

Supporting information
for

**Synthesis of 3-(pyridin-2-yl)quinazolin-2,4(1*H*,3*H*)-diones via annulation of
anthranilic esters with *N*-pyridyl ureas**

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Saint Petersburg, Russia*

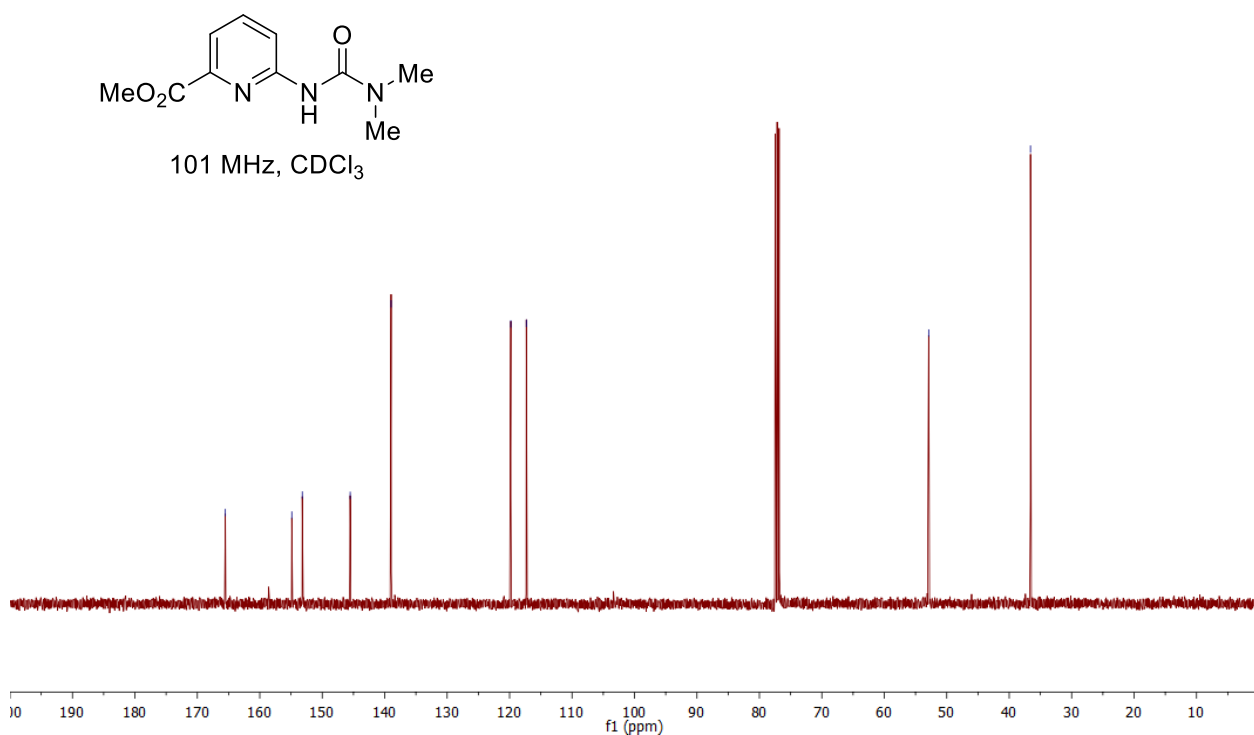
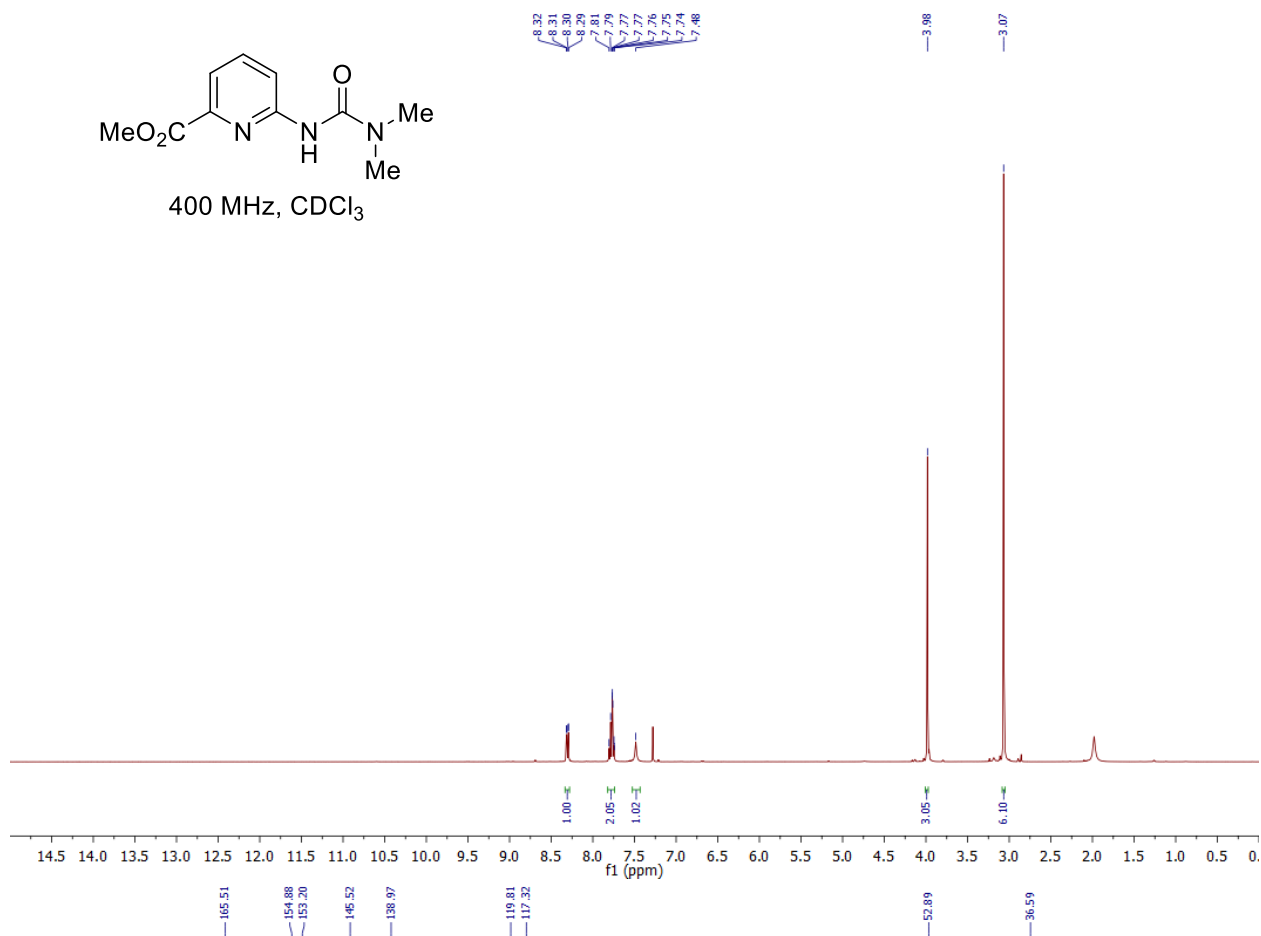
*Corresponding authors: v.boyarskii@spbu.ru.

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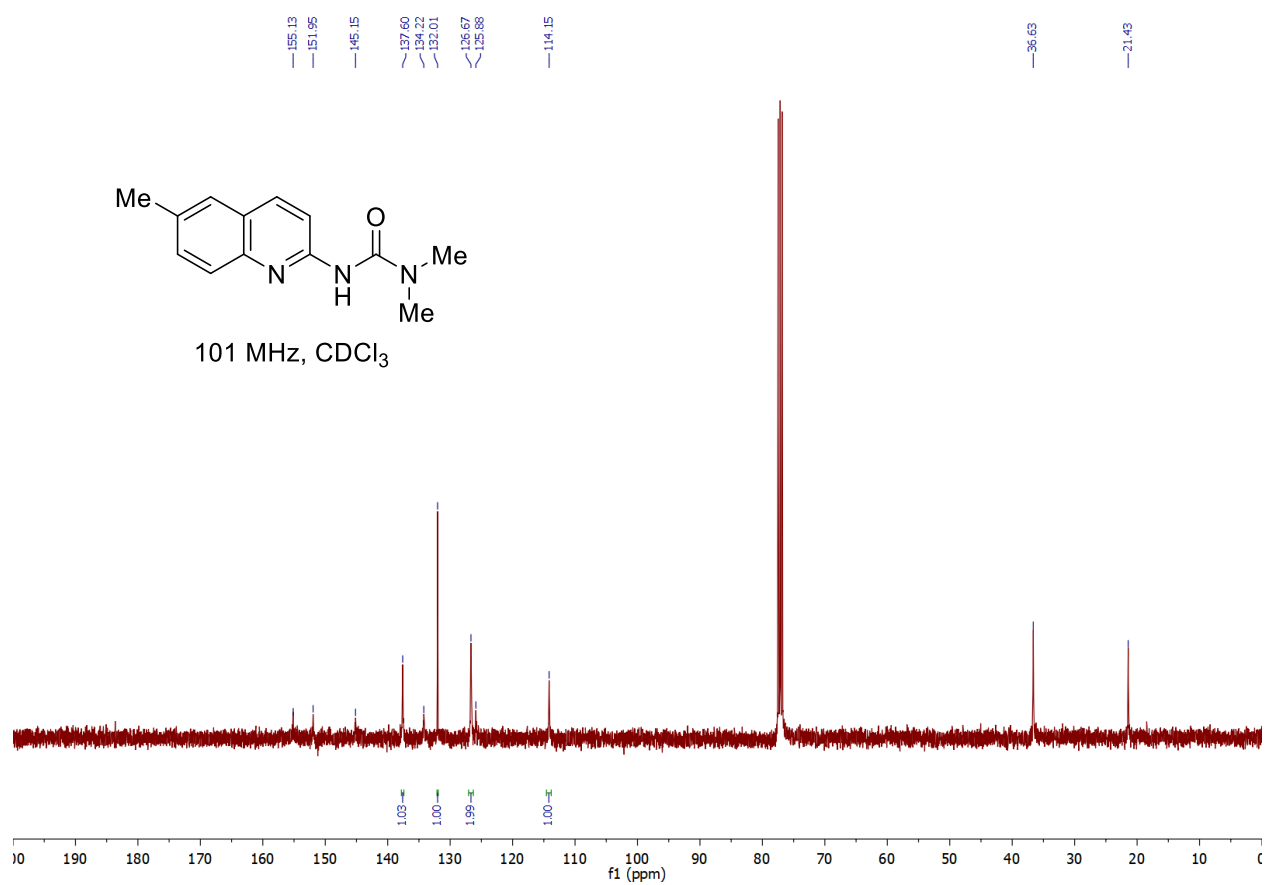
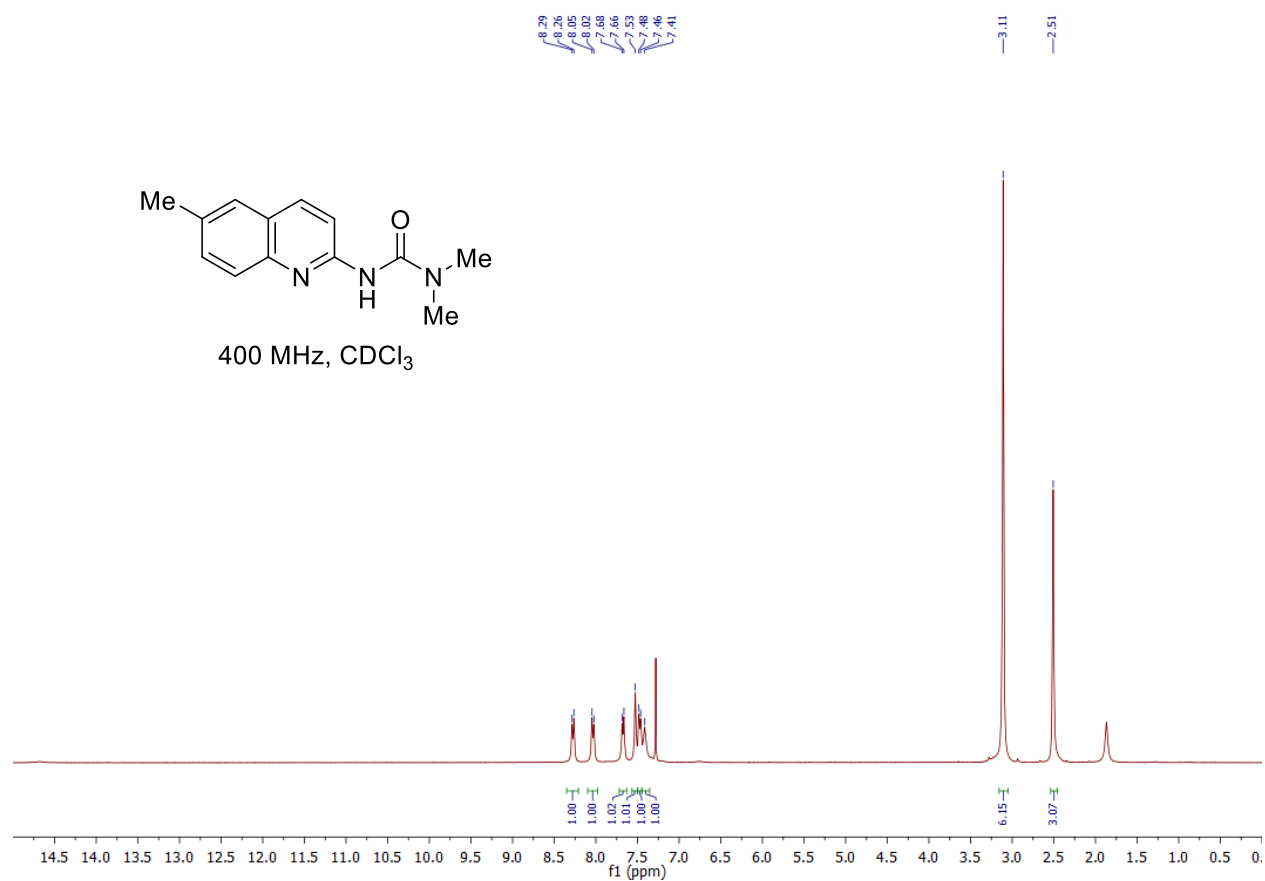
Copies of ^1H , ^{13}C , and ^{19}F NMR spectra.....	3
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Copies of ^1H , ^{13}C , and ^{19}F NMR spectra

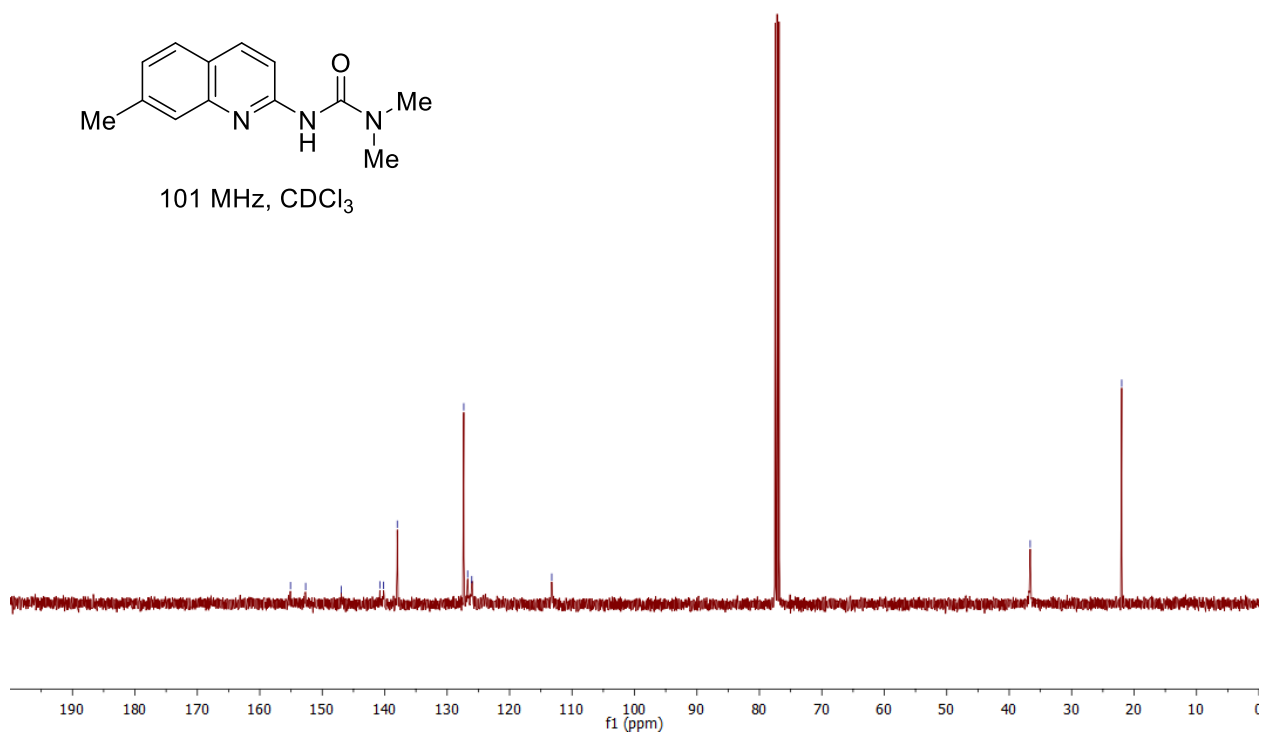
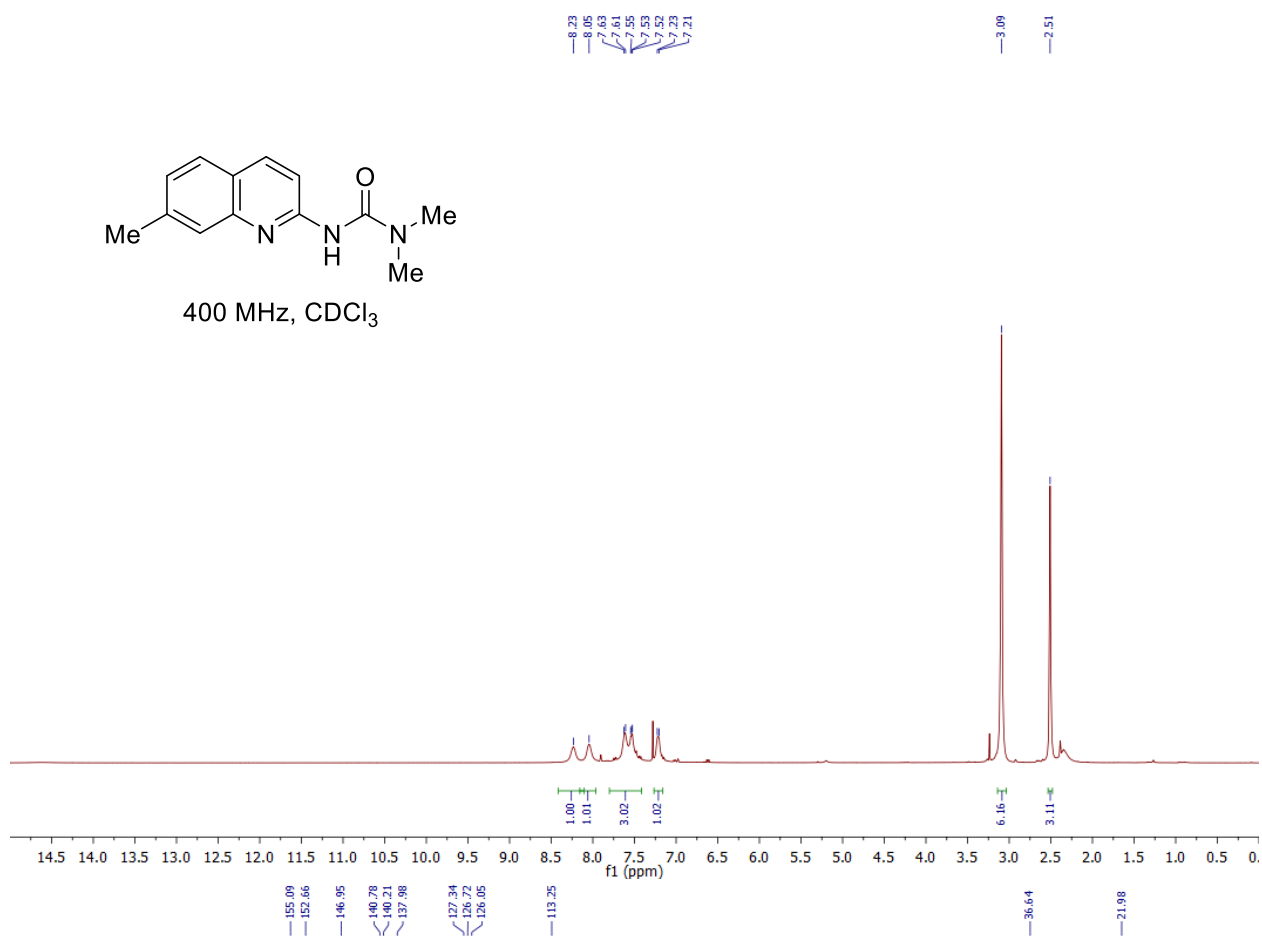
^1H and ^{13}C spectra of methyl 6-(3,3-dimethylureido)picolinate **1h**



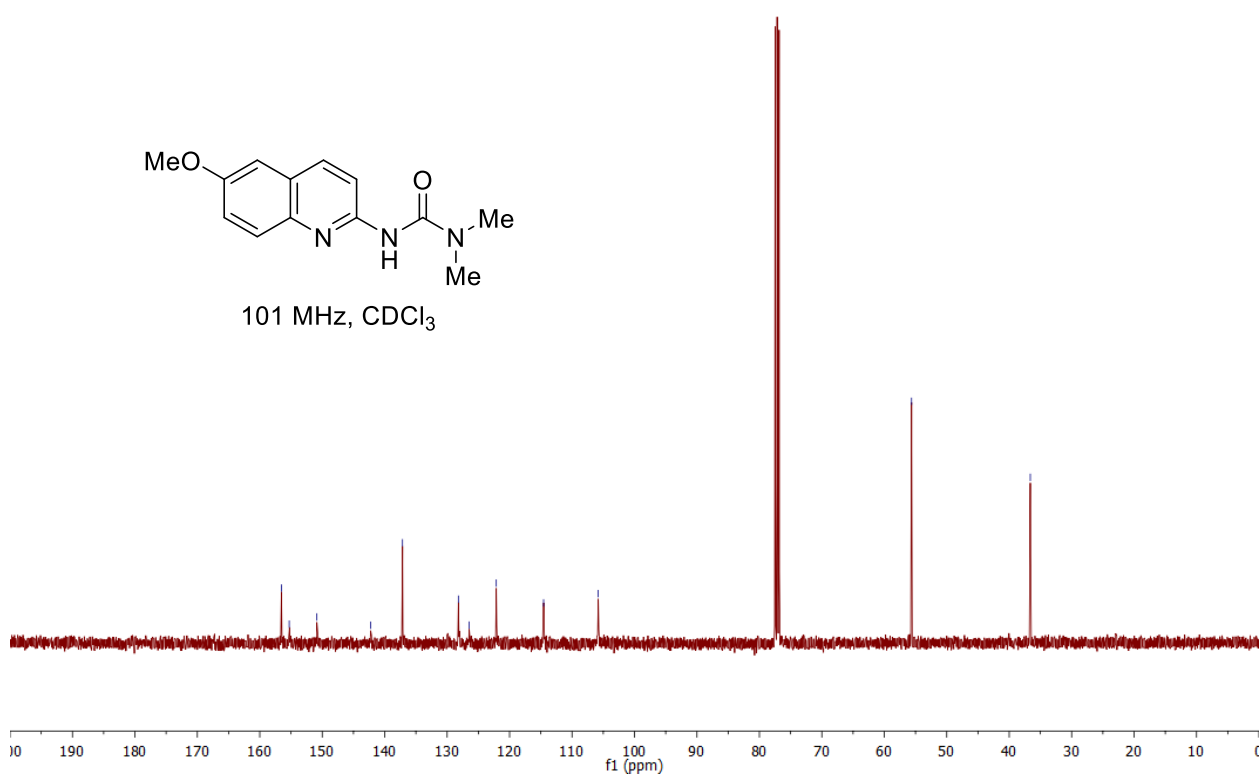
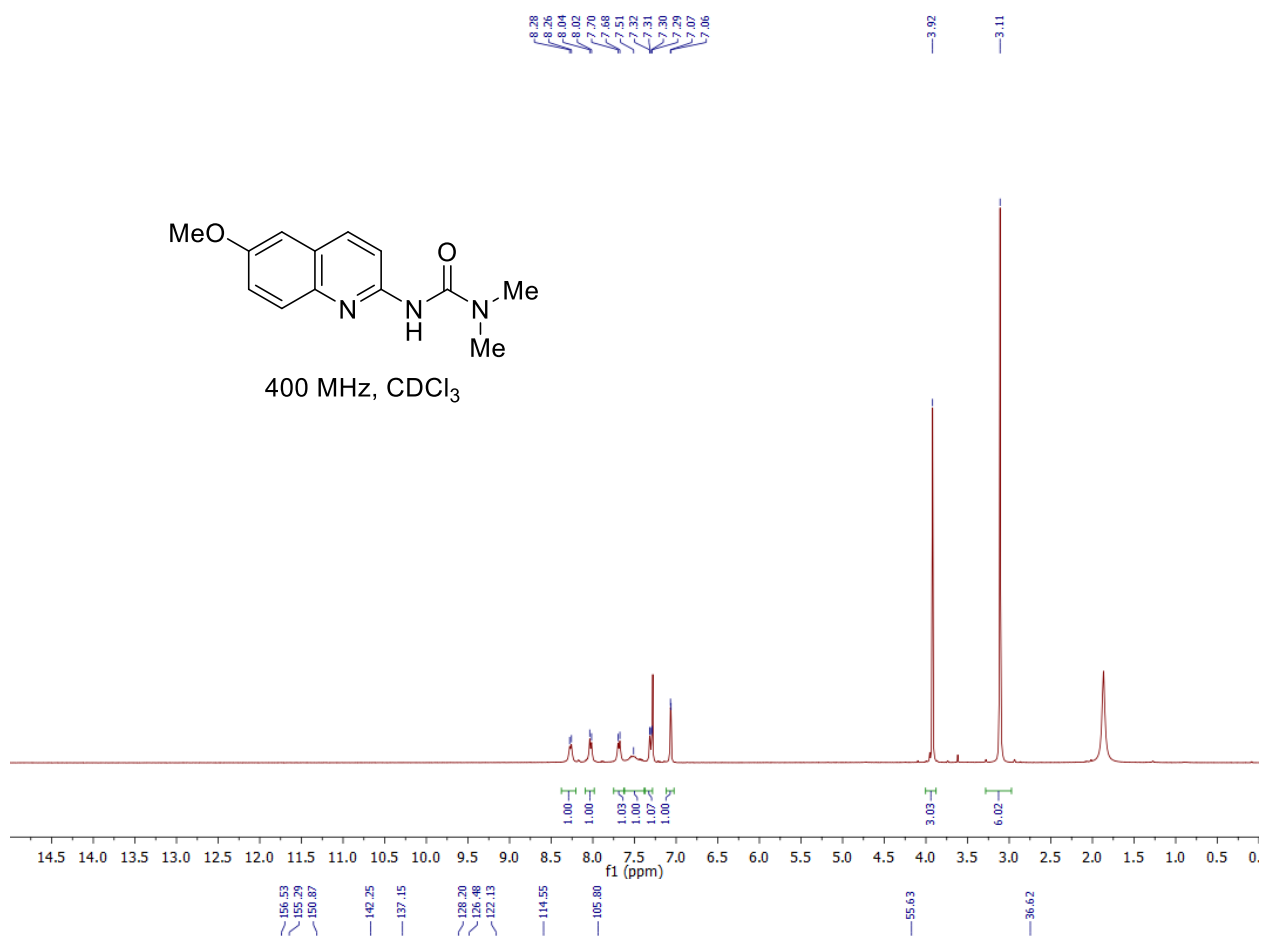
^1H and ^{13}C spectra of 1,1-dimethyl-3-(6-methylquinolin-2-yl)urea **1n**



