

Supplementary Information

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

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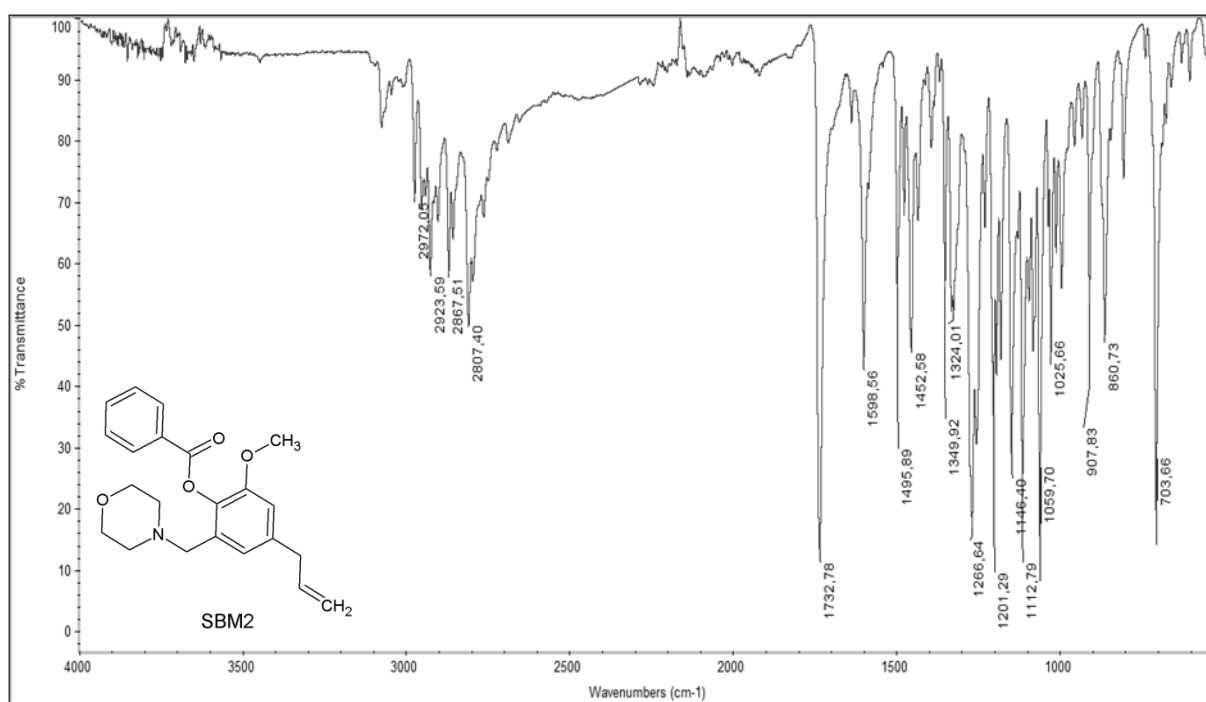


Figure S1. FTIR spectrum of compound 4a.

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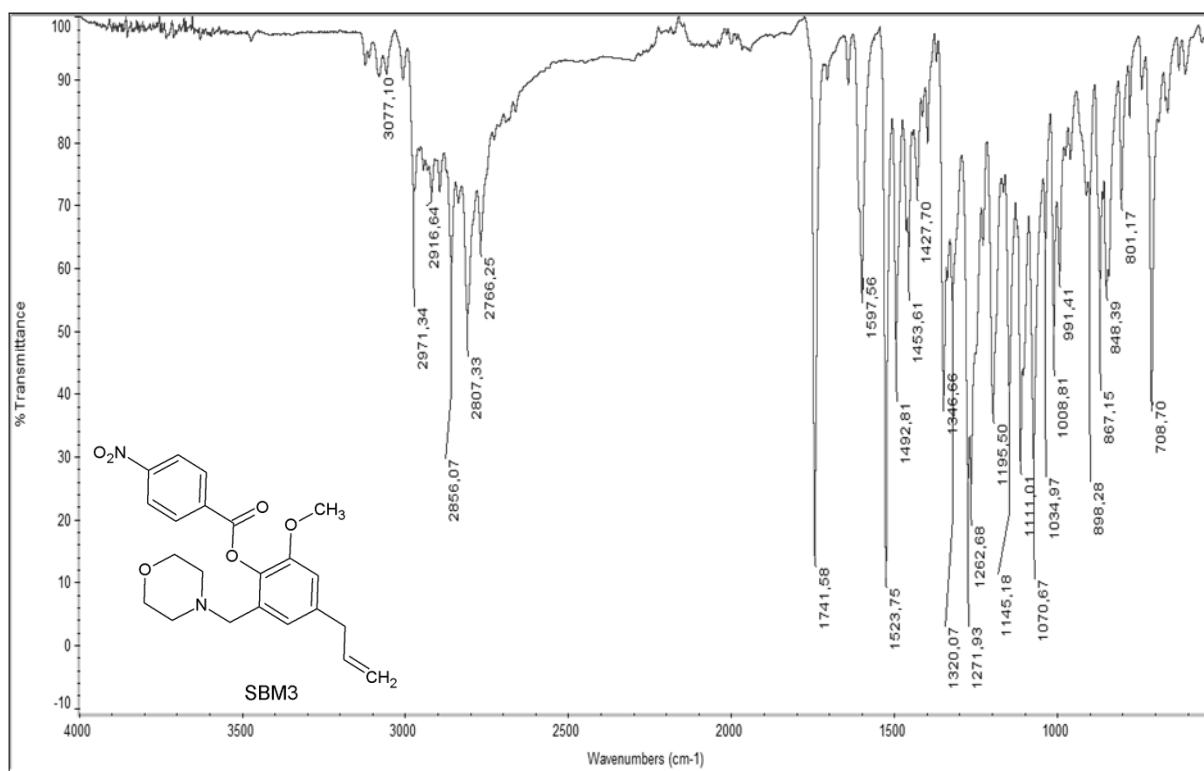


Figure S2. FTIR spectrum of compound **4b**.

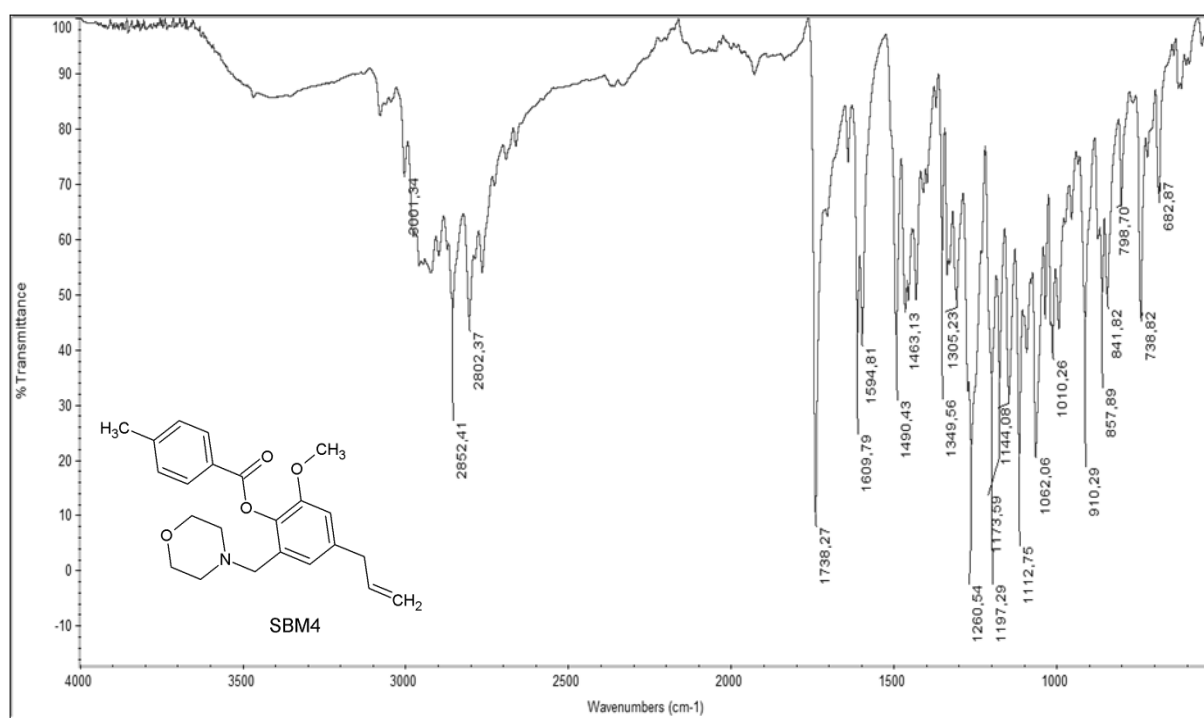


Figure S3. FTIR spectrum of compound **4c**.

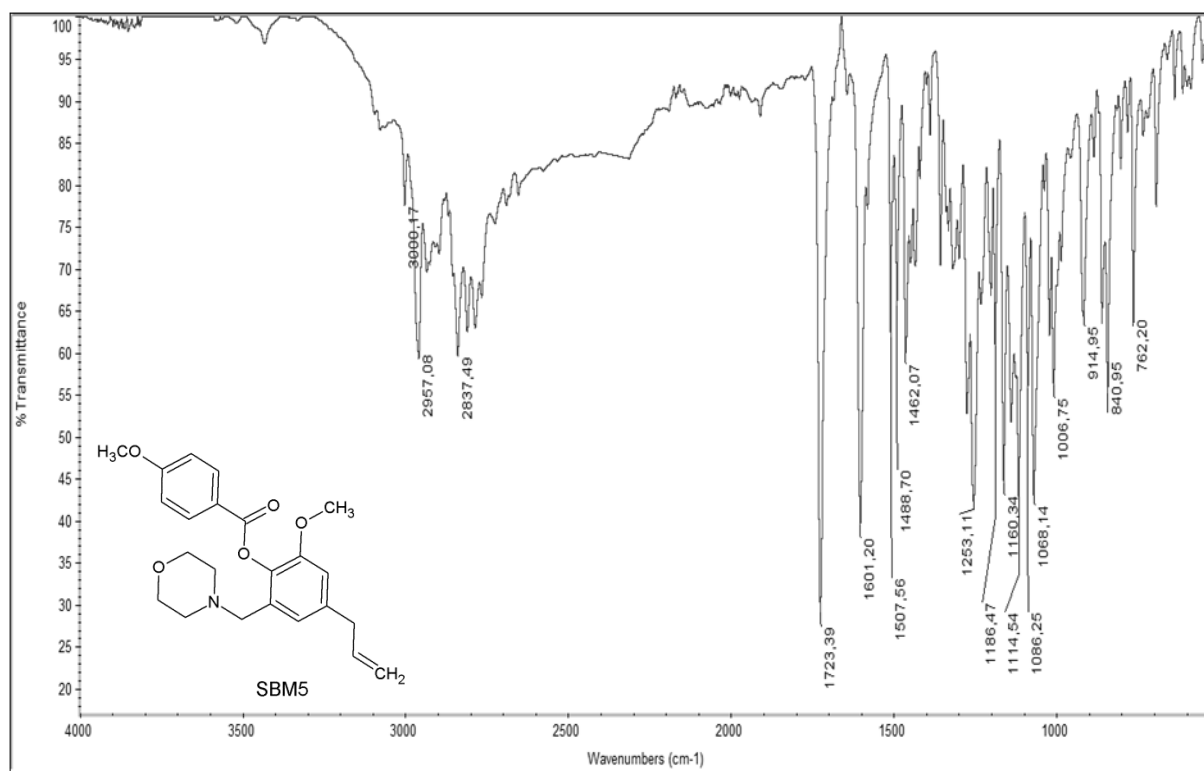


Figure S4. FTIR spectrum of compound **4d**.

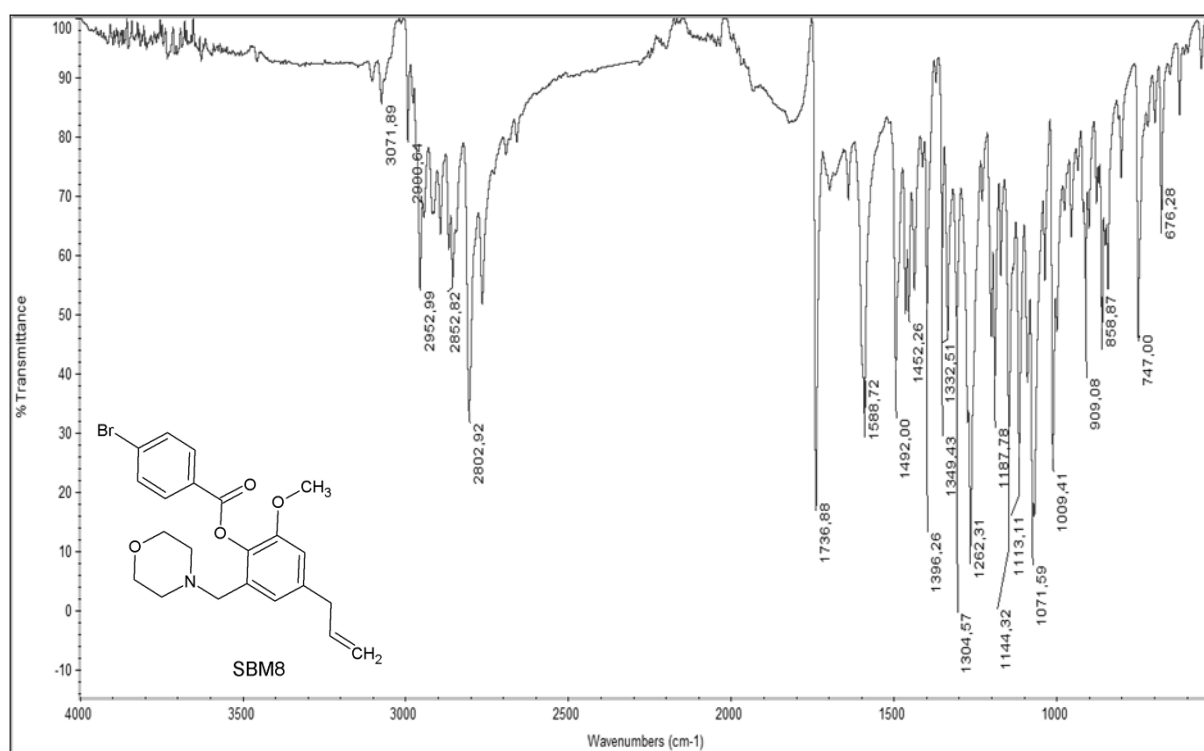


Figure S5. FTIR spectrum of compound **4e**.

