

Supplementary materials

Synthesis, Antitumor Evaluation, Molecular Modeling and Quantitative Structure–Activity Relationship (QSAR) of Novel 2-[(4-Amino-6-*N*-substituted-1,3,5-triazin-2-yl)methyl thio]-4-chloro-5-methyl-*N*-(1*H*-benzo[*d*]imidazol-2(3*H*)-ylidene)Benzenesulfonamides

Łukasz Tomorowicz ¹, Jarosław Sławiński ^{1,*}, Beata Żołnowska ^{1,*}, Krzysztof Szafranski ¹ and Anna Kawiak ²

¹ Department of Organic Chemistry, Medical University of Gdańsk, Al. Gen. J. Hallera 107, 80-416 Gdańsk, Poland; ltomorowicz@gumed.edu.pl (Ł.T.); k.szafranski@gumed.edu.pl (K.S.)

² Department of Biotechnology, Intercollegiate Faculty of Biotechnology, University of Gdańsk and Medical University of Gdańsk, ul. Abrahama 58, 80-307 Gdańsk, Poland; anna.kawiak@biotech.ug.edu.pl

* Correspondence: jaroslaw@gumed.edu.pl (J.S.); zolnowska@gumed.edu.pl (B.Ż.); Tel.: +48 58 349 10 98 (J.S.); +48 58 349 12 29 (B.Ż.)

Spectrum 1. ¹H NMR of compd **6 AGS-655** (500 MHz, DMSO-*d*₆).

Spectrum 2. ¹³C NMR of compd **6 AGS-655** (125 MHz, DMSO-*d*₆).

Spectrum 3. ¹H NMR of compd **9 AGS-649** (500 MHz, DMSO-*d*₆).

Spectrum 4. ¹³C NMR of compd **9 AGS-649** (125 MHz, DMSO-*d*₆).

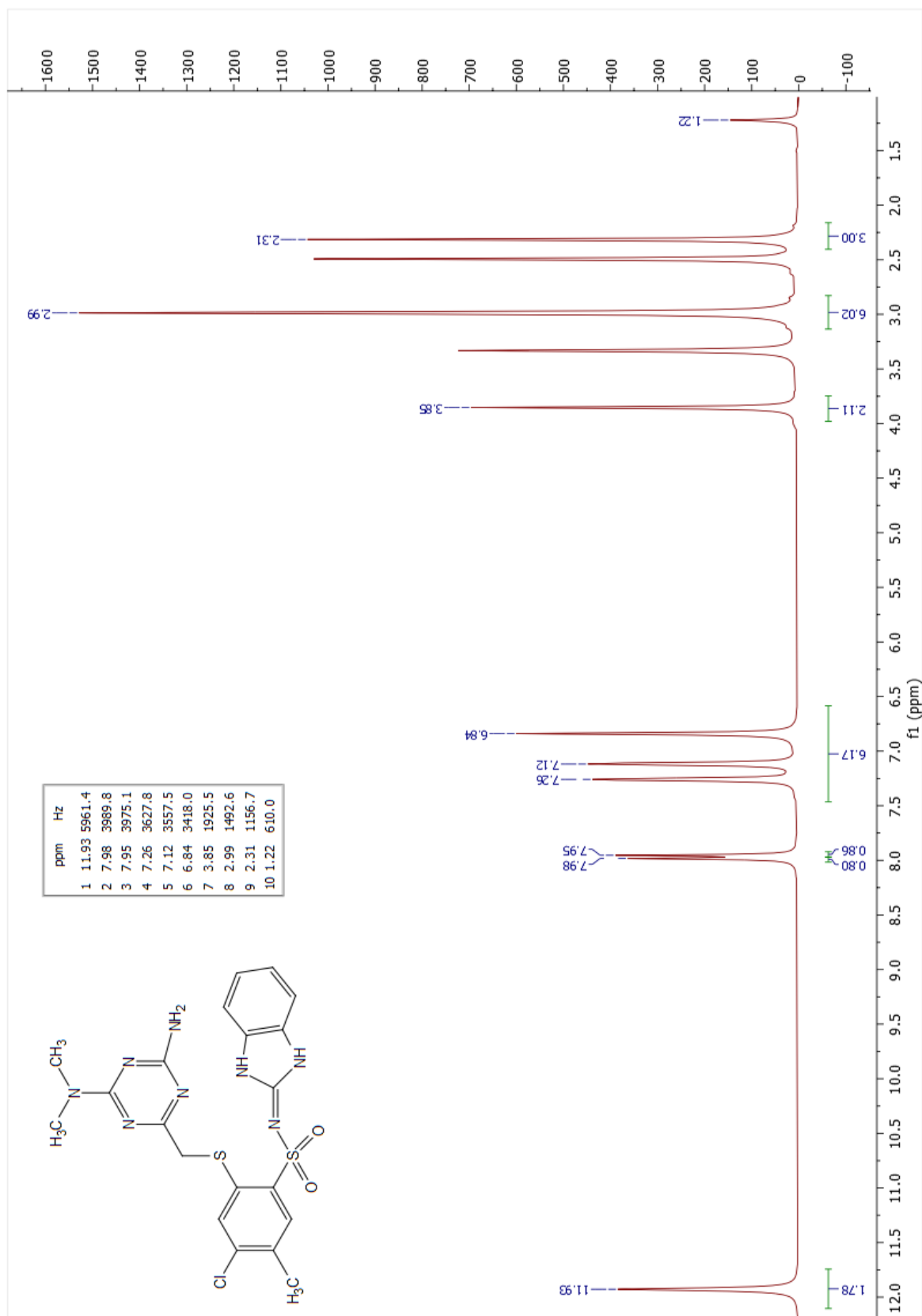
Spectrum 5. ¹H NMR of compd **11 AGS-659** (500 MHz, DMSO-*d*₆).

