

4,4-Difluoro-3-(3-phenyl-5-oxazolyl)-8-trifluoromethyl-5-(2-naphthyl)-4-bora-3a,4a-diaza-s-indacene

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¹H NMR spectrum of compound **1**

¹³C NMR spectrum of compound **1**

¹⁹F NMR spectrum of compound **1**

¹¹B NMR spectrum of compound **1**

2D ¹H-¹⁵N HMBC spectrum of of compound **1**

2D COSY spectrum of of compound **1**

2D NOESY spectrum of of compound **1**

2D ¹H-¹³C HMBC spectrum of of compound **1**

2D ¹H-¹³C HSQC spectrum of of compound **1**

IR spectrum of compound **1**

Normalized absorption and fluorescence spectra of compound **1**

¹H NMR spectrum of compound **4**

¹³C NMR spectrum of compound **4**

¹⁹F NMR spectrum of compound **4**

IR spectrum of compound **4**

¹H NMR spectrum of compound **2**

¹³C NMR spectrum of compound **2**

¹⁹F NMR spectrum of compound **2**

2D ¹H-¹⁵N HMBC spectrum of compound **2**

2D COSY spectrum of compound **2**

2D NOESY spectrum of compound **2**

IR spectrum of compound **2**

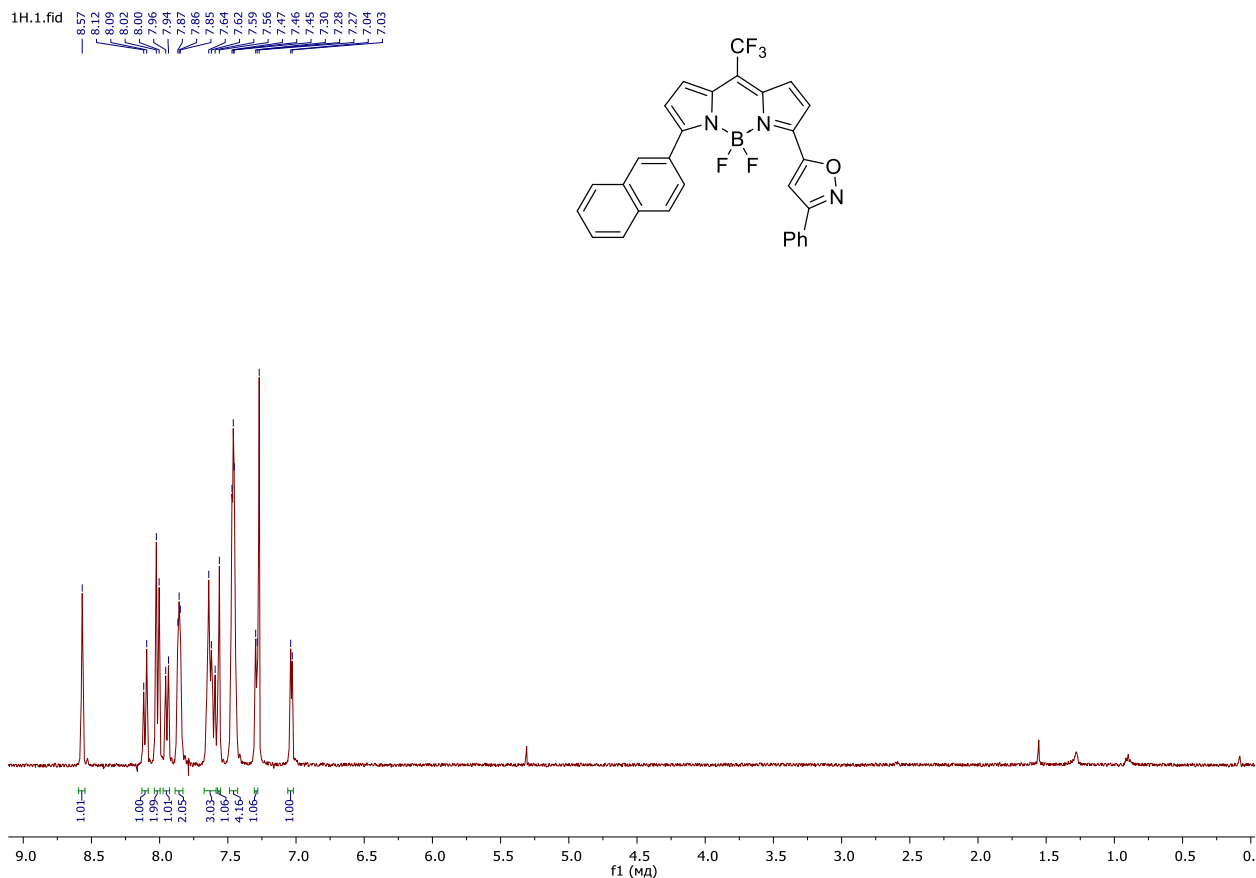


Figure S1. ¹H NMR spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalene-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) in CDCl₃.

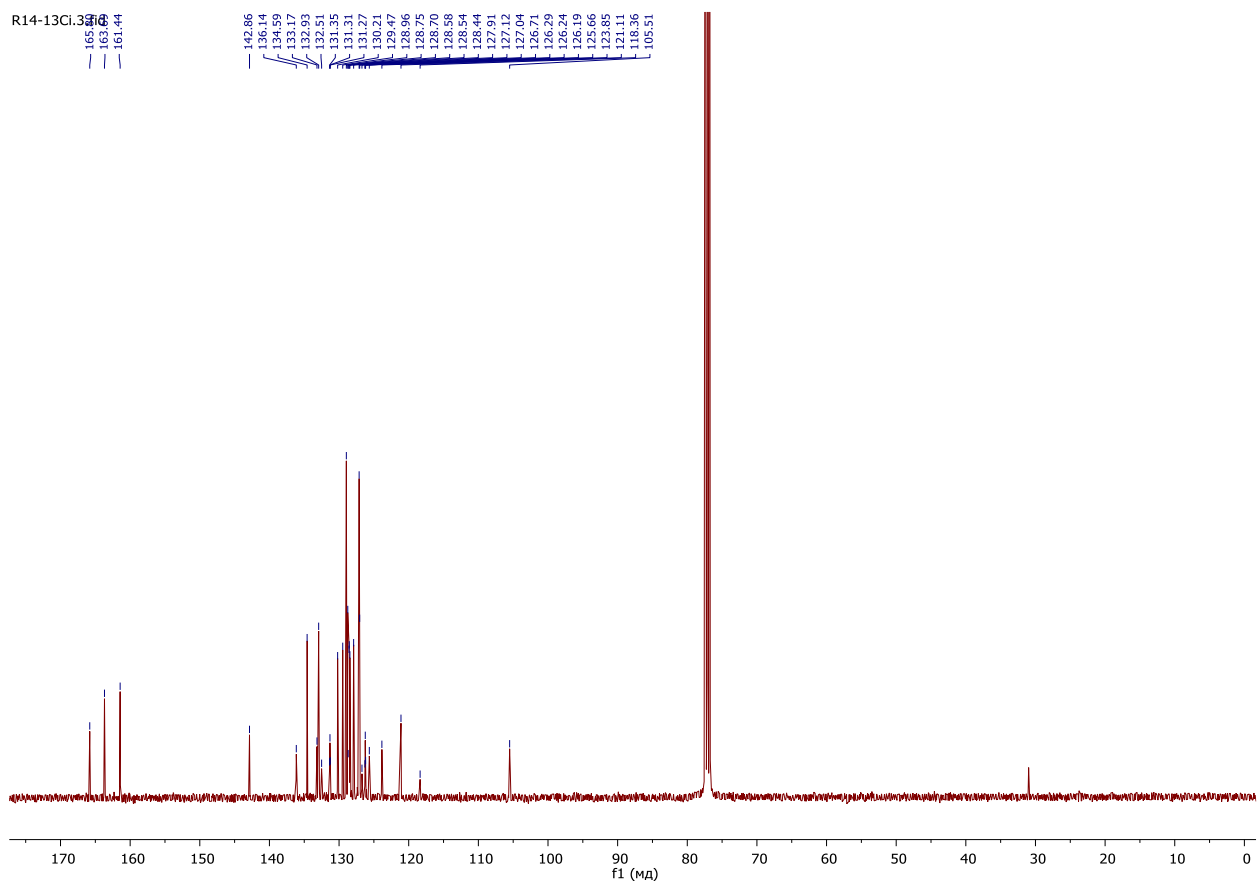


Figure S2. ¹³C NMR spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) in CDCl₃.