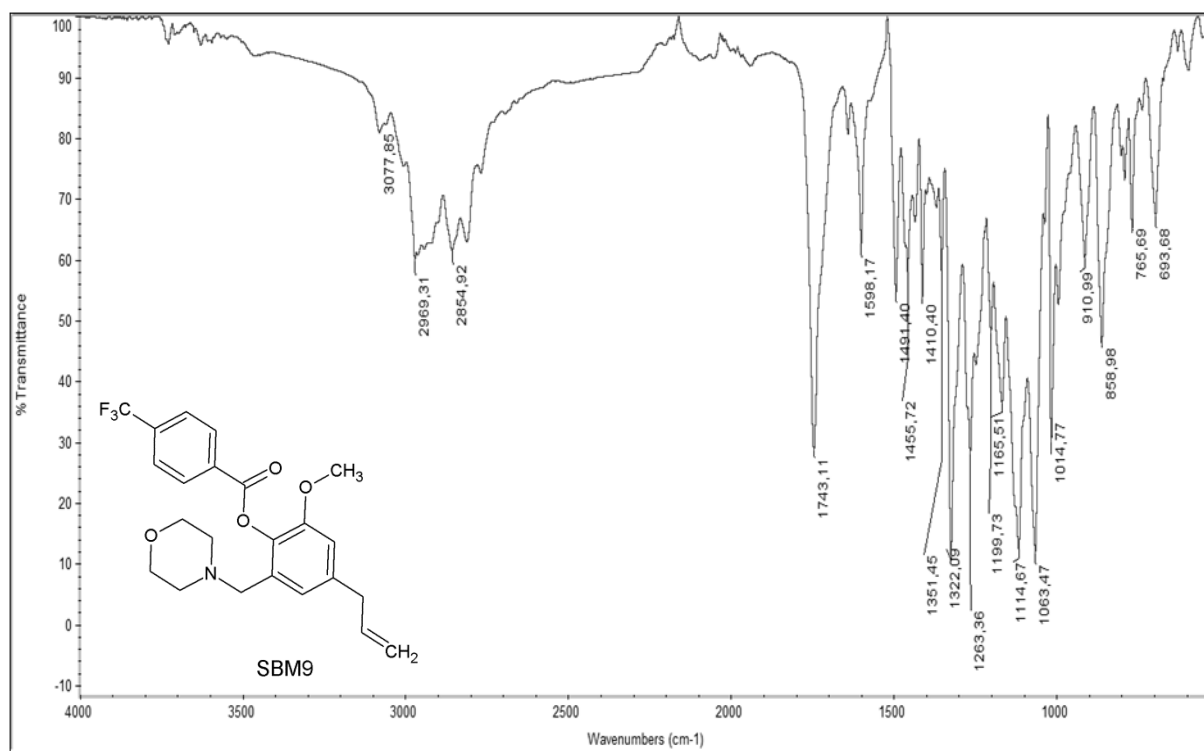


Figure S6. FTIR spectrum of compound **4f**.

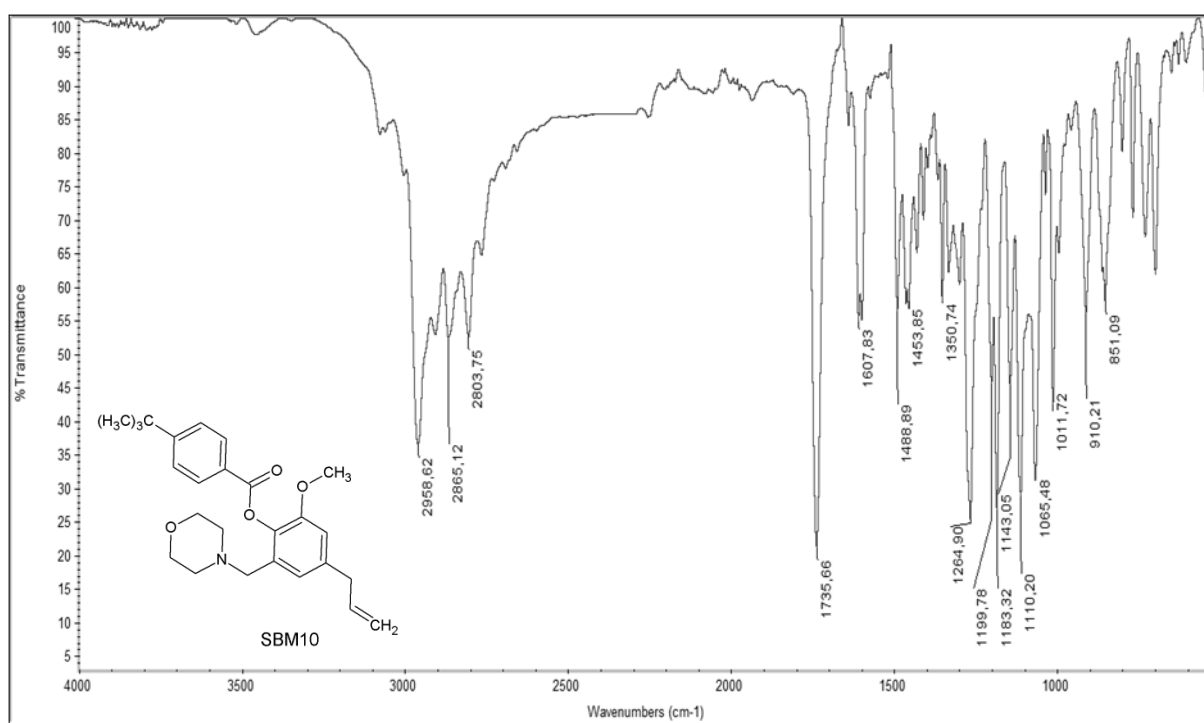


Figure S7. FTIR spectrum of compound **4g**.

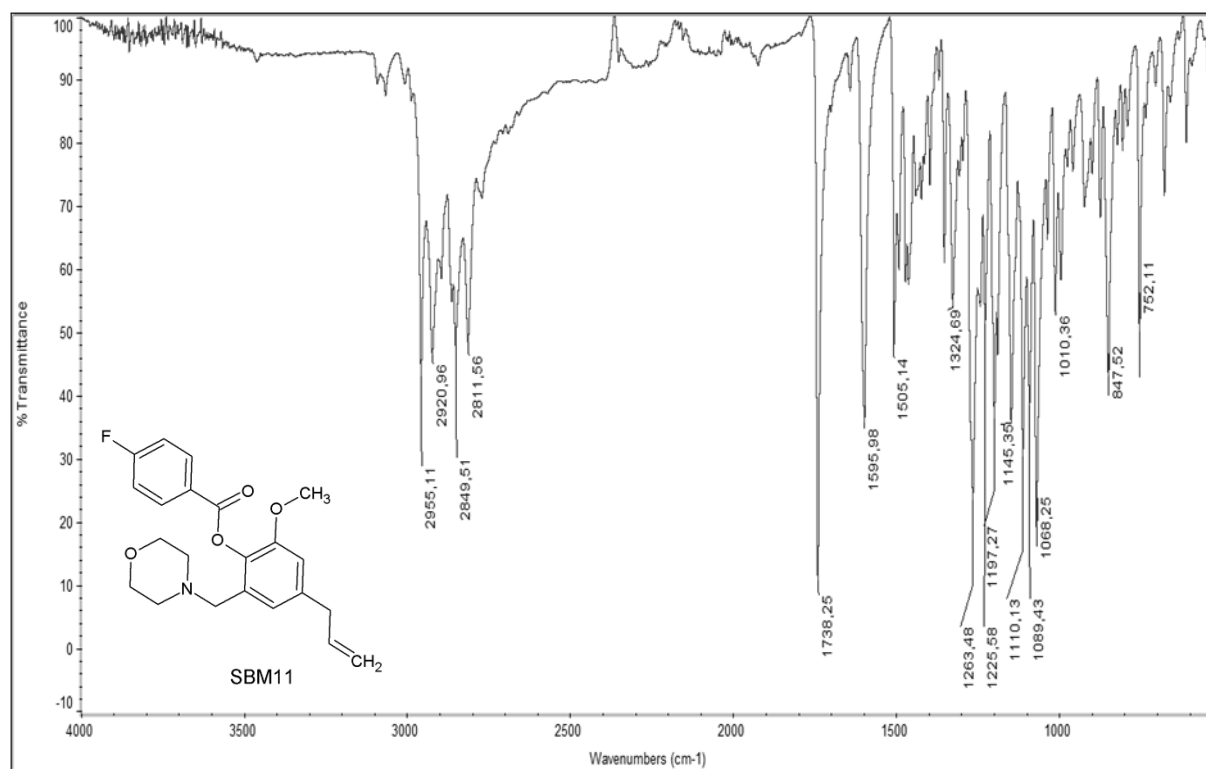


Figure S8. FTIR spectrum of compound **4h**.

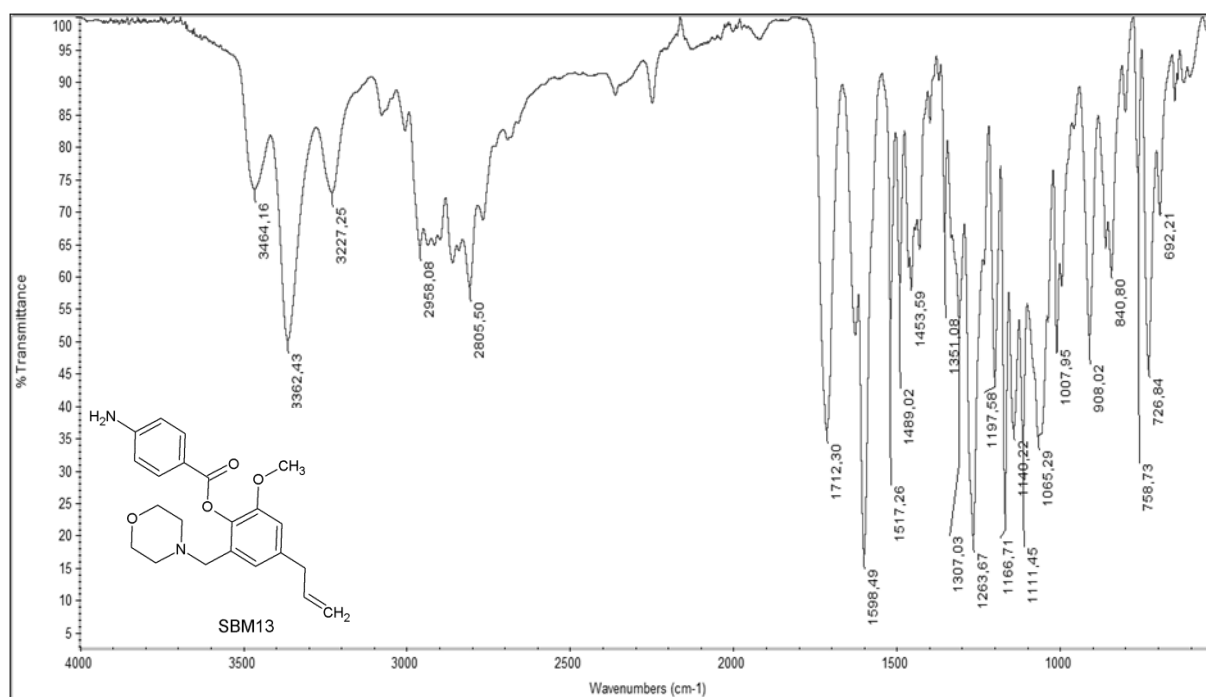


Figure S9. FTIR spectrum of compound **4i**.

