



Supporting Information

for

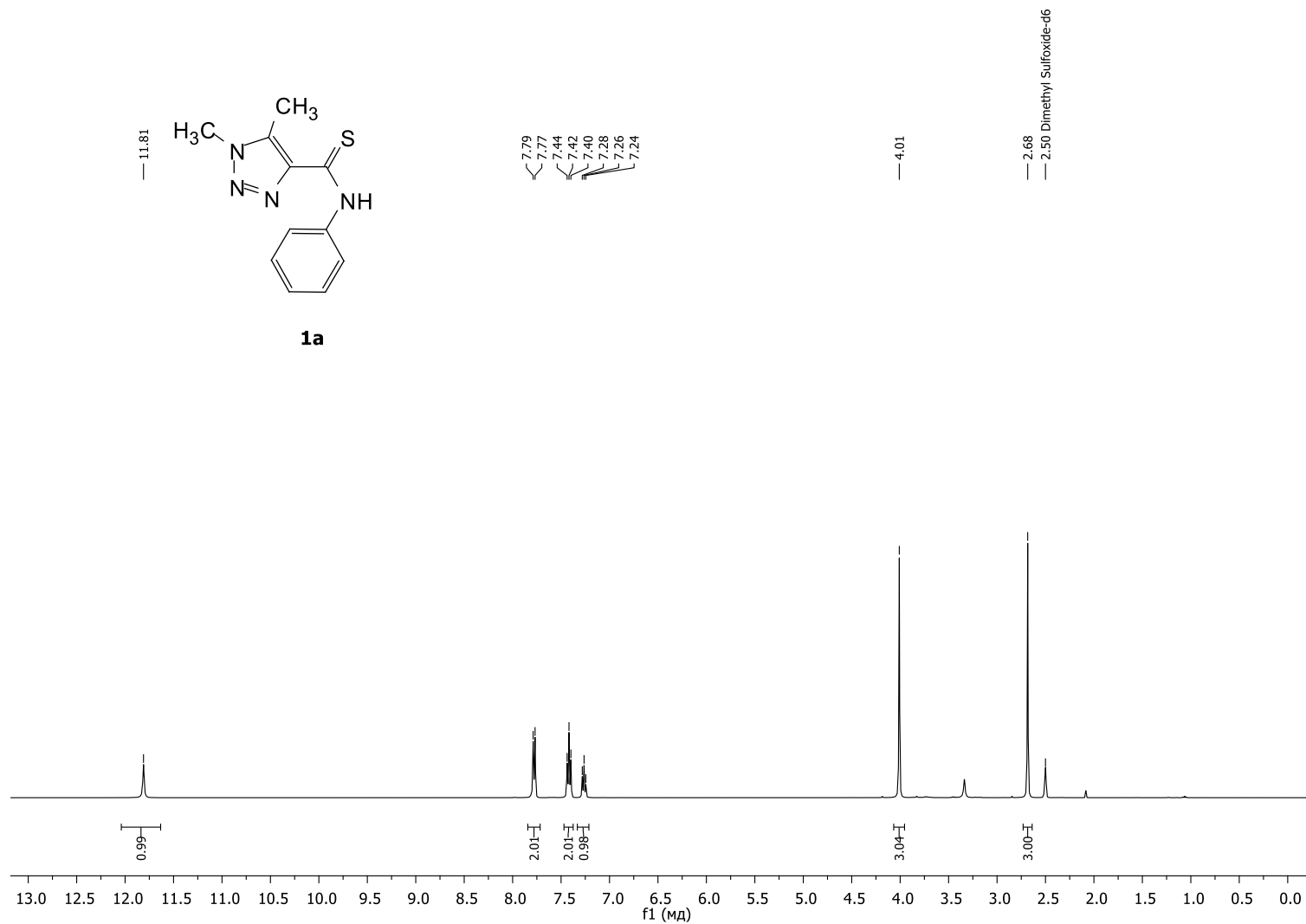
Regioselective synthesis of heterocyclic *N*-sulfonyl amidines from heteroaromatic thioamides and sulfonyl azides

Vladimir Ilkin, Vera Berseneva, Tetyana Beryozkina, Tatiana Glukhareva, Lidia Dianova, Wim Dehaen, Eugenia Seliverstova and Vasiliy Bakulev

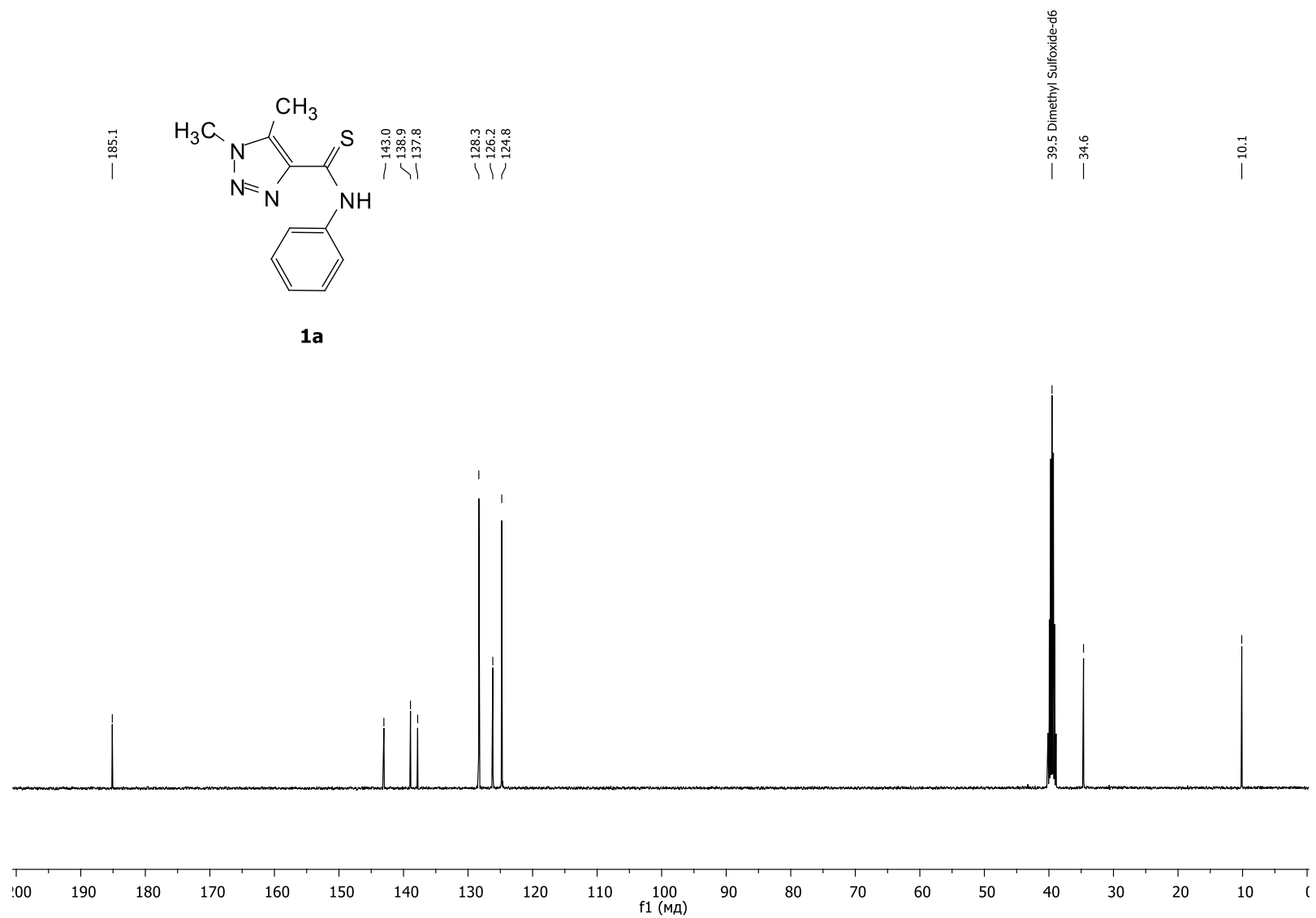
Beilstein J. Org. Chem. **2020**, *16*, 2937–2947. doi:10.3762/bjoc.16.243

Copies of NMR spectra of all new compounds

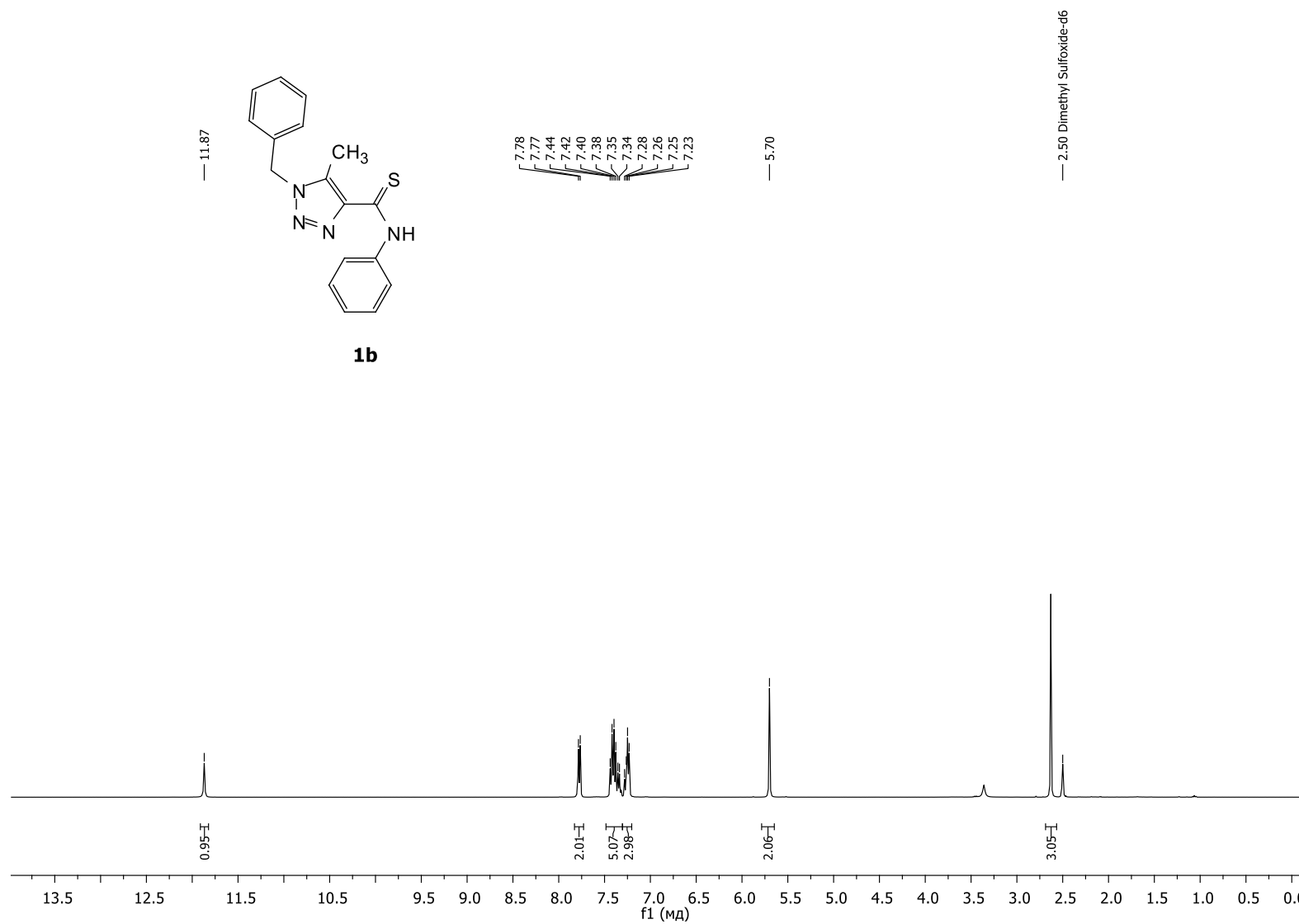
NMR spectra



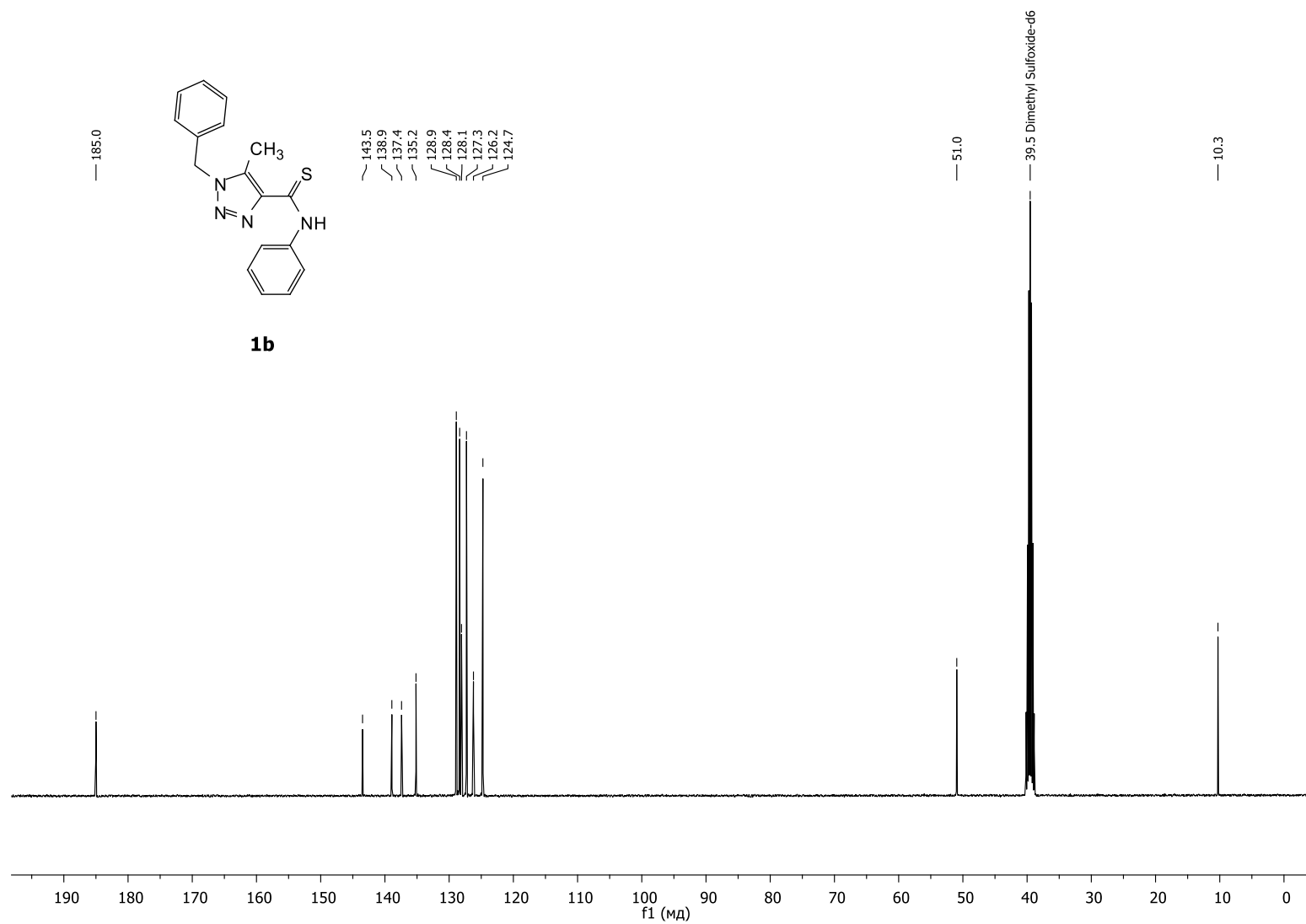
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **1a**.



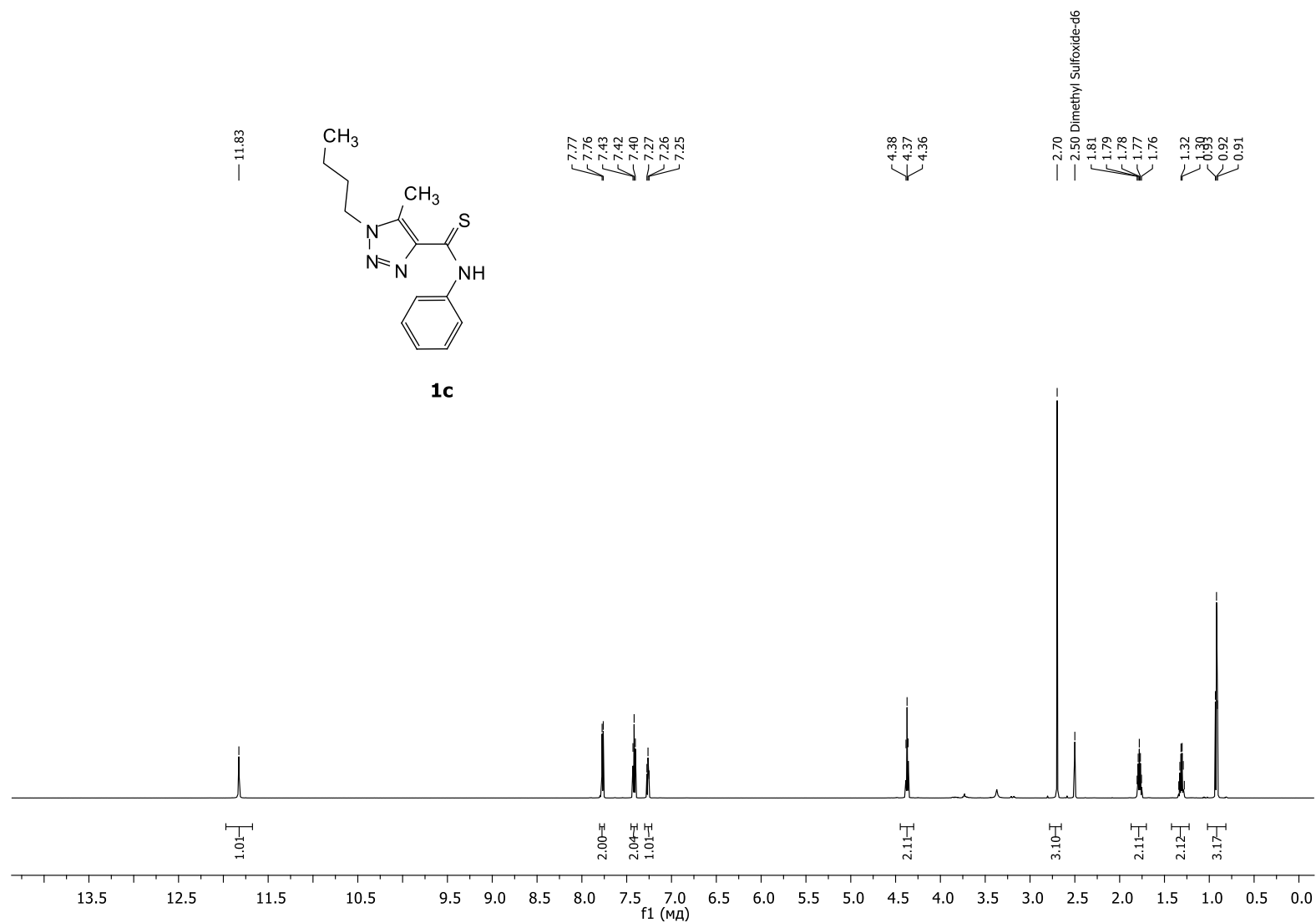
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **1a**.



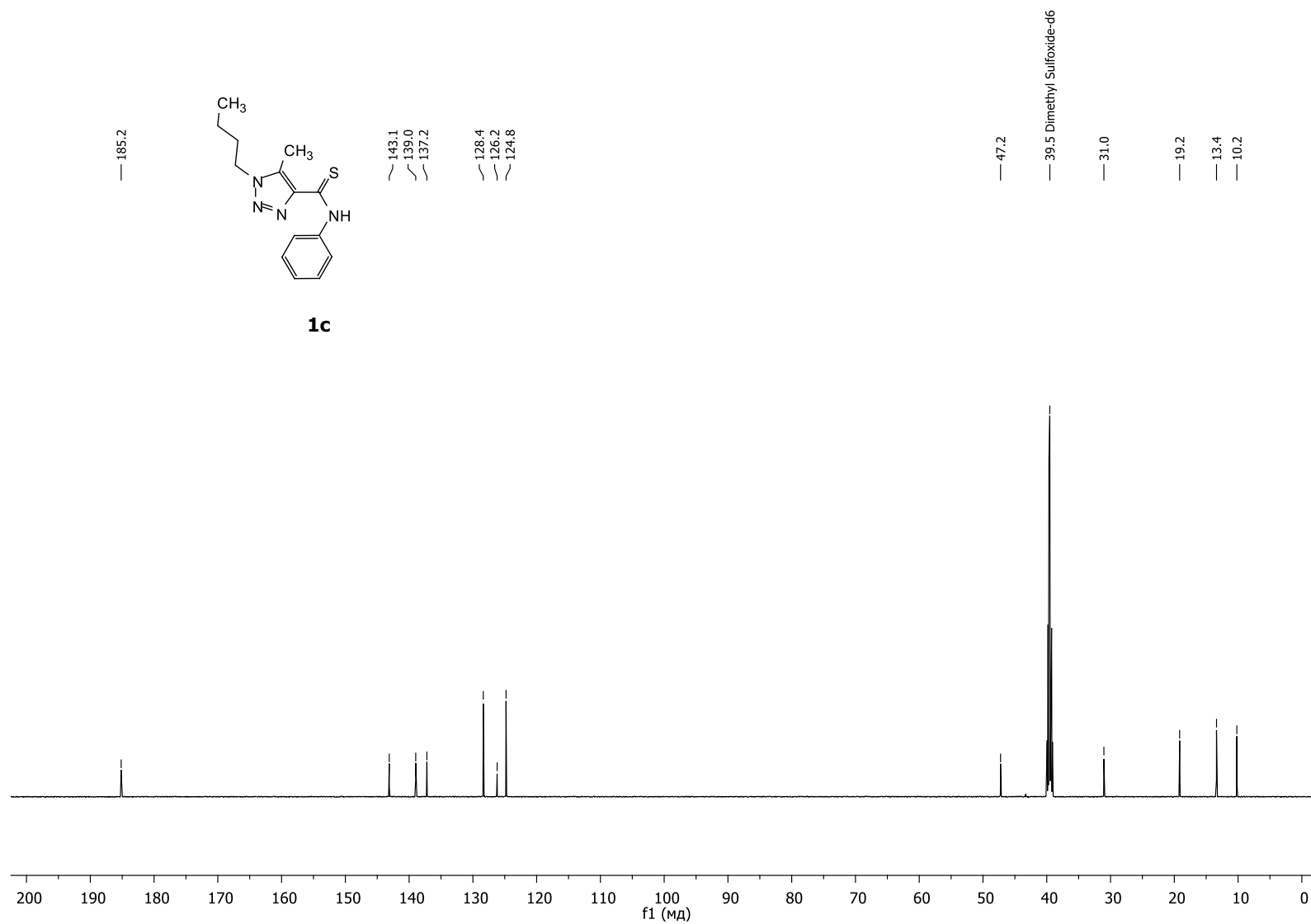
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **1b**.



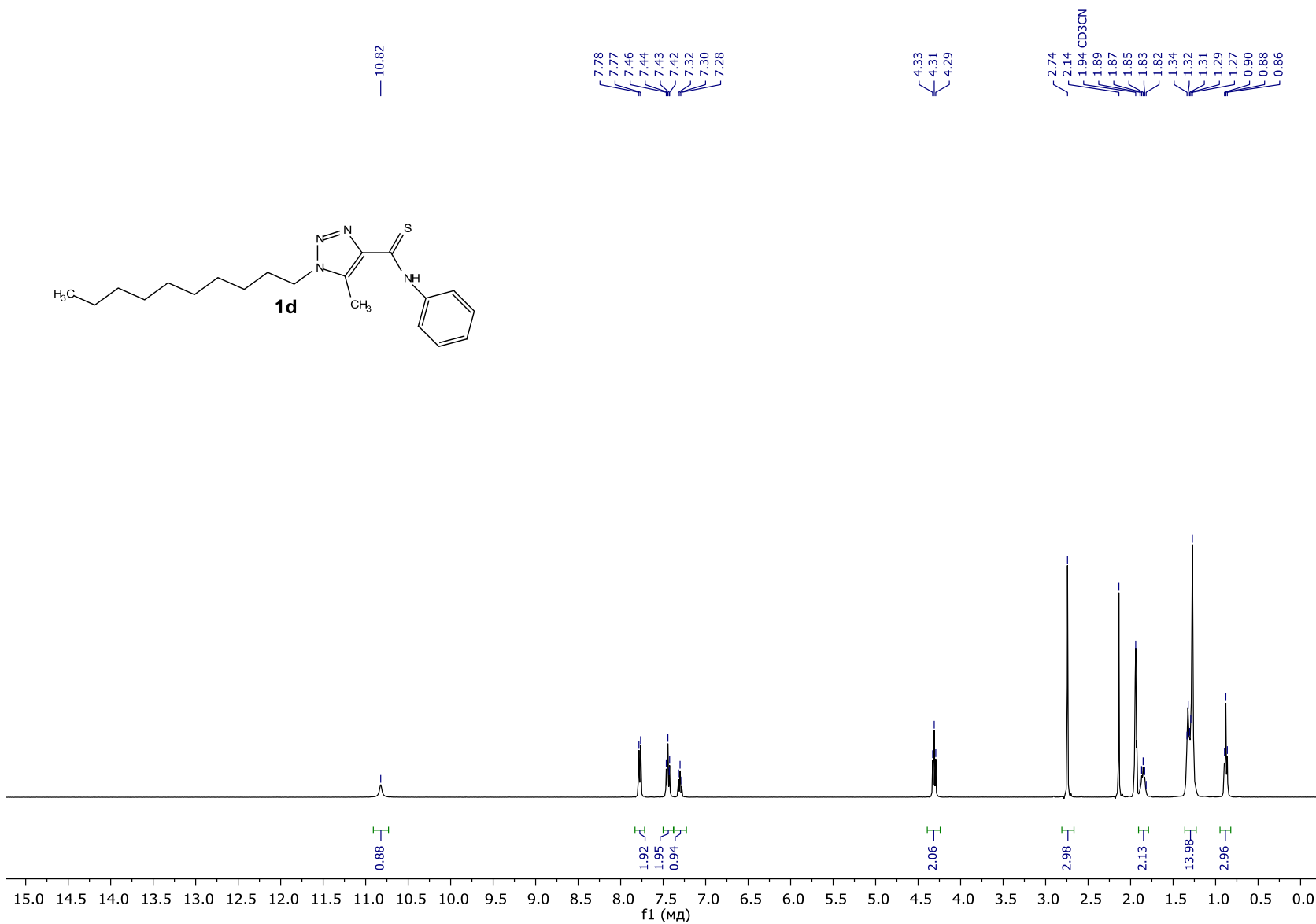
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **1b**.



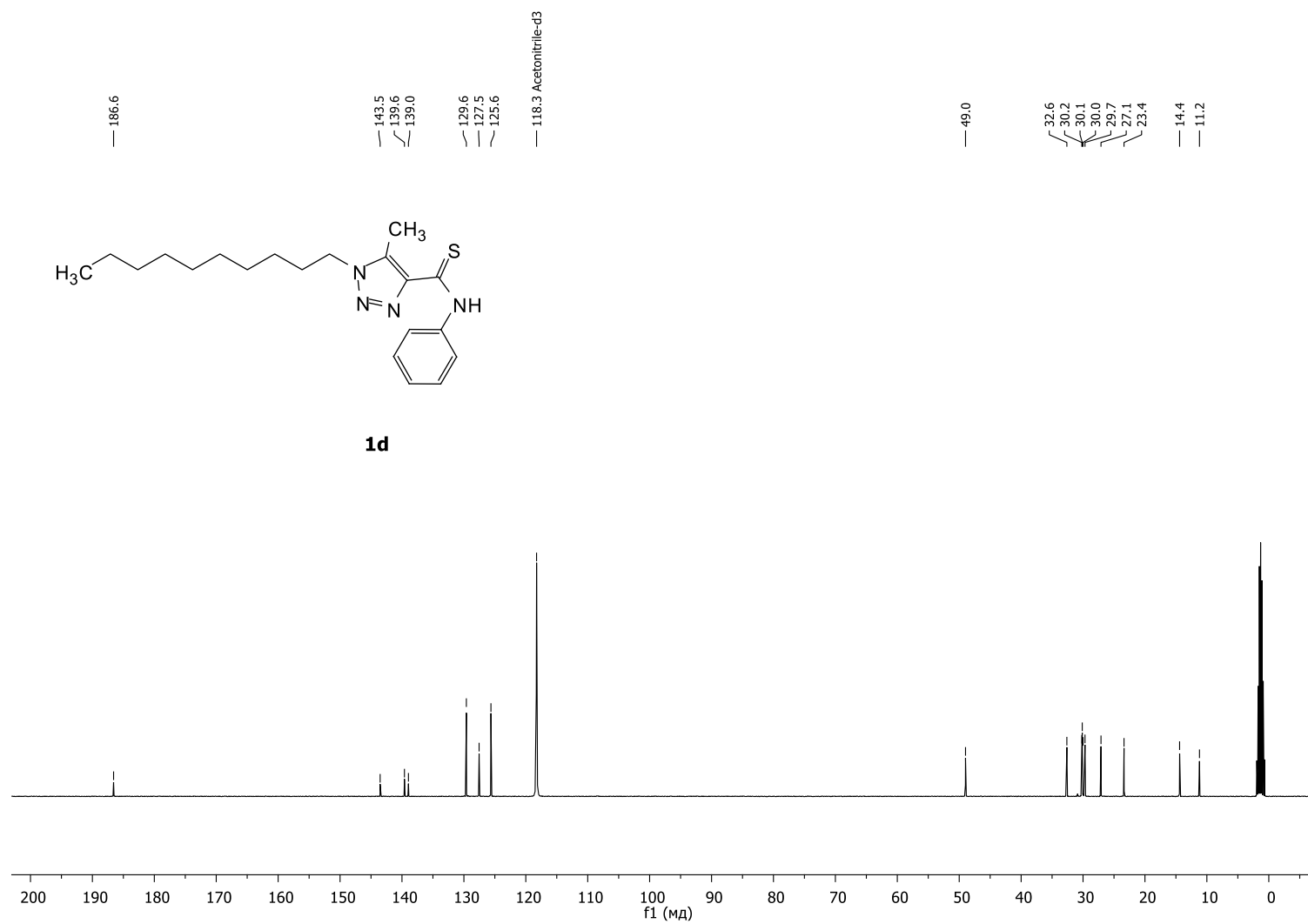
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **1c**.



The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **1c**.

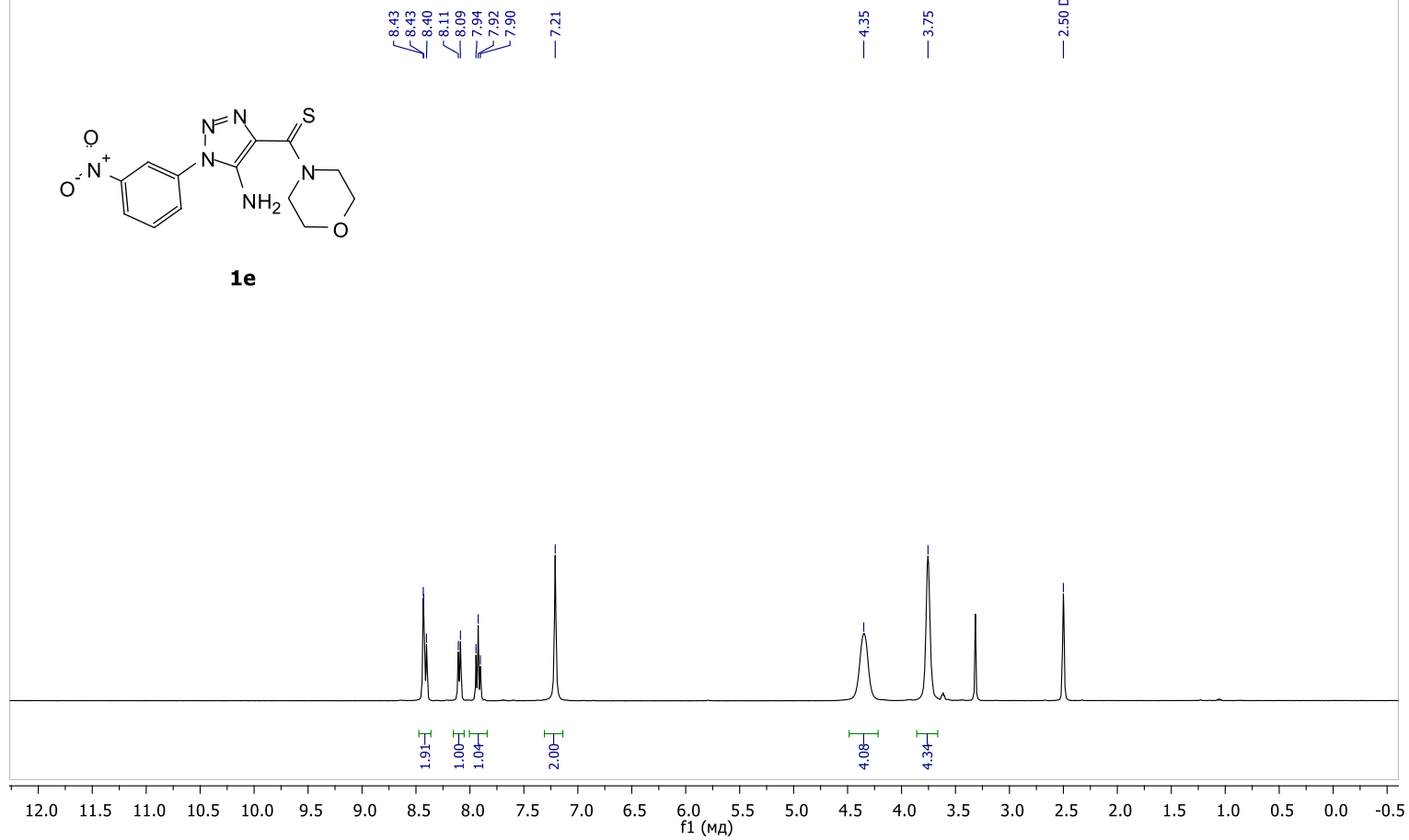


The ¹H NMR (400 MHz, CD₃CN) spectrum of compound **1d**. 7



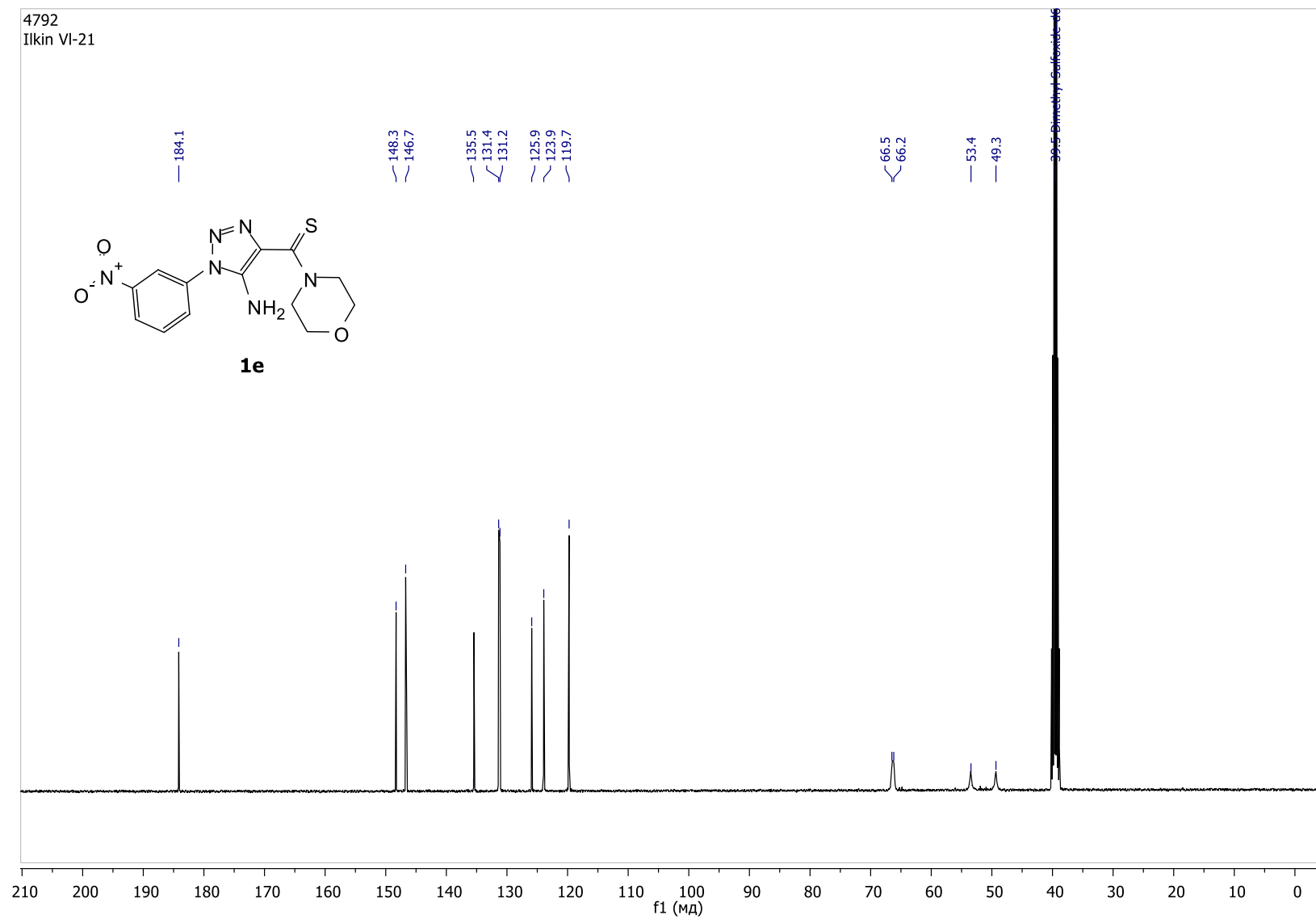
The ^{13}C NMR (100 MHz, CD_3CN) spectrum of compound **1d**.

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Ilkin VI-21

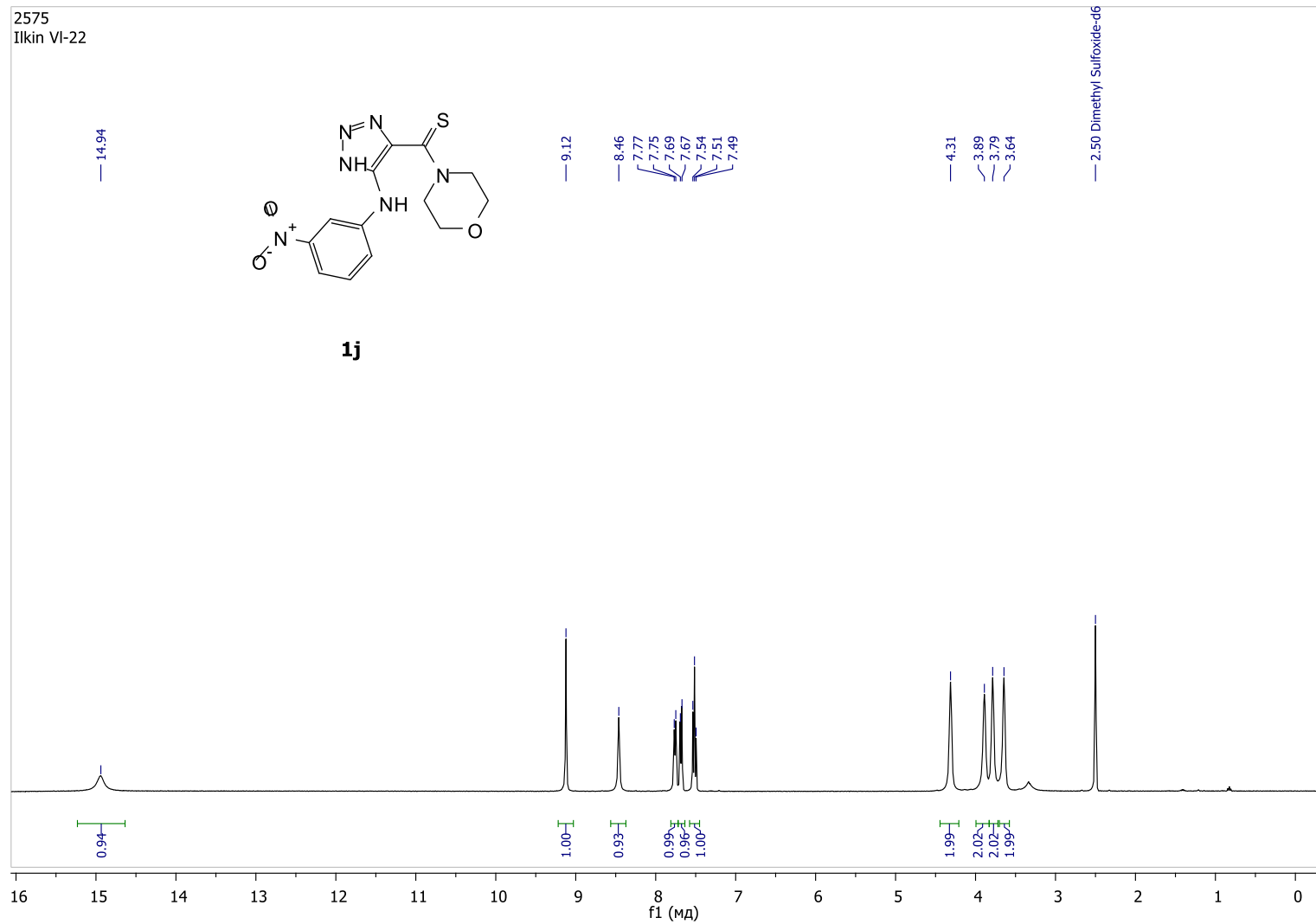


The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **1e**.

4792
Ilkin VI-21

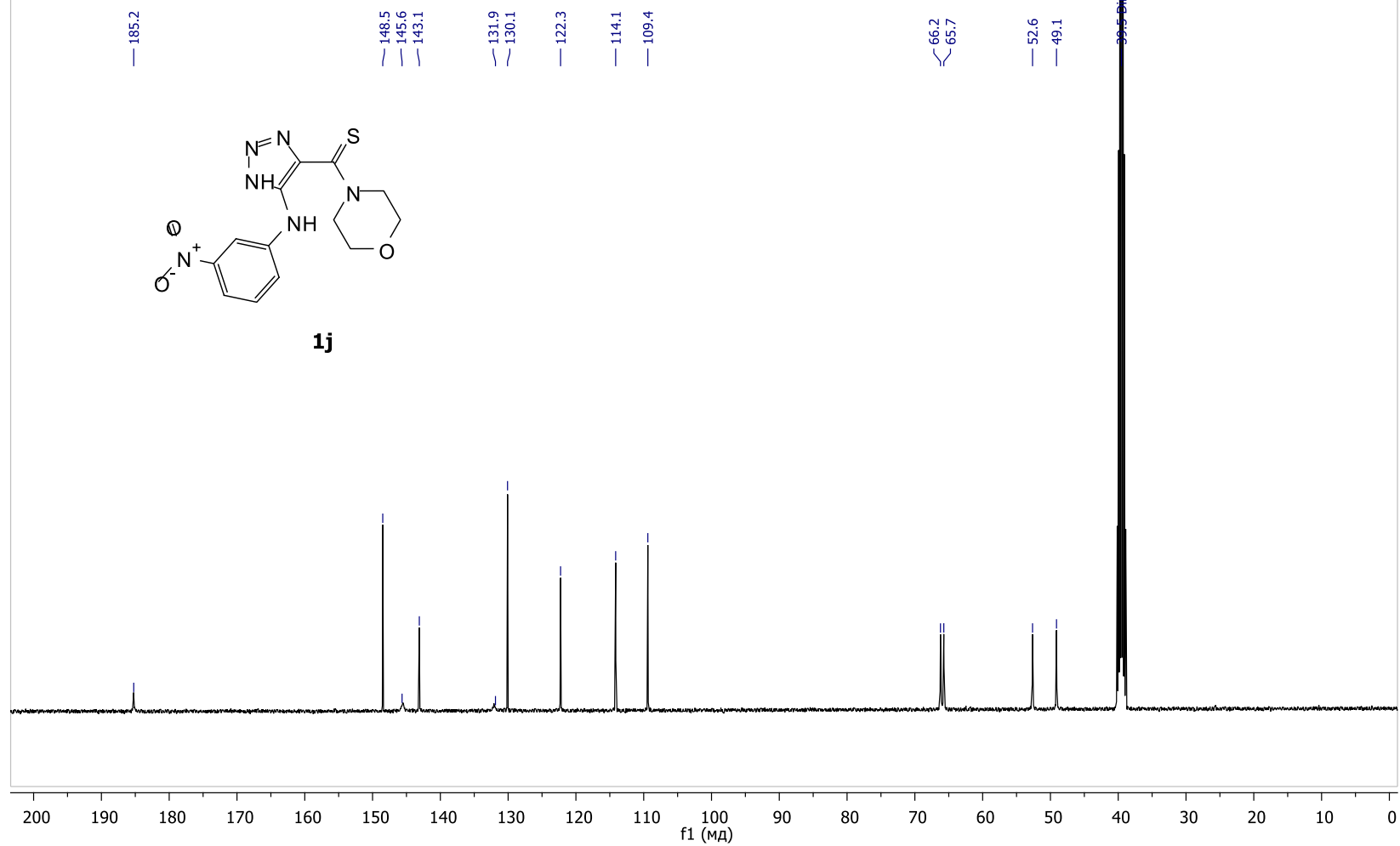


The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **1e**.

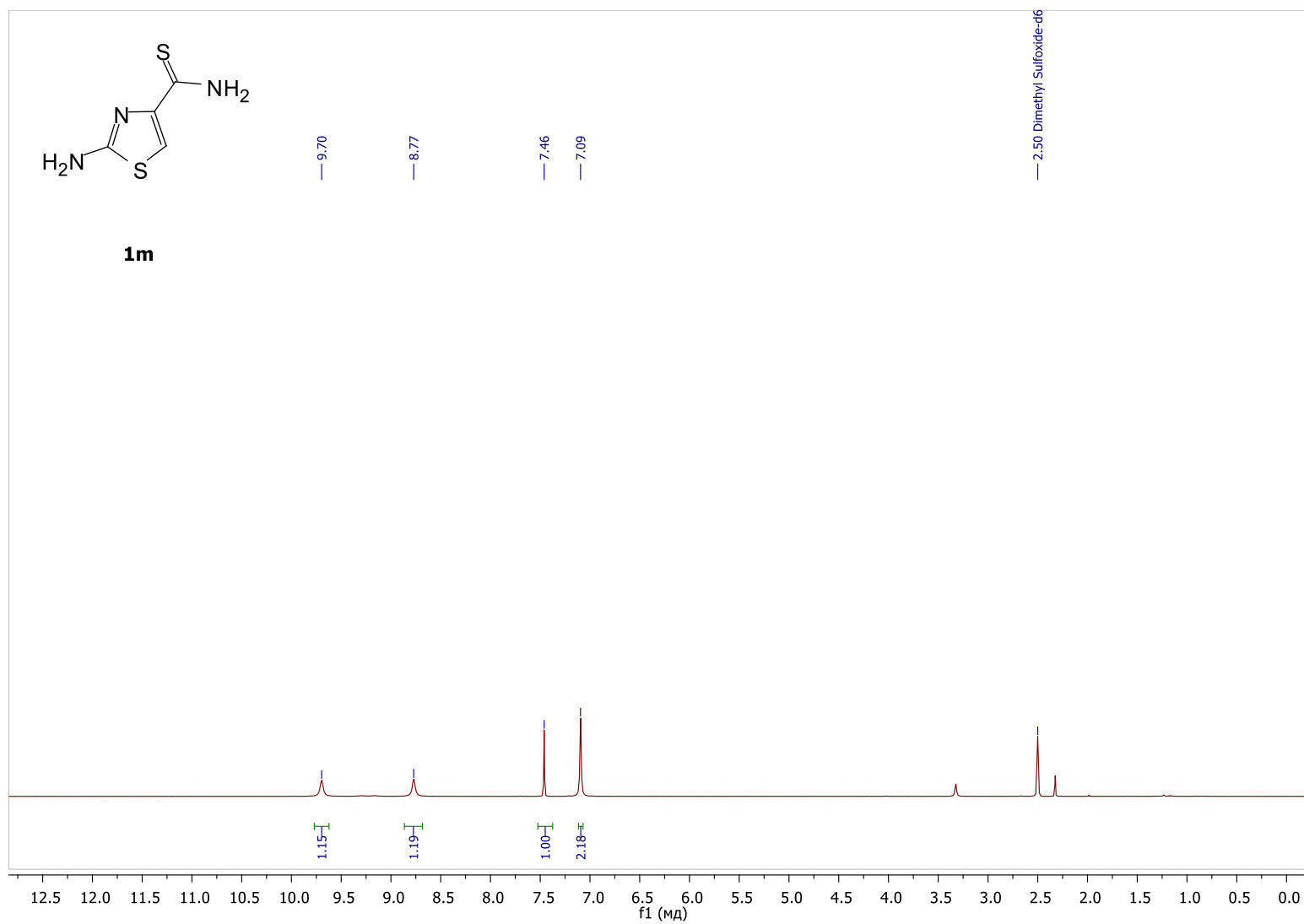


The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **1j**.

