

Supplementary materials

Synthesis and photophysical properties of 2-alkylamino-4-(2-hydroxynaphthalene-1-yl)quinazolinium tetrafluoroborates

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¹H NMR Spectra

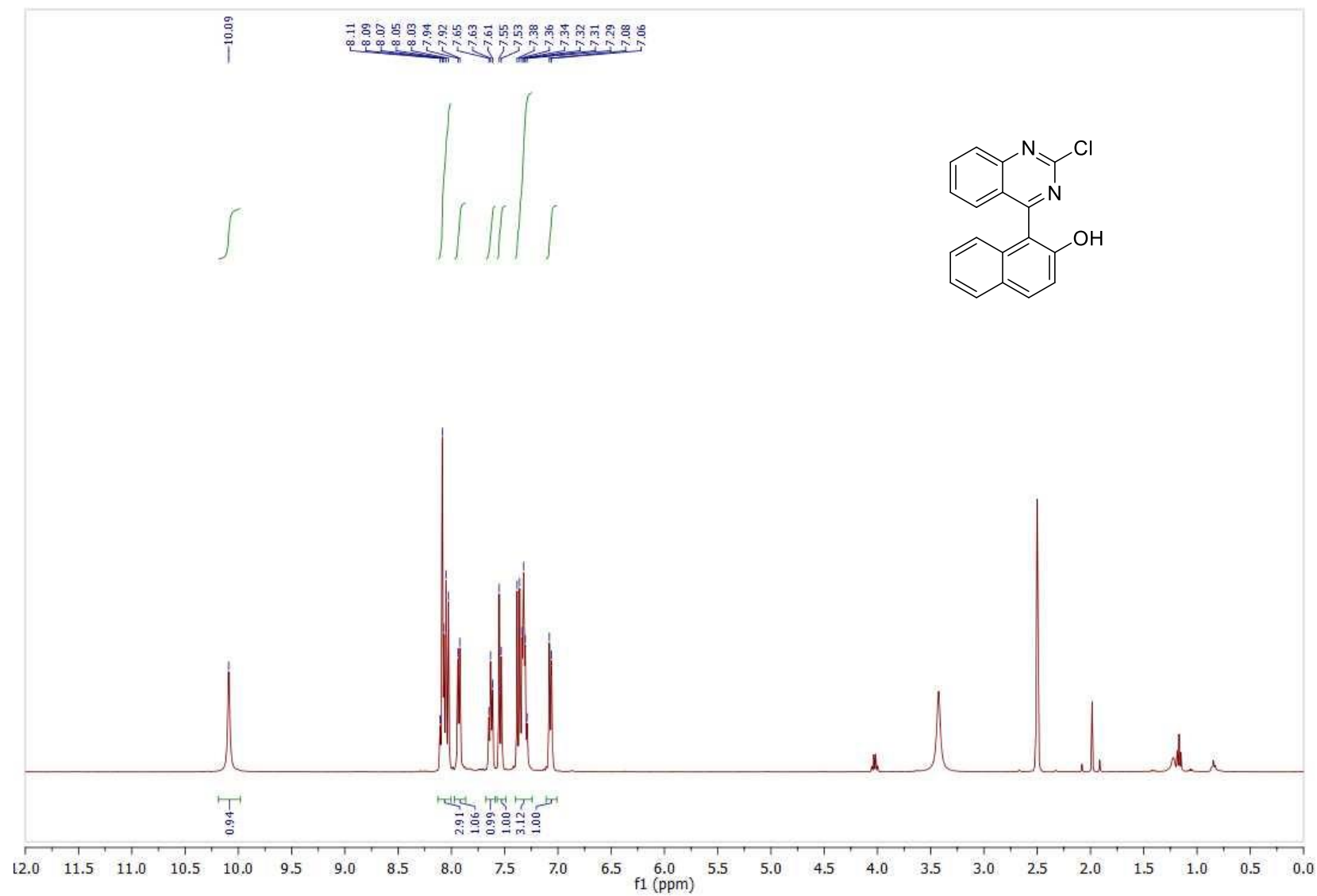


Fig. S1. ¹H NMR Spectrum 2-hydroxy-1-(2-chloroquinazolin-4-yl)naphthalene (**3**)

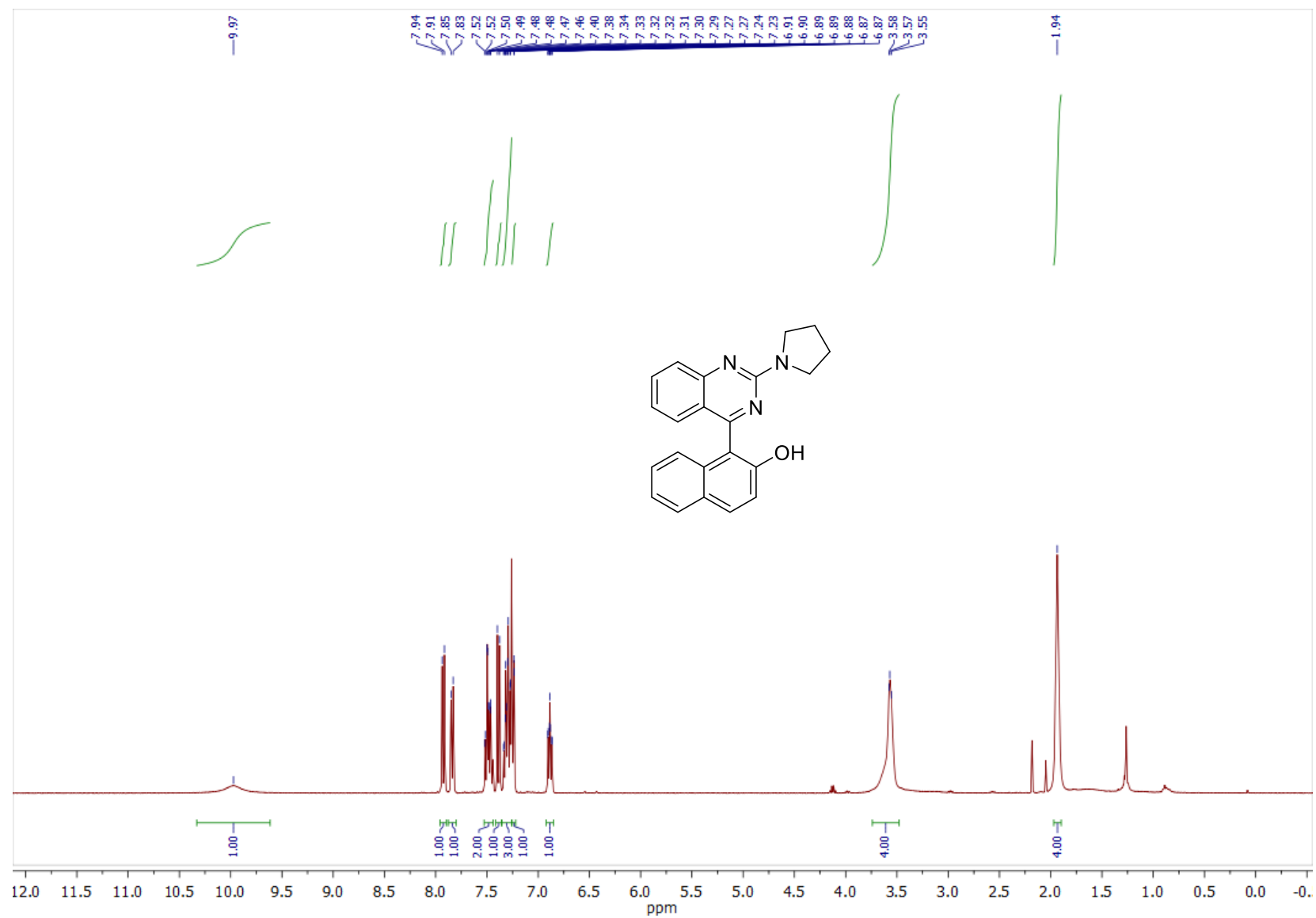


Fig. S2. ¹H NMR Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5a**)

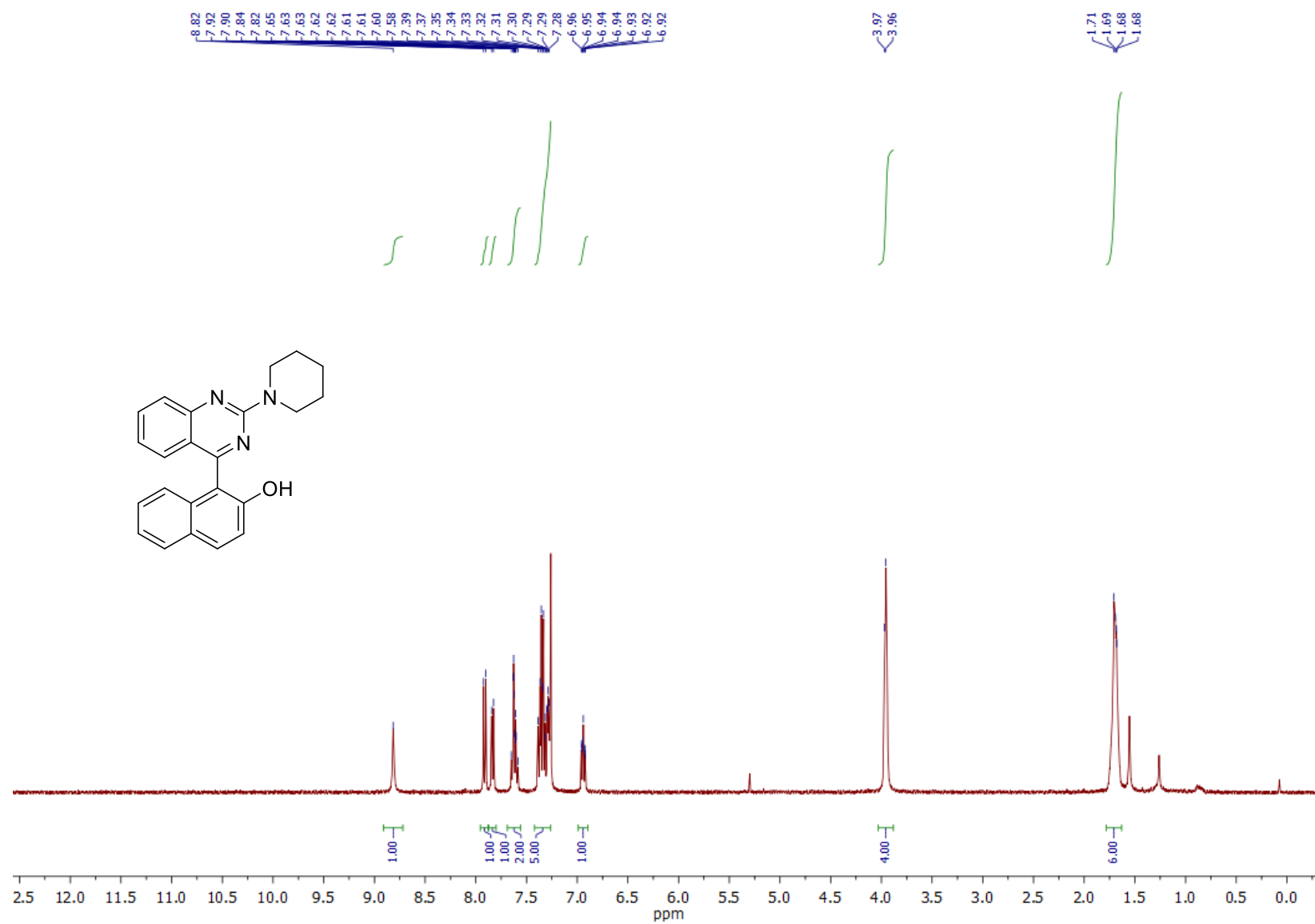


Fig. S3. ¹H NMR Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5b**)

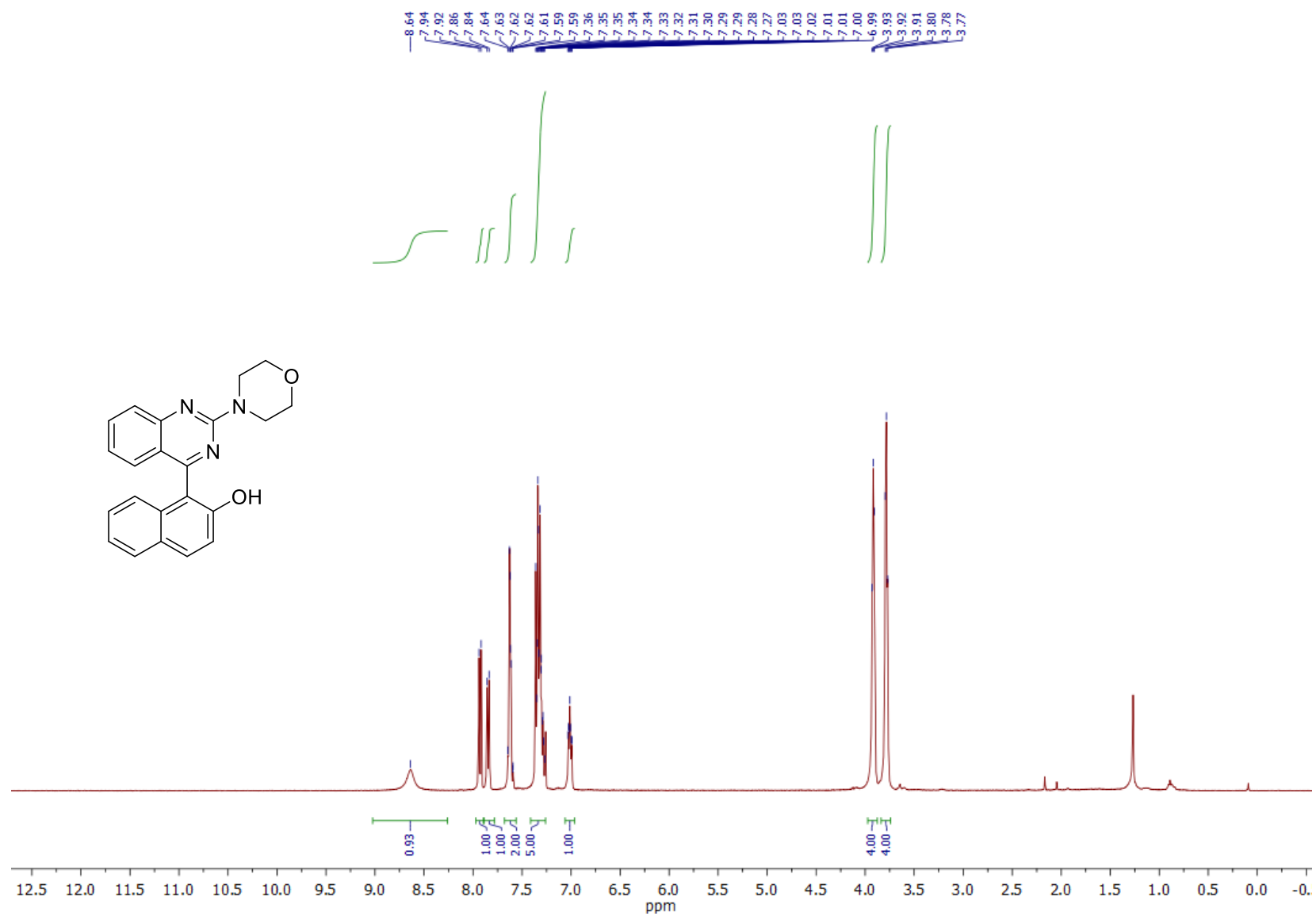


Fig. S4. ¹H NMR Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5c**)

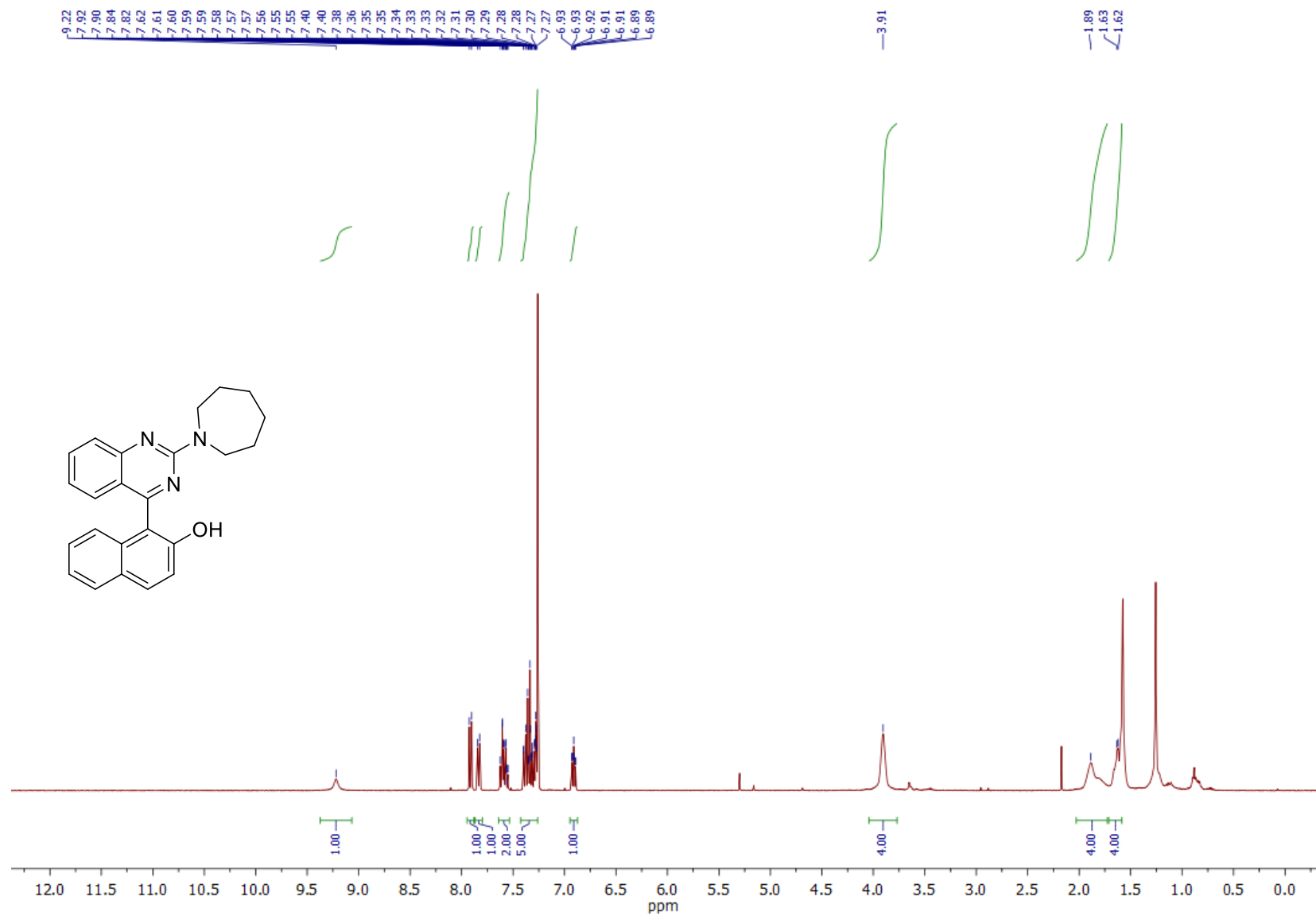


Fig. S5. ¹H NMR Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5d**)

