



Supporting Information

for

Base-promoted deacylation of 2-acetyl-2,5-dihydrothiophenes and their oxygen-mediated hydroxylation

Vladimir G. Ilkin, Margarita Likhacheva, Igor V. Trushkov, Tetyana V. Beryozkina, Vera S. Berseneva, Vladimir T. Abaev, Wim Dehaen and Vasiliy A. Bakulev

Beilstein J. Org. Chem. **2026**, 22, 192–204. doi:10.3762/bjoc.22.13

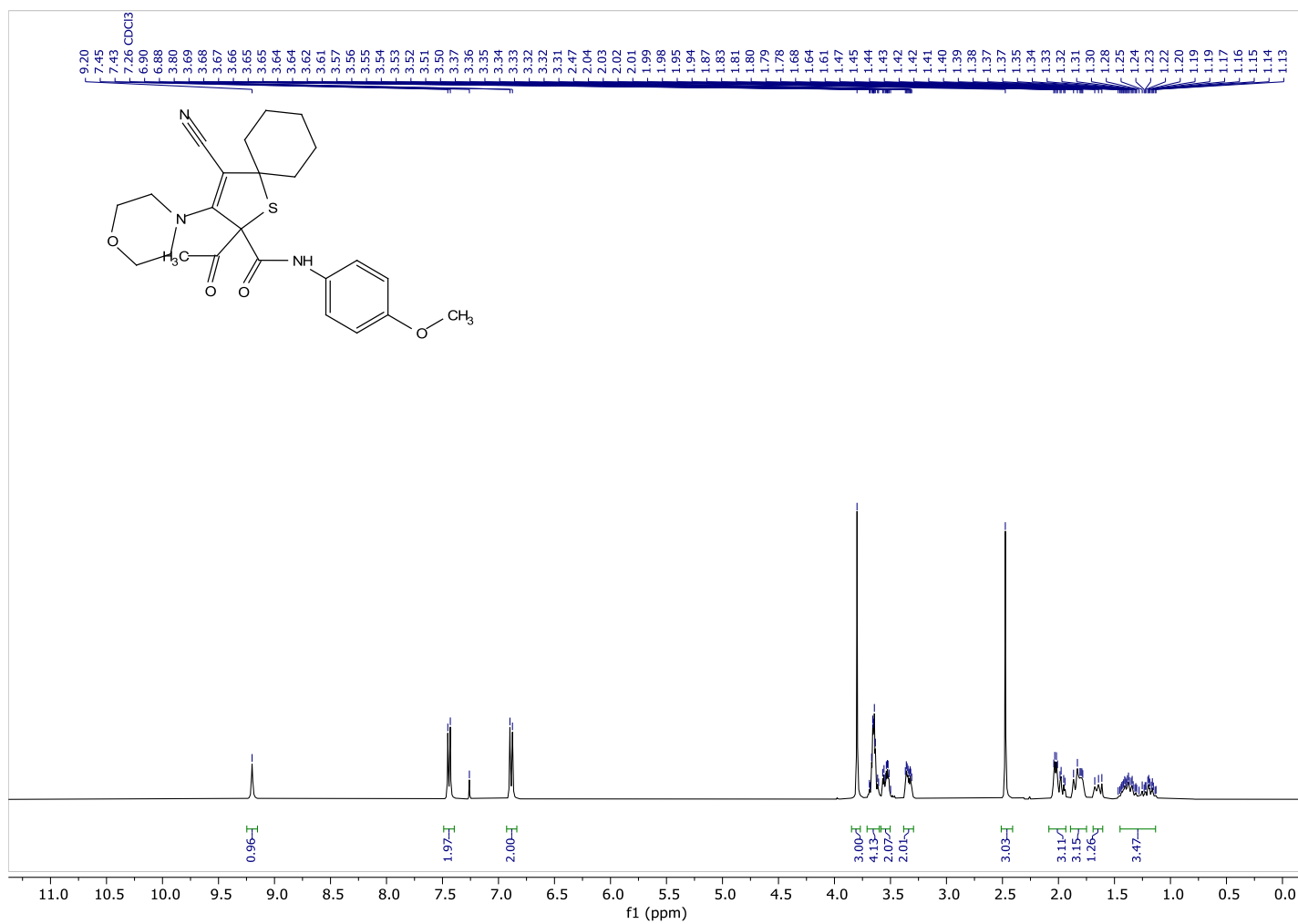
Copies of NMR spectra of all new compounds

Table of contents

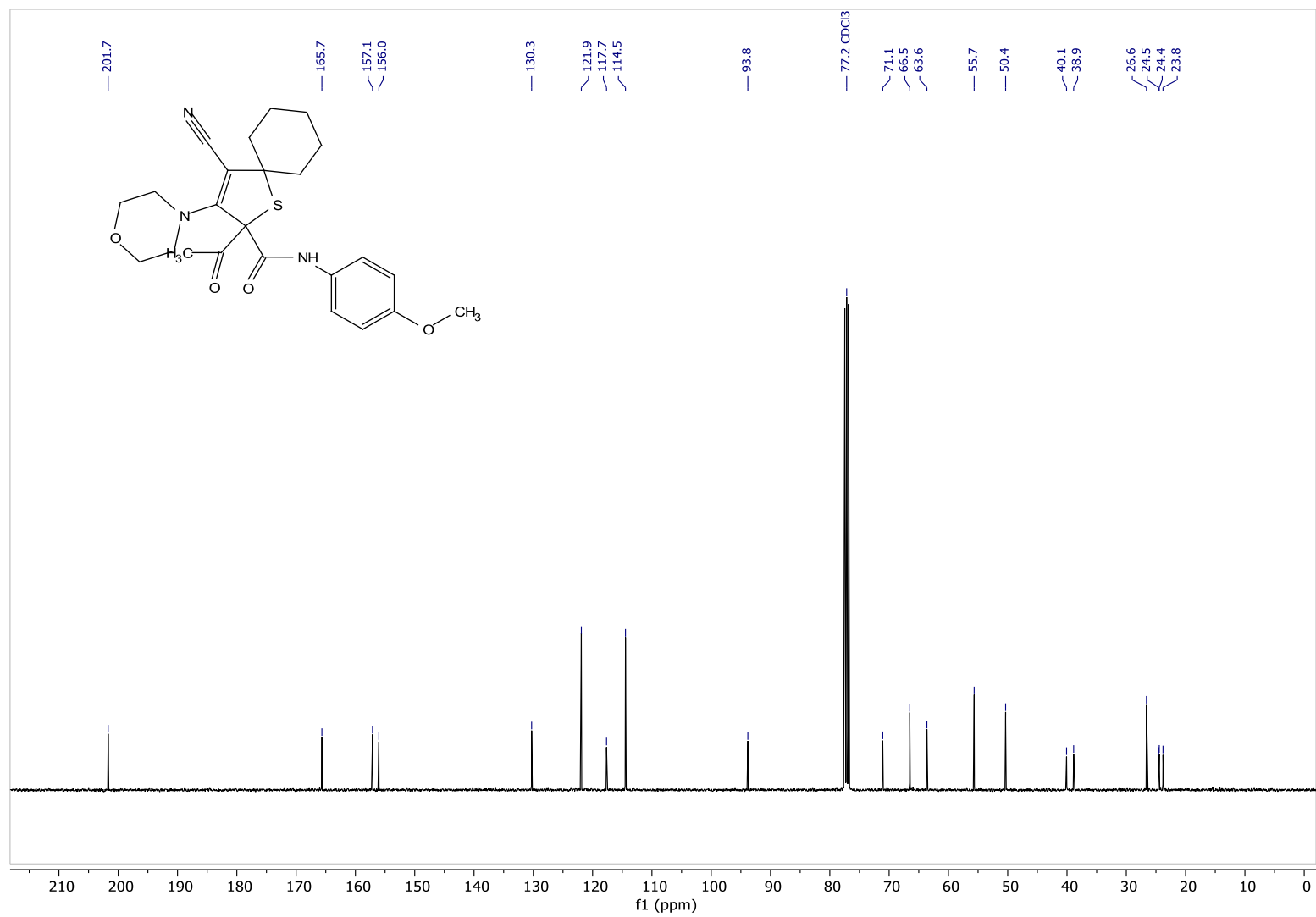
Copies of NMR spectra

S3

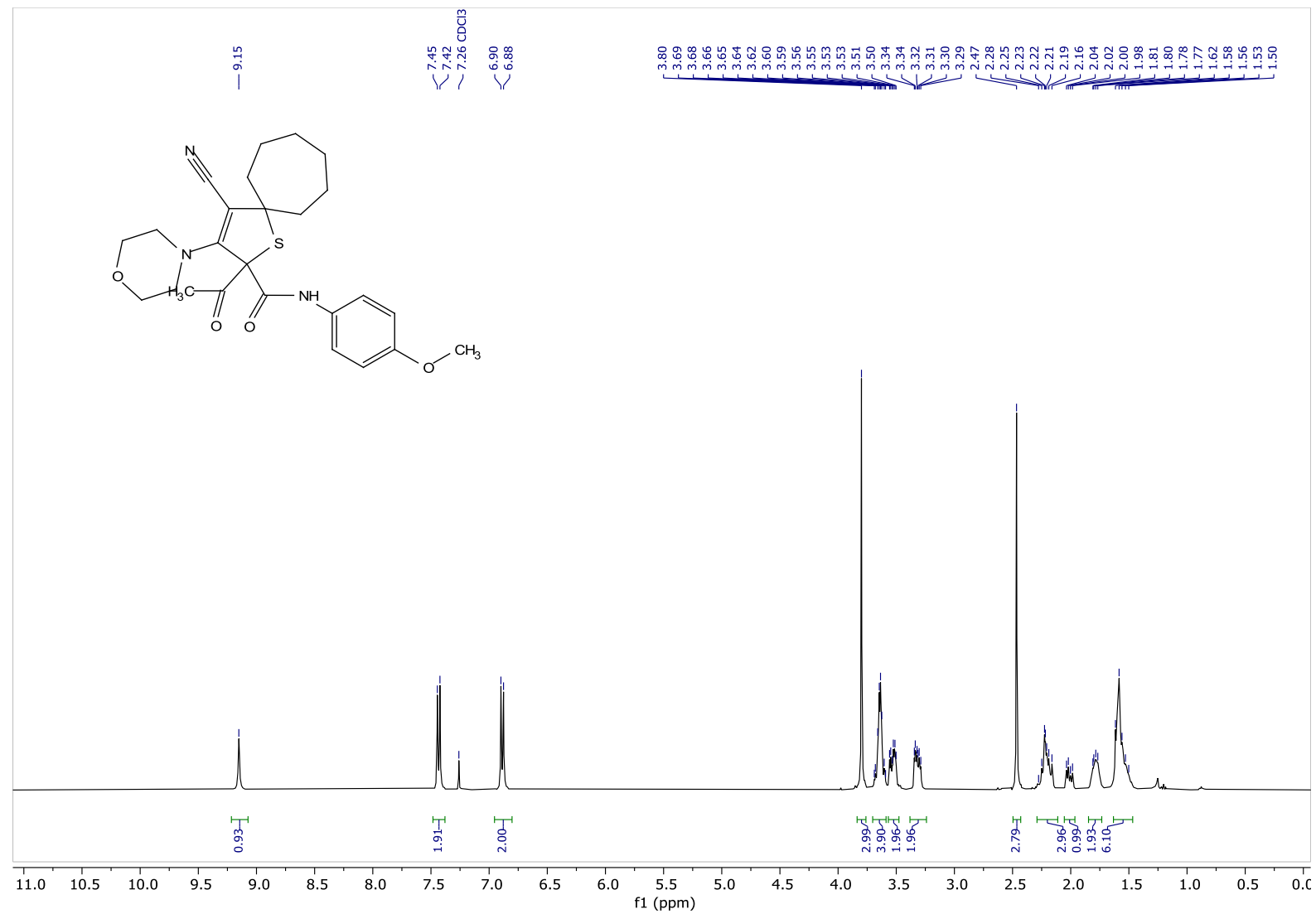
Copies of NMR spectra



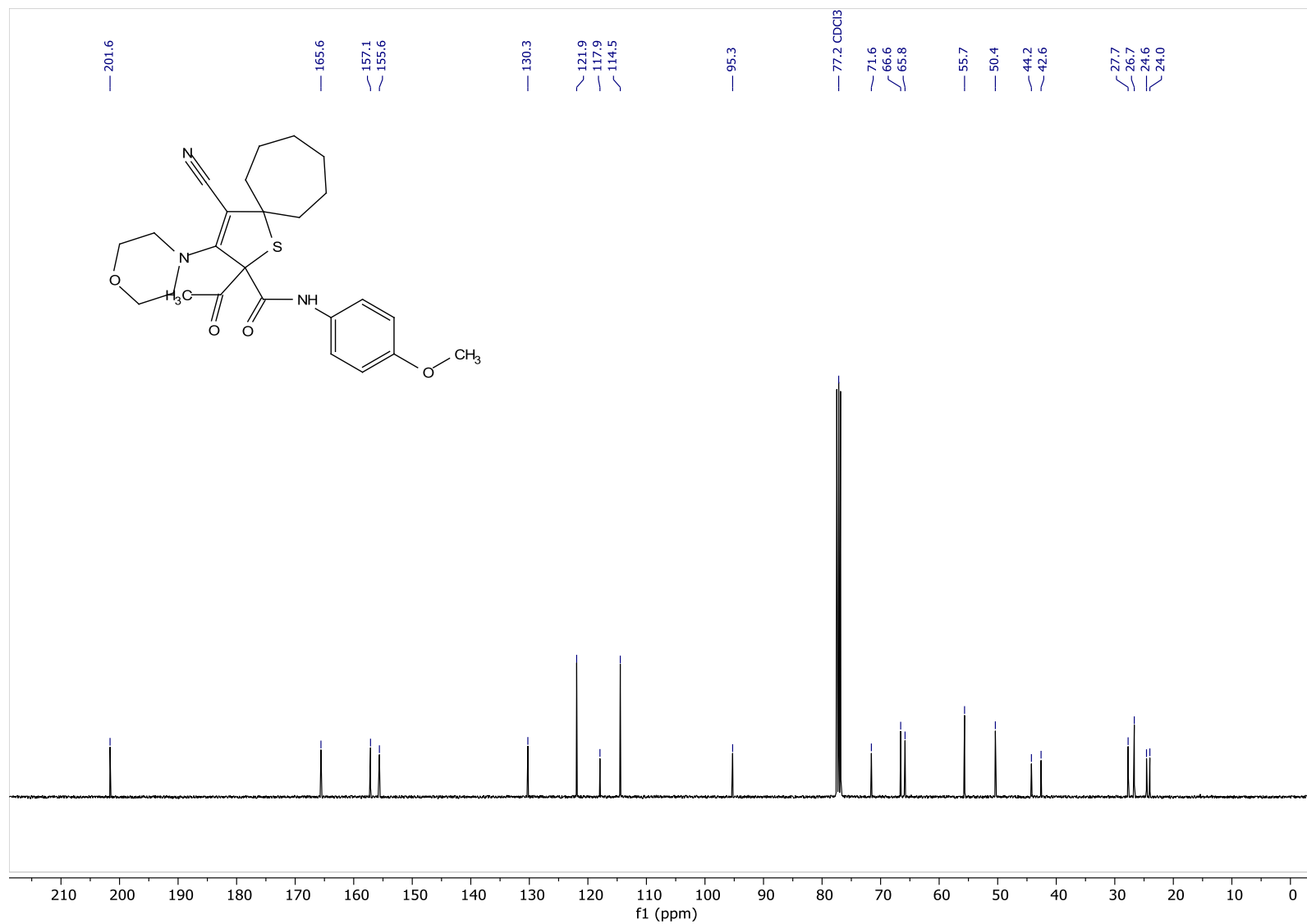
¹H NMR (400 MHz, CDCl₃-d) of **1b**



¹³C NMR (100 MHz, CDCl₃-*d*) of **1b**

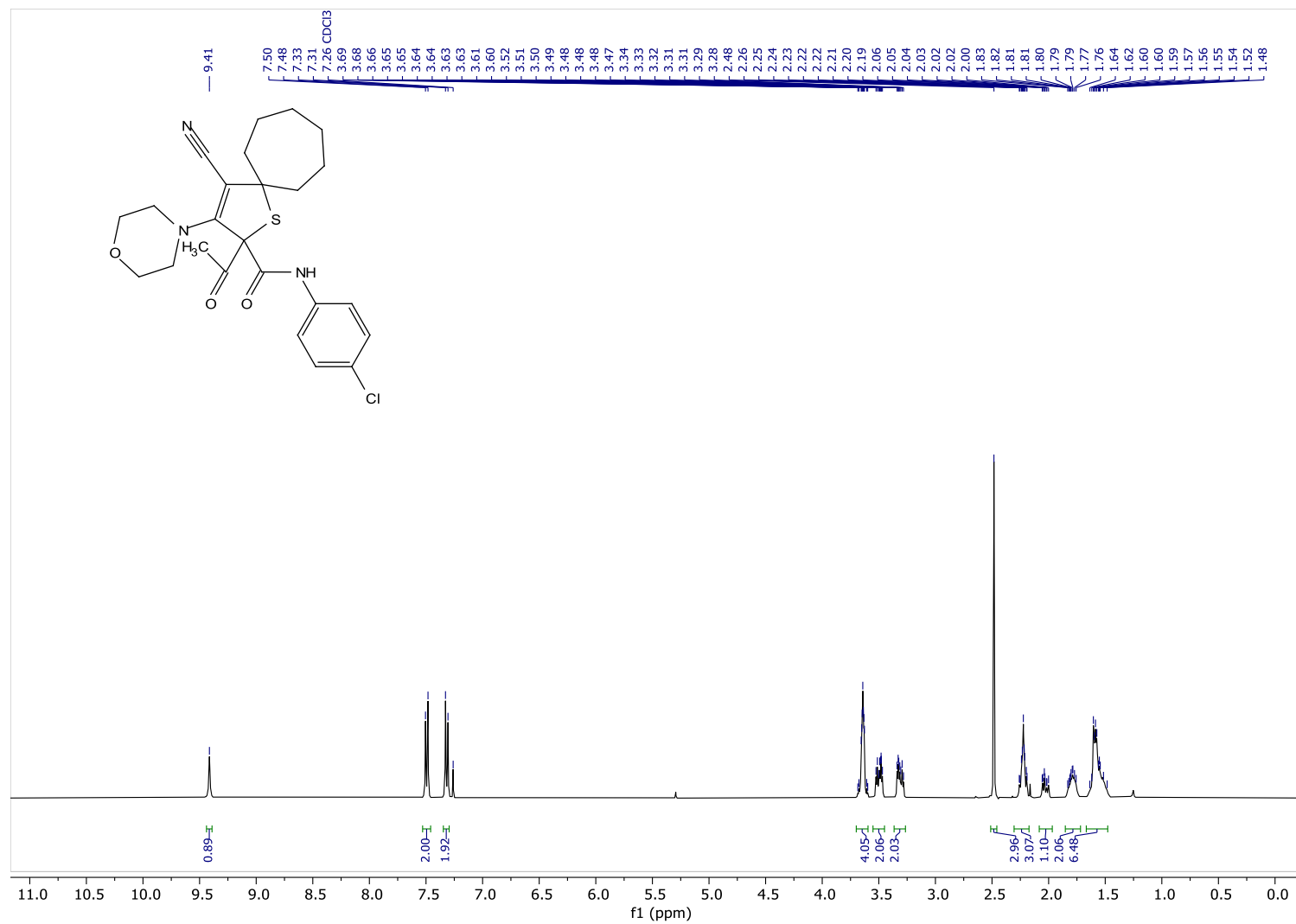


^1H NMR (400 MHz, CDCl_3 -d) of **1d**

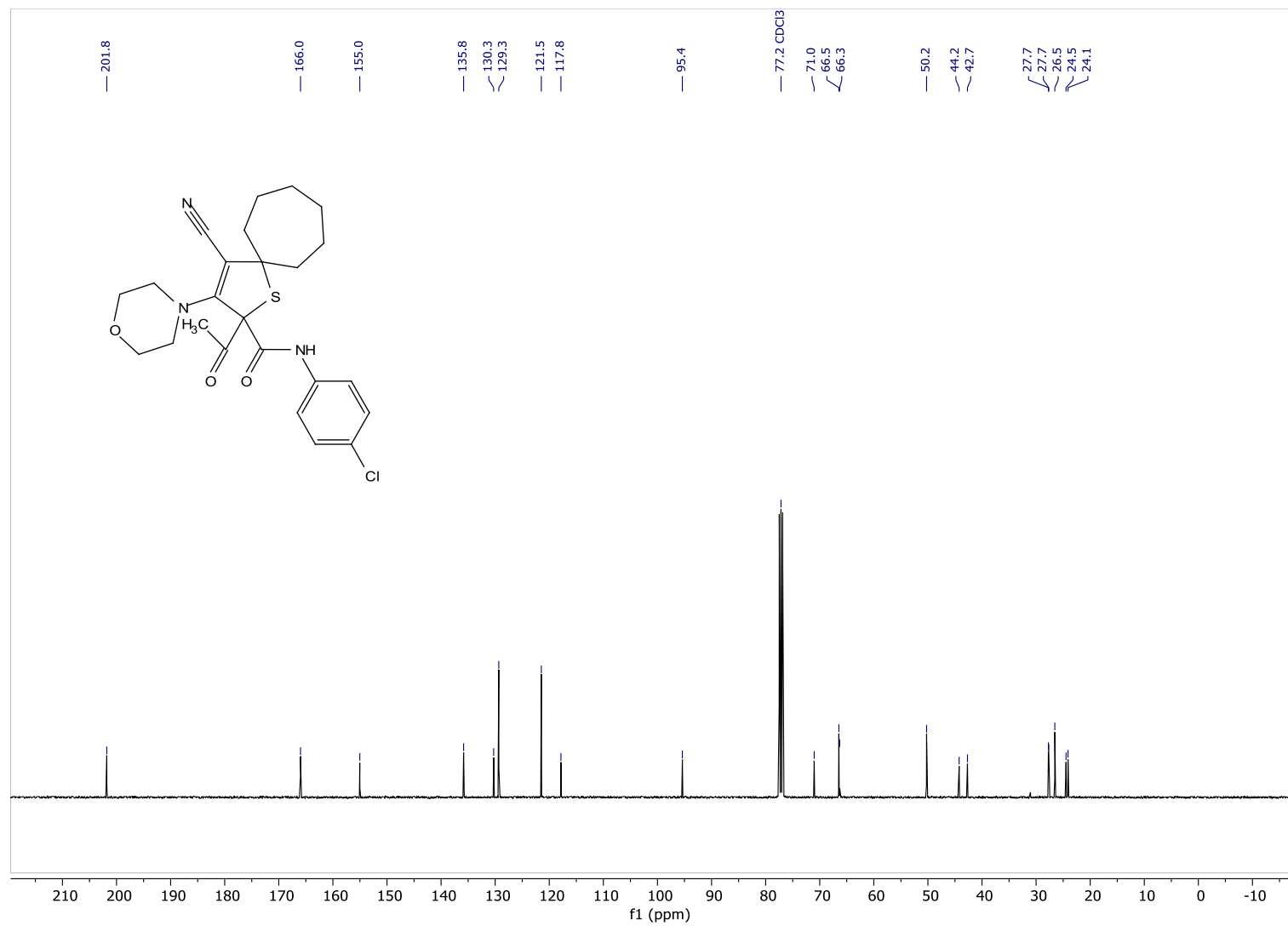


¹³C NMR (100 MHz, CDCl₃-d) of **1d**

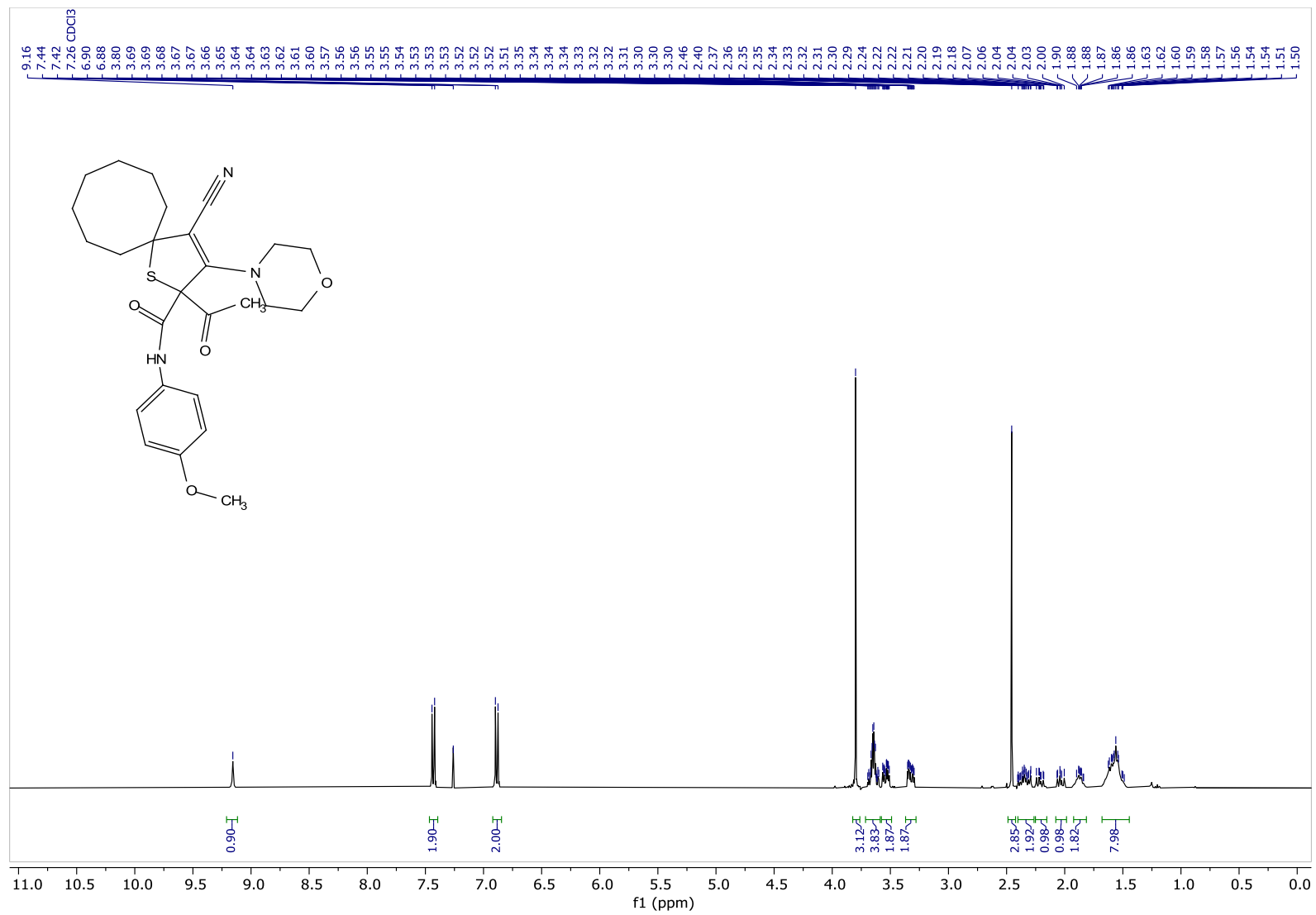
S6



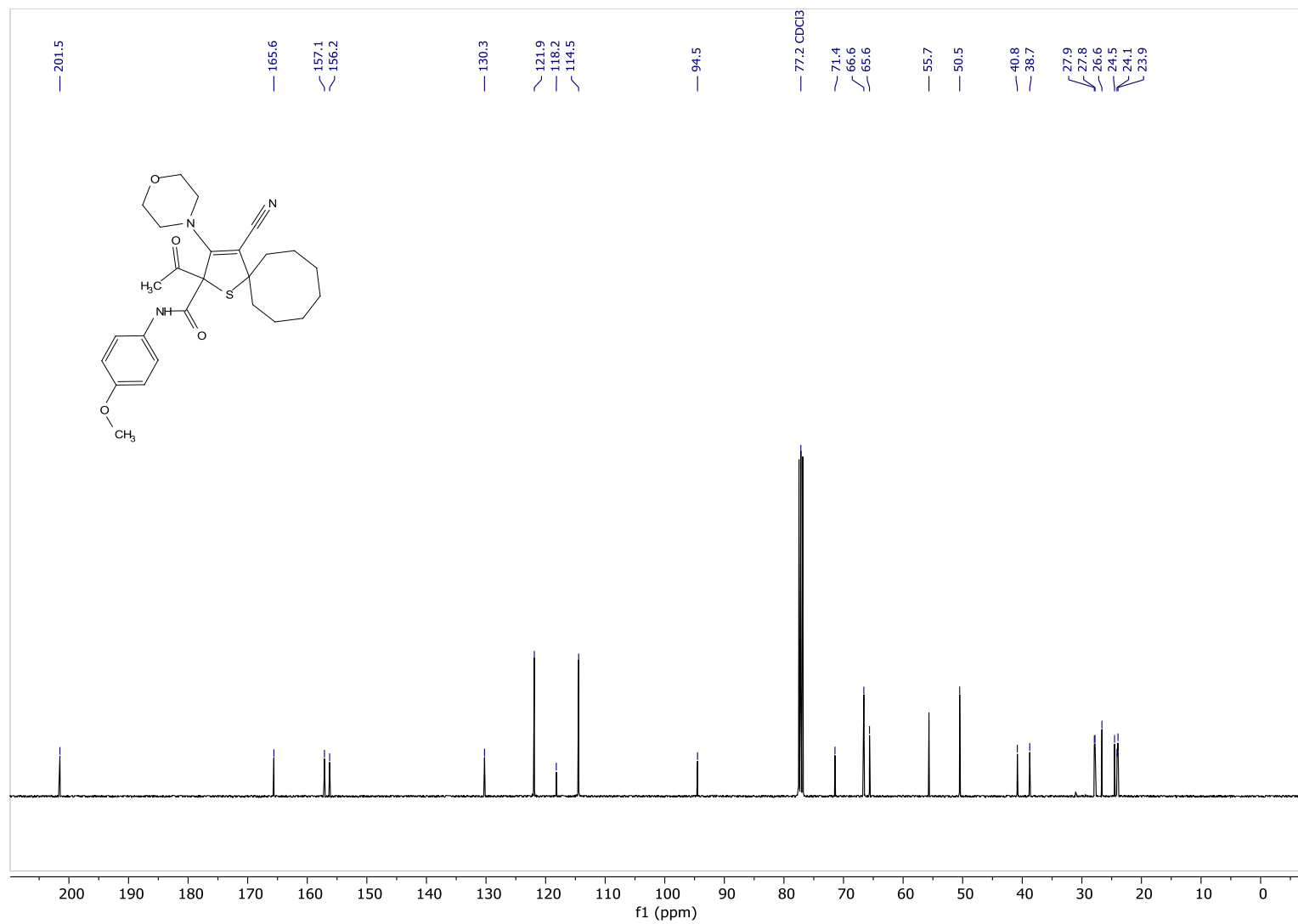
^1H NMR (400 MHz, CDCl_3 -*d*) of **1e**



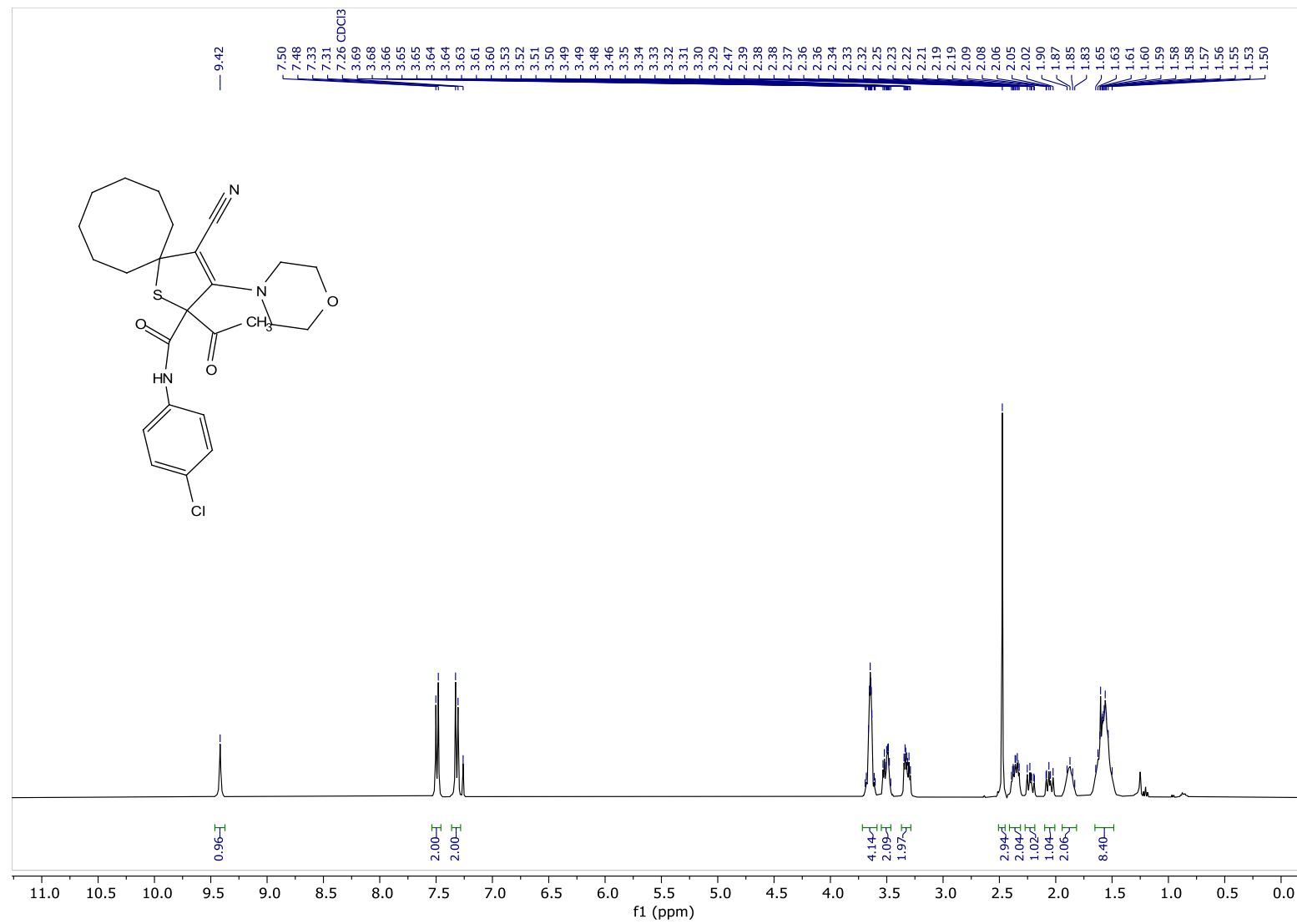
^{13}C NMR (100 MHz, CDCl_3 -*d*) of **1e**



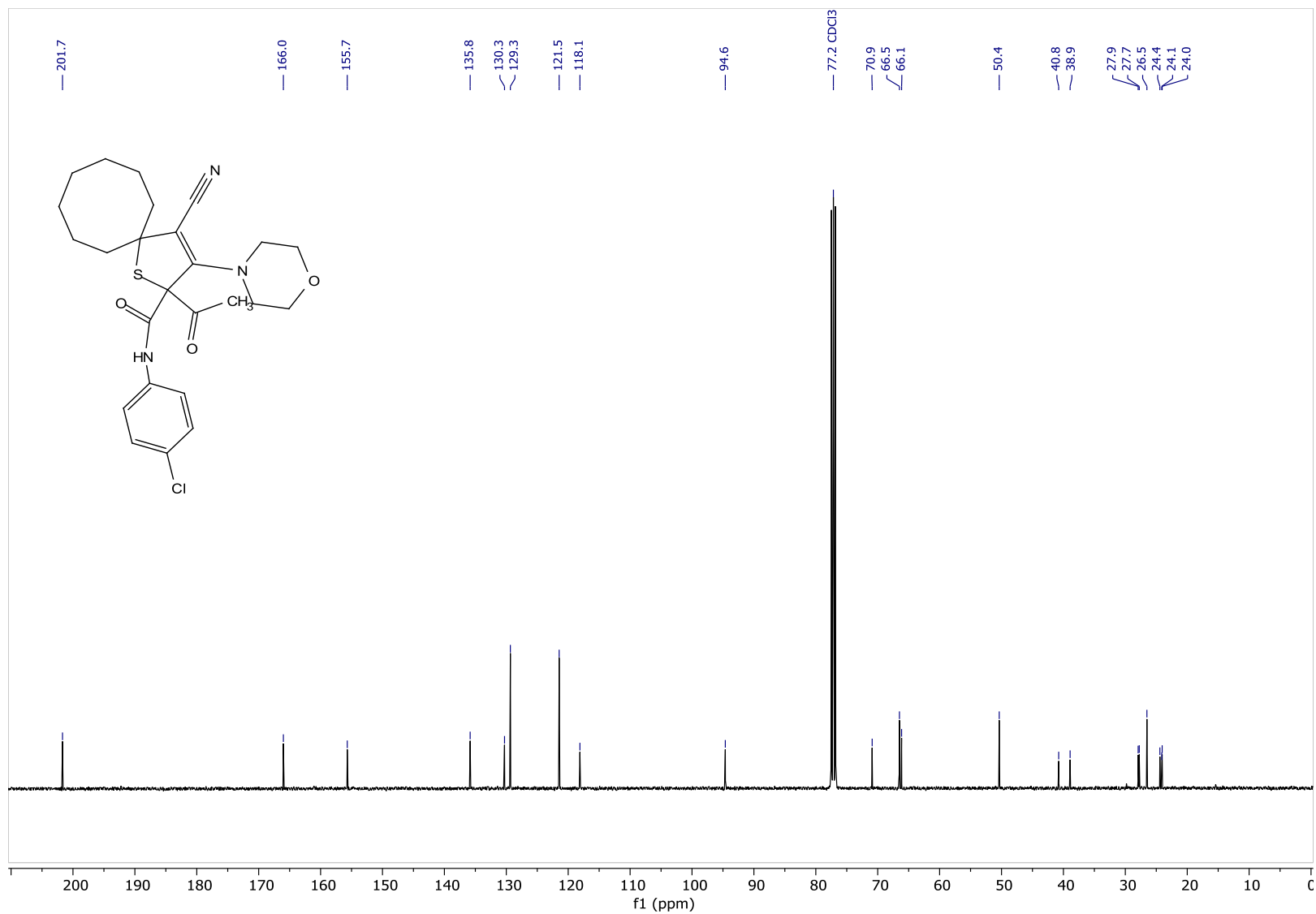
^1H NMR (400 MHz, CDCl_3 -d) of **1g**



¹³C NMR (100 MHz, CDCl₃-d) of **1g**

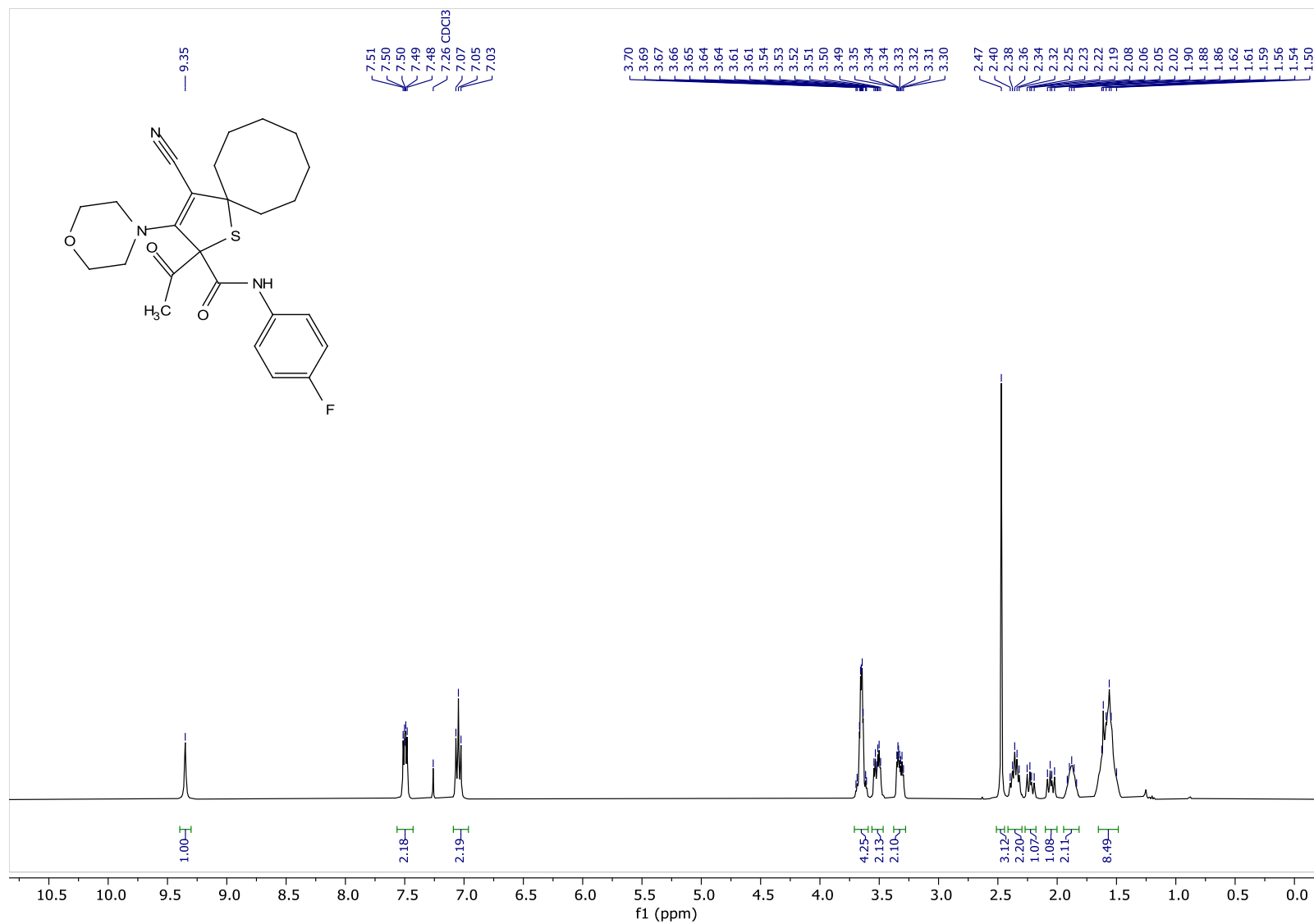


^1H NMR (400 MHz, CDCl_3 -d) of **1h**



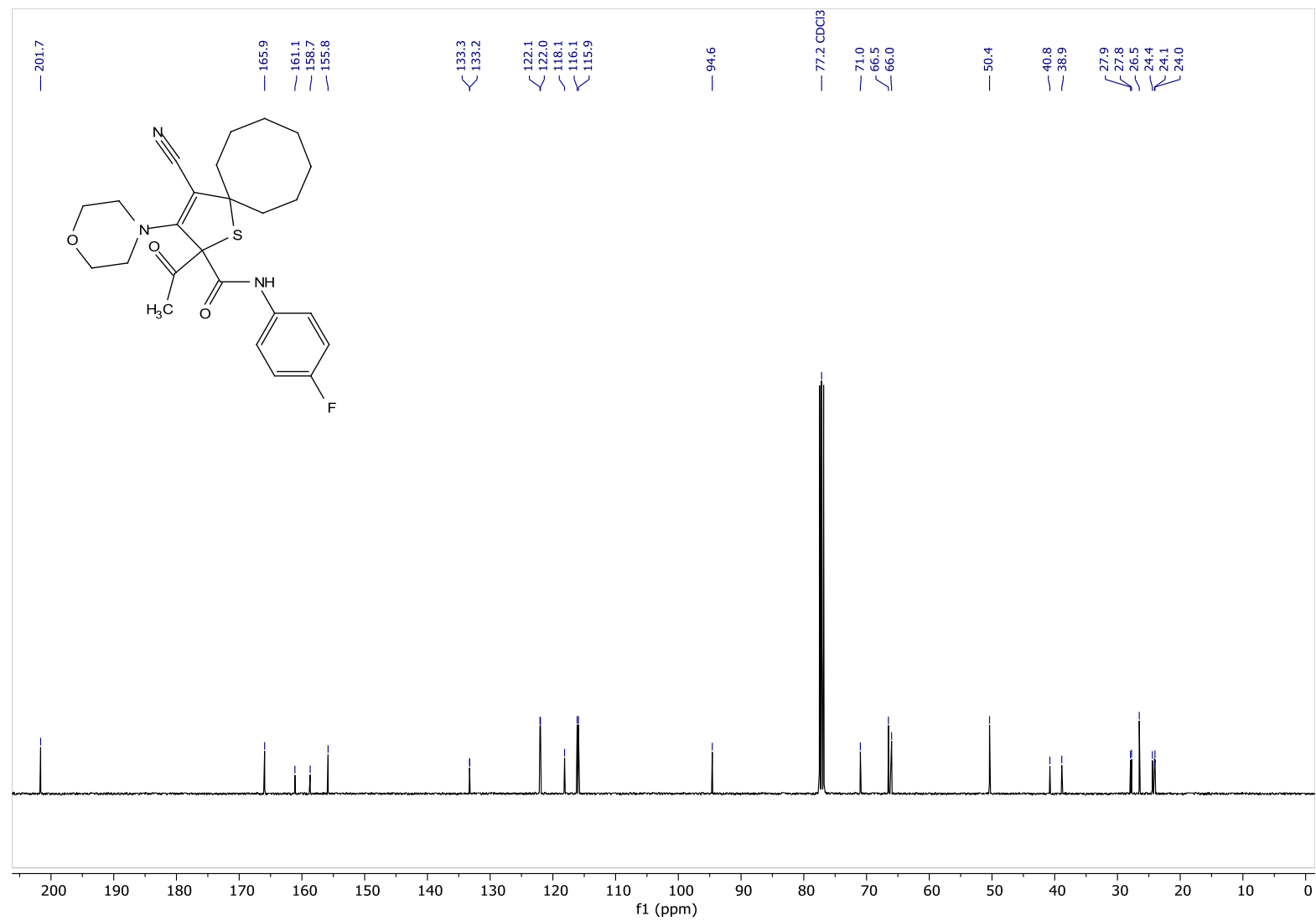
^{13}C NMR (100 MHz, CDCl_3 -*d*) of **1h**

