

Supporting Information

Metal-Free Synthesis of 2-Substituted Quinazolines via Green Oxidation of *o*-Aminobenzylamines: Practical Construction of *N*-Containing Heterocycles Based on a Salicylic Acid-Catalyzed Oxidation System

Yuki Yamamoto¹, Chihiro Yamakawa¹, Riku Nishimura¹, Chun-ping Dong¹,

Shintaro Kodama^{1*}, Akihiro Nomoto¹, Michio Ueshima¹, and Akiya Ogawa^{1*}

¹Department of Applied Chemistry, Graduate School of Engineering, Osaka Prefecture University, 1-1 Gakuen-cho, Nakaku, Sakai, Osaka 599-8531, Japan

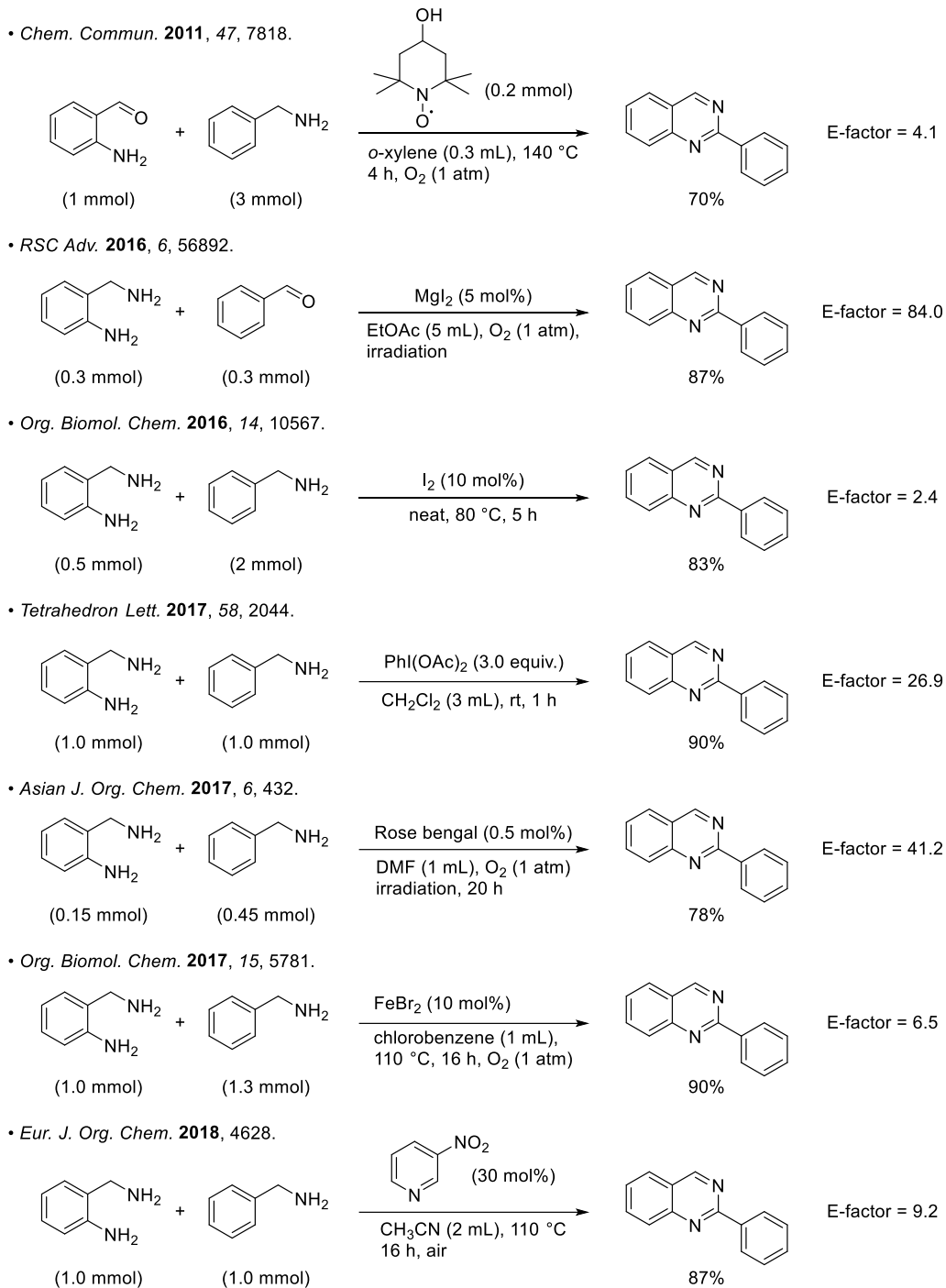
skodama@chem.osakafu-u.ac.jp, ogawa@chem.osakafu-u.ac.jp

CONTENTS

	Pages
Scheme S1. Comparison of the E-factor of some alternative methods for synthesis of quinazolines and this work	S2
Figure S1. ¹ H NMR spectrum of crude 3aa after the reaction (entry 17 in Table 1)	S3
Table S1. Optimization of reaction conditions for salicylic acid-catalyzed oxidation of benzylamine to the corresponding imine	S3
Copies of ¹ H and ¹³ C{ ¹ H} NMR spectra of compounds 3aa–3ah , 3aj–3at , and 3ba	S4–S23
Copies of ¹ H and ¹³ C{ ¹ H} NMR spectra of compounds 4a–4d	S24–S27
Copies of ¹ H and ¹³ C{ ¹ H} NMR spectra of compounds 6a–6e , 8 , and 9	S28–S34

Scheme S1. Comparison of the E-factor of some alternative methods for synthesis of quinazolines and this work

(a) Previously reported methods for synthesis of quinazolines from amines



(b) This work

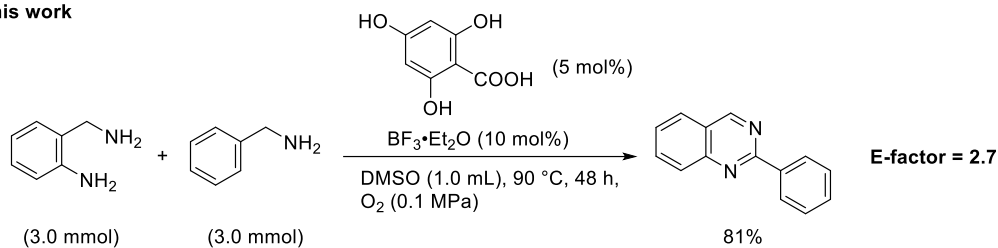


Figure S1. ^1H NMR spectrum of crude **3aa** after the reaction (entry 17 in Table 1, in CDCl_3)

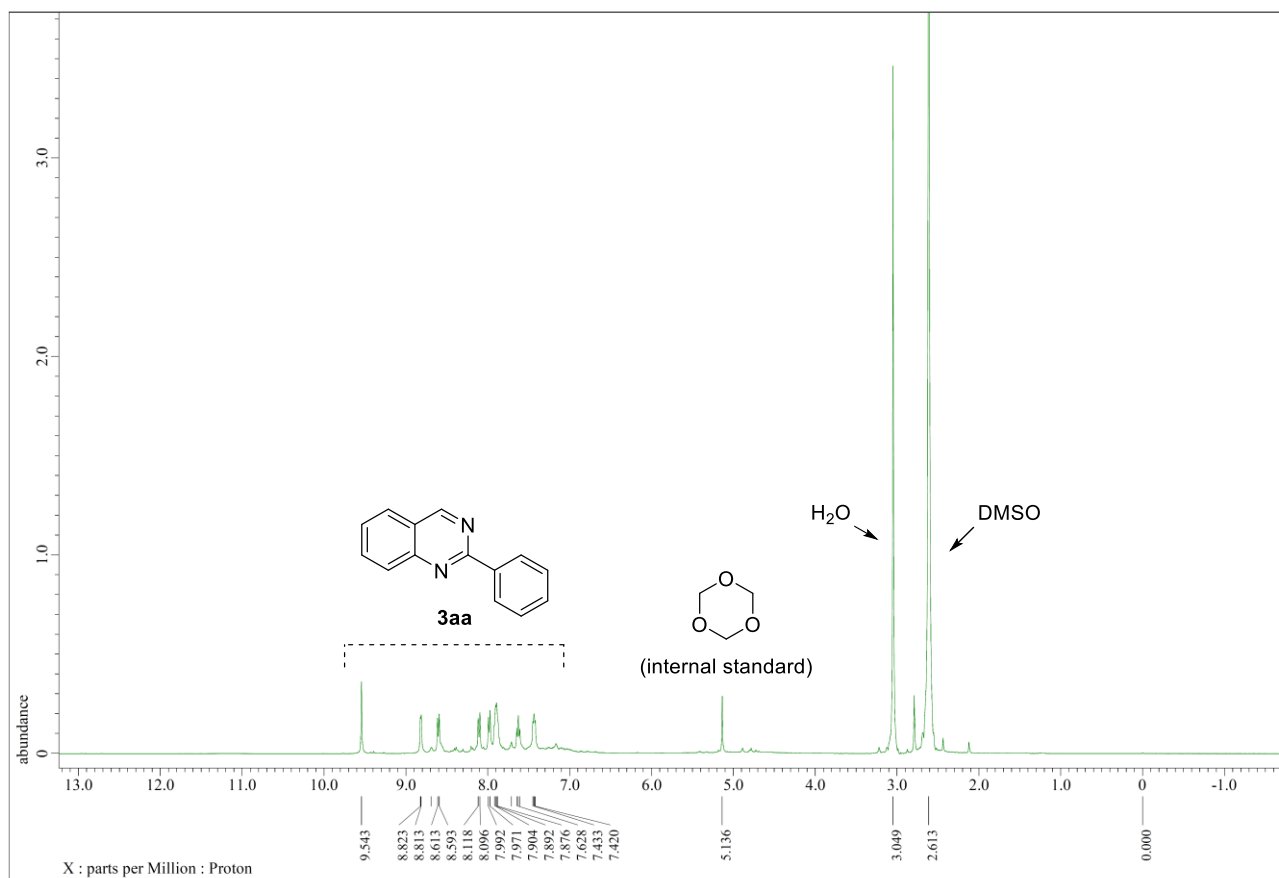


Table S1. Optimization of reaction conditions for salicylic acid-catalyzed oxidation of benzylamine to the corresponding imine

c1ccc(cc1)CN (2a, 3.0 mmol) + O=C(O)c1ccccc1O (5 mol%), additive $\xrightarrow[\text{O}_2 (0.1 \text{ MPa})]{\text{toluene (1.5 mL), 90 }^\circ\text{C, time}}$ c1ccc(cc1)/C=N/c2ccccc2 (4a)

Entry	Additive (mg)	Time (h)	Yield 4a (%) ^a
1	-	2	14
2	-	4	26
3	-	16	79
4	-	24	73
5	4A MS (100)	16	98 (87)

^aYields were determined by ^1H NMR spectroscopy (isolated yield)

Figure S2: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3aa**

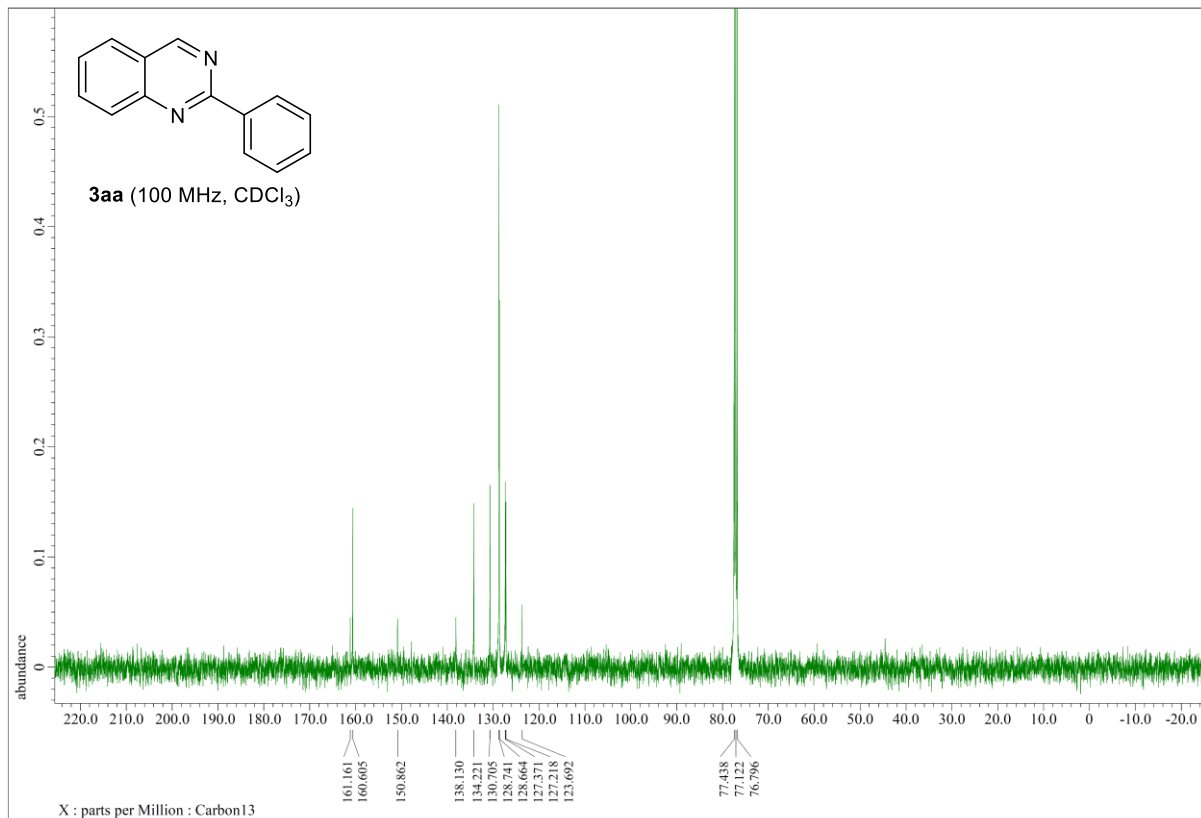
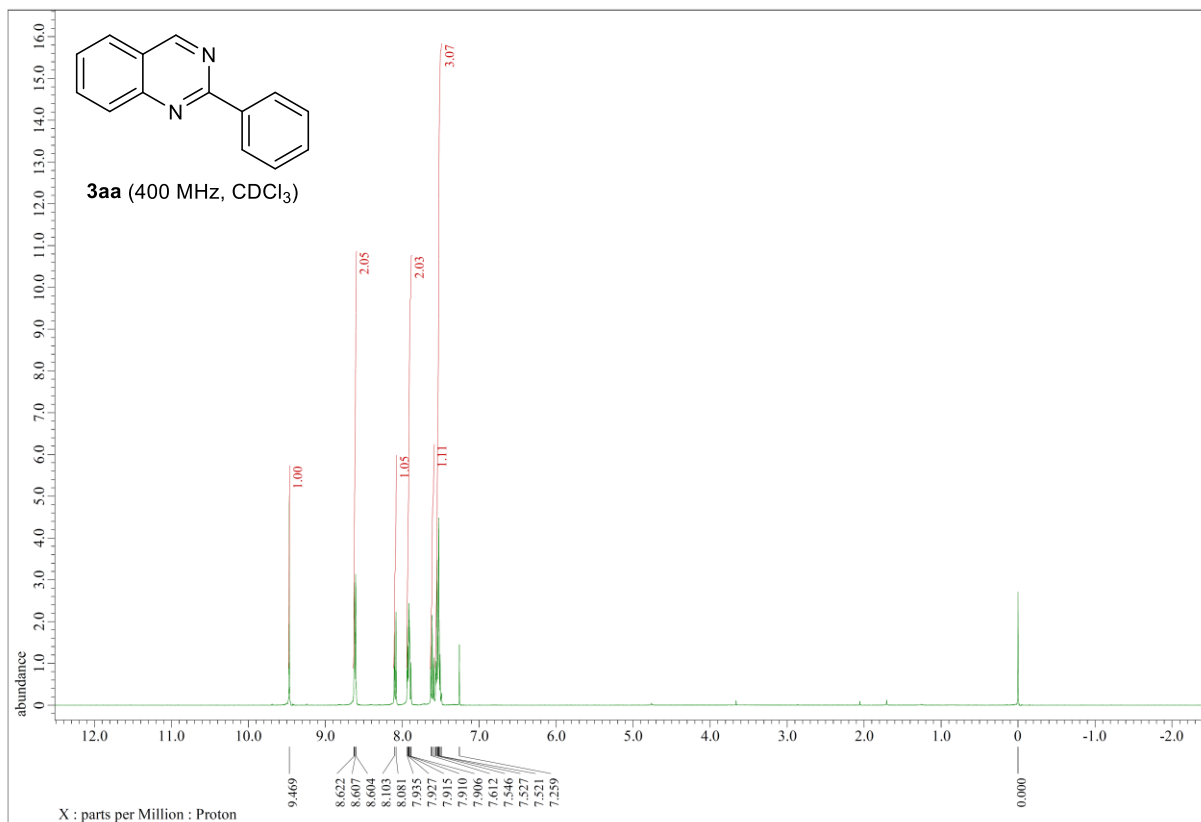


Figure S3: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ab**

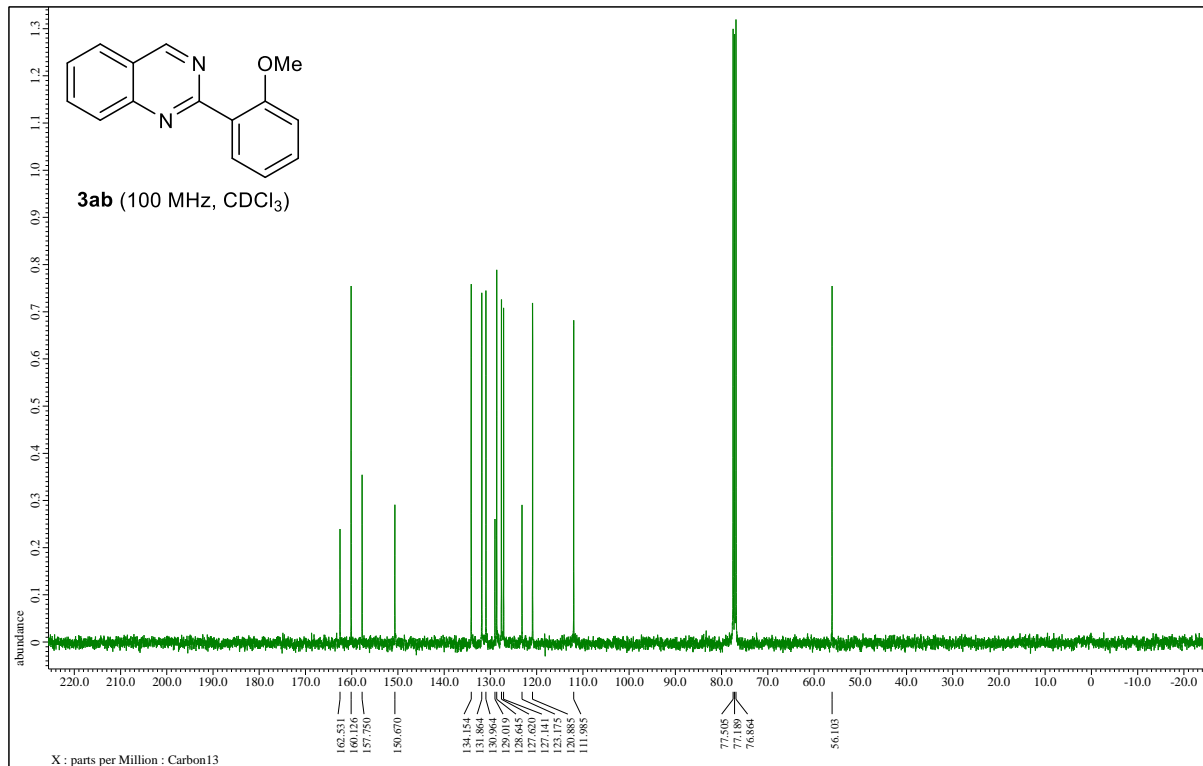
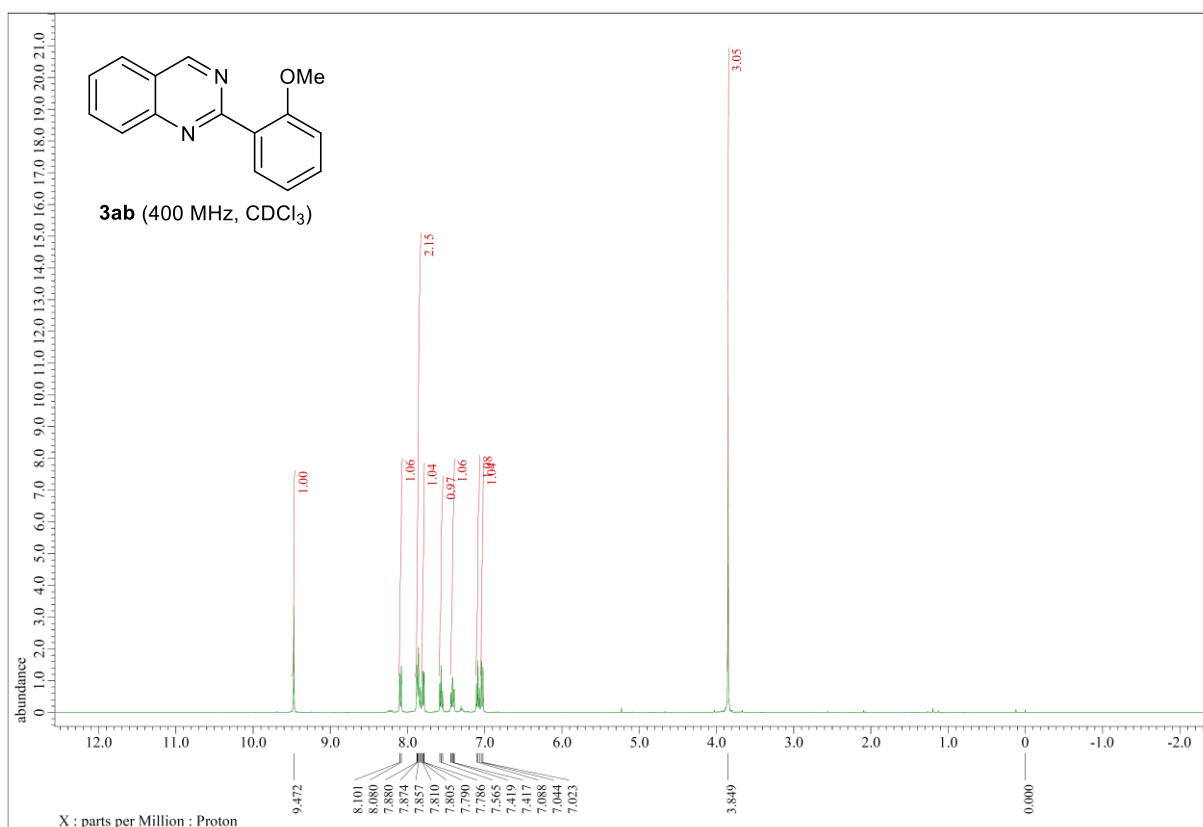


