

Supporting Information

Regulation of Axial Chirality through Dynamic Covalent Bond Constrained Biaryls

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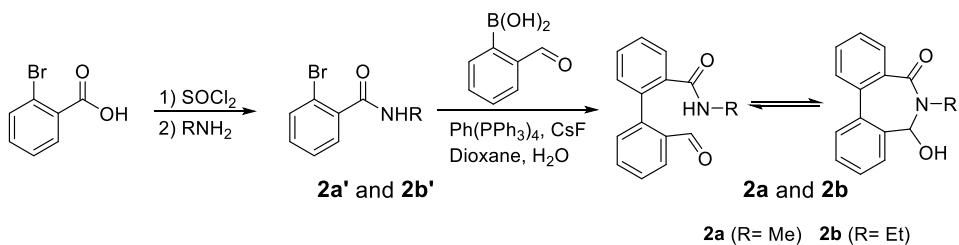
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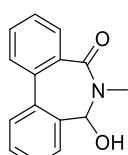
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1. Synthesis and Characterization

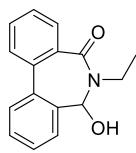
Scheme S1. Synthesis of **2a** and **2b**.



Amides **2a** and **2b** was prepared according to the literature methods.^{S1}

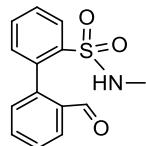


(2a): Under an argon atmosphere, 2-bromo-*N*-methyl-benzamide (0.22 g, 1.0 mmol), 2-formylphenylboronic acid (0.25 g, 1.7 mmol), and Pd(PPh₃)₄ (30 mg) were dissolved in 1,4-dioxane (15 mL). A solution of aqueous CsF (2 M, 2.0 mL) was added, and the mixture was stirred at 80 °C overnight. After the reaction was cooled to room temperature, brine (15 mL) was added, and the mixture was extracted with ethyl acetate (30 mL × 2). The combined organic layers were washed with water, dried over Na₂SO₄, and purified by column chromatography (silica gel, petroleum ether/ethyl acetate 10: 1 to 2: 1) to afford the title compound as a light yellow solid. The product powder was then crystallized from CH₃CN to afford a white crystalline solid (0.21 g, 83%). For the ring form a mixture of diastereomers (1.6: 1) was obtained. ¹H-NMR (CD₃CN): δ = 7.83-7.86 (m, 1.6H), 7.40-7.70 (m, 11.2H), 5.83 (d, J = 5.2 Hz, 1H), 5.80 (d, J = 4.0 Hz, 0.6H), 5.11 (d, J = 5.2 Hz, 1H), 4.25 (d, J = 4.0 Hz, 0.6H), 3.22 (s, 1.8H), 2.91 (s, 3H). ¹³C-NMR (CD₃CN): δ = 167.6, 166.3, 140.0, 139.6, 136.1, 135.9, 135.7, 135.5, 135.4, 130.9, 130.5, 130.0, 129.9, 129.3, 129.2, 128.6, 128.5, 128.2, 128.1, 128.0, 127.9, 127.4, 126.7, 121.6, 86.6, 77.2, 35.2, 24.3. HRMS: *m/z* Calcd. for C₁₅H₁₄NO₂ [M + H]⁺: 240.1025; found: 240.1019; HRMS: *m/z* Calcd. For C₁₅H₁₃NO₂Na [M + Na]⁺: 262.0844; found: 262.0840.

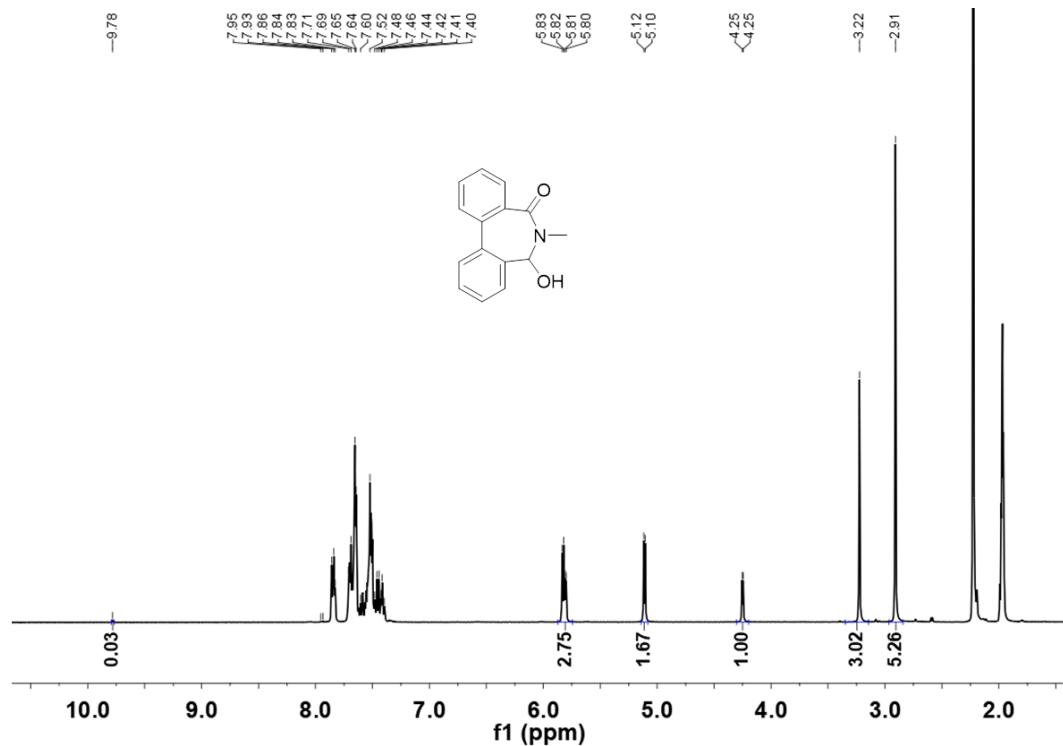


(2b): The same procedure was used as described above for **2a** (0.22 g, 85%). For the ring form a mixture of diastereomers (1.3: 1) was obtained. ¹H-NMR (CD₃CN): δ = 7.83-7.86 (m, 2.3H), 7.43-7.74 (m, 16.1 H), 5.86 (d, J = 4.0 Hz, 1.3H), 5.80 (d, J = 5.6 Hz, 1H), 5.10 (d, J = 5.6 Hz, 1H), 4.13 (d, J = 4.0 Hz, 1.3H), 3.47-3.81 (m, 4.6H), 1.16 (t, J = 7.2 Hz, 3.9H), 1.07 (t, J = 7.2 Hz, 3H). ¹³C-NMR

(DMSO-*d*₆): δ = 191.6, 168.5, 167.2, 166.1, 133.3, 131.1, 131.0, 130.5, 130.0, 129.8, 129.4, 129.1, 128.5, 128.4, 128.2, 128.1, 128.0, 127.9, 127.4, 127.1, 126.8, 126.5, 121.5, 85.2, 77.2, 43.5, 34.3, 34.0, 14.5, 13.6, 13.4. HRMS: *m/z* Calcd. for C₁₆H₁₅NO₂Na [M + Na]⁺: 276.1000; found: 276.0997.



(2c): The reported procedure^{S2} was used to afford the title compound as a light yellow oil (yield: 84%). Because of the fast inversion, the *d.r.* can't be calculated. ¹H NMR (CD₃CN): δ 9.65 (d, *J* = 0.5 Hz, 1H), 8.10-8.05 (m, 1H), 8.01-7.97 (dd, *J* = 7.7, 1.2 Hz, 1H), 7.91-7.89 (dd, *J* = 7.6, 1.0 Hz, 0.5H), 7.80-7.47 (m, 7.5H), 7.40-7.37 (m, 2H), 5.41 (d, *J* = 4.8 Hz, 0.5H), 4.75 (br, 1H), 4.59 (d, *J* = 5.2 Hz, 0.5H), 2.99 (s, 1.5H), 2.43 (d, *J* = 5.2 Hz, 3H).



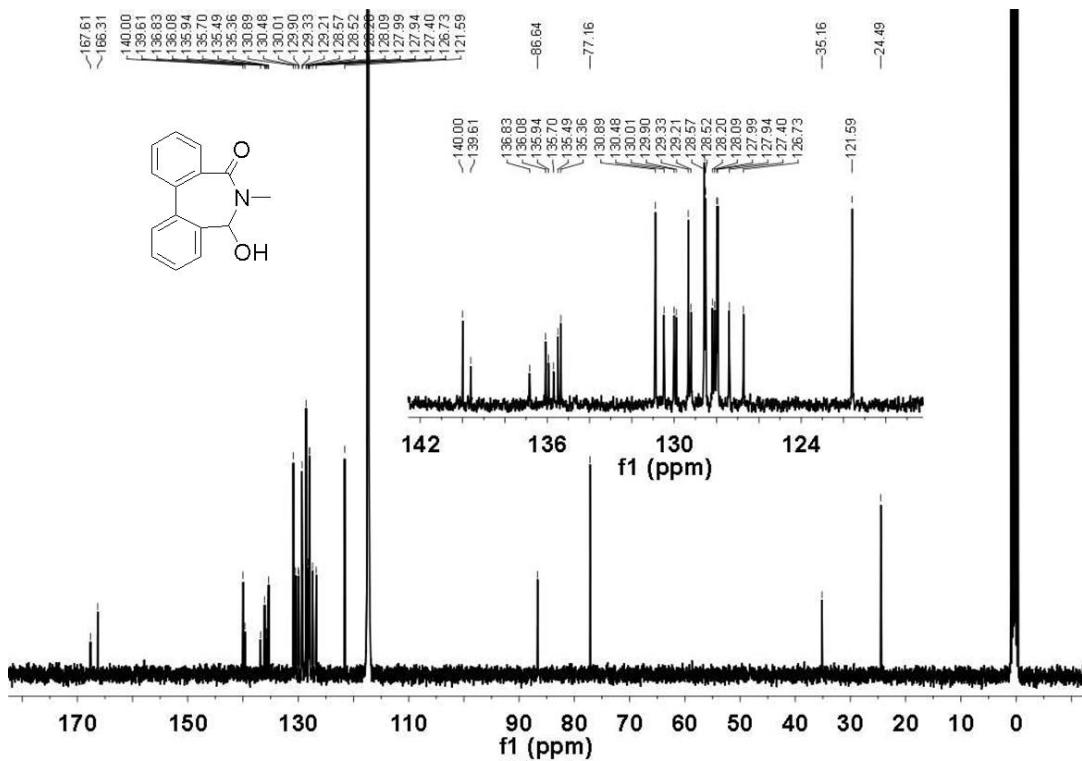


Figure S1. ^1H -NMR and ^{13}C -NMR spectra of **2a** in CD_3CN . Due to the presence of one chiral center and one chiral axis, two enantiomeric pairs of diastereomers were observed for the ring form of **2a** and **2b** (see more details in Figure S6).

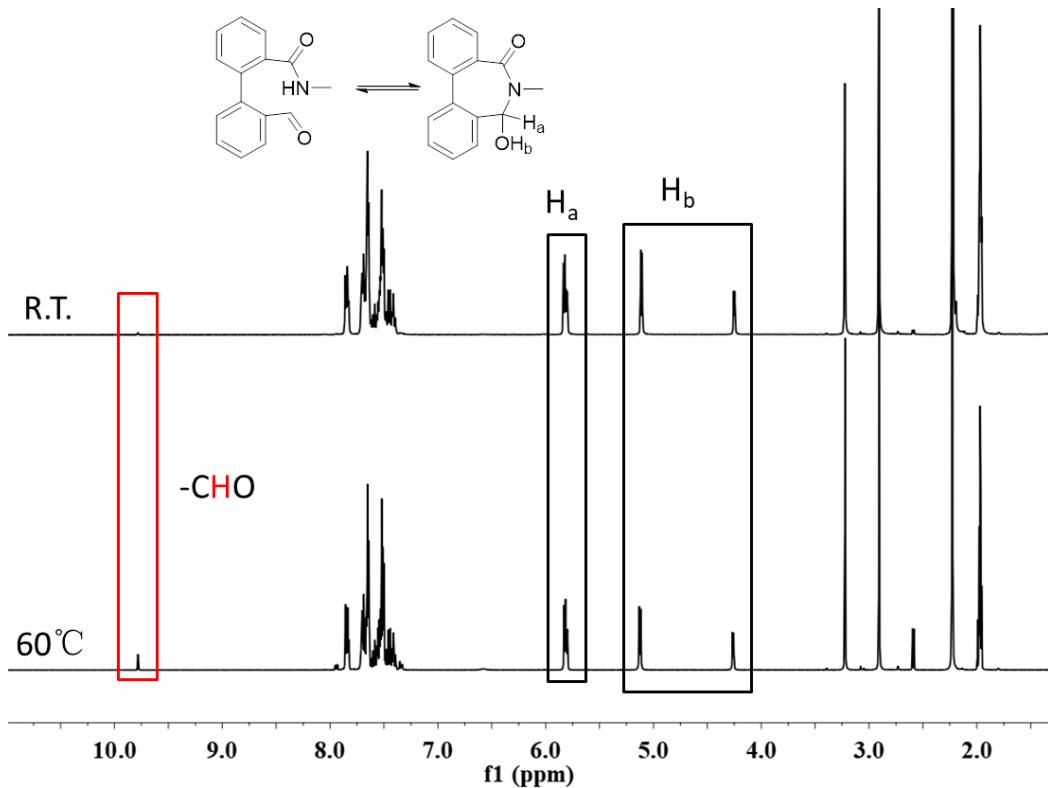


Figure S2. ^1H -NMR spectra of **2a** in CD_3CN at room temperature (top), and after heating at 60°C for 20 h (bottom).

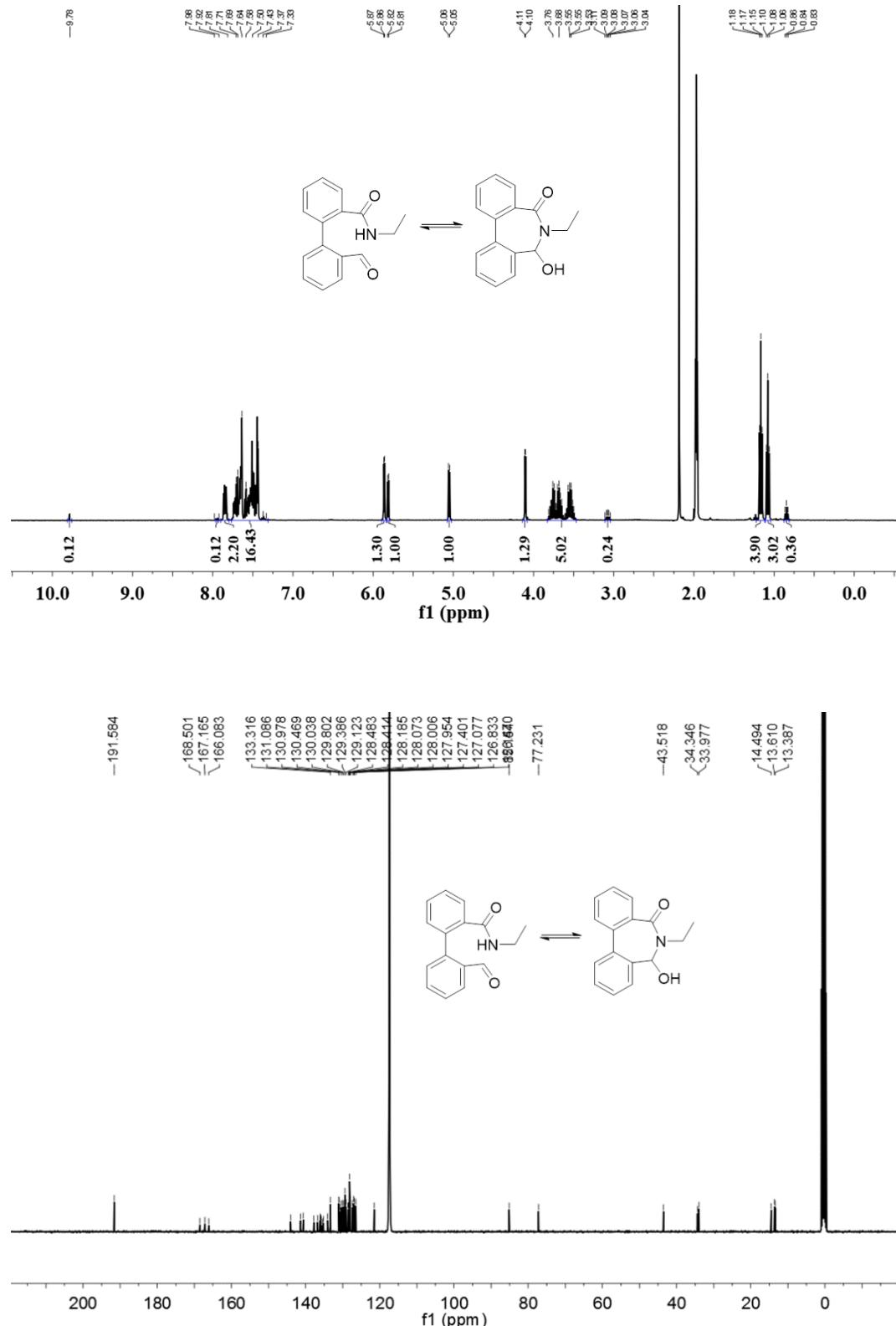


Figure S3. ¹H-NMR and ¹³C-NMR spectra of **2b** in CD₃CN.

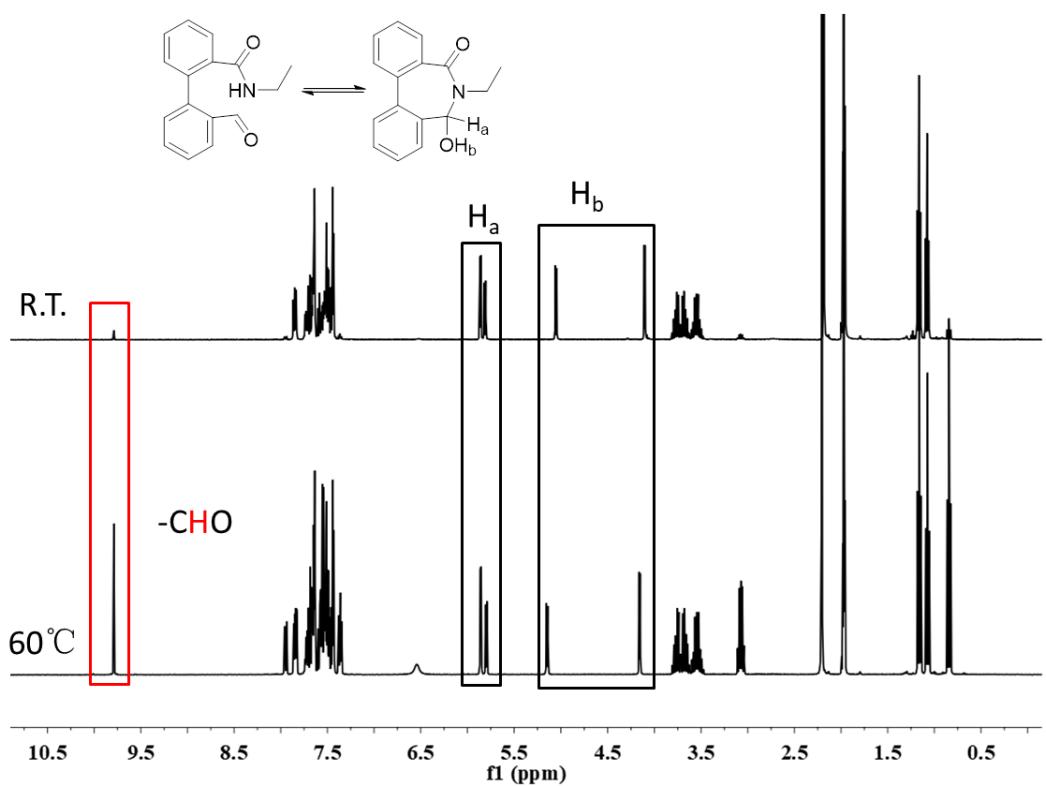


Figure S4. ¹H-NMR spectra of **2b** in CD_3CN at room temperature (bottom), and after heating at 60°C for 20 h (top).

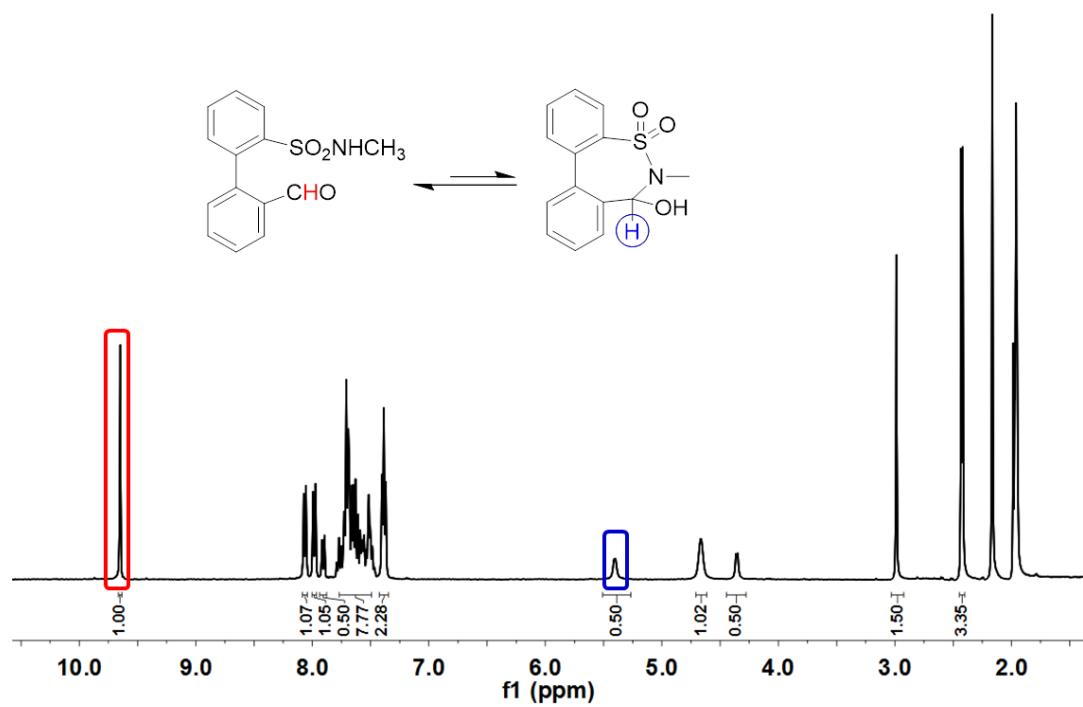


Figure S5. ¹H-NMR spectra of **2c** in CD_3CN .

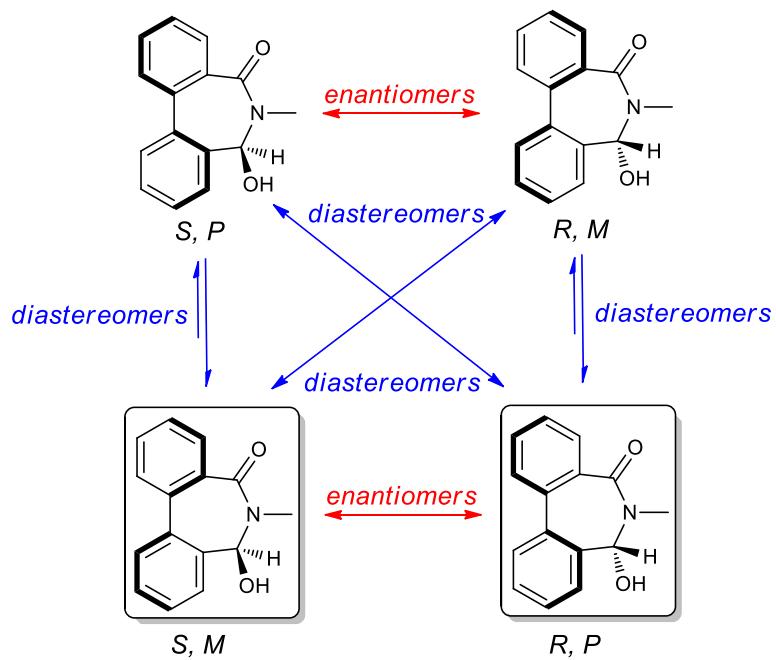


Figure S6. The relationship of enantiomers for the cyclic form of **2a**.

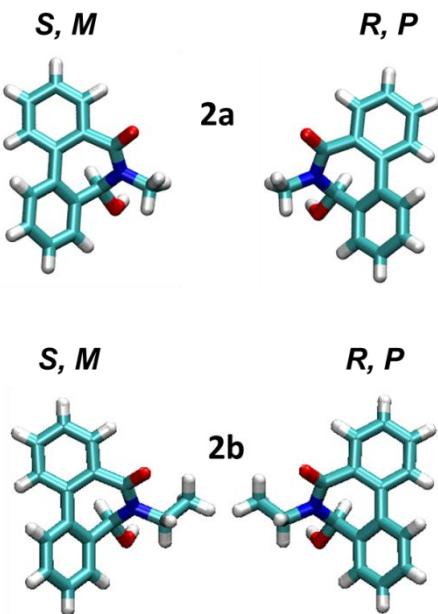


Figure S7. The X-ray crystal structures of **2a**, and **2b**, respectively.

2. Dynamic Covalent Reactions

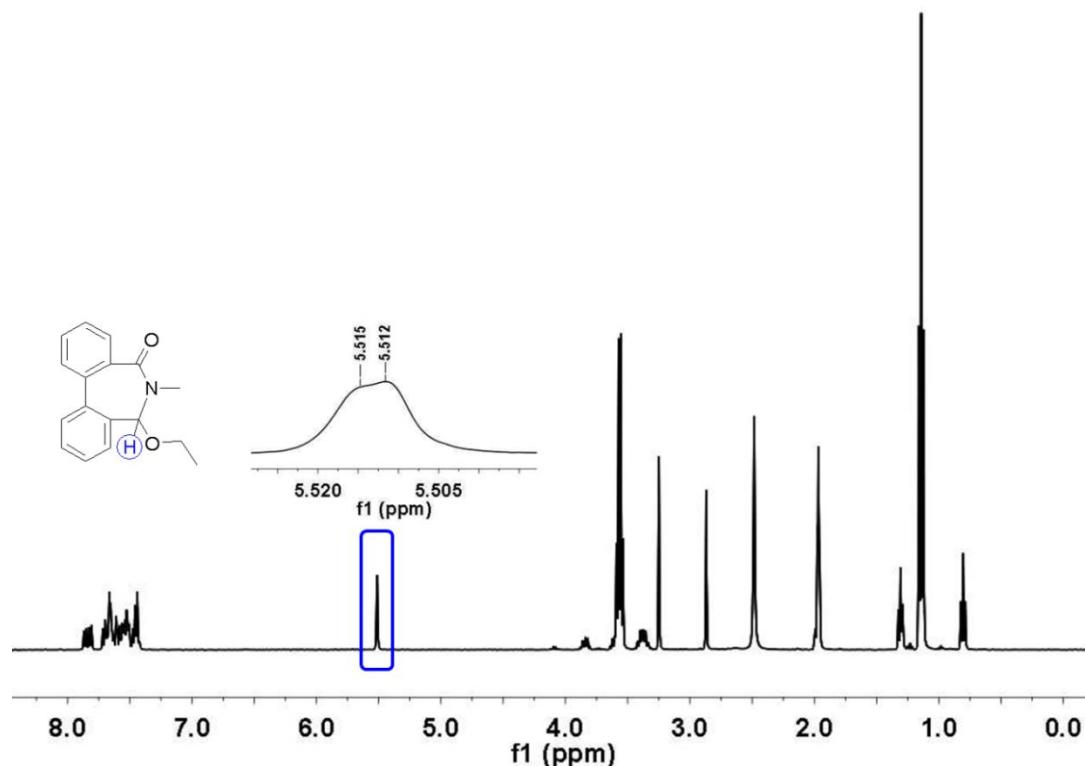


Figure S8. ¹H-NMR spectrum of the reaction of **2a** and ethanol in the presence of MA in CD₃CN at R.T.

