Supplementary Information

Design, Synthesis, Biological Evaluation and Molecular Modeling Studies of Novel Eugenol Esters as Leishmanicidal Agents

Camila M. Coelho,*[a,b] Thiago dos Santos,[a] Poliany G. Freitas,[b] Juliana B. Nunes,[c] Marcos J. Marques,[c] Camila G. D. Padovani,[d] Wagner A. S. Júdice,[d] Ihosvany Camps,[e] Nelson J. F. da Silveira,[b] Diogo T. Carvalho[a] and Marcia P. Veloso[a,b]

[a]Laboratório de Pesquisa em Química Farmacêutica, Faculdade de Ciências Farmacêuticas, [b]Laboratório de Modelagem Molecular e Simulação Computacional, Instituto de Química and [c]Laboratório de Biologia Molecular de Microorganismos, Instituto de Ciências Biomédicas, Universidade Federal de Alfenas, Rua Gabriel Monteiro da Silva, 700, 37130-000 Alfenas-MG, Brazil

[d]Centro Interdisciplinar de Investigação Bioquímica, Universidade de Mogi das Cruzes, 08780-911 Mogi das Cruzes-SP, Brazil

[e]Laboratório de Modelagem Computacional (LaModel), Instituto de Ciências Exatas (ICEx), Universidade Federal de Alfenas, 37130-000 Alfenas-MG, Brazil

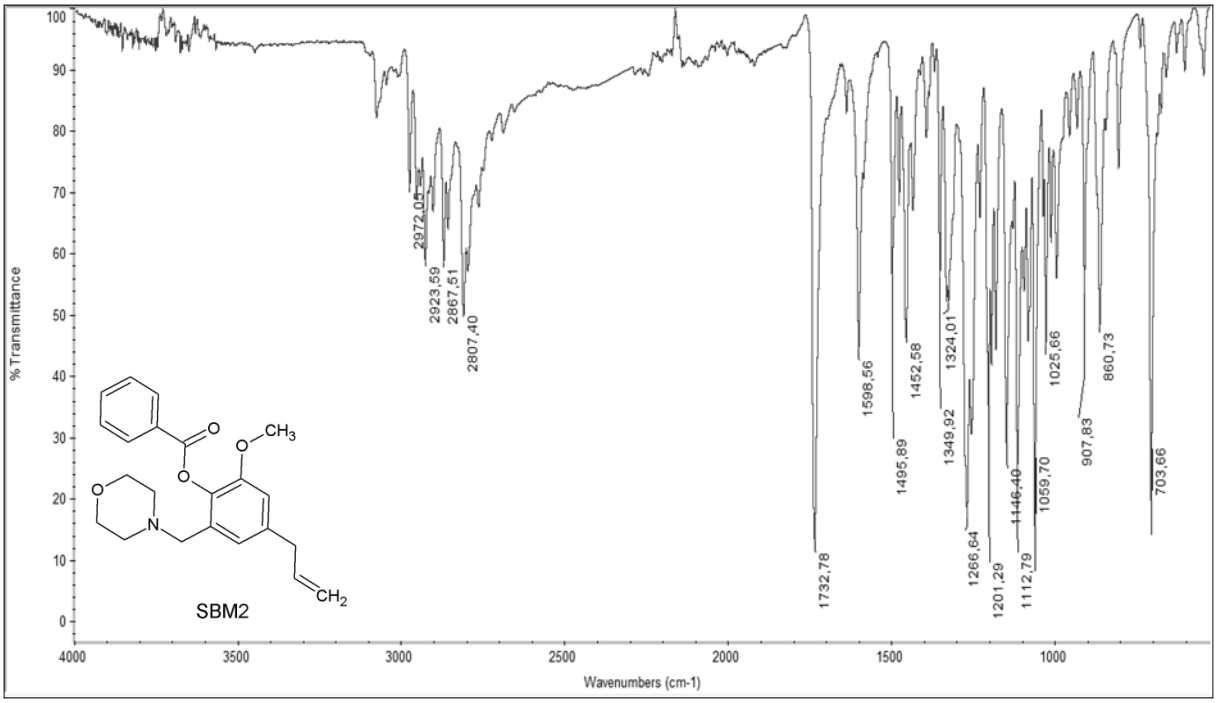

Figure S1. FTIR spectrum of compound **4a**.

*e-mail: camilademoraiscoelho@gmail.com

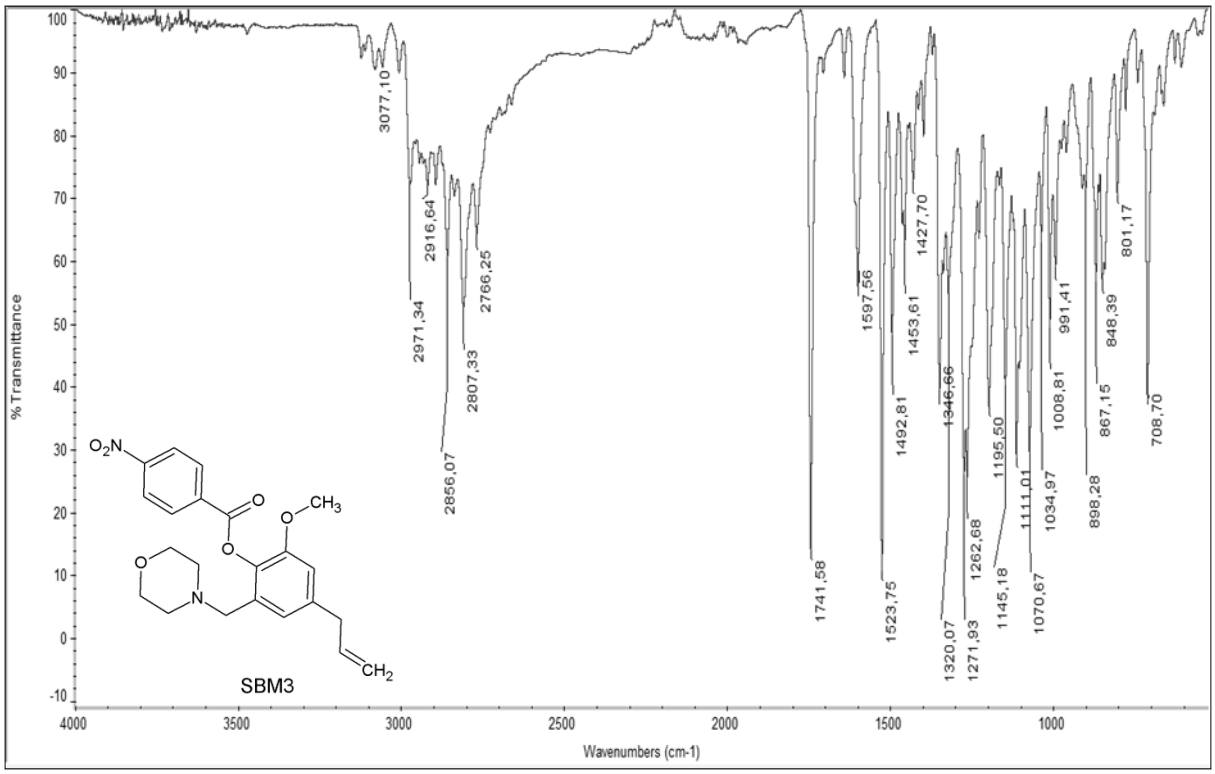

Figure S2. FTIR spectrum of compound **4b**.

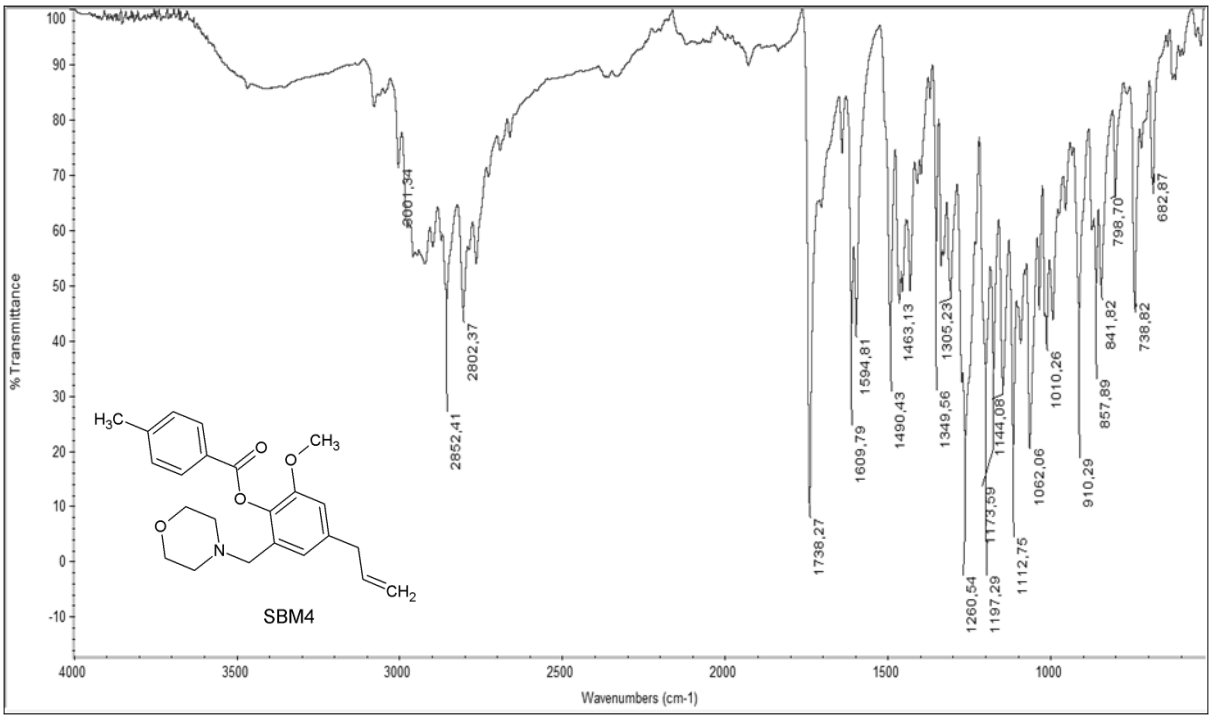

Figure S3. FTIR spectrum of compound **4c**.

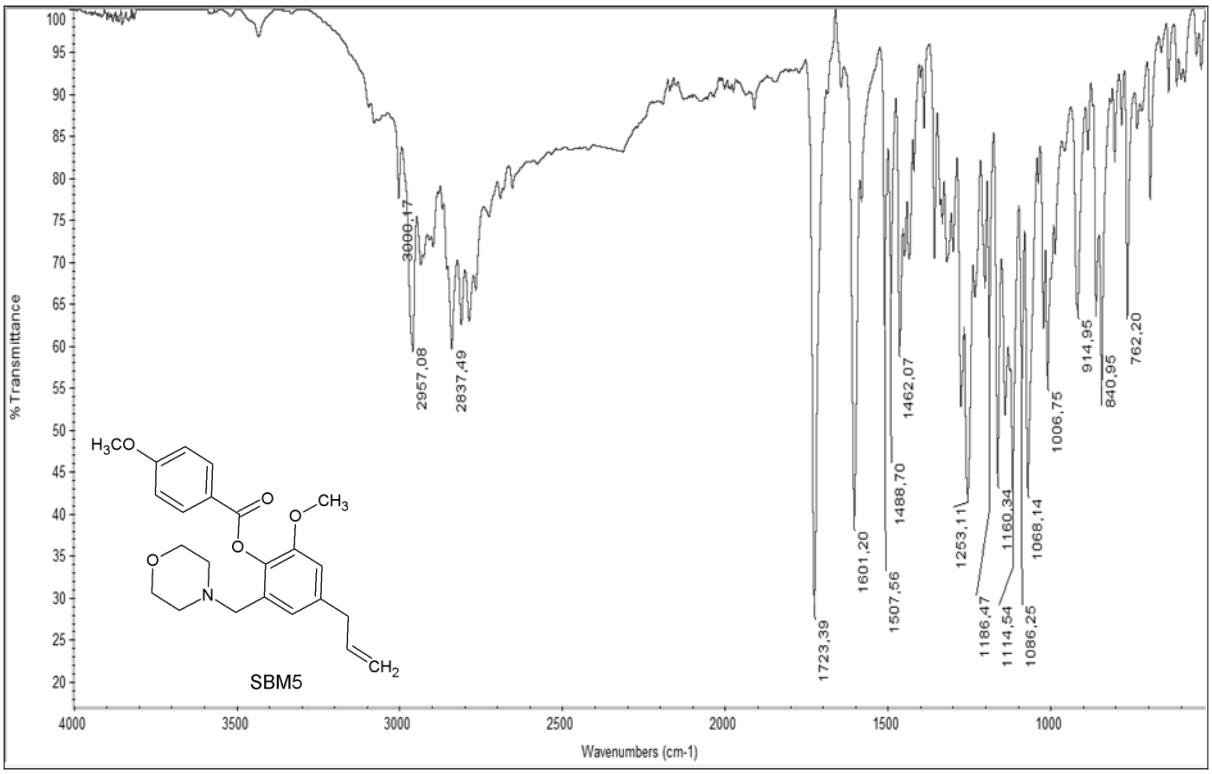

Figure S4. FTIR spectrum of compound **4d**.