S12

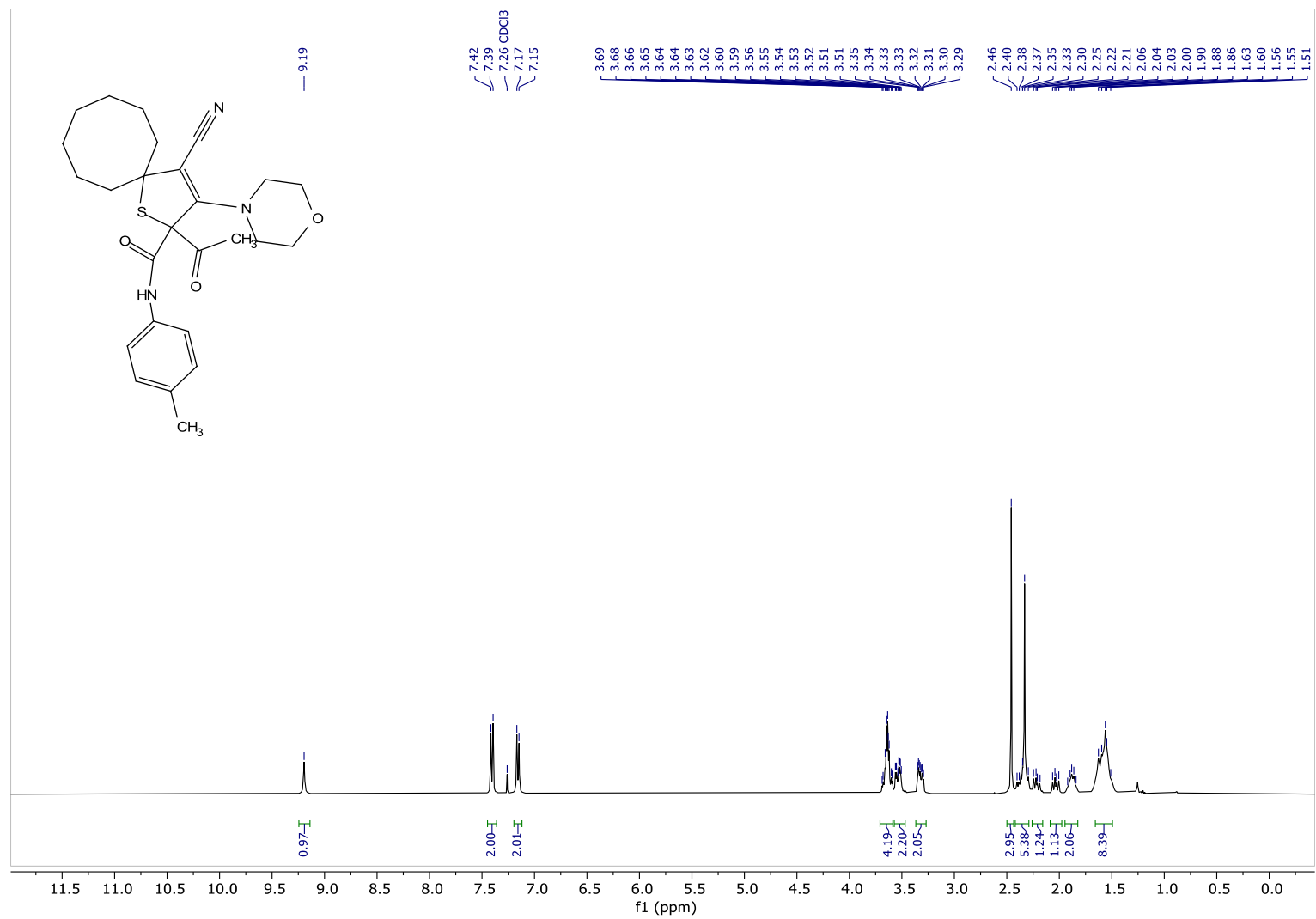


¹H NMR (400 MHz, CDCl₃-d) of **1i**

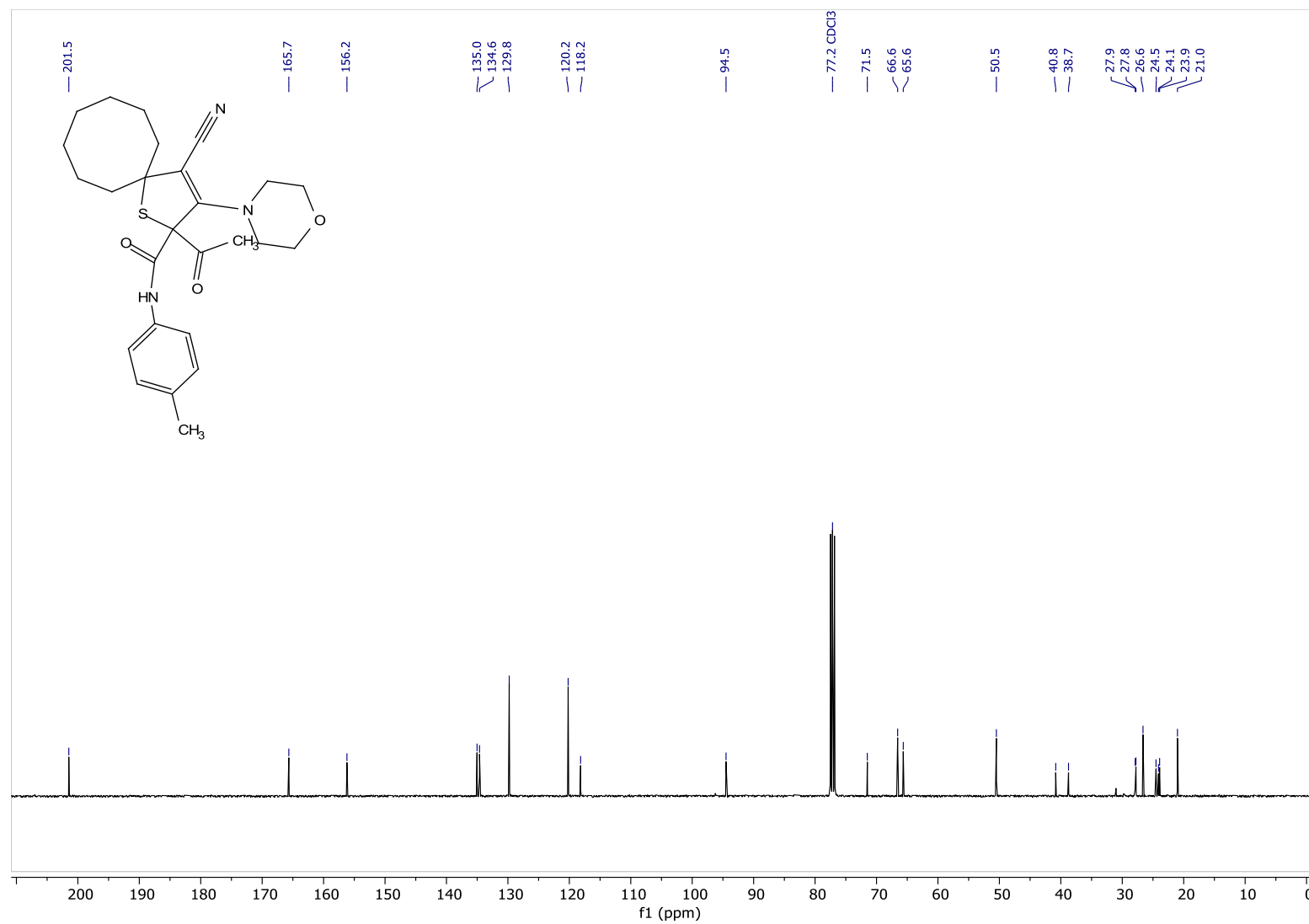
S13



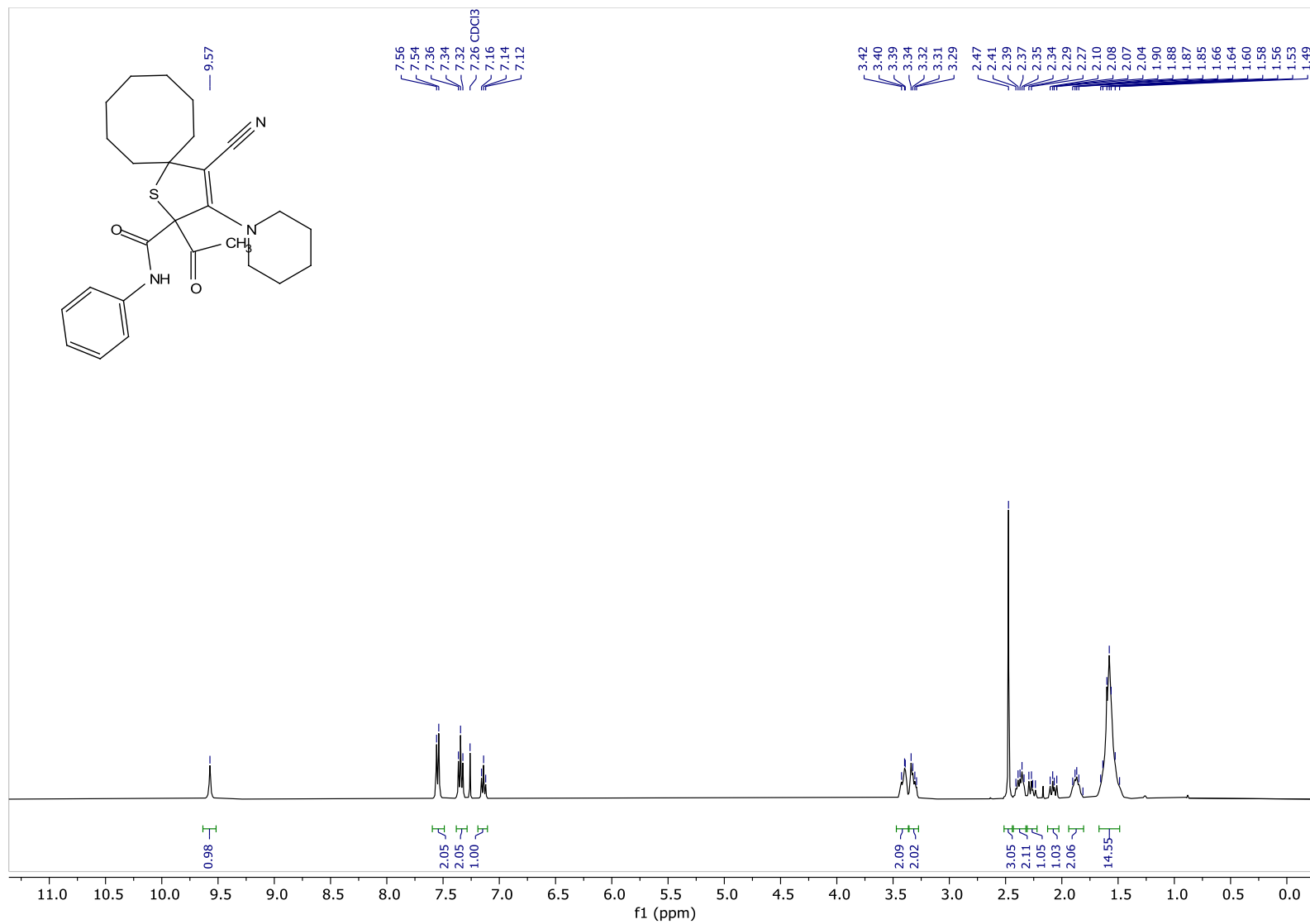
¹³C NMR (100 MHz, CDCl₃-d) of **1i**



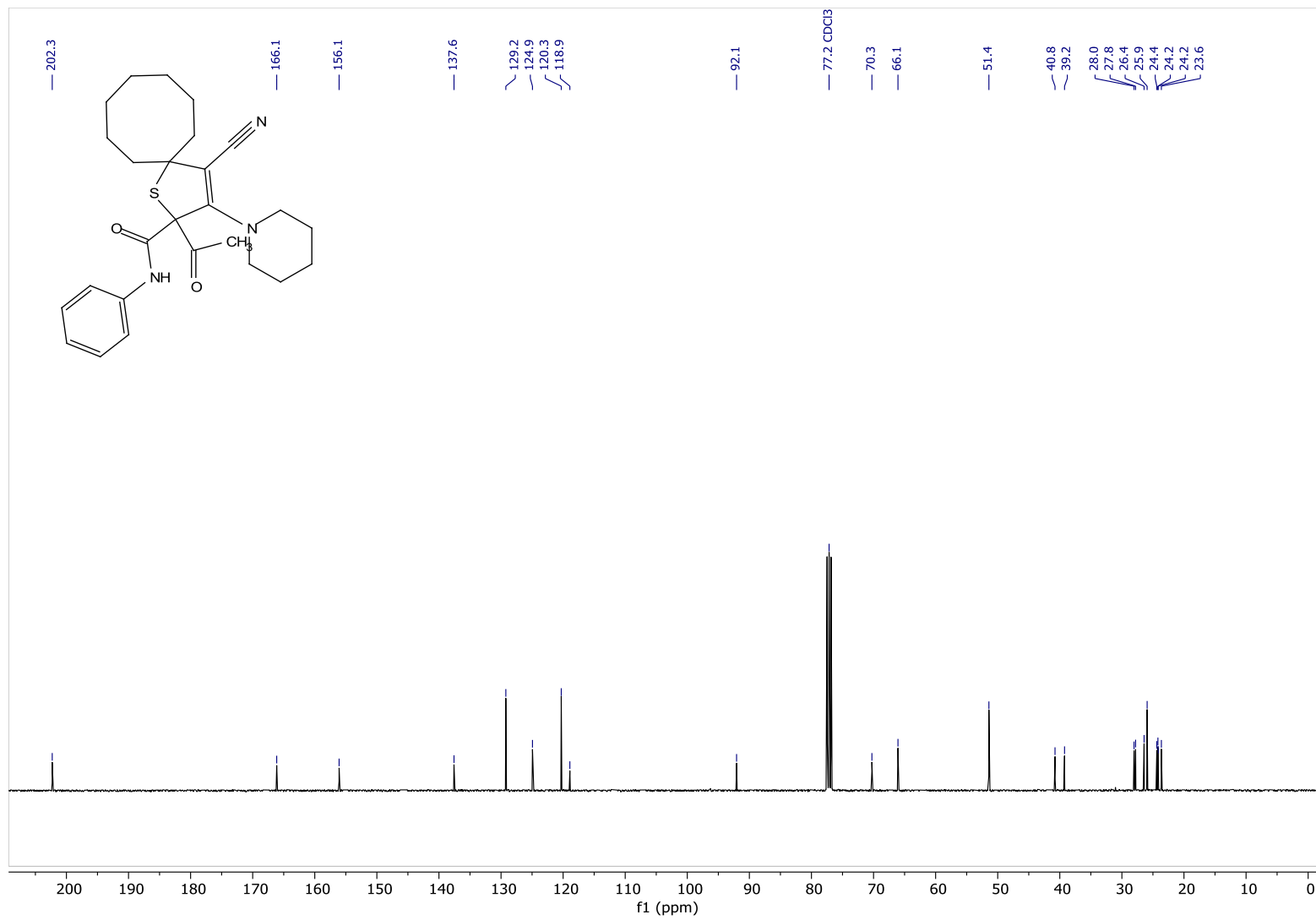
¹H NMR (400 MHz, CDCl₃-d) of **1j**



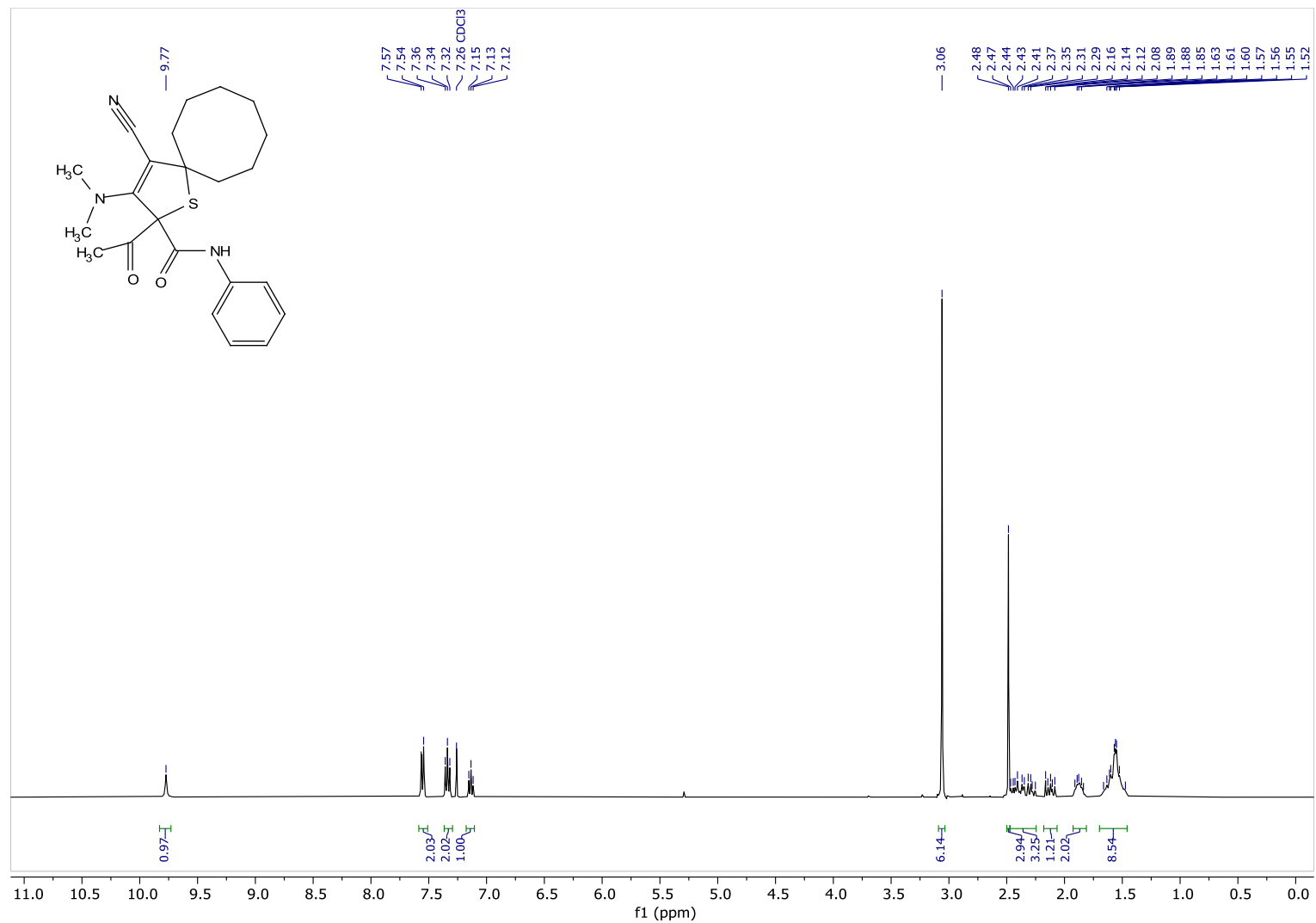
^{13}C NMR (100 MHz, CDCl_3 -d) of **1j**