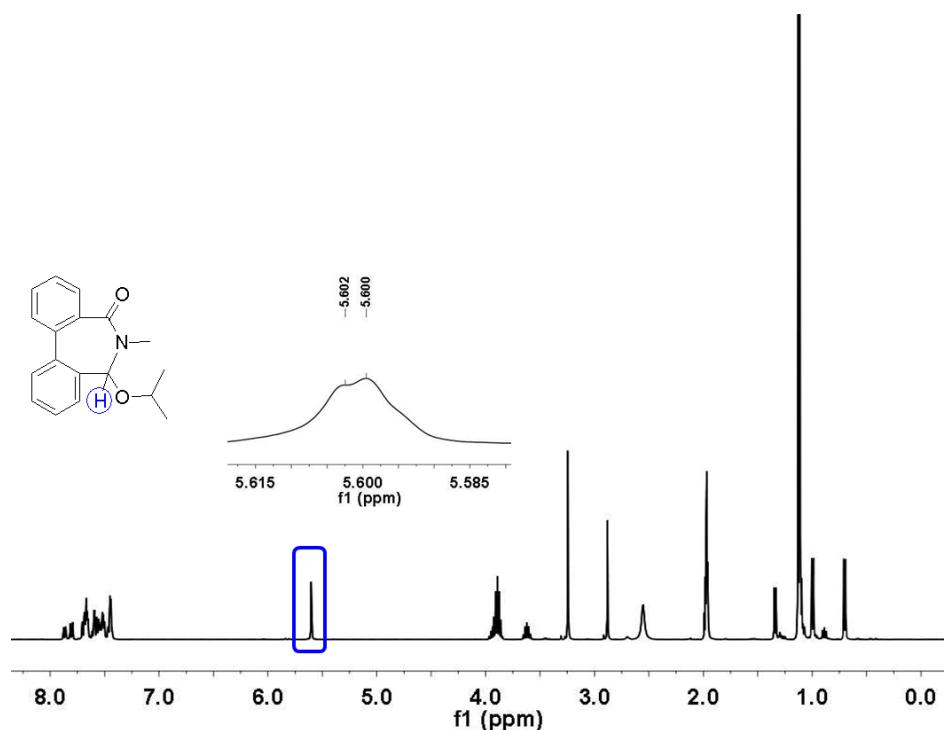


Figure S9. ¹H-NMR spectrum of the reaction of **2a** and 2-propanol in the presence of MA in CD₃CN at R.T.

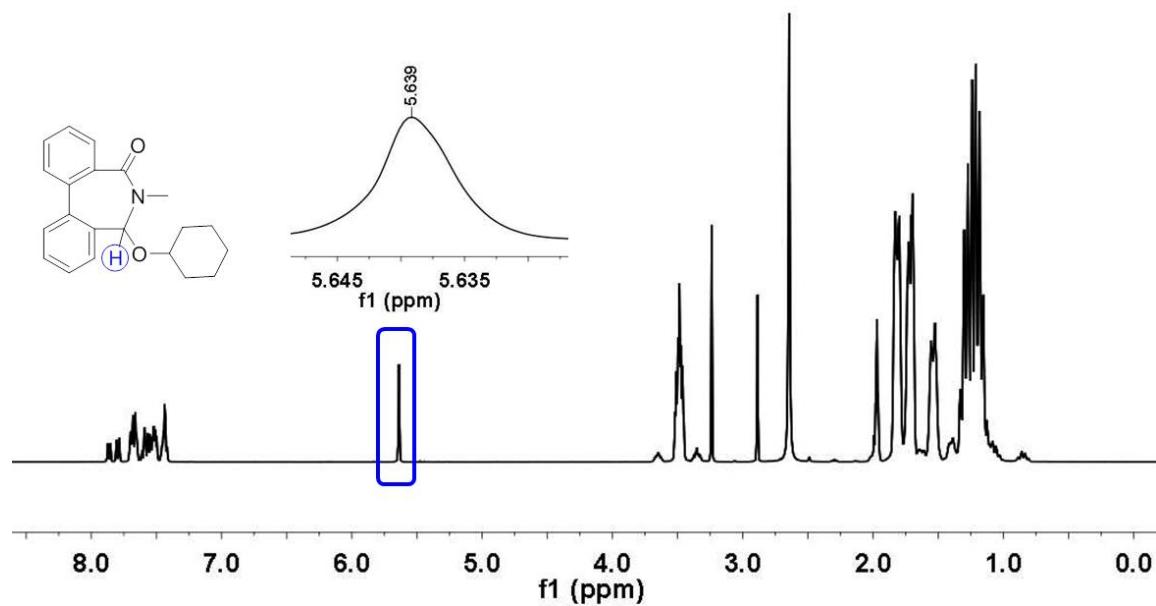


Figure S10. ^1H -NMR spectrum of the reaction of **2a** and cyclohexanol in the presence of MA in CD_3CN at R.T.

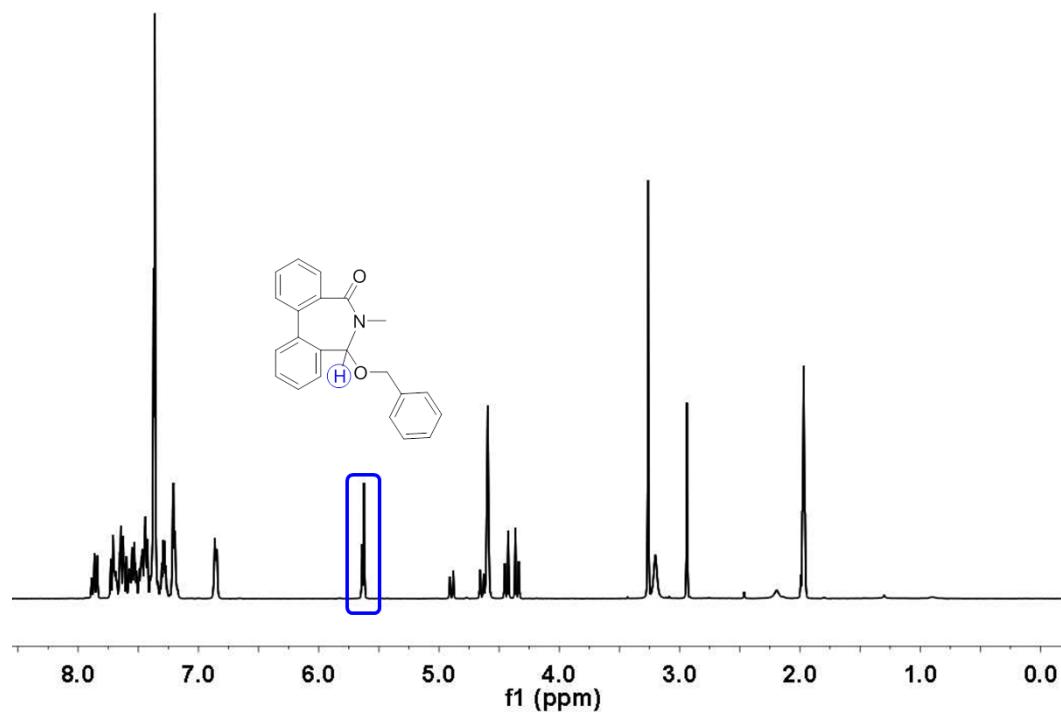


Figure S11. ^1H -NMR spectrum of the reaction of **2a** and benzyl alcohol in the presence of MA in CD_3CN at R.T.

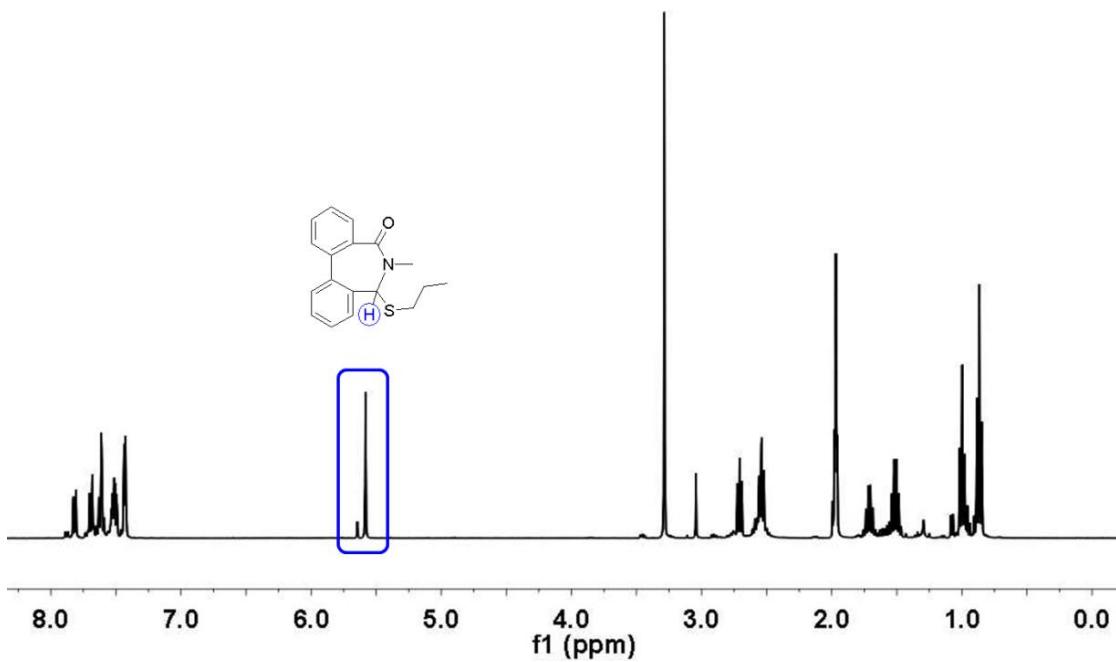


Figure S12. ¹H NMR spectrum of the reaction of **2a** and 1-propanethiol in the presence of MA in CD₃CN at R.T.

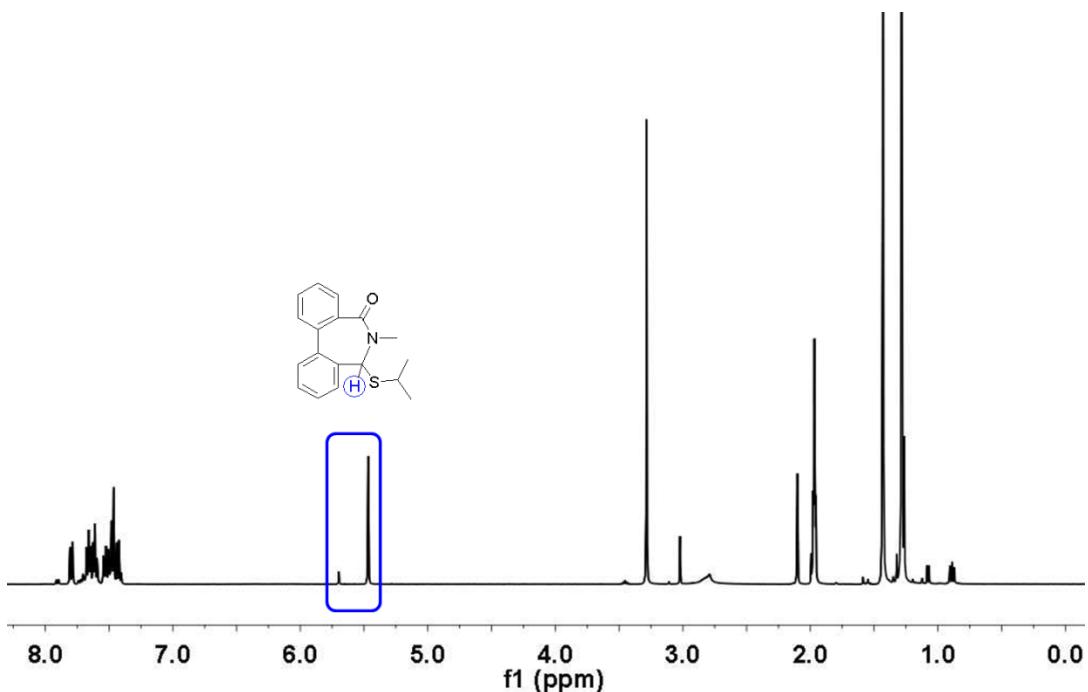


Figure S13. ¹H NMR spectrum of the reaction of **2a** and 2-propanethiol in the presence of MA in CD₃CN at R.T.

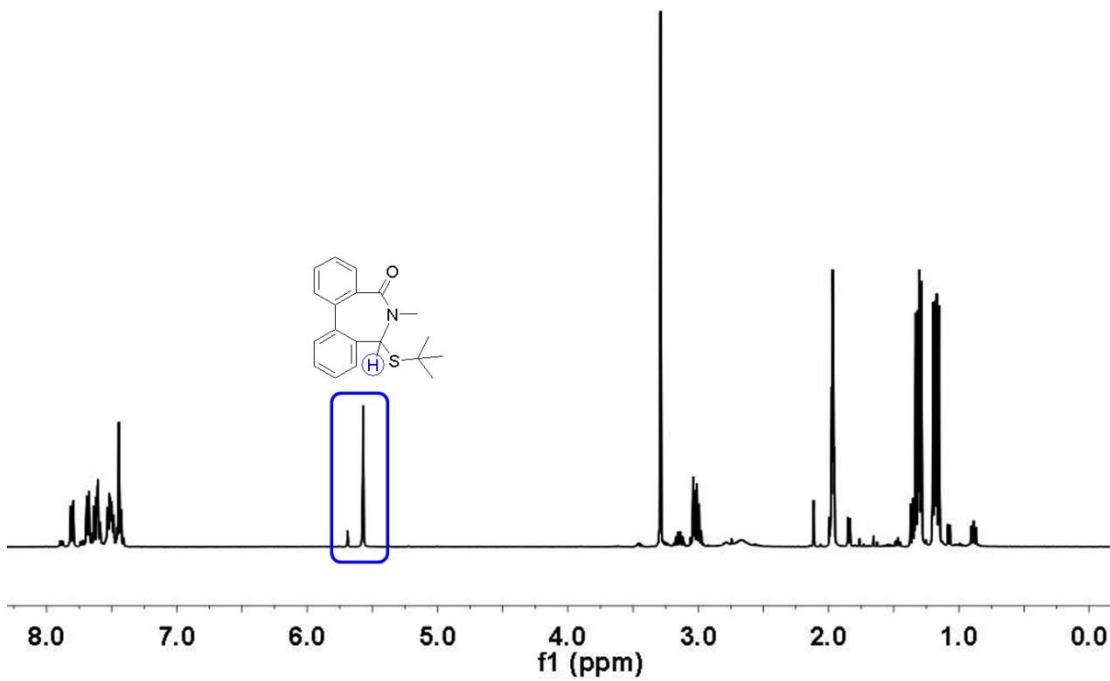


Figure S14. ¹H NMR spectrum of the reaction of **2a** and *tert*-butylthiol in the presence of MA in CD₃CN at R.T.

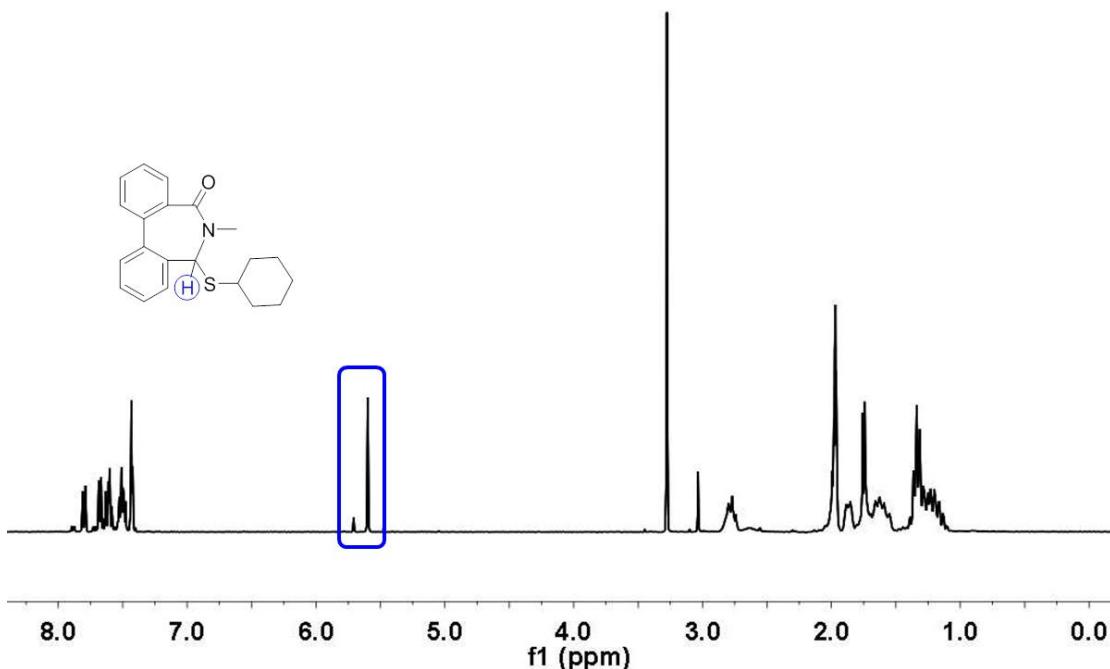


Figure S15. ¹H NMR spectrum of the reaction of **2a** and cyclohexanethiol in the presence of MA in CD₃CN at R.T.

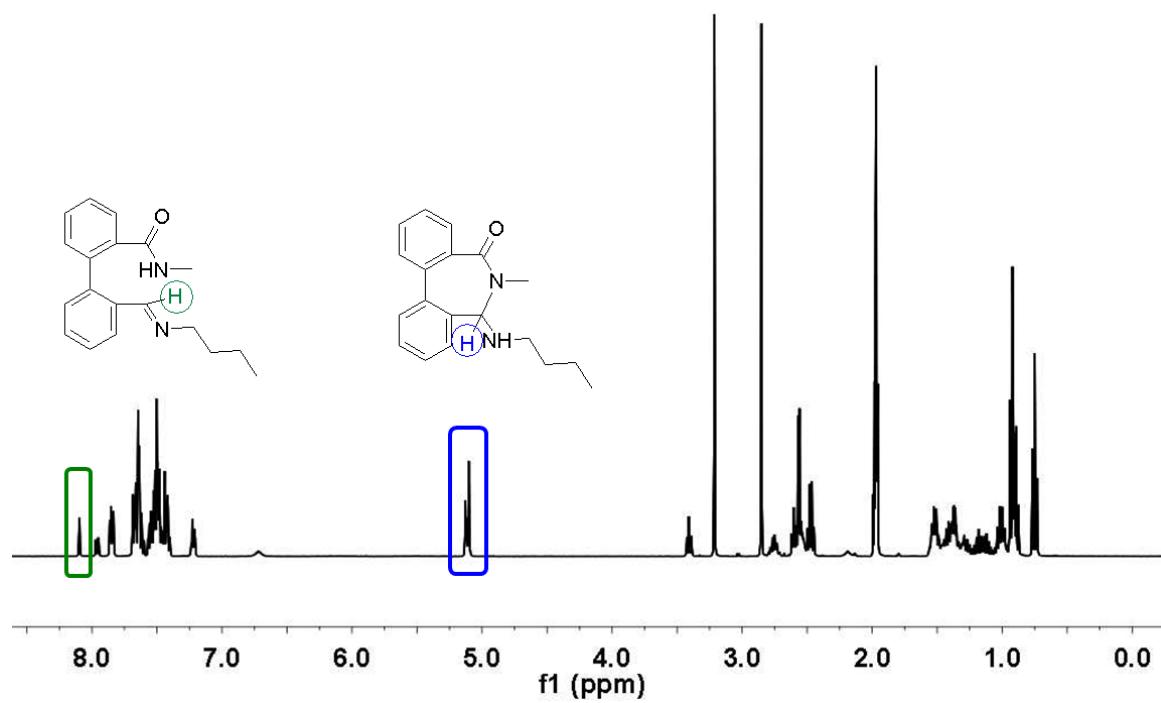


Figure S16. ^1H NMR spectrum of the reaction of **2a** and 1-butylamine in CD_3CN at 60°C .

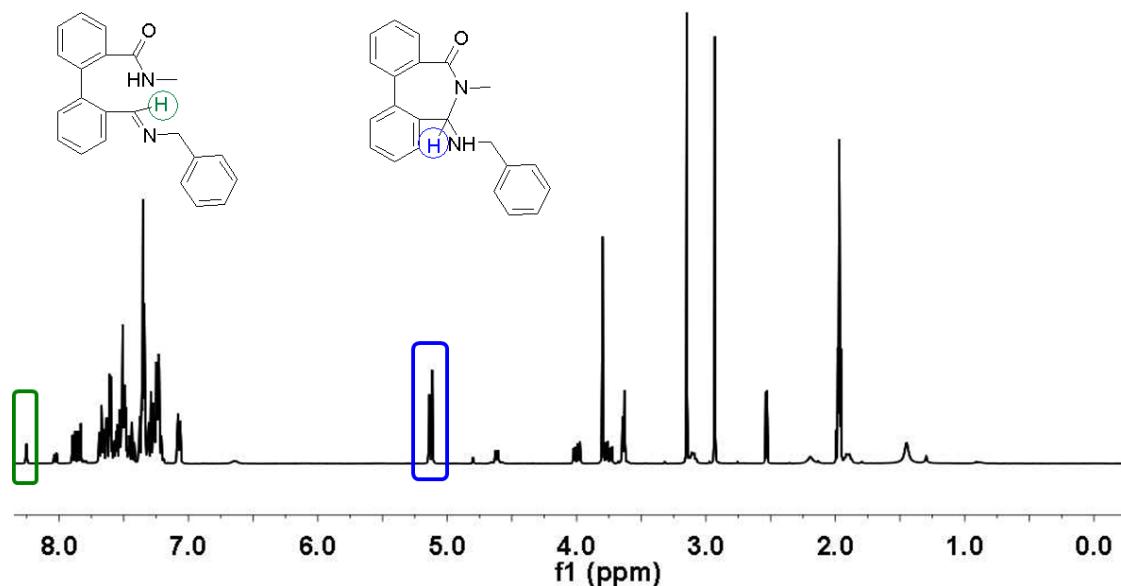


Figure S17. ^1H -NMR spectrum of the reaction of **2a** and phenylmethanamine in CD_3CN at 60°C .

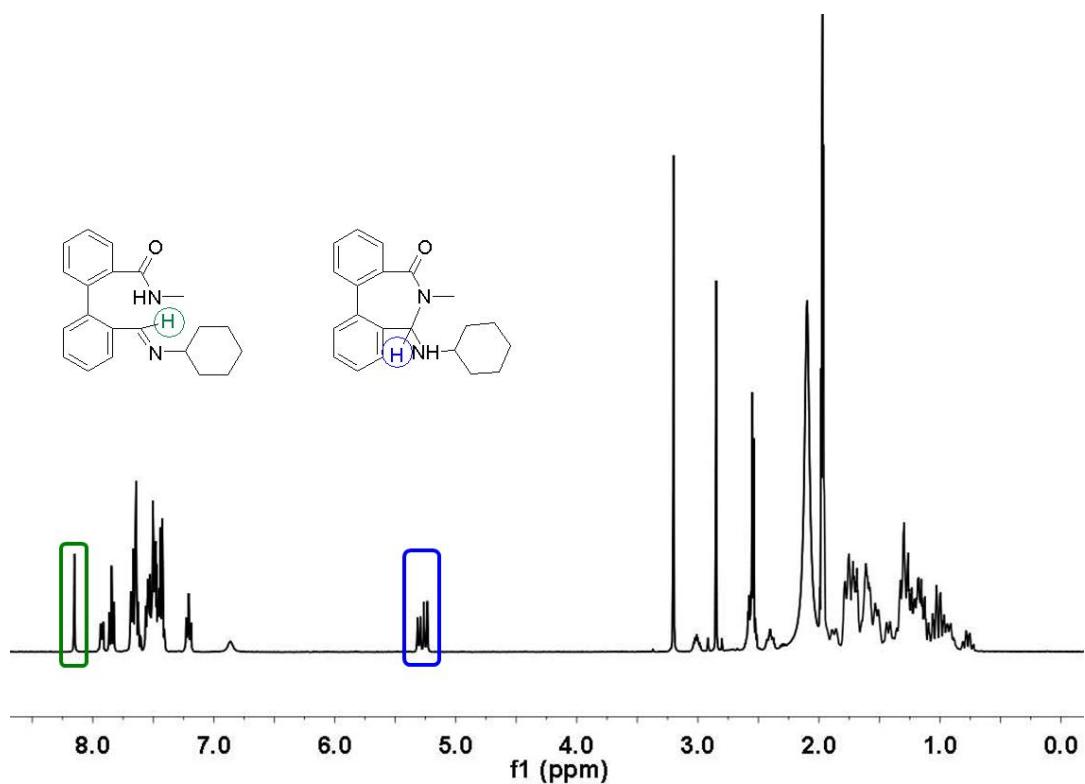


Figure S18. ^1H -NMR spectrum of the reaction of **2a** and cyclohexylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

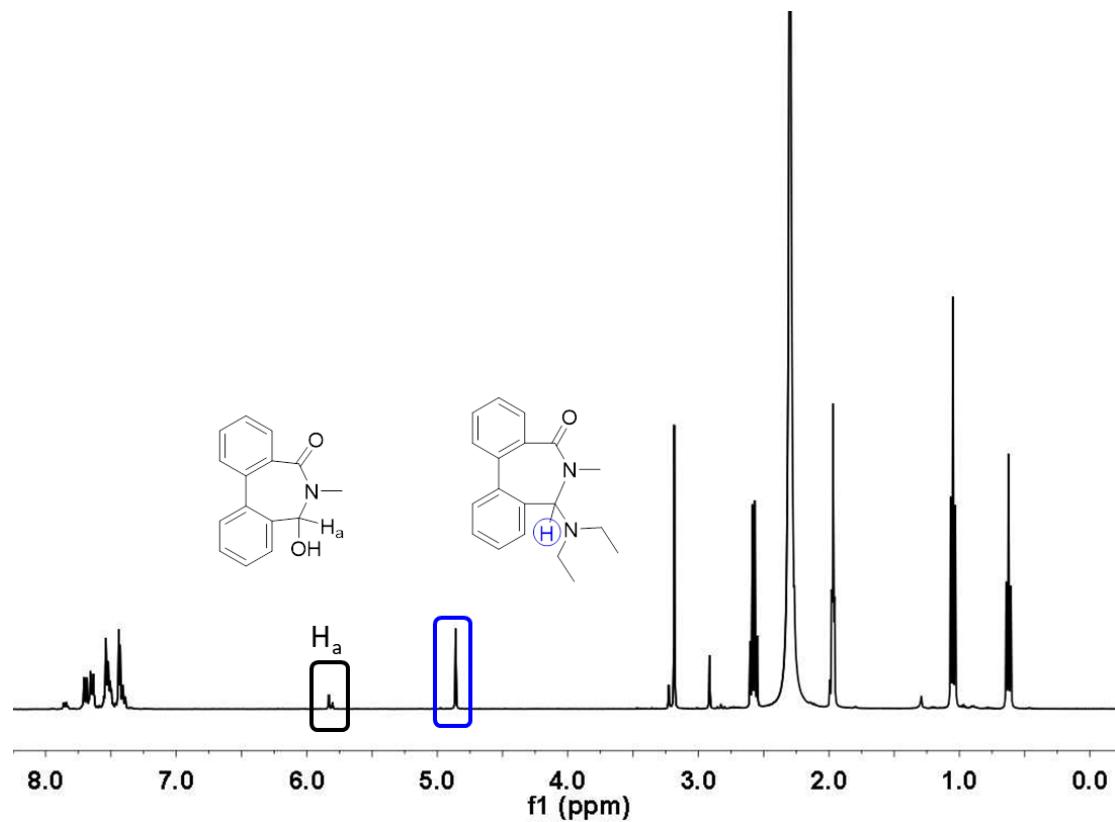


Figure S19. ^1H -NMR spectrum of the reaction of **2a** and diethylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

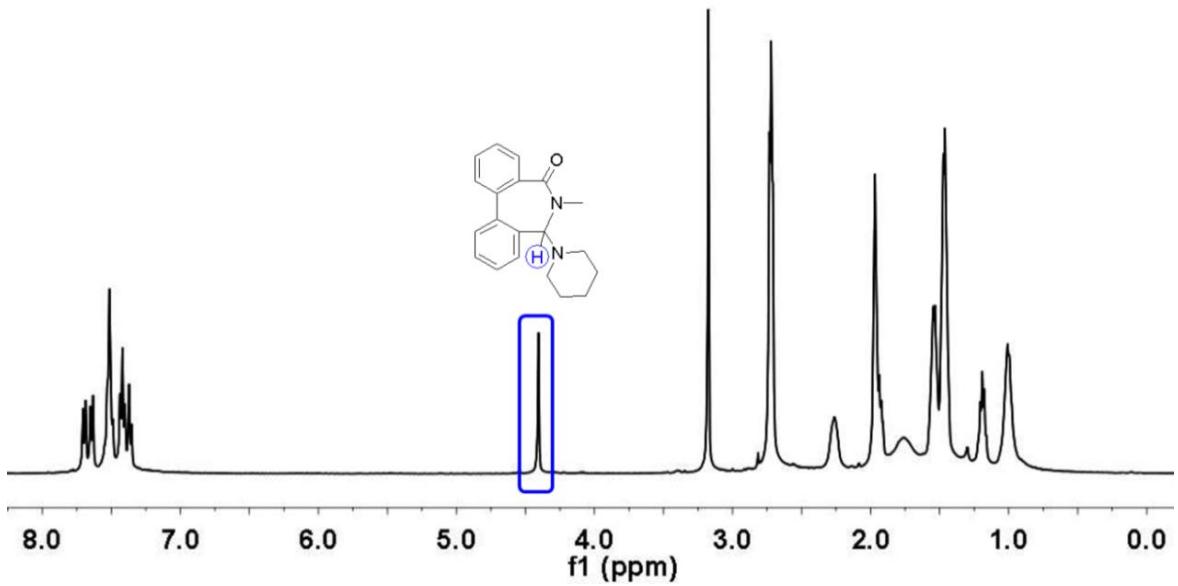


Figure S20. ^1H -NMR spectrum of the reaction of **2a** and piperidine in CD_3CN at $60\text{ }^\circ\text{C}$.