Figure S4: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ac**

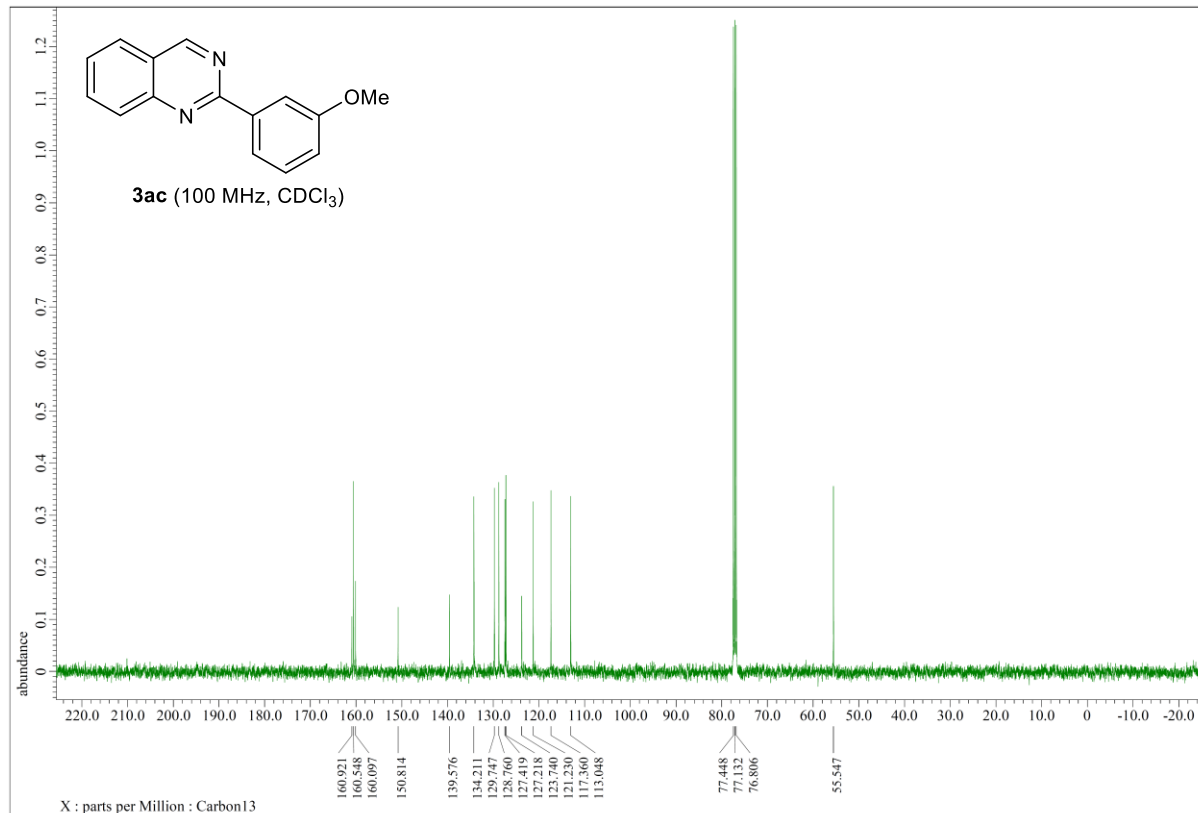
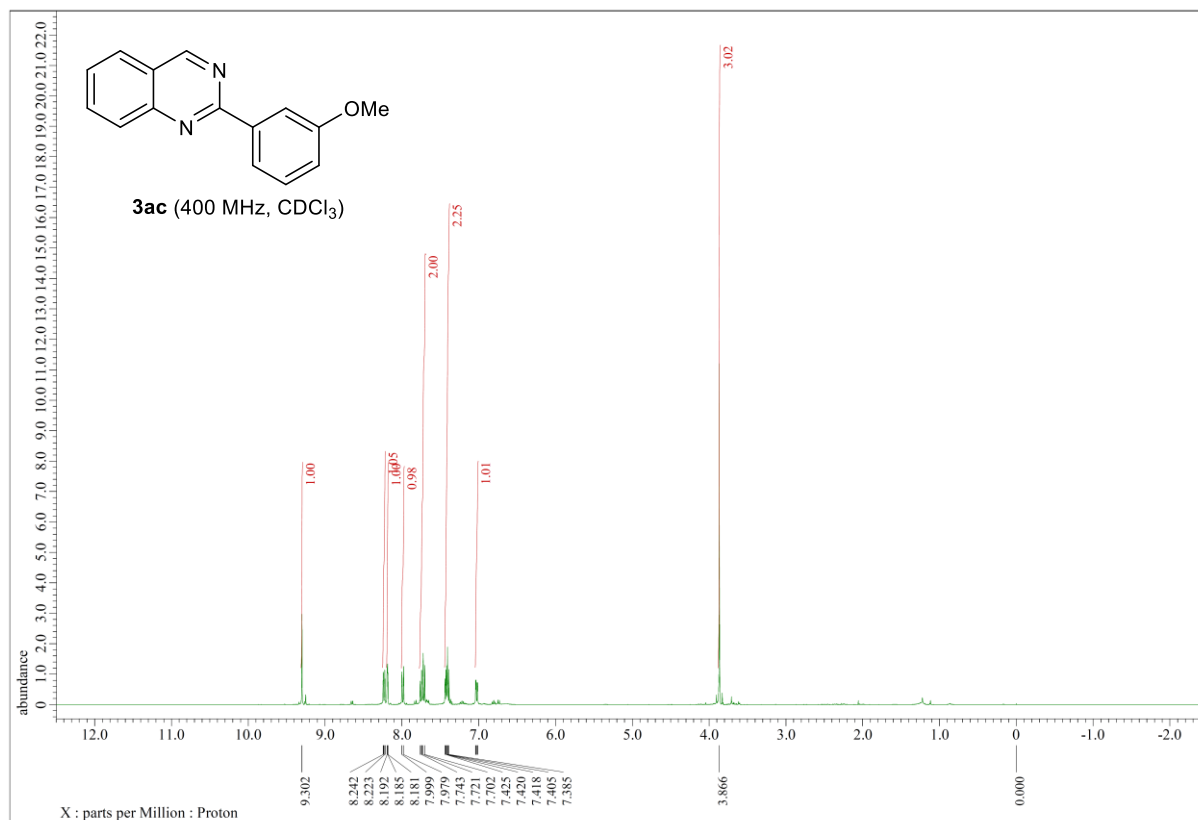


Figure S5: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ad**

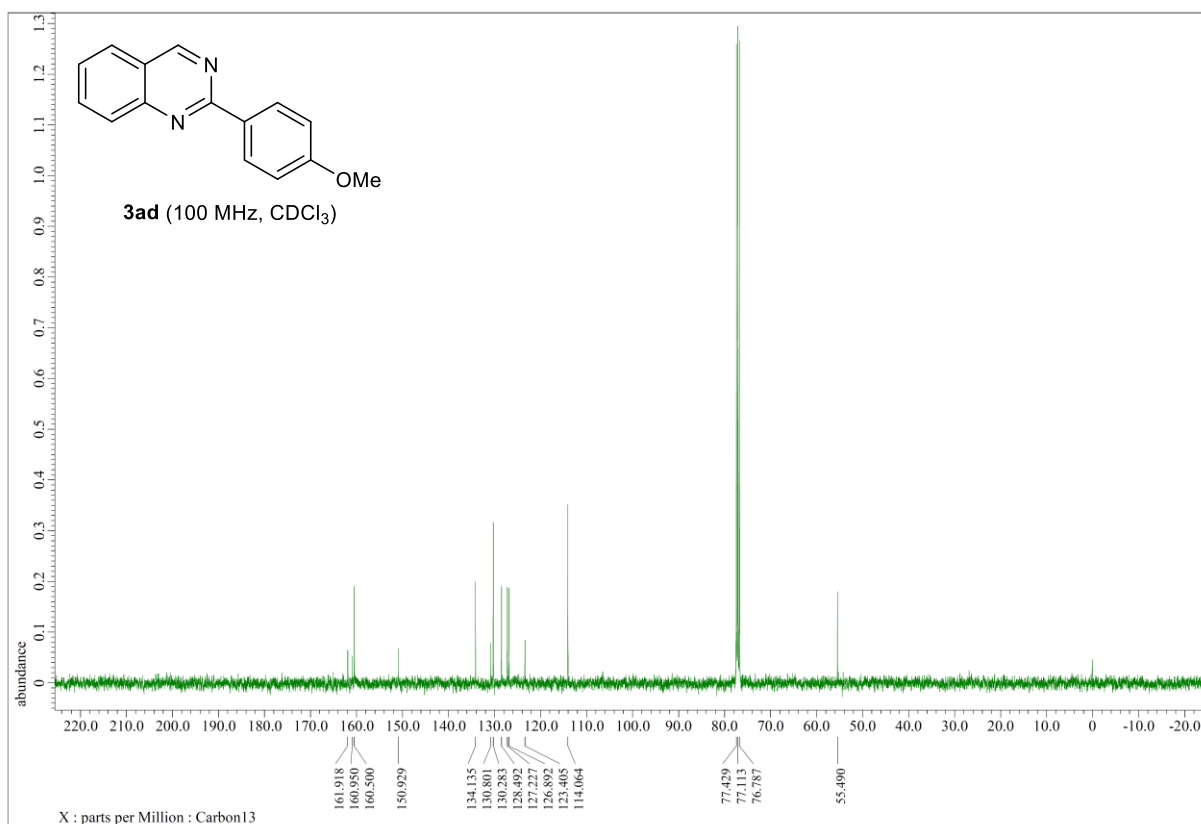
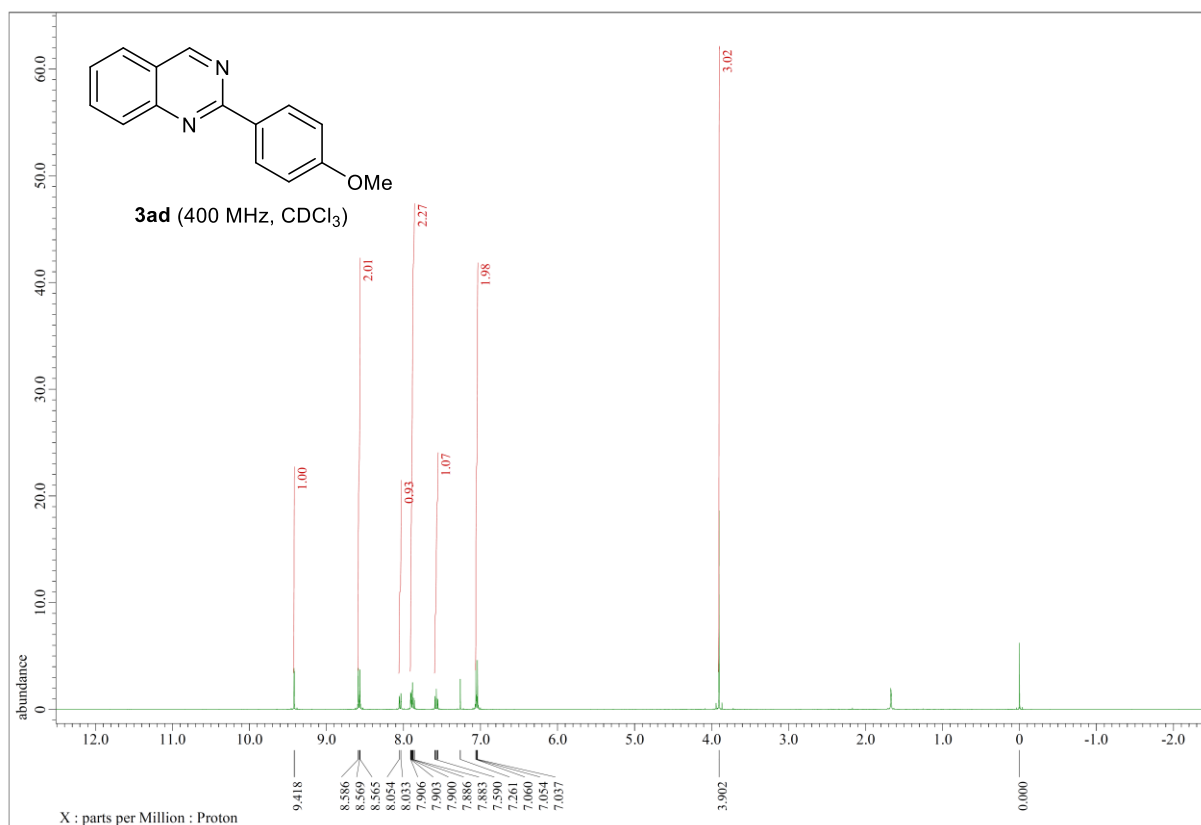


Figure S6: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ae**

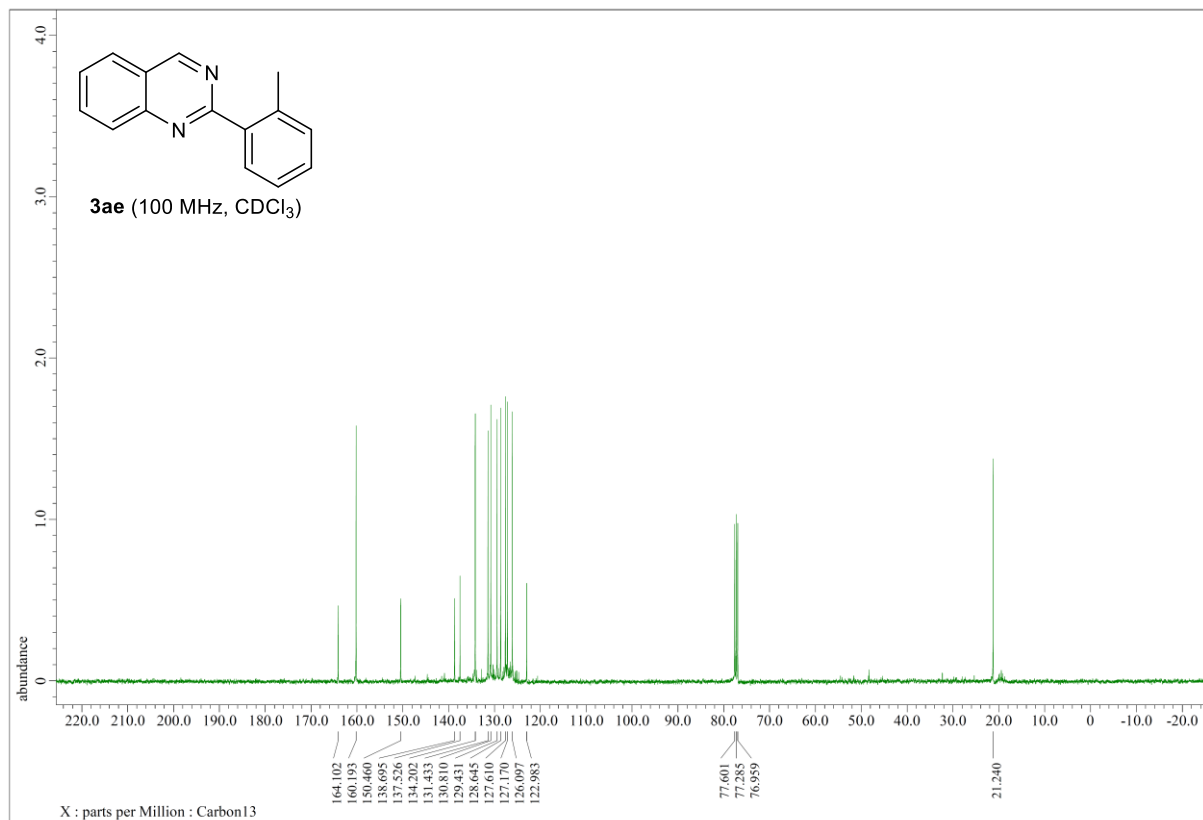
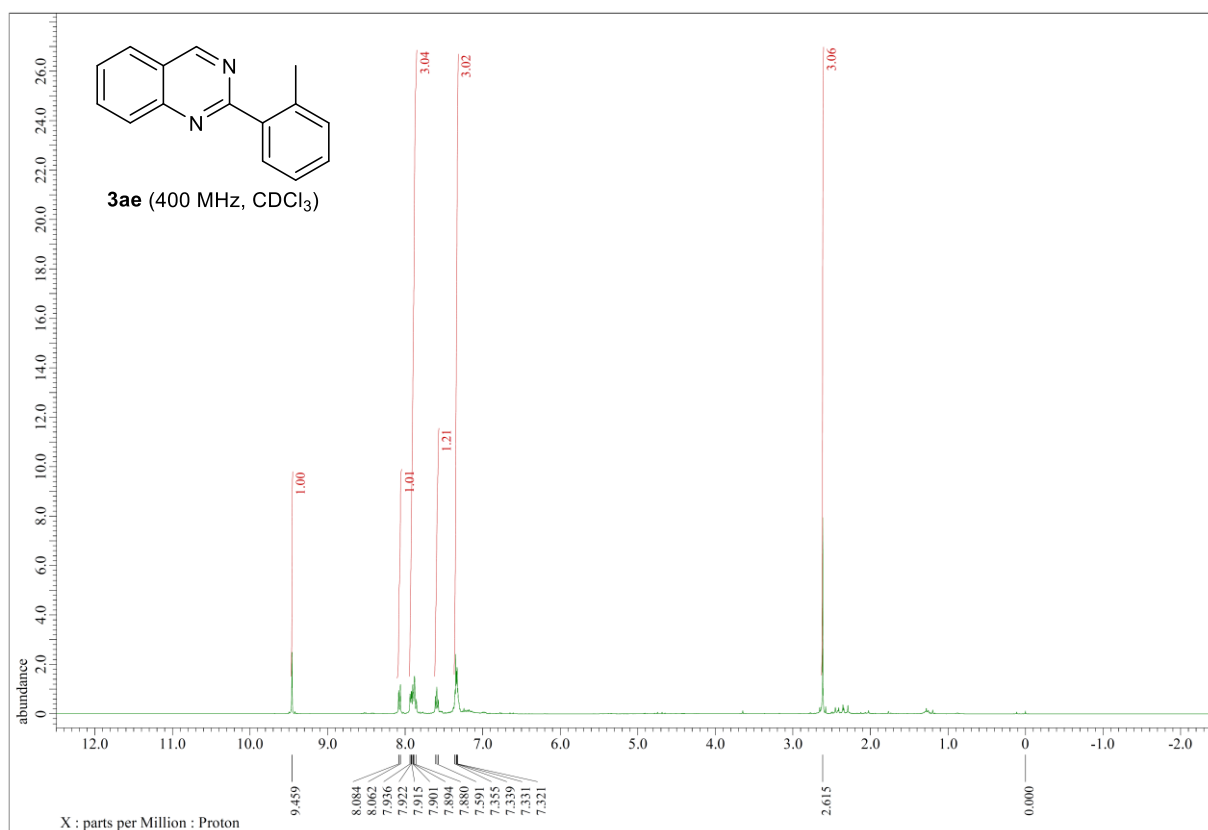


Figure S7: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3af**

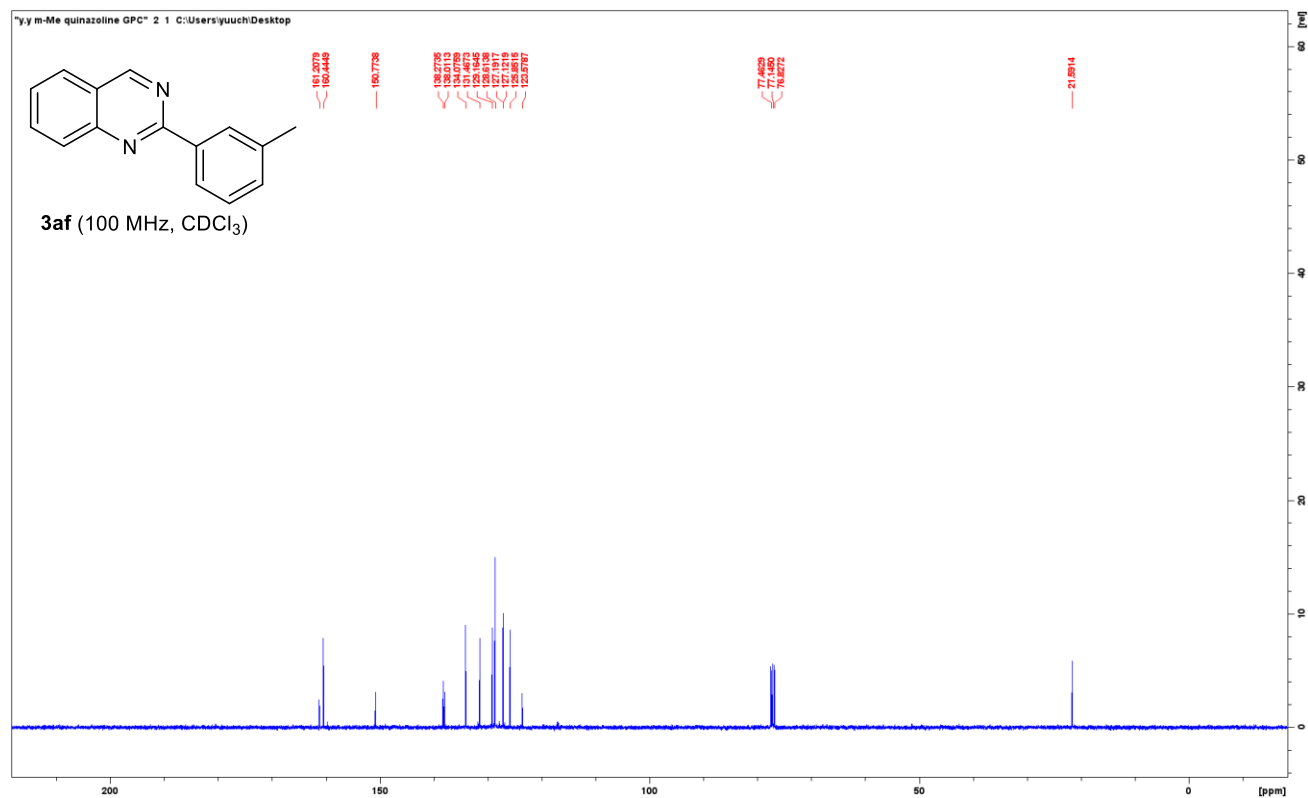
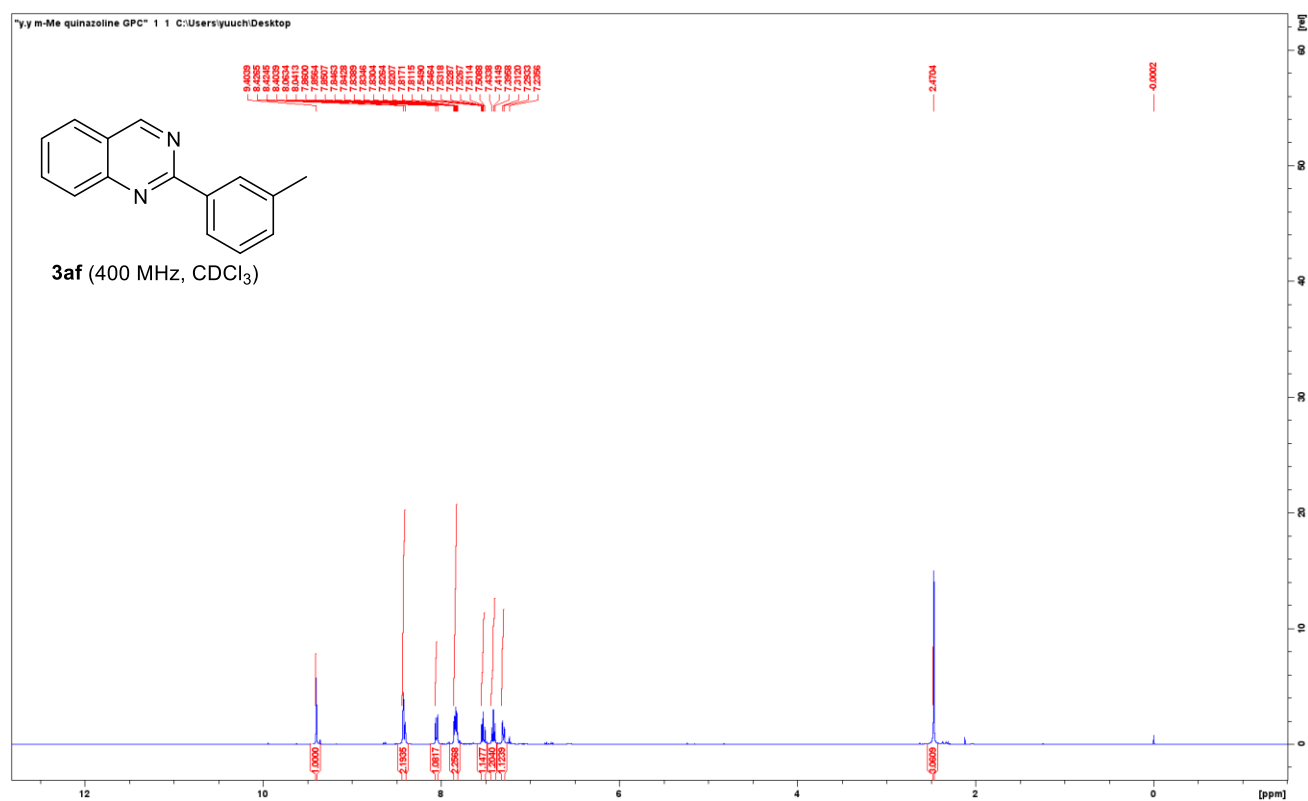