Spectrum 6. ¹H NMR of compd **19 AGS-651** (500 MHz, DMSO-*d*₆).

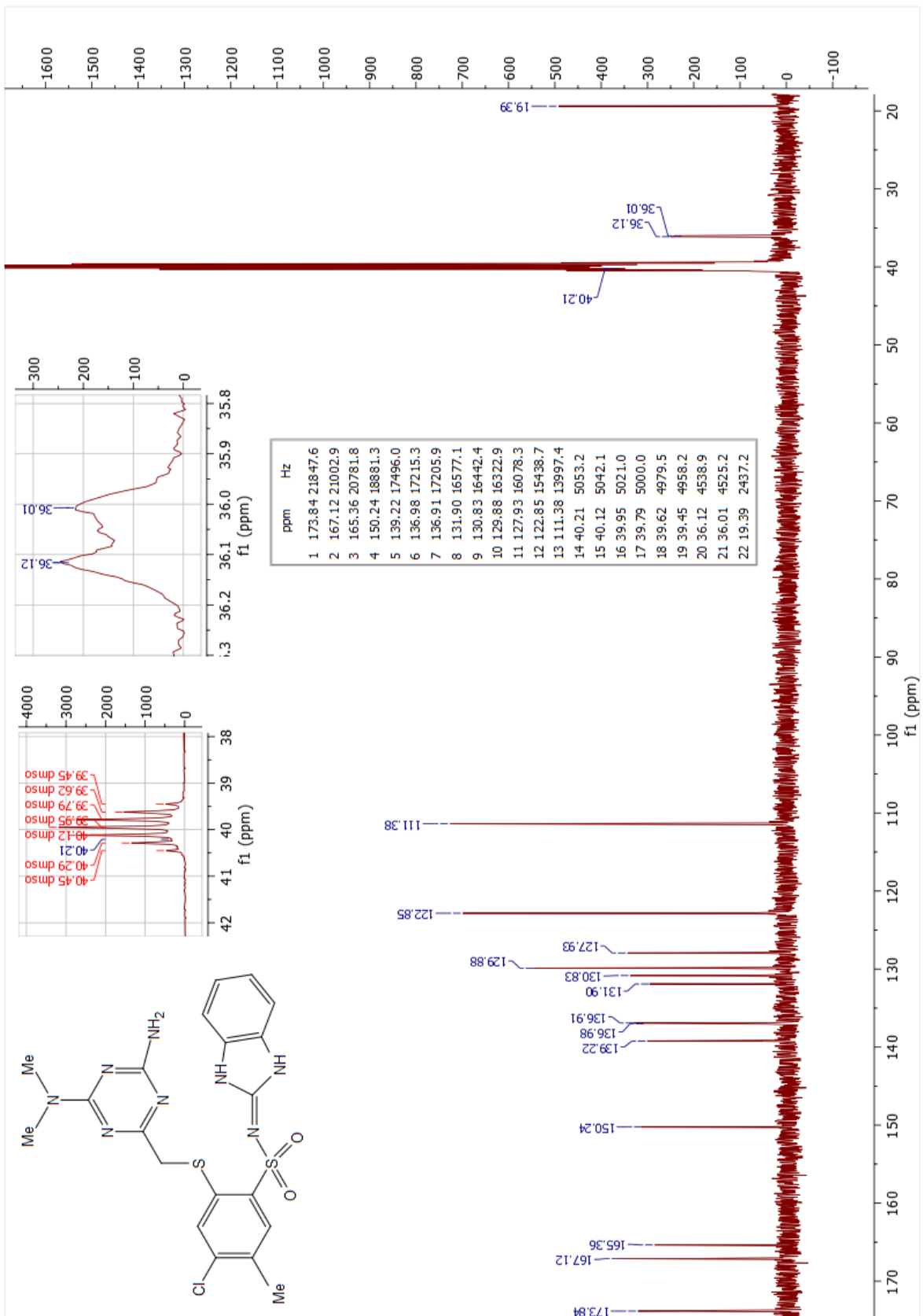
Spectrum 7. ¹³C NMR of compd **19 AGS-651** (125 MHz, DMSO-*d*₆).