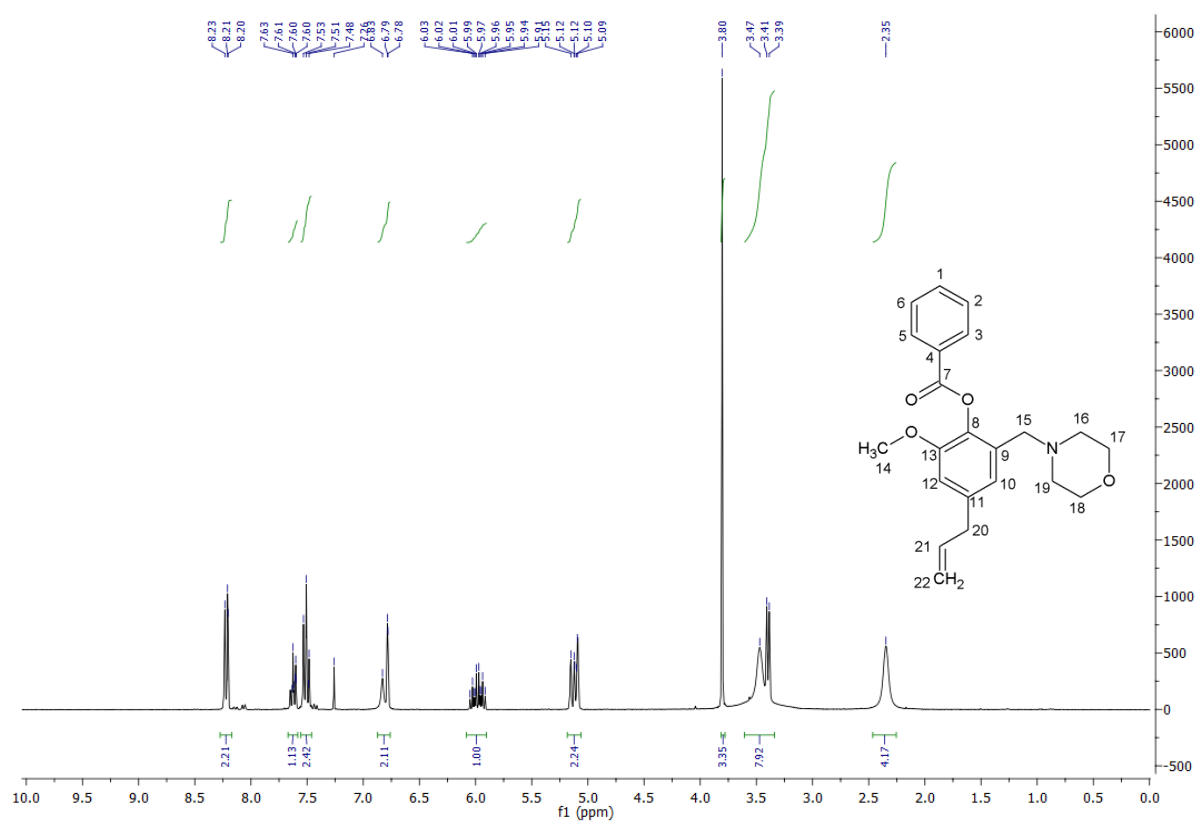


Figure S10. ^1H NMR spectrum (300 MHz, CDCl_3) of compound **4a**.

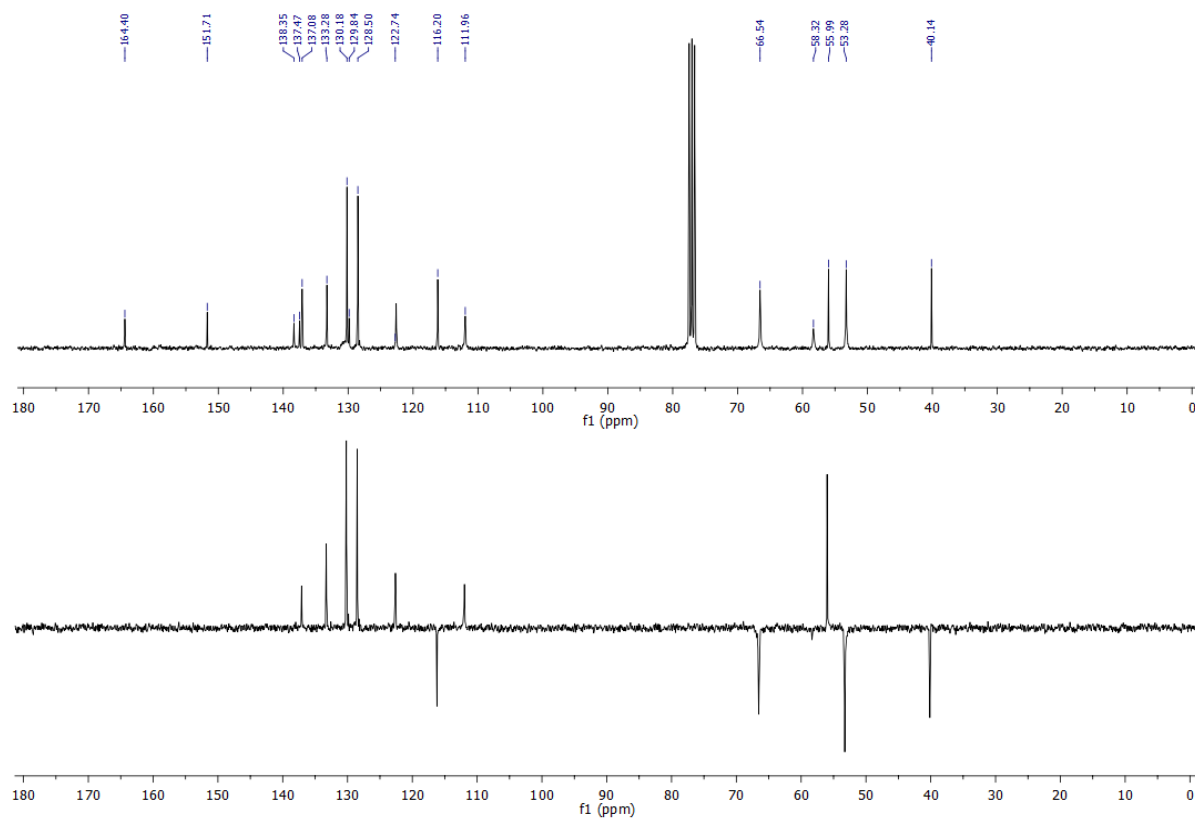


Figure S11. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl_3) of compound **4a**.

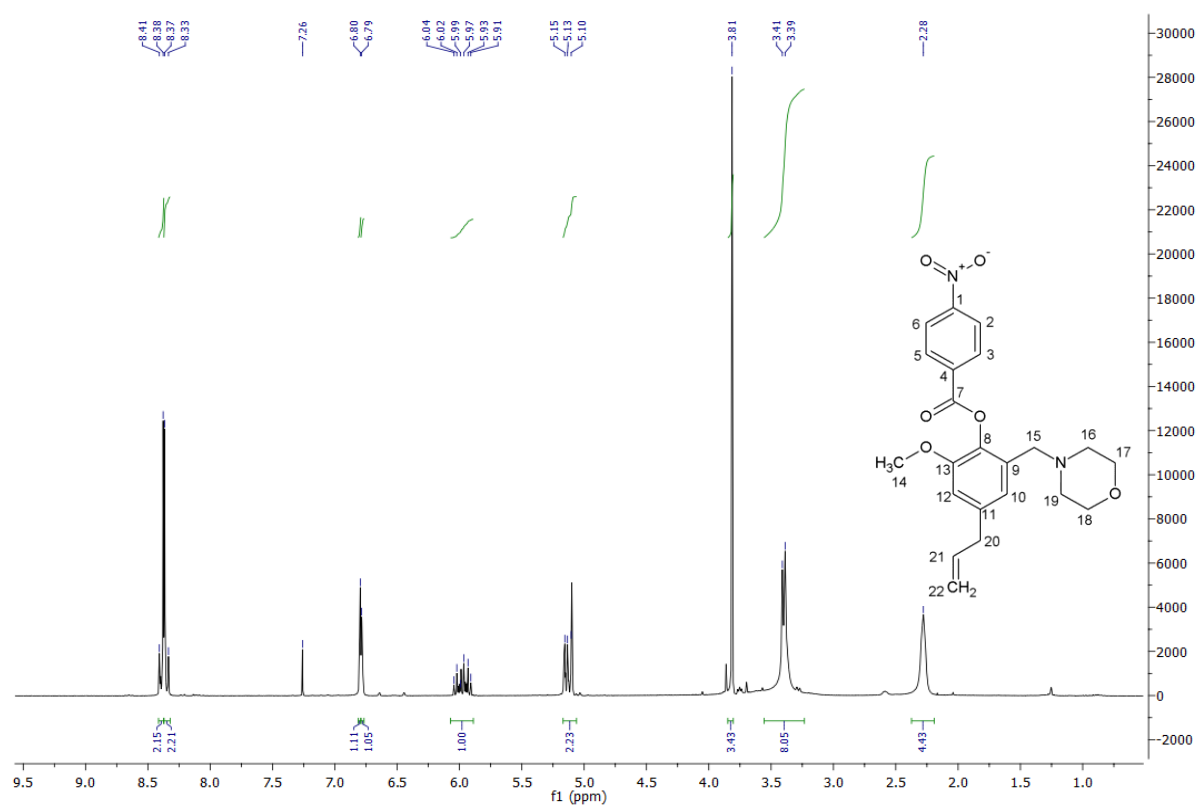


Figure S12. ^1H NMR spectrum (300 MHz, CDCl_3) of compound **4b**.

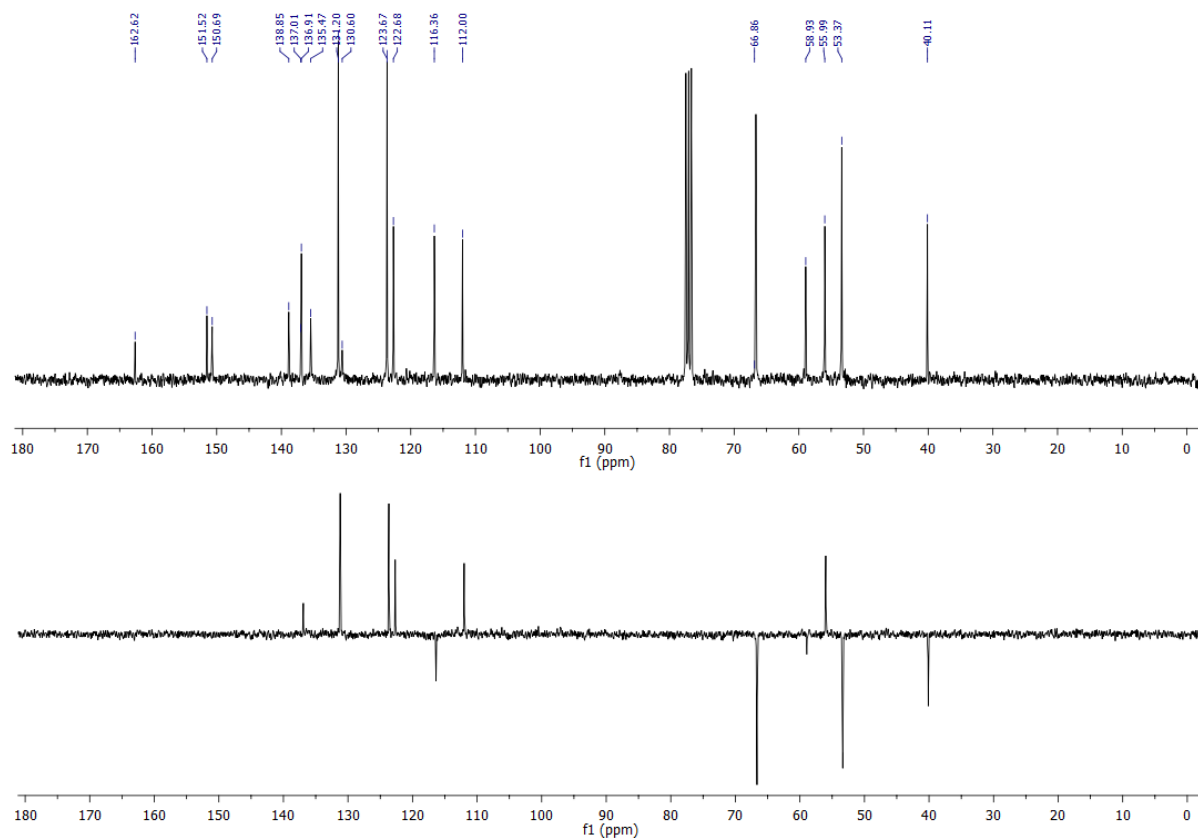


Figure S13. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl_3) of compound **4b**.

