

Supplementary Materials

Synthesis of spin-labeled ibuprofen and its interaction with lipid membrane

Denis S. Baranov,^{1*} Anna S. Smorygina,¹ Sergei A. Dzuba^{1,2*}

¹V.V. Voevodsky Institute of Chemical Kinetics and Combustion, SB RAS, 630090 Novosibirsk, Russian Federation

^{1,2}Novosibirsk State University, 630090 Novosibirsk, Russian Federation

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NMR spectra

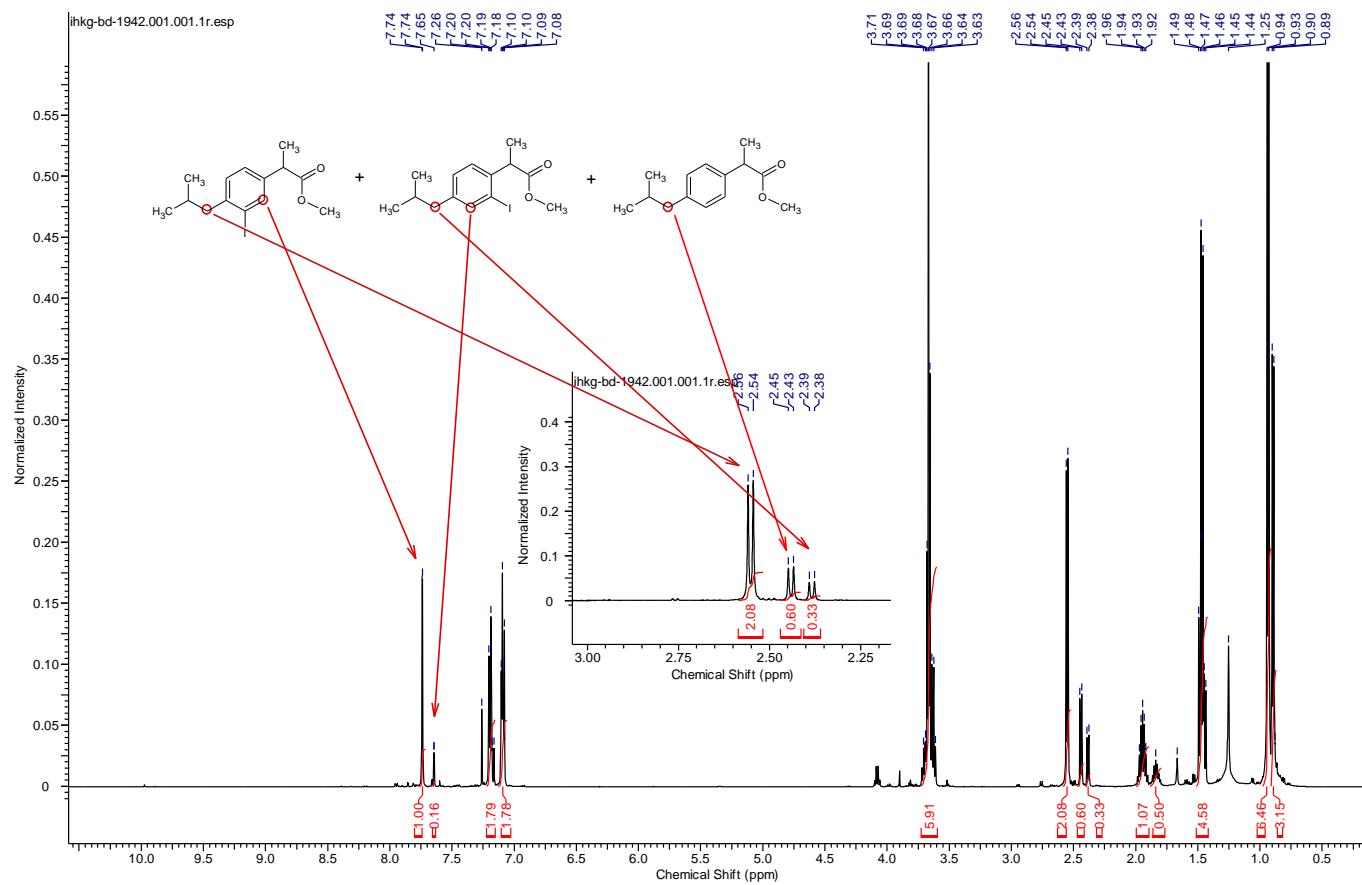
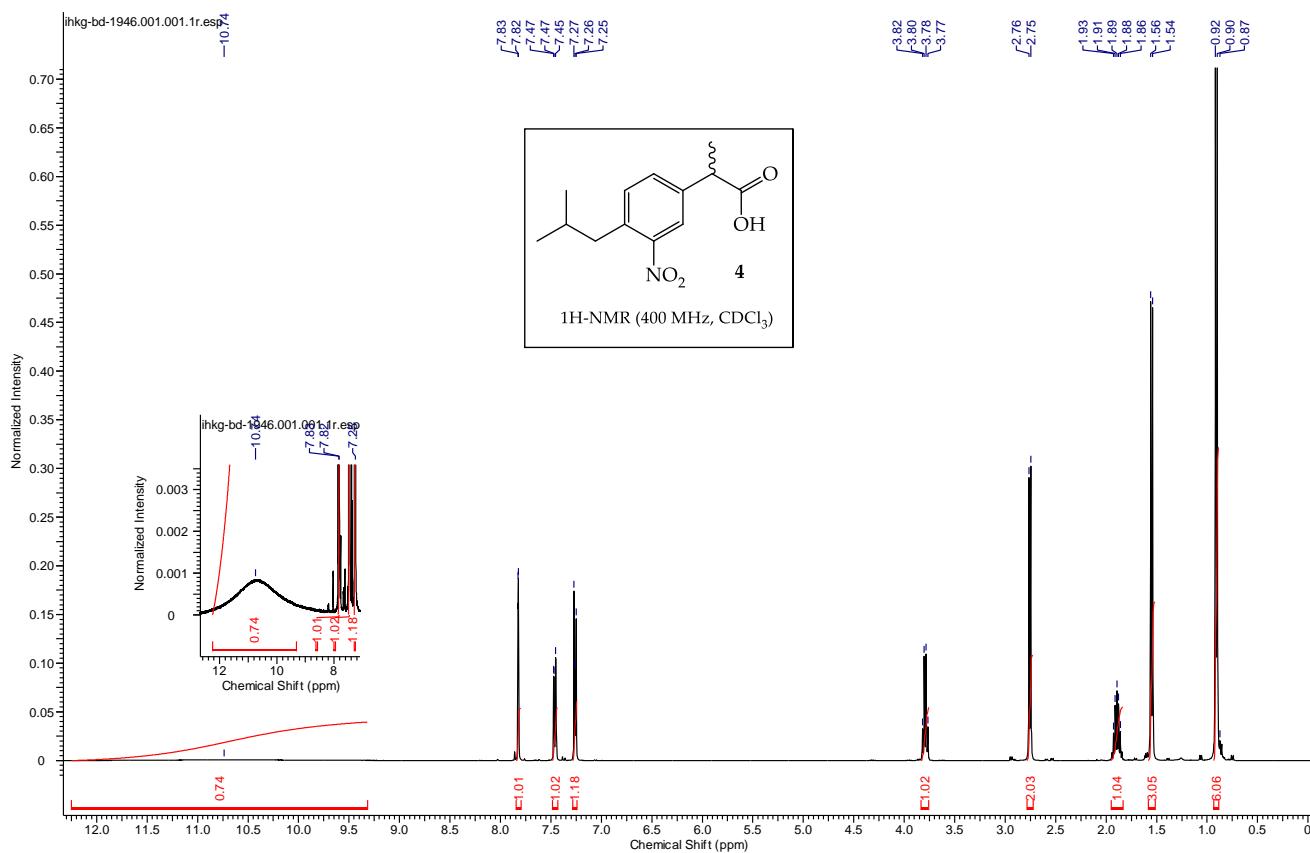


Figure S1. ^1H -NMR spectrum (500 MHz, CDCl_3) of a mixture of products isolated by the iodination reaction of ibuprofen with iodine and iodic acid in acetic acid at 70 °C, followed by methylation with methanol.



