

Synthesis of imidazo[4,5-*e*]thiazolo[2,3-*c*]-1,2,4-triazine-2,8-diones via a rearrangement of imidazo[4,5-*e*]thiazolo[3,2-*b*]-1,2,4-triazine-2,7-diones in the reaction with isatins

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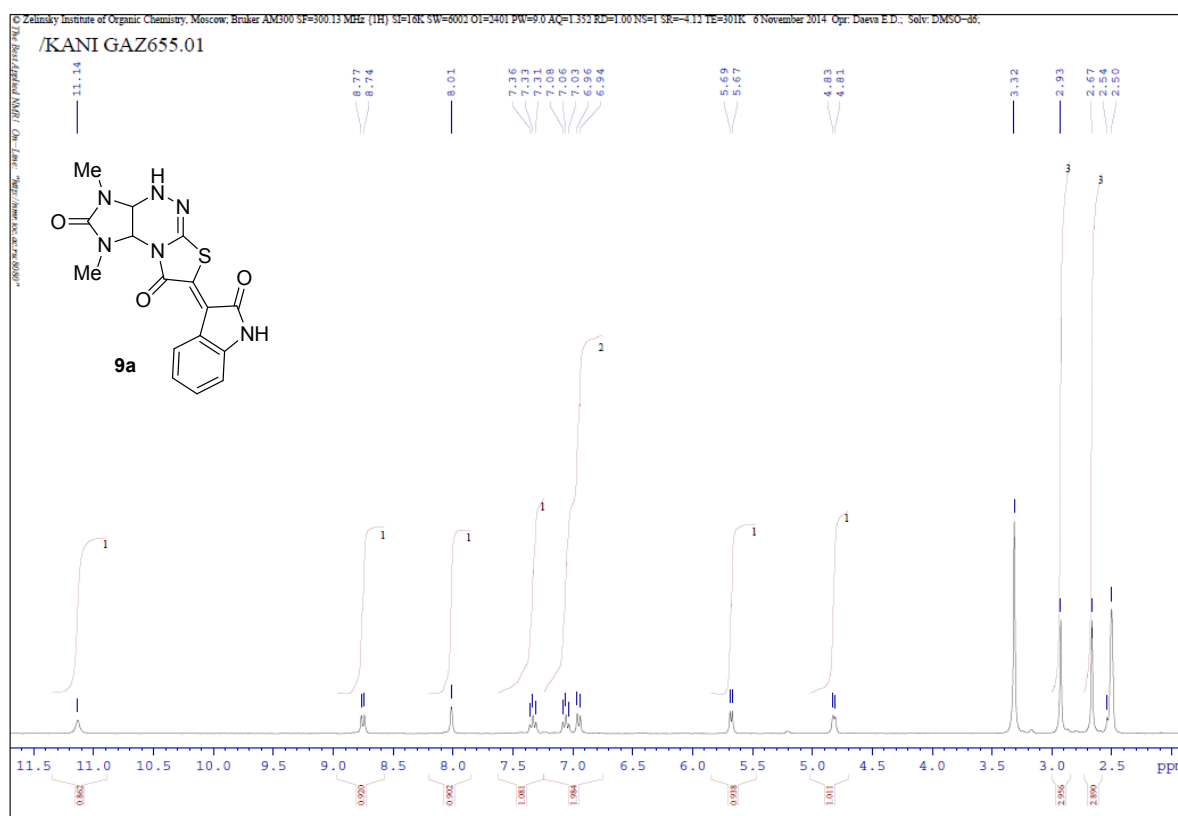
^aN.D. Zelinsky Institute of Organic Chemistry, Russian Academy of Sciences, Moscow 119991, Russian Federation. E-mail: gaz@ioc.ac.ru

^bA.N. Nesmeyanov Institute of Organoelement Compounds, Russian Academy of Sciences, Moscow 119991, Russian Federation. E-mail: unelya@xrlab.ineos.ac.ru

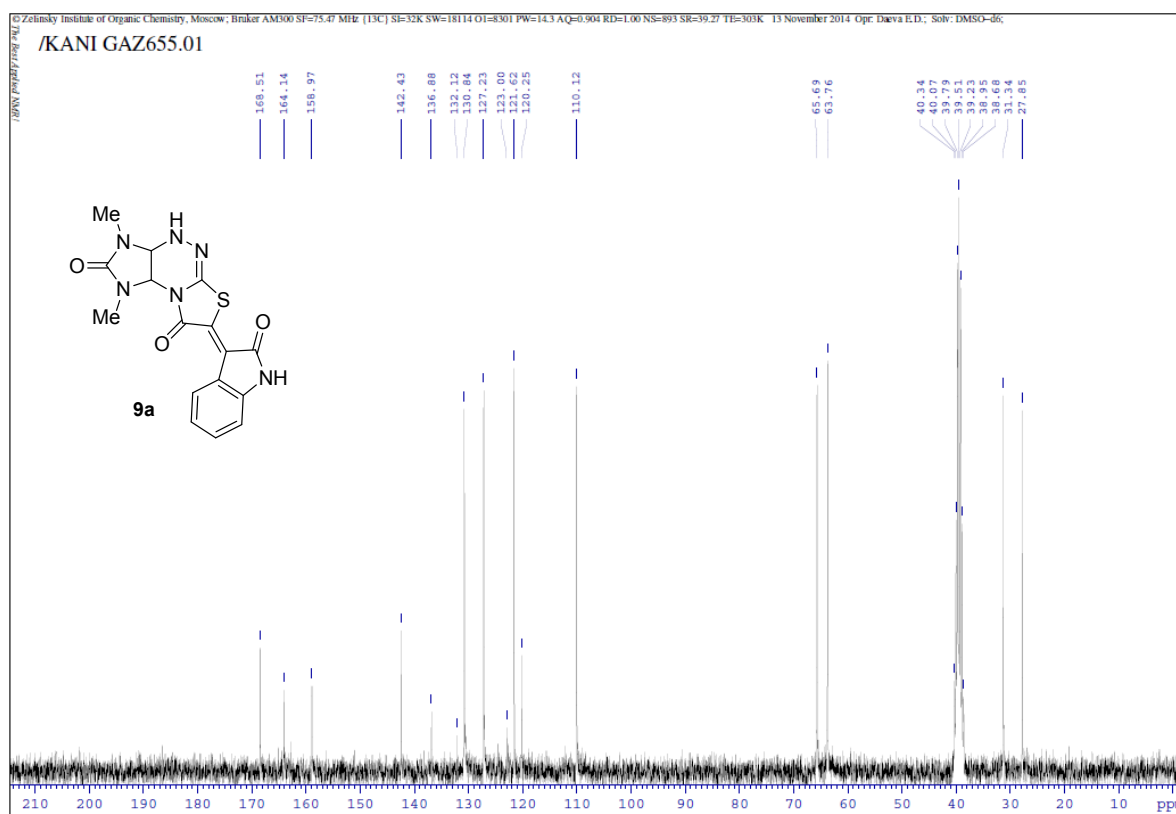
^cVoronezh State University, Voronezh, 394000, Russian Federation. E-mail: iezan@mail.ru

1. Spectra ¹ H, ¹³ C NMR, NOESY (for 11o), HMBC (for 11o)	2
2. Powder diffraction pattern for compounds 9b,d,e,n,11c,b	48

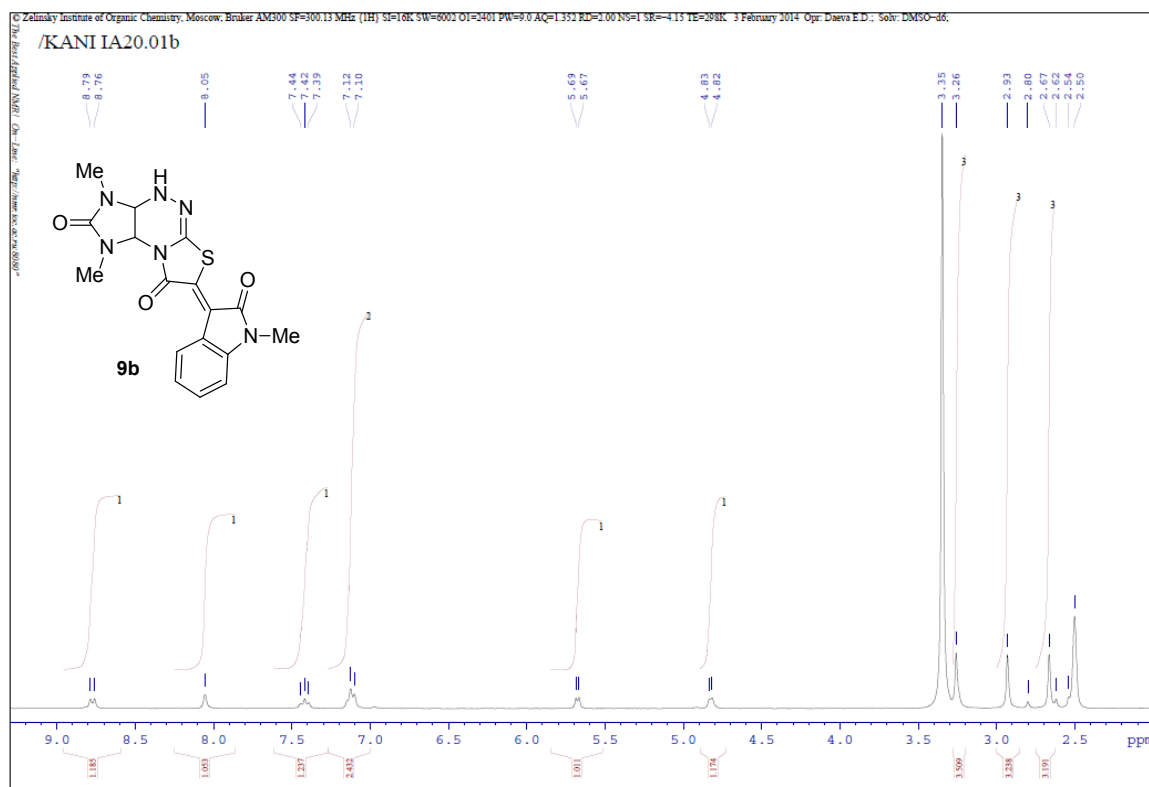
H NMR spectrum of **9a**



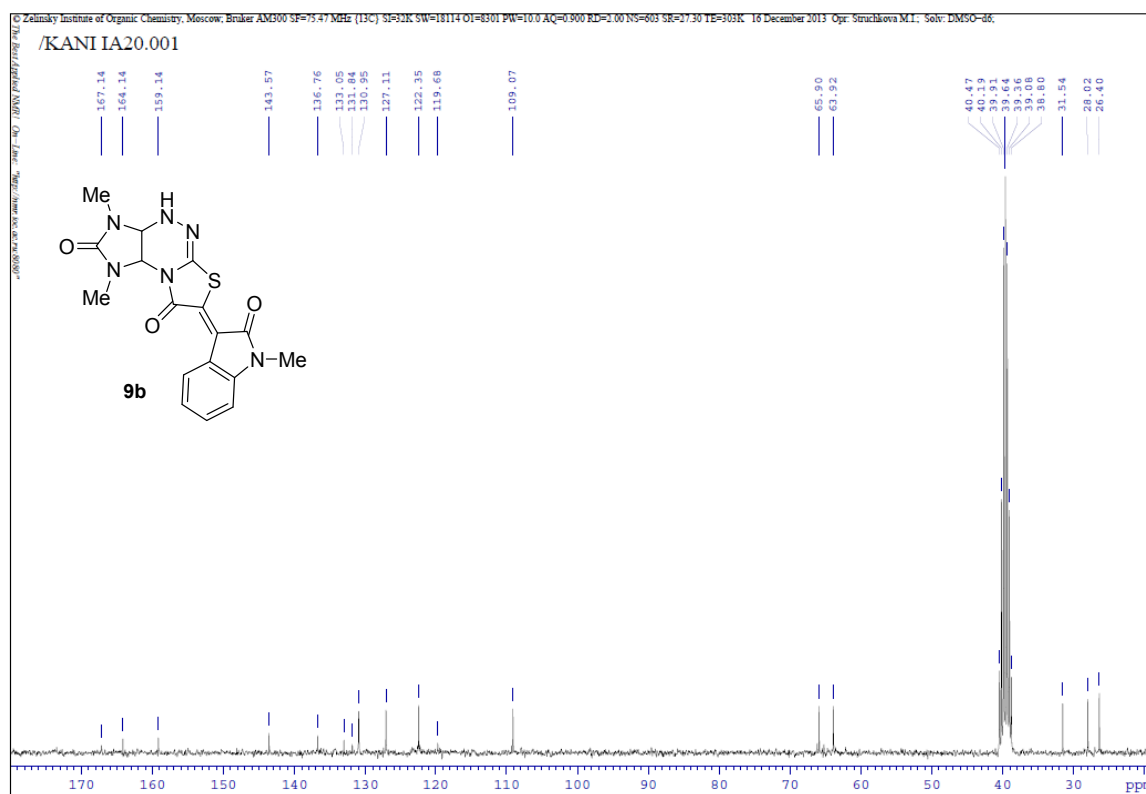
¹³C NMR spectrum of **9a**



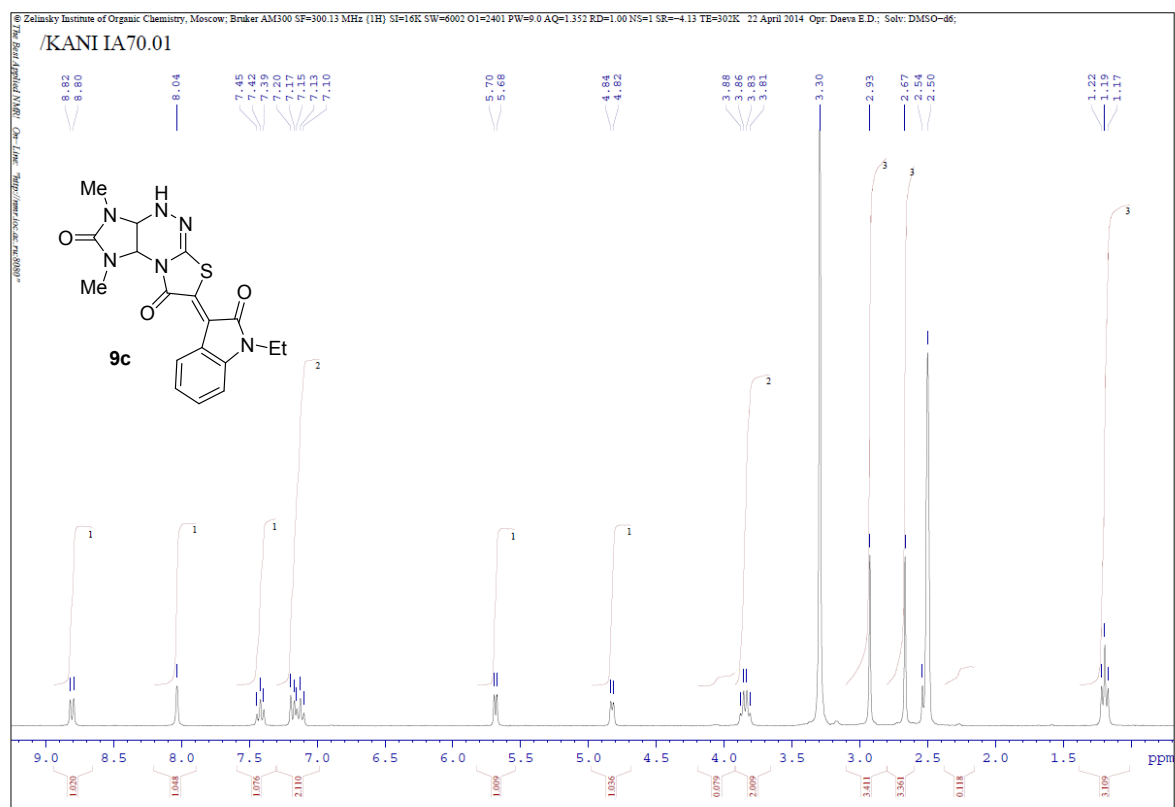
¹H NMR spectrum of **9b**



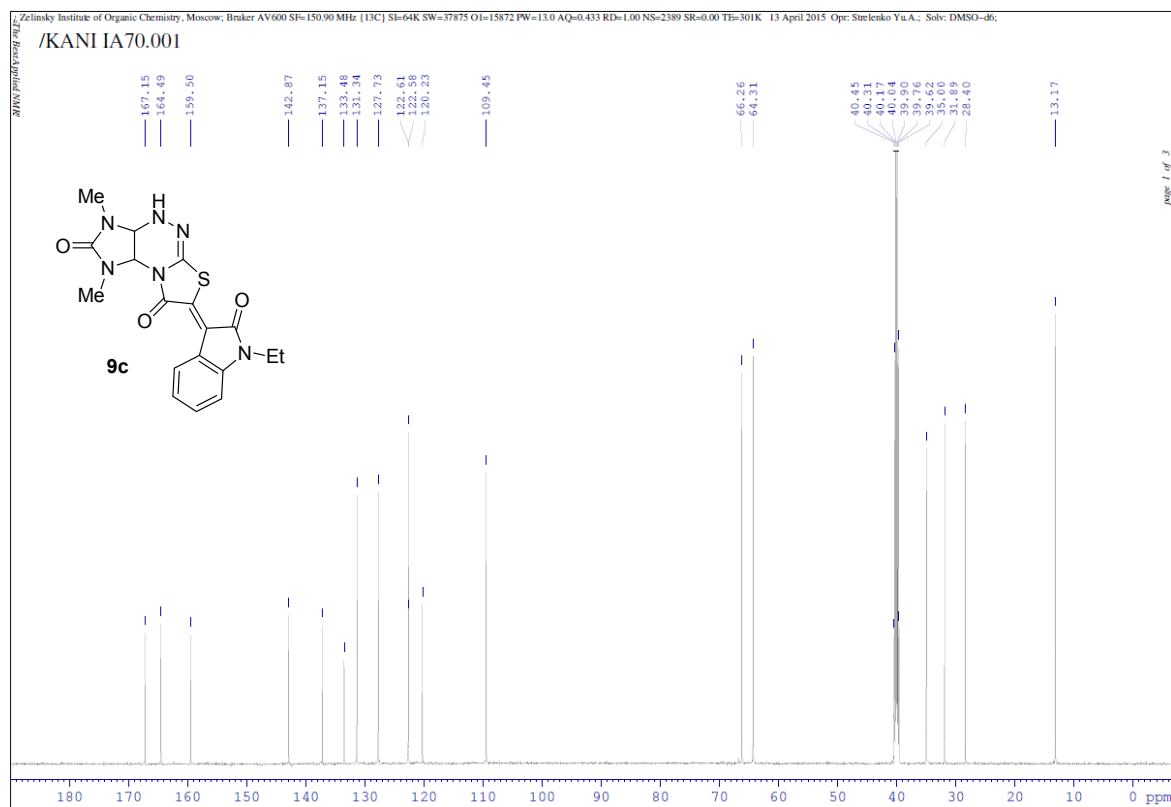
¹³C NMR spectrum of **9b**



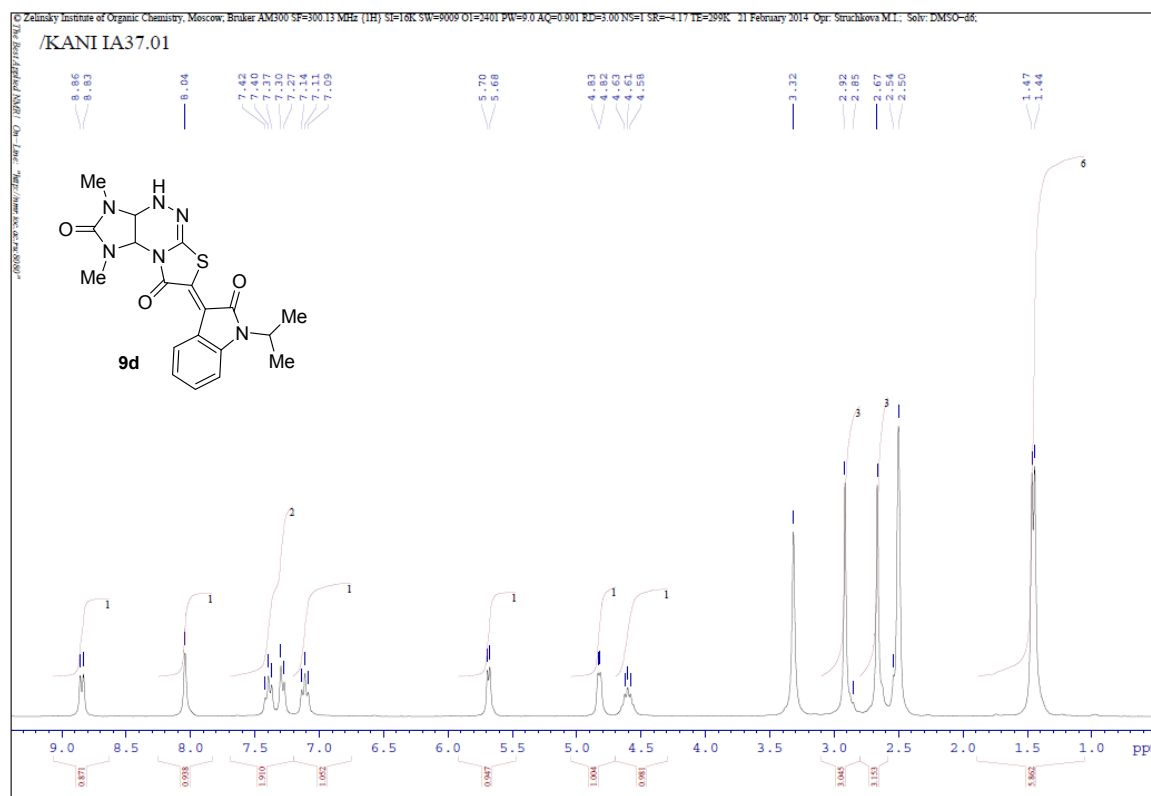
¹H NMR spectrum of **9c**



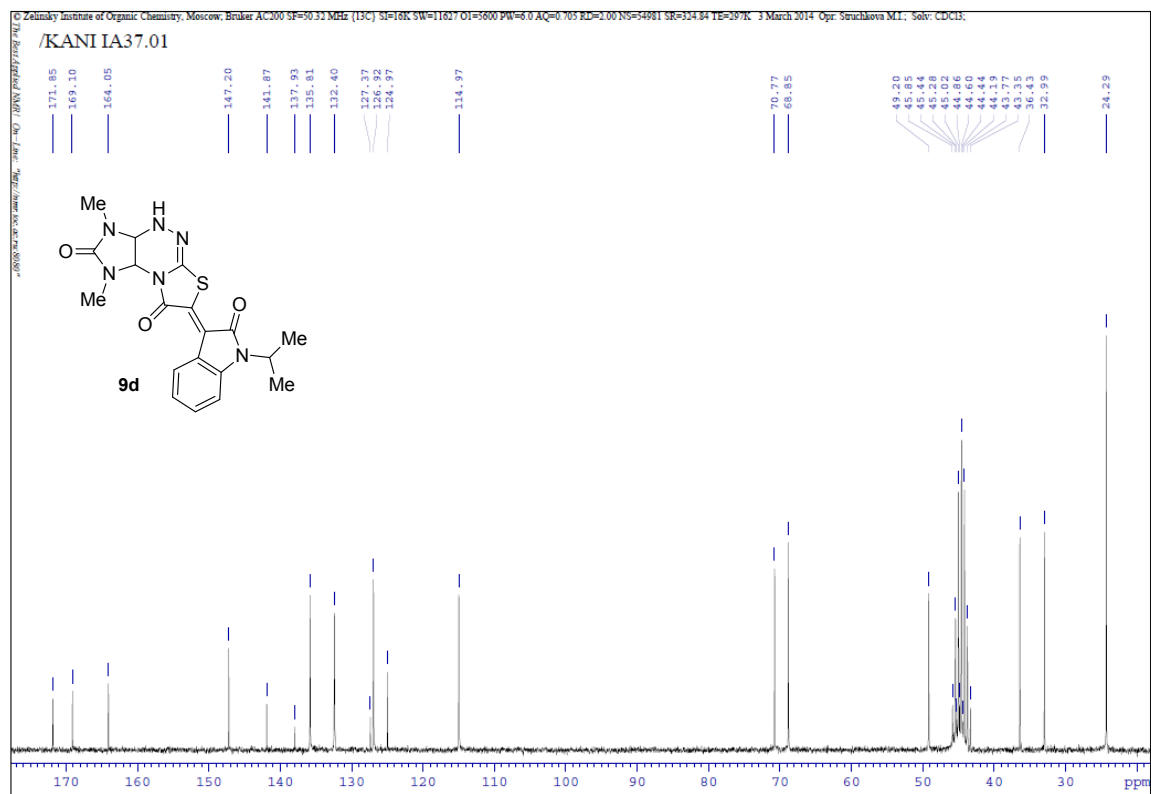
¹³C NMR spectrum of **9c**



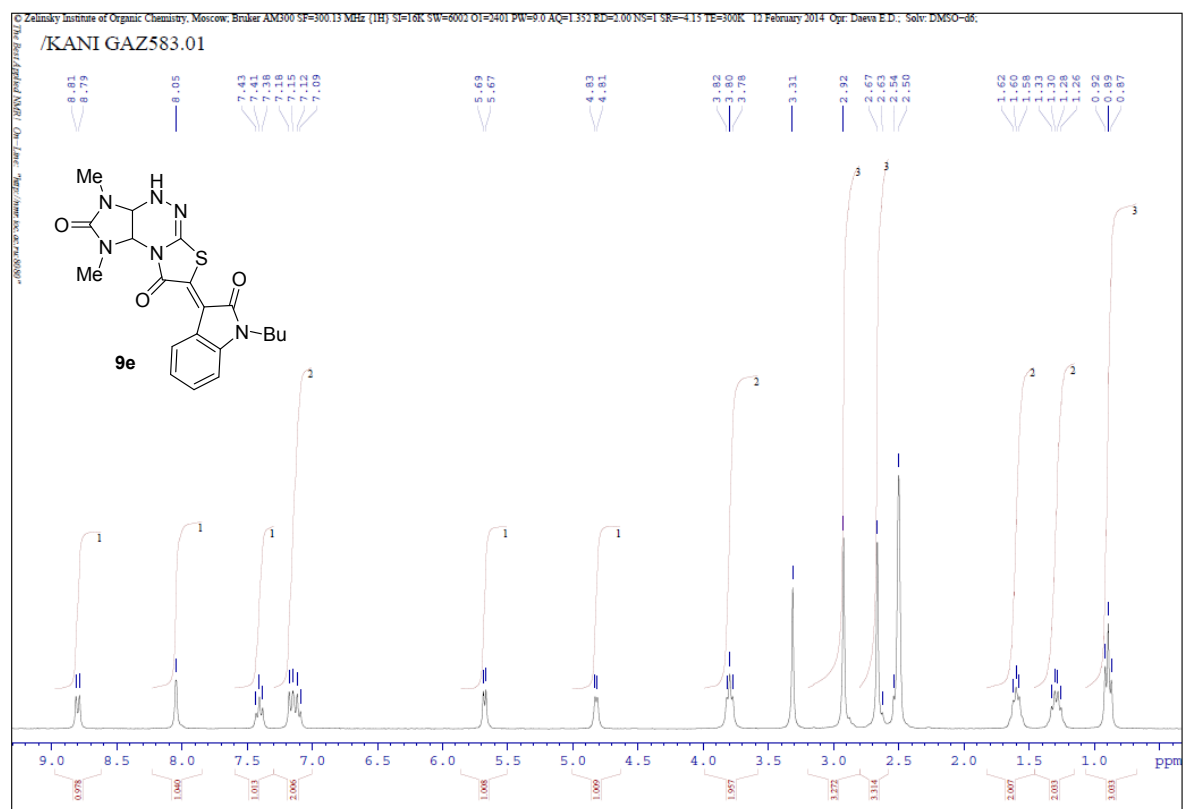
¹H NMR spectrum of **9d**



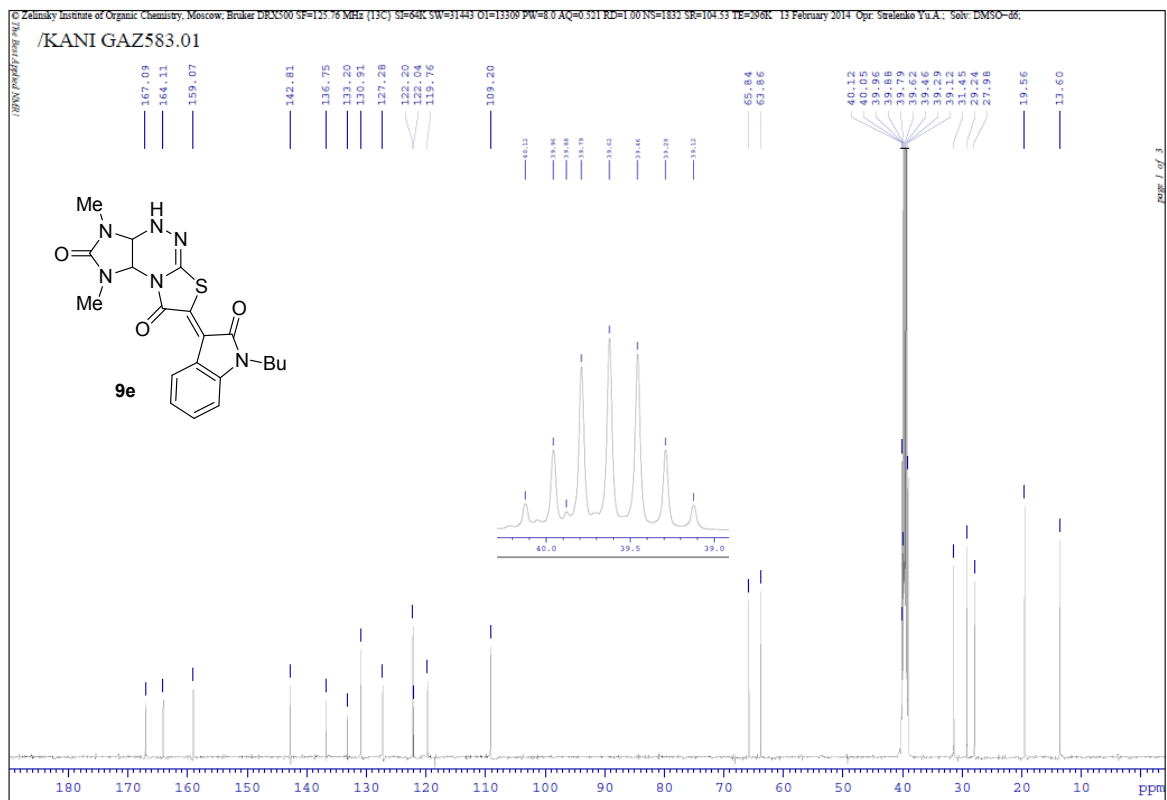
¹³C NMR spectrum of **9d**



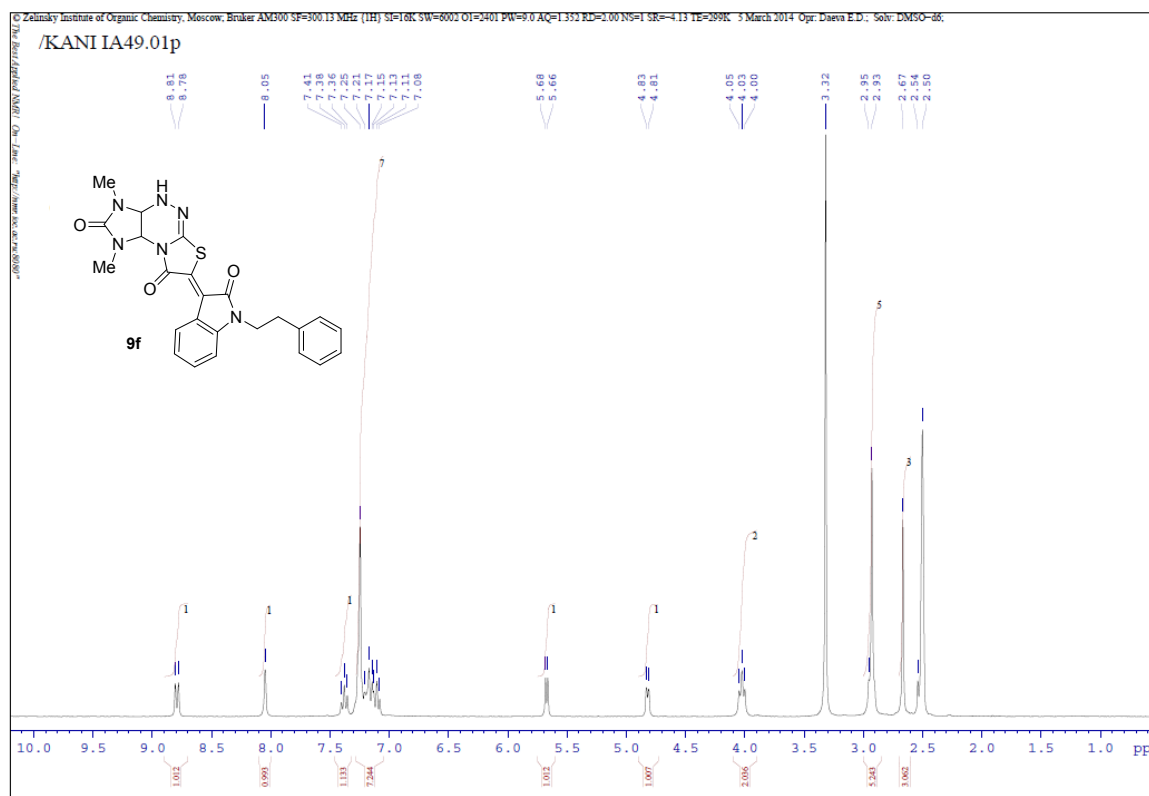
¹H NMR spectrum of **9e**



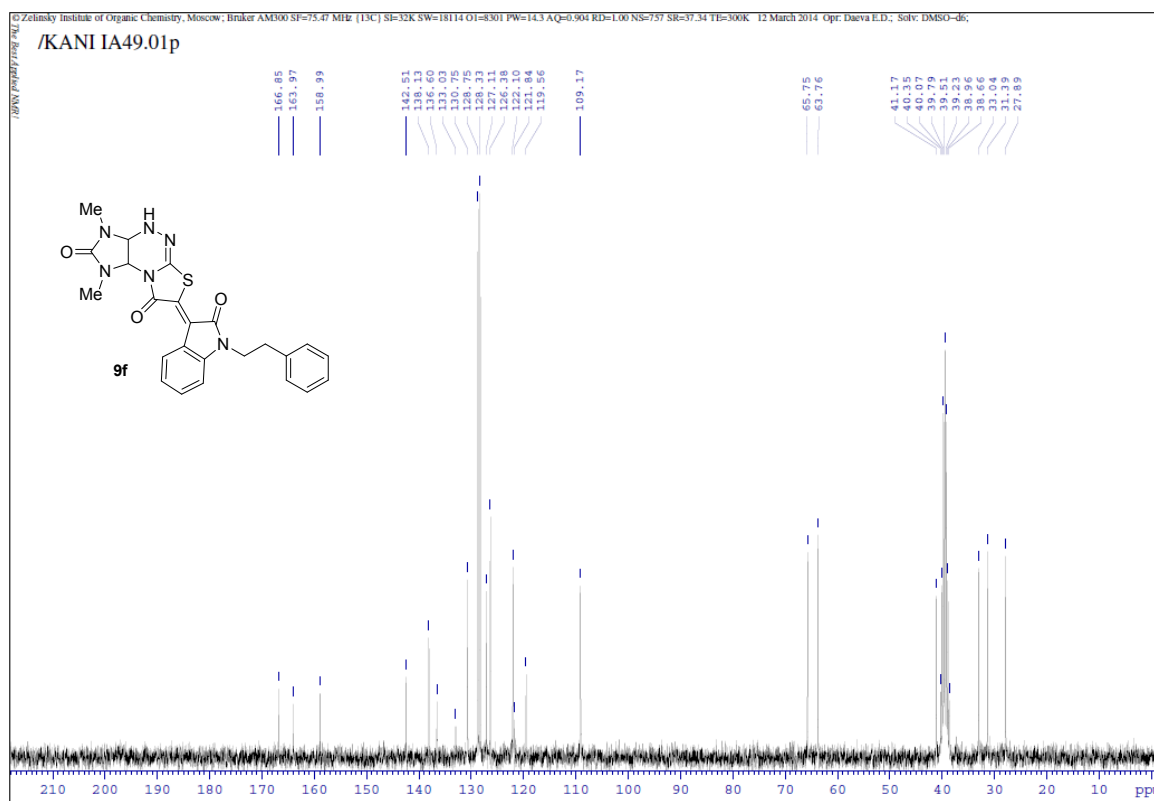
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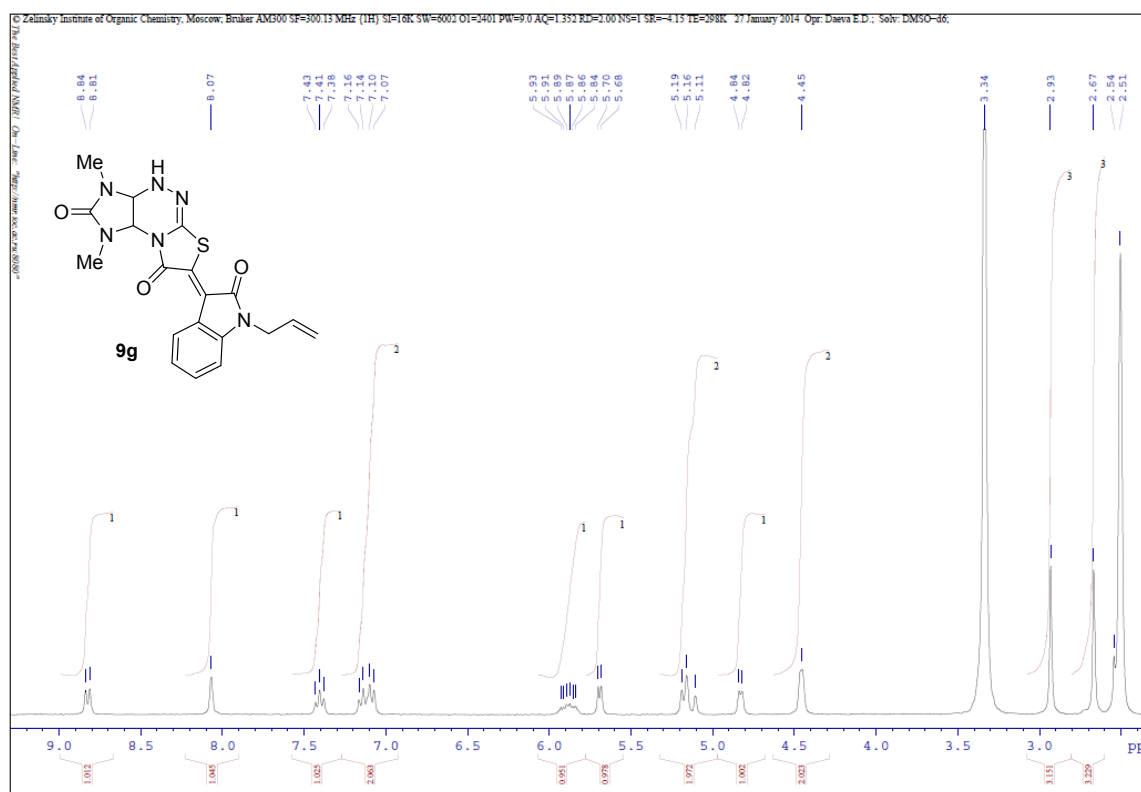
¹H NMR spectrum of **9f**