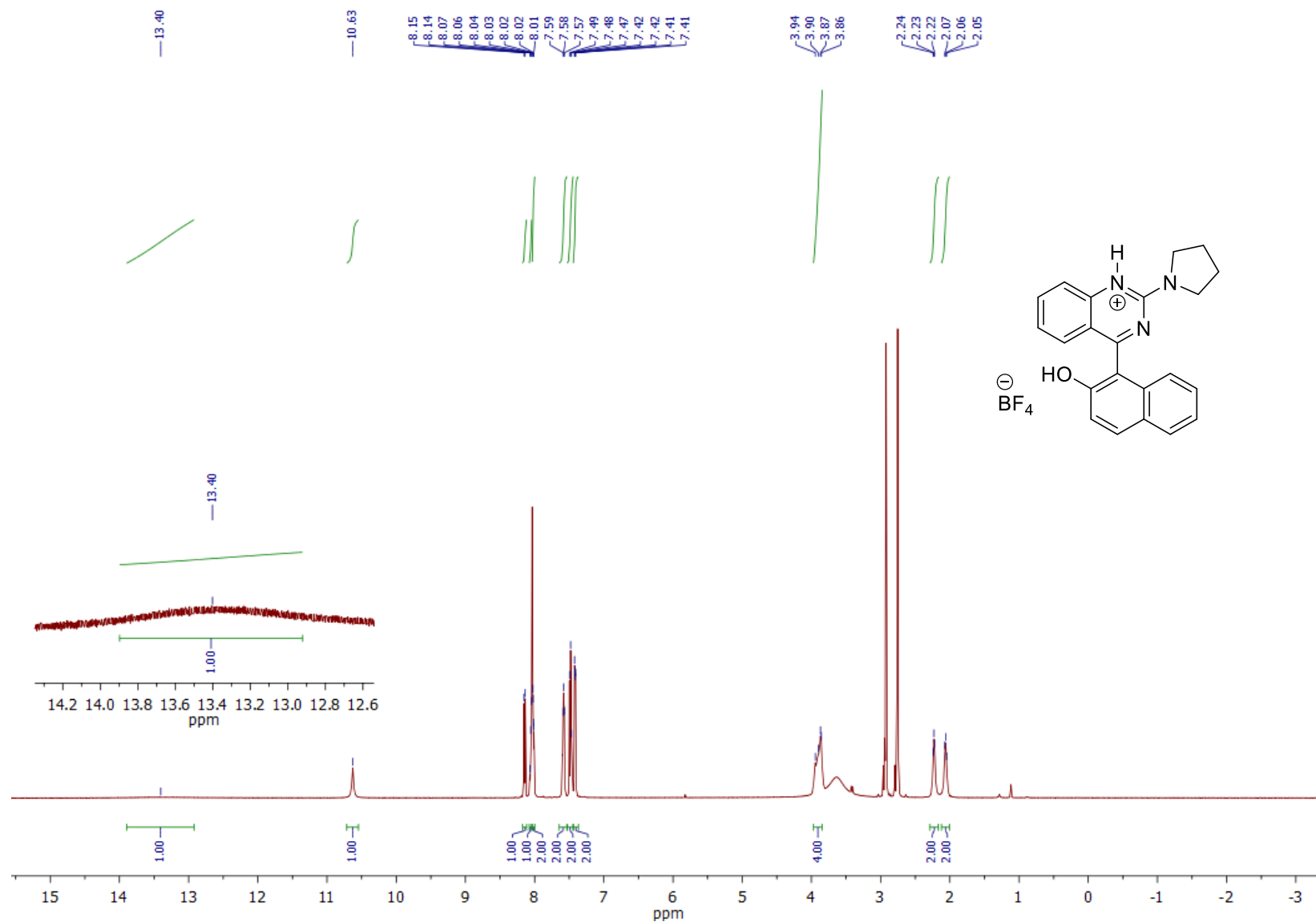


Fig. S6. ¹H NMR Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6a**)

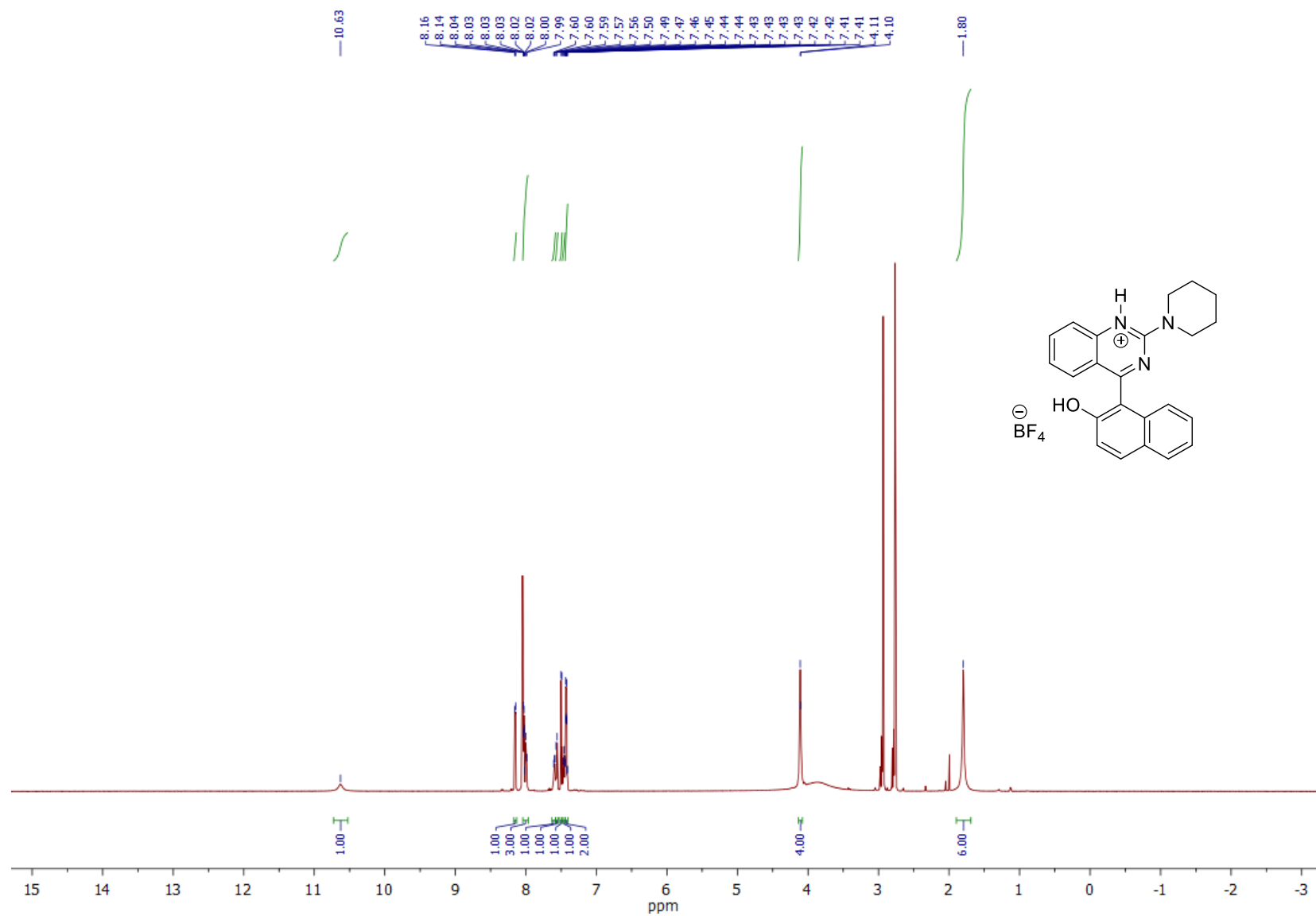


Fig. S7. ^1H NMR Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6b**)

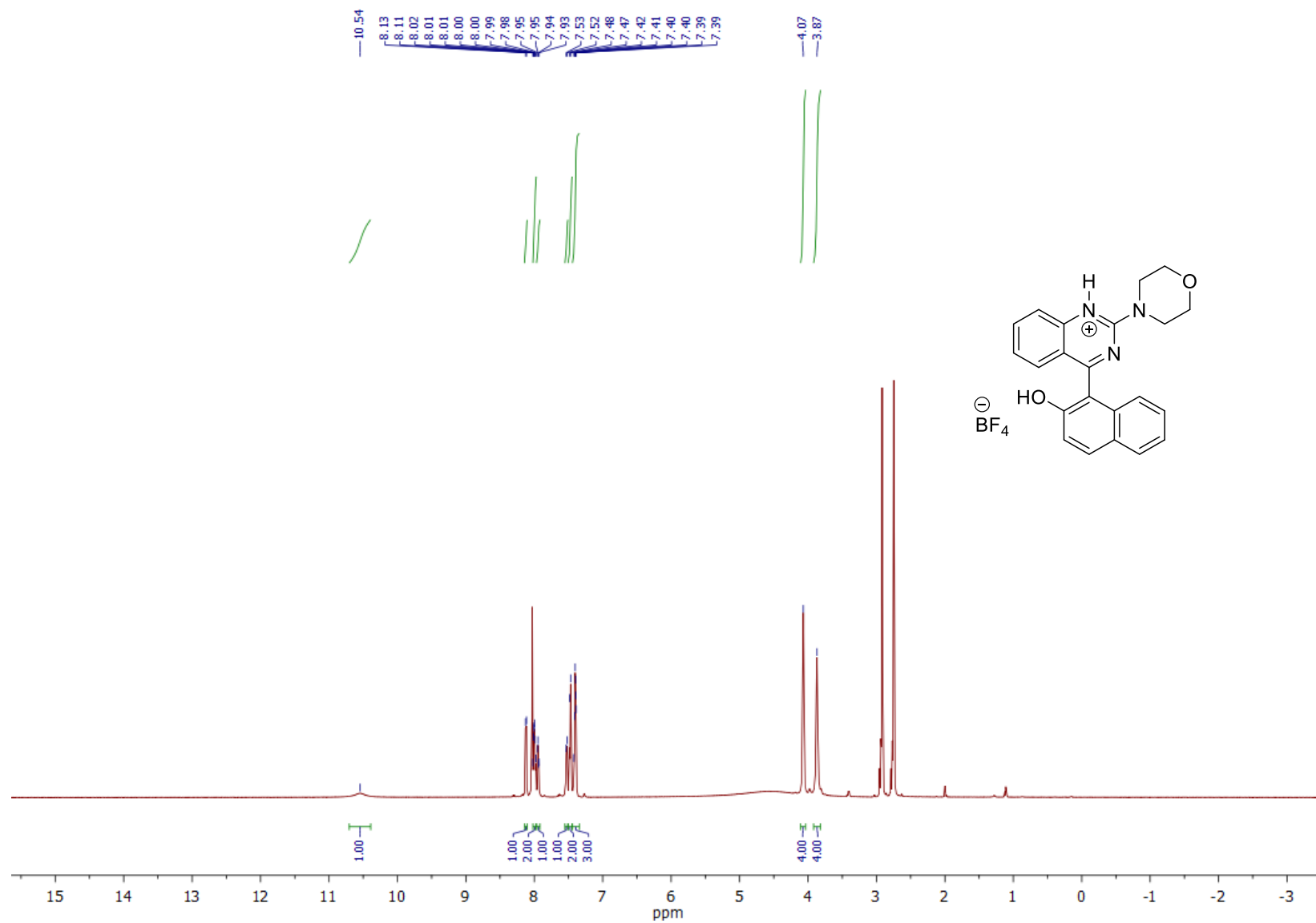


Fig. S8. ^1H NMR Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6c**)

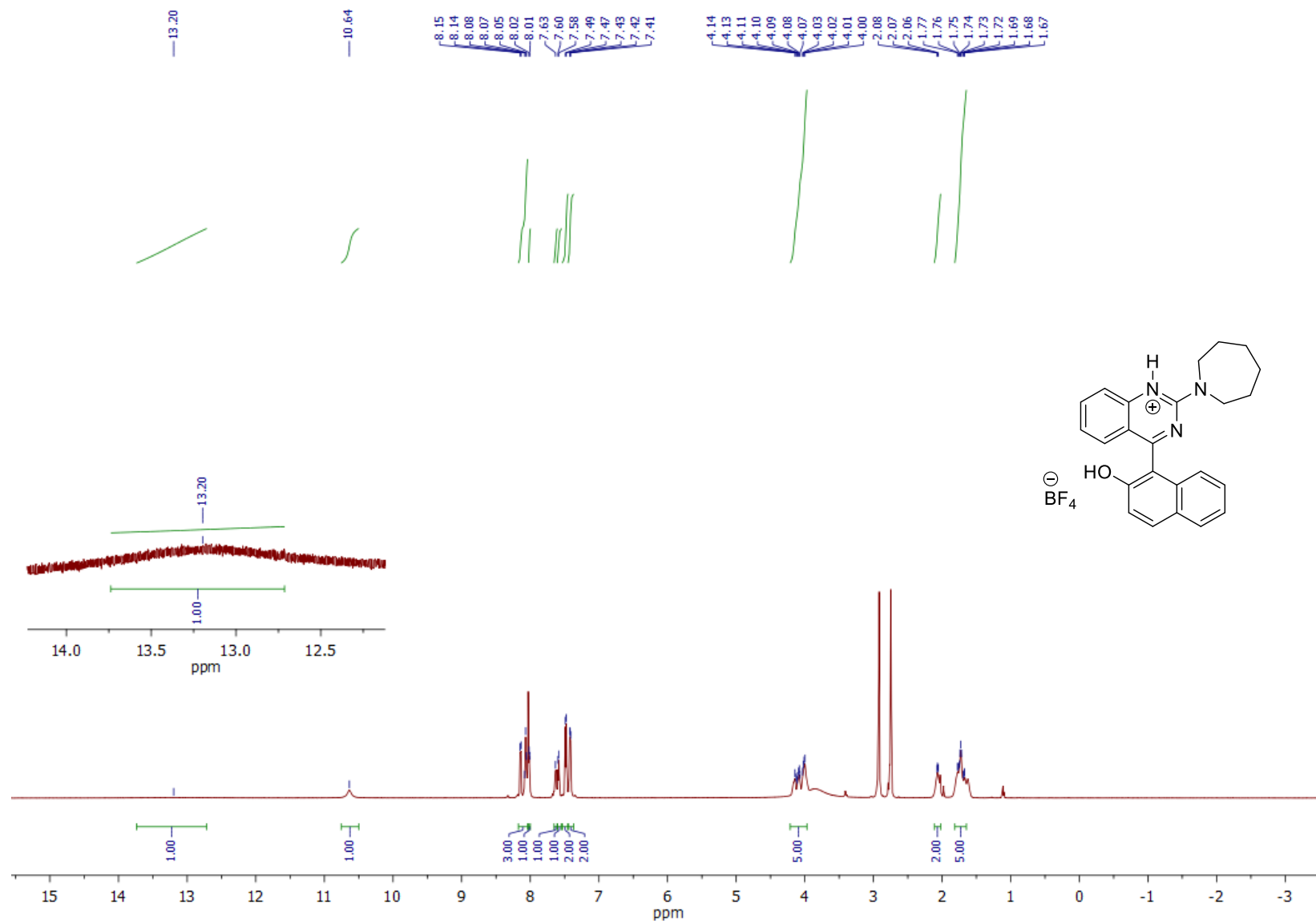


Fig. S9. ^1H NMR Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6d**)

¹³C NMR Spectra

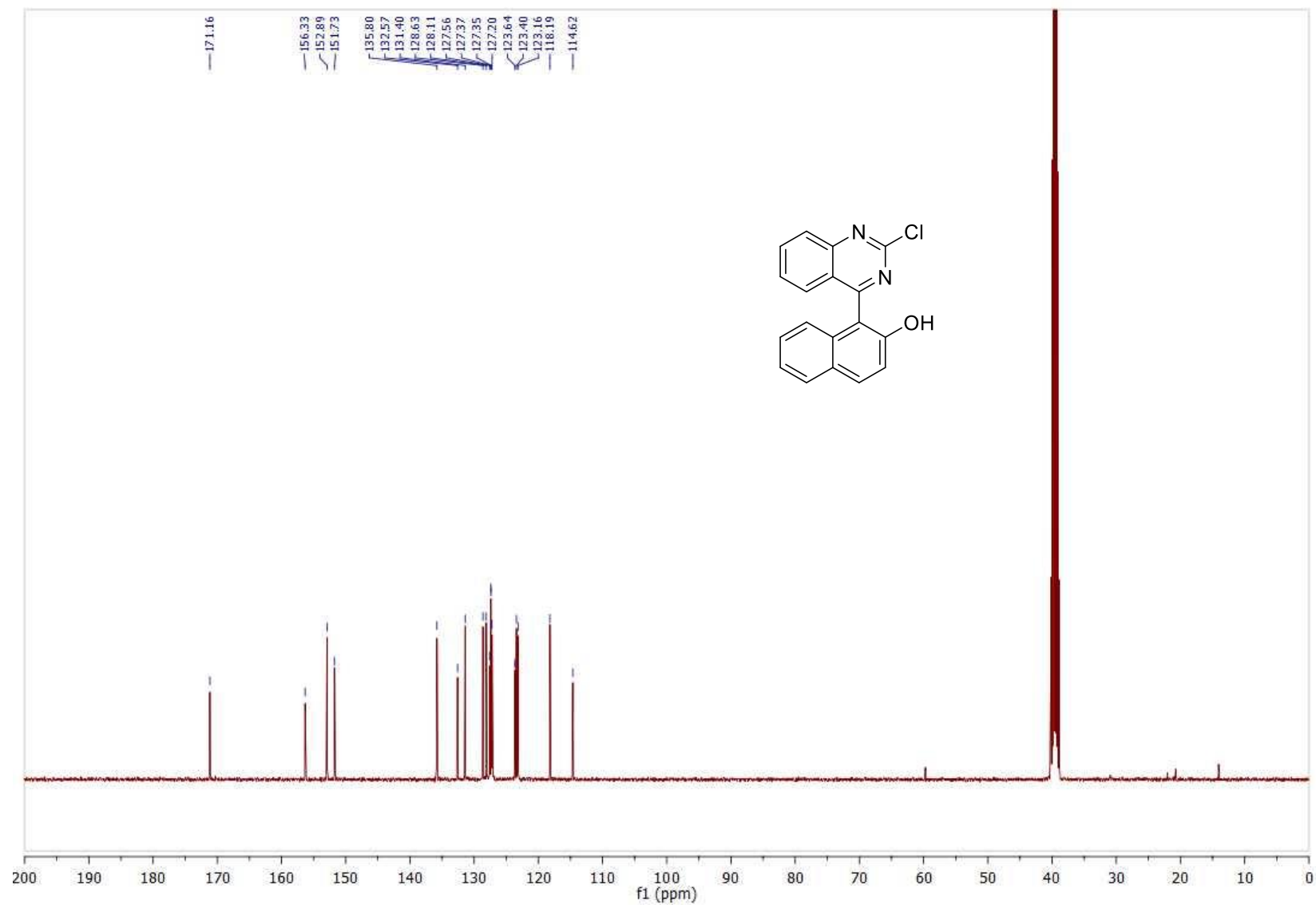


Fig. S10. ¹³C NMR Spectrum 2-hydroxy-1-(2-chloroquinazolin-4-yl)naphthalene (3)

