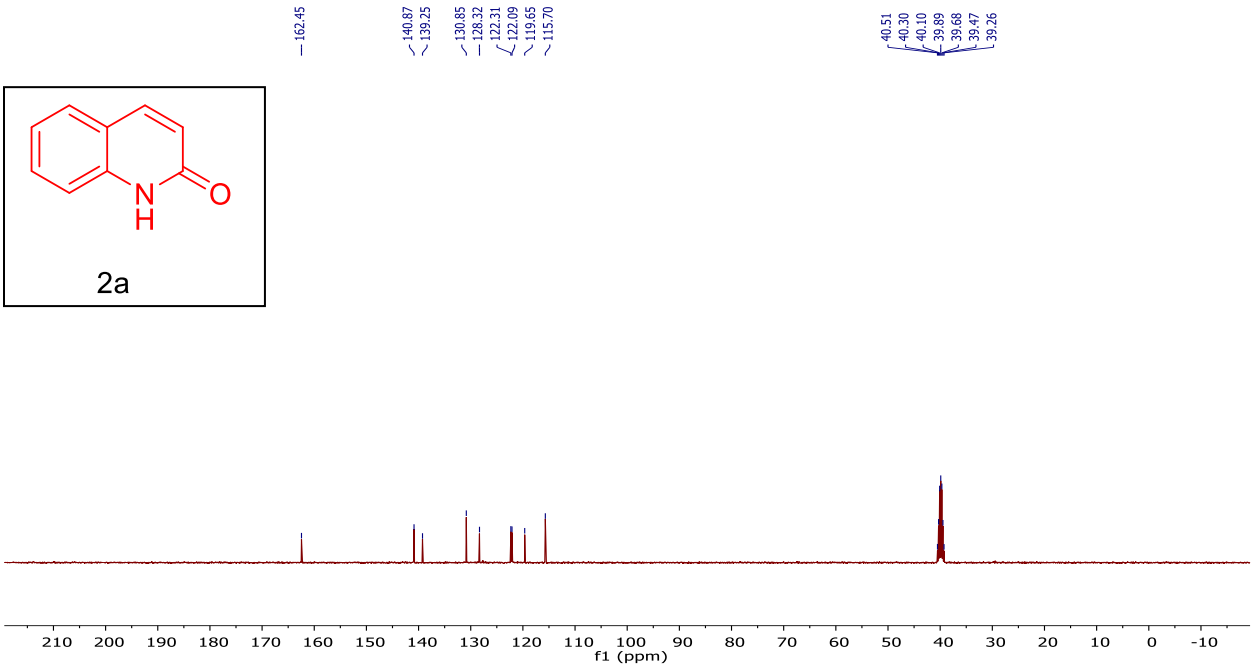



**Figure S2**. $^{13}$C NMR spectrum of **quinolin-2(1H)-one (2a).**

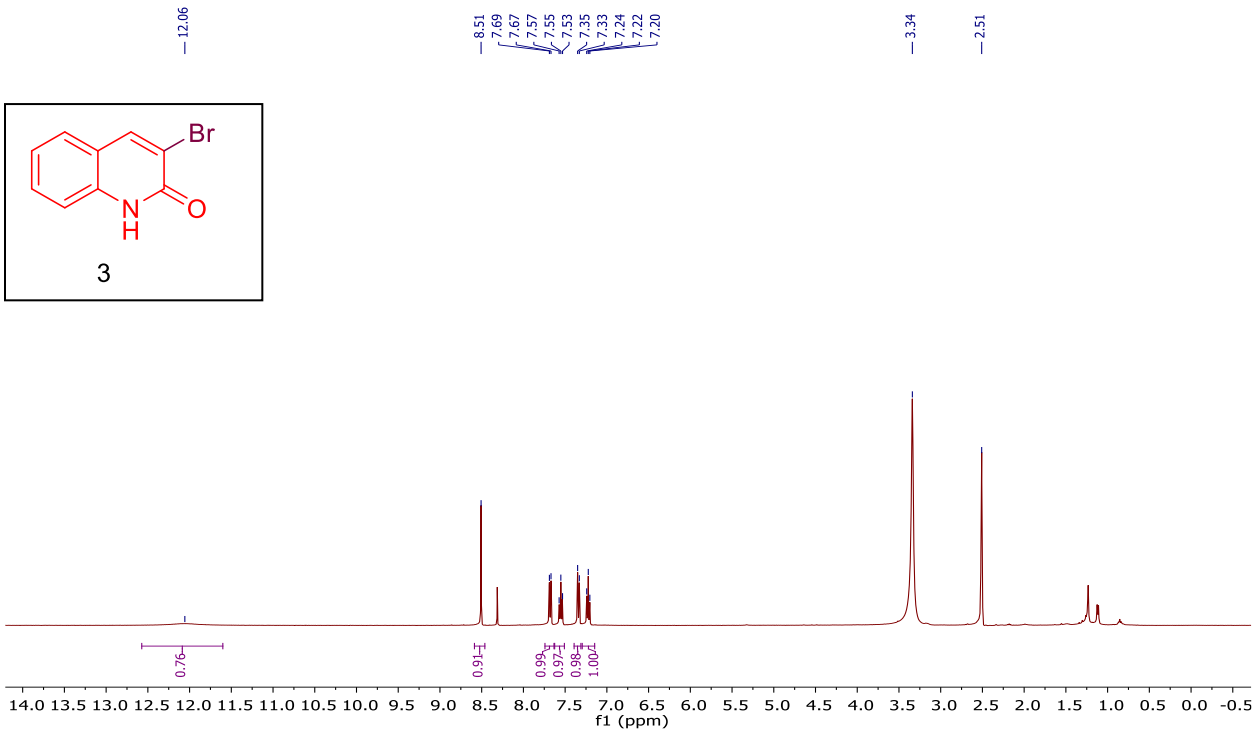



**Figure S3**. $^{1}$H NMR spectrum of **3-bromoquinolin-2(1H)-one (3).**

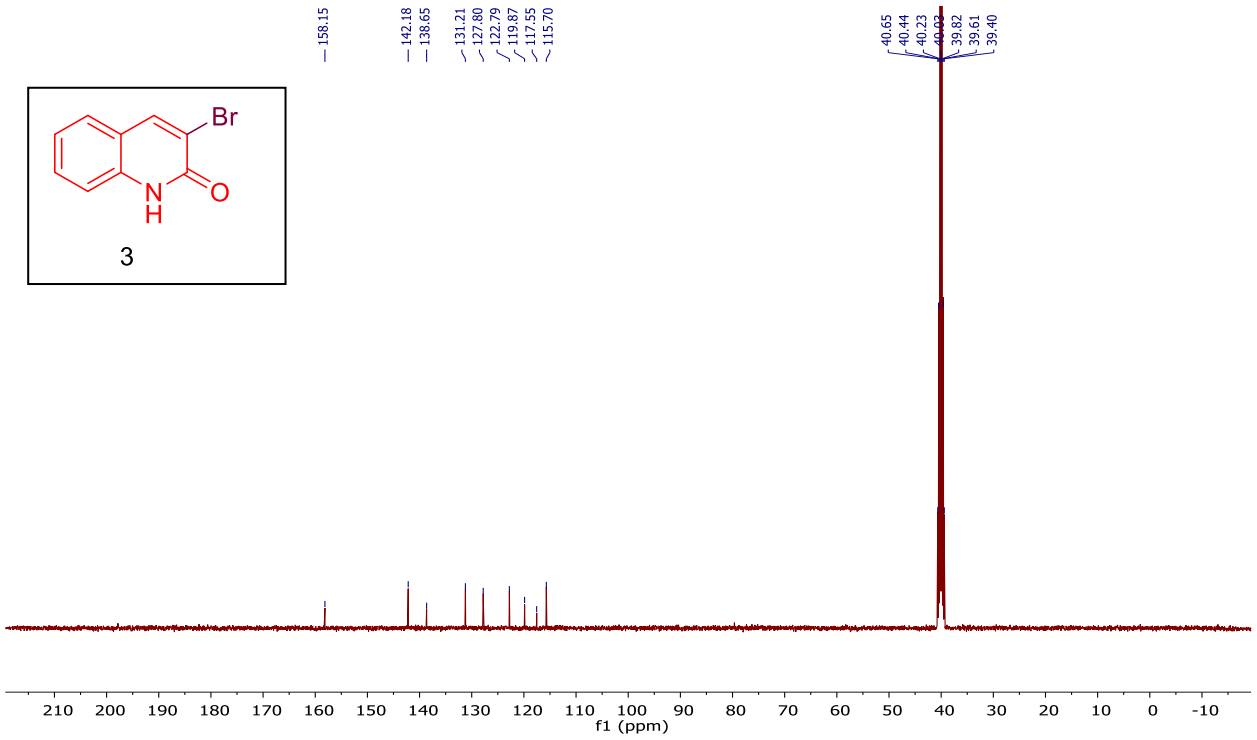



**Figure S4**. $^{13}$C NMR spectrum of **3-bromoquinolin-2(1H)-one (3).**

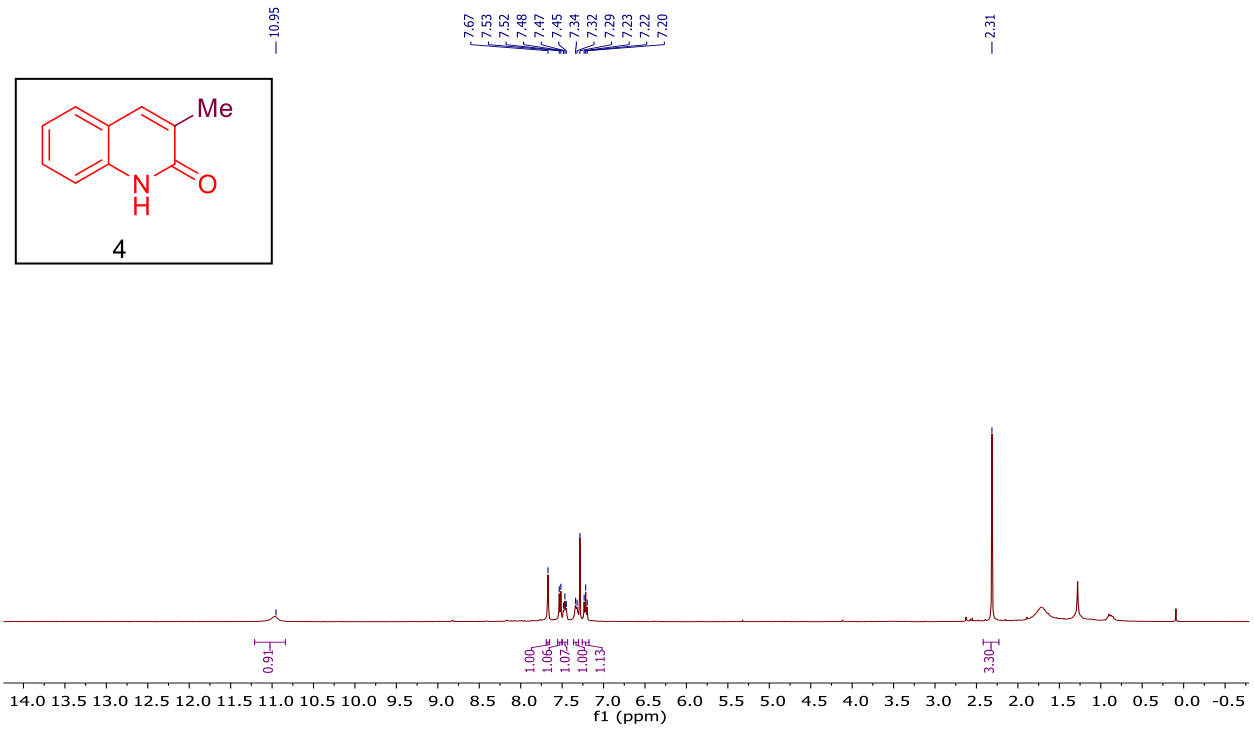



**Figure S5**. $^{1}$H NMR spectrum of **3-methylquinolin-2(1H)-one (4).**

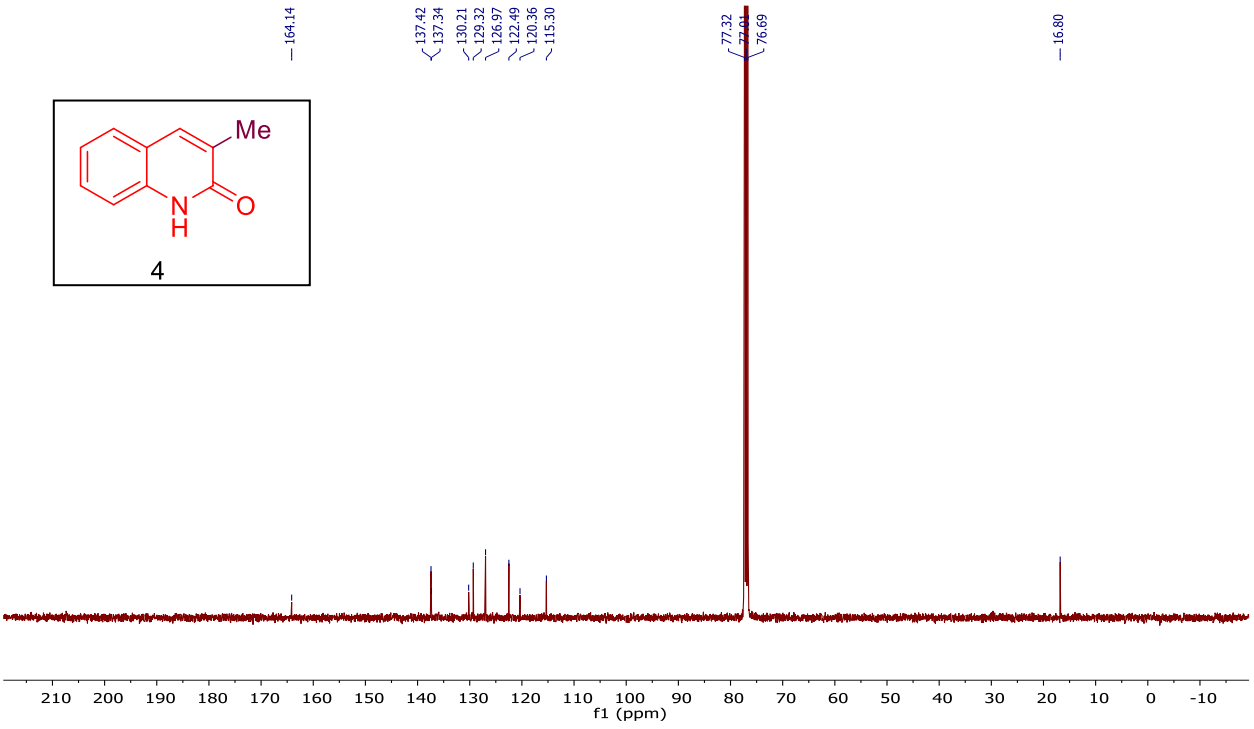



**Figure S6**. $^{13}$C NMR spectrum of **3-methylquinolin-2(1H)-one (4).**

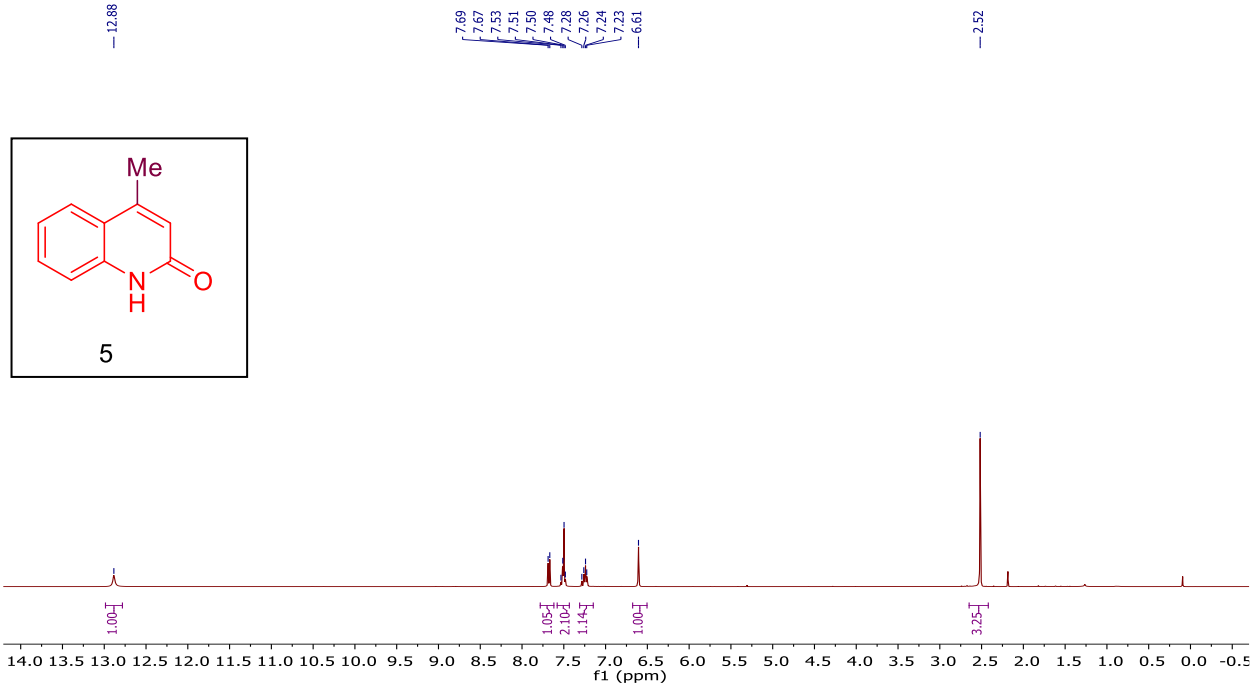



**Figure S7**. $^{1}$H NMR spectrum of **4-methylquinolin-2(1H)-one (5).**

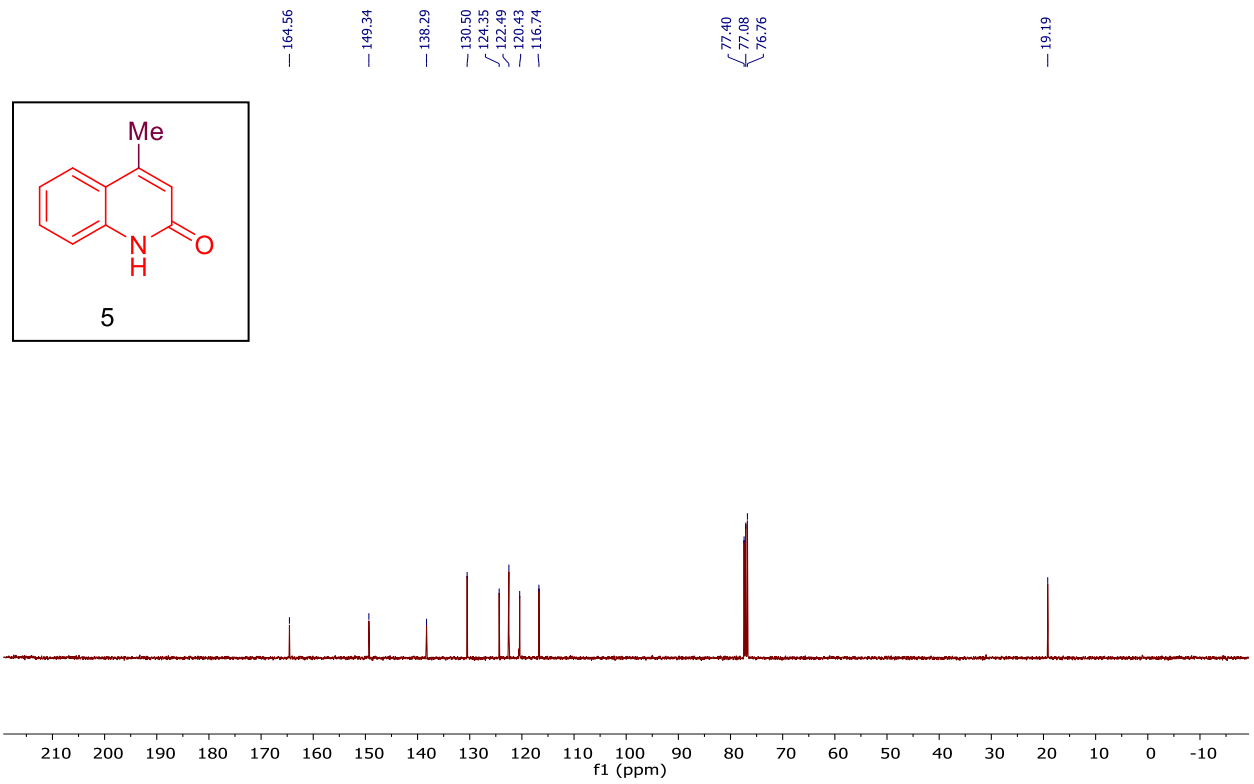



**Figure S8**. $^{13}$C NMR spectrum of **4-methylquinolin-2(1H)-one (5).**

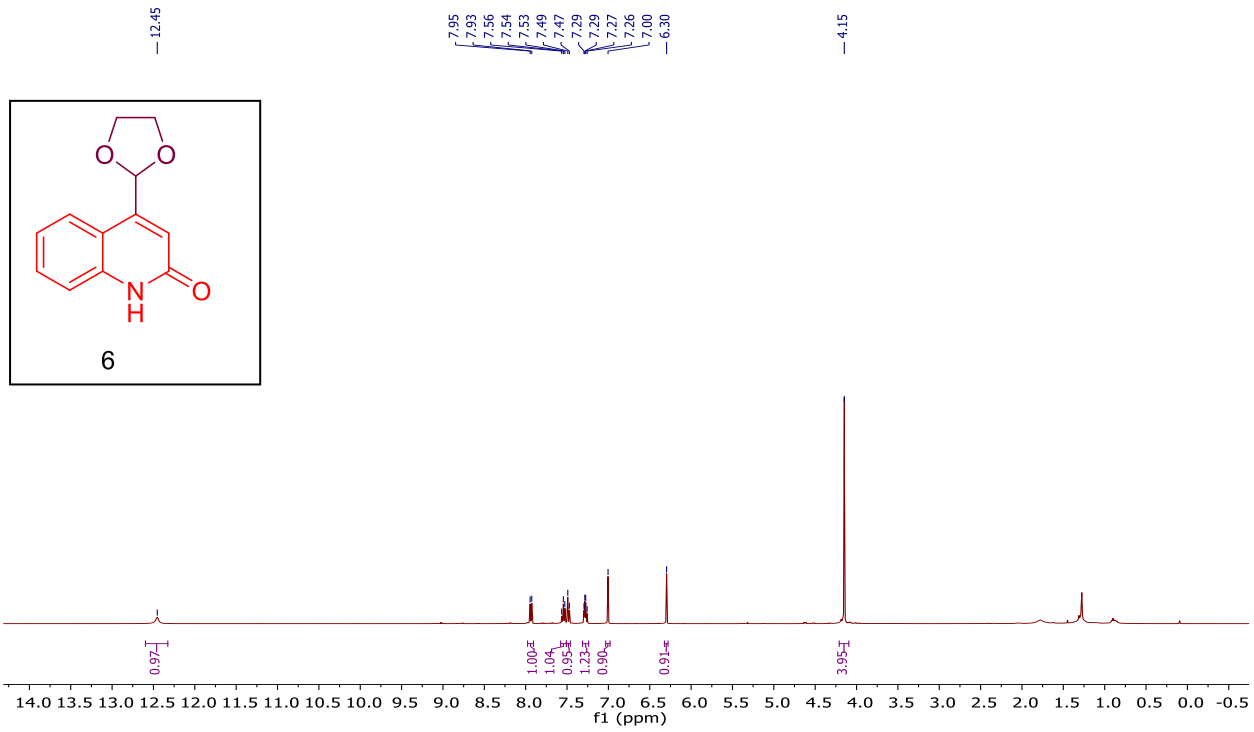