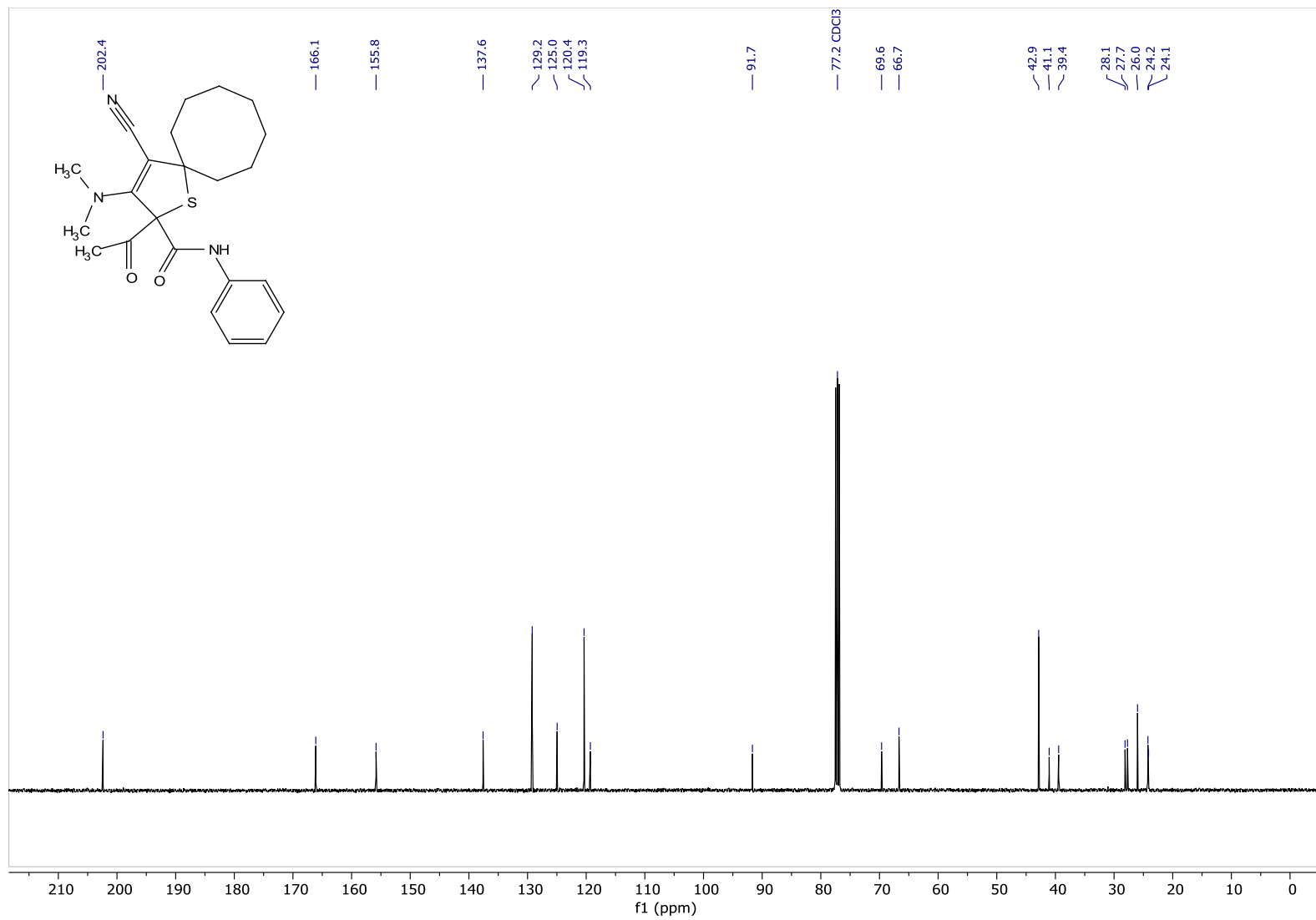
¹H NMR (400 MHz, CDCl₃-d) of **1k**



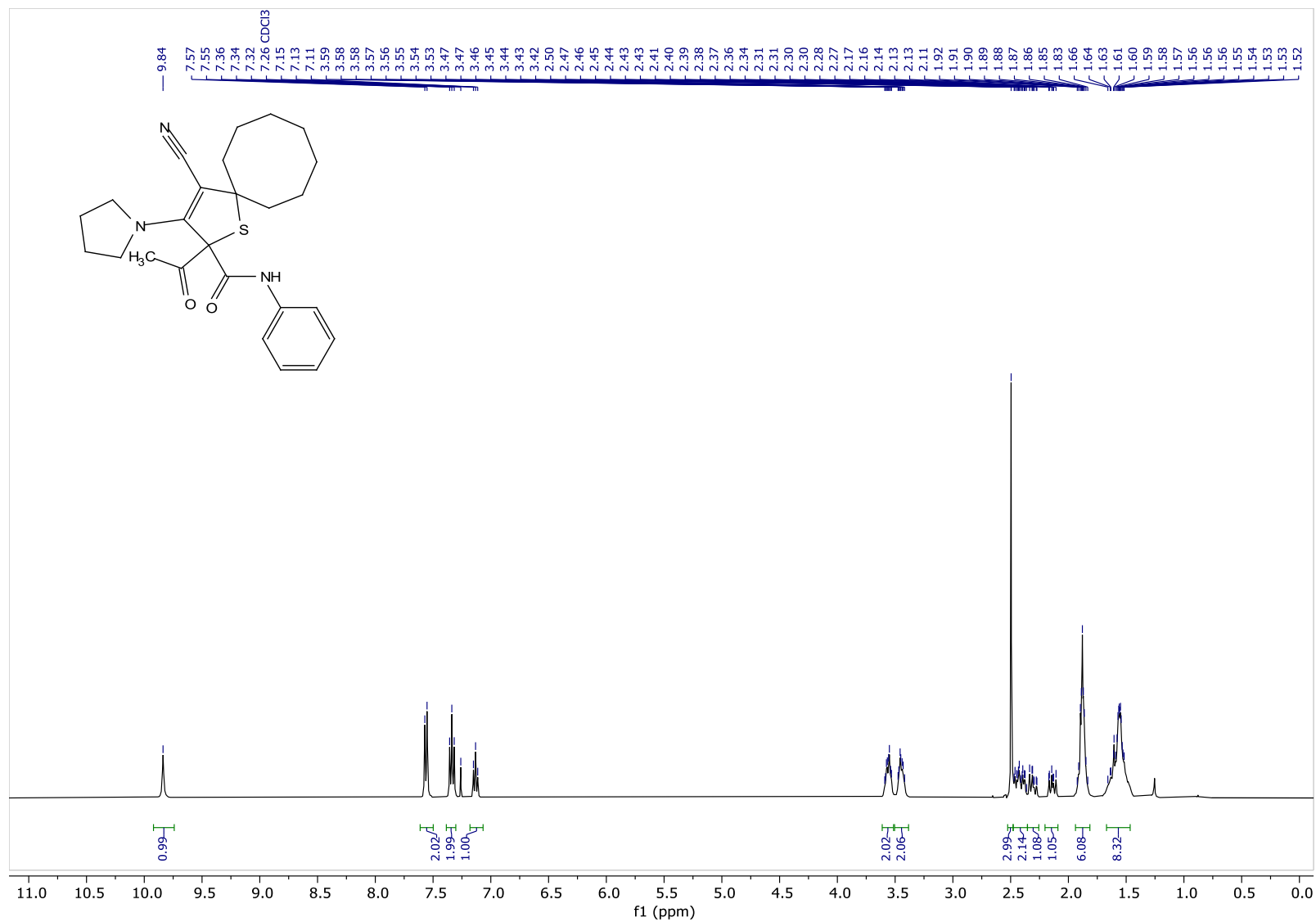
¹³C NMR (100 MHz, CDCl₃-d) of **1k**



^1H NMR (400 MHz, CDCl_3 -*d*) of **11**

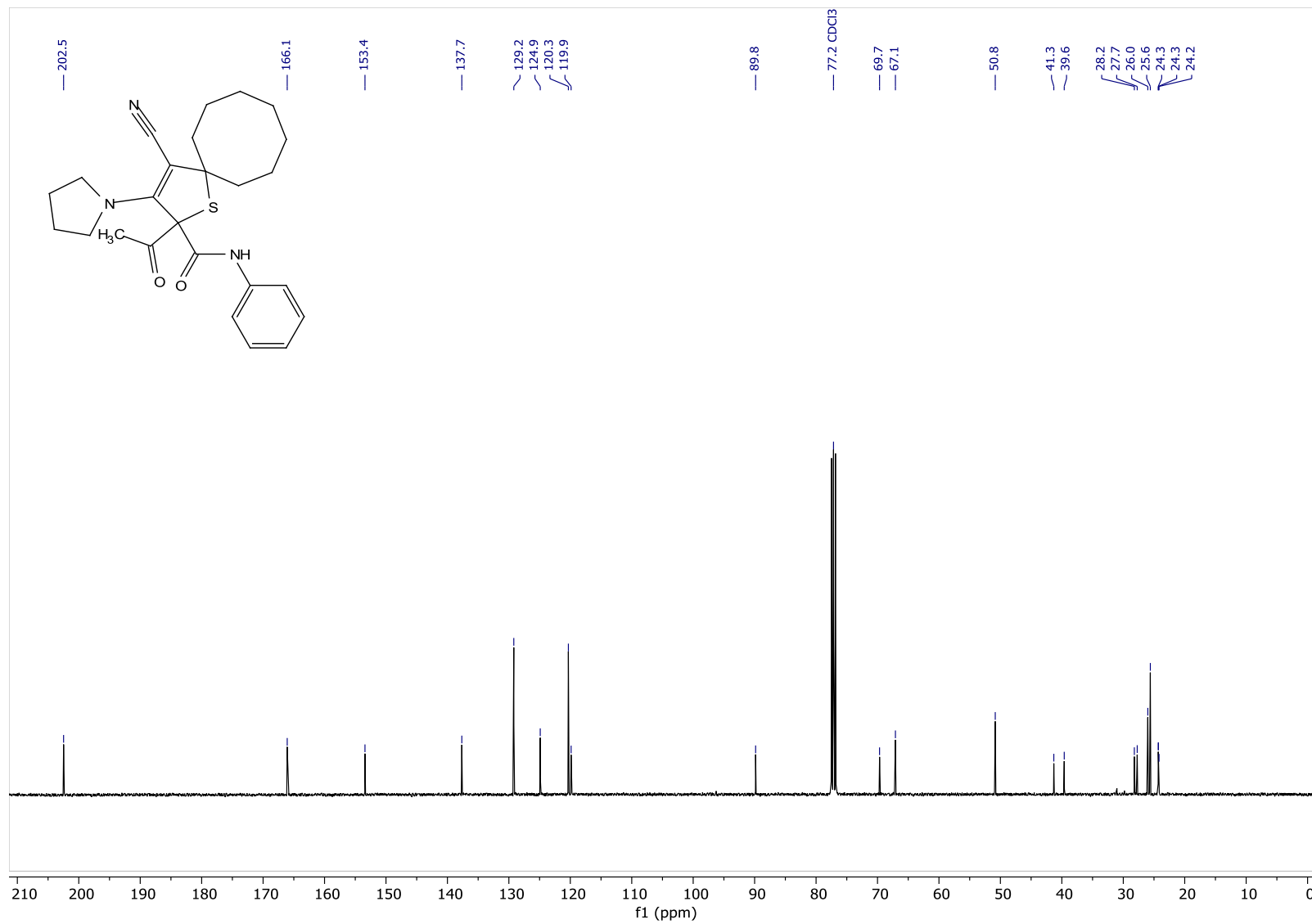


¹³C NMR (100 MHz, CDCl₃-d) of **11**



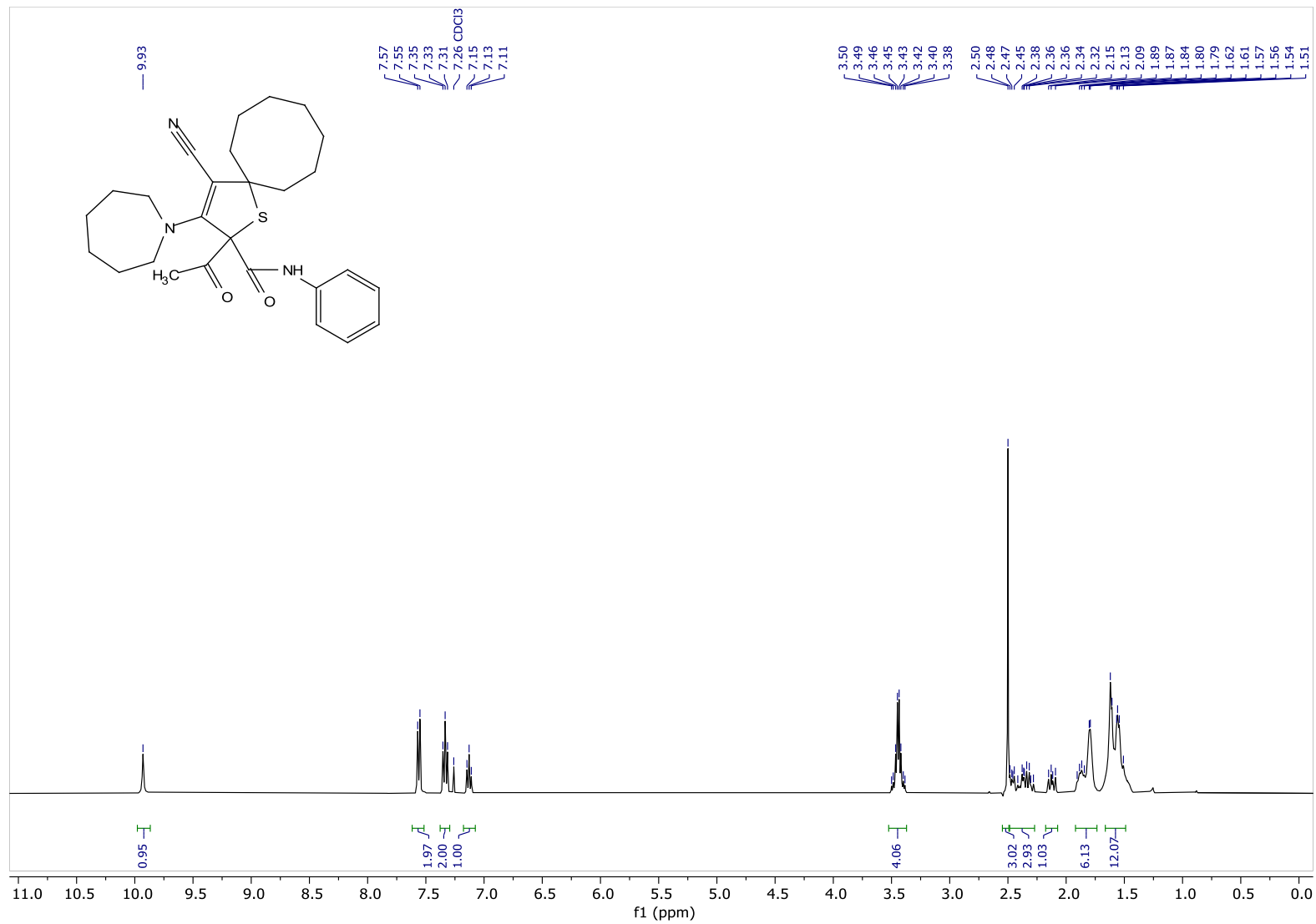
¹H NMR (400 MHz, CDCl₃-d) of **1m**

S21

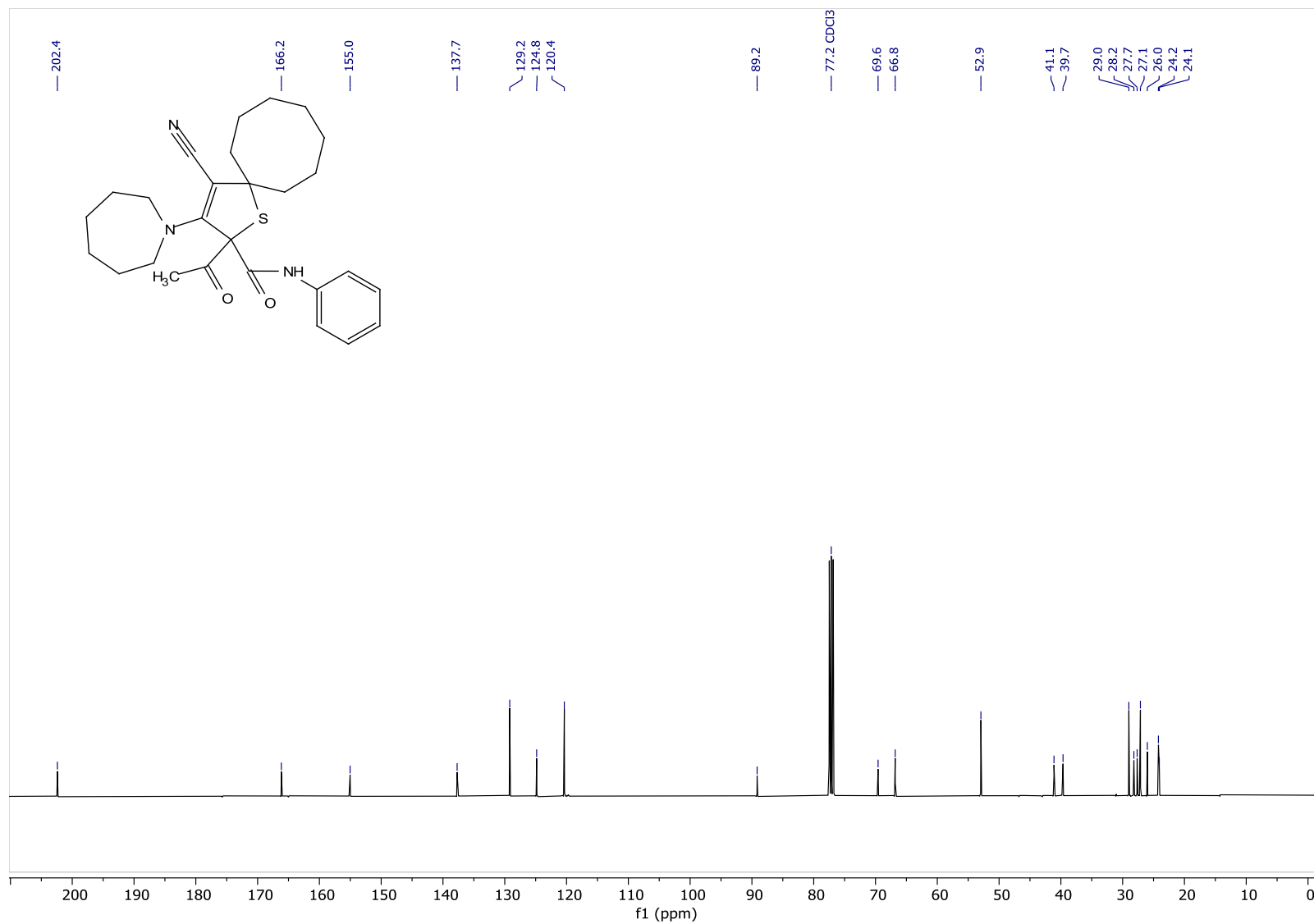


¹³C NMR (100 MHz, CDCl₃-d) of **1m**

S22

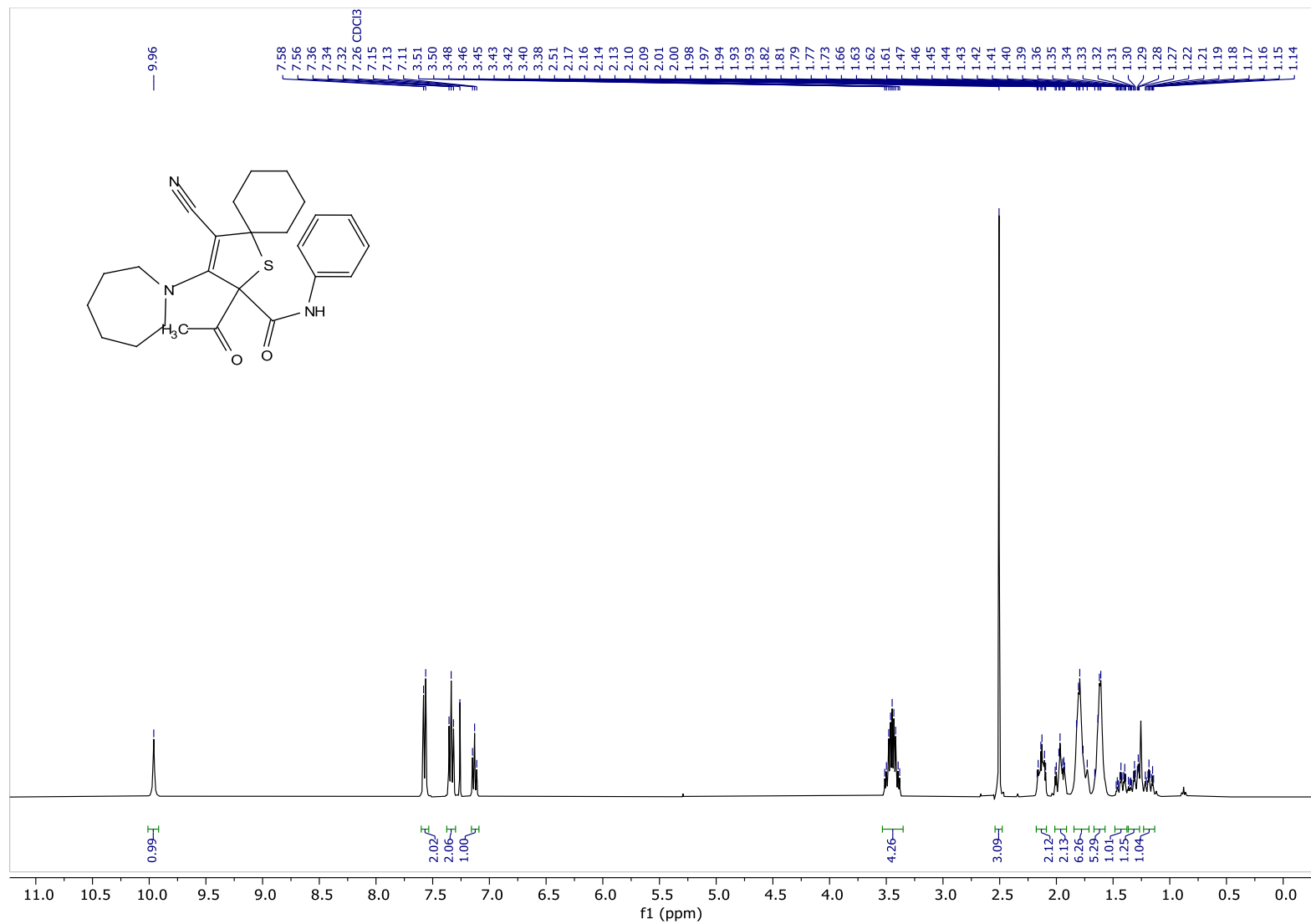


^1H NMR (400 MHz, CDCl_3 -d) of **1n**

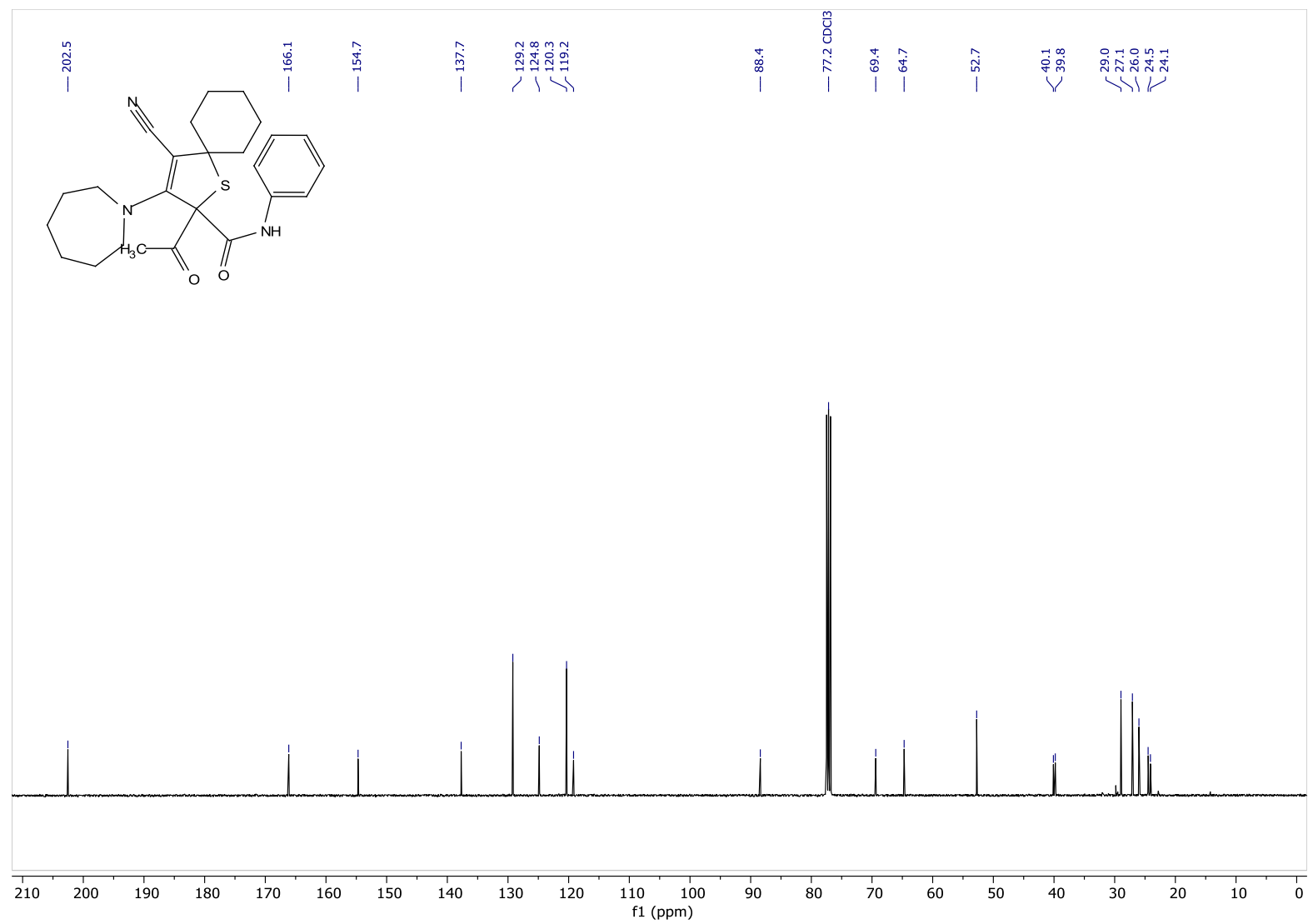


¹³C NMR (100 MHz, CDCl₃-d) of **1n**

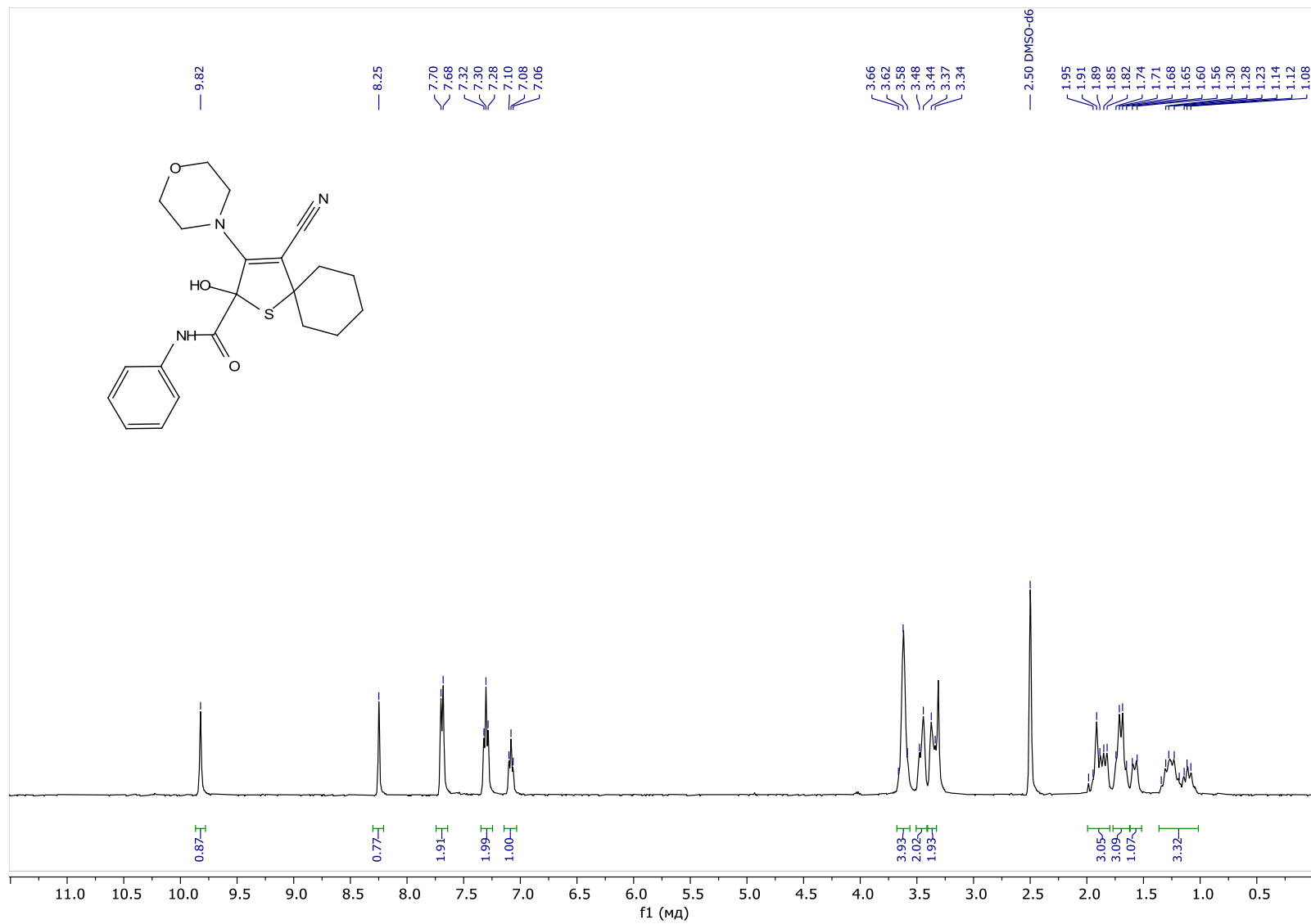
S24



¹H NMR (400 MHz, CDCl₃-d) of **1o**

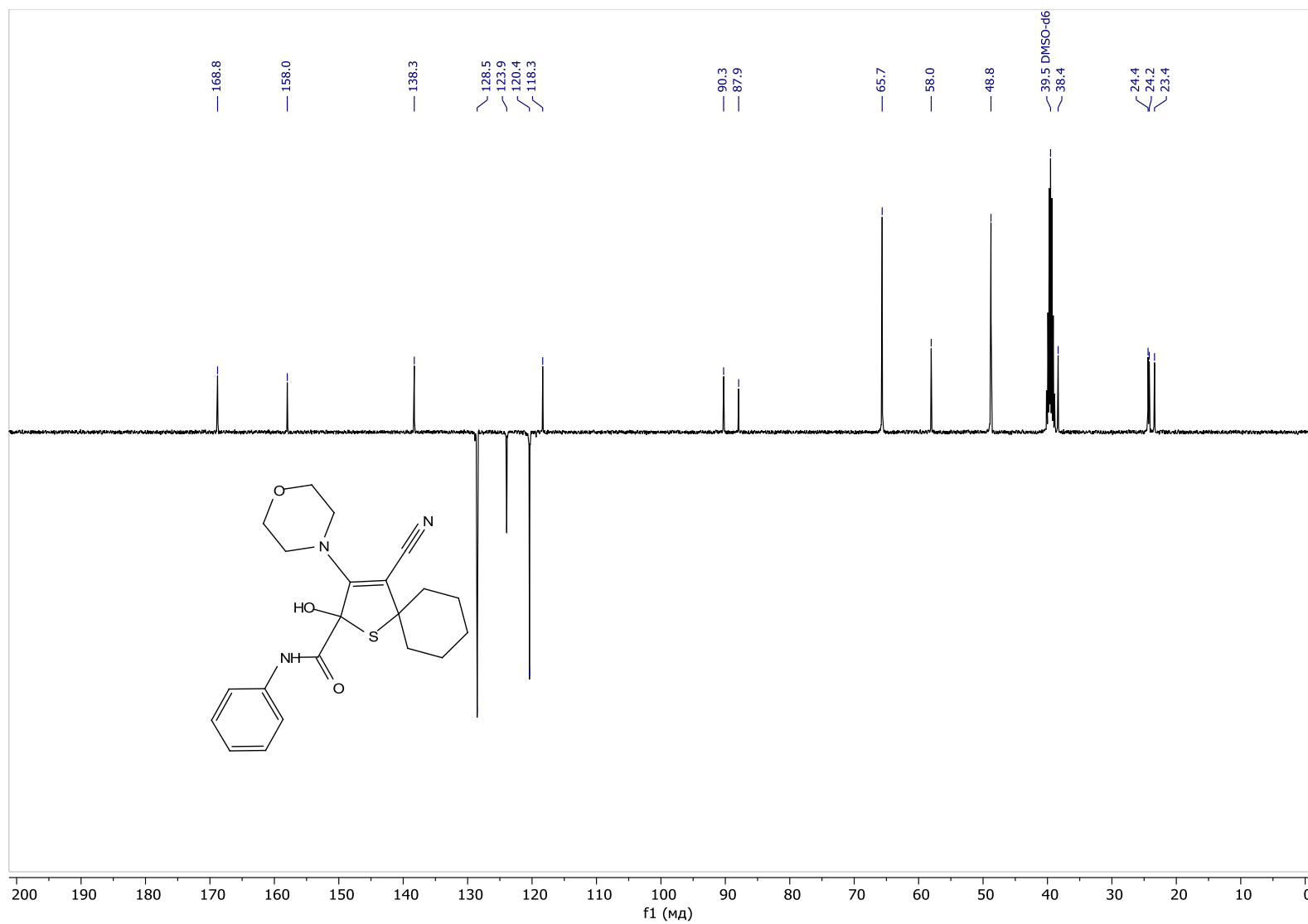


¹³C NMR (100 MHz, CDCl₃-d) of **1o**

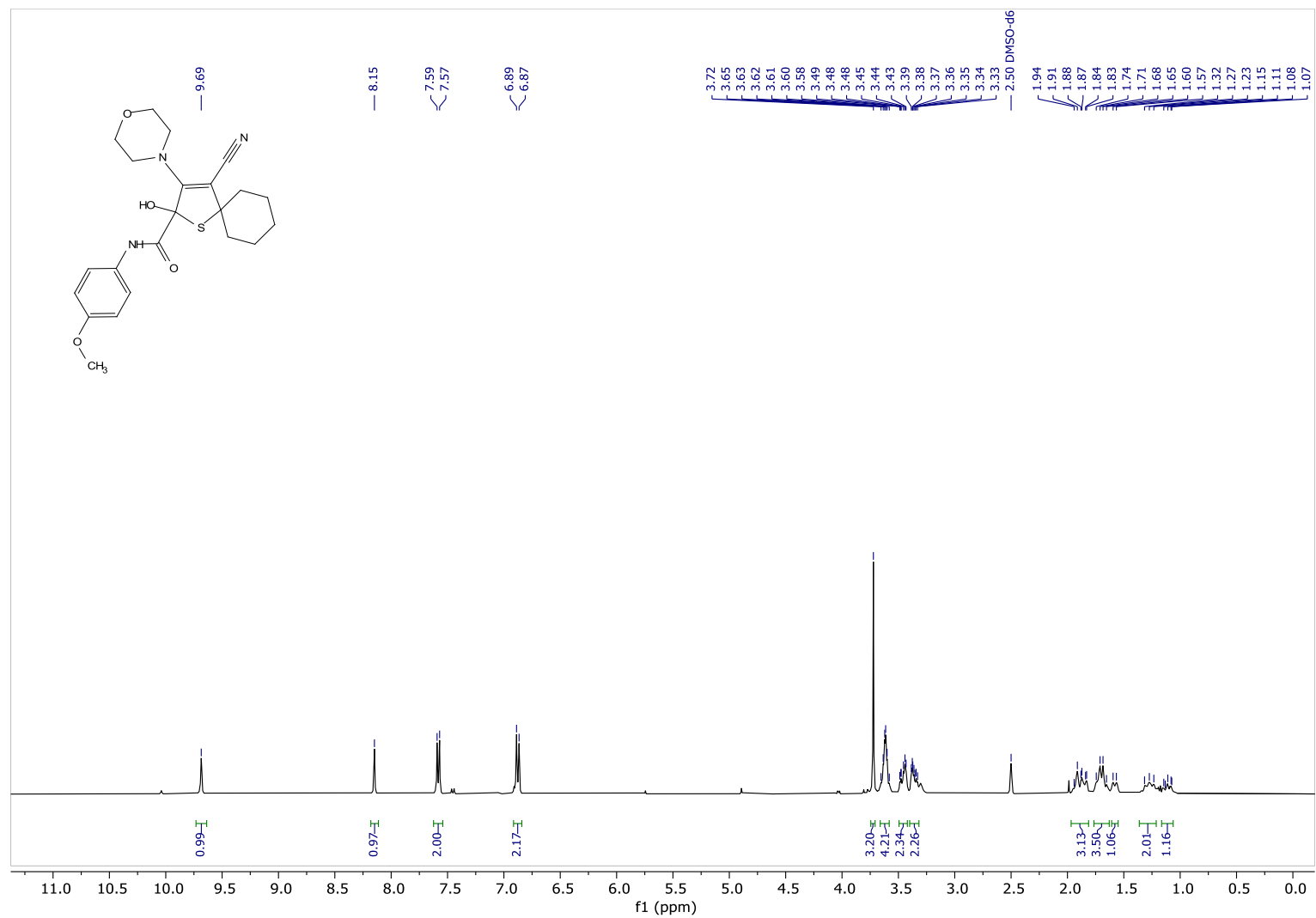


¹H NMR (400 MHz, DMSO-*d*₆) of **2a**

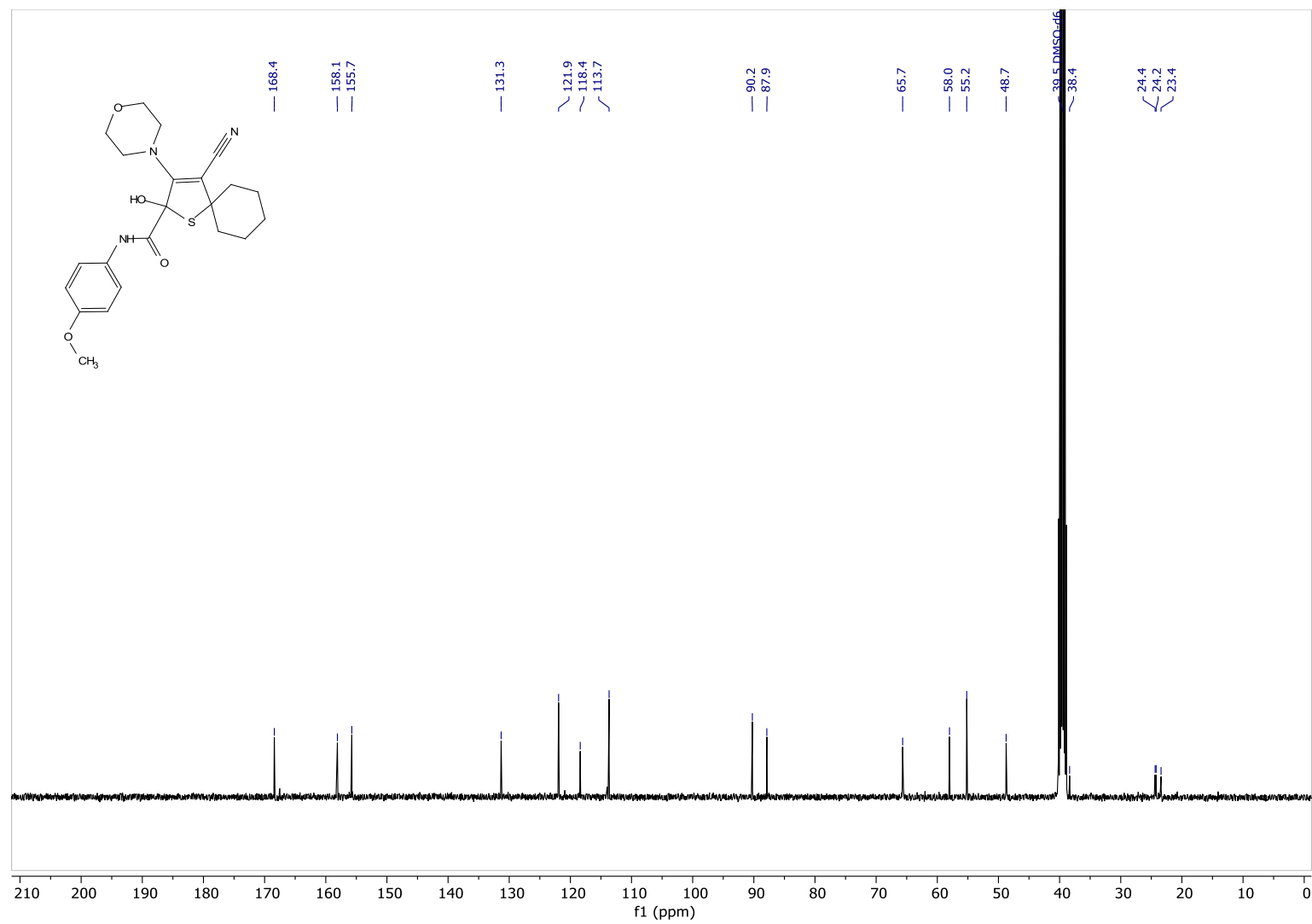
S27



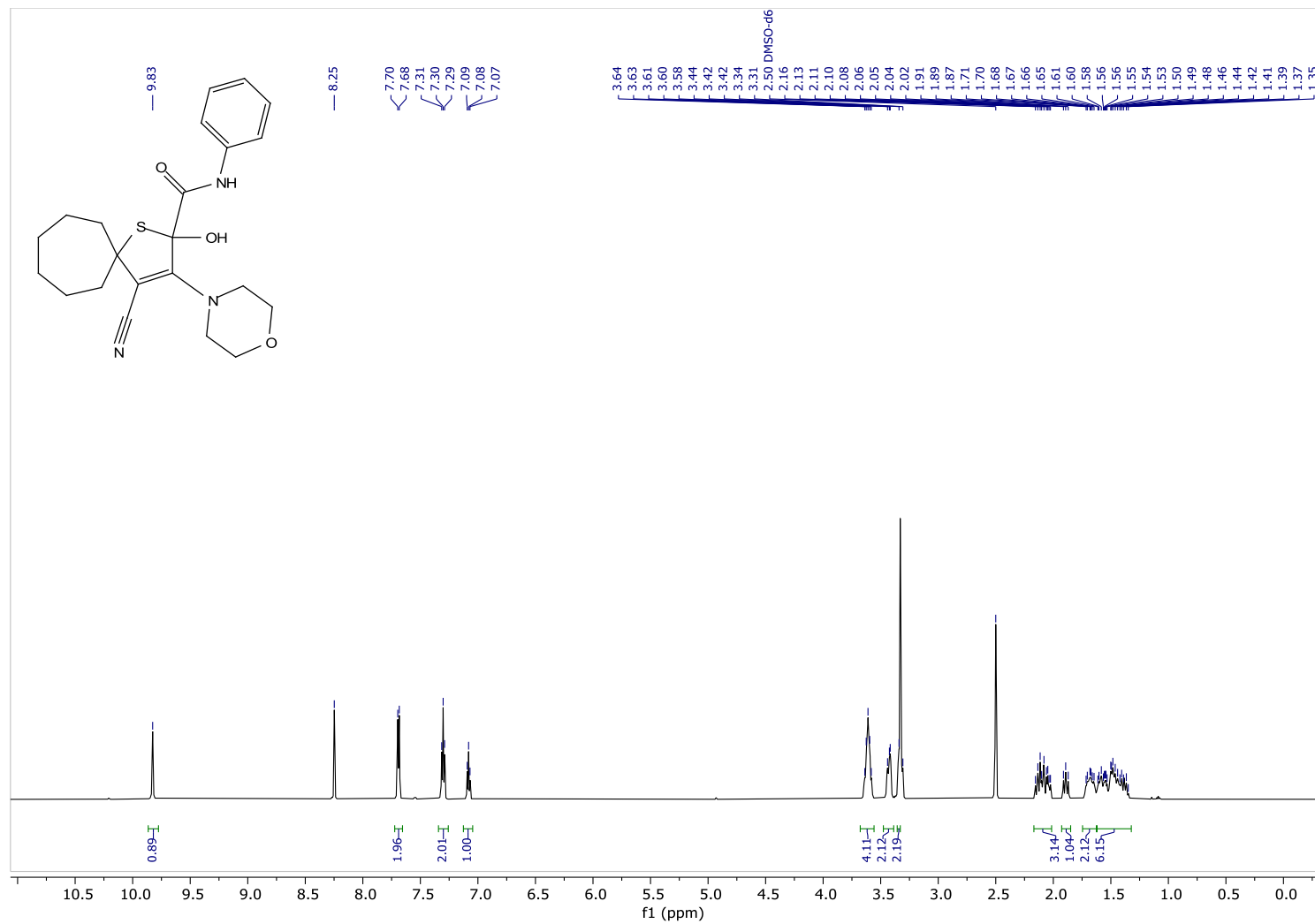
^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) of **2a**

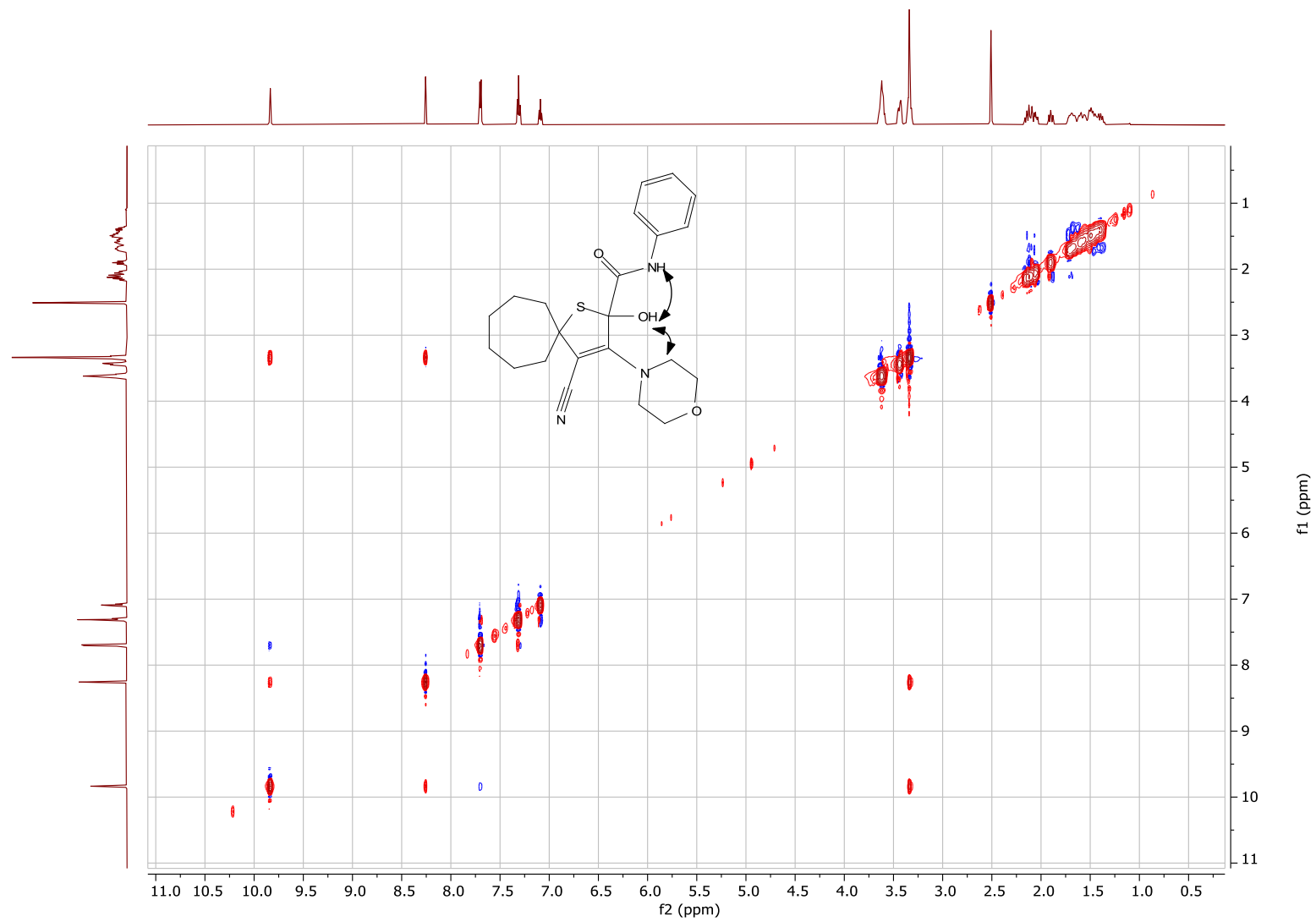


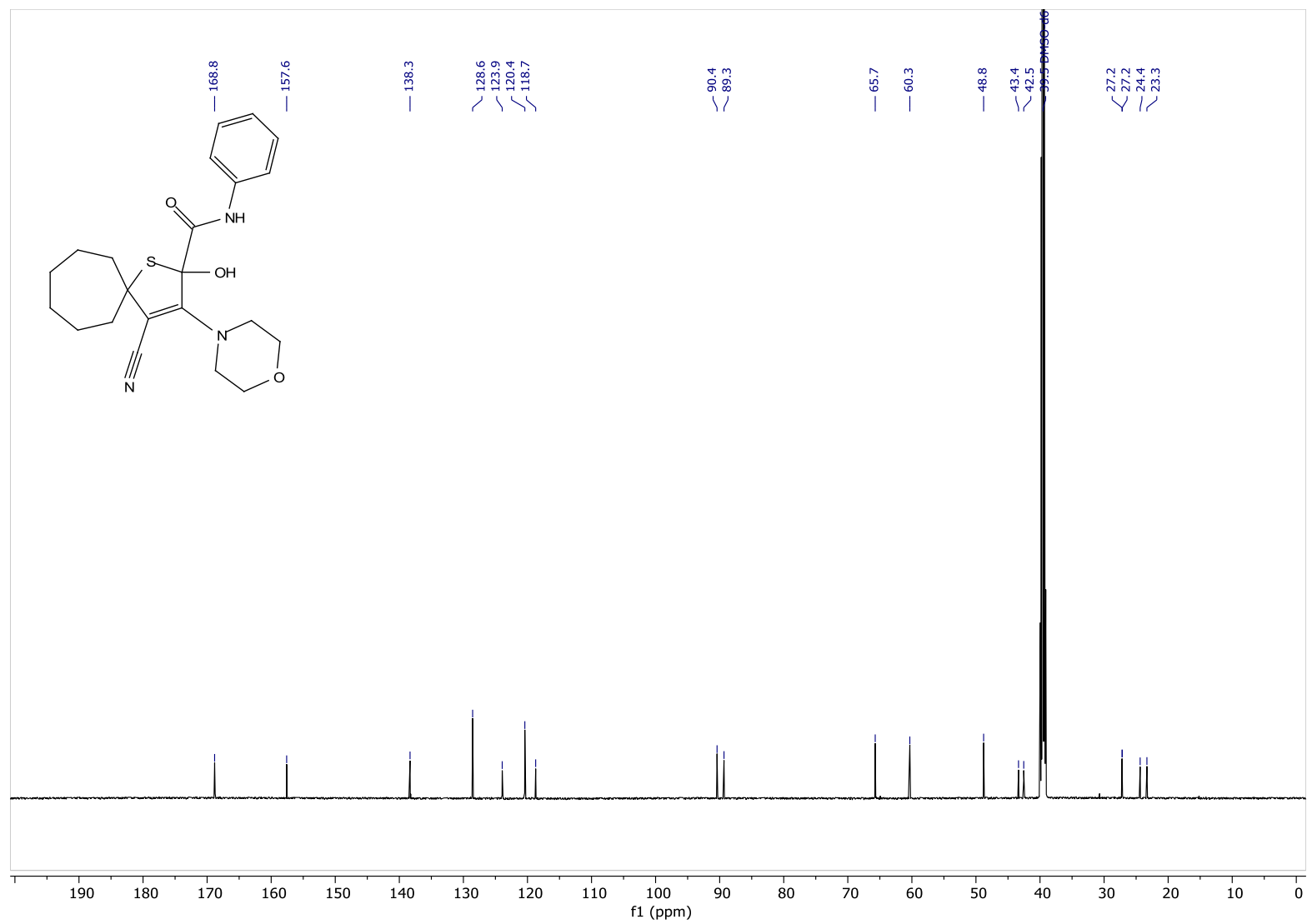
^1H NMR (400 MHz, $\text{DMSO}-d_6$) of **2b**



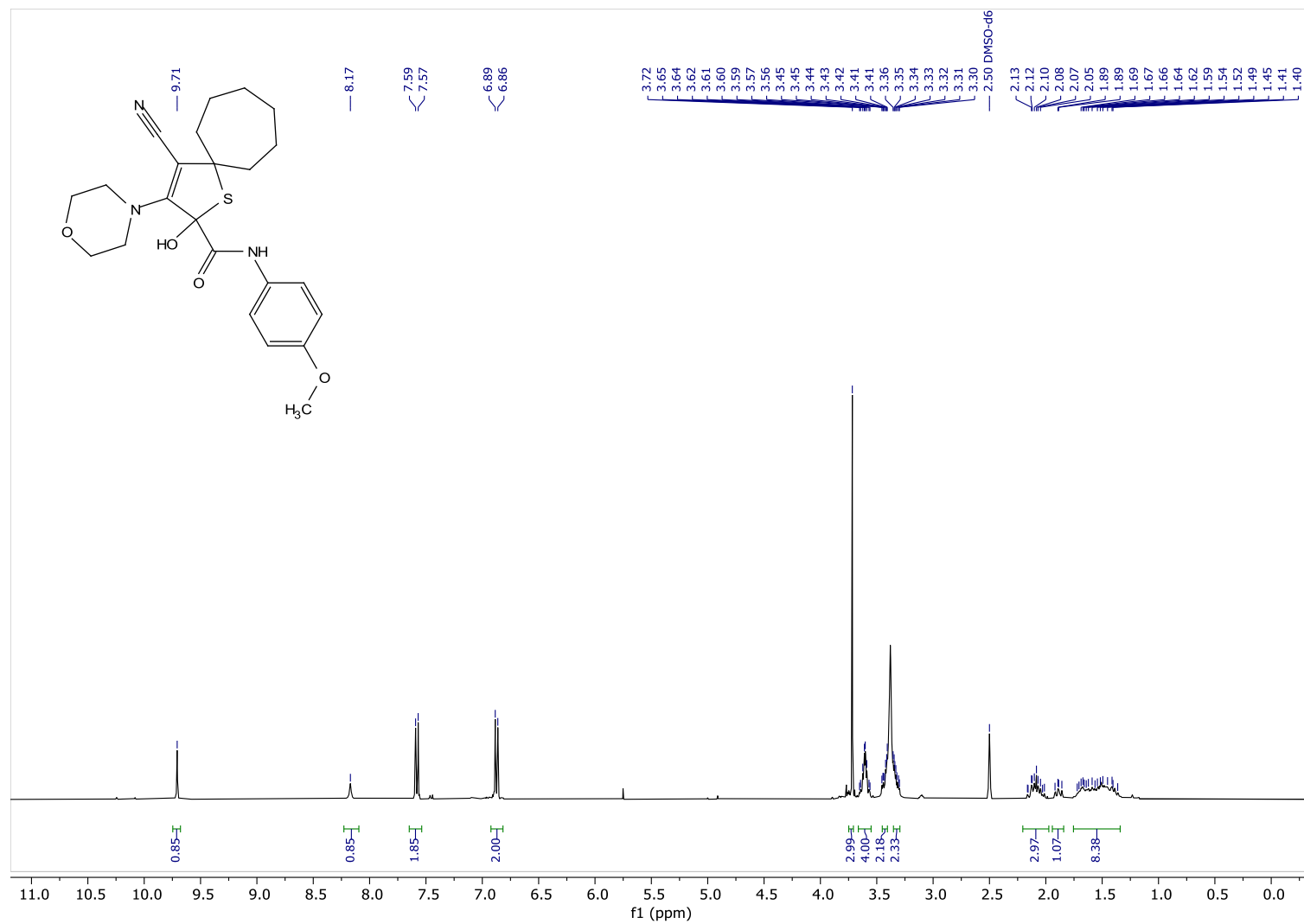
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **2b**