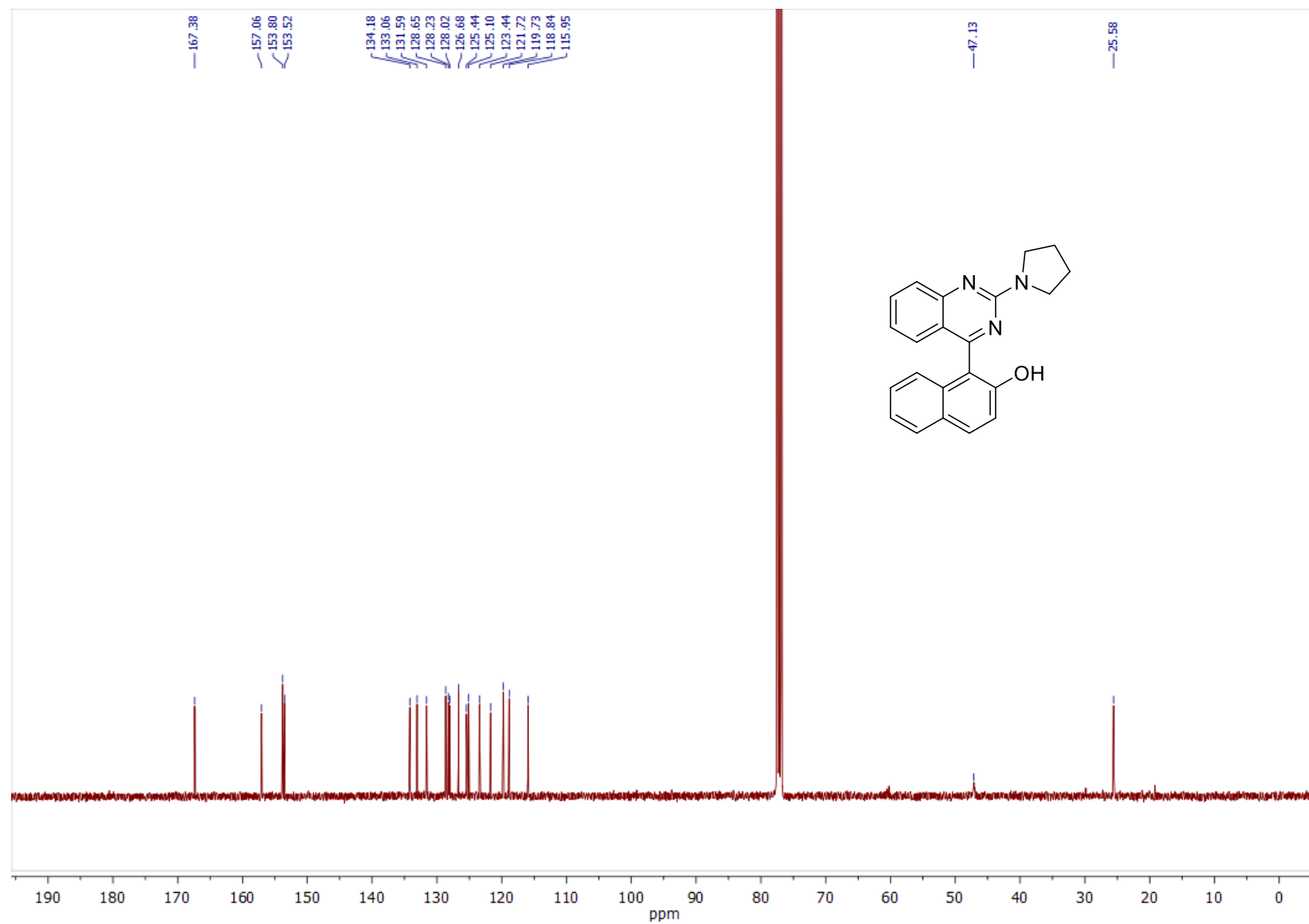


Fig. S11. ^{13}C NMR Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5a**)

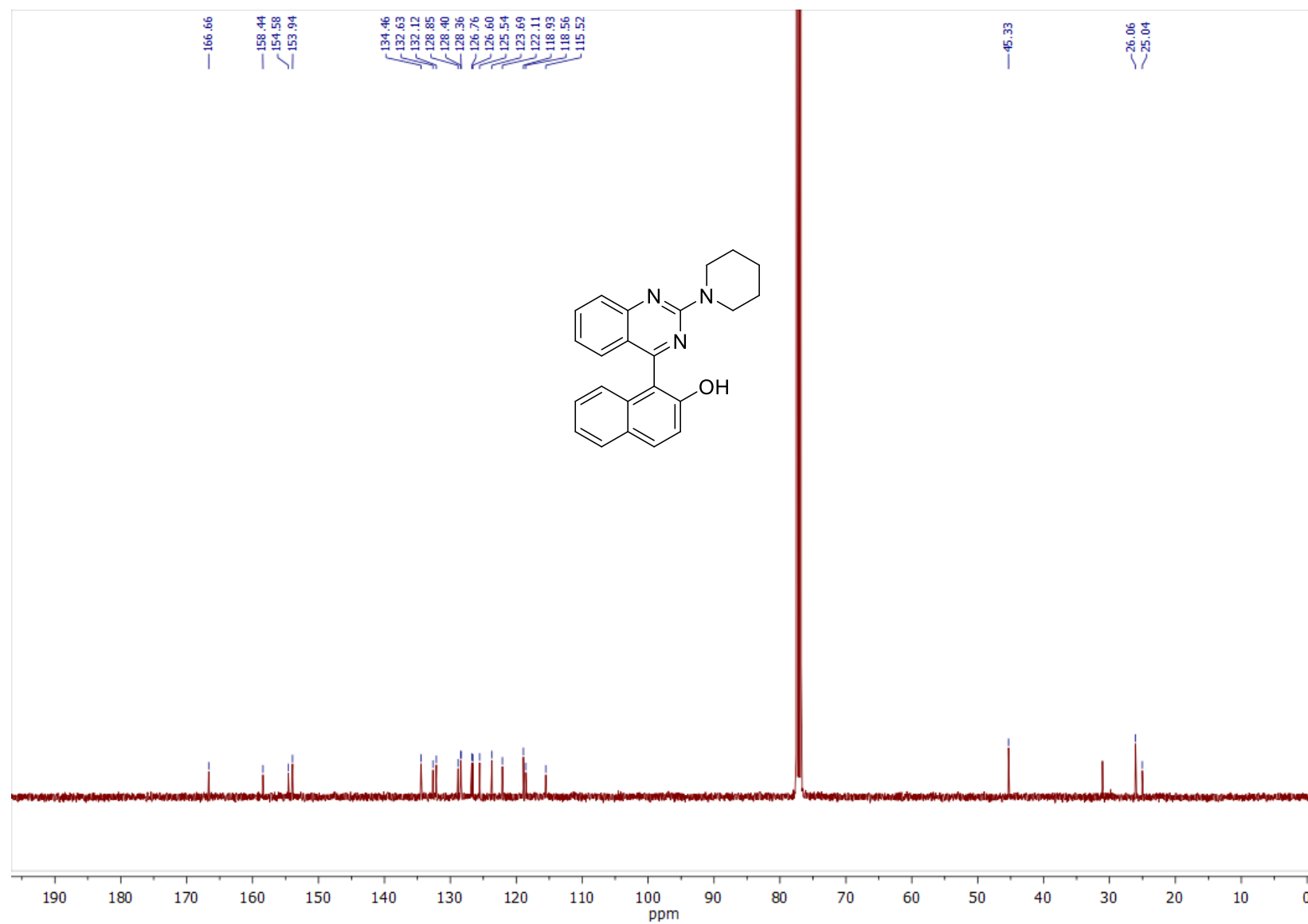


Fig. S12. ¹³C NMR Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5b**)

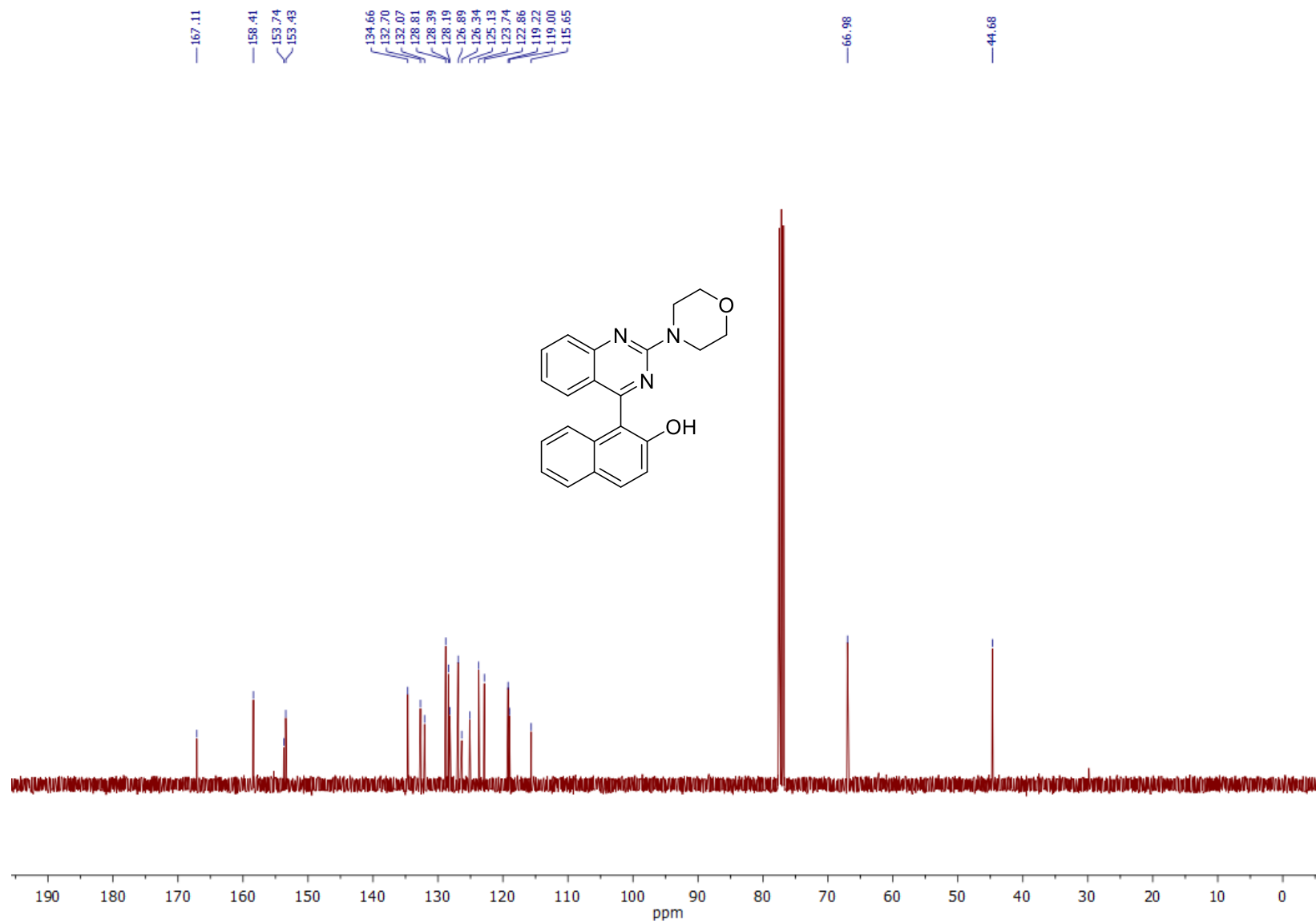


Fig. S13. ¹³C NMR Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5c**)

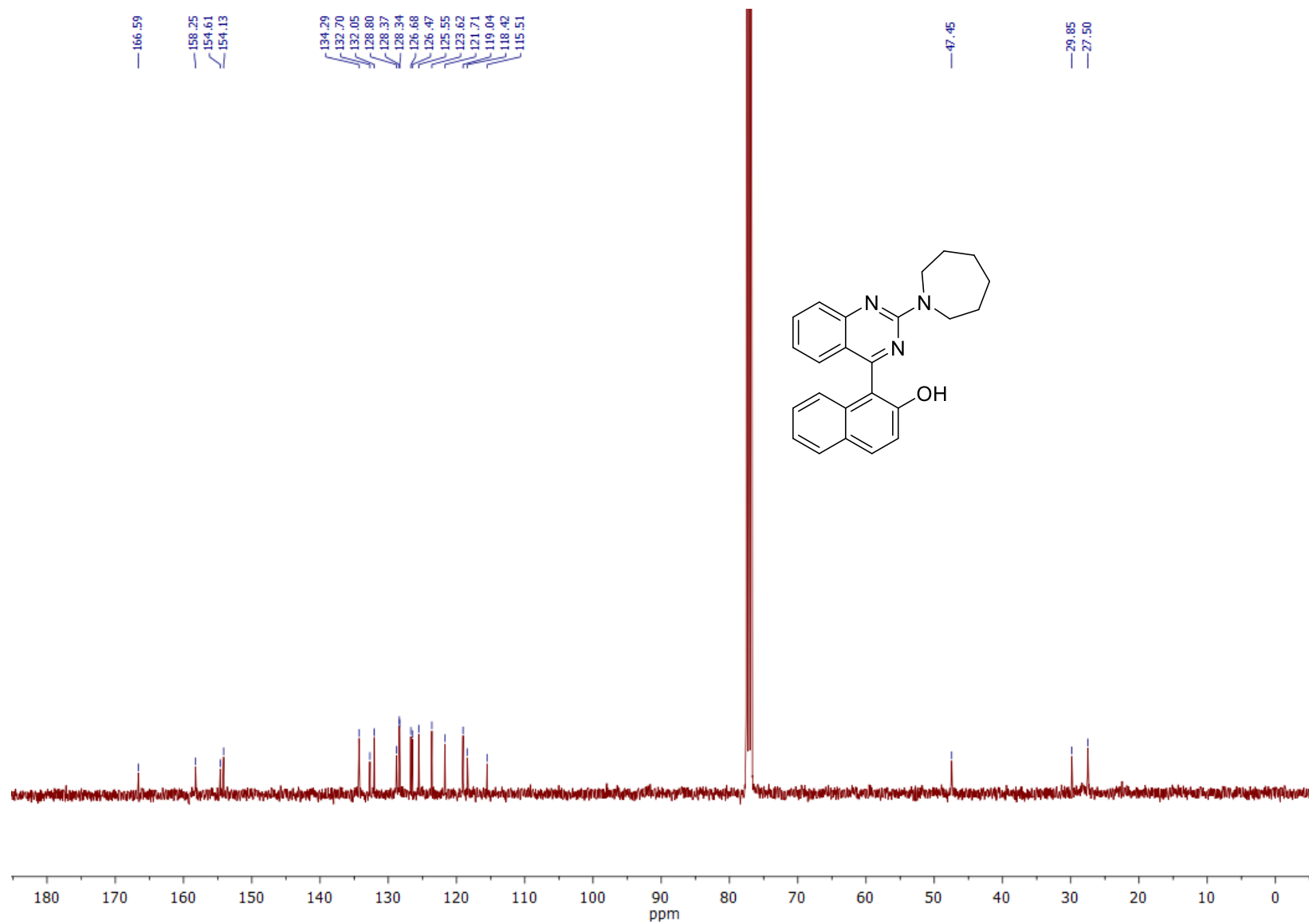


Fig. S14. ¹³C NMR Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)quinazoline (**5d**)

