

Decoration of A-ring of a lupane-type triterpenoid with different oxygen and nitrogen heterocycles

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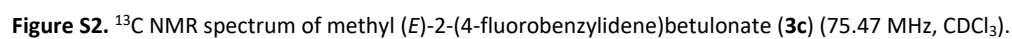
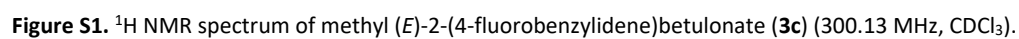
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† J.L.C.S. and H.M.T.A. contributed equally to this work.

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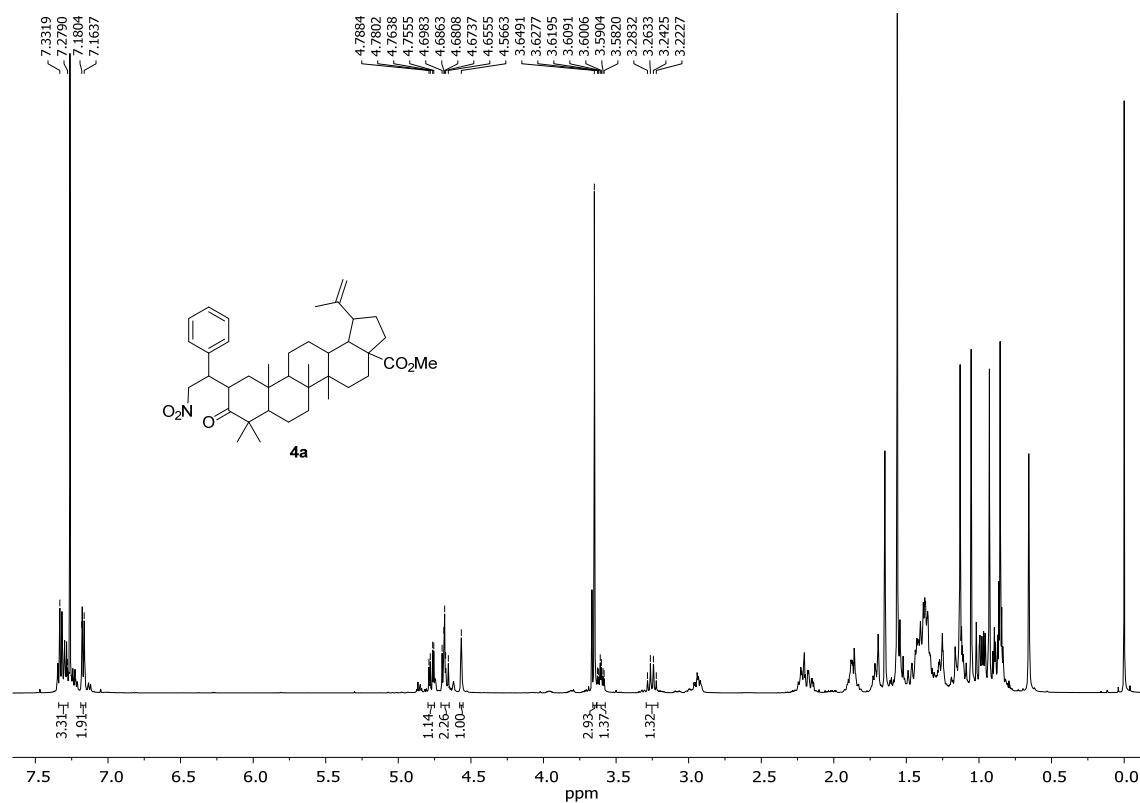


Figure S3. ¹H NMR spectrum of methyl 2-(1-phenyl-2-nitroethyl)betulonate (**4a**) (500.13 MHz, CDCl₃).

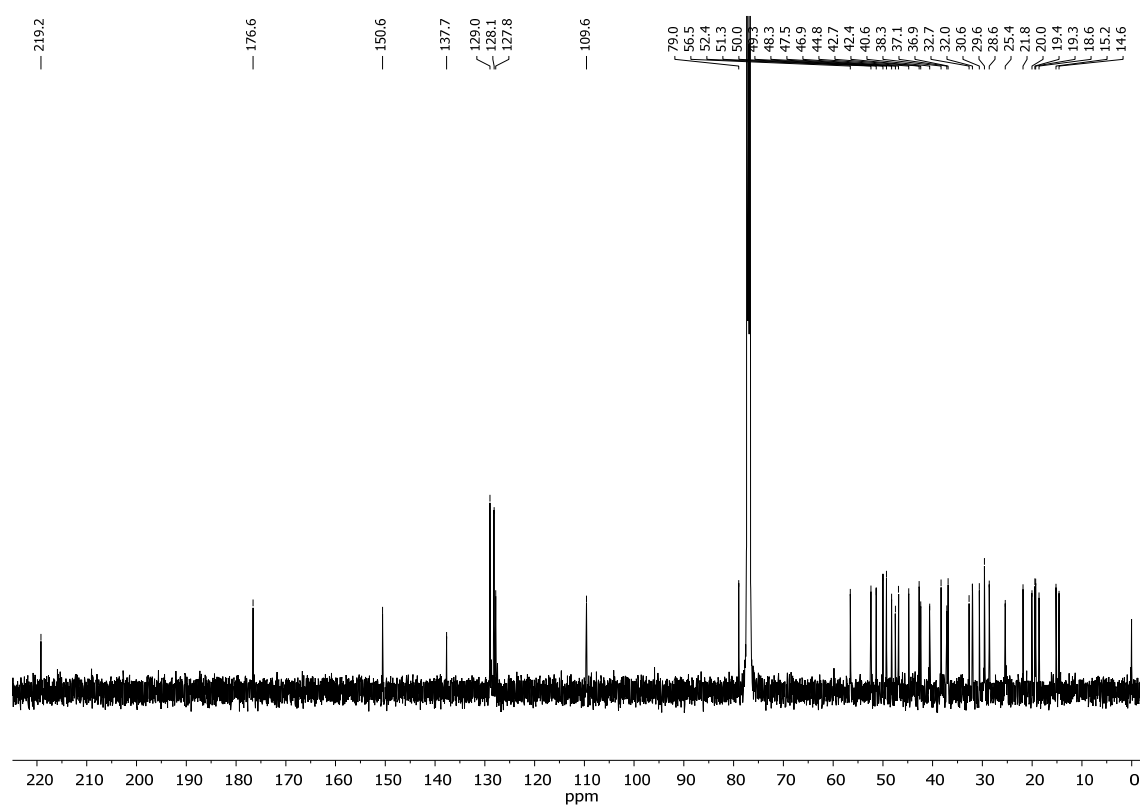


Figure S4. ¹³C NMR spectrum of methyl 2-(1-phenyl-2-nitroethyl)betulonate (**4a**) (125.77 MHz, CDCl₃).