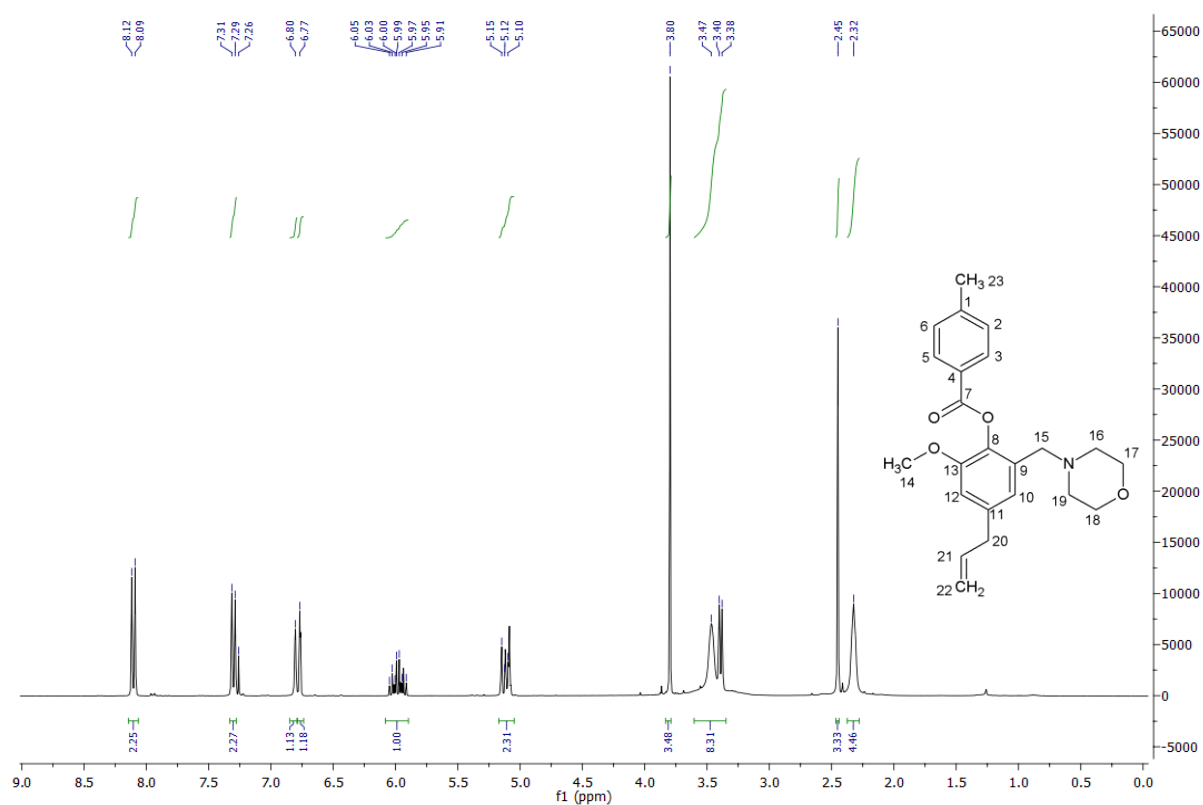


Figure S14. ¹H NMR spectrum (300 MHz, CDCl₃) of compound **4c**.

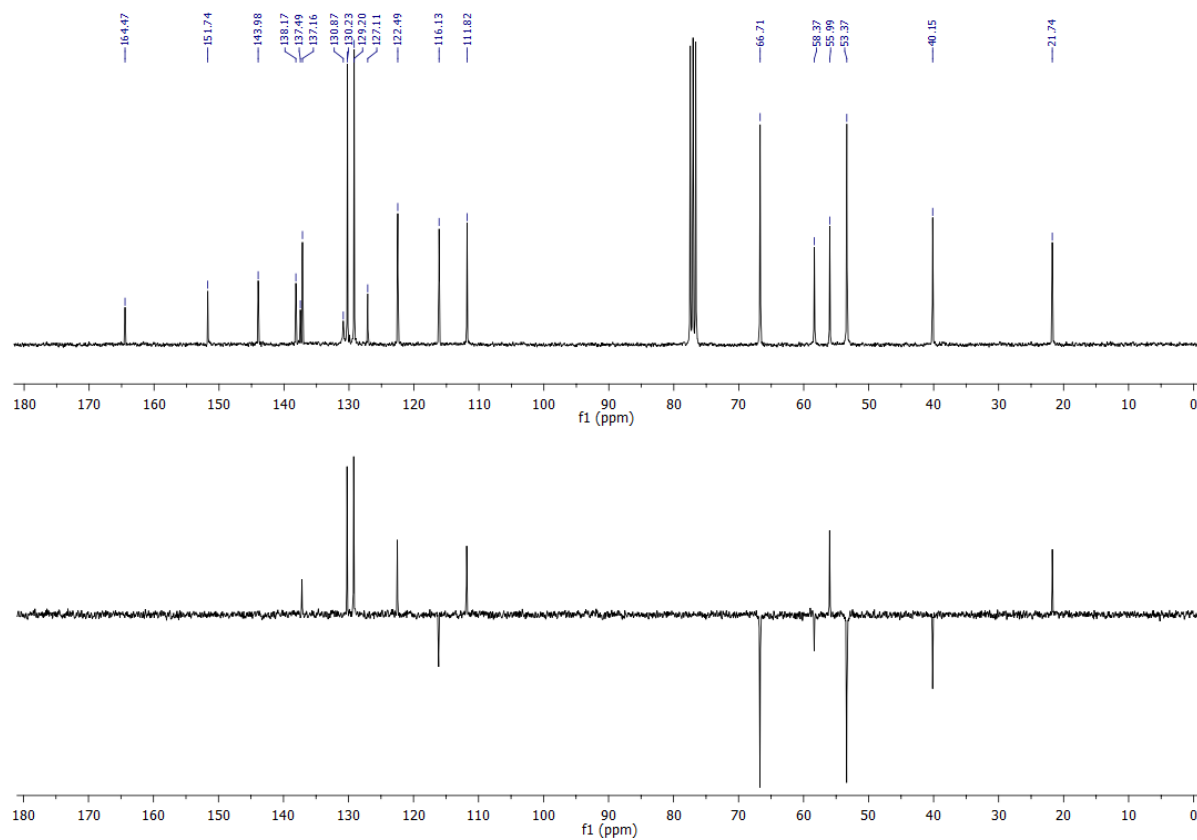


Figure S15. ¹³C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl₃) of compound **4c**.

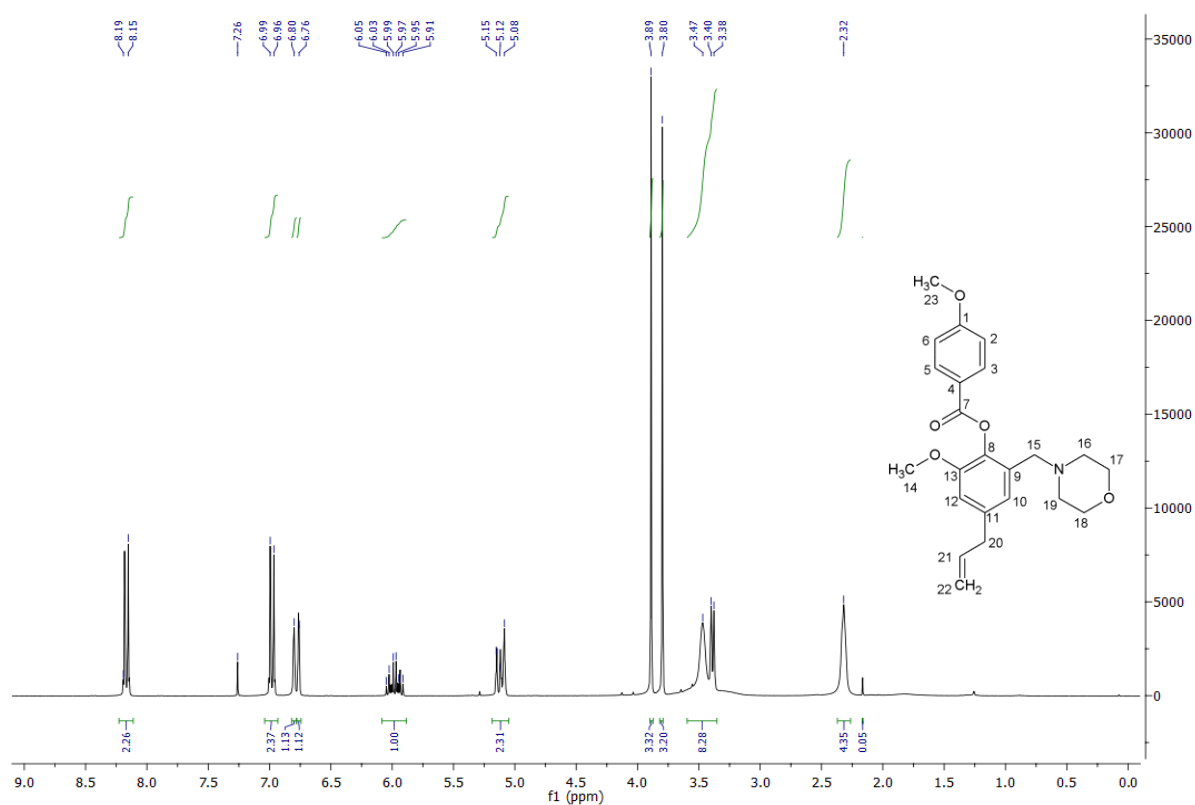


Figure S16. ¹H NMR spectrum (300 MHz, CDCl₃) of compound **4d**.

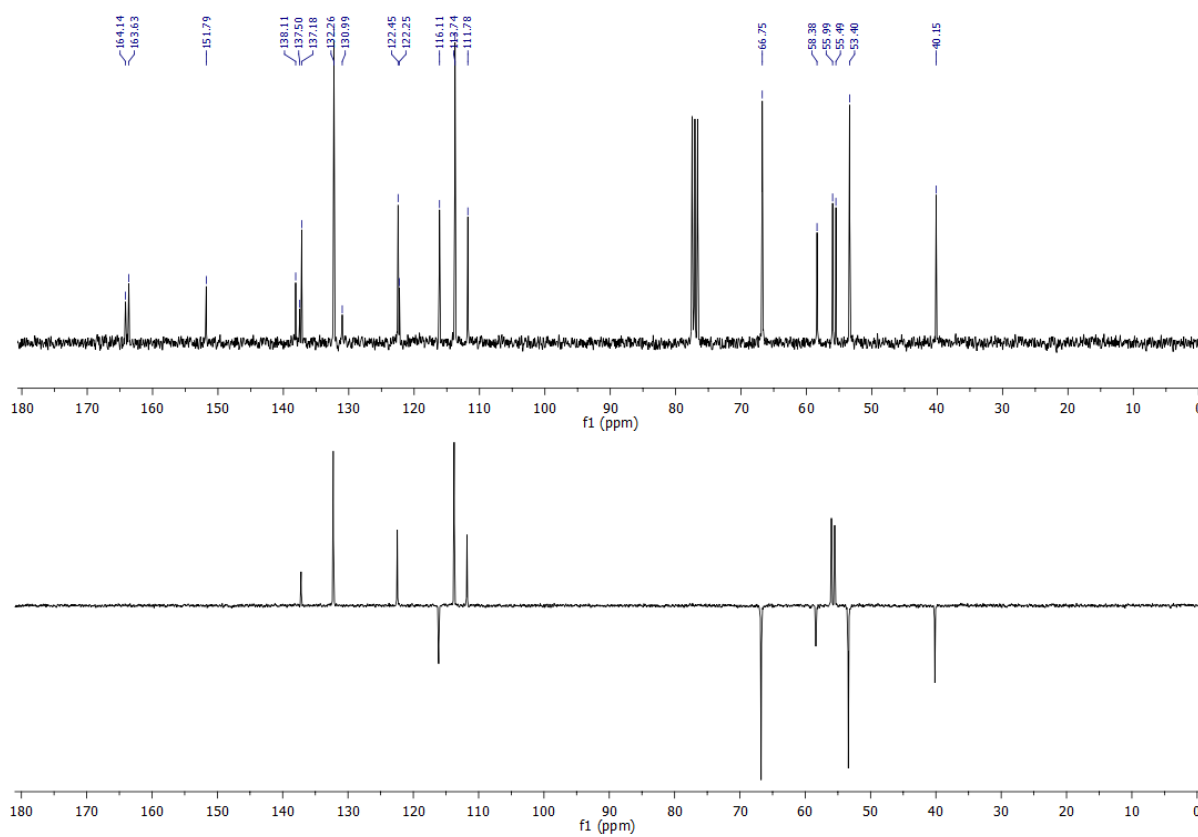


Figure S17. ¹³C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl₃) of compound **4d**.