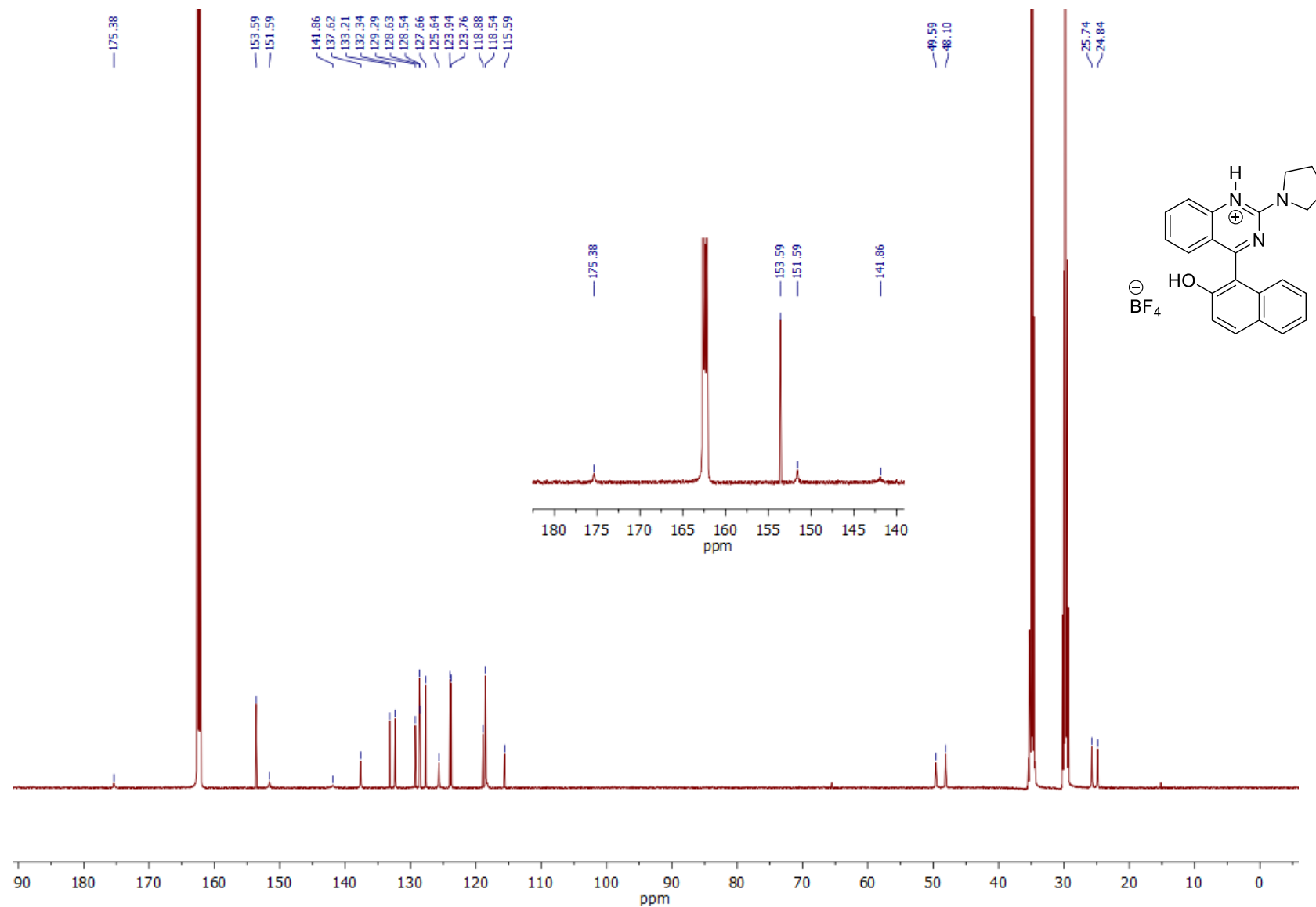


Fig. S15. ^{13}C NMR Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6a**)

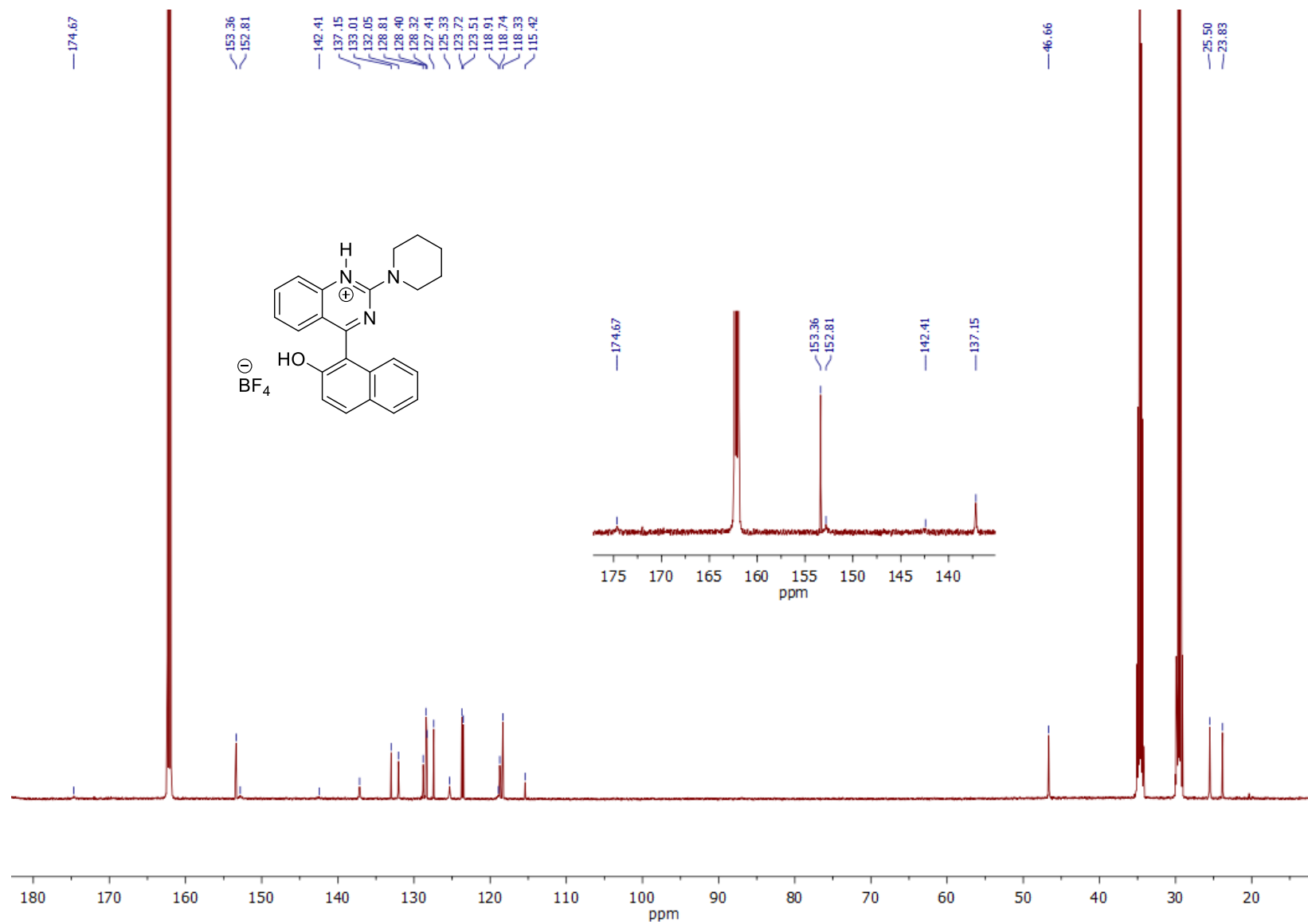


Fig. S16. ¹³C NMR Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6b**)

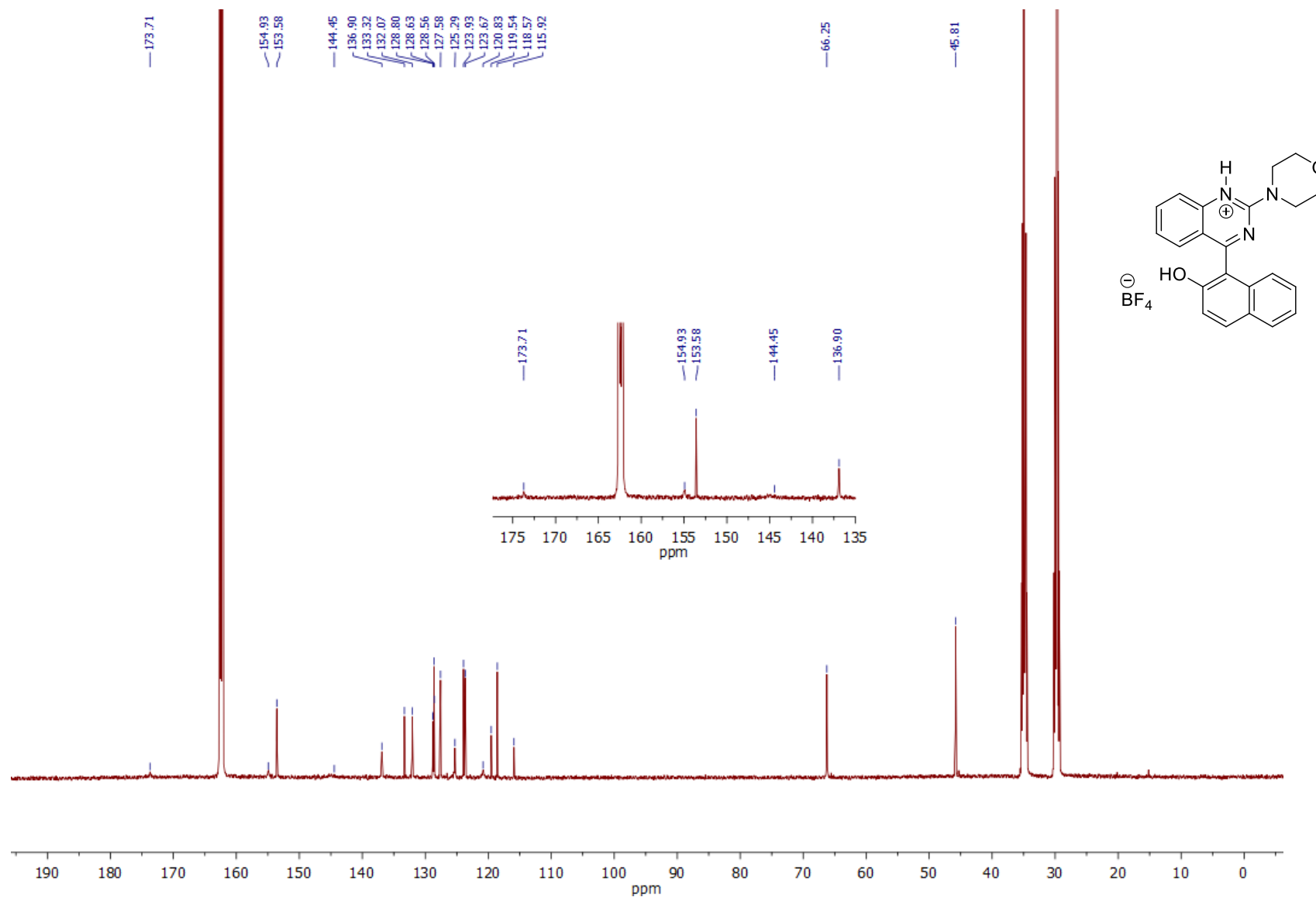


Fig. S17. ^{13}C NMR Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6c**)

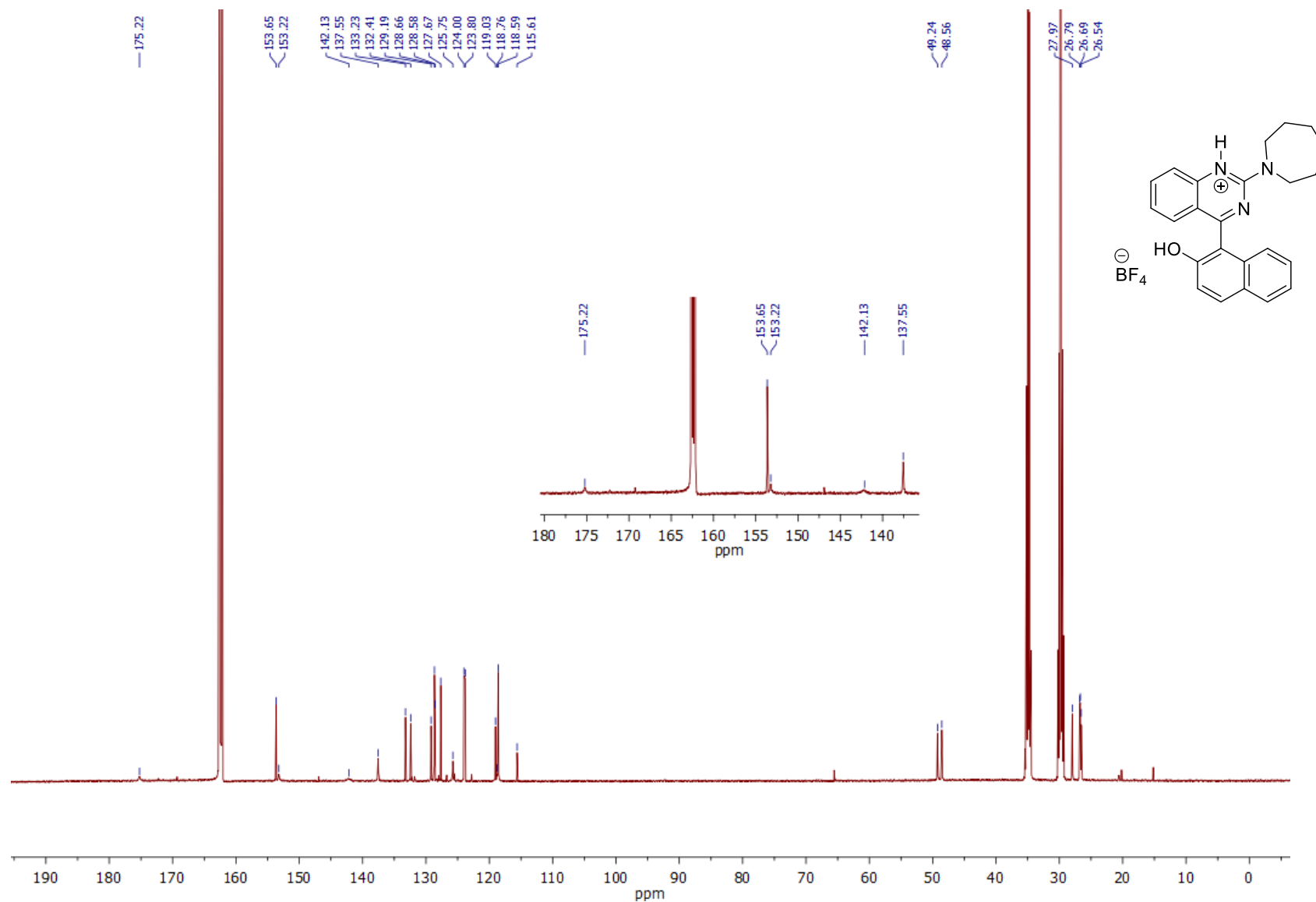


Fig. S18. ^{13}C NMR Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6d**)

HSQC and HMBC Spectra

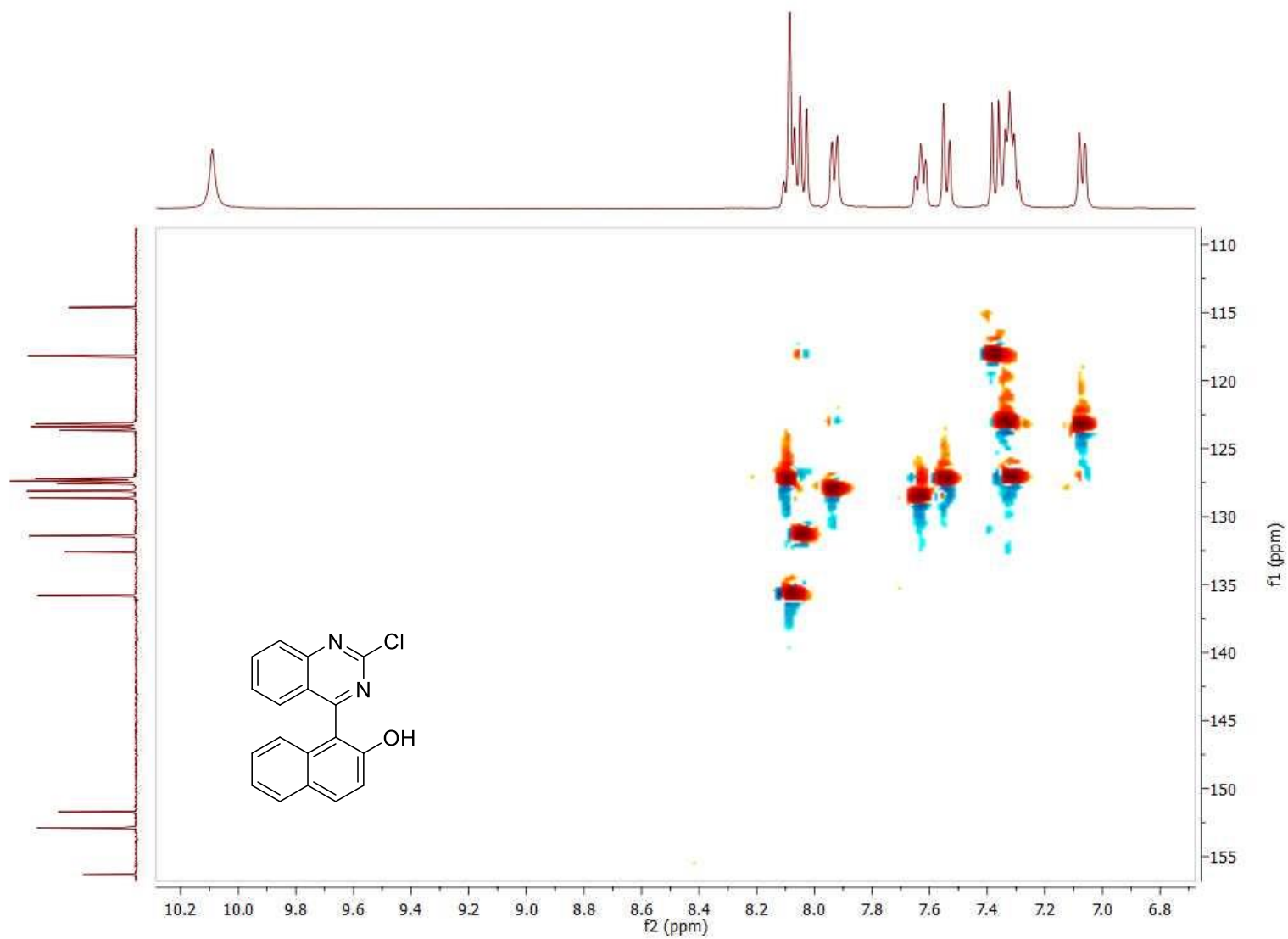


Fig. S19. HSQC Spectrum 2-hydroxy-1-(2-chloroquinazolin-4-yl)naphthalene (**3**)