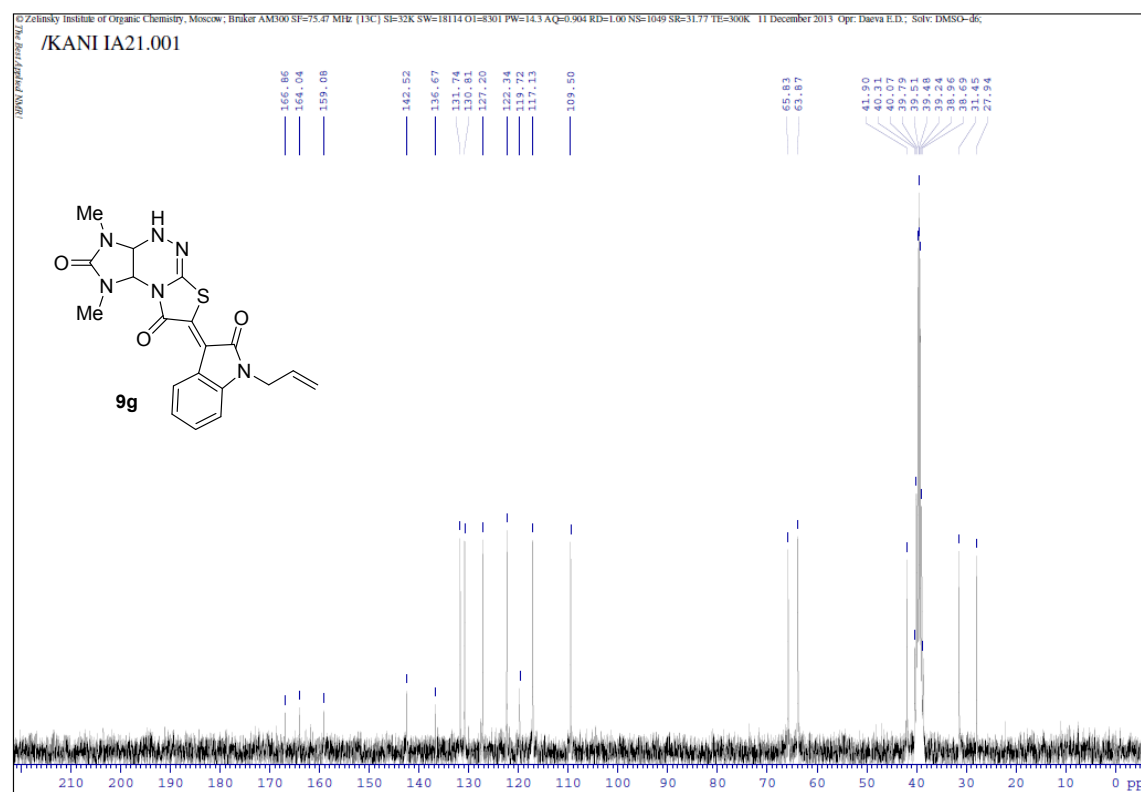
¹³C NMR spectrum of **9f**



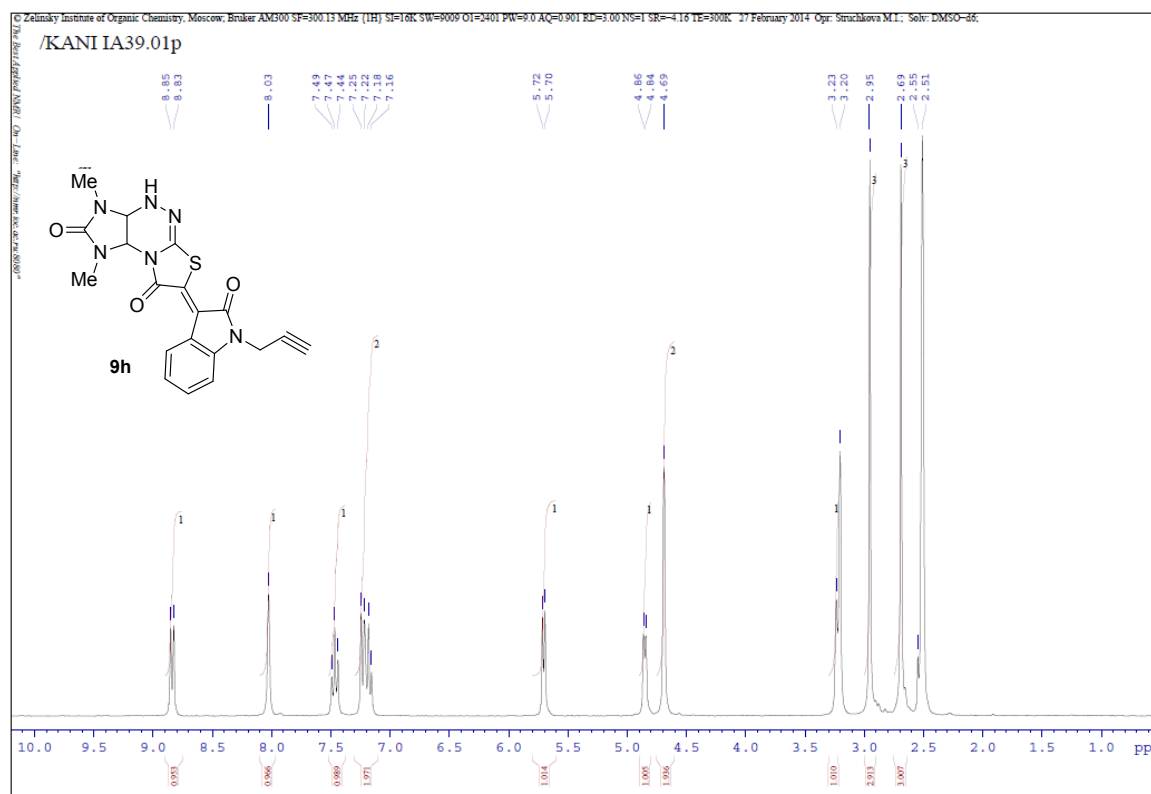
¹H NMR spectrum of **9g**



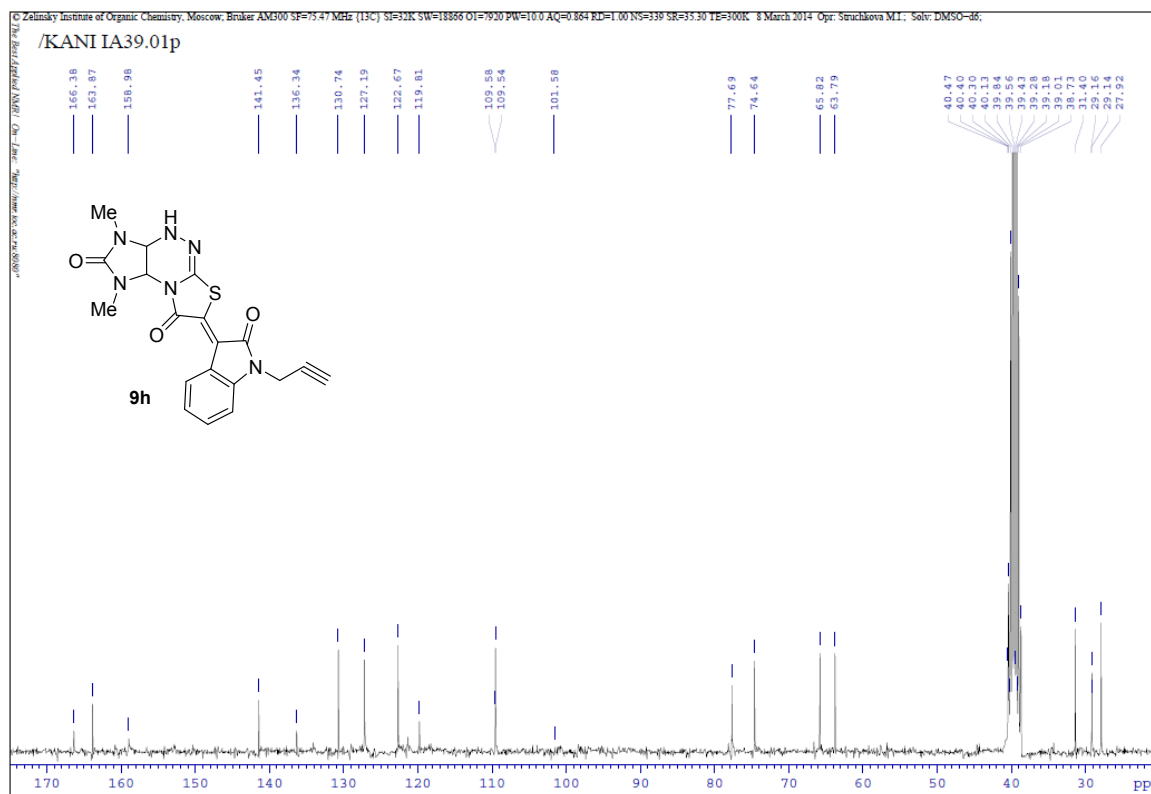
¹³C NMR spectrum of **9g**



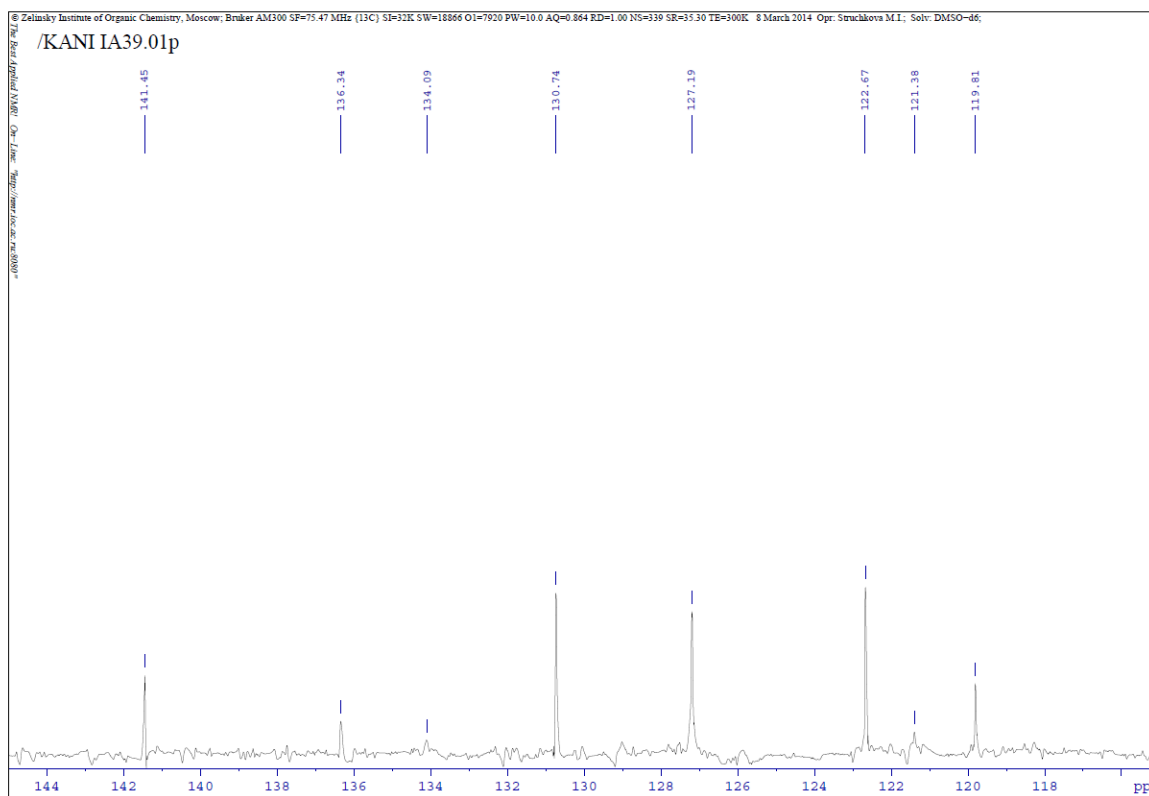
¹H NMR spectrum of **9h**



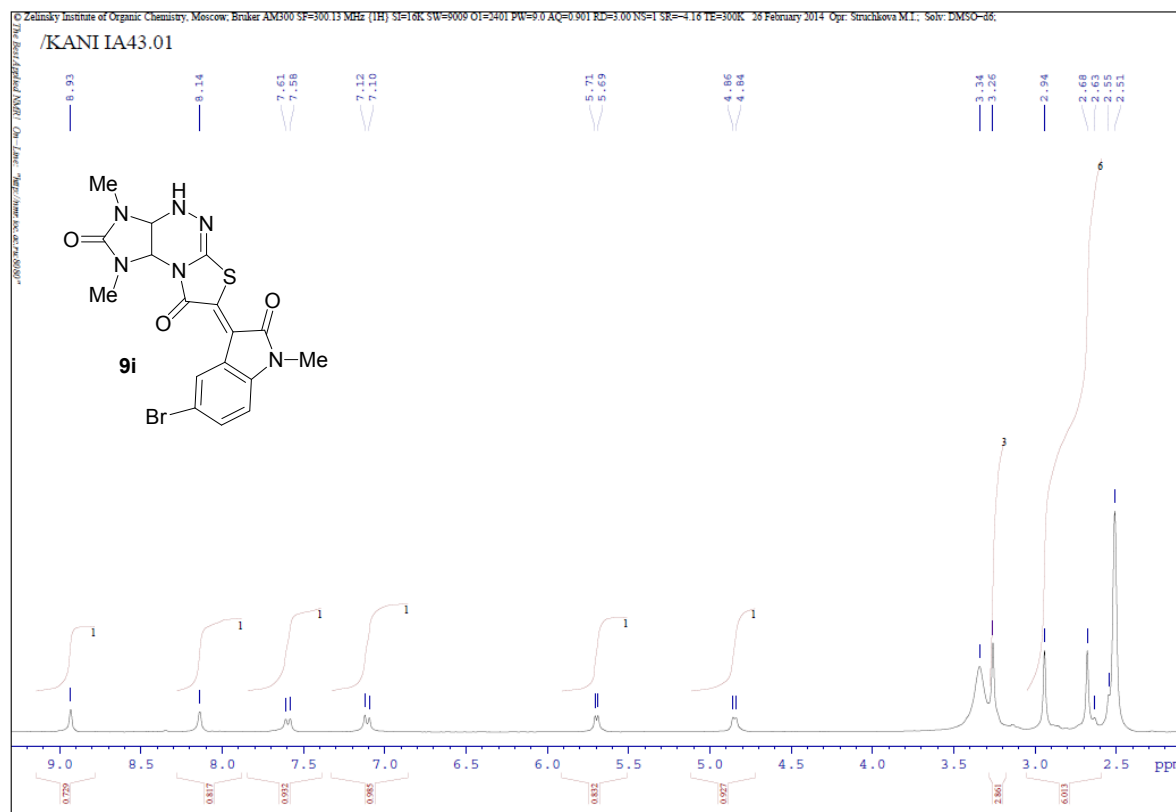
¹³C NMR spectrum of **9h**



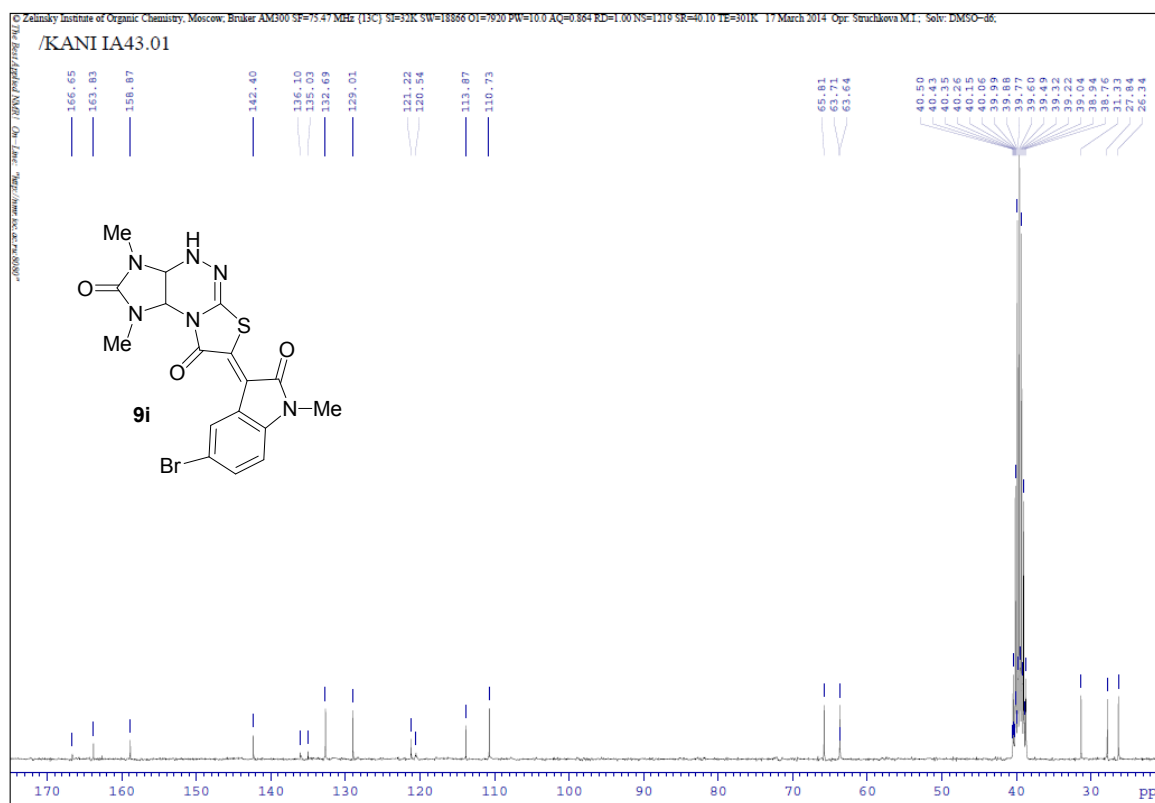
^{13}C NMR spectrum of **9h** in the region of 115-145 ppm



