

Supporting Information

Optimization of 2-aminoquinazolin-4(3H)-one derivatives as potent inhibitors of SARS-CoV-2: efficient synthesis and improved pharmacokinetic properties

Young Sup Shin^{1,2,†}, Jun Young Lee^{1,2,†}, Sangeun Jeon³, Jung-Eun Cho², Subeen Myung^{2,4}, Min Seong Jang⁵, Seungtaek Kim³, Jong Hwan Song², Hyoung Rae Kim², Hyeung-geun Park^{1,*}, Lak Shin Jeong^{1,*}, Chul Min Park^{2,4,*}

¹*Research Institute of Pharmaceutical Sciences, College of Pharmacy, Seoul National University, Seoul 08826, Korea*

²*Center for Convergent Research of Emerging Virus Infection (CEVI), Korea Research Institute of Chemical Technology, 141 Gajeong-ro, Yuseong-gu, Daejeon 34114, Korea*

³*Zoonotic Virus Laboratory, Institut Pasteur Korea, Seongnam-si, Gyeonggi-do 13488, Korea*

⁴*Medicinal Chemistry and Pharmacology, Korea University of Science and Technology, Daejeon 34114, Korea*

⁵*Department of Non-Clinical Studies, Korea Institute of Toxicology, Yuseong-gu, Daejeon 34114, Korea*

*Correspondence: parkcm@kRICT.re.kr (C.M. Park), lakjeong@snu.ac.kr (L.S. Jeong), hgpk@snu.ac.kr (H.-g. Park)

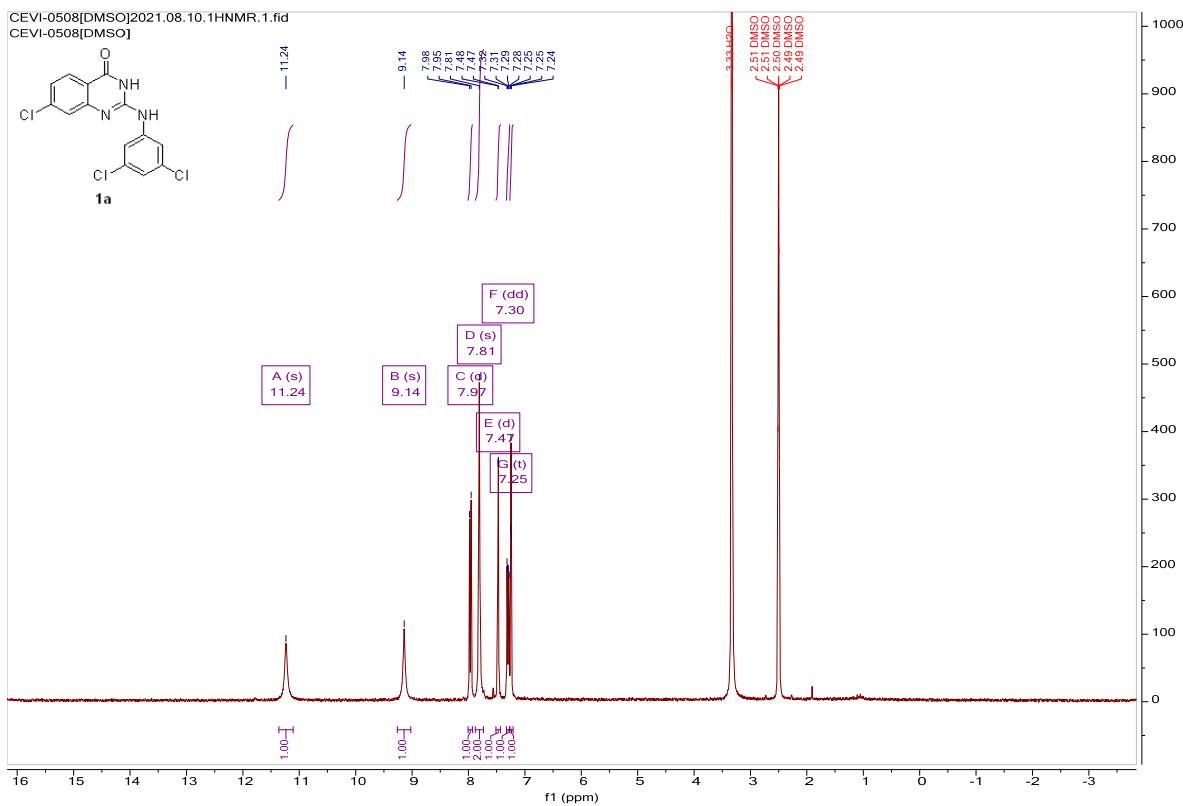
† These authors contributed equally to this work

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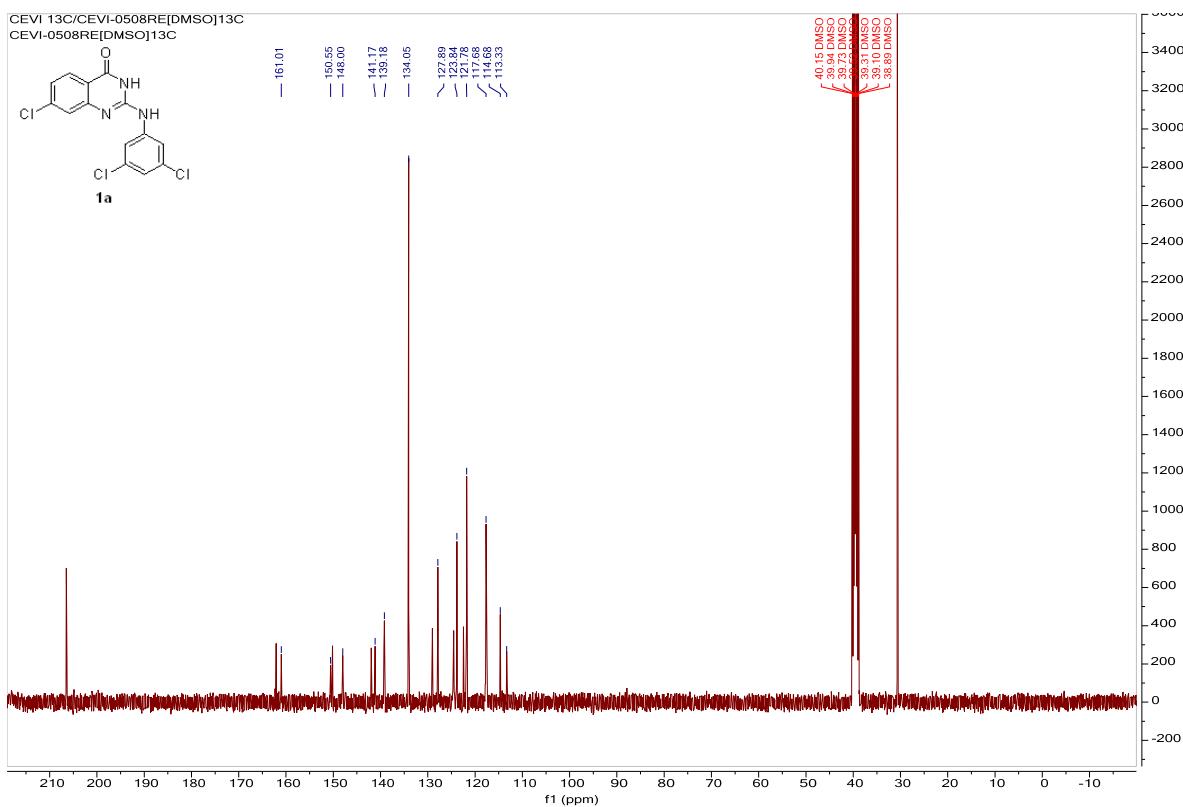
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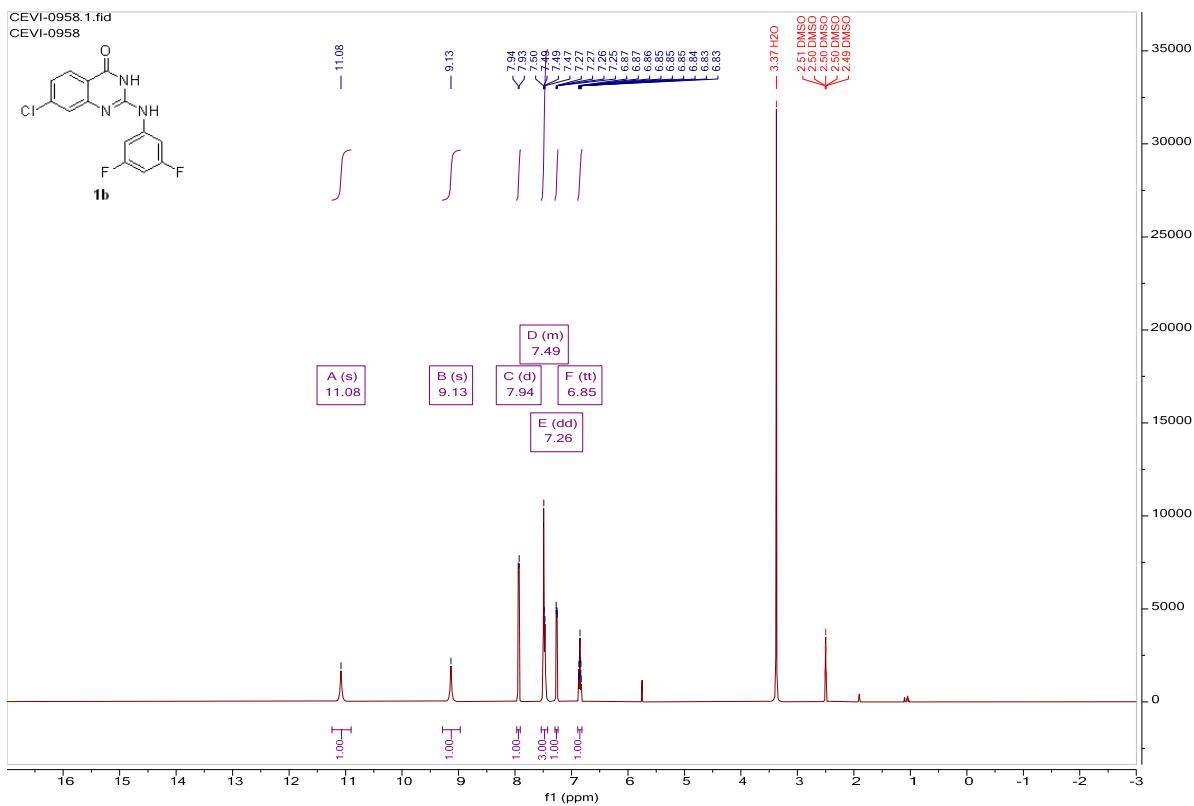
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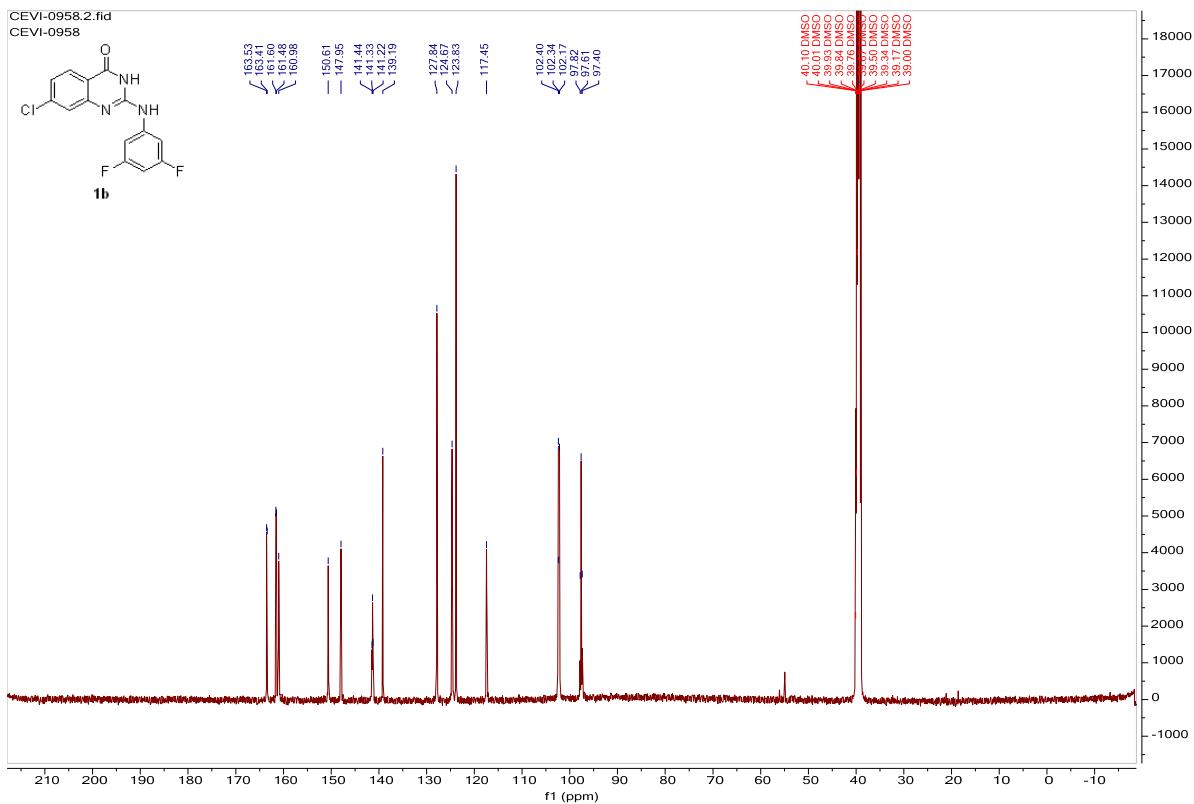
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **1a**



