

Bimetallic [Co/K] hydrogen evolution catalyst for electrochemical terminal C-H functionalization

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Supporting Information

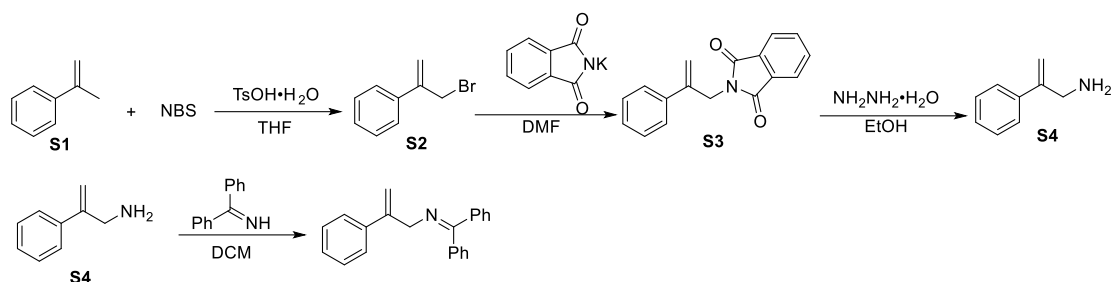
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1. General Information

^1H NMR and ^{13}C NMR were recorded on a Bruker 400 MHz and 600 MHz spectrometer (^1H NMR: 400MHz, 600MHz, ^{13}C NMR: 101MHz, 151MHz). The chemical shifts (δ) and coupling constants (J) were expressed in ppm and Hz respectively. ^1H NMR spectra were referenced to the solvent residual peak (TMS, δ 0 ppm; CD_3OD , δ 3.3 ppm) and $^{13}\text{C}\{^1\text{H}\}$ NMR spectra were referenced to the solvent residual peak (CDCl_3 , δ 77.0 ppm; CD_3OD , δ 50.0 ppm). High resolution mass spectra and liquid phase mass spectrometry were obtained using Waters G2-XS Qtof mass spectrometer with time of flight (TOF) analyzers. Cyclic voltammograms were recorded on electrochemical workstation CHI660E (Shanghai CH Instruments Co., Ltd.). The single crystal X-ray diffraction (SCXRD) data was obtained by using a Stoe Stadivari diffractometer. GC analysis was conducted using CEAULIGHT GC-7920 spectrometer. The structures were solved and refined using the SHELXT software. All solvents were purified and dried according to the standard procedures unless otherwise noted. Commercially substrates were purchased and used directly. *N*-Allylimine¹ and Ellman imine² were prepared according to the literature procedures.

2. General procedure for *N*-allylimine preparation^{3,4}



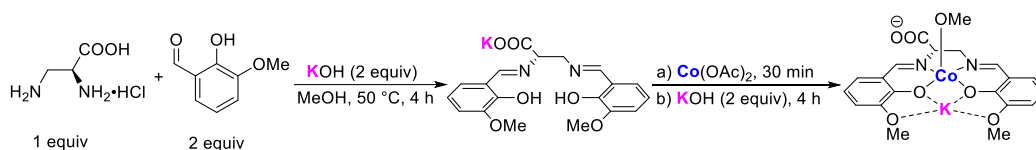
In an oven dried flask, **S1** (10.0 mmol, 1.0 eq.) and dry THF (30 mL) were added. To the resulting solution *N*-bromosuccinimide (11 mmol, 1.1 eq.) and TsOH (1 mmol, 0.1 eq.) were added and the solution was refluxed for 4h. Reaction mixture was cooled to room temperature and the reaction mixture was concentrated under reduced pressure. The residue was taken in ethyl acetate (75 mL), washed with H₂O (3×30 mL). Organic phase was dried over Na₂SO₄, concentrated under reduced pressure to obtain crude product **S2**.

Potassium phthalimide (11 mmol) were added to the solution of crude **S2** (obtained above) in DMF (20 mL) at room temperature. The resulting mixture was stirred for 16 h, after which a dark brown color was formed. Dichloromethane (25 mL) was added and the mixture poured into water (60 mL). The aqueous phase was separated and extracted with dichloromethane (3 × 50 mL). The combined organic extract was dried over anhydrous Na₂SO₄. The dichloromethane was removed in vacuo to afford the crude product **S3**.

Hydrazine hydrate (20.0 mmol) was added to a suspension of **S3** (obtained above) in ethanol (60 mL). The resulting mixture was heated under reflux for 1 h. Then 12 mL HCl aq. (2.0 M) was added and the reaction heated to reflux for a further 1 h. The reaction mixture was then cooled to 4 °C and the phthalhydrazide removed by filtration. The ethanol was removed in vacuum and the solid residue was treated with an excess of NaOH aq. (2.0 M) until the solid residue dissolved. The solution was extracted with ethyl acetate (5 × 30 mL) and the organic extract was dried over Na₂SO₄, filtered and the solvent removed in vacuo. The residue was purified by column chromatography (DCM/Methanol = 20/1 as eluent) to give the **S4** as a colorless oil.

To a solution of 0.91 g (6.8 mmol) of amine **S4** in 30 mL of dry dichloromethane was added 1.24 g (6.8 mmol; 1 equiv) of diphenylmethylenamine. The solution was stirred at room temperature for 16 h, the solvent was evaporated, to afford the pure *N*-(diphenylmethylenidene)amine.

3. Preparation and characterization of bimetallic catalysts



To the solution of (*L*)-3-aminoalanine hydrochloride (1.40 g, 10 mmol) in methanol (30 mL), KOH (1.12 g, 20 mmol) was added. The resulting mixture was allowed to stirred at room temperature for 10 min. o-Vanillin (3.04 g, 20 mmol) was further added to the solution. After stirring for 4 hours at 50 °C, Co(OAc)₂ (1.77 g, 10 mmol) was added to the resulting orange solution and allowed to stirred for 30 min at the same temperature. Additional KOH (1.12 g, 20 mmol) was further added to neutralize the in situ formed acetic acid. After further stirring for 4 hours under air atmosphere, the dark red precipitate was isolated by hot filtration and washed with methanol to remove the potassium acetate byproduct. The precipitate was further dried in vacuum to afford the desired **cat 2** in 62% yield (3.09 g). The single crystal can be accessed via evaporating the solution of **cat 2** in methanol and ethyl ether.

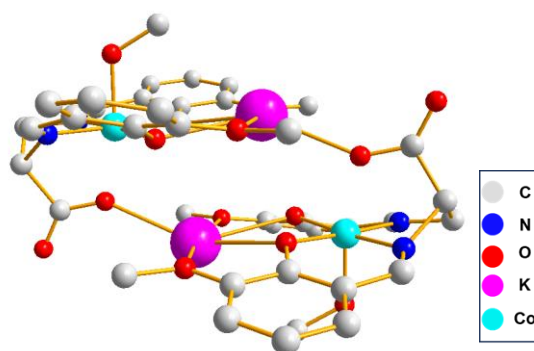


Fig. S1. Single crystal structure of **cat 2** (CCDC NO 2422475)

Table S1 Crystal data and structure refinement for **cat 2**.

Identification code	cat 2
Empirical formula	C ₄₂ H ₄₇ Co ₂ K ₂ N ₄ O ₁₆
Formula weight	1059.89
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	P1 2 ₁ /c 1
a/Å	11.6744(2)
b/Å	21.7762(4)
c/Å	9.08477(18)
α/°	90
β/°	106.474(2)
γ/°	90
Volume/Å ³	2214.75(8)
Z	2
ρ _{calc} /g/cm ³	1.589
μ/mm ⁻¹	8.214
F(000)	1094
Crystal size/mm ³	0.02 × 0.01 × 0.01
Radiation	Cu Kα (λ = 1.54184)
2θ range for data collection/°	3.942 to 75.260
Index ranges	-14 ≤ h ≤ 14, -26 ≤ k ≤ 26, -11 ≤ l ≤ 10
Reflections collected	39864
Independent reflections	4622 [R _{int} = 0.0739, R _{sigma} = 0.0302]
Data/restraints/parameters	4622/19/302
Goodness-of-fit on F ²	1.093
Final R indexes [I ≥ 2σ (I)]	R ₁ = 0.0754, wR ₂ = 0.1629
Final R indexes [all data]	R ₁ = 0.0825, wR ₂ = 0.1681
Largest diff. peak/hole / e Å ⁻³	1.074 / -1.051

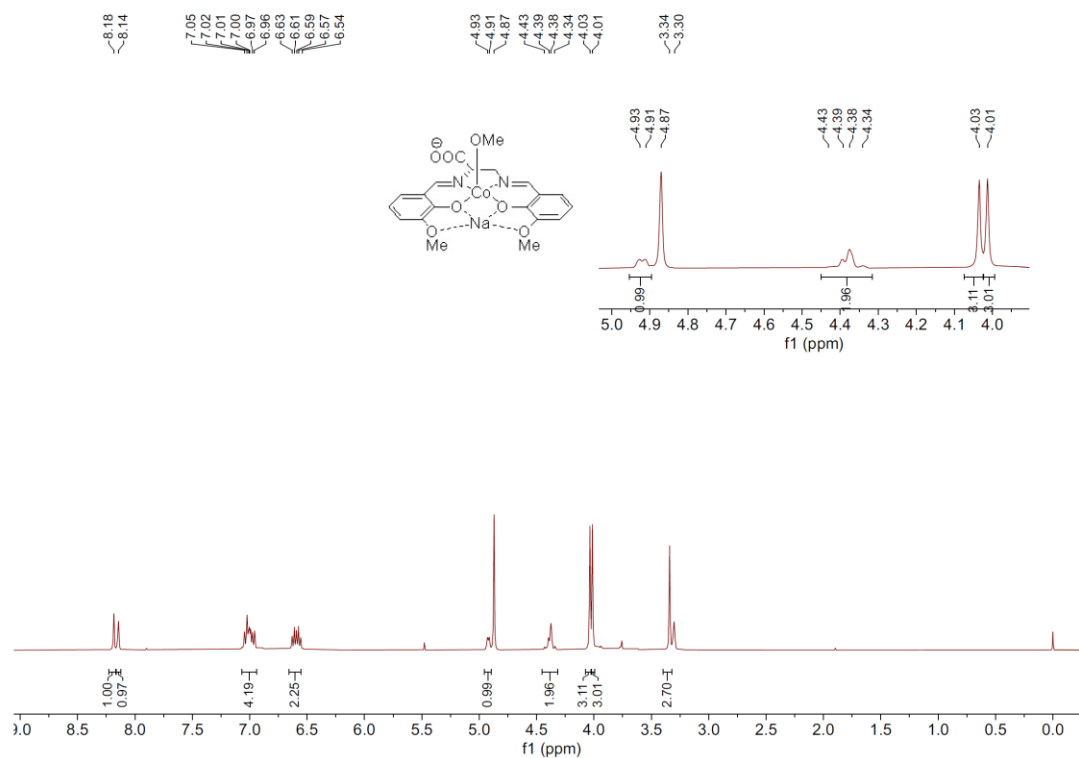


Fig. S2. The ¹H NMR spectra of **cat 1** in methanol-D₄

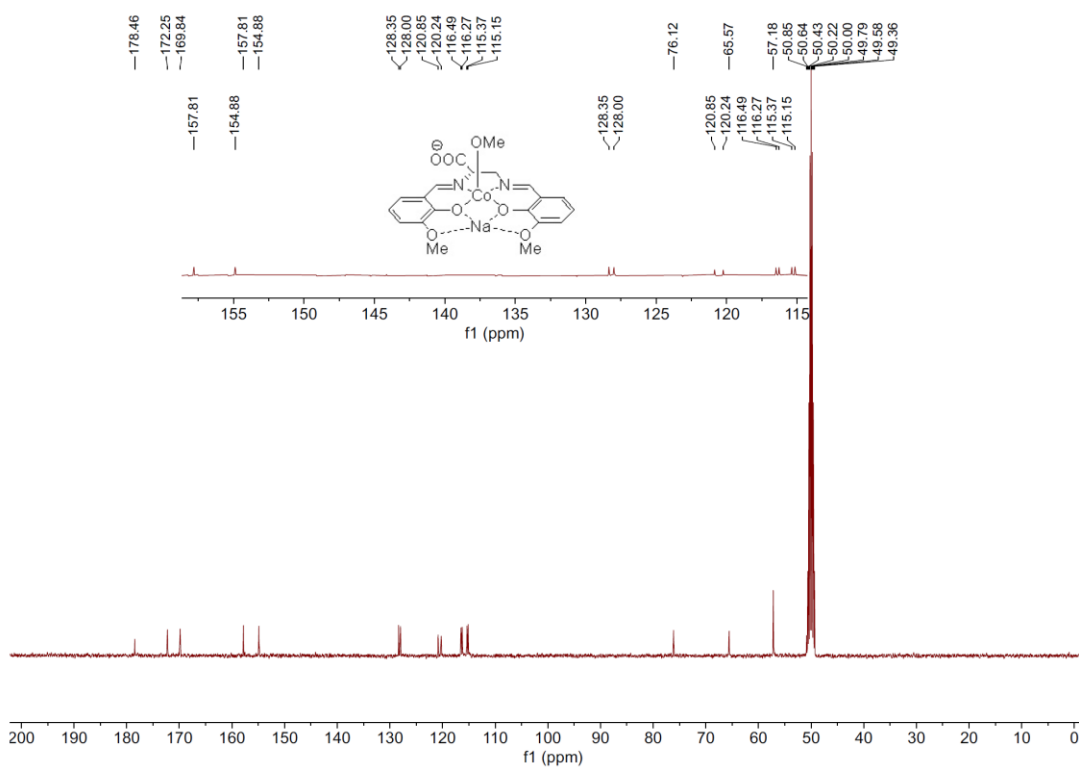


Fig. S3. The ¹³C NMR spectra of **cat 1** in methanol-D₄

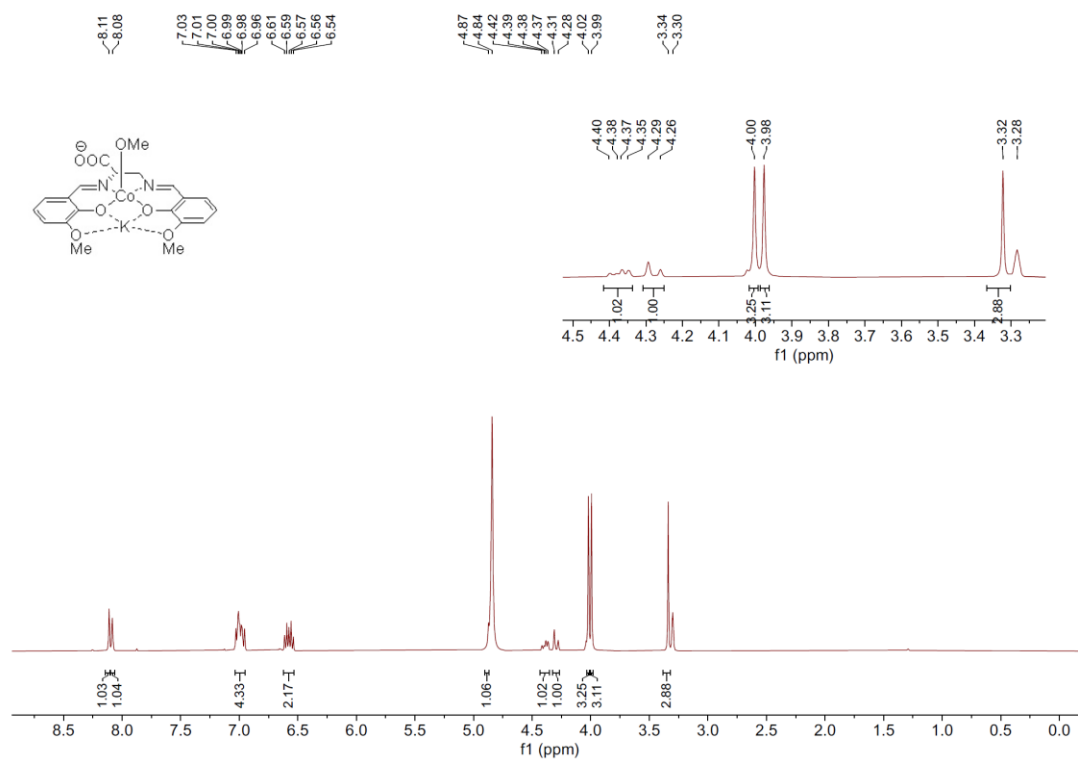


Fig. S4. The ¹H NMR spectra of **cat 2** in methanol-D₄

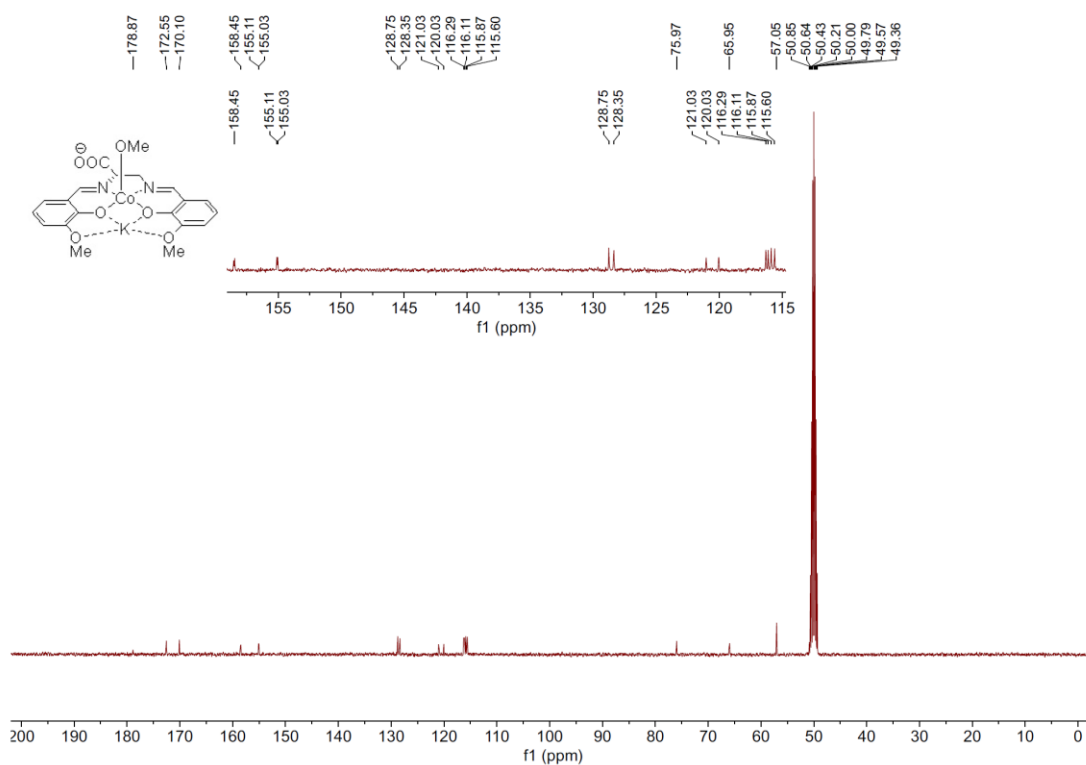


Fig. S5. The ¹³C NMR spectra of **cat 2** in methanol-D₄

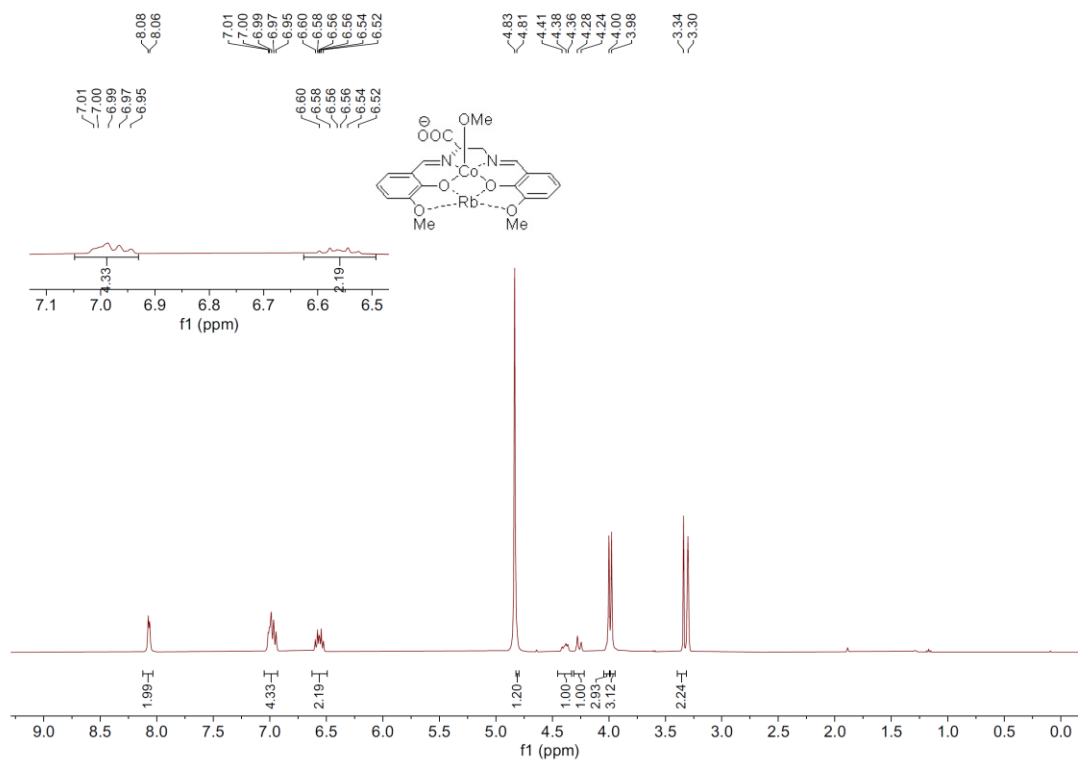


Fig. S6. The ¹H NMR spectra of **cat 3** in methanol-D₄

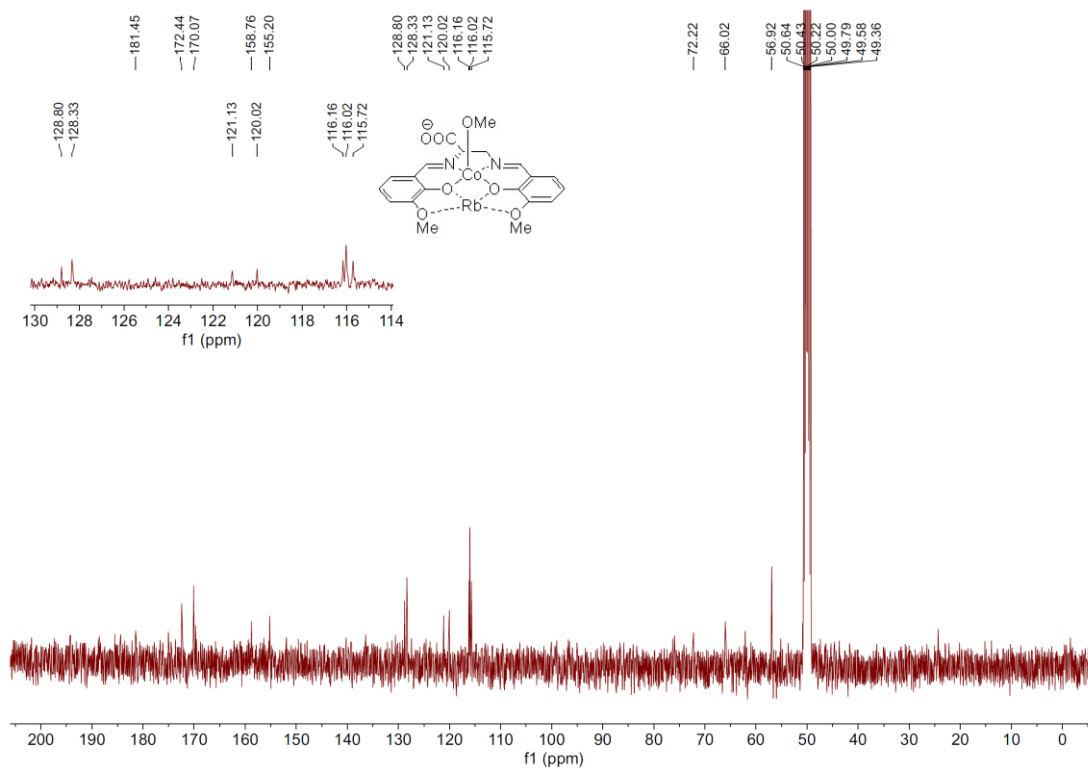


Fig. S7. The ¹³C NMR spectra of **cat 3** in methanol-D₄

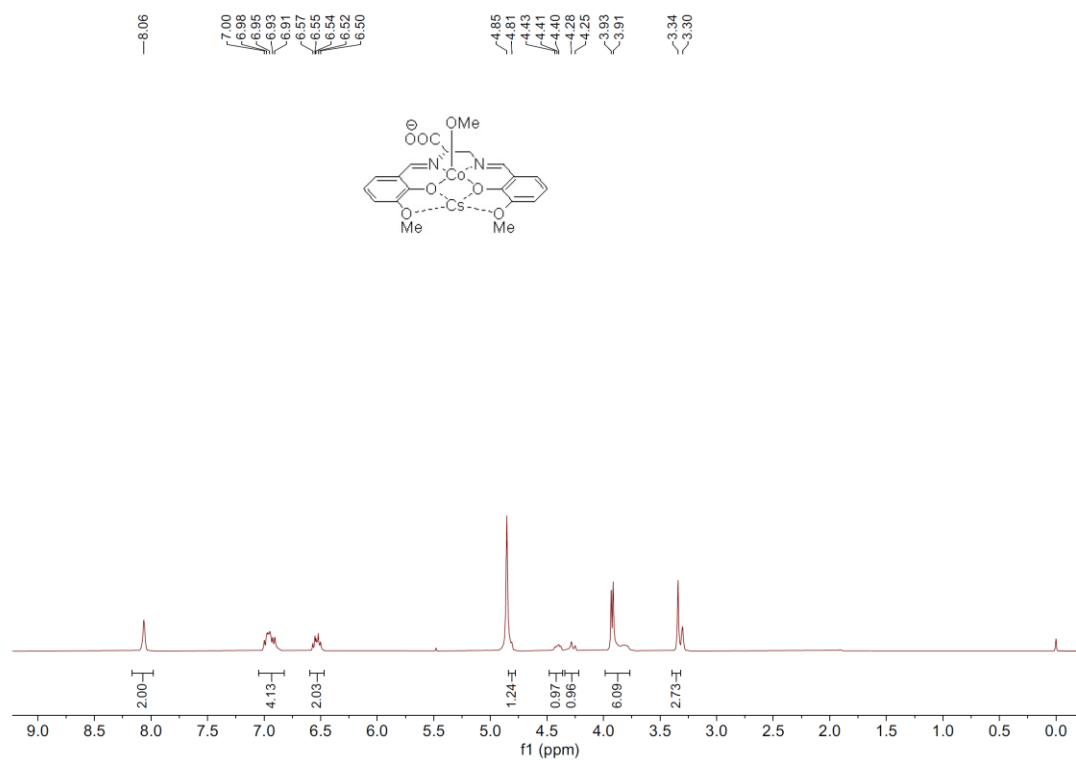


Fig. S8. The ¹H NMR spectra of **cat 4** in methanol-D₄

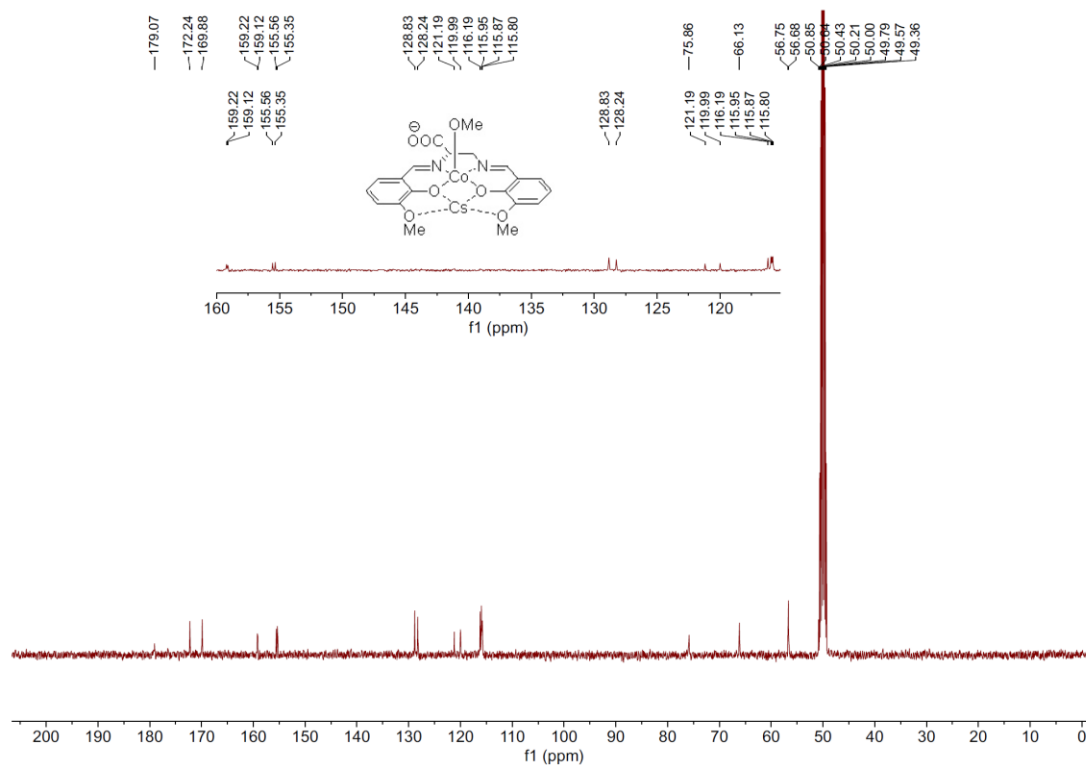
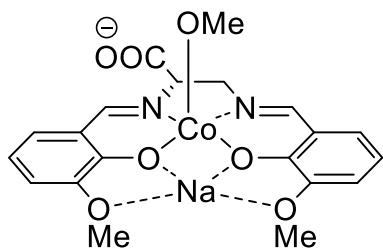
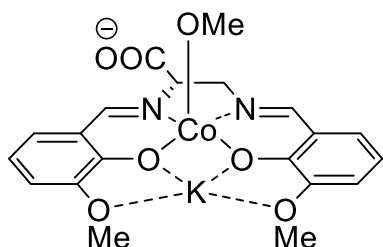


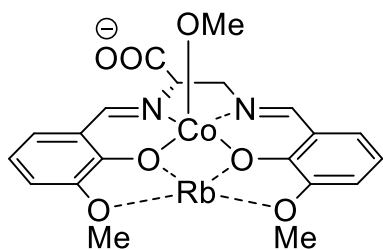
Fig. S9. The ¹³C NMR spectra of **cat 4** in methanol-D₄



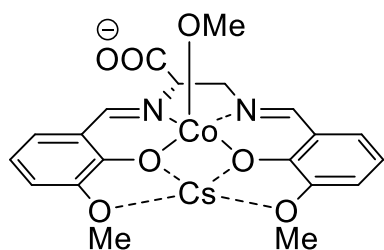
cat 1: 1.59 g, 66% yield (5 mmol scale); brown solid; ^1H NMR (400 MHz, methanol- d_4) δ 8.18 (s, 1H), 8.14 (s, 1H), 7.01 (m, 4H), 6.59 (m, 2H), 4.92 (d, $J = 8.0$ Hz, 1H), 4.39 (dd, $J = 16.0$ Hz, $J = 20.0$ Hz, 2H), 4.03 (s, 3H), 4.01 (s, 3H), 3.34 (s, 3H); ^{13}C NMR (101 MHz, methanol- d_4) δ 178.5, 172.3, 169.8, 157.8, 154.9, 128.4, 128.0, 120.9, 120.2, 116.5, 116.3, 115.4, 115.2, 76.1, 65.6, 57.2, 50.9; HRMS (ESI): calc for $\text{C}_{20}\text{H}_{20}\text{CoN}_2\text{NaO}_7$ ($\text{M}+\text{H}$) $^+$ 483.0578, found 483.0574.



cat 2: 3.09 g, 62% yield; dark red solid; ^1H NMR (400 MHz, methanol- d_4) δ 8.11 (s, 1H), 8.08 (s, 1H), 7.00 (m, 4H), 6.58 (m, 2H), 4.87 (s, 1H), 4.40 (dd, $J = 12.0$ Hz, $J = 8.0$ Hz, 1H), 4.30 (d, $J = 12.0$ Hz, 1H), 4.02 (s, 3H), 3.99 (s, 3H), 3.34 (s, 3H); ^{13}C NMR (101 MHz, methanol- d_4) δ 178.9, 172.6, 170.1, 158.5, 155.1, 155.0, 128.8, 128.4, 121.0, 120.0, 116.3, 116.1, 115.9, 115.6, 76.0, 66.0, 57.1, 50.9; HRMS (ESI): calc for $\text{C}_{20}\text{H}_{20}\text{CoKN}_2\text{O}_7$ ($\text{M}+\text{H}$) $^+$ 499.0318, found 499.0320.



cat 3: 1.25 g, 46% yield (5 mmol scale); brown solid; ^1H NMR (400 MHz, methanol- d_4) δ 8.18 (s, 1H), 8.15 (s, 1H), 7.02 (m, 4H), 6.60 (m, 2H), 4.93 (d, $J = 4.0$ Hz, 1H), 4.39 (m, 2H), 4.04 (s, 3H), 4.02 (s, 3H), 3.34 (s, 3H); ^{13}C NMR (101 MHz, methanol- d_4) δ 181.5, 172.4, 170.1, 158.8, 155.2, 128.8, 128.3, 121.1, 120.0, 116.2, 116.0, 115.7, 72.2, 66.0, 56.9, 50.9; HRMS (ESI): calc for $\text{C}_{20}\text{H}_{20}\text{CoRbN}_2\text{O}_7$ ($\text{M}+\text{H}$) $^+$ 544.9799, found 544.9800.



cat 4: 1.27 g, 43% yield (5 mmol scale); brown solid; ^1H NMR (400 MHz, methanol- d_4) δ 8.06 (s, 2H), 6.96 (m, 4H), 6.54 (m, 2H), 4.82 (d, J = 8.0 Hz, 1H), 4.42 (m, 1H), 4.27 (d, J = 12.0 Hz, 1H), 3.93 (s, 3H), 3.91 (s, 3H), 3.34 (s, 3H); ^{13}C NMR (101 MHz, methanol- d_4) δ 179.1, 172.2, 169.9, 159.2, 159.1, 155.6, 155.4, 128.8, 128.2, 121.2, 120.0, 116.2, 116.0, 115.9, 115.8, 75.9, 66.1, 56.8, 56.7, 50.9; HRMS (ESI): calc for $\text{C}_{20}\text{H}_{20}\text{CoCsN}_2\text{O}_7$ ($\text{M}+\text{H}$) $^+$ 592.9735, found 592.9730.

4. Cyclic voltammograms of bimetallic catalysts and substrates

The electrochemical analysis was demonstrated with Ag/AgNO₃ as a reference electrode, which is not a stable reference electrode. CVs can be calibrated using ferrocene as an external reference. (Fig. S10) $E_0(\text{Fc}/\text{Fc}^+) = (0.164 - 0.045)/2 = 0.060\text{V}$.

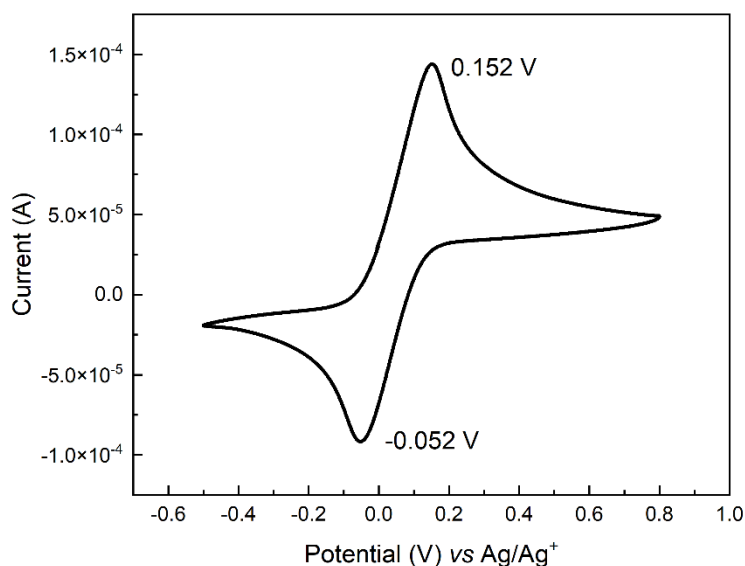


Fig. S10. Cyclic voltammograms of ferrocene (0.005 mmol) in 0.1 M ⁿBu₄NClO₄ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO₃ (0.1 M in CH₃CN) as counter and reference electrodes at a 100 mV/s scan rate.

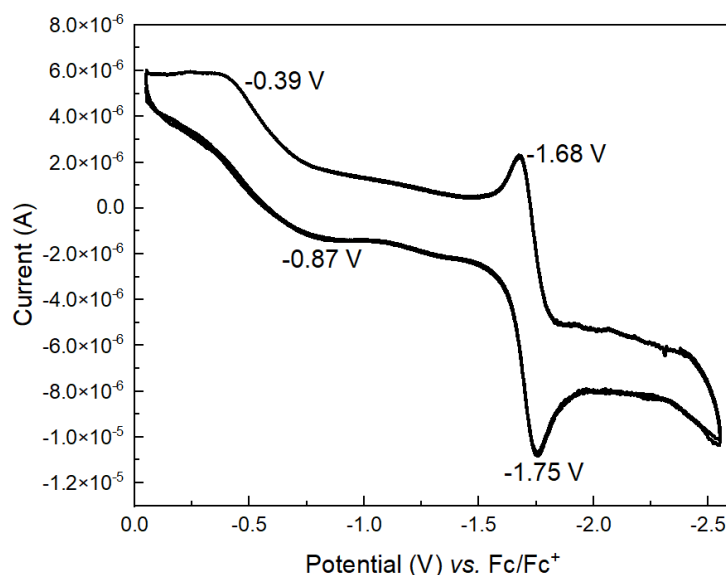


Fig. S11. Cyclic voltammogram of **cat 1** (0.01 mmol) in 0.1 M ⁿBu₄NClO₄ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO₃ (0.1 M in CH₃CN) as counter and reference electrodes at a 100 mV/s scan rate.

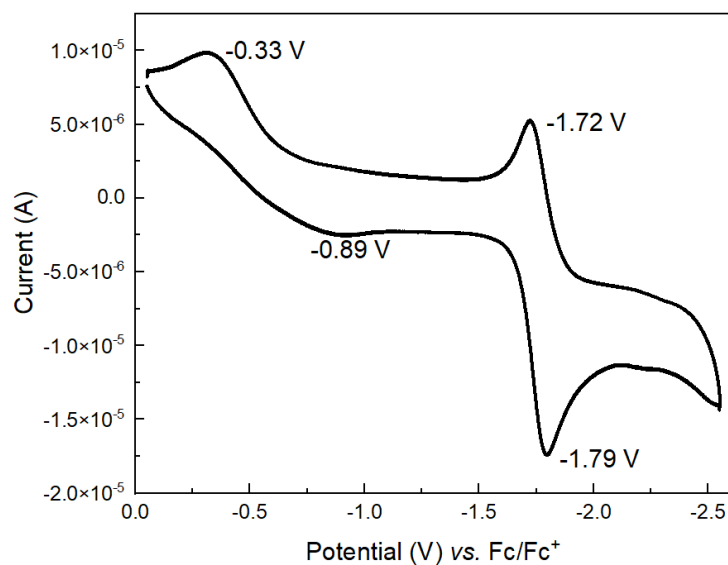


Fig. S12. Cyclic voltammogram of **cat 2** (0.01 mmol) in 0.1 M $n\text{BuNCIO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

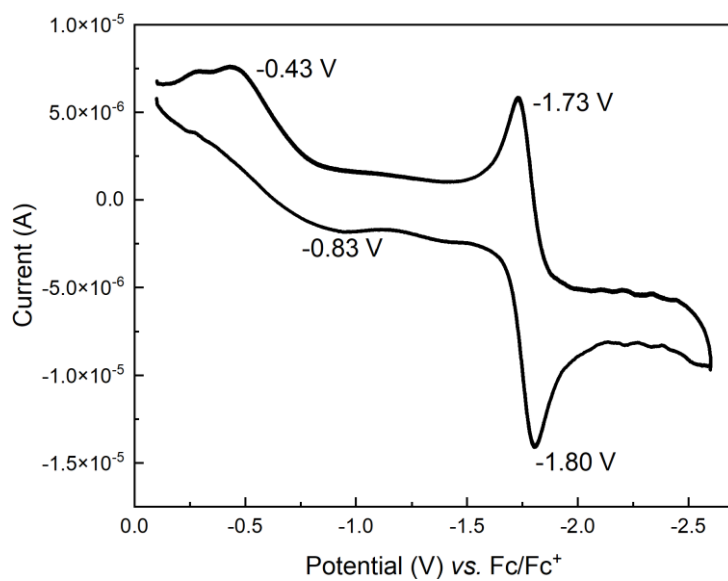


Fig. S13. Cyclic voltammogram of **cat 3** (0.01 mmol) in 0.1 M $n\text{BuNCIO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

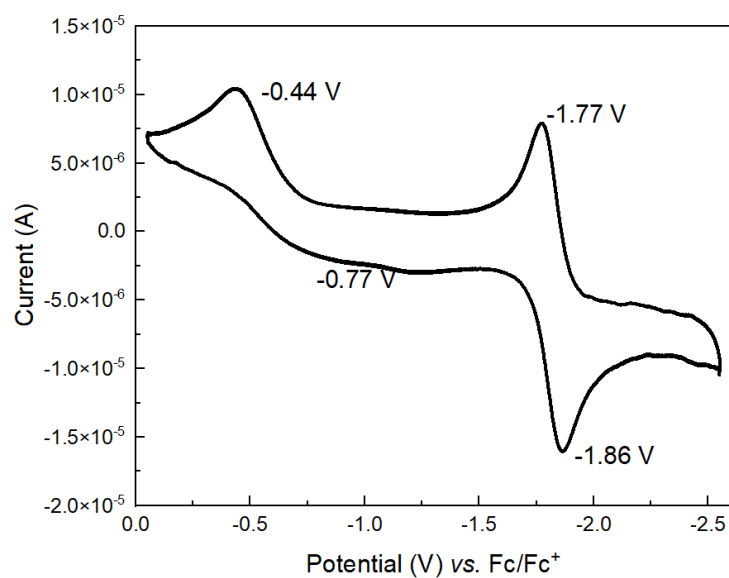


Fig. S14. Cyclic voltammogram of **cat 4** (0.01 mmol) in 0.1 M $n\text{BuNClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

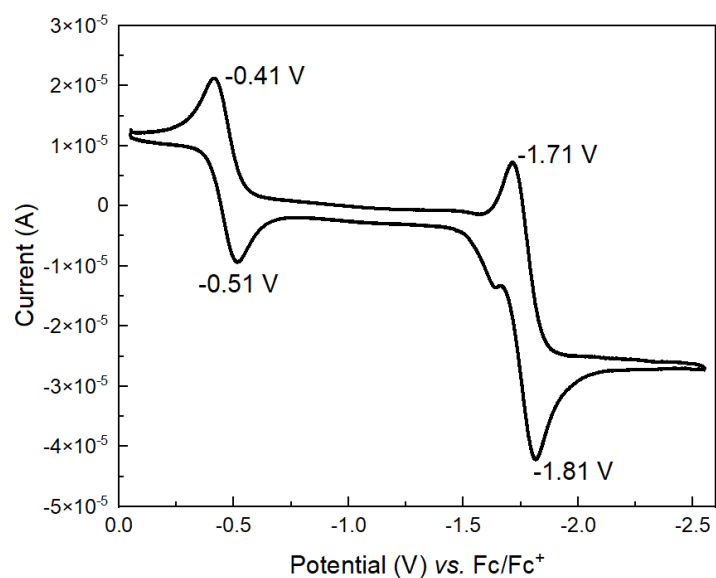


Fig. S15. Cyclic voltammogram of **cat 5** (0.01 mmol) in 0.1 M $n\text{BuNClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

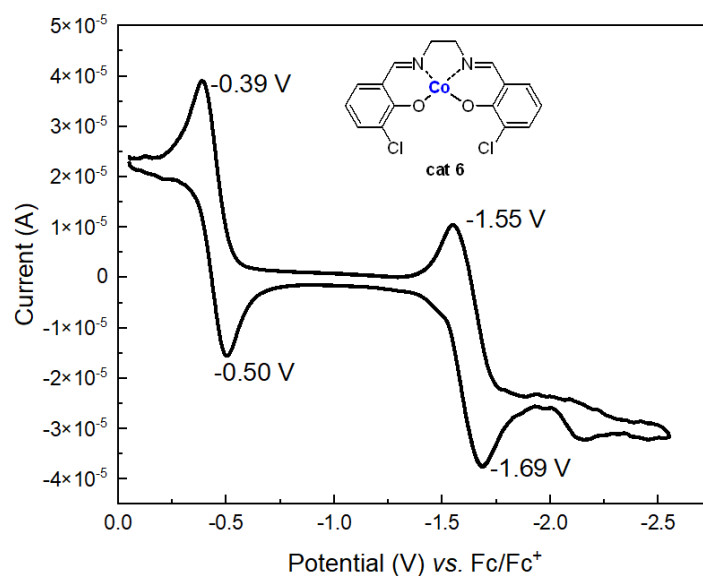


Fig. S16. Cyclic voltammogram of **cat 6** (0.01 mmol) in 0.1 M $n\text{BuNCIO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

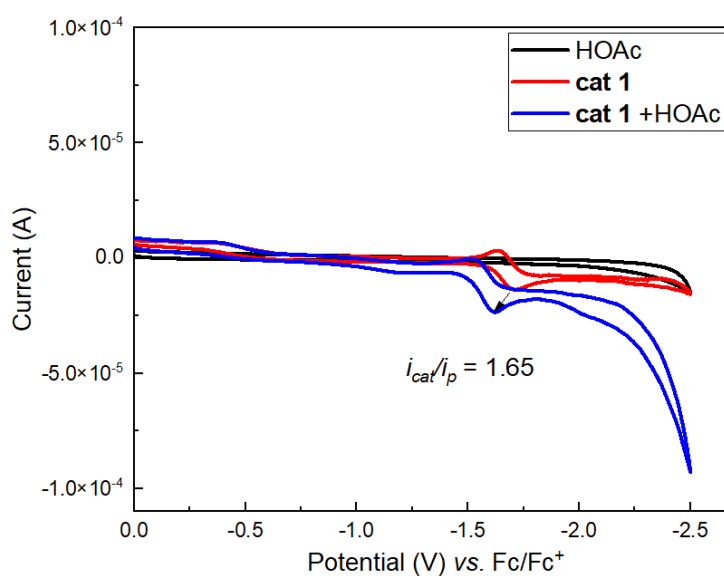


Fig. S17. Cyclic voltammogram of **cat 1** (0.01 mmol) and acetic acid (0.18 mmol) in 0.1 M $n\text{BuNCIO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

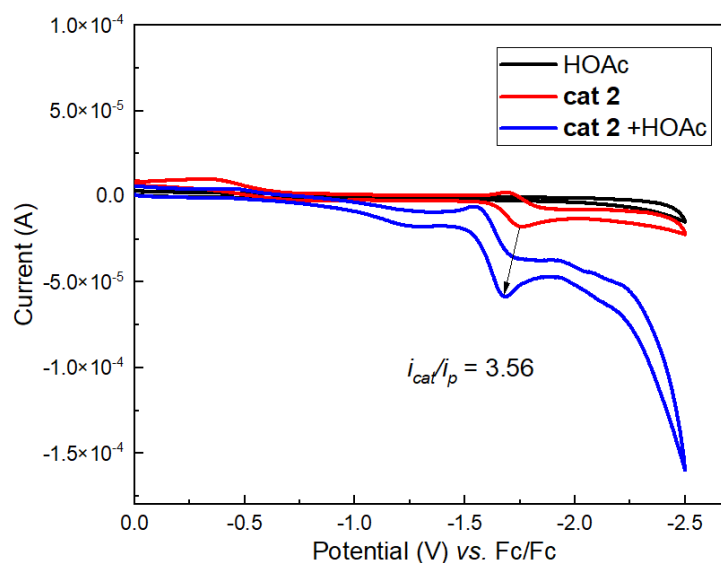


Fig. S18. Cyclic voltammogram of **cat 2** (0.01 mmol) and acetic acid (0.18 mmol) in 0.1 M $n\text{BuNClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

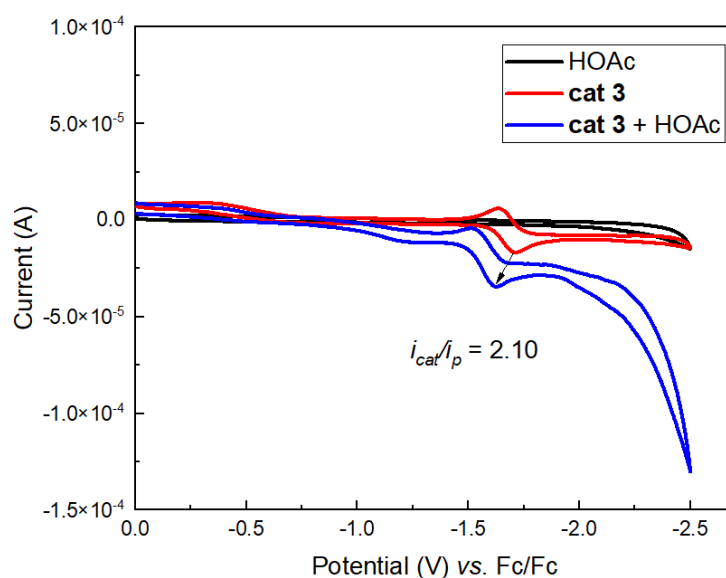


Fig. S19. Cyclic voltammogram of **cat 3** (0.01 mmol) and acetic acid (0.18 mmol) in 0.1 M $n\text{BuNClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

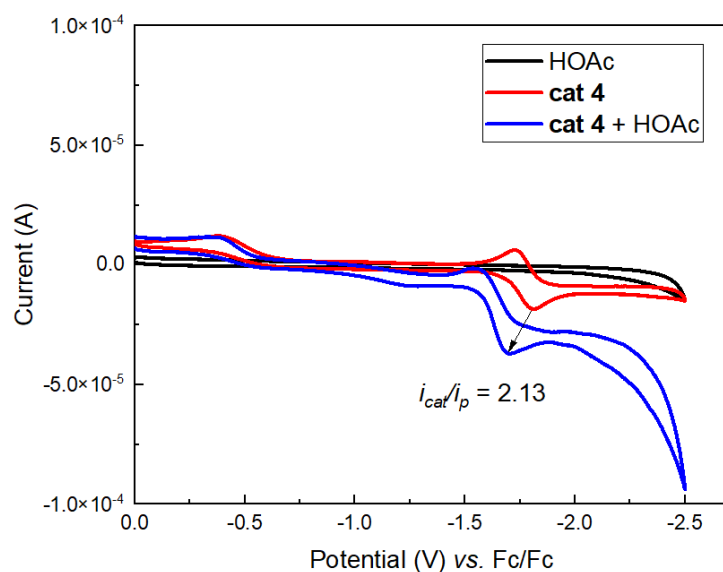


Fig. S20. Cyclic voltammogram of **cat 4** (0.01 mmol) and acetic acid (0.18 mmol) in 0.1 M $n\text{Bu}_4\text{NClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

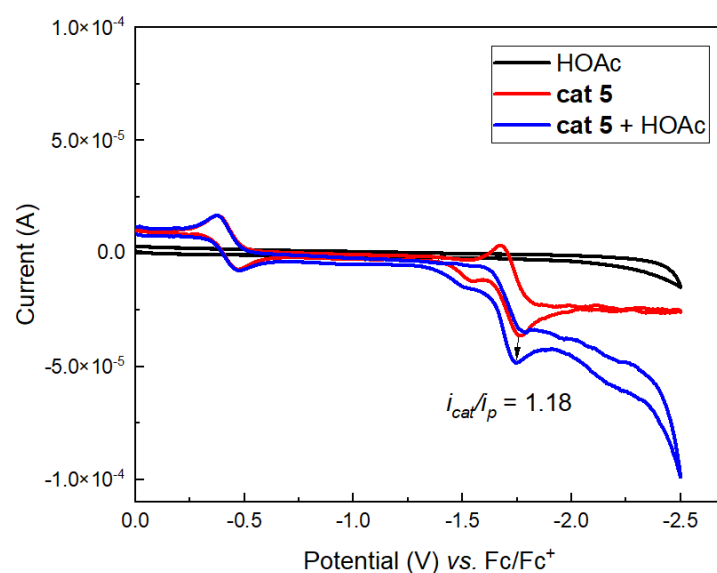


Fig. S21. Cyclic voltammogram of **cat 5** (0.01 mmol) and acetic acid (0.18 mmol) in 0.1 M $n\text{Bu}_4\text{NClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

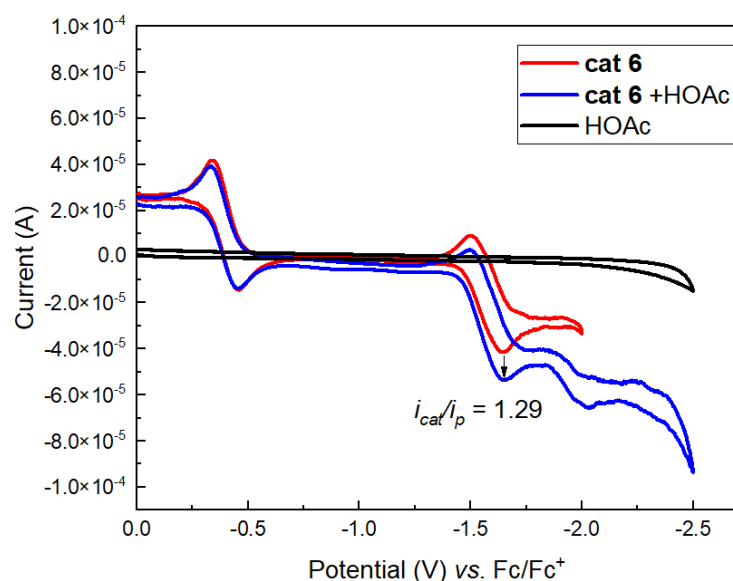


Fig. S22. Cyclic voltammogram of **cat 6** (0.01 mmol) and acetic acid (0.18 mmol) in 0.1 M $n\text{BuNClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

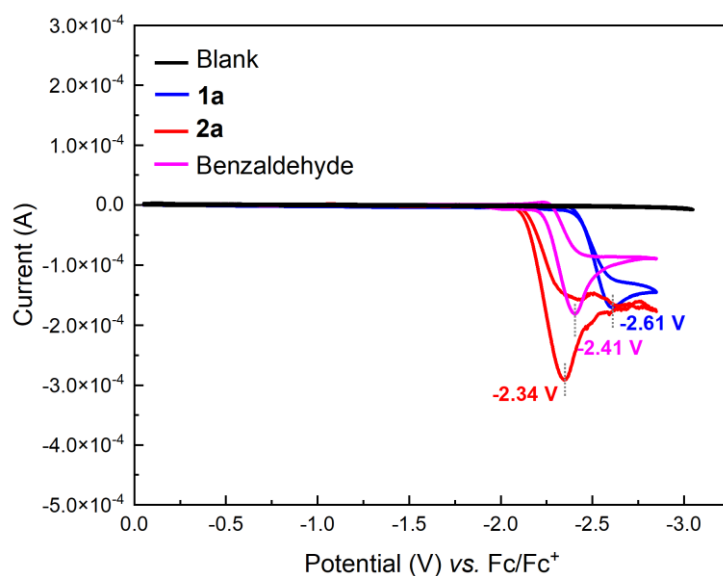


Fig. S23. Cyclic voltammogram of **1a** (0.05 mmol), **2a** (0.05 mmol) and benzaldehyde (0.05 mmol) in 0.1 M $n\text{BuNClO}_4$ (DMF 3.0 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

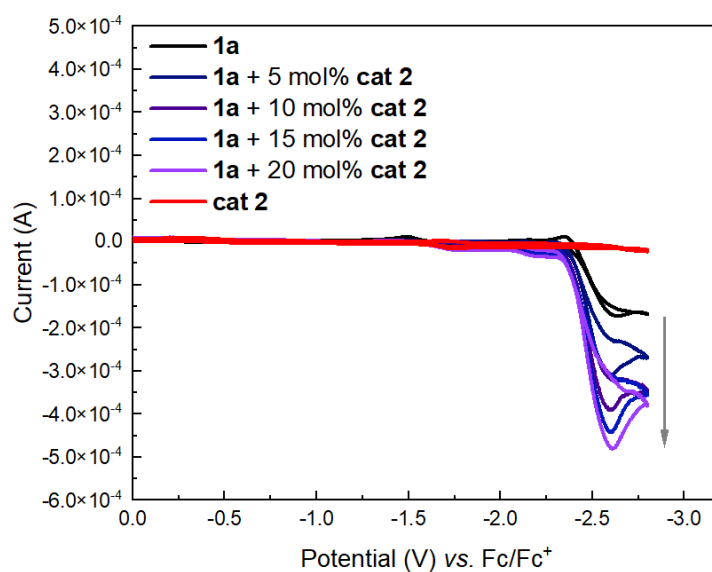


Fig. S24. Cyclic voltammograms of **1a** (0.05 mmol) and **cat 2** in 0.1 M $n\text{Bu}_4\text{NClO}_4$ (DMF 3 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

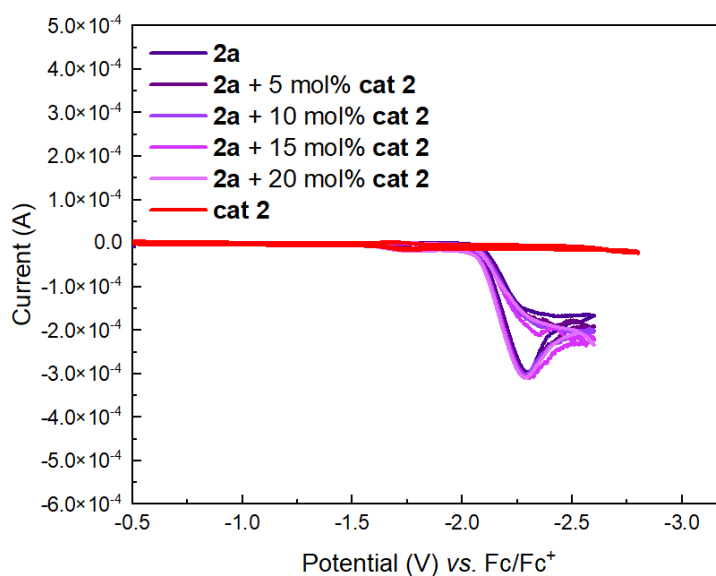


Fig. S25. Cyclic voltammogram of **2a** (0.05 mmol) and **cat 2** in 0.1 M $n\text{Bu}_4\text{NClO}_4$ (DMF 3.0 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

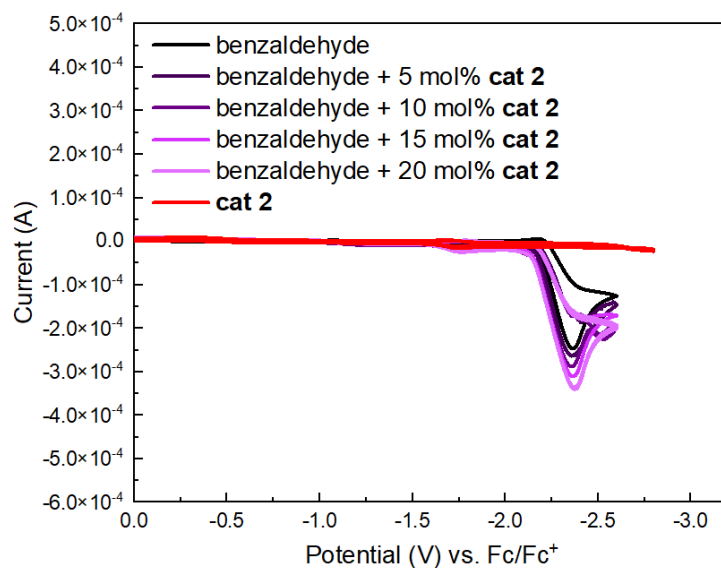


Fig. S26. Cyclic voltammogram of benzaldehyde (0.05 mmol) and **cat 2** in 0.1 M $n\text{BuNClO}_4$ (DMF 3.0 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

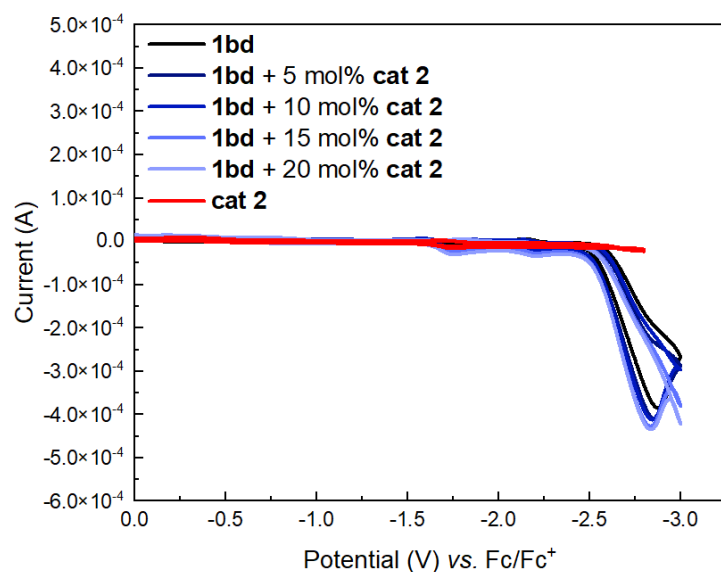


Fig. S27. Cyclic voltammogram of **1bd** (0.05 mmol) and **cat 2** in 0.1 M $n\text{BuNClO}_4$ (DMF 3.0 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

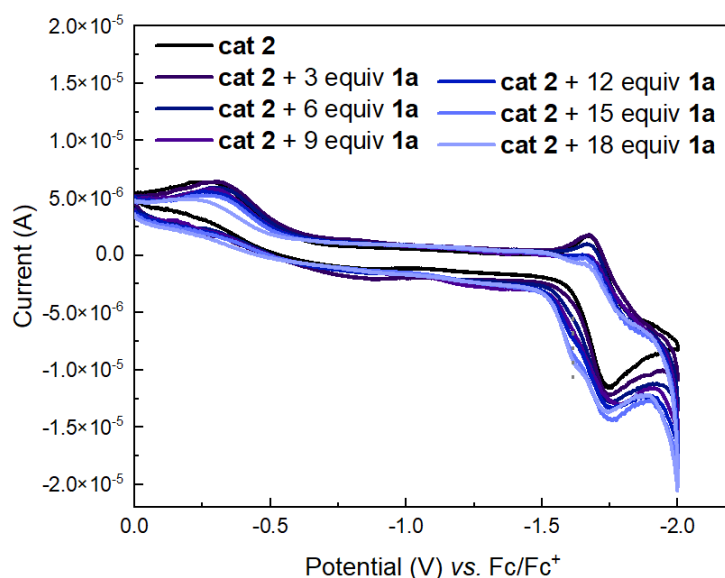


Fig. S28. Cyclic voltammogram of **1a** and **cat 2** (0.01 mmol) in 0.1 M $n\text{BuNCIO}_4$ (DMF 3.0 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

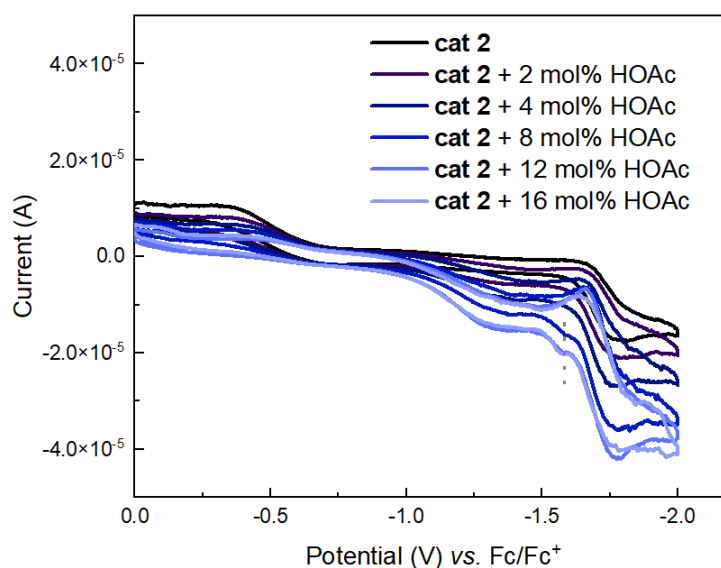
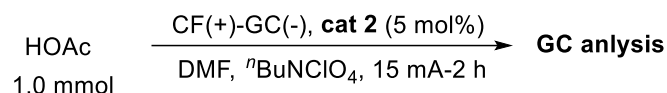


Fig. S29. Cyclic voltammogram of HOAc and **cat 2** (0.01 mmol) in 0.1 M $n\text{BuNCIO}_4$ (DMF 3.0 mL), using a glassy carbon working electrode and Pt wire, Ag/AgNO_3 (0.1 M in CH_3CN) as counter and reference electrodes at a 100 mV/s scan rate.