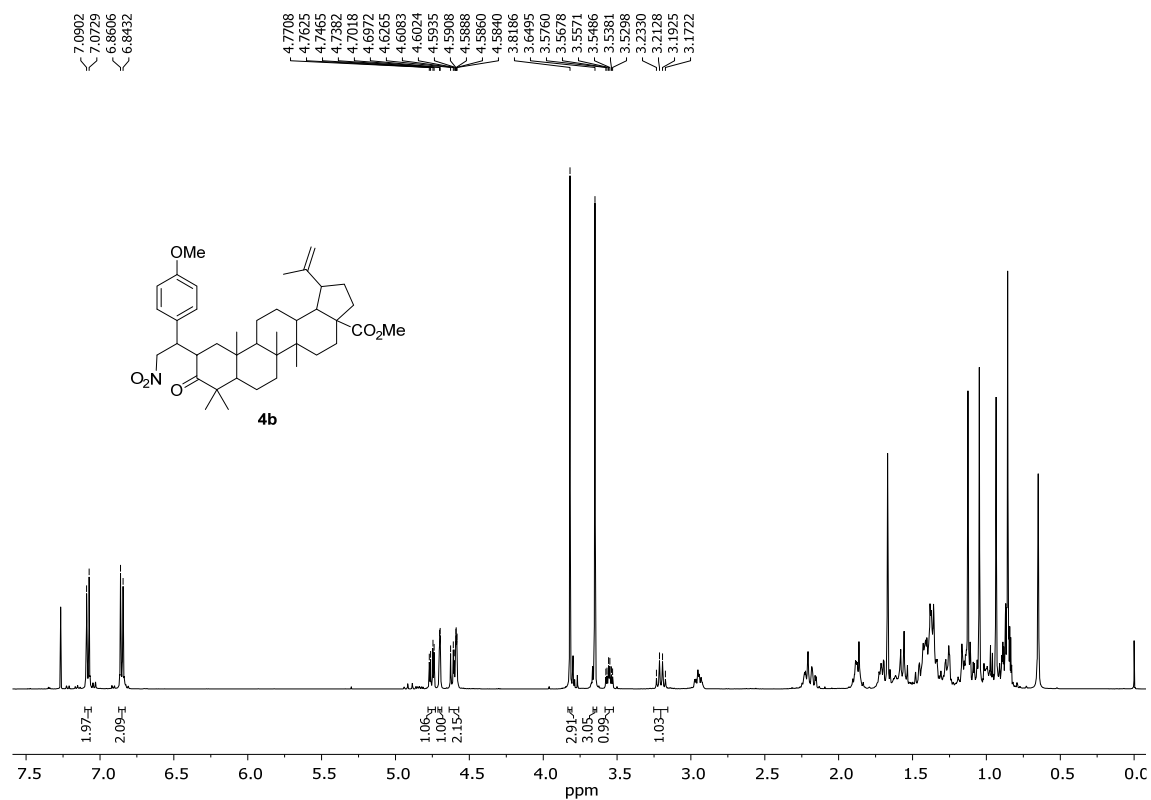


Figure S5. ¹H NMR spectrum of methyl 2-[1-(4-methoxyphenyl)-2-nitroethyl]betulonate (**4b**) (500.13 MHz, CDCl₃).

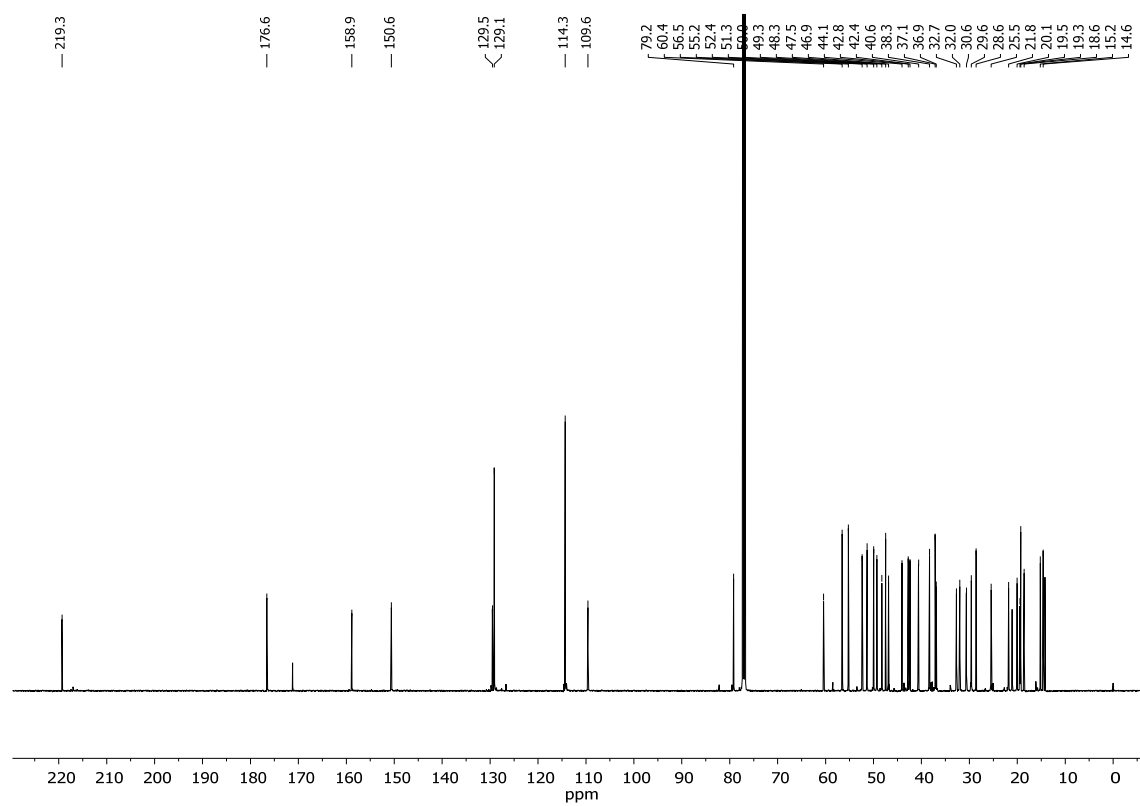


Figure S6. ¹³C NMR spectrum of methyl 2-[1-(4-methoxyphenyl)-2-nitroethyl]betulonate (**4b**) (125.77 MHz, CDCl₃).

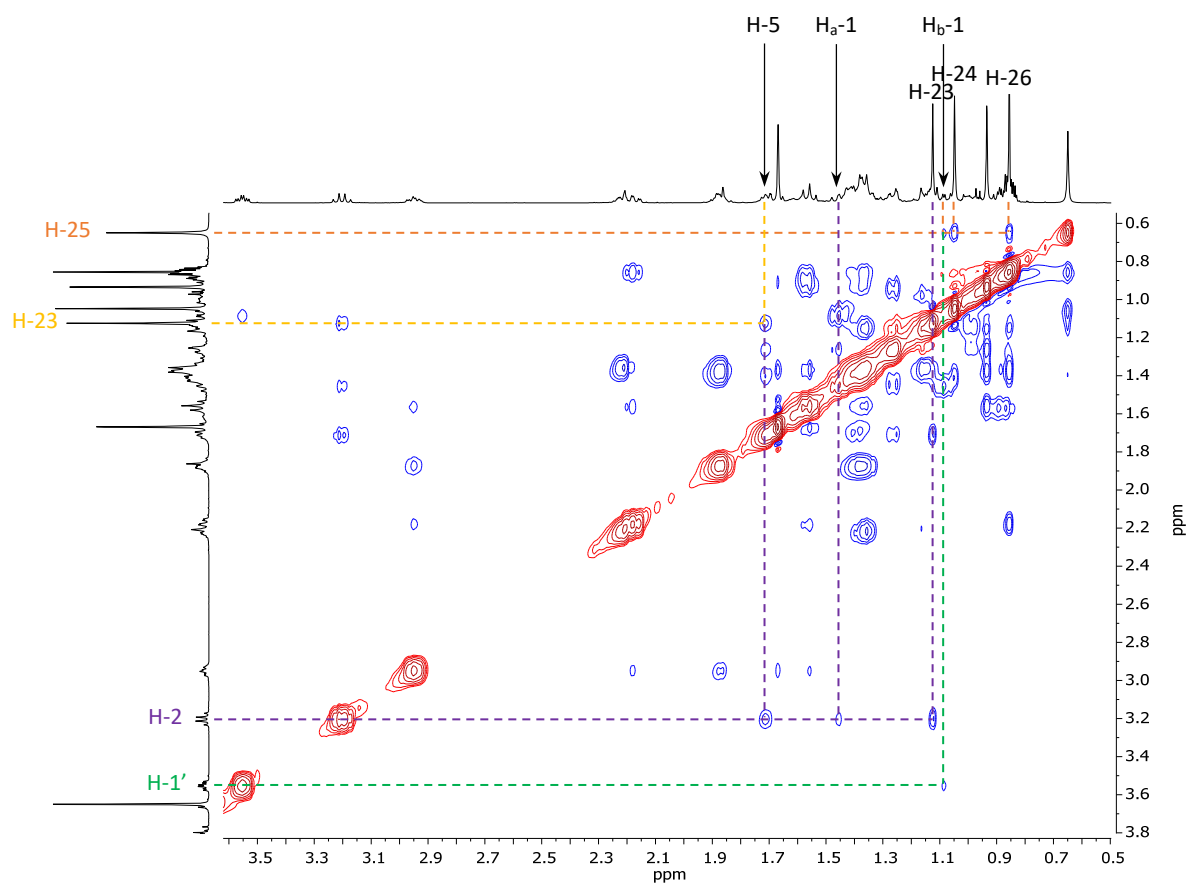
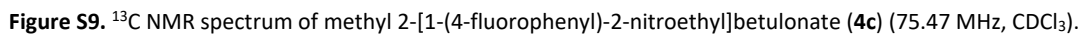
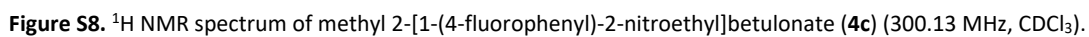


Figure S7. NOESY spectrum of the methyl 2-[1-(4-methoxyphenyl)-2-nitroethyl]betulonate (**4b**) (500.13 MHz, CDCl₃).



