

Supporting Information

Bioisosteric replacement of central 1,2,4-oxadiazole ring of high affinity CB₂ ligands by regioisomeric 1,3,4-oxadiazole ring

Dominik Heimann,^{a,§} Corinna Lueg,^{a,§} Henk de Vries,^b Bastian Frehland,^a Dirk Schepmann,^a Laura H. Heitman^b and Bernhard Wünsch^{a,c}

§ Both authors contributed equally to this work.

^a Institut für Pharmazeutische und Medizinische Chemie der Universität Münster, Corrensstraße 48, D-48149 Münster, Germany.

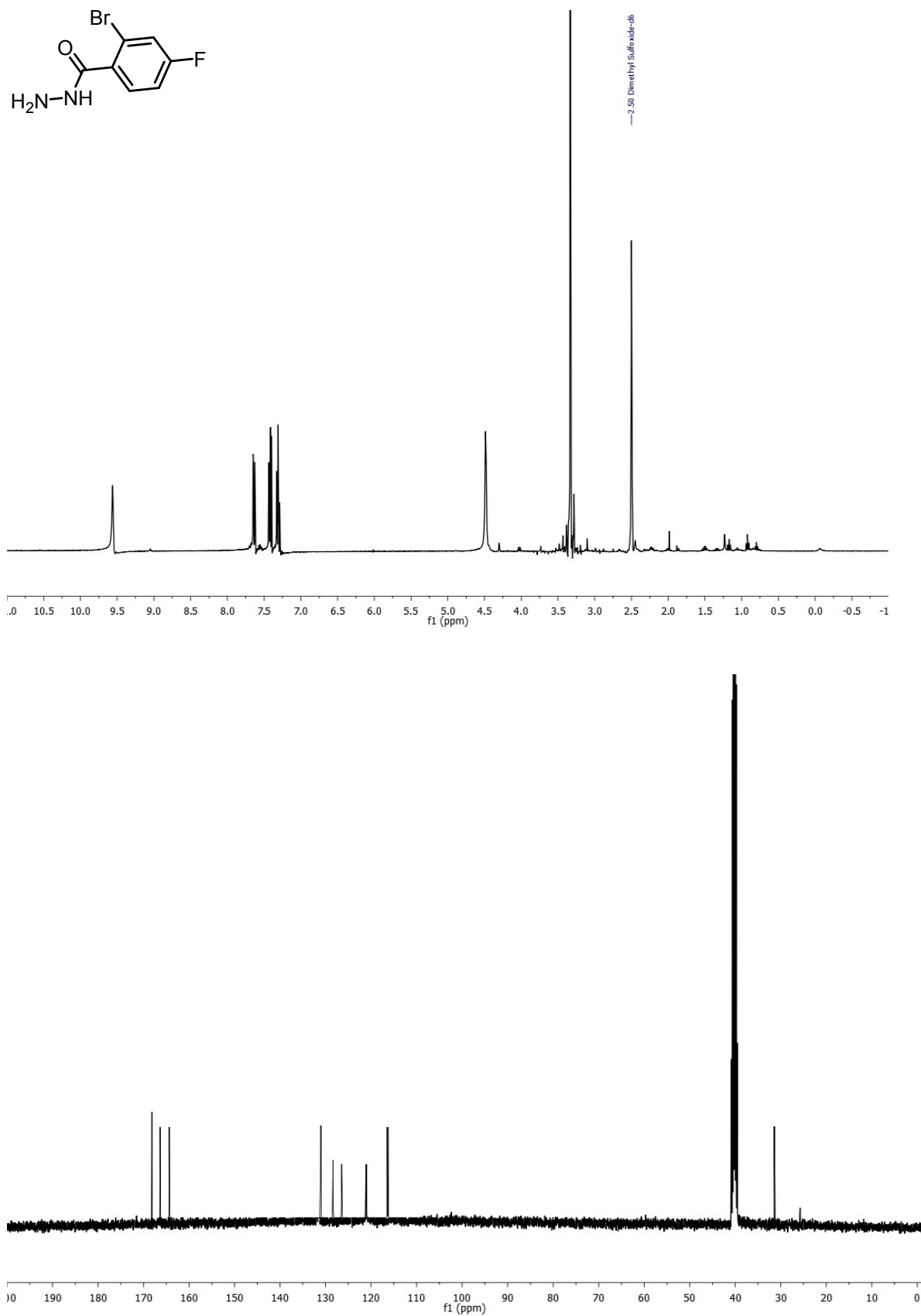
Tel.: +49-251-8333311; Fax: +49-251-8332144; E-mail: wuensch@uni-muenster.de

^b Division of Medicinal Chemistry, Leiden Academic Centre for Drug Research, Leiden University, P.O. Box 9502, 2300 RA Leiden, The Netherlands.

^c Cells-in-Motion Cluster of Excellence (EXC 1003 – CiM), Westfälische Wilhelms-Universität Münster, Germany.

Content

¹H and ¹³C NMR spectra

1. ^1H and ^{13}C NMR spectraFigure 1. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **3a**.

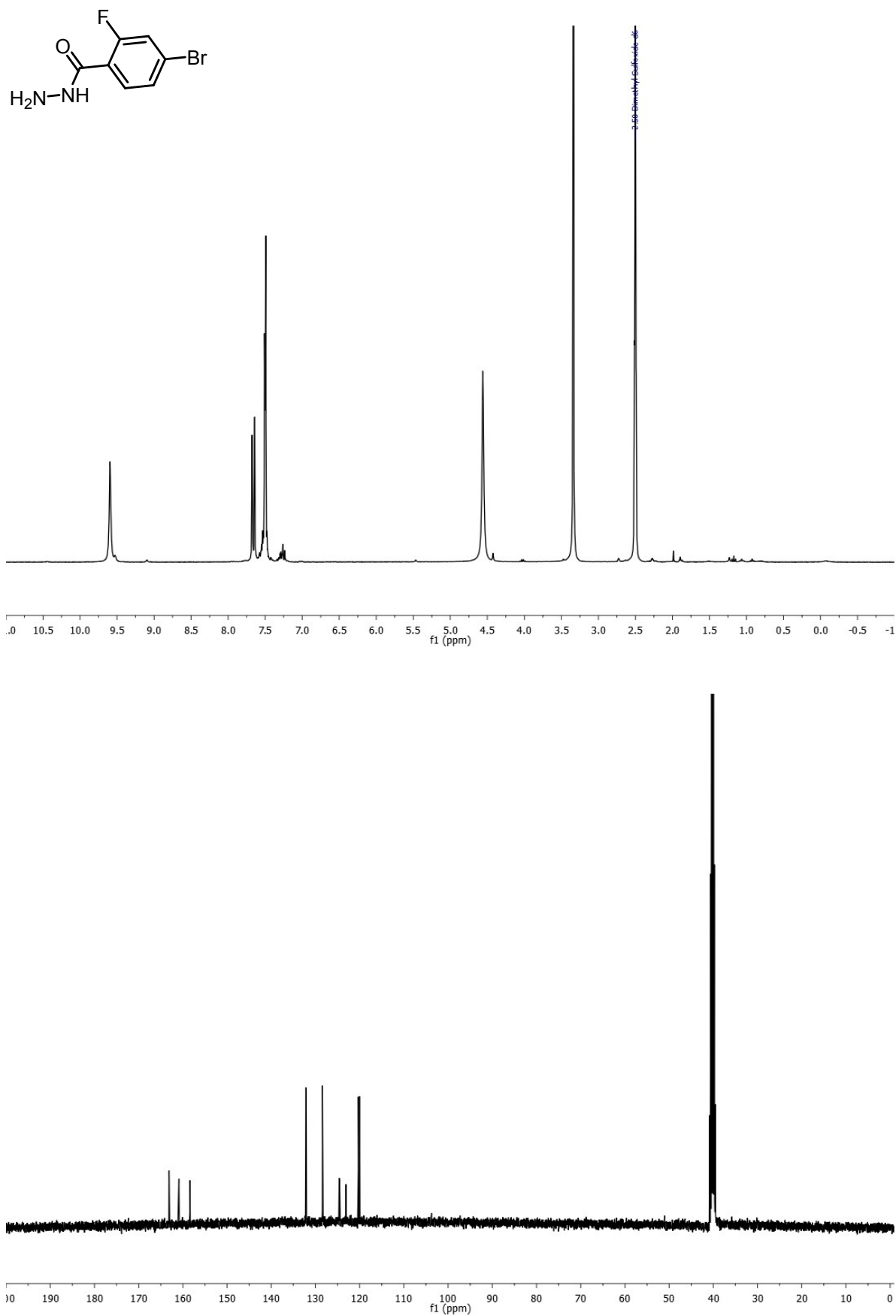


Figure 2. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **3b**.