Figure S8: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ag**

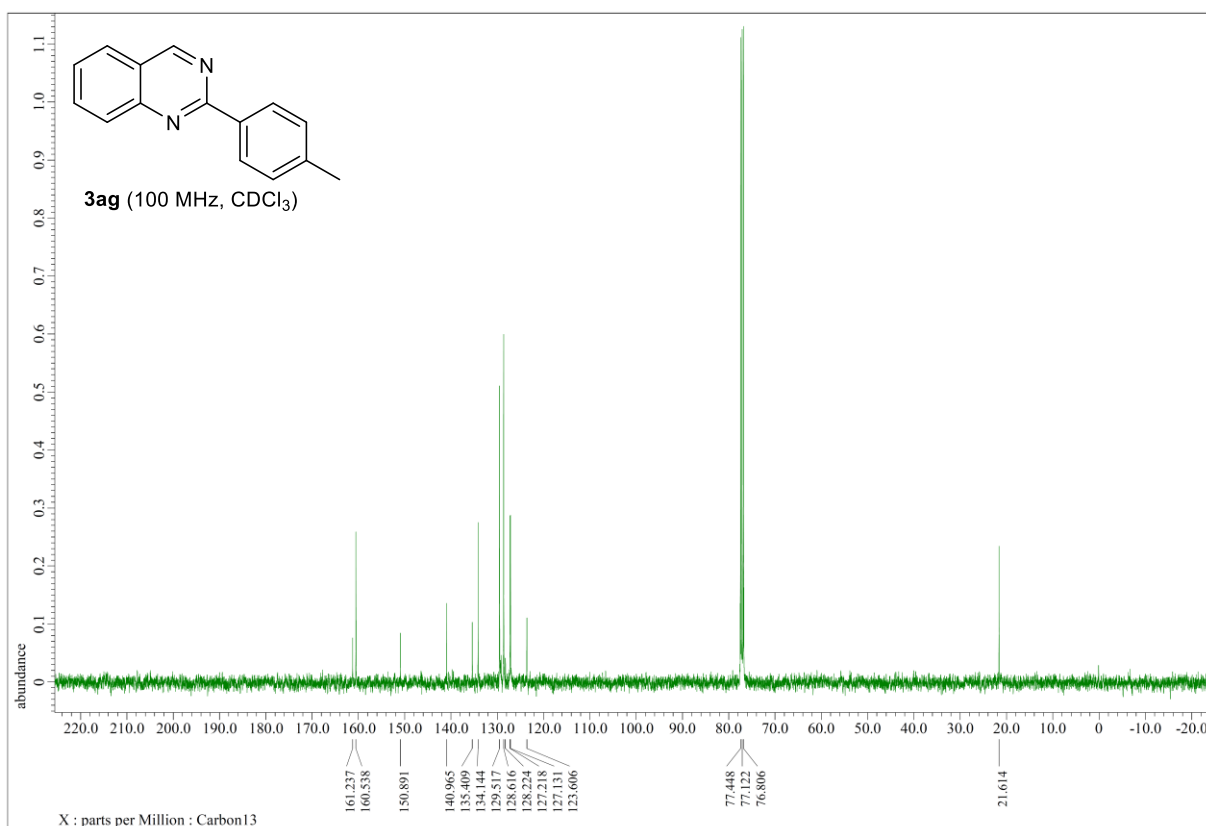
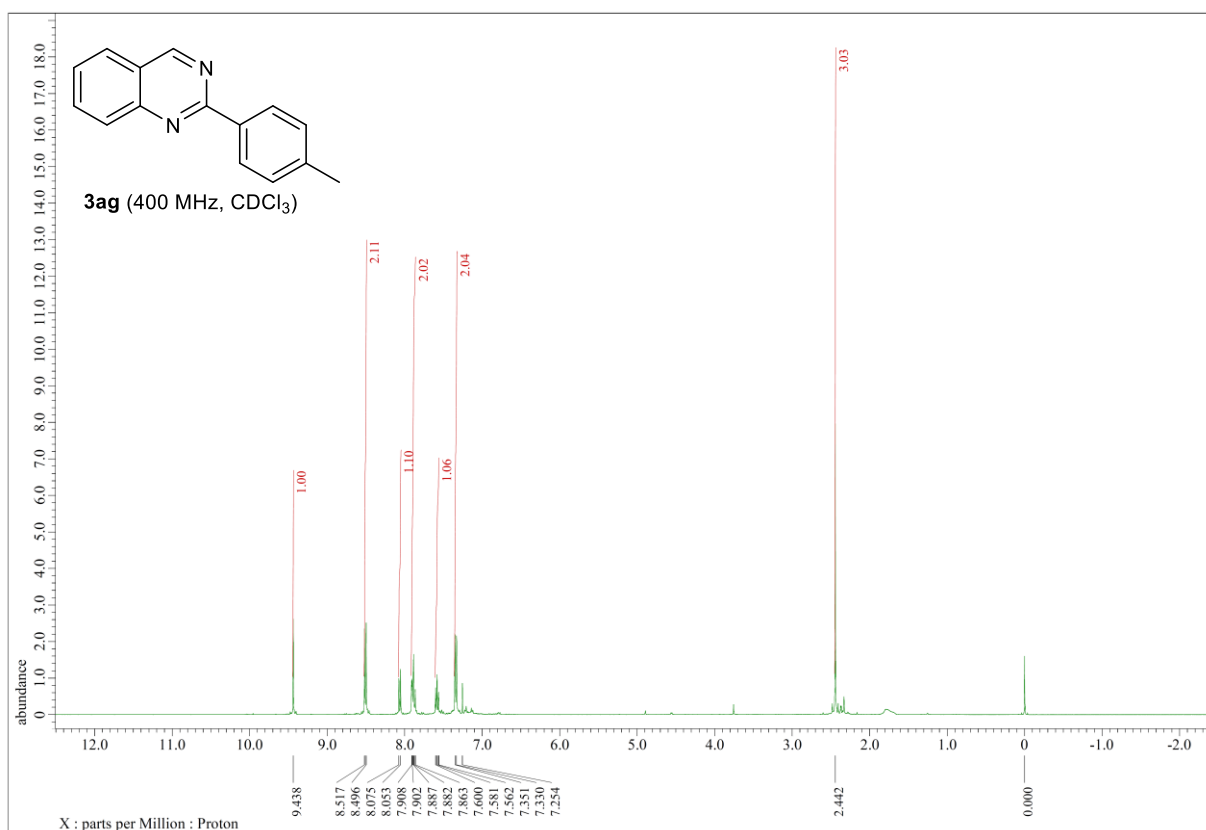


Figure S9: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ah**

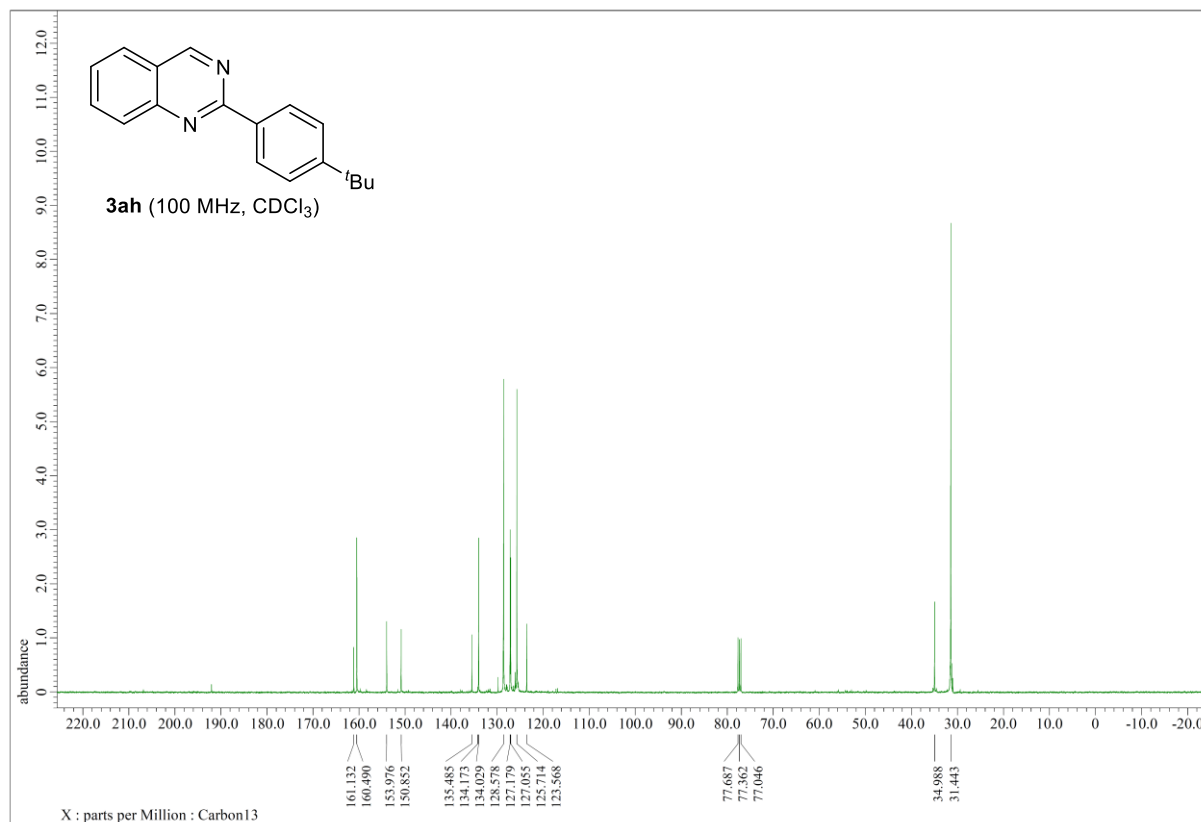
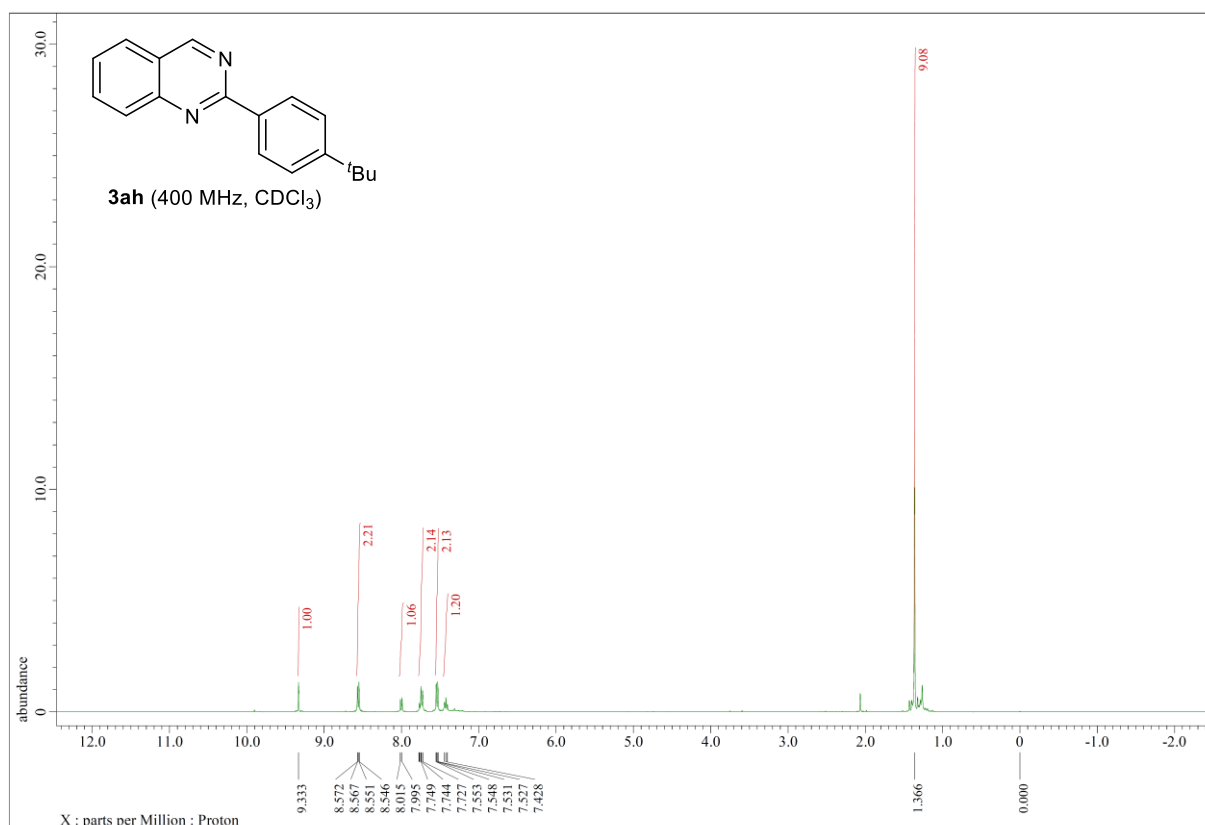


Figure S10: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3aj**

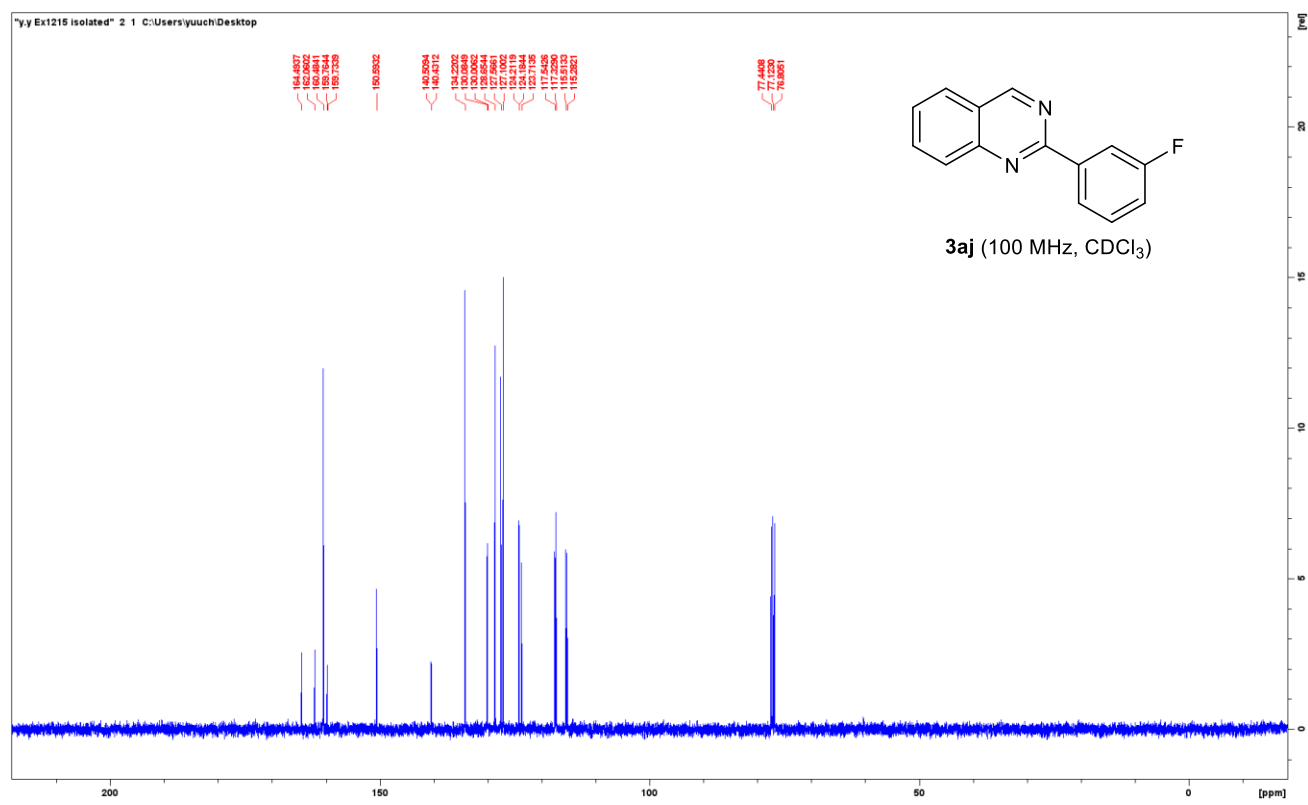
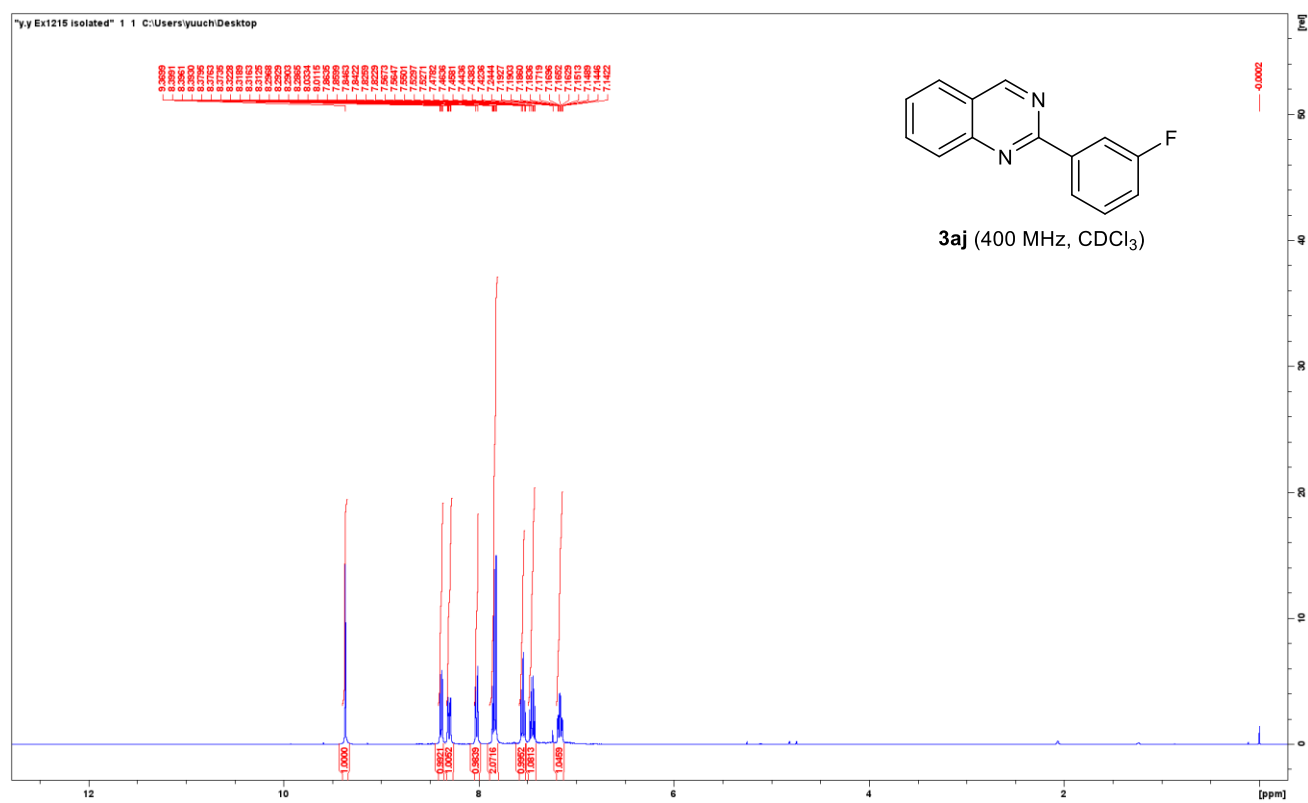