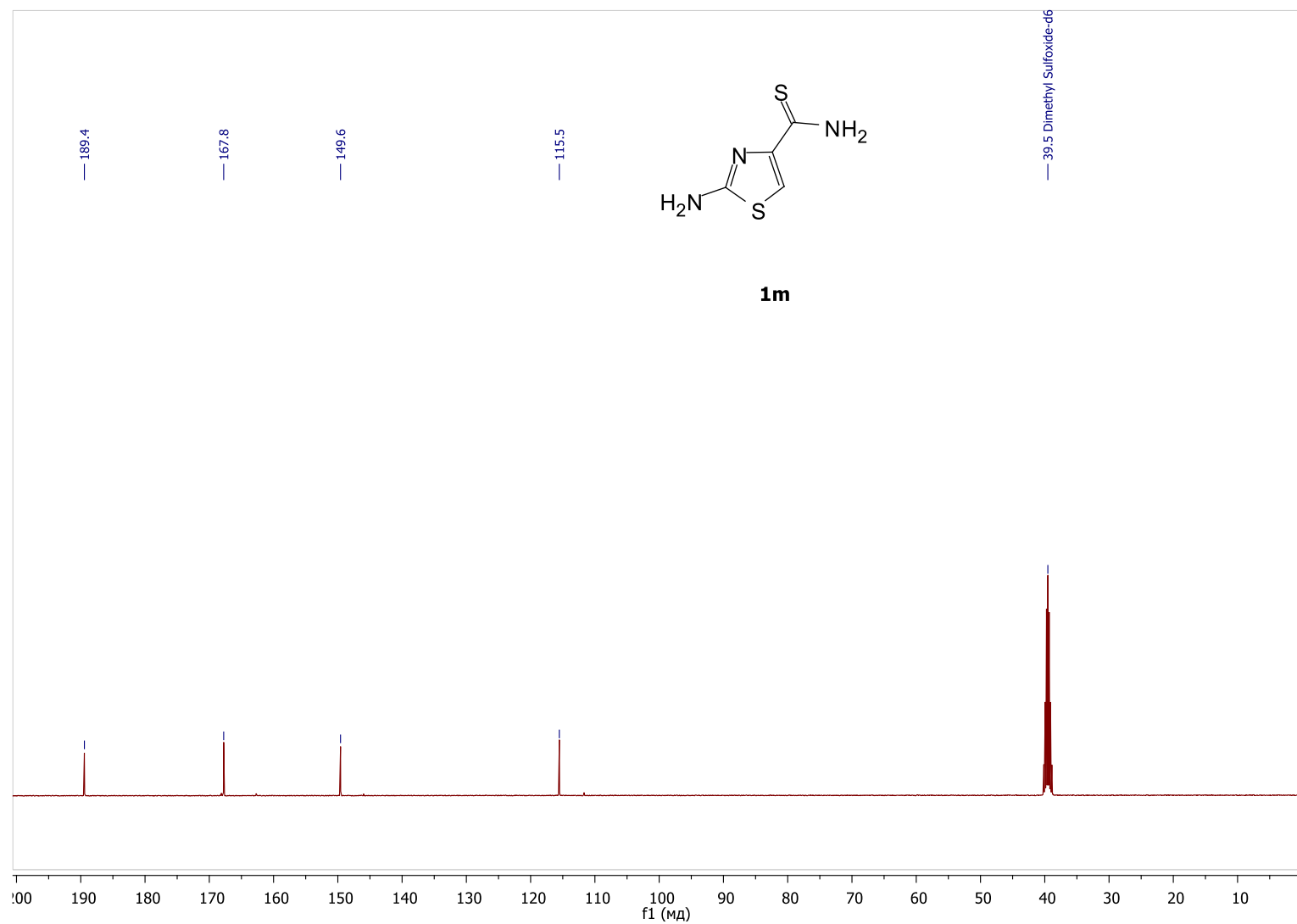
4788
Ilkin VI-22



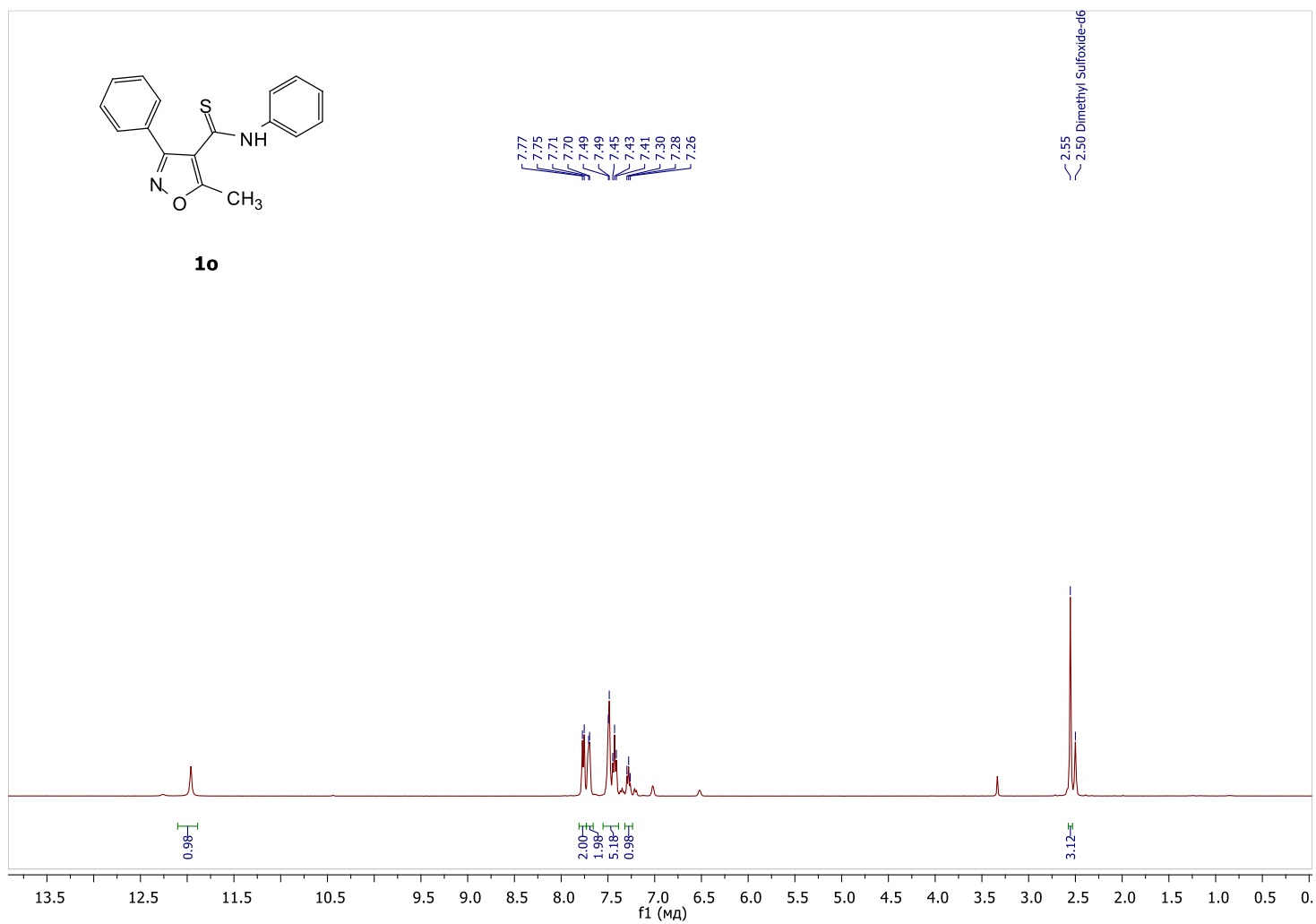
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **1j**.



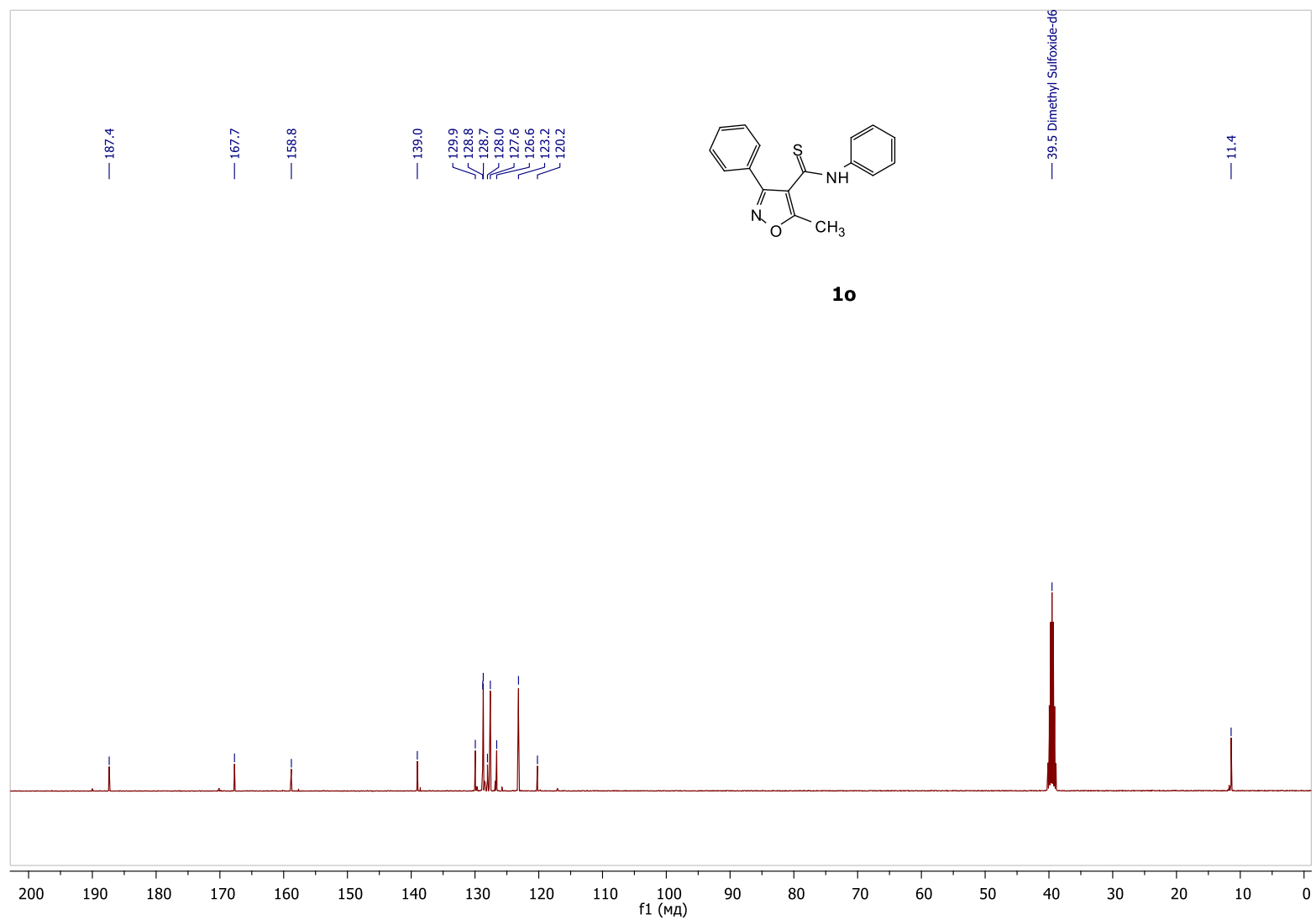
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **1m**.



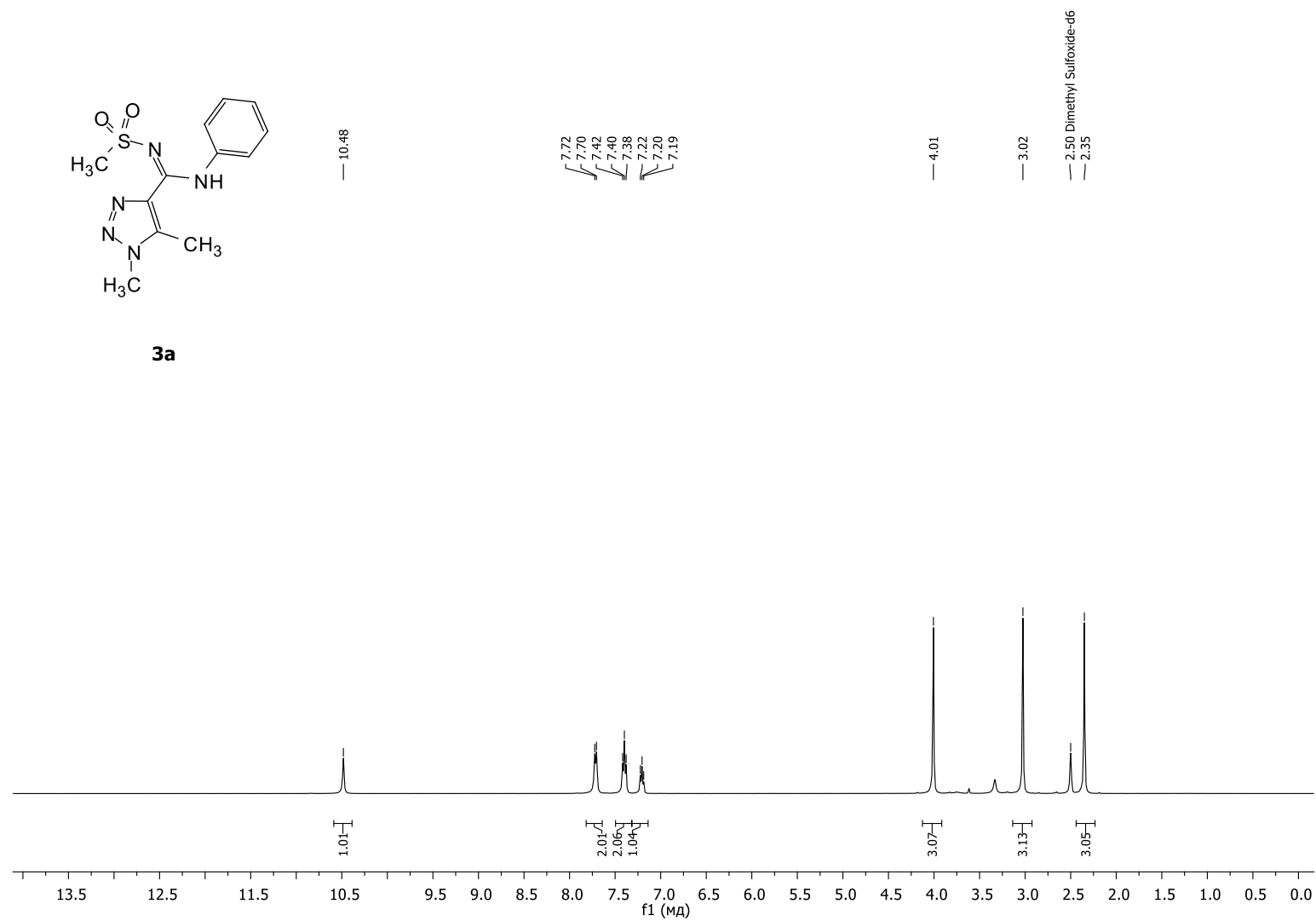
The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of compound **1m**.



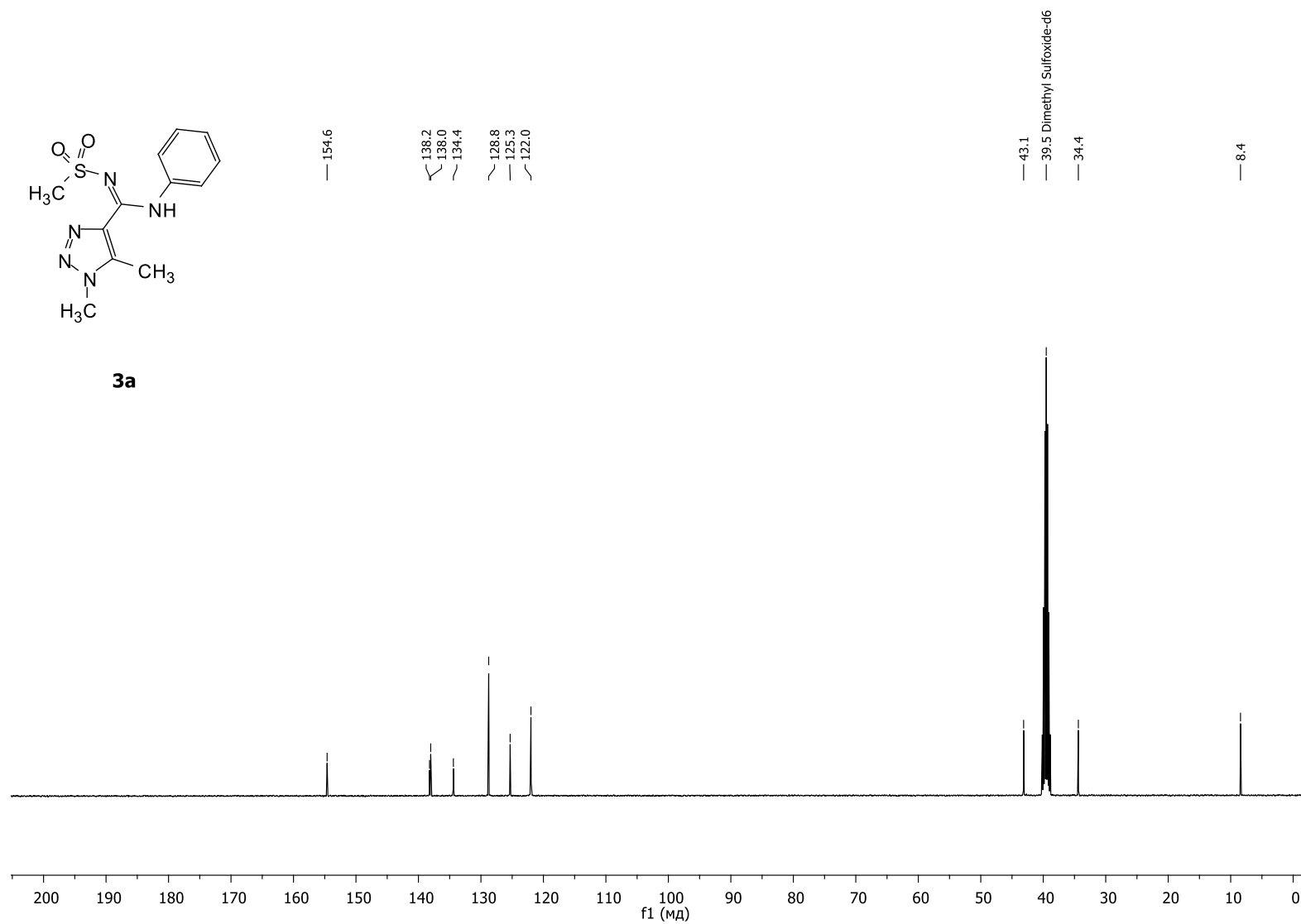
The ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **1o**.



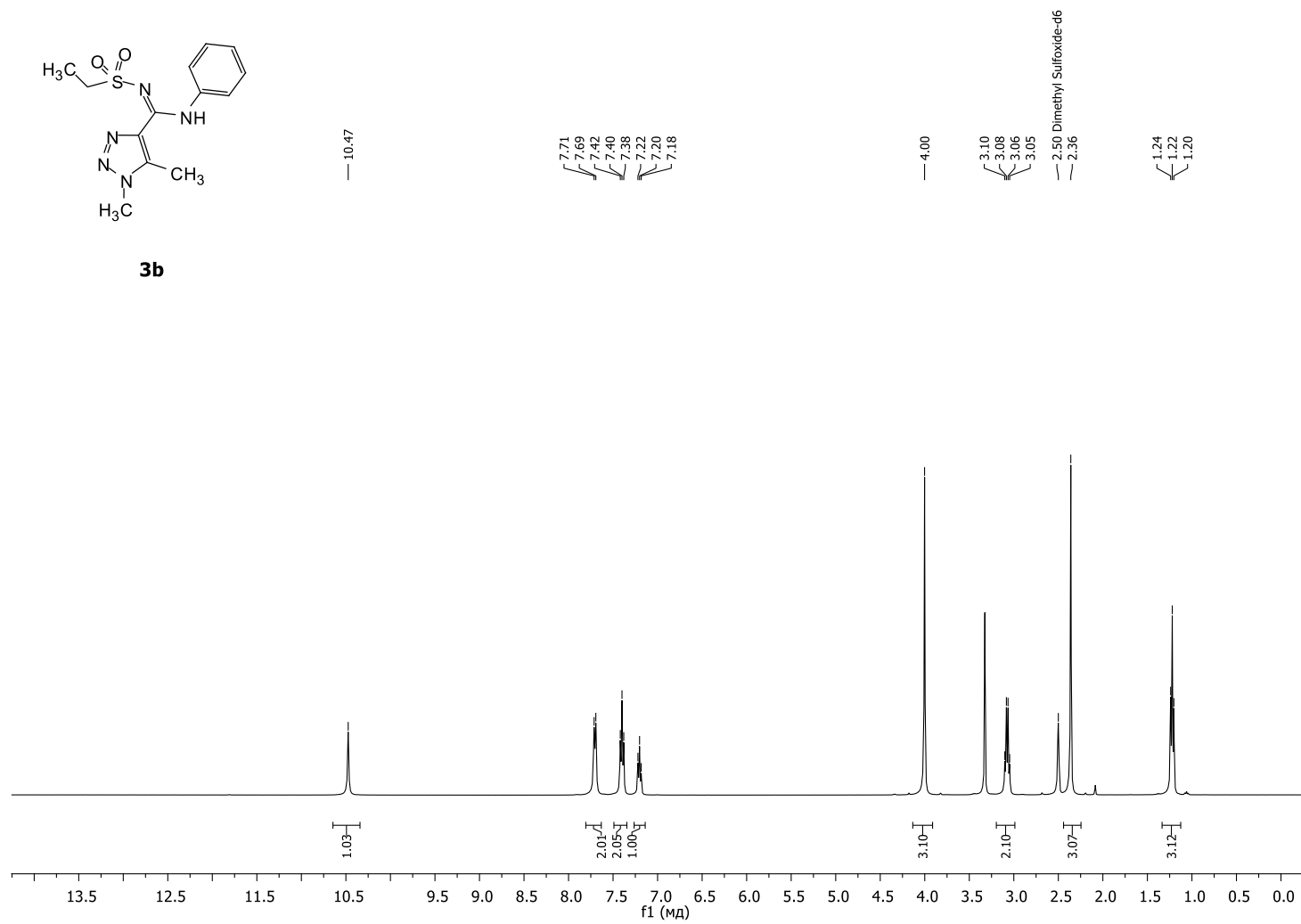
The ¹³C NMR (100 MHz, DMSO-d₆) spectrum of compound **1o** .



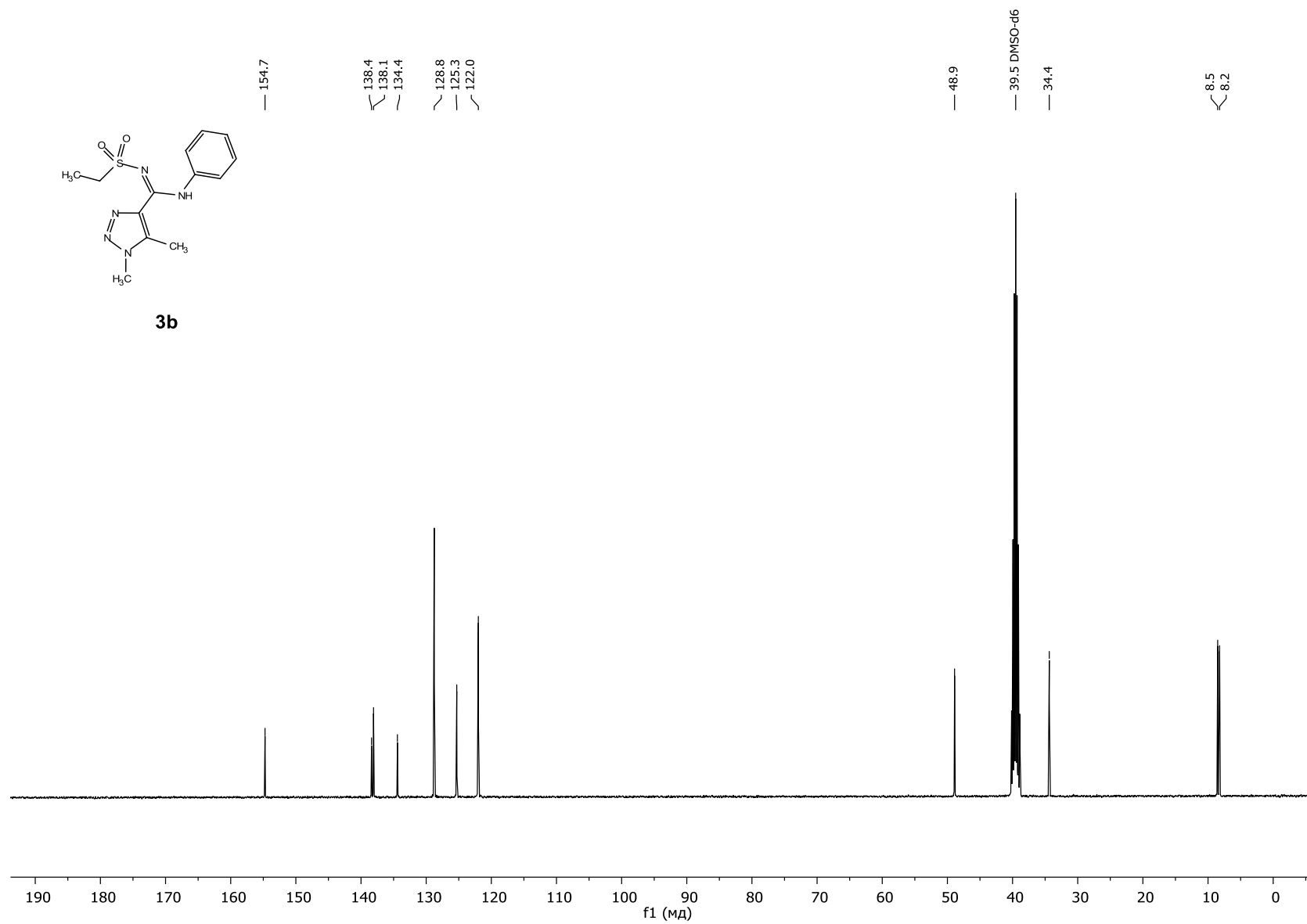
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3a**.



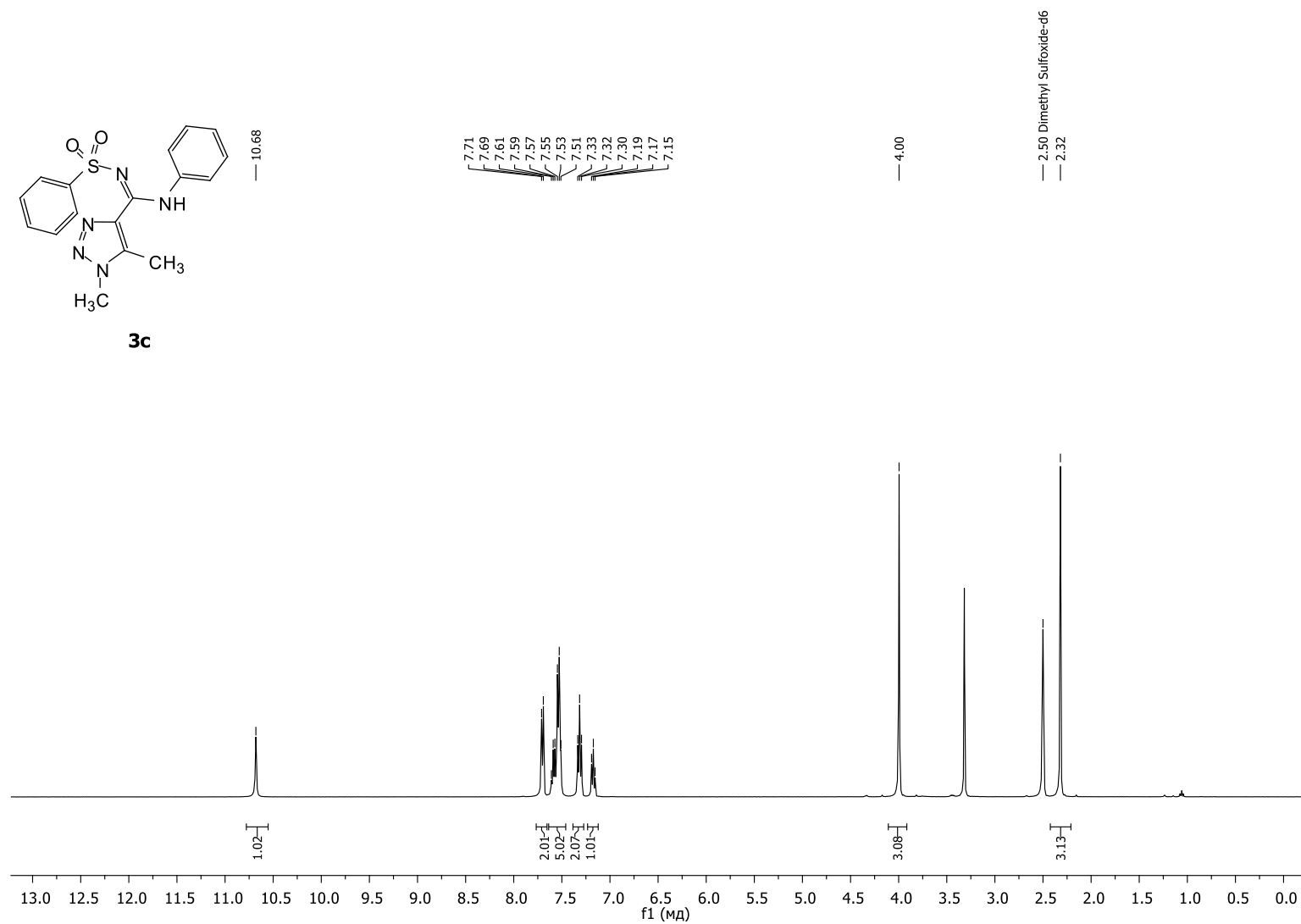
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3a**.



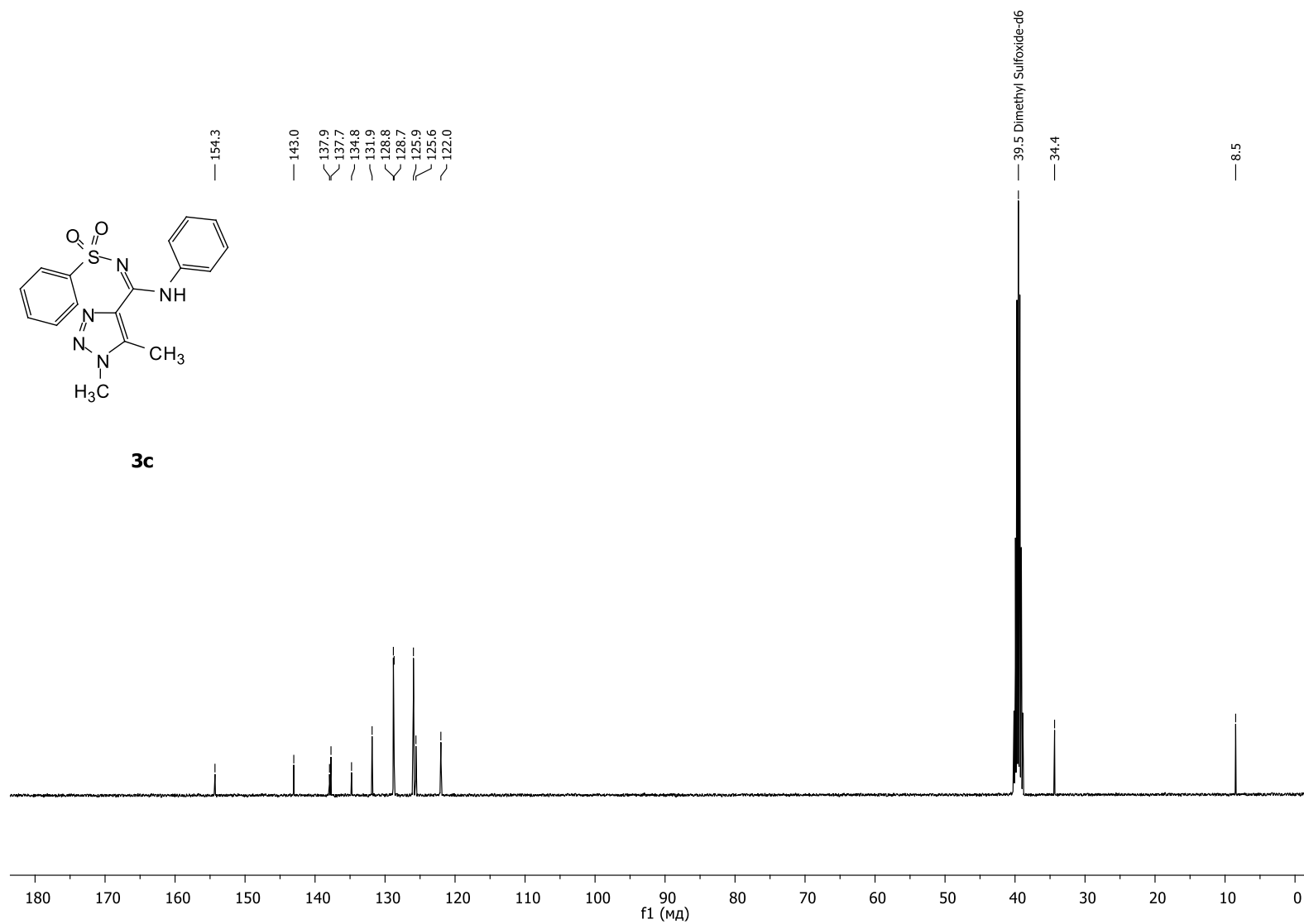
The ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **3b**.



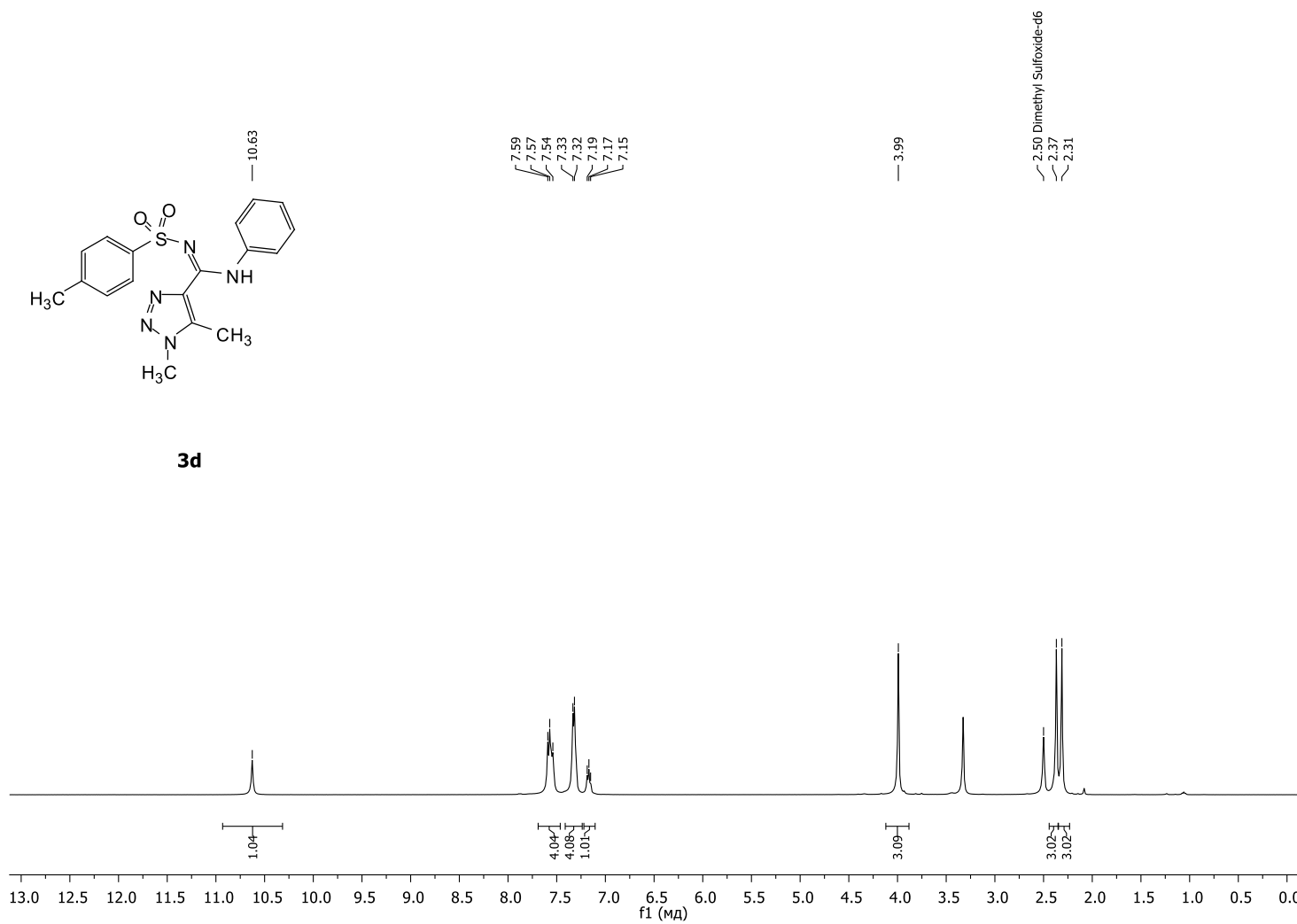
The ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of compound **3b**.



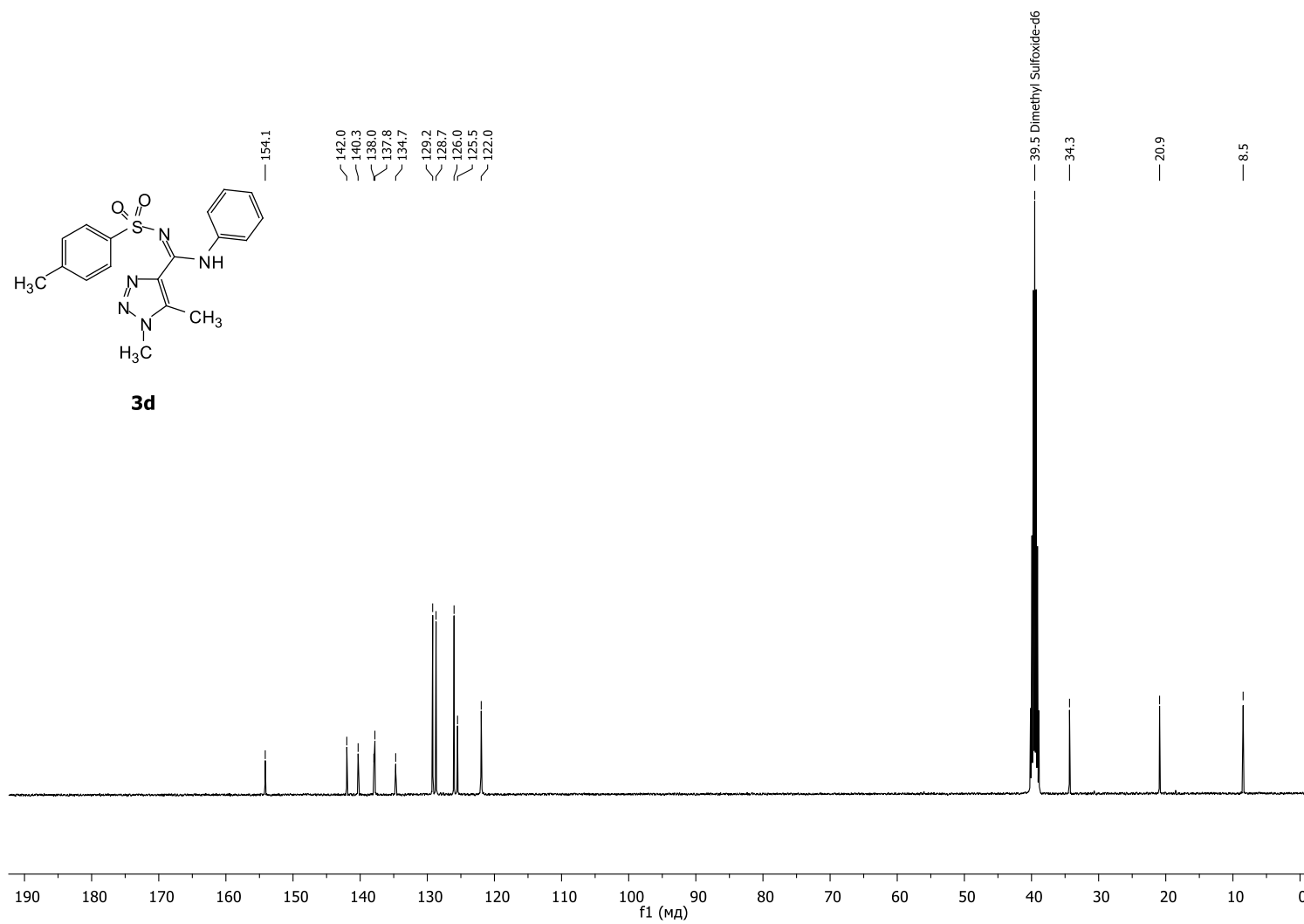
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3c**.



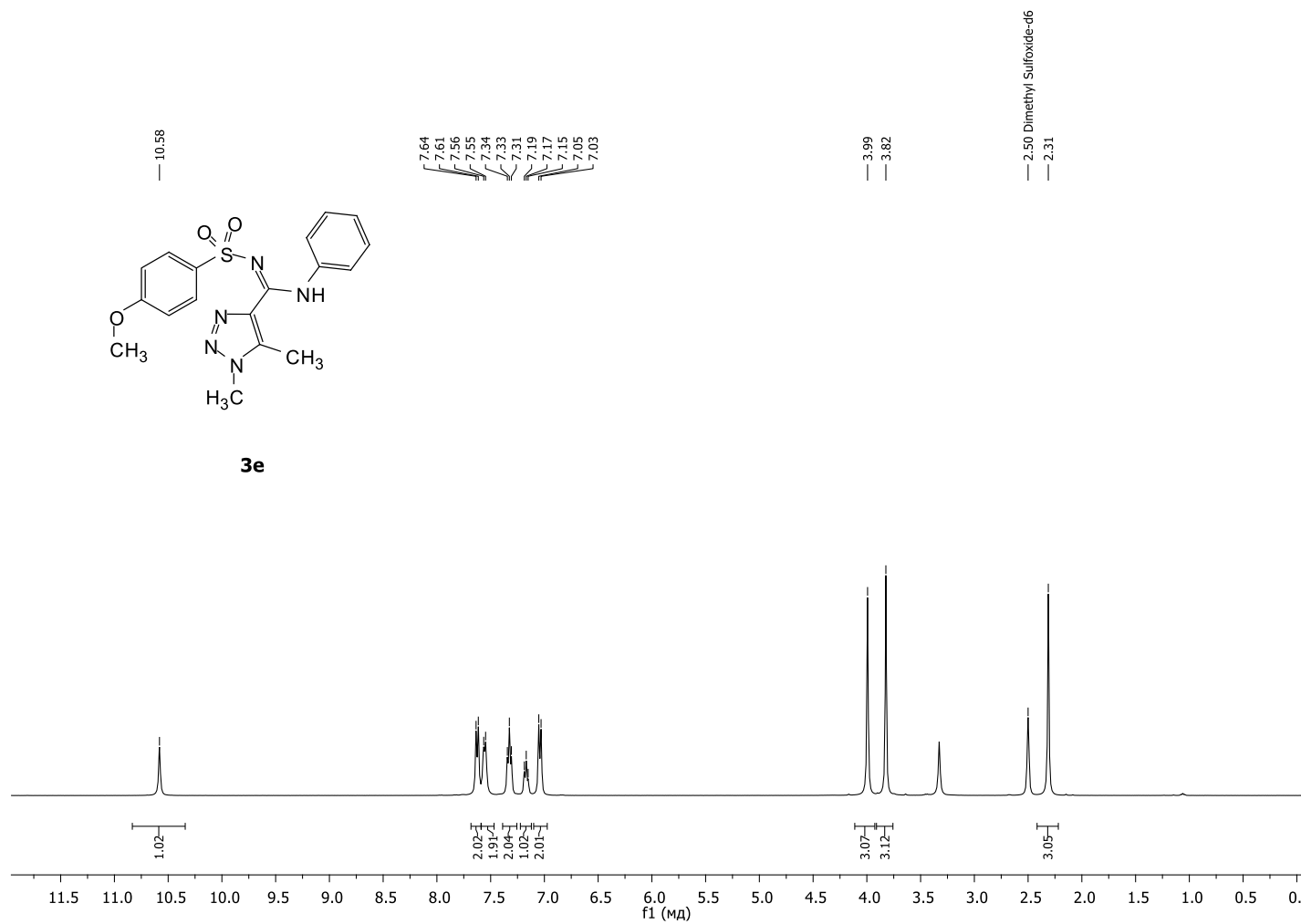
The ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of compound **3c**.



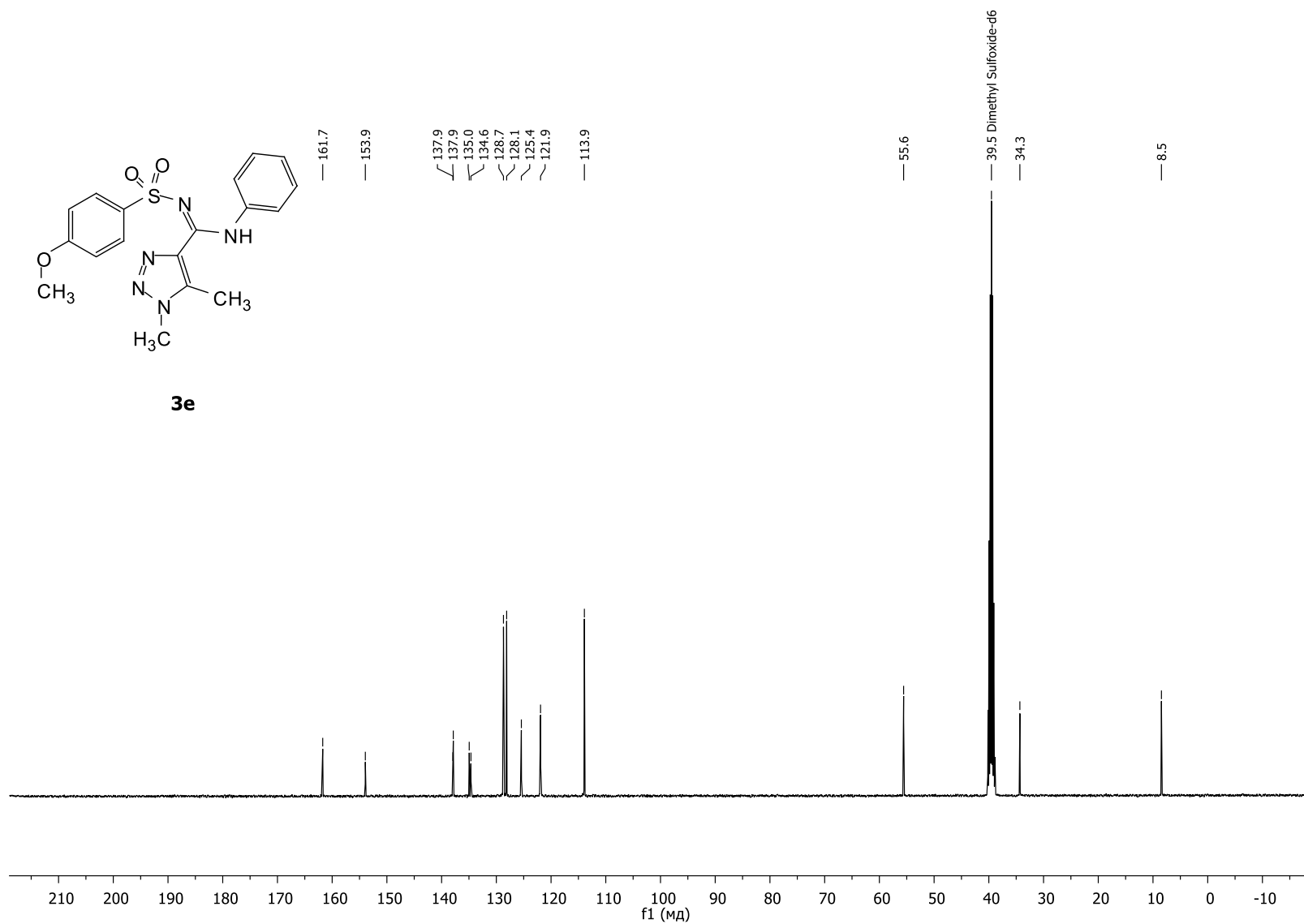
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3d**.