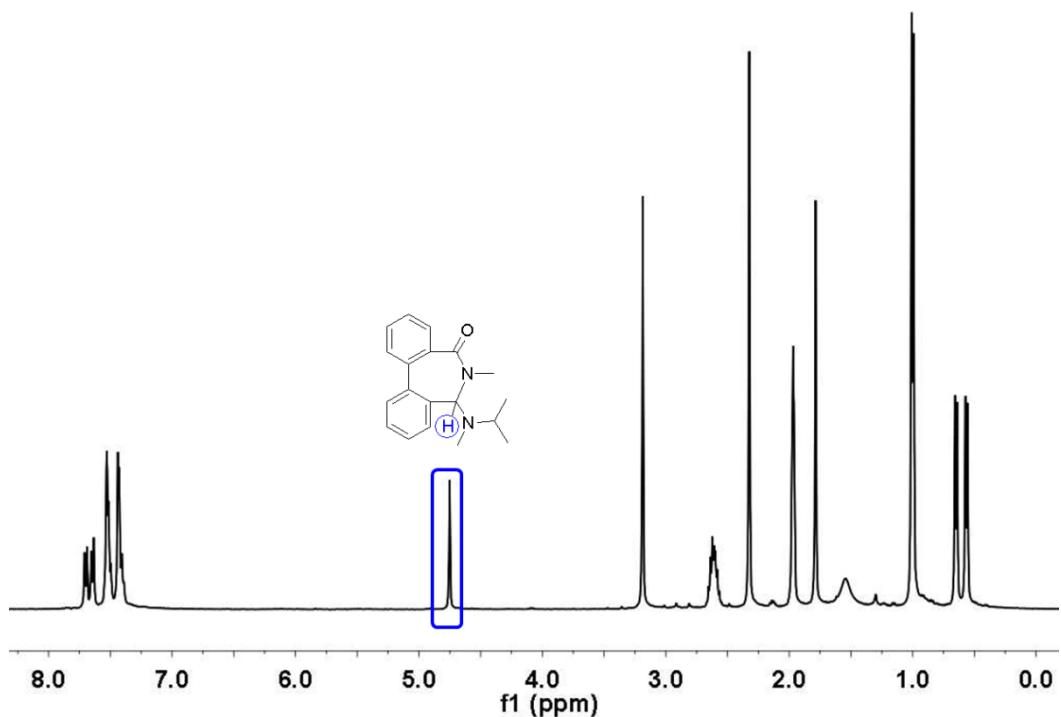


Figure S21. ^1H -NMR spectrum of the reaction of **2a** and *N*-isopropyl-methylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

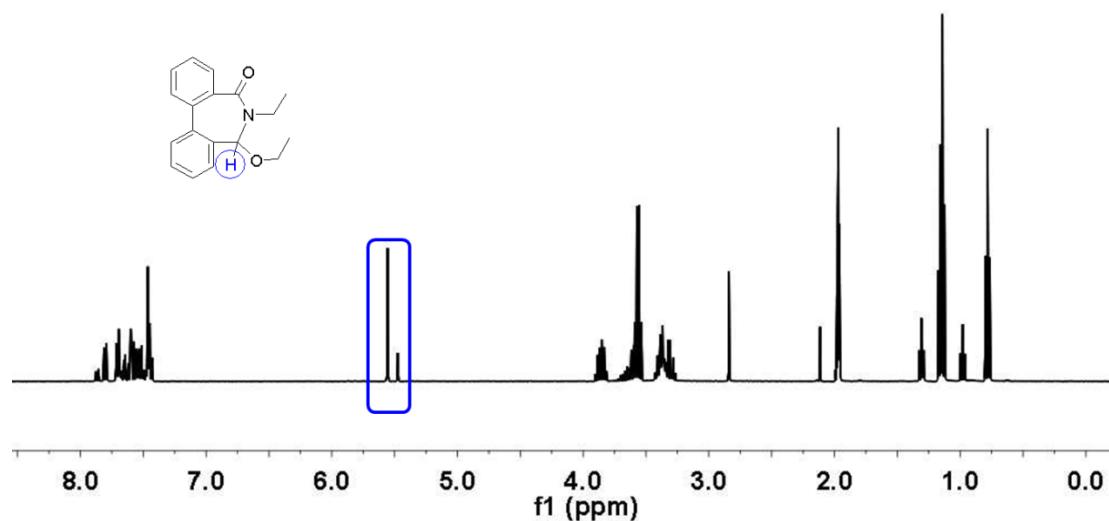


Figure S22. ¹H-NMR spectrum of the reaction of **2b** and ethanol in the presence of MA in CD₃CN at R.T.

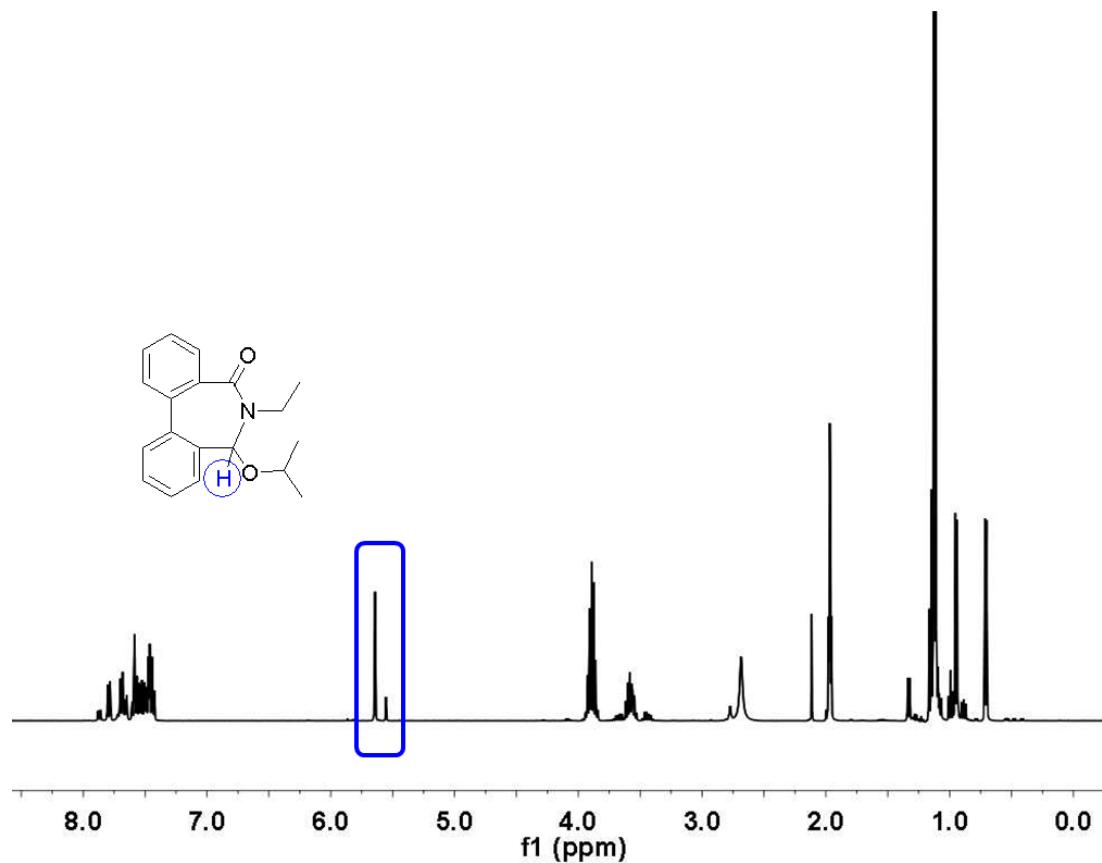


Figure S23. ¹H-NMR spectrum of the reaction of **2b** and 2-propanol in the presence of MA in CD₃CN at R.T.

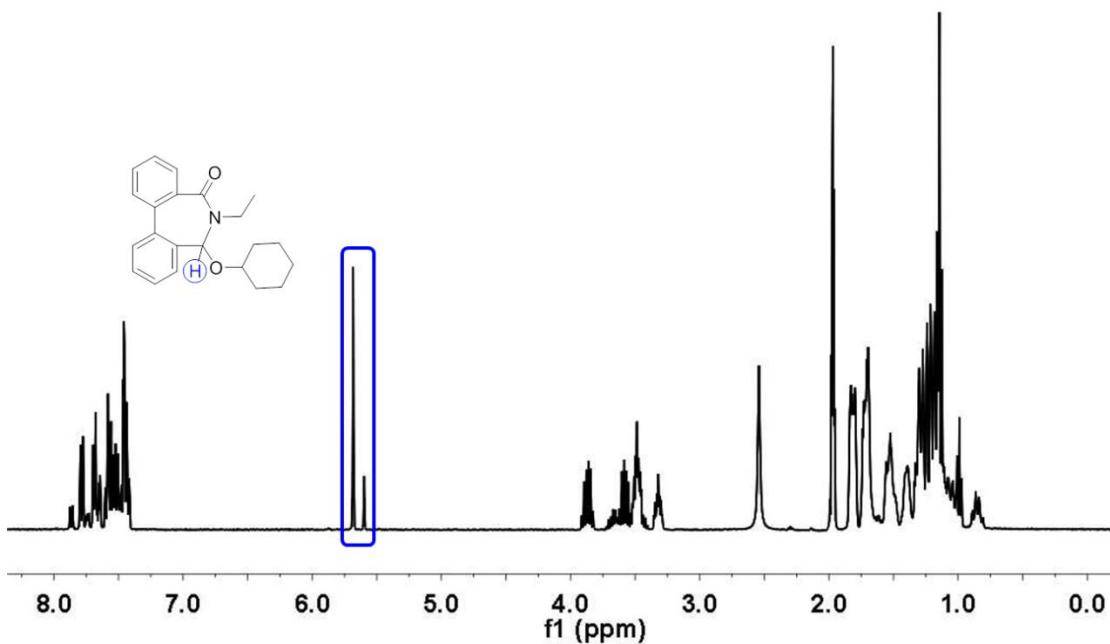


Figure S24. ¹H-NMR spectrum of the reaction of 2b and cyclohexanol in the presence of MA in CD₃CN at R.T.

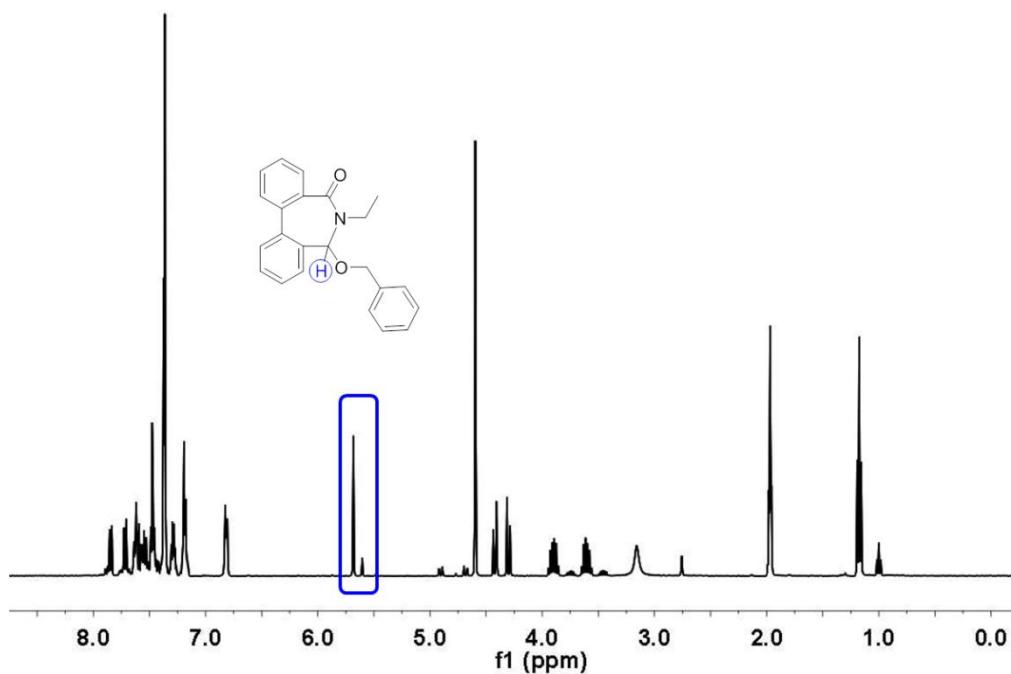


Figure S25. ¹H-NMR spectrum of the reaction of **2b** and benzyl alcohol in the presence of MA in CD₃CN at R.T.

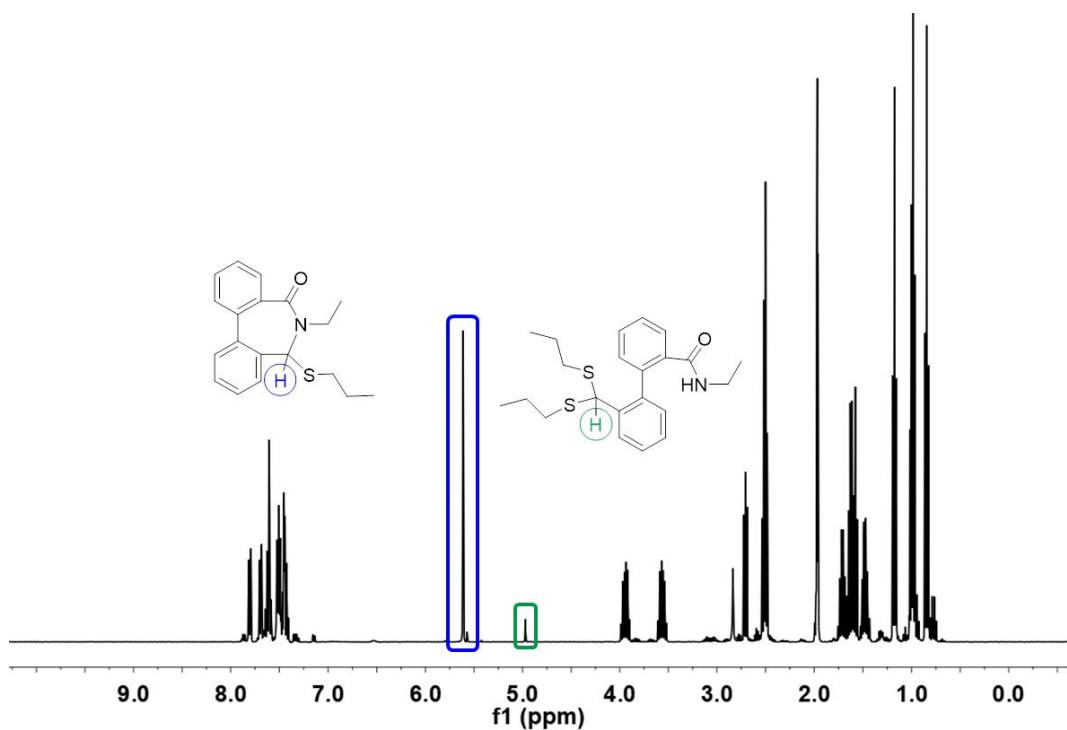


Figure S26. ^1H NMR spectrum of the reaction of **2b** and 1-propanethiol in the presence of MA in CD_3CN at R.T.

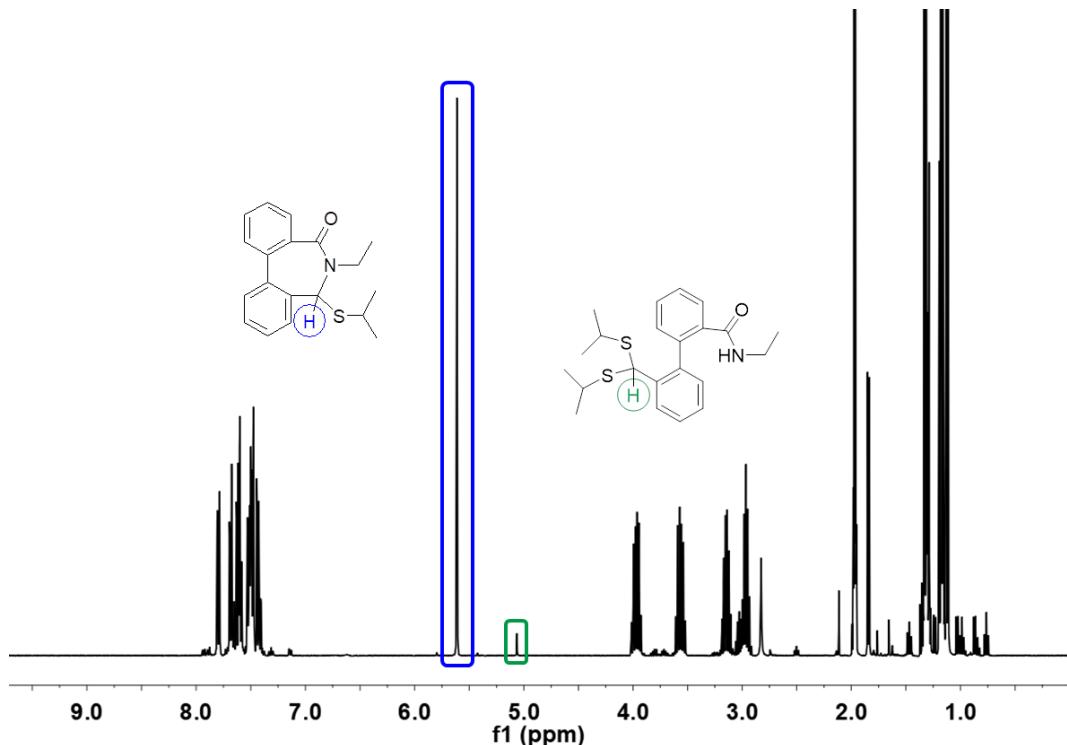


Figure S27. ^1H NMR spectrum of the reaction of **2b** and 2-propanethiol in the presence of MA in CD_3CN at R.T.

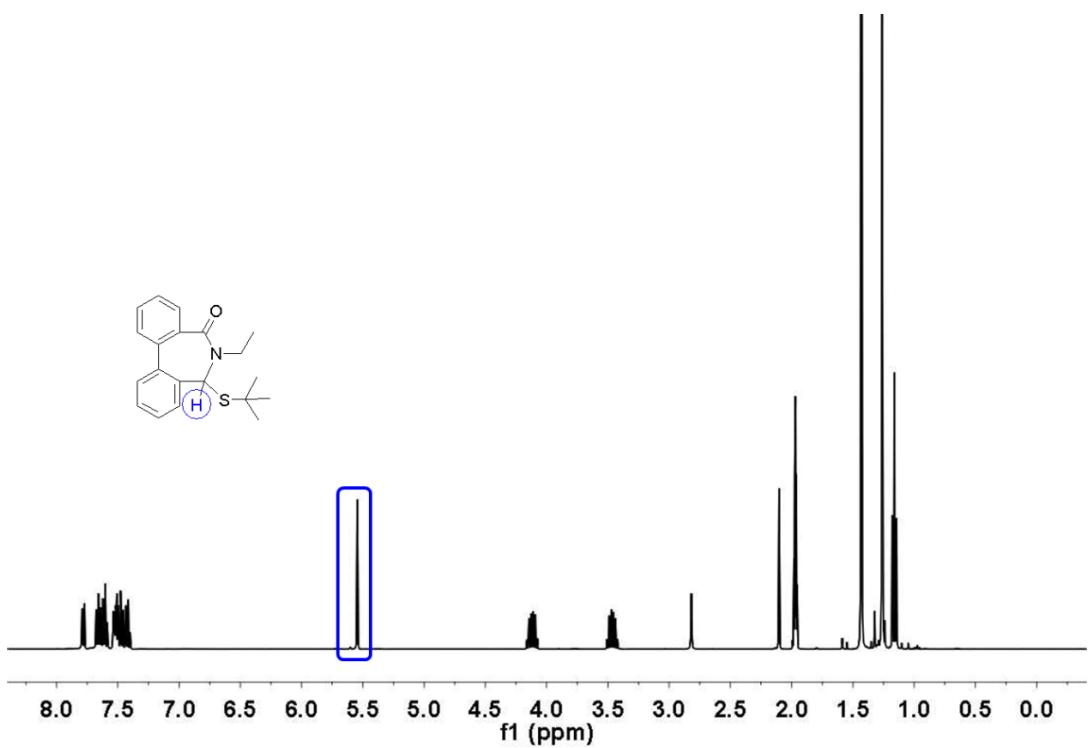


Figure S28. ¹H NMR spectrum of the reaction of **2b** and *tert*-butylthiol in the presence of MA in CD₃CN at R.T.

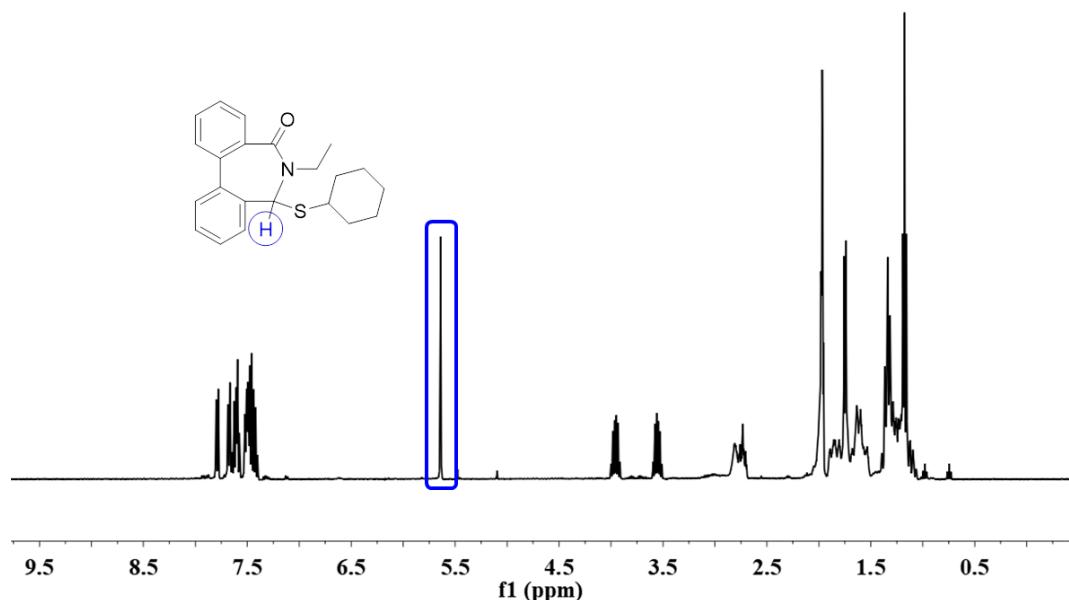


Figure S29. ¹H NMR spectrum of the reaction of **2b** and cyclohexanethiol in the presence of MA in CD₃CN at R.T.

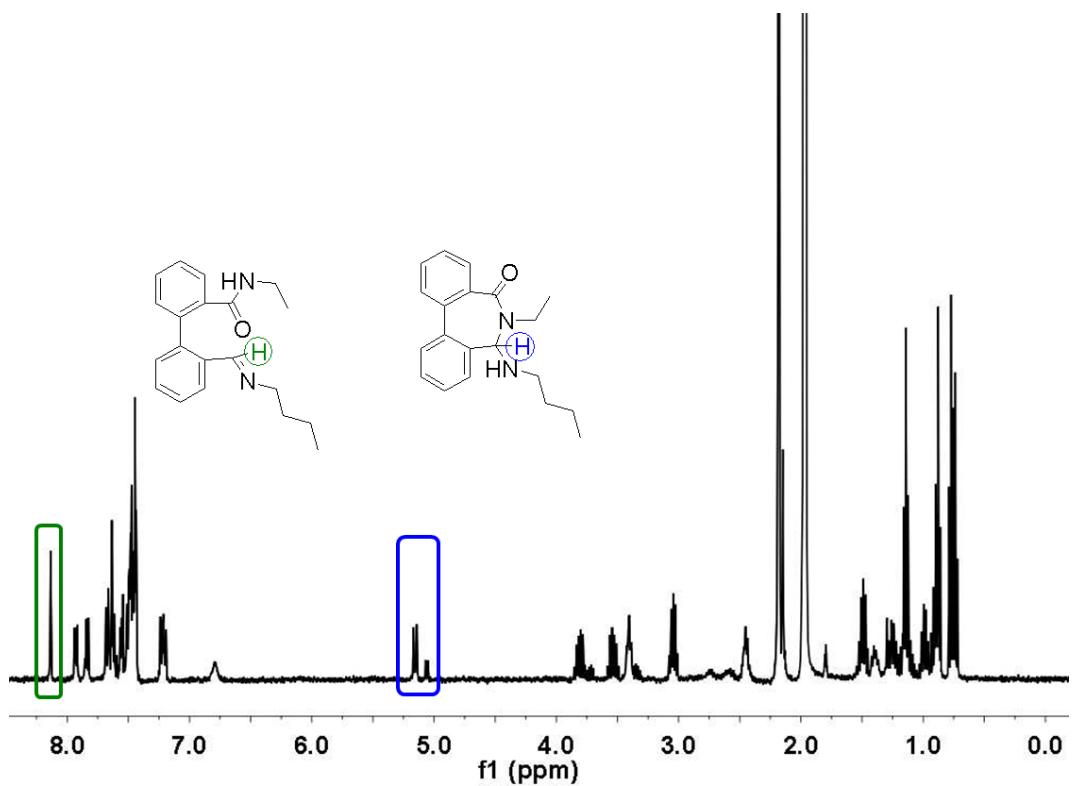


Figure S30. ^1H NMR spectrum of the reaction of **2b** and 1-butylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

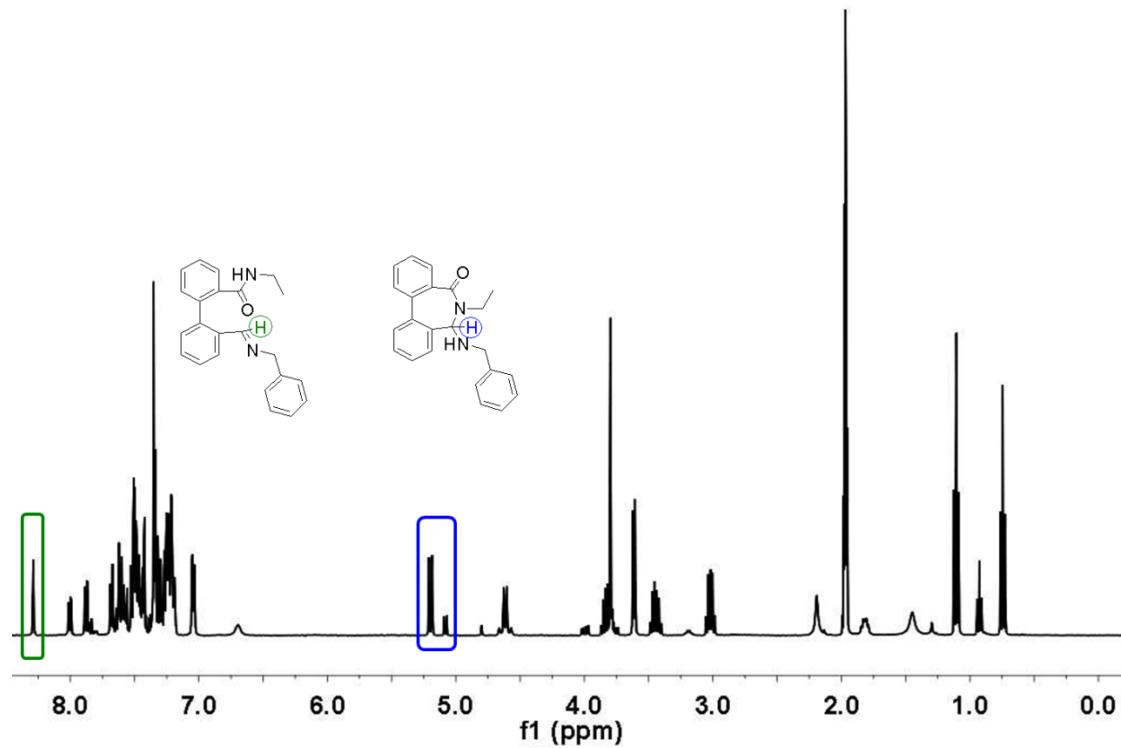


Figure S31. ^1H NMR spectrum of the reaction of **2b** and phenylmethanamine in CD_3CN at $60\text{ }^\circ\text{C}$.