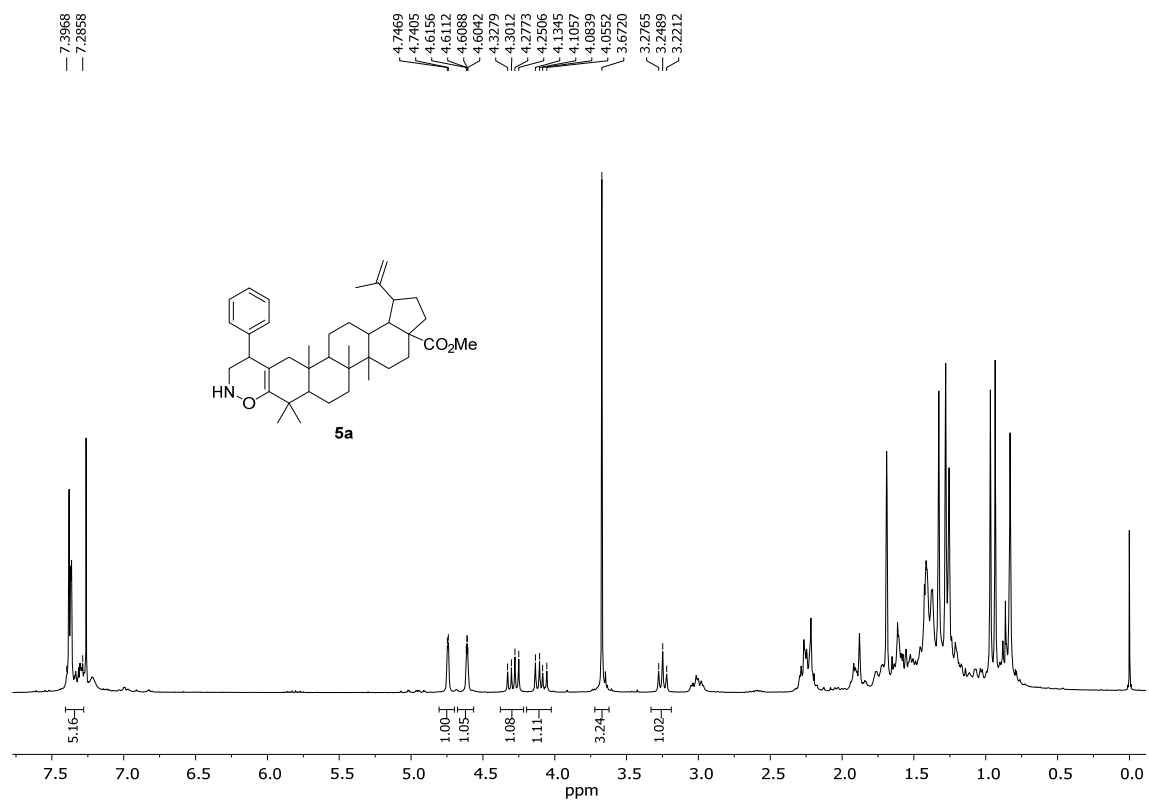


Figure S10. ¹H NMR spectrum of the 4-phenyl-1,2-oxazine-fused BoOMe compound **5a** (300.13 MHz, CDCl₃).

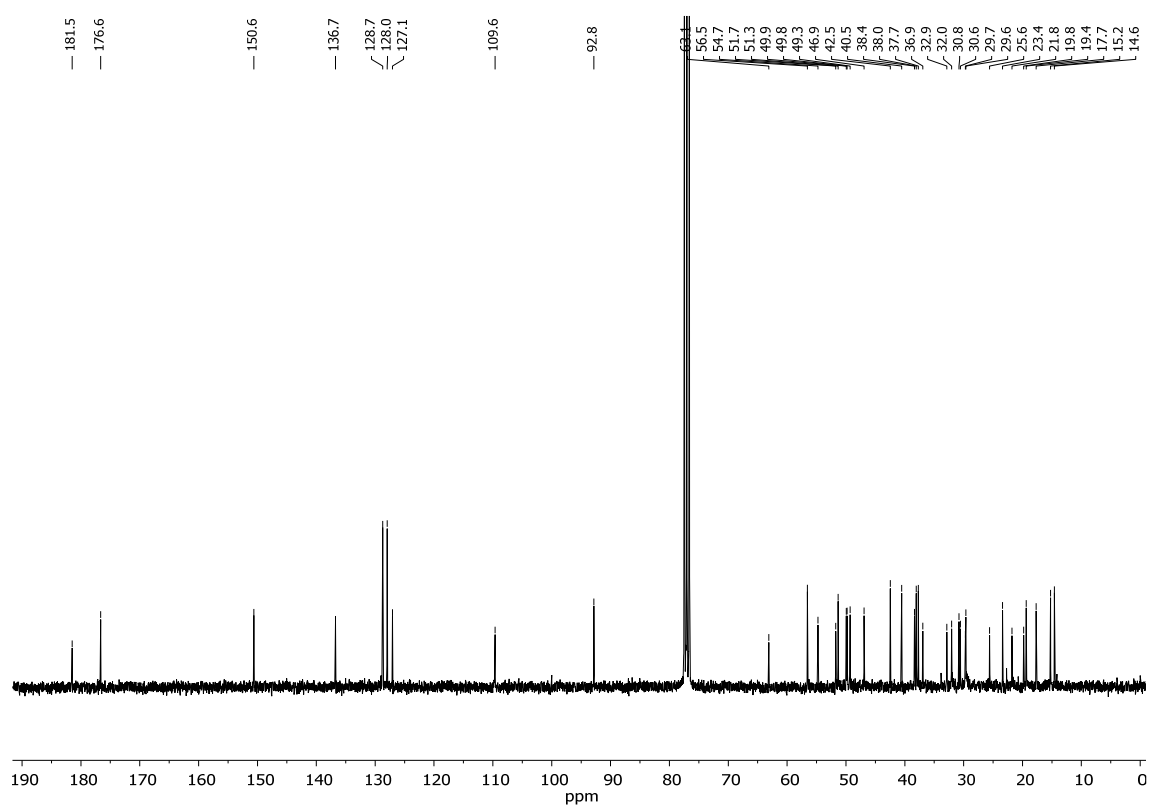


Figure S11. ¹³C NMR spectrum of the 4-phenyl-1,2-oxazine-fused BoOMe compound **5a** (75.47 MHz, CDCl₃).