**Figure S9**. $^{1}$H NMR spectrum of **4-(1,3-dioxolan-2-yl)quinolin-2(1H)-one (6).**

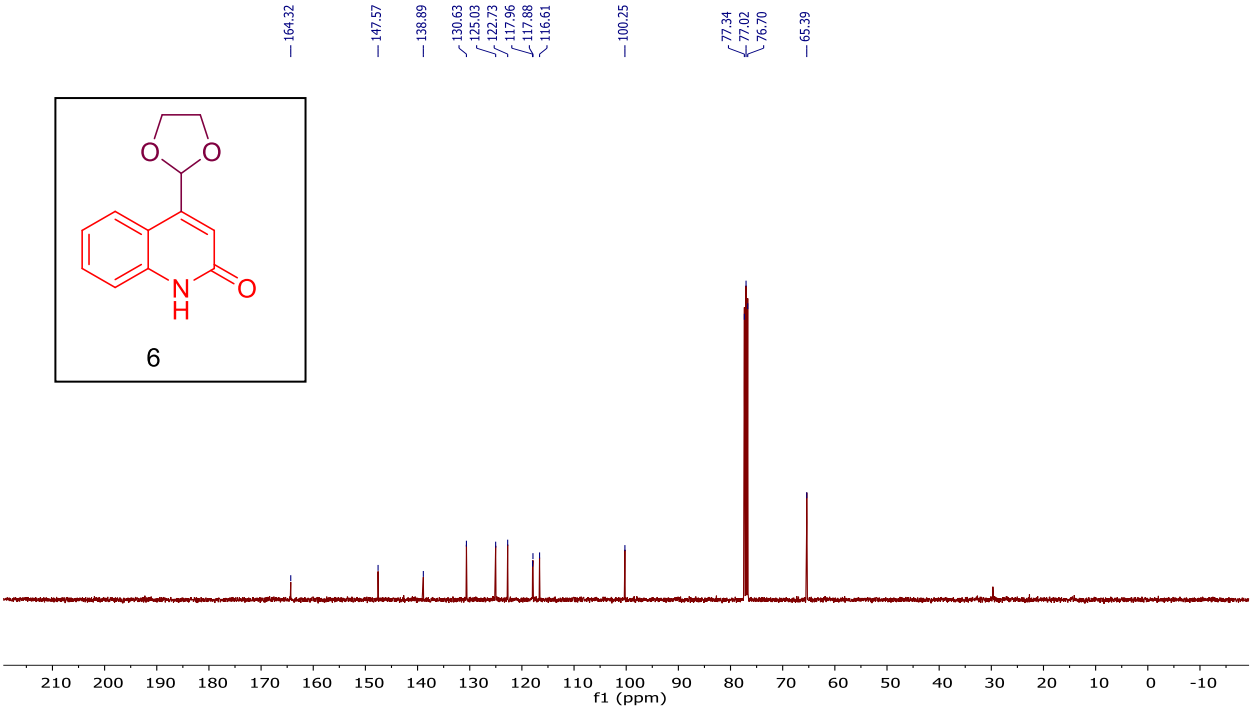



**Figure S10**. $^{13}$C NMR spectrum of **4-(1,3-dioxolan-2-yl)quinolin-2(1H)-one (6).**

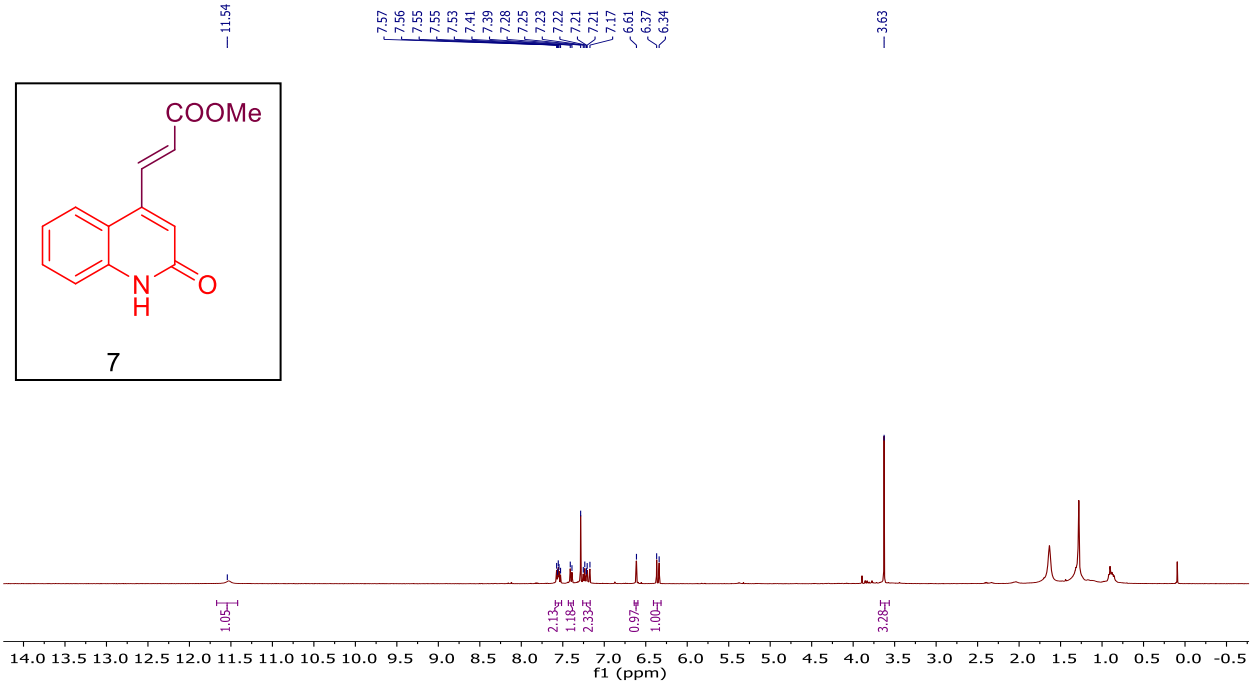



**Figure S11**. $^{1}$H NMR spectrum of **methyl (E)-3-(2-oxo-1,2-dihydroquinolin-4-yl)acrylate (7).**

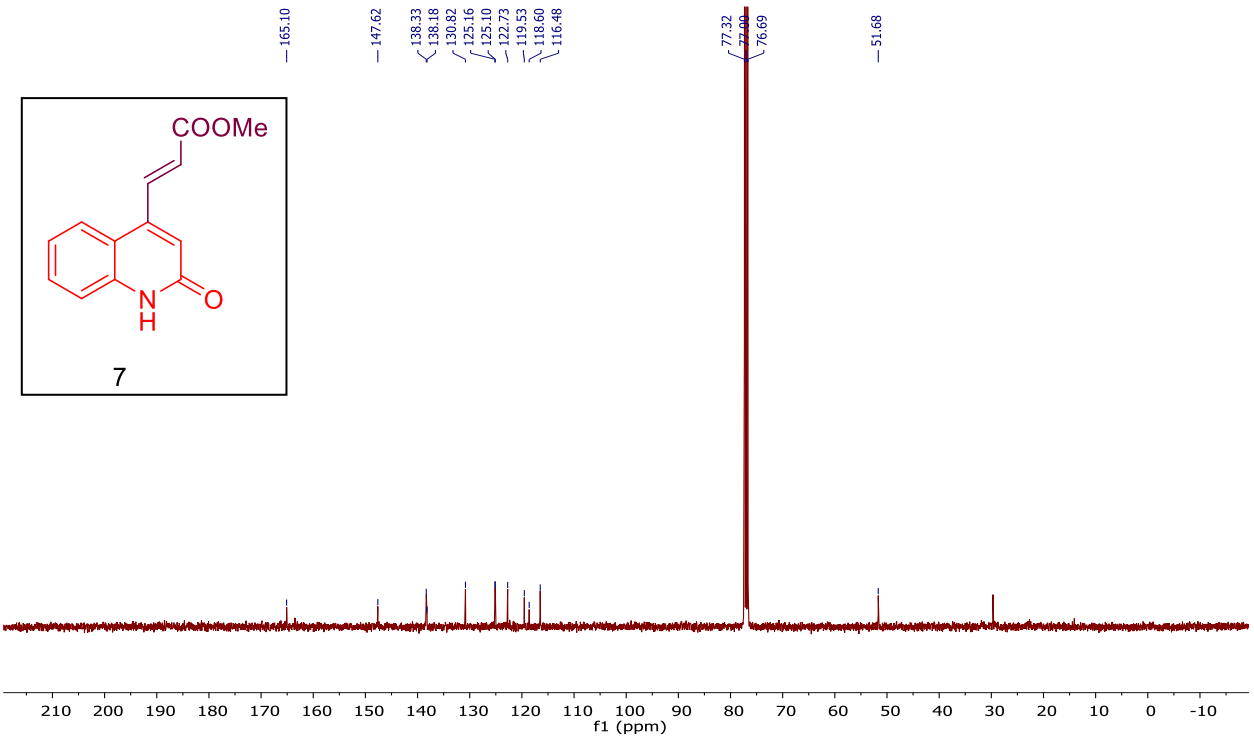



**Figure S12**. $^{13}$C NMR spectrum of **methyl (E)-3-(2-oxo-1,2-dihydroquinolin-4-yl)acrylate (7).**

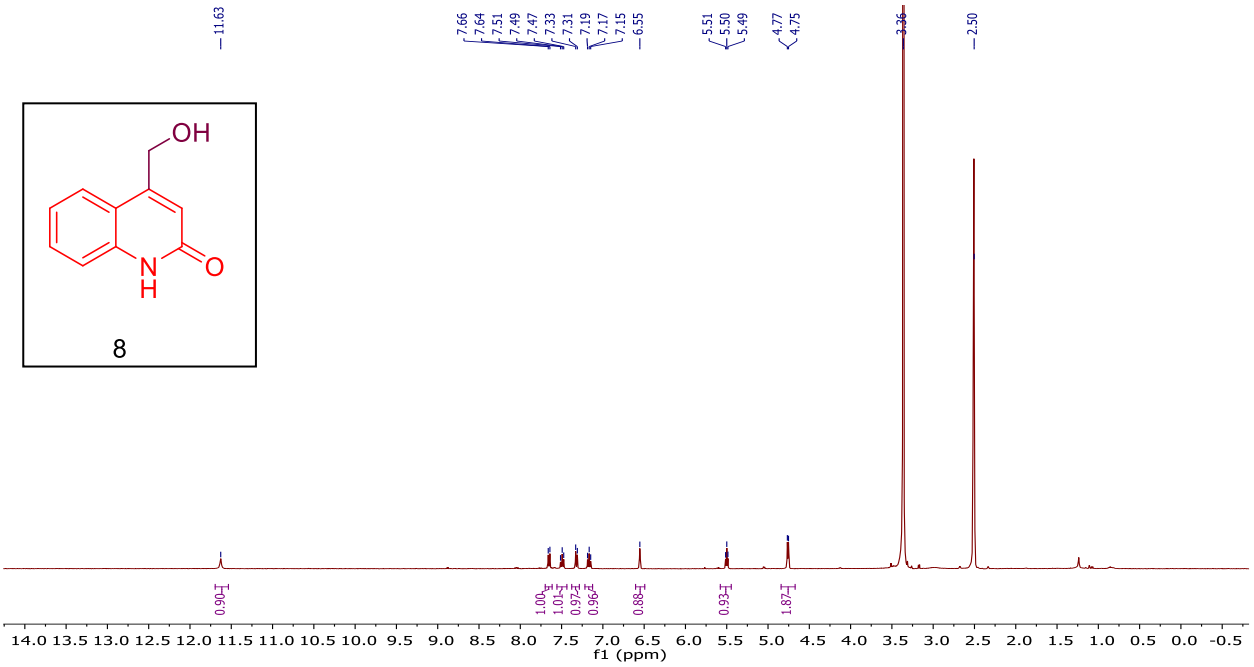



**Figure S13**. $^{1}$H NMR spectrum of **4-(hydroxymethyl)quinolin-2(1H)-one (8).**

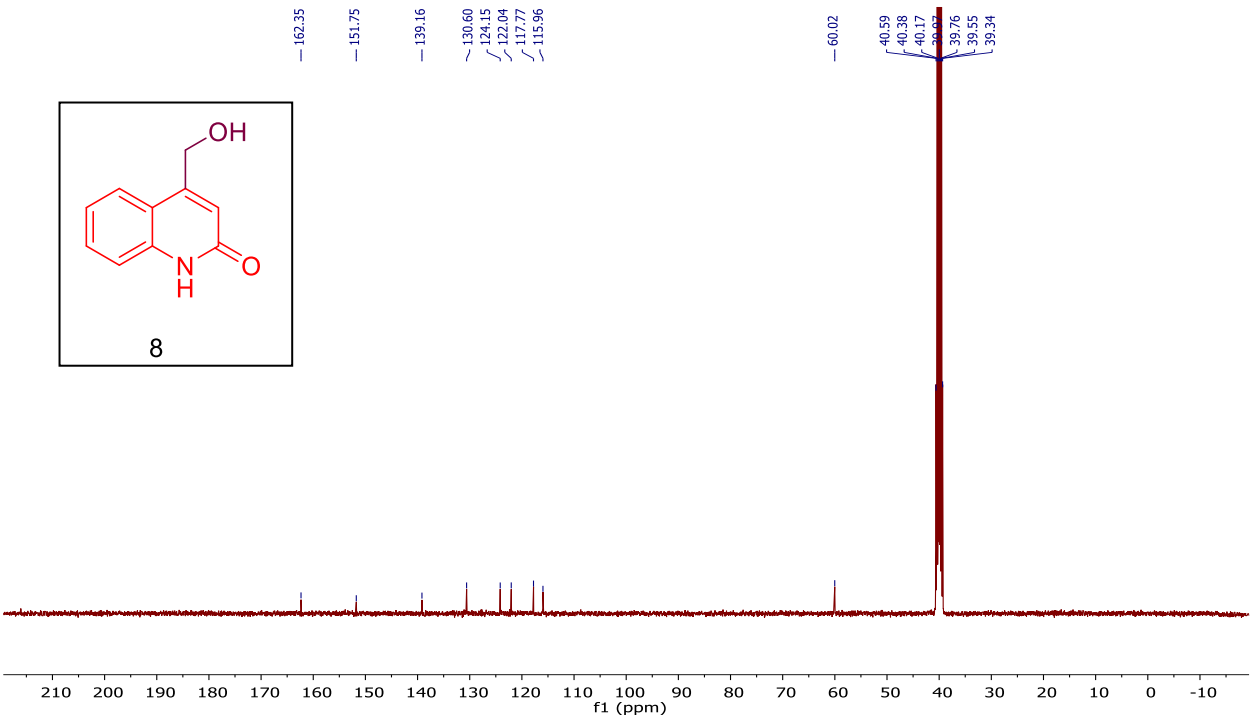



**Figure S14**. $^{13}$C NMR spectrum of **4-(hydroxymethyl)quinolin-2(1H)-one (8).**

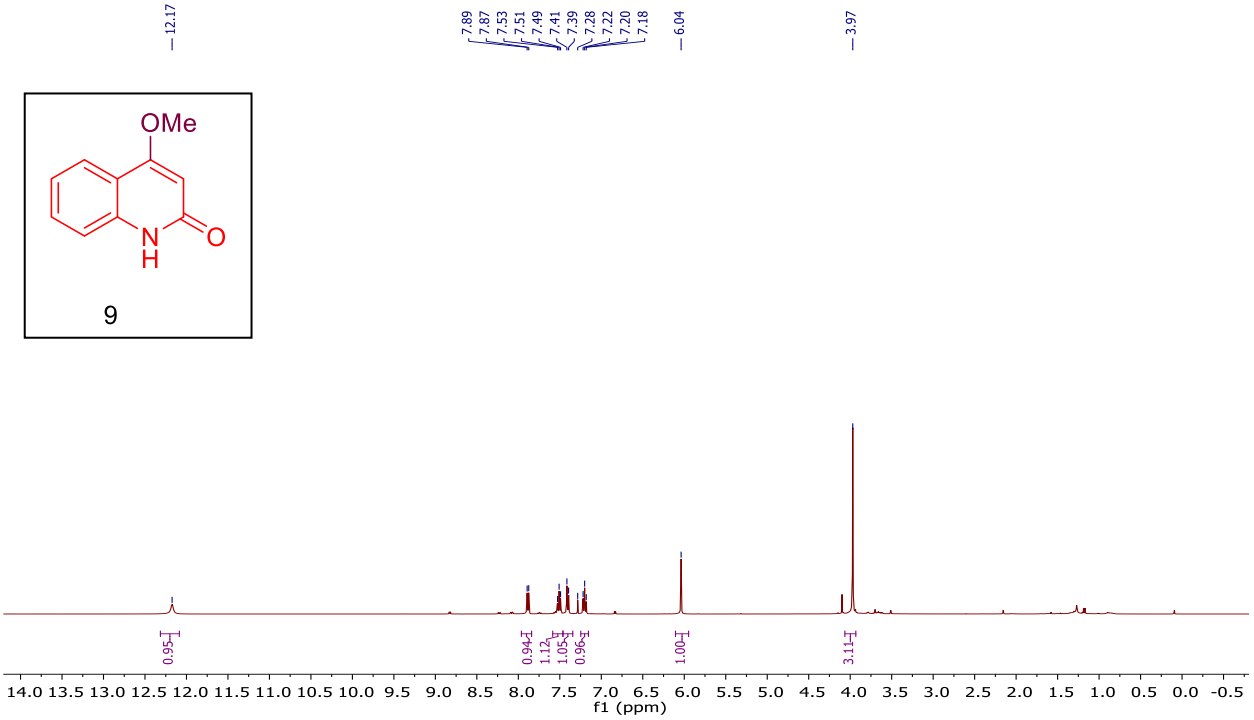