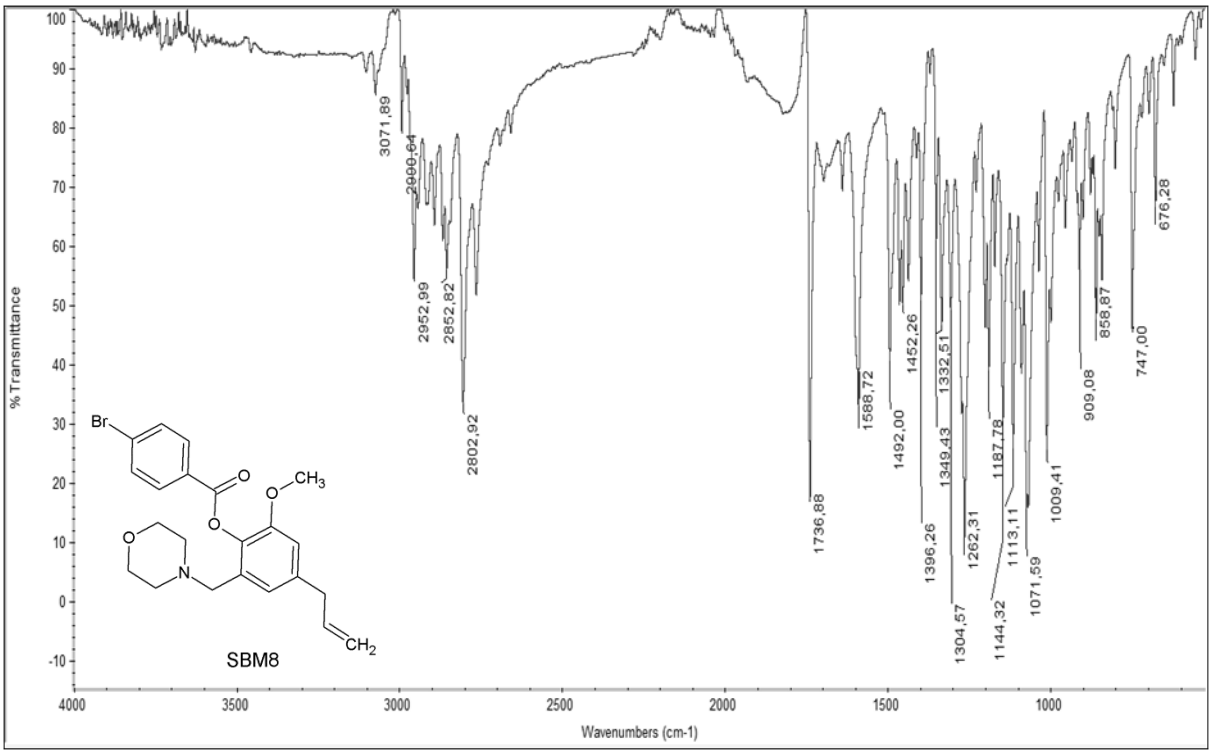

Figure S5. FTIR spectrum of compound **4e**.

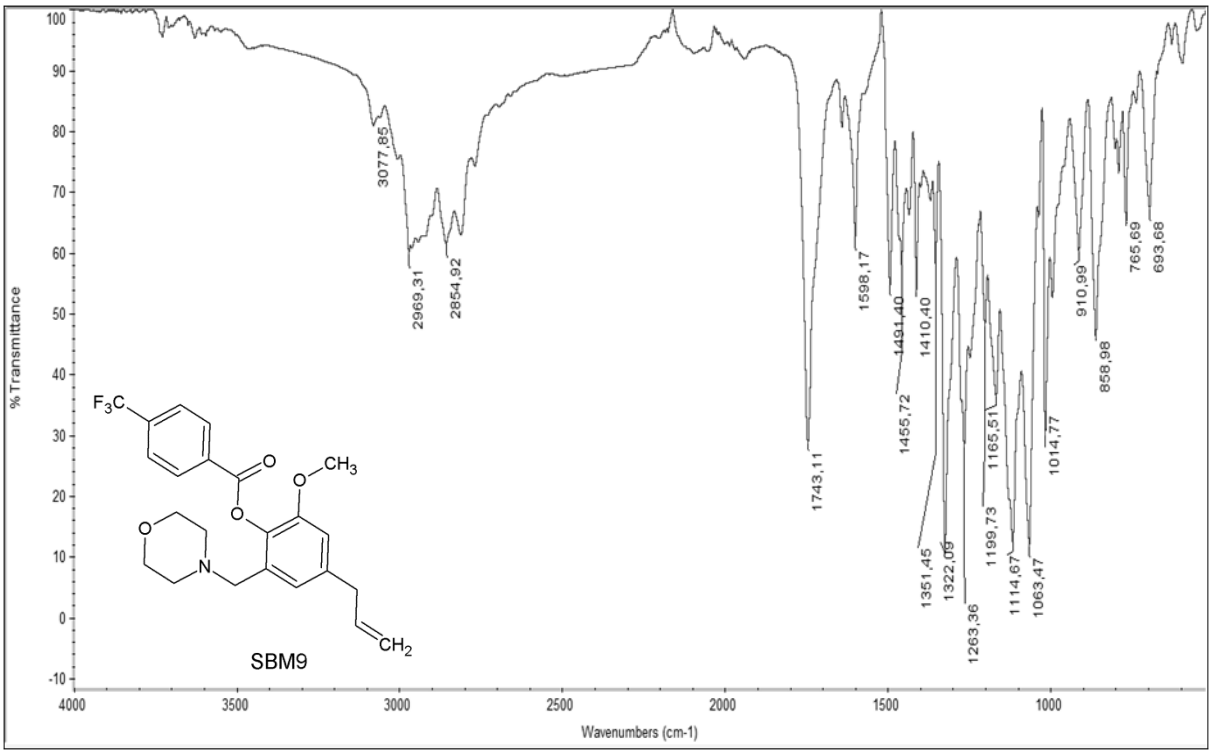

Figure S6. FTIR spectrum of compound **4f**.

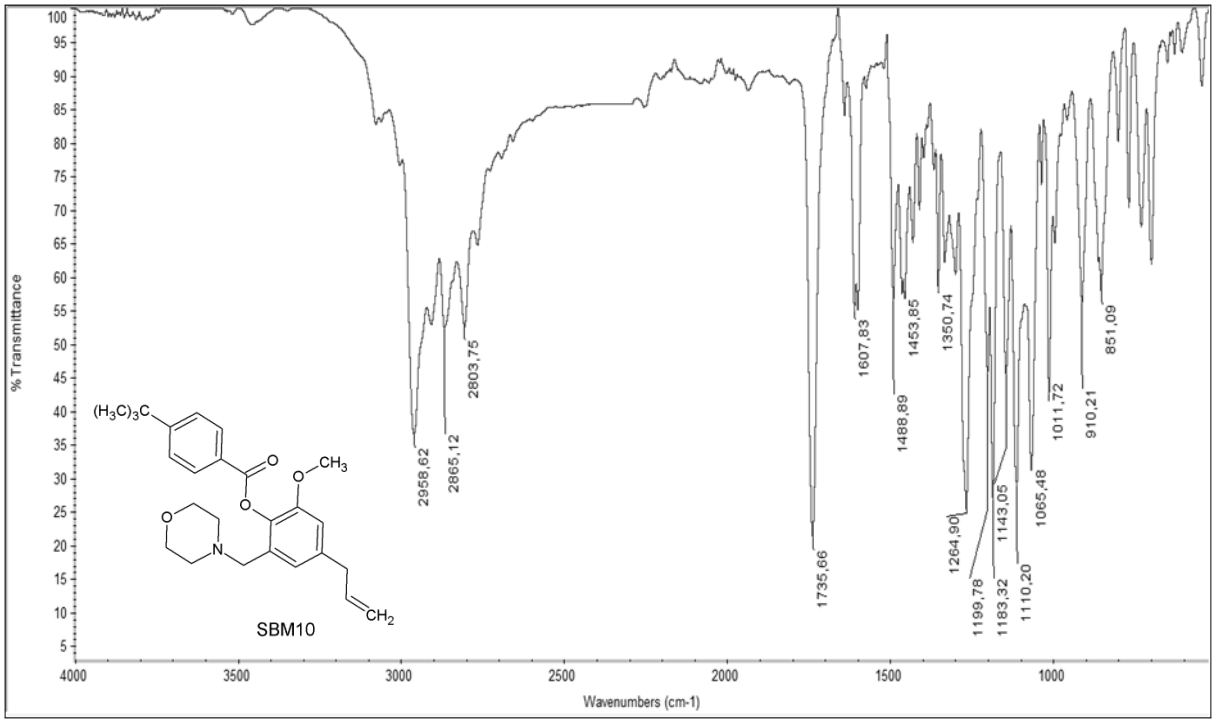

Figure S7. FTIR spectrum of compound **4g**.

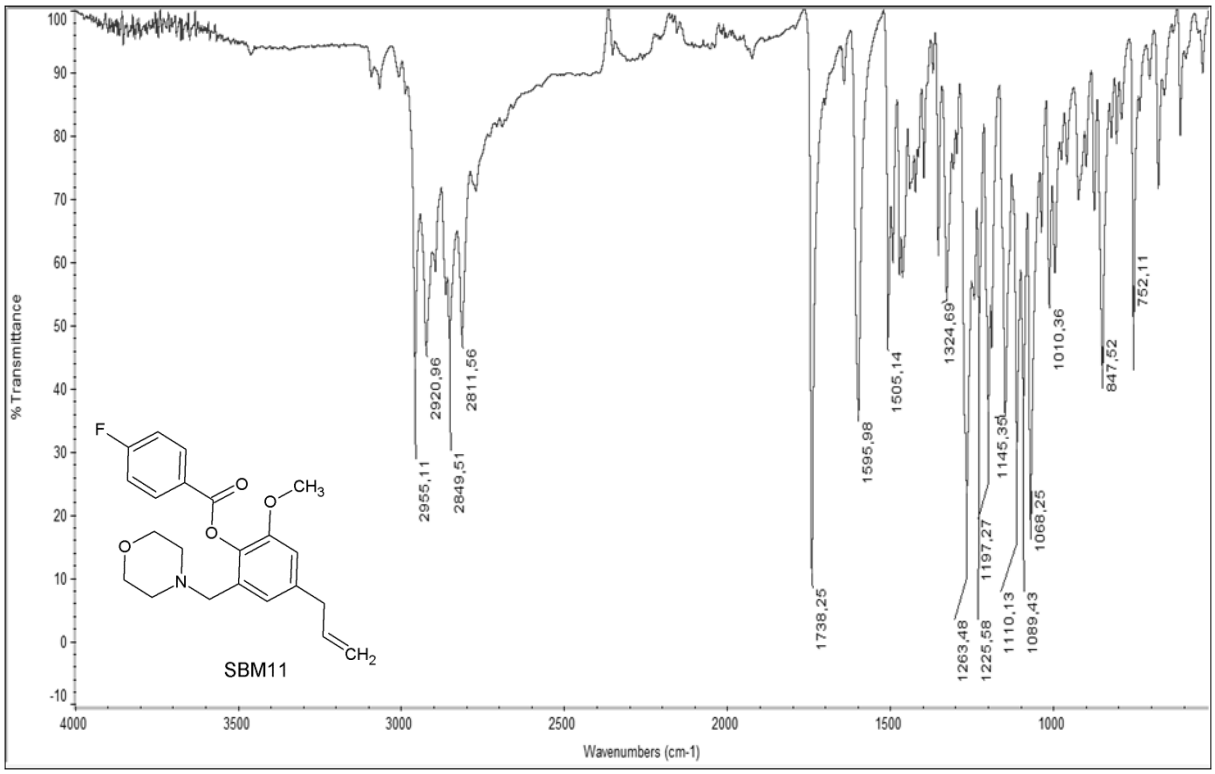

Figure S8. FTIR spectrum of compound **4h**.

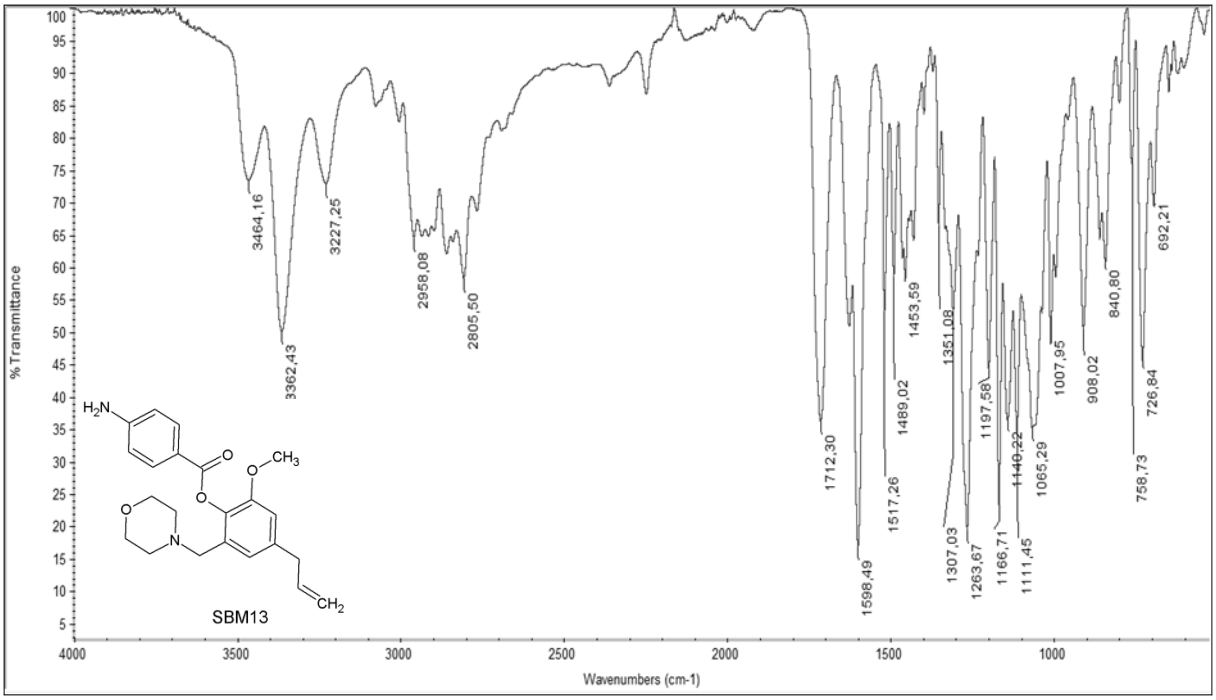

Figure S9. FTIR spectrum of compound **4i**.