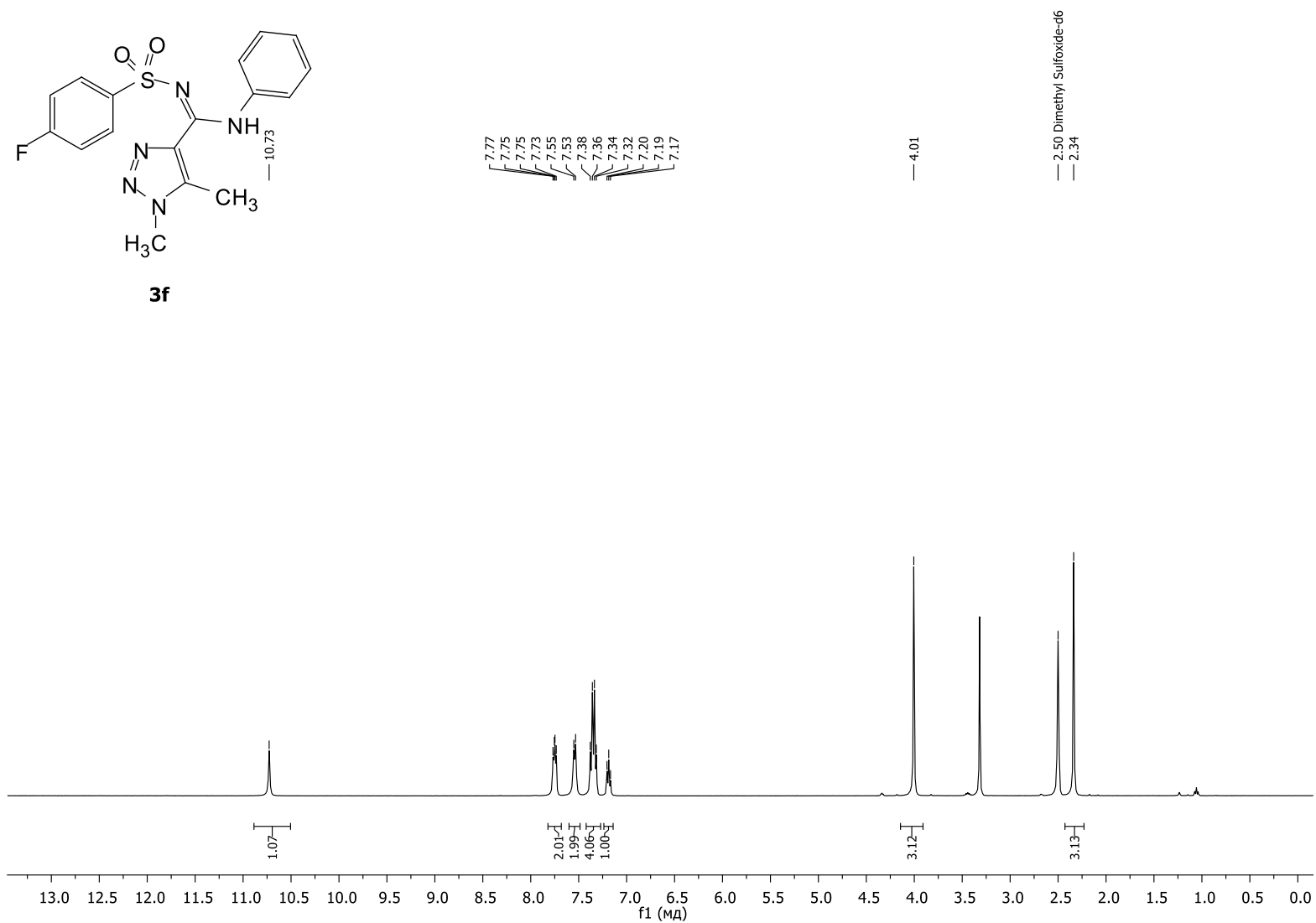
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3d**.



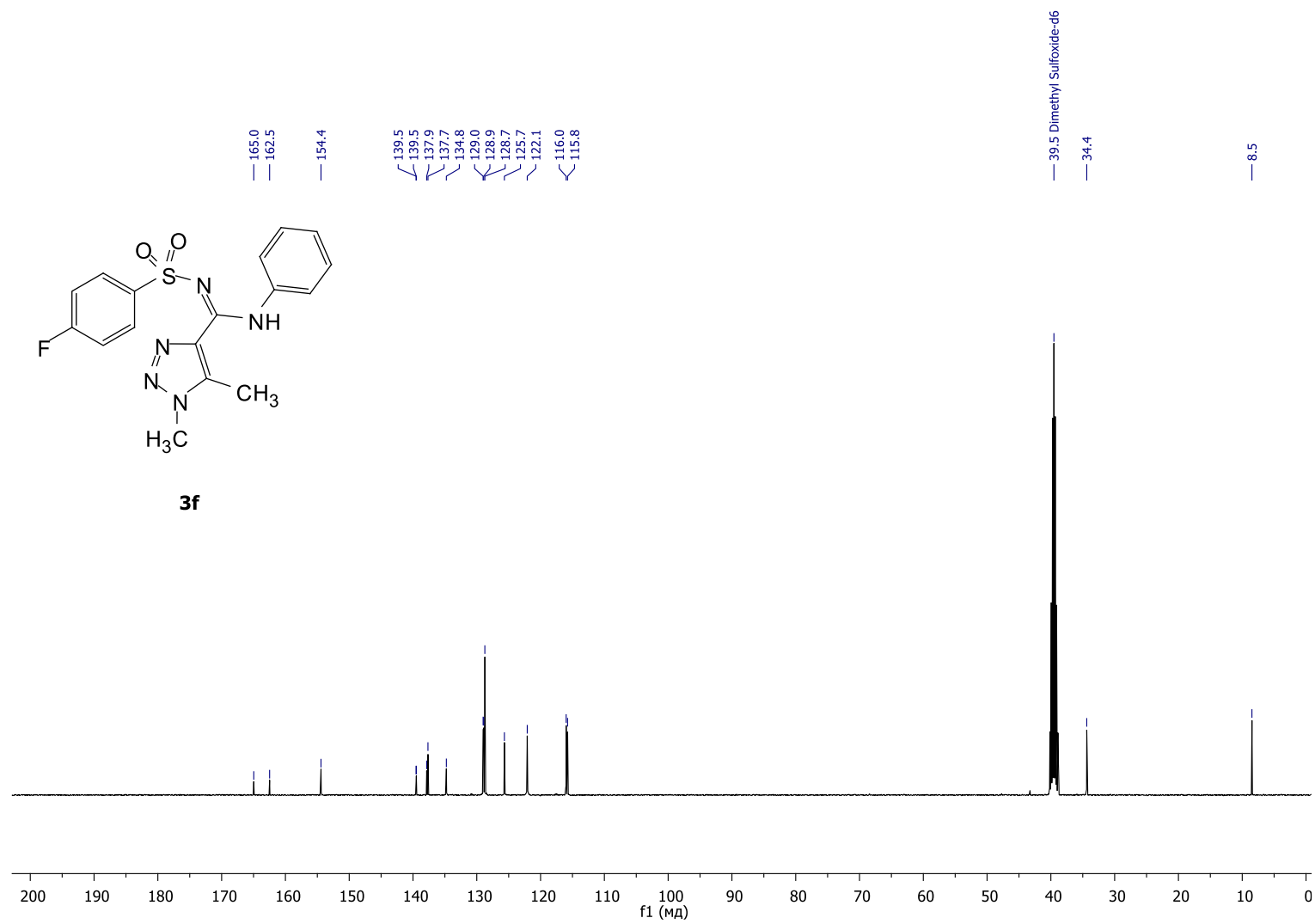
The ¹H NMR (400 MHz, DMSO-d₆) spectrum of compound **3e**.



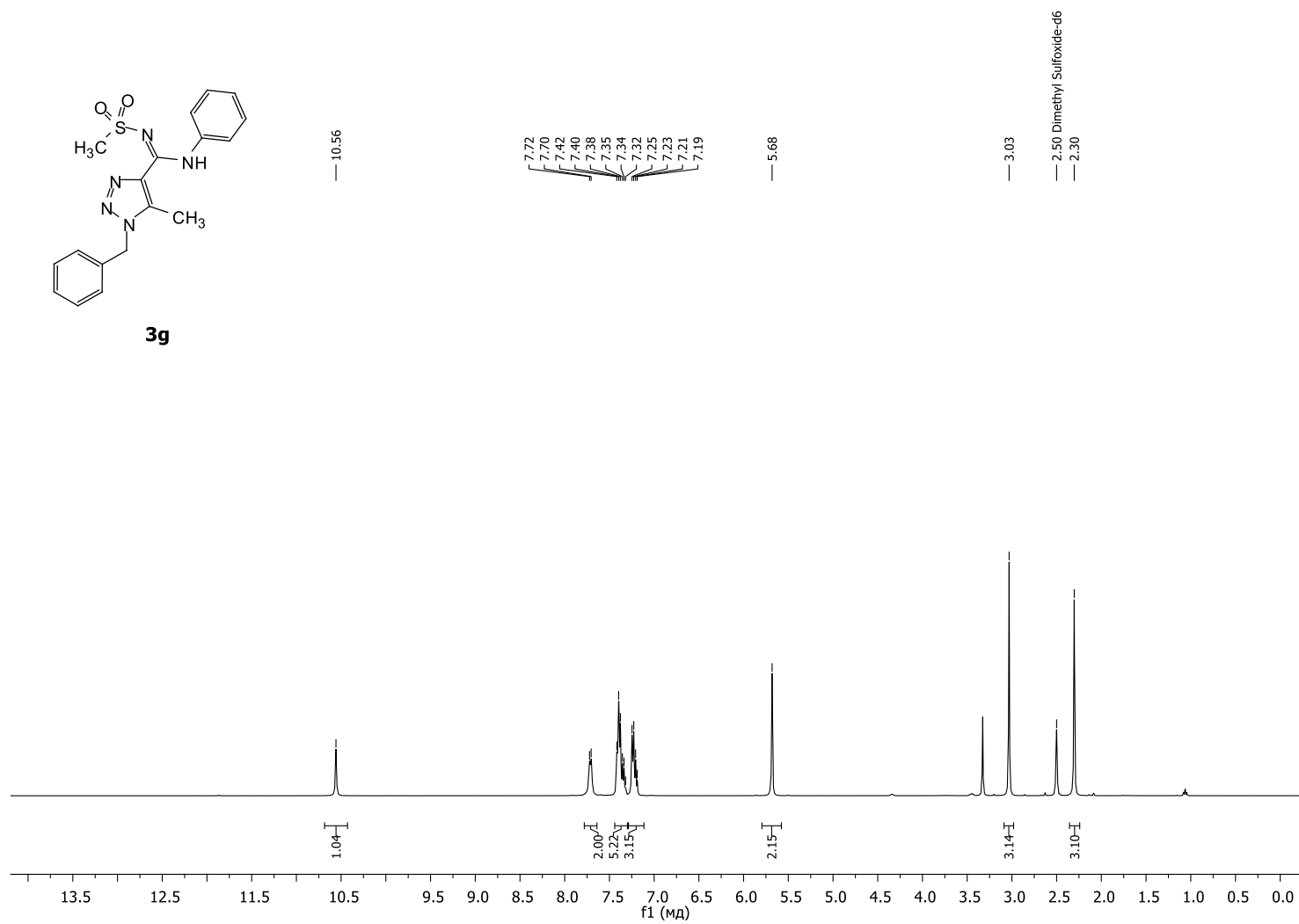
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3e**.



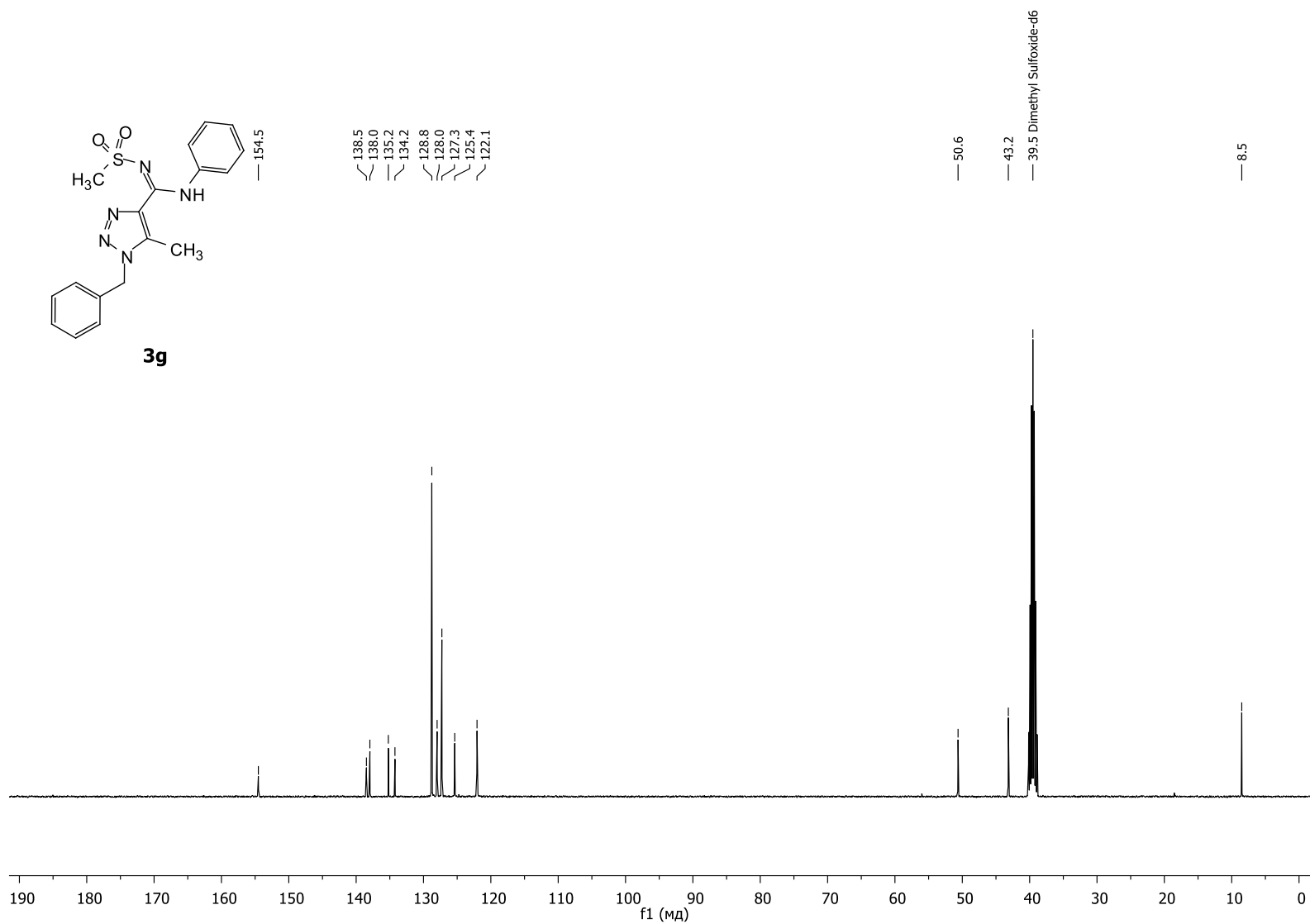
The ^1H NMR (400 MHz, DMSO- d_6) spectrum of compound **3f**.



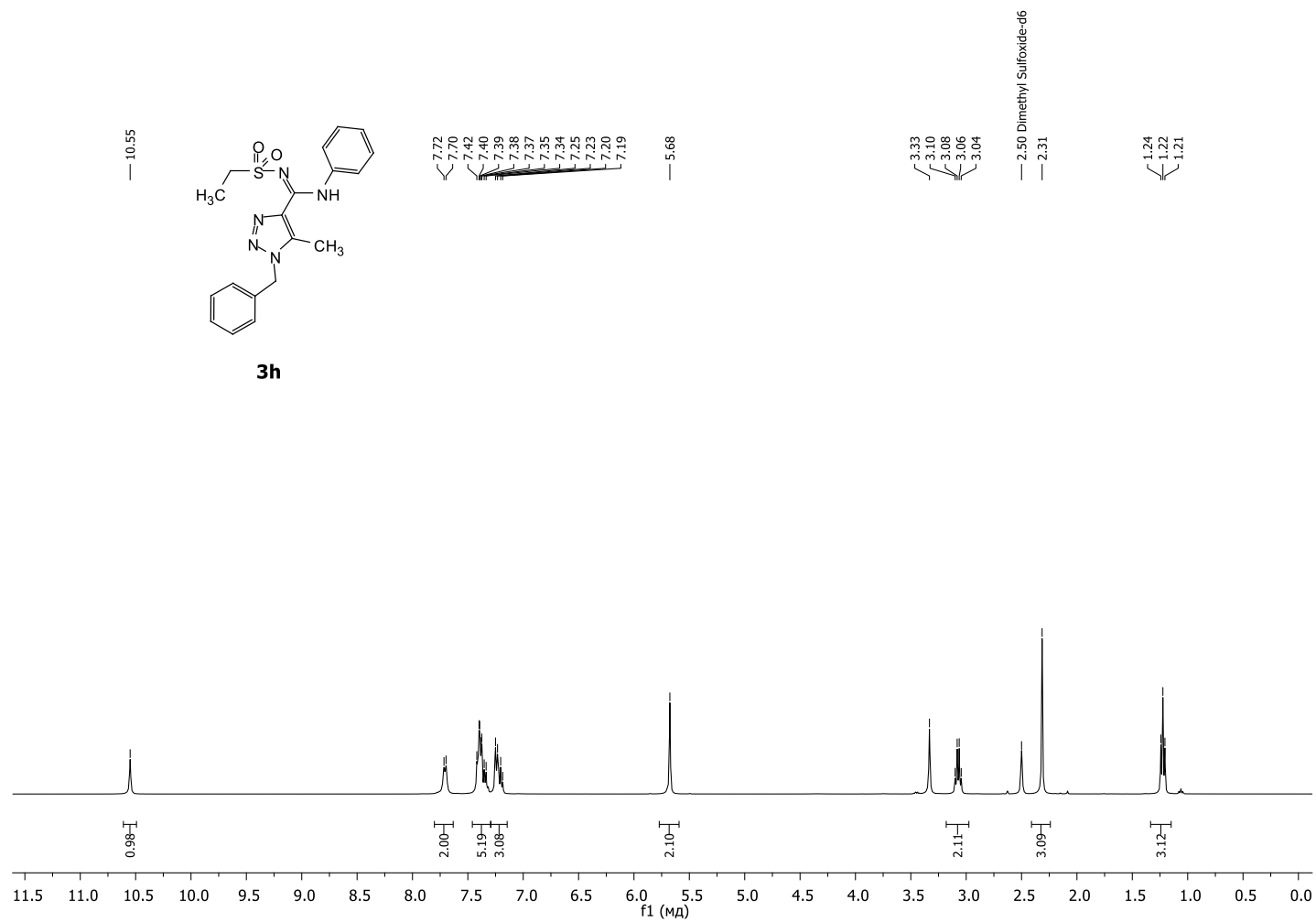
The ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of compound **3f**.



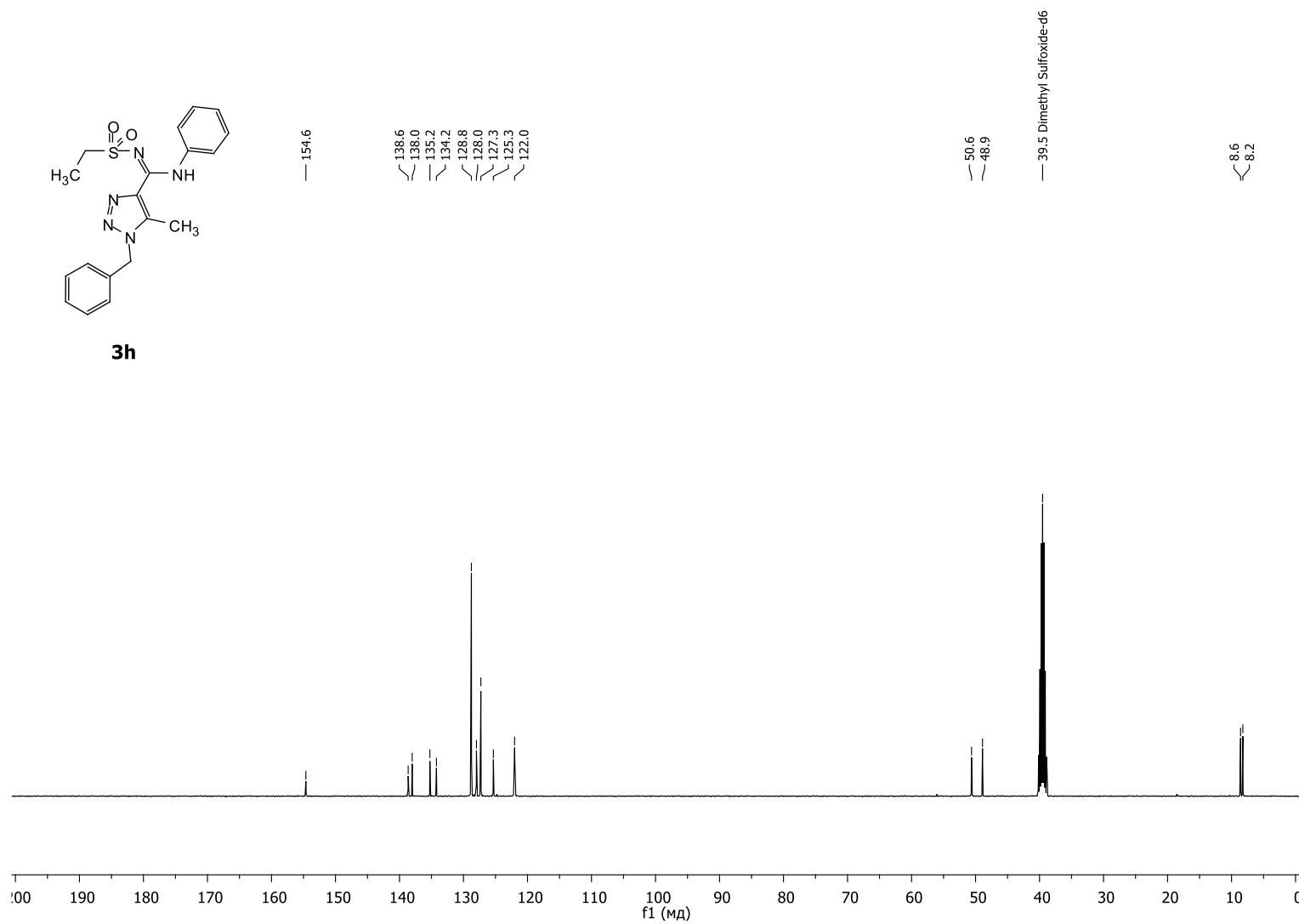
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3g**.



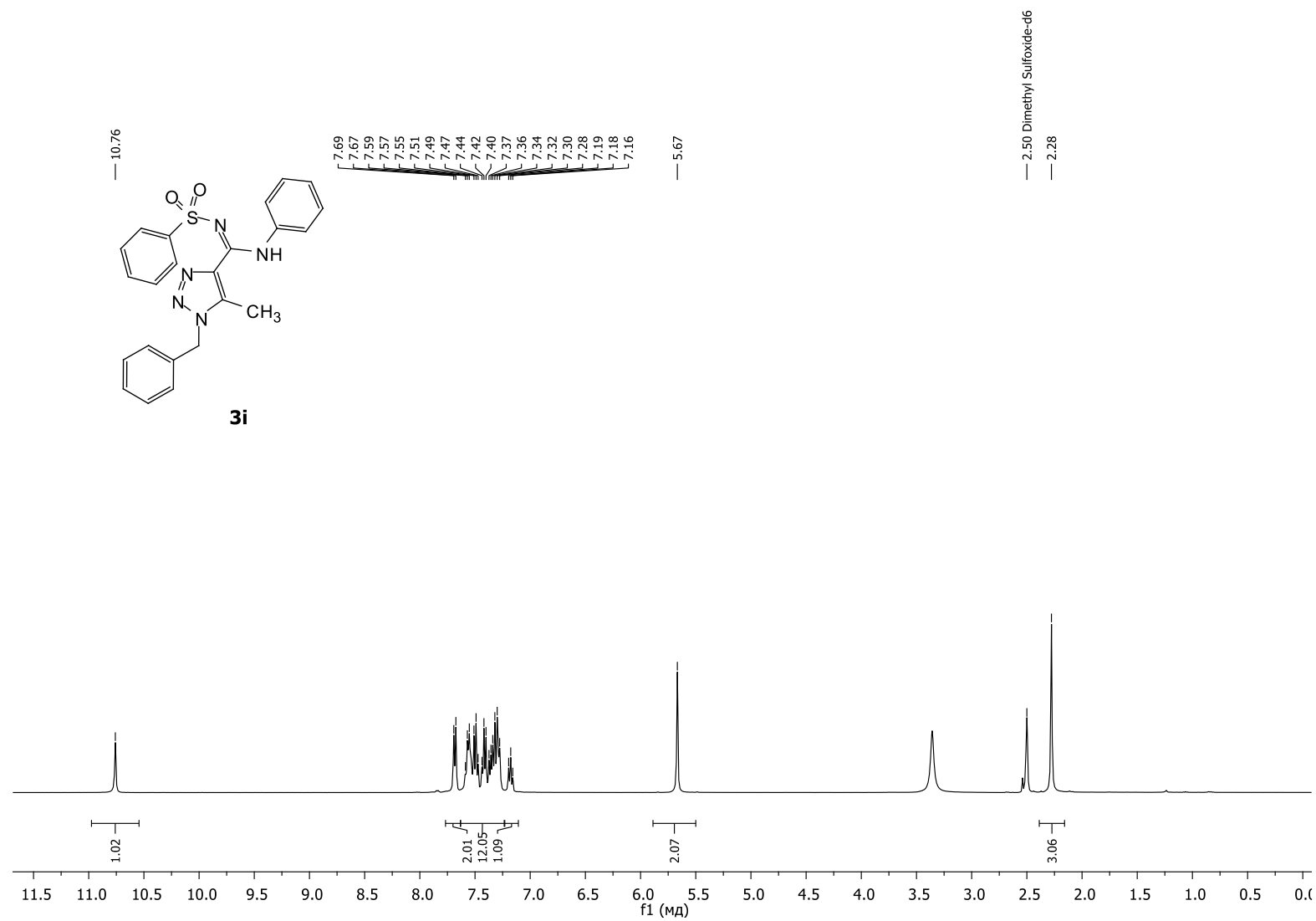
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3g**.



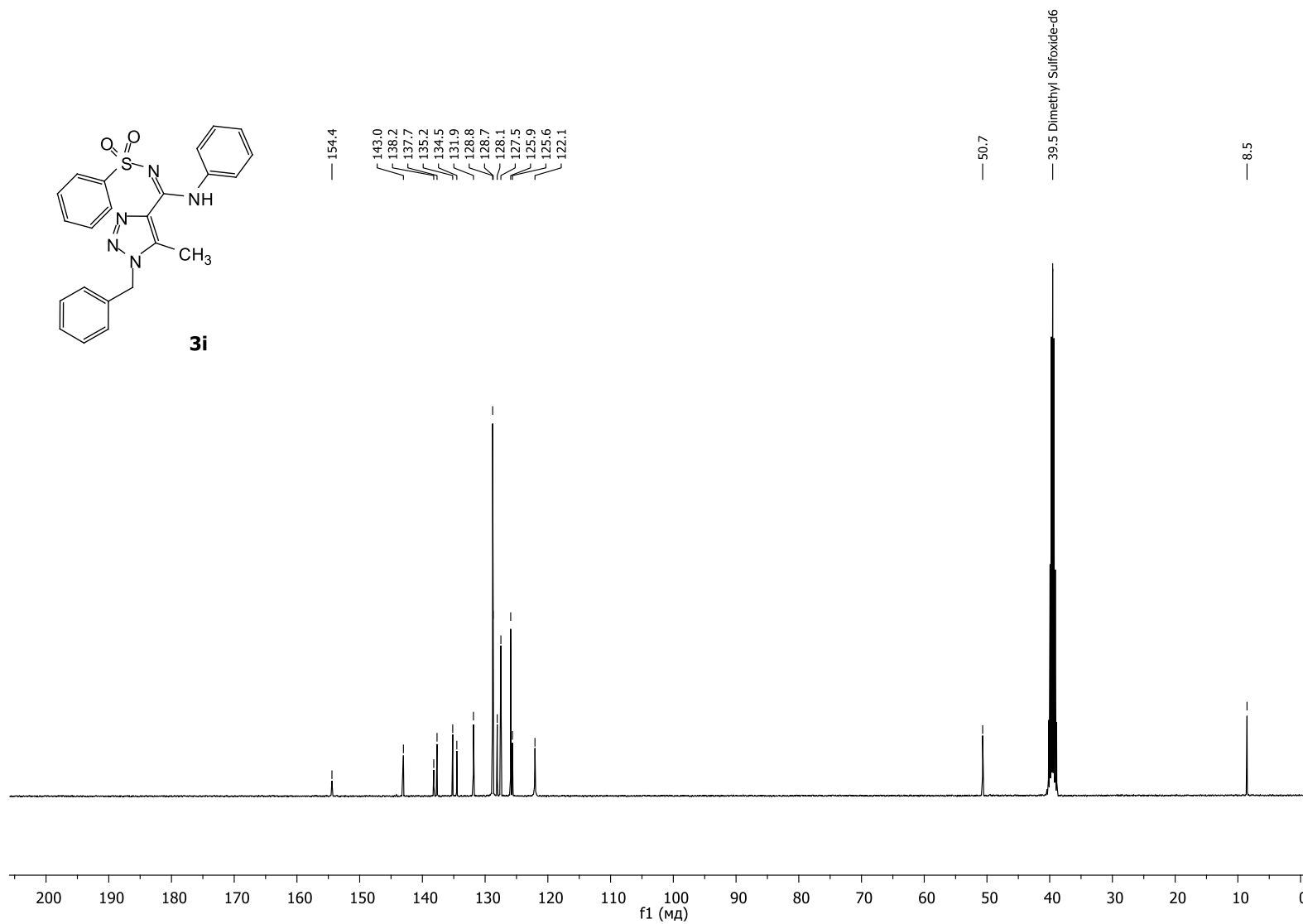
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3h**.



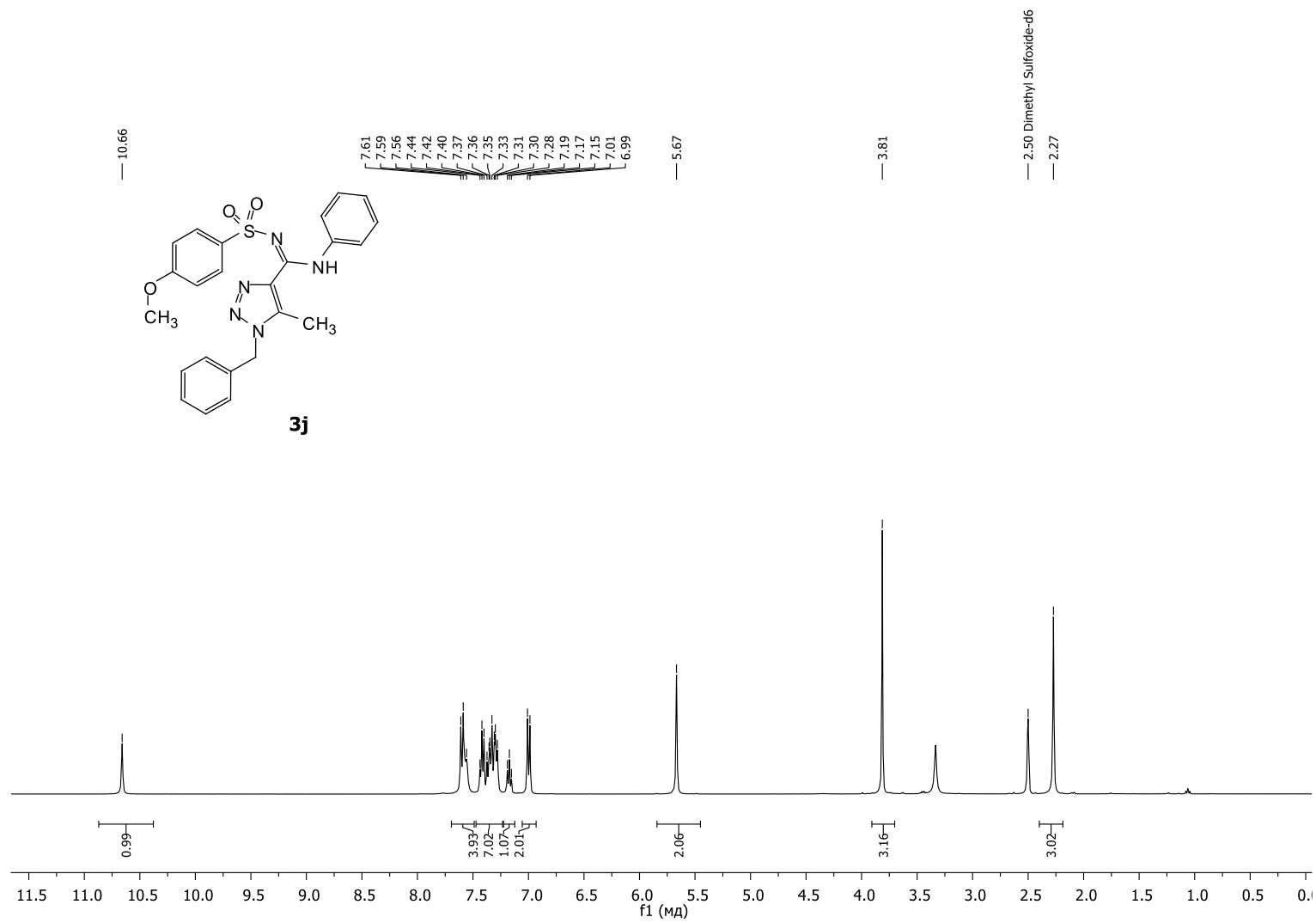
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3h**.



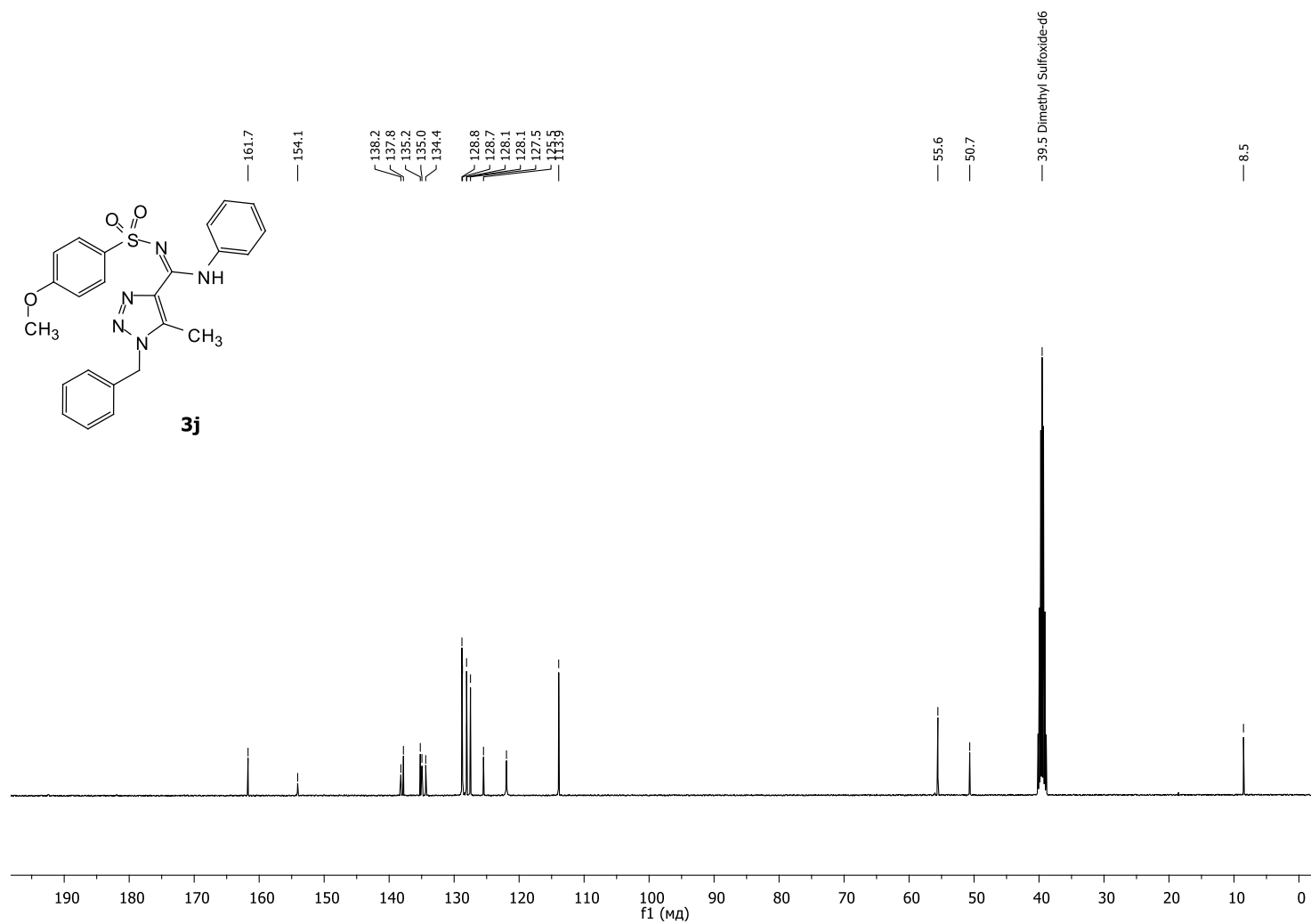
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3i**.



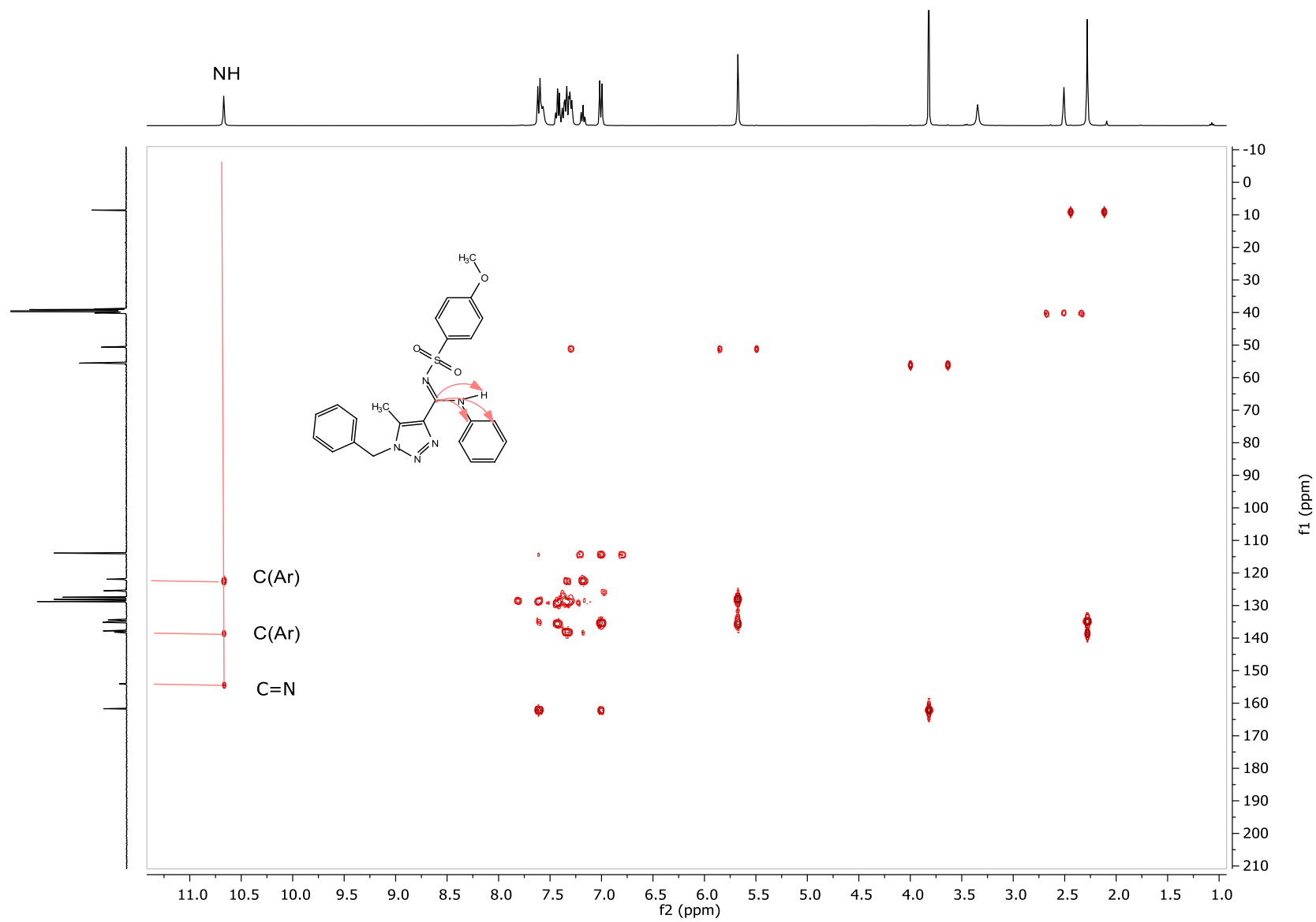
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3i**.



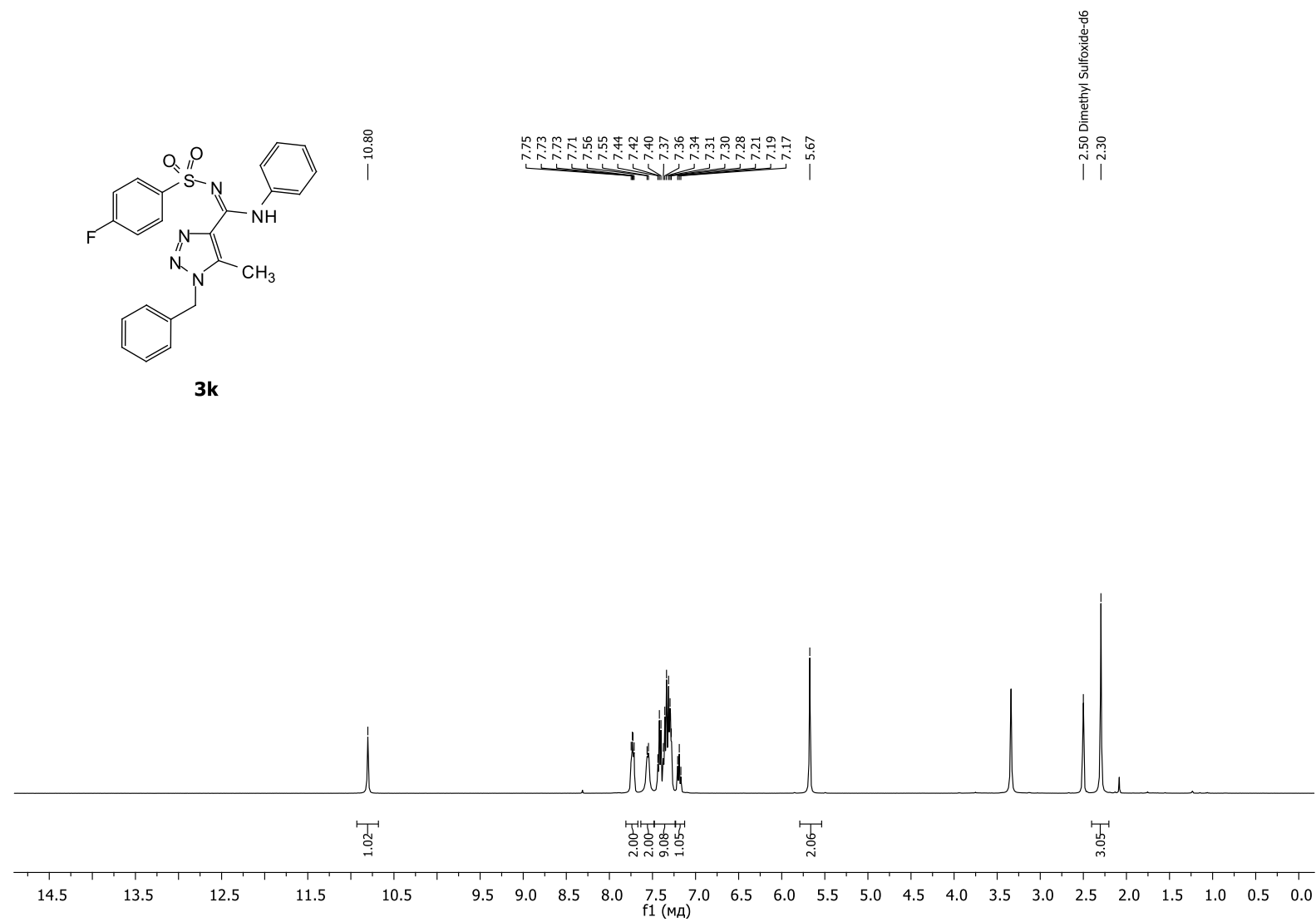
The ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **3j**.



