

Supplementary Material

The Effect of 4-(Dimethylamino)phenyl-5-oxopyrrolidines on Breast and Pancreatic Cancer Cell Colony Formation, Migration, and Growth of Tumor Spheroids

Karolina Kairytė ¹, Rita Vaickelionienė ¹, Birutė Grybaitė ¹, Kazimieras Anusevičius ¹,
Vytautas Mickevičius ¹ and Vilma Petrikaitė ^{2,3,4,*}

¹ Department of Organic Chemistry, Kaunas University of Technology, Radvilėnų Rd. 19,
LT-50254 Kaunas, Lithuania; karolina.kairyte@ktu.lt (K.K.); rita.vaickelioniene@ktu.lt (R.V.);
birute.grybaite@ktu.lt (B.G.); kazimieras.anusevicius@ktu.lt (K.A.);
vytautas.mickevicius@ktu.lt (V.M.)

² Institute of Biotechnology, Life Sciences Center, Vilnius University, Saulėtekio Al. 7,
LT-10257 Vilnius, Lithuania

³ Faculty of Medicine, Lithuanian University of Health Sciences, A. Mickevičiaus 9,
LT-44307 Kaunas, Lithuania

⁴ Laboratory of Drug Targets Histopathology, Institute of Cardiology, Lithuanian University
of
Health Sciences, Sukilėlių Pr. 13, LT-50162 Kaunas, Lithuania

* Correspondence: vilma.petrikaite@lsmuni.lt or vilma.petrikaite@bt.vu.lt; Tel.: +370-
68629383

4-(1*H*-benzo[d]imidazol-2-yl)-1-(dimethylamino)phenyl)pyrrolidin-2-one (3a)

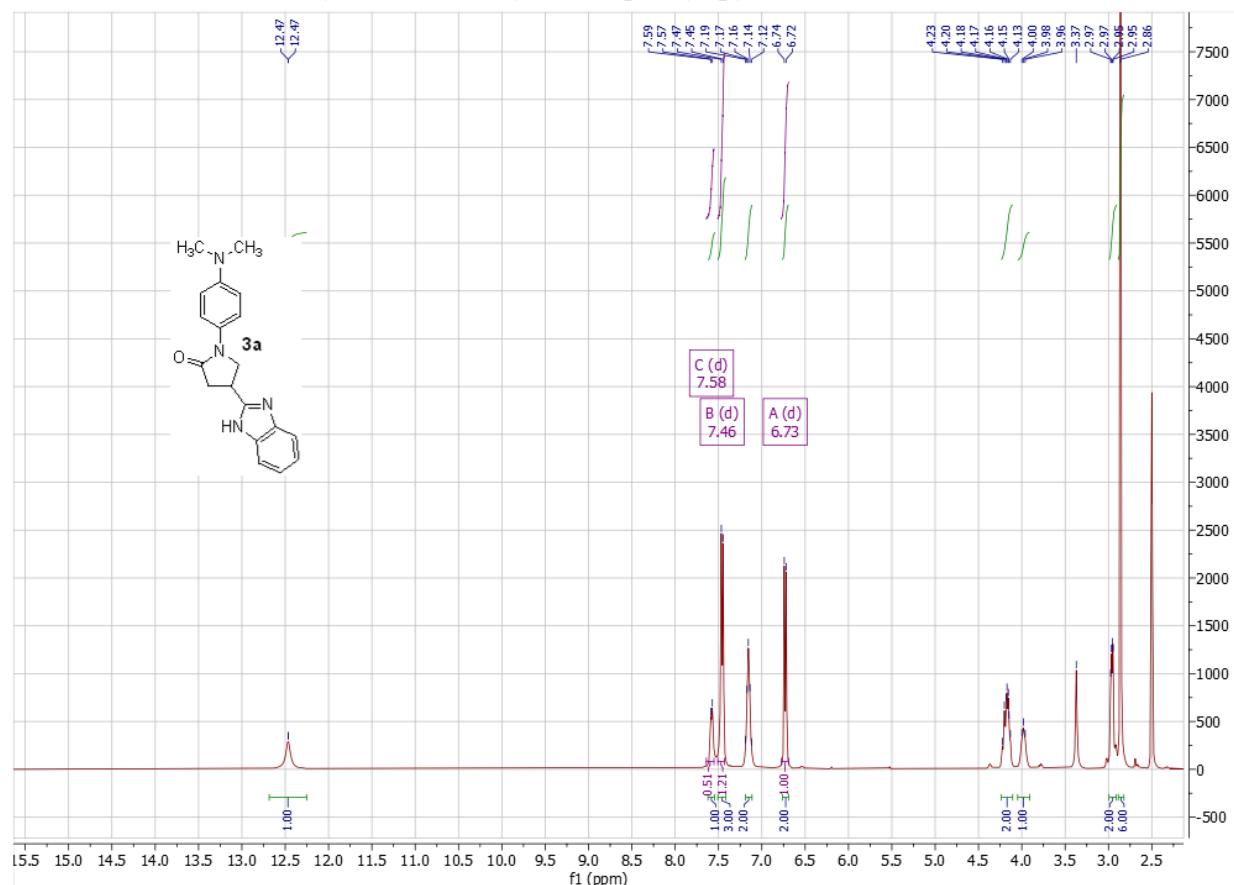


Figure S1. ¹H NMR spectrum of compound 3a.

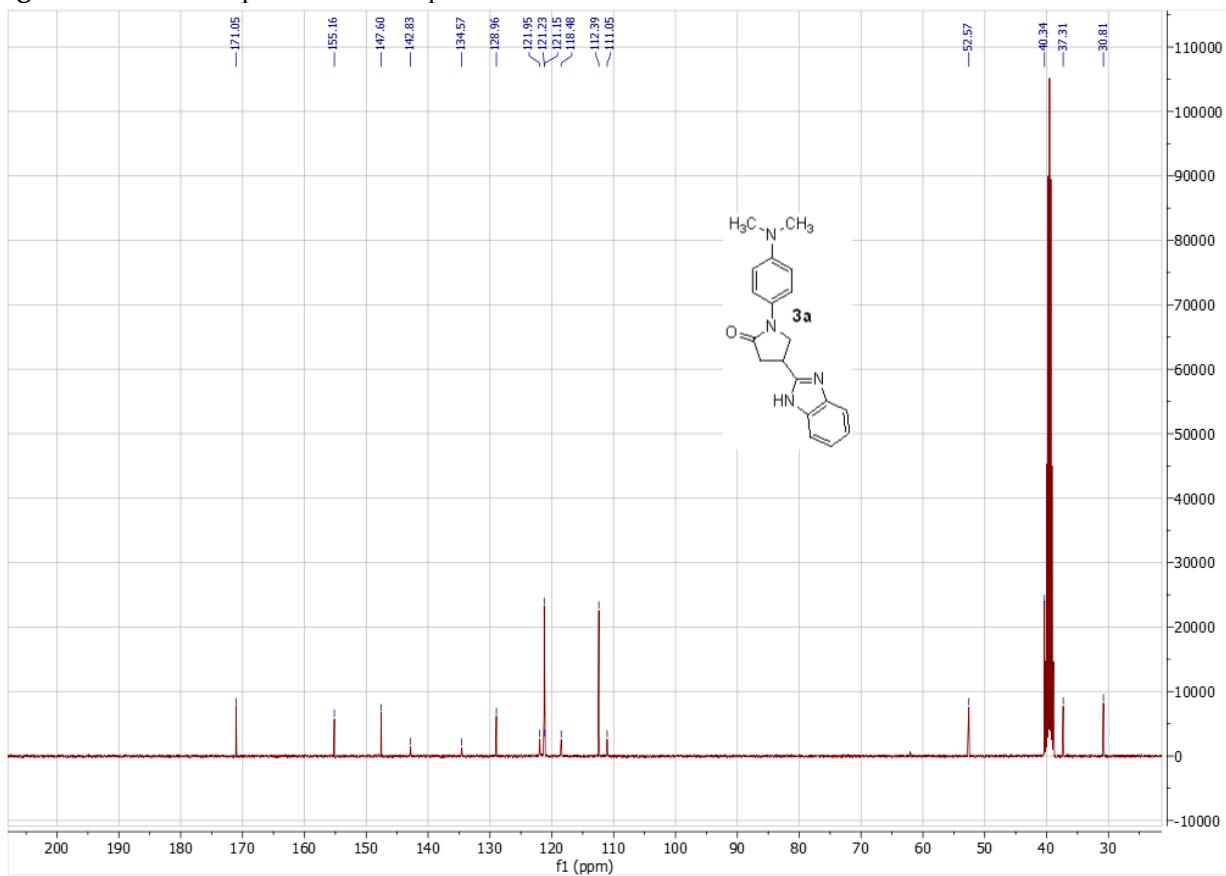


Figure S2. ¹³C NMR spectrum of compound 3a.

1-(4-(Dimethylamino)phenyl)-4-(5-fluoro-1H-benzo[d]imidazol-2-yl)pyrrolidin-2-one (3b)

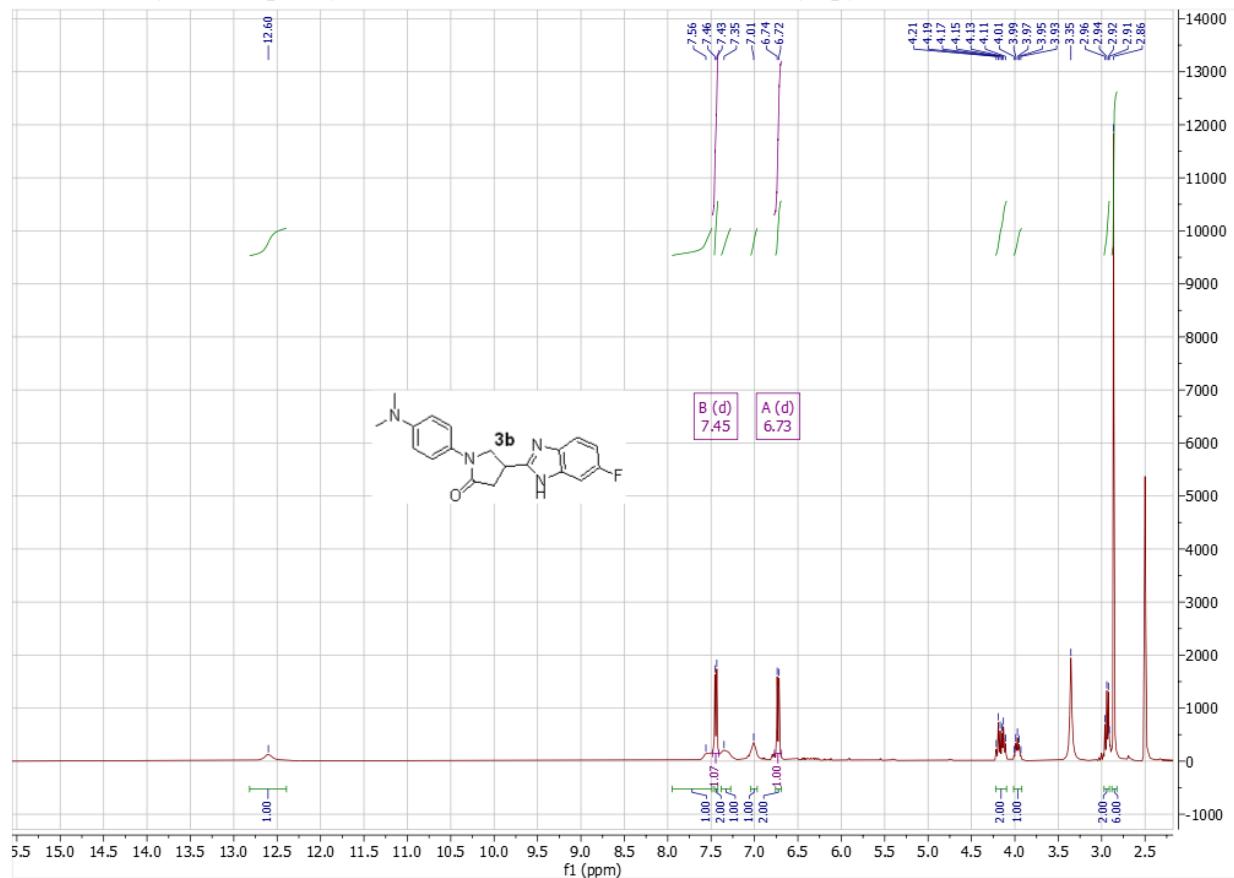


Figure S3. ^1H NMR spectrum of compound 3b.

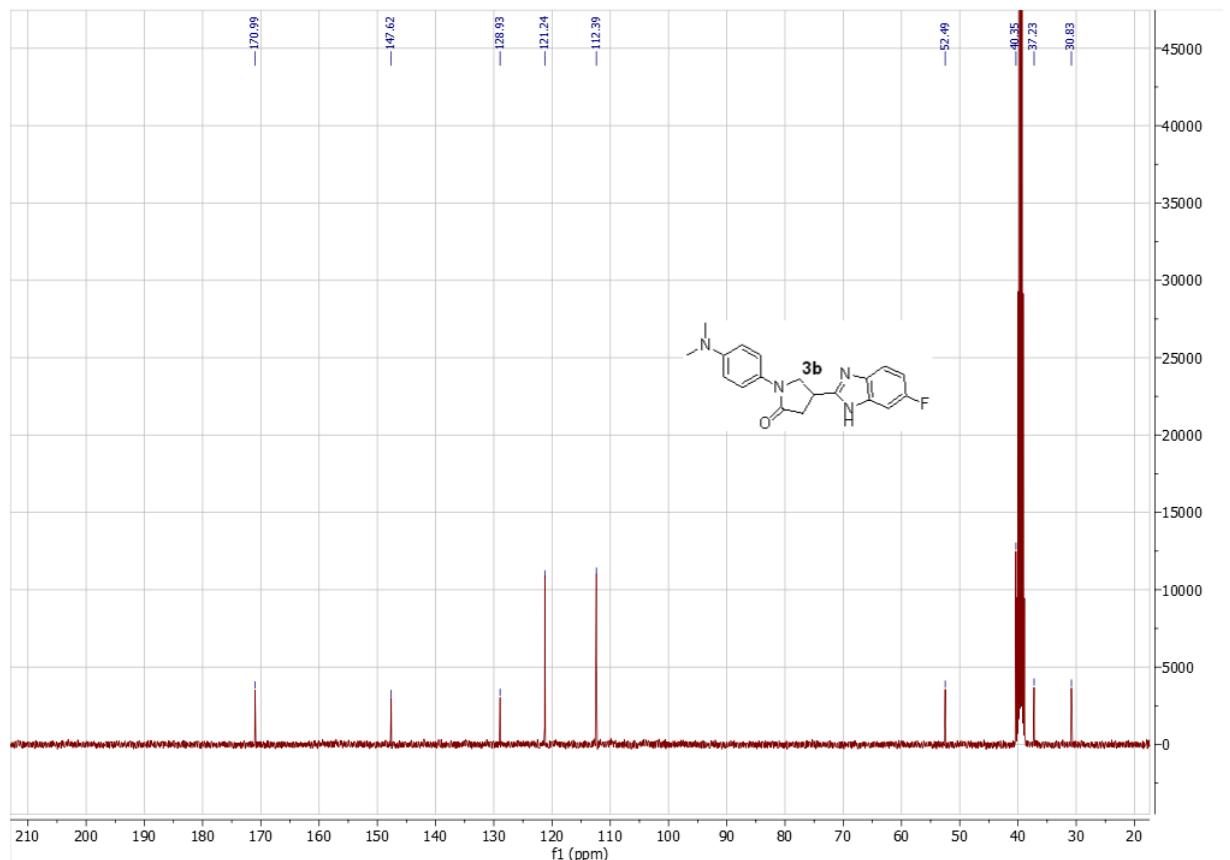


Figure S4. ^{13}C NMR spectrum of compound 3b.

1-(4-(Dimethylamino)phenyl)-4-(5-chloro-1H-benzo[d]imidazol-2-yl)pyrrolidin-2-one (3c)

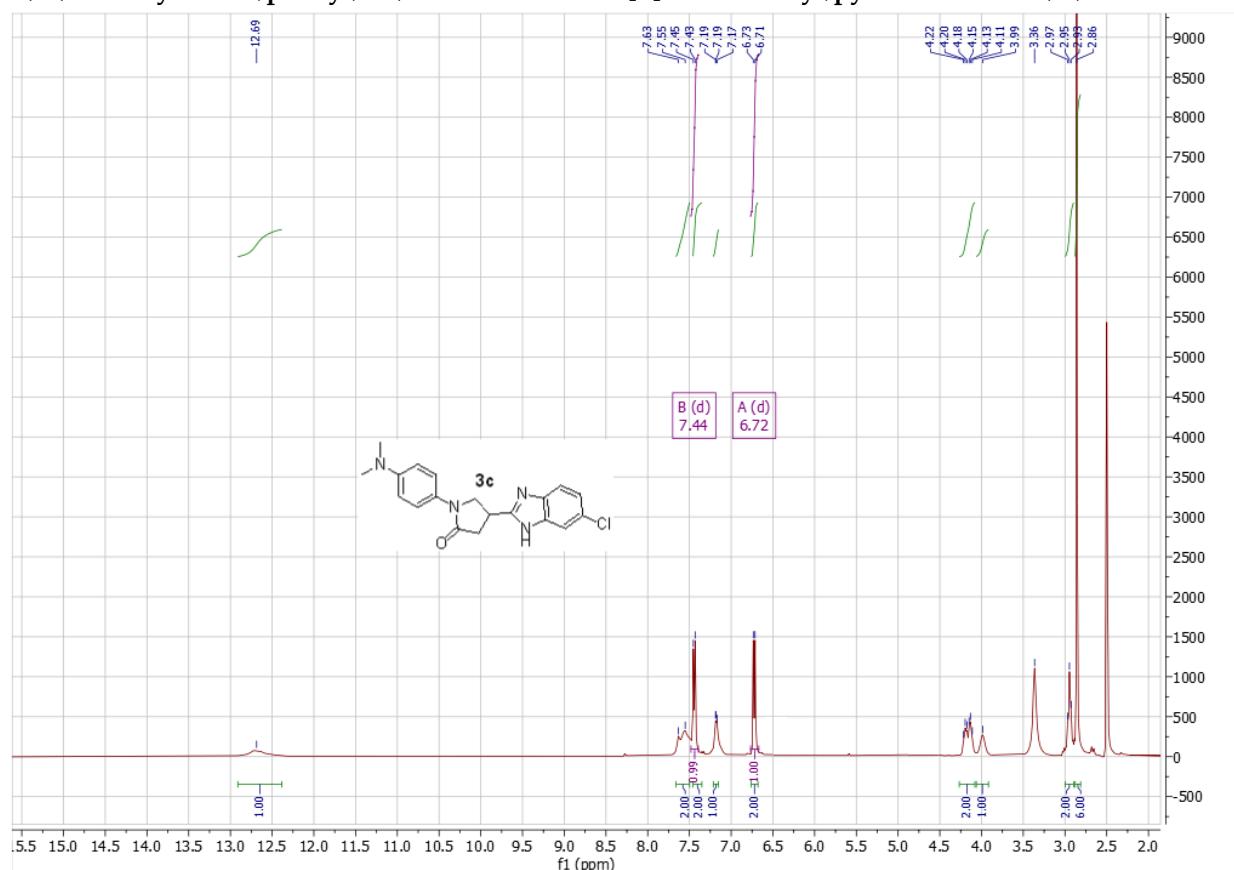


Figure S5. ¹H NMR spectrum of compound 3c.

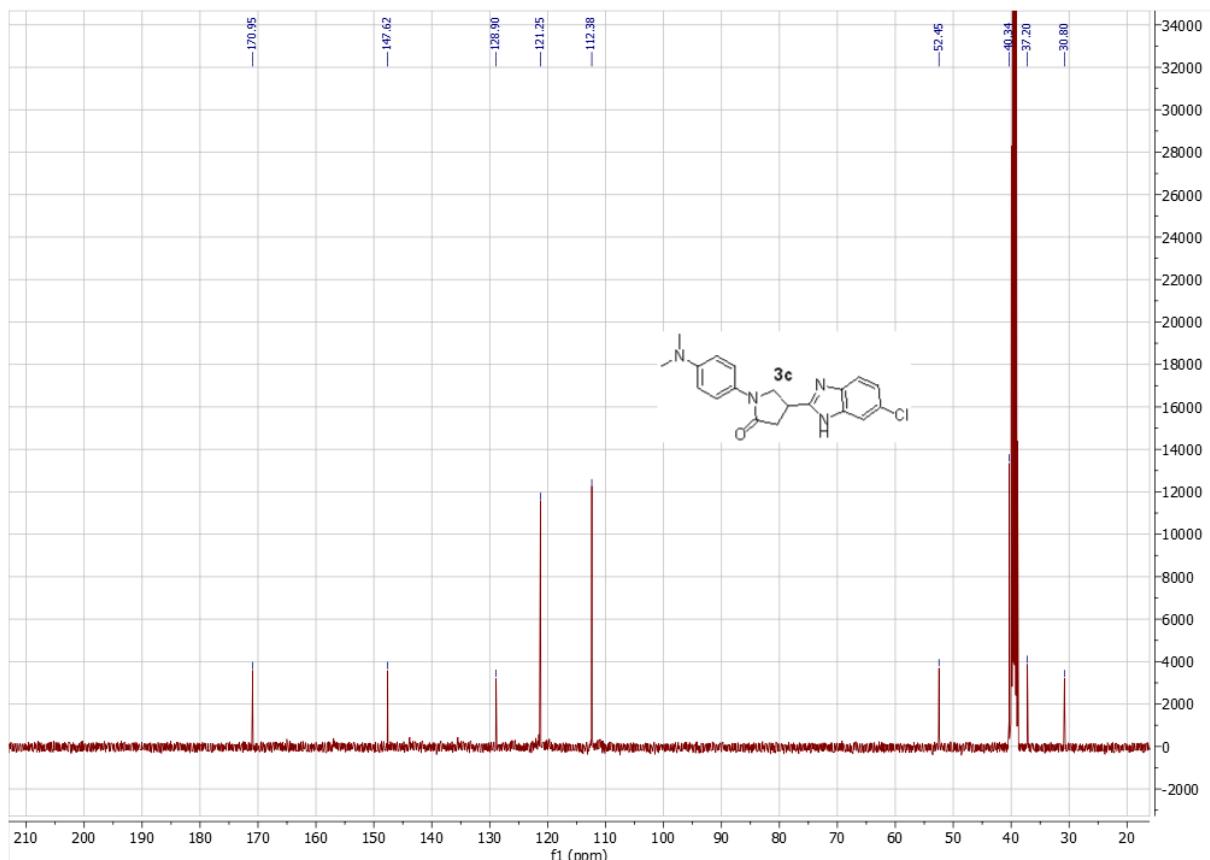


Figure S6. ¹³C NMR spectrum of compound 3c.