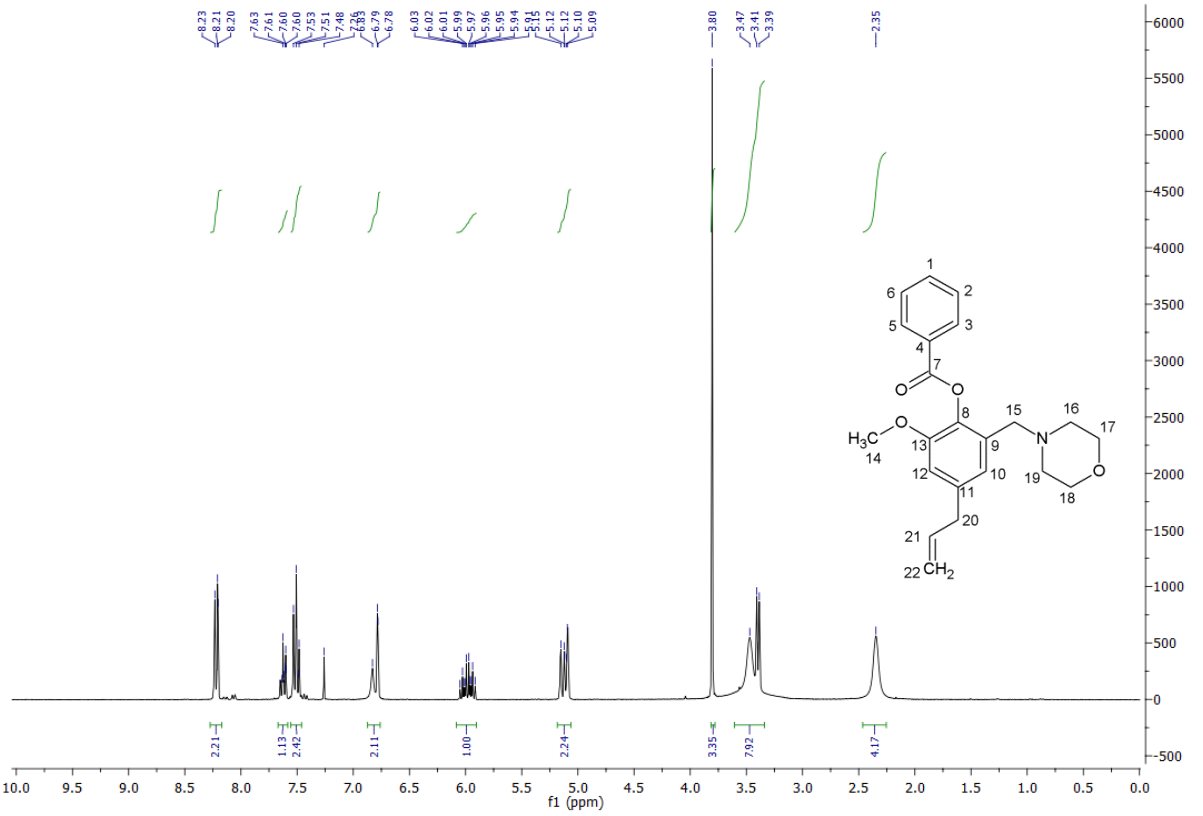

Figure S10. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4a**.

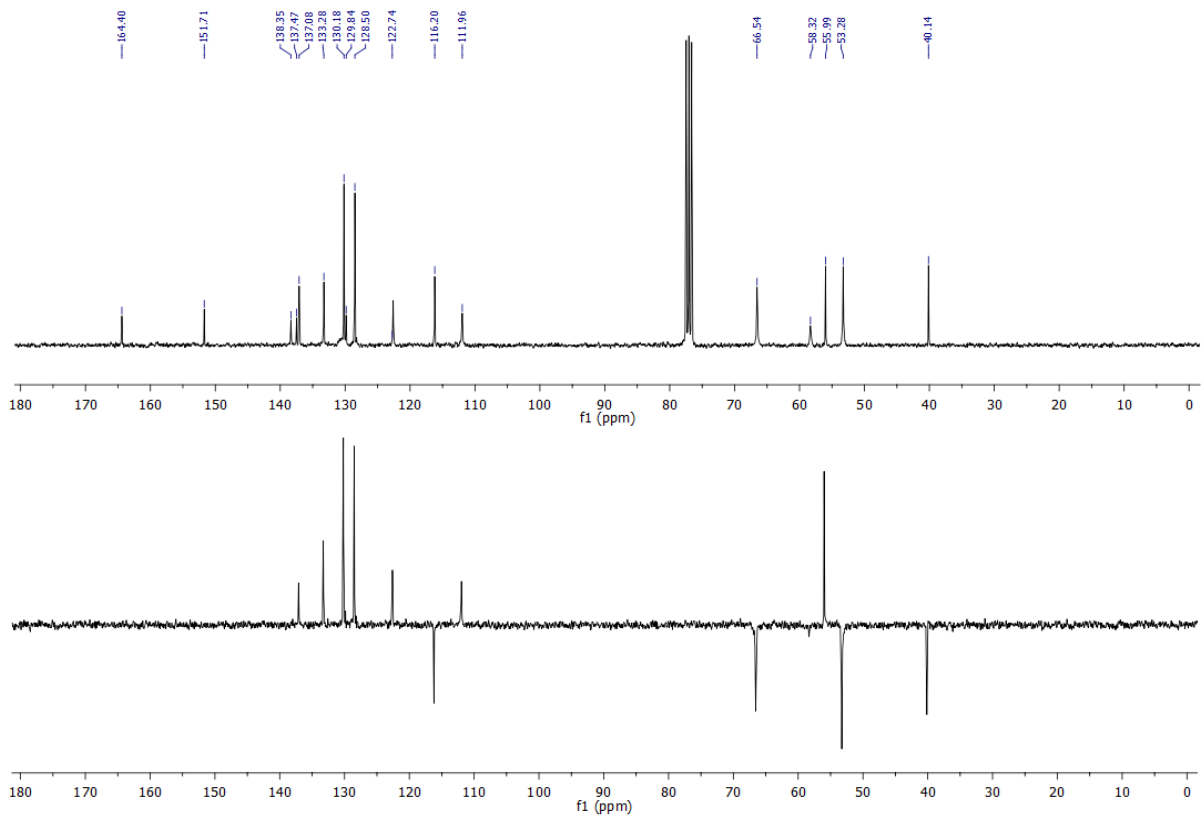

Figure S11. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4a**.

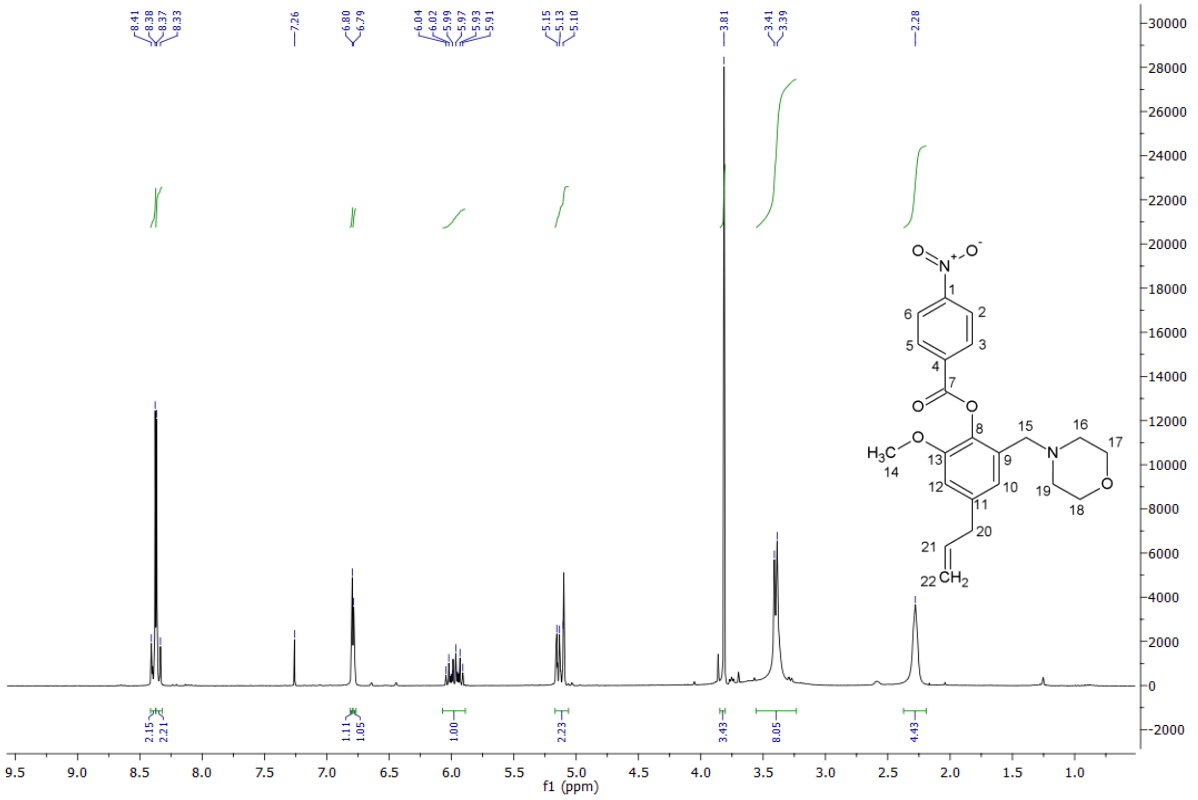

Figure S12. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4b**.

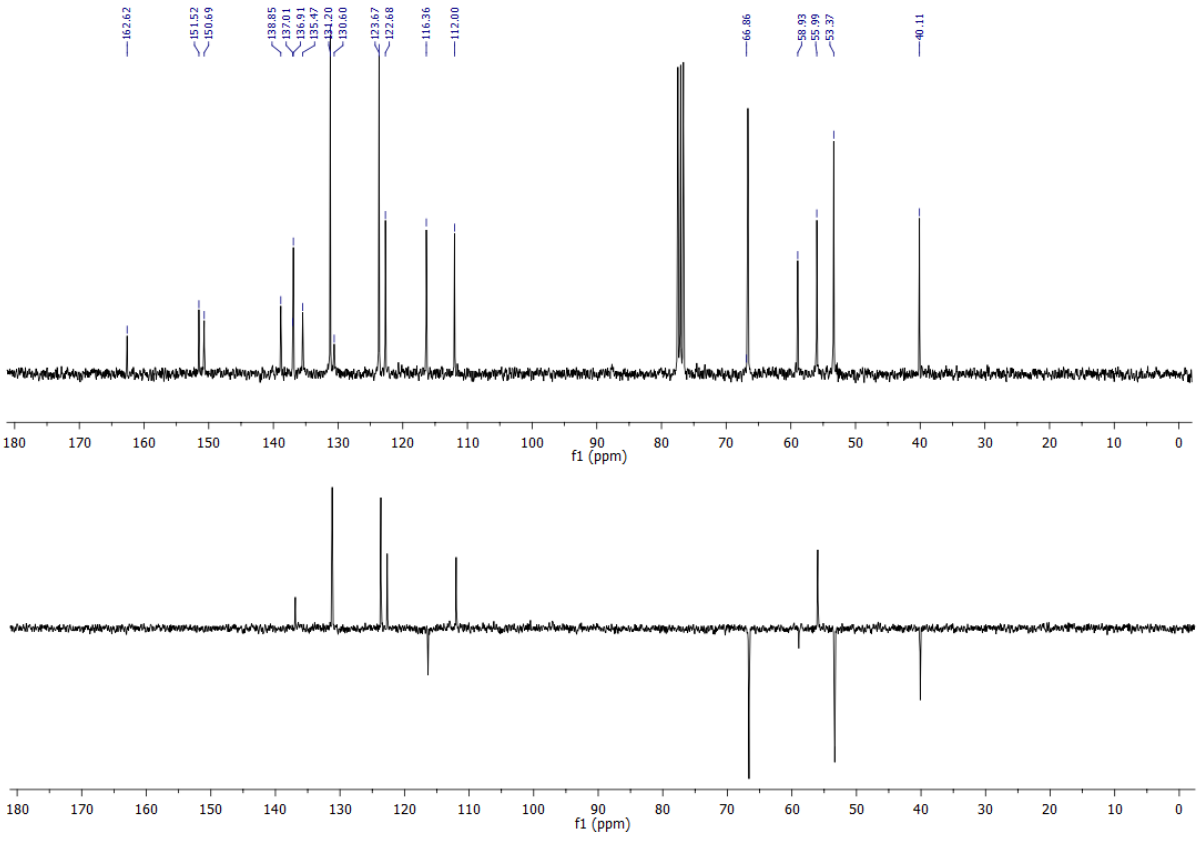

Figure S13. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4b**.

