

# Synthesis of 3,5-Bis(trifluoromethyl)phenyl-Substituted Pyrazole Derivatives as Potent Growth Inhibitors of Drug-Resistant Bacteria

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## Characterization data (I-B)

### 4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-formyl-pyrazol-1-yl] benzoic acid (III).

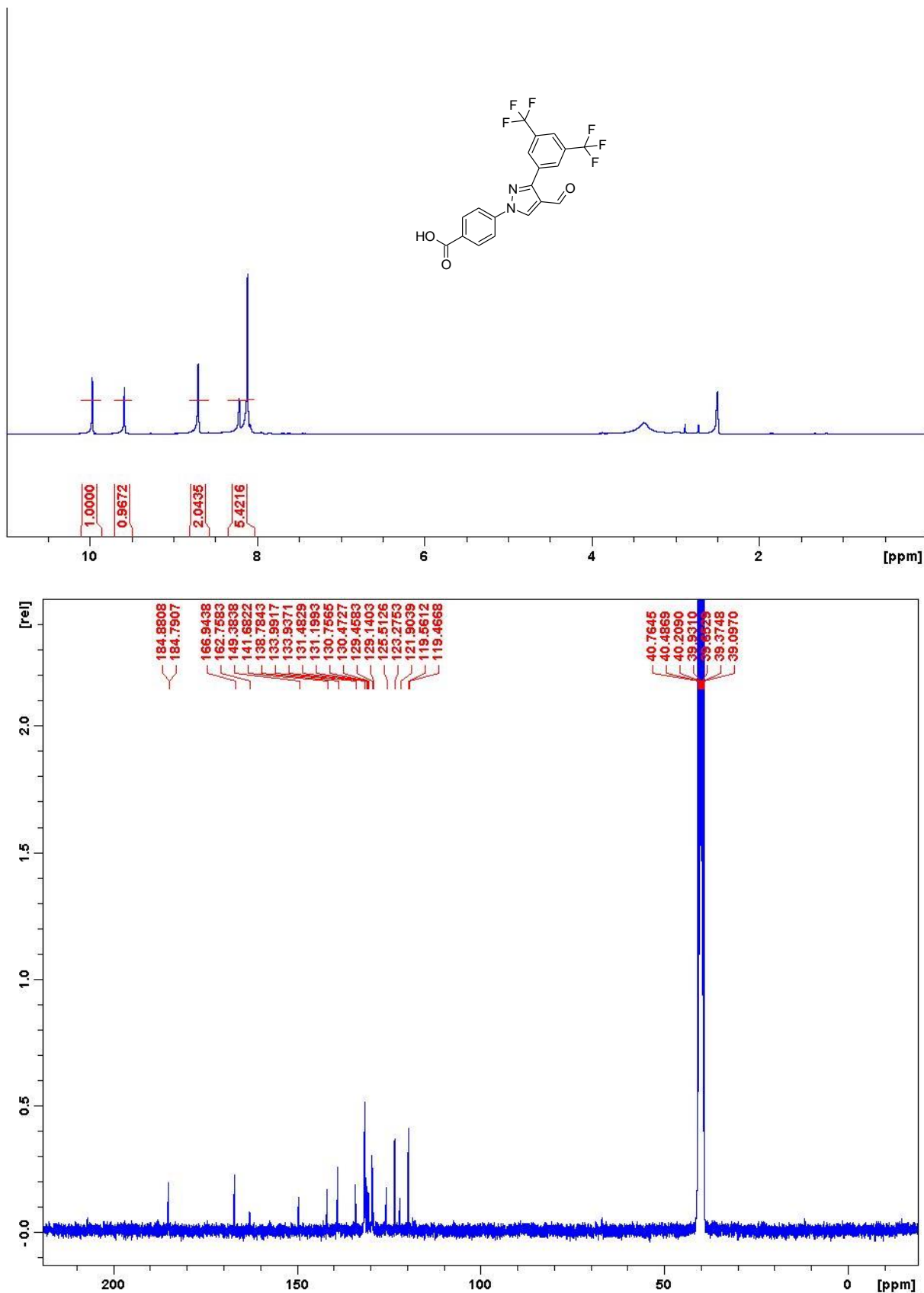


Figure S1. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound III

4-[4-(Anilinomethyl)-3-[3,5-bis(trifluoromethyl) phenyl] pyrazol-1-yl] benzoic acid (1).

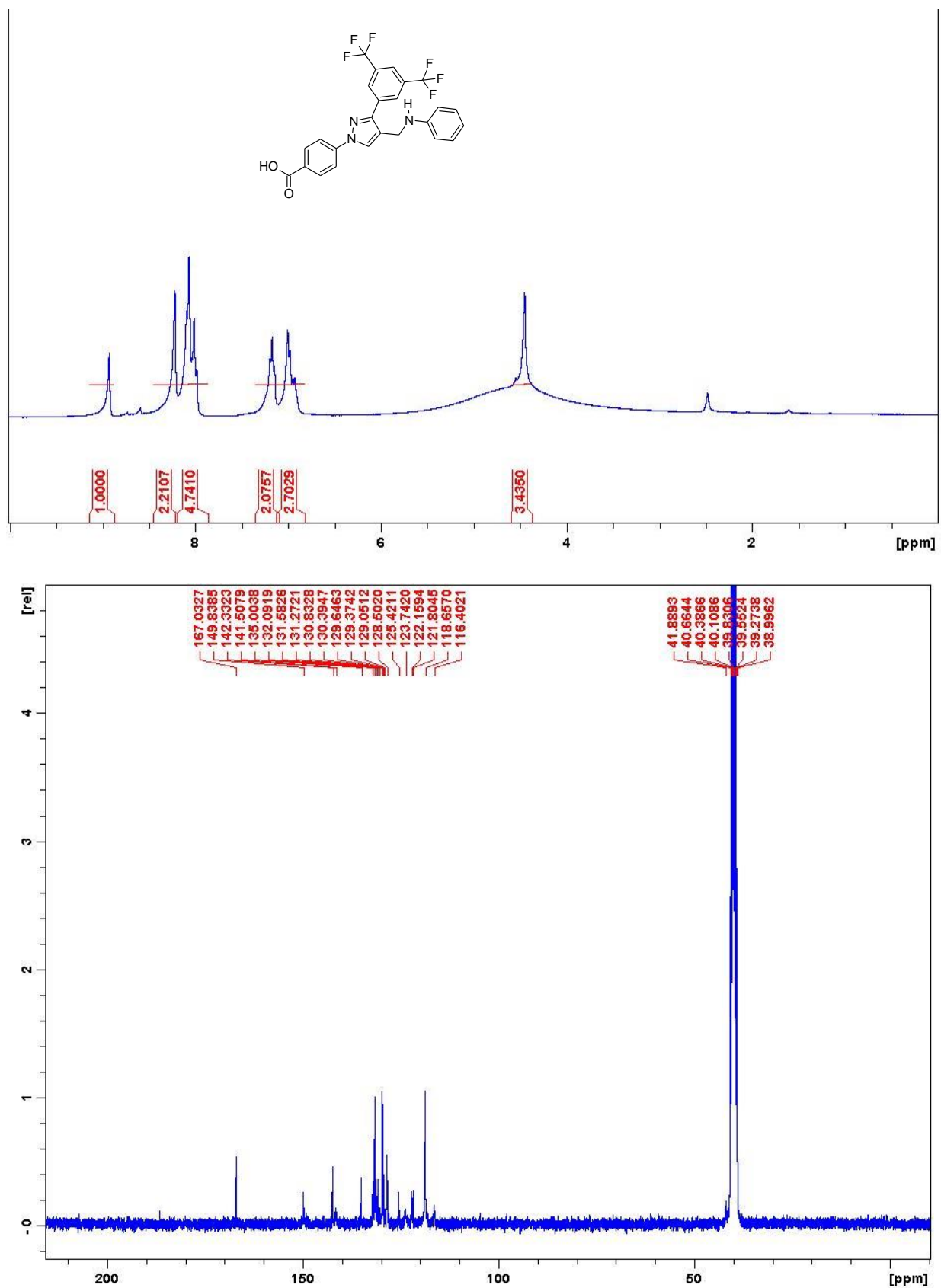


Figure S2. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 1

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-isopropylanilino) methyl] pyrazol-1-yl] benzoic acid (2).

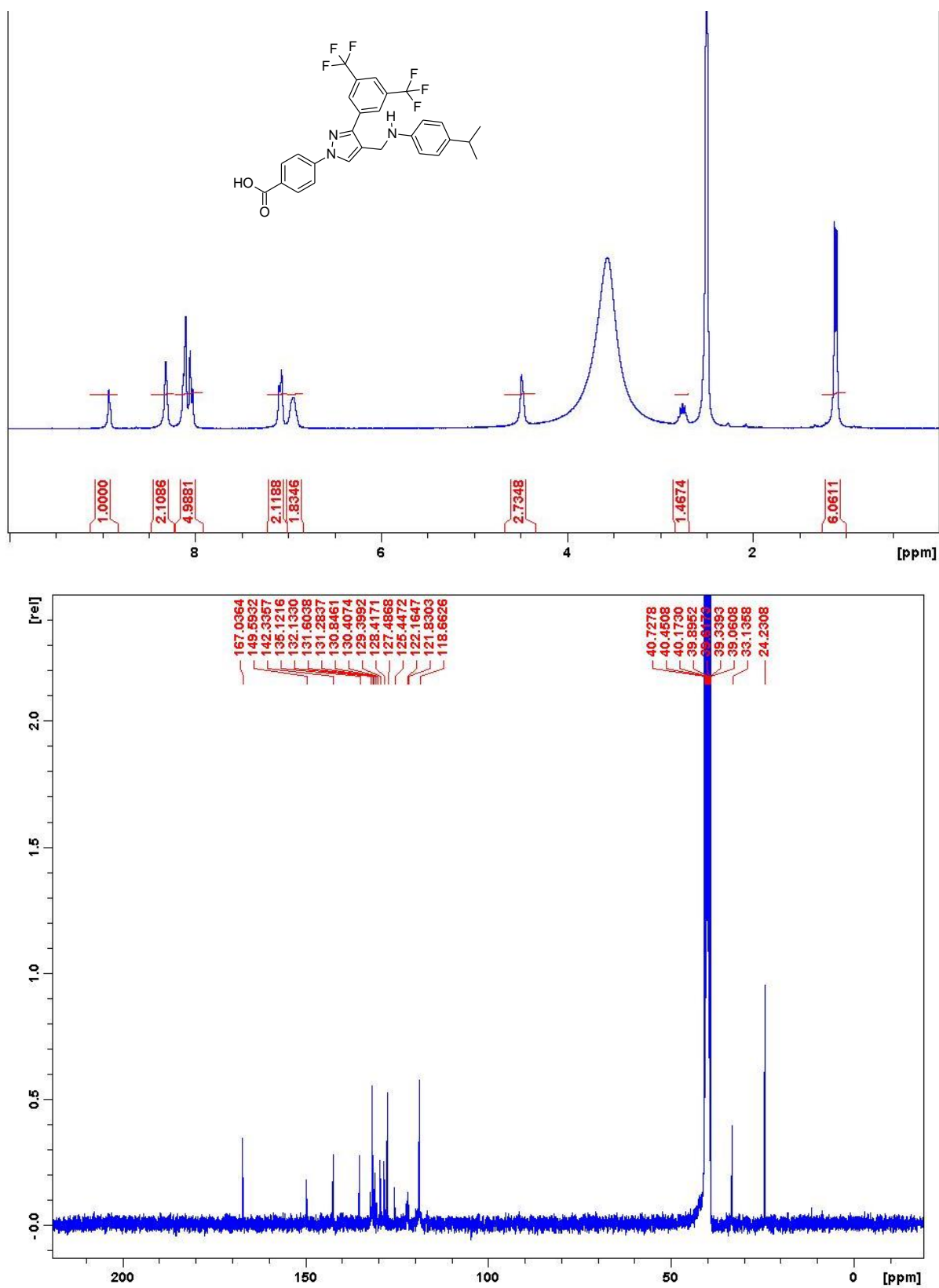


Figure S3. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 2

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-tert-butylanilino) methyl] pyrazol-1-yl] benzoic acid (3).

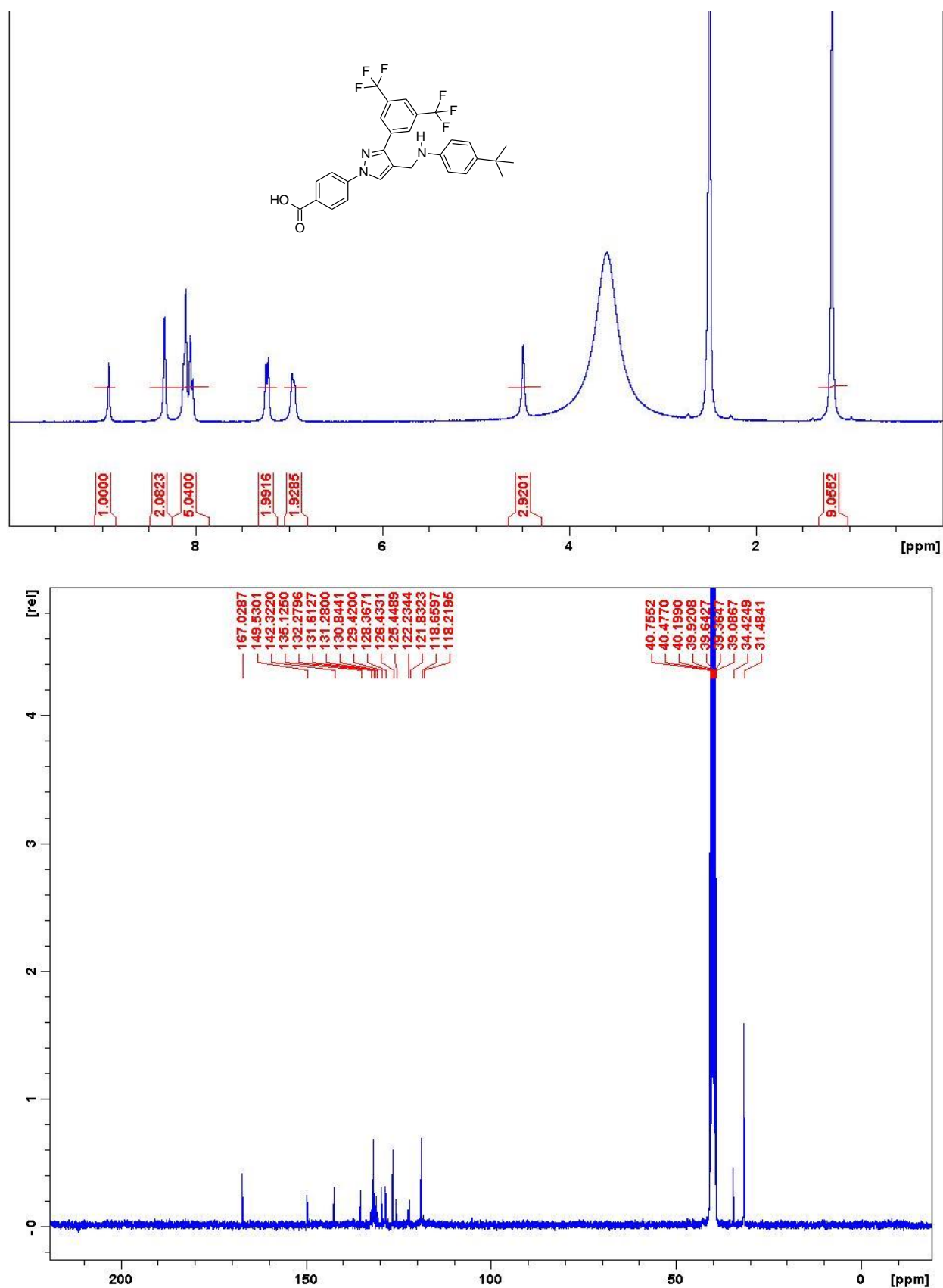


Figure S4. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 3

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-methoxyanilino) methyl] pyrazol-1-yl] benzoic acid (4).