**Figure S15**. $^{1}$H NMR spectrum of **4-methoxyquinolin-2(1H)-one (9).**

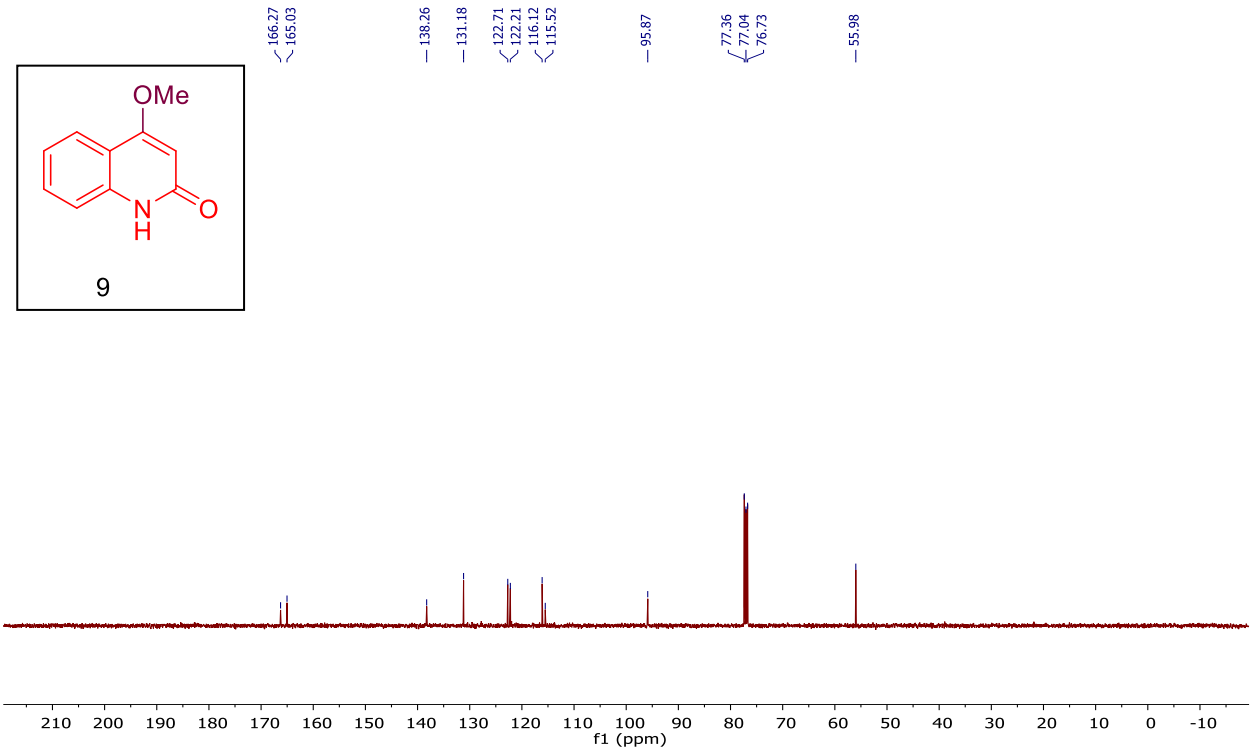



**Figure S16**. $^{13}$C NMR spectrum of **4-methoxyquinolin-2(1H)-one (9).**

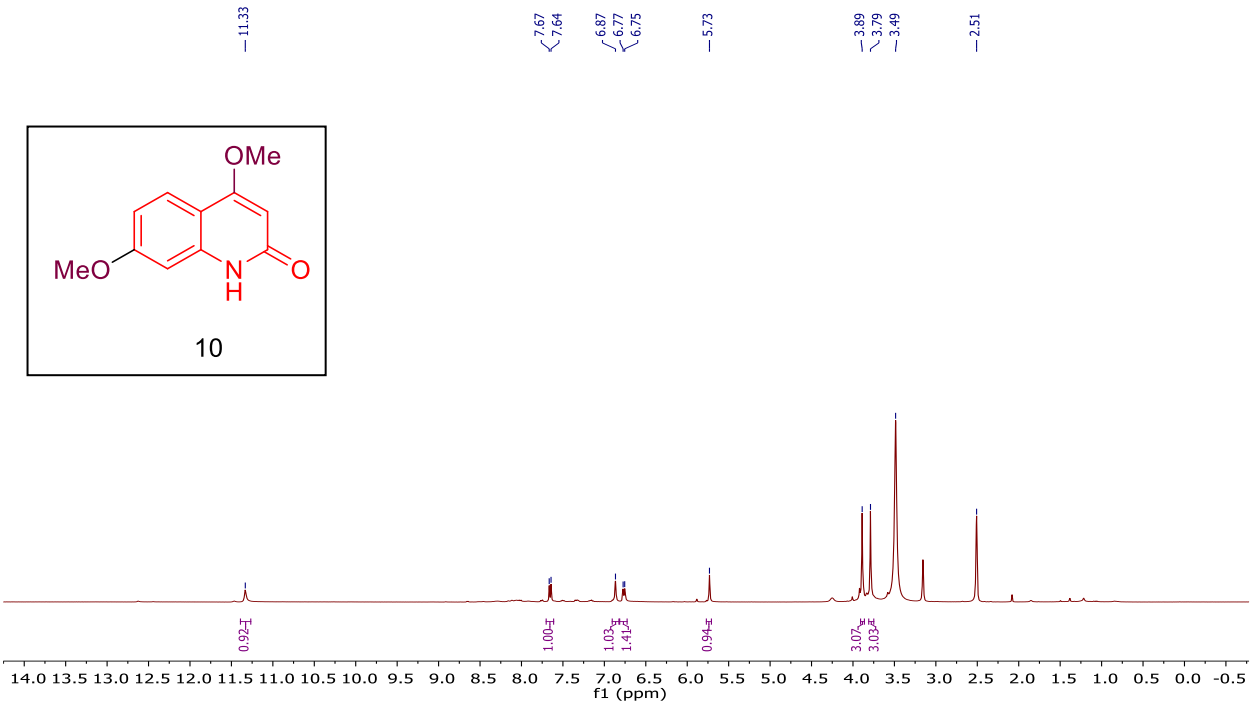



**Figure S17**. $^{1}$H NMR spectrum of **4,7-dimethoxyquinolin-2(1H)-one (10).**

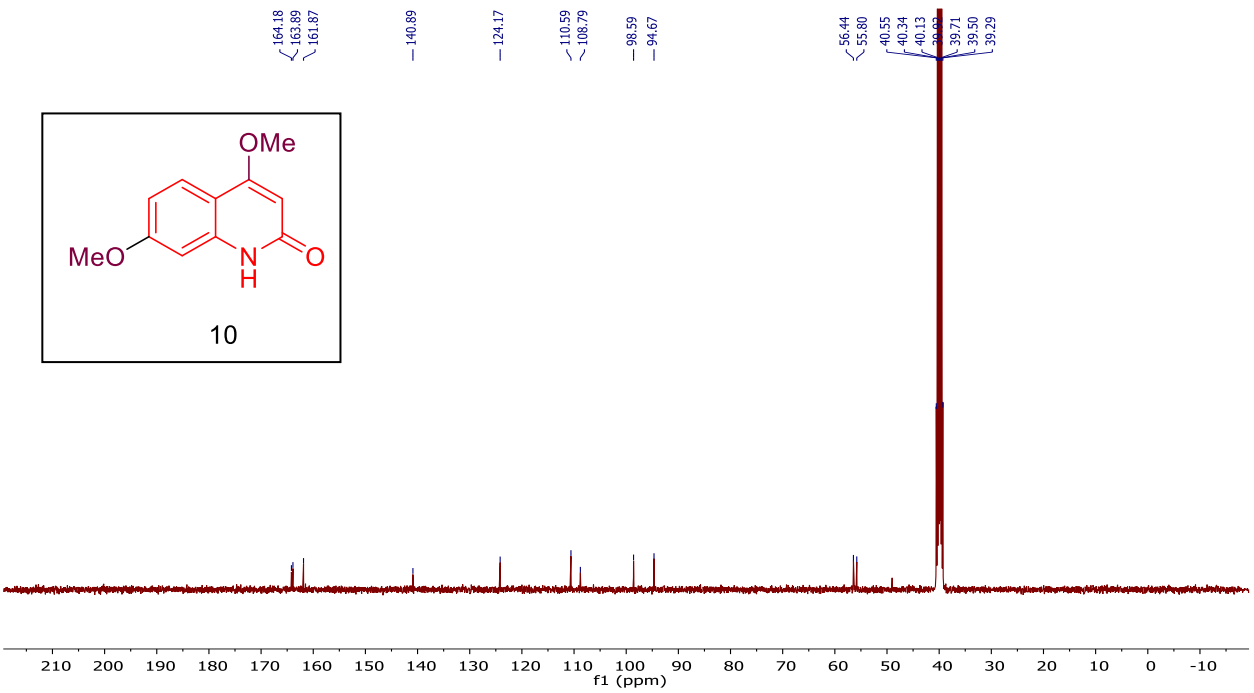



**Figure S18**. $^{13}$C NMR spectrum of **4,7-dimethoxyquinolin-2(1H)-one (10).**

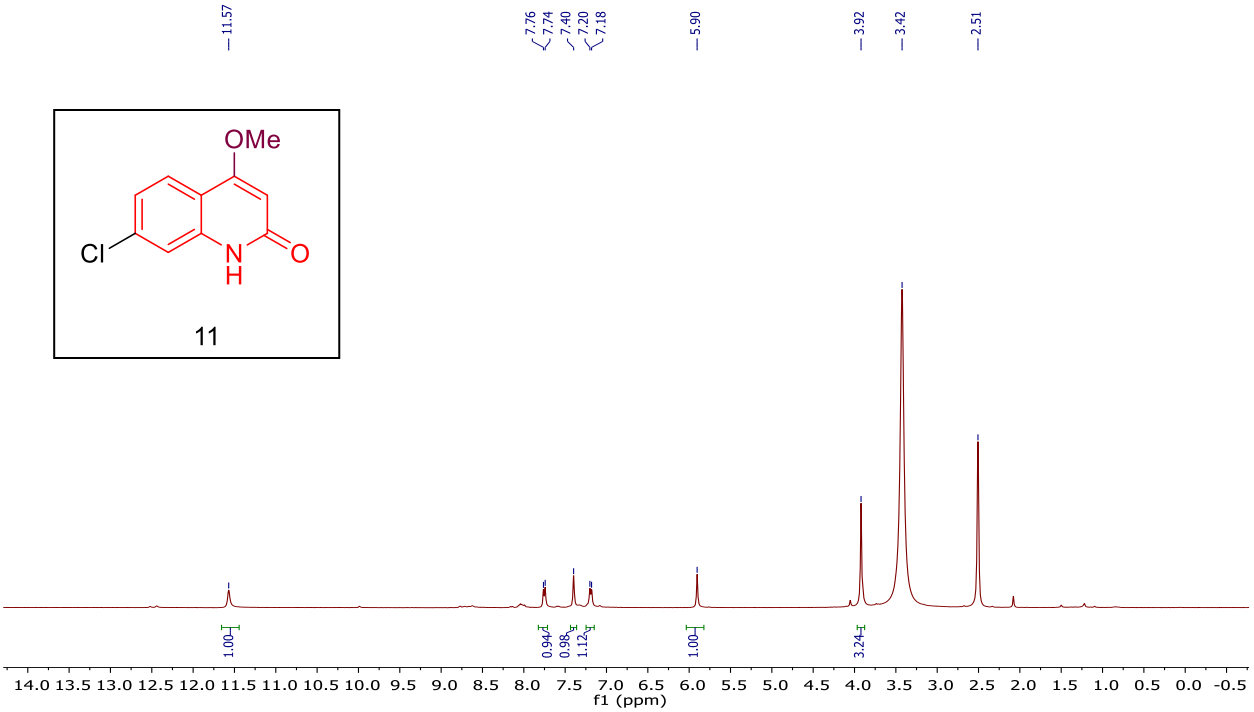



**Figure S19**. [1]H NMR spectrum of **7-chloro-4-methoxyquinolin-2(1H)-one (11).**

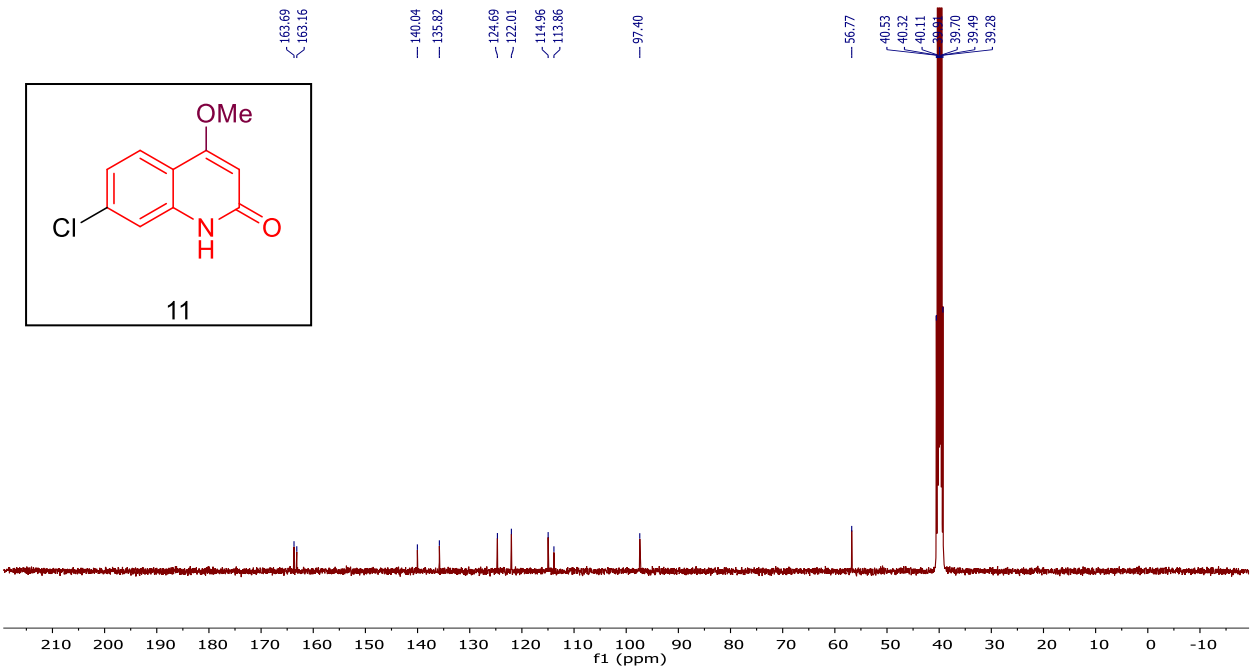



**Figure S20**. [13]C NMR spectrum of **7-chloro-4-methoxyquinolin-2(1H)-one (11).**

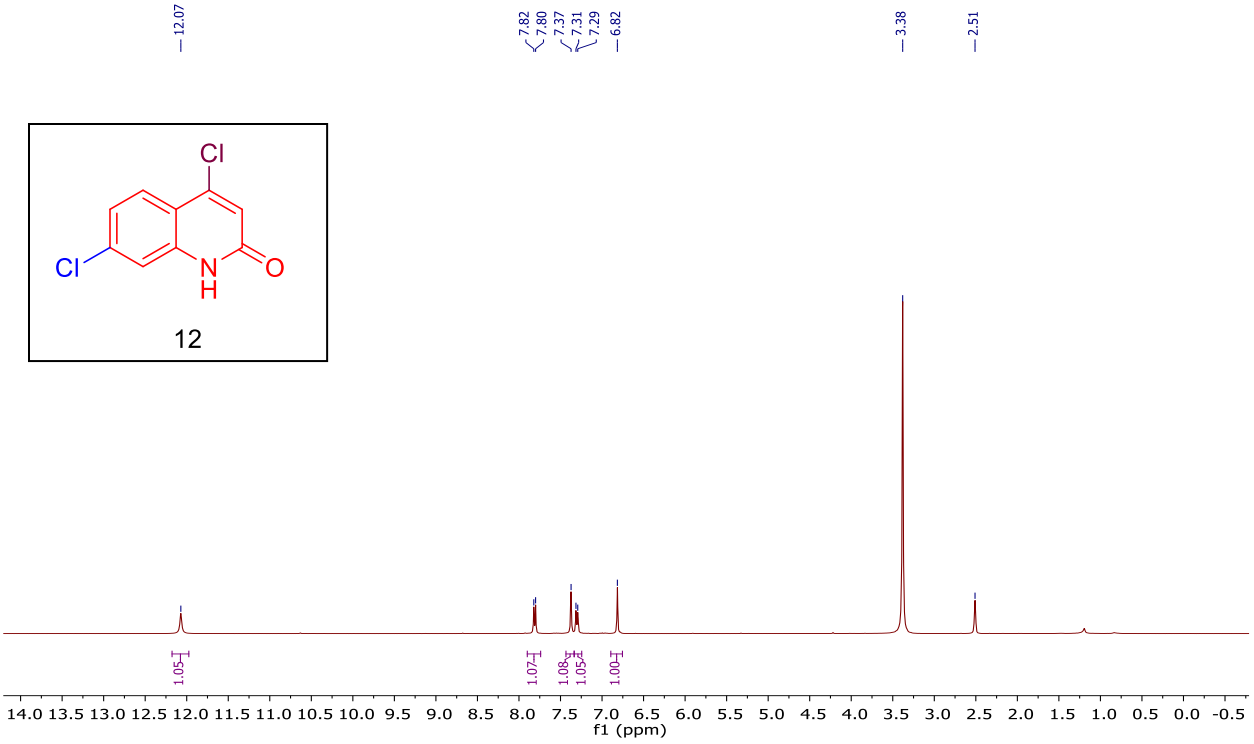