19F.3.fid
F19

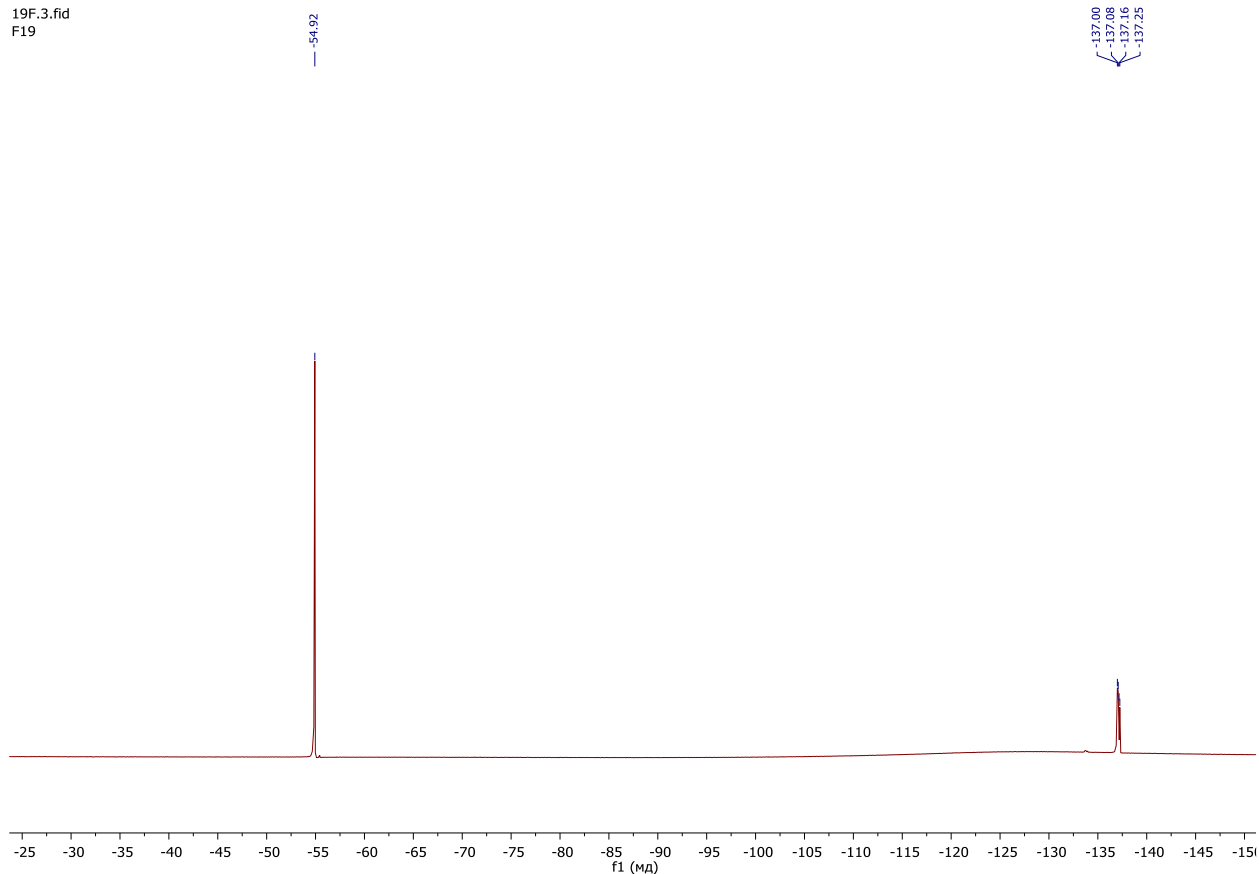


Figure S3. ^{19}F NMR spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) in CDCl_3 .

13c.1.fid

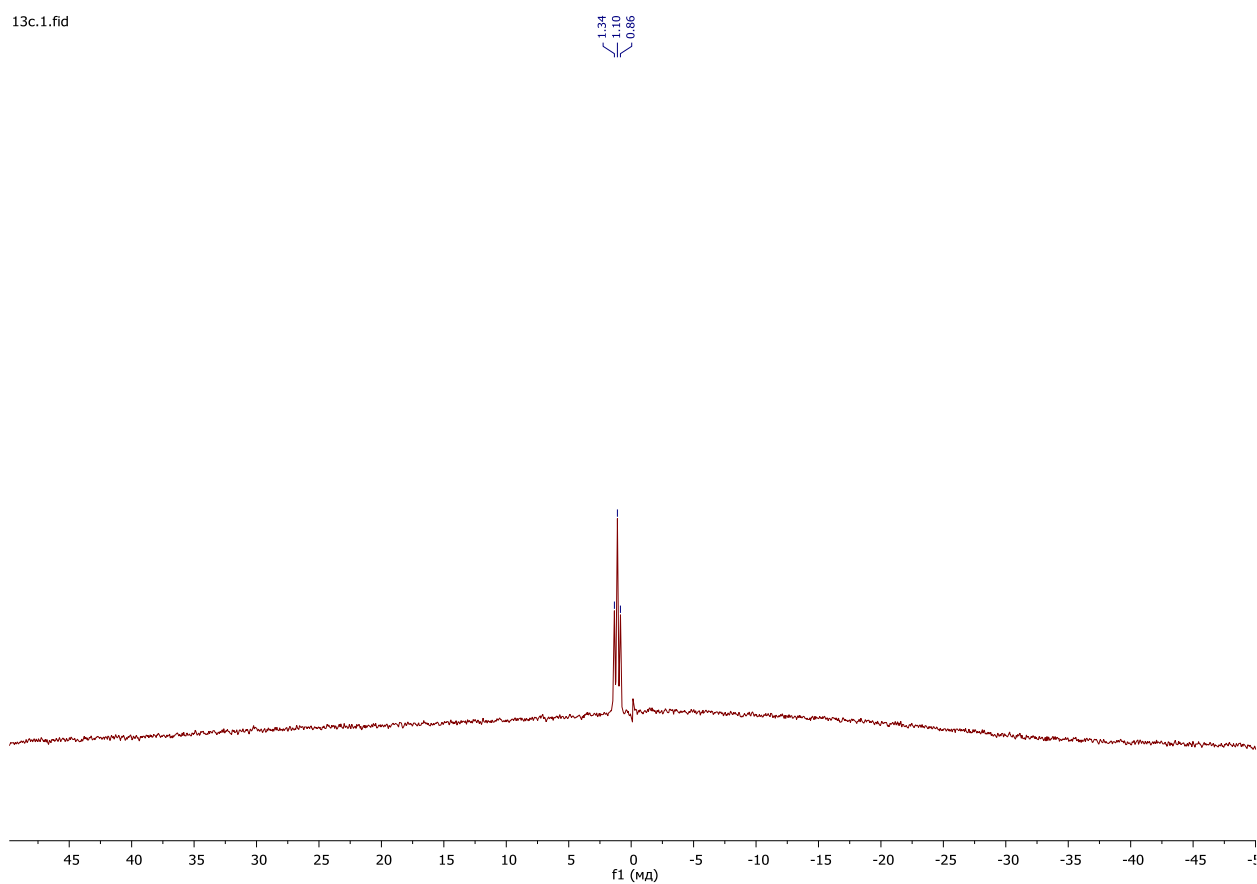


Figure S4. ^{11}B NMR spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) in CDCl_3 .

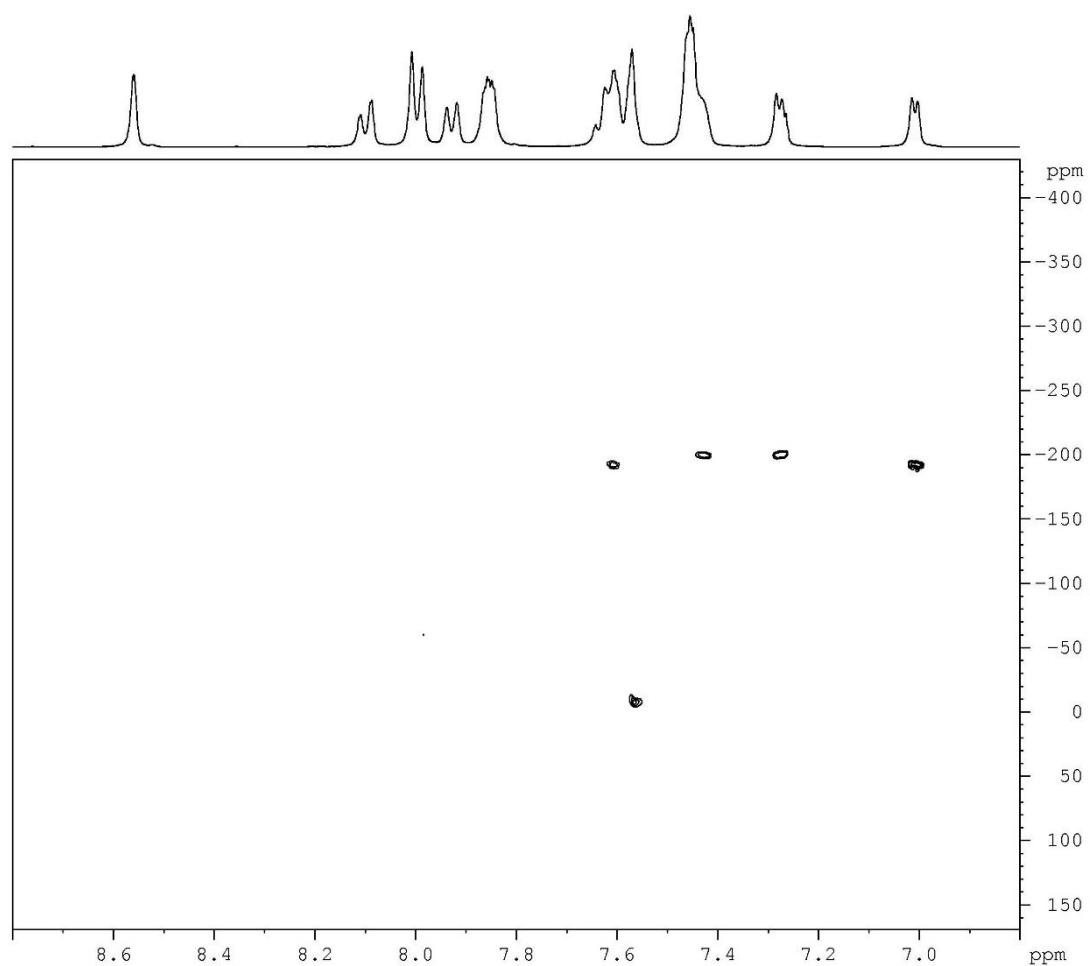


Figure S5. 2D ^1H - ^{15}N HMBC spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) (CDCl_3)