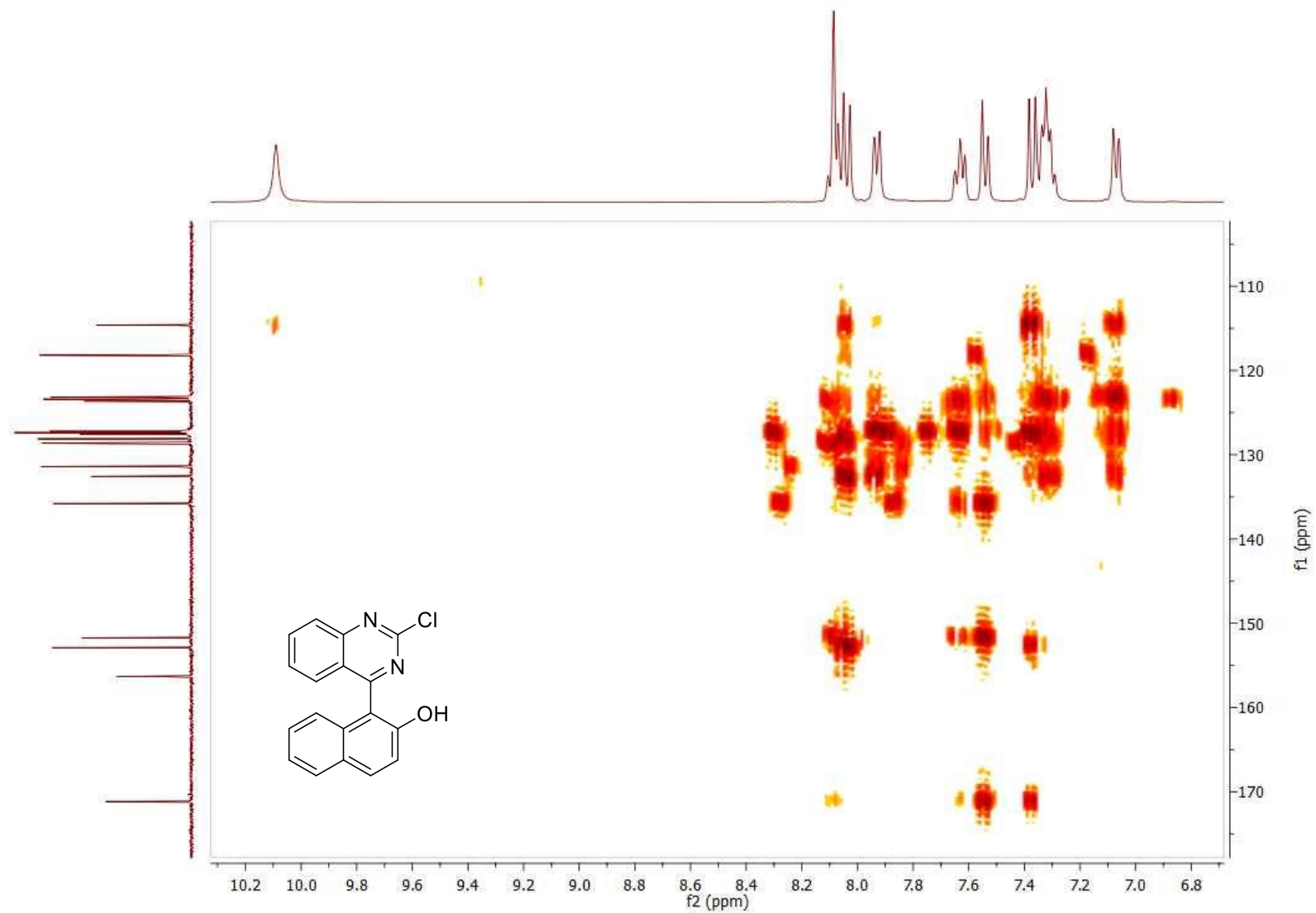


Fig. S20. HMBC Spectrum 2-hydroxy-1-(2-chloroquinazolin-4-yl)naphthalene (**3**)

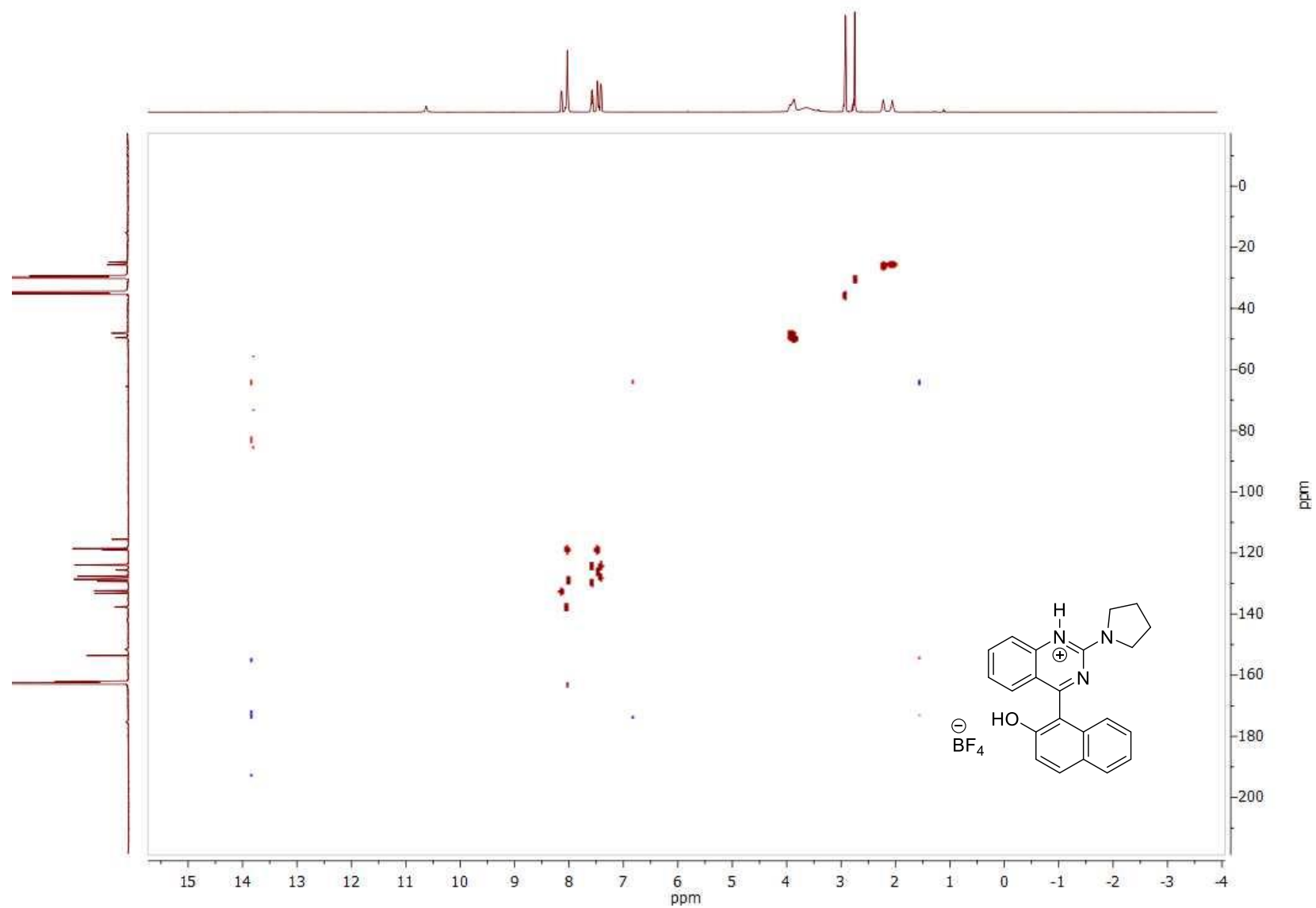


Fig. S21. HSQC Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6a**)

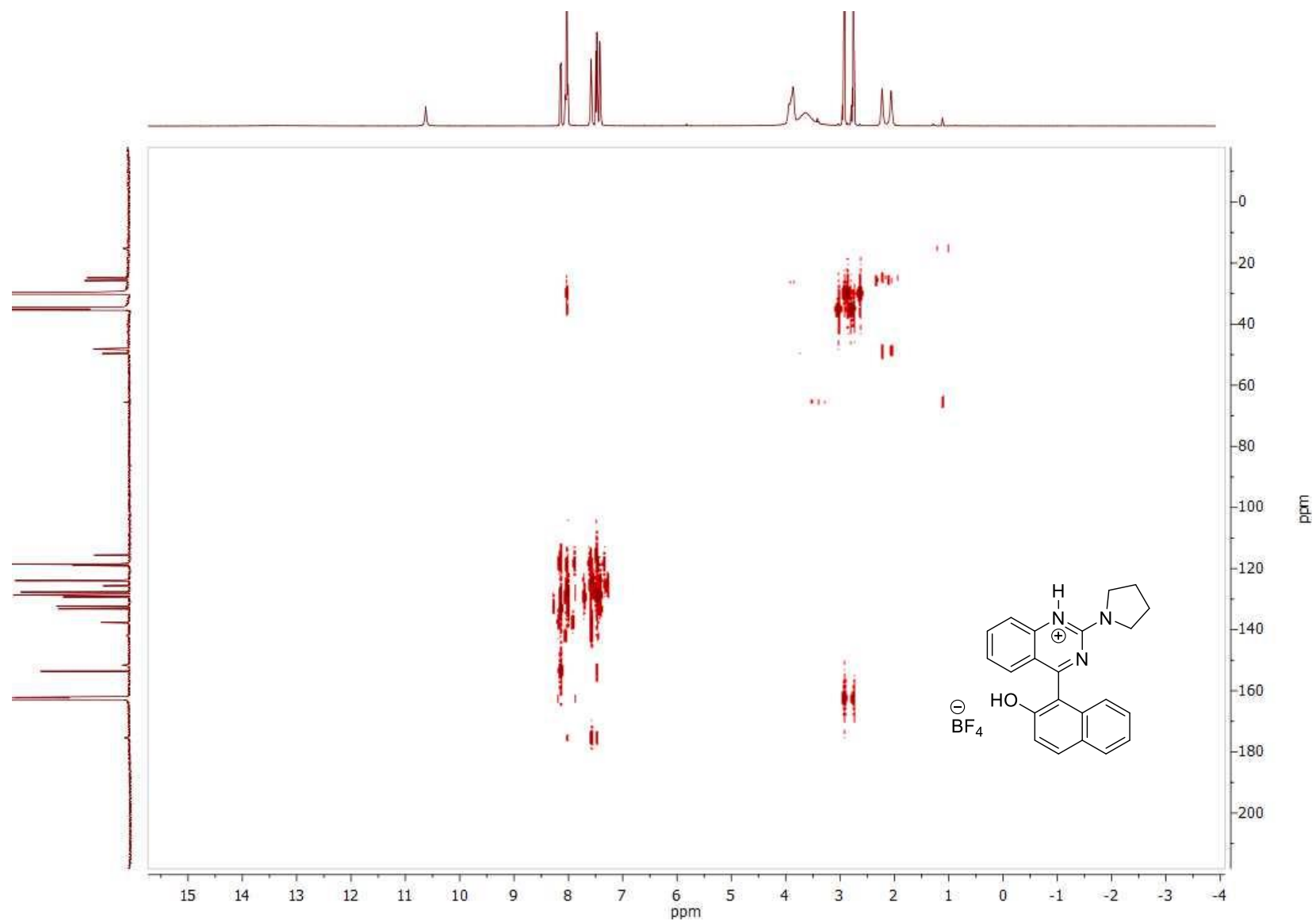


Fig. S22. HMBC Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6a**)

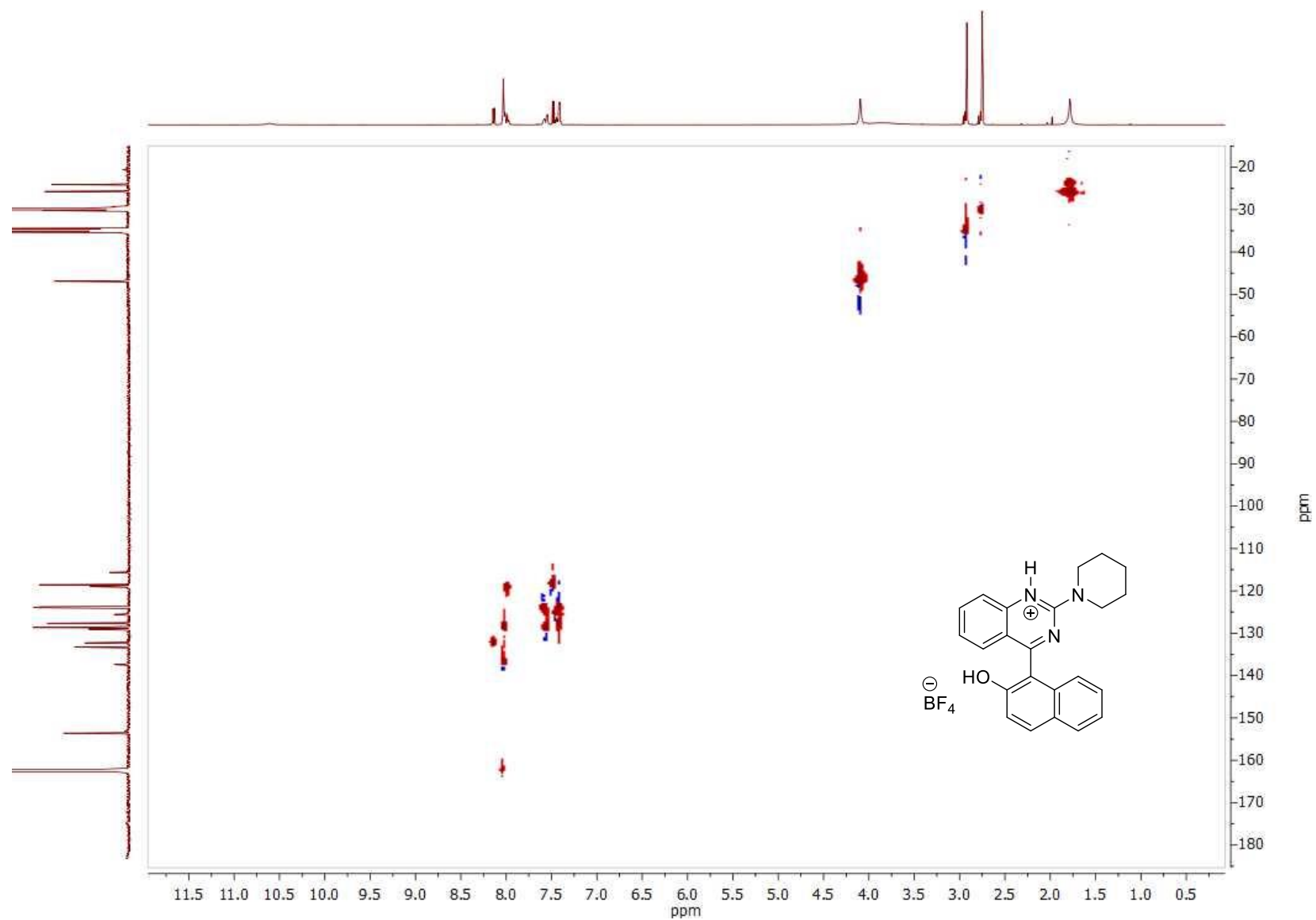


Fig. S23. HSQC Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6b**)

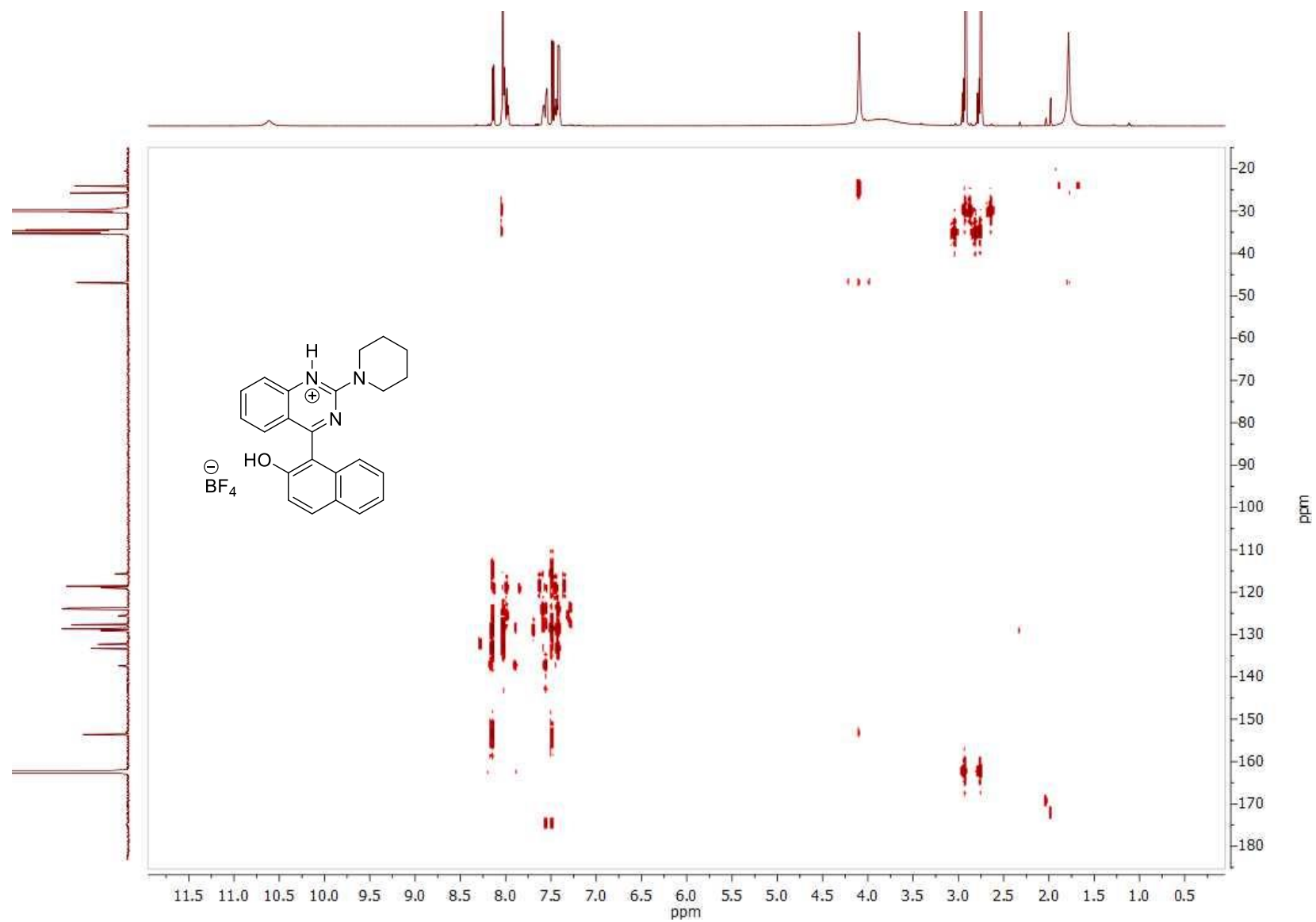


Fig. S24. HMBC Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6b**)