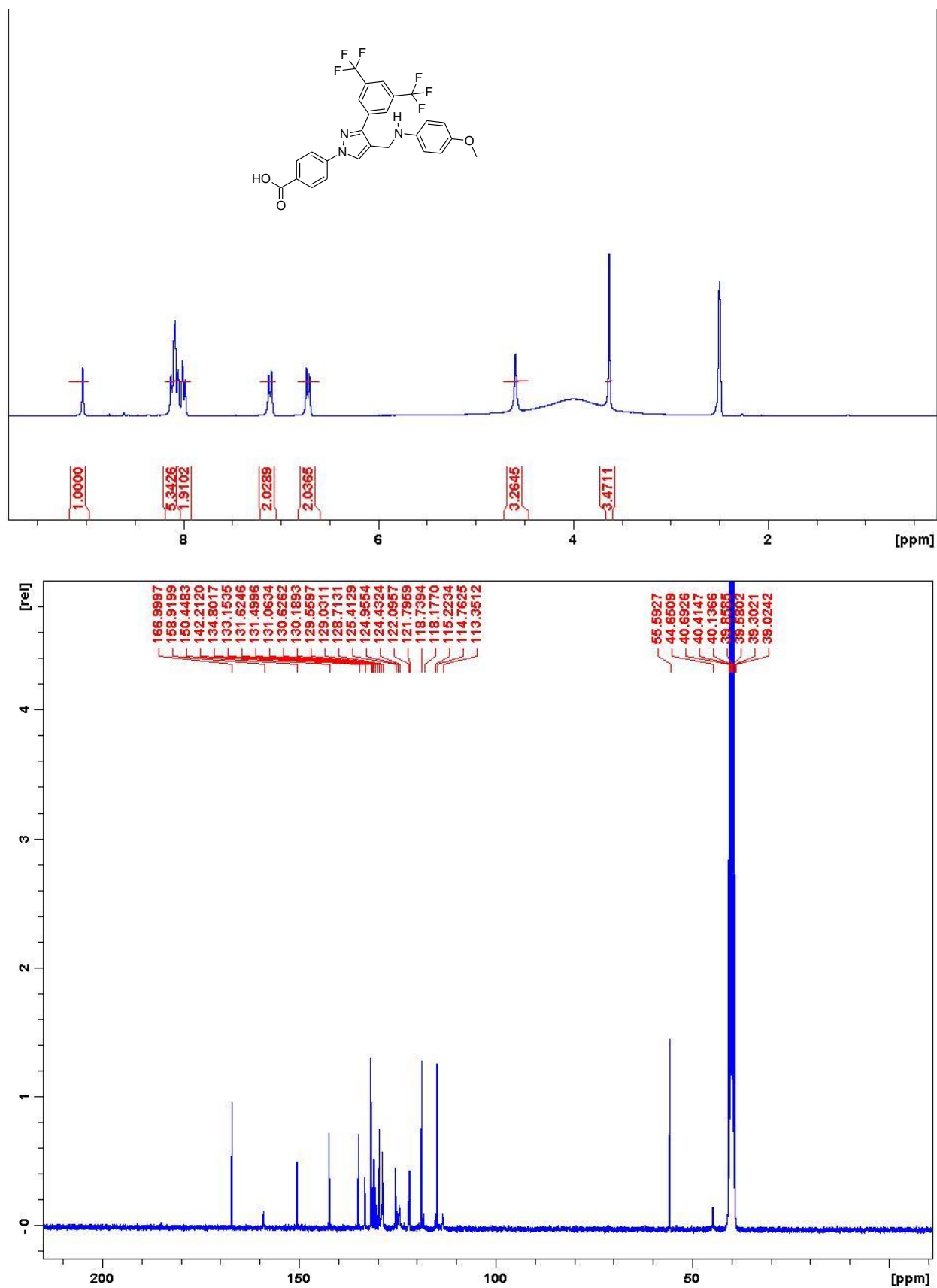


Figure S5. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 4

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-phenoxyanilino) methyl] pyrazol-1-yl] benzoic acid (5).

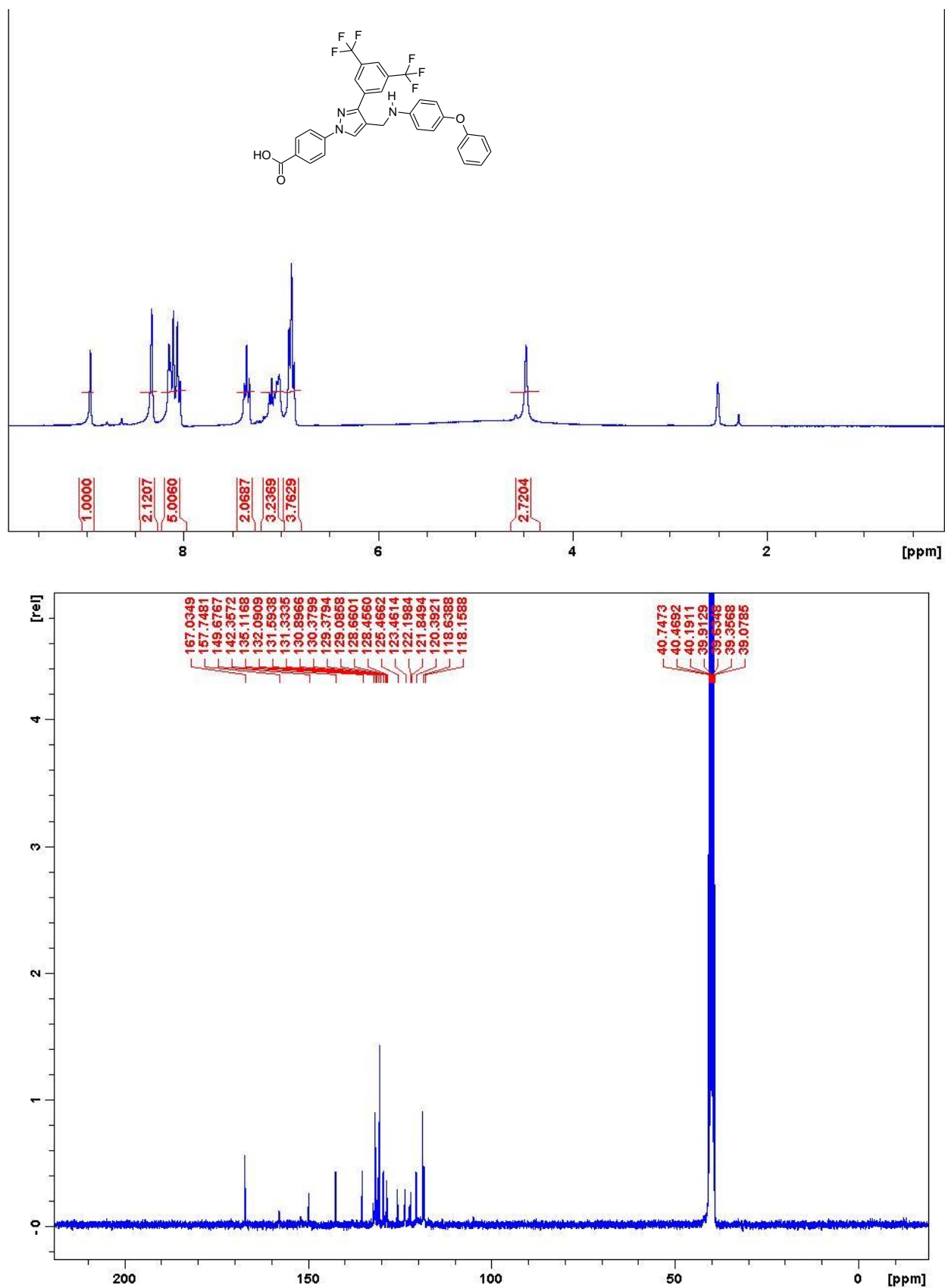


Figure S6. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 5

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-methylsulfonylanilino) methyl] pyrazol-1-yl] benzoic acid (6).

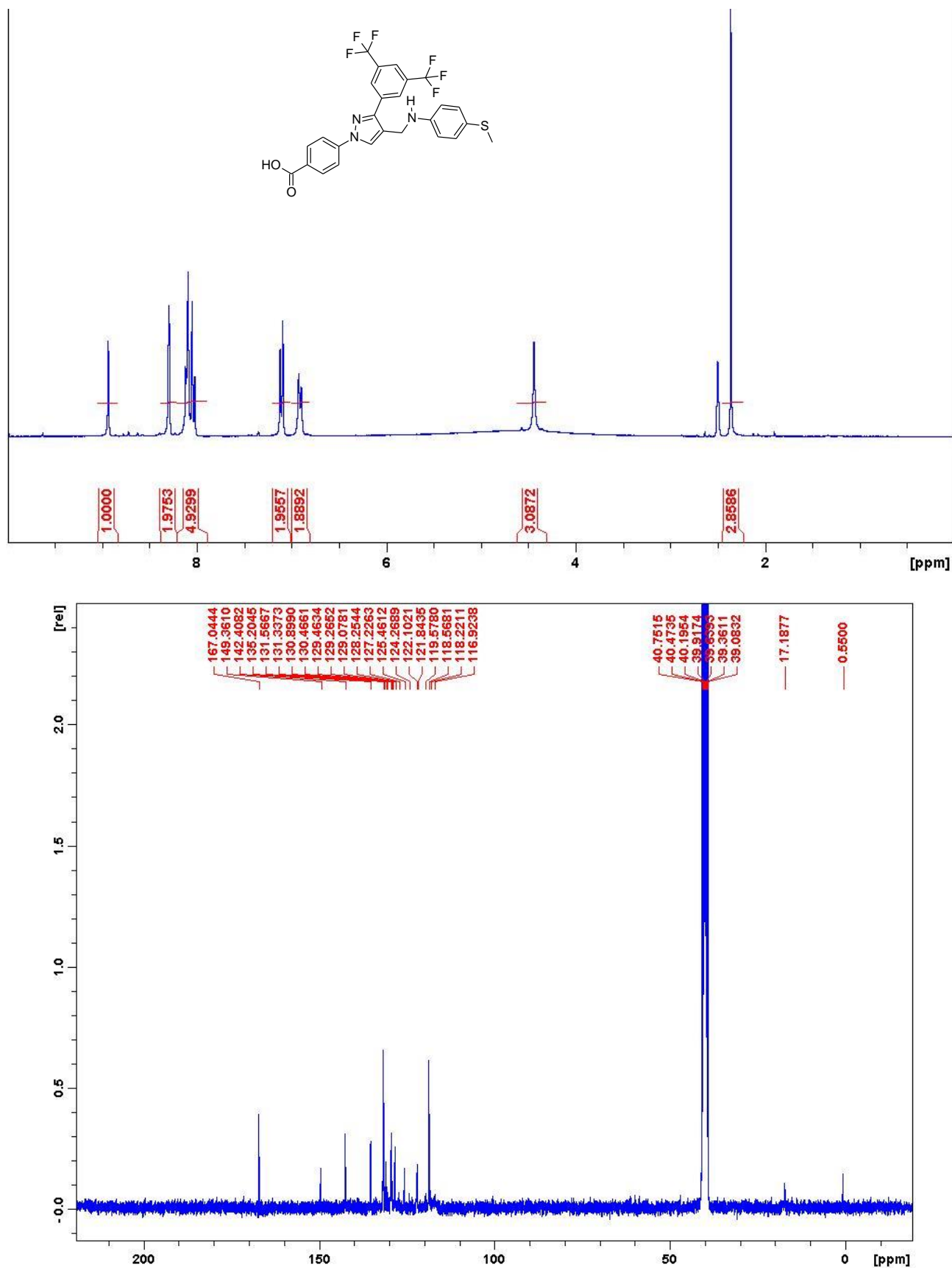
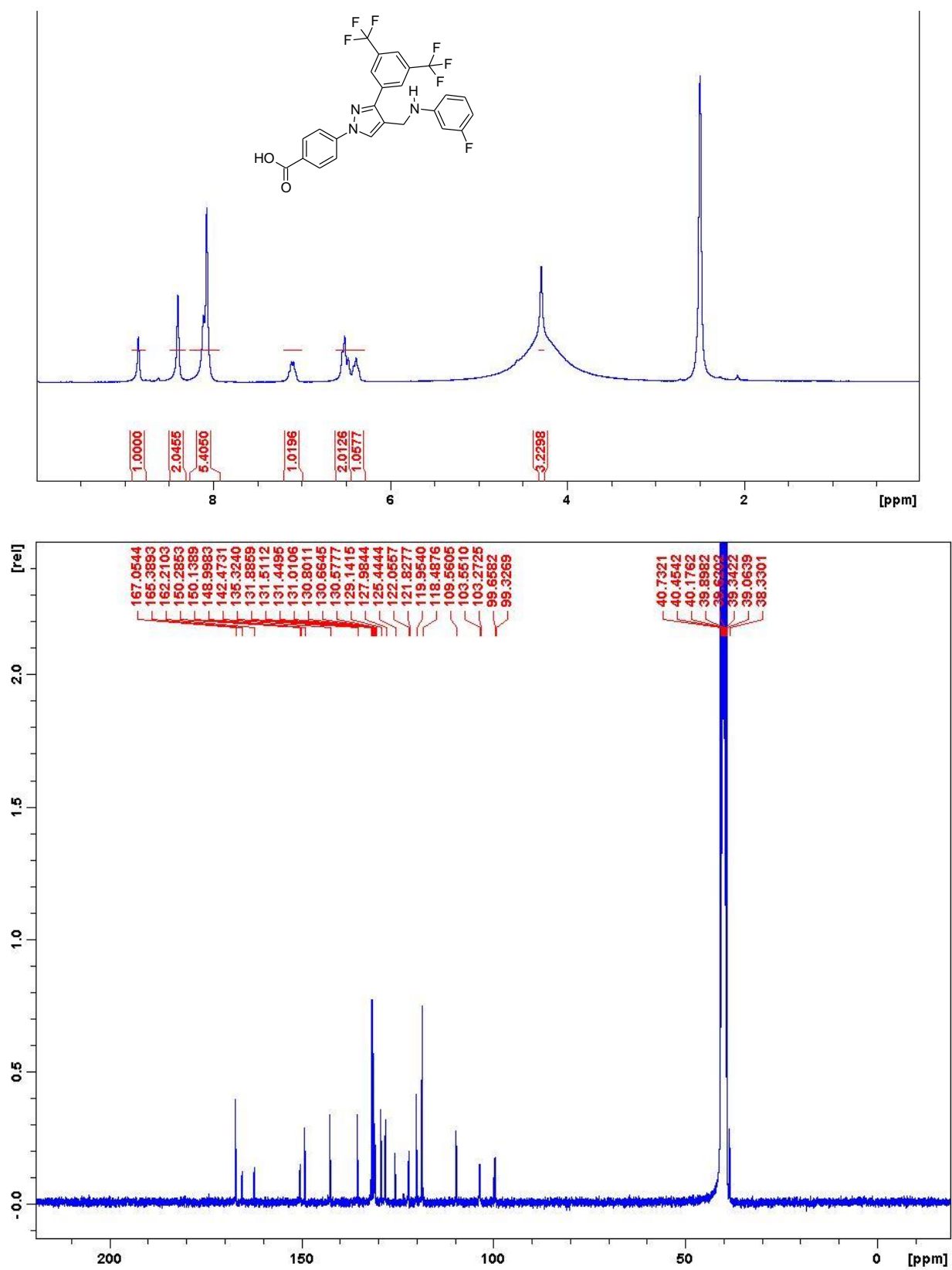


Figure S7. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 6



**4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(3-fluoroanilino) methyl] pyrazol-1-yl] benzoic acid (7).**



**Figure S8.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **7**

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-fluoroanilino) methyl] pyrazol-1-yl] benzoic acid (8).