5. GC experiment for hydrogen detection



To verify the hydrogen product during reduction of HOAc, we also conducted a GC analysis for the reaction atmosphere. After electrolysis, the headspace atmosphere of the reaction tube was subjected to GC analysis. As shown in the GC spectra, substantial amount of hydrogen was detected by comparing with the standard sample containing H₂, O₂, N₂. The result clearly confirmed the HER process (Fig. S30).

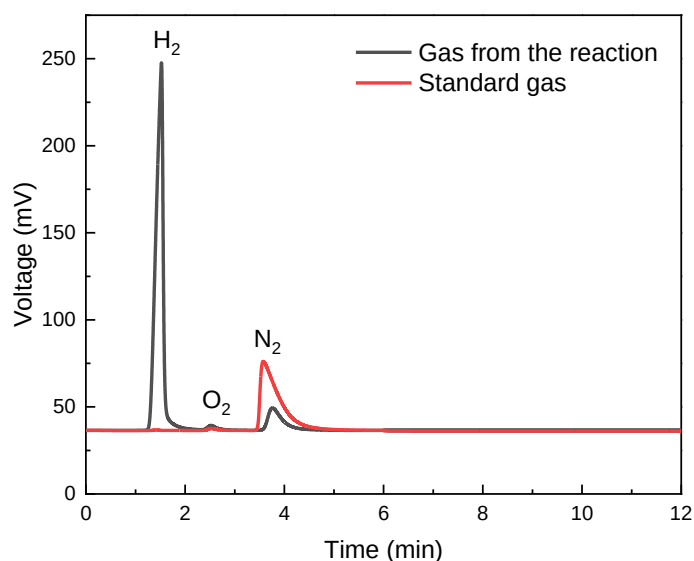
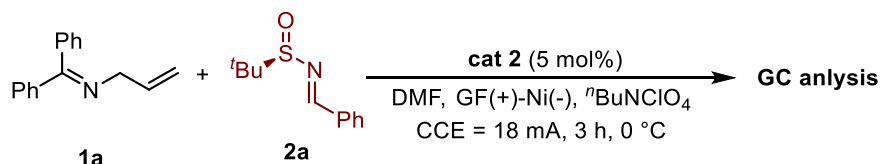


Fig. S30. GC spectra of standard sample (containing H₂, O₂, N₂) and the reaction atmosphere (after reaction)



To verify the hydrogen byproduct during the C-H functionalization between **1a** and **2a**, we also conducted a GC analysis for the reaction atmosphere. After electrolysis, the headspace atmosphere of the reaction tube was subjected to GC analysis. As shown in the GC spectra, substantial amount of hydrogen was detected by comparing with the standard sample containing H₂, O₂, N₂. The result clearly confirmed the HER process in the transformation (Fig. S31).

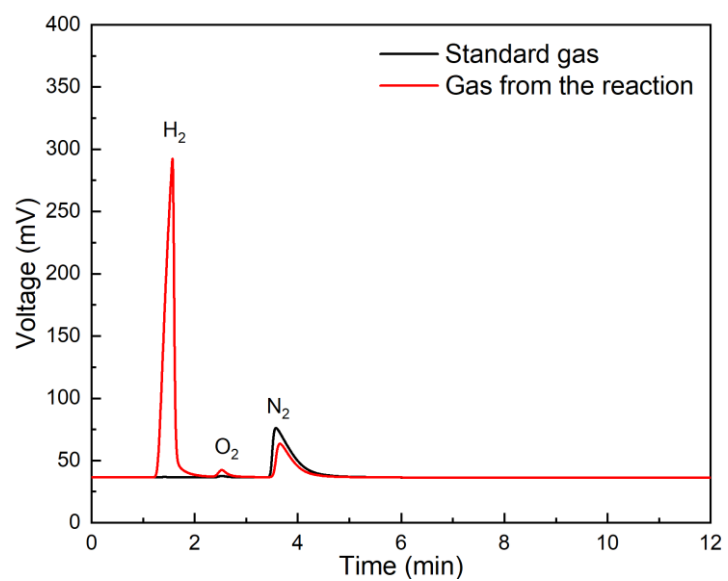
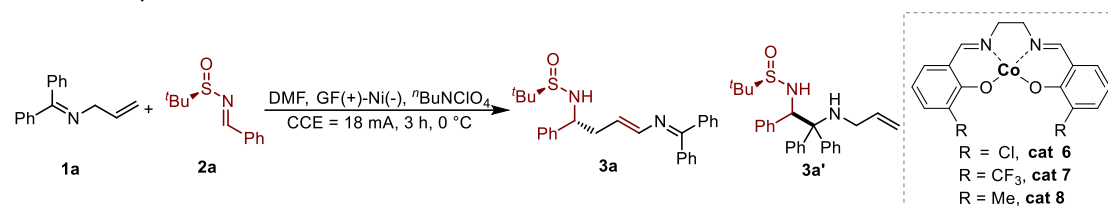


Fig. S31. GC spectra of standard sample (containing H_2 , O_2 , N_2) and the reaction atmosphere (after reaction)

6. Optimization of reaction conditions

Table S2. Optimization of C-H functionalization of **1a** with **2a**^a



Entry	Variations of the optimal conditions	Product	Yield (%) ^b
1	None	3a'	21
2	50 °C	3a'	28
3	50 °C, ⁿ Bu ₄ NOAc as electrolyte	3a'	35
4	50 °C, ⁿ Bu ₄ NBF ₄ as electrolyte	3a'	29
5	50 °C, ⁿ Bu ₄ NOAc as electrolyte, CH ₃ CN as solvent	3a'	38
6	50 °C, ⁿ Bu ₄ NOAc as electrolyte, THF as solvent	3a'	36
7	50 °C, ⁿ Bu ₄ NOAc as electrolyte, DMSO as solvent	3a'	42
8	cat 2 (5 mol%) as catalyst	3a	81
9	cat 6 (5 mol%) as catalyst	3a	35
10	cat 7 (5 mol%) as catalyst	3a	32
11	cat 8 (5 mol%) as catalyst	3a	28
12	cat 6 (5 mol%) as catalyst, Cs ₂ CO ₃ (1 equiv)	3a	48
13	cat 6 (5 mol%) as catalyst, K ₂ CO ₃ (1 equiv)	3a	46
14	cat 2 (5 mol%) as catalyst, CH ₃ CN as solvent	-	-
15	cat 2 (5 mol%) as catalyst, THF as solvent	3a	trace
16	cat 2 (5 mol%) as catalyst, lead plate as cathode	3a	32
17	cat 2 (5 mol%) as catalyst, zinc plate as cathode	3a	53
18	cat 2 (5 mol%) as catalyst, ⁿ Bu ₄ NPF ₆ as electrolyte	3a	65
19	cat 2 (5 mol%) as catalyst, ⁿ Bu ₄ NOAc as electrolyte	3a	17
20	cat 2 (5 mol%) as catalyst, ⁿ Bu ₄ NBr as electrolyte	3a	60

^a Reaction conditions: **1a** (1.5 mmol), **2a** (0.5 mmol), ⁿBu₄NClO₄ (1.0 mmol), DMF (10 mL), graphite felt anode, nickel plate cathode, CCE = 18 mA, 3 h (4.03 F/mol), 0 °C; ^b Isolated yield.

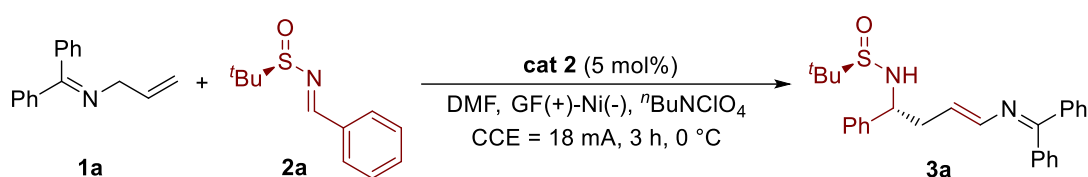
At the outset, we conducted the reaction in the absence of hydrogen evolution catalyst and only 21% yield of crossing-Pinacol coupling product was observed (Entry 1). Upon increasing reaction temperature to 50 °C, the product yield was delivered in 28% yield (Entry 2). Varying the electrolyte and solvents failed to give any **3a** product, although it slightly benefited the generation of **3a'** (Entry 3-7). Hydrogen evolution catalyst significantly changed the product distribution; the [Co/K] catalyst afforded the C-H functionalized product **3a** in 81% yield (Entry 8). In sharp contrast, mononuclear Salen catalysts (**cat 6-8**) only afforded the product in 28-35% yield (Entry 9-11). Despite the additional introduction of base additives, the yield remained unsatisfactory (Entry 12-13). Additionally, variations on the other parameters including solvent, cathode and electrolyte were also concluded and listed on the table (Entry 14-20).

7. General procedure for the electrochemical C-H functionalization of *N*-allylimine



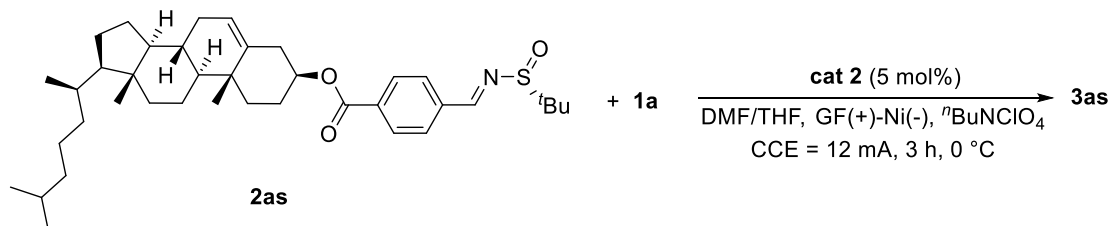
Fig. S32. Electrolysis setup (graphite felt, nickel plate: width 1.8 cm, immersion depth 1.5 cm)

3a as example



An undivided cell was equipped with a magnetic stirrer, nickel plate (1.8*1.5 cm²), graphite felt (1.8*1.5 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S32). The substrate *N*-allylimine **1a** (332 mg, 1.5 mmol), Ellman imine **2a** (105 mg, 0.5 mmol), **cat 2** (12 mg, 0.025 mmol) and ⁿBu₄NClO₄ (342 mg, 1.0 mmol) were added to the solvent DMF (10 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (18 mA, *J* = 6.7 mA•cm⁻²) at 0 °C for 3 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3a** (174 mg) in 81% yield. To prevent it from decomposing, the obtained product should be stored at 0 °C.

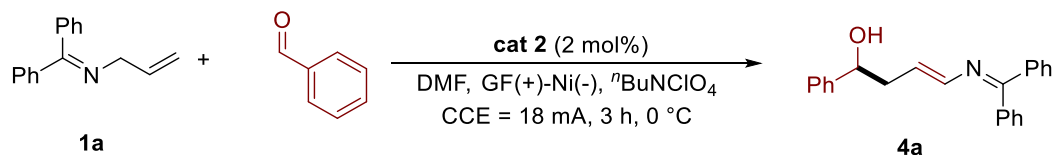
3as as example (0.3 mmol)



An undivided cell was equipped with a magnetic stirrer, nickel plate (1.8*1.5 cm²), graphite felt (1.8*1.5 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S32). The substrate *N*-allylimine **1a** (199 mg, 0.9 mmol), Ellman imine **2as** (187 mg, 0.3 mmol), **cat 2** (7 mg, 0.015 mmol) and ⁿBu₄NClO₄ (342 mg, 1.0 mmol) were added to the mixed solvent DMF/THF (10 mL, 8/2 v/v). The resulting mixture was allowed to stir and electrolyze under constant current condition (12 mA, *J* = 4.4 mA•cm⁻²) at 0 °C for 3 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then

removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3as** (177 mg) in 70% yield. To prevent it from decomposing, the obtained product should be stored at 0 °C.

3j as example



An undivided cell was equipped with a magnetic stirrer, nickel plate (1.8*1.5 cm²), graphite felt (1.8*1.5 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S32). The substrate *N*-allylimine **1a** (221 mg, 1.0 mmol), benzaldehyde (51 μL , 0.5 mmol), **cat 2** (5 mg, 0.01 mmol) and $n\text{Bu}_4\text{NClO}_4$ (342 mg, 1.0 mmol) were added to the solvent DMF (10 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (18 mA, $J = 6.7 \text{ mA}\cdot\text{cm}^{-2}$) at 0 °C for 3 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 8/1-4/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **4a** (142 mg) in 87% yield. To prevent it from decomposing, the obtained product should be stored at 0 °C.

The reaction forming **4r** was conducted following the procedure of **3as**.

Gram-scale reaction procedure

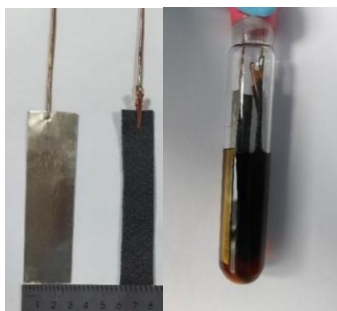
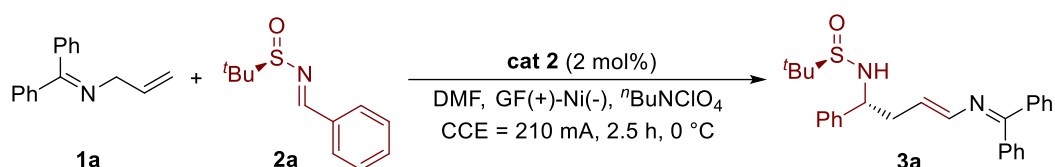
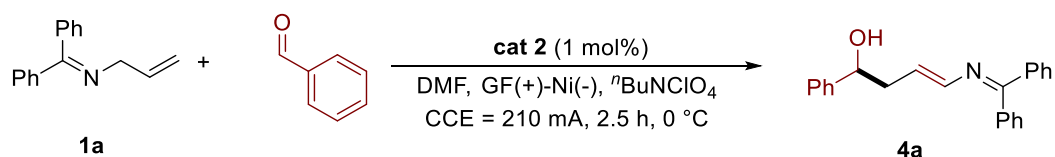


Fig. S33. Electrolysis setup of gram-scale reaction (graphite felt: width 2.0 cm, immersion depth 1.5 cm; nickel plate: width 3.0 cm, immersion depth 7.0 cm)



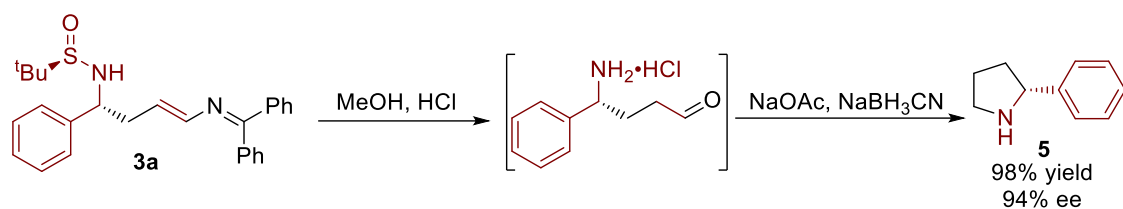
An undivided cell was equipped with a magnetic stirrer, nickel plate (3.0*7.0 cm²), graphite felt (2.0*7.0 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S33). The substrate *N*-allylimine **1a** (3.32 g, 15 mmol), Ellman imine **2a** (1.05 g, 5 mmol), **cat 2** (50.0 mg, 0.1 mmol) and *n*Bu₄NClO₄ (1.37 g, 4.0 mmol) were added to the solvent DMF (40 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (210 mA, *J* = 10.0 mA•cm⁻²) at 0 °C for 2.5 hours. The reaction mixture was subsequently poured into water (300 mL) and extracted with ethyl acetate (80 mL*3). The combined organic phases were washed with saturated brine solution (200 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3a** (1.46 g) in 68% yield.



An undivided cell was equipped with a magnetic stirrer, nickel plate (3.0*7.0 cm²), graphite felt (2.0*7.0 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S33). The substrate *N*-allylimine **1a** (2.21 g, 10 mmol), benzaldehyde (510 μL, 5 mmol), **cat 2** (25.0 mg, 0.05 mmol) and *n*Bu₄NClO₄ (1.37 g, 4.0 mmol) were added to the solvent DMF (40 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (210 mA, *J* = 10.0 mA•cm⁻²) at 0 °C for 2.5 hours. The reaction mixture was subsequently poured into water (300 mL) and extracted with ethyl acetate (80 mL*3). The combined organic phases were washed with saturated brine solution (200 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **4a** (1.30 g) in 79% yield.

8. Procedure for the derivatization of products

Synthesis of chiral pyrroline



To a cooled solution of **3a** (215 mg, 0.5 mmol) in methanol (5 mL) at 0 °C, 37% HCl (167 μL , 2 mmol) was added dropwise. The mixture was stirred at 0 °C for 4 hours, after which the excess HCl was removed using a rotary evaporator to yield the amino aldehyde hydrochloride intermediate. The intermediate was dissolved in an additional 10 mL of methanol, and the resulting solution was cooled to -10 °C with stirring. NaOAc (82 mg, 1 mmol) was then added to neutralize the hydrochloride intermediate. After stirring for 30 minutes, NaBH_3CN (63 mg, 1 mmol) was added at the same temperature. The reaction was allowed to proceed for 4 hours before being quenched with saturated ammonium chloride solution. The volatile solvents were removed using a rotary evaporator, and the residue was extracted with ethyl ether (10 mL*3). The combined organic phases were washed with saturated brine (30 mL) and dried over anhydrous Na_2SO_4 . After concentrating the solution, the residue was purified by column chromatography on silica gel (DCM/methanol = 30/1 to 15/1, v/v) to afford the desired product **5** (72 mg) in 98% yield. The enantiomeric excess of the product **5** was determined by HPLC with a chiral stationary phase (HPLC: Daicel Chiralpak AD-H, *n*-hexane/*i*-propanol = 90/10, flow rate = 1.0 mL/min, T = 23 °C, UV = 250 nm, t_R = 5.9 min (major), t_R = 6.7 min (minor)). The absolute configuration of **5** was determined by comparison with the HPLC spectra of the commercially available *R*-2-phenylpyrrolidine (Fig. S34-36).

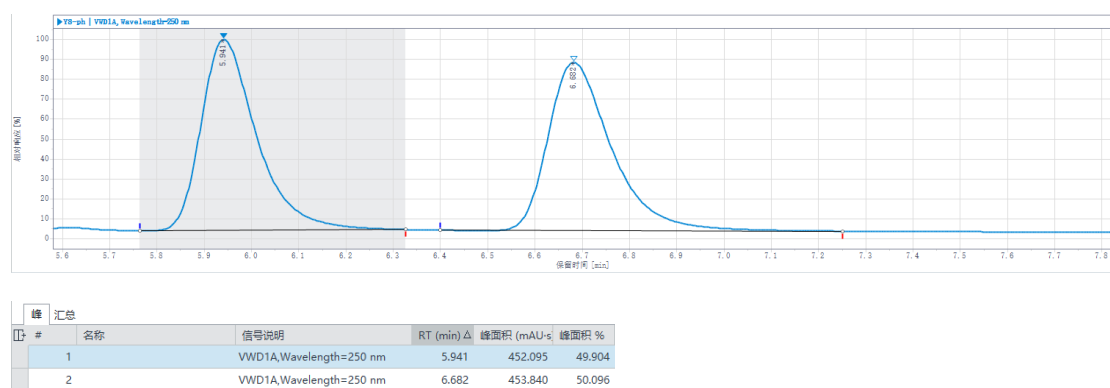


Fig. S34. HPLC spectra of racemic sample of 2-phenylpyrrolidine.

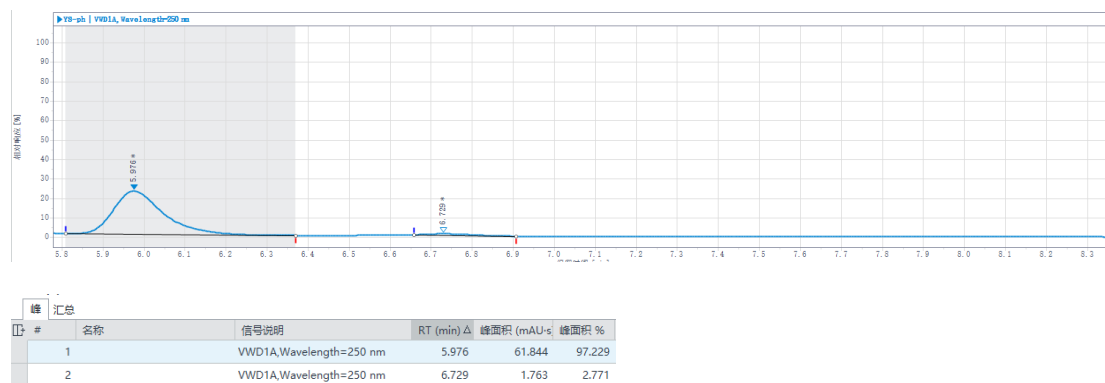


Fig. S35. HPLC spectra of the product 5.

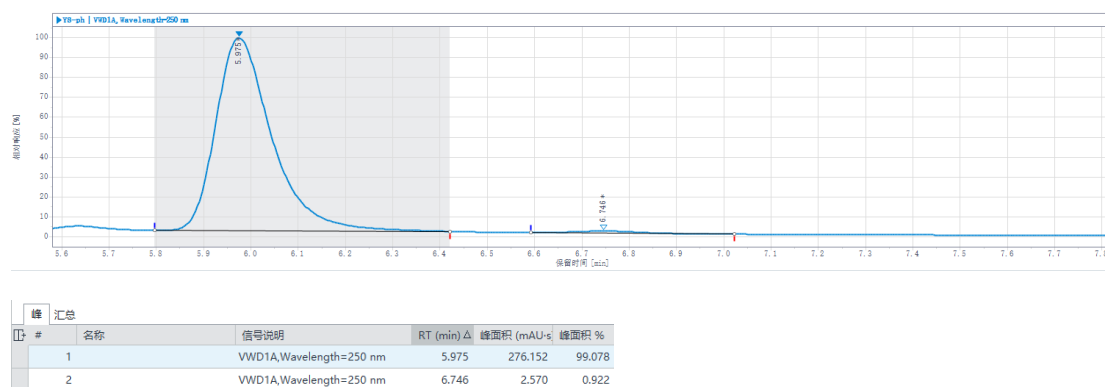


Fig. S36. HPLC spectra of standard sample of *R*-2-phenylpyrrolidine.

The chiral pyrroline **6** was prepared according to the above procedure, and its HPLC spectra are listed below (Fig. S37-38). HPLC condition: Daicel Chiralpak AD-H, *n*-hexane/*i*-propanol = 90/10, flow rate = 1.0 mL/min, T = 23°C, UV = 250 nm, t_R = 4.9 min (minor), t_R = 5.3 min (major).

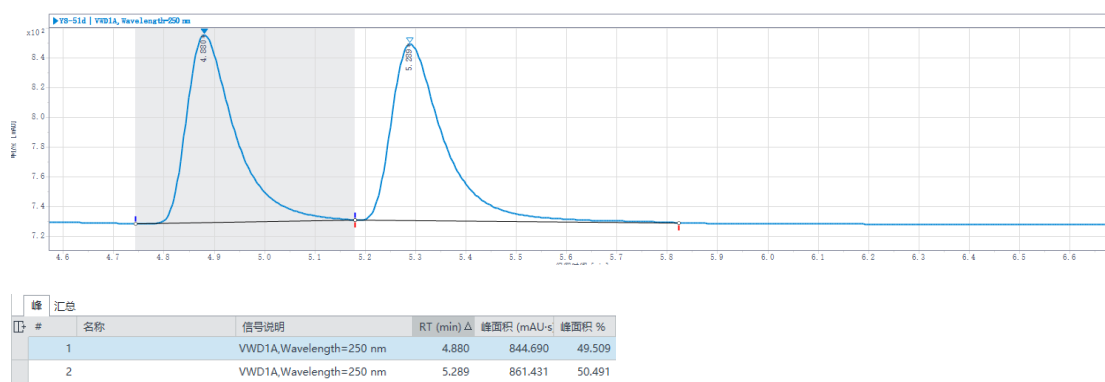
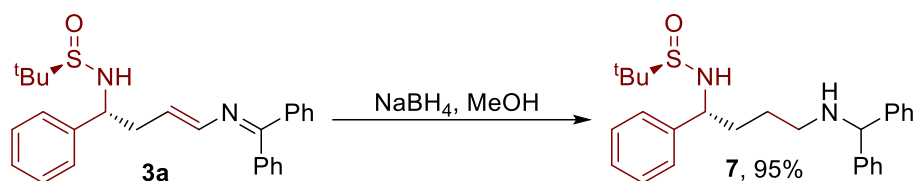


Fig. S37. HPLC spectra of racemic sample of 2-(2,5-difluorophenyl)pyrrolidine



Fig. S38. HPLC spectra of the product **6**.

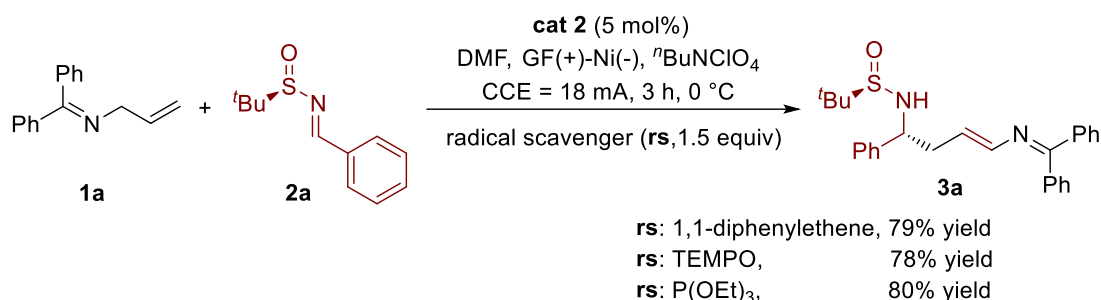
Reduction of the product **3a**



To the cooled solution of **3a** (215 mg, 0.5 mmol) in methanol (5 mL) at 0 °C, excessive NaBH_4 (190 mg, 5 mmol) was added in portions. The resulting reaction mixture was allowed to be warmed to room temperature and stirred for 5 hours before being quenched with saturated ammonium chloride solution. The reaction mixture was extracted with ethyl acetate (20 mL×3). The combined organic phases were washed with saturated brine solution (50 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 3/1-1/1, v/v) on silica gel to afford the desired product **7** (206 mg) in 95 % yield.

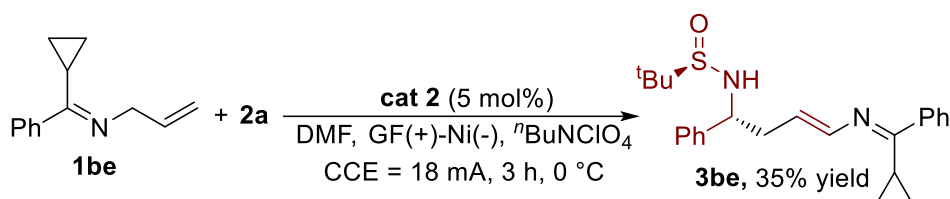
9. Procedure and details for control experiments

Radical suppression experiment



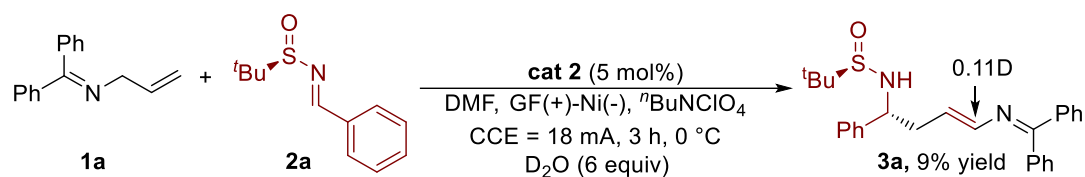
An undivided cell was equipped with a magnetic stirrer, nickel plate (1.8*1.5 cm²), graphite felt (1.8*1.5 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S32). The substrate *N*-allylimine **1a** (332 mg, 1.5 mmol), Ellman imine **2a** (105 mg, 0.5 mmol), **cat 2** (12 mg, 0.025 mmol), ⁿBu₄NClO₄ (342 mg, 1.0 mmol) and radical scavenger (0.75 mmol) were added to the solvent DMF (10 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (18 mA, $J = 6.7 \cdot \text{mA} \cdot \text{cm}^{-2}$) at 0 °C for 3 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3a**.

Radical clock experiment



An undivided cell was equipped with a magnetic stirrer, nickel plate (1.8*1.5 cm²), graphite felt (1.8*1.5 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S32). The substrate *N*-allylimine **1be** (278 mg, 1.5 mmol), Ellman imine **2a** (105 mg, 0.5 mmol), **cat 2** (12 mg, 0.025 mmol) and ⁿBu₄NClO₄ (342 mg, 1.0 mmol) were added to the solvent DMF (10 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (18 mA, $J = 6.7 \text{ mA} \cdot \text{cm}^{-2}$) at 0 °C for 3 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3be** (69 mg) in 35% yield.

Deuterium incorporating experiment



An undivided cell was equipped with a magnetic stirrer, nickel plate (1.8*1.5 cm²), graphite felt (1.8*1.5 cm²), as cathode and anode, respectively (the electrolysis setup is shown in Fig. S32). The substrate *N*-allylimine **1a** (332 mg, 1.5 mmol), Ellman imine **2a** (105 mg, 0.5 mmol), **cat 2** (12 mg, 0.025 mmol), *n*Bu₄NClO₄ (342 mg, 1.0 mmol) and D₂O (60 μL, 3 mmol) were added to the solvent DMF (10 mL). The resulting mixture was allowed to stir and electrolyze under constant current condition (18 mA, *J* = 6.7 mA•cm⁻²) at 0 °C for 3 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3a** (19 mg) in 9% yield. The deuteration was determined by ¹H NMR (Fig. S39).

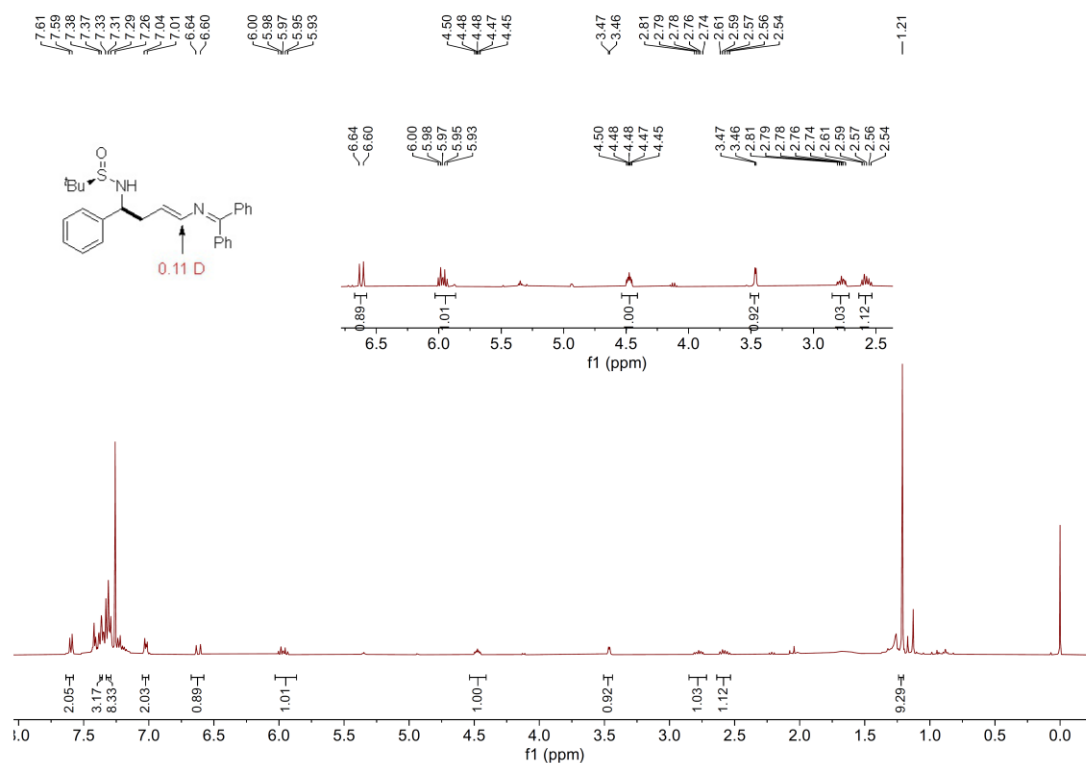
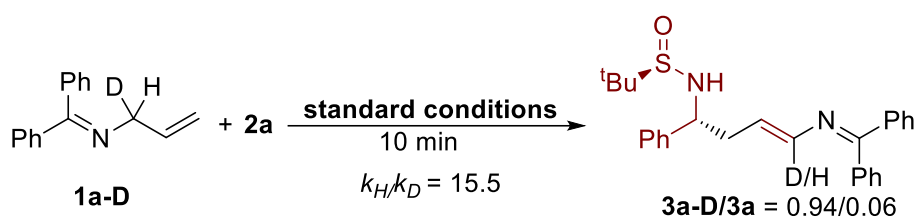


Fig. S39. ¹H NMR spectra of the product **3a**.

Kinetic isotope effect study using **1a-D** as substrate



We conducted KIE study by using **1a-D** as substrate. Under standard conditions, the crude product **3a-d** (<10 mg) was isolated after electrolyzing 10 min. The deuteration was detected by the crude ^1H NMR spectra (Fig. S40).

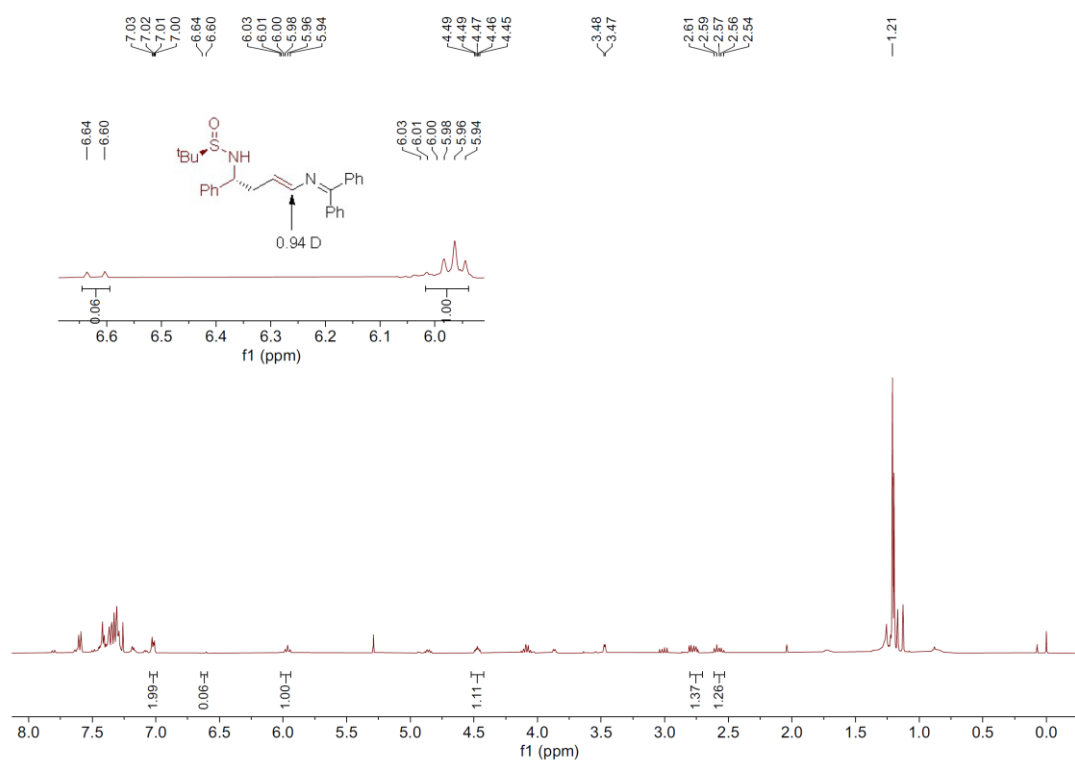
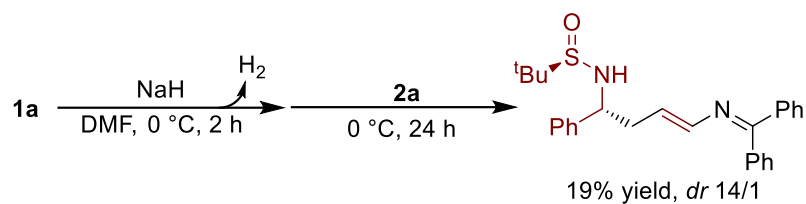


Fig. S40. ^1H NMR spectra of product **3a-D/3a**

Replacing electrolysis with NaH



To the cooled solution (0 °C) of **1a** (332 mg, 1.5 mmol) in DMF (5 mL), sodium hydride (1.5 mmol) was added under nitrogen atmosphere. After stirring for 2 hours, substrate **2a** (105 mg, 0.5 mmol) was added, and the resulting mixture was allowed to be stirred at same temperature for additional 24 hours. The reaction mixture was subsequently poured into water (200 mL) and extracted with ethyl acetate (40 mL*3). The combined organic phases were washed with saturated brine solution (100 mL). The volatile solvent was then removed with a rotary evaporator, and the residue was purified by column chromatography (PE/EA = 5/1-2/1, v/v basified with 1% triethylamine) on silica gel to afford the desired product **3a** (41 mg) in 19% yield. The ¹H NMR of the product was shown below (Fig. S41).

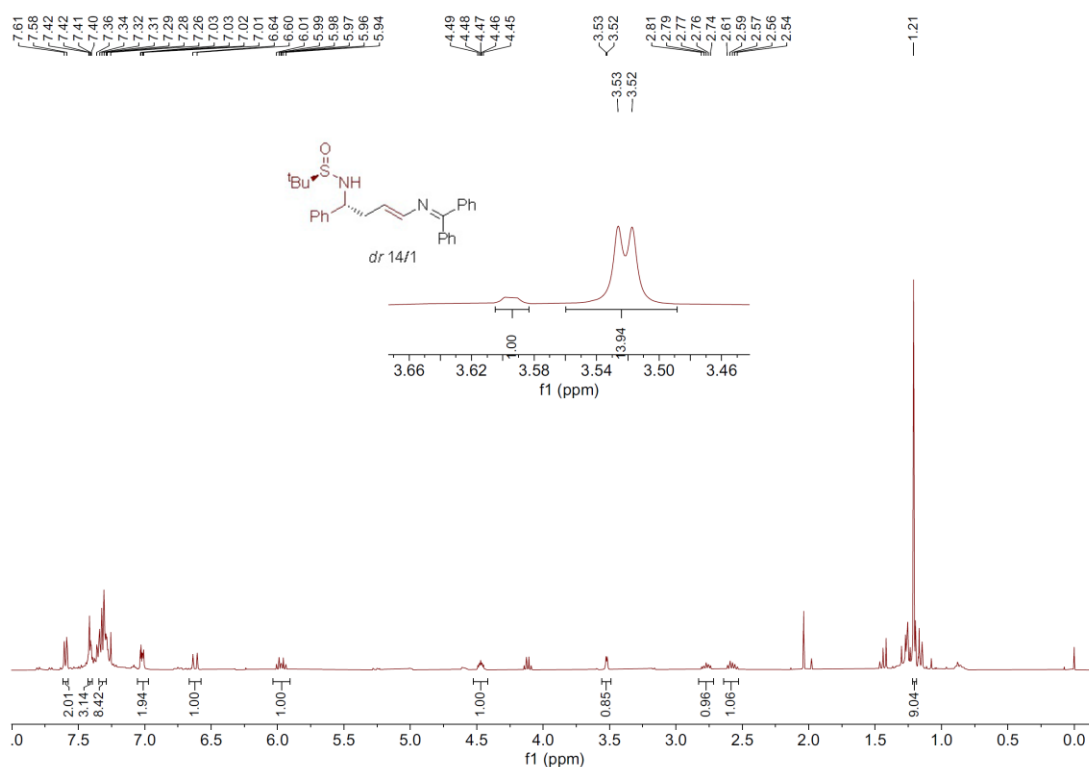


Fig. S41. ¹H NMR spectra of product **3a**

10. Density functional theory (DFT) calculations

All the calculations were performed with Gaussian 16 program (Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Petersson, G. A.; Nakatsuji, H.; Li, X.; Caricato, M.; Marenich, A. V.; Bloino, J.; Janesko, B. G.; Gomperts, R.; Mennucci, B.; Hratchian, H. P.; Ortiz, J. V.; Izmaylov, A. F.; Sonnenberg, J. L.; Williams; Ding, F.; Lipparini, F.; Egidi, F.; Goings, J.; Peng, B.; Petrone, A.; Henderson, T.; Ranasinghe, D.; Zakrzewski, V. G.; Gao, J.; Rega, N.; Zheng, G.; Liang, W.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Throssell, K.; Montgomery Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M. J.; Heyd, J. J.; Brothers, E. N.; Kudin, K. N.; Staroverov, V. N.; Keith, T. A.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A. P.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Millam, J. M.; Klene, M.; Adamo, C.; Cammi, R.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Farkas, O.; Foresman, J. B.; Fox, D. J. Gaussian 16 Rev. C.01, Wallingford, CT, 2016), and the structures were illustrated by CYLview (CYLview20; Legault, C. Y., Université de Sherbrooke, 2020).

The optimization of catalyst intermediate and transition state geometries with Gaussian 16 program was conducted using the B3LYP-D3(BJ) functional with a basis-set of 6-31G(d,p)^{7,8} for H, C, N, O and SDD for Na, K, Rb, Cs and Co. In order to improve the accuracy of calculation, single-point energy calculations were performed using the B3LYP-D3(BJ) functional with a basis-set of 6-311+g(d) for H, C, N, O and SDD for Na, K, Rb, Cs and Co within the SMD implicit solvation model⁹, with *N,N*-dimethylformamide as the solvent.

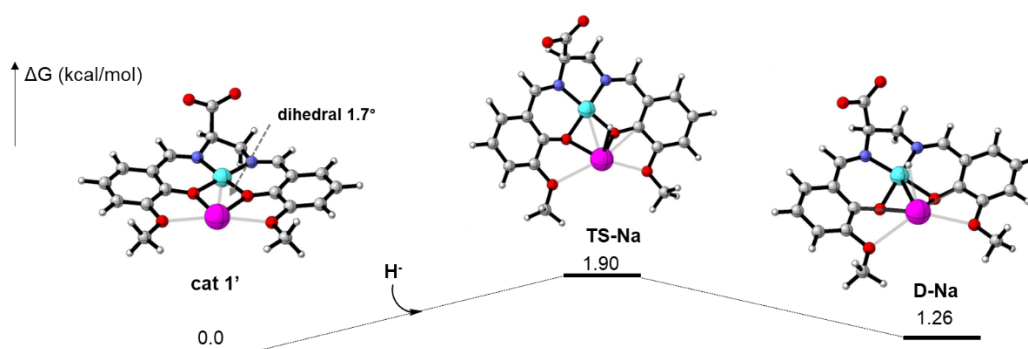


Fig. S42. Gibbs free energy profile (in kcal/mol) for the step forming **D-Na** from **cat 1'** at the B3LYP-D3(BJ)/6-31G(d,p) (SMD, solvent = DMF)//B3LYP-D3(BJ)/6-311+g(d) level.

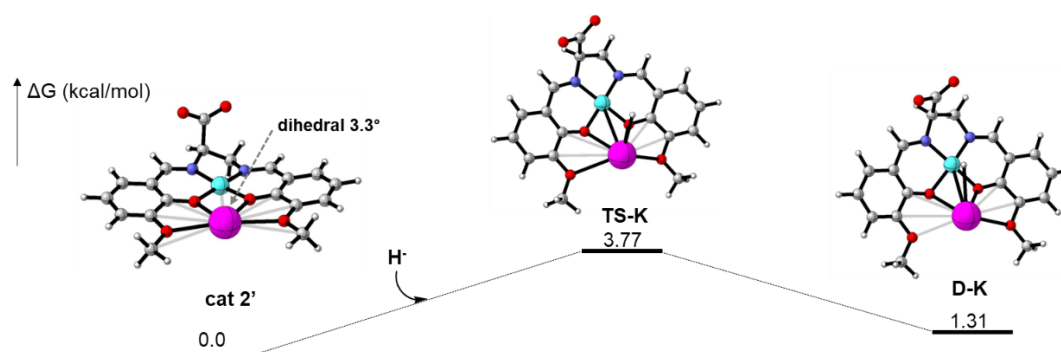


Fig. S43. Gibbs free energy profile (in kcal/mol) for the step forming **D-K** from **cat 2'** at the B3LYP-D3(BJ)/6-31G(d,p) (SMD, solvent = DMF)//B3LYP-D3(BJ)/6-311+g(d) level.

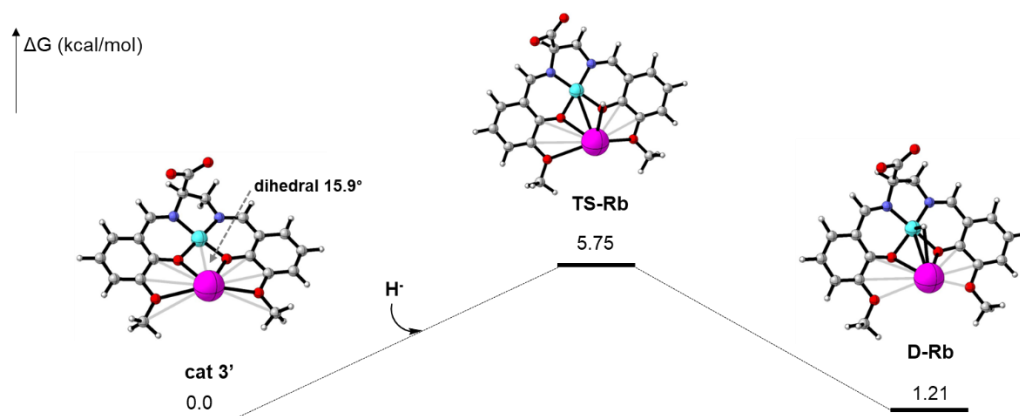


Fig. S44. Gibbs free energy profile (in kcal/mol) for the step forming **D-Rb** from **cat 3'** at the B3LYP-D3(BJ)/6-31G(d,p) (SMD, solvent = DMF)//B3LYP-D3(BJ)/6-311+g(d) level.

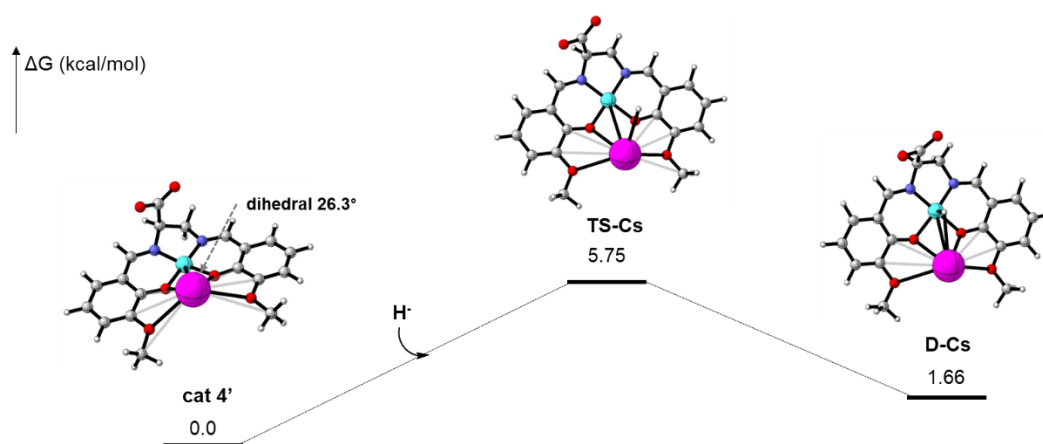


Fig. S45. Gibbs free energy profile (in kcal/mol) for the step forming **D-Cs** from **cat 4'** at the B3LYP-D3(BJ)/6-31G(d,p) (SMD, solvent = DMF)//B3LYP-D3(BJ)/6-311+g(d) level.