**Figure S21**. $^{1}$H NMR spectrum of **4,7-dichloroquinolin-2(1H)-one (12).**

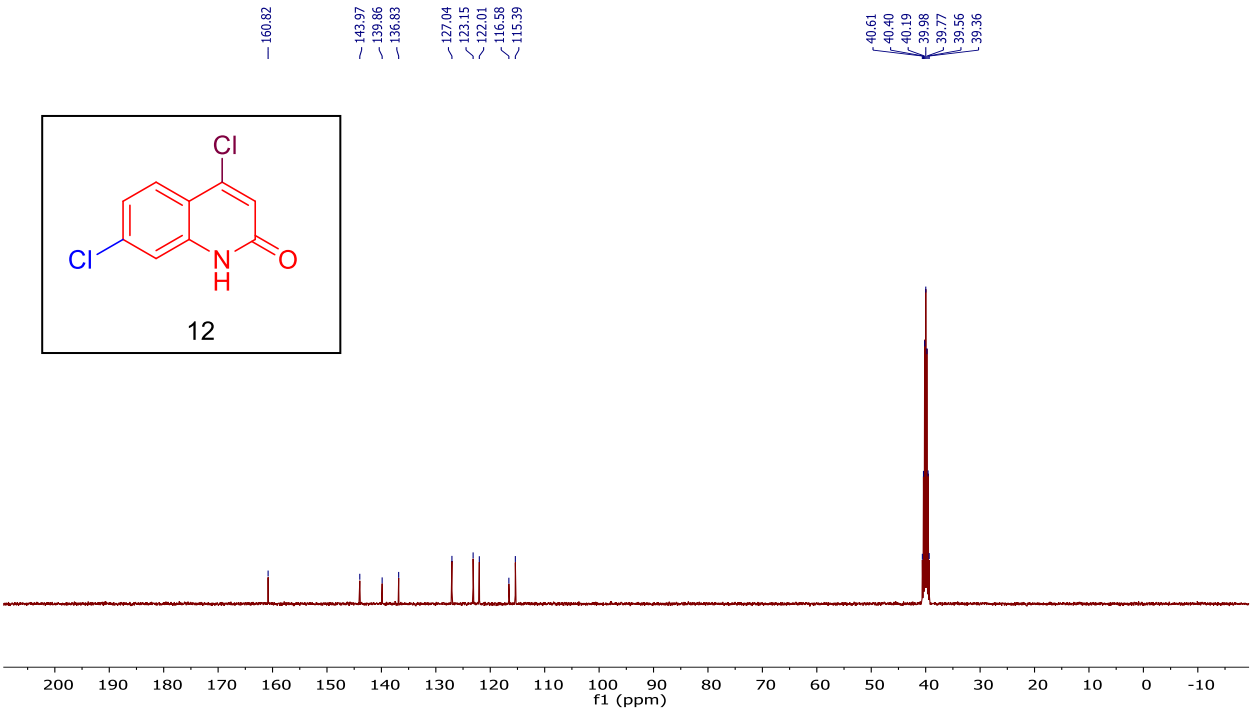



**Figure S22**. $^{13}$C NMR spectrum of **4,7-dichloroquinolin-2(1H)-one (12).**

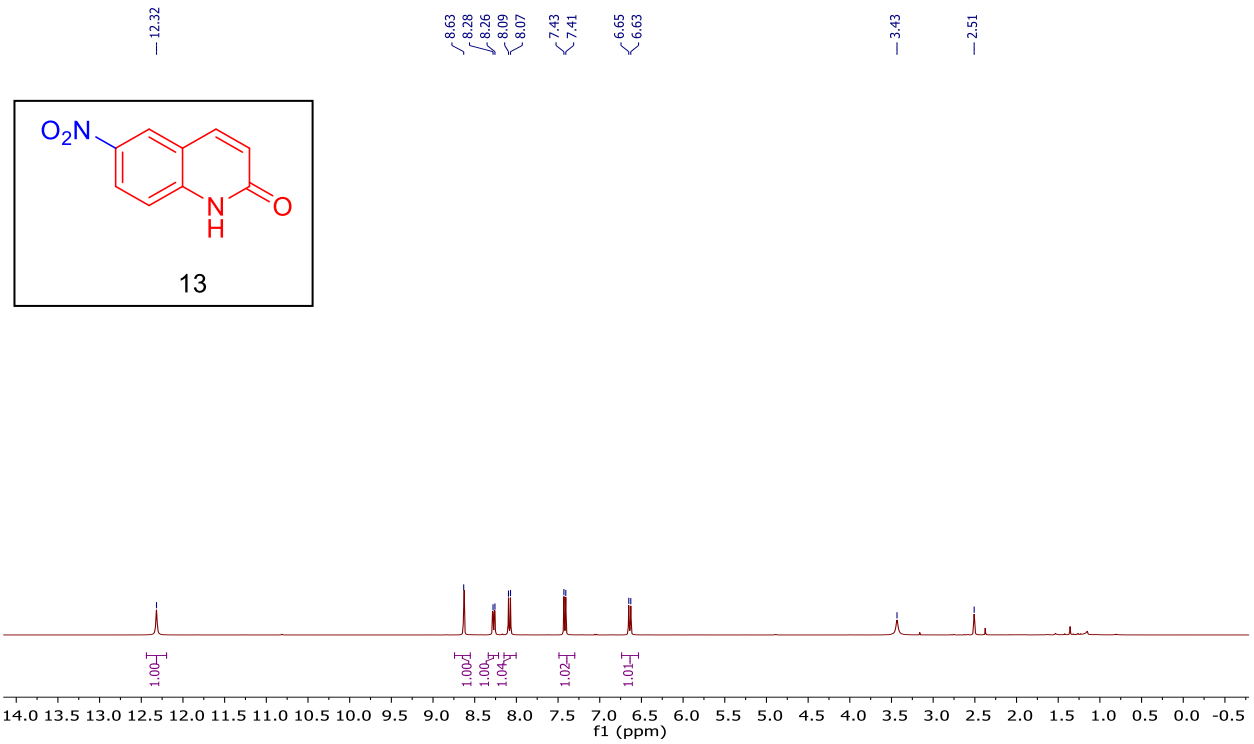



**Figure S23**. [1]H NMR spectrum of **6-nitroquinolin-2(1H)-one (13).**

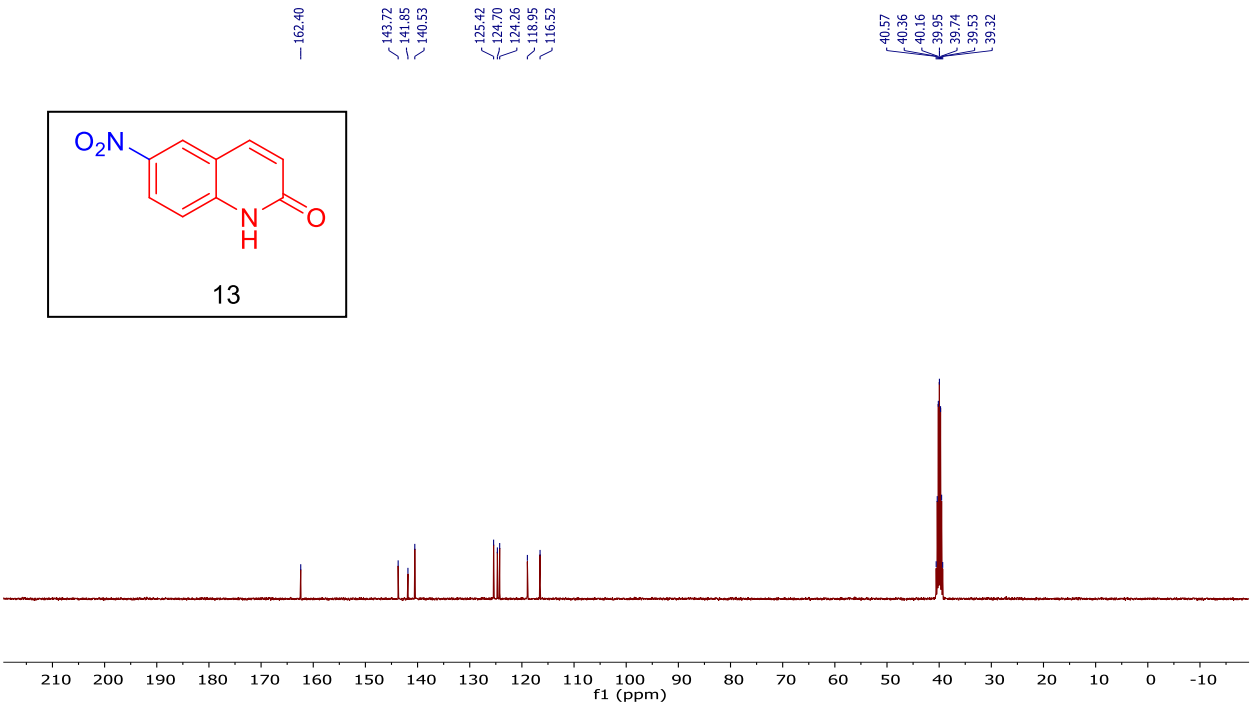



**Figure S24**. [13]C NMR spectrum of **6-nitroquinolin-2(1H)-one (13).**

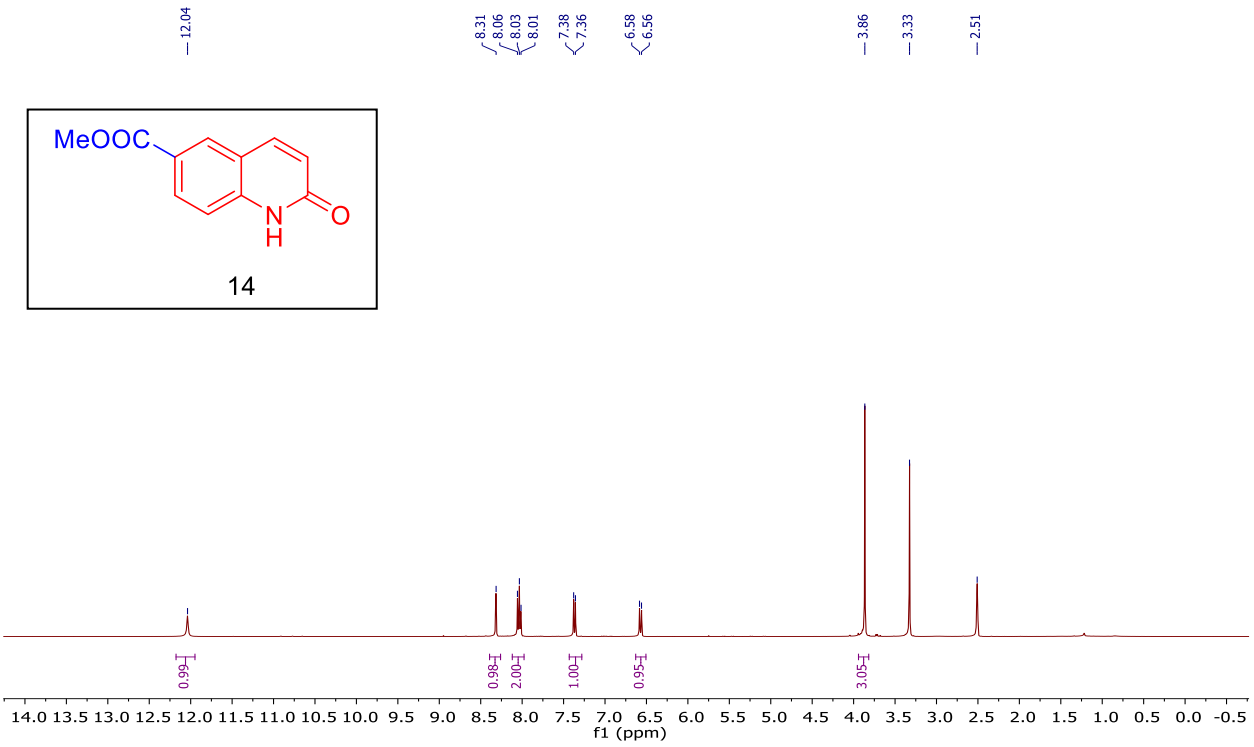



**Figure S25**. $^{1}$H NMR spectrum of **methyl 2-oxo-1,2-dihydroquinoline-6-carboxylate (14).**

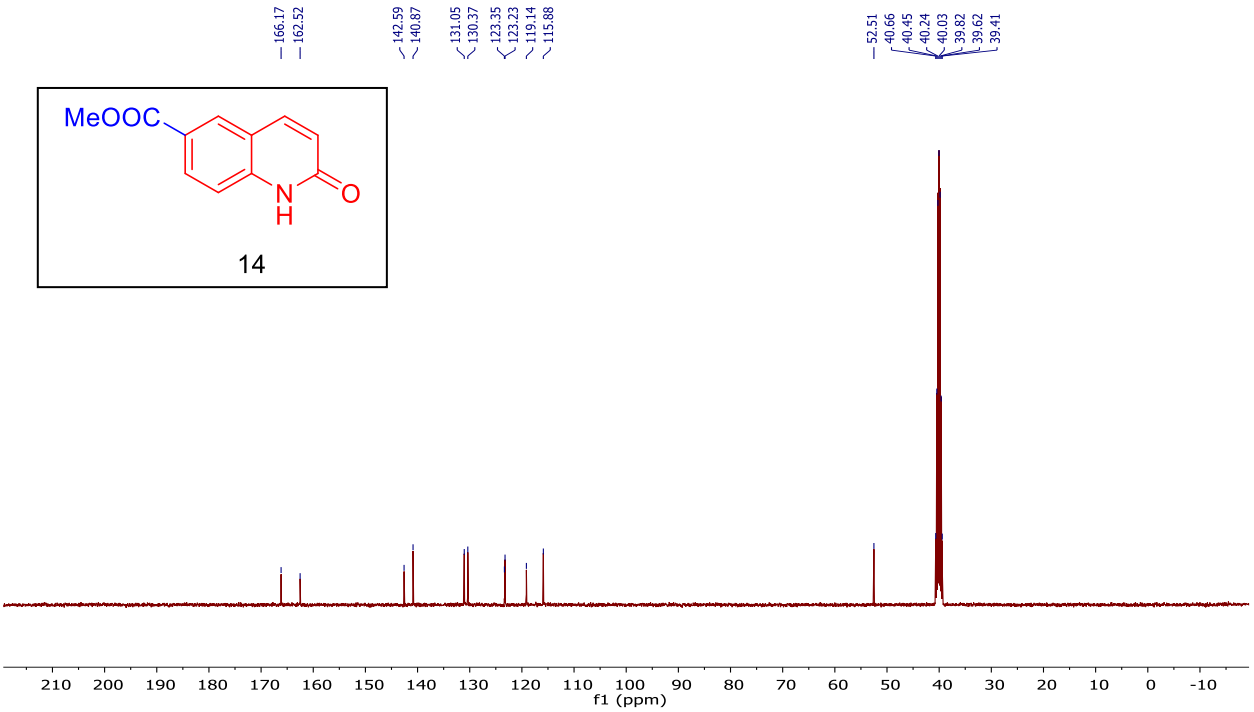



**Figure S26**. $^{13}$C NMR spectrum of **methyl 2-oxo-1,2-dihydroquinoline-6-carboxylate (14).**

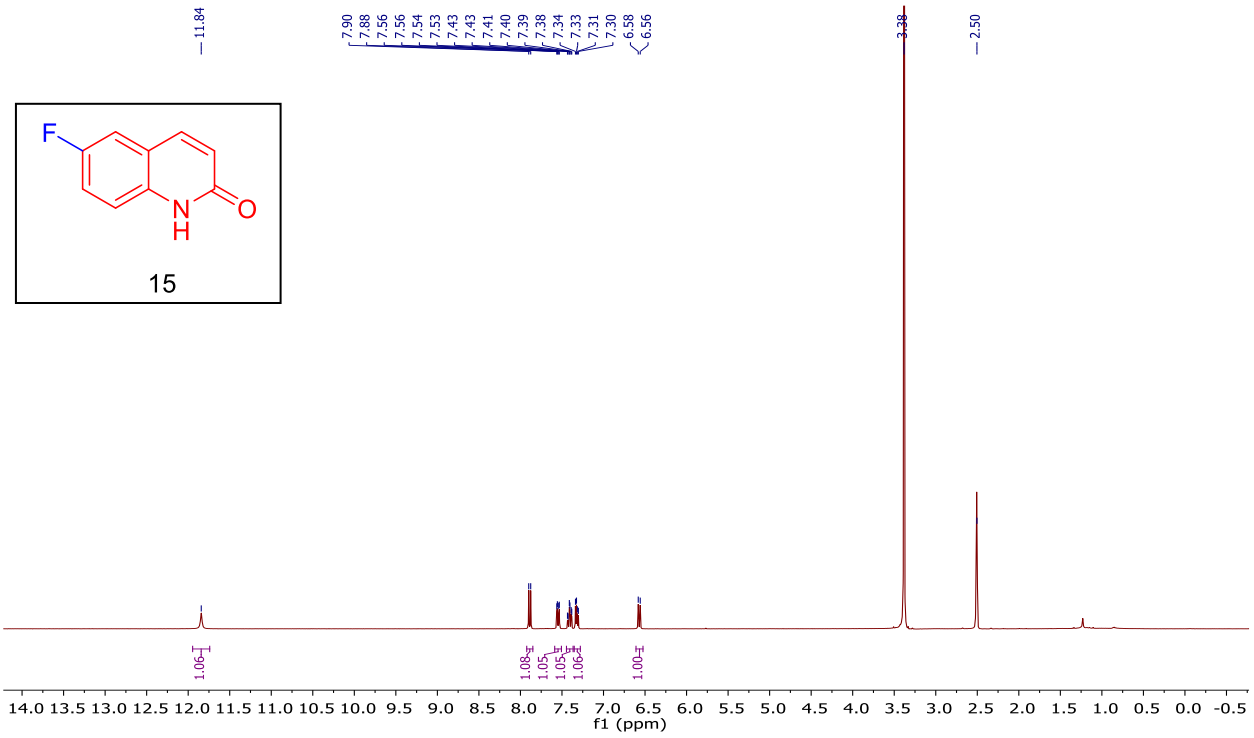



**Figure S27**. $^{1}$H NMR spectrum of **6-fluoroquinolin-2(1H)-one (15).**

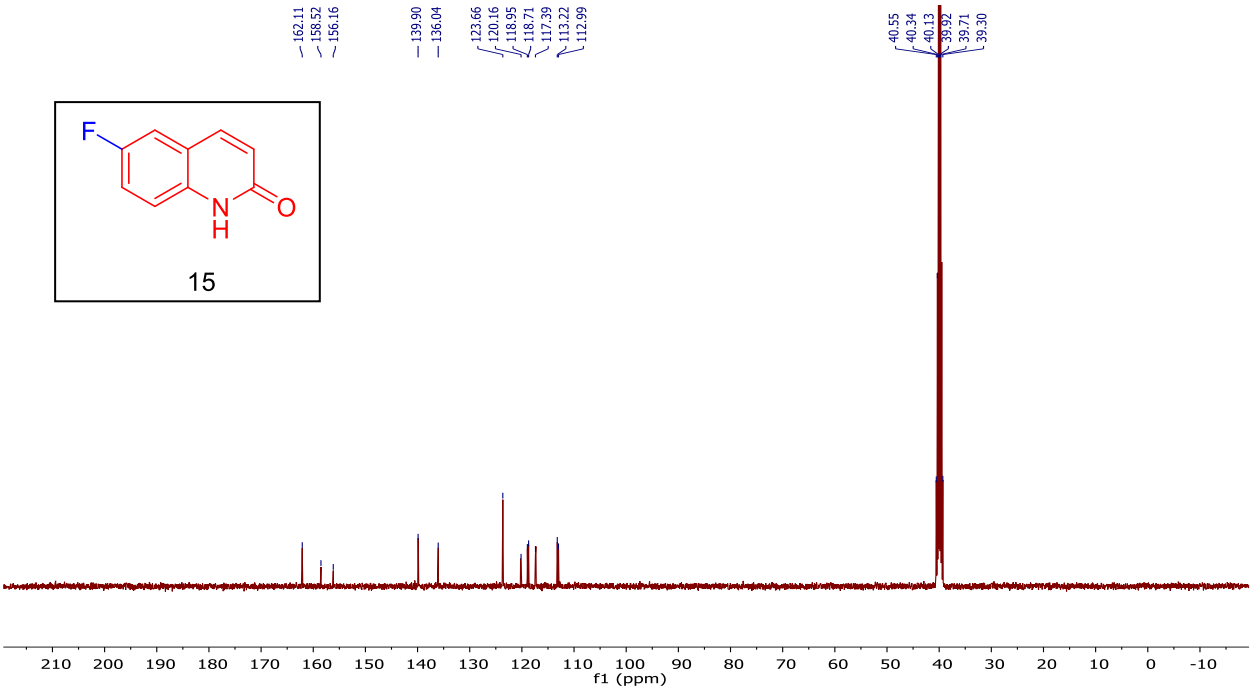