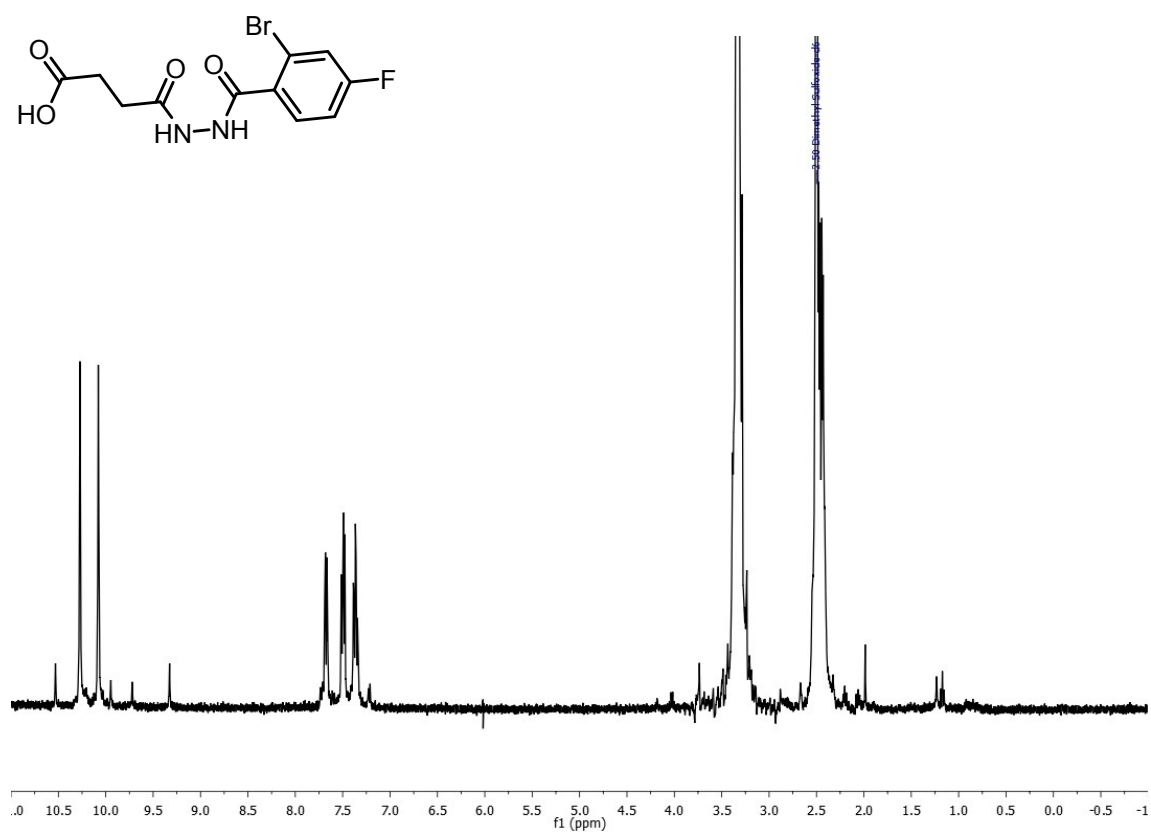


Figure 3. ¹H NMR spectrum of compound **4a**.

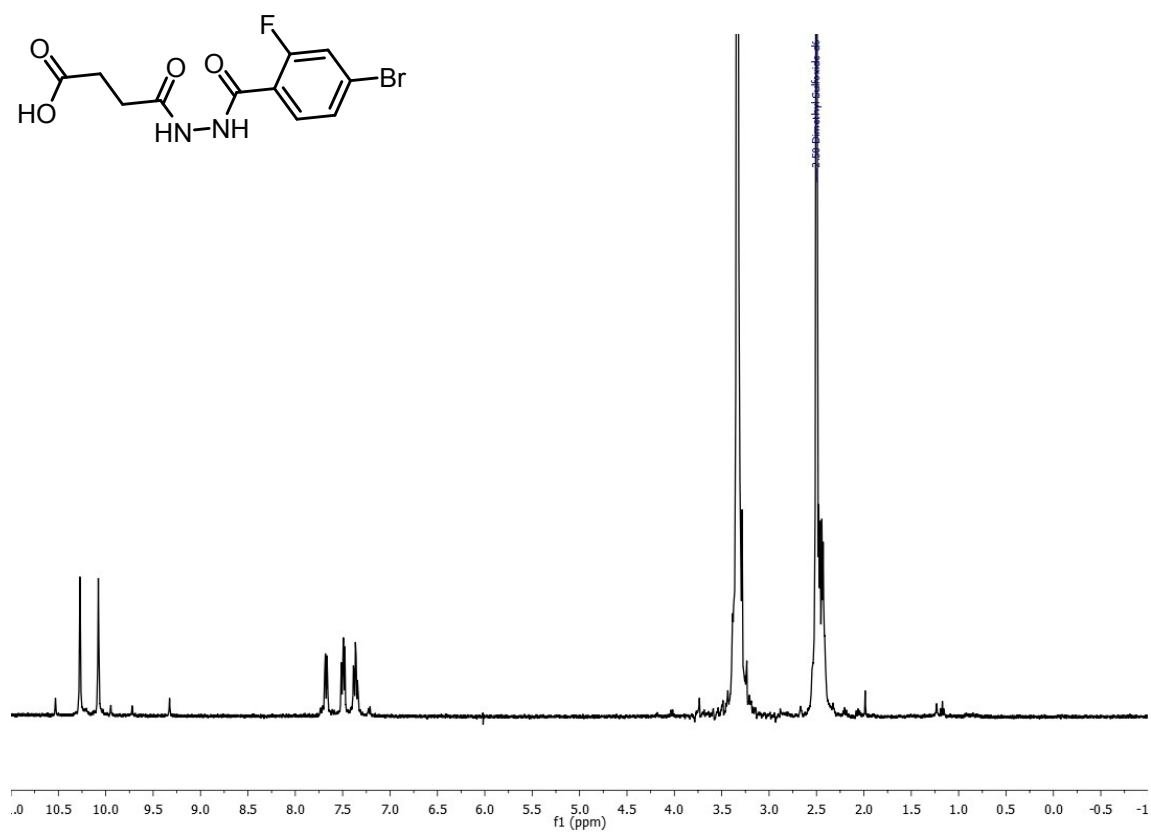


Figure 4. ¹H NMR spectrum of compound **4b**.