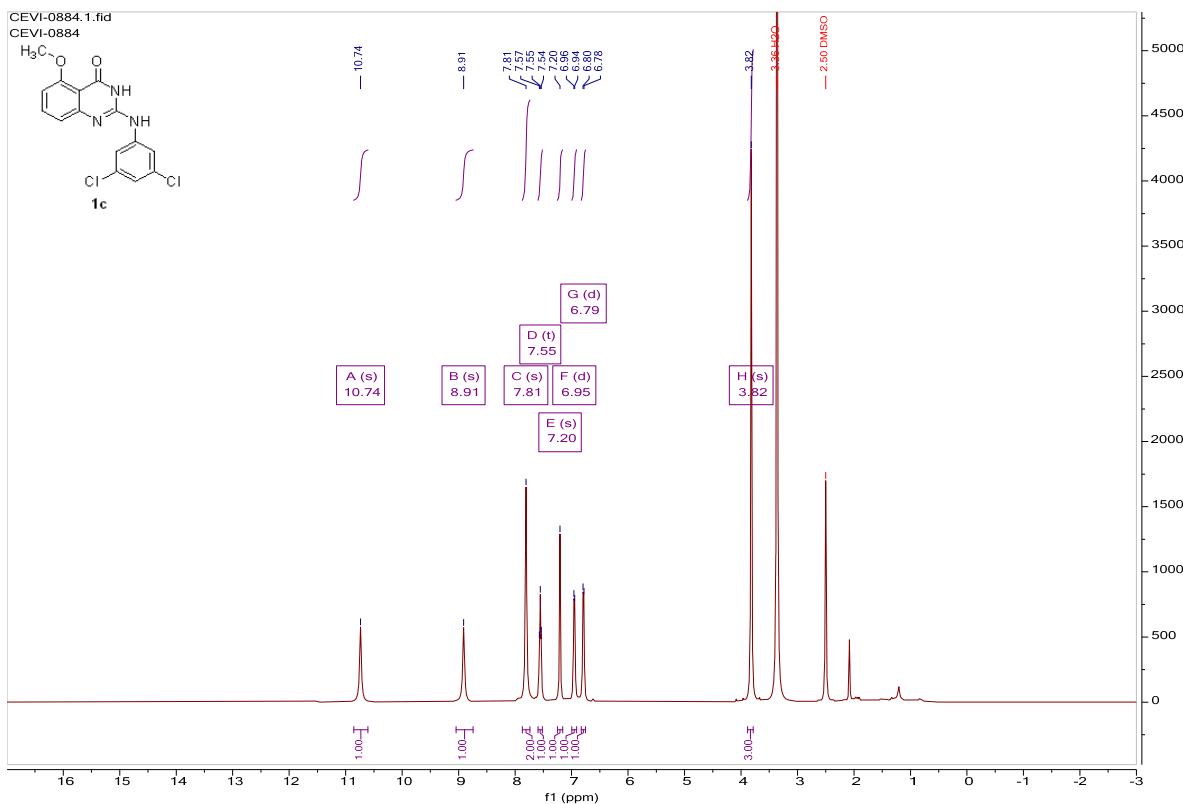
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of **1a**



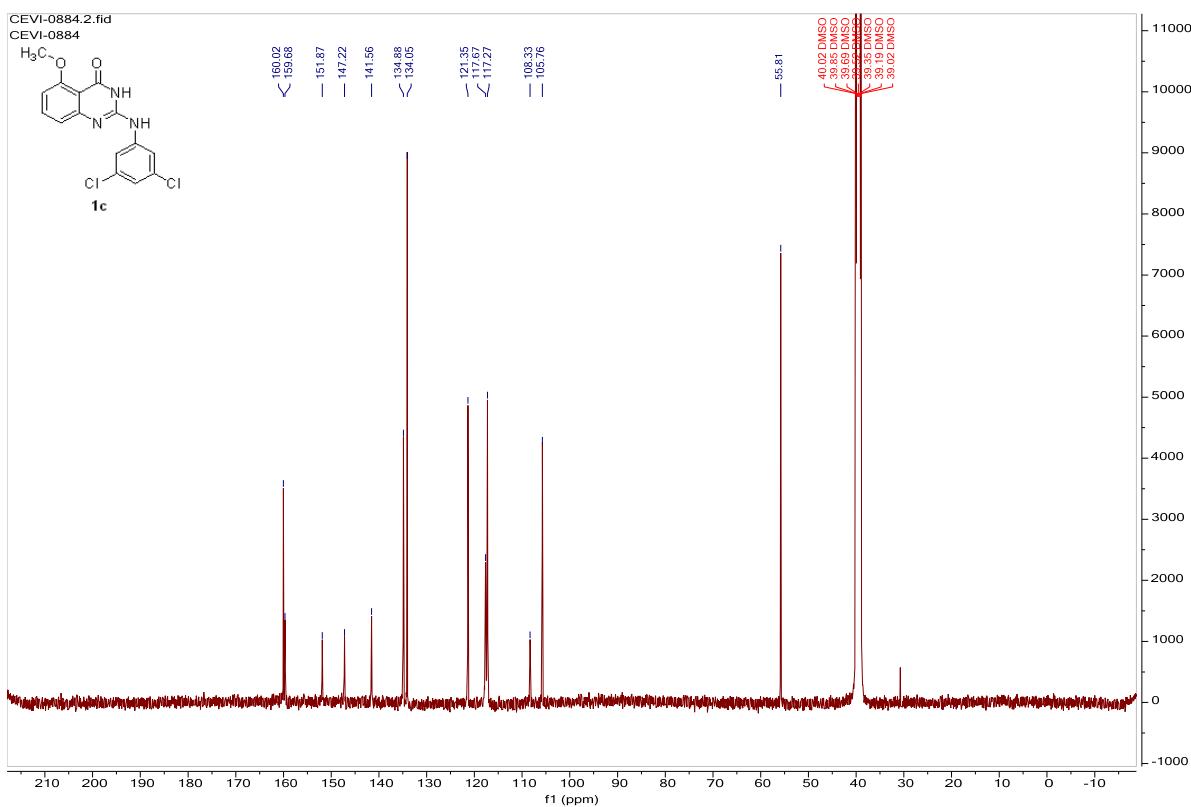
¹H NMR spectrum (500 MHz, DMSO-*d*₆) of **1b**



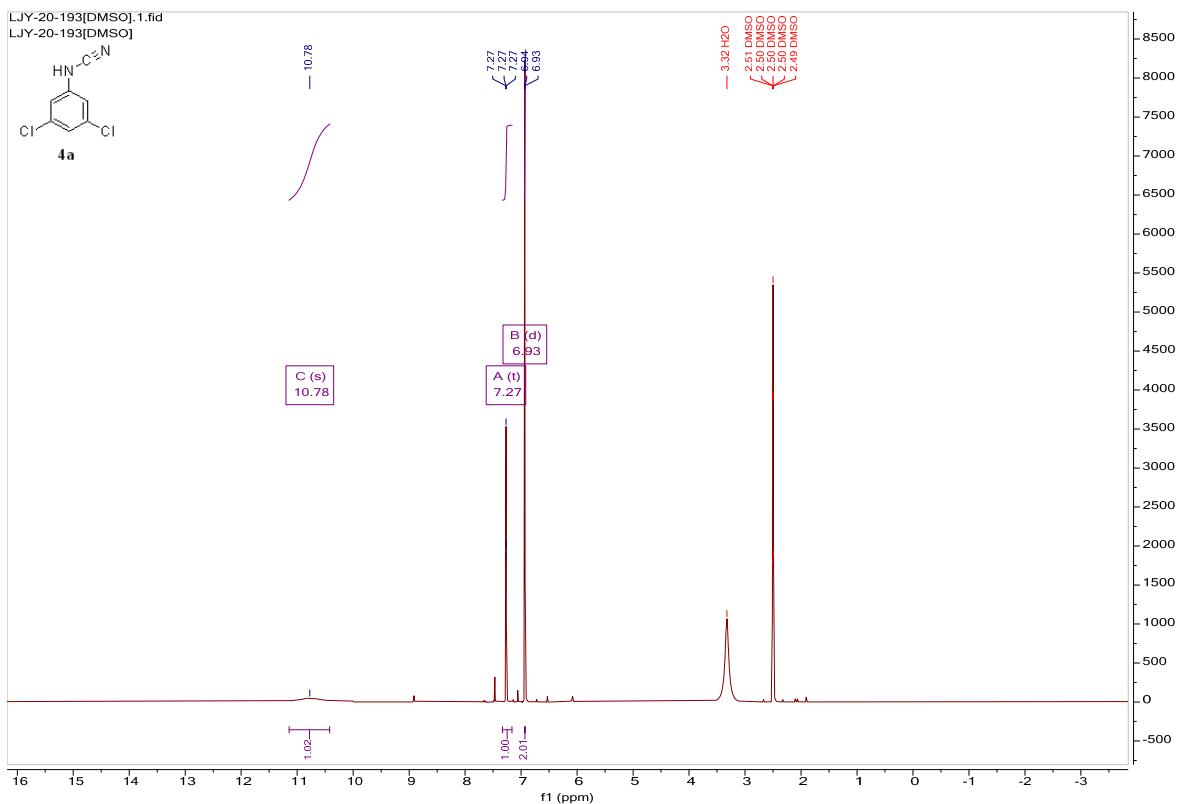
¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of **1b**