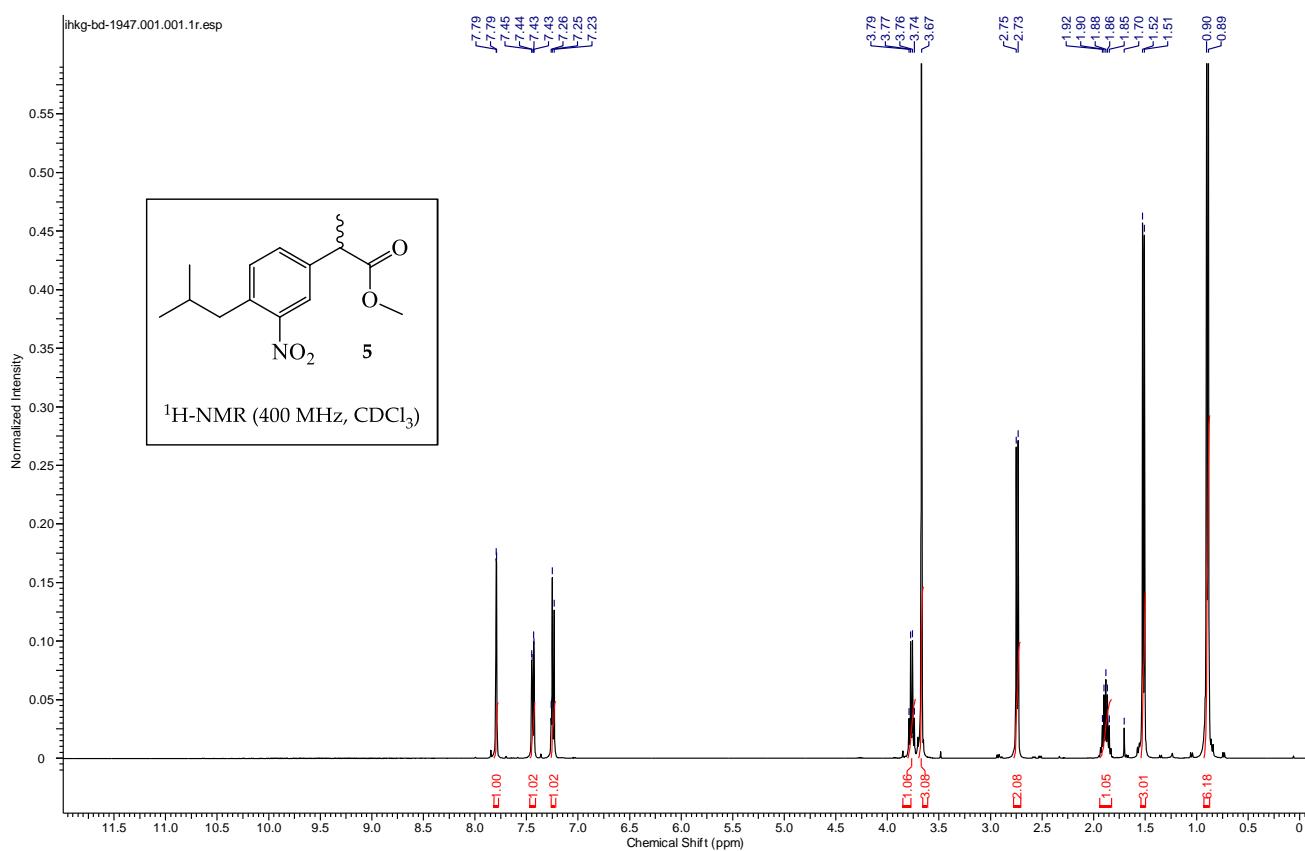


Figure S4. ^1H -NMR spectrum of compound 5.

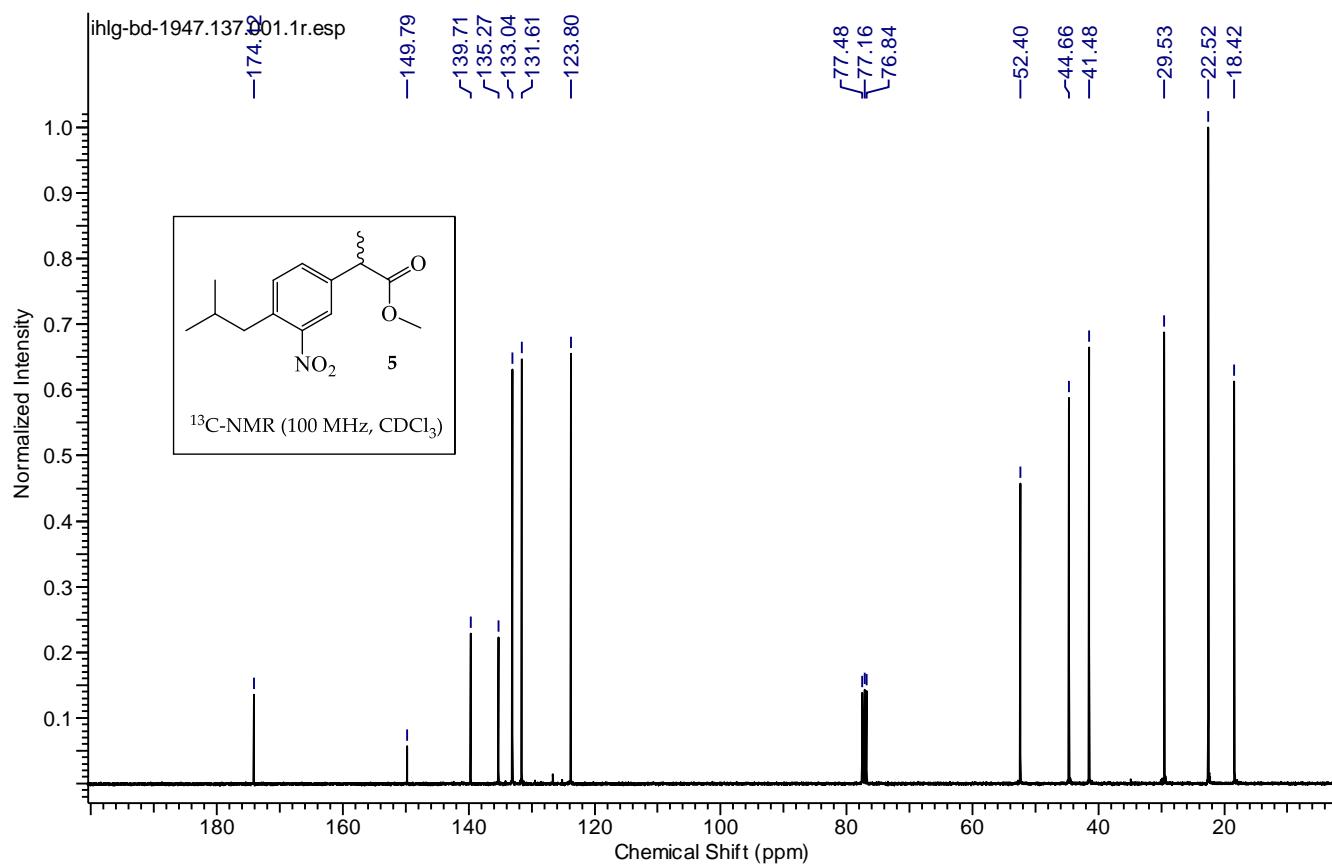


Figure S5. ^{13}C -NMR spectrum of compound 5.

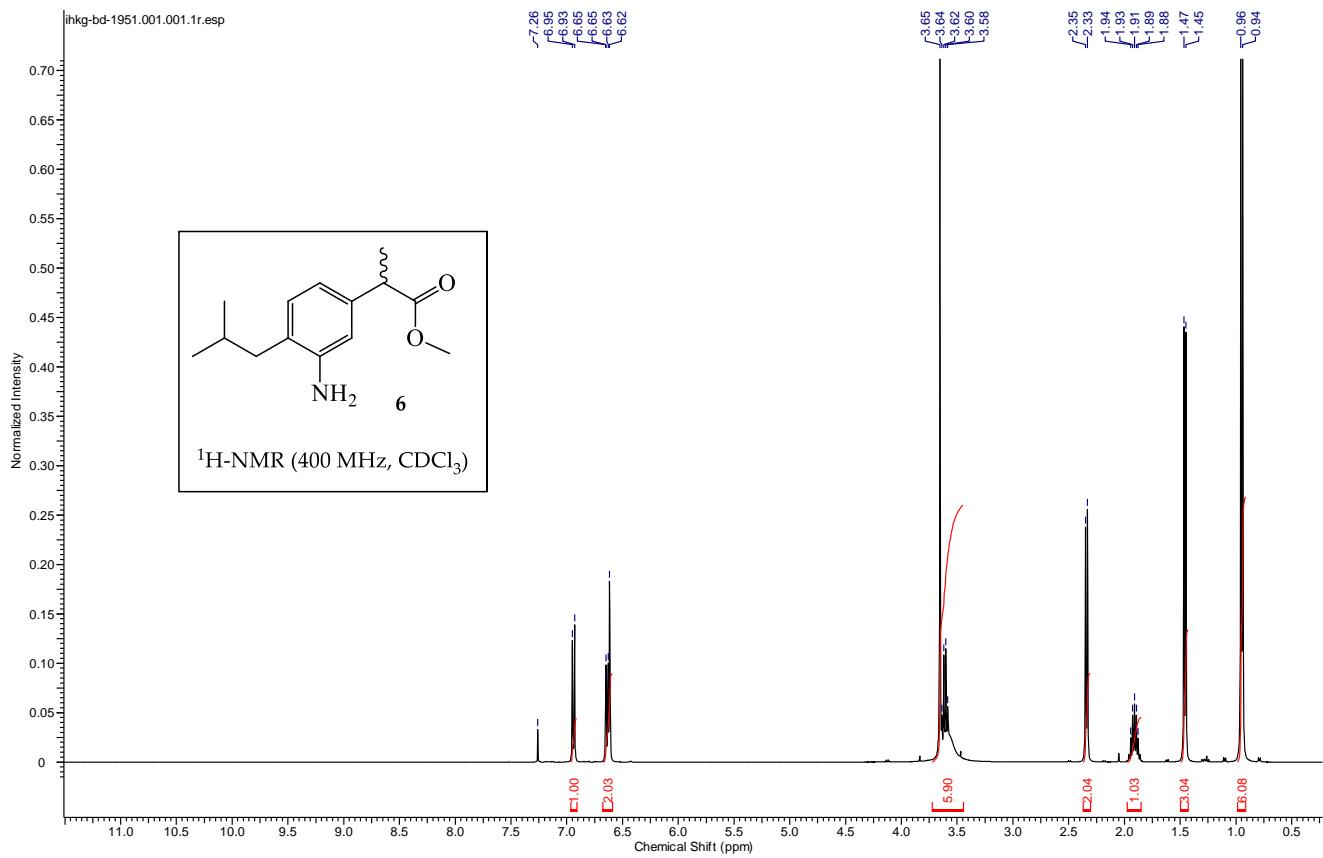


Figure S6. ¹H-NMR spectrum of compound 6.