Spectrum 8. ¹H NMR of compd **31 AGS-676**(500 MHz, DMSO-*d*₆).

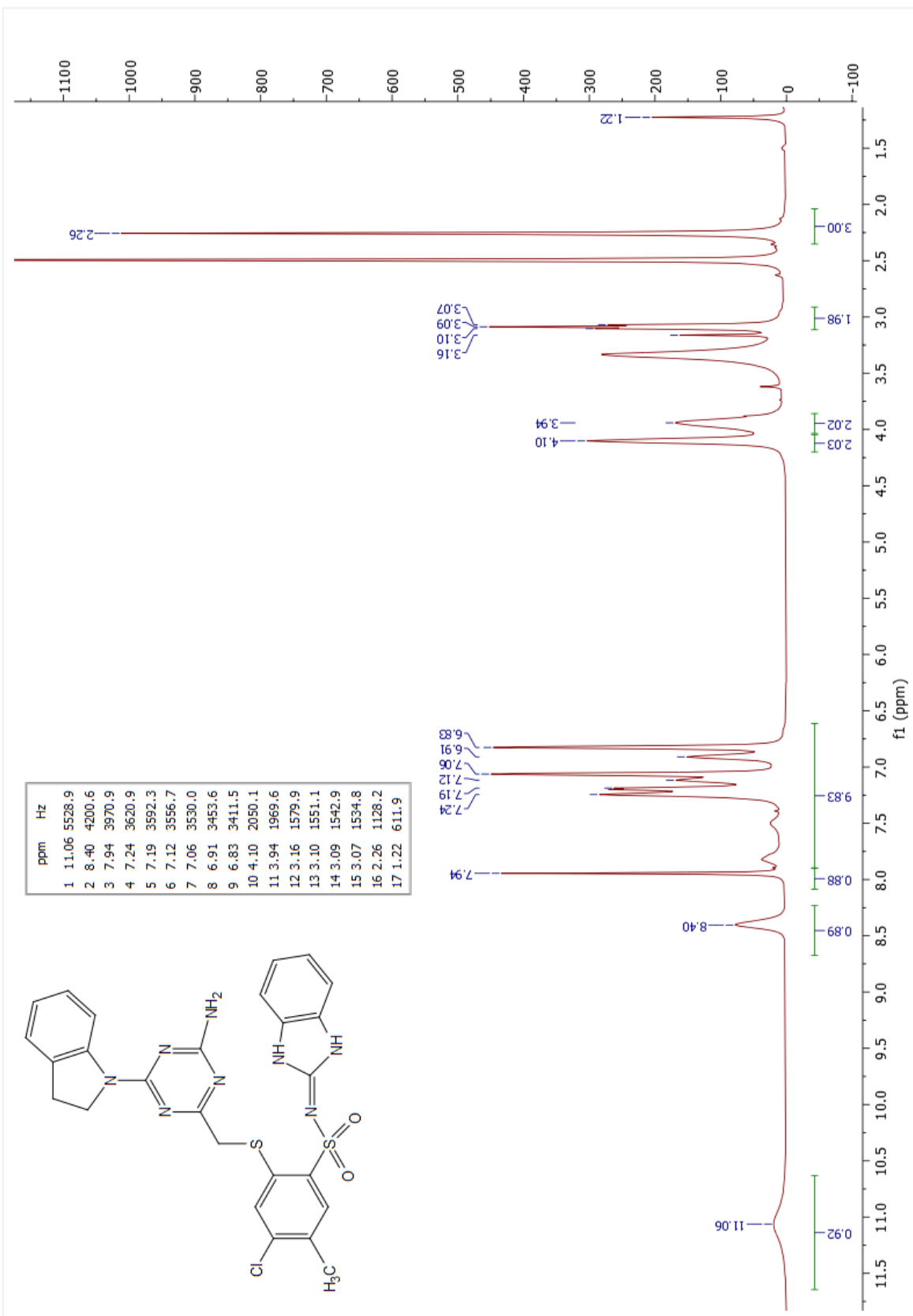
Spectrum 9. ¹³C NMR of compd **31 AGS-676** (125 MHz, DMSO-*d*₆).



