

SUPPLEMENTARY MATERIALS

Features on the Way to the Synthesis of 1-Benzoyl-2-Phenyl-3a,6a-Diazapentalene And 1-Pivaloyl-2-Tert-Butyl-3a,6a-Diazapentalene

Nazym A. Alzhapparova^{1*} , Svetlana Yu. Panshina¹ , Marat K. Ibrayev¹ , Eugene V. Babaev² 

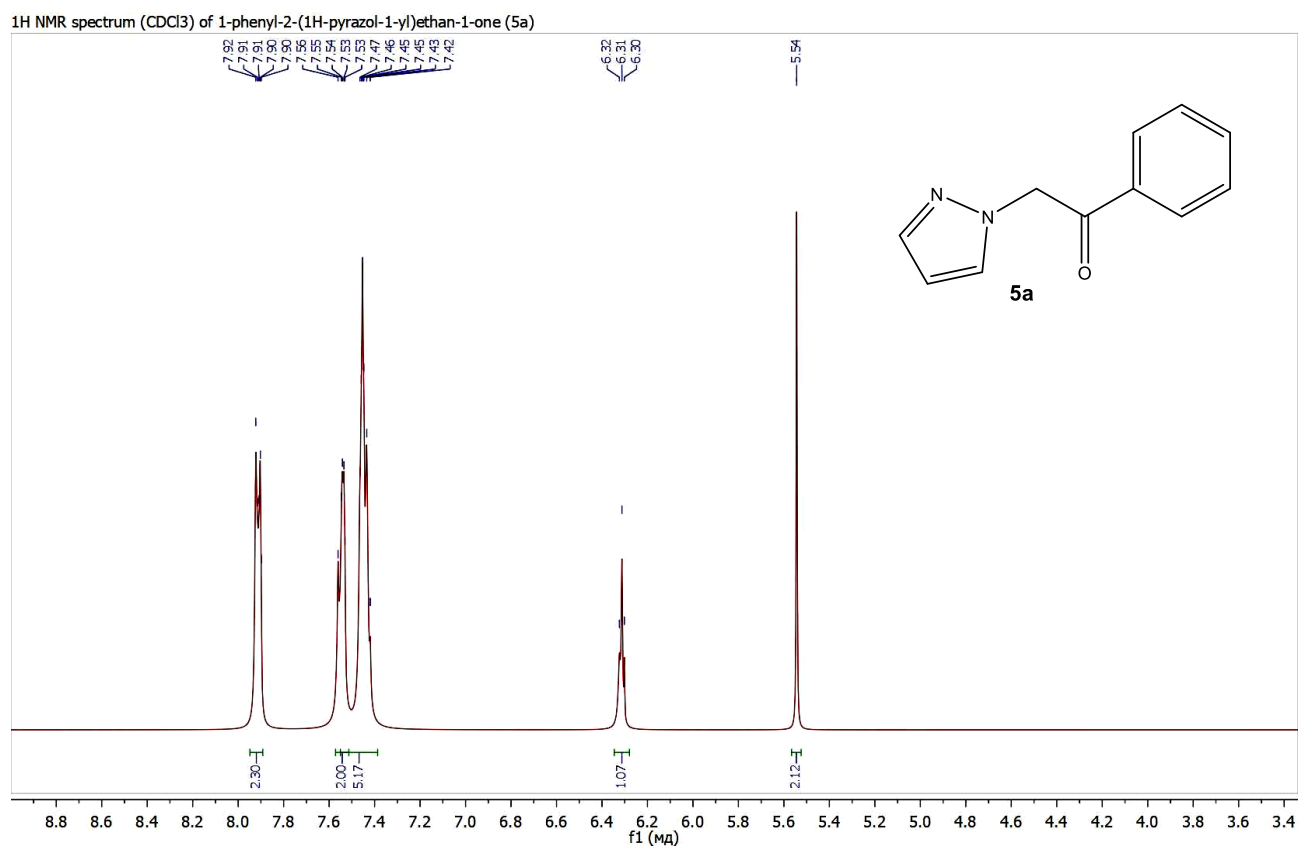
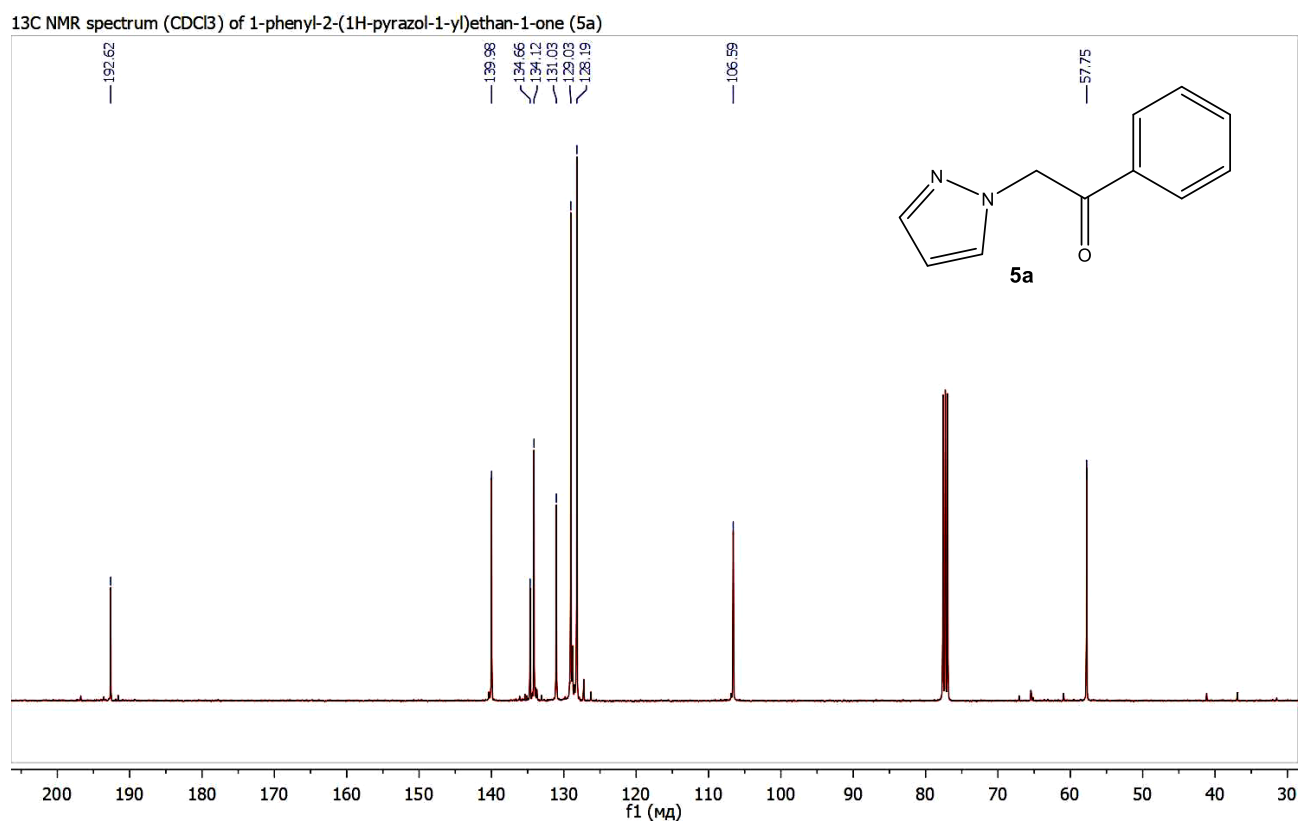
¹*Buketov Karaganda National Research University, Karaganda, Kazakhstan*

²*Lomonosov Moscow State University, Moscow, Russia*

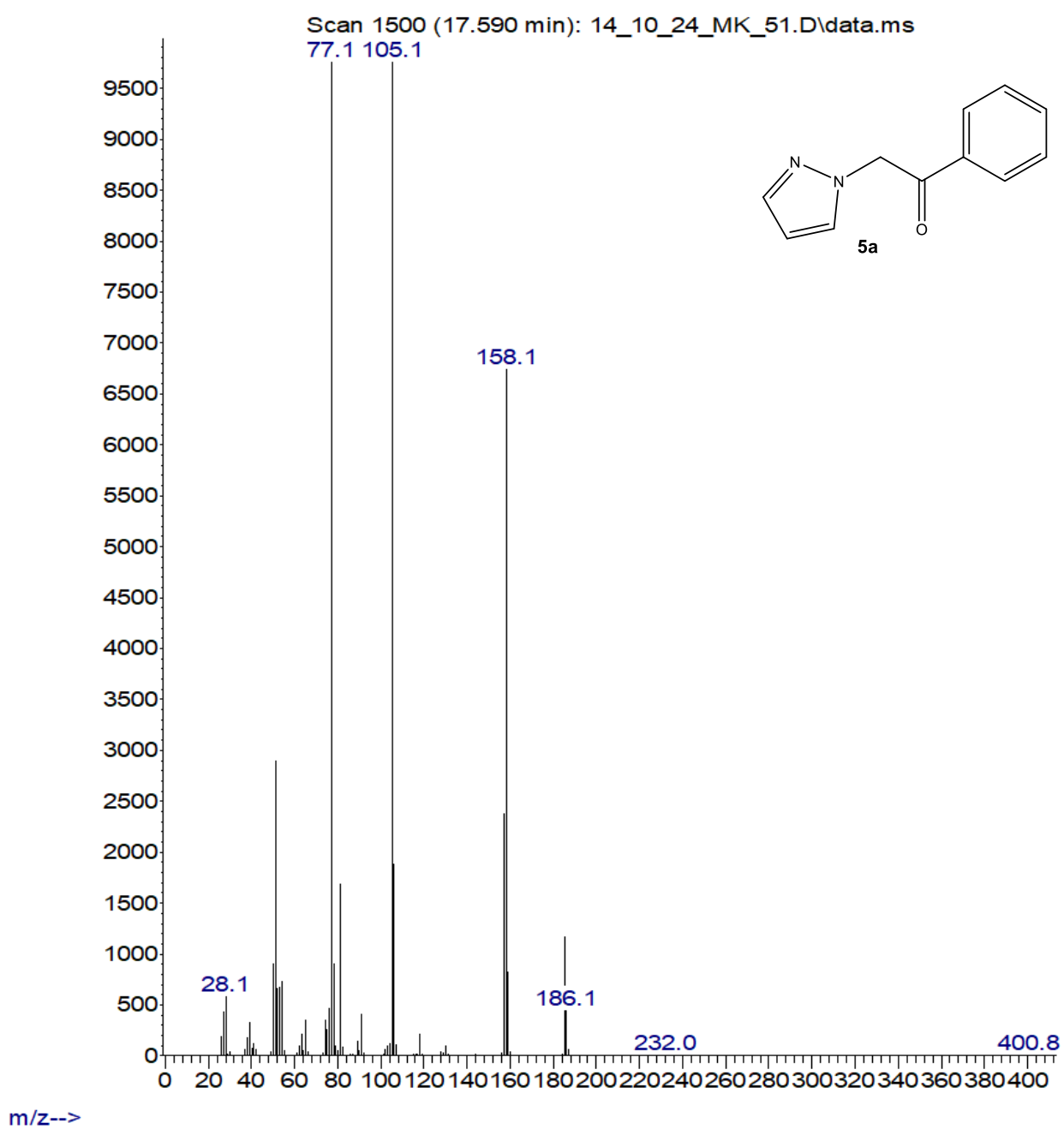
(*Corresponding author's e-mail: nazym285@mail.ru)