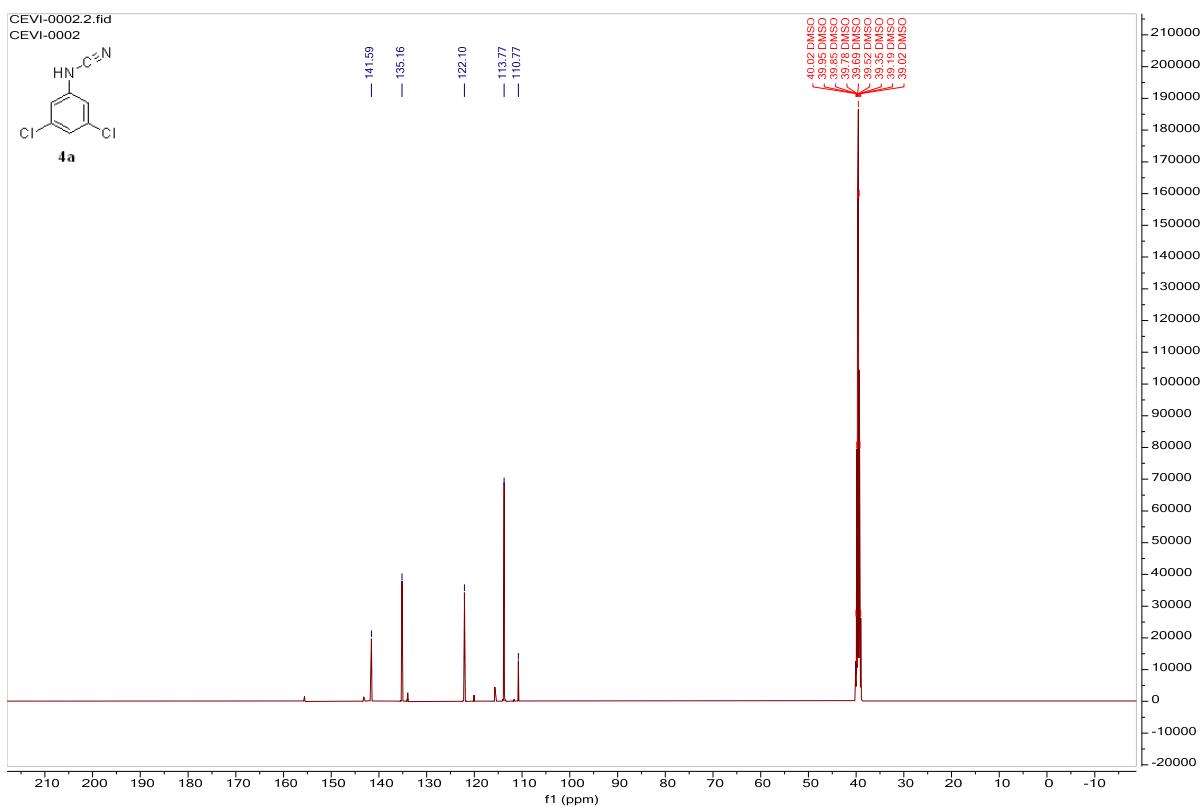
^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of **1c**



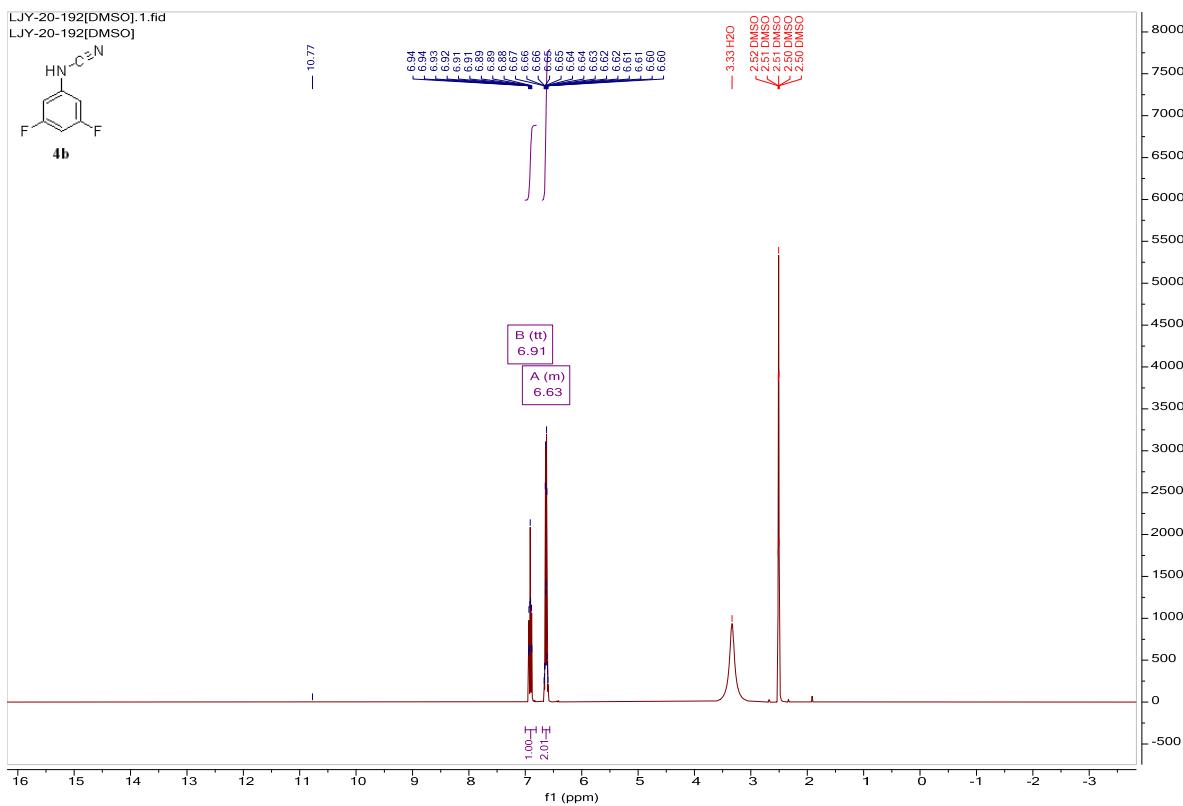
^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of **1c**



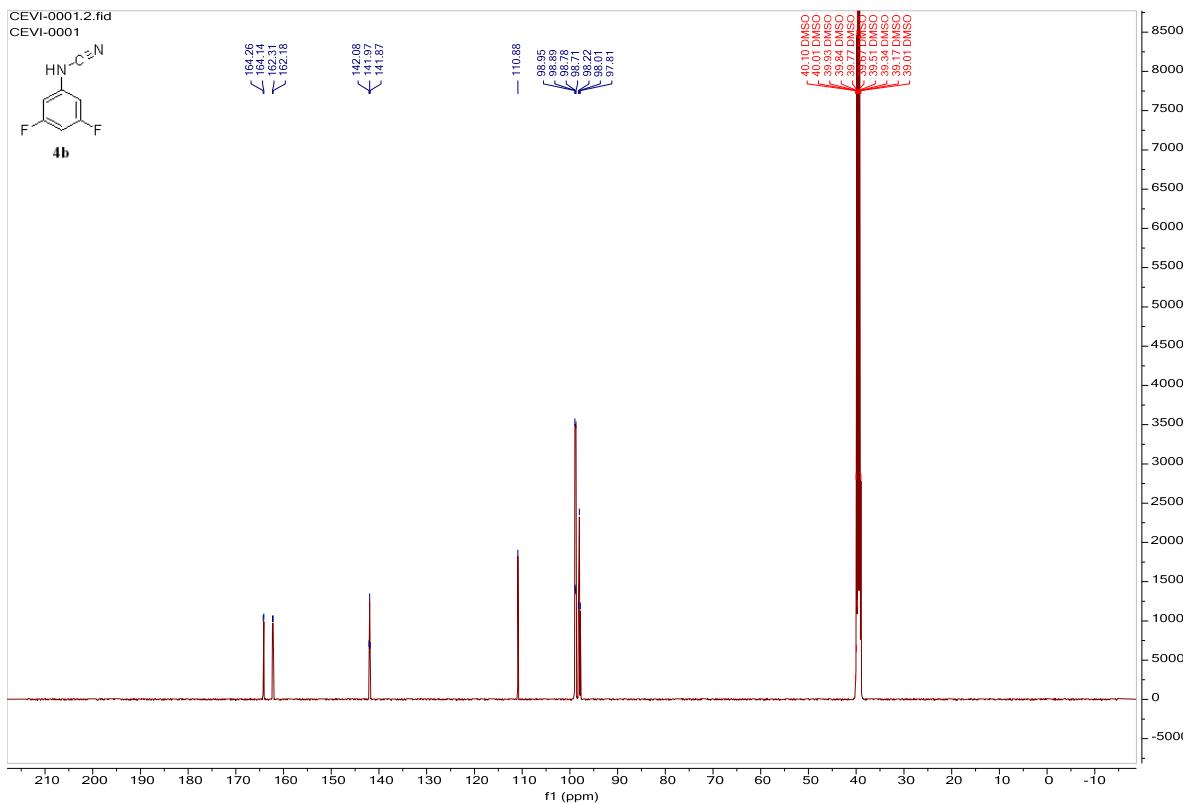
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **4a**



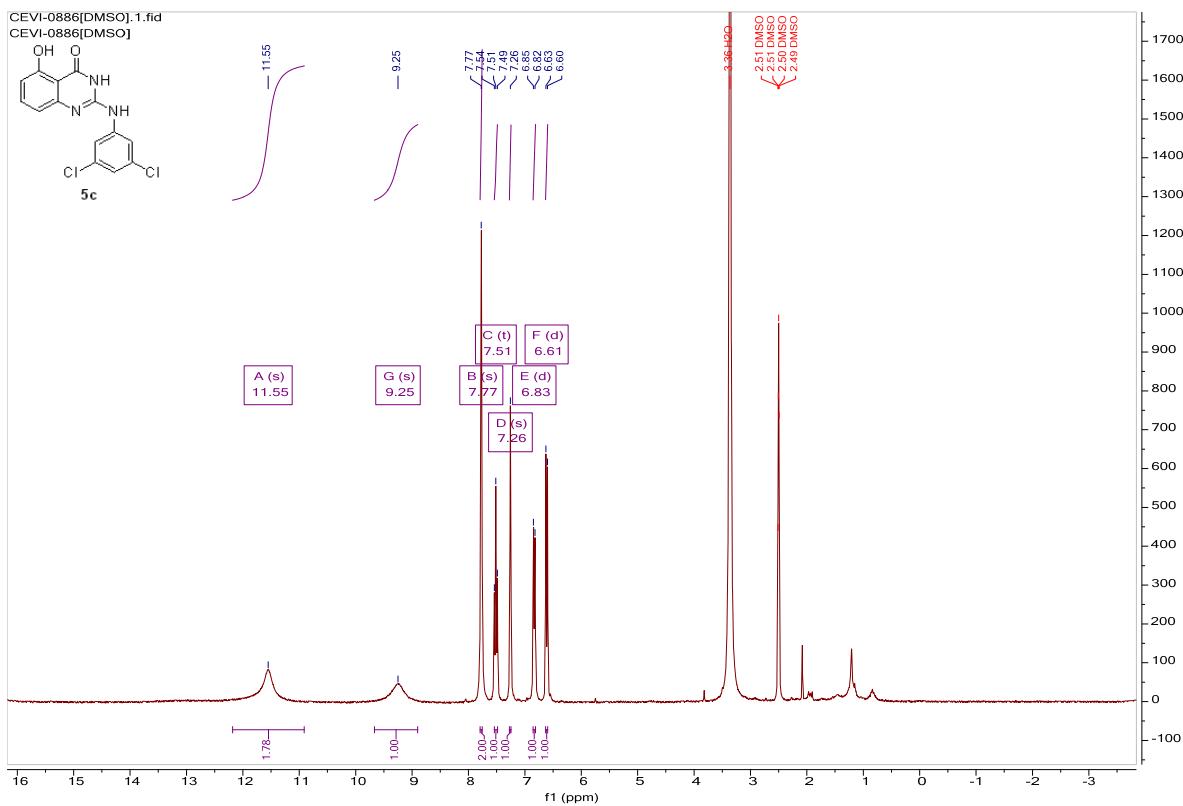
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of **4a**