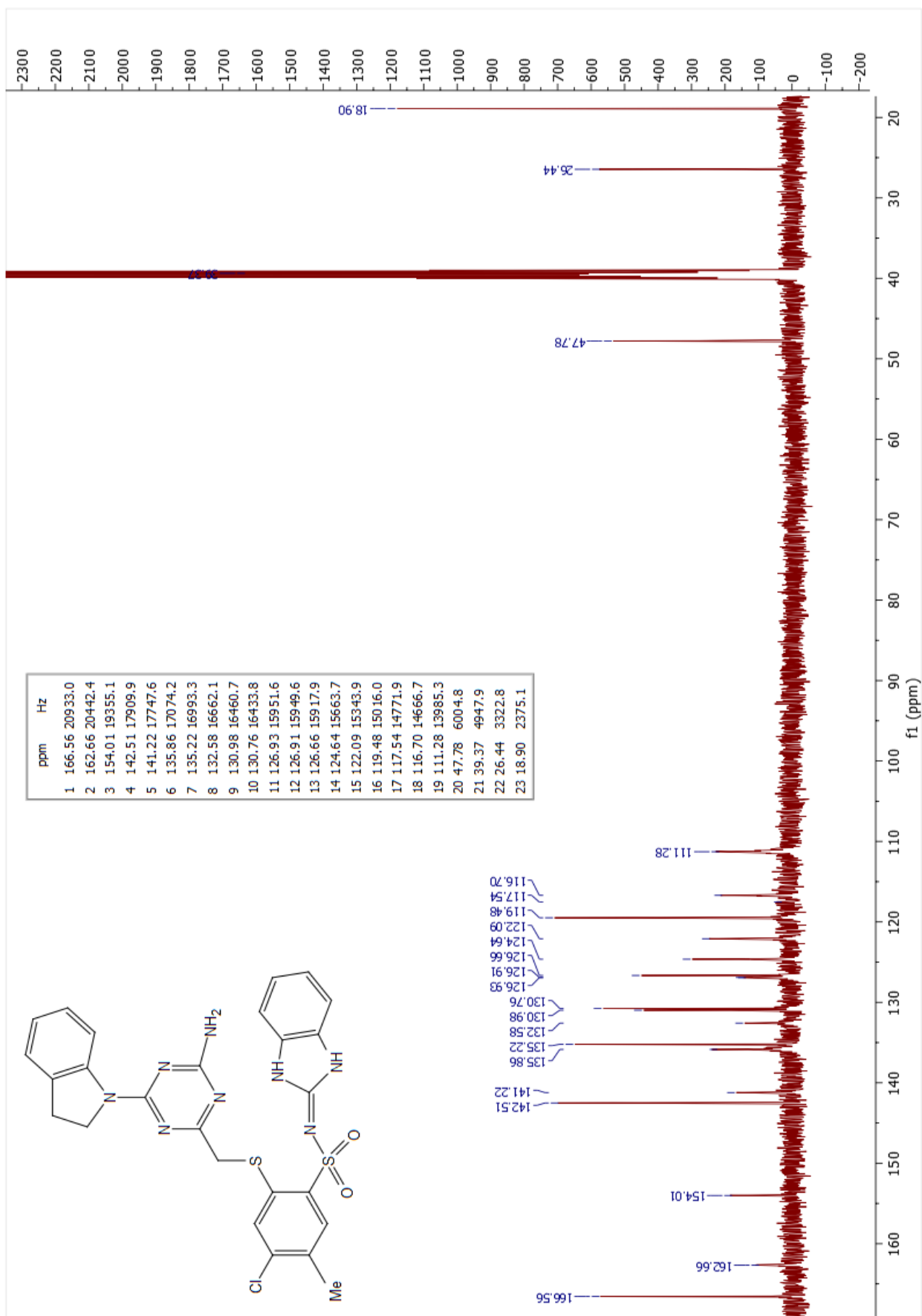
Spectrum 1. ^1H NMR of compd 6 (AGS-655) (500 MHz, $\text{DMSO-}d_6$)