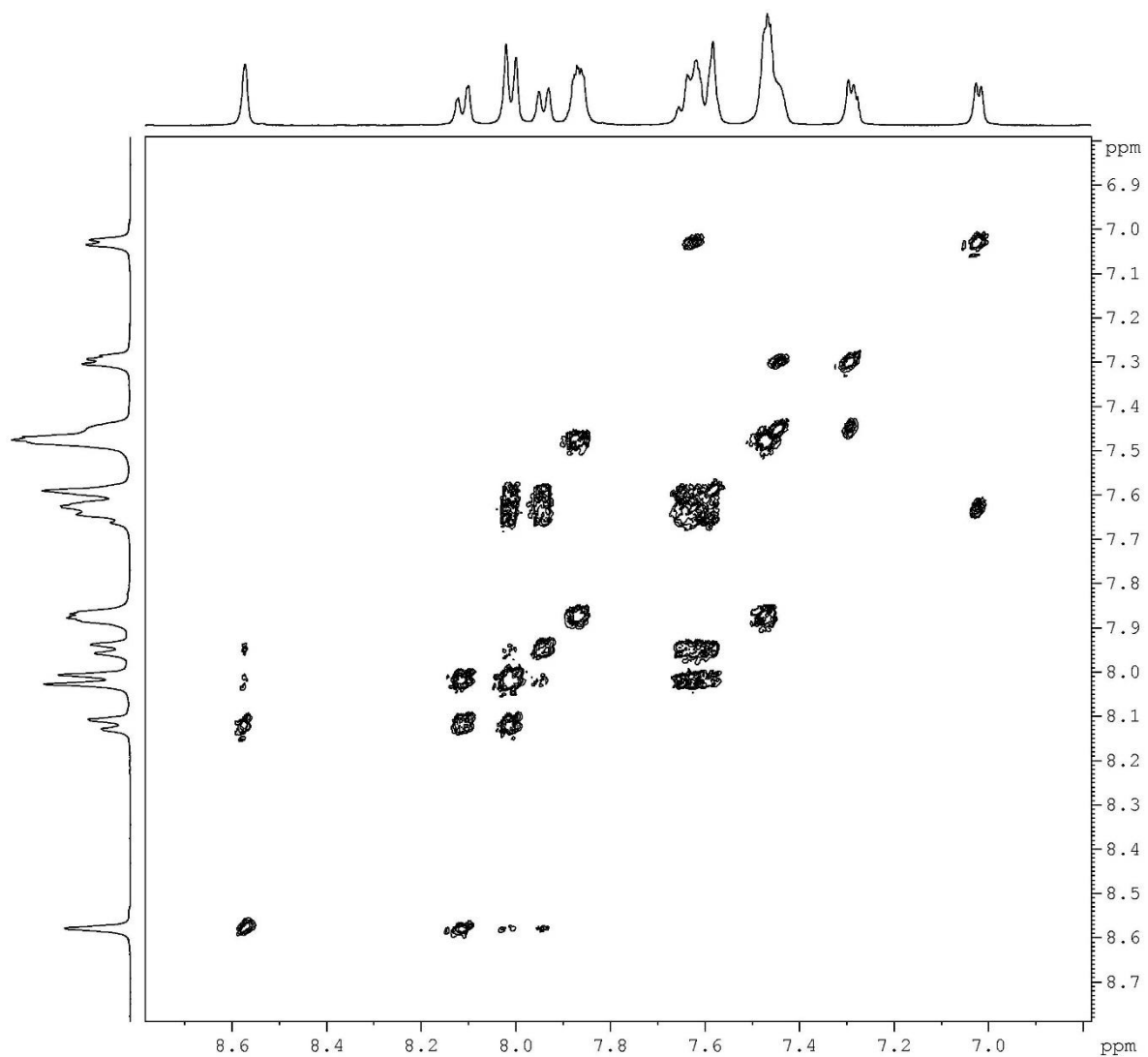


Figure S6. 2D COSY spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) (CDCl₃)

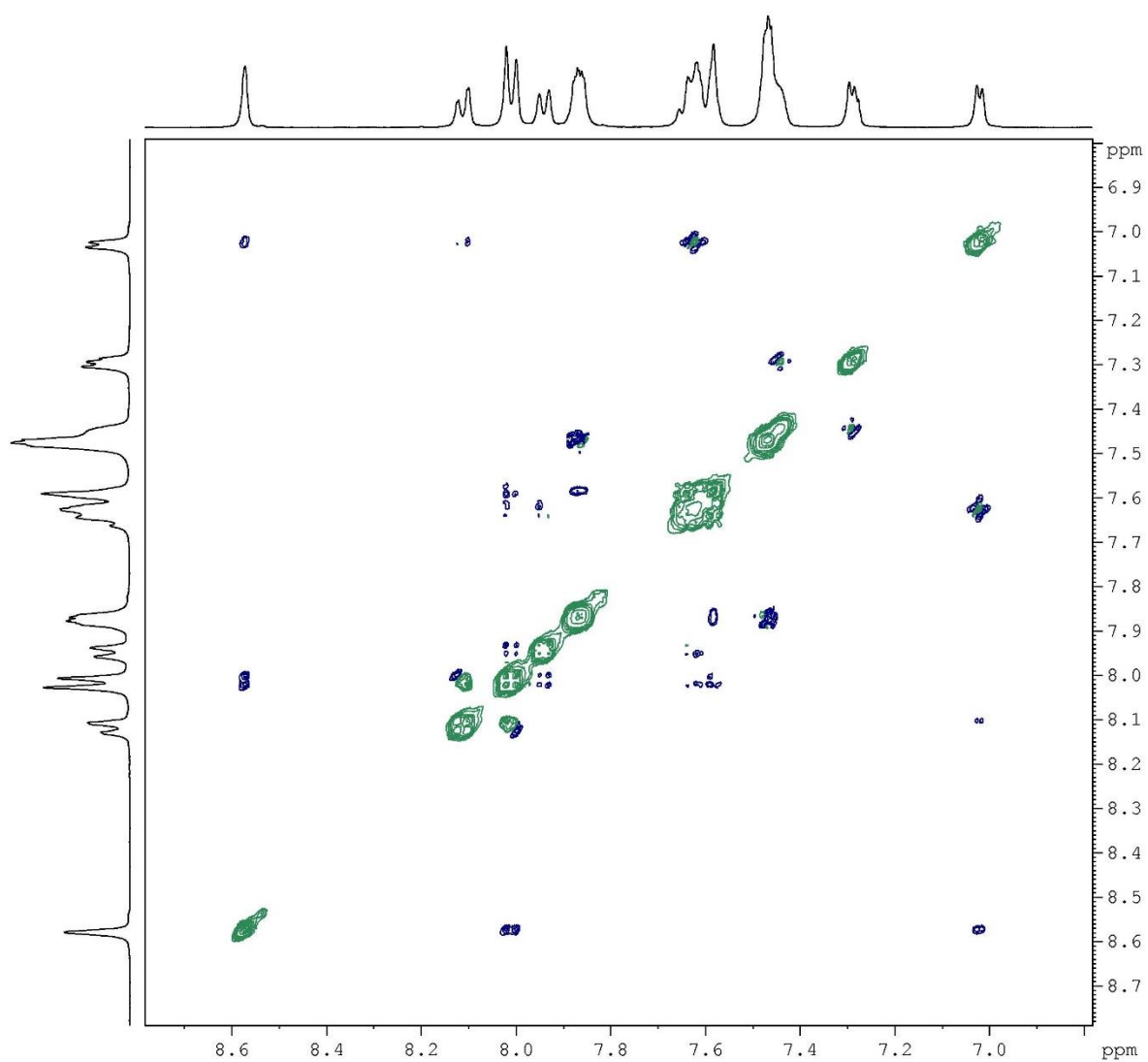


Figure S7. 2D NOESY spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) (CDCl₃)