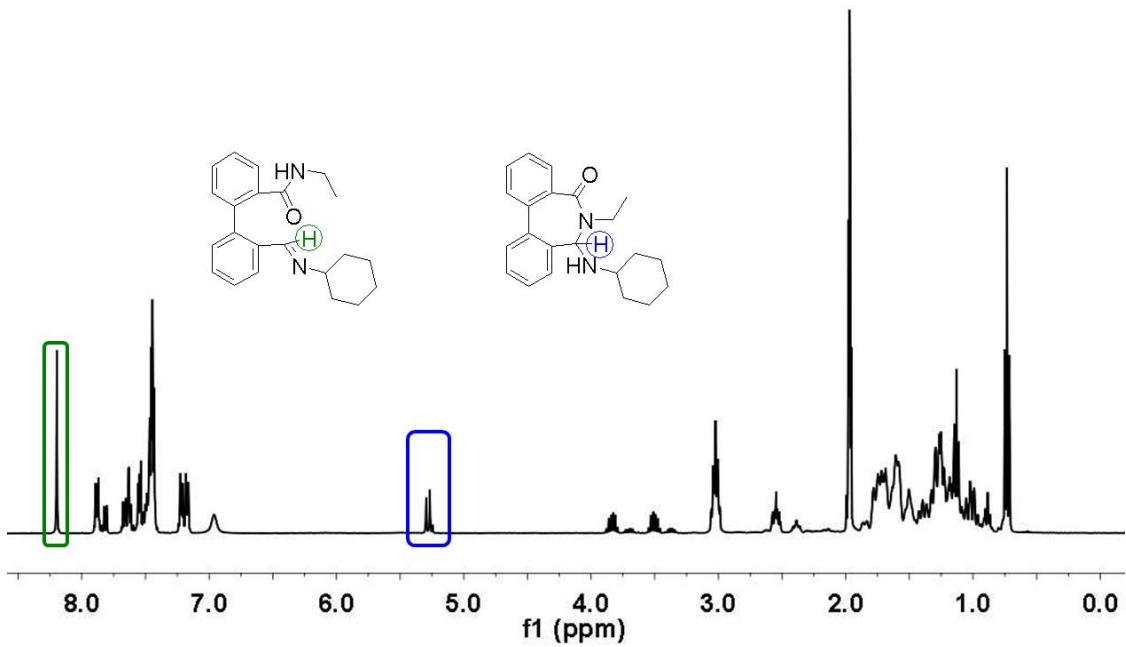


Figure S32. ^1H NMR spectrum of the reaction of **2b** and cyclohexylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

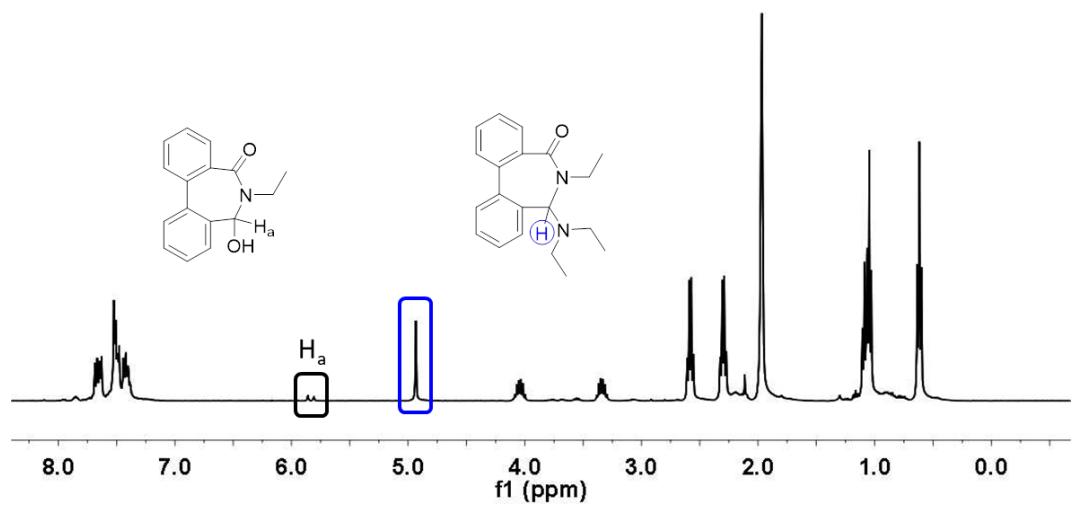


Figure S33. ^1H -NMR spectrum of the reaction of **2b** and diethylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

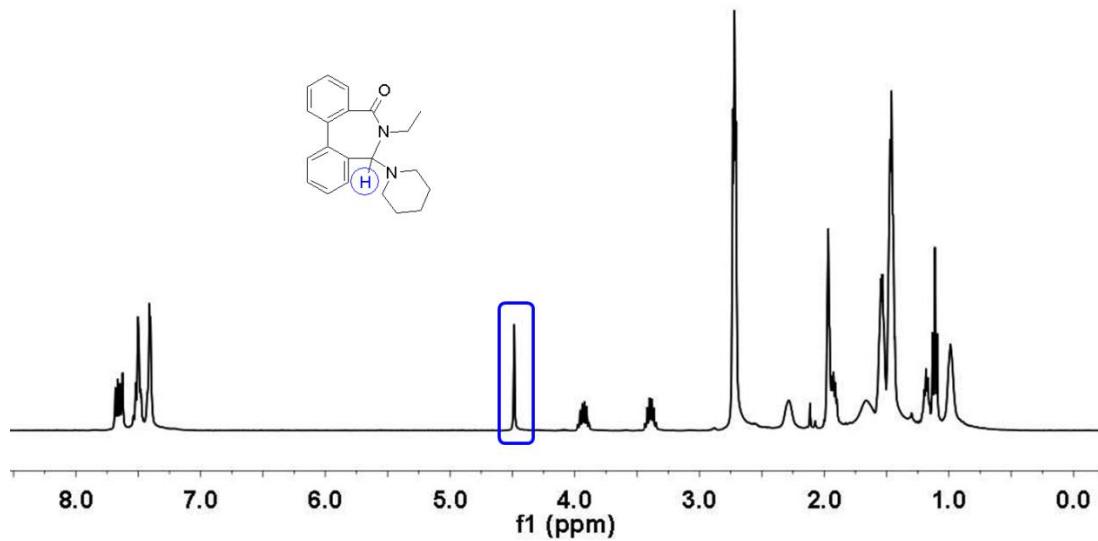


Figure S34. ^1H -NMR spectrum of the reaction of **2b** and piperidine in CD_3CN at $60\text{ }^\circ\text{C}$.

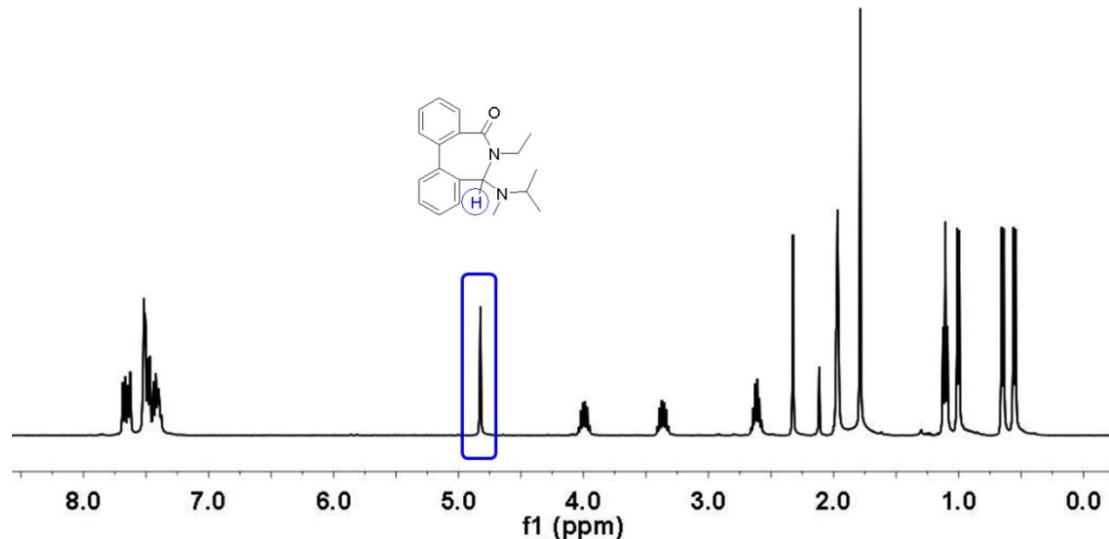


Figure S35. ^1H -NMR spectrum of the reaction of **2b** and *N*-isopropyl-methylamine in CD_3CN at $60\text{ }^\circ\text{C}$.

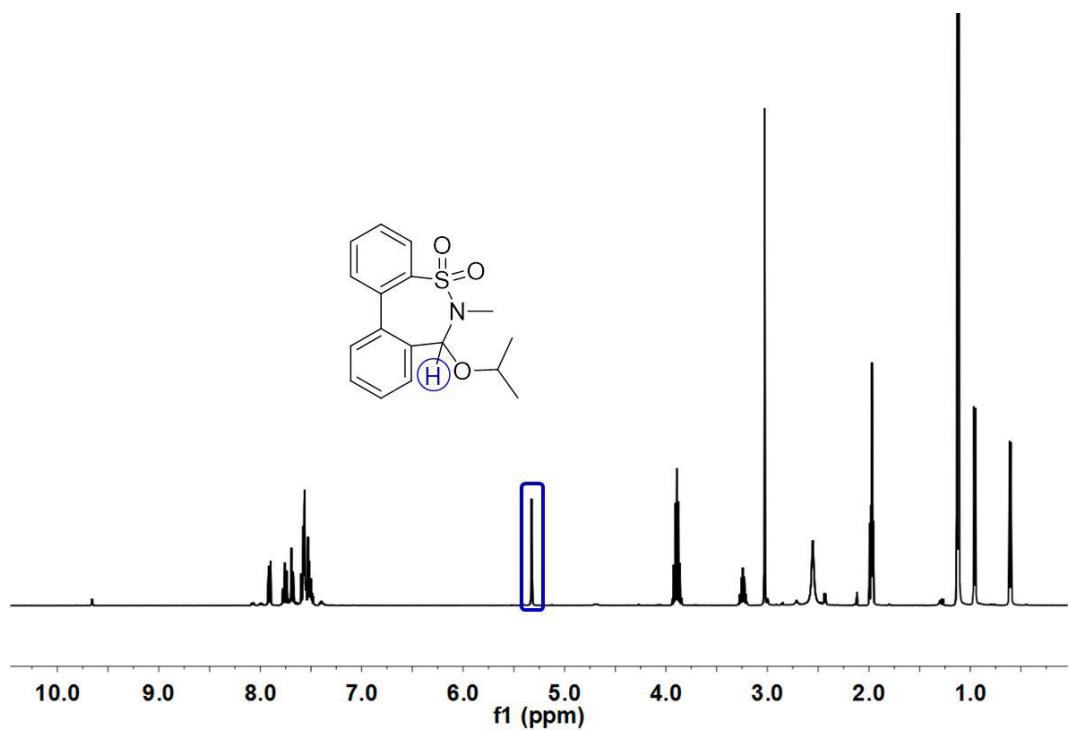


Figure S36. ¹H-NMR spectrum of the reaction of **2c** and 2-propanol in the presence of MA in CD₃CN at R.T.

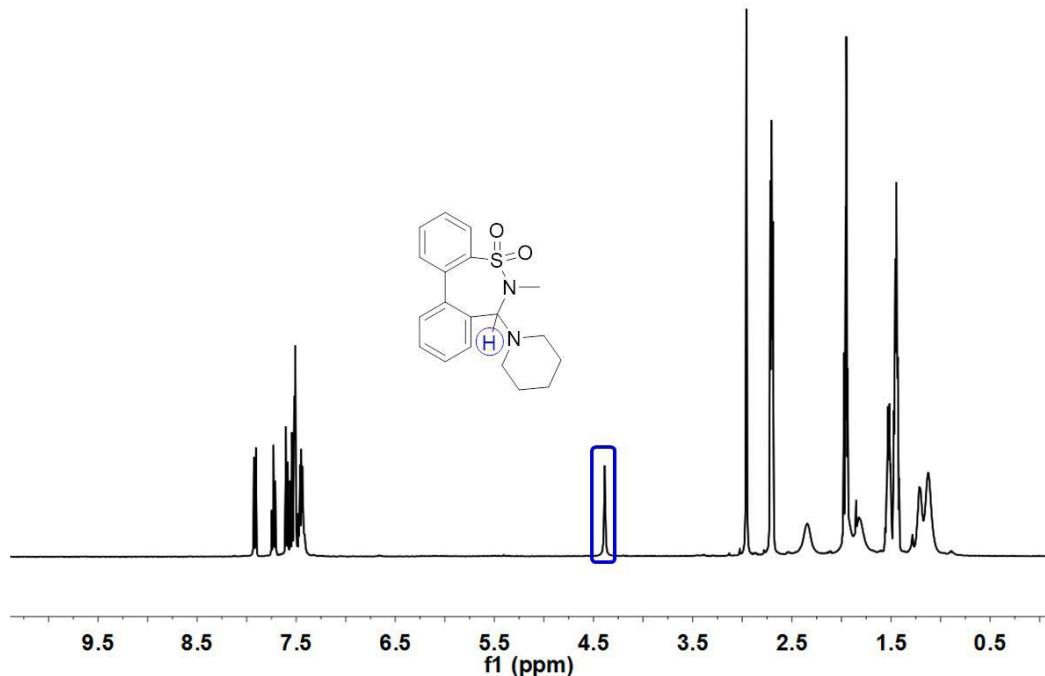


Figure S37. ¹H-NMR spectrum of the reaction of **2c** and piperidine in CD₃CN at R.T.

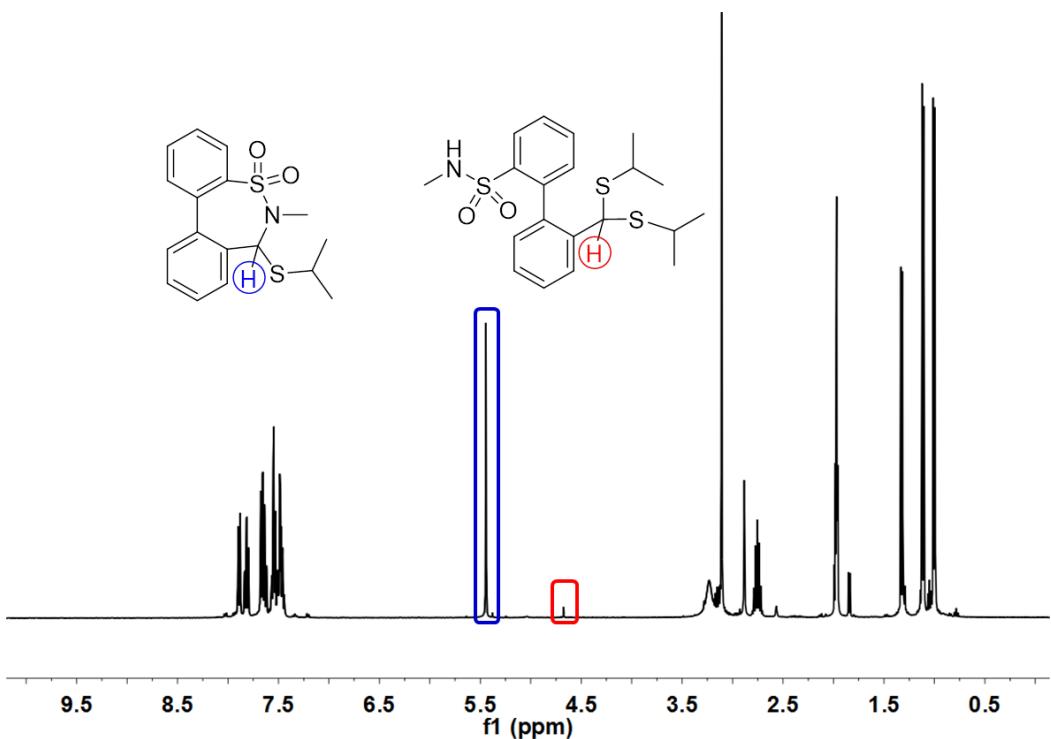


Figure S38. ¹H NMR spectrum of the reaction of **2k** and 2-propanethiol in the presence of MA in CD₃CN at R.T.

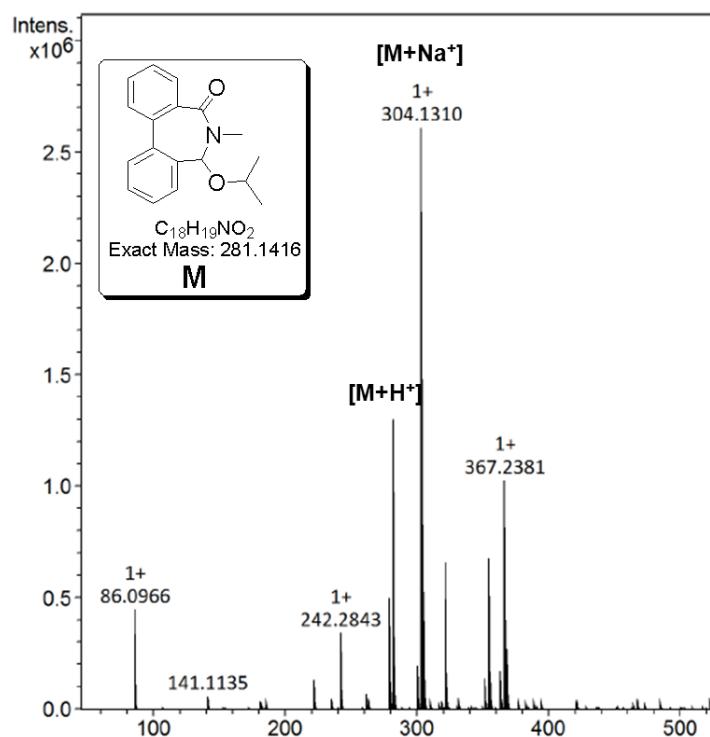


Figure S39. Mass spectrum of the solution of DCR of **2a** with 2-propanol.

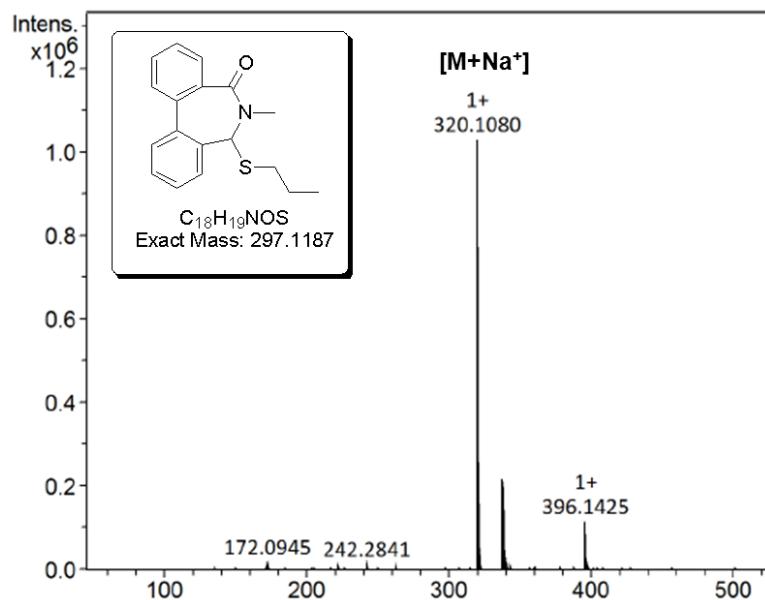


Figure S40. Mass spectrum of the solution of DCR of **2a** with 1-propanethiol.

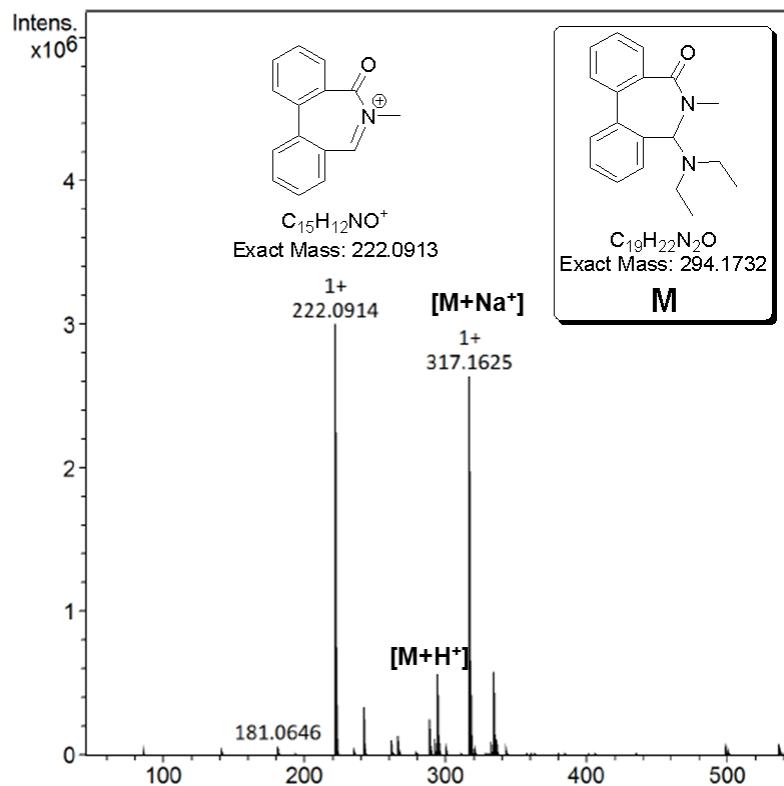


Figure S41. Mass spectrum of the solution of DCR of **2a** with diethylamine.

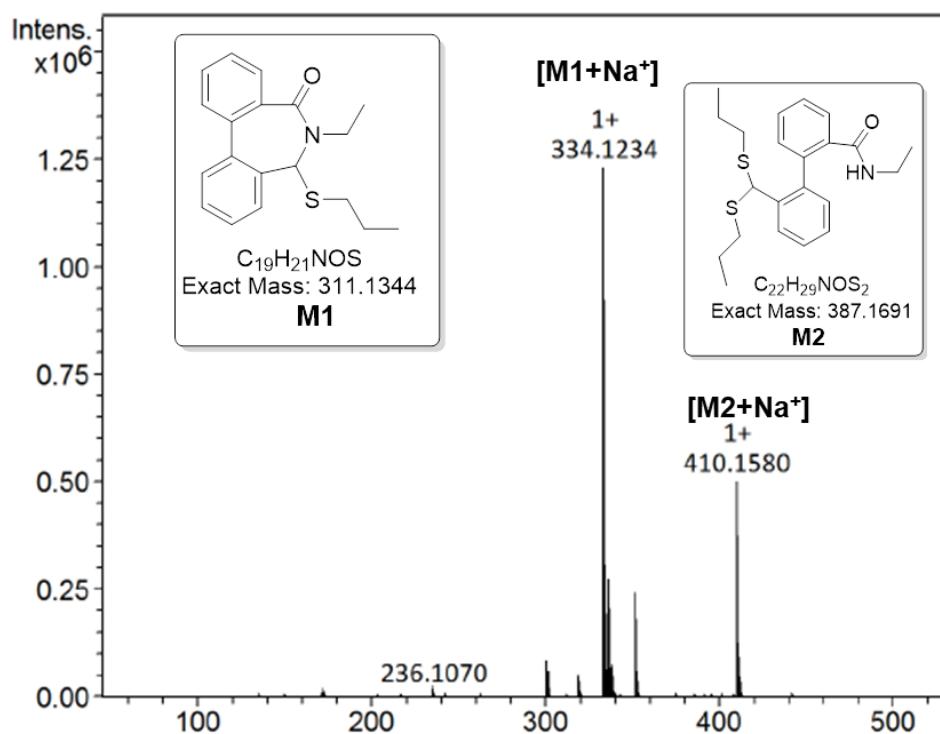


Figure S42. Mass spectrum of the solution of DCR of **2b** with 1-propanethiol.

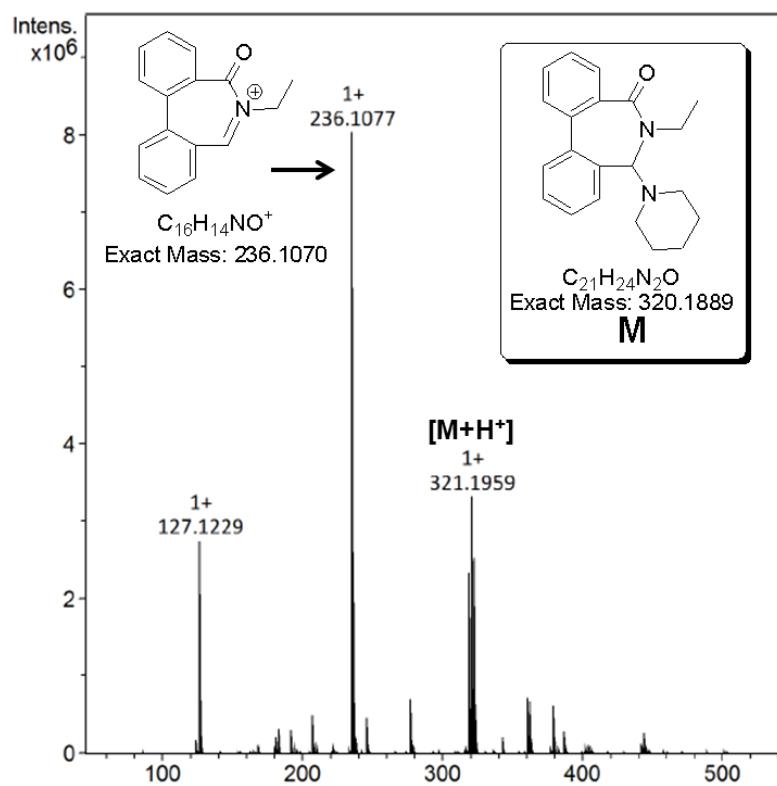


Figure S43. Mass spectrum of the solution of DCR of **2b** with piperidine.

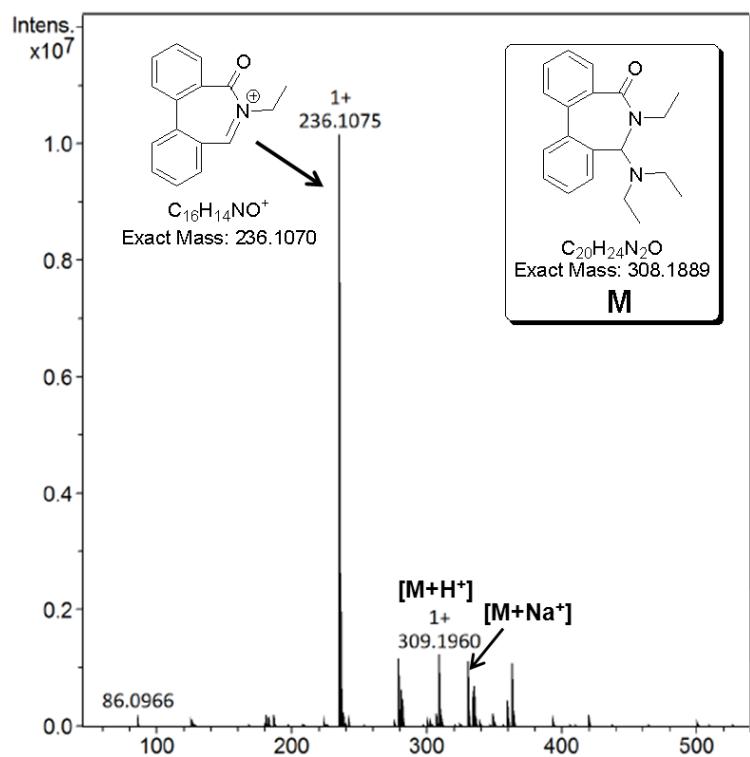


Figure S44. Mass spectrum of the solution of DCR of **2b** with diethylamine.