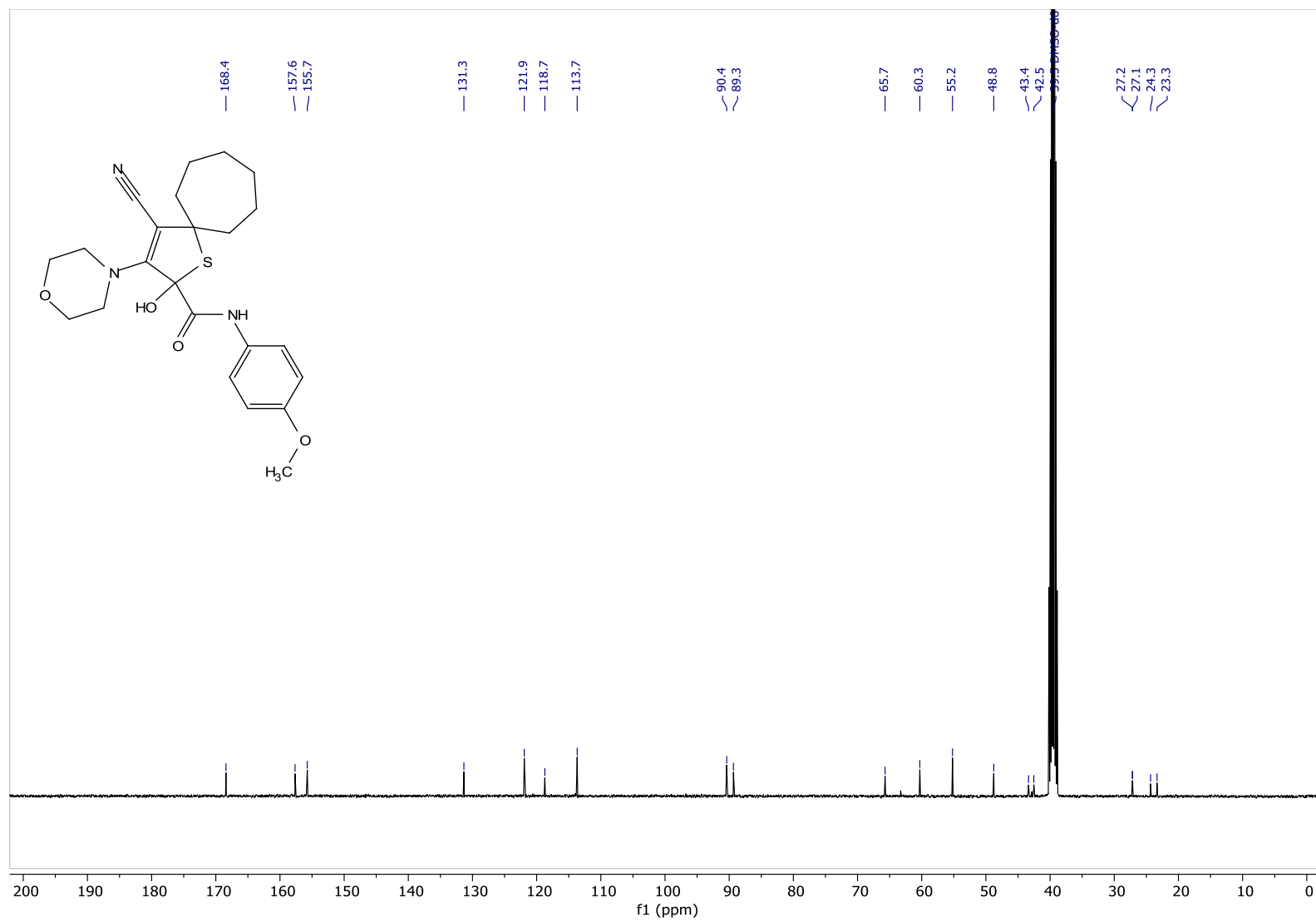




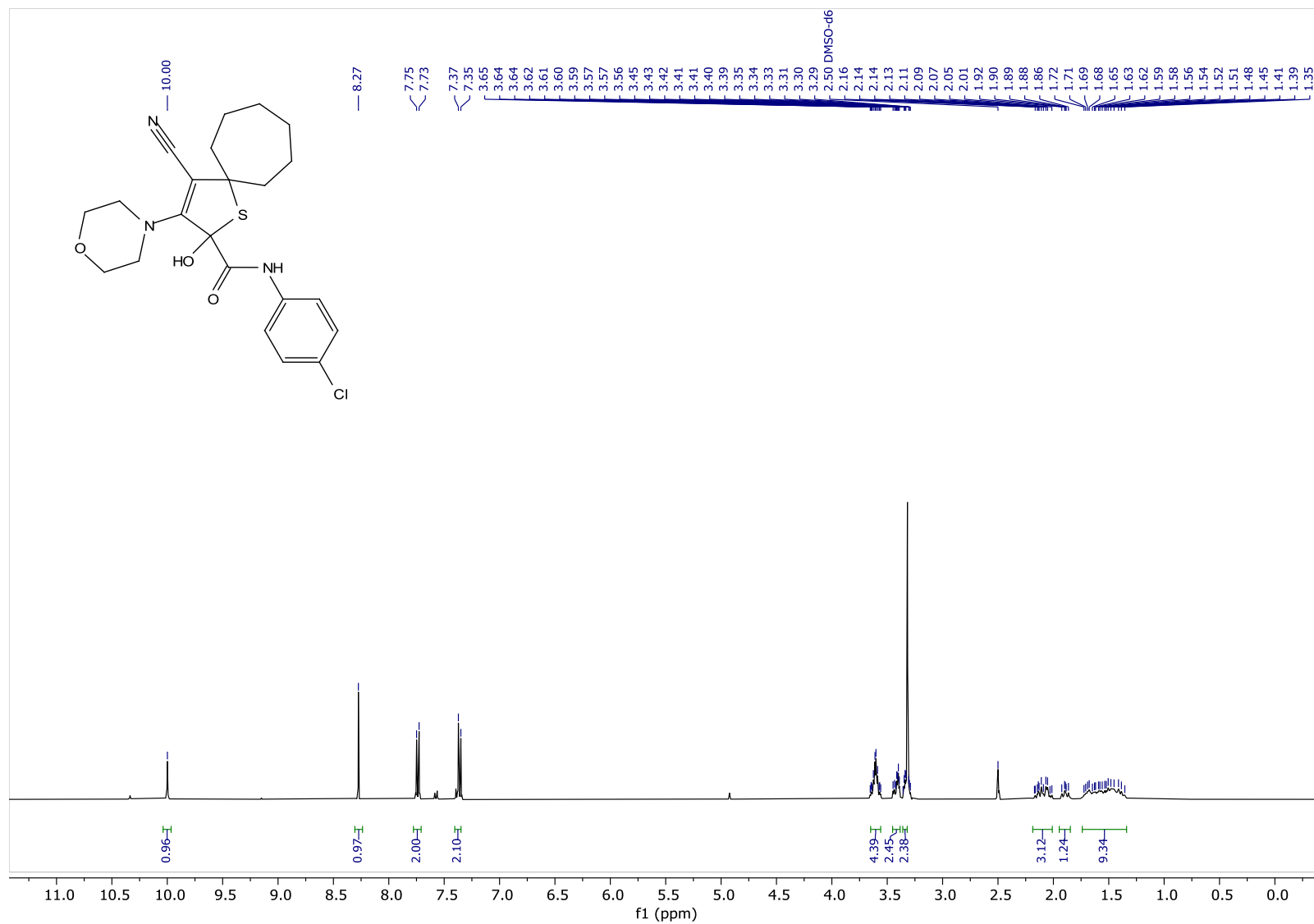


¹³C NMR (100 MHz, DMSO-*d*₆) of **2c**



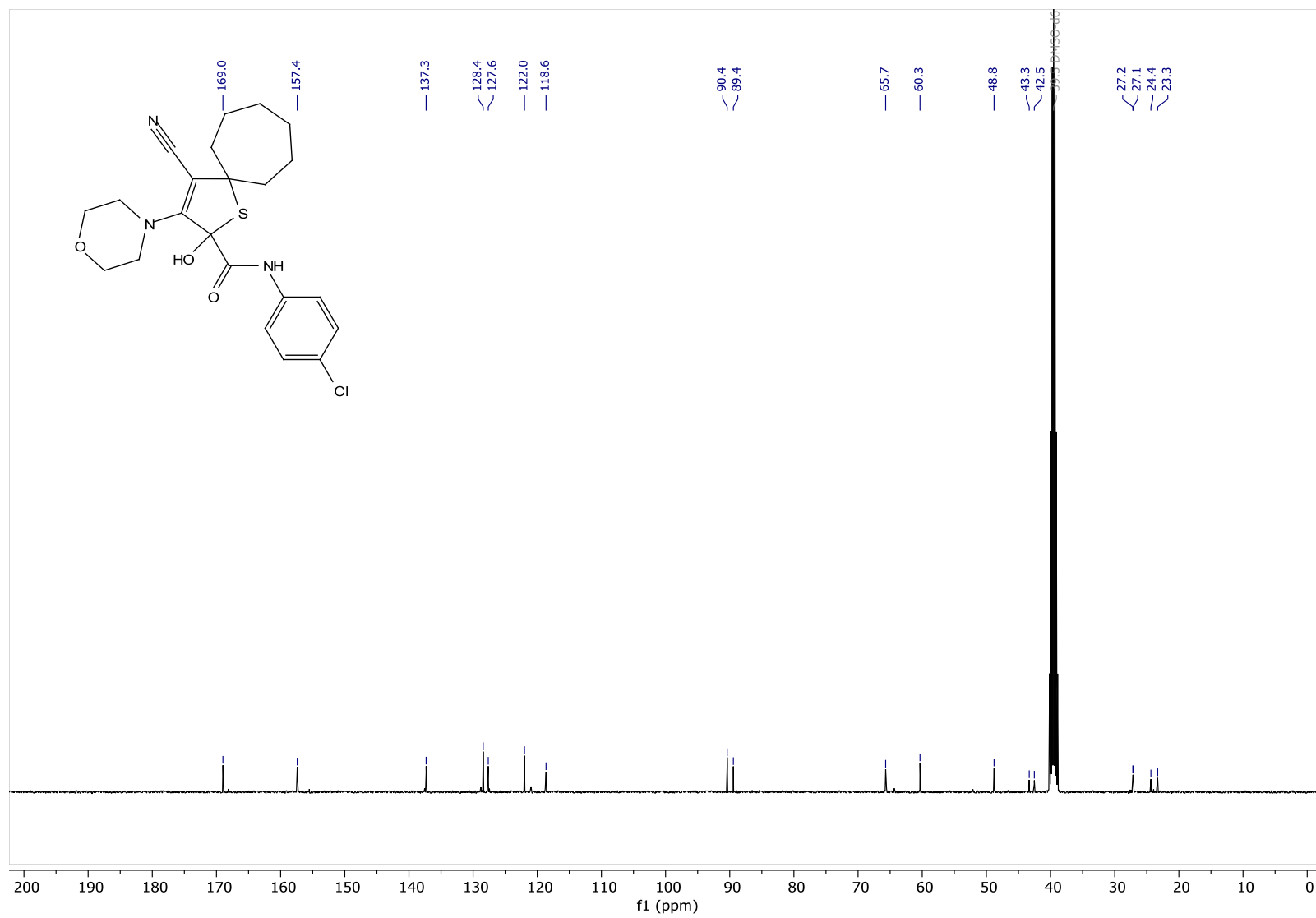


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **2d**

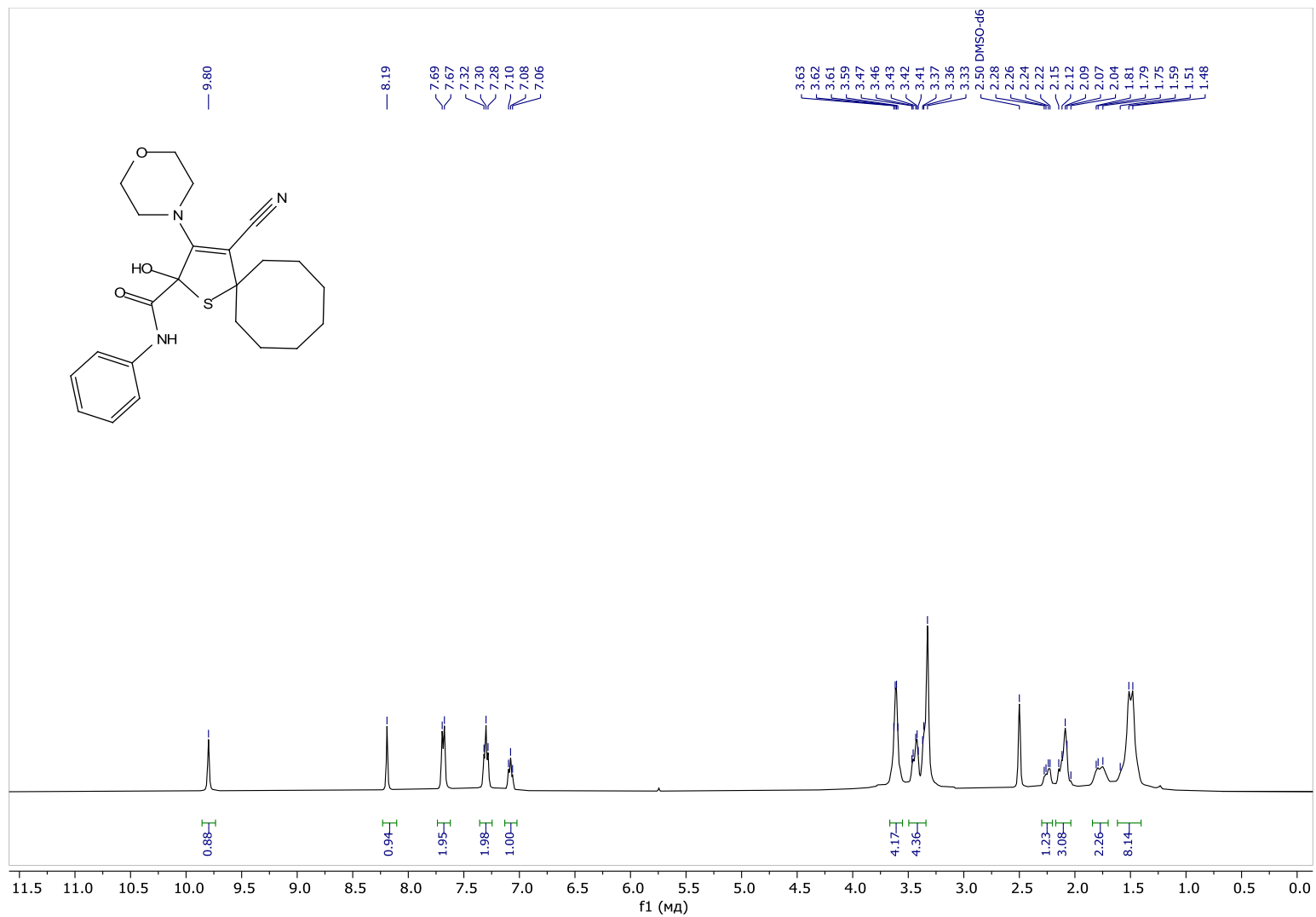


^1H NMR (400 MHz, $\text{DMSO}-d_6$) of **2e**

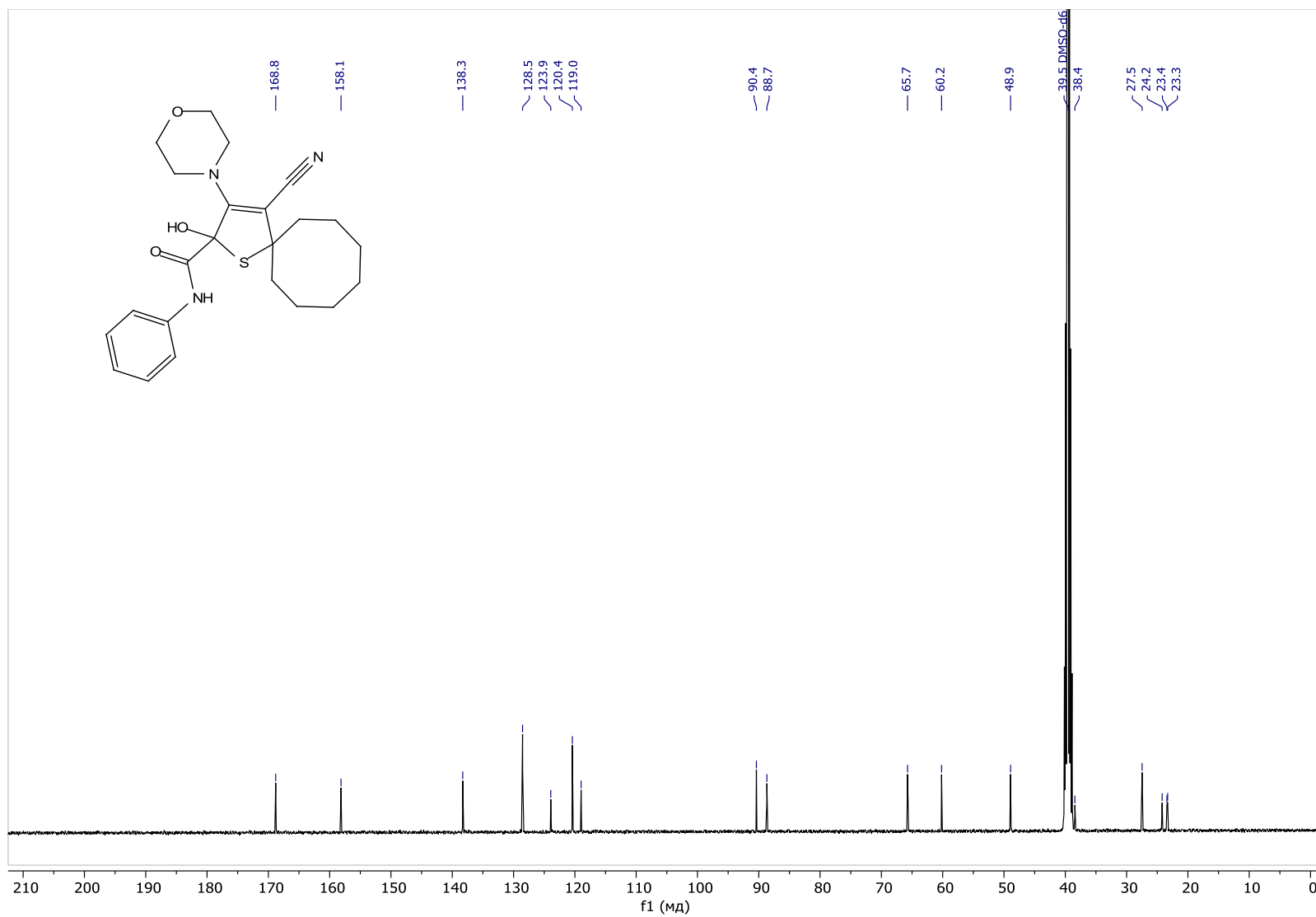
S36



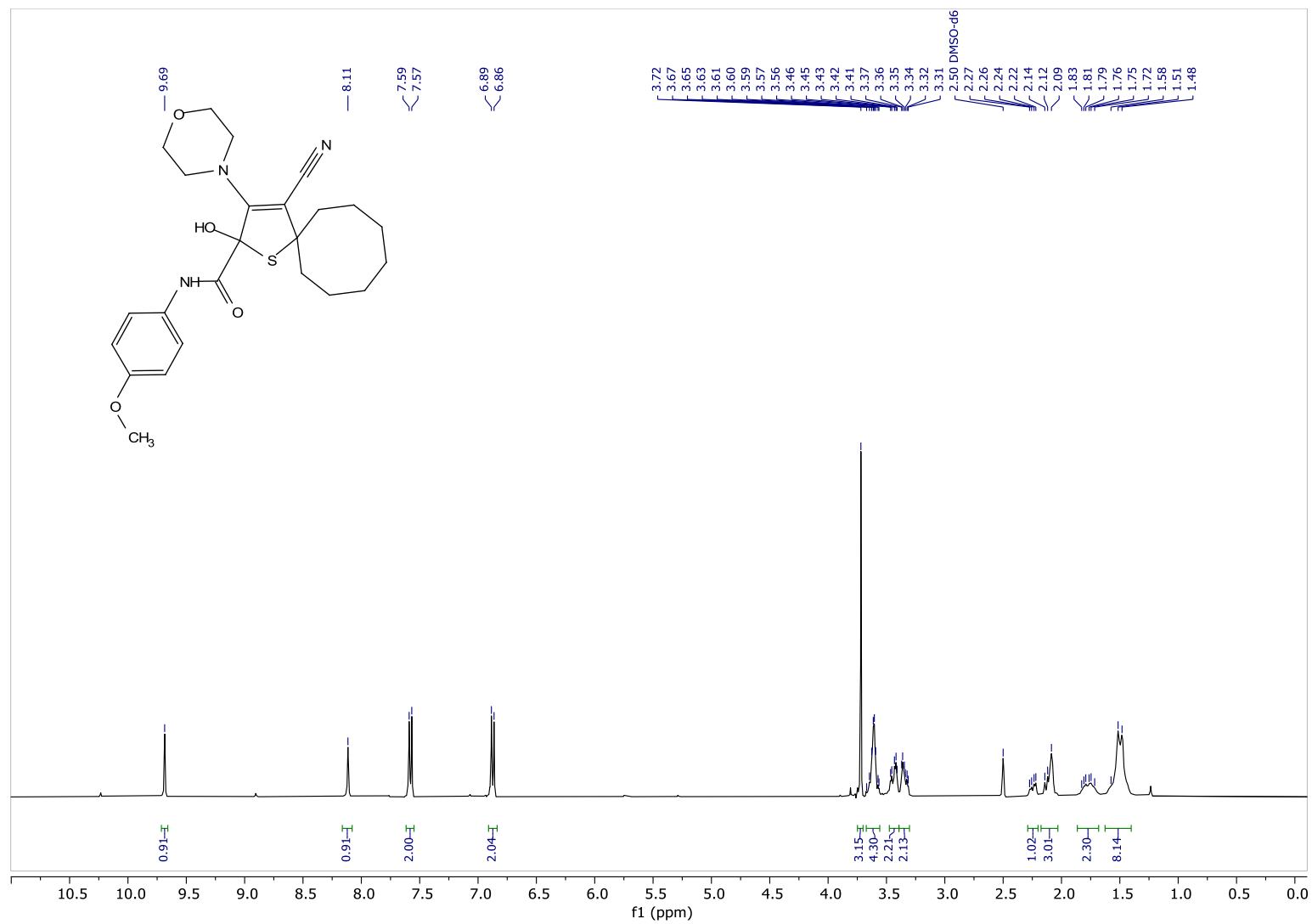
¹³C NMR (100 MHz, DMSO-*d*₆) of **2e**



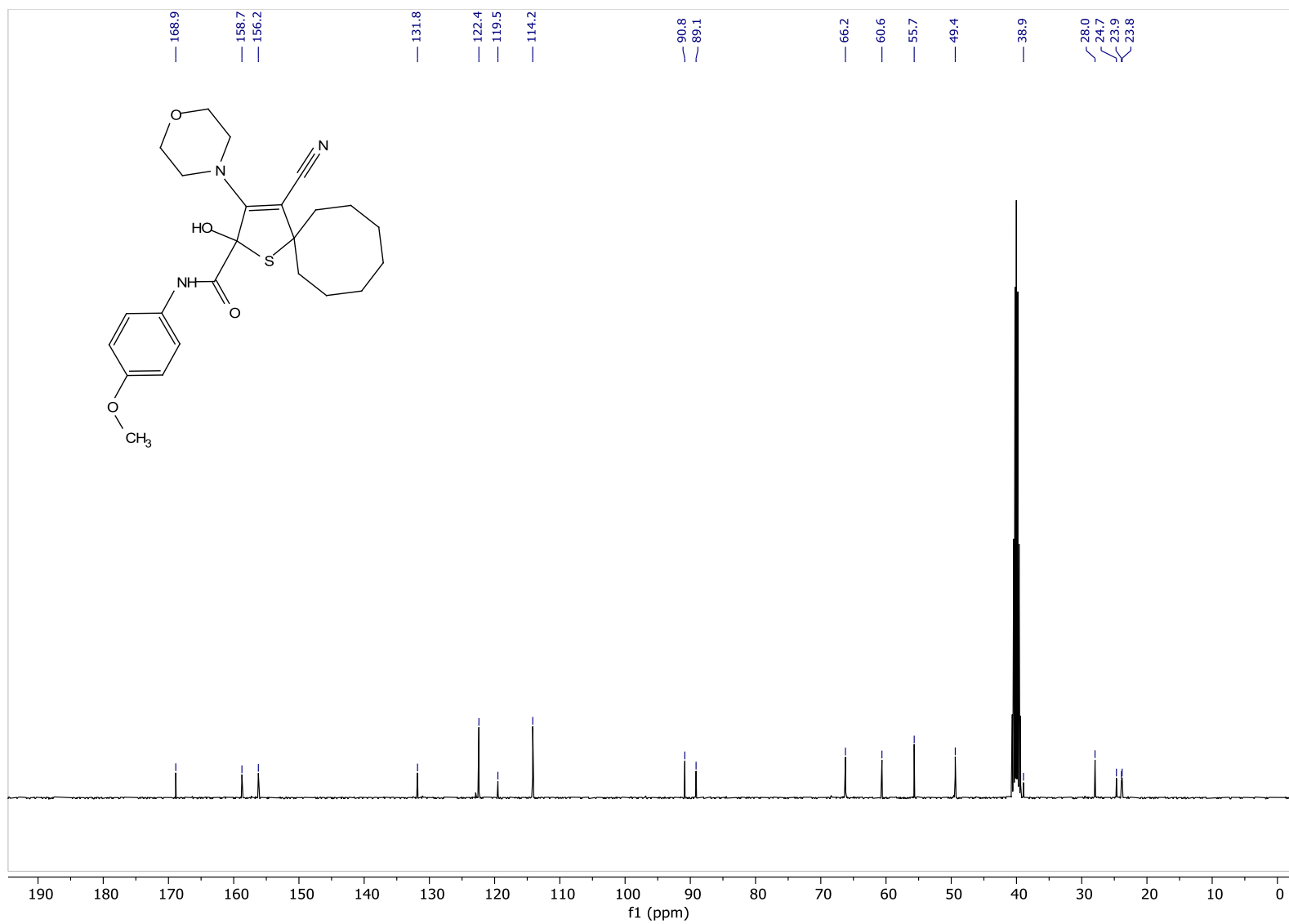
¹H NMR (400 MHz, DMSO-*d*₆) of **2f**



^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **2f**

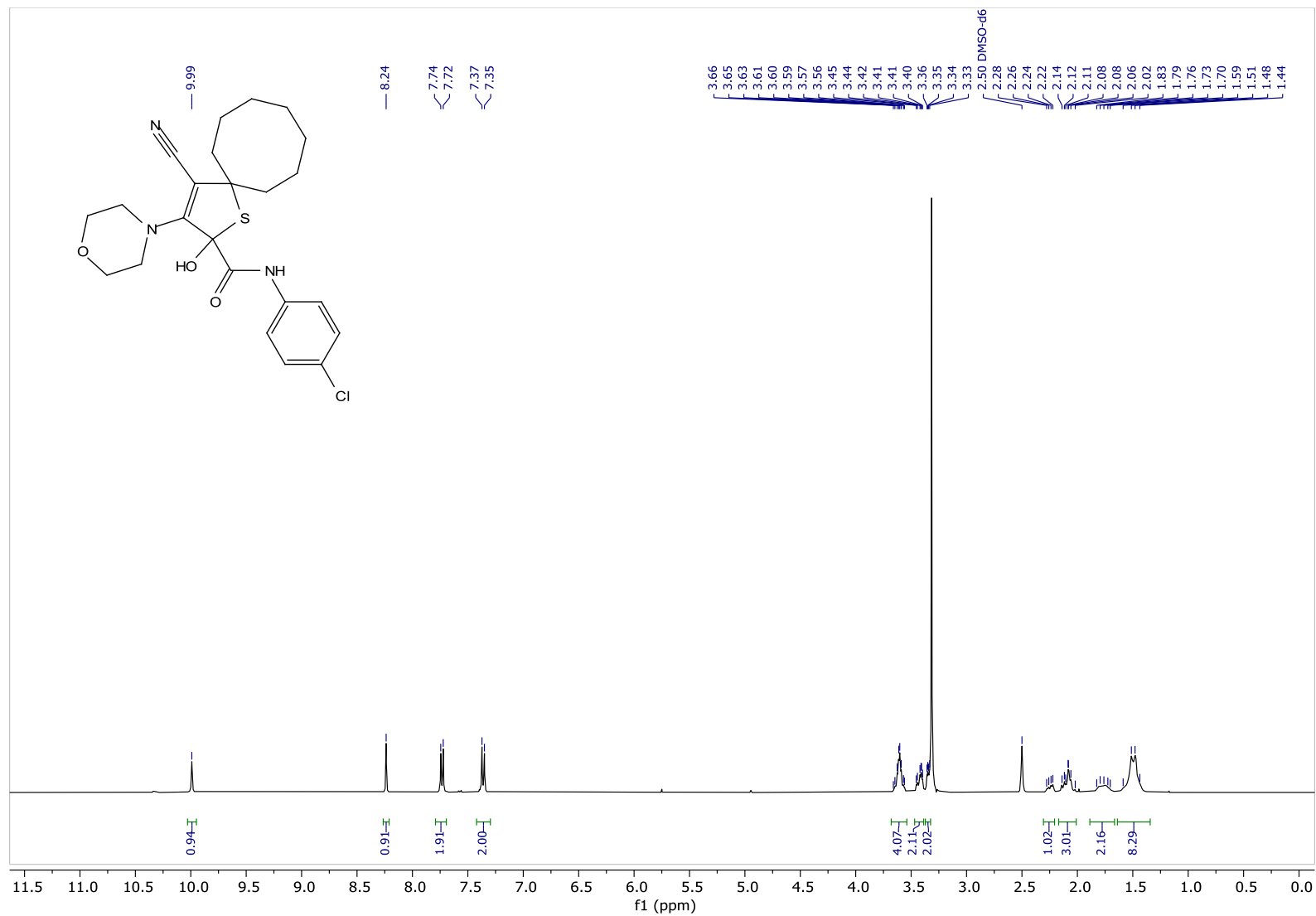


¹H NMR (400 MHz, DMSO-*d*₆) of **2g**

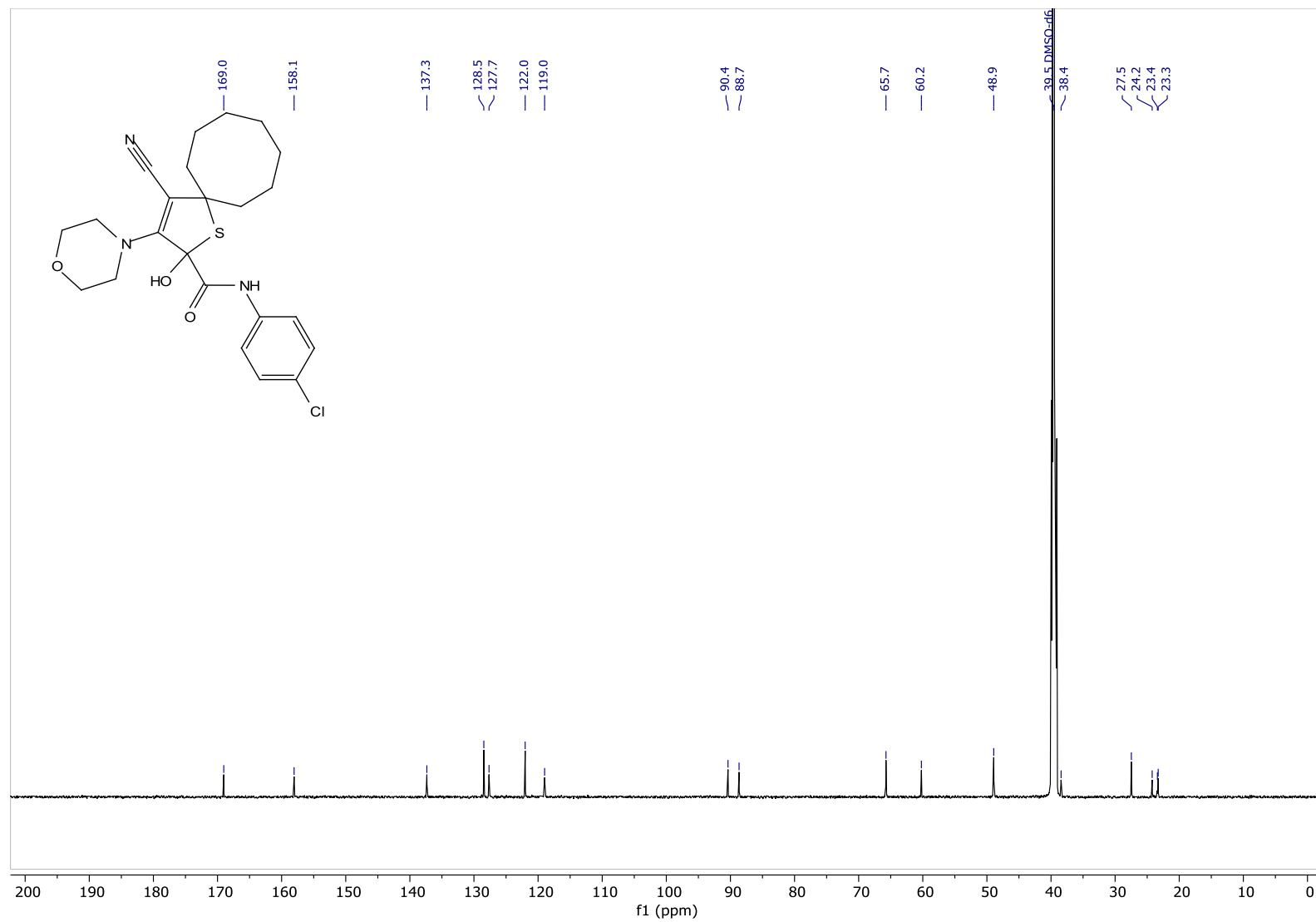


¹³C NMR (100 MHz, DMSO-*d*₆) of **2g**

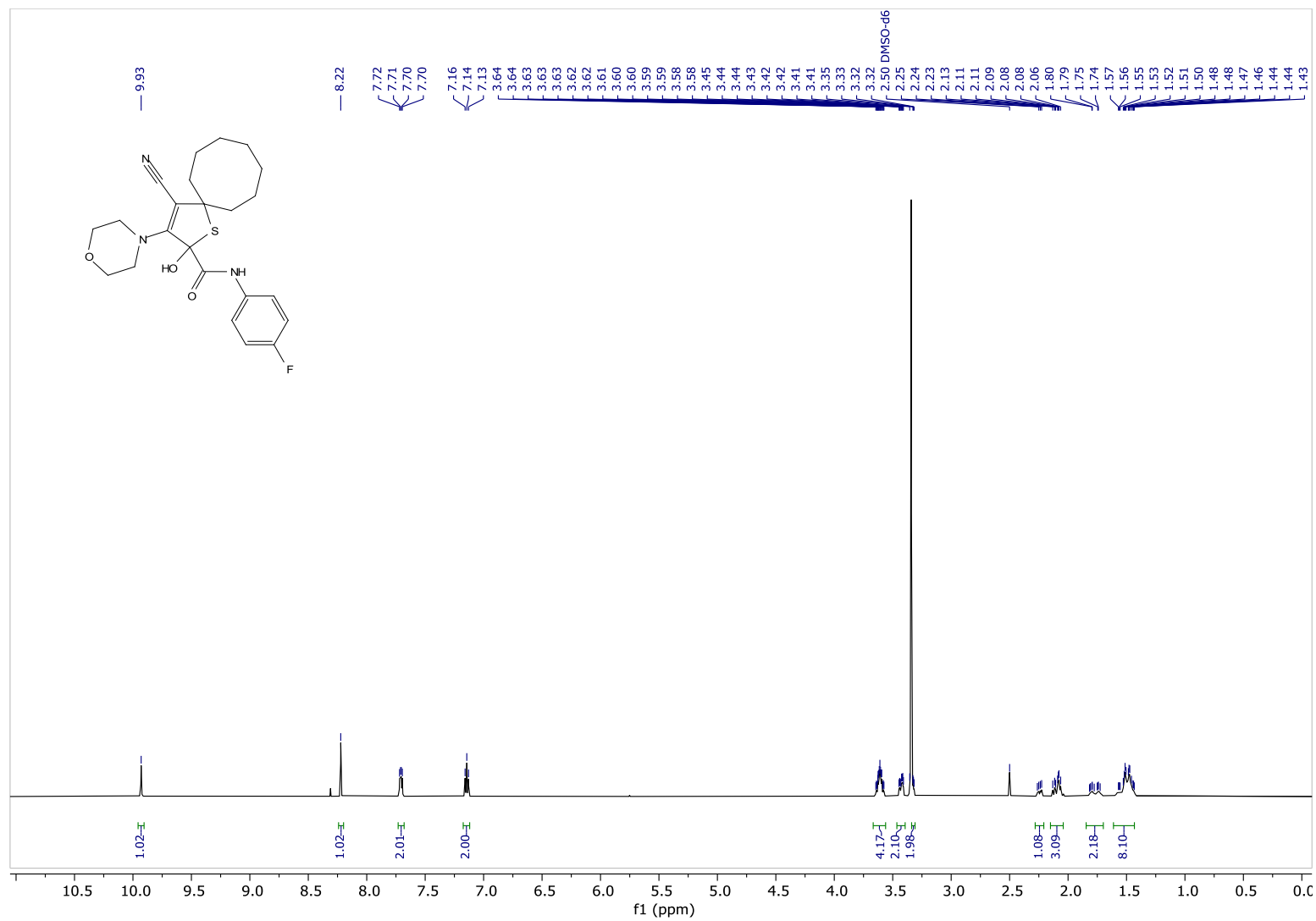
S41



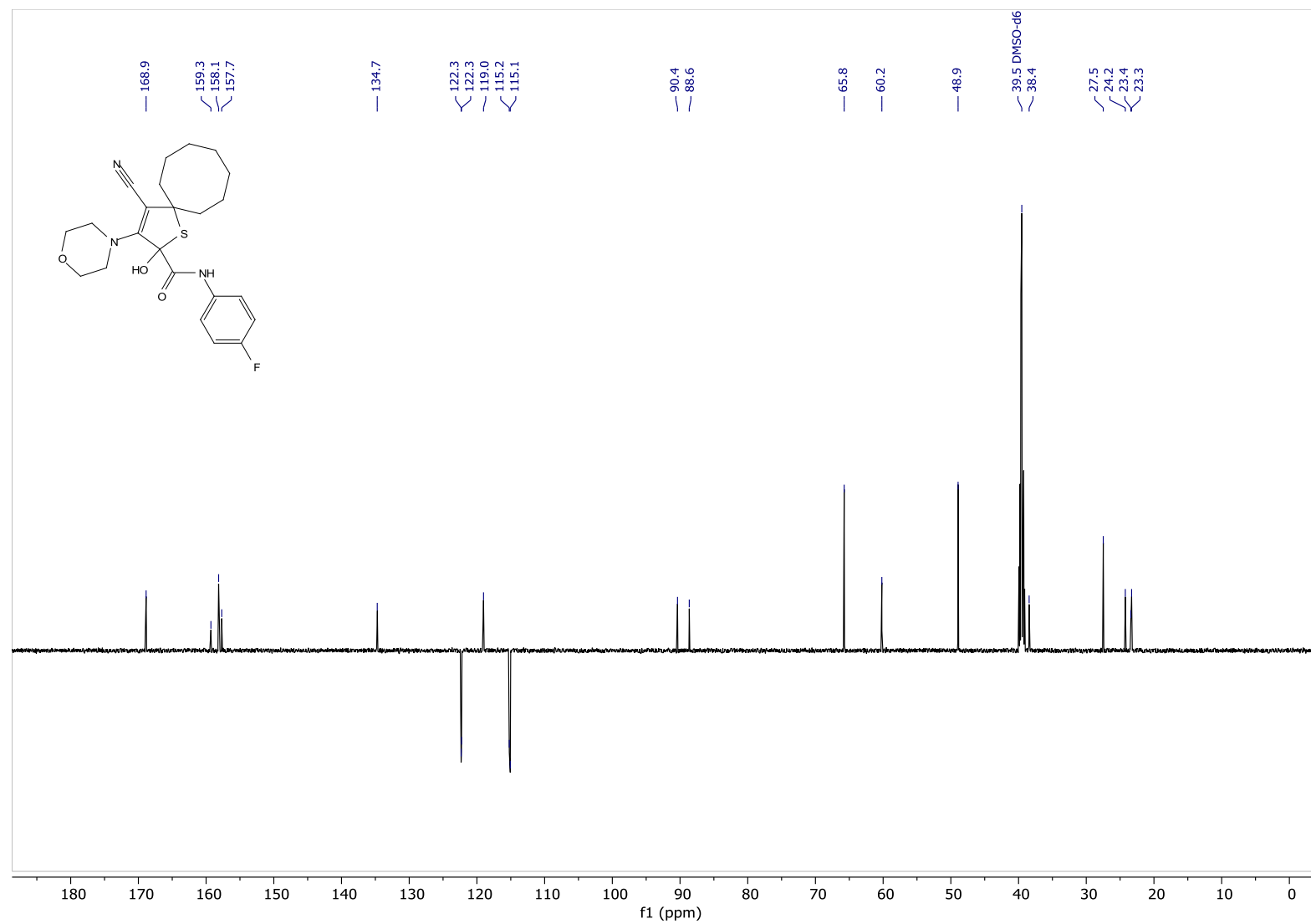
^1H NMR (400 MHz, DMSO- d_6) of **2h**



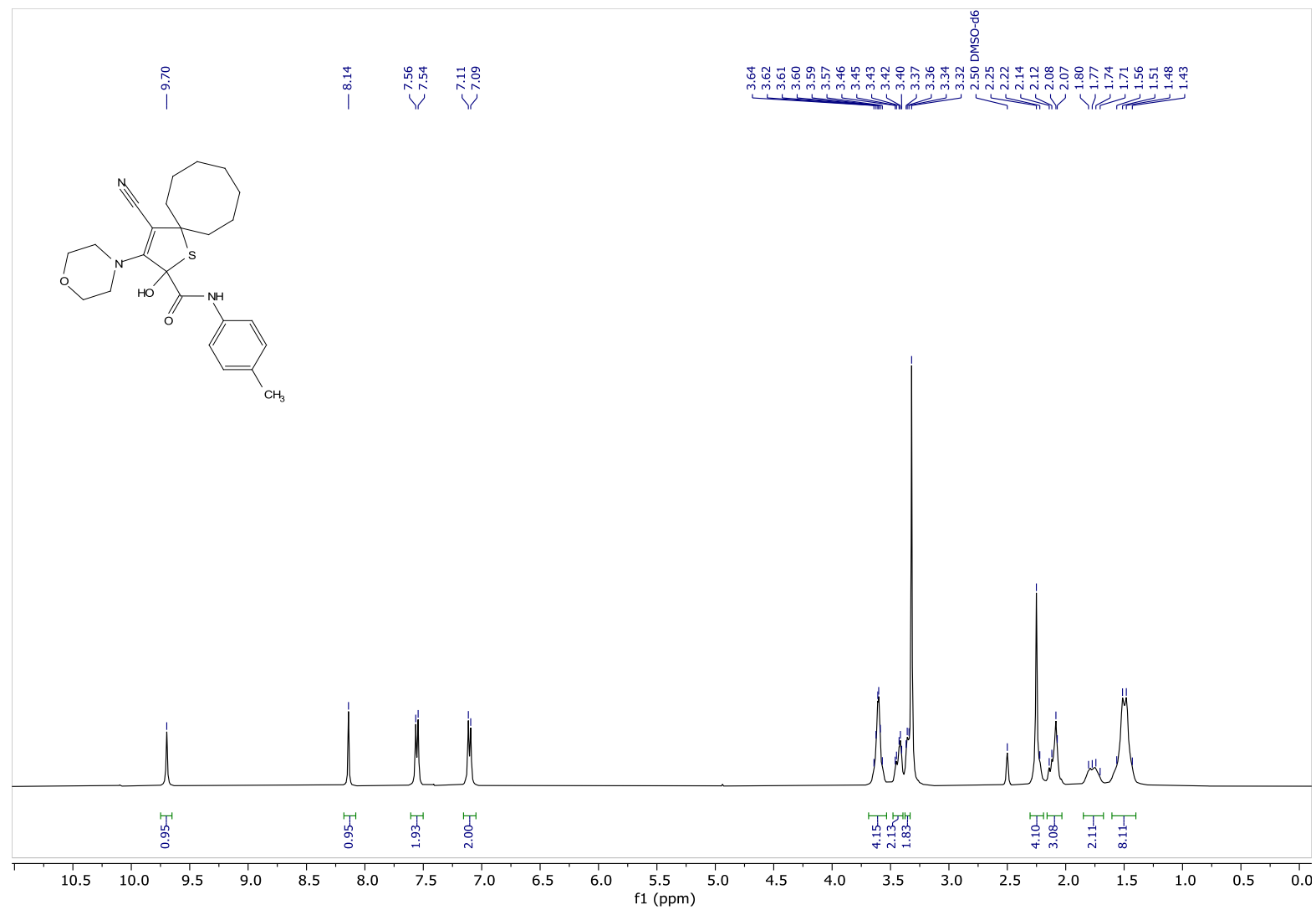
¹³C NMR (100 MHz, DMSO-*d*₆) of **2h**



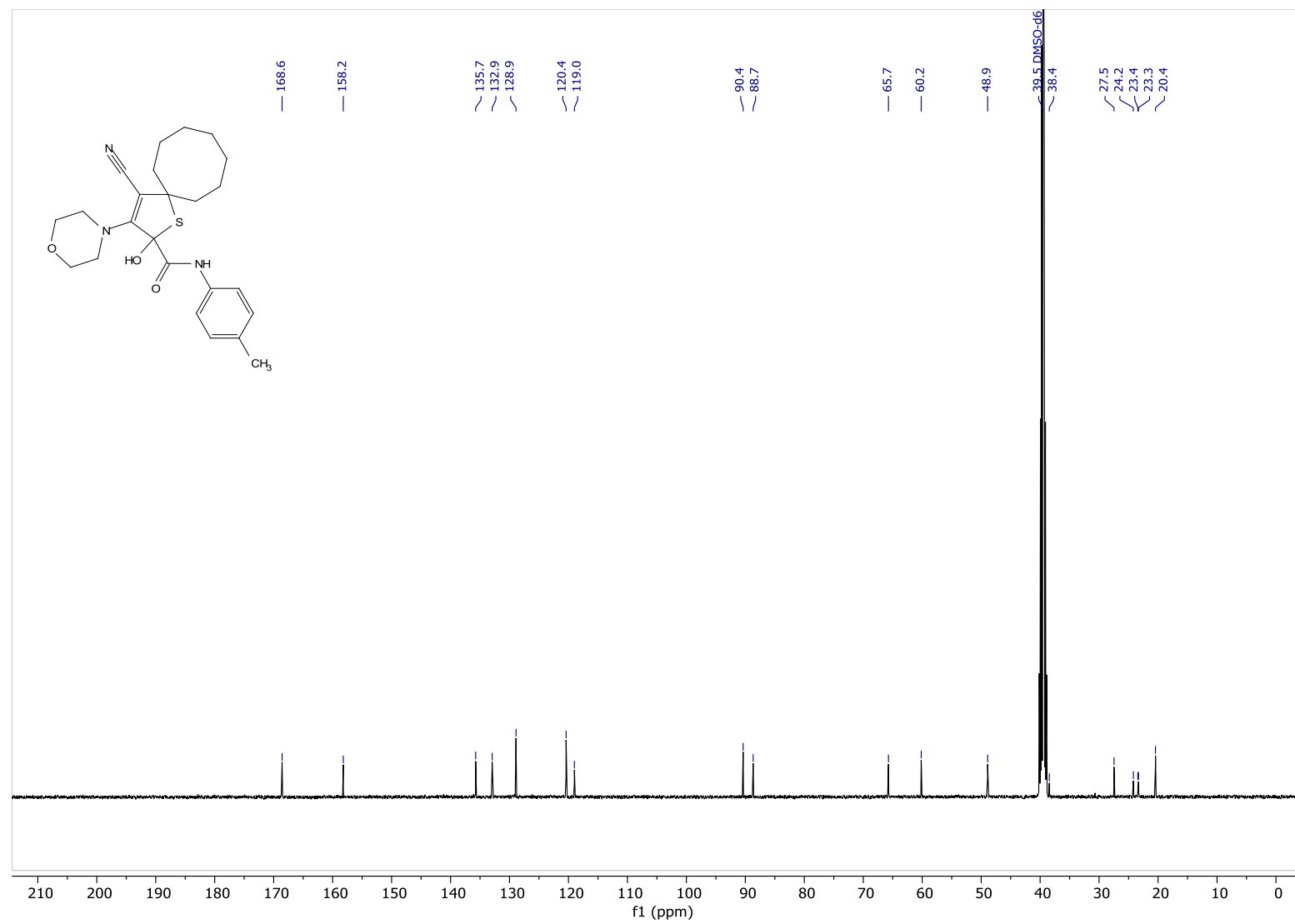
¹H NMR (600 MHz, DMSO-*d*₆) of **2i**



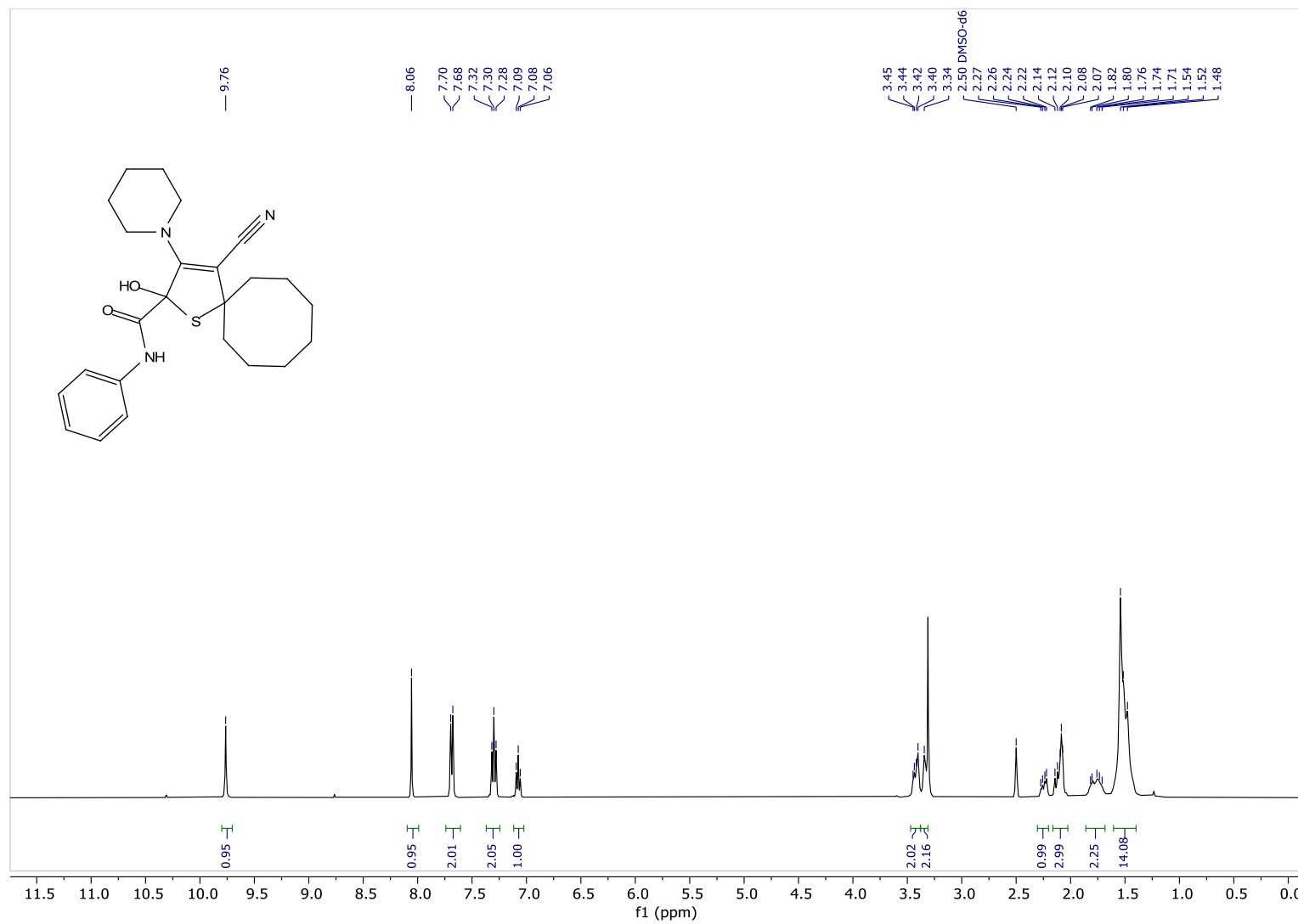
^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **2i**