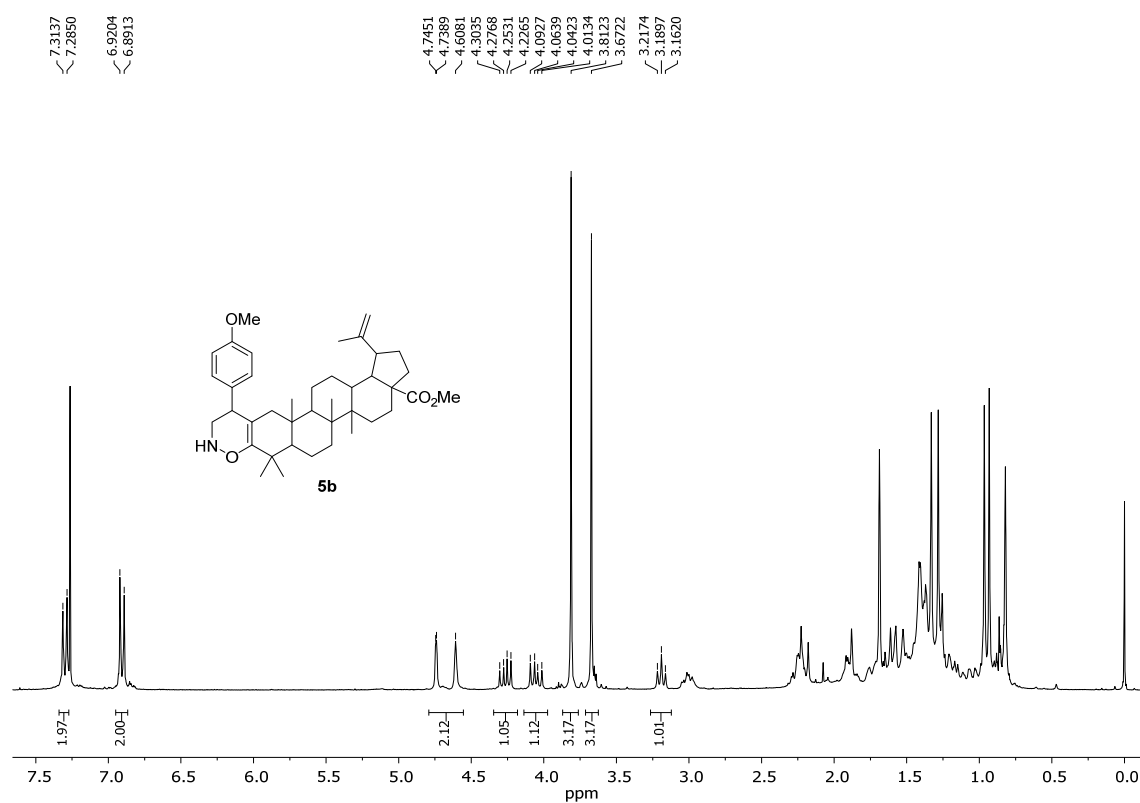


Figure S12. ¹H NMR spectrum of the 4-(4-methoxyphenyl)-1,2-oxazine-fused BoOMe compound **5b** (300.13 MHz, CDCl₃).

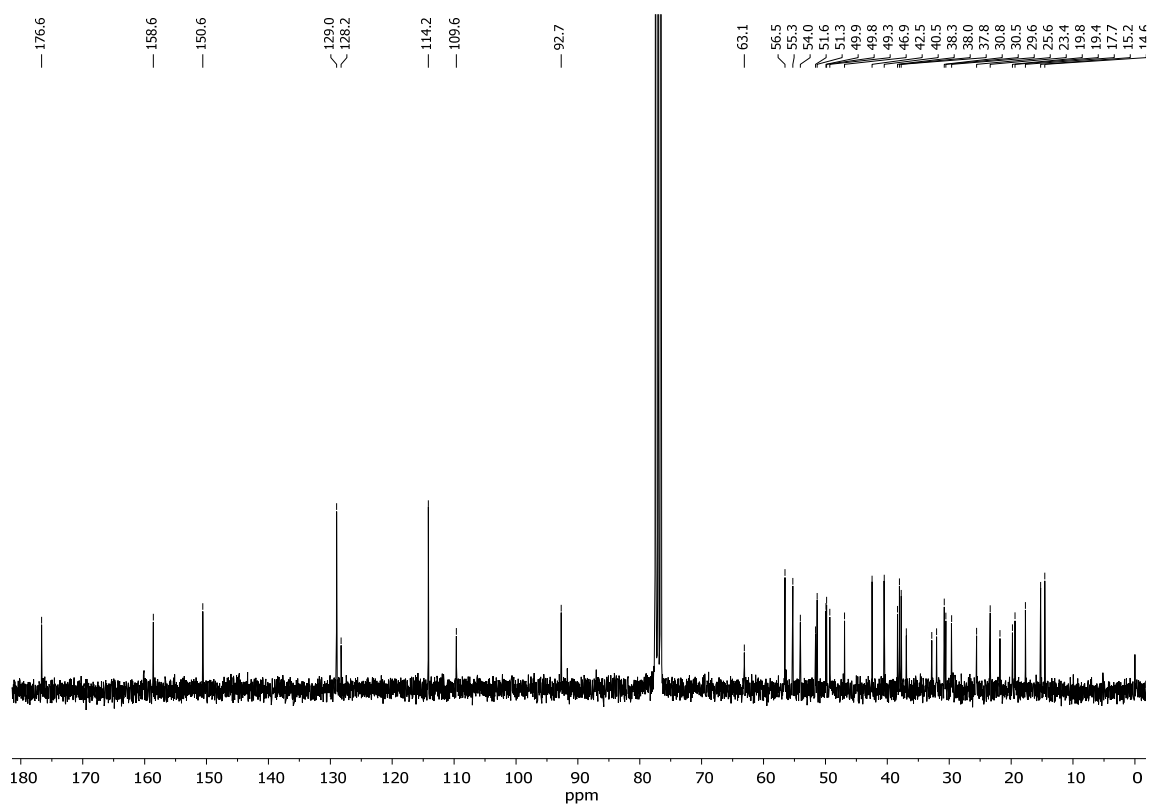


Figure S13. ¹³C NMR spectrum of the 4-(4-methoxyphenyl)-1,2-oxazine-fused BoOMe compound **5b** (75.47 MHz, CDCl₃).

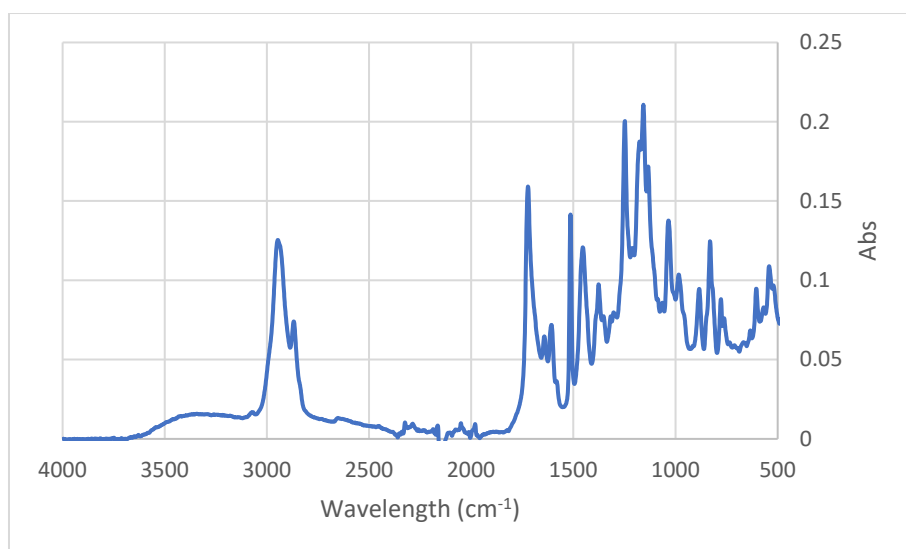


Figure S14. ATR-FTIR spectrum of the 4-(4-methoxyphenyl)-1,2-oxazine-fused BoOMe compound **5b** (FTIR Bruker Tensor 27, with ATR Golden Gate accessory, Diamond (Specac), Absorbance mode, resolution 4 cm⁻¹, 256 scans, 4000-500 cm⁻¹).