1-(4-(Dimethylamino)phenyl)-4-(5-methyl-1*H*-benzo[d]imidazol-2-yl)pyrrolidin-2-one (3d)

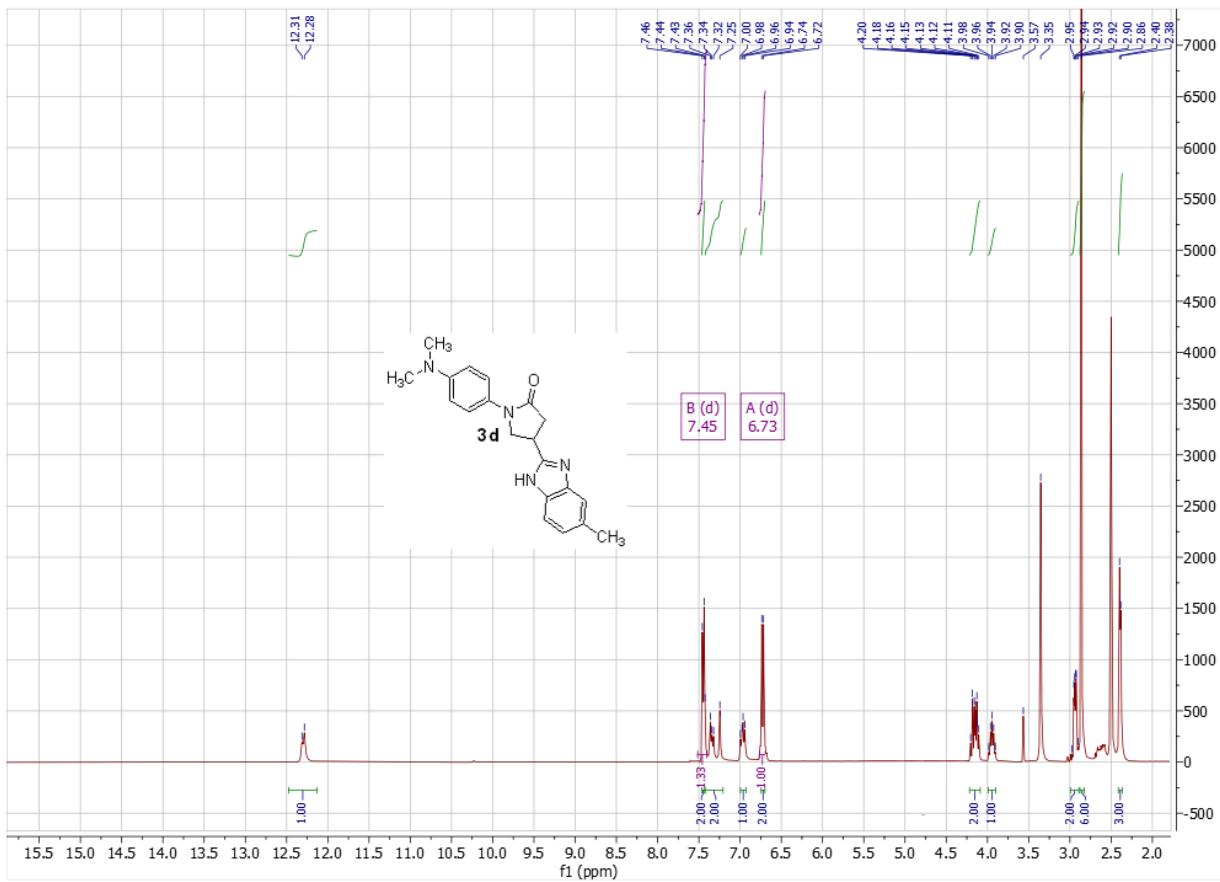


Figure S7. ^1H NMR spectrum of compound 3d.

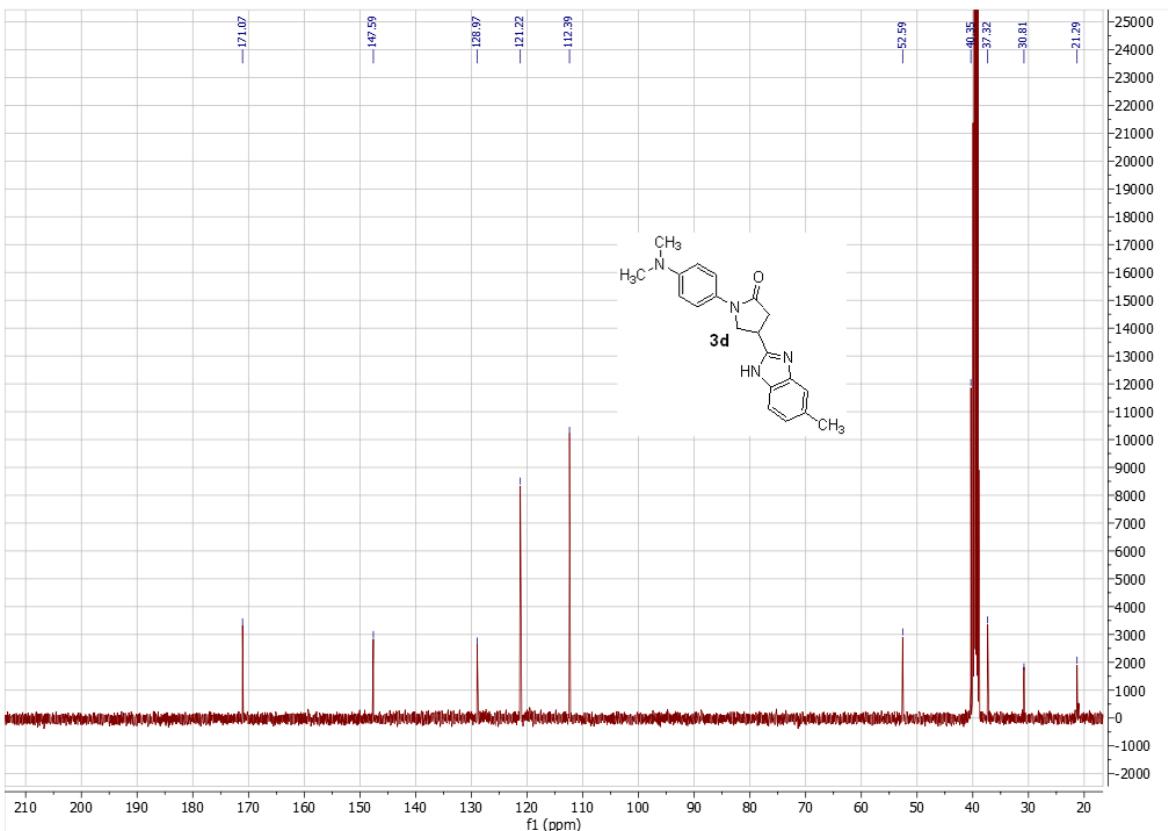


Figure S8. ^{13}C NMR spectrum of compound **3d**.

1-(4-(Dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (4)

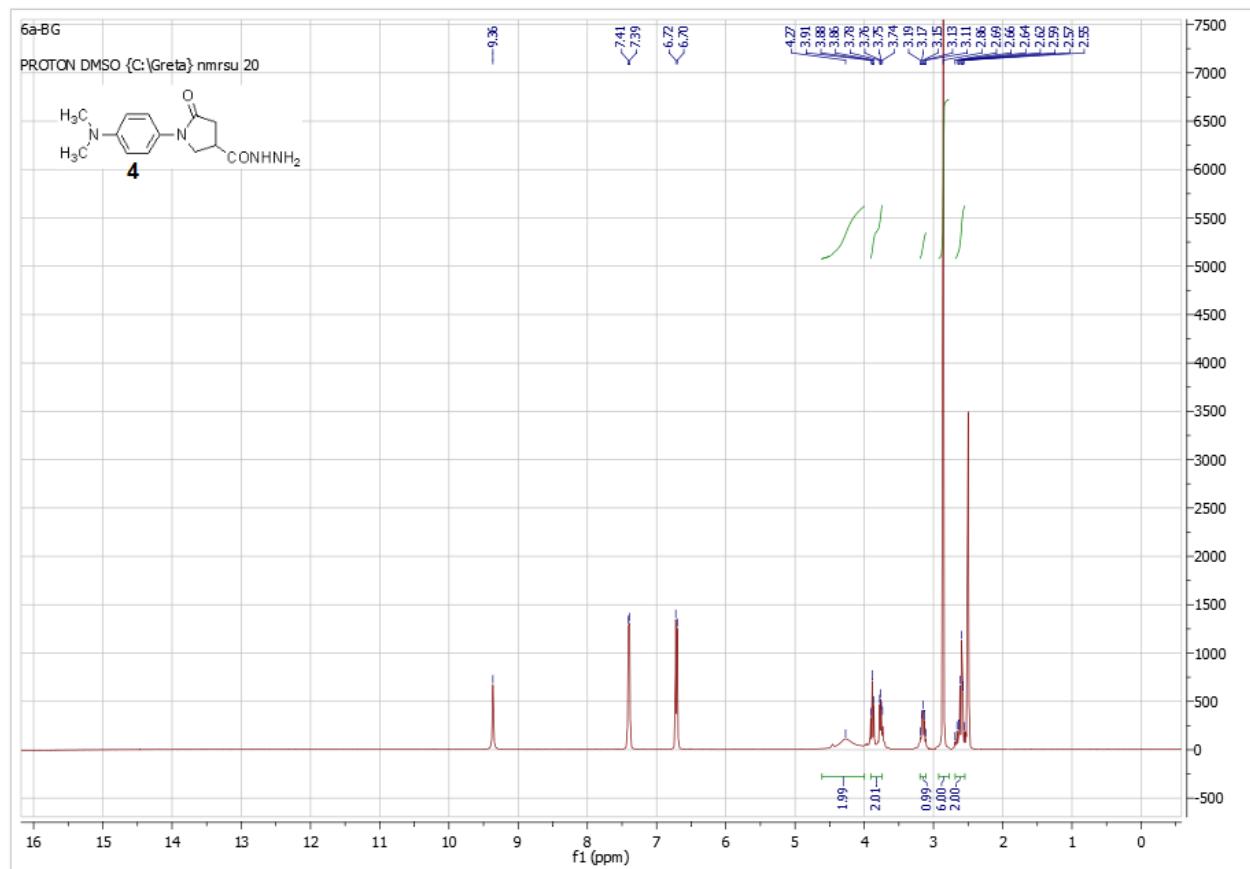


Figure S9. ^1H NMR spectrum of compound 4.

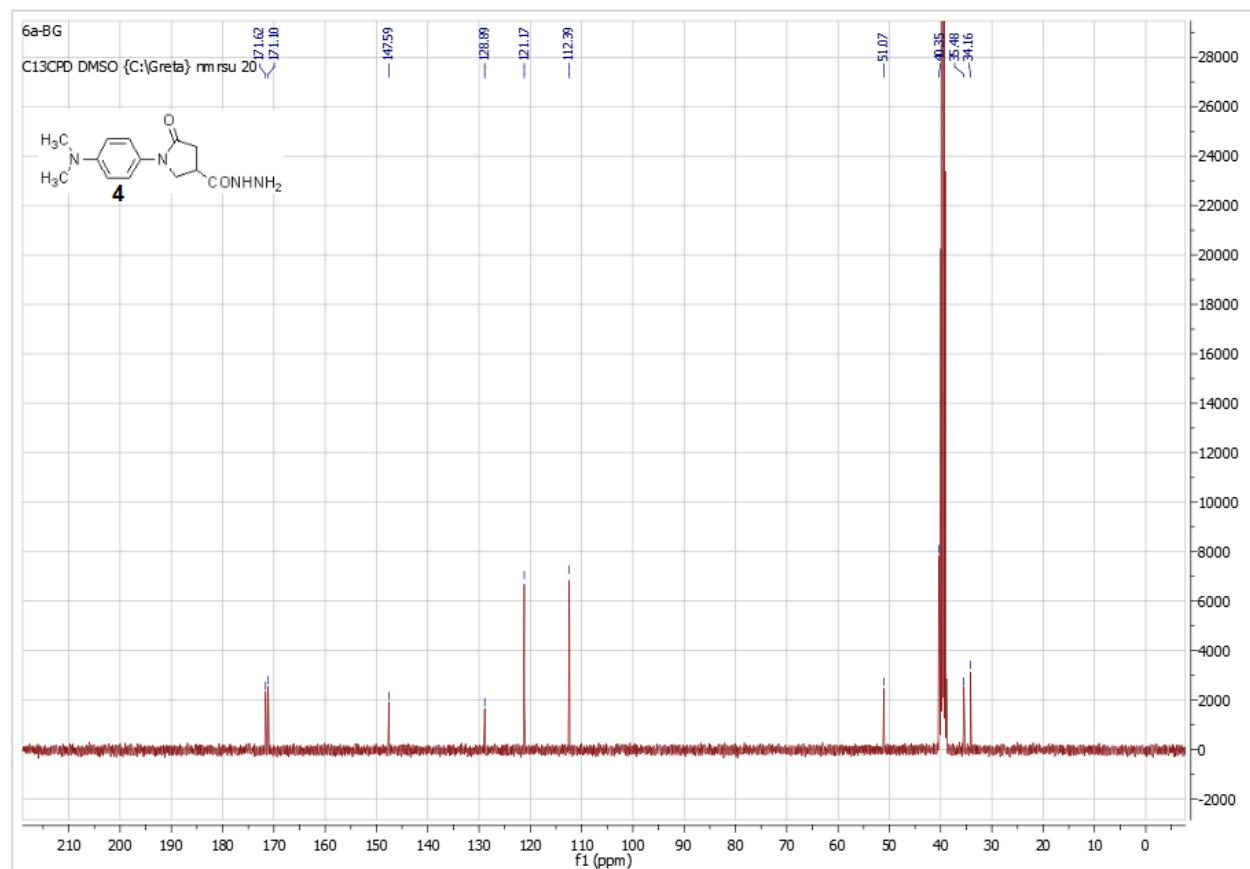


Figure S10. ^{13}C NMR spectrum of compound 4.

***N'*-benzylidene-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5a)**

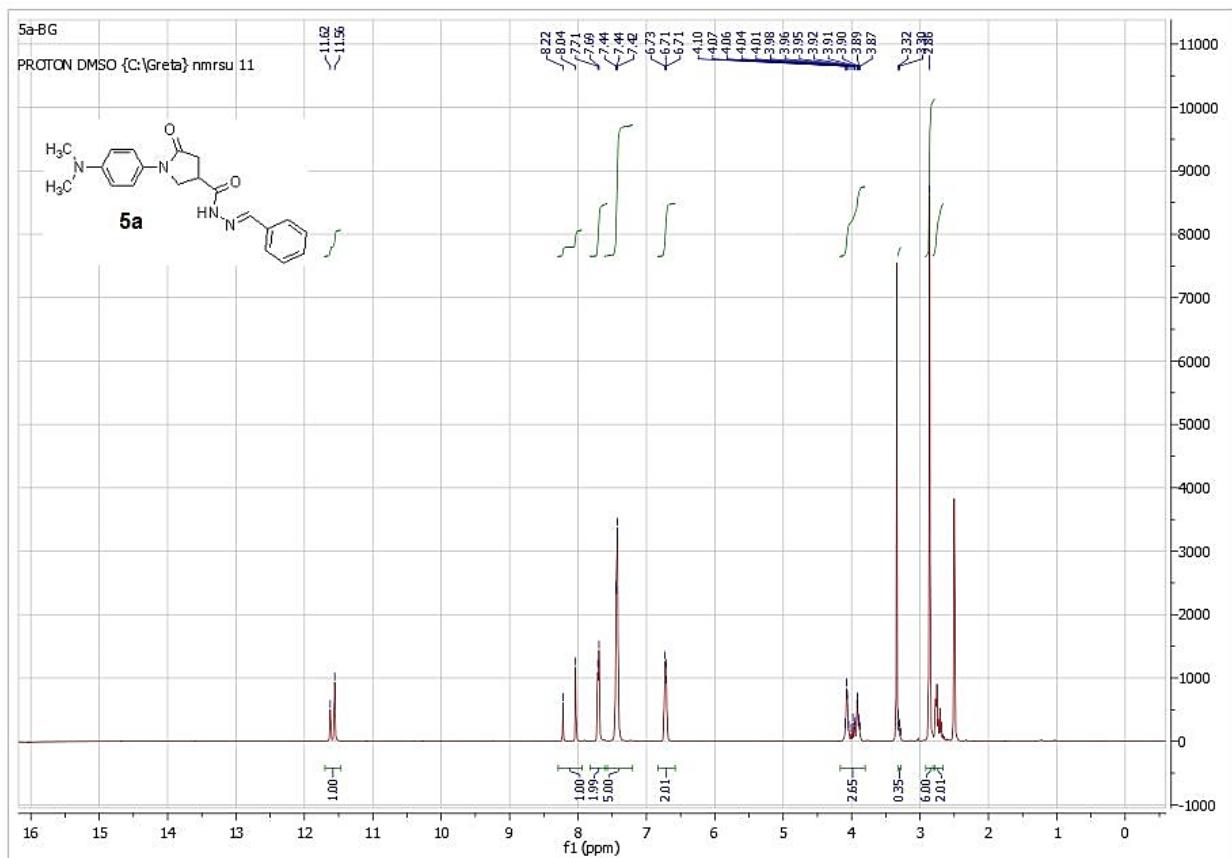


Figure S11. ^1H NMR spectrum of compound 5a.

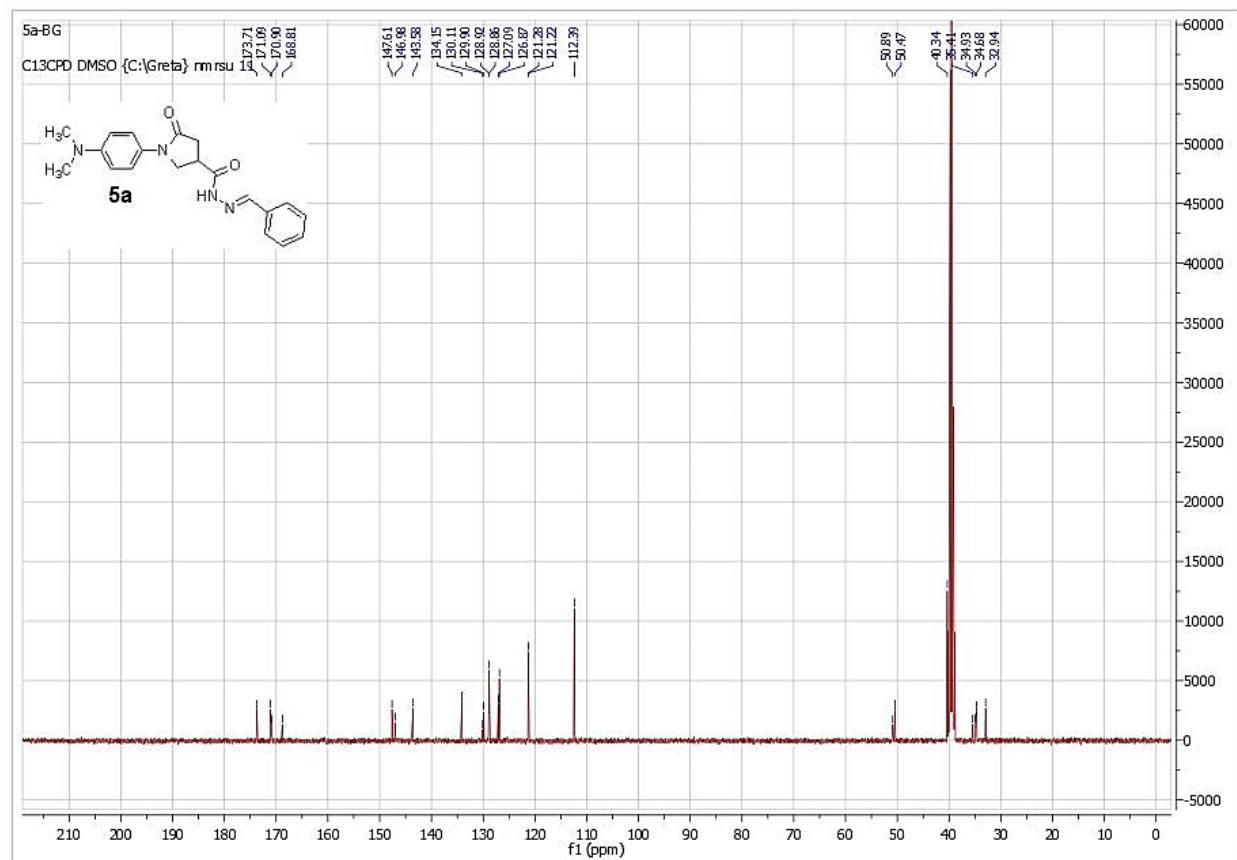


Figure S12. ^{13}C NMR spectrum of compound 5a.