Figure S11: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ak**

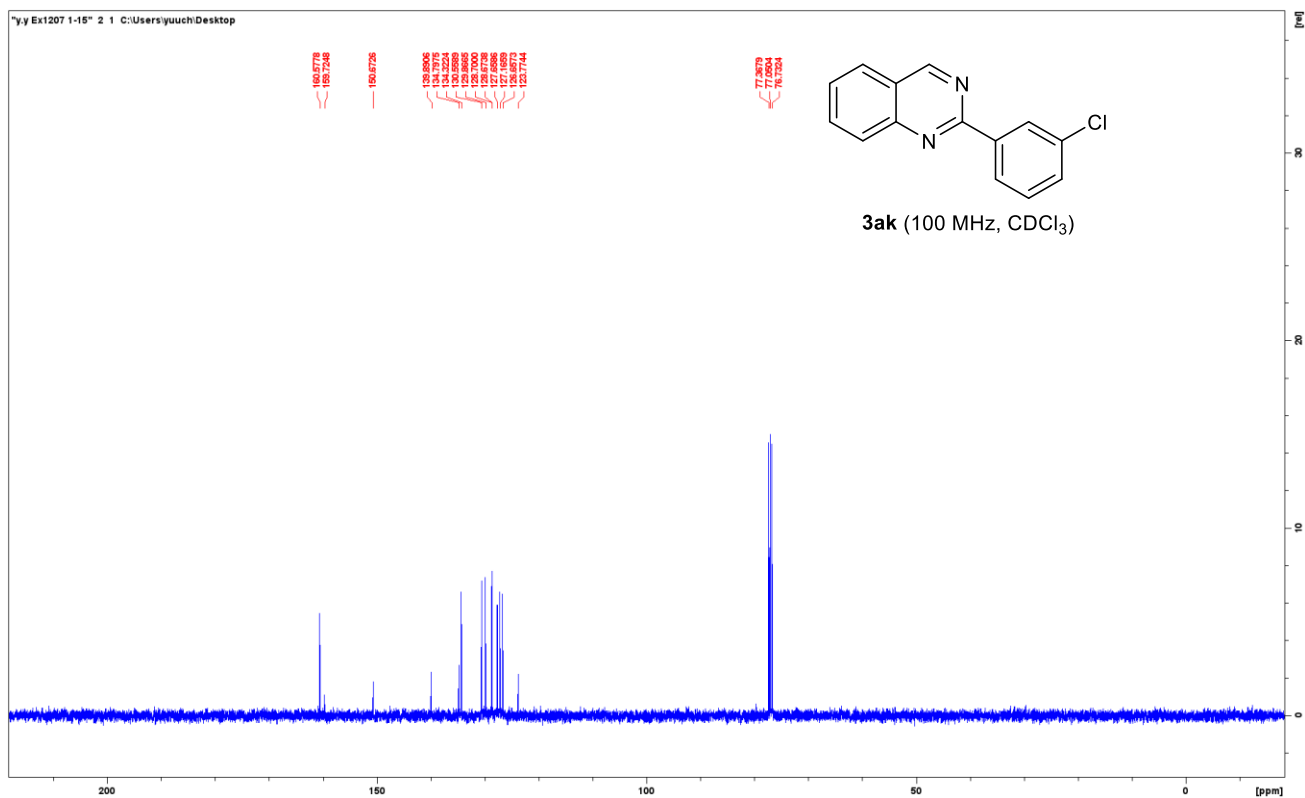
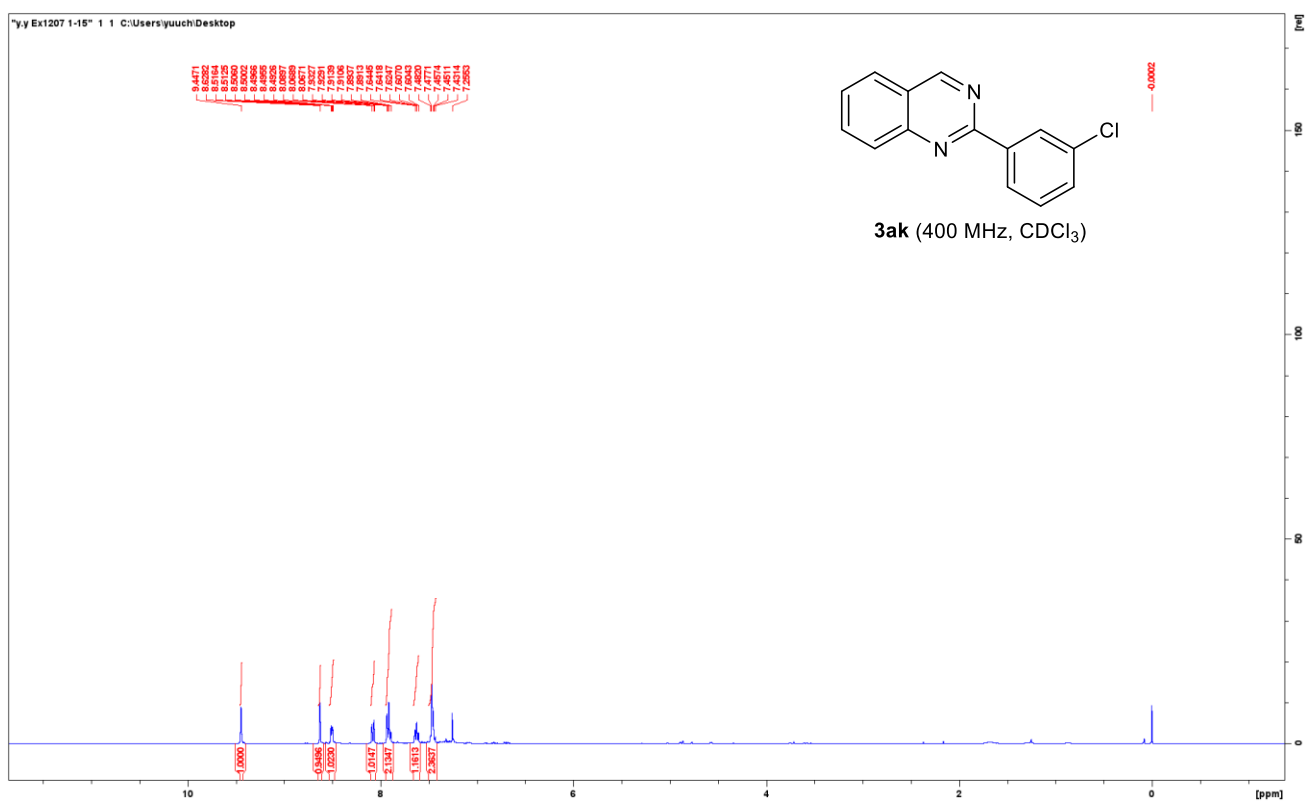


Figure S12: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3aI**

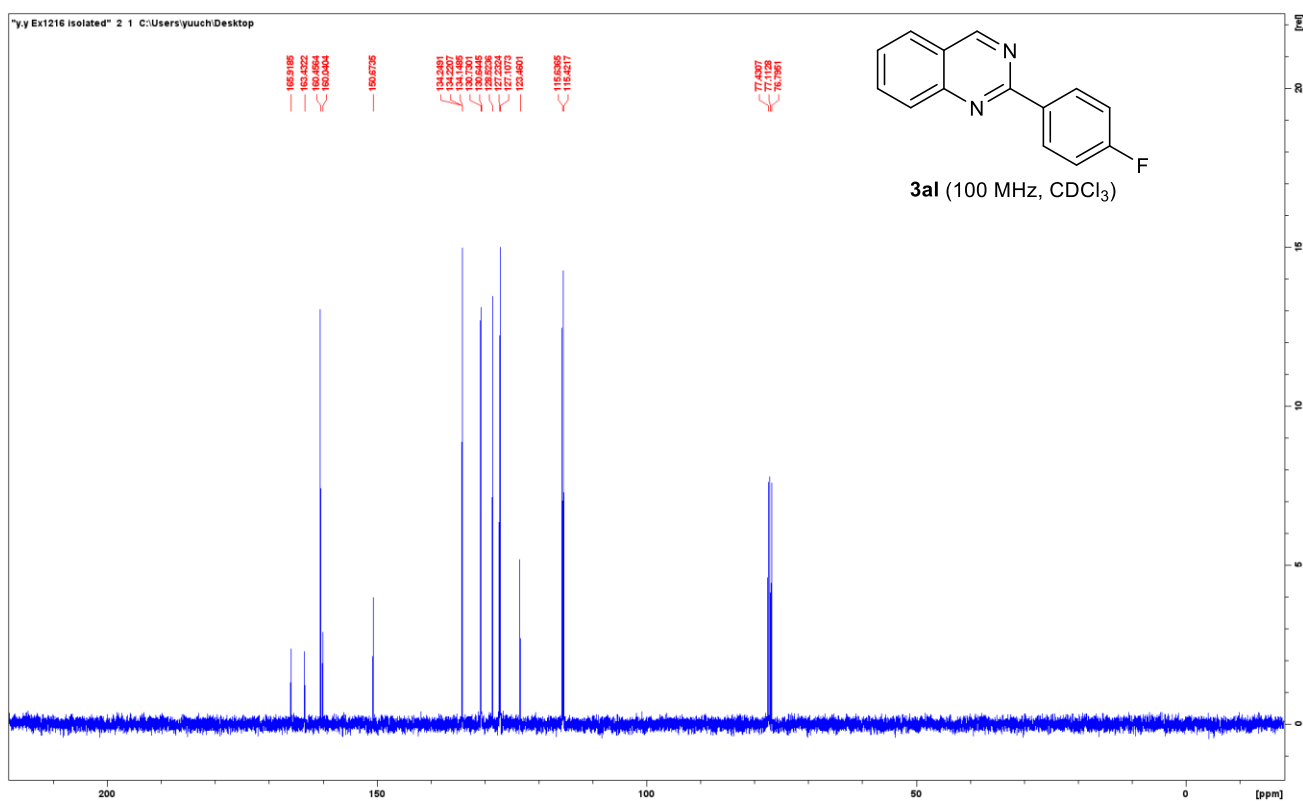
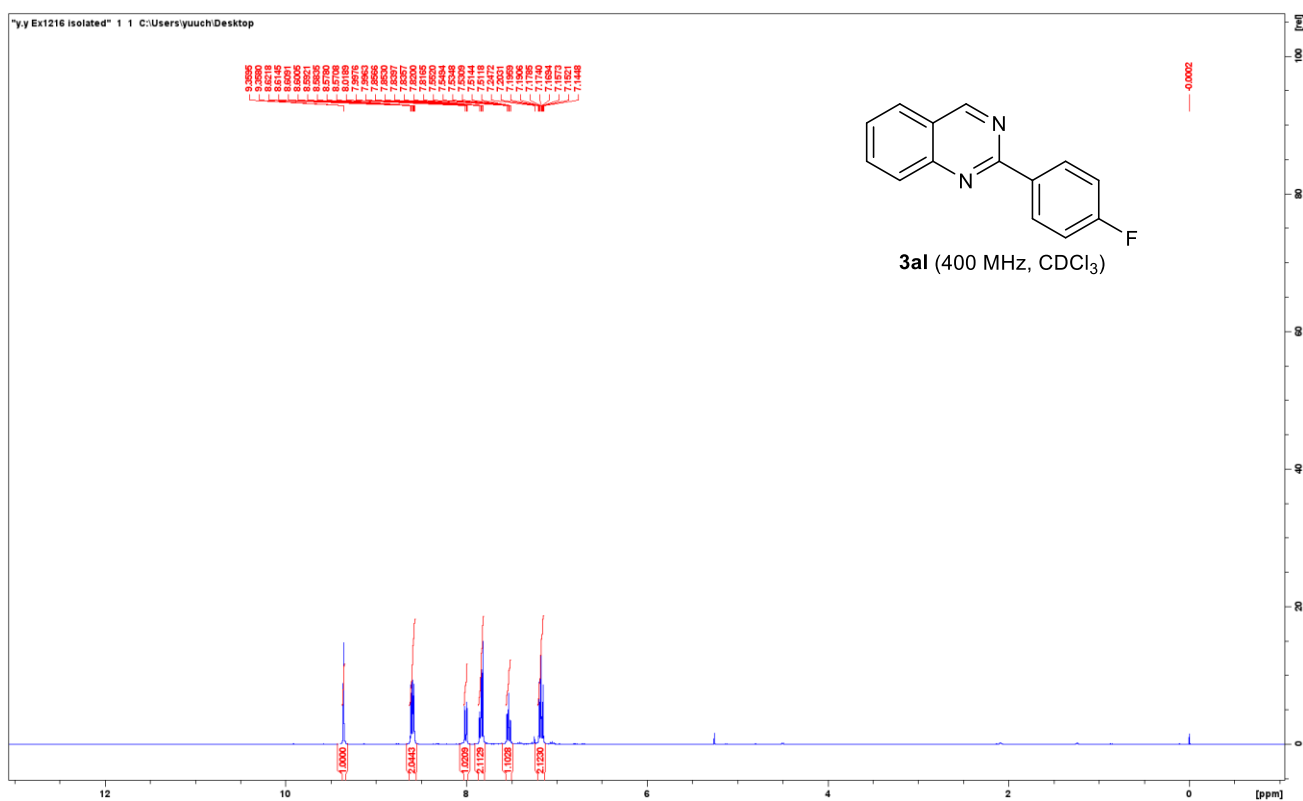


Figure S13: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3am**

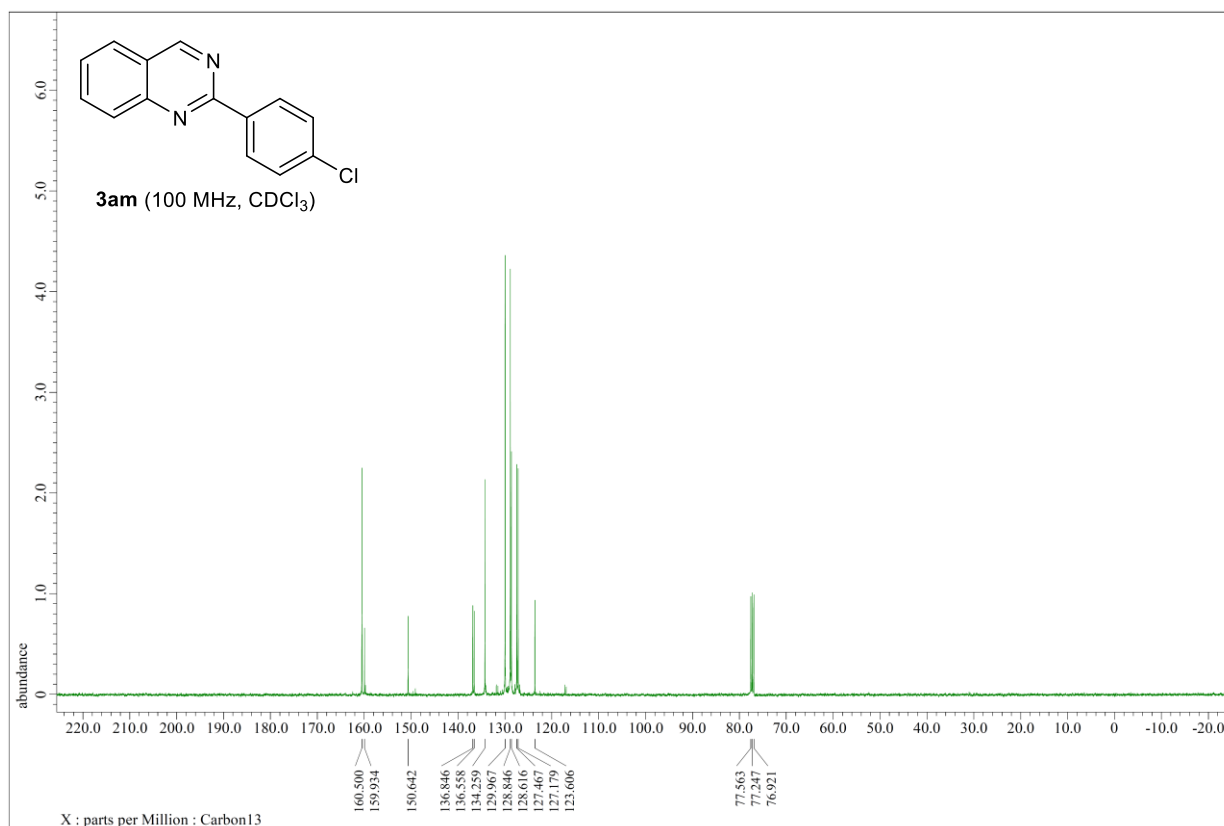
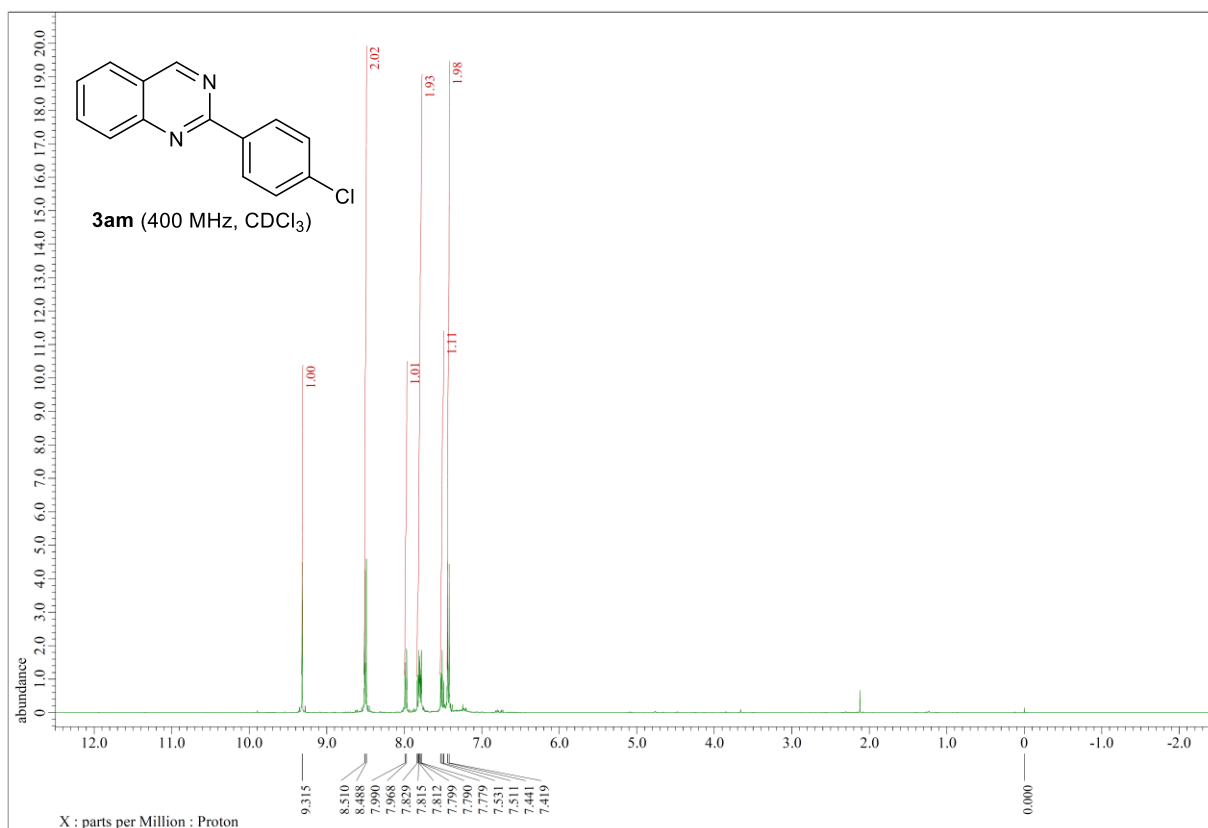


Figure S14: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3an**

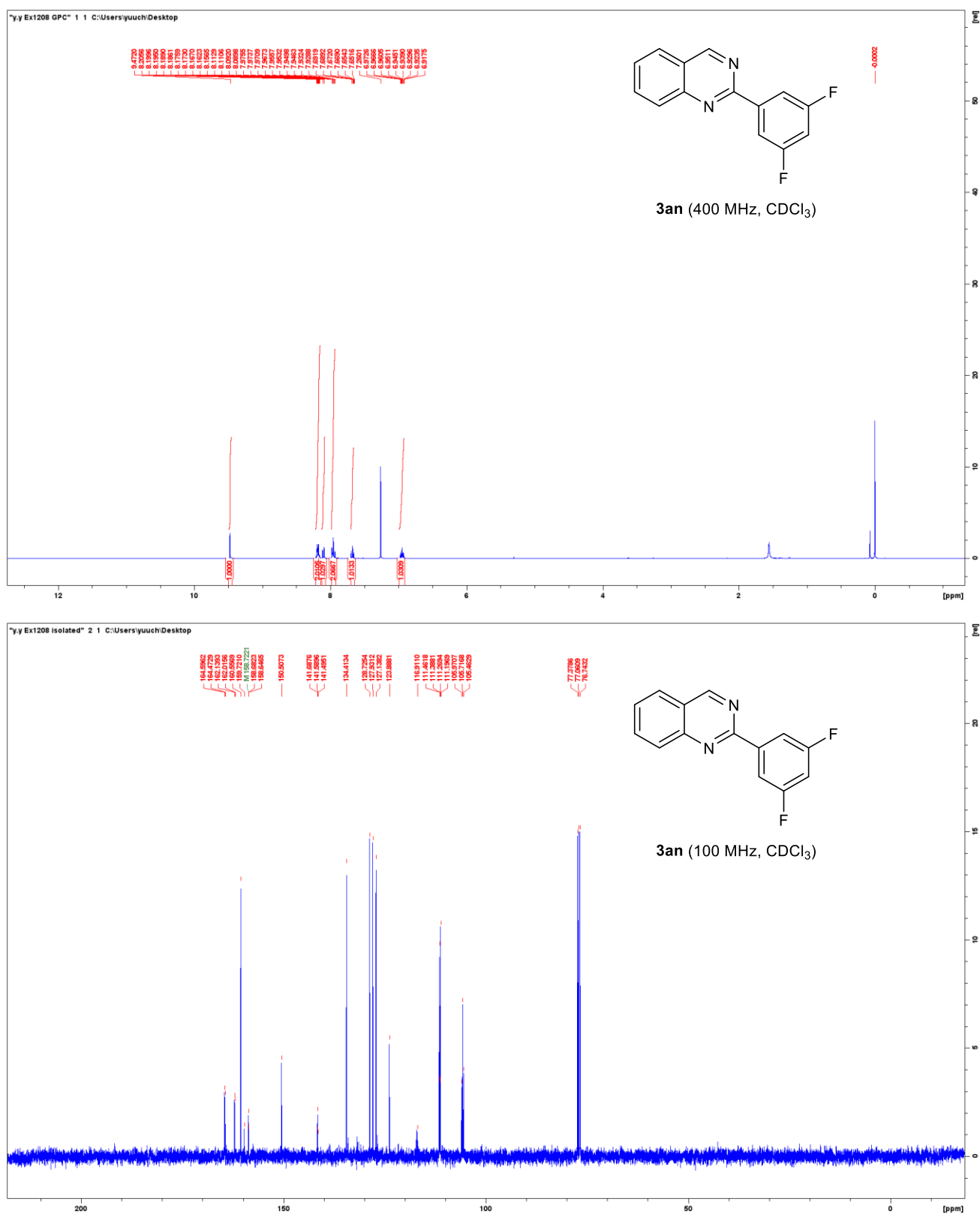


Figure S15: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ao**

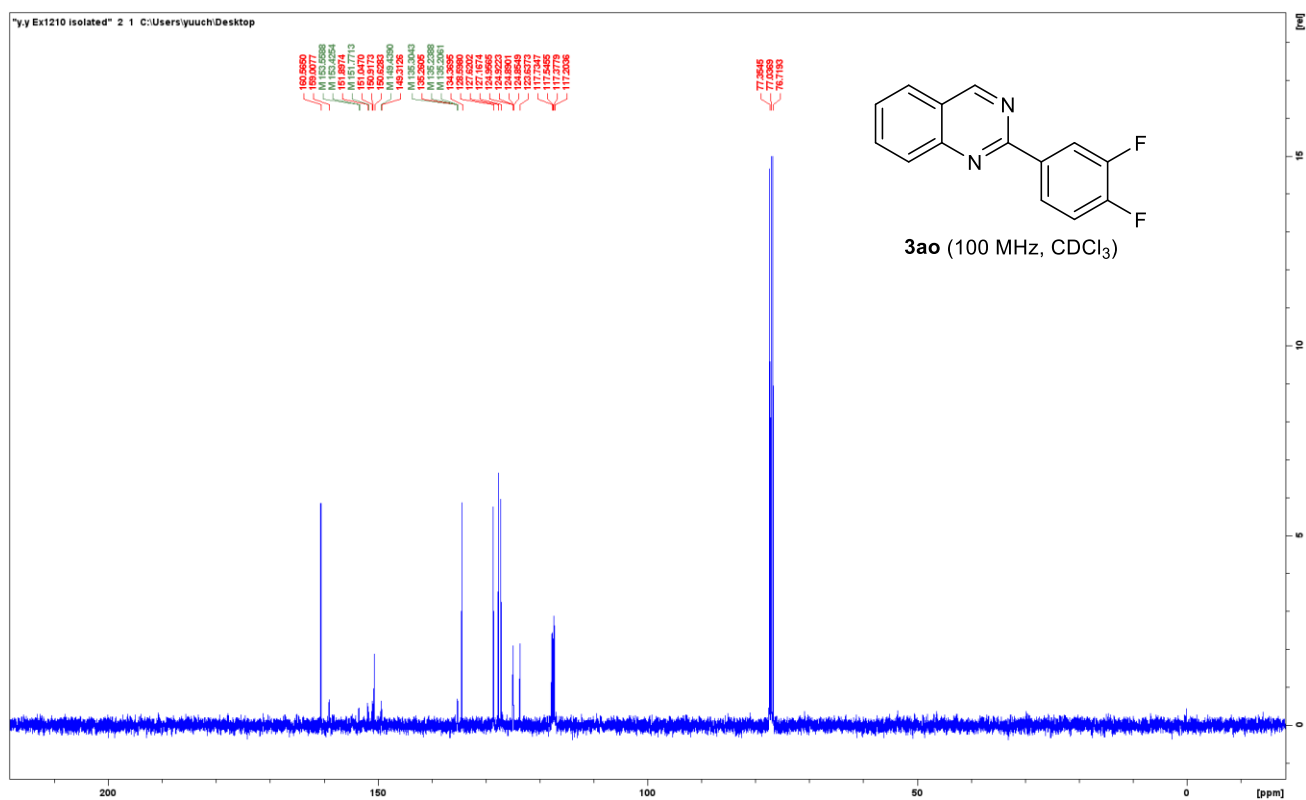
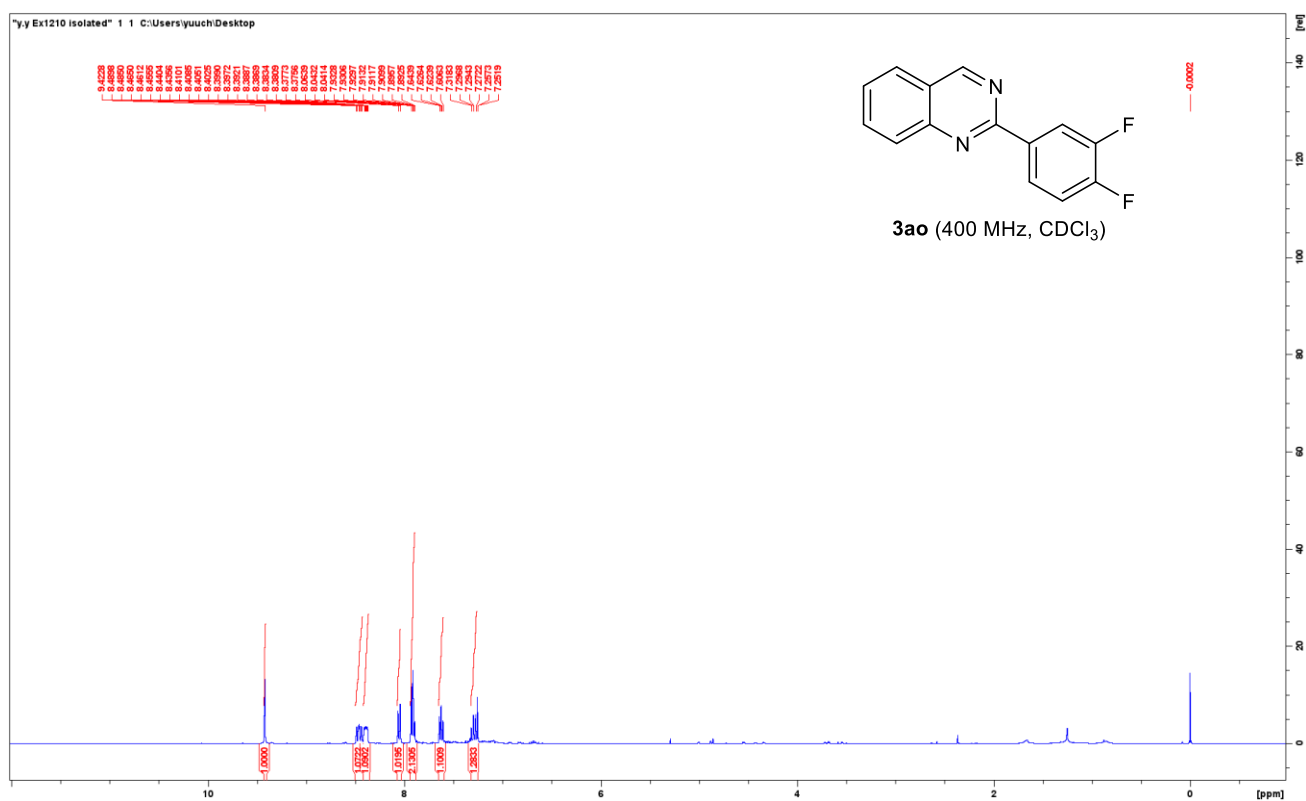