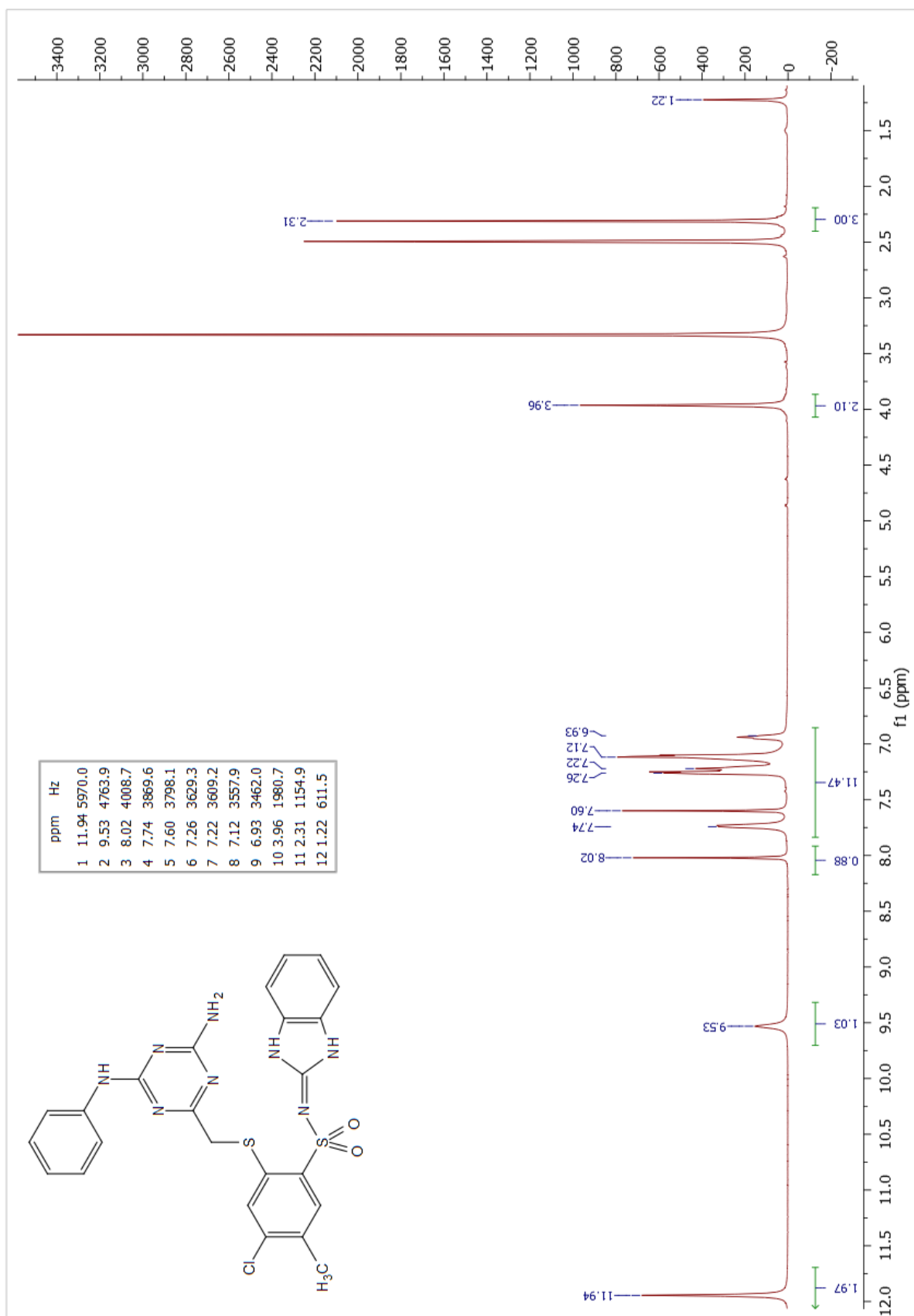
Spectrum 2. ^{13}C NMR of compd 6 AGS-655 (125 MHz, $\text{DMSO-}d_6$)