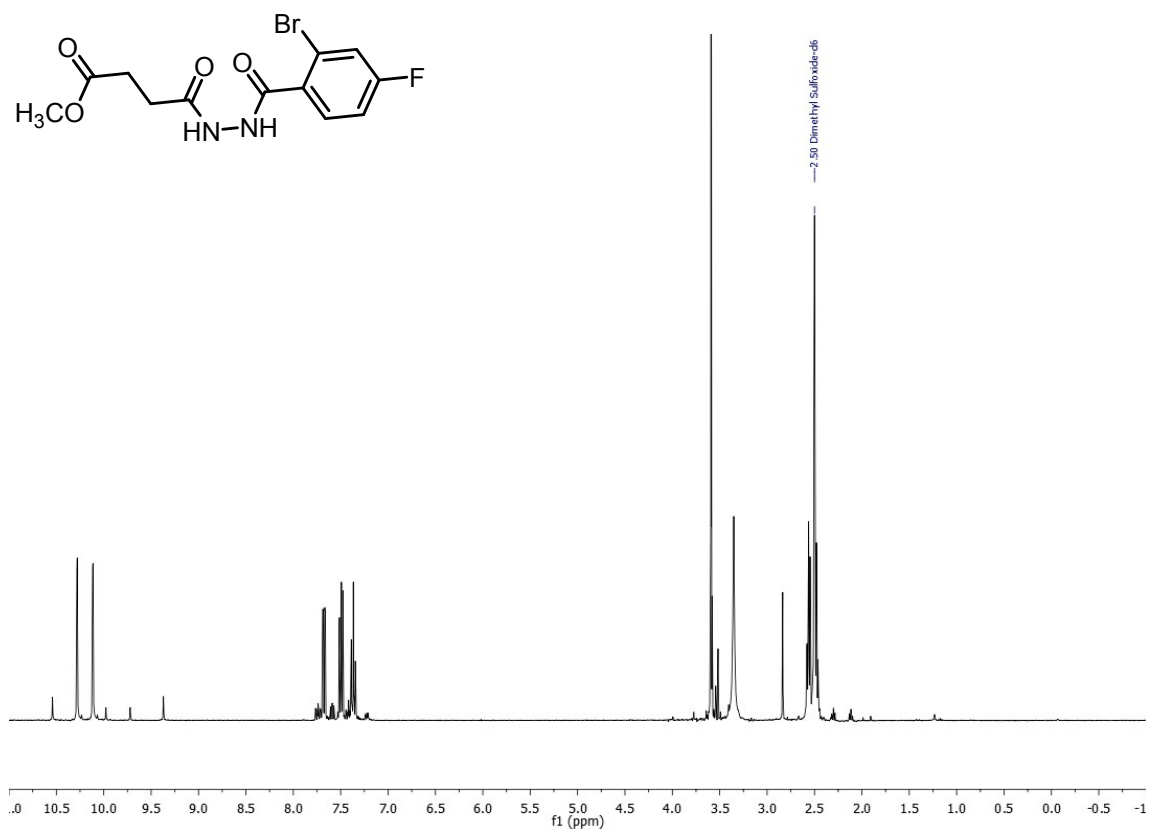


Figure 5. ¹H NMR spectrum of compound **5a**.

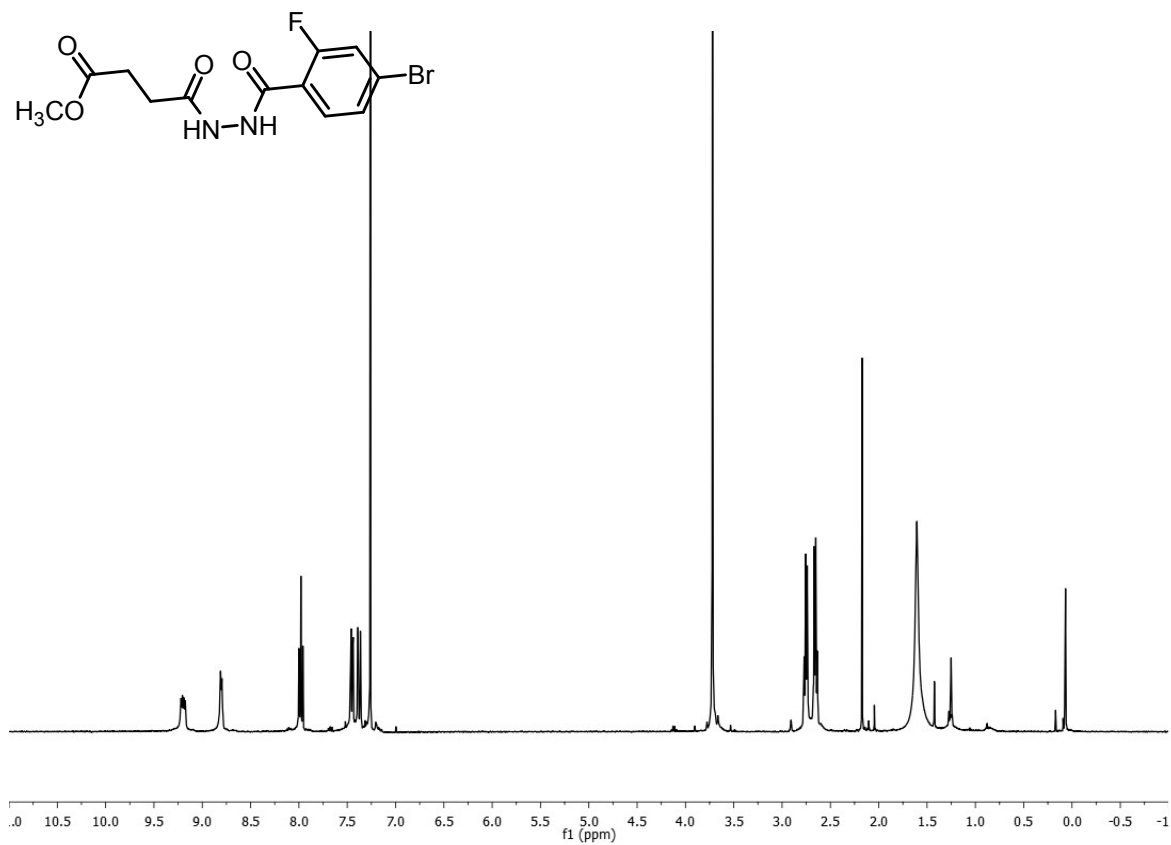


Figure 6. ¹H NMR spectrum of compound **5b**.

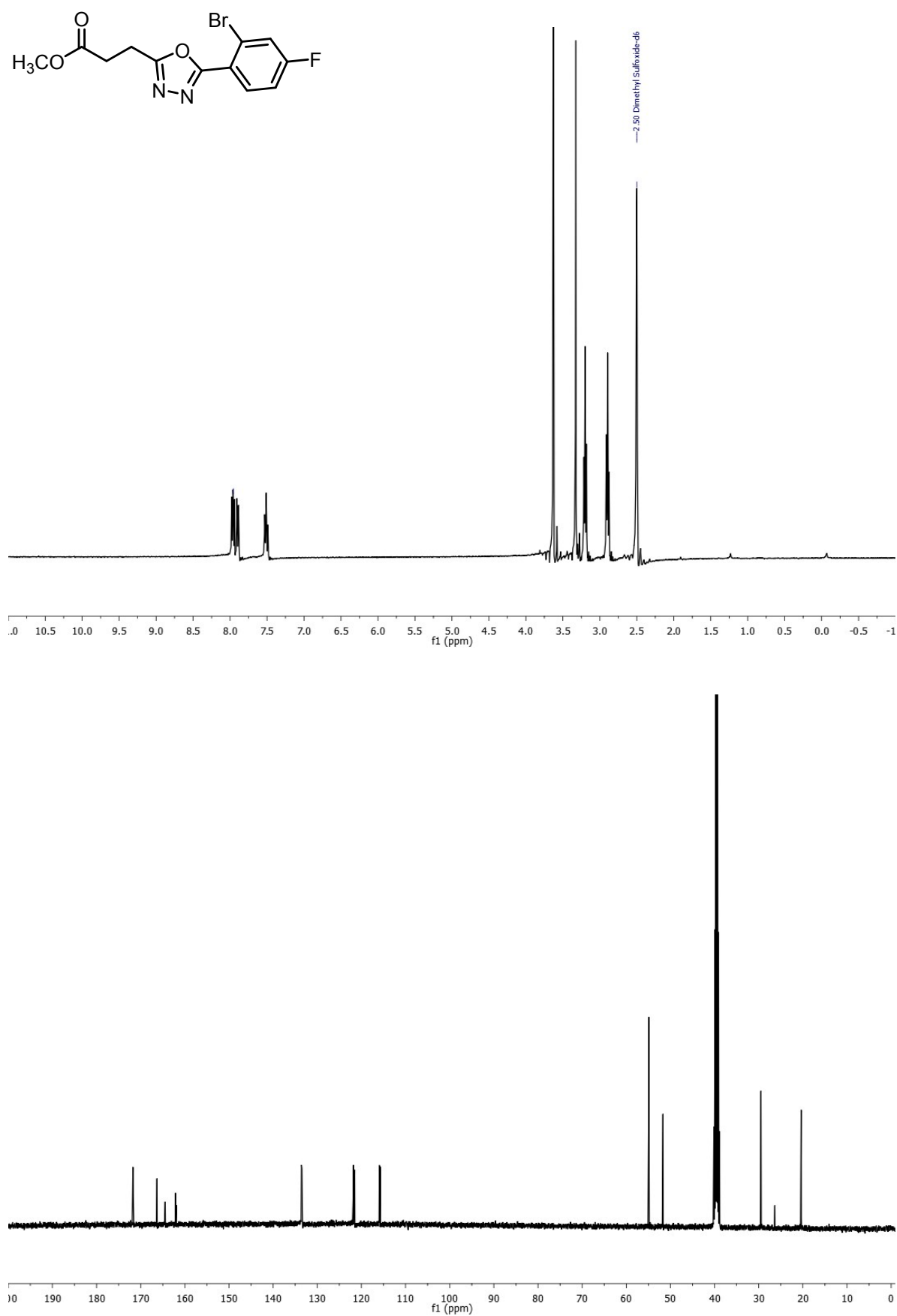


Figure 7. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **6a**.