H⁻

Cartesian coordinates

ATOM X Y Z

H 0.00000000 0.00000000 0.00000000

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -0.471817 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -0.459457 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -0.461817 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -0.667141 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -0.654781 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -0.657141 a.u.

cat 1'

Cartesian coordinates

ATOM X Y Z

C -4.82947100 1.42201600 0.34276900

C -3.46531200 1.55556700 0.15183900

C -2.65114900 0.42343000 -0.13883200

C -3.26350800 -0.85414400 -0.21629400

C -4.66120000 -0.96735600 -0.01718500

C -5.43107600 0.14687500 0.25386700

H -5.44905900 2.28217500 0.56707600

H -5.12064900 -1.94980000 -0.07550200

H -6.50042800 0.05320900 0.40789800

C -2.48822100 -2.03763200 -0.49983000

H -3.03796300 -2.97944900 -0.56510000

N -1.20599900 -2.06886700 -0.68377000

C 4.46361000 2.13714900 0.12215100

C 3.08506500 2.05059100 0.00857200

C 2.44323100 0.79683100 -0.17341800

C 3.23077600 -0.37848300 -0.21906000

C 4.63545100 -0.26987300 -0.09484900

C 5.24261000 0.96258300 0.06656400

H 4.95572300 3.09224800 0.26221000

H 5.23243400 -1.17663800 -0.11518100

H 6.32040800 1.03588500 0.16346800

C 2.62772800 -1.68438900 -0.35264400

H 3.29359900 -2.54241500 -0.28283500

N 1.35971200 -1.91261900 -0.53352100

C -0.52622000 -3.32915400 -1.02856300

H -1.06439300 -4.18705700 -0.61908100

H -0.47886000 -3.38732600 -2.12377200

C 0.86486600 -3.27504700 -0.41874100

H 1.53808000 -3.97710500 -0.92492200

O	-1.36939000	0.62966900	-0.30591600
O	1.13126500	0.79953200	-0.26904000
O	-2.76160100	2.75164300	0.23353900
O	2.21058900	3.13447000	0.07398200
C	-3.51830500	3.92627700	0.51820200
H	-2.80703200	4.75410000	0.53527800
H	-4.26772400	4.10866200	-0.26039900
H	-4.01109500	3.85019300	1.49423800
C	2.79607800	4.42204100	0.24822600
H	1.97078400	5.13668500	0.26736600
H	3.34844100	4.47954900	1.19325000
H	3.46583700	4.66523200	-0.58460500
Co	-0.01325100	-0.64569800	-0.48677400
Na	-0.23044800	2.49490800	0.03769800
C	0.87283300	-3.71646500	1.14269200
O	-0.14286600	-4.35098500	1.49278700
O	1.91474000	-3.38717700	1.74178100

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1603.283975 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1603.200064 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1603.568162 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1603.625695 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1603.541785 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1603.909883 a.u.

Lowest frequency: 26.73 cm⁻¹

TS-Na

Cartesian coordinates

ATOM	X	Y	Z
C	4.95178400	-1.07719500	0.38931900
C	3.63768100	-1.33023200	0.03639600
C	2.72751500	-0.26881200	-0.28047700
C	3.21161400	1.06504100	-0.14615800
C	4.56345500	1.29940800	0.20265600
C	5.42673300	0.25229600	0.45938200
H	5.62547300	-1.89098100	0.63310800
H	4.90853700	2.32724000	0.28434200
H	6.45903700	0.43861900	0.73789600
C	2.34585300	2.19671200	-0.37415100
H	2.81865900	3.18354600	-0.39008900
N	1.06931400	2.12973300	-0.55895200
C	-4.23503500	-2.54114800	0.17751000
C	-2.88187300	-2.36500700	-0.06423300
C	-2.32862600	-1.06983200	-0.31157900

C	-3.20265800	0.04854800	-0.22699700
C	-4.58165200	-0.15505400	0.01341100
C	-5.09790100	-1.42416100	0.20319700
H	-4.64116200	-3.52872000	0.36584800
H	-5.22865300	0.71579600	0.07500100
H	-6.15569300	-1.56860900	0.39938800
C	-2.72181300	1.40664000	-0.35536700
H	-3.46797800	2.19846800	-0.31632500
N	-1.47752700	1.75367700	-0.46520000
C	0.31033100	3.33674300	-0.91638900
H	0.72245400	4.22659500	-0.43120500
H	0.37204800	3.44341000	-2.00879800
C	-1.14289500	3.17735600	-0.47573800
H	-1.79292100	3.69674400	-1.19210600
O	1.52464400	-0.58678000	-0.65589300
O	-1.05549000	-0.99519600	-0.58463100
O	3.06642900	-2.58757400	-0.01425500
O	-1.94288100	-3.38336500	-0.05955200
C	3.86993000	-3.68154600	0.38696200
H	3.23844000	-4.56904100	0.30689100
H	4.74243900	-3.80078600	-0.26988400
H	4.21055000	-3.56700000	1.42472400
C	-2.40229000	-4.68561900	0.24684900
H	-1.52345700	-5.33384900	0.22067300
H	-2.85635400	-4.72644100	1.24629900
H	-3.13213600	-5.03881900	-0.49462800
Co	0.00858800	0.57333400	-0.48972700
Na	0.44685100	-2.12182100	0.68209900
C	-1.47407400	3.91704400	0.91838100
O	-0.63958200	4.79097300	1.24507800
O	-2.56510400	3.58315800	1.42524100
H	0.45038200	-0.70683000	2.15172000

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1603.880068 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1603.794265 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1604.16404 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1604.289802 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1604.203999 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1604.573774 a.u.

Lowest frequency: -311.44 cm⁻¹

D-Na

Cartesian coordinates

ATOM	X	Y	Z
C	-4.92405000	1.18426600	0.47258600
C	-3.61128500	1.41083200	0.09074300
C	-2.74676100	0.34740300	-0.32812200
C	-3.25616800	-0.98086200	-0.21216300
C	-4.60180400	-1.18988100	0.16259600
C	-5.43456000	-0.13156300	0.48696400
H	-5.56396700	2.00383400	0.78118500
H	-4.97301000	-2.21081300	0.21537200
H	-6.46462400	-0.30526900	0.78189000
C	-2.41369700	-2.13227700	-0.47274800
H	-2.91476500	-3.10323400	-0.54378500
N	-1.12990000	-2.08934200	-0.59159900
C	4.31554200	2.43060800	0.23905600
C	2.96709200	2.29723700	-0.05705700
C	2.38170600	1.02910200	-0.36512900
C	3.21215600	-0.12175400	-0.24058800
C	4.58505800	0.03620100	0.05054700
C	5.13984500	1.28669800	0.27321000
H	4.74401600	3.40111800	0.46496300
H	5.20061800	-0.85613400	0.12924700
H	6.19491600	1.39155700	0.50647000
C	2.68965600	-1.46916900	-0.37881900
H	3.41660000	-2.28020800	-0.35209100
N	1.43554200	-1.77748200	-0.45990400
C	-0.38755400	-3.31201300	-0.93424300
H	-0.83406900	-4.19413100	-0.46561400
H	-0.42020000	-3.41078300	-2.02861700
C	1.05849600	-3.18883900	-0.45668700
H	1.70960200	-3.74174500	-1.14746600
O	-1.56006000	0.64966800	-0.76170500
O	1.12700200	0.99981800	-0.71334900
O	-2.98893200	2.65389600	0.11510000
O	2.05147100	3.34506000	-0.04245200
C	-3.78082900	3.76738900	0.48065300
H	-3.12933200	4.64202700	0.41624200
H	-4.62773100	3.89730100	-0.20657100
H	-4.16409600	3.67272200	1.50640600
C	2.55674500	4.63945800	0.21508400
H	1.70311400	5.31951900	0.16022300
H	3.01250200	4.70689100	1.21329400
H	3.30172400	4.93519100	-0.53635300

Co	-0.02652000	-0.55642400	-0.44873000
Na	-0.37313100	2.00362600	0.58681400
C	1.33423500	-3.90931800	0.95772100
O	0.45635900	-4.73661700	1.29578400
O	2.43377600	-3.61724700	1.47355400
H	-0.17016200	-0.13423000	1.28940800

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1603.890731 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1603.804139 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1604.178223 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1604.290827 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1604.204235 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1604.578319 a.u.

Lowest frequency: 21.81 cm⁻¹

cat 2'

Cartesian coordinates

ATOM	X	Y	Z
C	4.93331100	-1.29225100	0.24607700
C	3.56475500	-1.46747100	0.12278600
C	2.69049600	-0.36390100	-0.13567700
C	3.29102100	0.91894800	-0.26705300
C	4.69192200	1.07518000	-0.13423400
C	5.50528900	-0.00946100	0.11842400
H	5.58242700	-2.13595900	0.44689500
H	5.11622400	2.07010500	-0.23341100
H	6.57793900	0.11122200	0.22222900
C	2.50114700	2.08241400	-0.56336000
H	3.04144500	3.02535900	-0.67182600
N	1.21783600	2.10031800	-0.72426300
C	-4.68464700	-1.82888600	0.03785600
C	-3.30004600	-1.84423700	-0.04311200
C	-2.54601100	-0.63700800	-0.15427200
C	-3.27060600	0.58360900	-0.17926900
C	-4.68157300	0.57834400	-0.08524300
C	-5.38355900	-0.60636900	0.01834100
H	-5.24459300	-2.75214900	0.12493100
H	-5.20473800	1.52989400	-0.08950400
H	-6.46570600	-0.60675300	0.09089500
C	-2.60016500	1.85112300	-0.29437000
H	-3.21934600	2.74305200	-0.21662500
N	-1.32714900	2.01545900	-0.48854500
C	0.55670100	3.36120700	-1.09607100
H	1.14110200	4.22021300	-0.75961500

H	0.44837300	3.36887800	-2.18862500
C	-0.79246200	3.36567300	-0.40980100
H	-1.47368200	4.07766800	-0.89062600
O	1.40039200	-0.58313200	-0.22965400
O	-1.23116700	-0.71030500	-0.20963400
O	2.93467000	-2.69942500	0.24695700
O	-2.54398900	-3.01315200	-0.00950100
C	3.76611200	-3.83546300	0.45901700
H	3.10079700	-4.70094700	0.50232600
H	4.47390800	-3.96825200	-0.36744400
H	4.31598600	-3.75622500	1.40421800
C	-3.25586300	-4.24499300	0.00831500
H	-2.50351700	-5.03715700	-0.01735600
H	-3.85591500	-4.34776500	0.92041200
H	-3.90576000	-4.33940000	-0.86945700
Co	0.00750200	0.69337400	-0.44047500
C	-0.70153000	3.82281100	1.13957700
O	0.35592200	4.41880800	1.43186500
O	-1.72395500	3.54301200	1.79586600
K	0.17878700	-2.82817800	0.31790900

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1469.314123 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1469.228072 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1469.59585 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1469.657644 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1469.571593 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1469.939371 a.u.

Lowest frequency: 15.55 cm⁻¹

TS-K

Cartesian coordinates

ATOM	X	Y	Z
C	5.08358900	-0.81923900	0.12389700
C	3.75332100	-1.13328600	-0.09134200
C	2.75484000	-0.11438200	-0.27189500
C	3.19970800	1.23928800	-0.18479100
C	4.56731700	1.53440700	0.03193600
C	5.50154700	0.52970800	0.18125700
H	5.81898400	-1.60297100	0.26670900
H	4.86967300	2.57732900	0.08801200
H	6.54735500	0.76137000	0.35560800
C	2.28387500	2.33532500	-0.36344200
H	2.72360100	3.33688600	-0.39786300
N	1.00417100	2.23191900	-0.50937200

C	-4.31661000	-2.51339100	-0.07374600
C	-2.94480600	-2.33334600	-0.15462800
C	-2.36271900	-1.03068000	-0.29737000
C	-3.25319200	0.08067600	-0.30348200
C	-4.64947300	-0.12786100	-0.21824500
C	-5.18205200	-1.39922200	-0.11176500
H	-4.73890300	-3.50618300	0.03433500
H	-5.30049300	0.74222500	-0.21867100
H	-6.25458000	-1.54908400	-0.03873500
C	-2.77532400	1.43991300	-0.39938400
H	-3.53083900	2.22353500	-0.41463500
N	-1.53149900	1.80232600	-0.44487100
C	0.22488000	3.43061700	-0.85707600
H	0.60224000	4.31646000	-0.33689400
H	0.31764600	3.57107800	-1.94337000
C	-1.23537000	3.23359200	-0.46589900
H	-1.87380500	3.72004800	-1.21500500
O	1.53128100	-0.47839000	-0.49947900
O	-1.06772500	-0.94136900	-0.40298300
O	3.25787700	-2.42501400	-0.12749600
O	-2.02110200	-3.36630400	-0.08500700
C	4.18639200	-3.48138600	0.02288100
H	3.61125900	-4.40705700	-0.05637900
H	4.94760100	-3.46251000	-0.76904400
H	4.68511200	-3.44486400	1.00131600
C	-2.52740700	-4.68338600	0.00714800
H	-1.65814800	-5.34558600	0.02079100
H	-3.11043600	-4.83077100	0.92695800
H	-3.15606700	-4.93319700	-0.85843700
Co	-0.01895600	0.65159200	-0.38891800
C	-1.64857600	3.99156300	0.89671500
O	-0.86816500	4.91357600	1.22352400
O	-2.74089800	3.62105100	1.37455100
H	0.67385500	-0.41247300	2.60315200
K	0.54417100	-2.38151600	1.12858700

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1469.899317 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1469.812171 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1470.181432 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1470.318775 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1470.231629 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1470.60089 a.u.

Lowest frequency: -287.10 cm⁻¹

D-K

Cartesian coordinates

ATOM	X	Y	Z
C	5.06328200	-1.10226300	0.19940700
C	3.71350600	-1.34971700	0.00592800
C	2.77841100	-0.30181700	-0.30203200
C	3.29820200	1.03118100	-0.31720600
C	4.67929500	1.25705900	-0.12505400
C	5.55921900	0.21655100	0.11969100
H	5.74884200	-1.91095300	0.42856600
H	5.04435200	2.28097000	-0.16265100
H	6.61759200	0.40455000	0.26993000
C	2.43990200	2.17386400	-0.55245900
H	2.94156400	3.13936000	-0.67737600
N	1.15101500	2.13827200	-0.60771900
C	-4.51938000	-2.24182700	-0.00587600
C	-3.14582800	-2.16939900	-0.18325100
C	-2.46284000	-0.92072100	-0.36985000
C	-3.25696200	0.26418900	-0.28577600
C	-4.65452200	0.16537300	-0.11035600
C	-5.28854100	-1.06017700	0.01875500
H	-5.01217500	-3.19850400	0.13253800
H	-5.23080300	1.08568600	-0.05618000
H	-6.36317300	-1.11897100	0.16145600
C	-2.67990400	1.59032900	-0.38995200
H	-3.38193100	2.42374200	-0.39475000
N	-1.41662400	1.86510500	-0.43322100
C	0.41946500	3.37004400	-0.94252600
H	0.88580300	4.24655700	-0.48240500
H	0.43686900	3.46725000	-2.03755600
C	-1.01912300	3.27102700	-0.44364400
H	-1.67172600	3.82520700	-1.13208700
O	1.54517300	-0.61800700	-0.53698900
O	-1.18300700	-0.93650300	-0.58130000
O	3.13280300	-2.60925900	0.11928400
O	-2.30134800	-3.27768000	-0.15492400
C	4.00234700	-3.70901700	0.29699100
H	3.37310300	-4.60282400	0.29485300
H	4.73051500	-3.77971800	-0.52259000
H	4.54621300	-3.65053000	1.25113700
C	-2.90898000	-4.55240900	-0.18244600
H	-2.09654500	-5.28016900	-0.25534500
H	-3.49161900	-4.75146700	0.72900900
H	-3.56983000	-4.65961100	-1.05345900

Co	0.02479300	0.62736100	-0.33971900
C	-1.27320400	4.00781200	0.96491100
O	-0.37860300	4.82126800	1.29353200
O	-2.37817900	3.74435700	1.48528300
H	0.08597500	0.43467500	1.40753600
K	0.29663300	-2.20797600	1.11514500

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1469.917099 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1469.828972 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1470.203459 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1470.322697 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1470.23457 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1470.609057 a.u.

Lowest frequency: 22.93 cm⁻¹

cat 3'

Cartesian coordinates

ATOM	X	Y	Z
C	4.95098300	-1.06486200	-0.09767900
C	3.57696700	-1.23987600	-0.11911700
C	2.68405800	-0.13125600	-0.28273400
C	3.27492900	1.15664600	-0.41604900
C	4.68222900	1.31219400	-0.38312000
C	5.51265800	0.22220800	-0.23011300
H	5.61241300	-1.91393000	0.02663300
H	5.09757300	2.31102000	-0.48190000
H	6.59026200	0.34171600	-0.20721300
C	2.46649400	2.32865800	-0.60403000
H	2.99808100	3.27920400	-0.68826300
N	1.17599200	2.34933400	-0.69366800
C	-4.67731900	-1.69231500	-0.32355600
C	-3.29032200	-1.68217700	-0.30668600
C	-2.55343900	-0.45809900	-0.31567100
C	-3.29974200	0.75010300	-0.32888400
C	-4.71356800	0.71775500	-0.33100300
C	-5.39766500	-0.48187300	-0.33582500
H	-5.22237100	-2.62876200	-0.31858700
H	-5.25399200	1.65974500	-0.32552100
H	-6.48207100	-0.50337900	-0.34156500
C	-2.64402900	2.02975200	-0.32742500
H	-3.27822200	2.90767500	-0.21268200
N	-1.36743900	2.21993300	-0.45990300
C	0.49845100	3.63189700	-0.94775100
H	1.07727500	4.46262600	-0.53852100

H	0.38133200	3.73767300	-2.03432600
C	-0.84534500	3.56069100	-0.25506500
H	-1.53609100	4.31031500	-0.65935800
O	1.39149500	-0.35046800	-0.29014000
O	-1.23769700	-0.50757600	-0.28732800
O	2.96003700	-2.47373300	0.02619700
O	-2.51658500	-2.83575700	-0.25979600
C	3.79720000	-3.62406400	0.02213400
H	3.13106900	-4.48919500	0.05785900
H	4.39789800	-3.67160200	-0.89360100
H	4.46066700	-3.64264300	0.89554700
C	-3.18517100	-4.07475800	-0.45995800
H	-2.40777500	-4.84174200	-0.49364700
H	-3.87773200	-4.29793200	0.36131000
H	-3.73393700	-4.07762800	-1.40900300
Co	-0.01454500	0.91478200	-0.46410100
C	-0.74656200	3.85886300	1.33146000
O	0.30406900	4.43967200	1.67519700
O	-1.75617300	3.49331300	1.96572500
Rb	0.16412000	-2.55318000	0.90530200

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1465.091976 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1465.00464 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1465.372207 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1465.448706 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1465.36137 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1465.728937 a.u.

Lowest frequency: 17.67 cm⁻¹

TS-Rb

Cartesian coordinates

ATOM	X	Y	Z
C	5.09493400	-0.35259800	-0.12218900
C	3.77760800	-0.73883300	-0.29573000
C	2.71059100	0.22303500	-0.38106100
C	3.08131800	1.59669900	-0.25938900
C	4.43704700	1.96556900	-0.08348200
C	5.43480600	1.01517500	-0.01663600
H	5.88135300	-1.09551900	-0.05063800
H	4.67871400	3.02199600	0.00478100
H	6.47162600	1.30247000	0.12564500
C	2.10170300	2.64379900	-0.37011500
H	2.48449200	3.66902700	-0.36930800
N	0.82700800	2.47645900	-0.50140600

C	-4.25177100	-2.55133100	-0.32541000
C	-2.88830500	-2.30298700	-0.35166400
C	-2.36483900	-0.96764700	-0.40403800
C	-3.31144300	0.09708000	-0.39348500
C	-4.69788300	-0.18172900	-0.36264800
C	-5.17050700	-1.48024100	-0.33417600
H	-4.62699700	-3.56783200	-0.28536400
H	-5.39026900	0.65566200	-0.34567400
H	-6.23600800	-1.68496900	-0.30404500
C	-2.90265800	1.48079400	-0.42512000
H	-3.69777800	2.22428900	-0.42025100
N	-1.67932300	1.90896000	-0.44451100
C	-0.01686200	3.64812600	-0.78656300
H	0.31293100	4.52454000	-0.21998900
H	0.06705500	3.85171700	-1.86349000
C	-1.46365900	3.35371900	-0.40874900
H	-2.12757200	3.83176200	-1.14091900
O	1.50032500	-0.20420600	-0.56281100
O	-1.07296000	-0.80880200	-0.45073500
O	3.36328800	-2.05574500	-0.37871000
O	-1.92134300	-3.29542300	-0.31127000
C	4.36299900	-3.05524800	-0.35830700
H	3.84260500	-4.00942100	-0.47156600
H	5.07181300	-2.93132200	-1.18859600
H	4.91886300	-3.05413500	0.58986500
C	-2.36547900	-4.63704600	-0.33741300
H	-1.46550500	-5.25712400	-0.34172400
H	-2.97113100	-4.88321200	0.54625900
H	-2.95229700	-4.84840100	-1.24183500
Co	-0.10710200	0.83940200	-0.41934100
C	-1.92424100	4.03451400	0.97930900
O	-1.20788200	4.99656600	1.33543900
O	-2.98751200	3.57446800	1.44479500
Rb	0.66294300	-2.30671200	1.18579400
H	0.81567700	-0.16293500	2.65361000

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1465.675304 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1465.586586 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1465.955699 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1466.106677 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1466.017959 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1466.387072 a.u.

Lowest frequency: -269.42 cm⁻¹

D-Rb

Cartesian coordinates

ATOM	X	Y	Z
C	5.06745600	-0.90984500	-0.06432800
C	3.70940600	-1.15865000	-0.19179500
C	2.75345700	-0.10587600	-0.40772700
C	3.27030100	1.22846600	-0.42574500
C	4.65847400	1.45548200	-0.29548000
C	5.55393700	0.41296000	-0.12549000
H	5.76684900	-1.72298100	0.09766700
H	5.01764100	2.48185300	-0.32565800
H	6.61804700	0.60220900	-0.02405700
C	2.39984000	2.37154300	-0.60273500
H	2.89157500	3.34570700	-0.69686100
N	1.11005800	2.32347000	-0.64125800
C	-4.53955900	-2.11248600	-0.30403500
C	-3.15951100	-2.02739500	-0.41488800
C	-2.47409900	-0.76728900	-0.50176800
C	-3.28144800	0.40769200	-0.39996500
C	-4.68478900	0.29545000	-0.29223700
C	-5.31687700	-0.93701900	-0.25288100
H	-5.03281000	-3.07675900	-0.24094000
H	-5.26843700	1.21003000	-0.22198900
H	-6.39660700	-1.00715900	-0.16377300
C	-2.70897600	1.73841400	-0.42735200
H	-3.41564500	2.56795400	-0.41142900
N	-1.44715700	2.02122000	-0.43750200
C	0.36495900	3.56252800	-0.90479500
H	0.83400700	4.42133600	-0.41462800
H	0.35885300	3.71053800	-1.99436100
C	-1.06153100	3.42796700	-0.38306400
H	-1.73230400	4.01075800	-1.02933700
O	1.50711200	-0.42003600	-0.56733200
O	-1.18569700	-0.76308900	-0.64503100
O	3.14475400	-2.42607800	-0.09702800
O	-2.31381300	-3.13351700	-0.41209500
C	4.02833200	-3.52642300	-0.03856800
H	3.40360700	-4.42344600	-0.04600000
H	4.69993100	-3.54809000	-0.90774700
H	4.63635000	-3.51679700	0.87811200
C	-2.91568300	-4.40807000	-0.48743300
H	-2.09824800	-5.13115000	-0.55304900
H	-3.52402700	-4.62979300	0.40230300
H	-3.55096000	-4.50004000	-1.37933100

Co	-0.00023000	0.80289000	-0.36885000
C	-1.29591800	4.08570500	1.06624400
O	-0.40101300	4.88632200	1.42521000
O	-2.39107100	3.78703600	1.58887300
Rb	0.27100700	-2.08679400	1.23336700
H	0.04201900	0.68233200	1.29022000

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1465.697986 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1465.608757 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1465.979656 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1466.11392 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1466.024691 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1466.39559 a.u.

Lowest frequency: 20.63 cm⁻¹

cat 4'

Cartesian coordinates

ATOM	X	Y	Z
C	4.90247900	-1.04270500	-0.44832700
C	3.52360900	-1.17013300	-0.41986600
C	2.66708700	-0.02380000	-0.50143900
C	3.29579200	1.25072800	-0.58062600
C	4.70868100	1.35604200	-0.59646100
C	5.50374600	0.23105600	-0.53995800
H	5.53713500	-1.91937800	-0.39376700
H	5.15656400	2.34406500	-0.65425700
H	6.58506300	0.31266900	-0.55784400
C	2.51956700	2.45741100	-0.63936800
H	3.07791500	3.39637000	-0.65480700
N	1.22713100	2.52248200	-0.67544300
C	-4.68726200	-1.42943900	-0.70637500
C	-3.30164800	-1.44212800	-0.64714800
C	-2.55086700	-0.22917200	-0.55836000
C	-3.27968600	0.98803700	-0.49405600
C	-4.69337400	0.97664000	-0.53747500
C	-5.39104900	-0.20943100	-0.65421800
H	-5.24386500	-2.35614600	-0.78312900
H	-5.22311400	1.92273200	-0.47392700
H	-6.47498100	-0.21417500	-0.69520400
C	-2.60163200	2.24747500	-0.34771200
H	-3.22145500	3.11998500	-0.14171100
N	-1.32016300	2.42361200	-0.43954800
C	0.57530400	3.84161700	-0.75463100
H	1.17859900	4.60159600	-0.25375000

H	0.44036400	4.08848200	-1.81587900
C	-0.75782600	3.70462700	-0.04792300
H	-1.43417300	4.52629700	-0.31352100
O	1.37053300	-0.20392600	-0.48190000
O	-1.23911000	-0.30317900	-0.50889000
O	2.86310300	-2.37971700	-0.29633100
O	-2.54007700	-2.59976900	-0.64249300
C	3.64243900	-3.56278500	-0.41390100
H	2.93743900	-4.39658100	-0.39099500
H	4.19055500	-3.58144200	-1.36332000
H	4.35202700	-3.66434500	0.41729500
C	-3.20161000	-3.81586400	-0.96258600
H	-2.42400900	-4.58070000	-1.01900800
H	-3.93163800	-4.09611900	-0.19197400
H	-3.70884600	-3.74529300	-1.93217800
Co	0.00546600	1.10031600	-0.57154900
C	-0.60696500	3.74305800	1.56212200
O	0.43885000	4.29876100	1.95855600
O	-1.57326400	3.23721300	2.16836800
Cs	0.04634600	-2.24930300	1.21102000

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1461.143789 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1461.054743 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1461.422152 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1461.4976 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1461.408554 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1461.775963 a.u.

Lowest frequency: 13.41 cm⁻¹

TS-Cs

Cartesian coordinates

ATOM	X	Y	Z
C	5.04139900	0.31332200	-0.39298800
C	3.76130000	-0.19380100	-0.52842300
C	2.60146100	0.65768700	-0.50398100
C	2.84383900	2.05437300	-0.33363800
C	4.16395800	2.54764900	-0.19584900
C	5.25158900	1.70017500	-0.22316500
H	5.89891500	-0.35002700	-0.40220900
H	4.30500600	3.61741100	-0.06219000
H	6.26108900	2.08199200	-0.10966000
C	1.76782500	3.00588400	-0.36063900
H	2.05281600	4.06112200	-0.30875500
N	0.51096400	2.72736100	-0.47824300

C	-4.08078700	-2.75165700	-0.59279300
C	-2.74500600	-2.38188400	-0.56099300
C	-2.34308600	-1.00398200	-0.51714900
C	-3.38427300	-0.03168300	-0.48862300
C	-4.74014200	-0.43455000	-0.51515800
C	-5.09339300	-1.76930800	-0.57019200
H	-4.36179300	-3.79839300	-0.62529800
H	-5.50573500	0.33578300	-0.47824300
H	-6.13616400	-2.07016200	-0.58541000
C	-3.10529900	1.38304300	-0.44620800
H	-3.96679000	2.04780000	-0.41627900
N	-1.92748500	1.92398400	-0.43487400
C	-0.44159600	3.83182500	-0.67868800
H	-0.19126700	4.69358300	-0.05205100
H	-0.38530600	4.11932900	-1.73804900
C	-1.85172300	3.37772900	-0.32131100
H	-2.56172800	3.82822400	-1.02722700
O	1.42952000	0.12089200	-0.64475700
O	-1.06989300	-0.72569600	-0.50221000
O	3.47690100	-1.53837700	-0.67526900
O	-1.69558900	-3.28479900	-0.55196300
C	4.56961400	-2.42871300	-0.77767000
H	4.13997100	-3.42175500	-0.93080400
H	5.21285200	-2.17903300	-1.63279000
H	5.17822700	-2.43275700	0.13778000
C	-2.01301800	-4.65562700	-0.68126800
H	-1.05936000	-5.18923100	-0.69746200
H	-2.61605600	-5.01669100	0.16413500
H	-2.55418000	-4.85674900	-1.61606500
Co	-0.26202600	1.00795900	-0.45331400
C	-2.37475900	3.93275000	1.10067100
O	-1.77387000	4.95639300	1.49539800
O	-3.36970500	3.32759100	1.55104700
H	1.11915200	0.13348400	2.70707500
Cs	0.89480700	-2.20264800	1.20827700

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1461.721317 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1461.631245 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1462.000182 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1462.155448 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1462.065376 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1462.434313 a.u.

Lowest frequency: -243.84 cm⁻¹

D-Cs

Cartesian coordinates

ATOM	X	Y	Z
C	5.06799200	-0.70221800	-0.24653000
C	3.71126700	-0.95958100	-0.37279700
C	2.73873400	0.09107900	-0.51512900
C	3.24308100	1.43068200	-0.48468100
C	4.63019100	1.66564100	-0.35558700
C	5.53904400	0.62705600	-0.24254000
H	5.77738600	-1.51535300	-0.13574600
H	4.97795700	2.69627100	-0.34121800
H	6.60175000	0.82357700	-0.13986300
C	2.36417800	2.57435300	-0.60967300
H	2.84814200	3.55624200	-0.64703100
N	1.07492500	2.51555800	-0.66201400
C	-4.54606400	-1.97815500	-0.50990500
C	-3.16733500	-1.88097400	-0.62764900
C	-2.48444500	-0.61555500	-0.63859600
C	-3.29788100	0.54838000	-0.46993400
C	-4.69996100	0.42359700	-0.35933300
C	-5.32737000	-0.81155100	-0.38300600
H	-5.03468500	-2.94681500	-0.50121900
H	-5.28692300	1.33046600	-0.23602400
H	-6.40606900	-0.89117900	-0.28926900
C	-2.73611000	1.88378500	-0.43776700
H	-3.44974300	2.70531100	-0.37878300
N	-1.47716500	2.17863100	-0.44428400
C	0.31653300	3.75823300	-0.85663900
H	0.78264900	4.59753900	-0.33093200
H	0.29640100	3.95846800	-1.93766600
C	-1.10357400	3.58486100	-0.32679600
H	-1.78681600	4.19080000	-0.93778100
O	1.49154700	-0.23029600	-0.65887300
O	-1.19607200	-0.59738300	-0.77880000
O	3.16474000	-2.23728000	-0.34736900
O	-2.32035000	-2.98207200	-0.70647500
C	4.05997400	-3.32853400	-0.34730200
H	3.44417900	-4.23048800	-0.39758600
H	4.72881300	-3.30059000	-1.21855700
H	4.67163900	-3.35892200	0.56683400
C	-2.91777700	-4.25366200	-0.83212100
H	-2.09772700	-4.96815200	-0.94381800
H	-3.51127000	-4.52022400	0.05571800
H	-3.56654700	-4.30841900	-1.71739500

Co	-0.02140200	0.97496700	-0.43094000
C	-1.32961300	4.16900500	1.15490600
O	-0.43909400	4.95997000	1.54477300
O	-2.41692300	3.83474400	1.67300200
H	0.01130200	0.84813600	1.20782800
Cs	0.25013000	-2.05800400	1.21197100

B3LYP+GD3(BJ)/Gen Gibbs Free Energy: -1461.748435 a.u.

B3LYP+GD3(BJ)/Gen Enthalpy: -1461.658265 a.u.

B3LYP+GD3(BJ)/Gen Electronic Energy: -1462.02914 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Gibbs Free Energy: -1462.162101 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Enthalpy: -1462.071931 a.u.

B3LYP+GD3(BJ)/Gen solvent = (DMF) Electronic Energy: -1462.442806 a.u.

Lowest frequency: 18.45 cm⁻¹

The optimization of reaction intermediate and transition state geometries with Gaussian 16 program was conducted using the B3LYP+GD3(BJ) functional with a basis-set of 6-311G** for H, C, N, O, S. The SMD implicit solvation model⁹, with *N,N*-dimethylformamide as the solvent.

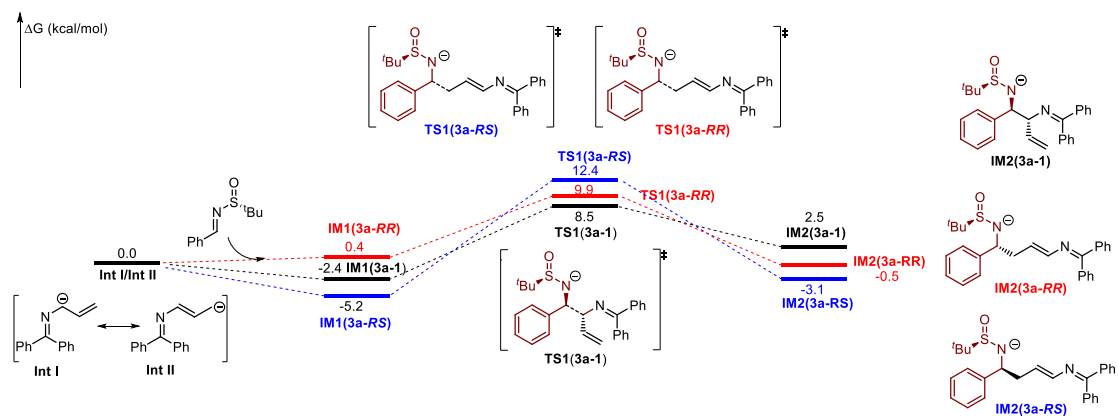


Fig. S46. Gibbs free energy profile (in kcal/mol) for the reaction between carbanions **Int I/Int II** and Ellman imine at the B3LYP+GD3(BJ)/6-311G** (SMD, solvent = DMF) level.

Int I

Cartesian coordinates

ATOM	X	Y	Z
N	-0.14009900	1.87317200	-0.00012200
C	0.24135400	0.59880800	-0.00004100
C	1.66253800	0.30534000	0.00006800
C	2.64242200	1.33544300	0.00027500
C	2.15561300	-1.02617300	-0.00013200
C	3.99875600	1.05130000	0.00021600
H	2.30064700	2.36292300	0.00049400
C	3.51922400	-1.30070900	-0.00019700
H	1.45411300	-1.85182800	-0.00026400
C	4.46217500	-0.27101700	-0.00004100
H	4.71114900	1.87116600	0.00039000
H	3.84940400	-2.33523800	-0.00037400
H	5.52417600	-0.48816100	-0.00011500
C	-0.71593300	-0.55300400	0.00004600
C	-1.18610400	-1.09819200	1.20193000
C	-1.18579100	-1.09858600	-1.20177700
C	-2.11348600	-2.13853600	1.20534900
H	-0.82658500	-0.69195300	2.14159800
C	-2.11313200	-2.13898500	-1.20510400
H	-0.82606100	-0.69263400	-2.14148900
C	-2.58469000	-2.65893100	0.00014600
H	-2.46939700	-2.54316500	2.14689700
H	-2.46873200	-2.54394800	-2.14662300
H	-3.30785500	-3.46699900	0.00019600
C	-1.34564500	2.43567800	-0.00017000
H	-1.32441400	3.52887900	-0.00012800
C	-2.66246200	1.86081400	-0.00025800
H	-2.74367800	0.77965500	-0.00042400
C	-3.82151500	2.56839400	-0.00016700
H	-4.78606500	2.07302000	-0.00031500
H	-3.82594800	3.65622300	0.00015200

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -672.980331 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -672.921134 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -673.185312 a.u.

Lowest frequency: 20.92 cm⁻¹

Int II

Cartesian coordinates

ATOM	X	Y	Z
C	2.66247200	1.86084500	-0.00010100
H	2.74358400	0.77967900	-0.00034800
C	1.34565900	2.43574800	0.00007300
H	1.32441500	3.52894000	0.00024000
N	0.14013400	1.87323000	0.00001800
C	-0.24130500	0.59887200	-0.00010400
C	-1.66251000	0.30537800	-0.00007800
C	-2.64241100	1.33546900	0.00013400
C	-2.15557400	-1.02613800	-0.00026600
C	-3.99874500	1.05130800	0.00017300
H	-2.30064000	2.36295100	0.00027300
C	-3.51918400	-1.30069600	-0.00022900
H	-1.45407200	-1.85178800	-0.00045000
C	-4.46214200	-0.27101500	-0.00000300
H	-4.71115500	1.87115800	0.00034500
H	-3.84935600	-2.33522800	-0.00037800
H	-5.52414200	-0.48817500	0.00003100
C	0.71598100	-0.55296600	-0.00006800
C	1.18611100	-1.09838200	-1.20185400
C	1.18578800	-1.09839100	1.20185800
C	2.11339100	-2.13883700	-1.20509300
H	0.82663900	-0.69228300	-2.14159900
C	2.11304600	-2.13885100	1.20535700
H	0.82604400	-0.69227700	2.14149100
C	2.58454700	-2.65905800	0.00019100
H	2.46922600	-2.54366900	-2.14658300
H	2.46861100	-2.54369900	2.14694100
H	3.30766200	-3.46717000	0.00029200
C	3.82155700	2.56834600	-0.00004600
H	4.78610900	2.07297400	-0.00022400
H	3.82603800	3.65618300	0.00017600

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -672.980333 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -672.921135 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -673.185312 a.u.

Lowest frequency: 20.90 cm⁻¹

2a

Cartesian coordinates

ATOM	X	Y	Z
C	-4.72087600	0.50561000	0.06407800
C	-4.34676500	-0.49150900	-0.83438300
C	-3.01764200	-0.89807800	-0.90338500
C	-2.05459200	-0.30813500	-0.07443800
C	-2.43875800	0.69657900	0.82723200
C	-3.76499300	1.09789400	0.89476900
H	-5.75557200	0.82396000	0.11936400
H	-5.08780800	-0.95037600	-1.47821000
H	-2.71732700	-1.67402400	-1.59913700
H	-1.68996600	1.14964200	1.46510700
H	-4.06033100	1.87335700	1.59185500
C	-0.66621300	-0.76139600	-0.17731100
H	-0.48319000	-1.54803000	-0.91805400
N	0.27208100	-0.26841400	0.54283800
S	1.84628700	-0.98876200	0.24785800
O	2.43198500	-1.24194200	1.61485300
C	2.67895300	0.56686400	-0.41597800
C	2.63783200	1.64267800	0.66099100
H	3.24755300	2.49406300	0.34418200
H	1.61932800	1.99108600	0.83684600
H	3.04228100	1.25984200	1.60047200
C	1.94917200	0.97165100	-1.69336200
H	0.94227500	1.33708900	-1.48724700
H	2.50813300	1.77555800	-2.18095100
H	1.88219800	0.13895700	-2.40046200
C	4.11361200	0.12511200	-0.71411300
H	4.14046600	-0.68766600	-1.44584000
H	4.66717400	0.97161000	-1.12959500
H	4.62537400	-0.20406200	0.19264500

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -956.372813 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -956.314144 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -956.567859 a.u.

Lowest frequency: 22.13 cm⁻¹

IM1(3a-RR)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.22774200	-1.17004000	-3.56493700
C	-0.10116300	-0.51301300	-3.07767300
C	0.40799900	-0.82826900	-1.81125400
C	-0.22910300	-1.80872200	-1.03635500
C	-1.35496000	-2.45824800	-1.52139100
C	-1.85588000	-2.14139400	-2.78730600
H	-1.61908000	-0.91956200	-4.54405700
H	0.38651400	0.25249000	-3.67123700
H	0.15472700	-2.03731900	-0.05075700
H	-1.85322500	-3.20152200	-0.91068900
H	-2.73939400	-2.64656300	-3.16054500
C	1.58969000	-0.11093700	-1.32778000
H	1.99821200	0.66313800	-1.98493000
N	2.13734000	-0.37565400	-0.20335300
S	3.50108900	0.60626900	0.22145400
O	3.96401000	1.40613600	-0.97912600
C	4.72204000	-0.82990200	0.39651500
C	6.04723700	-0.14745300	0.73979600
H	6.81124600	-0.91366100	0.89756100
H	6.37880900	0.50512400	-0.07008500
H	5.97033100	0.44500300	1.65637400
C	4.23457900	-1.70682100	1.54592700
H	4.09939300	-1.12707300	2.46382600
H	3.29244200	-2.19869400	1.30371900
H	4.98568200	-2.47703800	1.74681700
C	4.80871700	-1.57478400	-0.92801200
H	3.89610300	-2.13590800	-1.13478100
H	4.98717800	-0.87718400	-1.74991400
H	5.64442600	-2.27989600	-0.89192700
C	1.50672500	3.44603100	1.19630400
H	1.68193700	4.17961900	0.41750600
H	2.19924200	3.44267600	2.03434200
C	0.48547300	2.55850400	1.11542200
H	-0.15795800	2.61900800	0.24491400
C	0.23114400	1.50447400	2.05716900
H	0.98860200	1.39064100	2.83627200
N	-0.70777000	0.56663900	2.06714000
C	-1.80474800	0.42814100	1.31329900
C	-2.53009400	-0.82603800	1.41551200
C	-1.99592100	-1.93273500	2.13004800
C	-3.78927300	-1.03794900	0.79538600

C	-2.66131600	-3.14689500	2.20472800
H	-1.03433200	-1.80970800	2.61144200
C	-4.44595700	-2.26101600	0.86808700
H	-4.25462000	-0.22918500	0.24624000
C	-3.89441700	-3.33667300	1.56850600
H	-2.20841500	-3.96521200	2.75690200
H	-5.40543100	-2.37465700	0.37232200
H	-4.40609800	-4.29096800	1.61827500
C	-2.33033800	1.49076000	0.40906700
C	-2.70289000	2.74430200	0.92299700
C	-2.47165400	1.28539200	-0.97143100
C	-3.17193700	3.75574900	0.09099200
H	-2.60685700	2.92651600	1.98809400
C	-2.94159400	2.29483400	-1.80930300
H	-2.20036200	0.32600400	-1.39091400
C	-3.28976000	3.53863300	-1.28379000
H	-3.45159600	4.71508300	0.51379600
H	-3.03021300	2.10984600	-2.87491400
H	-3.65290300	4.32713600	-1.93356100

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.352547 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.255119 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.775053 a.u.

Lowest frequency: 16.83 cm⁻¹

IM1(3a-R5)

Cartesian coordinates

ATOM	X	Y	Z
C	1.42933900	2.40210200	-0.50399600
N	0.41151500	2.15660400	-1.24034100
S	-0.79397800	3.40692000	-1.30057700
O	-0.44306400	4.53022600	-0.34660600
C	-2.18710900	2.42773600	-0.46910100
C	-3.37956000	3.38487500	-0.50649800
H	-4.24471200	2.88579500	-0.06154100
H	-3.17968300	4.29407000	0.06410700
H	-3.64171600	3.66419700	-1.53117500
C	-2.44652400	1.18010400	-1.30679700
H	-2.63263700	1.43243900	-2.35534300
H	-1.60990500	0.48610700	-1.25474900
H	-3.33644900	0.67439600	-0.92231300
C	-1.76343400	2.12015200	0.95893900
H	-0.97982900	1.36407400	0.99863700
H	-1.41180200	3.02722700	1.45613800

H	-2.62606300	1.73984700	1.51144900
C	2.56380700	0.47988400	3.67944400
H	2.66990700	1.09678900	4.56470500
H	3.47655200	0.17845800	3.17528800
C	1.34112900	0.09637200	3.22975600
H	0.46117800	0.42314000	3.78560600
C	1.04768600	-0.70835100	2.08641600
H	1.88166200	-1.04981600	1.46830300
N	-0.21133000	-1.00722700	1.80435000
C	-0.66486100	-1.72586800	0.77236900
C	-2.10713900	-1.87294700	0.64496100
C	-2.99359600	-1.22294800	1.54569900
C	-2.71838900	-2.66989100	-0.35681500
C	-4.37037300	-1.33264900	1.42778700
H	-2.56440700	-0.62322200	2.33654300
C	-4.10091500	-2.77167700	-0.47110500
H	-2.09936300	-3.21789700	-1.05519700
C	-4.95024800	-2.10074600	0.41076100
H	-5.00480700	-0.80956900	2.13727800
H	-4.51974900	-3.39012500	-1.25930000
H	-6.02722000	-2.17908900	0.31618900
C	0.24508400	-2.36633600	-0.21602000
C	0.13599700	-2.11706400	-1.59455600
C	1.26411600	-3.23971300	0.20283800
C	0.99562200	-2.71654800	-2.51167400
H	-0.62947800	-1.43734100	-1.94953100
C	2.12835700	-3.83770700	-0.70949100
H	1.37110000	-3.45830000	1.25925100
C	1.99894000	-3.58099800	-2.07493600
H	0.88823900	-2.49922900	-3.56918800
H	2.90243100	-4.51011800	-0.35490900
H	2.67206900	-4.04535000	-2.78683800
H	1.48338400	3.32159000	0.08781900
C	2.57038800	1.49139100	-0.40944000
C	3.59976500	1.79282200	0.49063800
C	2.66068100	0.33441100	-1.19889400
C	4.69913600	0.94676200	0.60847500
H	3.52797300	2.68473400	1.10253900
C	3.75854700	-0.50421300	-1.08241600
H	1.86400900	0.10283100	-1.89235200
C	4.77908500	-0.20172200	-0.17538300
H	5.48888100	1.18190600	1.31221700
H	3.81978200	-1.39746300	-1.69109300
H	5.63433800	-0.86164900	-0.08428000

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.361509 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.265833 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.786031 a.u.

Lowest frequency: 22.77 cm⁻¹

IM1(3a-1)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.33061600	1.54052900	-0.13869800
N	-2.00569400	0.47066600	-0.36033000
S	-3.37882400	0.26726000	0.70147300
O	-3.25847100	-1.12895200	1.26989500
C	-4.68338600	0.17155500	-0.65446800
C	-6.00194700	-0.01851300	0.09820300
H	-6.82165900	-0.06857600	-0.62393100
H	-6.00011100	-0.94585900	0.67503700
H	-6.20131600	0.81533200	0.77772800
C	-4.66217600	1.49886700	-1.40710000
H	-4.76313900	2.35036500	-0.72682100
H	-3.74419000	1.62067600	-1.98361800
H	-5.50689800	1.52774000	-2.10164300
C	-4.37521700	-1.02257000	-1.54803100
H	-4.28009700	-1.93258600	-0.95211500
H	-5.19361700	-1.16058800	-2.26107900
H	-3.44948800	-0.87398300	-2.10500700
C	0.83513200	0.96063400	2.08624400
H	1.66320100	1.62746200	1.83514200
C	-0.20482900	1.48248300	2.91400800
H	-1.00628500	0.77619000	3.13170100
C	-0.28749600	2.73594100	3.43048300
H	0.48650700	3.47751100	3.25042600
H	-1.12671600	3.03848900	4.04623900
H	-1.61334100	2.26358300	0.63114000
C	-0.14728000	1.88505100	-0.92494300
C	0.53221300	3.07597100	-0.63568600
C	0.32370800	1.05085700	-1.94864600
C	1.66647900	3.42938000	-1.35780600
H	0.16972900	3.71109600	0.16525200
C	1.45226300	1.41110300	-2.67324700
H	-0.20023800	0.12789400	-2.16204900
C	2.12713300	2.59673800	-2.37802900
H	2.19388100	4.34696100	-1.12452300
H	1.81645400	0.76446000	-3.46259600

H	3.01422100	2.86749400	-2.93898800
N	0.76128200	-0.28101600	1.63501100
C	1.63480700	-0.92025200	0.85027400
C	1.22766200	-2.24752300	0.38071400
C	2.14845600	-3.20877000	-0.10053400
C	-0.13335600	-2.64414700	0.42027700
C	1.73754800	-4.47011000	-0.52039000
H	3.20398400	-2.96872500	-0.12994000
C	-0.53476600	-3.90677000	0.00628400
H	-0.87429300	-1.93857500	0.77107100
C	0.39182200	-4.83796800	-0.47479100
H	2.48028400	-5.17701900	-0.87732500
H	-1.58900600	-4.16436200	0.04692900
H	0.07292600	-5.81972600	-0.80628400
C	2.95924500	-0.37147400	0.47580000
C	3.45942500	-0.47439600	-0.83686500
C	3.77805700	0.28388600	1.41789500
C	4.69828000	0.04991800	-1.19079400
H	2.85806600	-0.96375000	-1.59191200
C	5.01679700	0.81077400	1.06641200
H	3.44329200	0.36559900	2.44457600
C	5.48738700	0.70243000	-0.24317300
H	5.04325000	-0.04051100	-2.21563200
H	5.62182200	1.30256700	1.82114400
H	6.45054000	1.11699100	-0.51876200

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.356869 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.259826 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.779808 a.u.

Lowest frequency: 13.30 cm⁻¹

TS1(3a-RR)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.03712600	4.31480500	1.19582400
C	-1.75294600	3.45562300	0.36796500
C	-1.68719200	2.06634500	0.54313800
C	-0.88859600	1.56056200	1.57653200
C	-0.17305200	2.42025800	2.40713800
C	-0.24100100	3.80020400	2.22129600
H	-1.10161000	5.38694600	1.04462500
H	-2.36987900	3.86011500	-0.42807000
H	-0.83507800	0.48882900	1.71814500
H	0.44320300	2.01100900	3.20034200

H	0.31794900	4.46797600	2.86711800
C	-2.43557200	1.16350500	-0.36781800
H	-3.25078600	1.64917000	-0.90691200
N	-2.60396300	-0.10626000	0.04244300
S	-3.64061000	-1.03043700	-0.90739500
O	-4.76133800	-0.17943300	-1.50944100
C	-4.45931700	-2.00057000	0.49706500
C	-5.47689200	-2.90701100	-0.19425800
H	-5.98637500	-3.52417100	0.55186100
H	-6.22863800	-2.31945700	-0.72527400
H	-4.99328300	-3.57762700	-0.91161100
C	-3.37636800	-2.81614800	1.19582100
H	-2.84401100	-3.46109300	0.48935700
H	-2.64865600	-2.16899900	1.68592300
H	-3.83479800	-3.46055800	1.95363200
C	-5.14144500	-1.00656200	1.42566900
H	-4.40630200	-0.38106900	1.93474900
H	-5.81140600	-0.35788300	0.85566700
H	-5.73110300	-1.53934900	2.17854200
C	-1.25177400	1.24456300	-2.06331800
H	-1.30641900	2.30031500	-2.31172300
H	-1.89467100	0.61107000	-2.67105100
C	0.00052900	0.72602700	-1.67062300
H	0.72198200	1.43367100	-1.28461400
C	0.25508900	-0.62894500	-1.57972100
H	-0.52454500	-1.28700300	-1.95971600
N	1.30500600	-1.32597200	-1.03650000
C	2.43824600	-0.88162700	-0.58064900
C	3.38218500	-1.85272600	0.00589800
C	3.02836800	-3.20982100	0.14943200
C	4.66290500	-1.46106100	0.43797900
C	3.91443000	-4.12702600	0.69547700
H	2.04463500	-3.52169300	-0.17677100
C	5.54941800	-2.38470200	0.98669700
H	4.96843200	-0.42702300	0.34091200
C	5.18387300	-3.72247300	1.12004500
H	3.61628900	-5.16527400	0.79557600
H	6.53097000	-2.05532600	1.31010200
H	5.87374400	-4.44062500	1.54841500
C	2.85632900	0.55440700	-0.61967300
C	3.35724300	1.11210200	-1.80043700
C	2.71560800	1.36673100	0.50942300
C	3.69085100	2.46300300	-1.85723900
H	3.47043900	0.48624100	-2.67877800

C	3.04338800	2.71973200	0.45250800
H	2.33038200	0.93988500	1.42768800
C	3.52781500	3.27191100	-0.73236100
H	4.07555600	2.88572800	-2.77882900
H	2.91627500	3.34249300	1.33043500
H	3.78088500	4.32515500	-0.77834000

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.337445 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.241878 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.761589 a.u.

Lowest frequency: -430.15 cm⁻¹

TS1(3a-RS)

Cartesian coordinates

ATOM	X	Y	Z
C	3.04142400	-0.72176400	-0.41469300
N	2.23777900	-0.88389300	0.66086500
S	1.94829000	-2.47041400	1.15402800
O	2.48195500	-3.49524600	0.15075700
C	0.04951100	-2.69996500	1.08203200
C	-0.18695400	-3.94668900	1.93672600
H	-1.25932100	-4.16096500	1.98214800
H	0.31424300	-4.81982000	1.51090400
H	0.17259900	-3.80781200	2.96076100
C	-0.60753700	-1.47428700	1.70042500
H	-0.26371300	-1.31144700	2.72726400
H	-0.39300700	-0.57886500	1.11978600
H	-1.69274500	-1.61758800	1.73133300
C	-0.36954200	-2.94347600	-0.35834000
H	-0.32593200	-2.02835300	-0.94195500
H	0.28541400	-3.68860300	-0.81600800
H	-1.39921400	-3.31544000	-0.38753500
C	2.16391600	0.23015300	-2.08227500
H	2.80407500	-0.17227300	-2.86180600
H	2.42250500	1.24143200	-1.78463600
C	0.78427800	-0.06492900	-2.14498700
H	0.45988000	-0.93667900	-2.70991700
C	-0.17620600	0.59643200	-1.41881600
H	0.11546800	1.46345500	-0.82571100
N	-1.47141200	0.16092000	-1.41646400
C	-2.41210200	0.71763900	-0.70909500
C	-3.75238300	0.10349300	-0.71439100
C	-3.96713700	-1.14597100	-1.33014600
C	-4.85437800	0.73683700	-0.11197900

C	-5.22417600	-1.73339500	-1.33629300
H	-3.12720200	-1.64257400	-1.79765600
C	-6.11441400	0.14359000	-0.11940300
H	-4.72585600	1.70172900	0.36160800
C	-6.30883700	-1.09436400	-0.72828200
H	-5.36221100	-2.69806800	-1.81270700
H	-6.94746500	0.65373700	0.35176800
H	-7.28908700	-1.55719500	-0.73024700
C	-2.18776100	1.93846600	0.12622900
C	-2.21019200	1.86306600	1.52370100
C	-1.92556400	3.17331900	-0.47836000
C	-1.96991300	2.99531100	2.29905800
H	-2.41398300	0.91289300	2.00292500
C	-1.69202400	4.30751900	0.29583700
H	-1.90696800	3.24261400	-1.56026100
C	-1.71093500	4.22103600	1.68733800
H	-1.98467600	2.91977900	3.38068900
H	-1.49476600	5.25801200	-0.18735700
H	-1.52542100	5.10268100	2.29036500
H	3.34067800	-1.62111900	-0.95506700
C	4.12869700	0.29017000	-0.31210400
C	5.22900200	0.22738900	-1.17899300
C	4.08522400	1.32323200	0.63448100
C	6.25102400	1.17012600	-1.10794900
H	5.28038400	-0.57184400	-1.91156200
C	5.10286100	2.27083600	0.70069100
H	3.24650100	1.36798600	1.31837700
C	6.19149700	2.20164500	-0.17002300
H	7.09725500	1.09850200	-1.78297500
H	5.04968800	3.06514400	1.43791200
H	6.98576000	2.93756600	-0.11409100

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.333506 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.239616 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.759432 a.u.

Lowest frequency: -307.31 cm⁻¹

TS1(3a-1)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.20382000	-1.27753800	0.06706000
N	-2.10940800	-0.27800700	0.24268300
S	-3.51479600	-0.47416200	-0.64091200
O	-3.57977800	0.52594900	-1.80215900

C	-4.71713700	0.25280800	0.62049900
C	-6.09741000	0.15622800	-0.03029100
H	-6.85828500	0.54238600	0.65530700
H	-6.13639600	0.74035100	-0.95186900
H	-6.35407000	-0.88093900	-0.26847500
C	-4.64360300	-0.60103300	1.88142500
H	-4.85112300	-1.65367800	1.66213100
H	-3.65645400	-0.53591900	2.34088500
H	-5.38989800	-0.25842800	2.60610400
C	-4.33116800	1.70434300	0.87359800
H	-4.26731600	2.24335800	-0.07434900
H	-5.08508900	2.18896000	1.50293900
H	-3.36404700	1.77170800	1.37395700
C	0.05663400	-0.99033900	-1.53764800
H	0.75642100	-1.80971100	-1.36846000
C	-0.85733900	-1.18318800	-2.65445100
H	-1.49572300	-0.33163300	-2.87608400
C	-1.01639300	-2.32790400	-3.33807200
H	-0.40220400	-3.20253400	-3.13903900
H	-1.76519800	-2.42074000	-4.11765200
H	-1.54224700	-2.23723400	-0.33981300
C	-0.17356100	-1.42538600	1.12168800
C	0.50603000	-2.64272500	1.27821200
C	0.14838300	-0.36589400	1.98009600
C	1.46331600	-2.80365400	2.27323400
H	0.27027100	-3.46906500	0.61548400
C	1.10704500	-0.52678000	2.97785200
H	-0.37380000	0.57436200	1.86486000
C	1.76715700	-1.74433900	3.13115000
H	1.97281100	-3.75465300	2.38332800
H	1.34360600	0.30410000	3.63389400
H	2.51527100	-1.86736600	3.90617400
N	0.47680400	0.30804300	-1.33194500
C	1.61981000	0.65493300	-0.83017800
C	1.77619200	2.08004000	-0.44378700
C	3.03040300	2.70810900	-0.38654000
C	0.63650700	2.84716500	-0.14129200
C	3.14095400	4.05346400	-0.04206300
H	3.92461800	2.14525100	-0.62363900
C	0.74862400	4.18864000	0.20185200
H	-0.33148600	2.36320300	-0.17567600
C	2.00298400	4.80097300	0.25600500
H	4.12003000	4.51899500	-0.01039300
H	-0.14367200	4.75796300	0.43892600

H	2.09091700	5.84587900	0.53145900
C	2.78715900	-0.26163800	-0.66123700
C	3.51471900	-0.29891500	0.53425800
C	3.19435200	-1.09479200	-1.71464800
C	4.59589900	-1.16318600	0.68658000
H	3.22256900	0.34257400	1.35445800
C	4.28006900	-1.95161200	-1.56780600
H	2.65800700	-1.06272500	-2.65552800
C	4.98166600	-1.99561100	-0.36196900
H	5.13465500	-1.18731400	1.62738200
H	4.58191100	-2.58367700	-2.39564100
H	5.82428100	-2.66773900	-0.24511100

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.339463 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.247923 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.767904 a.u.