List of Content

¹ H NMR spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (5a) (Figure S1).	S2
¹³ C NMR spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (5a) (Figure S2).	S2
Mass spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (5a) (Figure S3)	S3
IR spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (5a) (Figure S4)	S4
¹ H NMR spectrum of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (6a) (Figure S5)	S5
¹³ C NMR spectrum of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (6a) (Figure S6)	S5
IR spectrum of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (6a) (Figure S7)	S6
¹ H NMR spectrum of 1-benzoyl-2-phenyl-3a,6a-diazapentalene (8a) (Figure S8)	S7
¹³ C NMR spectrum of 1-benzoyl-2-phenyl-3a,6a-diazapentalene (8a) (Figure S9)	S7
¹ H NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (5b) (Figure S10)	S8
¹³ C NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (5b) (Figure S11)	S8
Mass spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (5b) (Figure S12)	S9
IR spectrum of 1-(1H-pyrazol-1-yl)-3,3-dimethylbutan-2-one (5b) (Figure S13)	S10
¹ H NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (6b) (Figure S14)	S11
¹³ C NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (6b) (Figure S15)	S11
IR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (6b) (Figure S16)	S12
¹ H NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b) (Figure S17)	S13
¹³ C NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b) (Figure S18)	S13
¹ H – ¹ H COSY NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b) (Figure S19)	S14
¹ H – ¹³ C HMBC NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b) (Figure S20)	S14
¹ H – ¹³ C HSQC NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b) (Figure S21)	S15

Figure S1. ¹H NMR spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (5a)Figure S2. ¹³C NMR spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (5a)

Abundance



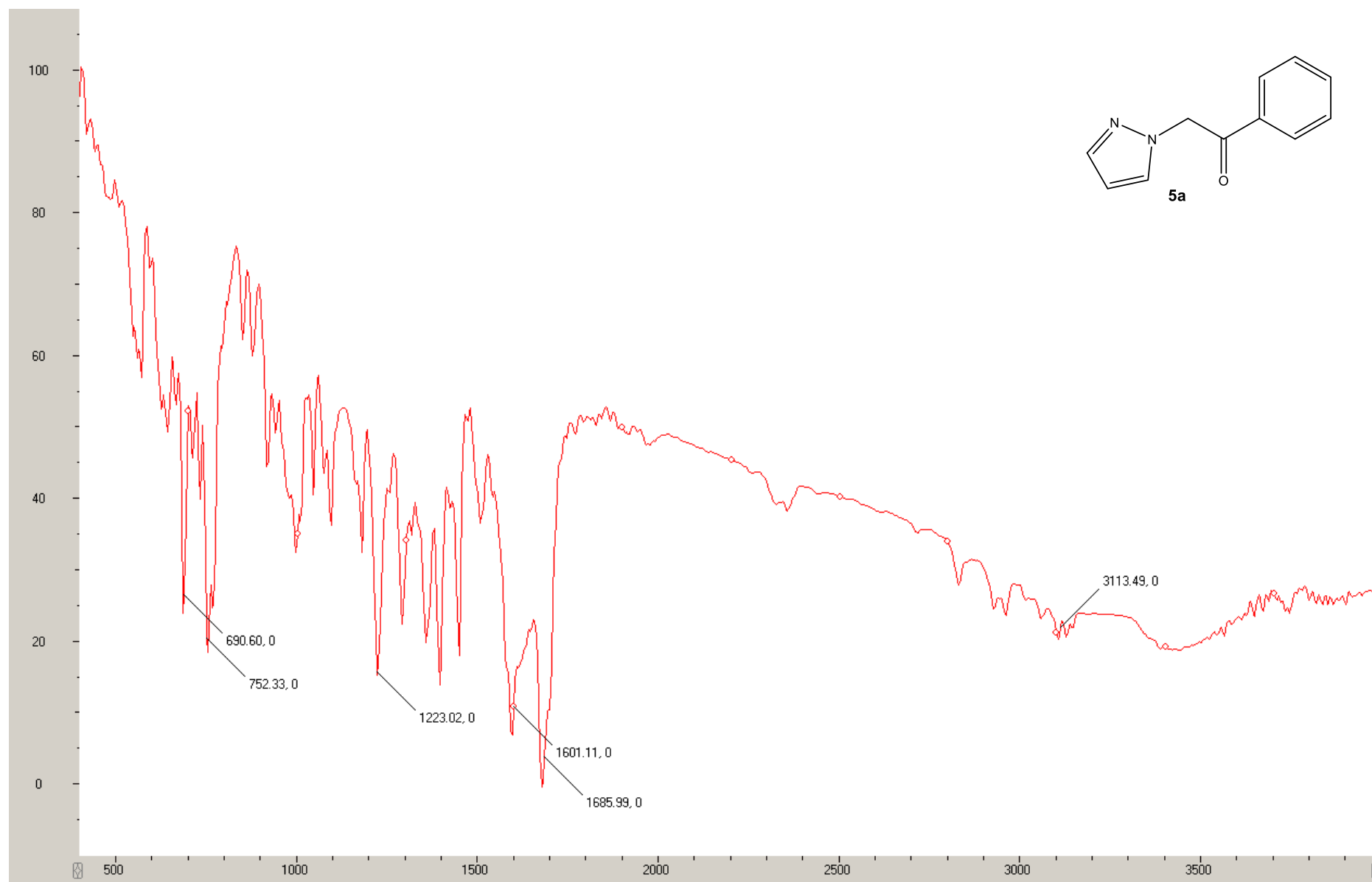


Figure S4. IR spectrum of 1-phenyl-2-(1H-pyrazol-1-yl)ethan-1-one (**5a**)

¹H NMR spectrum (DMSO-d₆) of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (**6a**)

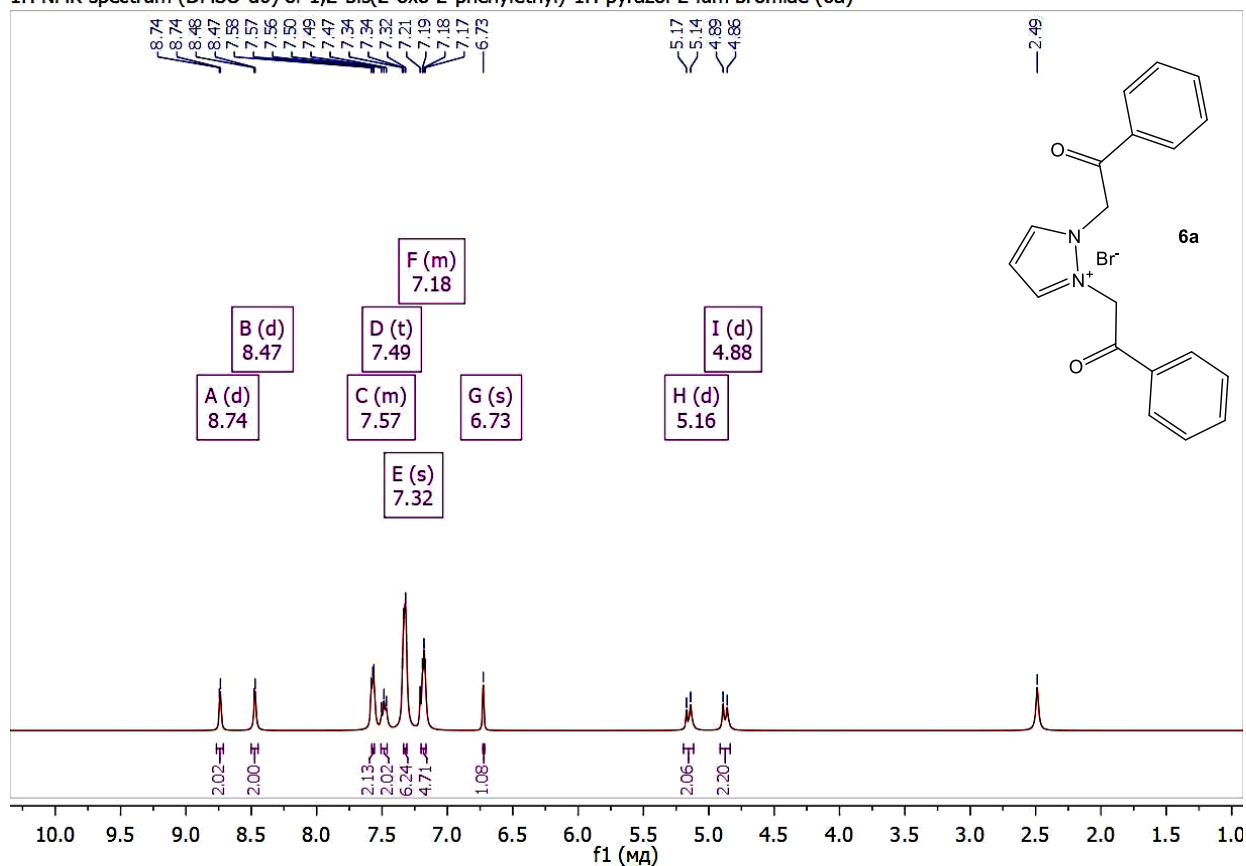


Figure S5. ¹H NMR spectrum of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (**6a**)

