

Supporting Information

Synthesis and Structural Analysis of Chiral Bis-dihydro[1,3]-naphthoxazines and Imidazolidine Derivatives Prepared by Three-Component Mannich-Type Condensation

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NMR and HRMS Spectra of compound **3**

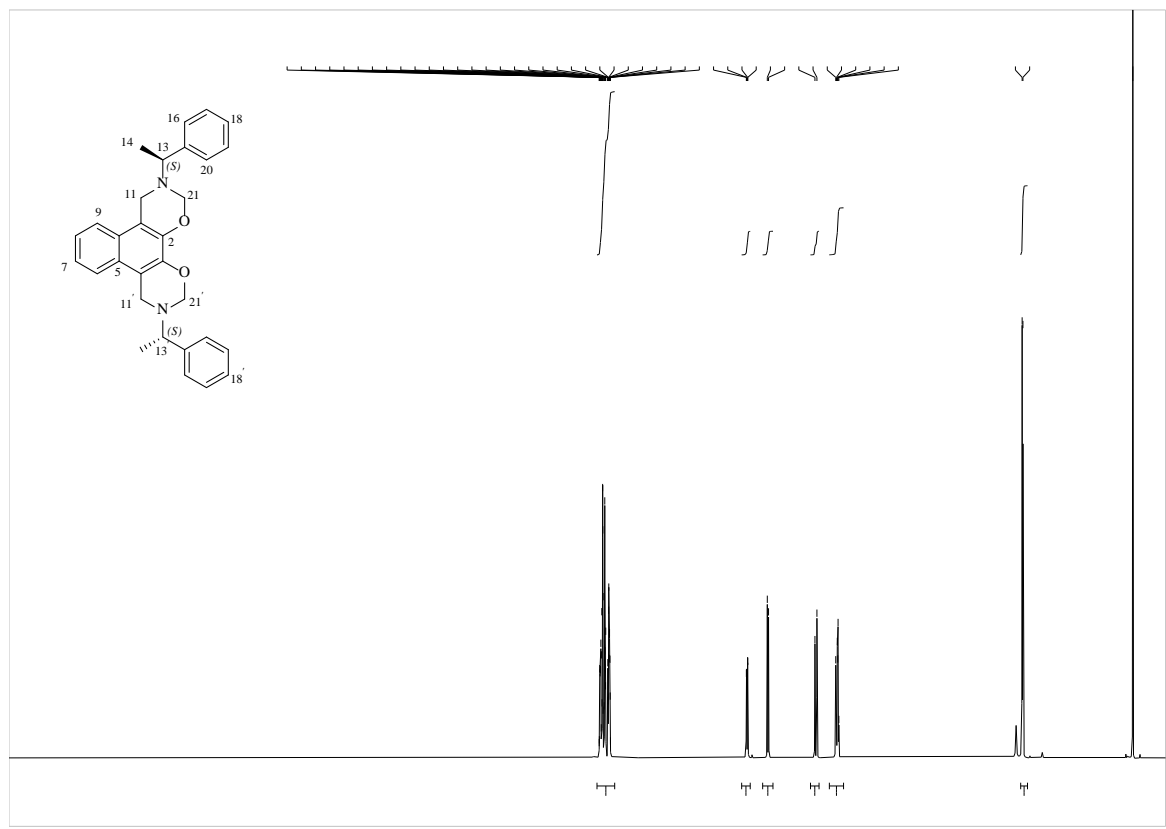


Figure S1. The ^1H NMR spectrum of compound **3**.

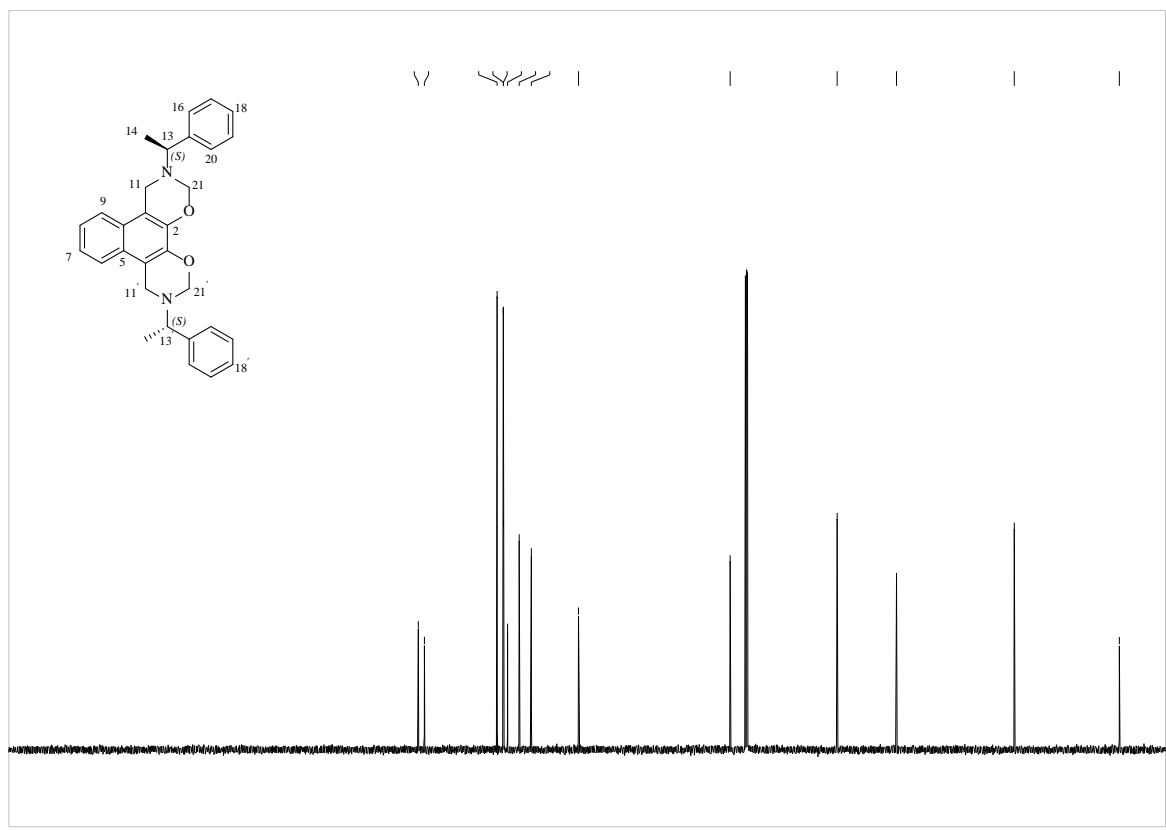


Figure S2. The ^{13}C NMR spectrum of compound **3**.

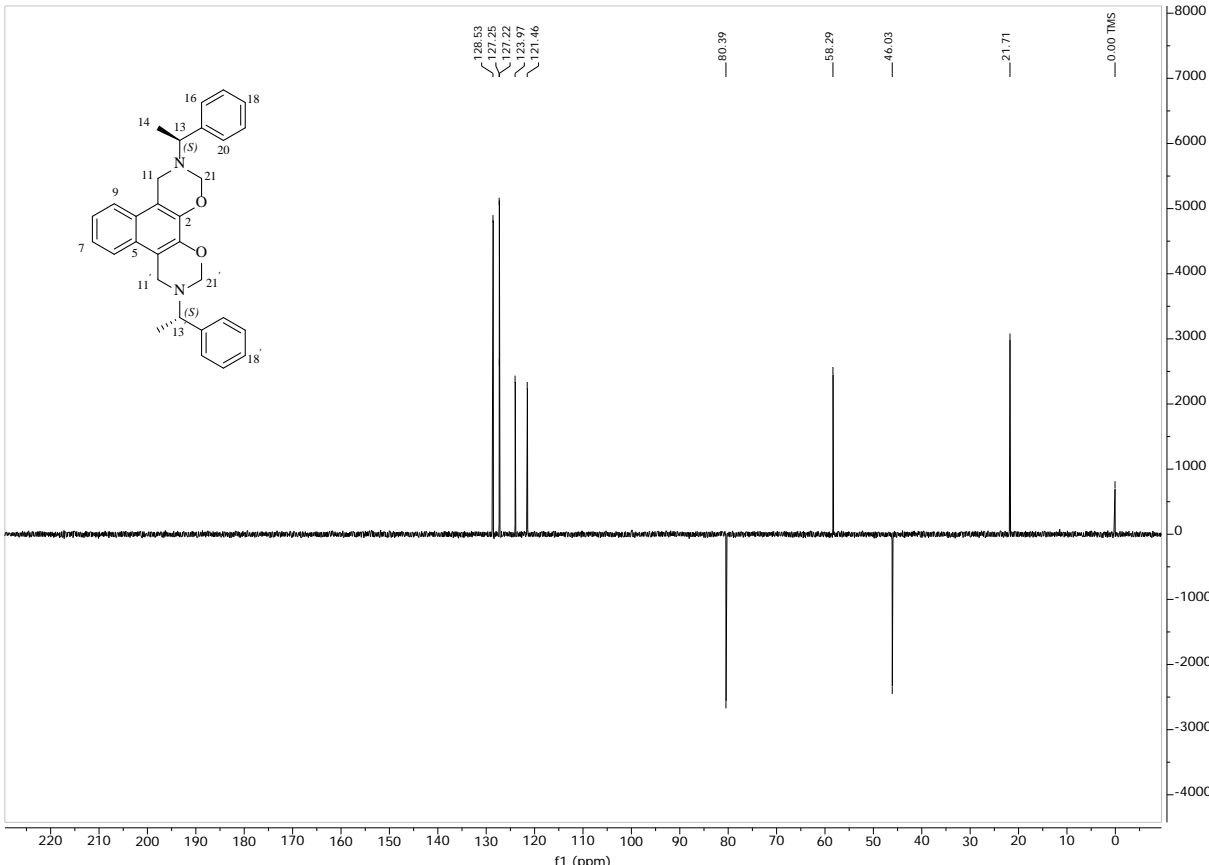


Figure S3. The DEPT 135 NMR spectrum of compound **3**.