Figure S16: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ap**

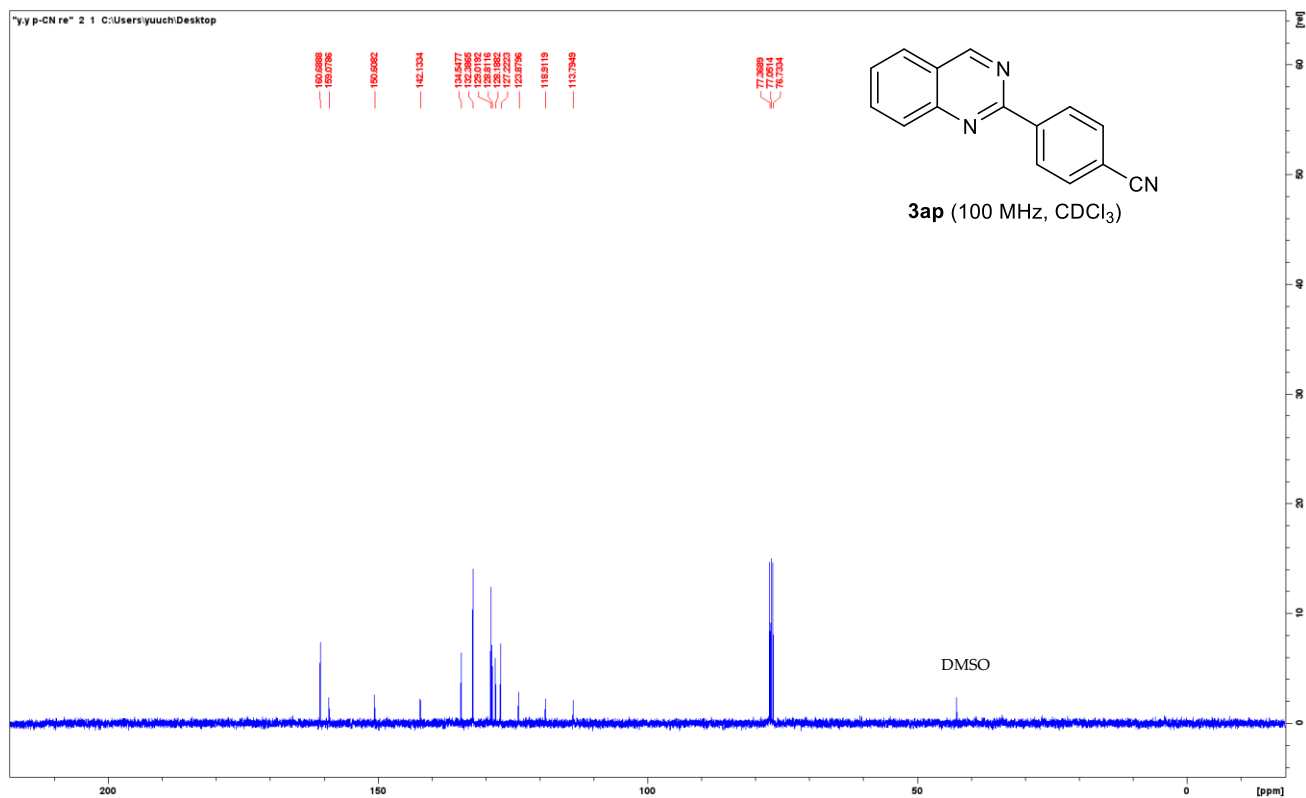
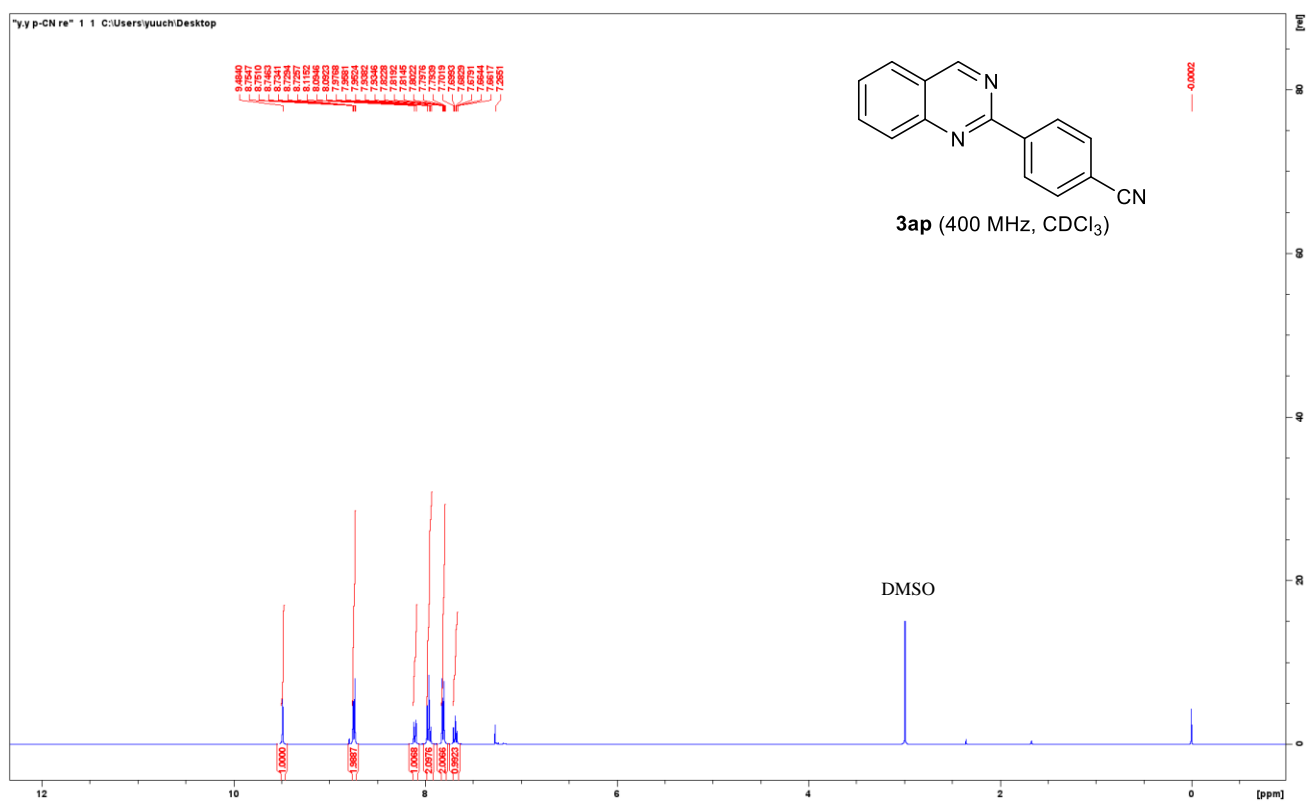


Figure S17: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3aq**

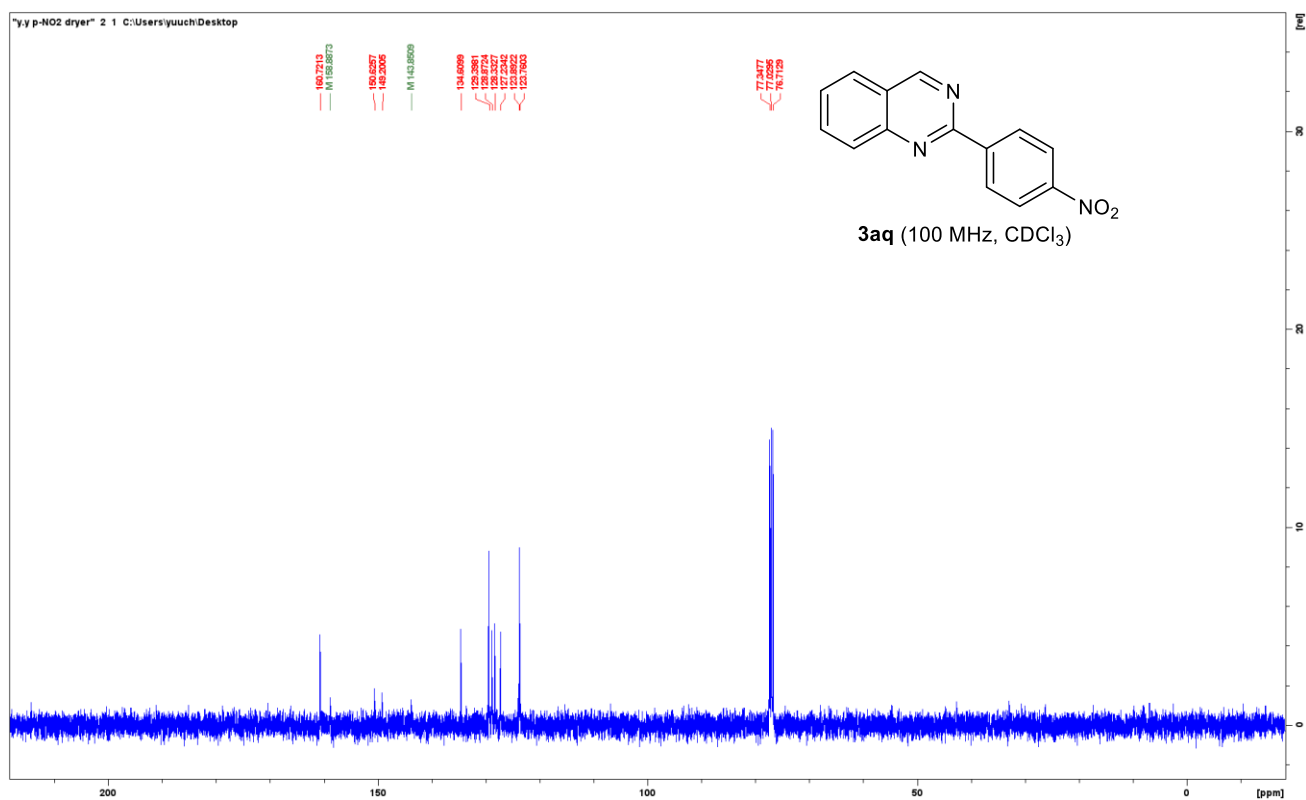
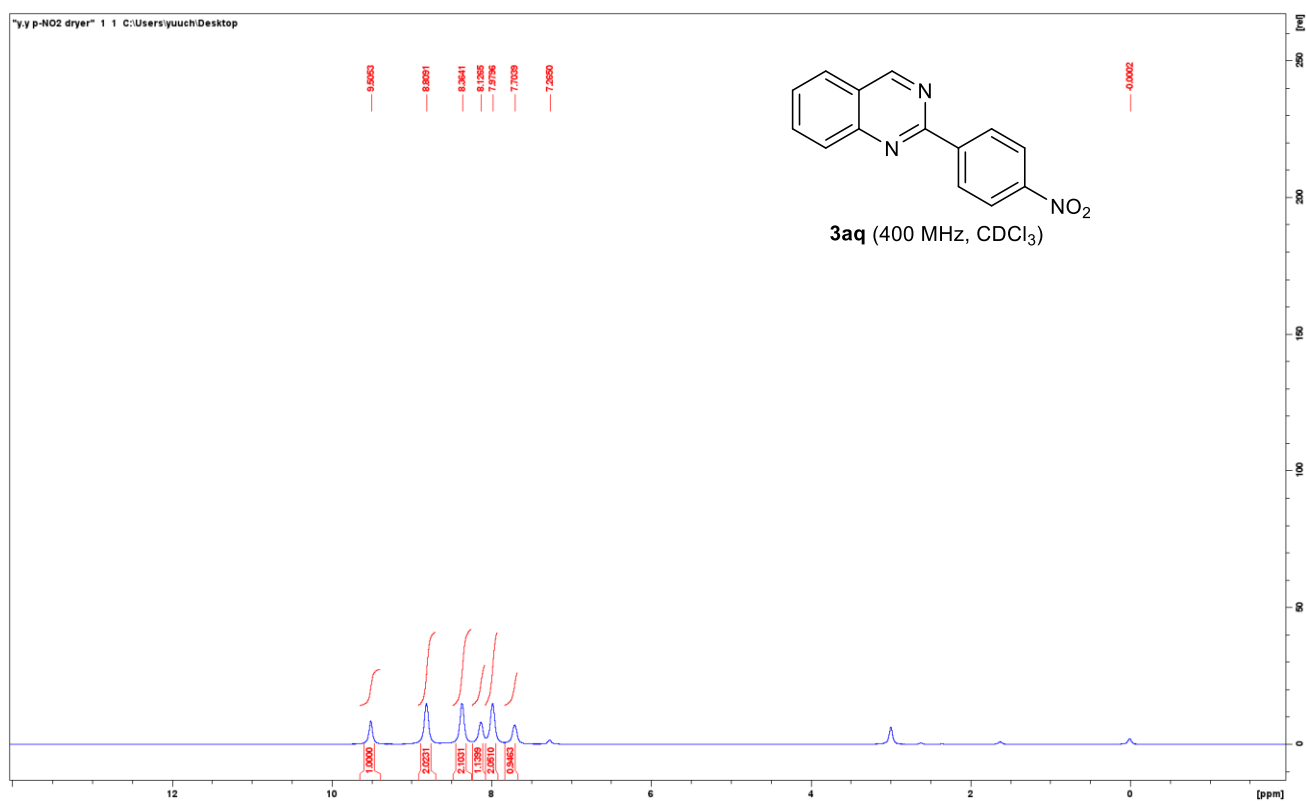


Figure S18: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ar**

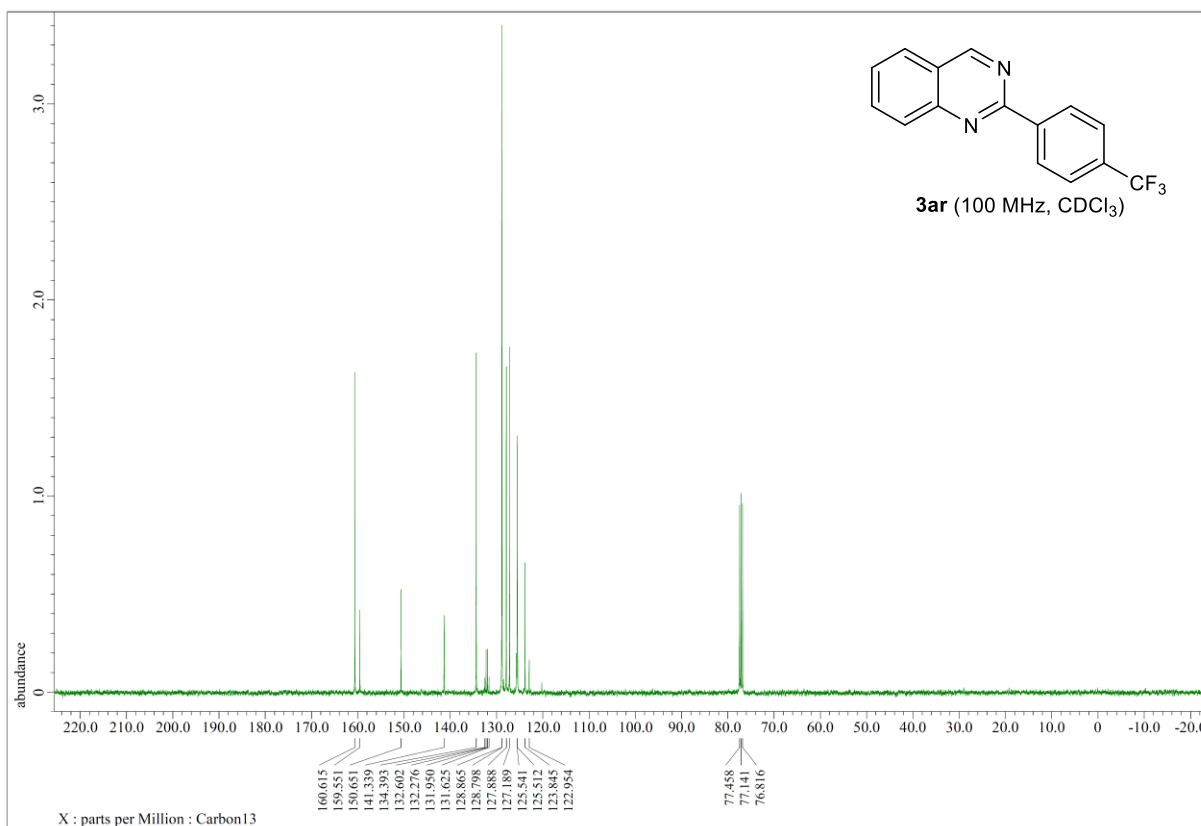
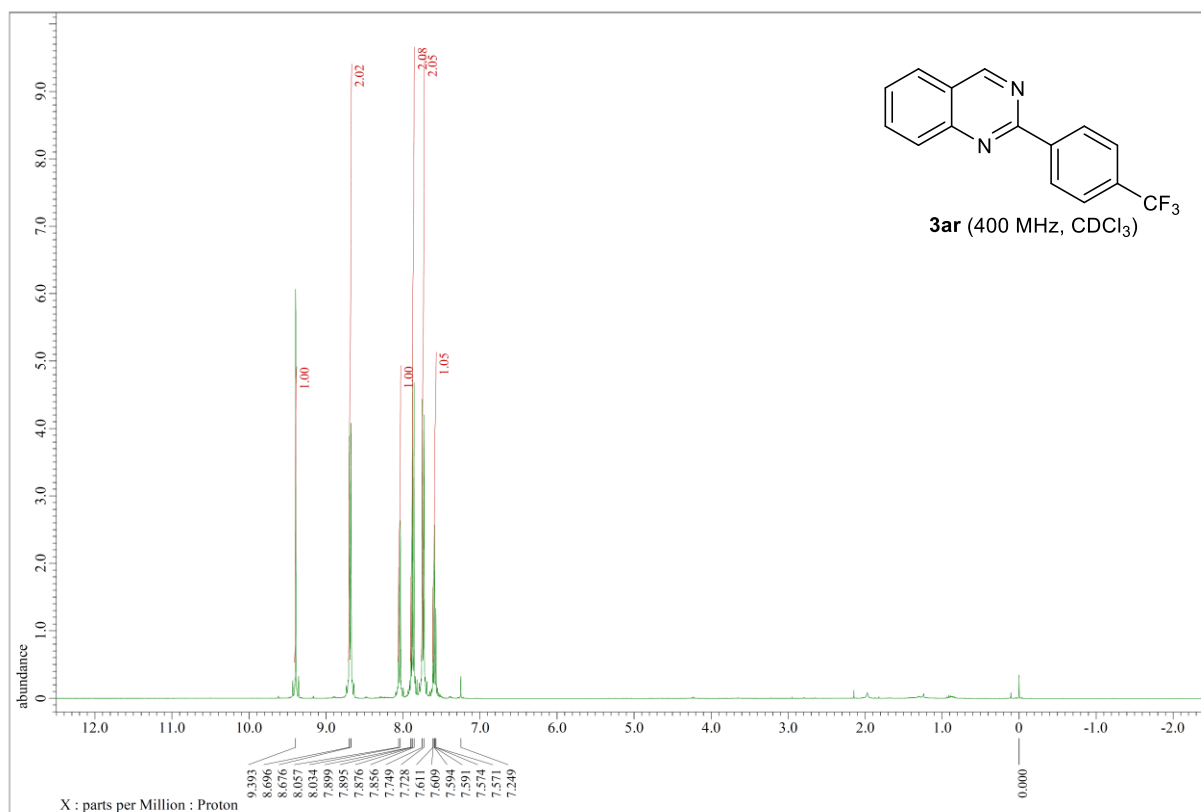