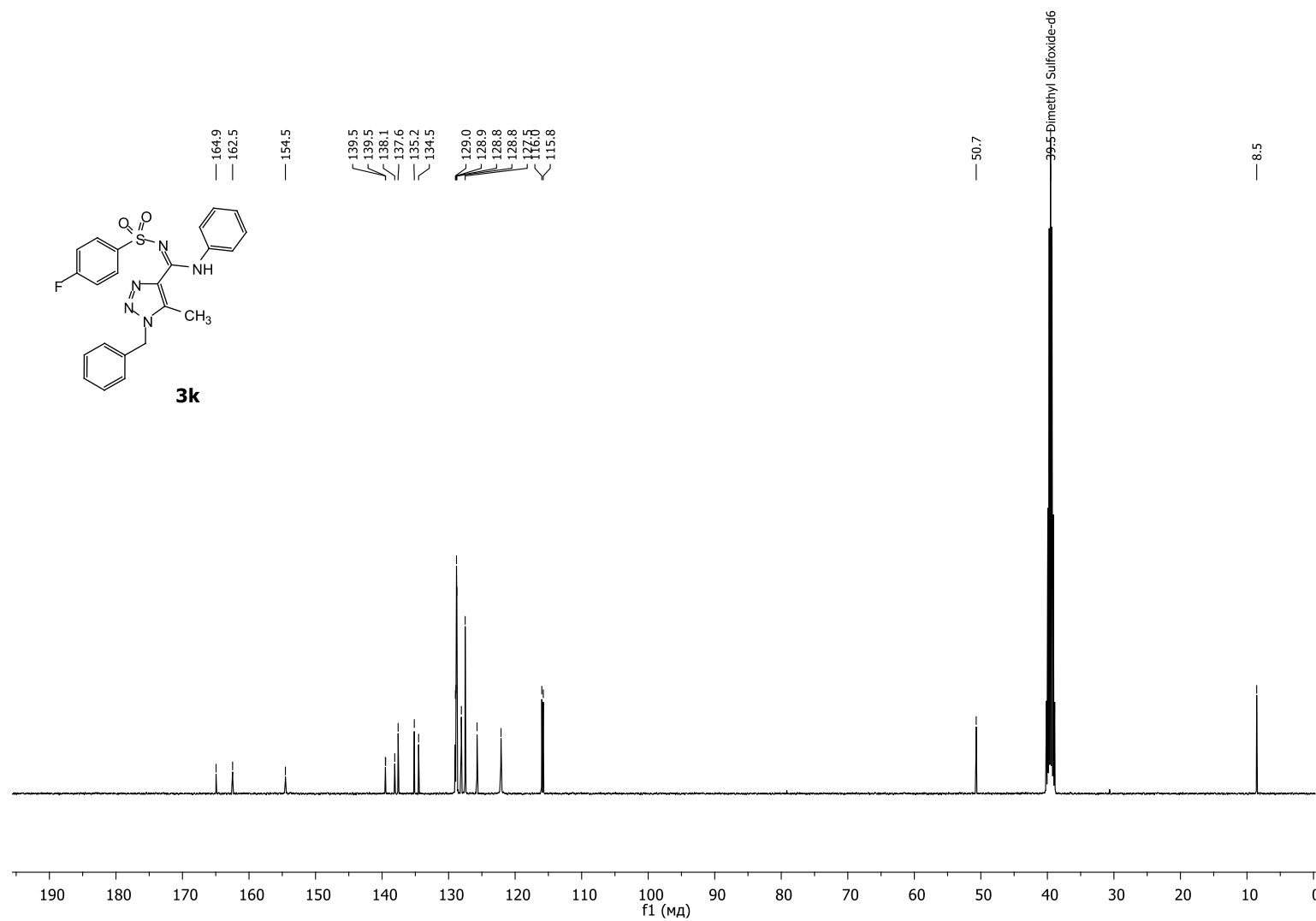
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3j**.



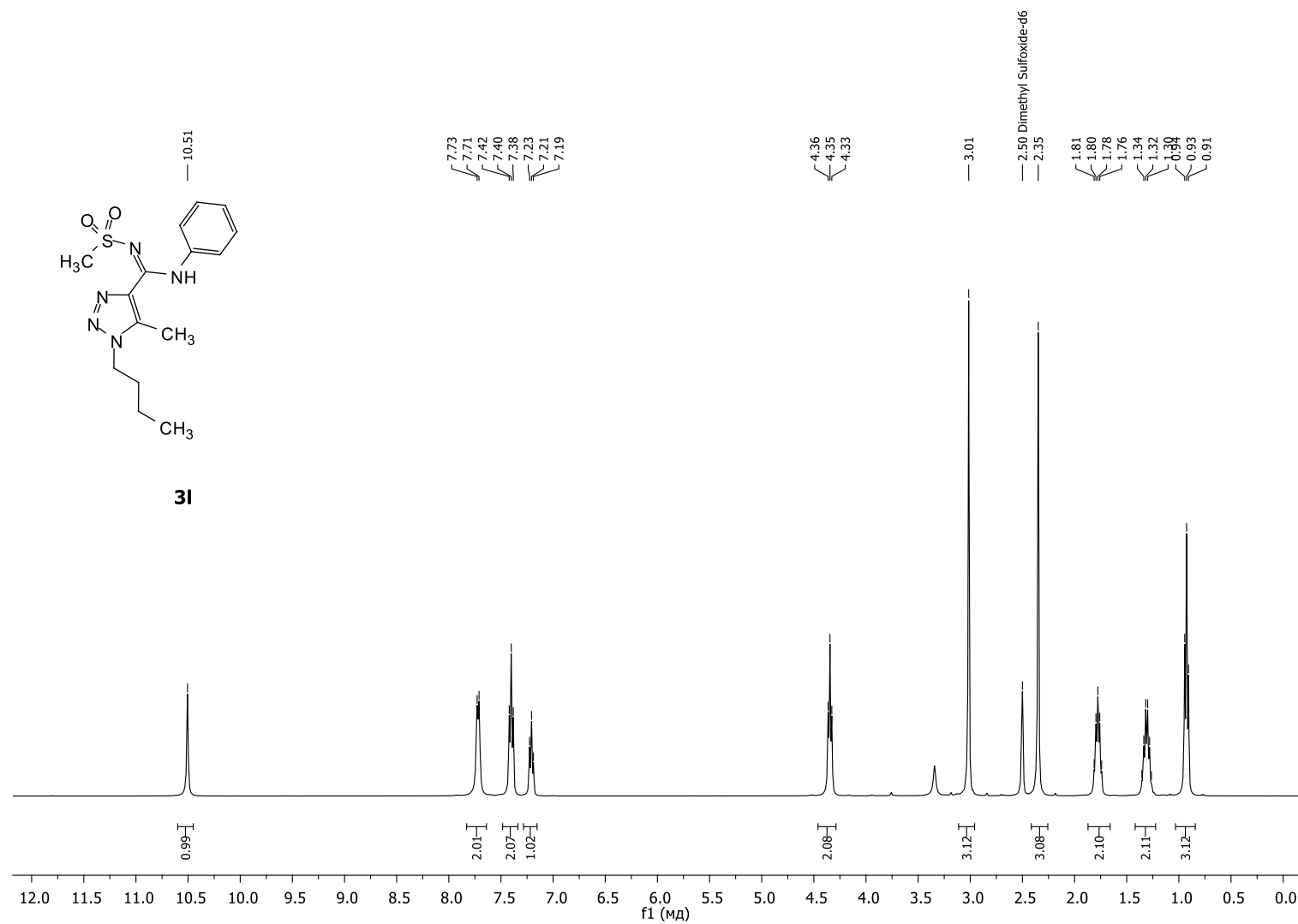
The HMBC NMR spectrum of compound **3j**.



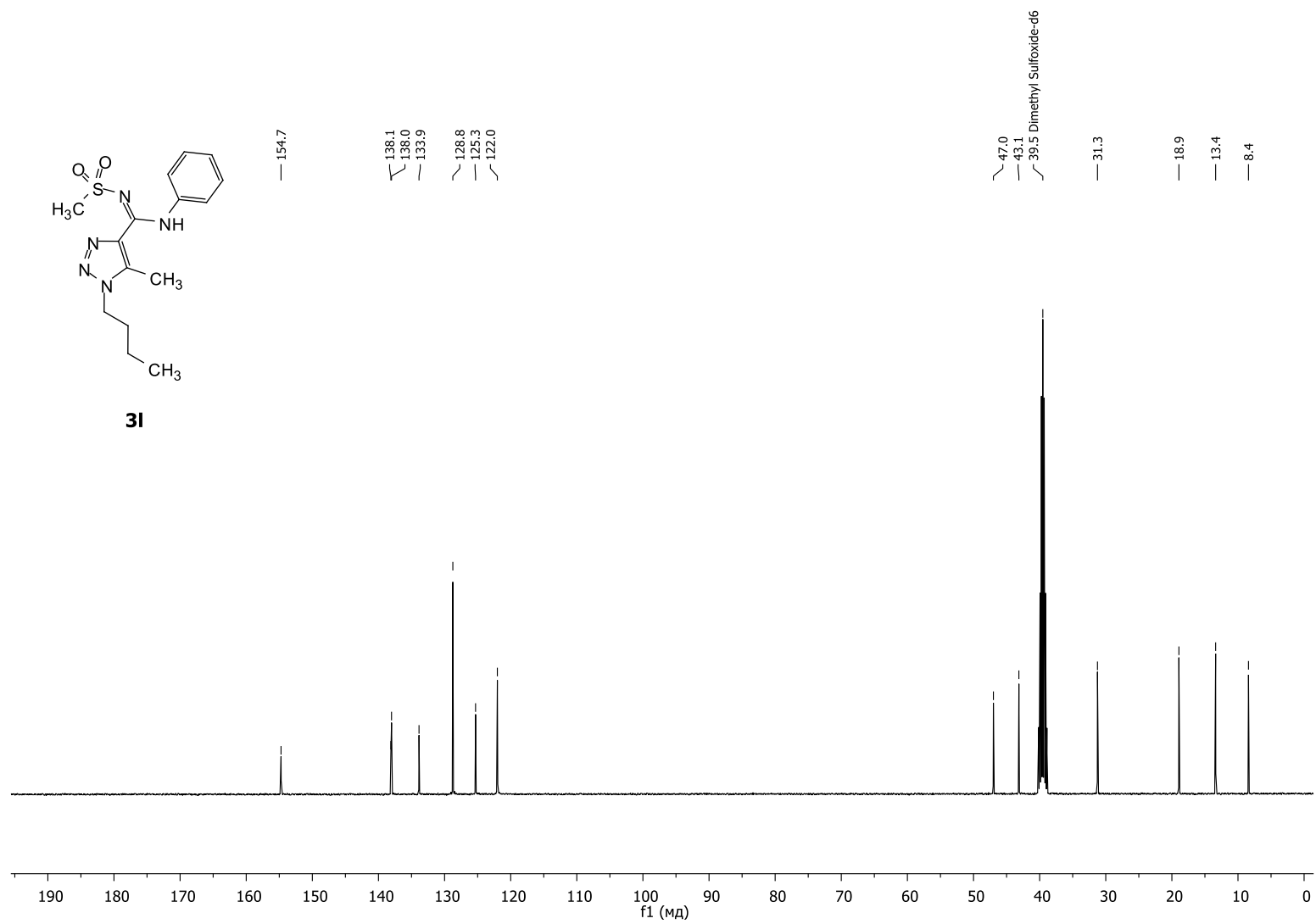
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3k**.



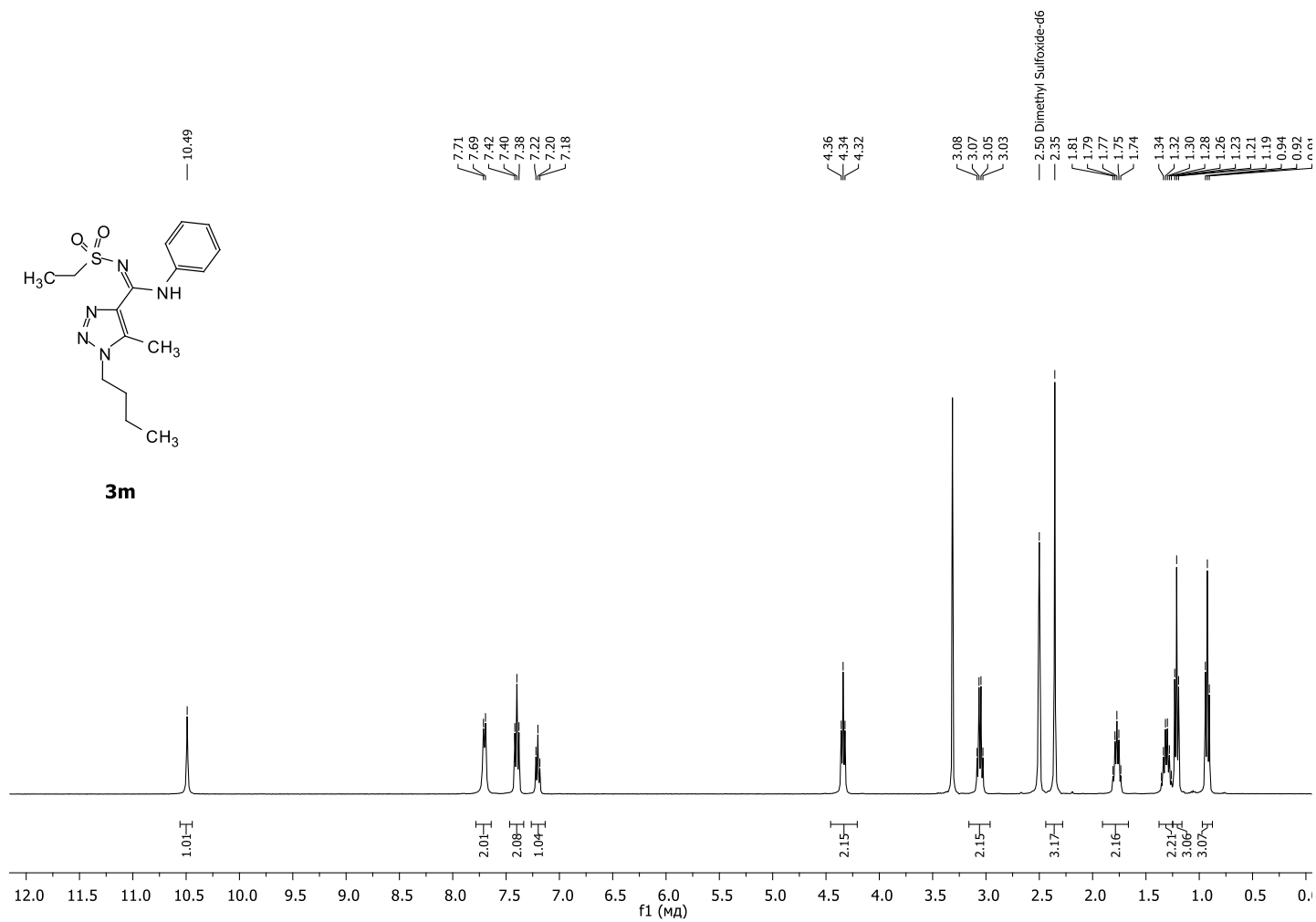
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3k**.



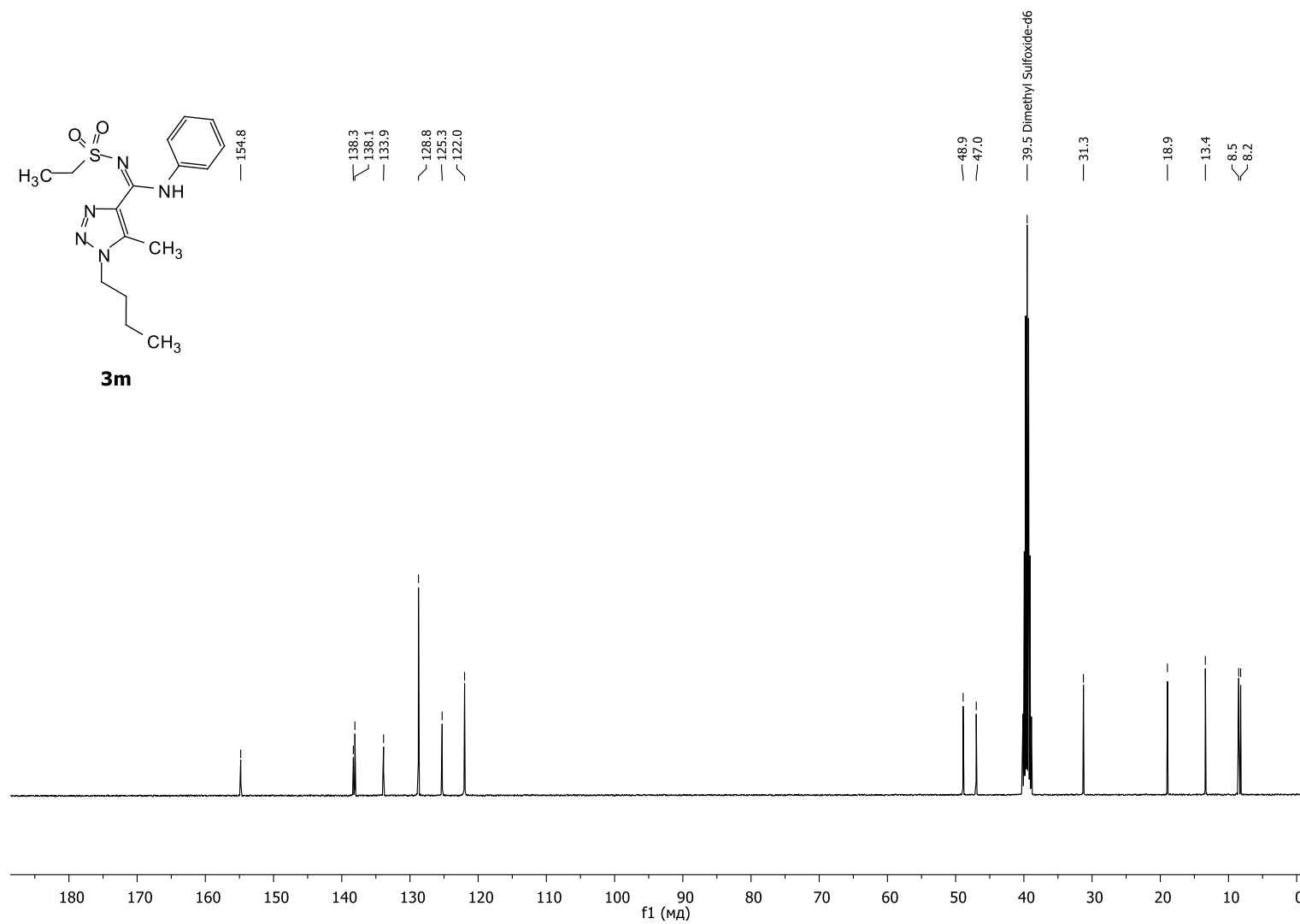
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3I**.



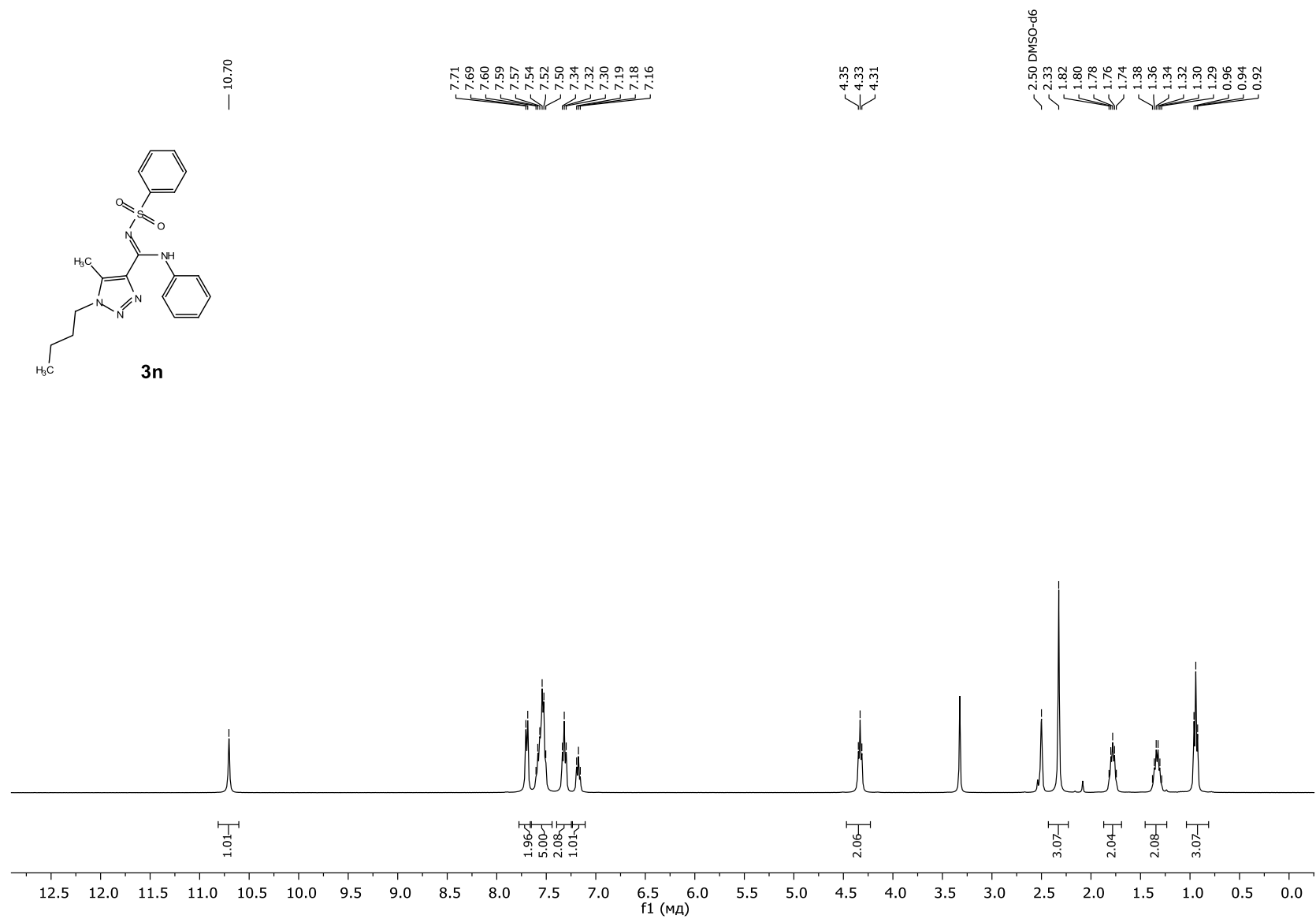
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **31**.



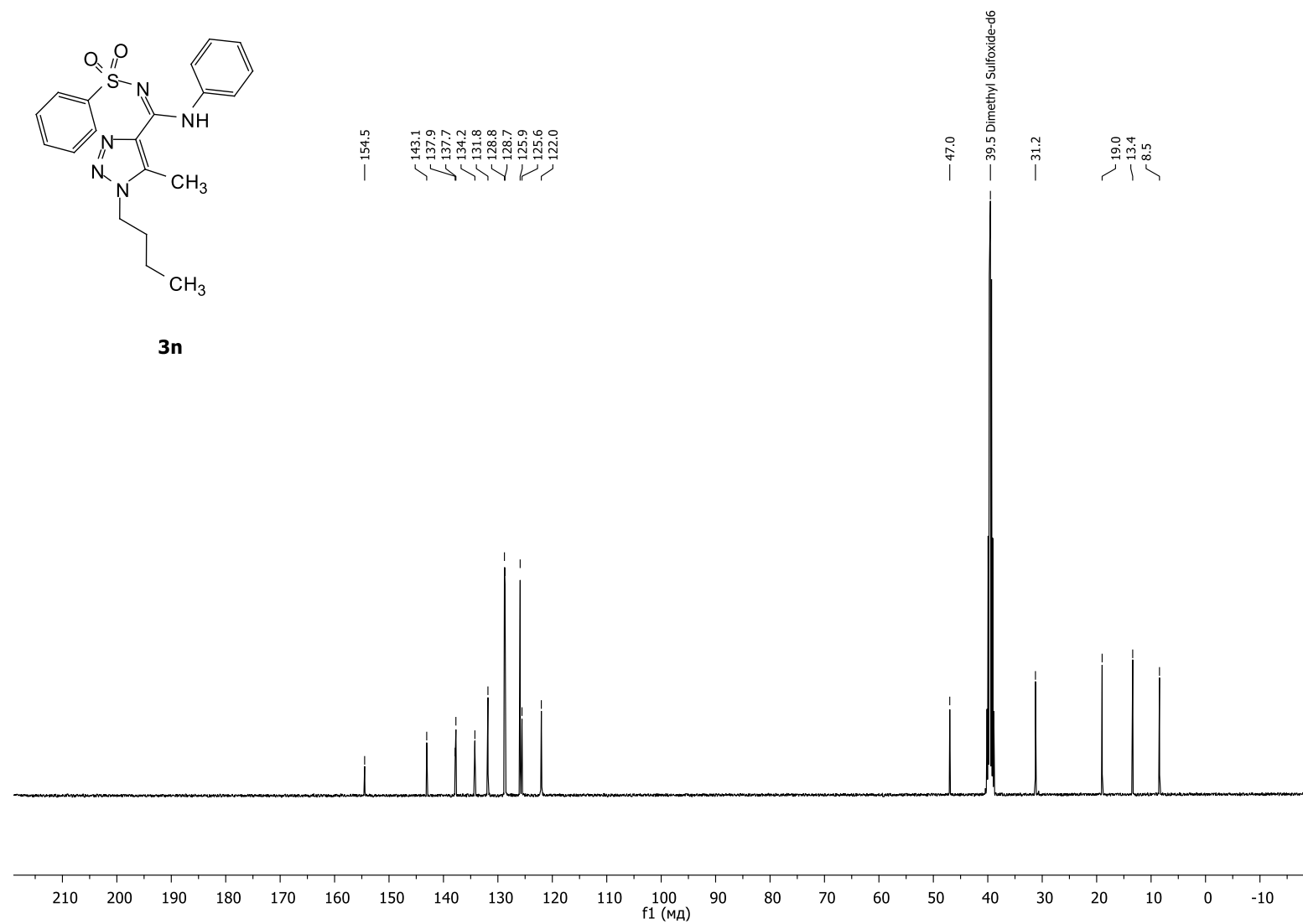
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3m**.



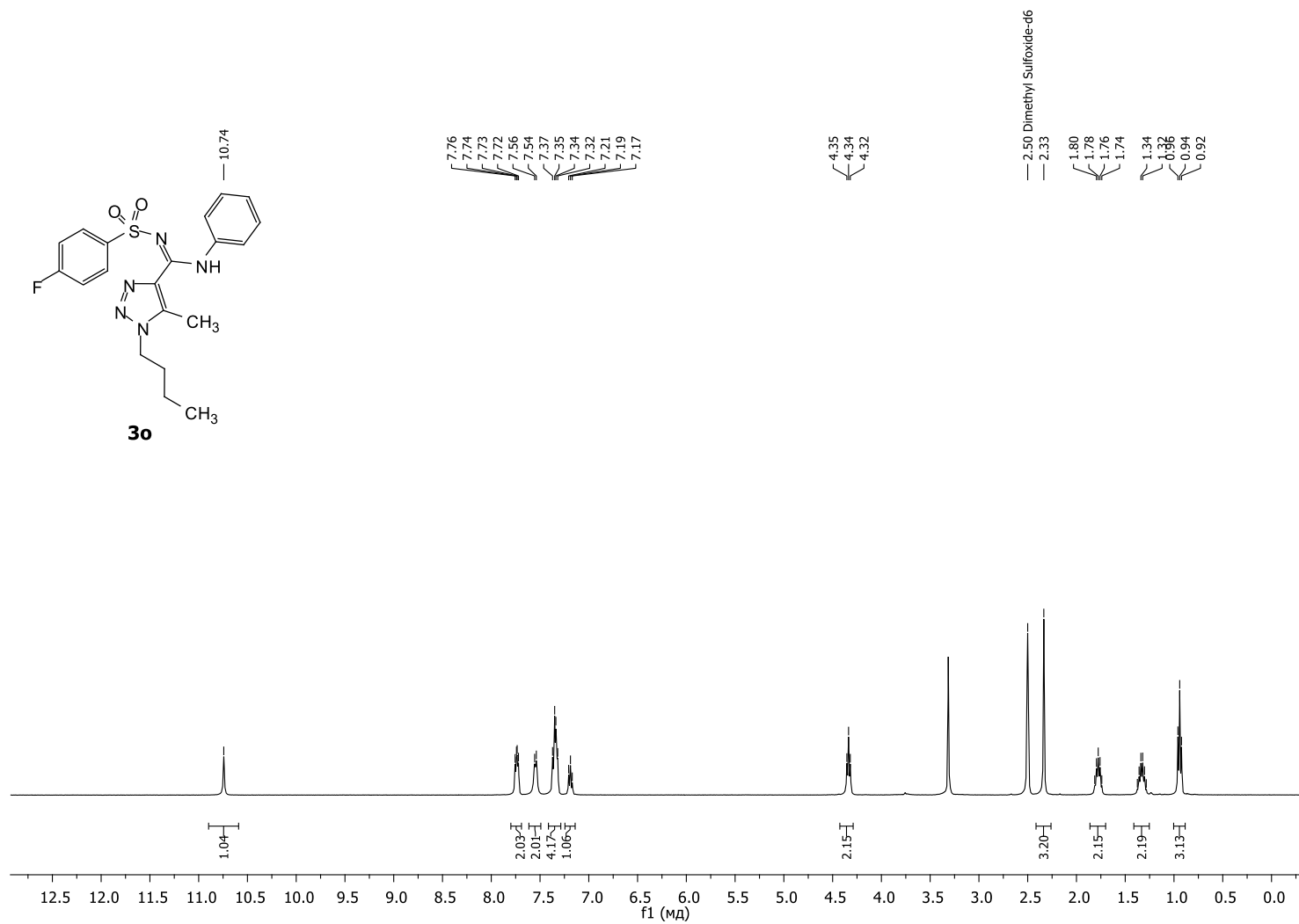
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3m**.



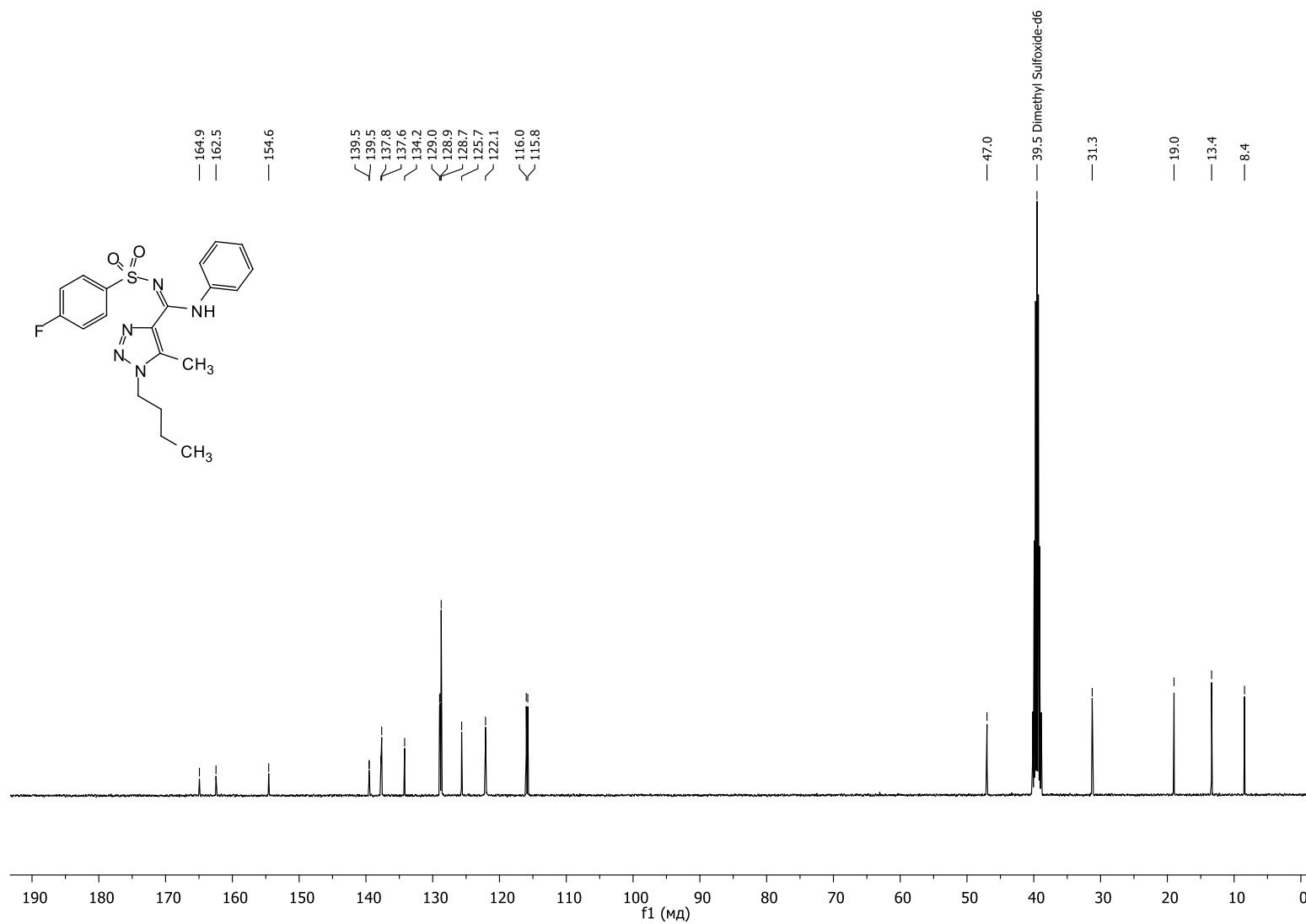
The ¹H NMR (400 MHz, DMSO-d₆) spectrum of compound **3n**.



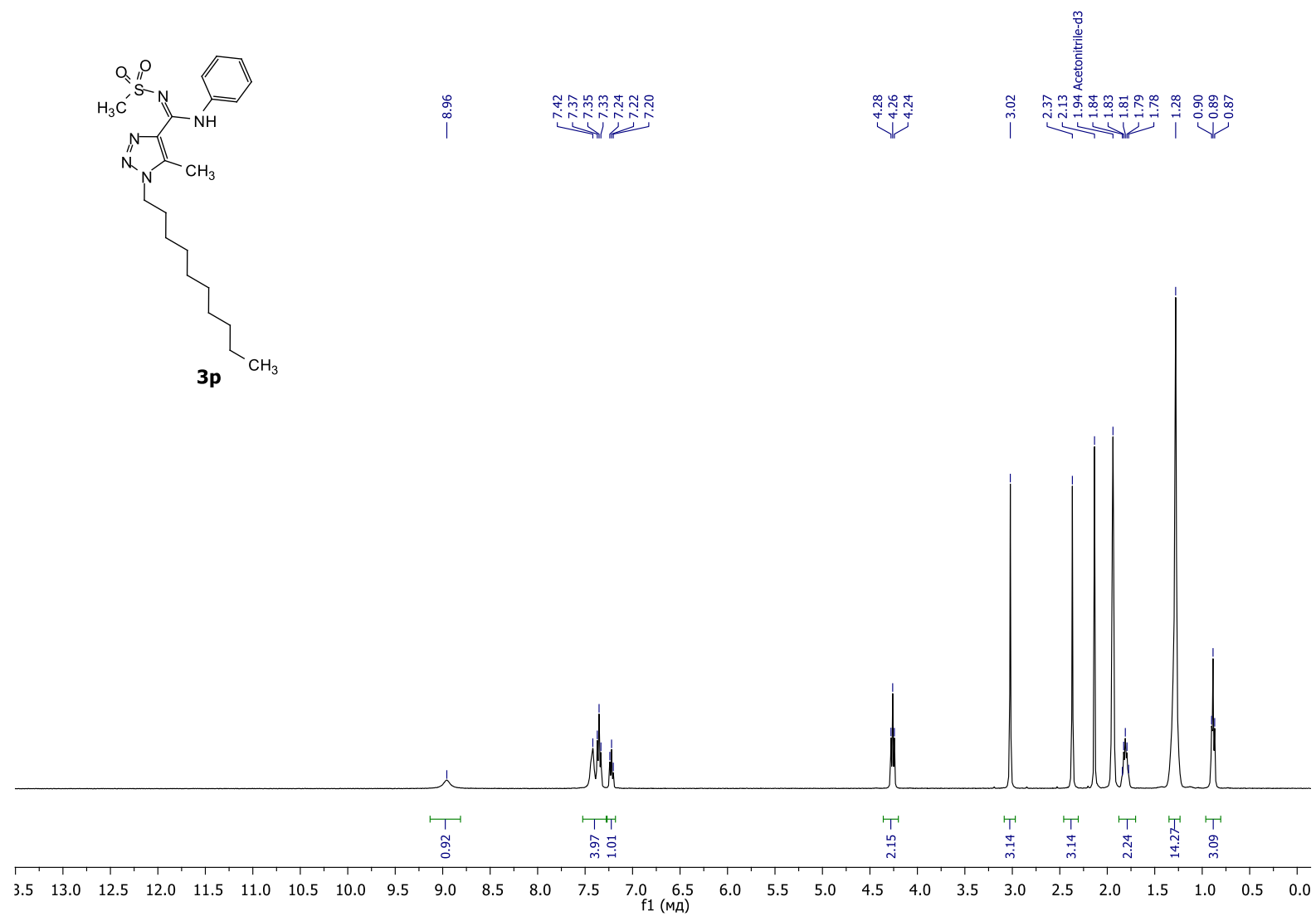
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3n**.



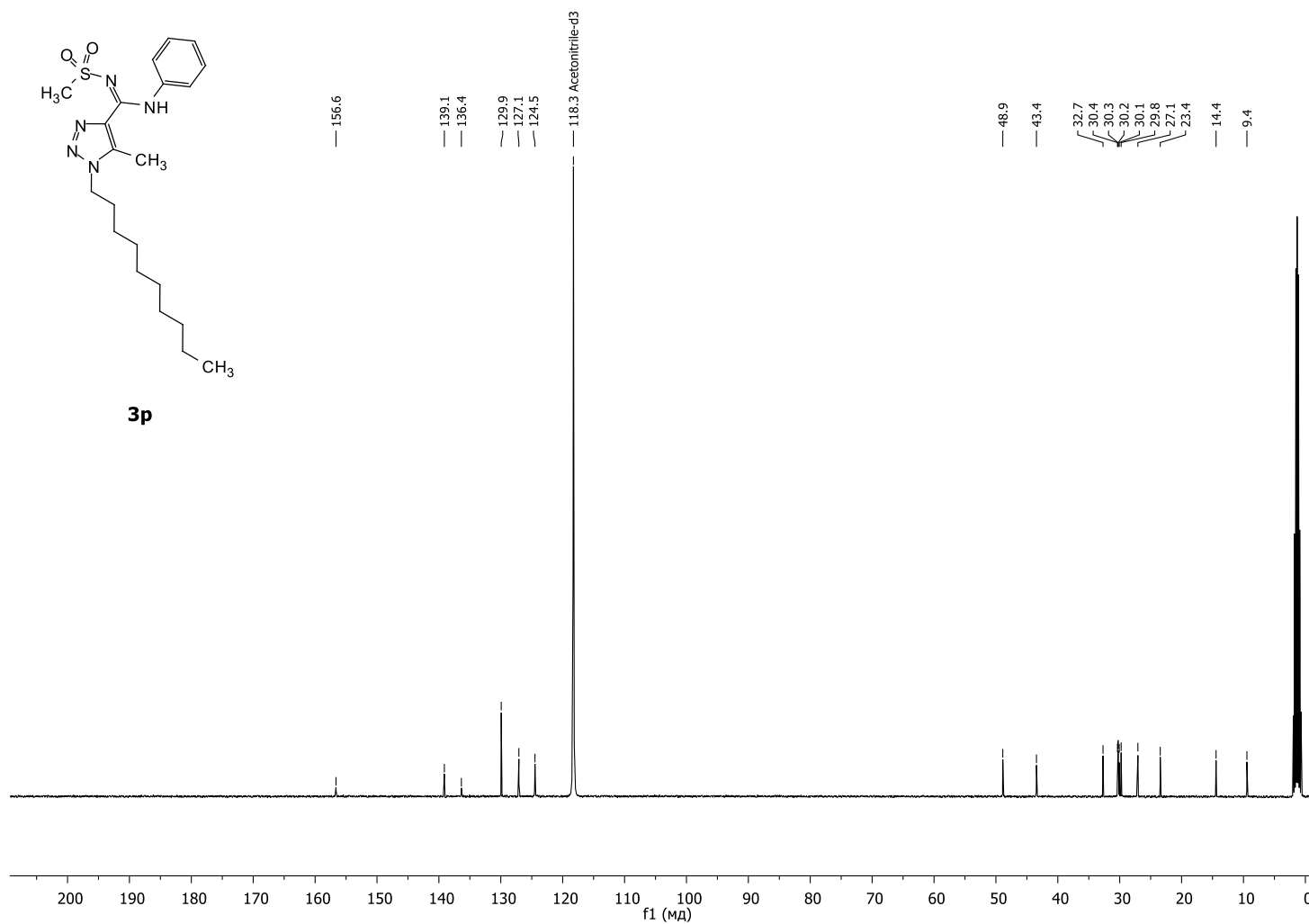
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3o**.



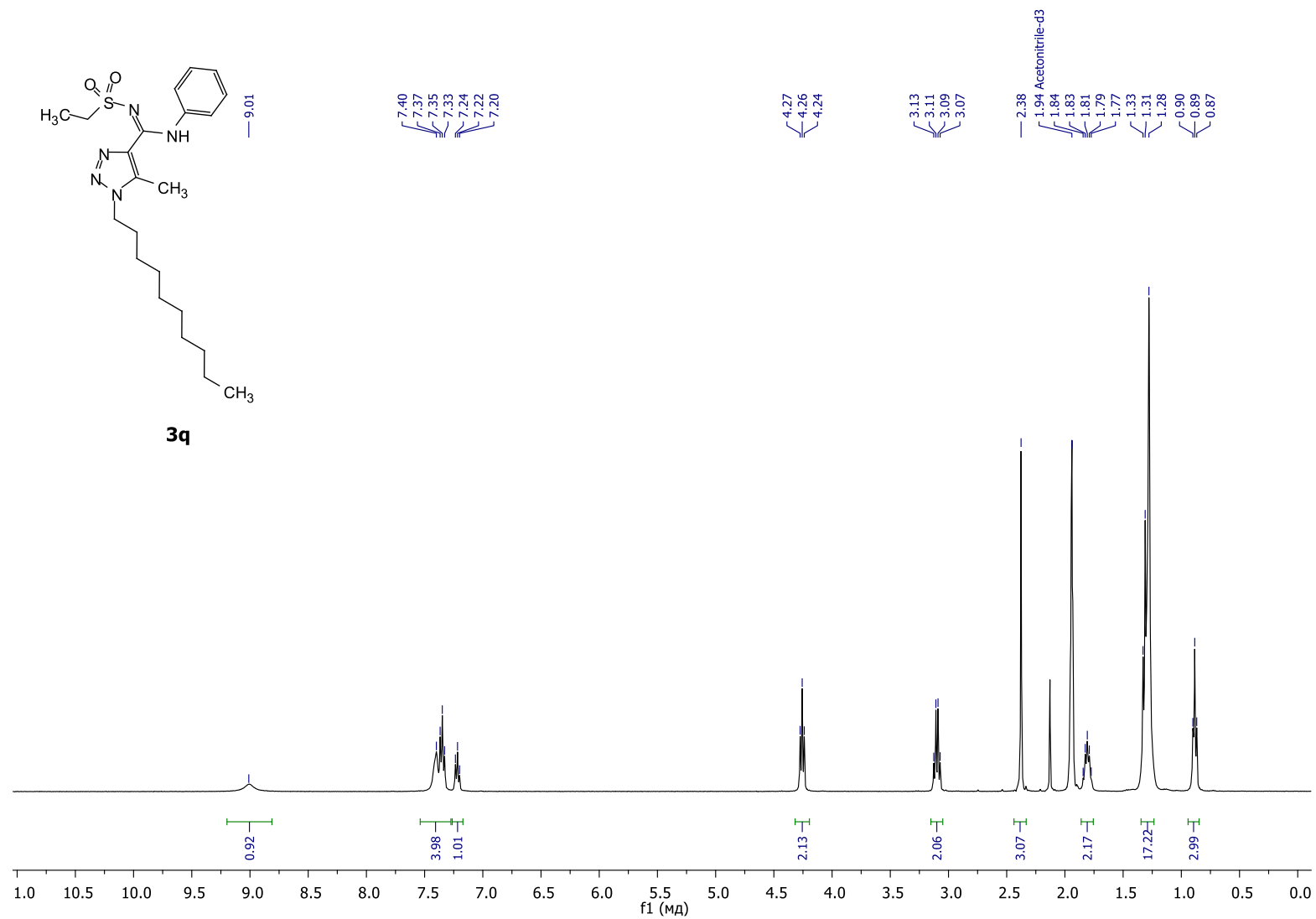
The ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of compound **3o**.



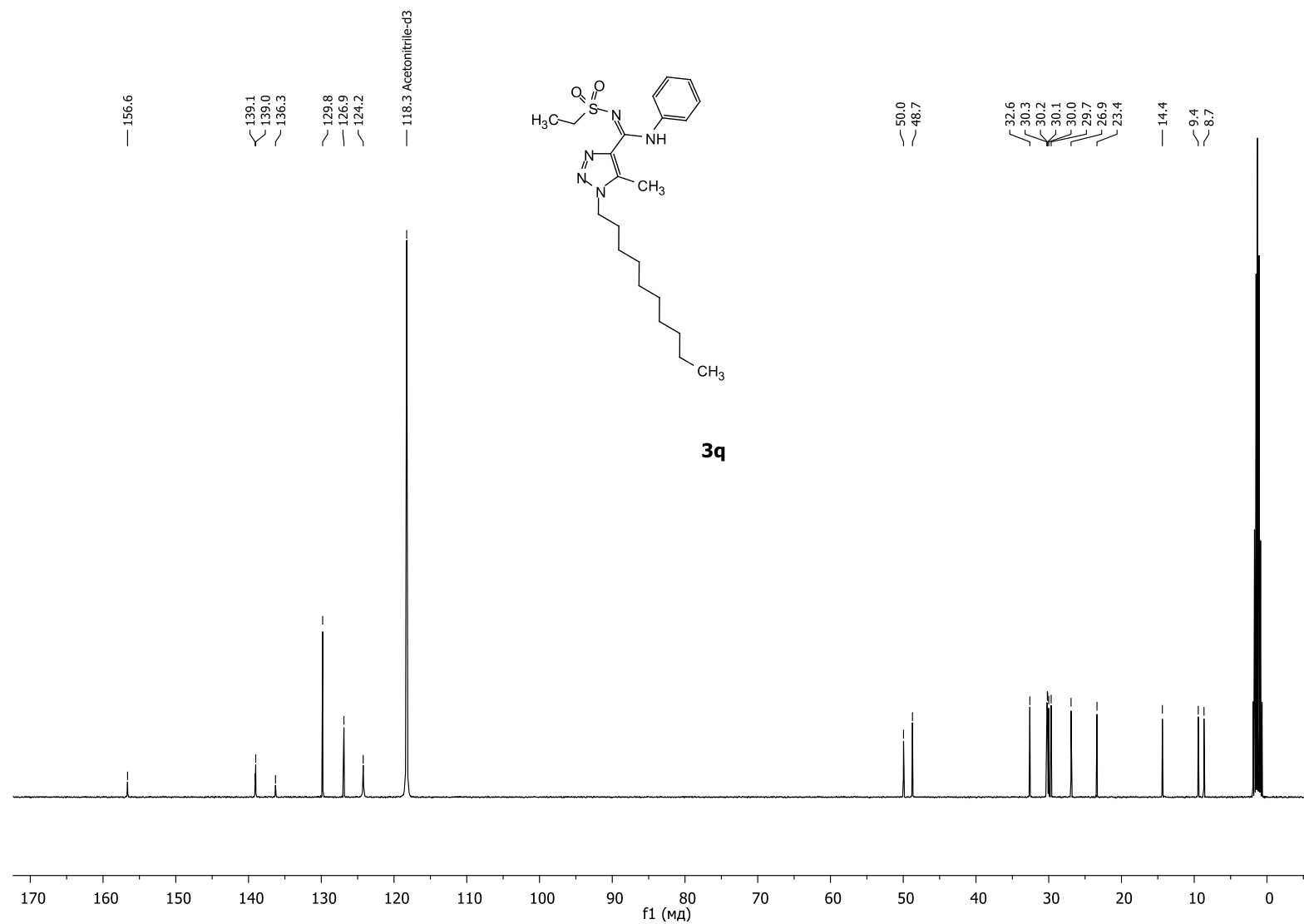
The ¹H NMR (400 MHz, CD₃CN, 40 °C) spectrum of compound **3p**.