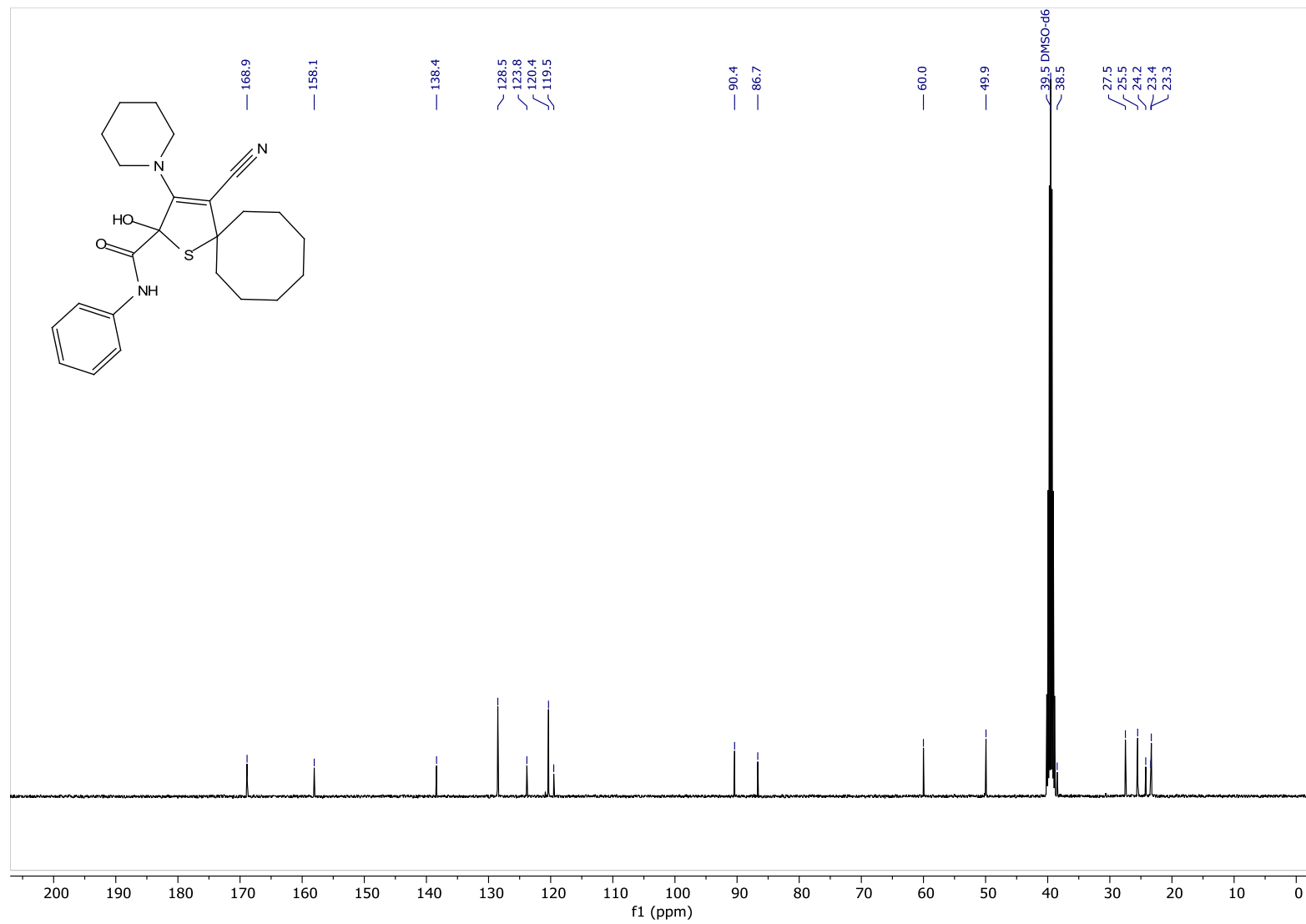
¹H NMR (400 MHz, DMSO-*d*₆) of **2j**



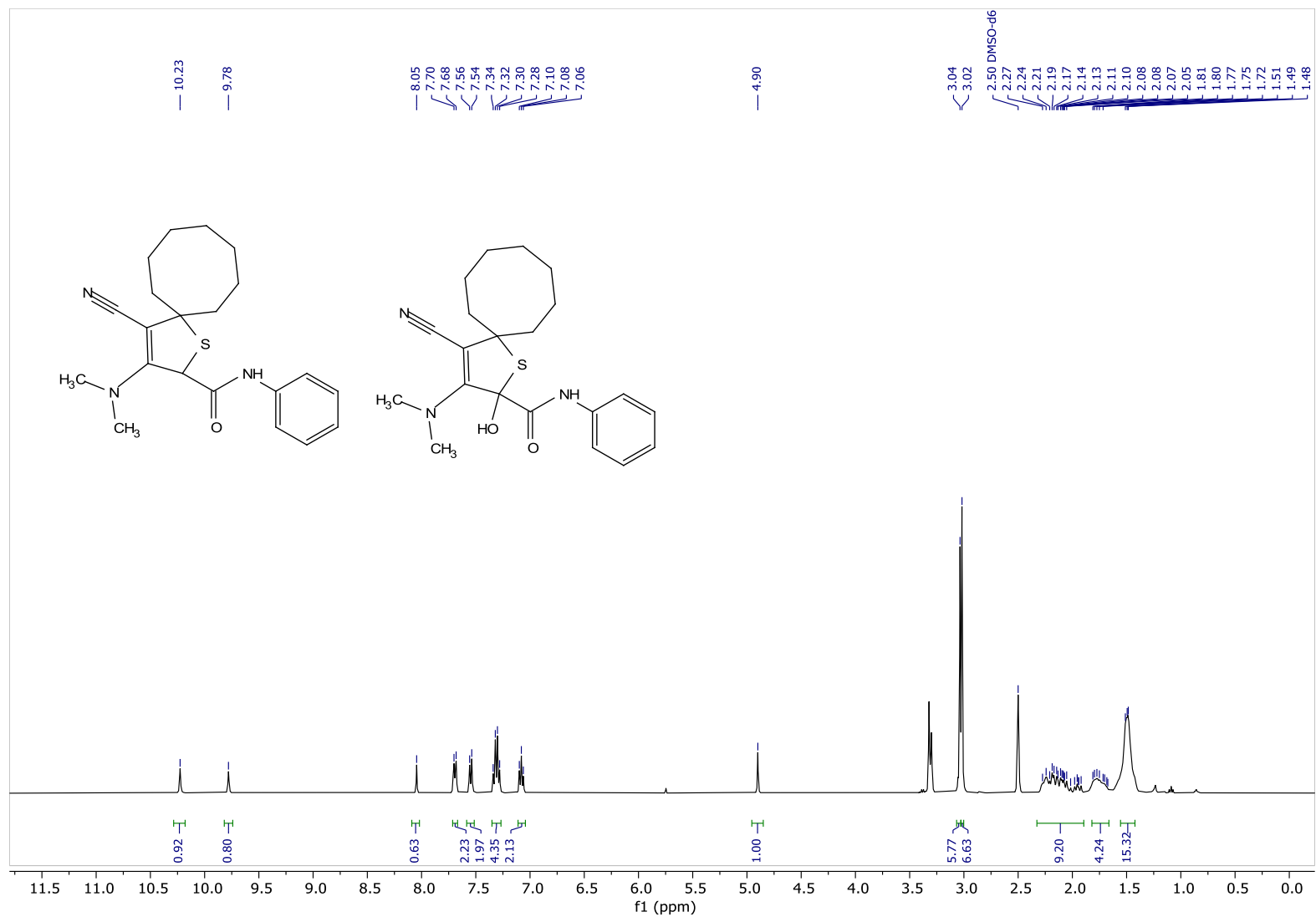
¹³C NMR (100 MHz, DMSO-*d*₆) of **2j**



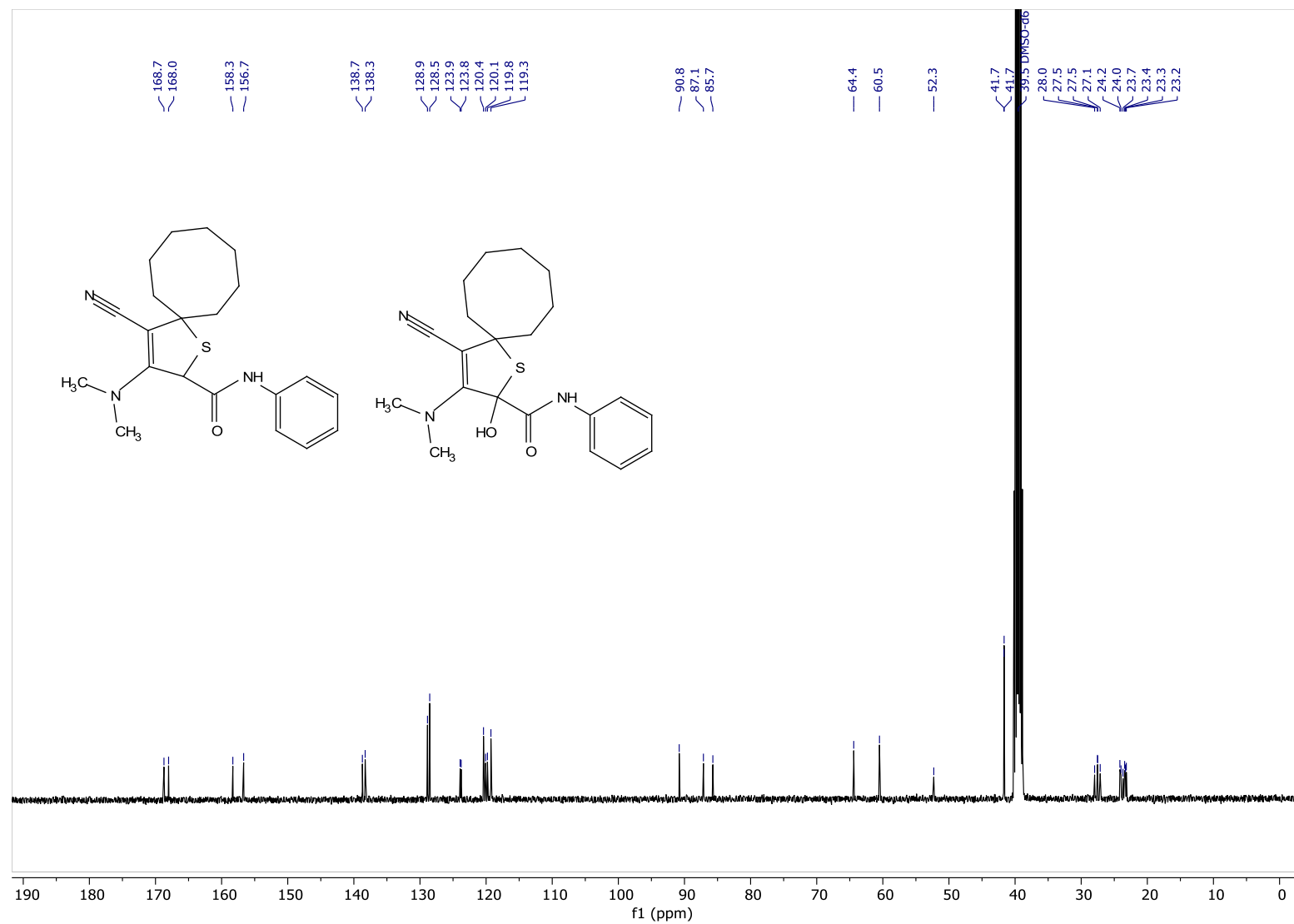
¹H NMR (400 MHz, DMSO-*d*₆) of **2k**



¹³C NMR (100 MHz, DMSO-*d*₆) of **2k**

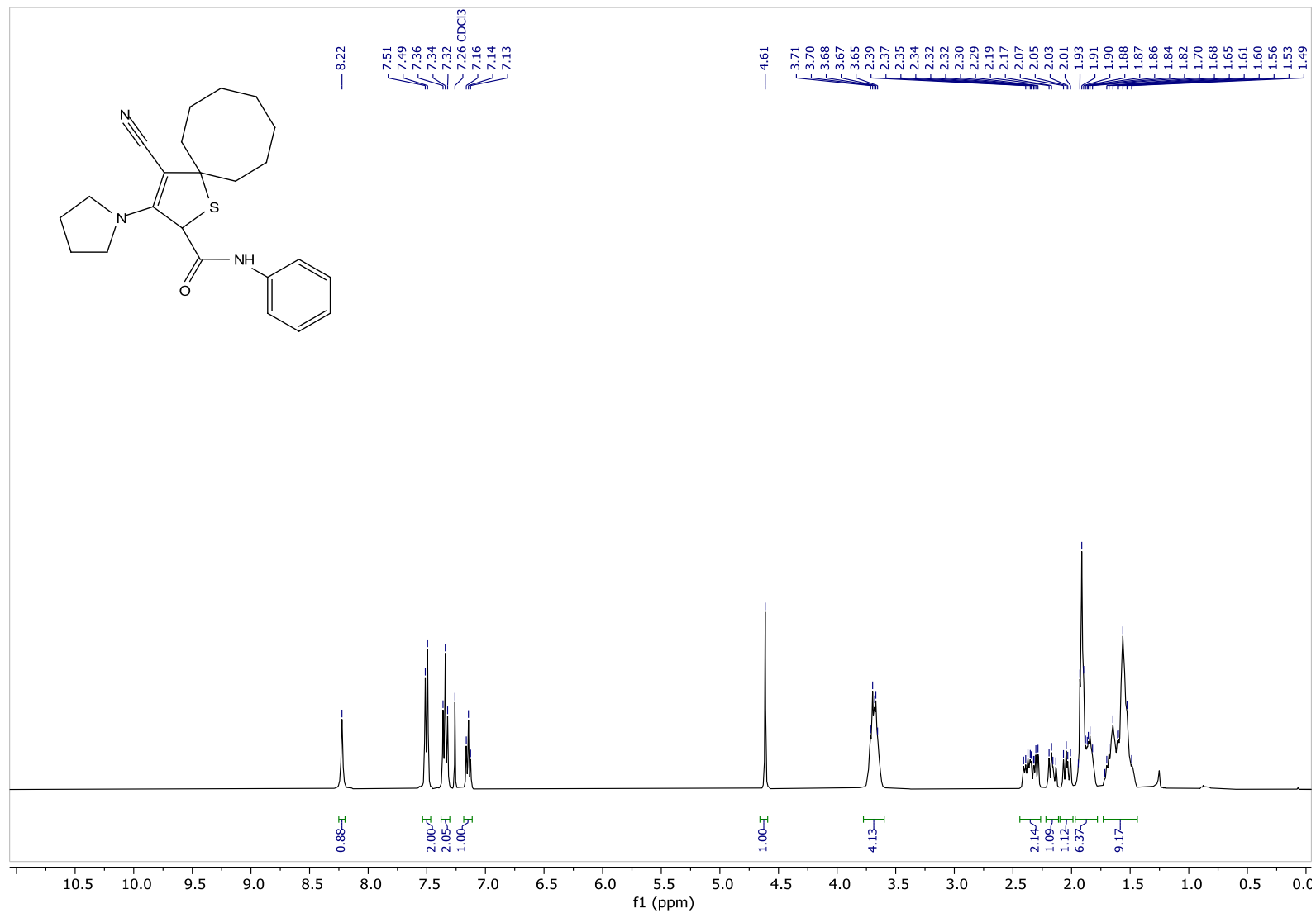


¹H NMR (400 MHz, DMSO-*d*₆) of **2I, I'**

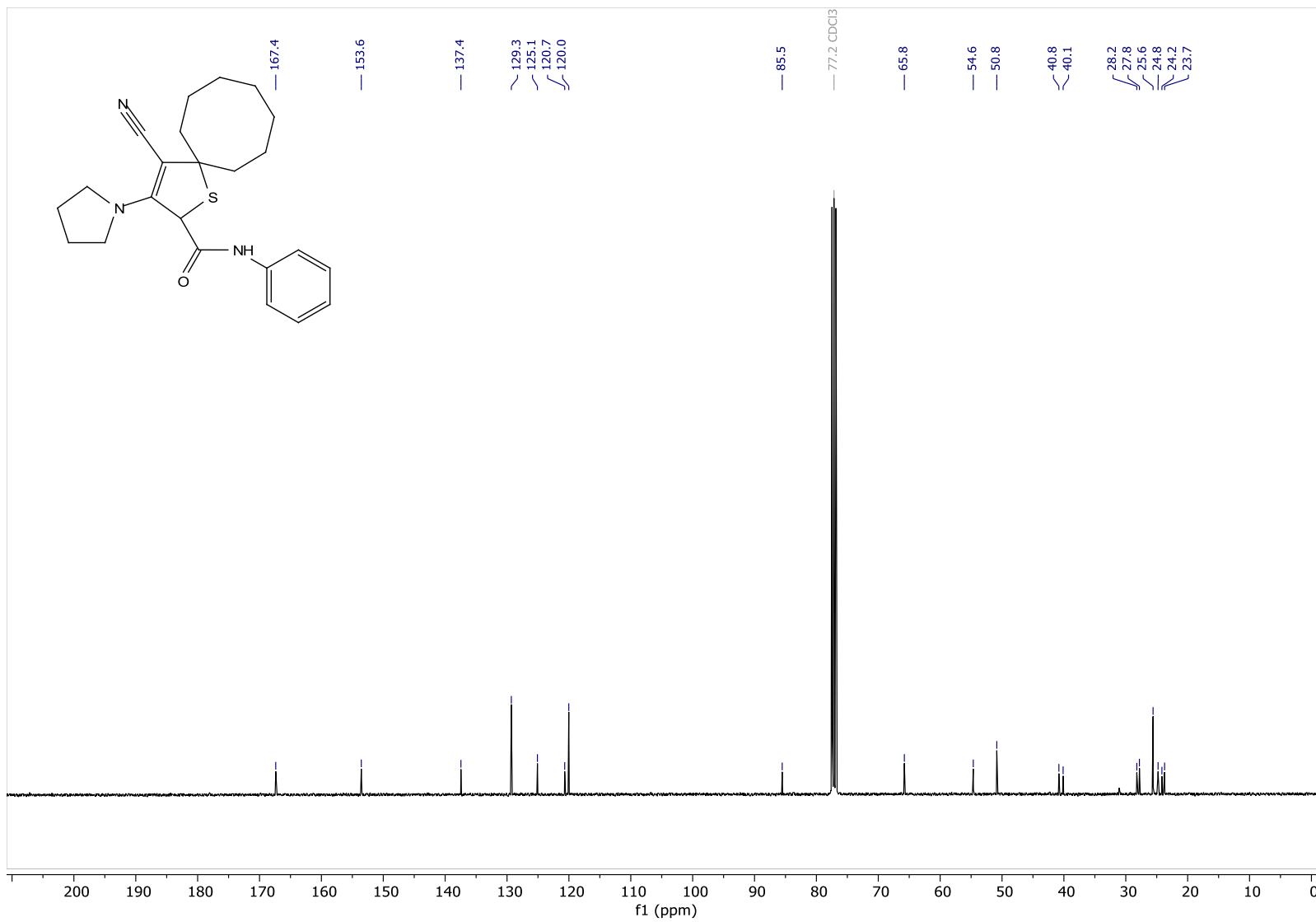


¹³C NMR (100 MHz, DMSO-*d*₆) of 2I, I'