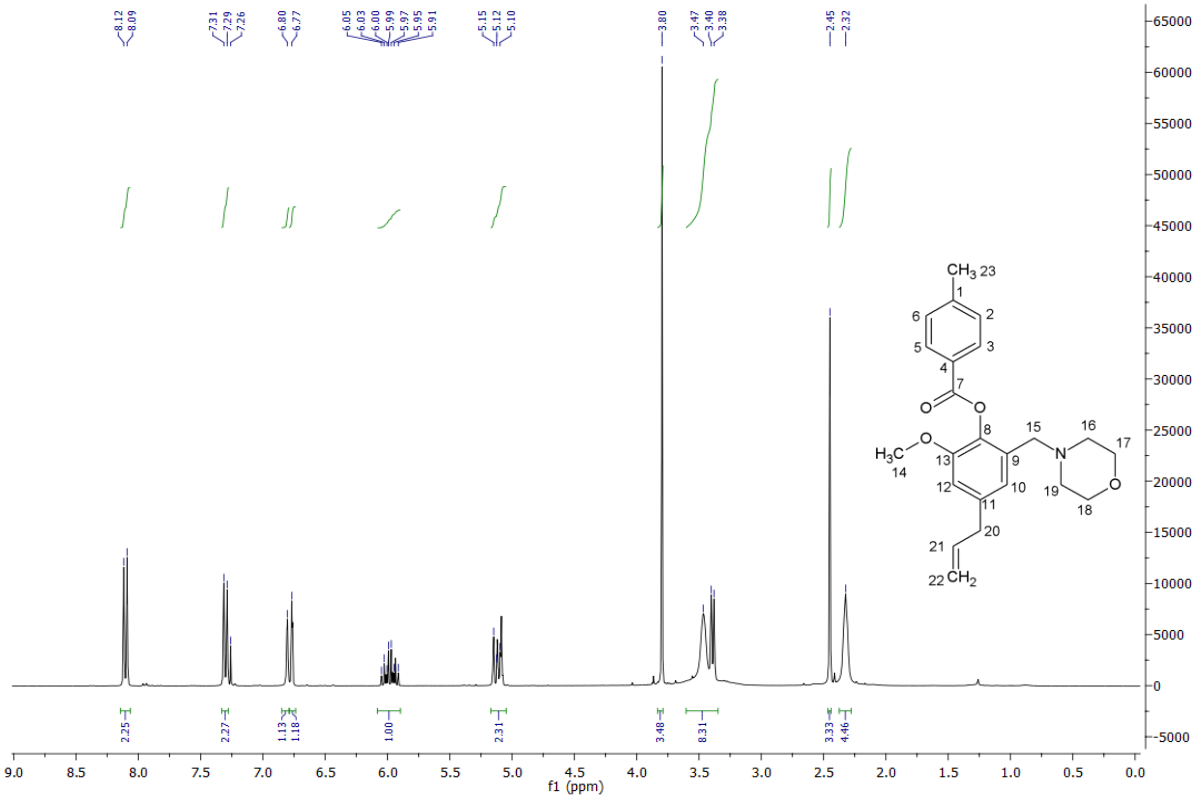

Figure S14. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4c**.

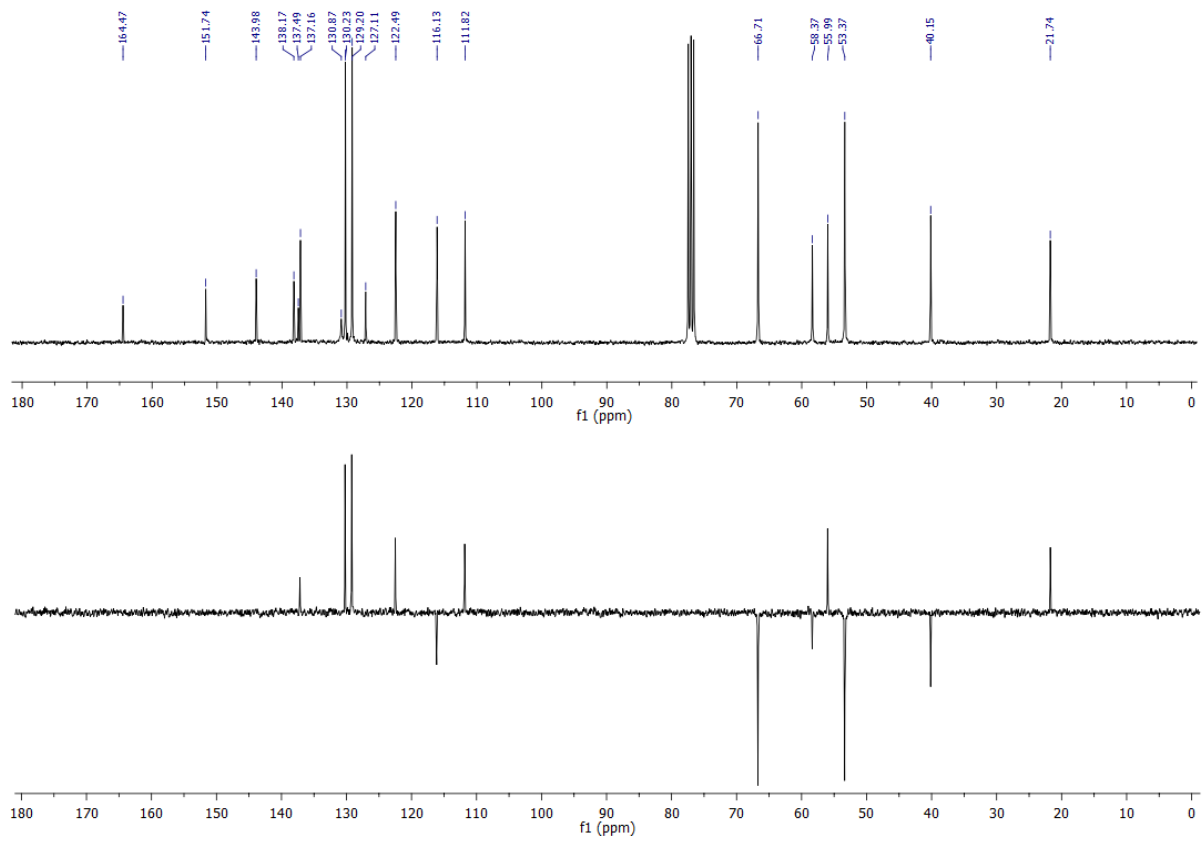

Figure S15. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4c**.

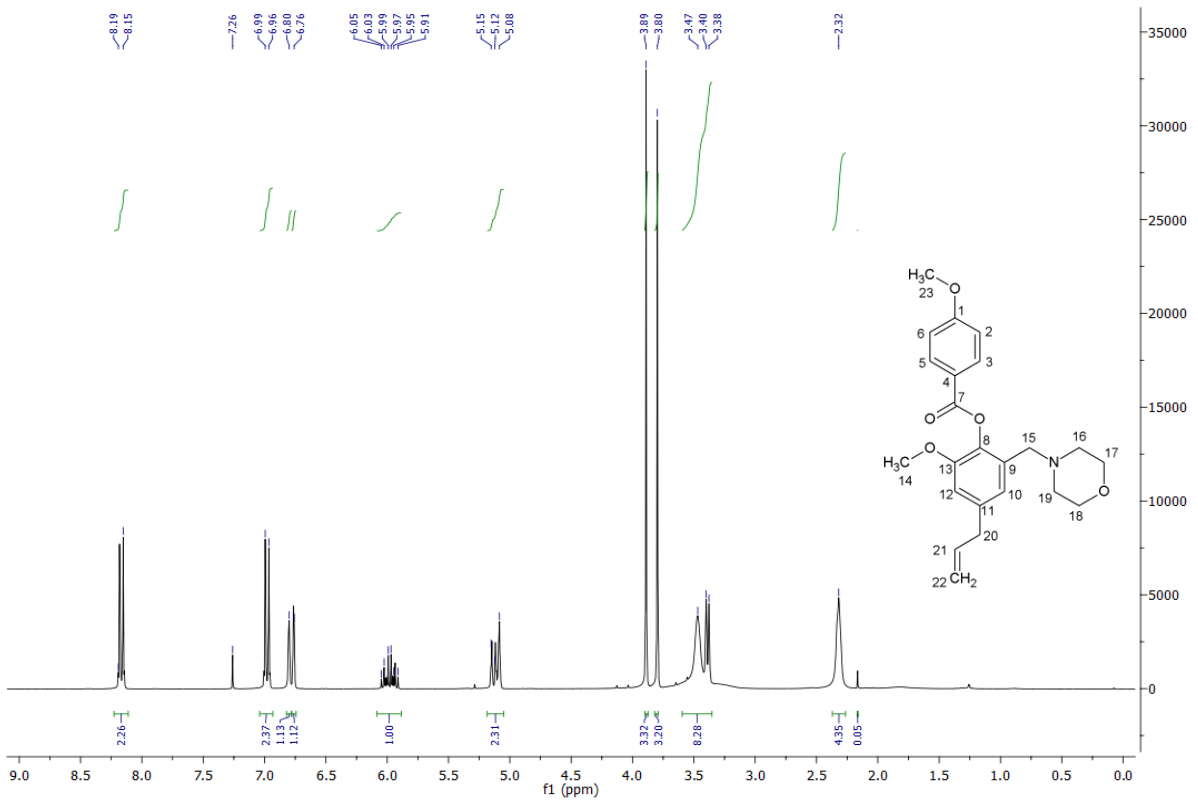

Figure S16. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4d**.

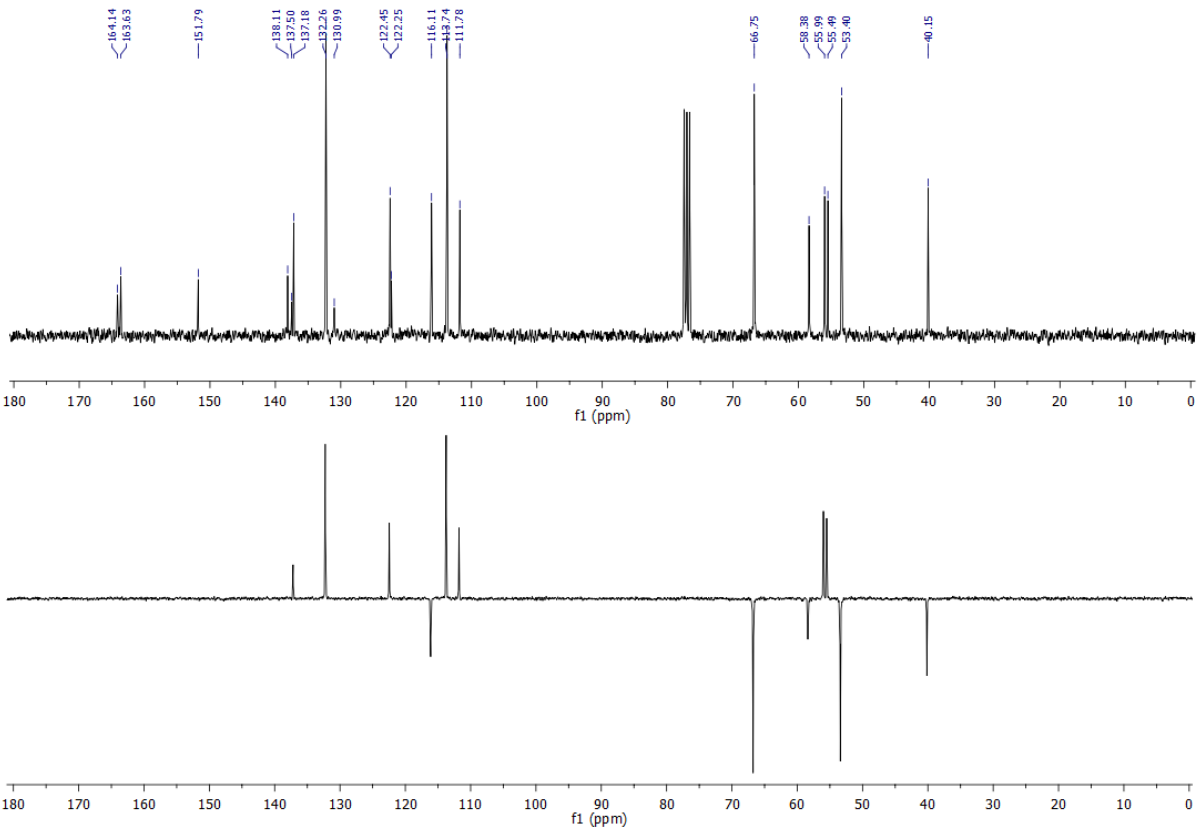

Figure S17. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4d**.