***N'*-(4-chlorobenzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5b)**

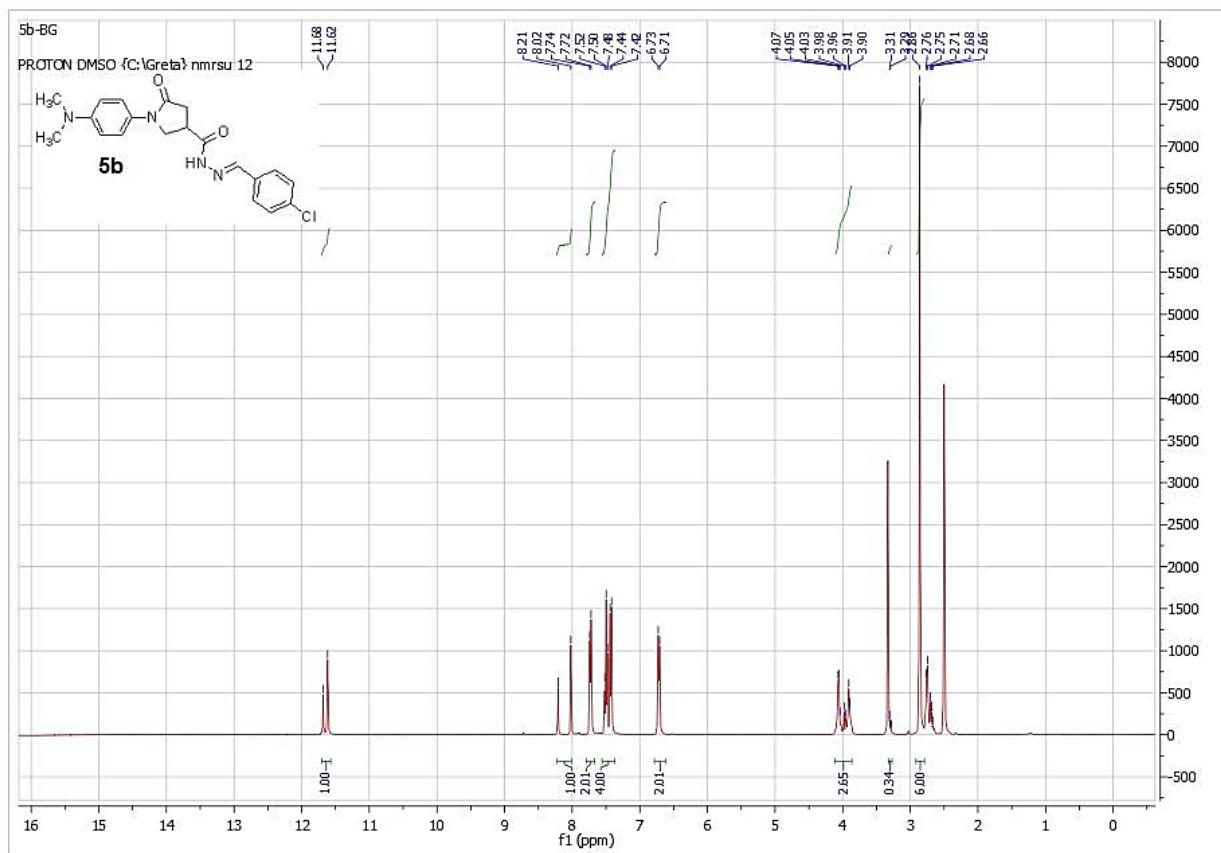


Figure S13. ^1H NMR spectrum of compound 5b.

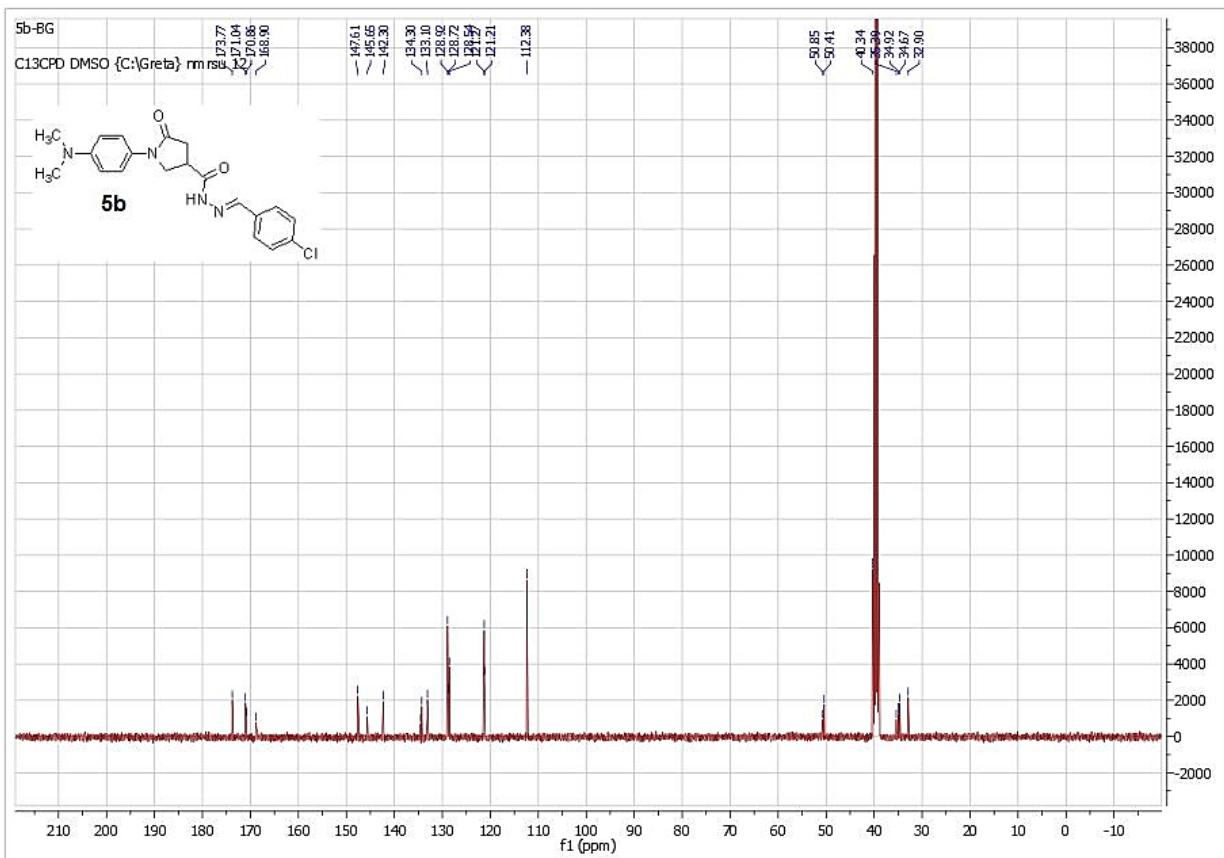


Figure S14. ^{13}C NMR spectrum of compound 5b.

N'-(4-bromobenzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5c)

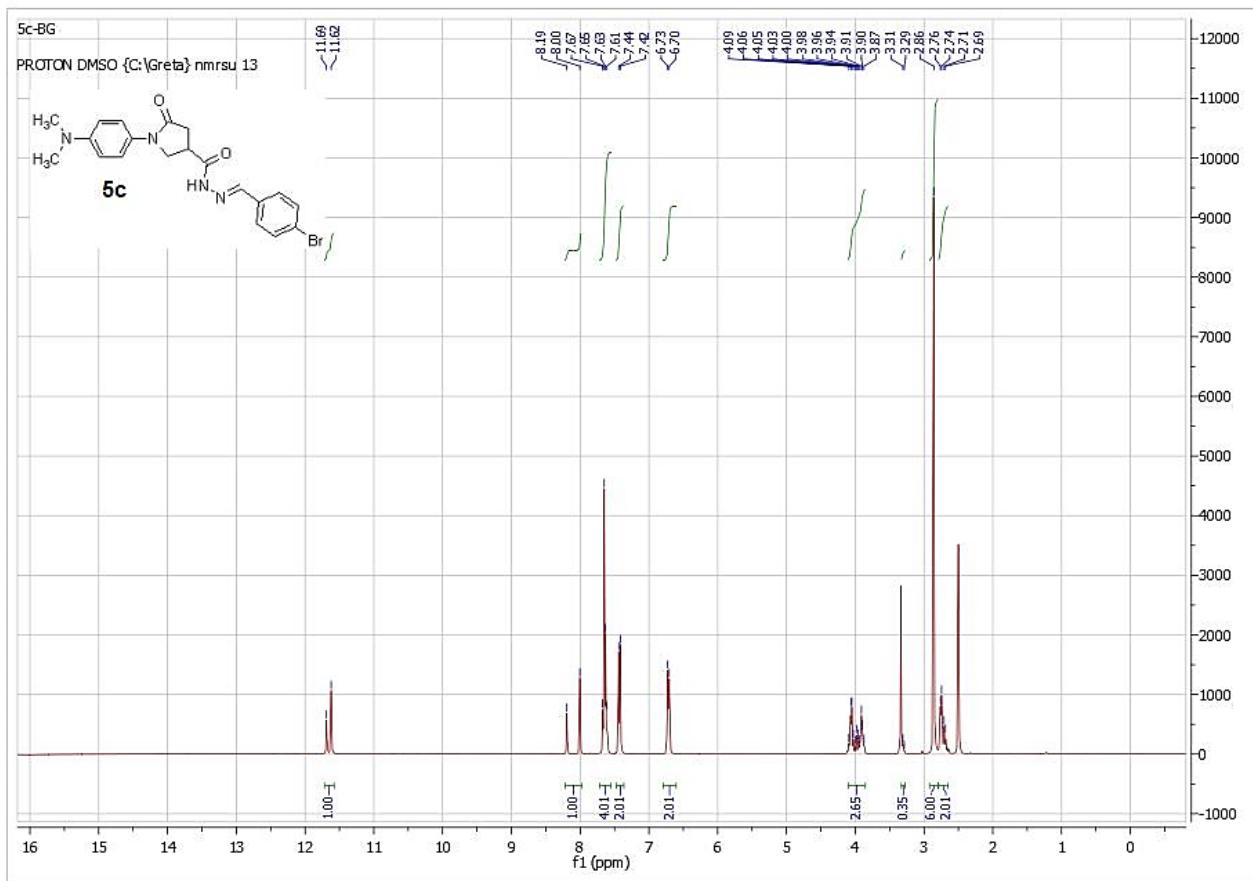


Figure S15. ^1H NMR spectrum of compound 5c.

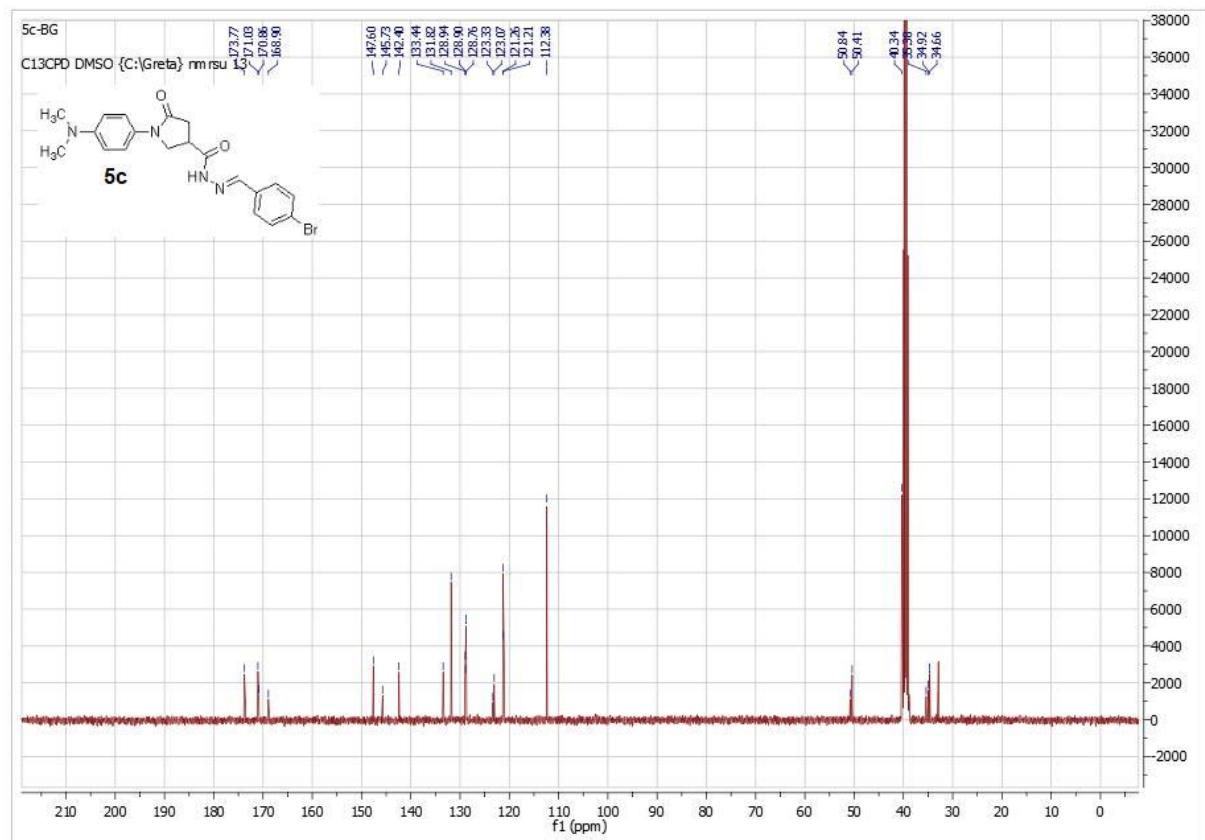


Figure S16. ^{13}C NMR spectrum of compound **5c**.

***N'*-(4-dimethylamino)benzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5d)**

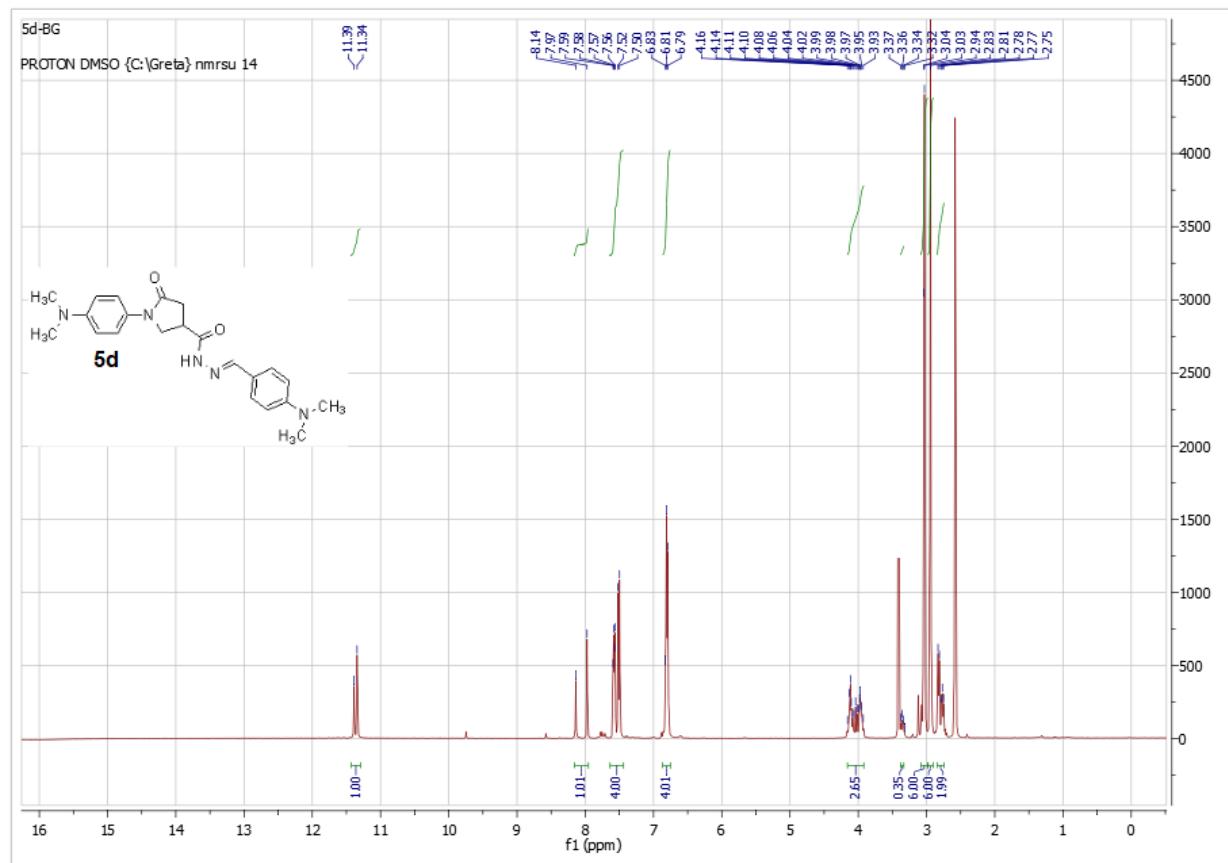


Figure S17. ^1H NMR spectrum of compound 5d.

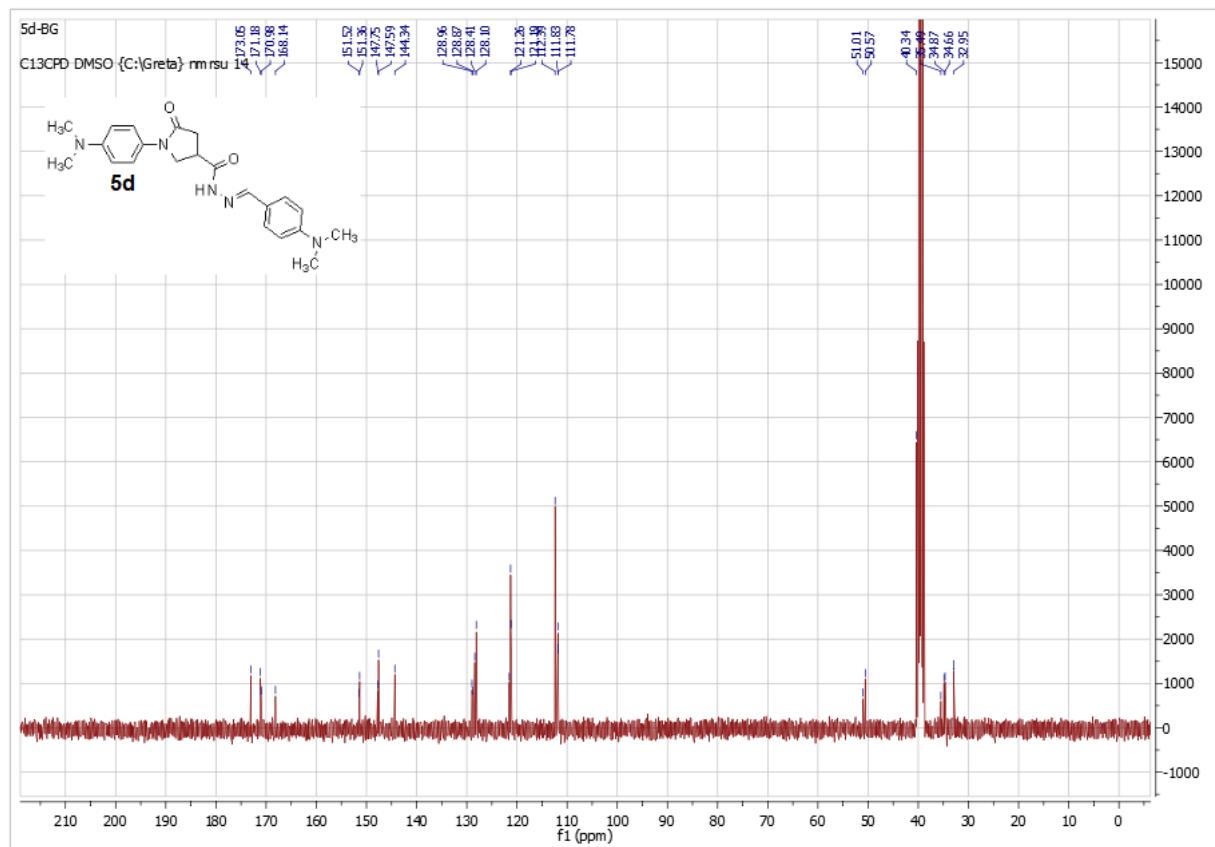


Figure S18. ^{13}C NMR spectrum of compound 5d.