Lowest frequency: -373.43 cm⁻¹

IM2(3a-RR)

Cartesian coordinates

ATOM	X	Y	Z
C	1.85146100	3.56417000	-0.25334800
C	2.14963000	2.44713300	0.52473400
C	1.94678600	1.15052200	0.03780100
C	1.43522100	1.00395700	-1.25381000
C	1.13128800	2.11711000	-2.03701300
C	1.33742300	3.40307100	-1.54033500
H	2.02219500	4.55968900	0.14247300
H	2.55075900	2.58121600	1.52484400
H	1.28747700	0.00199300	-1.63585100
H	0.73014500	1.97955500	-3.03558600
H	1.10220800	4.26983000	-2.14793000
C	2.21732000	-0.05569200	0.93430400
H	3.09969500	0.17509900	1.54257500
N	2.37991200	-1.31240300	0.20921200
S	3.83123900	-2.02429500	0.27940300
O	4.49515200	-1.89399400	1.67132900
C	5.10691900	-1.04022800	-0.79180800
C	6.35046300	-1.92817800	-0.80787300
H	7.12405800	-1.49416600	-1.45268500
H	6.76143000	-2.03690200	0.19807000
H	6.12023900	-2.92850600	-1.19056200
C	4.52268900	-0.90040000	-2.19023900
H	4.21698200	-1.87302200	-2.59177900

H	3.65101600	-0.24482200	-2.19478700
H	5.26718200	-0.47867100	-2.87673200
C	5.41670800	0.30452000	-0.15078100
H	4.58065100	0.99966900	-0.24344500
H	5.63652600	0.16161600	0.91038200
H	6.29064400	0.76638600	-0.62750000
C	1.04308200	-0.18738800	1.94712700
H	0.96752000	0.75677500	2.50615200
H	1.28968400	-0.97179200	2.66794000
C	-0.27502000	-0.45713700	1.29630100
H	-0.47293200	0.09049900	0.38267200
C	-1.21831700	-1.28396400	1.76353300
H	-1.02851600	-1.88144300	2.65291000
N	-2.44535500	-1.58832100	1.15467100
C	-3.19919300	-0.72335400	0.57433500
C	-4.41709300	-1.21225700	-0.12400700
C	-4.55474800	-2.57485900	-0.43316100
C	-5.45506400	-0.33584900	-0.47014100
C	-5.69666400	-3.04492200	-1.06788500
H	-3.75186800	-3.25142600	-0.17010800
C	-6.60303000	-0.81034100	-1.10040700
H	-5.37045500	0.71804800	-0.23833900
C	-6.72726500	-2.16401200	-1.40364000
H	-5.78472200	-4.09879400	-1.30679700
H	-7.39982000	-0.12063100	-1.35445400
H	-7.61773900	-2.53201800	-1.90049200
C	-2.93181800	0.75149700	0.55731800
C	-2.90330900	1.48047900	1.74925200
C	-2.65068200	1.39949300	-0.64875600
C	-2.57683000	2.83336300	1.73688000
H	-3.12133200	0.98119600	2.68614300
C	-2.30939400	2.74977400	-0.65875400
H	-2.67159500	0.83868900	-1.57608200
C	-2.26713900	3.46874700	0.53423600
H	-2.55565900	3.39039800	2.66672200
H	-2.06981800	3.23722000	-1.59633400
H	-1.99744700	4.51852100	0.52714900

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.354075 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.259195 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.782336 a.u.

Lowest frequency: 14.14 cm⁻¹

IM2(3a-R5)

Cartesian coordinates

ATOM	X	Y	Z
C	2.64219700	-0.03884900	0.73968700
N	2.08431500	-0.19432200	-0.60200600
S	2.38585100	0.94908600	-1.70504200
O	3.80785100	1.54802400	-1.60945200
C	1.32631200	2.52701900	-1.31227900
C	1.51668100	3.40992600	-2.54521000
H	0.89305400	4.30889700	-2.47170500
H	2.55910800	3.72111200	-2.64210100
H	1.23358100	2.88083800	-3.46161800
C	-0.12440900	2.08974100	-1.17665300
H	-0.45285800	1.52832900	-2.05788600
H	-0.26899900	1.45695400	-0.30109800
H	-0.78171400	2.96271800	-1.07818800
C	1.84553500	3.23637300	-0.06859400
H	1.53256500	2.73080600	0.84692900
H	2.93818000	3.26777700	-0.09831700
H	1.46922200	4.26661600	-0.02496900
C	1.74061000	-0.80447800	1.75423100
H	2.24319300	-0.80048700	2.72900700
H	1.66402000	-1.84514400	1.42339400
C	0.38473900	-0.19835200	1.87688500
H	0.31221700	0.78683300	2.33319900
C	-0.73032300	-0.74572500	1.37257000
H	-0.68242600	-1.72108100	0.89098100
N	-1.94307000	-0.06648400	1.42299400
C	-2.94486100	-0.40457600	0.68282000
C	-4.21960100	0.33556900	0.86564500
C	-4.46399800	1.03093200	2.06068700
C	-5.18778400	0.38125200	-0.14789200
C	-5.64164800	1.74556700	2.23693300
H	-3.71810200	0.99696800	2.84431700
C	-6.36462200	1.10495500	0.02760300
H	-5.01532700	-0.13824100	-1.08168300
C	-6.59776600	1.78652900	1.21991000
H	-5.81902900	2.26937400	3.16952200
H	-7.09830600	1.13717700	-0.76984600
H	-7.51692300	2.34432800	1.35853900
C	-2.90095900	-1.47585000	-0.35836400
C	-1.94332600	-1.43989700	-1.37956500
C	-3.81876700	-2.53280800	-0.32284400
C	-1.90800100	-2.44026400	-2.34695700

H	-1.22517800	-0.63033900	-1.41545700
C	-3.77033900	-3.54177100	-1.28073700
H	-4.56615700	-2.56666100	0.46138300
C	-2.81824600	-3.49500400	-2.29840500
H	-1.16597200	-2.39659800	-3.13606000
H	-4.47848500	-4.36139700	-1.23537700
H	-2.78595200	-4.27648500	-3.04908300
H	2.67673100	1.00315800	1.07537900
C	4.06219400	-0.57841300	0.86984700
C	5.04123600	0.14400000	1.55594200
C	4.40596300	-1.82988100	0.34749700
C	6.33172500	-0.36172500	1.71452100
H	4.79086000	1.12026800	1.95935800
C	5.69104000	-2.34342900	0.50578600
H	3.66006700	-2.39101700	-0.20350700
C	6.66222500	-1.61040200	1.19038300
H	7.07962100	0.22110100	2.24208400
H	5.93826400	-3.31585900	0.09250100
H	7.66476900	-2.00651200	1.30898900

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.358255 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.263897 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.787118 a.u.

Lowest frequency: 15.38 cm⁻¹

IM2(3a-1)

Cartesian coordinates

ATOM	X	Y	Z
C	-1.37381200	0.17424600	0.32278400
N	-1.98374600	-1.13706000	0.45013000
S	-3.39360900	-1.44116400	-0.28179200
O	-3.43634200	-1.11471200	-1.79265600
C	-4.72496000	-0.18840400	0.37608000
C	-6.05429300	-0.85218800	0.01219900
H	-6.89351600	-0.24966200	0.37917400
H	-6.15534400	-0.95179000	-1.07141400
H	-6.13734100	-1.85013300	0.45443800
C	-4.57290300	-0.07873300	1.88598700
H	-4.59765300	-1.06577100	2.35969600
H	-3.63286800	0.39999900	2.16360600
H	-5.39452500	0.51227600	2.31028600
C	-4.59609500	1.14990900	-0.34355700
H	-3.83735300	1.78991300	0.11038100
H	-4.31695200	0.96784500	-1.38552600

H	-5.54855100	1.69426600	-0.32499700
C	-0.22968600	0.33472100	1.38973400
H	0.14594100	1.35635700	1.28226600
C	-0.76880300	0.16297200	2.78172900
H	-1.10161700	-0.83902200	3.03289600
C	-0.86485400	1.15415800	3.66412500
H	-0.53375700	2.16124700	3.42482100
H	-1.28248600	0.99710100	4.65367300
H	-2.06537000	0.98772100	0.58023300
C	-0.79572100	0.52348600	-1.04328100
C	-0.80191000	1.84935000	-1.48389500
C	-0.18956800	-0.44160500	-1.85113300
C	-0.22879800	2.20603800	-2.70476200
H	-1.26532800	2.61111800	-0.86410300
C	0.39017700	-0.09290700	-3.06723000
H	-0.19293300	-1.47170700	-1.52160800
C	0.37160900	1.23405500	-3.50250600
H	-0.25131500	3.24034500	-3.03125700
H	0.85768100	-0.85660600	-3.68017100
H	0.81990600	1.50509200	-4.45209900
N	0.79335600	-0.67109000	1.16307800
C	1.96505100	-0.36196700	0.76025400
C	2.90379800	-1.47261200	0.42655000
C	4.28301000	-1.25639700	0.31653400
C	2.40415100	-2.76702300	0.21753000
C	5.14320900	-2.30995300	0.01223100
H	4.68770100	-0.26483800	0.47513500
C	3.26157400	-3.81488400	-0.09182600
H	1.33690300	-2.92795700	0.29926500
C	4.63634700	-3.59039200	-0.19524500
H	6.20928300	-2.12796900	-0.06332000
H	2.85996200	-4.80805500	-0.25893700
H	5.30466700	-4.40837900	-0.43939600
C	2.46620000	1.03853900	0.57474000
C	2.76641500	1.51208900	-0.70502200
C	2.62312300	1.88830800	1.67398900
C	3.19772600	2.82344400	-0.88615500
H	2.64474100	0.85787500	-1.55916300
C	3.06769300	3.19609100	1.49364900
H	2.39204400	1.52382200	2.66841700
C	3.35107000	3.66802800	0.21257800
H	3.41194600	3.18522700	-1.88540900
H	3.18850800	3.84681900	2.35234600
H	3.69033400	4.68801900	0.07175000

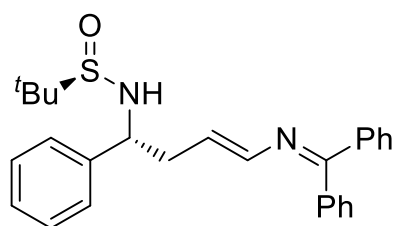
B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Gibbs Free Energy: -1629.349083 a.u.

B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Enthalpy: -1629.255603 a.u.

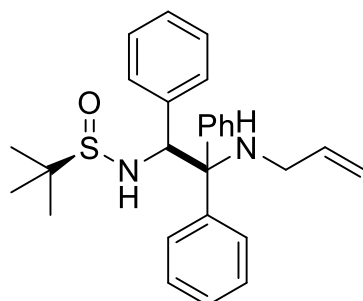
B3LYP+GD3(BJ)/6-311G** solvent = (DMF) Electronic Energy: -1629.778452 a.u.

Lowest frequency: 16.48 cm⁻¹

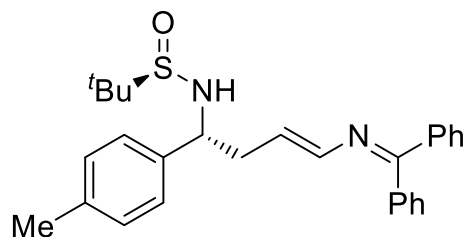
11. Experimental data



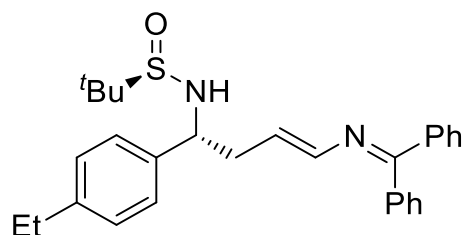
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3a**): 174 mg, 81% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.40 (m, 3H), 7.31 (m, 8H), 7.01 (m, 2H), 6.63 (d, J = 12.0 Hz, 2H), 5.99 (m, 1H), 4.47 (m, 1H), 3.52 (d, J = 4.0 Hz, 1H), 2.77 (m, 1H), 2.57 (m, 1H), 1.2 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 141.5, 140.5, 139.3, 135.9, 130.1, 128.64, 128.56, 128.5, 128.2, 127.9, 127.7, 127.6, 127.2, 58.5, 55.7, 37.7, 22.5. These data are in accordance with the literature.⁵



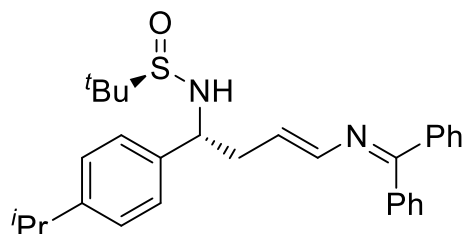
(*R*)-*N*-(2-(Allylamino)-1,2,2-triphenylethyl)-2-methylpropane-2-sulfonamide (**3a'**): 61 mg, 28% yield; foam solid; ^1H NMR (600 MHz, CDCl_3) δ 7.30 (m, 8H), 7.18 (m, 3H), 7.10 (t, J = 6.0 Hz, 2H), 6.62 (d, J = 12.0 Hz, 2H), 5.74 (m, 1H), 5.38 (d, J = 12.0 Hz, 1H), 5.07 (dd, J = 18.0 Hz, J = 2.0 Hz, 1H), 4.96 (dd, J = 12.0 Hz, J = 2.0 Hz, 1H), 3.74 (d, J = 8.0 Hz, 1H), 2.72 (m, 2H), 1.03 (s, 9H); ^{13}C NMR (151 MHz, CDCl_3) δ 141.3, 140.0, 138.9, 136.5, 130.0, 129.8, 128.9, 127.6, 127.49, 127.45, 127.4, 127.3, 127.0, 114.9, 70.2, 65.0, 56.6, 45.9, 22.7; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{32}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$)⁺ 433.2314, found 433.2314.



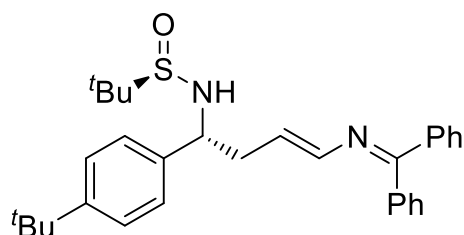
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(*p*-tolyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3b**): 163 mg, 73% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.39 (m, 4H), 7.30 (t, J = 8.0 Hz, 2H), 7.19 (d, J = 8.0 Hz, 2H), 7.14 (d, J = 8.0 Hz, 2H), 7.03 (m, 2H), 6.63 (d, J = 16.0 Hz, 1H), 5.98 (m, 1H), 4.43 (m, 1H), 4.43 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.55 (m, 1H), 2.35 (s, 3H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 140.5, 139.5, 138.6, 137.4, 136.1, 130.1, 129.3, 128.8, 128.71, 128.66, 128.3, 128.02, 127.96, 127.2, 58.3, 55.7, 37.8, 22.6, 21.1. These data are in accordance with the literature.⁵



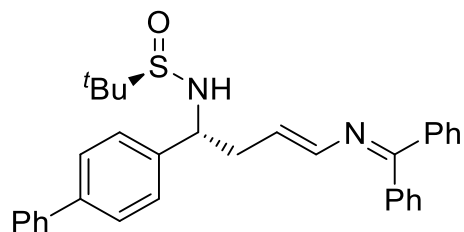
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-ethylphenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3c**): 163 mg, 71% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.41 (m, 3H), 7.33 (m, 3H), 7.22 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 7.04 (m, 2H), 6.65 (d, J = 12.0 Hz, 1H), 5.98 (m, 1H), 4.44 (m, 1H), 3.43 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.66 (q, J = 8.0 Hz, 2H), 2.56 (m, 1H), 1.24 (t, J = 8.0 Hz, 3H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 143.8, 140.5, 139.5, 138.9, 136.1, 130.2, 128.8, 128.71, 128.67, 128.3, 128.1, 128.0, 127.3, 58.4, 55.8, 37.8, 28.5, 22.6, 15.5; HRMS (ESI): calc for $\text{C}_{29}\text{H}_{34}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 459.2470, found 459.2474.



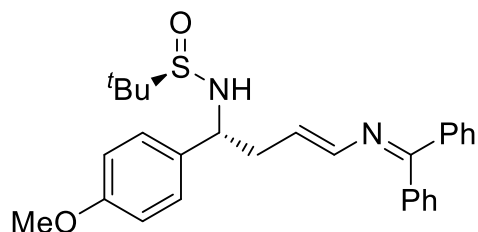
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-isopropylphenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3d**): 175 mg, 74% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.41 (m, 3H), 7.34 (m, 3H), 7.22 (d, J = 8.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 7.04 (m, 2H), 6.64 (d, J = 12.0 Hz, 1H), 5.97 (m, 1H), 4.45 (m, 1H), 3.45 (d, J = 4.0 Hz, 1H), 2.91 (m, 1H), 2.76 (m, 1H), 2.57 (m, 1H), 1.25 (d, J = 8.0 Hz, 6H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 148.3, 140.4, 139.5, 138.9, 136.1, 130.1, 128.73, 128.68, 128.66, 128.3, 128.1, 128.0, 127.2, 126.6, 58.4, 55.7, 37.8, 33.7, 23.94, 23.89, 22.6; HRMS (ESI): calc for $\text{C}_{30}\text{H}_{36}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 473.2627, found 473.2632.



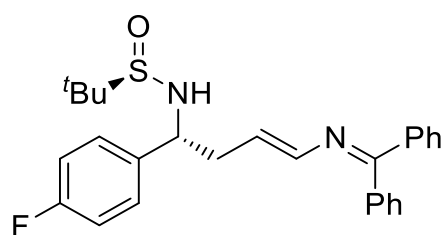
(*R*)-*N*-((*R,E*)-1-(4-(*tert*-Butyl)phenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3e**): 175 mg, 72% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.43 (t, J = 4.0 Hz, 3H), 7.33 (m, 6H), 7.23 (s, 1H), 7.07 (q, J = 4.0 Hz, 2H), 6.79 (d, J = 12.0 Hz, 1H), 5.99 (m, 1H), 4.45 (m, 1H), 3.46 (d, J = 2.0 Hz, 1H), 2.76 (m, 1H), 2.58 (m, 1H), 1.32 (s, 9H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 150.6, 140.4, 139.5, 138.5, 136.1, 130.1, 128.72, 128.66, 128.4, 128.2, 128.0, 126.9, 125.5, 58.3, 55.8, 37.7, 34.5, 31.3, 22.6; HRMS (ESI): calc for $\text{C}_{31}\text{H}_{38}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 487.2783, found 487.2785.



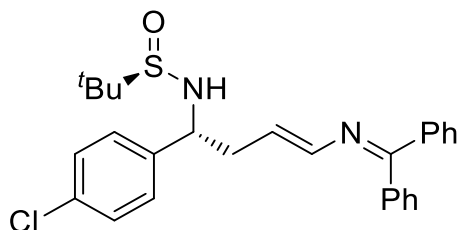
(*R*)-*N*-((*R,E*)-1-([1,1'-Biphenyl]-4-yl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3f**): 200 mg, 79% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.59 (m, 6H), 7.44 (t, J = 8.0 Hz, 2H), 7.33 (m, 9H), 7.03 (q, J = 4.0 Hz, 2H), 6.65 (d, J = 12.0 Hz, 1H), 6.02 (m, 1H), 4.53 (m, 1H), 3.54 (d, J = 4.0 Hz, 1H), 2.81 (m, 1H), 2.61 (m, 1H), 1.22 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 140.7, 140.64, 140.61, 140.58, 139.4, 136.0, 130.2, 128.8, 128.7, 128.6, 128.3, 128.0, 127.7, 127.6, 127.31, 127.27, 127.0, 58.3, 55.8, 37.8, 22.6; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{34}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 507.2470, found 507.2473.



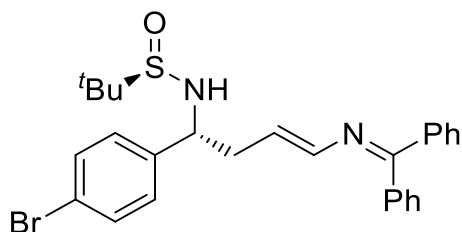
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-methoxyphenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3g**): 166 mg, 72% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (m, 2H), 7.42 (m, 3H), 7.32 (m, 3H), 7.22 (d, J = 8.0 Hz, 2H), 7.03 (m, 2H), 6.87 (d, J = 8.0 Hz, 2H), 6.62 (d, J = 12.0 Hz, 1H), 5.98 (m, 1H), 4.42 (m, 1H), 3.81 (s, 3H), 3.44 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.54 (m, 1H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 159.1, 140.5, 139.5, 136.1, 133.7, 130.1, 128.73, 128.67, 128.4, 128.3, 128.0, 127.9, 113.9, 58.0, 55.7, 55.2, 37.8, 22.6; These data are in accordance with the literature.⁵



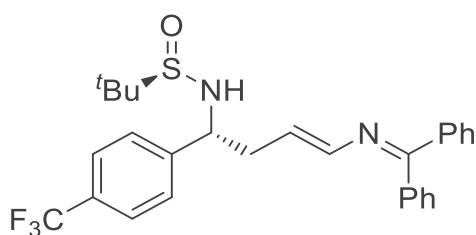
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-fluorophenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3h**): 218 mg, 97% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.42 (m, 3H), 7.31 (m, 5H), 7.02 (m, 4H), 6.59 (d, J = 16.0 Hz, 1H), 5.96 (m, 1H), 4.46 (m, 1H), 3.48 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.54 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.2, 162.2 (d, $J_{\text{F-C}}$ = 247.5 Hz), 140.8, 139.3, 137.4 (d, $J_{\text{F-C}}$ = 3.0 Hz), 136.0, 130.2, 128.9 (d, $J_{\text{F-C}}$ = 8.1 Hz), 128.72, 128.67, 128.6, 128.3, 128.0, 127.2, 115.4 (d, $J_{\text{F-C}}$ = 21.2 Hz), 58.0, 55.8, 37.8, 22.5; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{29}\text{N}_2\text{OSF}$ ($\text{M}+\text{H}$) $^+$ 449.2063, found 449.2068.



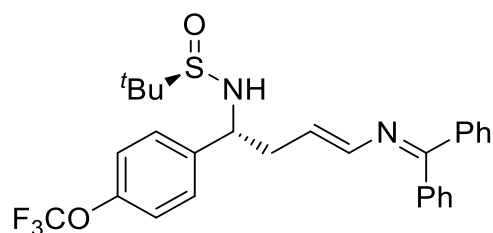
(*R*)-*N*-((*R,E*)-1-(4-Chlorophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3i**): 188 mg, 81% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.43 (m, 3H), 7.37 (d, J = 8.0 Hz, 1H), 7.31 (m, 4H), 7.23 (d, J = 8.0 Hz, 2H), 7.00 (m, 2H), 6.57 (d, J = 12.0 Hz, 1H), 5.95 (m, 1H), 4.45 (m, 1H), 3.48 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.53 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 141.0, 140.1, 139.4, 136.0, 133.5, 130.3, 128.8, 128.73, 128.71, 128.6, 128.4, 128.1, 126.9, 58.0, 55.9, 37.8, 22.5; These data are in accordance with the literature.⁵



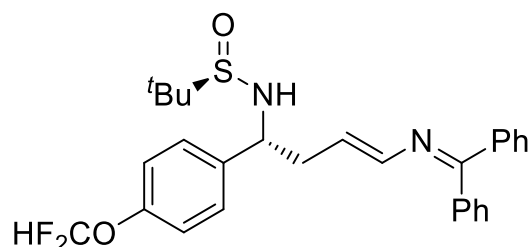
(*R*)-*N*-((*R,E*)-1-(4-Bromophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3j**): 232 mg, 91% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.46 (m, 5H), 7.38 (t, J = 6.0 Hz, 1H), 7.32 (d, J = 6.0 Hz, 2H), 7.17 (d, J = 8.0 Hz, 2H), 7.00 (m, 2H), 6.56 (d, J = 12.0 Hz, 1H), 5.95 (m, 1H), 4.44 (m, 1H), 3.46 (s, 1H), 2.76 (m, 1H), 2.53 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4, 141.1, 140.7, 139.4, 136.0, 131.7, 130.3, 129.1, 128.81, 128.76, 128.6, 128.4, 128.1, 126.9, 121.7, 58.1, 56.0, 37.7, 22.6; These data are in accordance with the literature.⁵



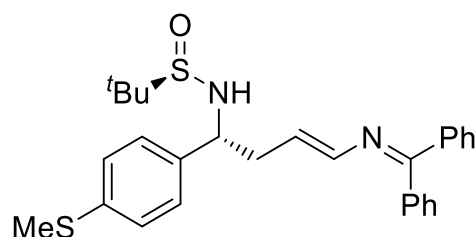
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-(trifluoromethyl)phenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3k**): 177 mg, 71% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 4H), 7.41 (m, 5H), 7.33 (m, 2H), 7.24 (t, J = 8.0 Hz, 1H), 7.00 (d, J = 8.0 Hz, 2H), 6.59 (d, J = 12.0 Hz, 1H), 5.95 (m, 1H), 4.54 (m, 1H), 3.57 (d, J = 4.0 Hz, 1H), 2.78 (m, 1H), 2.58 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 145.7, 141.1, 139.3, 136.0, 130.4, 128.8, 128.7, 128.5, 128.4, 128.1, 127.7, 127.3, 126.6, 125.6 (q, $J_{\text{F-C}}$ = 4.0 Hz), 124.0 (q, $J_{\text{F-C}}$ = 272.7 Hz), 58.4, 56.1, 37.8, 22.6; HRMS (ESI): calc for $\text{C}_{28}\text{H}_{29}\text{N}_2\text{OSF}_3$ ($\text{M}+\text{H}$)⁺ 499.2031, found 499.2032.



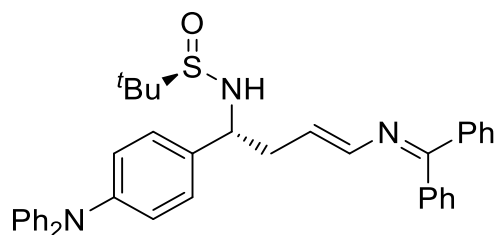
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-(trifluoromethoxy)phenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**4l**): 185 mg, 72% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, $J = 12.0$ Hz, 2H), 7.42 (m, 3H), 7.33 (m, 5H), 7.19 (d, $J = 8.0$ Hz, 2H), 7.03 (m, 2H), 6.62 (d, $J = 12.0$ Hz, 1H), 5.96 (m, 1H), 4.49 (m, 1H), 3.52, (d, $J = 4.0$ Hz, 1H), 2.77 (m, 1H), 2.56 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 148.6 (q, $J_{\text{F-C}} = 3.0$ Hz), 140.9, 140.3, 139.3, 136.0, 130.3, 128.74, 128.72, 128.5, 128.3, 128.0, 127.0, 121.0, 120.4 (q, $J_{\text{F-C}} = 257.6$ Hz), 58.0, 55.9, 37.8, 22.5; HRMS (ESI): calc for $\text{C}_{28}\text{H}_{29}\text{N}_2\text{O}_2\text{SF}_3$ ($\text{M}+\text{H}$) $^+$ 515.1980, found 515.1985.



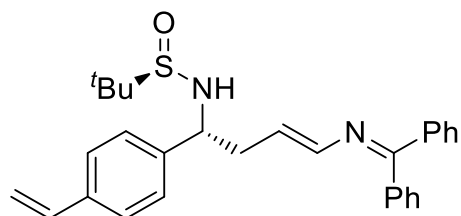
(*R*)-*N*-((*R,E*)-1-(4-(Difluoromethoxy)phenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3m**): 174 mg, 70% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 8.0$ Hz, 2H), 7.43 (m, 3H), 7.37 (t, $J = 8.0$ Hz, 1H), 7.31 (m, 4H), 7.09 (d, $J = 8.0$ Hz, 2H), 7.03 (m, 2H), 6.61 (t, $J = 16.0$ Hz, 1H), 6.52 (t, $J_{\text{F-H}} = 74.0$ Hz, 1H), 5.95 (m, 1H), 4.47 (m, 1H), 3.47 (d, $J = 4.0$ Hz, 1H), 2.77 (m, 1H), 2.55 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 150.6 (t, $J_{\text{F-C}} = 3.0$ Hz), 140.9, 139.3, 138.8, 136.0, 130.3, 128.79, 128.75, 128.73, 128.6, 128.4, 128.1, 127.2, 119.6, 115.8 (t, $J_{\text{F-C}} = 261.1$ Hz), 58.1, 55.9, 37.8, 22.6; HRMS (ESI): calc for $\text{C}_{28}\text{H}_{30}\text{N}_2\text{O}_2\text{SF}_2$ ($\text{M}+\text{H}$) $^+$ 497.2074, found 497.2078.



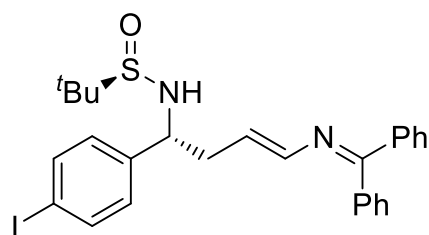
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-(methylthio)phenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3n**): 181 mg, 76% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, $J = 8.0$ Hz, 2H), 7.43 (m, 3H), 7.37 (m, 1H), 7.31 (t, $J = 8.0$ Hz, 2H), 7.22 (s, 4H), 7.01 (m, 2H), 6.60 (d, $J = 12.0$ Hz, 1H), 5.97 (m, 1H), 4.43 (m, 1H), 3.45 (d, $J = 4.0$ Hz, 1H), 2.77 (m, 1H), 2.55 (m, 1H), 2.49 (s, 3H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 140.8, 139.4, 138.4, 138.0, 136.0, 130.2, 128.8, 128.70, 128.67, 128.4, 128.0, 127.8, 127.5, 126.6, 58.1, 55.8, 37.7, 22.6, 15.7; HRMS (ESI): calc for $\text{C}_{28}\text{H}_{32}\text{N}_2\text{OS}_2$ ($\text{M}+\text{H}$) $^+$ 477.2034, found 477.2039.



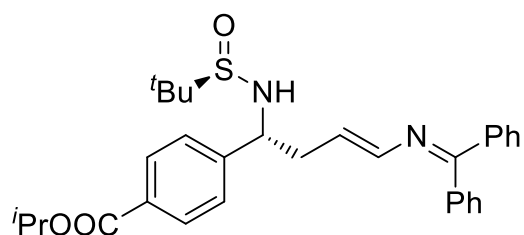
(*R*)-*N*-((*R,E*)-1-(4-(Diphenylamino)phenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3o**): 161 mg, 54% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, J = 8.0 Hz, 2H), 7.44 (t, J = 4.0 Hz, 3H), 7.35 (m, 3H), 7.24 (m, 4H), 7.13 (m, 8H), 7.01 (m, 4H), 6.73 (d, J = 12.0 Hz, 1H), 6.01 (m, 1H), 4.42 (m, 1H), 3.44 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.58 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 147.6, 147.4, 140.4, 139.5, 136.2, 135.3, 130.2, 129.2, 128.74, 128.68, 128.4, 128.2, 128.1, 124.41, 123.35, 122.9, 58.2, 55.8, 37.8, 22.6; HRMS (ESI): calc for $\text{C}_{39}\text{H}_{39}\text{N}_3\text{OS}$ ($\text{M}+\text{H}$) $^+$ 598.2892, found 598.2895.



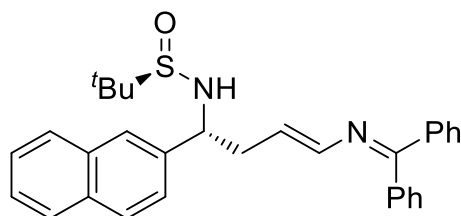
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-vinylphenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3p**): 123 mg, 53% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.59 (d, J = 8.0 Hz, 2H), 7.39 (m, 5H), 7.32 (m, 3H), 7.25 (m, 2H), 7.16 (t, J = 8.0 Hz, 1H), 7.00 (m, 1H), 6.74 (q, J = 8.0 Hz, 1H), 6.59 (d, J = 12.0 Hz, 1H), 5.98 (m, 1H), 5.77 (d, J = 16.0 Hz, 1H), 5.27 (d, J = 8.0 Hz, 1H), 4.46 (m, 1H), 3.50 (d, J = 4.0 Hz, 1H), 2.79 (m, 1H), 2.57 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 141.2, 140.8, 139.5, 137.1, 136.3, 136.0, 130.2, 128.8, 128.7, 128.3, 128.0, 127.5, 126.4, 114.1, 58.3, 55.8, 37.8, 22.6; HRMS (ESI): calc for $\text{C}_{29}\text{H}_{32}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 457.2314, found 457.2315.



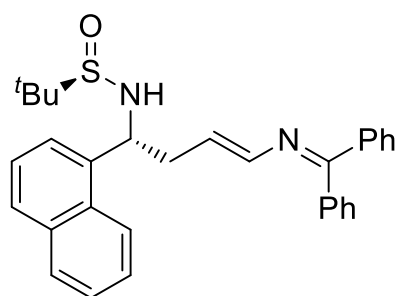
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(4-iodophenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3q**): 175 mg, 63% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.67 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 8.0 Hz, 2H), 7.44 (m, 3H), 7.33 (m, 3H), 7.04 (d, J = 8.0 Hz, 2H), 7.00 (m, 2H), 6.56 (d, J = 16.0 Hz, 1H), 5.94 (m, 1H), 4.42 (m, 1H), 3.46 (d, J = 4.0 Hz, 1H), 2.74 (m, 1H), 2.52 (m, 1H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4, 141.4, 141.1, 139.4, 137.7, 136.1, 130.3, 129.4, 128.82, 128.77, 128.6, 128.5, 128.1, 126.9, 93.3, 58.2, 56.0, 37.7, 22.6; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{29}\text{N}_2\text{OSI}$ ($\text{M}+\text{H}$) $^+$ 557.1124, found 557.1128.



Isopropyl 4-((*R,E*)-1-(((*R*)-tert-butylsulfinyl)amino)-4-((diphenylmethylene)amino)but-3-en-1-yl)benzoate (**3r**): 191 mg, 74% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 8.02 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 8.0 Hz, 2H), 7.39 (m, 6H), 7.29 (m, 2H), 6.98 (m, 2H), 6.58 (m, 1H), 5.95 (m, 1H), 5.27 (m, 1H), 4.53 (m, 1H), 3.54 (d, J = 4.0 Hz, 1H), 2.79 (m, 1H), 2.58 (m, 1H), 1.39 (d, J = 4.0 Hz, 3H), 1.37 (d, J = 2.0 Hz, 3H) 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 165.7, 146.5, 141.0, 139.3, 136.0, 130.4, 130.3, 129.9, 128.8, 128.7, 128.6, 128.3, 128.0, 127.2, 126.8, 68.4, 58.3, 56.0, 37.8, 22.6, 21.9; HRMS (ESI): calc for $\text{C}_{31}\text{H}_{36}\text{N}_2\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 517.2525, found 517.2529.

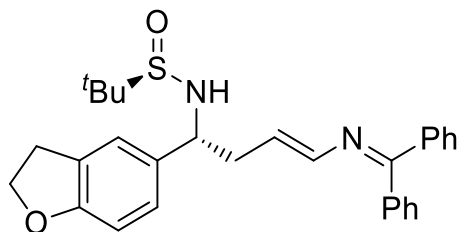


(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(naphthalen-2-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3s**): 209 mg, 87% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.84 (m, 3H), 7.75 (s, 1H), 7.56 (d, J = 4.0 Hz, 2H), 7.50 (q, J = 4.0 Hz, 2H), 7.43 (d, J = 12.0 Hz, 1H), 7.35 (t, J = 6.0 Hz, 2H), 7.28 (t, J = 8.0 Hz, 2H), 7.21 (t, J = 8.0 Hz, 2H), 6.87 (d, J = 8.0 Hz, 2H), 6.57 (d, J = 16.0 Hz, 1H), 6.02 (m, 1H), 4.65 (m, 1H), 3.58 (d, J = 4.0 Hz, 1H), 2.88 (m, 1H), 2.68 (m, 1H), 1.23 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 140.8, 139.5, 139.0, 136.0, 133.3, 133.1, 130.2, 128.8, 128.6, 128.5, 128.2, 128.1, 128.0, 127.6, 127.5, 126.4, 126.2, 126.1, 125.2, 58.7, 55.9, 37.7, 22.6; HRMS (ESI): calc for $\text{C}_{31}\text{H}_{32}\text{N}_2\text{O}_5$ ($\text{M}+\text{H}$) $^+$ 481.2314, found 481.2318.

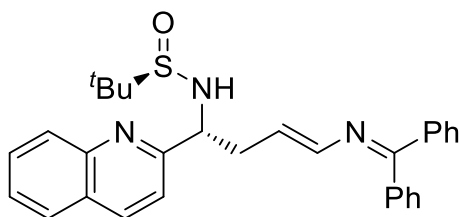


(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(naphthalen-1-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3t**): 185 mg, 77% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 8.15 (d, J = 8.0 Hz, 1H), 7.88 (d, J = 8.0 Hz, 1H), 7.81 (d, J = 8.0 Hz, 1H), 7.57 (m, 3H), 7.49 (m, 3H), 7.36 (m, 4H), 7.28 (t, J = 8.0 Hz, 2H), 6.98 (d, J = 8.0 Hz, 2H), 6.65 (d, J = 16.0 Hz, 1H), 6.04 (m, 1H), 5.32 (t, J = 8.0 Hz, 1H), 3.69 (d, J = 4.0 Hz, 1H), 2.90 (t, J = 8.0 Hz, 2H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.9, 140.7, 139.4, 136.5, 136.0, 133.9, 130.7, 130.1, 128.9, 128.7, 128.62, 128.58, 128.4, 128.3, 128.0, 127.7, 126.3, 125.6, 125.2, 124.8, 123.0, 55.8, 53.8, 36.7, 22.6; HRMS (ESI): calc for

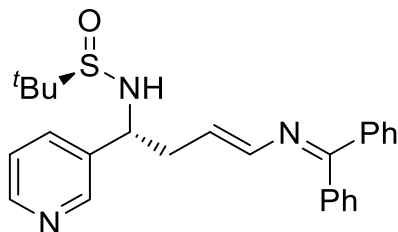
C₃₁H₃₂N₂O₂S (M+H)⁺ 481.2314, found 481.2318.



(*R*)-*N*-((*R,E*)-1-(2,3-Dihydrobenzofuran-5-yl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3u**): 161 mg, 68% yield; foam solid; *dr* 5/1; ¹H NMR (400 MHz, CDCl₃) δ 7.60 (d, *J* = 8.0 Hz, 2H), 7.43 (m, 3H), 7.34 (m, 3H), 7.13 (s, 1H), 7.04 (m, 3H), 6.74 (d, *J* = 8.0 Hz, 1H), 6.64 (d, *J* = 12.0 Hz, 1H), 5.98 (m, 1H), 4.57 (t, *J* = 8.0 Hz, 2H), 4.39 (m, 1H), 3.41 (d, *J* = 4.0 Hz, 1H), 3.18 (t, *J* = 8.0 Hz, 2H), 2.76 (m, 1H), 2.53 (m, 1H), 1.20 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 165.8, 159.7, 140.4, 139.4, 136.1, 133.7, 130.1, 128.7, 128.6, 128.3, 128.1, 128.0, 127.2, 127.0, 124.1, 109.2, 71.3, 58.4, 55.7, 37.9, 29.6, 22.6; HRMS (ESI): calc for C₂₉H₃₂N₂O₂S (M+H)⁺ 473.2263, found 473.2266.

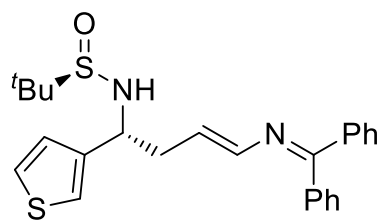


(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(quinolin-2-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3v**): 185 mg, 77% yield; foam solid; ¹H NMR (400 MHz, CDCl₃) δ 8.10 (d, *J* = 4.0 Hz, 1H), 8.02 (d, *J* = 8.0 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.69 (t, *J* = 4.0 Hz, 2H), 7.59 (d, *J* = 4.0 Hz, 2H), 7.52 (t, *J* = 4.0 Hz, 1H), 7.36 (m, 3H), 7.29 (t, *J* = 4.0 Hz, 4H), 6.95 (d, *J* = 4.0 Hz, 2H), 6.63 (d, *J* = 8.0 Hz, 1H), 6.11 (m, 1H), 5.52 (d, *J* = 2.0 Hz, 1H), 4.77 (q, *J* = 4.0 Hz, 1H), 2.75 (m, 2H), 1.30 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 165.8, 160.0, 147.1, 140.6, 139.4, 136.6, 136.1, 130.2, 129.5, 129.3, 128.7, 128.6, 128.5, 128.3, 128.0, 127.5, 127.4, 126.4, 119.9, 59.6, 56.1, 38.7, 22.9; HRMS (ESI): calc for C₃₀H₃₁N₃O₂S (M+H)⁺ 482.2266, found 482.2270.

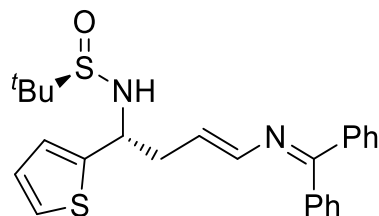


(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(pyridin-3-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3w**): 164 mg, 76% yield; foam solid; ¹H NMR (400 MHz, CDCl₃) δ 8.57 (s, 2H), 7.65 (d, *J* = 8.0 Hz, 1H), 7.61 (d, *J* = 8.0 Hz, 2H), 7.43 (m, 3H), 7.38 (t, *J* = 6.0 Hz, 1H), 7.30 (m, 3H), 7.04 (m, 2H), 6.64 (d, *J* = 12.0 Hz, 1H), 5.96 (m, 1H), 4.52 (m, 1H), 3.60 (d, *J* = 4.0 Hz, 1H), 2.80 (m, 1H), 2.62 (m, 1H), 1.21 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 166.6, 149.2, 148.9, 141.2, 139.3, 137.1, 136.0, 135.1, 130.3, 128.8, 128.6, 128.4, 128.1, 126.5, 123.5, 56.7, 56.1, 37.6, 22.5; HRMS (ESI):

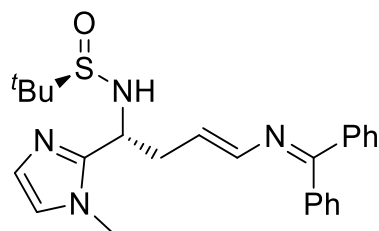
calc for C₂₆H₂₉N₃OS (M+H)⁺ 432.2110, found 432.2114.



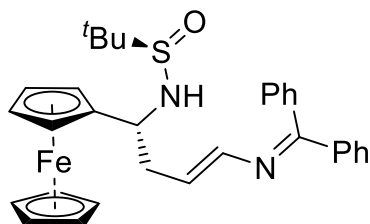
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(thiophen-3-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3x**): 146 mg, 67% yield; foam solid; ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.45 (d, *J* = 4.0 Hz, 3H), 7.37 (t, *J* = 8.0 Hz, 1H), 7.31 (m, 3H), 7.21 (s, 1H), 7.10 (t, *J* = 2.0 Hz, 2H), 7.07 (d, *J* = 4.0 Hz, 1H), 6.70 (d, *J* = 8.0 Hz, 1H), 6.04 (m, 1H), 4.59 (q, *J* = 4.0 Hz, 1H), 3.45 (d, *J* = 4.0 Hz, 1H), 2.73 (m, 1H), 2.61 (m, 1H), 1.20 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 166.0, 142.9, 140.6, 139.4, 136.1, 130.2, 128.74, 128.68, 128.65, 128.4, 128.1, 127.9, 126.5, 126.2, 122.3, 55.9, 54.9, 37.7, 22.6; HRMS (ESI): calc for C₂₅H₂₈N₂OS₂ (M+H)⁺ 437.1721, found 437.1722.



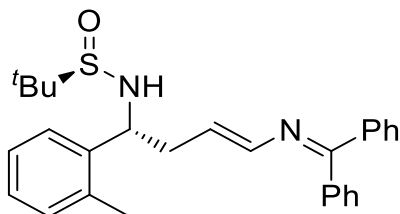
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(thiophen-2-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3y**): 177 mg, 81% yield; foam solid; ¹H NMR (400 MHz, CDCl₃) δ 7.62 (d, *J* = 8.0 Hz, 2H), 7.44 (t, *J* = 4.0 Hz, 3H), 7.35 (m, 3H), 7.25 (m, 1H), 7.10 (m, 2H), 7.04 (d, *J* = 4.0 Hz, 1H), 6.96 (q, *J* = 4.0 Hz, 1H), 6.73 (d, *J* = 16.0 Hz, 1H), 6.06 (m, 1H), 4.76 (m, 1H), 3.56 (d, *J* = 4.0 Hz, 1H), 2.82 (m, 1H), 2.61 (m, 1H), 1.21 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 166.2, 145.3, 140.8, 139.4, 136.0, 130.2, 128.8, 128.70, 128.66, 128.4, 128.0, 127.4, 126.7, 125.7, 125.0, 56.0, 54.8, 38.7, 22.6; HRMS (ESI): calc for C₂₅H₂₈N₂OS₂ (M+H)⁺ 437.1721, found 437.1722.



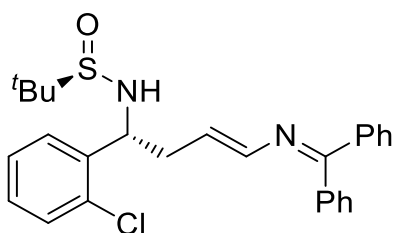
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(1-methyl-1H-imidazol-2-yl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3z**): 167mg, 77% yield; foam solid; ¹H NMR (400 MHz, CDCl₃) δ 7.63 (d, *J* = 8.0 Hz, 2H), 7.45 (m, 3H), 7.35 (m, 3H), 7.11 (q, *J* = 4.0 Hz, 2H), 6.95 (d, *J* = 2.0 Hz, 1H), 6.77 (d, *J* = 4.0 Hz, 1H), 6.73 (d, *J* = 16.0 Hz, 1H), 6.06 (m, 1H), 4.44 (q, *J* = 8.0 Hz, 1H), 4.12 (d, *J* = 4.0 Hz, 1H), 3.66 (s, 3H), 2.75 (m, 2H), 1.20 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 166.1, 147.4, 140.6, 139.3, 136.0, 130.2, 128.7, 128.6, 128.3, 128.0, 127.7, 127.4, 121.0, 56.1, 51.6, 37.9, 32.7, 22.7; HRMS (ESI): calc for C₂₅H₃₀N₄OS (M+H)⁺ 435.2219, found 435.2222.



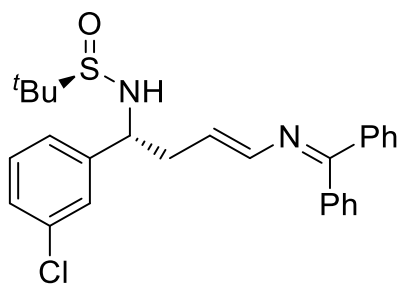
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-ferrocenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3aa**): 102 mg, 38% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, J = 8.0 Hz, 2H), 7.43 (m, 3H), 7.34 (m, 3H), 7.11 (m, 2H), 6.63 (d, J = 16.0 Hz, 1H), 6.10 (m, 1H), 4.28 (m, 1H), 4.20 (s, 5H), 4.17 (m, 4H), 3.96 (d, J = 4.0 Hz, 1H), 2.48 (m, 2H), 1.28 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.5, 140.2, 139.6, 136.2, 130.1, 128.8, 128.74, 128.72, 128.65, 128.3, 128.1, 91.2, 68.6, 68.1, 67.9, 67.8, 65.7, 55.6, 53.4, 37.8, 22.7; HRMS (ESI): calc for $\text{C}_{31}\text{H}_{34}\text{N}_2\text{OSFe}$ ($\text{M}+\text{H}$) $^+$ 539.1820, found 539.1821.



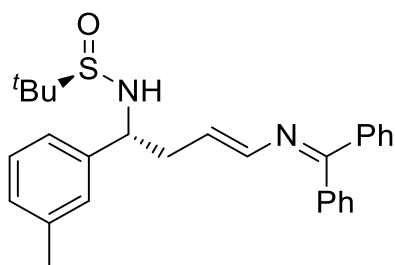
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(*o*-tolyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ab**): 176 mg, 79% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.41 (m, 3H), 7.32 (m, 4H), 7.18 (m, 3H), 7.03 (m, 2H), 6.64 (d, J = 12.0 Hz, 1H), 5.99 (m, 1H), 4.74 (m, 1H), 3.40 (d, J = 2.0 Hz, 1H), 2.74 (m, 1H), 2.62 (m, 1H), 2.35 (s, 3H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.9, 140.6, 139.5, 136.1, 135.8, 130.7, 130.2, 128.8, 128.70, 128.66, 128.4, 128.0, 127.7, 127.5, 126.3, 55.7, 53.8, 37.1, 22.6, 19.5. These data are in accordance with the literature.⁵



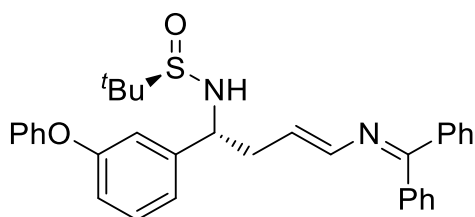
(*R*)-*N*-((*R,E*)-1-(2-Chlorophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ac**): 205 mg, 88% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 8.0 Hz, 2H), 7.37 (m, 8H), 7.23 (m, 2H), 7.06 (m, 2H), 6.68 (d, J = 12.0 Hz, 1H), 6.01 (m, 1H), 4.95 (dd, J = 12.0 Hz, J = 8.0 Hz, 1H), 3.73 (d, J = 4.0 Hz, 1H), 2.68 (t, J = 10.0 Hz, 2H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.2, 141.0, 139.4, 139.0, 136.1, 132.9, 130.2, 129.8, 128.8, 128.7, 128.6, 128.5, 128.4, 128.1, 127.1, 126.9, 56.2, 55.5, 36.7, 22.5; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{29}\text{N}_2\text{OSCl}$ ($\text{M}+\text{H}$) $^+$ 465.1767, found 465.1772.



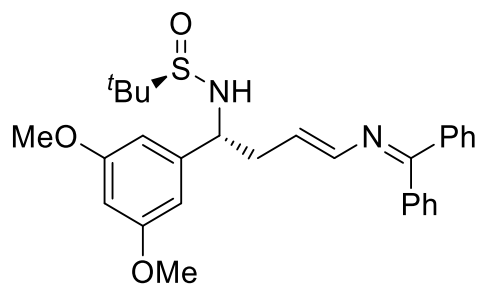
(*R*)-*N*-((*R,E*)-1-(3-chlorophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ad**): 198mg, 85% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.43 (m, 3H), 7.37 (t, J = 6.0 Hz, 1H), 7.30 (m, 5H), 7.19 (m, 1H), 7.04 (m, 2H), 6.63 (d, J = 12.0 Hz, 1H), 5.96 (m, 1H), 4.44 (m, 1H), 3.52 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.55 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 143.7, 140.9, 139.3, 136.0, 134.4, 130.2, 129.9, 128.74, 128.70, 128.6, 128.4, 128.02, 127.96, 127.2, 126.9, 125.7, 58.2, 55.9, 37.7, 22.5; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{29}\text{N}_2\text{OSCl}$ ($\text{M}+\text{H}$) $^+$ 465.1767, found 465.1770.



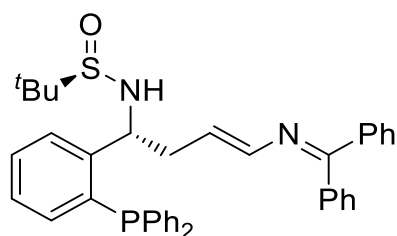
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(*m*-tolyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ae**): 178 mg, 80% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.60 (d, J = 8.0 Hz, 2H), 7.42 (m, 3H), 7.36 (t, J = 8.0 Hz, 1H), 7.30 (t, J = 8.0 Hz, 2H), 7.23 (t, J = 8.0 Hz, 1H), 7.11 (m, 3H), 7.04 (m, 2H), 6.64 (d, J = 12.0 Hz, 1H), 5.98 (m, 1H), 4.43 (m, 1H), 3.46 (d, J = 4.0 Hz, 1H), 2.77 (m, 1H), 2.57 (m, 1H), 2.35 (s, 3H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.9, 141.5, 140.5, 139.5, 138.2, 136.1, 130.2, 128.72, 128.67, 128.64, 128.55, 128.50, 128.3, 128.02, 128.00, 127.9, 124.3, 58.6, 55.8, 37.8, 22.6, 21.5; HRMS (ESI): calc for $\text{C}_{28}\text{H}_{32}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 445.2314, found 445.2318.



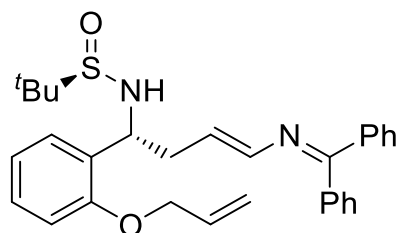
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(3-phenoxyphenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3af**): 196 mg, 75% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 12.0 Hz, 2H), 7.42 (m, 3H), 7.33 (m, 6H), 7.07 (m, 4H), 6.96 (m, 4H), 6.64 (d, J = 16.0 Hz, 1H), 5.97 (m, 1H), 4.44 (m, 1H), 3.52 (d, J = 4.0 Hz, 1H), 2.75 (m, 1H), 2.53 (m, 1H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 157.4, 156.8, 143.7, 140.7, 139.4, 136.0, 130.2, 129.9, 129.7, 128.73, 128.68, 128.62, 128.4, 128.0, 127.4, 123.3, 122.1, 118.9, 117.9, 117.4, 58.2, 55.9, 37.8, 22.5; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{34}\text{N}_2\text{O}_2\text{S}$ ($\text{M}+\text{H}$) $^+$ 523.2419, found 523.2421.



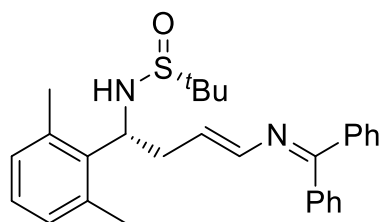
(*R*)-*N*-((*R,E*)-1-(3,5-Dimethoxyphenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ag**): 211 mg, 86% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.44 (m, 3H), 7.34 (m, 3H), 7.07 (m, 2H), 6.67 (d, J = 16.0 Hz, 1H), 6.48 (d, J = 4.0 Hz, 2H), 6.40 (t, J = 2.0 Hz, 1H), 6.00 (m, 1H), 4.39 (m, 1H), 3.77 (s, 6H), 3.49 (d, J = 4.0 Hz, 1H), 2.76 (m, 1H), 2.56 (m, 1H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.9, 160.8, 144.0, 140.5, 139.4, 136.0, 130.2, 128.71, 128.65, 128.3, 128.0, 127.7, 105.3, 99.6, 58.7, 55.8, 55.3, 37.7, 22.6; HRMS (ESI): calc for $\text{C}_{29}\text{H}_{34}\text{N}_2\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 491.2368, found 491.2371.



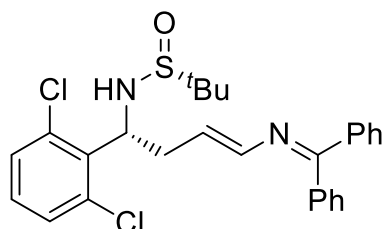
(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-1-(2-(diphenylphosphaneyl)phenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ah**): 163 mg, 53% yield; foam solid; $dr \sim 3/1$; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (m, 2H), 7.39 (m, 11H), 7.18 (m, 8H), 6.99 (m, 3H), 6.47 (d, J = 12.0 Hz, 1H), 5.96 (m, 1H), 5.39 (br, 1H), 3.76 (br, 1H), 2.57 (m, 1H), 2.38 (m, 1H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 146.6 (d, $J_{\text{P-C}}$ = 23.2 Hz), 140.8, 139.5, 136.6 (d, $J_{\text{P-C}}$ = 10.1 Hz), 136.3 (d, $J_{\text{P-C}}$ = 10.1 Hz), 136.1, 135.2 (d, $J_{\text{P-C}}$ = 14.1 Hz), 134.5, 134.0, 133.8, 133.6, 130.2, 129.3, 128.8 (d, $J_{\text{P-C}}$ = 1.0 Hz), 128.70, 128.67, 128.60, 128.5 (d, $J_{\text{P-C}}$ = 7.1 Hz), 128.4, 128.0, 127.7 (d, $J_{\text{P-C}}$ = 13.1 Hz), 127.4, 56.0, 55.7, 37.8, 22.5; HRMS (ESI): calc for $\text{C}_{39}\text{H}_{39}\text{N}_2\text{OSP}$ ($\text{M}+\text{H}$) $^+$ 615.2599, found 615.2598.