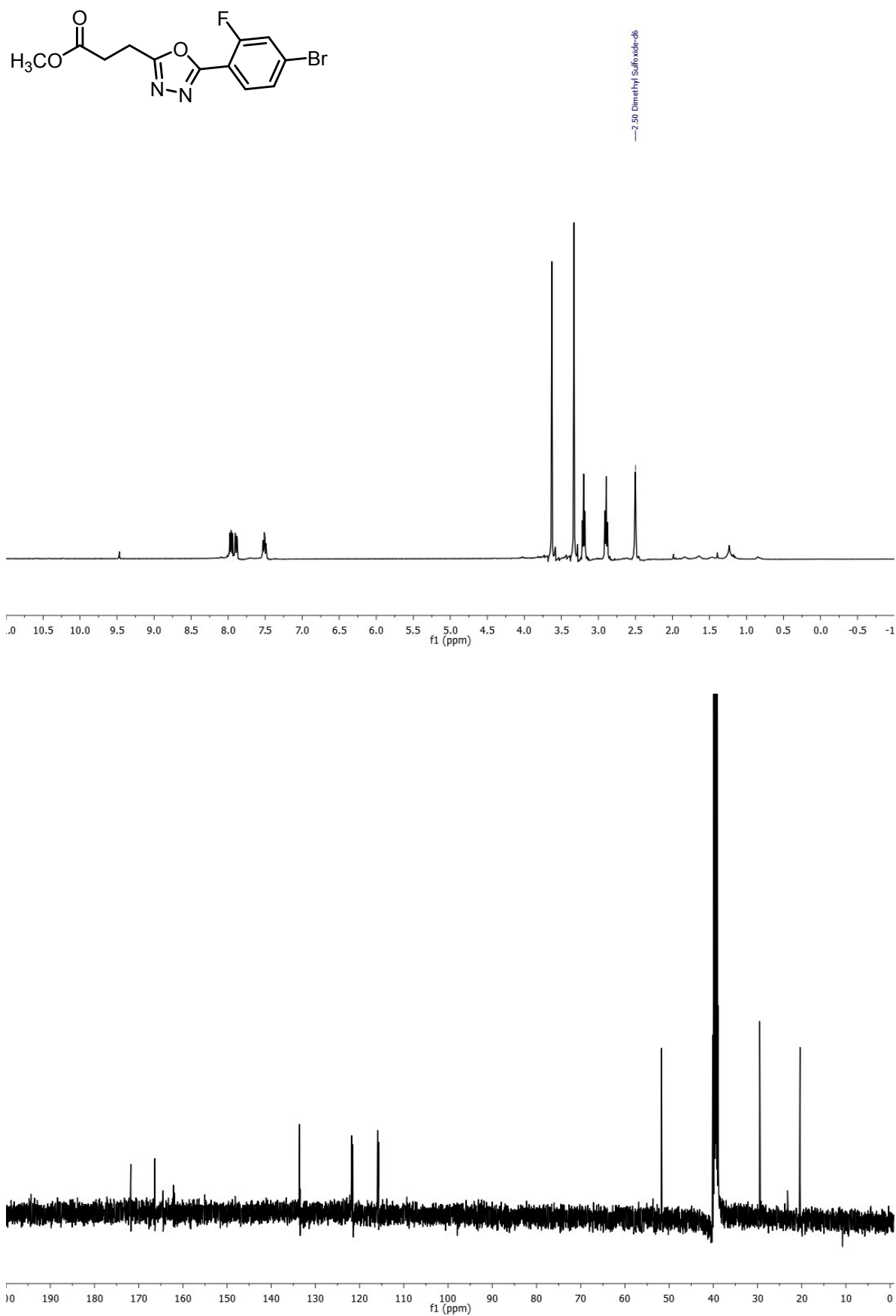


Figure 8. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **6b**.

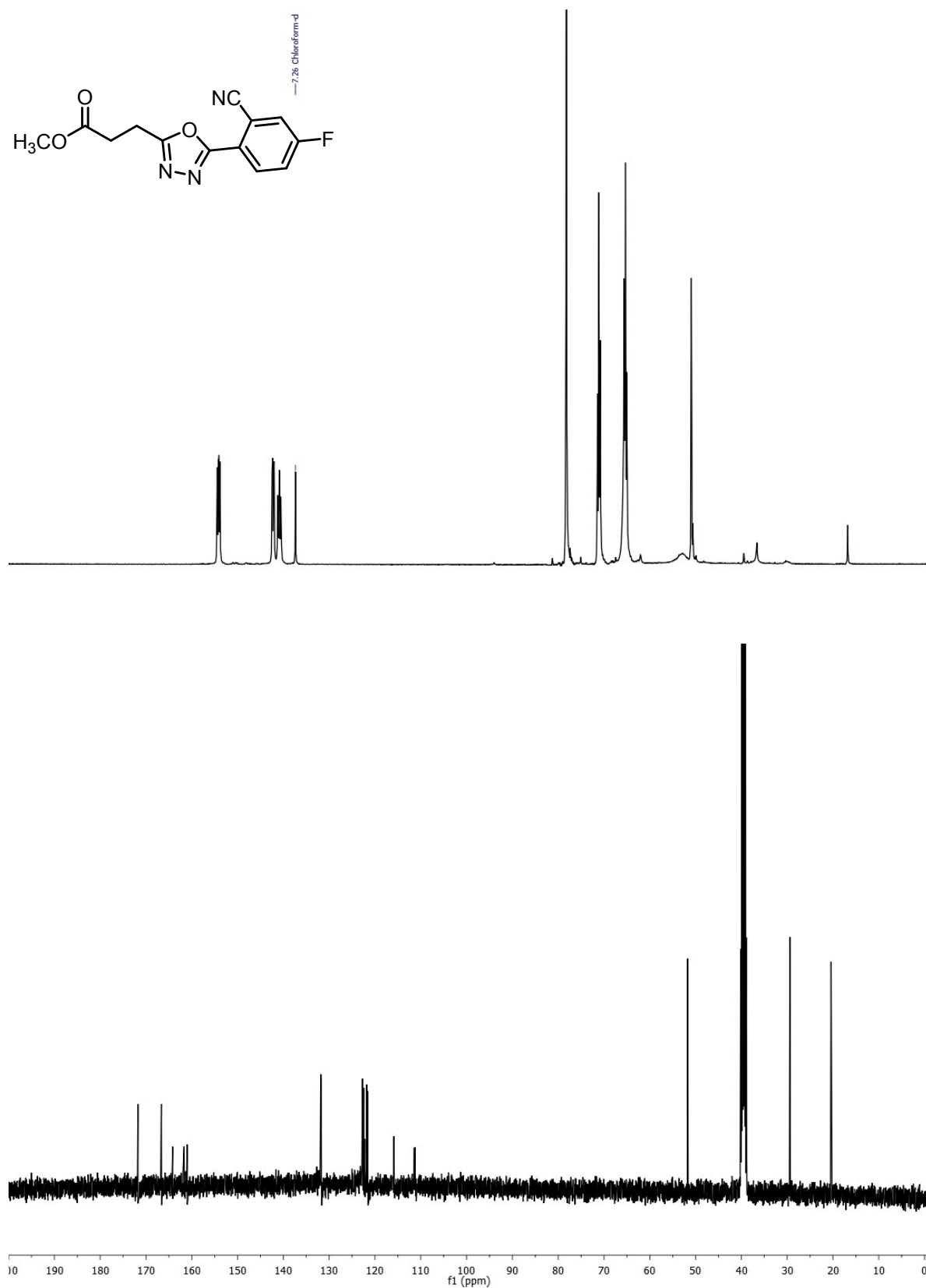


Figure 9. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **6c**.