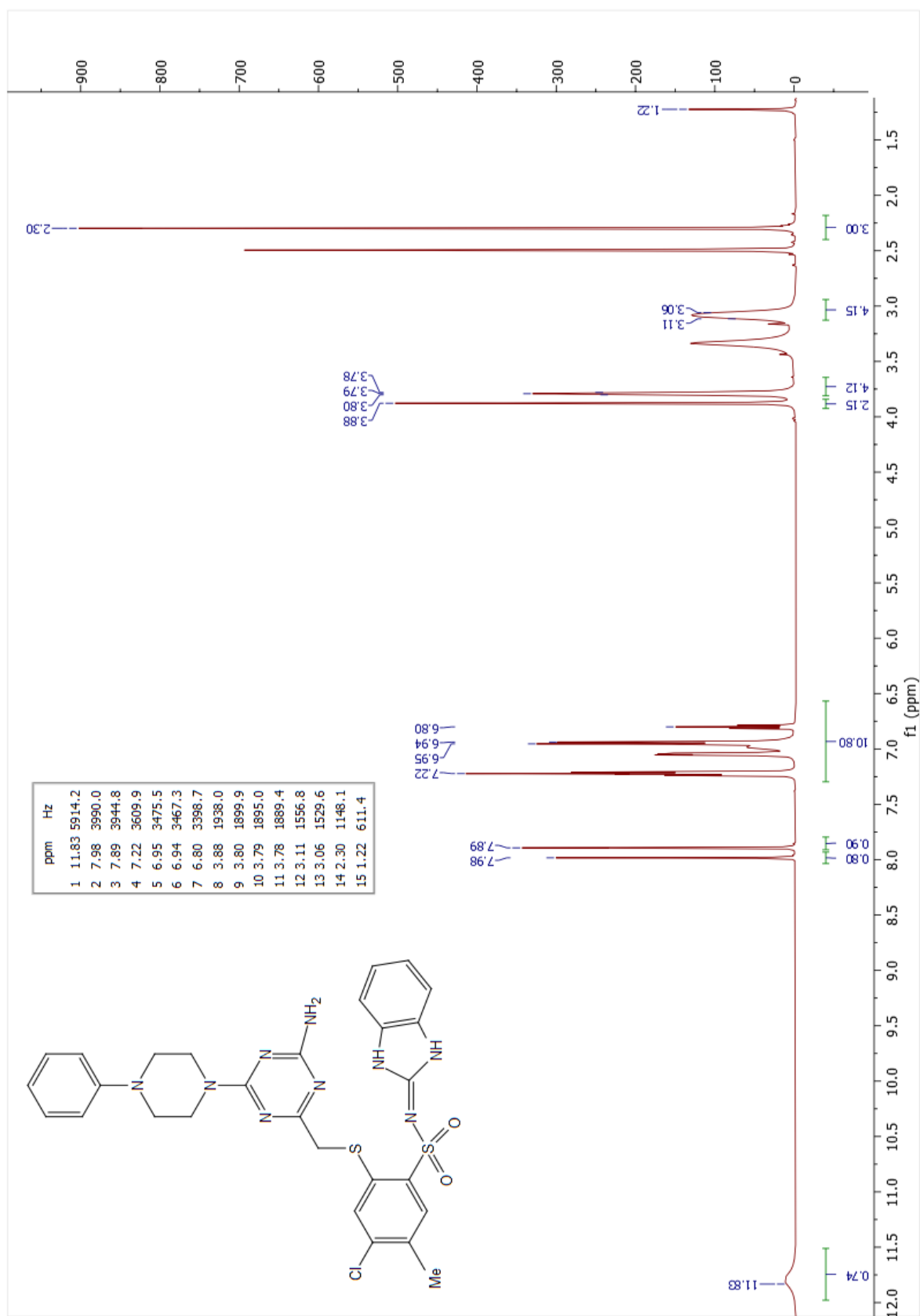
Spectrum 3. ^1H NMR of compd **9** AGS-649 (500 MHz, $\text{DMSO-}d_6$)



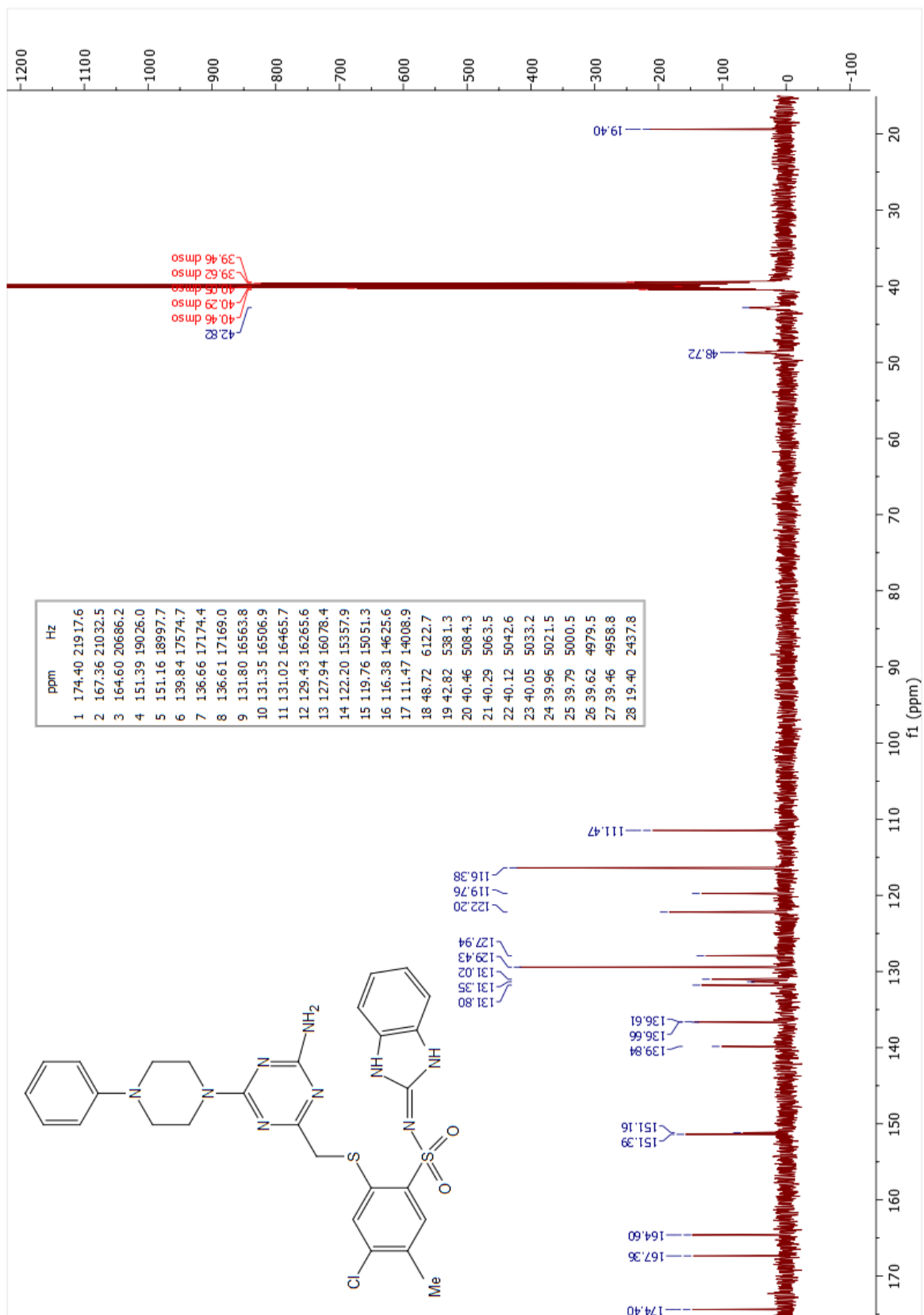
Spectrum 4. ^{13}C NMR of compd 9 AGS-649 (125 MHz, $\text{DMSO}-d_6$)