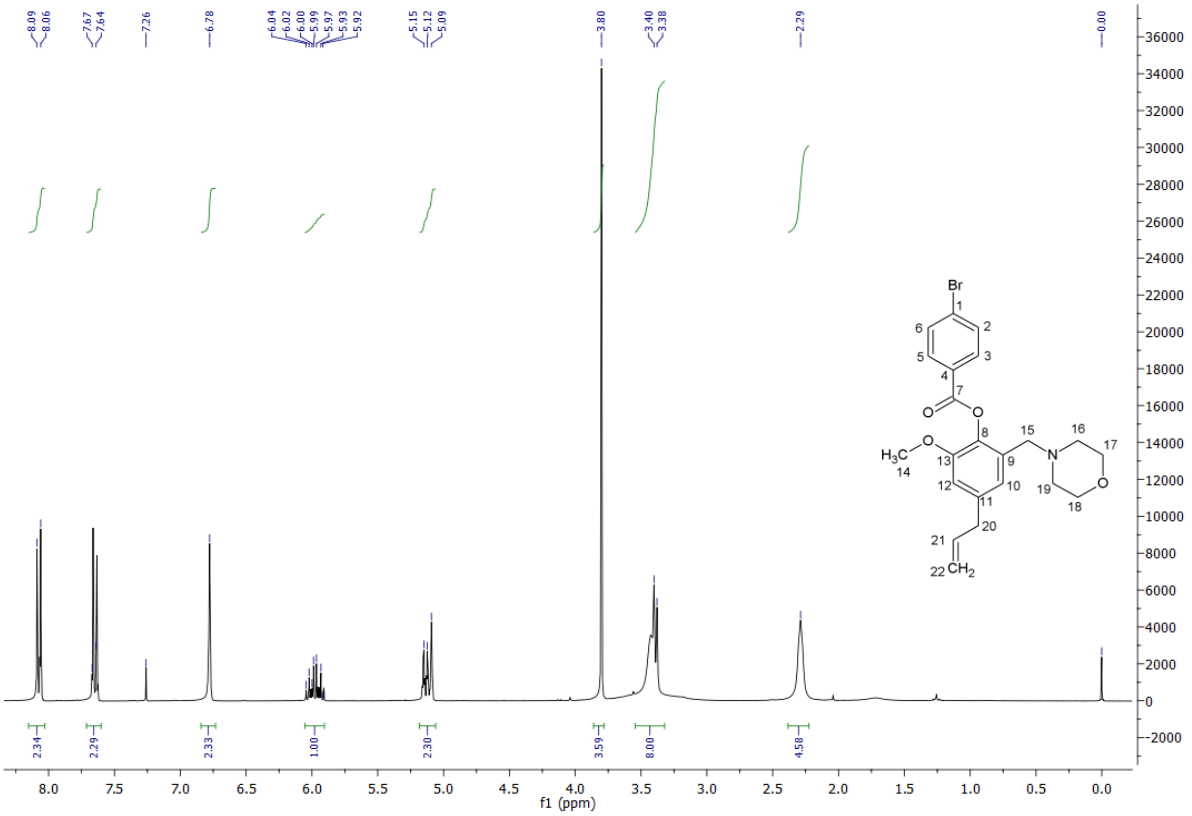

Figure S18. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4e**.

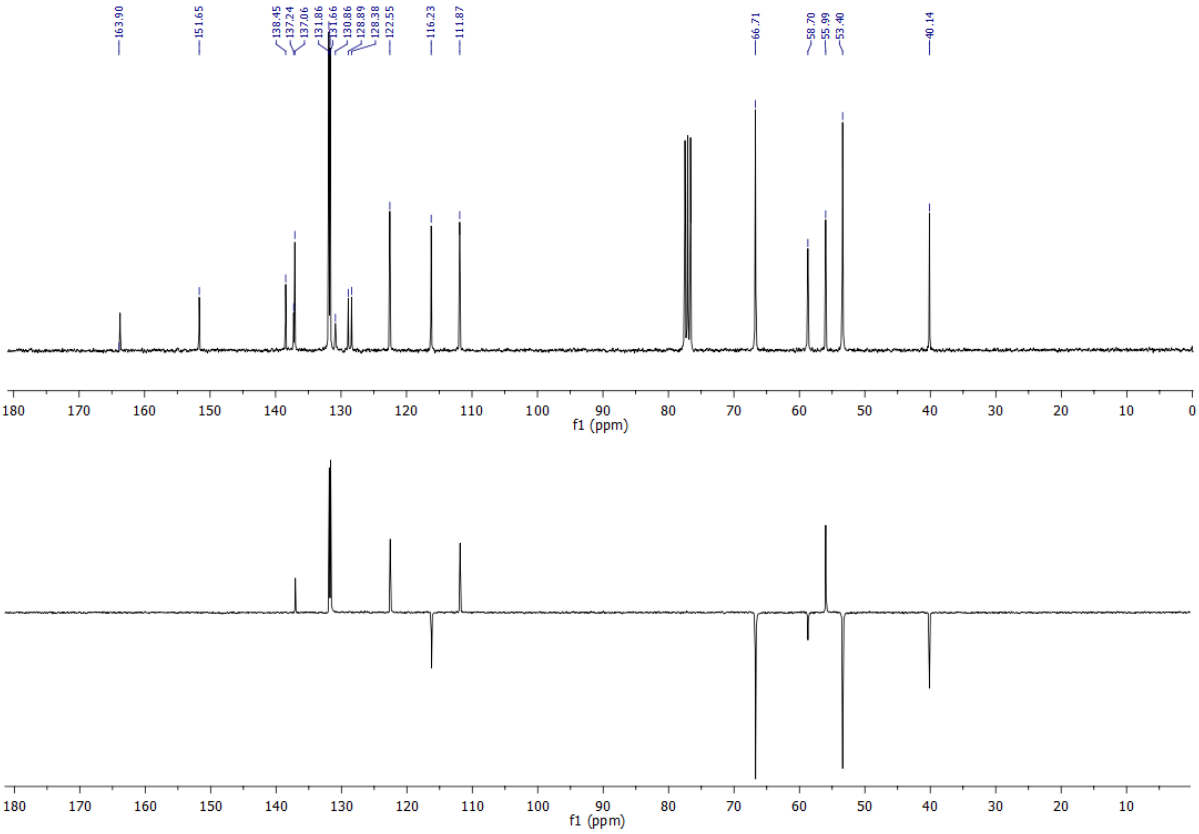

Figure S19. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4e**.

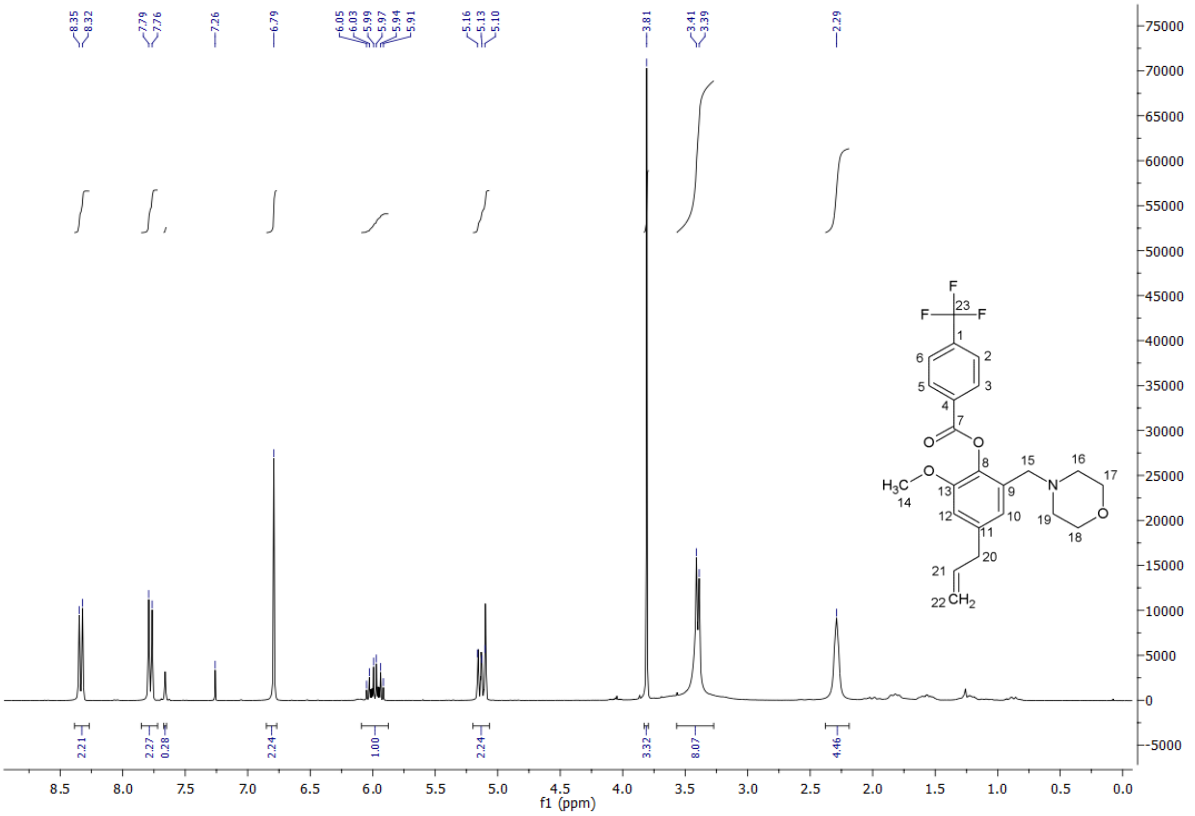

Figure S20. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4f**.

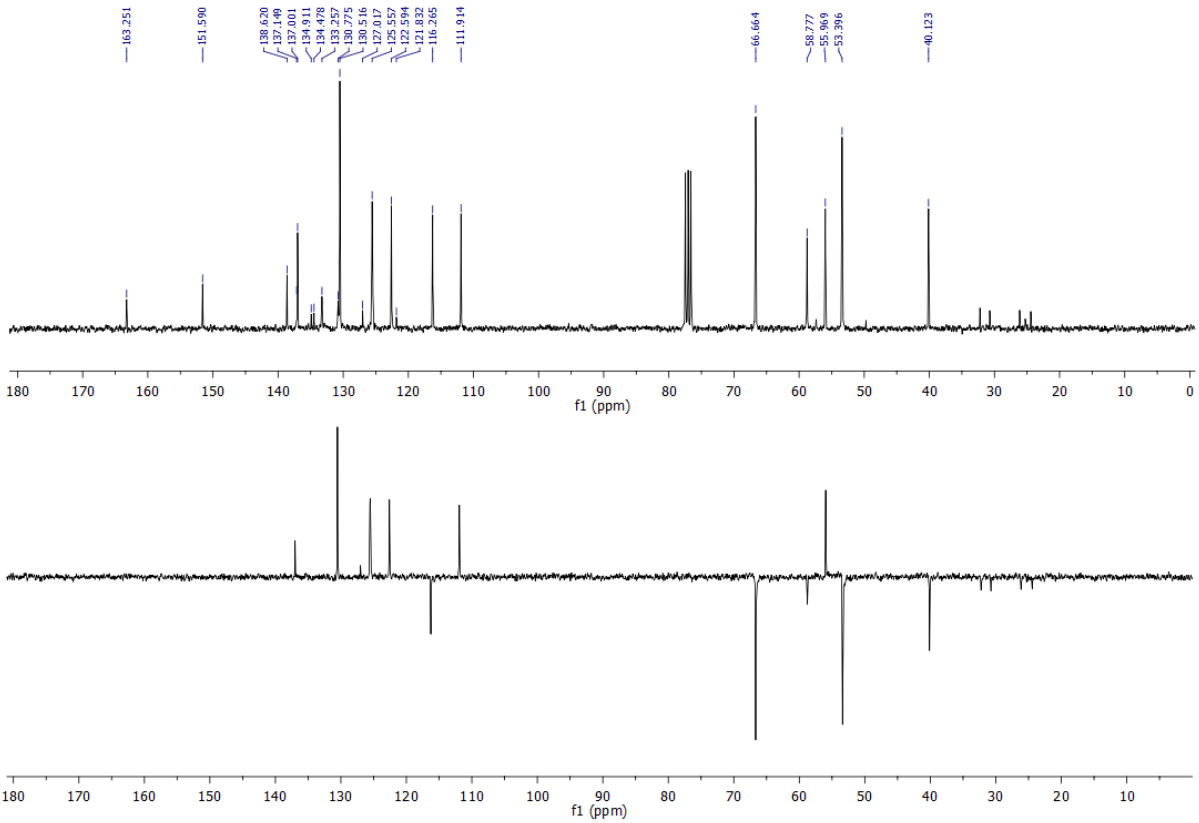

Figure S21. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4f**.