¹³C NMR spectrum (D₂O) of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (**6a**)

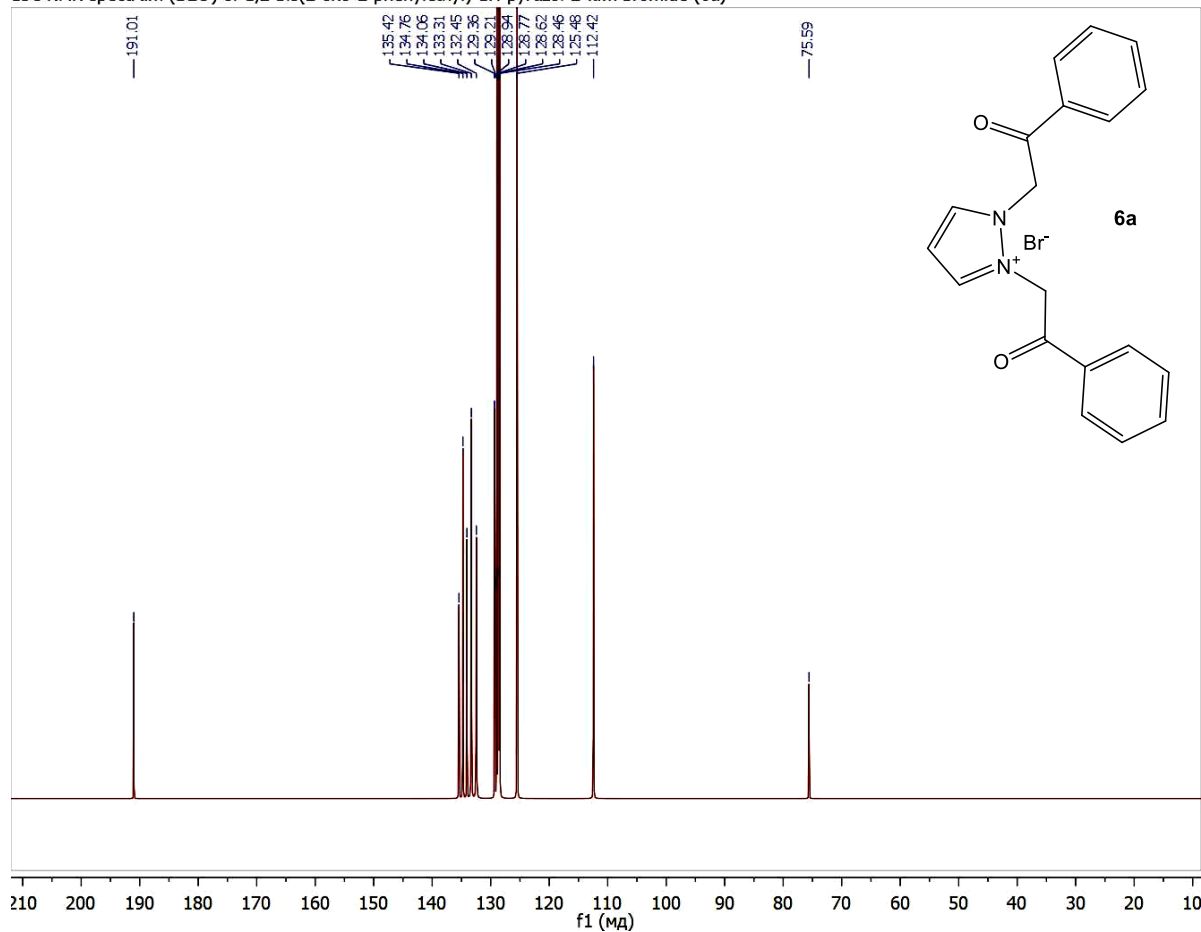


Figure S6. ¹³C NMR spectrum of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (**6a**)

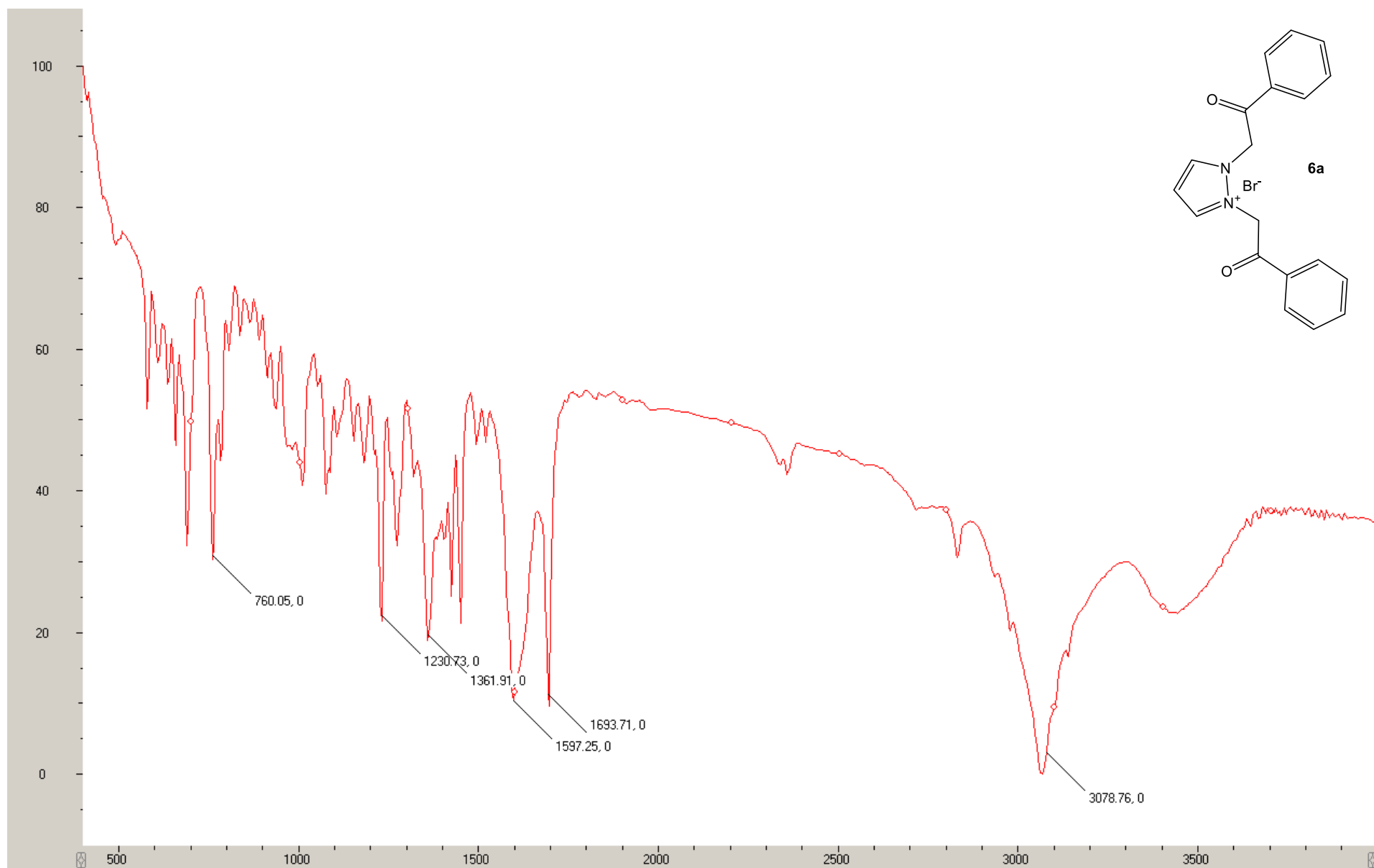


Figure S7. IR spectrum of 1,2-bis(2-oxo-2-phenylethyl)-1H-pyrazol-2-ium bromide (**6a**)

¹H NMR spectrum (DMSO-d₆) of 1-benzoyl-2-phenyl-3a,6a-diazapentalene (8a)