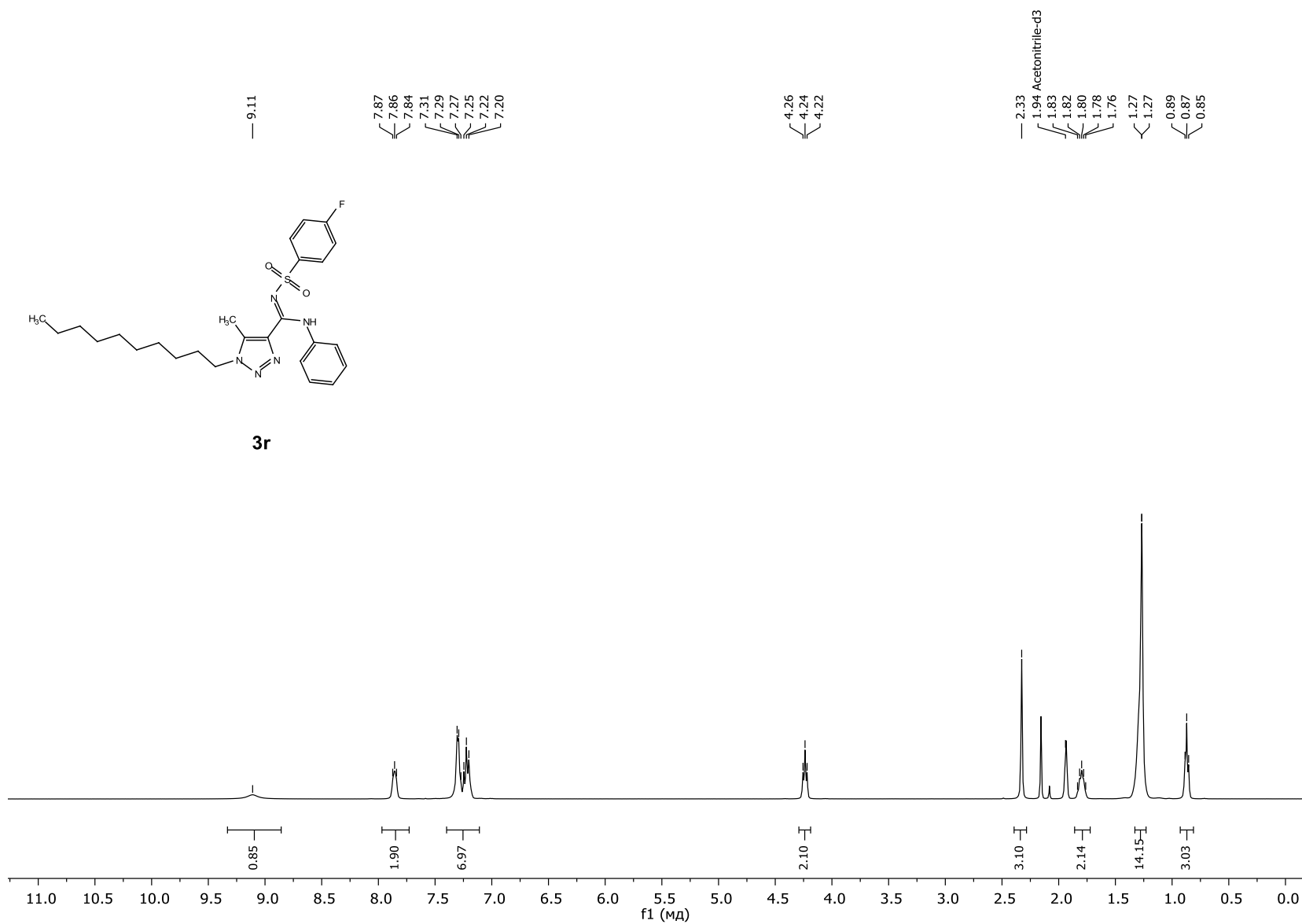
The ^{13}C NMR (100 MHz, CD_3CN , 40 °C) spectrum of compound **3p**.



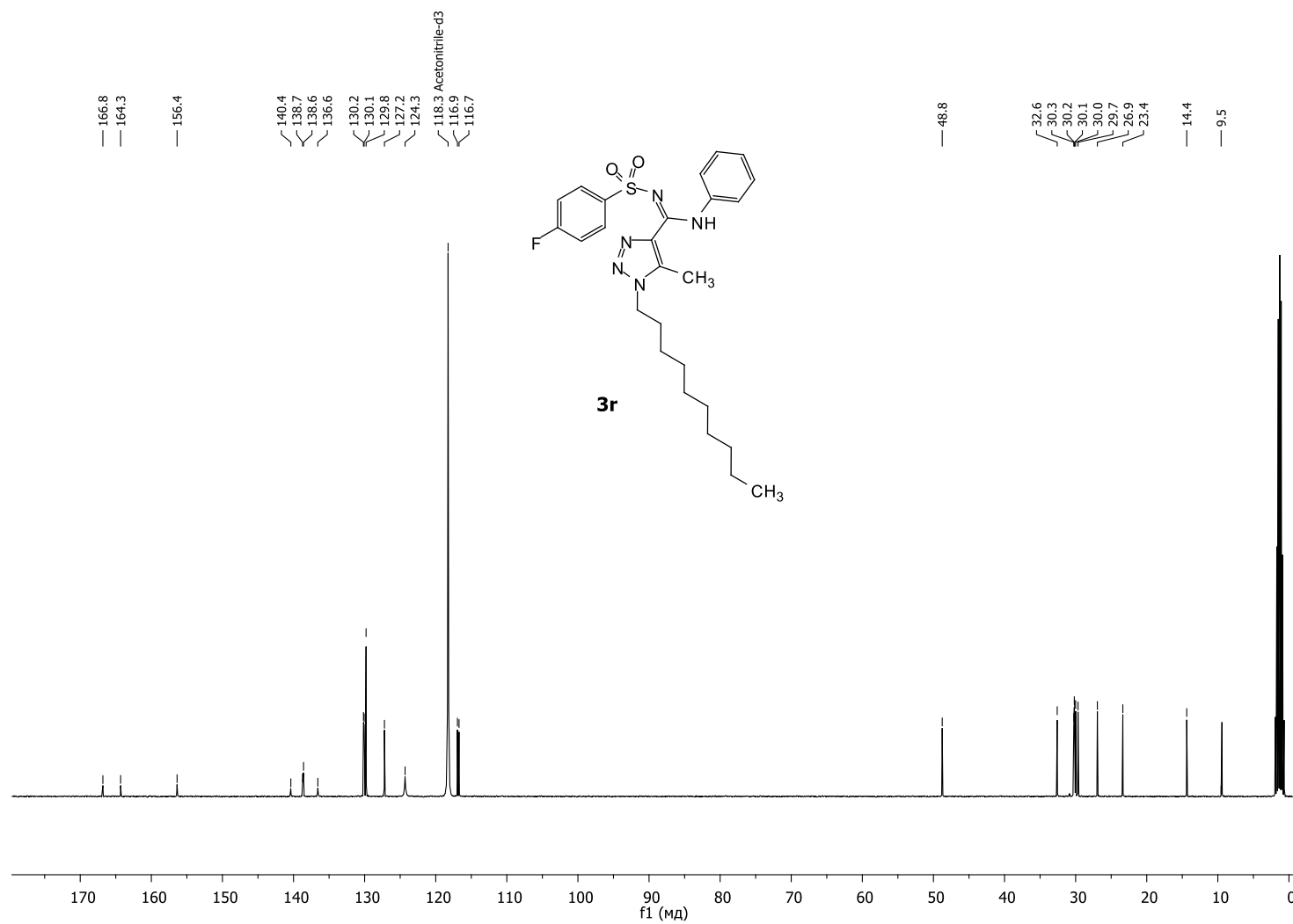
The ^1H NMR (400 MHz, CD_3CN) spectrum of compound **3q**.



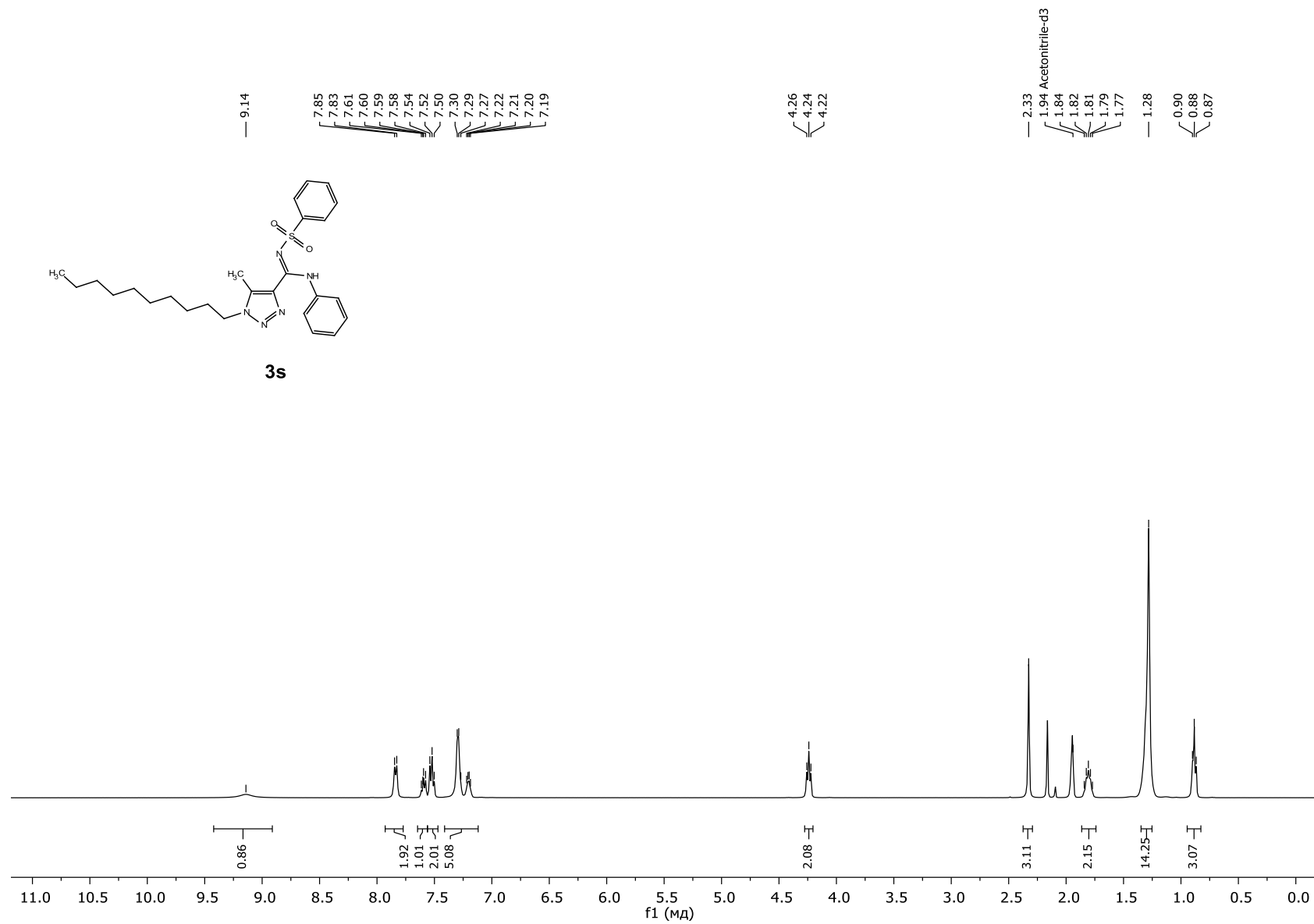
The ^{13}C NMR (100 MHz, CD_3CN) spectrum of compound **3q**.



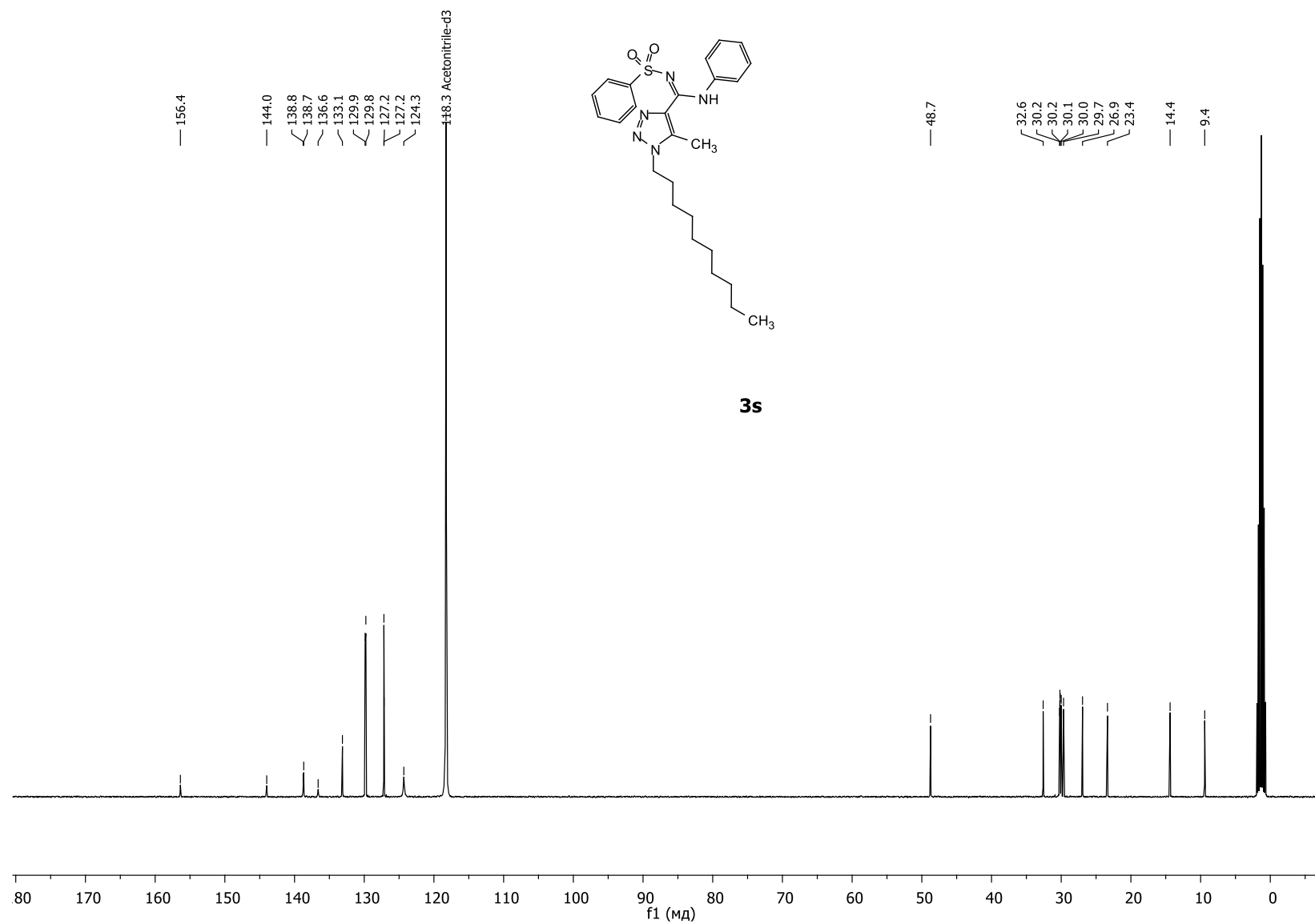
The ¹H NMR (400 MHz, CD₃CN) spectrum of compound **3r**.



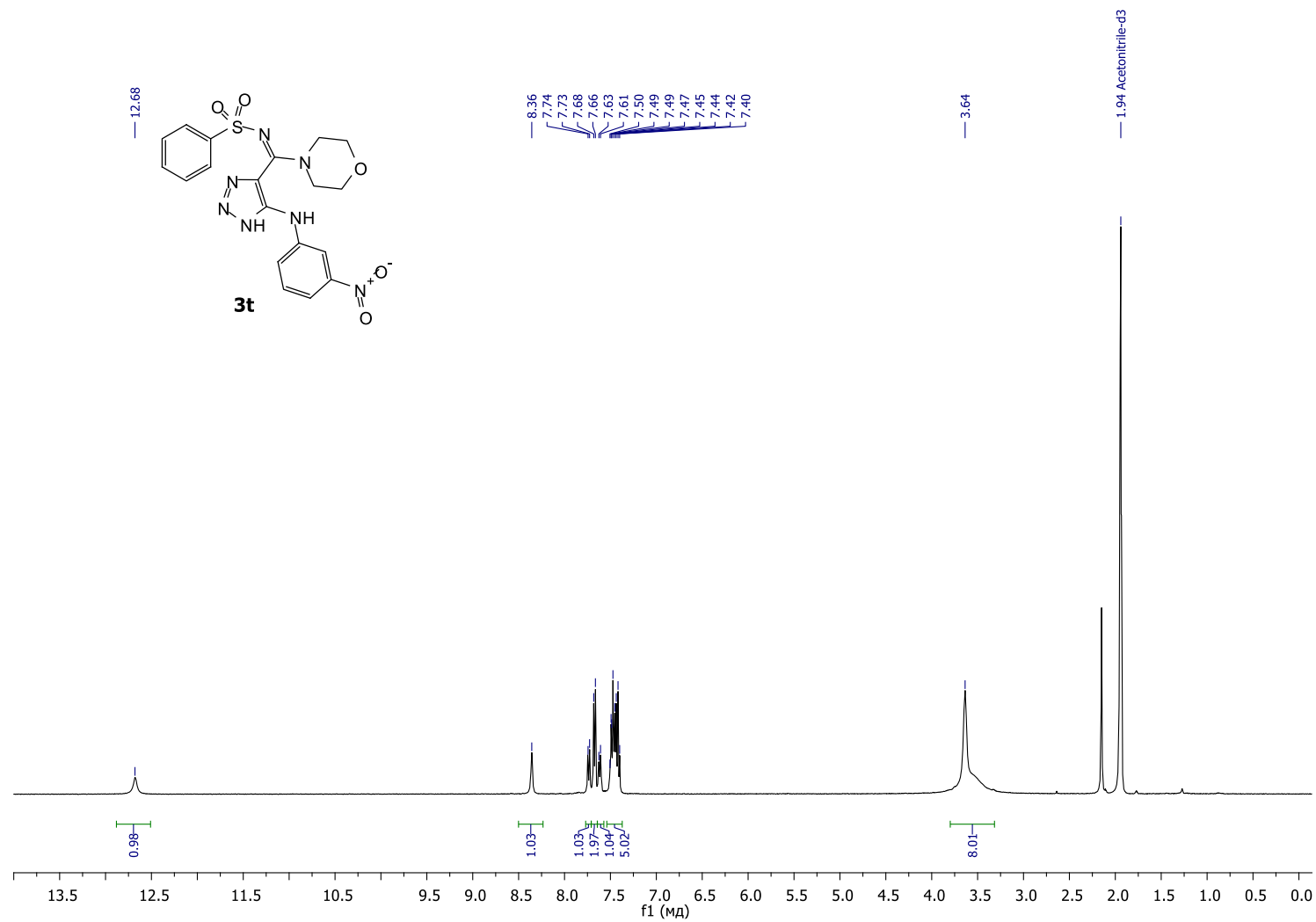
The ^{13}C NMR (100 MHz, CD_3CN) spectrum of compound **3r**.



The ¹H NMR (400 MHz, CD₃CN) spectrum of compound **3s**.

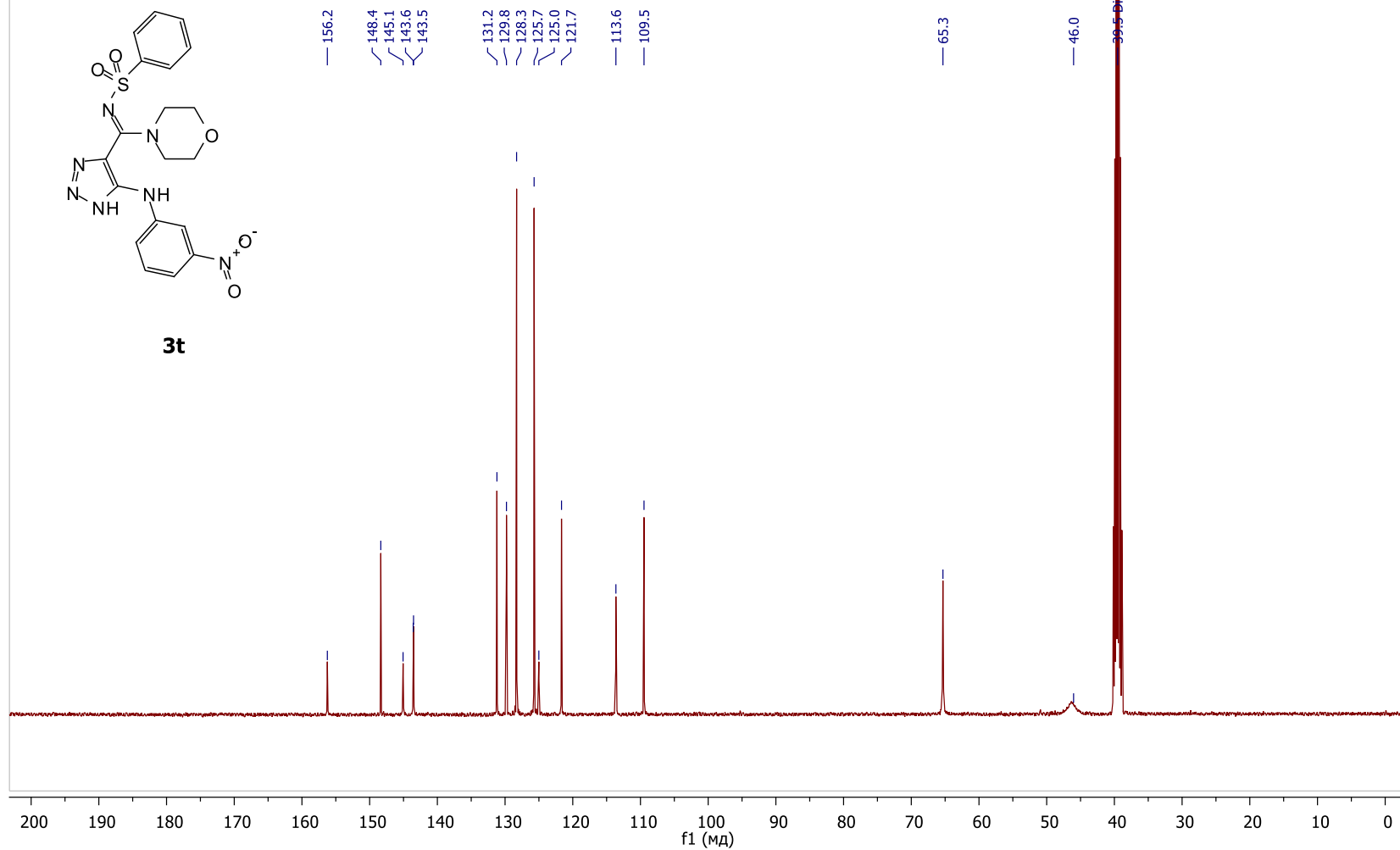


The ^{13}C NMR (100 MHz, CD_3CN) spectrum of compound **3s**.

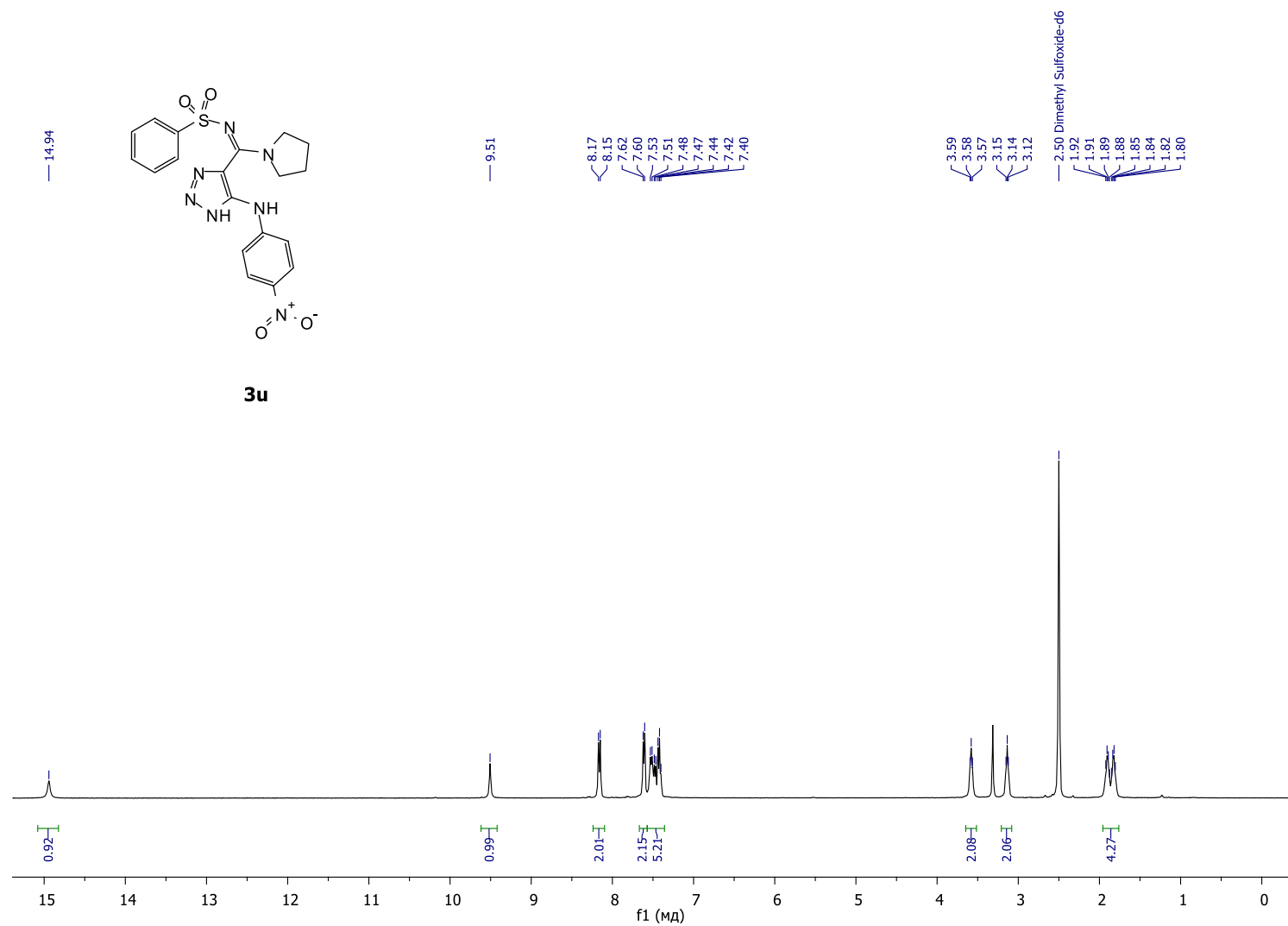


The ^1H NMR (400 MHz, CD_3CN) spectrum of compound **3t**.

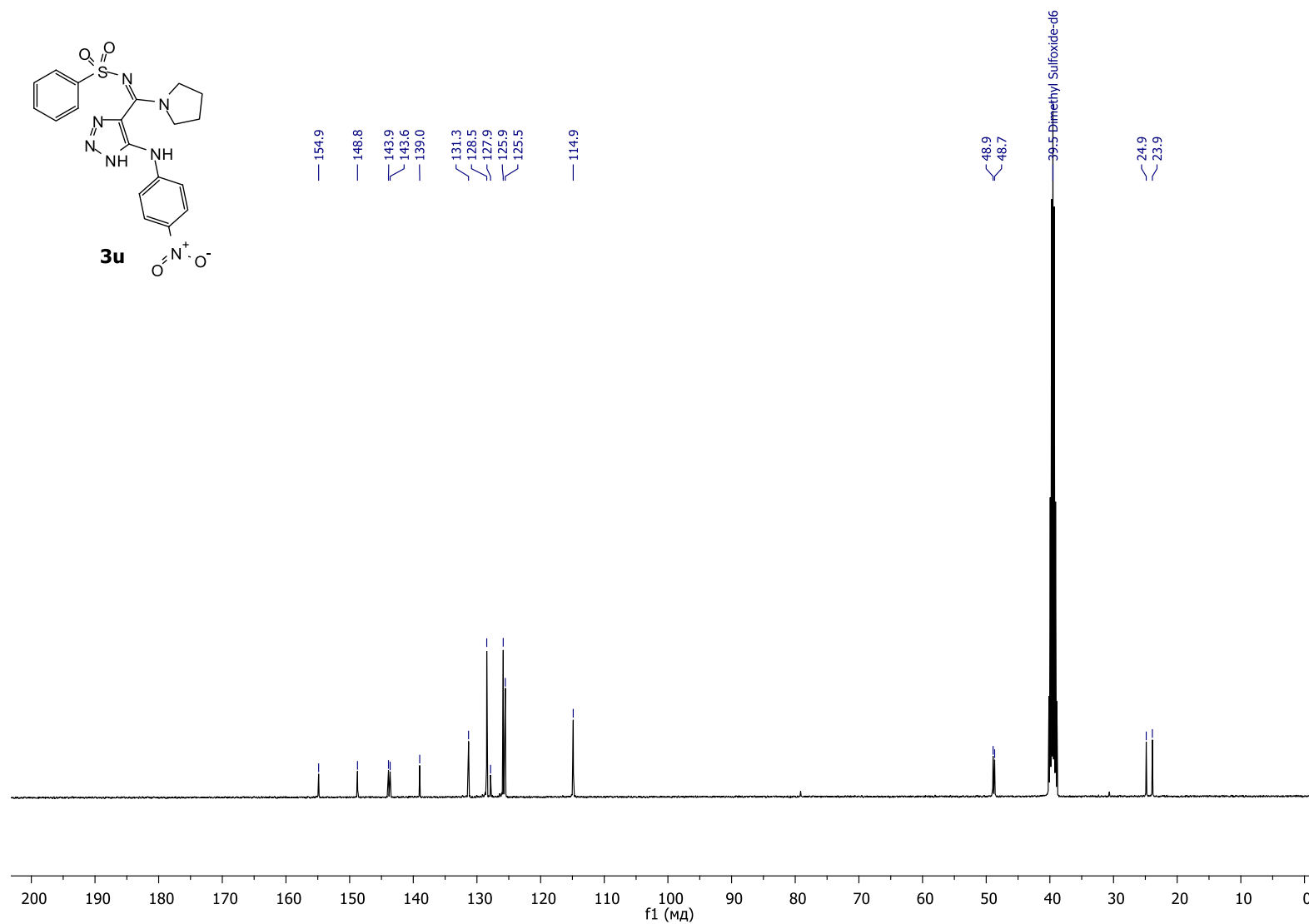
2572
Ilkin VL-1



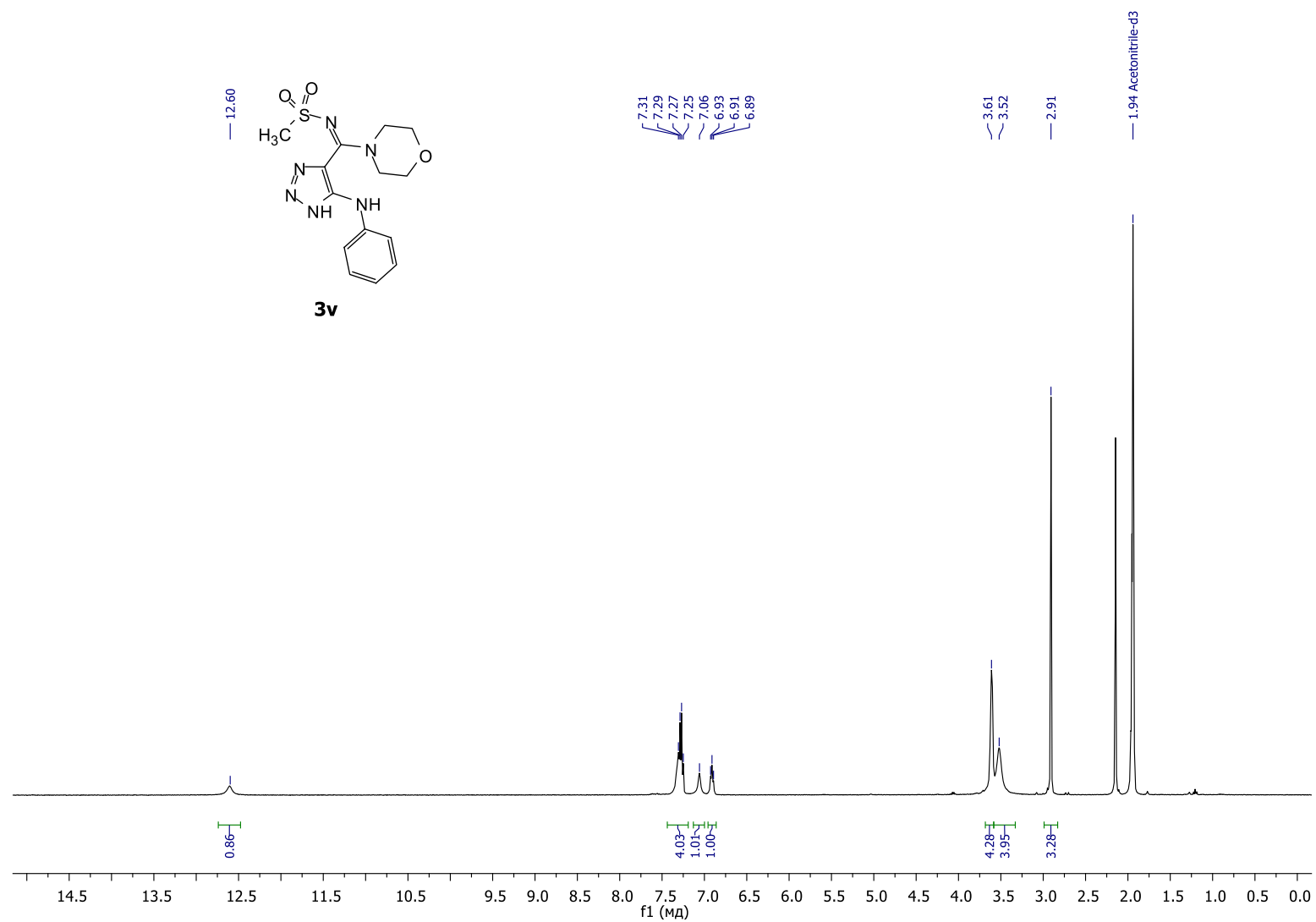
The ^{13}C NMR (100 MHz, DMSO- d_6 , 50 °C) spectrum of compound **3t**.



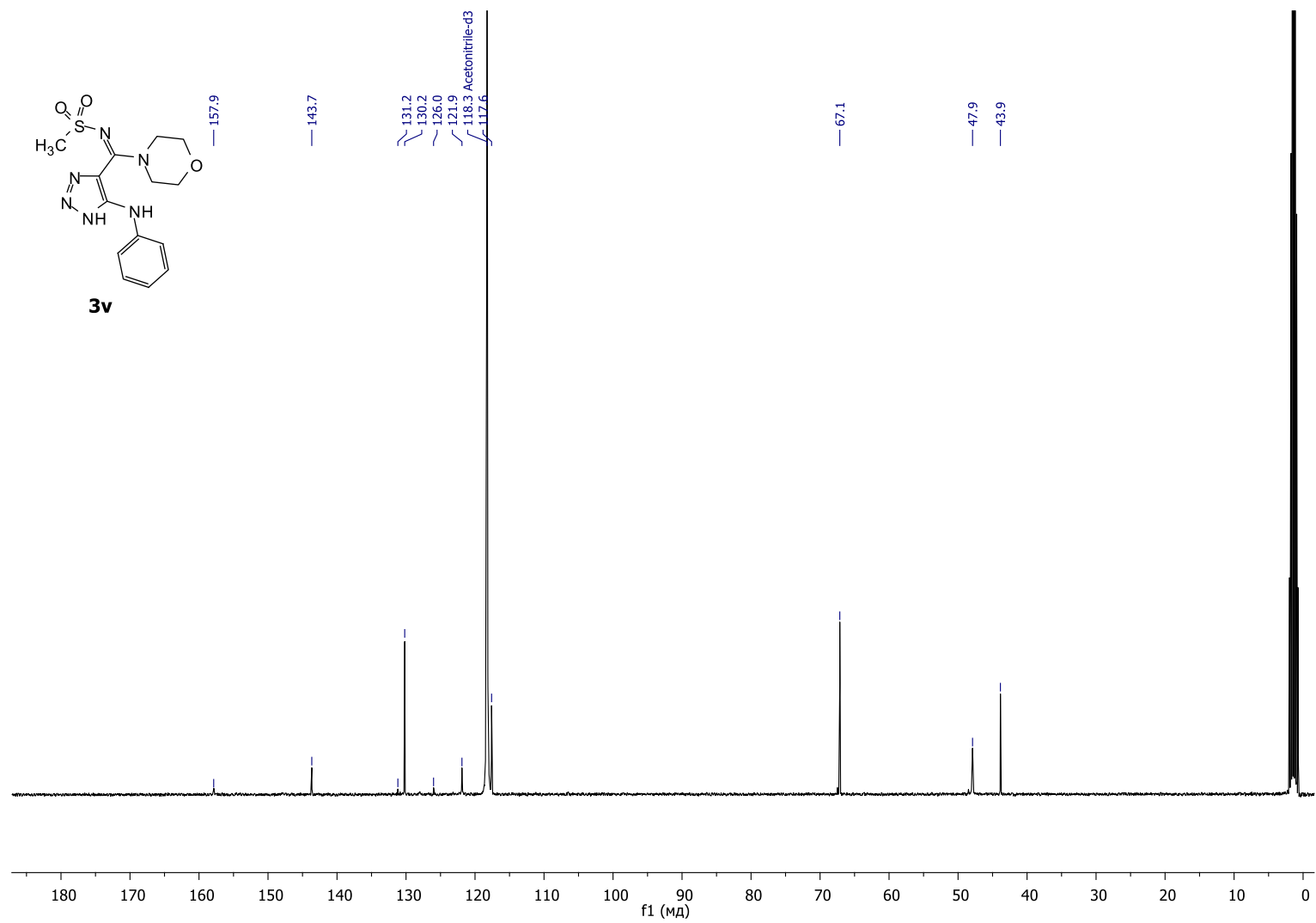
The ^1H NMR (400 MHz, $\text{DMSO-}d_6$) spectrum of compound **3u**.



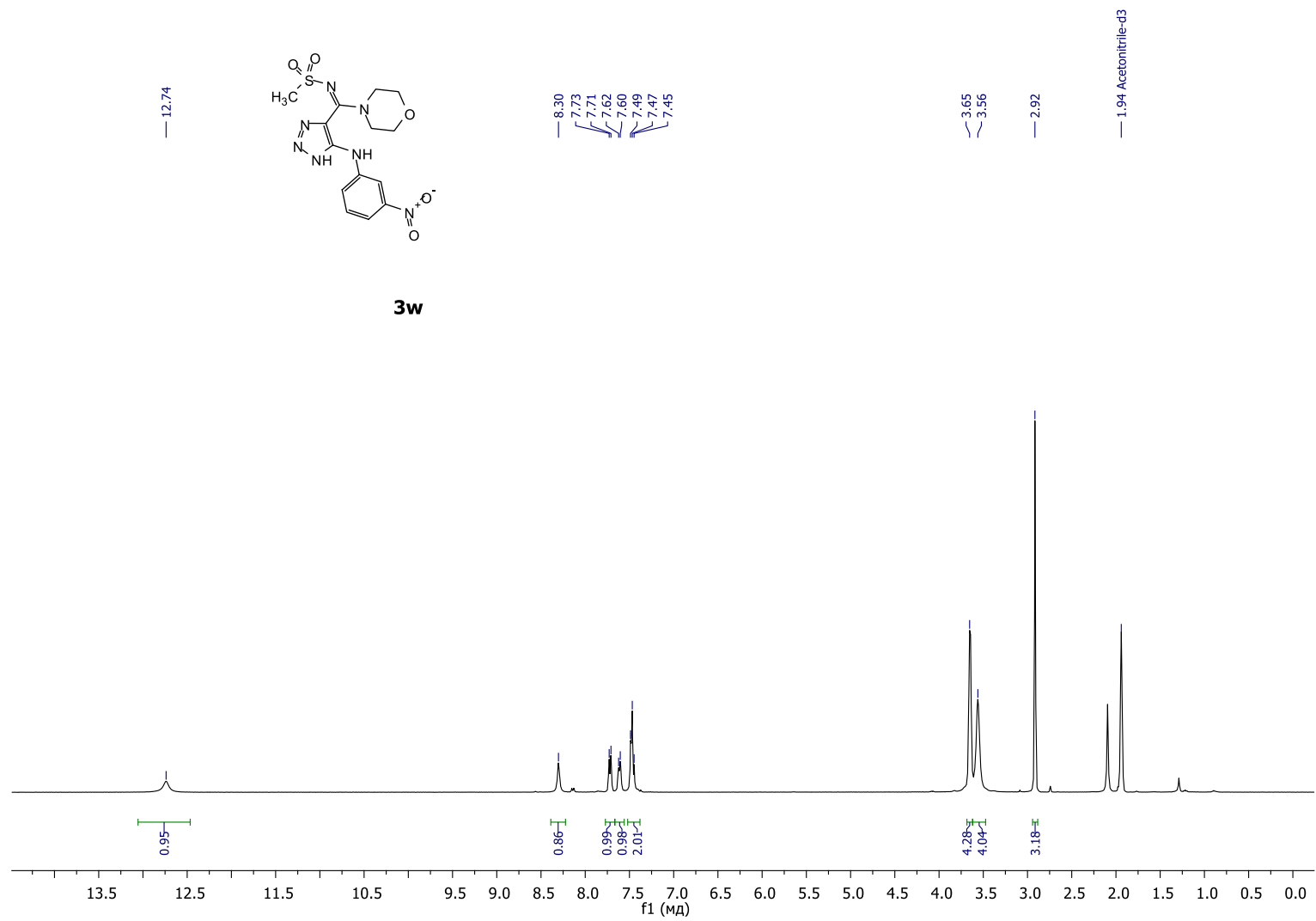
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3u**.



The ¹H NMR (400 MHz, CD₃CN) spectrum of compound **3v**.

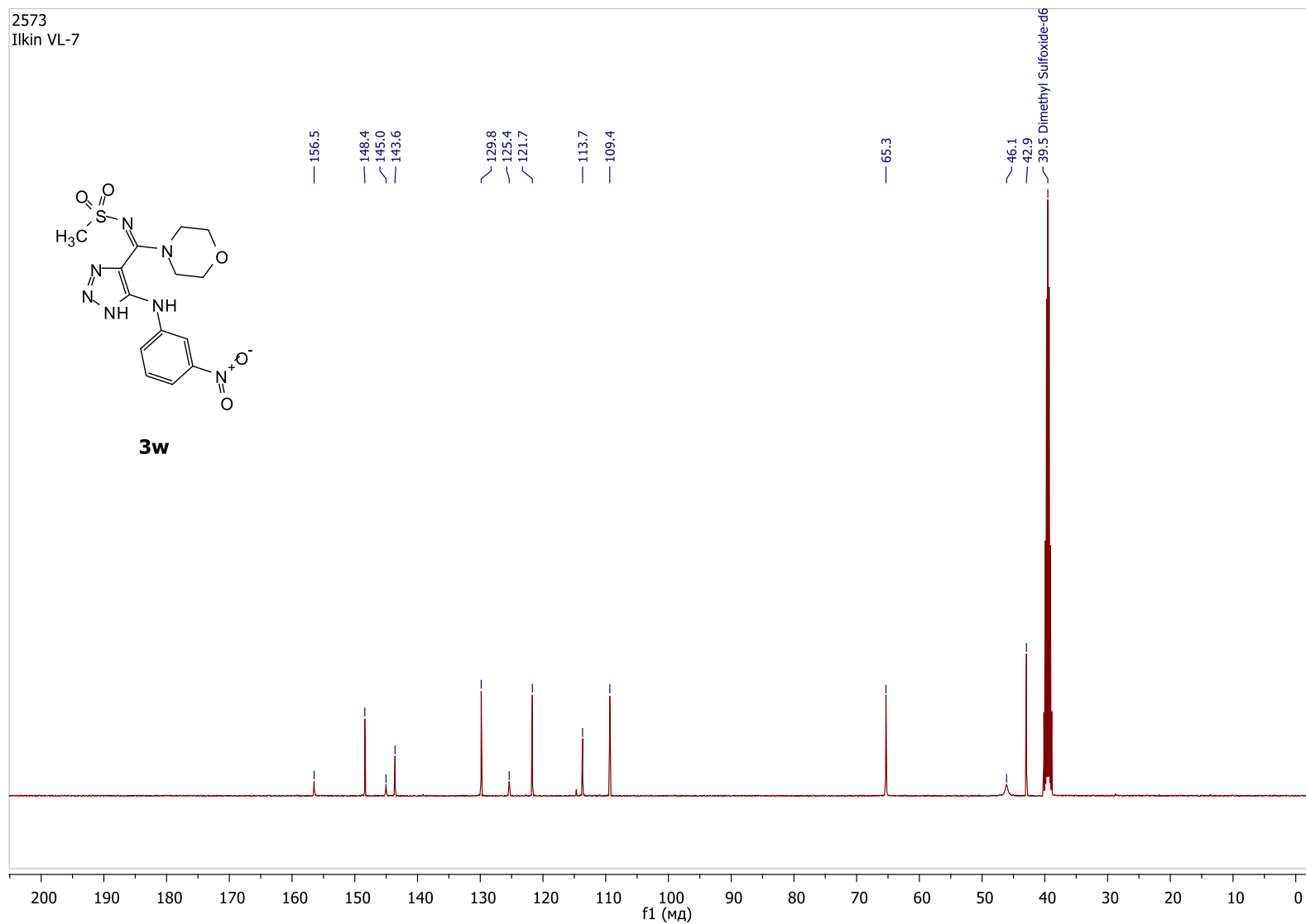


The ^{13}C NMR (100 MHz, CD_3CN , 50 °C) spectrum of compound **3v**.

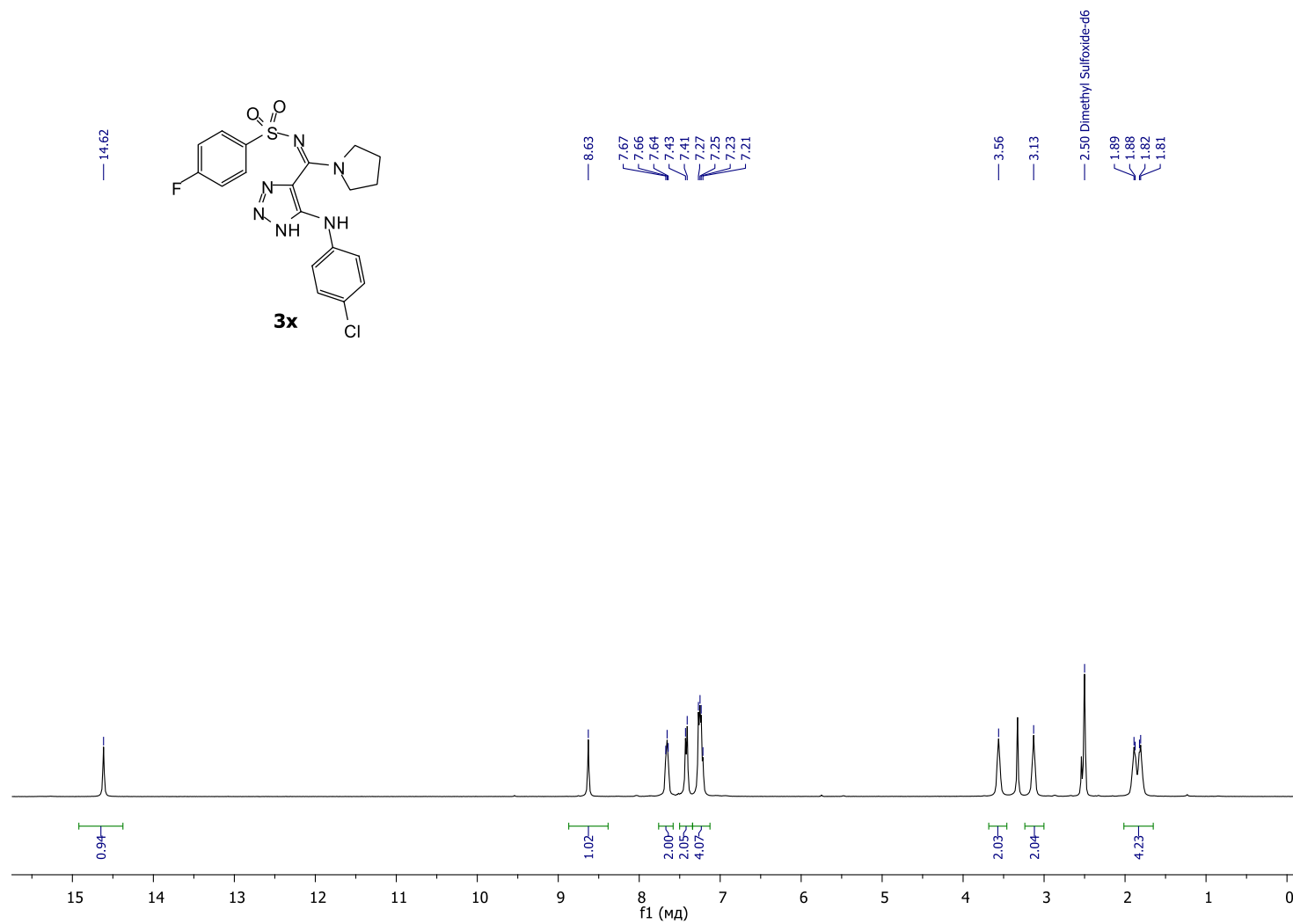


The ¹H NMR (400 MHz, CD₃CN) spectrum of compound **3w**.