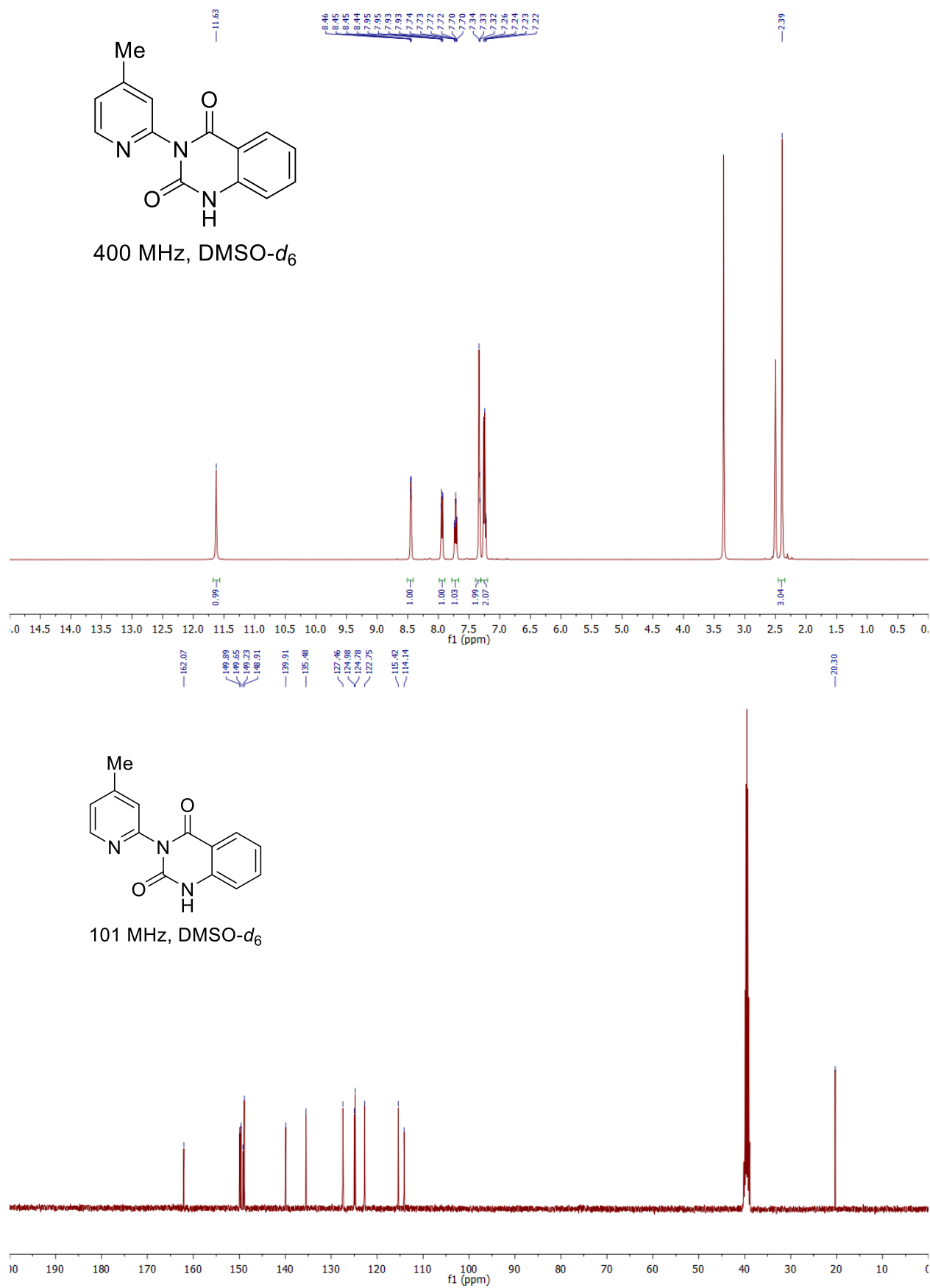
^1H and ^{13}C spectra of 1,1-dimethyl-3-(7-methylquinolin-2-yl)urea **1o**



^1H and ^{13}C spectra of 3-(6-methoxyquinolin-2-yl)-1,1-dimethylurea **1p**



^1H and ^{13}C spectra of 3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3a**

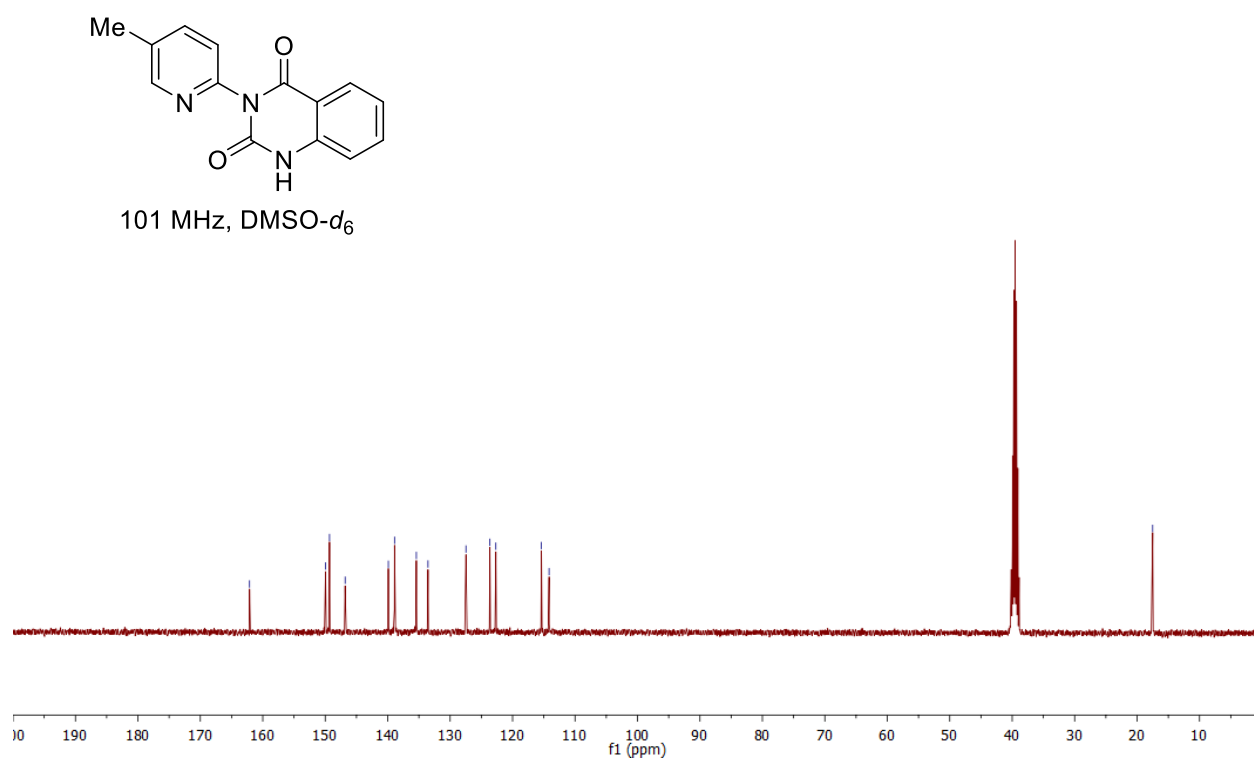
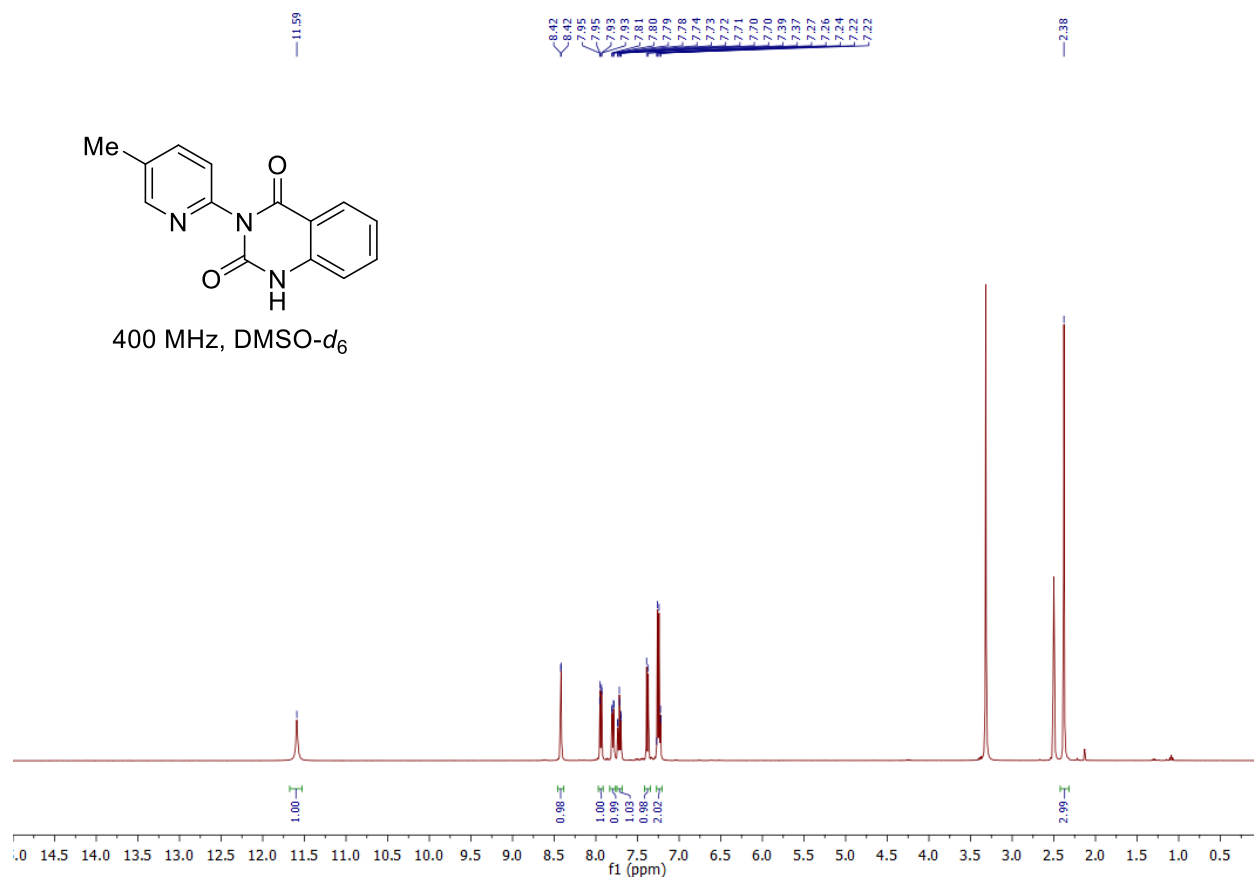


Chemical structure of 2-(pyridin-2-yl)-1,2,3,4-tetrahydroquinolin-4(1H)-one is shown. The spectrum is recorded at 400 MHz in DMSO- d_6 . The x-axis represents the chemical shift in ppm, ranging from 0.0 to 14.5. The spectrum displays several peaks, with the most prominent ones in the aromatic region (7.0-8.7 ppm) and a sharp peak at approximately 3.4 ppm. Integration values are provided below the baseline for several peak groups.

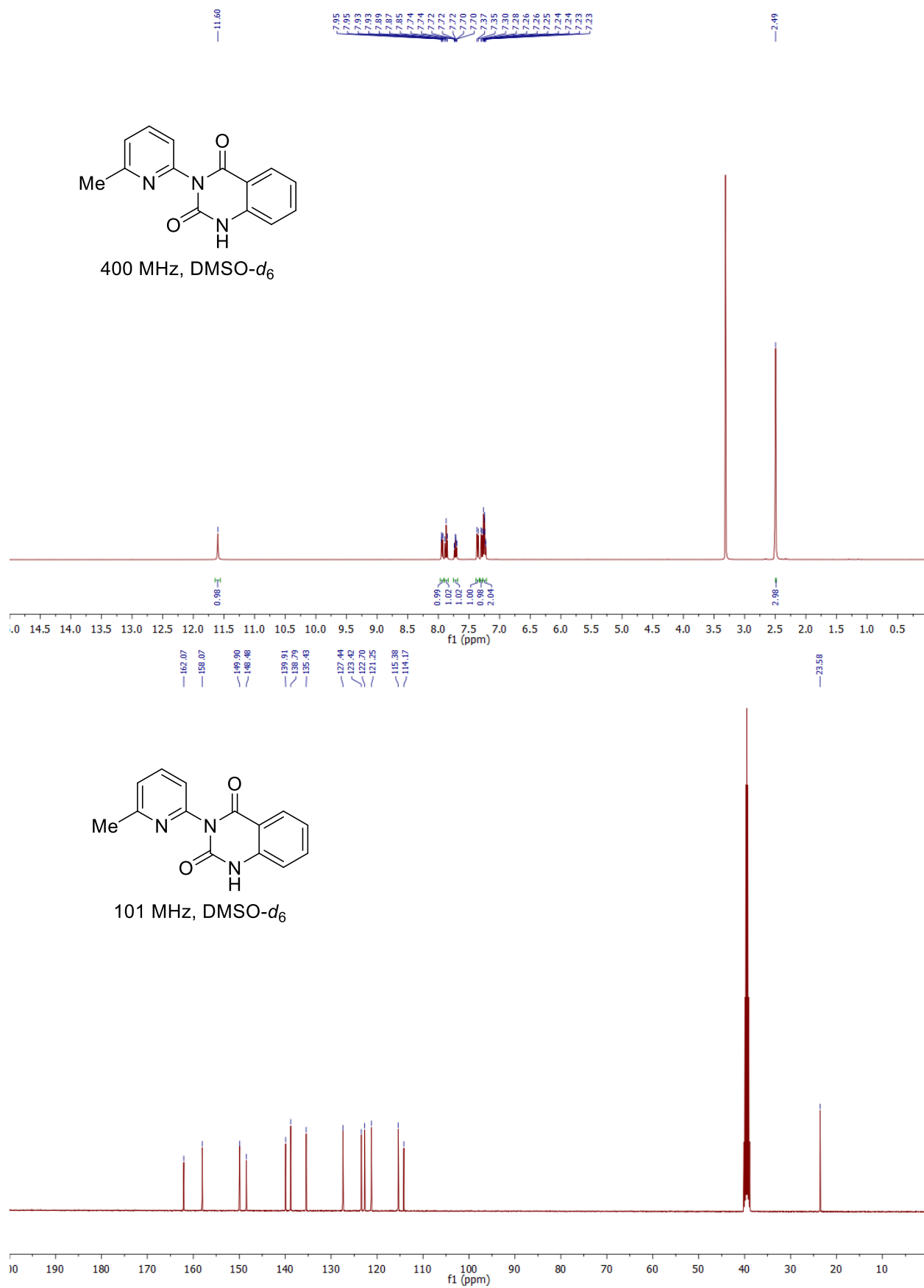
Chemical Shift (ppm)	Integration
~11.53	1.00
~8.61	1.00
~8.02	1.01
~7.98	1.03
~7.94	1.01
~7.75	2.04
~7.23	2.04
~3.4	-



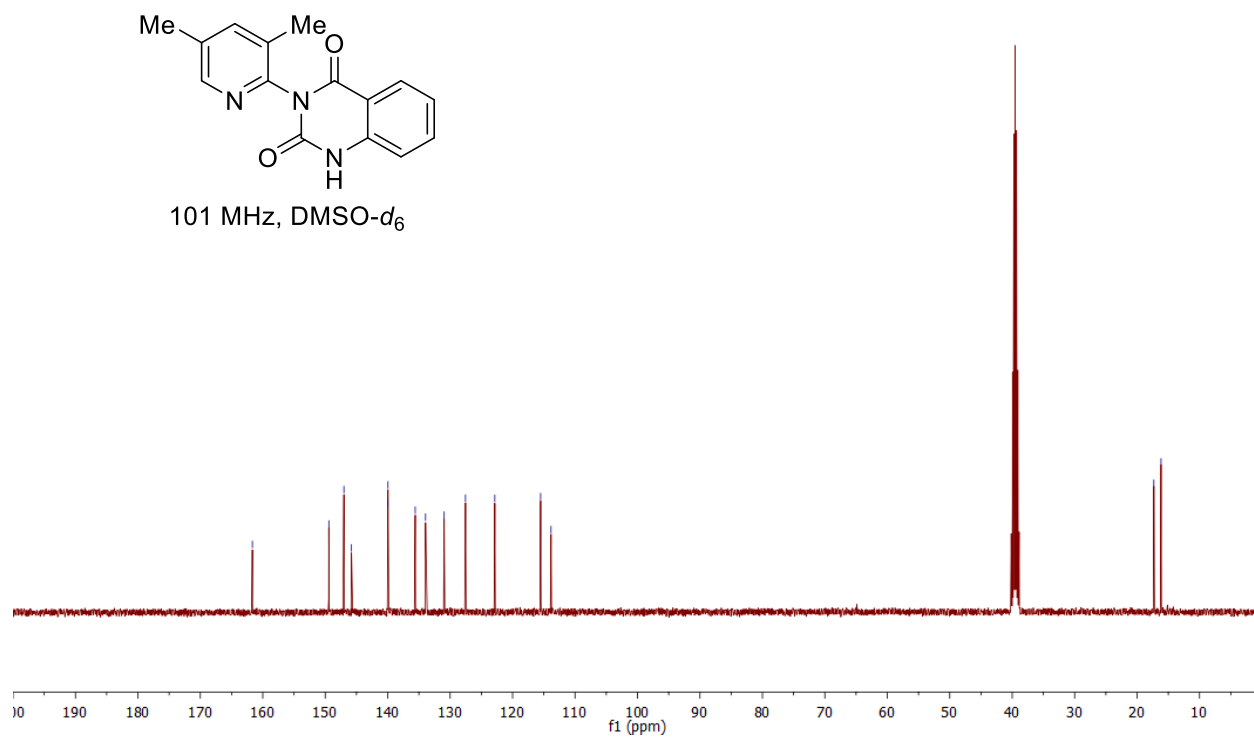
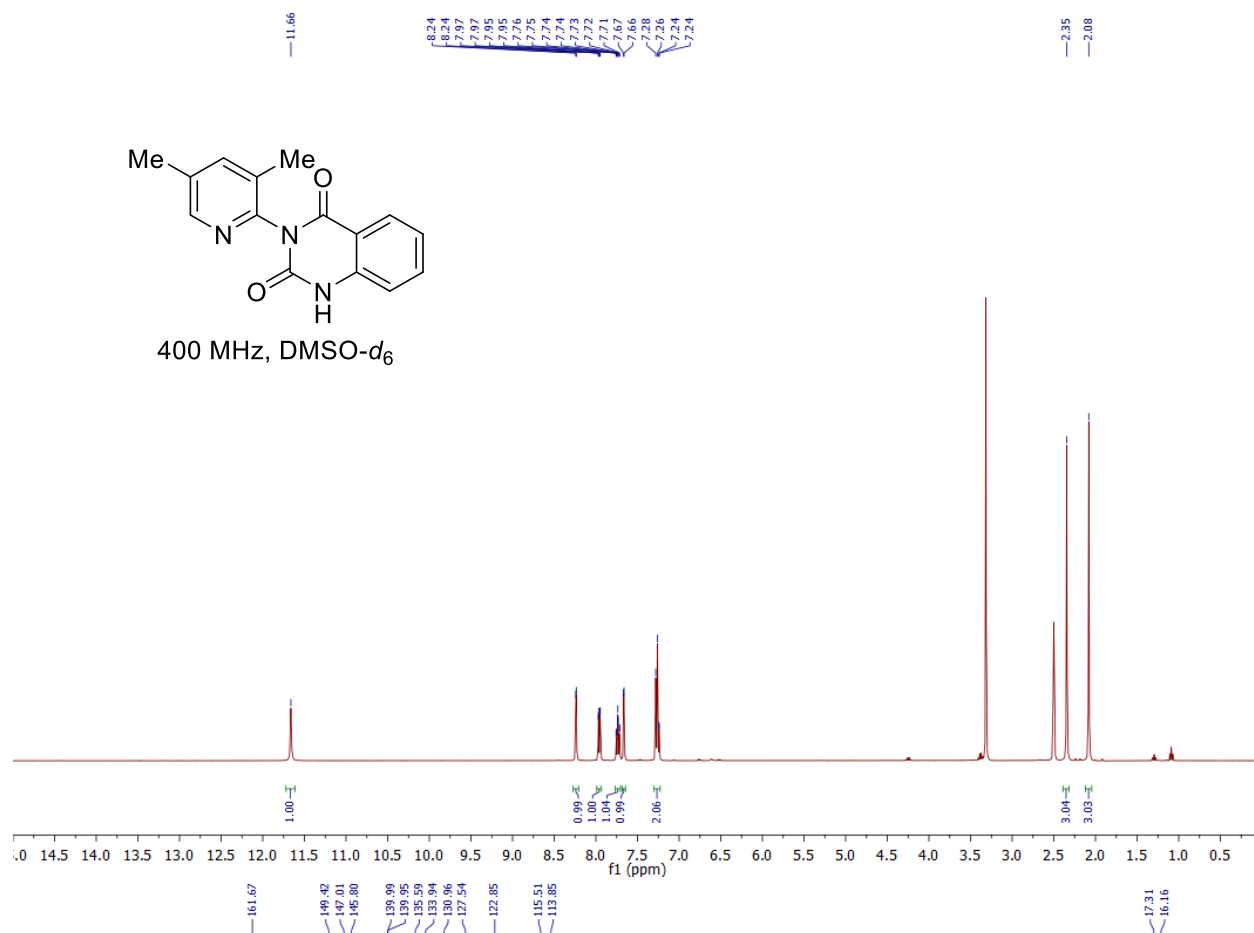
^1H and ^{13}C spectra of 3-(5-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3c**



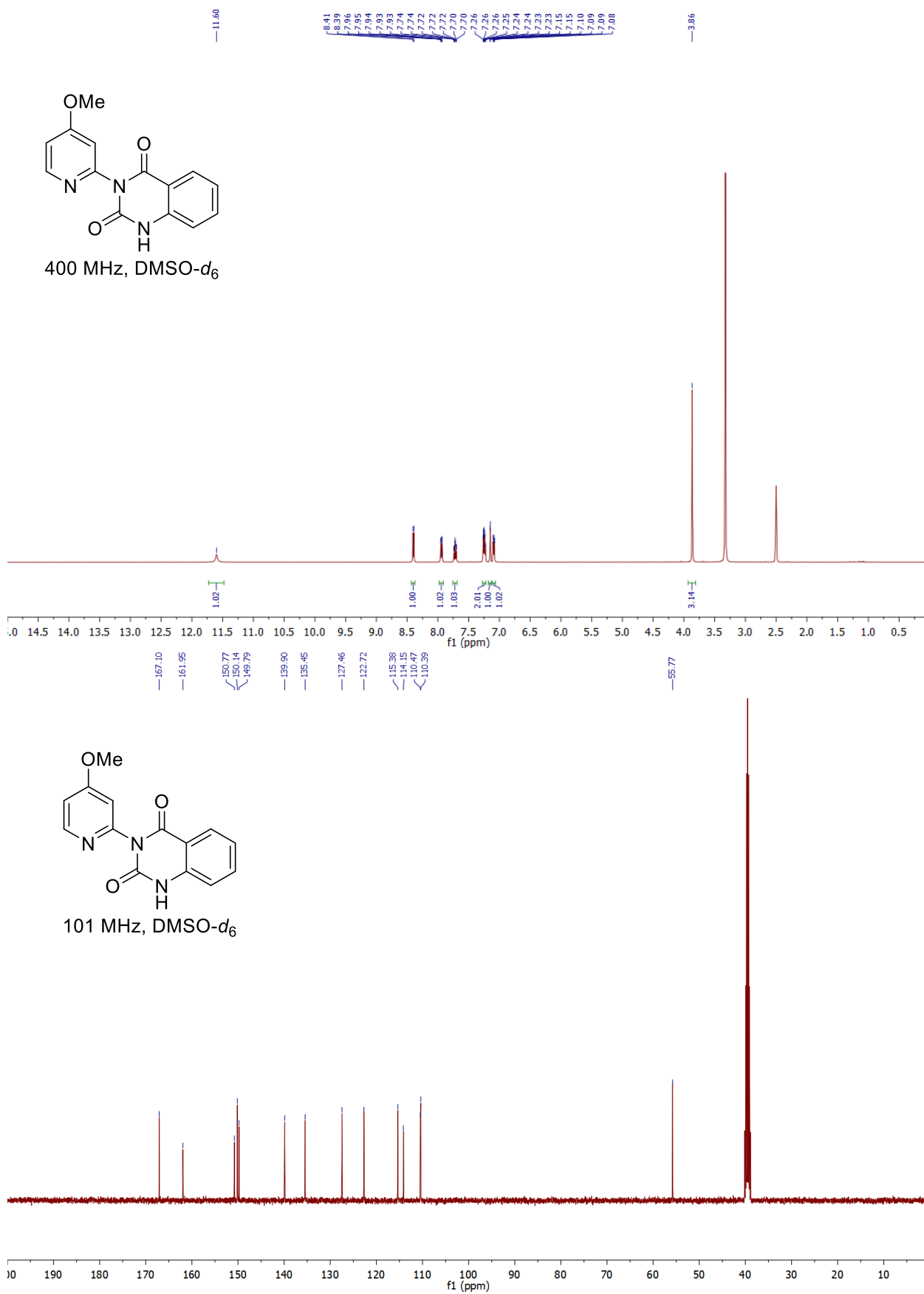
^1H and ^{13}C spectra of 3-(6-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3d**