S51

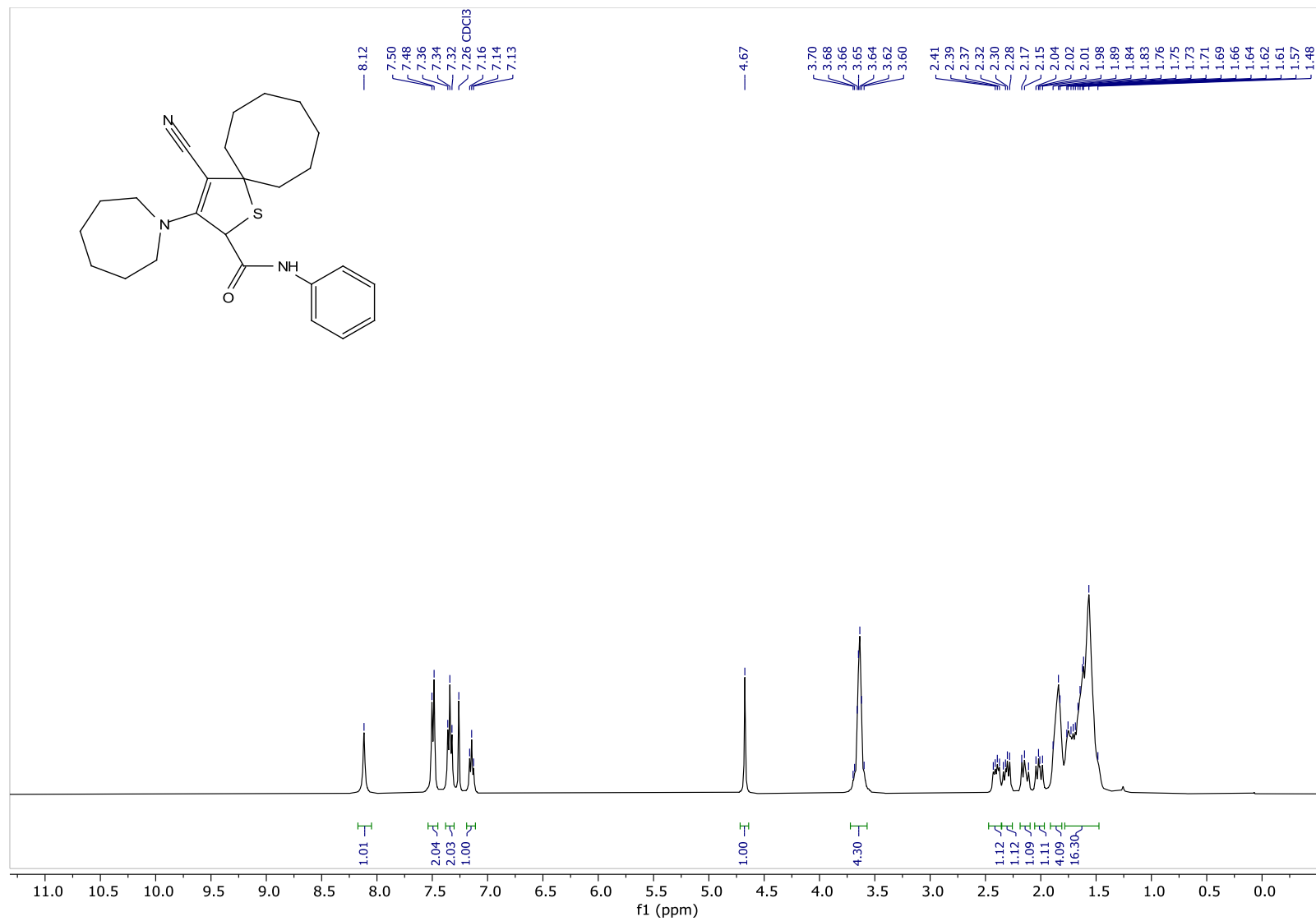


¹H NMR (400 MHz, CDCl₃-d) of **2m**

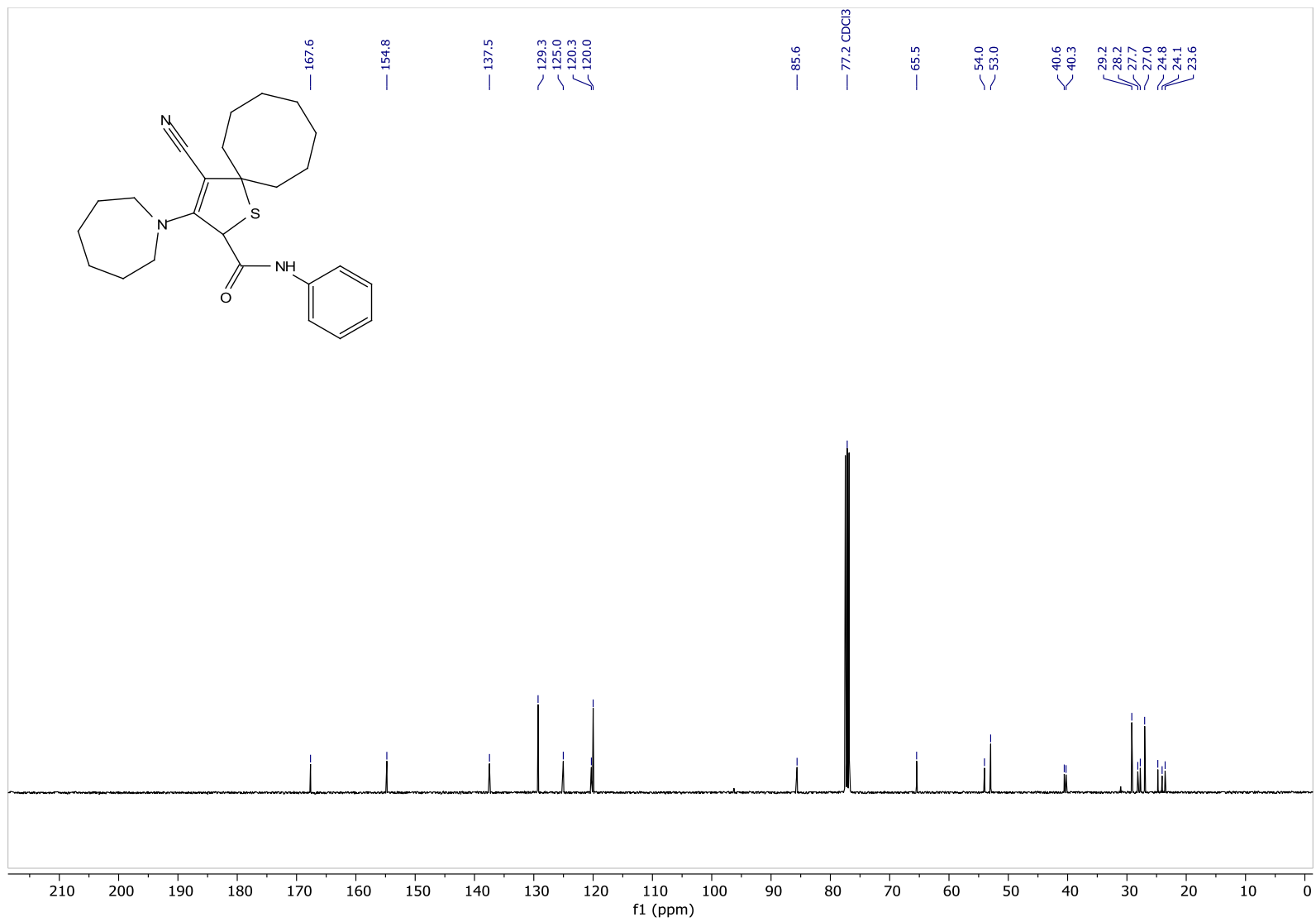


^{13}C NMR (100 MHz, CDCl_3 -d) of **2m**

S53

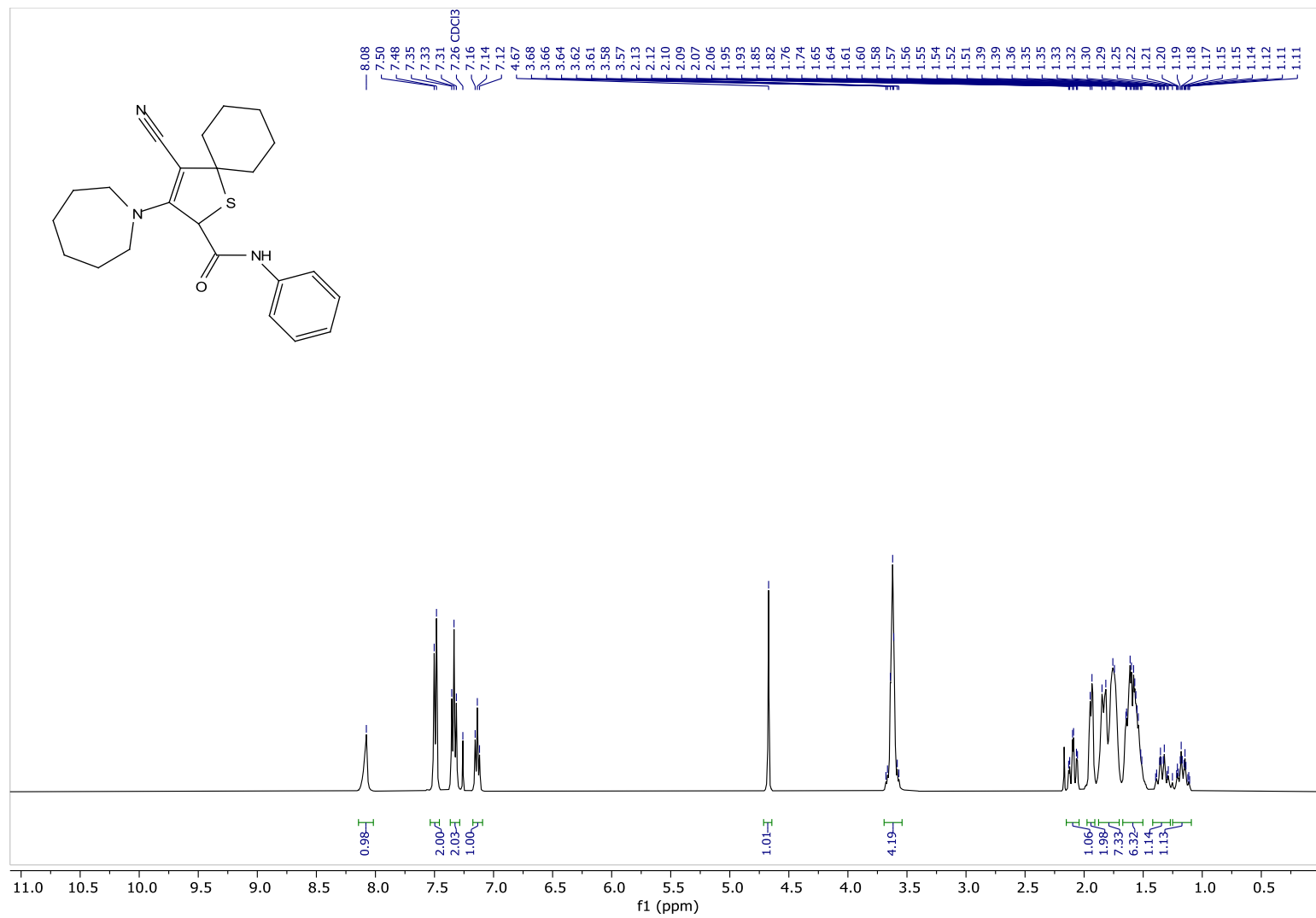


¹H NMR (400 MHz, CDCl₃-d) of **2n**

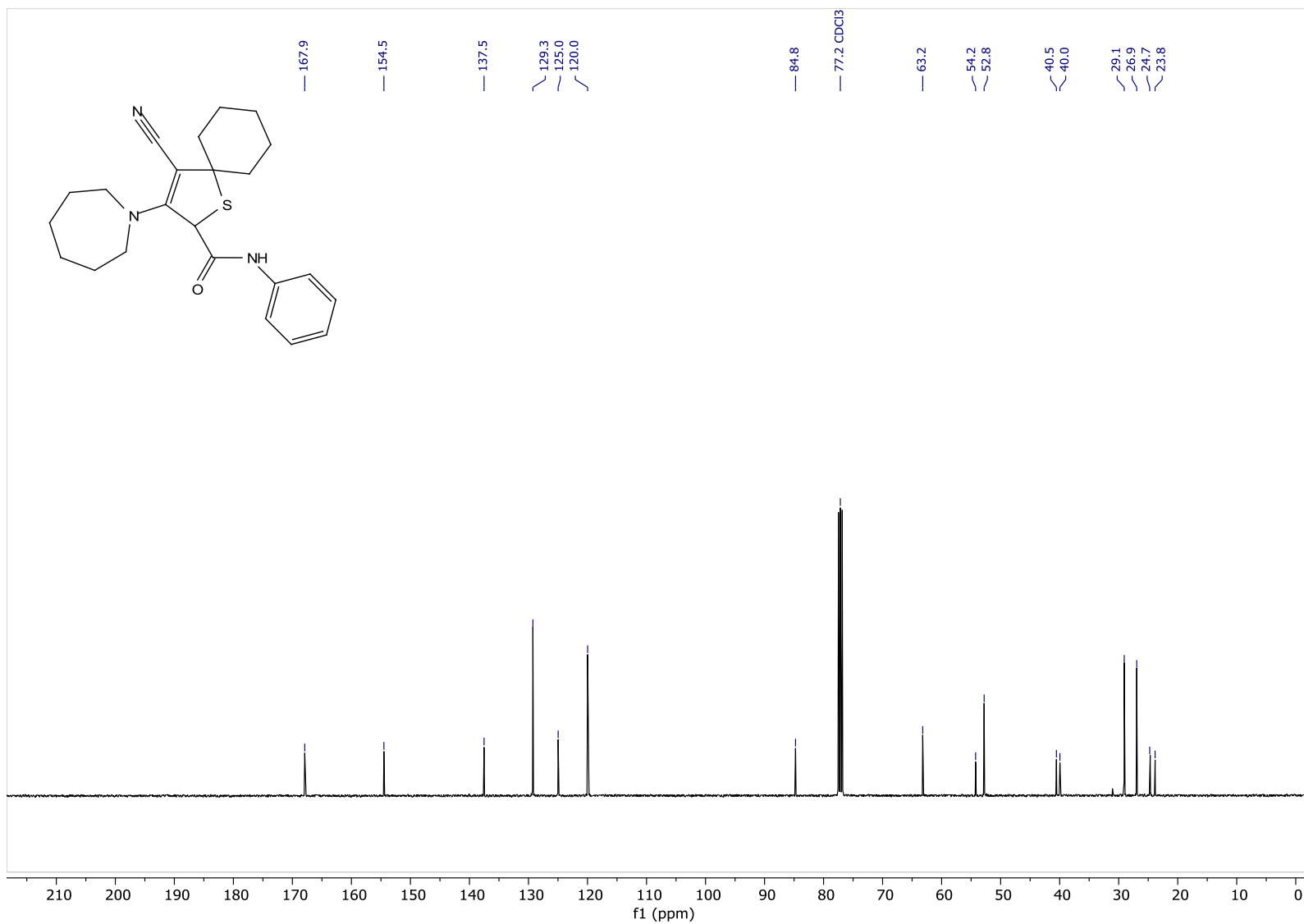


^{13}C NMR (100 MHz, CDCl_3 -*d*) of **2n**

S55

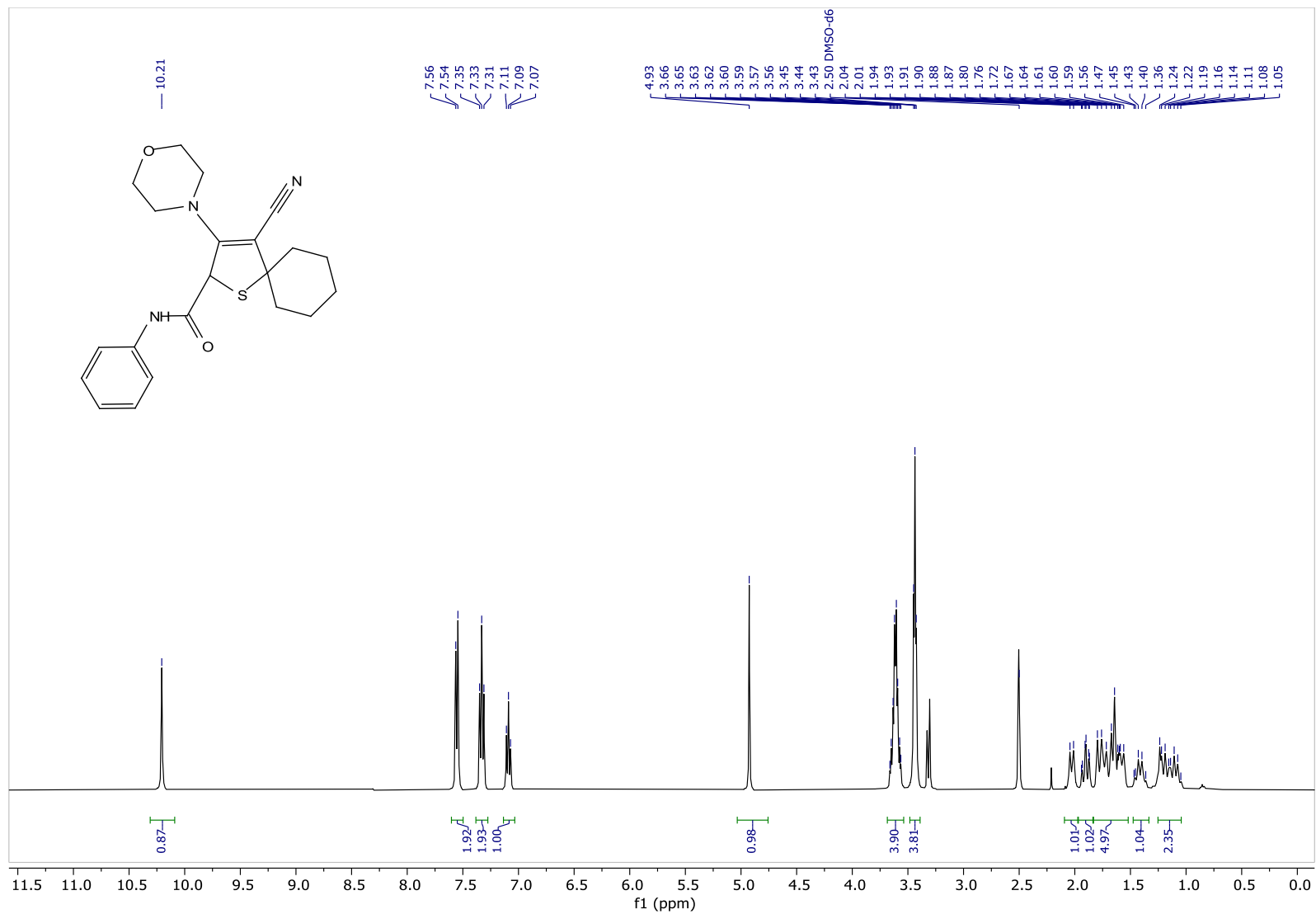


¹H NMR (400 MHz, CDCl₃-d) of **2o**

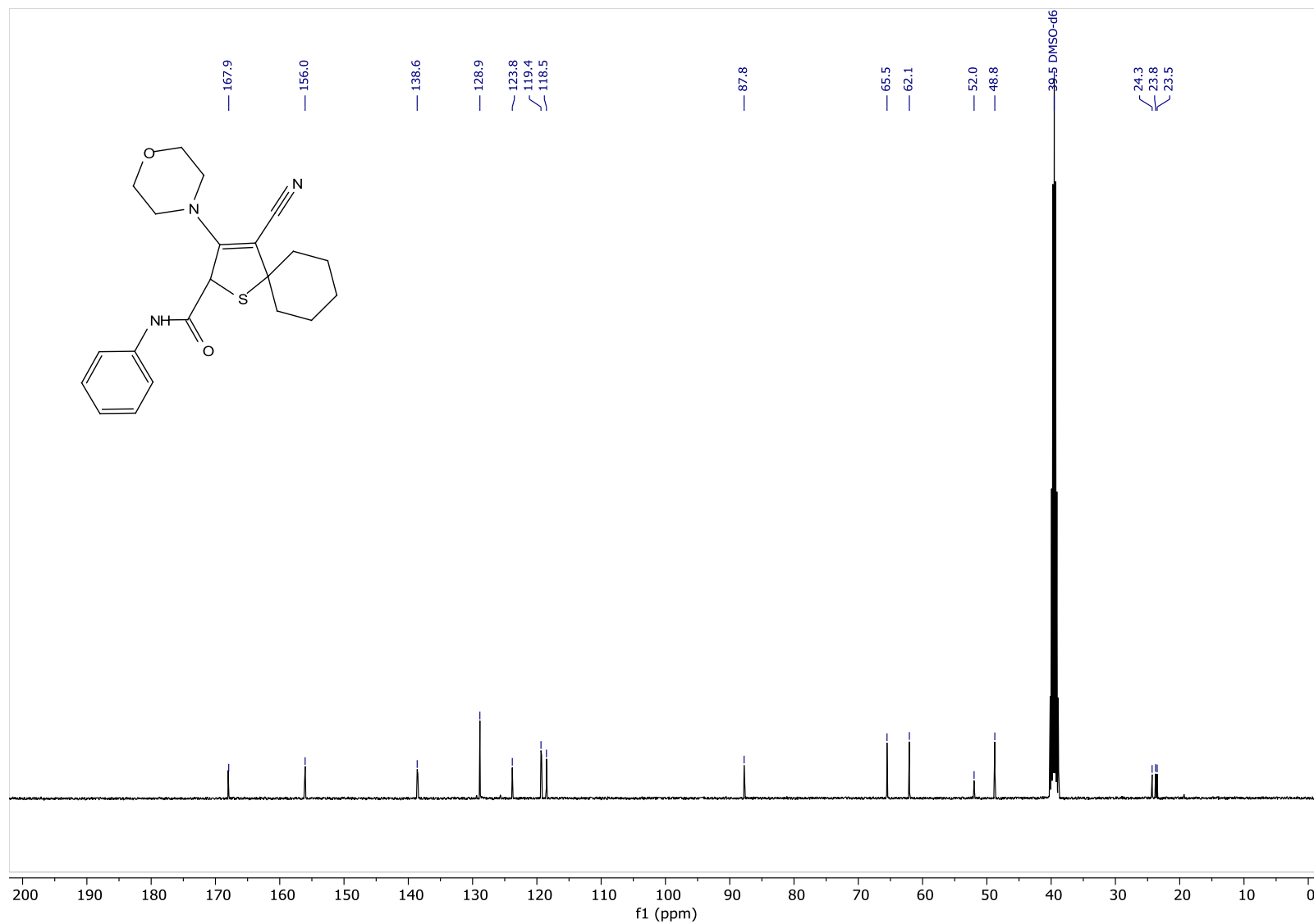


^{13}C NMR (100 MHz, CDCl_3 -d) of **2o**

S57

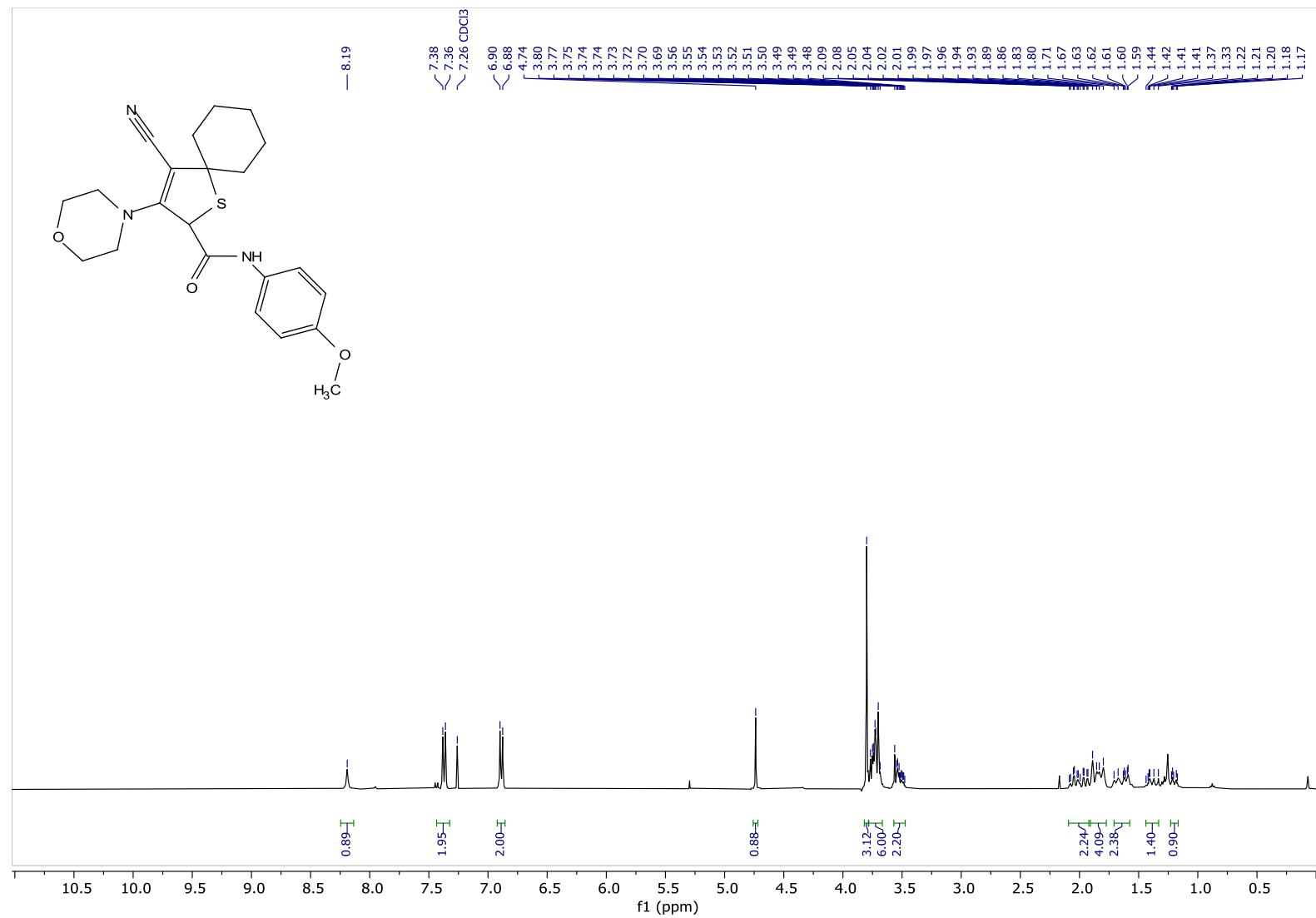


^1H NMR (400 MHz, $\text{DMSO}-d_6$) of **3a**

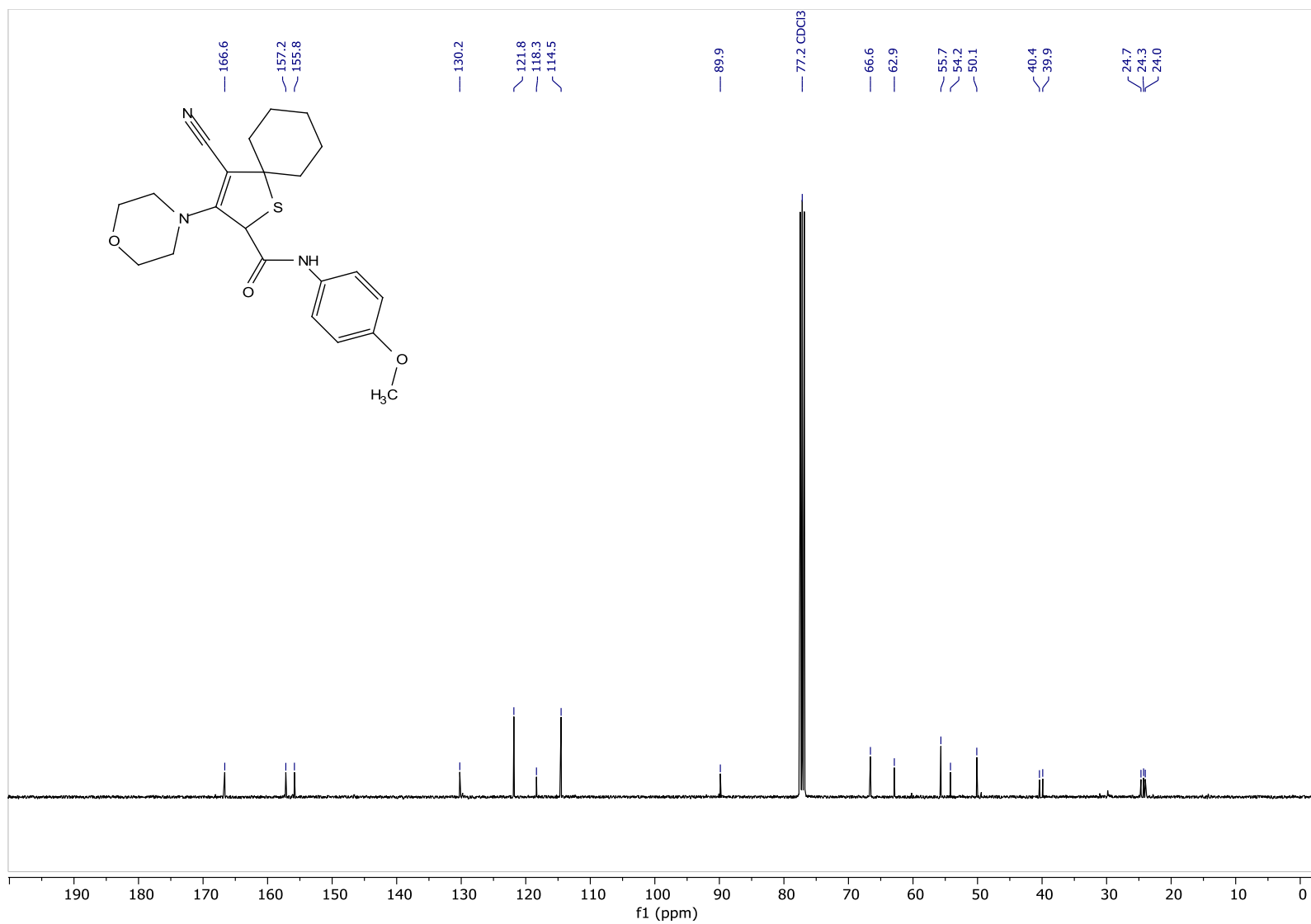


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **3a**

S59

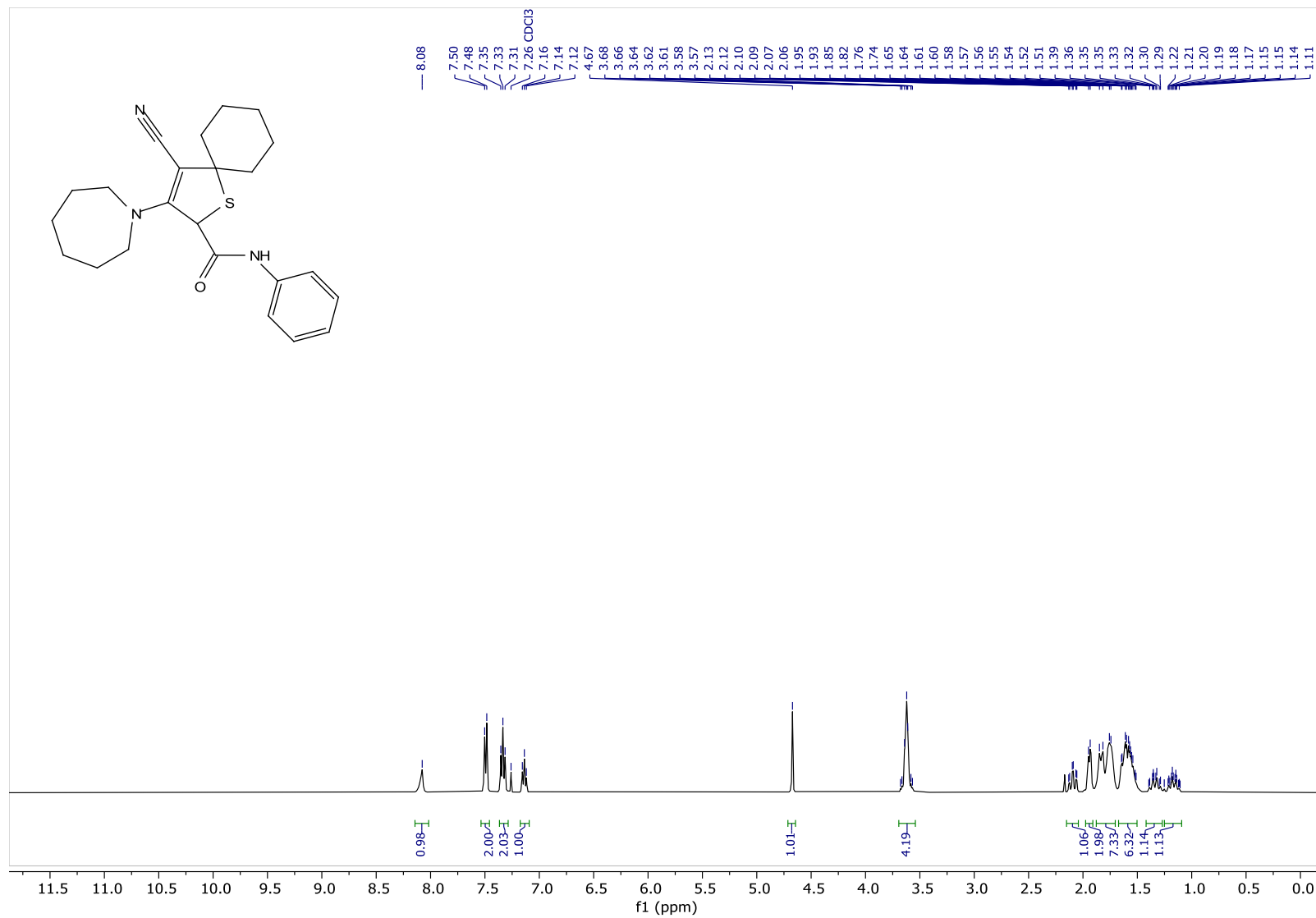


¹H NMR (400 MHz, CDCl₃-d) of **3b**

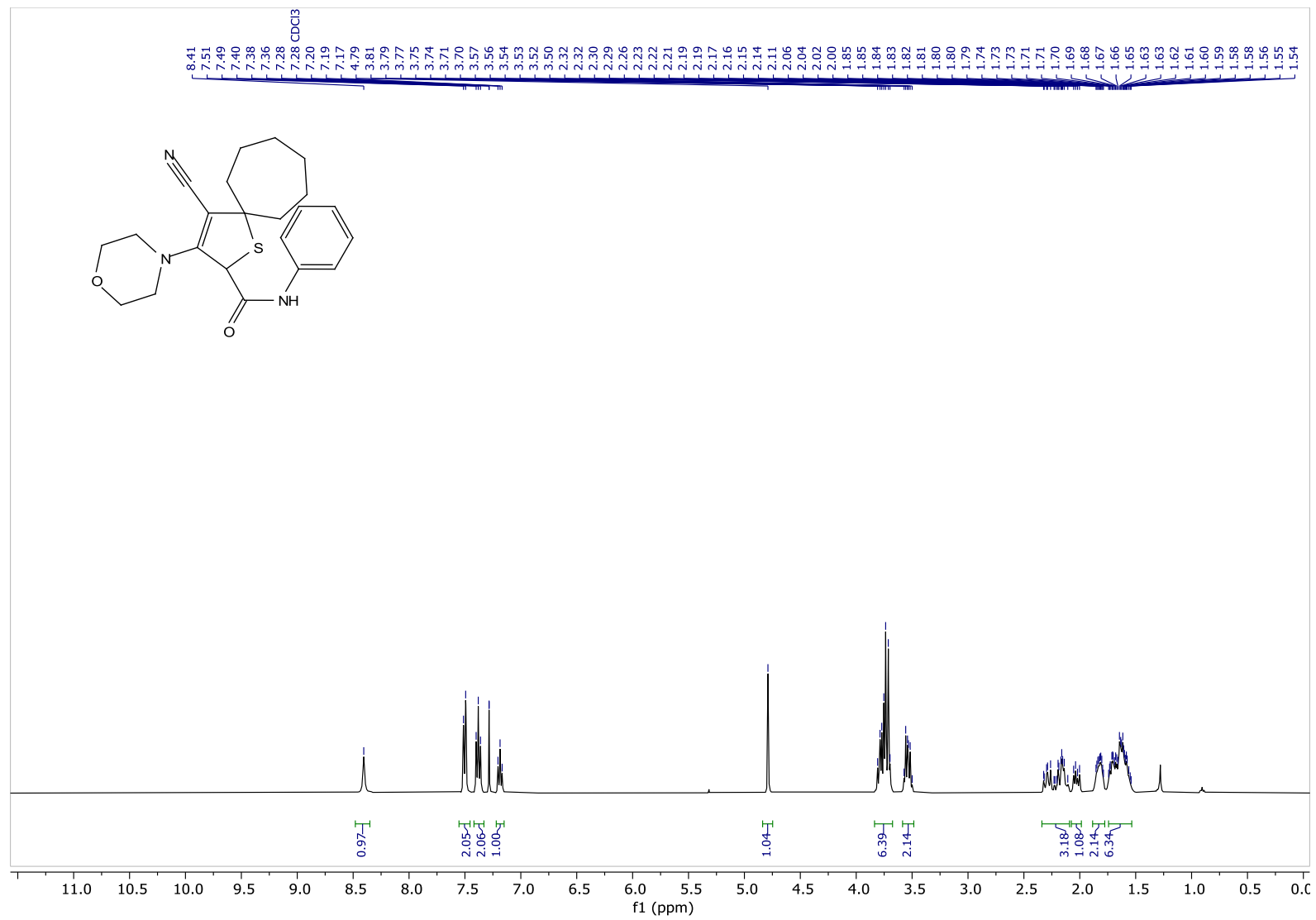


^{13}C NMR (100 MHz, CDCl_3 -d) of **3b**

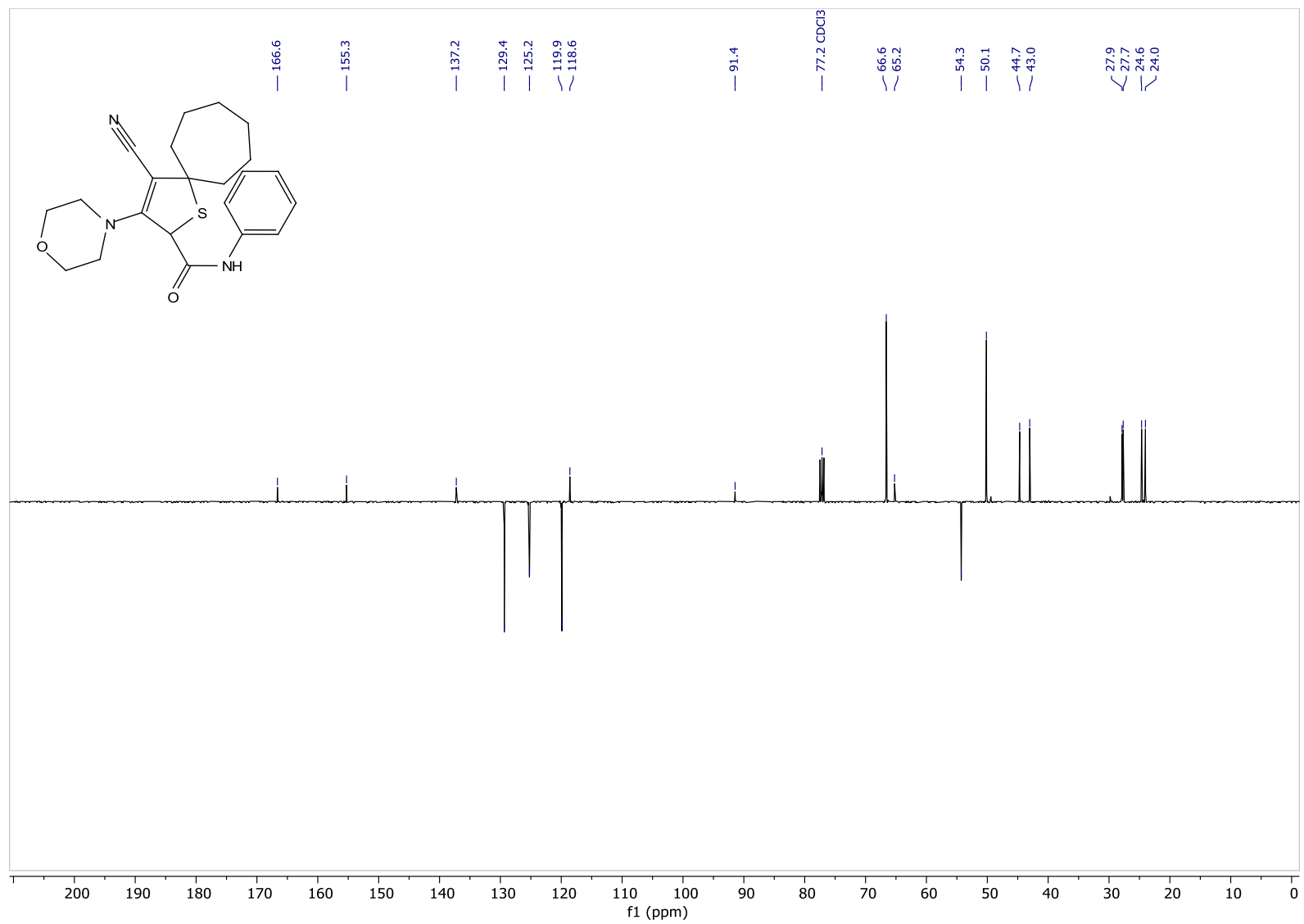
S61



¹H NMR (400 MHz, CDCl₃-d) of **2o**

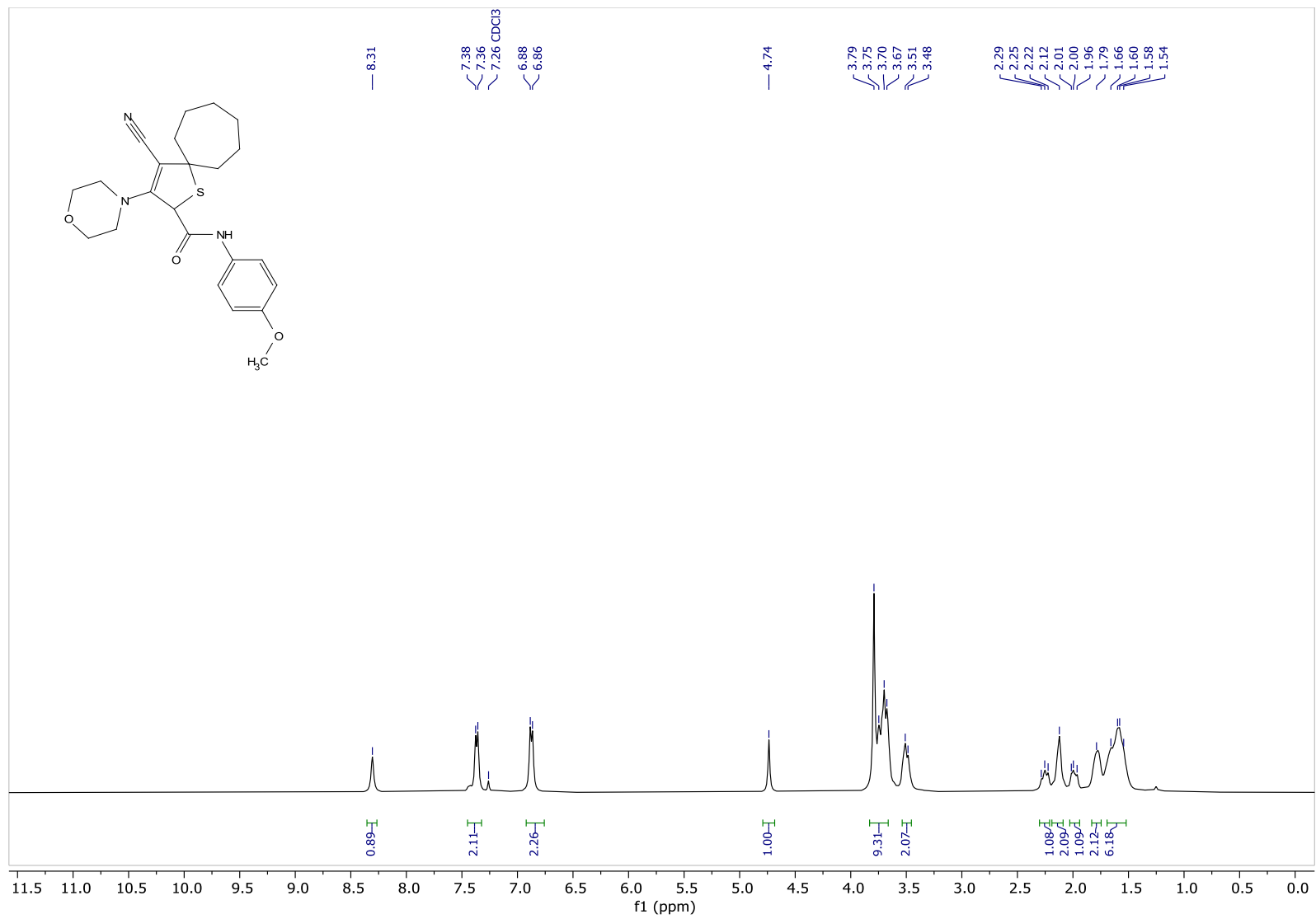


¹H NMR (400 MHz, CDCl₃-d) of **3c**

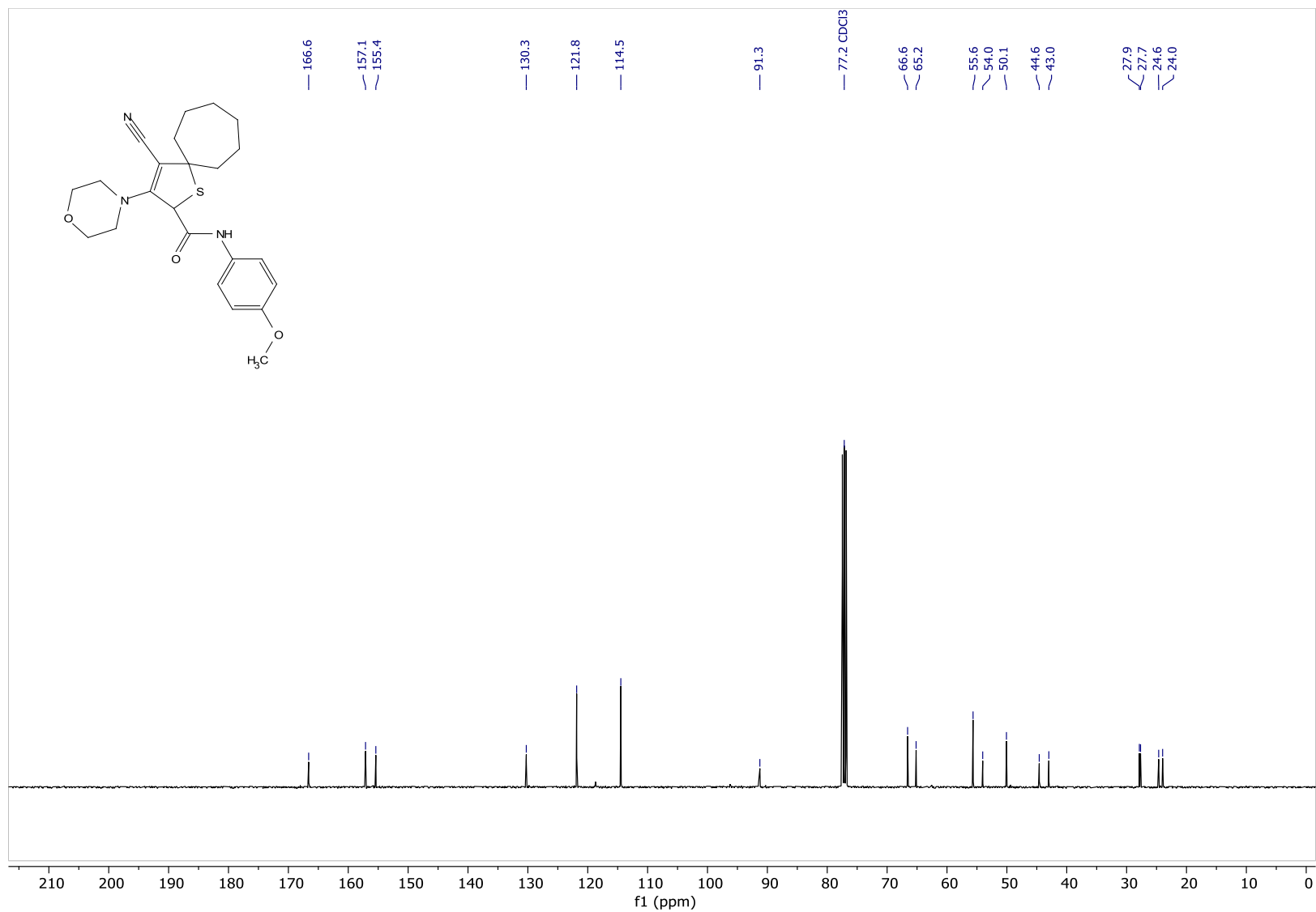


^{13}C NMR (100 MHz, CDCl_3 -d) of **3c**

S64

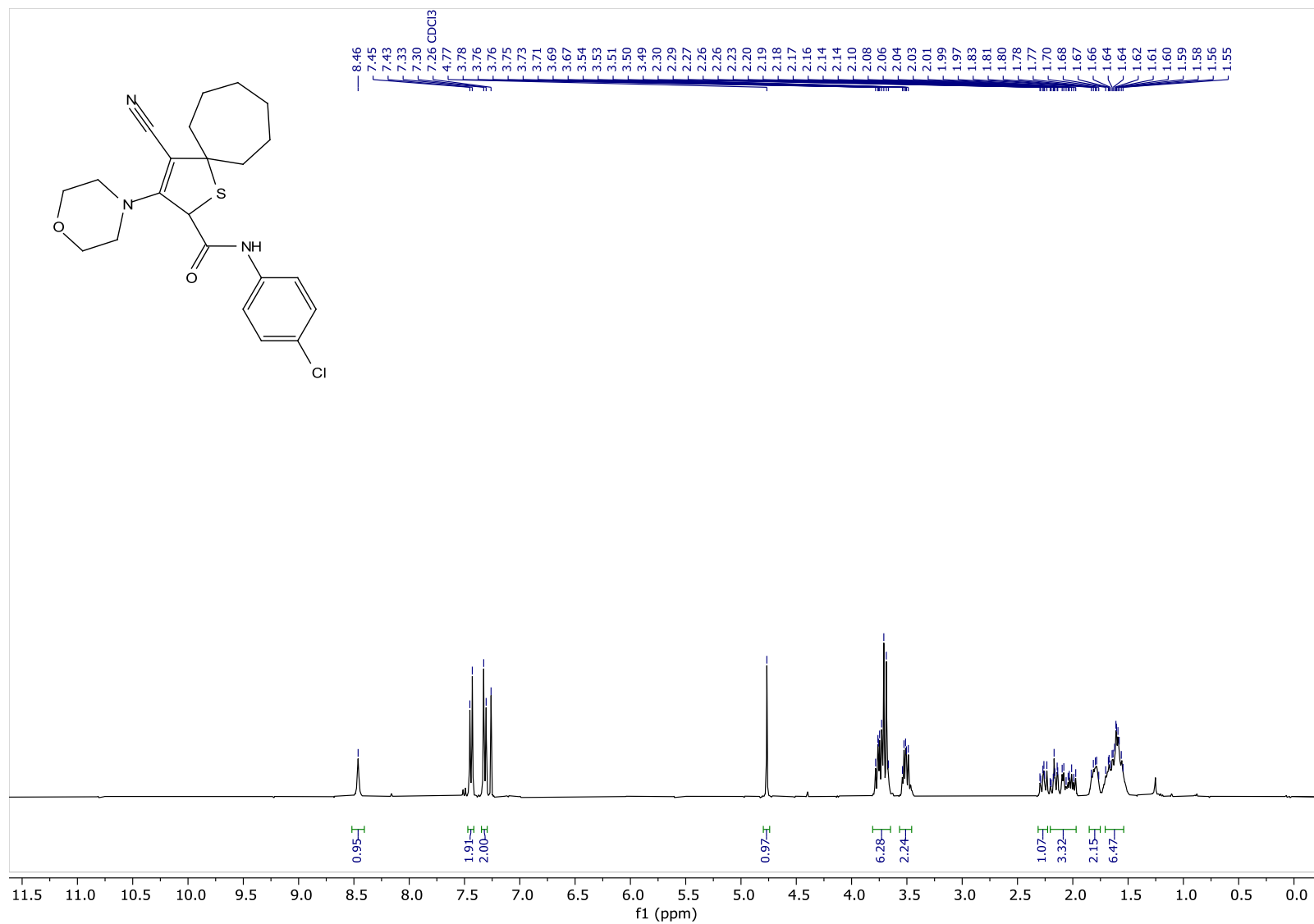


¹H NMR (400 MHz, CDCl₃-d) of **3d**



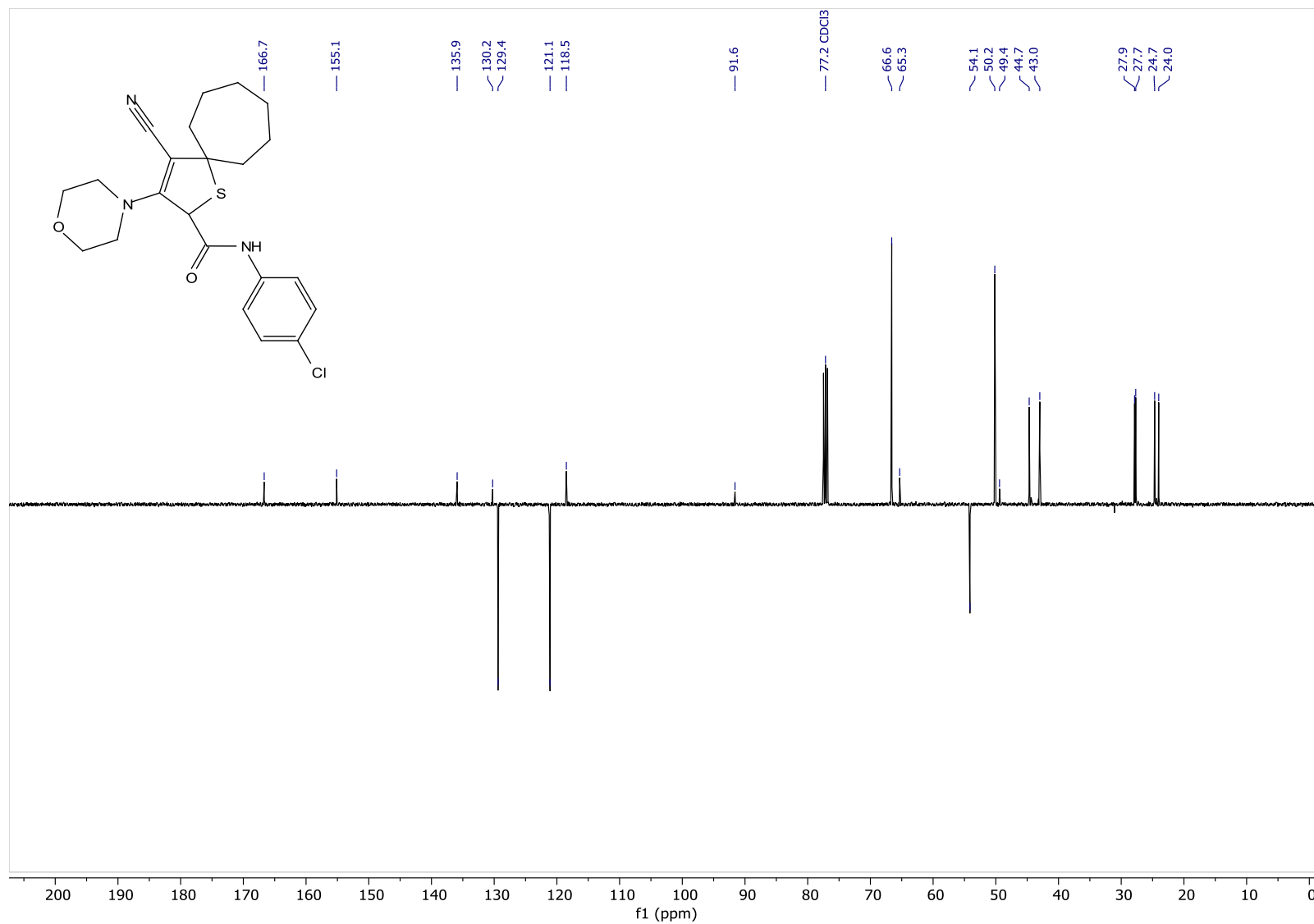
^{13}C NMR (100 MHz, CDCl_3 -*d*) of **3d**