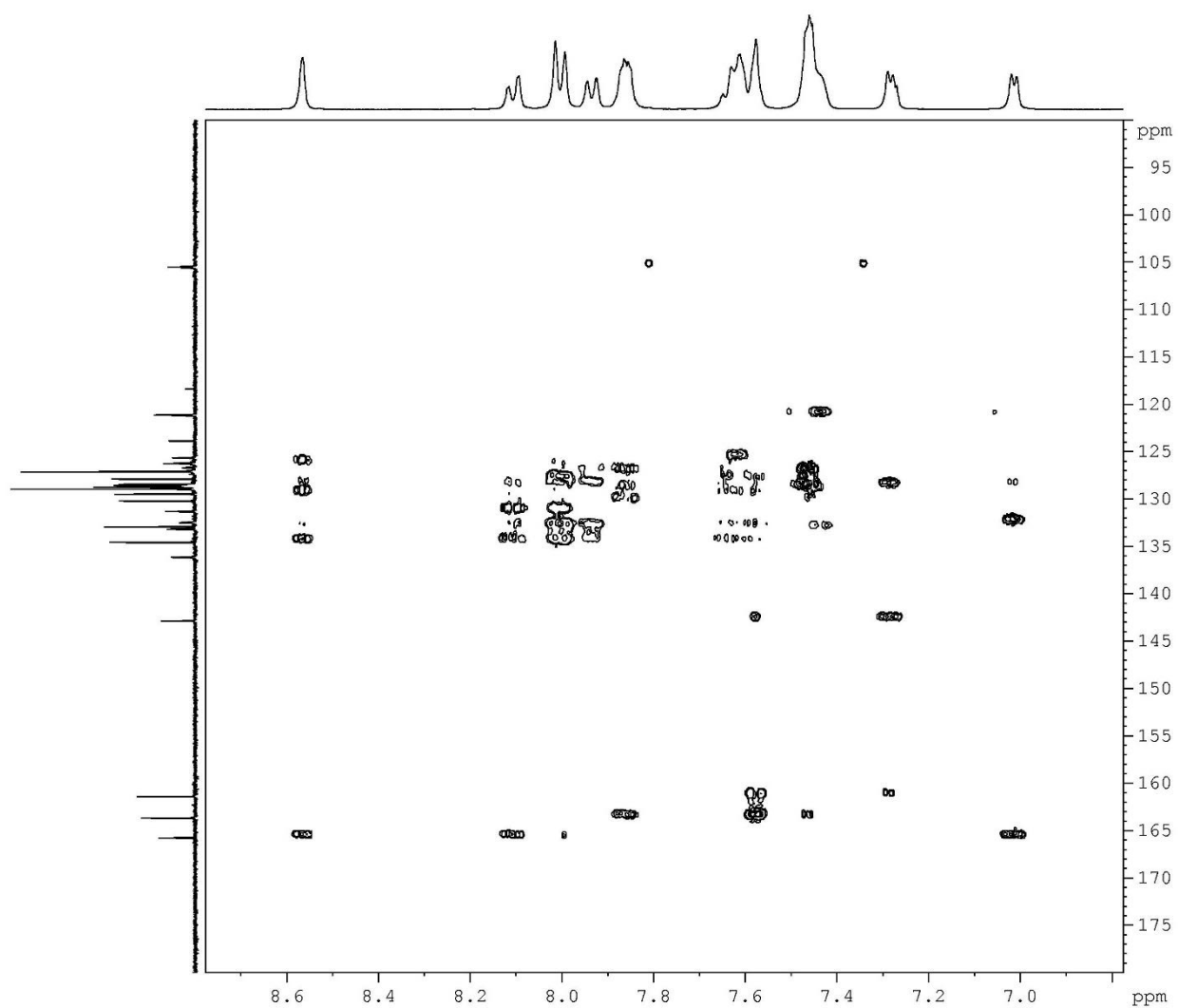


Figure S8. 2D ^1H - ^{13}C HMBC spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) (CDCl_3)

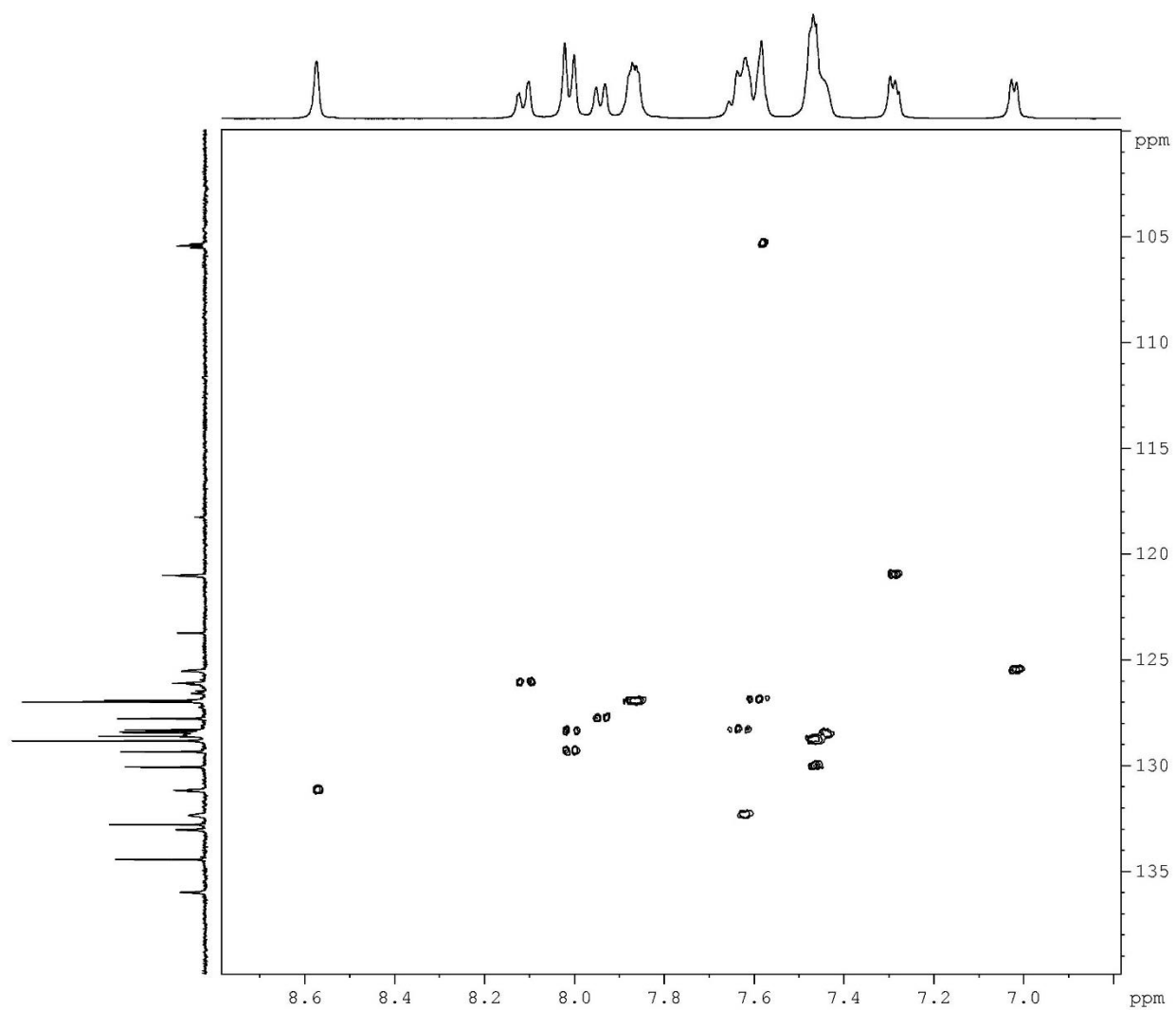


Figure S9. 2D ^1H - ^{13}C HSQC spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) (CDCl_3)

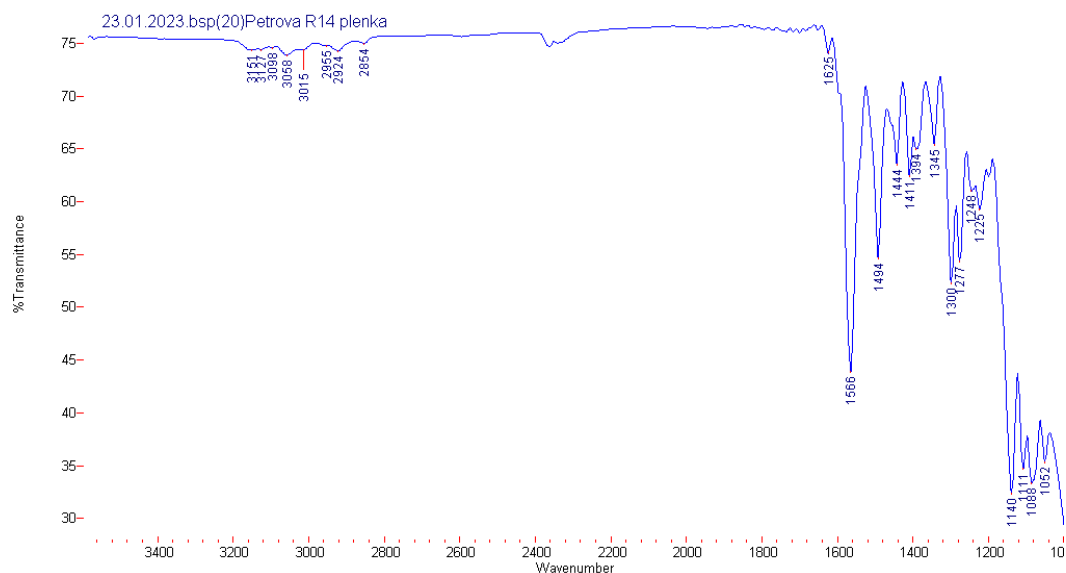


Figure S10. IR spectrum of 4,4-difluoro-3-(3-phenylisoxazol-5-yl)-8-trifluoromethyl-5-(naphthalen-2-yl)-4-bora-3a,4a-diaza-s-indacene (**1**) (film).