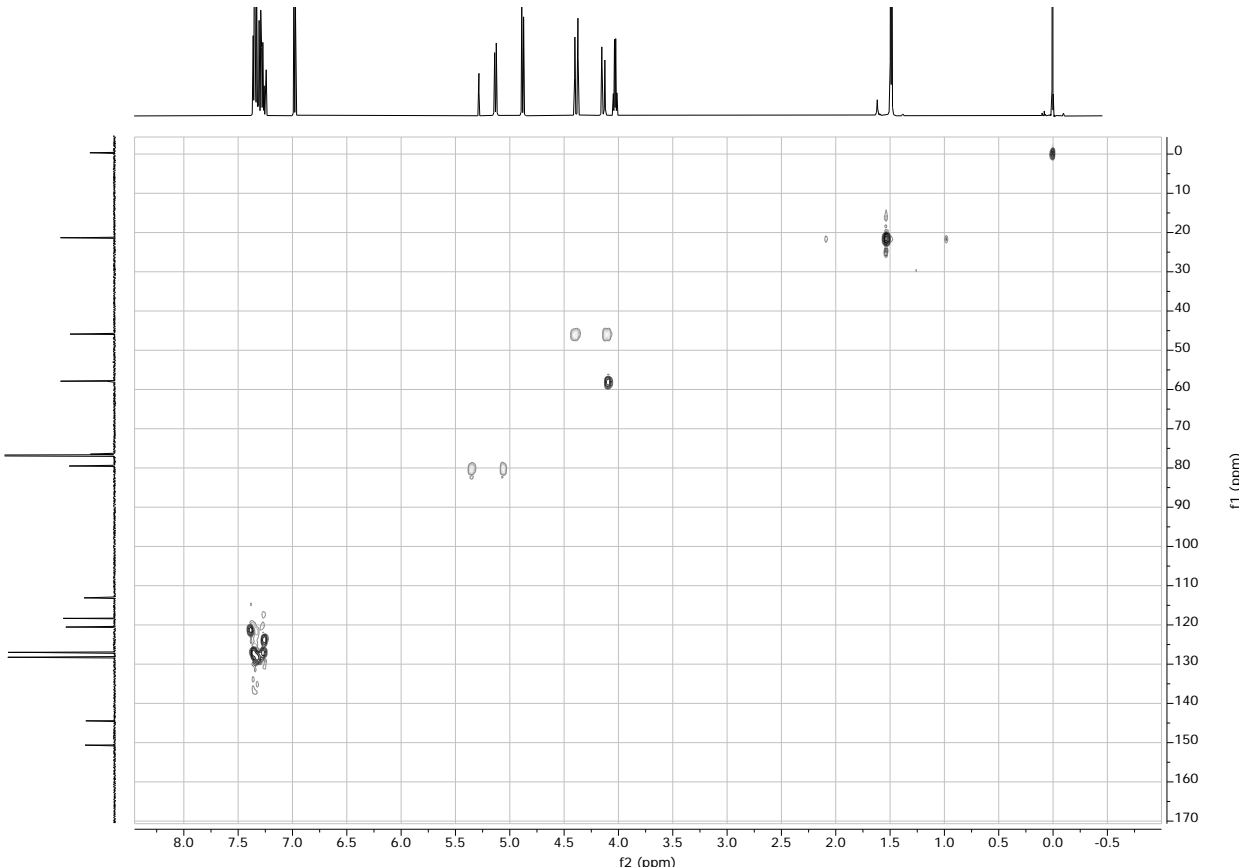


Figure S4. The HSQC NMR spectrum of compound **3**.

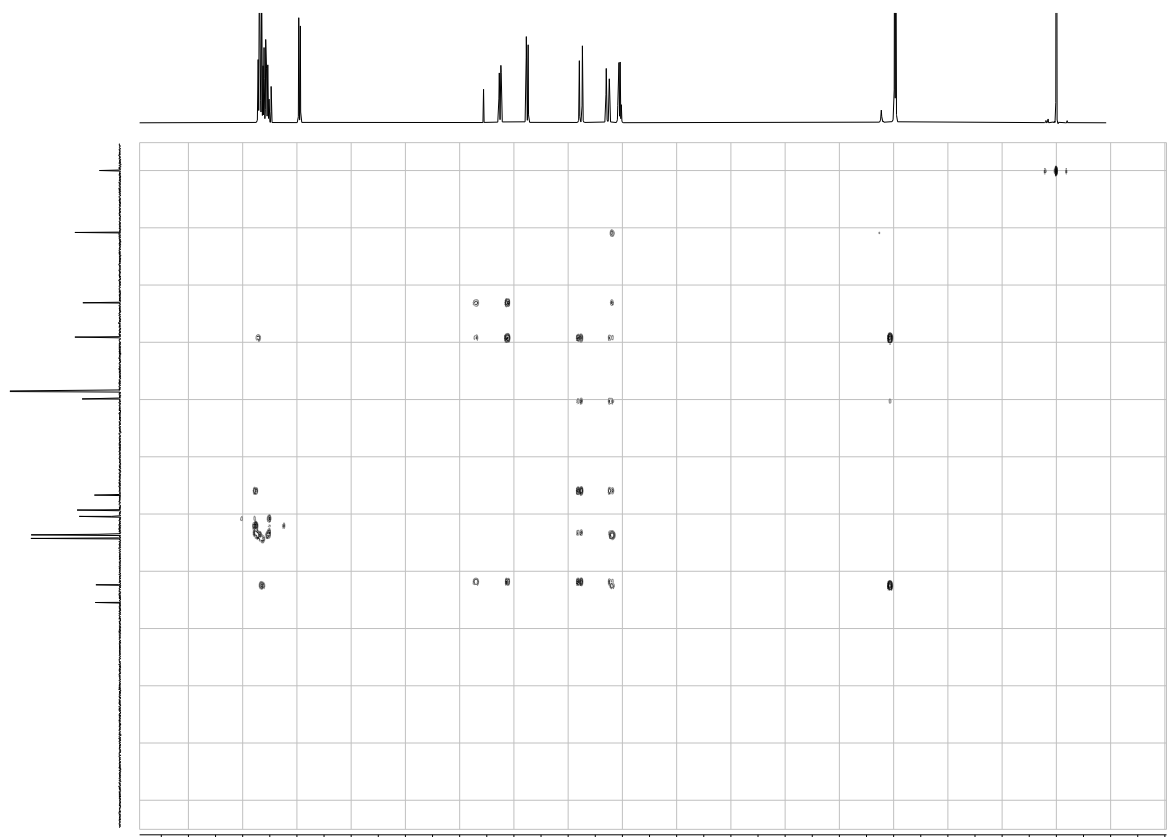


Figure S5. The HMBC NMR spectrum of compound **3**.

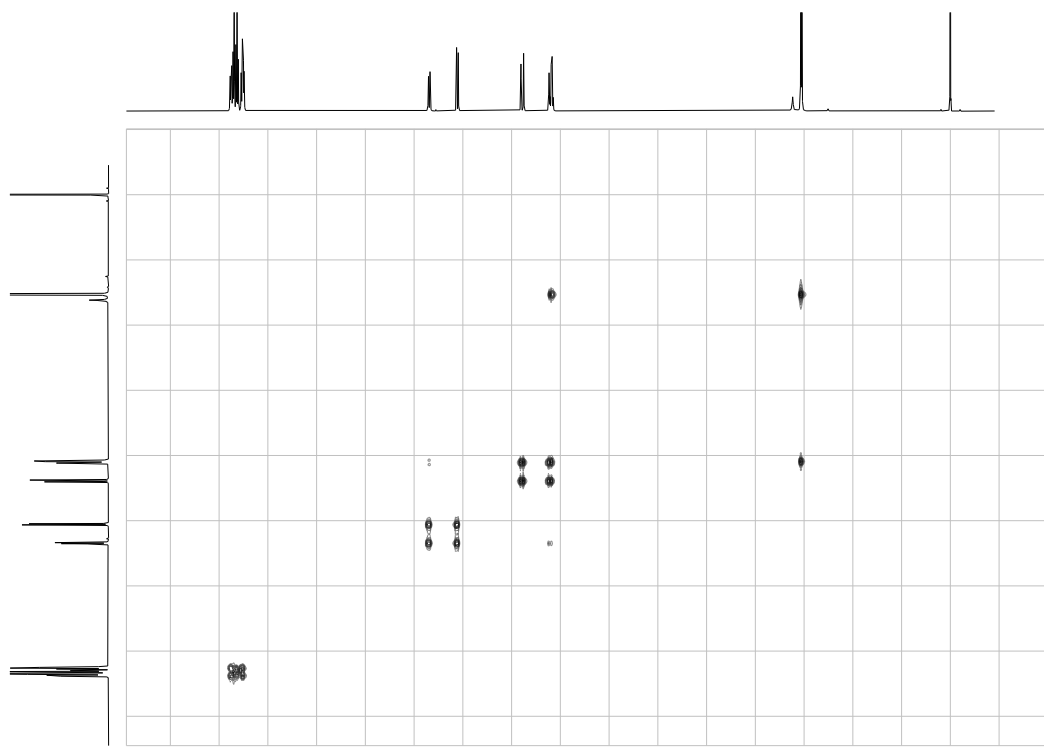


Figure S6. The COSY NMR spectrum of compound **3**.