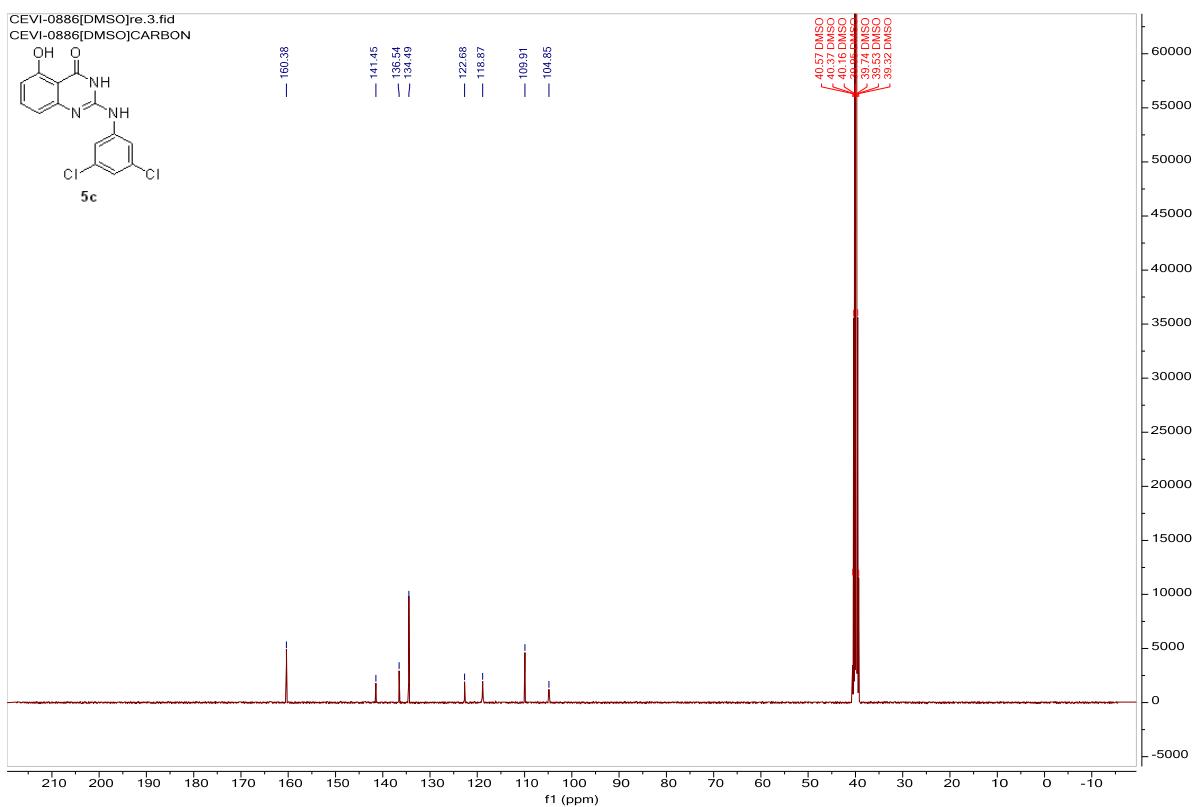
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **4b**



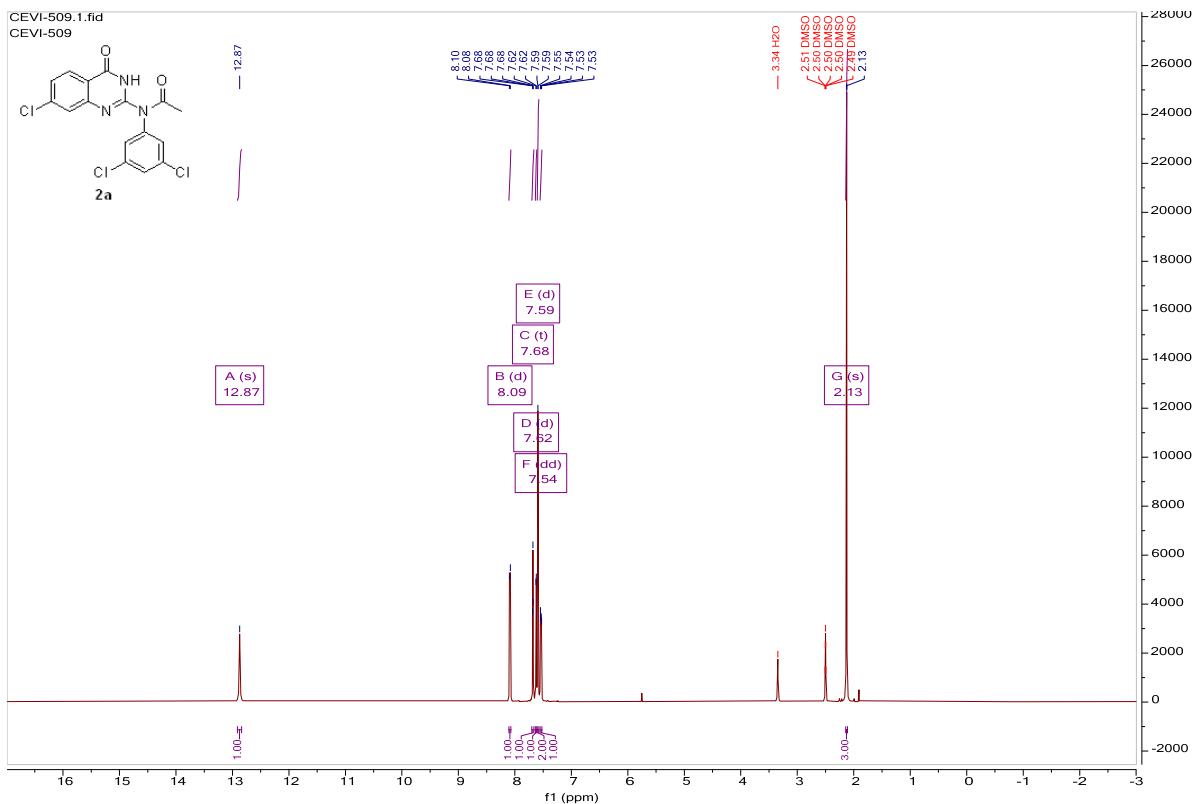
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of **4b**



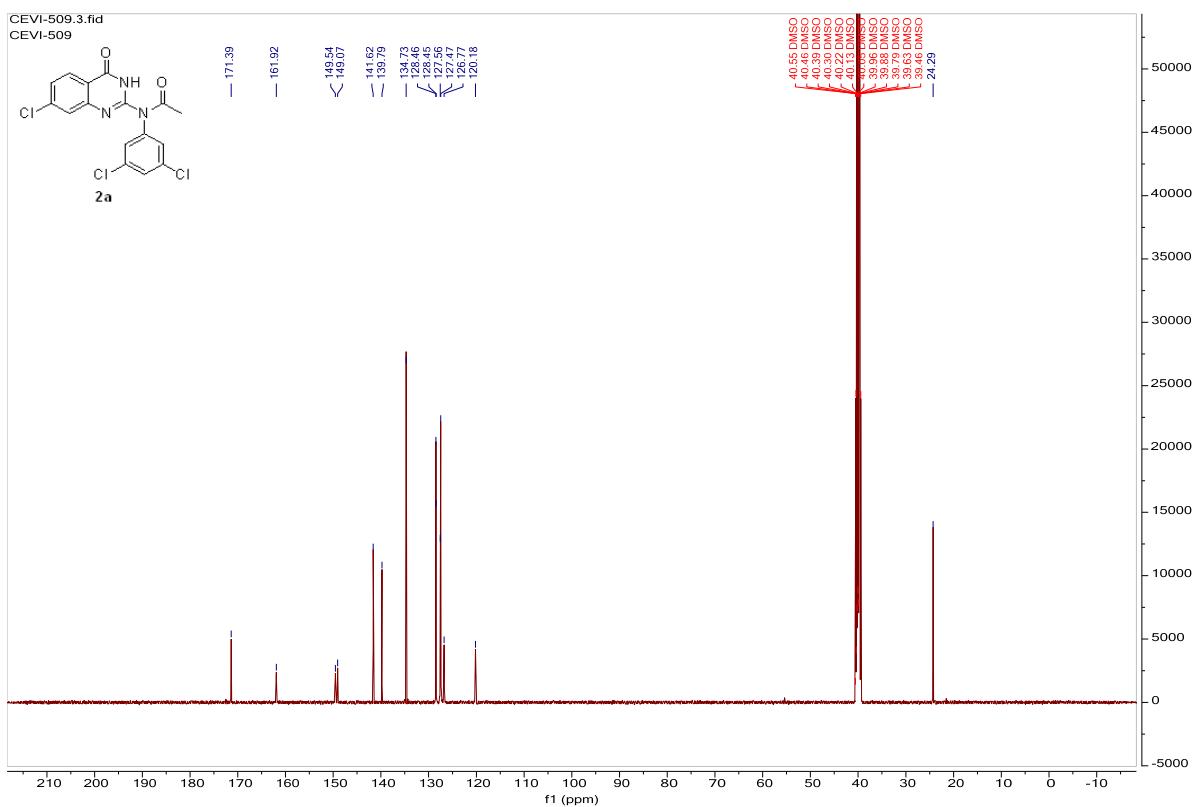
^1H NMR spectrum (300 MHz, $\text{DMSO}-d_6$) of **5c**



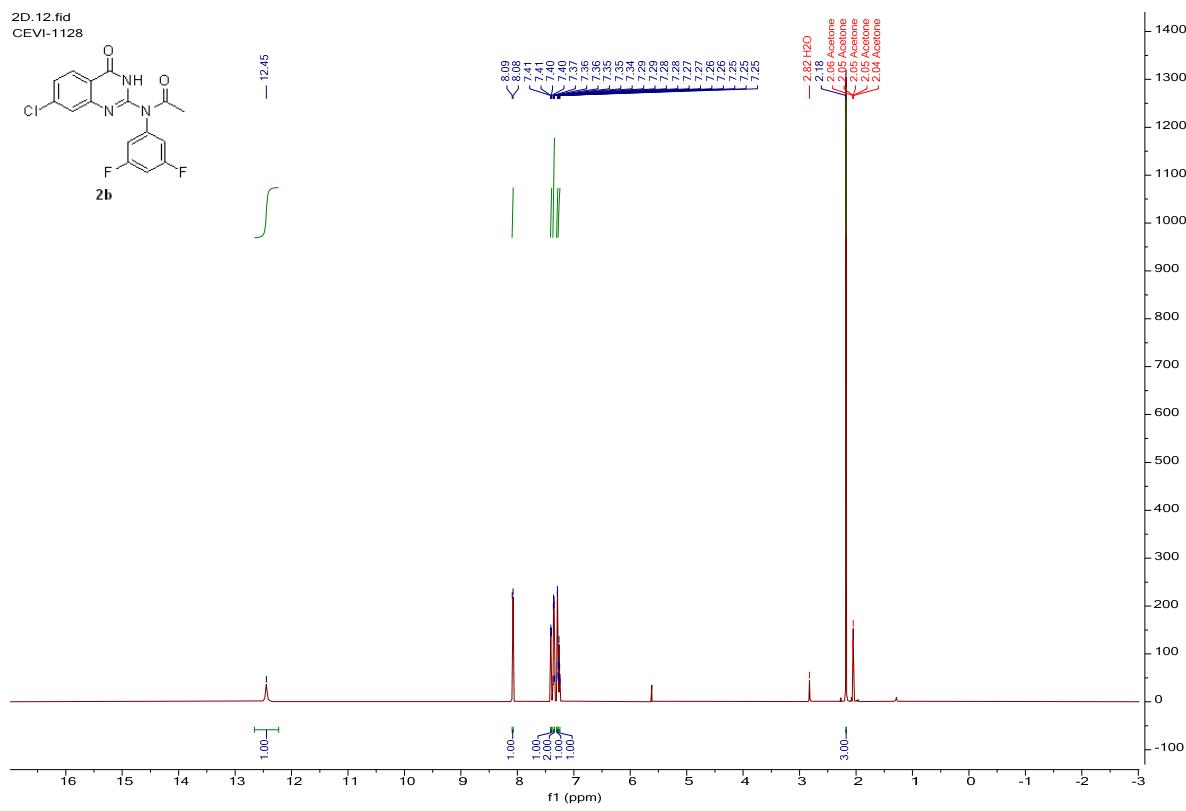
^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of **5c**