S66



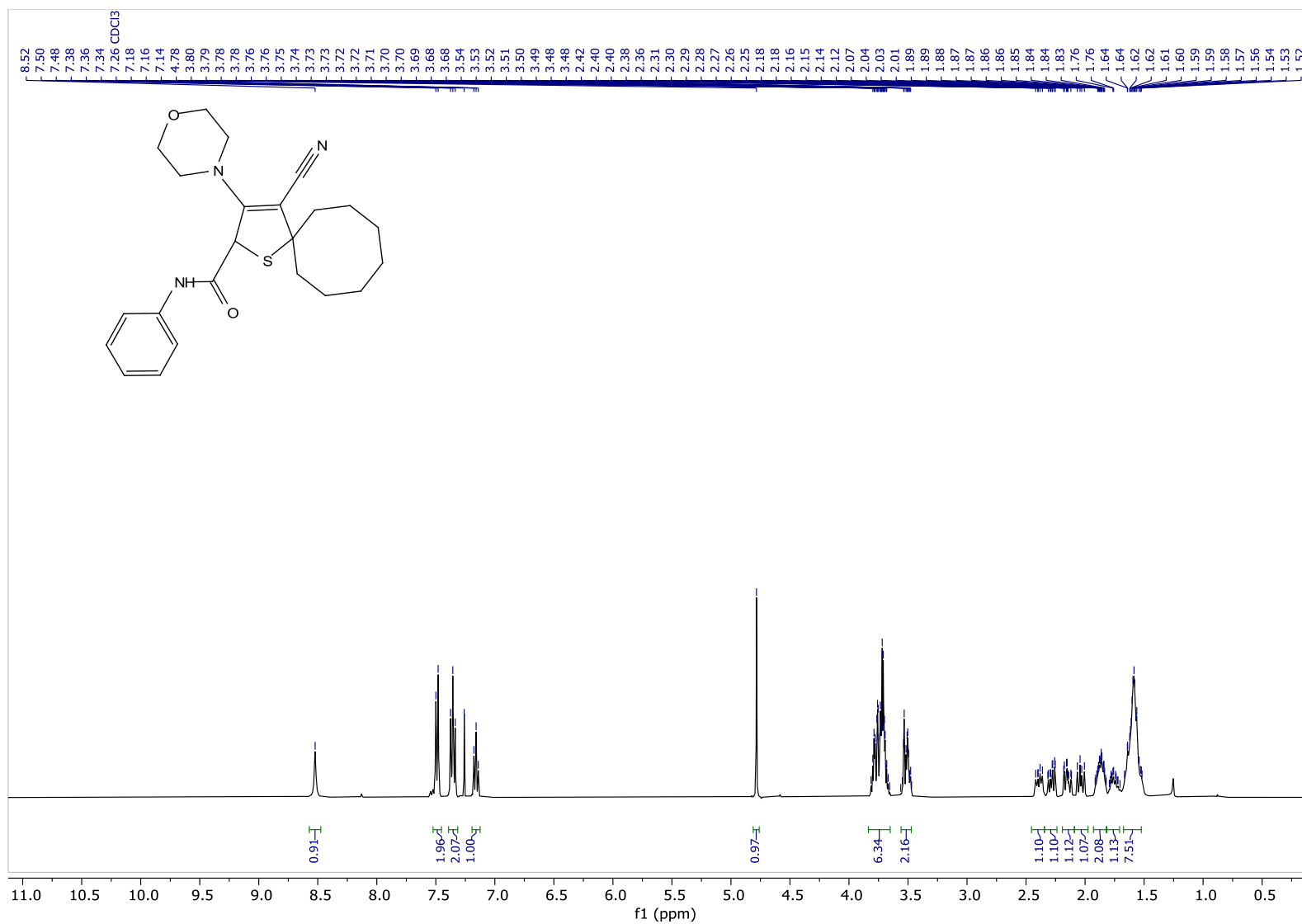
¹H NMR (400 MHz, CDCl₃-d) of **3e**

S67

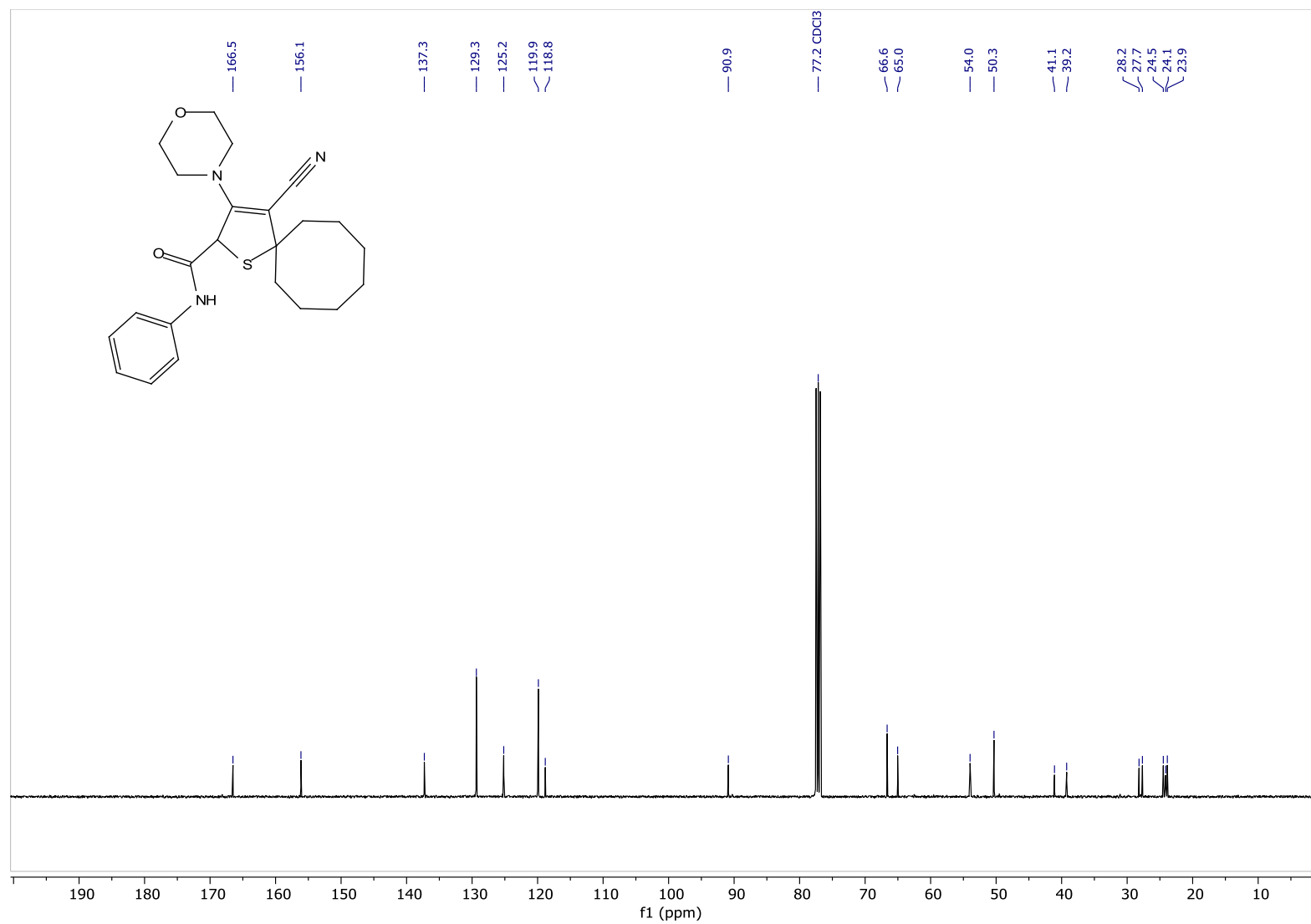


¹³C NMR (100 MHz, CDCl₃-d) of **3e**

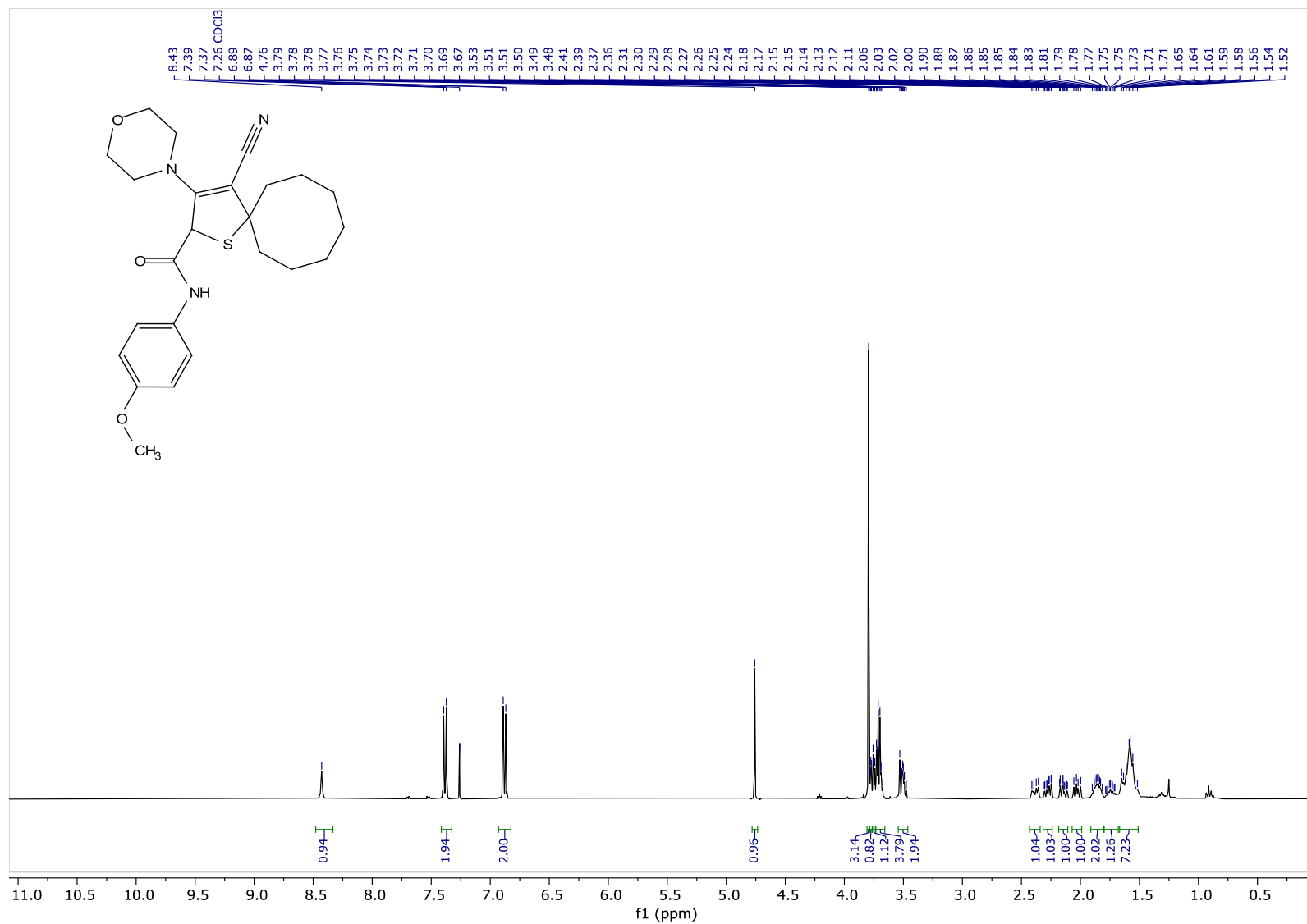
S68



^1H NMR (400 MHz, CDCl_3 -d) of **3f**

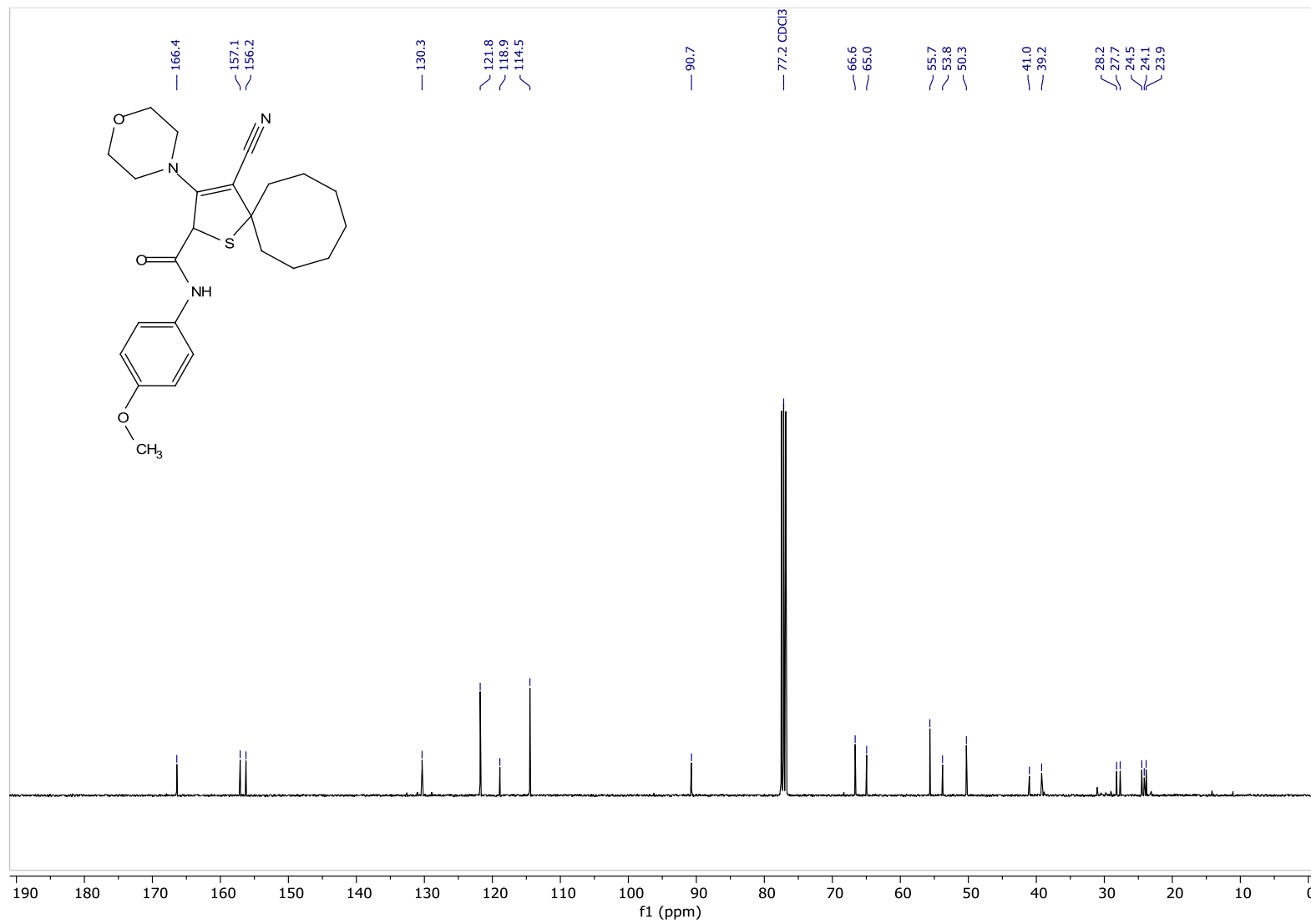


¹³C NMR (100 MHz, CDCl₃-d) of **3f**

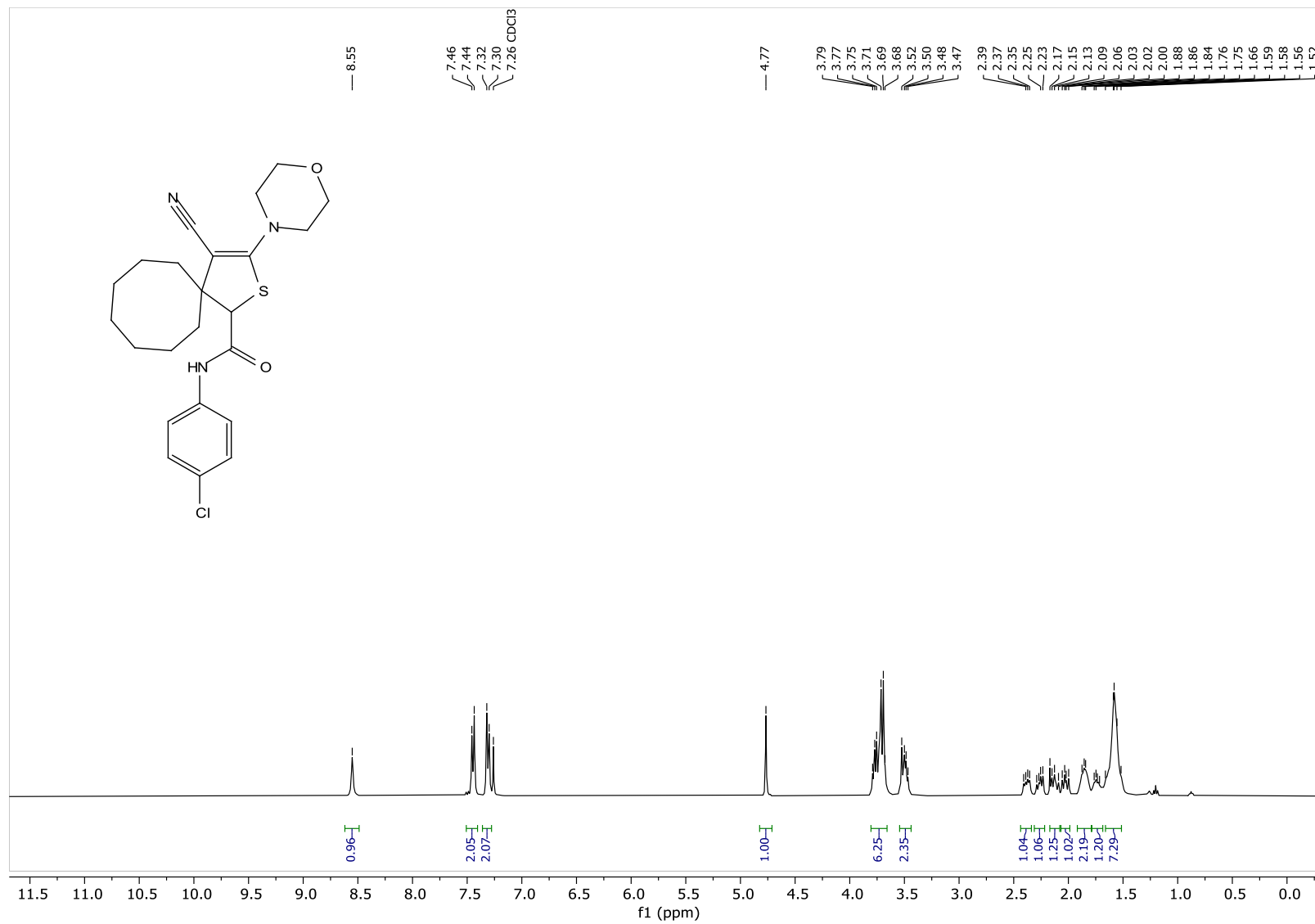


^1H NMR (400 MHz, CDCl_3 -d) of **3g**

S71

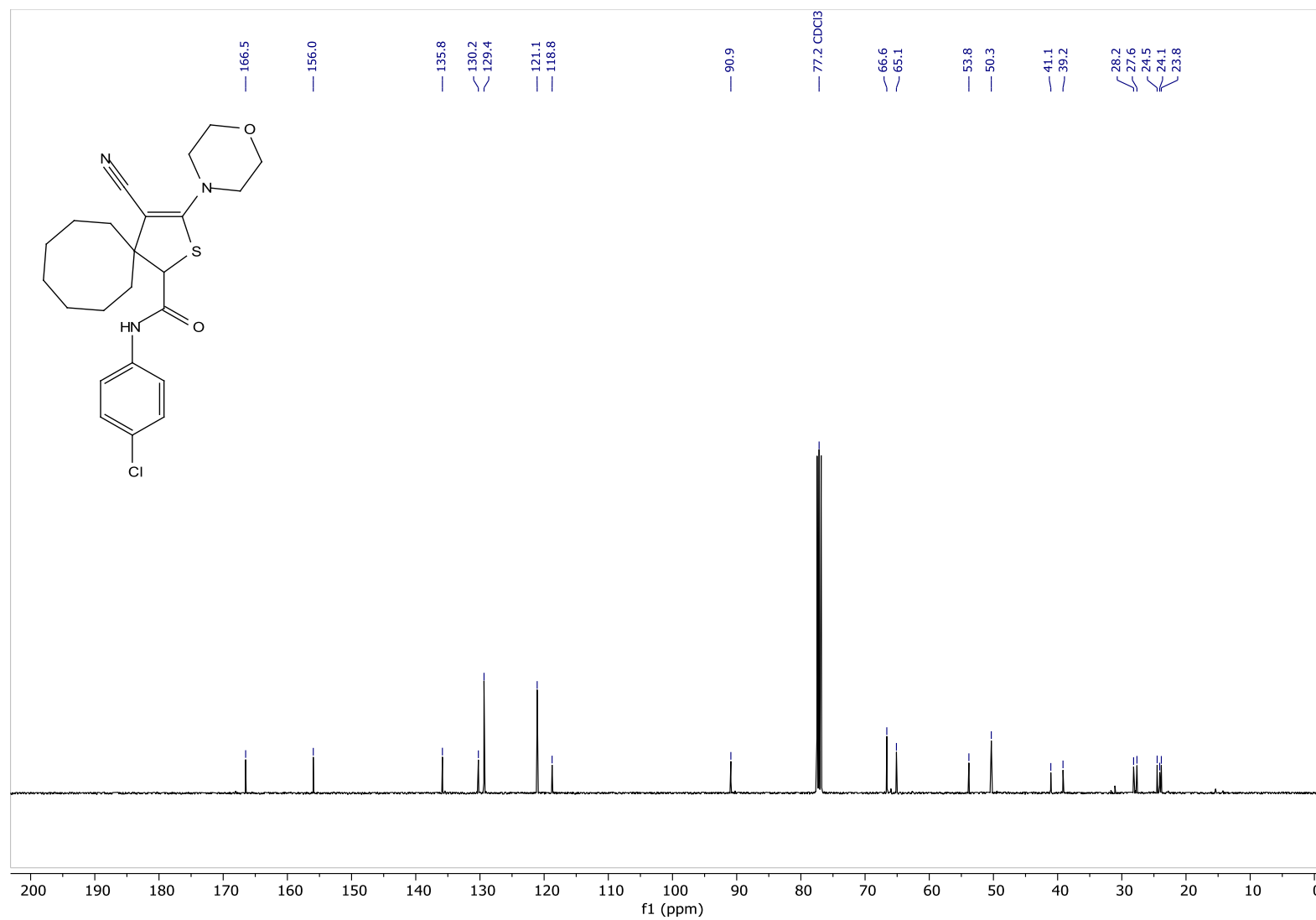


¹³C NMR (100 MHz, CDCl₃-d) of **3g**

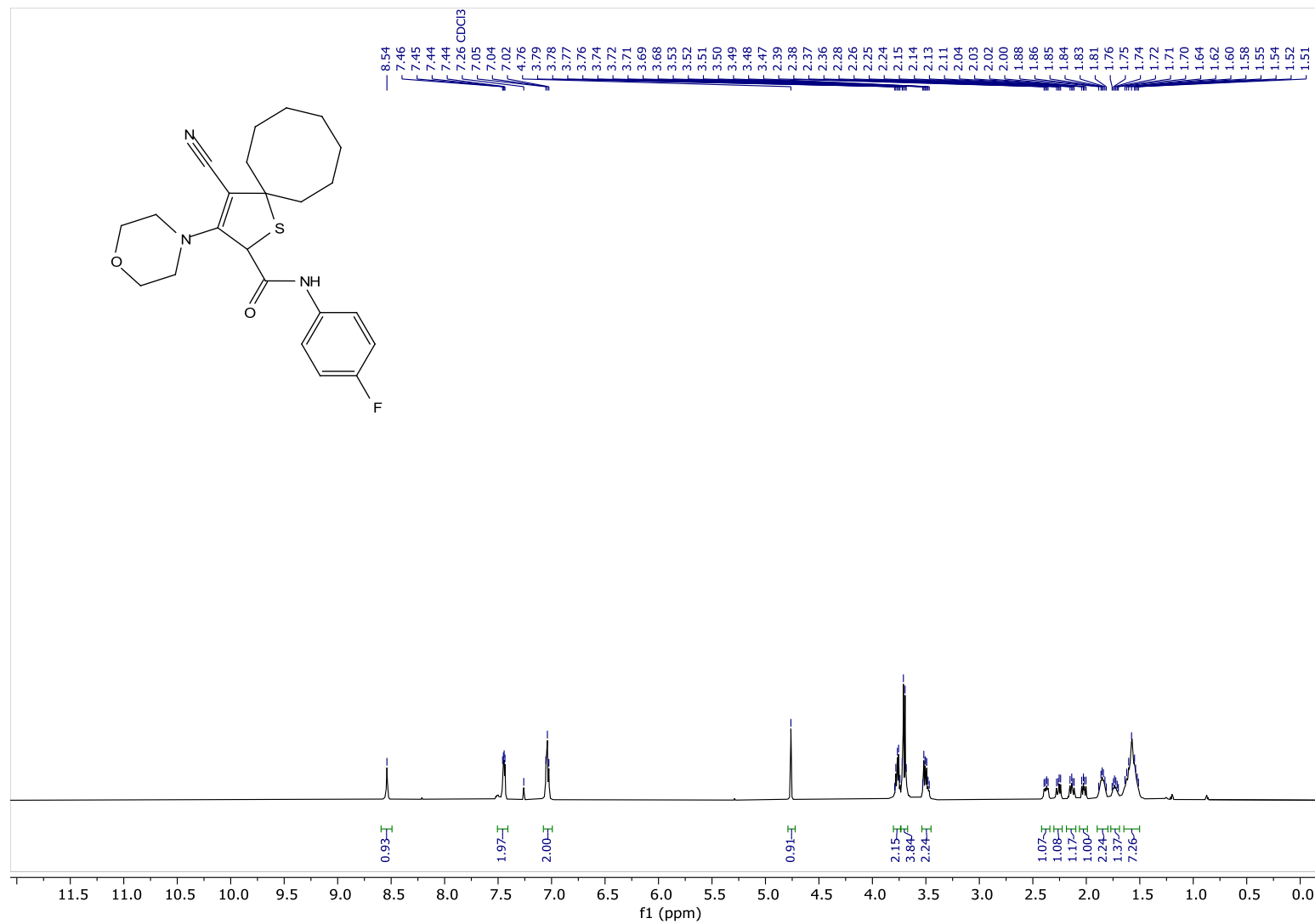


¹H NMR (400 MHz, CDCl₃-d) of **3h**

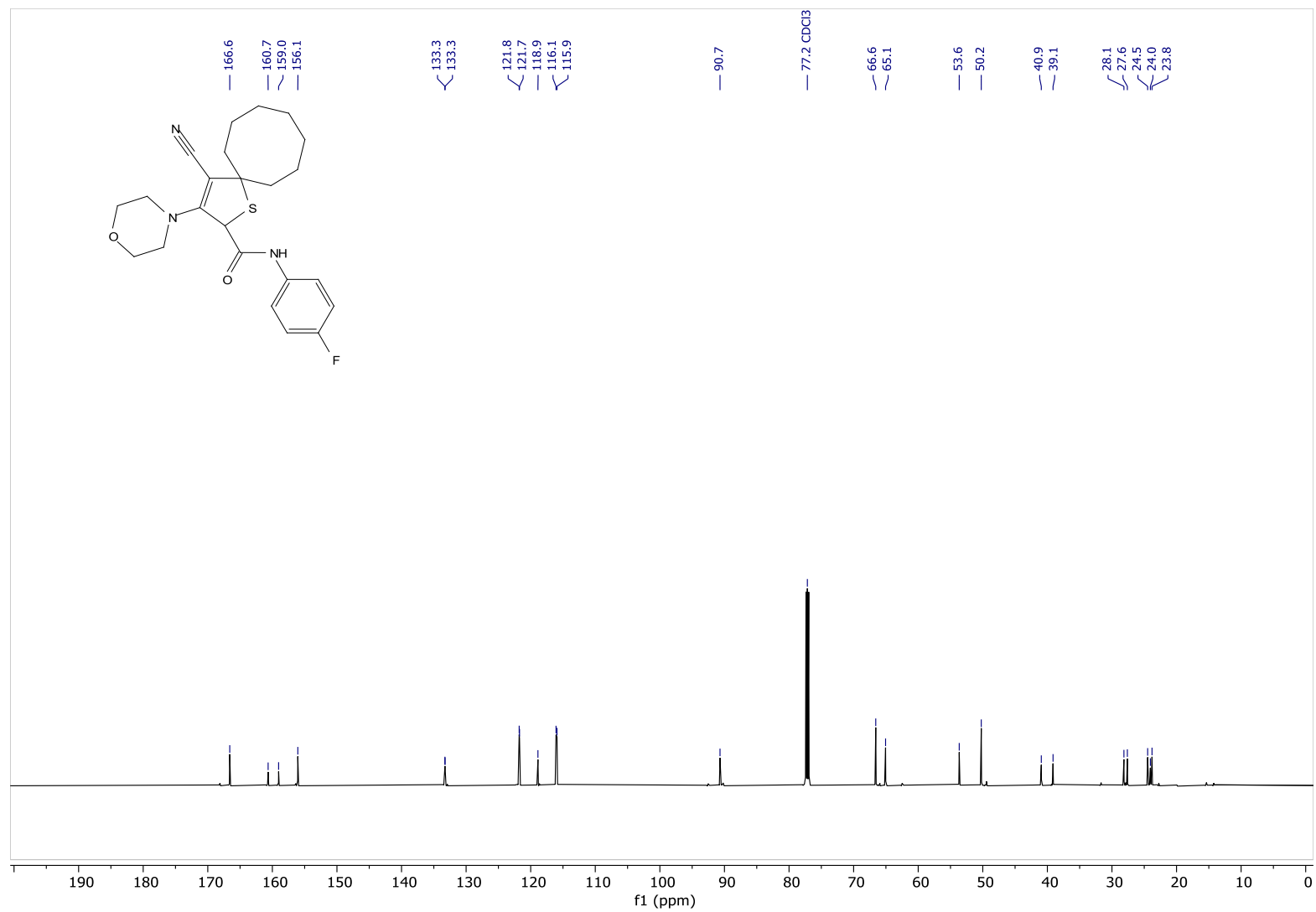
S73



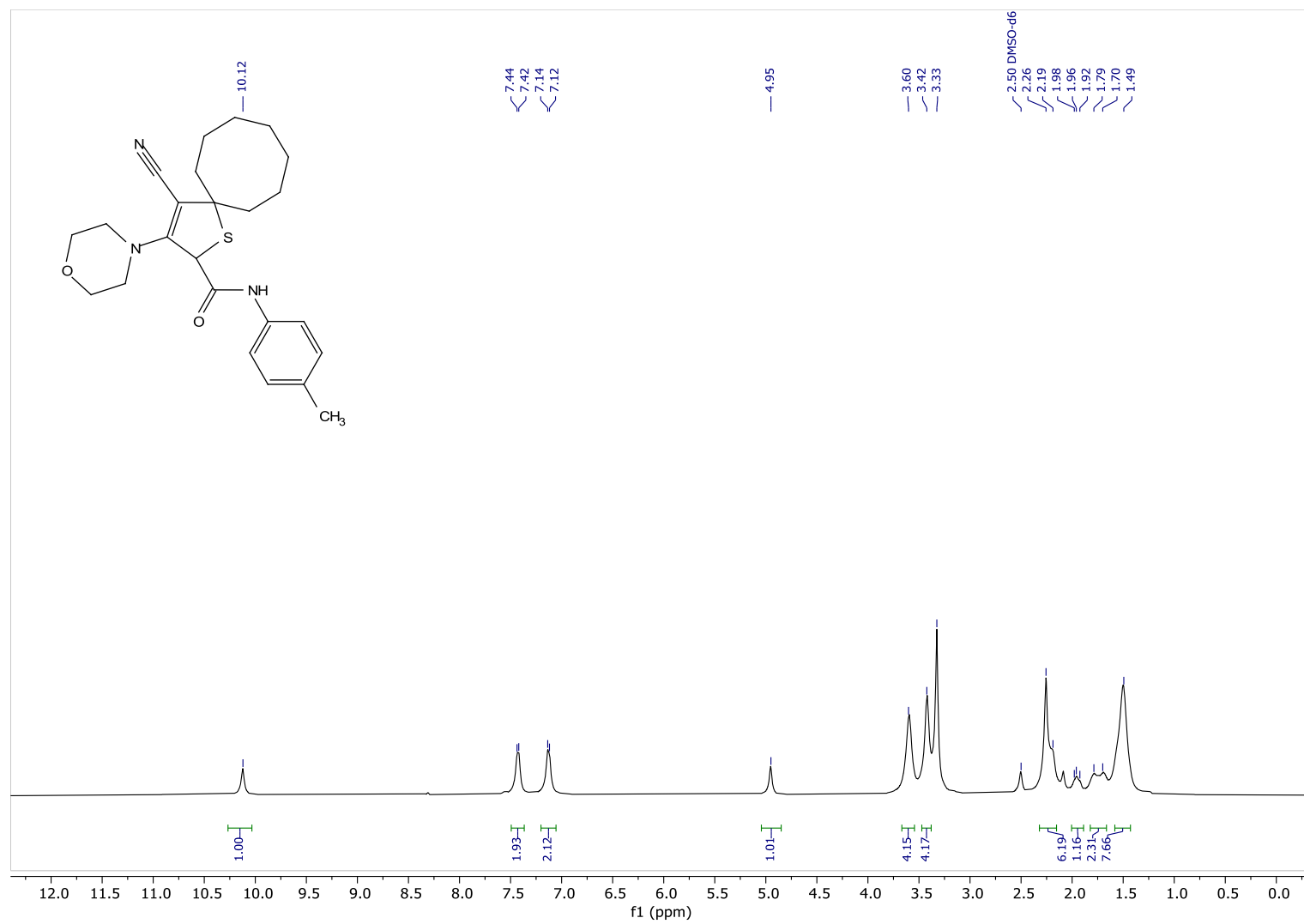
¹³C NMR (100 MHz, CDCl₃-d) of **3h**



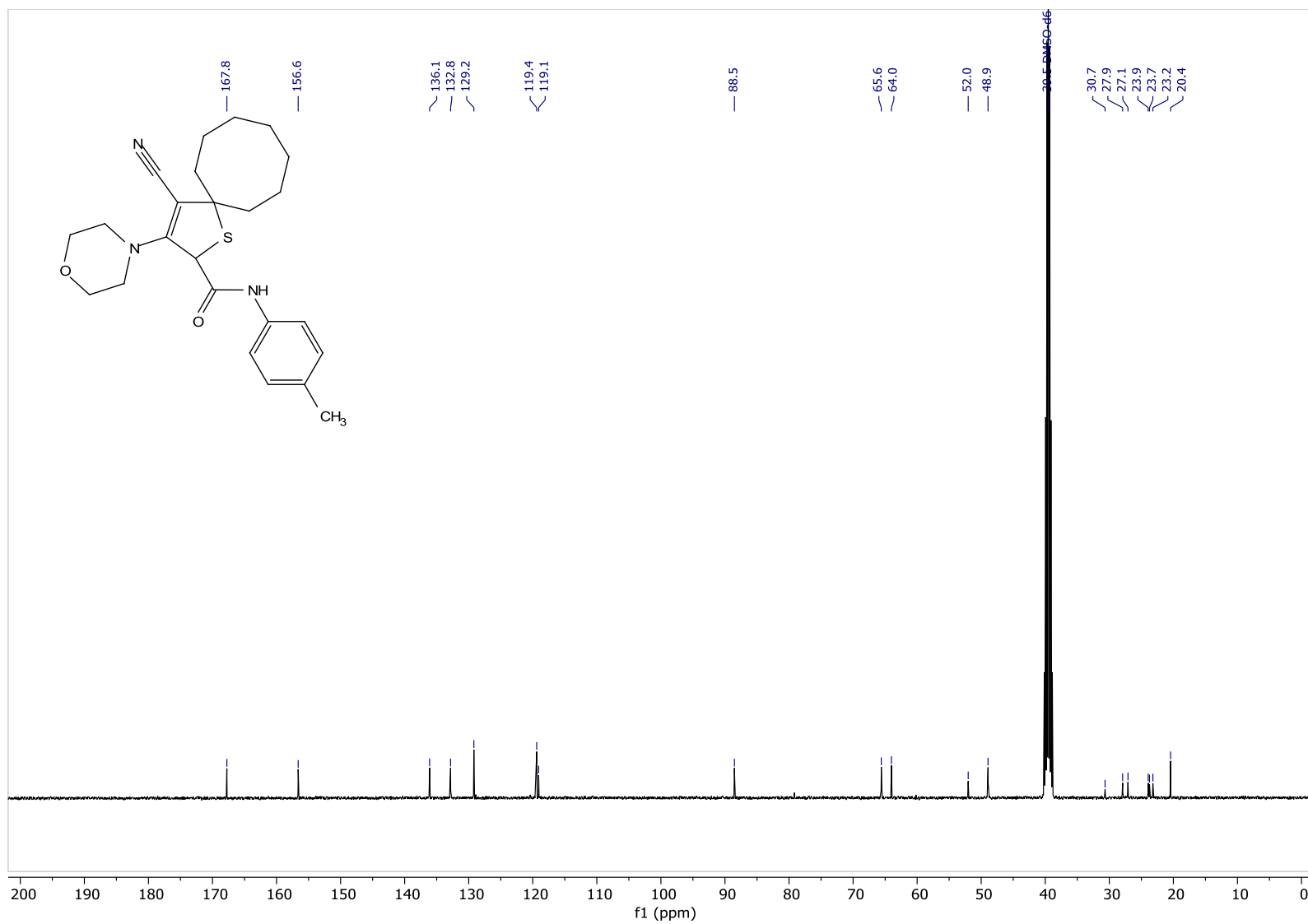
¹H NMR (600 MHz, CDCl₃-d) of **3i**



¹³C NMR (150 MHz, CDCl₃-d) of **3i**

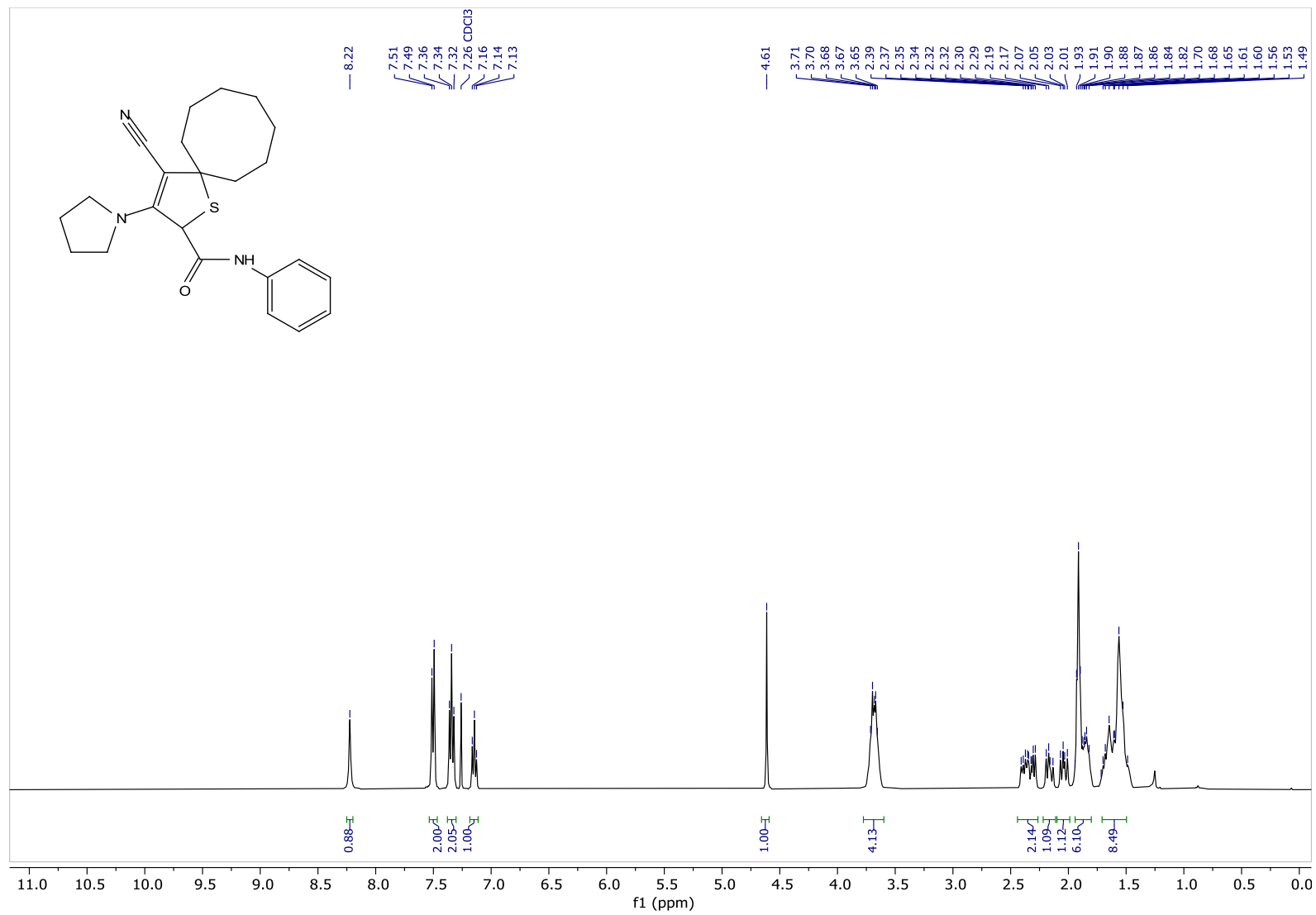


¹H NMR (400 MHz, DMSO-*d*₆) of **3j**

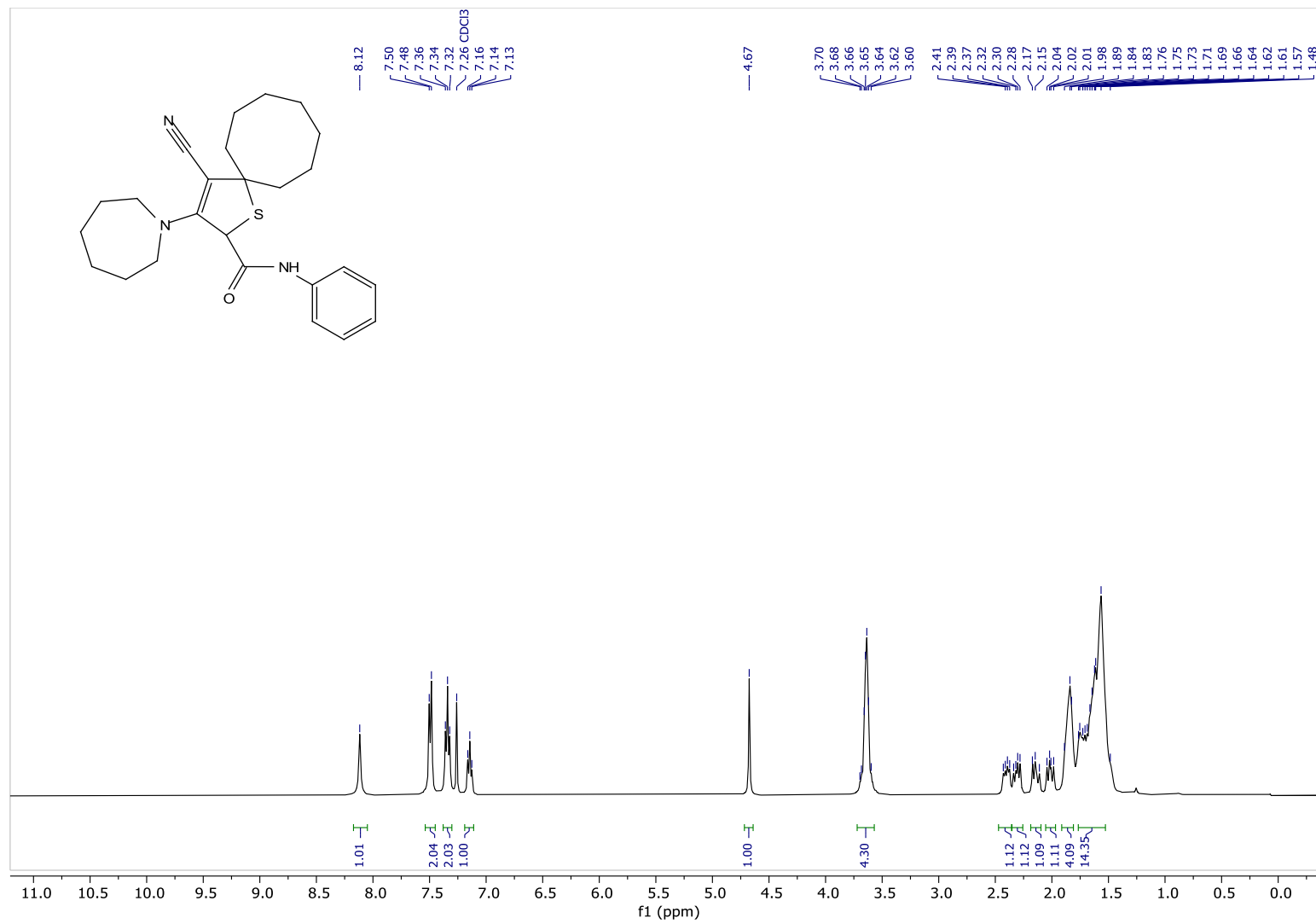


¹³C NMR (100 MHz, DMSO-*d*₆) of **3j**

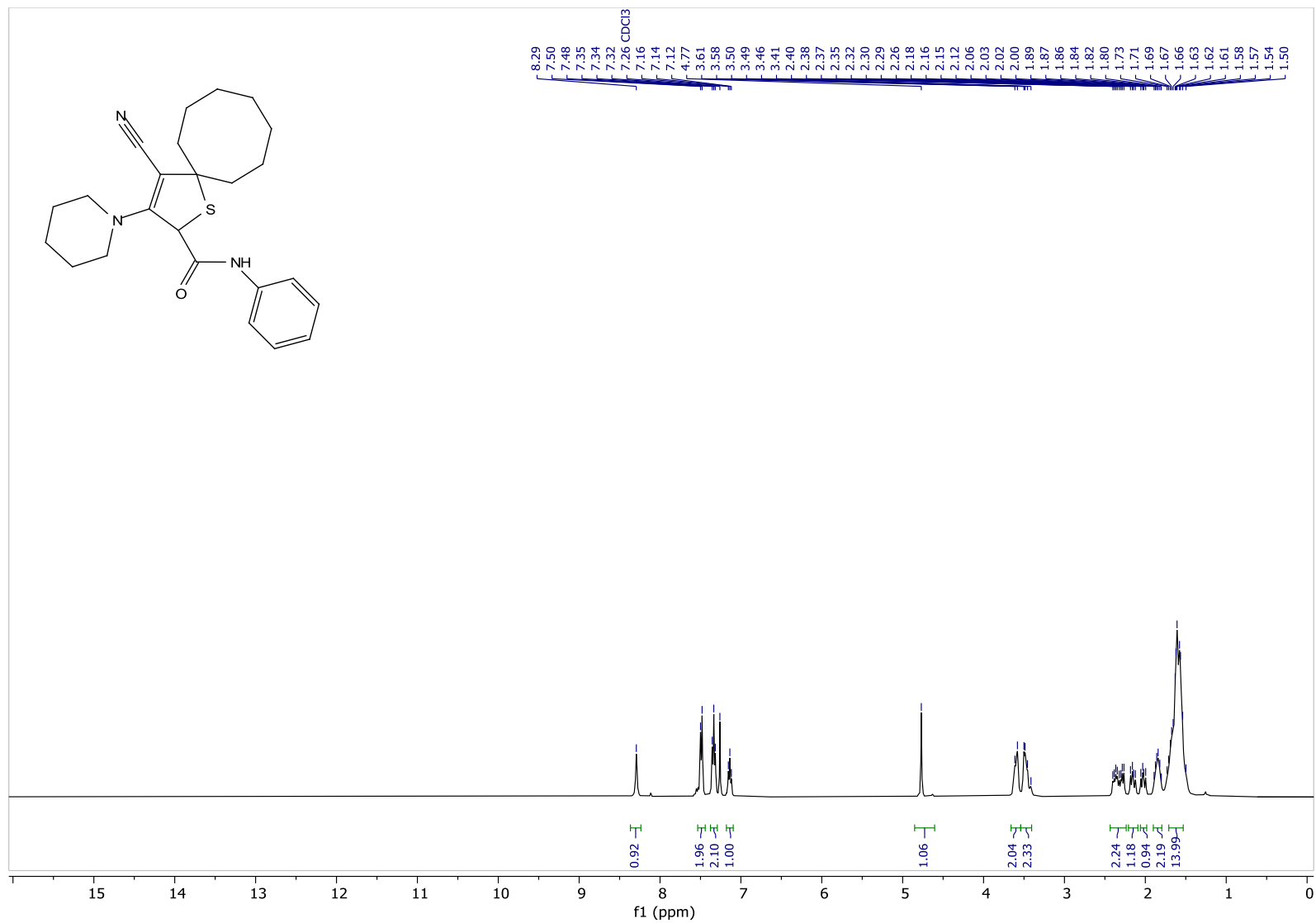
S78



¹H NMR (400 MHz, CDCl₃-d) of **2m**

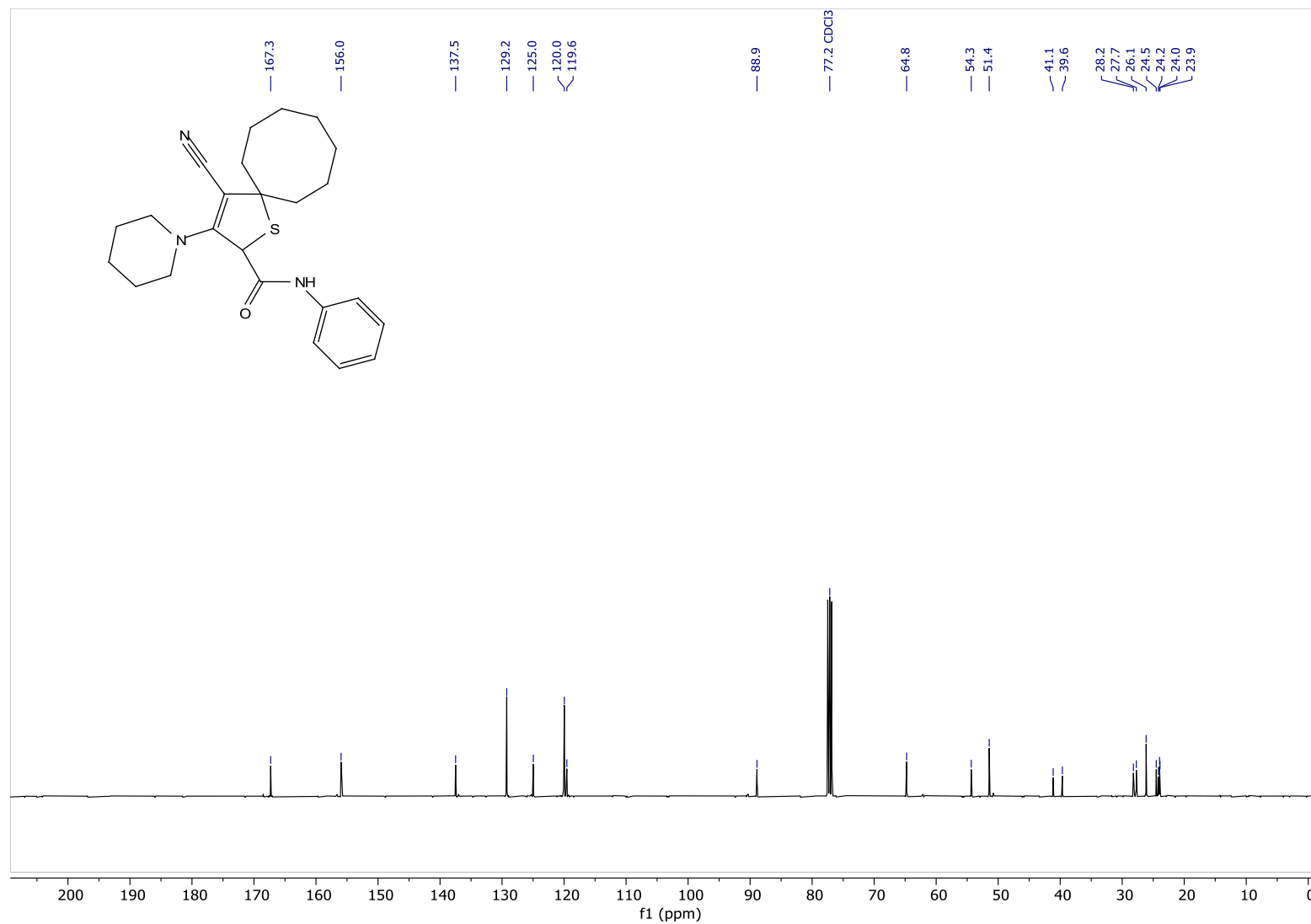


^1H NMR (400 MHz, CDCl_3 -d) of **2n**

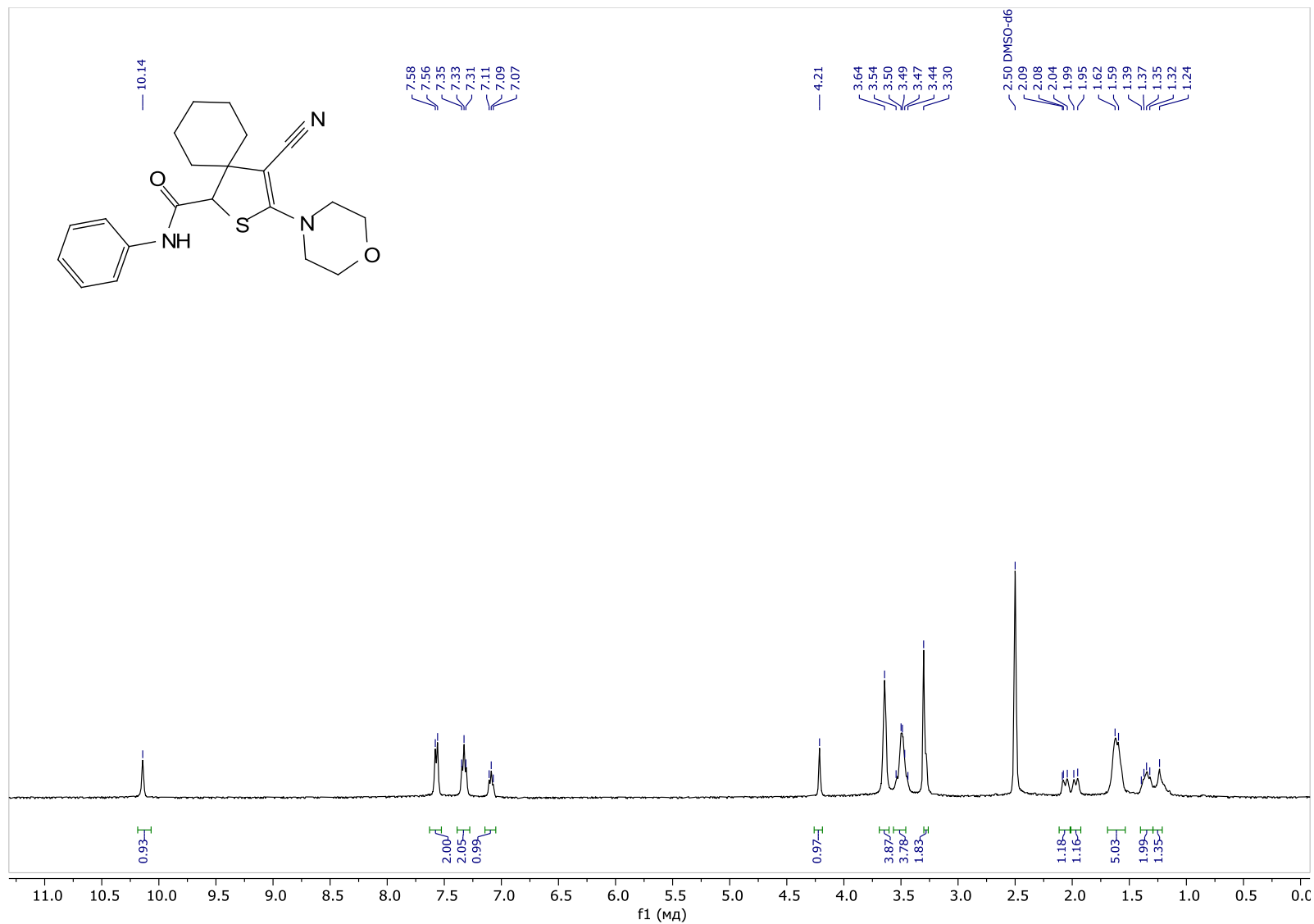


¹H NMR (400 MHz, CDCl₃-d) of **3k**