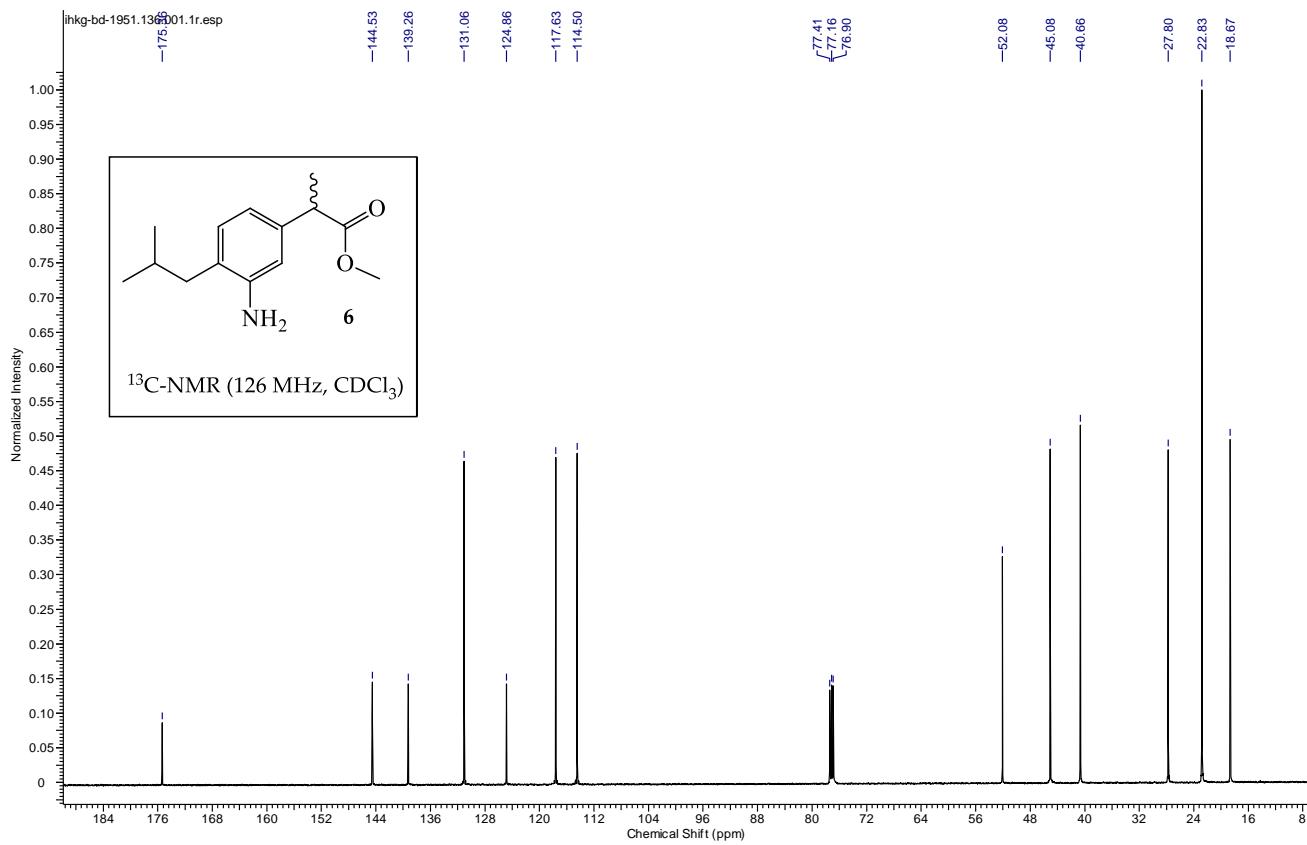


Figure S7. ¹³C-NMR spectrum of compound 6.

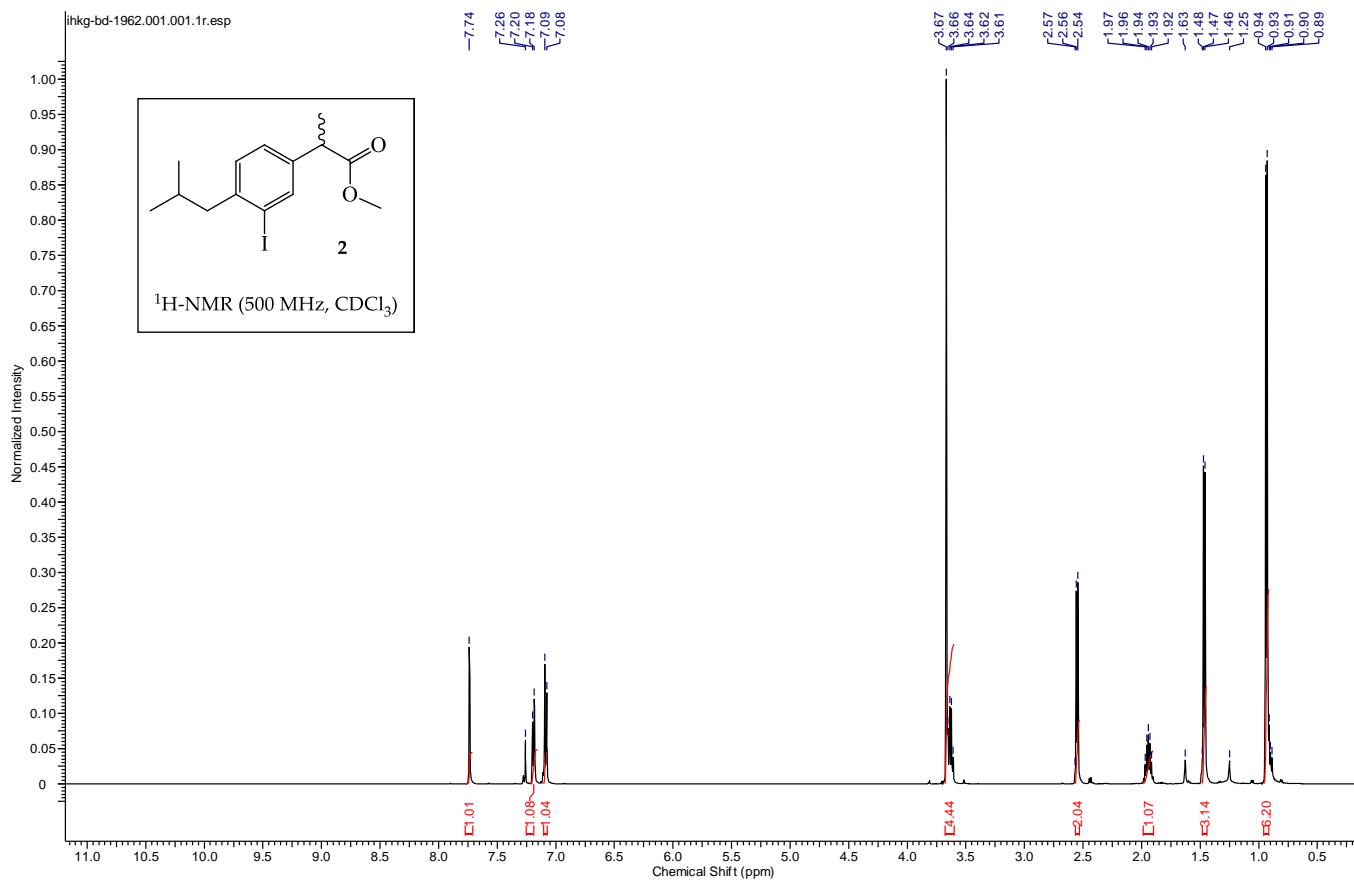


Figure S8. ¹H-NMR spectrum of compound 2.