Figure S19: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3as**

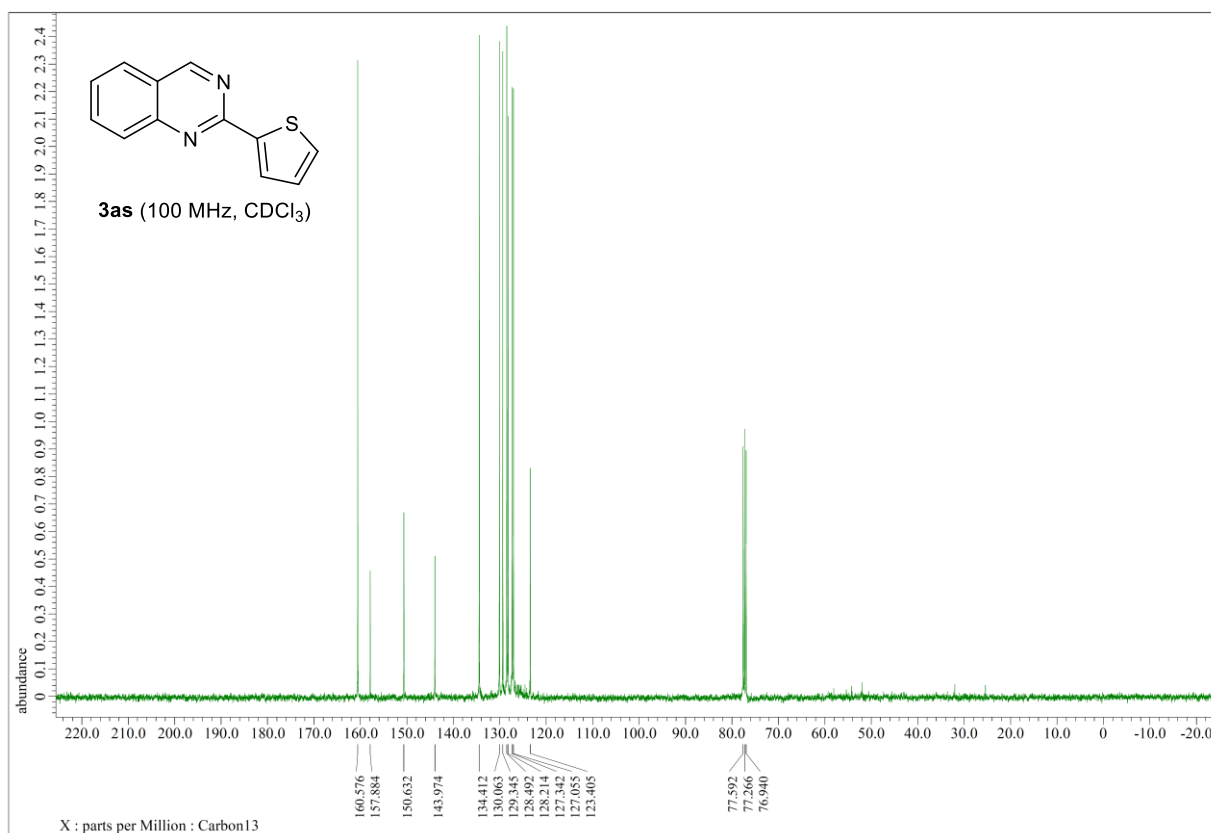
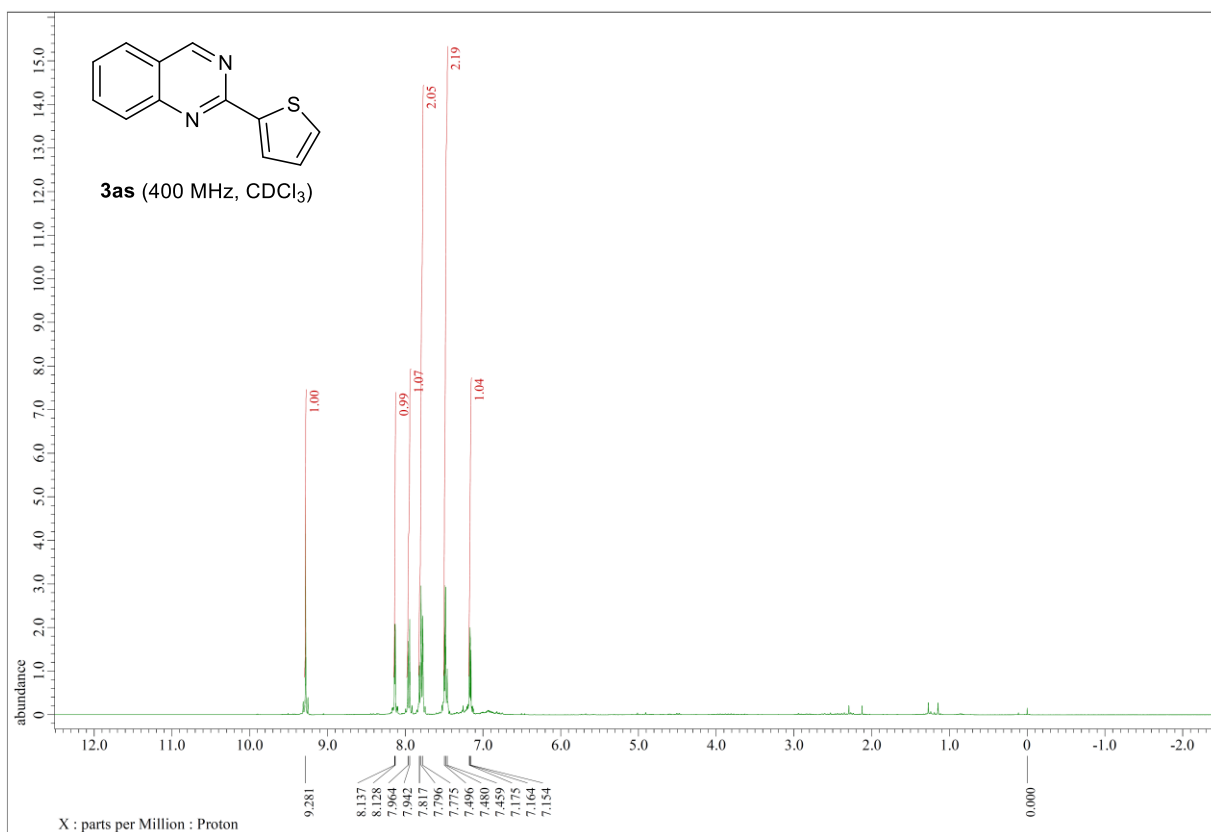


Figure S21: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **3ba**

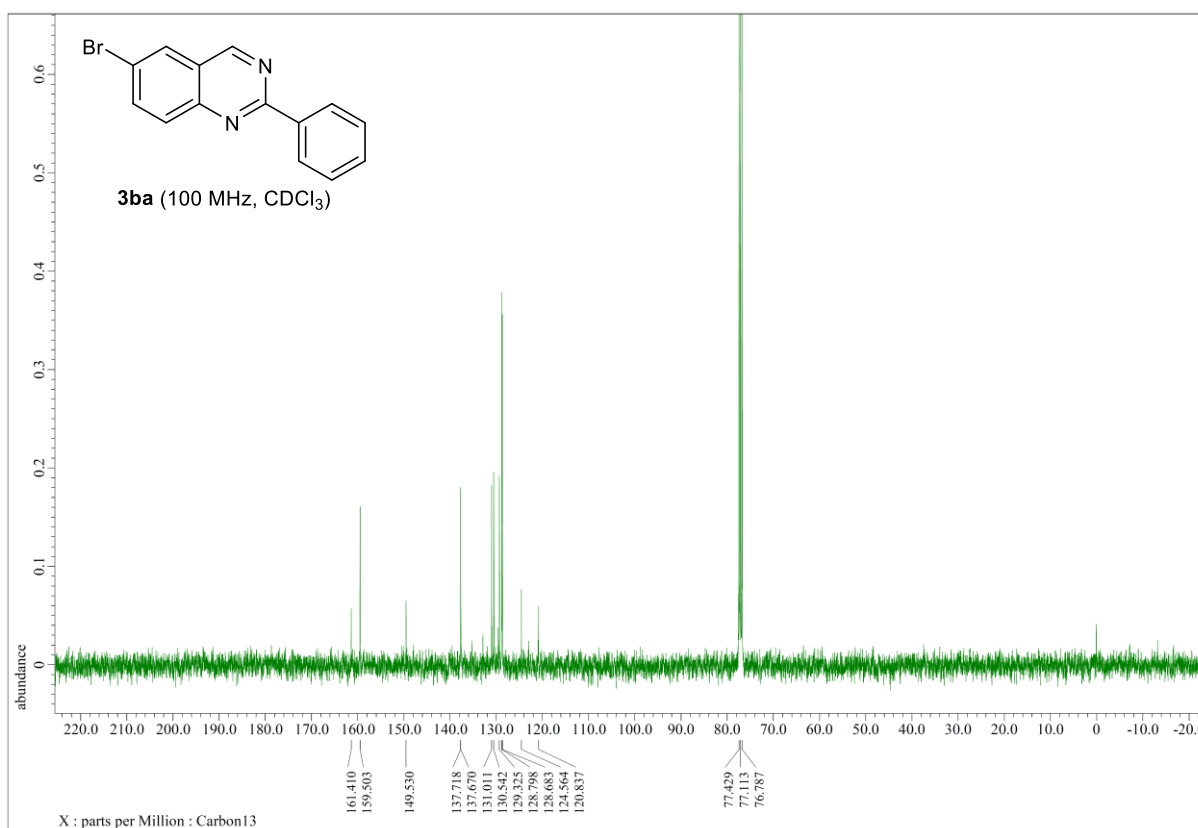
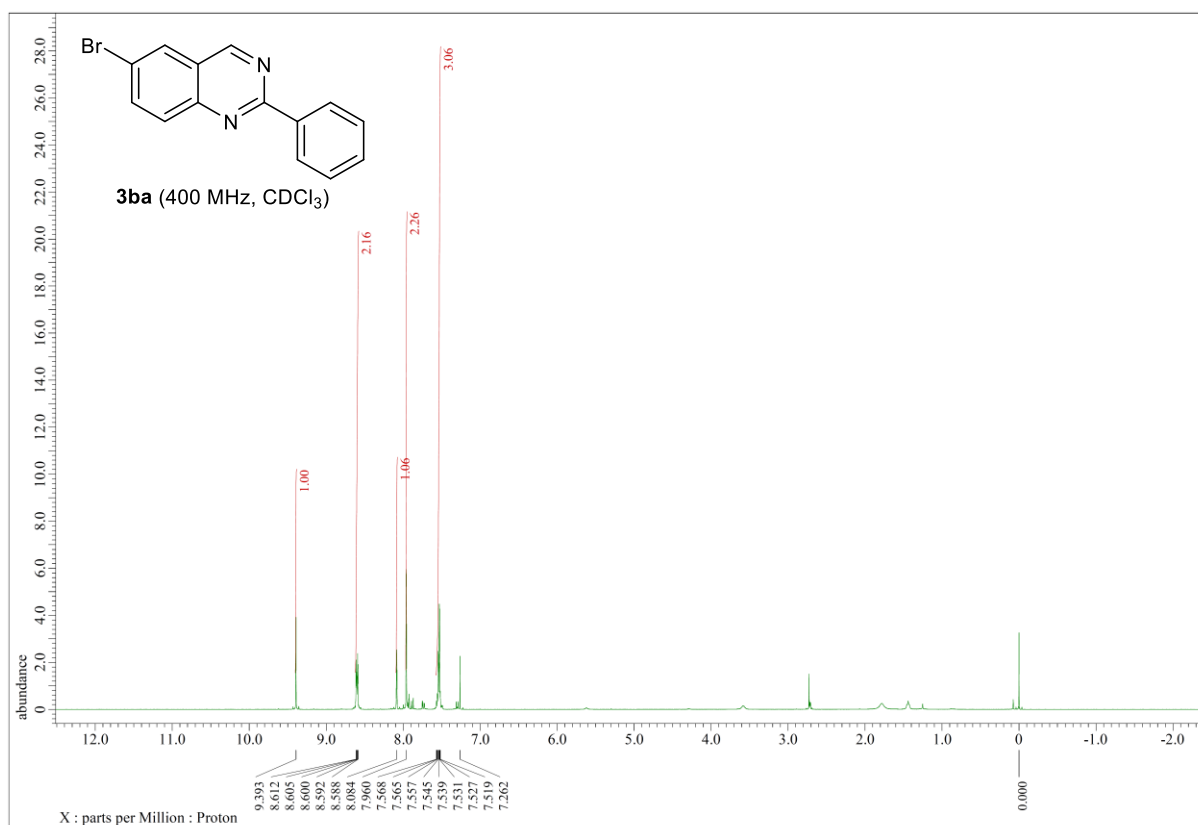


Figure S22: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **4a**

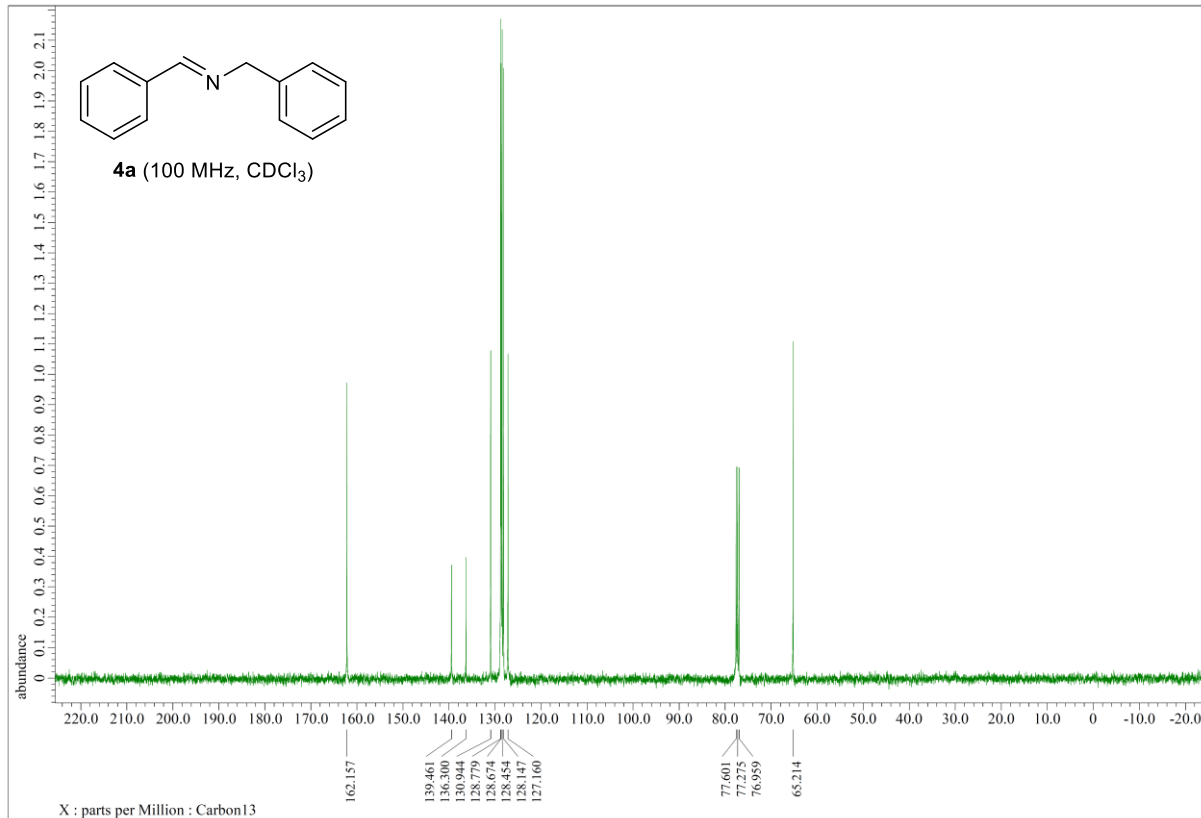
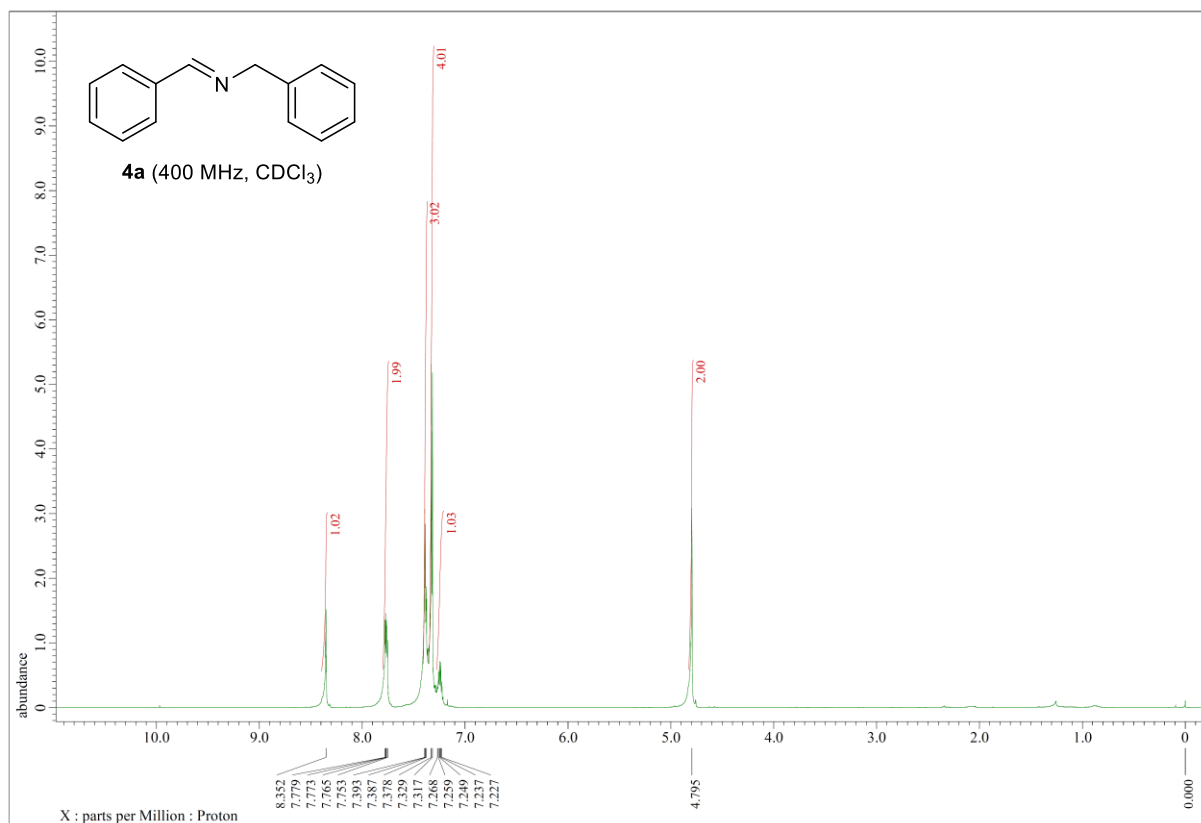


Figure S23: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **4b**

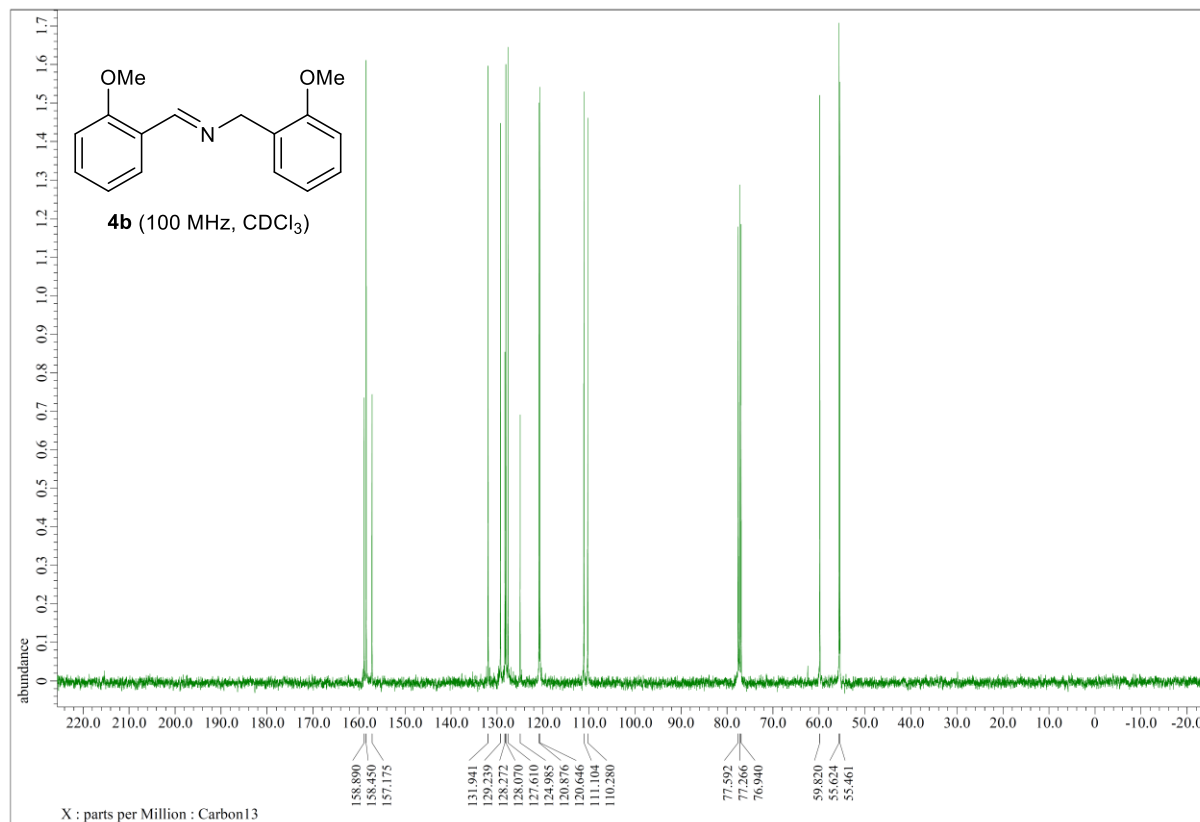
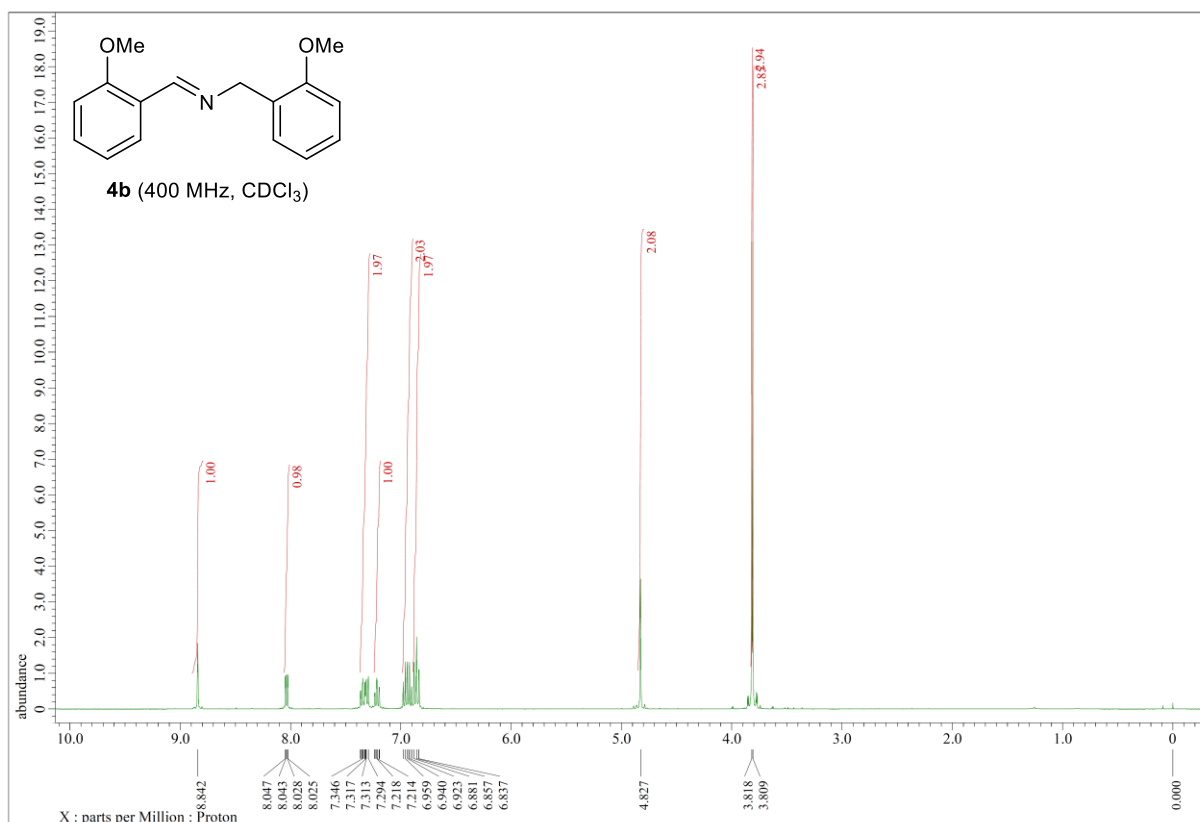