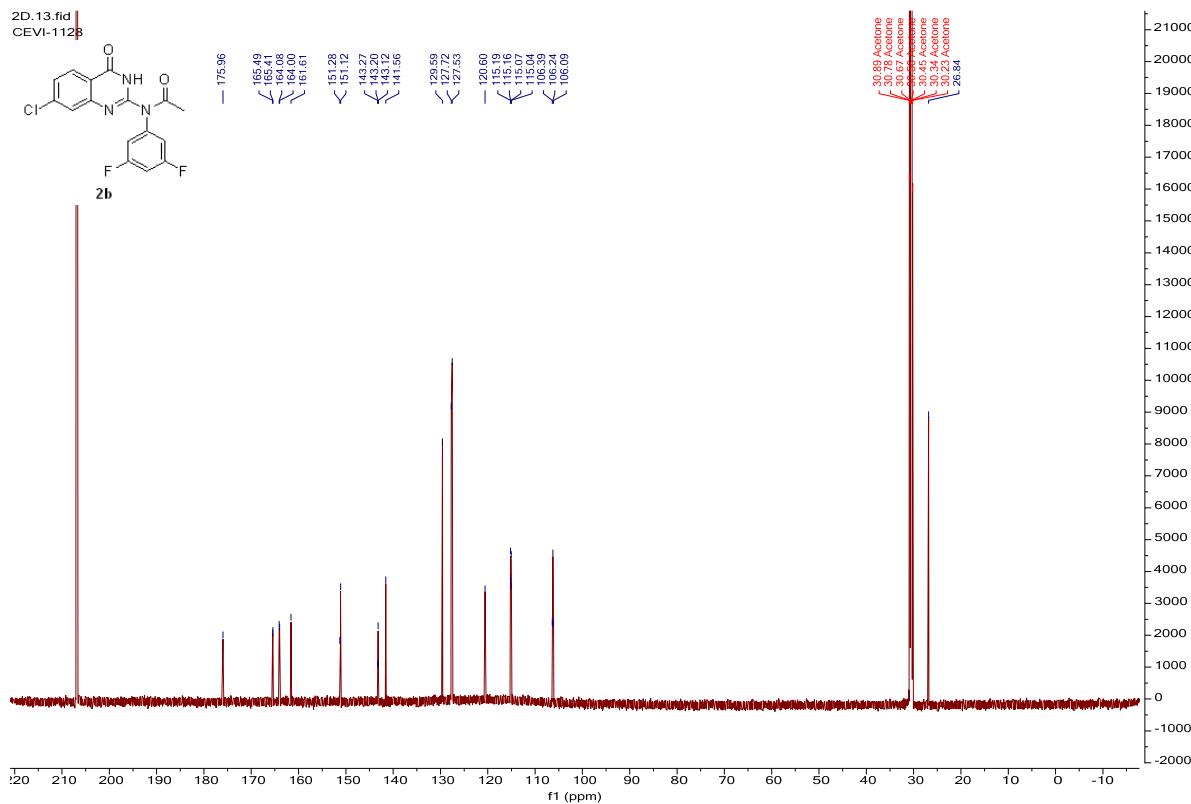
¹H NMR spectrum (500 MHz, DMSO-*d*₆) of **2a**



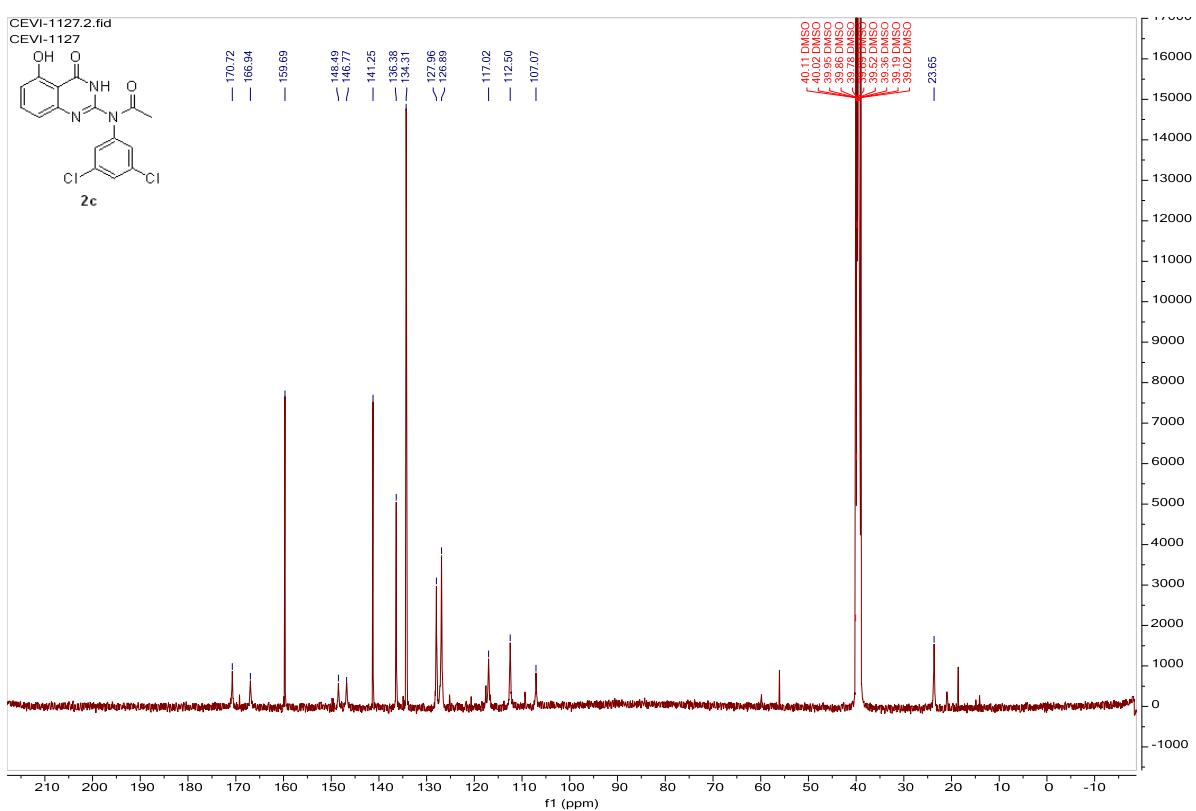
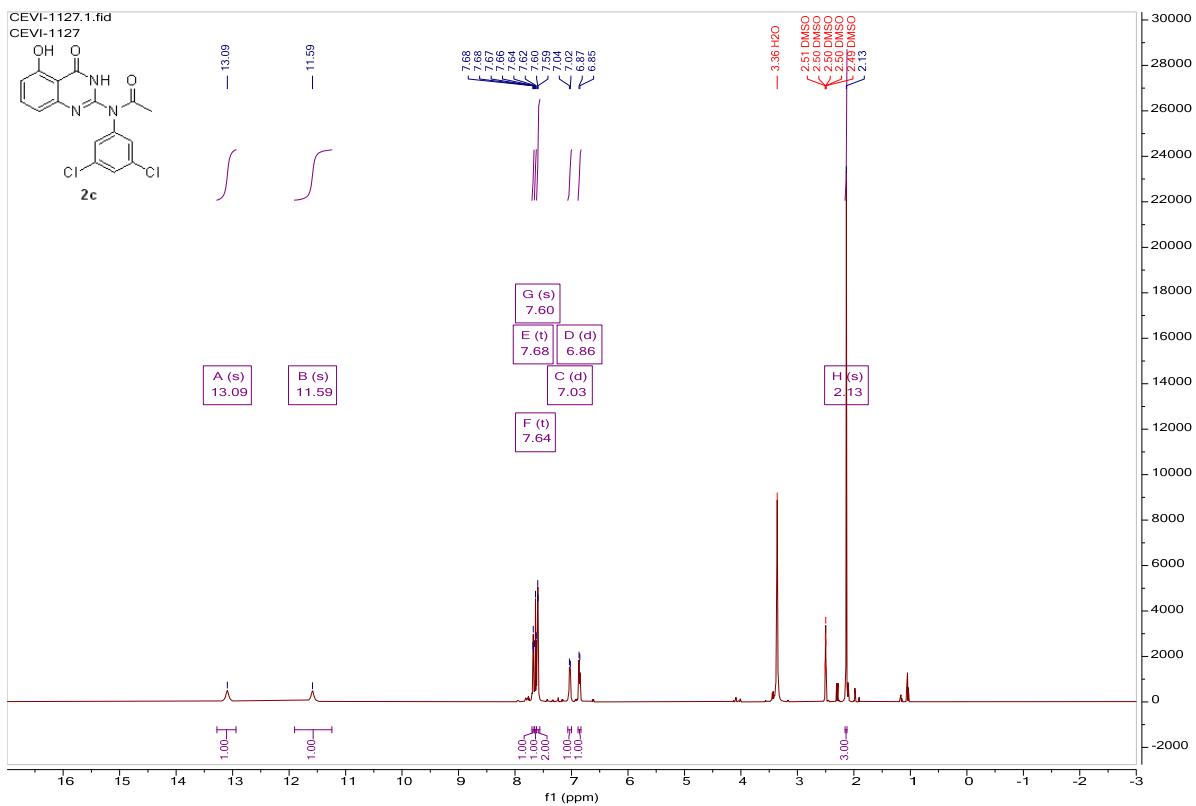
¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of **2a**



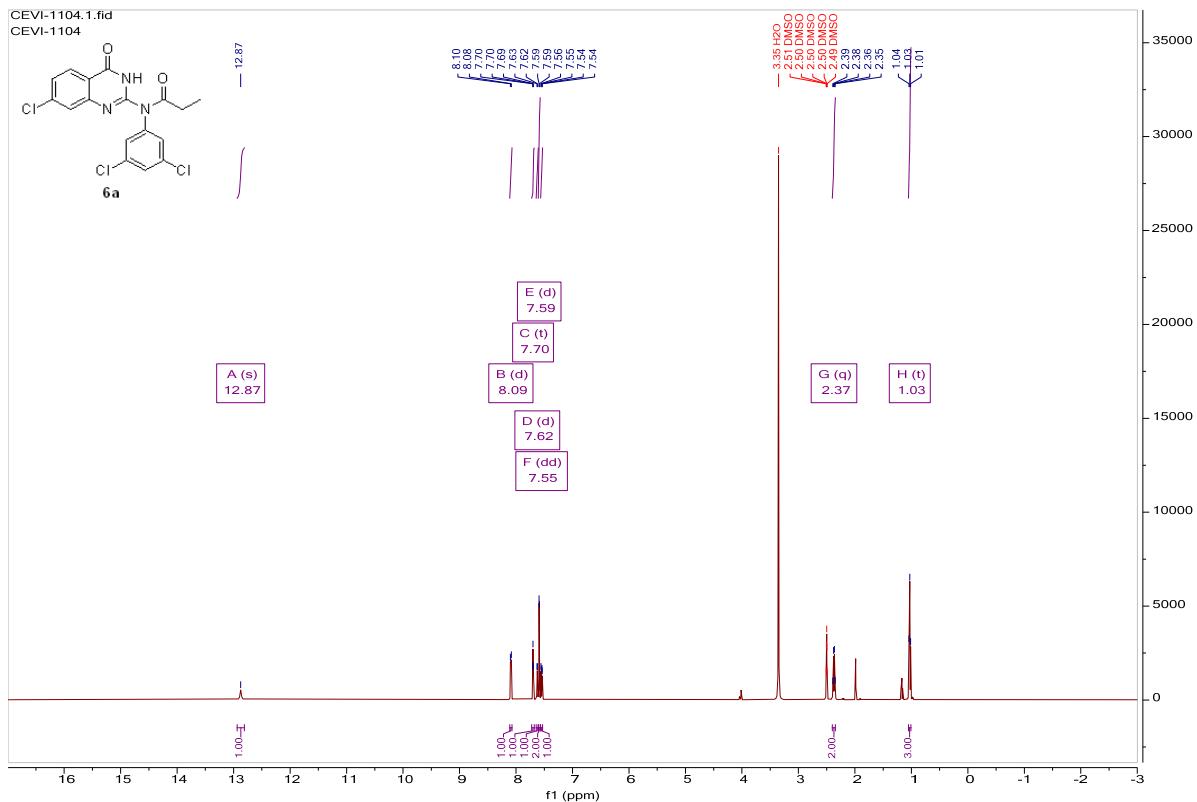
¹H NMR spectrum (700 MHz, Acetone-*d*₆) of **2b**