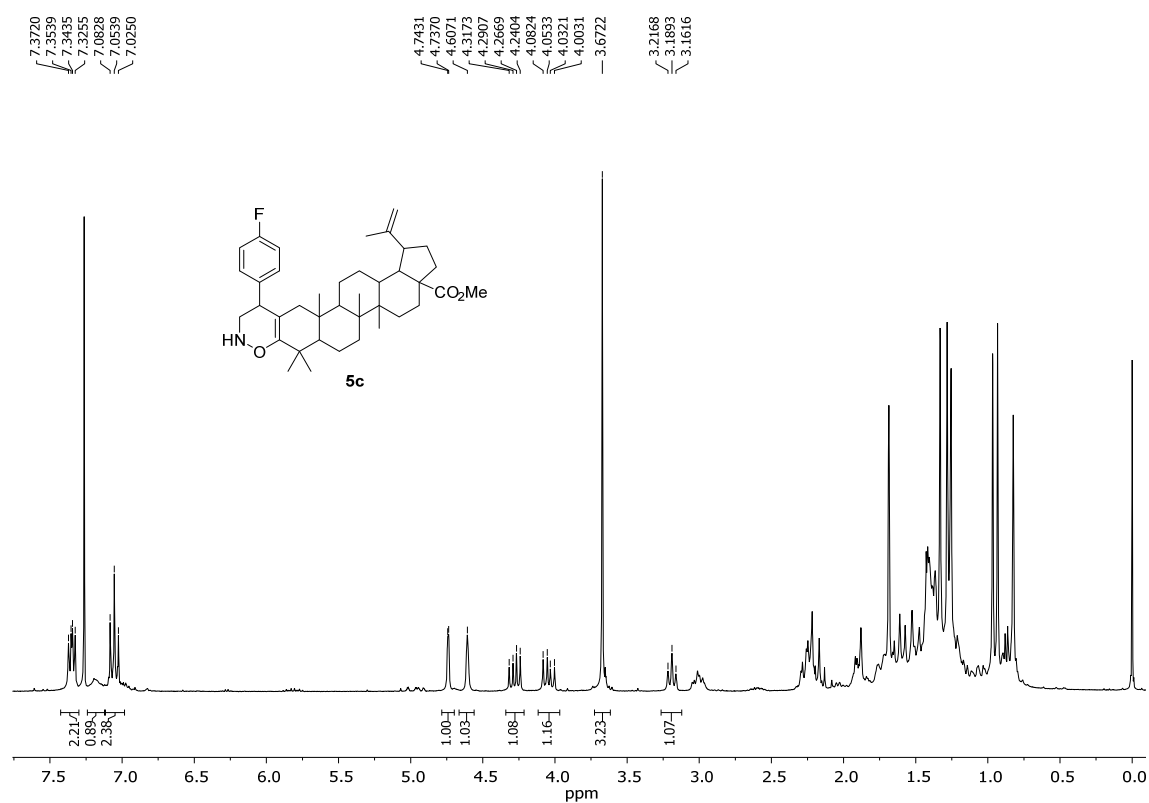


Figure S15. ¹H NMR spectrum of the 4-(4-fluorophenyl)-1,2-oxazine-fused BoOMe compound **5c** (300.13 MHz, CDCl₃).

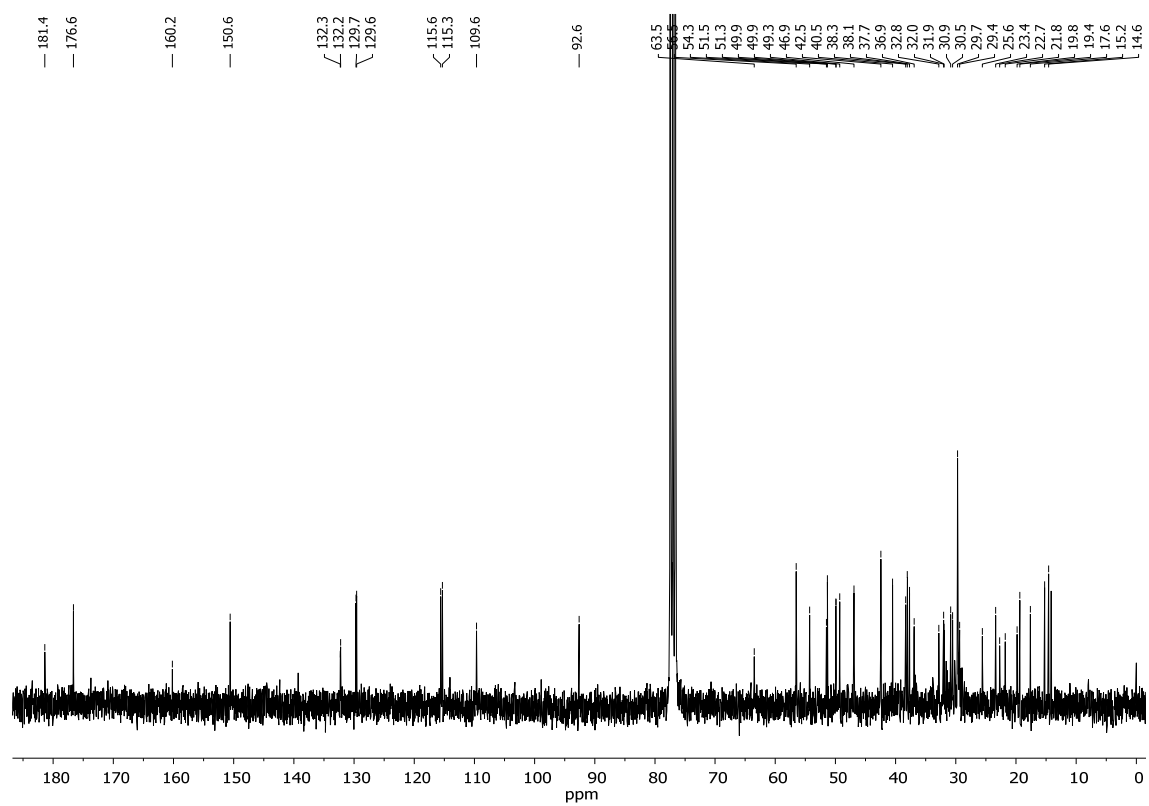


Figure S16. ¹³C NMR spectrum of the 4-(4-fluorophenyl)-1,2-oxazine-fused BoOMe compound **5c** (75.47 MHz, CDCl₃).

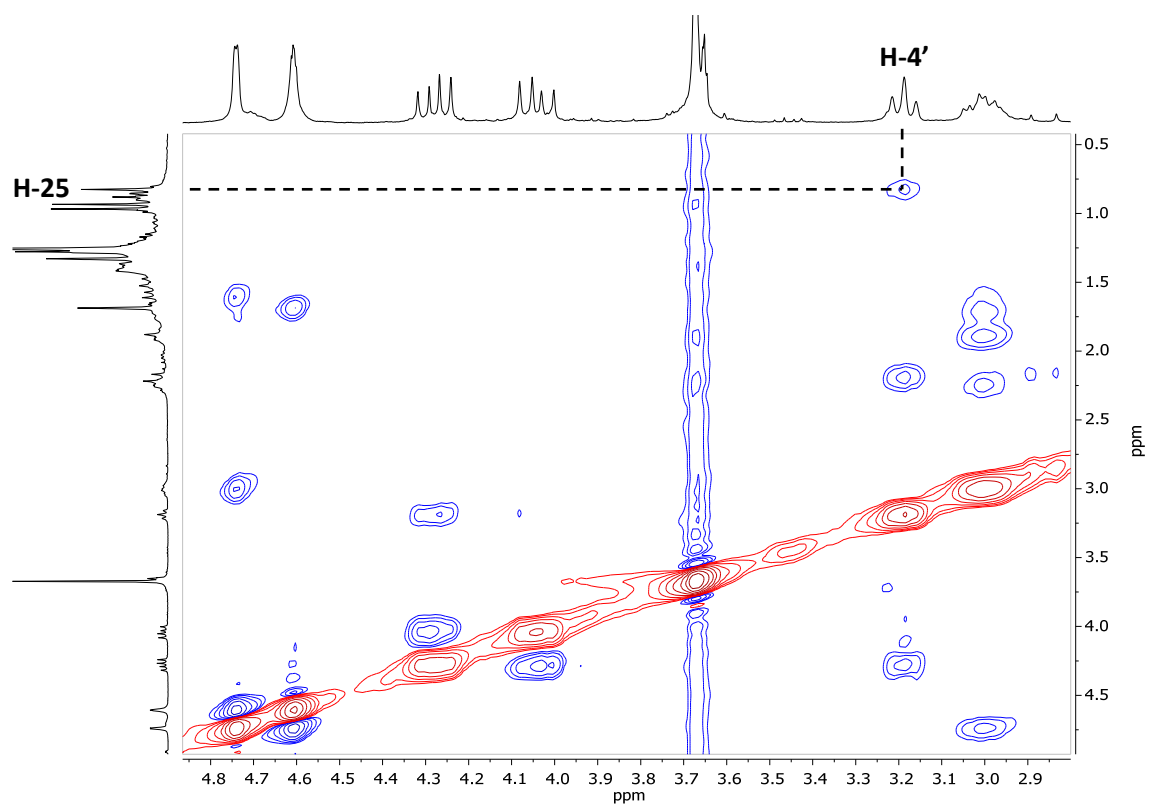


Figure S17. NOESY spectrum of the 4-(4-fluorophenyl)-1,2-oxazine-fused BoOMe compound **5c** (300.13 MHz, CDCl₃).