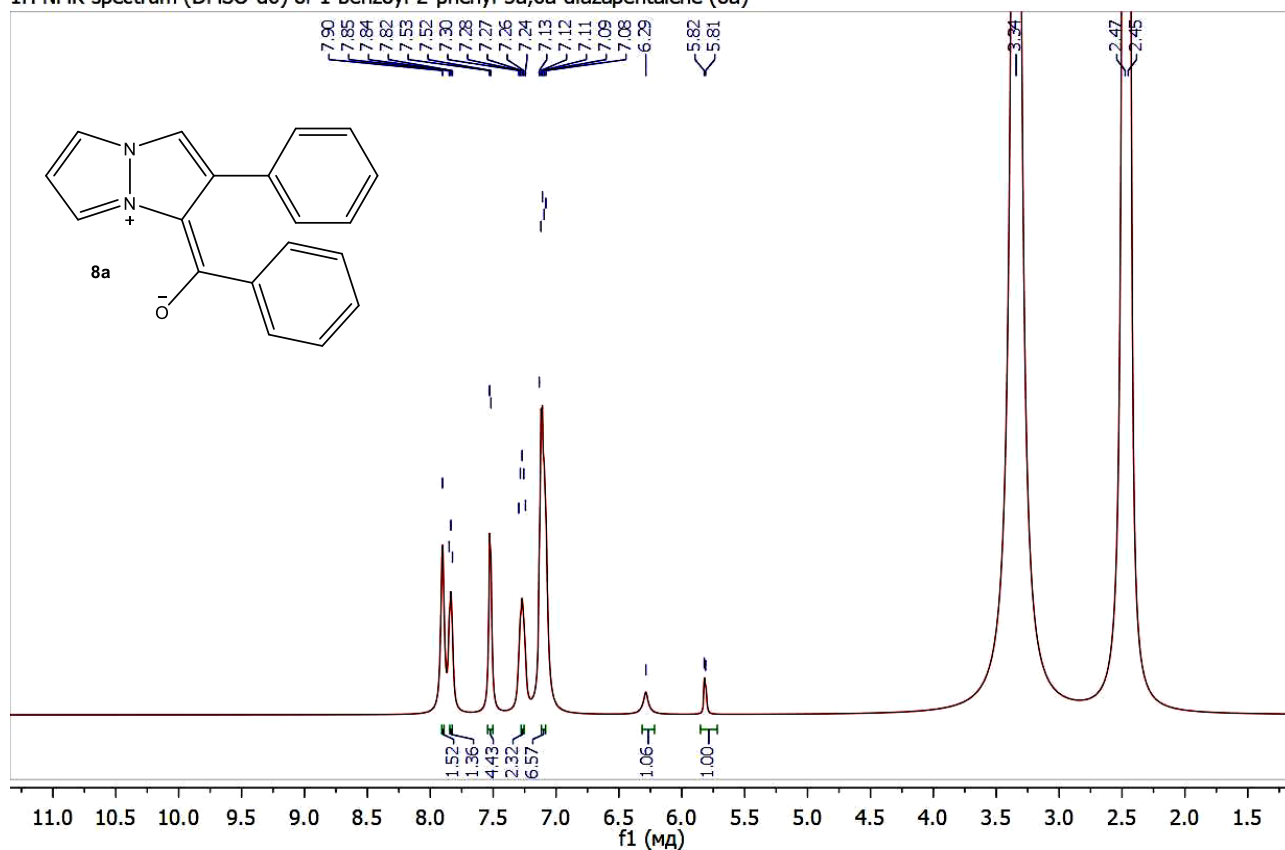


Figure S8. ¹H NMR spectrum of 1-benzoyl-2-phenyl-3a,6a-diazapentalene (8a)

¹³C NMR spectrum (DMSO-d₆) of 1-benzoyl-2-phenyl-3a,6a-diazapentalene (8a)

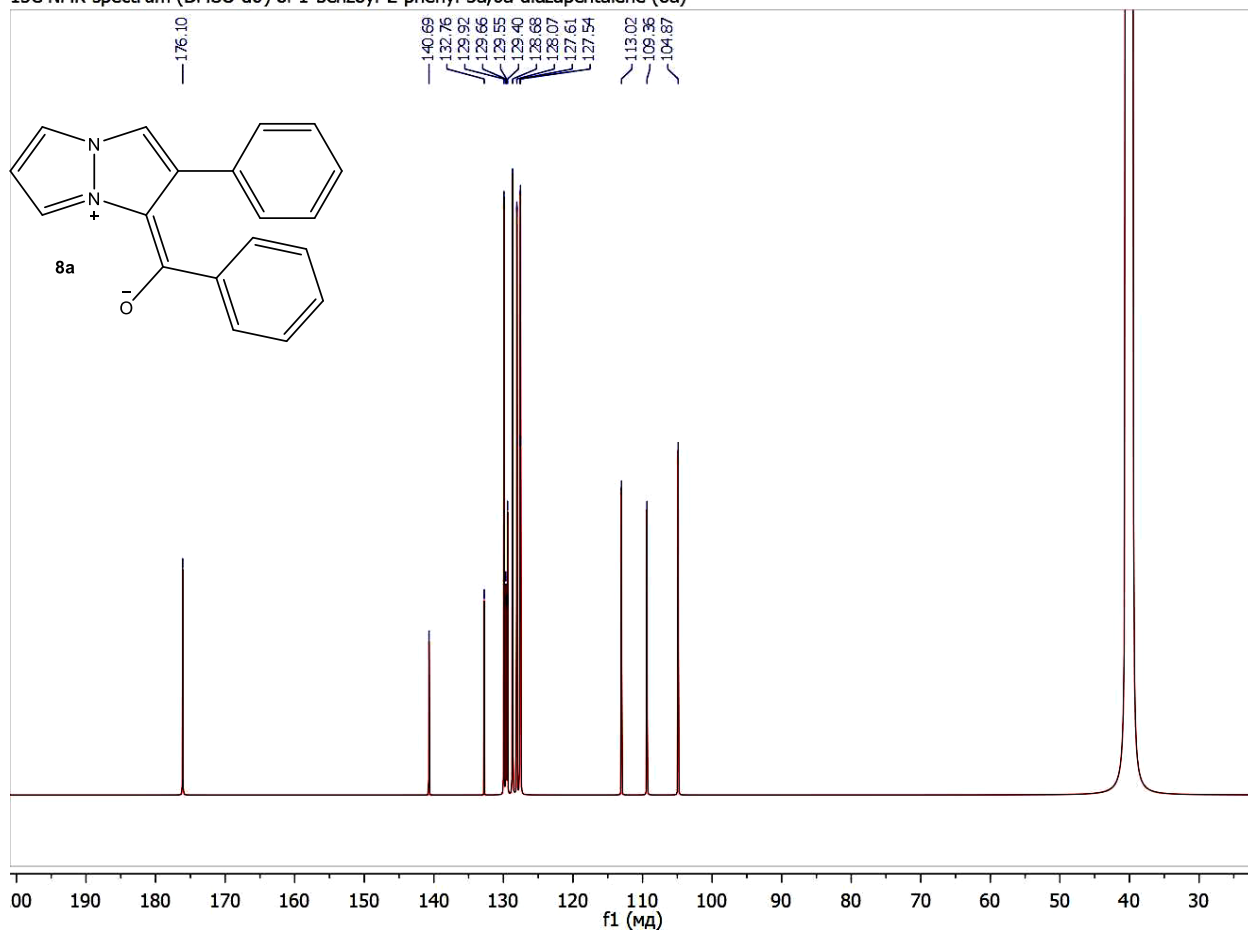


Figure S9. ¹³C NMR spectrum of 1-benzoyl-2-phenyl-3a,6a-diazapentalene (8a)

¹H NMR spectrum (CDCl₃) of 1-(1H-pyrazol-1-yl)-3,3-dimethylbutan-2-one (5b)

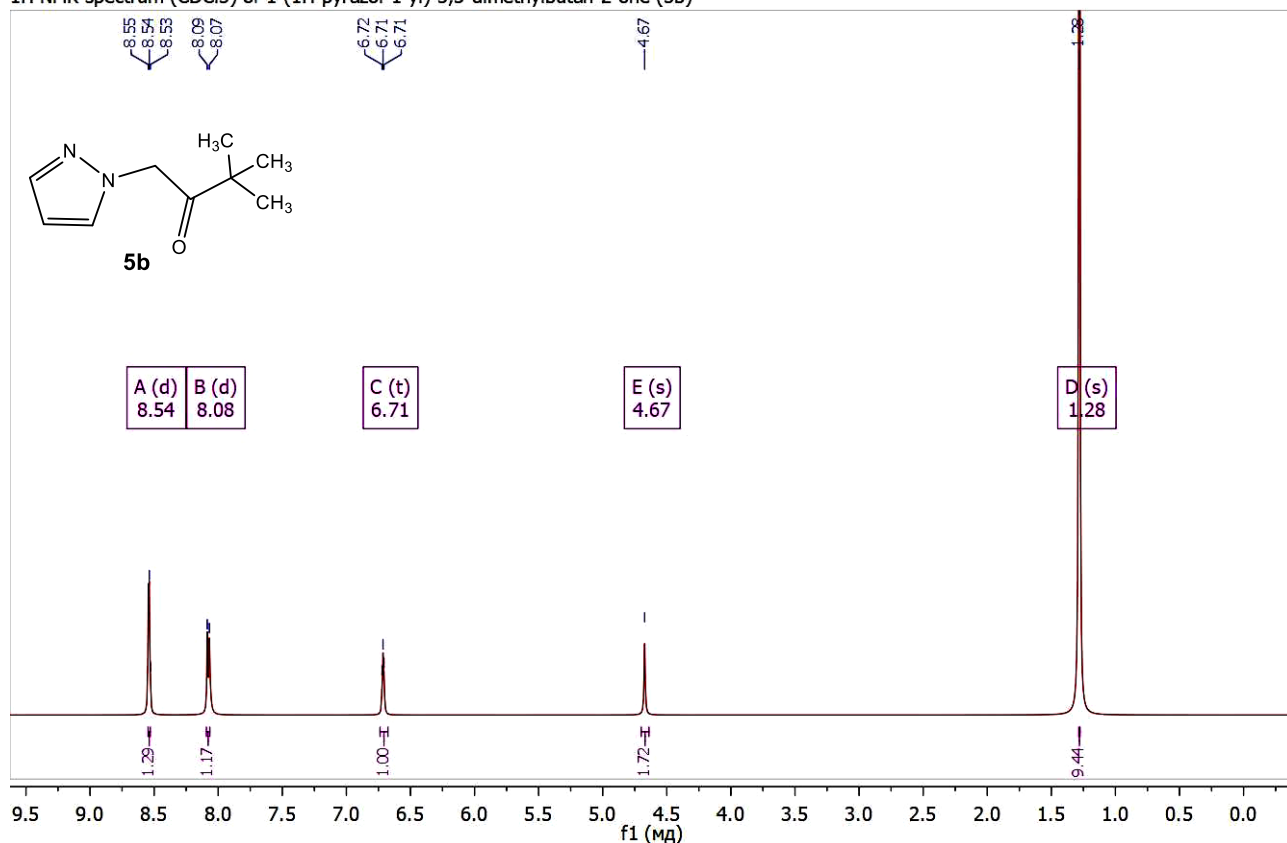


Figure S10. ¹H NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (5b)