S81

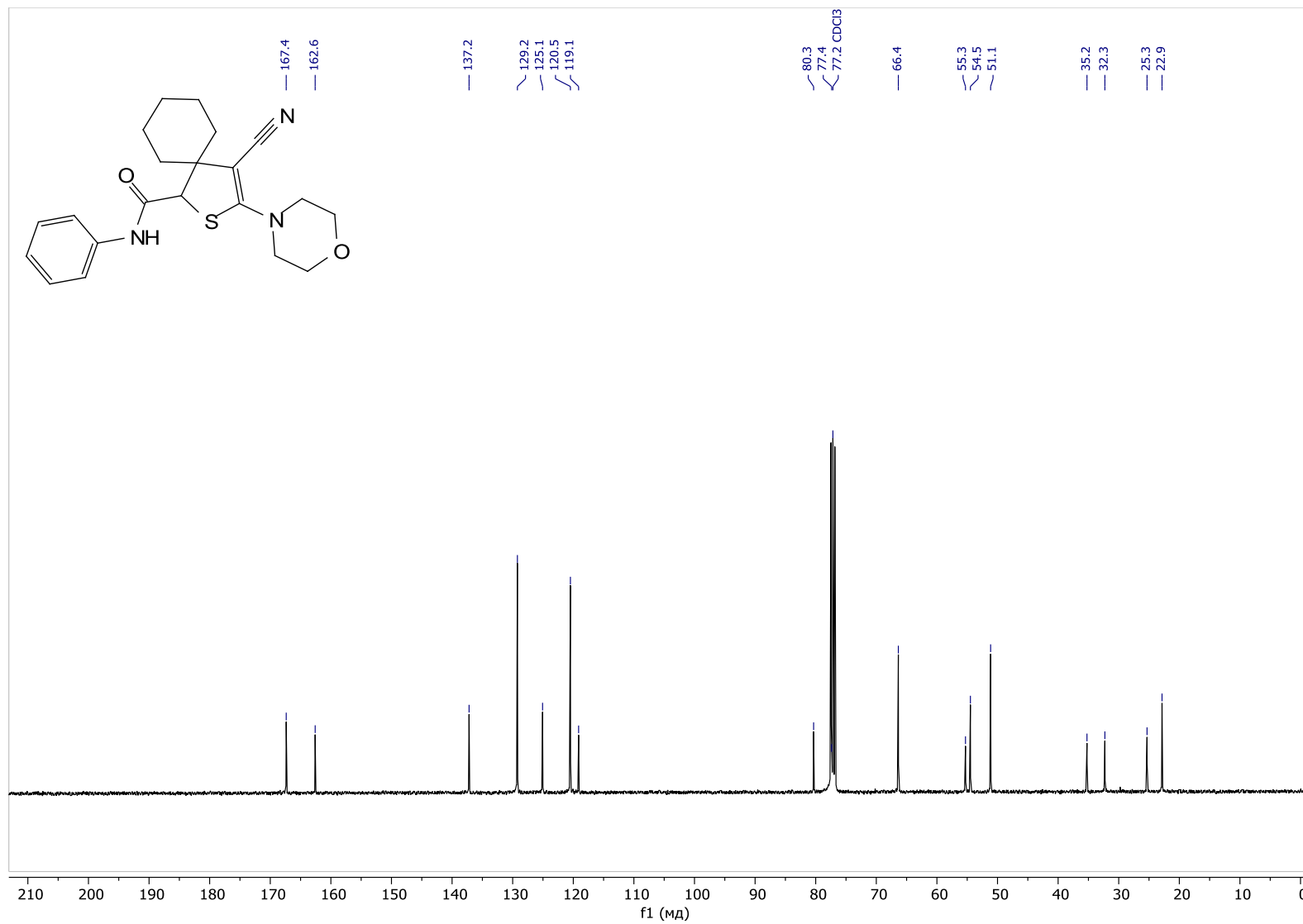


^{13}C NMR (100 MHz, CDCl_3 -*d*) of **3k**

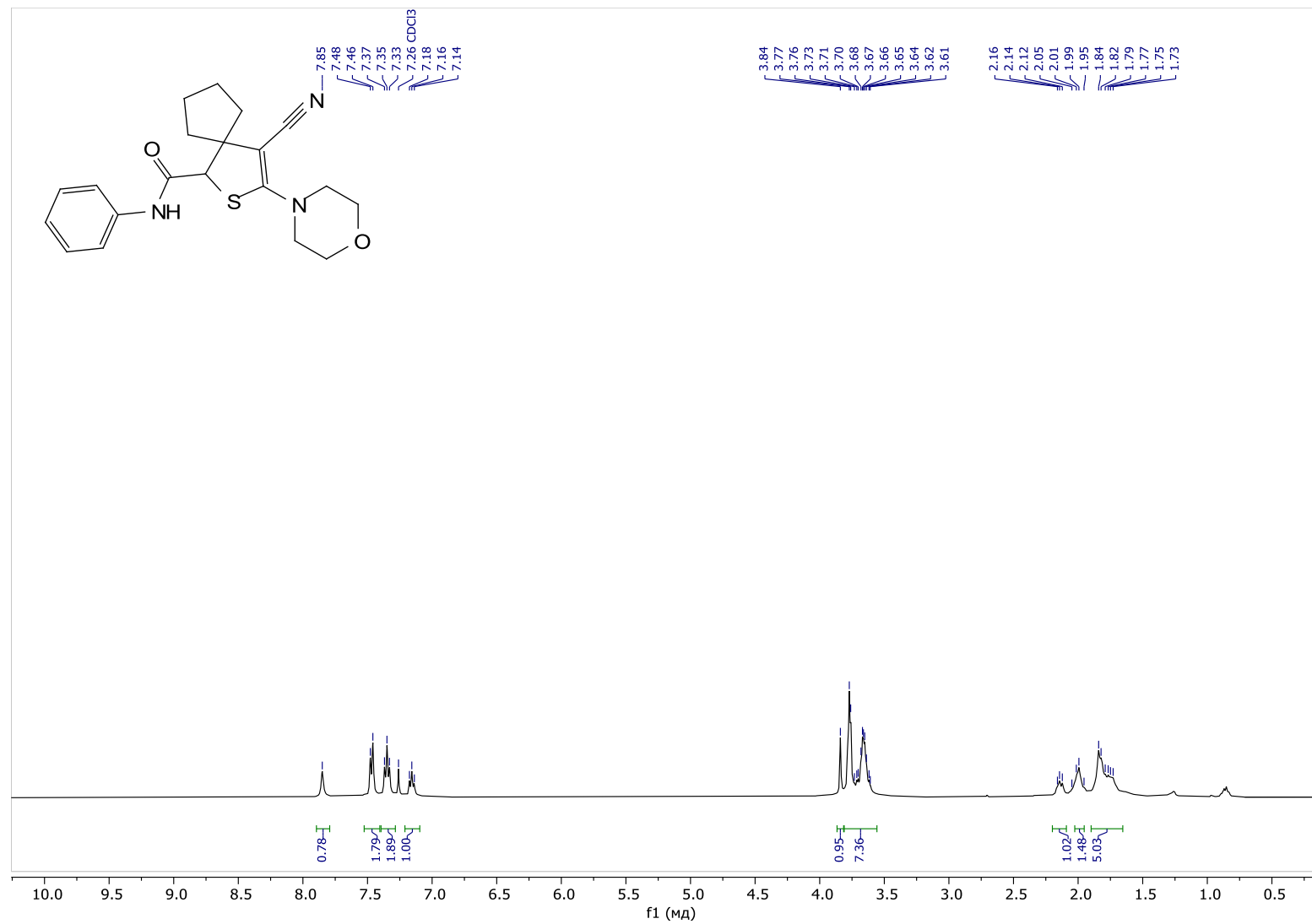


¹H NMR (400 MHz, DMSO-*d*₆) of **5a**

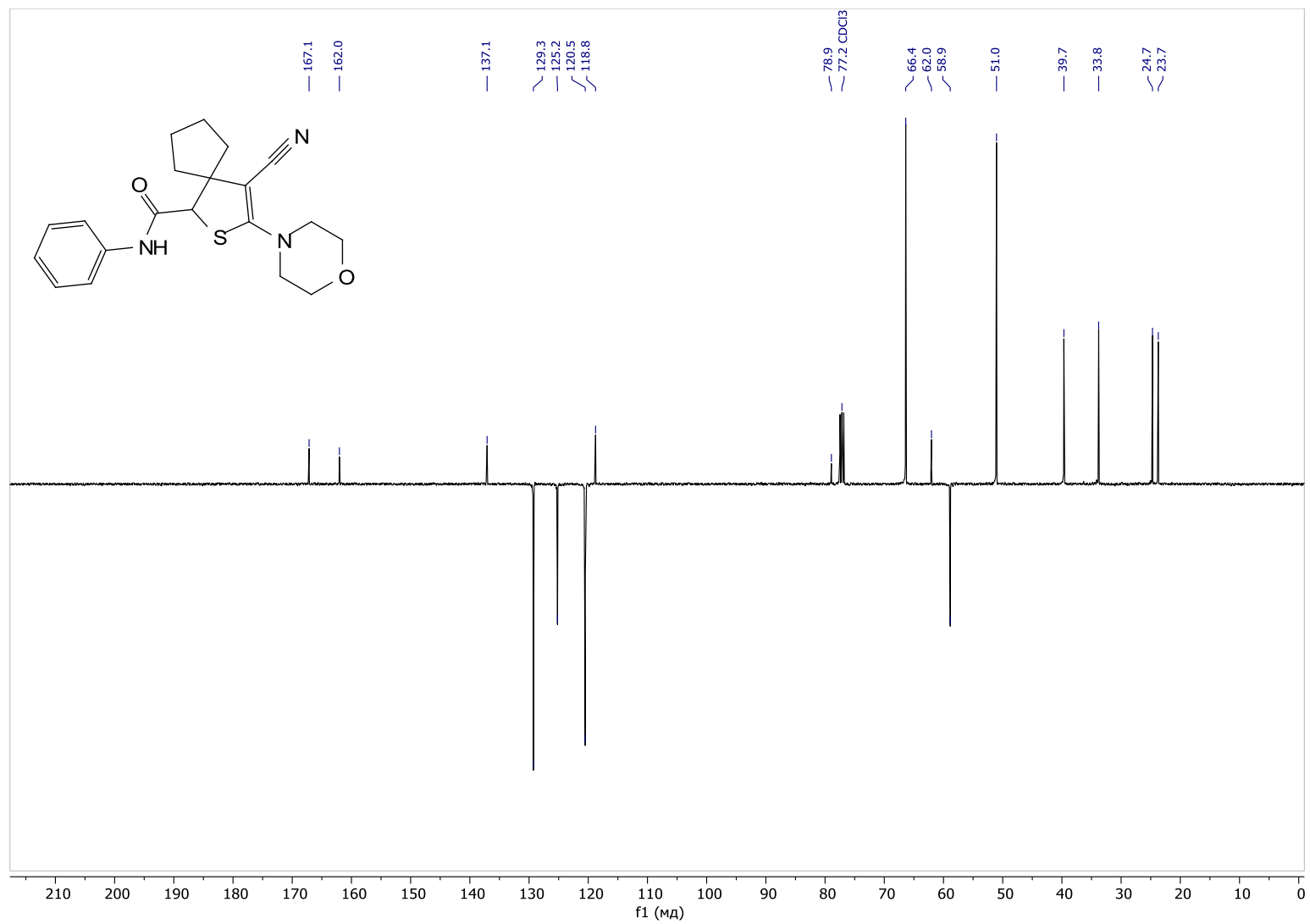
S83



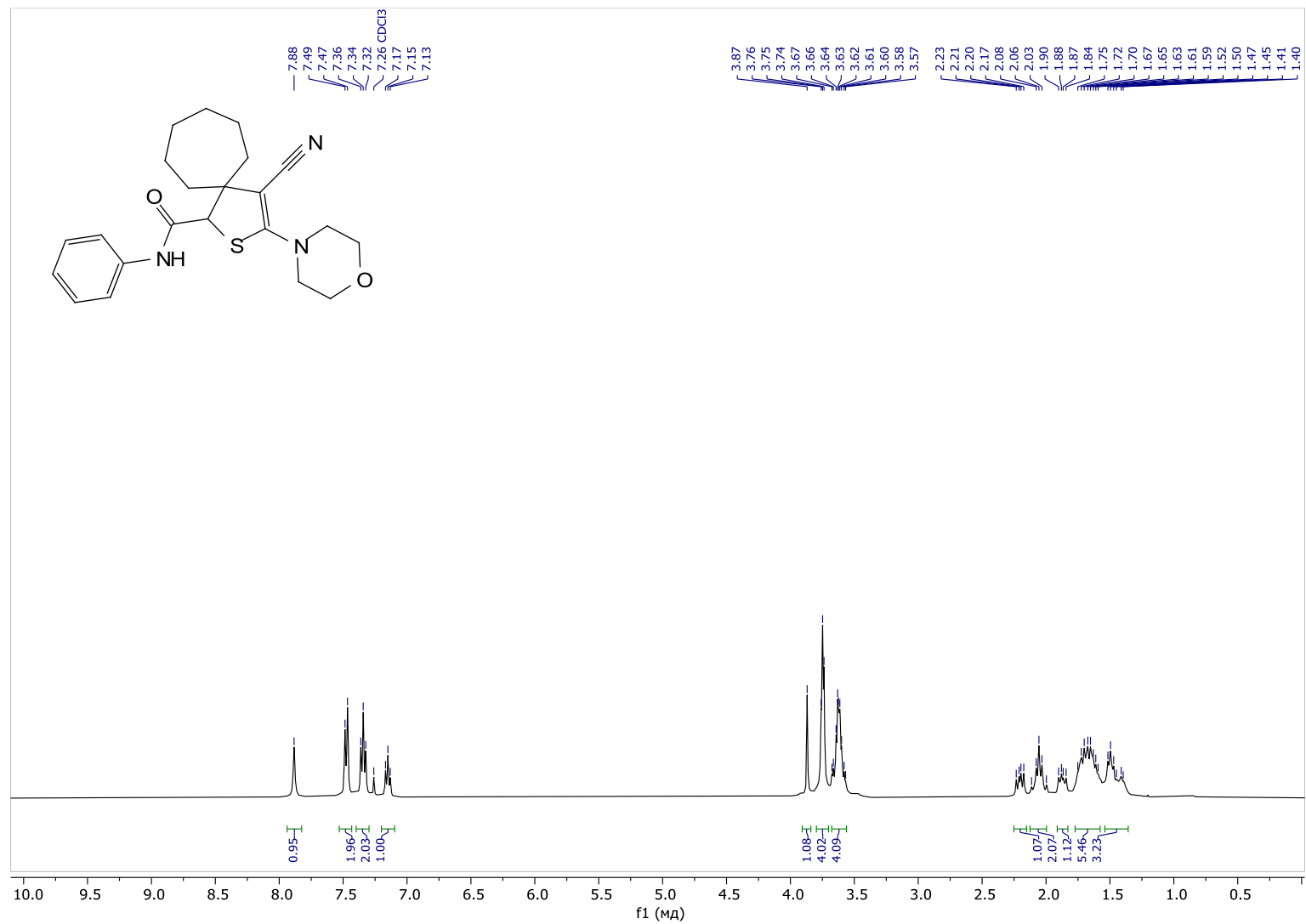
^{13}C NMR (100 MHz, CDCl_3 -*d*) of **5a**



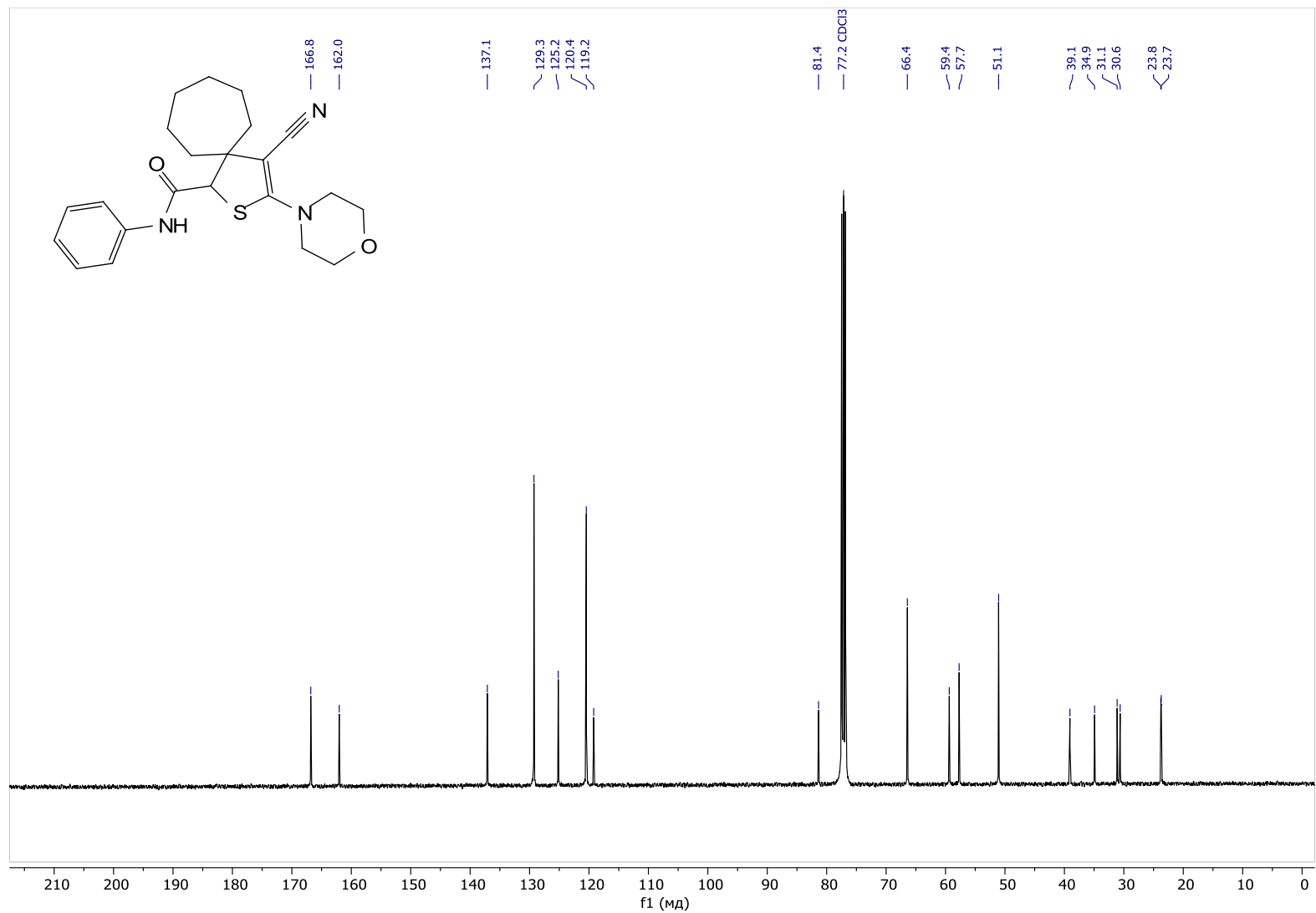
^1H NMR (400 MHz, CDCl_3 -*d*) of **5b**



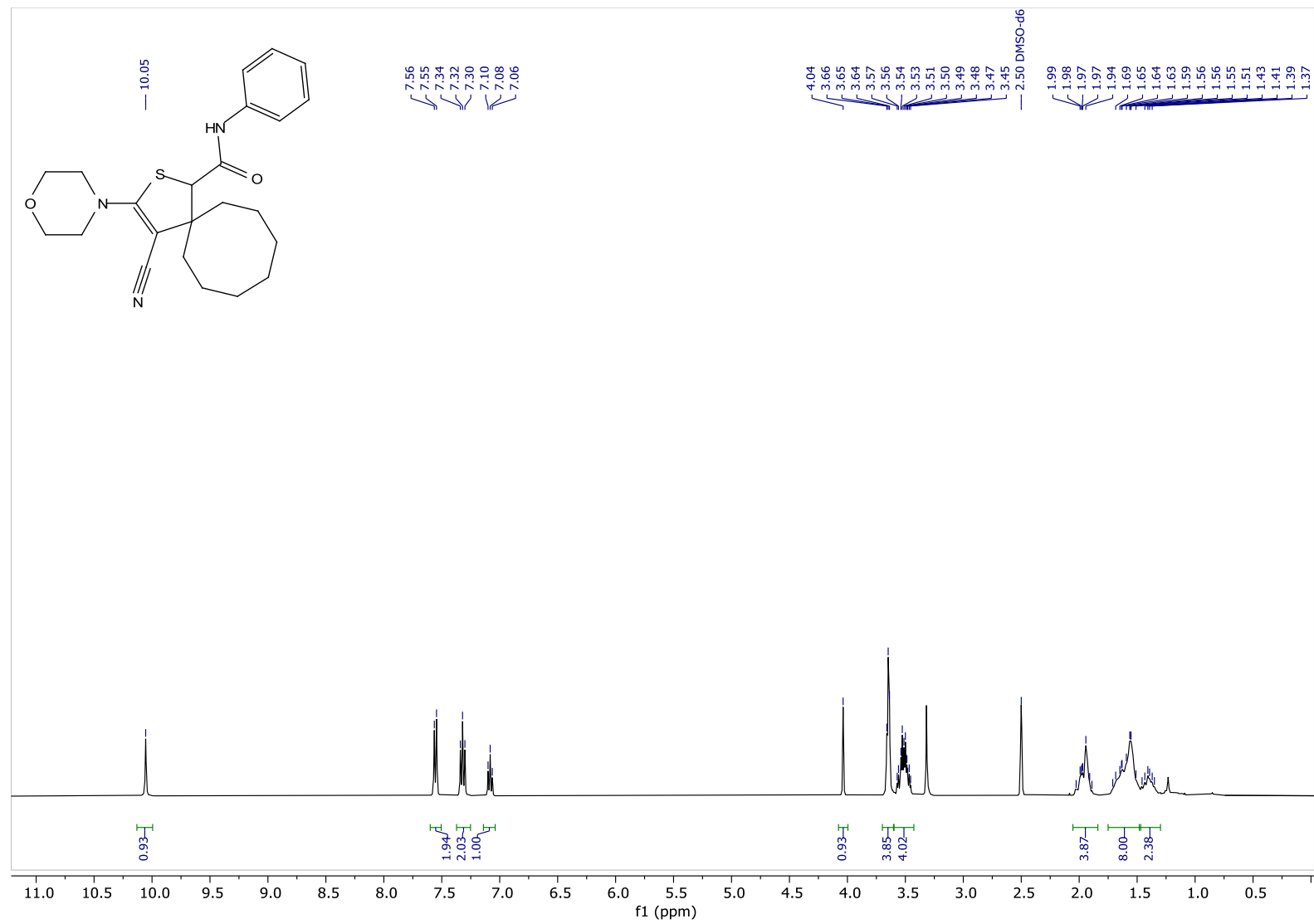
¹³C NMR (100 MHz, CDCl₃-*d*) of **5b**



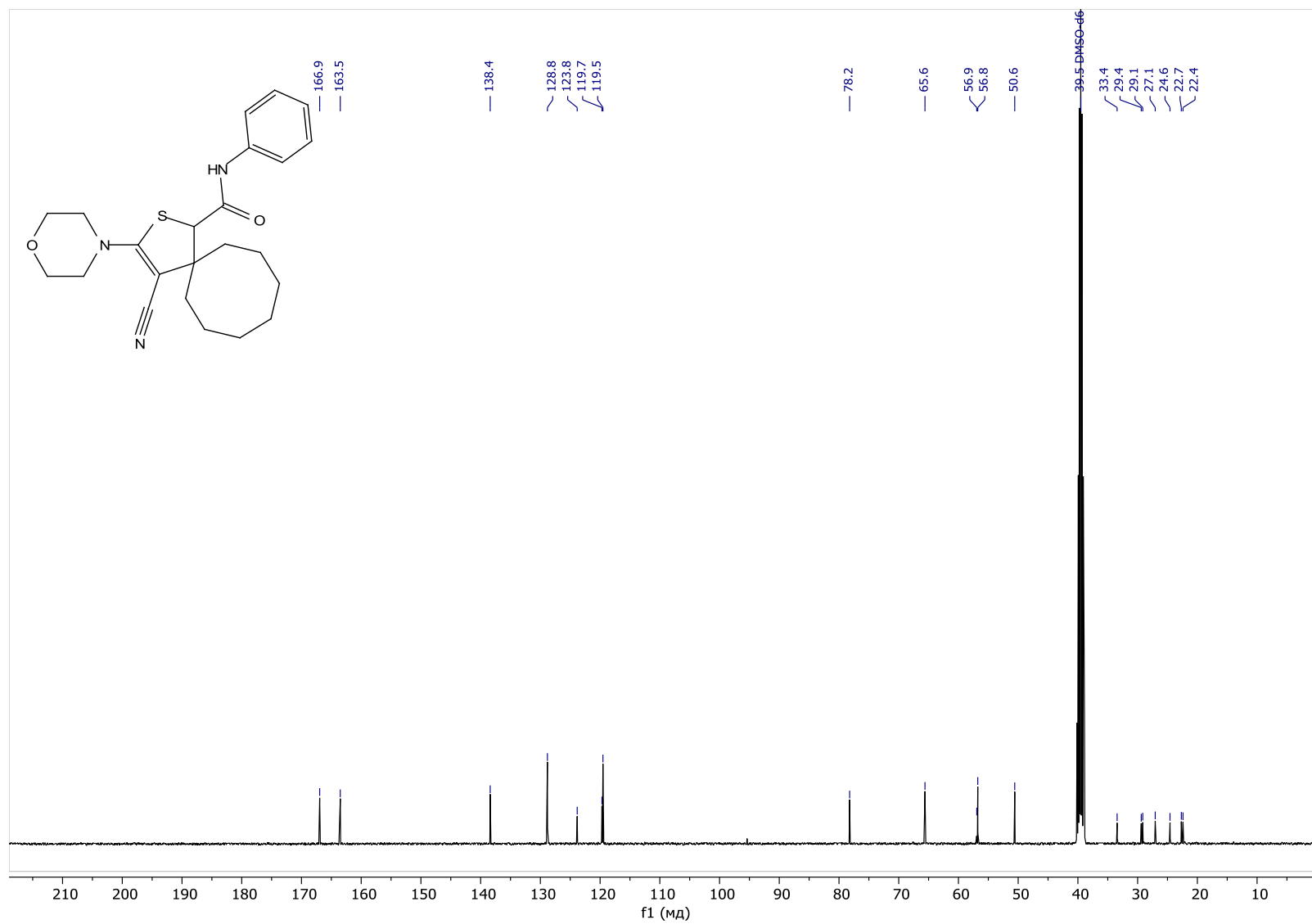
¹H NMR (400 MHz, CDCl₃-d) of **5c**



^{13}C NMR (100 MHz, CDCl_3 -*d*) of **5c**

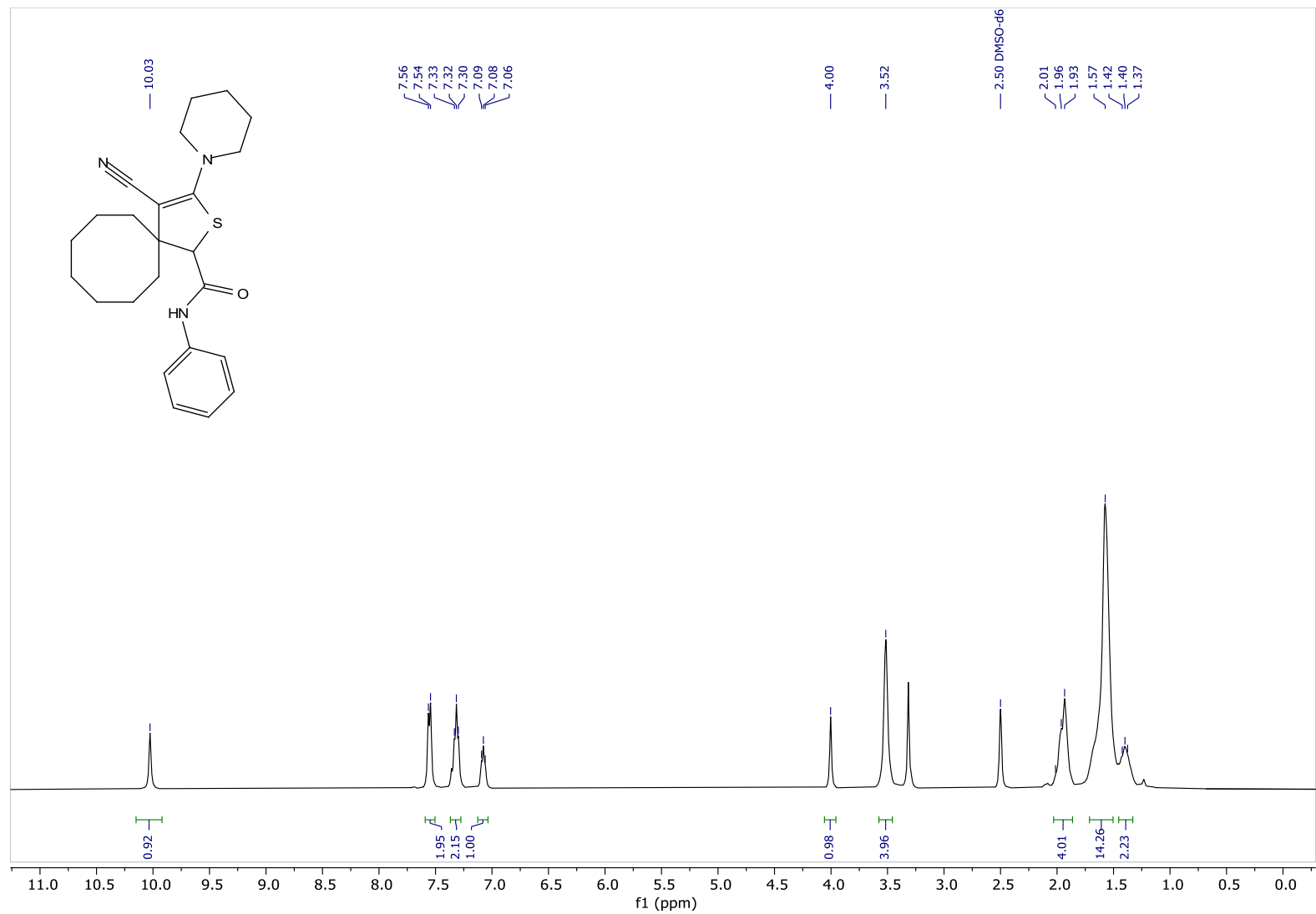


^1H NMR (400 MHz, $\text{DMSO}-d_6$) of **5d**

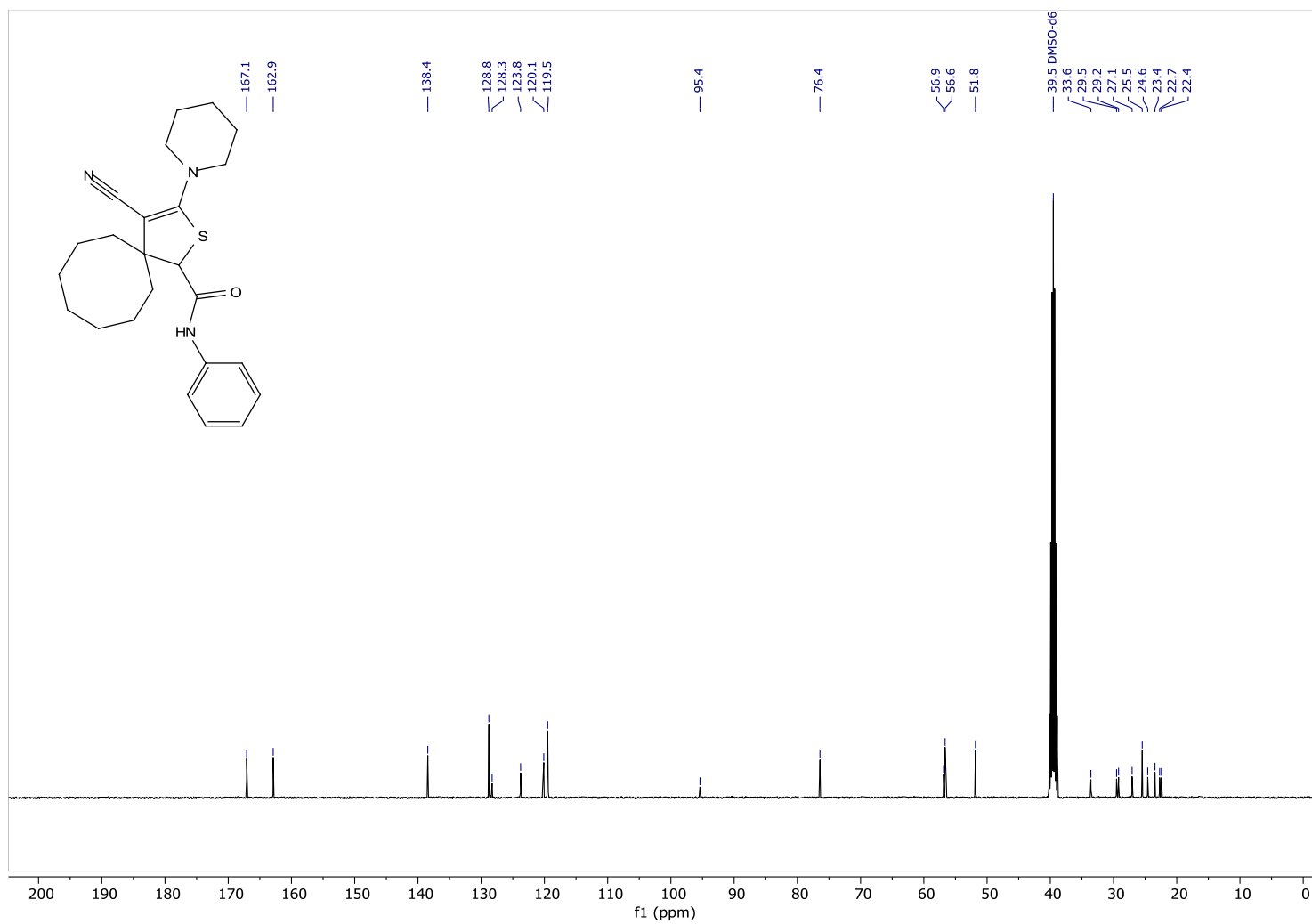


^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **5c**

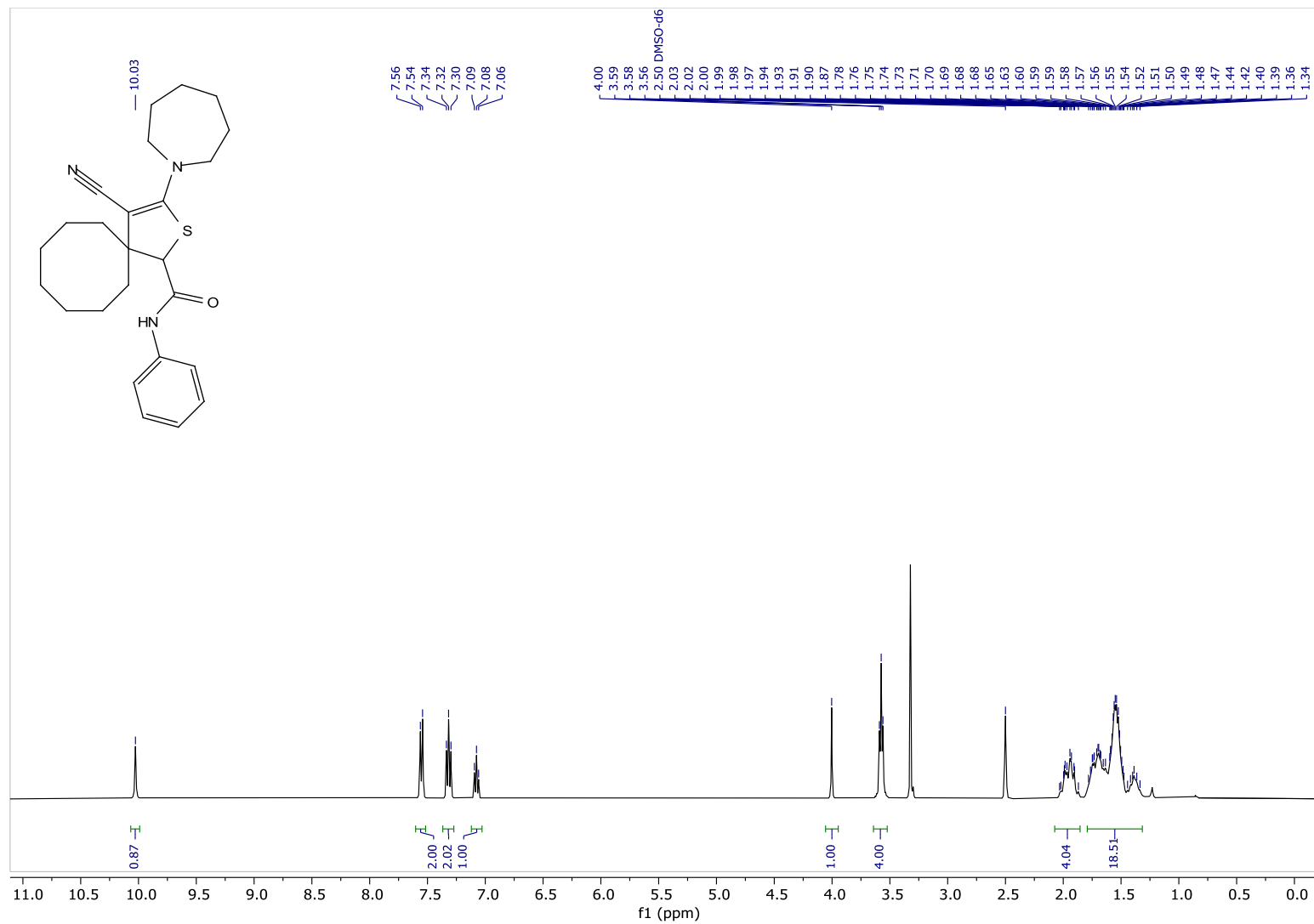
S90



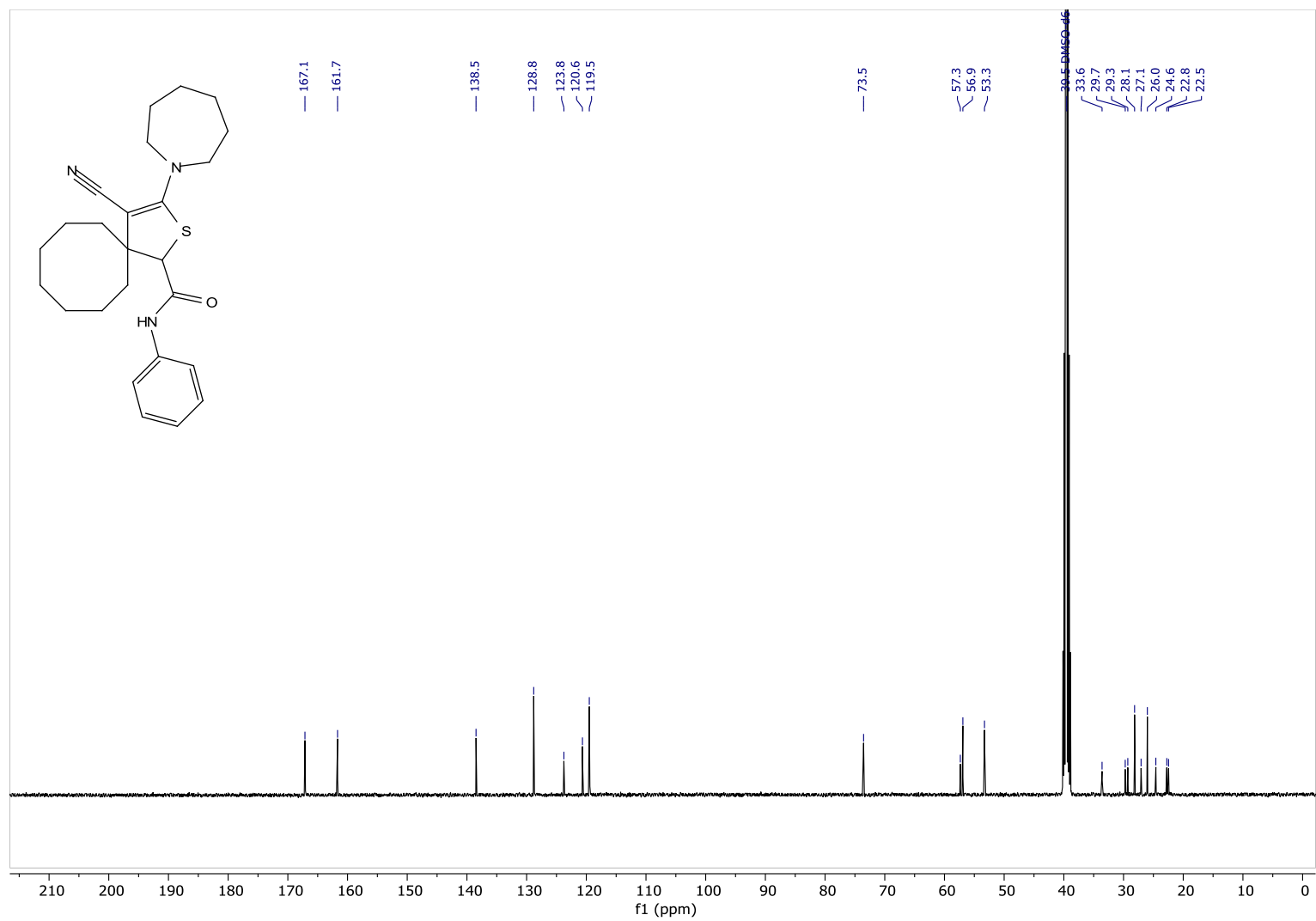
¹H NMR (400 MHz, DMSO-*d*₆) of **5e**



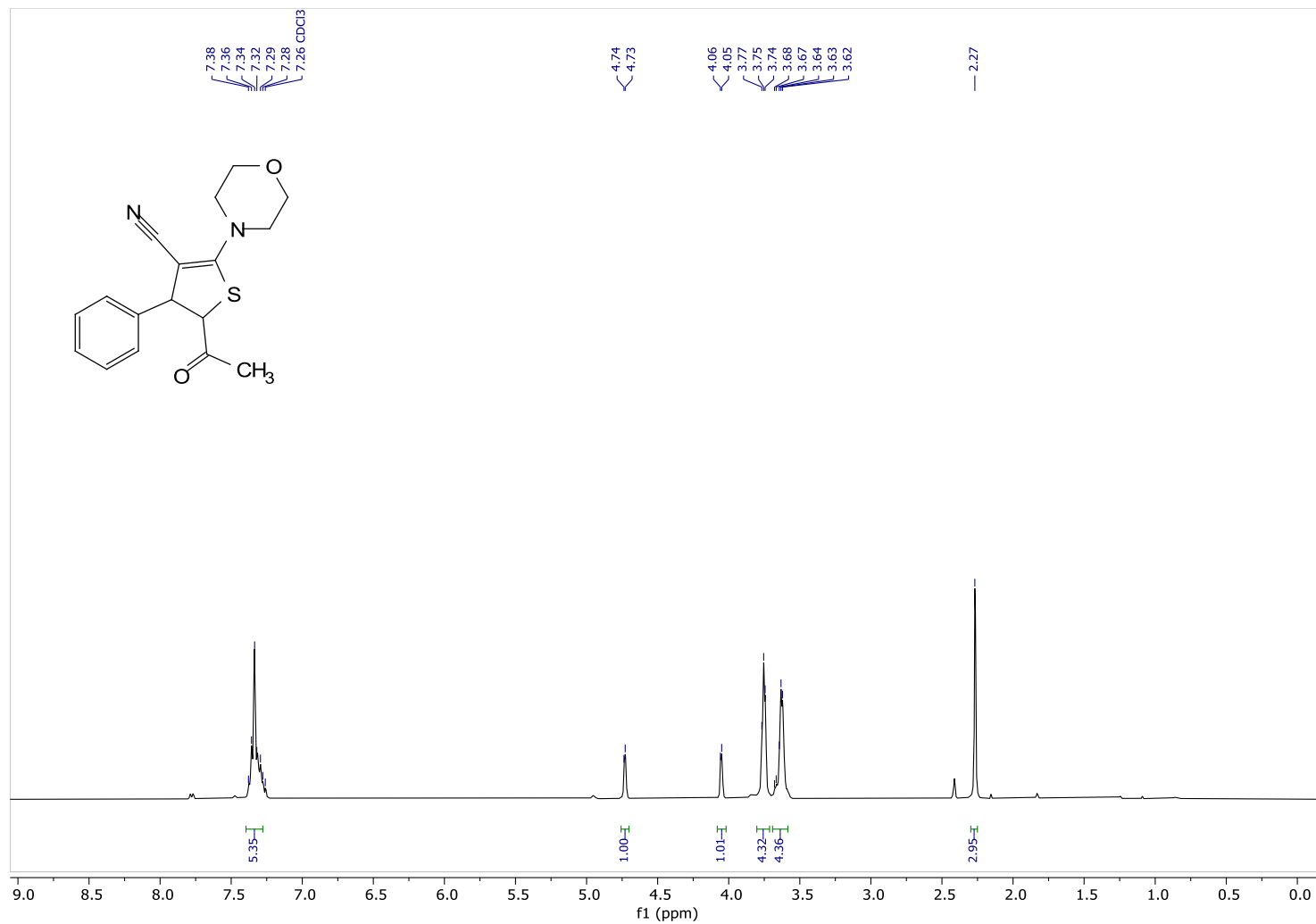
¹³C NMR (100 MHz, DMSO-*d*₆) of **5e**



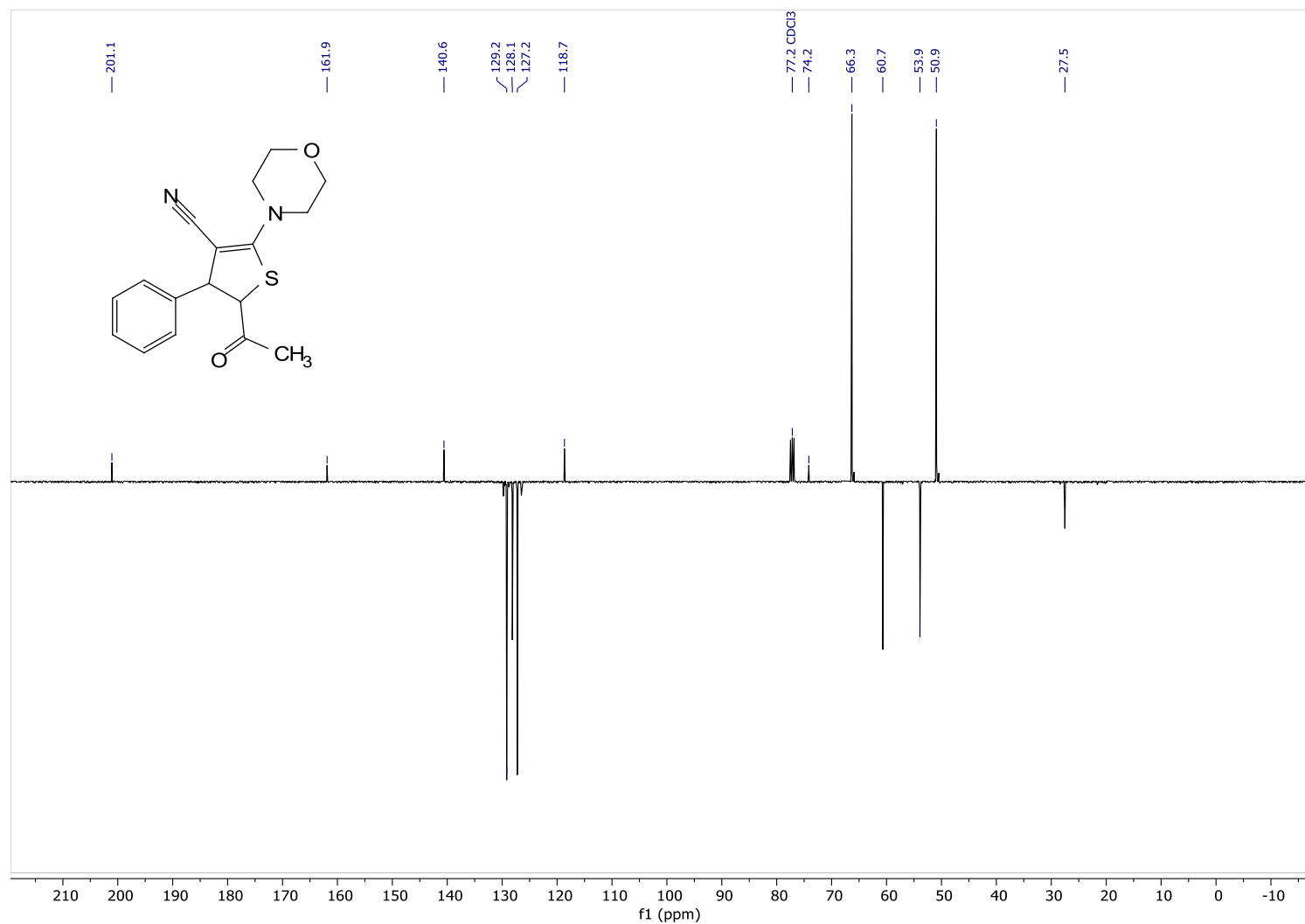
¹H NMR (400 MHz, DMSO-*d*₆) of **5f**



^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) of **5f**



^1H NMR (400 MHz, CDCl_3 -d) of **5g**



¹³C NMR (100 MHz, CDCl₃-d) of **5g**