^1H and ^{13}C spectra of 3-(3,5-dimethylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3e**



^1H and ^{13}C spectra of 3-(4-methoxypyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3f**

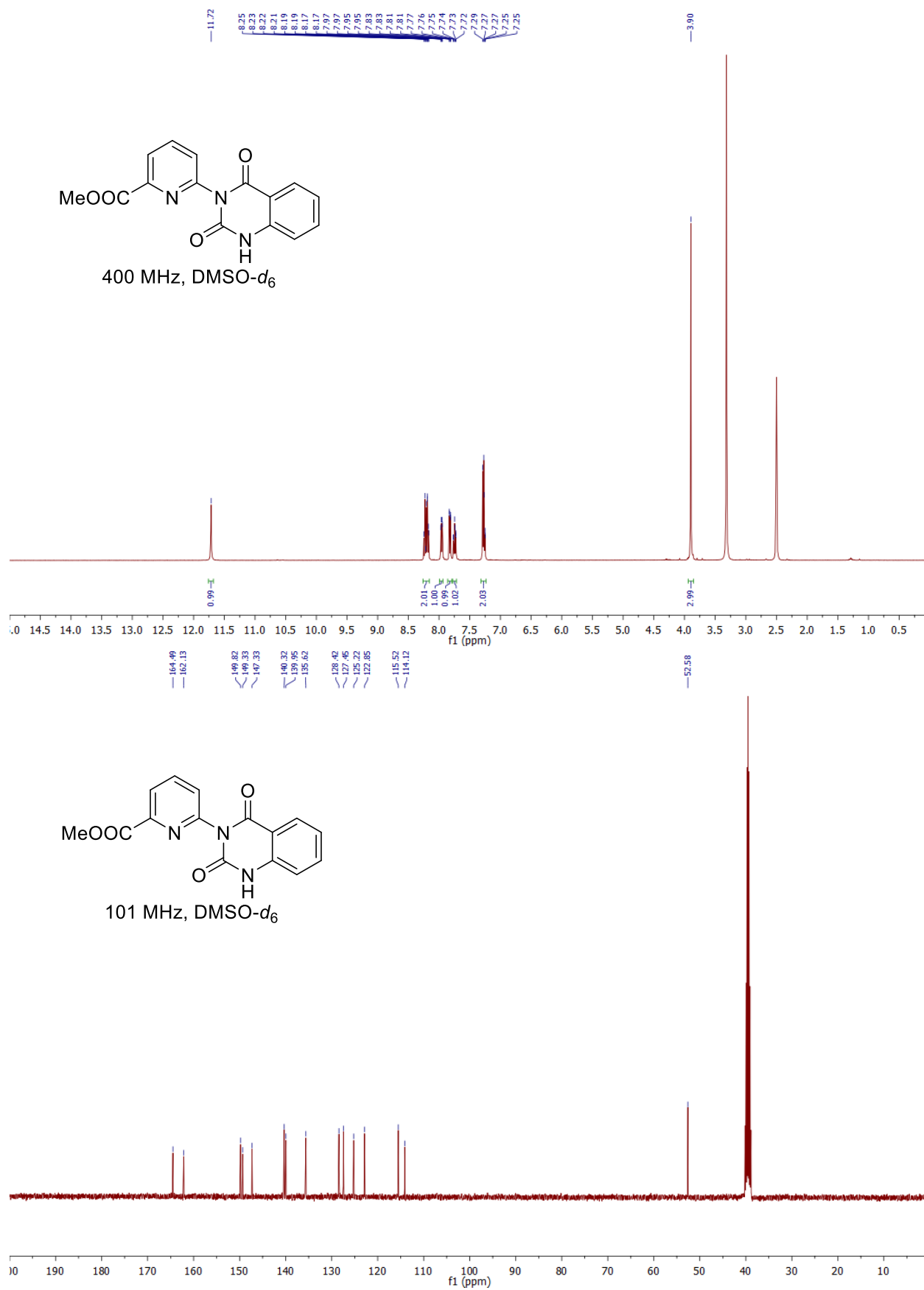


c1ccc(cc1)c2ccc(cc2)n3c(=O)[nH]c(=O)n3c4ccccc4

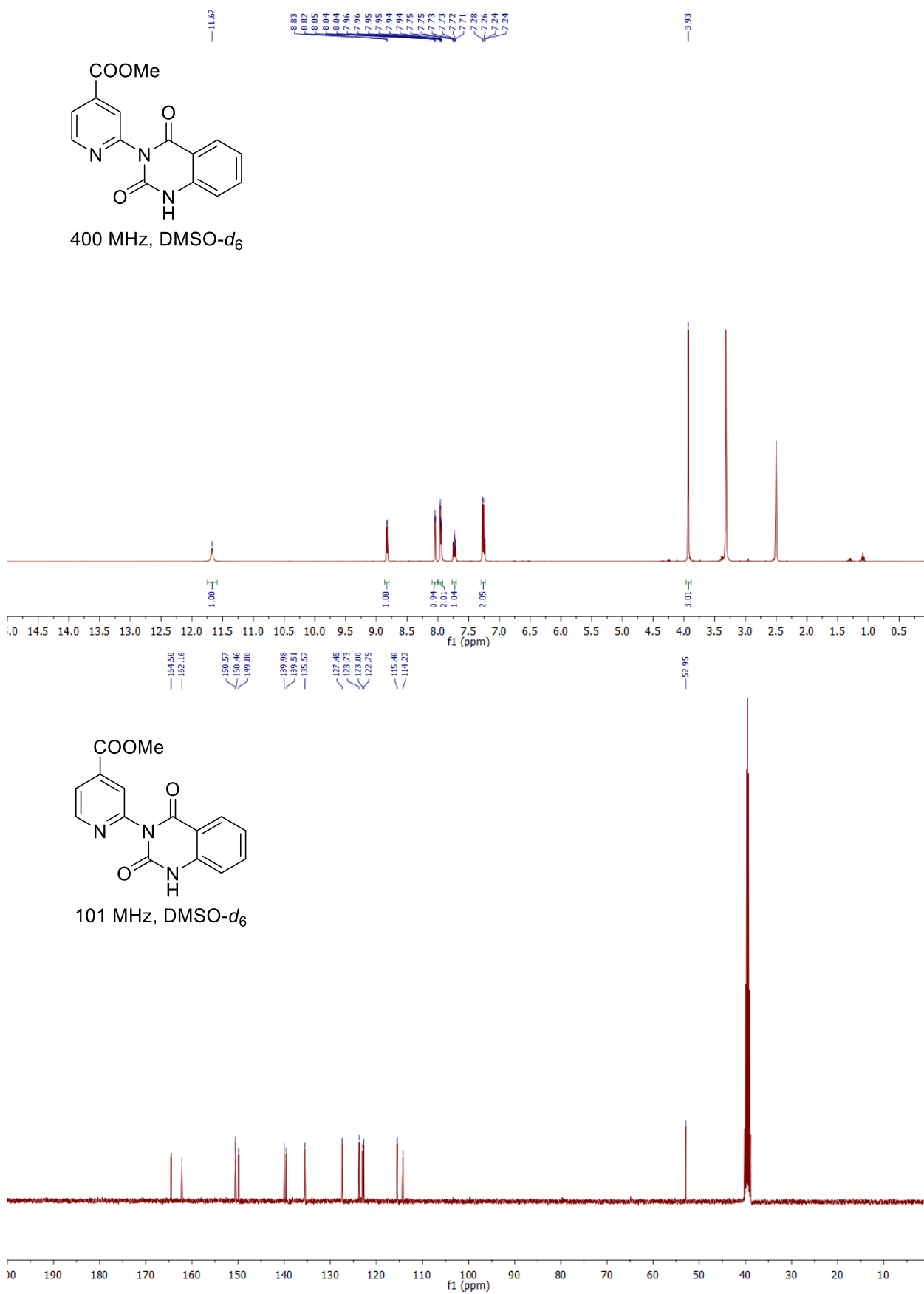
400 MHz, DMSO- d_6

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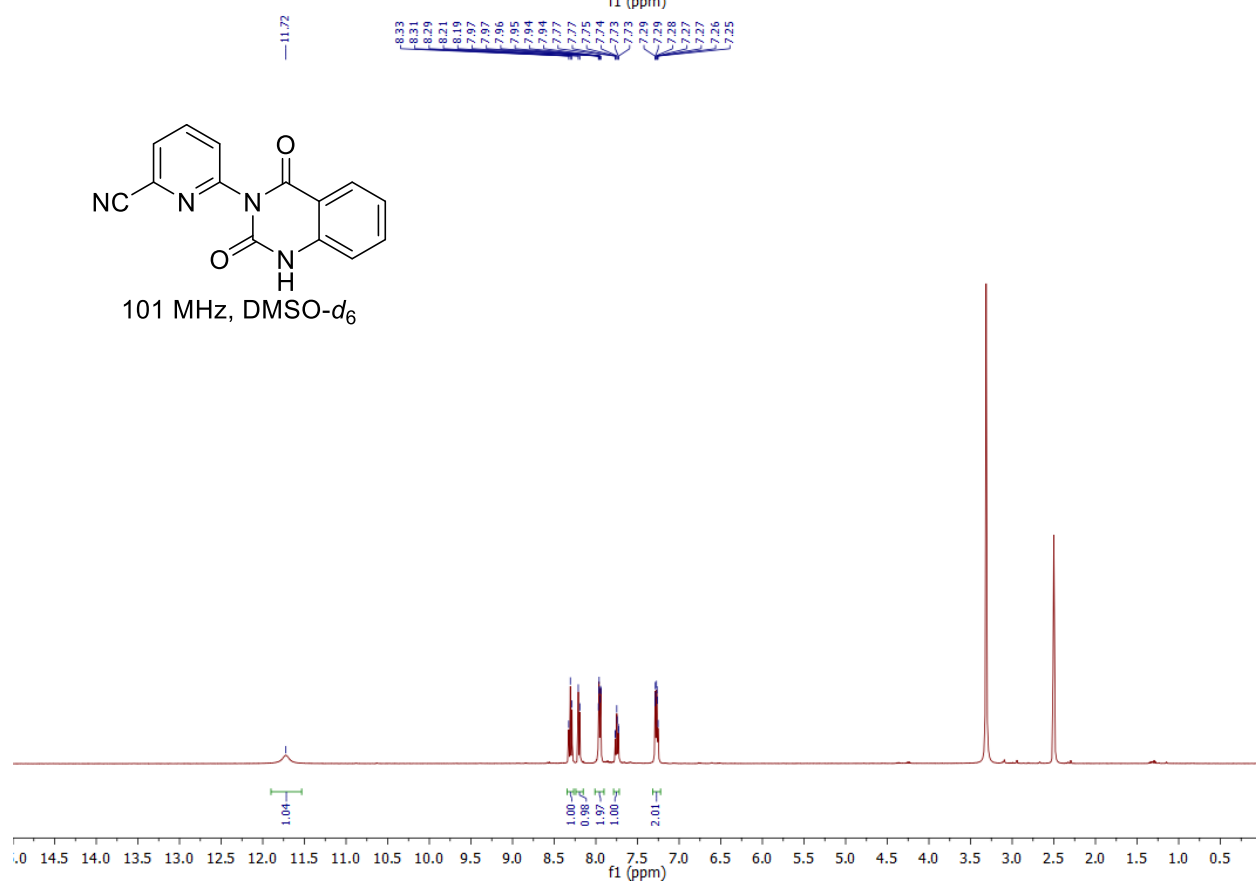
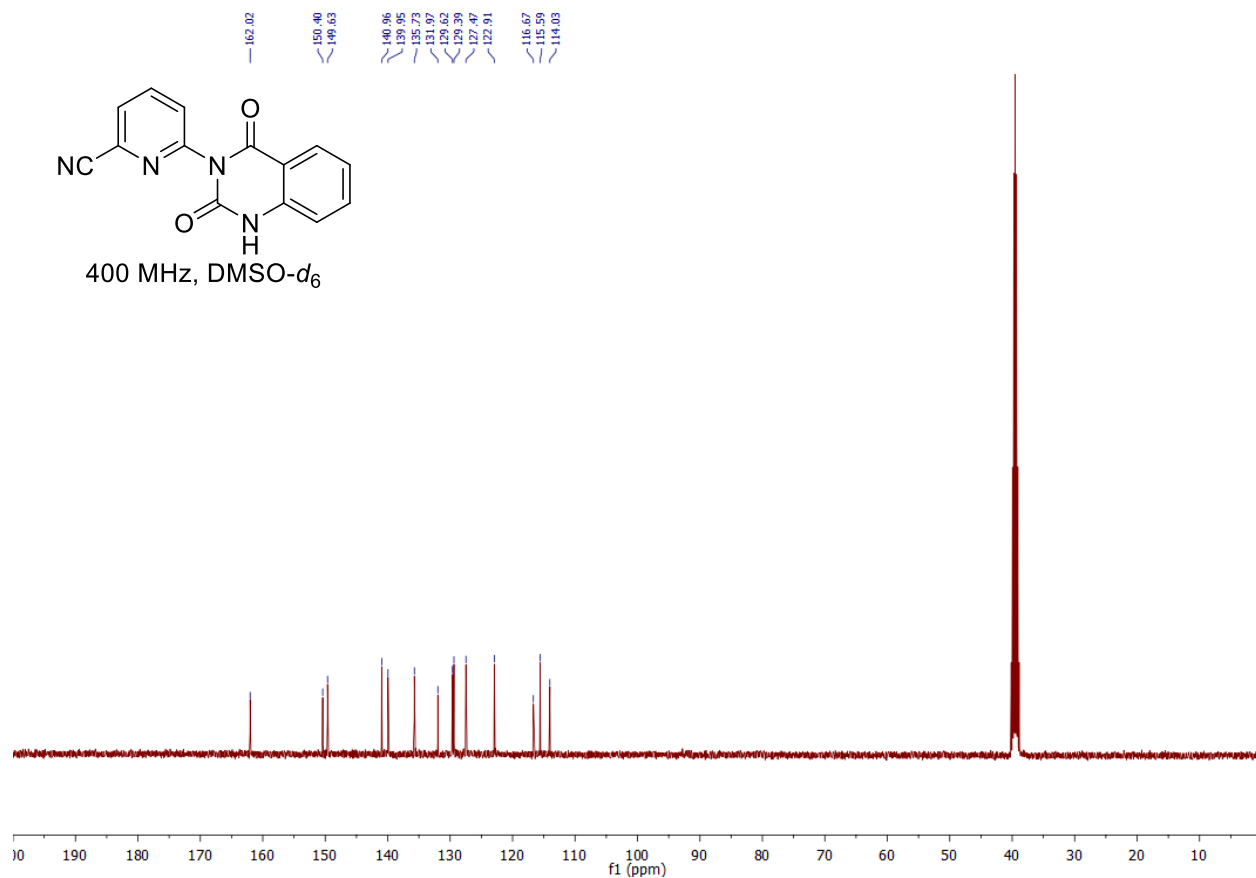
^1H and ^{13}C spectra of methyl 6-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)picolinate **3h**



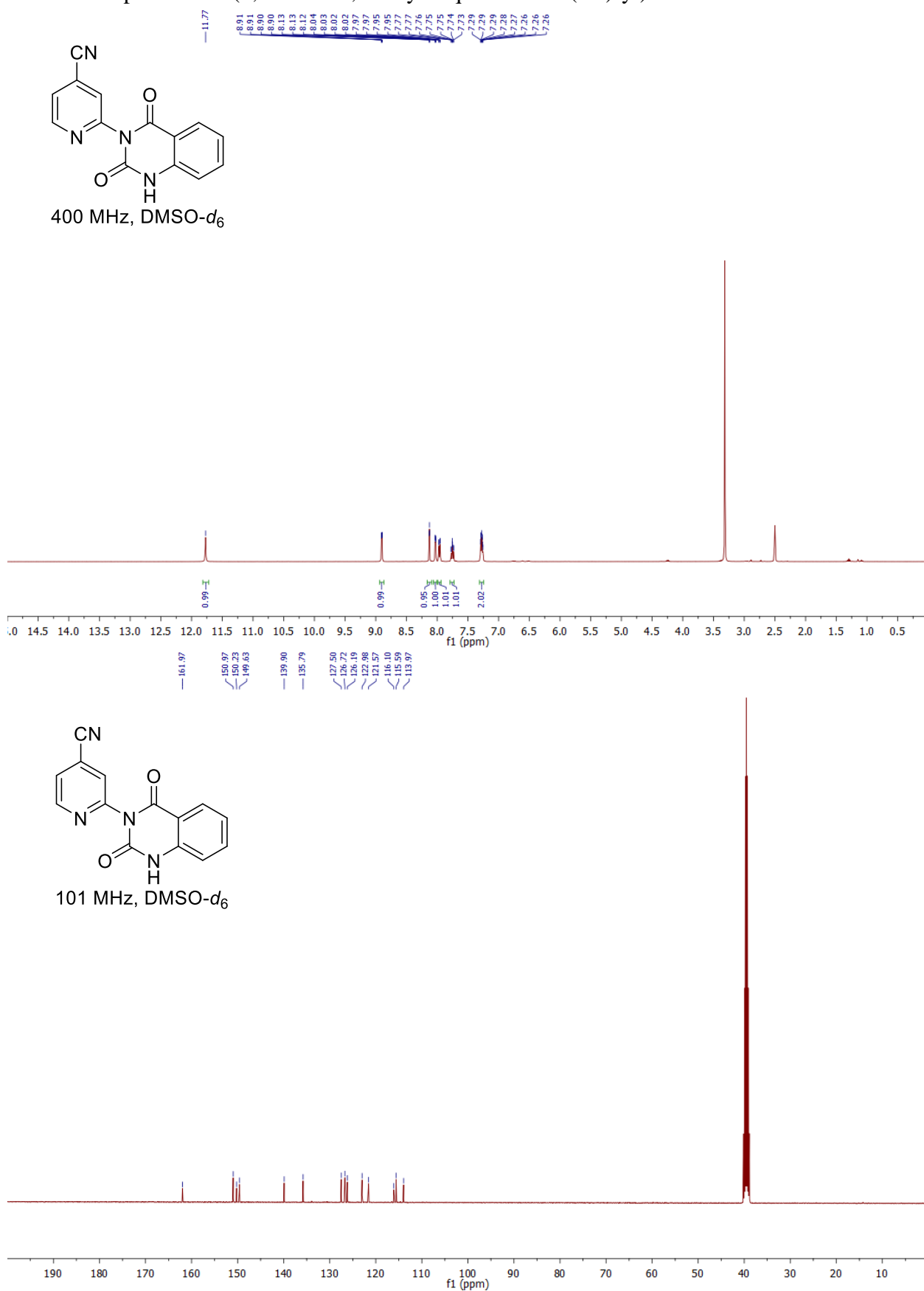
^1H and ^{13}C spectra of methyl 2-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)isonicotinate **3i**



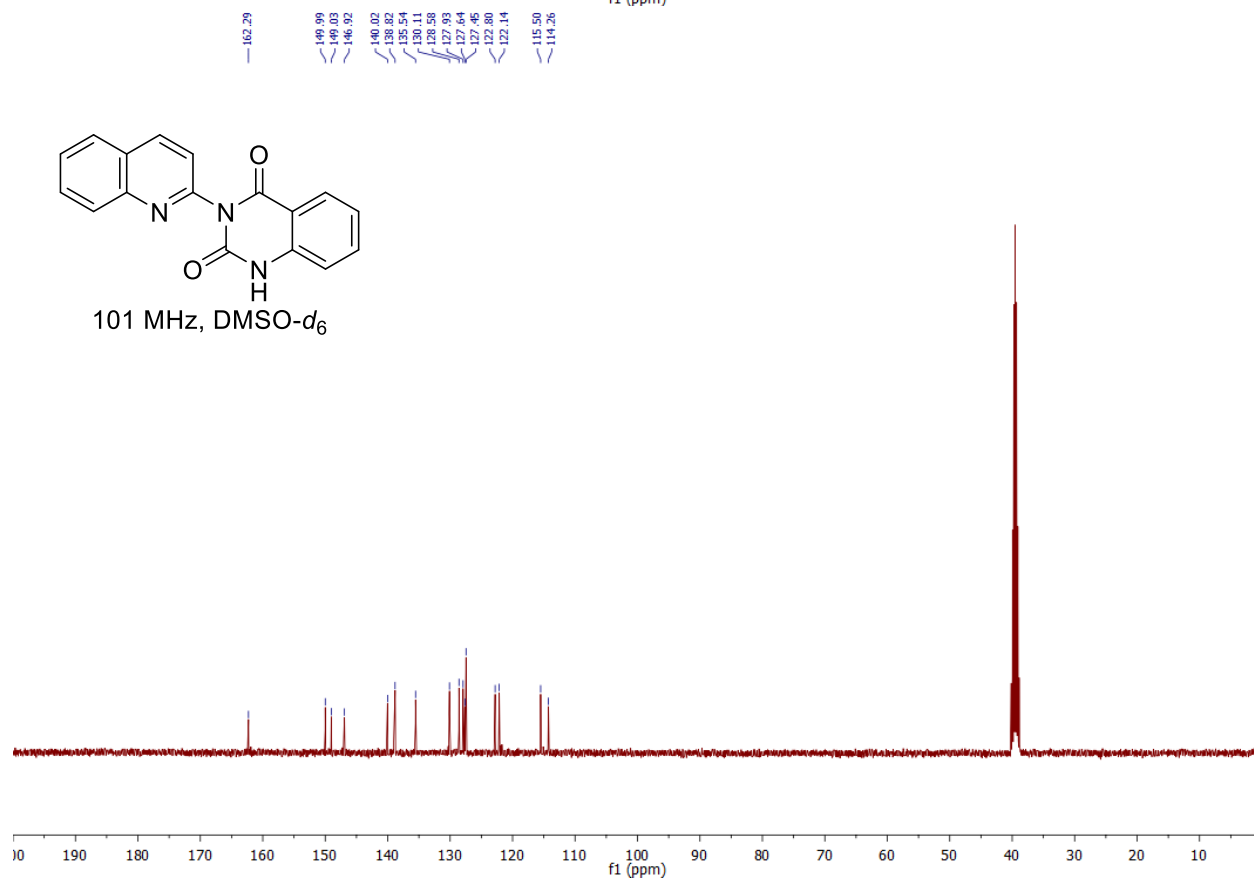
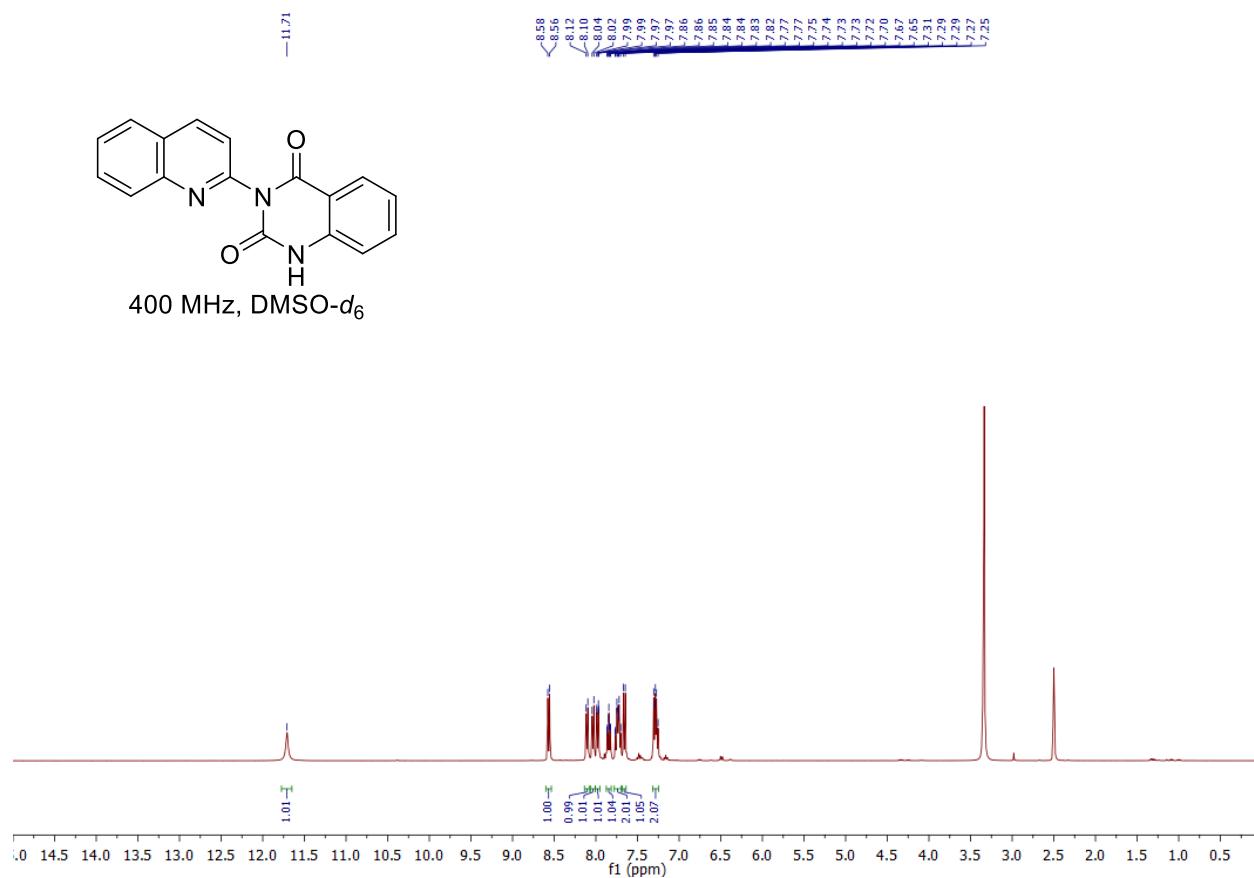
^1H and ^{13}C spectra of 6-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)picolinonitrile **3j**