¹³C NMR spectrum (CDCl₃) 1-(1H-pyrazol-1-yl)-3,3-dimethylbutan-2-one (5b)

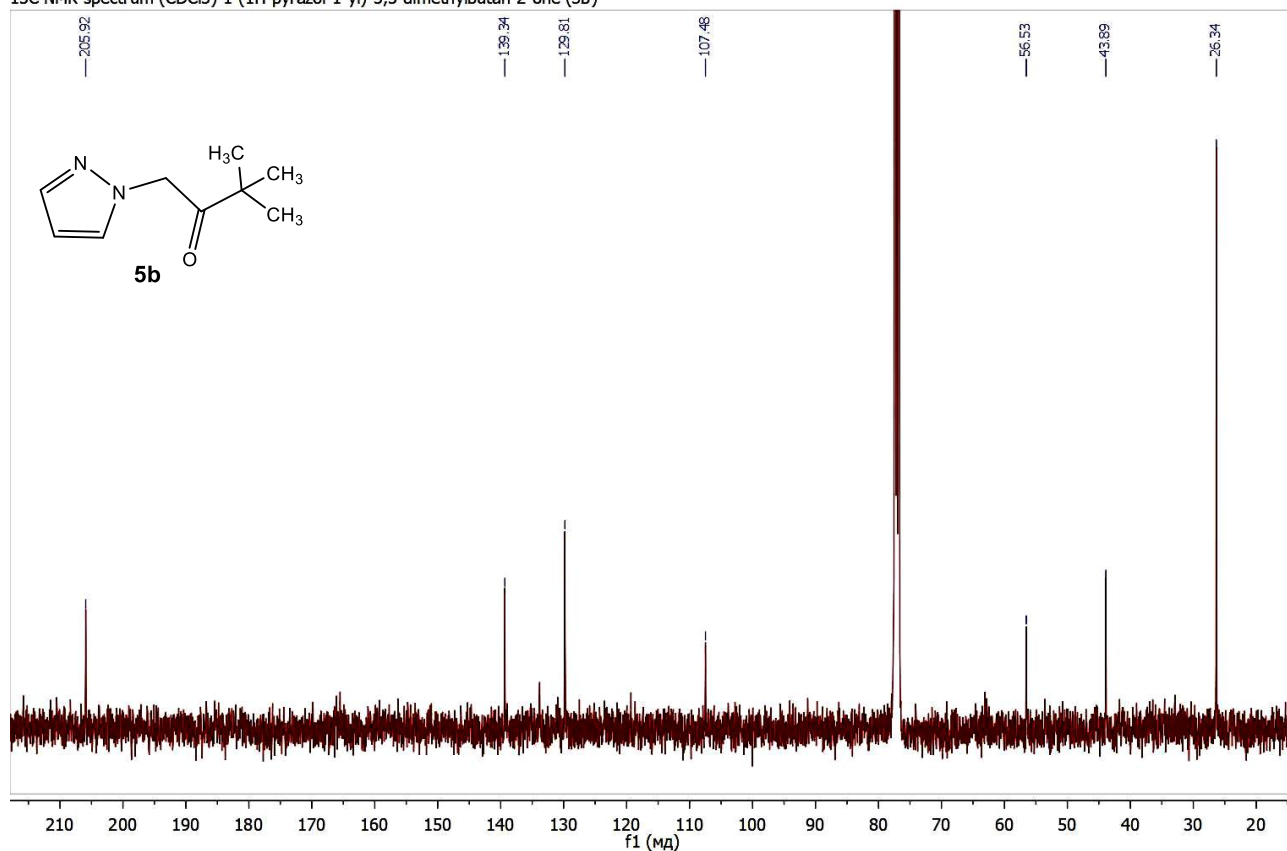
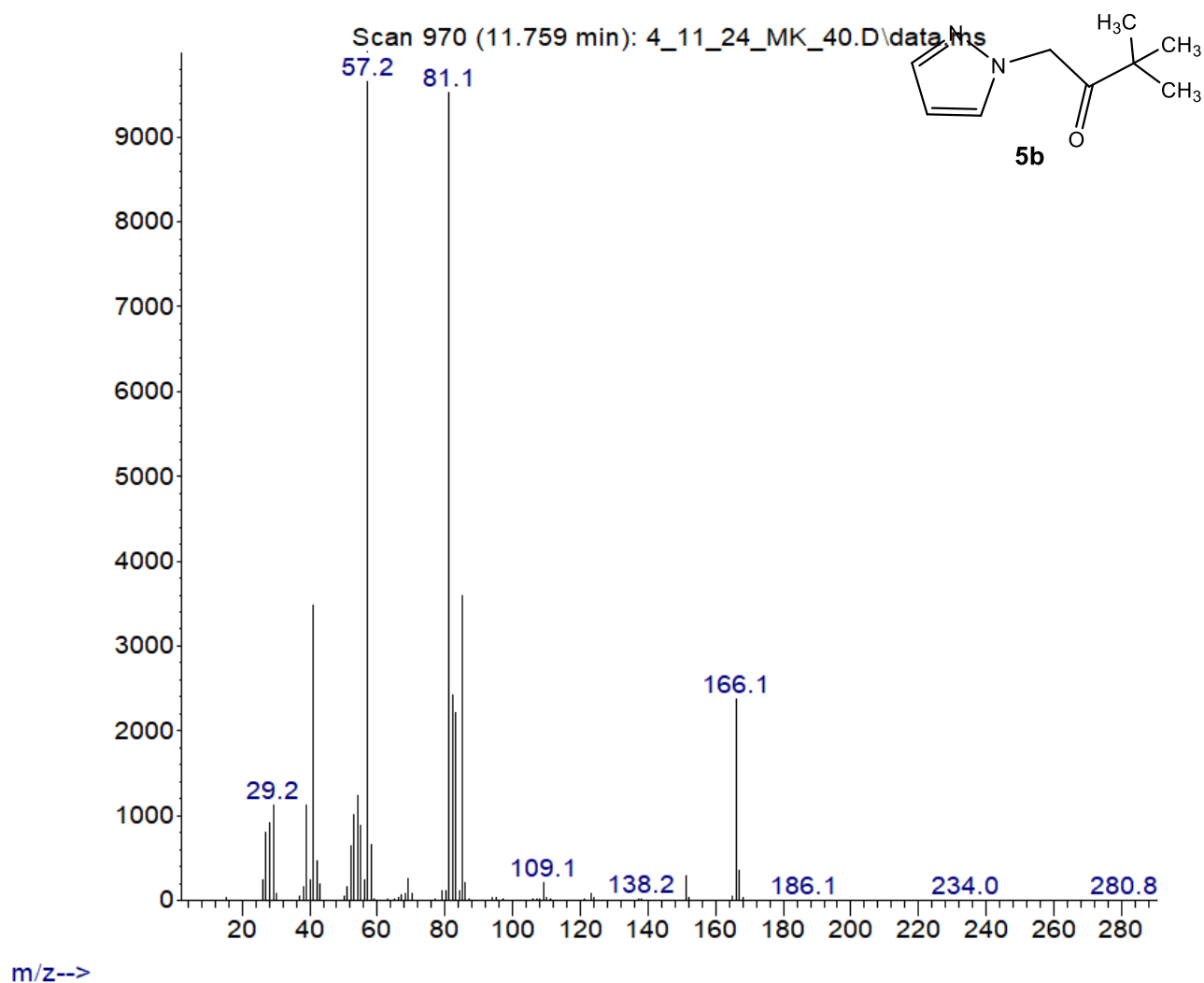
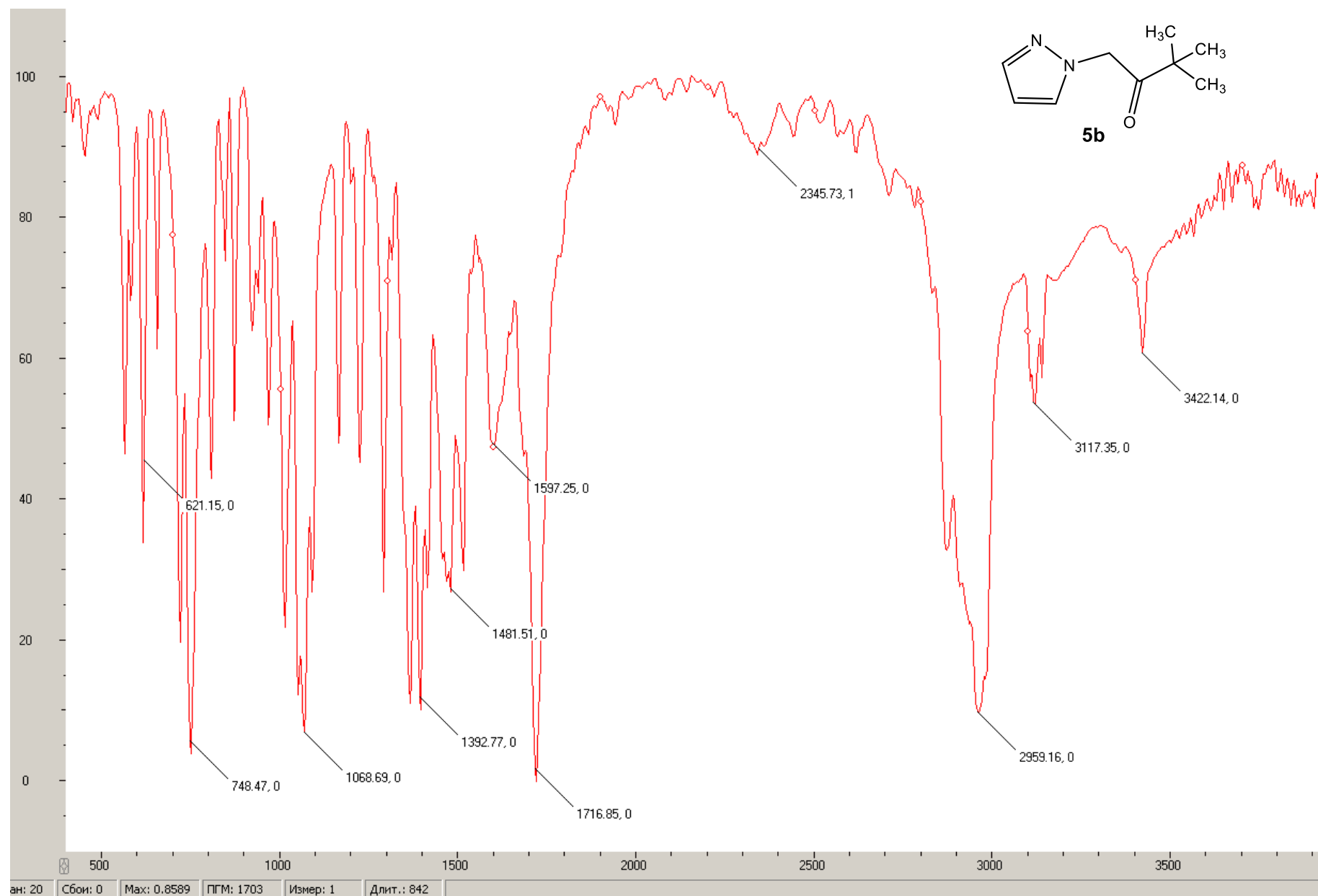
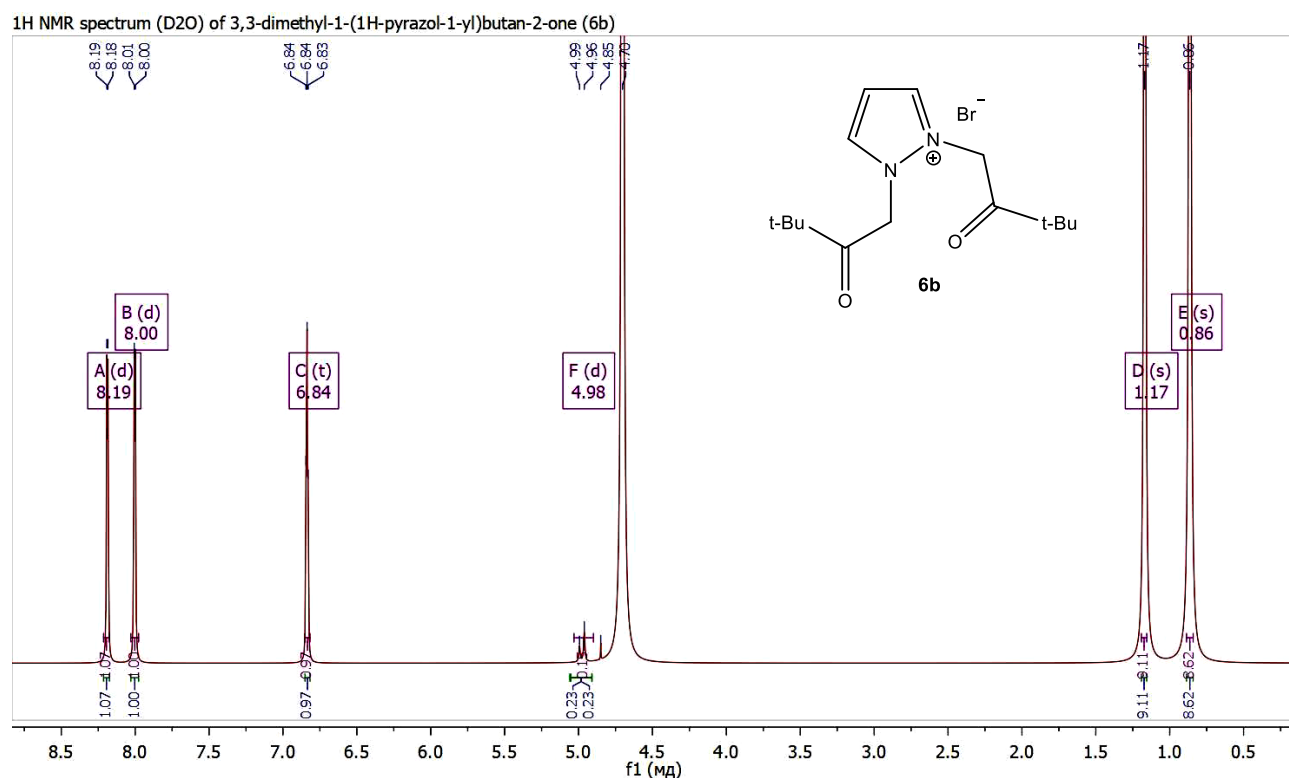
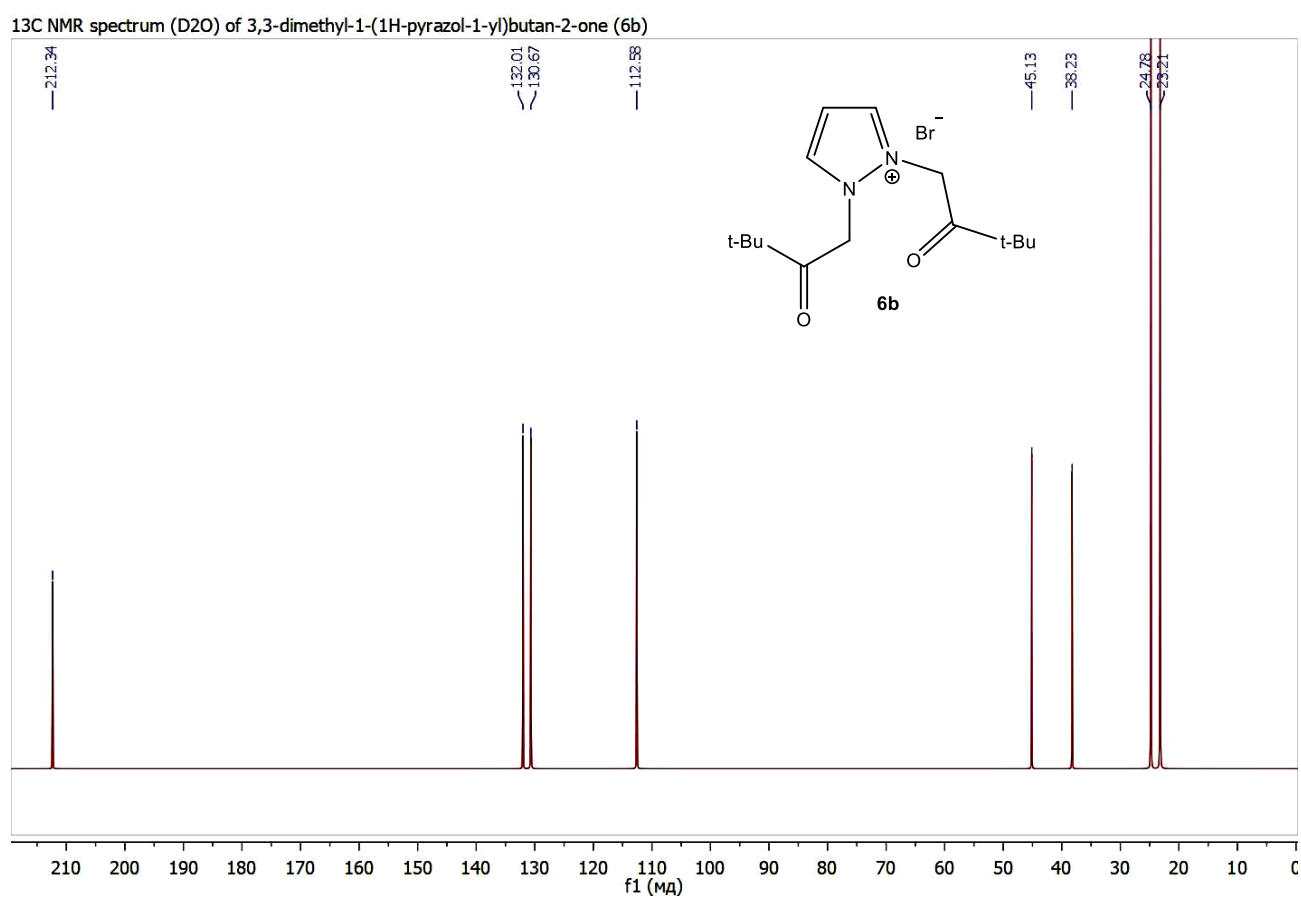


Figure S11. ¹³C NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (5b)

Abundance

Figure S12. Mass spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (**5b**)

Figure S13. IR spectrum of 1-(1H-pyrazol-1-yl)-3,3-dimethylbutan-2-one (**5b**)

Figure S14. ¹H NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (**6b**)Figure S15. ¹³C NMR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (**6b**)