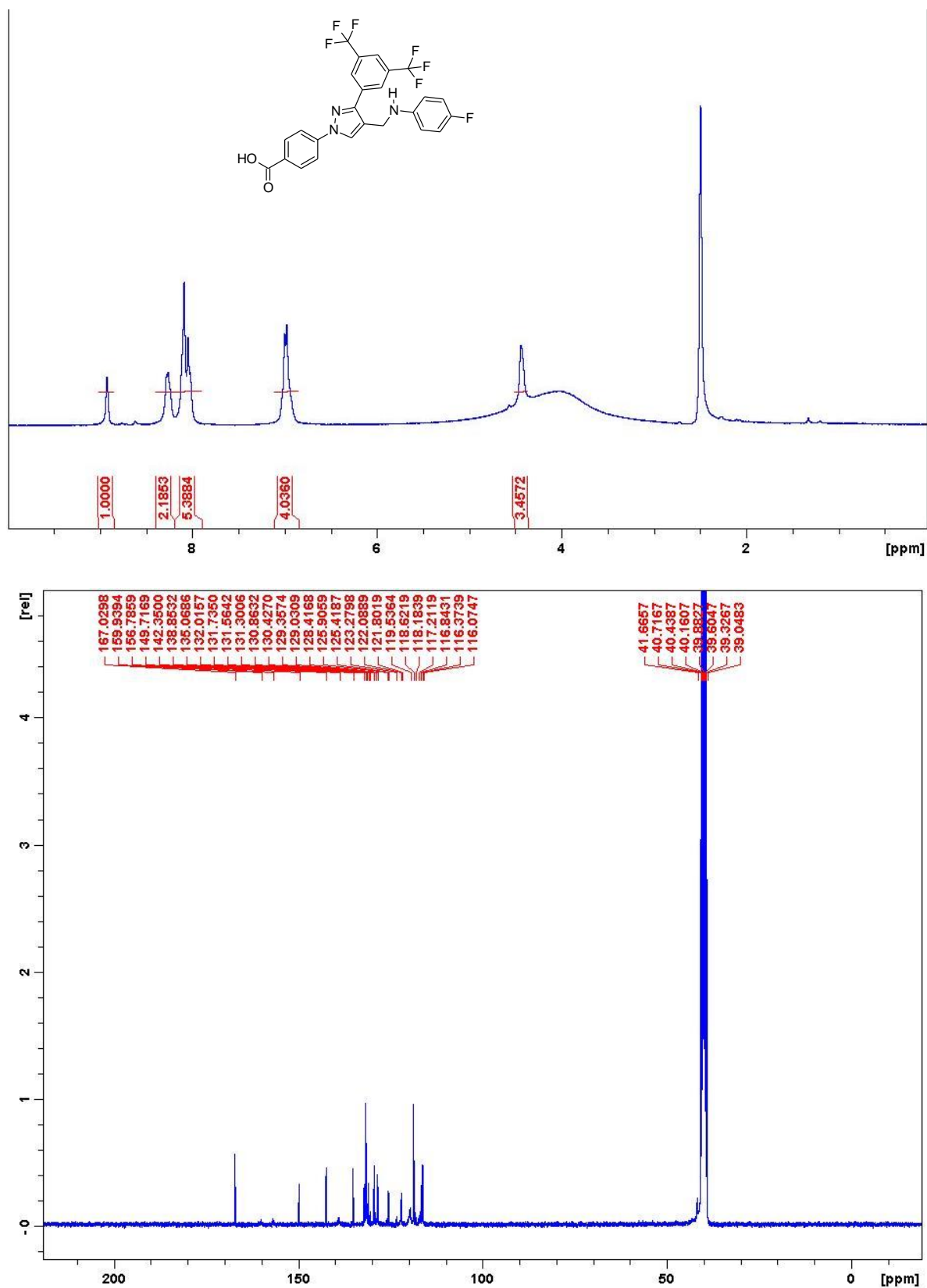


Figure S9. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 8

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-chloroanilino) methyl] pyrazol-1-yl] benzoic acid (9).

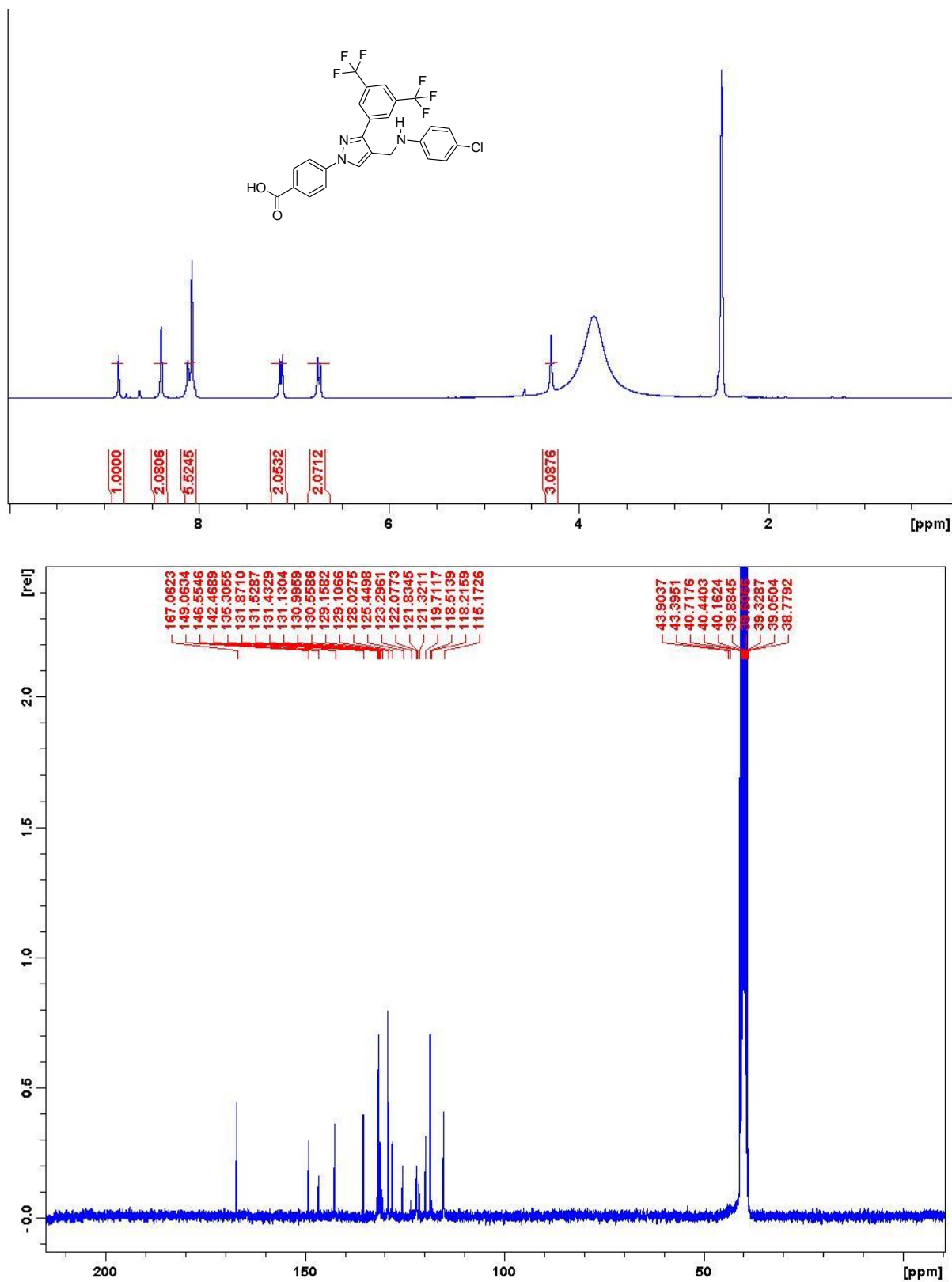


Figure S10. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 9

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(3-bromoanilino) methyl] pyrazol-1-yl] benzoic acid (10).

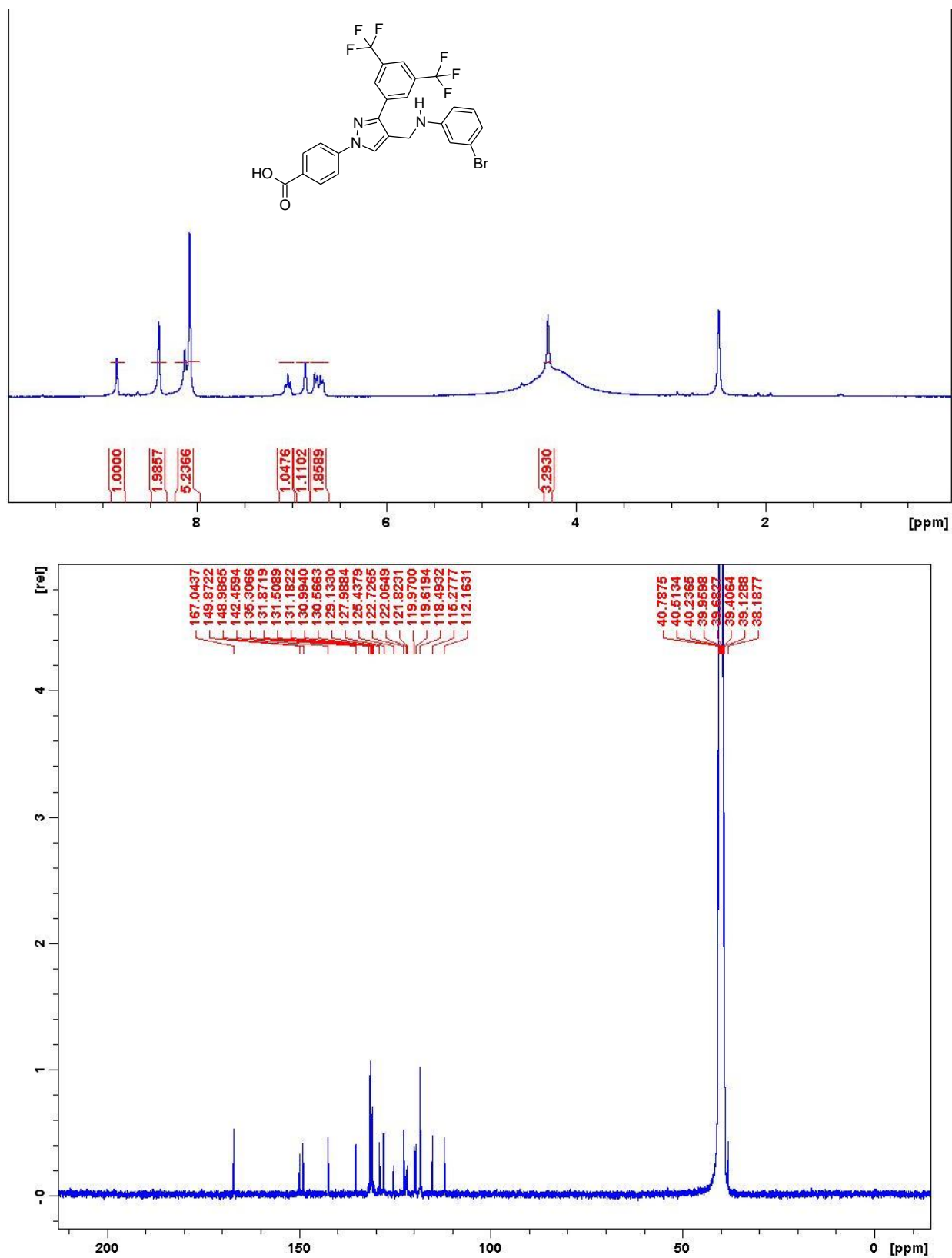
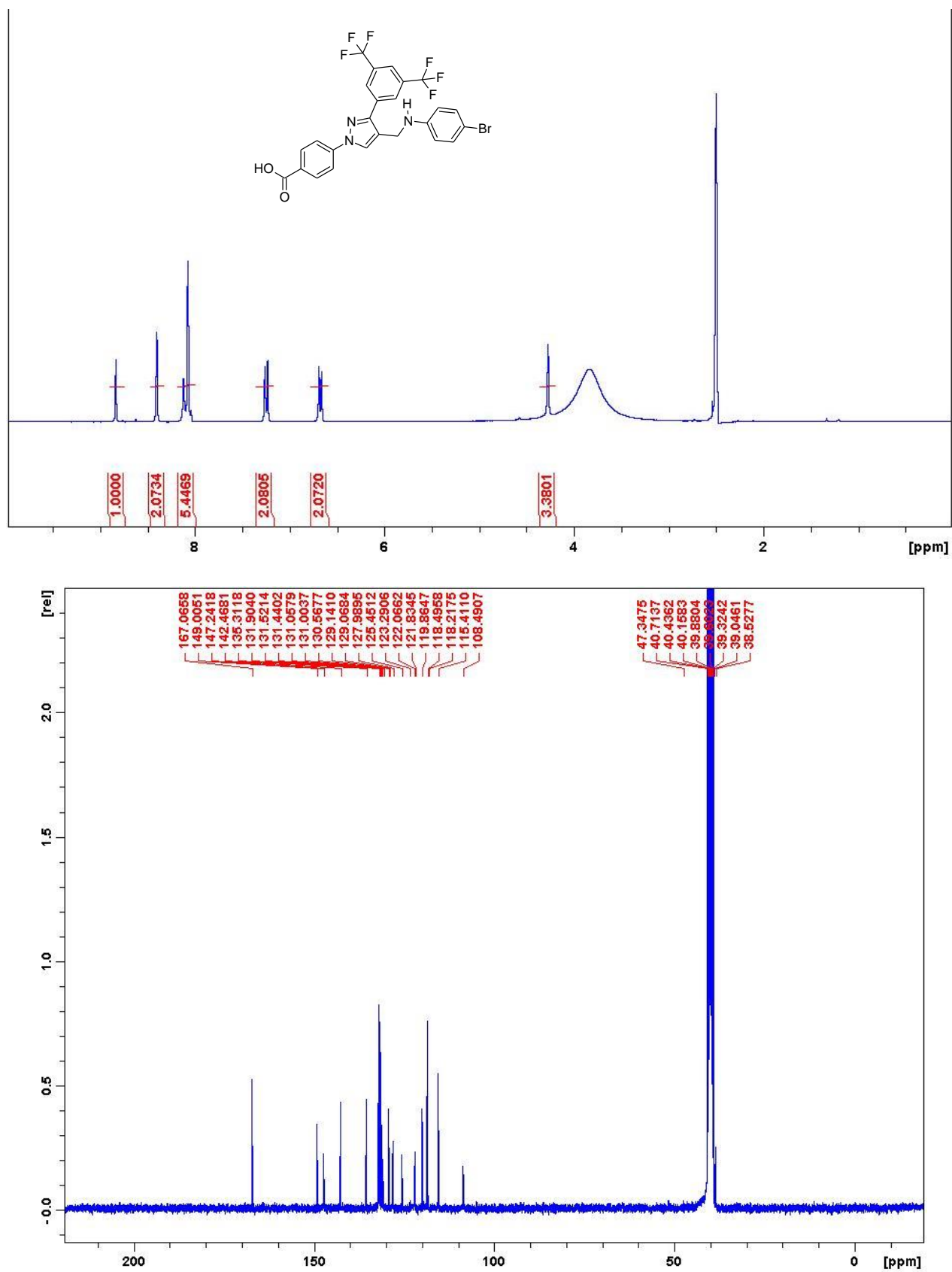


Figure S11. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 10

**4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-bromoanilino) methyl] pyrazol-1-yl] benzoic acid (11).**



**Figure S12.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **11**

3-[[3-[3,5-Bis(trifluoromethyl)phenyl]-1-(4-carboxyphenyl)pyrazol-4-yl]methylamino] benzoic acid (12).