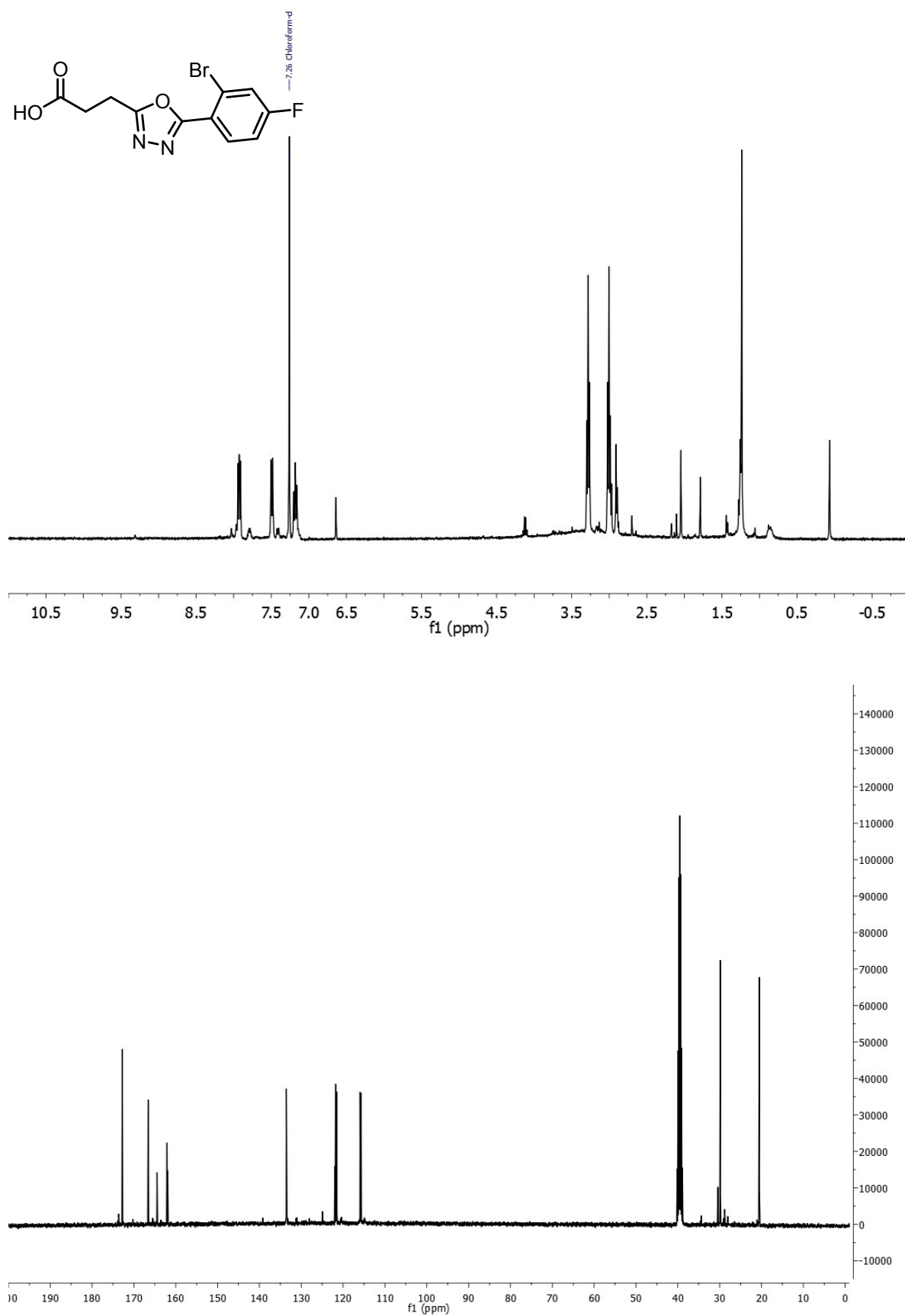


Figure 10. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **7a**.

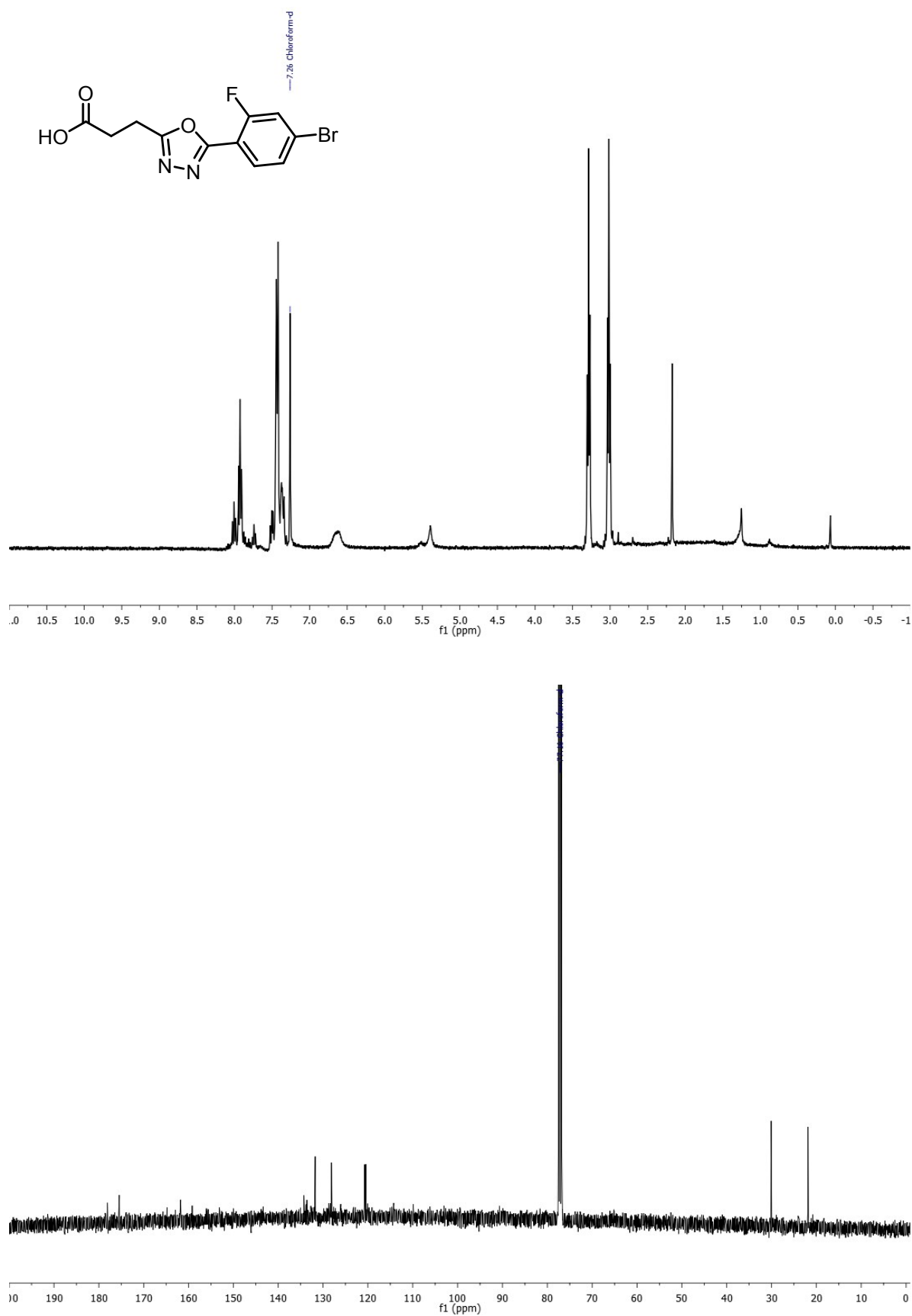


Figure 11. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **7b**.