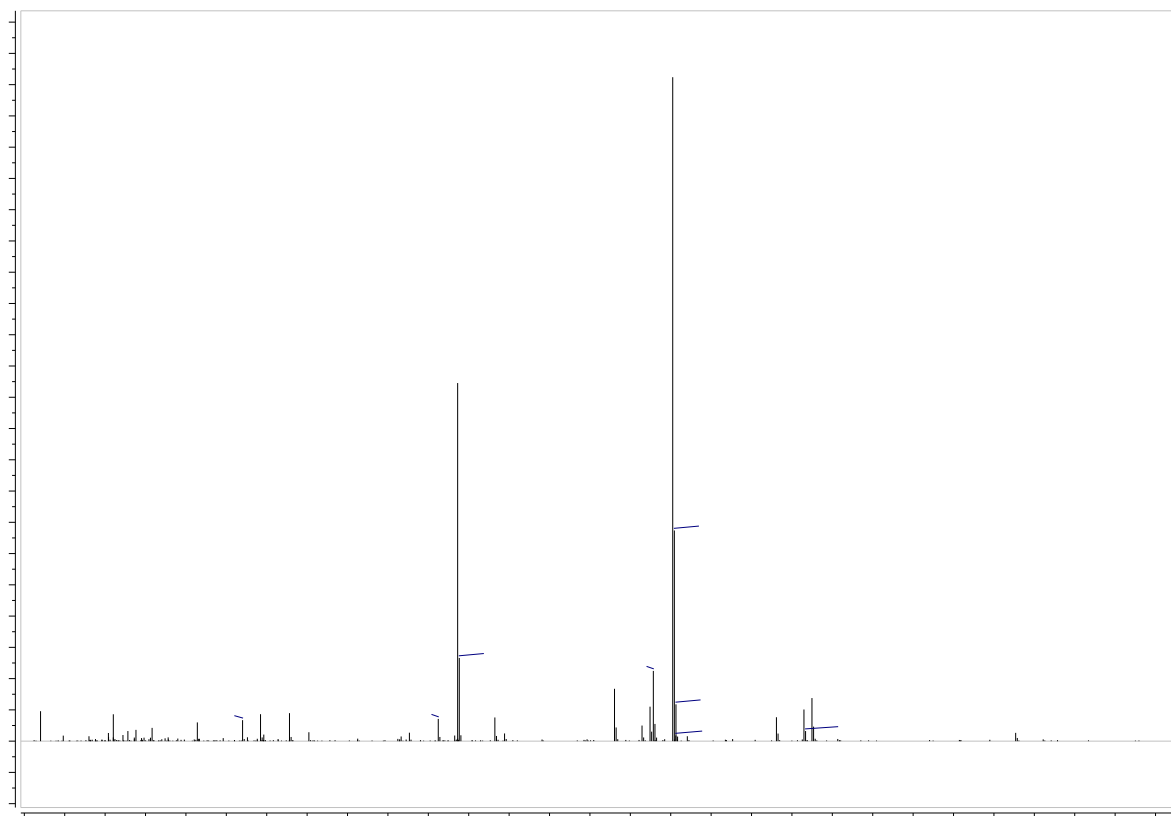


Figure S7. The HRMS spectrum of compound **3**.

NMR and HRMS Spectra of compound **5**

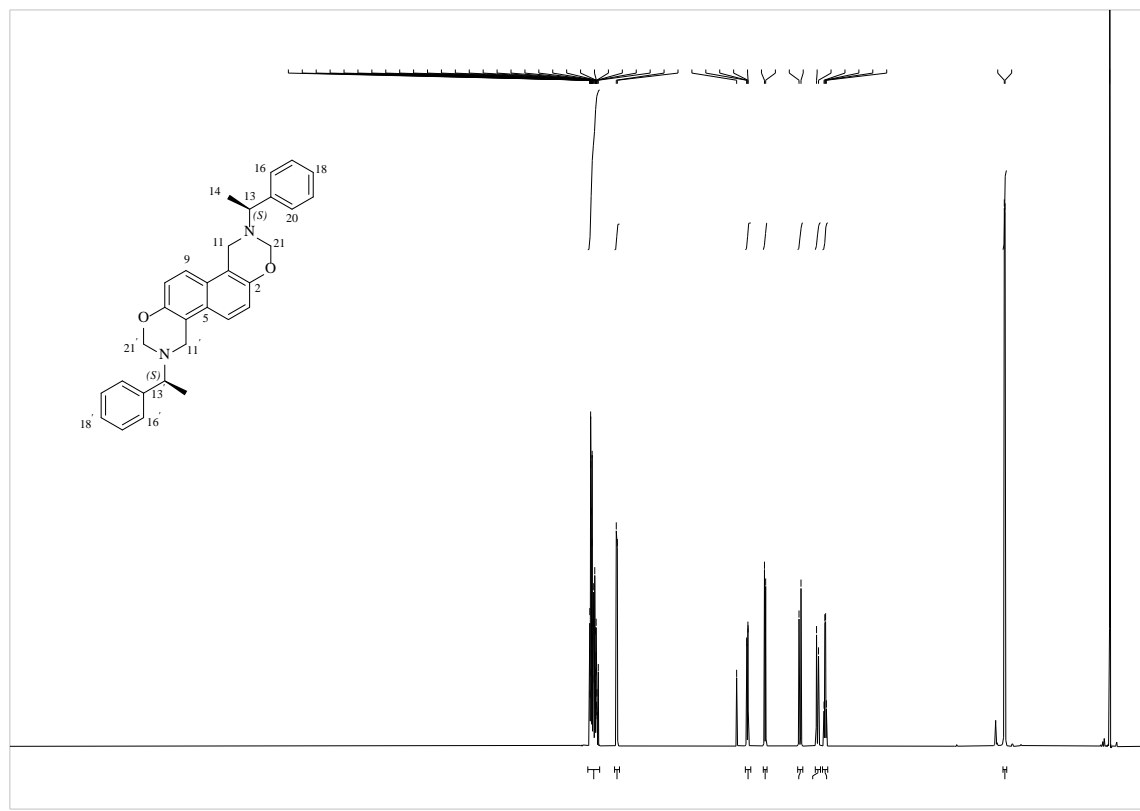


Figure S8. The ^1H NMR spectrum of compound **5**.

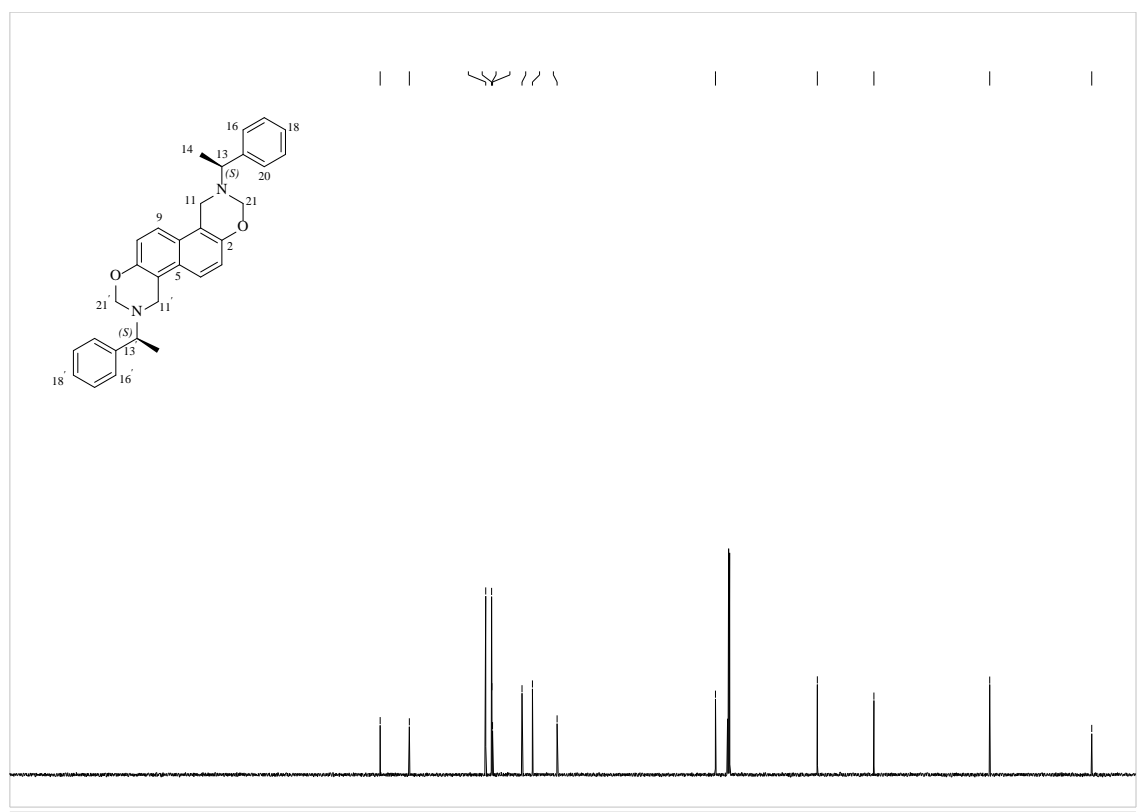


Figure S9. The ^{13}C NMR spectrum of compound **5**.