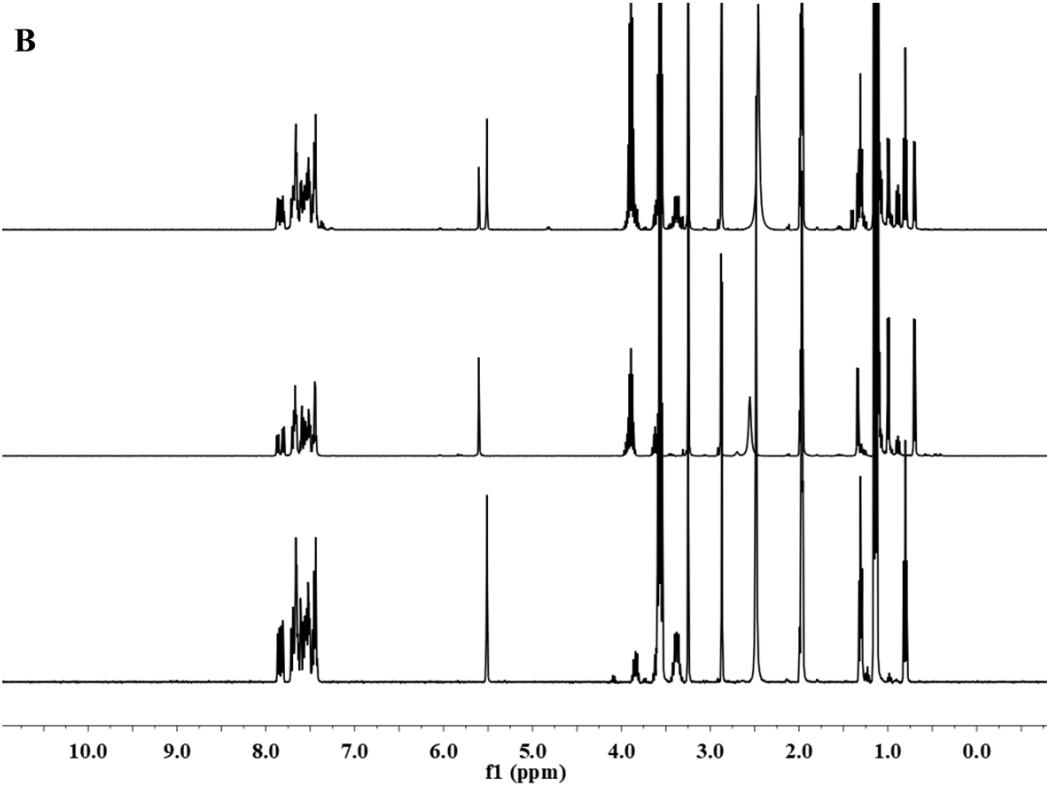
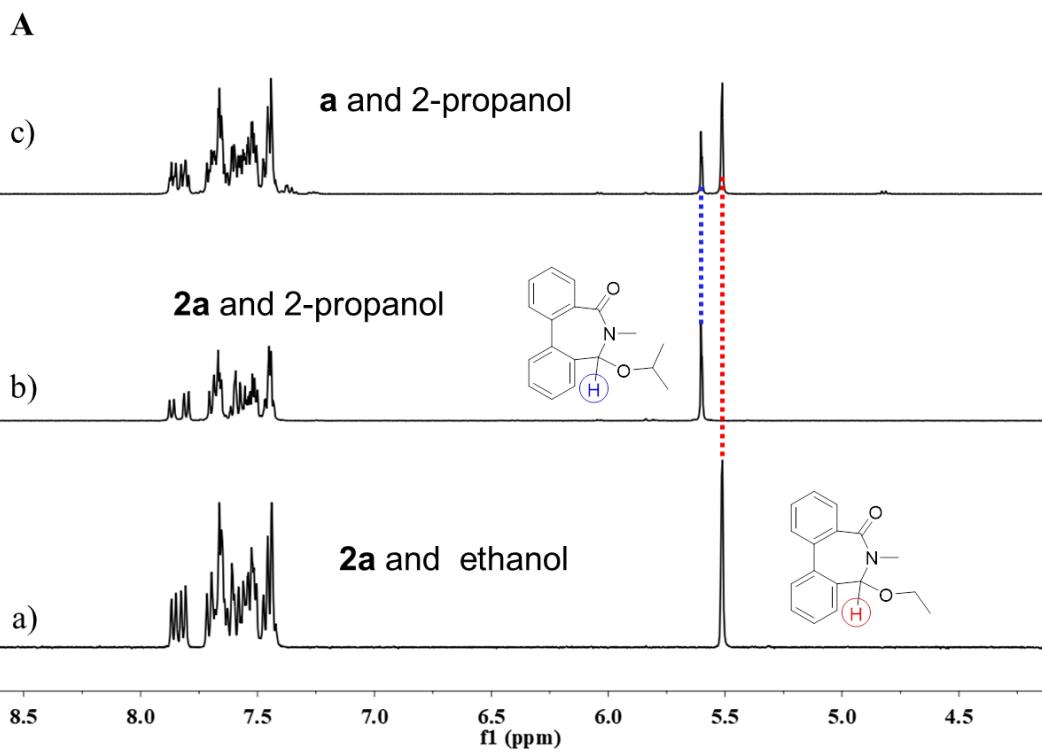


Figure S45. (A) Dynamic component exchange of alcohols: the reaction of **2a** with ethanol (a); the reaction of **2a** with 2-propanol (b); the addition of 2-propanol into panel a (c). (B) The full ^1H NMR spectra of A.

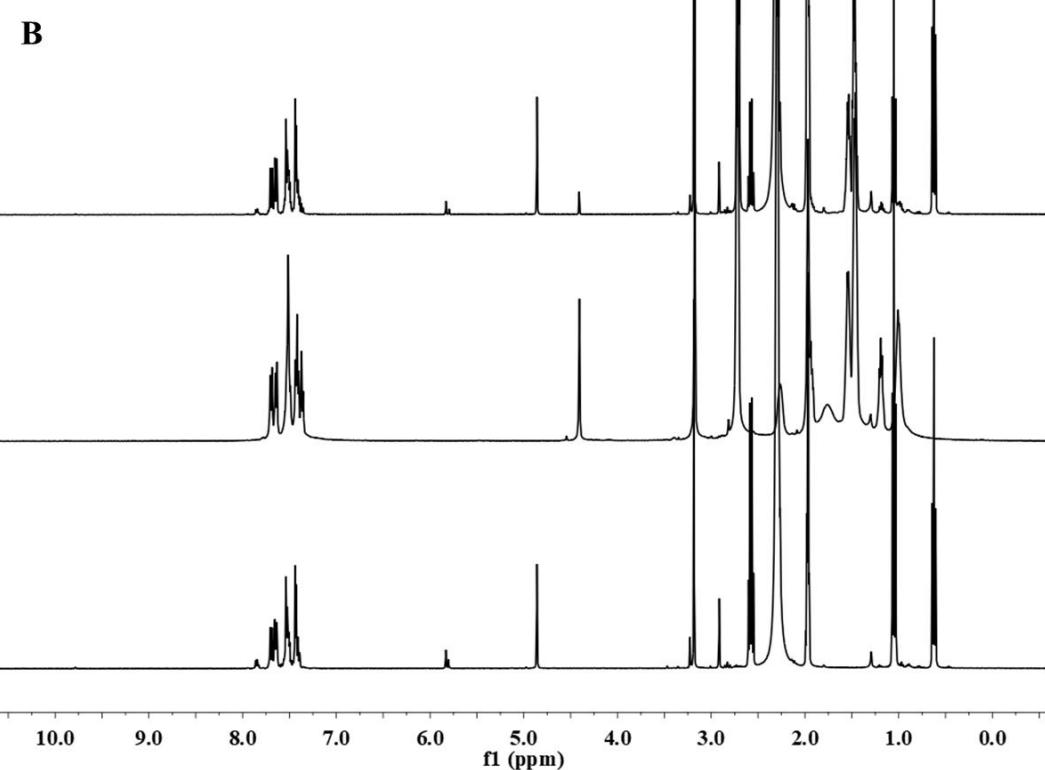
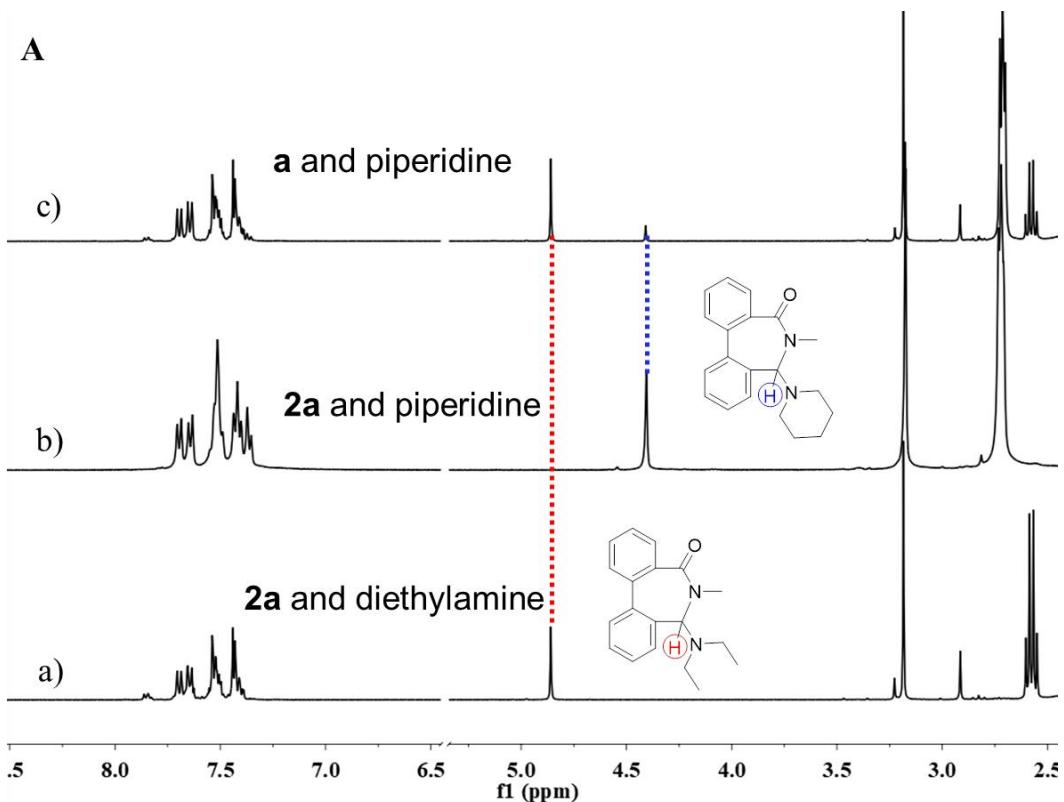


Figure S46. (A) Dynamic component exchange of secondary amines: the reaction of **2a** with diethylamine (a); the reaction of **2a** with piperidine (b); the addition of piperidine into panel a (c). (B) The full ^1H NMR spectra of A.

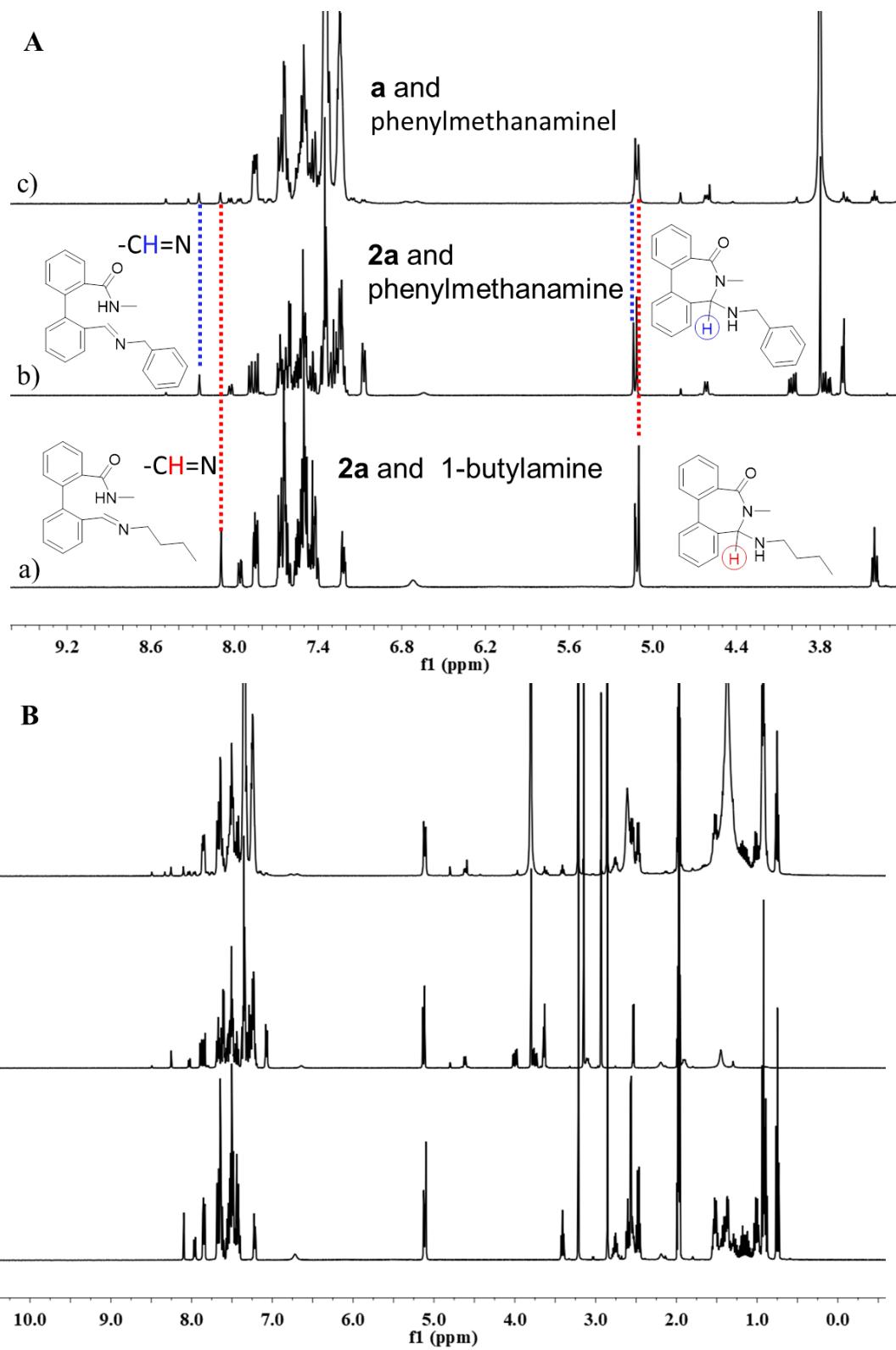
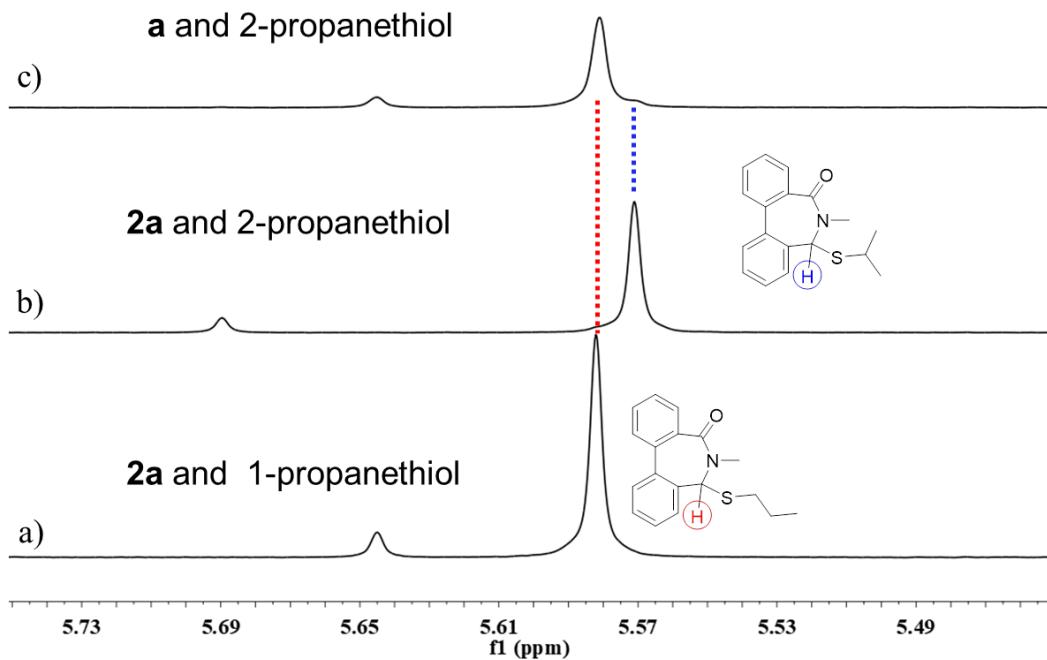


Figure S47. (A) Dynamic component exchange of primary amines: the reaction of **2a** with 1-butylamine (a); the reaction of **2a** with benzylamine (b); the addition of benzylamine into panel a (c). (B) The full ^1H NMR spectra of A.

A



B

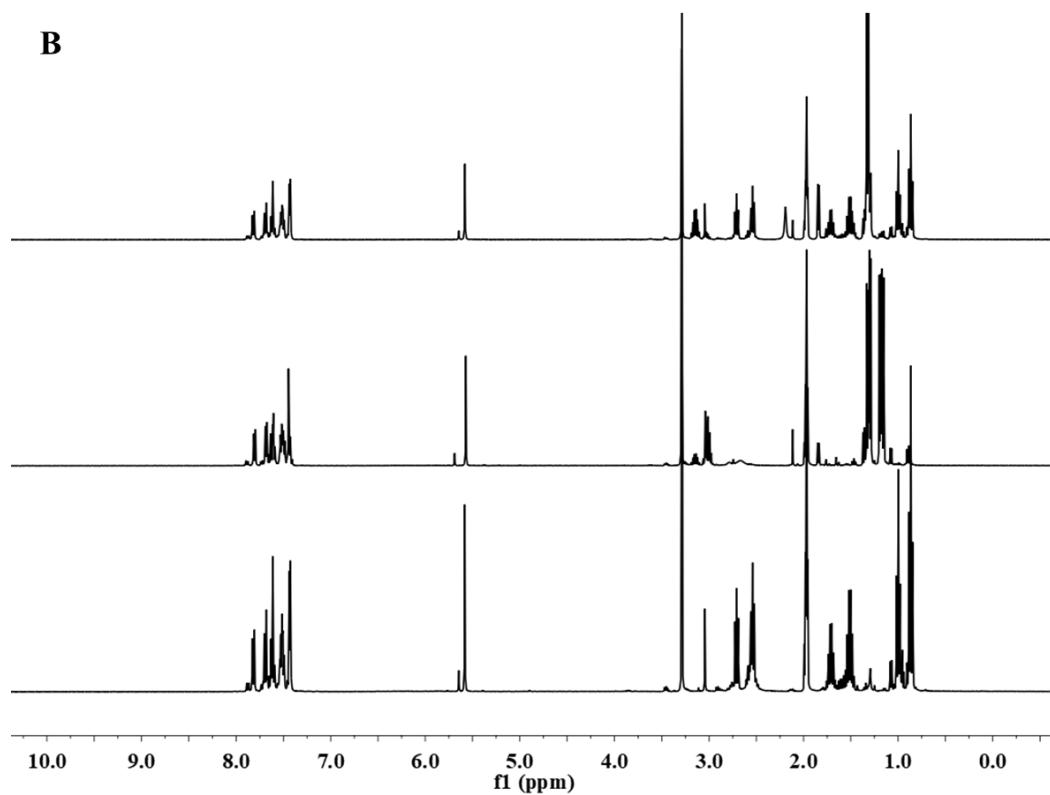


Figure S48. (A) Dynamic component exchange of thiols: the reaction of **2a** with 1-propanethiol (a); the reaction of **2a** with 2-propanethiol (b); the addition of 2-propanethiol into panel b (c). (B) The full ¹H NMR spectra of A.

3. The Regulation of Axial Chirality

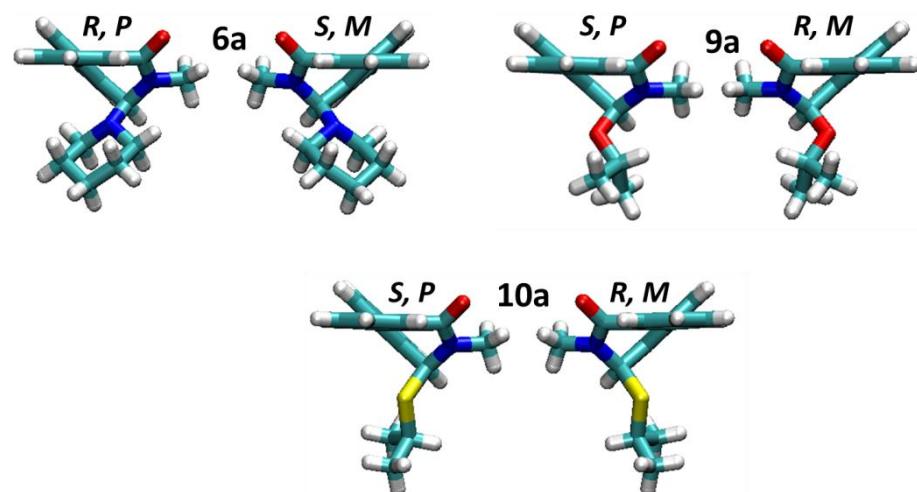


Figure S49. X-ray crystal structures of **6a**, **9a**, and **10a**, respectively.

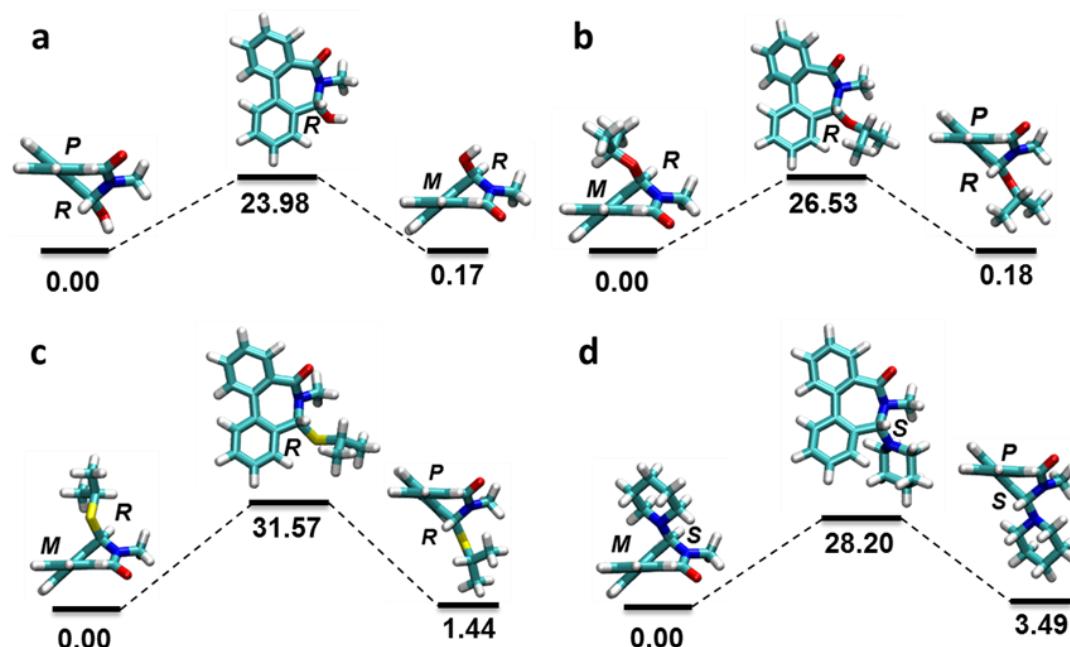


Figure S50. Calculated structures of atropisomers and the transition state for their interconversion of **2a** (a), **9a** (b), **10a** (c), and **6a** (d), with relative free energy listed in kcal/mol.

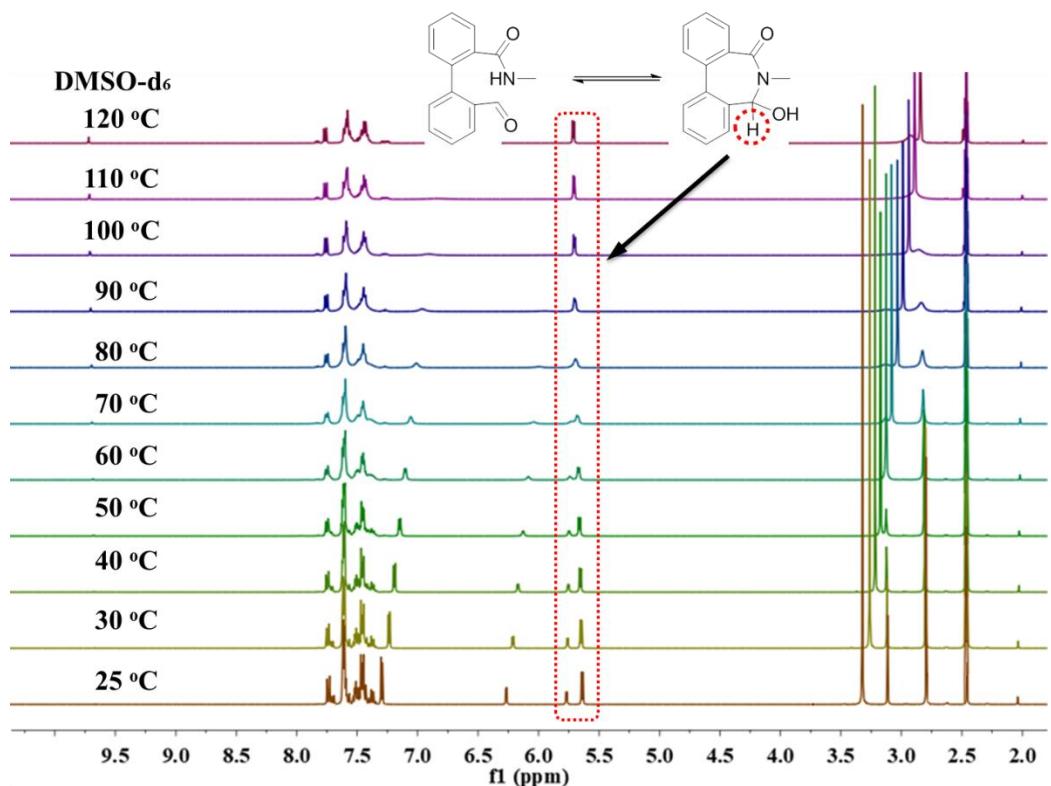


Figure S51. VT-NMR spectra of **2a** in DMSO-d₆.

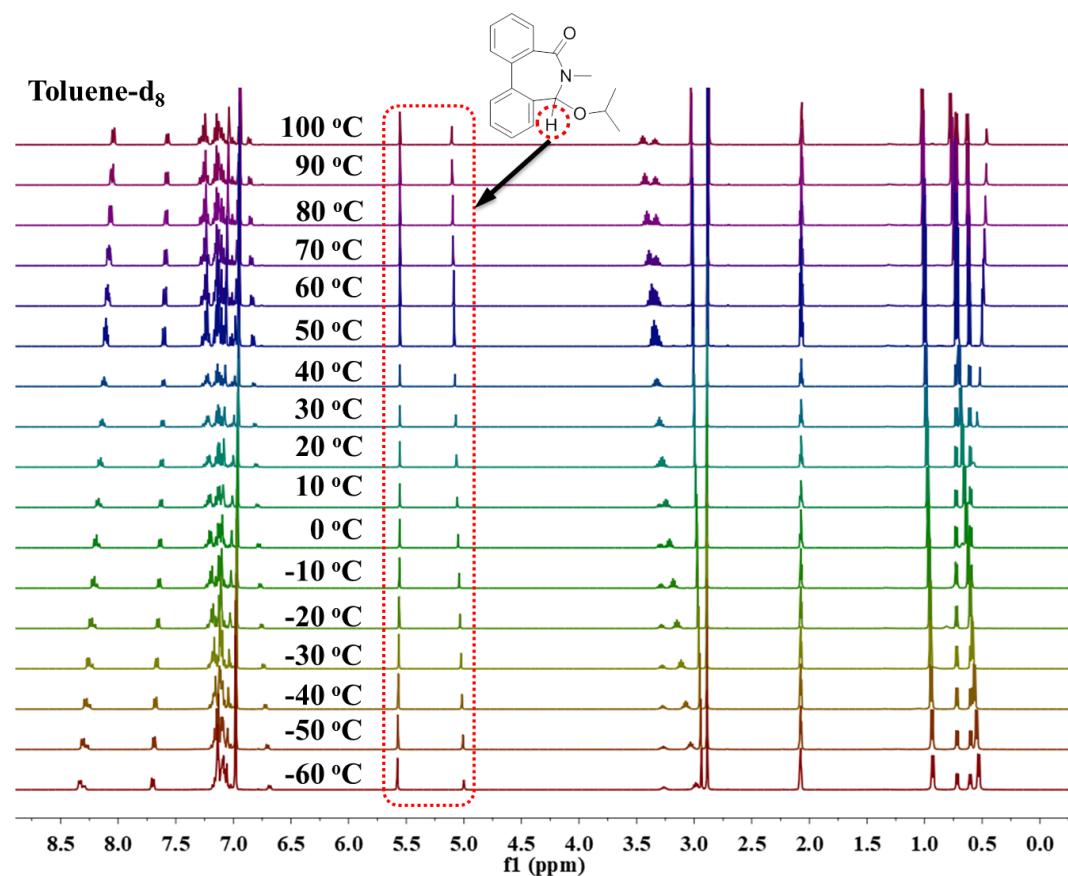


Figure S52. VT-NMR spectra of **9a** in toluene-d₈.