N'-(4-methoxybenzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5e)

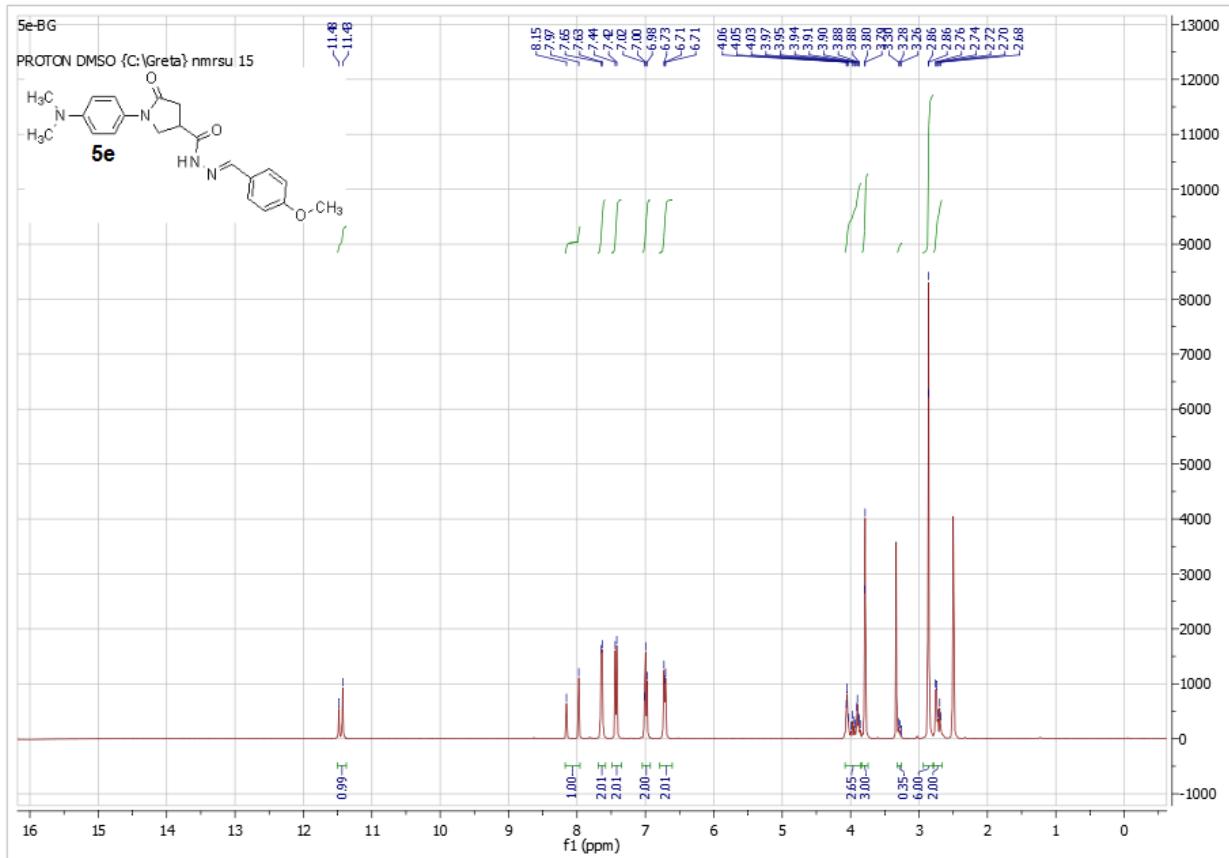


Figure S19. ^1H NMR spectrum of compound 5e.

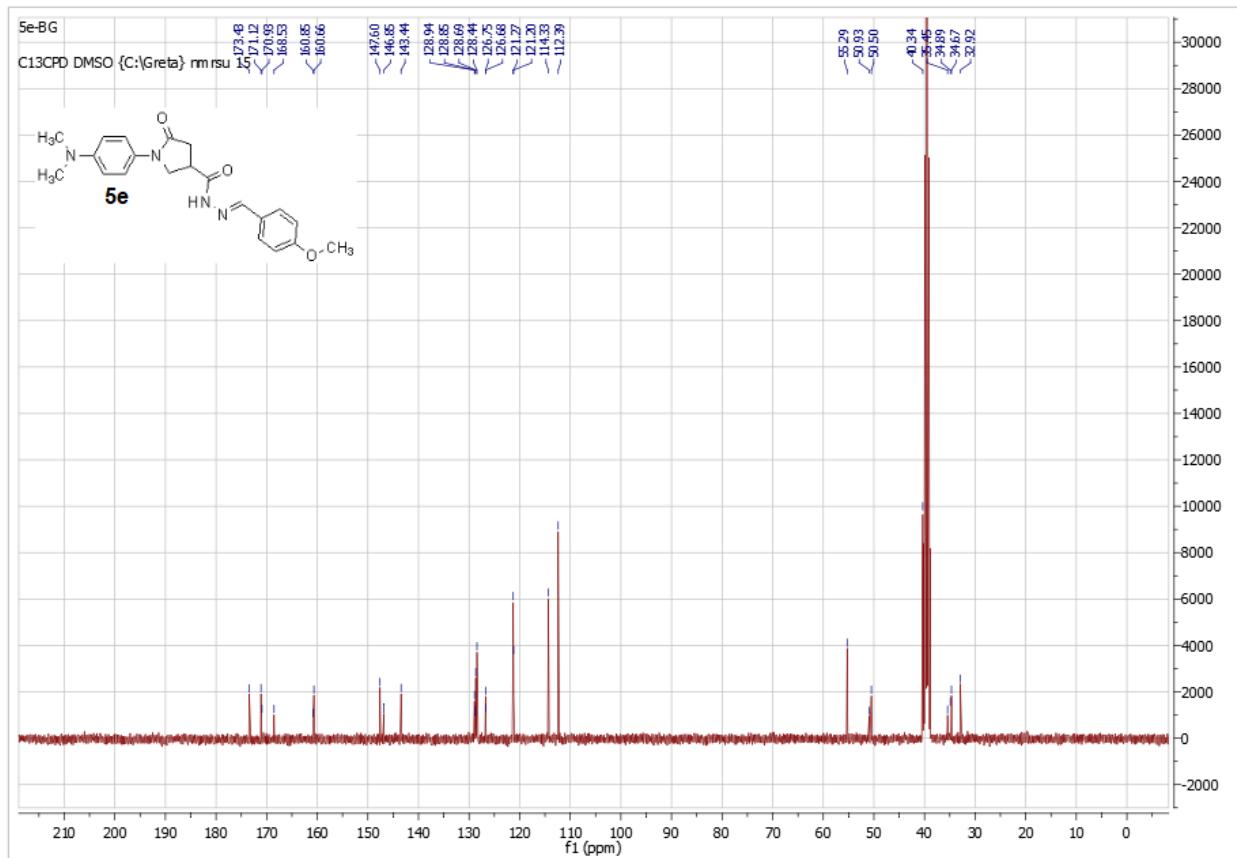


Figure S20. ^{13}C NMR spectrum of compound 5e.

N'-(2,5-dimethoxybenzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5f)

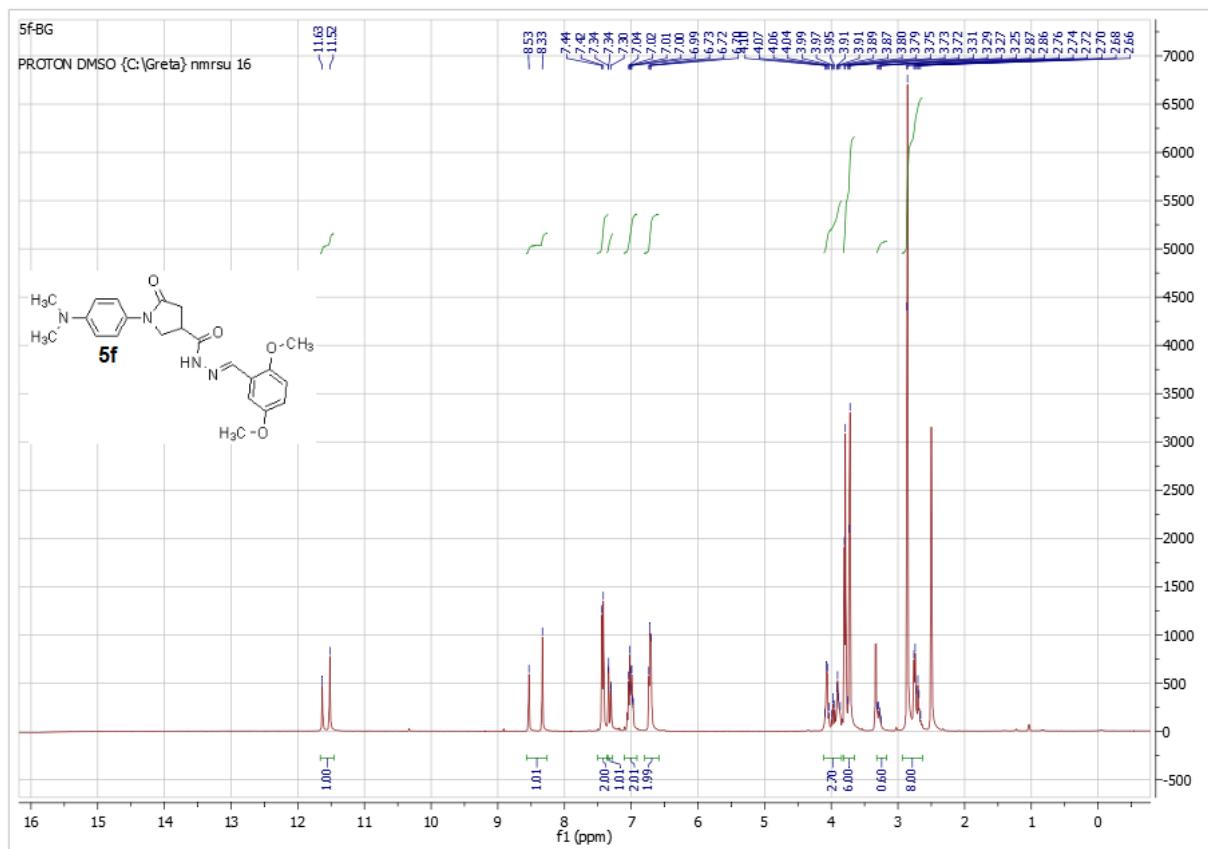


Figure S21. ^1H NMR spectrum of compound 5f.

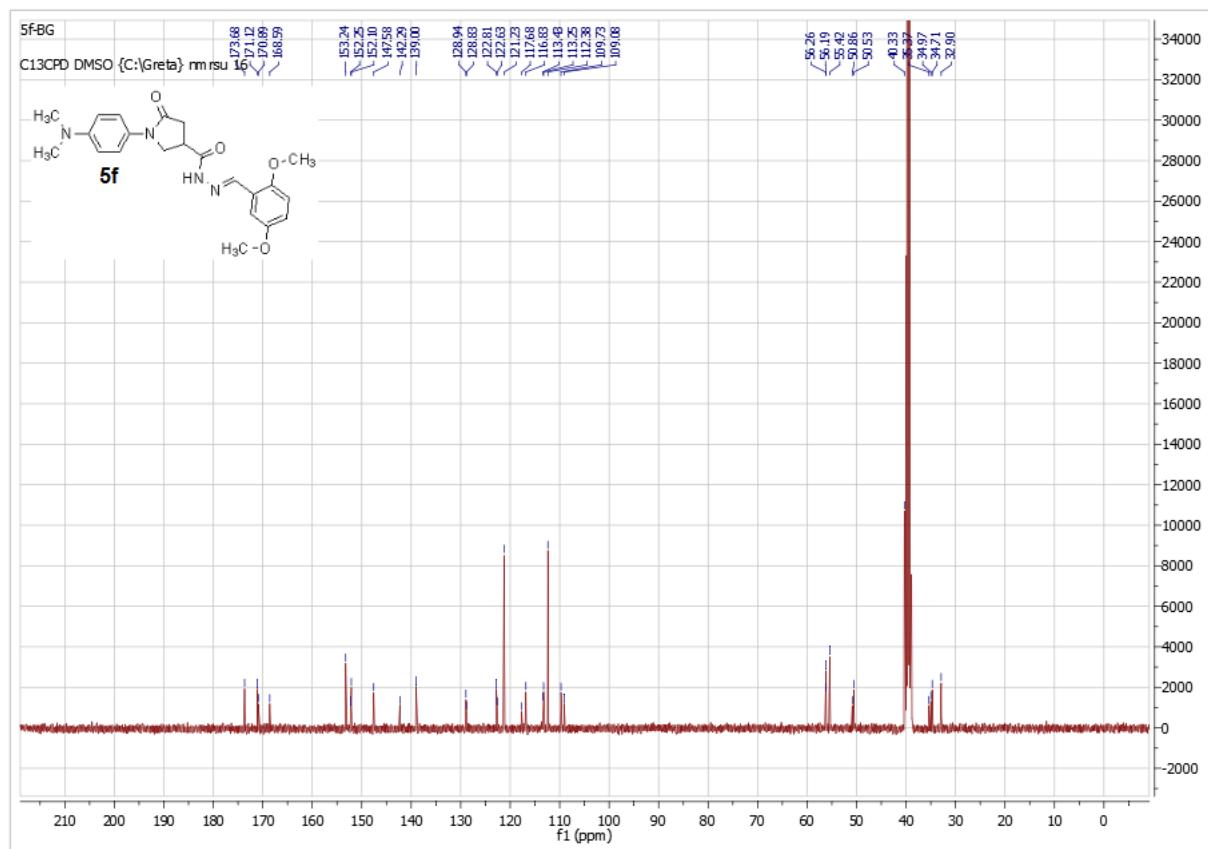


Figure S22. ^{13}C NMR spectrum of compound 5f.

***N'*-(2,4,6-trimethoxybenzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide
(5g)**

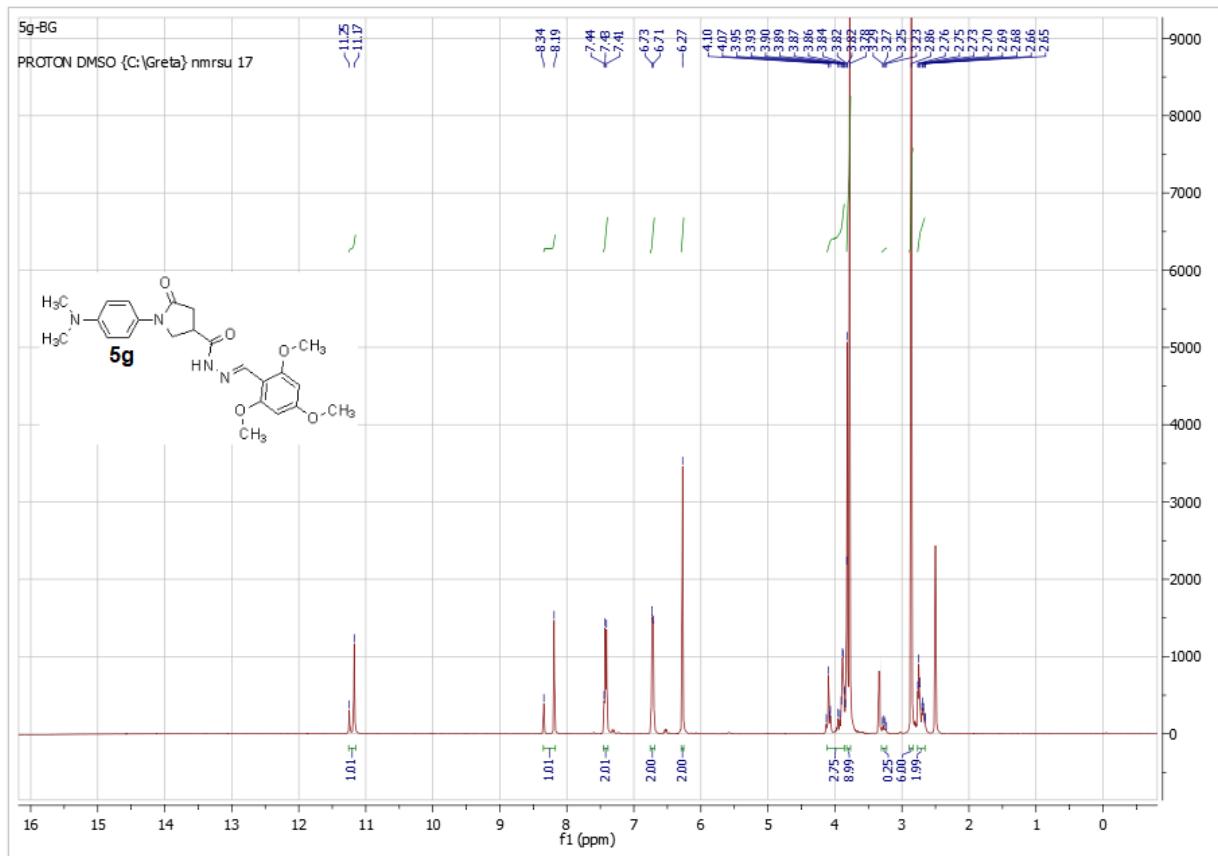


Figure S23. ^1H NMR spectrum of compound 5g.

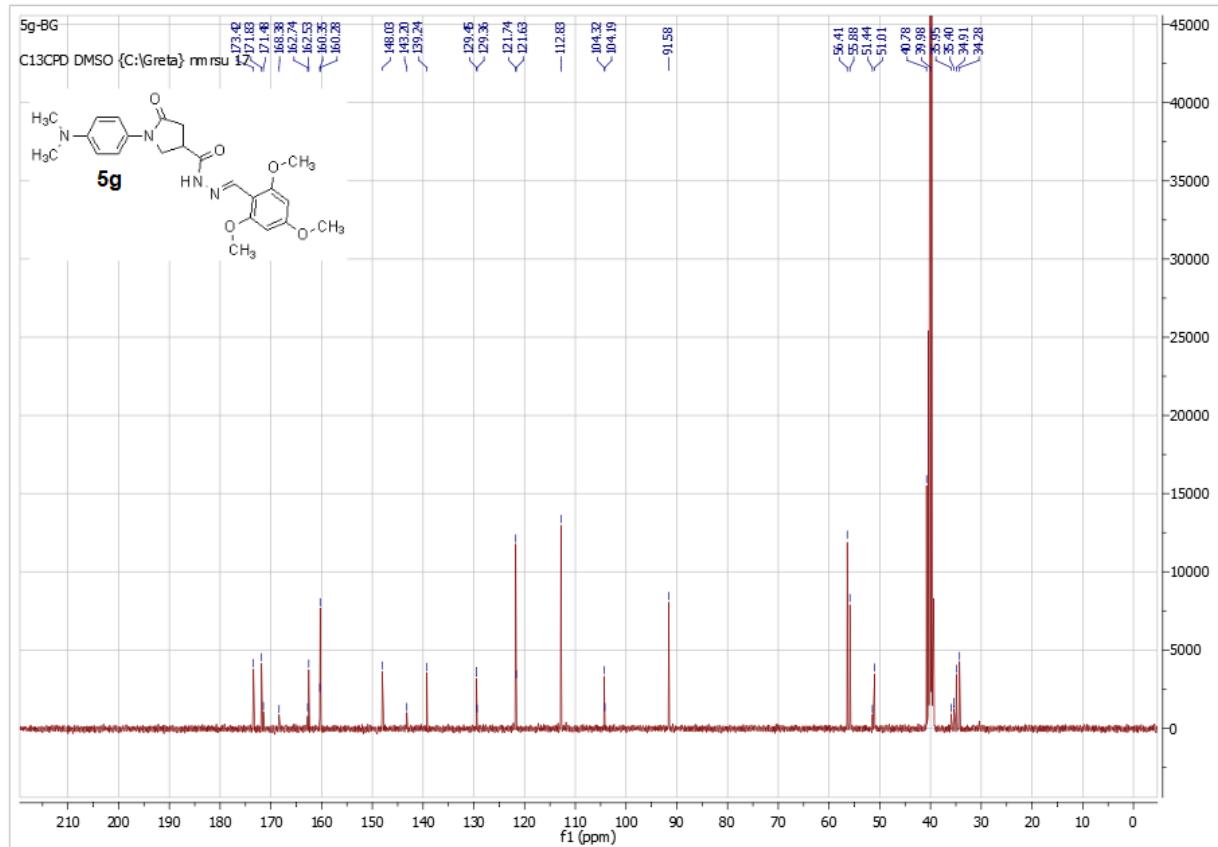


Figure S24. ^{13}C NMR spectrum of compound 5g.