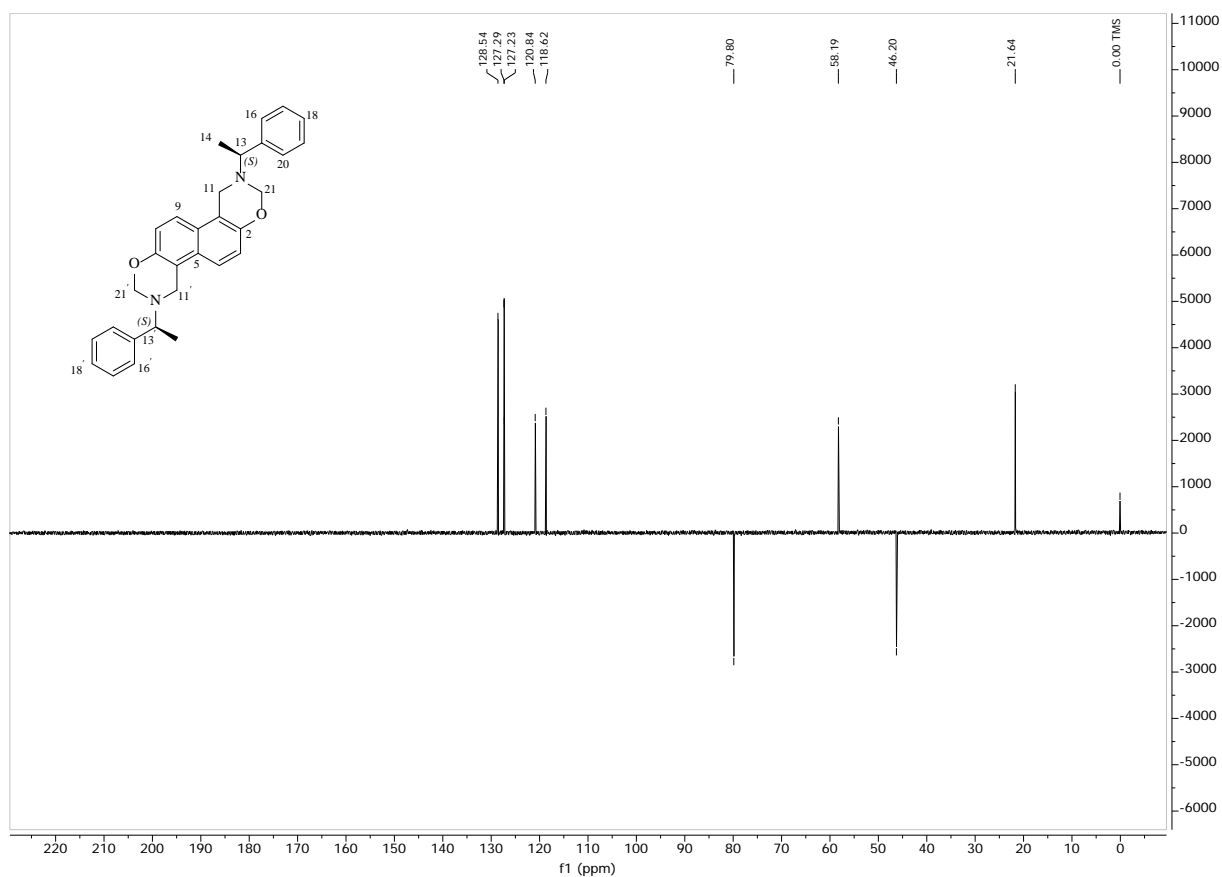


Figure S10. The DEPT 135 NMR spectrum of compound **5**.

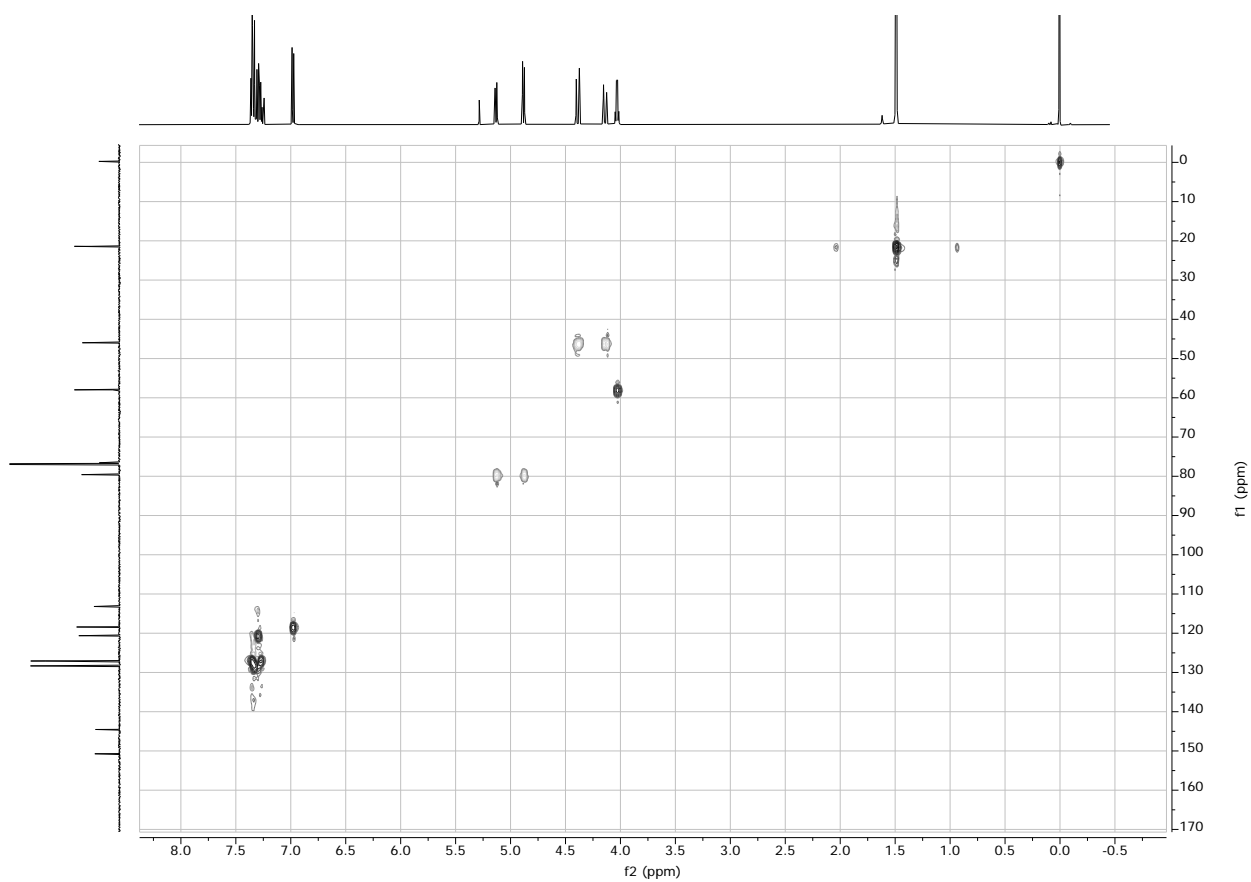


Figure S11. The HSQC NMR spectrum of compound **5**.

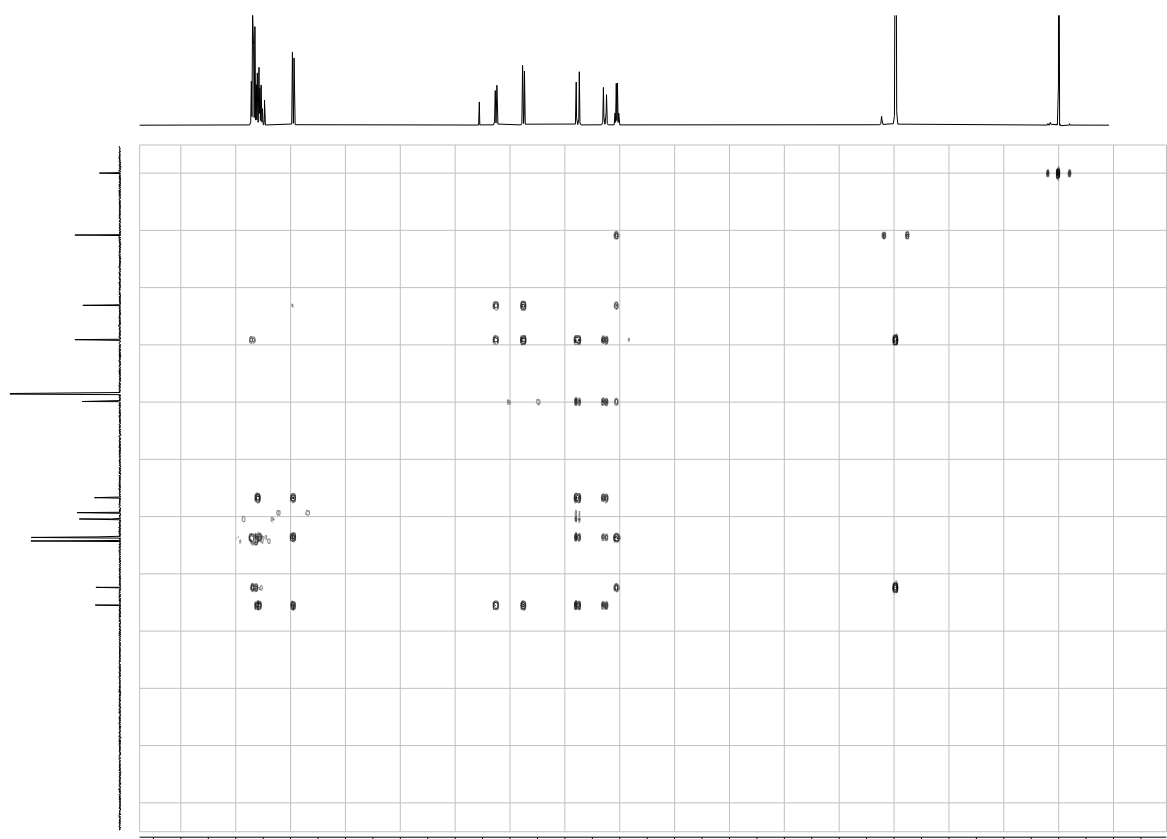


Figure S12. The HMBC NMR spectrum of compound **5**.

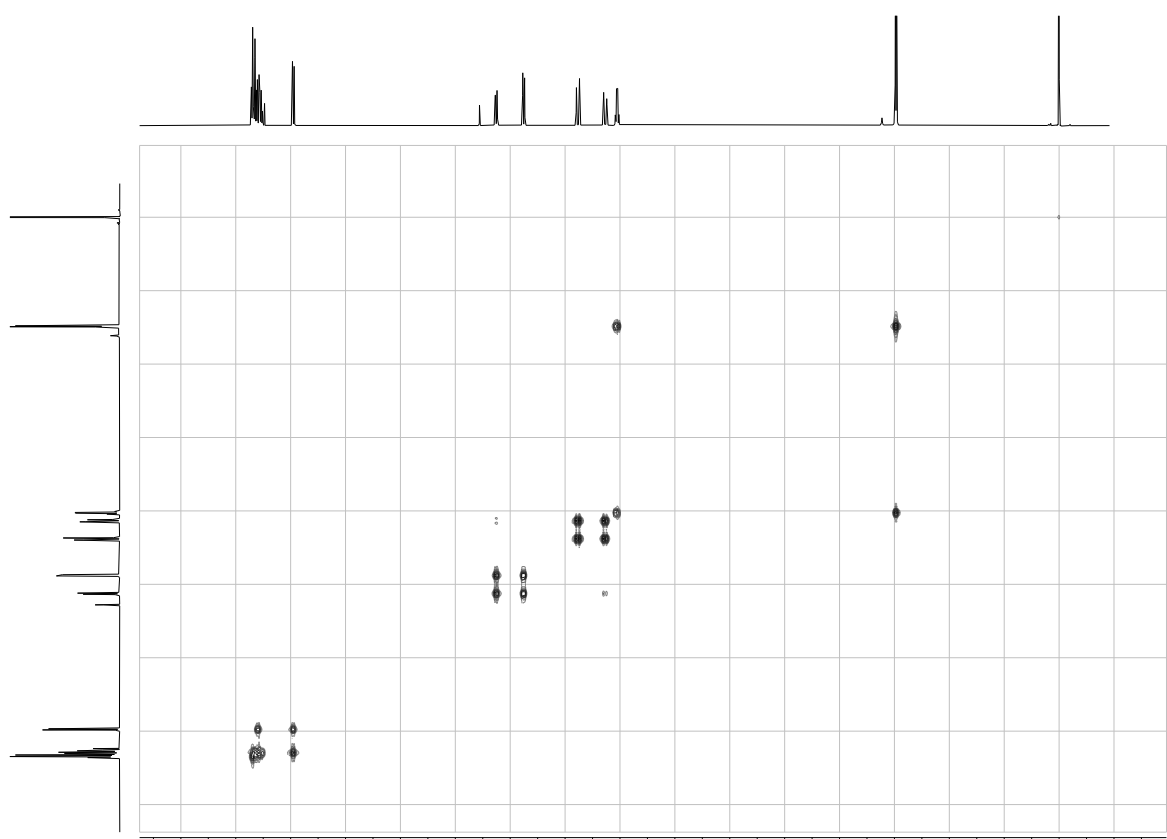


Figure S13. The COSY NMR spectrum of compound **5**.