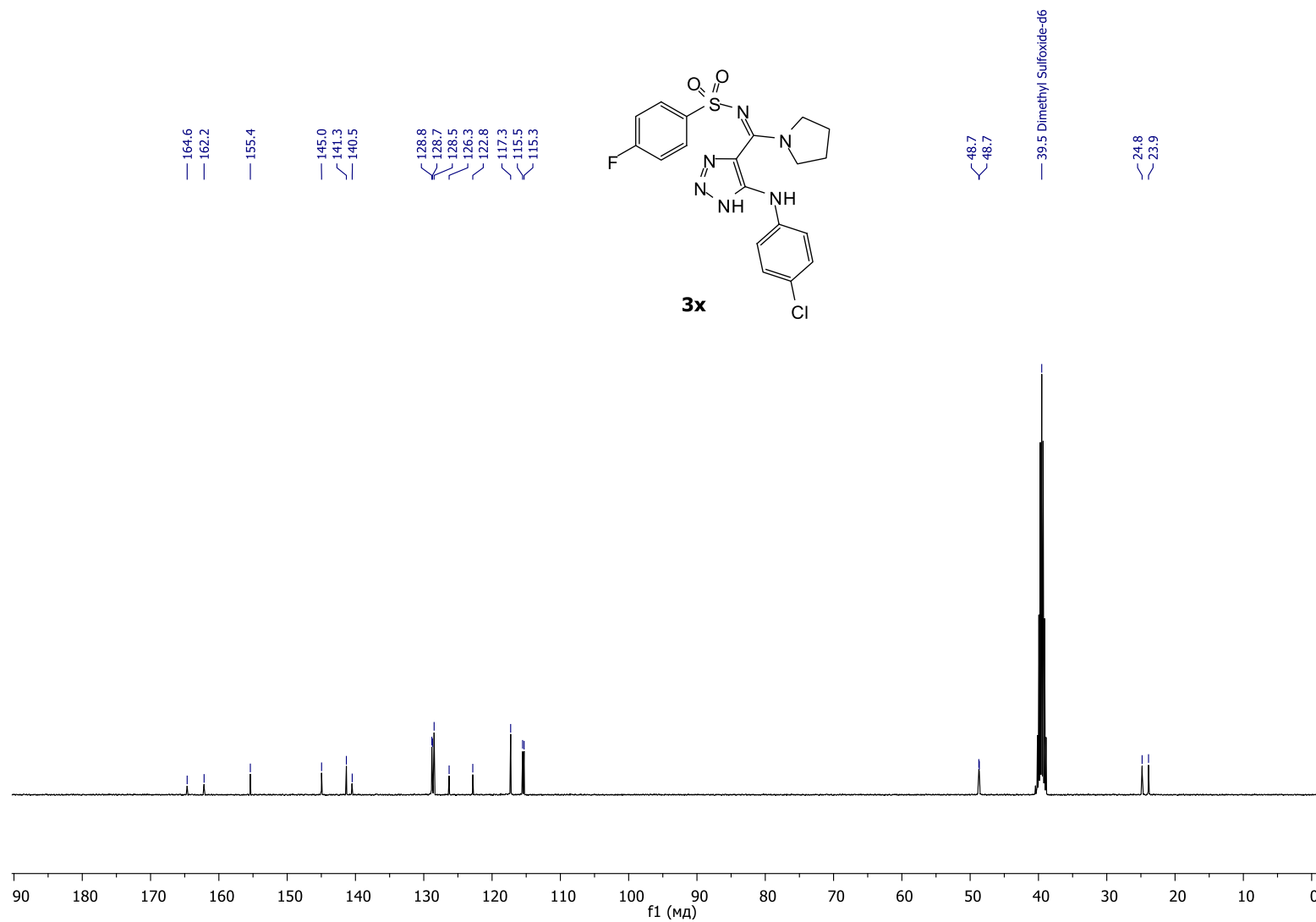
2573
Ilkin VL-7



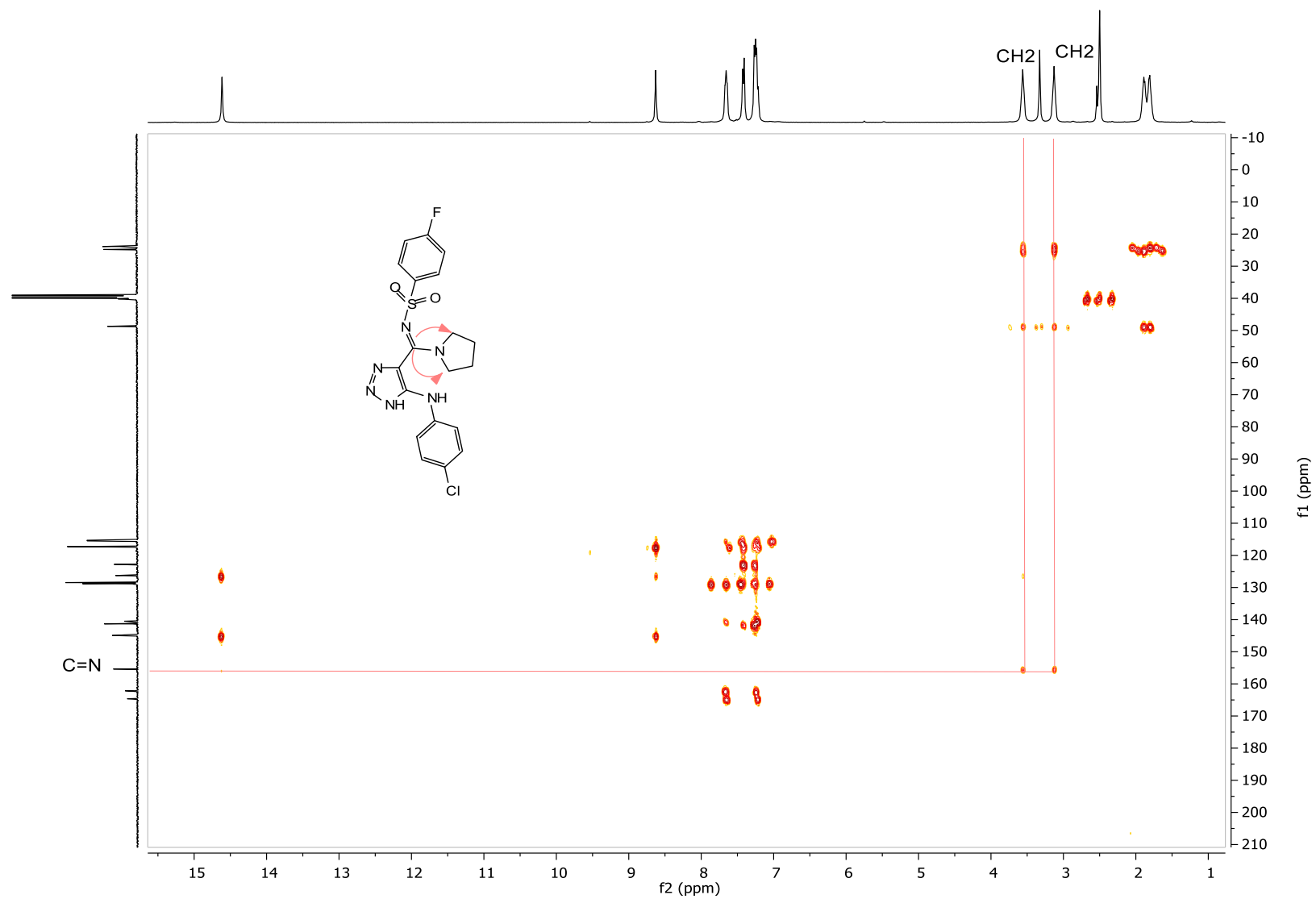
The ¹³C NMR (100 MHz, DMSO-*d*₆, 50 °C) spectrum of compound **3w**.



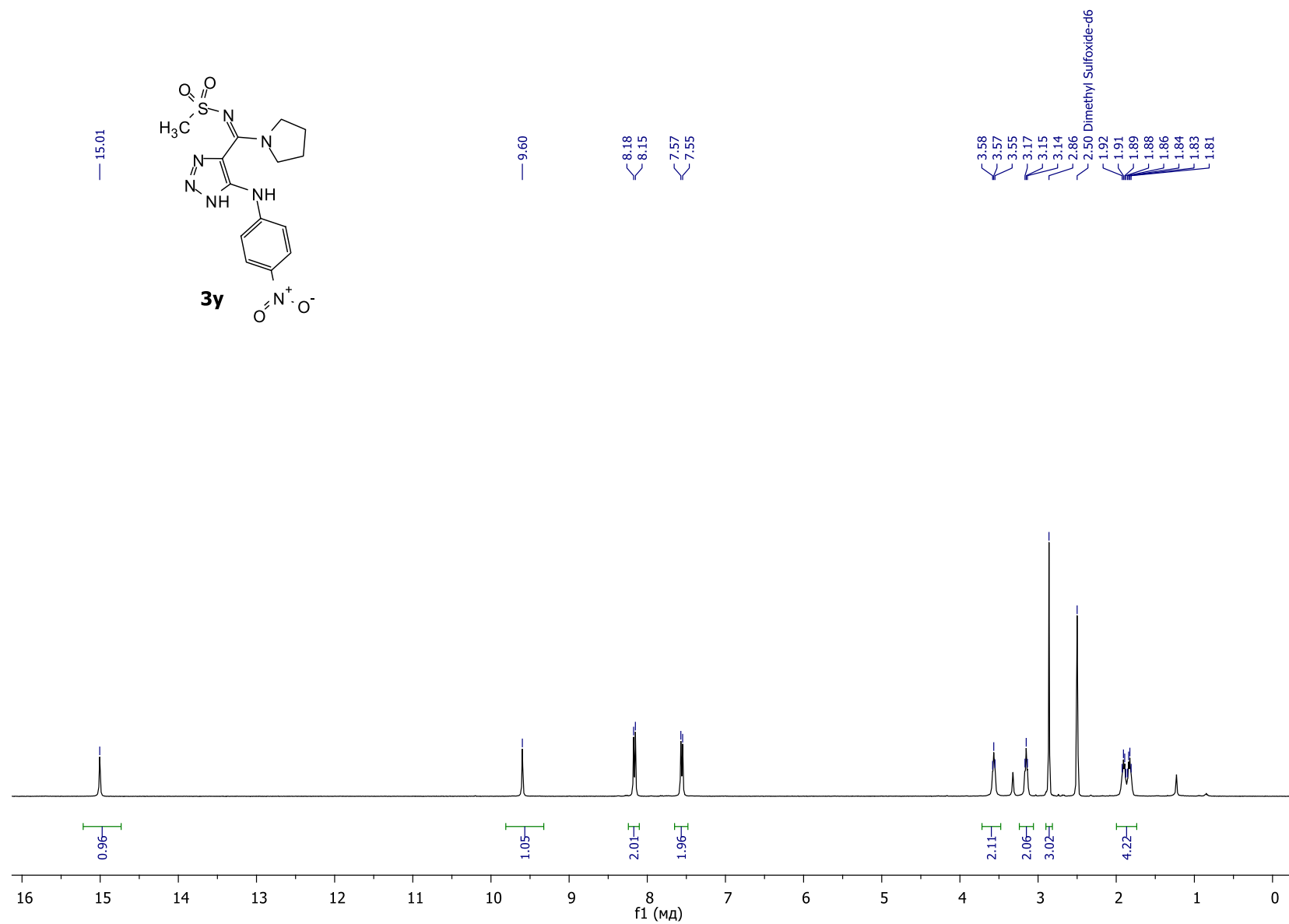
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3x**.



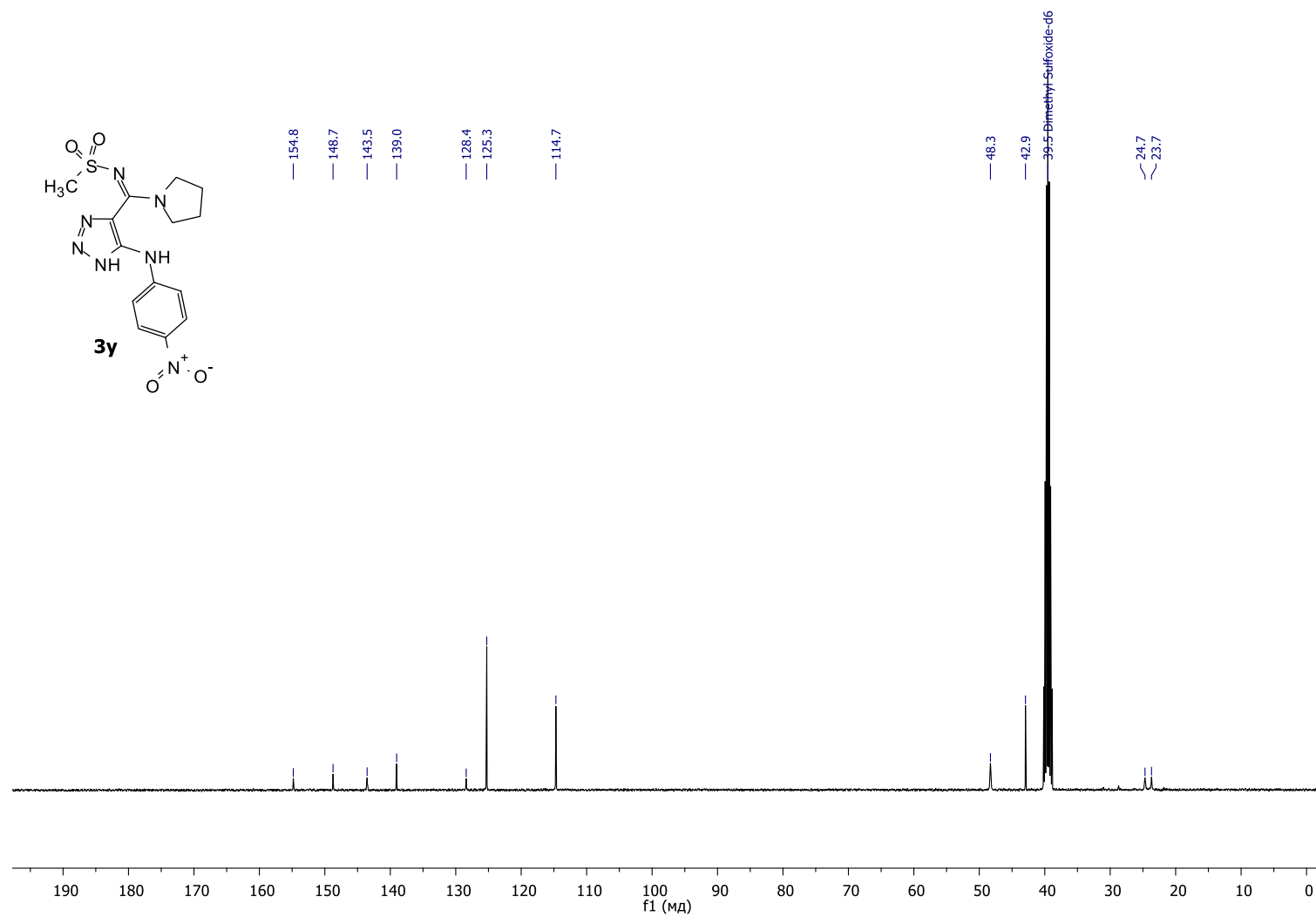
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3x**.



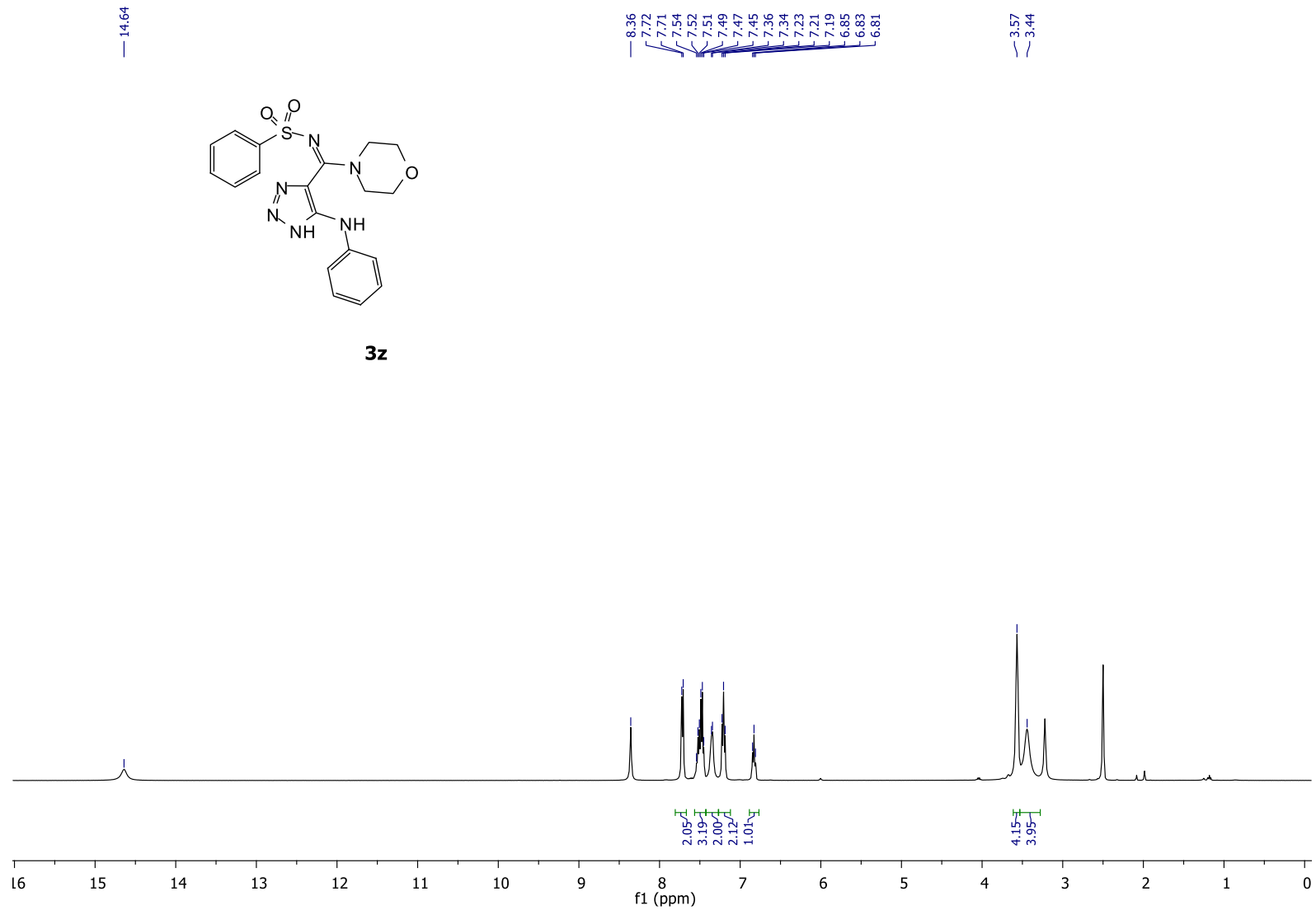
The HMBC NMR spectrum of compound **3x**.



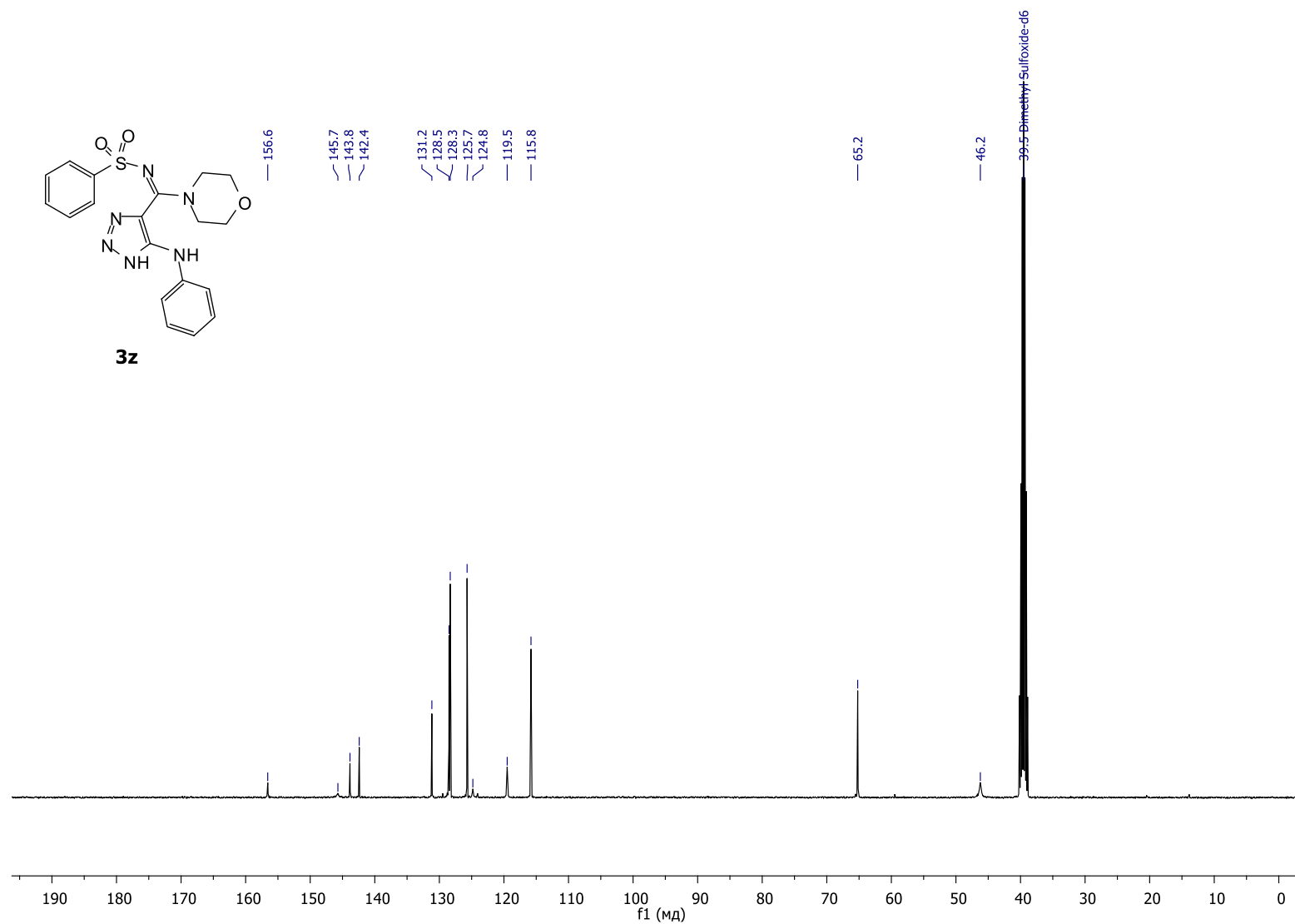
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3y**.



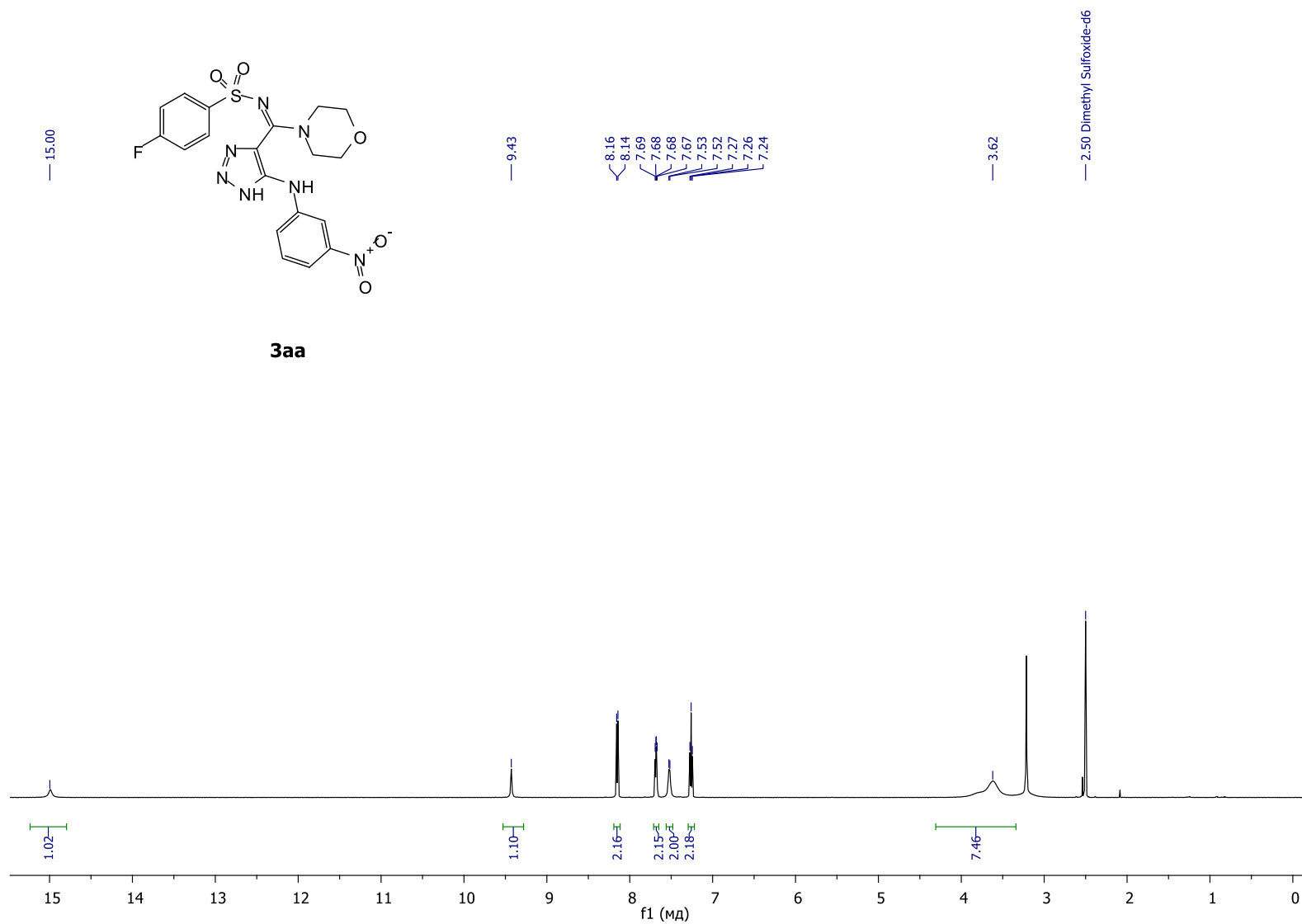
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3y**.



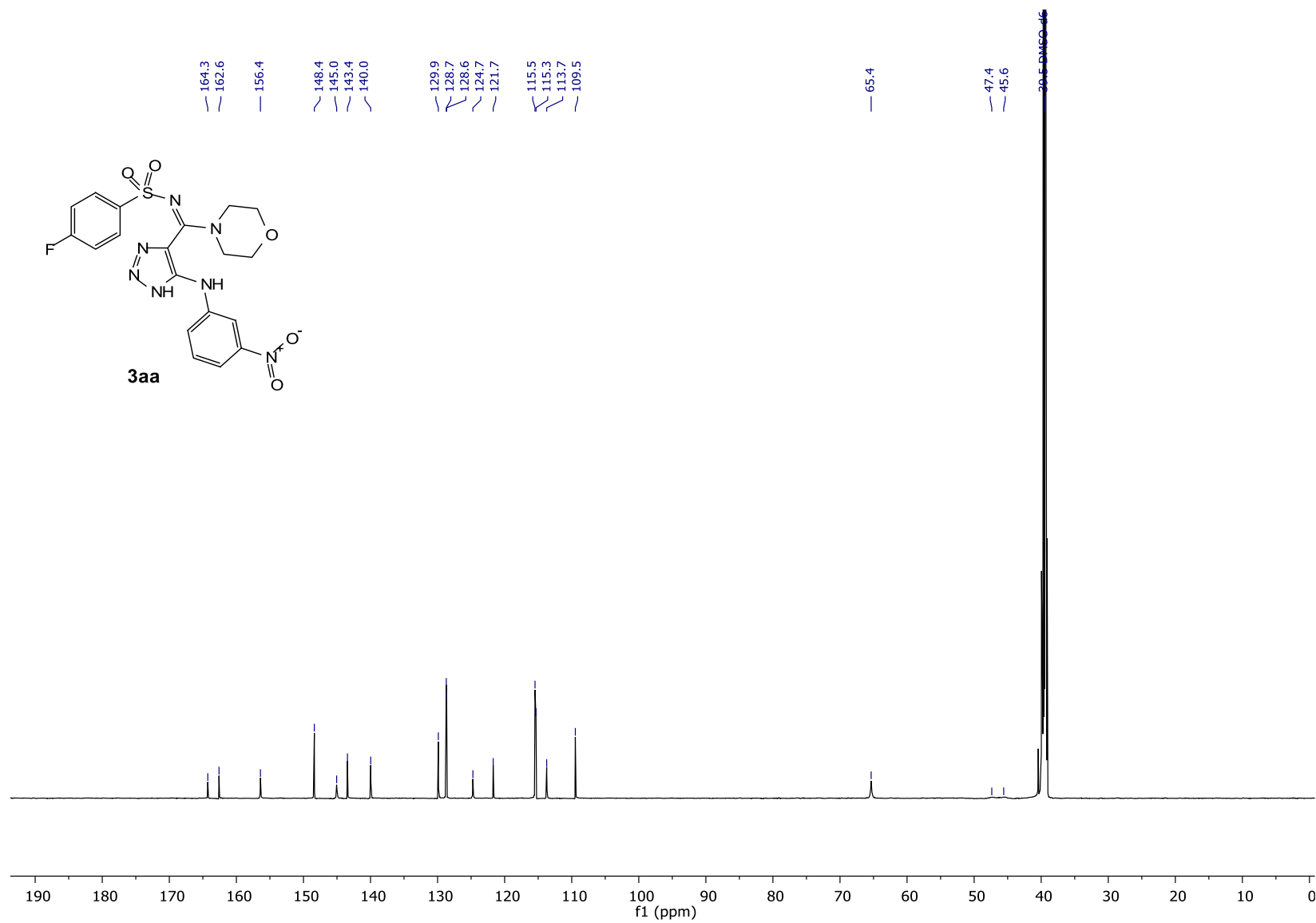
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3z**.



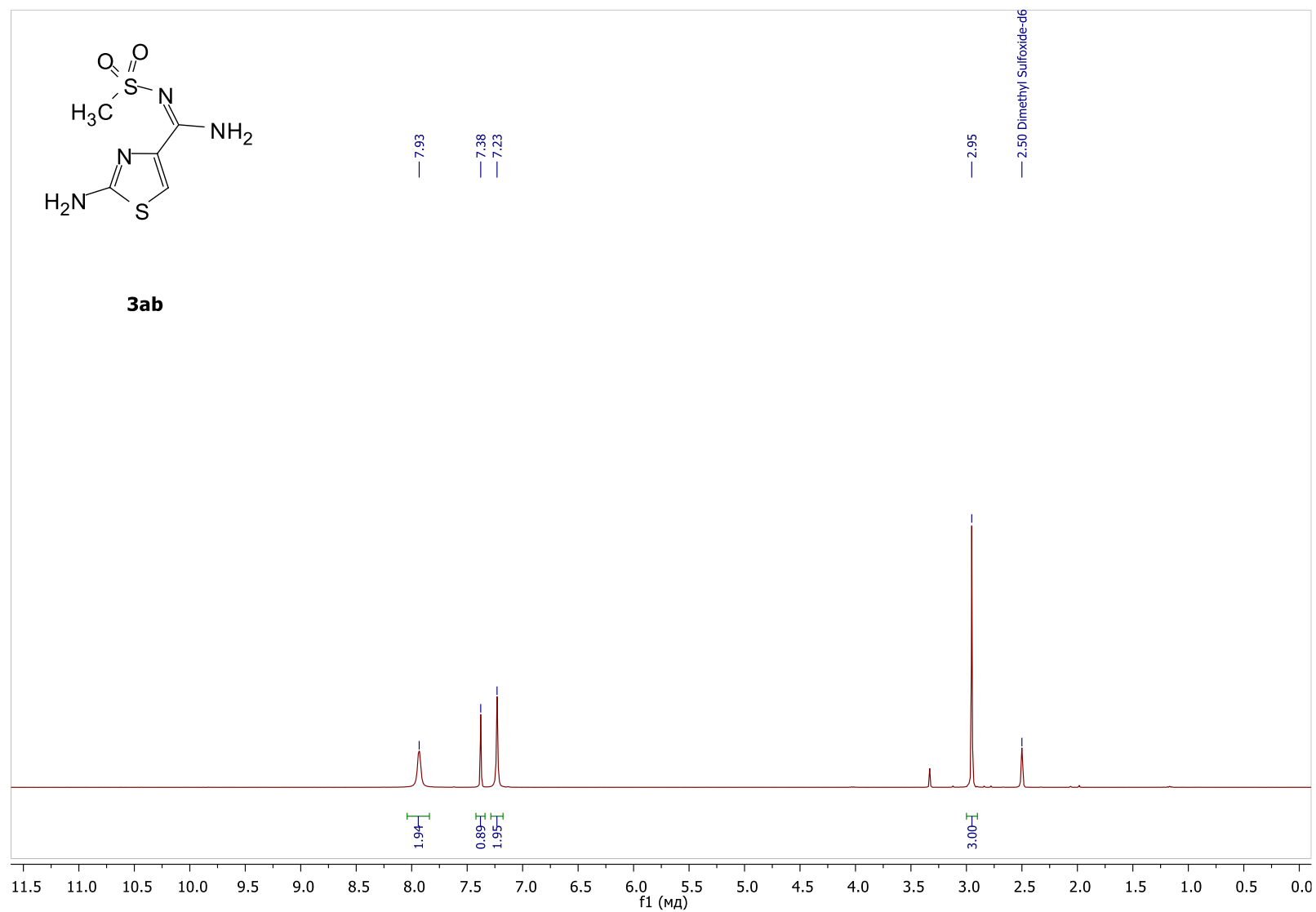
The ^{13}C NMR (100 MHz, DMSO- d_6 , 50 °C) spectrum of compound **3z**.



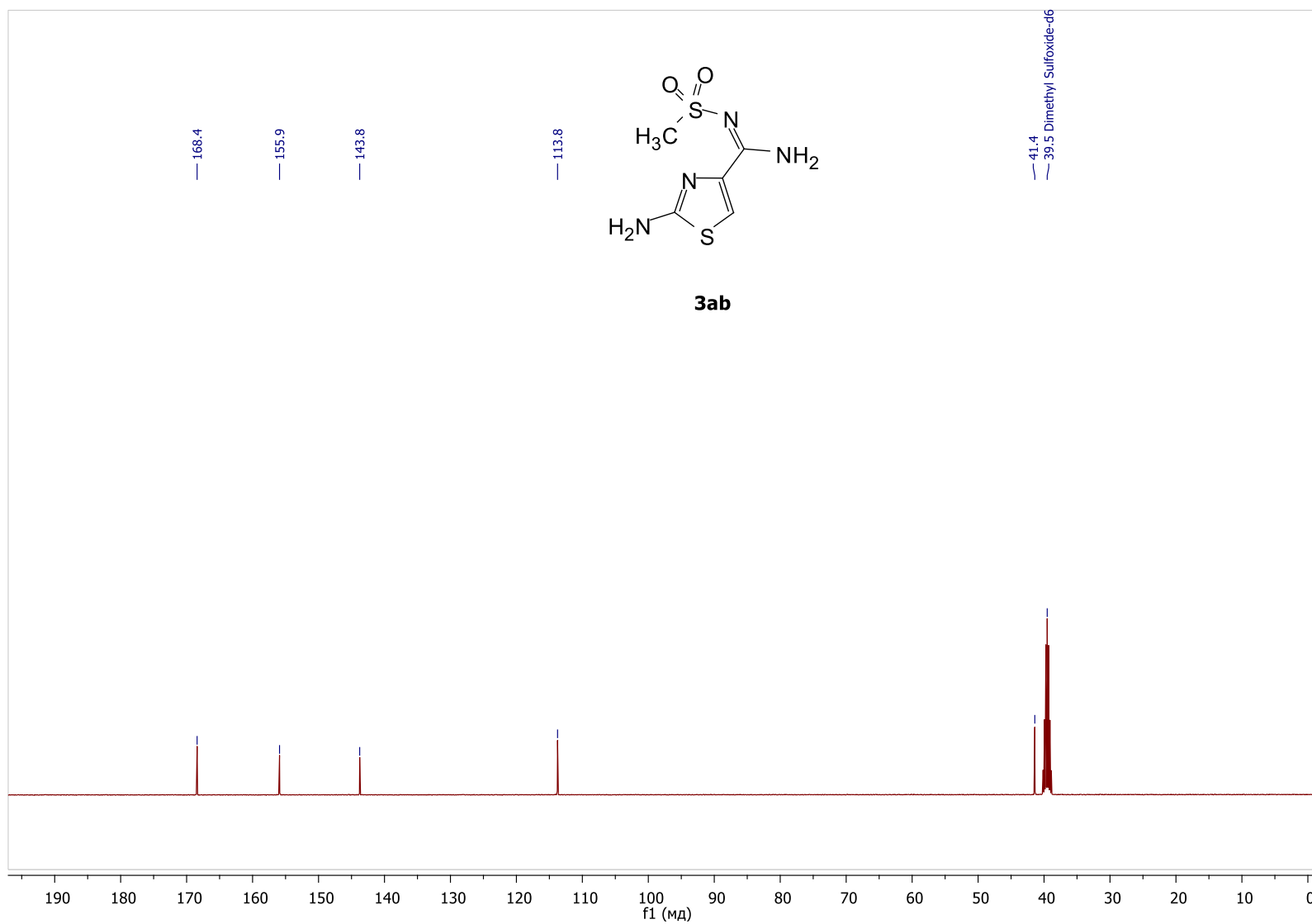
The ^1H NMR (400 MHz, DMSO- d_6) spectrum of compound **3aa**.



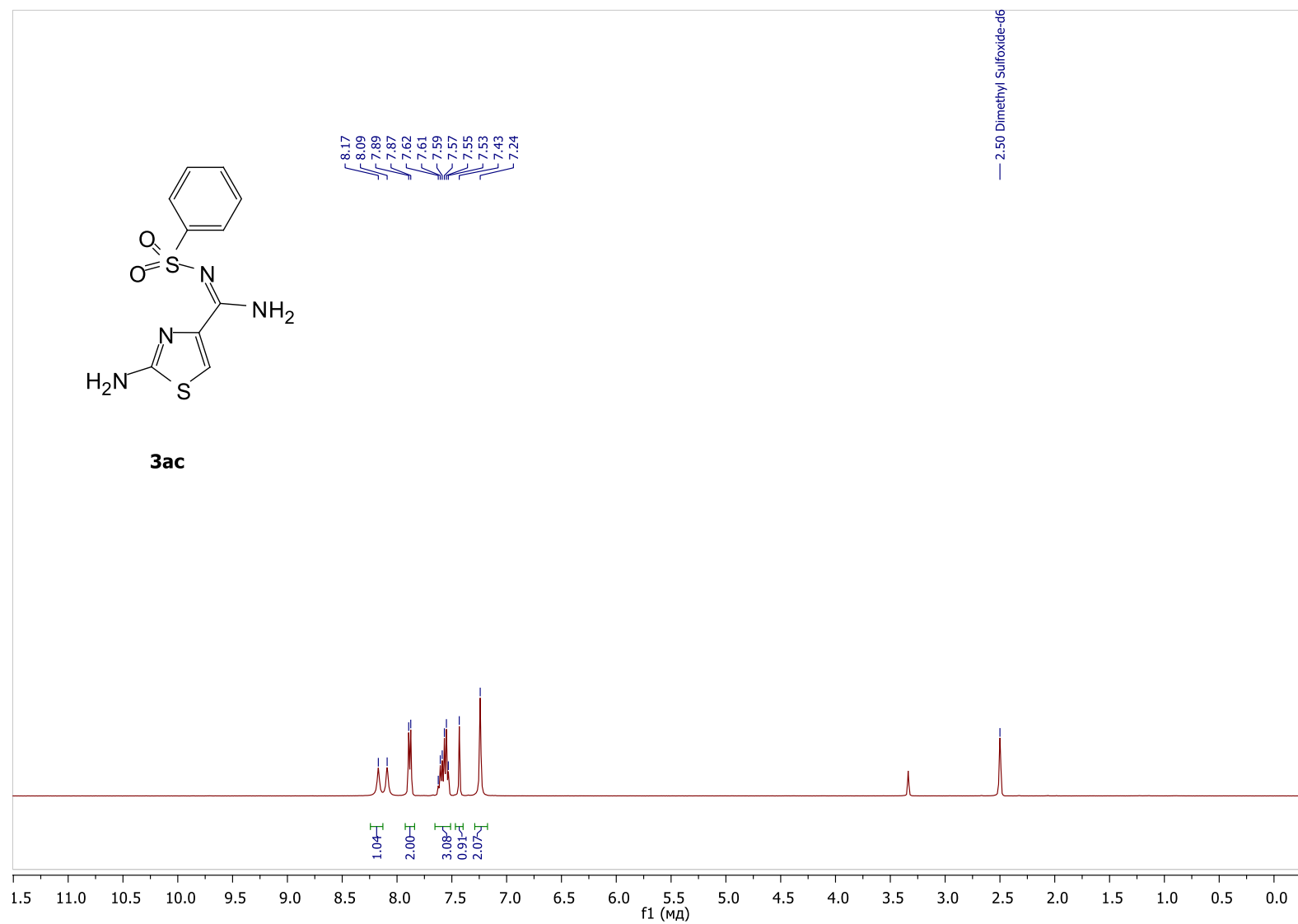
The ¹³C NMR (150 MHz, DMSO-*d*₆) spectrum of compound **3aa**.



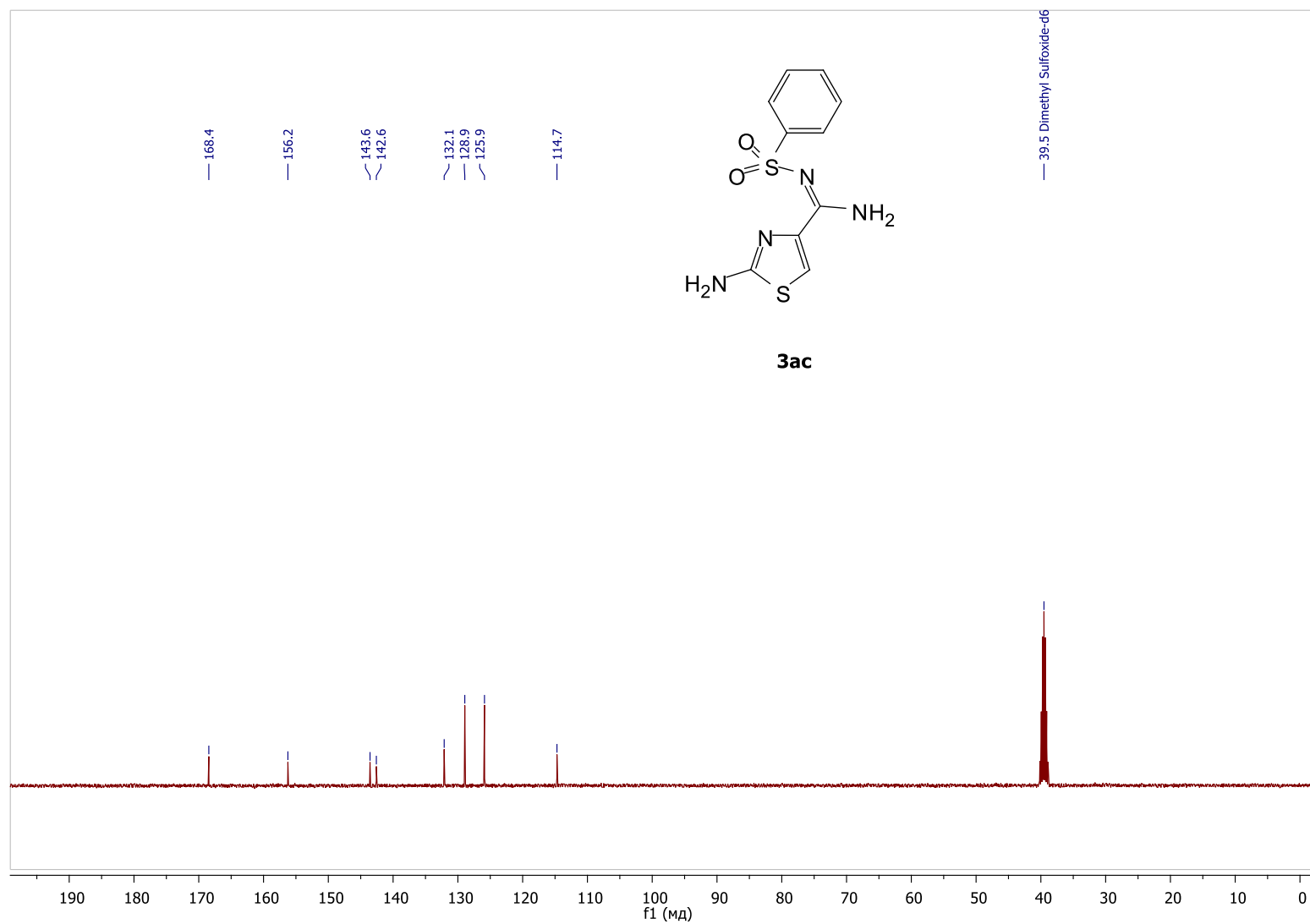
The ^1H NMR (400 MHz, DMSO- d_6) spectrum of compound **3ab**.



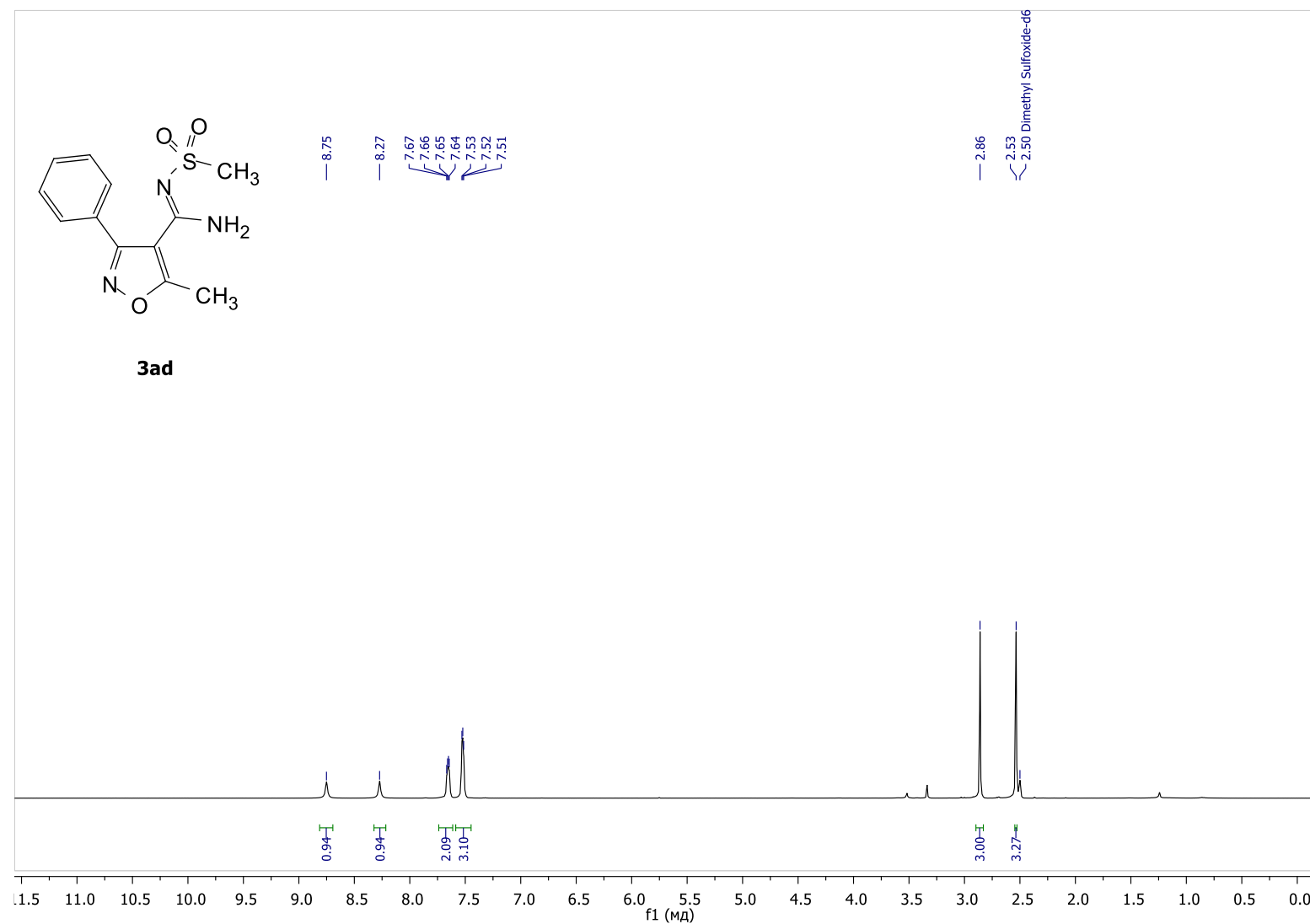
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3ab**.