***N'*-(3,4,5-trimethoxybenzylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (5h)**

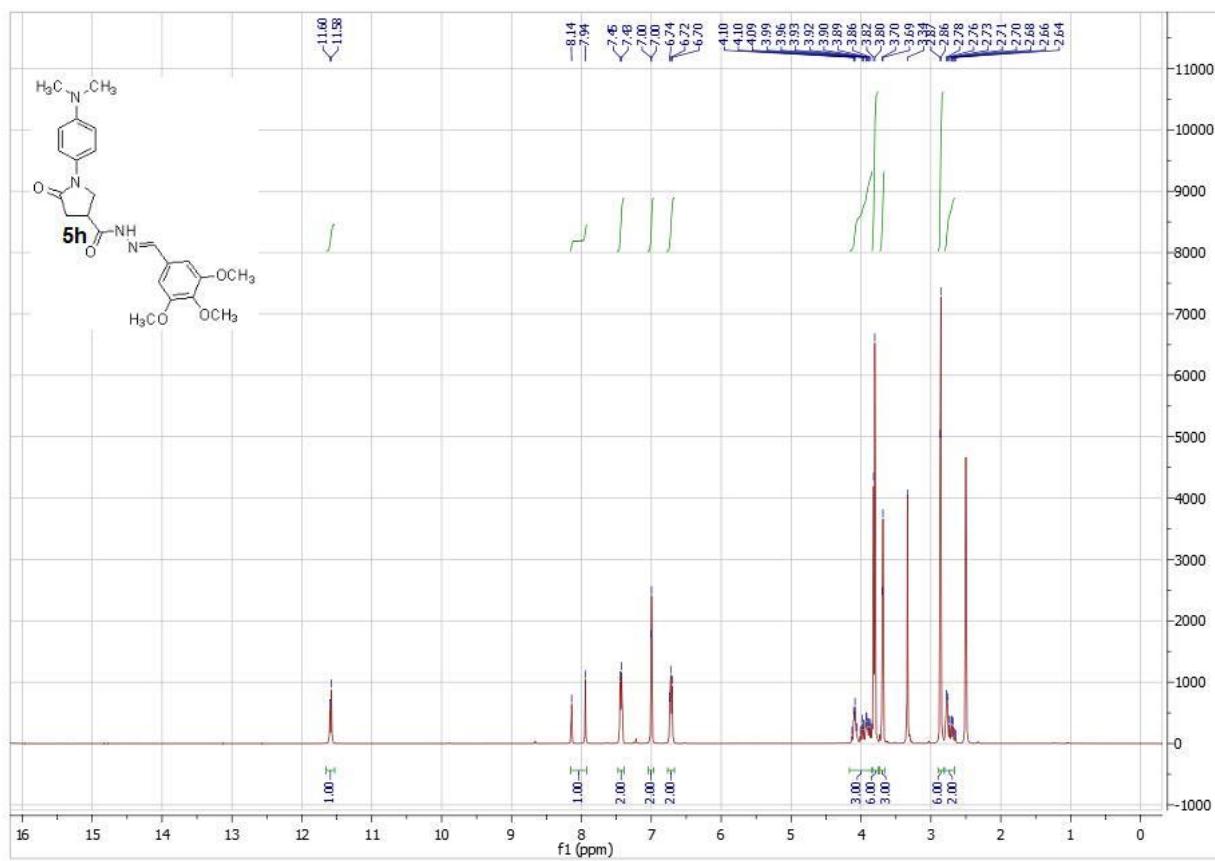


Figure S25. ^1H NMR spectrum of compound 5h.

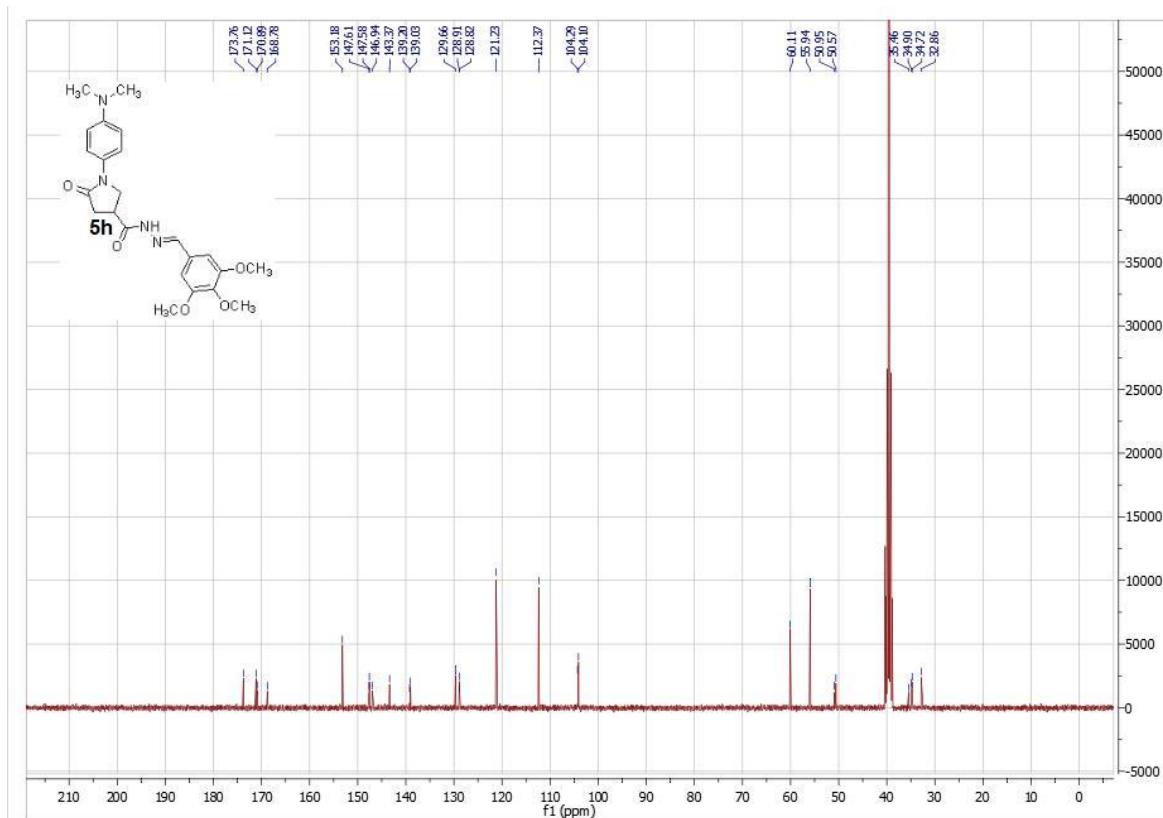


Figure S26. ^{13}C NMR spectrum of compound 5h.

1-(4-(Dimethylamino)phenyl)-N'-(4-nitrobenzylidene)-5-oxopyrrolidine-3-carbohydrazide (5i)

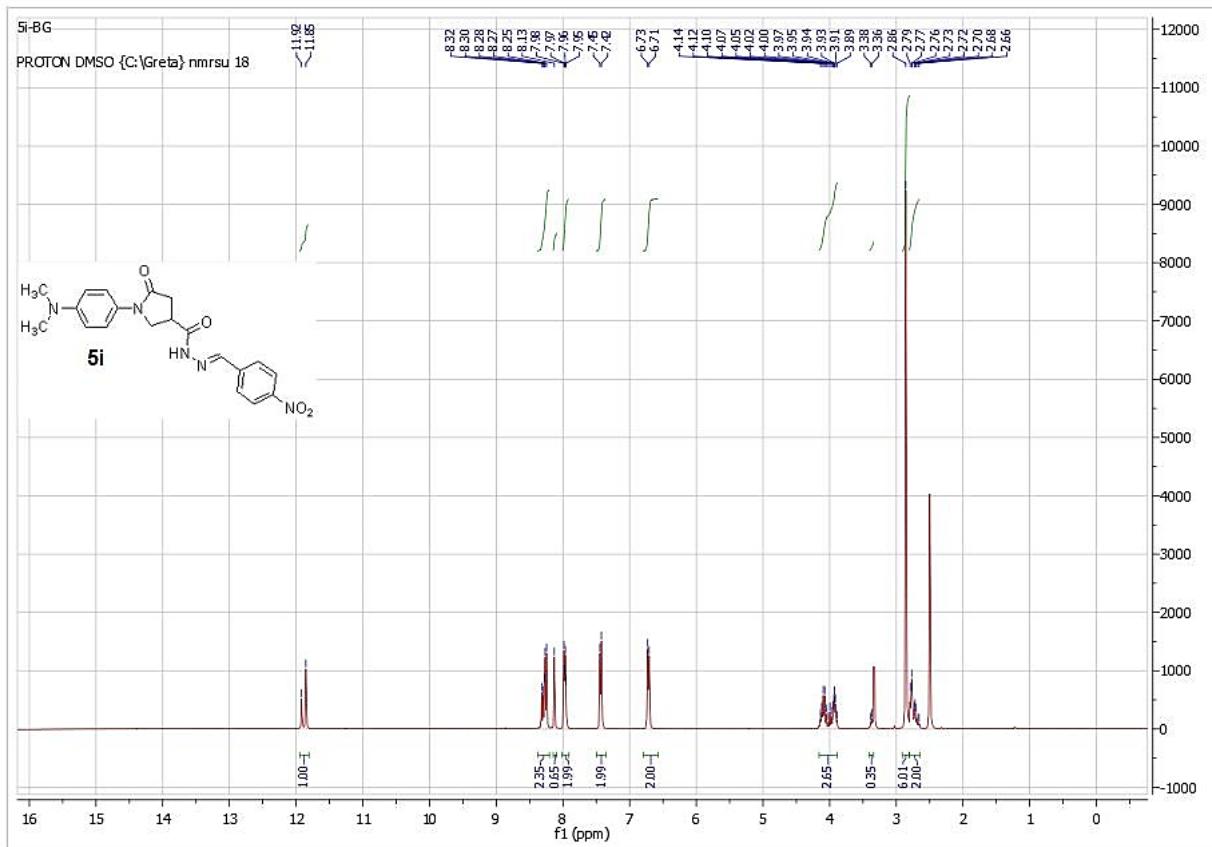


Figure S27. ^1H NMR spectrum of compound 5i.

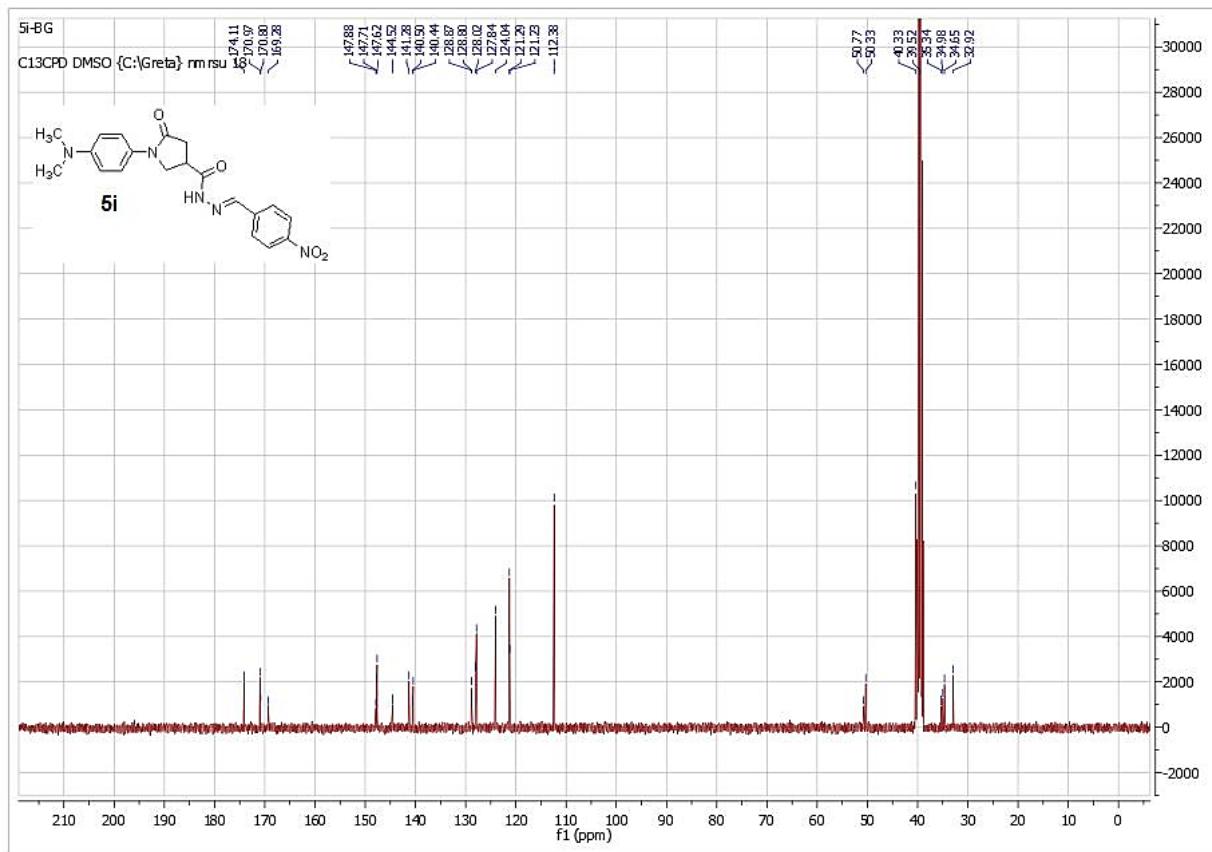


Figure S28. ^{13}C NMR spectrum of compound 5i.

1-(4-(Dimethylamino)phenyl)-5-oxo-N'-(thiophen-2-ylmethylene)pyrrolidine-3-carbohydrazide (5j)

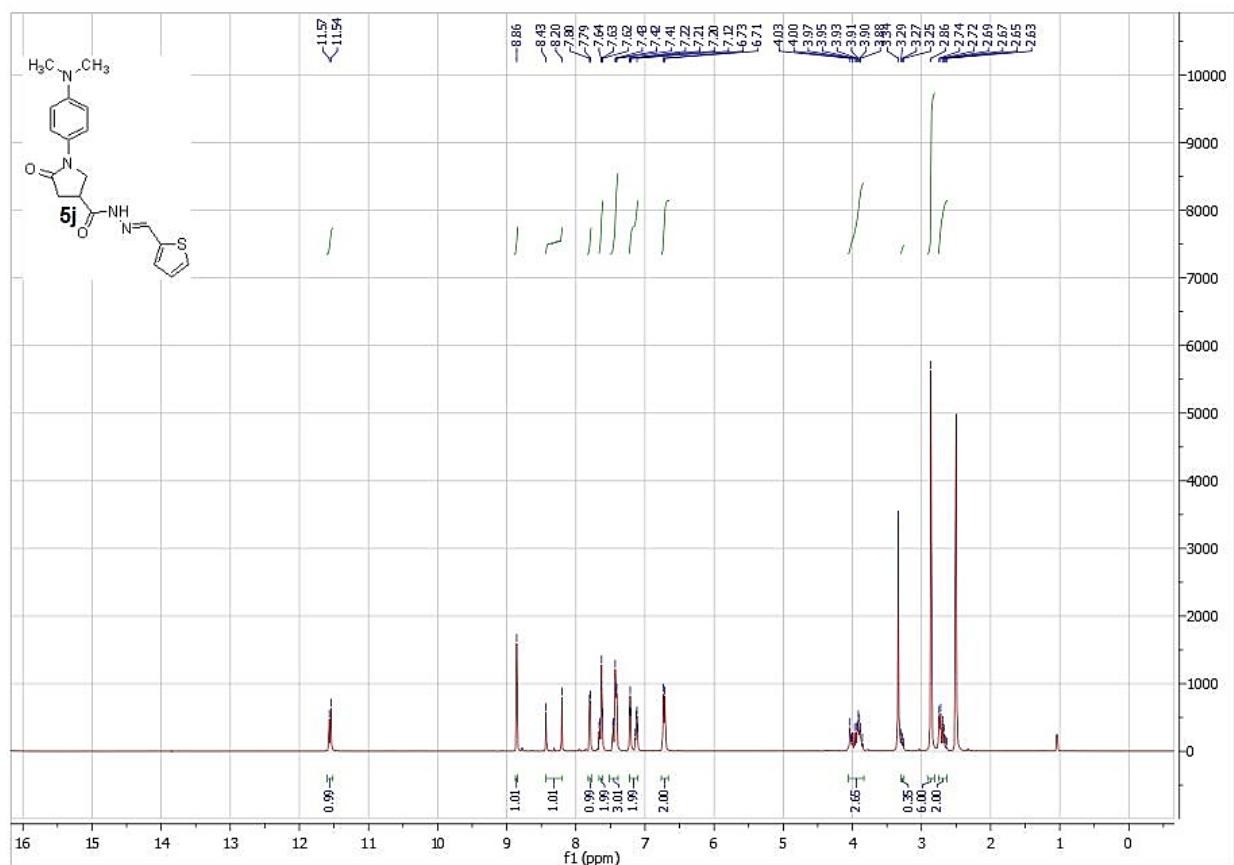


Figure S29. ^1H NMR spectrum of compound 5j.

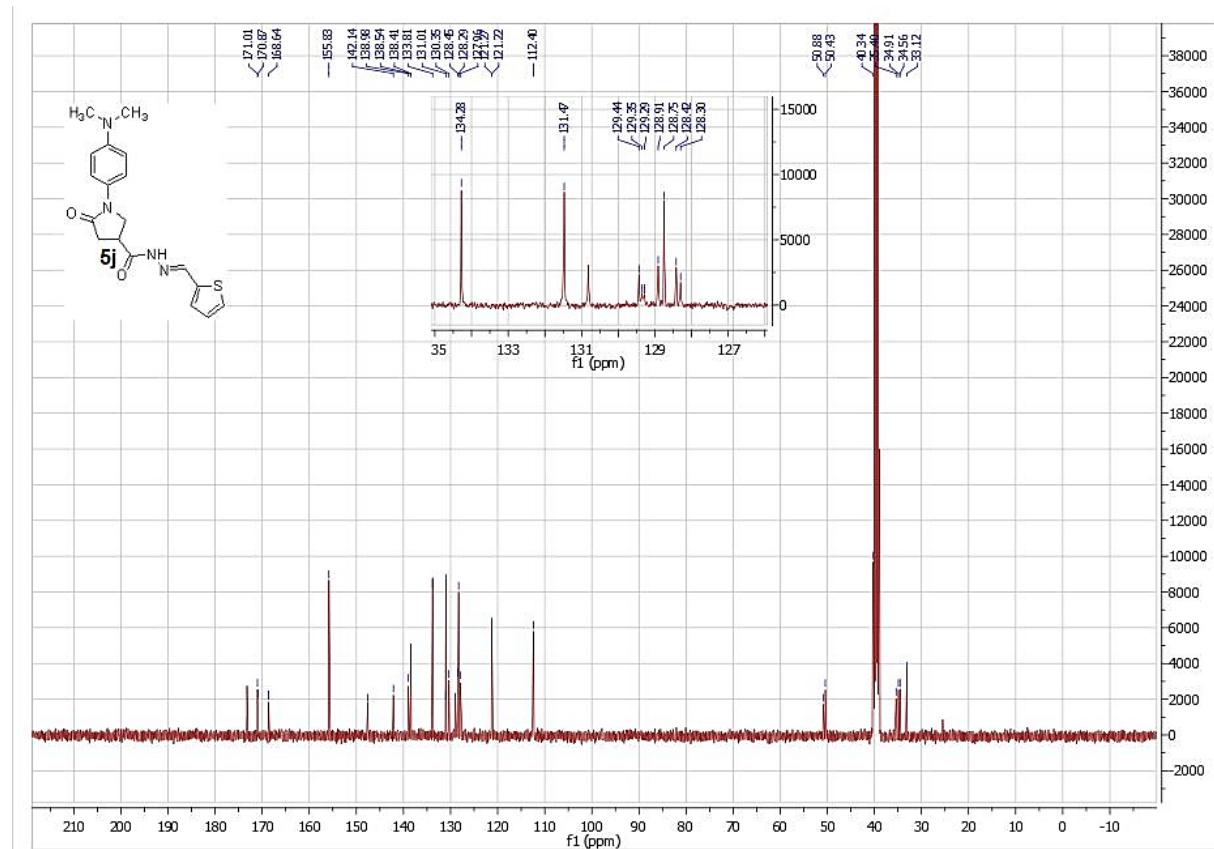


Figure S30. ^{13}C NMR spectrum of compound 5j.