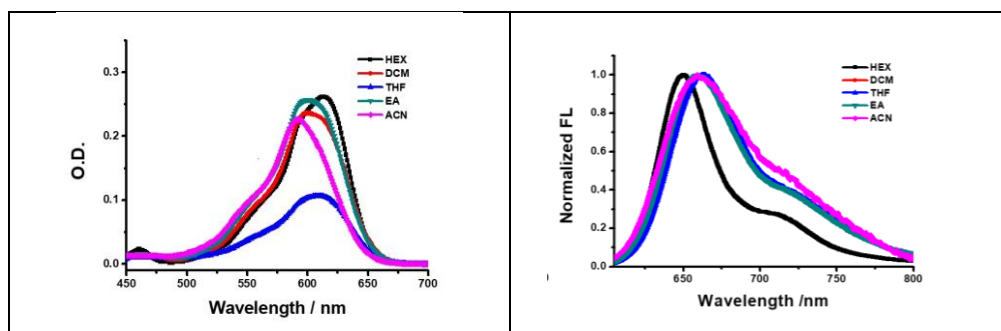
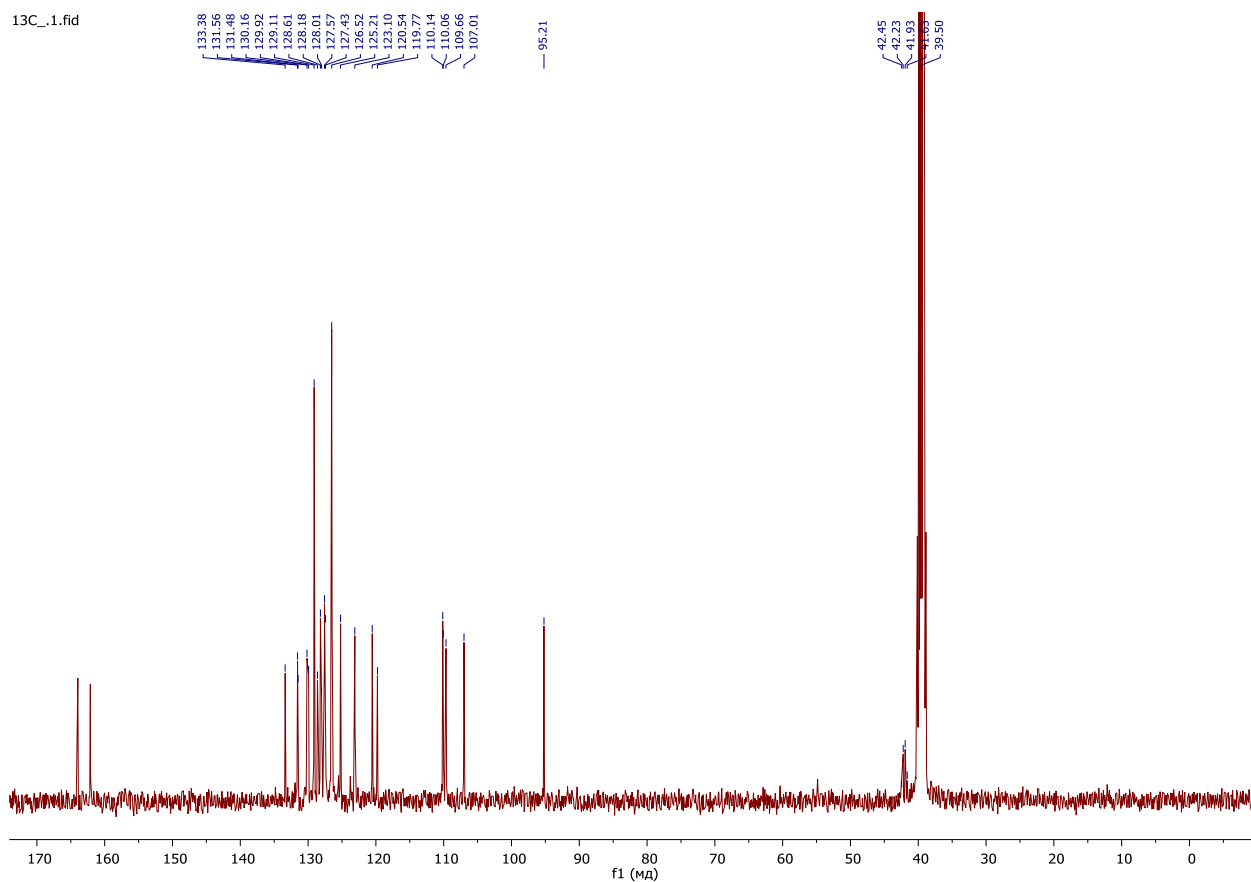
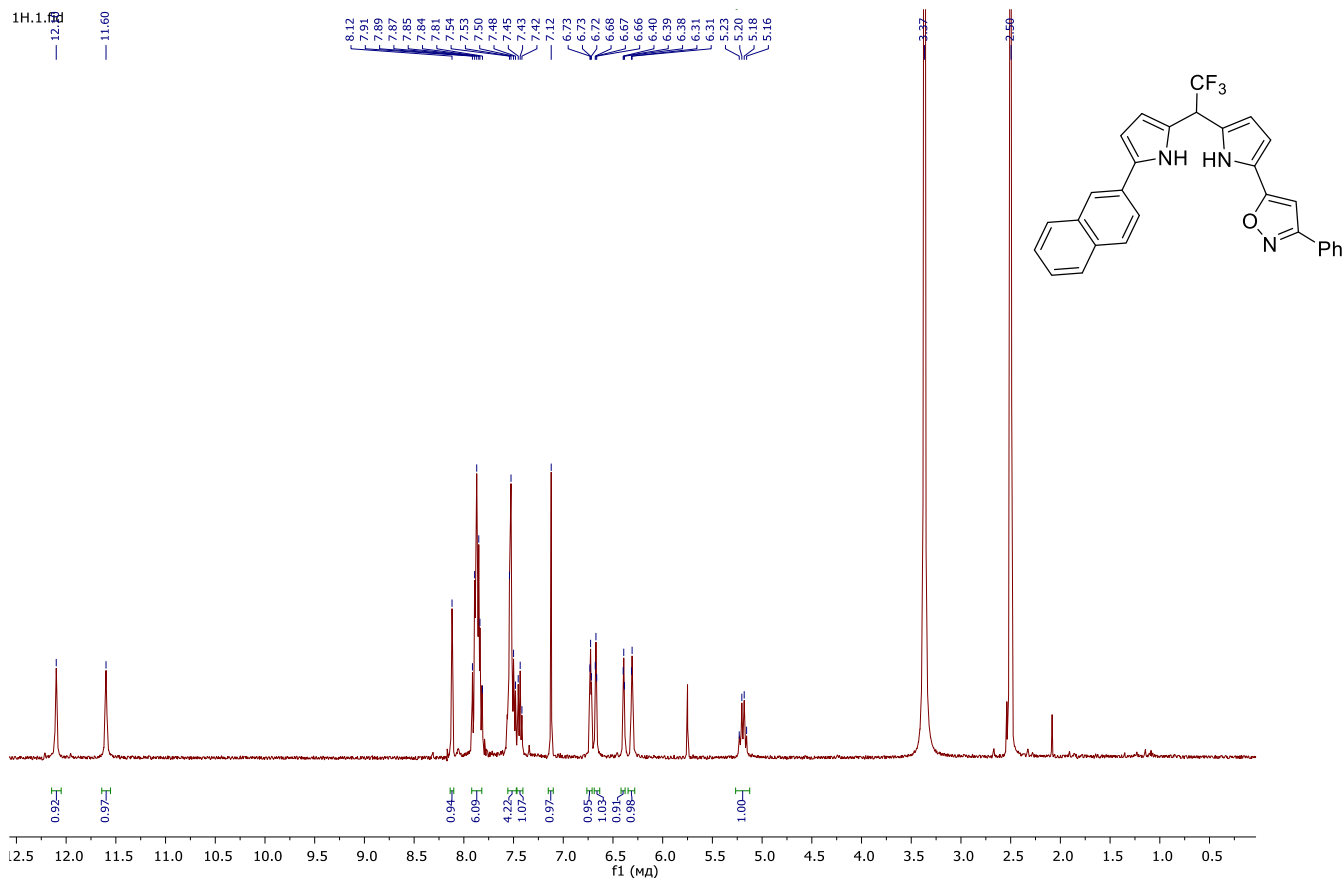


Figure S11. Normalized absorption and fluorescence spectra of compound **1** in different solvents (concentration 5×10^{-6} M)