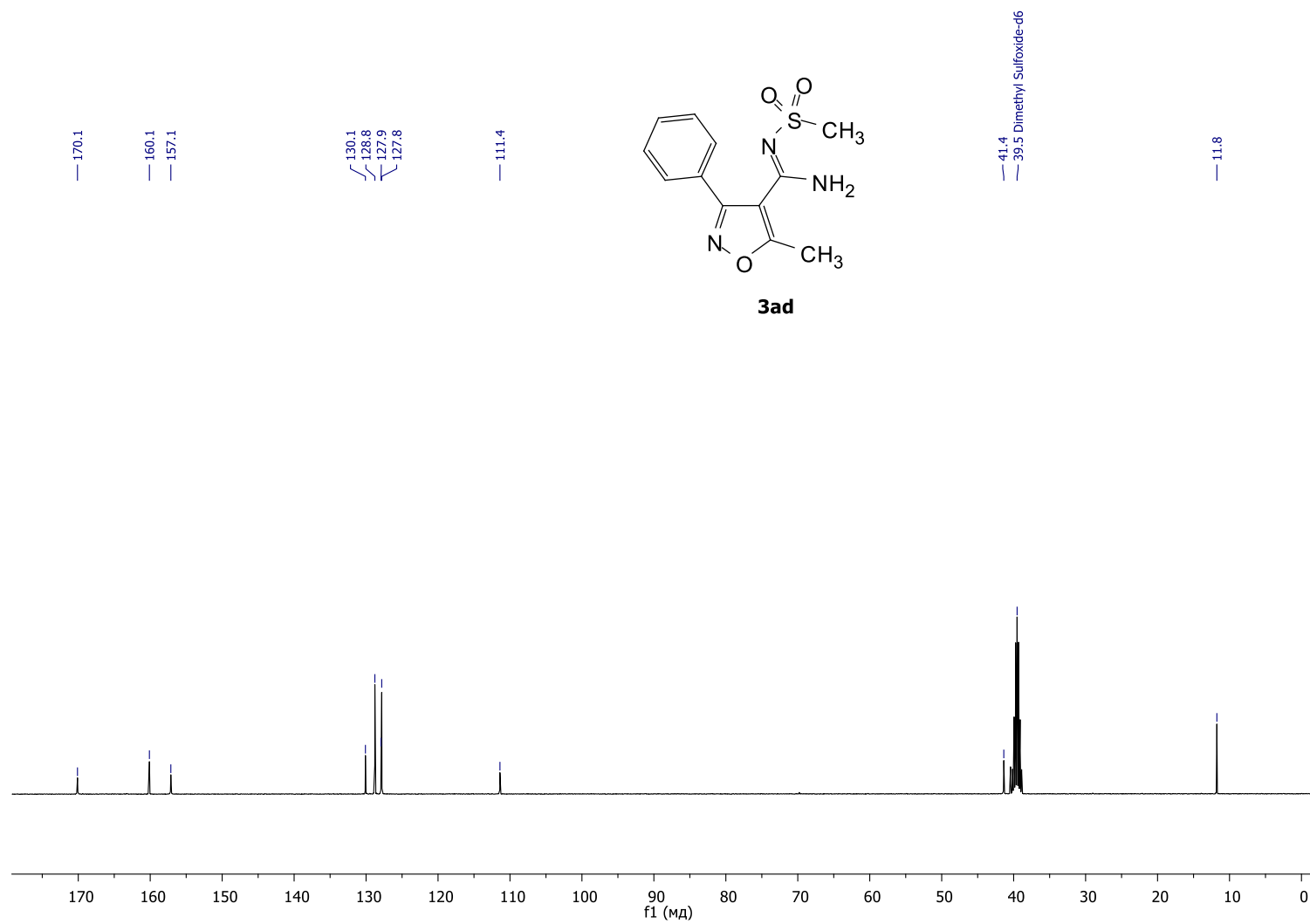
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3ac**.



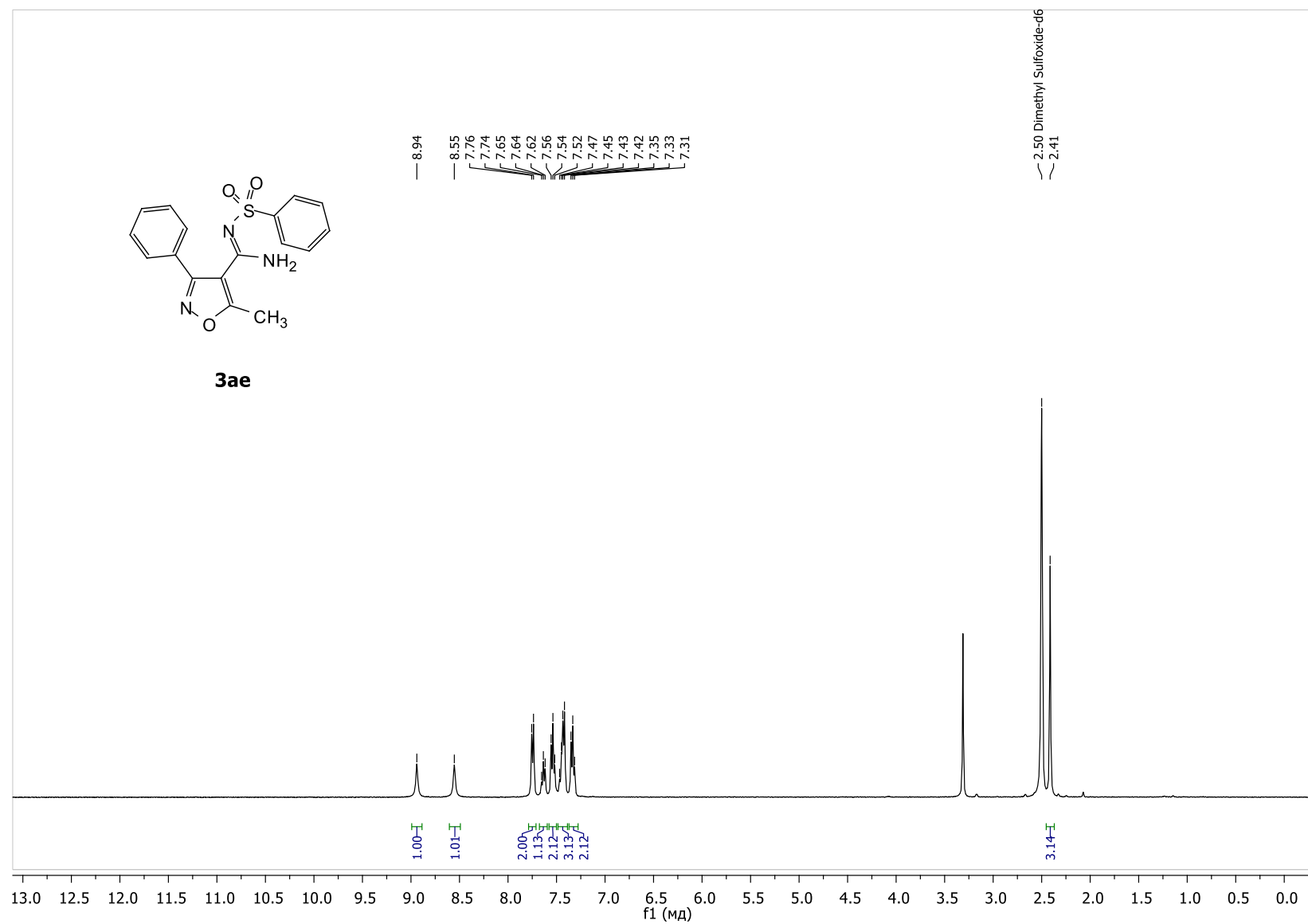
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3ac**.



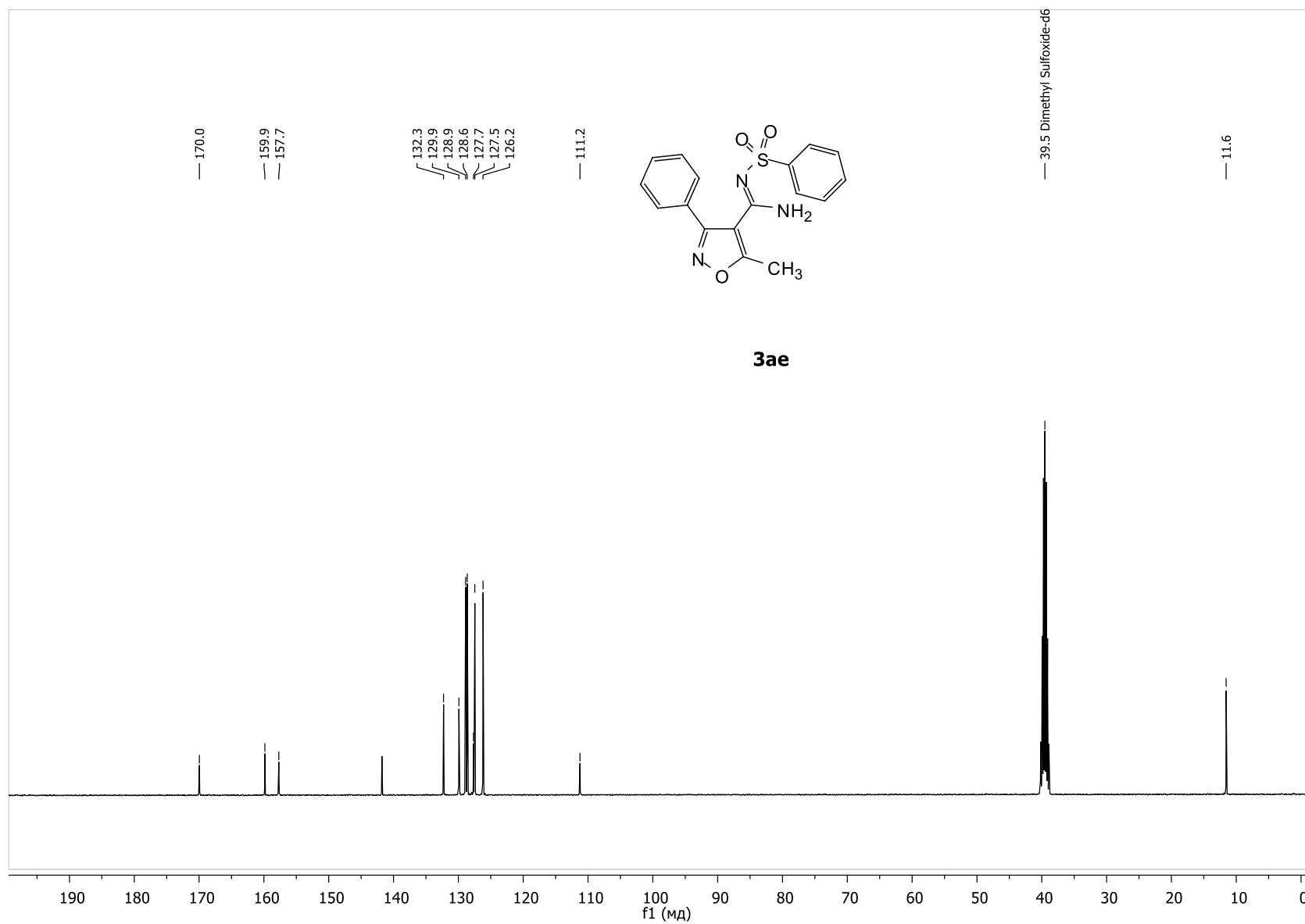
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **3ad**.



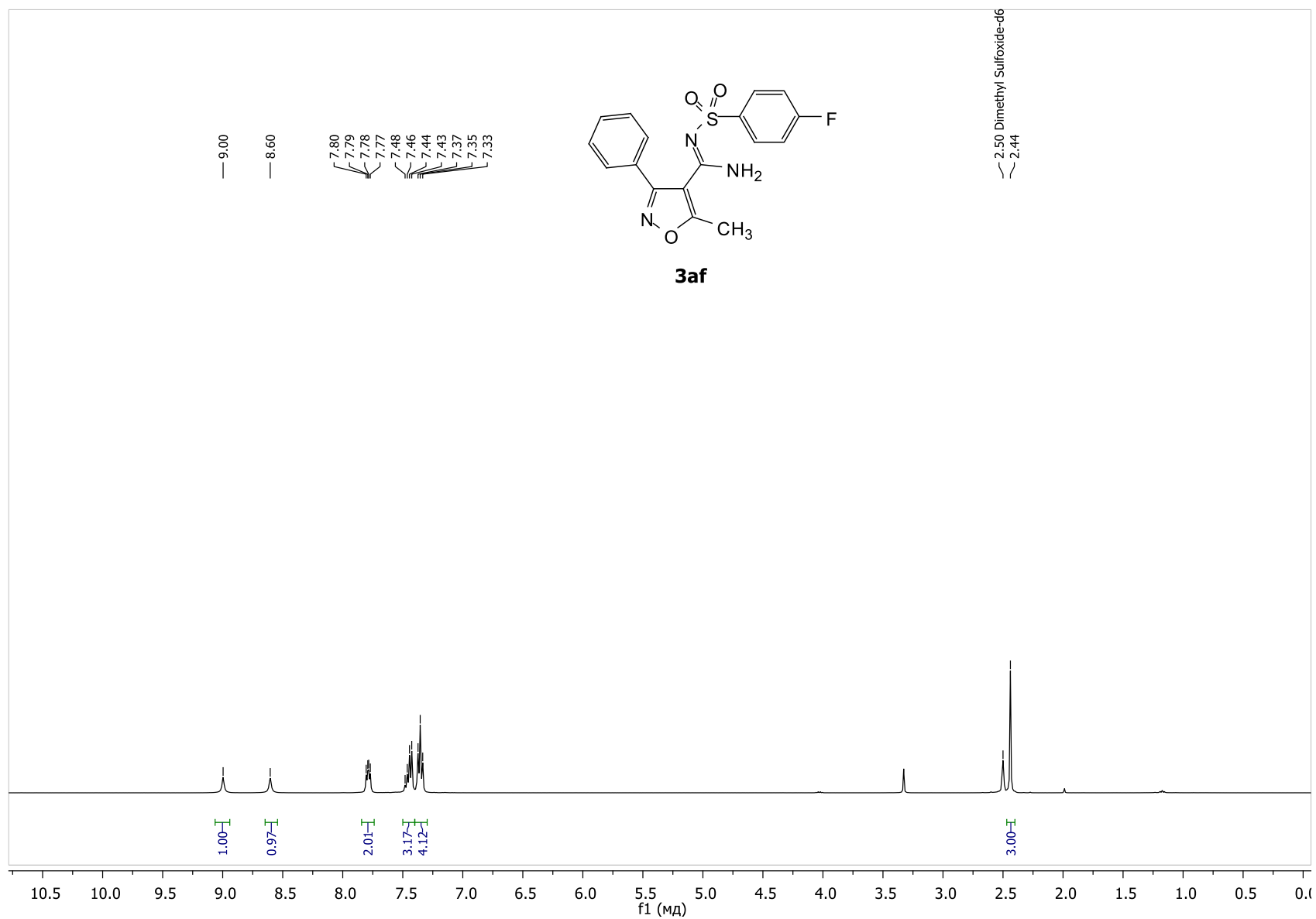
The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of compound **3ad**.



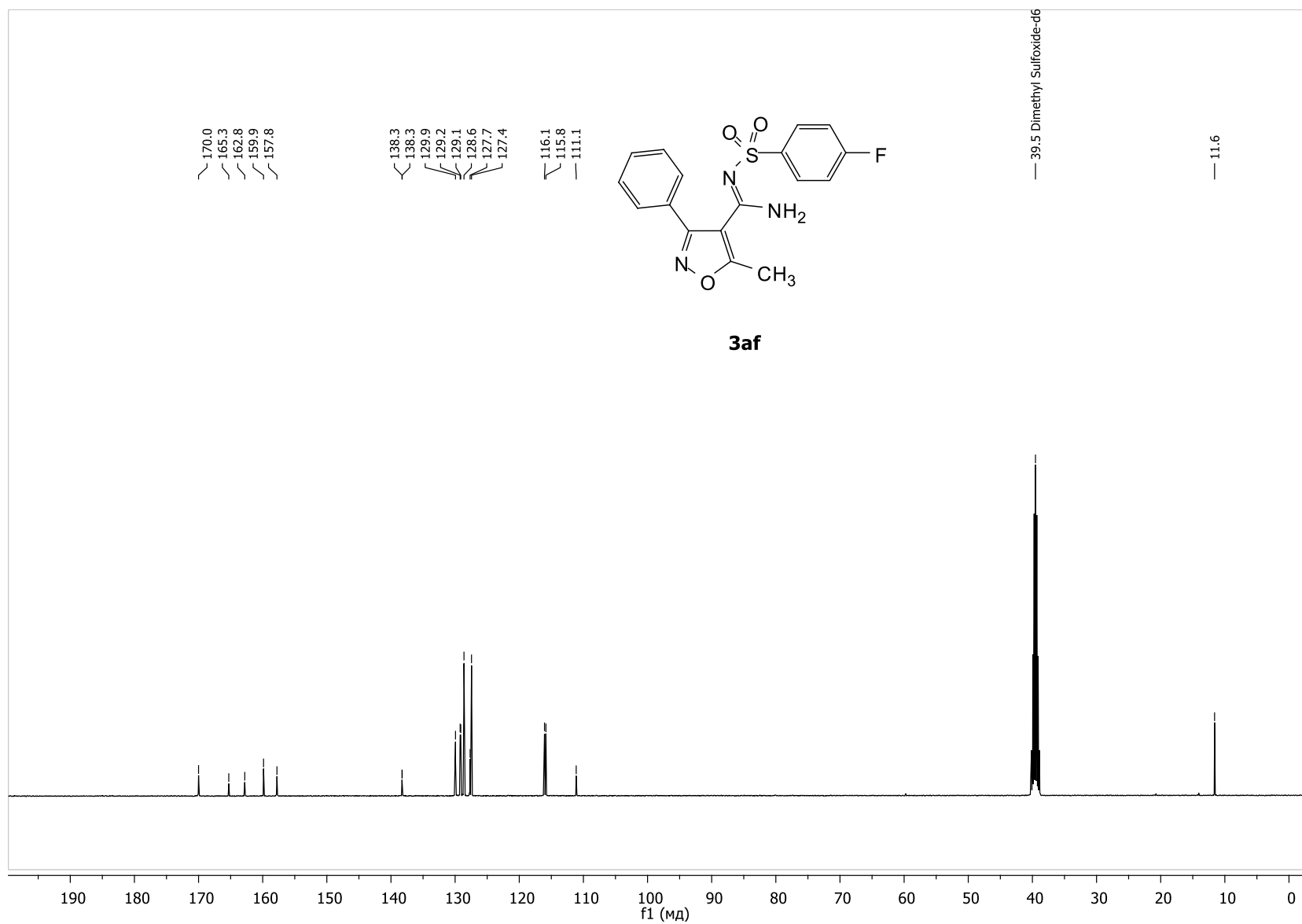
The ¹H NMR (400 MHz, DMSO-d₆) spectrum of compound **3ae**.



The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3ae**.

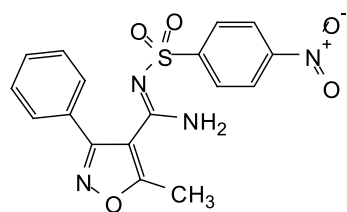


The ^1H NMR (400 MHz, DMSO- d_6) spectrum of compound **3af**.

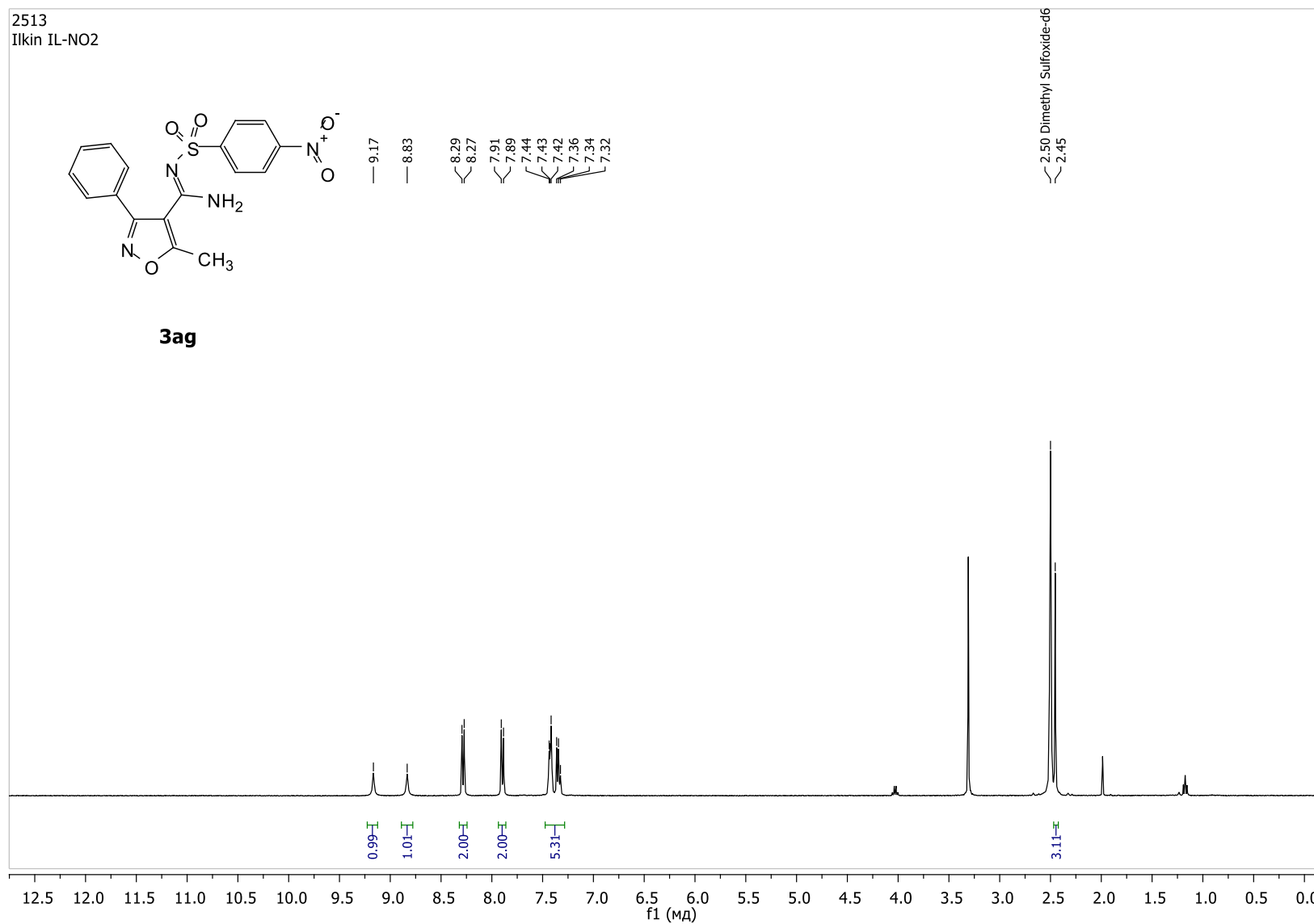


The ¹³C NMR (100 MHz, DMSO-d₆) spectrum of compound **3af**.

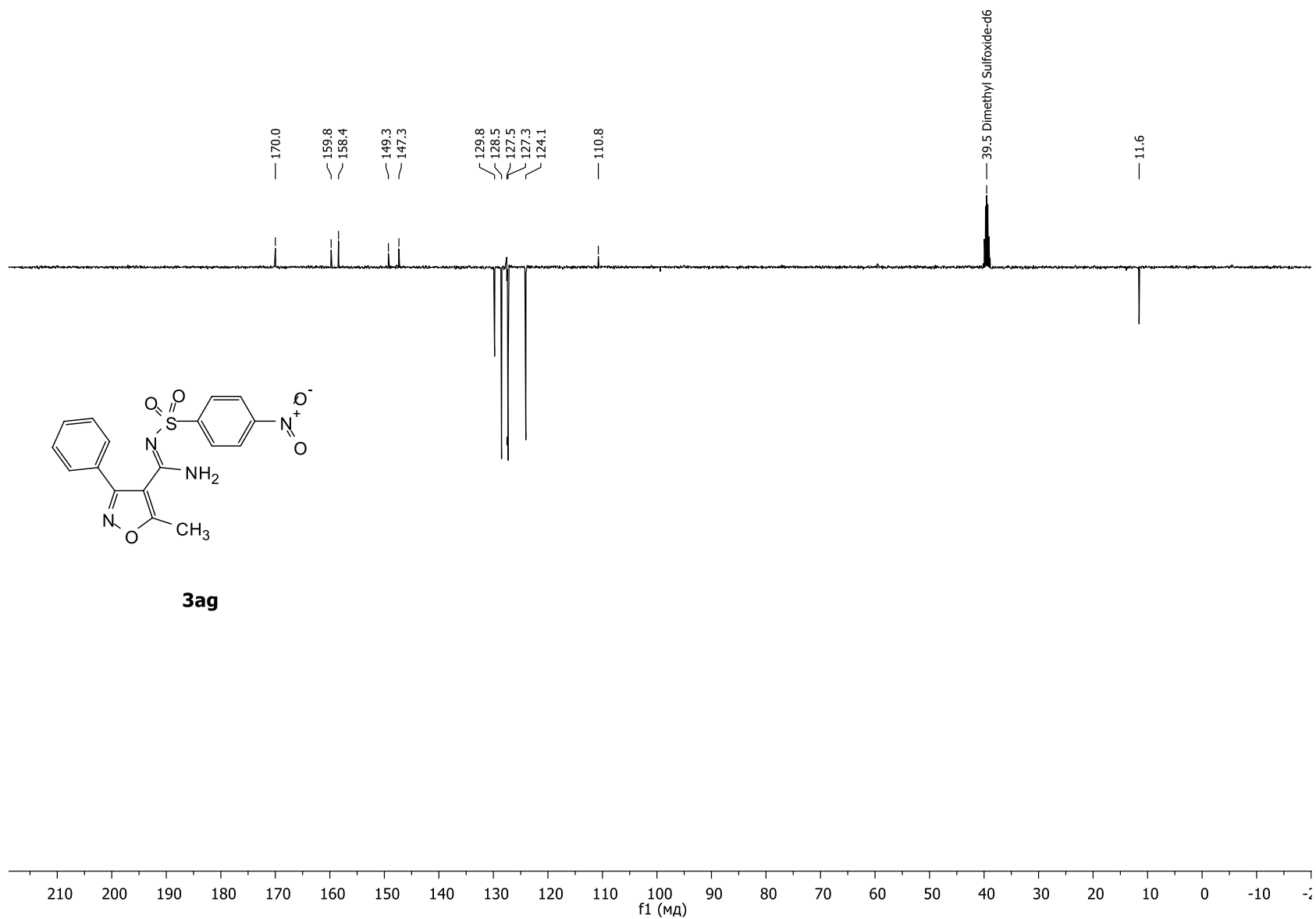
2513
Ilkin IL-NO2



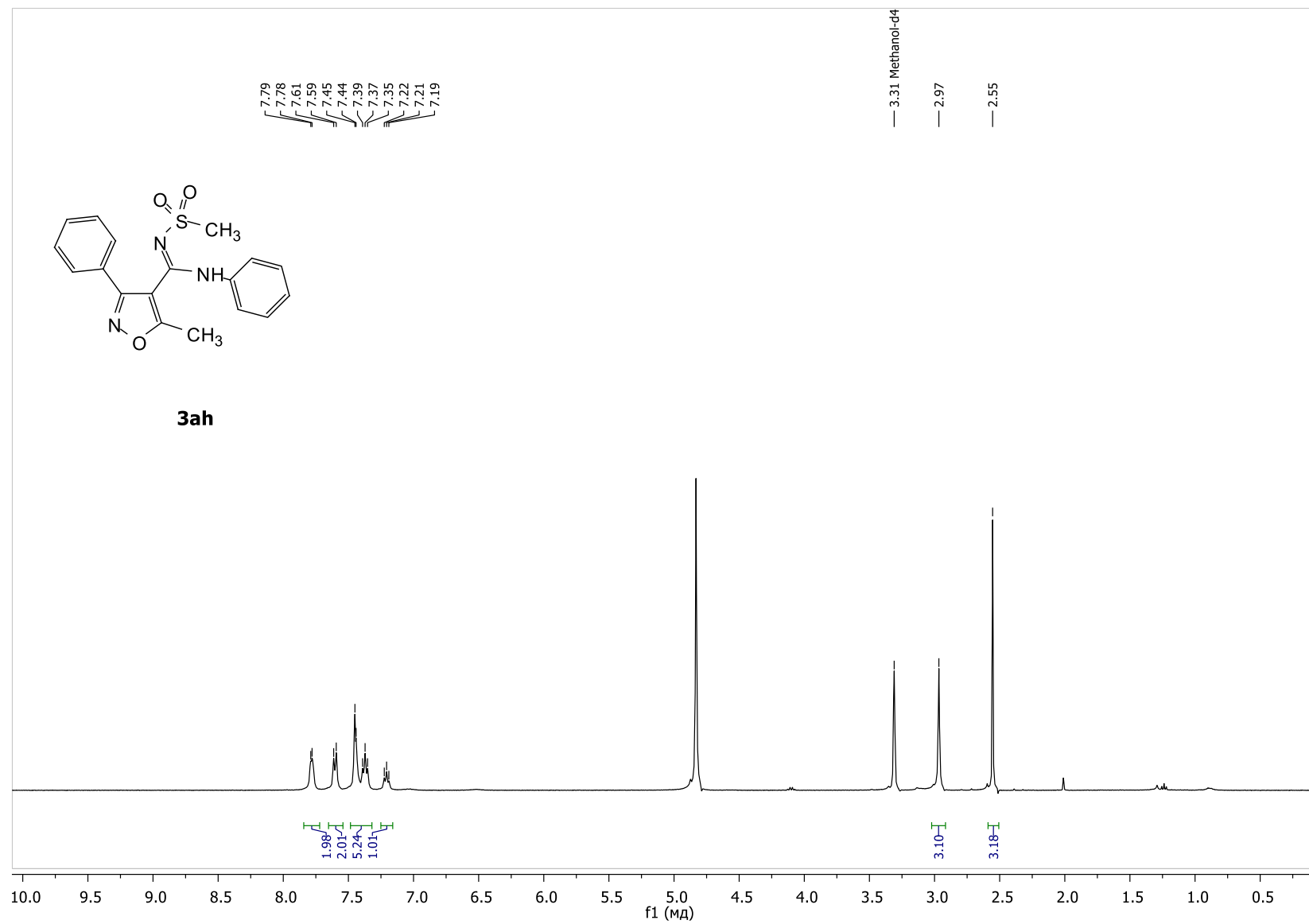
3ag



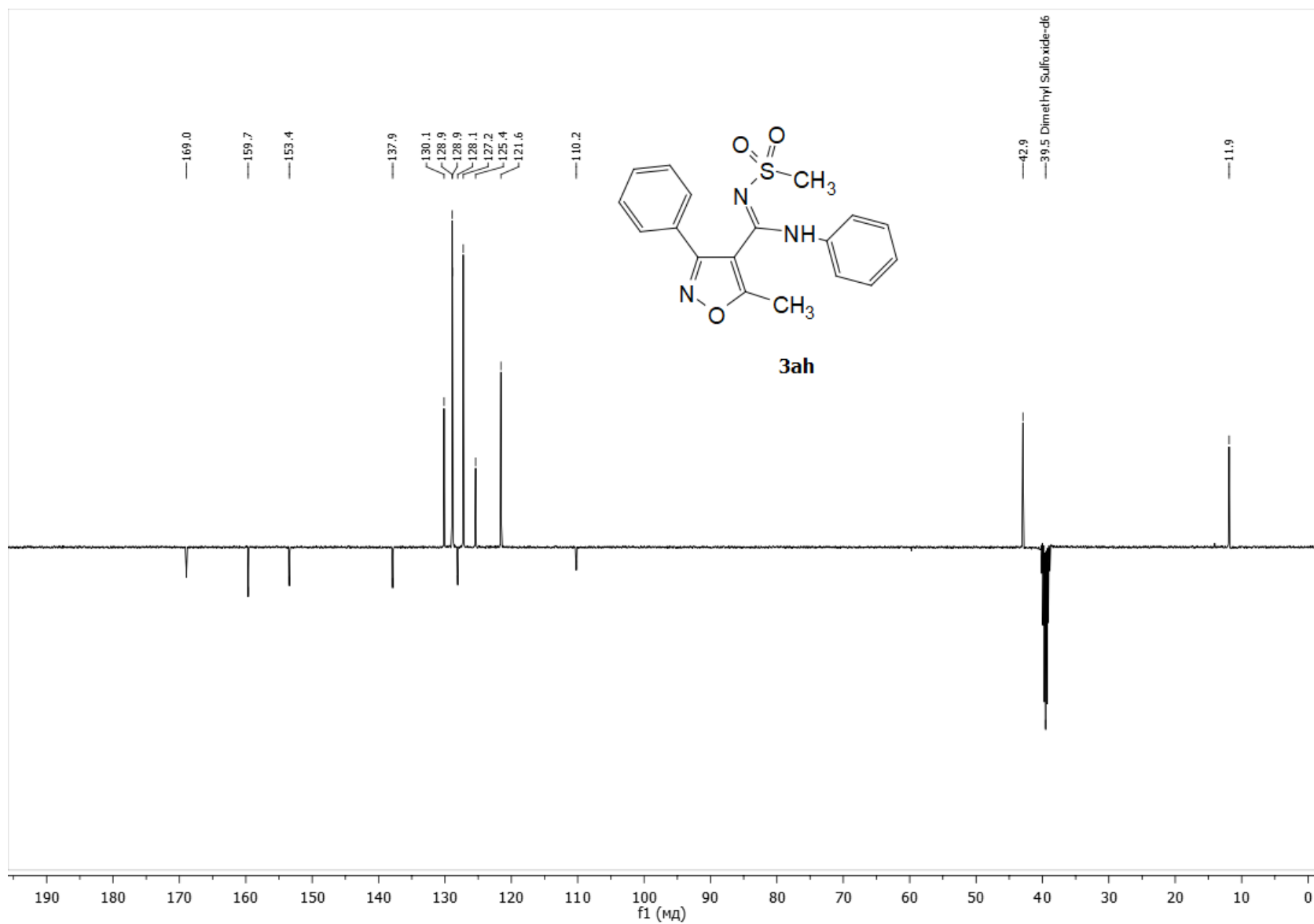
The ^1H NMR (400 MHz, DMSO-d_6) spectrum of compound **3ag**.



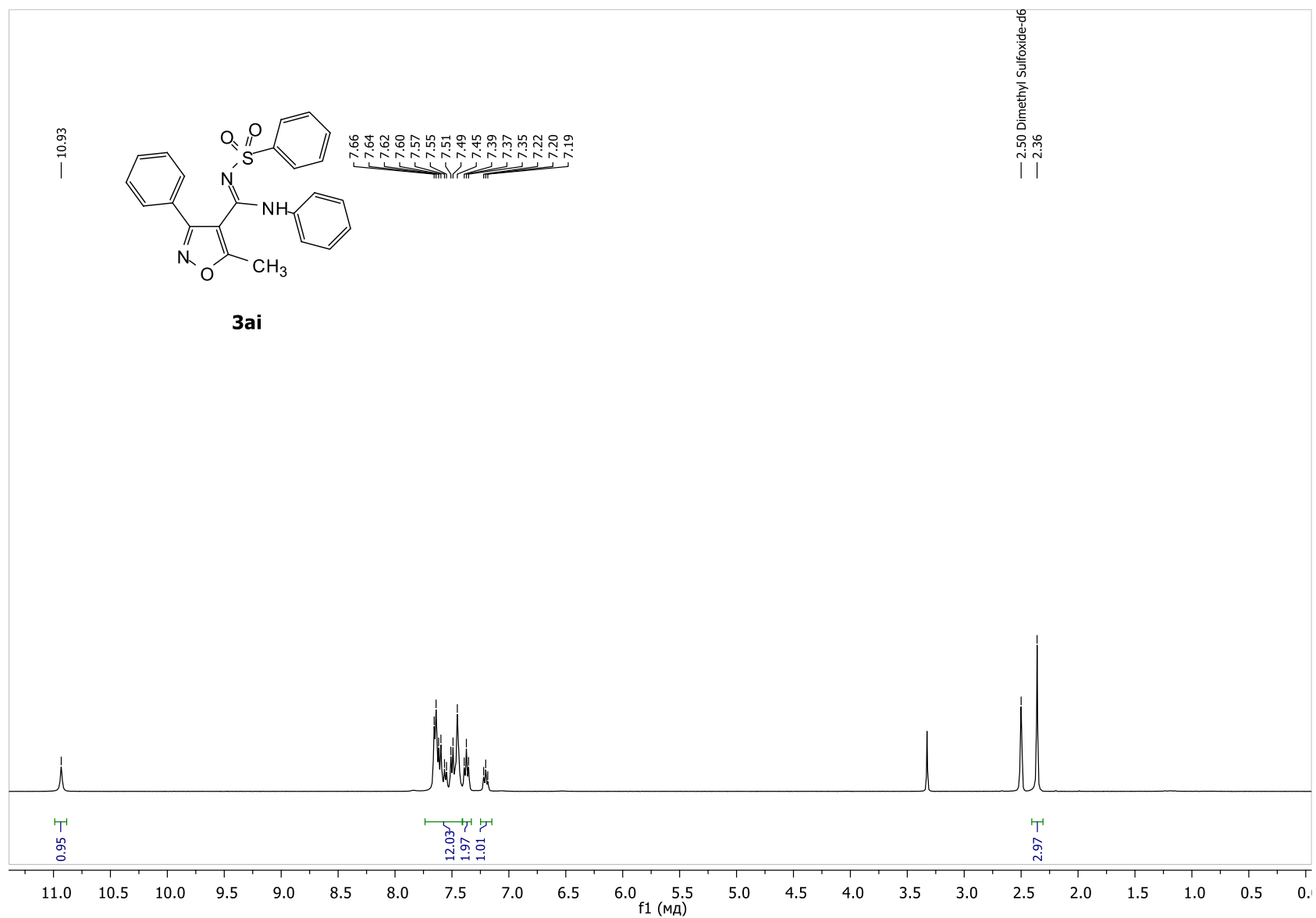
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3ag**.



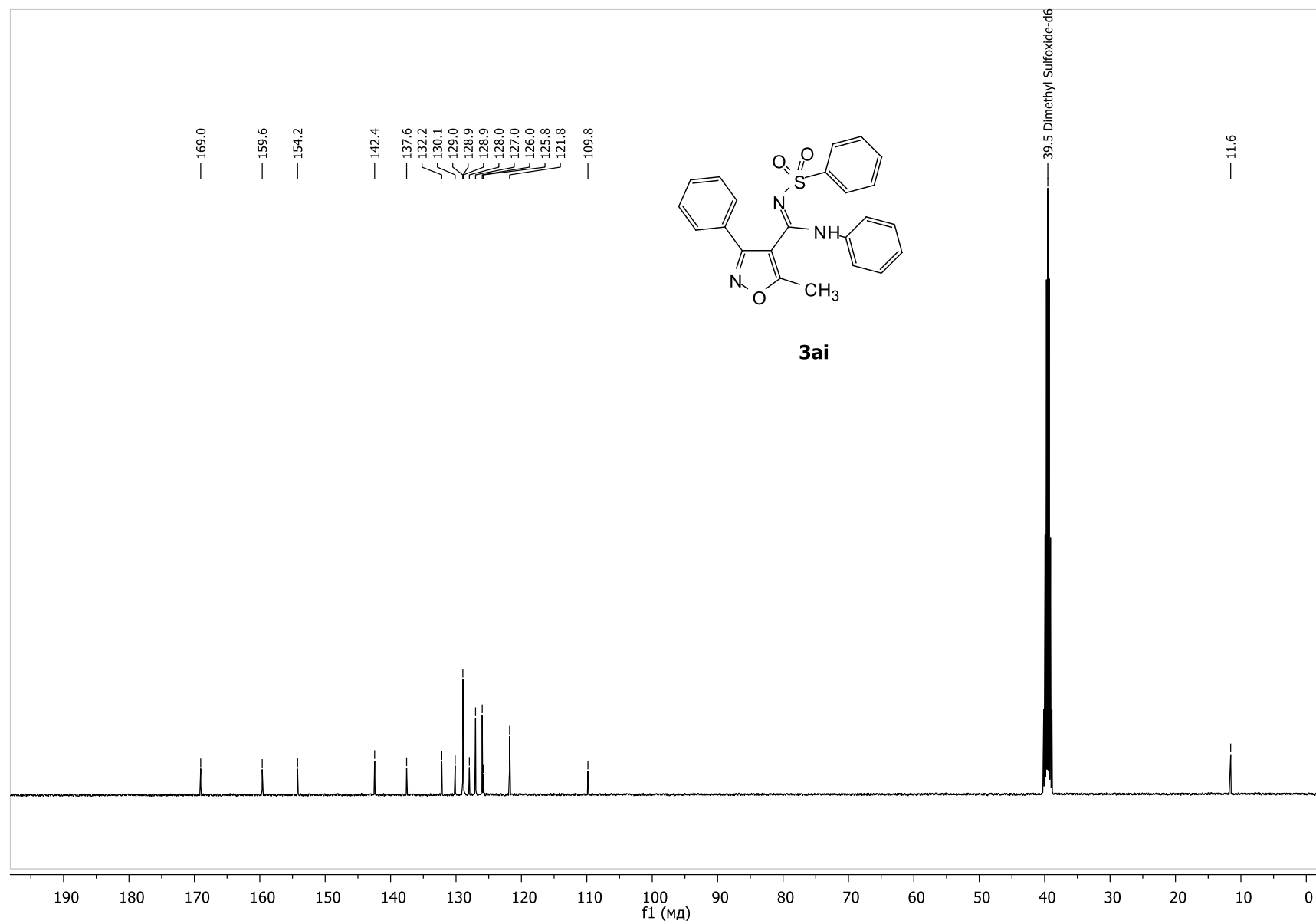
The ¹H NMR (400 MHz, CD₃OD) spectrum of compound **3ah**.



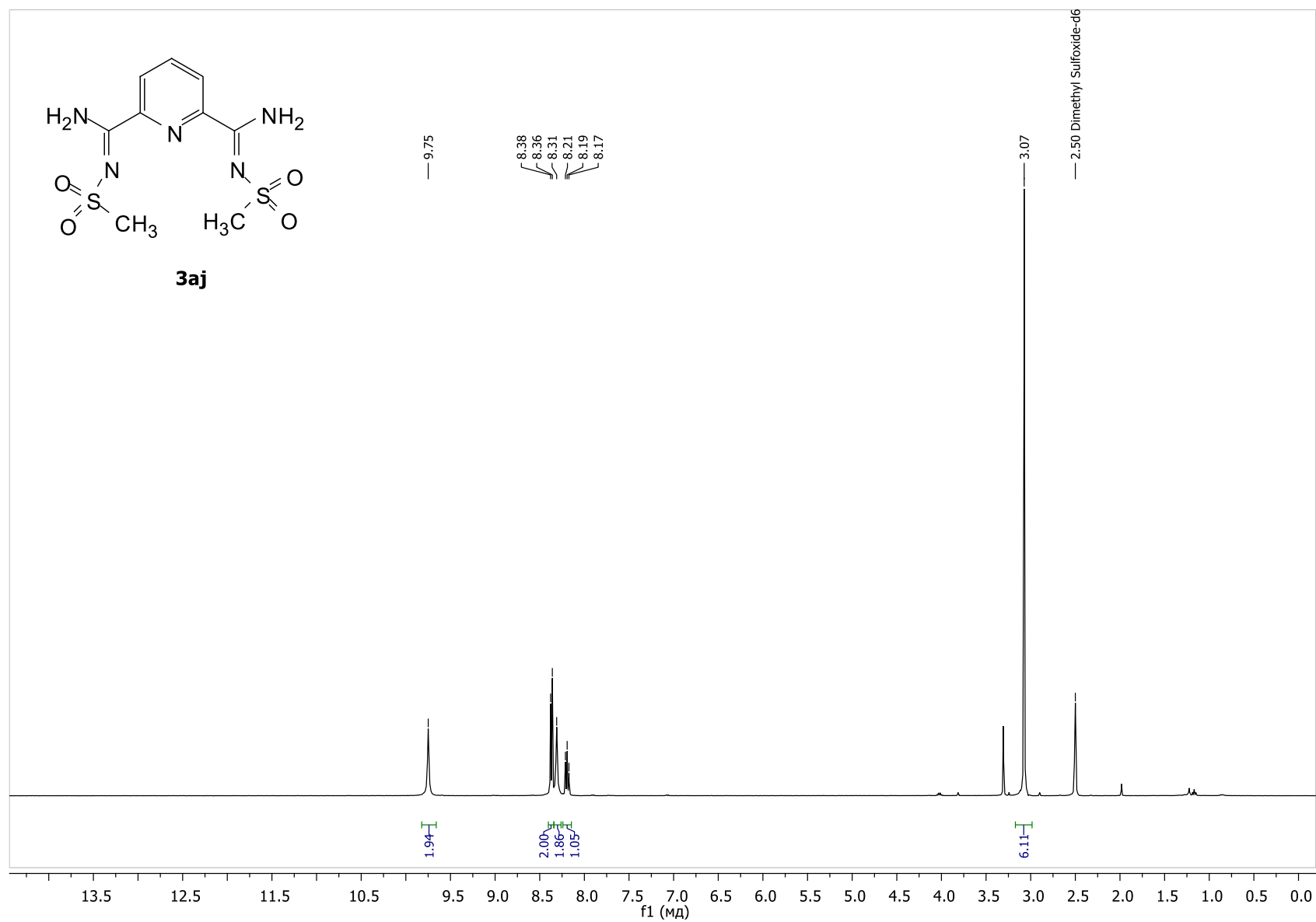
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3ah**.