**Figure S28**. $^{13}$C NMR spectrum of **6-fluoroquinolin-2(1H)-one (15).**

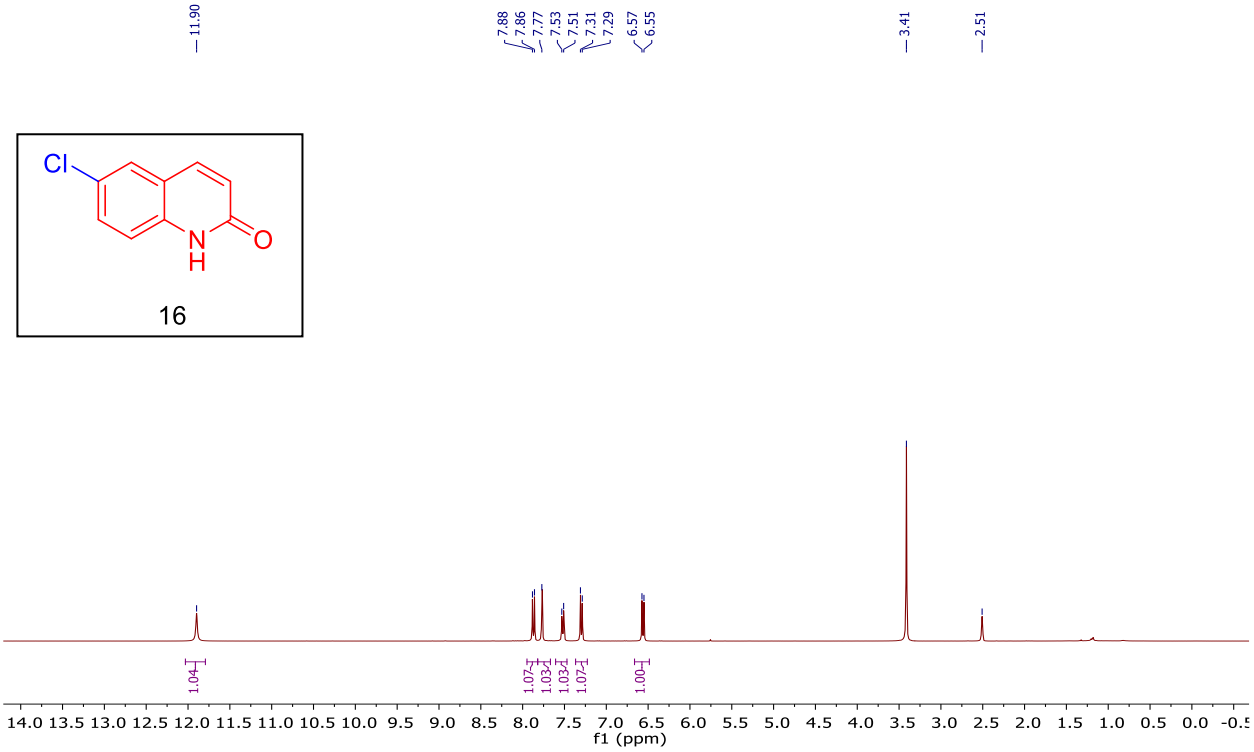



**Figure S29**. [1]H NMR spectrum of **6-chloroquinolin-2(1H)-one (16).**

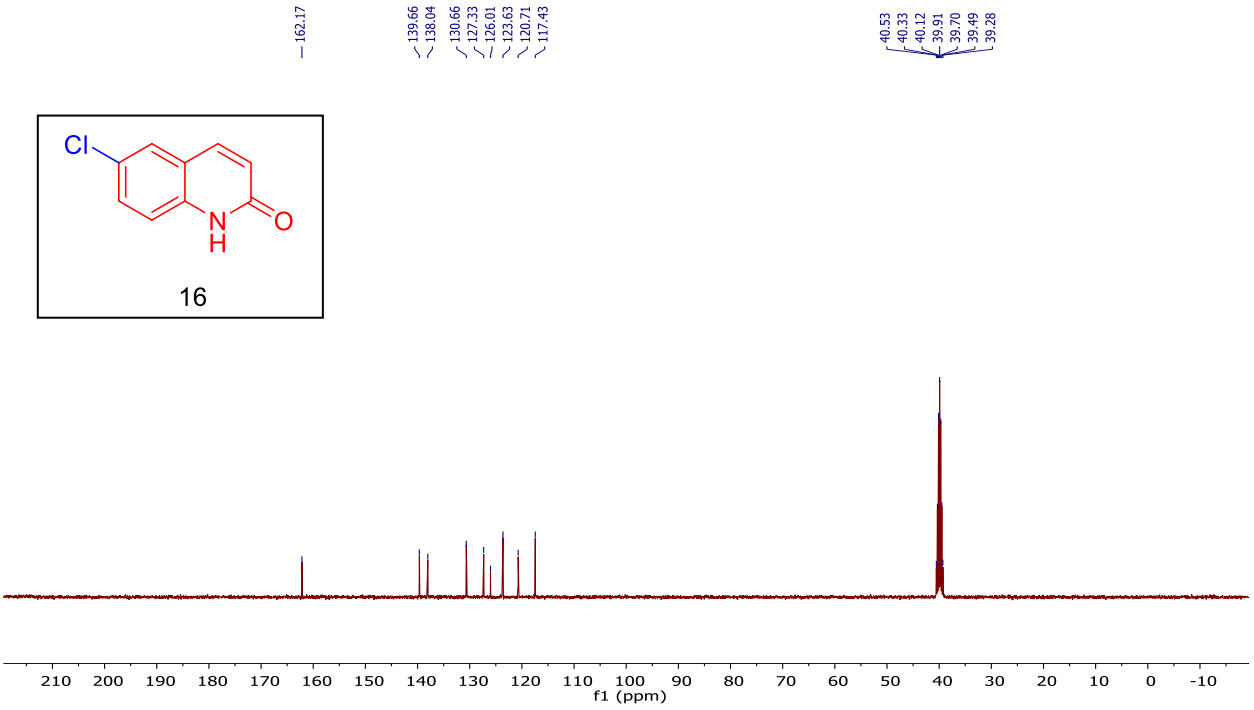



**Figure S30**. [13]C NMR spectrum of **6-chloroquinolin-2(1H)-one (16).**

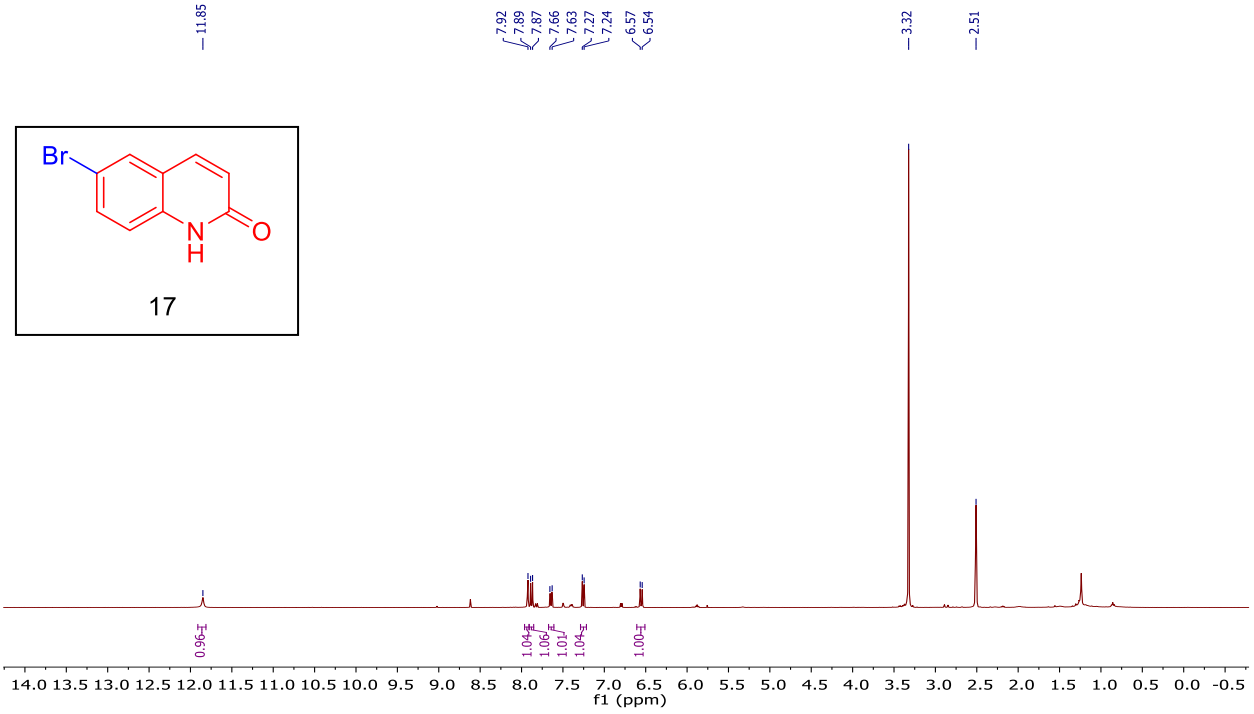



**Figure S31**. $^{1}$H NMR spectrum of **6-bromoquinolin-2(1H)-one (17).**

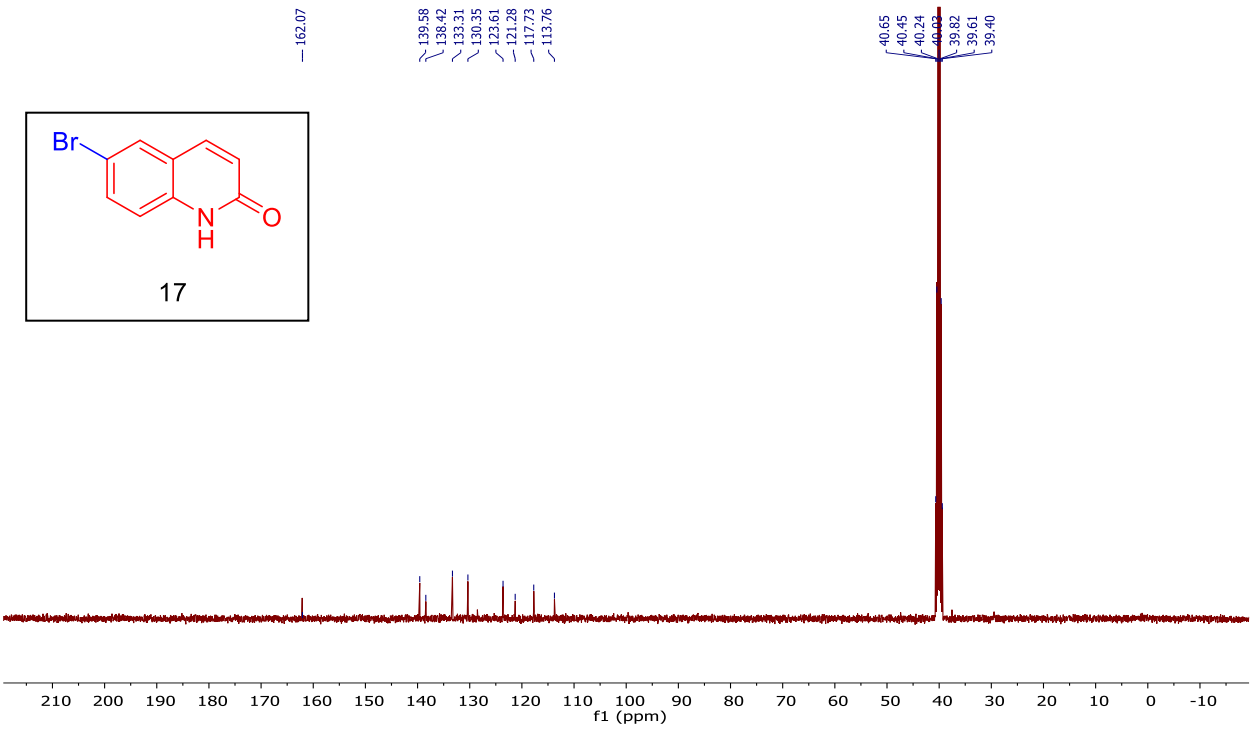



**Figure S32**. $^{13}$C NMR spectrum of **6-bromoquinolin-2(1H)-one (17).**

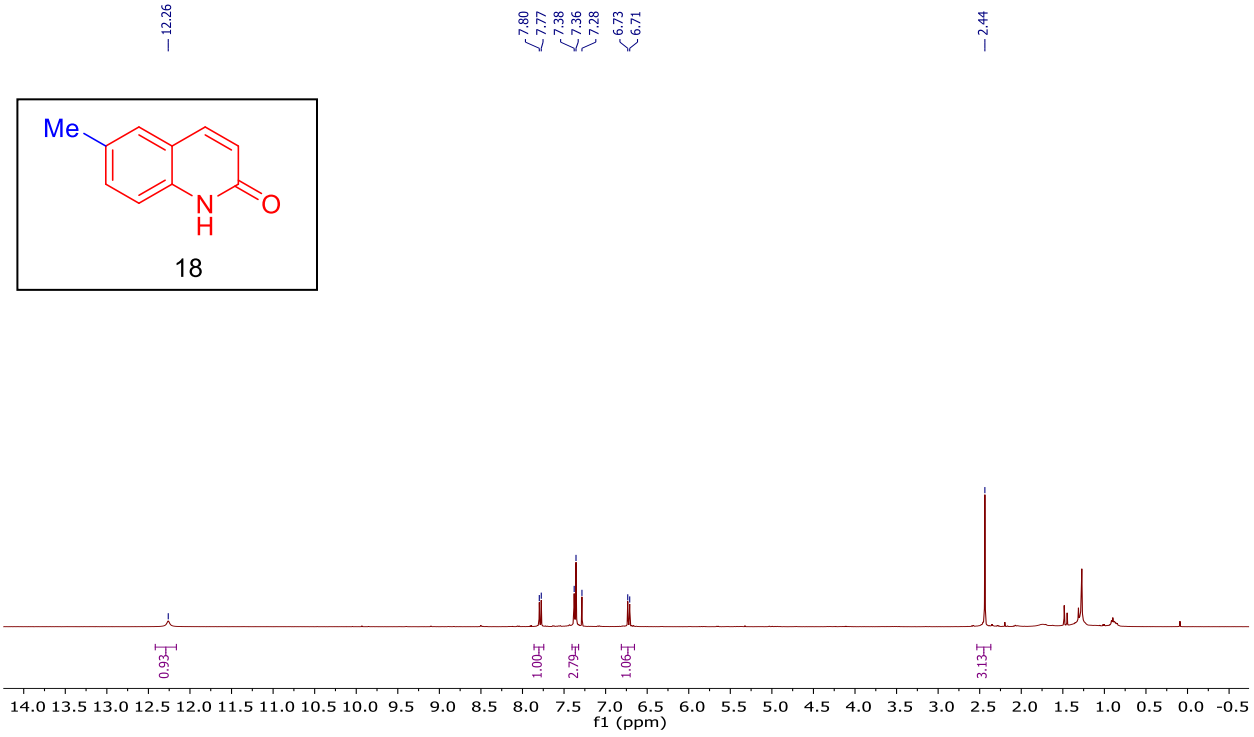



**Figure S33**. $^{1}$H NMR spectrum of **6-methylquinolin-2(1H)-one (18).**

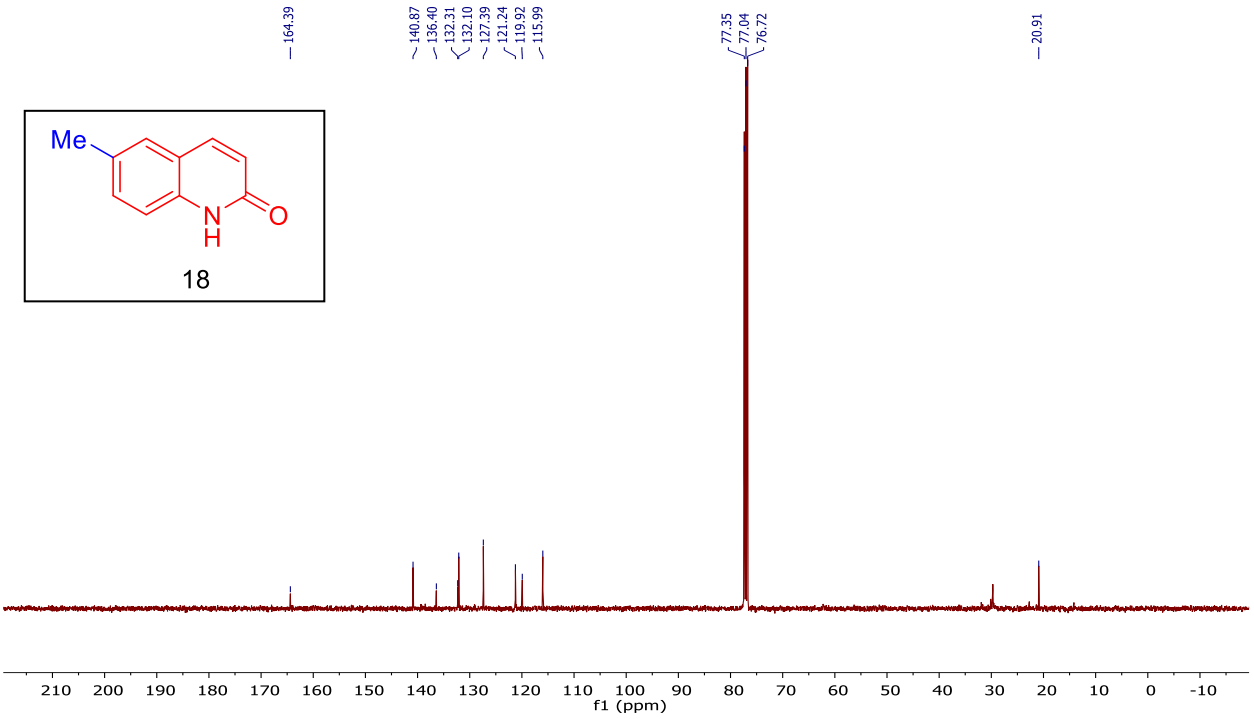



**Figure S34**. $^{13}$C NMR spectrum of **6-methylquinolin-2(1H)-one (18).**

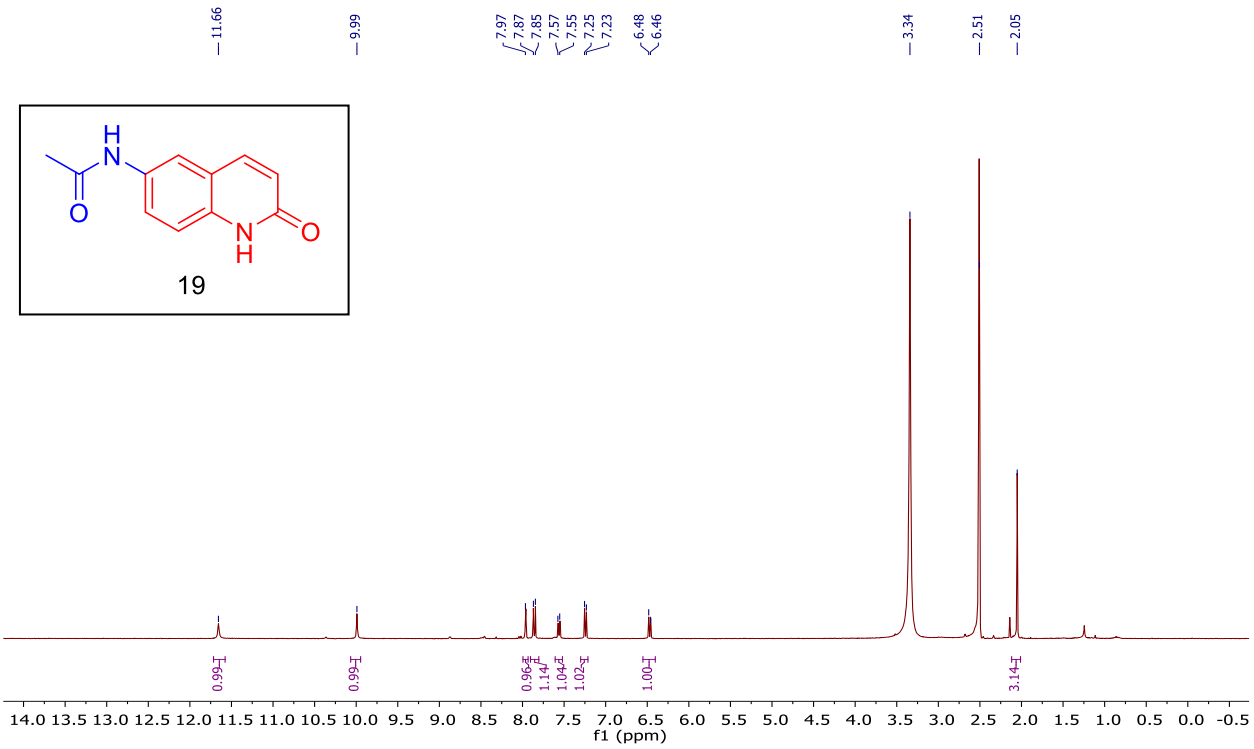