1-(4-(Dimethylamino)phenyl)-N'-(5-nitrothiophen-2-yl)methylene)-5-oxopyrrolidine-3-carbohydrazide (5k)

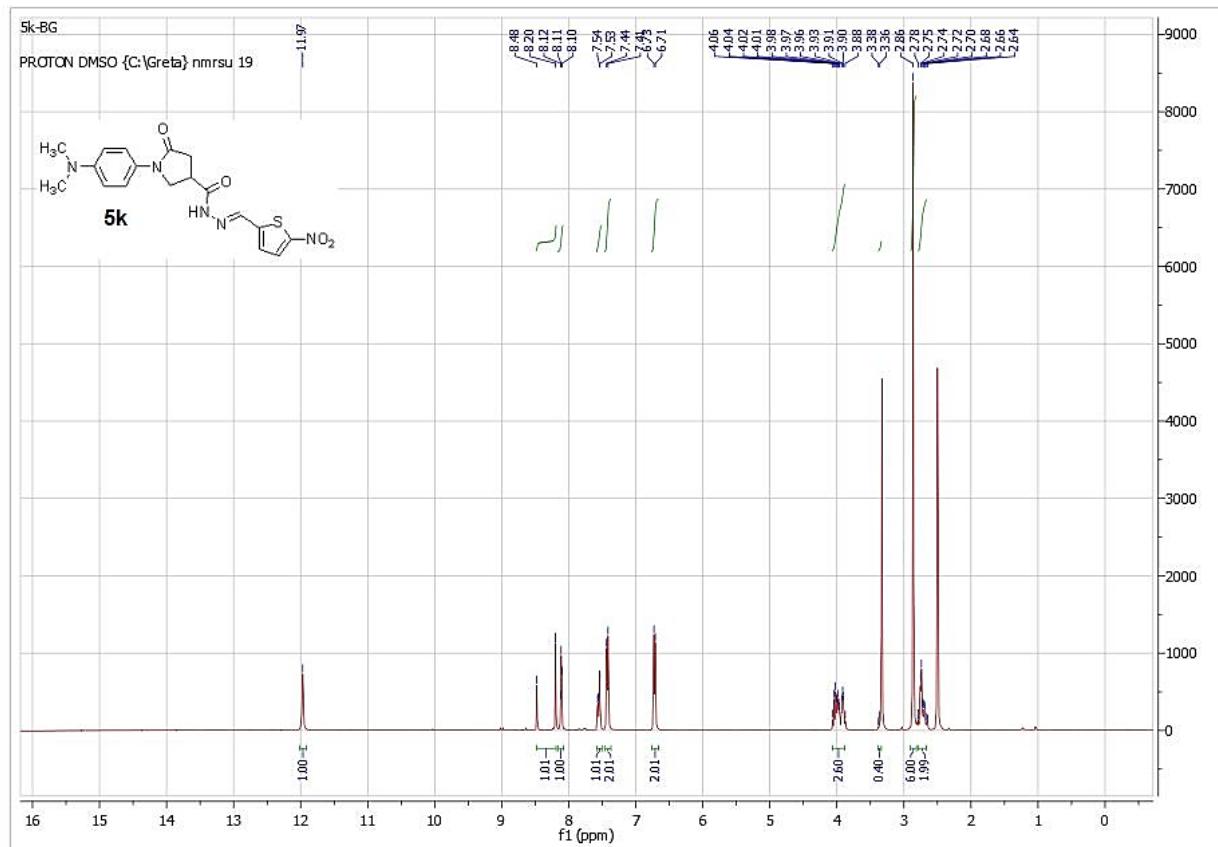


Figure S31. ^1H NMR spectrum of compound 5k.

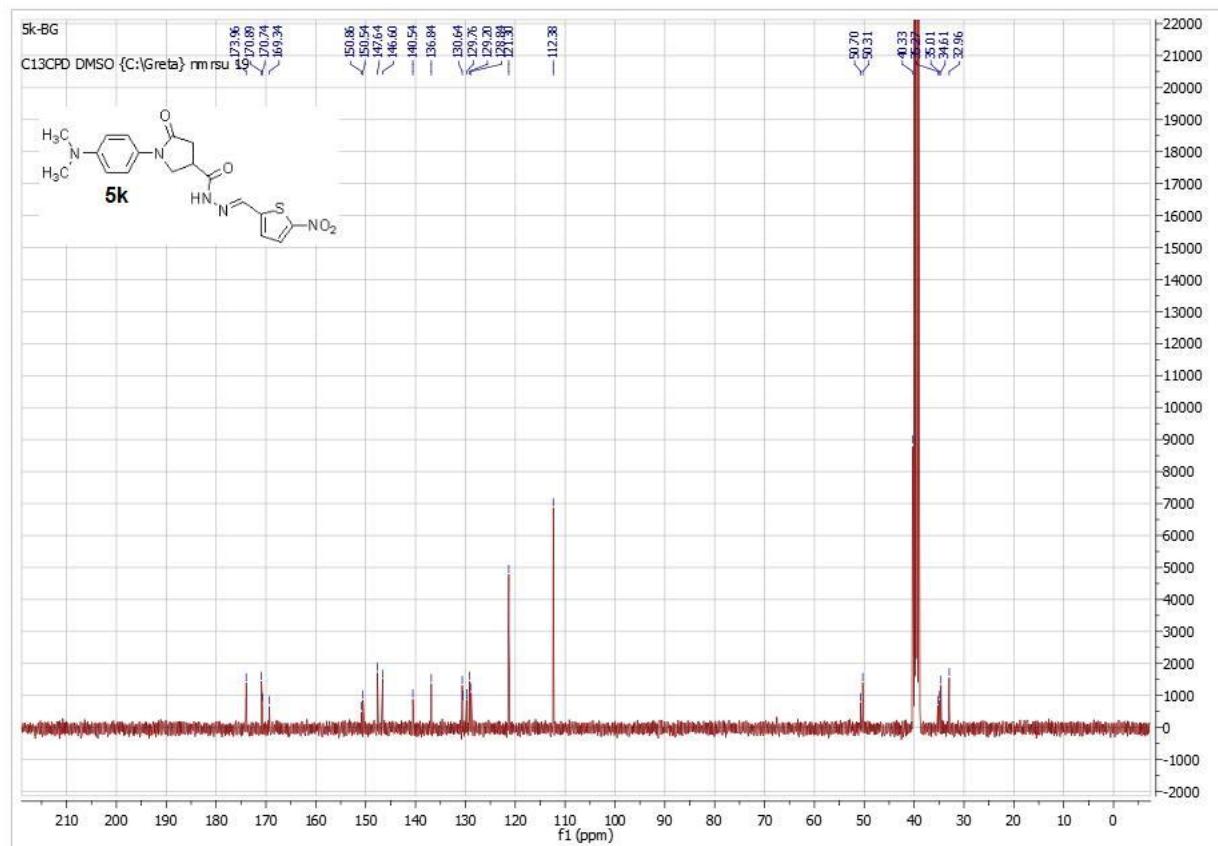


Figure S32. ^{13}C NMR spectrum of compound 51.

1-(4-(Dimethylamino)phenyl)-N'-(naphthalen-1-ylmethylene)-5-oxopyrrolidine-3-carbohydrazide (5l)

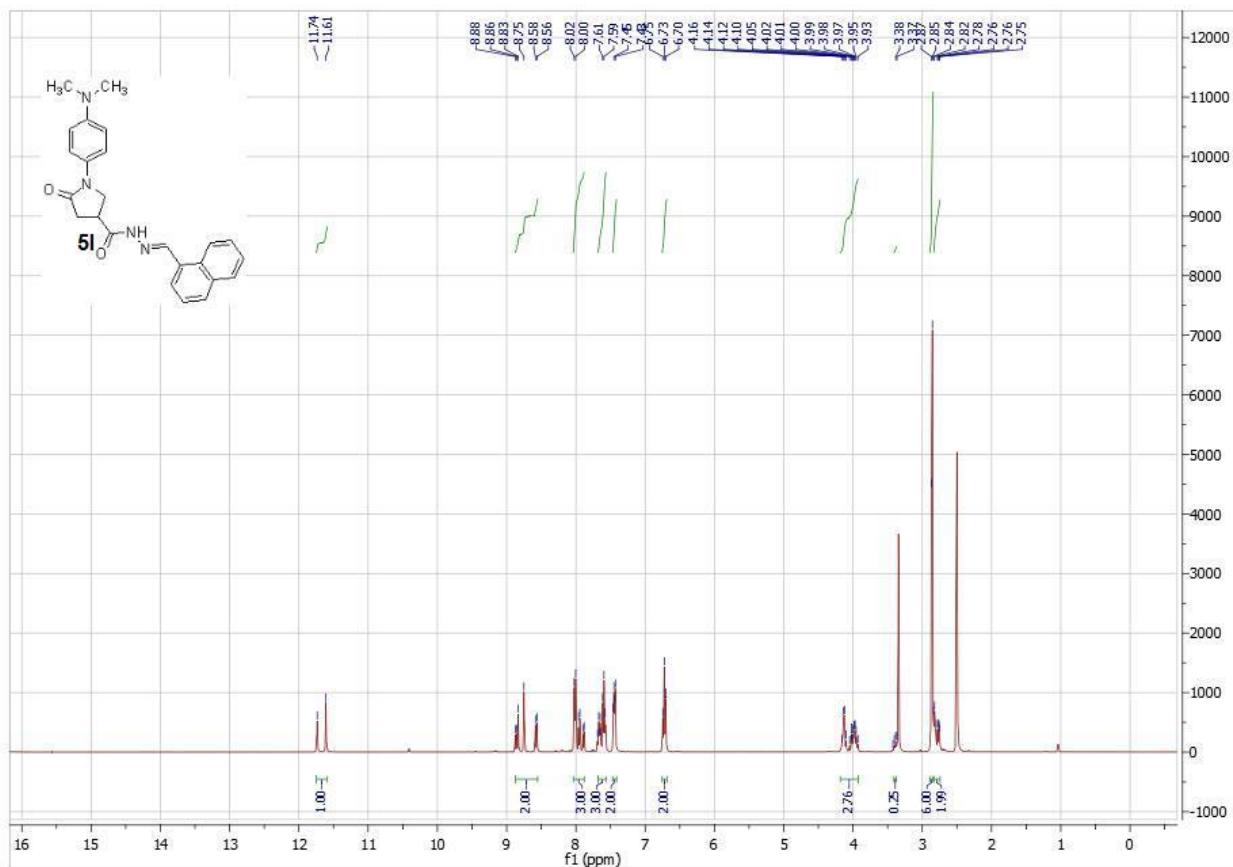


Figure S33. ^1H NMR spectrum of compound 5l.

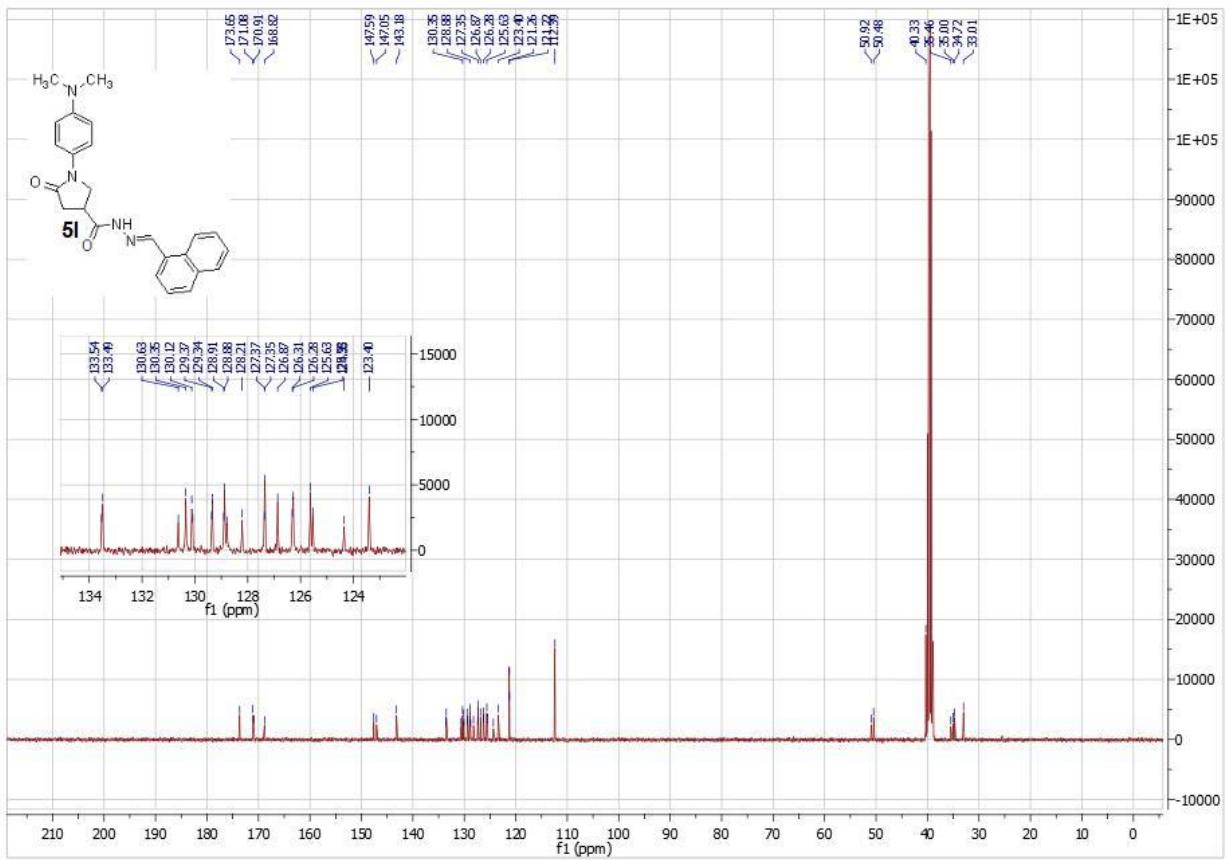


Figure S34. ^{13}C NMR spectrum of compound 5l.

1-(4-(Dimethylamino)phenyl)-5-oxo-N'-(propan-2-ylidene)pyrrolidine-3-carbohydrazide (6a)

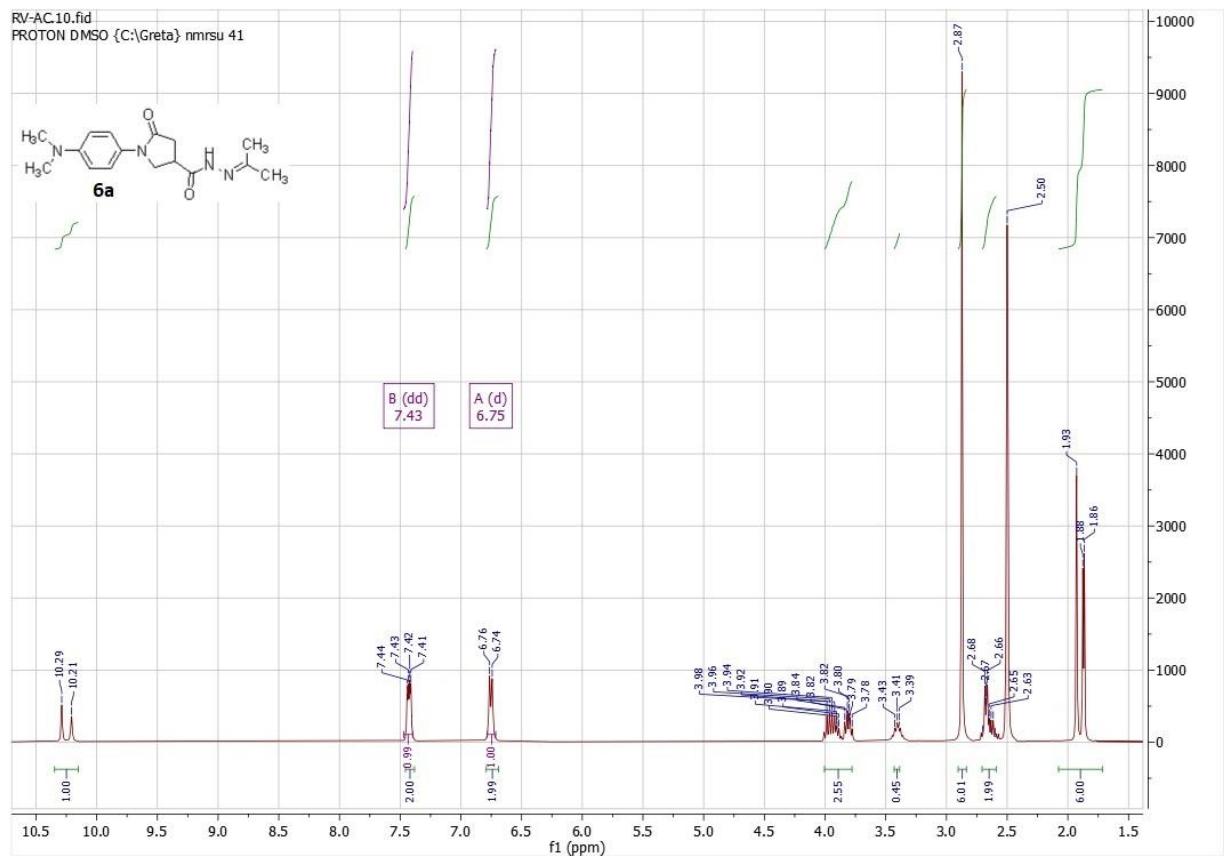


Figure S35. ^1H NMR spectrum of compound **6a**.

N'-(butan-2-ylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide (6b)

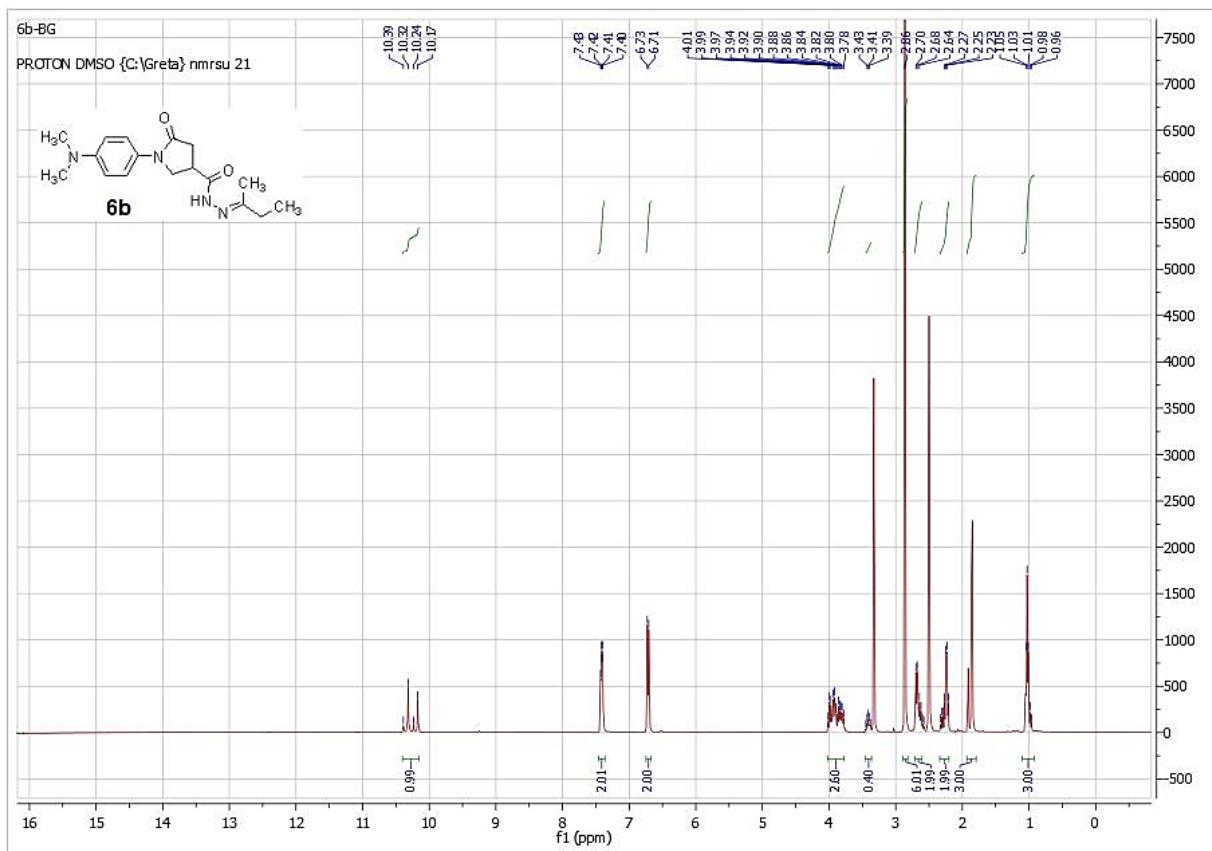


Figure S36. ^1H NMR spectrum of compound **6b**.

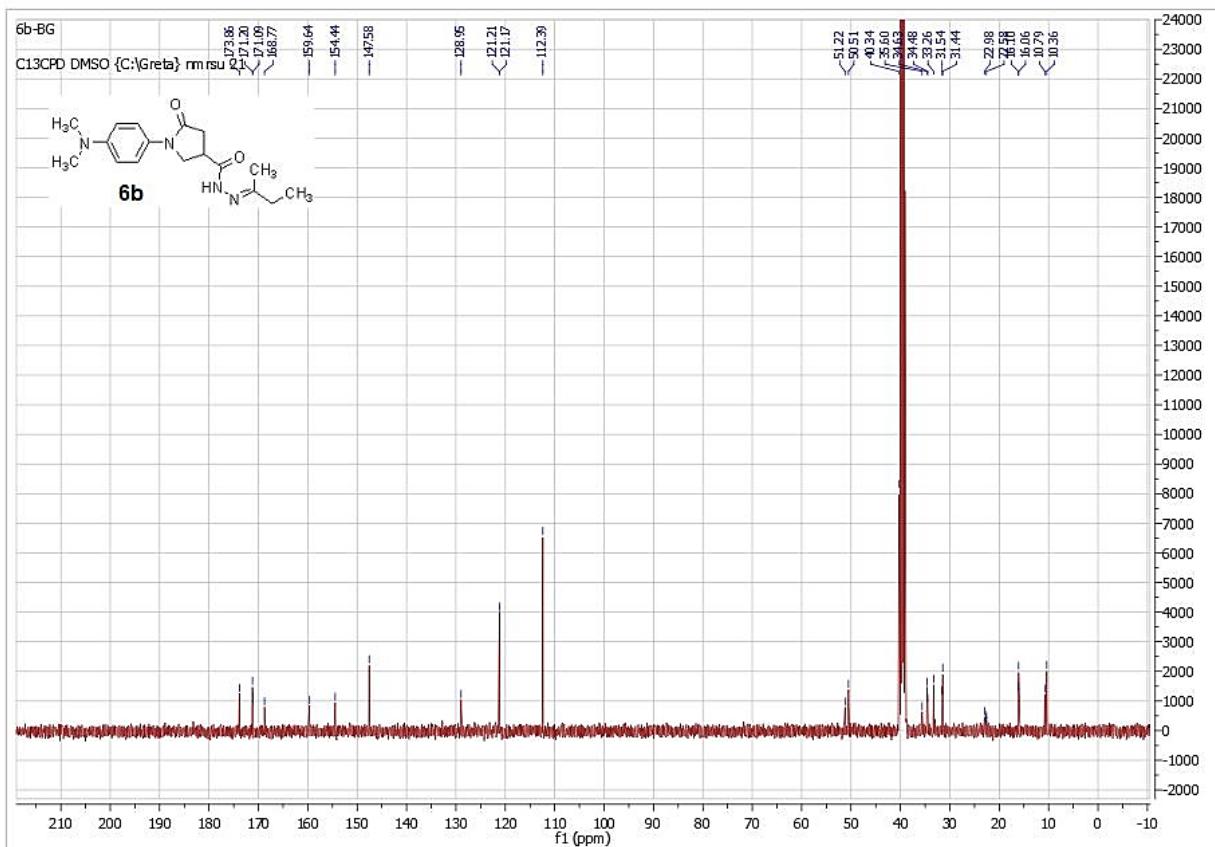


Figure S37. ^{13}C NMR spectrum of compound **6b**.