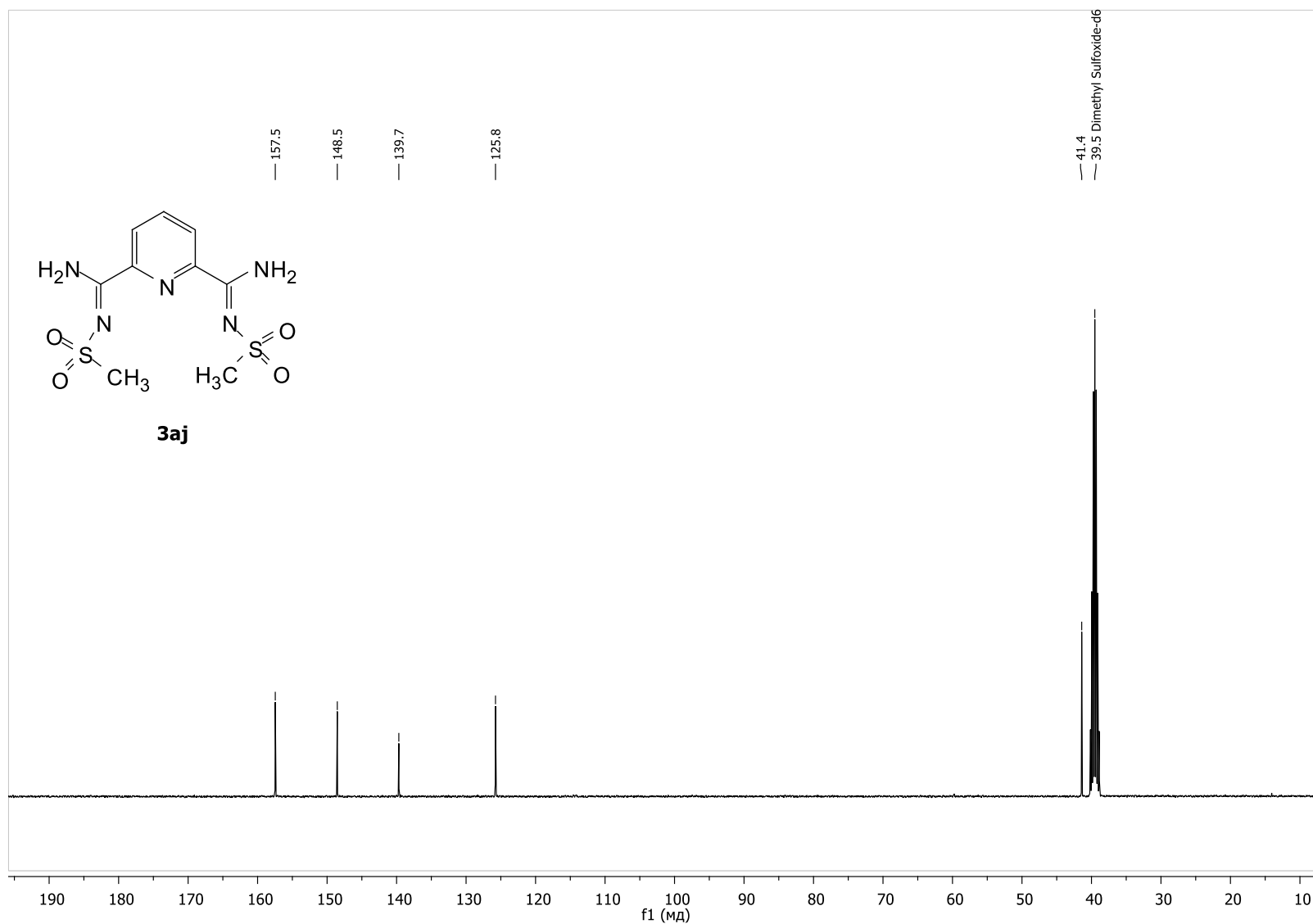
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3ai**.



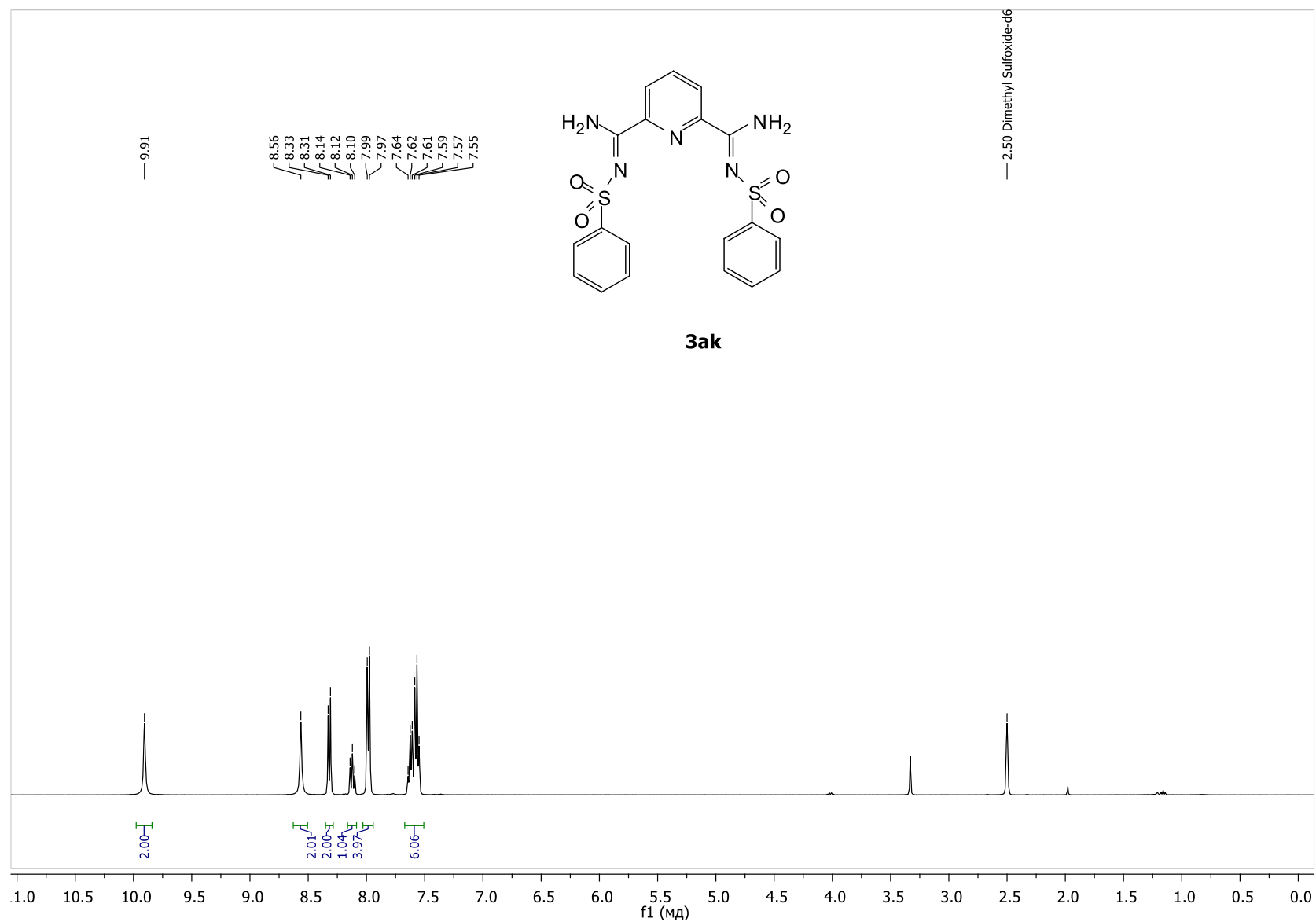
The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of compound **3ai**.



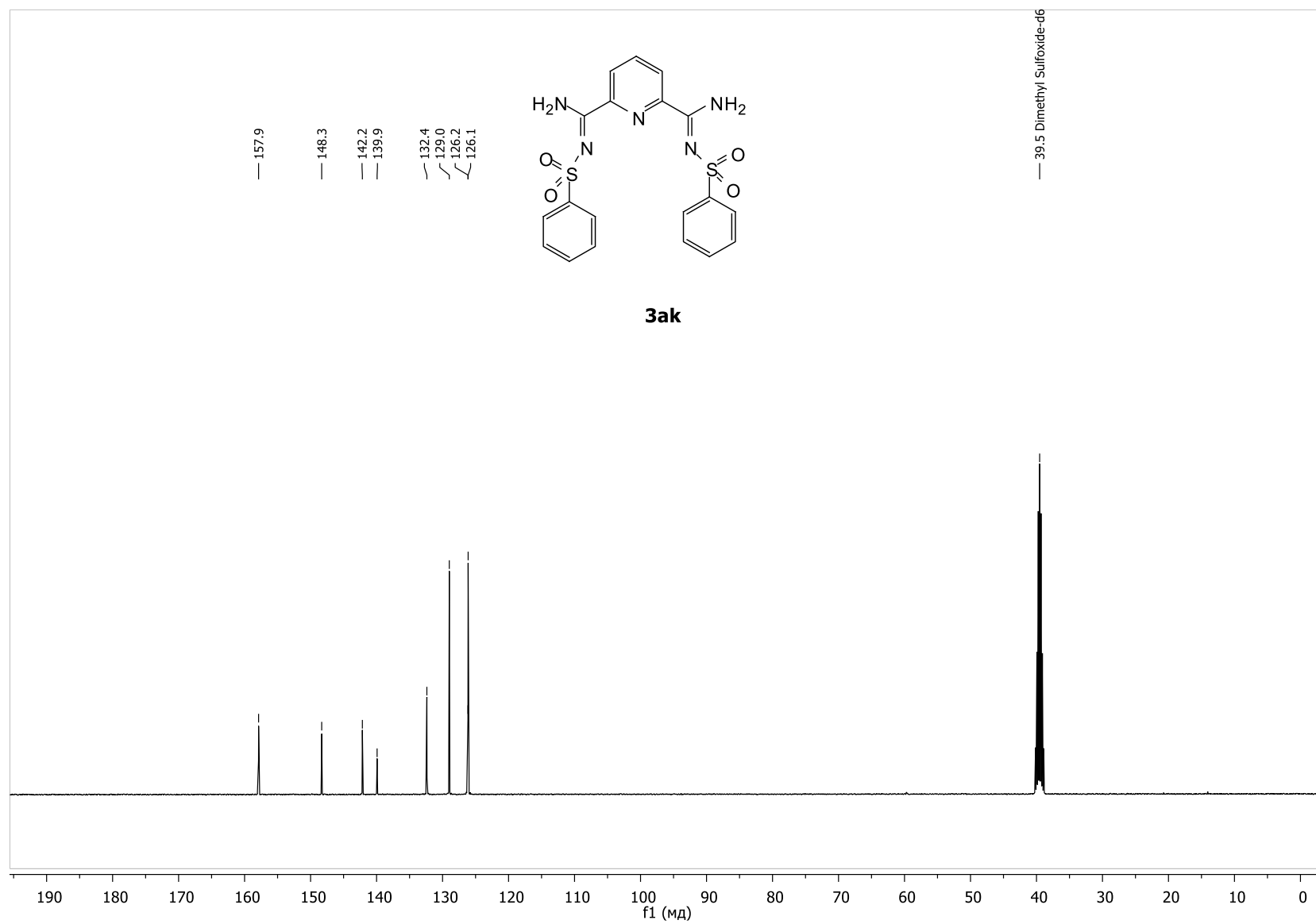
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3aj**.



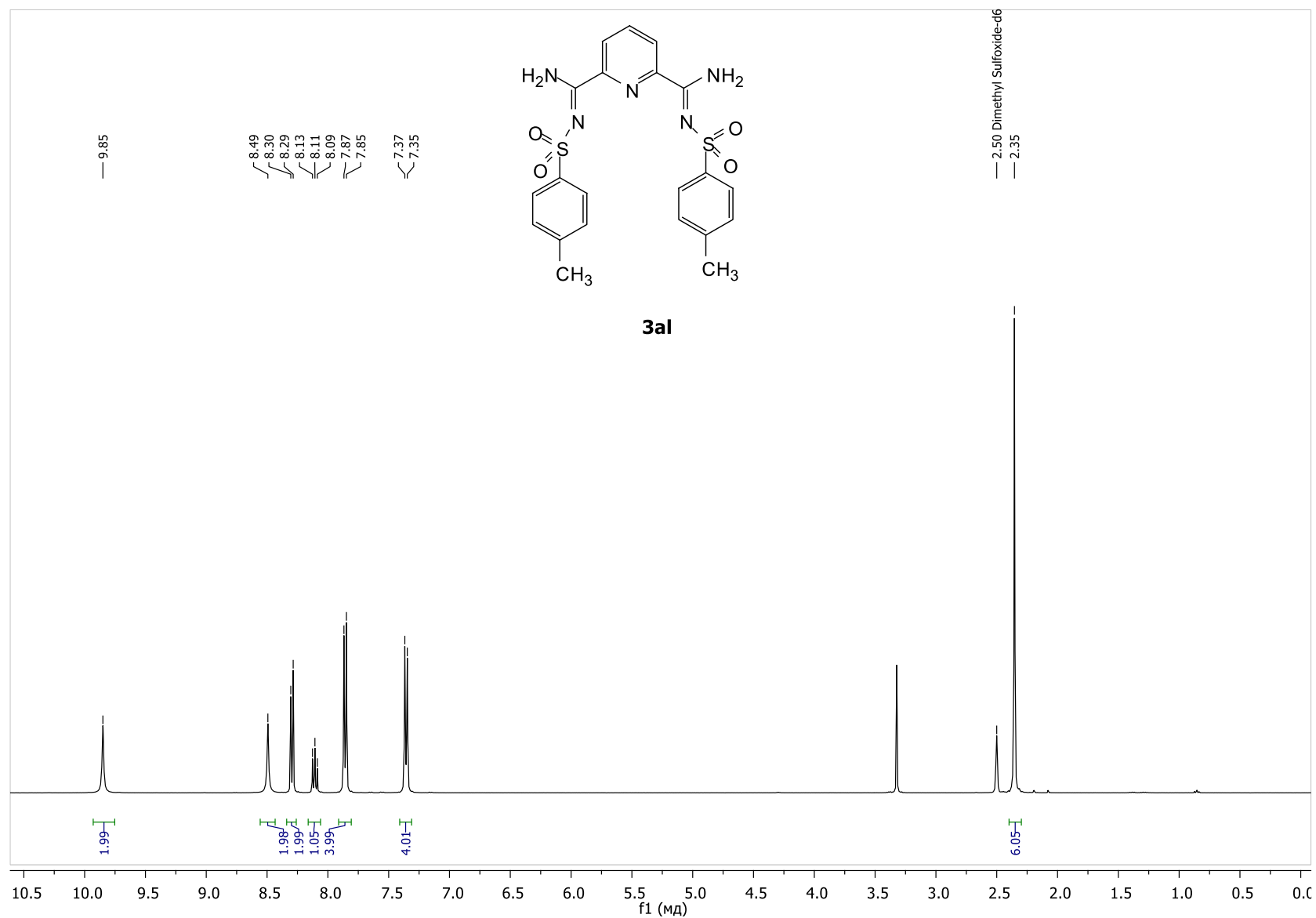
The ¹³C NMR (100 MHz, DMSO-d₆) spectrum of compound **3aj**.



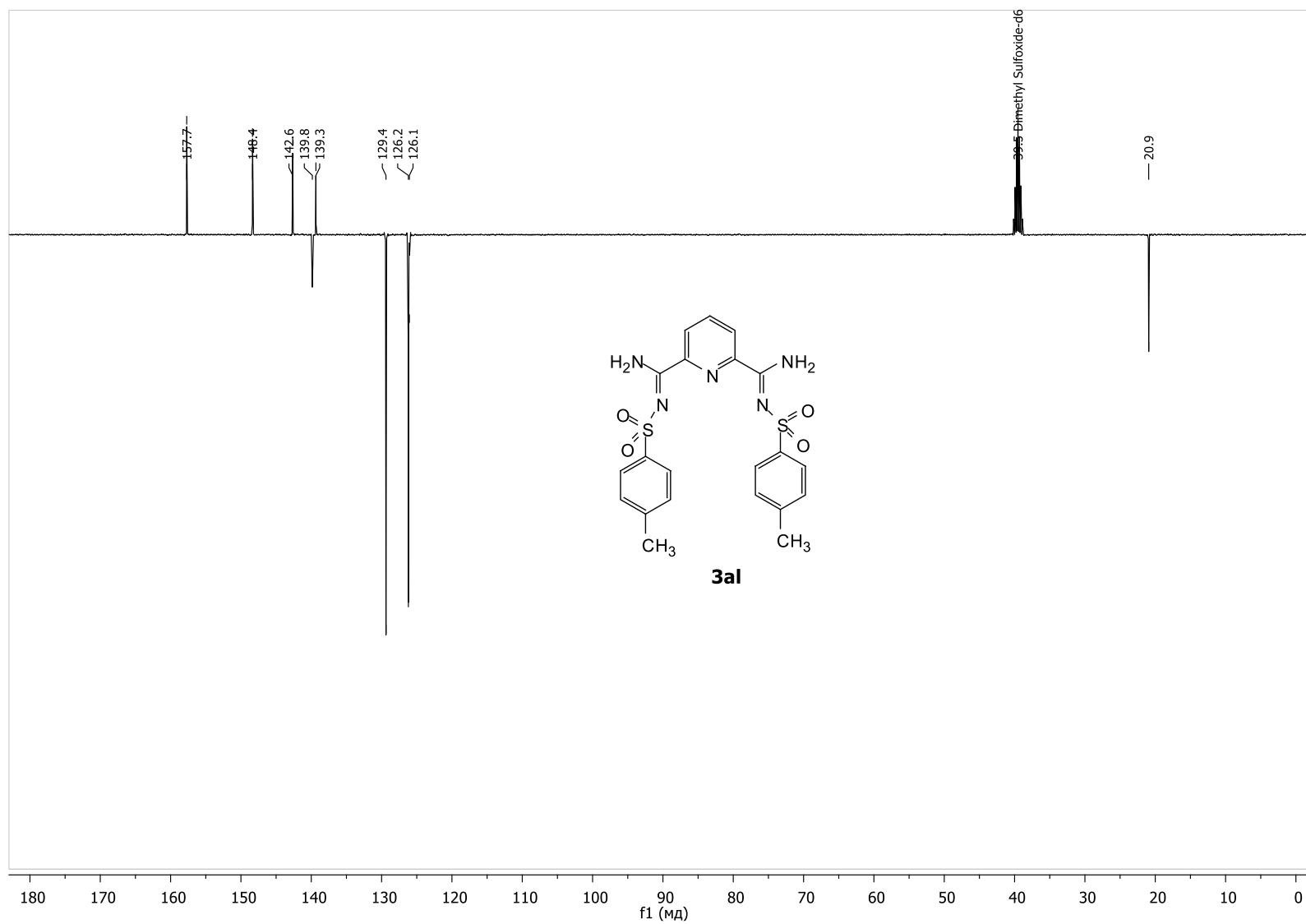
The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3ak**.



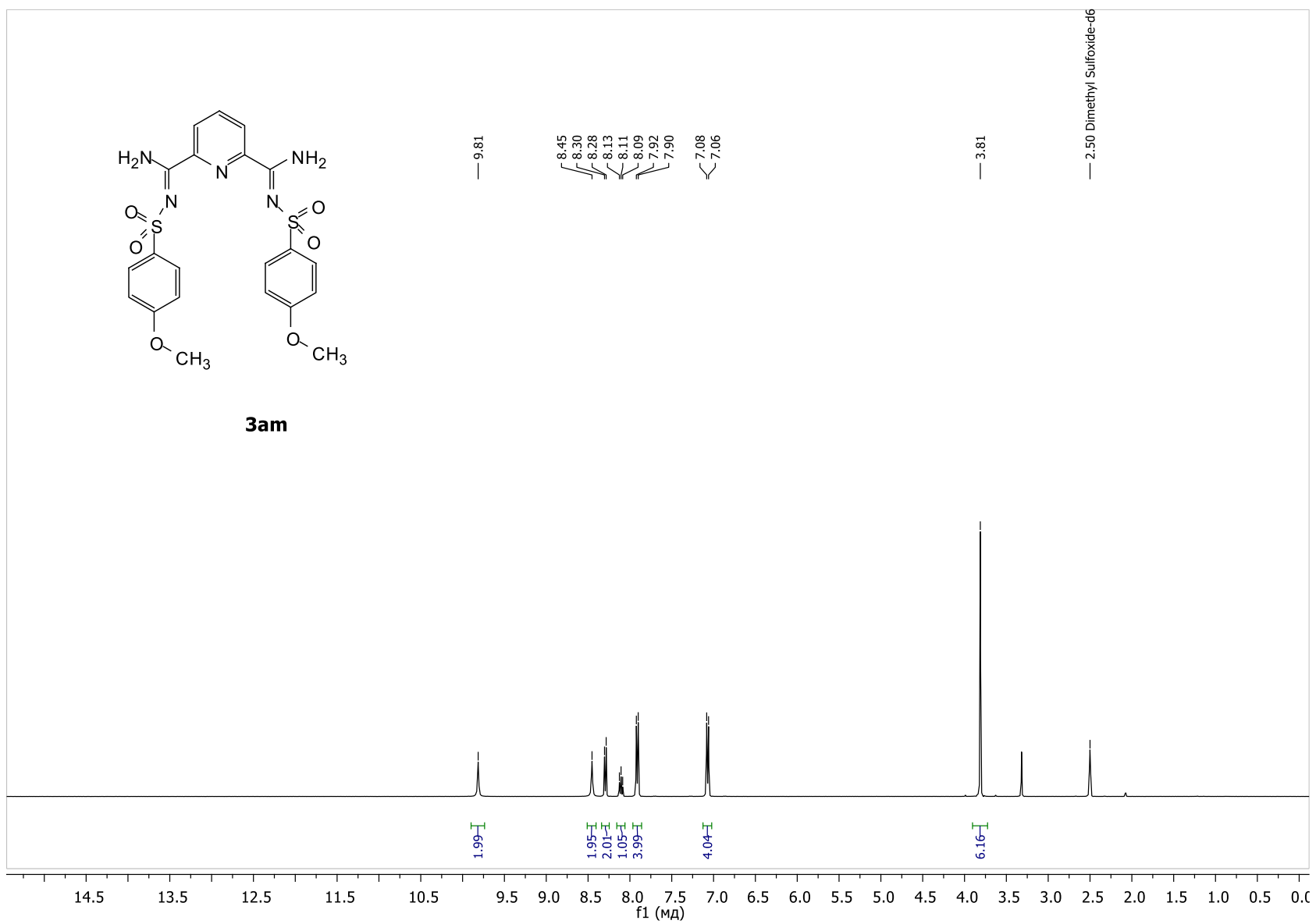
The ¹³C NMR (100 MHz, DMSO-*d*₆) spectrum of compound **3ak**.



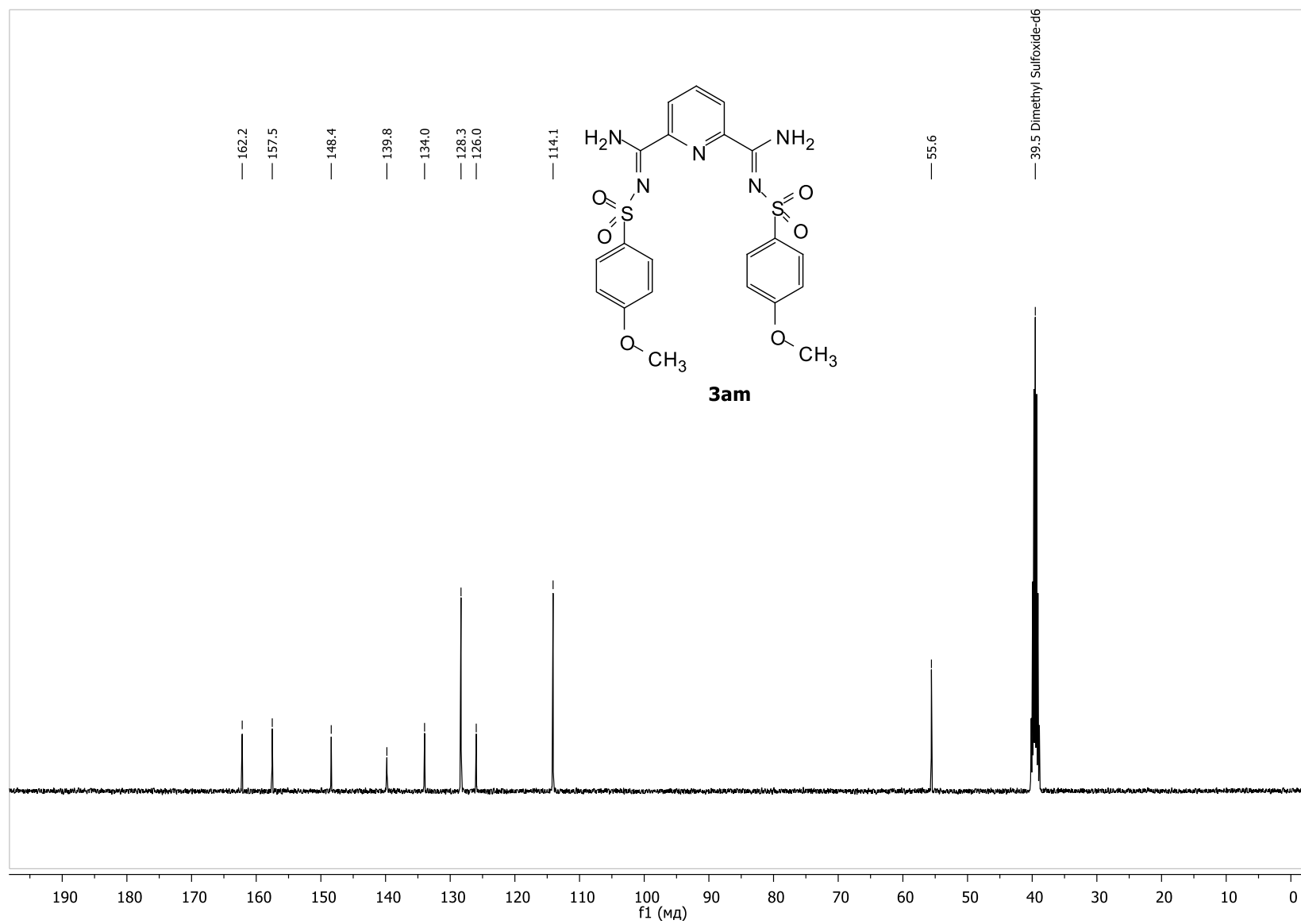
The ^1H NMR (400 MHz, DMSO- d_6) spectrum of compound **3al**.



The ^{13}C NMR (100 MHz, $\text{DMSO-}d_6$) spectrum of compound **3al**.

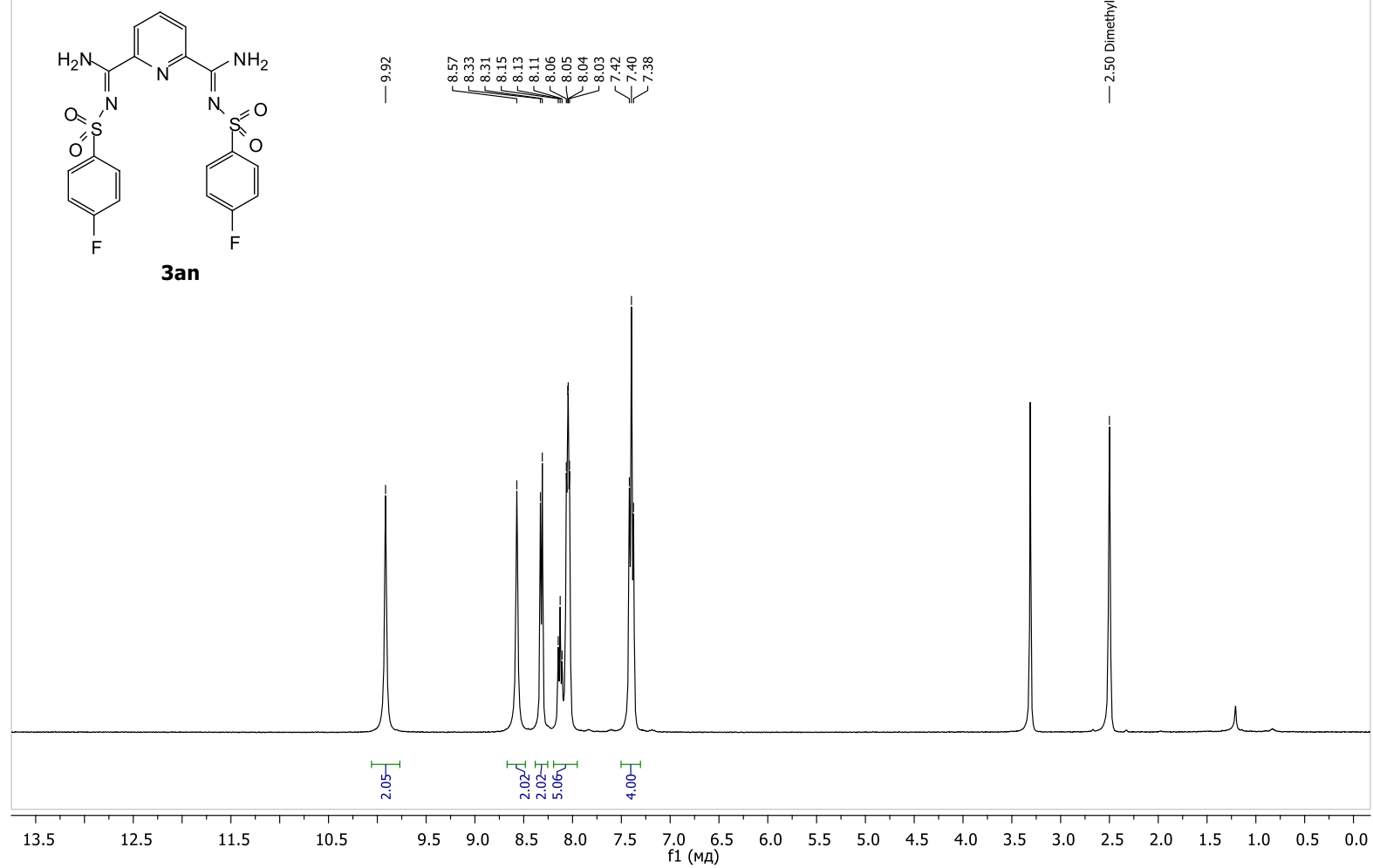


The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3am**.



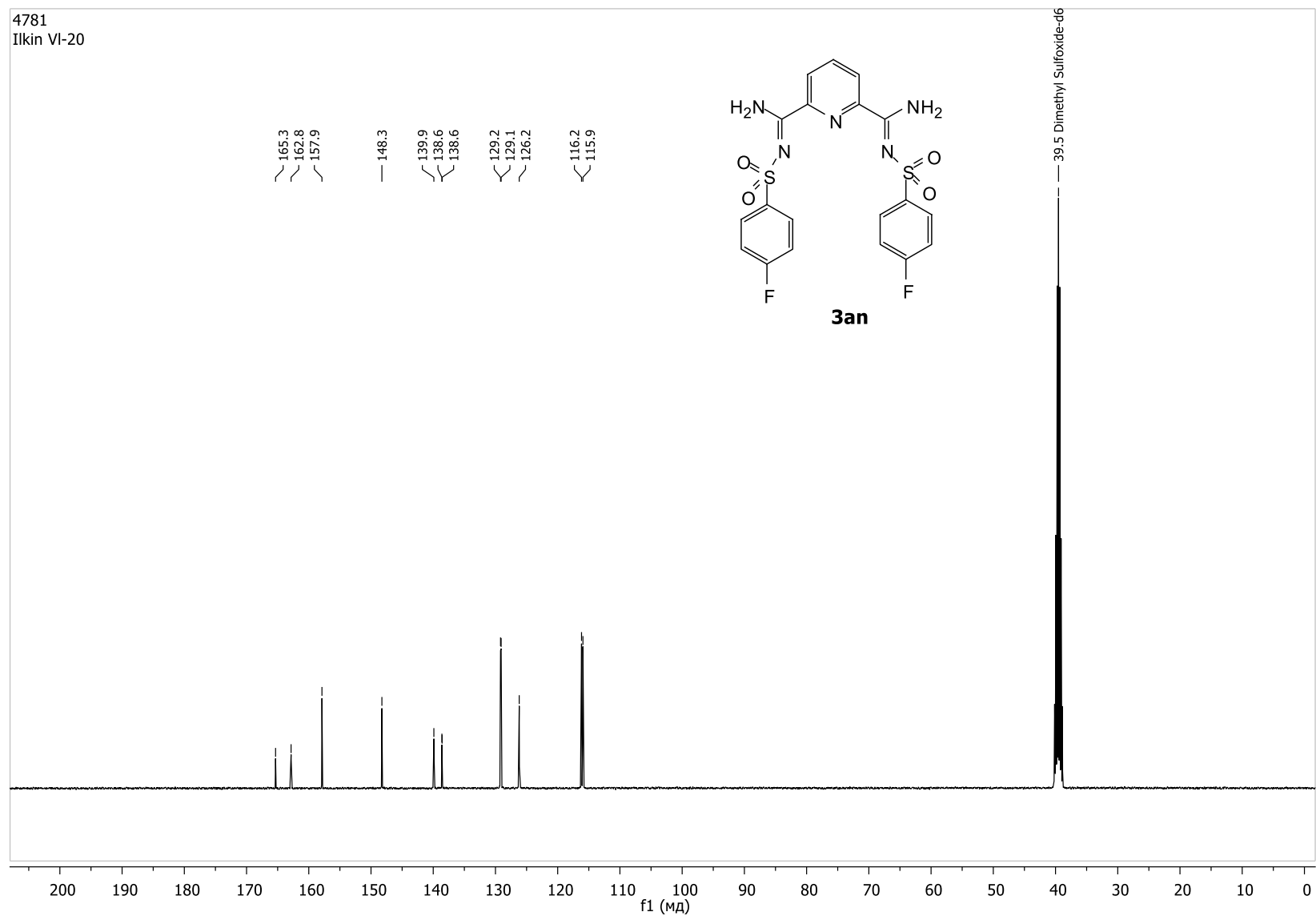
The ^{13}C NMR (100 MHz, $\text{DMSO}-d_6$) spectrum of compound **3am**.

2565
Ilkin VI-20

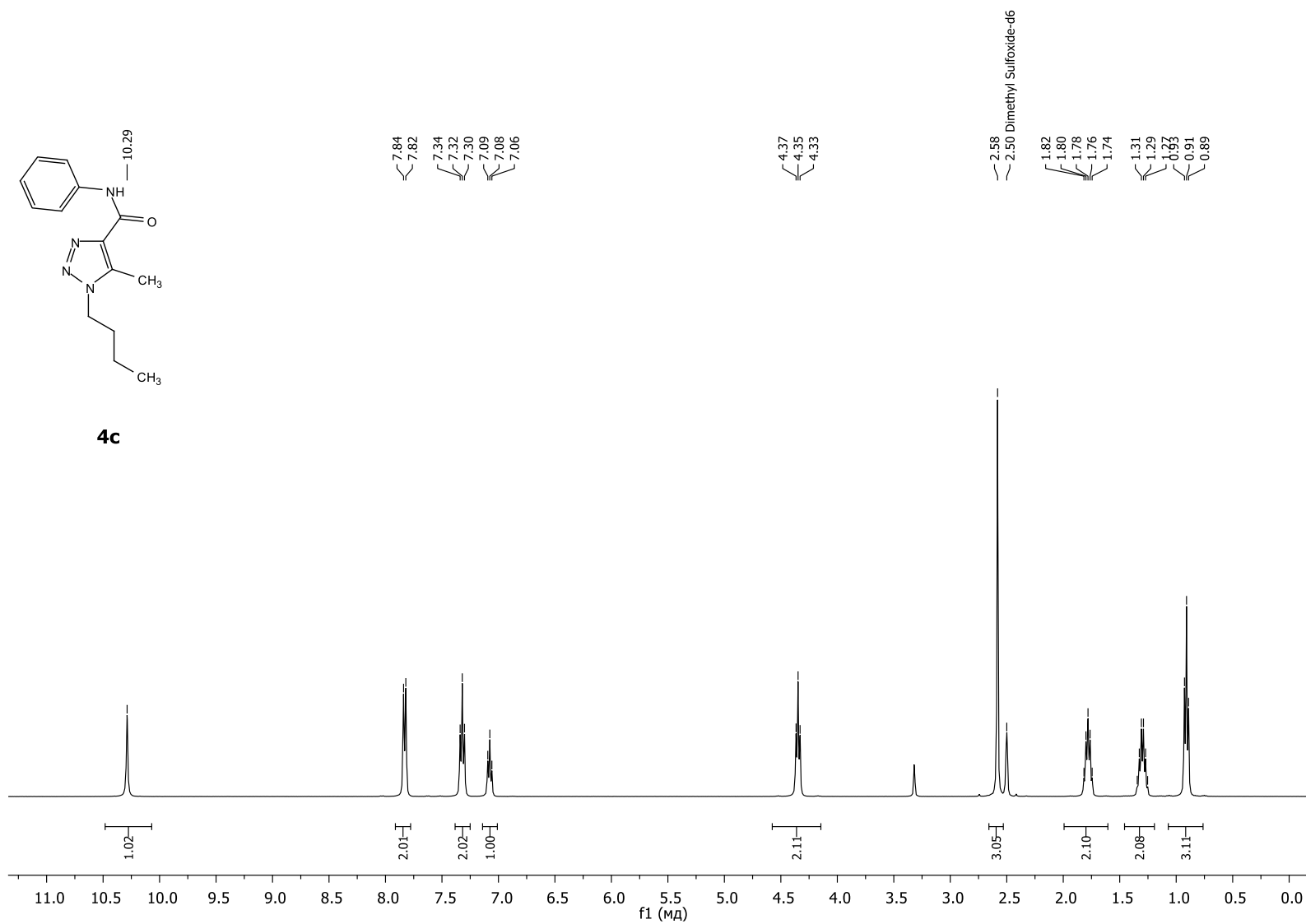


The ^1H NMR (400 MHz, $\text{DMSO}-d_6$) spectrum of compound **3an**.

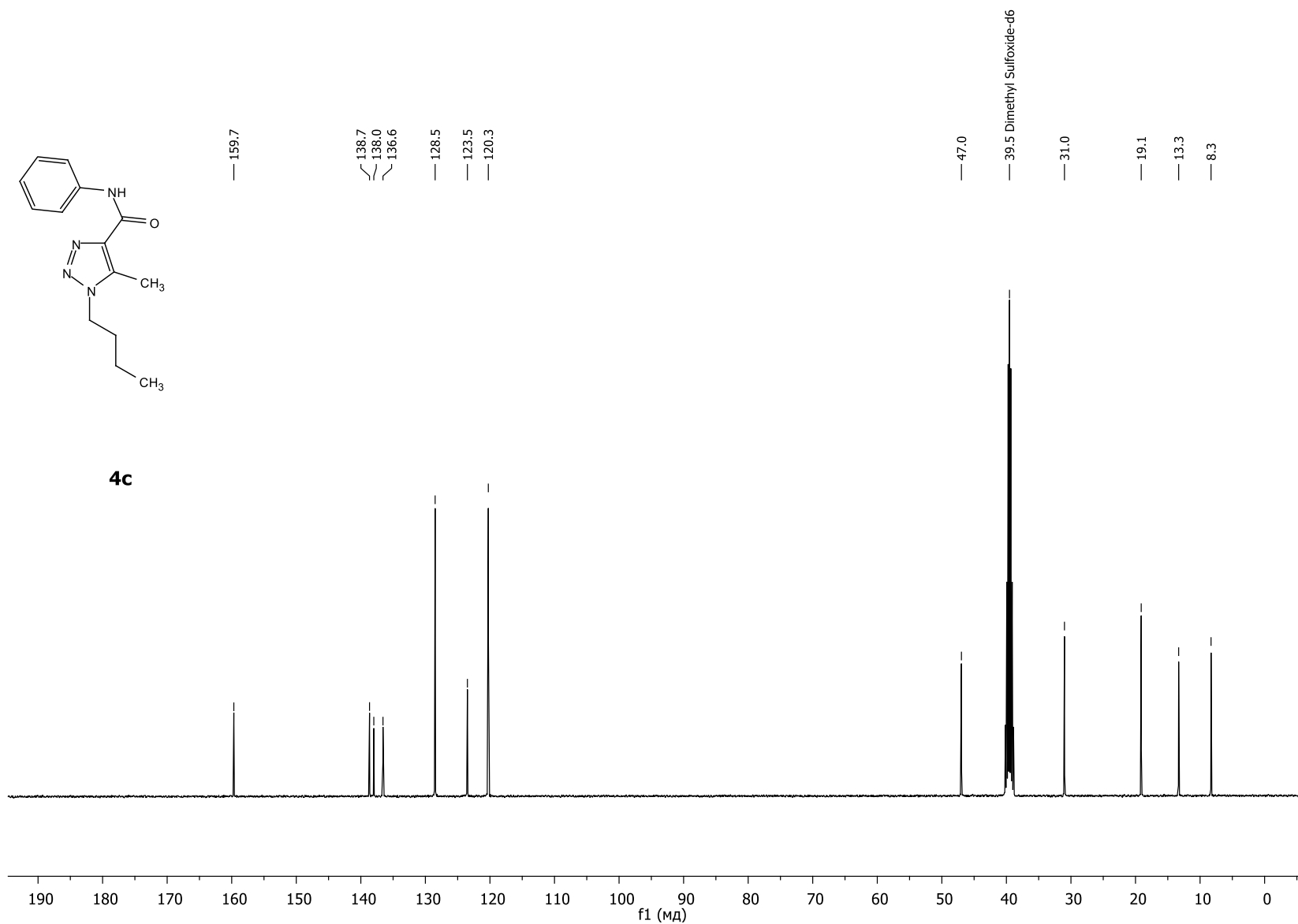
4781
Ilkin VI-20



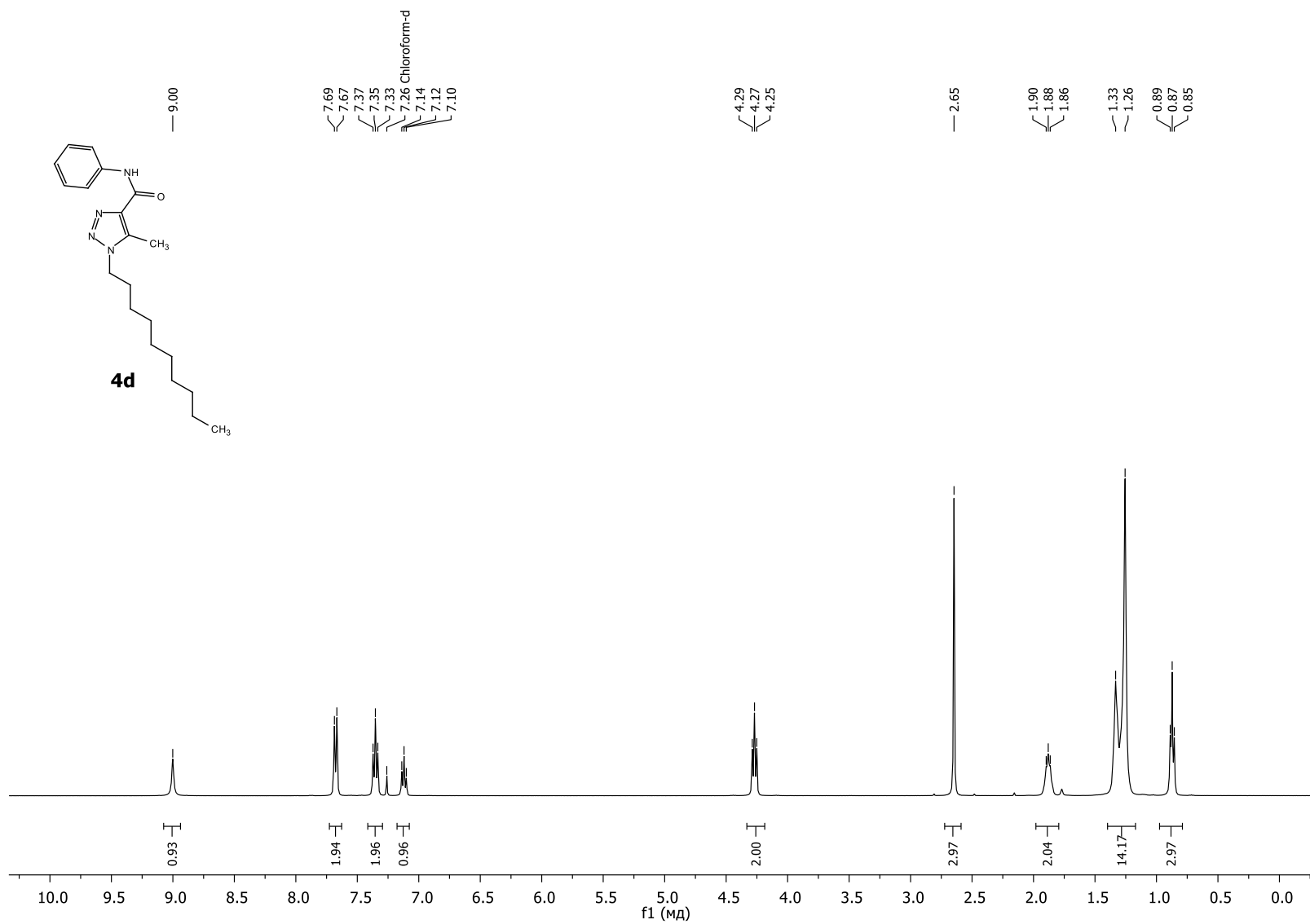
The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **3an**.



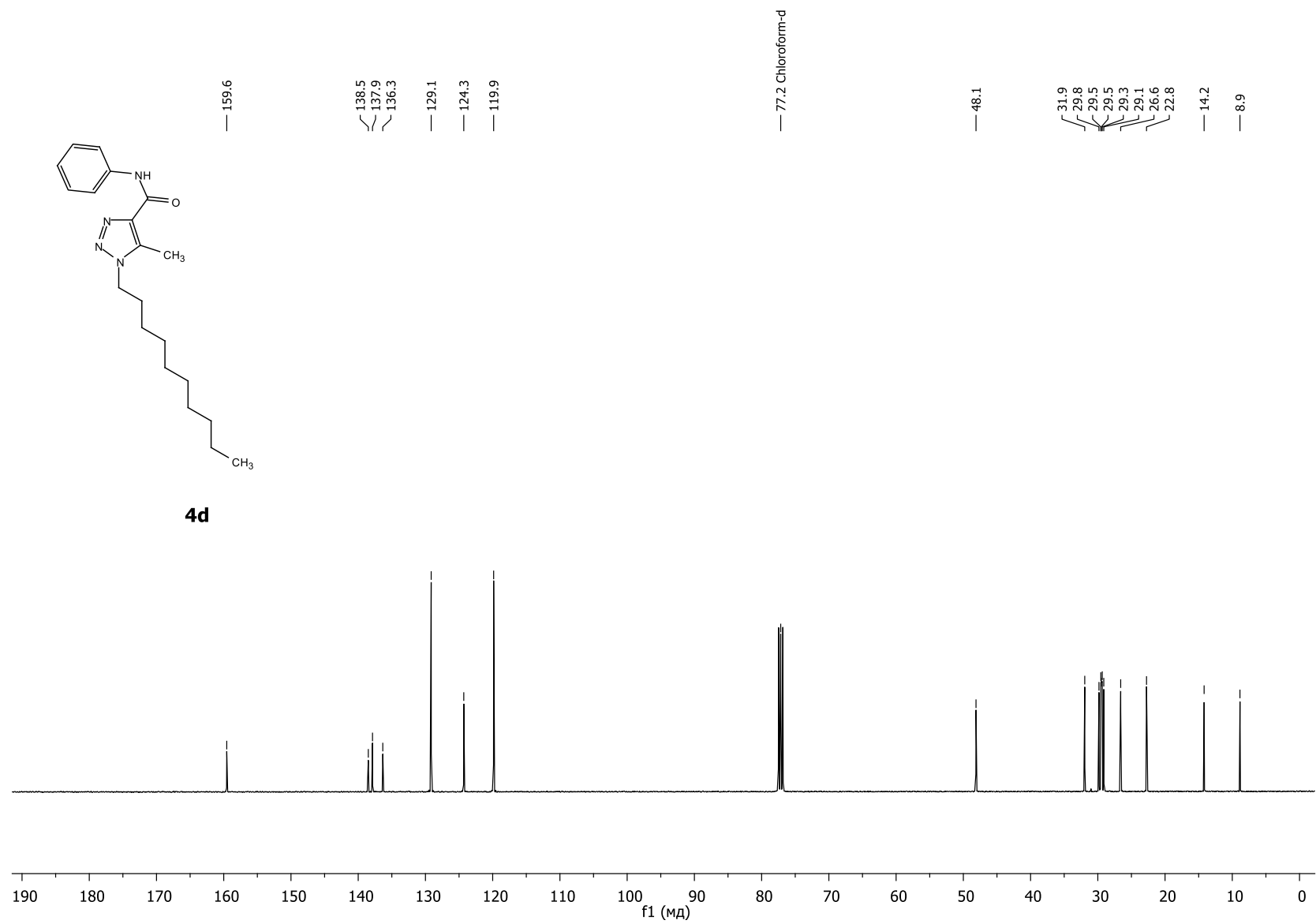
The ¹H NMR (400 MHz, DMSO-*d*₆) spectrum of compound **4c**.



The ^{13}C NMR (100 MHz, DMSO- d_6) spectrum of compound **4c**.



The ^1H NMR (400 MHz, CDCl₃) spectrum of compound **4d**.



The ^{13}C NMR (100 MHz, CDCl_3) spectrum of compound **4d**.