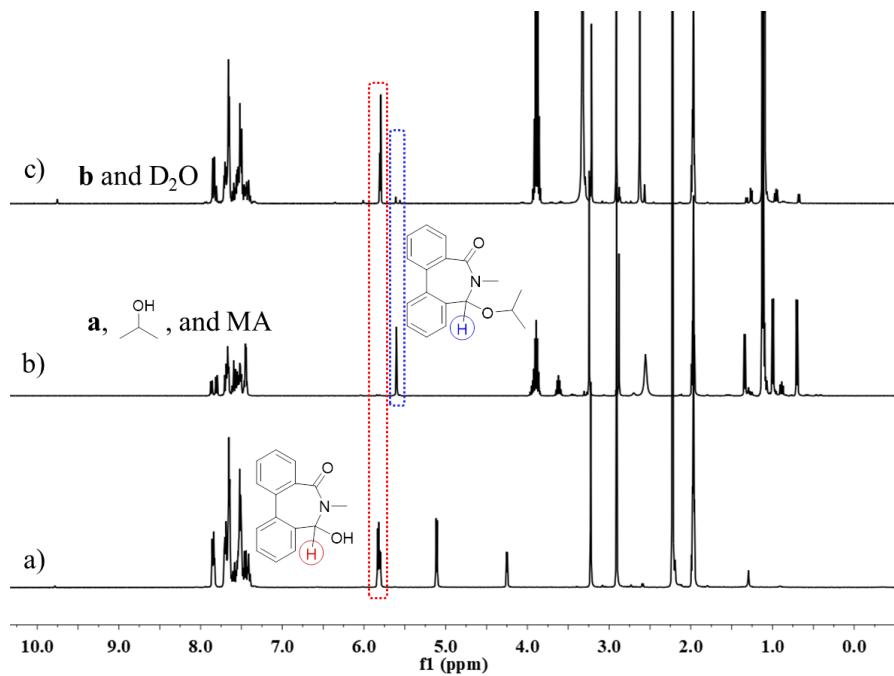


Figure S53. (a) ¹H-NMR spectrum of **2a**; (b) The DCR of **2a** (1.0 equiv.) and 2-propanol (3.0 equiv.) in the presence of methanesulfonic acid (1.0 equiv.) in CD_3CN (0.6 mL); (c) the addition of D_2O (0.2 mL) into panel b.

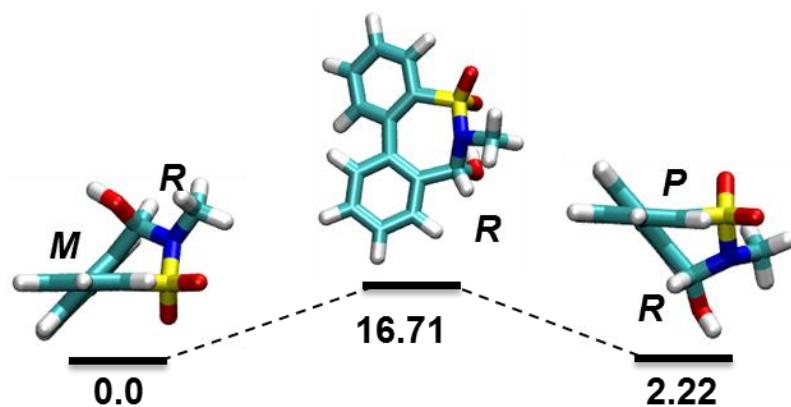


Figure S54. Calculated structures of atropisomers and the transition state for their interconversion of **2c** with relative free energy listed in kcal/mol.

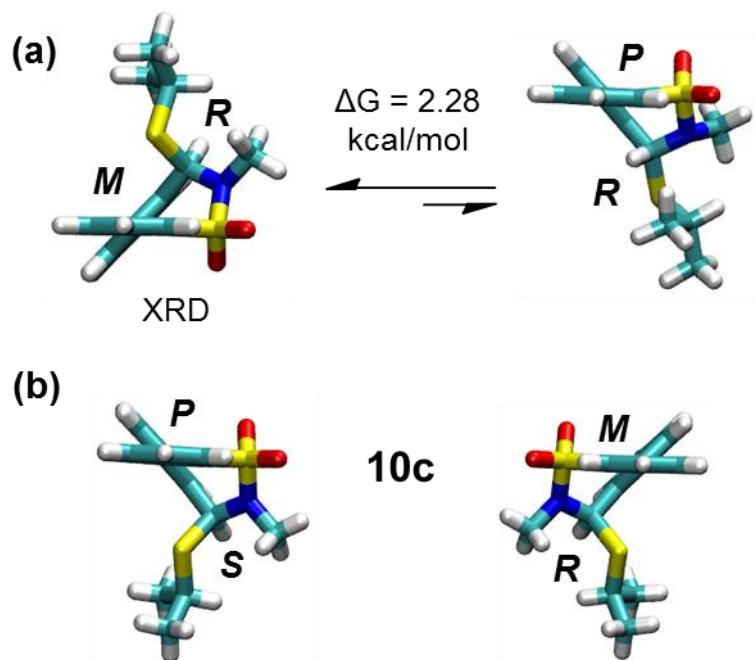
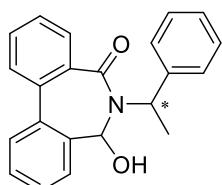
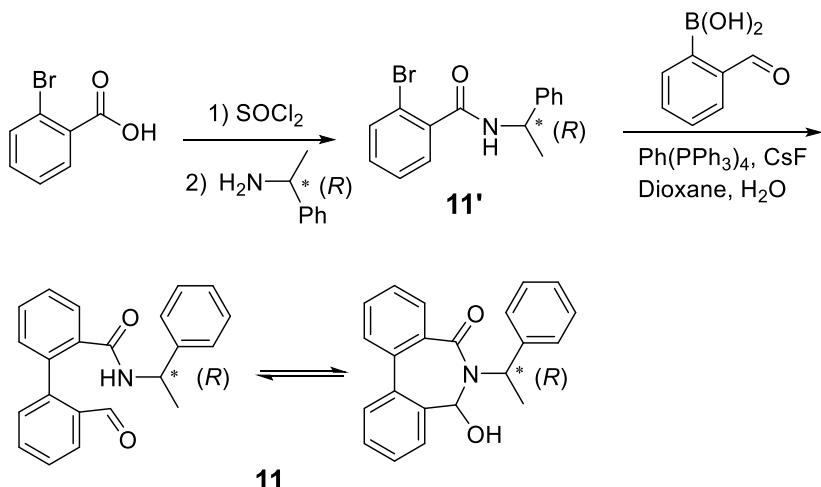


Figure S55. Calculated structure of atropisomers for interconversion of **10c** (a) and its crystal structures (b).

4. Studies on Chiroptical Switching

Scheme S2. Synthesis of **11**.



(11): (*R*)-*N*-(2-bromobenzoyl)methylbenzylamine (**11'**) was prepared according to the literature method.^{S3} **11** was then synthesized by using the same procedure as described above for **2a**. The product was crystallized from CH_3CN to afford a white crystalline solid (0.30 g, 85%). For the ring form a mixture of diastereomers (1.3: 1) was obtained. $^1\text{H-NMR}$ (CD_3CN): $\delta = 9.78\text{-}9.77$ (m, 1.8H), 7.95-7.88 (m, 1.9H), 7.64-7.19 (m, 19.6H), 7.09-7.00 (m, 3.7H), 6.93-6.84 (m, 1.8H), 6.26-6.15 (m, 0.3H), 5.70 (d, $J = 4.8$ Hz, 0.1H), 5.65 (d, $J = 4.4$ Hz, 0.1H), 4.91-4.81 (m, 1.8H), 3.90 (d, $J = 4.4$ Hz, 0.1H), 3.50 (d, $J = 4.8$ Hz, 0.1H), 1.76 (d, $J = 7.2$ Hz, 0.4H), 1.50 (d, $J = 7.2$ Hz, 0.3H), 1.26 (d, $J = 6.8$ Hz, 2.8H), 1.20 (d, $J = 6.8$ Hz, 2.6H). $^{13}\text{C-NMR}$ (CD_3CN): $\delta = 191.6, 191.5, 167.9, 144.1, 144.0, 143.9, 137.7, 137.6, 136.1, 134.2, 134.0, 133.4, 131.1, 130.1, 129.4, 128.4, 128.2, 127.7, 127.3, 127.2, 127.0, 126.9, 126.8, 125.9, 125.8, 49.0, 48.9, 21.4$. HRMS: m/z Calcd. for $\text{C}_{22}\text{H}_{19}\text{NO}_2\text{Na} [\text{M} + \text{Na}^+]$: 352.1313; found: 352.1380.

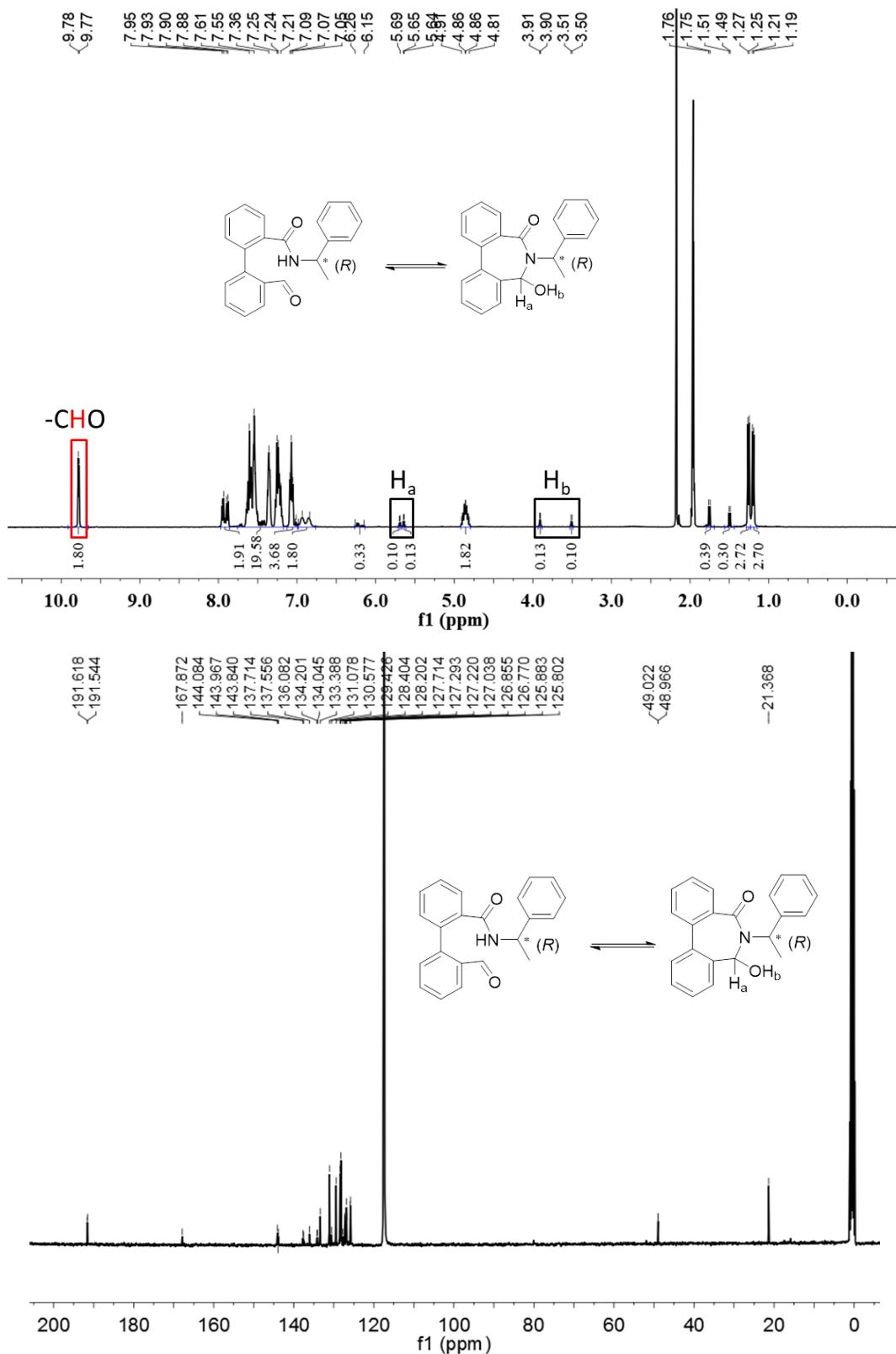


Figure S56. ¹H-NMR and ¹³C-NMR spectra of **11** in CD₃CN. The spectra was recorded after the compound was equilibrated in CD₃CN at 60 °C for 20 h.

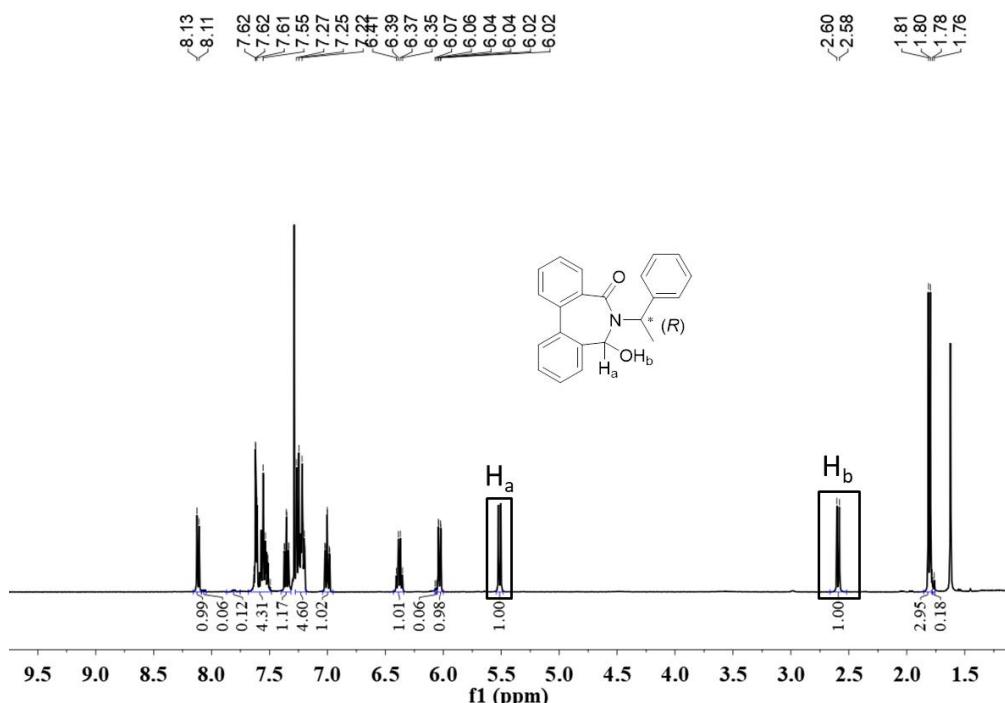


Figure S57. ^1H -NMR spectra of **11** in CDCl_3 . The spectra was recorded after the compound was equilibrated in CDCl_3 at 55°C for 20 h.

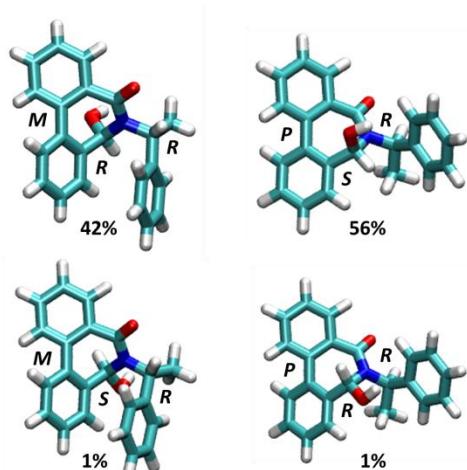


Figure S58. Calculated structures and distribution of four diastereomers of **11**.

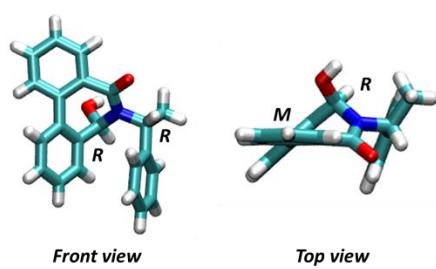


Figure S59. X-ray crystal structure of **11**, shown in front and top view, respectively.

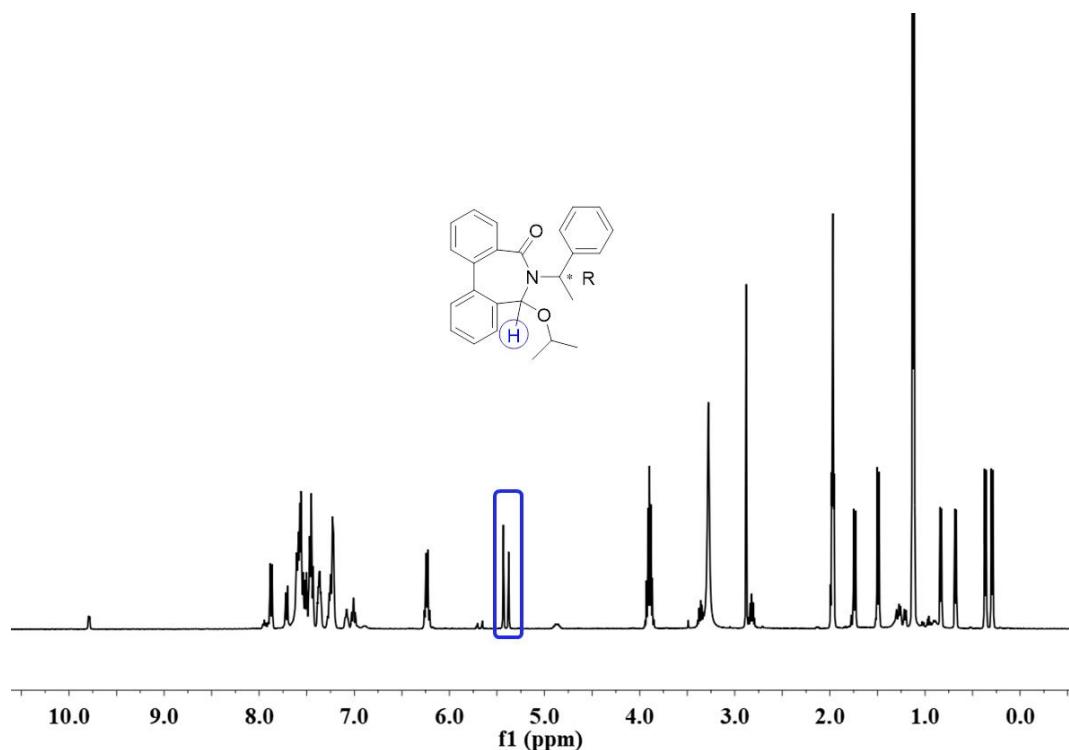


Figure S60. ^1H -NMR spectrum of the reaction of **11** and 2-propanol in the presence of MA in CD_3CN at R.T (d.r. = 1.3).

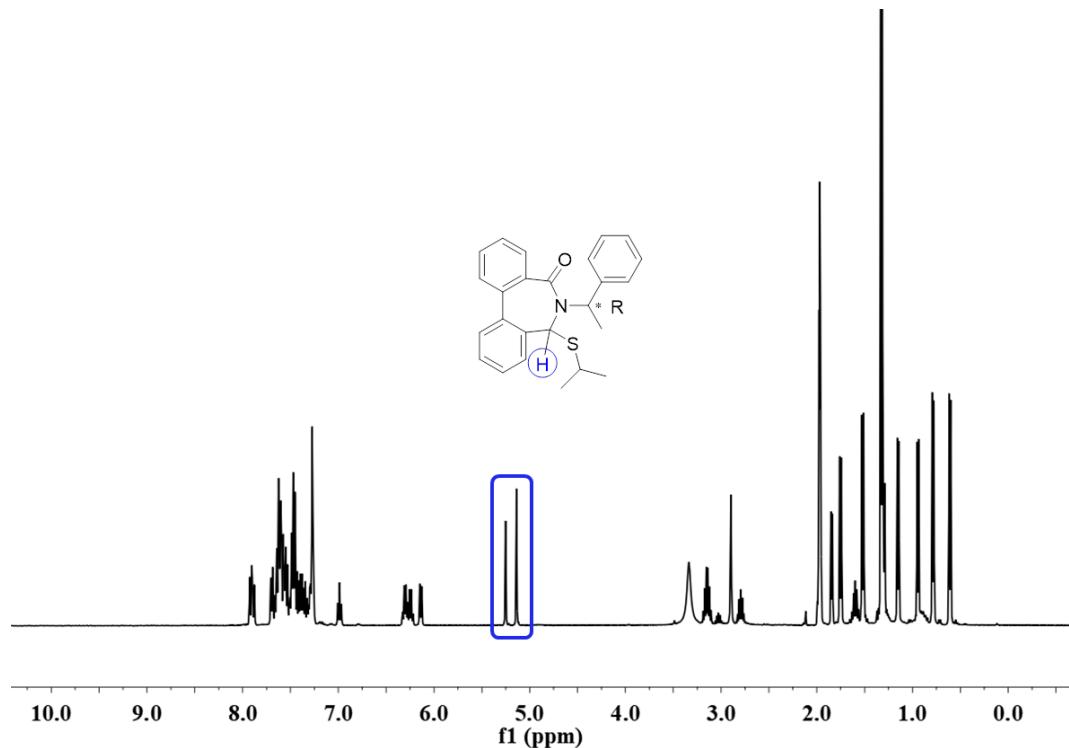


Figure S61. ^1H NMR spectrum of the reaction of **11** and 2-propanethiol in the presence of MA in CD_3CN at R.T (d.r. = 1.4).

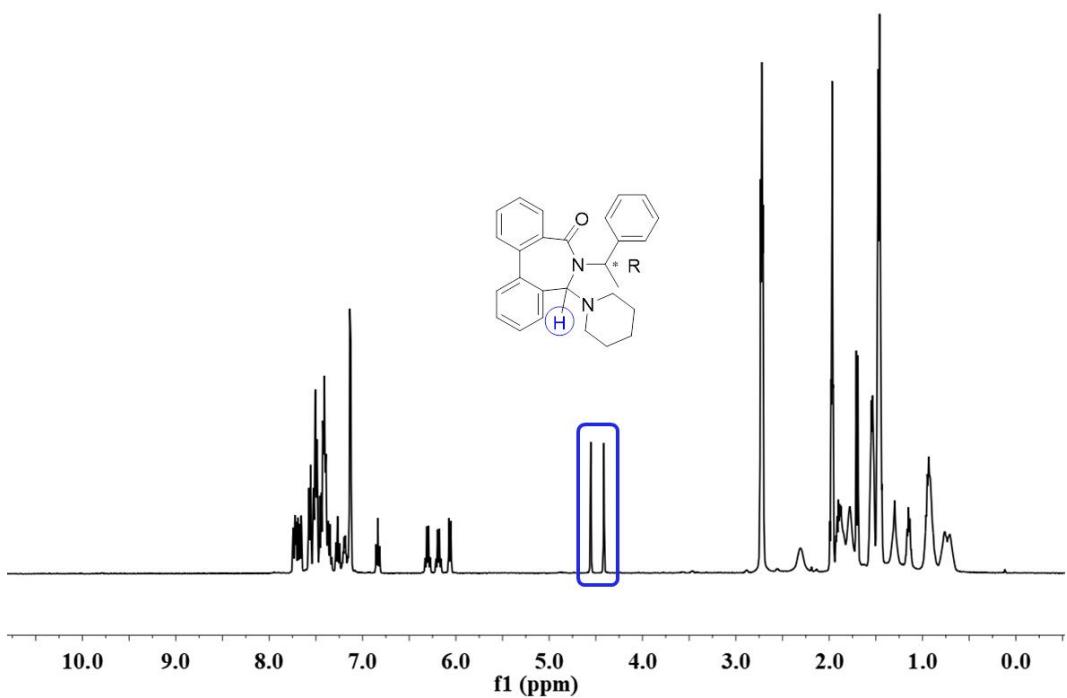


Figure S62. ^1H -NMR spectrum of the reaction of **11** and piperidine in CD_3CN at R.T (d.r. ~ 1.0).

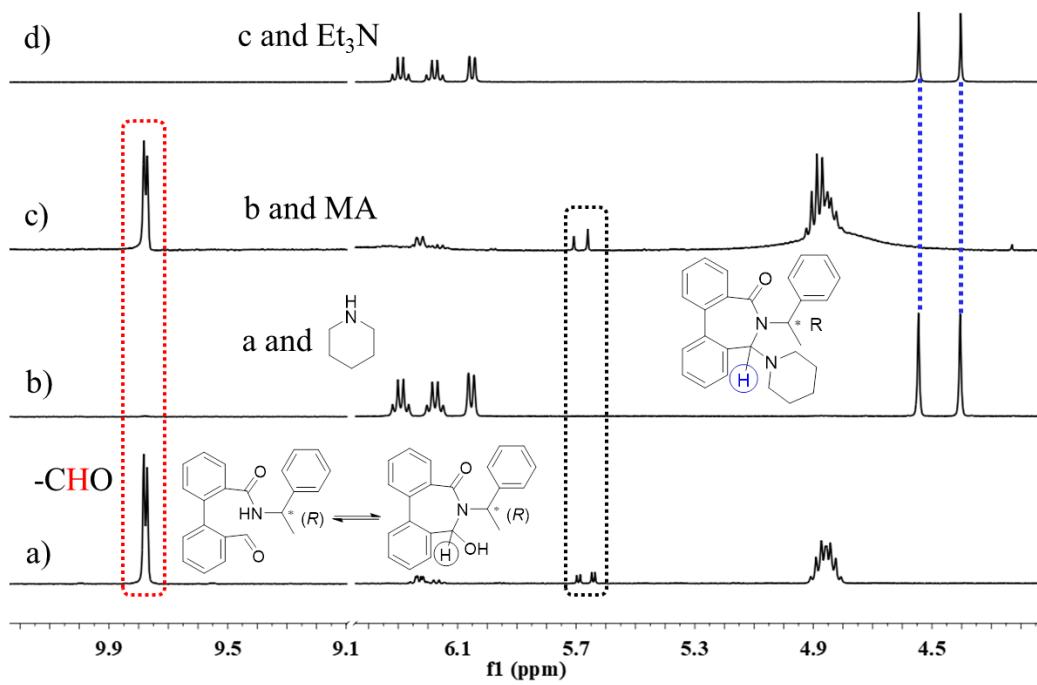
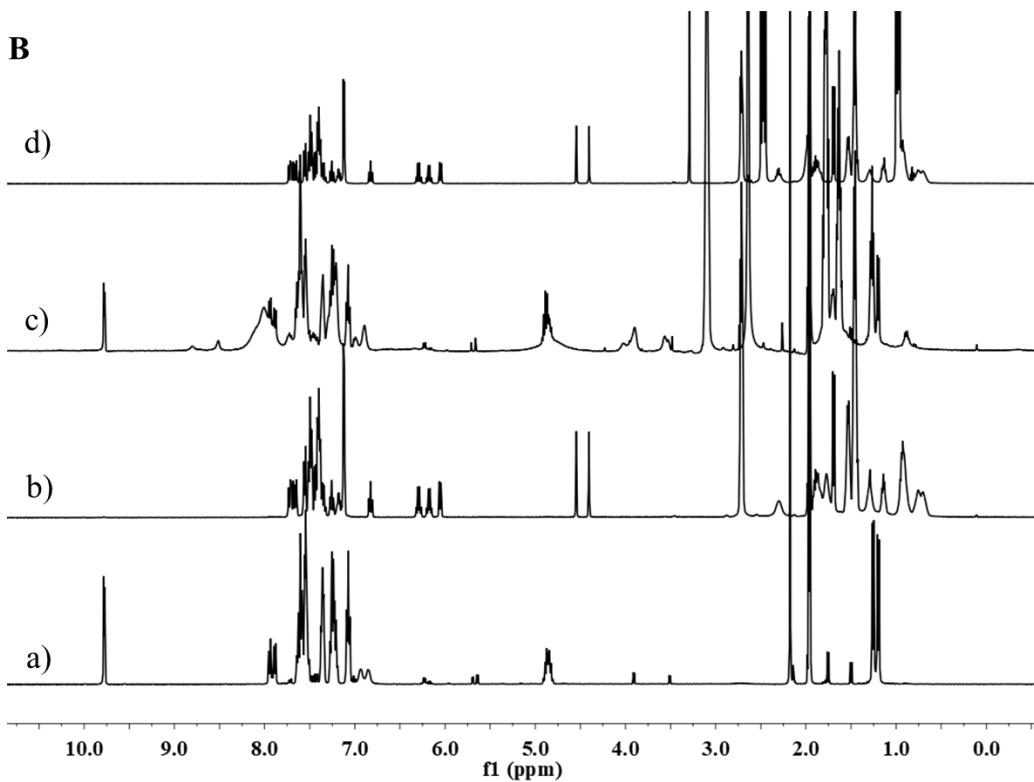
A**B**

Figure S63. (A) (a) ^1H -NMR spectrum of **11** in CD_3CN ; (b) the reaction of **11** (1.0 equiv.) and piperidine (3.0 equiv.); (c) the addition of MA (3.0 equiv.) into panel b; (d) the addition of triethylamine (3.0 equiv.) into panel c. (B) The full ^1H NMR spectra of A.