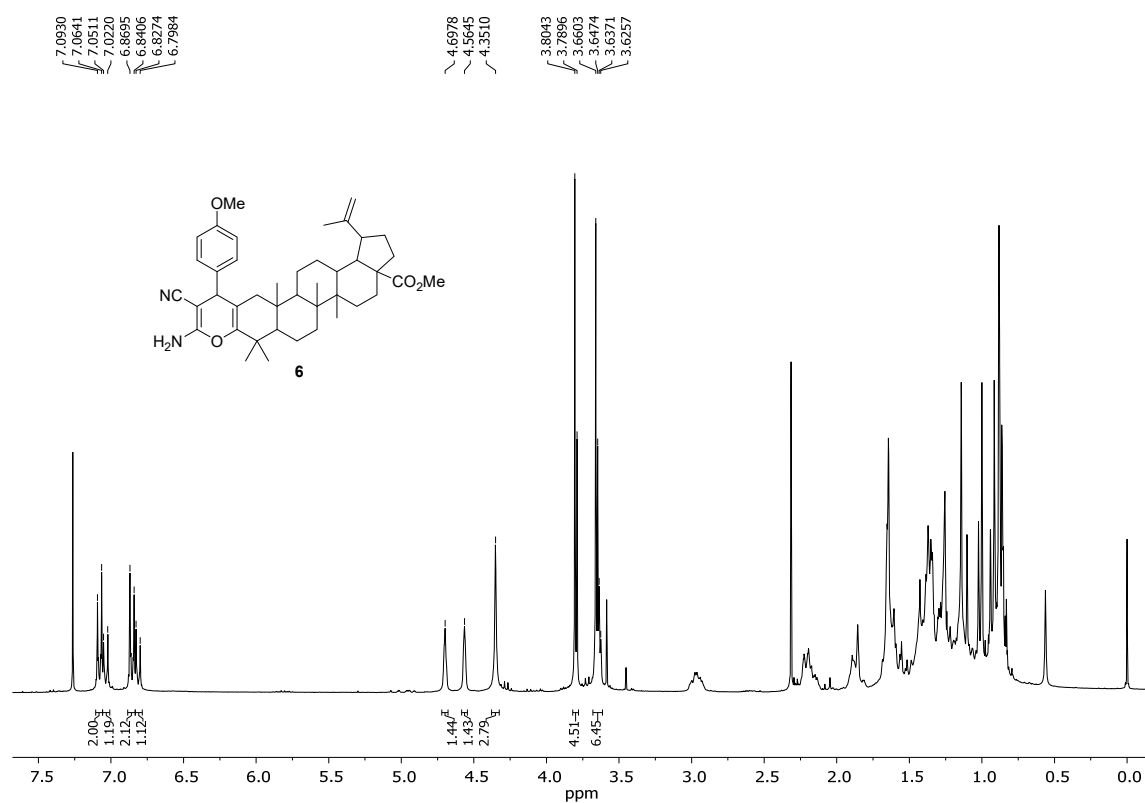


Figure S18. ¹H NMR spectrum of the pyran-fused BoOMe compound **6** (300.13 MHz, CDCl₃).

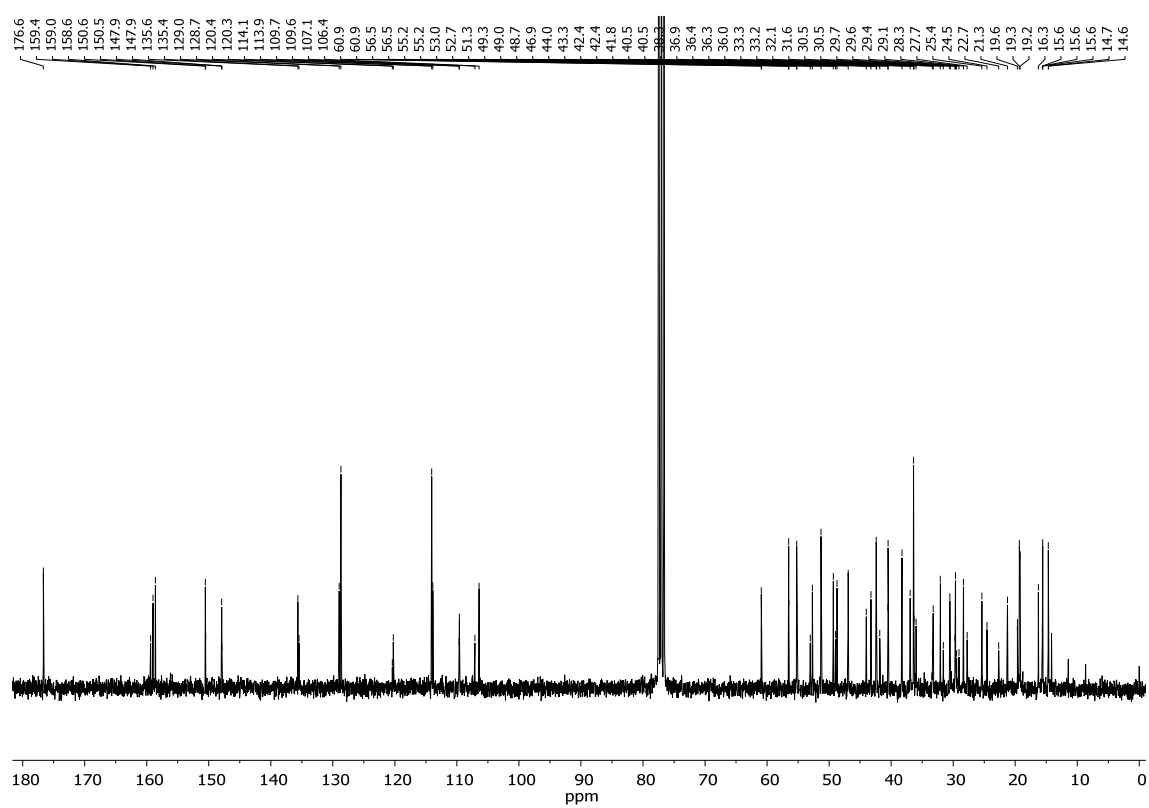


Figure S19. ¹³C NMR spectrum of the pyran-fused BoOMe compound **6** (75.47 MHz, CDCl₃).

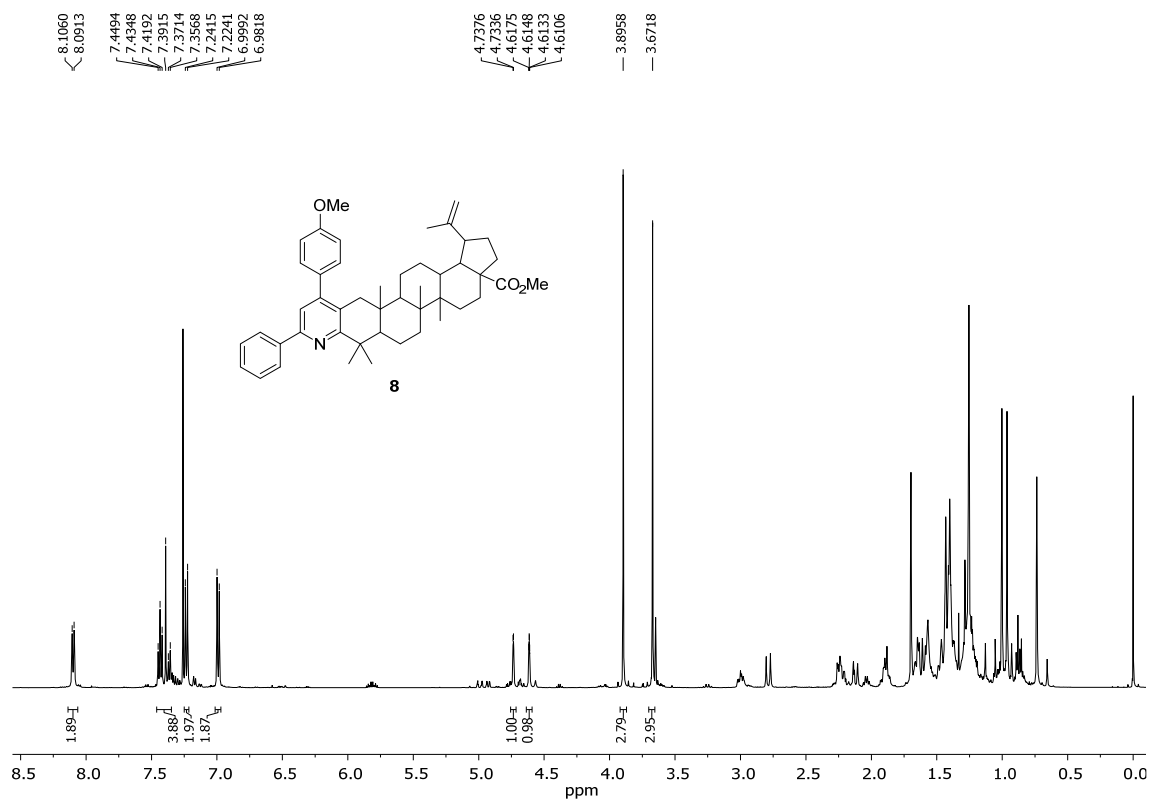


Figure S20. ¹H NMR spectrum of the diarylpyridine-fused BoOMe compound **8** (500.13 MHz, CDCl₃).