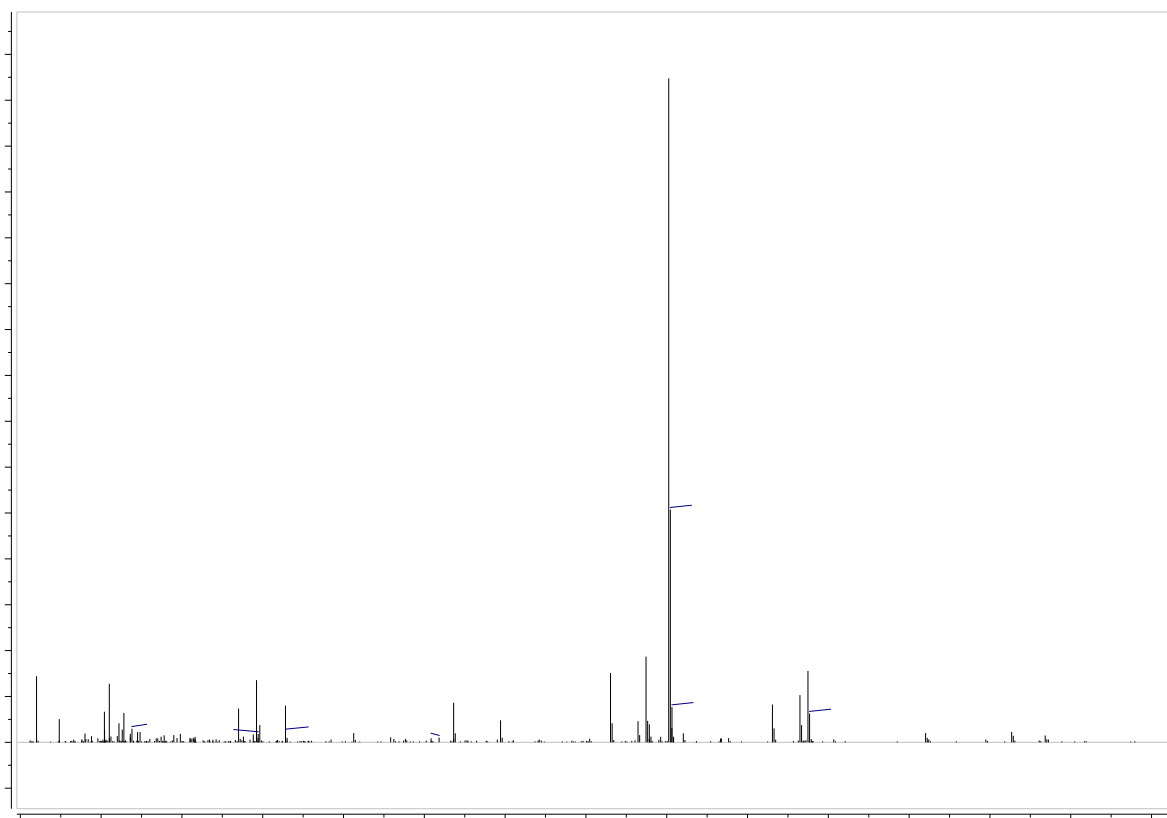


Figure S14. The HRMS spectrum of compound **5**.

NMR Spectrum of compound **8** (contains 16% of **9**)

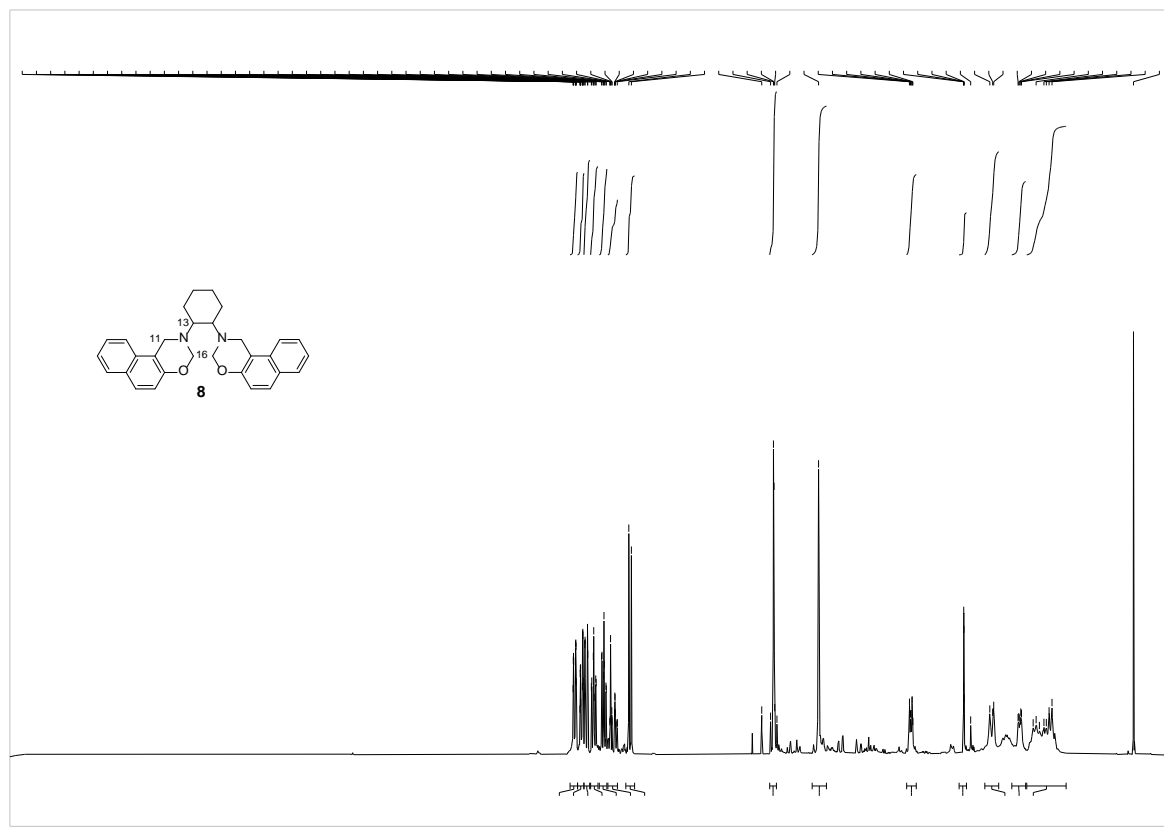


Figure S15. The ^1H NMR spectrum of compound **8** (contains 16% of **9**).

NMR and HRMS Spectra of a mixture of compounds **8** and **9** (20:19)