Figure S24: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **4c**

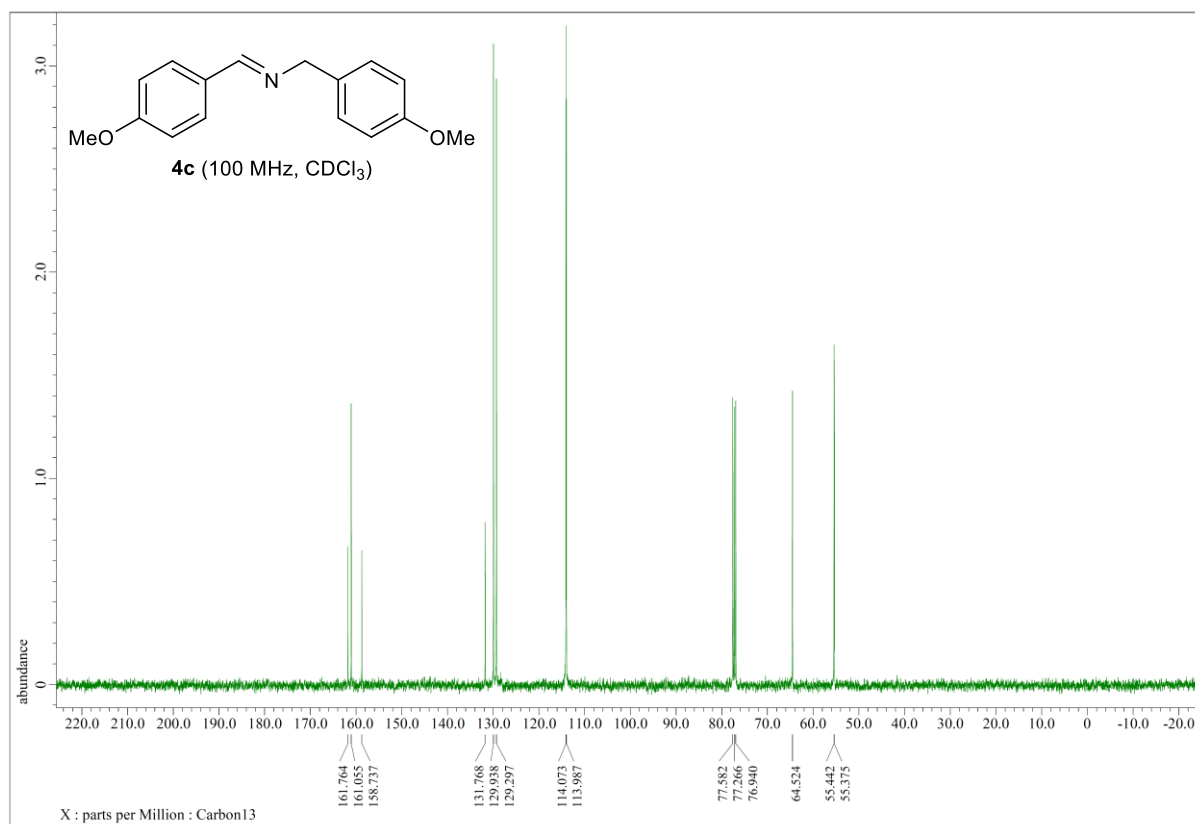
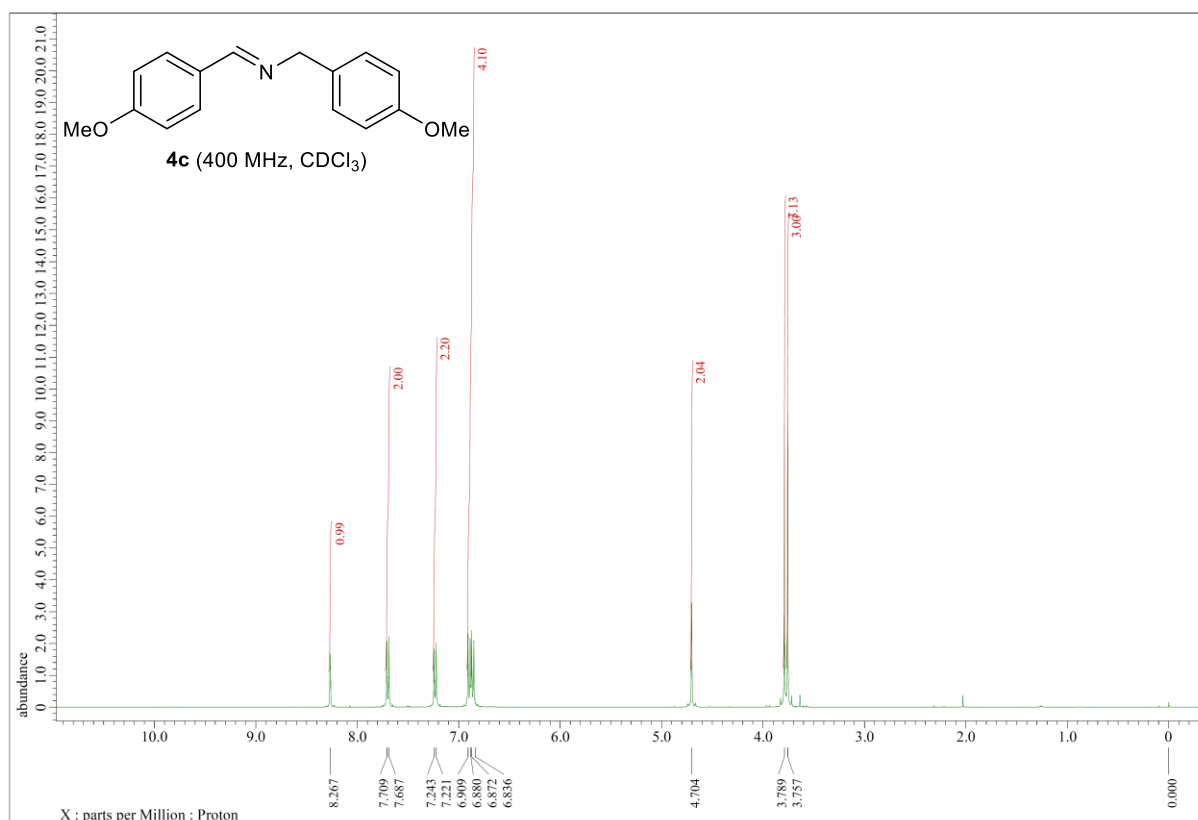


Figure S25: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **4d**

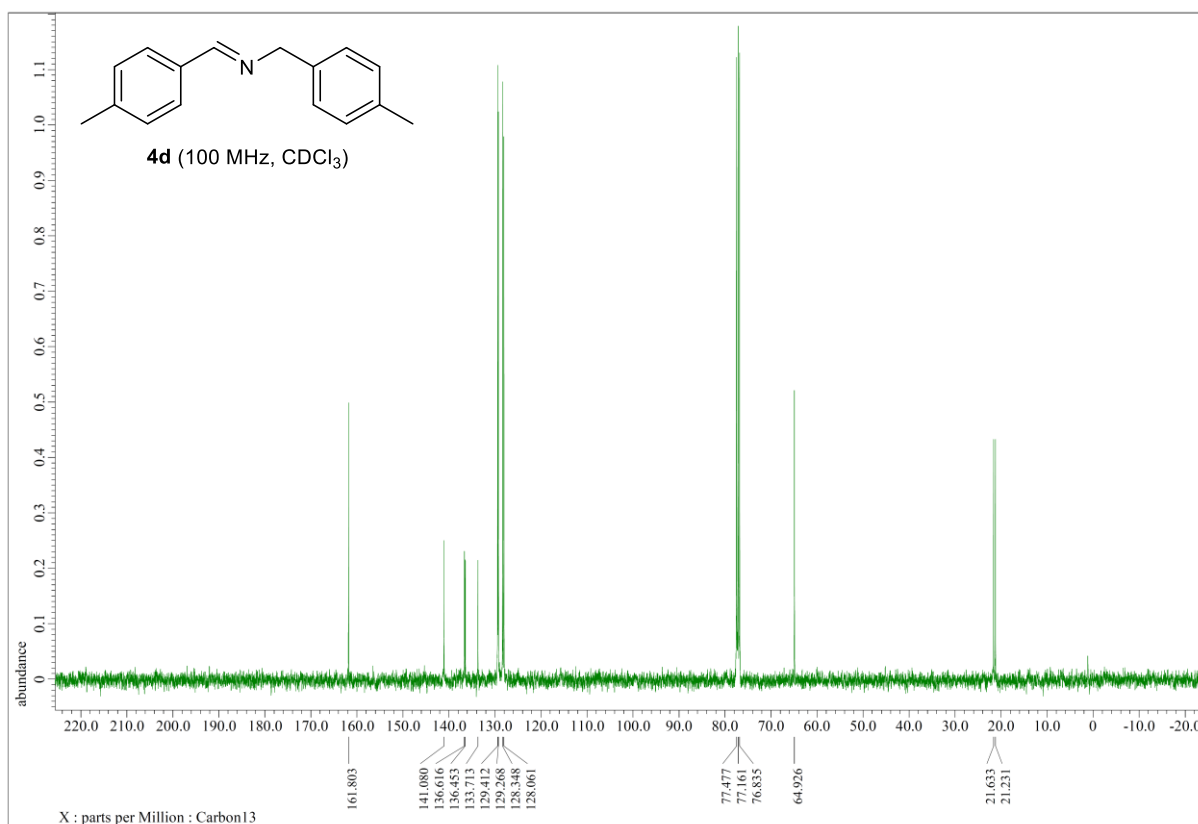
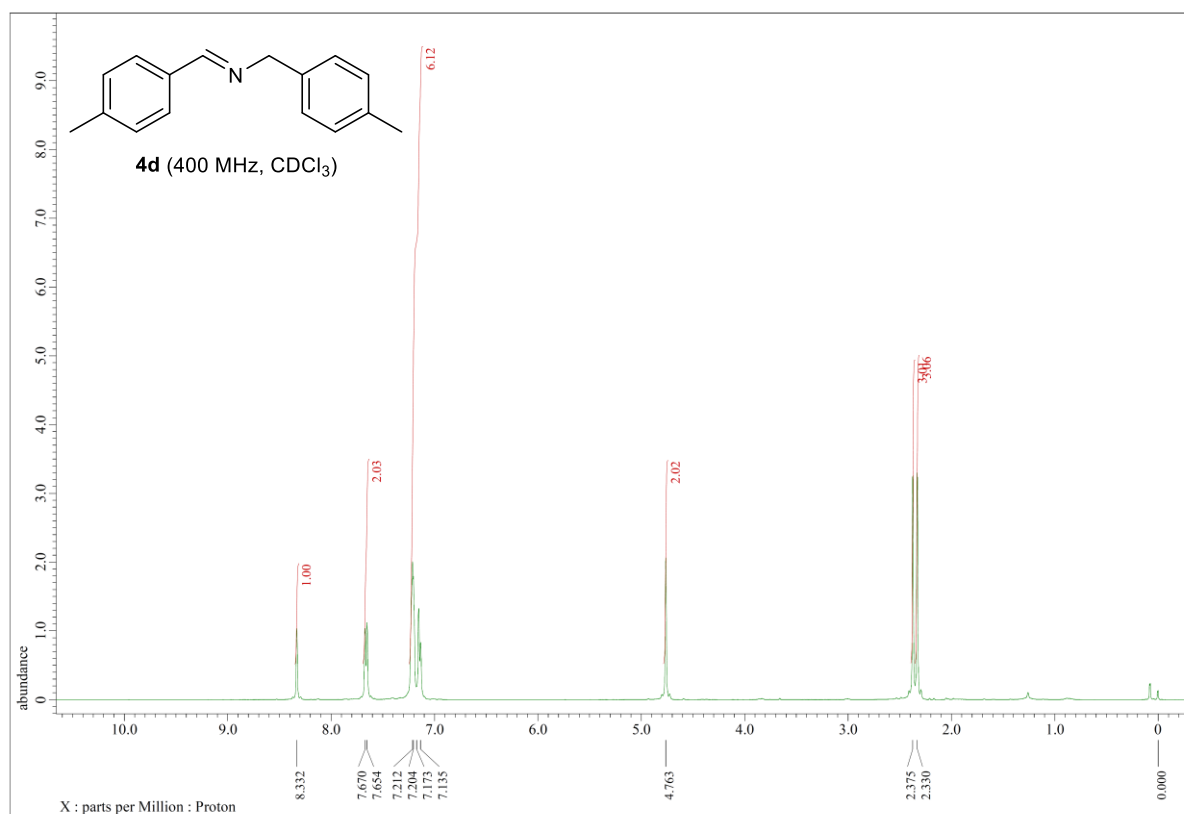


Figure S26: Copies of ¹H and ¹³C{¹H} NMR spectra of compound **6a**

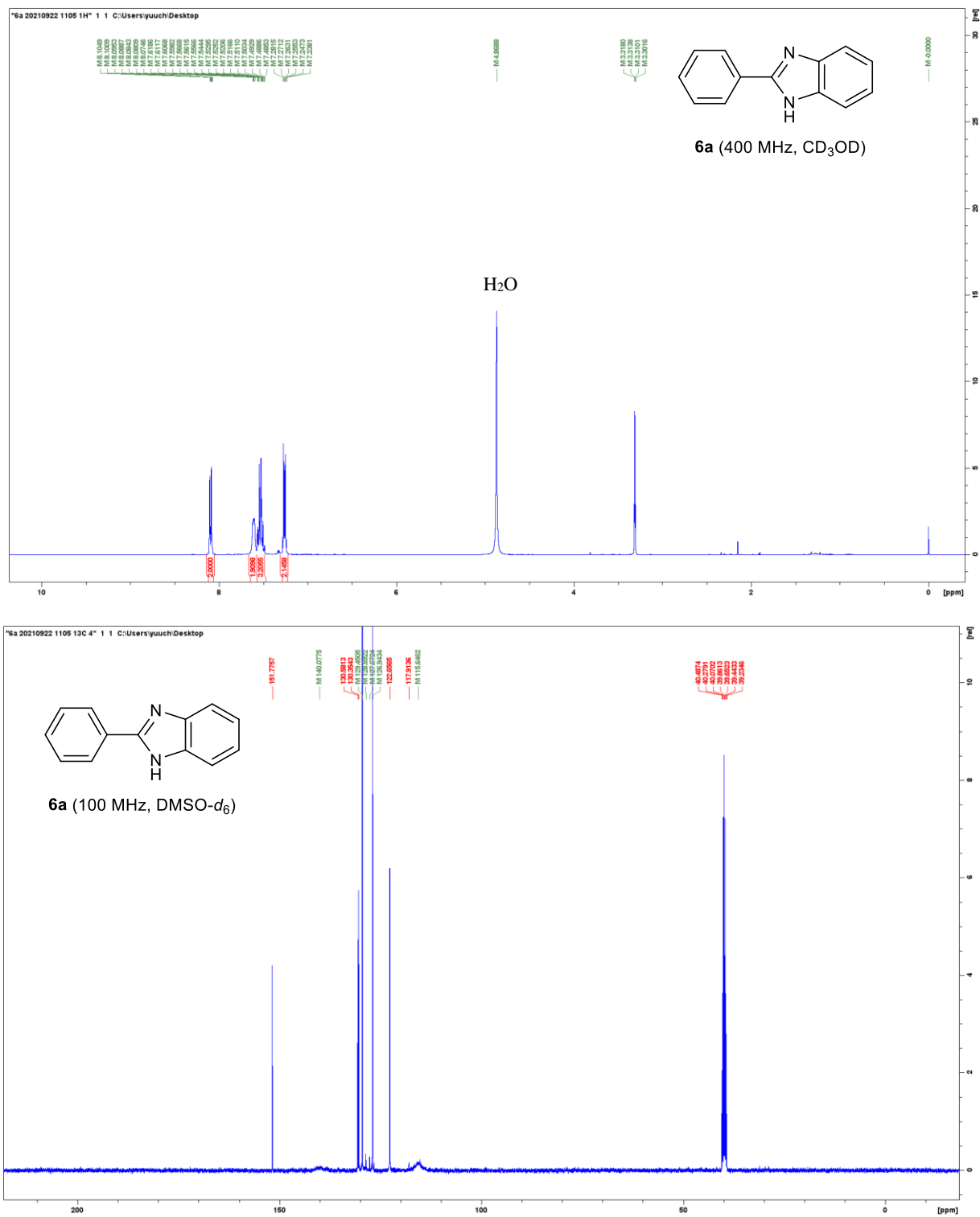


Figure S27: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **6b**

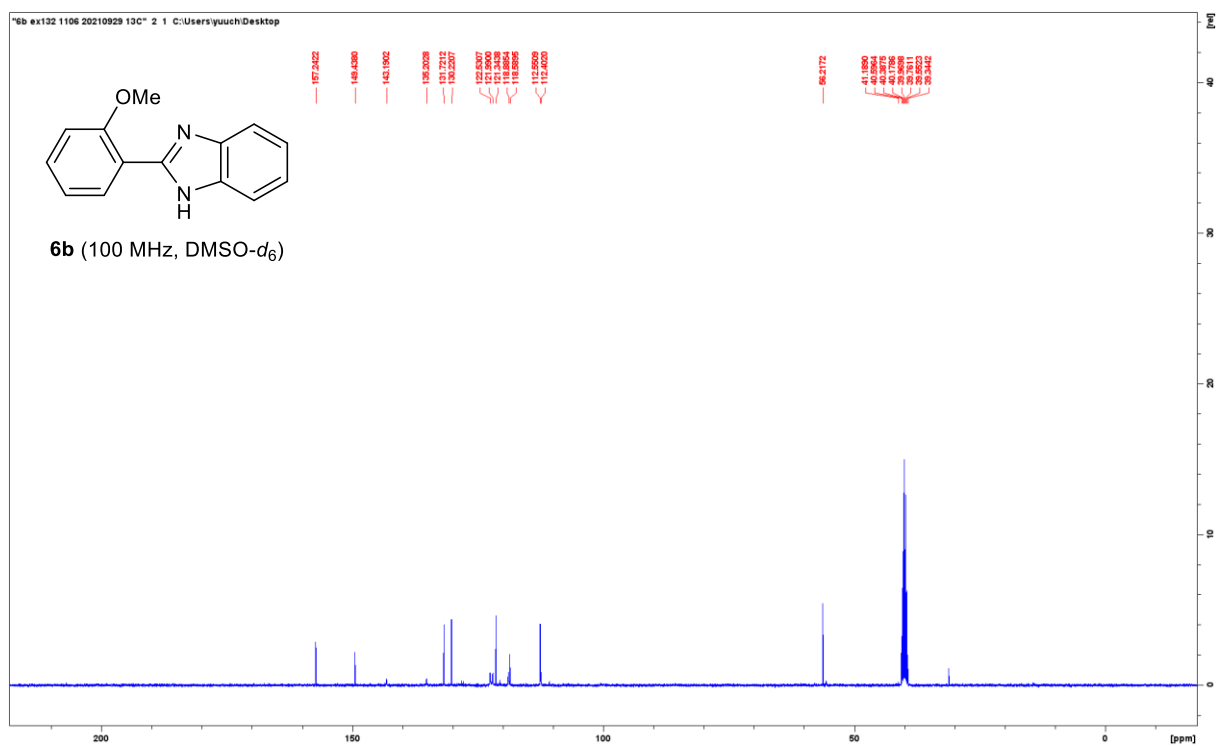
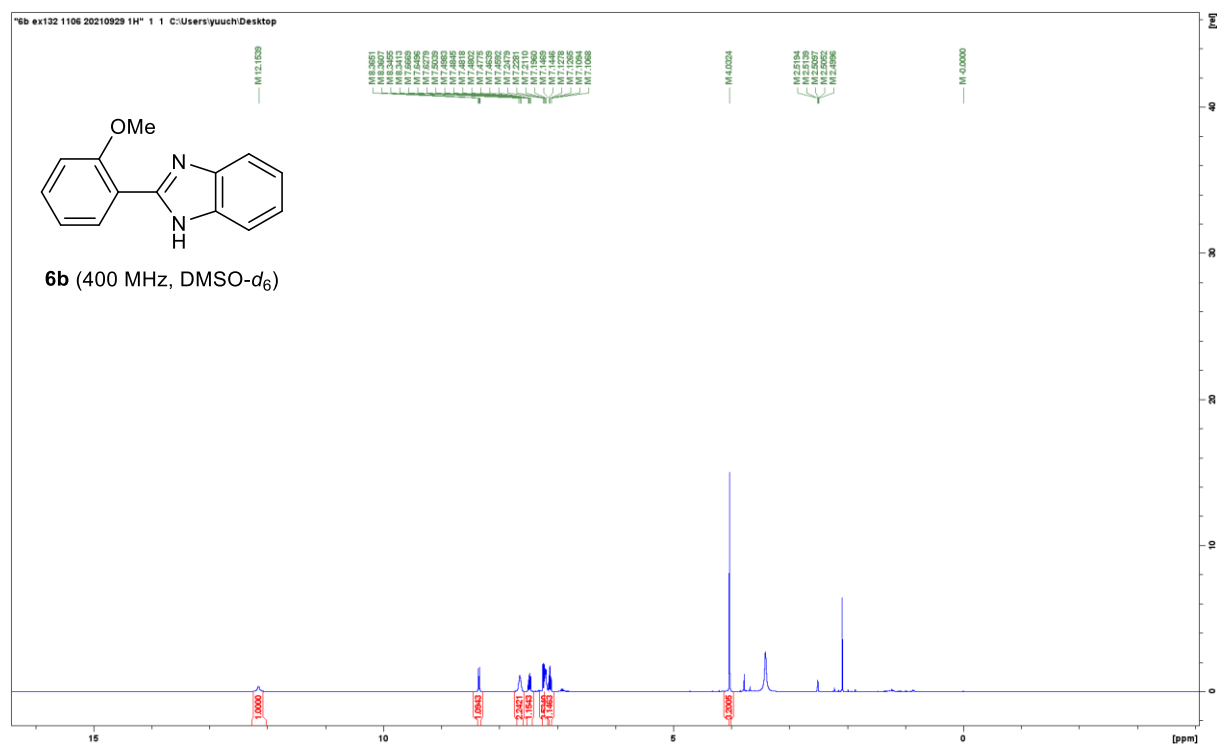