**Figure S35**. $^{1}$H NMR spectrum of **N-(2-oxo-1,2-dihydroquinolin-6-yl)acetamide (19).**

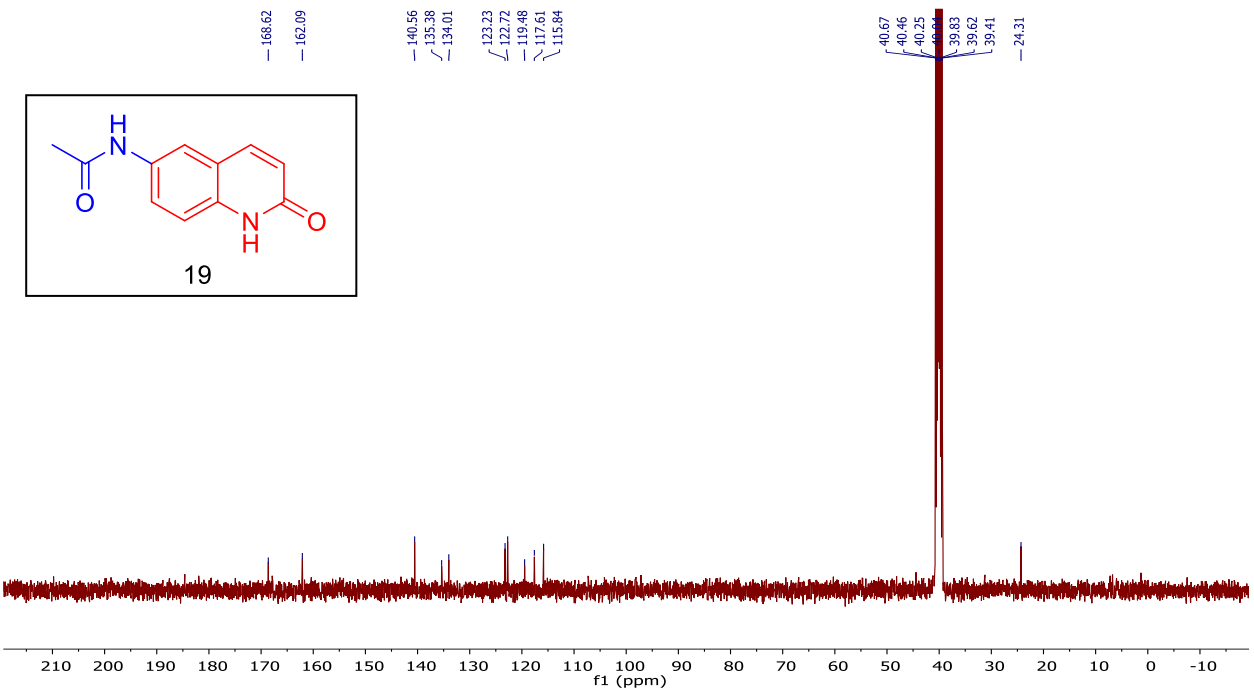



**Figure S36**. $^{13}$C NMR spectrum of **N-(2-oxo-1,2-dihydroquinolin-6-yl)acetamide (19).**

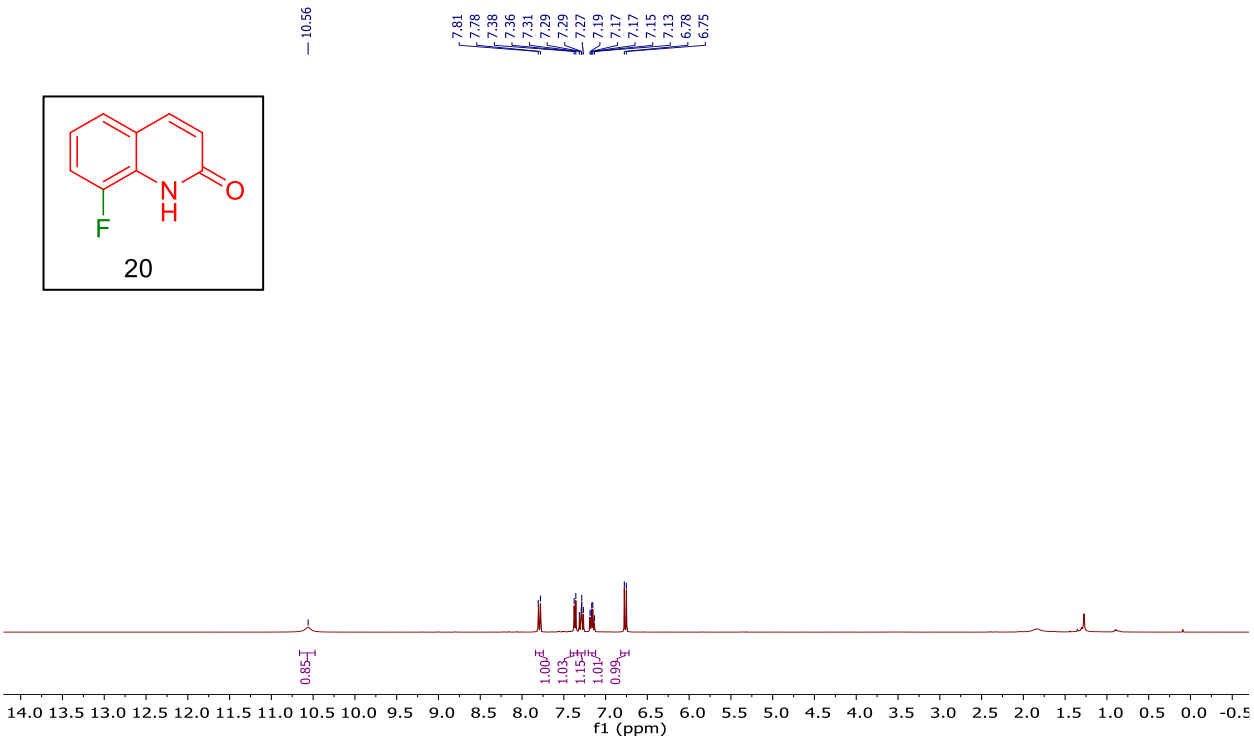



**Figure S37**. $^{1}$H NMR spectrum of **8-fluoroquinolin-2(1H)-one (20).**

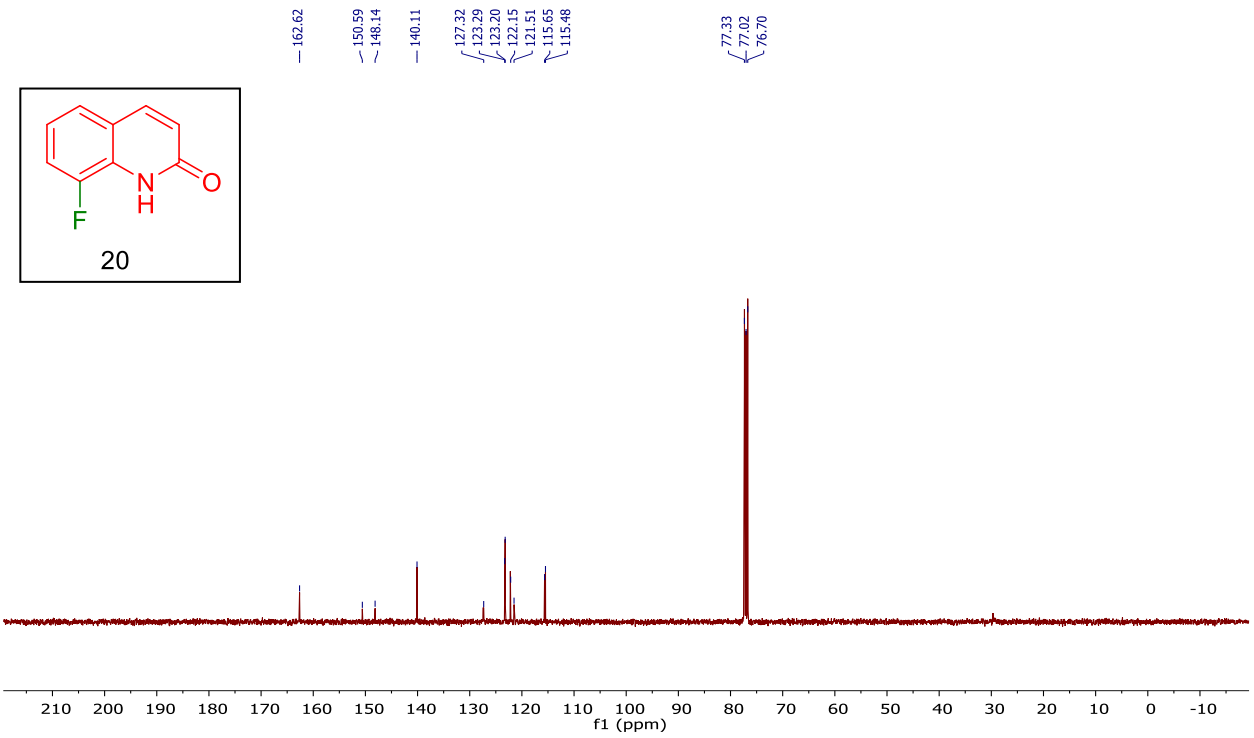



**Figure S38**. $^{13}$C NMR spectrum of **8-fluoroquinolin-2(1H)-one (20)**

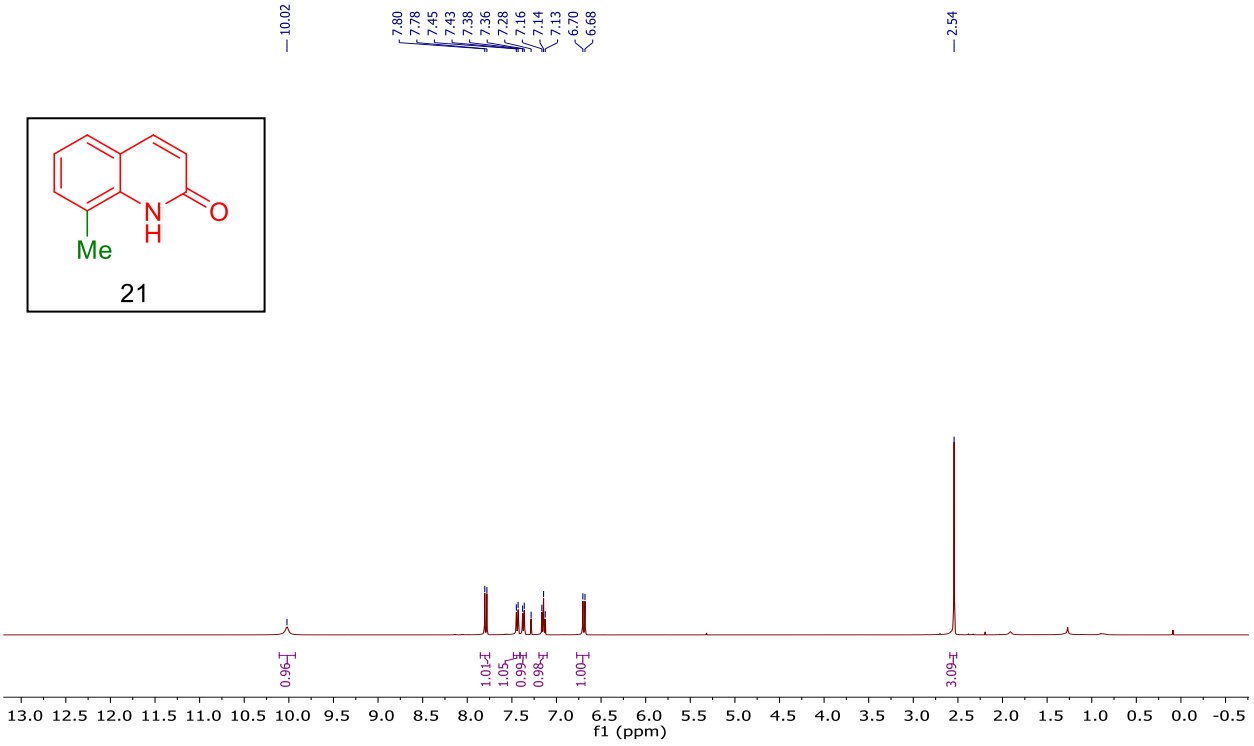



**Figure S39**. $^{1}$H NMR spectrum of **8-methylquinolin-2(1H)-one (21).**

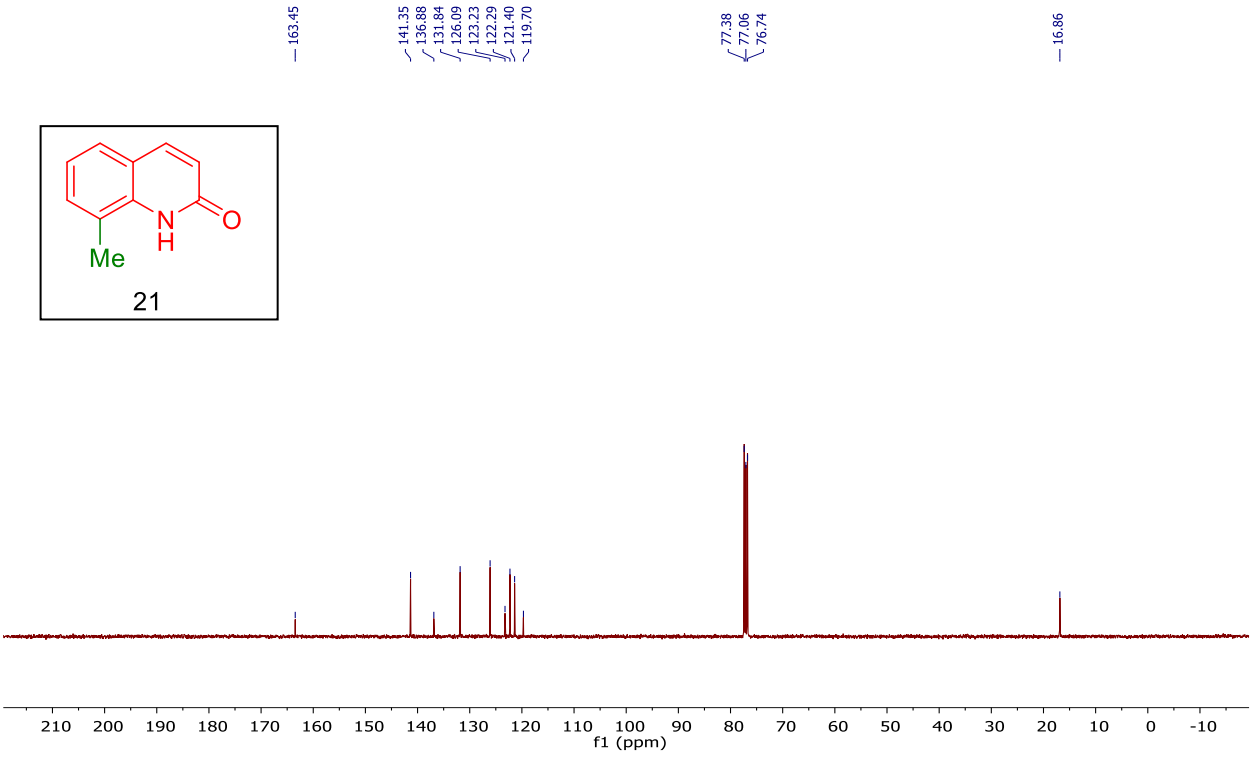



**Figure S40**. $^{13}$C NMR spectrum of **8-methylquinolin-2(1H)-one (21).**

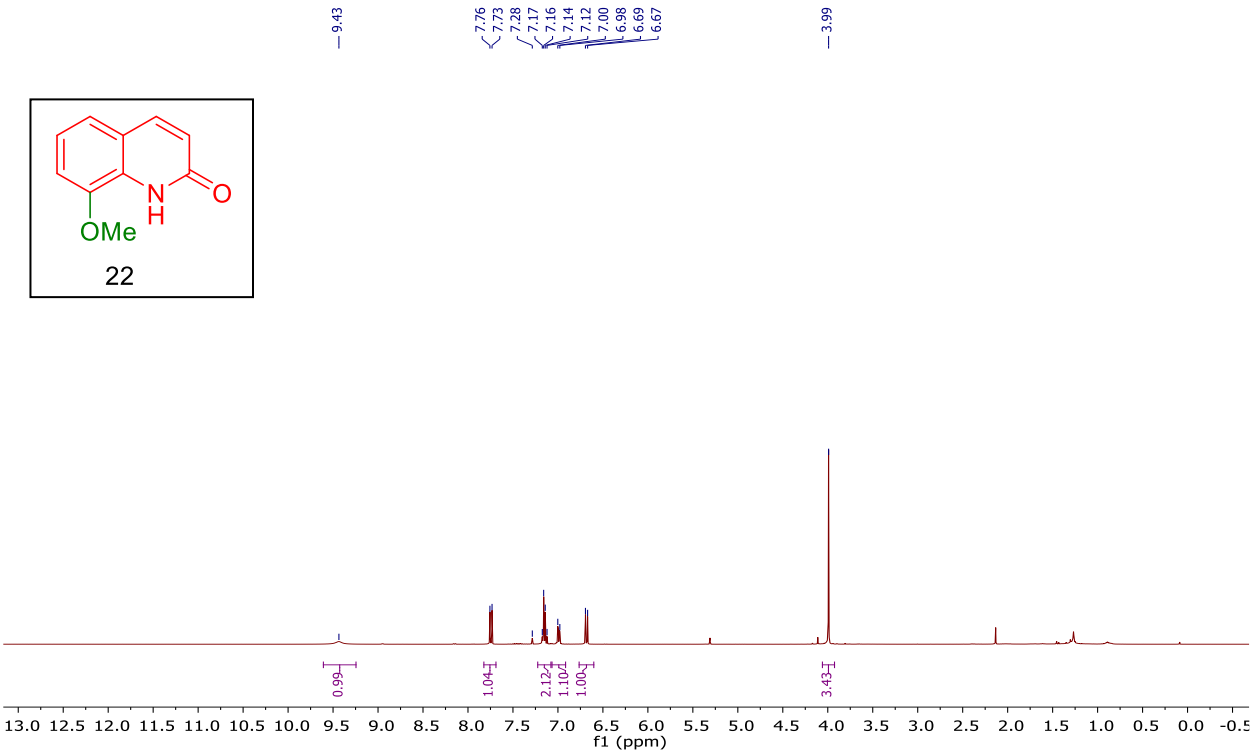