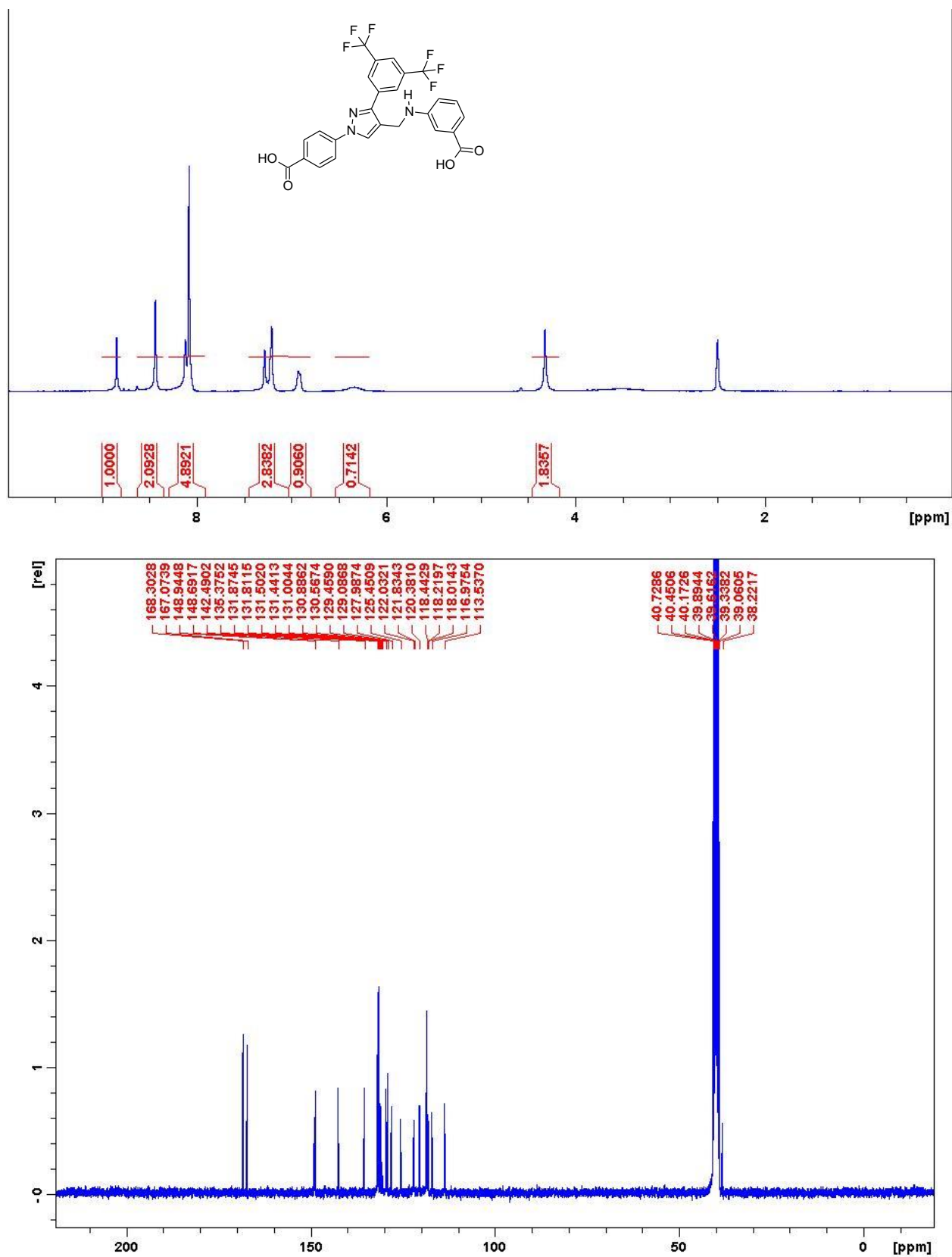


Figure S13. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 12

4-[[3-[3,5-Bis(trifluoromethyl) phenyl]-1-(4-carboxyphenyl) pyrazol-4-yl] methylamino] benzoic acid (13).

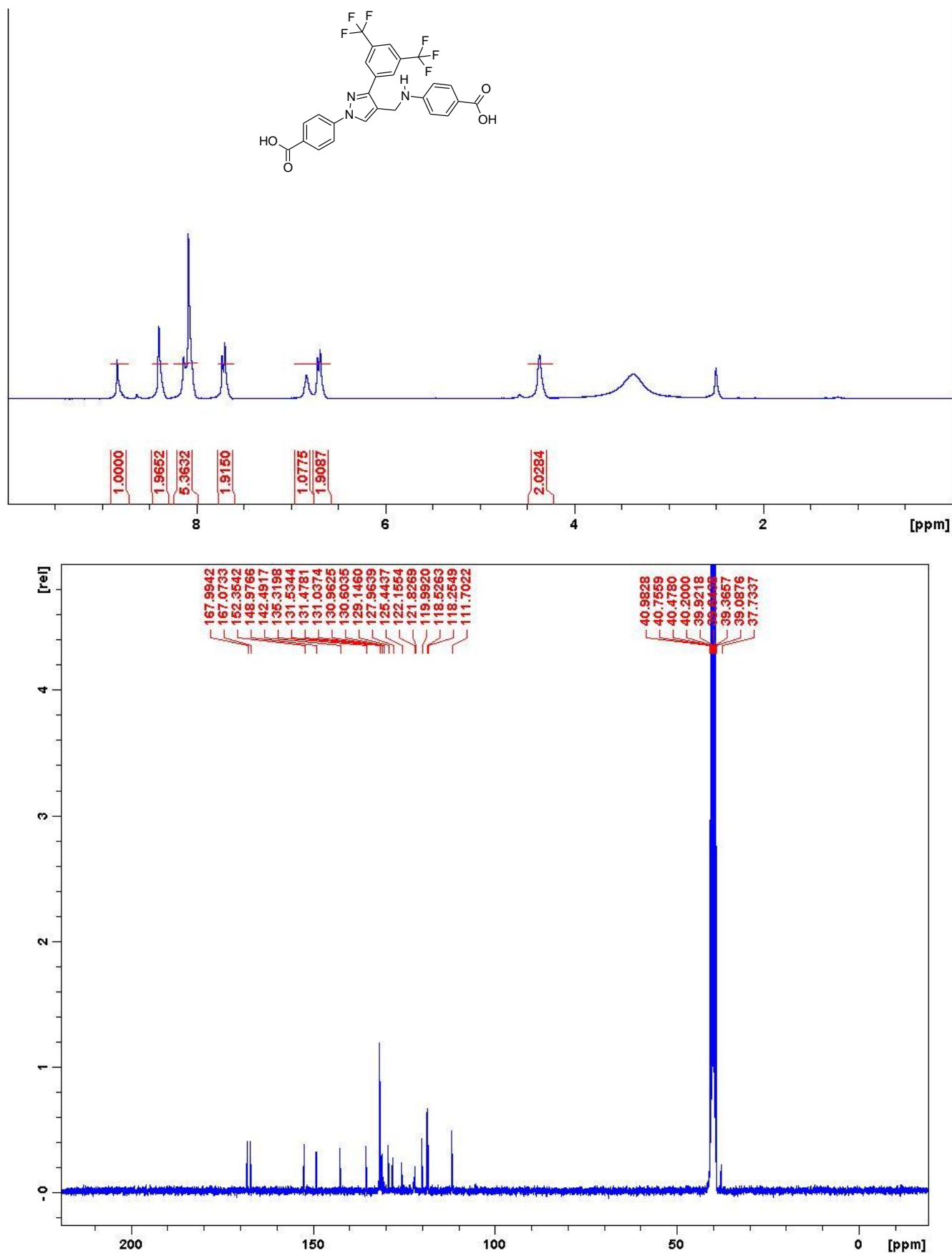


Figure S14. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 13

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(4-fluoro-3-methyl-anilino)methyl]pyrazol-1-yl] benzoic acid (14).

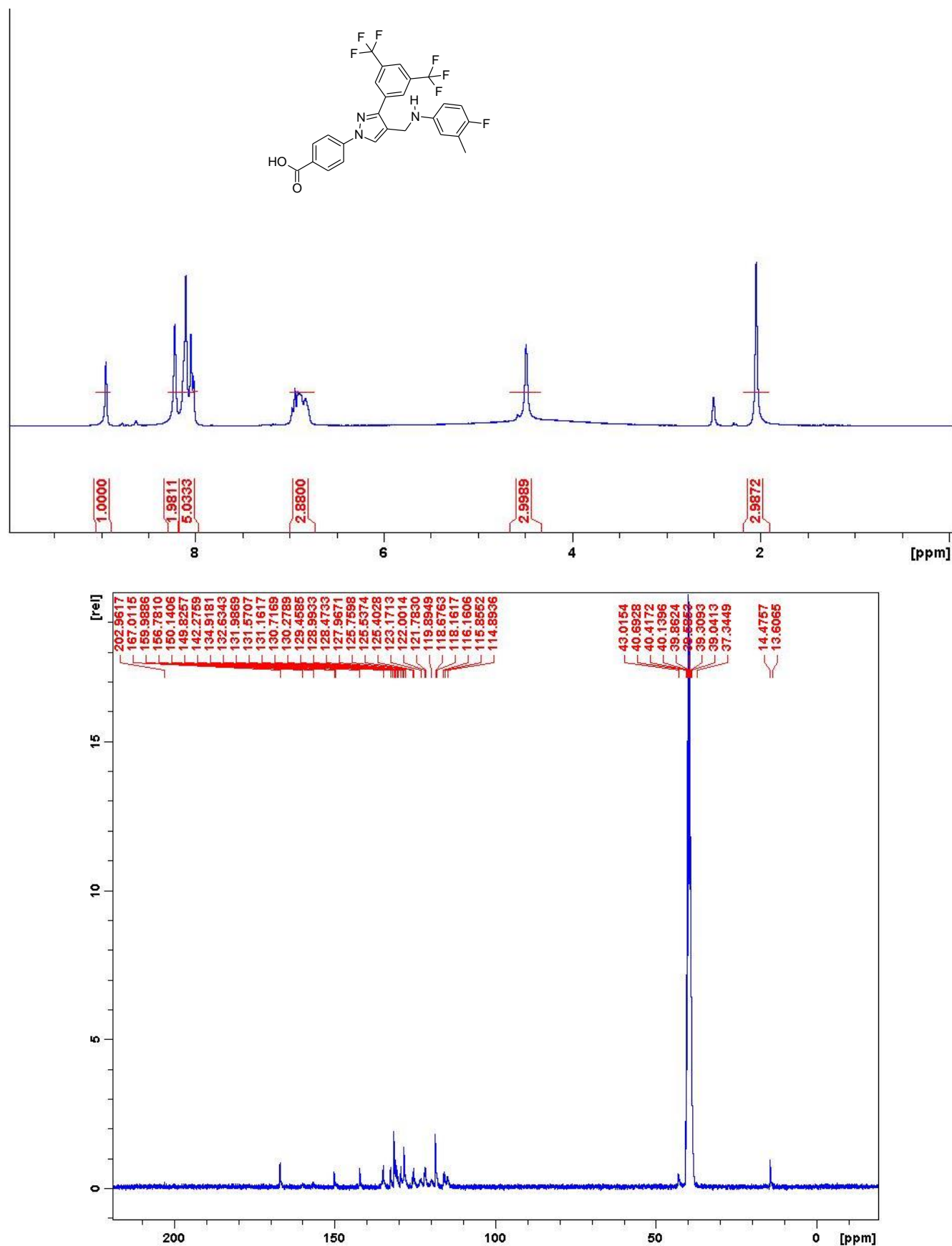


Figure S15. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 14



4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(3-chloro-4-methyl-anilino)methyl]pyrazol-1-yl] benzoic acid  
(15).

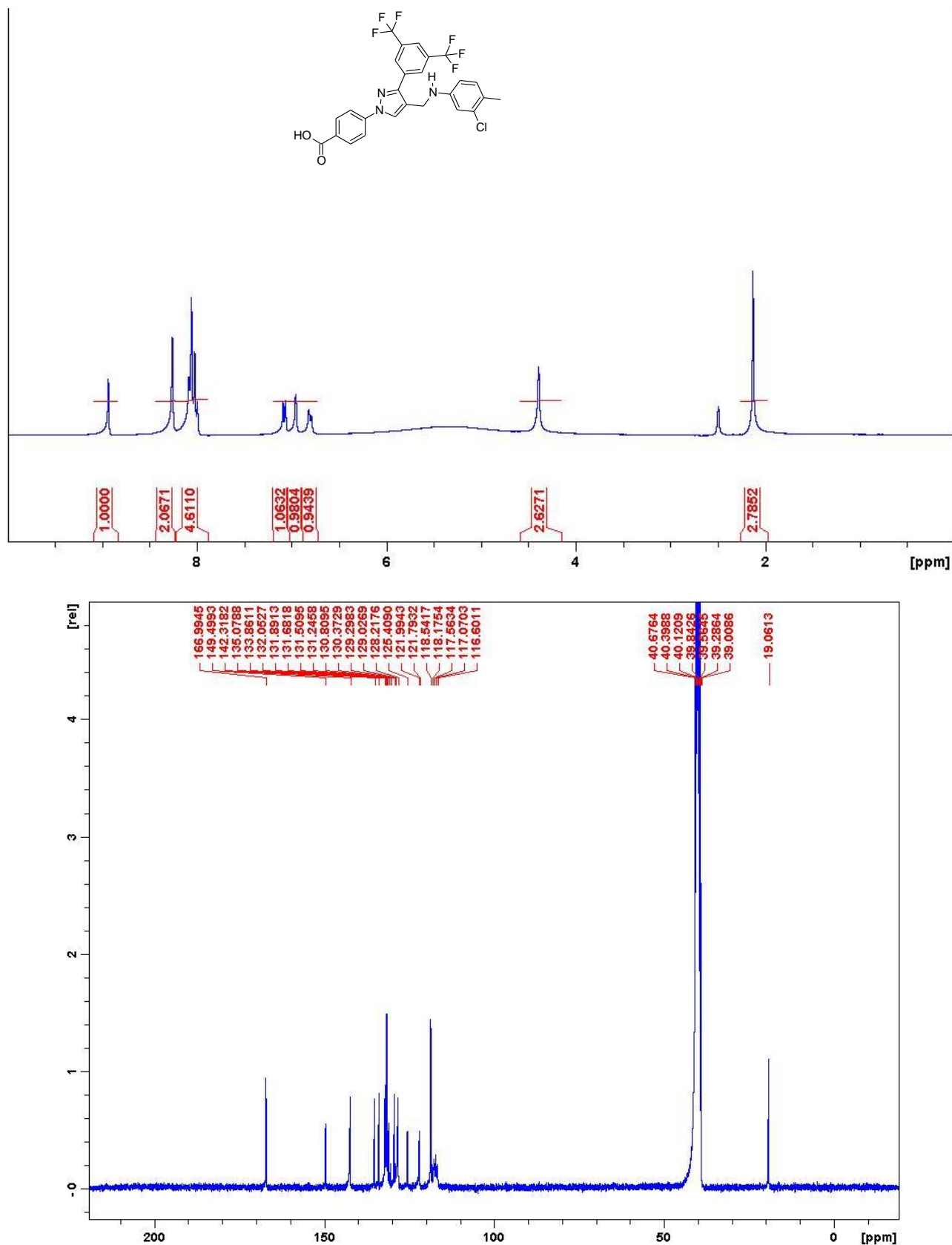


Figure S16. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 15

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(4-bromo-3-methyl-anilino)methyl]pyrazol-1-yl]benzoic acid (16).