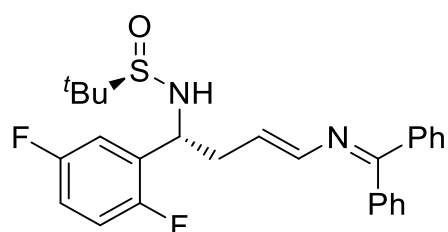
(*R*)-*N*-((*R,E*)-1-(2-(Allyloxy)phenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3al**): 215 mg, 88% yield; foam solid; dr 7/1; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.41 (m, 3H), 7.33 (m, 3H), 7.21 (m, 2H), 7.05 (m, 2H), 6.92 (t, J = 8.0 Hz, 1H), 6.84 (d, J = 8.0 Hz, 1H), 6.64 (d, J = 12 Hz, 1H), 6.04 (m, 2H), 5.38 (m, 1H), 5.23 (m, 1H), 4.63 (q, J = 8.0 Hz, 1H), 4.53 (d, J = 4.0 Hz, 2H), 4.11 (d, J = 8.0 Hz, 1H), 2.67 (m, 2H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.4, 155.6, 140.1, 139.5, 136.2, 133.0, 130.3, 130.1, 129.0, 128.7, 128.5, 128.4, 128.3, 128.2, 128.0, 120.9, 117.4, 112.0, 68.6, 57.0, 55.8, 37.3, 22.6; HRMS (ESI): calc for $\text{C}_{30}\text{H}_{34}\text{N}_2\text{O}_2\text{S}$ ($\text{M}+\text{H}$) $^+$ 487.2419, found 487.2421.



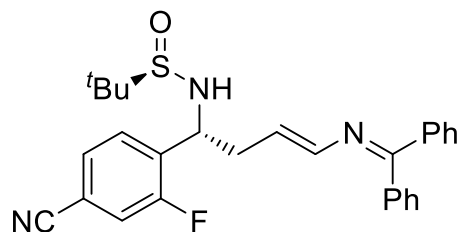
(*R*)-*N*-((*R,E*)-1-(2,6-Dimethylphenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3aj**): 128 mg, 56% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.59 (d, J = 8.0 Hz, 2H), 7.43 (m, 3H), 7.36 (m, 1H), 7.30 (t, J = 8.0 Hz, 2H), 7.09 (t, J = 6.0 Hz, 1H), 7.02 (m, 4H), 6.67 (d, J = 12.0 Hz, 1H), 5.95 (m, 1H), 4.97 (m, 1H), 3.88 (d, J = 4.0 Hz, 1H), 2.79 (m, 2H), 2.46 (s, 3H), 2.37 (s, 3H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.9, 140.0, 139.5, 137.0, 136.4, 136.1, 130.6, 130.1, 128.8, 128.7, 128.4, 128.3, 128.0, 127.5, 55.6, 54.1, 35.3, 22.6, 21.4; HRMS (ESI): calc for $\text{C}_{29}\text{H}_{34}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 459.2470, found 459.2475.



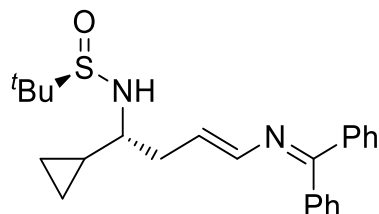
(*R*)-*N*-((*R,E*)-1-(2,6-Dichlorophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ak**): 152 mg, 61% yield; foam solid; *dr* 4/1; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 8.0 Hz, 2H), 7.43 (m, 3H), 7.35 (m, 4H), 7.25 (d, J = 8.0 Hz, 1H), 7.13 (d, J = 8.0 Hz, 1H), 7.09 (m, 2H), 6.73 (d, J = 12.0 Hz, 1H), 6.08 (m, 1H), 5.28 (m, 1H), 4.75 (d, J = 12.0 Hz, 1H), 2.80 (m, 2H), 1.21 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 140.3, 139.4, 136.8, 136.1, 135.1, 133.6, 130.2, 129.9, 129.0, 128.8, 128.7, 128.3, 128.0, 127.7, 60.3, 57.9, 35.7, 22.5; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{28}\text{N}_2\text{OSCl}_2$ ($\text{M}+\text{H}$) $^+$ 499.1378, found 499.1379.



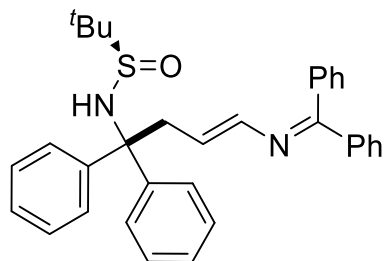
(*R*)-*N*-((*R,E*)-1-(2,5-Difluorophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3al**): 184 mg, 79% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 8.0 Hz, 2H), 7.44 (m, 3H), 7.35 (m, 3H), 7.01 (m, 5H), 6.67 (d, J = 12.0 Hz, 1H), 5.98 (m, 1H), 4.68 (q, J = 8.0 Hz, 1H), 3.66 (d, J = 8.0 Hz, 1H), 2.72 (m, 1H), 2.58 (m, 1H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 159.6 (d, $J_{\text{F-C}}$ = 244.4 Hz), 156.1 (dd, $J_{\text{F-C}}$ = 2.0 Hz, $J_{\text{F-C}}$ = 244.4 Hz), 141.1, 139.3, 136.0, 130.8 (dd, $J_{\text{F-C}}$ = 7.1 Hz, $J_{\text{F-C}}$ = 15.2 Hz), 130.3, 128.8 (d, $J_{\text{F-C}}$ = 2.0 Hz), 128.6, 128.460, 128.1, 126.7, 116.8 (dd, $J_{\text{F-C}}$ = 9.1 Hz, $J_{\text{F-C}}$ = 25.3 Hz), 115.5 (dd, $J_{\text{F-C}}$ = 9.1 Hz, $J_{\text{F-C}}$ = 24.2 Hz), 115.1 (dd, $J_{\text{F-C}}$ = 5.1 Hz, $J_{\text{F-C}}$ = 25.3 Hz), 56.2, 53.7, 37.2, 22.5; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{28}\text{N}_2\text{OSF}_2$ ($\text{M}+\text{H}$) $^+$ 467.1969, found 467.1973.



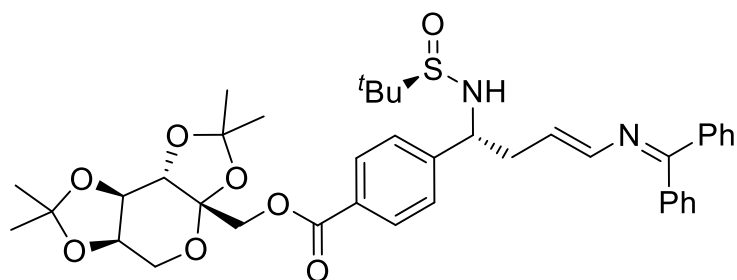
(*R*)-*N*-((*R,E*)-1-(4-Cyano-2-fluorophenyl)-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3am**): 147 mg, 62% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, $J = 8.0$ Hz, 2H), 7.46 (m, 5H), 7.38 (d, $J = 8.0$ Hz, 1H), 7.32 (m, 3H), 7.06 (m, 2H), 6.64 (d, $J = 12.0$ Hz, 1H), 5.95 (m, 1H), 4.72 (q, $J = 8.0$ Hz, 1H), 3.76 (d, $J = 8.0$ Hz, 1H), 2.66 (m, 2H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.9, 159.6 (d, $J_{\text{F-C}} = 251.5$ Hz), 141.4, 139.2, 136.0, 135.2 (d, $J_{\text{F-C}} = 13.1$ Hz), 130.5, 129.9, 128.9, 128.8, 128.5, 128.3, 128.1, 125.9, 119.4 (d, $J_{\text{F-C}} = 26.3$ Hz), 117.3, 112.8 (d, $J_{\text{F-C}} = 9.1$ Hz), 56.5, 54.4, 37.1, 22.5. HRMS (ESI): calc for $\text{C}_{28}\text{H}_{28}\text{N}_3\text{OSF}$ ($\text{M}+\text{H}$) $^+$ 474.2015, found 474.2018



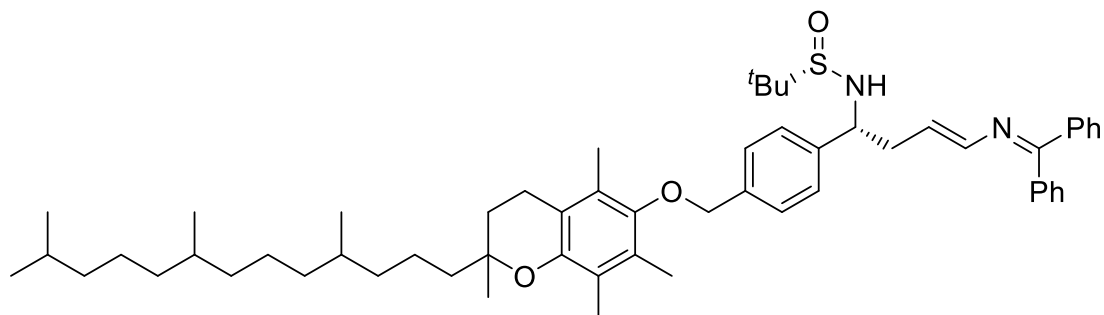
(*R*)-*N*-((*R,E*)-1-Cyclopropyl-4-((diphenylmethylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3an**): 89 mg, 45% yield; foam solid; *dr* 6/1; ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, $J = 8.0$ Hz, 2H), 7.47 (m, 3H), 7.33 (m, 3H), 7.19 (m, 2H), 6.79 (d, $J = 12.0$ Hz, 1H), 6.25 (m, 1H), 3.23 (d, $J = 4.0$ Hz, 1H), 2.51 (m, 1H), 2.42 (m, 2H), 1.19 (s, 9H), 0.91 (m, 1H), 0.59 (dd, $J = 16.0$ Hz, $J = 4.0$ Hz, 2H), 0.36 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.6, 140.2, 139.5, 136.3, 130.2, 128.9, 128.71, 128.67, 128.61, 128.4, 128.1, 61.0, 55.5, 36.8, 22.6, 16.8, 4.7, 4.3; HRMS (ESI): calc for $\text{C}_{24}\text{H}_{30}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 395.2157, found 395.2161.



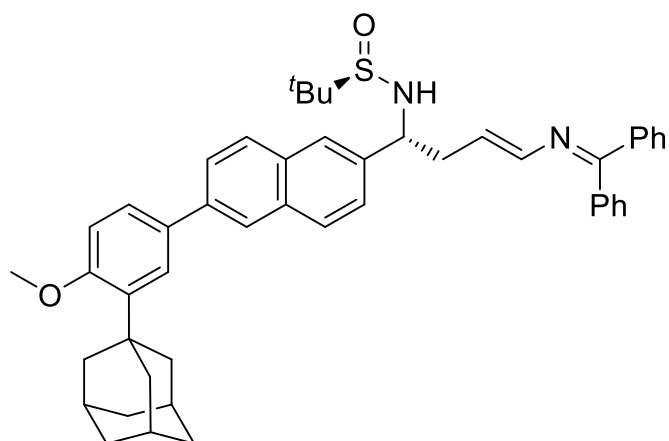
(*R,E*)-*N*-(4-((Diphenylmethylene)amino)-1,1-diphenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ao**): 106 mg, 42% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.58 (d, $J = 8.0$ Hz, 2H), 7.42 (m, 3H), 7.36 (t, $J = 6.0$ Hz, 3H), 7.27 (m, 10H), 7.06 (q, $J = 4.0$ Hz, 2H), 6.83 (d, $J = 12.0$ Hz, 1H), 5.86 (m, 1H), 4.19 (s, 1H), 3.44 (m, 1H), 3.30 (m, 1H), 1.19 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 145.5, 143.8, 142.9, 139.6, 135.9, 130.2, 128.9, 128.82, 128.79, 128.5, 128.3, 128.2, 128.04, 128.00, 127.3, 126.89, 126.85, 66.4, 56.3, 42.5, 22.9; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{34}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 507.2470, found 507.2473.



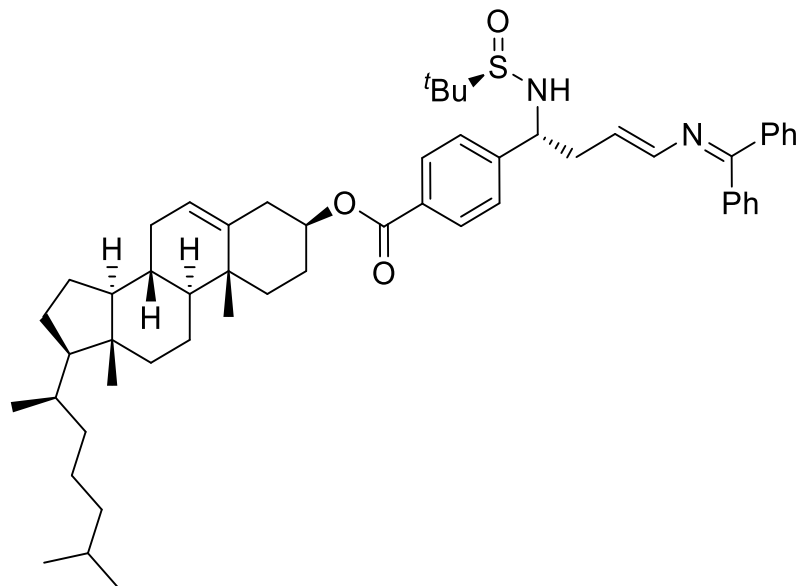
((3a*S*,5a*R*,8a*R*,8b*S*)-2,2,7,7-Tetramethyltetrahydro-3a*H*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-3a-yl)methyl 4-((*R,E*)-1-(((*R*)-tert-butylsulfinyl)amino)-4-((diphenylmethylene)amino)but-3-en-1-yl)benzoate (**3ap**): 247 mg, 69% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 8.06 (d, J = 8.0 Hz, 2H), 7.59 (d, J = 8.0 Hz, 2H), 7.39 (m, 6H), 7.32 (m, 2H), 7.00 (m, 2H), 6.60 (d, J = 12.0 Hz, 1H), 5.94 (m, 1H), 4.66 (m, 2H), 4.54 (m, 1H), 4.46 (d, J = 4.0 Hz, 1H), 4.36 (d, J = 12.0 Hz, 1H), 4.26 (d, J = 8.0 Hz, 1H), 3.97 (d, J = 12.0 Hz, 1H), 3.81 (d, J = 12.0 Hz, 1H), 3.53 (d, J = 4.0 Hz, 1H), 2.79 (m, 1H), 2.59 (m, 1H), 1.55 (s, 3H), 1.47 (s, 3H), 1.38 (s, 3H), 1.35 (s, 3H), 1.22 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4, 165.6, 147.0, 141.0, 139.3, 136.0, 130.3, 130.1, 129.3, 128.8, 128.6, 128.4, 128.1, 127.4, 126.8, 109.1, 108.8, 101.6, 70.8, 70.5, 70.0, 65.4, 61.3, 58.3, 56.0, 37.8, 26.5, 25.9, 25.6, 24.0, 22.6; HRMS (ESI): calc for $\text{C}_{40}\text{H}_{48}\text{N}_2\text{O}_8\text{S}$ ($\text{M}+\text{H}$) $^+$ 717.3210, found 717.3214.



(*S*)-*N*-((1*R,E*)-4-((Diphenylmethylene)amino)-1-(4-(((2,5,7,8-tetramethyl-2-(4,8,12-trimethyltridecyl)chroman-6-yl)oxy)methyl)phenyl)but-3-en-1-yl)-2-methylpropane-2-sulfinamide (**3aq**): 136 mg, 52% yield (0.3 mmol); foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.61 (d, J = 8.0 Hz, 2H), 7.49 (d, J = 8.0 Hz, 2H), 7.43 (m, 3H), 7.33 (m, 5H), 7.04 (m, 2H), 6.66 (d, J = 12.0 Hz, 1H), 6.00 (m, 1H), 4.70 (s, 2H), 4.51 (m, 1H), 3.50 (d, J = 4.0 Hz, 1H), 2.80 (m, 1H), 2.60 (m, 3H), 2.23 (s, 3H), 2.18 (s, 3H), 2.11 (s, 3H), 1.80 (m, 2H), 1.56 (m, 3H), 1.40 (m, 10H), 1.22 (s, 9H), 1.09 (m, 8H), 0.86 (t, J = 6.0 Hz, 15H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 148.0, 147.9, 141.1, 140.7, 139.5, 137.7, 136.1, 130.2, 128.8, 128.7, 128.4, 128.0, 127.90, 127.85, 127.7, 127.5, 125.9, 122.9, 117.6, 74.8, 74.3, 58.3, 55.8, 40.0, 39.3, 37.8, 37.43, 37.41, 37.38, 37.2, 32.8, 32.7, 31.3, 27.9, 24.8, 24.4, 23.9, 22.7, 22.61, 22.60, 21.0, 20.6, 19.7, 19.6, 12.9, 12.0, 11.8; HRMS (ESI): calc for $\text{C}_{57}\text{H}_{80}\text{N}_2\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 873.5968, found 873.5962.

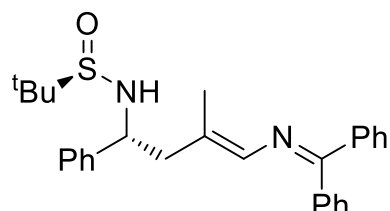


(*R*)-*N*-((*R,E*)-1-(6-(3-((3*R*,5*R*,7*R*)-Adamantan-1-yl)-4-methoxyphenyl)naphthalen-2-yl)-4-((diphenyl-methylene)amino)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ar**): 180 mg, 50% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 8.0 (s, 1H), 7.86 (d, J = 8.0 Hz, 2H), 7.76 (d, J = 4.0 Hz, 2H), 7.57 (m, 4H), 7.43 (d, J = 8.0 Hz, 1H), 7.34 (t, J = 6.0 Hz, 2H), 7.28 (t, J = 6.0 Hz, 2H), 7.23 (m, 2H), 6.99 (d, J = 12.0 Hz, 1H), 6.89 (d, J = 8.0 Hz, 2H), 6.59 (d, J = 12.0 Hz, 1H), 6.04 (m, 1H), 4.65 (m, 1H), 3.89 (s, 3H), 3.60 (d, J = 4.0 Hz, 1H), 2.89 (m, 1H), 2.69 (m, 1H), 2.19 (s, 6H), 2.10 (s, 3H), 1.80 (s, 6H), 1.23 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 158.6, 140.8, 139.4, 139.2, 138.8, 138.6, 135.9, 133.4, 133.0, 132.0, 130.2, 128.7, 128.6, 128.4, 128.2, 128.0, 127.6, 126.8, 126.2, 126.0, 125.8, 125.54, 125.46, 124.7, 112.1, 58.6, 55.9, 55.1, 40.6, 37.7, 37.13, 37.08, 29.1, 22.6; HRMS (ESI): calc for $\text{C}_{48}\text{H}_{52}\text{N}_2\text{O}_2\text{S}$ ($\text{M}+\text{H}$) $^+$ 721.3828, found 721.3829.

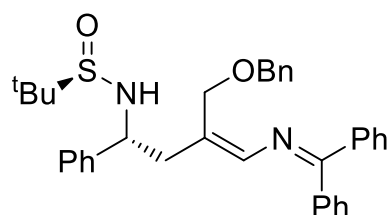


(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[*a*]phenanthren-3-yl 4-((*R,E*)-1-(((*R*)-tert-butylsulfinyl)amino)-4-((diphenylmethylene)amino)but-3-en-1-yl)benzoate (**3as**): 177 mg, 70% yield (0.3 mmol); foam solid; ^1H NMR (400 MHz, CDCl_3) δ 8.02 (d, J = 8.0 Hz, 2H), 7.60 (d, J = 4.0 Hz, 2H), 7.39 (m, 6H), 7.31 (t, J = 8.0 Hz, 2H), 6.97 (d, J = 8.0 Hz, 2H), 6.57 (d, J = 12.0 Hz, 1H), 5.95 (m, 1H), 5.43 (d, J = 8.0 Hz, 1H), 4.88 (m, 1H), 4.53 (m, 1H), 3.54 (d, J = 4.0 Hz, 1H), 2.79 (m, 1H), 2.57 (m, 1H), 2.48 (d, J = 8.0 Hz, 2H), 1.97 (m, 4H), 1.78 (m, 2H), 1.58 (m, 2H), 1.51 (m, 4H), 1.36

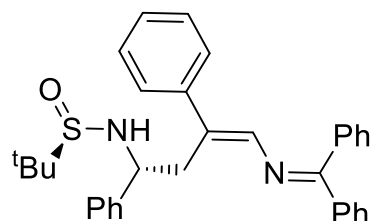
(m, 5H), 1.21 (s, 9H), 1.12 (m, 4H), 1.07 (s, 3H), 1.01 (m, 4H), 0.93 (m, 4H), 0.88 (d, $J = 4.0$ Hz, 3H), 0.86 (d, $J = 2.0$ Hz, 3H), 0.69 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 165.6, 146.5, 141.0, 139.5, 139.3, 136.0, 130.3, 129.9, 128.8, 128.7, 128.6, 128.3, 128.0, 127.3, 126.8, 122.8, 74.6, 58.3, 56.6, 56.1, 56.0, 50.0, 42.3, 39.7, 39.5, 38.2, 37.8, 37.0, 36.6, 36.1, 35.7, 31.9, 31.8, 28.2, 28.0, 27.8, 24.2, 23.8, 22.8, 22.6, 22.5, 21.0, 19.3, 18.7, 11.8; HRMS (ESI): calc for $\text{C}_{55}\text{H}_{74}\text{N}_2\text{O}_3\text{S}$ ($\text{M}+\text{H}$) $^+$ 843.5498, found 843.5496.



(*R*)-*N*-((*R,E*)-4-((Diphenylmethylene)amino)-3-methyl-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3at**): 160 mg, 72% yield; foam solid; $E/Z = 9/1$; ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, $J = 8.0$ Hz, 2H), 7.42 (m, 3H), 7.28 (m, 8H), 6.93 (m, 2H), 6.35 (s, 1H), 4.55 (dd, $J = 4.0$ Hz, $J = 12.0$ Hz, 1H), 3.43 (d, $J = 4.0$ Hz, 1H), 2.74 (dd, $J = 4.0$ Hz, $J = 12.0$ Hz, 1H), 2.42 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 2.12 (s, 3H), 1.17 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 162.9, 142.0, 139.8, 136.1, 135.6, 135.0, 129.8, 128.62, 128.55, 128.32, 128.26, 127.9, 127.7, 127.1, 57.5, 55.8, 45.2, 22.5, 16.4; HRMS (ESI): calc for $\text{C}_{28}\text{H}_{32}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 445.2314, found 445.2318.

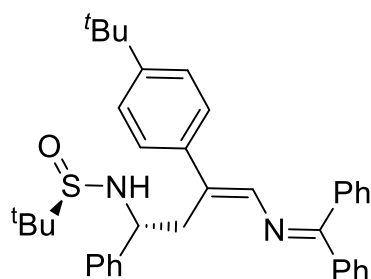


(*R*)-*N*-((*R,Z*)-3-((Benzyloxy)methyl)-4-((diphenylmethylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3au**): 168 mg, 61% yield; foam solid; ^1H NMR (400 MHz, CDCl_3) δ 7.58 (d, $J = 4.0$ Hz, 2H), 7.42 (m, 4H), 7.37 (m, 3H), 7.28 (m, 7H), 7.21 (d, $J = 4.0$ Hz, 2H), 6.93 (d, $J = 8.0$ Hz, 2H), 6.49 (s, 1H), 4.62 (s, 2H), 4.59 (q, $J = 4.0$ Hz, 1H), 4.56 (s, 2H), 3.64 (d, $J = 4.0$ Hz, 1H), 2.87 (q, $J = 4.0$ Hz, 1H), 2.58 (q, $J = 4.0$ Hz, 1H), 1.15 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 164.7, 142.2, 139.5, 138.6, 138.0, 135.7, 134.2, 130.2, 128.8, 128.63, 128.61, 128.5, 128.34, 128.29, 128.0, 127.9, 127.6, 127.5, 127.2, 72.1, 66.4, 58.1, 55.8, 40.8, 22.5; HRMS (ESI): calc for $\text{C}_{35}\text{H}_{38}\text{N}_2\text{O}_2\text{S}$ ($\text{M}+\text{H}$) $^+$ 551.2732, found 551.2736.

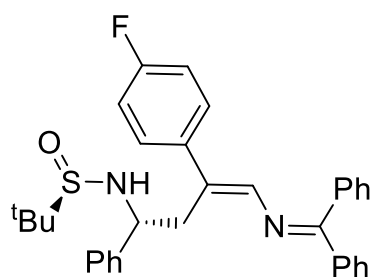


(*R*)-*N*-((*R*)-4-((Diphenylmethylene)amino)-1,3-diphenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3av**): *E* isomer 102 mg, 40%; *Z* isomer 106 mg, 42% yield; foam solid; *E* isomer ^1H NMR

(400 MHz, CDCl₃) δ 7.74 (q, J = 4.0 Hz, 2H), 7.42 (m, 6H), 7.34 (d, J = 8.0 Hz, 2H), 7.25 (m, 7H), 7.19 (t, J = 8.0 Hz, 1H), 7.05 (m, 2H), 7.02 (s, 1H), 4.53 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 4.06 (d, J = 4.0 Hz, 1H), 3.77 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 3.52 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 1.13 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 165.9, 142.9, 140.0, 139.5, 137.1, 136.8, 136.1, 130.3, 128.9, 128.8, 128.7, 128.5, 128.4, 128.24, 128.16, 127.51, 127.48, 127.3, 126.5, 58.6, 56.0, 37.3, 22.5; *Z* isomer dr = 5/1; ¹H NMR (400 MHz, CDCl₃) δ 7.56 (q, J = 8.0 Hz, 3H), 7.43 (m, 5H), 7.29 (m, 9H), 7.12 (m, 2H), 6.90 (d, J = 8.0 Hz, 1H), 6.51 (s, 1H), 4.35 (t, J = 8.0 Hz, 1H), 3.43 (d, J = 4.0 Hz, 1H), 3.31 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 2.71 (dd, J = 8.0 Hz, J = 16.0 Hz, 1H), 1.15 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 165.1, 141.9, 139.4, 137.6, 136.2, 135.8, 135.0, 130.0, 129.0, 128.6, 128.5, 128.3, 128.0, 127.7, 127.6, 127.4, 127.2, 58.2, 55.8, 44.0, 22.5; HRMS (ESI): calc for C₃₃H₃₄N₂OS (M+H)⁺ 507.2470, found 507.2473.

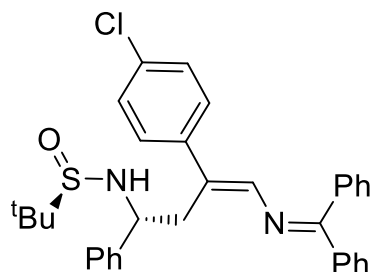


(*R*)-*N*-((*R,E*)-3-(4-(*tert*-Butyl)phenyl)-4-((diphenylmethylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3aw**): 132 mg, 47% yield; foam solid; ¹H NMR (400 MHz, CDCl₃) δ 7.72 (d, J = 8.0 Hz, 2H), 7.40 (m, 8H), 7.30 (d, J = 8.0 Hz, 2H), 7.22 (m, 5H), 7.04 (m, 3H), 4.55 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 4.07 (d, J = 8.0 Hz, 1H), 3.75 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 3.51 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 1.30 (s, 9H), 1.12 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 165.3, 150.6, 143.0, 139.6, 137.03, 137.00, 136.3, 136.2, 130.2, 128.8, 128.7, 128.4, 128.2, 128.1, 127.4, 127.3, 126.1, 125.5, 58.8, 56.0, 37.3, 34.5, 31.2, 22.5; HRMS (ESI): calc for C₃₇H₄₂N₂OS (M+H)⁺ 563.3096, found 563.3096.

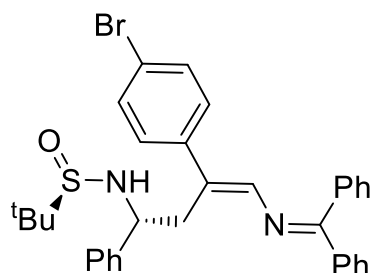


(*R*)-*N*-((*R*)-4-((Diphenylmethylene)amino)-3-(4-fluorophenyl)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ax**): *E* isomer 100 mg, 38% yield; *Z* isomer 98 mg, 37% yield; foam solid; *E* isomer ¹H NMR (400 MHz, CDCl₃) δ 7.73 (d, J = 8.0 Hz, 2H), 7.42 (m, 6H), 7.31 (d, J = 8.0 Hz, 3H), 7.20 (m, 4H), 7.04 (m, 2H), 6.96 (m, 3H), 4.52 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 4.04 (d, J = 4.0 Hz, 1H), 3.73 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 3.50 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 1.14 (s, 9H); ¹³C NMR (101 MHz, CDCl₃) δ 166.0, 162.2 (d, J_{F-C} = 249.5 Hz), 142.7, 139.5, 136.7, 136.2, 136.0 (d, J_{F-C} = 7.1 Hz), 130.4, 128.9, 128.8, 128.7, 128.4, 128.3, 128.2, 128.1 (d, J_{F-C} = 8.1 Hz), 127.6, 127.3, 115.4 (d, J_{F-C} = 22.2 Hz), 58.2, 56.0, 37.4, 22.6; *Z* isomer dr = 6/1; ¹H NMR (400 MHz, CDCl₃) δ 7.53 (m, 4H), 7.41 (m, 3H), 7.27 (m, 7H), 7.10 (m, 3H), 6.89 (dd, J = 2.0 Hz, J = 8.0 Hz, 2H), 6.50 (s, 1H),

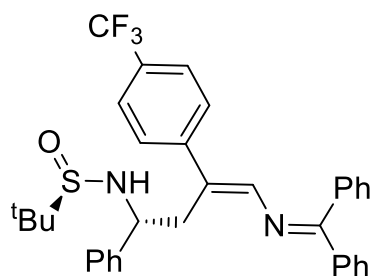
4.33 (m, 1H), 3.41 (d, $J = 4.0$ Hz, 1H), 3.31 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 2.68 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 1.16 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.4, 162.1 (d, $J_{\text{F-C}} = 247.5$ Hz), 141.8, 139.3, 136.2, 135.7, 133.9, 133.6 (d, $J_{\text{F-C}} = 3.0$ Hz), 131.6 (d, $J_{\text{F-C}} = 8.1$ Hz), 130.1, 128.9, 128.6, 128.5, 128.4, 128.0, 127.7, 127.6, 127.2, 114.6 (d, $J_{\text{F-C}} = 21.2$ Hz), 57.9, 55.8, 43.8, 22.5; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{33}\text{FN}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 525.2376, found 525.2379.



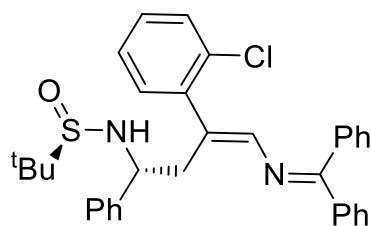
(*R*)-*N*-((*R*)-3-(4-Chlorophenyl)-4-((diphenylmethylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ay**): 192 mg, 71% yield; foam solid; $dr = 6/1$ ^1H NMR (400 MHz, CDCl_3) δ 7.53 (d, $J = 8.0$ Hz, 2H), 7.50 (d, $J = 4.0$ Hz, 2H), 7.39 (m, 5H), 7.28 (m, 6H), 7.09 (s, 2H), 6.89 (d, $J = 4.0$ Hz, 2H), 6.51 (s, 1H), 4.32 (t, $J = 4.0$ Hz, 1H), 3.41 (s, 1H), 3.31 (dd, $J = 4.0$ Hz, $J = 12.0$ Hz, 1H), 2.67 (q, $J = 4.0$ Hz, 1H), 1.16 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.7, 141.7, 139.3, 136.6, 136.1, 135.7, 133.6, 133.1, 131.3, 130.2, 129.0, 128.6, 128.5, 128.4, 128.1, 127.9, 127.8, 127.6, 127.2, 57.9, 55.8, 43.6, 22.5; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{33}\text{ClN}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 541.2080, found 541.2082.



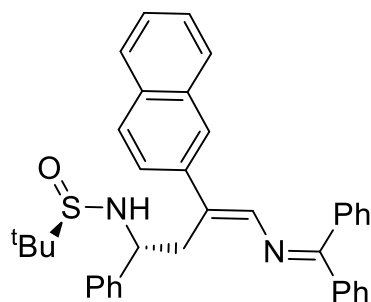
(*R*)-*N*-((*R*)-3-(4-Bromophenyl)-4-((diphenylmethylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3az**): *E* isomer 100 mg, 34% yield; *Z* isomer 99 mg, 34% yield; foam solid; *E* isomer ^1H NMR (400 MHz, CDCl_3) δ 7.73 (d, $J = 8.0$ Hz, 2H), 7.41 (m, 8H), 7.31 (m, 2H), 7.21 (m, 3H), 7.09 (d, $J = 8.0$ Hz, 2H), 7.03 (m, 2H), 6.97 (s, 1H), 4.52 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 4.02 (d, $J = 4.0$ Hz, 1H), 3.71 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 3.50 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 142.6, 139.4, 139.1, 137.1, 136.0, 135.8, 131.6, 130.5, 129.0, 128.9, 128.7, 128.4, 128.3, 128.2, 128.0, 127.6, 127.3, 121.4, 58.1, 56.0, 37.1, 22.6; *Z* isomer $dr = 6/1$; ^1H NMR (400 MHz, CDCl_3) δ 7.54 (m, 4H), 7.42 (m, 6H), 7.28 (m, 5H), 7.08 (m, 2H), 6.88 (dd, $J = 2.0$ Hz, $J = 4.0$ Hz, 2H), 6.51 (s, 1H), 4.32 (m, 1H), 3.39 (d, $J = 4.0$ Hz, 1H), 3.32 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 2.66 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 1.16 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 141.7, 139.2, 136.63, 136.58, 135.6, 133.6, 131.6, 130.8, 130.2, 129.0, 128.6, 128.5, 128.3, 128.1, 127.8, 127.5, 127.1, 121.4, 57.9, 55.8, 43.5, 22.5; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{33}\text{BrN}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 585.1575, found 585.1578.



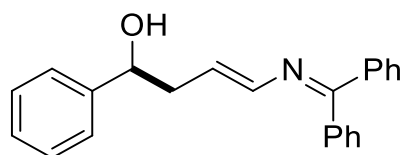
(*R*)-*N*-((*R*)-4-((Diphenylmethylene)amino)-1-phenyl-3-(4-(trifluoromethyl)phenyl)but-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3ba**): *E* isomer 95 mg, 33% yield; *Z* isomer 100 mg, 34% yield; foam solid; *E* isomer ^1H NMR (400 MHz, CDCl_3) δ 7.75 (d, J = 4.0 Hz, 2H), 7.51 (d, J = 8.0 Hz, 2H), 7.44 (m, 6H), 7.31 (t, 4H), 7.20 (m, 3H), 7.03 (m, 2H), 7.01 (s, 1H), 4.53 (dd, J = 8.0 Hz, J = 10.0 Hz, 1H), 4.00 (d, J = 4.0 Hz, 1H), 3.75 (dd, J = 4.0 Hz, J = 8.0 Hz, 1H), 3.56 (dd, J = 4.0 Hz, J = 8.0 Hz, 1H), 1.15 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 167.3, 143.9, 142.4, 139.3, 138.3, 135.9, 135.3, 130.7, 129.1, 129.0, 128.7, 128.4, 128.3, 128.2, 127.7, 127.4, 126.6, 125.5 (q, $J_{\text{F-C}}$ = 3.0 Hz), 124.1 (q, $J_{\text{F-C}}$ = 181.8 Hz), 58.0, 56.0, 37.1, 22.6; *Z* isomer dr = 7/ 1; ^1H NMR (400 MHz, CDCl_3) δ 7.65 (s, 3H), 7.53 (d, J = 4.0 Hz, 2H), 7.42 (m, 4H), 7.28 (m, 6H), 7.08 (dd, J = 4.0 Hz, J = 5.0 Hz, 2H), 6.89 (dd, J = 2.0 Hz, J = 4.0 Hz, 2H), 6.57 (s, 1H), 4.31 (m, 1H), 4.32 (d, J = 4.0 Hz, 1H), 4.31 (dd, J = 4.0 Hz, J = 8.0 Hz, 1H), 2.71 (dd, J = 8.0 Hz, J = 16.0 Hz, 1H), 1.16 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 141.6, 141.5, 139.1, 137.5, 135.6, 133.3, 130.4, 130.2, 129.1, 128.7, 128.6, 128.4, 128.1, 127.8, 127.2, 124.5 (q, $J_{\text{F-C}}$ = 3.0 Hz), 124.3 (q, $J_{\text{F-C}}$ = 272.7 Hz), 57.9, 55.8, 43.4, 22.5; HRMS (ESI): calc for $\text{C}_{34}\text{H}_{33}\text{F}_3\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 575.2344, found 575.2347.



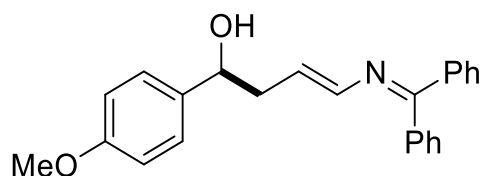
(*R*)-*N*-((*R*)-3-(2-Chlorophenyl)-4-((diphenylmethylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3bb**): *E* isomer 99 mg, 37% yield; *Z* isomer 90 mg, 33% yield; foam solid; *E* isomer ^1H NMR (400 MHz, CDCl_3) δ 7.44 (t, J = 4.0 Hz, 3H), 7.41 (m, 3H), 7.27 (m, 4H), 7.23 (m, 2H), 7.19 (m, 4H), 7.11 (m, 1H), 7.00 (d, J = 4.0 Hz, 2H), 6.63 (s, 1H), 4.33 (m, 1H), 3.39 (d, J = 4.0 Hz, 1H), 3.27 (d, J = 8.0 Hz, 1H), 2.90 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 1.13 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.2, 141.5, 139.3, 138.2, 137.9, 135.9, 134.7, 133.1, 132.2, 130.0, 129.4, 128.8, 128.59, 128.55, 128.47, 128.4, 128.2, 127.9, 127.7, 127.6, 125.8, 58.3, 55.7, 42.9, 22.5; *Z* isomer dr = 3/1; ^1H NMR (400 MHz, CDCl_3) δ 7.78 (d, J = 8.0 Hz, 2H), 7.43 (m, 6H), 7.31 (m, 4H), 7.22 (m, 3H), 7.10 (m, 3H), 6.92 (dd, J = 4.0 Hz, J = 8.0 Hz, 1H), 6.69 (s, 1H), 4.54 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 4.13 (m, 1H), 3.81 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 3.43 (dd, J = 8.0 Hz, J = 12.0 Hz, 1H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.7, 142.6, 139.9, 139.2, 136.2, 135.9, 132.9, 131.0, 130.5, 129.7, 129.1, 128.79, 128.76, 128.6, 128.5, 128.3, 128.22, 128.19, 127.6, 127.5, 126.5, 57.9, 55.9, 38.7, 22.6; HRMS (ESI): calc for $\text{C}_{33}\text{H}_{33}\text{ClN}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 541.2080, found 541.2085.



(*R*)-*N*-((*R*)-4-((Diphenylmethylene)amino)-3-(naphthalen-2-yl)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3bc**): *E* isomer 100 mg, 36% yield; *Z* isomer 89 mg, 32% yield; foam solid; *E* isomer ^1H NMR (400 MHz, CDCl_3) δ 7.77 (m, 4H), 7.72 (t, $J = 4.0$ Hz, 2H), 7.44 (m, 8H), 7.36 (d, $J = 8.0$ Hz, 3H), 7.25 (t, $J = 4.0$ Hz, 2H), 7.21 (d, $J = 8.0$ Hz, 1H), 7.18 (s, 1H), 7.09 (m, 2H), 4.62 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 4.09 (d, $J = 4.0$ Hz, 1H), 3.88 (dd, $J = 8.0$ Hz, $J = 16.0$ Hz, 1H), 3.63 (dd, $J = 8.0$ Hz, $J = 16.0$ Hz, 1H), 1.13 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 142.9, 139.5, 137.3, 136.9, 136.1, 133.4, 132.8, 130.4, 129.0, 128.9, 128.8, 128.4, 128.3, 128.2, 128.1, 127.53, 127.46, 127.4, 126.2, 126.0, 125.4, 124.5, 58.8, 56.0, 37.3, 22.5; *Z* isomer *dr* = 7/1; ^1H NMR (400 MHz, CDCl_3) δ 8.01 (s, 1H), 7.87 (m, 3H), 7.76 (dd, $J = 4.0$ Hz, 12.0 Hz, 1H), 7.56 (d, $J = 8.0$ Hz, 2H), 7.49 (t, $J = 6.0$ Hz, 2H), 7.44 (m, 3H), 7.30 (m, 4H), 7.24 (m, 2H), 7.11 (m, 2H), 6.95 (dd, $J = 2.0$ Hz, $J = 8.0$ Hz, 2H), 6.61 (s, 1H), 4.39 (m, 1H), 3.41 (m, 2H), 2.83 (dd, $J = 8.0$ Hz, $J = 12.0$ Hz, 1H), 1.14 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.3, 141.9, 139.4, 136.5, 135.8, 135.4, 135.0, 133.2, 132.8, 130.1, 129.0, 128.9, 128.6, 128.54, 128.50, 128.43, 128.38, 128.0, 127.7, 127.5, 127.2, 126.9, 126.0, 125.8, 58.3, 55.8, 44.0, 22.5; HRMS (ESI): calc for $\text{C}_{37}\text{H}_{36}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 557.2627, found 557.2629.

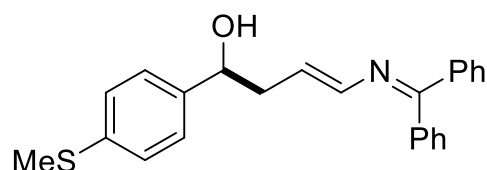


(*E*)-4-((Diphenylmethylene)amino)-1-phenylbut-3-en-1-ol (**4a**): 142 mg, 87% yield; pale yellow solid, m.p. 89-91 $^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, $J = 8.0$ Hz, 2H), 7.42 (t, $J = 4.0$ Hz, 3H), 7.33 (m, 7H), 7.25 (m, 1H), 7.10 (m, 2H), 6.75 (d, $J = 12.0$ Hz, 1H), 6.15 (m, 1H), 4.71 (t, $J = 6.0$ Hz, 1H), 2.51 (t, $J = 6.0$ Hz, 2H), 2.34 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 143.8, 140.6, 139.4, 136.1, 130.2, 128.8, 128.7, 128.5, 128.4, 128.3, 128.1, 127.4, 125.9, 73.6, 40.5; HRMS (ESI): calc for $\text{C}_{23}\text{H}_{21}\text{NO}$ ($\text{M}+\text{H}$) $^+$ 328.1701, found 328.1706.

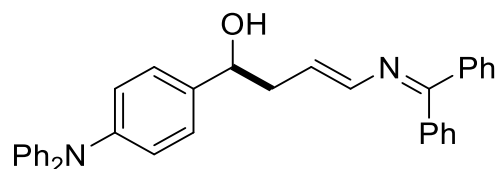


(*E*)-4-((Diphenylmethylene)amino)-1-(4-methoxyphenyl)but-3-en-1-ol (**4b**): 127 mg, 71% yield; pale yellow solid, m.p. 106-108 $^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, $J = 8.0$ Hz, 2H), 7.43 (t, $J = 2.0$ Hz, 3H), 7.35 (m, 3H), 7.23 (d, $J = 8.0$ Hz, 2H), 7.11 (m, 2H), 6.85 (d, $J = 8.0$ Hz, 2H), 6.74 (d, $J = 12.0$ Hz, 1H), 6.13 (m, 1H), 4.67 (t, $J = 6.0$ Hz, 1H), 3.79 (s, 3H), 2.50 (t, $J = 6.0$ Hz, 2H), 2.22 (br, 1H);

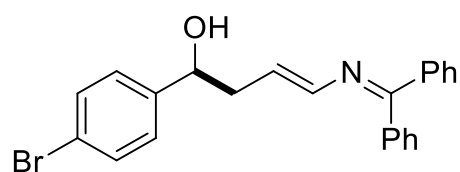
^{13}C NMR (101 MHz, CDCl_3) δ 166.0, 158.9, 140.5, 139.4, 136.1, 135.9, 130.2, 128.8, 128.71, 128.69, 128.6, 128.4, 128.1, 127.1, 113.7, 73.3, 55.2, 40.5; HRMS (ESI): calc for $\text{C}_{24}\text{H}_{23}\text{NO}_2$ ($\text{M}+\text{H}$) $^+$ 358.1807, found 358.1810.



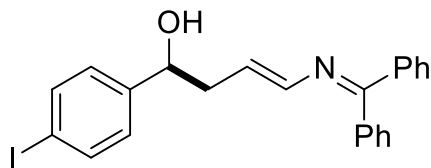
(*E*)-4-((Diphenylmethylene)amino)-1-(4-(methylthio)phenyl)but-3-en-1-ol (**4c**): 105 mg, 56% yield; pale yellow solid, m.p. 139-141 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.64 (d, J = 8.0 Hz, 2H), 7.45 (m, 3H), 7.36 (m, 3H), 7.24 (m, 4H), 7.11 (m, 2H), 6.74 (d, J = 12.0 Hz, 1H), 6.13 (m, 1H), 4.71 (t, J = 6.0 Hz, 1H), 2.51 (t, J = 8.0 Hz, 2H), 2.48 (s, 3H), 2.07 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.2, 140.9, 140.6, 139.4, 137.5, 136.1, 130.3, 128.9, 128.8, 128.7, 128.4, 128.1, 126.6, 126.5, 73.3, 40.5, 15.9; HRMS (ESI): calc for $\text{C}_{24}\text{H}_{23}\text{NOS}$ ($\text{M}+\text{H}$) $^+$ 374.1579, found 374.1579.



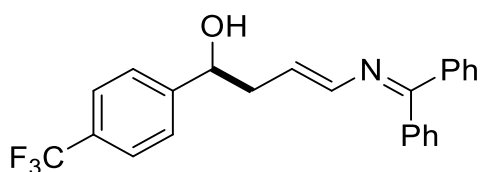
(*E*)-1-(4-(Diphenylamino)phenyl)-4-((diphenylmethylene)amino)but-3-en-1-ol (**4d**): 131 mg, 53% yield; pale yellow solid, m.p. 124-126 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (m, 2H), 7.39 (m, 6H), 7.21 (m, 8H), 7.02 (m, 8H), 6.82 (d, J = 16.0 Hz, 1H), 6.22 (m, 1H), 4.67 (q, J = 8.0 Hz, 1H), 2.52 (m, 2H), 2.15 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 147.7, 147.2, 140.6, 139.4, 137.8, 136.2, 130.3, 129.2, 128.80, 128.76, 128.70, 128.66, 128.5, 128.1, 126.8, 124.1, 123.8, 122.7, 73.3, 40.4; HRMS (ESI): calc for $\text{C}_{35}\text{H}_{30}\text{N}_2\text{O}$ ($\text{M}+\text{H}$) $^+$ 495.2436, found 495.2441.



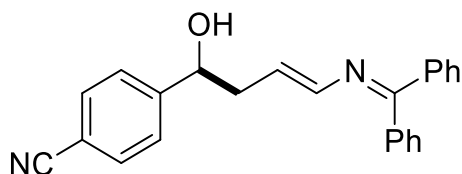
(*E*)-1-(4-Bromophenyl)-4-((diphenylmethylene)amino)but-3-en-1-ol (**4e**): 146 mg, 72% yield; pale yellow solid, m.p. 135-137 $^{\circ}\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.62 (d, J = 8.0 Hz, 2H), 7.44 (m, 5H), 7.38 (t, J = 8.0 Hz, 1H), 7.32 (t, J = 6.0 Hz, 2H), 7.17 (d, J = 12.0 Hz, 2H), 7.08 (m, 2H), 6.69 (d, J = 16.0 Hz, 1H), 6.12 (m, 1H), 4.69 (t, J = 6.0 Hz, 1H), 2.47 (t, J = 8.0 Hz, 2H), 2.38 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 142.7, 141.0, 139.3, 136.1, 131.4, 130.3, 128.83, 128.79, 128.66, 128.4, 128.1, 127.68, 127.66, 121.2, 73.0, 40.5; HRMS (ESI): calc for $\text{C}_{23}\text{H}_{20}\text{NOBr}$ ($\text{M}+\text{H}$) $^+$ 406.0807, found 406.0808.



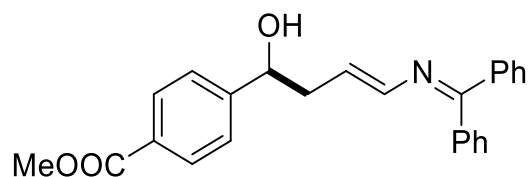
(*E*)-4-((Diphenylmethylene)amino)-1-(4-iodophenyl)but-3-en-1-ol (**4f**): 145 mg, 64% yield; pale yellow solid, m.p. 150-152 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.65 (d, J = 4.0 Hz, 2H), 7.63 (d, J = 4.0 Hz, 2H), 7.46 (m, 3H), 7.39 (t, J = 6.0 Hz, 1H), 7.33 (t, J = 6.0 Hz, 2H), 7.10 (m, 2H), 7.07 (d, J = 8.0 Hz, 2H), 6.70 (d, J = 12.0 Hz, 1H), 6.10 (m, 1H), 4.69 (t, J = 4.0 Hz, 1H), 2.48 (m, 2H), 2.14 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.5, 143.4, 141.1, 139.4, 137.4, 136.1, 130.4, 128.9, 128.8, 128.7, 128.5, 128.1, 127.9, 127.6, 92.8, 73.1, 40.5; HRMS (ESI): calc for $\text{C}_{23}\text{H}_{20}\text{NOI}$ ($\text{M}+\text{H}$) $^+$ 454.0668, found 454.0669.



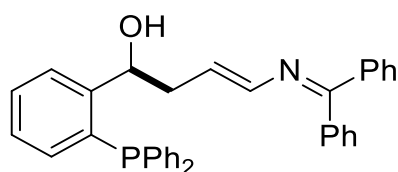
(*E*)-4-((Diphenylmethylene)amino)-1-(4-(trifluoromethyl)phenyl)but-3-en-1-ol (**4g**): 162 mg, 82% yield; pale yellow solid, m.p. 133-135 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, J = 8.0 Hz, 2H), 7.58 (d, J = 8.0 Hz, 2H), 7.42 (m, 6H), 7.32 (d, J = 8.0 Hz, 2H), 7.09 (q, J = 4.0 Hz, 2H), 6.73 (d, J = 12.0 Hz, 1H), 6.13 (m, 1H), 2.52 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.7, 147.7, 141.2, 139.3, 136.1, 130.4, 129.6 (q, $J_{\text{F-C}}$ = 32.3 Hz), 128.9, 128.8, 128.6, 128.5, 128.1, 127.4, 126.2, 125.3 (q, $J_{\text{F-C}}$ = 4.0 Hz), 124.2 (q, $J_{\text{F-C}}$ = 273.7 Hz), 73.0, 40.6; HRMS (ESI): calc for $\text{C}_{24}\text{H}_{20}\text{NOF}_3$ ($\text{M}+\text{H}$) $^+$ 396.1575, found 396.1579.



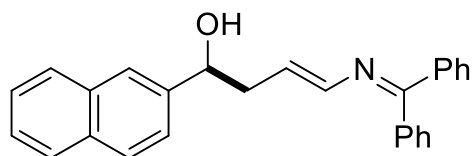
(*E*)-4-((Diphenylmethylene)amino)-1-(4-cyanophenyl)but-3-en-1-ol (**4h**): 122 mg, 69% yield; pale yellow solid, m.p. 106-108 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.59 (t, J = 8.0 Hz, 4H), 7.41 (m, 6H), 7.30 (t, J = 8.0 Hz, 2H), 7.09 (m, 2H), 6.71 (d, J = 12.0 Hz, 1H), 6.14 (m, 1H), 4.77 (t, J = 8.0 Hz, 1H), 2.87 (br, 1H), 2.47 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.8, 149.2, 141.1, 139.2, 136.0, 132.1, 130.4, 128.9, 128.8, 128.6, 128.4, 128.1, 127.2, 126.5, 118.8, 110.9, 72.7, 40.5; HRMS (ESI): calc for $\text{C}_{24}\text{H}_{20}\text{N}_2\text{O}$ ($\text{M}+\text{H}$) $^+$ 353.1654, found 353.1658.



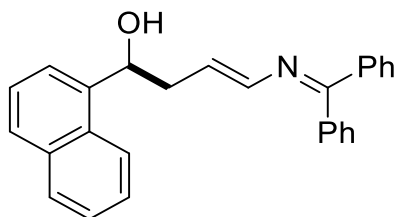
Methyl (*E*)-4-(4-((diphenylmethylene)amino)-1-hydroxybut-3-en-1-yl)benzoate (**4i**): 131 mg, 68% yield; pale yellow solid, m.p. 162-164 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, J = 8.0 Hz, 2H), 7.63 (d, J = 8.0 Hz, 2H), 7.41 (m, 6H), 7.33 (t, J = 6.0 Hz, 2H), 7.10 (q, J = 4.0 Hz, 2H), 6.74 (d, J = 12.0 Hz, 1H), 6.14 (m, 1H), 4.81 (t, J = 6.0 Hz, 1H), 3.92 (s, 3H), 2.53 (m, 2H), 2.32 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.9, 166.5, 148.9, 141.1, 139.3, 136.1, 130.4, 129.7, 129.2, 128.84, 128.80, 128.7, 128.4, 128.1, 127.6, 125.8, 73.2, 52.1, 40.6; HRMS (ESI): calc for $\text{C}_{25}\text{H}_{23}\text{NO}_3$ ($\text{M}+\text{H}$) $^+$ 386.1756, found 386.1760.



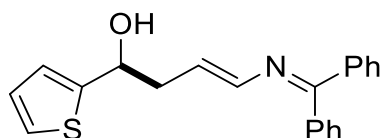
(*E*)-4-((Diphenylmethylene)amino)-1-(2-(diphenylphosphaneyl)phenyl)but-3-en-1-ol (**4j**): 207 mg, 81% yield; pale yellow solid, m.p. 78-80 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.56 (m, 10H), 7.44 (m, 7H), 7.34 (m, 3H), 7.23 (t, J = 8.0 Hz, 1H), 7.05 (m, 3H), 6.60 (d, J = 12.0 Hz, 1H), 5.97 (m, 1H), 5.36 (d, J = 4.0 Hz, 1H), 5.05 (d, J = 4.0 Hz, 1H), 2.63 (t, J = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.3, 149.0 (d, $J_{\text{P-C}}$ = 8.1 Hz), 139.7 (d, $J_{\text{P-C}}$ = 21.2 Hz), 136.2, 133.9 (d, $J_{\text{P-C}}$ = 13.1 Hz), 132.8 (d, $J_{\text{P-C}}$ = 25.3 Hz), 132.5, 132.2, 132.1, 131.9, 131.8 (d, $J_{\text{P-C}}$ = 10.1 Hz), 131.6, 130.8, 130.1, 129.8, 129.3, 128.8 (d, $J_{\text{P-C}}$ = 10.1 Hz), 128.7, 128.6 (d, $J_{\text{P-C}}$ = 5.1 Hz), 128.2 (d, $J_{\text{P-C}}$ = 29.3 Hz), 126.8 (d, $J_{\text{P-C}}$ = 13.1 Hz), 71.4 (d, $J_{\text{P-C}}$ = 5.1 Hz), 36.7; HRMS (ESI): calc for $\text{C}_{35}\text{H}_{30}\text{NOP}$ ($\text{M}+\text{H}$) $^+$ 512.2143, found 512.2144.



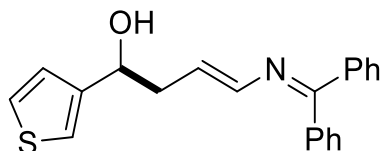
(*E*)-4-((Diphenylmethylene)amino)-1-(naphthalen-2-yl)but-3-en-1-ol (**4k**): 145 mg, 77% yield; pale yellow solid, m.p. 110-112 °C; ^1H NMR (400 MHz, CDCl_3) δ 7.79 (m, 3H), 7.71 (s, 1H), 7.59 (d, J = 8.0 Hz, 2H), 7.42 (m, 3H), 7.35 (m, 2H), 7.25 (m, 4H), 6.97 (d, J = 8.0 Hz, 2H), 6.69 (d, J = 16.0 Hz, 1H), 6.20 (m, 1H), 4.84 (t, J = 6.0 Hz, 1H), 2.67 (br, 1H), 2.58 (t, J = 6.0 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 141.2, 140.6, 139.4, 136.0, 133.2, 132.9, 130.2, 128.8, 128.6, 128.33, 128.25, 128.0, 127.9, 127.6, 126.0, 125.7, 124.6, 124.1, 73.7, 40.6; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{23}\text{NO}$ ($\text{M}+\text{H}$) $^+$ 378.1858, found 378.1861.