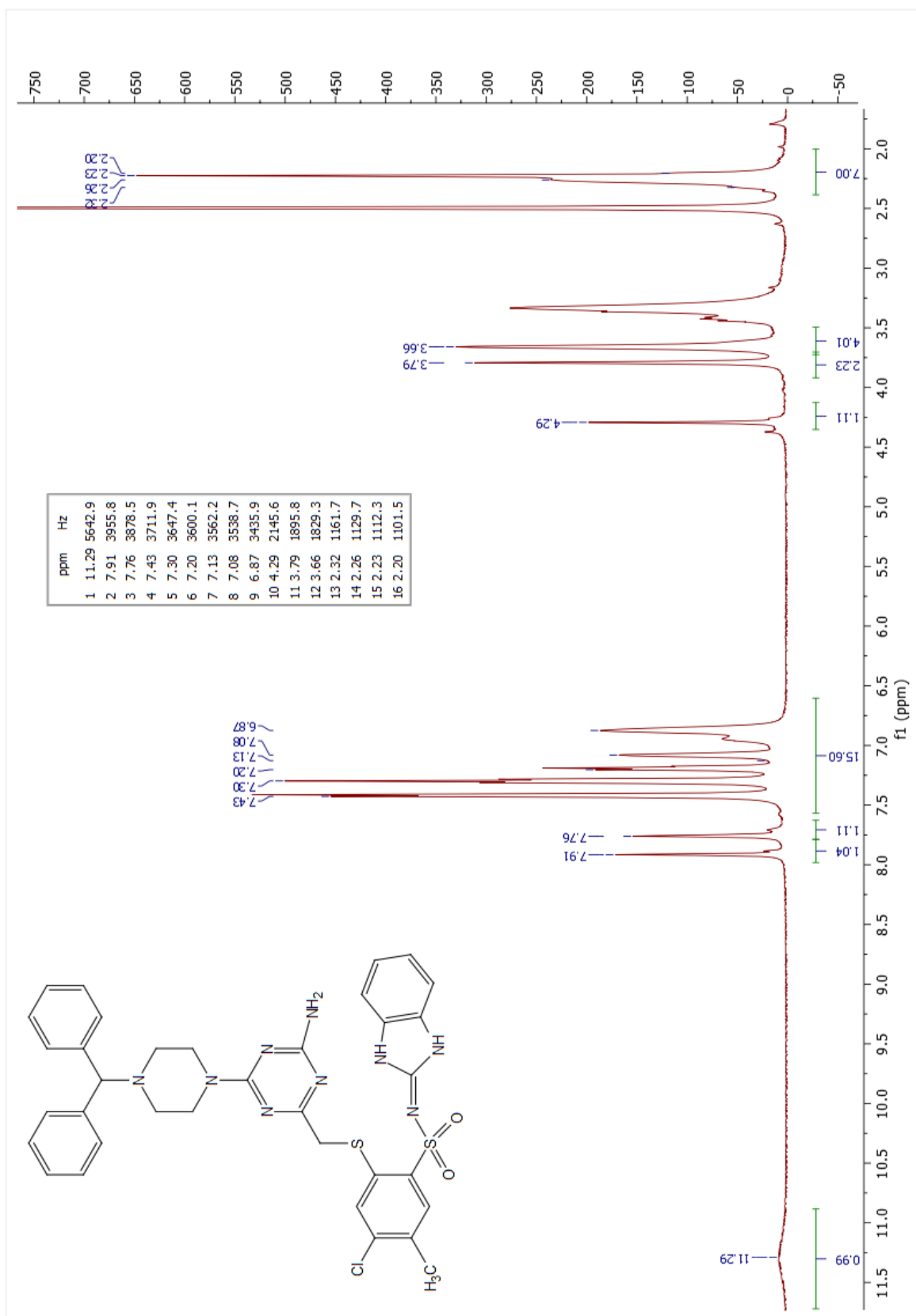
Spectrum 5. ¹H NMR of compd 11 (AGS-659) (500 MHz, DMSO-*d*₆)