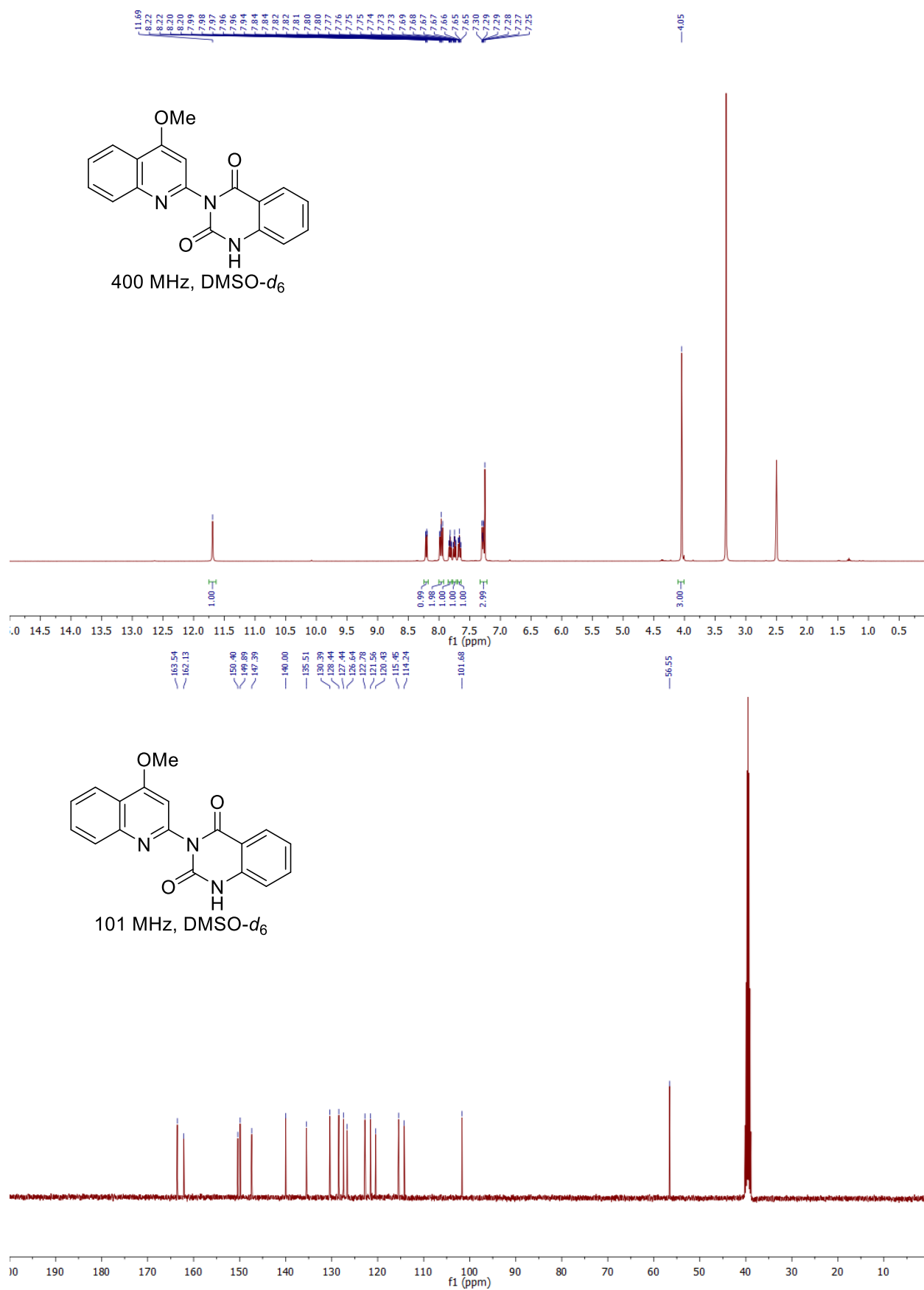
^1H and ^{13}C spectra of 2-(2,4-dioxo-1,4-dihydroquinazolin-3(2*H*)-yl)isonicotinonitrile **3k**



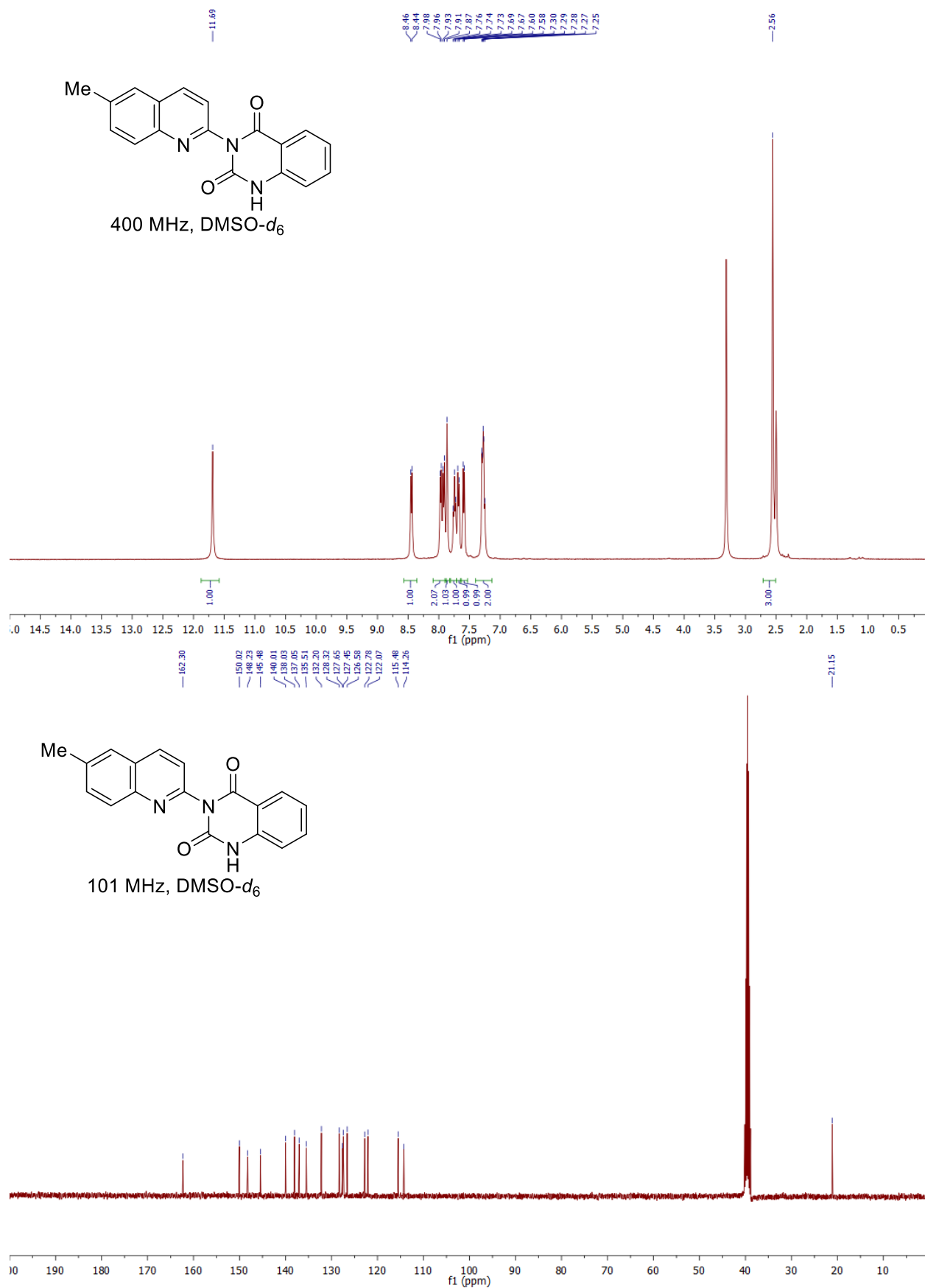
^1H and ^{13}C spectra of 3-(quinolin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3l**



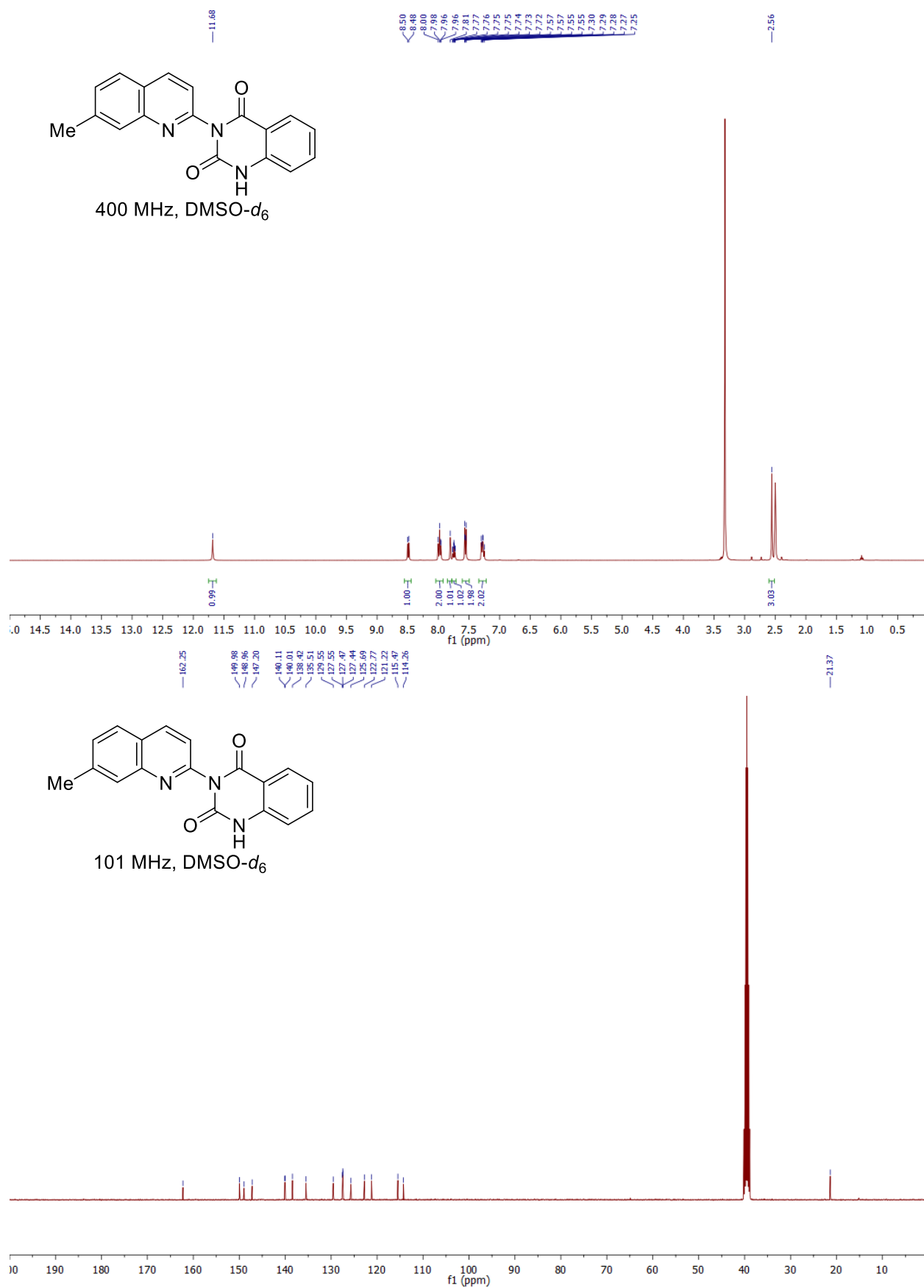
^1H and ^{13}C spectra of 3-(4-methoxyquinolin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3m**



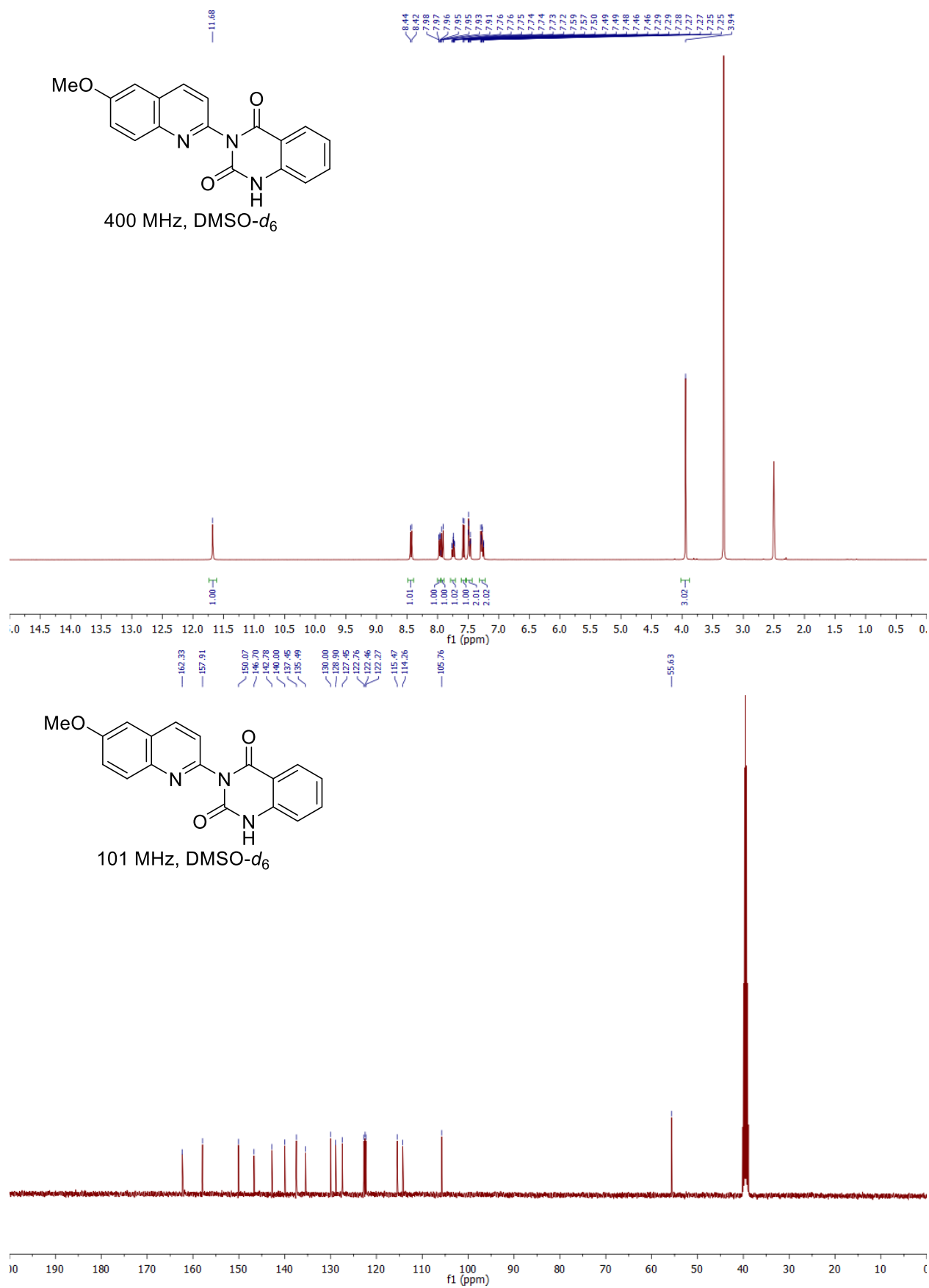
^1H and ^{13}C spectra of 3-(6-methylquinolin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3n**



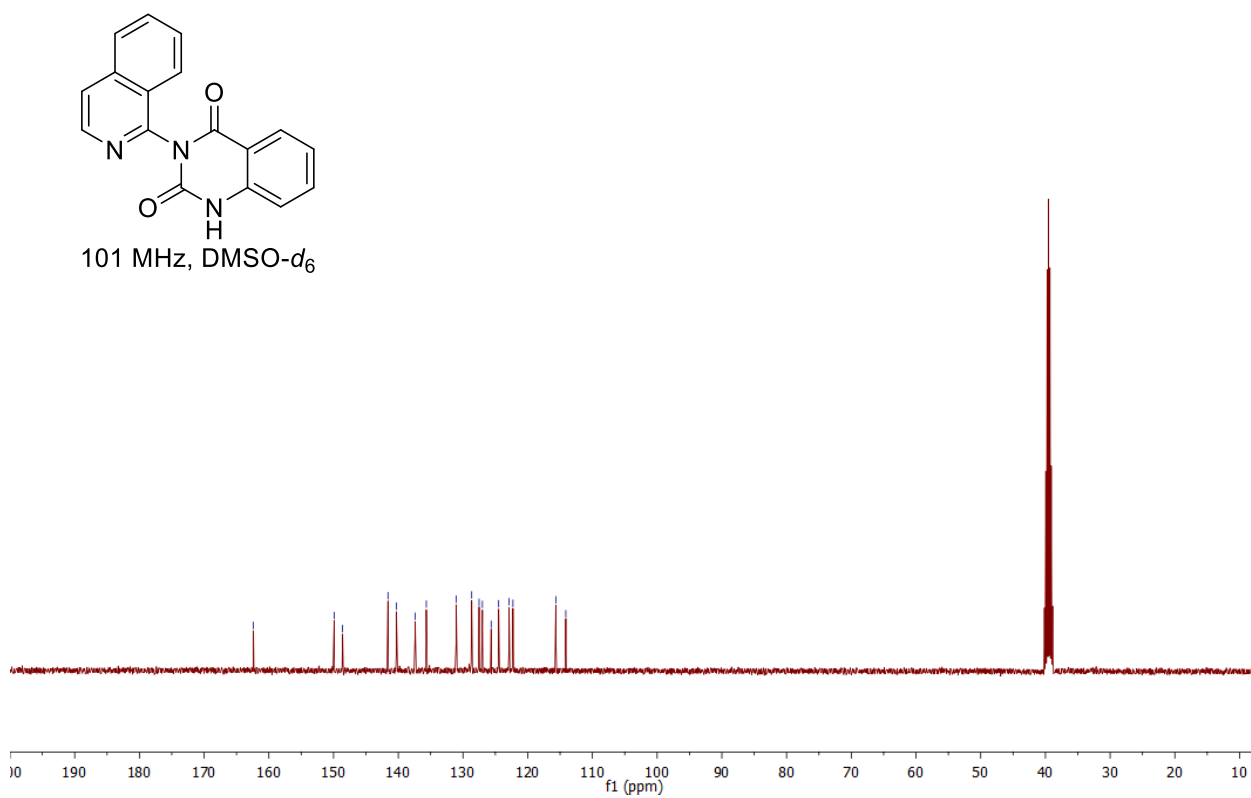
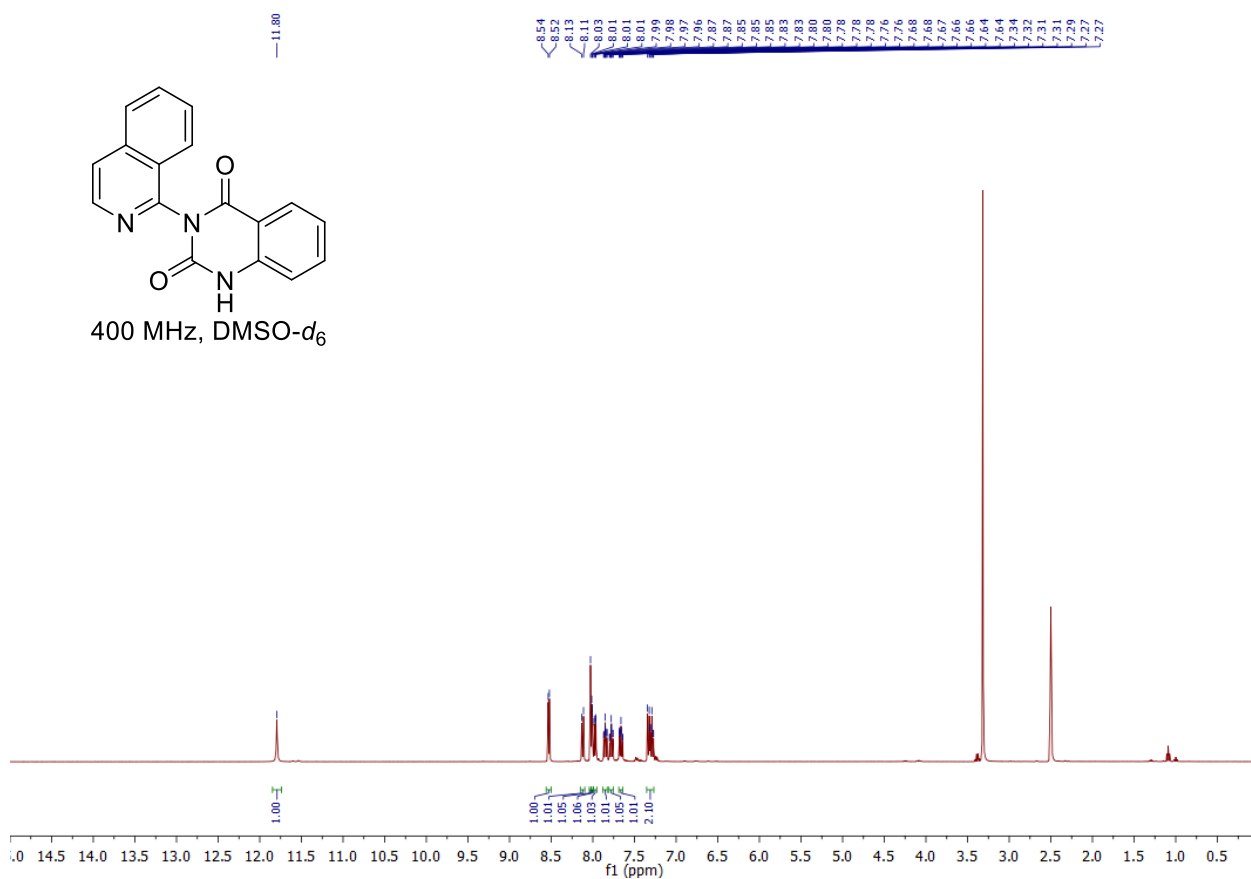
^1H and ^{13}C spectra of 3-(7-methylquinolin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3o**



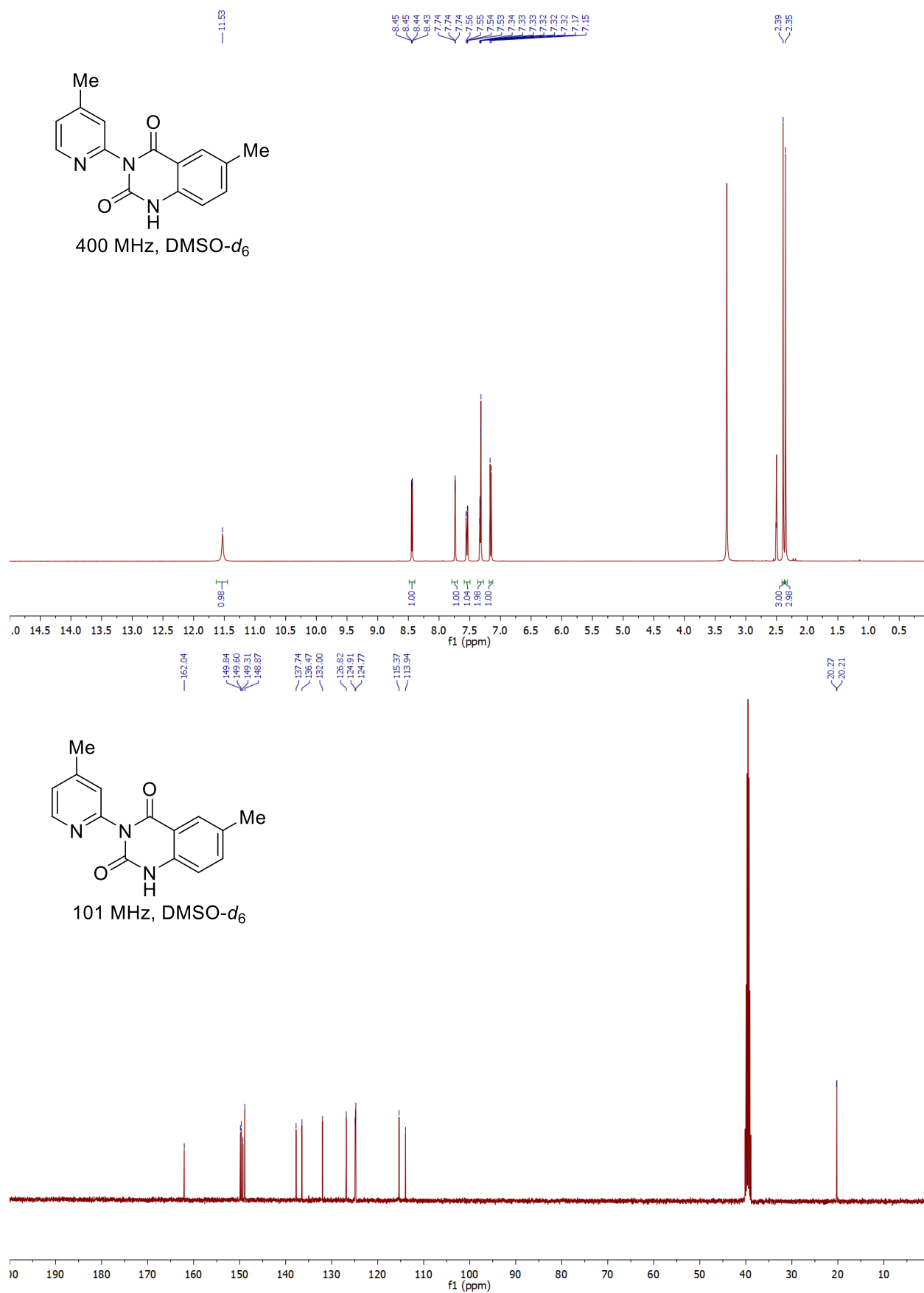
^1H and ^{13}C spectra of 3-(6-methoxyquinolin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3p**