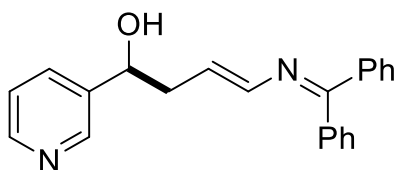
(*E*)-4-((Diphenylmethylene)amino)-1-(naphthalen-1-yl)but-3-en-1-ol (**4l**): 155 mg, 82% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.00 (t, $J = 4.0$ Hz, 1H), 7.84 (t, $J = 4.0$ Hz, 1H), 7.73 (d, $J = 8.0$ Hz, 1H), 7.60 (t, $J = 8.0$ Hz, 3H), 7.44 (m, 3H), 7.36 (m, 4H), 7.28 (t, $J = 6.0$ Hz, 2H), 7.06 (m, 2H), 6.77 (d, $J = 12.0$ Hz, 1H), 6.31 (m, 1H), 5.47 (q, $J = 4.0$ Hz, 1H), 2.72 (m, 1H), 2.58 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.1, 140.4, 139.40, 139.36, 136.1, 133.7, 130.2, 128.9, 128.8, 128.7, 128.3, 128.0, 127.8, 125.9, 125.38, 125.35, 123.00, 122.96, 70.4, 39.6; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{23}\text{NO}$ ($\text{M}+\text{H}$) $^+$ 378.1858, found 378.1862.



(*E*)-4-((Diphenylmethylene)amino)-1-(thiophen-2-yl)but-3-en-1-ol (**4m**): 140 mg, 84% yield; white solid, m.p. 95-97 $^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.63 (d, $J = 8.0$ Hz, 2H), 7.44 (m, 3H), 7.34 (m, 3H), 7.20 (dd, $J = 2.0$ Hz, $J = 8.0$ Hz, 1H), 7.13 (m, 2H), 6.92 (t, $J = 4.0$ Hz, 2H), 6.79 (d, $J = 12.0$ Hz, 1H), 6.17 (m, 1H), 4.93 (t, $J = 6.0$ Hz, 1H), 2.59 (t, $J = 8.0$ Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.3, 147.8, 140.7, 139.3, 136.1, 130.2, 128.8, 128.71, 128.67, 128.4, 128.0, 127.9, 126.5, 124.4, 123.7, 69.6, 40.5; HRMS (ESI): calc for $\text{C}_{21}\text{H}_{19}\text{NOS}$ ($\text{M}+\text{H}$) $^+$ 334.1266, found 334.1269.

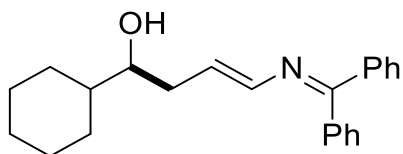


(*E*)-4-((Diphenylmethylene)amino)-1-(thiophen-3-yl)but-3-en-1-ol (**4n**): 132 mg, 79% yield; white solid, m.p. 113-115 $^\circ\text{C}$; ^1H NMR (400 MHz, CDCl_3) δ 7.64 (d, $J = 8.0$ Hz, 2H), 7.45 (m, 3H), 7.35 (m, 3H), 7.27 (q, $J = 4.0$ Hz, 1H), 7.14 (m, 3H), 7.03 (d, $J = 4.0$ Hz, 1H), 6.78 (d, $J = 16.0$ Hz, 1H), 6.15 (m, 1H), 4.81 (t, $J = 8.0$ Hz, 1H), 2.54 (m, 2H), 2.27 (br, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.2, 145.2, 140.7, 139.4, 136.1, 130.3, 128.8, 128.72, 128.68, 128.4, 128.2, 128.1, 125.9, 125.6, 120.8, 69.9, 39.7; HRMS (ESI): calc for $\text{C}_{21}\text{H}_{19}\text{NOS}$ ($\text{M}+\text{H}$) $^+$ 334.1266, found 334.1270.

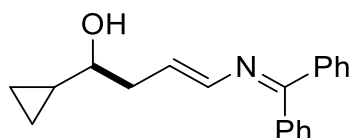


(*E*)-4-((Diphenylmethylene)amino)-1-(pyridin-3-yl)but-3-en-1-ol (**4o**): 135 mg, 82% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.47 (d, $J = 4.0$ Hz, 1H), 8.43 (dd, $J = 4.0$ Hz, $J = 2.0$ Hz, 1H), 7.66 (d, $J = 8.0$ Hz, 1H), 7.62 (d, $J = 4.0$ Hz, 2H), 7.43 (m, 3H), 7.38 (t, $J = 6.0$ Hz, 1H), 7.31 (t, $J = 8.0$

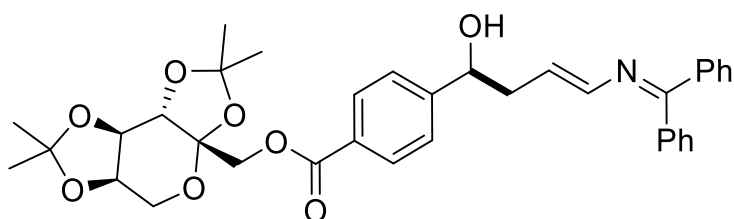
Hz, 2H), 7.21 (dd, $J = 8.0$ Hz, $J = 3.2$ Hz, 1H), 7.10 (m, 2H), 6.73 (d, $J = 12.0$ Hz, 1H), 6.16 (m, 1H), 4.74 (t, $J = 8.0$ Hz, 1H), 2.51 (t, $J = 6.0$ Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4, 148.3, 147.6, 140.7, 139.6, 139.3, 136.0, 133.8, 130.3, 128.8, 128.7, 128.6, 128.4, 128.0, 127.8, 123.3, 71.2, 40.4; HRMS (ESI): calc for $\text{C}_{22}\text{H}_{20}\text{N}_2\text{O}$ ($\text{M}+\text{H}$) $^+$ 329.1654, found 329.1658.



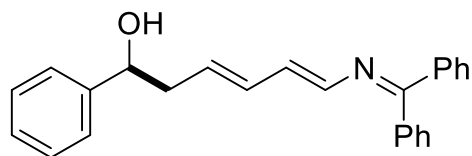
(*E*)-1-Cyclohexyl-4-((diphenylmethylene)amino)but-3-en-1-ol (**4p**): 88 mg, 53% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, $J = 4.0$ Hz, 2H), 7.46 (m, 3H), 7.36 (m, 3H), 7.20 (m, 2H), 6.80 (d, $J = 12.0$ Hz, 1H), 6.19 (m, 1H), 3.42 (m, 1H), 2.32 (m, 1H), 2.18 (m, 1H), 1.84 (d, $J = 12.0$ Hz, 1H), 1.74 (m, 2H), 1.65 (m, 2H), 1.36 (m, 1H), 1.09 (m, 6H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.8, 140.4, 139.5, 136.3, 130.2, 129.6, 128.8, 128.71, 128.65, 128.5, 128.1, 75.2, 42.9, 35.5, 29.2, 27.9, 26.5, 26.2, 26.1; HRMS (ESI): calc for $\text{C}_{23}\text{H}_{27}\text{NO}$ ($\text{M}+\text{H}$) $^+$ 334.2171, found 334.2175.



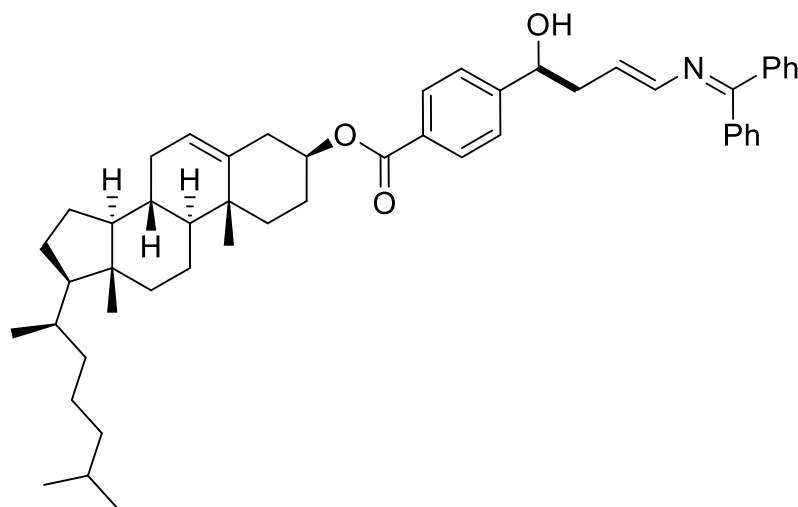
(*E*)-1-Cyclopropyl-4-((diphenylmethylene)amino)but-3-en-1-ol (**4q**): 82 mg, 56% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.66 (d, $J = 8.0$ Hz, 2H), 7.46 (m, 3H), 7.36 (m, 3H), 7.20 (m, 2H), 6.82 (d, $J = 16.0$ Hz, 1H), 6.25 (m, 1H), 2.96 (m, 1H), 2.44 (m, 1H), 2.33 (m, 1H), 1.88 (br, 1H), 0.92 (m, 1H), 0.50 (m, 2H), 0.30 (m, 1H), 0.22 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 165.7, 140.2, 139.5, 136.3, 130.2, 129.2, 128.74, 128.66, 128.4, 128.1, 76.0, 38.4, 17.3, 2.7, 2.5; HRMS (ESI): calc for $\text{C}_{20}\text{H}_{21}\text{NO}$ ($\text{M}+\text{H}$) $^+$ 292.1701, found 292.1705.



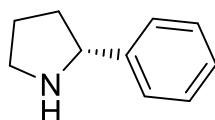
((3*aS*,5*aR*,8*aR*,8*bS*)-2,2,7,7-Tetramethyltetrahydro-3*aH*-bis([1,3]dioxolo)[4,5-*b*:4',5'-*d*]pyran-3*a*-yl)methyl 4-((*E*)-4-((diphenylmethylene)amino)-1-hydroxybut-3-en-1-yl)benzoate (**4s**): 193 mg, 63%; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 8.03 (d, $J = 12.0$ Hz, 2H), 7.62 (d, $J = 8.0$ Hz, 2H), 7.43 (t, $J = 4.0$ Hz, 3H), 7.38 (t, $J = 8.0$ Hz, 3H), 7.31 (t, $J = 8.0$ Hz, 2H), 7.09 (m, 2H), 6.73 (d, $J = 12.0$ Hz, 1H), 6.15 (m, 1H), 4.78 (t, $J = 6.0$ Hz, 1H), 4.68 (dd, $J = 4.0$ Hz, $J = 12.0$ Hz, 1H), 4.64 (m, 1H), 4.66 (t, $J = 2.0$ Hz, 1H), 4.33 (dd, $J = 4.0$ Hz, $J = 12.0$ Hz, 1H), 4.26 (d, $J = 8.0$ Hz, 1H), 3.95 (d, $J = 16.0$ Hz, 1H), 3.79 (d, $J = 12.0$ Hz, 1H), 2.50 (m, 2H), 1.54 (s, 3H), 1.47 (s, 3H), 1.36 (s, 3H), 1.34 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4, 165.7, 149.2, 140.9, 139.3, 136.0, 130.3, 129.8, 128.79, 128.77, 128.6, 128.4, 128.1, 127.7, 125.8, 109.1, 108.8, 101.6, 73.0, 70.7, 70.4, 70.0, 65.2, 61.3, 40.6, 26.5, 25.8, 25.5, 24.0, 20.7; HRMS (ESI): calc for $\text{C}_{36}\text{H}_{39}\text{NO}_8$ ($\text{M}+\text{H}$) $^+$ 614.2754, found 614.2758.



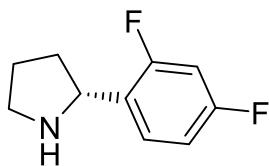
(3*E*,5*E*)-6-((Diphenylmethylene)amino)-1-phenylhexa-3,5-dien-1-ol (**4t**): 145 mg, 82% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.67 (d, J = 8.0 Hz, 2H), 7.46 (m, 4H), 7.32 (m, 6H), 7.28 (m, 1H), 7.19 (m, 2H), 6.88 (d, J = 12.0 Hz, 1H), 6.69 (t, J = 12.0 Hz, 1H), 6.15 (m, 1H), 5.80 (m, 1H), 4.71 (t, J = 8.0 Hz, 1H), 2.53 (t, J = 8.0 Hz, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.2, 143.9, 139.52, 139.45, 136.2, 132.1, 132.0, 131.3, 130.2, 128.8, 128.7, 128.5, 128.4, 128.3, 128.1, 127.5, 125.7, 73.6, 43.1; HRMS (ESI): calc for $\text{C}_{25}\text{H}_{23}\text{NO}$ ($\text{M}+\text{H}$) $^+$ 354.1858, found 354.1860.



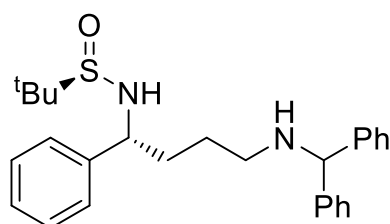
(3*S*,8*S*,9*S*,10*R*,13*R*,14*S*,17*R*)-10,13-Dimethyl-17-((*R*)-6-methylheptan-2-yl)-2,3,4,7,8,9,10,11,12,13,14,15,16,17-tetradecahydro-1H-cyclopenta[*a*]phenanthren-3-yl 4-((*E*)-4-((diphenylmethylene)amino)-1-hydroxybut-3-en-1-yl)benzoate (**4r**): 135 mg, 61% yield (0.3 mmol scale); pale yellow solid, m.p. 168-170 °C; ^1H NMR (400 MHz, CDCl_3) δ 8.00 (d, J = 8.0 Hz, 2H), 7.63 (d, J = 8.0 Hz, 2H), 7.37 (m, 8H), 7.09 (q, J = 4.0 Hz, 2H), 6.72 (d, J = 12.0 Hz, 1H), 6.13 (m, 1H), 5.42 (d, J = 8.0 Hz, 1H), 4.87 (m, 1H), 4.79 (t, J = 6.0 Hz, 1H), 2.50 (m, 4H), 1.86 (m, 8H), 1.53 (m, 6H), 1.37 (m, 3H), 1.20 (m, 7H), 1.07 (s, 3H), 1.02 (m, 3H), 0.92 (d, J = 4.0 Hz, 3H), 0.88 (d, J = 4.0 Hz, 3H), 0.86 (d, J = 2.0 Hz, 3H), 0.69 (s, 3H); ^{13}C NMR (101 MHz, CDCl_3) δ 166.4, 165.8, 148.7, 141.0, 139.6, 139.3, 136.1, 130.3, 129.9, 129.6, 128.8, 128.7, 128.4, 128.3, 128.1, 127.6, 125.7, 122.8, 74.5, 73.2, 56.7, 56.1, 50.0, 42.3, 40.6, 39.7, 39.5, 38.2, 37.0, 36.6, 36.2, 35.8, 31.9, 31.8, 28.2, 28.0, 27.9, 24.3, 23.8, 22.8, 22.5, 21.0, 19.4, 18.7, 11.8; HRMS (ESI): calc for $\text{C}_{51}\text{H}_{65}\text{NO}_3$ ($\text{M}+\text{H}$) $^+$ 740.5043, found 740.5044.



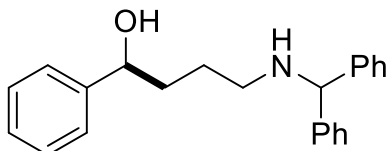
(*R*)-2-Phenylpyrrolidine (**5**): 72 mg, 98% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.31 (m, 4H), 7.20 (t, J = 6.0 Hz, 1H), 4.07 (t, J = 8.0 Hz, 1H), 3.17 (m, 1H), 2.97 (m, 1H), 2.11 (m, 1H), 2.02 (br, 1H), 1.85 (m, 2H), 1.64 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.7, 128.1, 126.5, 126.3, 62.4, 46.8, 34.7, 34.2, 25.4. These data are in accordance with the literature.⁶



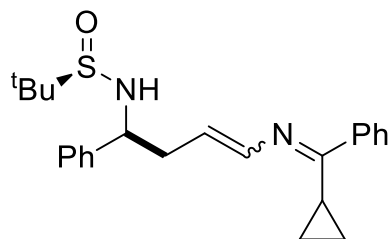
(*R*)-2-(2,4-Difluorophenyl)pyrrolidine (**6**): 84 mg, 92% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.25 (m, 1H), 6.94 (m, 1H), 6.84 (m, 1H), 4.39 (t, $J = 8.0$ Hz, 1H), 3.15 (m, 1H), 3.04 (dd, $J = 16.0$ Hz, $J = 8.0$ Hz, 1H), 2.25 (m, 1H), 1.97 (br, 1H), 1.85 (m, 2H), 1.61 (m, 1H); ^{13}C NMR (101 MHz, CDCl_3) δ 158.9 (d, $J_{\text{F-C}} = 242.4$ Hz), 156.3 (d, $J_{\text{F-C}} = 242.4$ Hz), 134.5 (dd, $J_{\text{F-C}} = 16.2$ Hz, $J_{\text{F-C}} = 7.1$ Hz), 115.9 (dd, $J_{\text{F-C}} = 25.3$ Hz, $J_{\text{F-C}} = 8.1$ Hz), 113.96 (m), 55.4, 46.7, 33.1, 25.5. These data are in accordance with the literature.⁶



(*R*)-*N*-((*R*)-4-(Benzhydrylamino)-1-phenylbutyl)-2-methylpropane-2-sulfonamide (**7**): 206 mg, 95% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.30 (m, 13 H), 7.18 (m, 2H), 4.72 (s, 1H), 4.33 (m, 1H), 3.44 (d, $J = 4.0$ Hz, 1H), 2.53 (m, 2H), 2.07 (m, 1H), 1.77 (m, 2H), 1.45 (m, 1H), 1.20 (s, 9H); ^{13}C NMR (101 MHz, CDCl_3) δ 144.1, 144.0, 142.3, 128.6, 128.4, 127.8, 127.1, 126.9, 67.4, 58.8, 55.6, 47.9, 34.2, 26.3, 22.6; HRMS (ESI): calc for $\text{C}_{27}\text{H}_{34}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$)⁺ 435.2470, found 435.2474.



4-(Benzhydrylamino)-1-phenylbutan-1-ol (**8**): 154 mg, 93% yield; pale yellow oil; ^1H NMR (400 MHz, CDCl_3) δ 7.34 (m, 12H), 7.21 (m, 3H), 4.80 (s, 1H), 4.67 (q, $J = 4.0$ Hz, 1H), 3.38 (br, 1H), 2.66 (m, 1H), 2.55 (m, 1H), 1.82 (m, 2H), 1.59 (m, 2H); ^{13}C NMR (101 MHz, CDCl_3) δ 145.4, 143.4, 143.2, 128.6, 128.5, 128.2, 127.24, 127.18, 127.14, 127.11, 126.9, 125.8, 73.9, 67.8, 48.2, 38.5, 26.9; HRMS (ESI): calc for $\text{C}_{23}\text{H}_{25}\text{NO}$ ($\text{M}+\text{H}$)⁺ 332.2014, found 332.2017.



(*R*)-*N*-((*S,E*)-4-((Cyclopropyl(phenyl)methylene)amino)-1-phenylbut-3-en-1-yl)-2-methylpropane-2-sulfonamide (**3be**): 69 mg, 35% yield; pale yellow oil; $E/Z = 4/1$; ^1H NMR (400 MHz, CDCl_3) δ 7.31 (m, 8H), 7.01 (m, 2H), 6.41 (d, $J = 8.0$ Hz, 1H), 5.65 (m, 1H), 4.42 (m, 1H), 3.44 (d, $J = 2.0$ Hz, 1H),

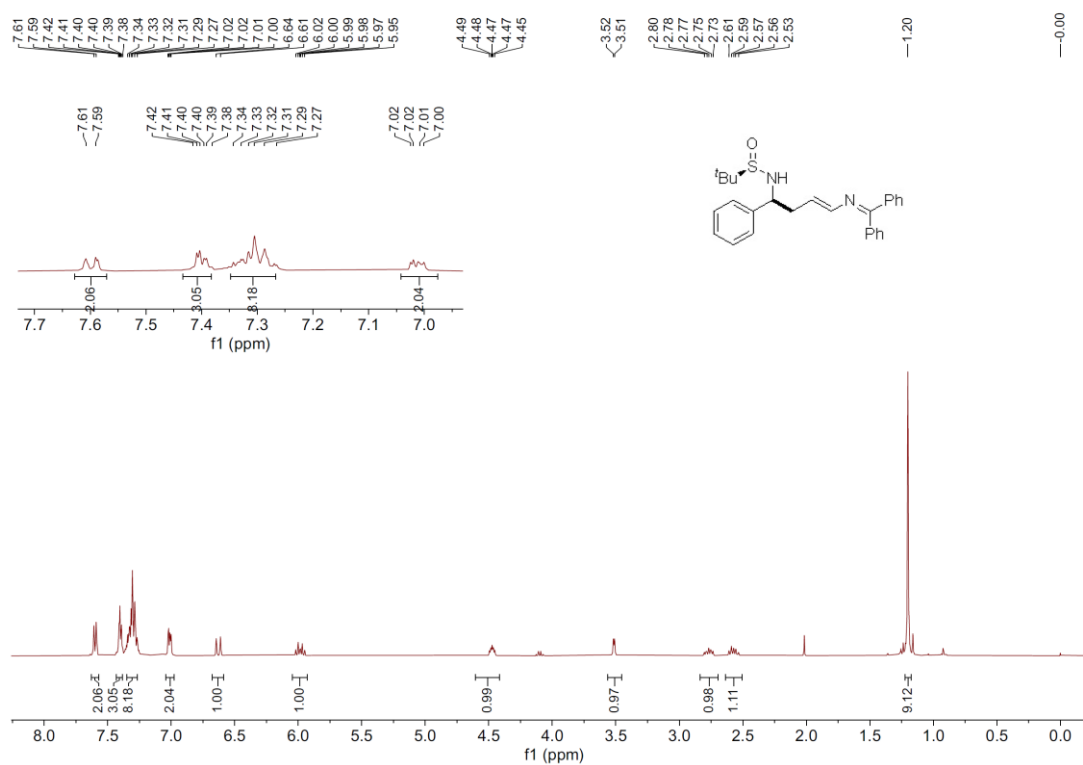
2.68 (m, 1H), 2.48 (m, 1H), 1.82 (m, 1H), 1.19 (s, 9H), 0.87 (m, 4H); ^{13}C NMR (101 MHz, CDCl_3) δ 172.2, 141.7, 139.9, 136.8, 128.6, 128.5, 128.2, 127.7, 127.5, 127.3, 123.9, 58.6, 55.8, 37.6, 22.6, 20.2, 8.2, 7.9; HRMS (ESI): calc for $\text{C}_{24}\text{H}_{30}\text{N}_2\text{OS}$ ($\text{M}+\text{H}$) $^+$ 395.2157, found 395.2159.

12. References

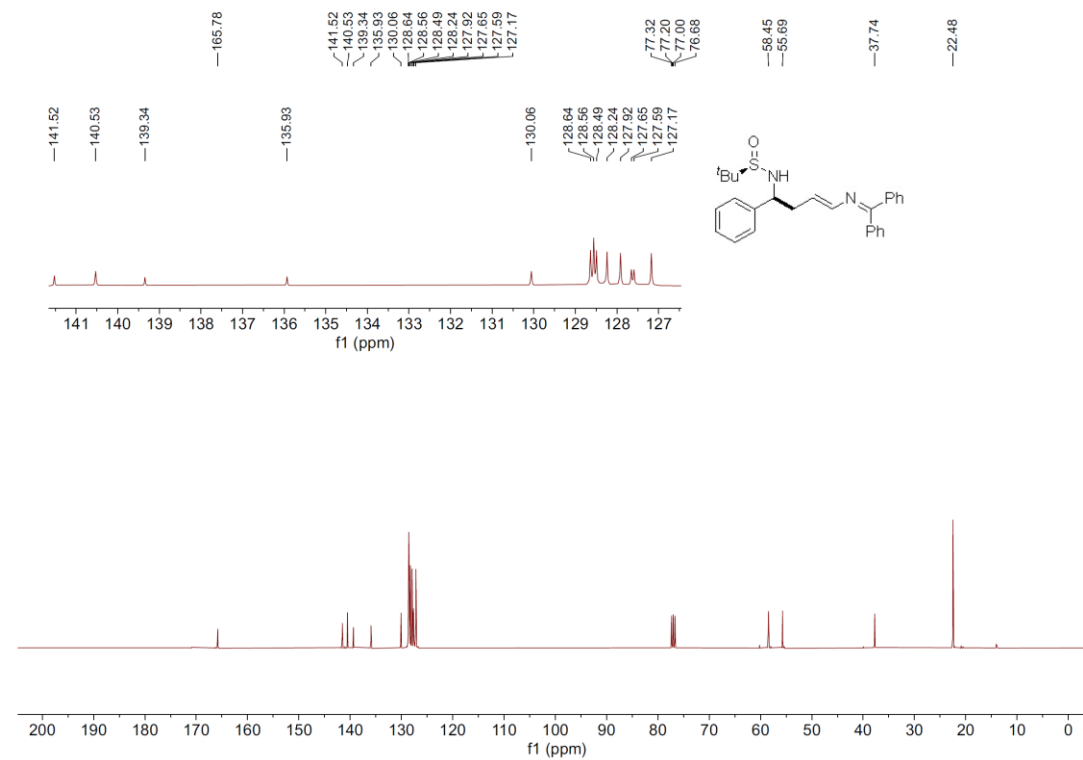
1. Serviano, J. M. I.; Phipps, E. J. T.; Holland, P. L. Intermolecular Hydroalkoxylation and Hydrocarboxylation of 2-Azadienes with High Efficiency. *J. Org. Chem.* **2023**, *88*, 3277–3281.
2. Bao, J.; Nick, S. J.; Lanin, A. S.; Molinero, N. I.; Sera, B. J.; Njardarson, J. T. Stereoselective Synthesis of Conjugated Di- and Trienamides via a Dienolate Enabled Anionic Cascade. *J. Org. Chem.* **2023**, *88*, 17485–17488.
3. Chen, S.-J.; Zhong, W.-Q.; Huang, J.-M. Electrochemical Trifluoromethylation and Sulfonylation of N-Allylamides: Synthesis of Oxazoline Derivatives. *J. Org. Chem.* **2023**, *88*, 12630–12640.
4. Hende, E. V.; Verniest, G.; Deroose, F.; Thuring, J.-W.; Macdonald, G.; De Kimpe, N. Synthesis of 1-Boc-3-fluoroazetidine-3-carboxylic Acid. *J. Org. Chem.* **2009**, *74*, 2250–2253.
5. Uphade, M. B.; Reddy, A. A.; Khandare, S. P.; Prasad, K. R. *Org. Lett.* **2019**, *21*, 9109–9113.
6. Yin, C.; Zhang, R.; Pan, Y.; Gao, S.; Ding, X.; Bai, S.-T.; Lang, Q.; Zhang, X. PPM Ir-f-phamidol-Catalyzed Asymmetric Hydrogenation of γ -Amino Ketones Followed by Stereoselective Cyclization for Construction of Chiral 2-Aryl-pyrrolidine Pharmacophores. *J. Org. Chem.* **2024**, *89*, 527–533.
7. Stephens, P. J.; Devlin, F. J.; Chabalowski, C. F.; Frisch, M. J. Ab initio calculation of vibrational absorption and circular dichroism spectra using density functional force fields. *J. Phys. Chem.* **1994**, *98*, 11623–11627.
8. Grimme, S.; Ehrlich, S.; Goerigk, L. Effect of the damping function in dispersion corrected density functional theory. *J. Comput. Chem.* **2011**, *32*, 1456–1465.
9. Marenich, A. V.; Cramer, C. J.; Truhlar, D. G. Universal Solvation Model Based on Solute Electron Density and on a Continuum Model of the Solvent Defined by the Bulk Dielectric Constant and Atomic Surface Tensions. *J. Phys. Chem. B.* **2009**, *113*, 6378–6396.

Part II NMR spectra

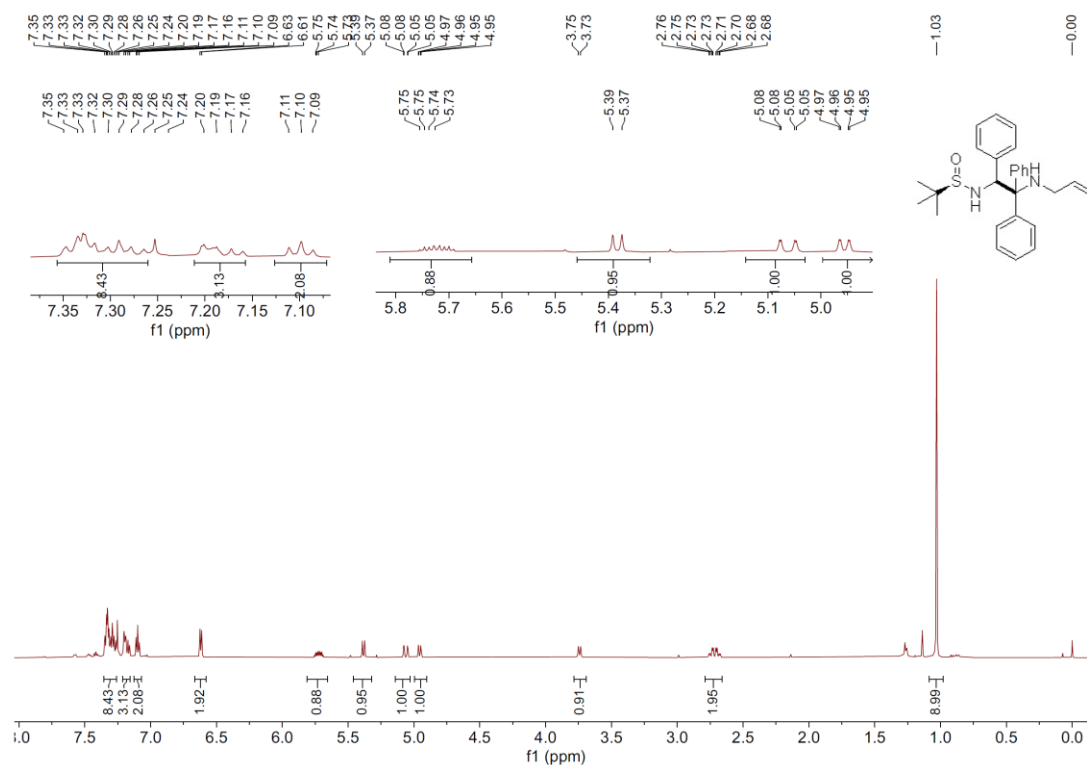
3a ^1H NMR



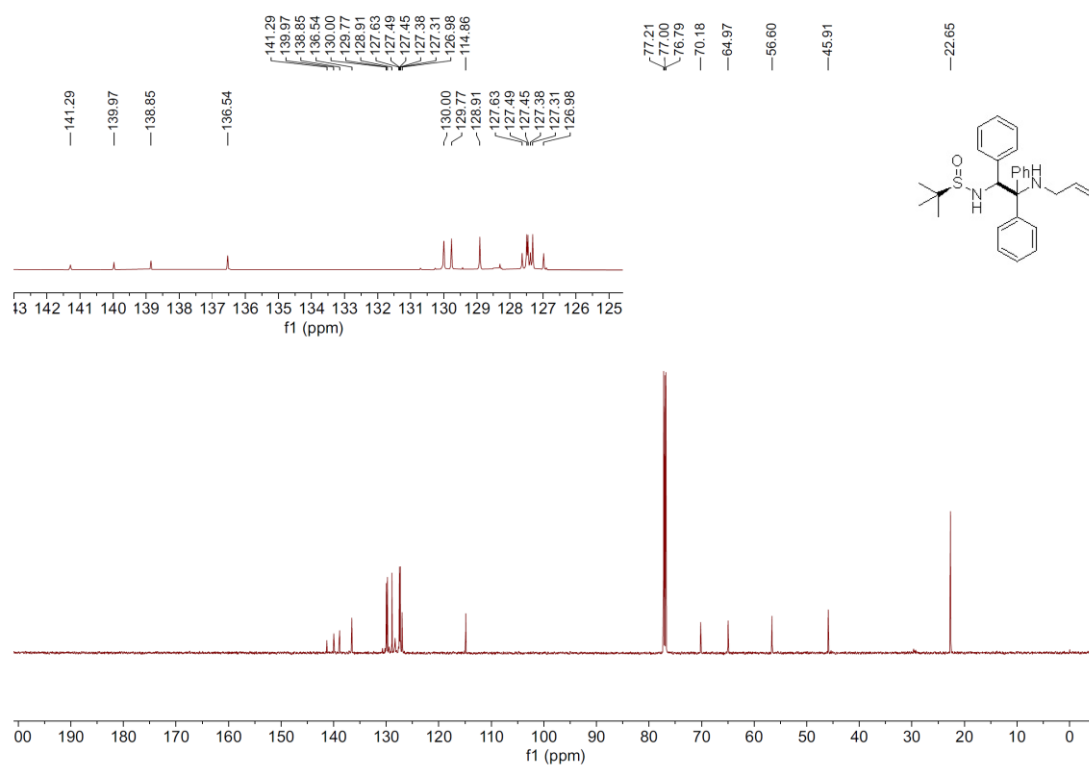
3a ^{13}C NMR



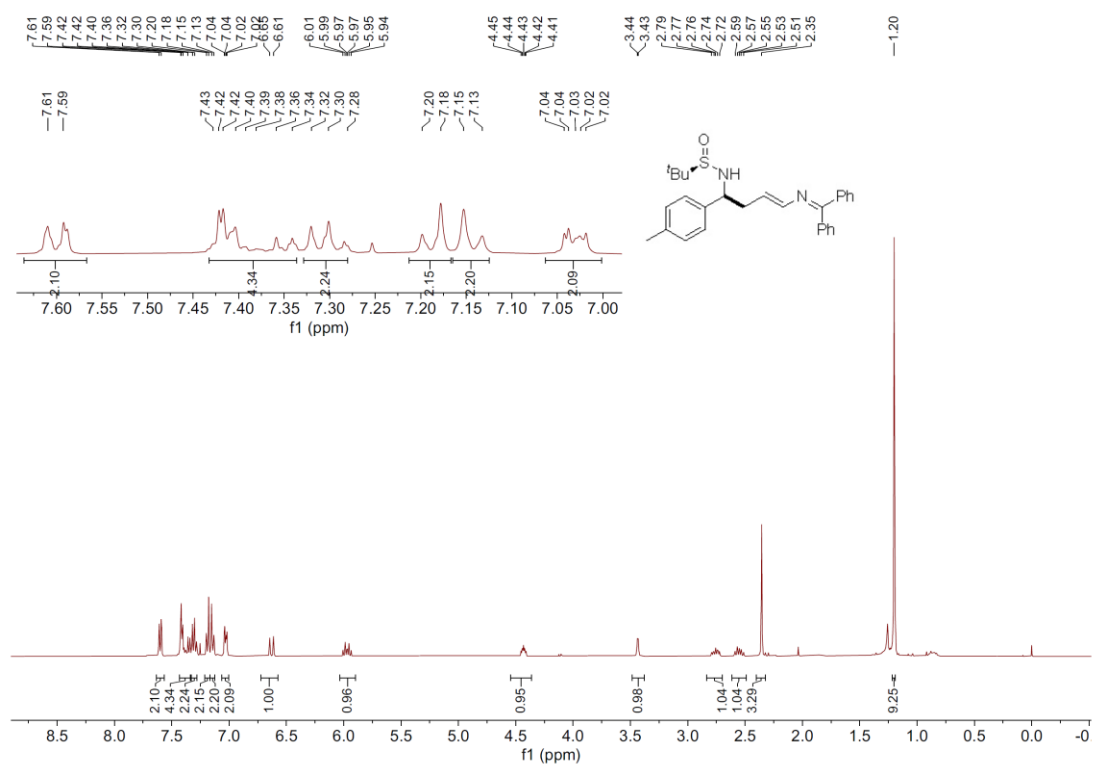
3a' ¹H NMR



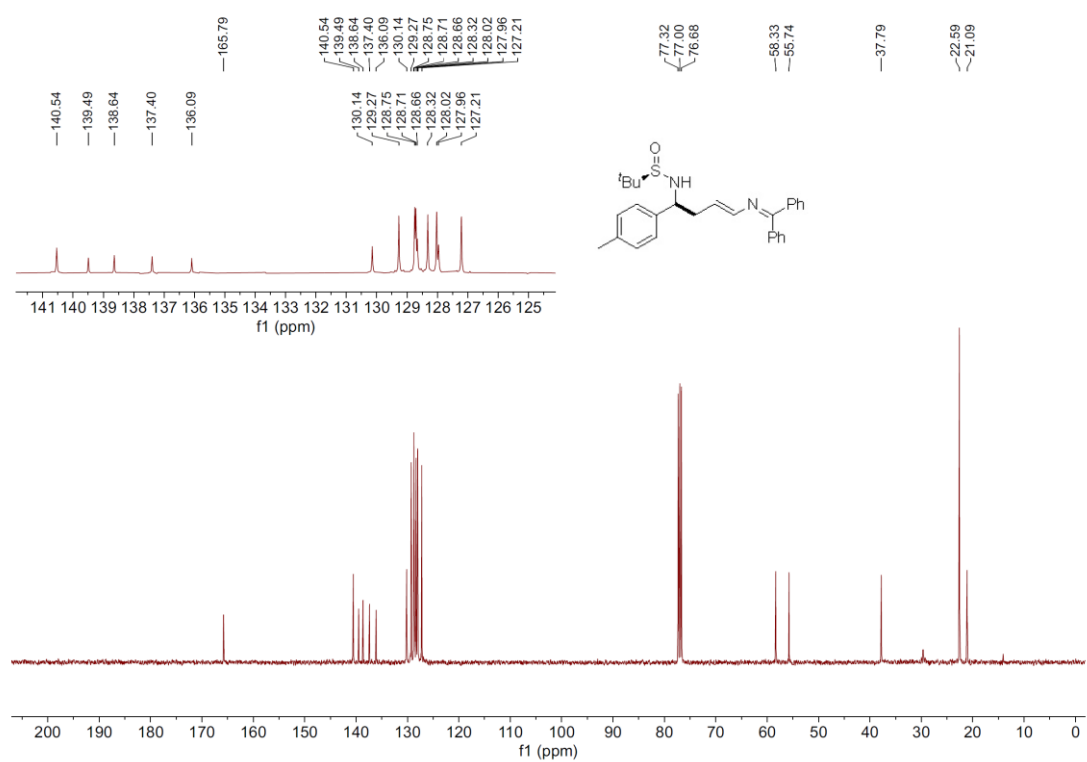
3a' ¹³C NMR



3b ¹H NMR



3b ¹³C NMR



Chemical structure of compound 10: CCc1ccc(cc1)[C@H](NC(=O)C(C)(C)C)C/C=C/N=C(c2ccccc2)c3ccccc3

¹H NMR spectrum (CDCl₃):

Chemical Shift (ppm)	Integration
7.61, 7.59	2.05
7.43, 7.42, 7.41, 7.32, 7.30, 7.23, 7.21, 7.18, 7.16, 7.15, 7.05, 7.04, 7.03, 6.92, 6.83, 6.63	3.06
6.01, 5.99, 5.98, 5.97, 5.96, 5.94	2.10
4.46, 4.44, 4.43, 4.42	2.18
3.44, 3.43	2.12
2.79, 2.78, 2.76, 2.75, 2.72, 2.68, 2.66, 2.65, 2.63, 2.60, 2.58, 2.56, 2.54, 2.53, 2.52, 2.51, 1.26, 1.24, 1.23, 1.20	2.07
1.26, 1.24, 1.23, 1.20	3.24, 9.22

Chemical structure of the compound is shown above the spectra. The structure is a substituted benzene ring with an ethyl group (Et), a sulfonamide group (SO₂NH-Bu), and a side chain containing a trans-alkene and a phenyl group (Ph).

¹³C NMR Spectrum (Top): The spectrum shows peaks in the aromatic region (127.27 to 143.76 ppm) and a carbonyl region (136.12 to 165.80 ppm). The peaks are labeled with their chemical shifts in ppm.

¹H NMR Spectrum (Bottom): The spectrum shows peaks in the aromatic region (7.668 to 7.732 ppm) and a carbonyl region (55.75 to 58.36 ppm). The peaks are labeled with their chemical shifts in ppm.

Chemical structure of compound 10: CC(C)c1ccc(cc1)C(=O)N[C@@H](C/C=C/N=C(c2ccccc2)c3ccccc3)C(=O)O

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis is labeled f1 (ppm) and ranges from 6.5 to 7.65. The spectrum shows several multiplets and doublets. Integration values are provided below the peaks: 2.09, 3.20, 2.28, 2.11, 2.22, 2.13, 2.13, 1.03, 0.96, 1.00, 0.98, 1.06, 1.02, 0.99, 6.07, 9.38.

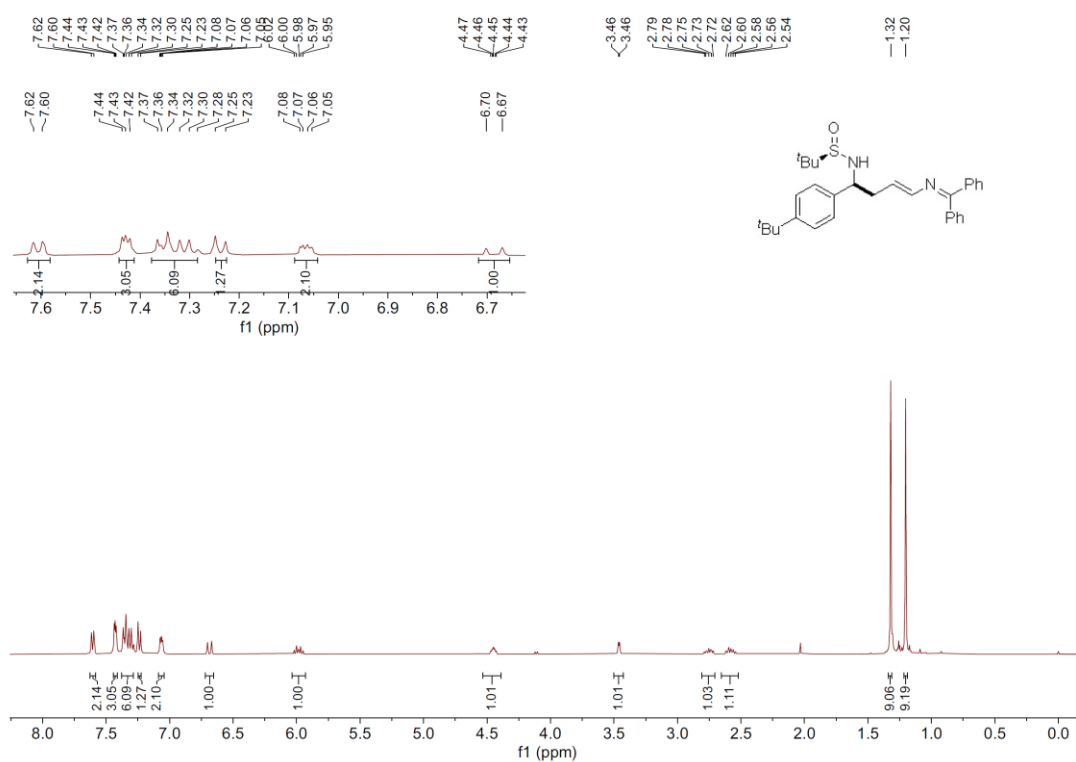
¹³C NMR spectrum (CDCl₃) of compound 10. The x-axis is labeled f1 (ppm) and ranges from 1.20 to 126.07. The spectrum shows several sharp peaks. Integration values are provided below the peaks: 1.26, 1.24, 1.20, 6.07, 9.38.

Chemical structure of compound 10: CC(C)c1ccc(cc1)[C@H](NC(=O)C(C)C)C/C=C/N=C(c2ccccc2)C(=O)c3ccccc3

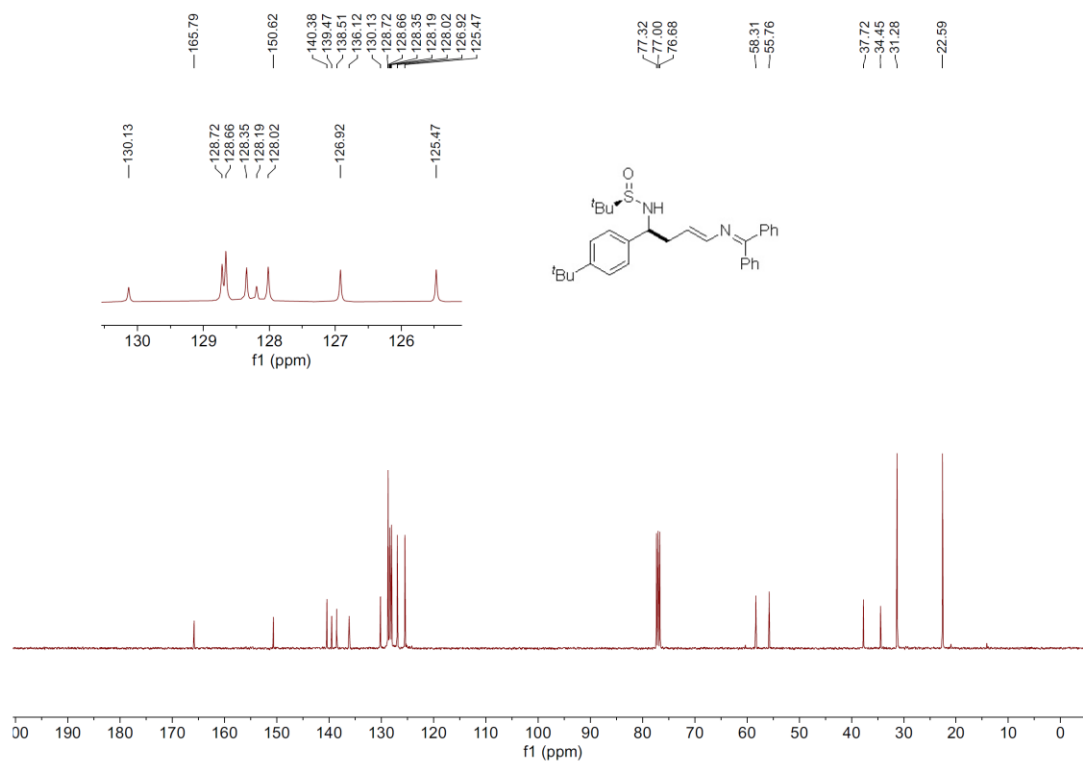
¹³C NMR spectrum (top): CDCl₃. Peaks (ppm): 148.36, 140.43, 139.49, 138.93, 136.12, 130.14, 128.73, 128.66, 128.34, 128.14, 128.02, 127.22, 126.63, 130.14, 128.73, 128.66, 128.34, 128.14, 128.02, 127.22, 126.63, 128.02, 127.22, 126.63.

¹³C NMR spectrum (bottom): DMSO-d₆. Peaks (ppm): 165.78, 148.36, 140.43, 139.49, 138.93, 136.12, 130.14, 128.73, 128.66, 128.34, 128.14, 128.02, 127.22, 126.63, 128.02, 127.22, 126.63, 77.32, 77.00, 76.68, 58.36, 55.74, 37.76, 33.74, 23.94, 23.89, 22.60.