***N'*-(1-(4-aminophenyl)ethylidene)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carbohydrazide
(6c)**

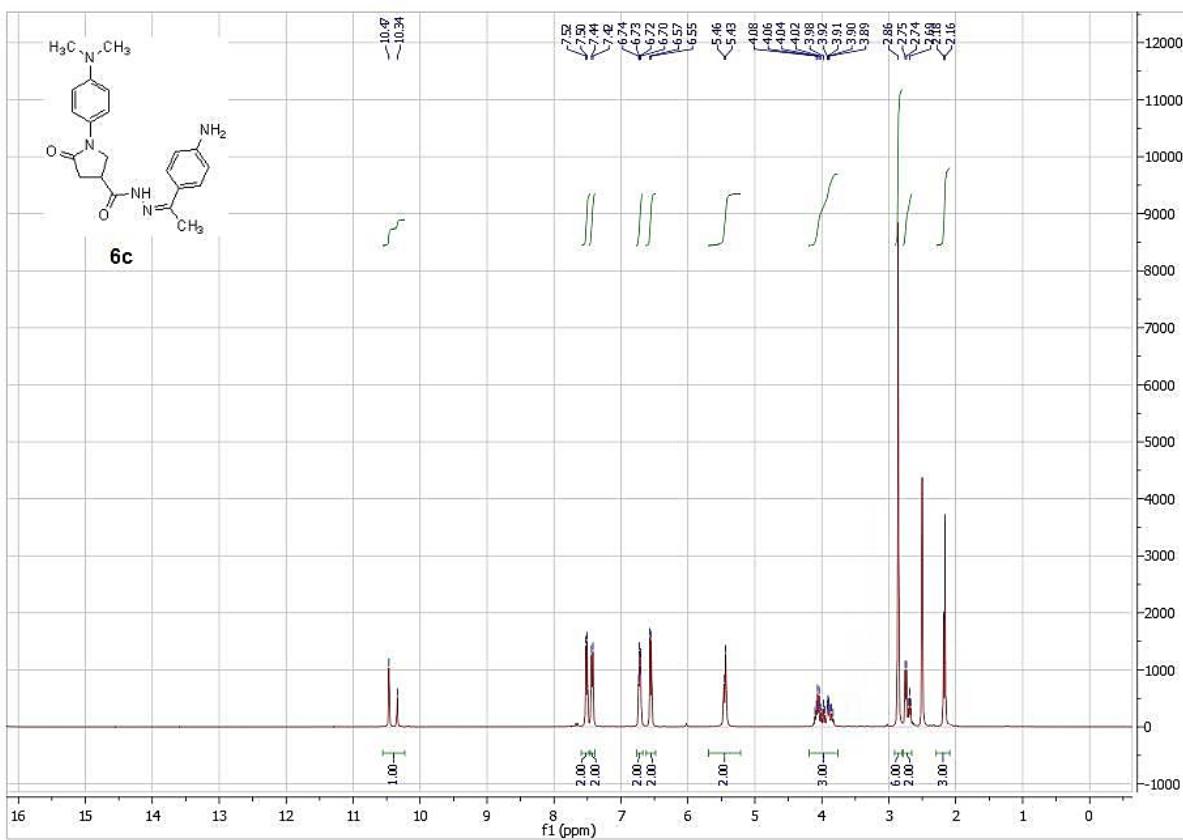


Figure S38. ^1H NMR spectrum of compound 6c.

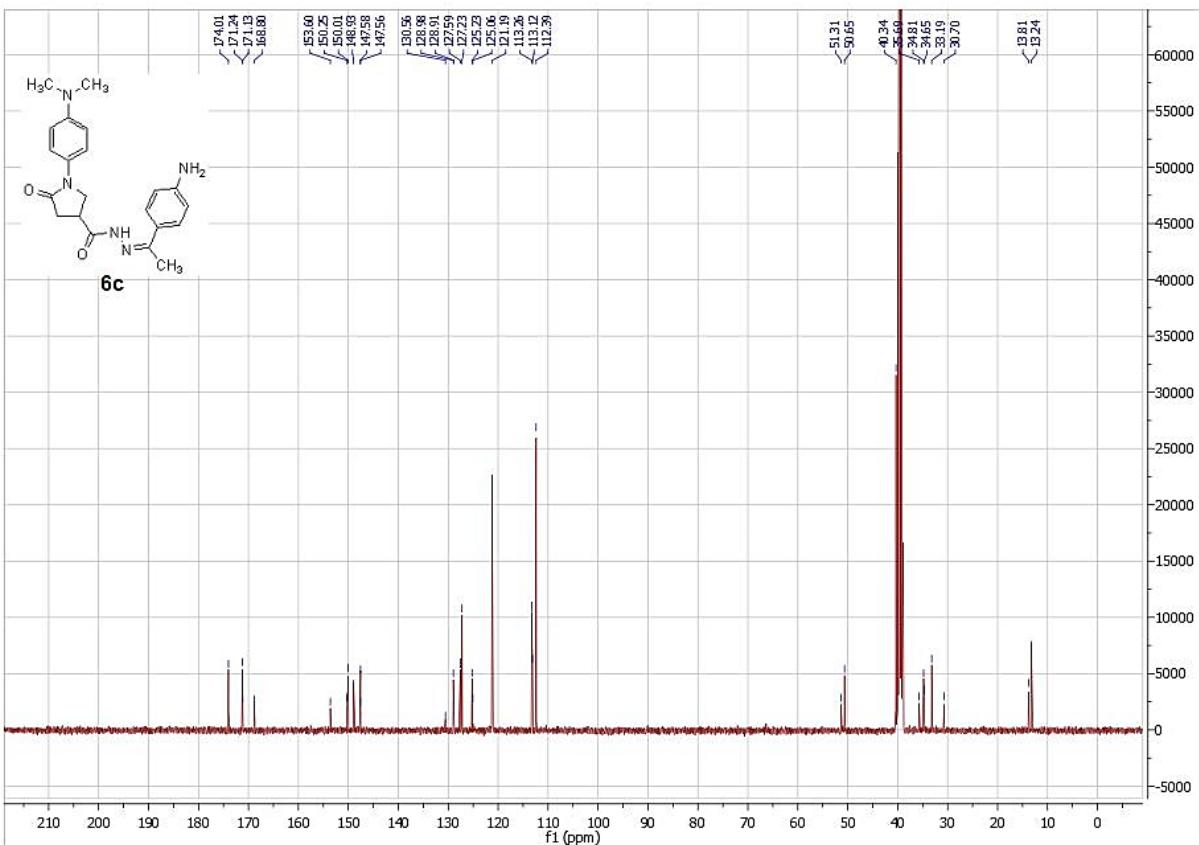


Figure S39. ^{13}C NMR spectrum of compound 6c.

N-(2,5-dimethyl-1*H*-pyrrol-1-yl)-1-(4-(dimethylamino)phenyl)-5-oxopyrrolidine-3-carboxamide (**7**)

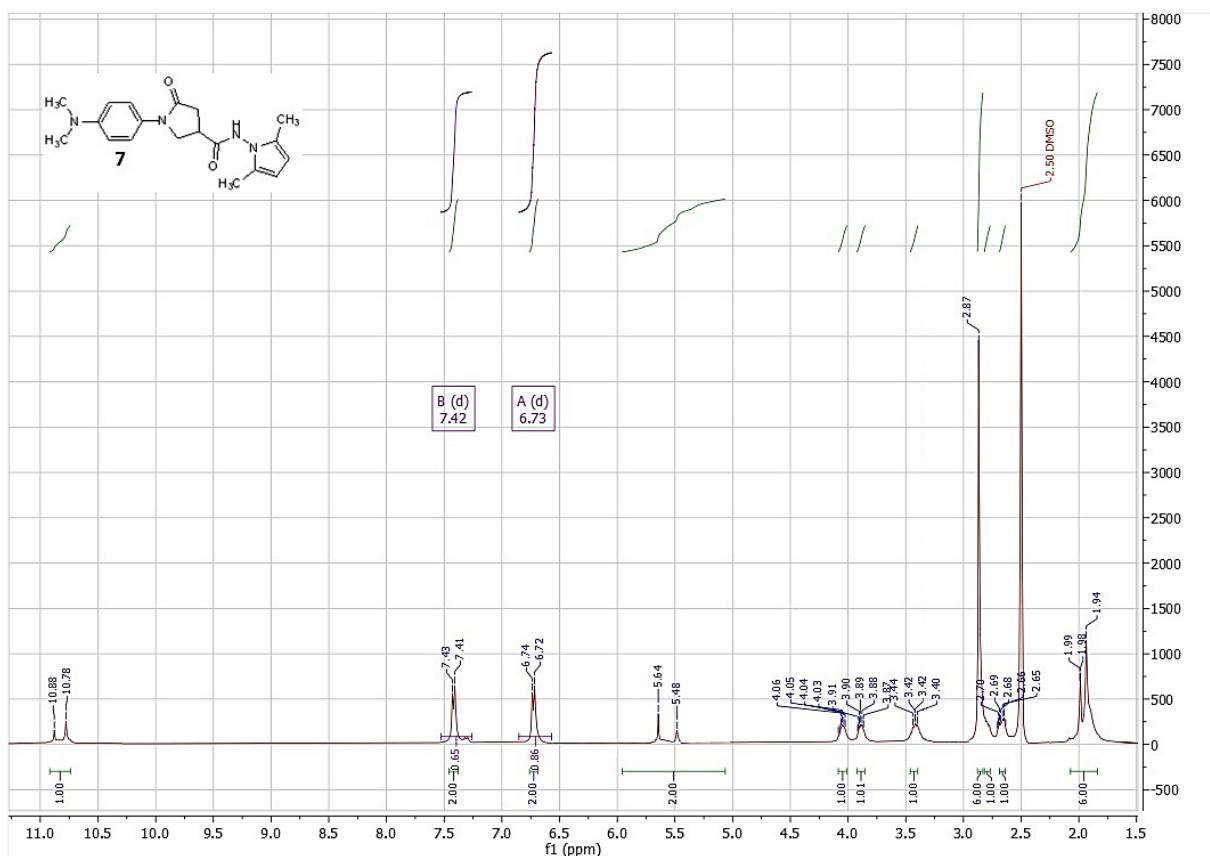


Figure S40. ^1H NMR spectrum of compound **7**.

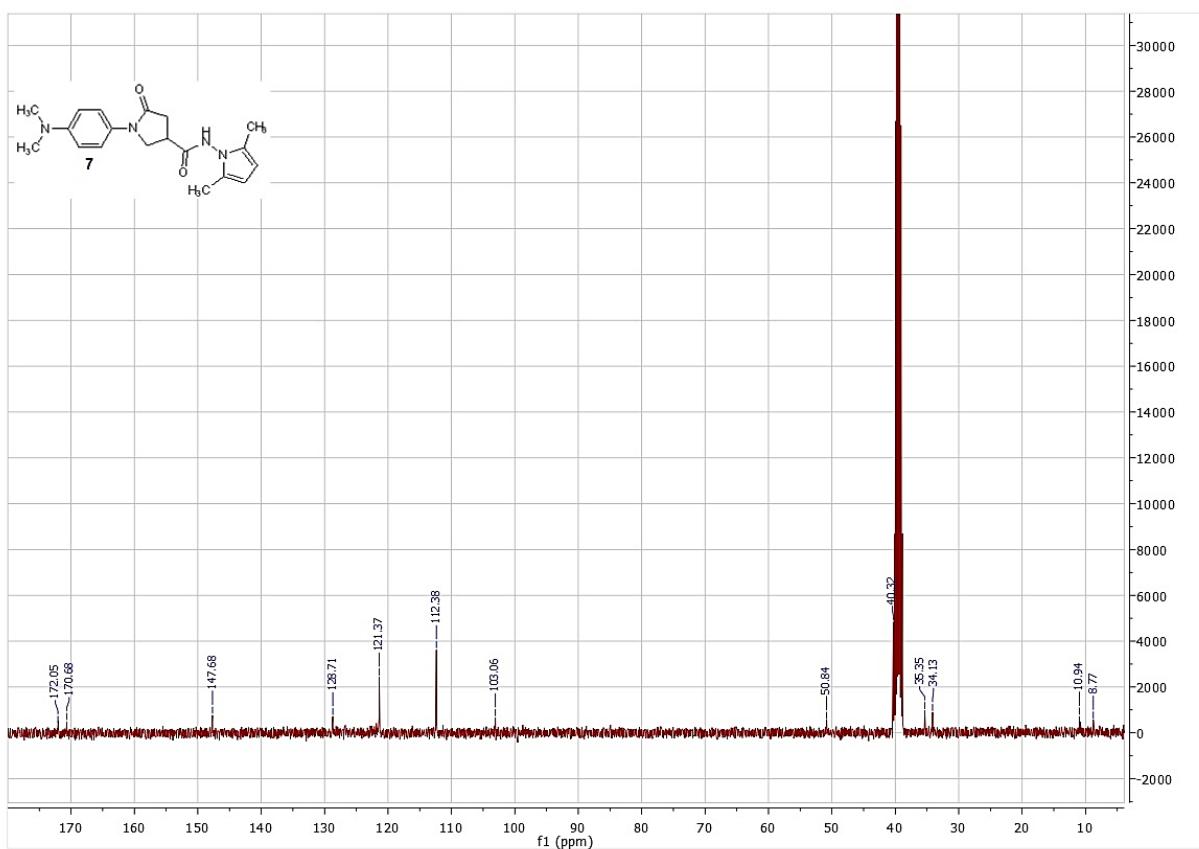


Figure S41. ^{13}C NMR spectrum of compound **7**.

1-(1-(4-(Dimethylamino)phenyl)-5-oxopyrrolidine-3-carboxamido)-5-oxopyrrolidine-3-carboxylic acid (8)

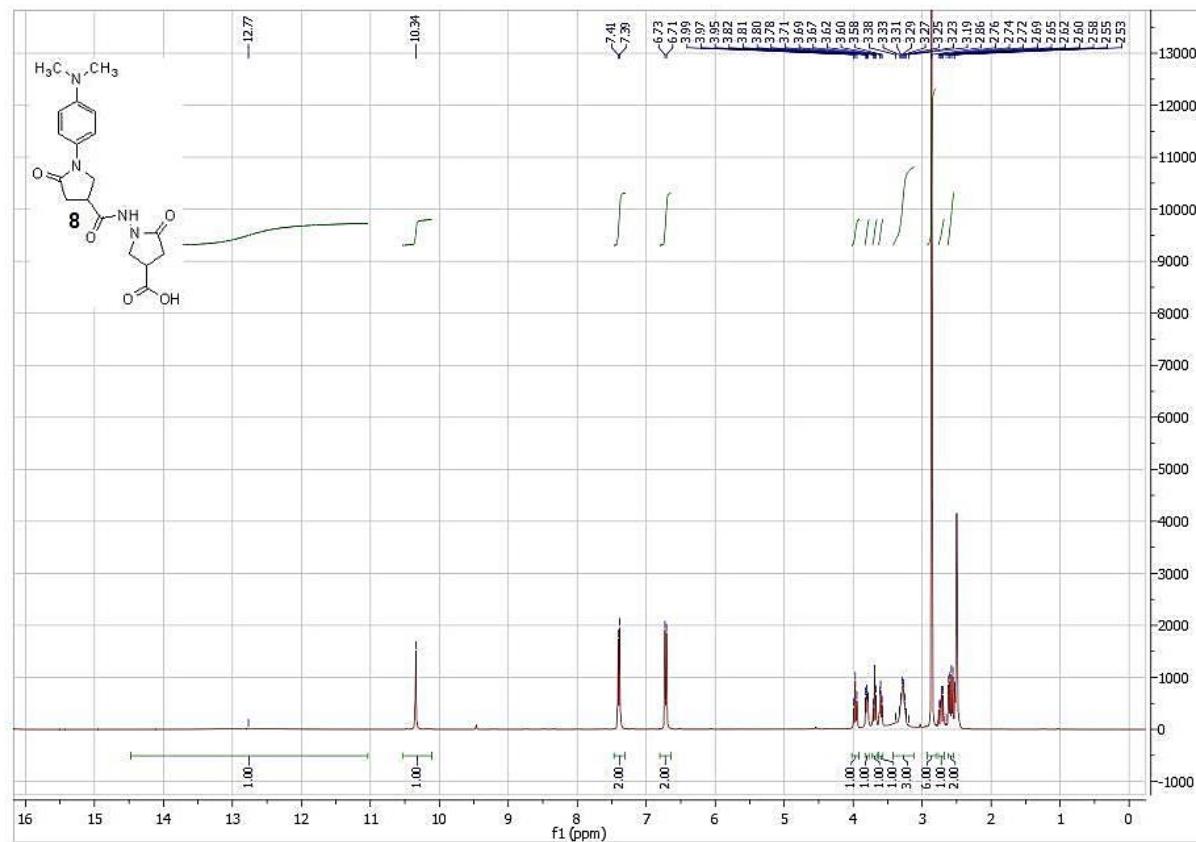


Figure S42. ^1H NMR spectrum of compound 8.

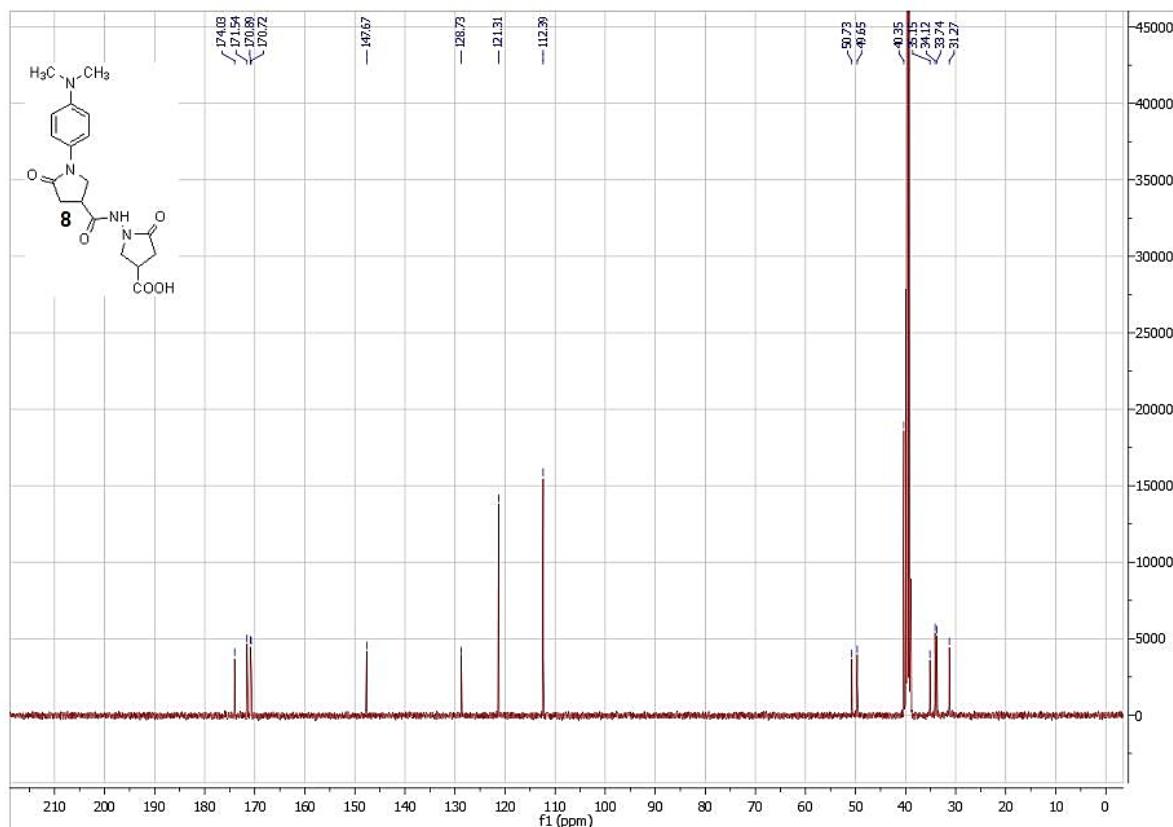


Figure S43. ^{13}C NMR spectrum of compound 8.