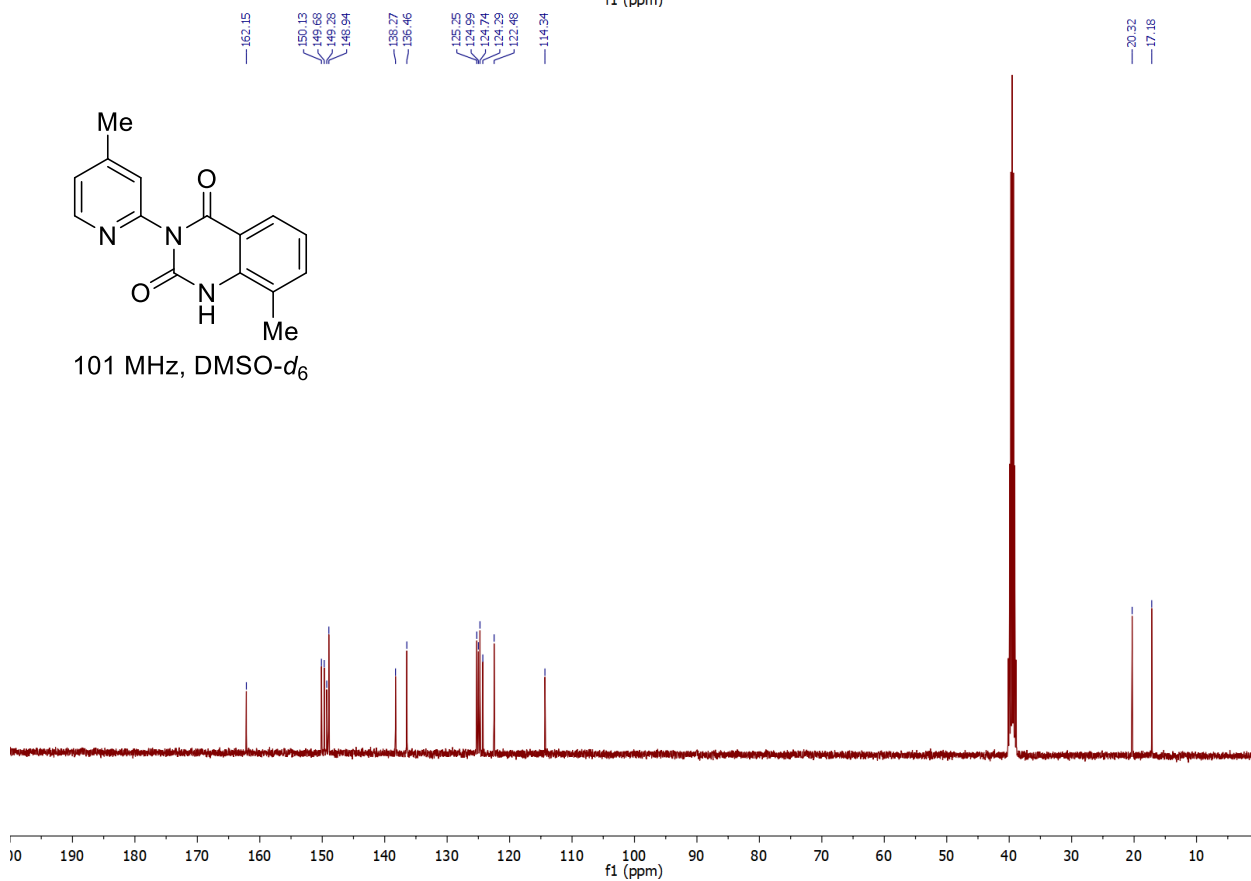
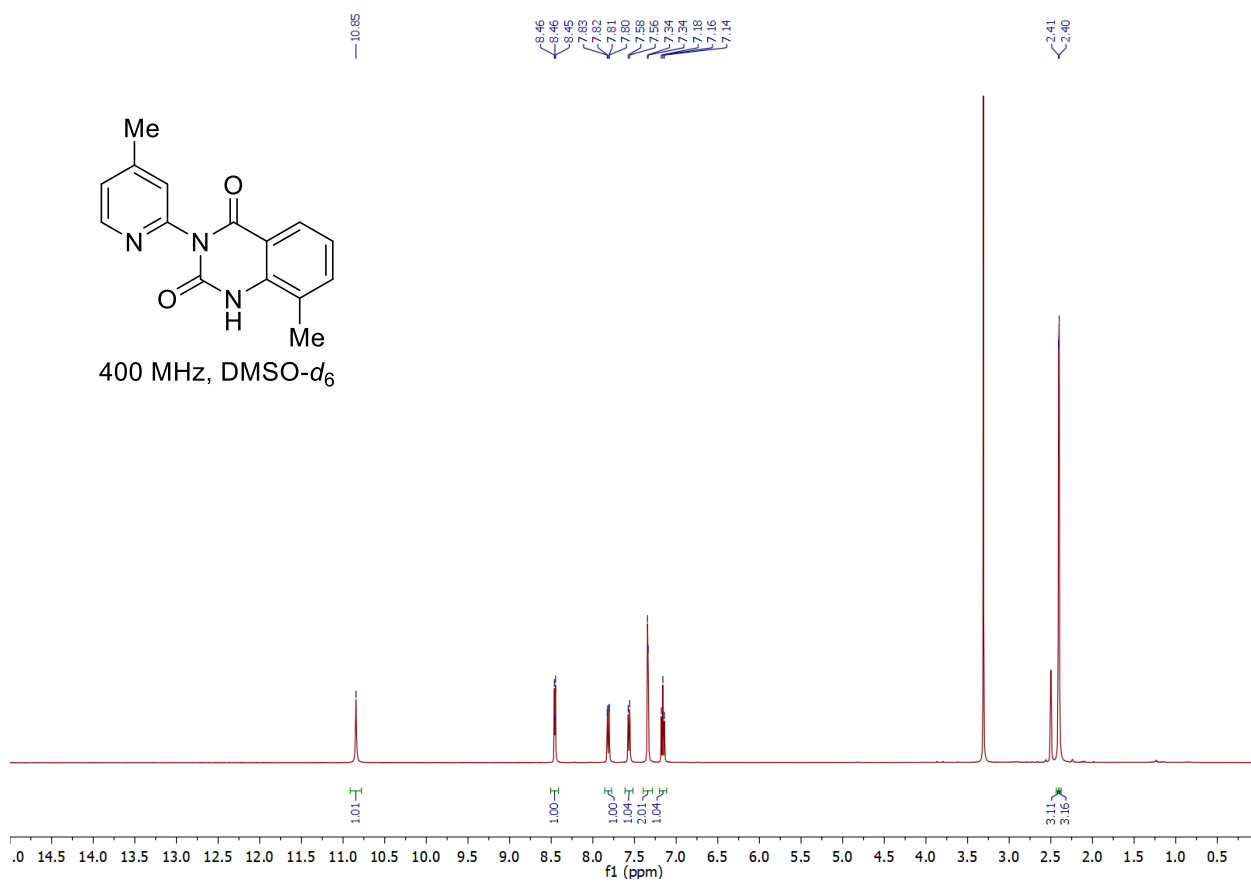
^1H and ^{13}C spectra of 3-(isoquinolin-1-yl)quinazoline-2,4(1*H*,3*H*)-dione **3q**



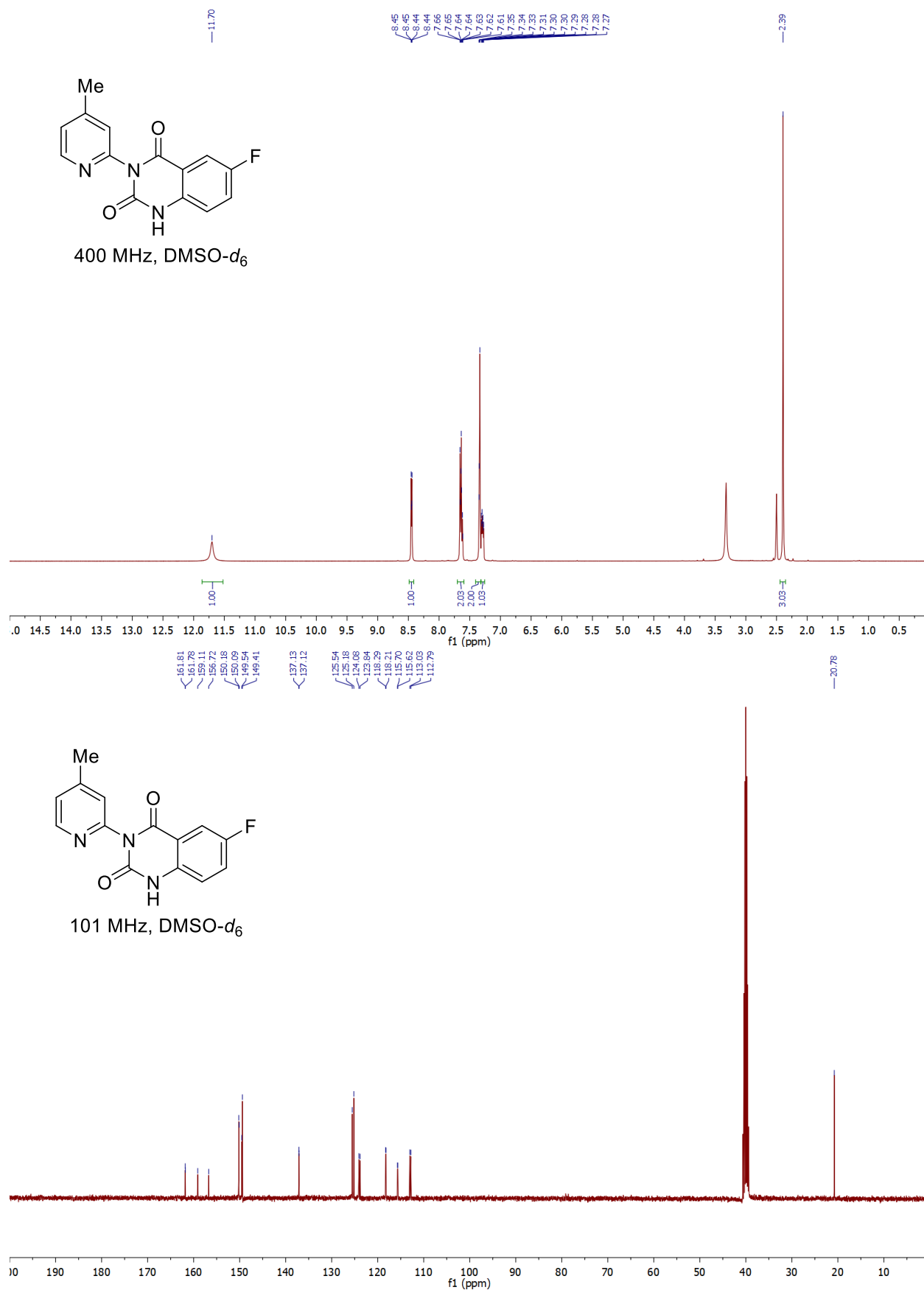
^1H and ^{13}C spectra of 6-methyl-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3r**

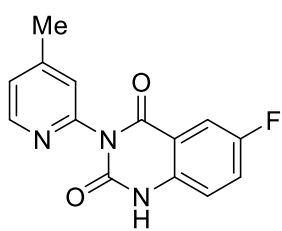


^1H and ^{13}C spectra of 8-methyl-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3s**

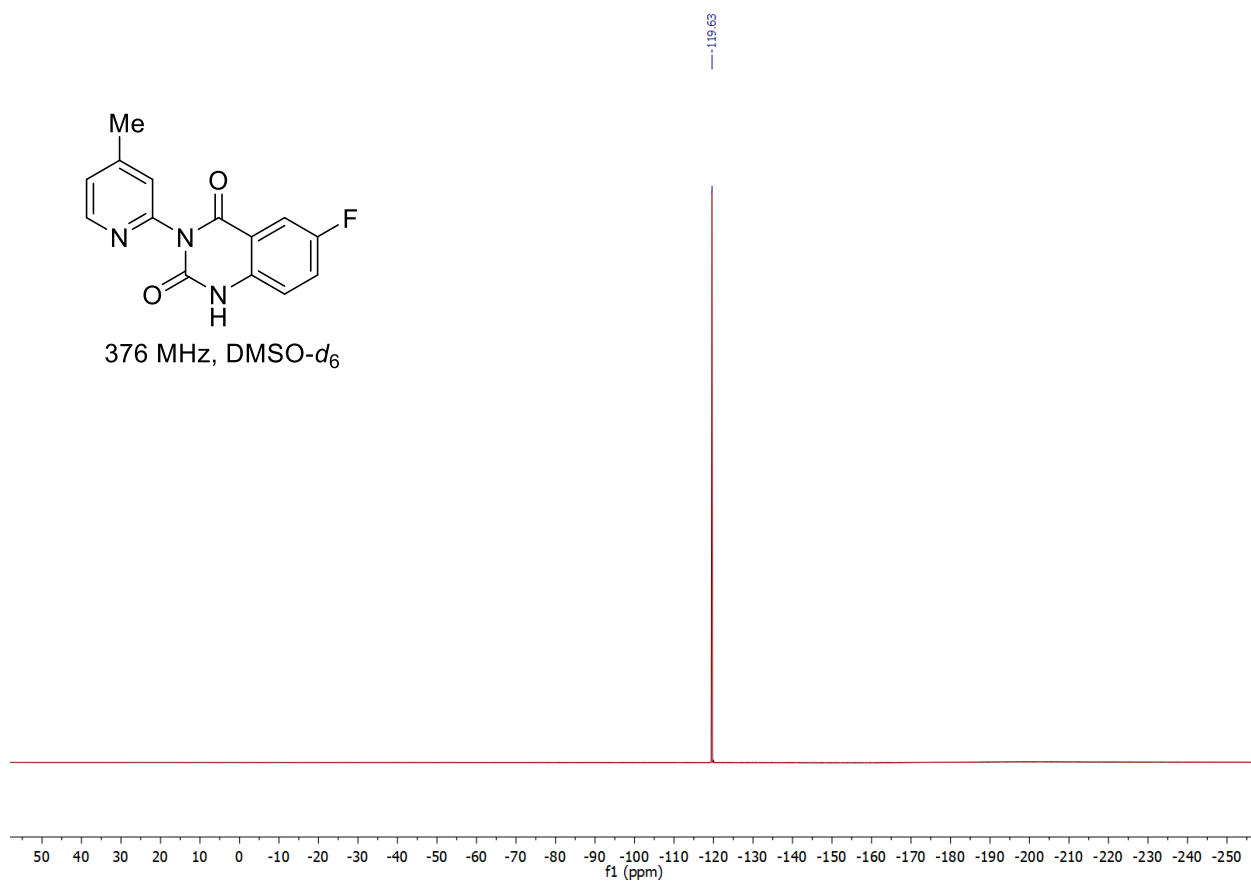


^1H , ^{13}C , and ^{19}F spectra of 6-fluoro-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3t**

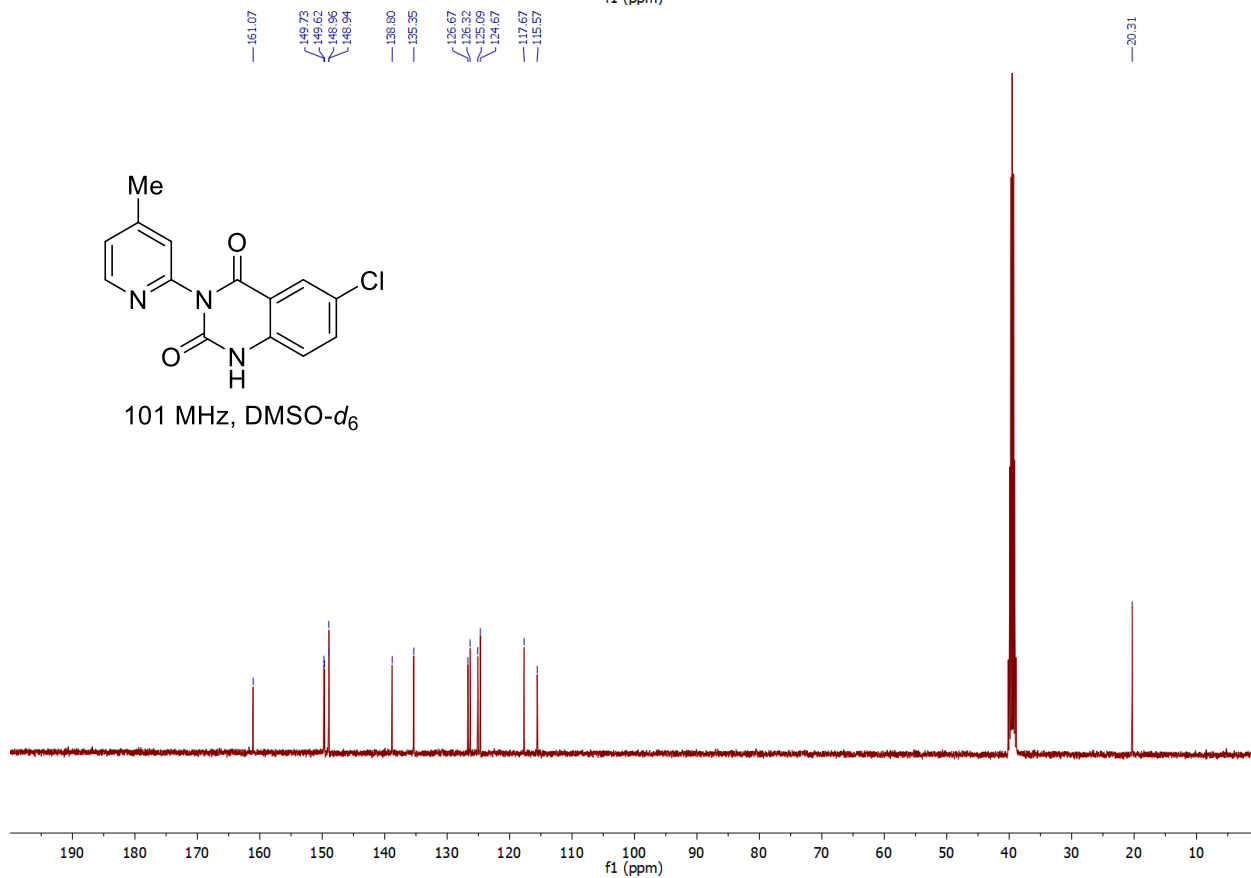
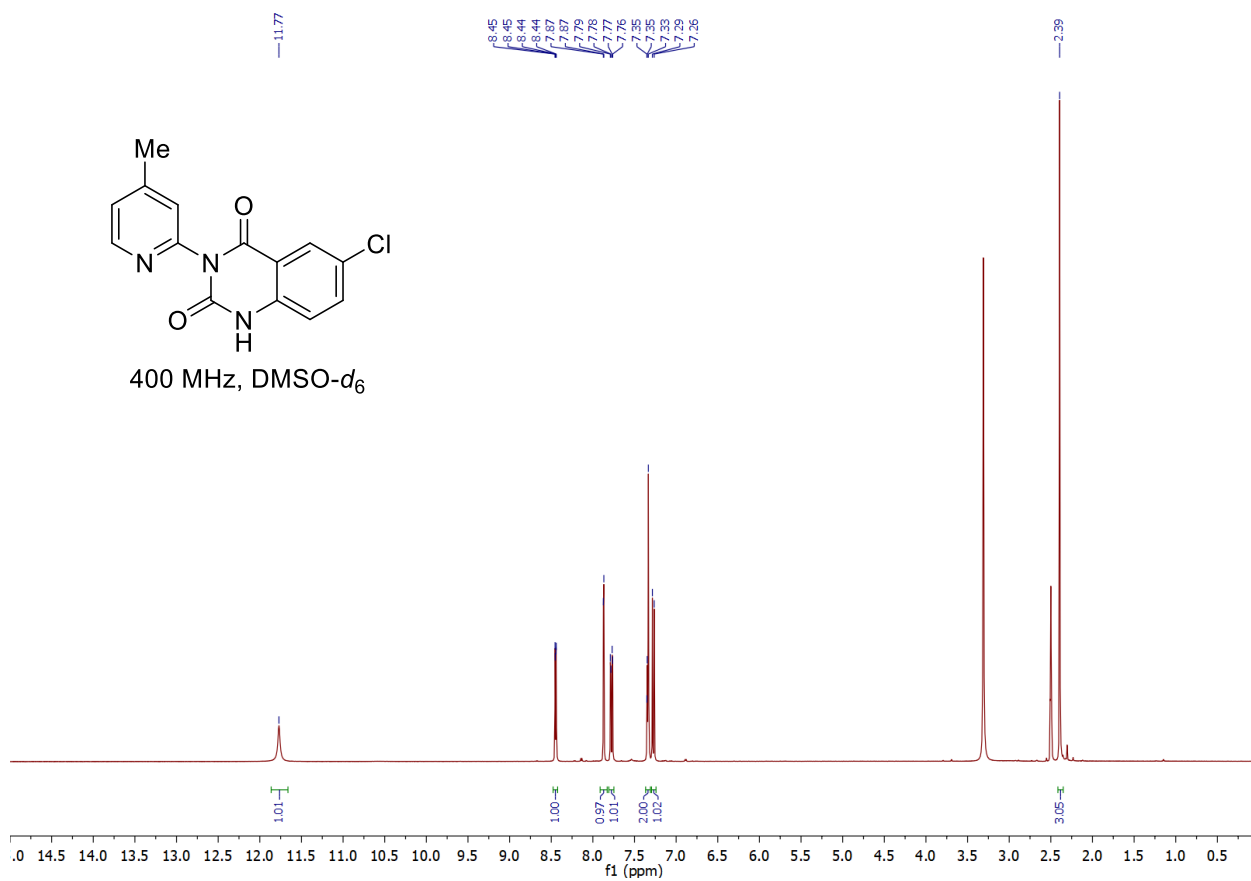




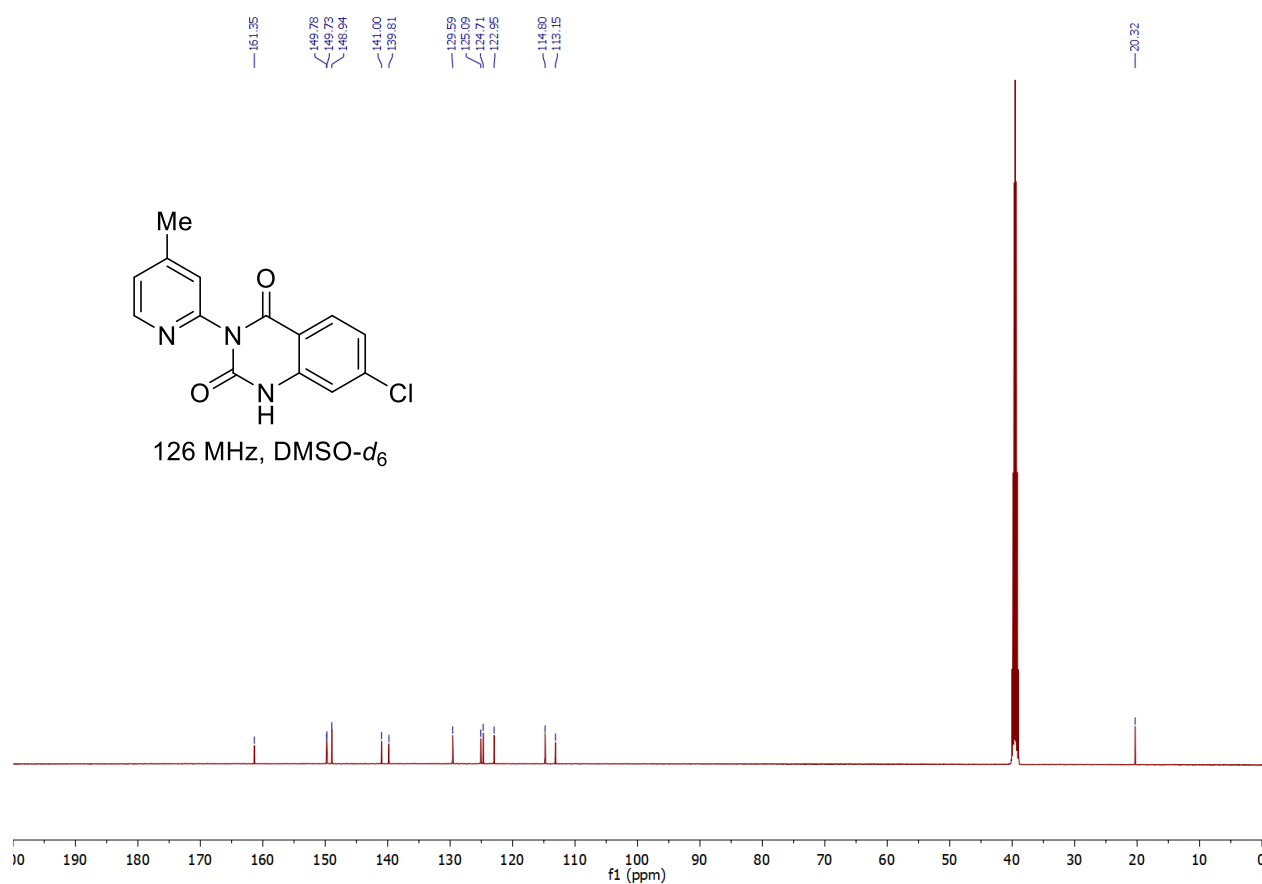
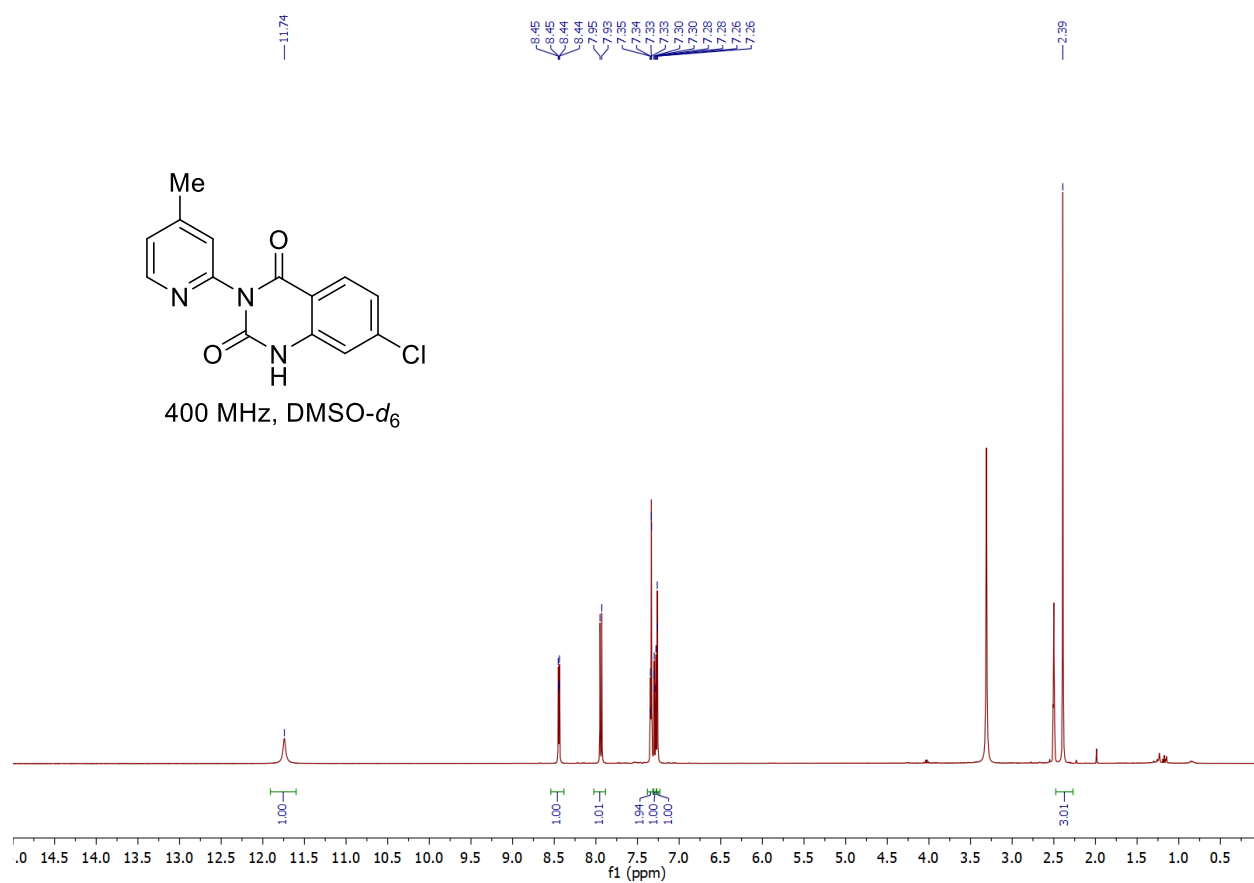
376 MHz, DMSO- d_6