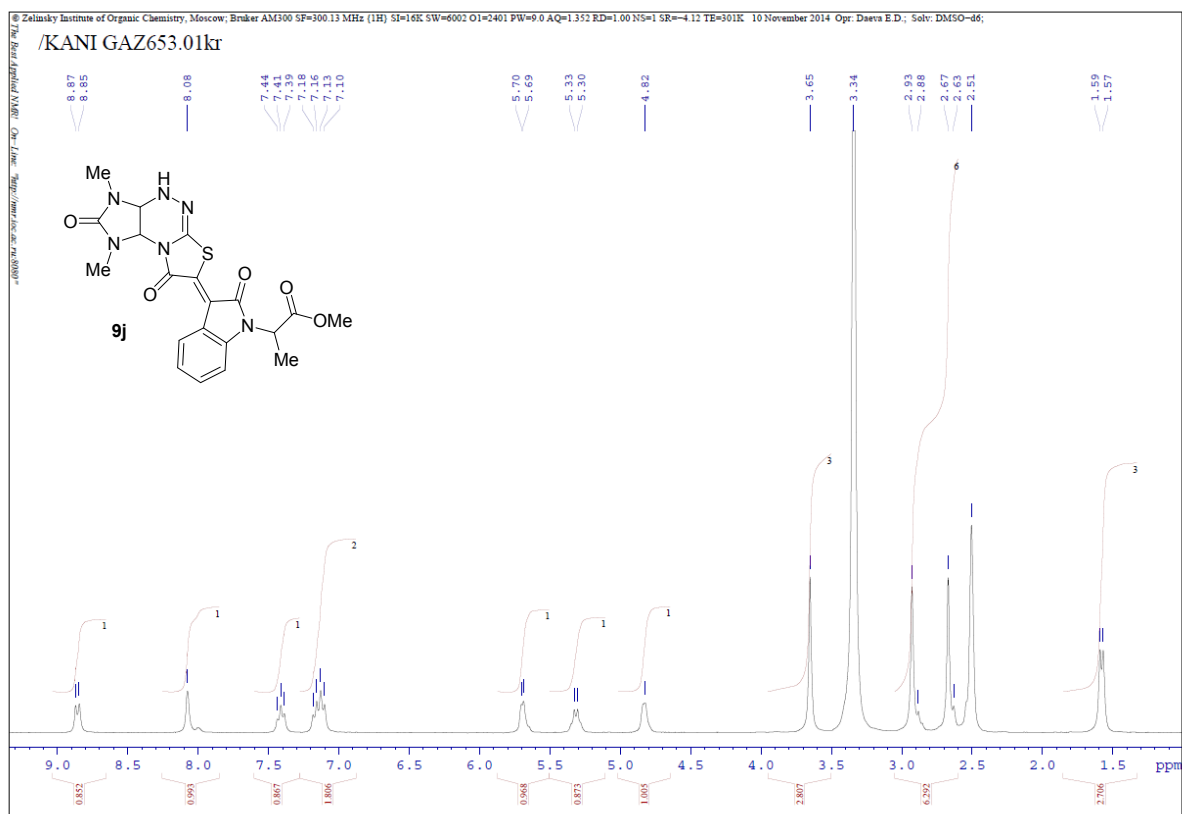
^1H NMR spectrum of **9i**



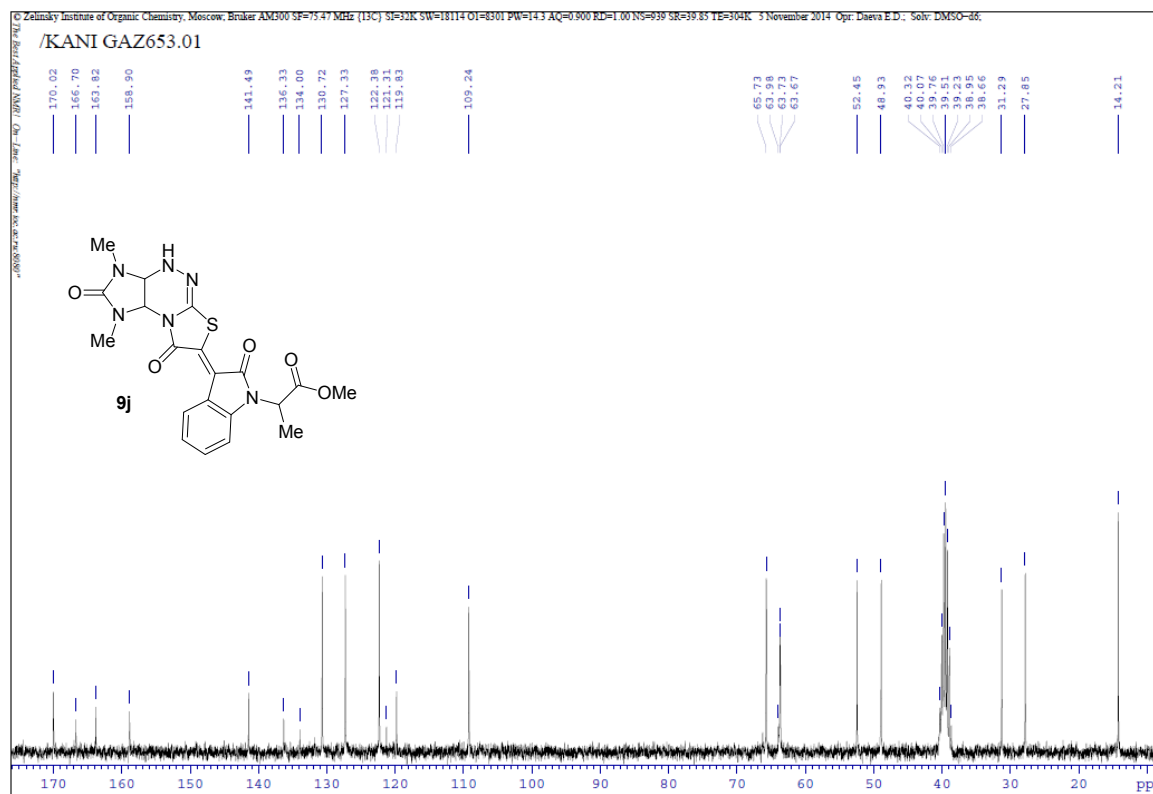
^{13}C NMR spectrum of **9i**



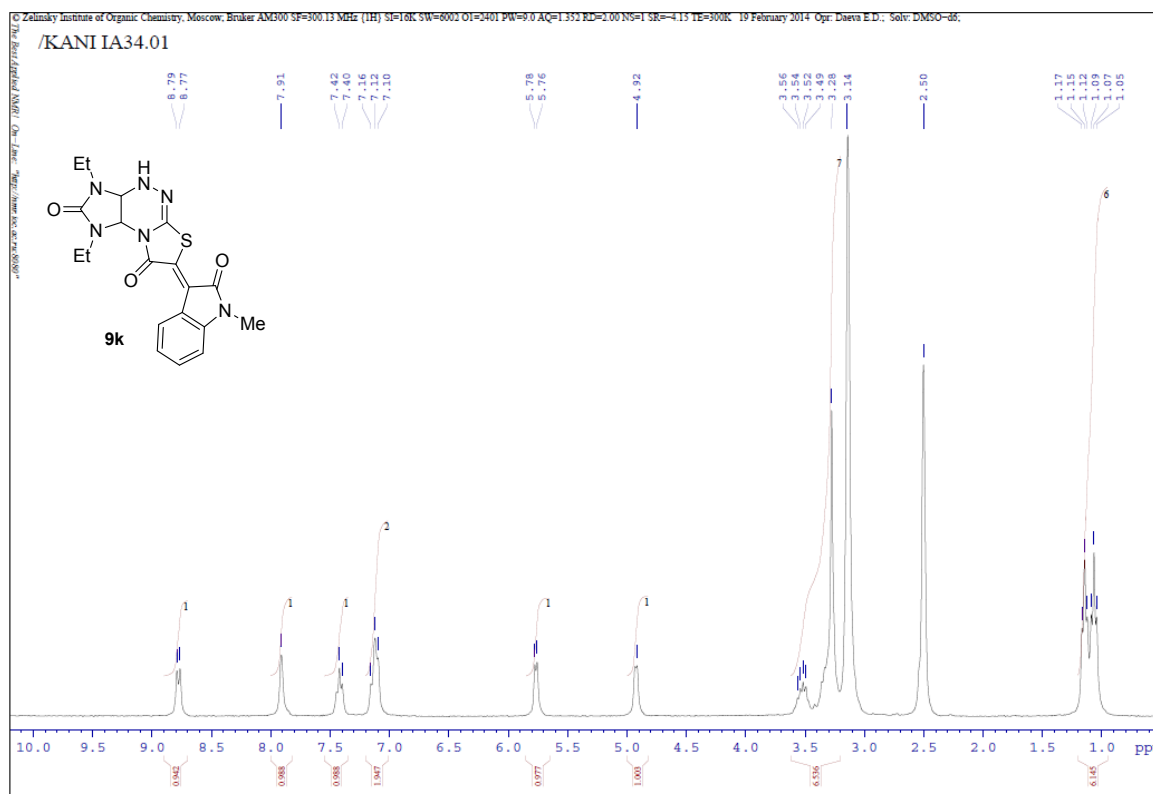
^1H NMR spectrum of **9j**



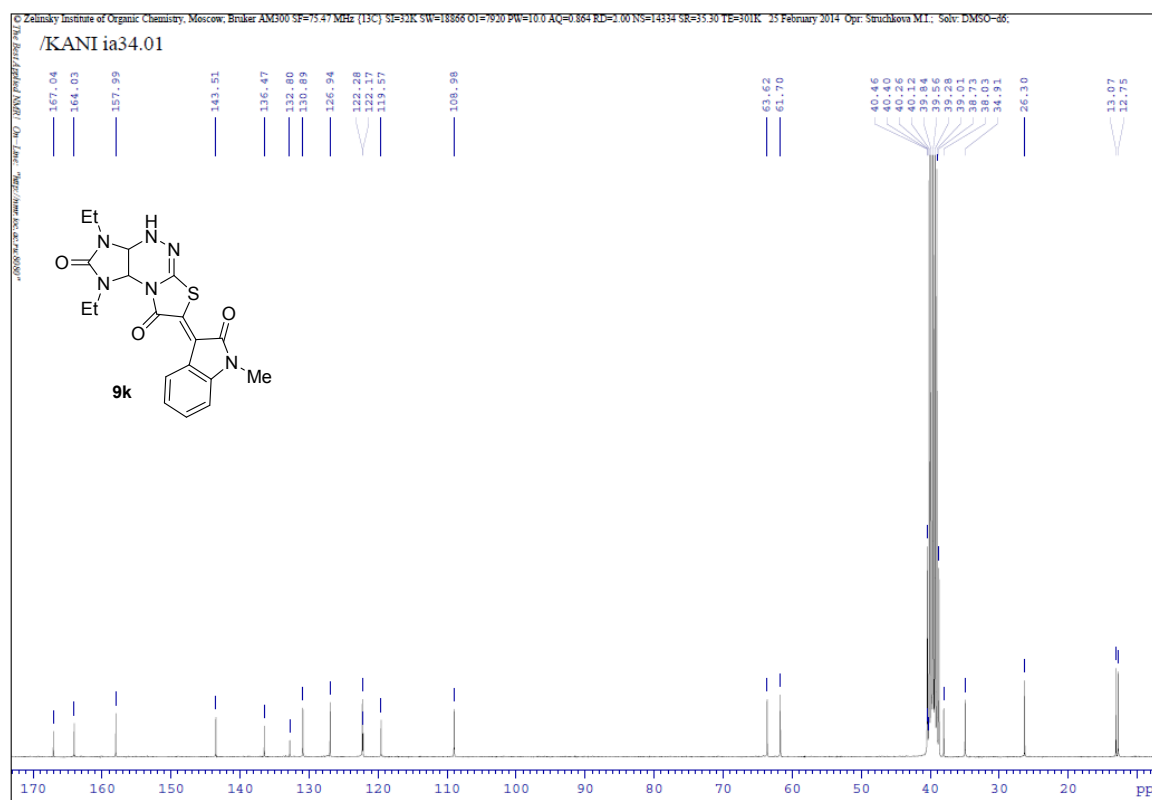
^{13}C NMR spectrum of **9j**



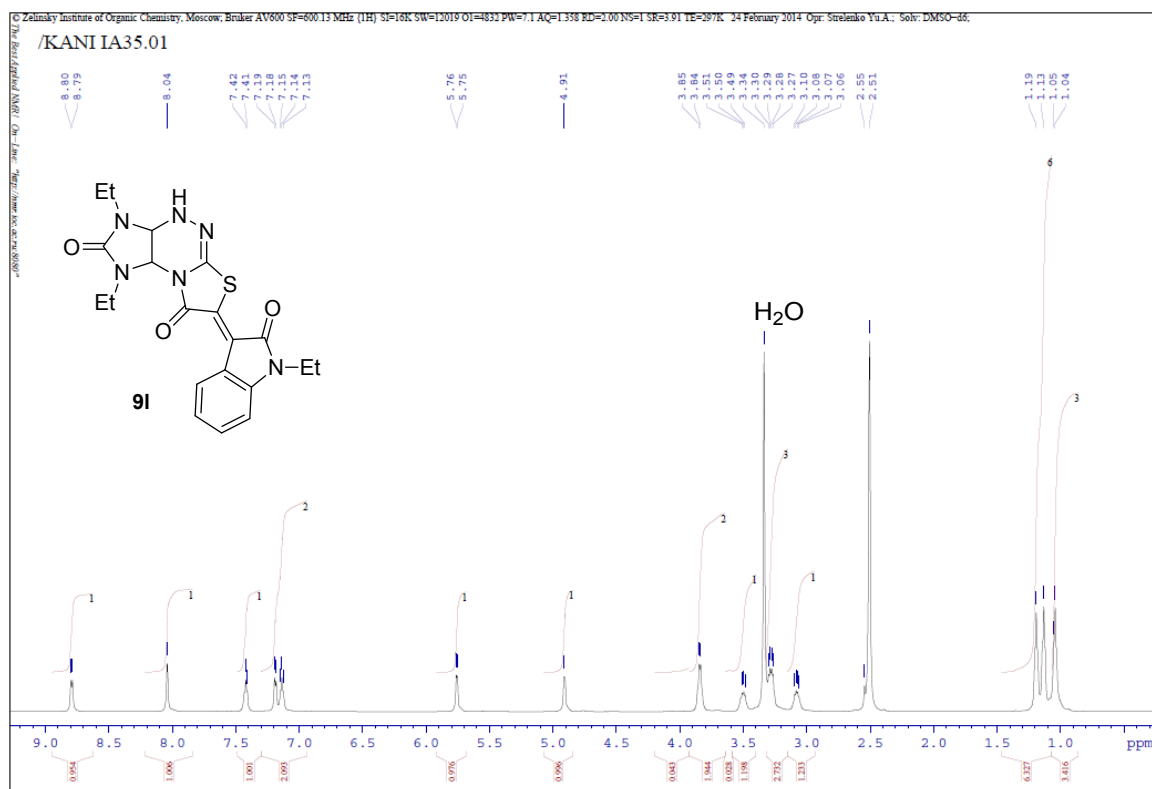
^1H NMR spectrum of **9k**



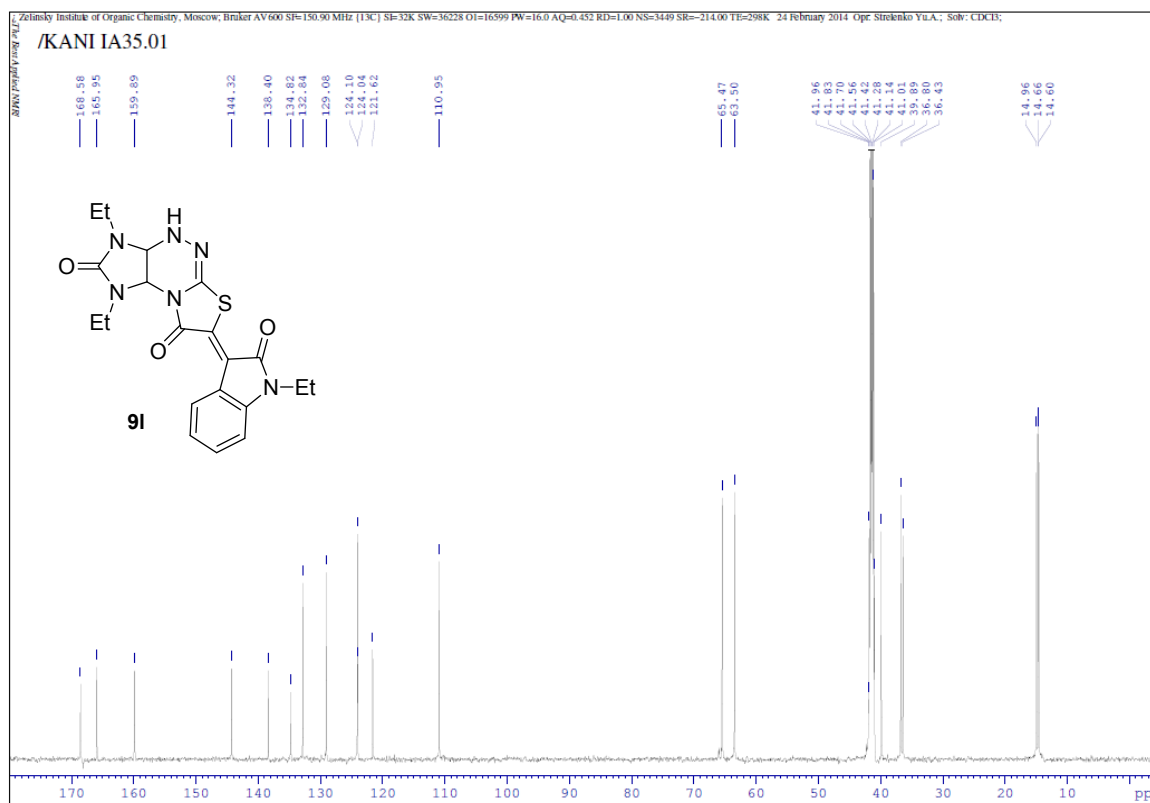
¹³C NMR spectrum of **9k**



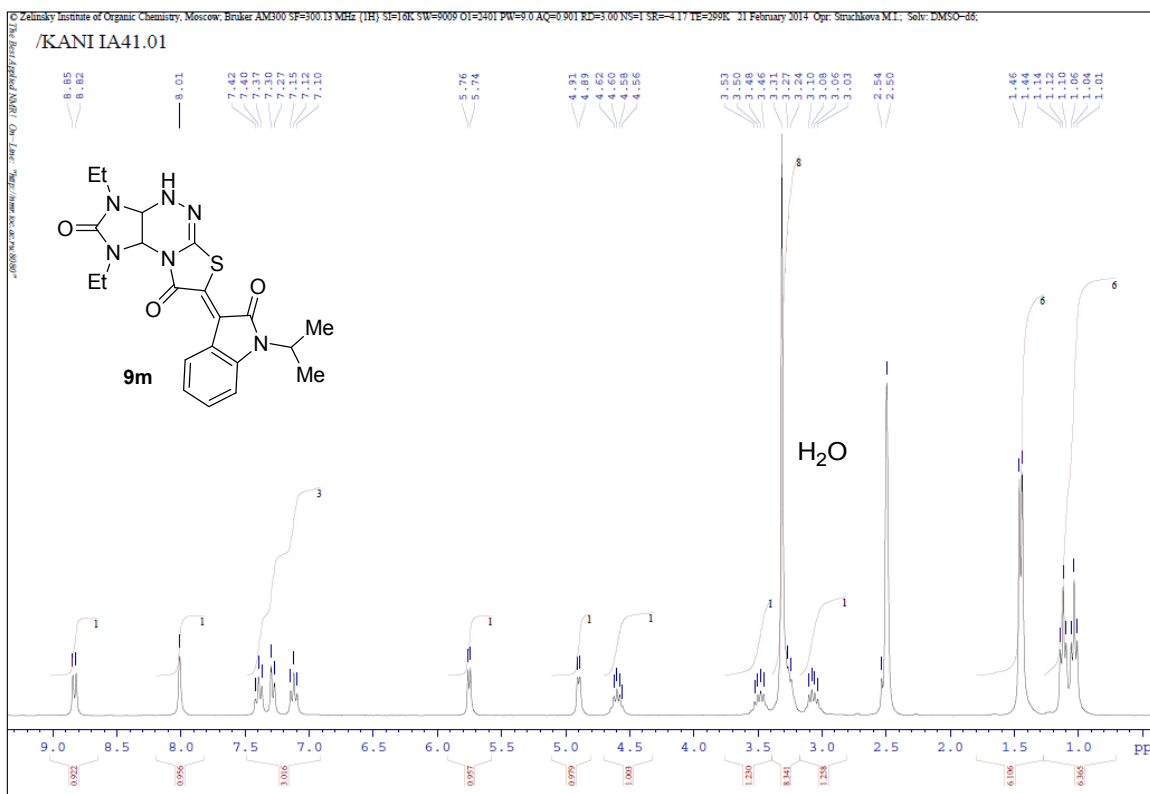
¹H NMR spectrum of **9l**



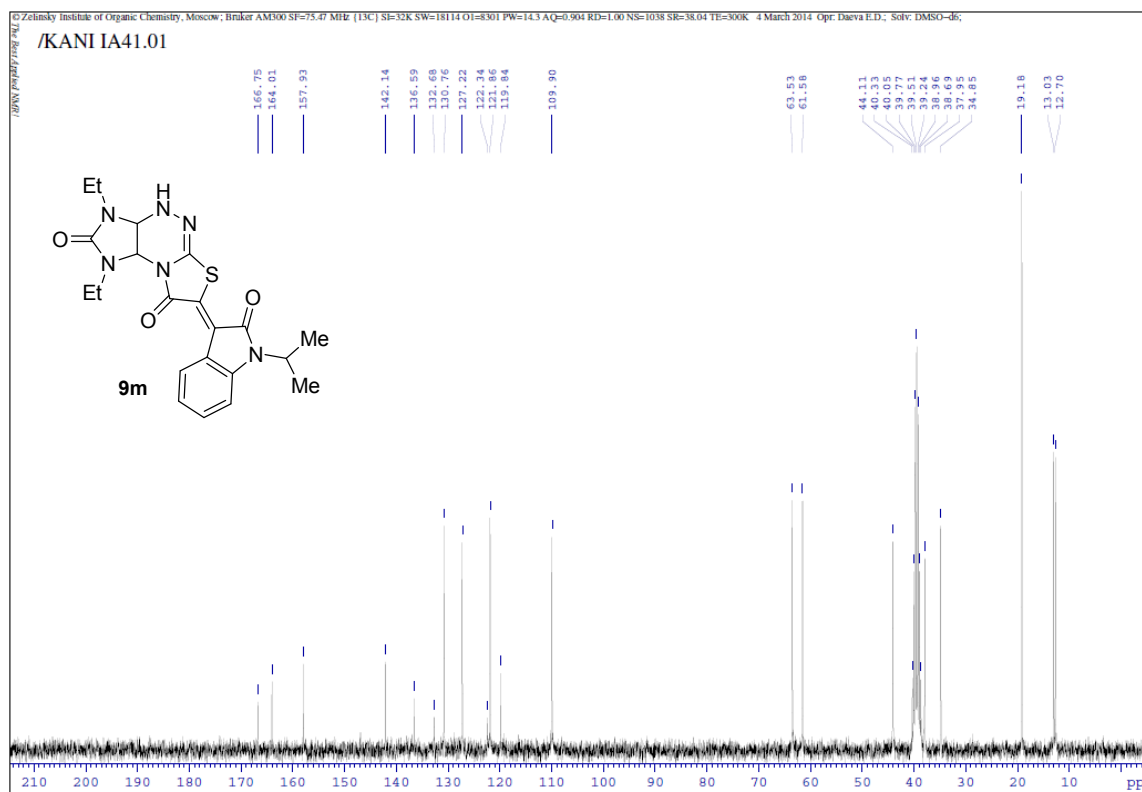
^{13}C NMR spectrum of **9l**



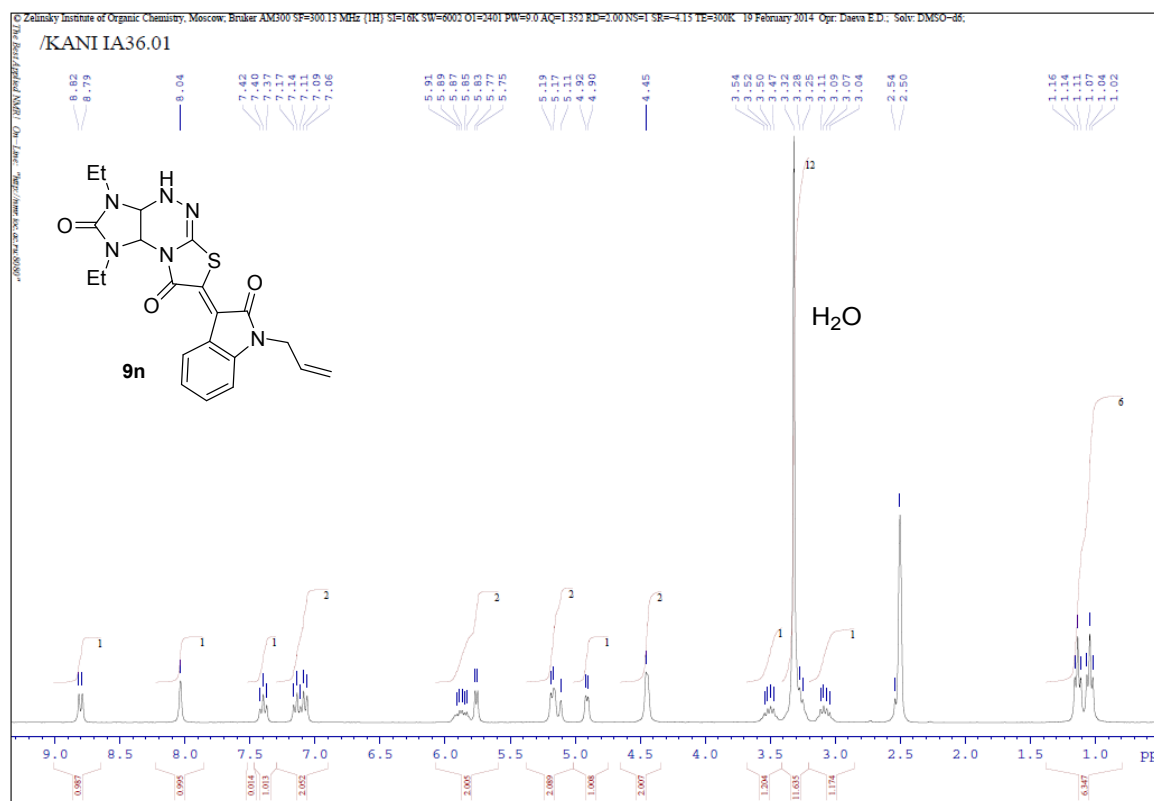
^1H NMR spectrum of **9m**



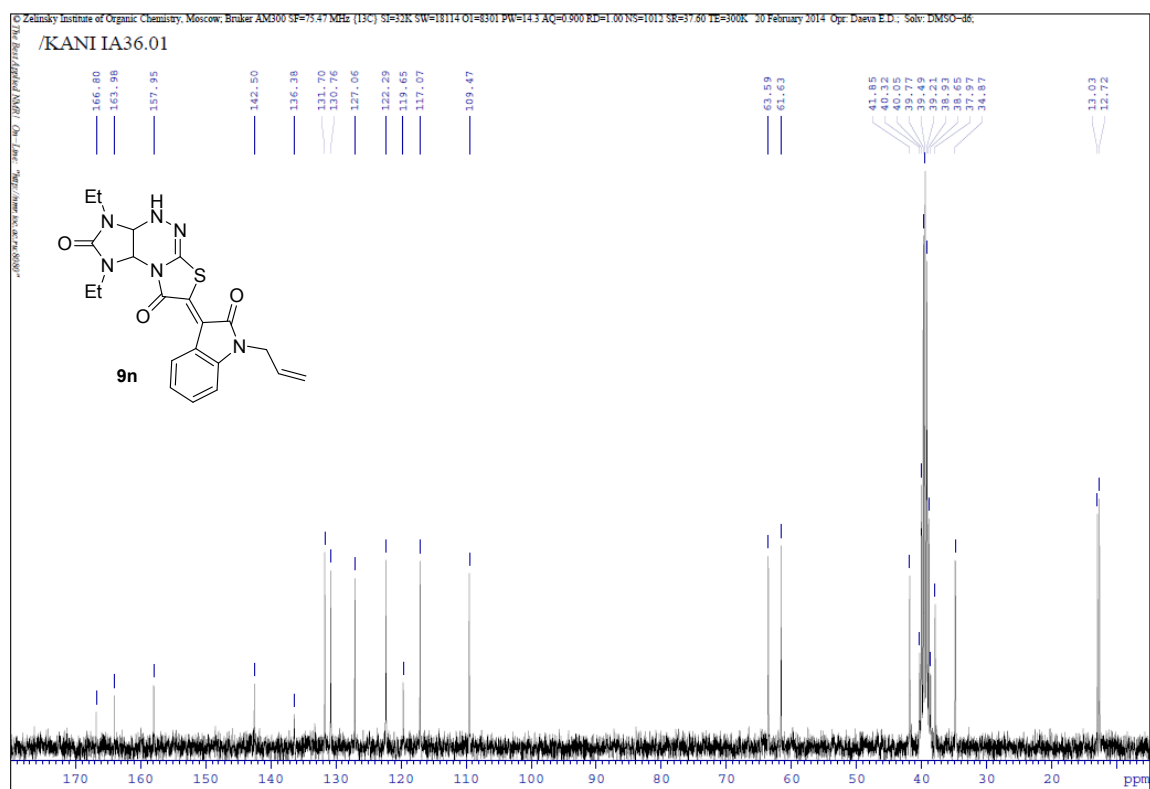
^{13}C NMR spectrum of **9m**



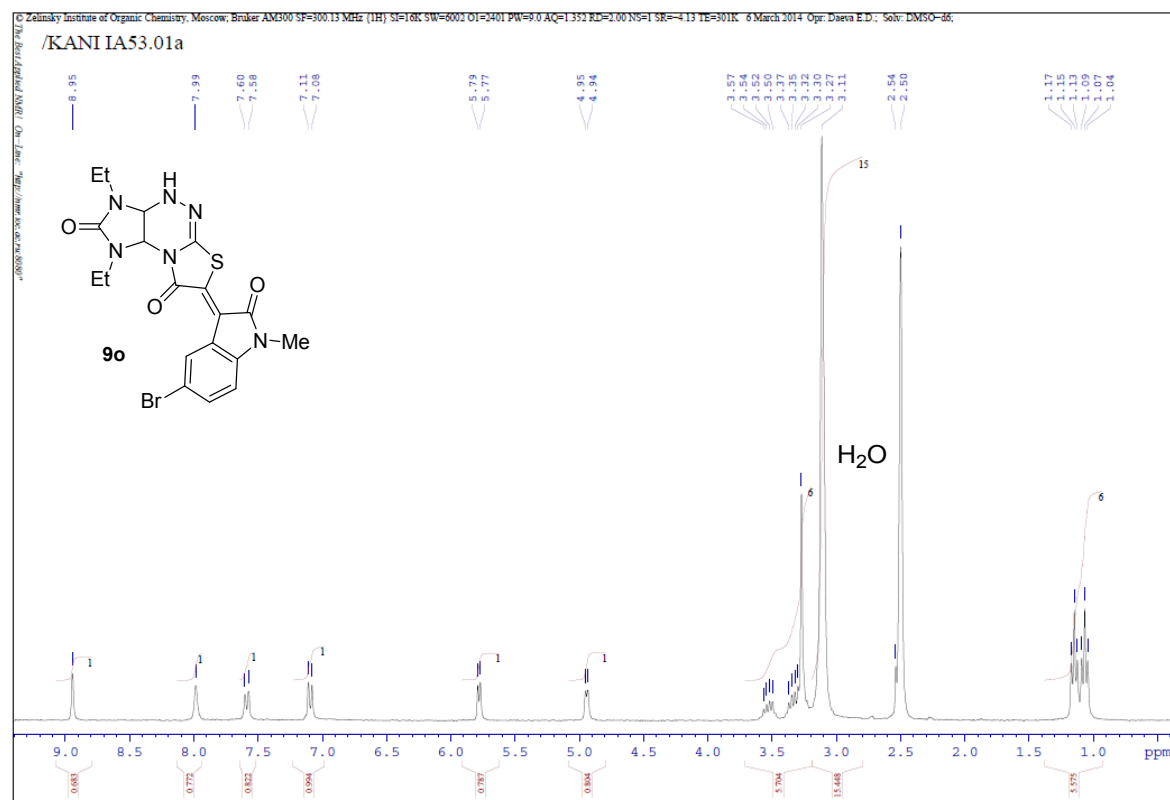
^1H NMR spectrum of **9n**



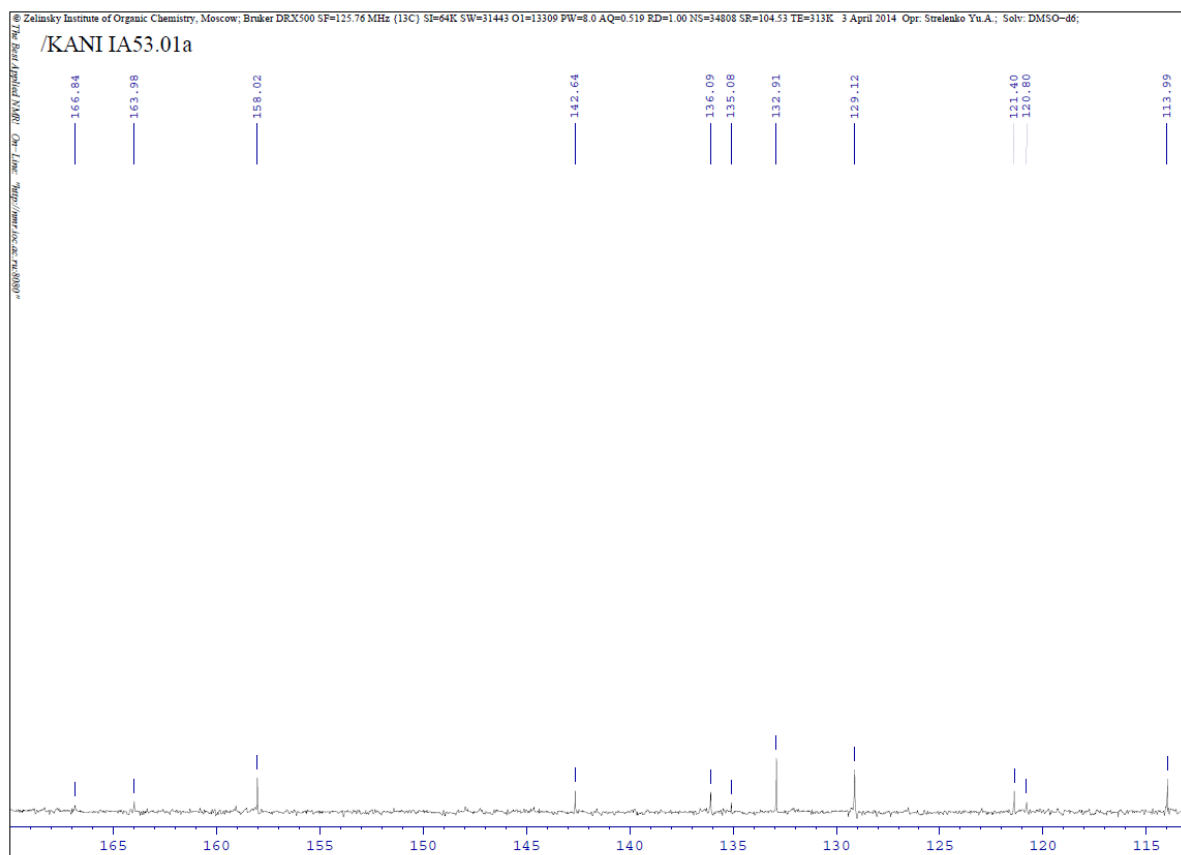
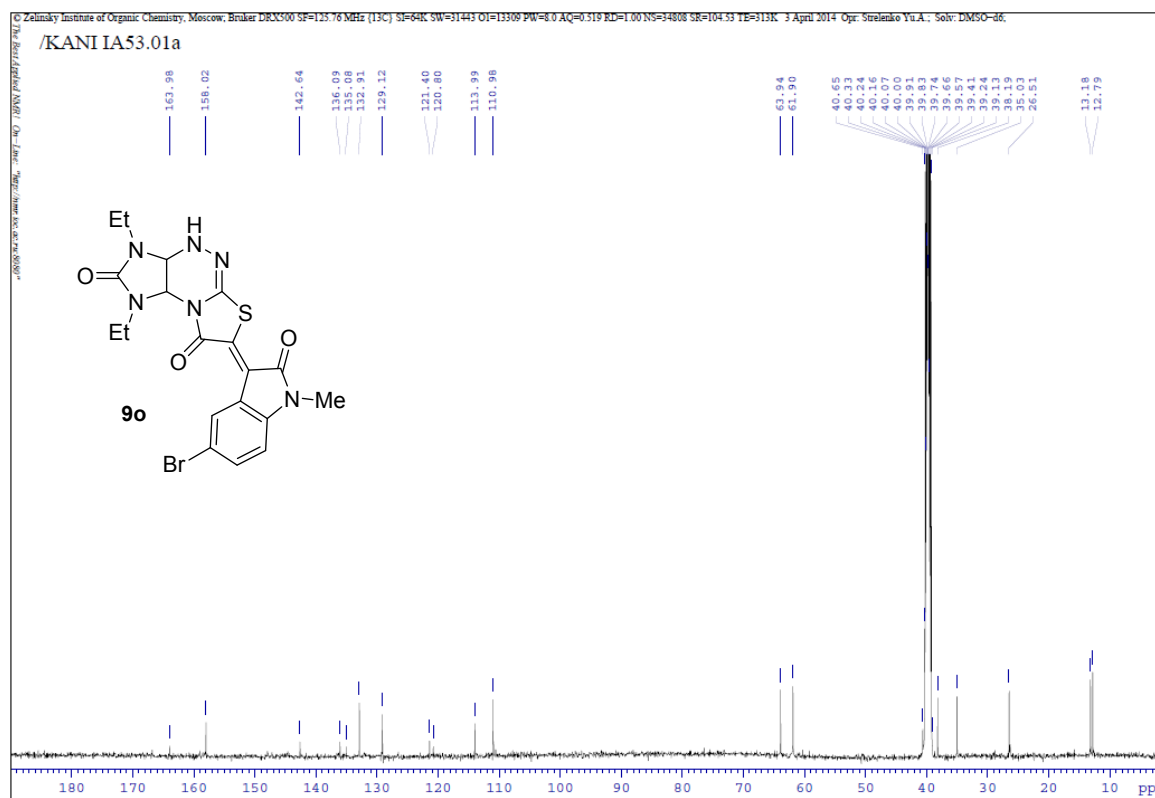
¹H NMR spectrum of **9n**