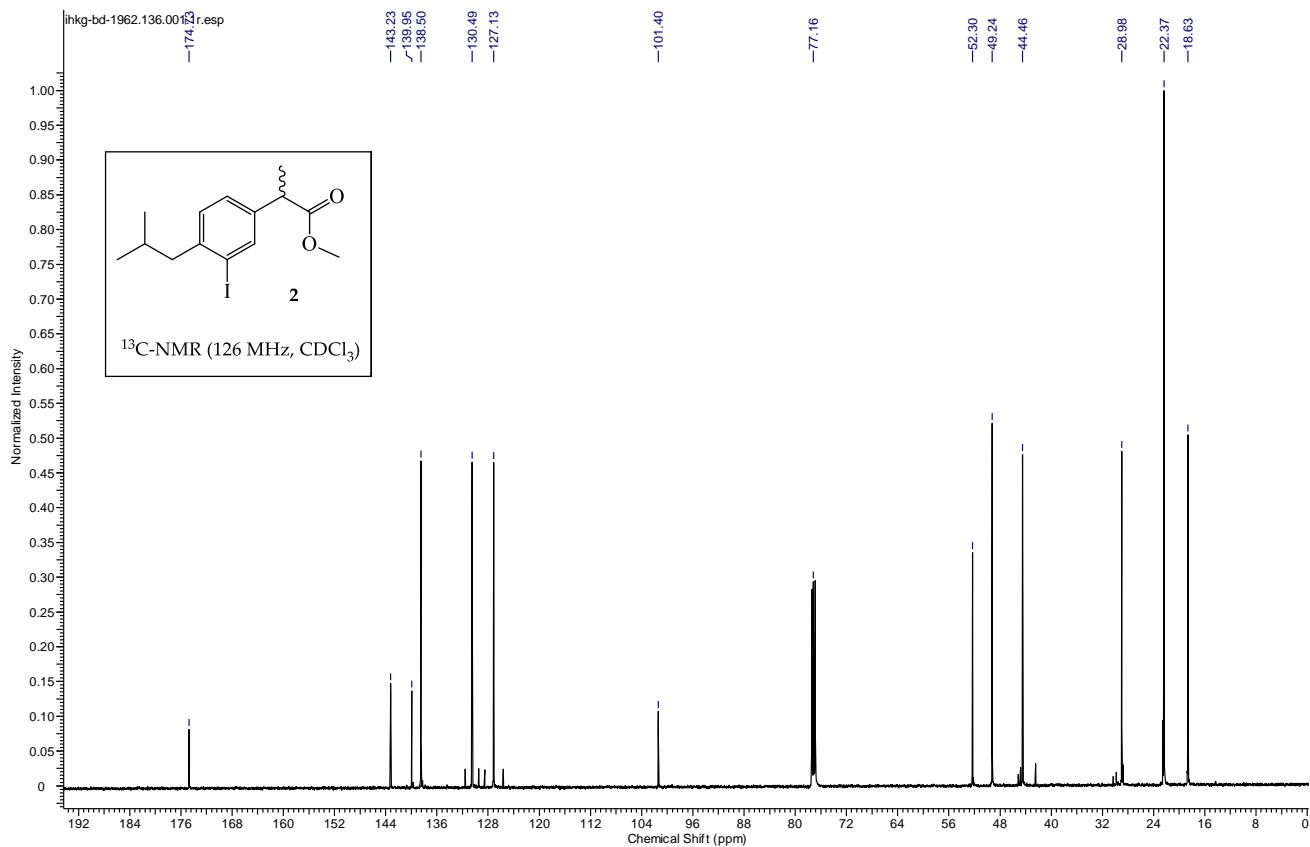


Figure S9. ¹³C-NMR spectrum of compound 2.

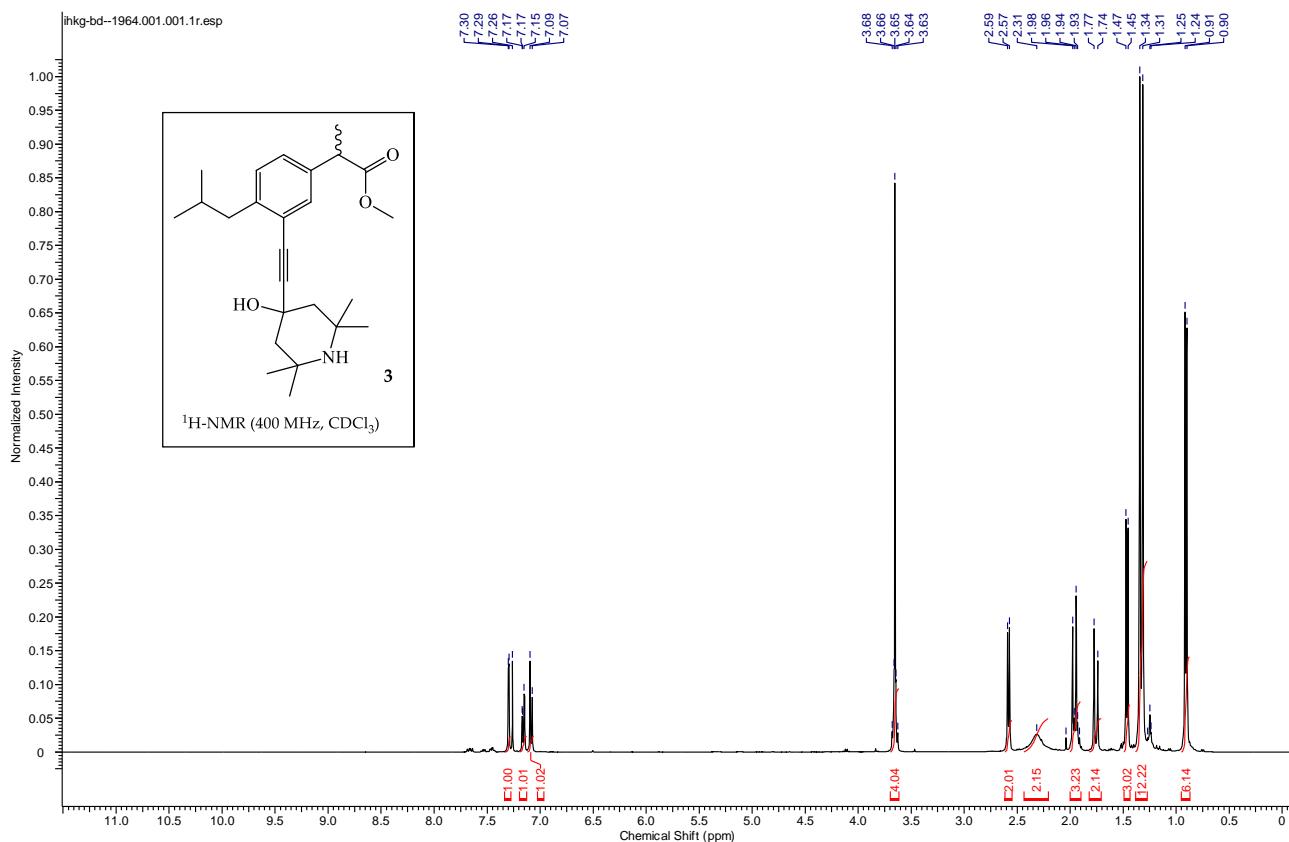


Figure S10. ^1H -NMR spectrum of compound 3.

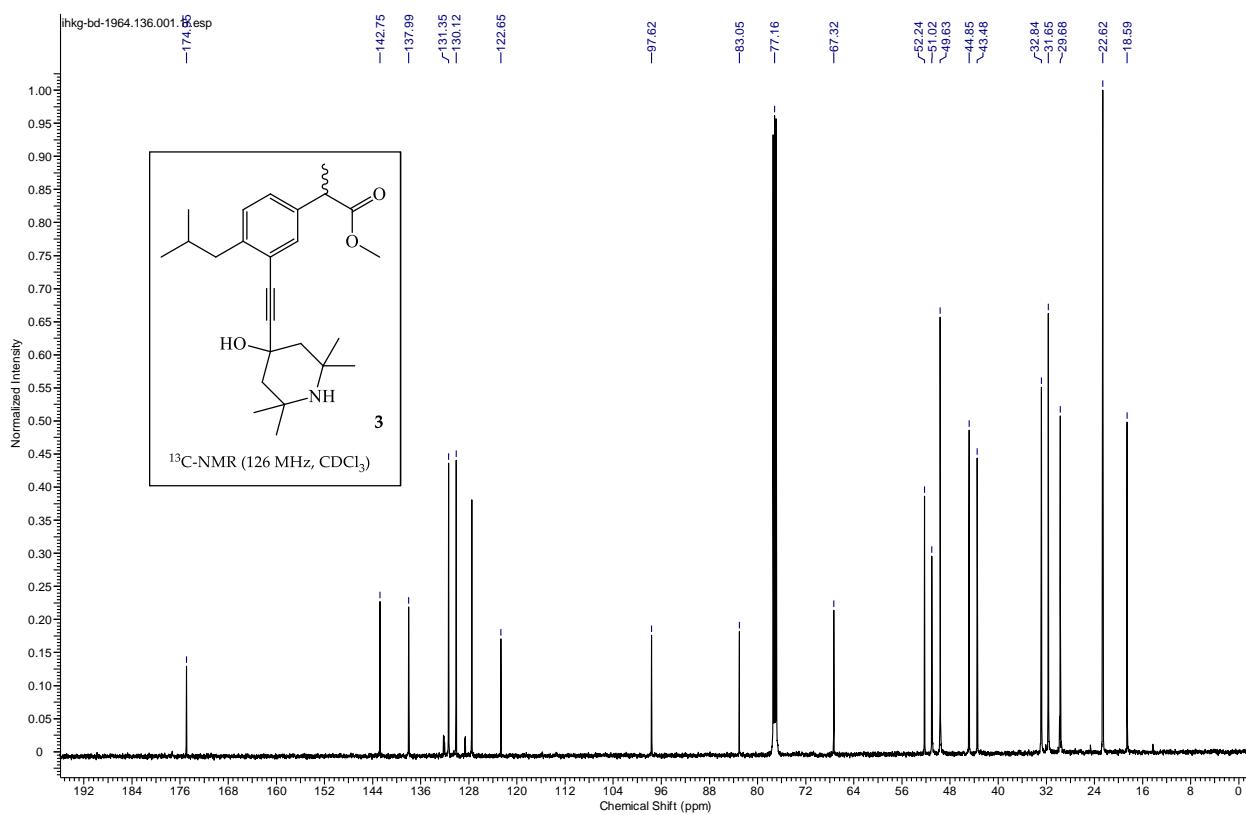


Figure S11. ^{13}C -NMR spectrum of compound 3.