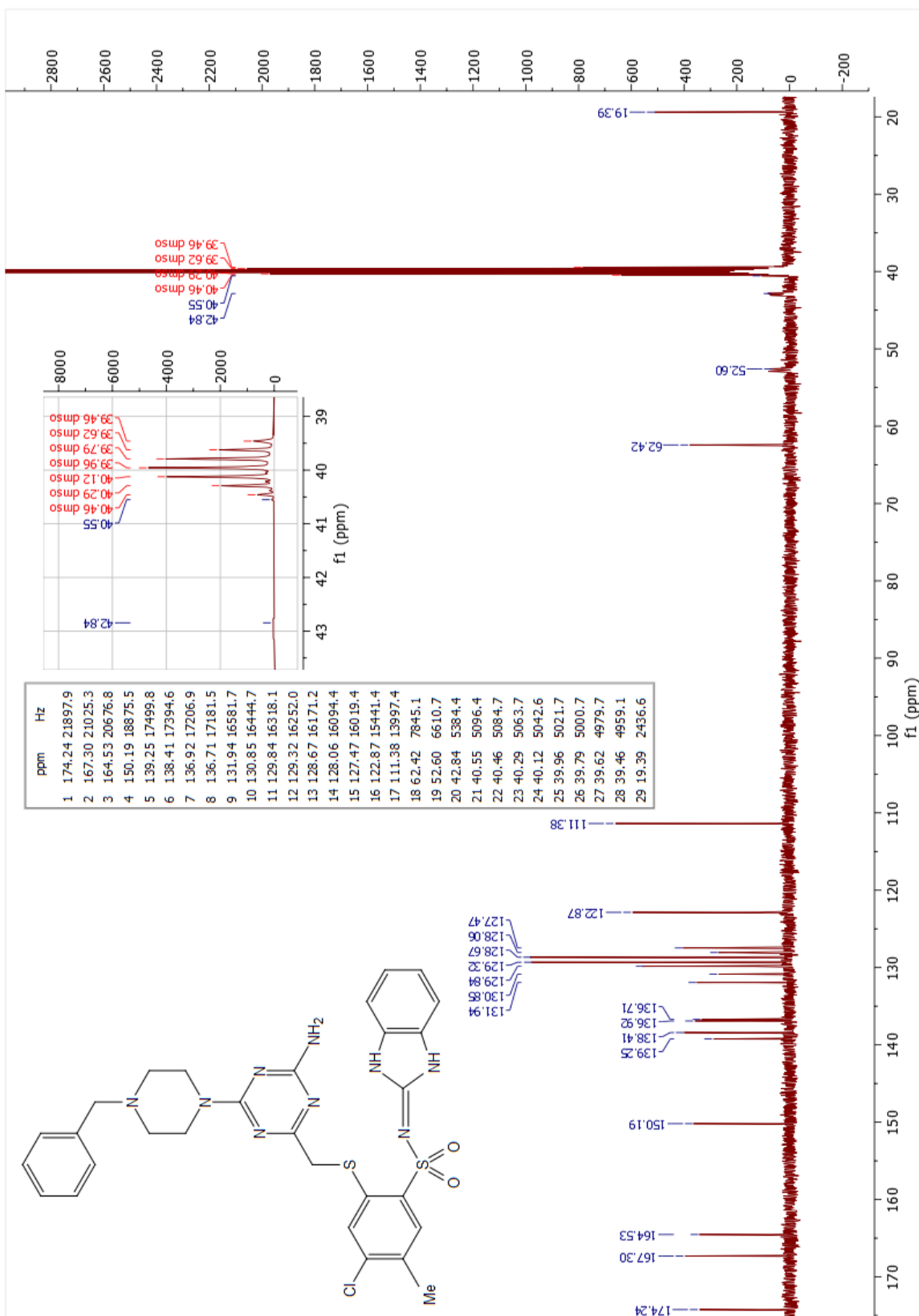
Spectrum 6. ¹H NMR of compd 19 AGS-651 (500 MHz, DMSO-*d*₆).



Spectrum 7. ^{13}C NMR of compd 19 AGS-651 (125 MHz, $\text{DMSO}-d_6$)



Spectrum 8. ¹H NMR of compd 31 AGS-676(500 MHz, DMSO-d₆)



Spectrum 9. ^{13}C NMR of compd 31 AGS-676 (125 MHz, $\text{DMSO}-d_6$)