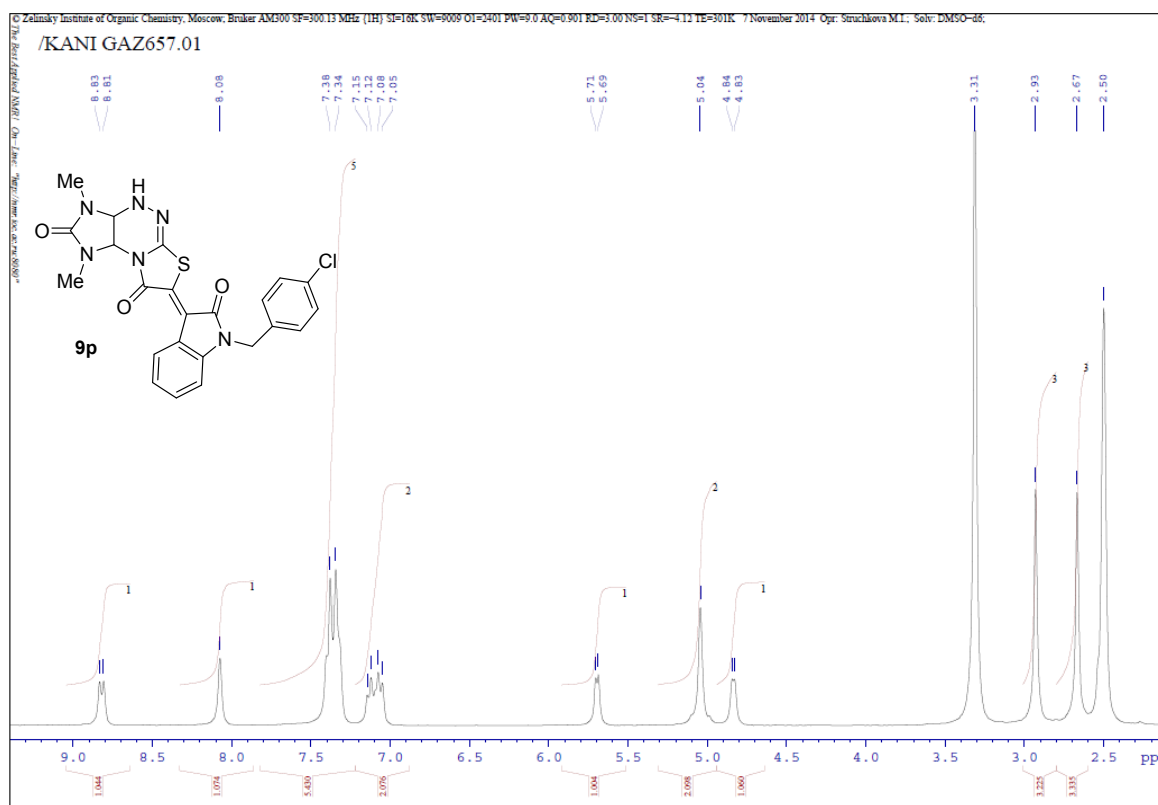
¹H NMR spectrum of **9o**



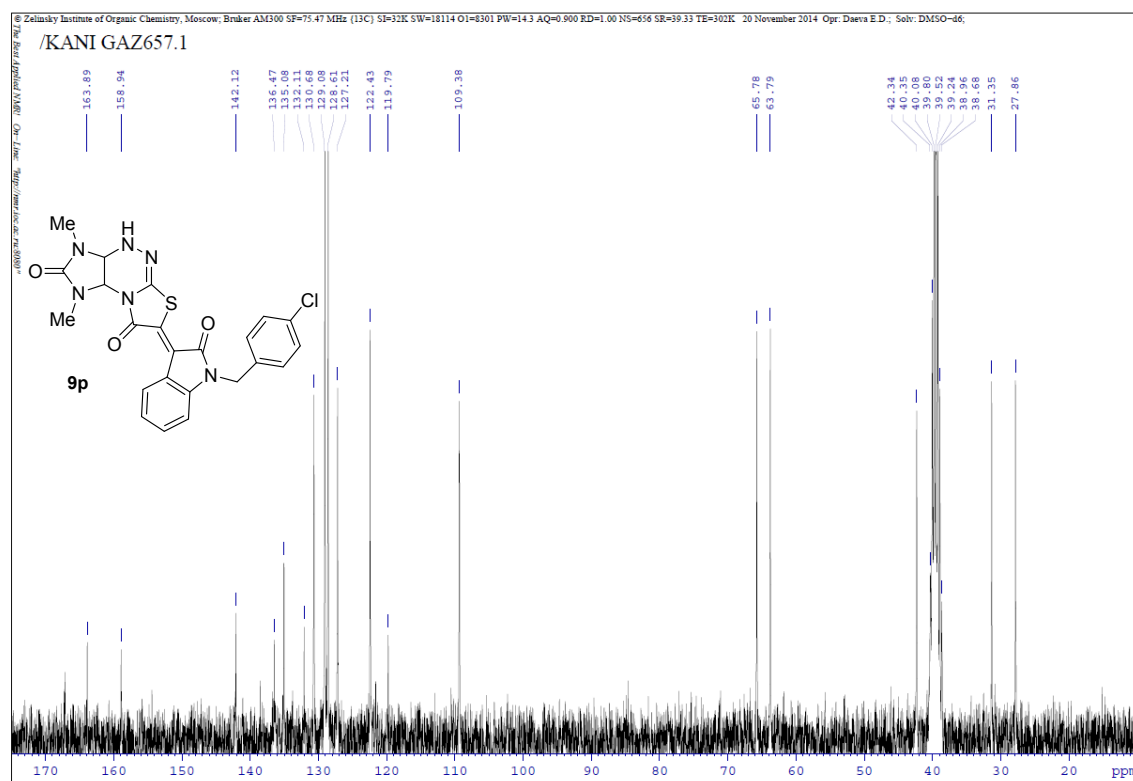
^{13}C NMR spectrum of **9o**



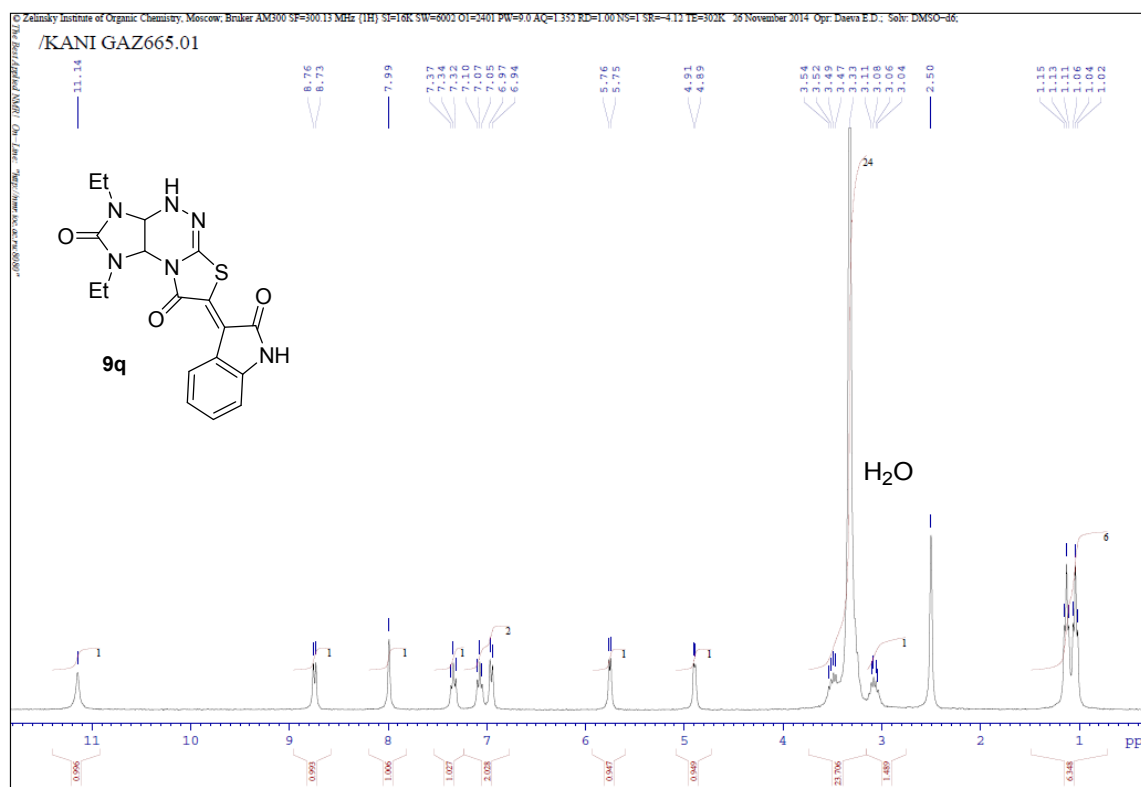
¹H NMR spectrum of **9p**



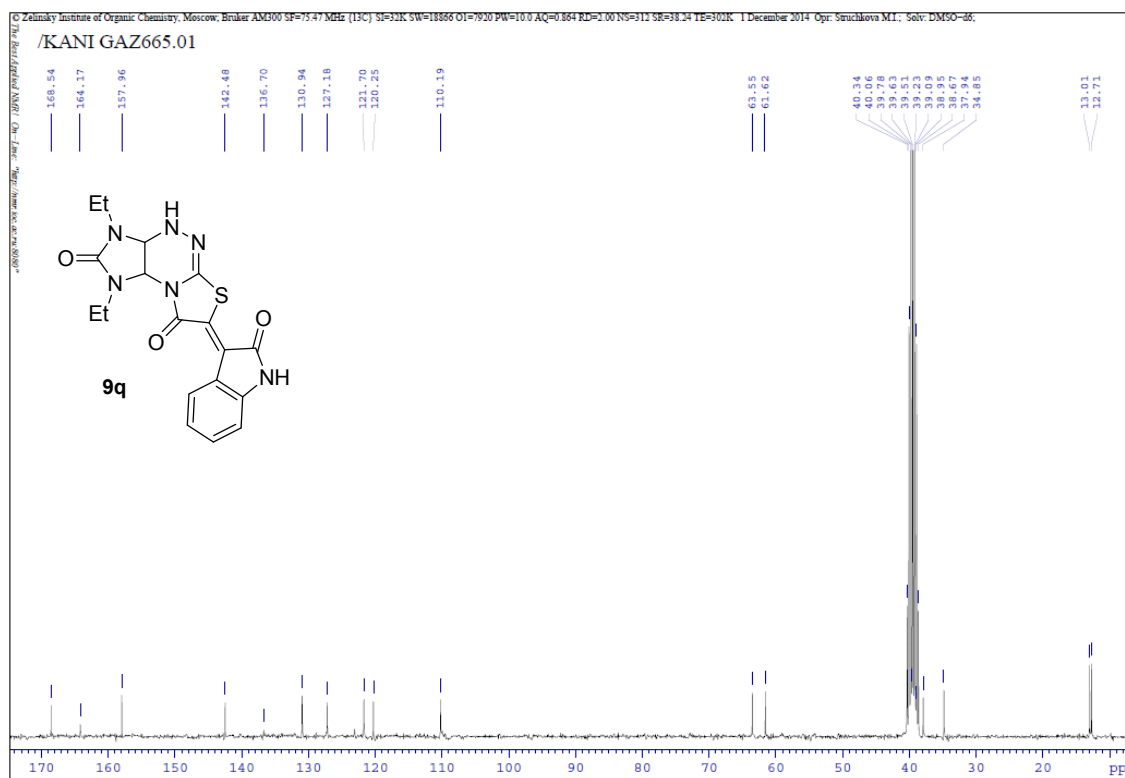
¹³C NMR spectrum of **9p**



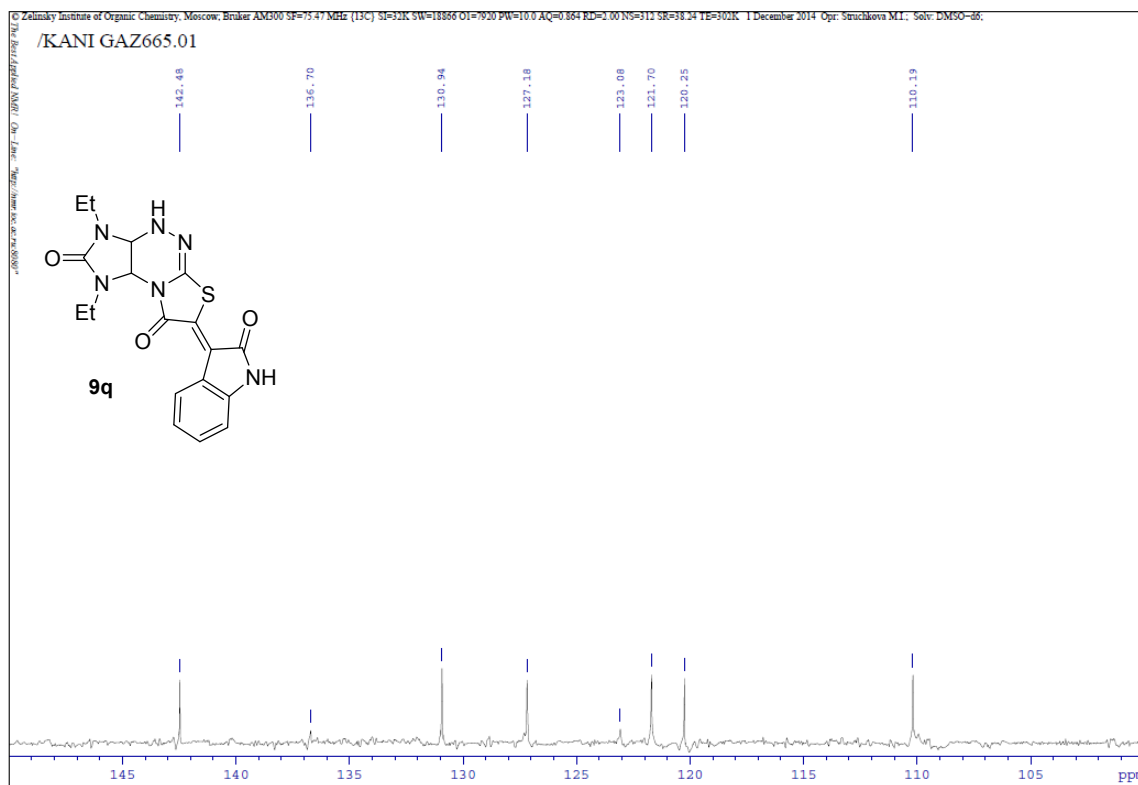
¹H NMR spectrum of **9q**



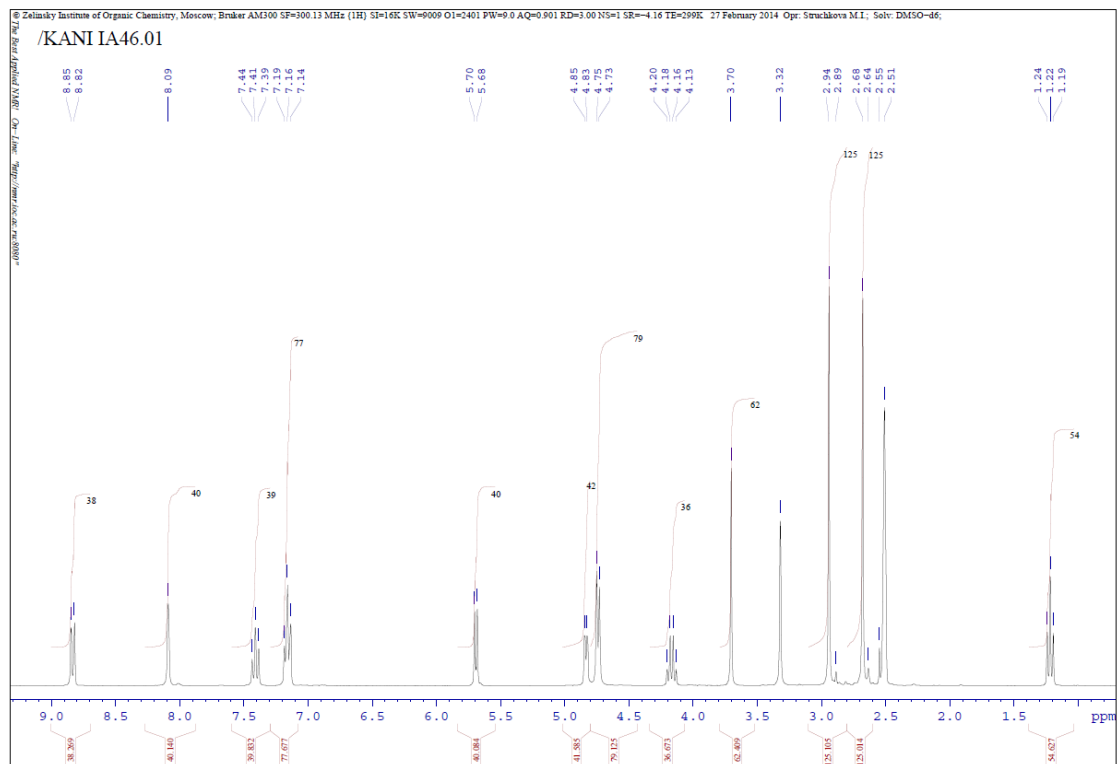
¹³C NMR spectrum of **9q**



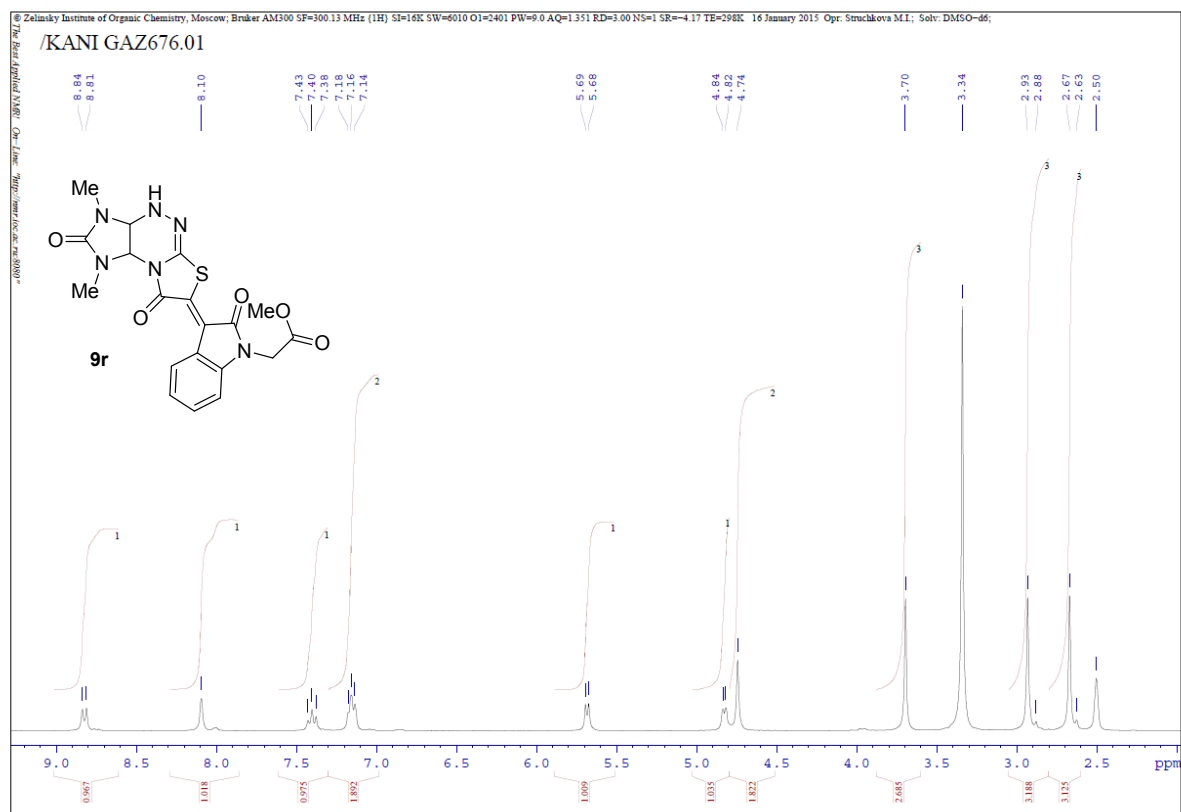
^{13}C NMR spectrum of **9q** in the region 100-150 ppm.



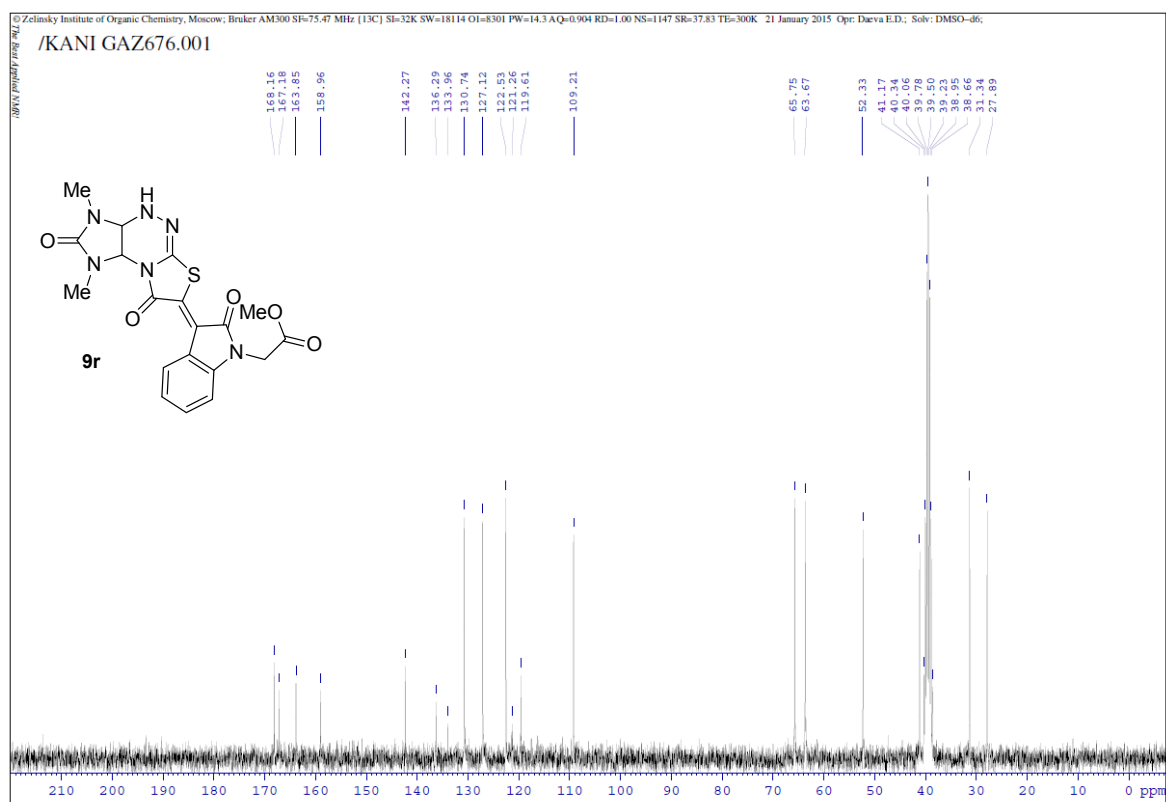
^1H NMR spectrum of the mixture of methyl (**9r**) and ethyl esters of 2-(3-(1,3-dimethyl-2,8-dioxo-1,2,3,3a,4,9a-hexahydroimidazo[4,5-e]thiazolo[2,3-c][1,2,4]triazin-7(8*H*)-ylidene)-2-oxo-1,2-dihydro-3*H*-indol-1-yl)acetic acid **9**