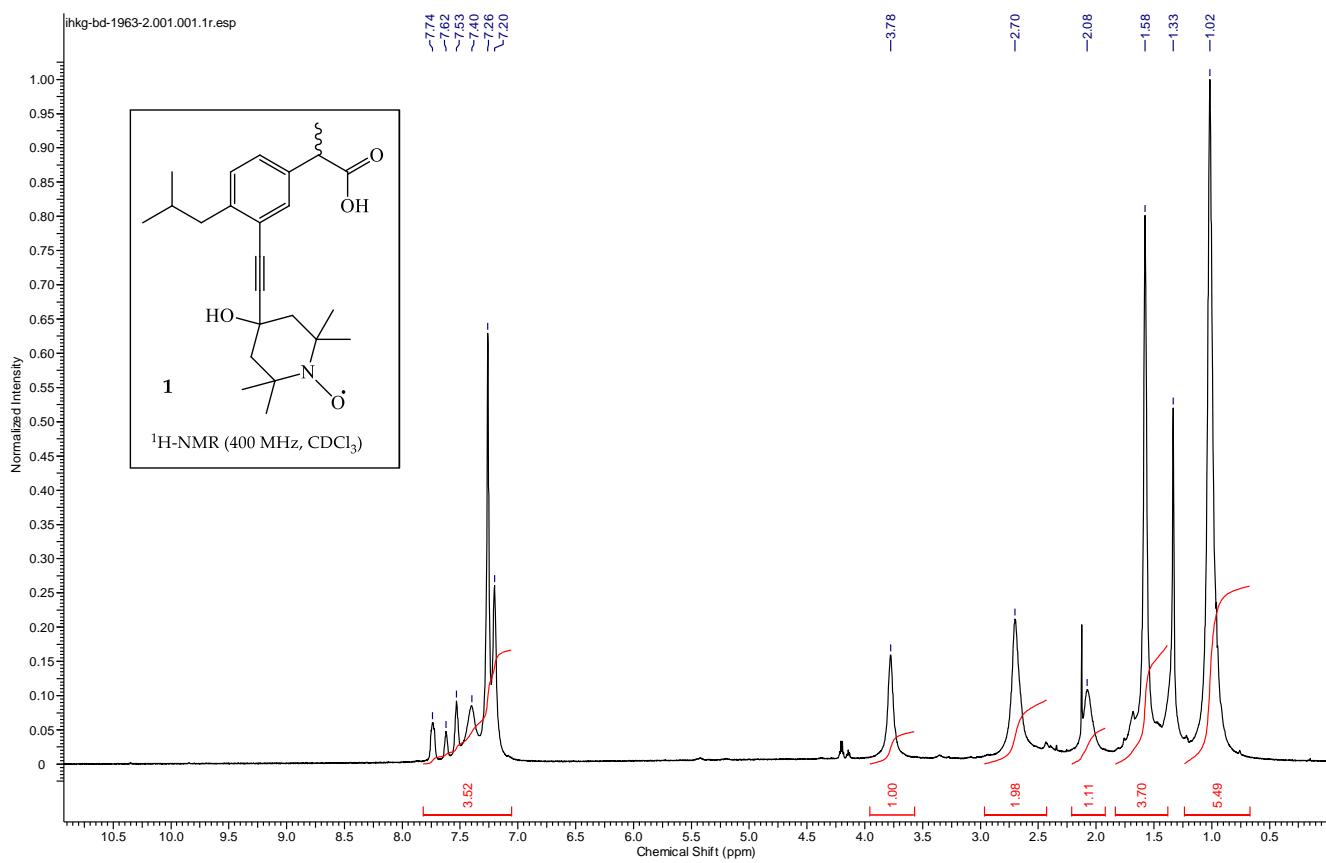


Figure S12. ¹H-NMR spectrum of compound 1.

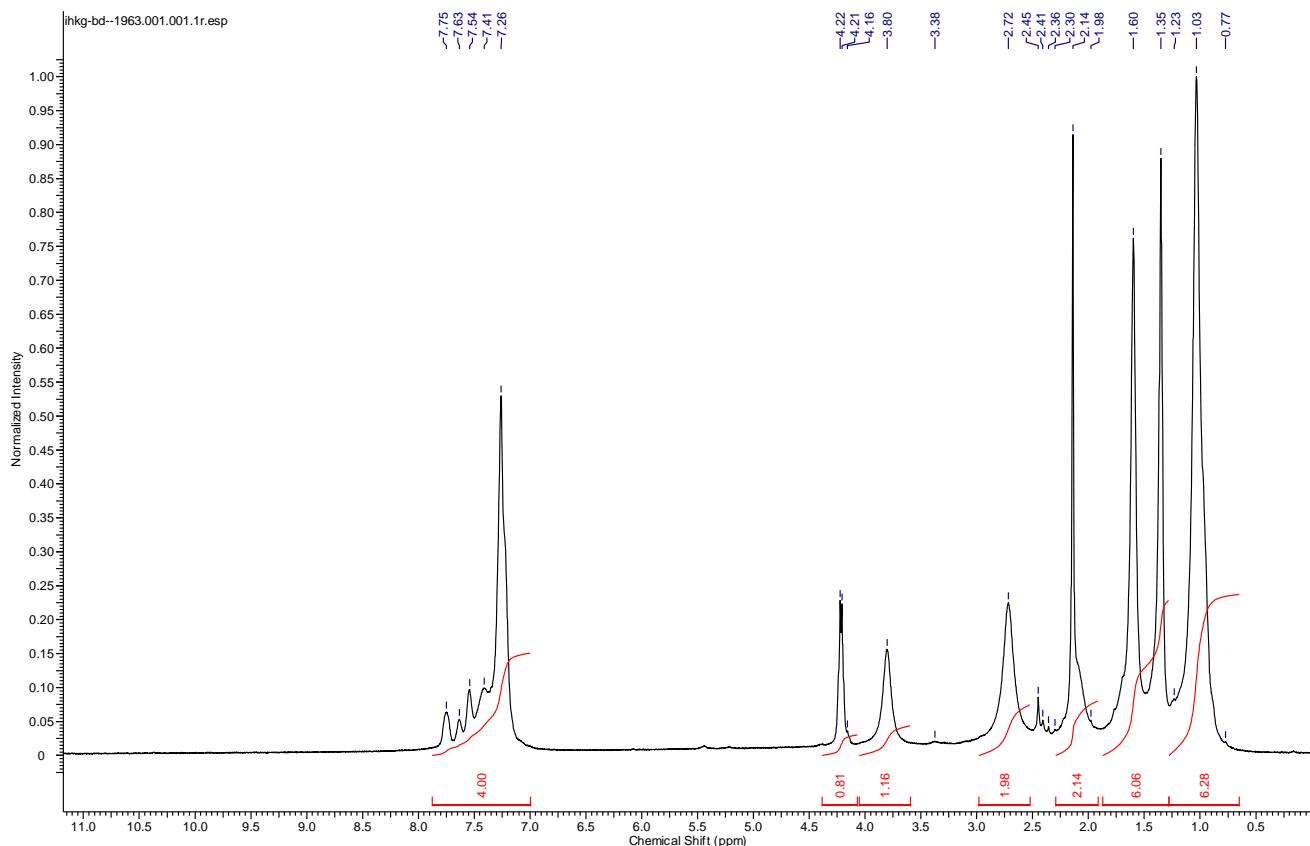


Figure S13. ¹H-NMR spectrum of mixture of compound 1 and ethyl acetate.