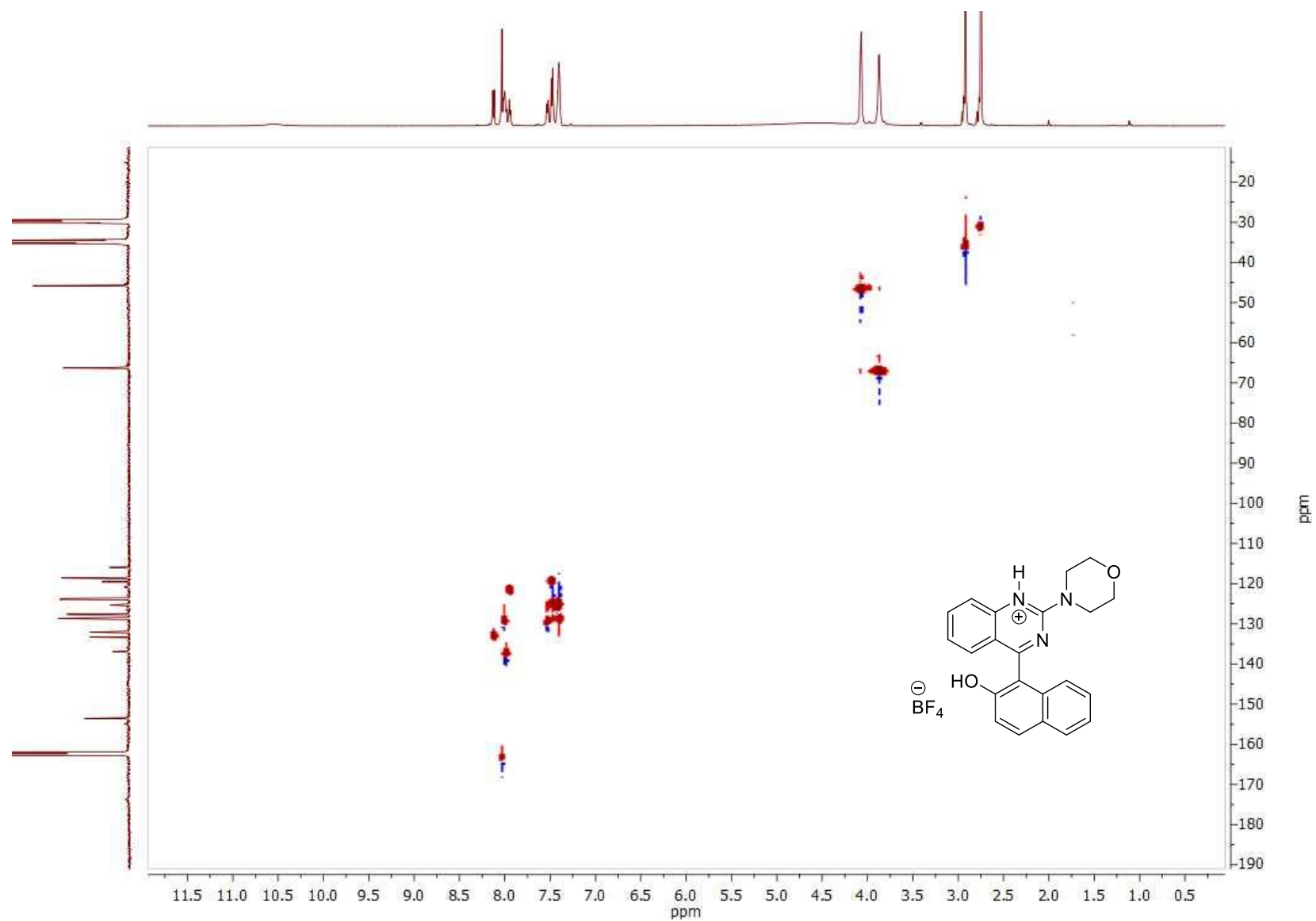


Fig. S25. HSQC Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6c**)

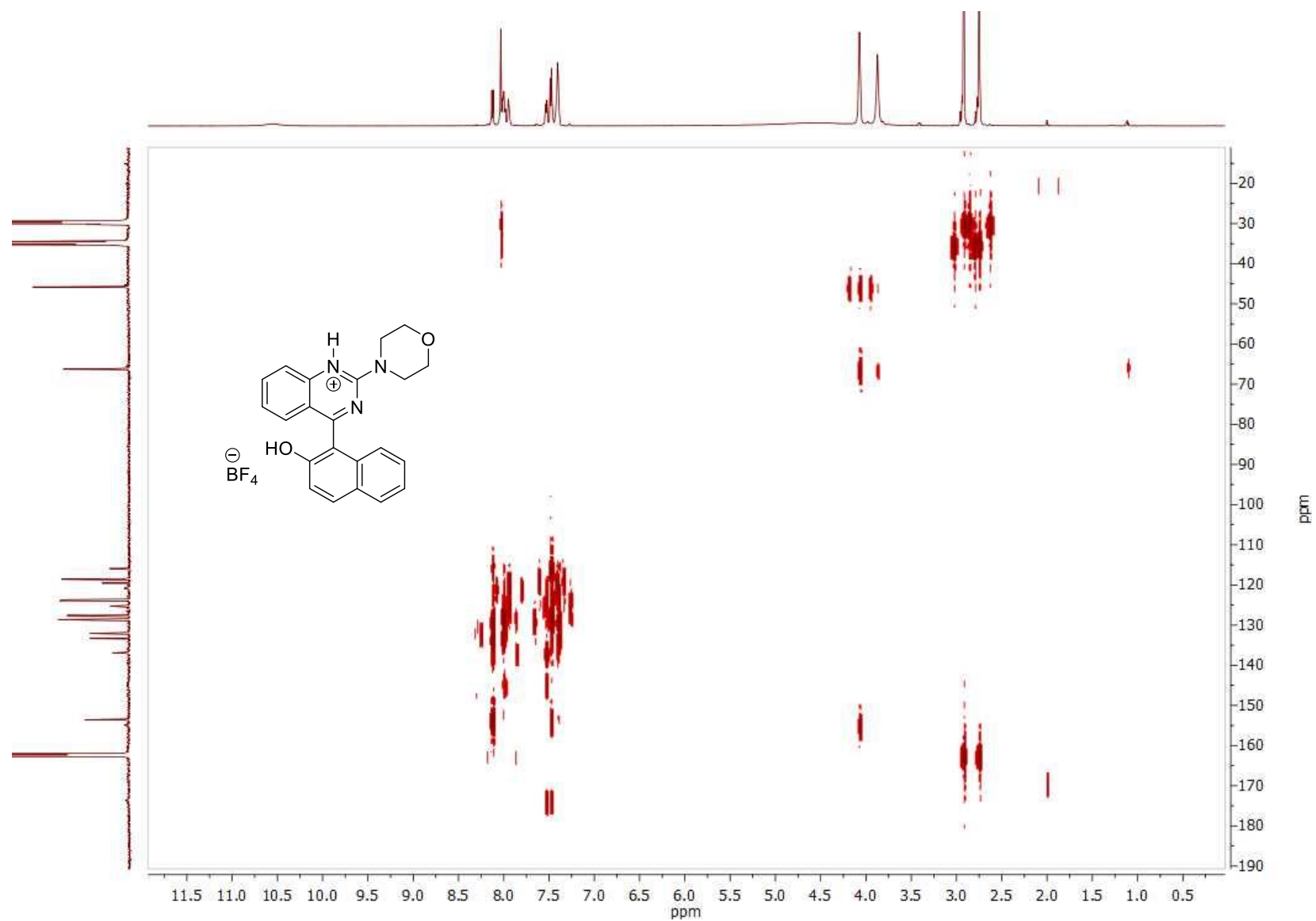


Fig. S26. HMBC Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6c**)

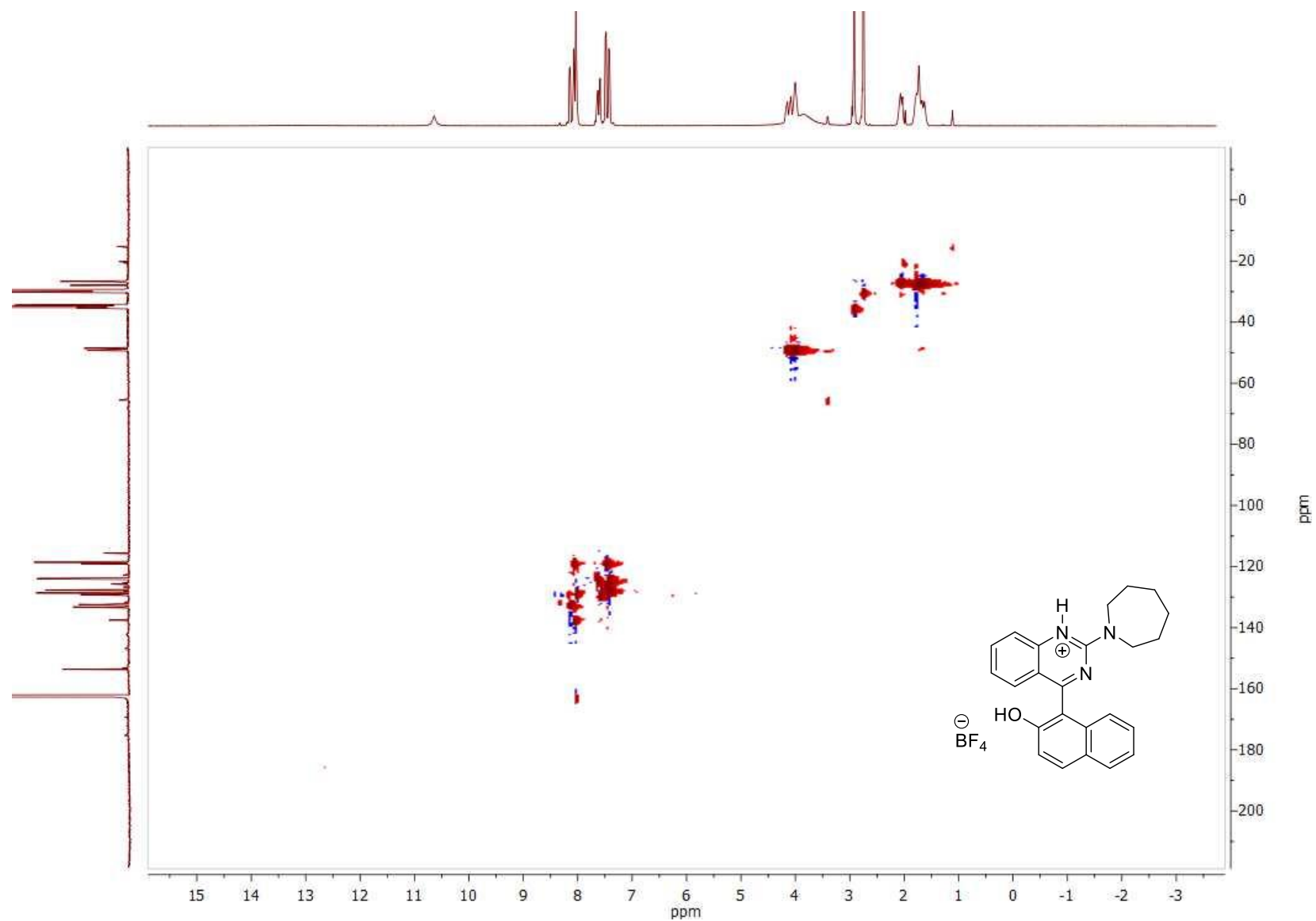


Fig. S27. HSQC Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6d**)

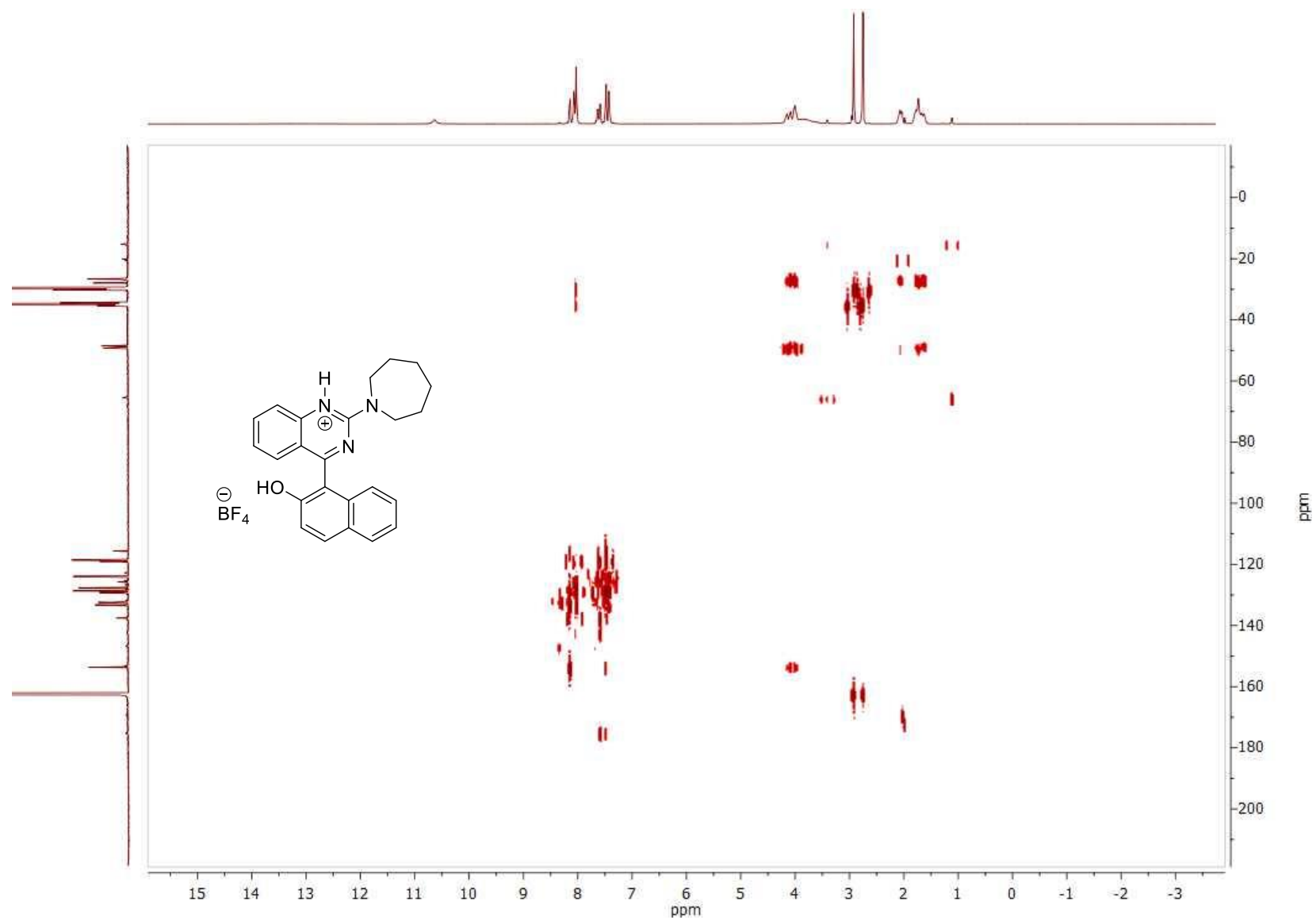


Fig. S28. HMBC Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6d**)

^{11}B and ^{19}F NMR Spectra

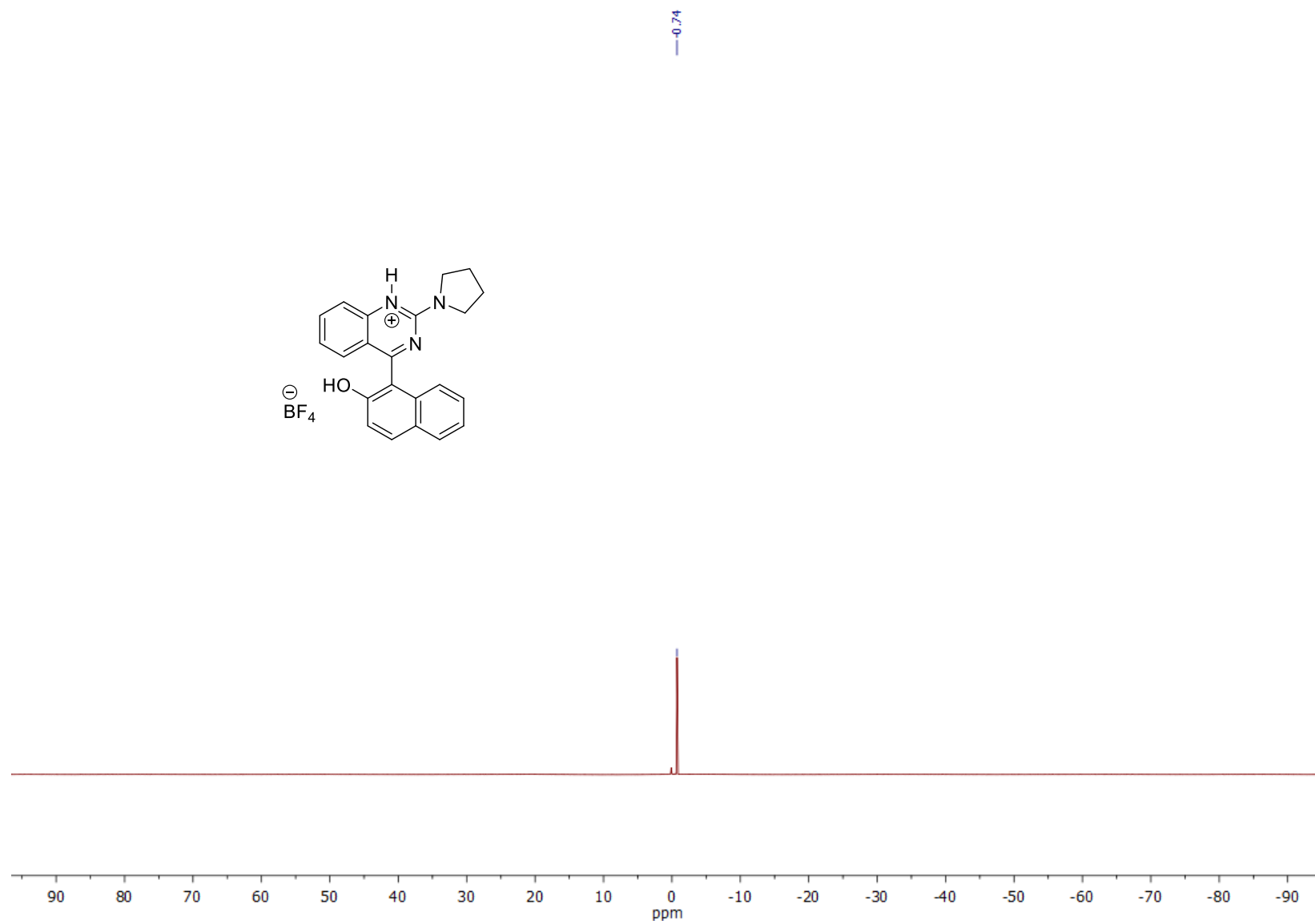


Fig. S29. ^{11}B NMR Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6a**)