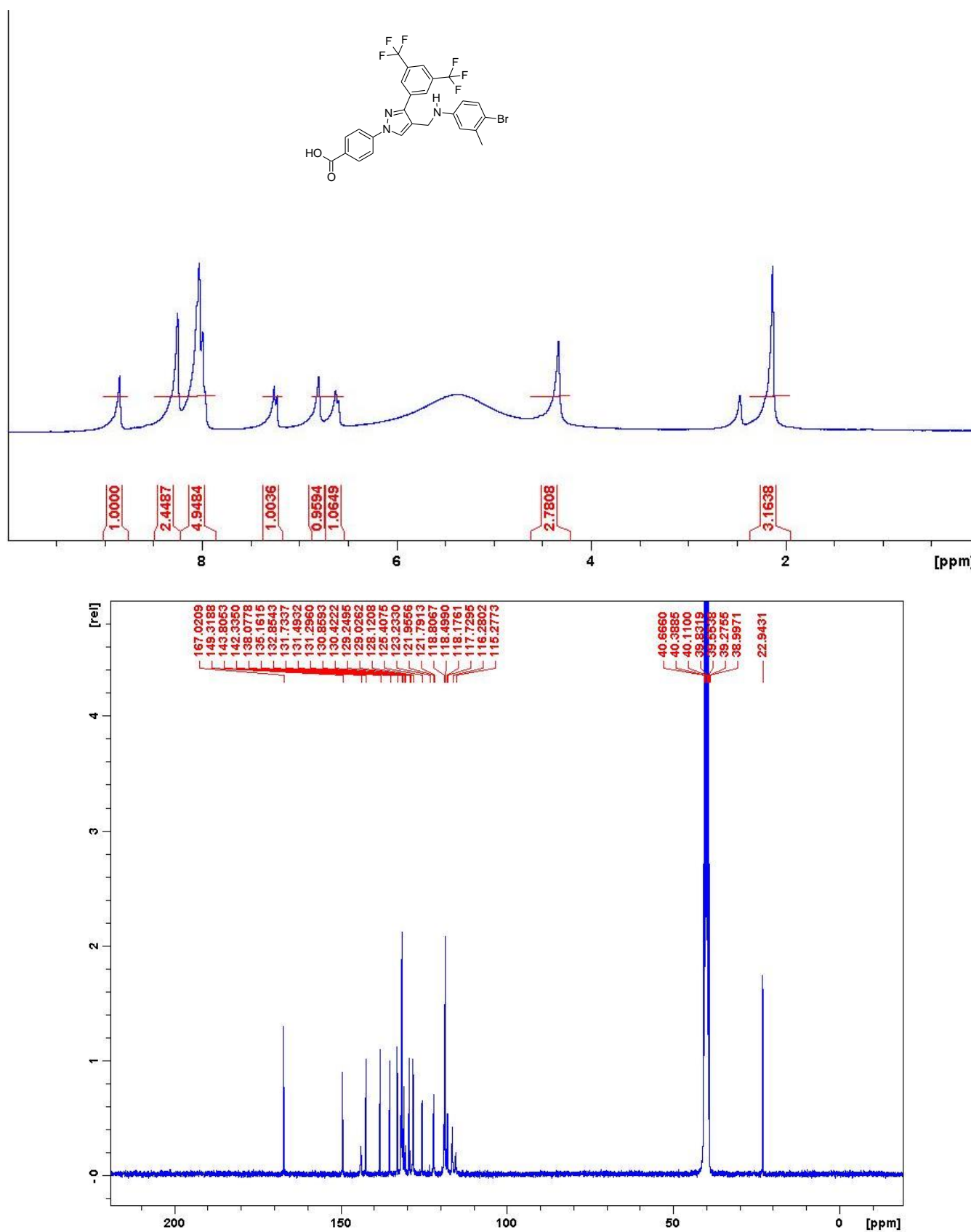
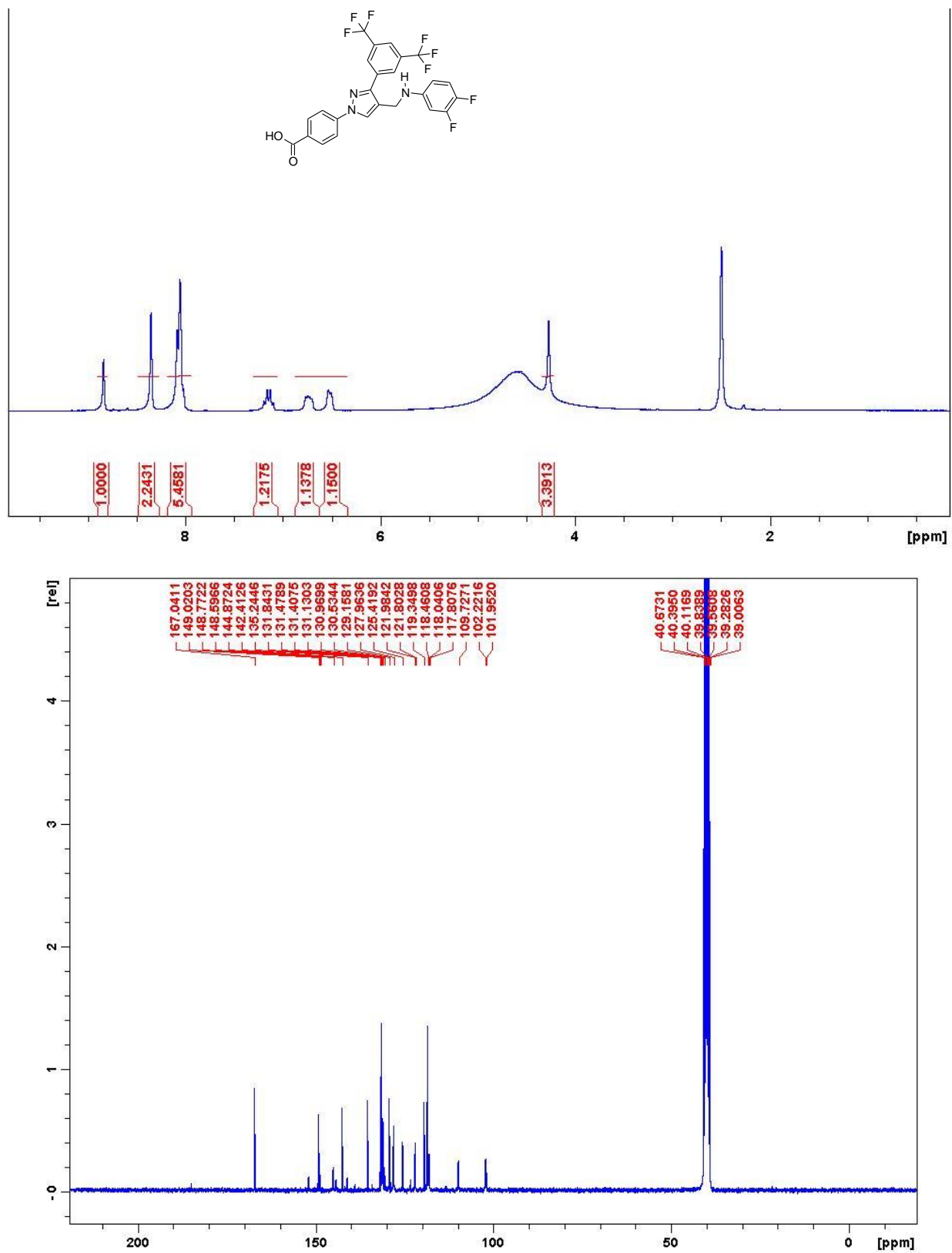


Figure S17. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 16

**4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(3,4-difluoroanilino) methyl] pyrazol-1-yl] benzoic acid (17).**



**Figure S18.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **17**

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(3-chloro-4-fluoro-anilino)methyl]pyrazol-1-yl] benzoic acid (18).

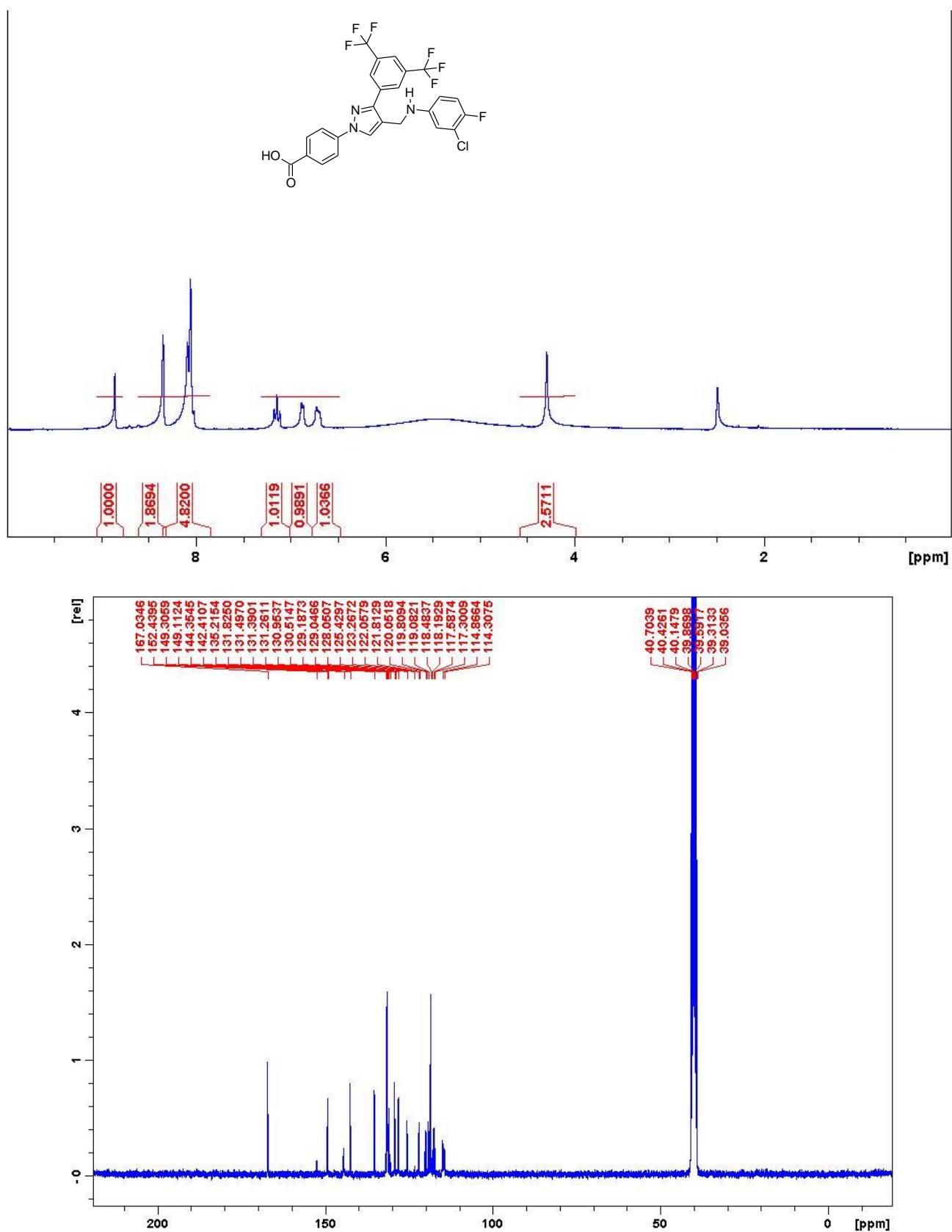


Figure S19. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 18

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(3,4-dichloroanilino)methyl]pyrazol-1-yl] benzoic acid (19).

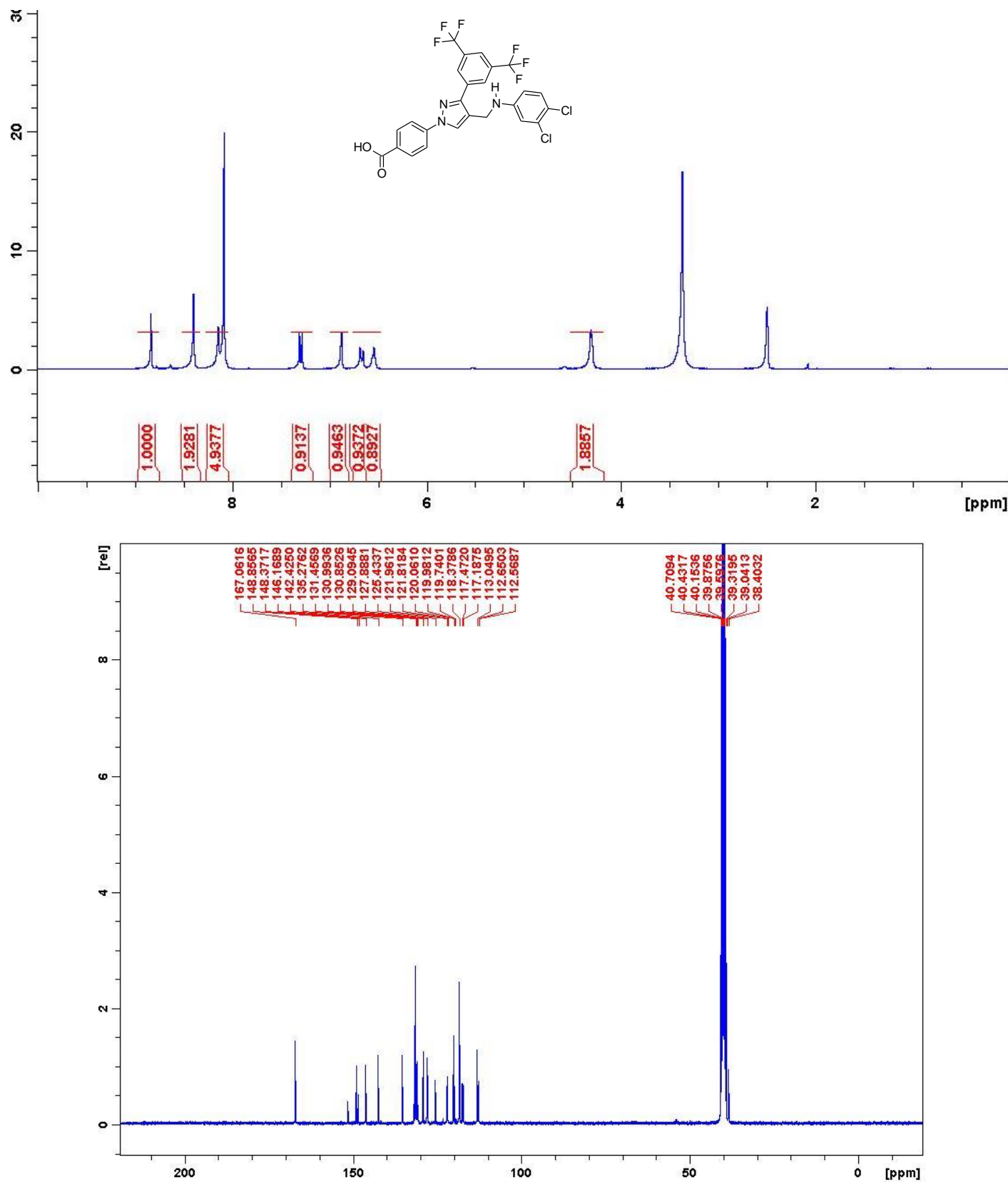


Figure S20. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 19

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(3,5-dichloroanilino) methyl] pyrazol-1-yl] benzoic acid (20).