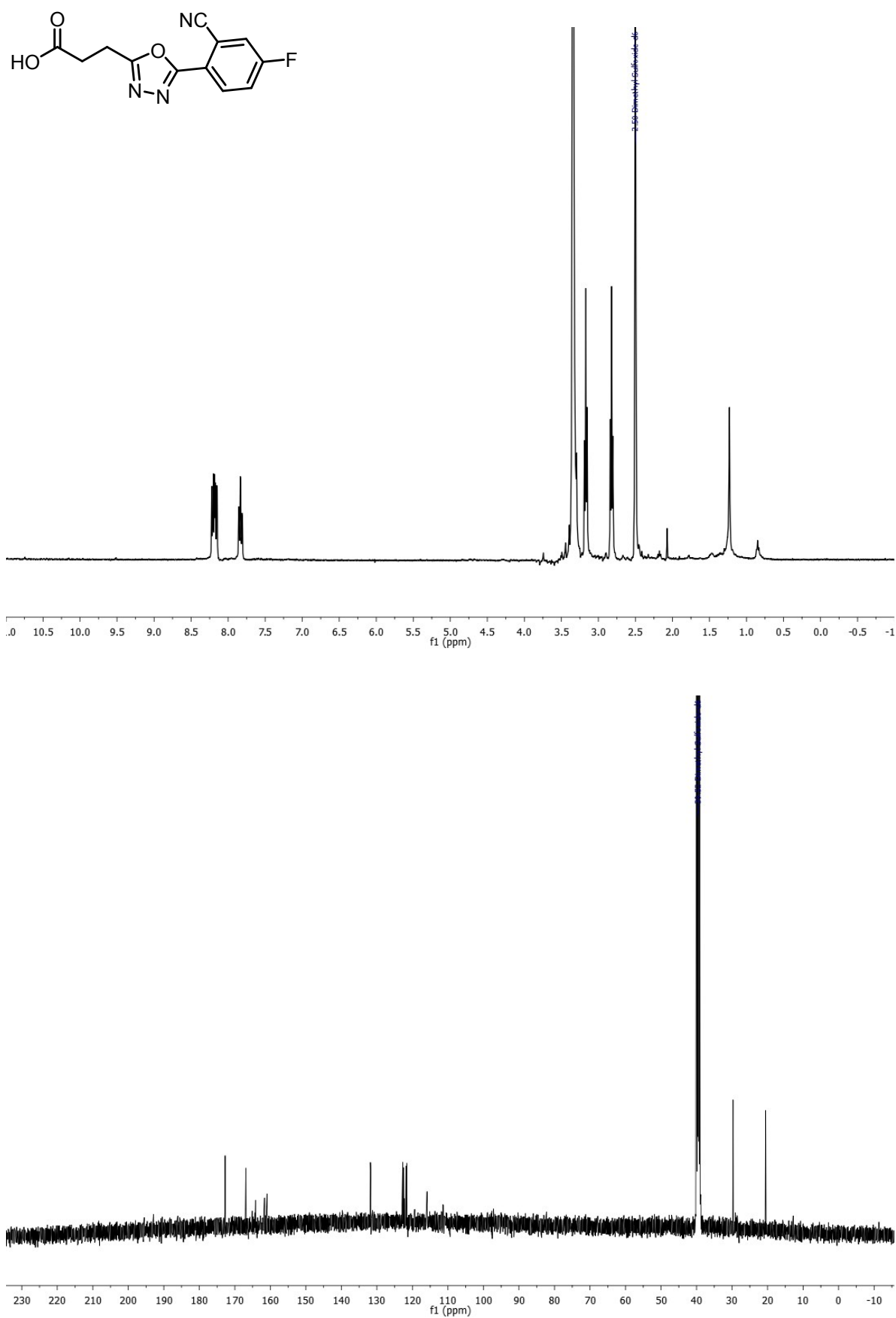


Figure 12. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **7c**.

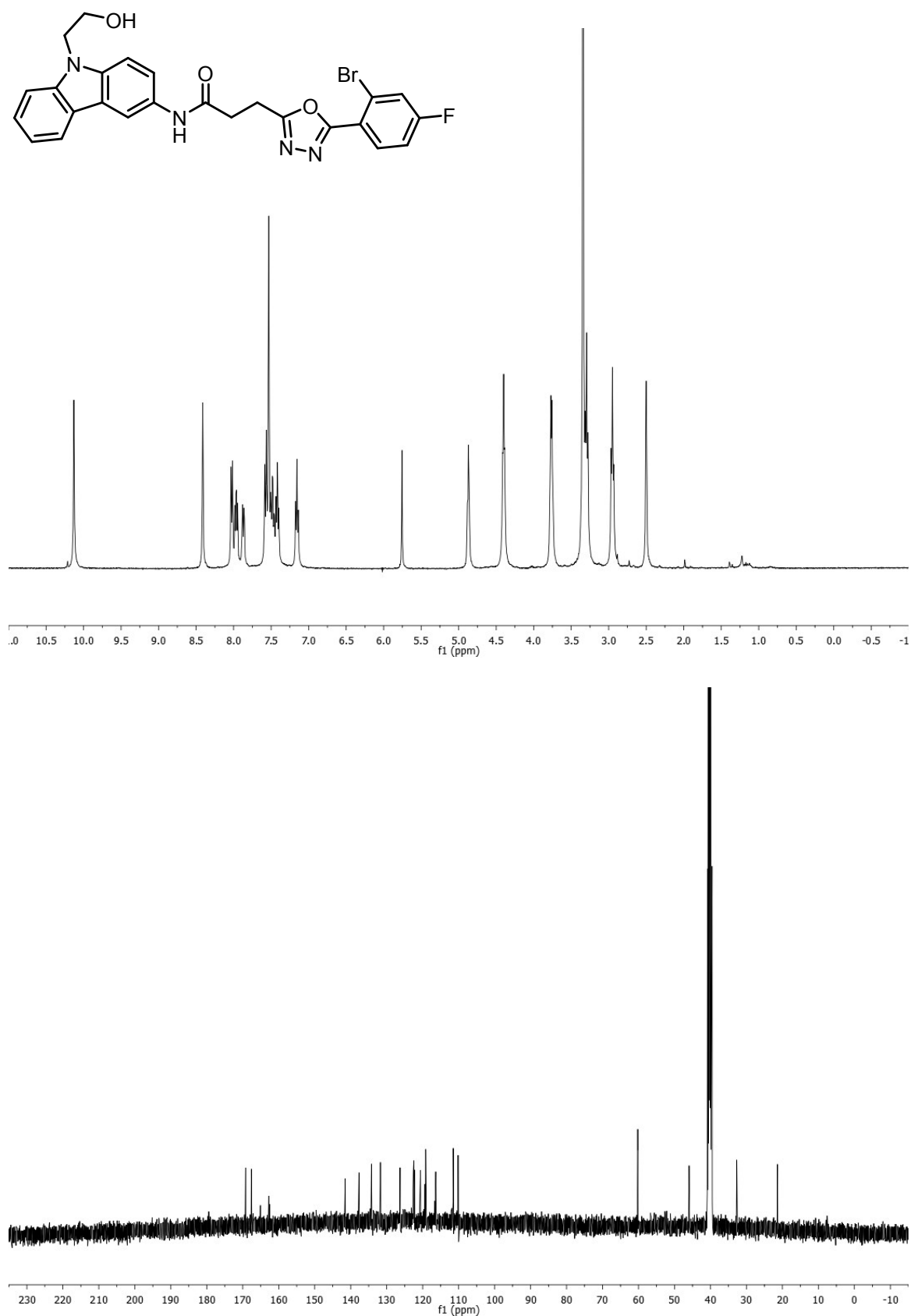


Figure 13. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **8a**.