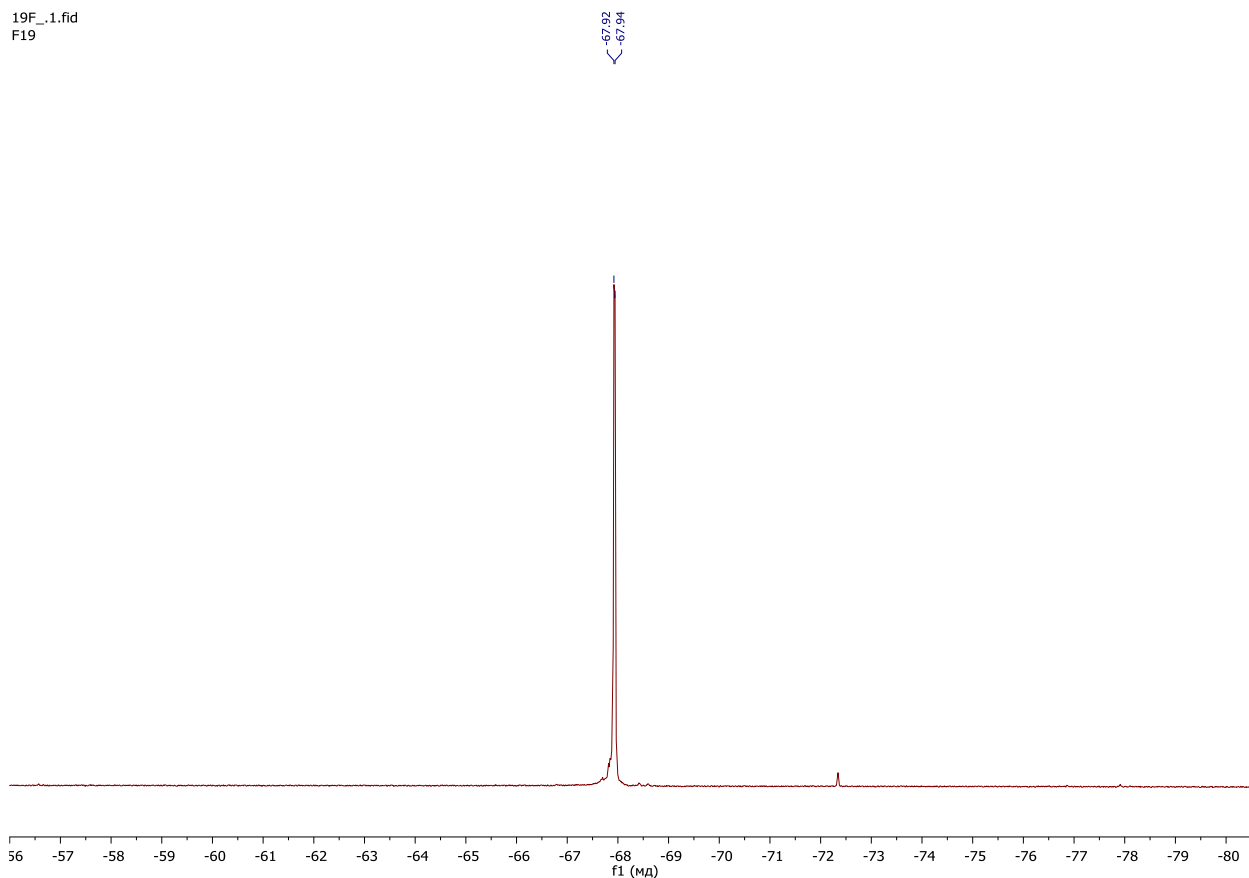


Figure S14. ^{19}F NMR spectrum of 3-phenyl-5-(5-{2,2,2-trifluoro-1-[5-(naphthalen-2-yl)-1H-pyrrol-2-yl]-ethyl}-1H-pyrrol-2-yl)isoxazole (**4**) in CDCl_3 .

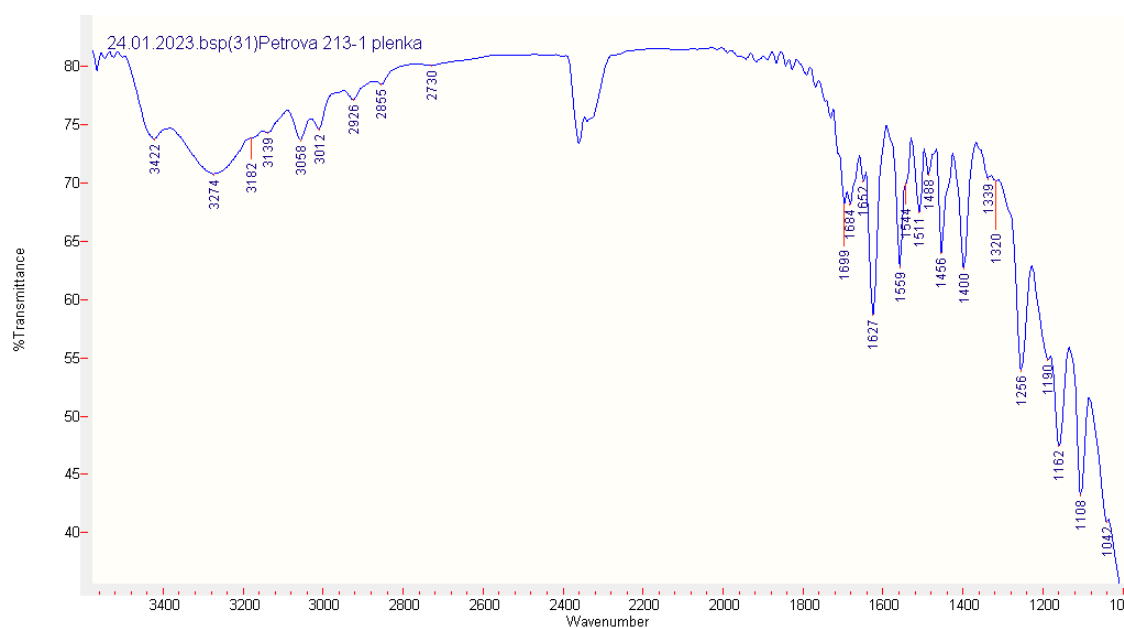


Figure S15. IR spectrum of 3-phenyl-5-(5-{2,2,2-trifluoro-1-[5-(naphthalen-2-yl)-1H-pyrrol-2-yl]-ethyl}-1H-pyrrol-2-yl)isoxazole (**4**) (film).

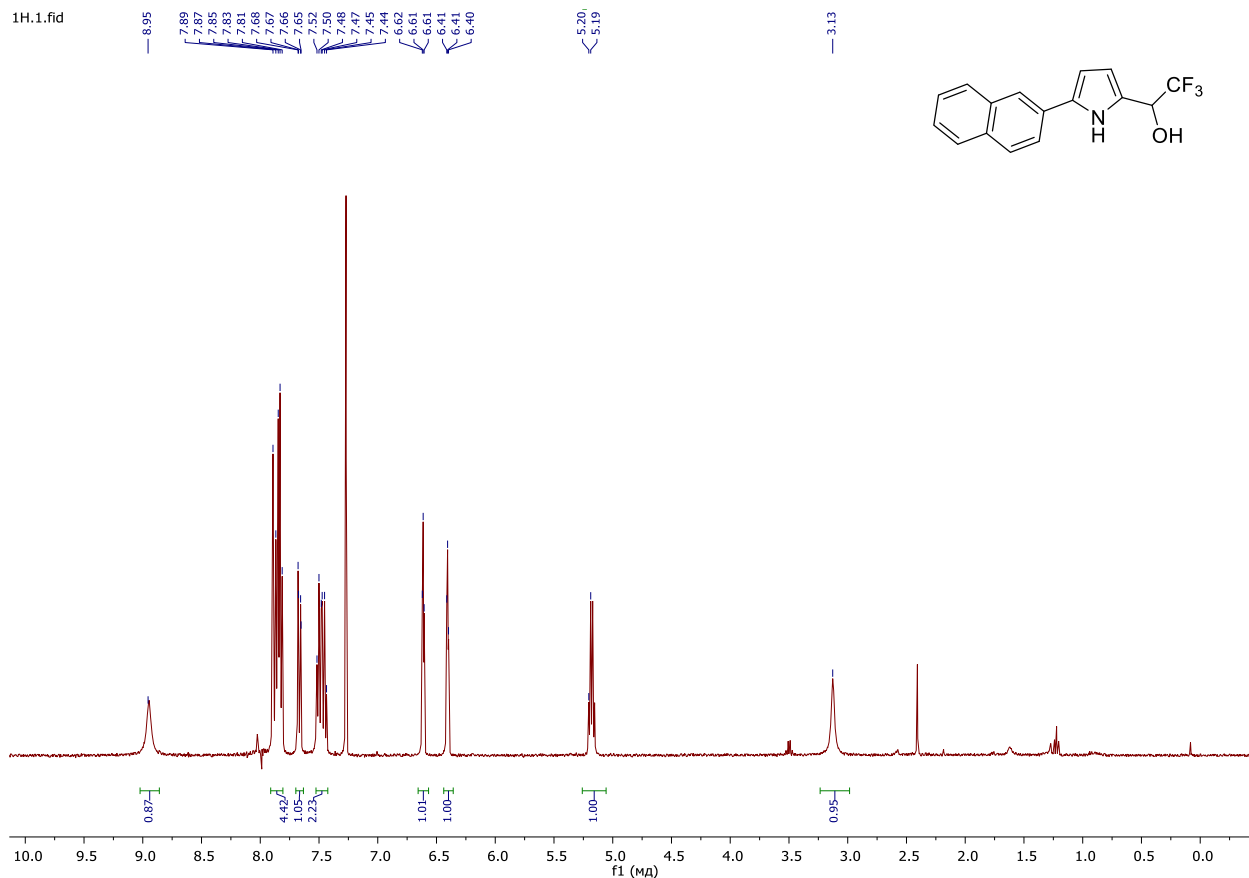


Figure S16. ¹H NMR spectrum of 2,2,2-trifluoro-1-[5-(naphthalen-2-yl)pyrrol-2-yl]ethan-1-ol (2) in CDCl₃.