**Figure S41**. $^{1}$H NMR spectrum of **8-methoxyquinolin-2(1H)-one (22).**

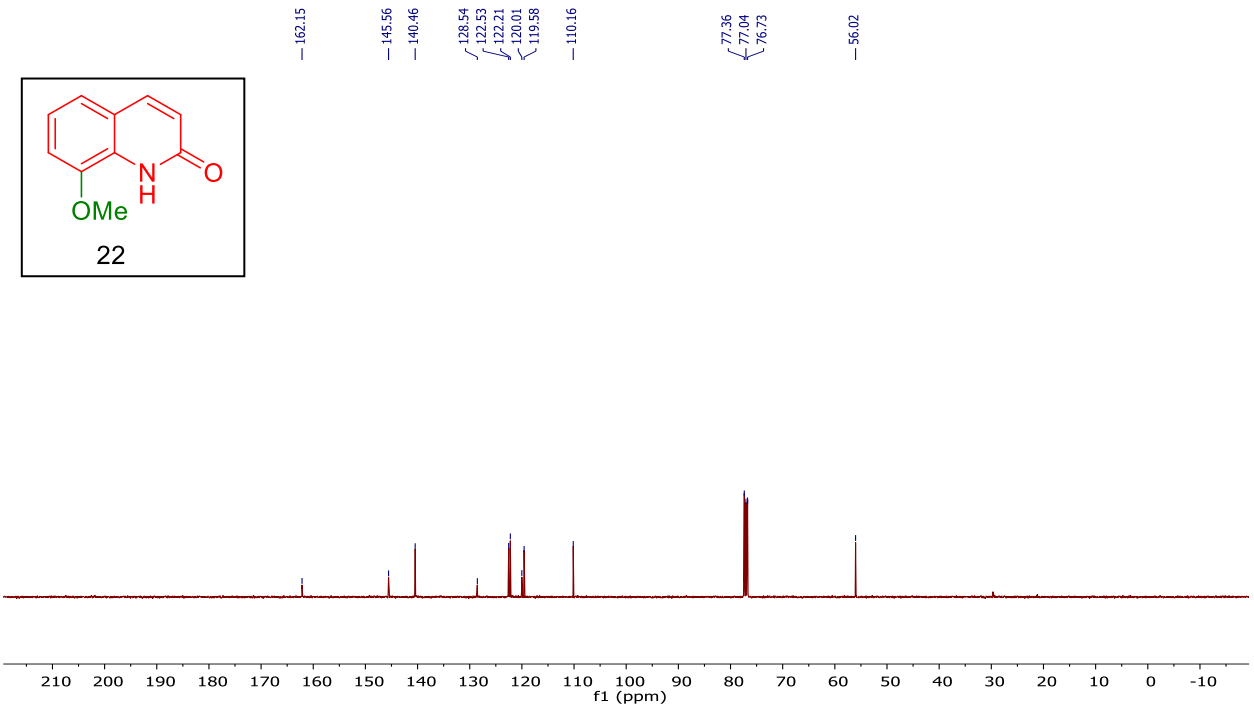



**Figure S42**. $^{13}$C NMR spectrum of **8-methoxyquinolin-2(1H)-one (22).**

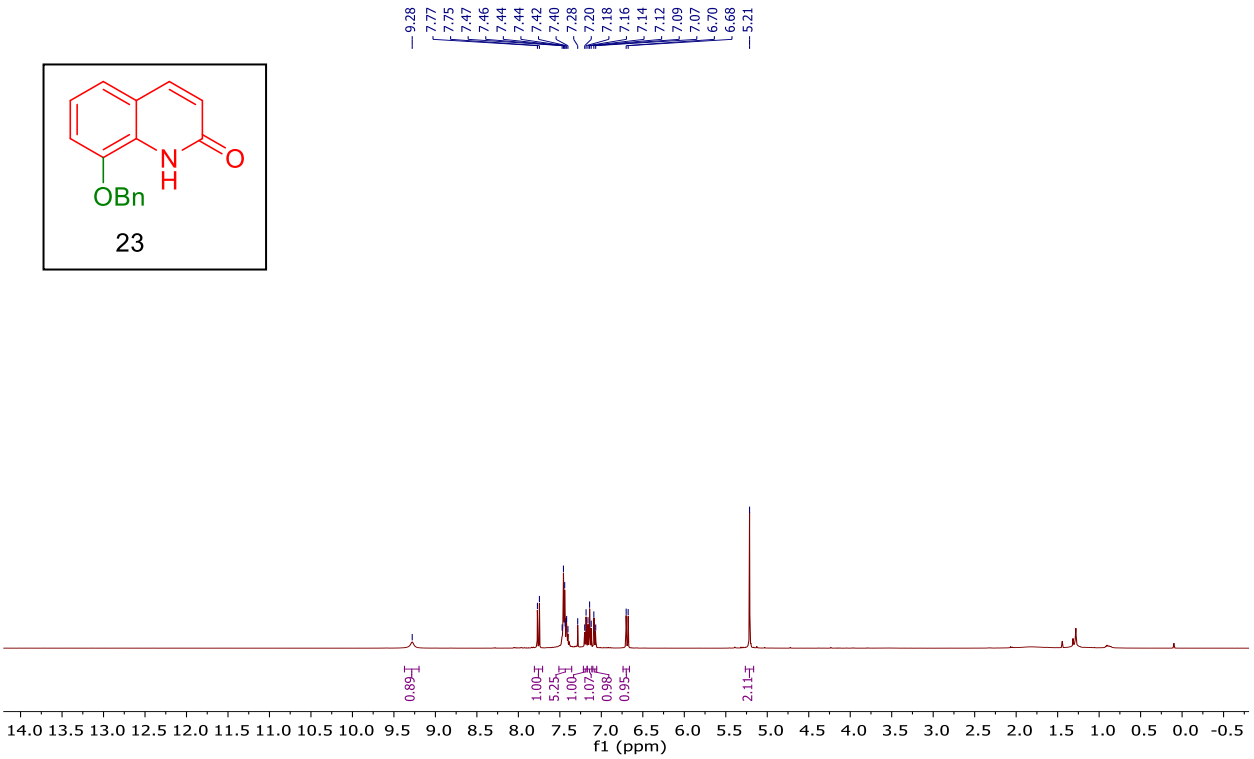



**Figure S43**. $^{1}$H NMR spectrum of **8-(benzyloxy)quinolin-2(1H)-one (23).**

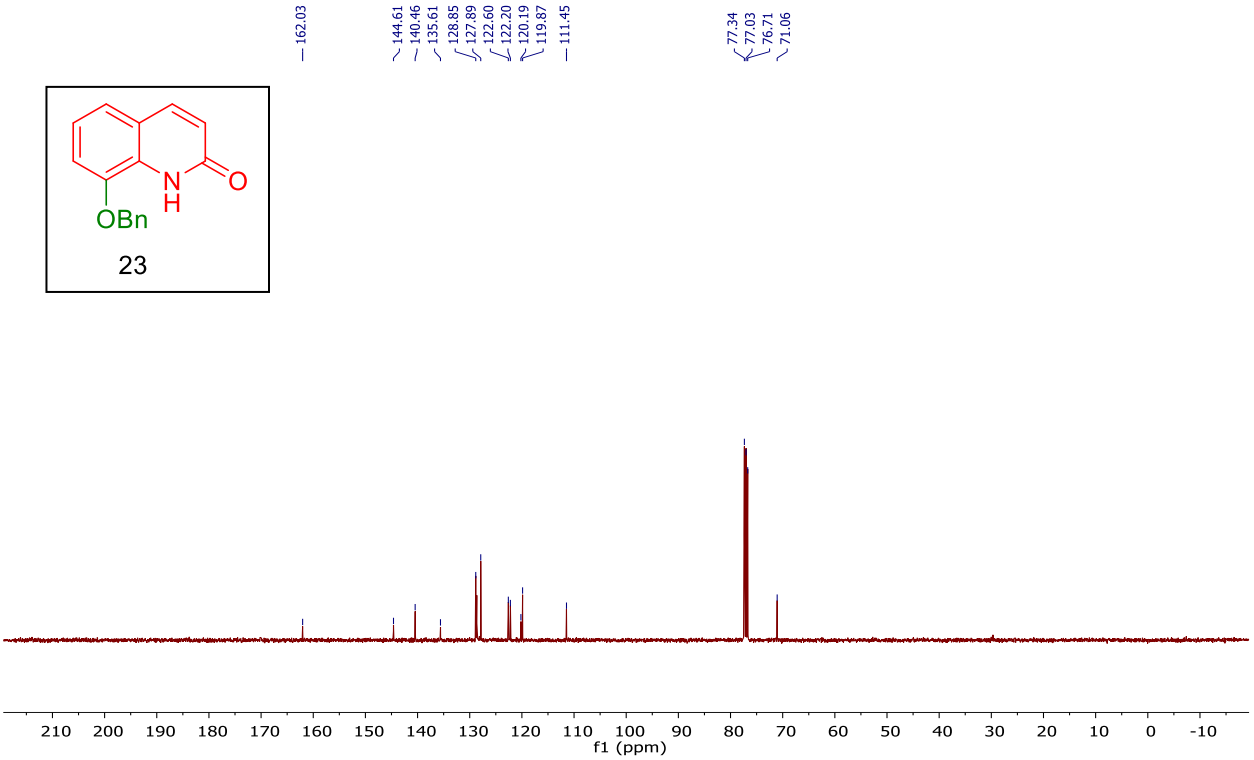



**Figure S44**. $^{13}$C NMR spectrum of **8-(benzyloxy)quinolin-2(1H)-one (23).**

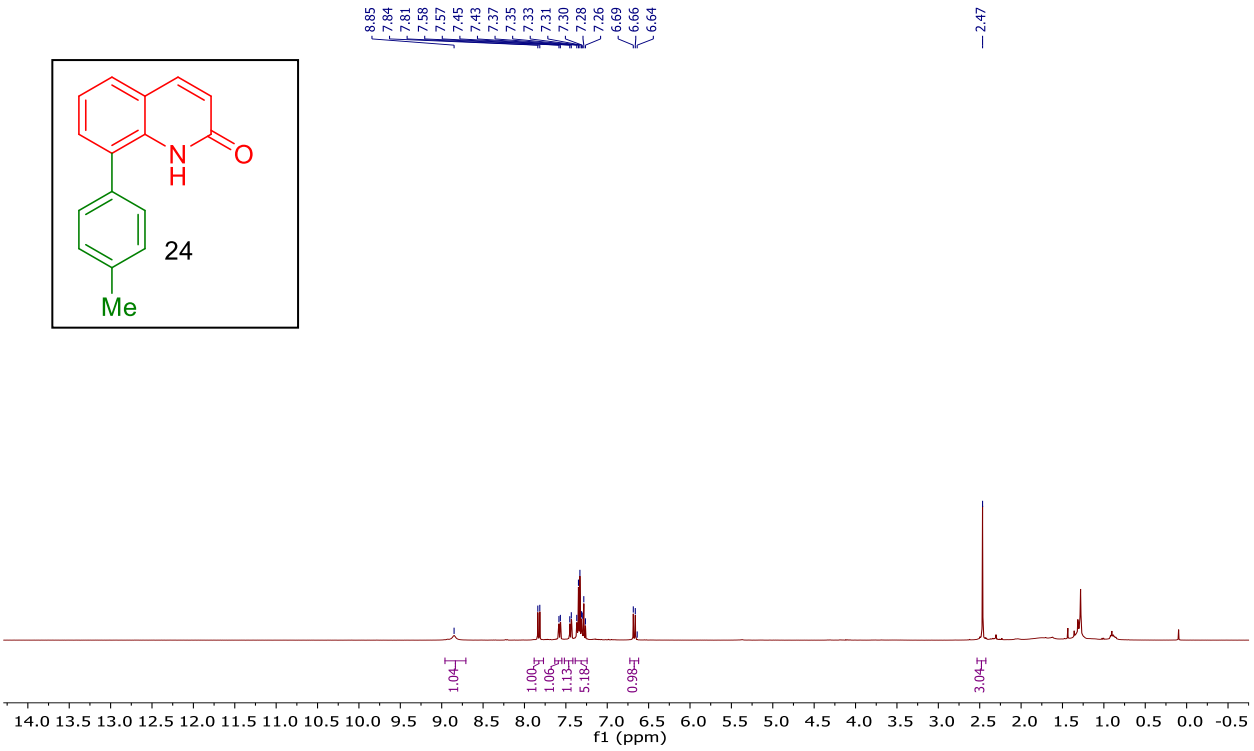



**Figure S45**. $^{1}$H NMR spectrum of **8-(p-tolyl)quinolin-2(1H)-one (24).**

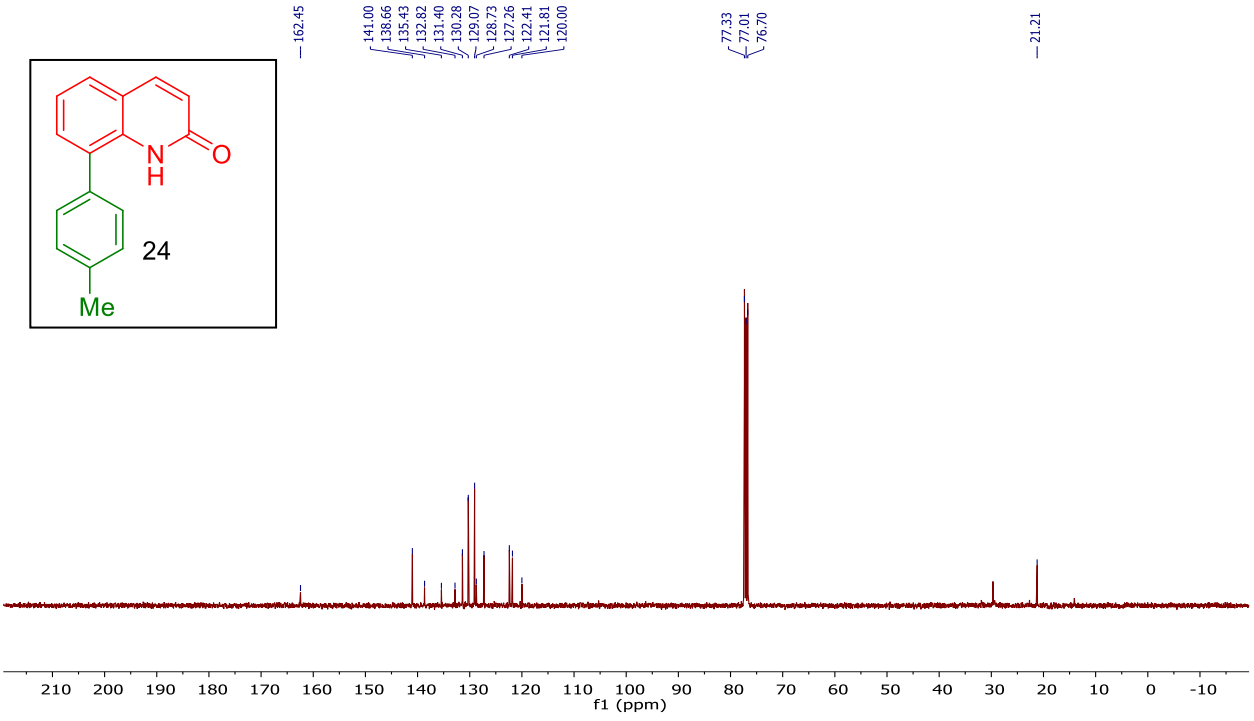



**Figure S46**. $^{13}$C NMR spectrum of **8-(p-tolyl)quinolin-2(1H)-one (24).**

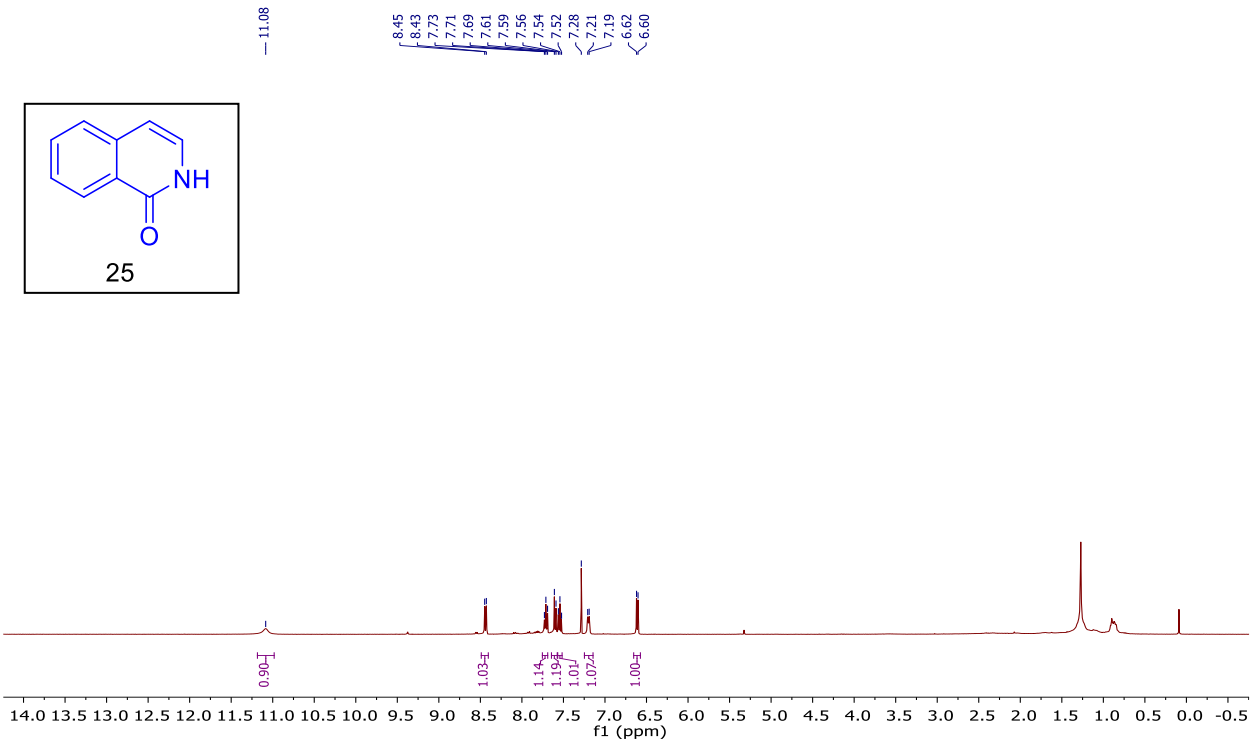



**Figure S47**. $^{1}$H NMR spectrum of **isoquinolin-1(2H)-one (25).**

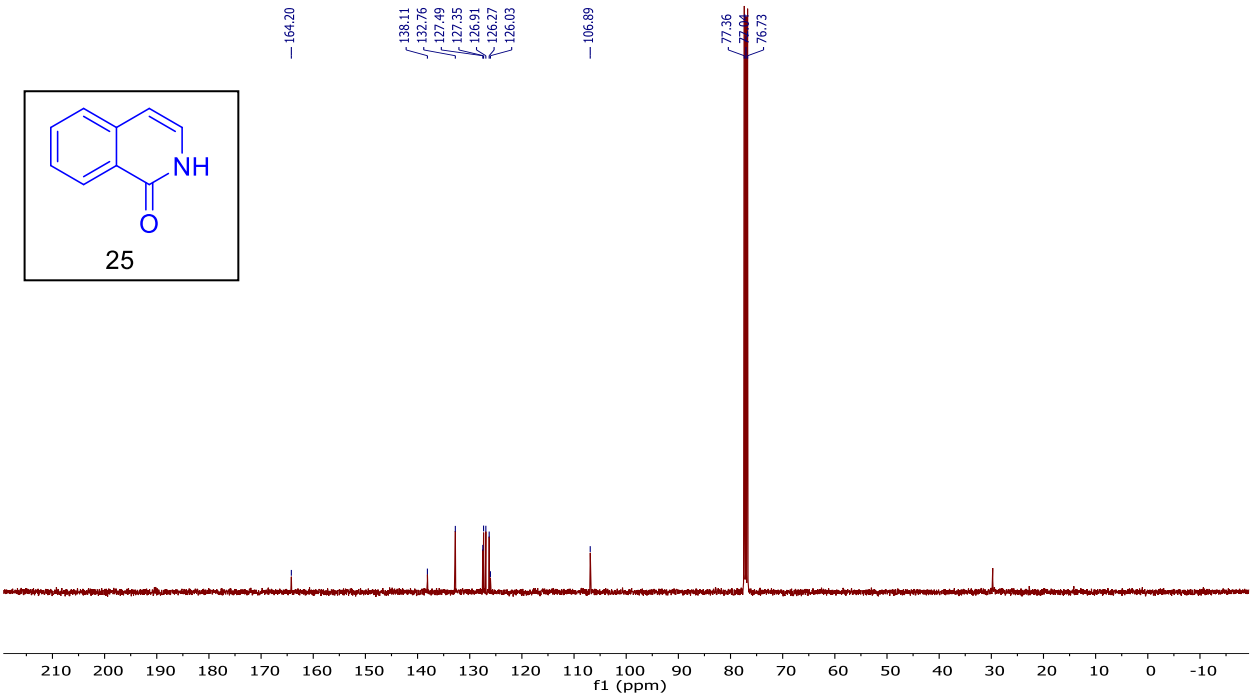