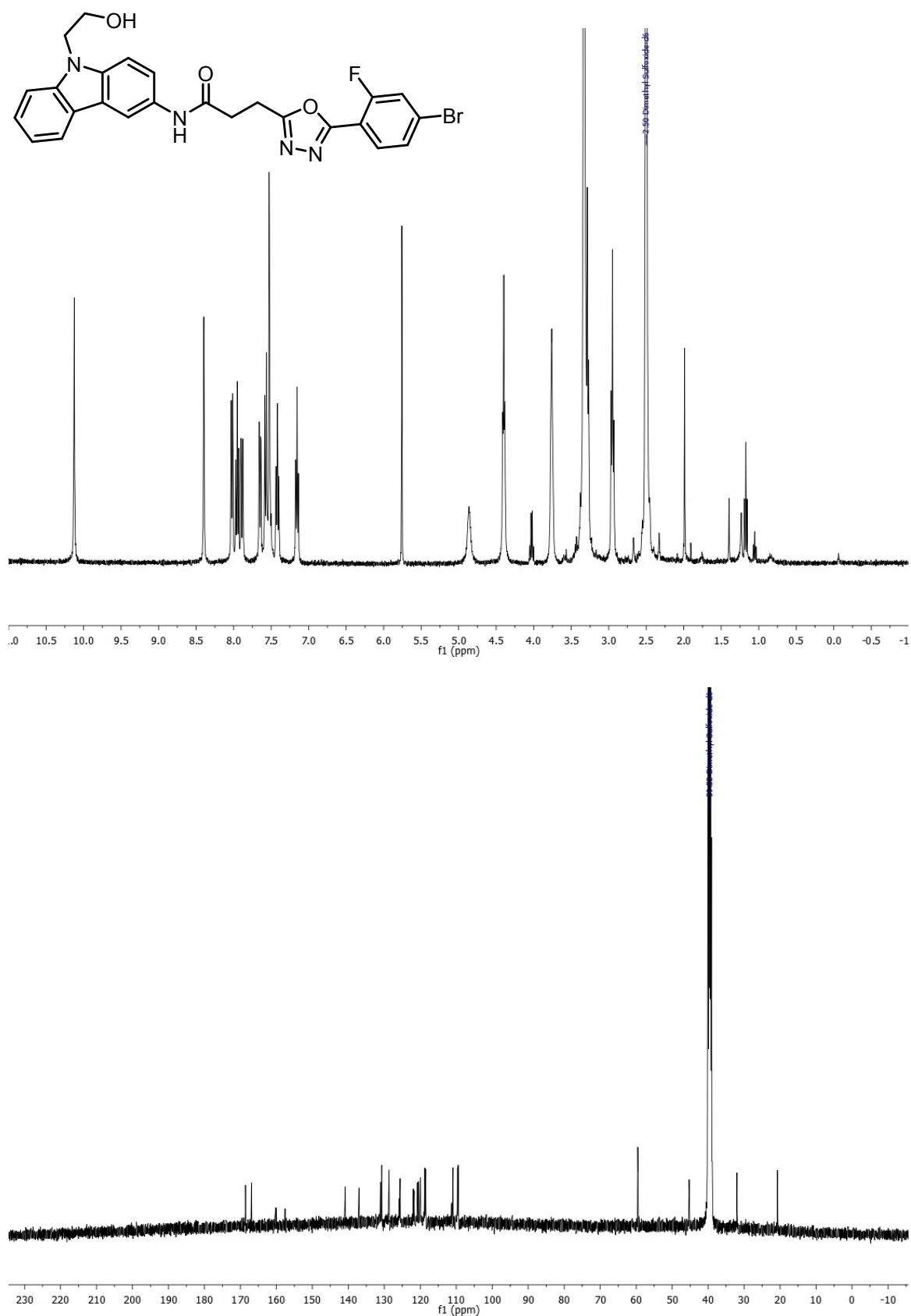


Figure 14. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **8b**.

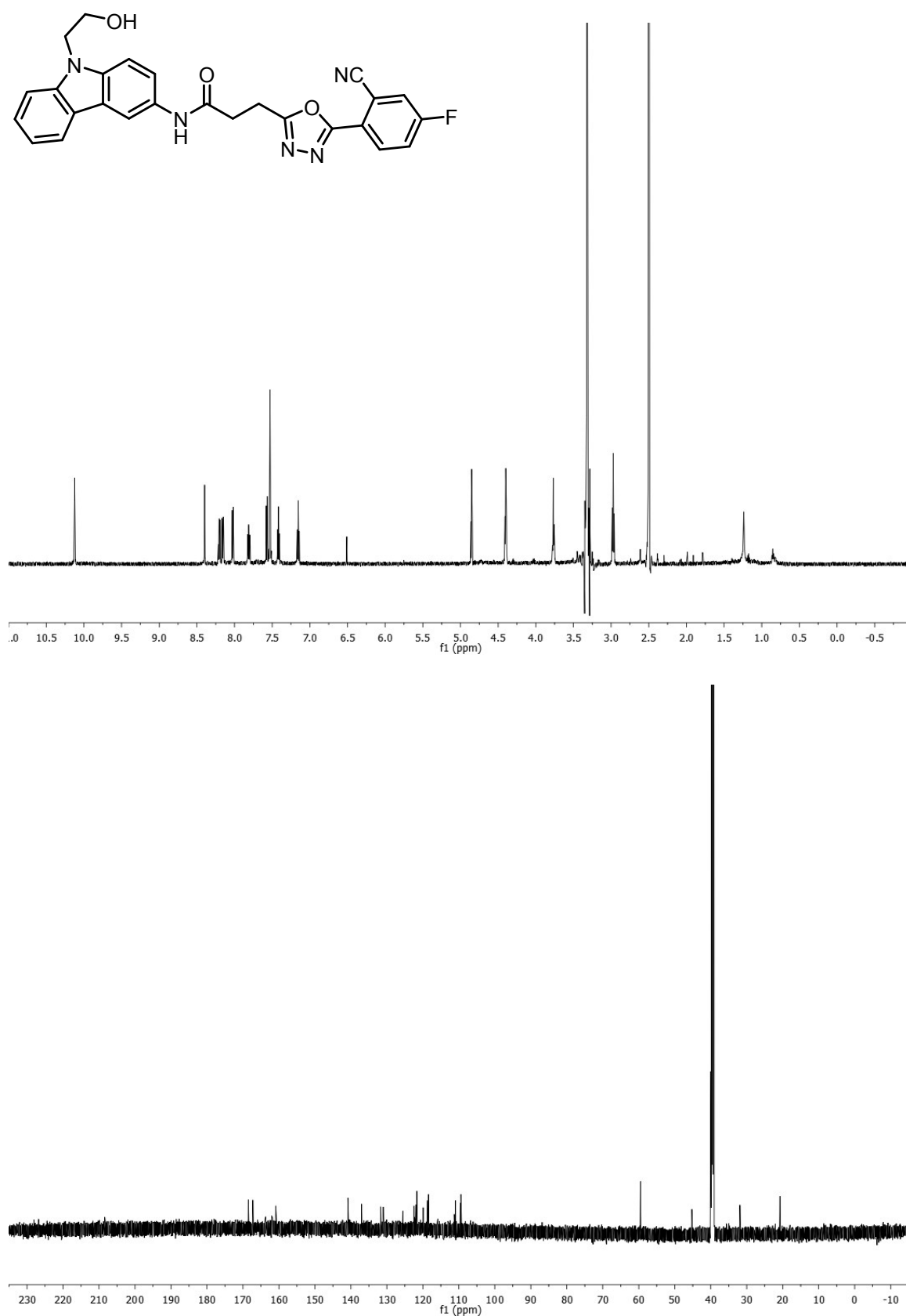


Figure 15. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **8c**.

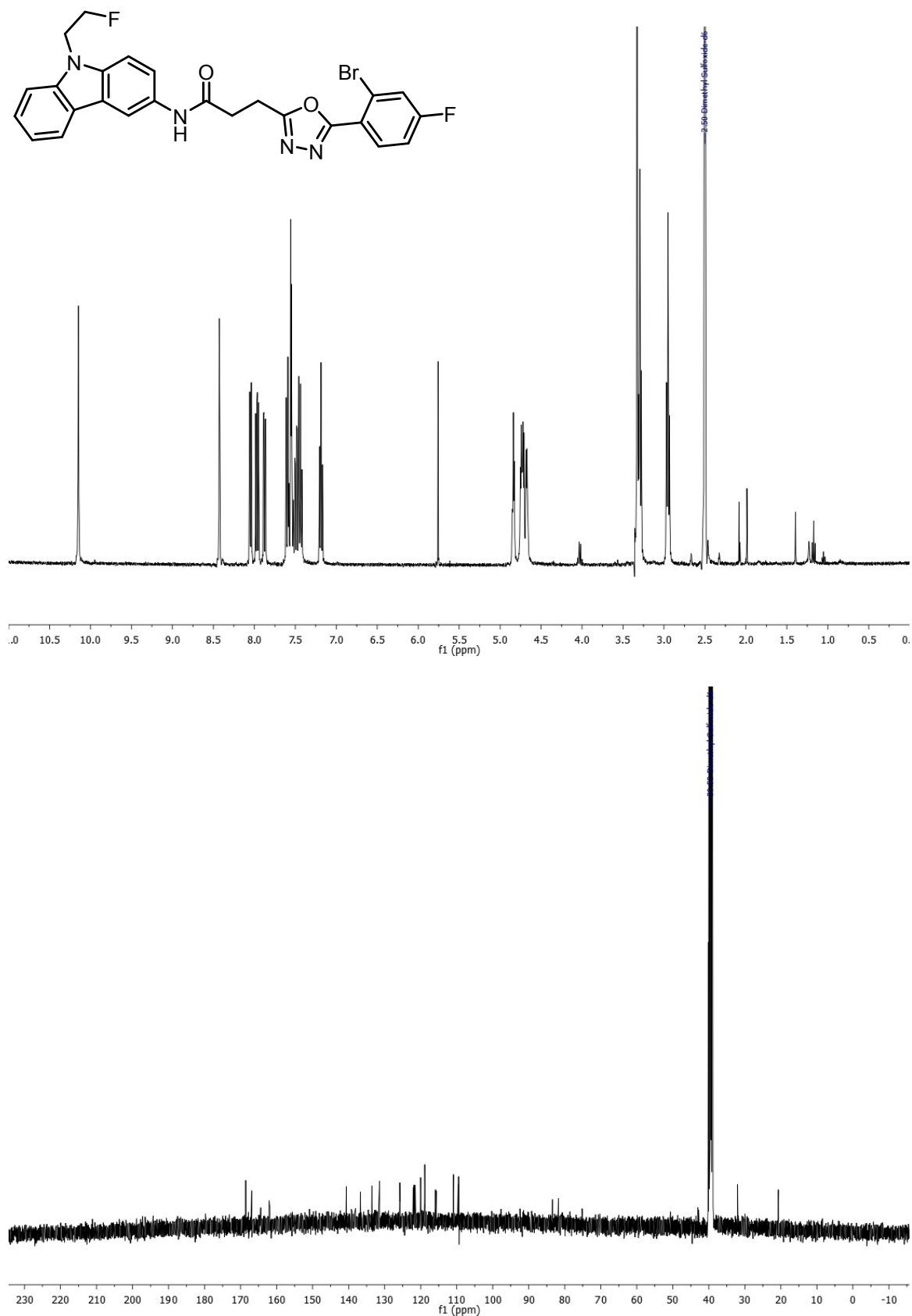


Figure 16. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **9a**.