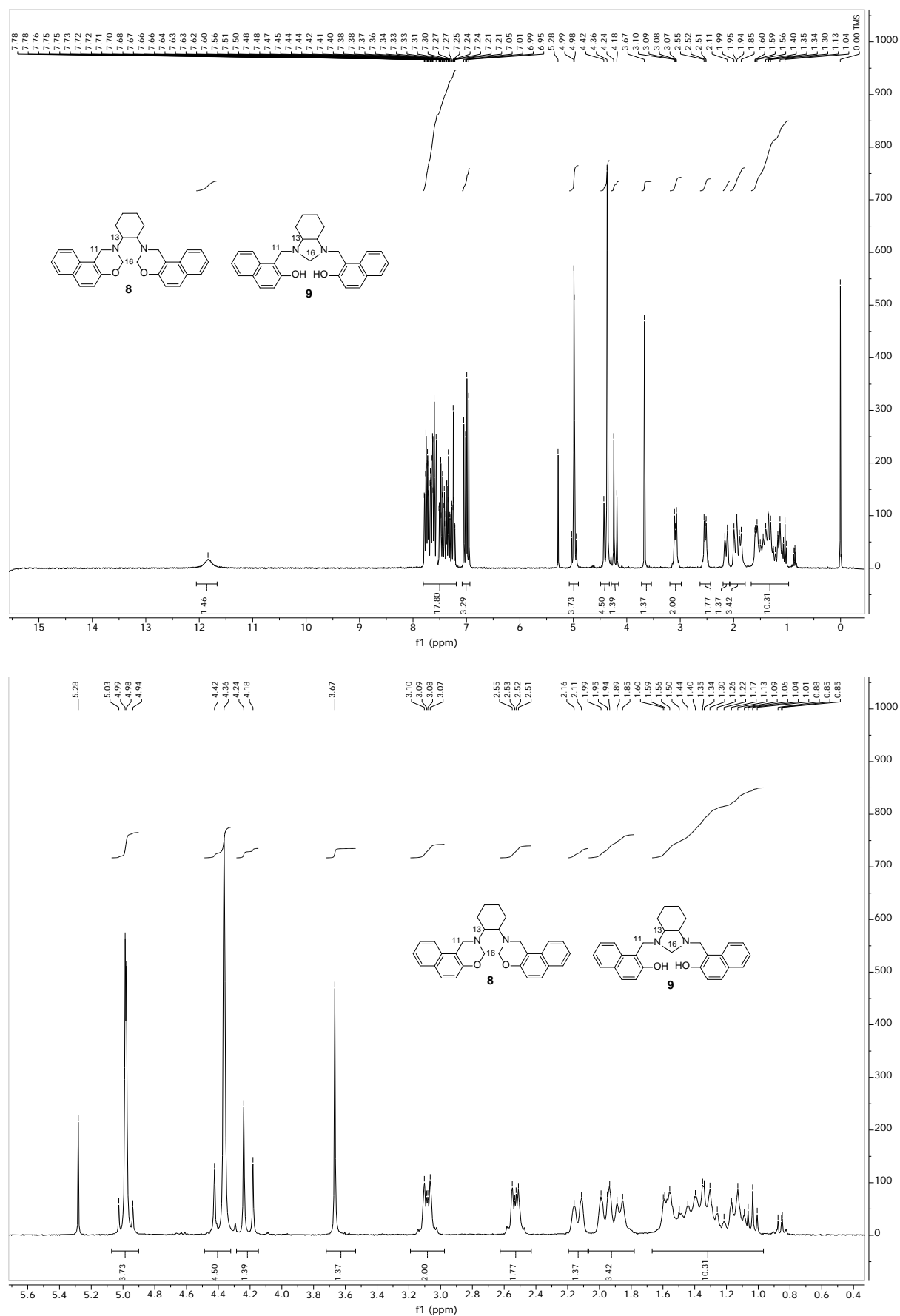


Figure S16. The ^1H NMR spectra of a mixture of compounds **8** and **9** (20:19).

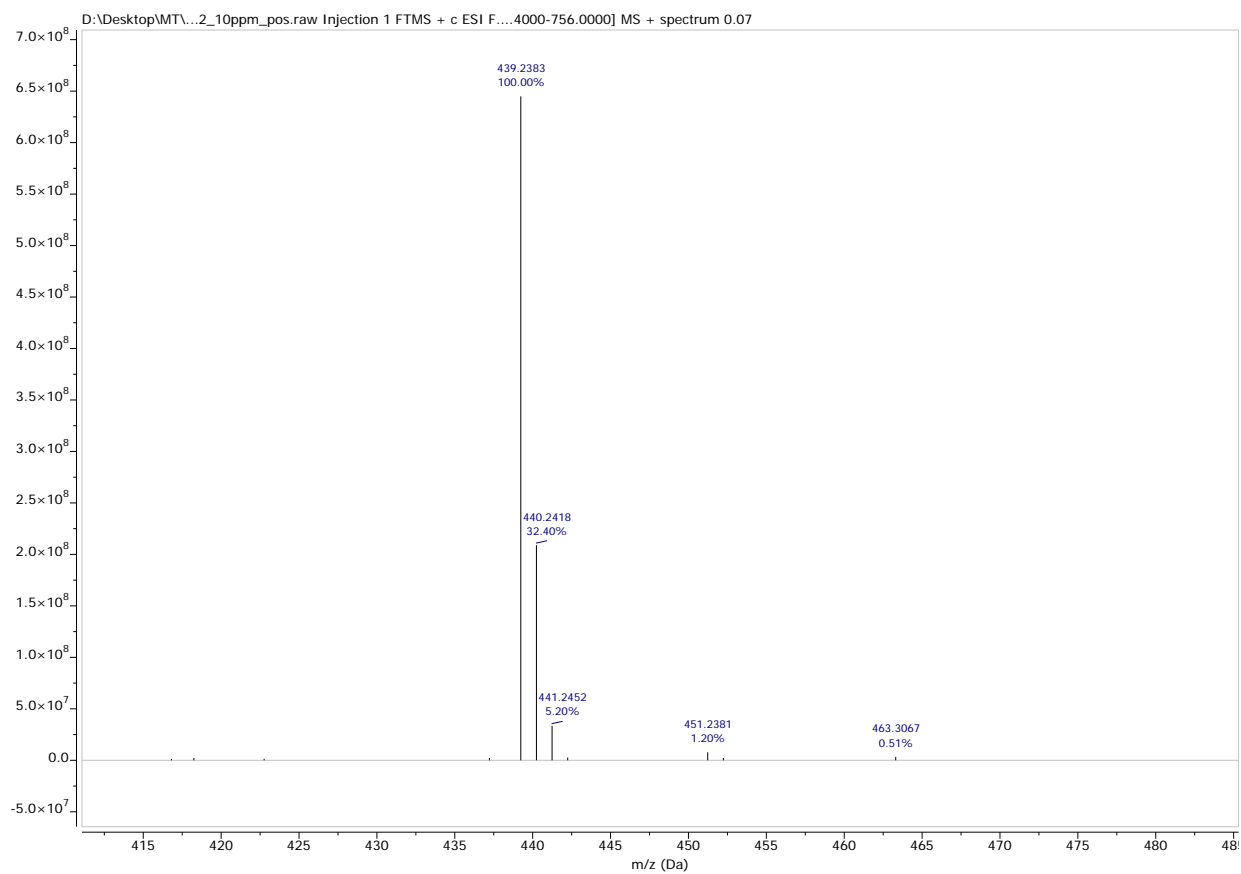


Figure S17. The HRMS spectrum of a mixture of compounds **8** and **9** (20:19).

NMR and HRMS Spectra of compound (*R,R*)-9

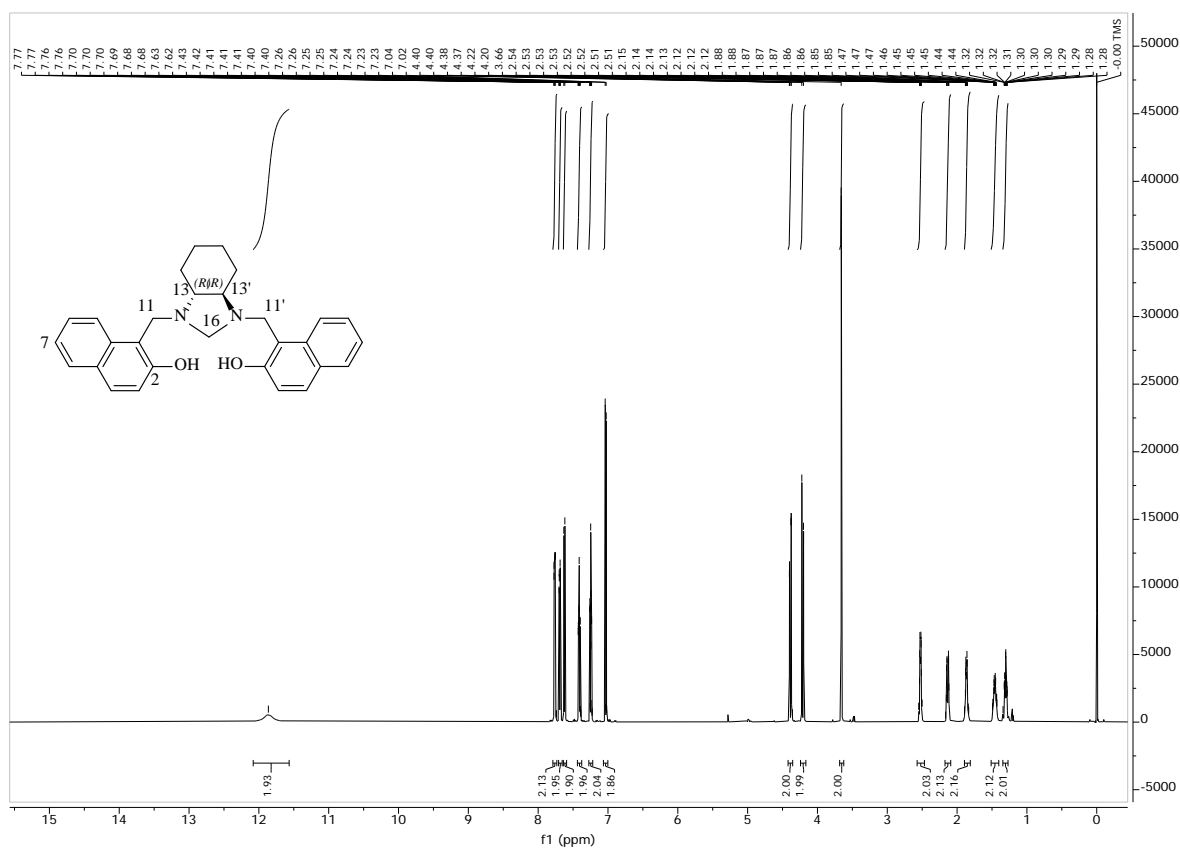


Figure S18. The ^1H NMR spectrum of compound (*R,R*)-9.