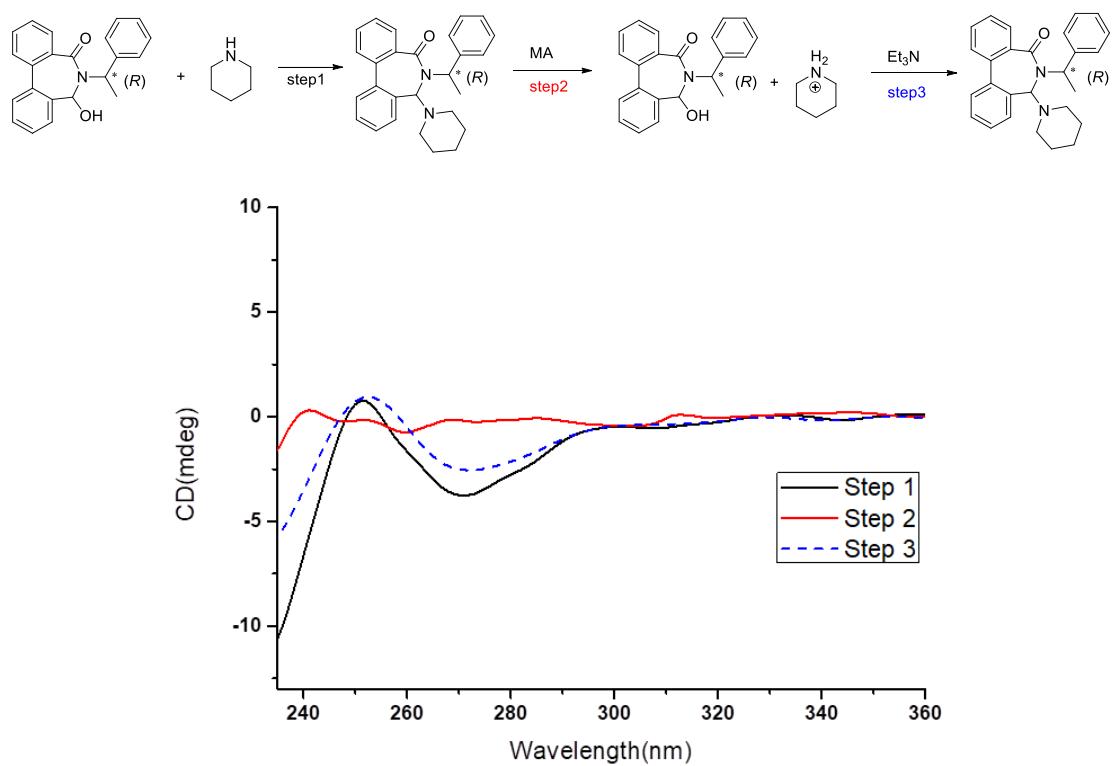


Figure S64. The switching of CD signal of the DCR of **11** (1.0 equiv.) and piperidine (3.0 equiv.) in CD₃CN (step 1) with MA (3.0 equiv., step 2) and triethylamine (3.0 equiv., step 3). The CD spectra was recorded after dilution (0.10 mM).

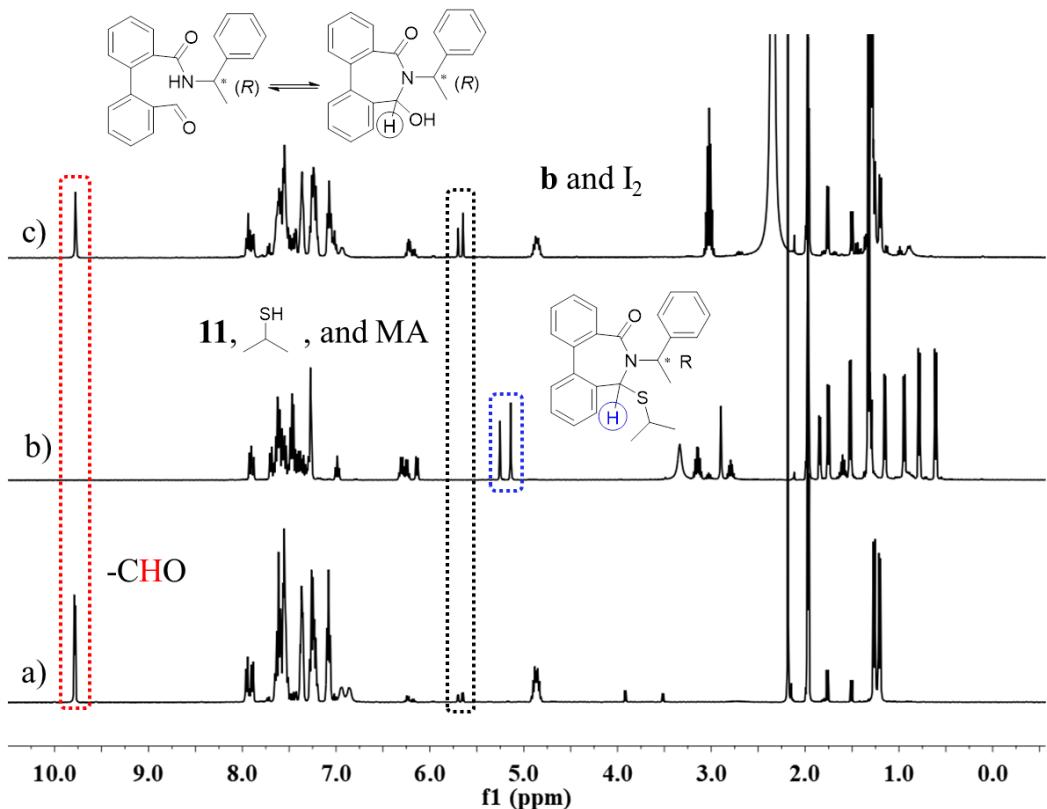


Figure S65. (a) ¹H-NMR spectrum of **11** in CD₃CN; (b) the reaction of **11** (1.0 equiv.), 2-propanethiol (3.0 equiv.), and MA (1.0 equiv.); (c) the addition of I₂ (0.75 equiv.) into panel b.

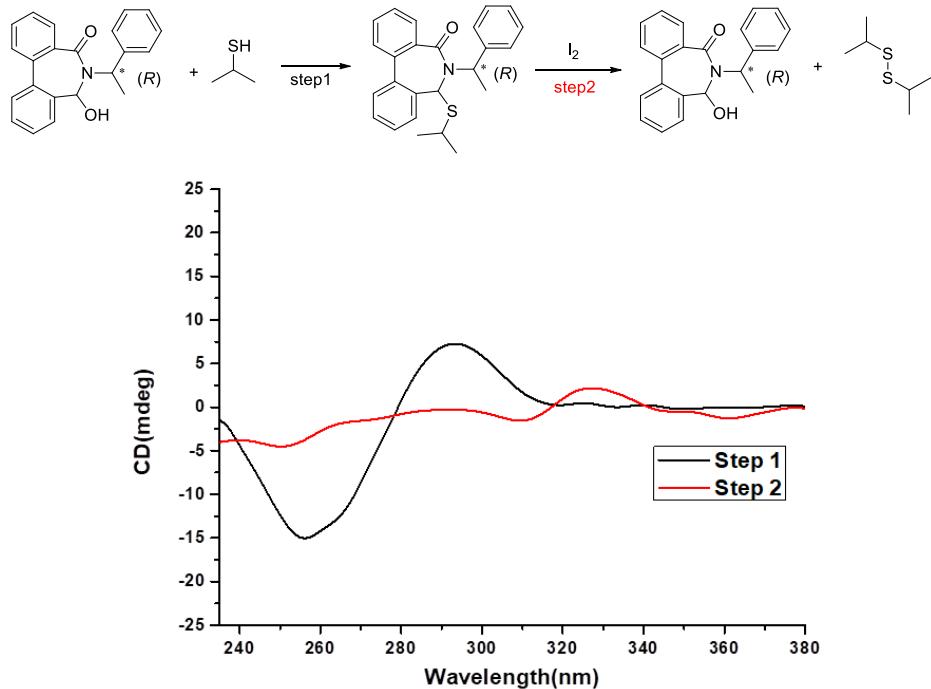
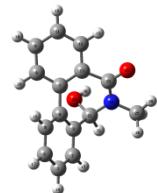
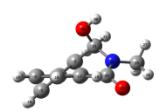


Figure S66. The switching of CD signal of the DCR of **11** (1.0 equiv.), 2-propanethiol (3.0 equiv.), and MA (1.0 equiv.) in CD₃CN (step 1) with I₂ (0.75 equiv., step 2). The CD spectra was recorded after dilution (0.10 mM).

5. Coordinates of DFT Calculations



Front view

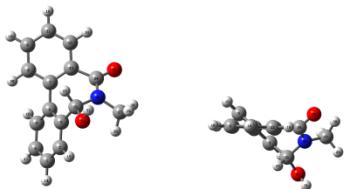


Top view

2a-(R, M) (G = -784.3354942 hartree)

Imaginary frequency: 0

C	-3.59404300	-1.06150900	-0.29990300
C	-2.95312600	0.02516000	0.28986100
C	-1.56496200	0.06468800	0.39005100
C	-0.78972600	-0.99584600	-0.10467600
C	-1.44663500	-2.07910800	-0.69978400
C	-2.83441800	-2.11506000	-0.79779000
C	0.69266000	-1.00249300	-0.00689800
C	1.33448300	-2.21403000	0.28341200
C	2.71893200	-2.30815400	0.34962800
H	3.18344200	-3.25869100	0.59102800
C	3.50190500	-1.18270700	0.10653300
C	2.88322200	0.02327200	-0.19518300
C	1.49053900	0.13498800	-0.23235500
H	-4.67624300	-1.08136200	-0.37205200
H	-3.53706700	0.85296500	0.68284500
H	-0.85926400	-2.89304100	-1.11342400
H	-3.31830000	-2.96298200	-1.27109400
H	4.58409900	-1.24408200	0.14936400
H	3.47221200	0.90751800	-0.41256500
H	0.72922400	-3.09299600	0.48134200
C	-0.89955300	1.27445900	0.99810100
C	0.98458900	1.49947900	-0.62414100
O	1.61296500	2.15005900	-1.45713000
N	-0.12230700	2.00355400	-0.00614000
C	-0.66496100	3.28395400	-0.44305100
H	-1.65202500	3.14514600	-0.89595900
H	-0.75798300	3.96247100	0.40911300
H	0.01234900	3.71243900	-1.17688100
O	-0.12322800	0.87496500	2.09492400
H	0.28369700	1.66654700	2.47228700
H	-1.67933300	1.97844400	1.31379100

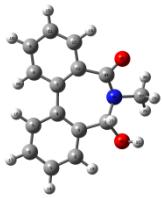


Front view Top view

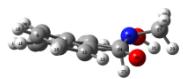
2a-(R, P) (G = -784.3357595 hartree)

Imaginary frequency: 0

C	-3.19887900	-1.73703700	0.34364500
C	-2.79184100	-0.55944300	-0.27980600
C	-1.43721500	-0.26821300	-0.40082700
C	-0.46548400	-1.15263700	0.09471200
C	-0.89074700	-2.33184200	0.71573900
C	-2.24611900	-2.62111200	0.84317600
C	0.98874200	-0.87679900	-0.07089500
C	1.83099700	-1.94645500	-0.41047700
C	3.20028100	-1.77486800	-0.56090700
H	3.82077200	-2.62071500	-0.83805300
C	3.77161500	-0.51932300	-0.35831000
C	2.95847300	0.54833600	-0.00619900
C	1.57445100	0.39299300	0.11808000
H	-4.25603900	-1.96190900	0.43983000
H	-3.51783400	0.13654000	-0.68561200
H	-0.15279700	-3.01836300	1.11937400
H	-2.55627200	-3.53649600	1.33639000
H	4.84115200	-0.37670600	-0.46994600
H	3.38288100	1.52827700	0.18501000
H	1.39148000	-2.92513600	-0.57549600
C	-0.94123500	1.01571300	-1.01507900
O	-1.98354900	1.67333100	-1.66248600
H	-0.12037000	0.79623100	-1.70774800
C	0.82696200	1.60786700	0.60535300
O	1.32753400	2.32018900	1.47419700
N	-0.38647100	1.86875100	0.05269500
C	-1.29637900	2.80214500	0.70301000
H	-2.23185000	2.29125100	0.95085100
H	-1.52355300	3.65211300	0.05669900
H	-0.81586100	3.15665200	1.61210100
H	-1.61001700	2.37289500	-2.21325200



Front view

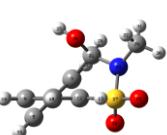


Top view

2a-TS (3a in the main text, G = -784.2975434 hartree)

Imaginary frequency: 1

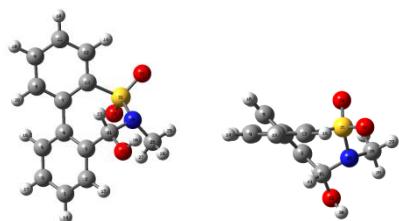
C	3.49258500	-1.56048900	0.14772100
C	2.97010200	-0.27690400	0.14746100
C	1.59292700	-0.02089000	0.07611500
C	0.69289500	-1.10332900	-0.01435900
C	1.25310500	-2.39715700	0.05266800
C	2.61564500	-2.63593100	0.11969500
C	-0.80375100	-1.02870800	-0.10130300
C	-1.49007600	-2.19905100	-0.48035700
C	-2.86829600	-2.33232000	-0.39751400
H	-3.33314700	-3.26290200	-0.70644000
C	-3.63493300	-1.27733400	0.08113000
C	-2.99913400	-0.07937000	0.36194200
C	-1.61125800	0.08194600	0.23486600
H	4.56549500	-1.71217000	0.20022200
H	3.64268700	0.56722800	0.21113600
H	0.60453100	-3.26033400	0.09280900
H	2.97966800	-3.65681500	0.16698200
H	-4.71088500	-1.36609300	0.18449400
H	-3.57539000	0.79176200	0.64677100
H	-0.93731400	-3.04005000	-0.87500700
C	1.23552800	1.44942000	0.26561700
O	2.29383300	2.20907100	-0.24960800
H	1.16177800	1.63301700	1.35099100
C	-1.21460900	1.53441600	0.25195500
O	-2.02447200	2.37893700	0.60761200
N	-0.02597300	1.91692300	-0.36124000
C	-0.01111800	3.35071900	-0.67519800
H	0.79147000	3.54530200	-1.38118300
H	0.11722500	3.97663400	0.21842700
H	-0.96597700	3.60819100	-1.12833800
H	2.36911700	3.02360700	0.26115400



Top view

Front view**2c-(R, M) (G = -1219.554331 hartree)****Imaginary frequency: 0**

C	3.89217500	-0.14601800	-0.25850200
C	2.90095900	-0.94026900	0.31271500
C	1.59415300	-0.47776500	0.44147900
C	1.26831200	0.81463200	-0.01094100
C	2.27220700	1.60739800	-0.57202900
C	3.57585800	1.13510000	-0.69620300
C	-0.11272400	1.35823600	0.06955200
C	-0.33124900	2.66149200	0.52030600
C	-1.61838700	3.18825700	0.60369800
H	-1.75808100	4.20168800	0.96466500
C	-2.72025100	2.42074400	0.23994600
C	-2.53156400	1.11852600	-0.21671200
C	-1.24125000	0.61038700	-0.30086800
H	4.90402000	-0.52535200	-0.35154800
H	3.14857200	-1.93345500	0.67682500
H	2.01909200	2.59803900	-0.93761100
H	4.33755600	1.76738800	-1.13999500
H	-3.72200000	2.82970300	0.30896500
H	-3.36907700	0.49929100	-0.51754500
H	0.52034700	3.25966100	0.82873100
C	0.58954100	-1.36256900	1.16008300
O	-0.06050800	-0.98816400	-2.02314000
N	-0.42005400	-1.96655200	0.29446300
O	-0.09012300	-0.66776700	2.18717400
H	0.56573800	-0.36408400	2.82825800
H	1.13627900	-2.21360000	1.58719900
S	-1.04612300	-1.03552200	-0.95008100
O	-2.36948200	-1.57576900	-1.24396400
C	-1.38965300	-2.79942800	1.02442000
H	-1.94451300	-3.41144700	0.31785300
H	-0.80971800	-3.44930800	1.68276300
H	-2.07772700	-2.20305500	1.62928500



Front view

Top view

2c-(*R*, *P*) (G = -1219.550798 hartree)

Imaginary frequency: 0

C	3.38192300	1.55362400	0.40504100
C	2.85437700	0.50838400	-0.34906100
C	1.47711600	0.38251200	-0.50874800
C	0.61180300	1.31255900	0.09285800
C	1.15316400	2.36517800	0.83497900
C	2.53011700	2.48358800	0.99517300
C	-0.86059200	1.21341800	-0.09030600
C	-1.59854900	2.34402800	-0.45086600
C	-2.97208500	2.26873700	-0.66906200
H	-3.51763300	3.16319900	-0.95039300
C	-3.64323100	1.05641300	-0.54138700
C	-2.93627500	-0.08616200	-0.17864800
C	-1.56603100	0.00444100	0.04136500
H	4.45629300	1.64338100	0.52725500
H	3.50756400	-0.21005200	-0.83266400
H	0.48593300	3.08334100	1.30215600
H	2.93604700	3.30082700	1.58206600
H	-4.71123600	0.99759300	-0.71795700
H	-3.43266800	-1.04162100	-0.05181300
H	-1.07915800	3.28797200	-0.58253500
C	0.88361600	-0.75434200	-1.31089200
O	1.84696700	-1.27201100	-2.16889600
H	0.01281600	-0.39713900	-1.86990600
O	-0.11056200	-1.06714900	1.95821900
N	0.38064000	-1.86950100	-0.44634200
C	1.44400700	-2.67506400	0.18261000
H	2.05443600	-2.08481700	0.87480100
H	2.06755100	-3.07650400	-0.61315200
H	0.98138900	-3.50475100	0.71971900
H	1.41237700	-1.89404900	-2.76769000
S	-0.76981900	-1.44369000	0.70606500
O	-1.74606000	-2.52905500	0.77182000



Front view

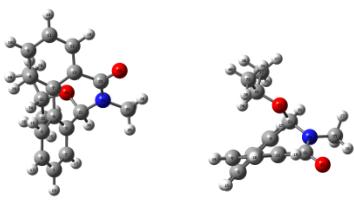


Top view

2c-TS (3c in the main text, G = -1219.5277 hartree)

Imaginary frequency: 1

C	4.09081100	0.06451700	-0.12974600
C	3.09598300	-0.86209800	0.13745500
C	1.73207900	-0.53956700	0.12476300
C	1.34441100	0.79903800	-0.09827700
C	2.36932700	1.69786400	-0.46388200
C	3.71146700	1.35446800	-0.47962700
C	-0.02497300	1.40737500	0.01624100
C	-0.07869600	2.78972400	0.29251900
C	-1.25308600	3.52737000	0.27631100
H	-1.21522800	4.58889300	0.49547500
C	-2.46231500	2.90894100	-0.01684600
C	-2.47134000	1.53640000	-0.20402800
C	-1.28320900	0.79906900	-0.15855800
H	5.13452500	-0.22967100	-0.11270600
H	3.37489400	-1.89177900	0.34374100
H	2.10667700	2.70014400	-0.77571300
H	4.45003100	2.09334200	-0.77159300
H	-3.38688100	3.47278600	-0.06166500
H	-3.40650100	1.01493400	-0.37624900
H	0.83520200	3.30801100	0.54933500
C	0.85923300	-1.78008900	0.27321700
O	-2.77403300	-1.24325400	-0.91525500
N	-0.33423500	-1.75653600	-0.59813300
O	0.64212200	-2.20099300	1.59039100
H	0.00114000	-1.61090400	2.01378700
H	1.45150700	-2.58365900	-0.16823700
S	-1.65823400	-0.93189100	-0.03024000
O	-1.85777700	-1.18333300	1.40545000
C	-0.68032400	-3.09748200	-1.12222300
H	-1.53630100	-3.01820200	-1.78749200
H	0.18033200	-3.44724000	-1.69264400
H	-0.89671200	-3.80318700	-0.31387600



Front view

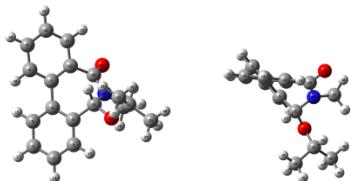
Top view

9a-(R, M) (G = -902.1620068 hartree)

Imaginary frequency: 0

C	3.35162600	1.54688500	-0.91529900
C	2.83366300	0.30535000	-0.55276800
C	1.46643200	0.13747300	-0.35329000
C	0.59060200	1.22327500	-0.50872100
C	1.12199600	2.46403600	-0.87383800
C	2.48988600	2.62675800	-1.07806400
C	-0.86610300	1.08149700	-0.25726500
C	-1.52717700	2.11198100	0.42395700
C	-2.89280100	2.05608500	0.67791400
H	-3.37415800	2.86261800	1.22122500
C	-3.63469200	0.96568800	0.23205600
C	-2.99641600	-0.05866700	-0.45695400
C	-1.61890000	-0.02841900	-0.68515300
H	4.41850800	1.66713600	-1.07075100
H	3.49832400	-0.54519600	-0.42225700
H	0.45150600	3.30571100	-1.01888000
H	2.87830800	3.59702100	-1.36950200
H	-4.70210300	0.91282300	0.41819100
H	-3.55873500	-0.90874500	-0.82766200
H	-0.94930200	2.96144700	0.77513300
C	0.92218200	-1.23462100	-0.01389200
C	-1.08604900	-1.20482100	-1.46404000
O	-1.77183500	-1.68472200	-2.36480800
N	0.11789400	-1.74034300	-1.11551300
C	0.66365900	-2.85668100	-1.87435400
H	1.62722600	-2.58016500	-2.31352200
H	0.80610100	-3.72250700	-1.22139000
H	-0.03660900	-3.10923300	-2.66637600
O	0.11977300	-1.29065900	1.14126100
H	1.77114400	-1.92584000	0.07890800
C	0.60828100	-0.62071800	2.30518600
C	1.87884100	-1.27586100	2.82958300
C	-0.53587200	-0.67059900	3.30147700
H	0.81622700	0.42876200	2.05273900
H	2.70507000	-1.17859000	2.11857900
H	2.18758900	-0.80152400	3.76466100

H	1.70084300	-2.33898400	3.01822300
H	-1.42567500	-0.20582000	2.86770100
H	-0.76971000	-1.70851100	3.55634000
H	-0.26826700	-0.13679000	4.21638900



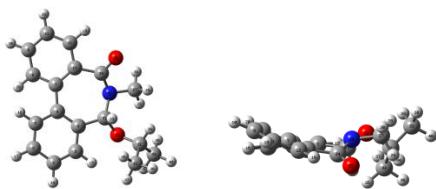
Front view Top view

9a-(R, P) (G = -902.1617222 hartree)

Imaginary frequency: 0

C	-0.37324300	3.71467500	-0.26165700
C	-1.03804300	2.49990500	-0.11048500
C	-0.31201600	1.32422700	0.04810300
C	1.09217100	1.34377000	0.06426100
C	1.74439500	2.57215200	-0.08666000
C	1.01874700	3.74818500	-0.25250700
C	1.87911600	0.09819600	0.28365400
C	3.00046100	0.16016300	1.12505600
C	3.79149900	-0.95505400	1.36565400
H	4.64234700	-0.87719300	2.03453700
C	3.48928600	-2.16950400	0.75177100
C	2.39573500	-2.24757900	-0.09842900
C	1.57402800	-1.13871300	-0.32257400
H	-0.94010900	4.63132800	-0.38753200
H	-2.12139400	2.45309100	-0.10212000
H	2.82972300	2.60215100	-0.09372400
H	1.54237900	4.69019500	-0.37770700
H	4.10369200	-3.04501200	0.93266800
H	2.15766700	-3.17331800	-0.61162100
H	3.23660000	1.10090300	1.61240300
C	-0.97752100	-0.02380200	0.15849800
O	-2.34233000	0.12189100	0.36309000
H	-0.51303400	-0.59483300	0.97311800
C	0.47985900	-1.34022900	-1.33982900
O	0.70708600	-1.99698000	-2.35459100
N	-0.73068600	-0.77959300	-1.08556700
C	-1.71460800	-0.66087000	-2.15221500
H	-2.04581900	0.37798800	-2.23198300
H	-2.58688600	-1.29240600	-1.96170300
H	-1.24264500	-0.97448100	-3.08100600
C	-3.00418200	-1.05555200	0.85579300

C	-2.82483600	-1.16746500	2.36328000
C	-4.46324100	-0.91646000	0.46288500
H	-2.56531100	-1.93279100	0.35895700
H	-1.77043300	-1.22880300	2.64504900
H	-3.32371600	-2.06625600	2.73455500
H	-3.26580600	-0.29444200	2.85285200
H	-4.56611700	-0.82293500	-0.62082800
H	-4.88878800	-0.02373800	0.93087000
H	-5.03123000	-1.78784700	0.79659100



Front view

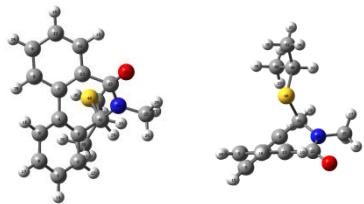
Top view

9a-TS (G = -902.1197311 hartree)

Imaginary frequency: 1

C	0.96974400	3.47915900	-0.07852200
C	1.36471100	2.15314200	0.00266500
C	0.45521800	1.08511800	0.00695800
C	-0.92424600	1.37680000	-0.00396200
C	-1.29718600	2.72925100	-0.15415200
C	-0.38359000	3.76879100	-0.19207800
C	-2.05438600	0.40410100	0.10978400
C	-3.28950500	0.89184800	0.57484100
C	-4.45040600	0.13061600	0.55971400
H	-5.37441900	0.55723100	0.93586400
C	-4.41798300	-1.16727700	0.06416700
C	-3.19797700	-1.69799600	-0.32528800
C	-2.01379400	-0.94958200	-0.27208000
H	1.71437500	4.26825500	-0.07917600
H	2.41881300	1.92765300	0.07206900
H	-2.34410900	2.97468700	-0.27565700
H	-0.73163700	4.78929700	-0.31139800
H	-5.31698700	-1.77248900	0.02282100
H	-3.12574700	-2.72938600	-0.64800900
H	-3.34690700	1.89385600	0.98023500
C	1.13519400	-0.28195500	-0.13107100
O	2.33005600	-0.25647600	0.60085400
H	1.38621300	-0.40114600	-1.20061500
C	-0.79116200	-1.80353500	-0.44197700
O	-0.88366300	-2.88951000	-0.99399700
N	0.35821800	-1.47534400	0.28259100

C	1.19206400	-2.66299100	0.50324400
H	1.96104900	-2.41636400	1.23041500
H	1.64843900	-3.04024700	-0.41978800
H	0.55562900	-3.45016500	0.90531100
C	3.51336000	-0.71444700	-0.08124500
C	4.05609100	0.33402900	-1.04309900
C	4.51566000	-1.05319300	1.00700800
H	3.26614500	-1.61958300	-0.64895600
H	3.30036200	0.65194600	-1.76764200
H	4.89929100	-0.08515200	-1.59832200
H	4.41074800	1.21340800	-0.49669000
H	4.12942700	-1.82945800	1.67189200
H	4.73095300	-0.16112300	1.60242700
H	5.44884600	-1.40719700	0.56279500



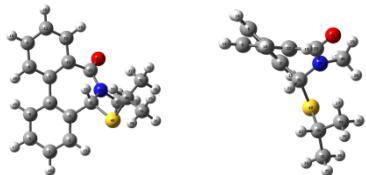
Front view Top view

10a-(R, M) (G = -1225.136128 hartree)

Imaginary frequency: 0

C	-0.81455400	-3.75065100	-0.27910600
C	-1.25921800	-2.47604300	-0.61988700
C	-0.47629400	-1.35258700	-0.35705800
C	0.78154100	-1.50271500	0.24709200
C	1.22072400	-2.78904400	0.57781400
C	0.43147500	-3.90563200	0.32085700
C	1.62896700	-0.32610900	0.56078300
C	2.33055100	-0.31245200	1.77557400
C	3.15526200	0.74695700	2.12736400
H	3.67134800	0.73409100	3.08176400
C	3.31351500	1.82235700	1.25493100
C	2.64101600	1.81859100	0.04215300
C	1.78435400	0.76914100	-0.31037600
H	-1.43495400	-4.61520300	-0.49006200
H	-2.22646600	-2.35097600	-1.09983400
H	2.20296000	-2.91543800	1.02270900
H	0.79501600	-4.89417200	0.58072900
H	3.95706900	2.65491700	1.51788600
H	2.76719800	2.63251800	-0.66301300
H	2.20311600	-1.14343400	2.46201200
C	-0.96793500	0.01072900	-0.77875600

C	1.16075400	0.92016800	-1.67521200
O	1.81505600	1.43005300	-2.58216800
N	-0.13832500	0.55061500	-1.84469300
C	-0.80447300	0.81805400	-3.11238500
H	-1.23895900	-0.10420100	-3.50794400
H	-1.60001800	1.55657200	-2.96822600
H	-0.07086100	1.20774500	-3.81311400
H	-1.96381200	-0.11111700	-1.21059000
C	-3.04993300	1.24501500	0.69489800
C	-3.43039700	2.39998700	1.61671500
C	-3.62294400	-0.07648200	1.19239200
H	-3.41057100	1.45720200	-0.31755900
H	-3.05591100	3.35482300	1.24098900
H	-4.51938300	2.46084000	1.69606800
H	-3.02757000	2.23864300	2.62172500
H	-3.33650100	-0.91738200	0.55516000
H	-3.26705400	-0.28333200	2.20613600
H	-4.71633200	-0.02365700	1.21041900
S	-1.21343500	1.21319500	0.61113500