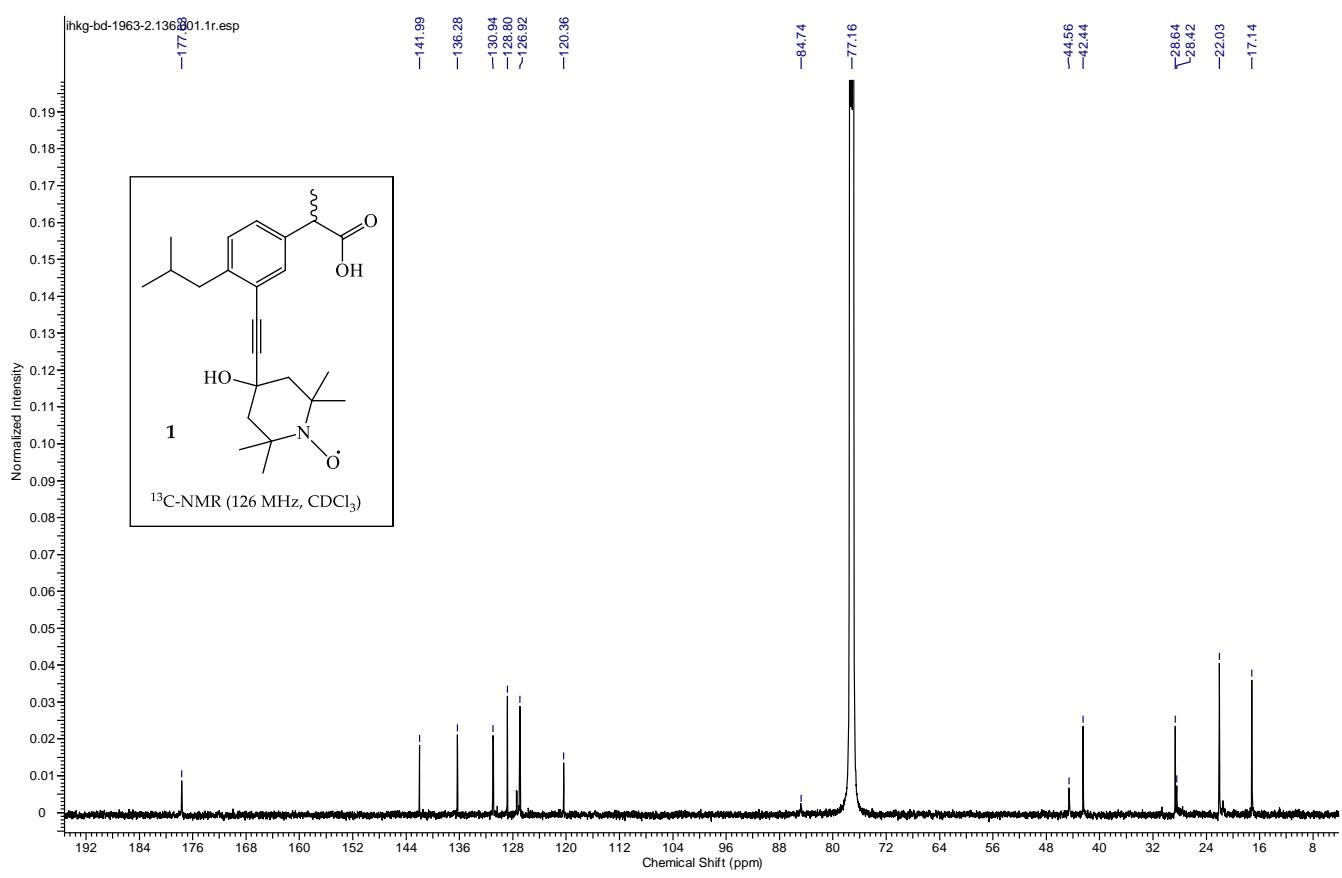


Figure S14. ^{13}C -NMR spectrum of compound **1**.

IR spectra

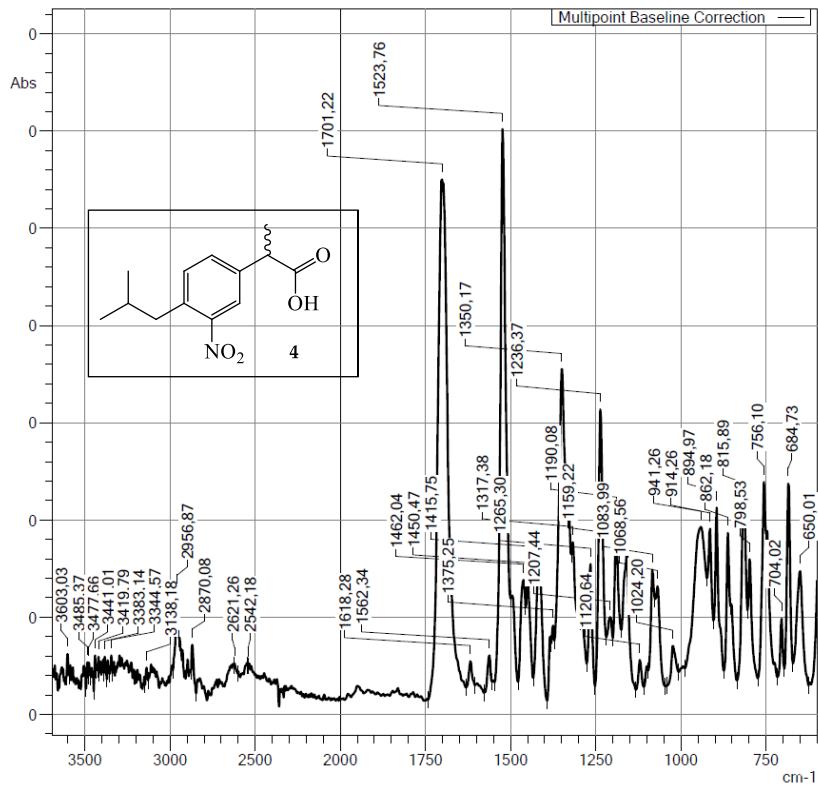


Figure S15. IR spectrum of compound 4.

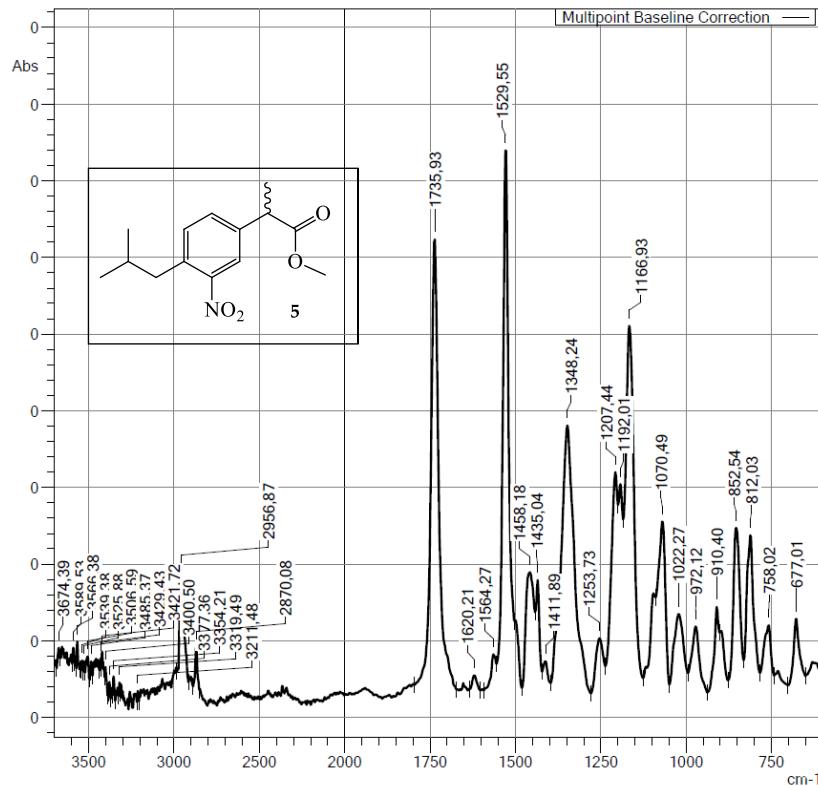


Figure S16. IR spectrum of compound 5.

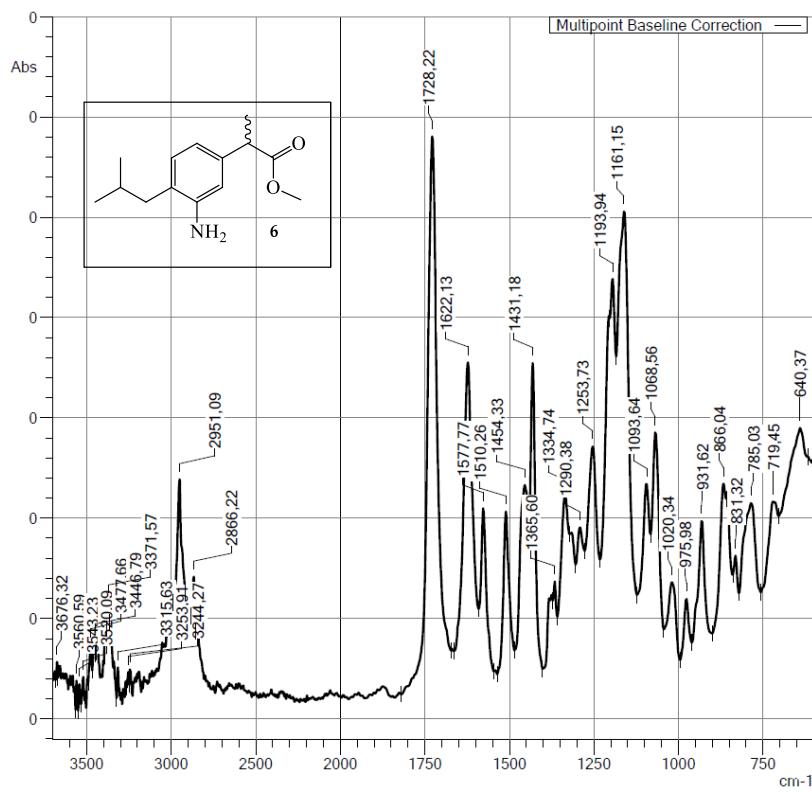


Figure S17. IR spectrum of compound 6.