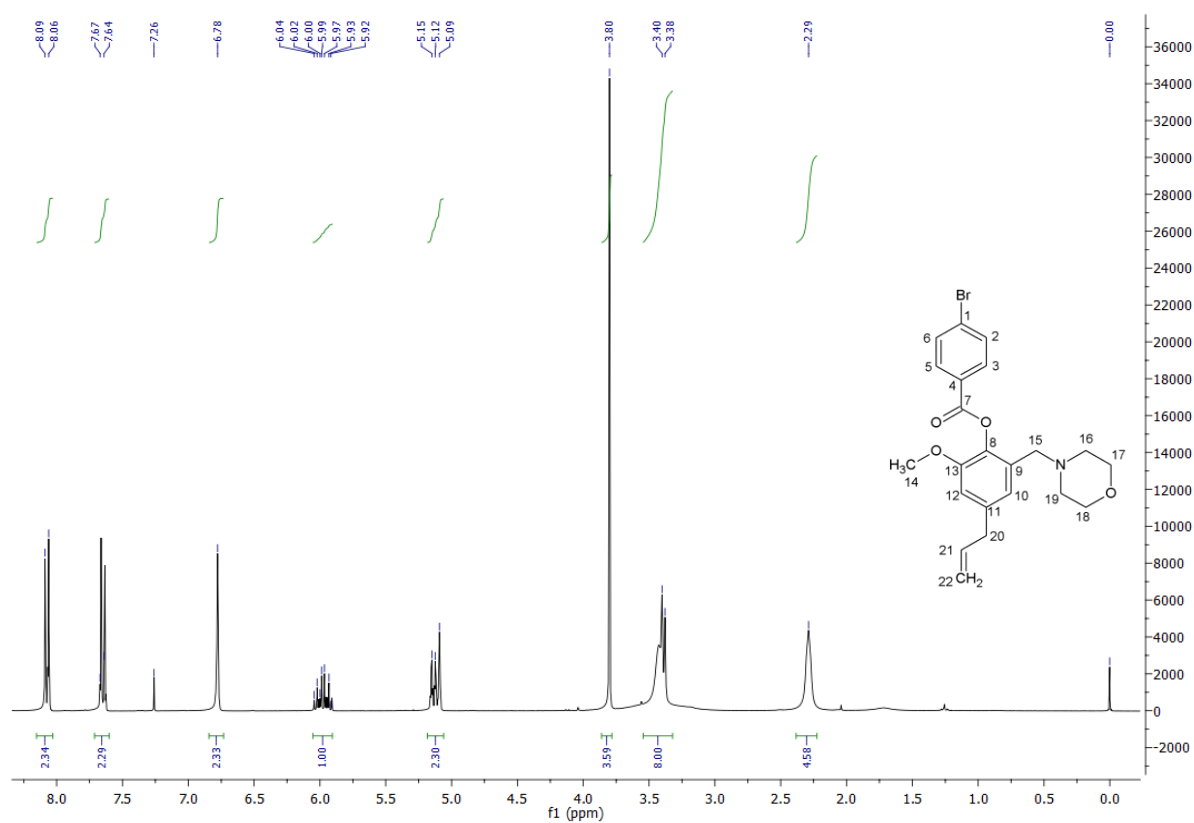


Figure S18. ^1H NMR spectrum (300 MHz, CDCl_3) of compound **4e**.

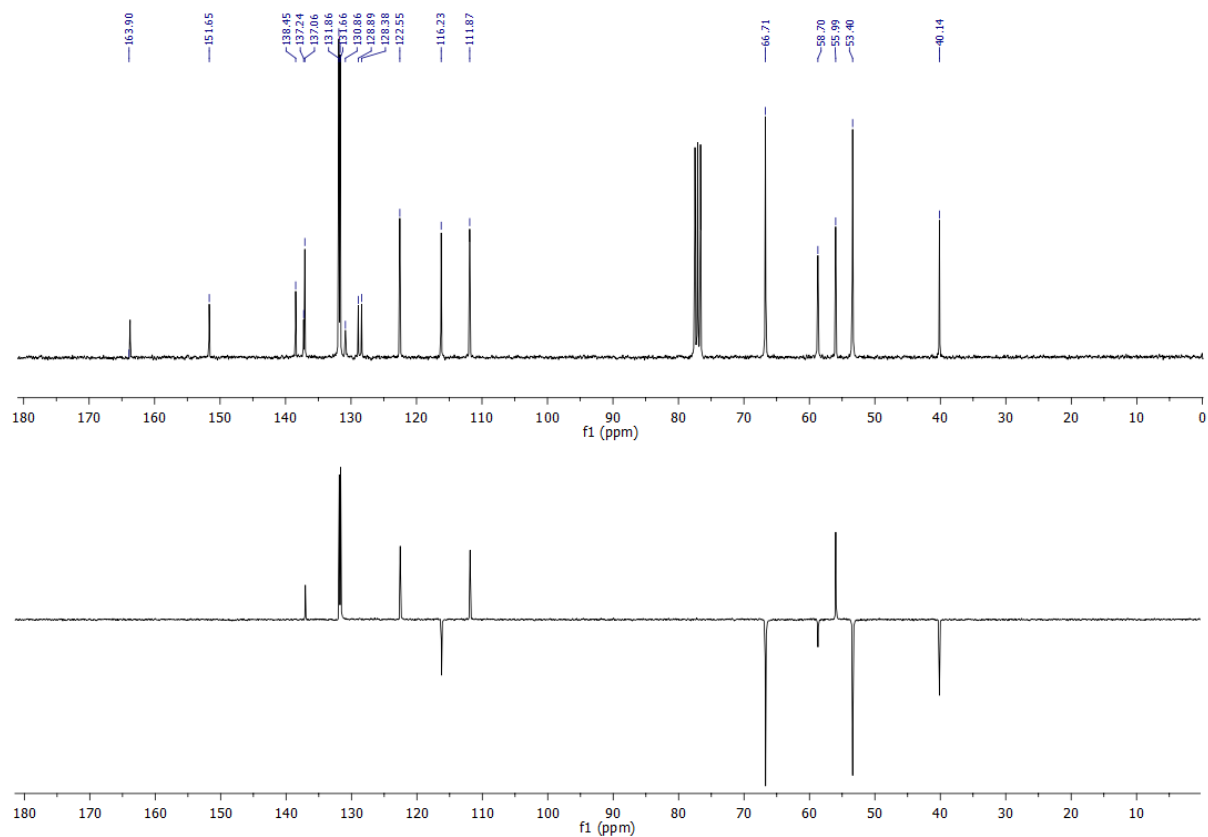


Figure S19. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl_3) of compound **4e**.

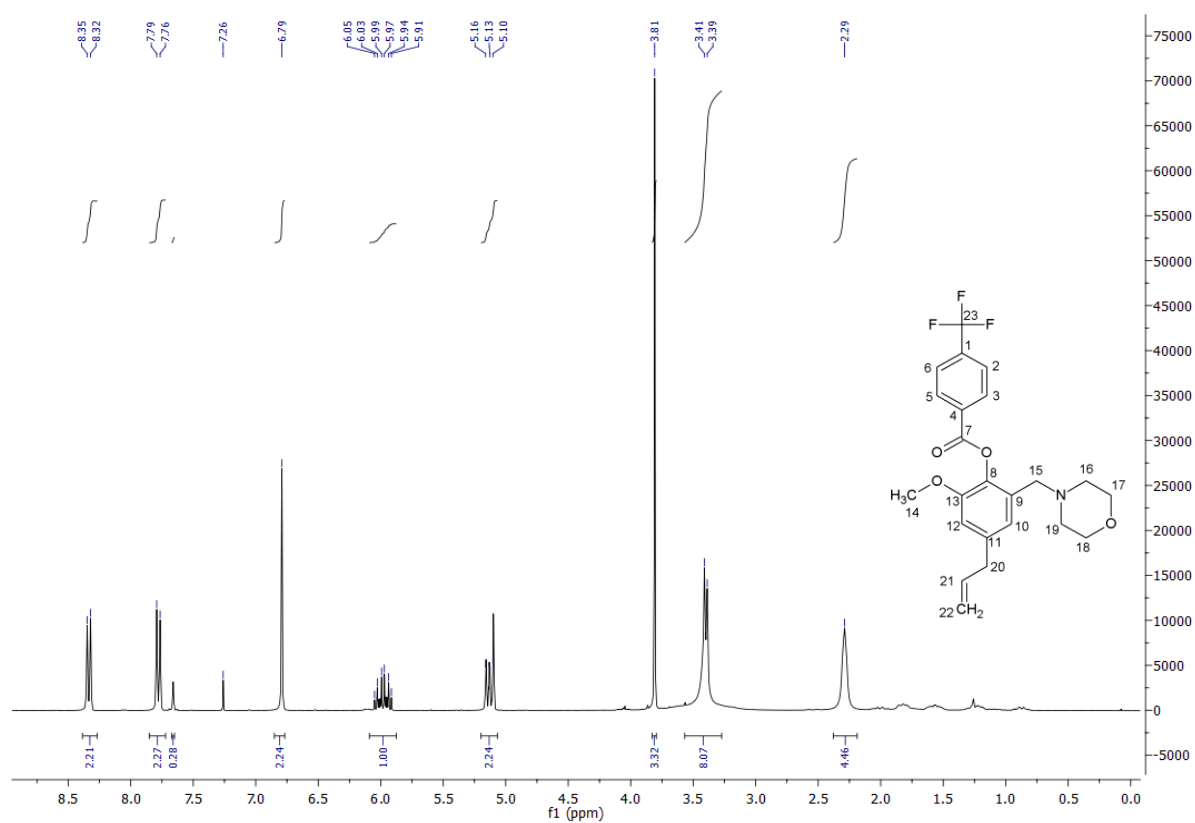


Figure S20. ¹H NMR spectrum (300 MHz, CDCl₃) of compound **4f**.

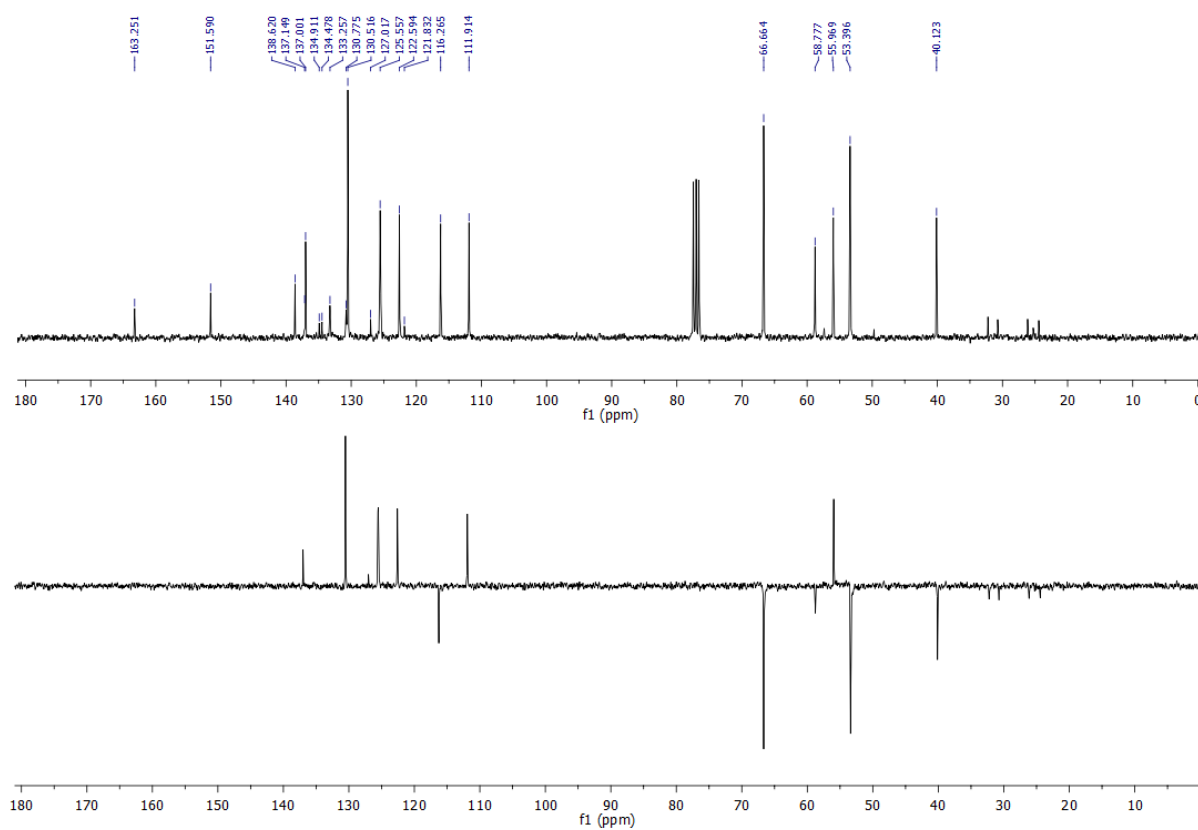


Figure S21. ¹³C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl₃) of compound **4f**.