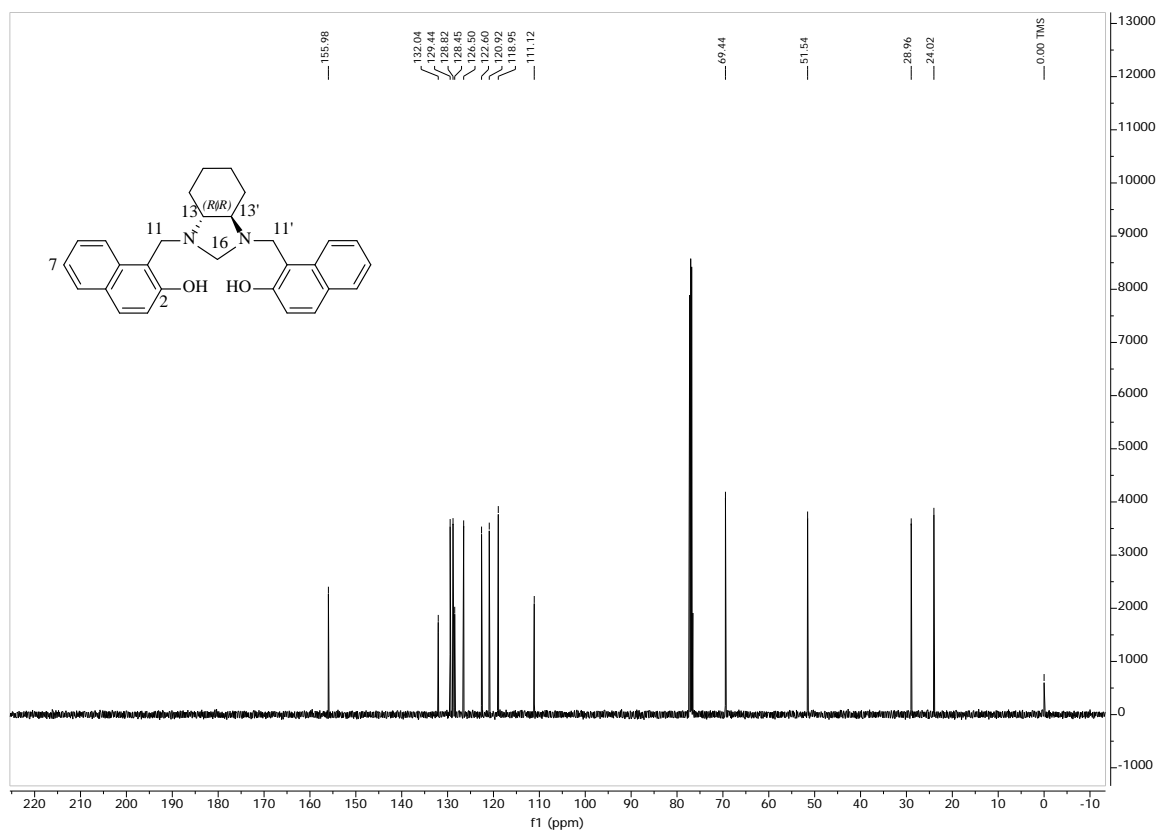


Figure S19. The ^{13}C NMR spectrum of compound (*R,R*)-9.

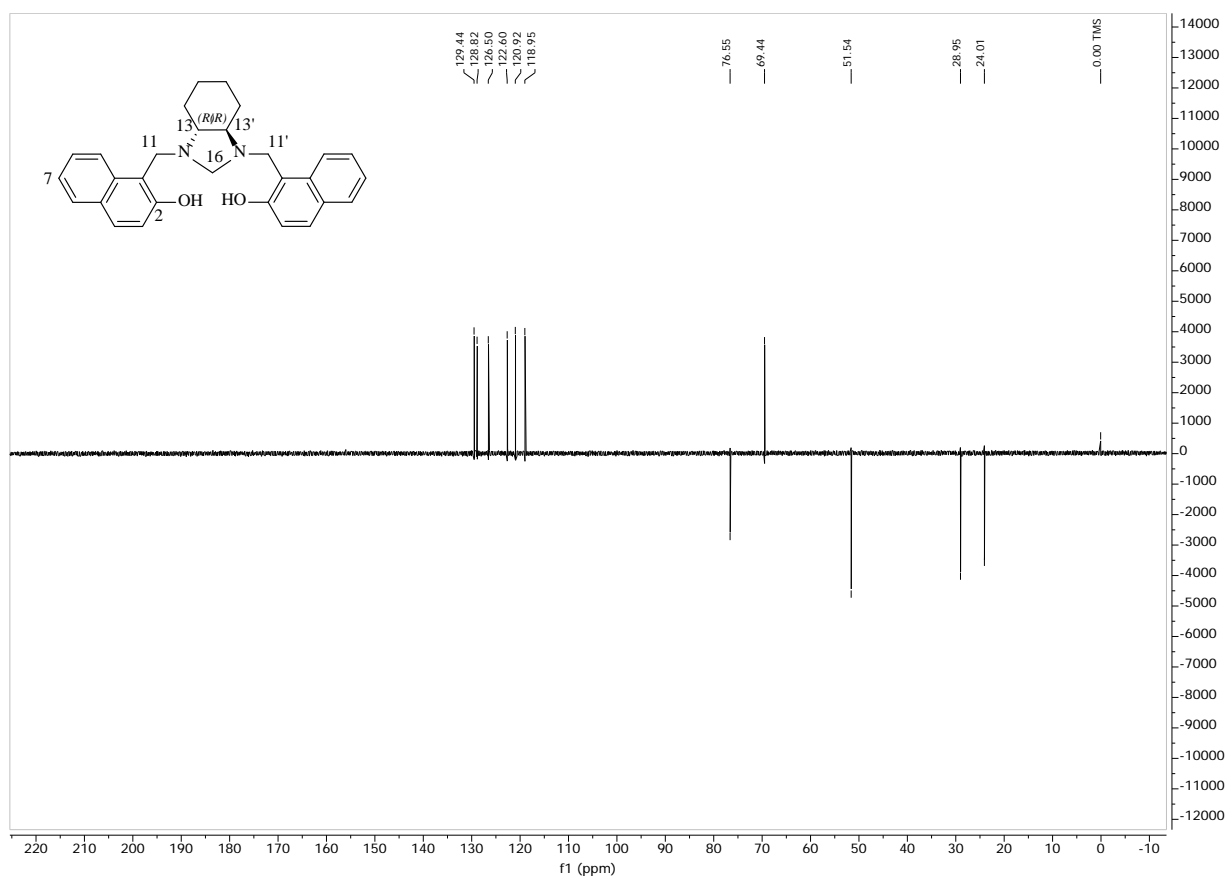


Figure S20. The DEPT 135 NMR spectrum of compound (R,R) -9.

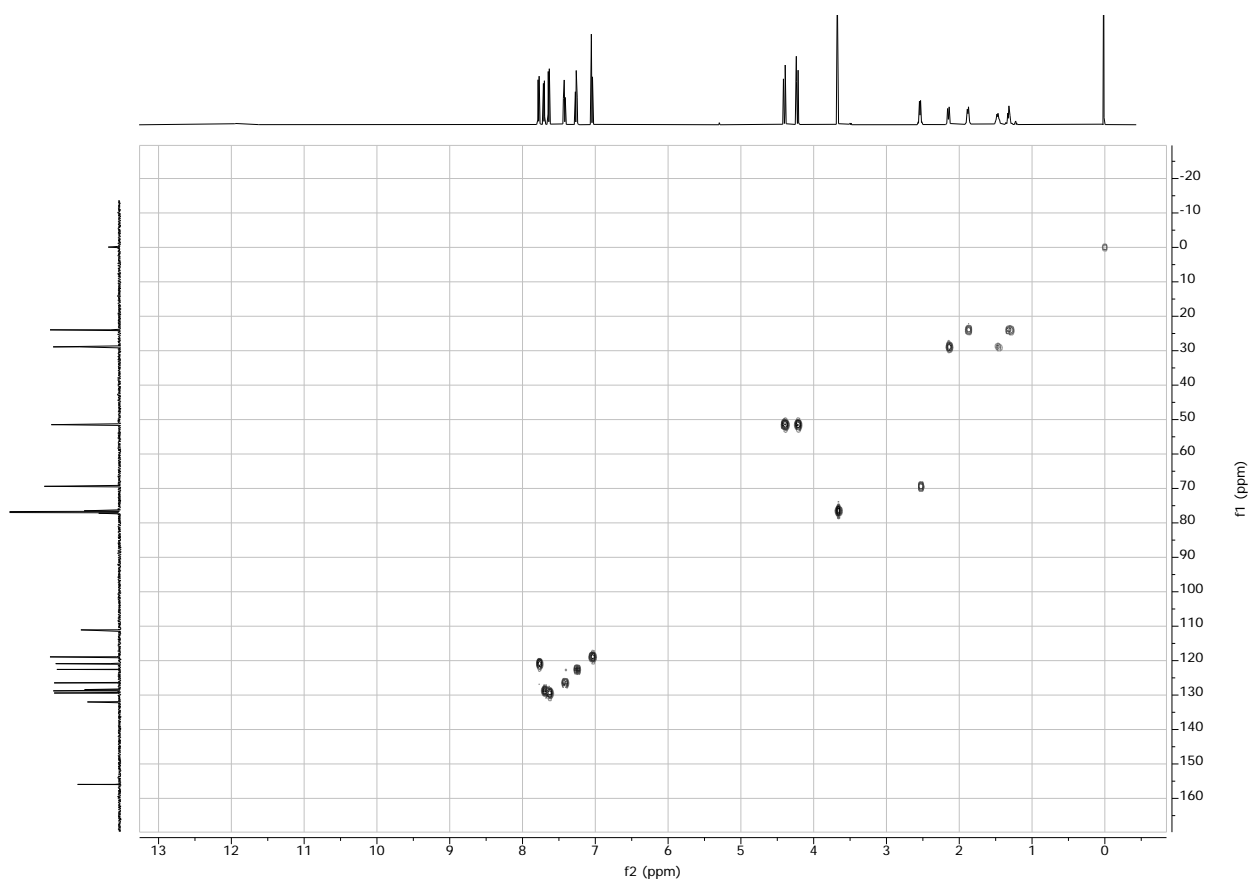


Figure S21. The HSQC NMR spectrum of compound (R,R) -9.