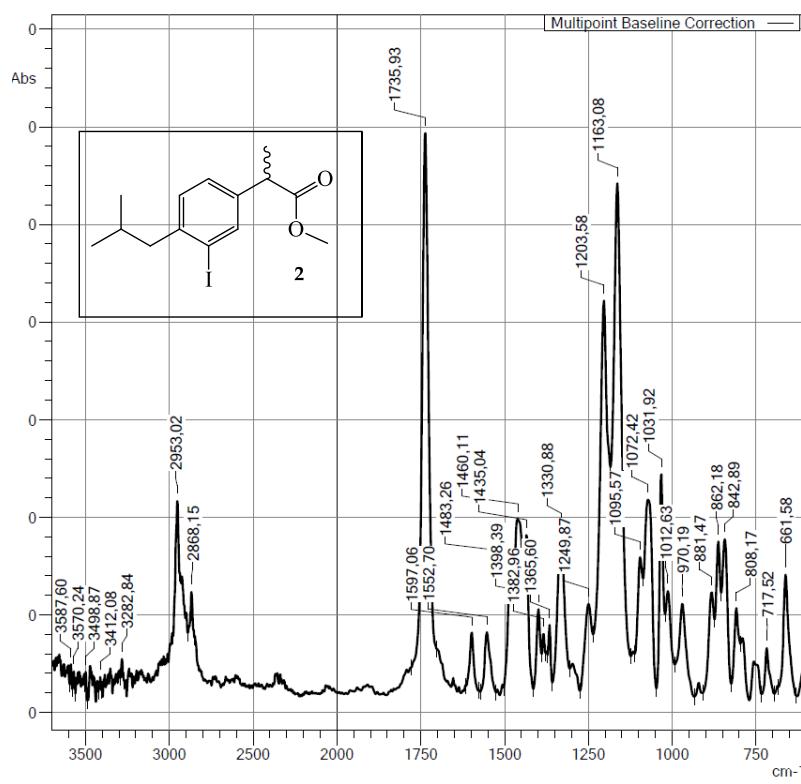


Figure S18. IR spectrum of compound 2.

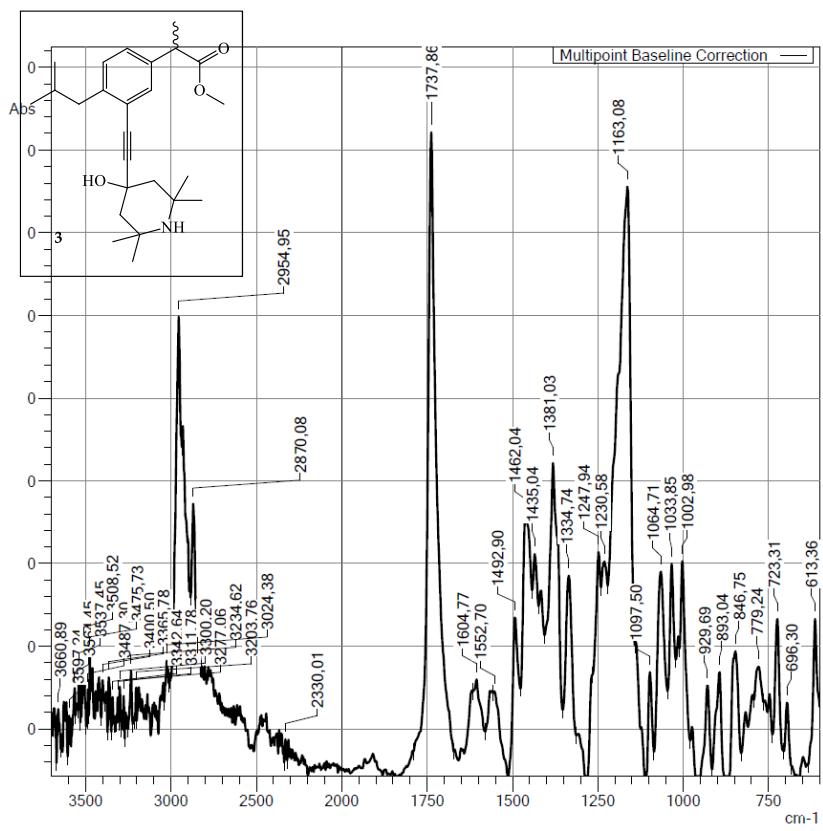


Figure S19. IR spectrum of compound 3.

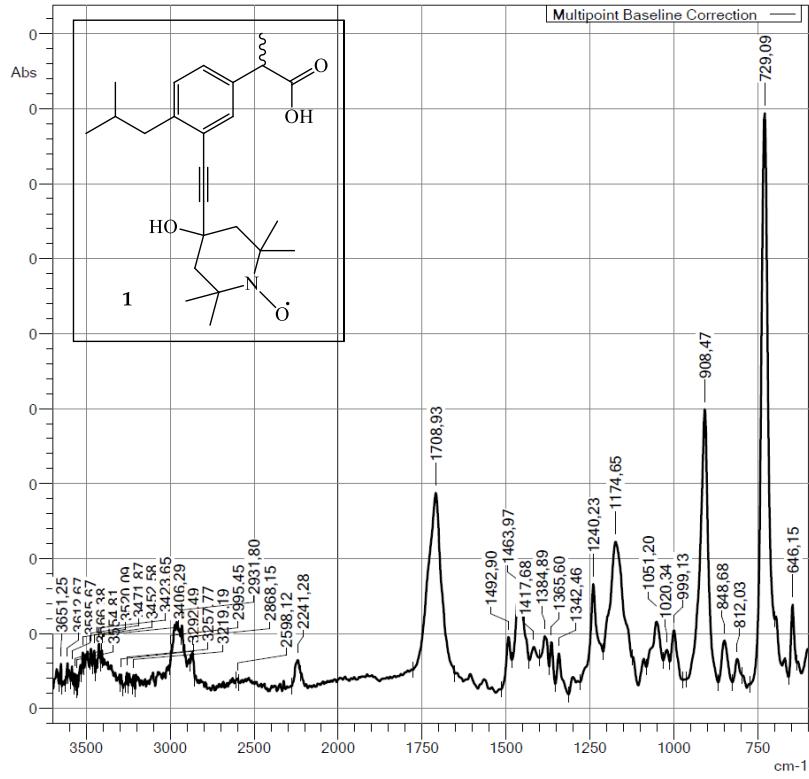


Figure S20. IR spectrum of compound 1.

HRMS spectra

BD-1963_ #62 RT: 3.59 AV: 1 NL: 2.57E6
T: + c EI Full ms [32.50-407.50]

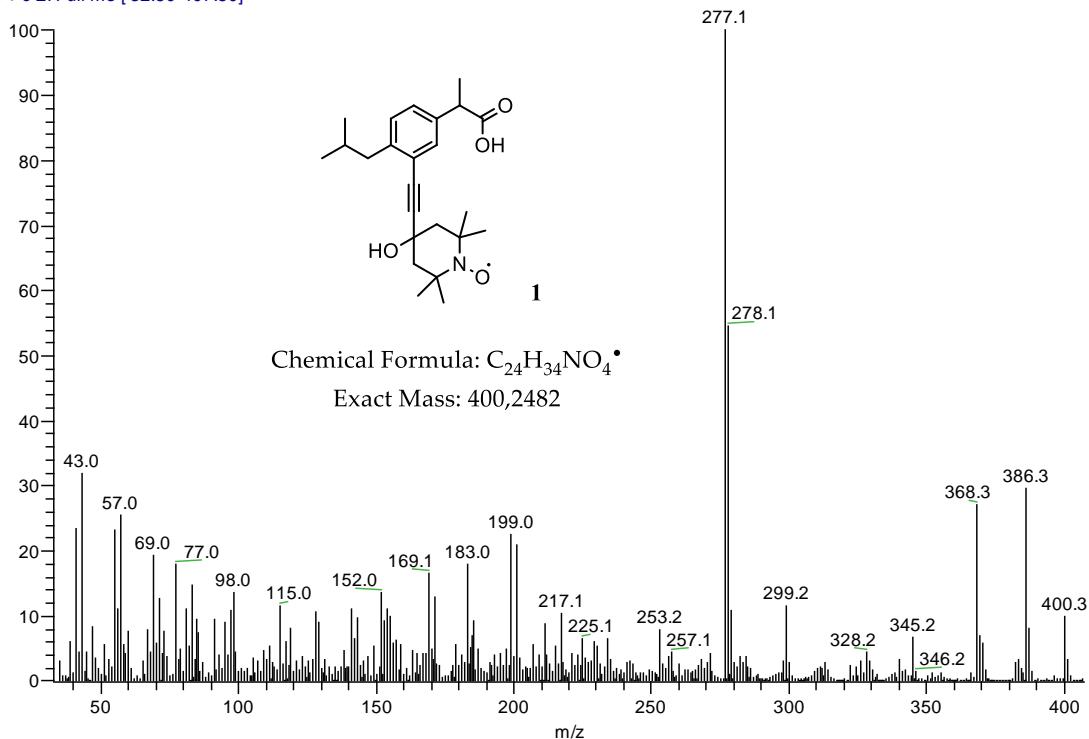


Figure S21. HRMS spectrum of compound 1.