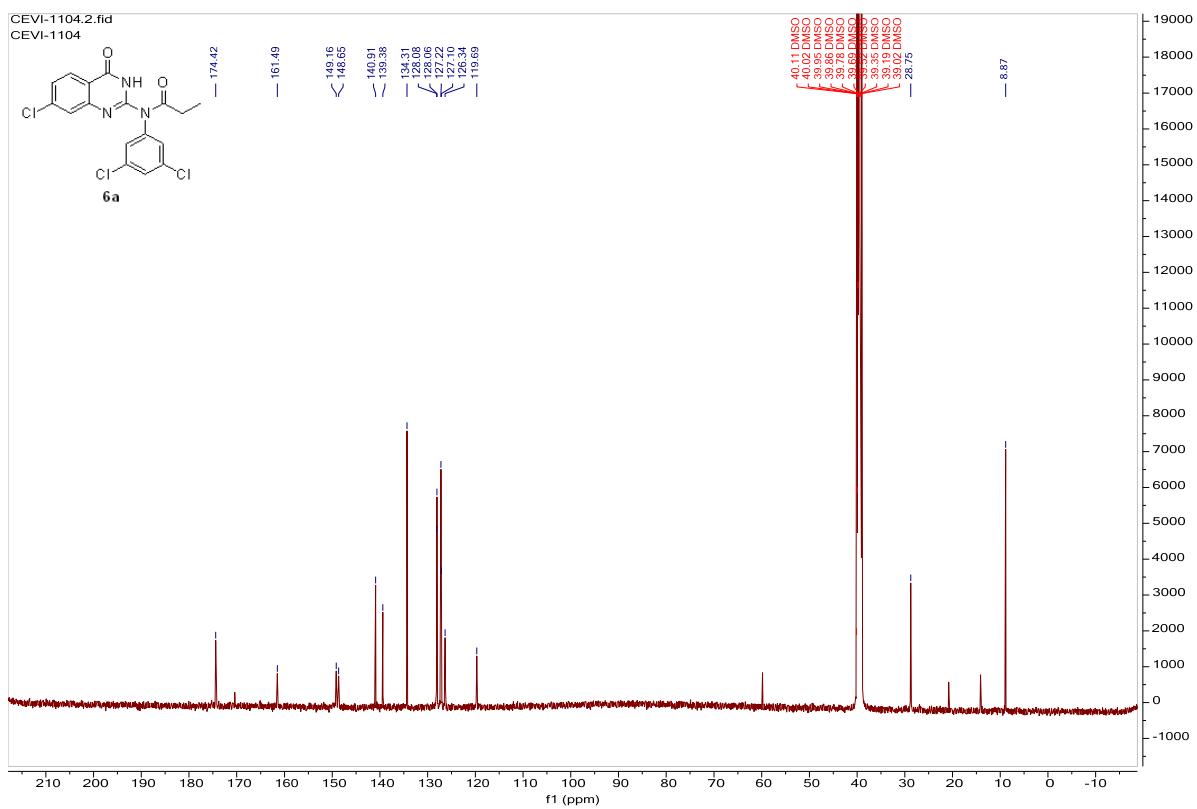
¹³C NMR spectrum (175 MHz, Acetone-*d*₆) of **2b**



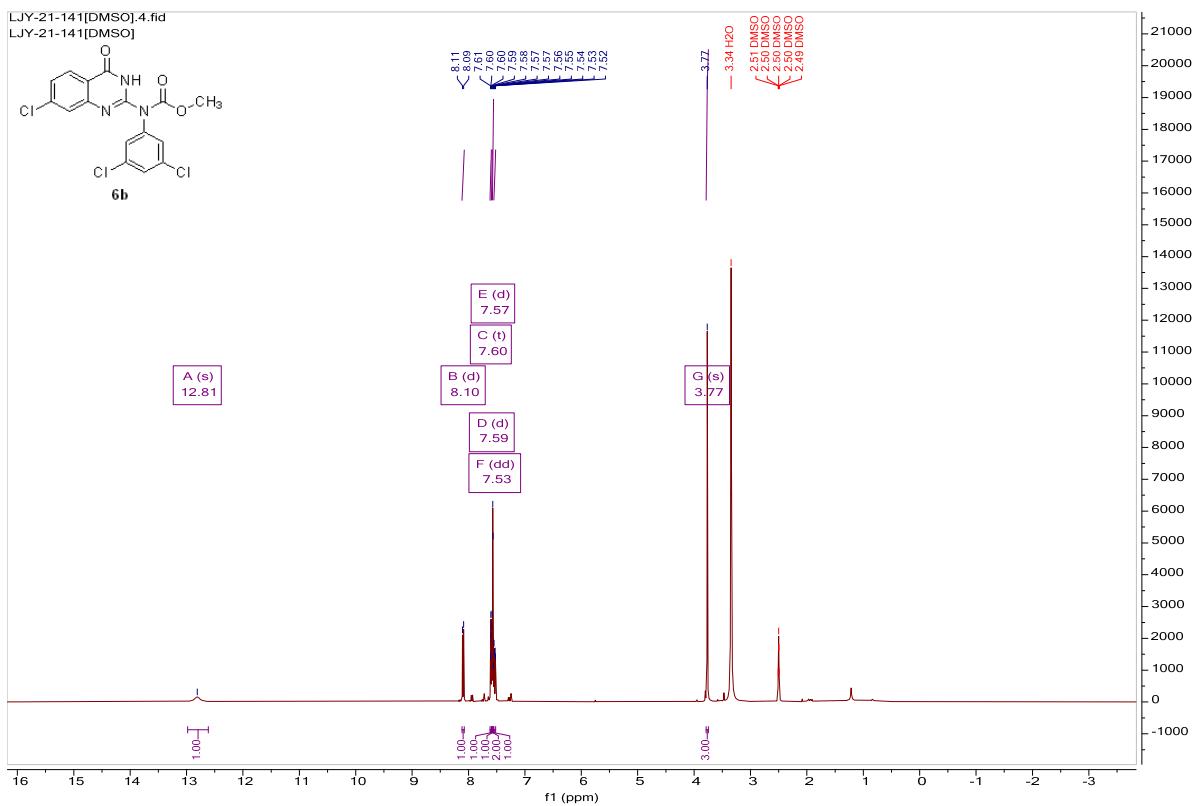
¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of **2c**



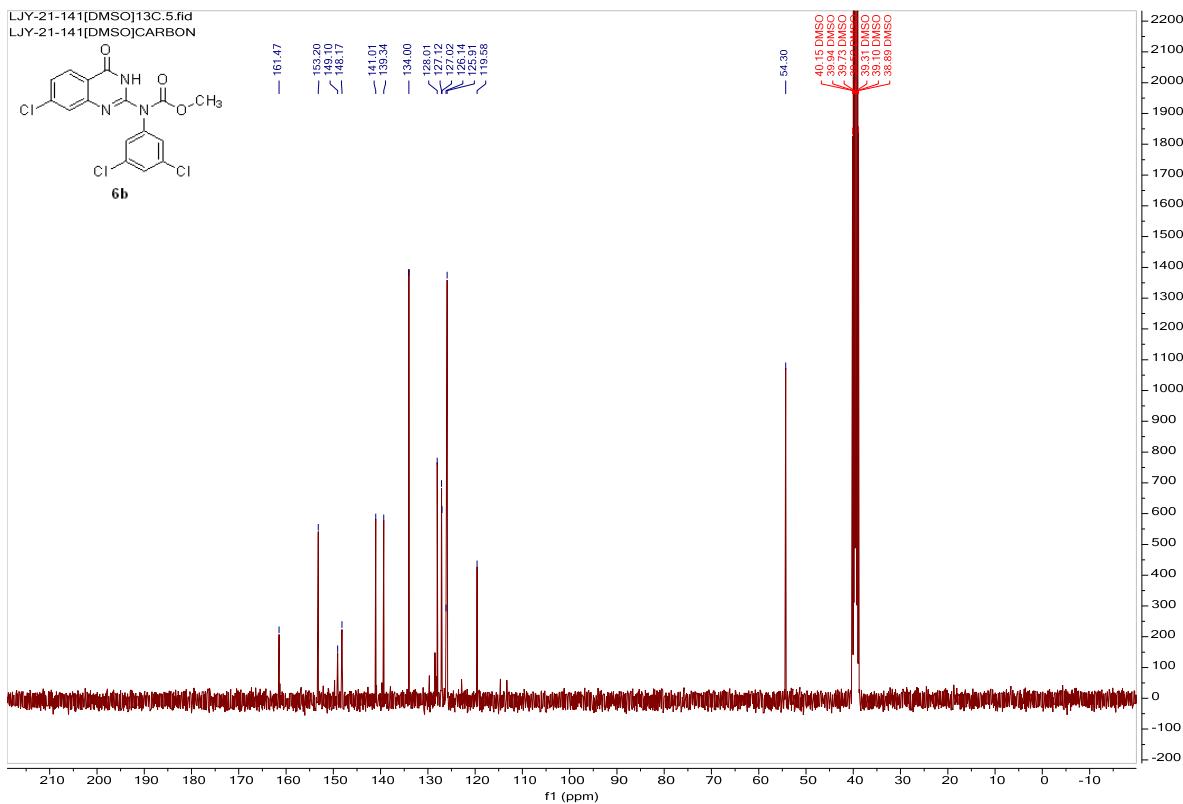
^1H NMR spectrum (500 MHz, $\text{DMSO}-d_6$) of **6a**



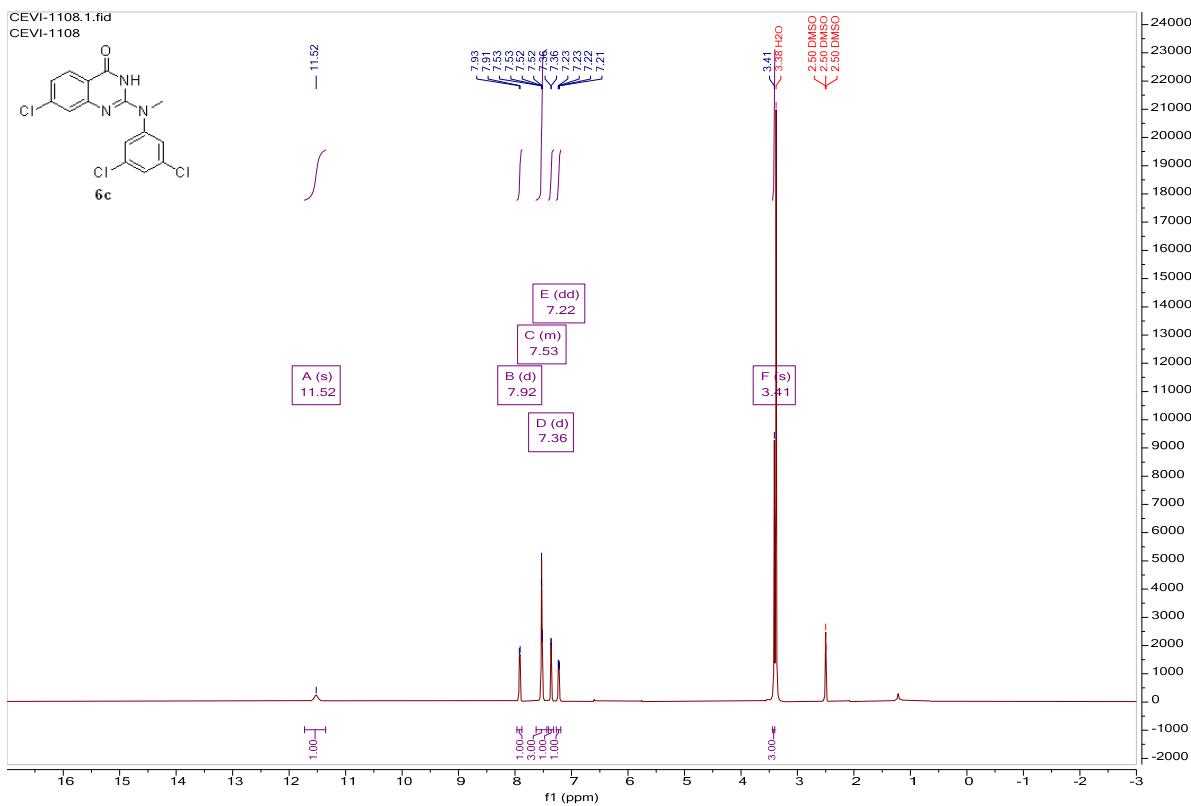
^{13}C NMR spectrum (125 MHz, $\text{DMSO}-d_6$) of **6a**