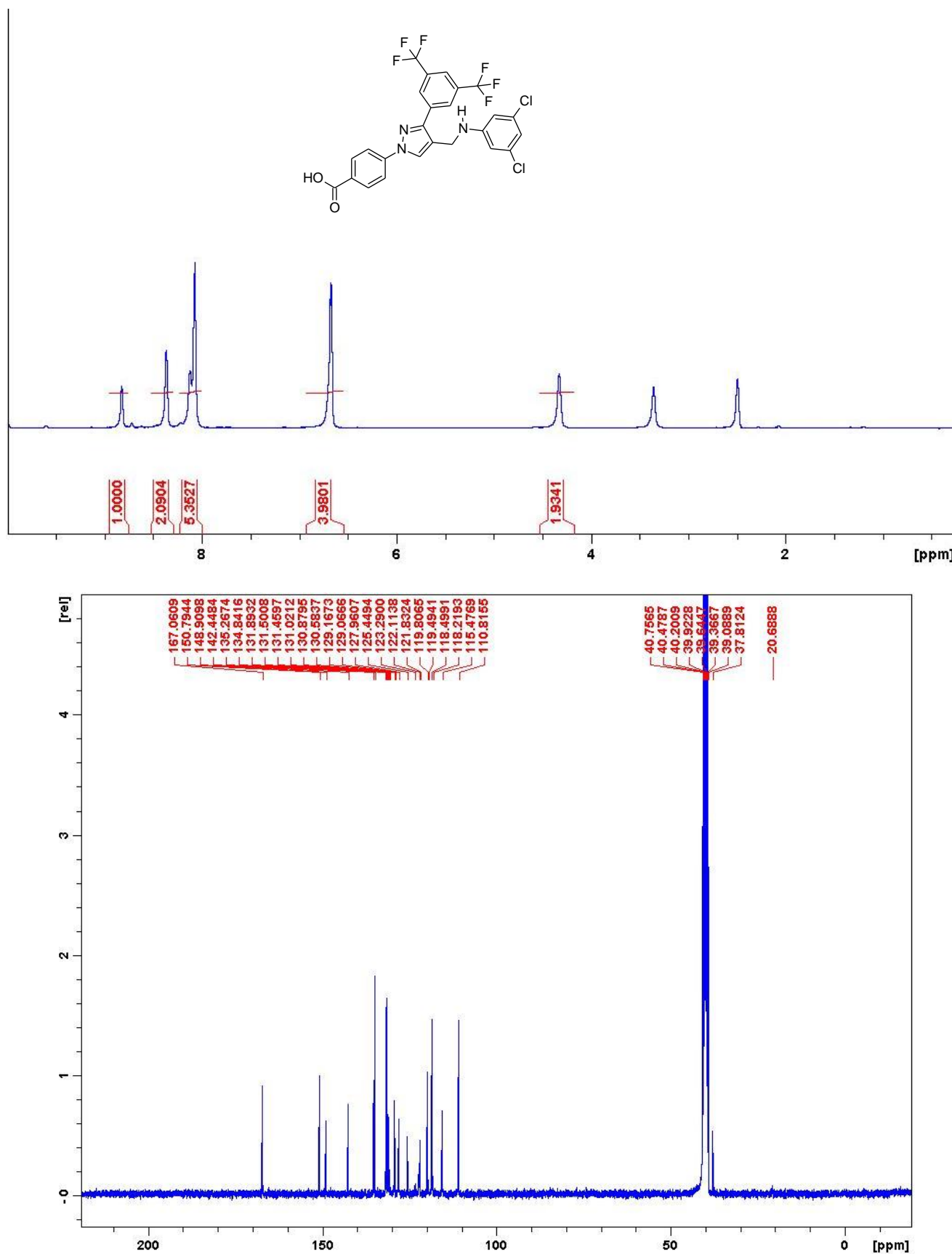


Figure S21. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 20

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(4-bromo-3-chloro-anilino)methyl]pyrazol-1-yl]benzoic acid (21).

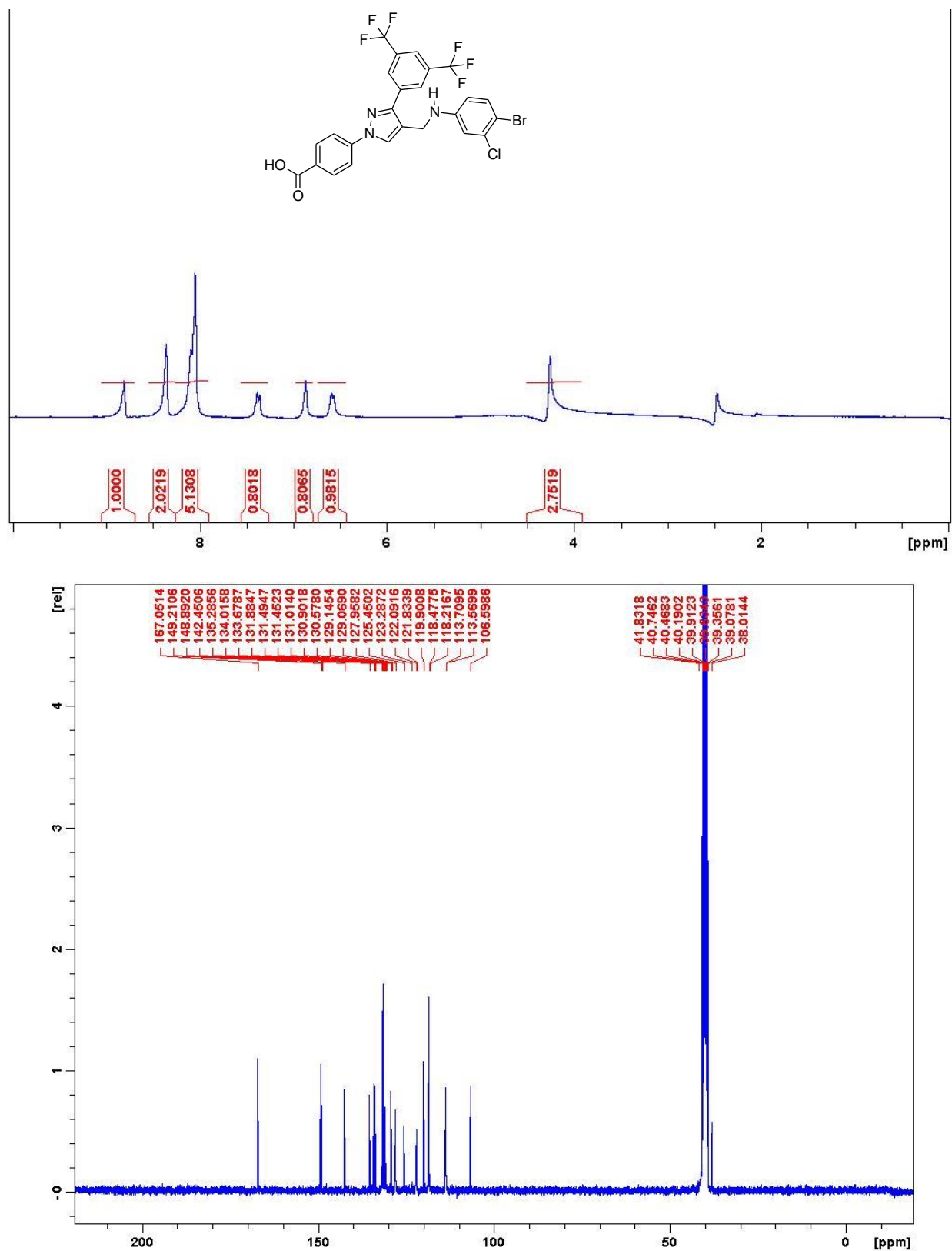
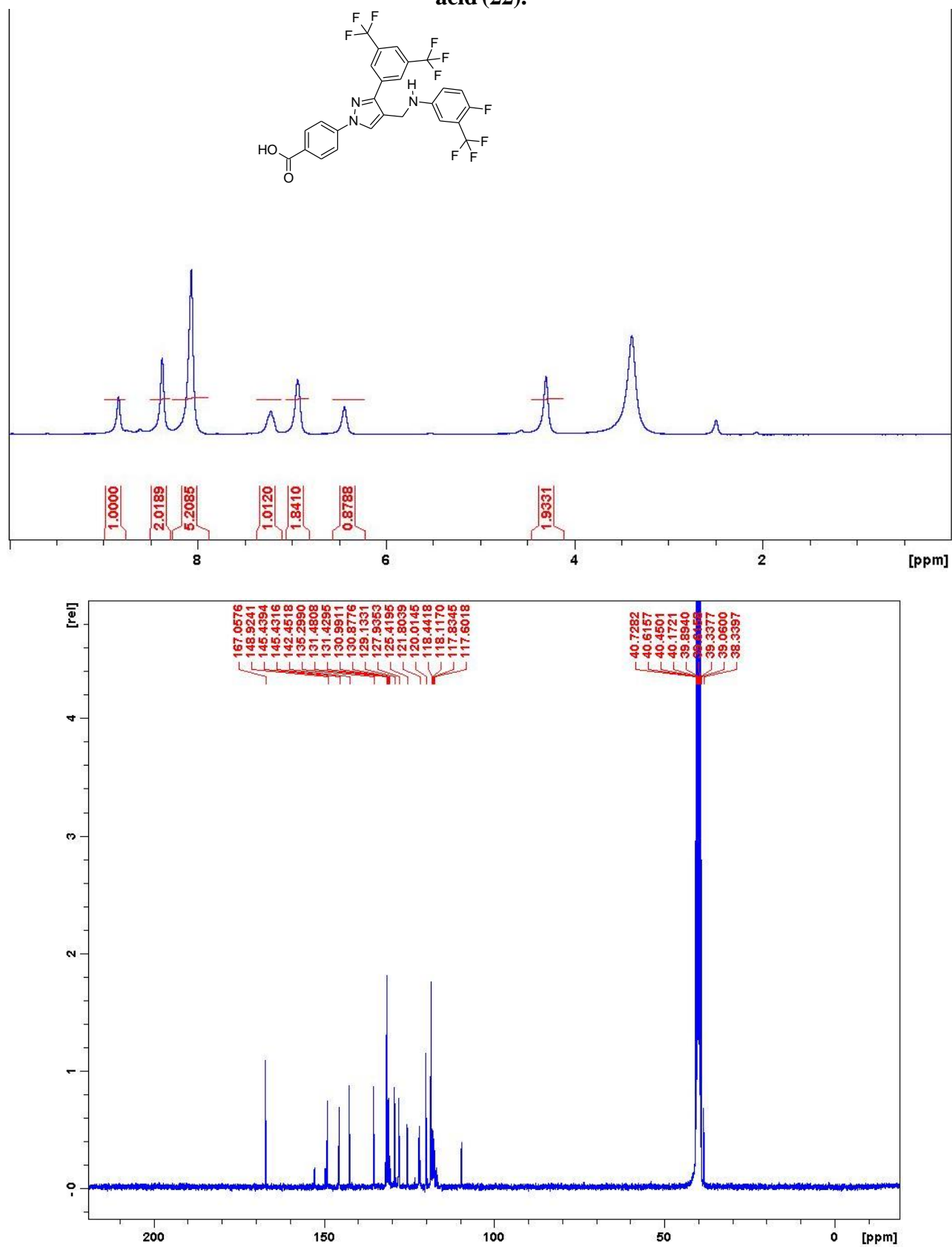


Figure S22. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 21

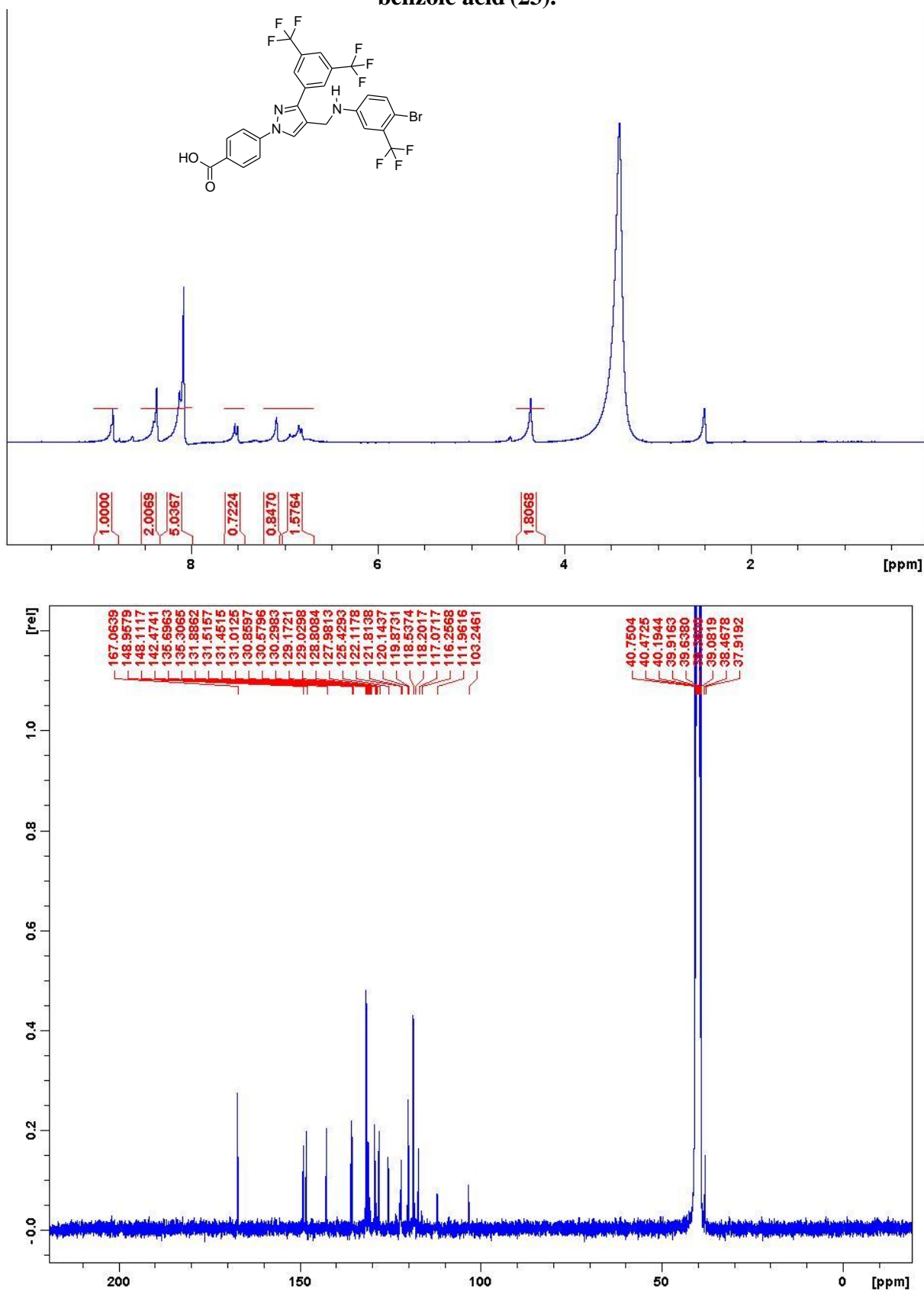
**4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[[4-fluoro-3-(trifluoromethyl)anilino]methyl]pyrazol-1-yl] benzoic acid (22).**



**Figure S23.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound **22**



**4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[[4-bromo-3-(trifluoromethyl)anilino]methyl]pyrazol-1-yl] benzoic acid (23).**



**Figure S24.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 23

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(2,3,4-trifluoroanilino) methyl] pyrazol-1-yl] benzoic acid (24).