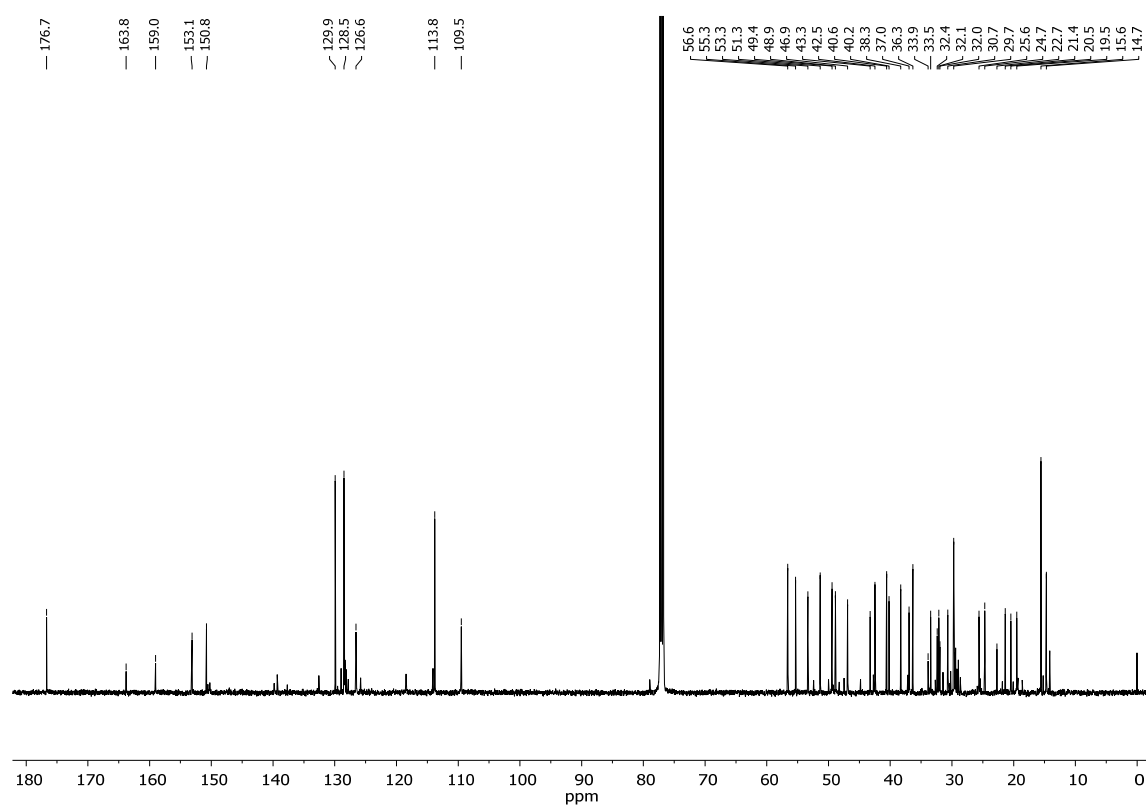


Figure S21. ¹³C NMR spectrum of the diarylpyridine-fused BoOMe compound **8** (125.77 MHz, CDCl₃).

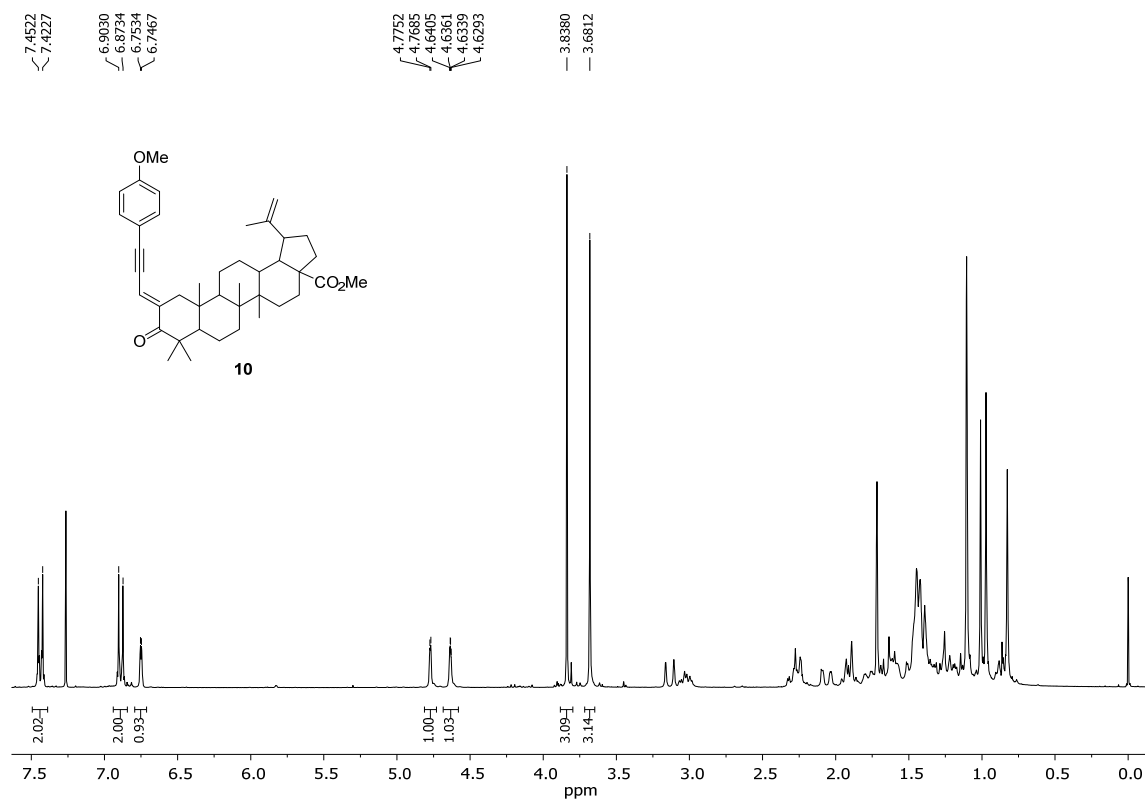


Figure S22. ¹H NMR spectrum of methyl (*E*)-2-[3-(4-methoxyphenyl)prop-2-yn-1-ylidene]betulonate (**10**) (300.13 MHz, CDCl₃).