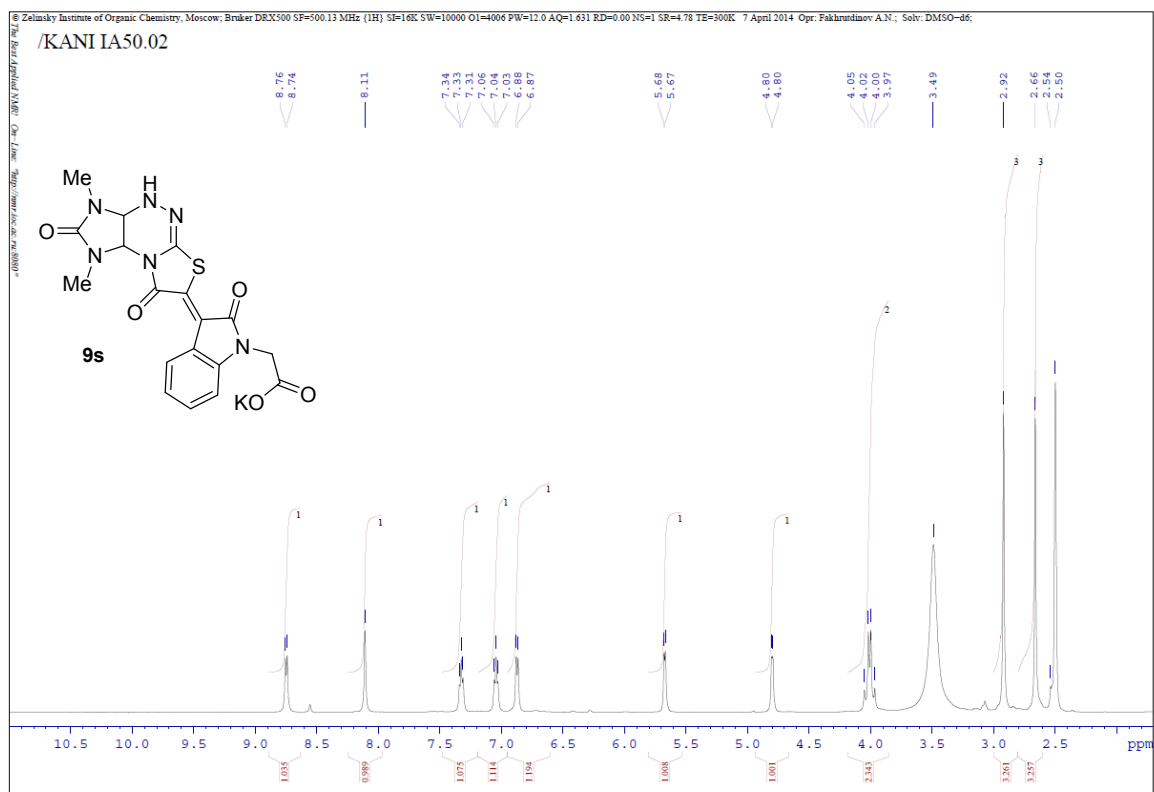
¹H NMR spectrum of **9r**



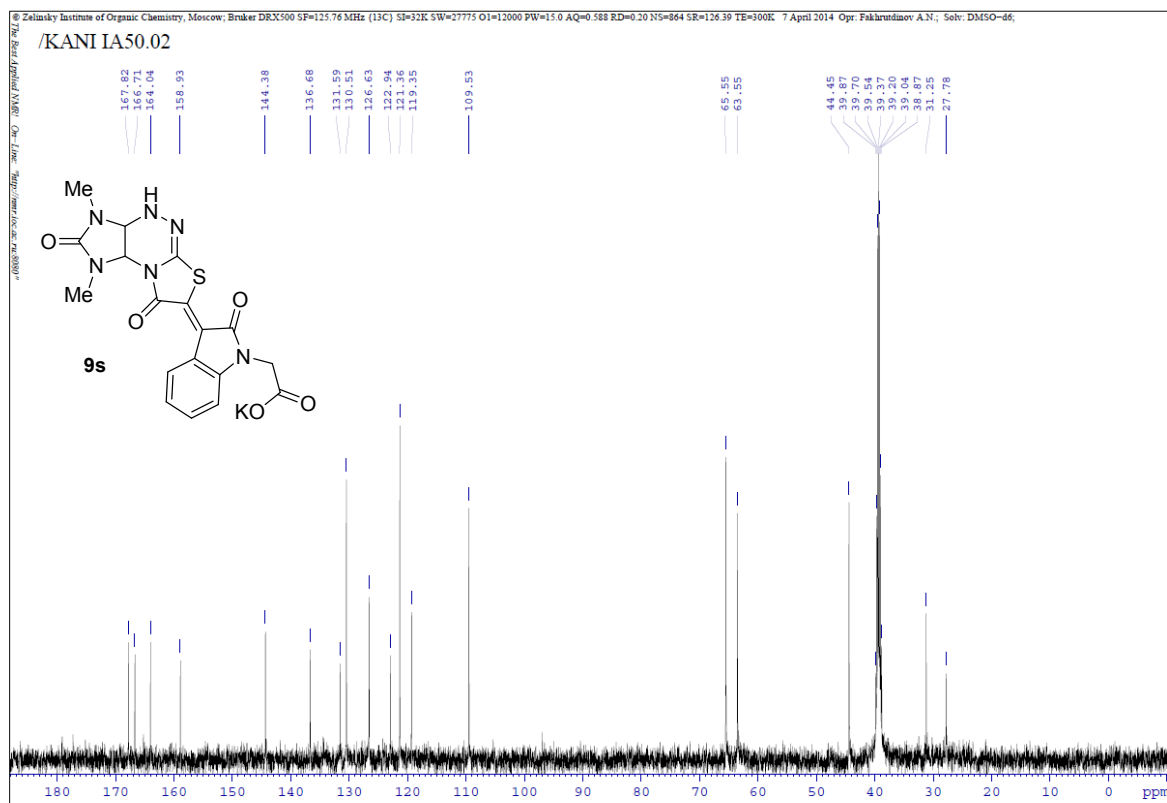
¹³C NMR spectrum of **9r**



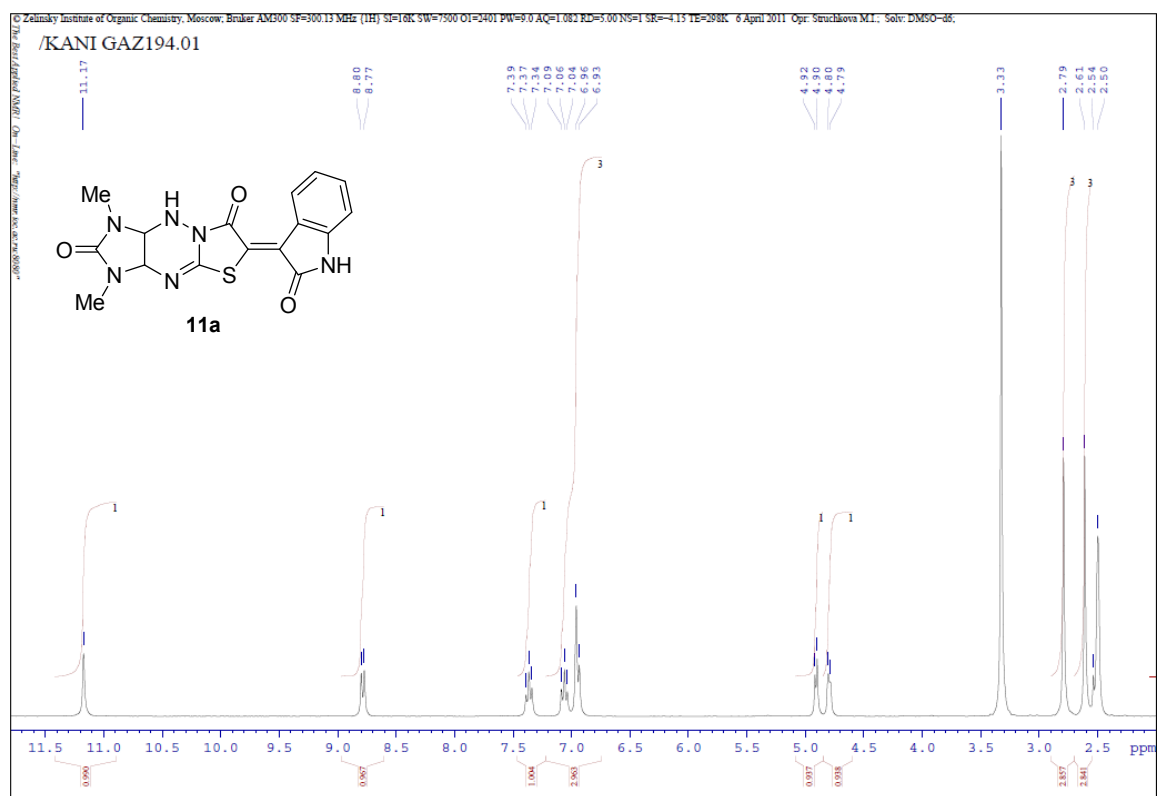
¹H NMR spectrum of **9s**



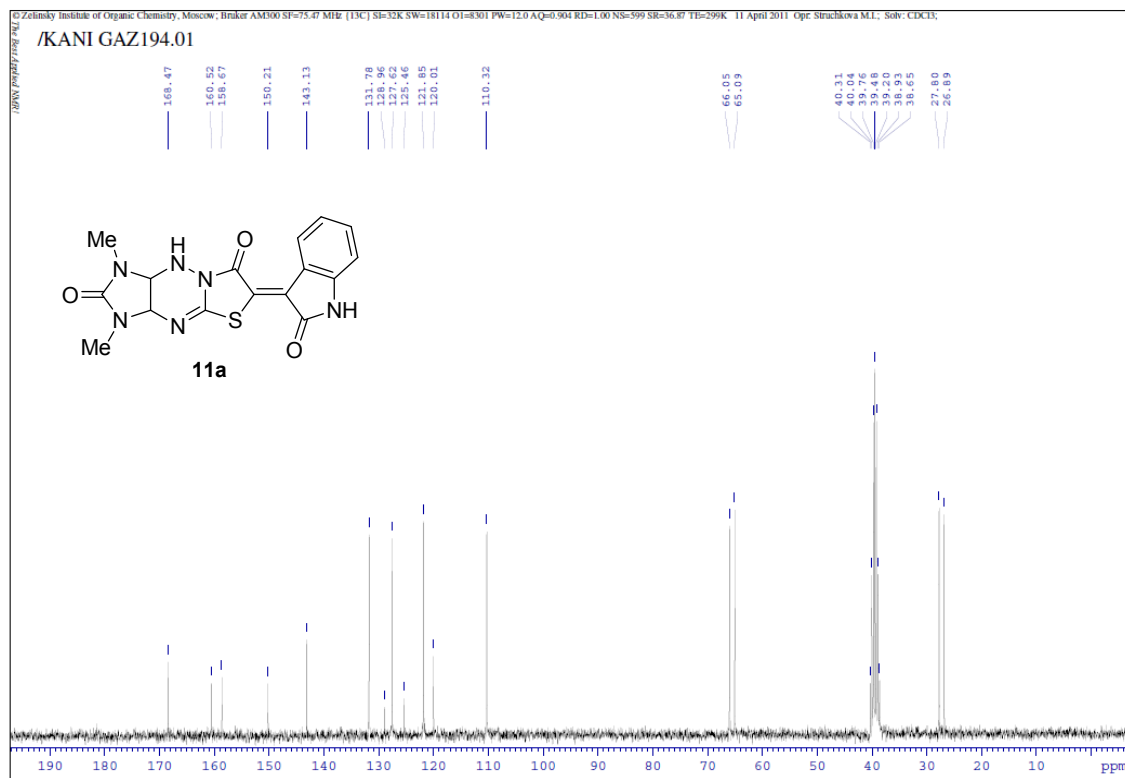
¹³C NMR spectrum of **9s**



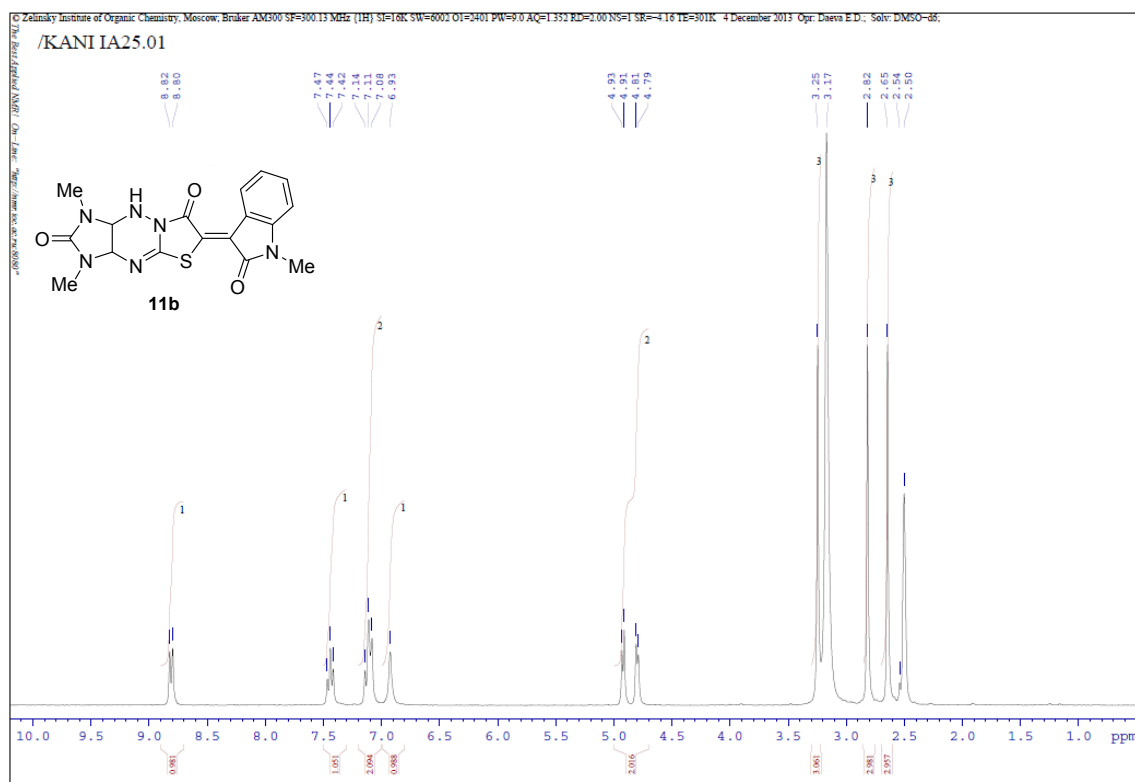
¹H NMR spectrum of **11a**



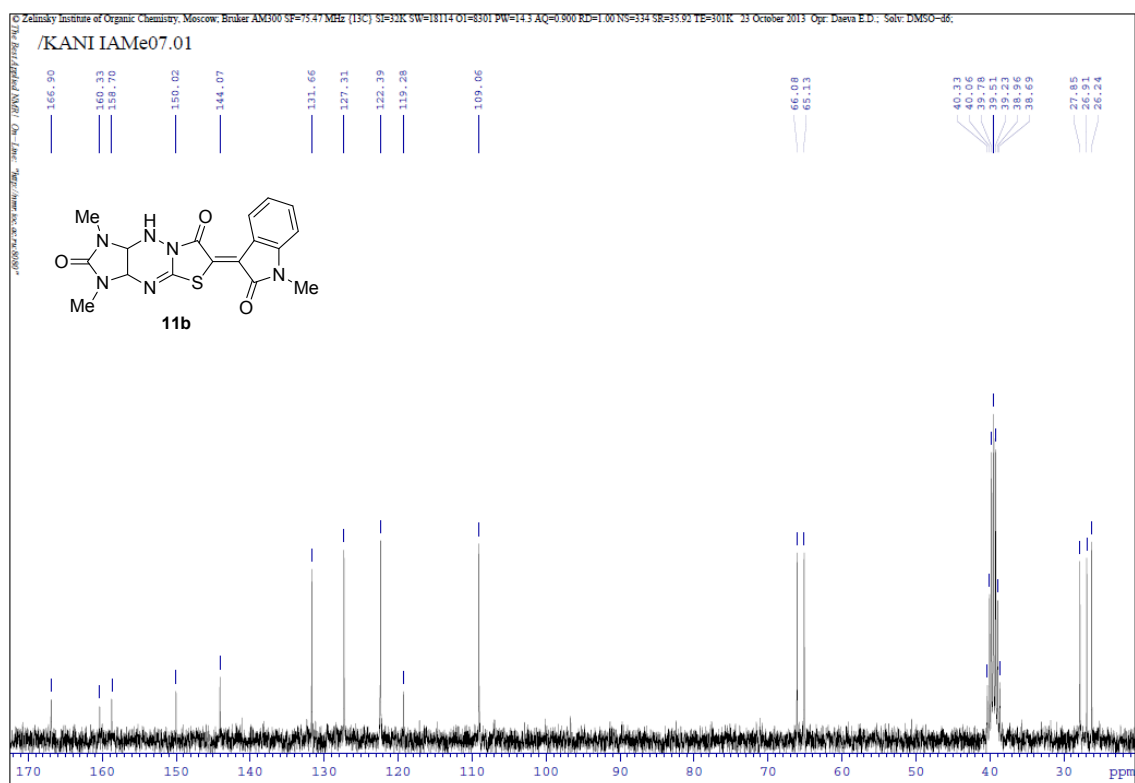
¹³C NMR spectrum of **11a**



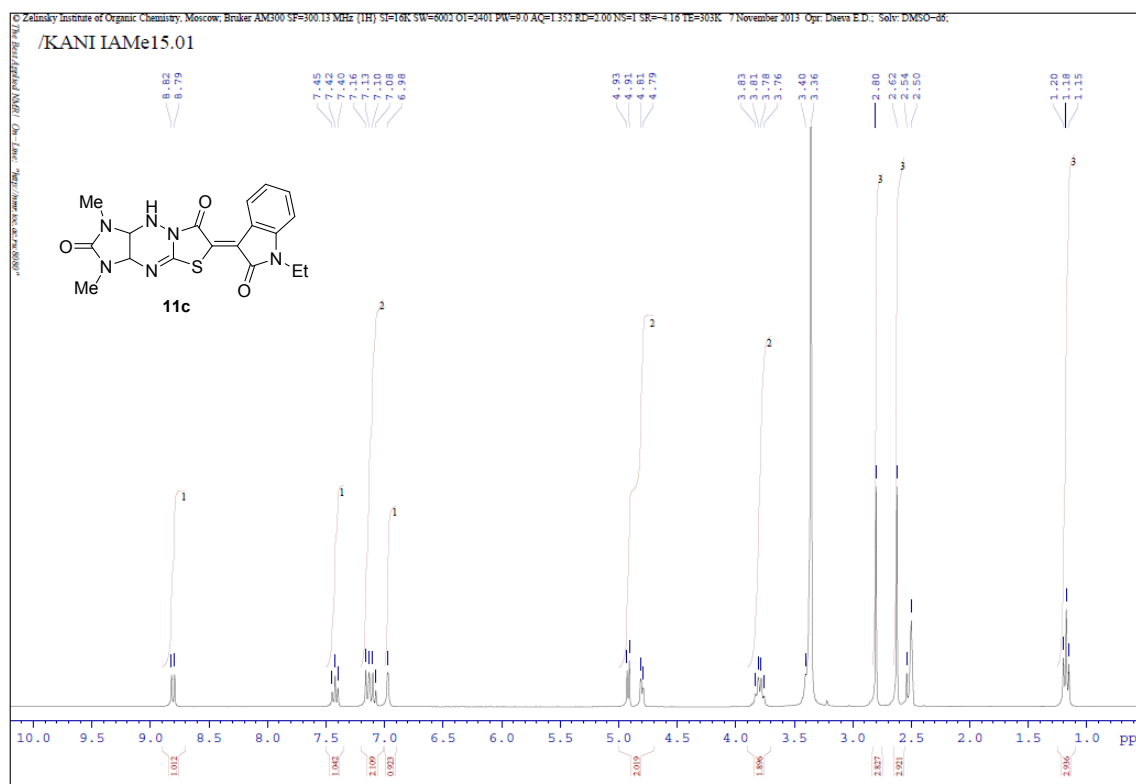
¹H NMR spectrum of **11b**



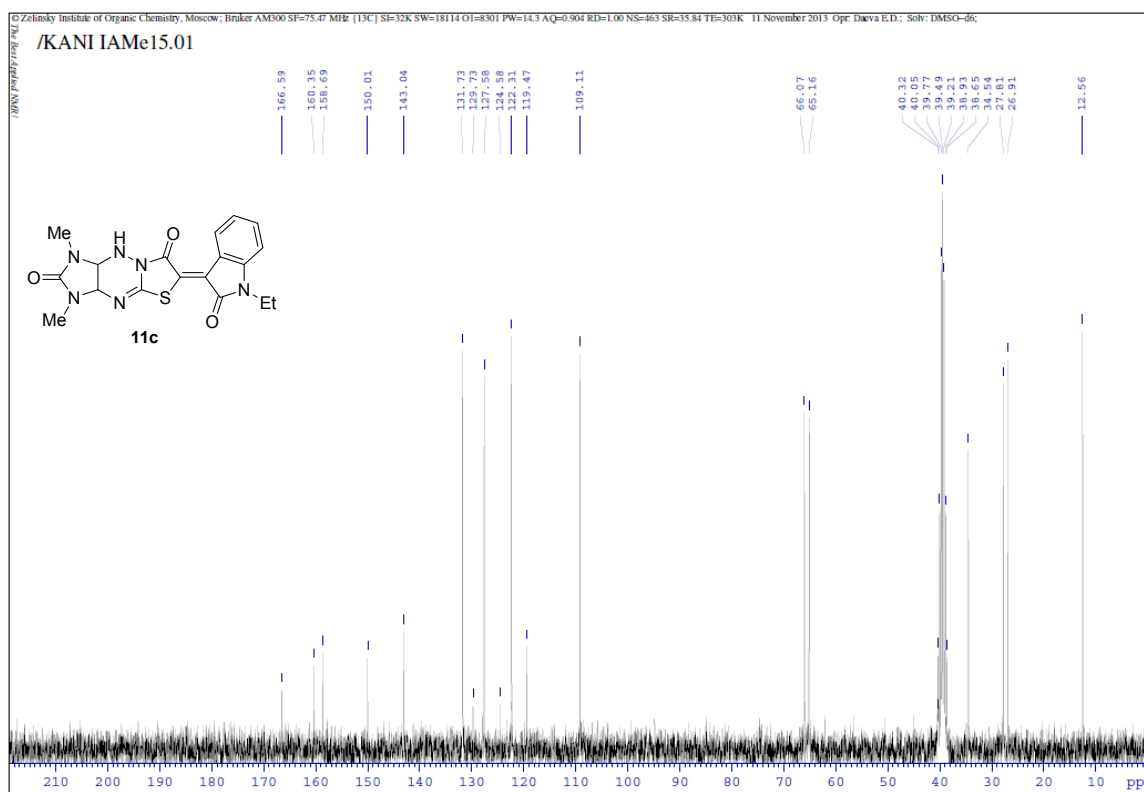
¹³C NMR spectrum of **11b**



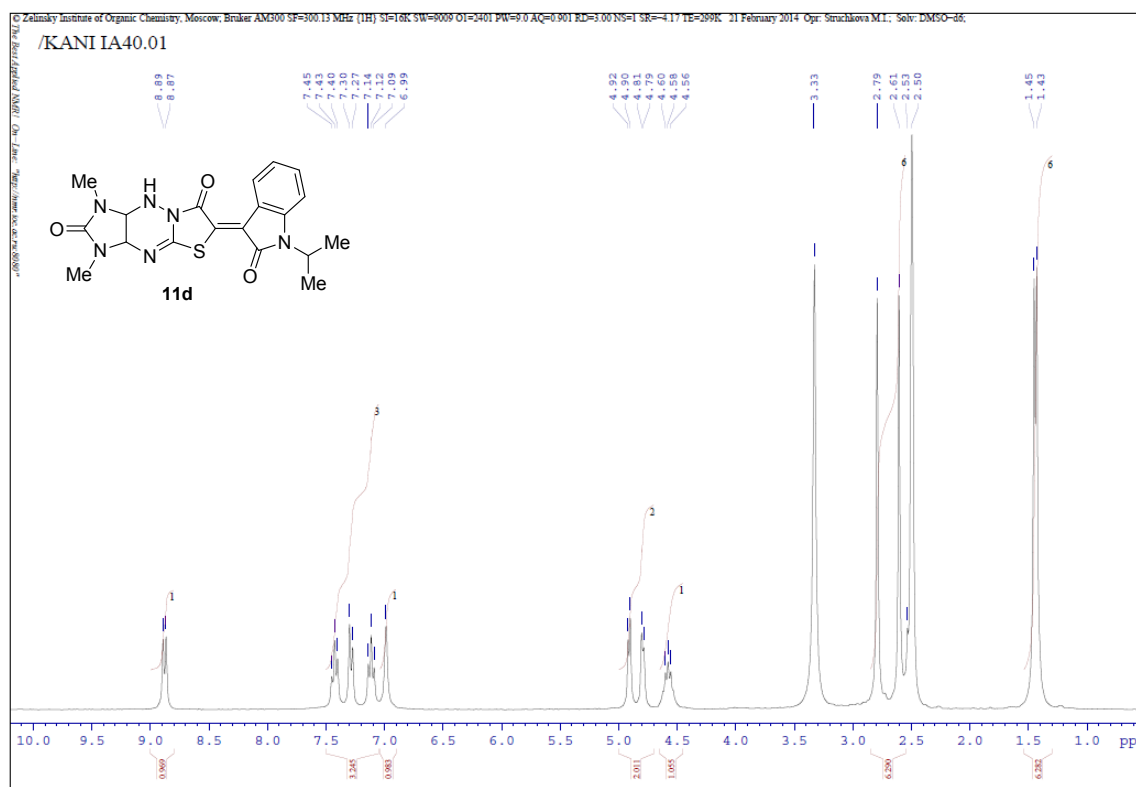
¹H NMR spectrum of **11c**



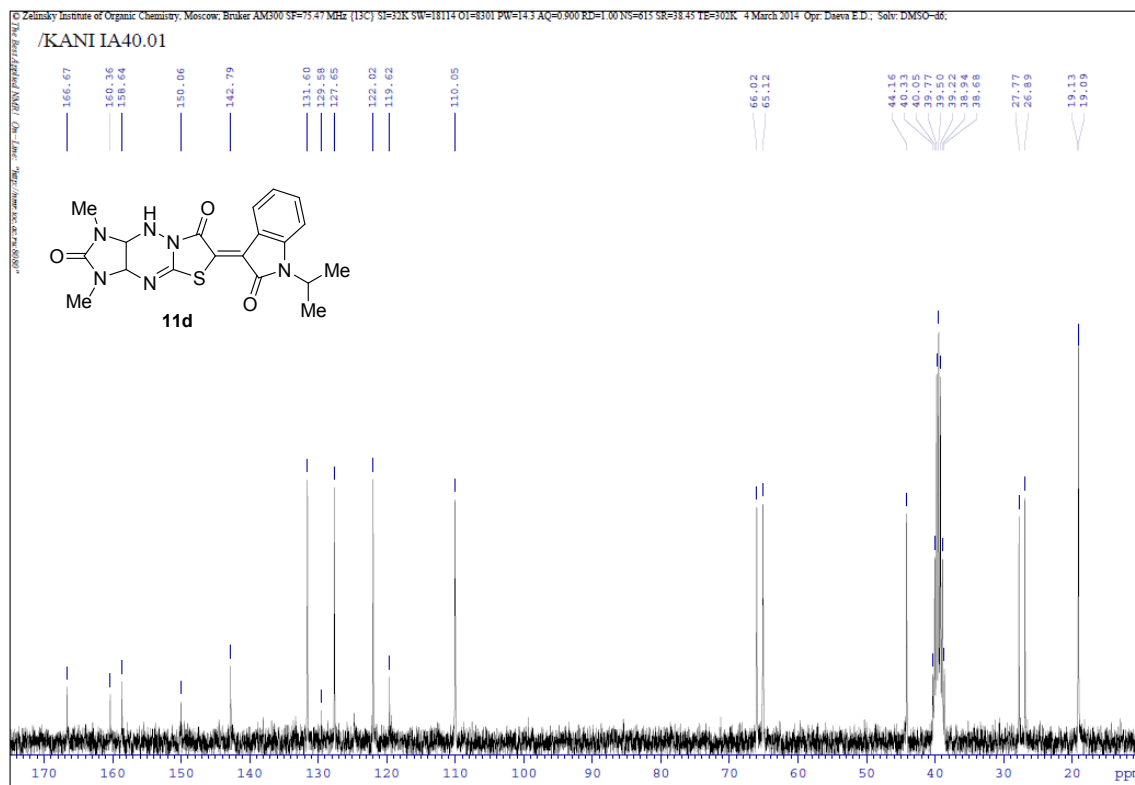
¹³C NMR spectrum of **11c**



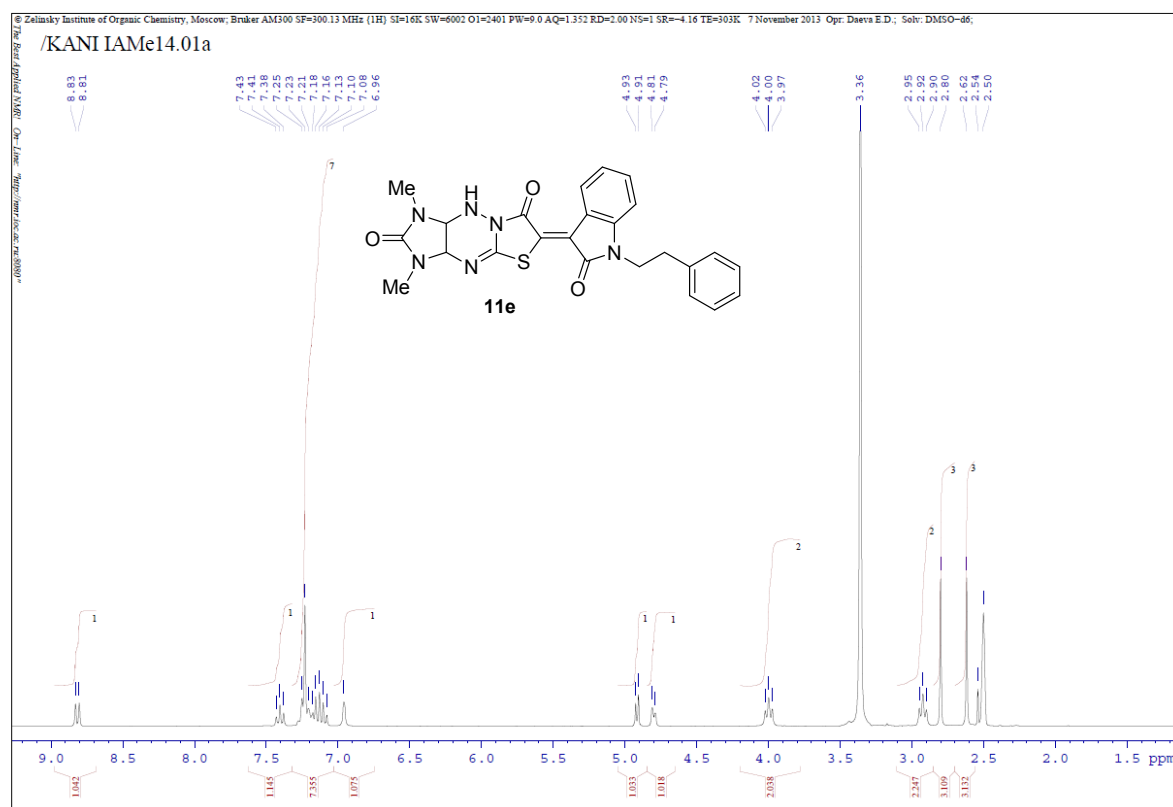
¹H NMR spectrum of **11d**



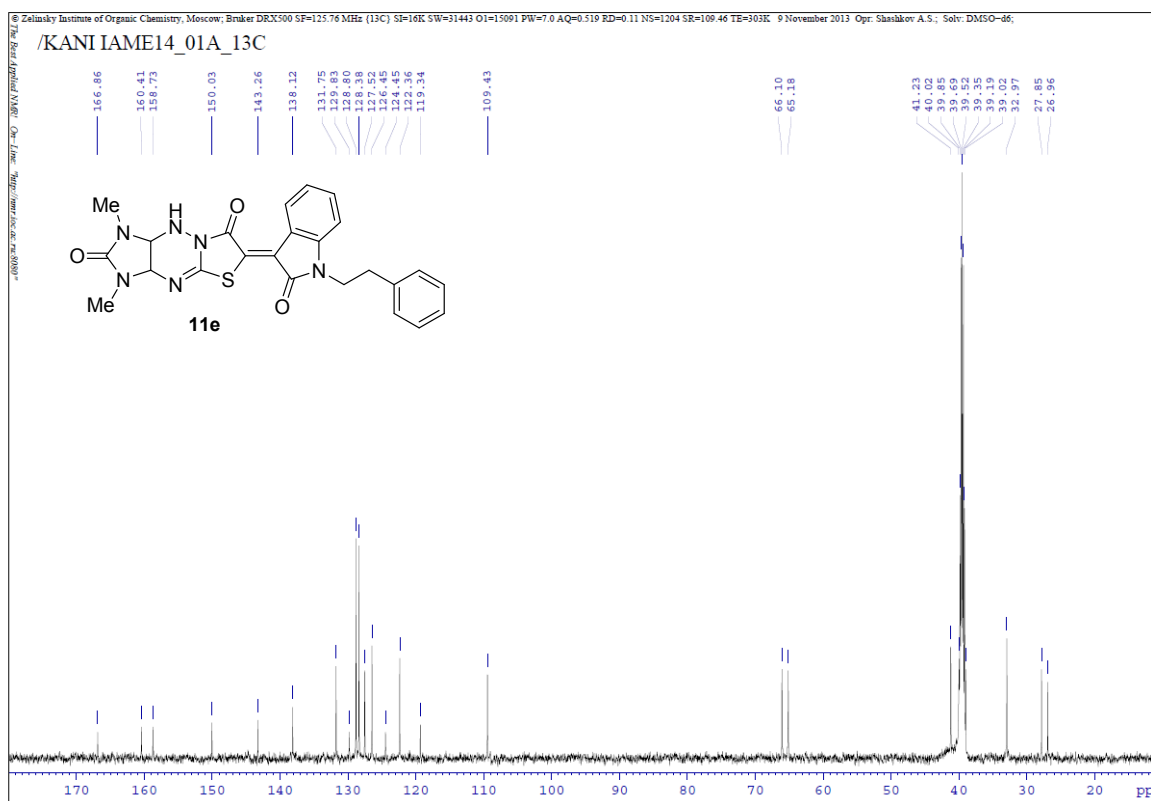
¹³C NMR spectrum of **11d**



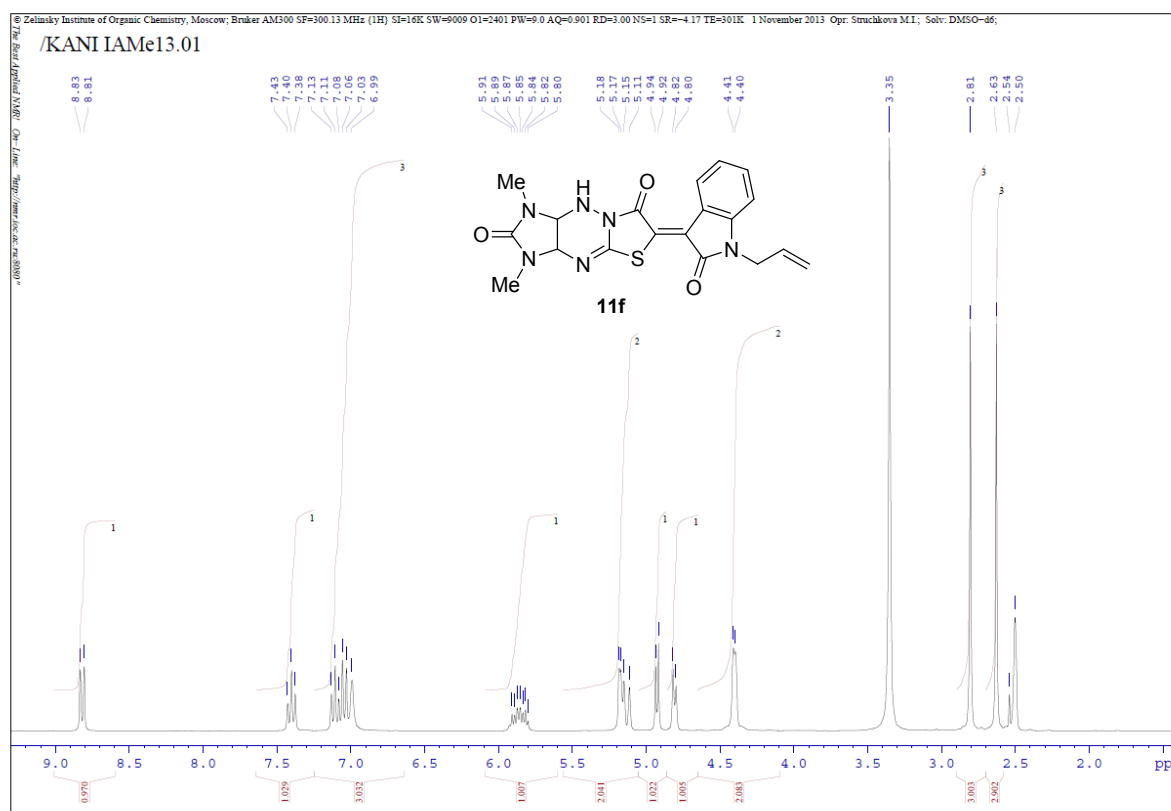
¹H NMR spectrum of **11e**



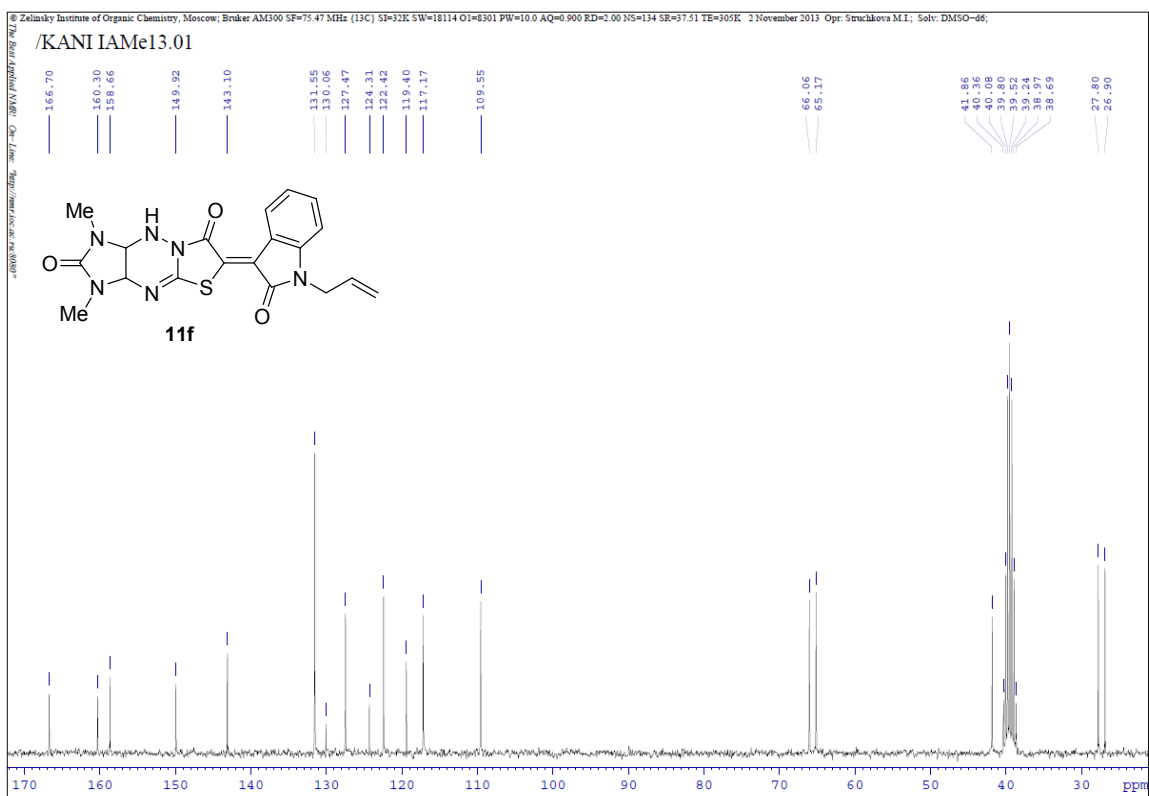
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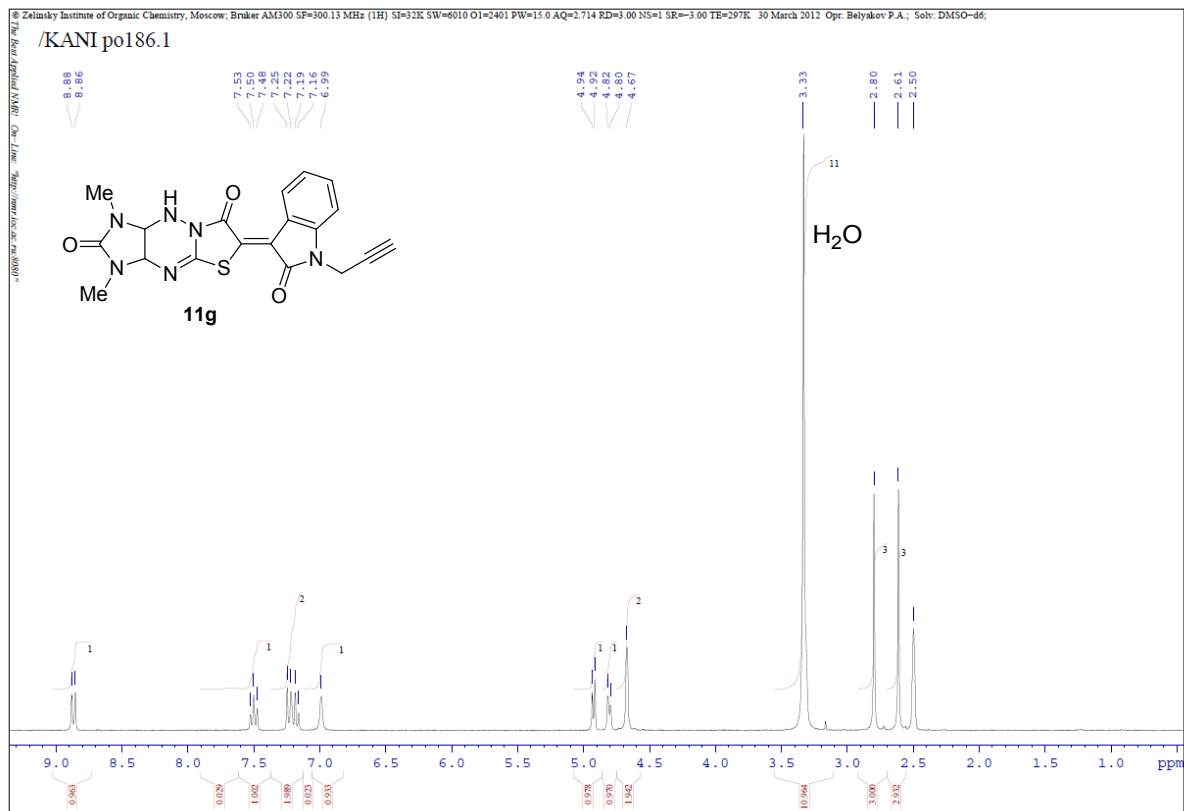
¹H NMR spectrum of **11f**