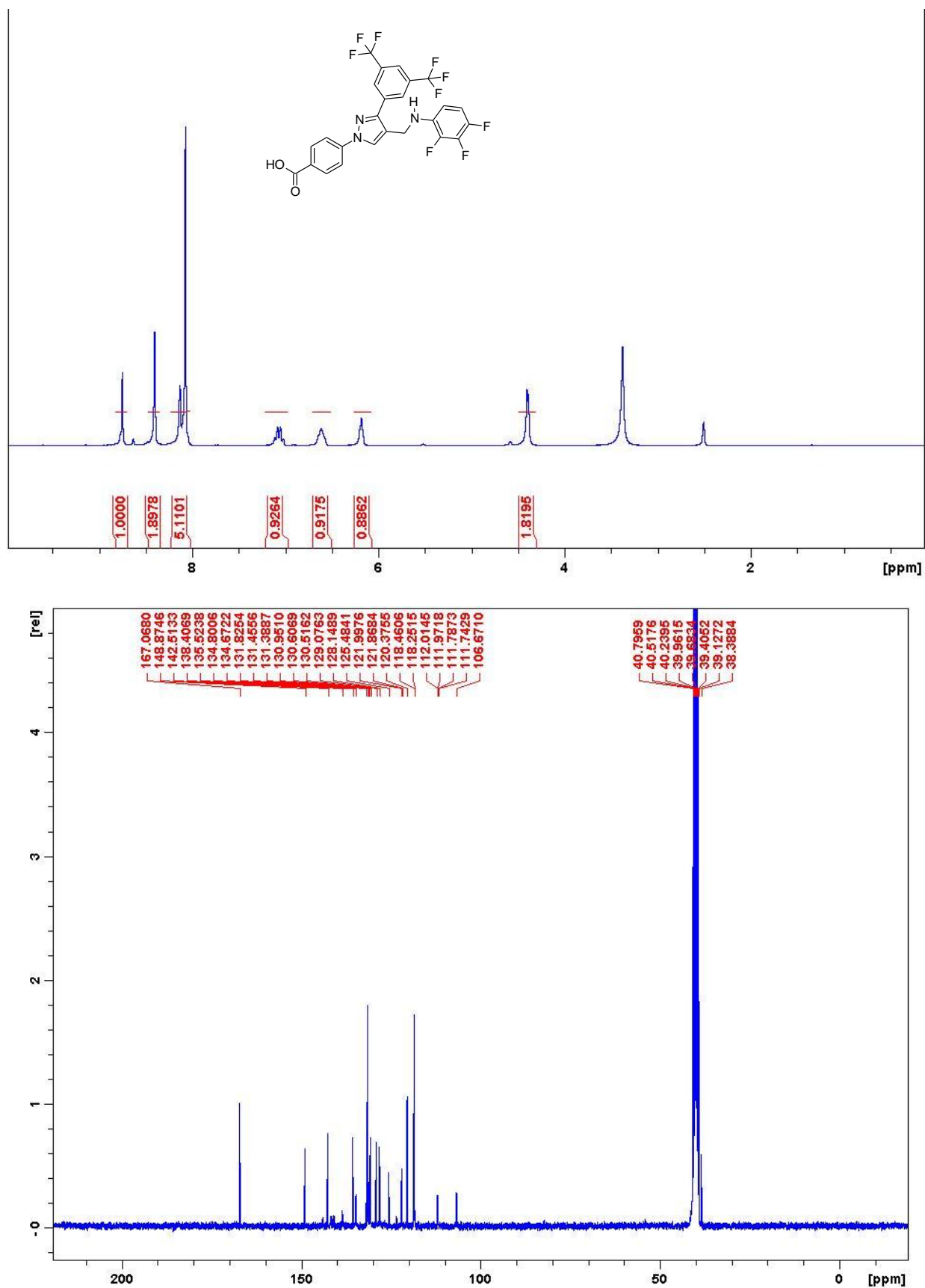


Figure S25. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 24

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(3,4,5-trifluoroanilino) methyl]pyrazol-1-yl]benzoic acid (25).

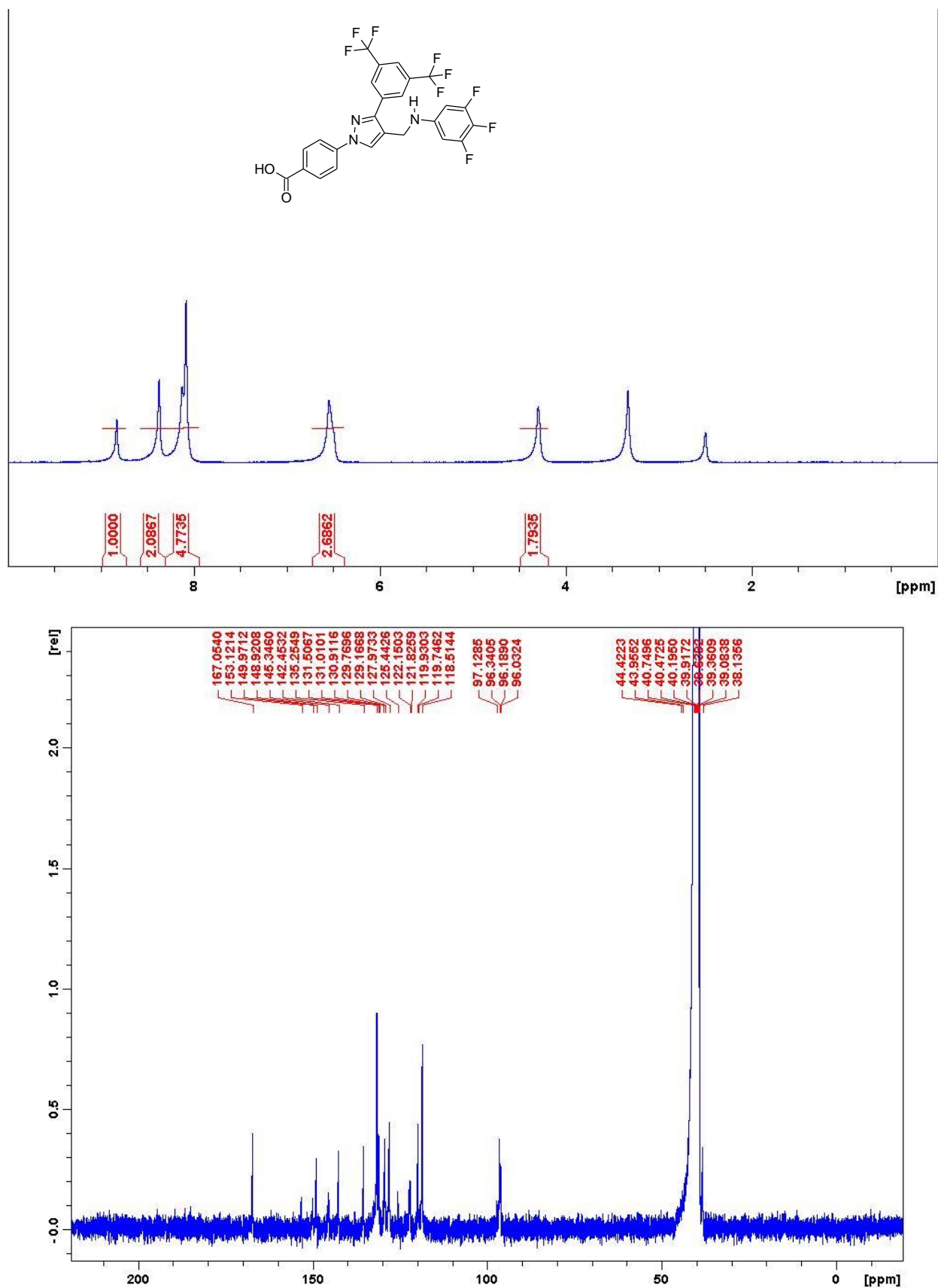


Figure S26. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 25

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(5-chloro-2,4-difluoro-anilino) methyl]pyraz-ol-1-yl] benzoic acid  
(26).

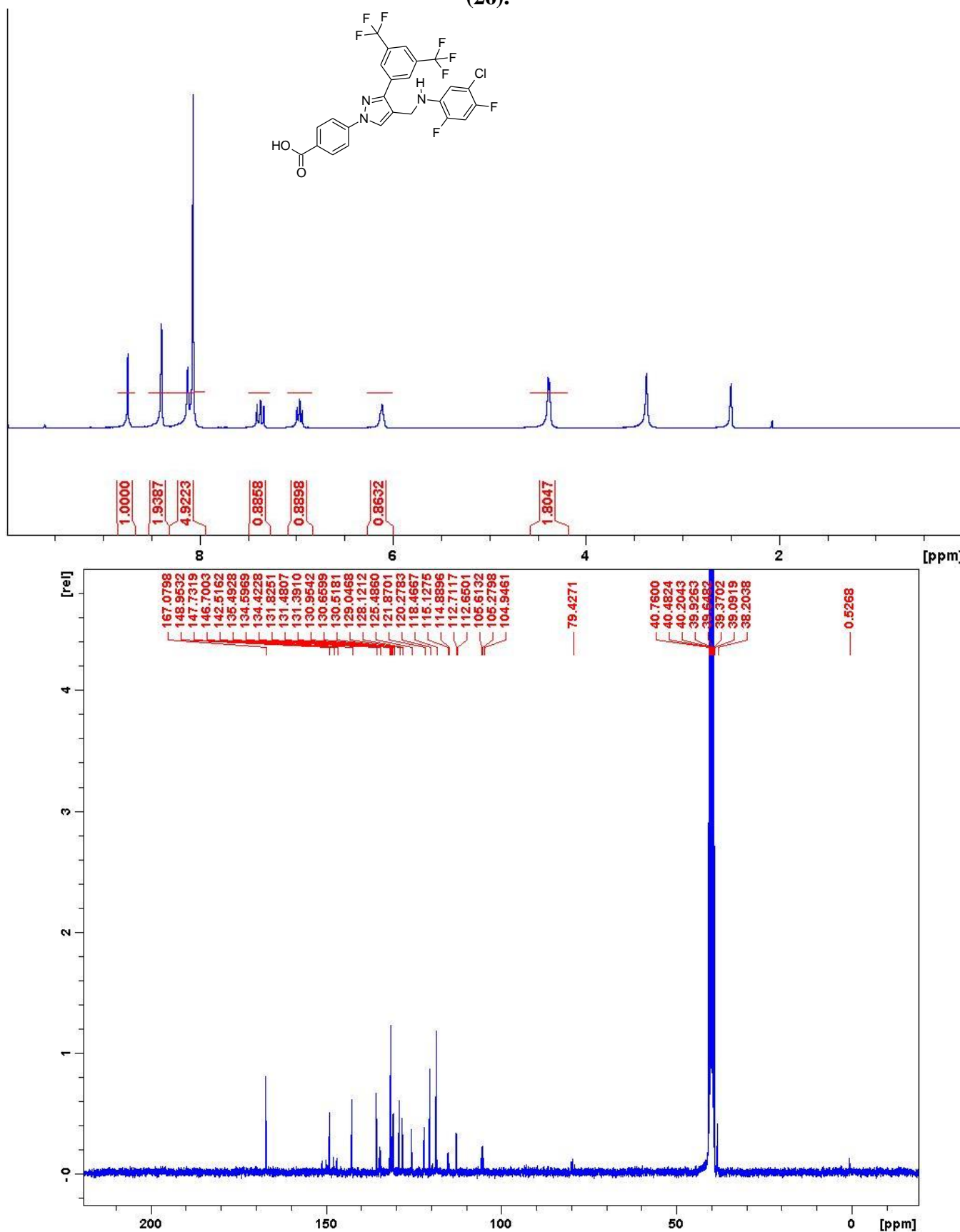


Figure S27. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 26

4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(3-chloro-2,4-difluoro-anilino) methyl] pyraz-ol-1-yl] benzoic acid (27).

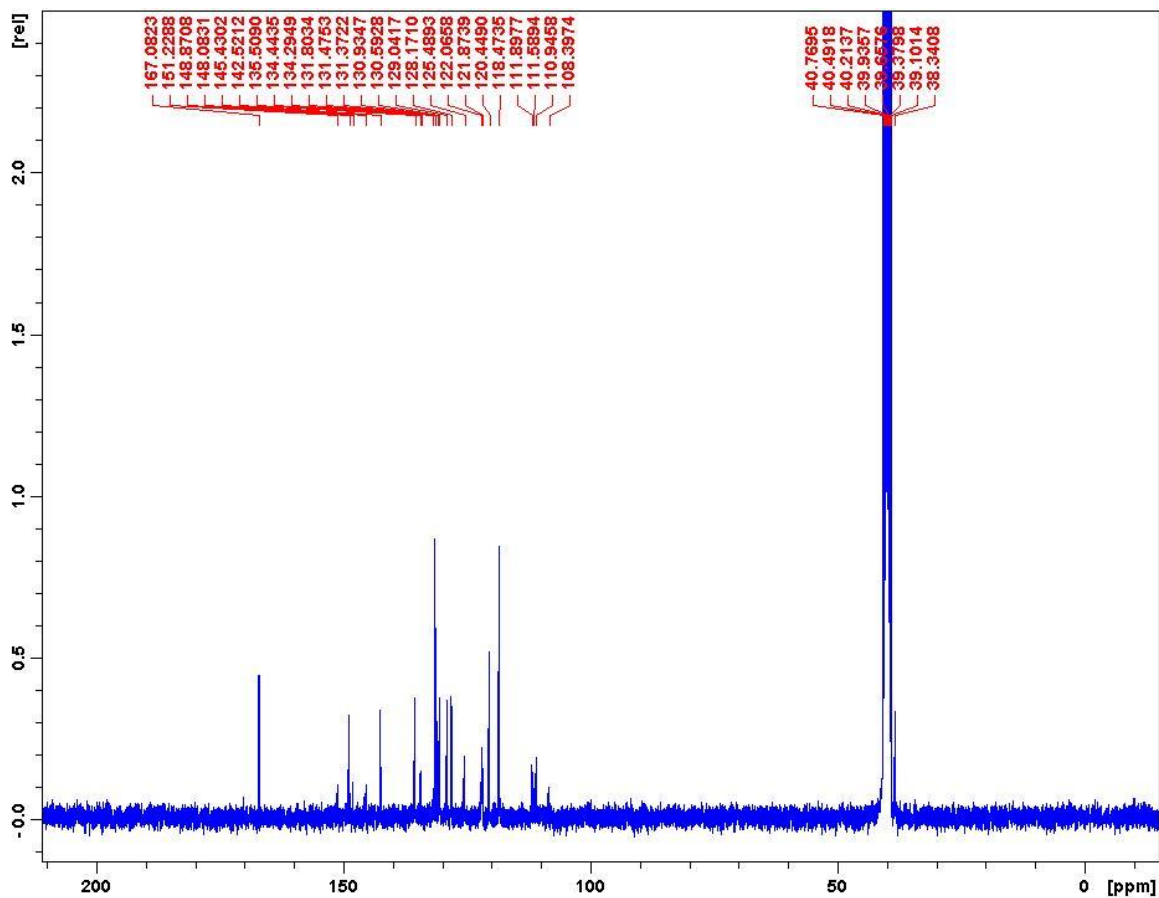
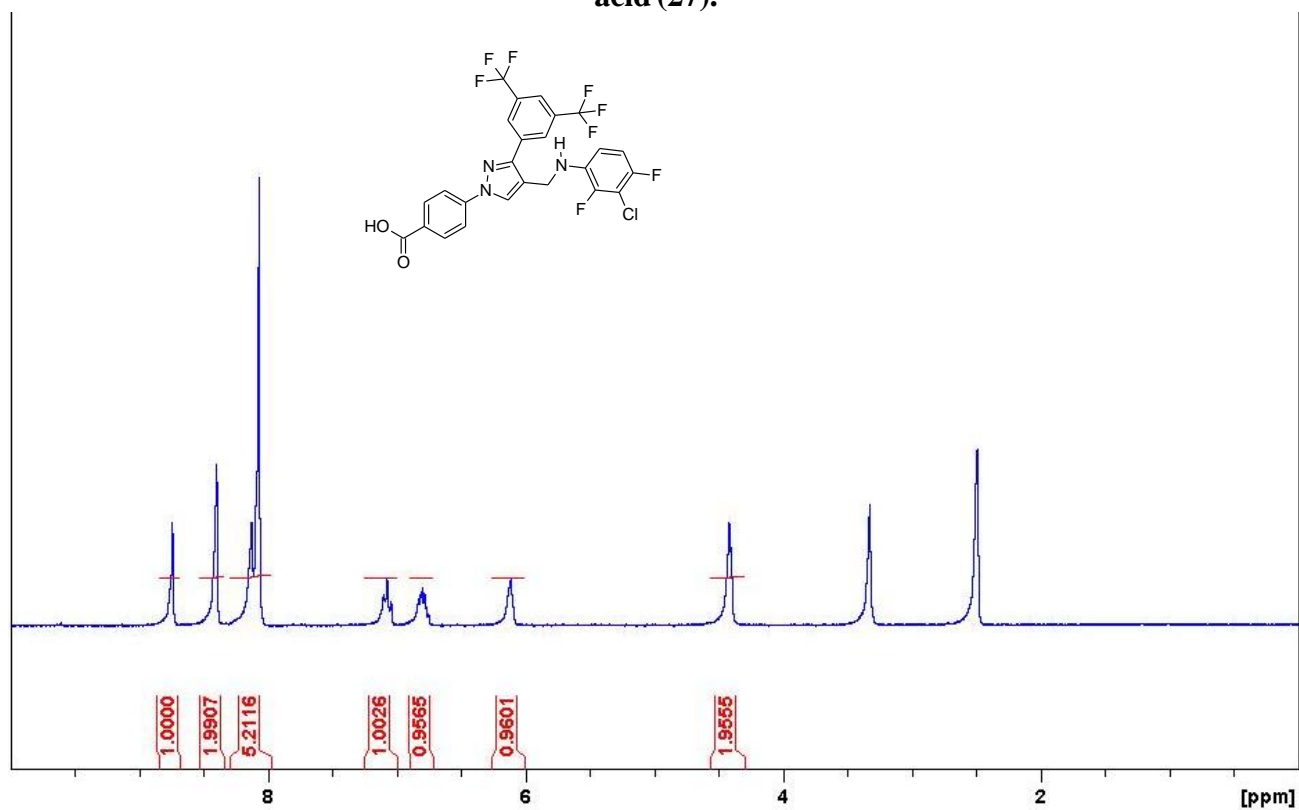


Figure S28. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 27

4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(3,5-dichloro-4-fluoro-anilino)methyl]pyraz-ol-1-yl]benzoic acid  
(28).