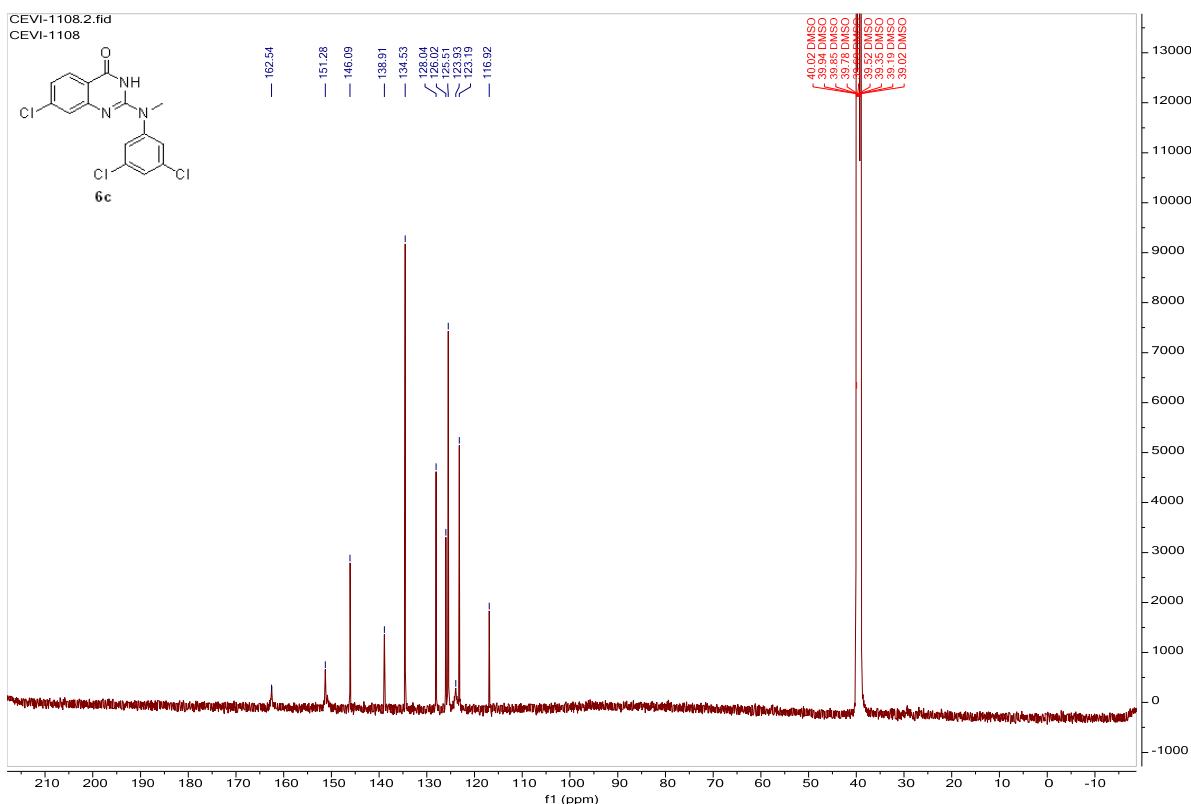
¹H NMR spectrum (400 MHz, DMSO-*d*₆) of **6b**



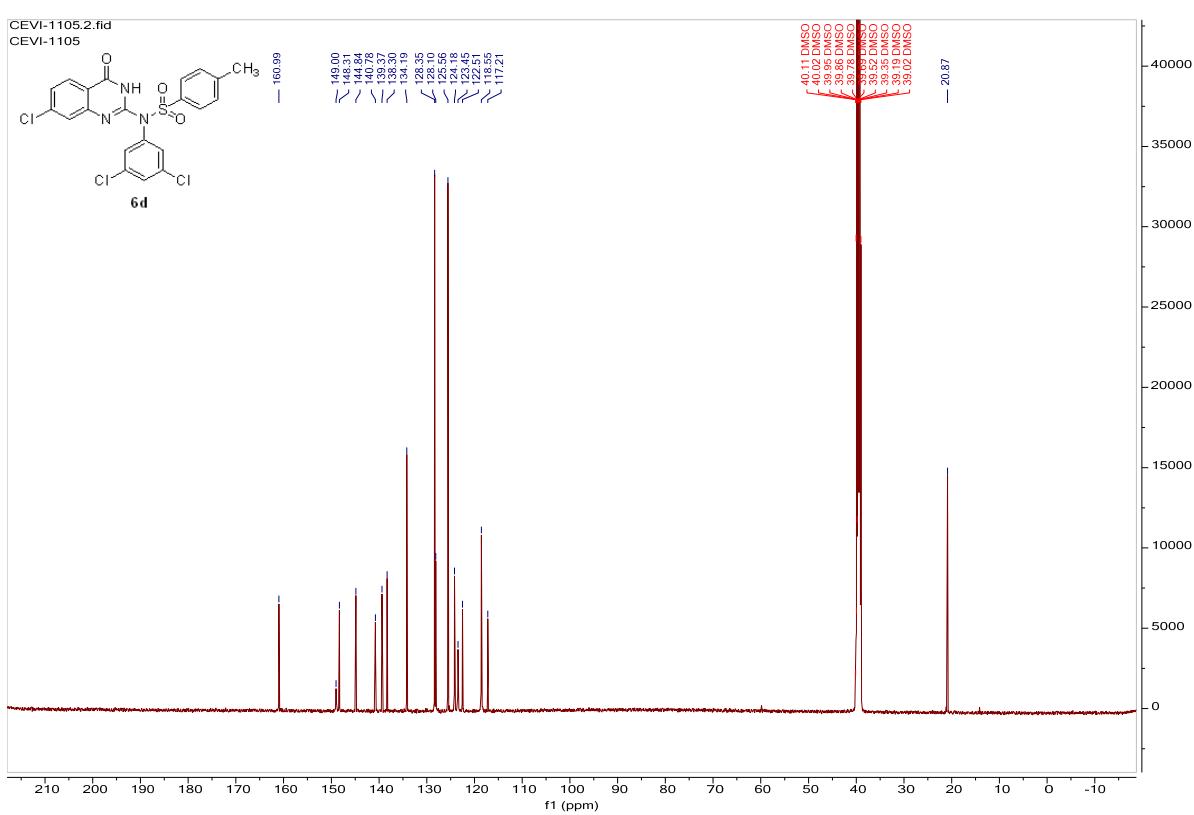
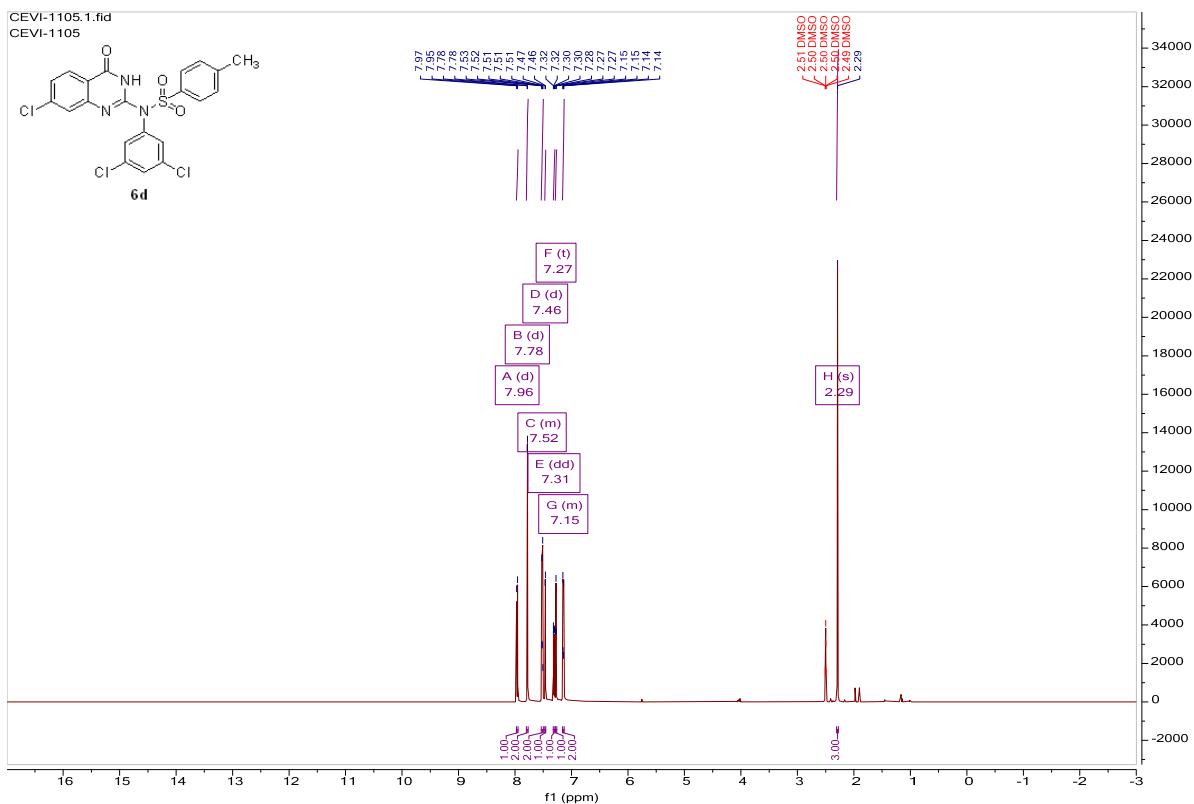
¹³C NMR spectrum (100 MHz, DMSO-*d*₆) of **6b**