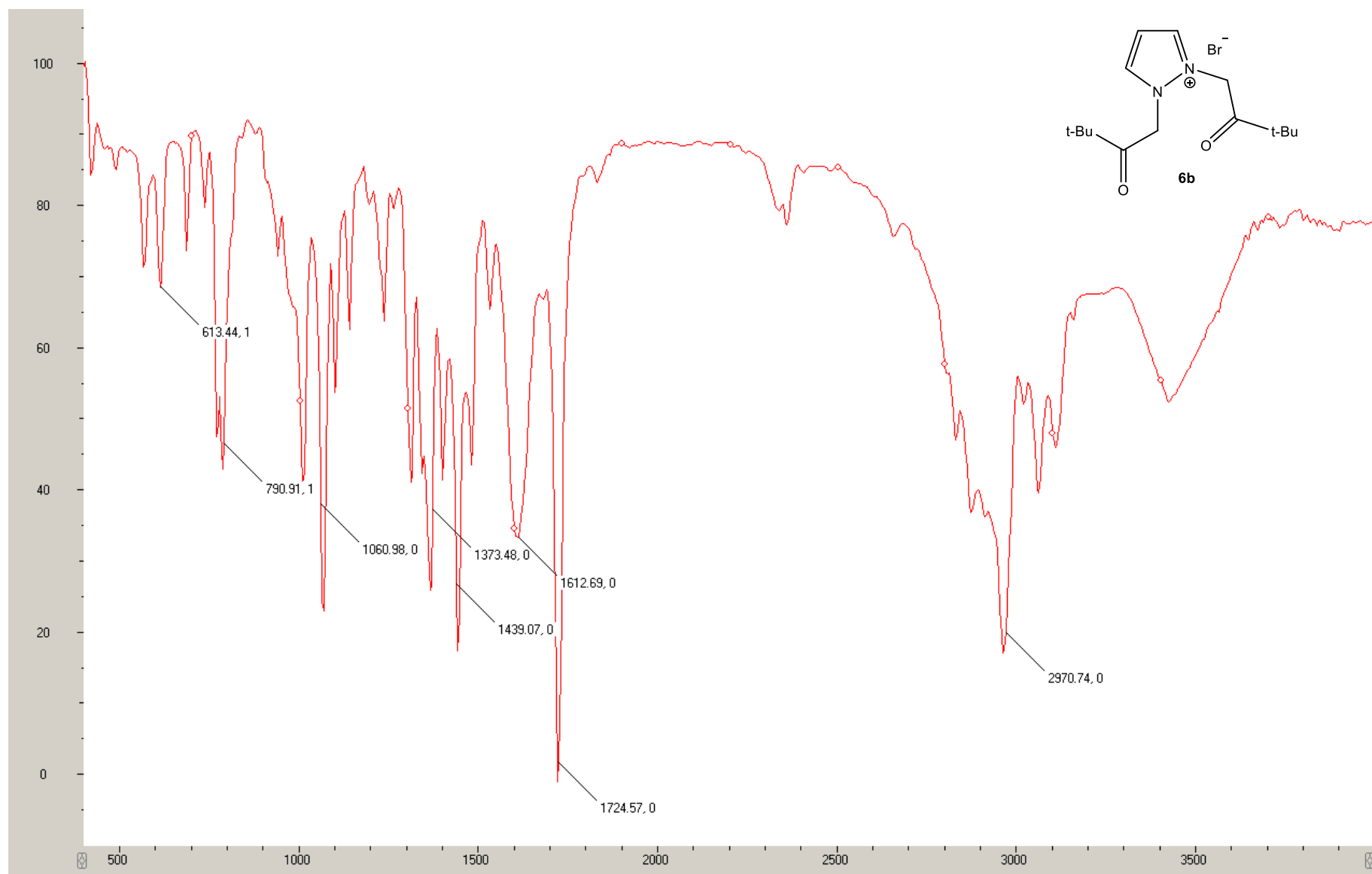


Figure S16. IR spectrum of 3,3-dimethyl-1-(1H-pyrazol-1-yl)butan-2-one (**6b**)

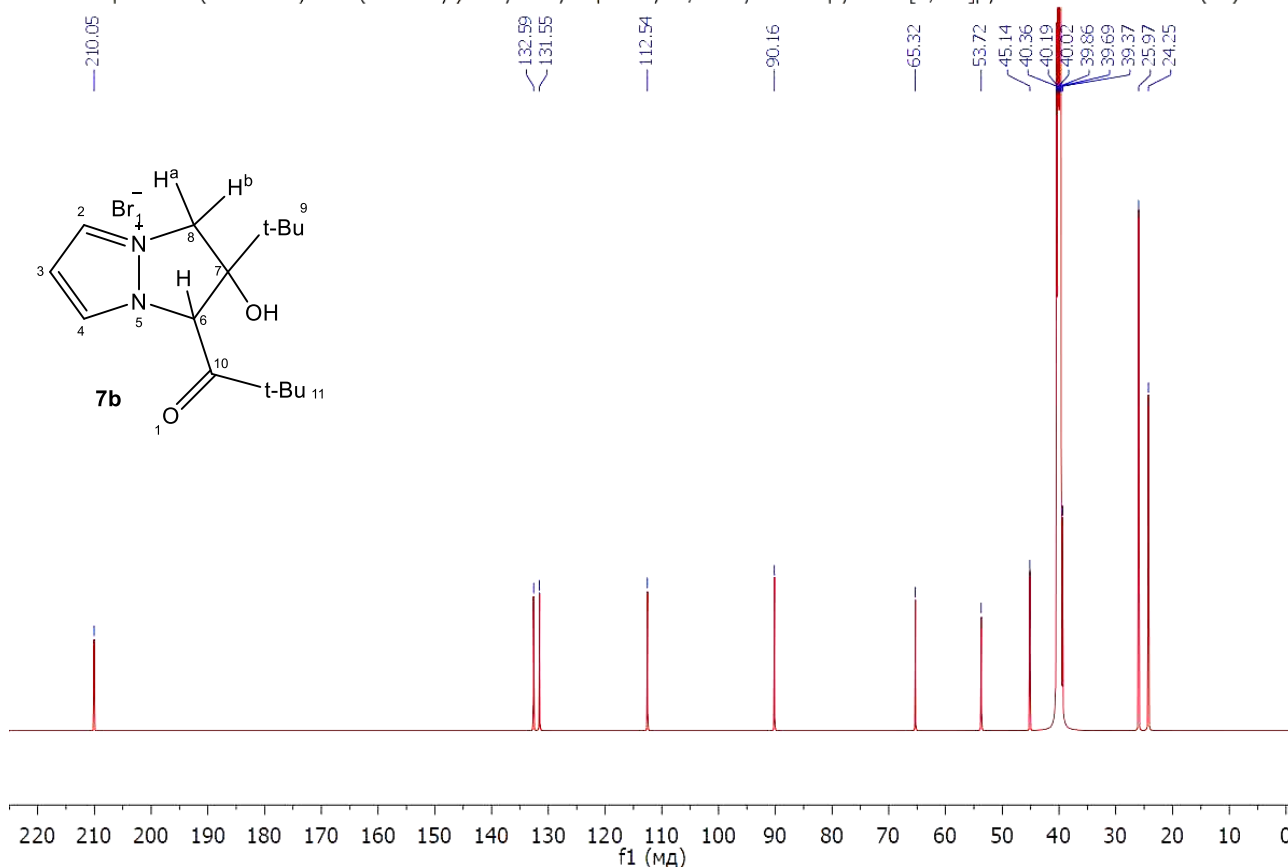
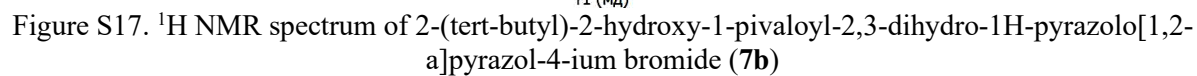


Figure S18. ¹³C NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (**7b**)