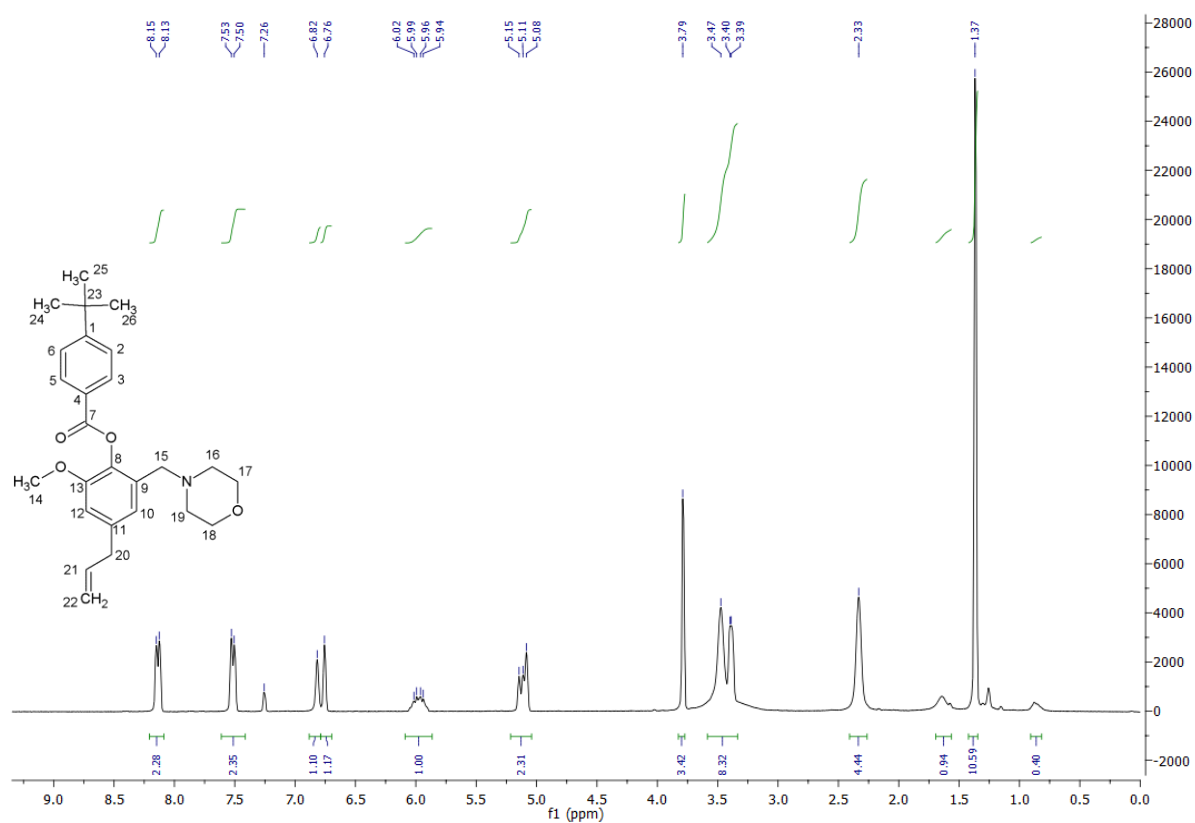


Figure S22. ^1H NMR spectrum (300 MHz, CDCl_3) of compound **4g**.

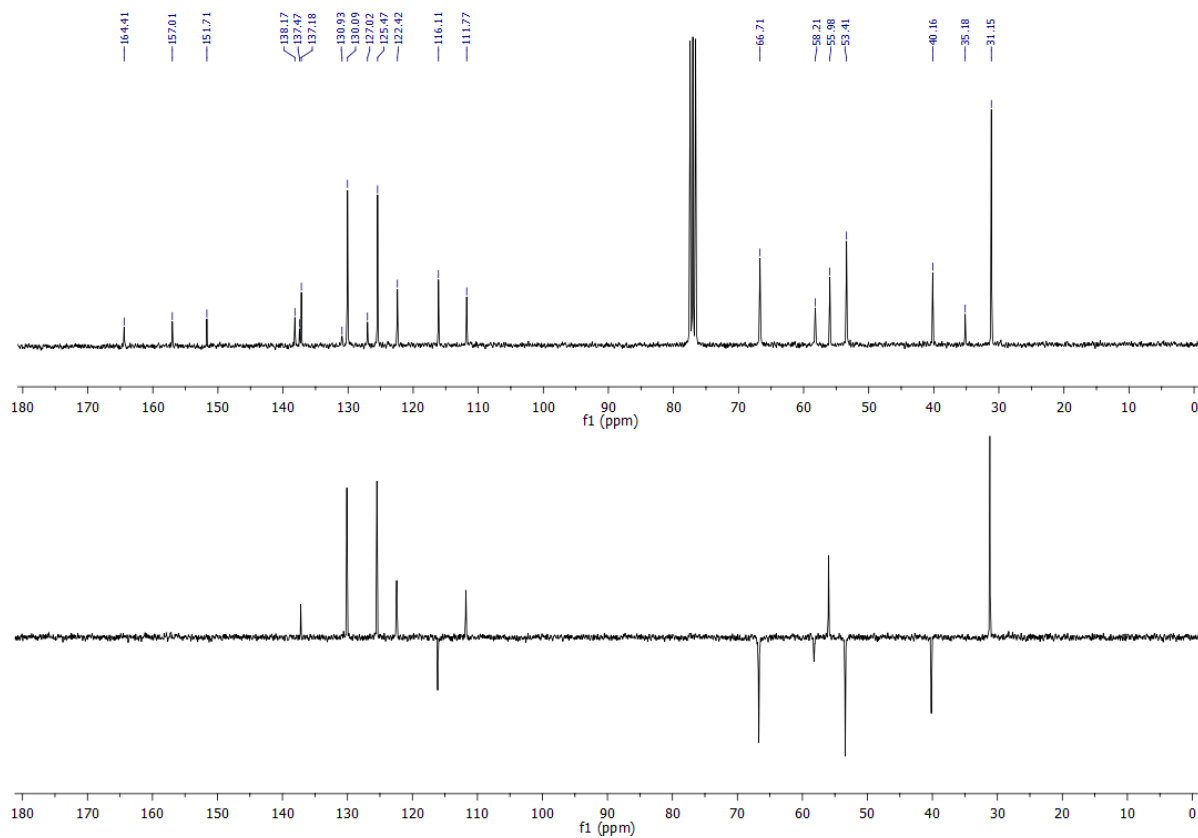


Figure S23. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl_3) of compound **4g**.

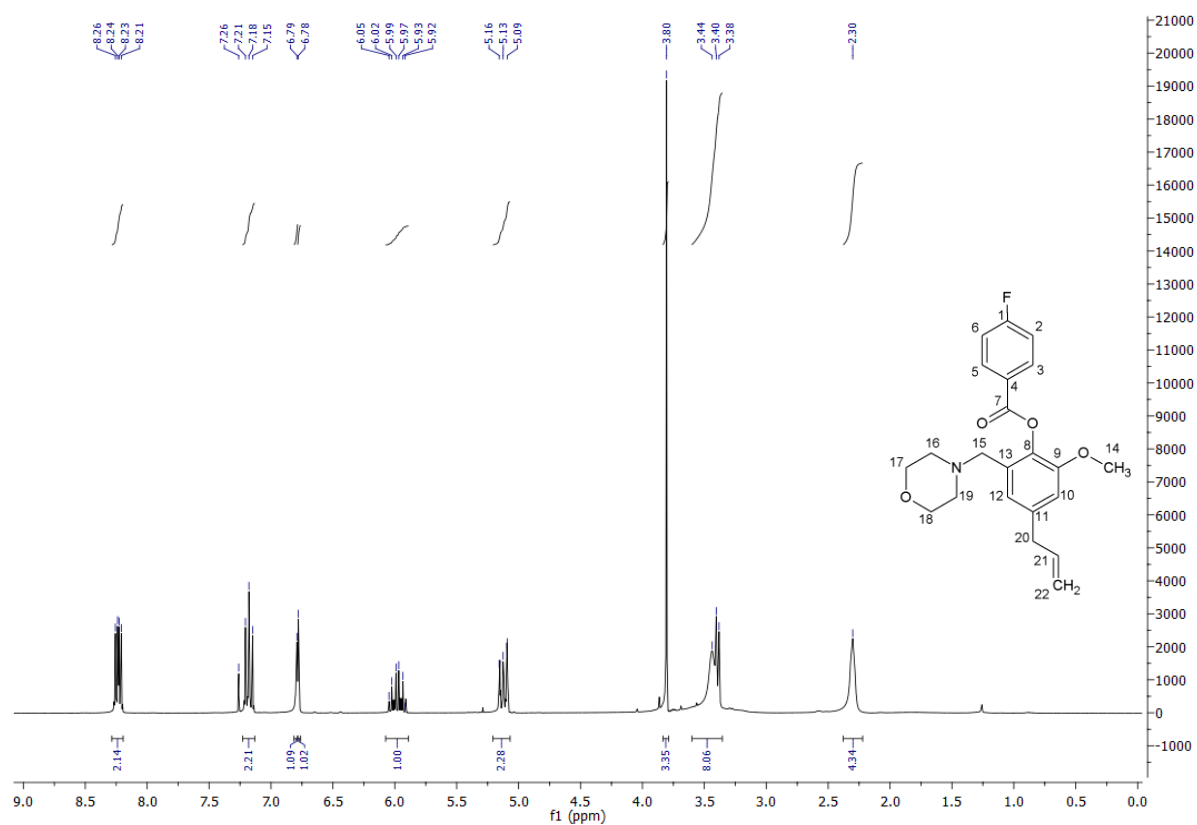


Figure S24. ^1H NMR spectrum (300 MHz, CDCl_3) of compound **4h**.

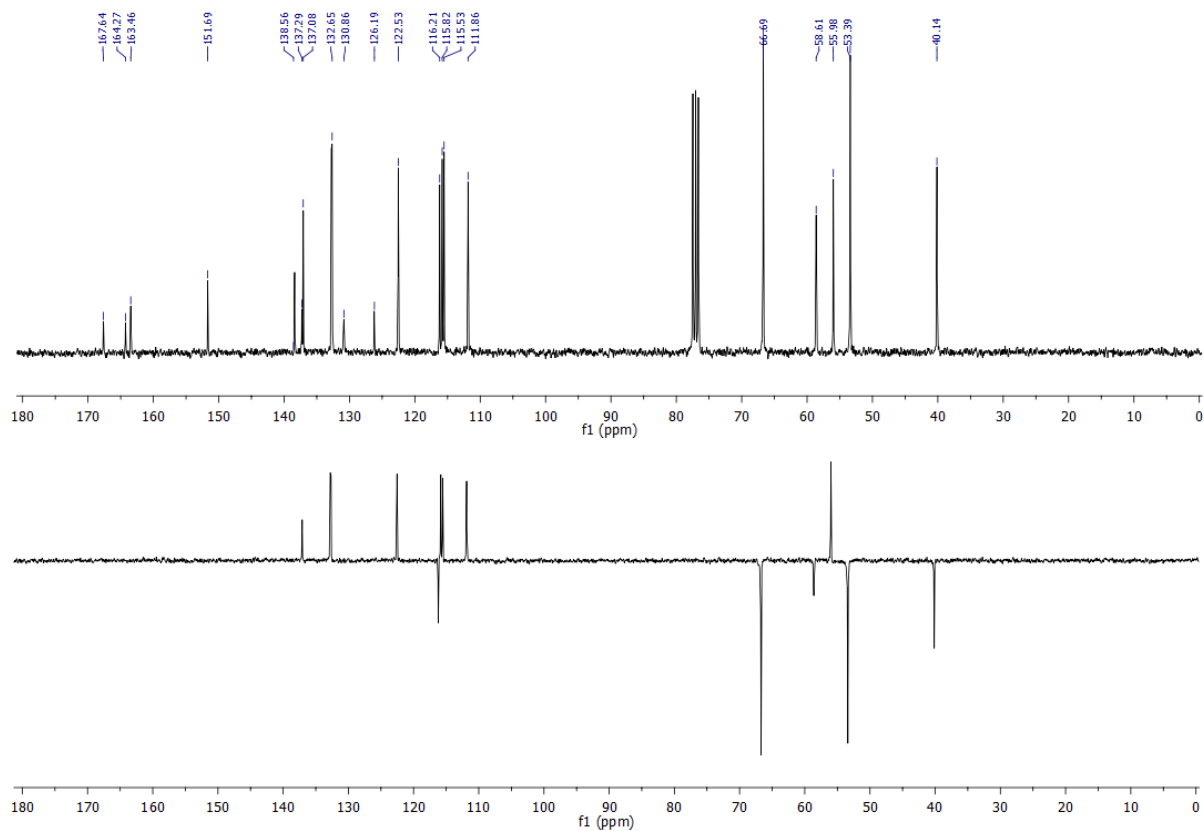


Figure S25. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl_3) of compound **4h**.