Figure S28: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **6c**

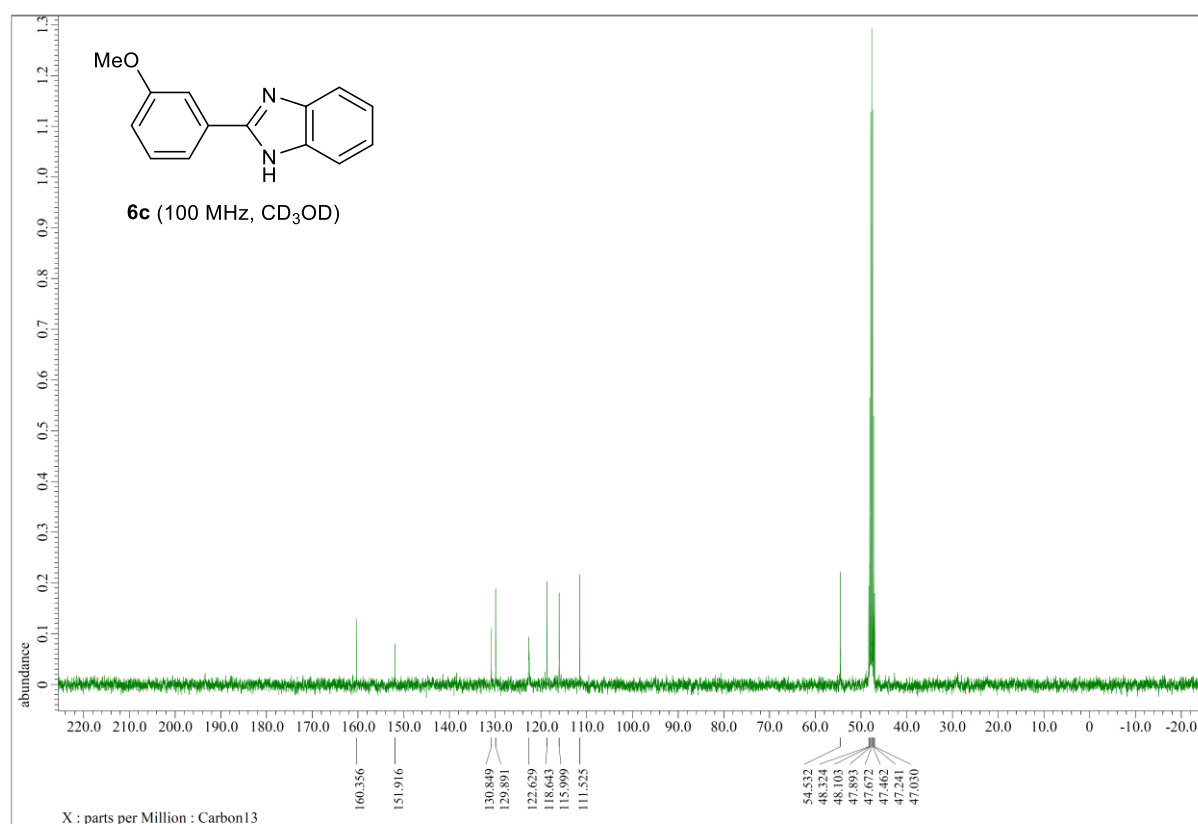
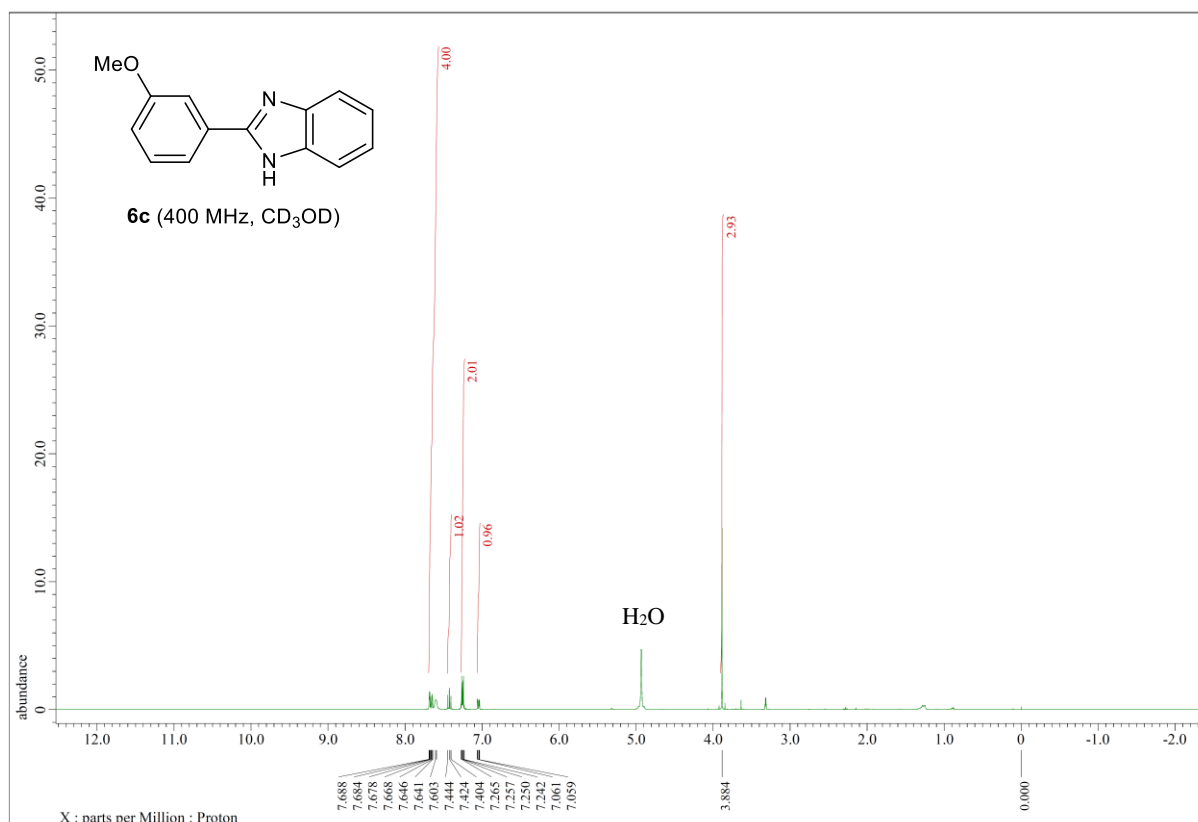


Figure S29: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **6d**

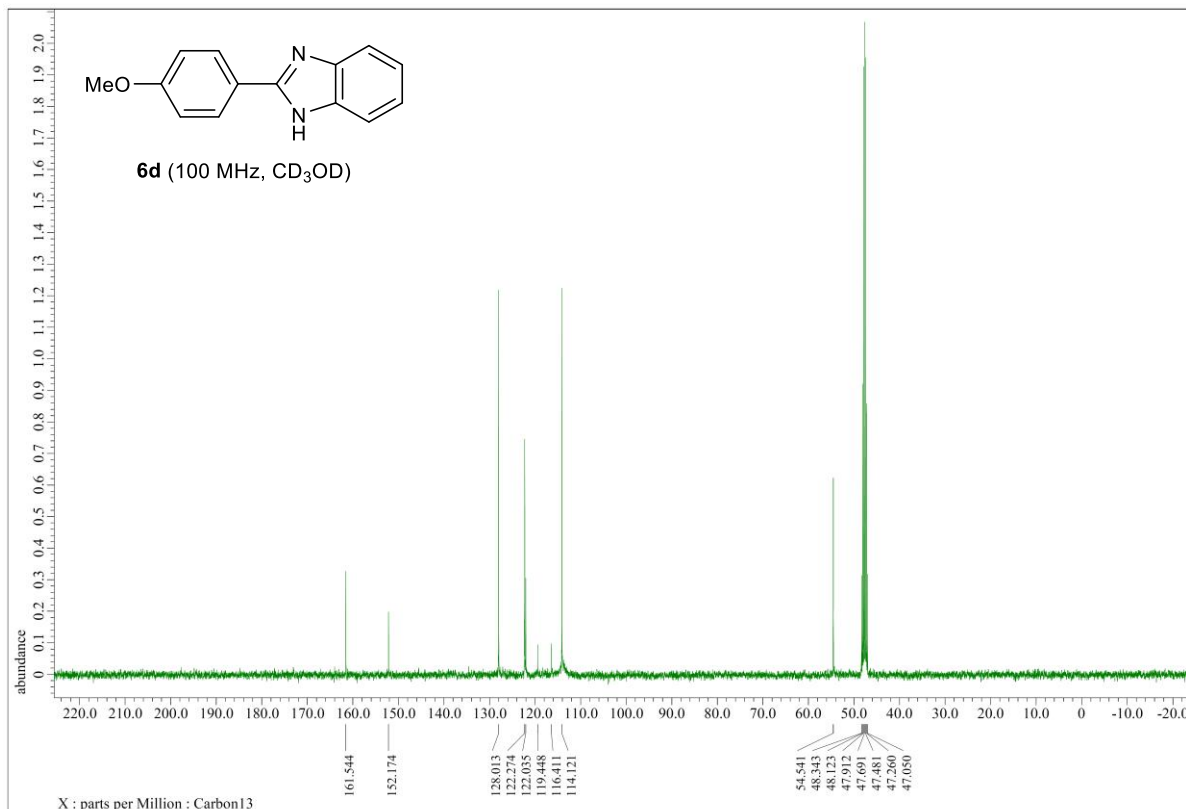
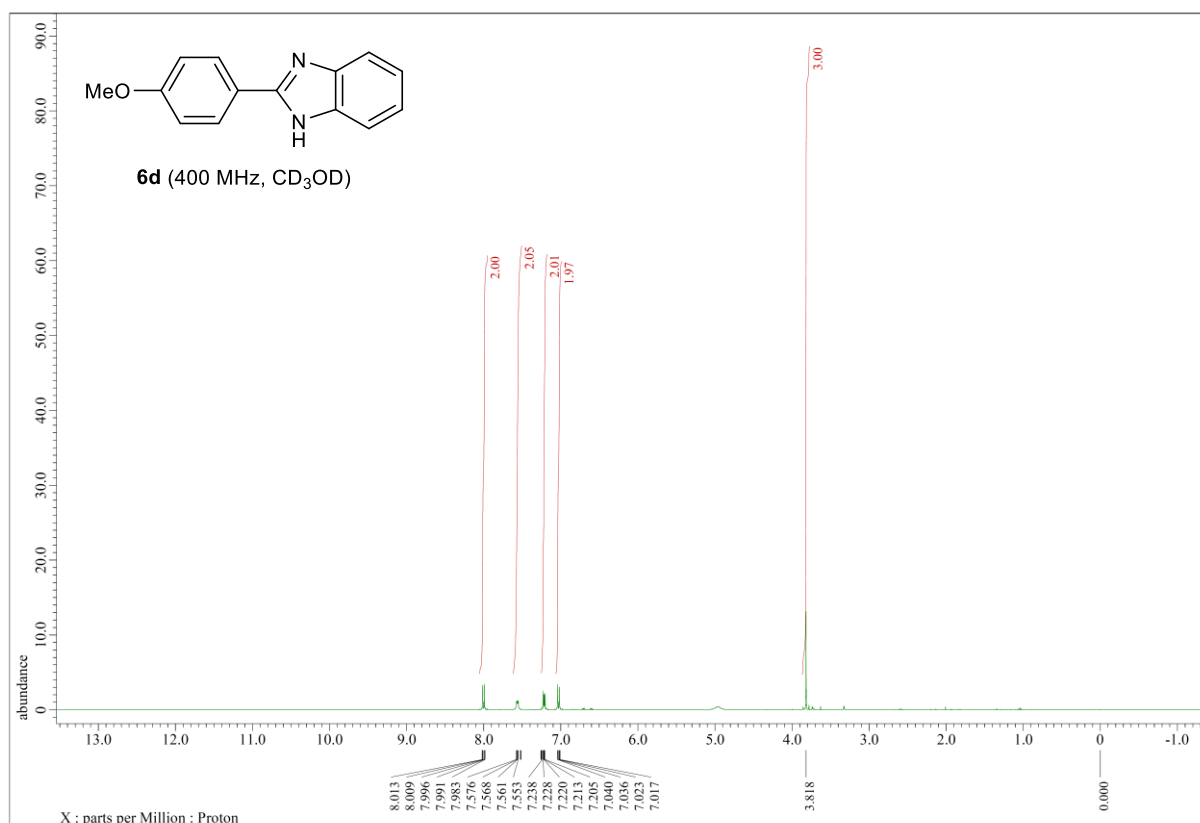


Figure S30: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **6e**

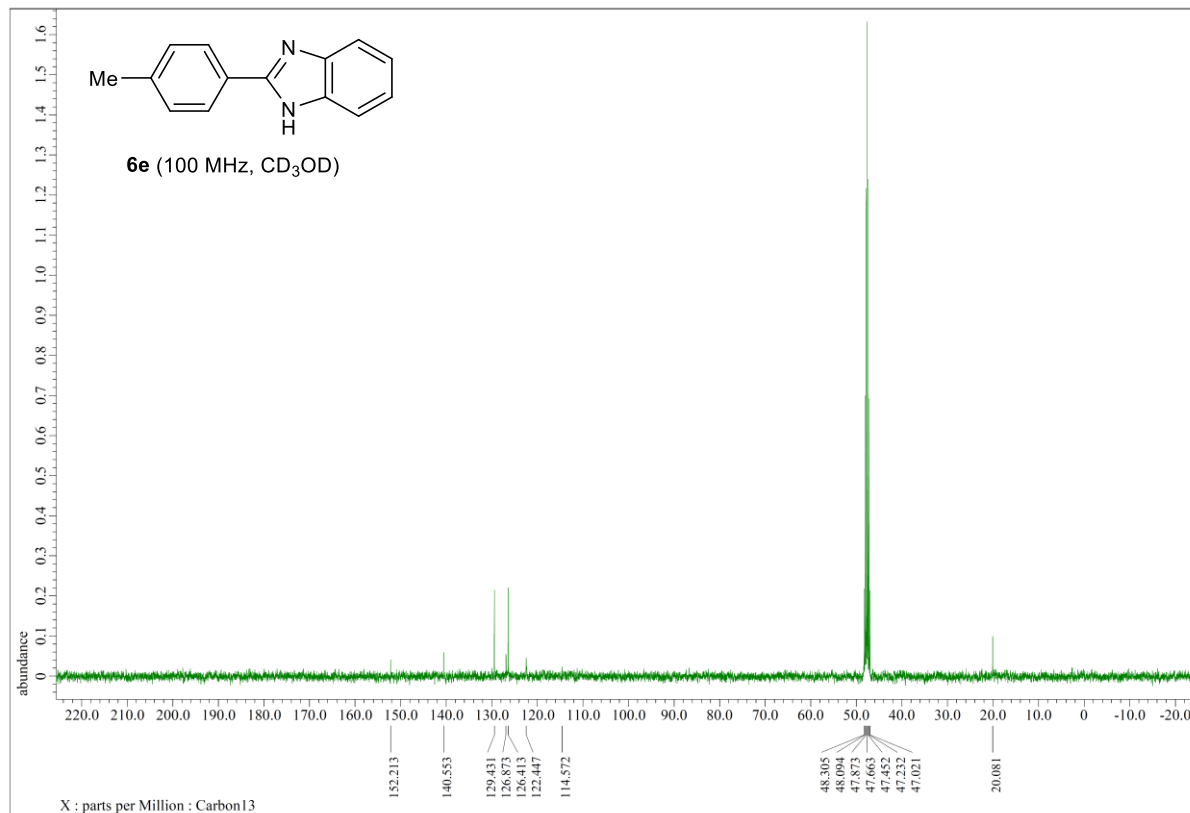
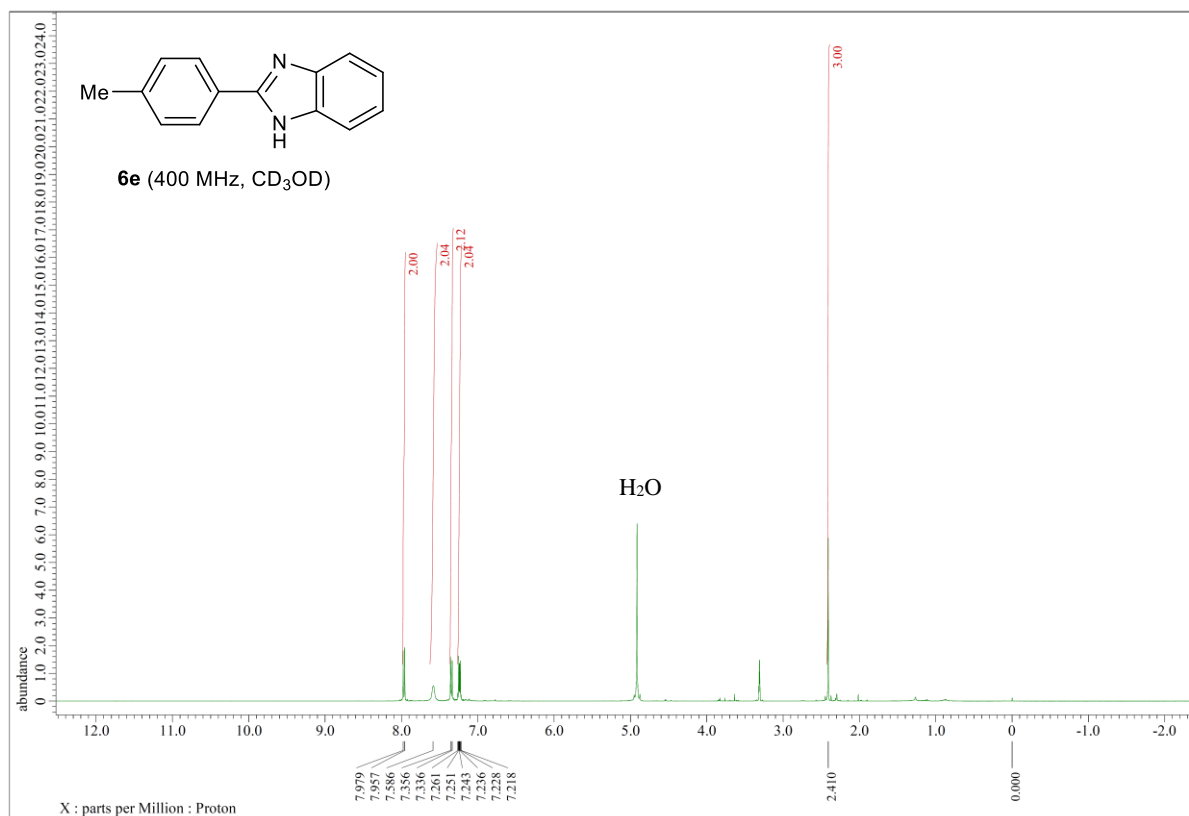


Figure S31: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **8**

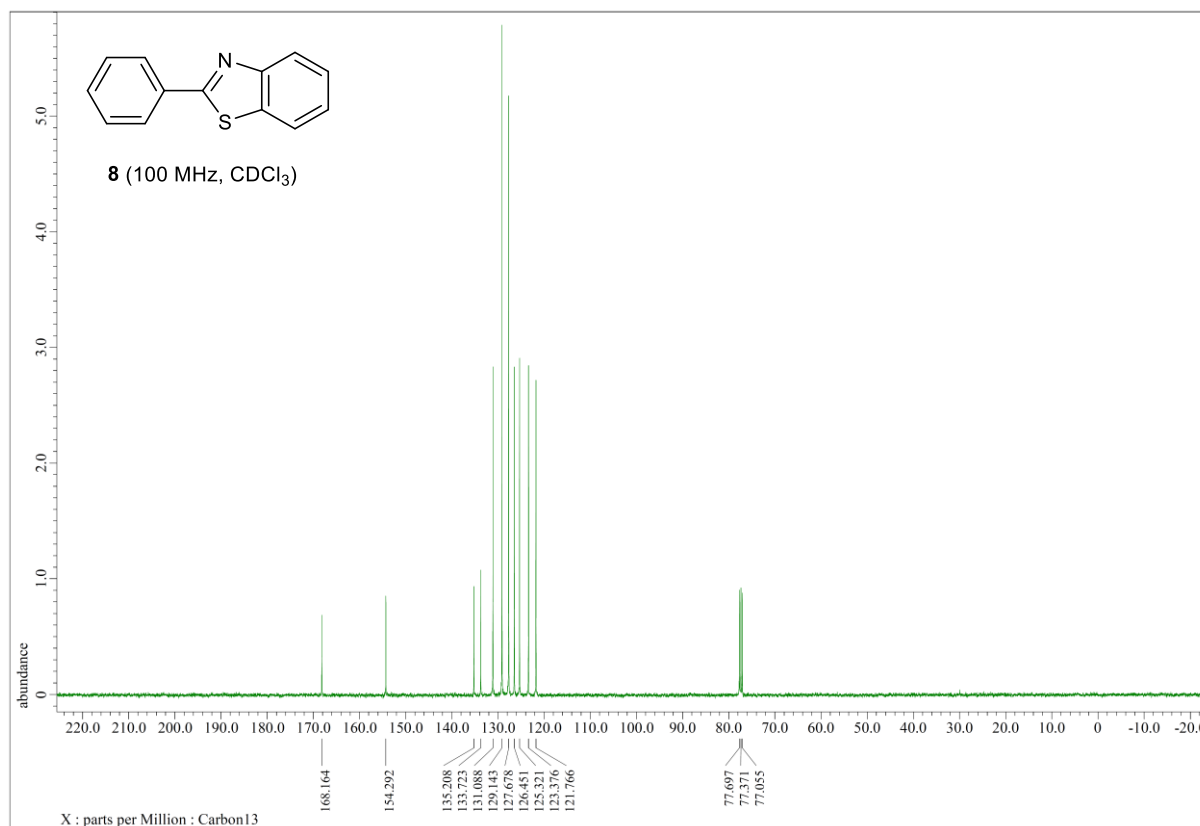
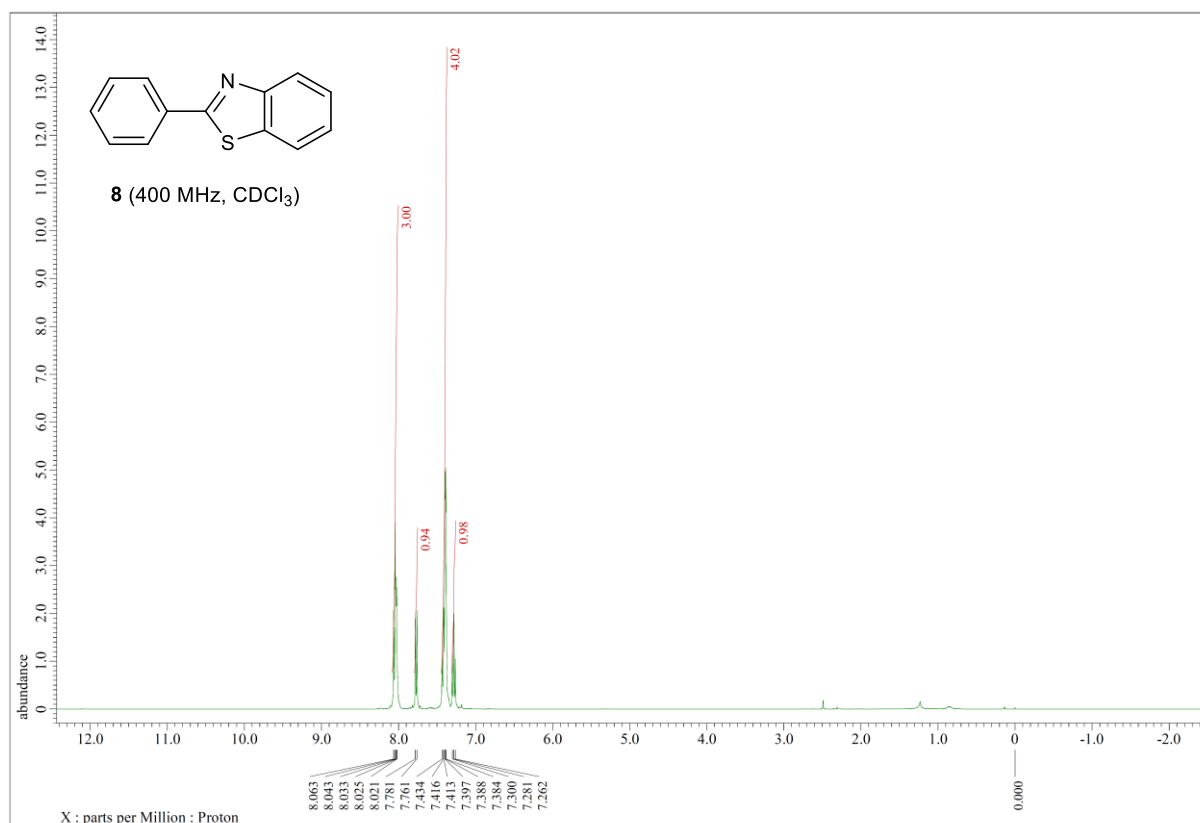


Figure S32: Copies of ^1H and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of compound **9**