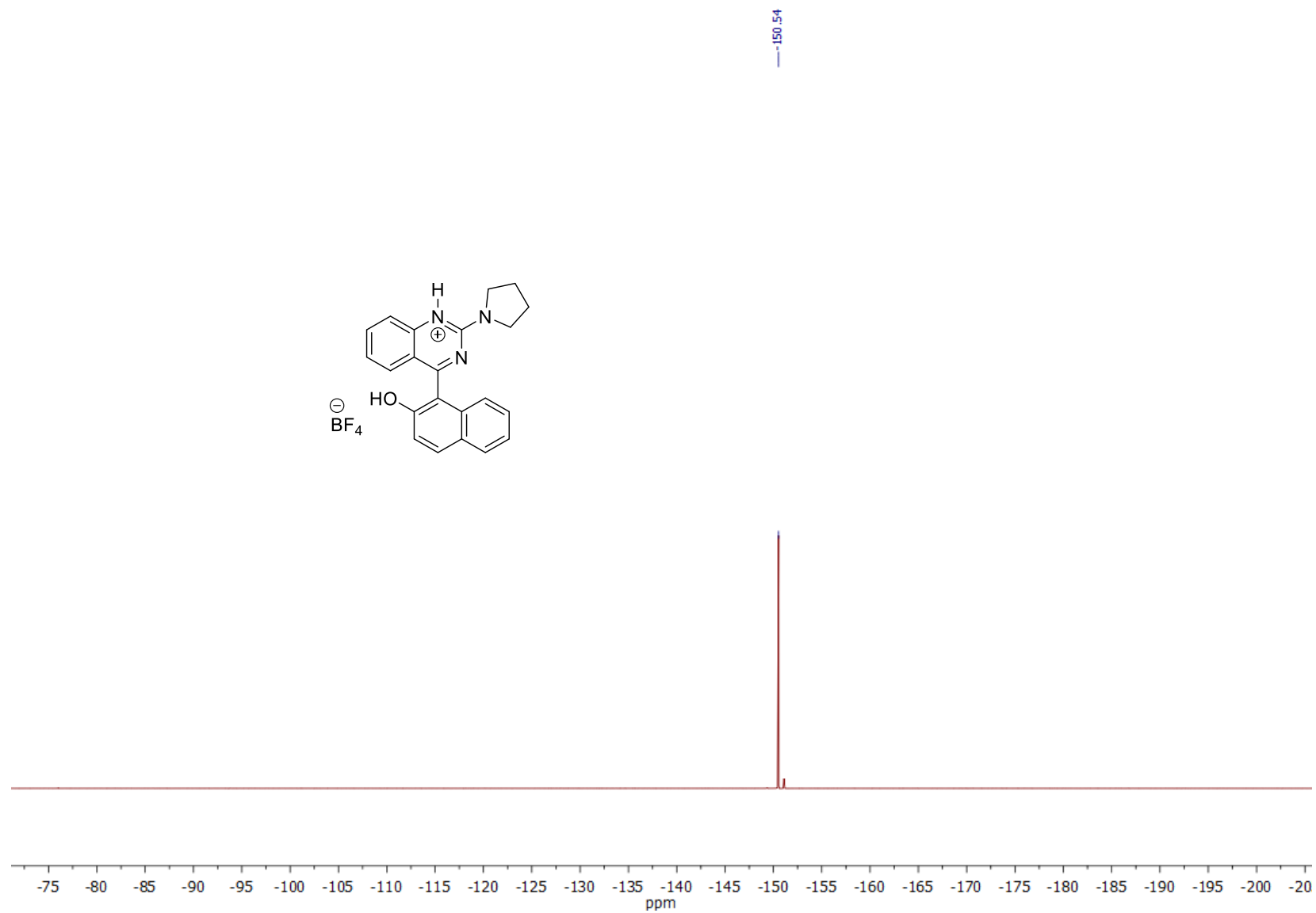


Fig. S30. ^{19}F NMR Spectrum 2-(pyrrolidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6a**)

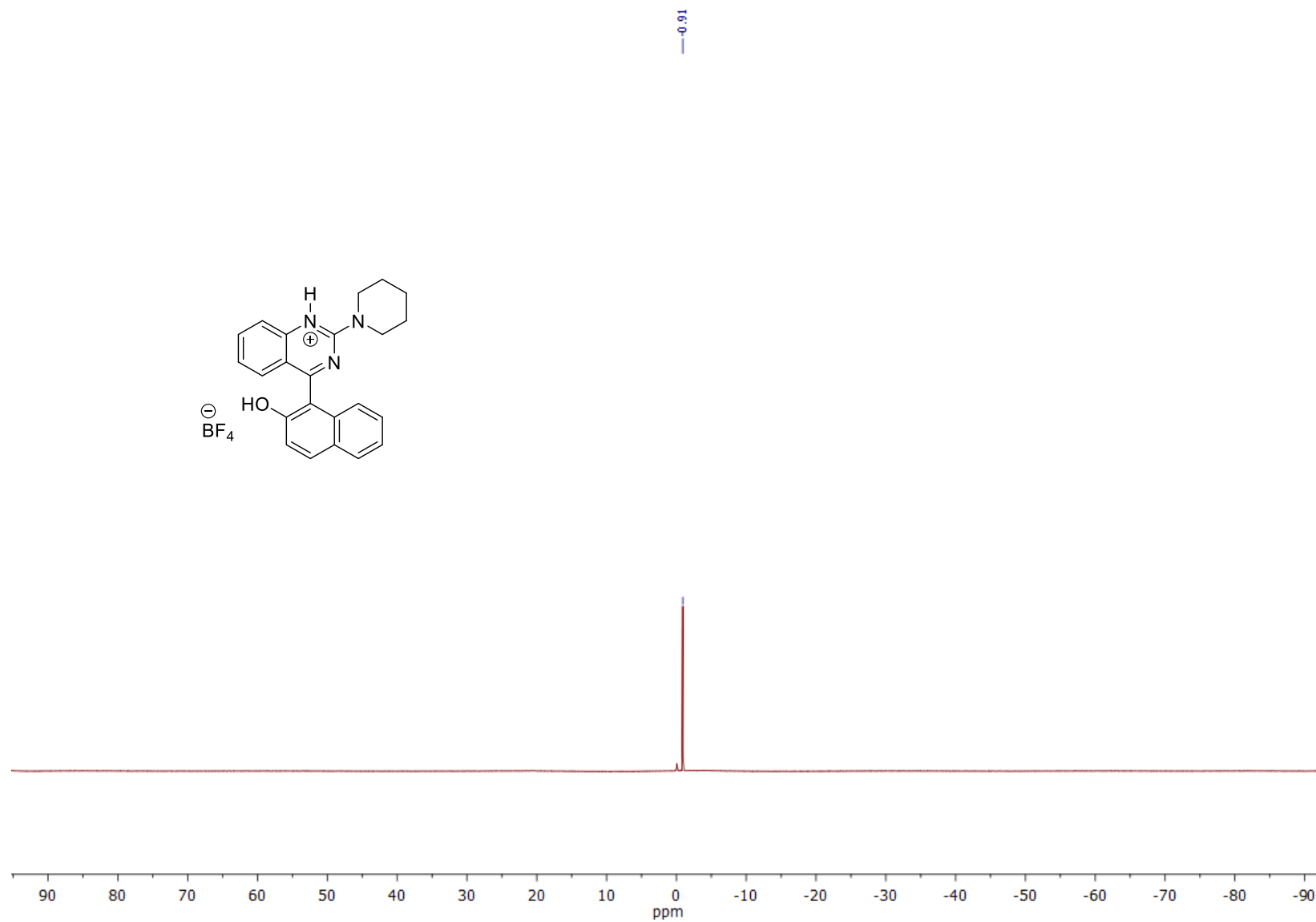


Fig. S31. ¹¹B NMR Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6b**)

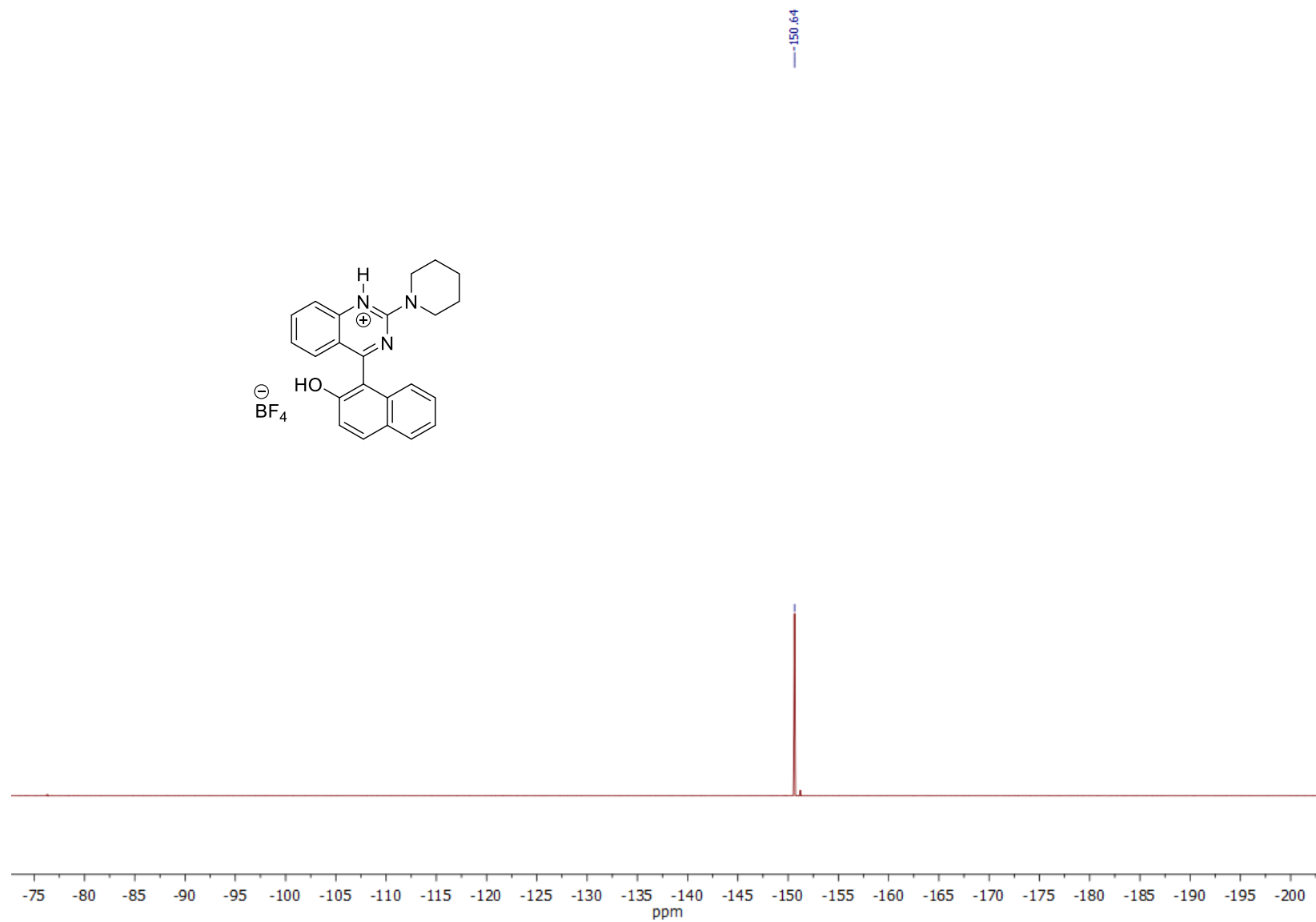


Fig. S32. ¹⁹F NMR Spectrum 2-(piperidin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6b**)

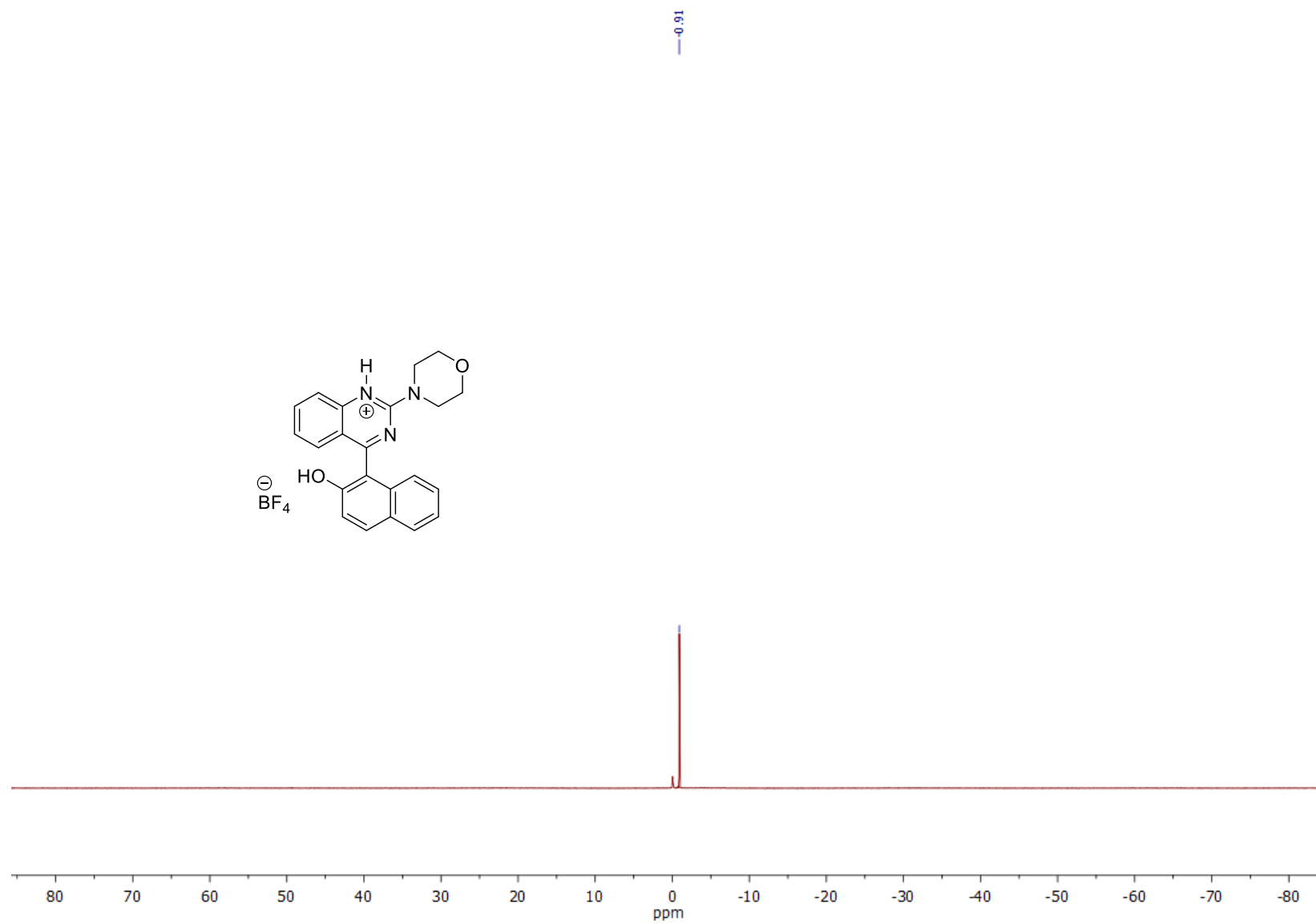


Fig. S33. ^{11}B NMR Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6c**)