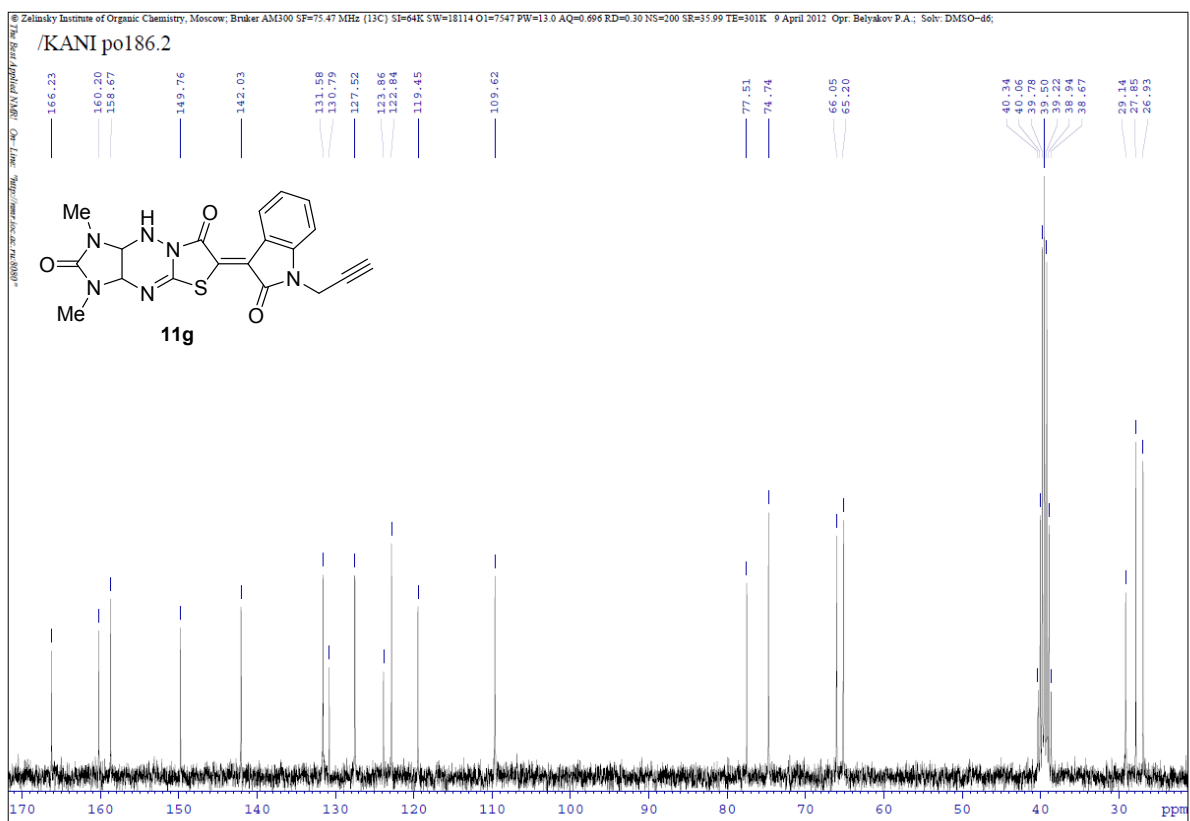
¹³C NMR spectrum of **11f**



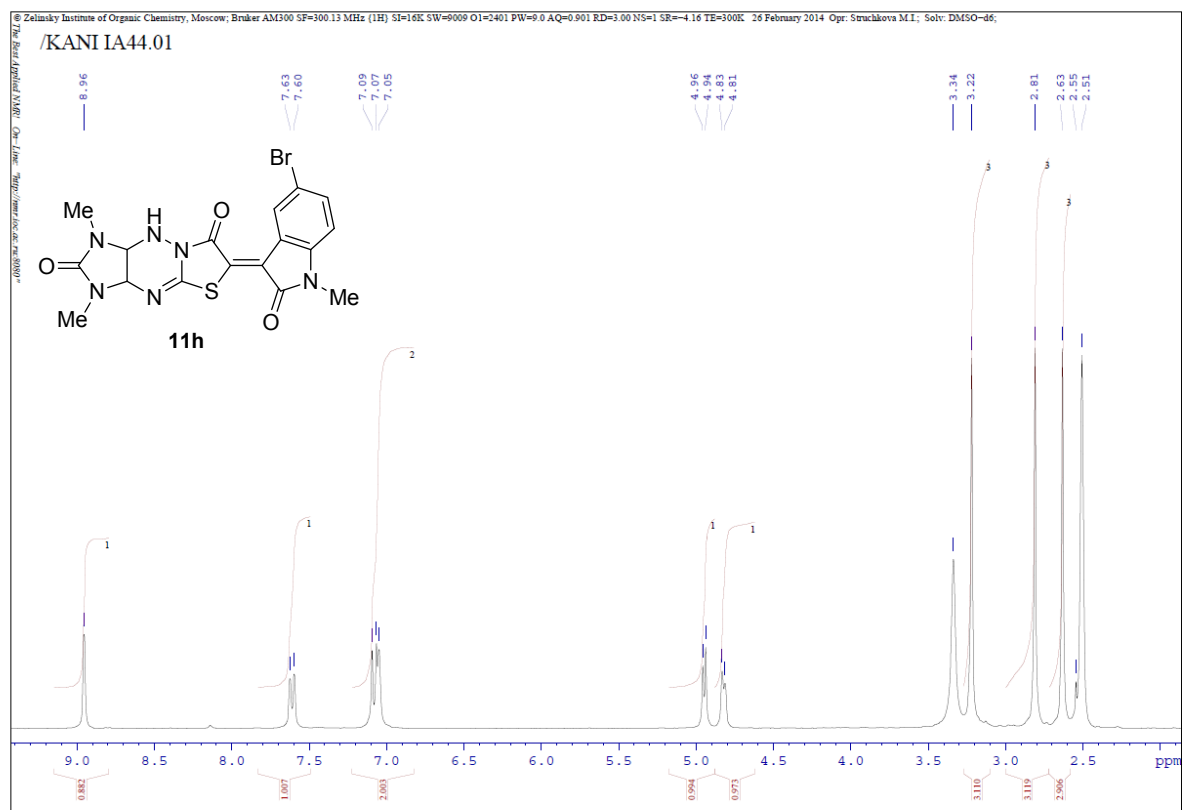
¹H NMR spectrum of **11g**



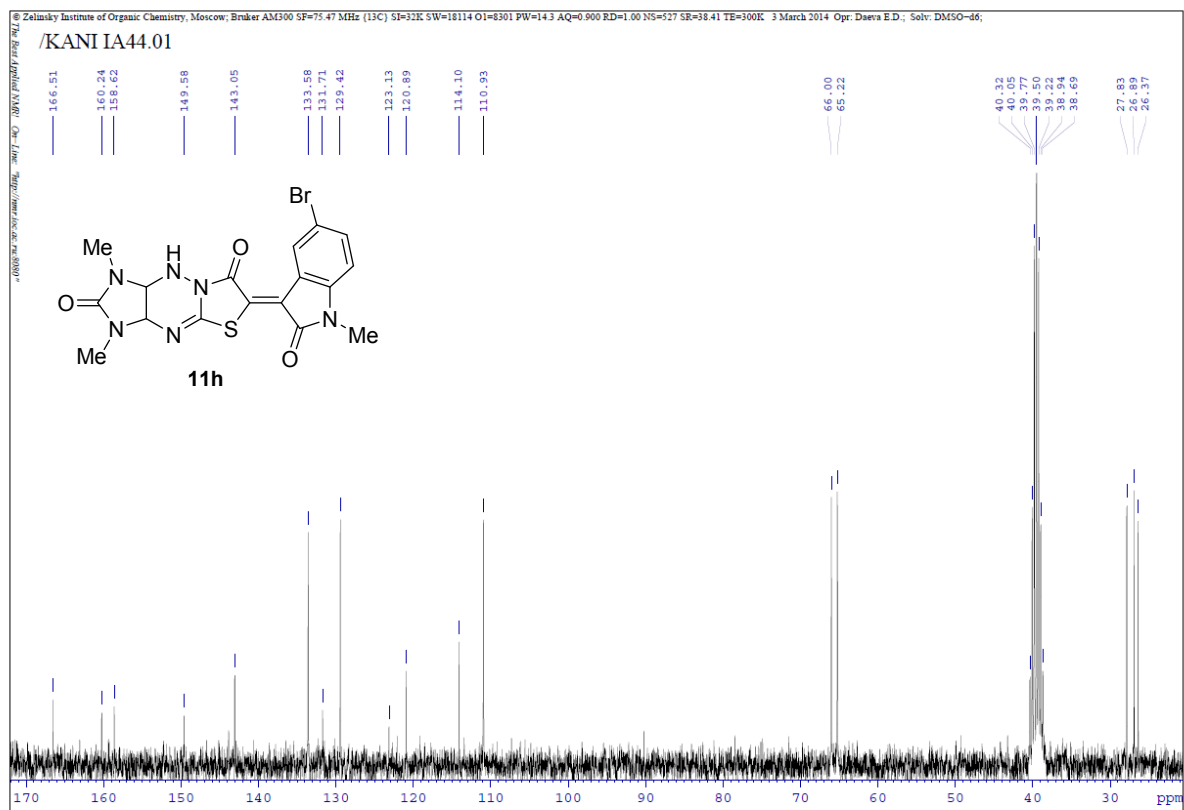
¹³C NMR spectrum of **11g**



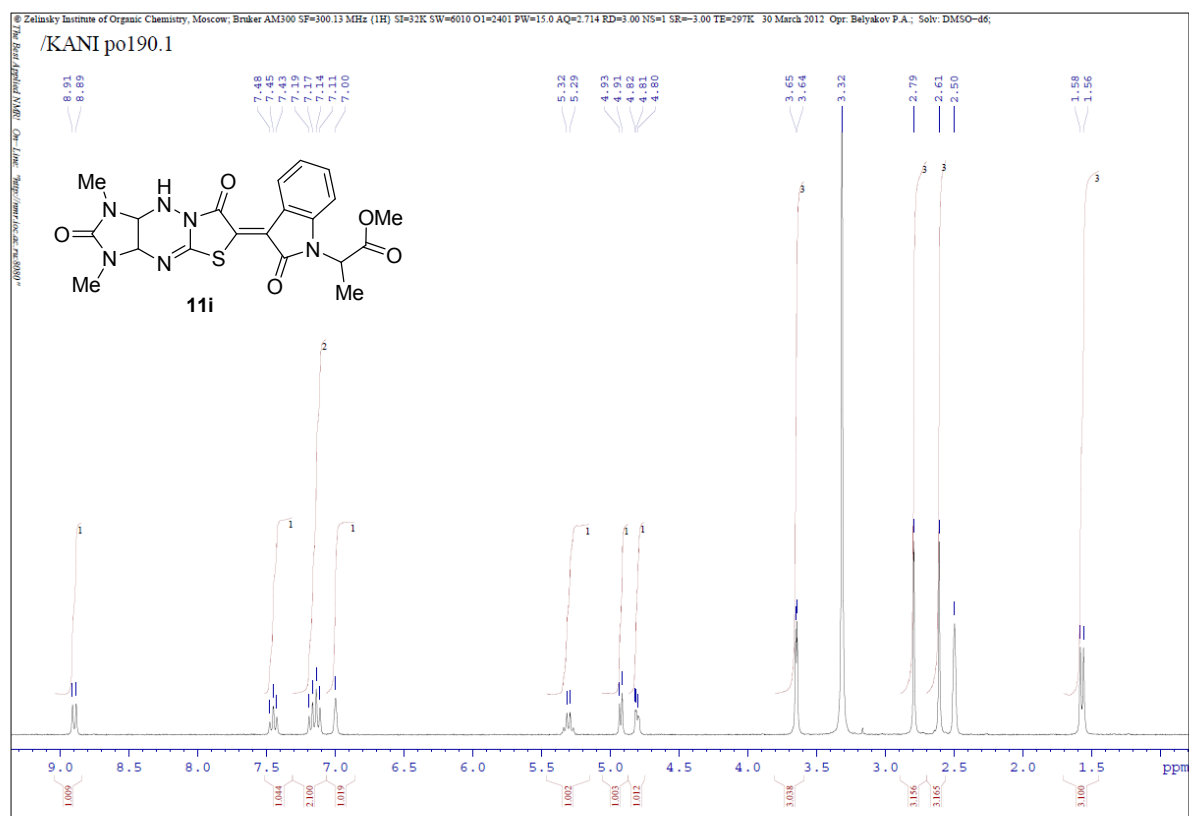
¹H NMR spectrum of **11h**



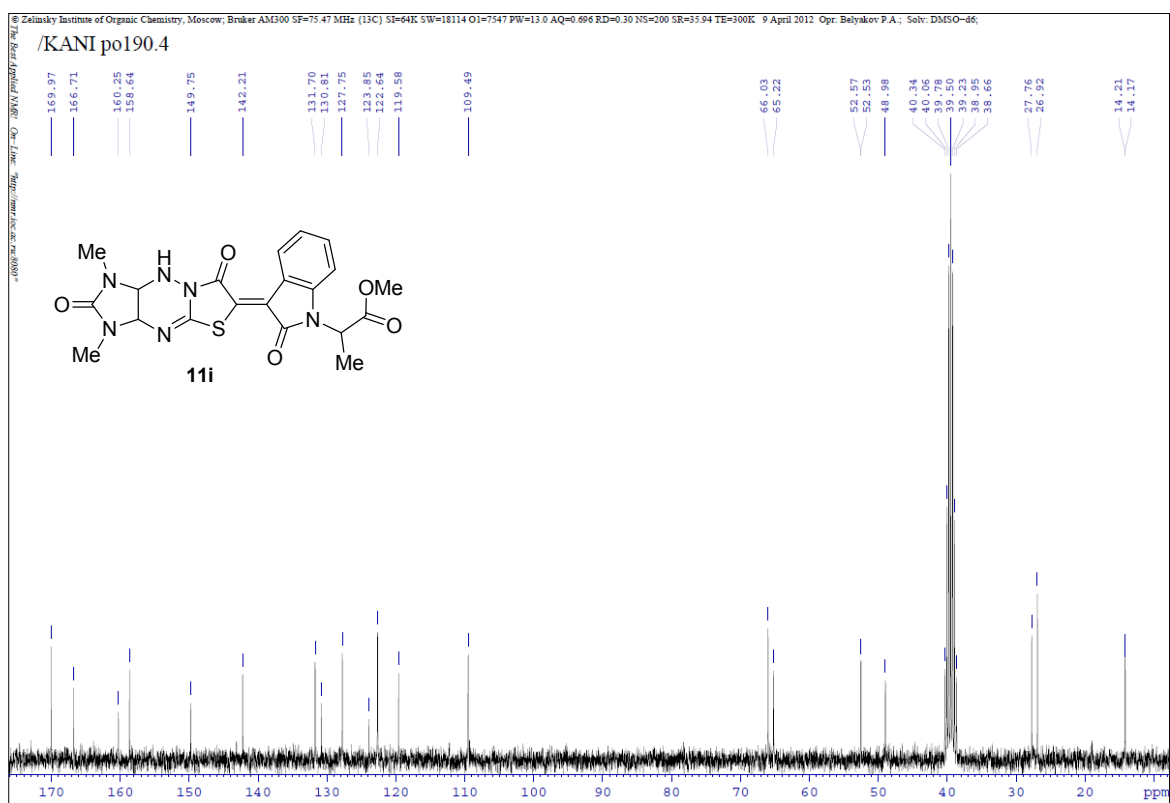
¹³C NMR spectrum of **11h**



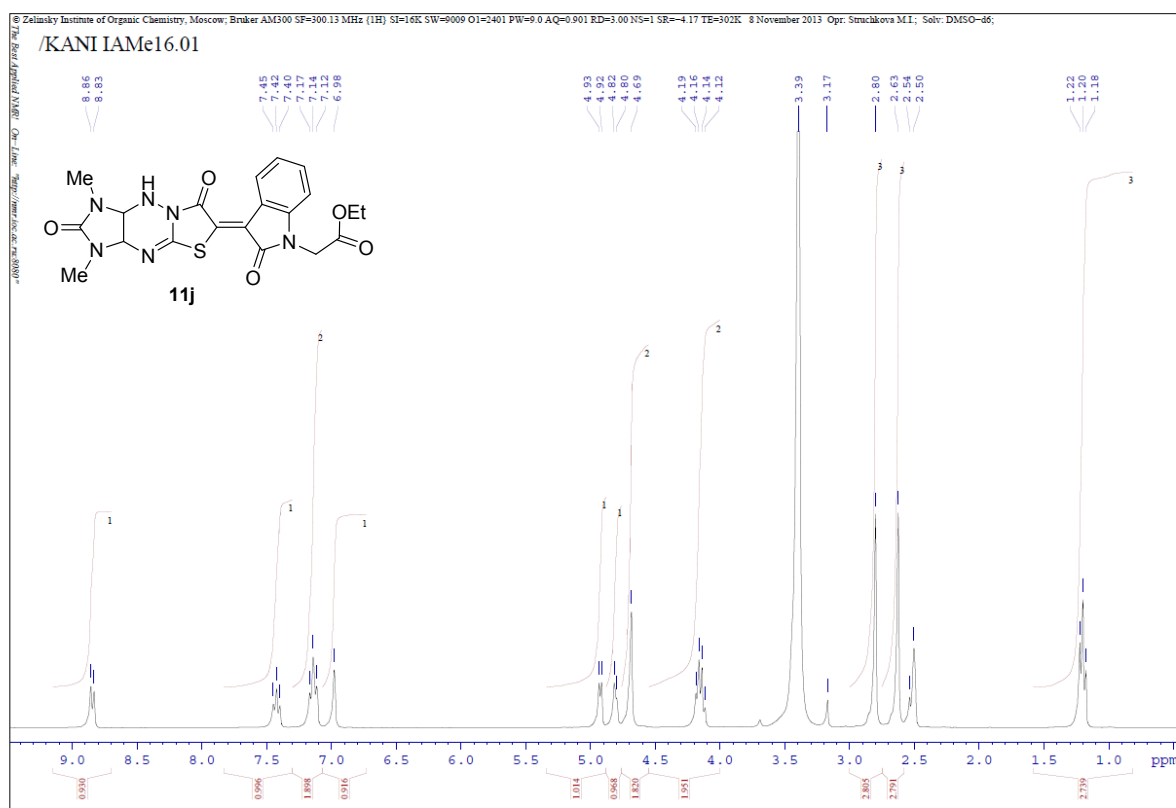
¹H NMR spectrum of **11i**



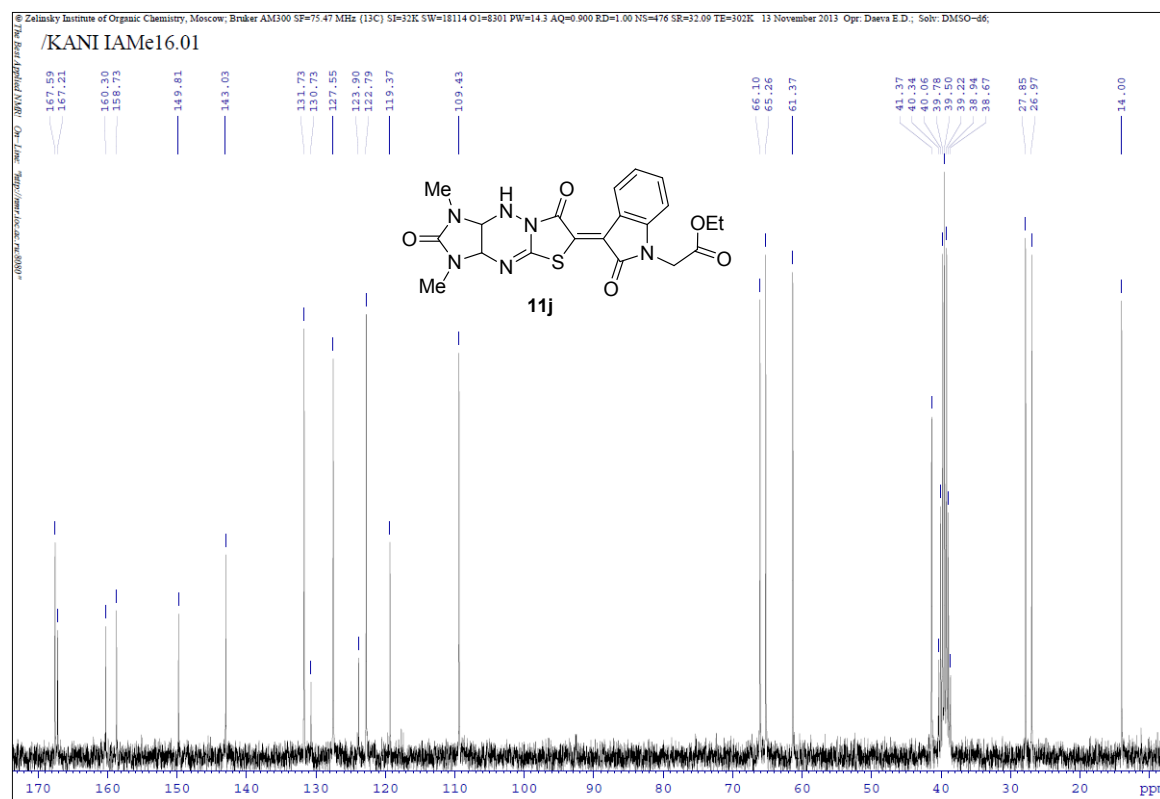
¹³C NMR spectrum of **11i**



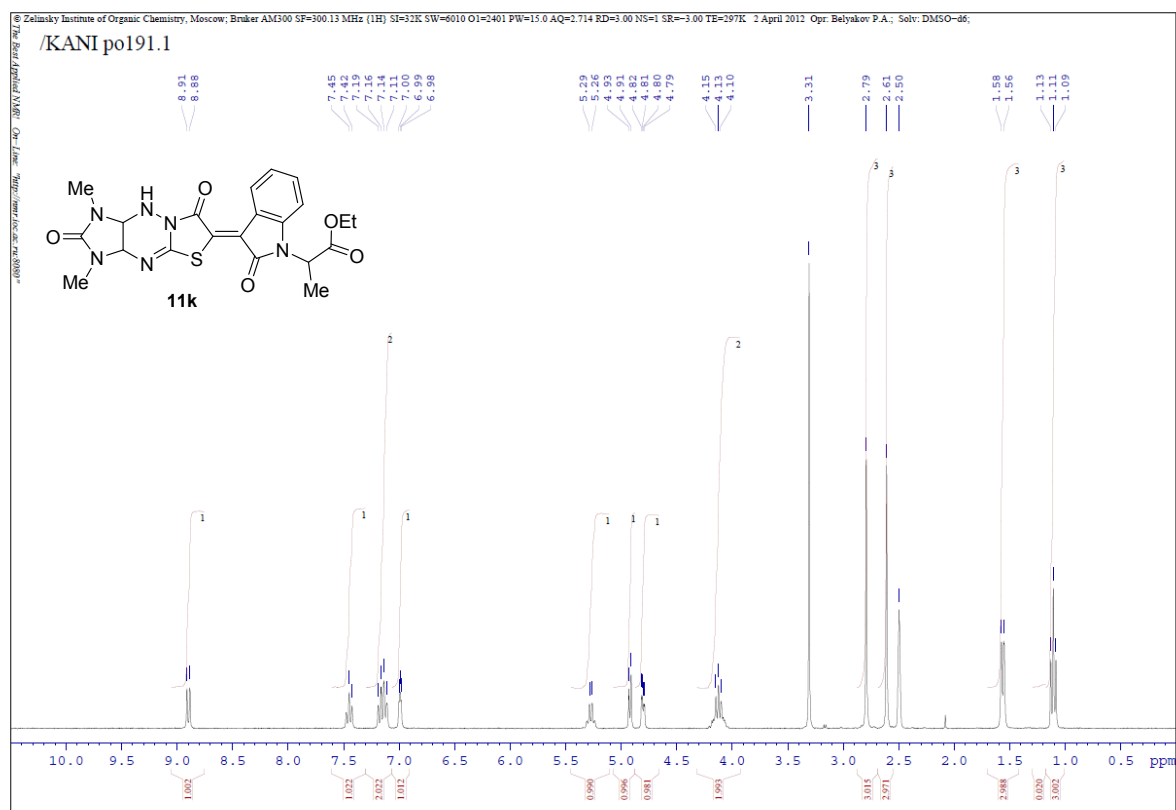
¹H NMR spectrum of **11j**



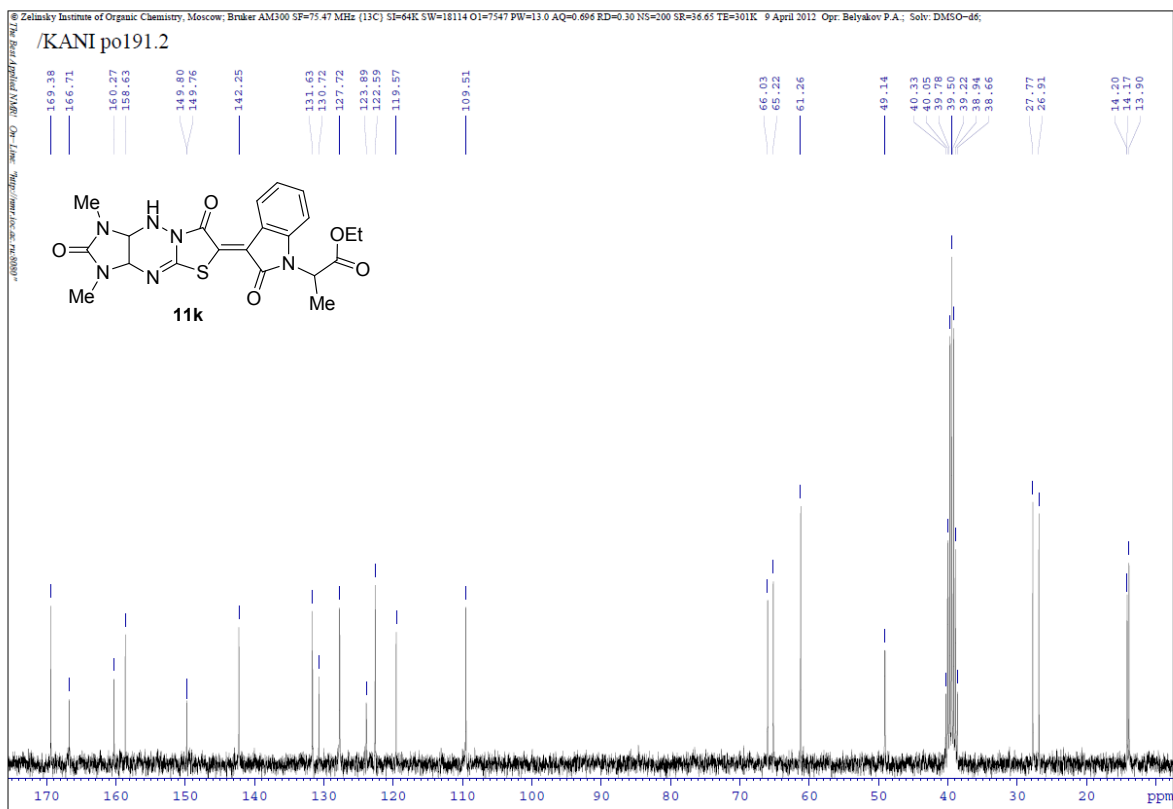
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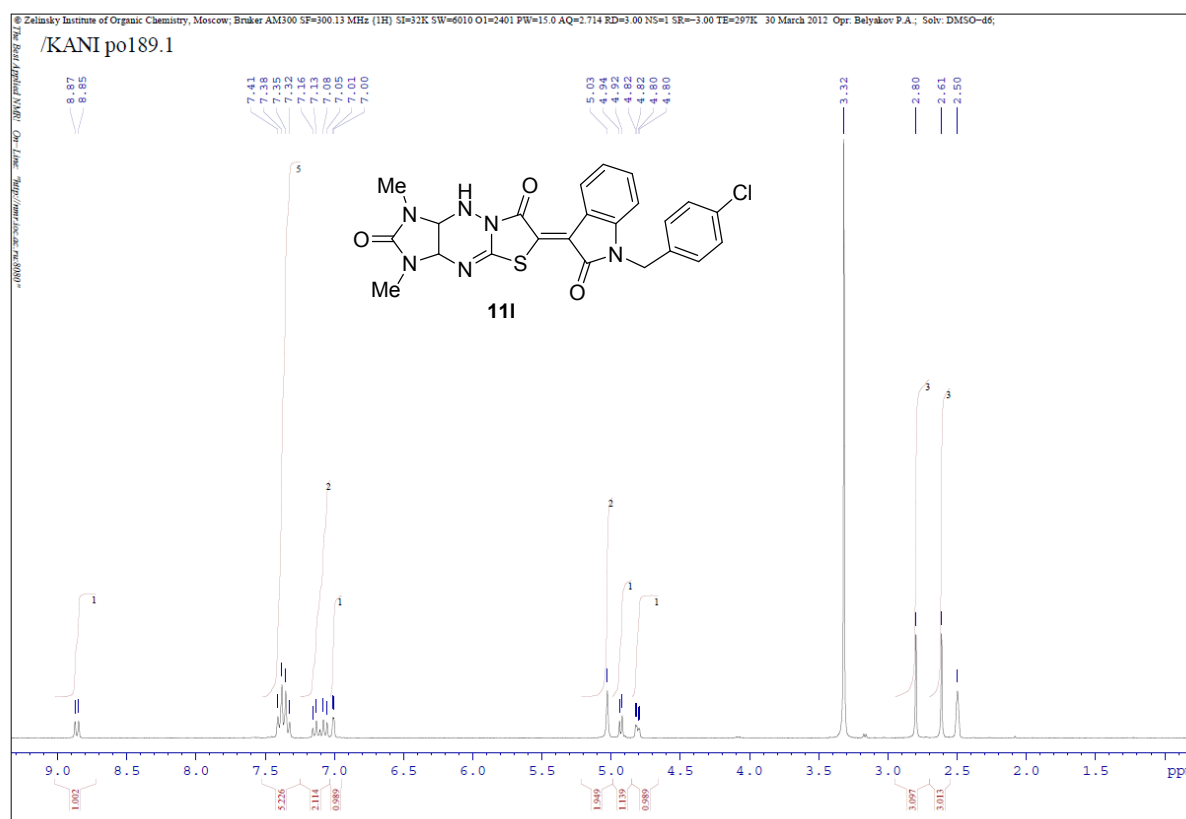
¹H NMR spectrum of **11k**



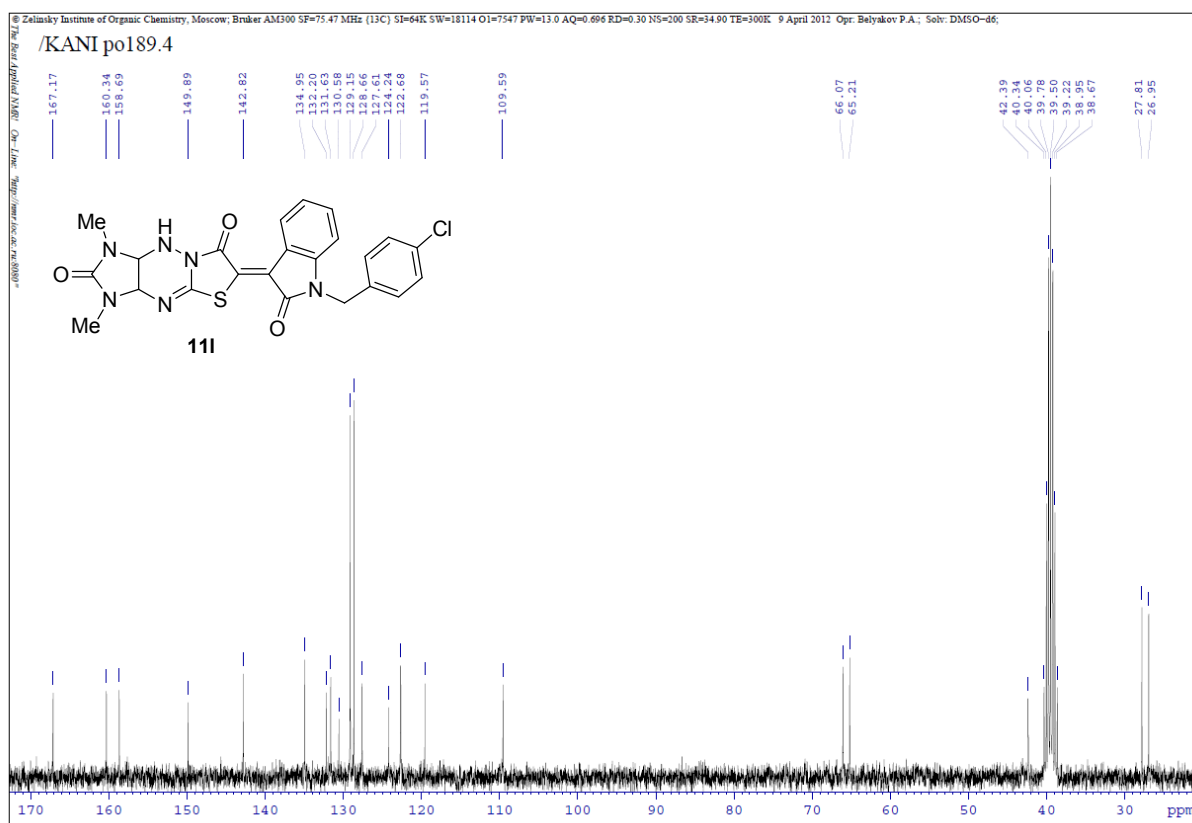
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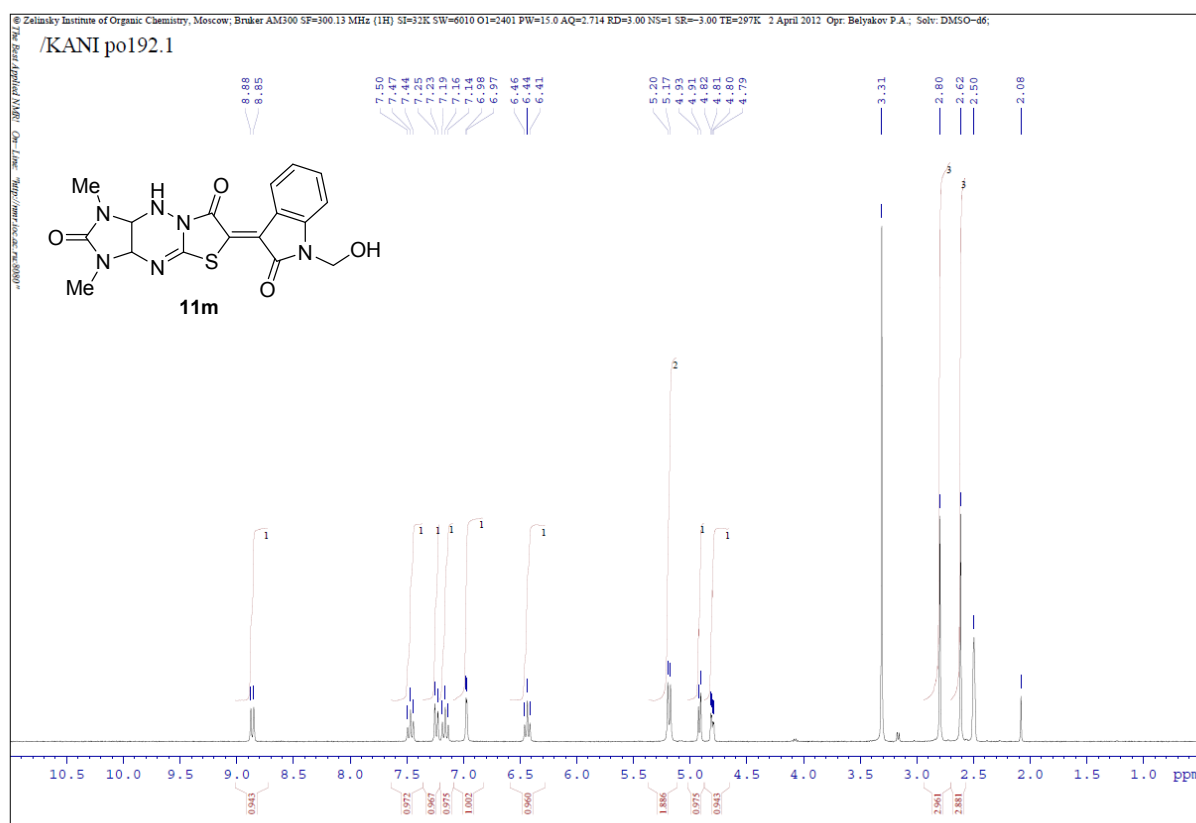
¹H NMR spectrum of **11l**



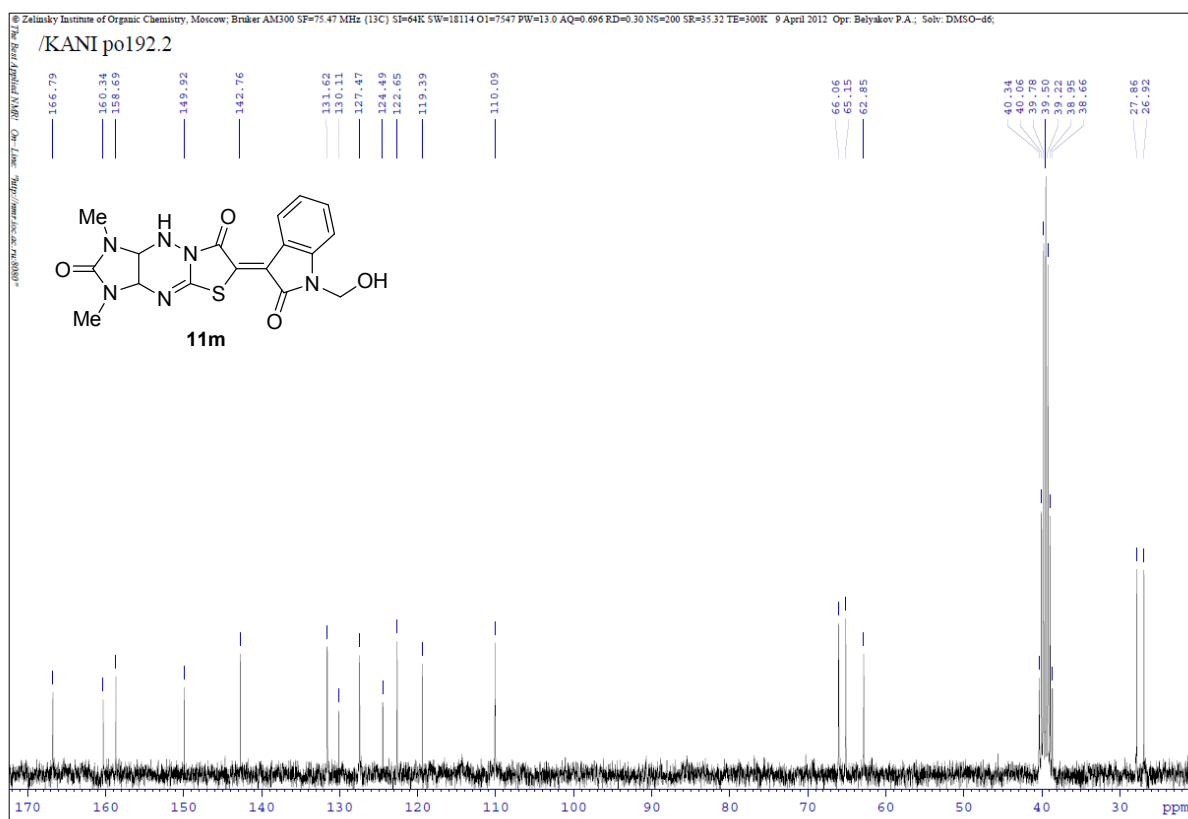
¹³C NMR spectrum of **11l**



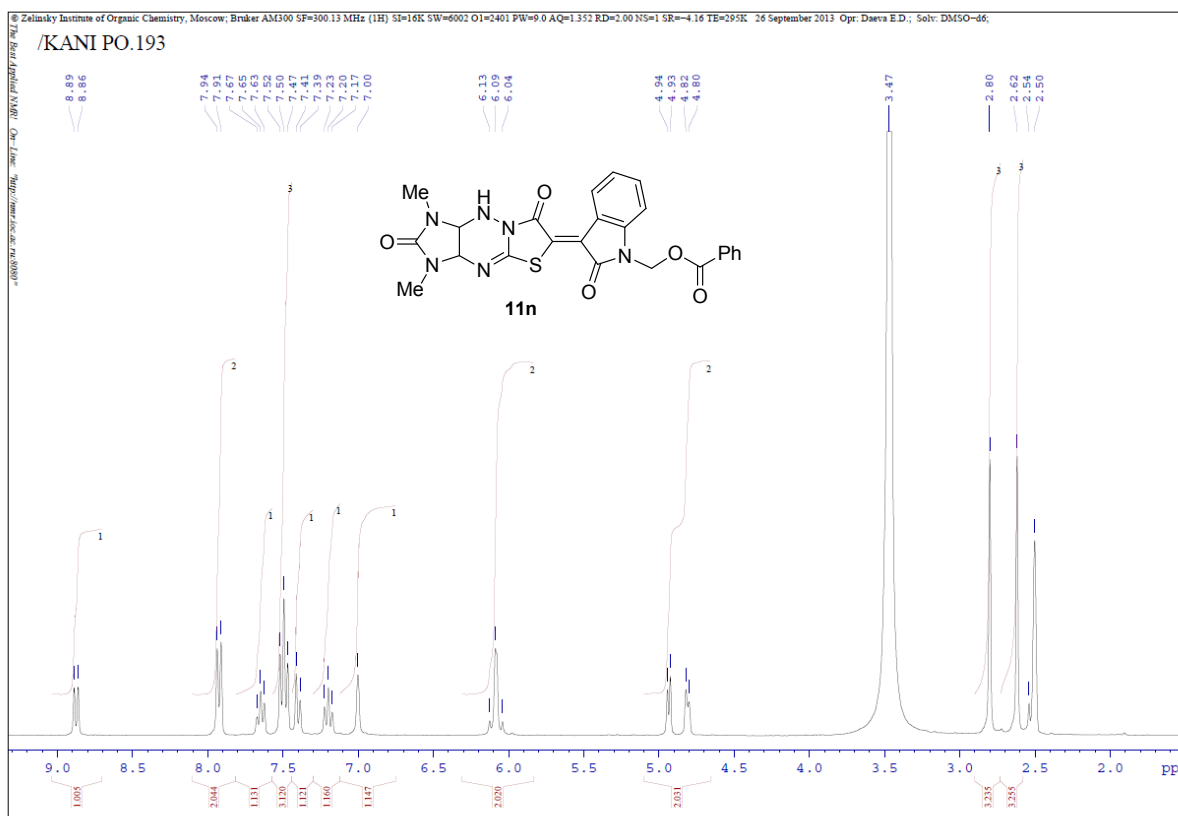
¹H NMR spectrum of **11m**



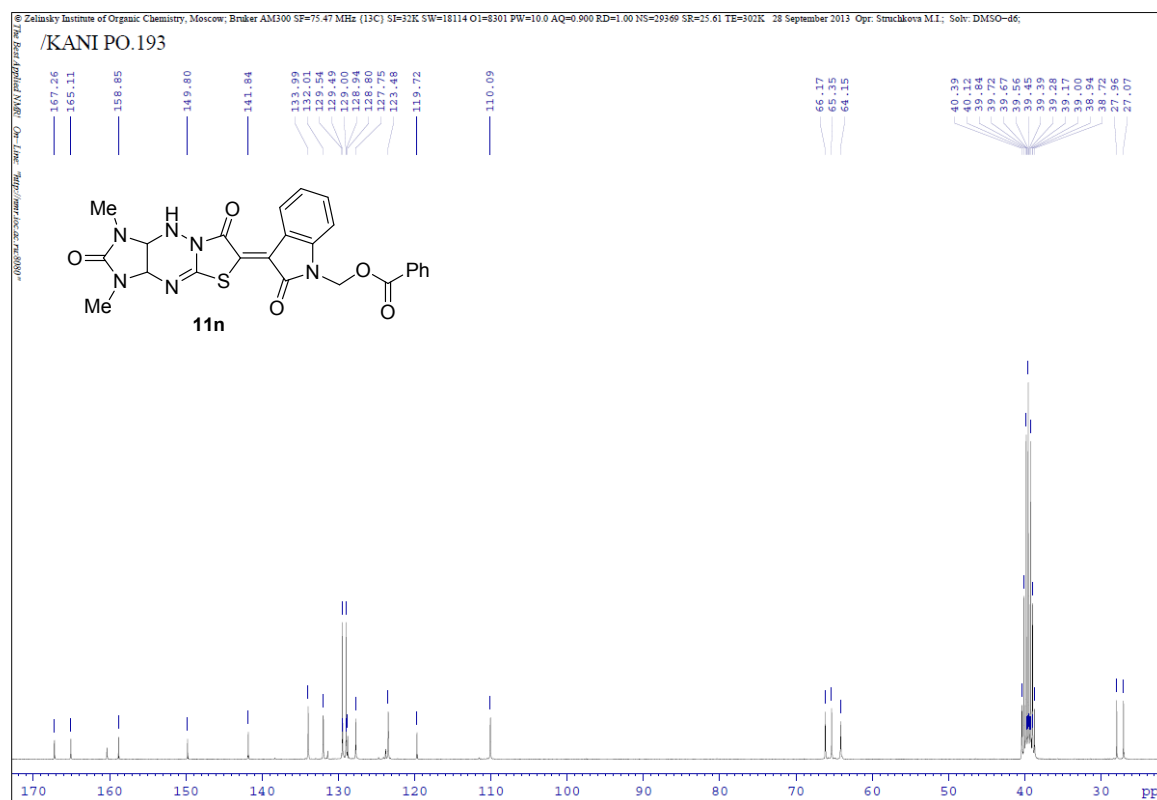
¹³C NMR spectrum of **11m**



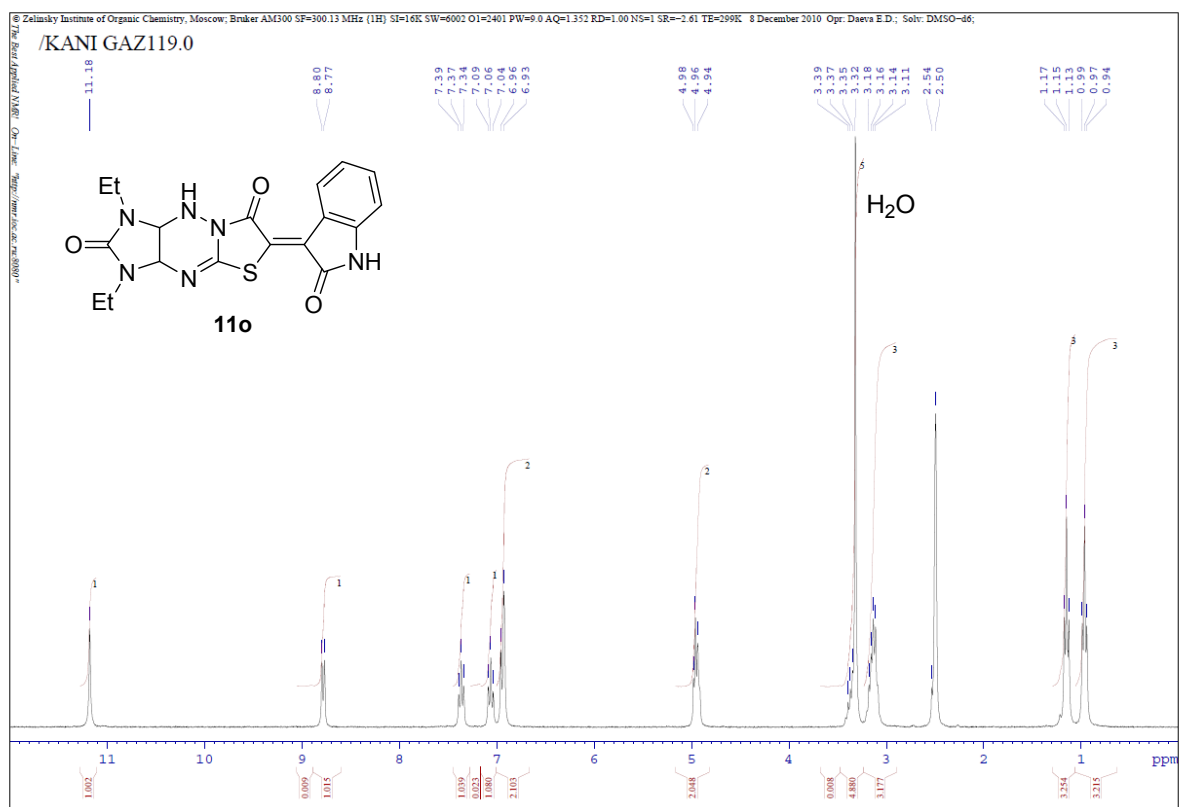
¹H NMR spectrum of **11n**



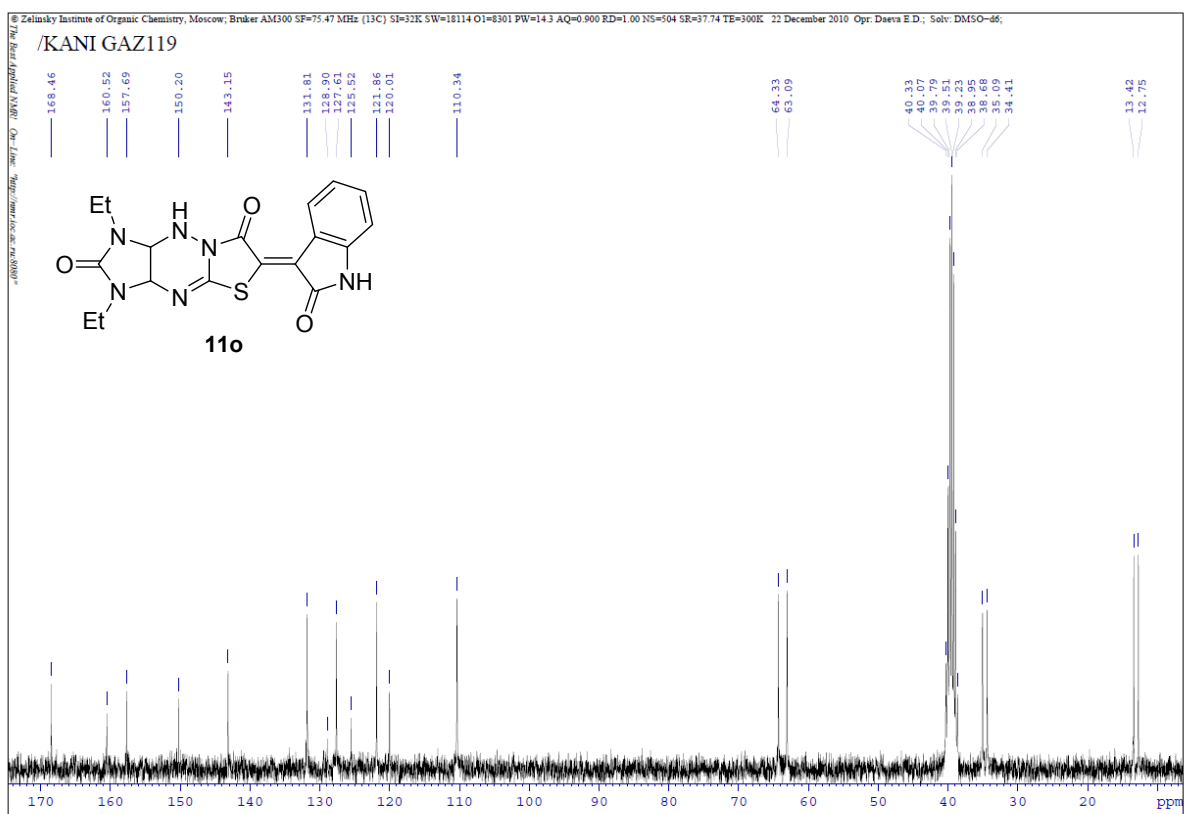
¹³C NMR spectrum of **11n**



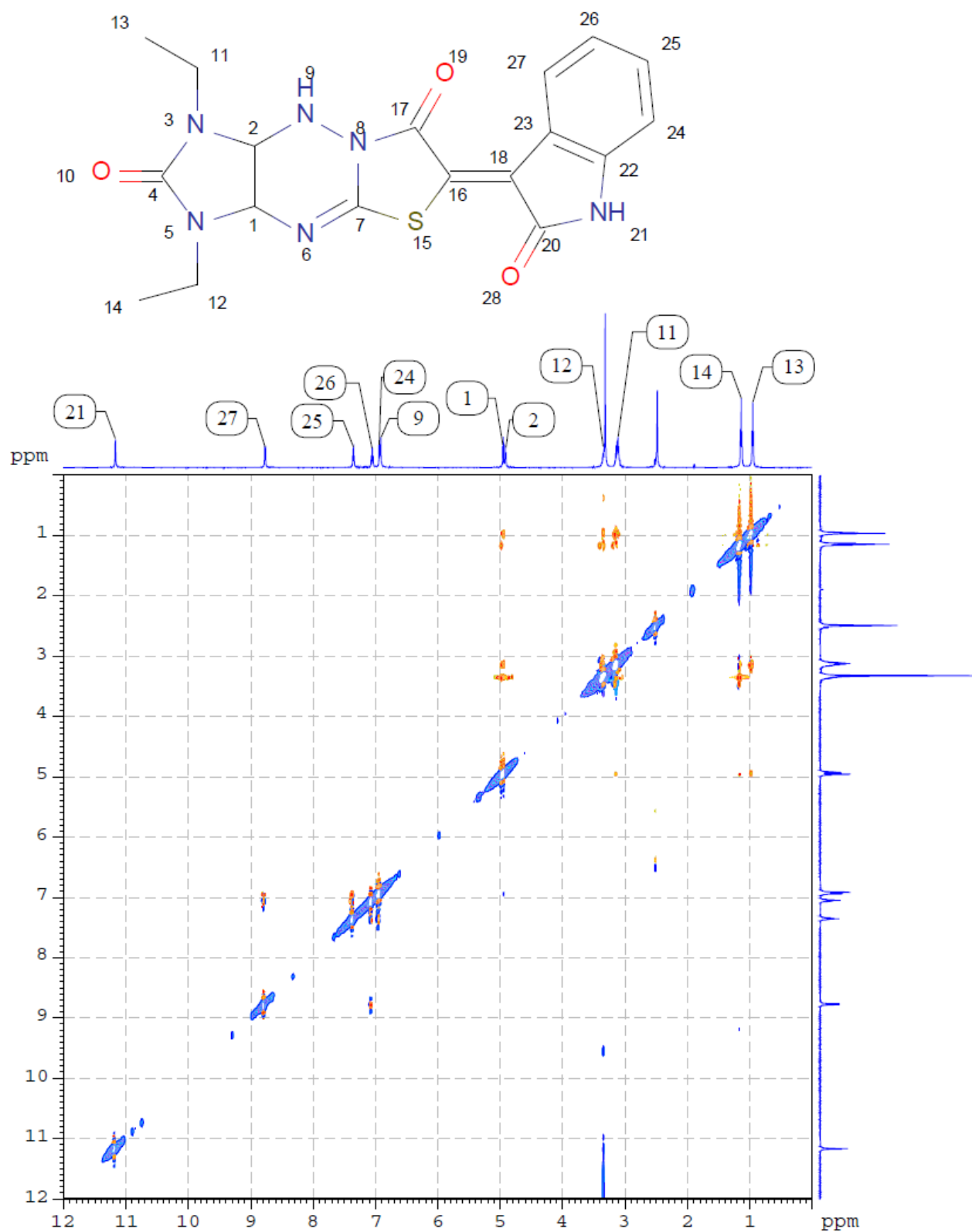
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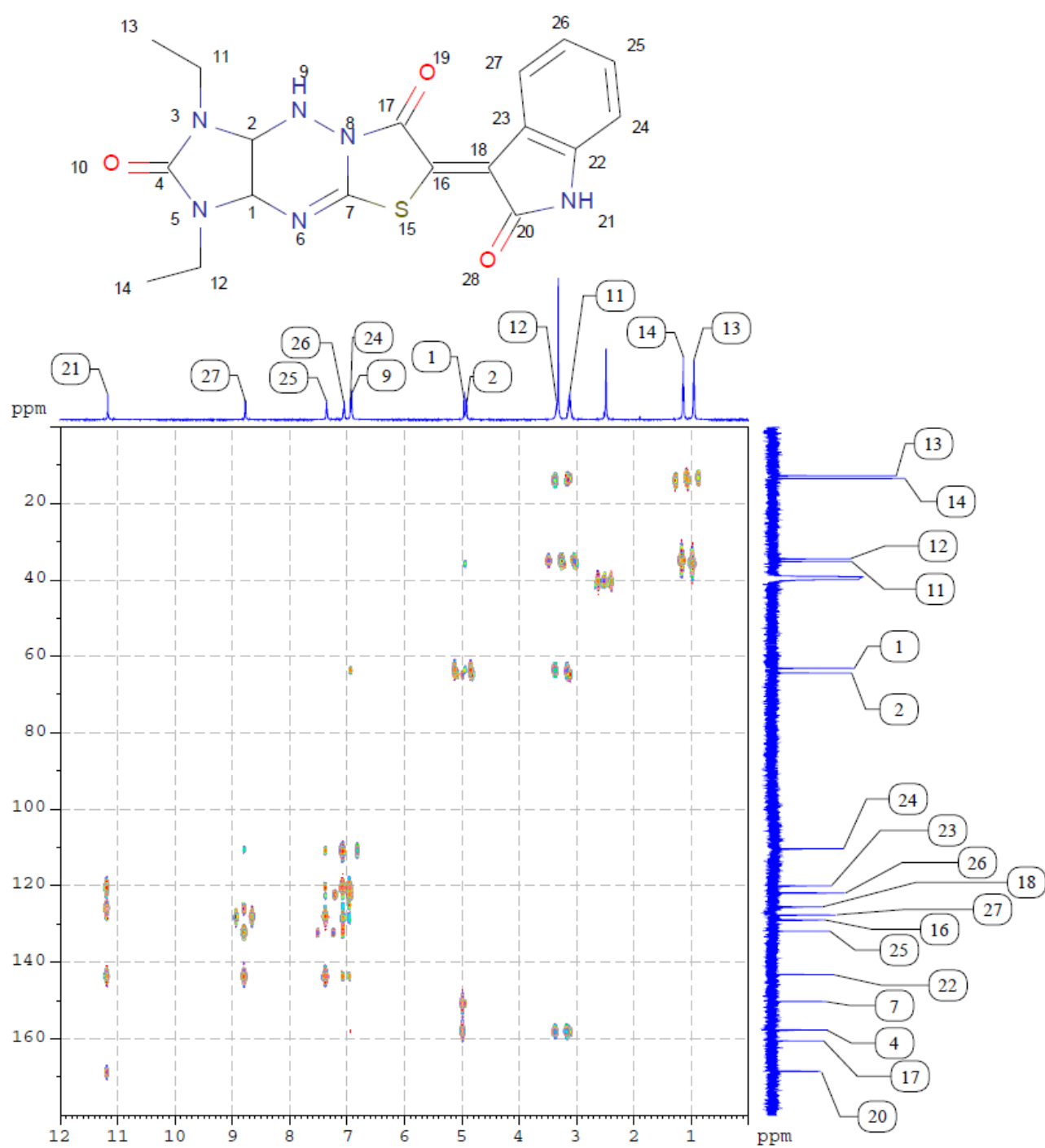
¹³C NMR spectrum of **11o**