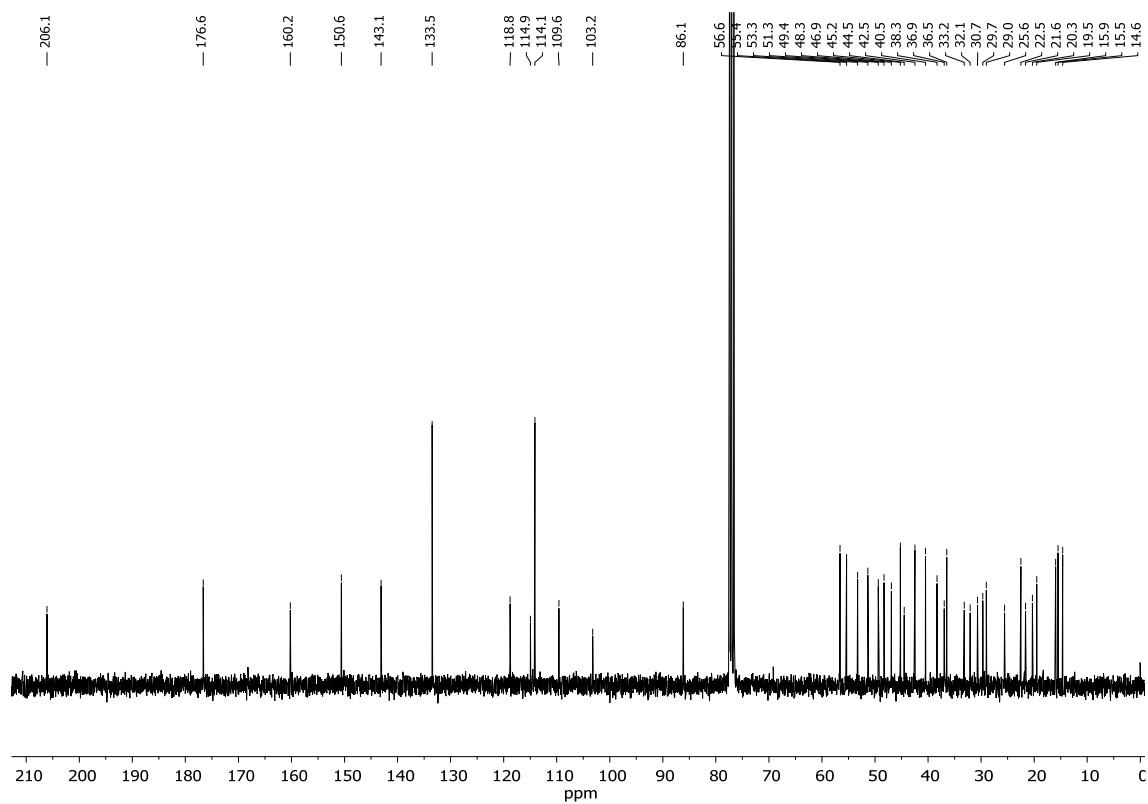


Figure S23. ¹³C NMR spectrum of methyl (*E*)-2-[3-(4-methoxyphenyl)prop-2-yn-1-ylidene]betulonate (**10**) (75.47 MHz, CDCl₃).

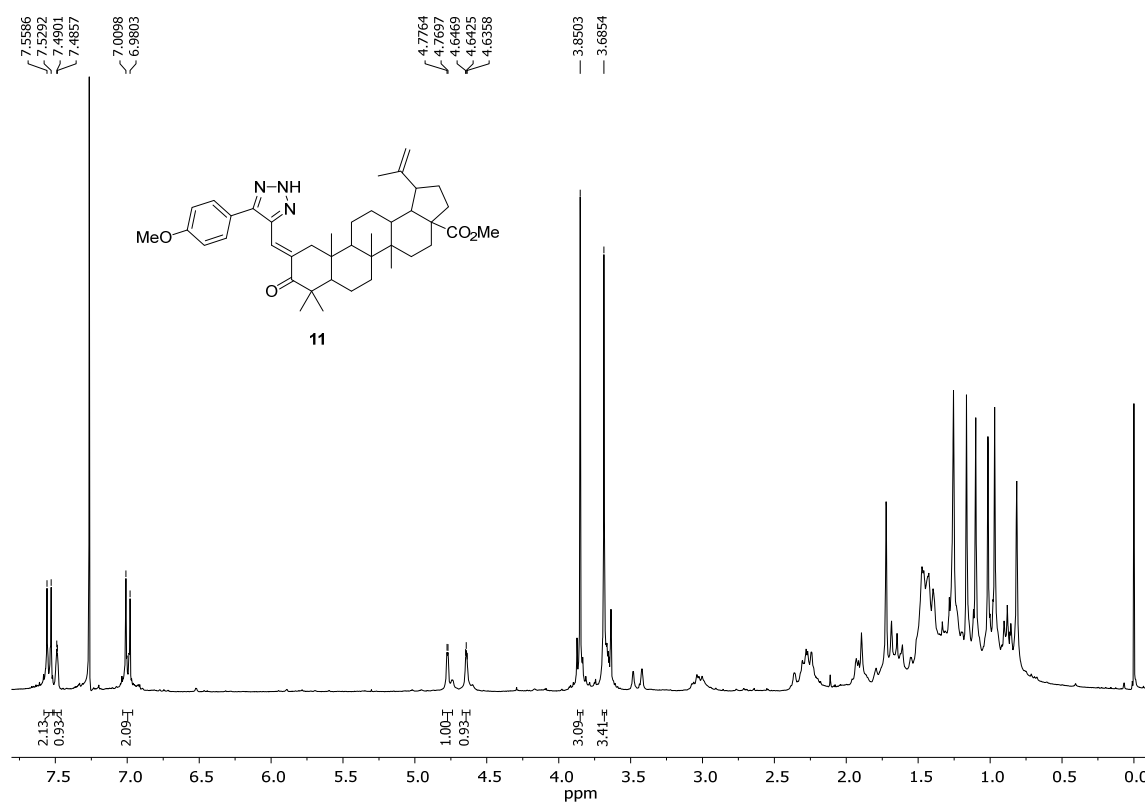


Figure S24. ^1H NMR spectrum of the 1,2,3-triazole–BoOMe compound **11** (300.13 MHz, CDCl_3).

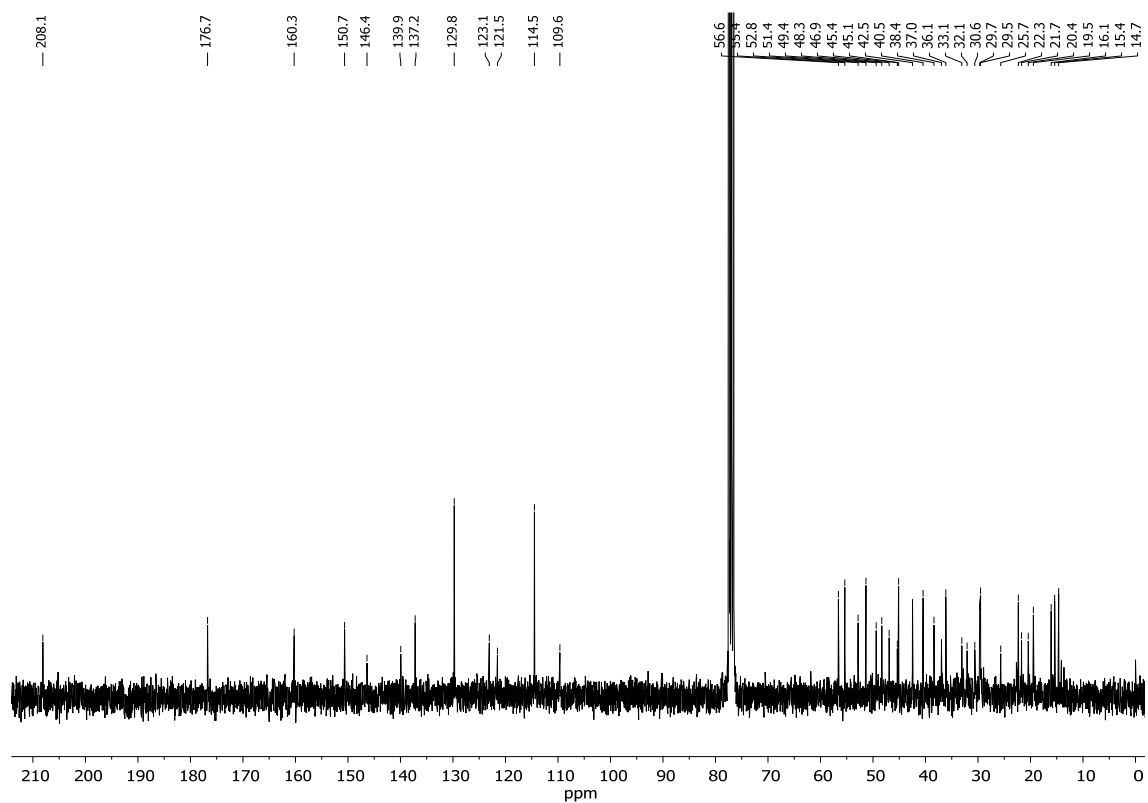


Figure S25. ^{13}C NMR spectrum of the 1,2,3-triazole–BoOMe compound **11** (75.47 MHz, CDCl_3).