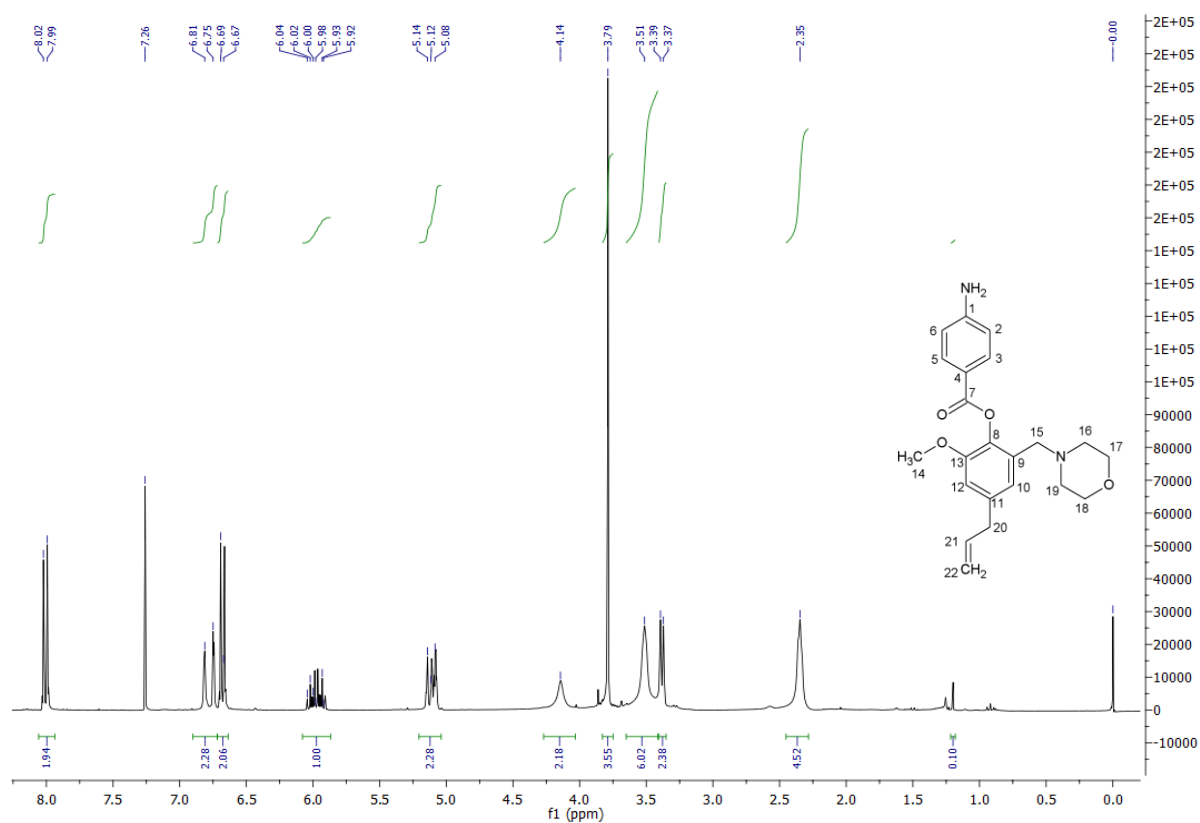


Figure S26. ^1H NMR spectrum (300 MHz, CDCl_3) of compound **4i**.

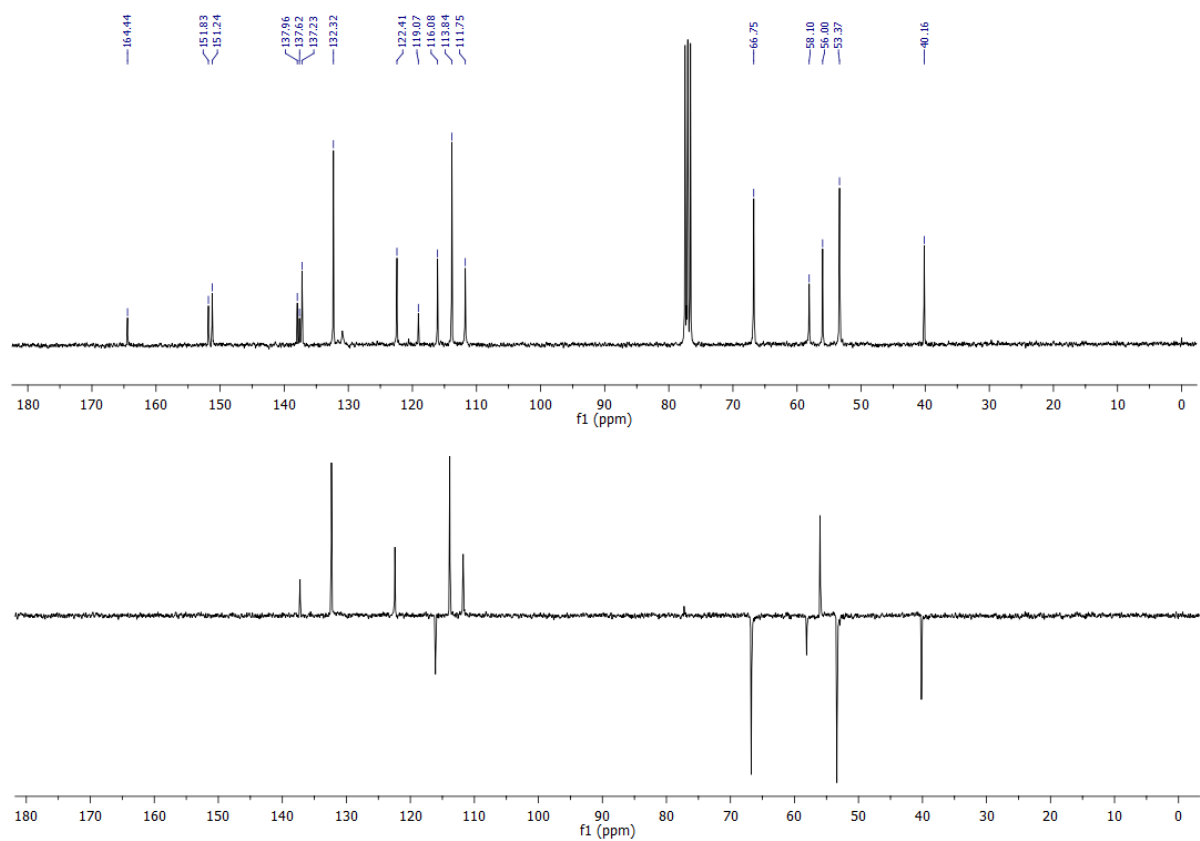


Figure S27. ^{13}C NMR spectrum and DEPT-135 subspectrum (75 MHz, CDCl_3) of compound **4i**.

Performance

Data: SBM20001.A2[c] 22 Jun 2017 14:13 Cal: SBL_tof 22 Jun 2017 14:12

Shimadzu Biotech Axima Performance 2.9.3.20110624: Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

%Int. 94 mV[sum= 28201 mV] Profiles 1-300 Smooth Gauss 5 -Baseline 15

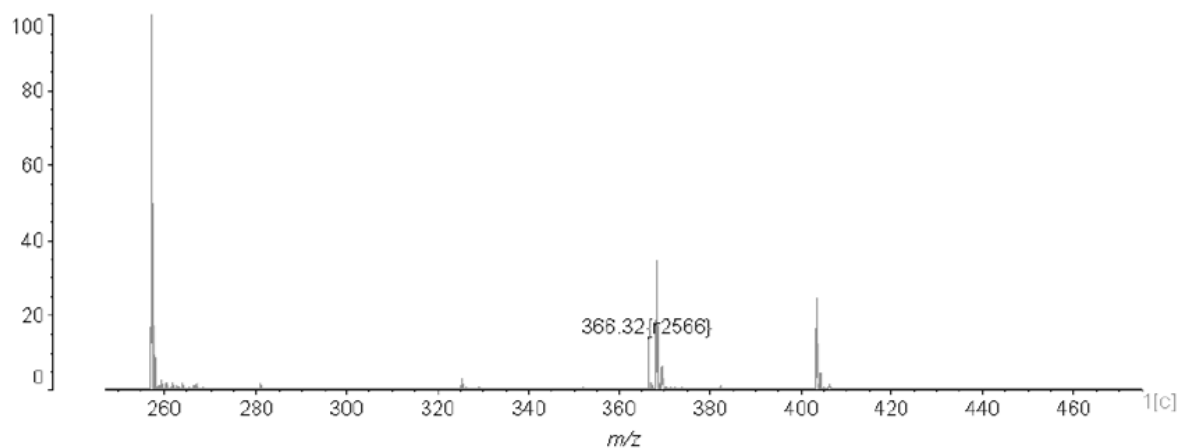


Figure S28. Mass spectrum of compound **4a**.

Performance

Data: SBM30001.A3[c] 22 Jun 2017 14:33 Cal: SBL_tof 22 Jun 2017 14:12

Shimadzu Biotech Axima Performance 2.9.3.20110624: Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

%Int. 43 mV[sum= 12986 mV] Profiles 1-300 Smooth Gauss 5 -Baseline 15

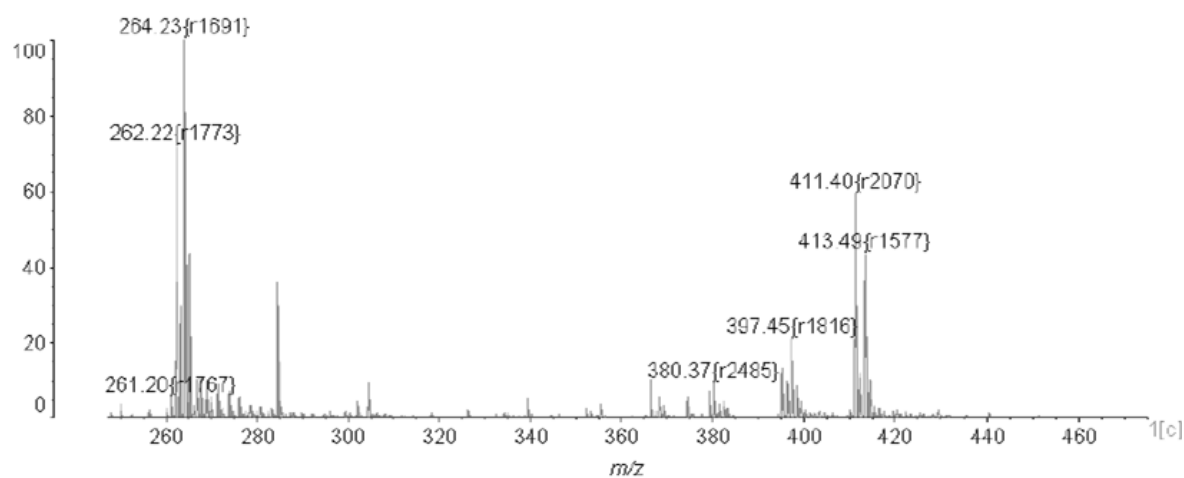


Figure S29. Mass spectrum of compound **4b**.

Performance
Data: SBM40002.B4[c] 22 Jun 2017 15:13 Cal: SBL_tof 22 Jun 2017 14:12
Shimadzu Biotech Axima Performance 2.9.3.20110624 Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

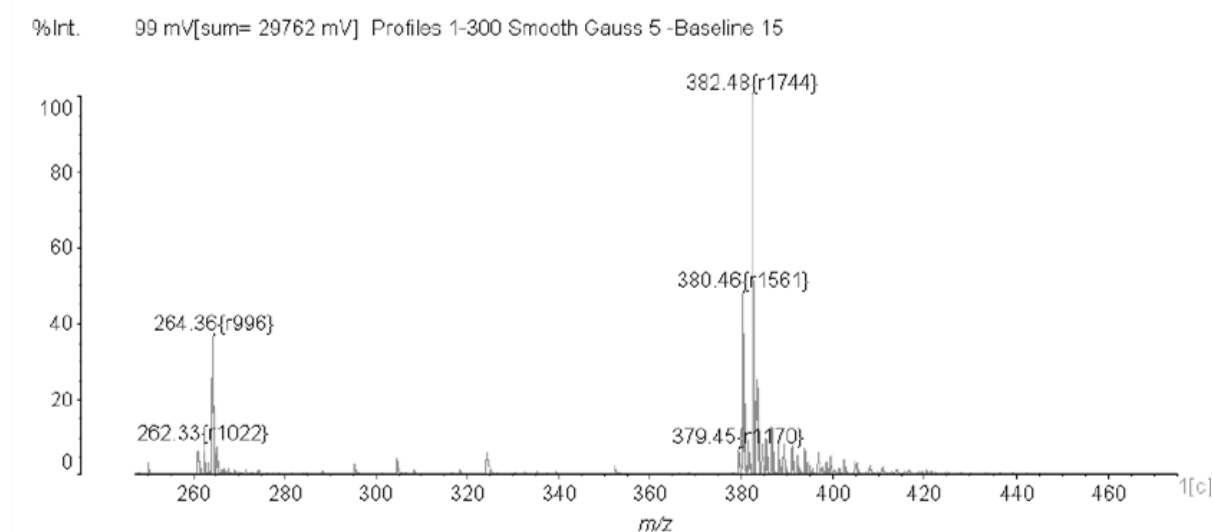


Figure S30. Mass spectrum of compound **4c**.