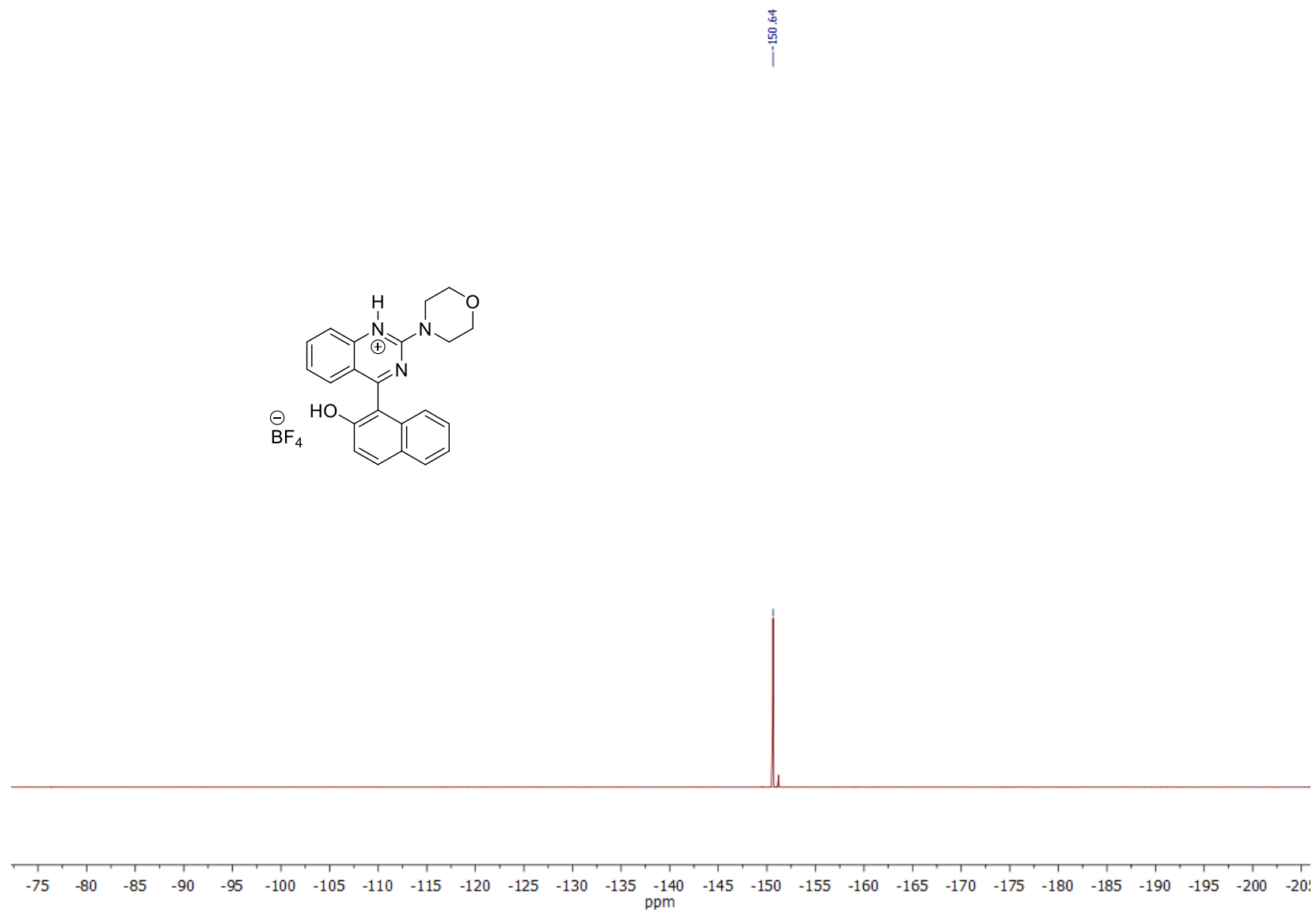


Fig. S34. ¹⁹F NMR Spectrum 2-(morpholin-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6c**)

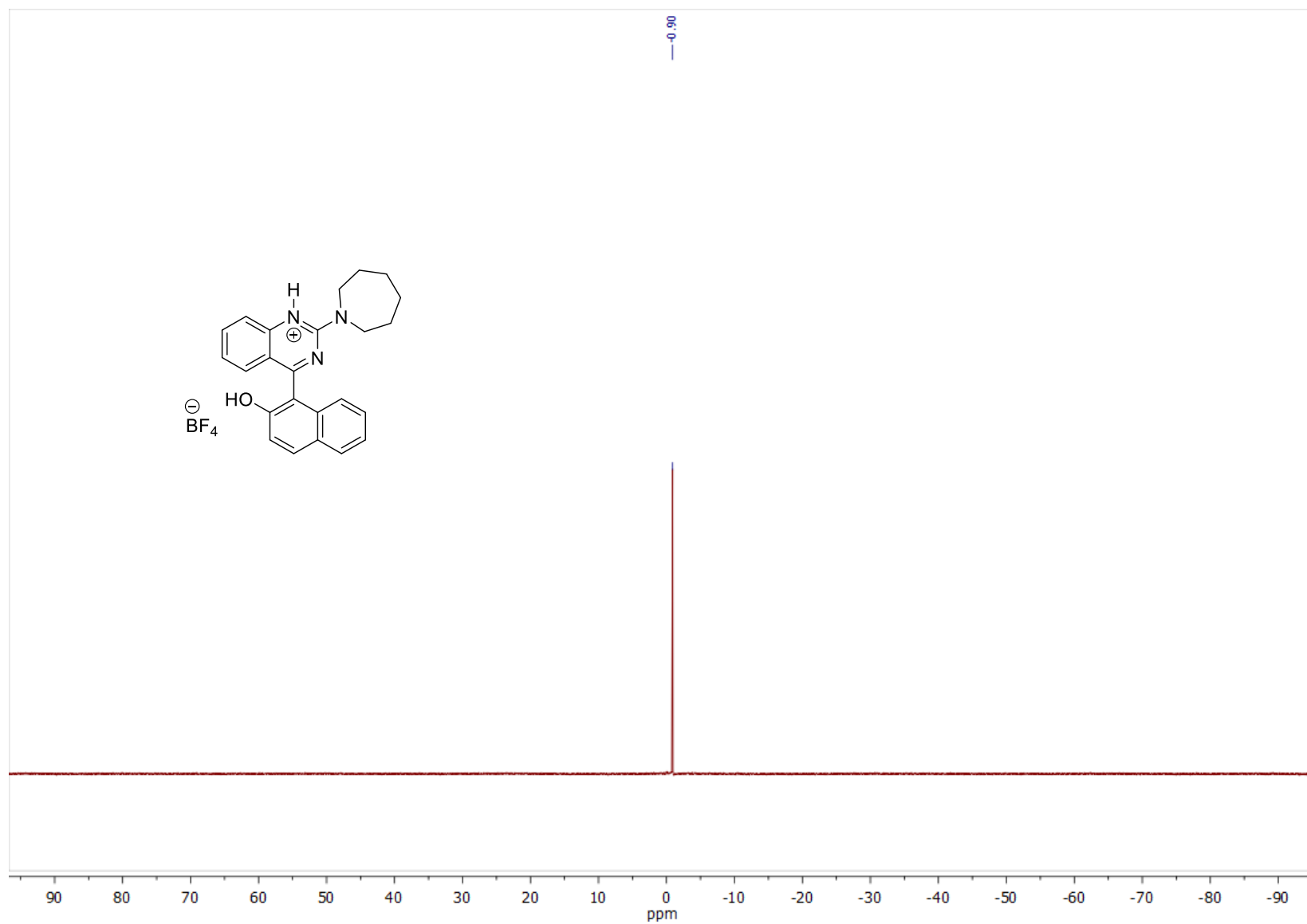


Fig. S35. ^{11}B NMR Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6d**)

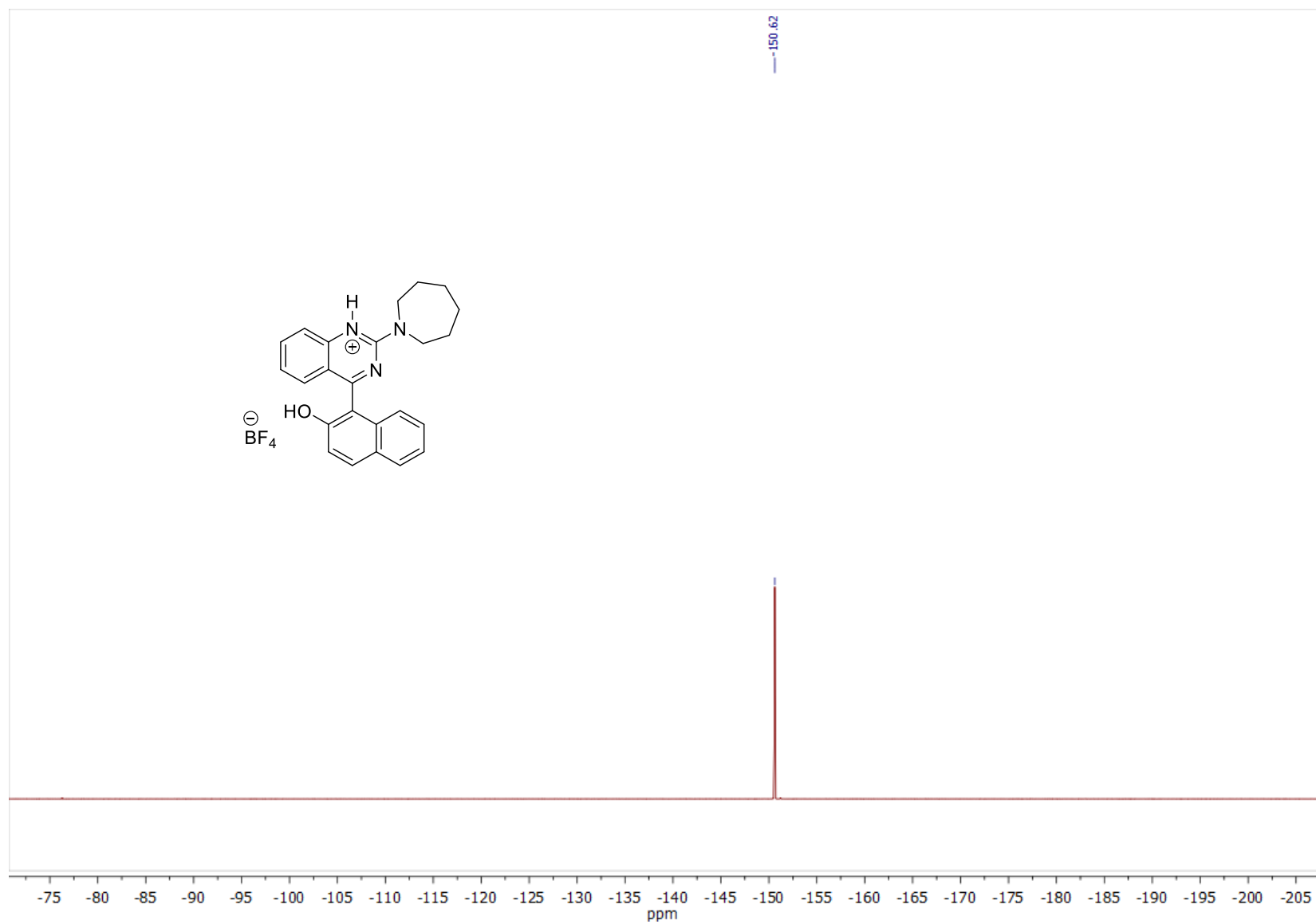


Fig. S36. ^{19}F NMR Spectrum 2-(azepan-1-yl)-4-(2-hydroxynaphthalen-1-yl)-1-quinazolinium tetrafluoroborate (**6d**)

Supplementary figures and tables showing the optical properties of the studied compounds

Calculation of Relative Fluorescence Quantum Yields

The relative fluorescence quantum yields (QY) were calculated using the following formula:

$$QY = \Phi_F^{ct} \times \left(\frac{I^{opp}}{I^{ct}} \right) \times \left(\frac{A^{ct}}{A^{opp}} \right) \times \left(\frac{n^{opp}}{n^{ct}} \right)^2$$

where I^{sam} and I^{st} are the integrated fluorescence intensities of the sample and the standard, respectively.

A^{sam} and A^{st} are the optical densities of the sample and the standard at the excitation wavelength.

n^{sam} and n^{st} are the refractive indices of the sample and standard solutions.

All measurements were carried out in 10-mm quartz cuvettes at room temperature. Quinine sulfate in an aqueous solution of H_2SO_4 (0.1 M) at a concentration of 5×10^{-5} M was used as the standard, which has a known quantum yield $\Phi_F = 0.546$ upon excitation at a wavelength of 350 nm.

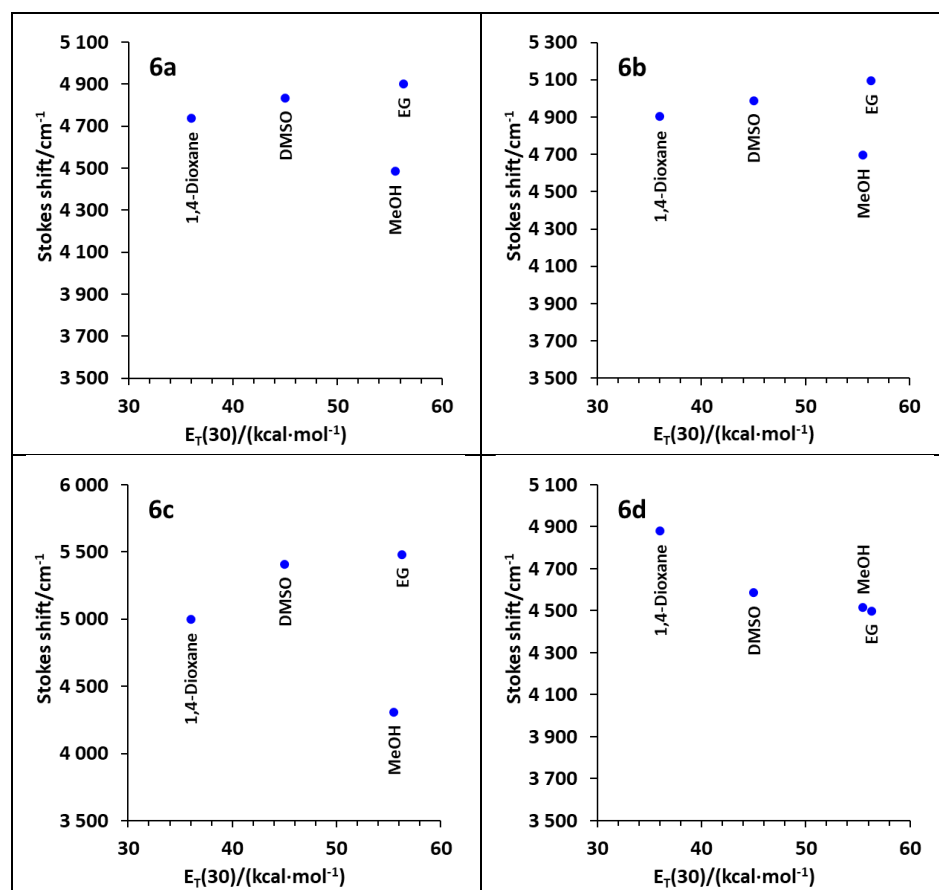


Fig. S37. Graphs of Stokes shift of fluorophores **6a–d** versus of the macroscopic solvent polarity $E_T(30)$ according to the Dimroth–Reichardt scale [1]. Solvents used: 1,4-dioxane, DMSO, MeOH, EG

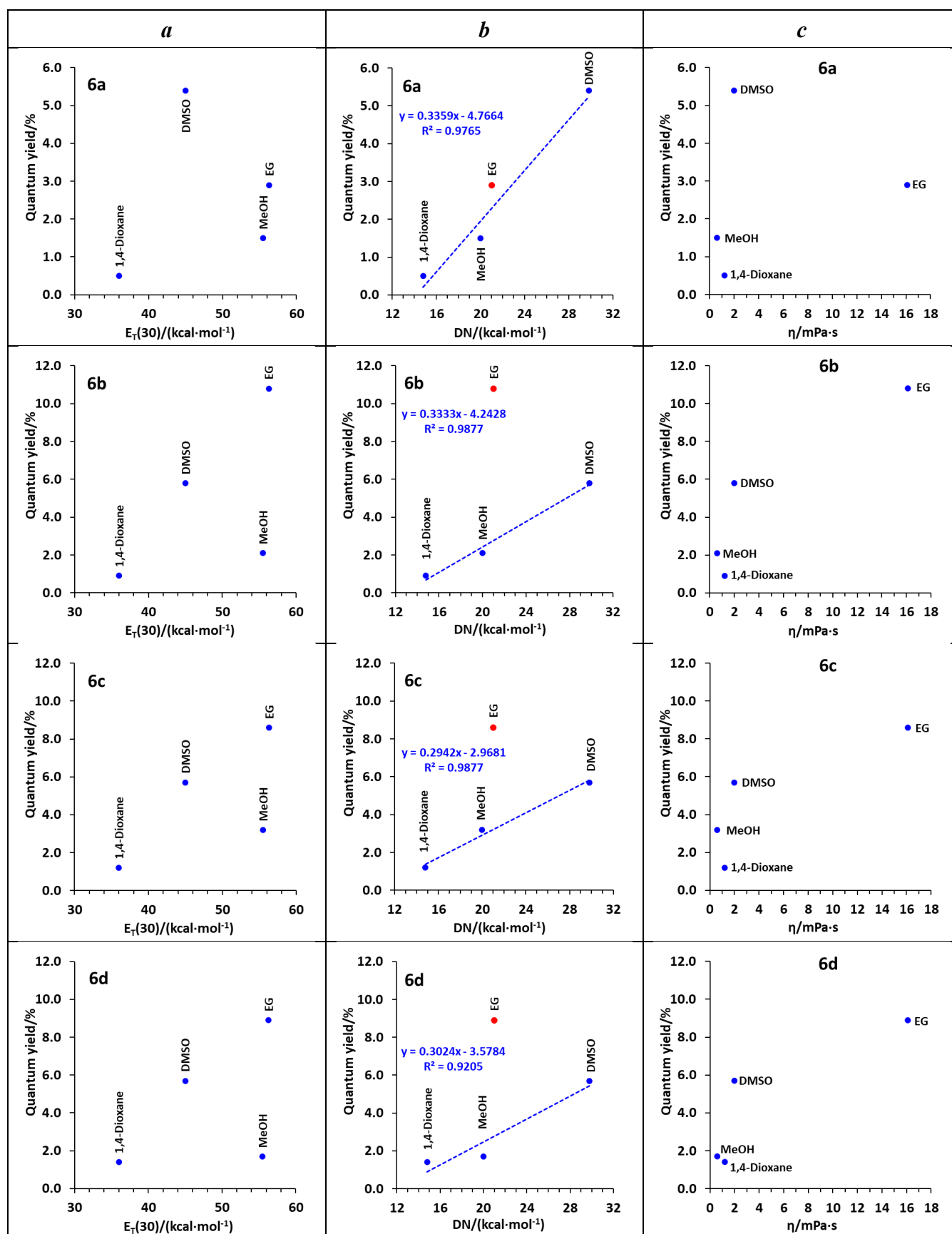


Fig. S38. Fluorescence quantum yield of fluorophores **6a–d** versus (a) the macroscopic solvent polarity $E_T(30)$ according to the Dimroth–Reichardt scale [1]; (b) the Gutmann donor number (DN) of the solvent [2]; (c) the solvent viscosity (η) [3]. Solvents used: 1,4-dioxane, DMSO, MeOH, ethylene glycol (EG)

References

1. C. Reichardt, *Angew. Chem. Int. Ed.*, 1979, **18**, 98.
2. V. Gutmann, *The Donor-Acceptor Approach to Molecular Interactions*, Springer, New York, 1978, 279 p.; ISBN 978-0-306-31064-5.
3. C. Wohlfarth, *Viscosity of Pure Organic Liquids and Binary Liquid Mixtures*, ed. M. D. Lechner (Landolt-Börnstein. Numerical Data and Functional Relationships in Science and Technology. New Series; vol. 25), Springer, Berlin, 2009, 382 p.; ISBN 978-3-540-56050-0.