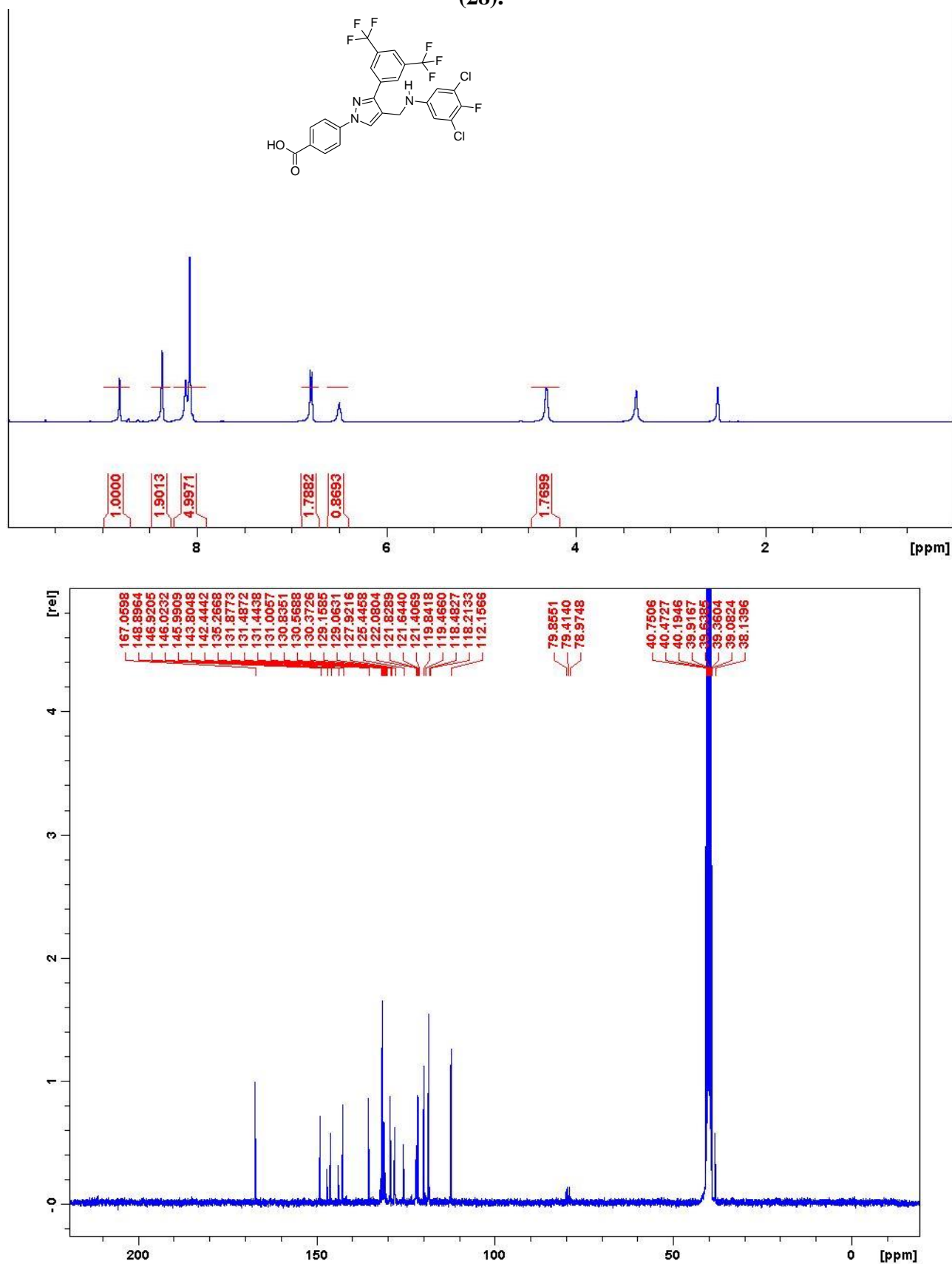
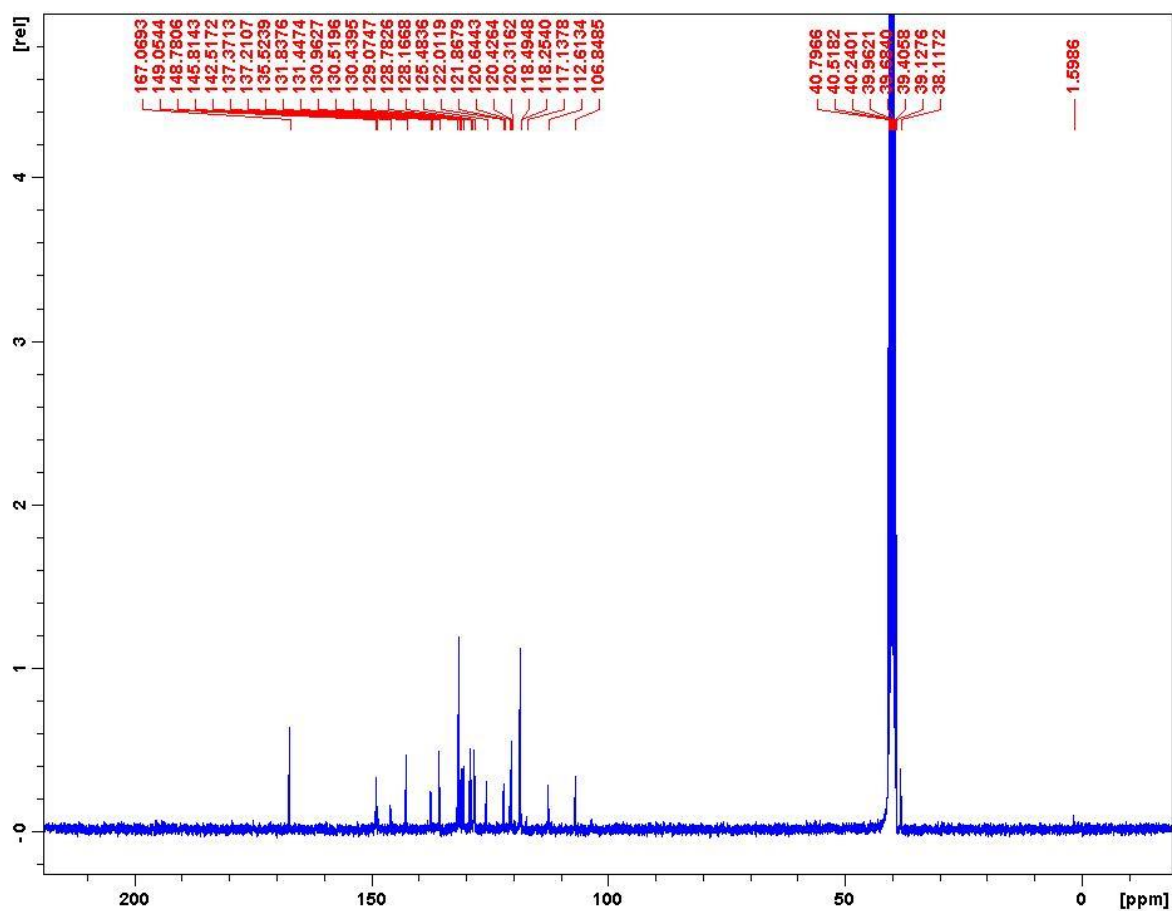
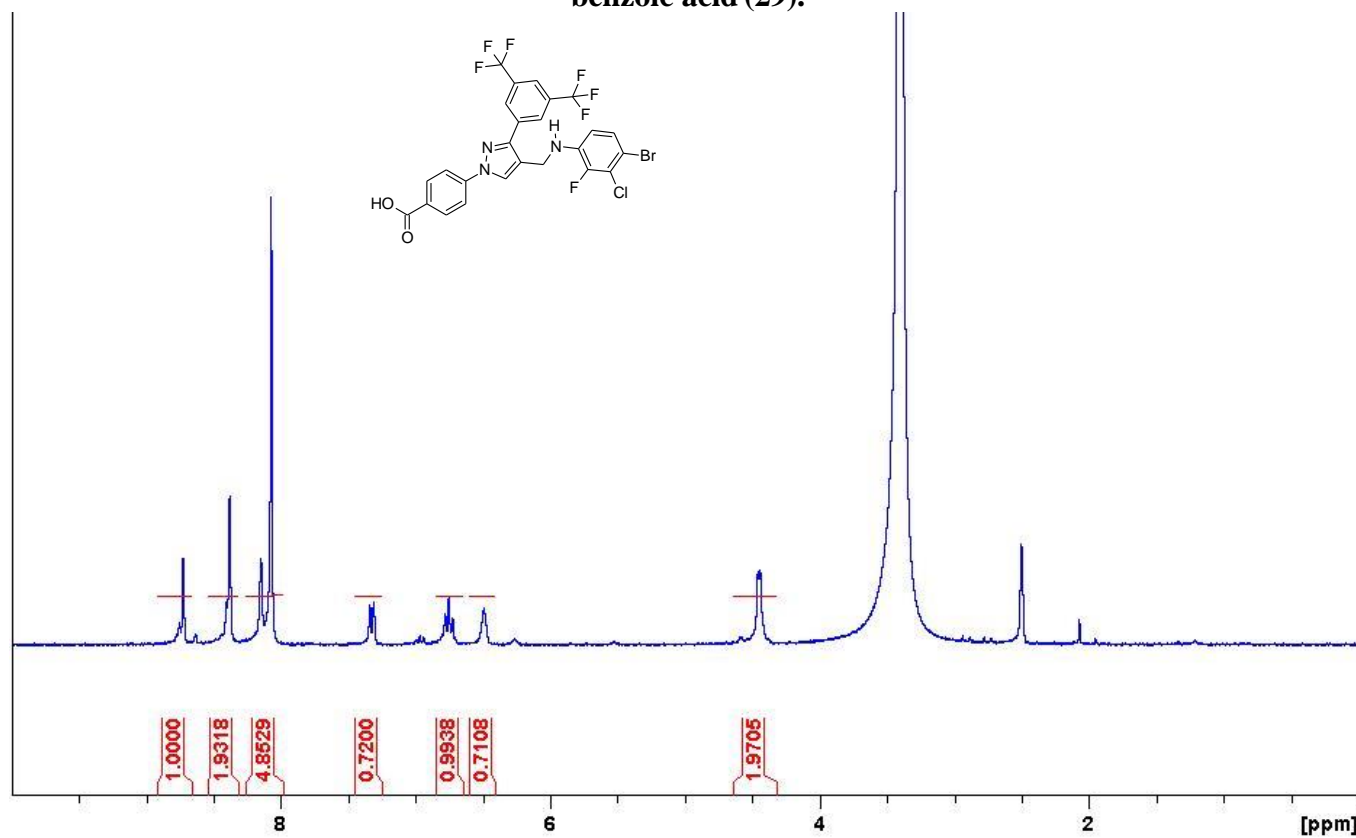


Figure S29. <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 28

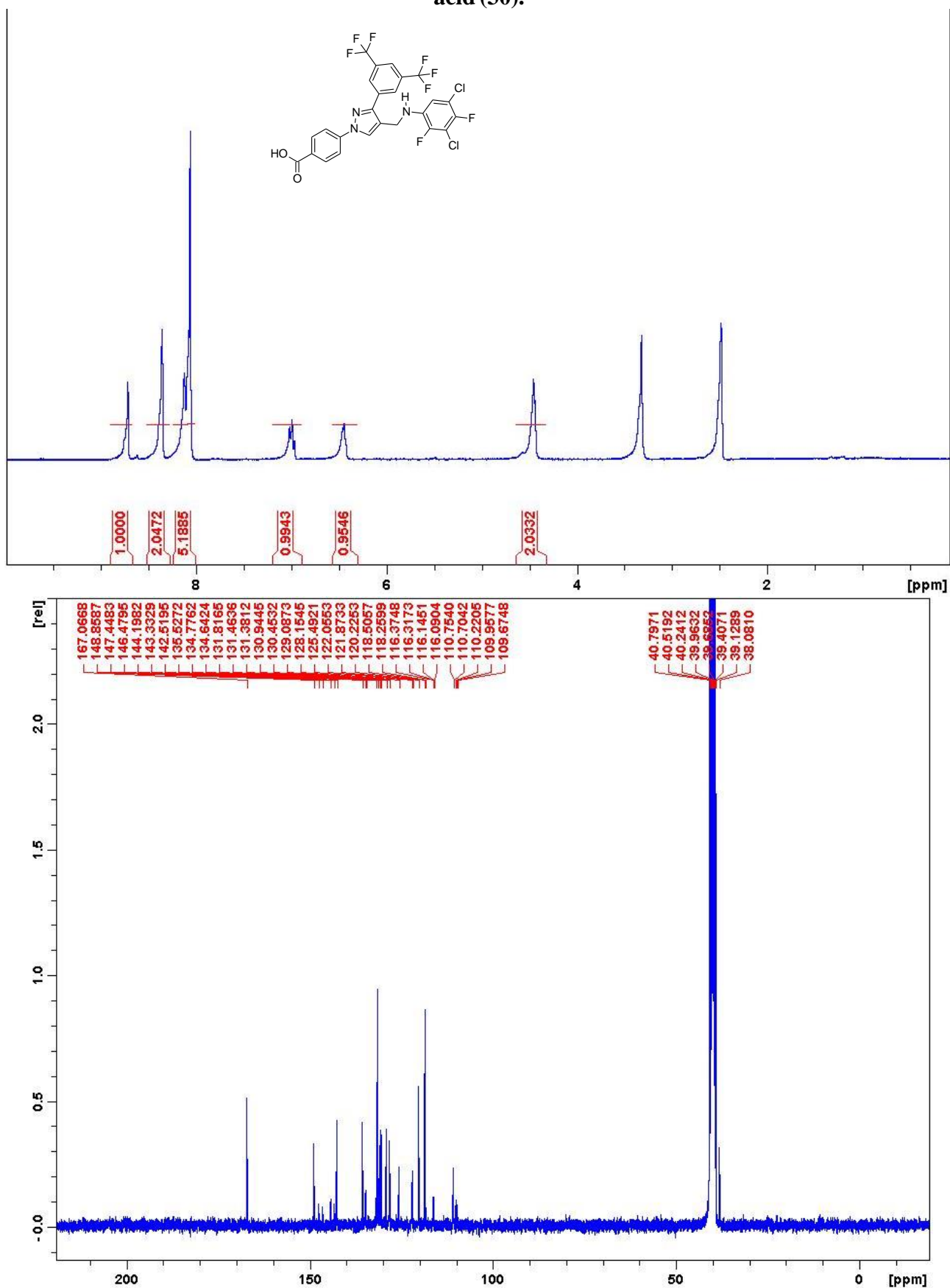
**4-[3-[3,5-Bis(trifluoromethyl) phenyl]-4-[(4-bromo-3-chloro-2-fluoro-anilino)methyl]pyrazol-1-yl] benzoic acid (29).**



**Figure S30.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 29



**4-[3-[3,5-Bis(trifluoromethyl)phenyl]-4-[(3,5-dichloro-2,4-difluoro-anilino)methyl] pyrazol-1-yl] benzoic acid (30).**



**Figure S31.** <sup>1</sup>H NMR and <sup>13</sup>C NMR spectra of compound 30