1-(4-(Dimethylamino)phenyl)-5-oxo-N'-(2-oxoindolin-3-ylidene)pyrrolidine-3-carbohydrazide (9)

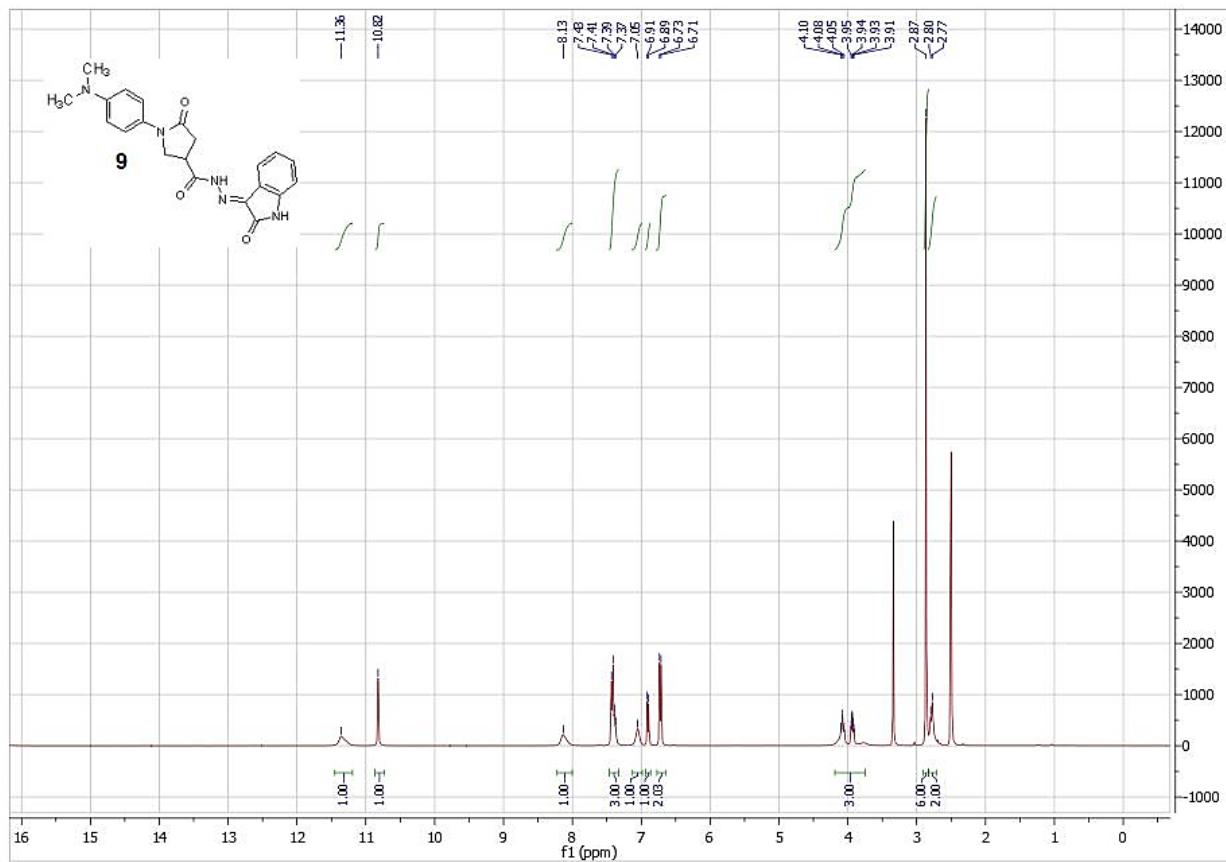


Figure S44. ^1H NMR spectrum of compound 9.

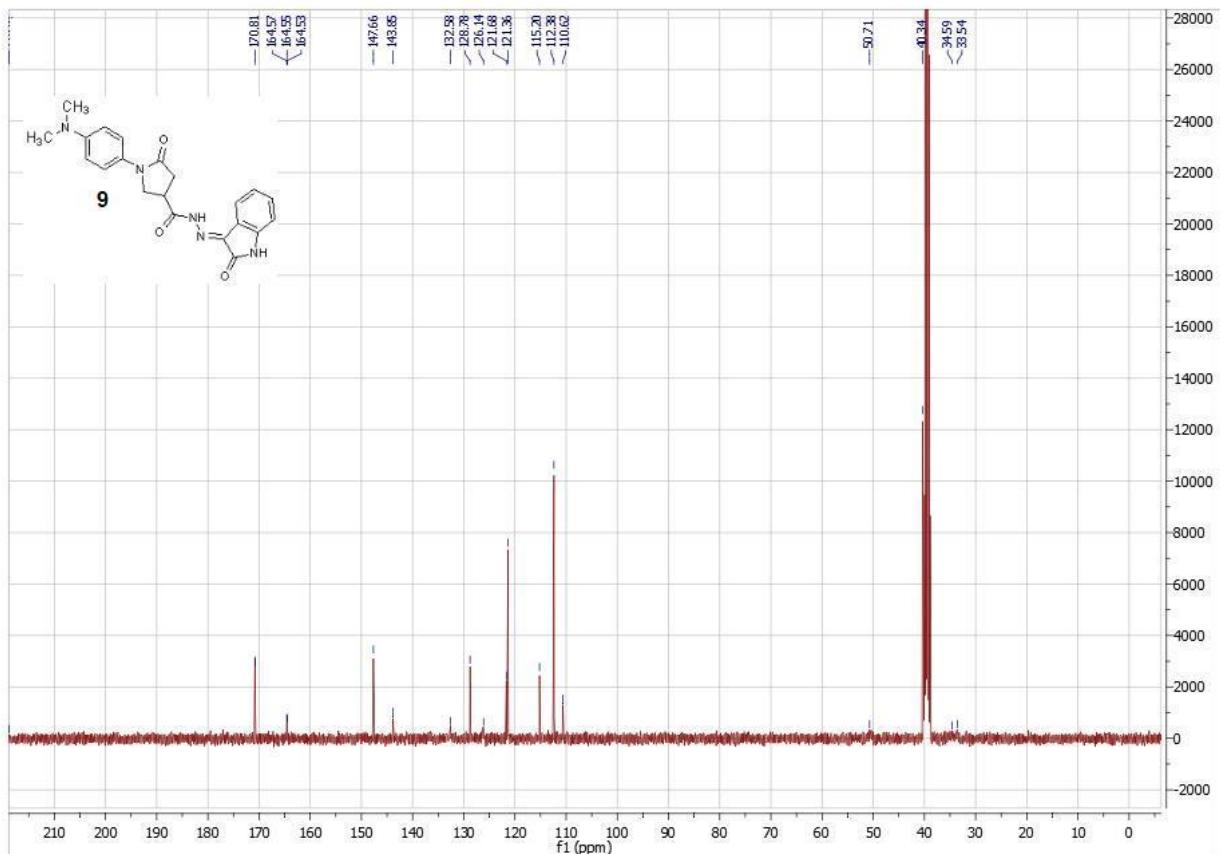


Figure S45. ^{13}C NMR spectrum of compound 9.

1-(4-(Dimethylamino)phenyl)-4-(5-thioxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)pyrrolidin-2-one (10)

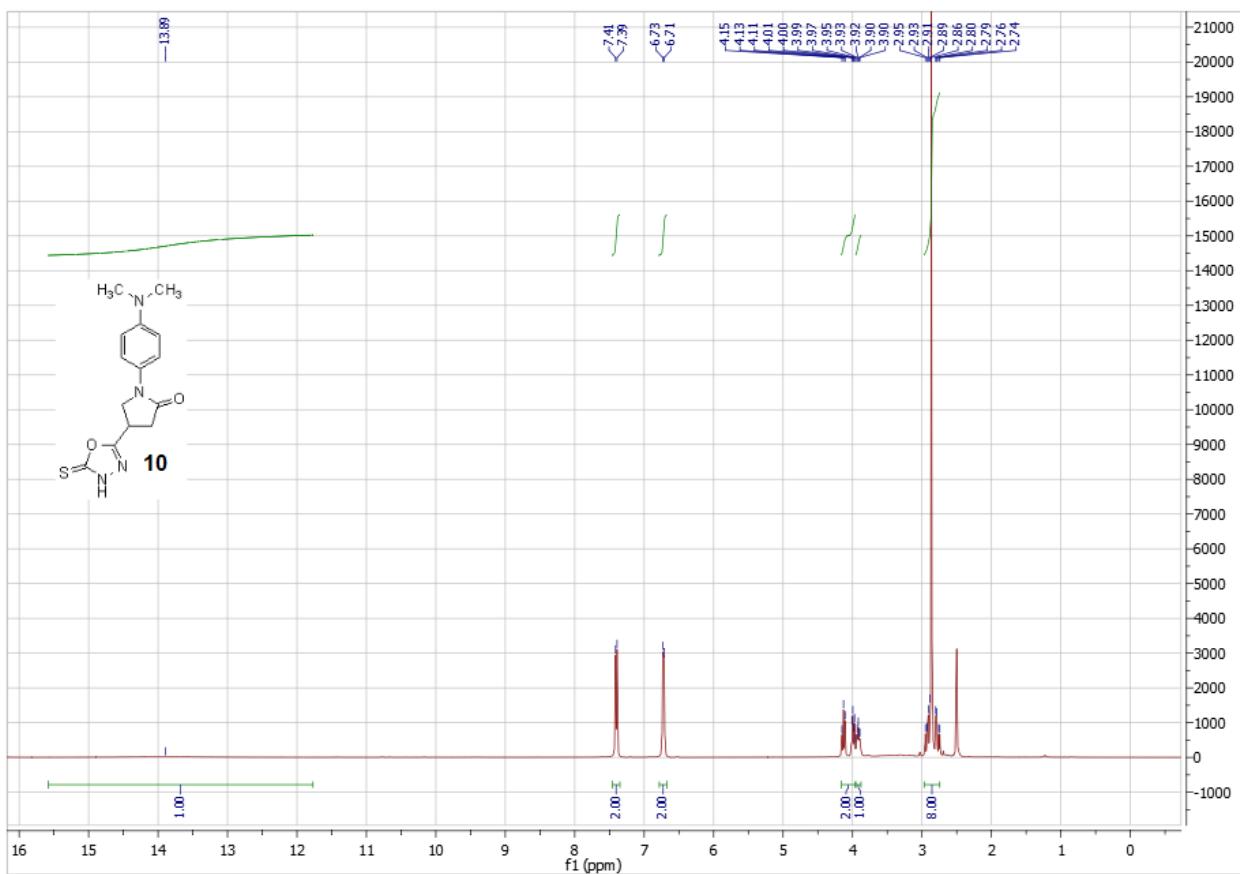


Figure S46. ¹H NMR spectrum of compound 10.

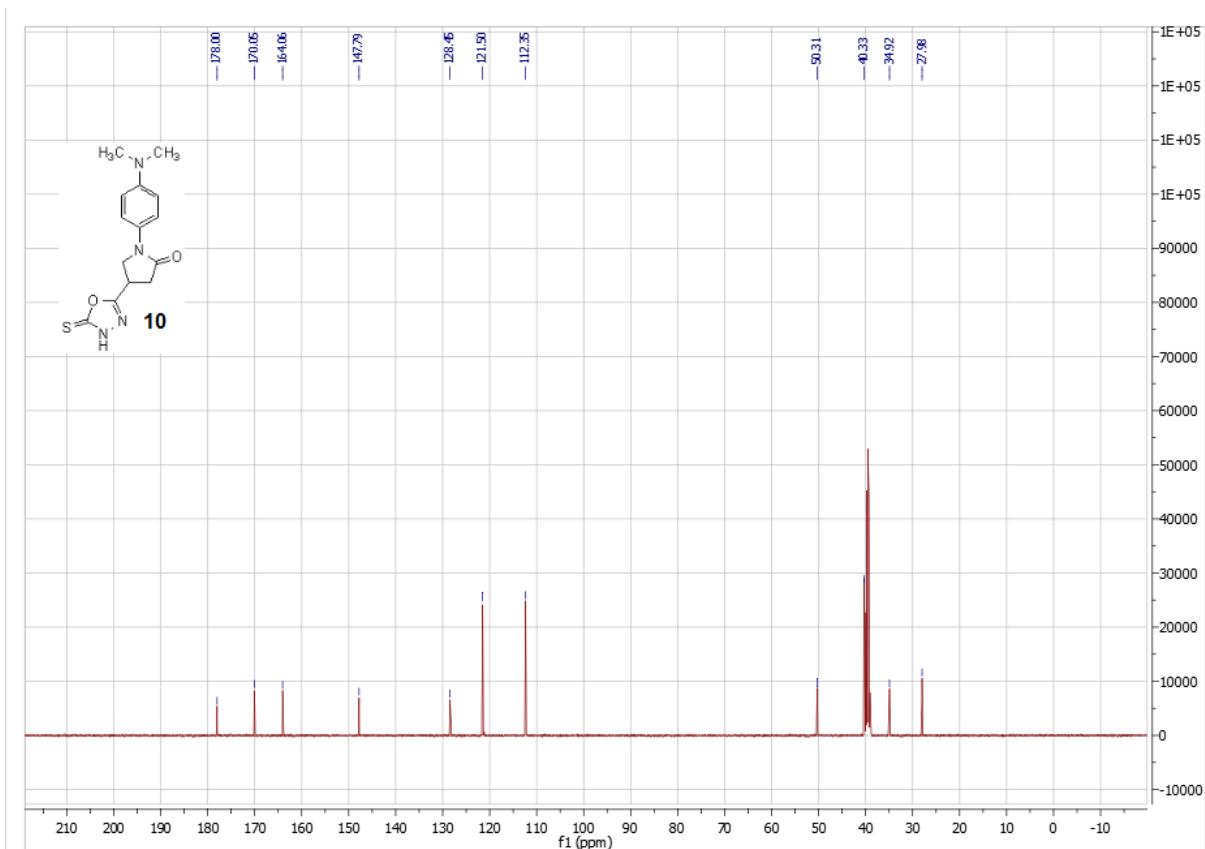


Figure S47. ¹³C NMR spectrum of compound 10.

1-(4-(Dimethylamino)phenyl)-4-(5,6-diphenyl-1,2,4-triazin-3-yl)pyrrolidin-2-one (11)

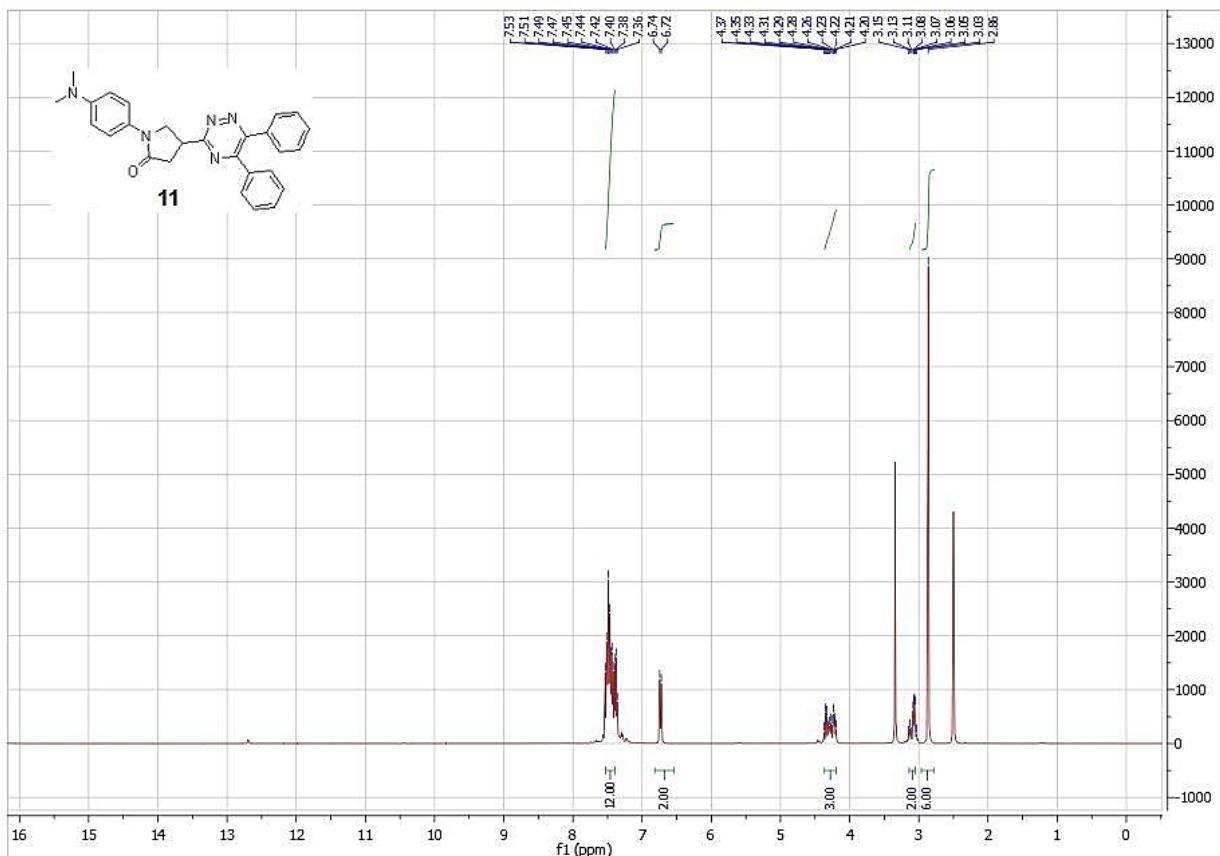


Figure S48. ^1H NMR spectrum of compound **11**.

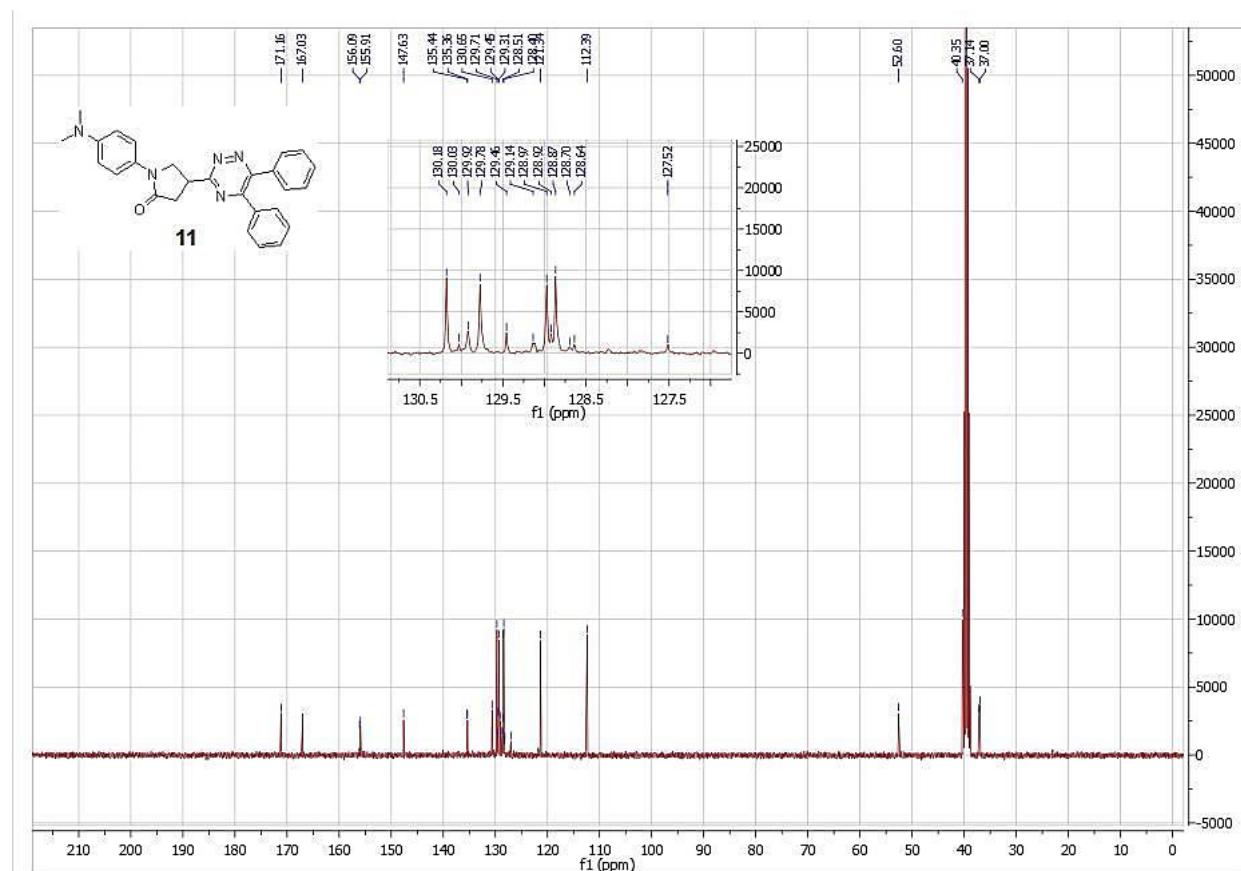


Figure S49. ^{13}C NMR spectrum of compound **11**.