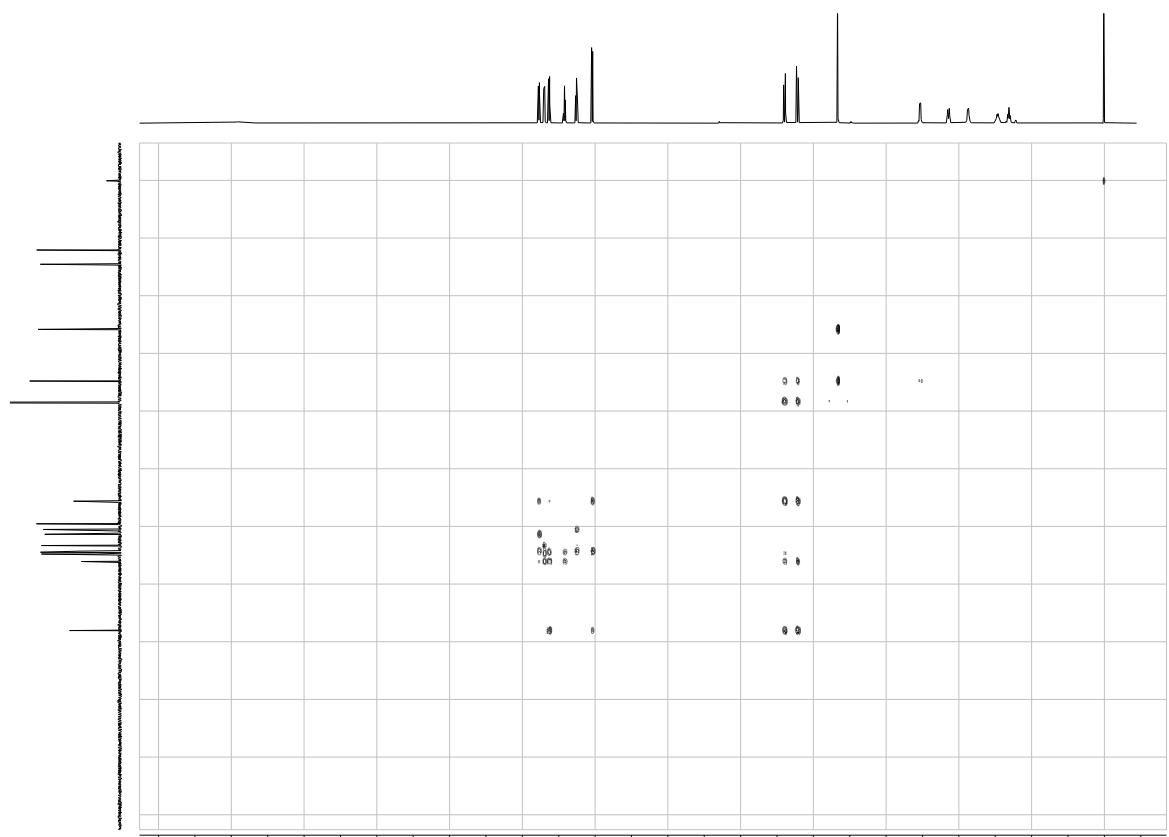


Figure S22. The HMBC NMR spectrum of compound (*R,R*)-**9**.

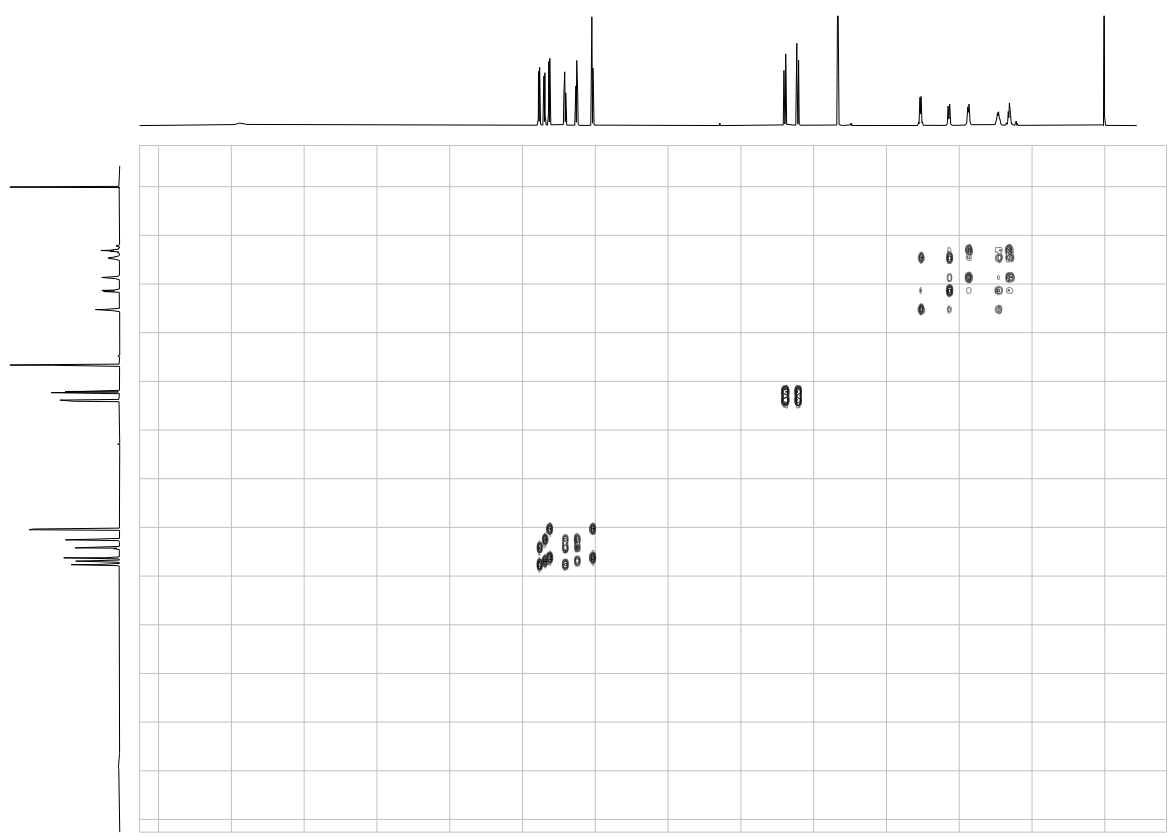


Figure S23. The COSY NMR spectrum of compound (*R,R*)-**9**.

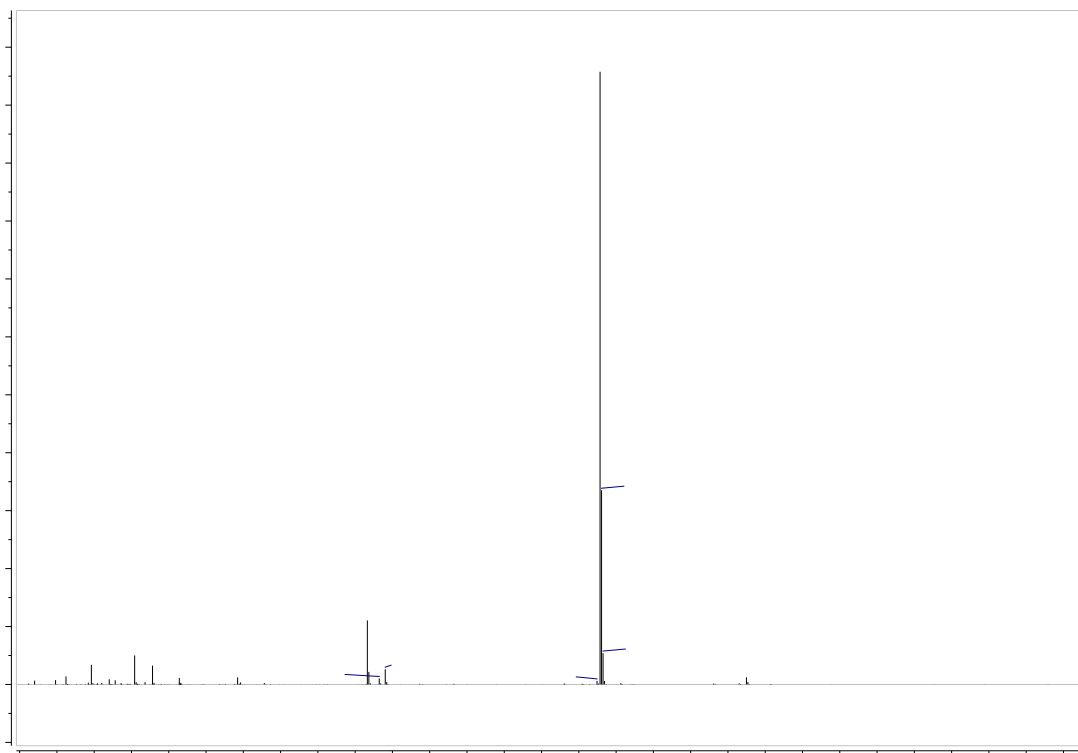


Figure S24. The HRMS spectrum of compound (R,R)-9.

Table S1. Most important data collection and refinement parameters for compounds **3** and (*R,R*)-**9**.

Compound	3	(<i>R,R</i>)-9
Empirical formula	C ₂₅ H ₃₀ N ₂ O ₂	C ₂₉ H ₃₀ N ₂ O ₂
Formula weight	450.56	438.55
Temperature	290 K	290 K
Crystal system	Monoclinic	Orthorhombic
Space group	<i>P</i> 2 ₁	<i>P</i> 2 ₁ 2 ₁ 2 ₁
<i>a</i> /Å	15.1999(9)	9.5093(3)
<i>b</i> /Å	5.1934(3)	9.9852(3)
<i>c</i> /Å	15.9835(12)	25.2395(9)
α /°	90	90
β /°	109.169(7)	90
γ /°	90	90
Volume/Å ³	1191.77(14)	2396.55(13)
<i>Z</i>	2	4
ρ_{calc} /cm ³	1.256	1.215
μ /mm ⁻¹	0.079	0.076
<i>F</i> (000)	480.0	936.0
Crystal size/mm ³	0.25 × 0.25 × 0.2	0.3 × 0.2 × 0.15
Radiation	MoK α (λ = 0.71073)	MoK α (λ = 0.71073)
2 θ range for data collection/°	5.424 to 57.972	4.578 to 56.614
Reflections collected/independent	5806/4188	38835/5910
<i>R</i> _{int} / <i>R</i> _{sigma}	0.0275/0.0549	0.0290, 0.0199
Data/restraints/parameters	4188/1/310	5910/0/298
Goodness-of-fit on <i>F</i> ²	1.061	1.075
Final <i>R</i> indexes [<i>I</i> ≥ 2 σ (<i>I</i>)]	<i>R</i> 1 = 0.0600, w <i>R</i> 2 = 0.1433	<i>R</i> 1 = 0.0509, w <i>R</i> 2 = 0.1253
Final <i>R</i> indexes [all data]	<i>R</i> 1 = 0.0947, w <i>R</i> 2 = 0.1643	<i>R</i> 1 = 0.0635, w <i>R</i> 2 = 0.1332
Largest diff. peak/hole / e Å ⁻³	0.18/-0.17	0.14/-0.13
Flack parameter	-1.8(10)	-0.4(3)
CCDC number	2294902	2294903