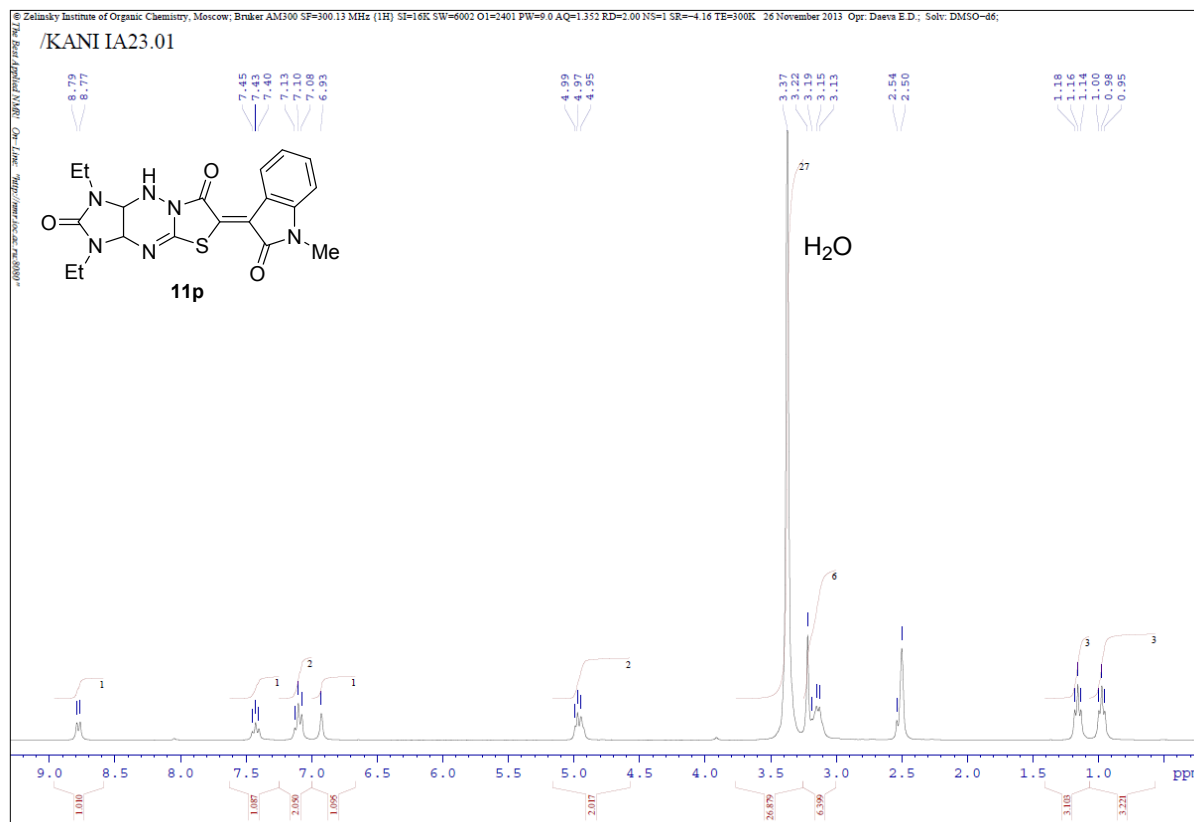
NOESY spectrum of **11o**



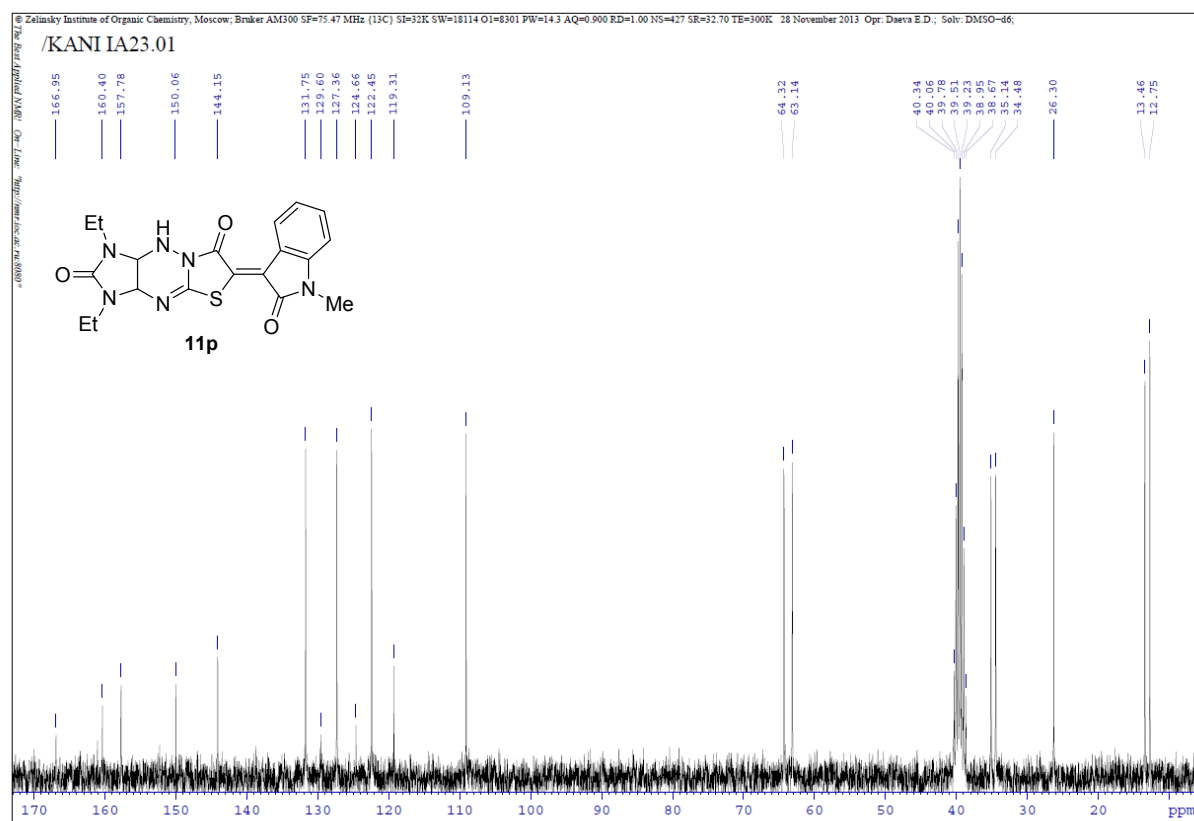
^1H - ^{13}C HMBC spectrum of **11o**



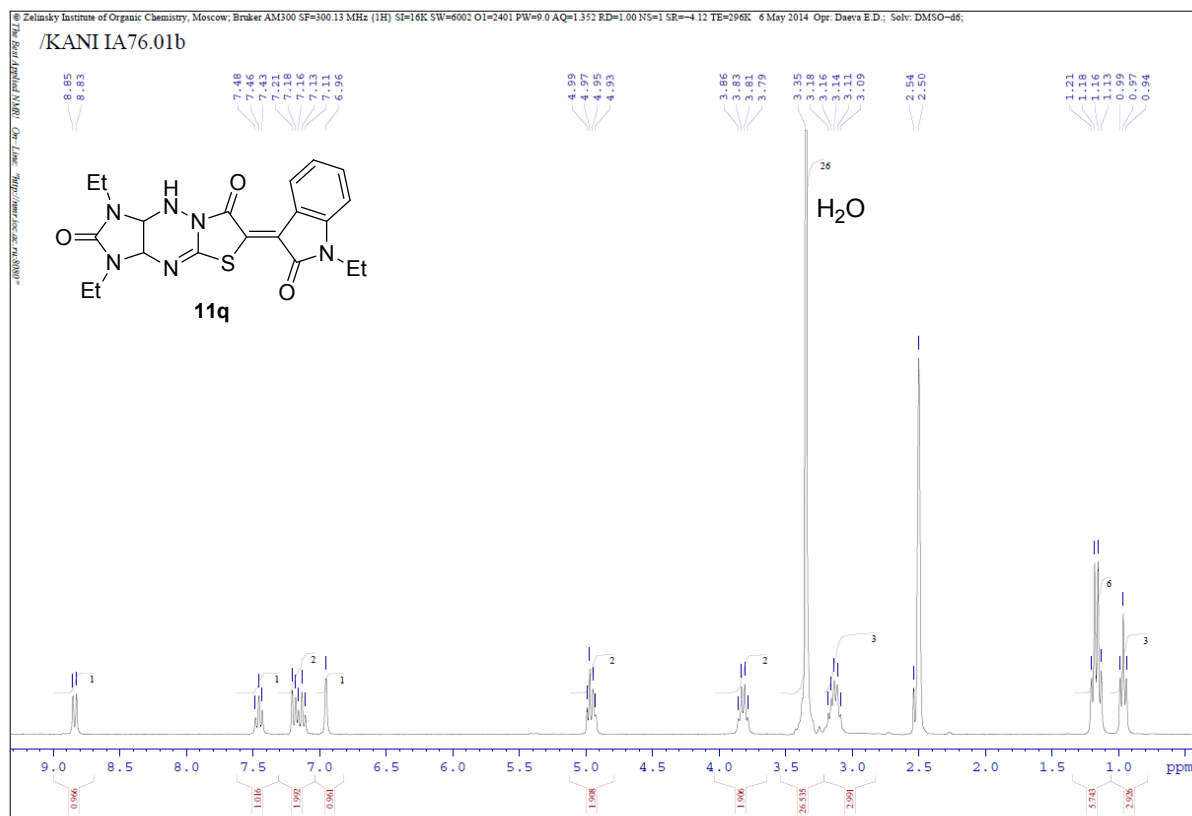
¹H NMR spectrum of **11p**



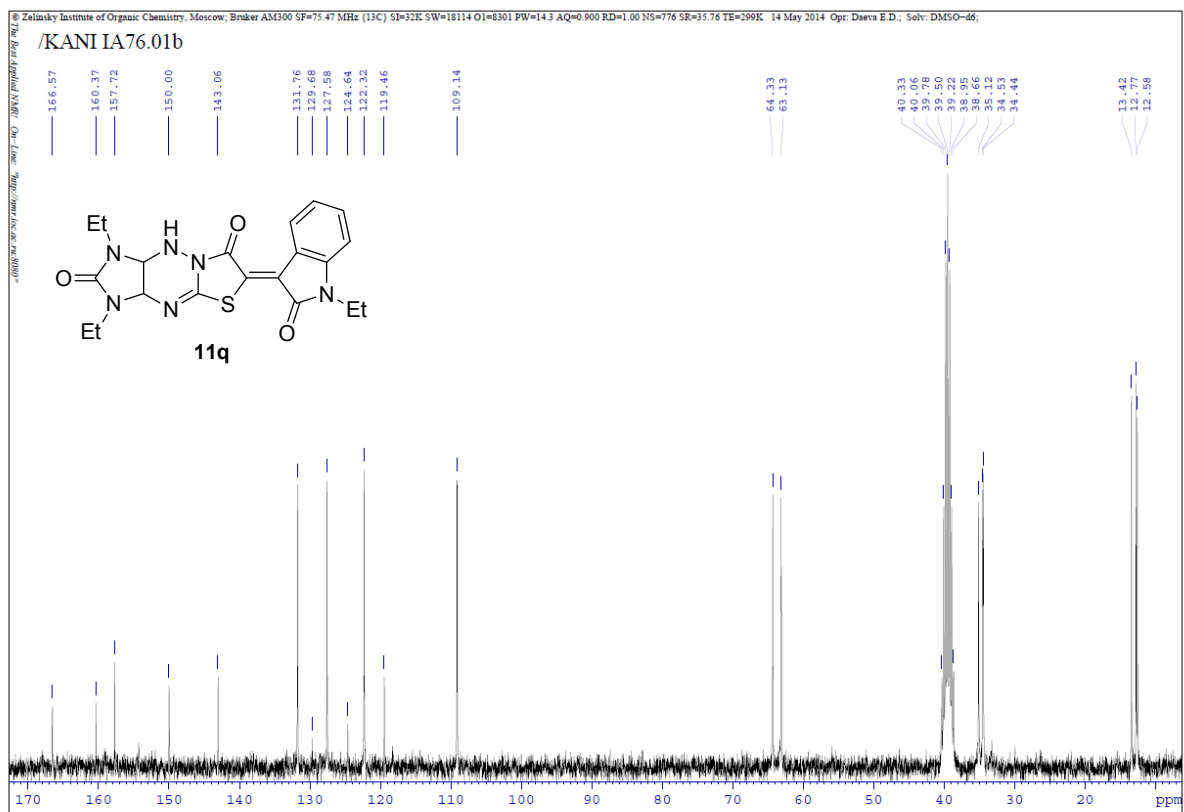
¹³C NMR spectrum of **11p**



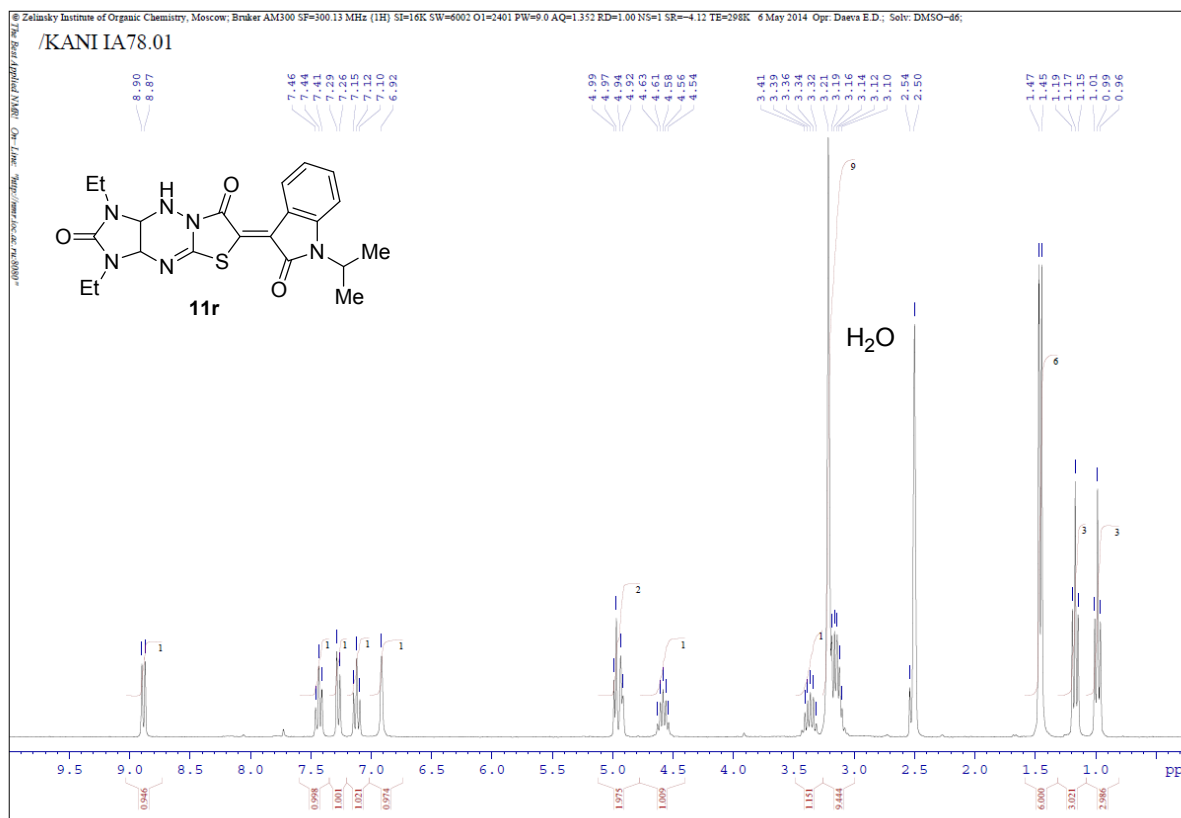
¹H NMR spectrum of **11q**



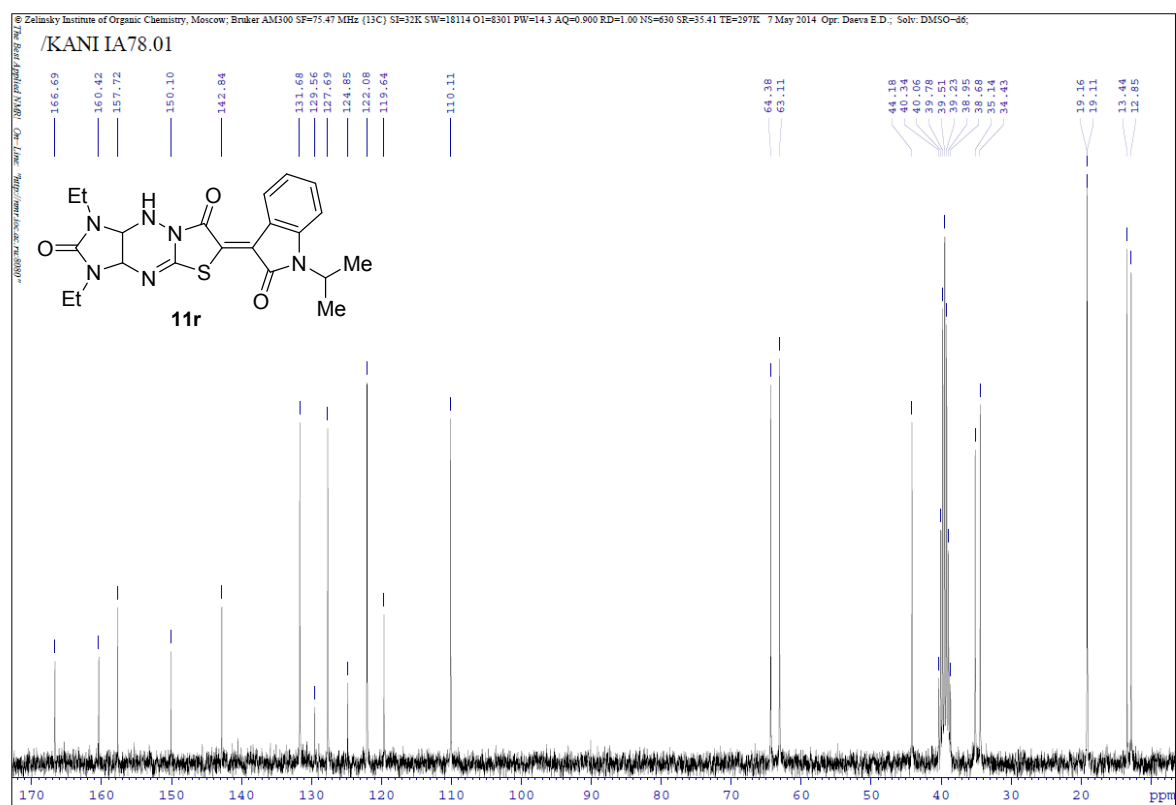
¹³C NMR spectrum of **11q**



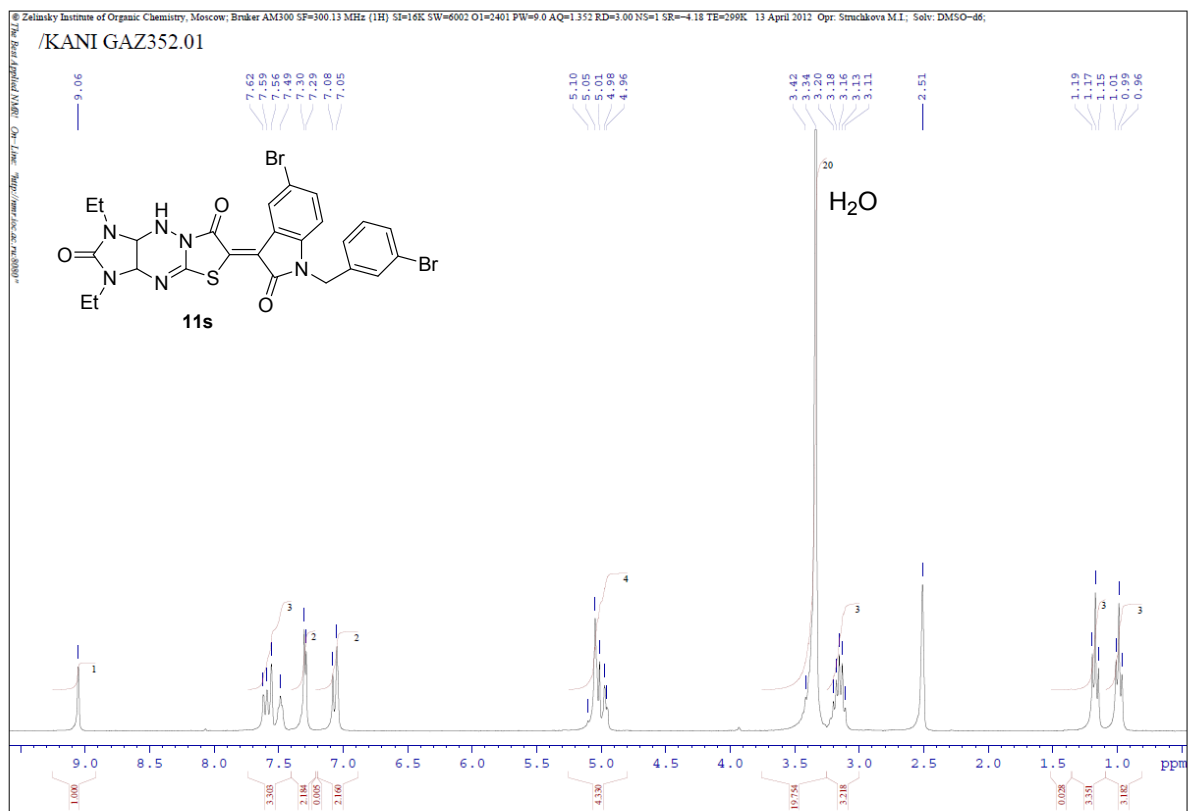
¹H NMR spectrum of **11r**



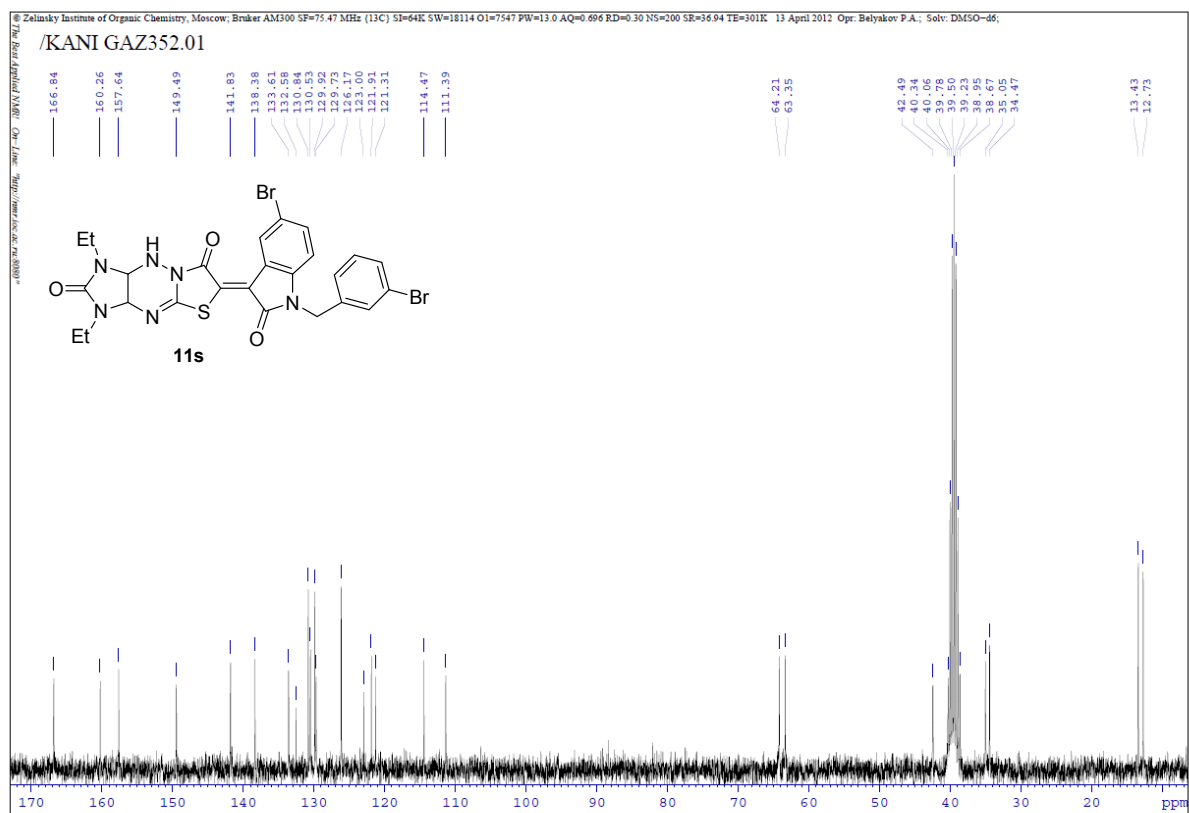
¹³C NMR spectrum of **11r**



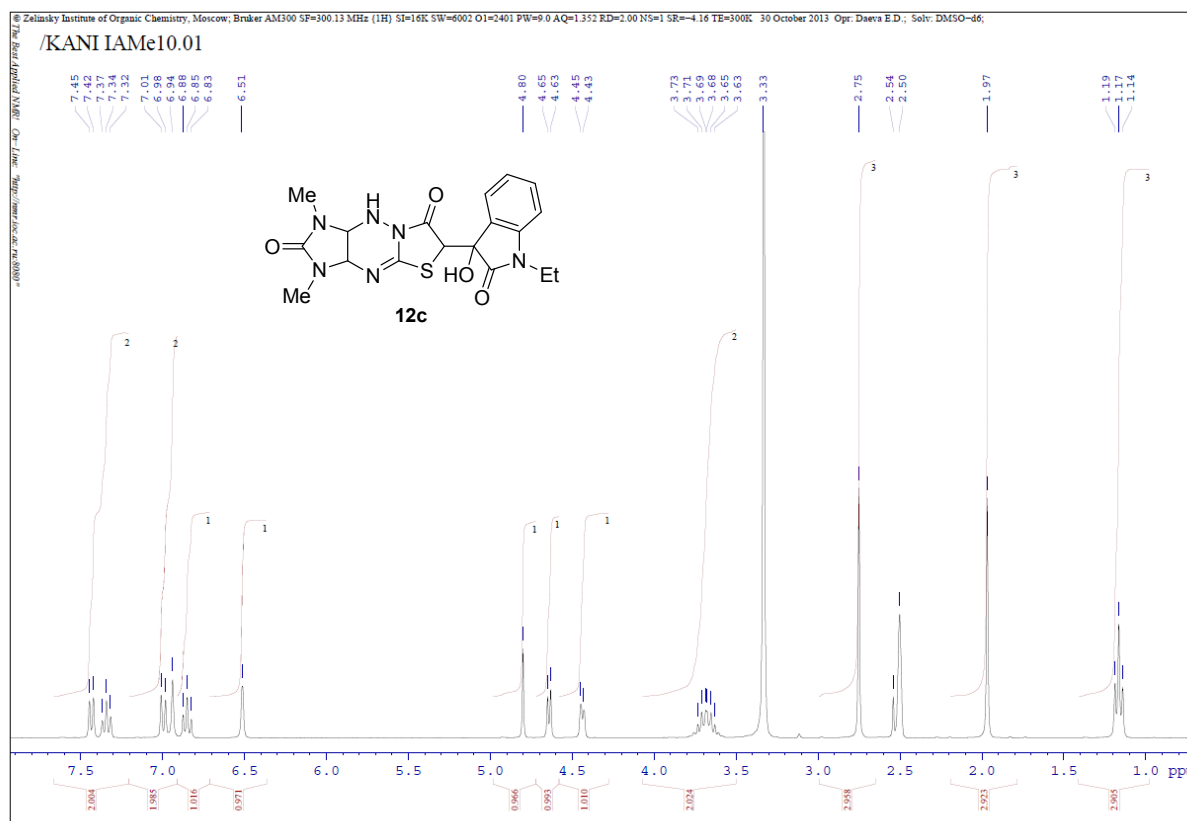
¹H NMR spectrum of **11s**



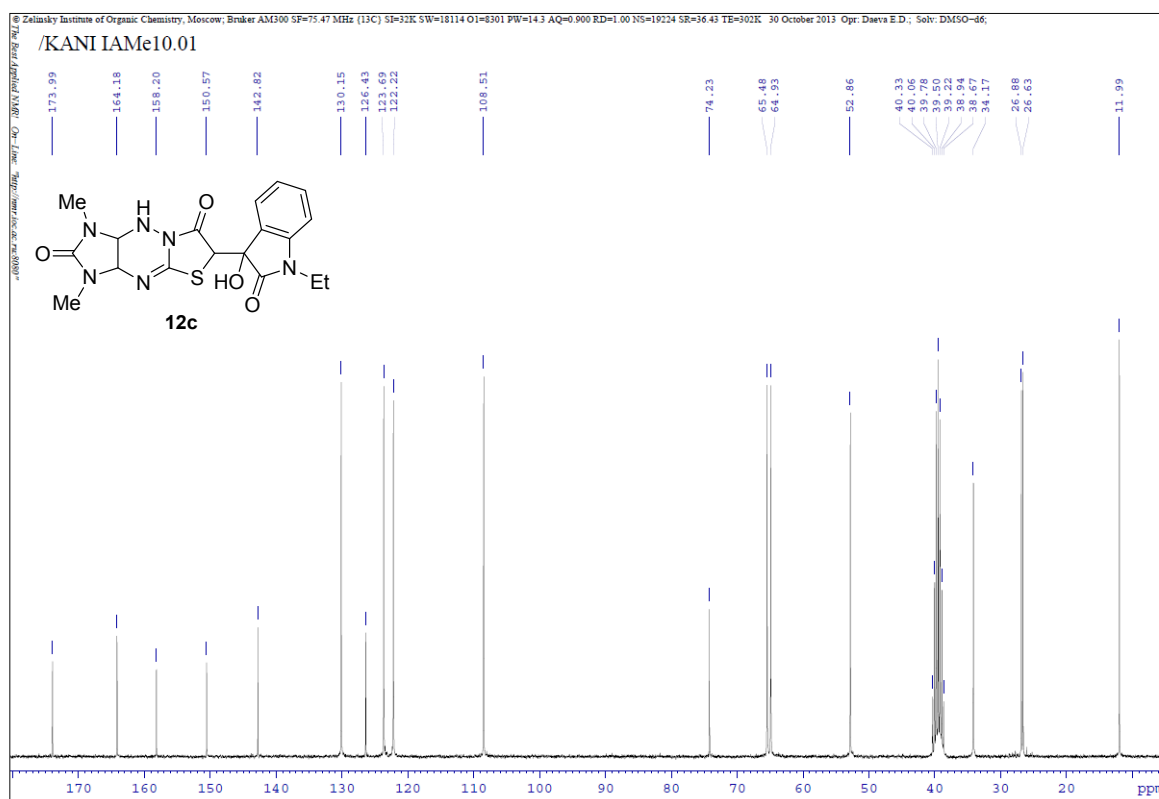
¹³C NMR spectrum of **11s**



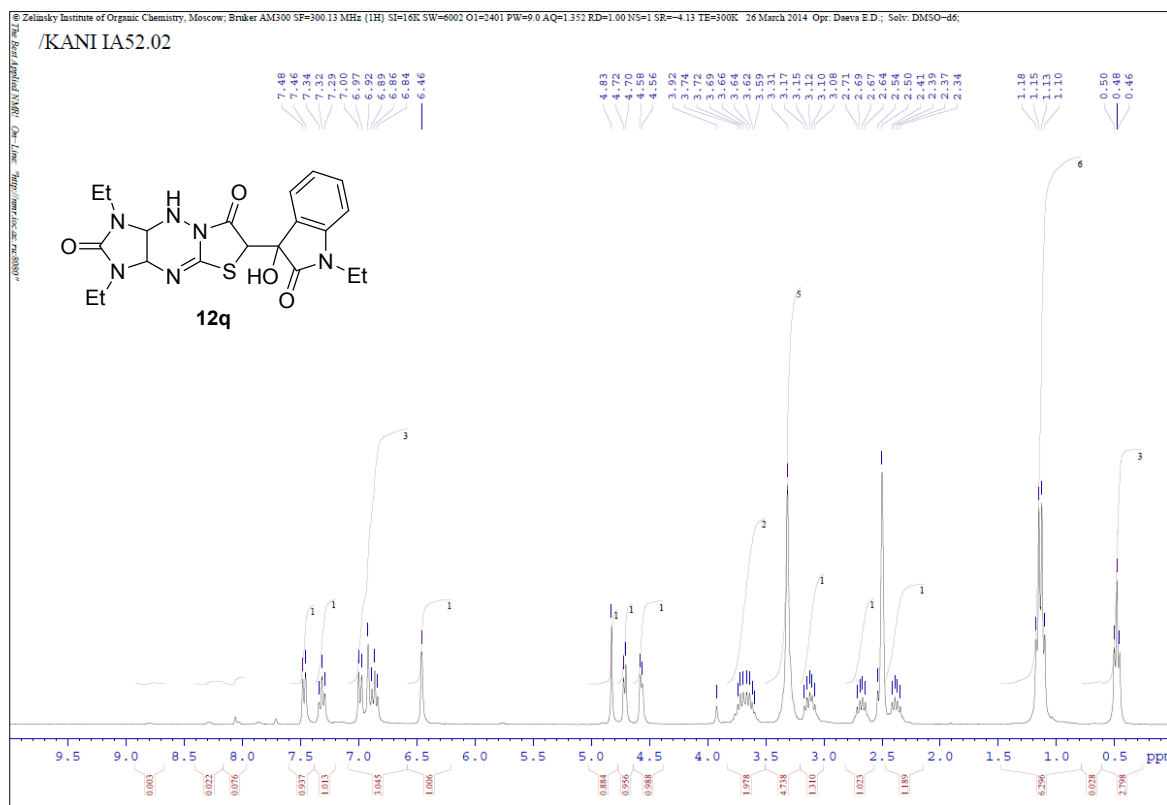
¹H NMR spectrum of **12c**



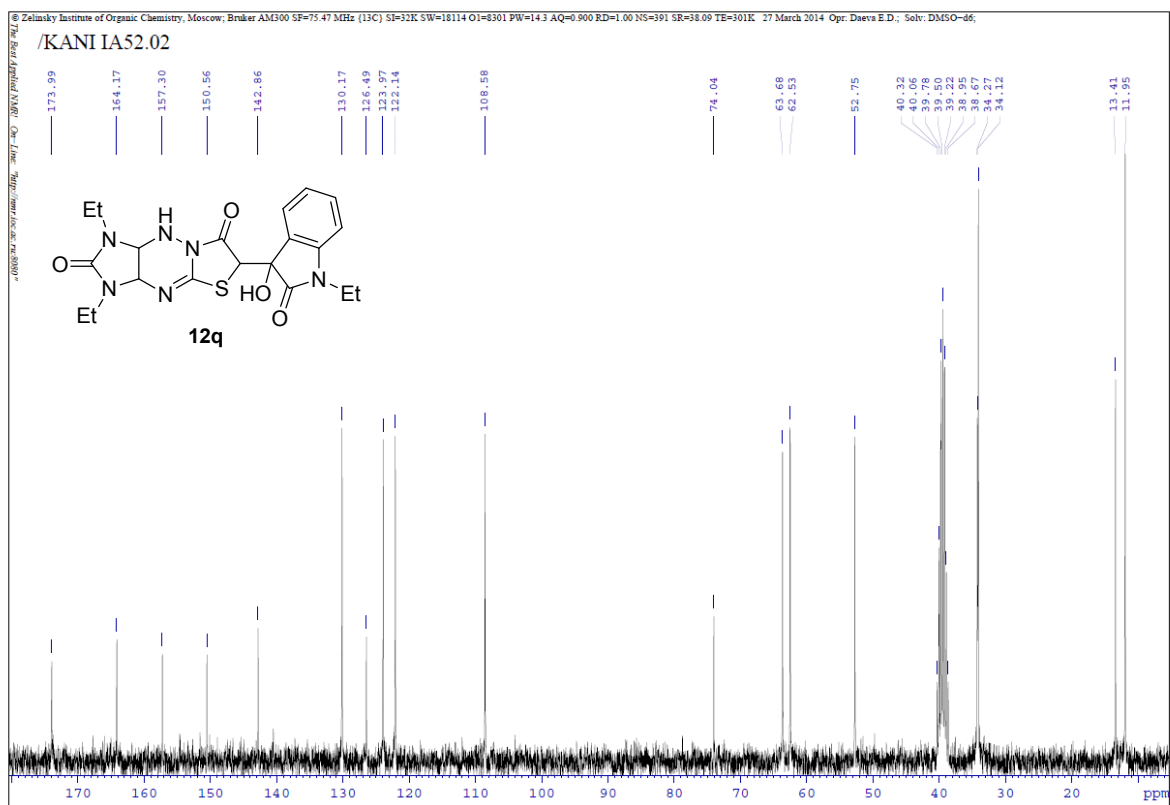
¹³C NMR spectrum of **12c**



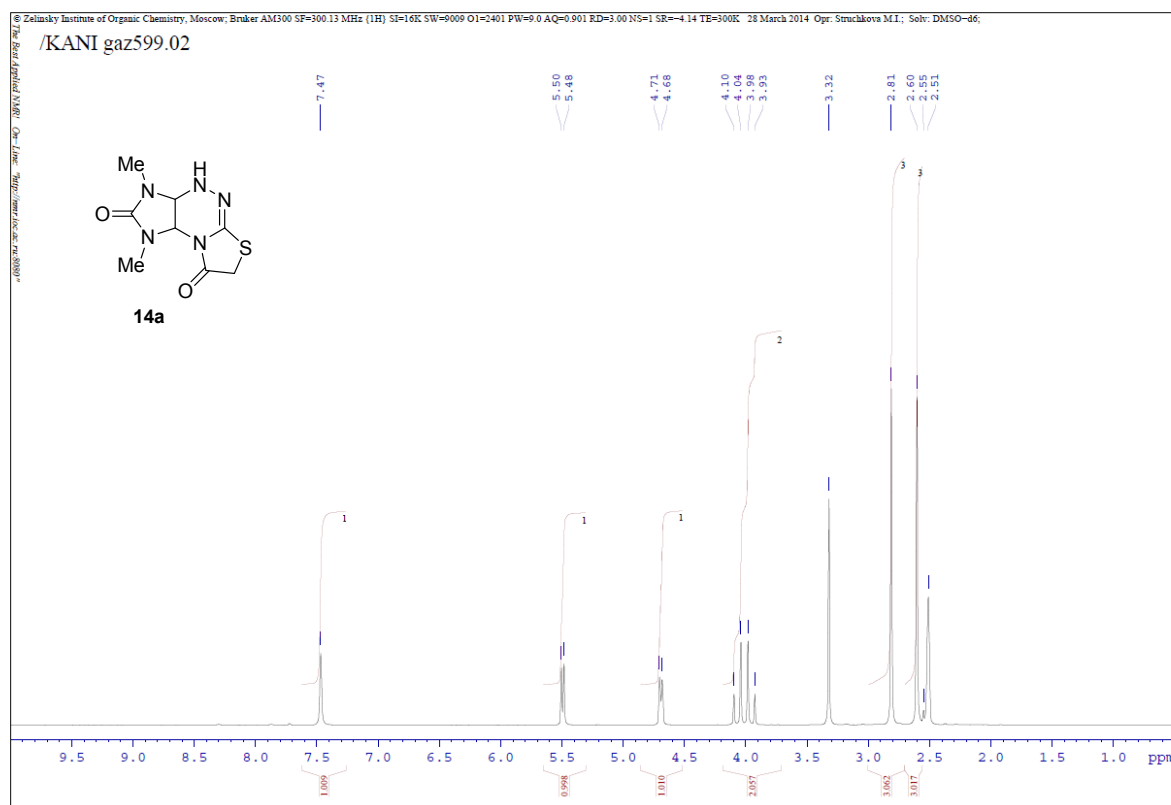