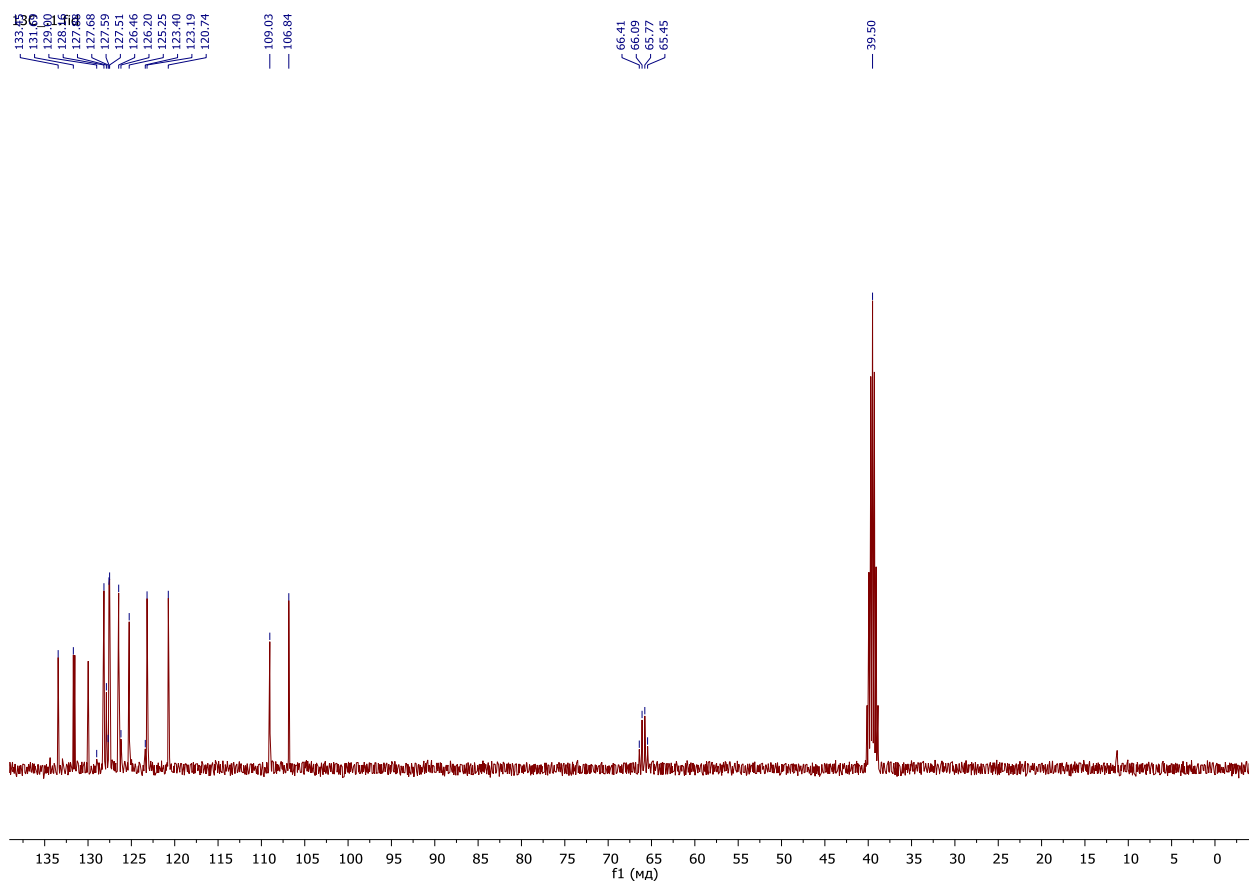


Figure S17. ¹³C NMR spectrum of 2,2,2-trifluoro-1-[5-(naphthalen-2-yl)pyrrol-2-yl]ethan-1-ol (2) in DMSO-d₆.

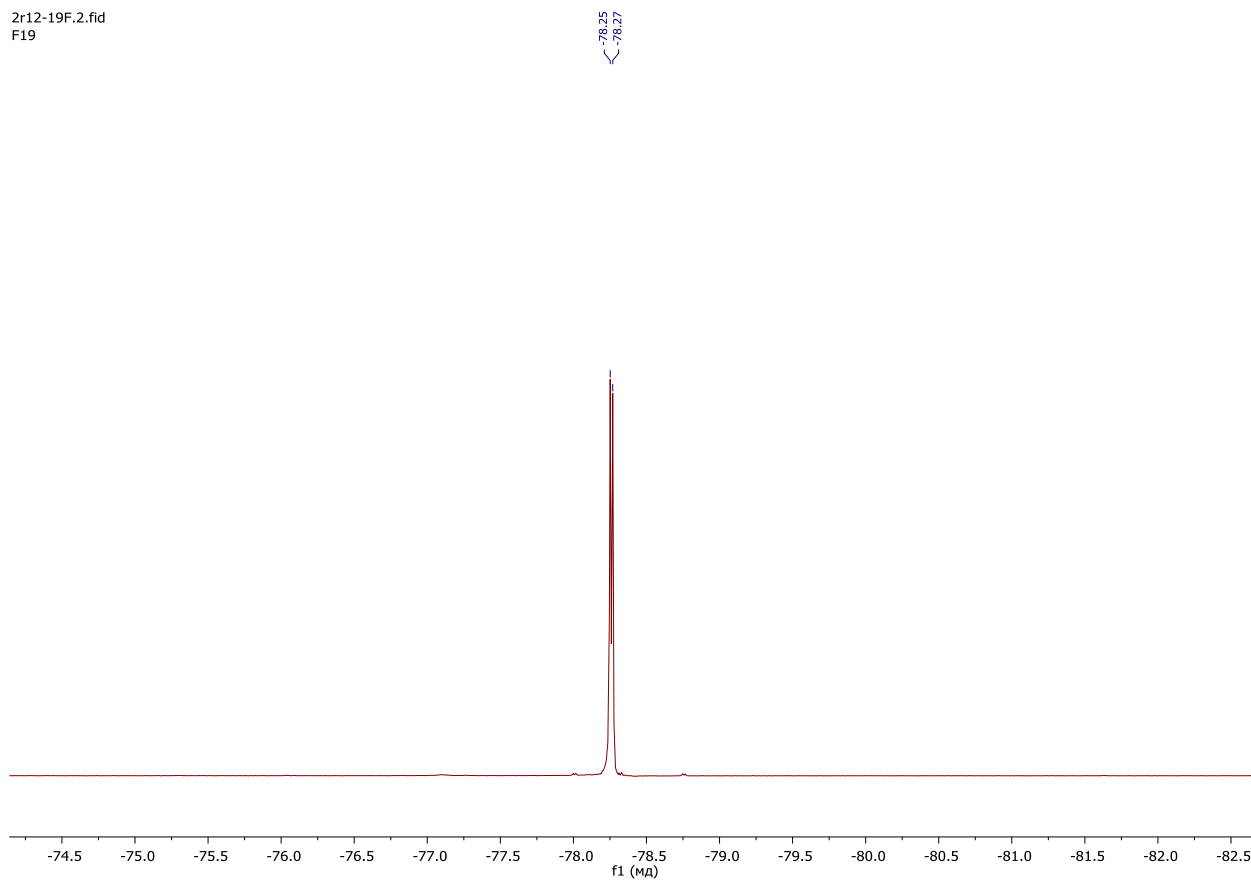


Figure S18. ^{19}F NMR spectrum of 2,2,2-trifluoro-1-[5-(naphthalen-2-yl)pyrrol-2-yl]ethan-1-ol (**2**) in CDCl_3 .

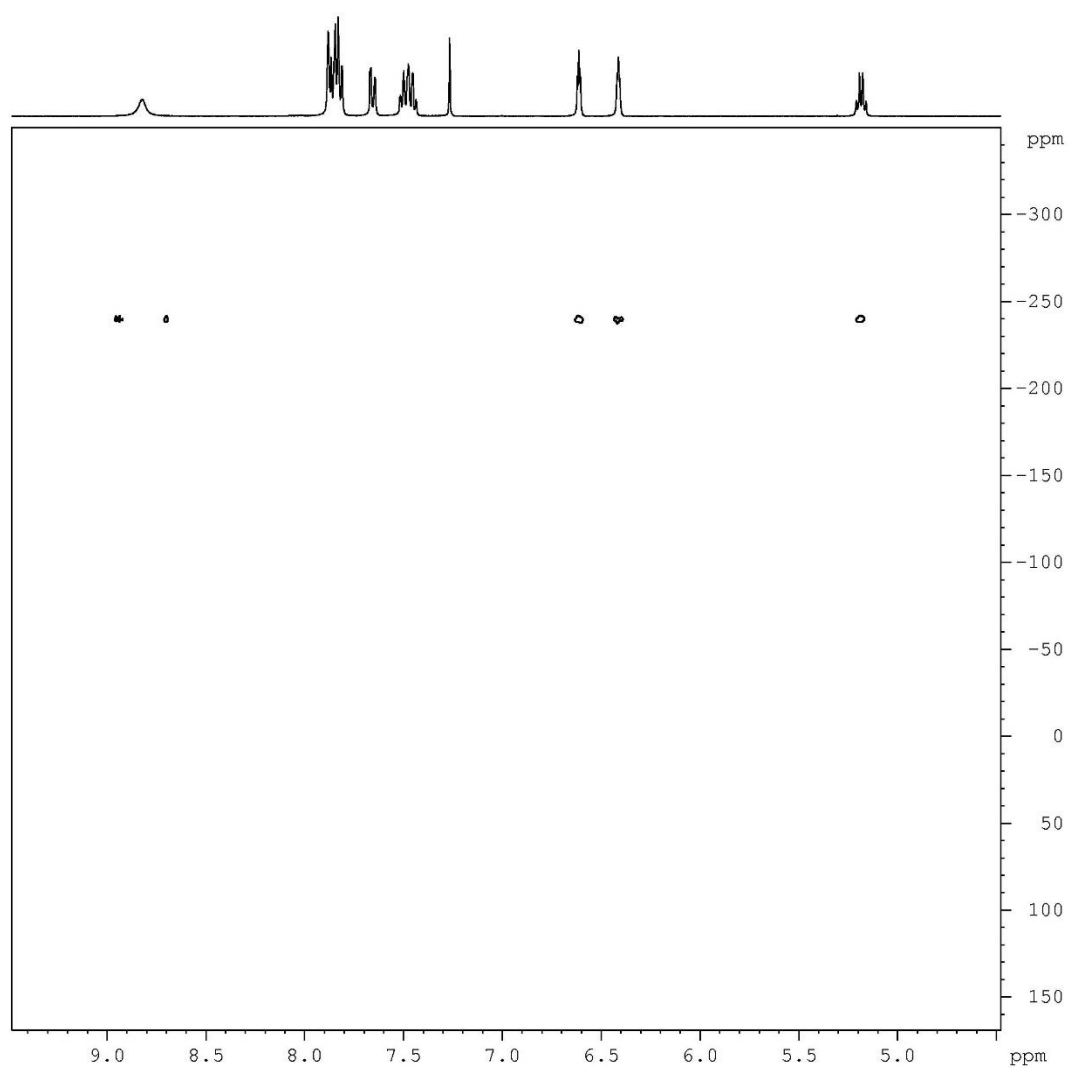
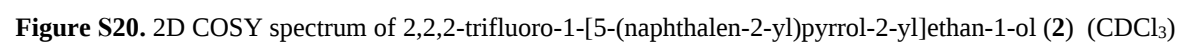