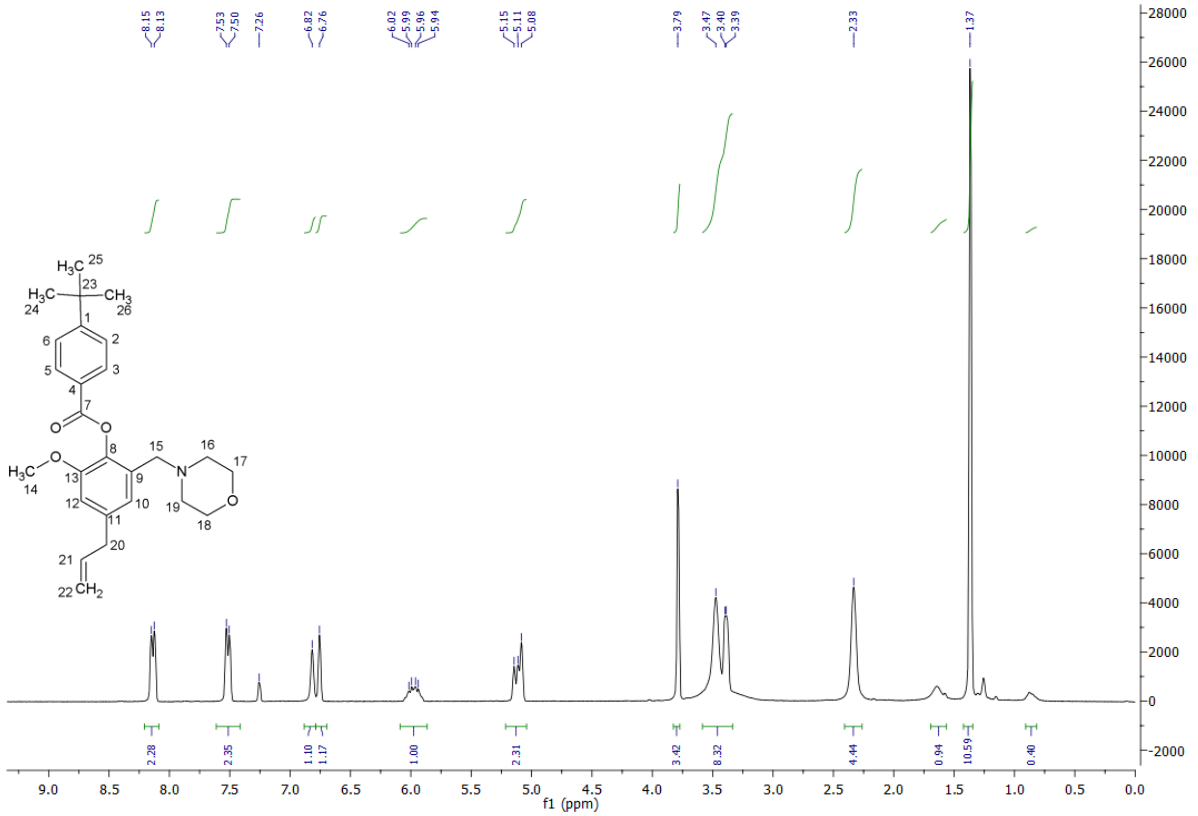

Figure S22. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4g**.

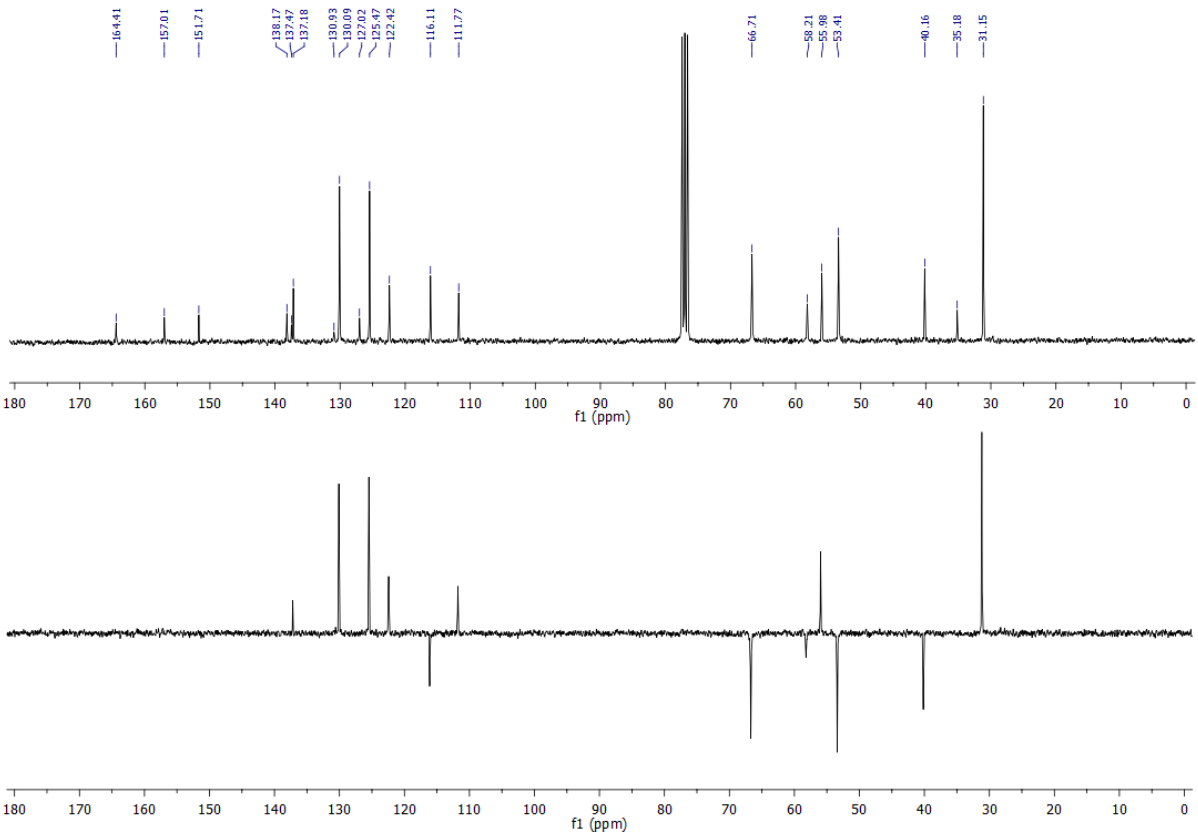

Figure S23. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4g**.

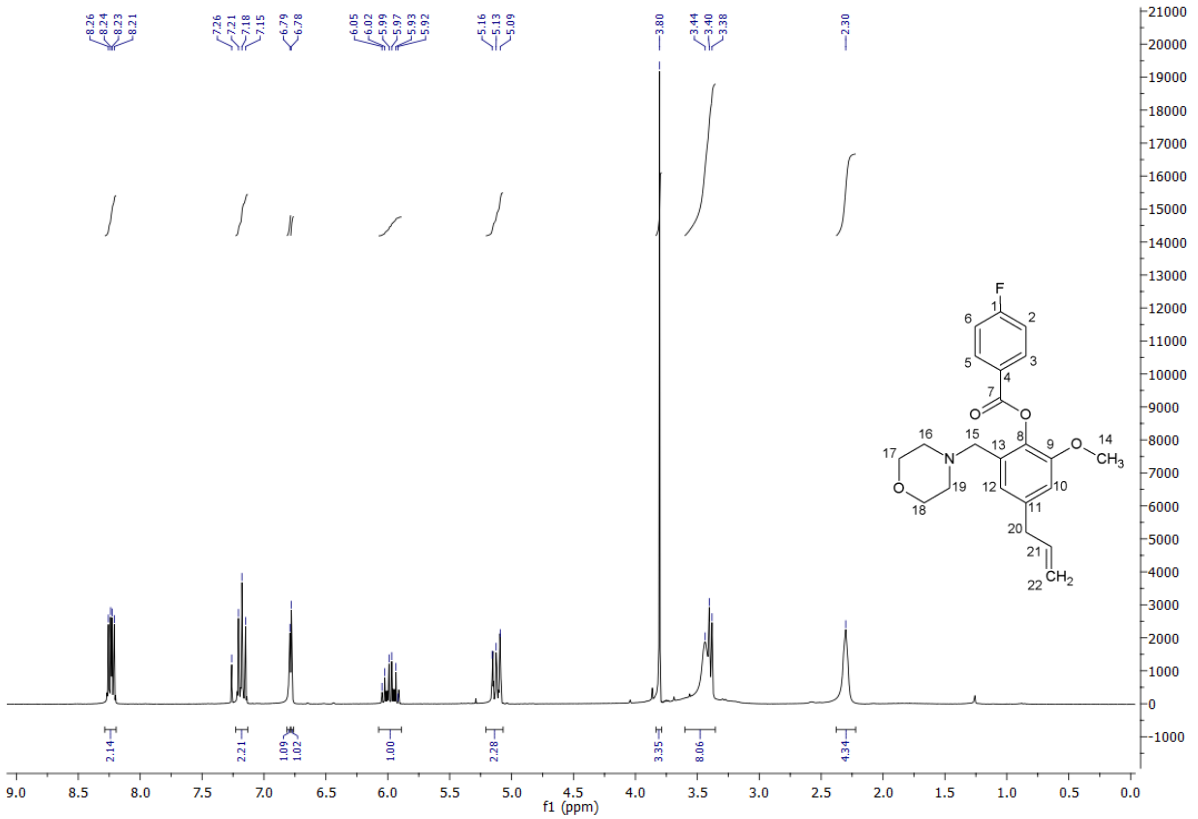

Figure S24. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4h**.

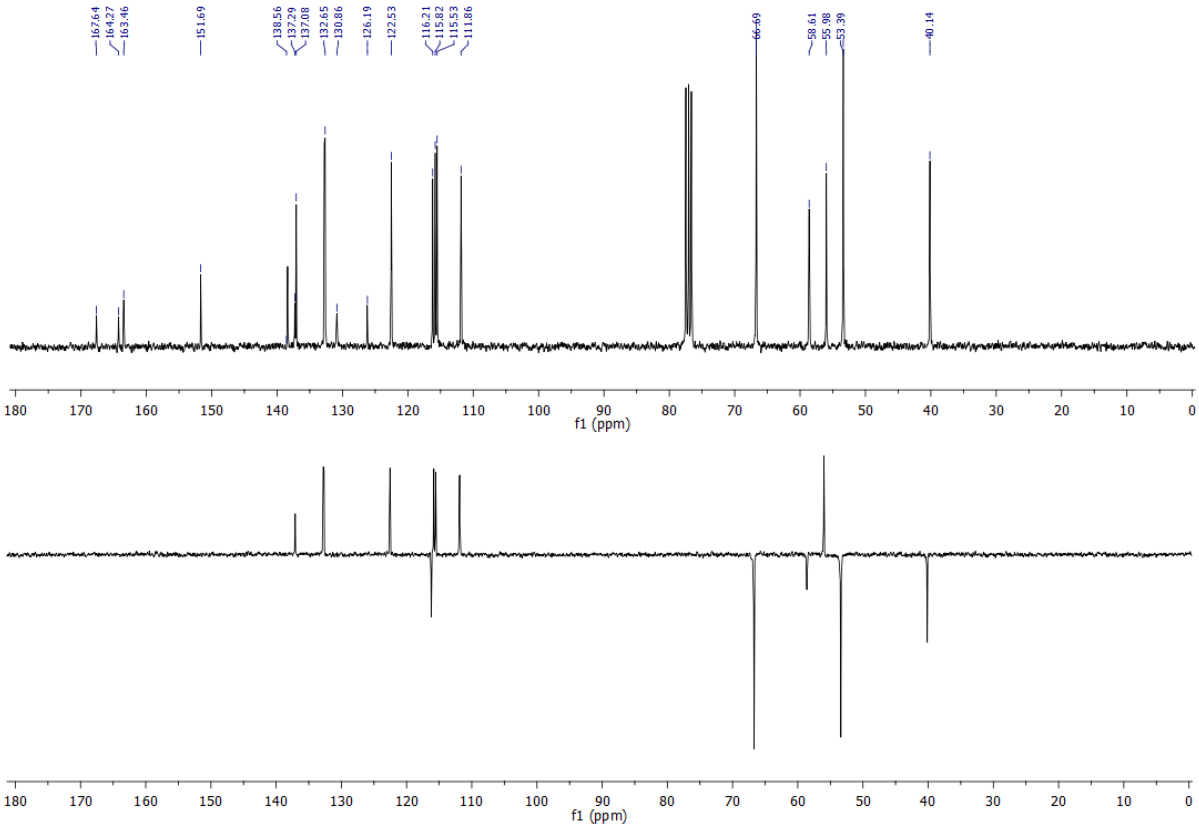

Figure S25. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4h**.

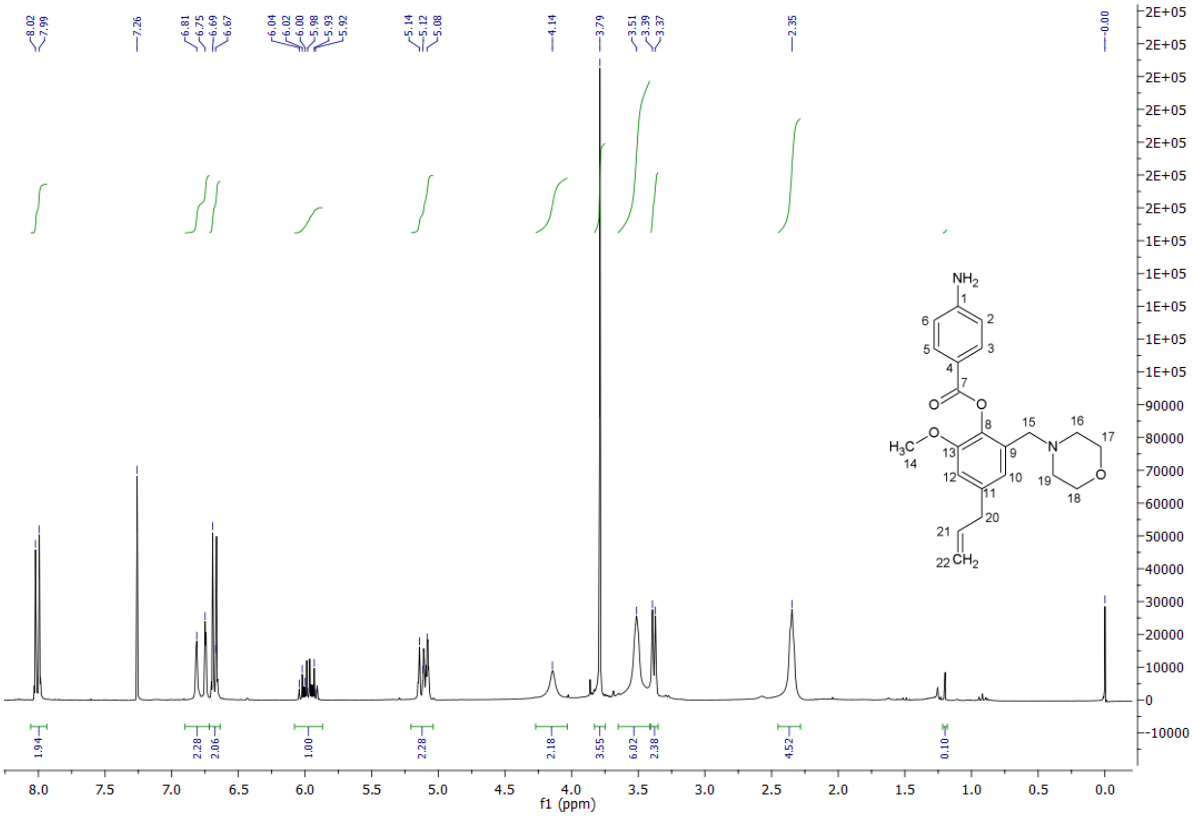

Figure S26. ^{1}H NMR spectrum (300 MHz, $CDCl_3$) of compound **4i**.