BD-1962_ #12 RT: 0.62 AV: 1 NL: 1.66E6
T: + c EI Full ms [14.50-380.50]

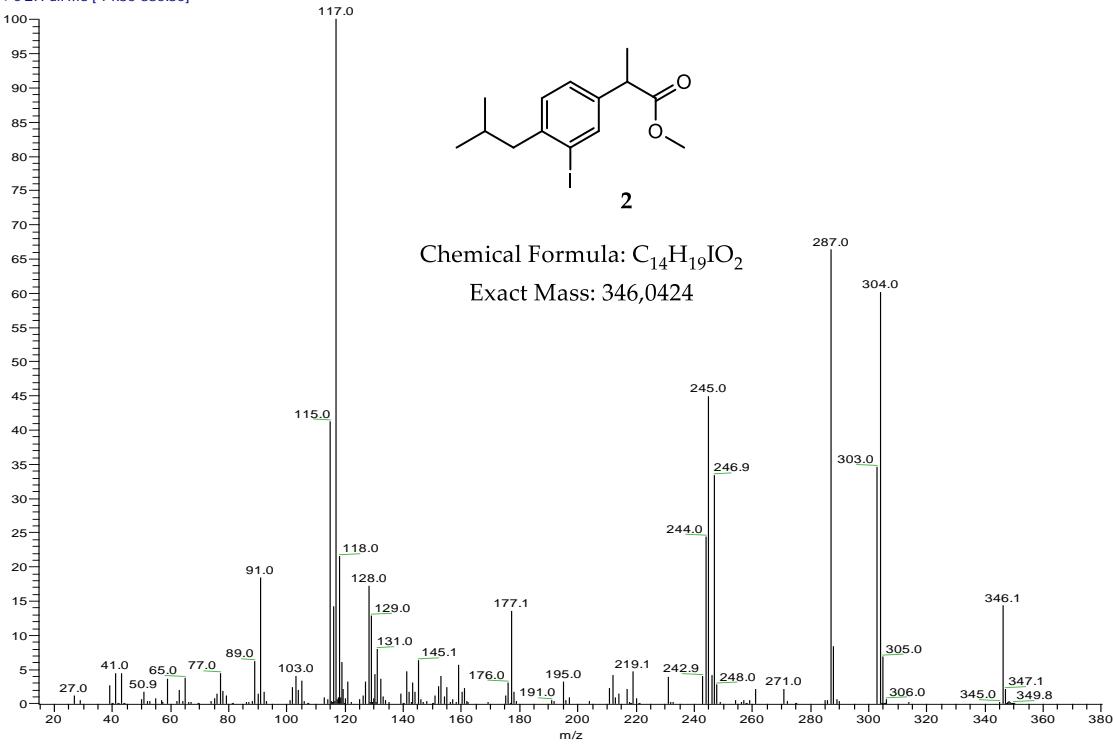


Figure S22. HRMS spectrum of compound 2.

BD-1964 #7 RT: 0.36 AV: 1 NL: 1.94E7
T: + c EI Full ms [32.50-420.50]

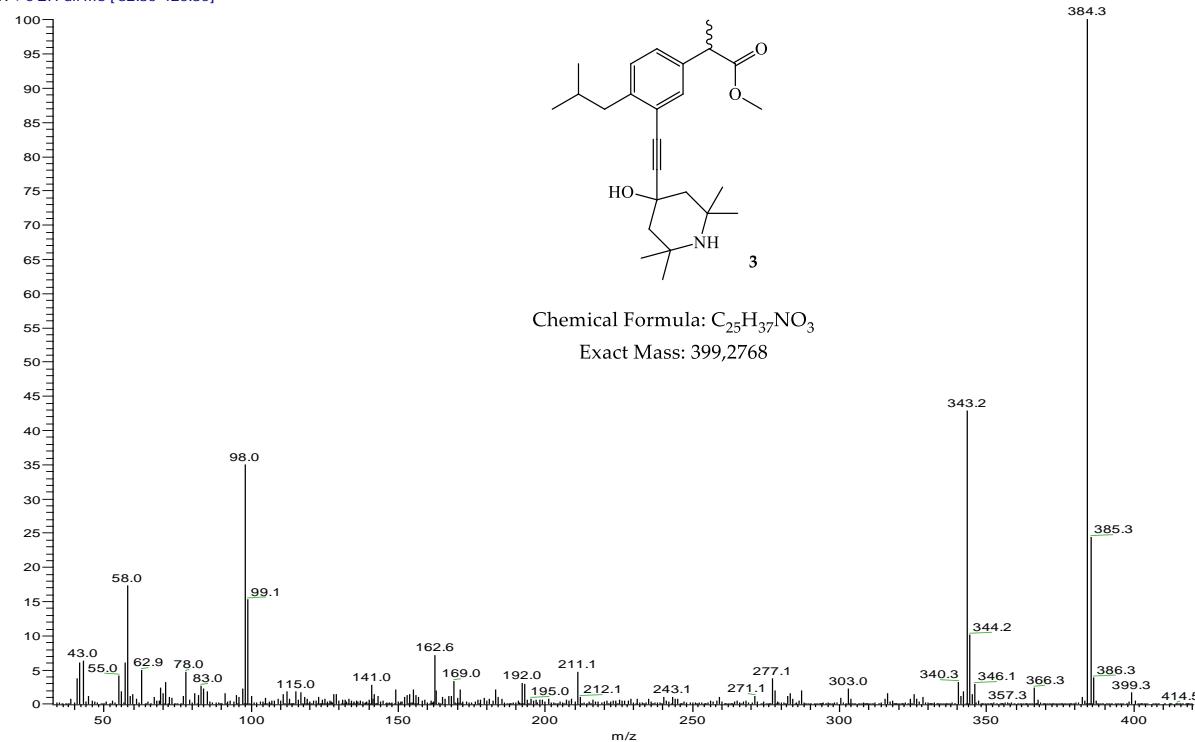


Figure S23. HRMS spectrum of compound 3.

BD-1951 #4 RT: 0.16 AV: 1 NL: 3.88E6
T: + c EI Full ms [32.50-280.50]

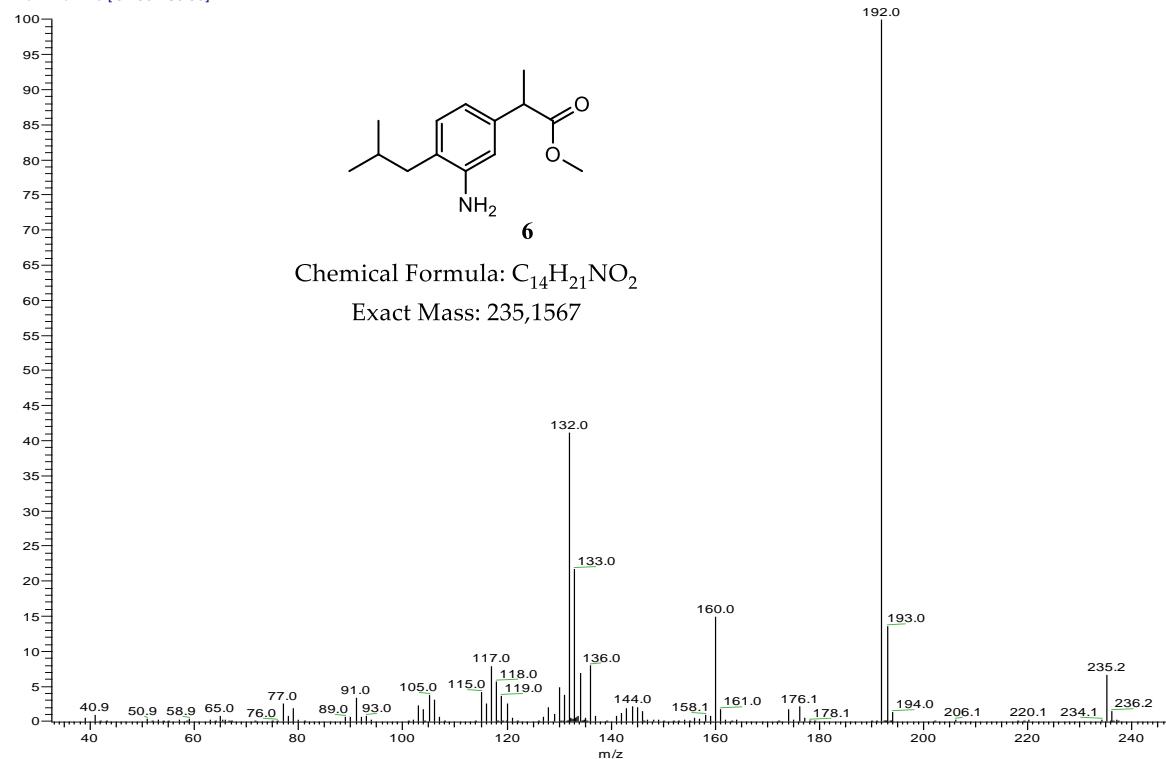


Figure S24. HRMS spectrum of compound 6.