Figure S19. 2D ^1H - ^{15}N HMBC spectrum of 2,2,2-trifluoro-1-[5-(naphthalen-2-yl)pyrrol-2-yl]ethan-1-ol (**2**) (CDCl_3)



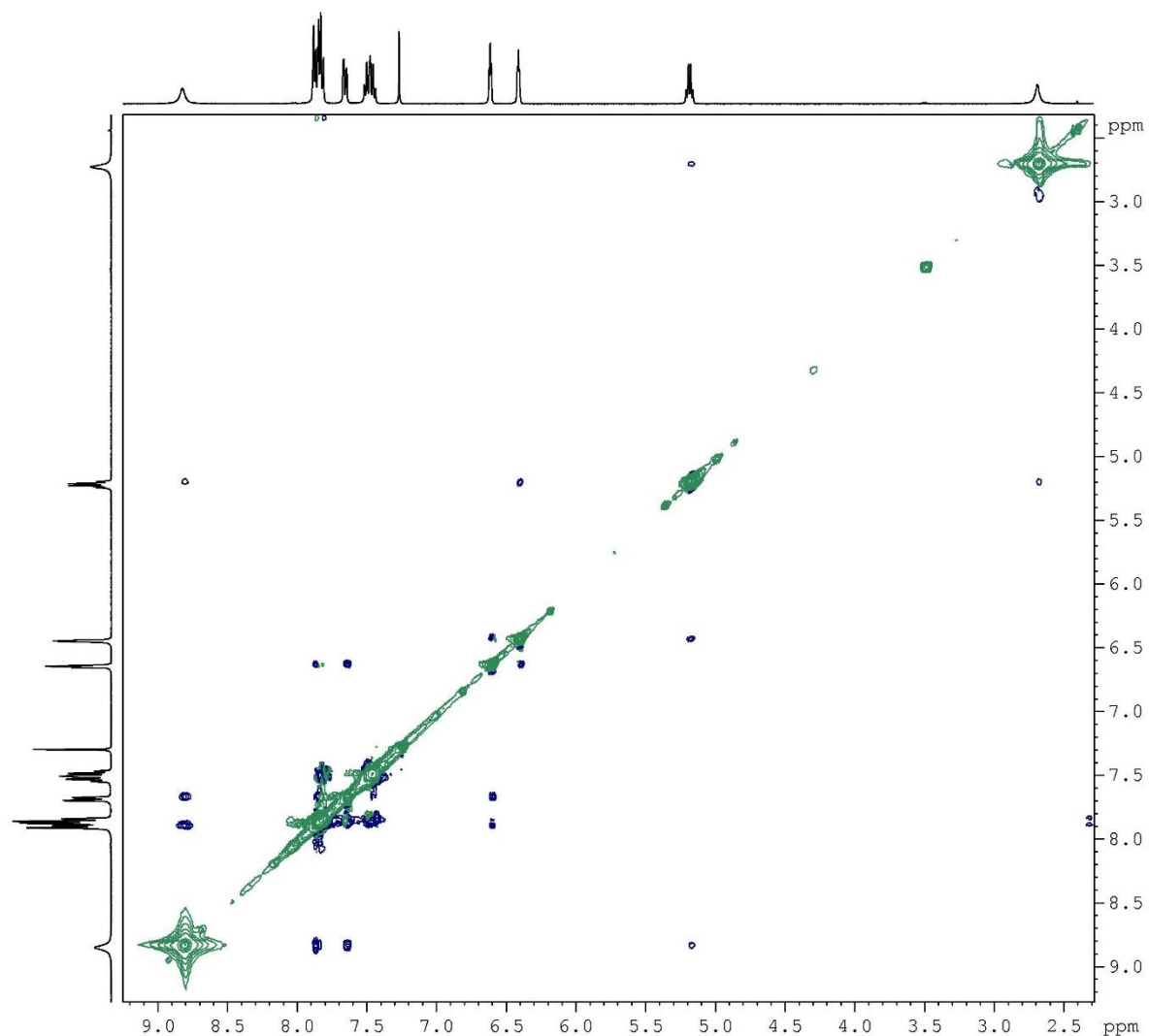


Figure S21. 2D NOESY spectrum of 2,2,2-trifluoro-1-[5-(naphthalen-2-yl)pyrrol-2-yl]ethan-1-ol (**2**) (CDCl_3)

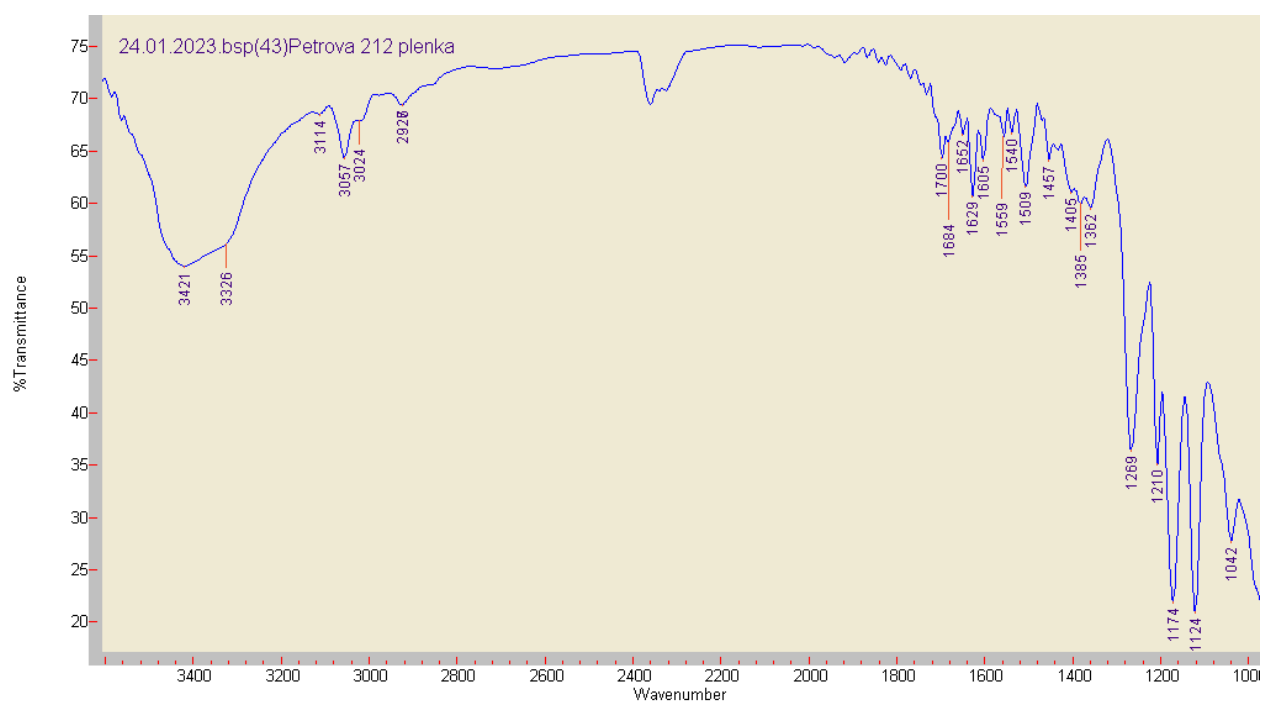


Figure S22. IR spectrum of 2,2,2-trifluoro-1-[5-(naphthalen-2-yl)pyrrol-2-yl]ethan-1-ol (**2**) (film).