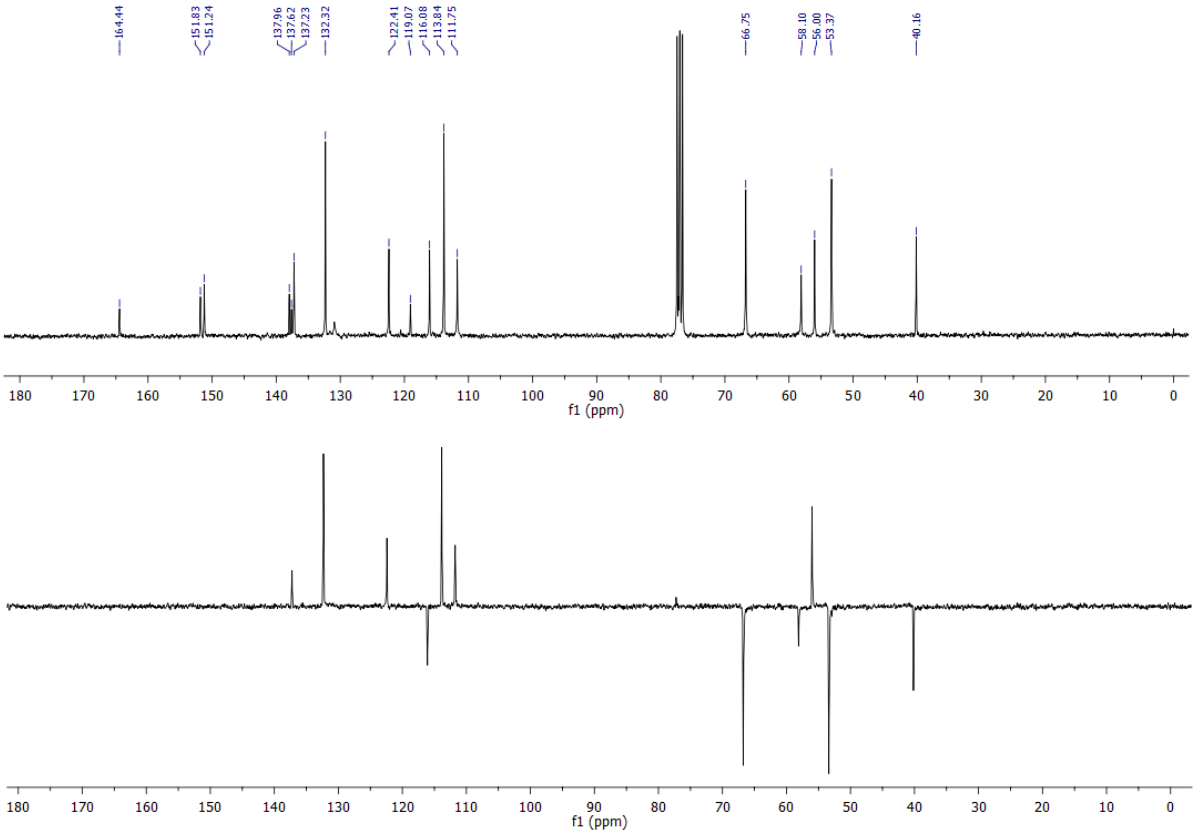

Figure S27. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, $CDCl_3$) of compound **4i**.

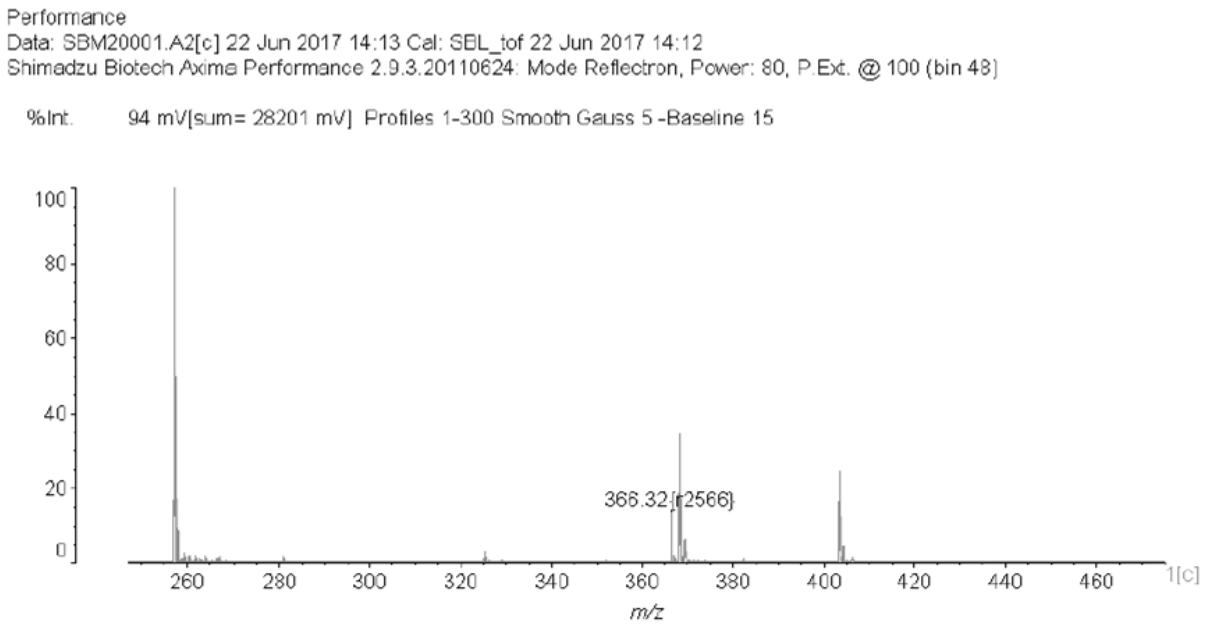

Figure S28. Mass spectrum of compound **4a**.

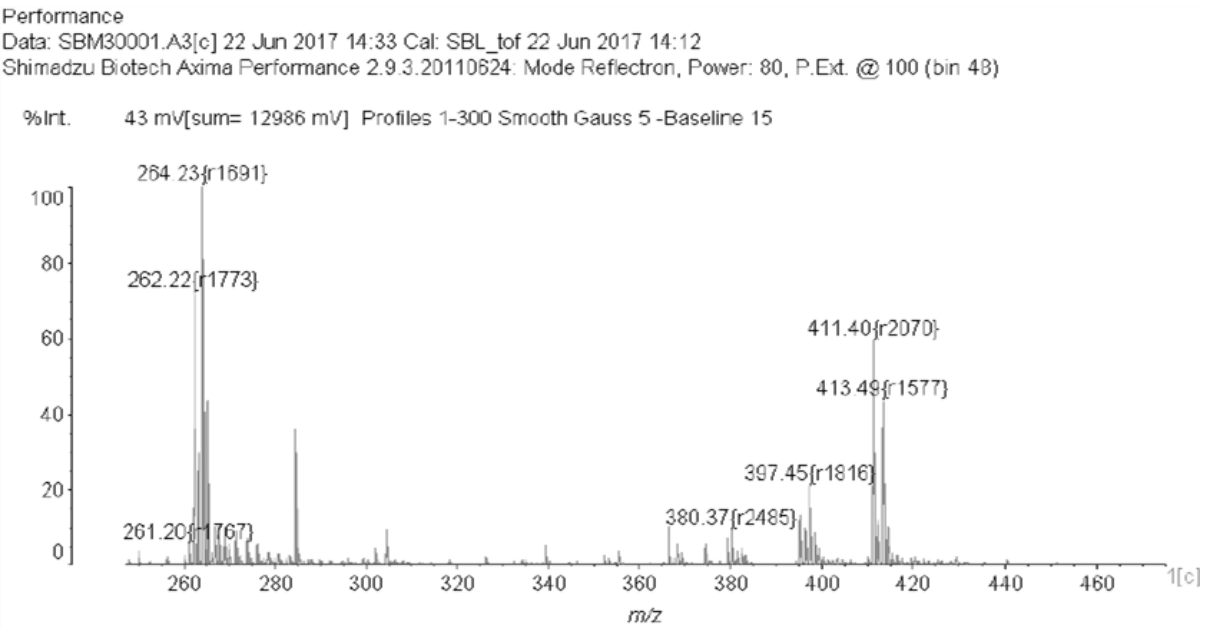

Figure S29. Mass spectrum of compound **4b**.

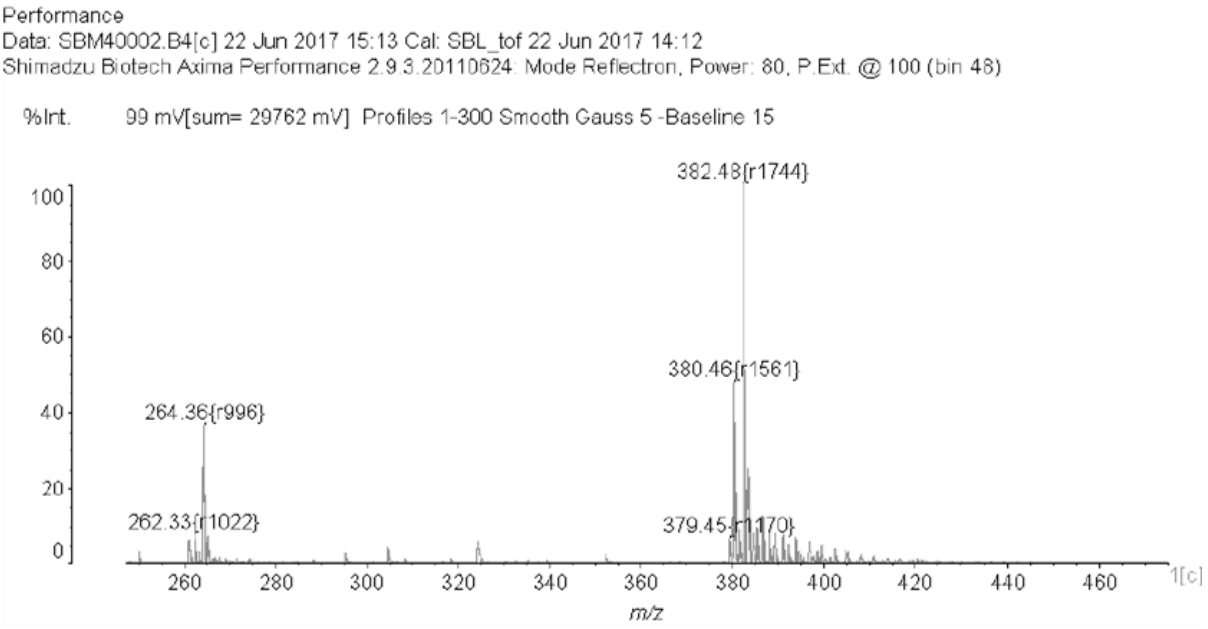

Figure S30. Mass spectrum of compound **4c**.

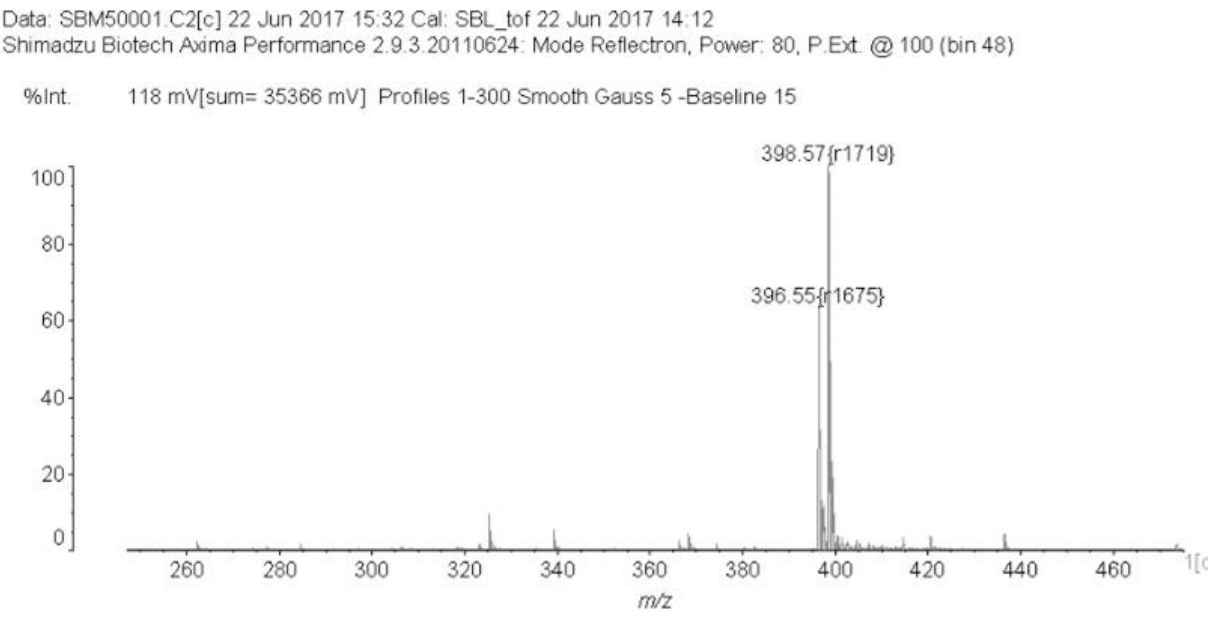

Figure S31. Mass spectrum of compound **4d**.