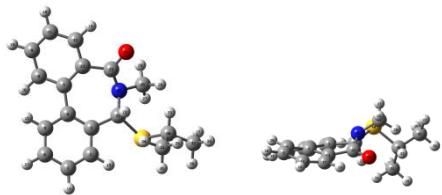
Front view Top view

10a-(R, P) (G = -1225.133834 hartree)

Imaginary frequency: 0

C	0.77668500	3.81422900	-0.14556400
C	-0.18635900	2.80887500	-0.10034200
C	0.18888400	1.47848700	0.06560900
C	1.54938200	1.13852500	0.18442700
C	2.50451600	2.15955900	0.14105300
C	2.12386100	3.48737500	-0.02475700
C	1.98174200	-0.27188200	0.38878400
C	3.00581900	-0.52760700	1.31243500
C	3.47339900	-1.81511000	1.54038300
H	4.25566800	-1.98029300	2.27387600
C	2.93546800	-2.88793900	0.83168900
C	1.93352500	-2.65413900	-0.09969200
C	1.43490400	-1.36598600	-0.31444000
H	0.47319100	4.84734300	-0.27791300
H	-1.23774900	3.06693200	-0.18848400
H	3.55761500	1.90626700	0.21642600

H	2.88057100	4.26380000	-0.06706600
H	3.29822700	-3.89605000	1.00117200
H	1.51879900	-3.46854900	-0.68431900
H	3.42414400	0.30248700	1.87307000
C	-0.78259600	0.31863400	0.04543800
H	-0.50403300	-0.38674600	0.83369500
C	0.42297800	-1.23586800	-1.42343900
O	0.56300700	-1.88703700	-2.45631700
N	-0.62445800	-0.38526400	-1.23445400
C	-1.42249600	0.02551000	-2.38019600
H	-1.48085200	1.11766500	-2.41273100
H	-2.43682700	-0.37663300	-2.32175500
H	-0.93503900	-0.34588500	-3.27907900
C	-3.15792100	-0.76353800	1.11356800
C	-4.51351200	-0.43018000	1.73001100
C	-3.27227800	-1.87068700	0.07270700
H	-2.46354700	-1.06400600	1.90559500
H	-4.42654700	0.33394200	2.50581700
H	-4.93961000	-1.33221300	2.17751500
H	-5.20872800	-0.07304800	0.96366200
H	-2.30479000	-2.11009300	-0.37550400
H	-3.96262400	-1.57402500	-0.72319200
H	-3.66409900	-2.77679800	0.54592400
S	-2.49703900	0.80559400	0.41868400



Front view

Top view

10a-TS (G = -1225.085812 hartree)

Imaginary frequency: 1

C	0.28424900	3.69113700	-0.04488100
C	0.86803400	2.43696500	0.05000200
C	0.12750100	1.24845300	0.14568100
C	-1.28673900	1.33417900	0.11967500
C	-1.84819900	2.62126700	-0.02040000
C	-1.09826900	3.78368400	-0.08308100
C	-2.27712300	0.20447100	0.08889000
C	-3.62336500	0.49495100	0.37615000
C	-4.65730600	-0.39861500	0.12670800
H	-5.67560300	-0.11615800	0.37305300
C	-4.38261100	-1.63816700	-0.43804900

C	-3.05638900	-1.99241600	-0.63135300
C	-2.00608600	-1.11574600	-0.33156900
H	0.90969000	4.57521800	-0.10889100
H	1.94756100	2.37442700	0.04767100
H	-2.91781700	2.72321500	-0.13697700
H	-1.59577500	4.74161700	-0.19083300
H	-5.17862400	-2.33752300	-0.66887000
H	-2.79412900	-2.98816500	-0.96863400
H	-3.88254100	1.44520500	0.82393100
C	0.93172500	-0.05763900	0.09522700
H	1.13632800	-0.25247300	-0.96853500
C	-0.68815100	-1.81627300	-0.20967200
O	-0.52872200	-2.93706400	-0.66033800
N	0.24577300	-1.24312100	0.67148100
C	1.06623200	-2.28031600	1.31073600
H	1.52963100	-1.86940800	2.20335600
H	1.84265800	-2.69775900	0.65890600
H	0.39579100	-3.08969100	1.59854100
C	3.62486500	-0.64204900	-0.50558700
C	3.80082900	0.29857500	-1.69145300
C	4.96109400	-1.03521300	0.11473400
H	3.09142900	-1.54585700	-0.81823200
H	2.84062600	0.62874700	-2.09923500
H	4.35105600	-0.20766600	-2.49085400
H	4.36523600	1.18571600	-1.38873300
H	4.82825600	-1.76314600	0.91839900
H	5.47305500	-0.15660400	0.52046800
H	5.60523800	-1.47471000	-0.65187400
S	2.61222200	0.13749300	0.81869600



Front view

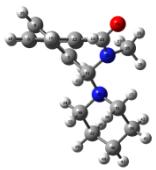
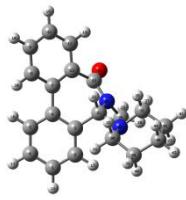
Top view

6a-(S, M) (G = -959.6456292 hartree)

Imaginary frequency: 0

C	-3.55689300	-1.95237300	-0.61909100
C	-2.31450200	-2.10521100	-0.00796900
C	-1.41433700	-1.04461300	0.05639300
C	-1.75315900	0.19954300	-0.50110300
C	-3.00631500	0.34125300	-1.10804500
C	-3.90275100	-0.72179700	-1.16763100

C	-0.80685400	1.34449400	-0.49262200
C	-0.71665900	2.14382000	-1.63888500
C	0.13608000	3.24100800	-1.69578100
H	0.19541500	3.83028800	-2.60502800
C	0.90753500	3.57621700	-0.58657300
C	0.81727400	2.80310100	0.56498000
C	-0.00903300	1.67899600	0.61787000
H	-4.24786200	-2.78763600	-0.66239500
H	-2.03305900	-3.06375800	0.41991400
H	-3.28843100	1.30525400	-1.52062800
H	-4.87111600	-0.58391800	-1.63726100
H	1.57144000	4.43364900	-0.61576800
H	1.39182900	3.05828300	1.44871800
H	-1.31125000	1.88150100	-2.50847000
C	-0.09142600	-1.23100500	0.76970500
C	-0.02001600	0.96870500	1.94605900
O	0.05448100	1.63474100	2.97872800
N	-0.06837900	-0.39169800	1.97167700
C	-0.15640900	-1.08294900	3.24959700
H	-1.05706900	-1.70415100	3.27779900
H	0.71881400	-1.72465800	3.39532400
H	-0.20021300	-0.34120700	4.04293200
H	-0.06448000	-2.26873800	1.14953000
C	2.30908400	-1.29928600	0.64347100
H	2.35441400	-2.38603700	0.86024700
H	2.30756000	-0.77277200	1.60208300
N	1.07230900	-0.97353200	-0.06813100
C	1.00558900	-1.68261000	-1.34659900
H	1.01349500	-2.78020400	-1.18854400
H	0.06488800	-1.43144900	-1.84265800
C	2.17842600	-1.28243100	-2.23684700
H	2.10897900	-1.81821100	-3.18858600
H	2.09458700	-0.20989700	-2.45223100
C	3.52880700	-0.88785100	-0.17496600
H	4.43808900	-1.14231800	0.37827100
C	3.50993200	-1.56442600	-1.54448200
H	3.62541300	-2.64879800	-1.41239100
H	4.34872500	-1.22367600	-2.15915100
H	3.51022600	0.20162000	-0.30124200



Front view

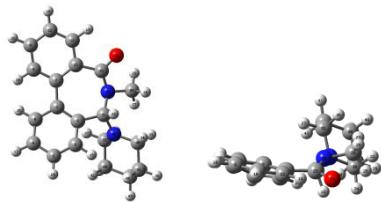
Top view

6a-(*S,P*) (G = -959.6400674 hartree)

Imaginary frequency: 0

C	-0.03998700	3.58043600	-0.72603900
C	-0.68295100	2.35320200	-0.58559300
C	0.02171300	1.23490600	-0.14494200
C	1.40061800	1.32557400	0.11163700
C	2.03241700	2.56670800	-0.02595900
C	1.31775700	3.68817700	-0.43495400
C	2.19188500	0.12609300	0.50227200
C	3.16565500	0.25034800	1.50257500
C	3.95838700	-0.82684000	1.87940100
H	4.69403400	-0.70368800	2.66736400
C	3.80764700	-2.05902000	1.24558100
C	2.86264200	-2.19662000	0.23741700
C	2.03782200	-1.12930700	-0.12516200
H	-0.59717100	4.44782600	-1.06453000
H	-1.74127300	2.25314300	-0.81004900
H	3.09952800	2.64491000	0.15944200
H	1.82524400	4.64094400	-0.54401800
H	4.42600000	-2.90325400	1.53098500
H	2.74908100	-3.13789400	-0.29019500
H	3.28575800	1.20783200	2.00016800
C	-0.58790200	-0.14906300	-0.05154500
H	-0.14312100	-0.67161600	0.81171200
C	1.13082100	-1.36428900	-1.30805600
O	1.56151400	-1.96990500	-2.28582100
N	-0.14522400	-0.88086900	-1.24719300
C	-0.86154100	-0.63113700	-2.49339700
H	-0.89738600	0.44552100	-2.69439800
H	-1.88411600	-1.00707500	-2.44183600
H	-0.32450400	-1.13640000	-3.29265100
C	-2.48993900	0.51468200	1.26732200
C	-2.52520600	-1.56774100	0.10894000
C	-4.01328700	0.58801400	1.29969700
H	-2.12434000	-0.01982300	2.16558000
H	-2.06696600	1.51925800	1.29690100
C	-4.04929800	-1.59641700	0.08238100
H	-2.15761000	-2.05596300	1.03223200

H	-2.11920800	-2.13254800	-0.73173100
C	-4.62457600	-0.81131400	1.26002100
H	-4.32885500	1.12734300	2.19811800
H	-4.35056300	1.16664800	0.43106300
H	-4.39152600	-2.63571000	0.10070100
H	-4.38860200	-1.15356500	-0.86202100
H	-5.71571600	-0.75795300	1.19698100
H	-4.38001400	-1.33576600	2.19333800
N	-2.03718100	-0.17931500	0.05059700

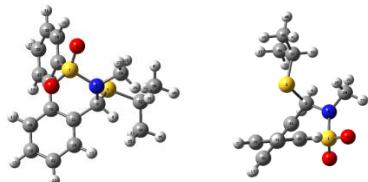


Front view Top view
6a-TS (G = -959.6006842 hartree)

Imaginary frequency: 1

C	-0.94072800	3.18655700	0.86137200
C	-1.09997300	1.81813100	0.97735900
C	-0.15171800	0.89002300	0.51260300
C	1.08255800	1.36797200	0.02319200
C	1.17391400	2.76637800	-0.17316300
C	0.19511600	3.66186100	0.21577600
C	2.33931000	0.56026800	-0.16344600
C	3.53052200	1.24762800	-0.47442800
C	4.77694400	0.64245200	-0.52141800
H	5.64641800	1.23955500	-0.77611400
C	4.90198400	-0.70750300	-0.22277100
C	3.75312700	-1.41574000	0.08021800
C	2.48107100	-0.82162300	0.09719300
H	-1.70293600	3.86218500	1.23471000
H	-2.01633800	1.42683400	1.40336800
H	2.04379300	3.19438000	-0.64608500
H	0.33677300	4.72226600	0.03559500
H	5.86758900	-1.20117200	-0.23342200
H	3.80759900	-2.47477300	0.29544800
H	3.52026900	2.30785200	-0.67046300
C	-0.69830100	-0.55078600	0.57075200
H	-0.75459000	-0.85772600	1.62750400
C	1.39733100	-1.85125100	0.27473200
O	1.70616400	-2.98509000	0.61890300
N	0.10262300	-1.58185700	-0.15307100
C	-0.65988500	-2.82301300	-0.33271200

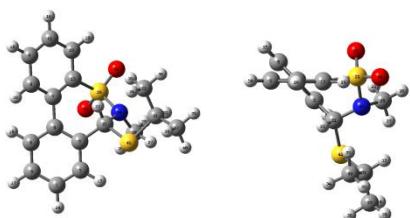
H	-1.52577200	-2.62274200	-0.95798600
H	-0.99203900	-3.25108700	0.62241200
H	-0.02304600	-3.55238400	-0.82801200
C	-3.10106500	-1.29809200	0.74155100
C	-2.31151700	-0.14487100	-1.27548100
C	-4.42009400	-0.52551100	0.70388100
H	-3.25622600	-2.27405900	0.24579100
H	-2.80291200	-1.50508500	1.77434400
C	-3.61594900	0.64646100	-1.37107100
H	-2.38323800	-1.03270700	-1.93109200
H	-1.46960700	0.45354600	-1.63623400
C	-4.76547000	-0.13776700	-0.73544400
H	-5.21469300	-1.13894200	1.14112500
H	-4.32379900	0.37971900	1.31624900
H	-3.83394400	0.87098600	-2.42017600
H	-3.48294200	1.60019300	-0.84500600
H	-5.69208500	0.44368600	-0.76615800
H	-4.94143200	-1.05278700	-1.31846500
N	-2.05393900	-0.52192400	0.10296600



Front view Top view
10c-(R, M) (G = -1660.353372 hartree)
Imaginary frequency: 0

S	-1.31142400	-0.82546600	-1.56056600
S	1.62228200	-0.60316400	0.74229500
O	-2.04783100	0.33677000	-2.04074500
O	-1.57464500	-2.11933000	-2.18120800
N	0.32757100	-0.52610500	-1.73865600
C	-1.41513100	0.14565400	1.02716000
C	-1.58400700	-0.96994700	0.19273400
C	0.98789300	0.32390600	-0.74632000
H	1.89431200	0.68026600	-1.24389200
C	-0.93199900	1.45478300	0.51928400
C	0.17920900	1.54023200	-0.33940200
C	-1.69645800	-0.02346600	2.38584700
H	-1.55584200	0.81667100	3.05866800
C	0.59582600	2.79037800	-0.79280500
H	1.45456000	2.85606500	-1.45495000
C	-1.58445200	2.62495900	0.91090300

H	-2.44917500	2.55406900	1.56388100
C	-1.15594000	3.86906600	0.45673300
H	-1.67881000	4.76691500	0.76849200
C	-2.11682100	-1.25330200	2.88403000
H	-2.32015900	-1.35894300	3.94434600
C	-0.06518200	3.95232400	-0.40151400
H	0.27641200	4.91563800	-0.76463900
C	1.14985200	-1.62023100	-2.26341100
H	1.39966900	-2.35510000	-1.49001600
H	2.06955700	-1.17401000	-2.65077700
H	0.62585000	-2.10800500	-3.08104800
C	-1.99951300	-2.20589100	0.67640600
H	-2.11773900	-3.03457700	-0.01253100
C	-2.26609000	-2.34667800	2.03461400
H	-2.59210600	-3.30436300	2.42457400
C	3.42271000	-0.60769600	0.36163200
H	3.52731400	-0.92891800	-0.68034700
C	4.04175200	0.77282500	0.54945900
H	3.55111500	1.53432400	-0.06412000
H	5.09992400	0.74707800	0.27027900
H	3.96496000	1.08048100	1.59641400
C	4.07515600	-1.64477000	1.27033100
H	3.92768800	-1.38280900	2.32295400
H	5.15131200	-1.67440400	1.07802800
H	3.66341900	-2.64196500	1.09913700



Front view

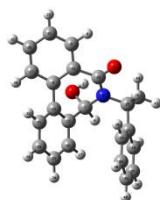
Top view

10c-(R, P) (G = -1660.349744 hartree)

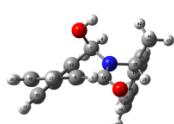
Imaginary frequency: 0

C	0.60653000	3.88520300	0.05622000
C	-0.32021600	2.84556500	0.03057000
C	0.08377900	1.52843200	0.24098100
C	1.44690700	1.24856400	0.46195100
C	2.36569000	2.29977500	0.49648000
C	1.94981600	3.61213900	0.29507700
C	1.91495500	-0.14552700	0.68467900
C	2.77462000	-0.43489700	1.74676600
C	3.19453600	-1.73891000	2.00026900

H	3.86041700	-1.93246600	2.83448200
C	2.75626700	-2.79084800	1.20243800
C	1.90169800	-2.53432200	0.13360300
C	1.49559000	-1.22736500	-0.11118900
H	0.27664400	4.90531300	-0.10888700
H	-1.36926400	3.06252400	-0.14848900
H	3.41635500	2.08155600	0.66193900
H	2.67627000	4.41749900	0.31743400
H	3.07781200	-3.80619200	1.40481600
H	1.55648500	-3.32927100	-0.51785000
H	3.09644600	0.37453300	2.39431700
C	-0.87686200	0.35660200	0.21154700
H	-0.53414200	-0.38581600	0.93233800
O	1.28128800	0.05780000	-2.40243400
N	-0.92052900	-0.33944900	-1.09818300
C	-1.54651100	0.40353800	-2.20644400
H	-1.03996400	1.35404700	-2.40638900
H	-2.58692900	0.58902100	-1.94245200
H	-1.51991800	-0.22002600	-3.10152600
S	0.57401400	-0.95107900	-1.61207600
O	0.31505900	-2.23768500	-2.25320800
C	-3.40621200	-0.80357600	0.62037400
H	-3.44603900	-1.05514900	-0.44429000
C	-2.68708500	-1.91276400	1.37669300
H	-2.53736300	-1.63570300	2.42468100
H	-1.71856000	-2.15132100	0.92893000
H	-3.29545300	-2.82190700	1.34379500
C	-4.82247000	-0.58252100	1.14594300
H	-4.80532300	-0.33000300	2.21049400
H	-5.40124600	-1.50170400	1.02243400
H	-5.33308300	0.21903600	0.60608800
S	-2.55441600	0.82150000	0.74987600



Front view



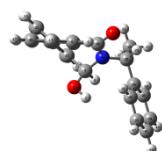
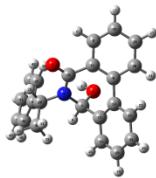
Top view

11-(R, R, M) (G = -1054.555361 hartree)

Imaginary frequency: 0

O	-0.91511400	-0.61956700	2.20289800
H	-0.81352800	-1.52873200	2.51553200
O	-1.01409400	-2.36078600	-1.54299200

N	0.07449000	-1.31428800	0.14645700
C	-3.45633200	-1.47437600	-0.58445700
H	-3.36546900	-2.51387000	-0.87942200
C	0.09965800	-0.37061600	1.26626600
H	1.08737200	-0.49757200	1.72346100
C	-2.36100300	0.62111400	-0.03847000
C	-1.01814300	-1.51911000	-0.64561700
C	-2.28280500	-0.74315800	-0.37872000
C	-0.00604000	1.05142700	0.77299600
C	-1.17133300	1.49503200	0.13042400
C	3.53993200	-0.96496100	0.53383200
H	3.62372100	-1.64214100	1.37861500
C	1.08667400	1.90335000	0.91398400
H	1.99103000	1.53138800	1.39068900
C	2.45890000	-1.06105800	-0.34172600
C	2.38483000	-0.17593700	-1.42275800
H	1.53574500	-0.23911200	-2.10022300
C	-4.70685100	-0.89374600	-0.42076800
H	-5.60523700	-1.48384700	-0.56751600
C	1.03912000	3.20631900	0.42761800
H	1.89839300	3.85969200	0.53734100
C	1.31956200	-2.05148000	-0.14484400
H	1.13273200	-2.54500300	-1.10008500
C	-3.63219100	1.19316700	0.10906300
H	-3.70478200	2.23870800	0.39117100
C	3.36427500	0.78902000	-1.62151800
H	3.28996200	1.47093200	-2.46263500
C	-1.20428100	2.80723000	-0.35735200
H	-2.08842600	3.15550100	-0.88243800
C	-0.11297800	3.65739300	-0.20993600
H	-0.16074200	4.66672200	-0.60536900
C	-4.79267400	0.45076200	-0.06978800
H	-5.76037400	0.92223200	0.06735100
C	4.52407400	0.00653200	0.33966800
H	5.35715200	0.07236400	1.03221900
C	4.43732700	0.88598200	-0.73421500
H	5.20148700	1.64194100	-0.88327600
C	1.56255500	-3.12391900	0.91217700
H	1.66705500	-2.69772700	1.91549100
H	2.47353400	-3.68488500	0.68847900
H	0.71896000	-3.81755600	0.92100700



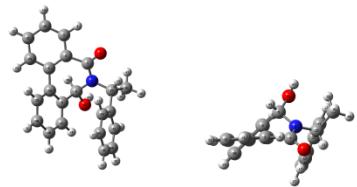
Front view Top view

11-(R, S, P) (G = -1054.55564 hartree)

Imaginary frequency: 0

O	0.10712500	-0.19991500	-1.66633600
H	0.94565800	-0.67003600	-1.78256700
O	-0.07177700	-1.72425500	2.19621900
N	0.49754500	-0.13359900	0.68607300
C	-1.93969000	-2.78106600	0.46032400
H	-1.27519900	-3.45603400	0.98816100
C	0.24776900	0.62635400	-0.54029100
H	1.12586200	1.27344900	-0.65221400
C	-2.47144000	-0.50894400	-0.20306100
C	-0.34824500	-1.08391200	1.18309600
C	-1.60986000	-1.42210300	0.43189200
C	-0.96692600	1.51132300	-0.40486900
C	-2.24316800	0.95804600	-0.22020300
C	-0.80564700	2.89442700	-0.44844800
H	0.18674300	3.30880400	-0.60546200
C	-3.08294000	-3.25946600	-0.16473500
H	-3.31035200	-4.31994600	-0.14657200
C	-1.89675600	3.74615600	-0.30206100
H	-1.75604500	4.82110500	-0.33931100
C	-3.62747100	-1.00864900	-0.81878300
H	-4.28813400	-0.31631700	-1.33072000
C	-3.33105700	1.82566400	-0.06507300
H	-4.31852200	1.40981100	0.10940200
C	-3.16386900	3.20598800	-0.10454900
H	-4.02251000	3.85669700	0.02416800
C	-3.93059700	-2.36410900	-0.81170800
H	-4.82651500	-2.71807100	-1.31132500
C	1.76917700	0.12184300	1.38569200
H	1.82129400	-0.64730200	2.15900600
C	1.74826900	1.48708900	2.06619500
H	0.88227700	1.54466600	2.72903000
H	2.65171000	1.63473900	2.66311000
H	1.68046800	2.30461700	1.34101700
C	2.92613900	-0.10374300	0.42040500
C	2.98046500	-1.31412300	-0.28465900
C	3.93045600	0.84015700	0.20819900

C	4.01003200	-1.57113800	-1.18333600
H	2.20660500	-2.06105600	-0.11712400
C	4.96719700	0.58215900	-0.69045100
H	3.91471700	1.78617500	0.73927500
C	5.00936300	-0.61896400	-1.38928600
H	4.03613000	-2.51406600	-1.72003800
H	5.73945100	1.32892100	-0.84451800
H	5.81357800	-0.81554400	-2.09061900



Front view

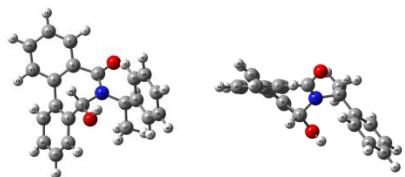
Top view

11-(R, S, M) (G = -1054.55218 hartree)

Imaginary frequency: 0

O	-1.27743800	-2.39081000	-1.47775200
N	-0.09146400	-1.39949700	0.19149000
C	-3.64881900	-1.36081300	-0.38553900
H	-3.64906000	-2.41933200	-0.62244200
C	-0.11263100	-0.47129500	1.34496600
C	-2.36900800	0.67147400	0.00148700
C	-1.21066800	-1.56923900	-0.56331500
C	-2.41474600	-0.71427900	-0.25816800
C	-0.01297400	0.95169300	0.85206300
C	-1.11009300	1.45568400	0.13653200
C	3.37024800	-0.90942300	0.38836600
H	3.47372300	-1.59139000	1.22605200
C	1.11913300	1.73254500	1.05847400
H	1.95218400	1.31498000	1.61401300
C	2.26393300	-1.00296100	-0.45432600
C	2.15327600	-0.10804500	-1.52299700
H	1.28941200	-0.17424300	-2.18179800
C	-4.84102600	-0.67118000	-0.22129200
H	-5.78883400	-1.19248700	-0.30235600
C	1.18690400	3.01655400	0.52693800
H	2.07902500	3.61660200	0.67600200
C	1.16308100	-2.03547300	-0.26129900
H	0.90667000	-2.41337600	-1.25358300
C	-3.58771300	1.35361900	0.14376900
H	-3.56871200	2.41632200	0.36332200
C	3.11436400	0.87406300	-1.73438800
H	3.00792200	1.56720500	-2.56302300

C	-1.02452800	2.74791800	-0.39620800
H	-1.85523100	3.14223200	-0.97381000
C	0.11708500	3.52007400	-0.20995400
H	0.17027900	4.51470500	-0.64061900
C	-4.80651500	0.69736700	0.04204800
H	-5.72953100	1.25244900	0.17398200
C	4.33892700	0.07154400	0.17852000
H	5.19311900	0.13513500	0.84549400
C	4.21124600	0.96854200	-0.87831900
H	4.96402500	1.73403000	-1.03817000
C	1.53896000	-3.24644900	0.58840900
H	1.79500600	-2.97457000	1.61264700
H	2.39789200	-3.75711600	0.14405000
H	0.69722300	-3.94256800	0.61185300
O	0.91784400	-0.75553900	2.23800100
H	0.63898200	-1.48492200	2.80496200
H	-1.08771400	-0.60790100	1.82640400



Front view

Top view

11-(R, R, P) (G = -1054.552141 hartree)

Imaginary frequency: 0

O	0.13844600	-1.91911400	1.83585200
N	0.44073800	-0.16390100	0.42277200
C	-1.86054600	-2.93544300	0.19041100
H	-1.10811700	-3.62602400	0.55504600
C	0.00235500	0.53424200	-0.80851300
C	-2.54910300	-0.63086600	-0.16747700
C	-0.26462500	-1.22293000	0.90306700
C	-1.57922500	-1.56563700	0.25007100
C	-1.15536300	1.44725500	-0.48468800
C	-2.36785600	0.84545300	-0.11551500
C	-1.03785200	2.83336000	-0.52830200
H	-0.09861700	3.27185700	-0.84719400
C	-3.06768100	-3.40135300	-0.30803300
H	-3.26067400	-4.46735200	-0.36179100
C	-2.11642000	3.63950700	-0.17568000
H	-2.01877200	4.71963600	-0.20871500
C	-3.76990400	-1.12420300	-0.65587100
H	-4.51752000	-0.41779300	-1.00192100

C	-3.44130500	1.66994600	0.24364900
H	-4.37740300	1.21869800	0.55801100
C	-3.31673100	3.05473600	0.22088700
H	-4.15847000	3.67523600	0.50996000
C	-4.02874800	-2.48534800	-0.73266900
H	-4.97846200	-2.83129800	-1.12731000
C	1.62583700	0.29966500	1.16539400
H	1.61640300	-0.31881100	2.06599800
C	1.49750600	1.75776200	1.59697700
H	0.53588700	1.90812200	2.09307100
H	2.29214200	2.00297100	2.30657700
H	1.56353000	2.43953000	0.74766200
C	2.90665700	-0.04512800	0.41329700
C	3.07440800	-1.35638200	-0.04817200
C	3.92230400	0.88355400	0.18115800
C	4.22844700	-1.72948600	-0.72913300
H	2.29036900	-2.08592100	0.14040200
C	5.08091800	0.51016900	-0.50068200
H	3.81474900	1.90731500	0.52436600
C	5.23737400	-0.79424100	-0.95895400
H	4.34218400	-2.75047800	-1.07963100
H	5.85947600	1.24599200	-0.67556400
H	6.13747500	-1.08194300	-1.49246300
O	1.04446000	1.27075600	-1.36218500
H	1.73314600	0.66116800	-1.65984300
H	-0.33841200	-0.24451400	-1.50273200

6. References

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- S2.** Ni, C.; Zha, D.; Ye, H.; Hai, Y.; Zhou, Y.; Anslyn, E. V.; You, L., Dynamic covalent chemistry within biphenyl scaffolds: reversible covalent bonding, control of selectivity, and chirality sensing with a single system. *Angew. Chem. Int. Ed.* **2018**, *57*, 1300-1305.
- S3.** Tinsley, I. C.; Spaniol, J. M.; Wheeler, K. A., Mapping the structural boundaries of quasiracemate fractional crystallization using 2-substituted diarylamides. *Chem. Commun.* **2017**, *53*, 4601-4604.