¹H NMR spectrum of **12q**



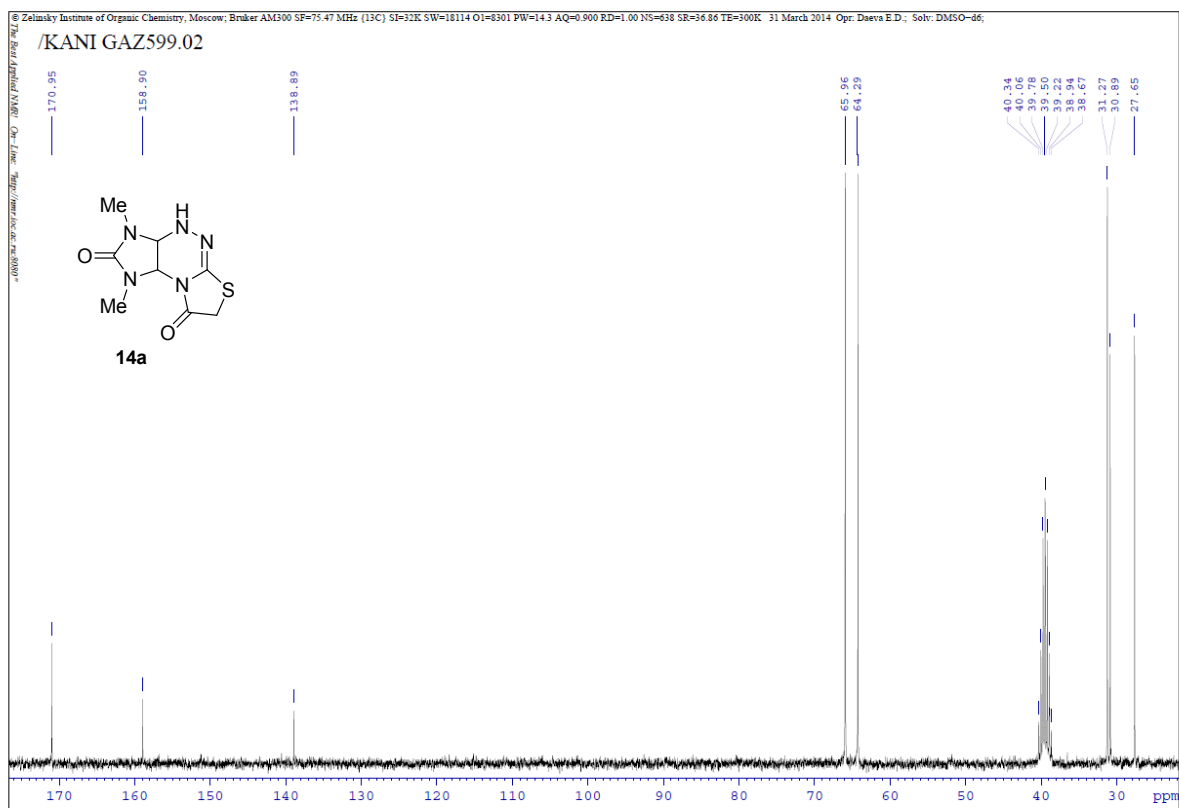
¹³C NMR spectrum of **12q**



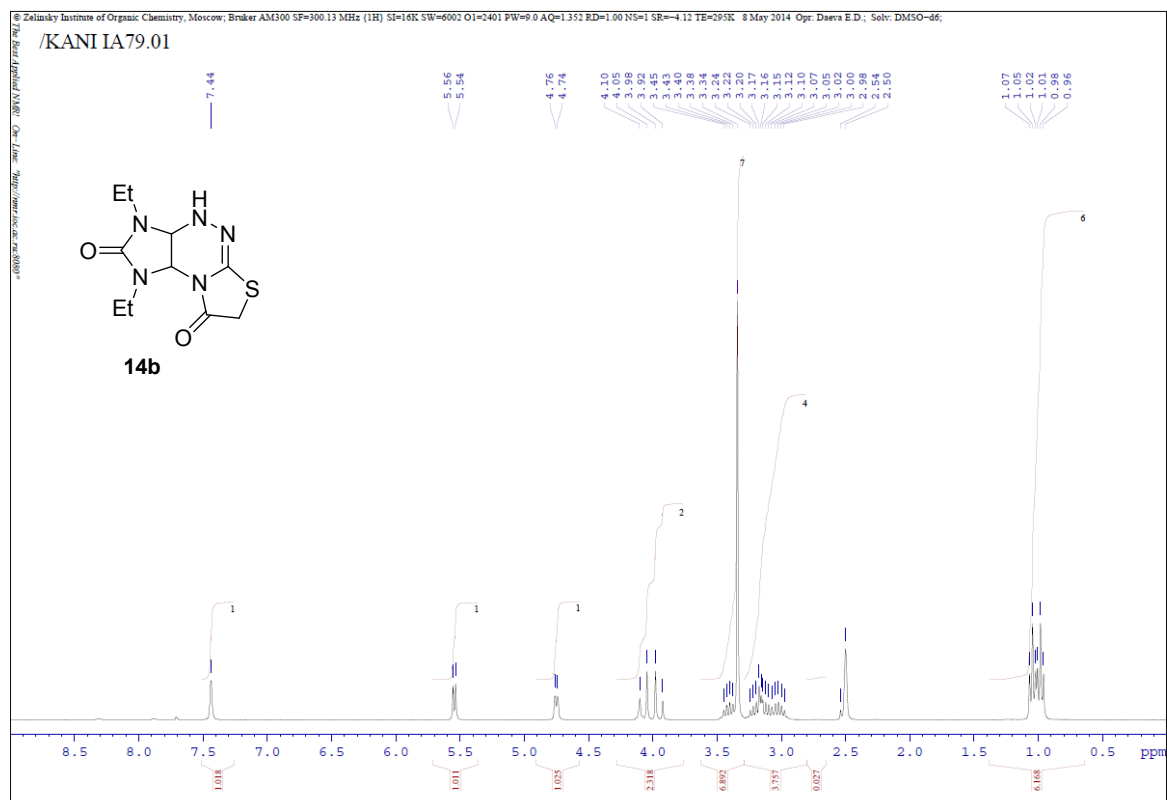
¹H NMR spectrum of **14a**



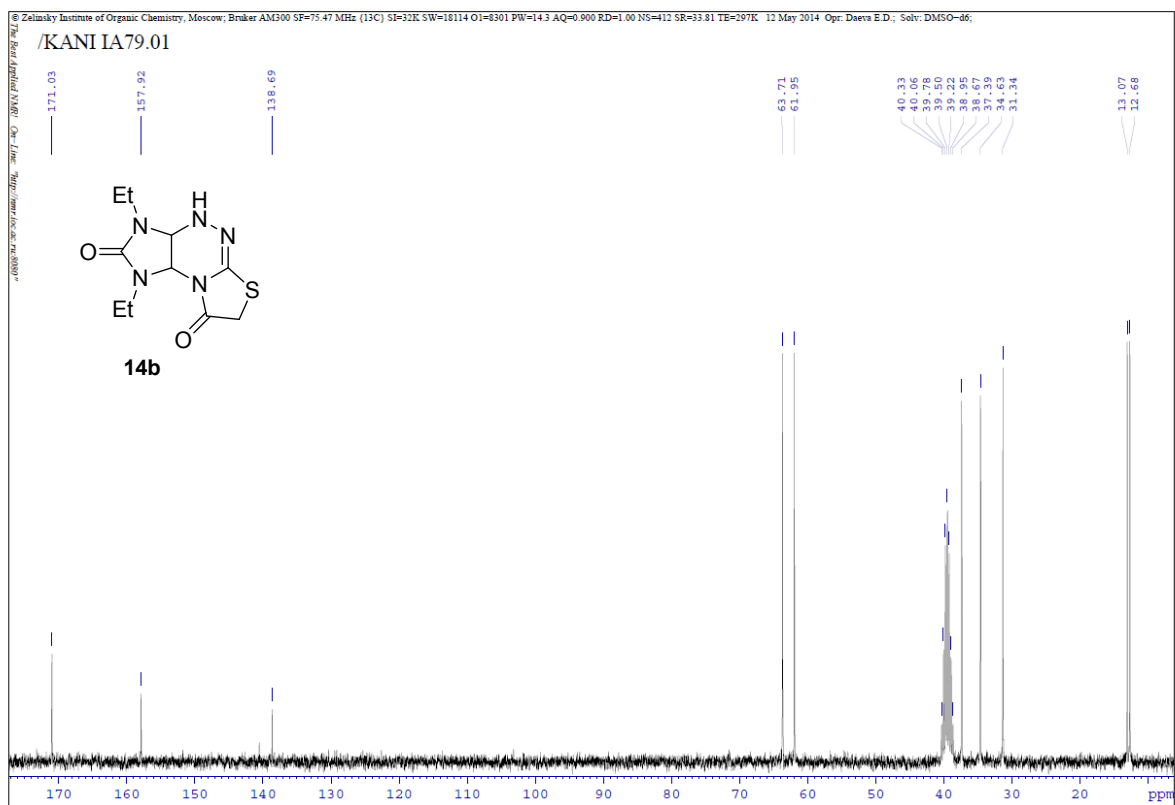
¹³C NMR spectrum of **14a**



¹H NMR spectrum of **14b**



¹³C NMR spectrum of **14b**



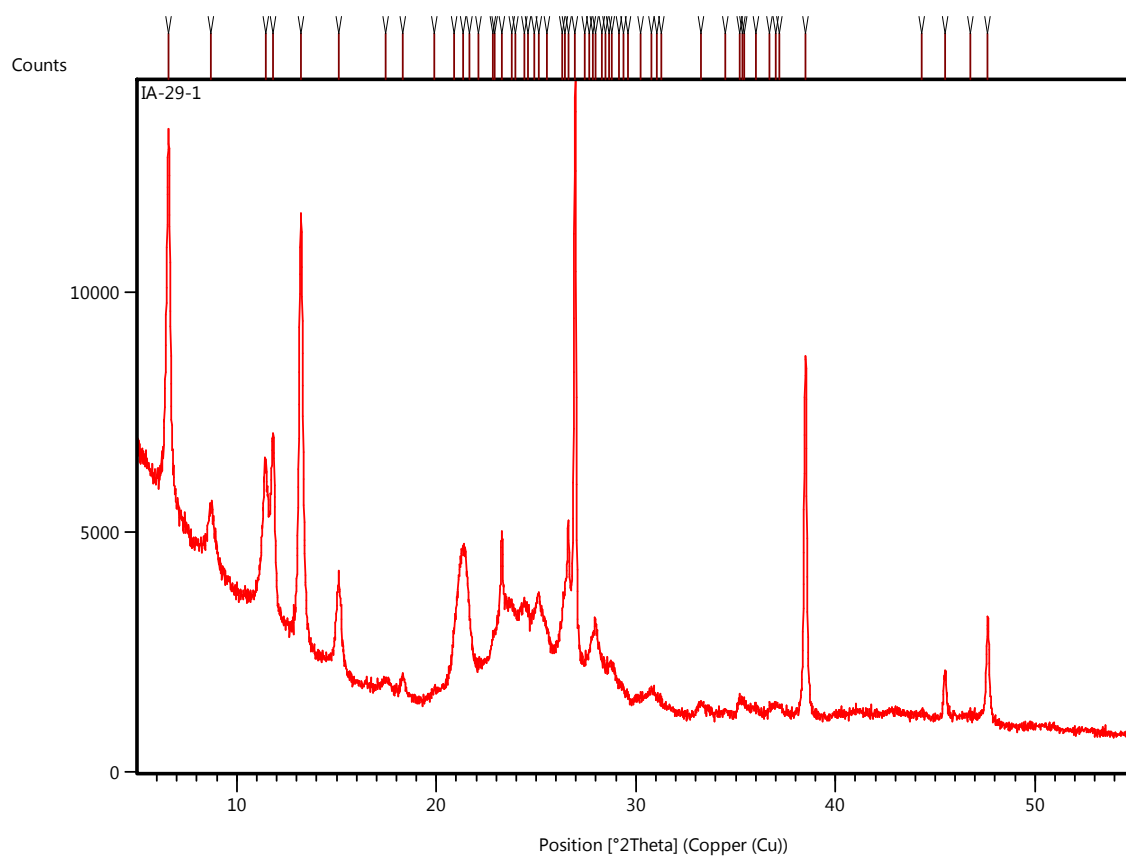


Figure 1. Powder diffraction pattern of **9b (IA29)**

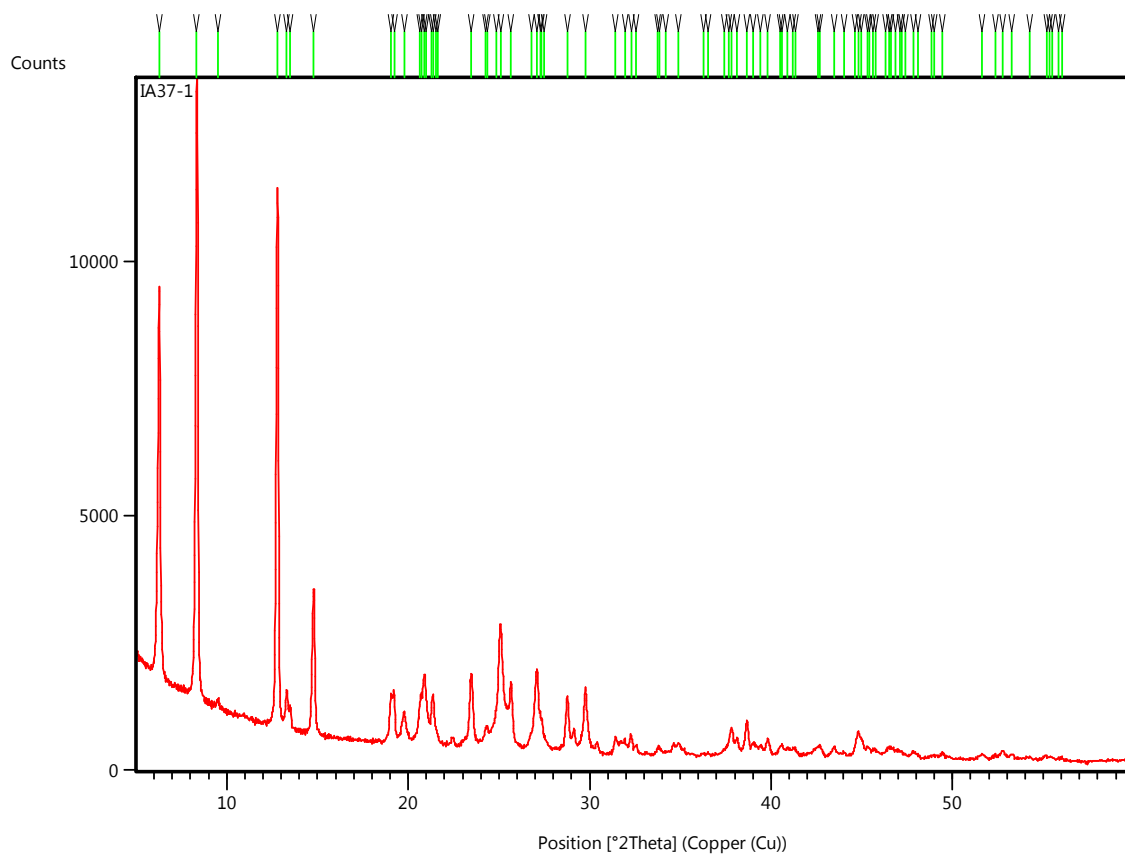


Figure 2. Powder diffraction pattern of **9d (IA37)**

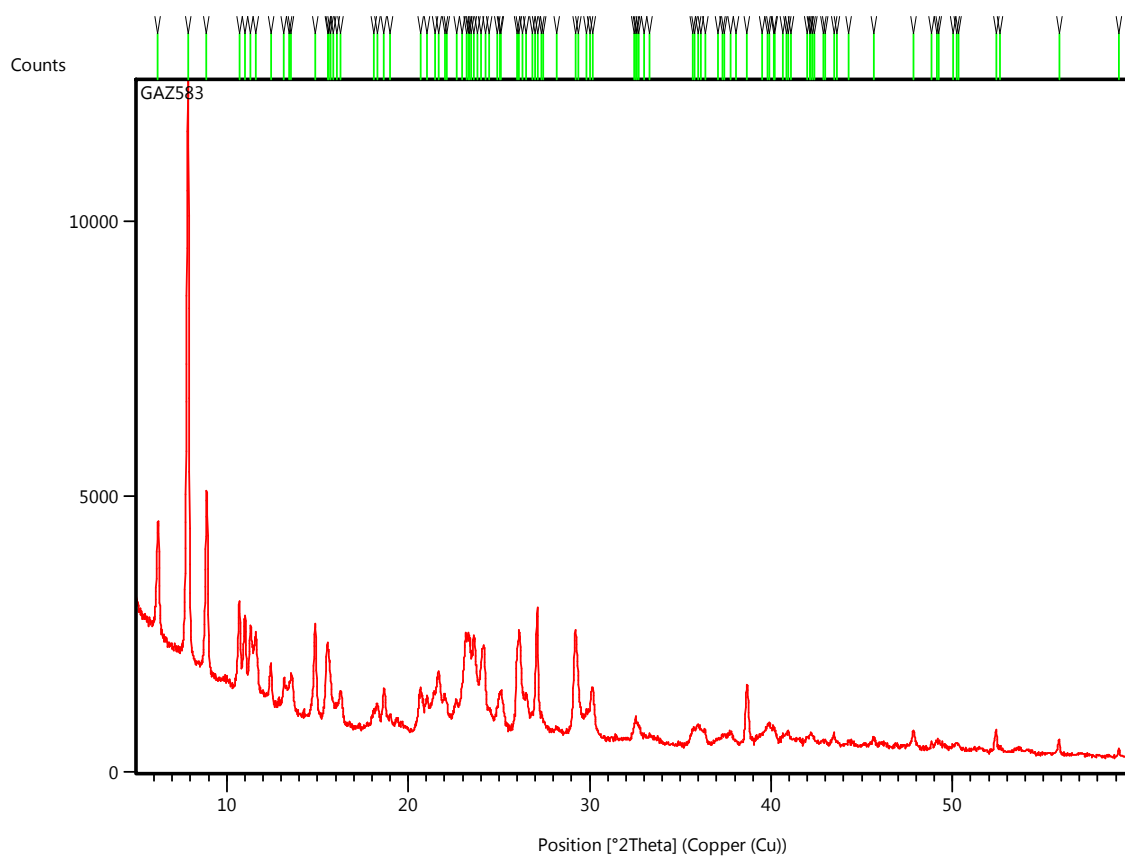


Figure 3. Powder diffraction pattern of **9e (GAZ583)**

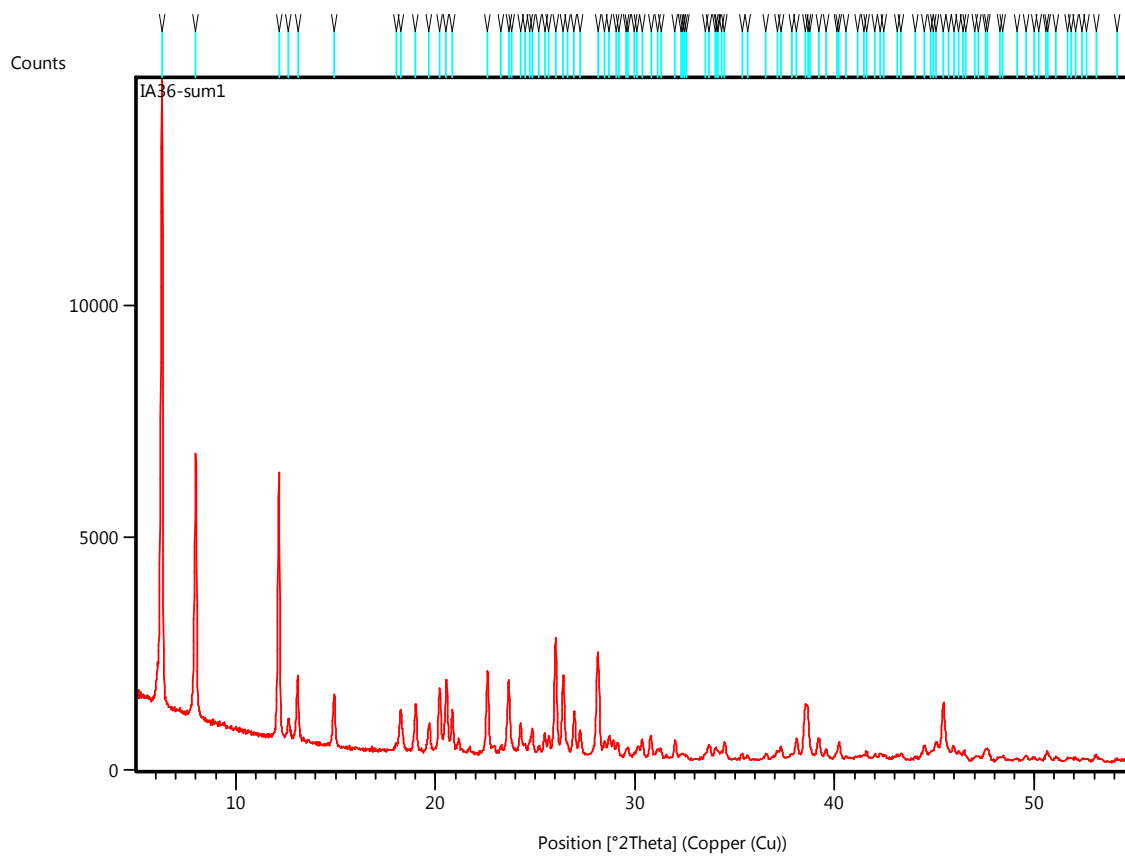


Figure 4. Powder diffraction pattern of **9n (IA36)**

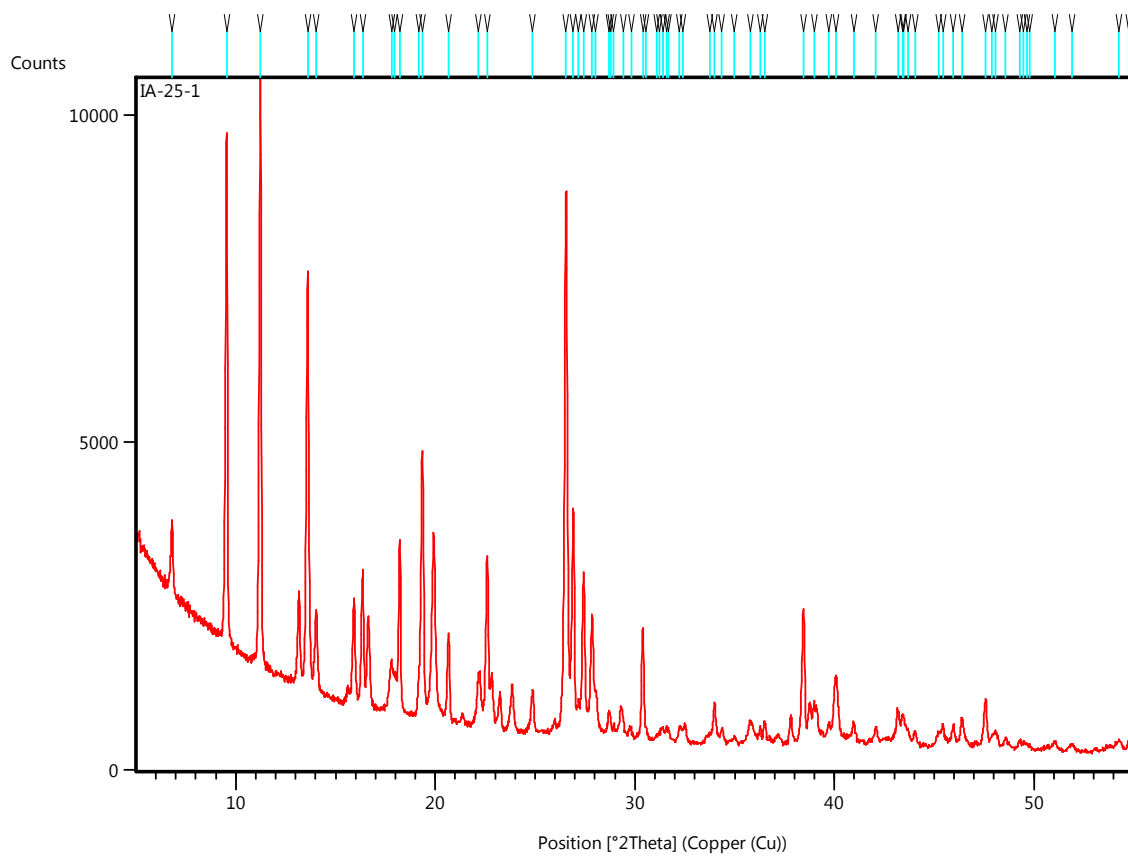


Figure 5. Powder diffraction pattern of **11b** (IA25)

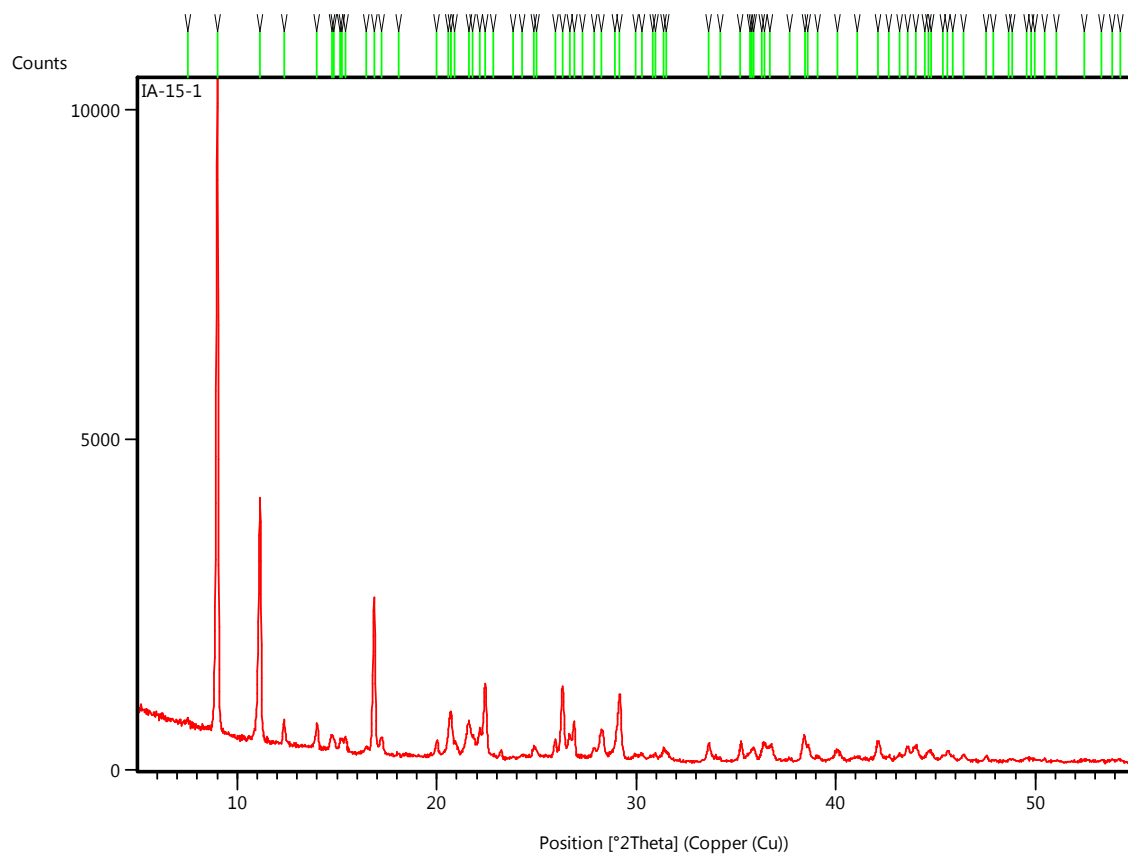


Figure 6. Powder diffraction pattern of **11c** (**IA15**)