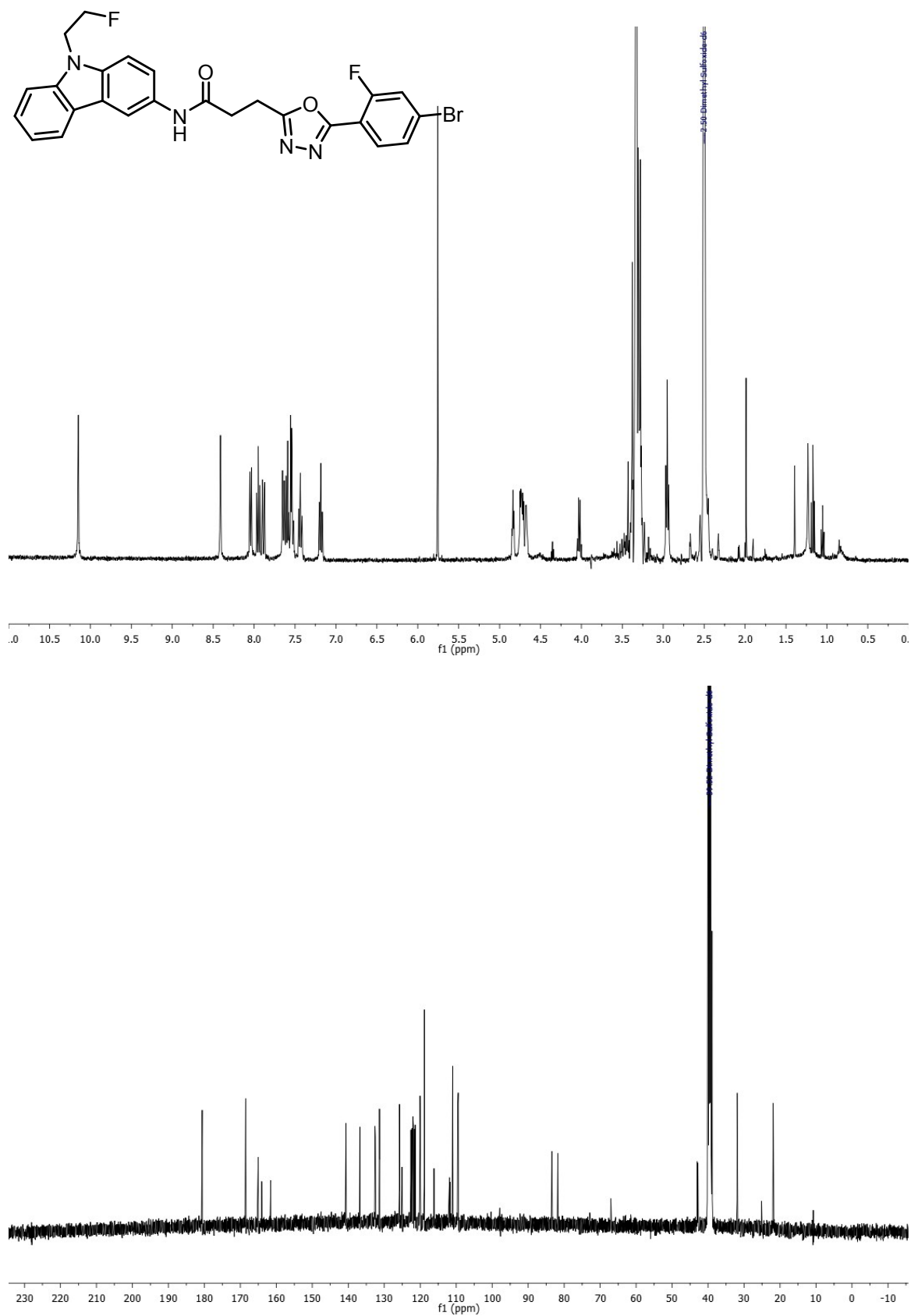


Figure 17. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **9b**.

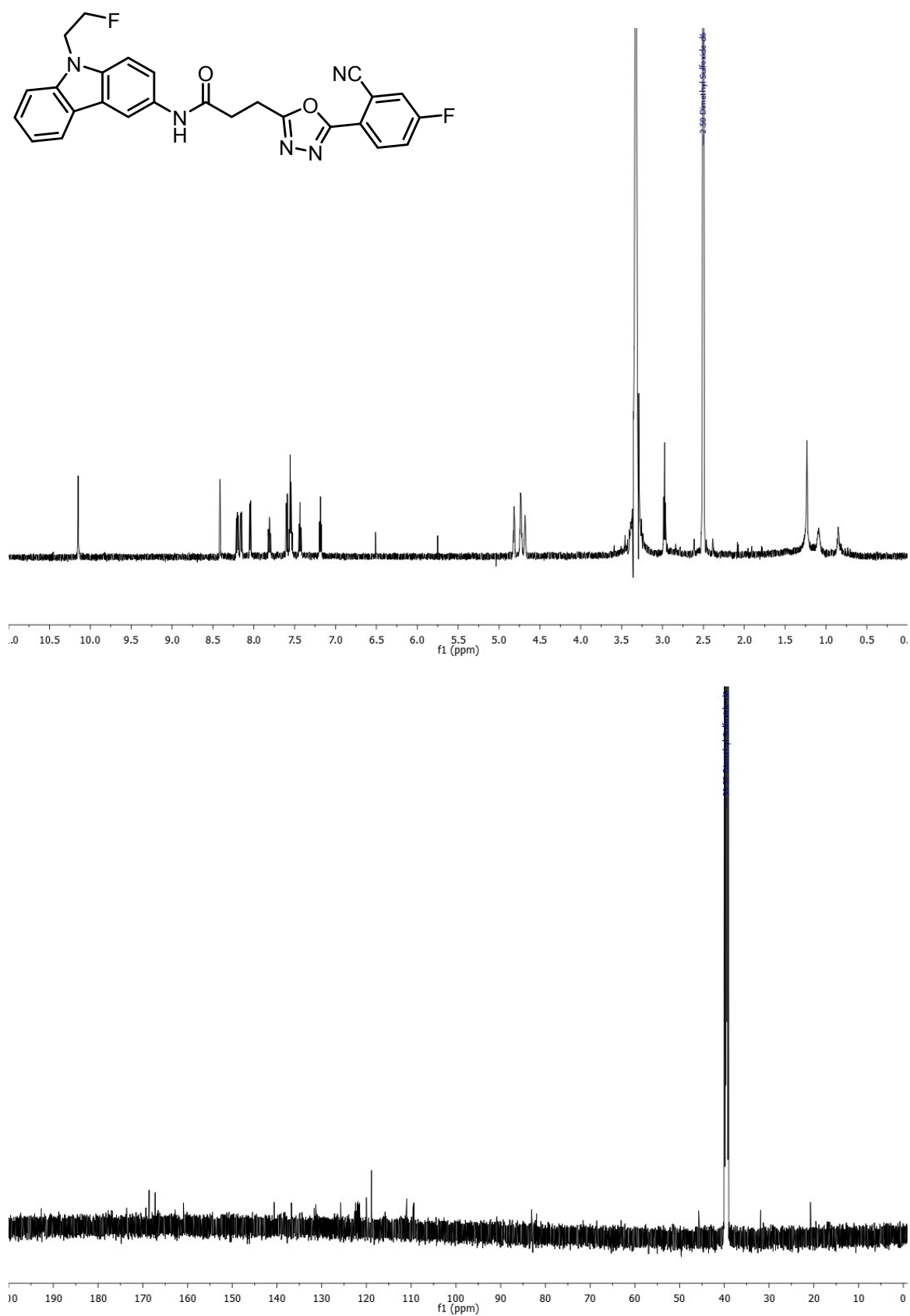


Figure 18. ^1H - (top) and ^{13}C -NMR spectrum (bottom) of compound **9c**.