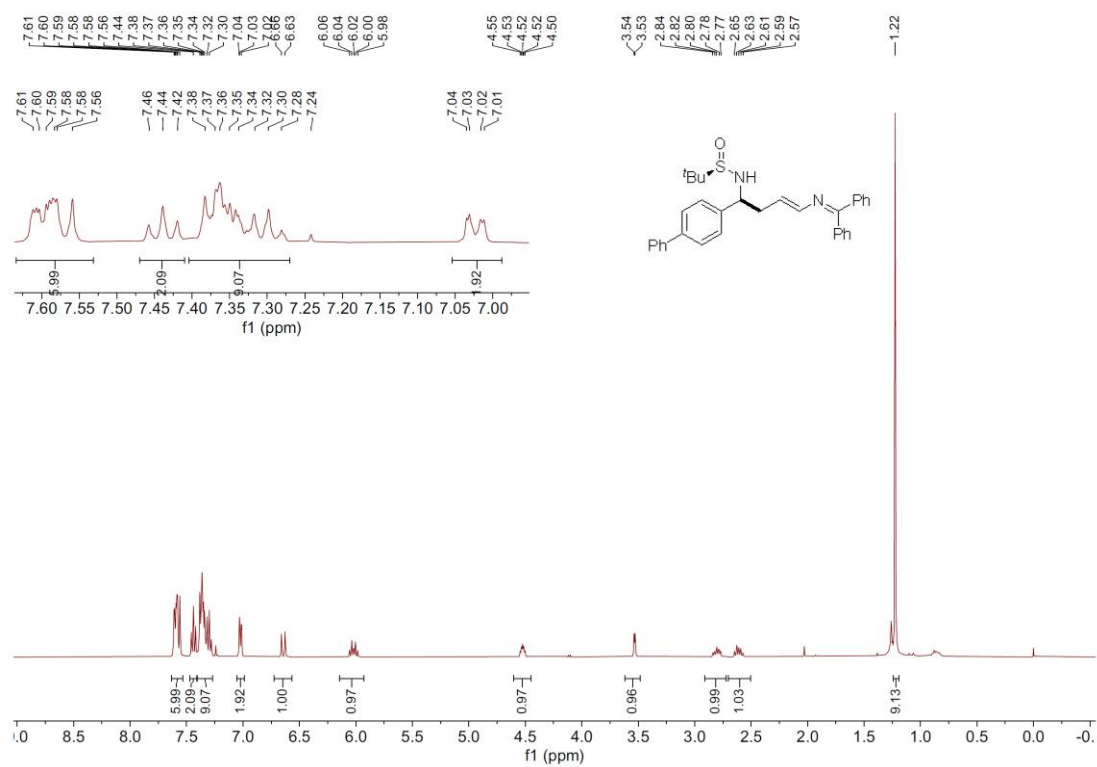
3e ¹H NMR



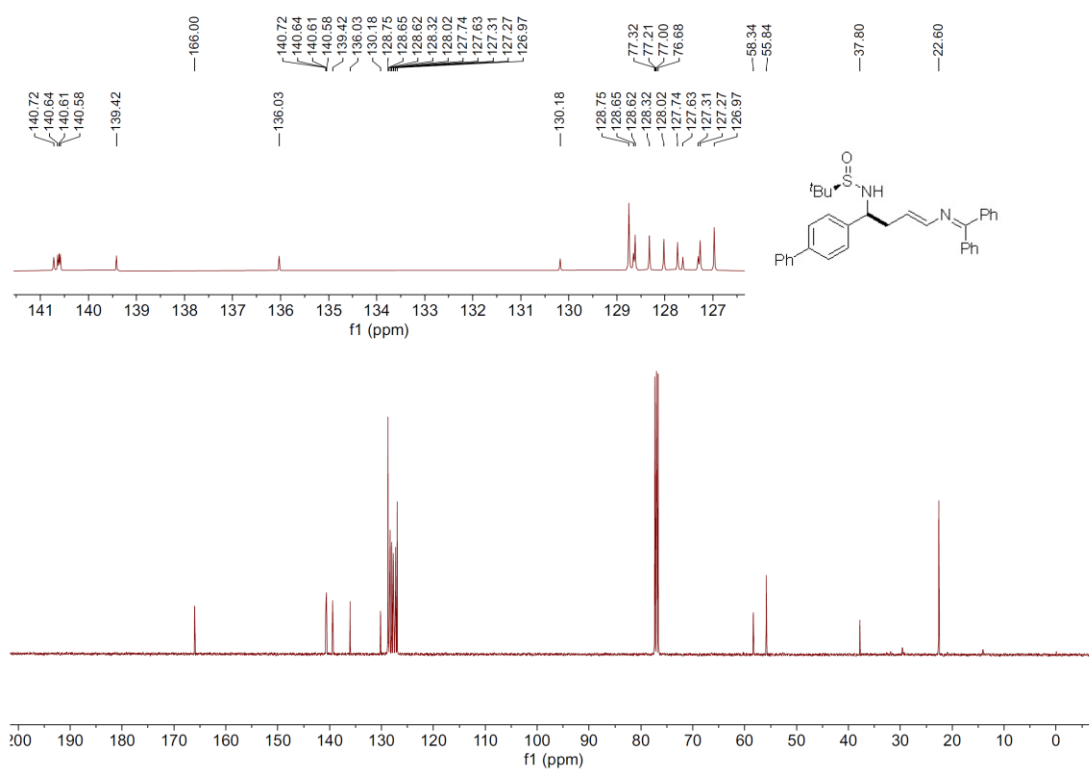
3e ¹³C NMR



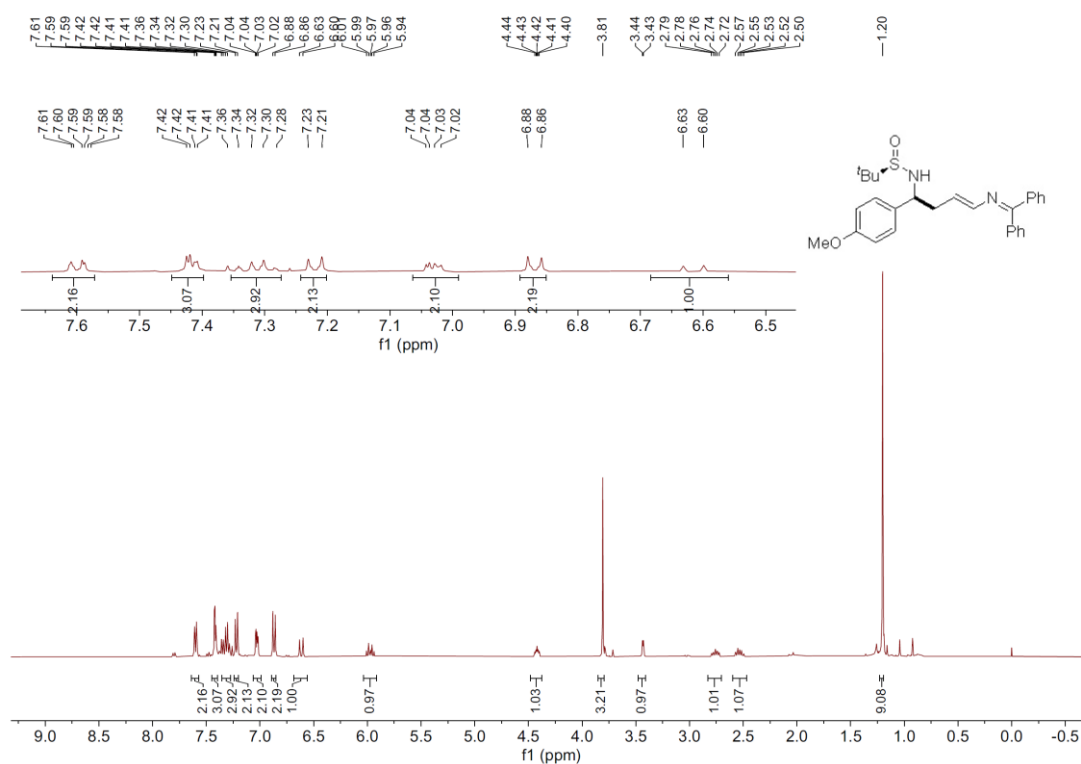
3f ¹H NMR



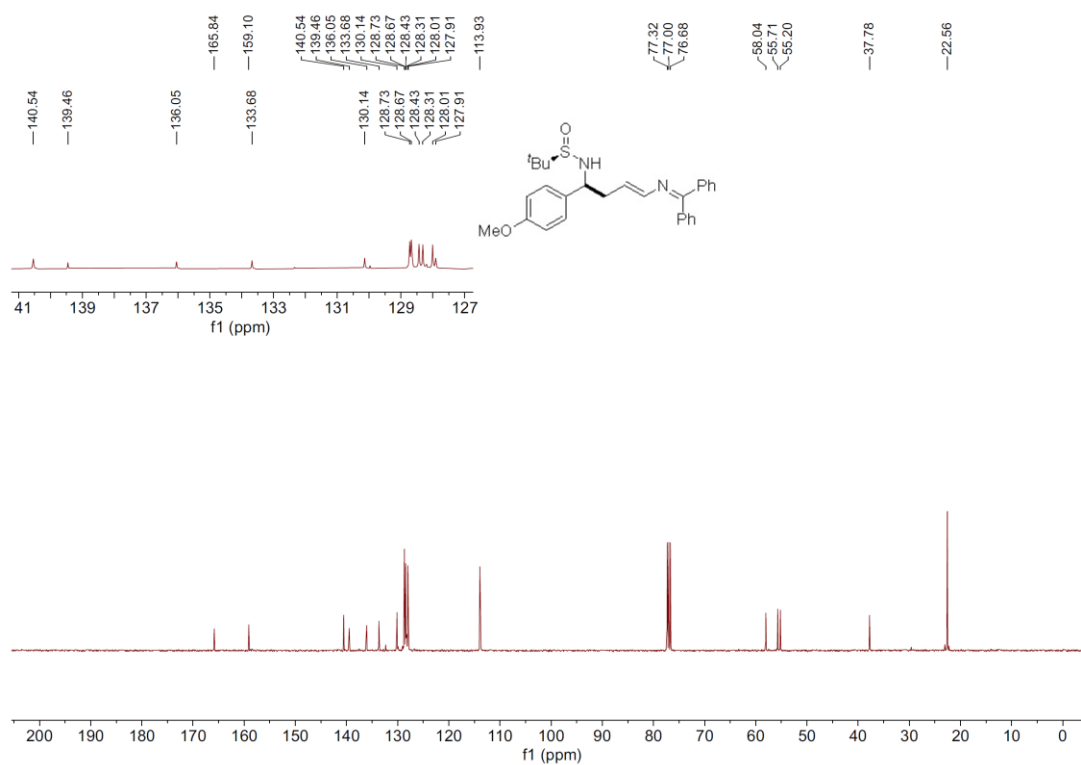
3f ¹³C NMR



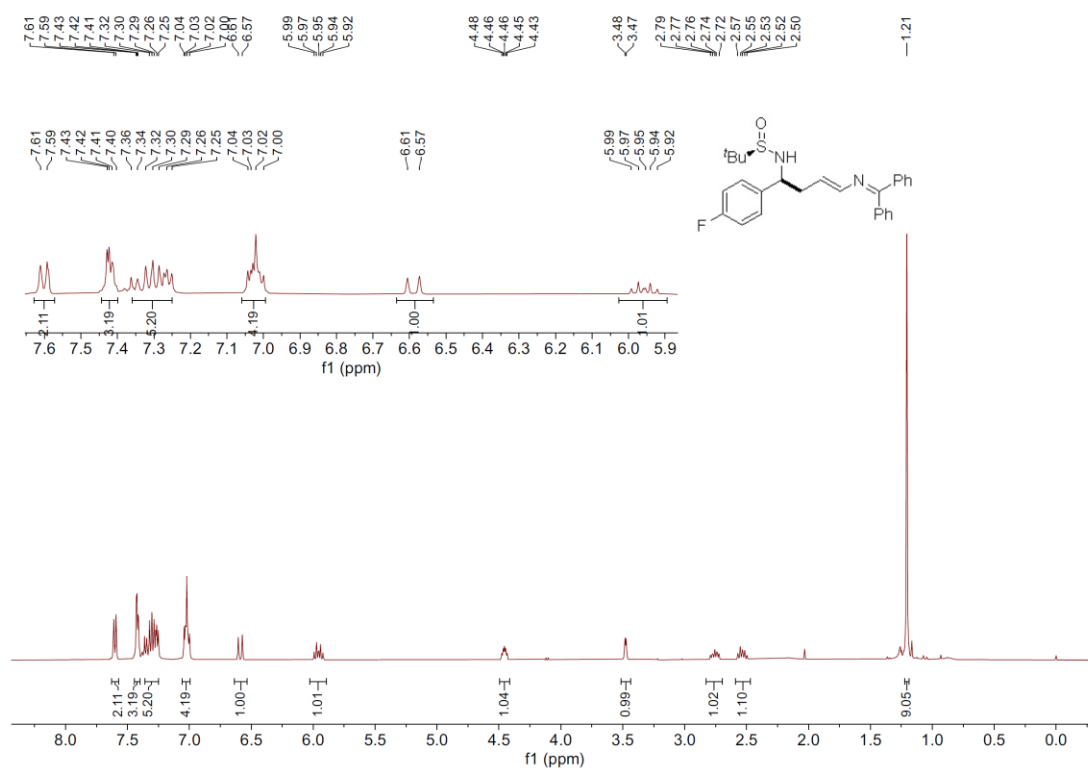
3g ¹H NMR



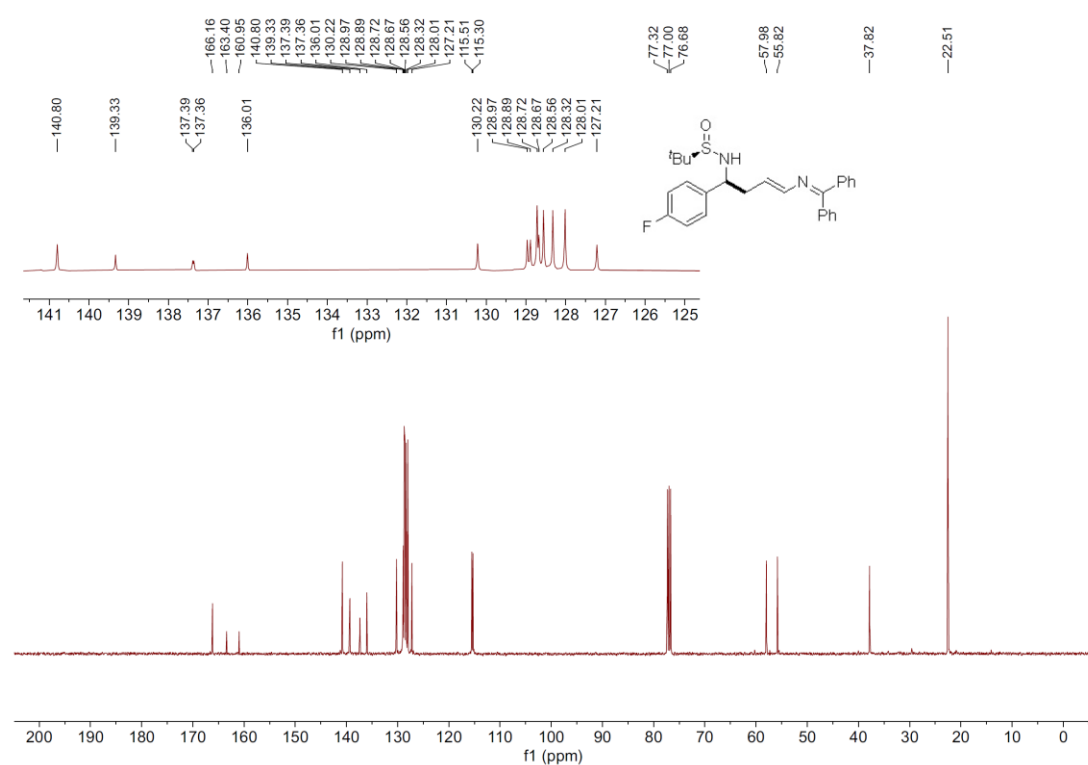
3g ¹³C NMR



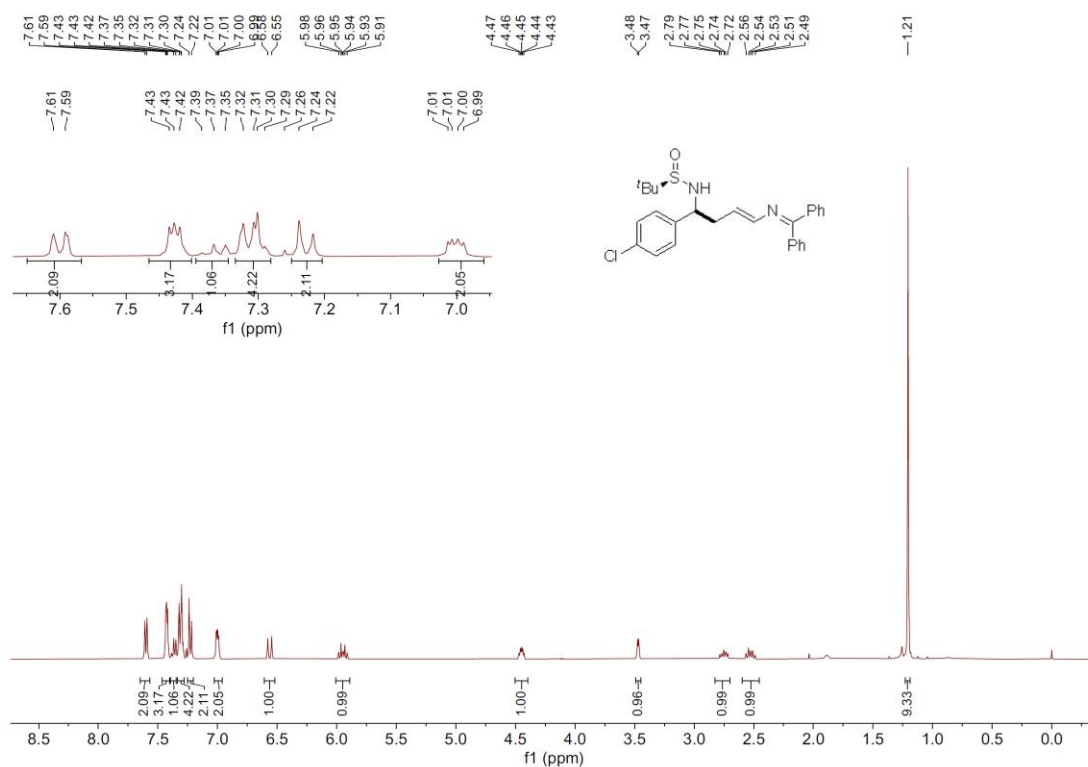
3h ^1H NMR



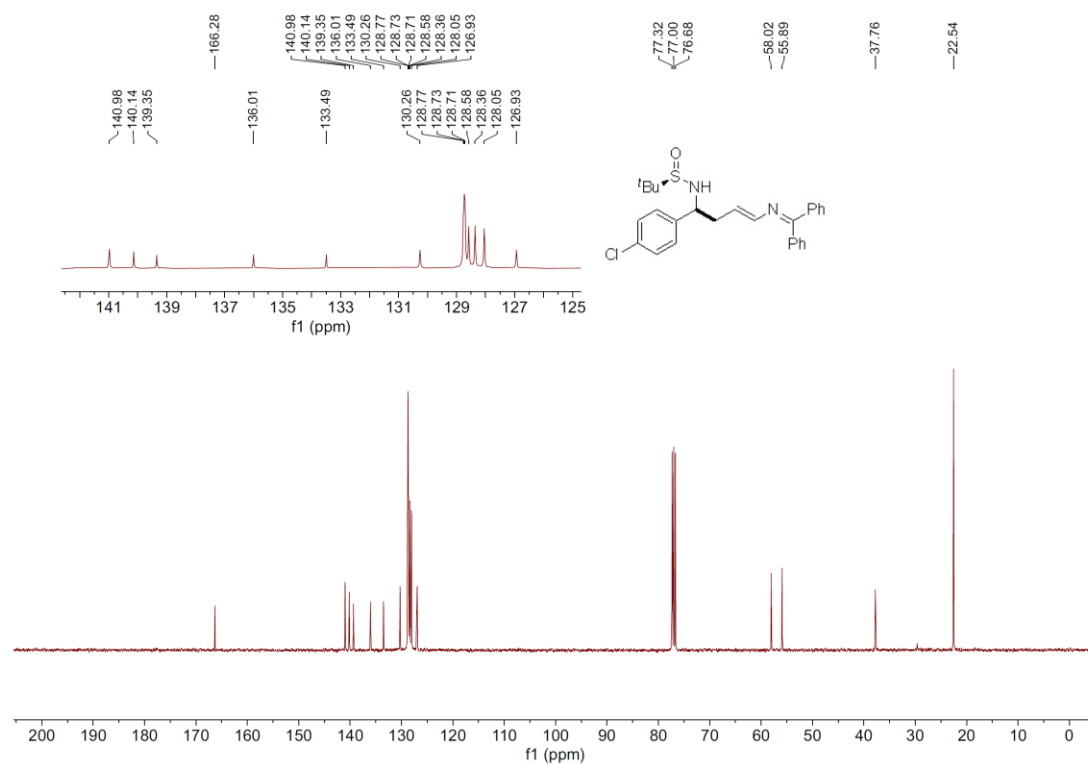
3h ^{13}C NMR



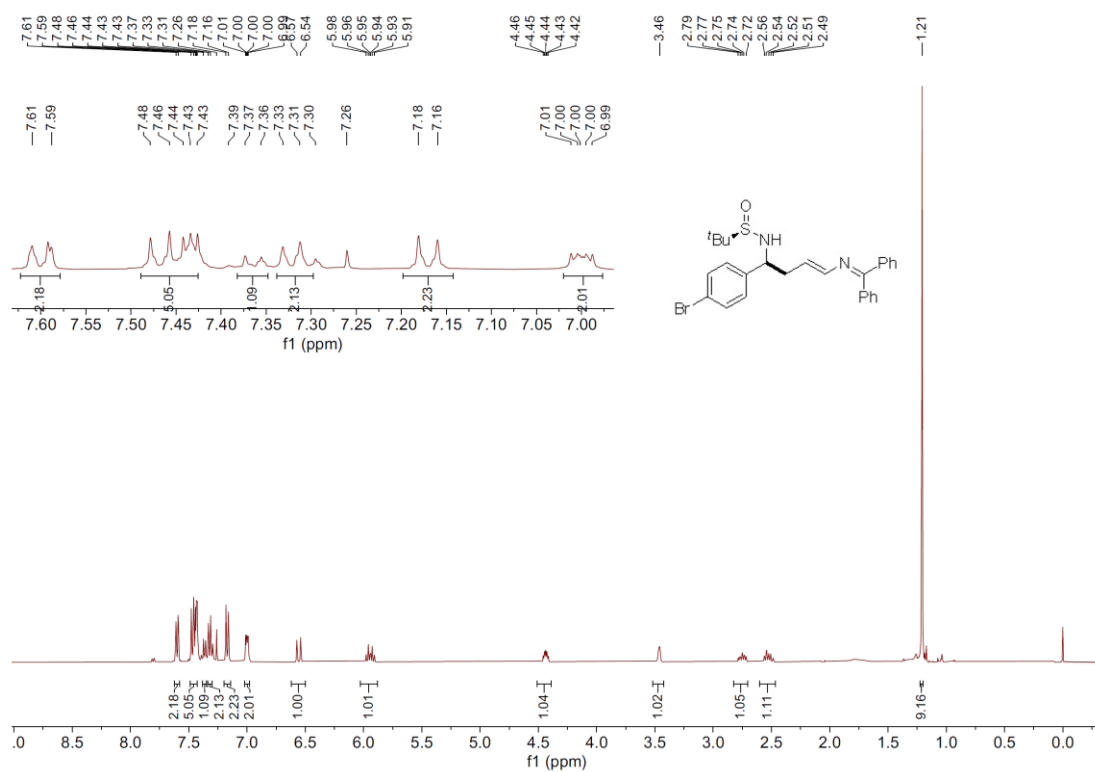
3i ¹H NMR



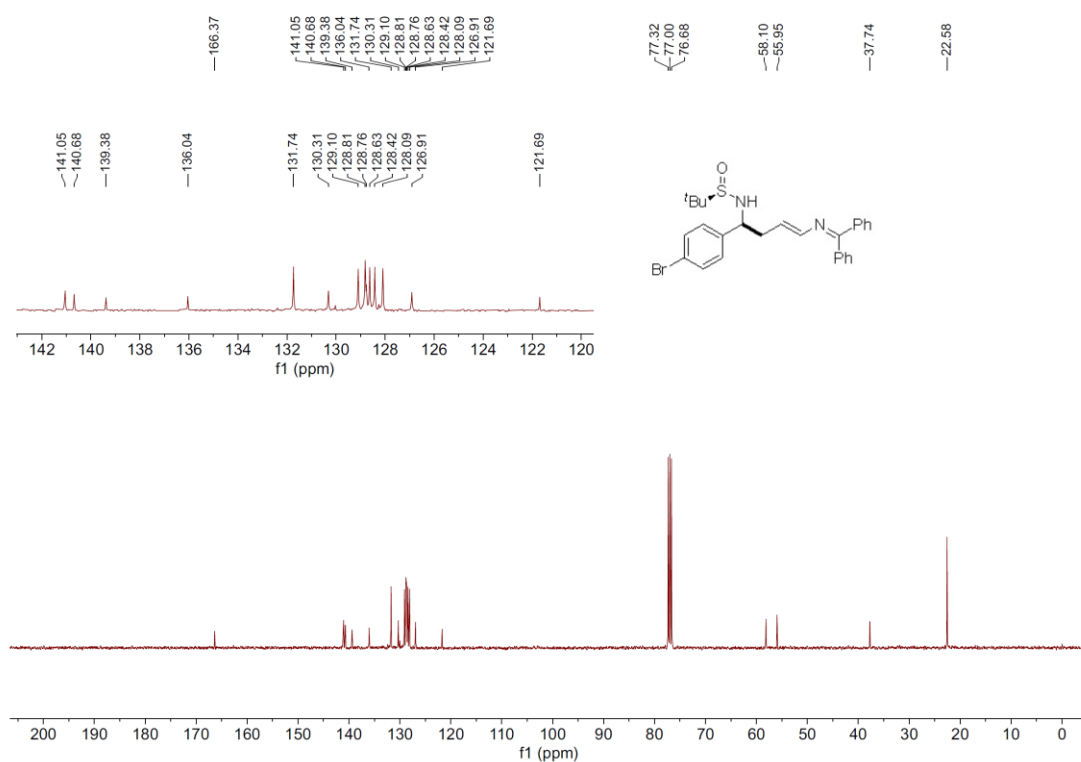
3i ¹³C NMR



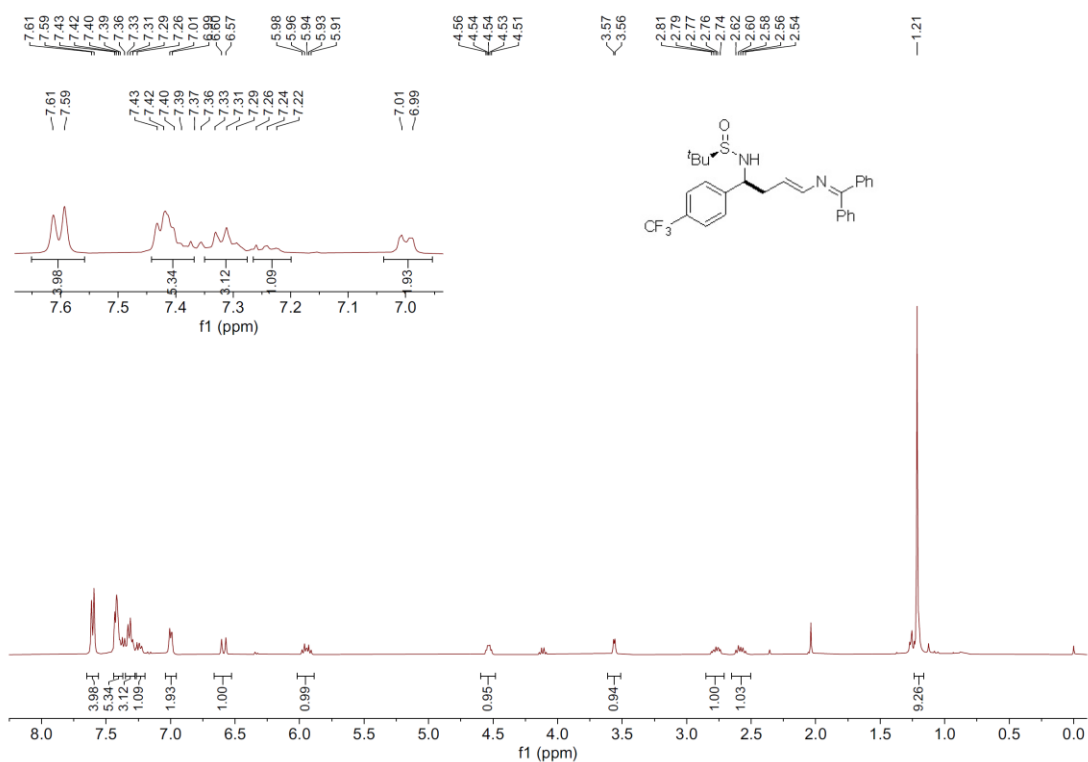
3j ¹H NMR



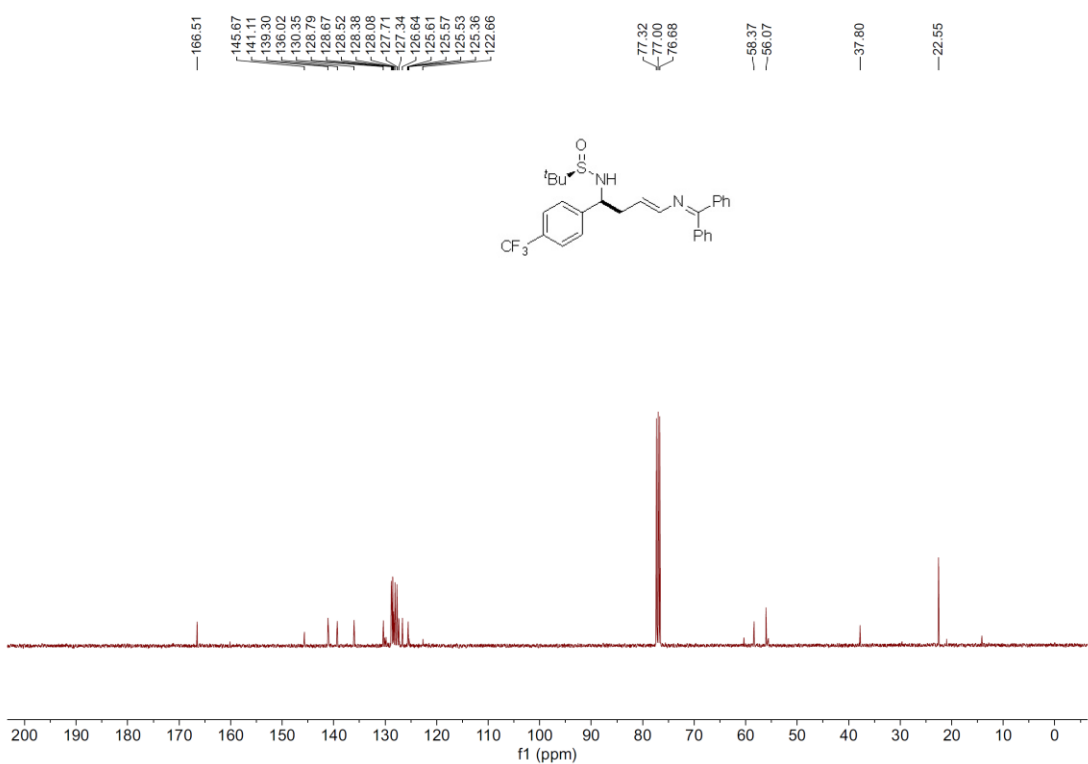
3j ¹³C NMR



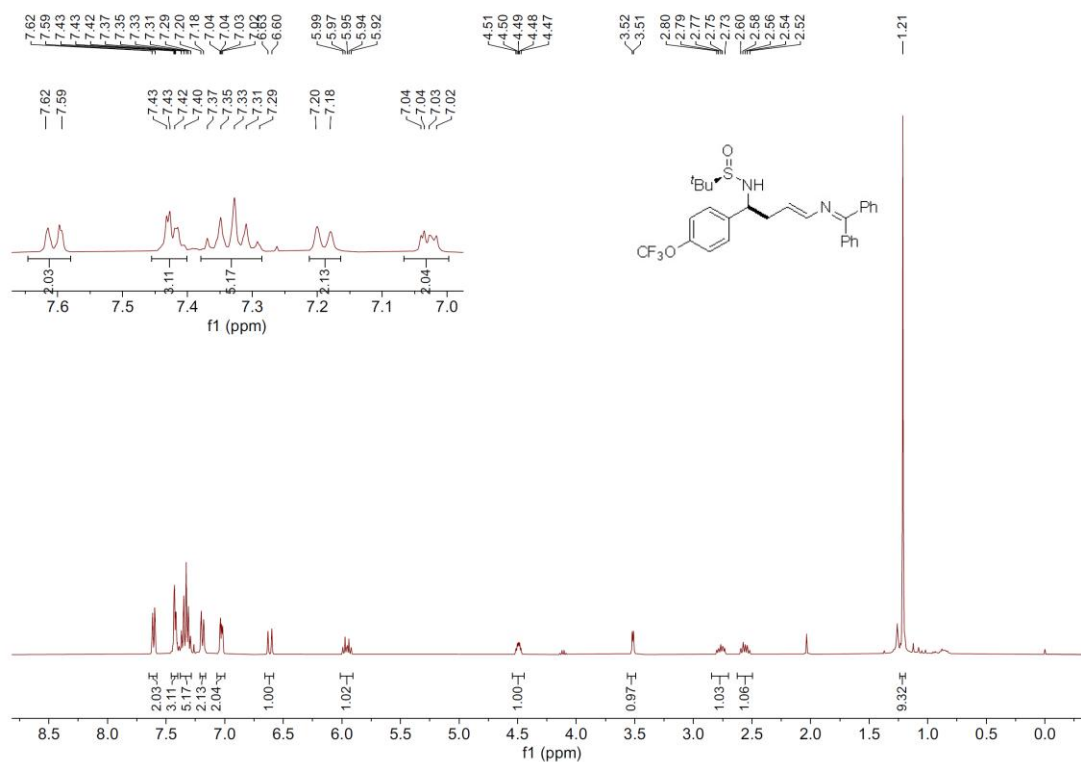
3k ¹H NMR



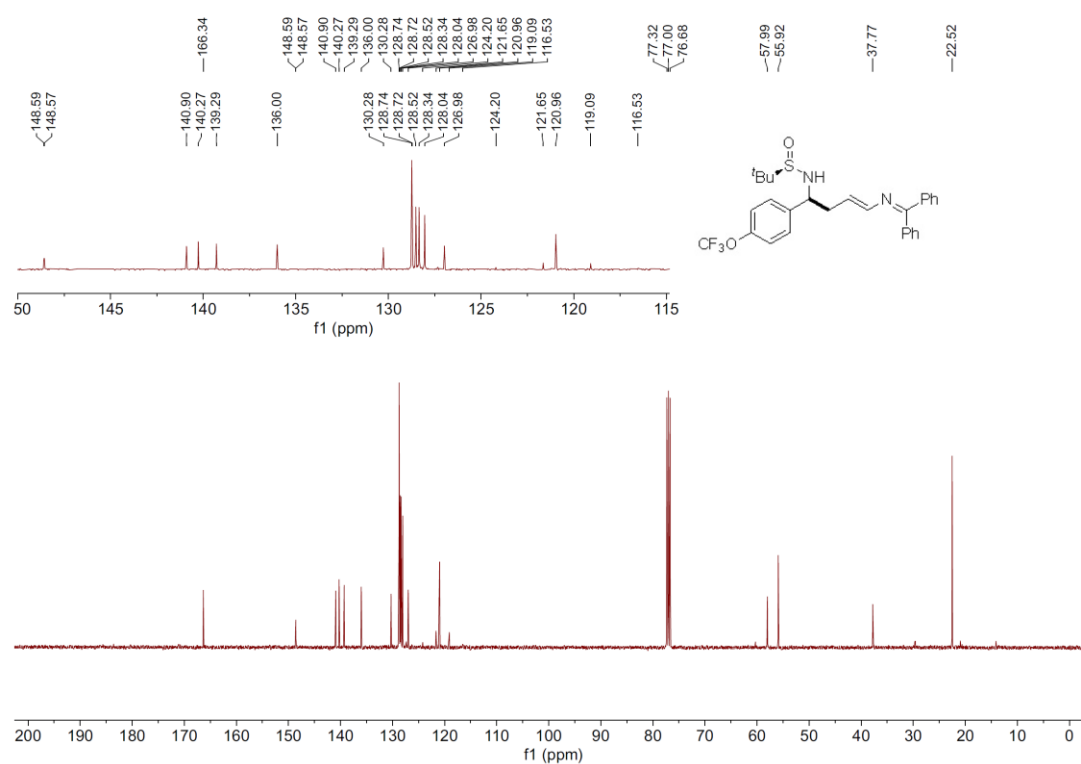
3k ¹³C NMR



31 ¹H NMR



31 ¹³C NMR



Chemical structure of compound 10:

CC(C)(C)C(=O)N[C@@H](Cc1ccc(cc1)C(F)(F)F)/C=C/N=C(c2ccccc2)c3ccccc3

¹H NMR spectrum (CDCl₃):

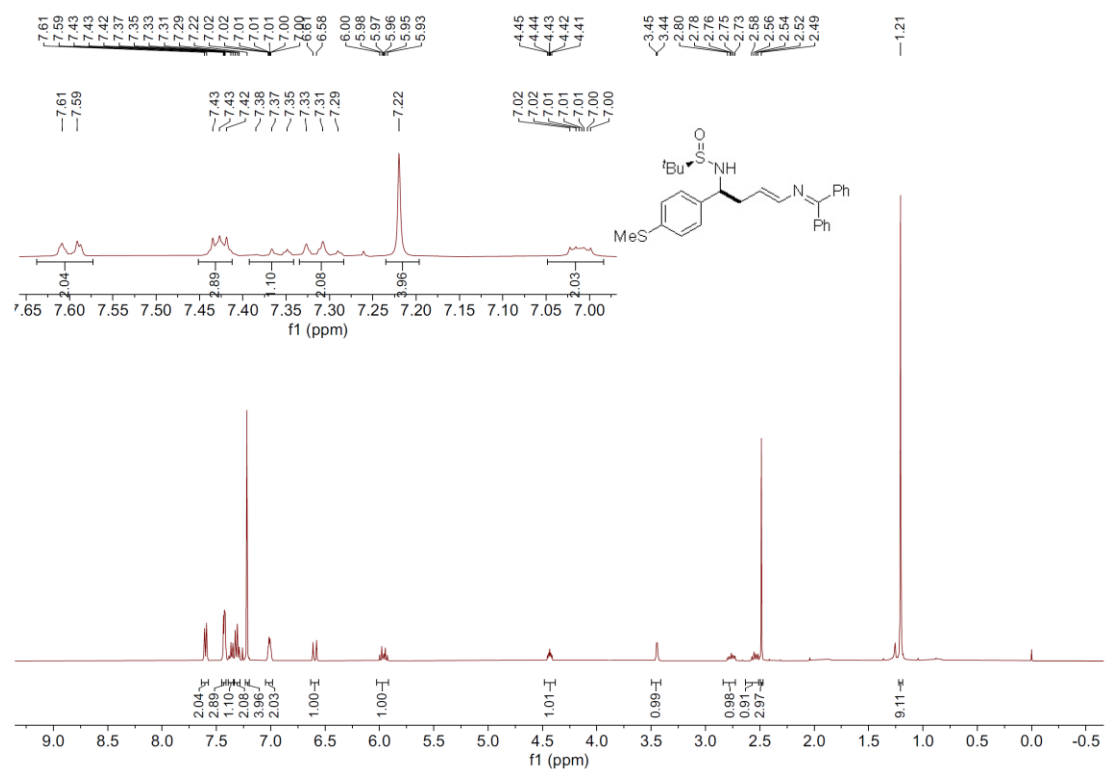
Chemical Shift (ppm)	Integration
7.61, 7.59, 7.44, 7.43, 7.42, 7.41, 7.39, 7.37, 7.35, 7.33, 7.31, 7.29, 7.26, 7.10, 7.08, 7.04, 7.03, 7.02	2.06, 3.05, 1.17, 2.11, 2.04
6.70, 6.63, 6.59, 6.52	2.09
6.33	1.01
5.99, 5.97, 5.95, 5.93, 5.91	0.98
4.47, 4.46	1.02, 1.04
3.47, 3.46	9.18
2.80, 2.79, 2.76, 2.74, 2.73, 2.59, 2.57, 2.55, 2.51	
1.21	

The figure displays the ¹³C NMR spectra of compound 10 in CDCl₃. The top spectrum is the ¹³C NMR spectrum, showing peaks from 130 to 140 ppm. The bottom spectrum is the ¹H NMR spectrum, showing peaks from 7 to 8 ppm. The chemical structure of compound 10 is shown on the right, featuring a 4-(difluoromethoxy)phenyl group, a tert-butyl group, and a 1-phenyl-2-((4-(difluoromethoxy)phenyl)amino)eth-1-en-1-yl group.

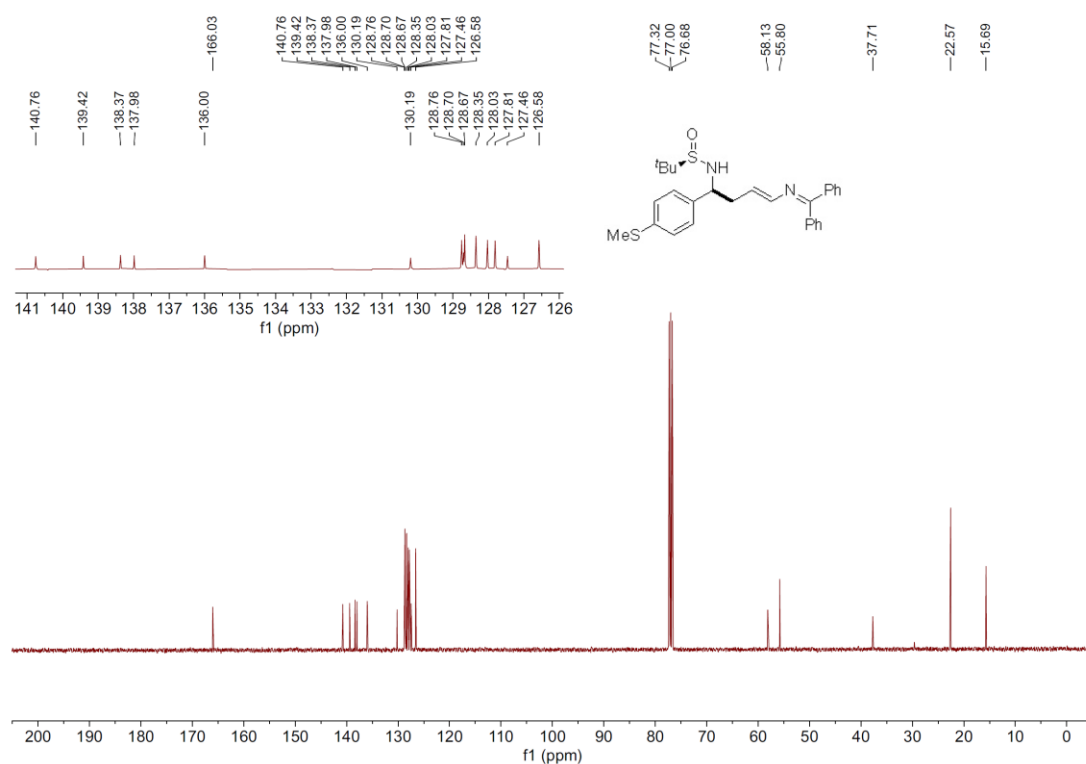
¹³C NMR peaks (ppm): 166.26, 140.85, 139.34, 138.78, 136.02, 130.27, 128.79, 128.75, 128.73, 128.36, 128.06, 127.18, 119.55, 118.37, 115.79, 113.20, 77.32, 77.20, 77.00, 76.68, 58.05, 55.89, 37.79, 22.55, -0.06.

¹H NMR peaks (ppm): 7.90, 7.85, 7.80, 7.75, 7.70, 7.65, 7.60, 7.55, 7.50, 7.45, 7.40, 7.35, 7.30, 7.25, 7.20, 7.15, 7.10, 7.05, 7.00, 6.95, 6.90, 6.85, 6.80, 6.75, 6.70, 6.65, 6.60, 6.55, 6.50, 6.45, 6.40, 6.35, 6.30, 6.25, 6.20, 6.15, 6.10, 6.05, 6.00, 5.95, 5.90, 5.85, 5.80, 5.75, 5.70, 5.65, 5.60, 5.55, 5.50, 5.45, 5.40, 5.35, 5.30, 5.25, 5.20, 5.15, 5.10, 5.05, 5.00, 4.95, 4.90, 4.85, 4.80, 4.75, 4.70, 4.65, 4.60, 4.55, 4.50, 4.45, 4.40, 4.35, 4.30, 4.25, 4.20, 4.15, 4.10, 4.05, 4.00, 3.95, 3.90, 3.85, 3.80, 3.75, 3.70, 3.65, 3.60, 3.55, 3.50, 3.45, 3.40, 3.35, 3.30, 3.25, 3.20, 3.15, 3.10, 3.05, 3.00, 2.95, 2.90, 2.85, 2.80, 2.75, 2.70, 2.65, 2.60, 2.55, 2.50, 2.45, 2.40, 2.35, 2.30, 2.25, 2.20, 2.15, 2.10, 2.05, 2.00, 1.95, 1.90, 1.85, 1.80, 1.75, 1.70, 1.65, 1.60, 1.55, 1.50, 1.45, 1.40, 1.35, 1.30, 1.25, 1.20, 1.15, 1.10, 1.05, 1.00, 0.95, 0.90, 0.85, 0.80, 0.75, 0.70, 0.65, 0.60, 0.55, 0.50, 0.45, 0.40, 0.35, 0.30, 0.25, 0.20, 0.15, 0.10, 0.05, 0.00.

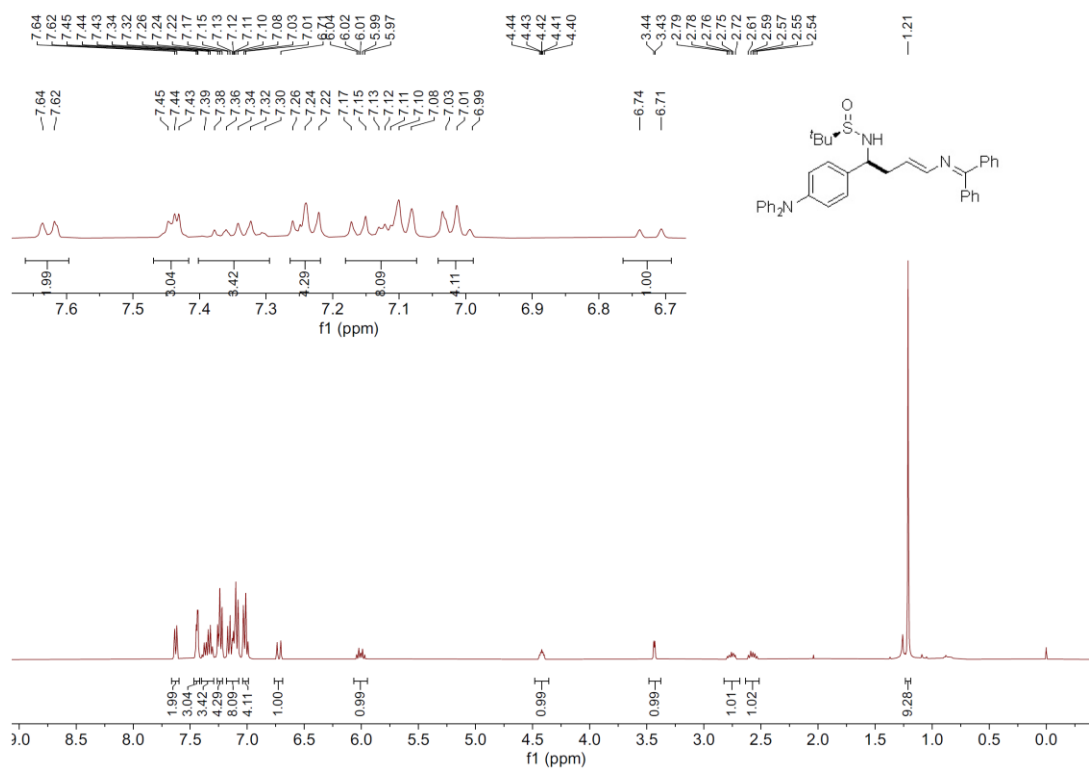
3n ¹H NMR



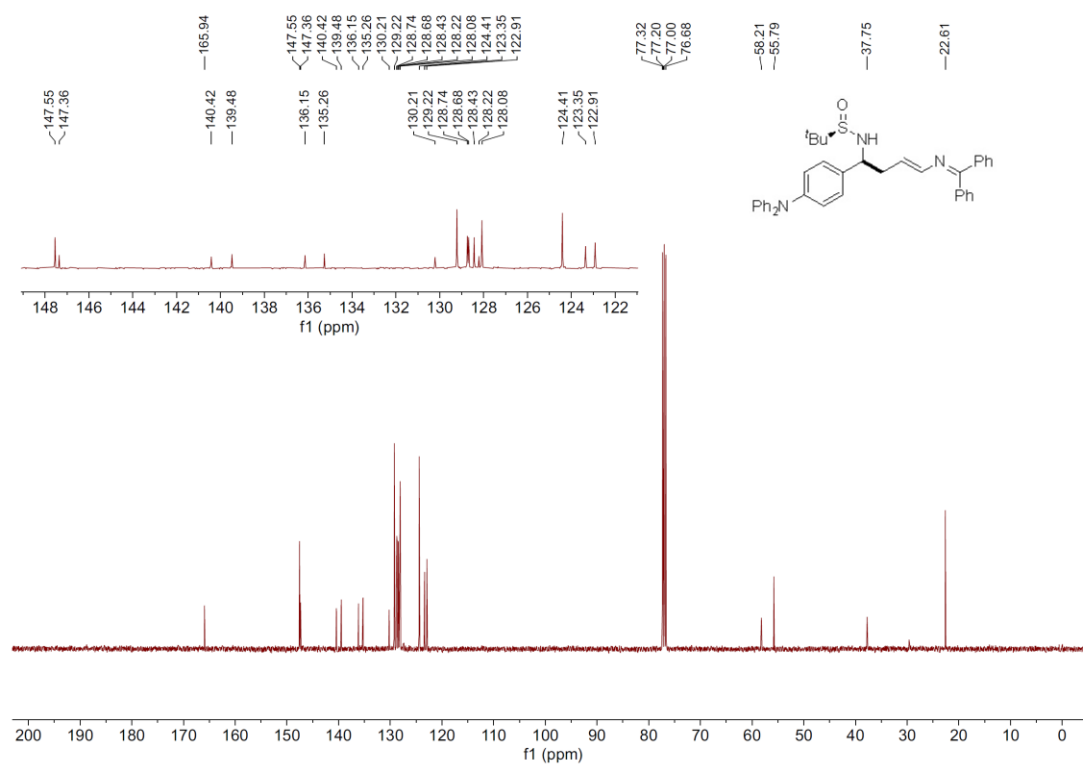
3n ¹³C NMR



3o ^1H NMR



3o ^{13}C NMR



Chemical structure of compound 10: CC(C)(C)N(C(=O)NCC/C=C/C(=N/C1=CC=CC=C1)C2=CC=CC=C2)C3=CC=CC=C3C=C

¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 0.0 to 8.6 ppm. The chemical structure of 10 is shown above the spectrum. The spectrum includes integration values and peak lists for both the main spectrum and an inset.

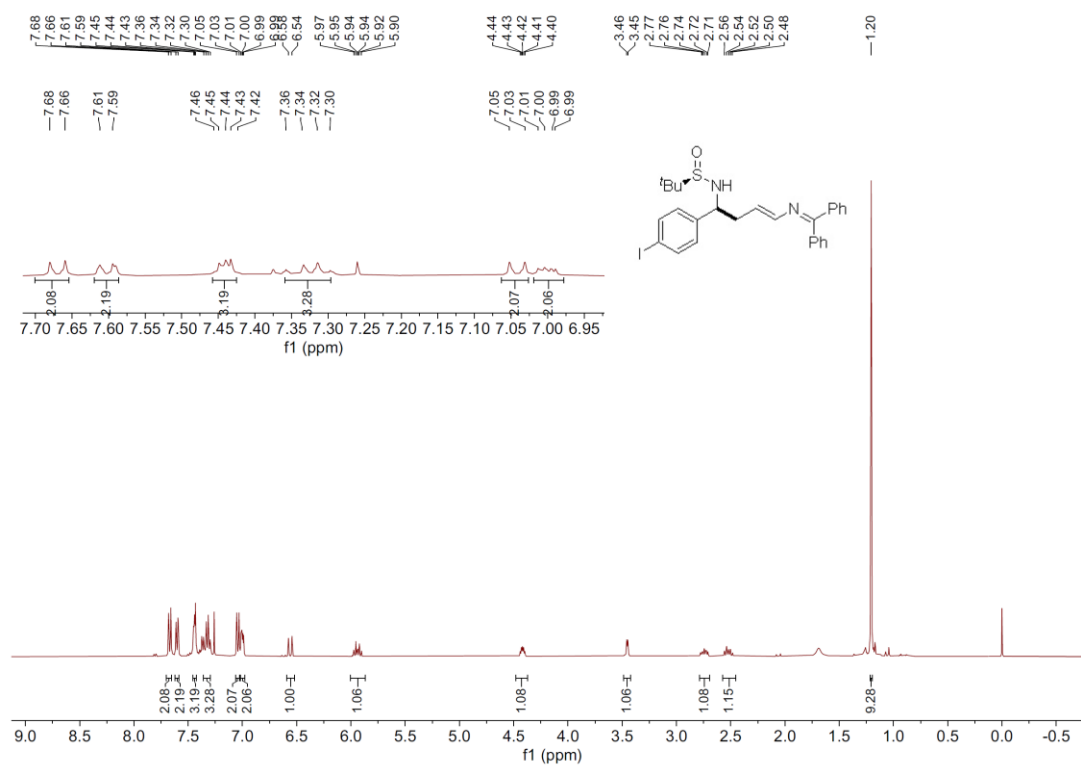
Integration values (from left to right): 2.09, 5.11, 3.09, 2.14, 0.91, 1.22, 1.02, 1.00, 1.07, 0.84, 0.92, 1.09, 1.09, 1.27, 1.24, 9.08.

Peak lists (ppm):

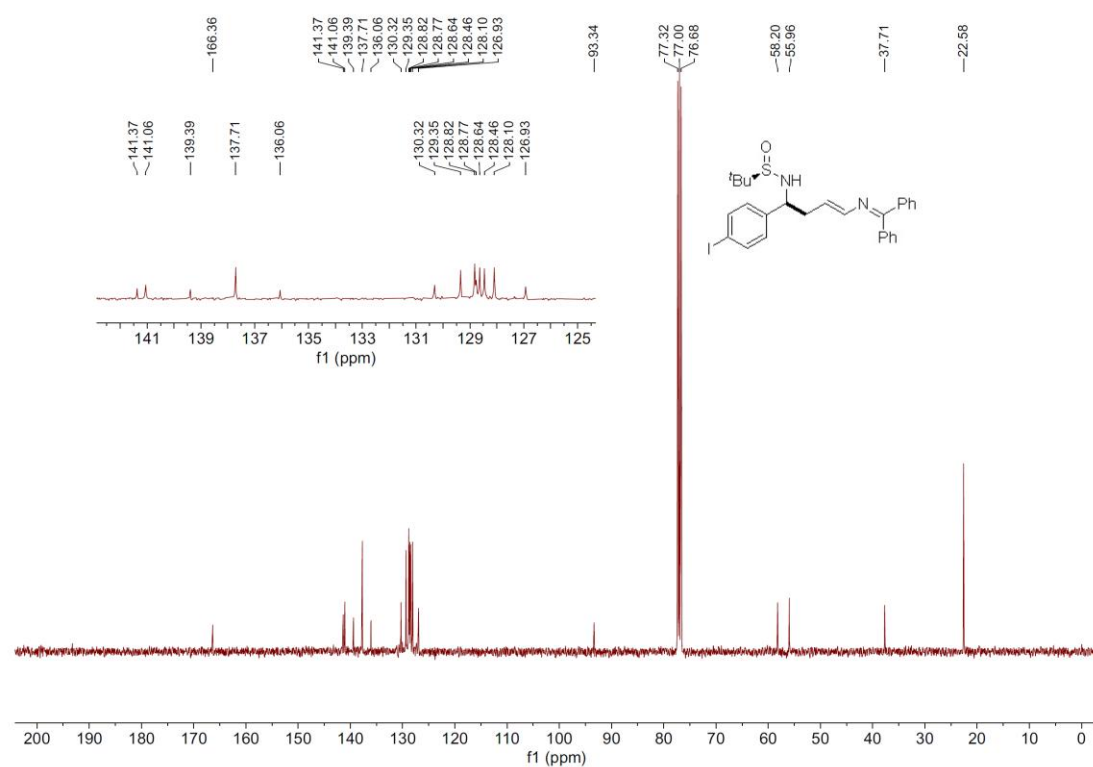
- Main spectrum (from left to right): 7.60, 7.58, 7.52, 7.42, 7.41, 7.38, 7.36, 7.35, 7.32, 7.31, 7.29, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.16, 7.14, 7.01, 6.99, 6.99, 6.98, 6.77, 6.74, 6.72, 6.70, 6.60, 6.57.
- Inset spectrum (from left to right): 7.60, 7.58, 7.52, 7.42, 7.41, 7.38, 7.36, 7.35, 7.32, 7.31, 7.29, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.16, 7.14, 7.01, 6.99, 6.99, 6.98, 6.77, 6.74, 6.72, 6.70, 6.60, 6.57.

[illegible]

3q ¹H NMR



3q ¹³C NMR



Chemical structure of compound 10: CCOC(=O)c1ccc(cc1)[C@H](NC(=O)C/C=C/N=C(c2ccccc2)C(=O)c3ccccc3)C

¹H NMR spectrum (CDCl₃) of compound 10. The x-axis represents the chemical shift in ppm, ranging from 0.0 to 9.0. The spectrum shows several peaks with corresponding integration values.

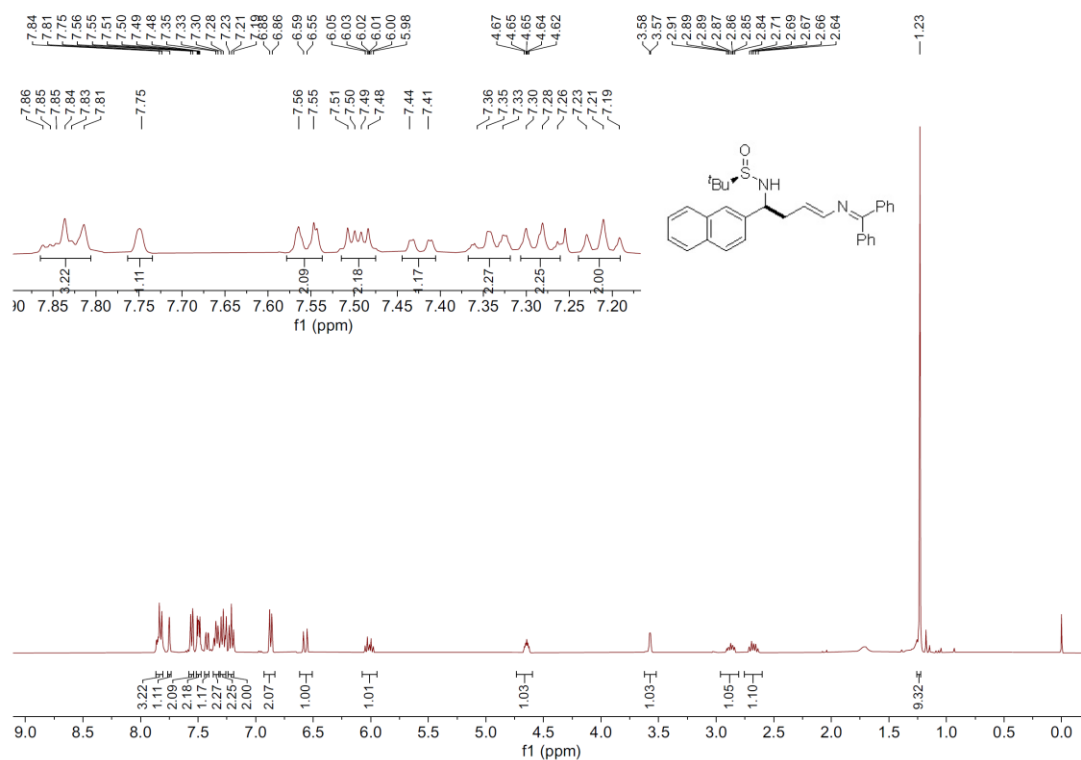
Chemical shift (ppm): 8.03, 8.01, 7.61, 7.59, 7.43, 7.42, 7.41, 7.39, 7.40, 7.37, 7.37, 7.35, 7.32, 7.31, 7.28, 7.26, 7.25, 7.24, 7.23, 7.22, 7.21, 7.20, 7.19, 7.18, 7.17, 7.16, 7.15, 7.14, 7.13, 7.12, 7.11, 7.10, 7.09, 7.08, 7.07, 7.06, 7.05, 7.04, 7.03, 7.02, 7.01, 7.00, 6.99, 6.98, 6.97, 6.96, 6.95, 6.94, 6.93, 6.92, 6.91, 6.90, 6.89, 6.88, 6.87, 6.86, 6.85, 6.84, 6.83, 6.82, 6.81, 6.80, 6.79, 6.78, 6.77, 6.76, 6.75, 6.74, 6.73, 6.72, 6.71, 6.70, 6.69, 6.68, 6.67, 6.66, 6.65, 6.64, 6.63, 6.62, 6.61, 6.60, 6.59, 6.58, 6.57, 6.56, 6.55, 6.54, 6.53, 6.52, 6.51, 6.50, 6.49, 6.48, 6.47, 6.46, 6.45, 6.44, 6.43, 6.42, 6.41, 6.40, 6.39, 6.38, 6.37, 6.36, 6.35, 6.34, 6.33, 6.32, 6.31, 6.30, 6.29, 6.28, 6.27, 6.26, 6.25, 6.24, 6.23, 6.22, 6.21, 6.20, 6.19, 6.18, 6.17, 6.16, 6.15, 6.14, 6.13, 6.12, 6.11, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 6.00, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91,

Chemical structure of compound 10: CC(C)(C)S(=O)(=O)N[C@@H](Cc1ccc(cc1)C(=O)OCC)/C=C/N=C(\)C2=CC=CC=C2

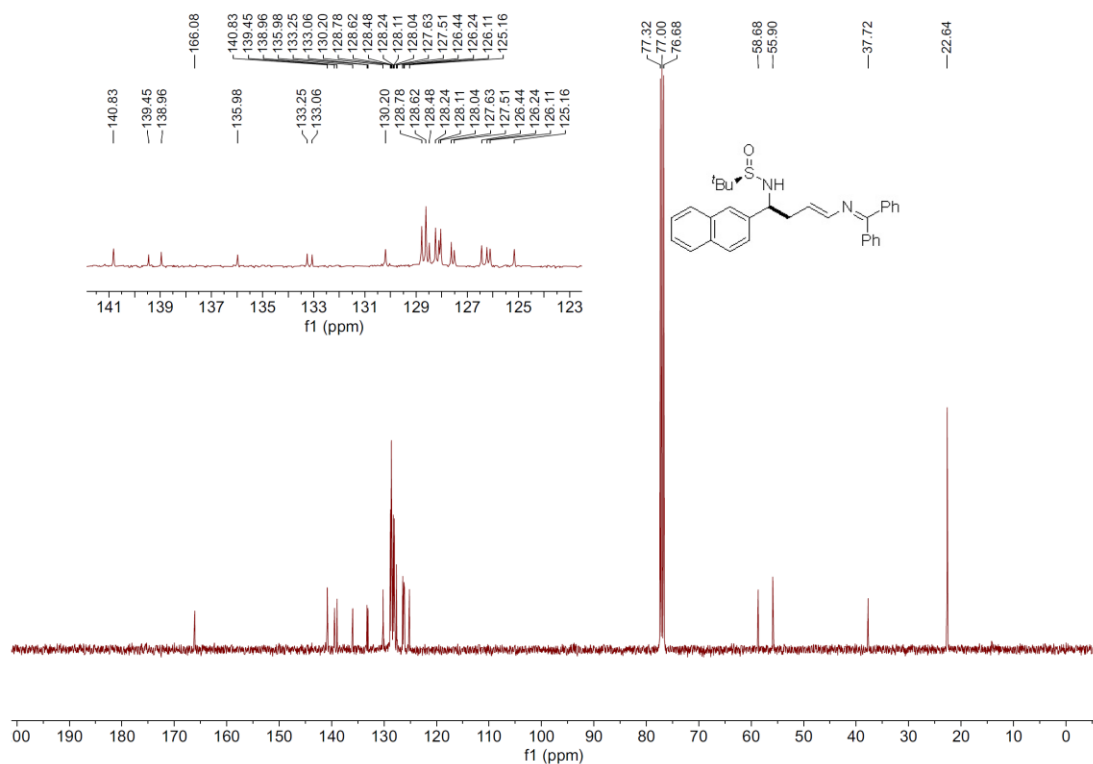
¹³C NMR spectrum (top): Peaks (ppm) are labeled at 130.37, 129.86, 128.77, 128.70, 128.59, 128.33, 128.04, 127.23, 126.82, 166.26, 165.70, 146.50, 141.02, 139.34, 135.99, 130.37, 130.25, 129.86, 128.77, 128.70, 128.59, 128.33, 127.23, 126.82, 77.32, 77.20, 77.00, 76.68, 68.35, 58.31, 55.97, 37.77, 22.55, and 21.89.

¹³C NMR spectrum (bottom): Peaks (ppm) are labeled at 166.26, 165.70, 146.50, 141.02, 139.34, 135.99, 130.37, 130.25, 129.86, 128.77, 128.70, 128.59, 128.33, 127.23, 126.82, 77.32, 77.20, 77.00, 76.68, 68.35, 58.31, 55.97, 37.77, 22.55, and 21.89.