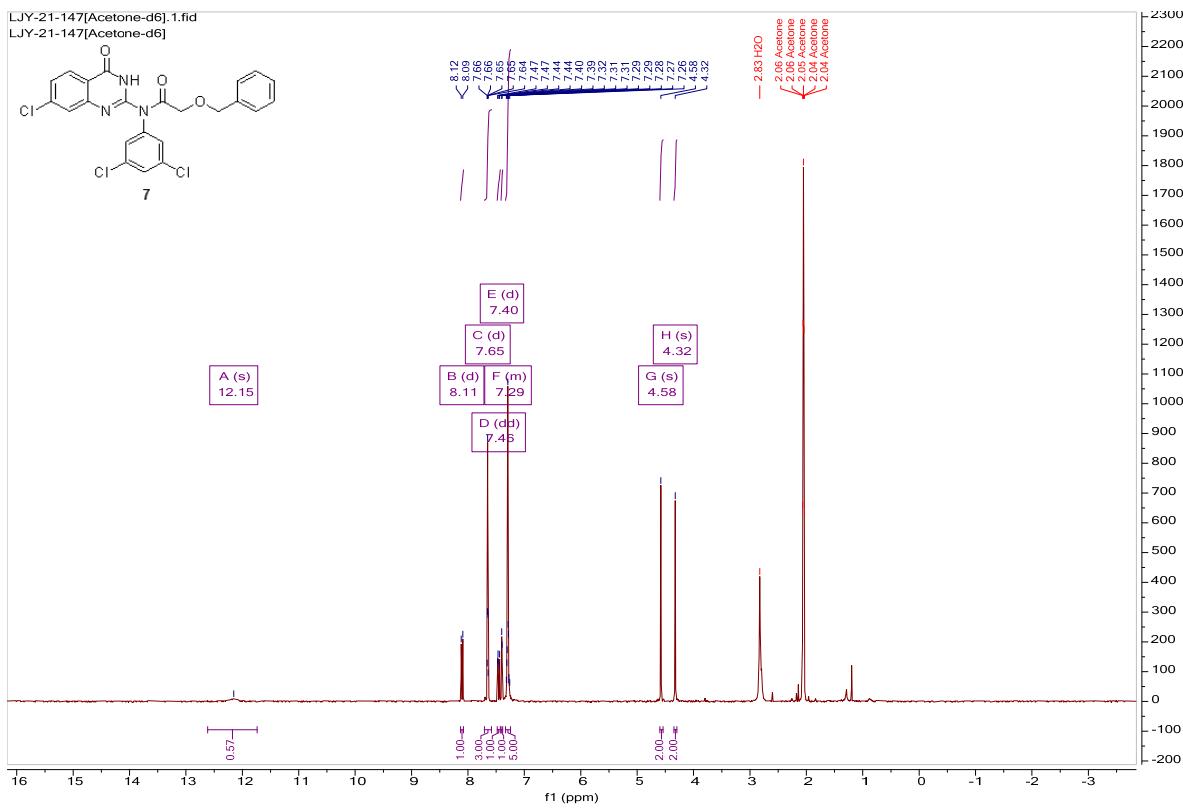


¹H NMR spectrum (500 MHz, DMSO-*d*₆) of **6c**

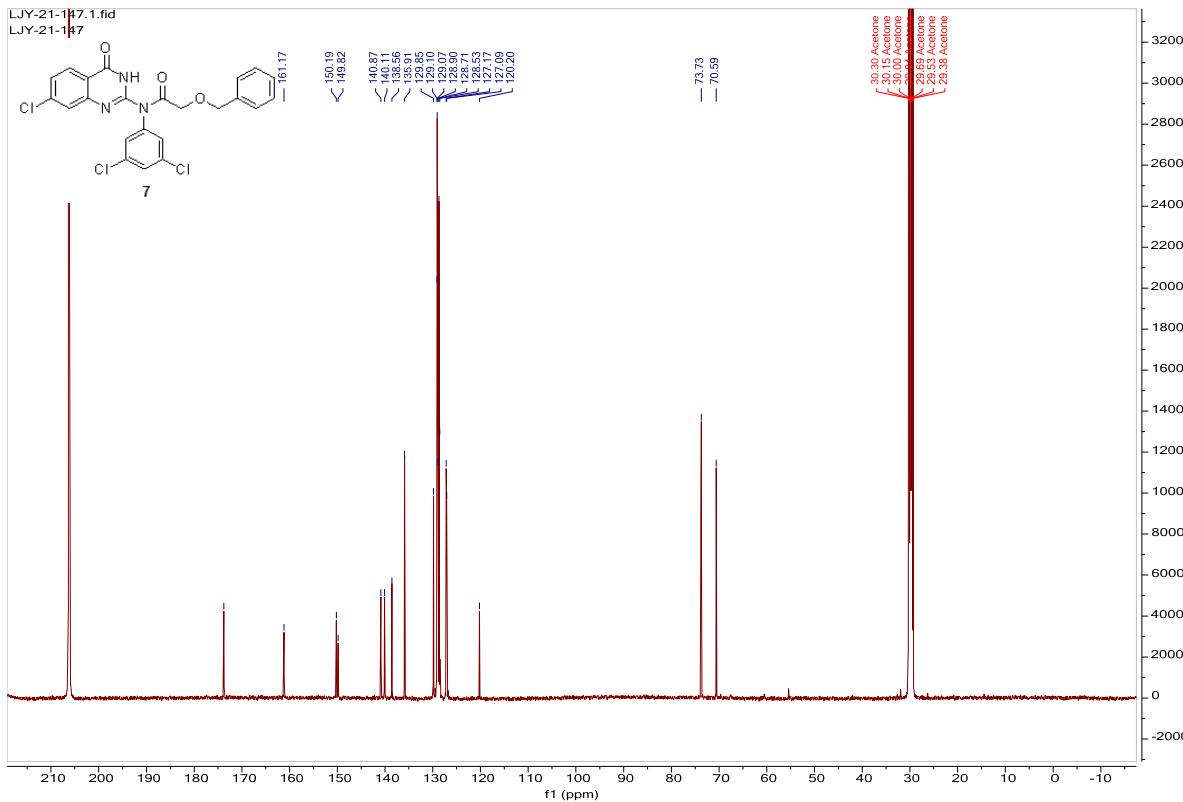


¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of **6c**

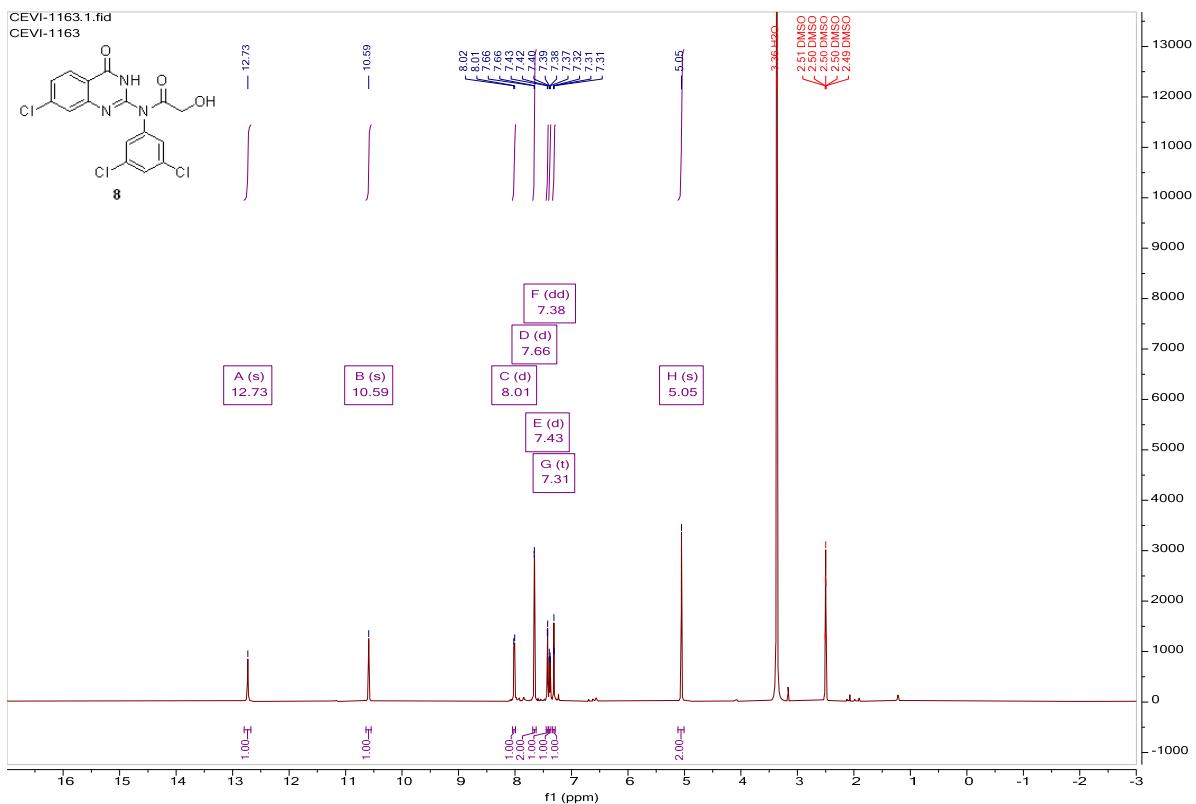




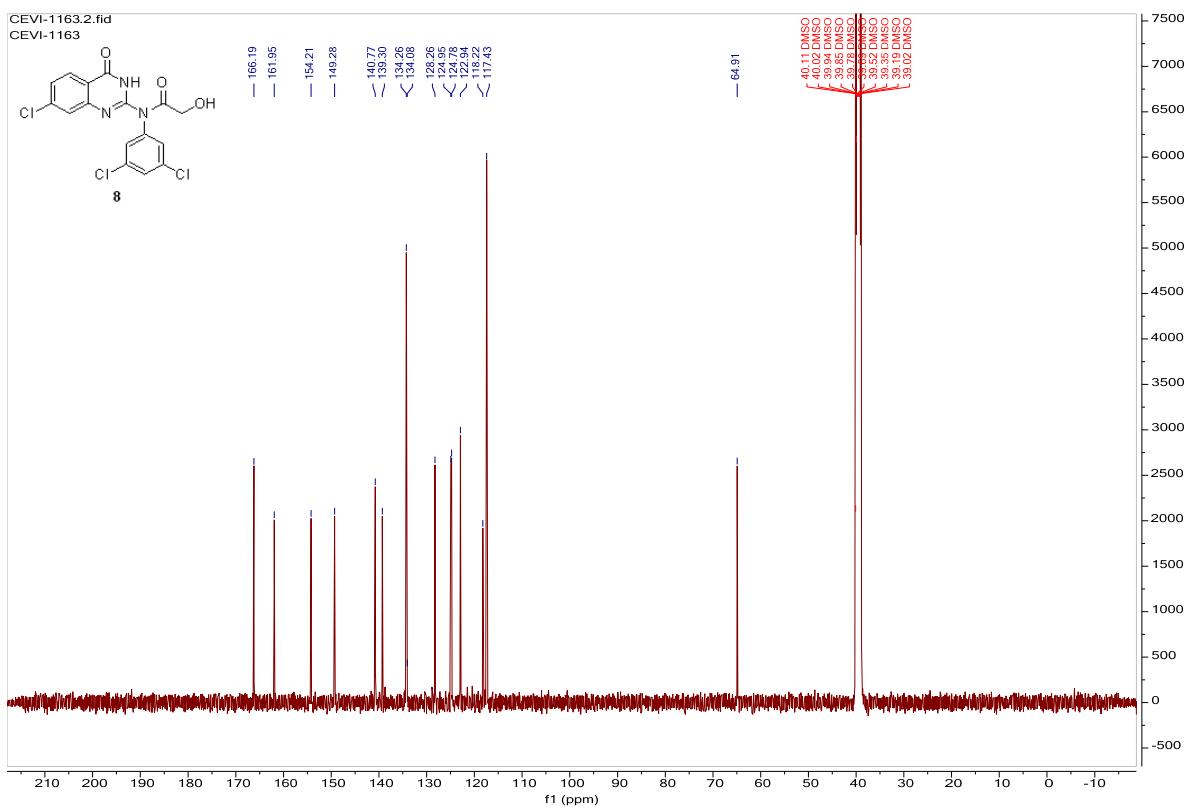
¹H NMR spectrum (300 MHz, Acetone-*d*6) of 7



¹³C NMR spectrum (125 MHz, Acetone-*d*6) of 7



¹H NMR spectrum (500 MHz, DMSO-*d*₆) of 8



¹³C NMR spectrum (125 MHz, DMSO-*d*₆) of 8

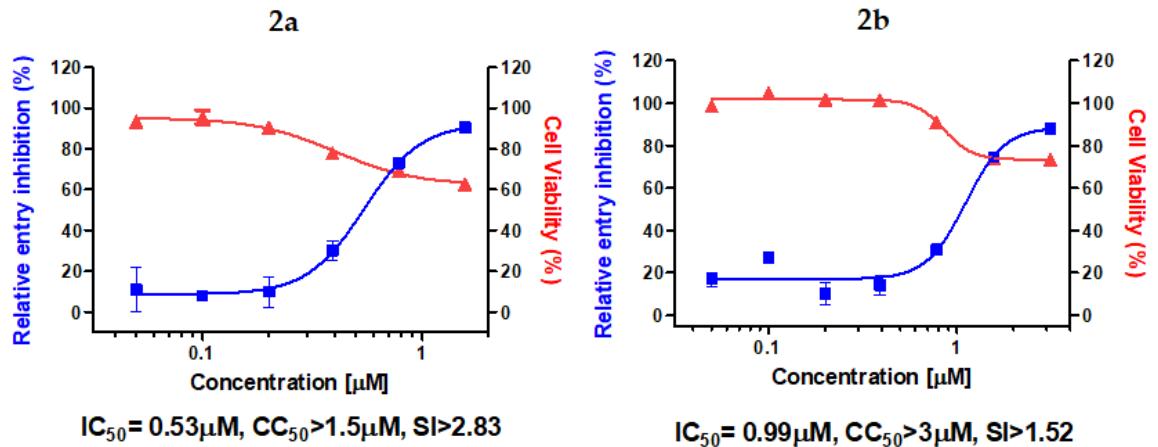


Figure 1S. Concentration-response inhibition curves of **2a** and **2b** against SARS-CoV-2 pseudovirus