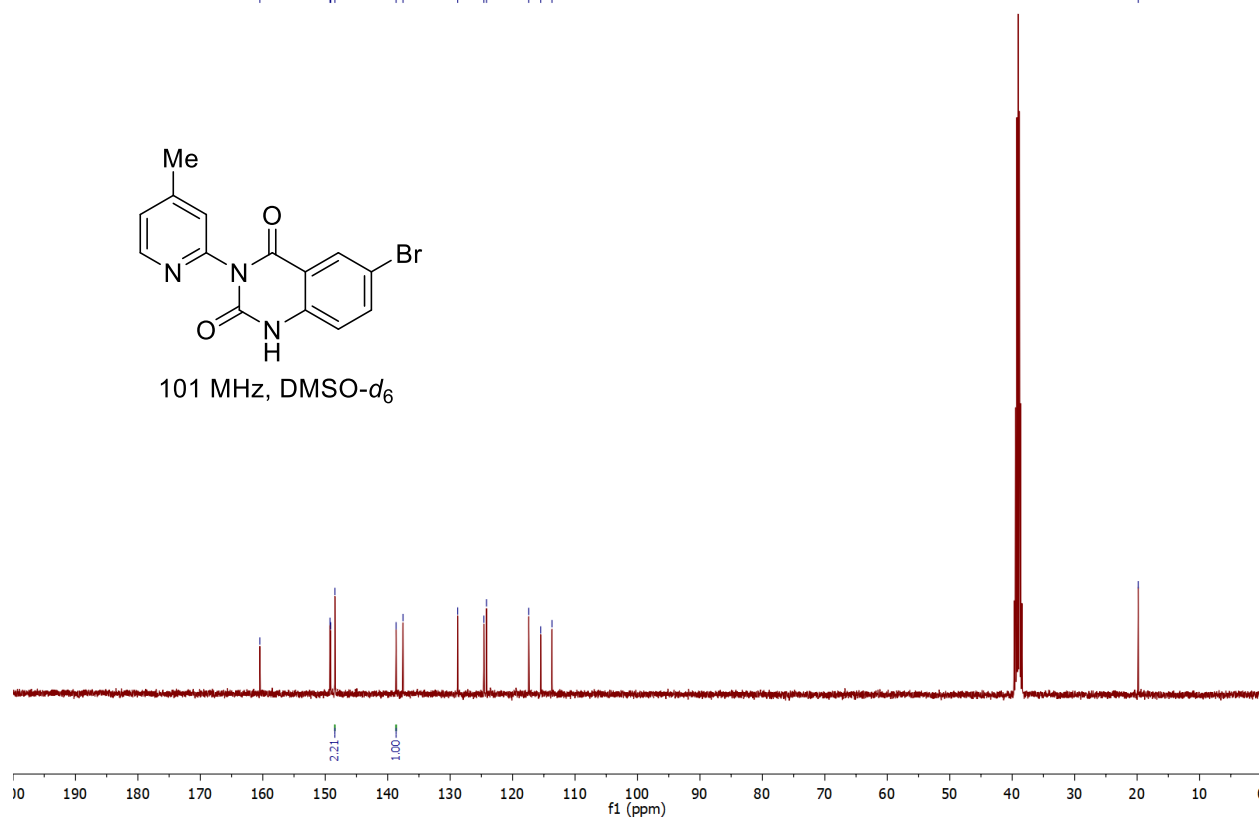
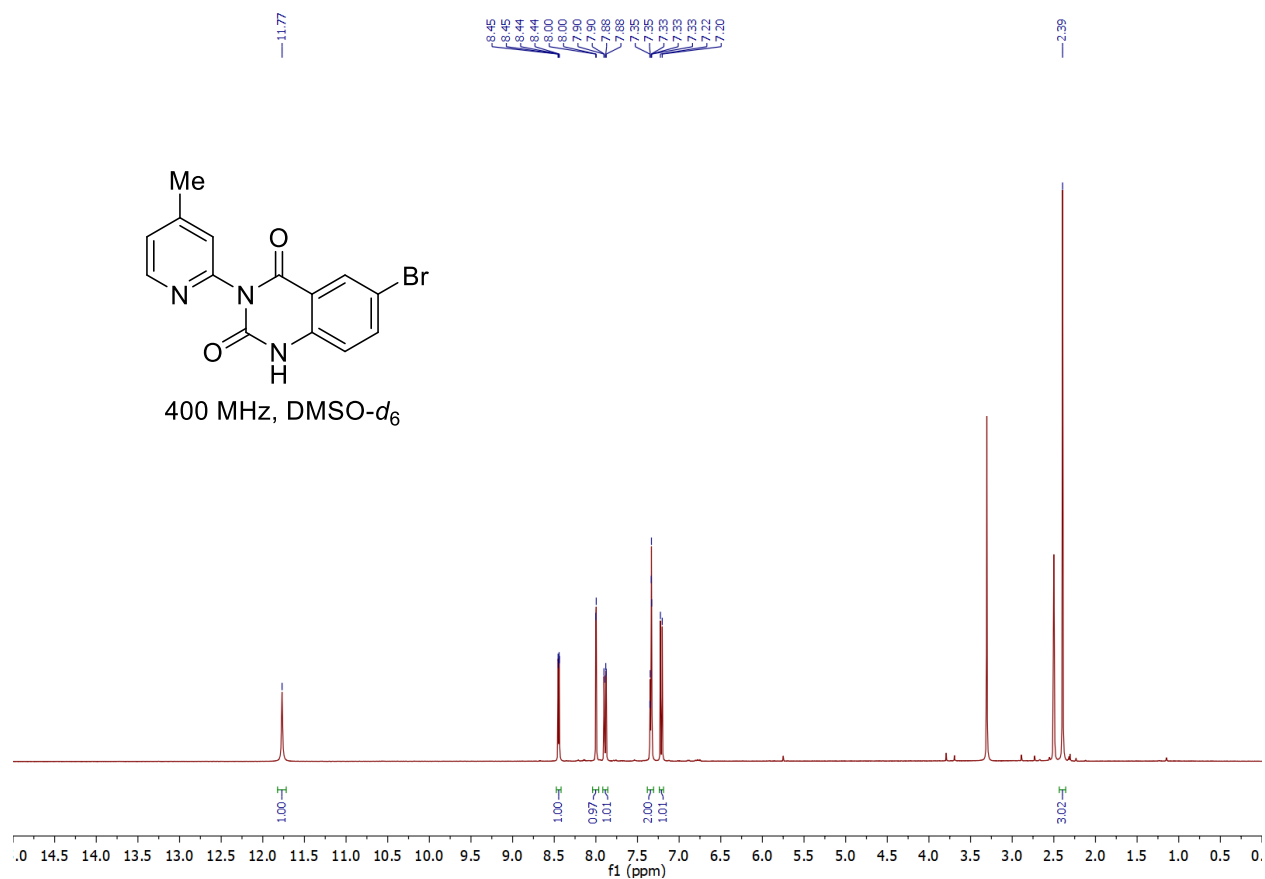
^1H and ^{13}C spectra of 6-chloro-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3u**



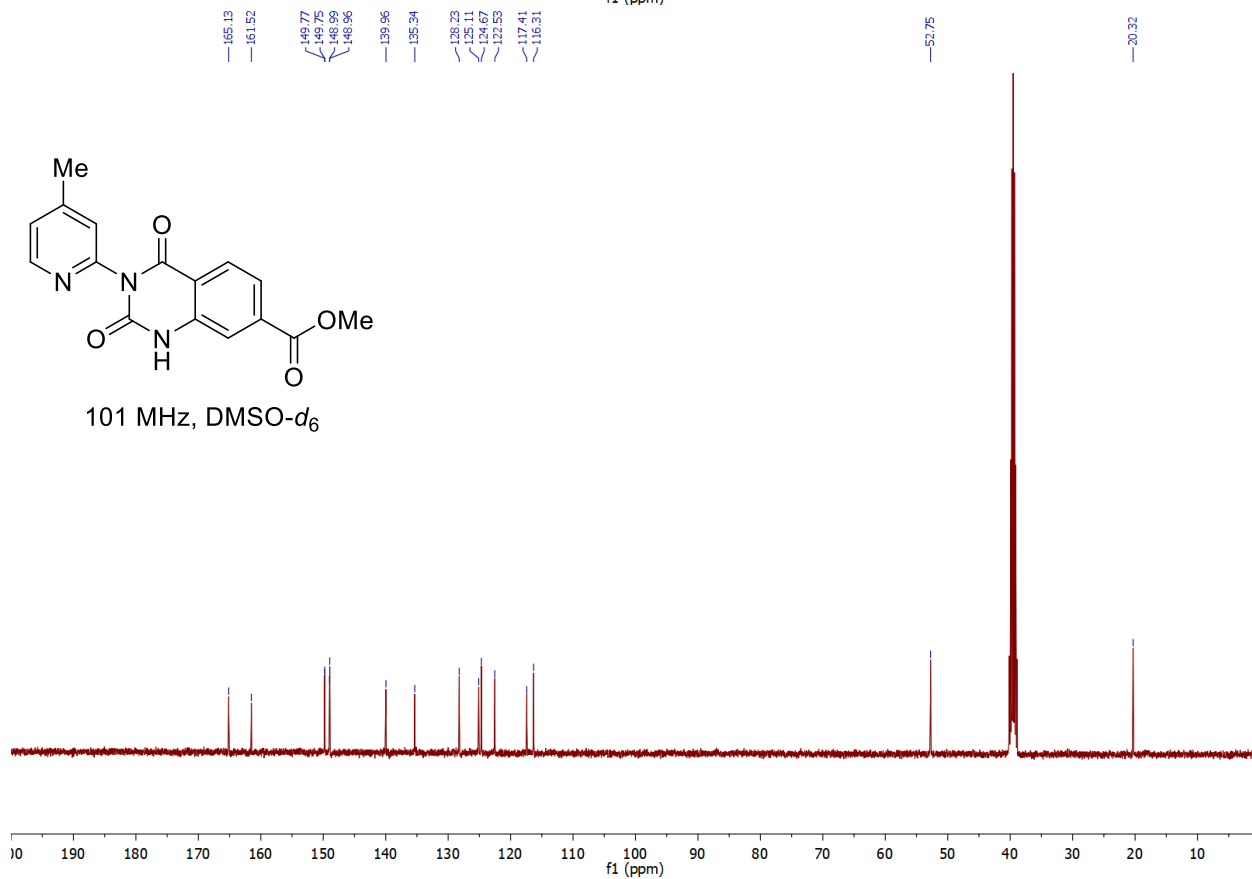
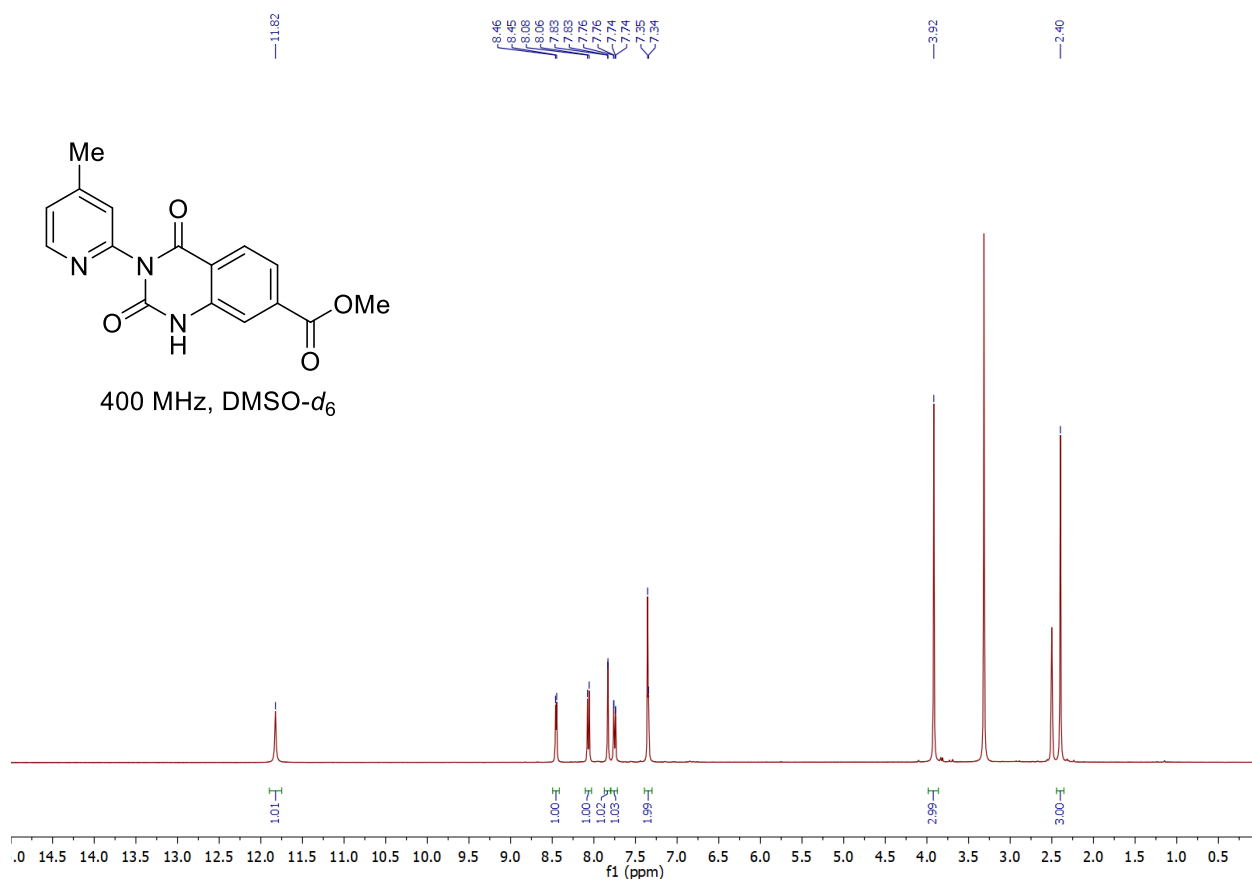
^1H and ^{13}C spectra of 7-chloro-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3v**



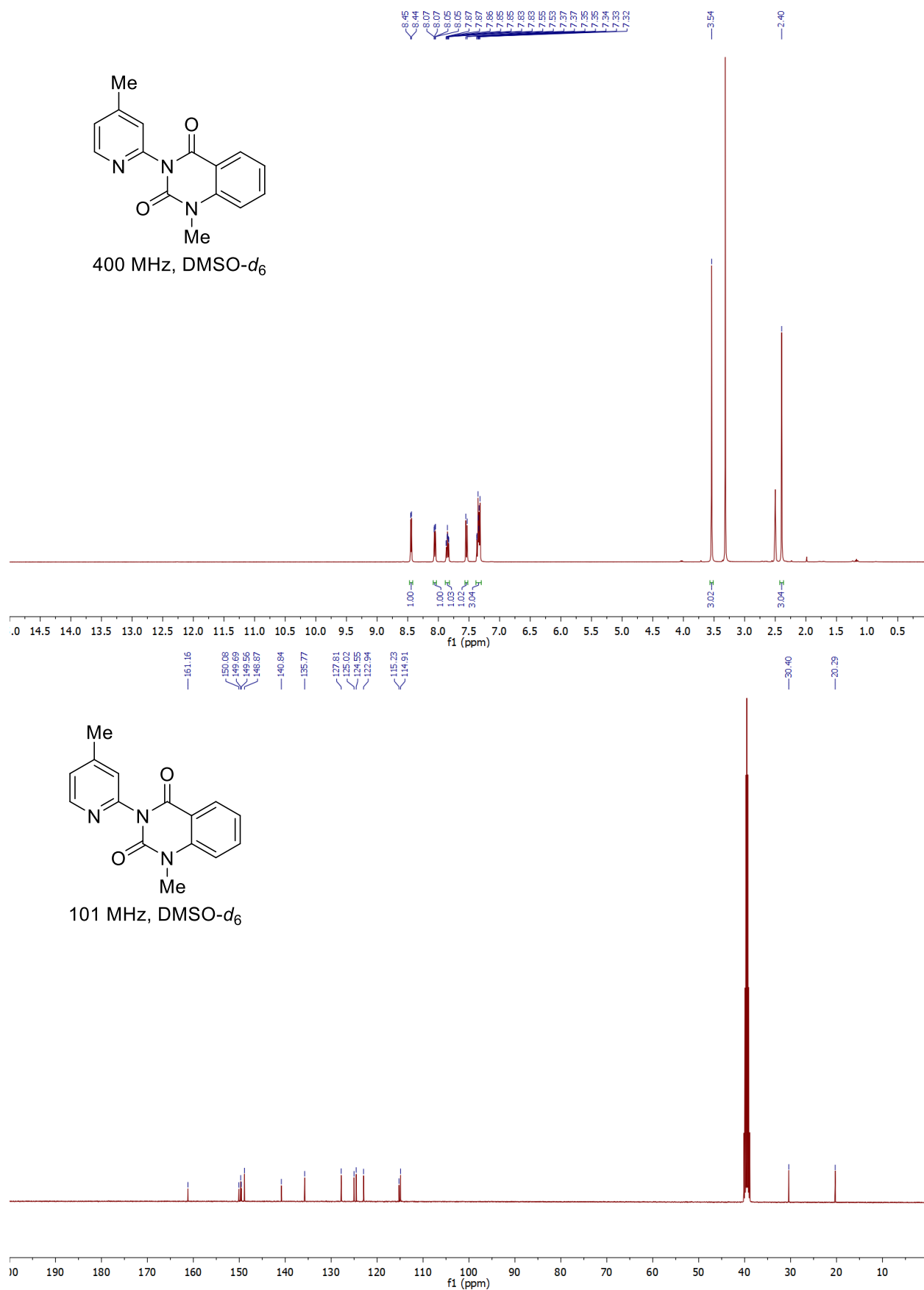
^1H and ^{13}C spectra of 6-bromo-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3w**



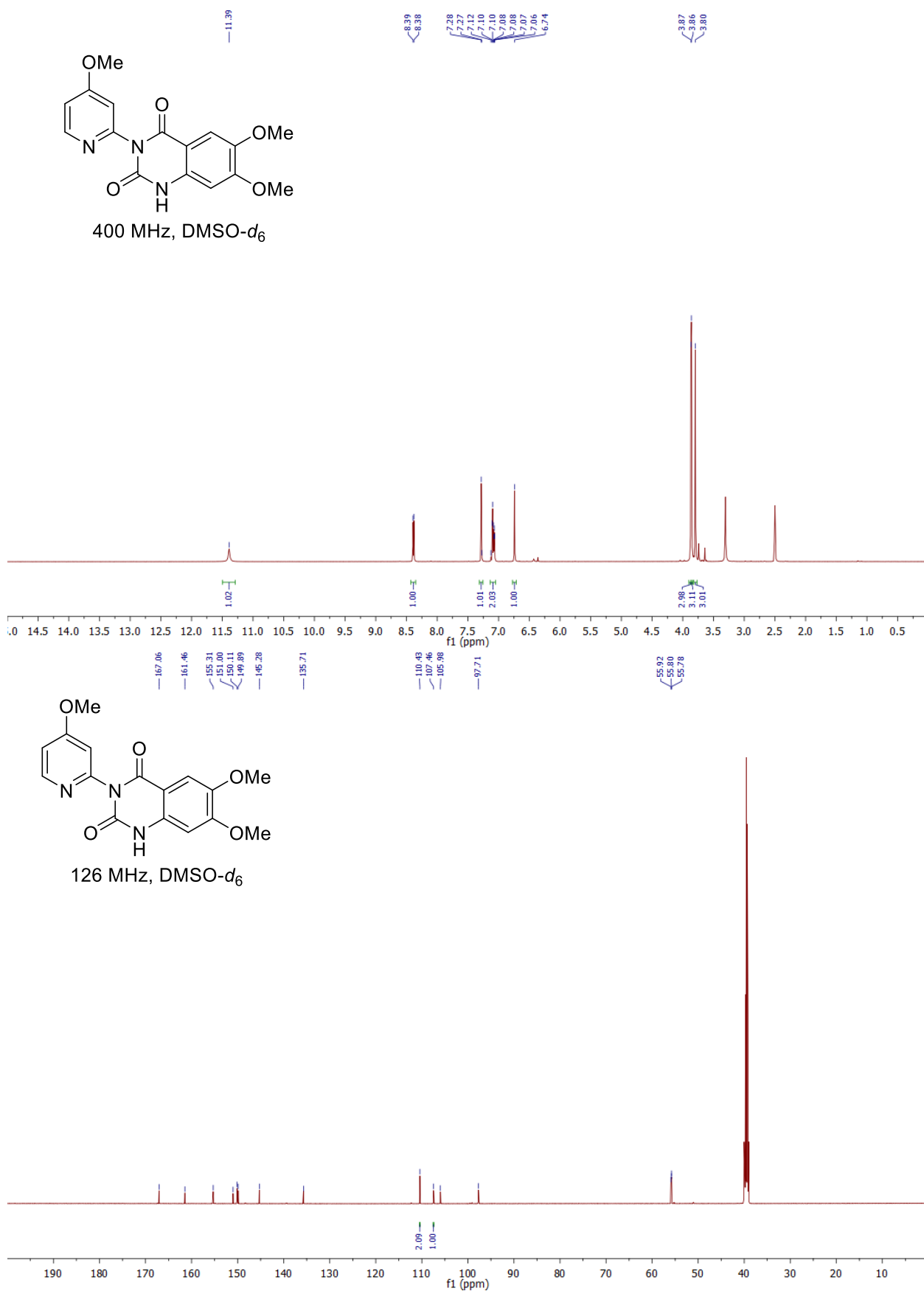
^1H and ^{13}C spectra of methyl 3-(4-methylpyridin-2-yl)-2,4-dioxo-1,2,3,4-tetrahydroquinazoline-7-carboxylate **3x**



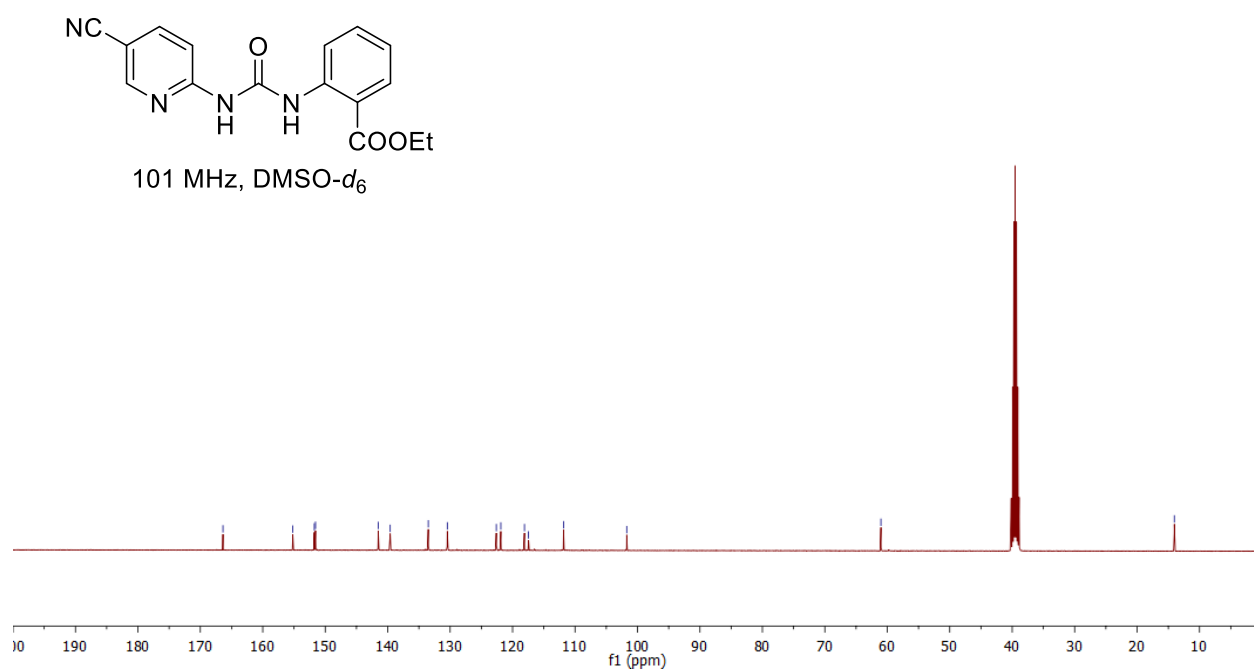
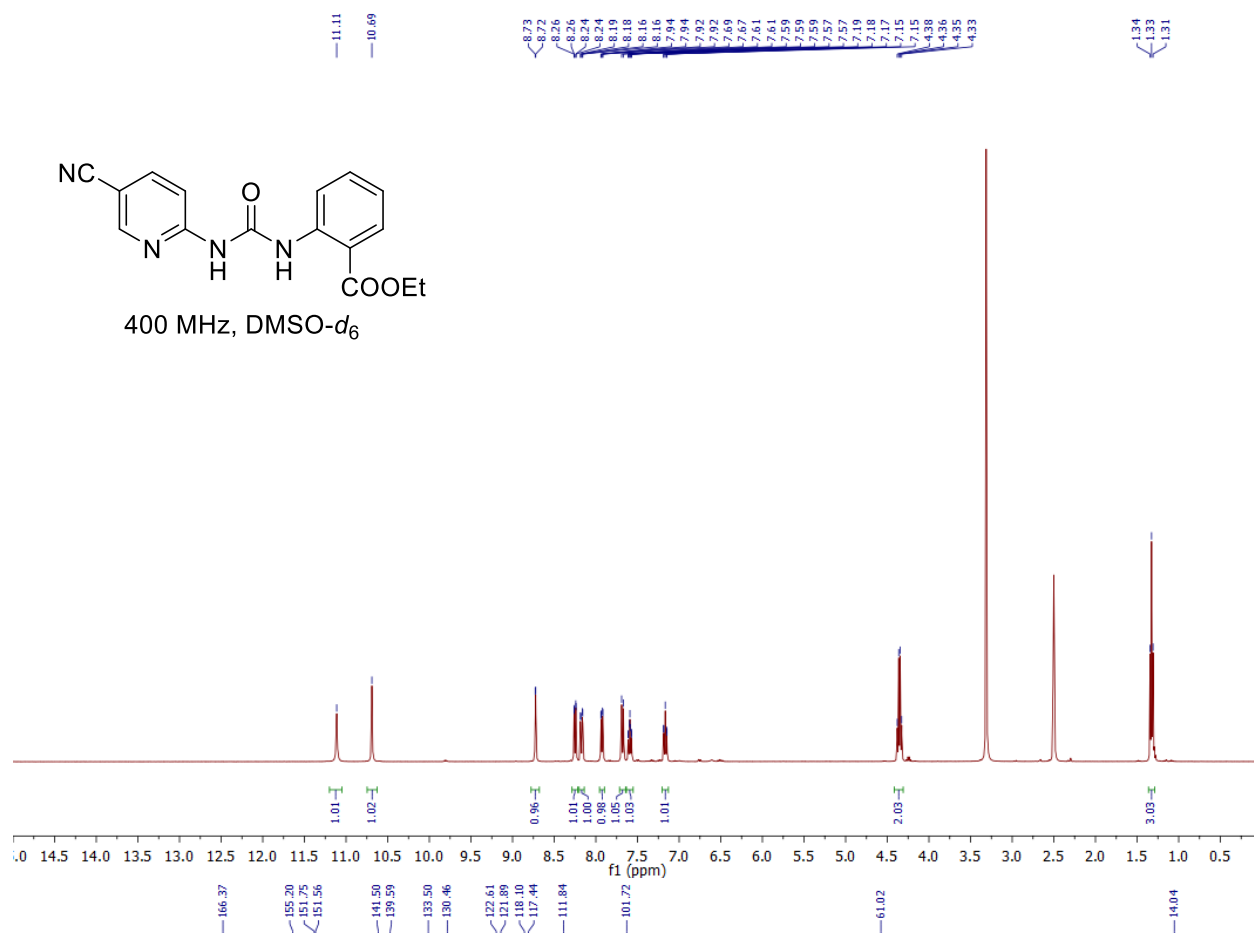
^1H and ^{13}C spectra of 1-methyl-3-(4-methylpyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3y**