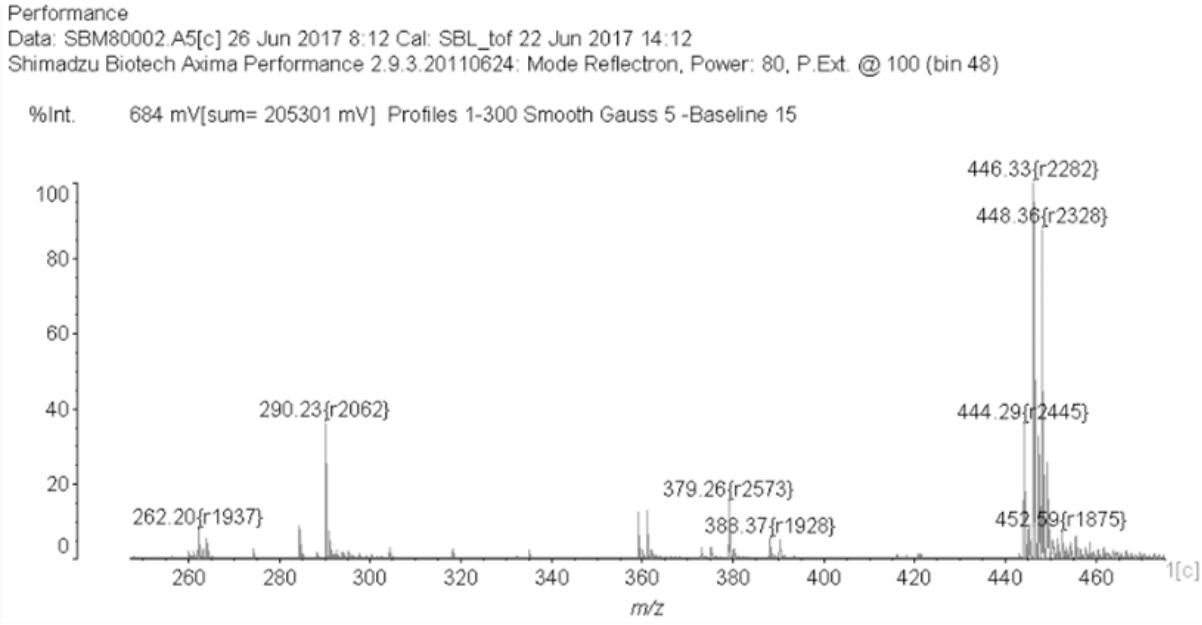

Figure S32. Mass spectrum of compound **4e**.

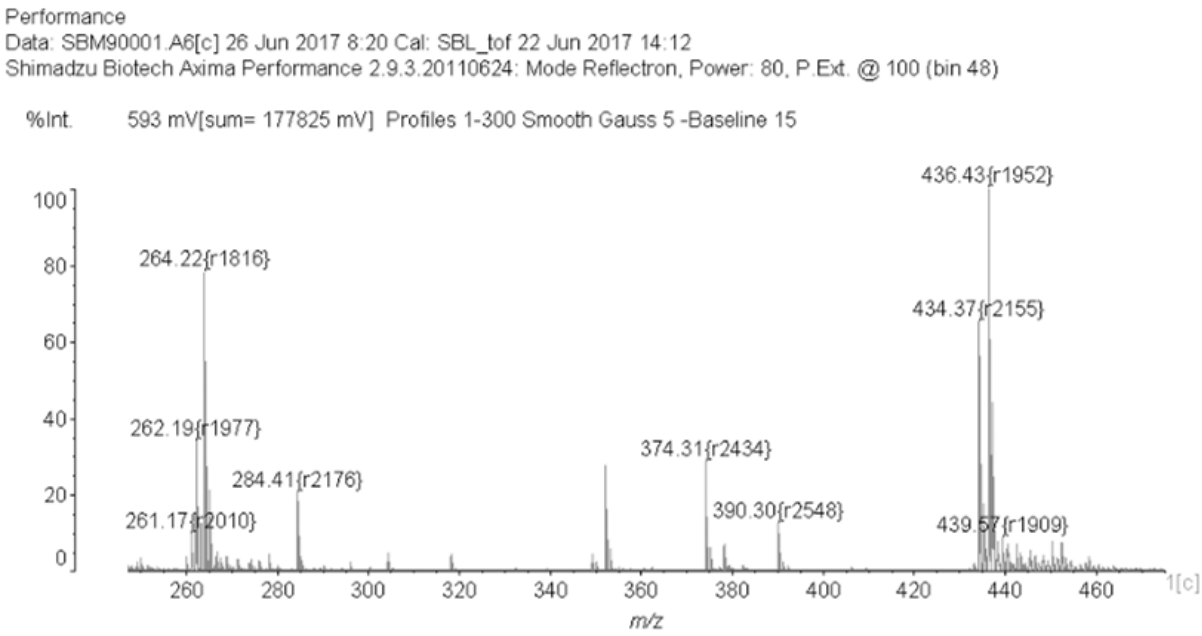

Figure S33. Mass spectrum of compound **4f**.

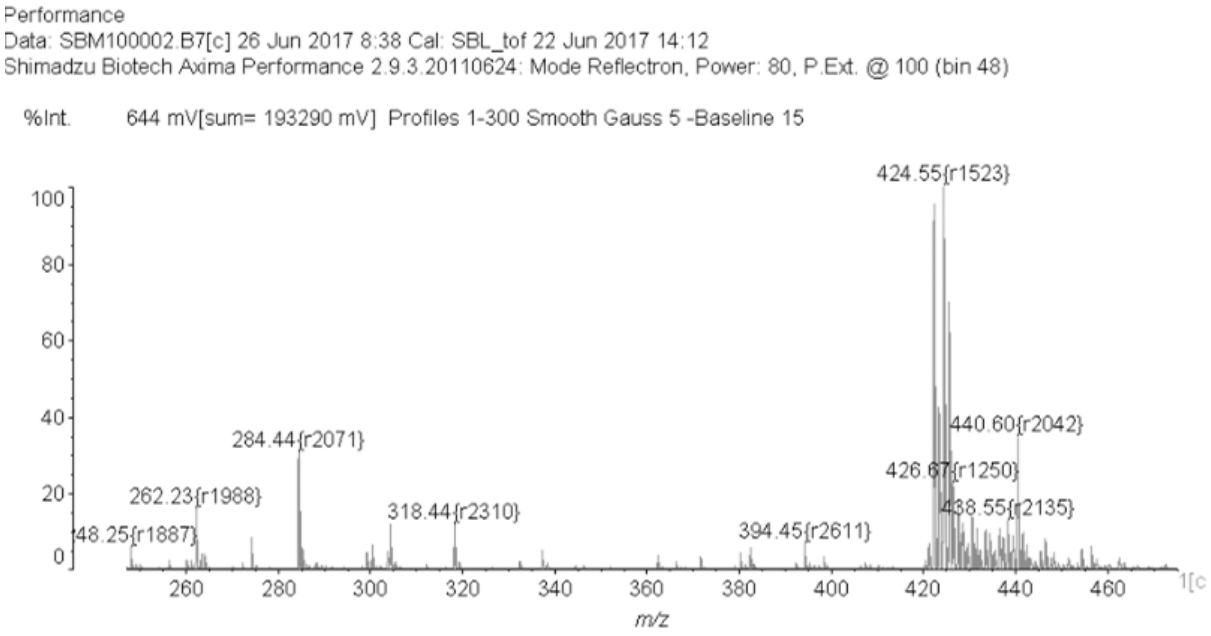

Figure S34. Mass spectrum of compound **4g**.

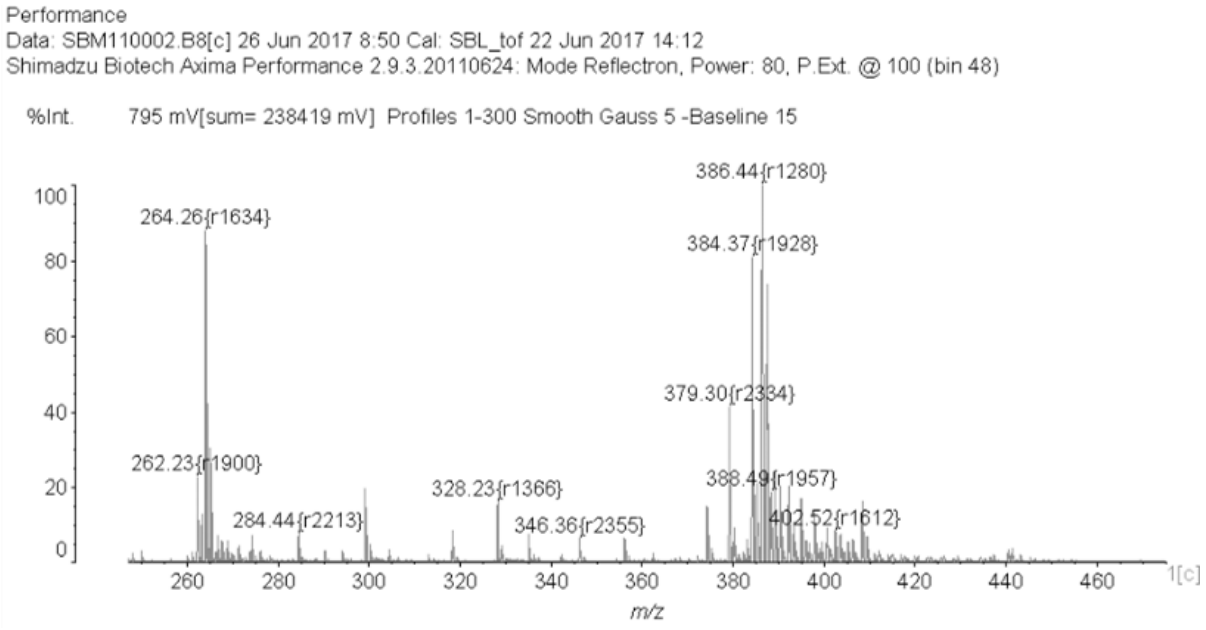

Figure S35. Mass spectrum of compound **4h**.

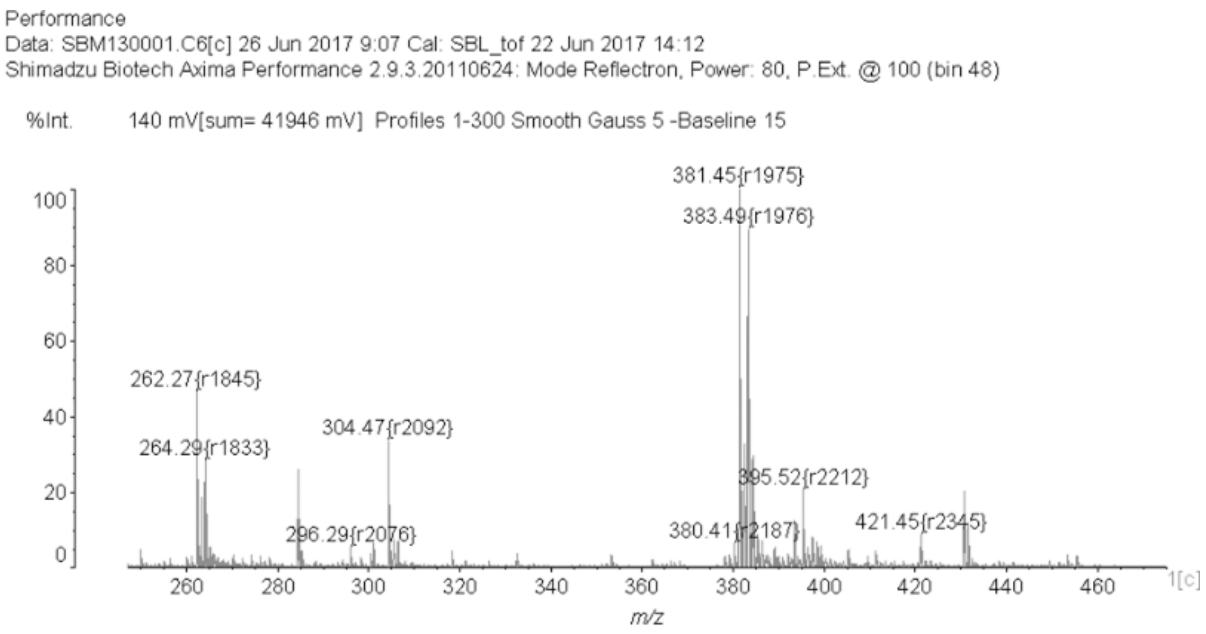

Figure S36. Mass spectrum of compound **4i**.