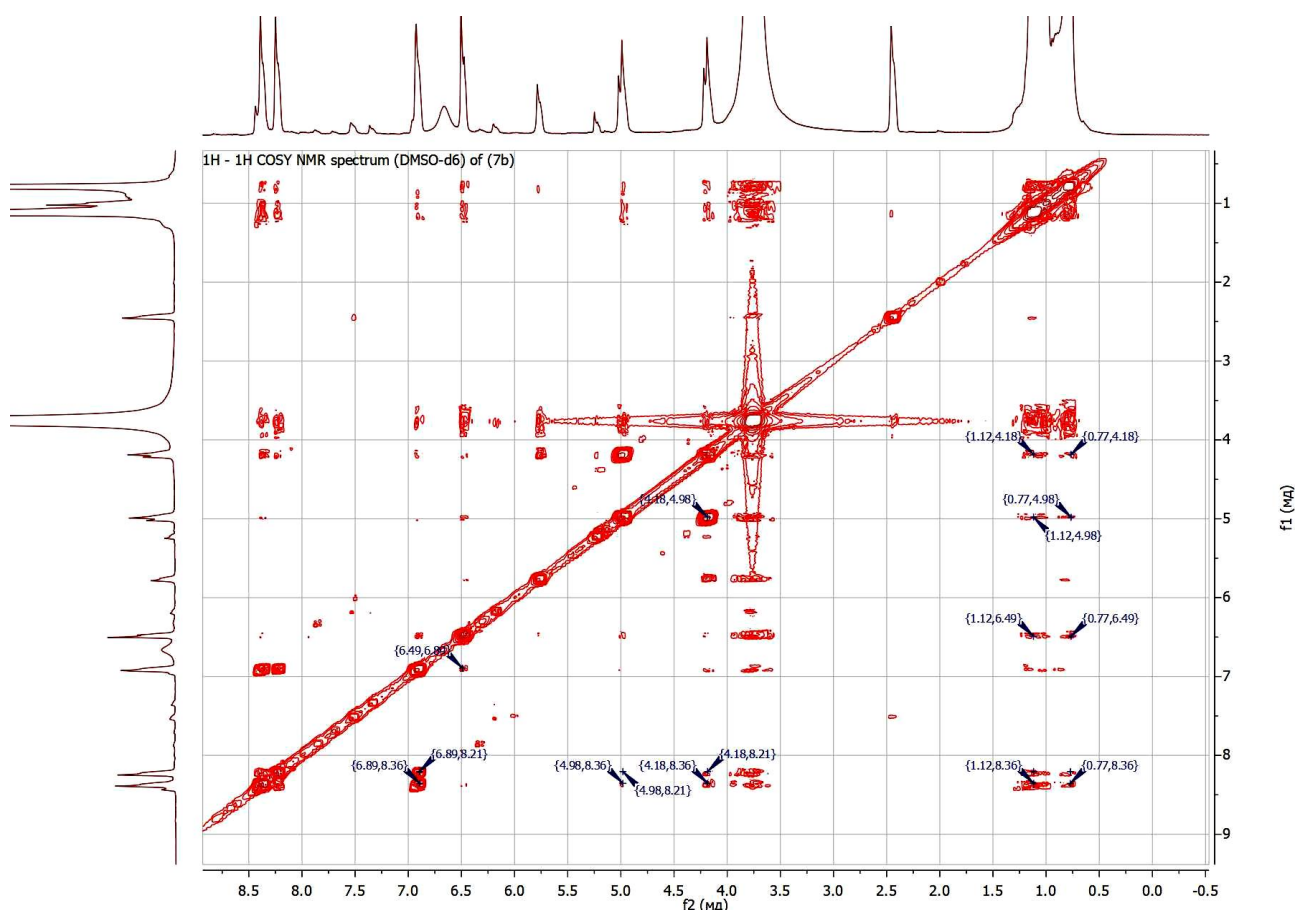


Figure S19. ¹H – ¹H COSY NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b)

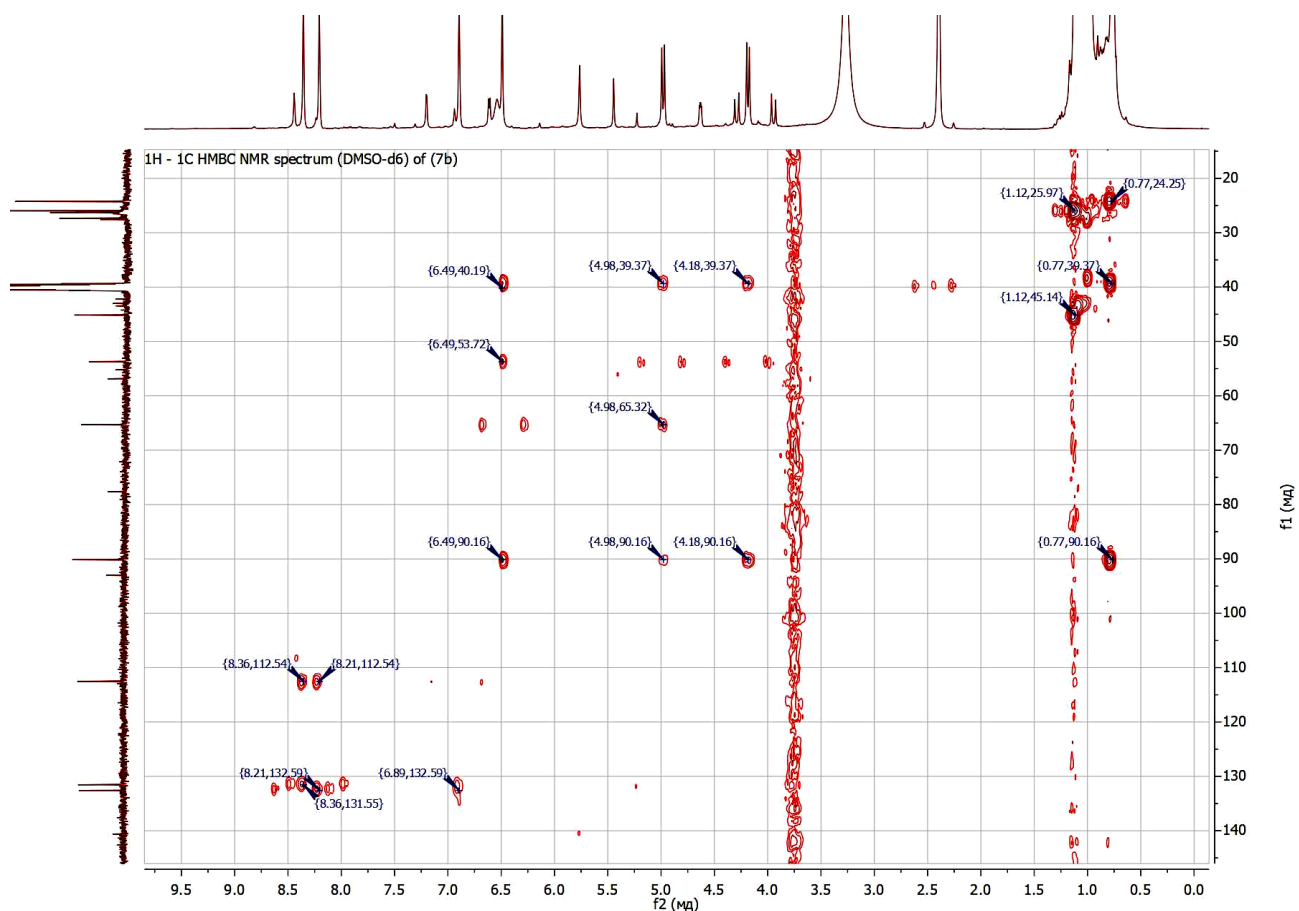


Figure S20. ¹H – ¹³C HMBC NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (7b)

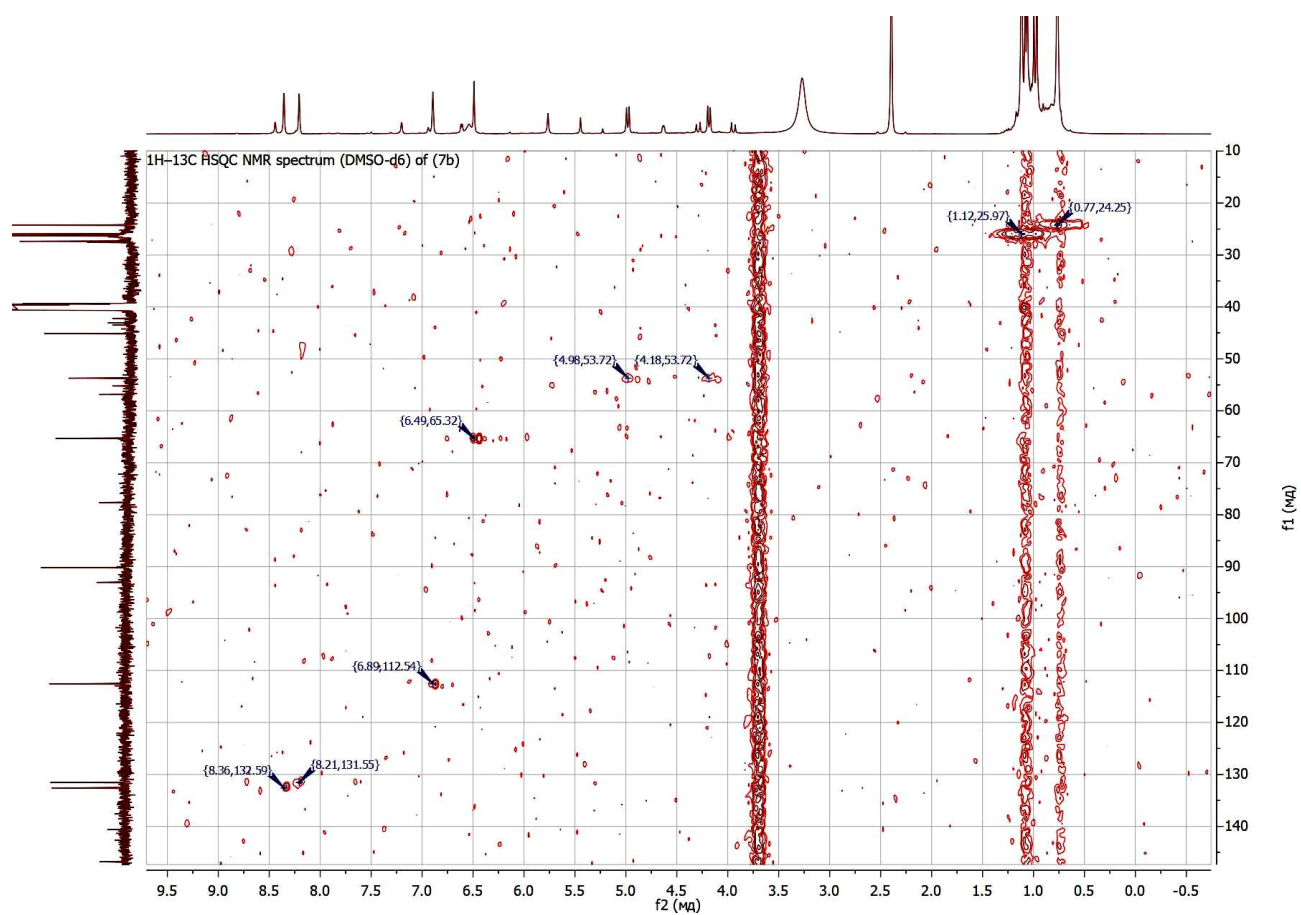


Figure S21. ¹H -¹³C HSQC NMR spectrum of 2-(tert-butyl)-2-hydroxy-1-pivaloyl-2,3-dihydro-1H-pyrazolo[1,2-a]pyrazol-4-ium bromide (**7b**)