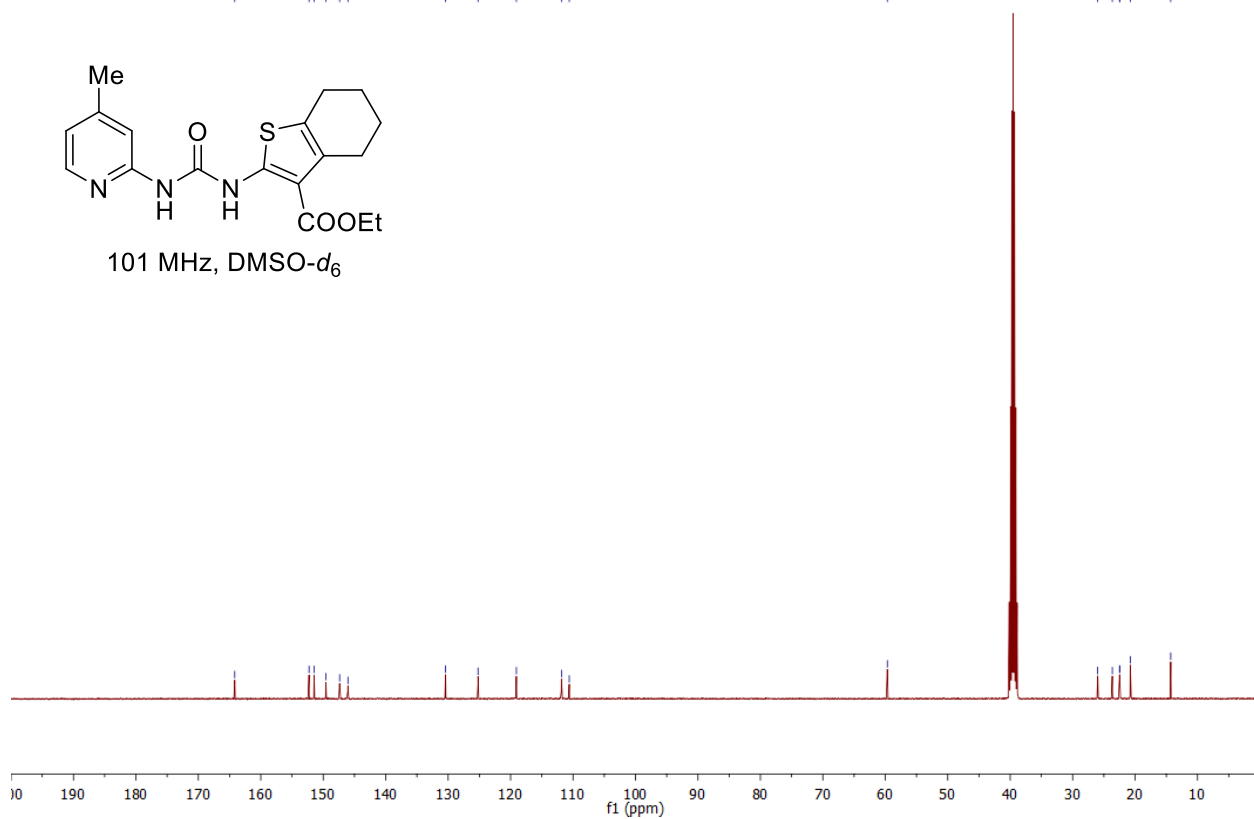
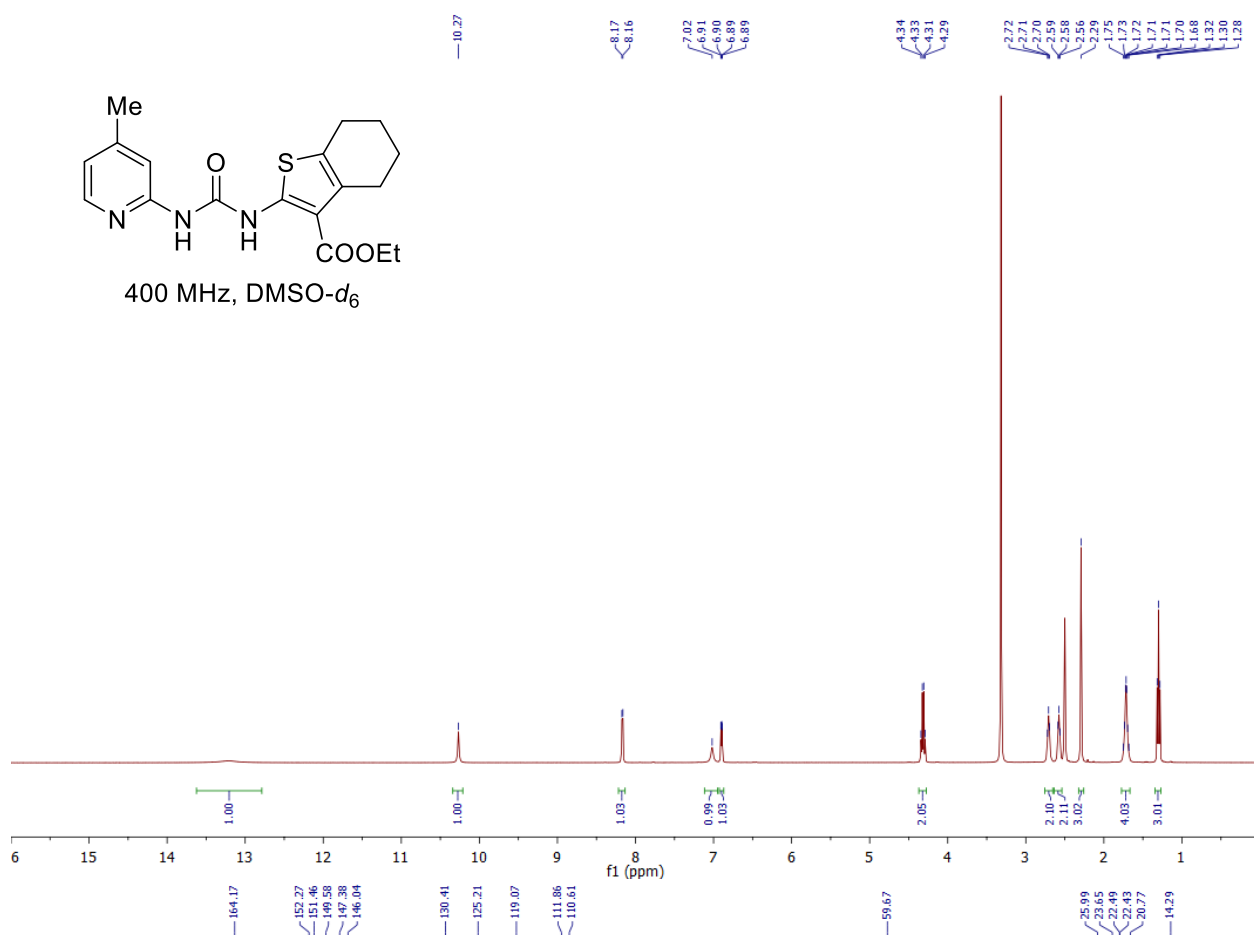
^1H and ^{13}C spectra of 6,7-dimethoxy-3-(4-methoxypyridin-2-yl)quinazoline-2,4(1*H*,3*H*)-dione **3z**



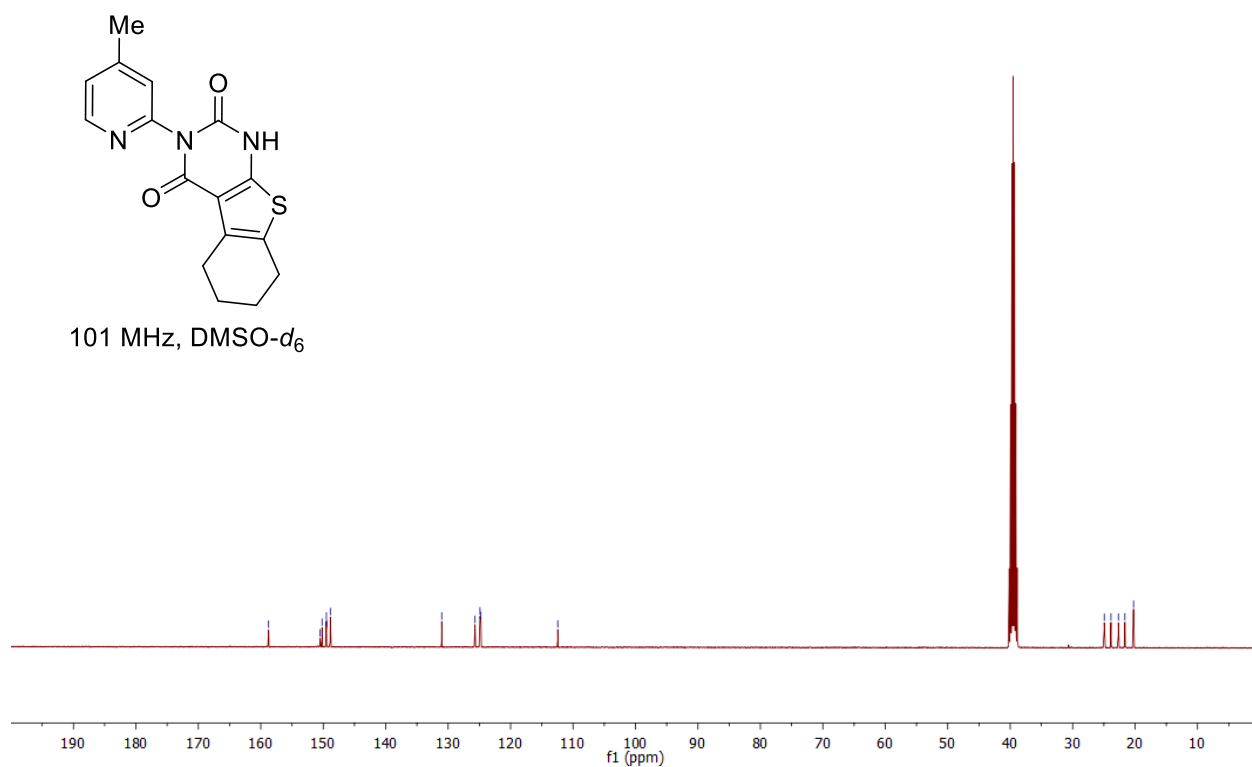
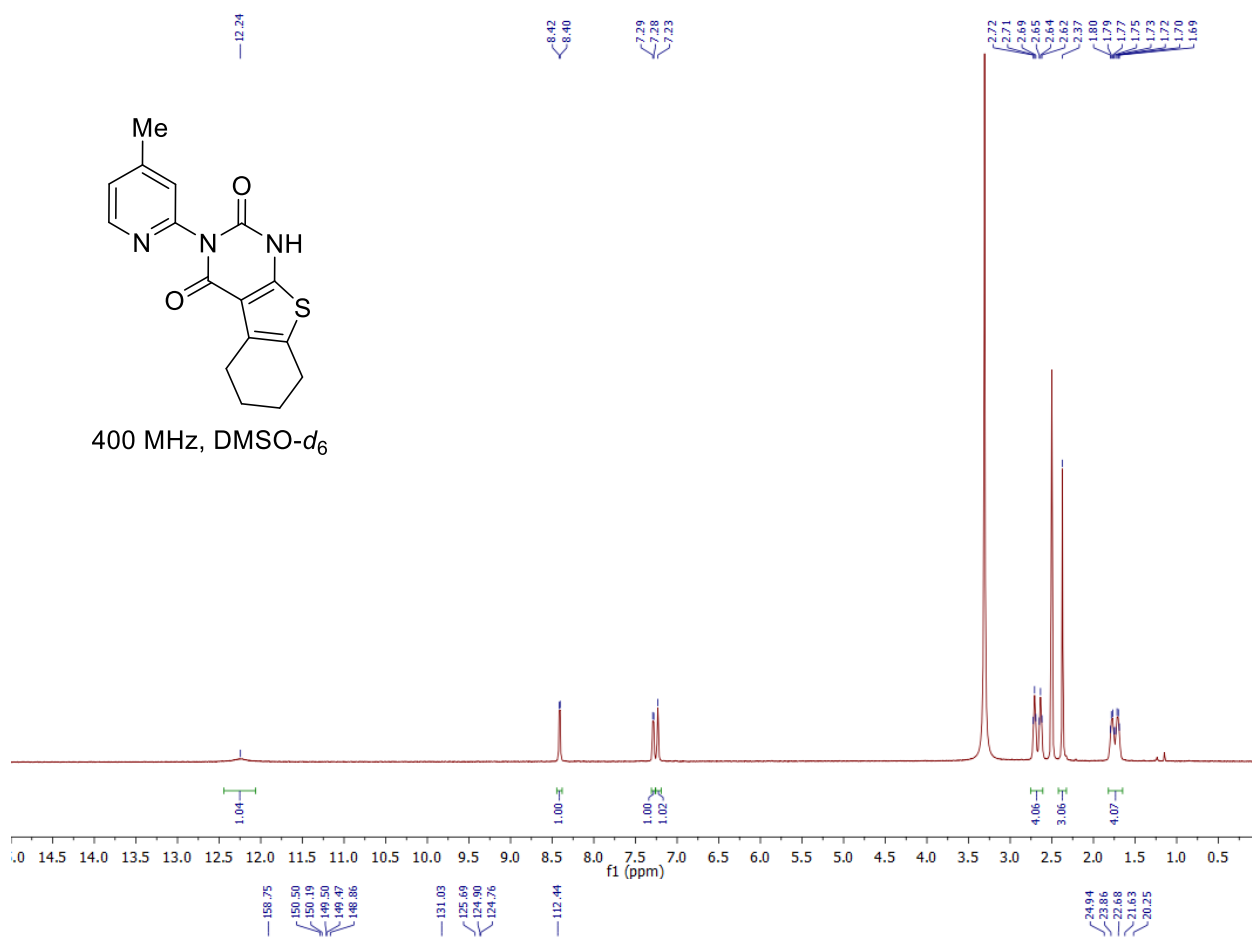
^1H and ^{13}C spectra of ethyl 2-(3-(5-cyanopyridin-2-yl)ureido)benzoate **4b**



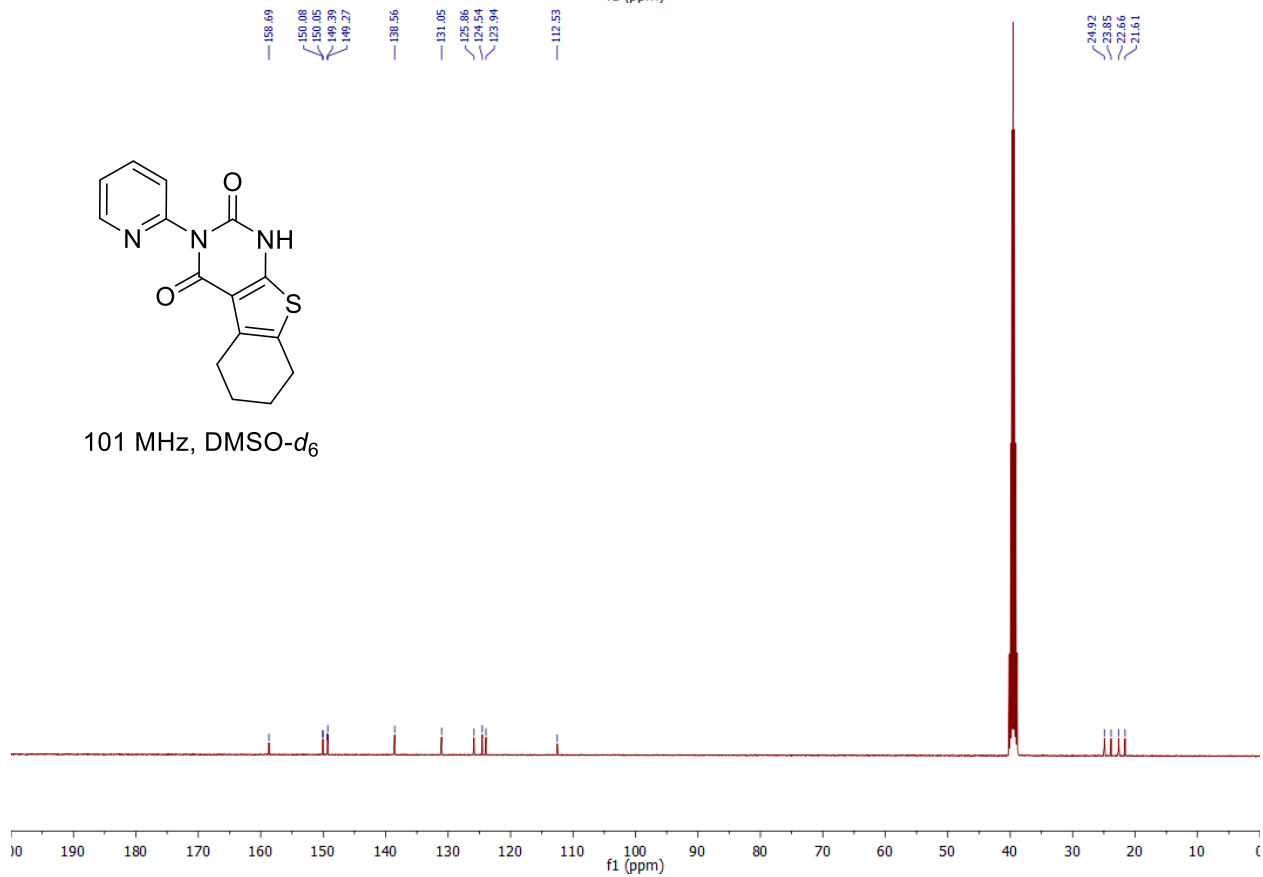
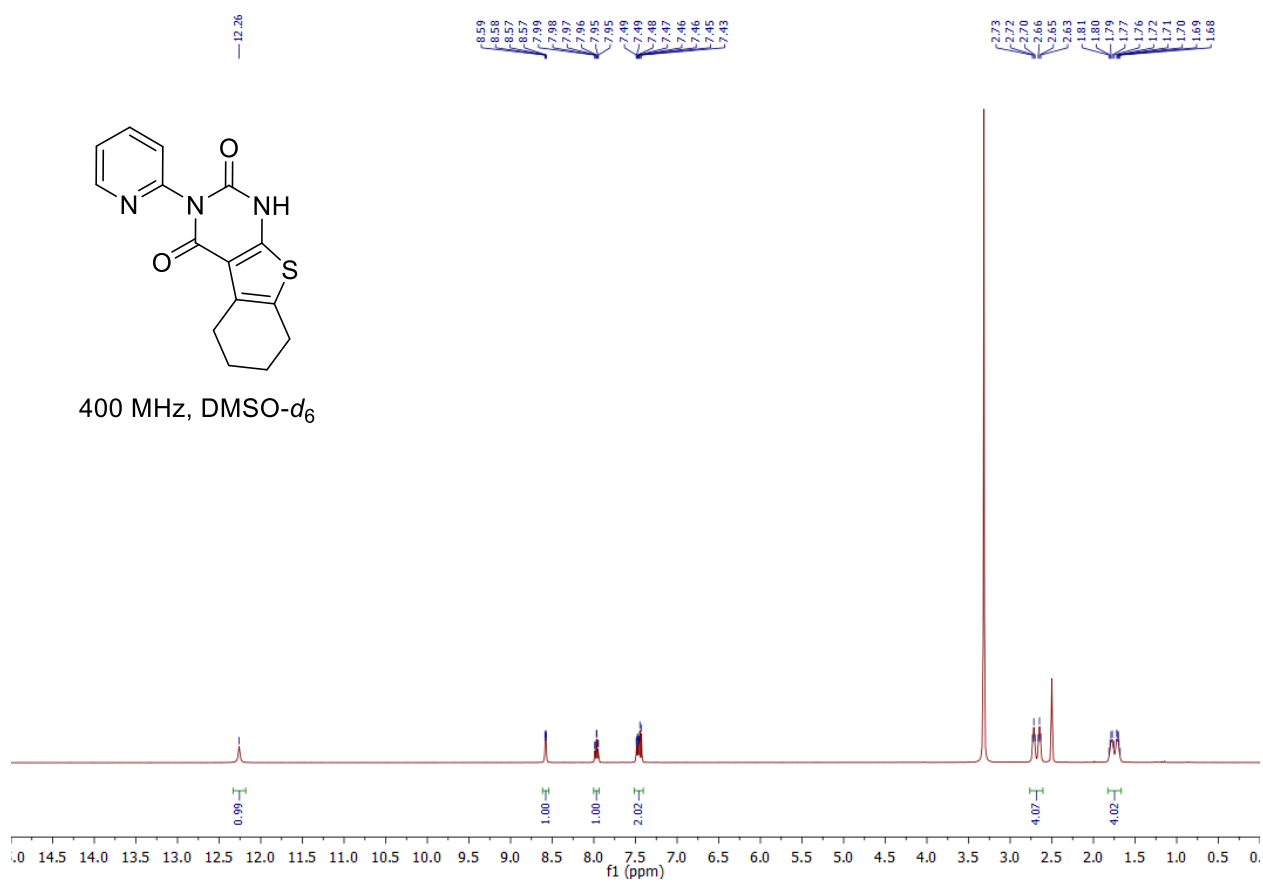
^1H and ^{13}C spectra of ethyl 2-(3-(4-methylpyridin-2-yl)ureido)-4,5,6,7-tetrahydrobenzo[*b*]thiophene-3-carboxylate **7a**