**Figure S48**. $^{13}$C NMR spectrum of **isoquinolin-1(2H)-one (25).**

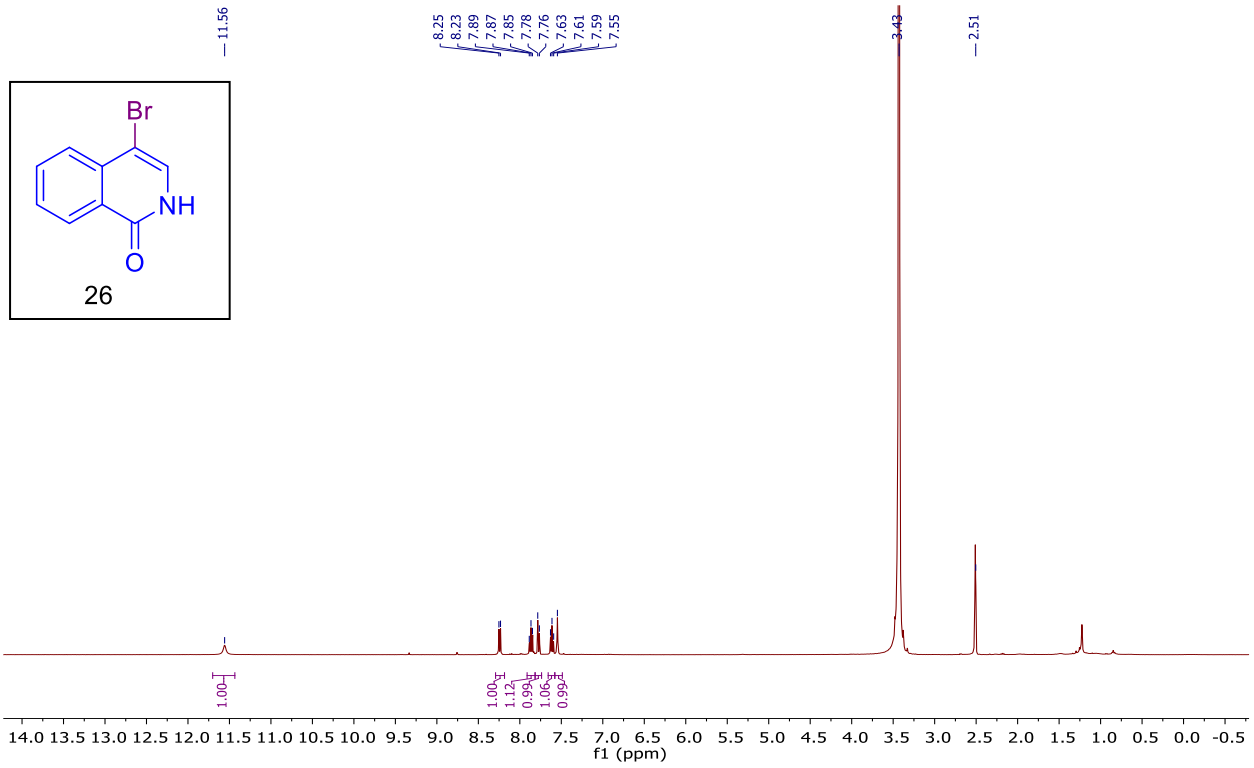



**Figure S49**. $^{1}$H NMR spectrum of **4-bromoisoquinolin-1(2H)-one (26).**

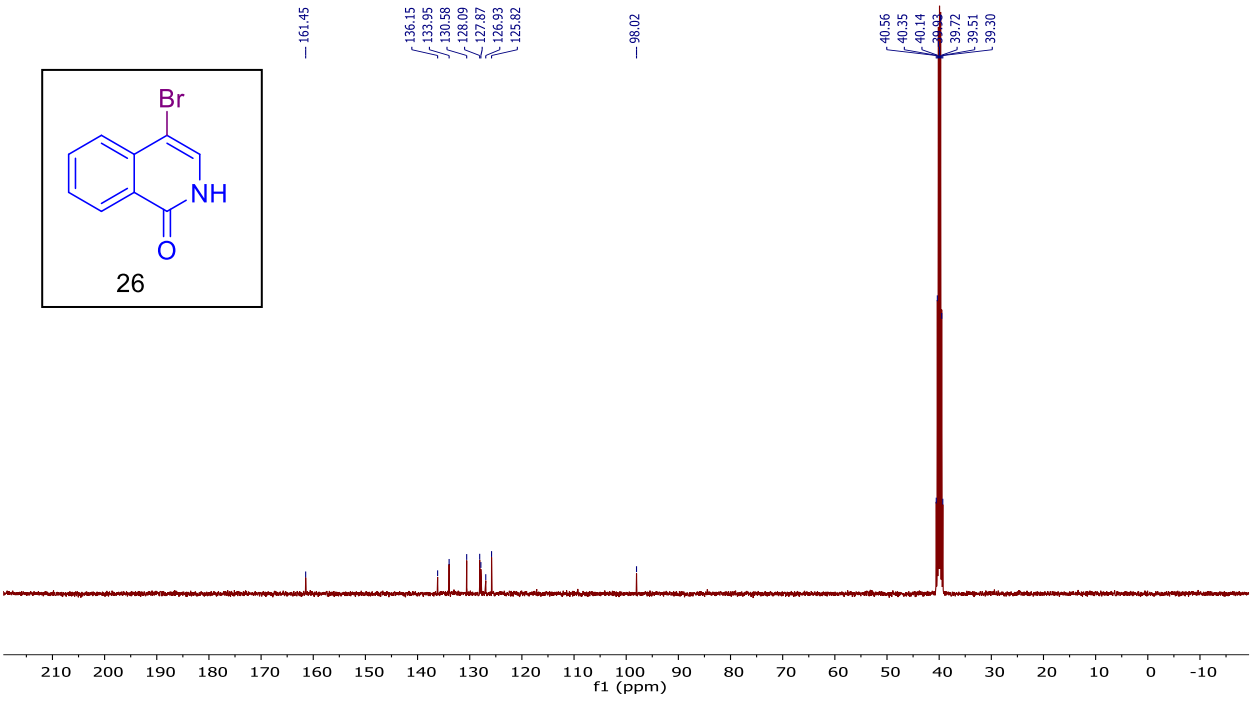



**Figure S50**. $^{13}$C NMR spectrum of **4-bromoisoquinolin-1(2H)-one (26).**

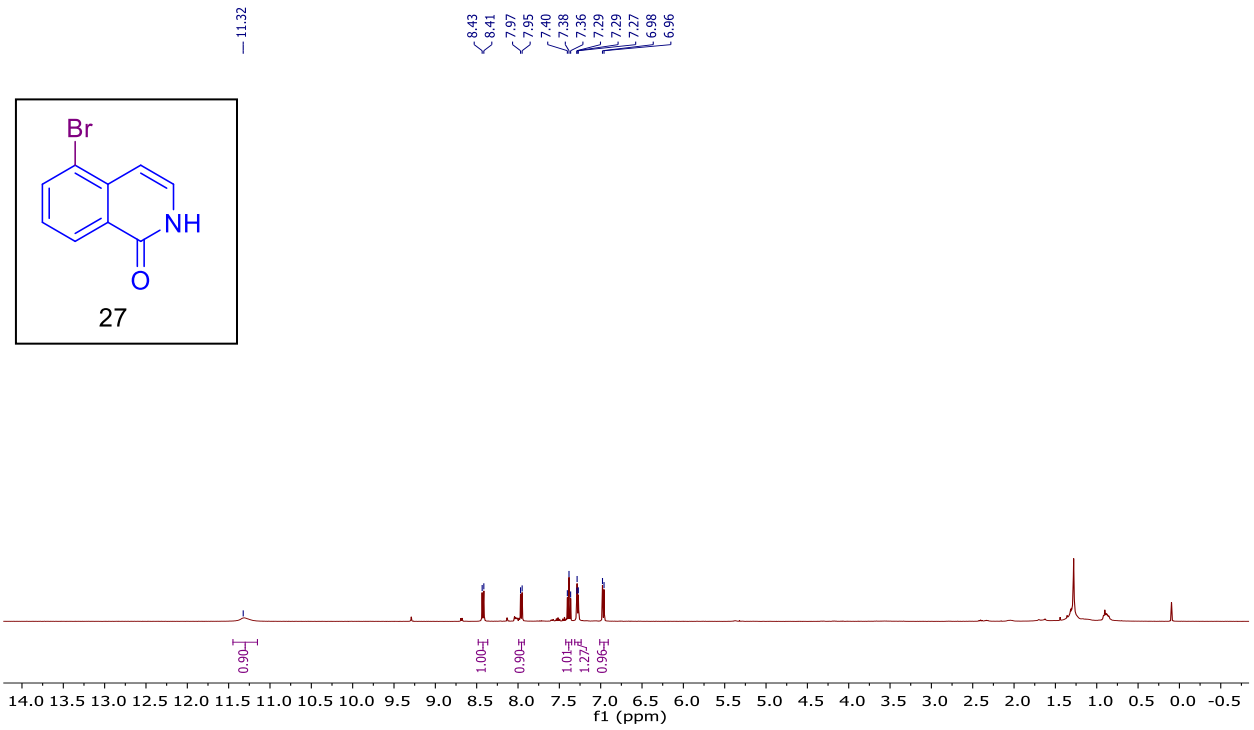



**Figure S51**. $^{1}$H NMR spectrum of **5-bromoisoquinolin-1(2H)-one (27).**

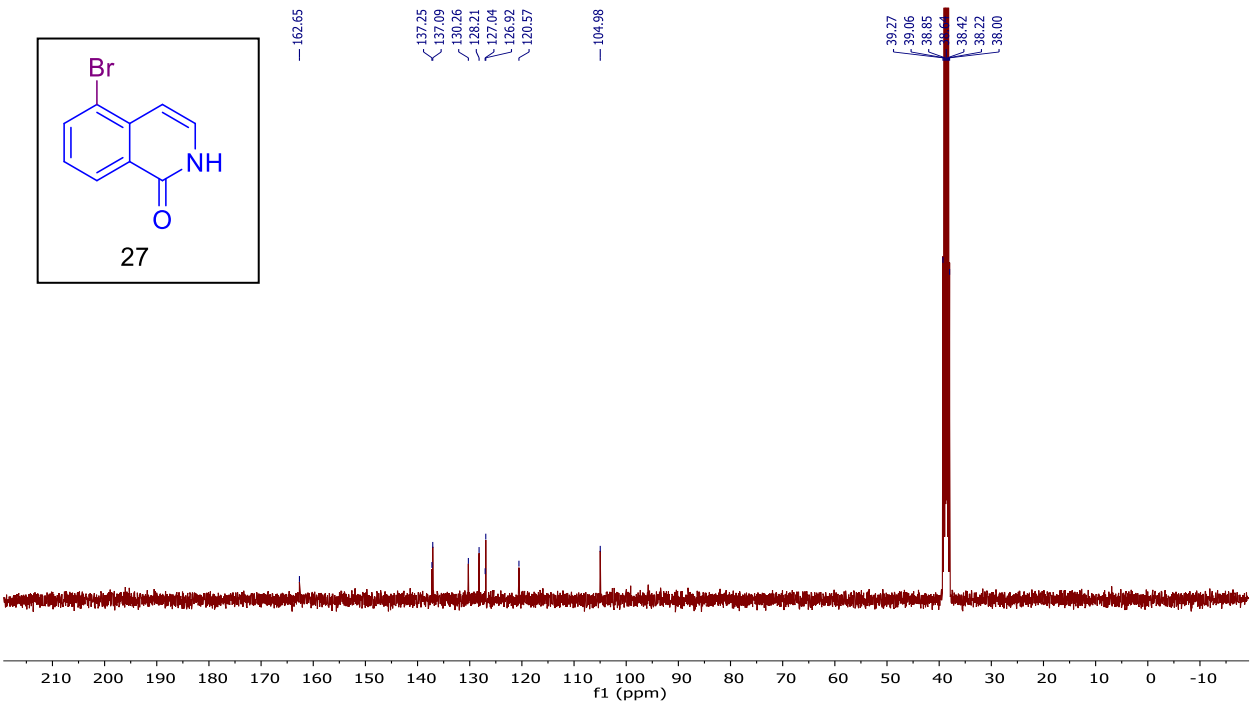



**Figure S52**. $^{13}$C NMR spectrum of **5-bromoisoquinolin-1(2H)-one (27).**

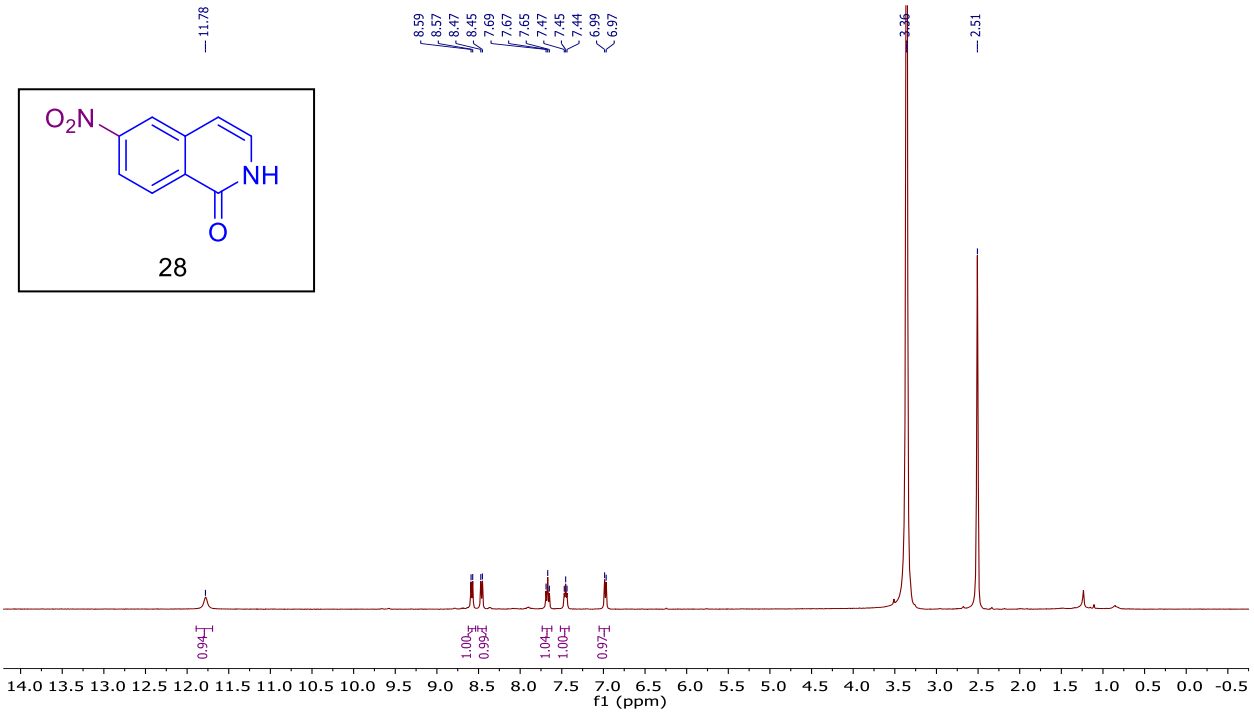



**Figure S53**. [1]H NMR spectrum of **6-nitroisoquinolin-1(2H)-one (28).**

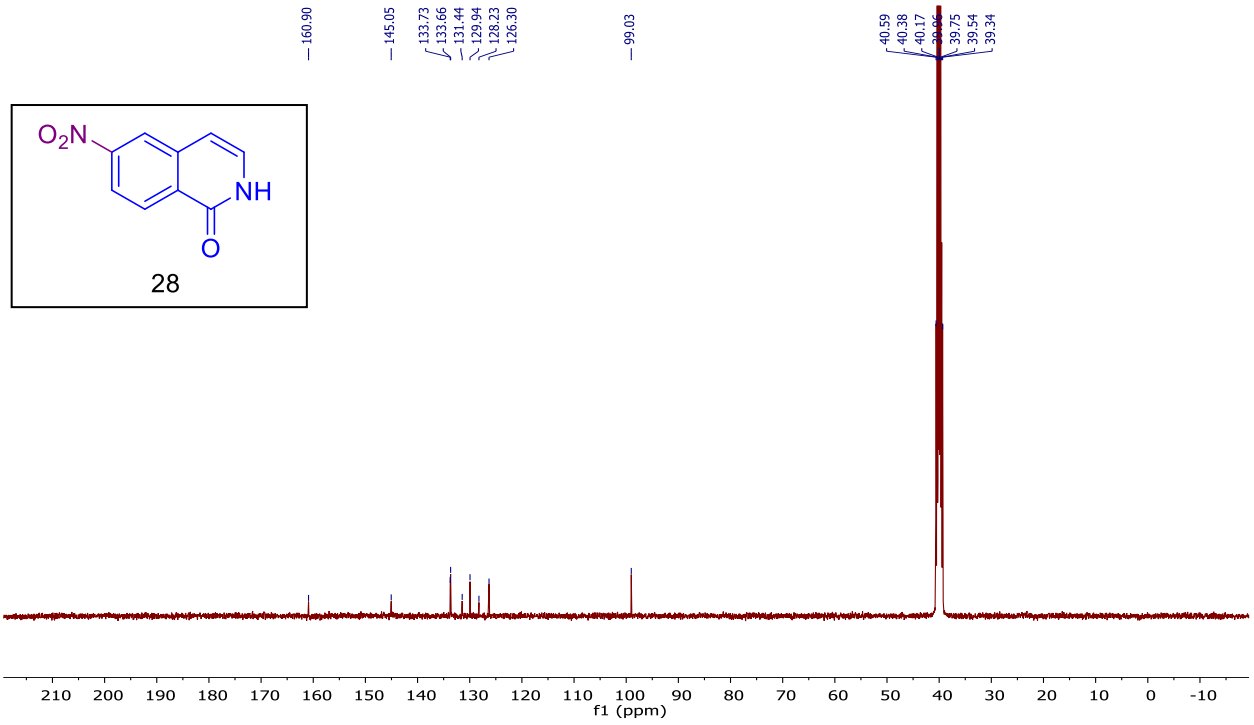



**Figure S54**. [13]C NMR spectrum of **6-nitroisoquinolin-1(2H)-one (28).**