Data: SBM50001.C2[c] 22 Jun 2017 15:32 Cal: SBL_tof 22 Jun 2017 14:12
Shimadzu Biotech Axima Performance 2.9.3.20110624 Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

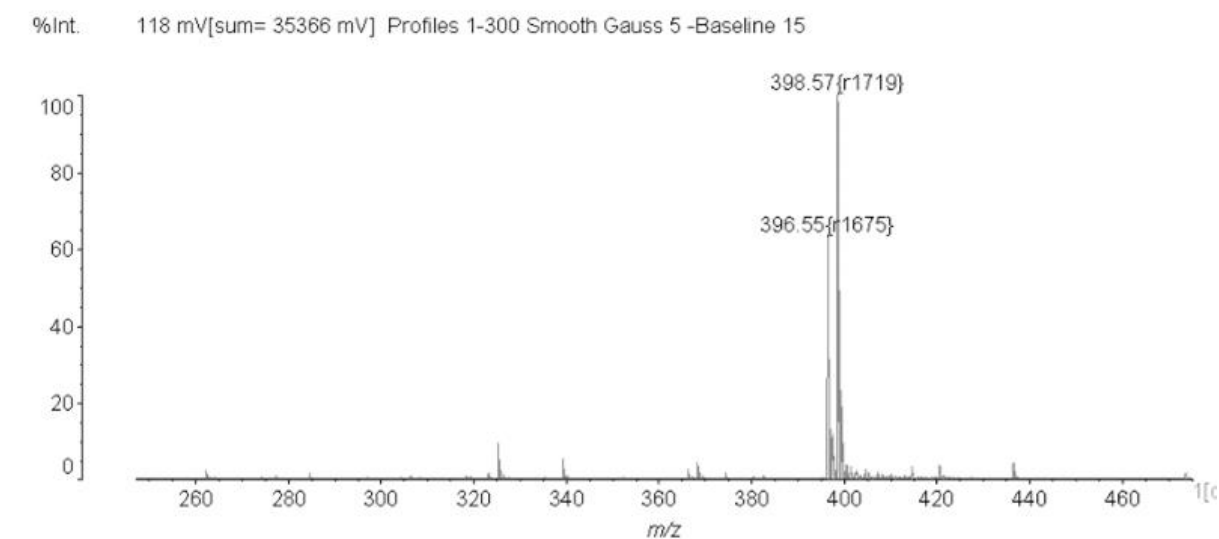


Figure S31. Mass spectrum of compound **4d**.

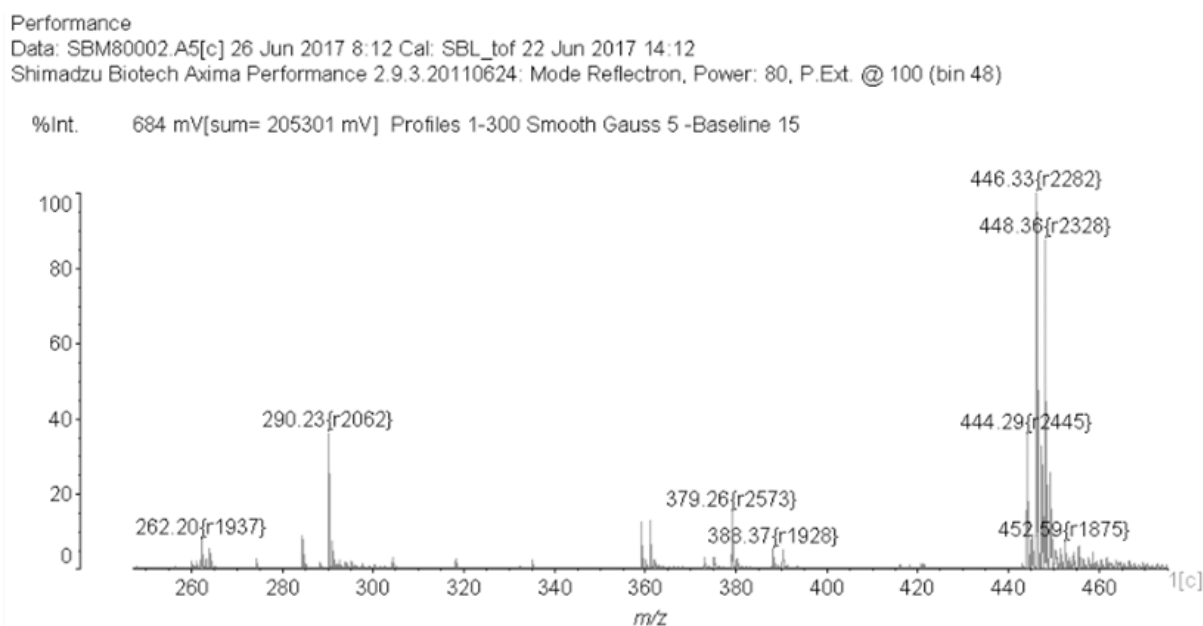


Figure S32. Mass spectrum of compound **4e**.

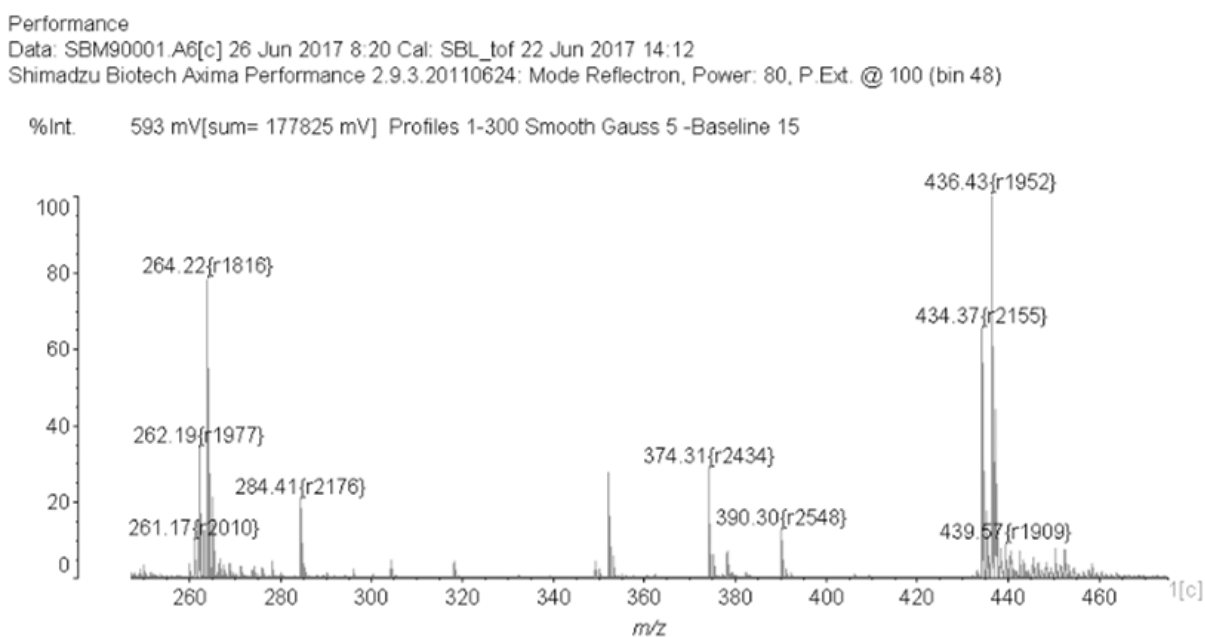


Figure S33. Mass spectrum of compound **4f**.

Performance
 Data: SBM100002.B7[c] 26 Jun 2017 8:38 Cal: SBL_tof 22 Jun 2017 14:12
 Shimadzu Biotech Axima Performance 2.9.3.20110624: Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

%Int. 644 mV[sum= 193290 mV] Profiles 1-300 Smooth Gauss 5 -Baseline 15

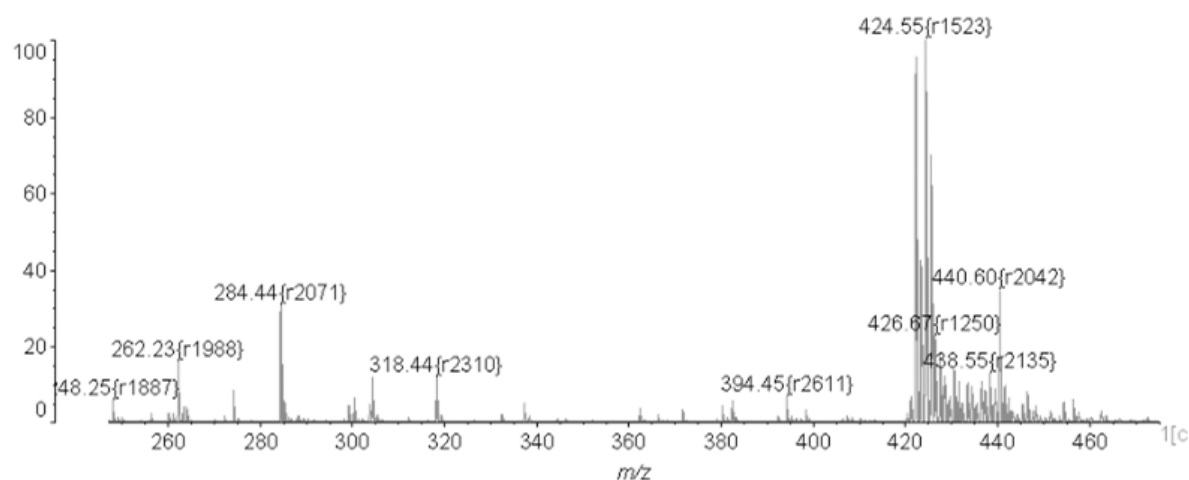


Figure S34. Mass spectrum of compound 4g.

Performance
 Data: SBM110002.B8[c] 26 Jun 2017 8:50 Cal: SBL_tof 22 Jun 2017 14:12
 Shimadzu Biotech Axima Performance 2.9.3.20110624: Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

%Int. 795 mV[sum= 238419 mV] Profiles 1-300 Smooth Gauss 5 -Baseline 15

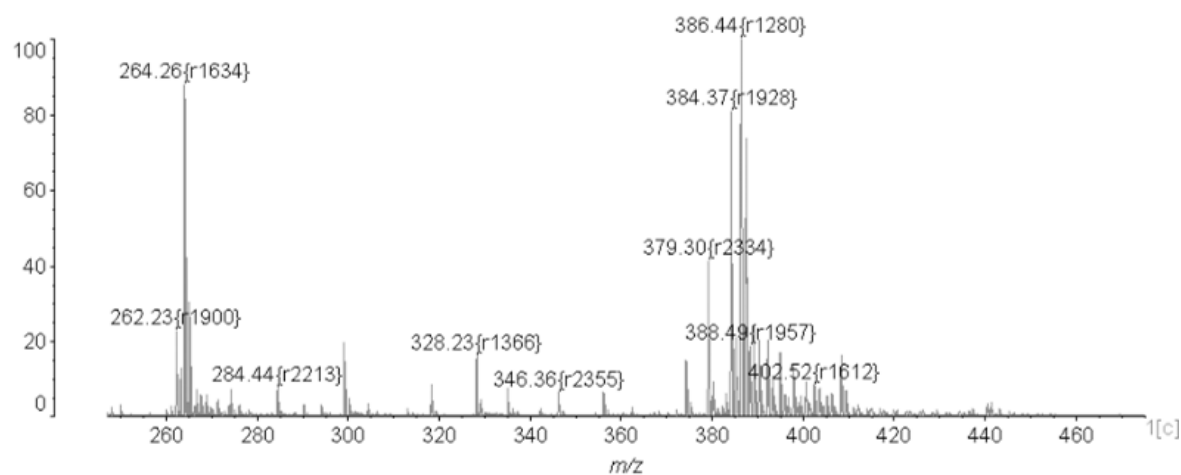


Figure S35. Mass spectrum of compound 4h.

Performance
Data: SBM130001.C6[c] 26 Jun 2017 9:07 Cal: SBL_tof 22 Jun 2017 14:12
Shimadzu Biotech Axima Performance 2.9.3.20110624: Mode Reflectron, Power: 80, P.Ext. @ 100 (bin 48)

%Int. 140 mV[sum= 41946 mV] Profiles 1-300 Smooth Gauss 5 -Baseline 15

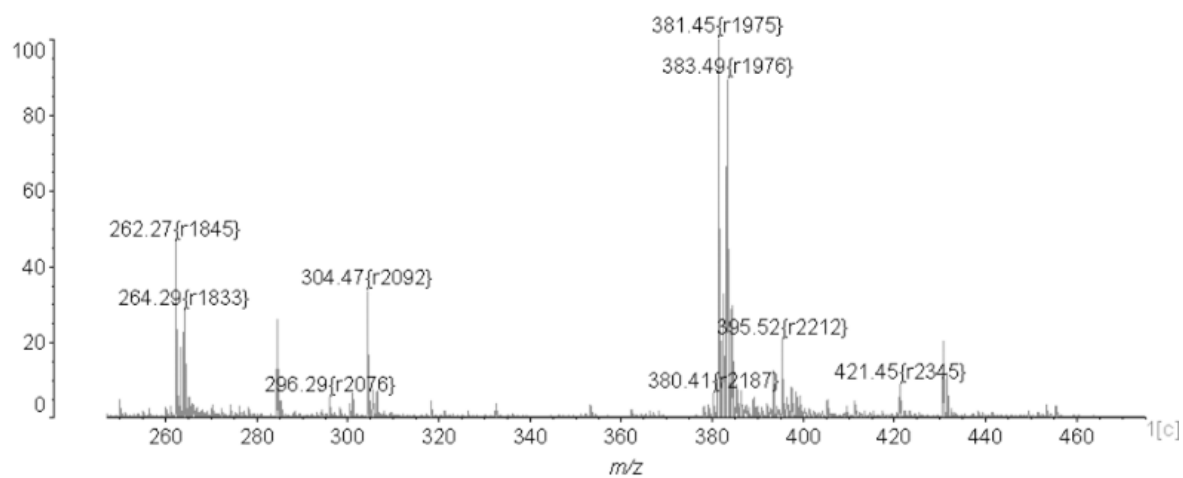


Figure S36. Mass spectrum of compound **4i**.