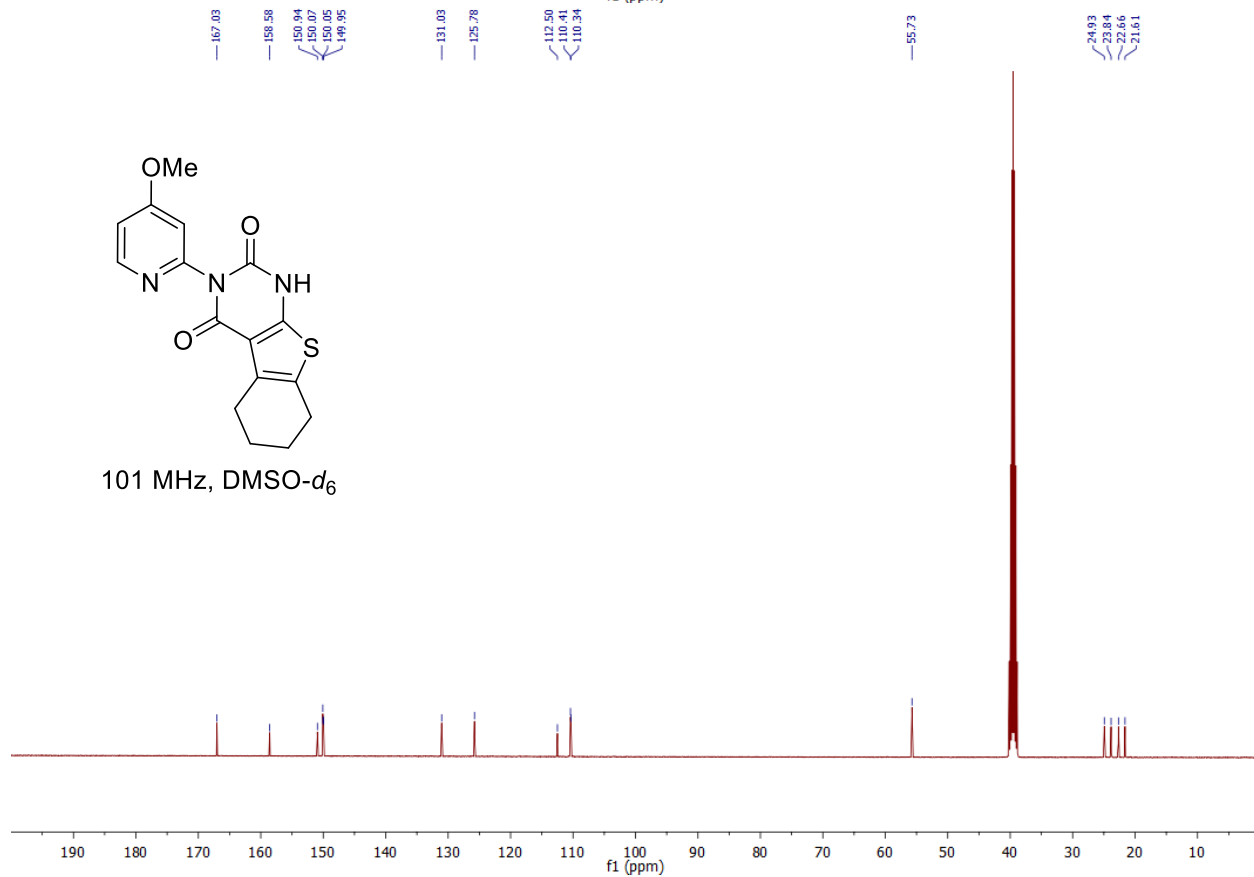
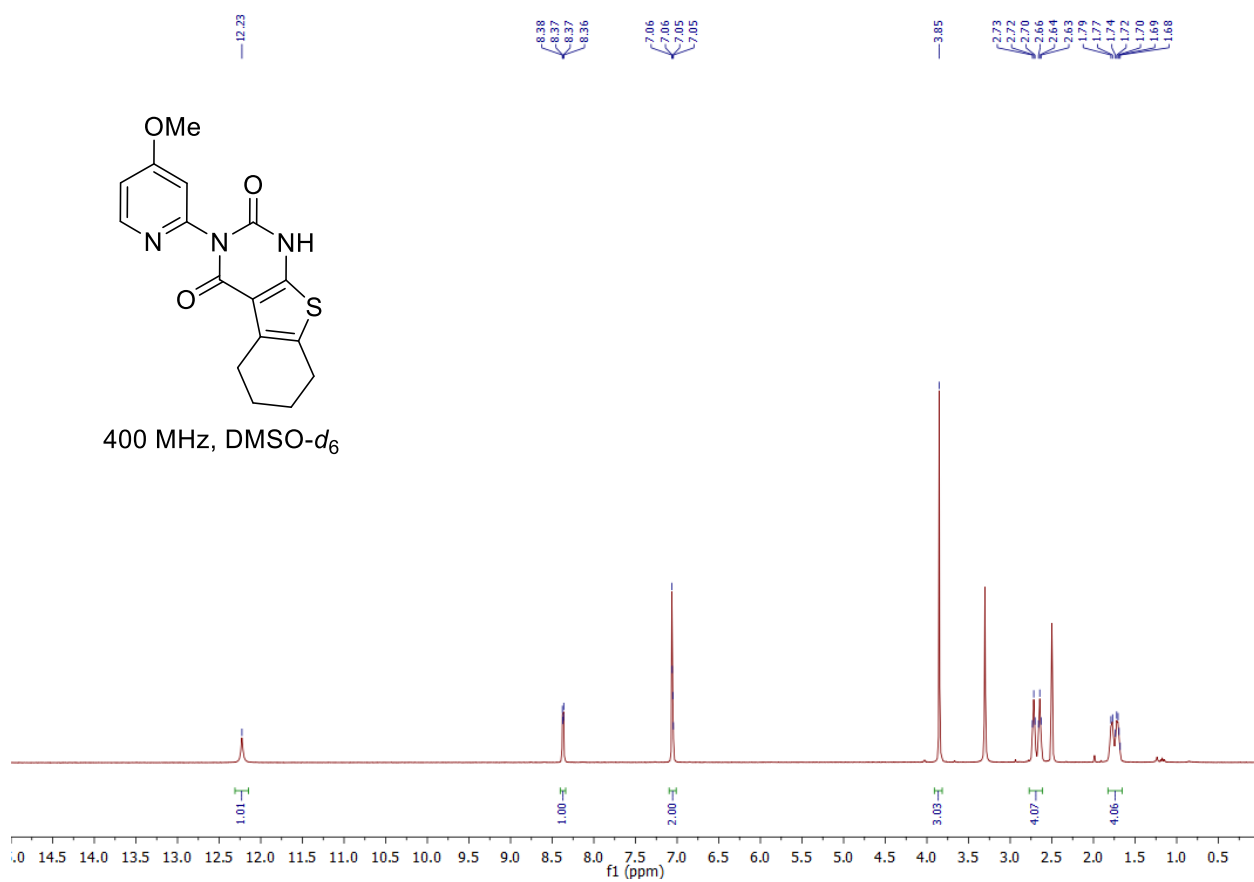
^1H and ^{13}C spectra of 3-(4-methylpyridin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione **8a**



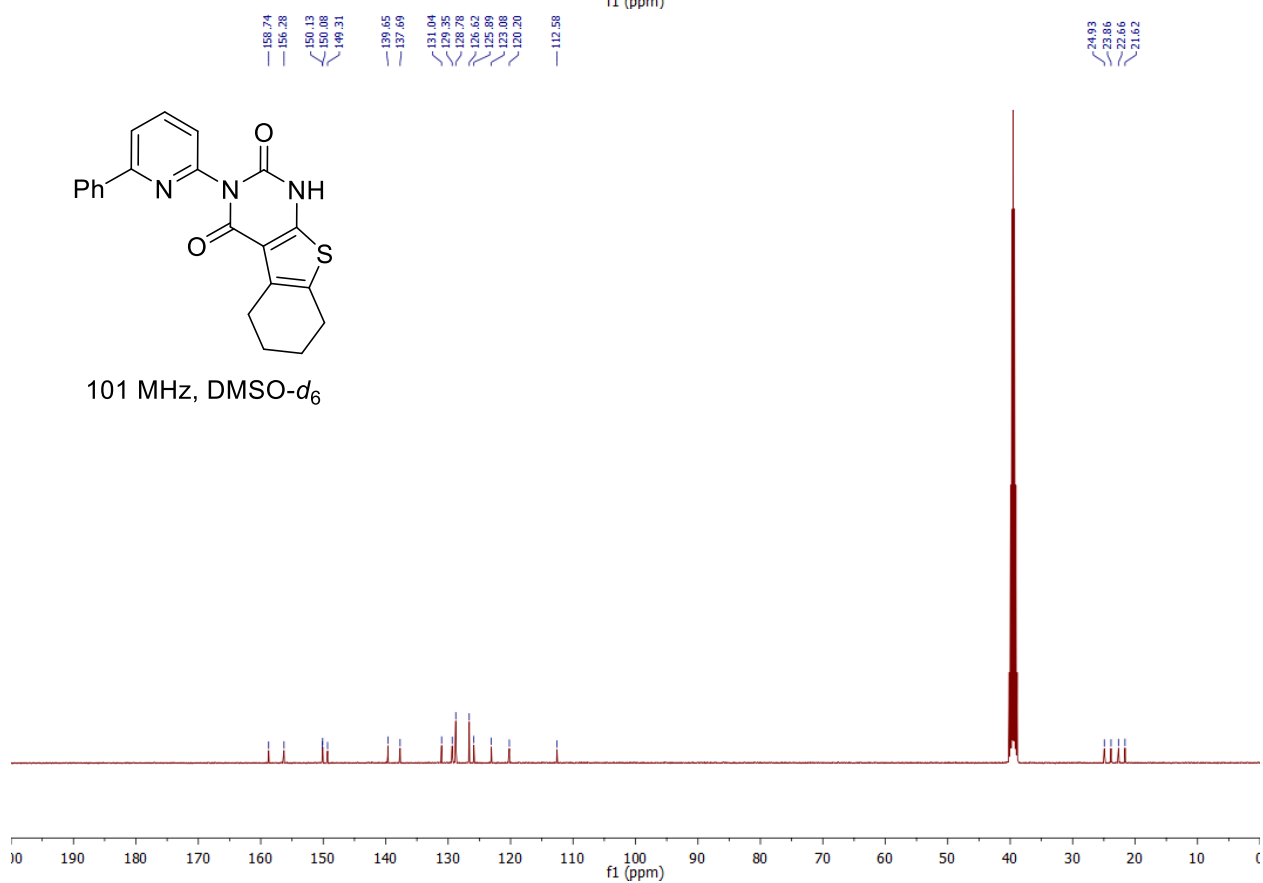
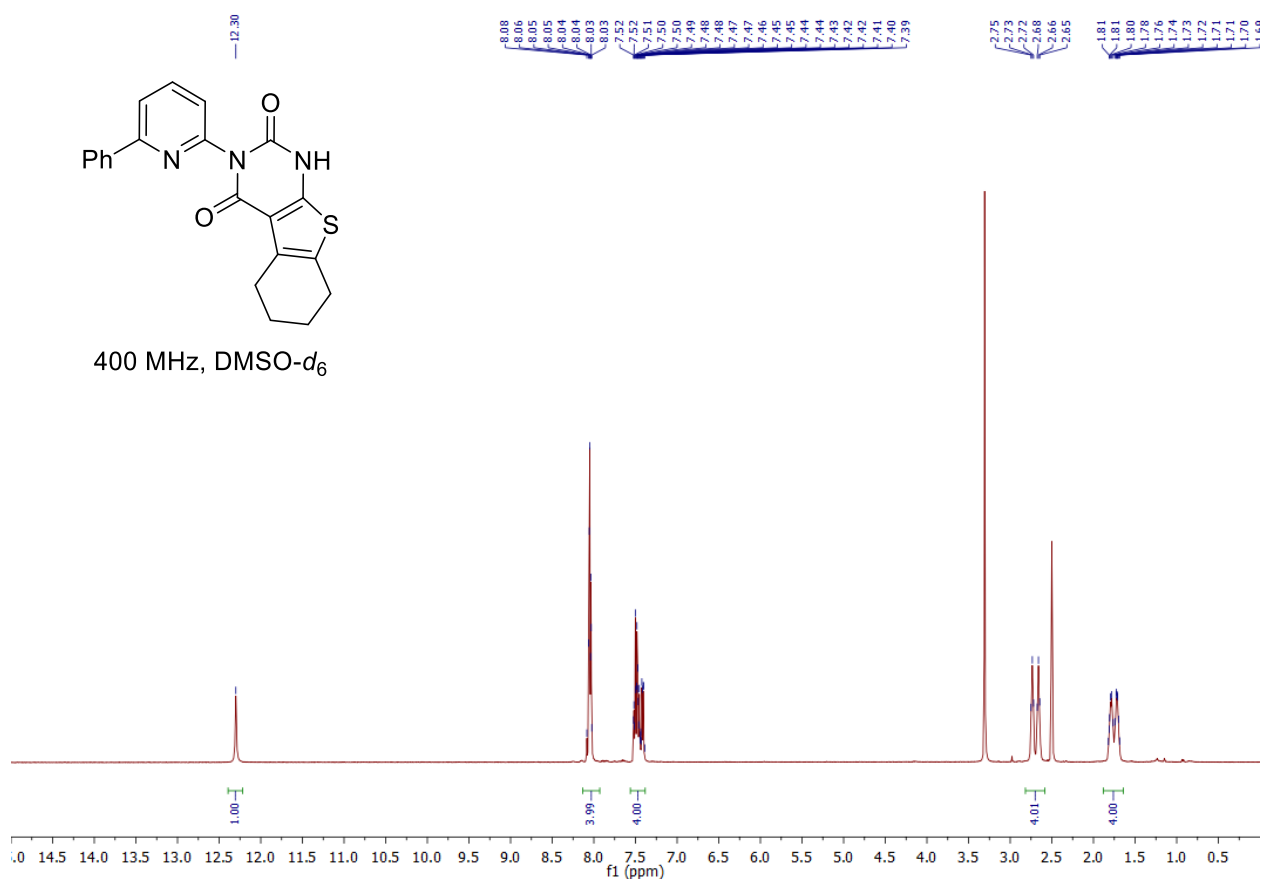
^1H and ^{13}C spectra of 3-(pyridin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione **8b**



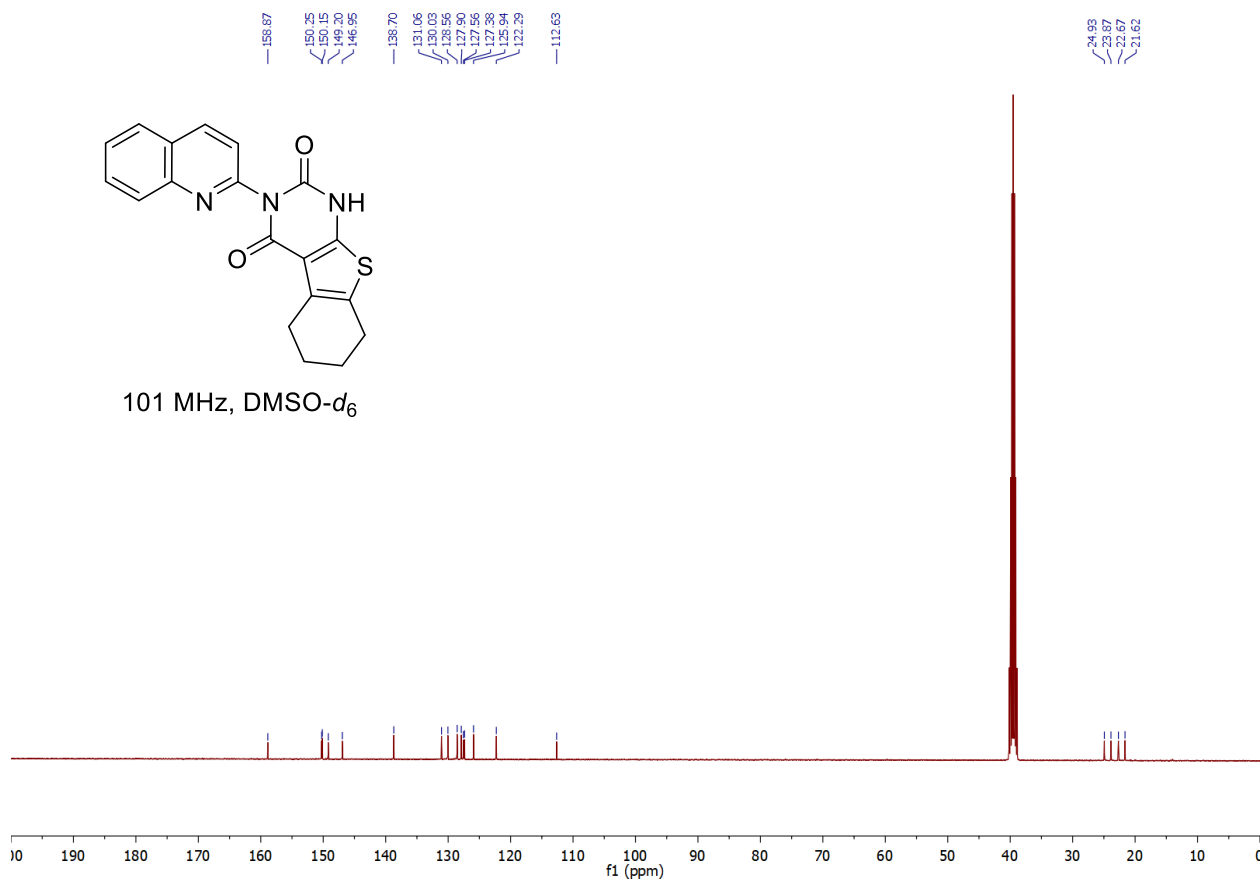
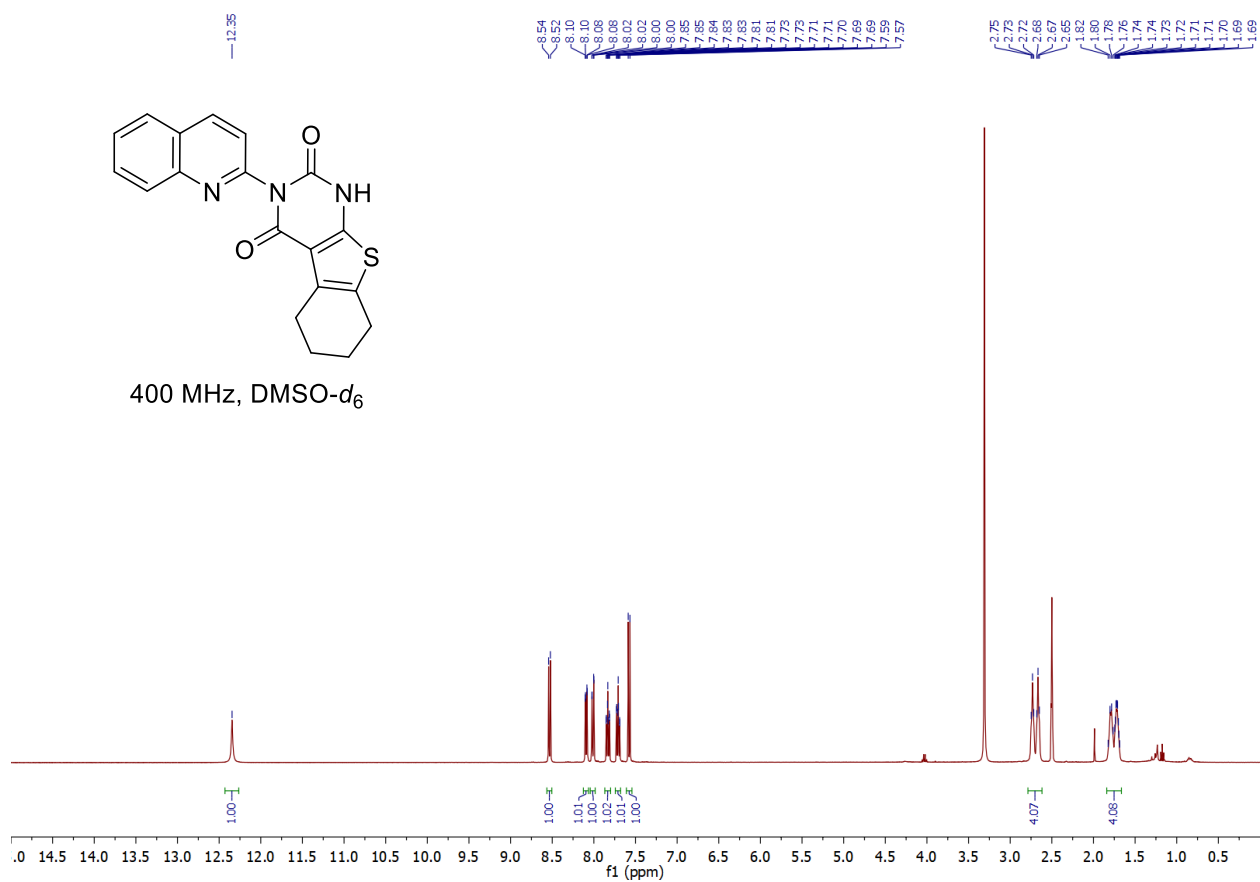
^1H and ^{13}C spectra of 3-(4-methoxypyridin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione **8c**



^1H and ^{13}C spectra of 3-(6-phenylpyridin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione **8d**



^1H and ^{13}C spectra of 3-(quinolin-2-yl)-5,6,7,8-tetrahydrobenzo[4,5]thieno[2,3-*d*]pyrimidine-2,4(1*H*,3*H*)-dione **8e**



^1H and ^{13}C spectra of 3-(4-methylpyridin-2-yl)-1,5,6,7-tetrahydro-2*H*-cyclopenta[4,5]thieno[2,3-*d*]pyrimidine-2,4(3*H*)-dione **8f**

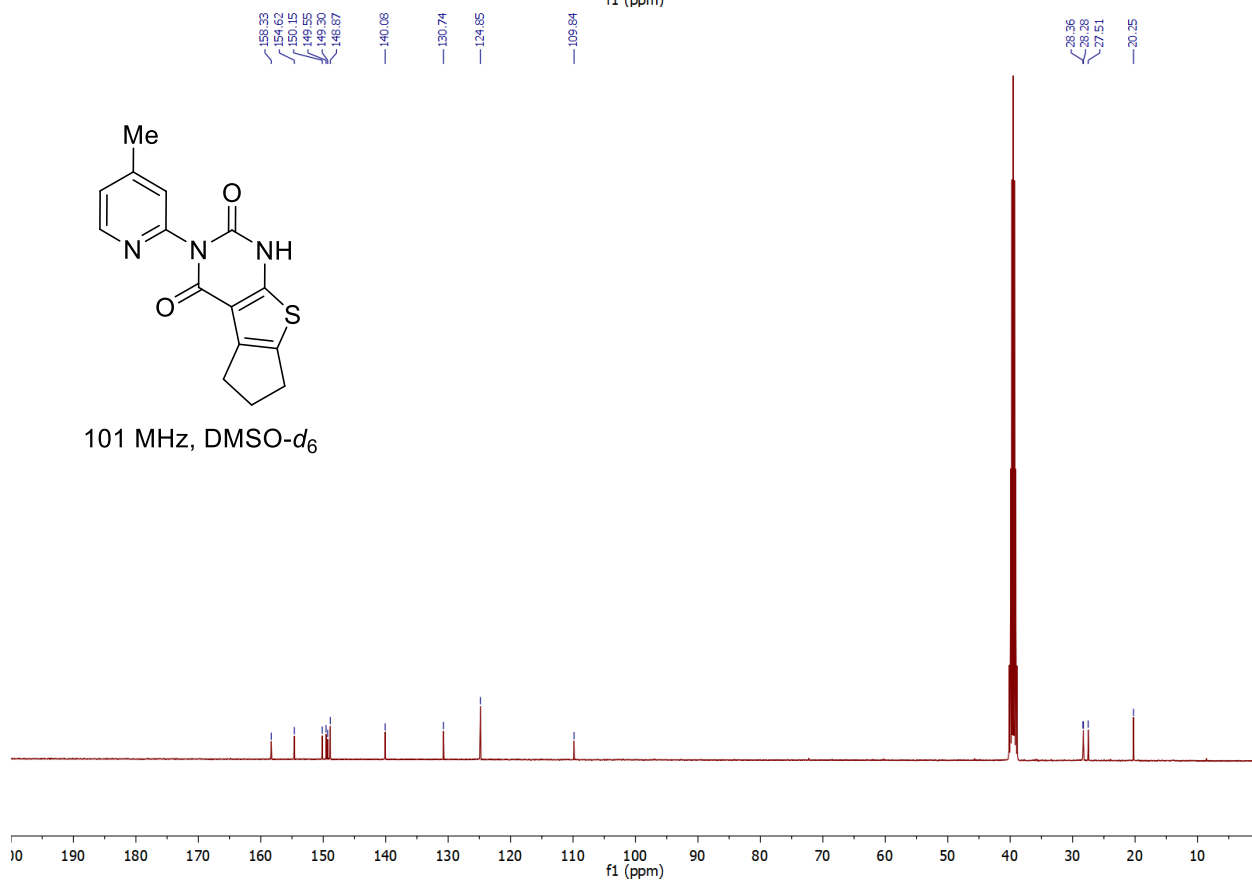
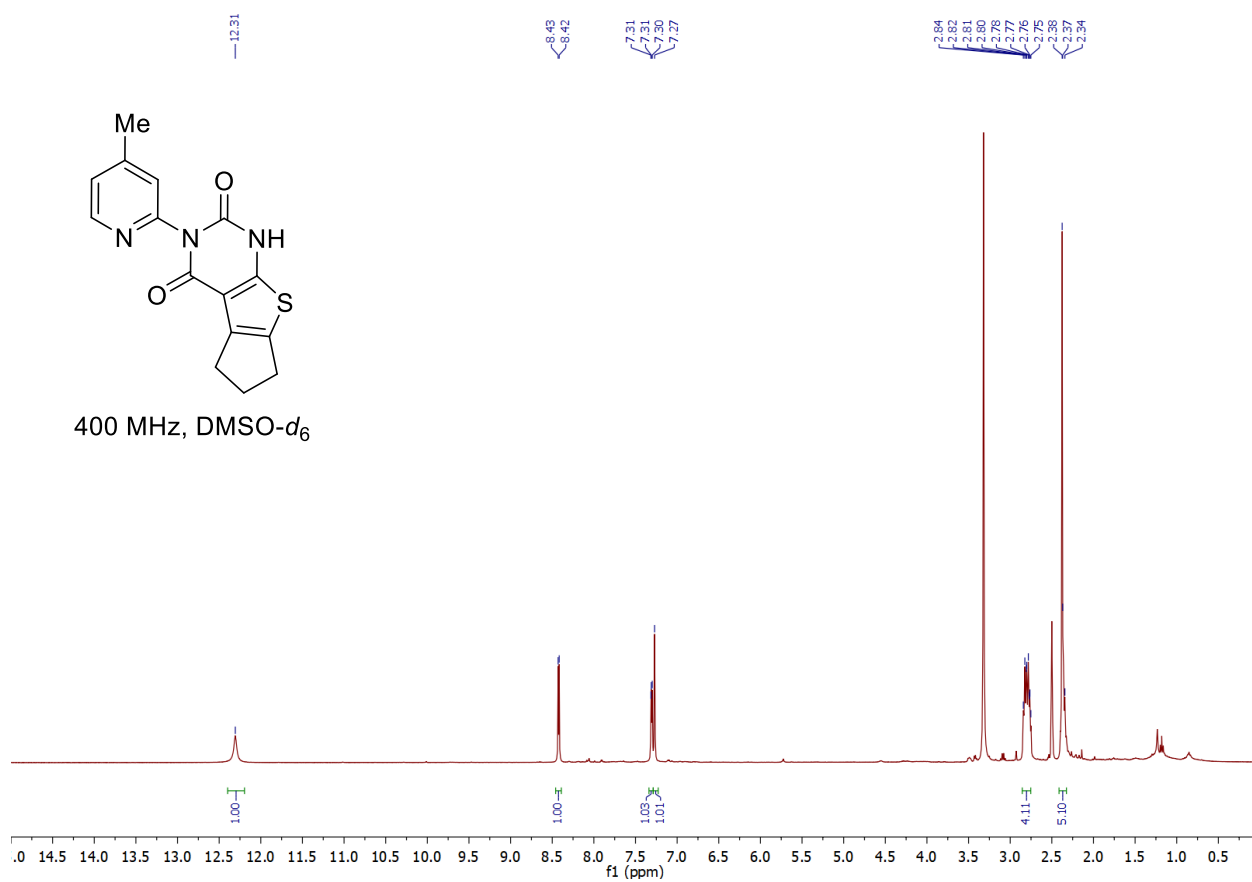


Table S1 Crystal data and structure refinement for 3a.

Identification code	CJL-278
CCDC number	2249286
Empirical formula	C ₁₄ H ₁₁ N ₃ O ₂
Formula weight	253.26
Temperature/K	100(2)
Crystal system	monoclinic
Space group	P2 ₁ /c
a/Å	11.4062(3)
b/Å	14.6246(3)
c/Å	6.9952(2)
α /°	90
β /°	94.055(2)
γ /°	90
Volume/Å ³	1163.96(5)
Z	4
$\rho_{\text{calc}}/\text{cm}^3$	1.445
μ/mm^{-1}	0.822
F(000)	528.0
Crystal size/mm ³	0.24 × 0.22 × 0.16
Radiation	Cu K α (λ = 1.54184)
2 Θ range for data collection/°	7.77 to 159.398
Index ranges	−14 ≤ h ≤ 10, −17 ≤ k ≤ 18, −8 ≤ l ≤ 8
Reflections collected	8636
Independent reflections	2434 [R_{int} = 0.0380, R_{sigma} = 0.0307]
Data/restraints/parameters	2434/0/173
Goodness-of-fit on F ²	1.045
Final R indexes [$I \geq 2\sigma(I)$]	R_1 = 0.0432, wR_2 = 0.1137
Final R indexes [all data]	R_1 = 0.0469, wR_2 = 0.1167
Largest diff. peak/hole / e Å ^{−3}	0.24/−0.32