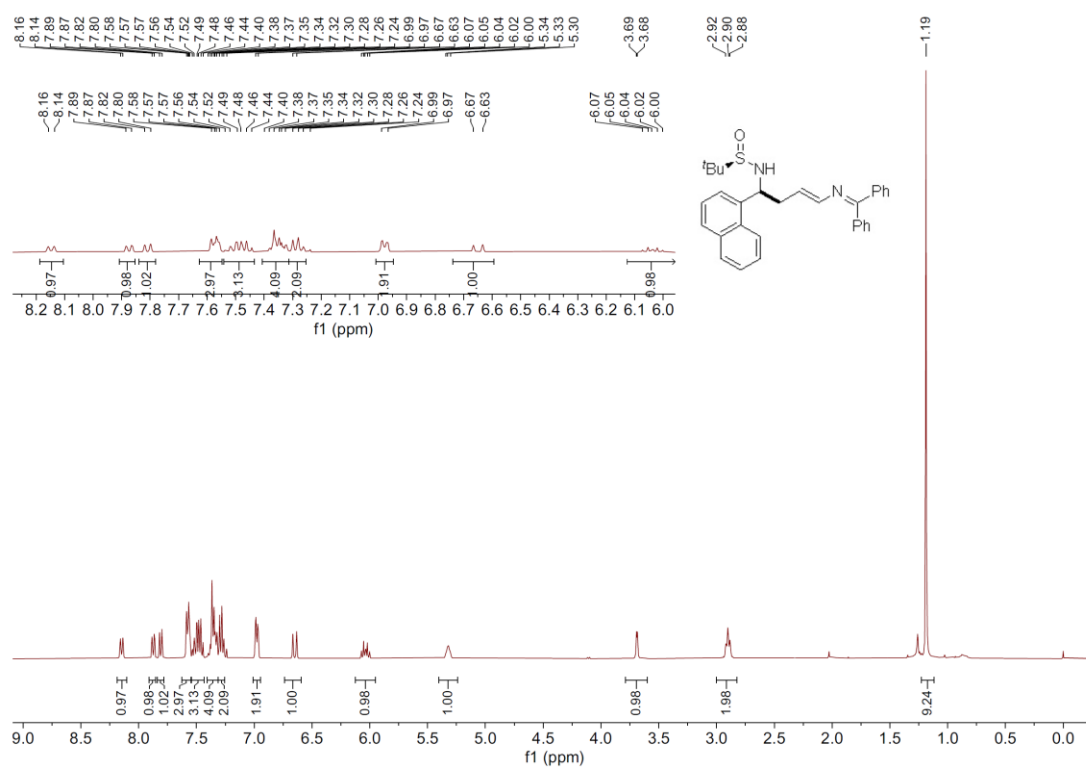
3s ¹H NMR



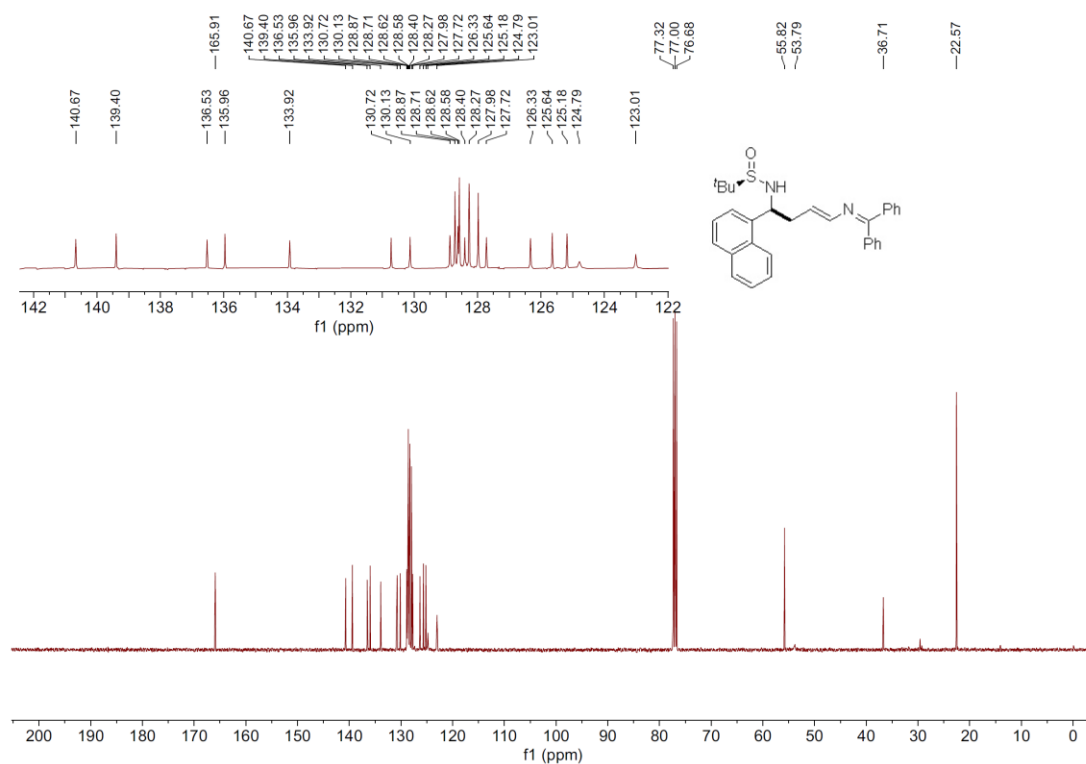
3s ¹³C NMR



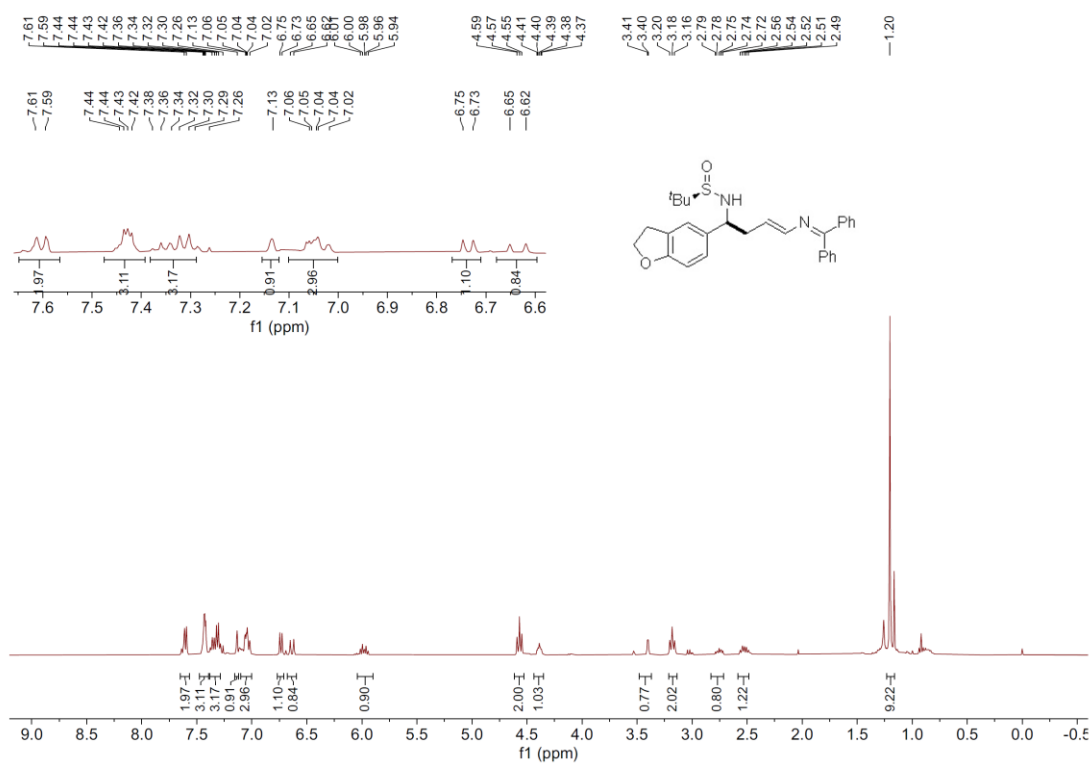
3t ¹H NMR



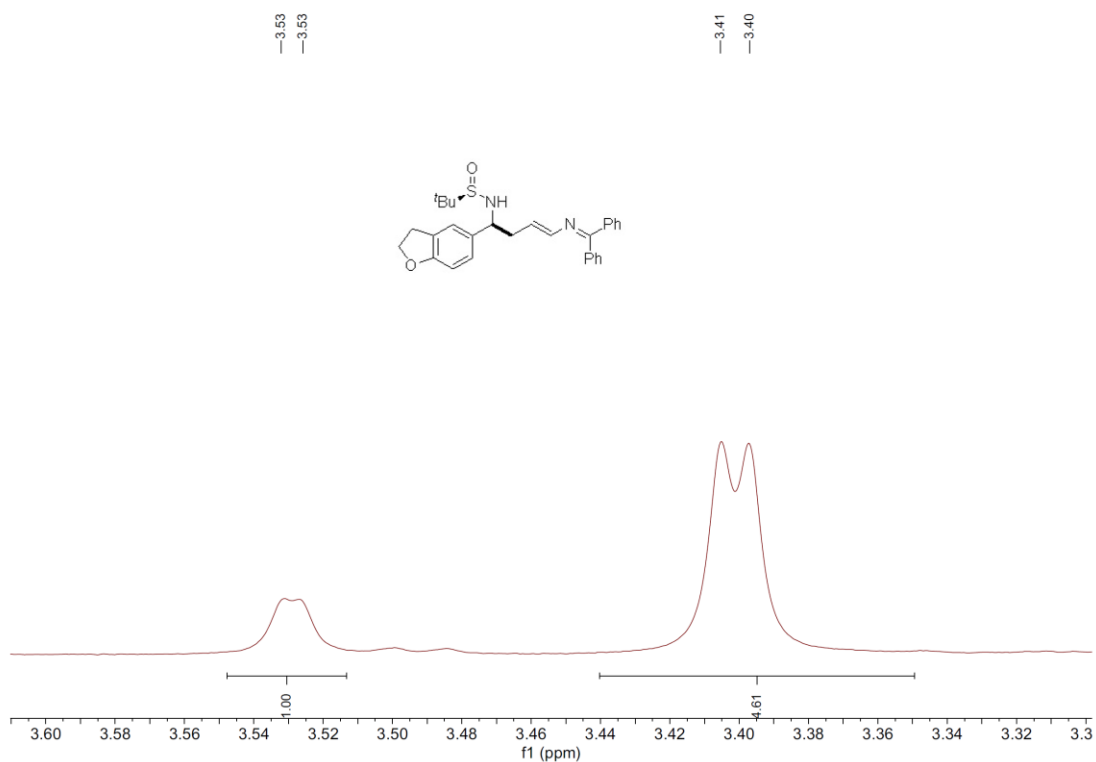
3t ¹³C NMR



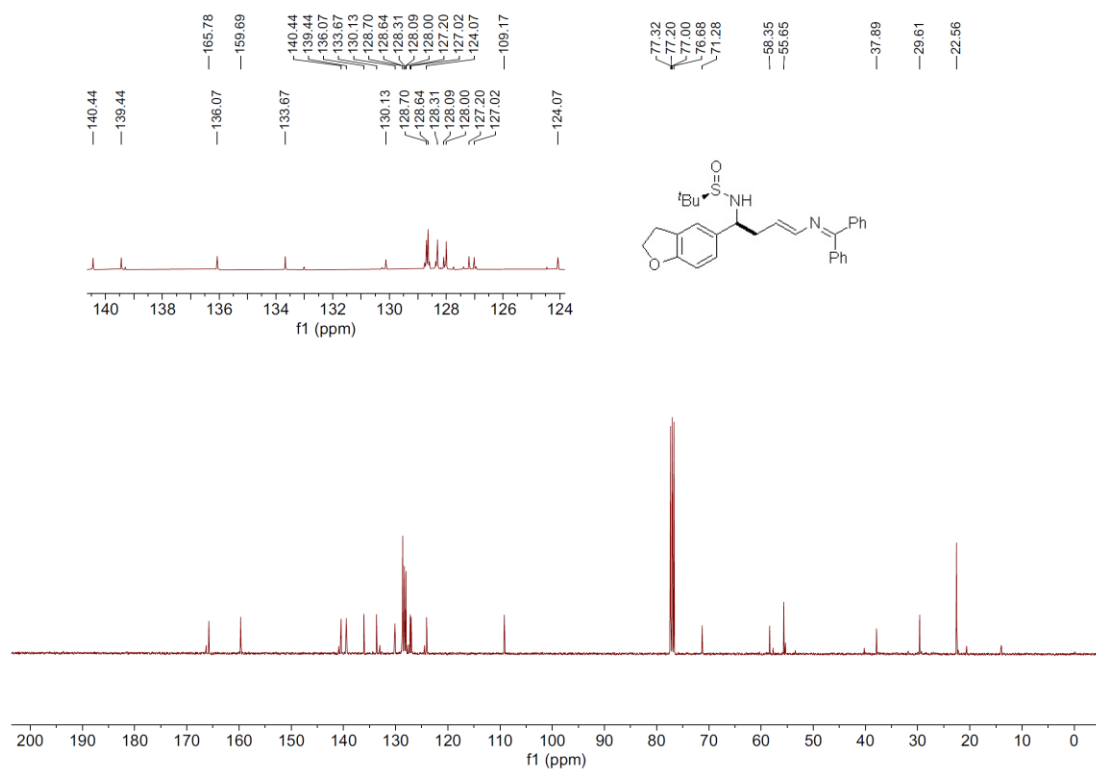
3u ¹H NMR



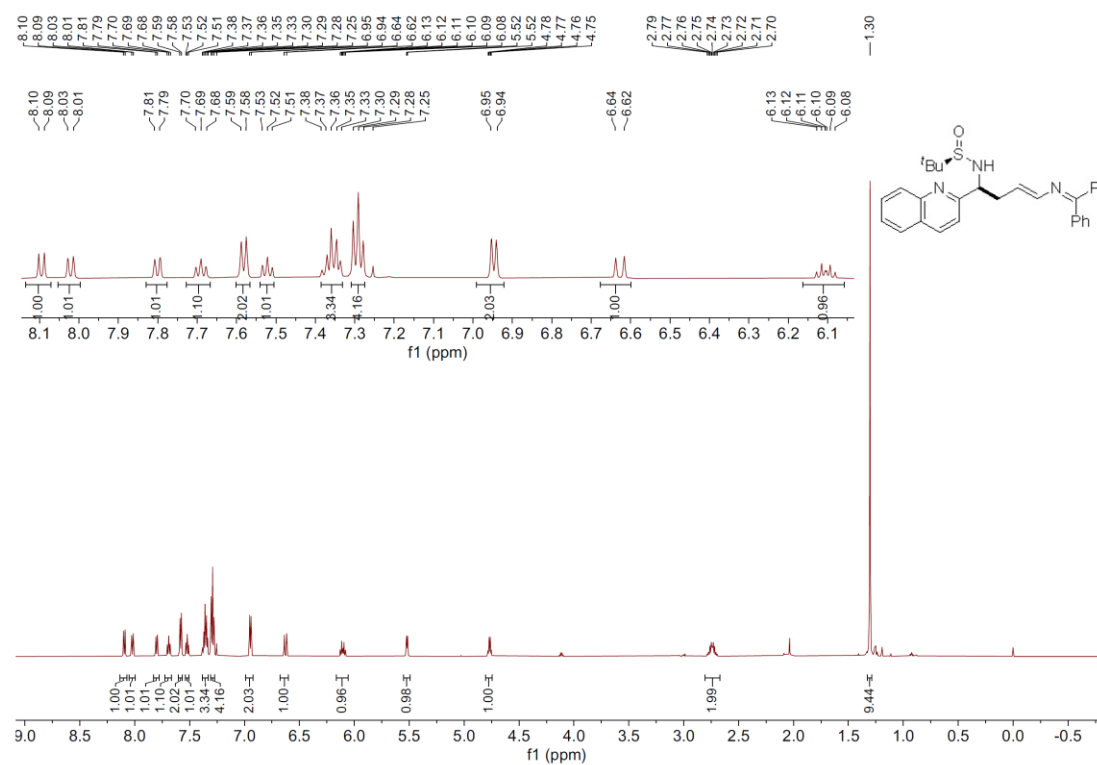
3u dr



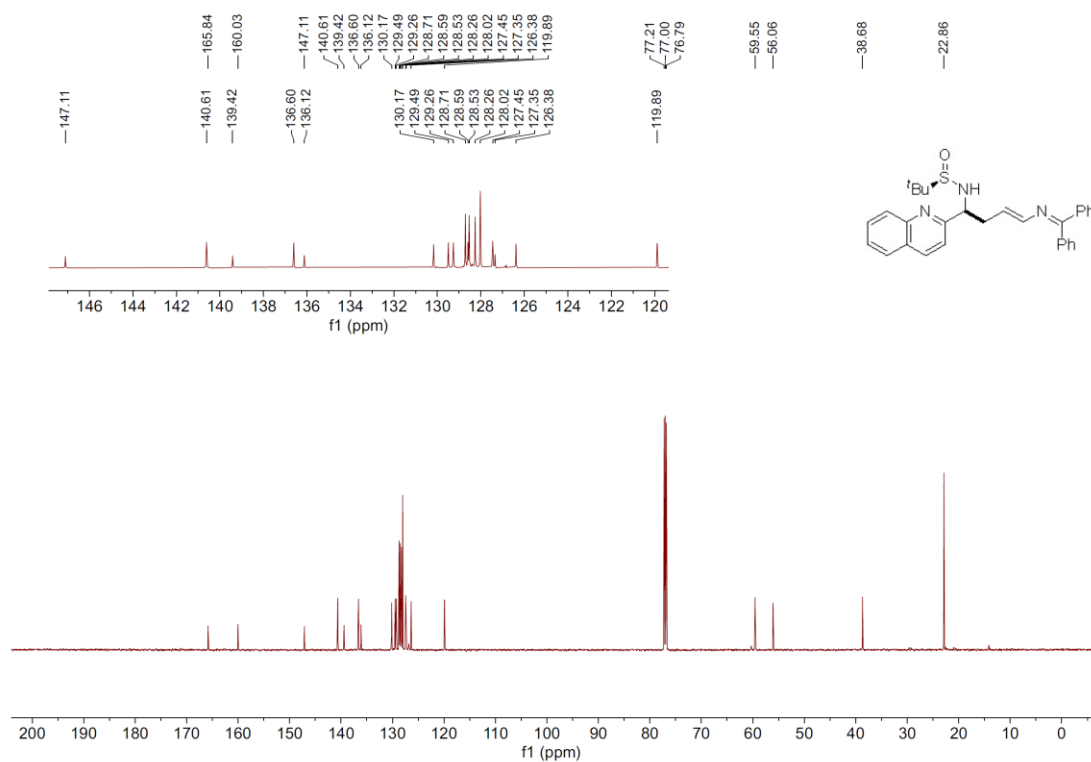
3u ¹³C NMR



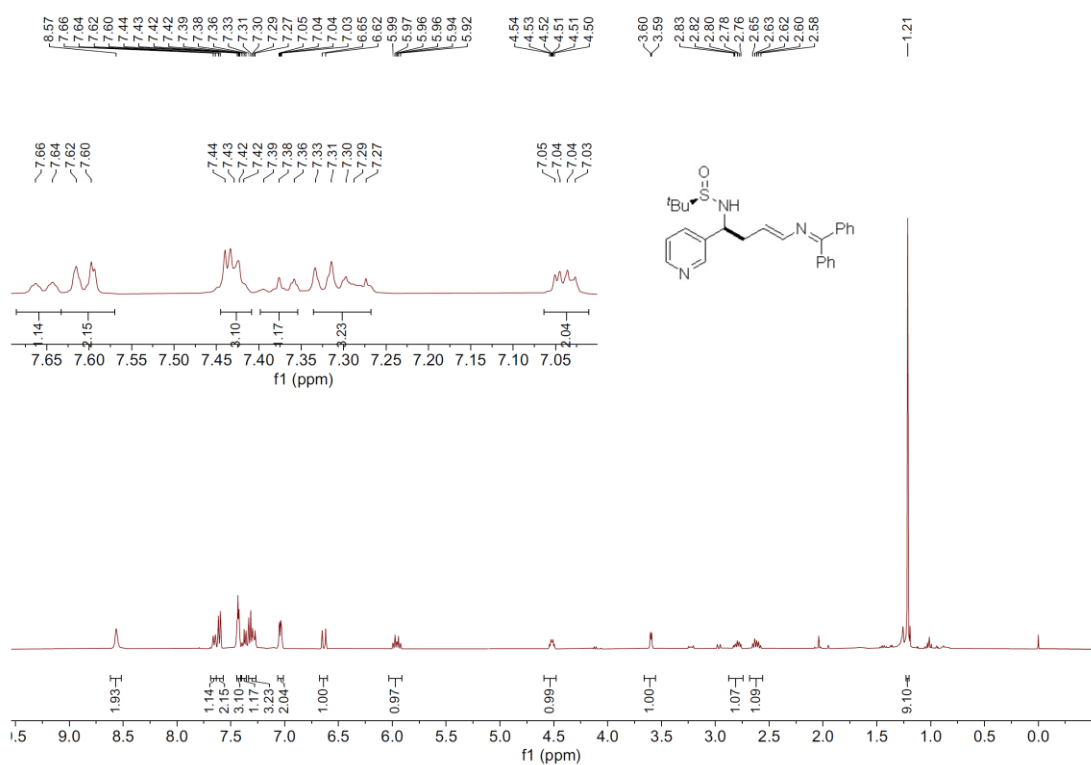
3v ¹H NMR



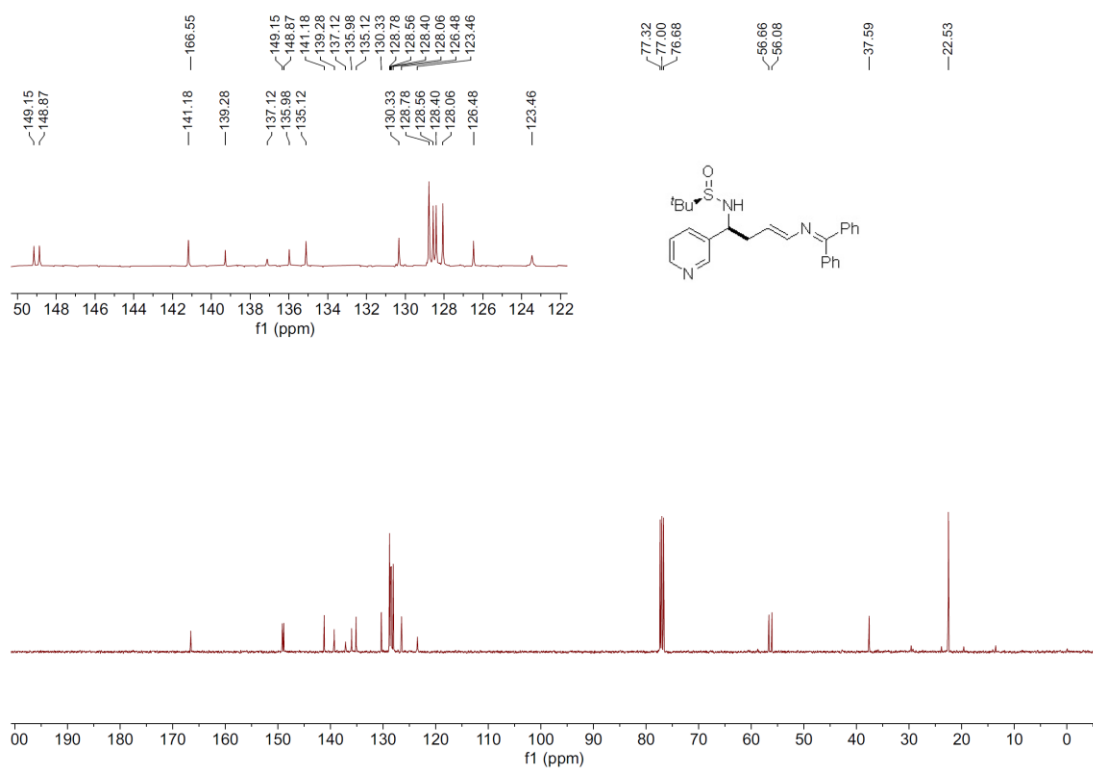
3v ¹³C NMR



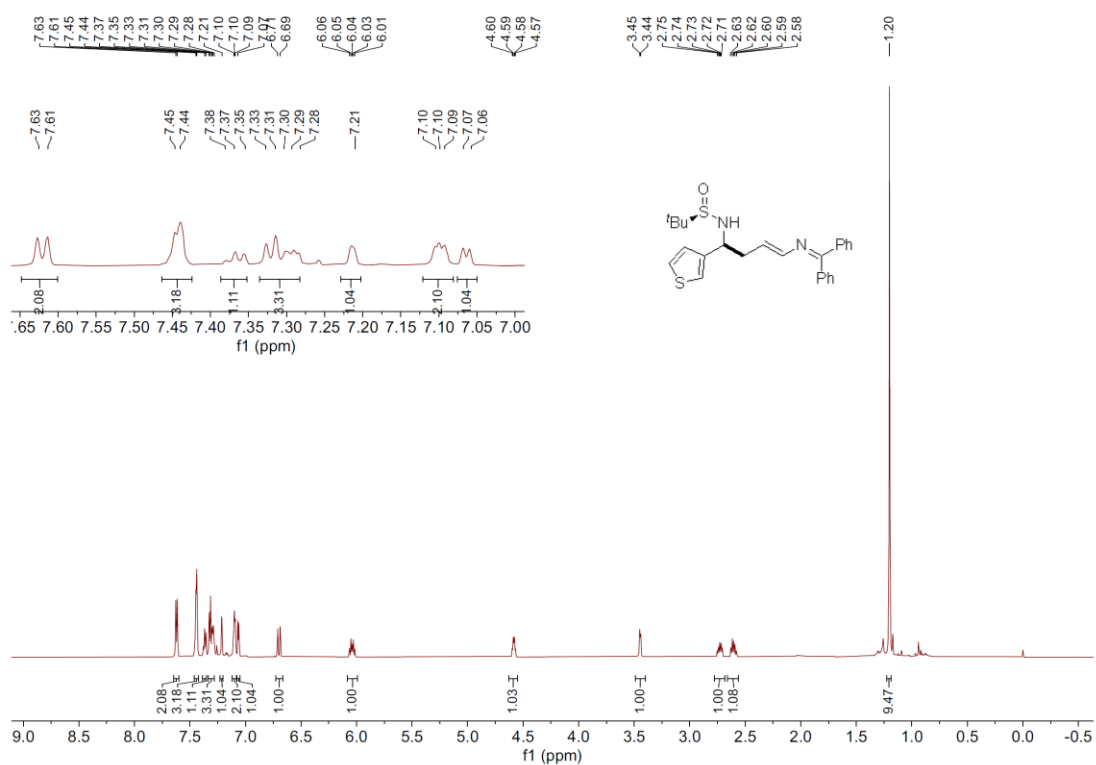
3w ¹H NMR



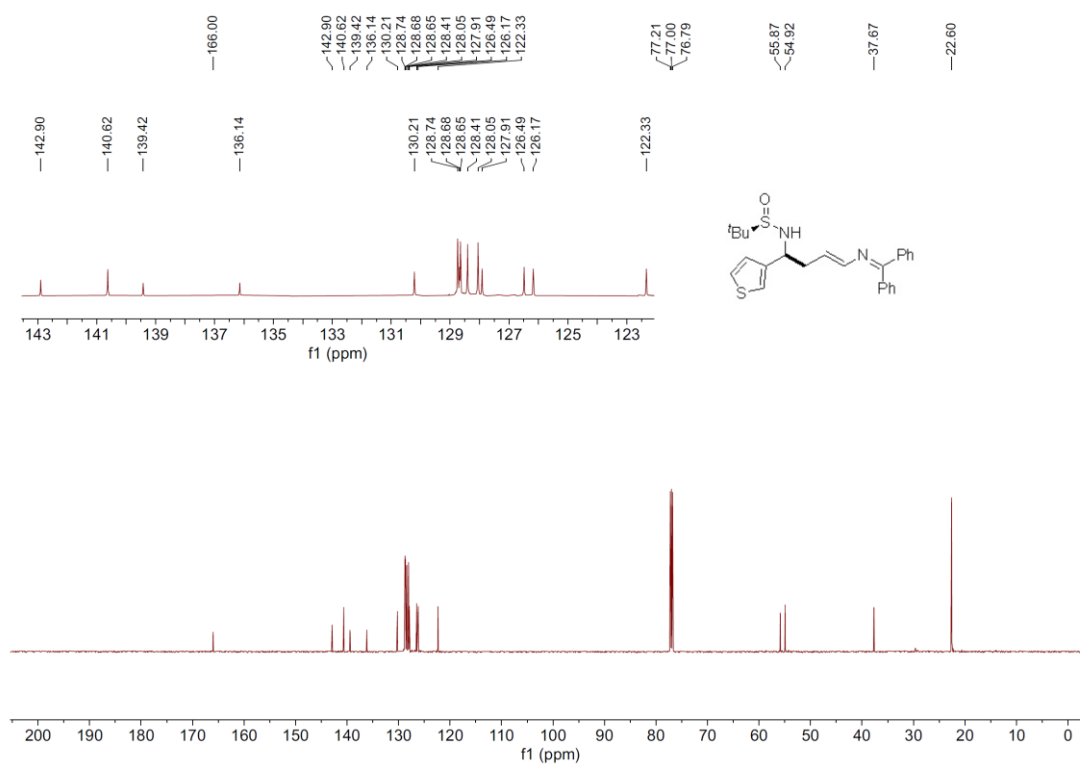
3w ¹³C NMR



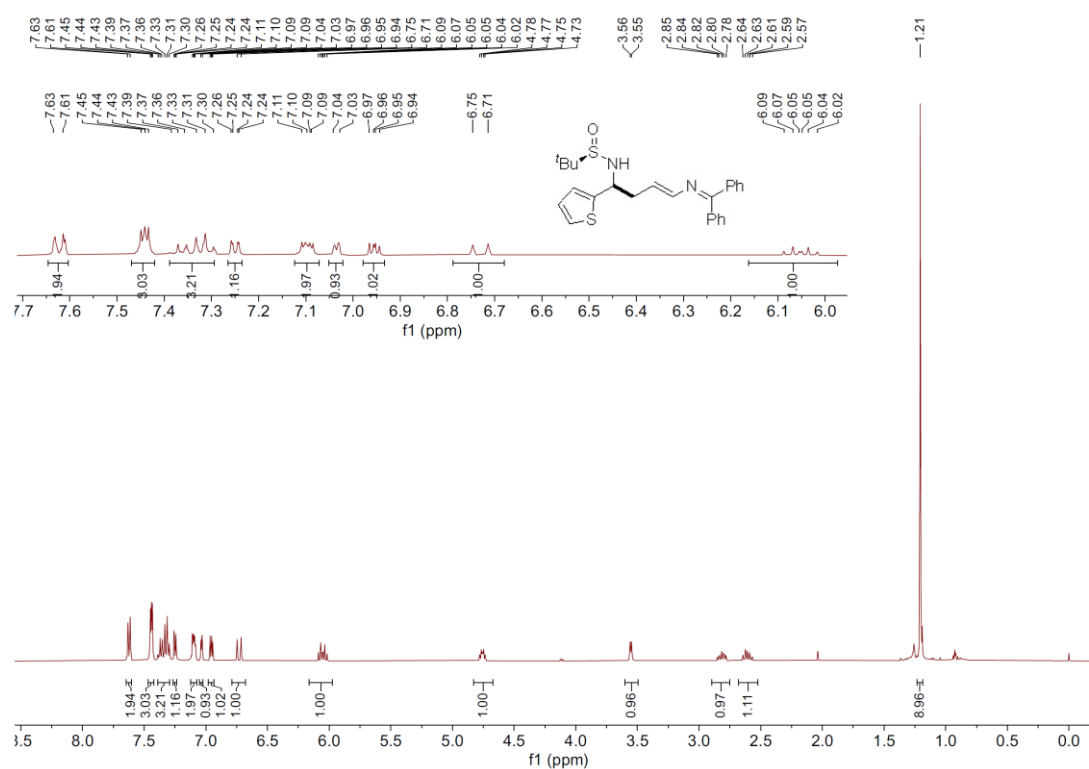
3x ¹H NMR



3x ¹³C NMR



3y ¹H NMR



Chemical Structure: CC(C)(C)S(=O)(=O)N[C@H](c1ccsc1)/C=C/N=C(c2ccccc2)c3ccccc3

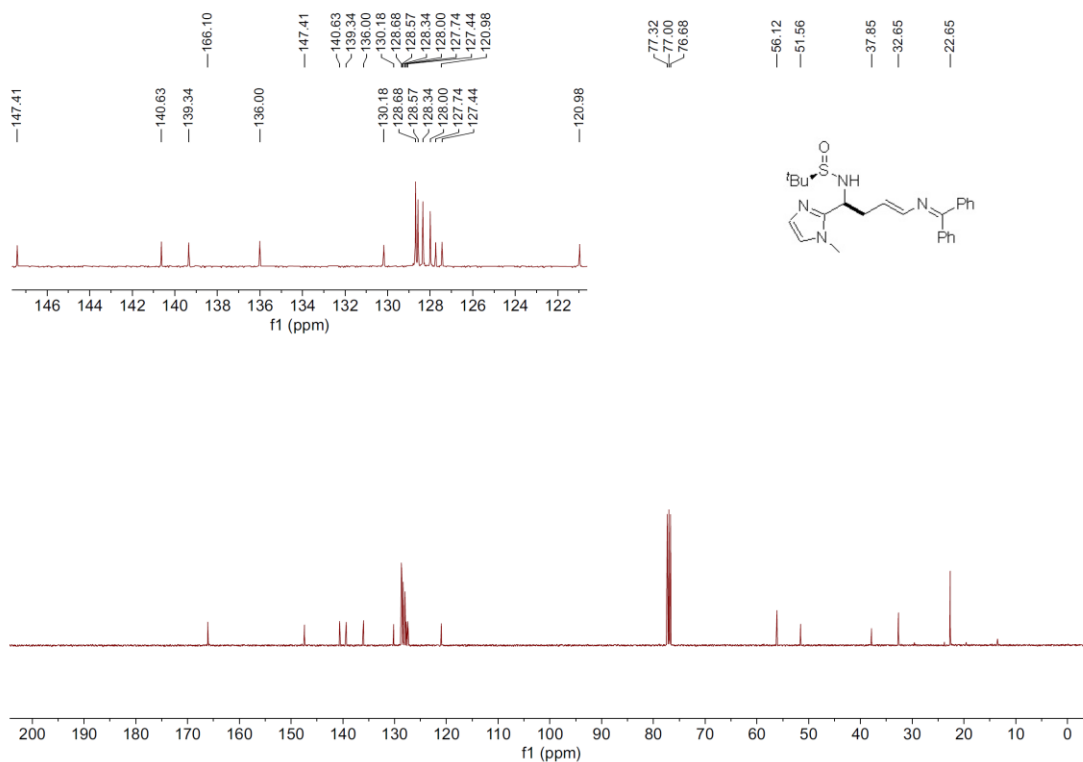
¹³C NMR Spectrum (ppm):

- 145.32
- 140.83
- 139.38
- 136.16
- 136.04
- 130.22
- 128.75
- 128.70
- 128.66
- 128.37
- 128.03
- 127.41
- 126.70
- 125.68
- 124.95
- 77.32
- 77.00
- 76.68
- 55.98
- 54.81
- 38.74
- 22.55

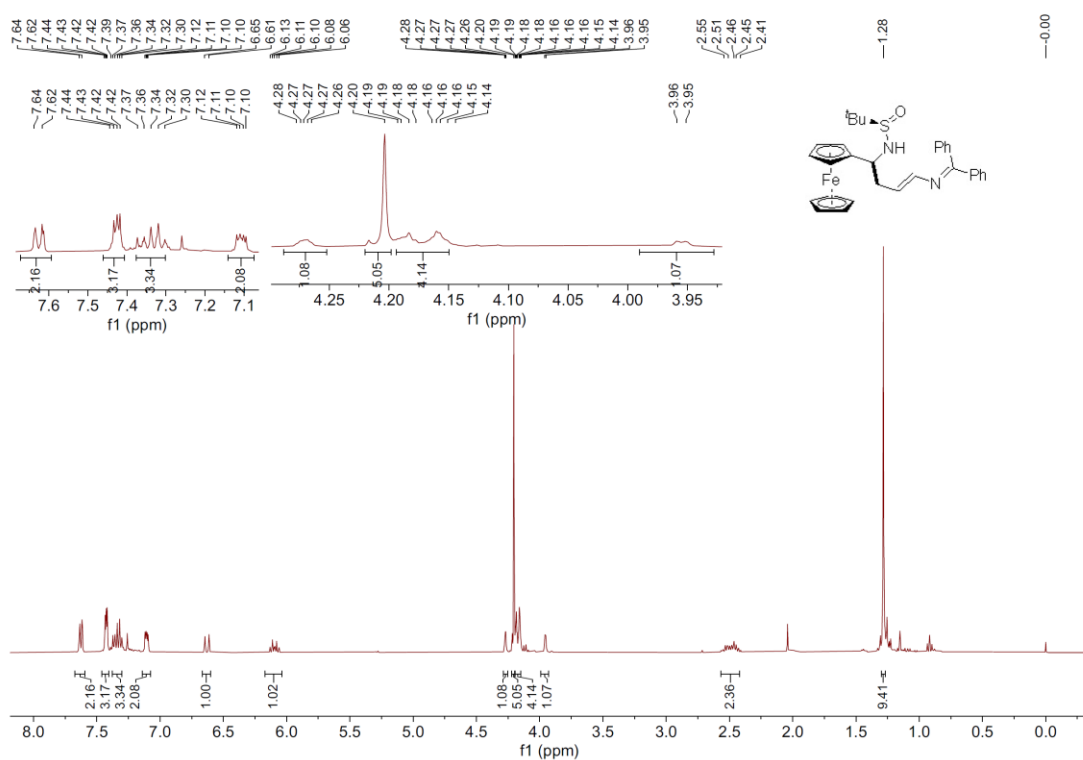
Chemical structure of compound 10: Cc1ccncc1[C@H](C(=O)N(C)C)C/C=C/C(=N/C1=CC=CC=C1)/N=C/C2=CC=CC=C2

¹H NMR spectrum (CDCl₃) of compound 10. The spectrum shows peaks from 0.0 to 8.0 ppm. Integration values are provided below the peaks: 2.02, 2.20, 2.29, 2.04, 2.04, 1.00, 1.06, 1.00, 3.19, 1.94, 9.16. A chemical structure of compound 10 is shown in the top right corner.

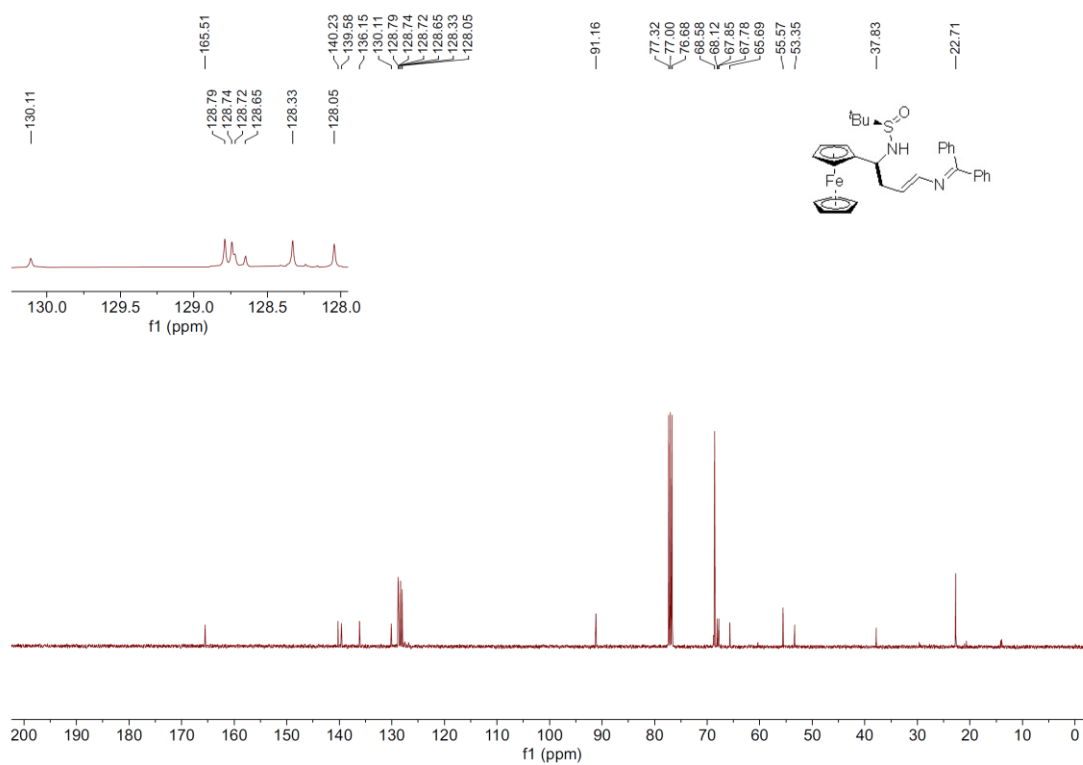
3z ¹³C NMR



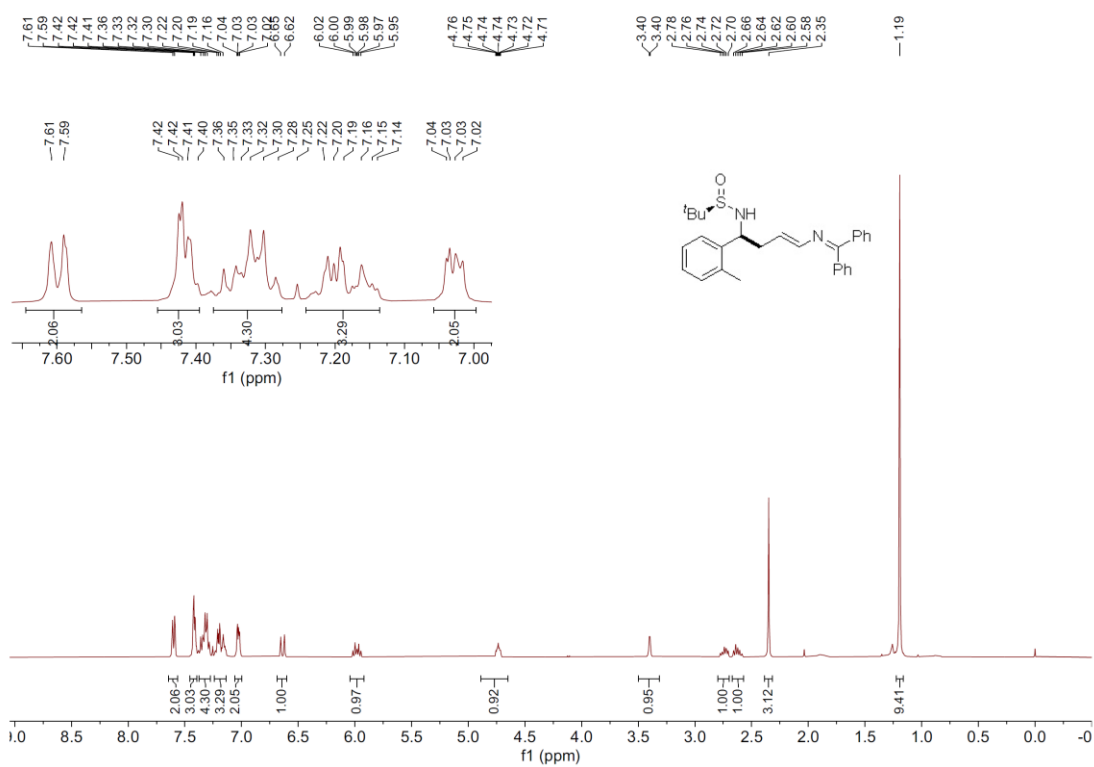
3aa ¹H NMR



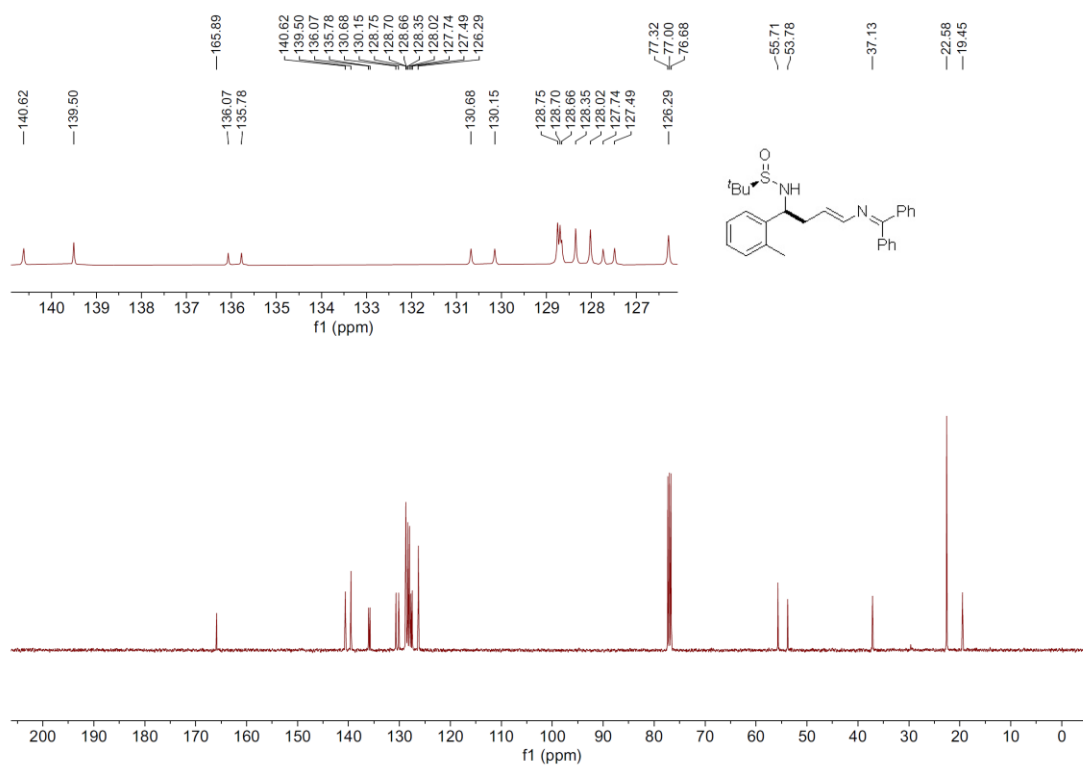
3aa ¹³C NMR



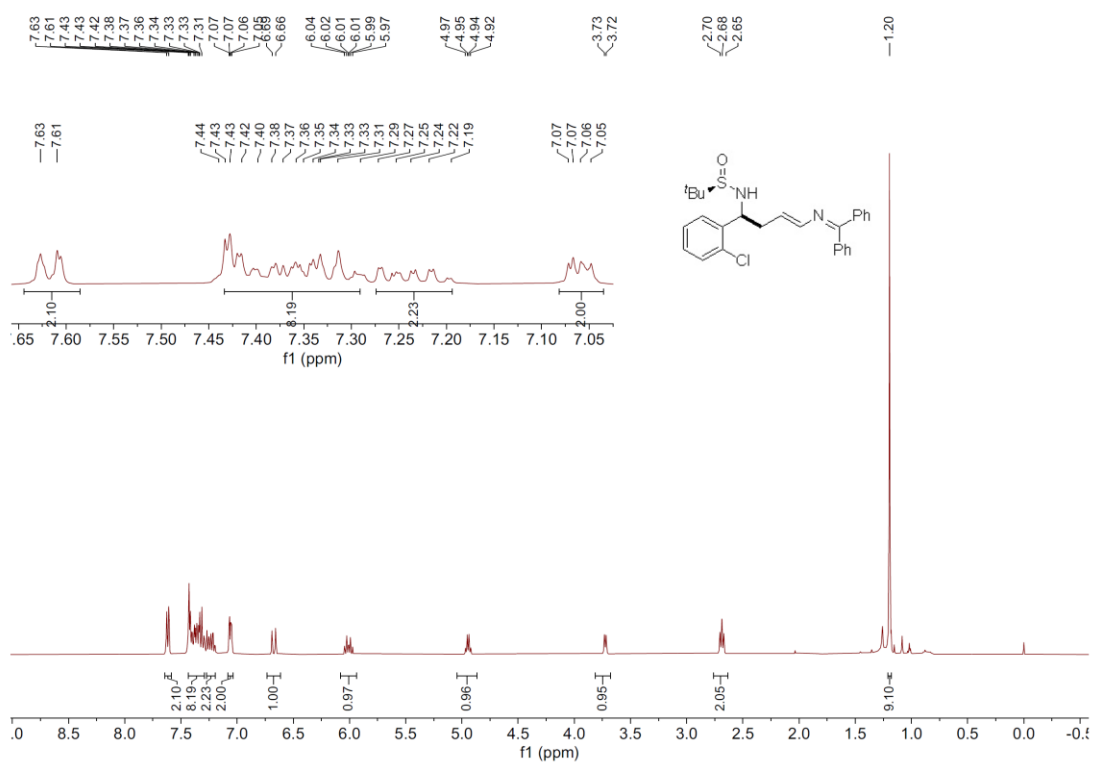
3ab ¹H NMR



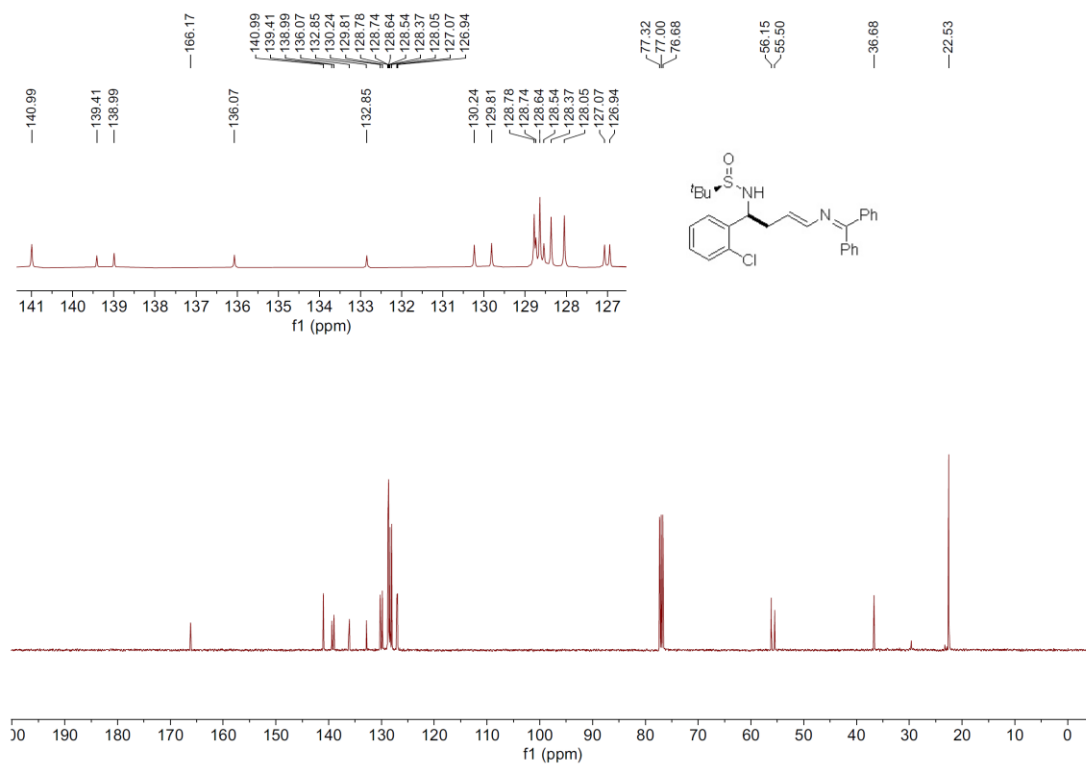
3ab ¹³CNMR



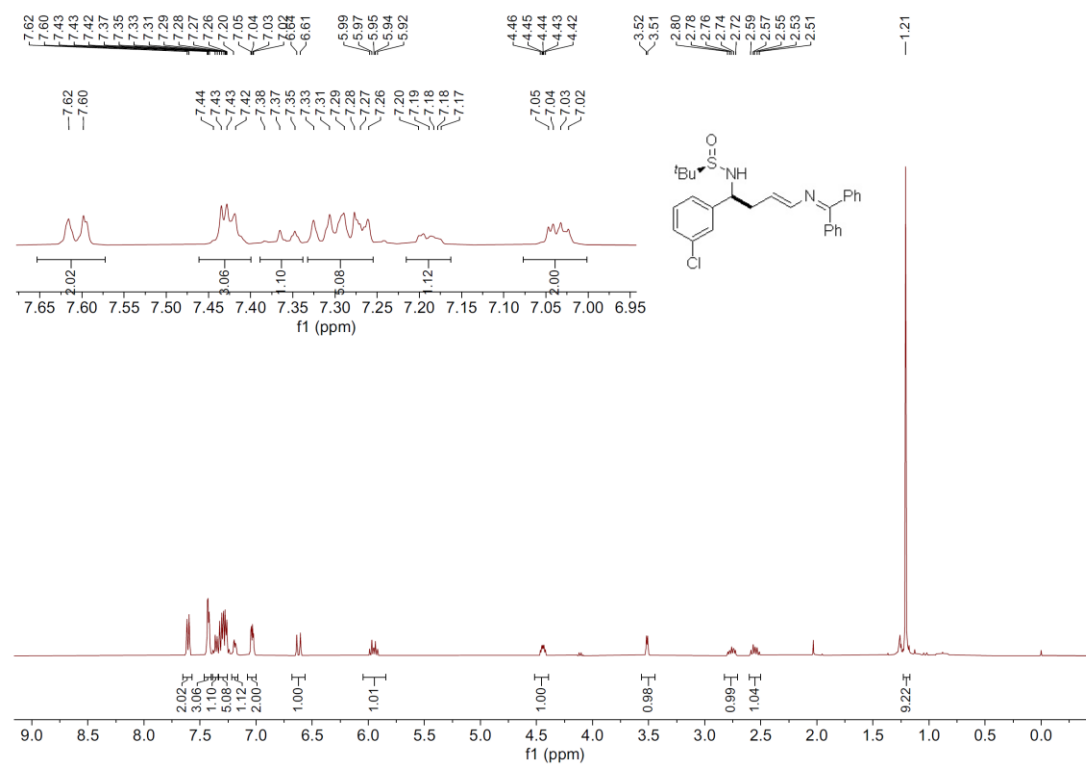
3ac ¹H NMR



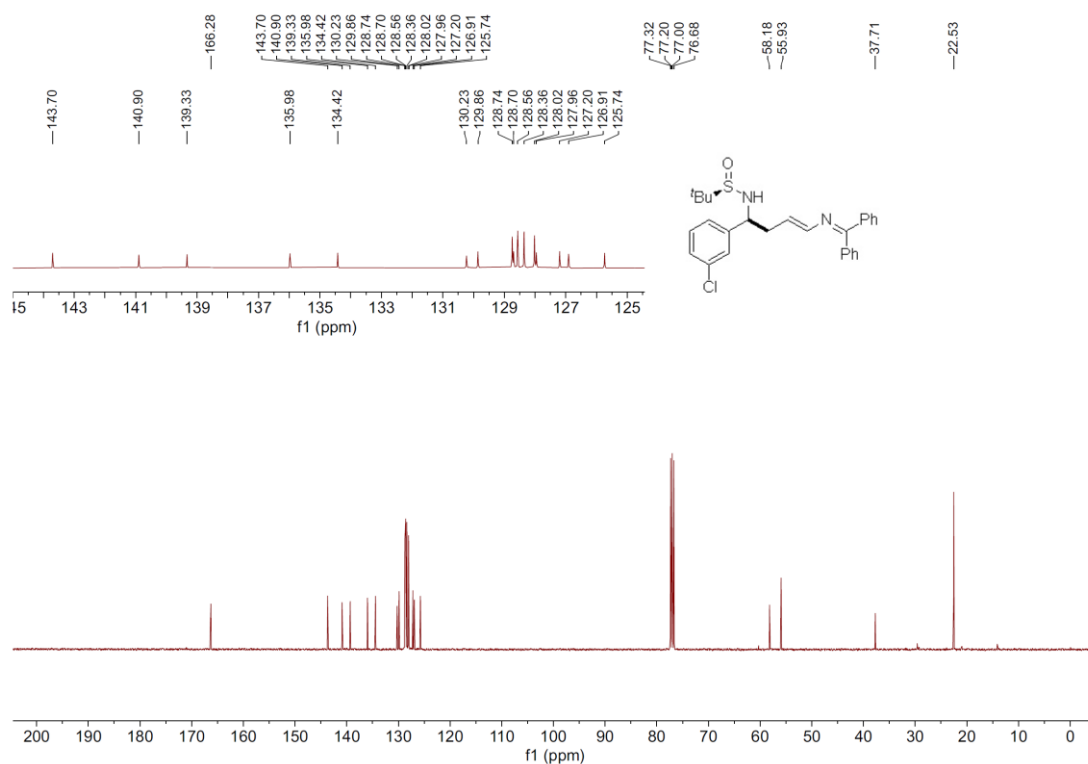
3ac ¹³C NMR



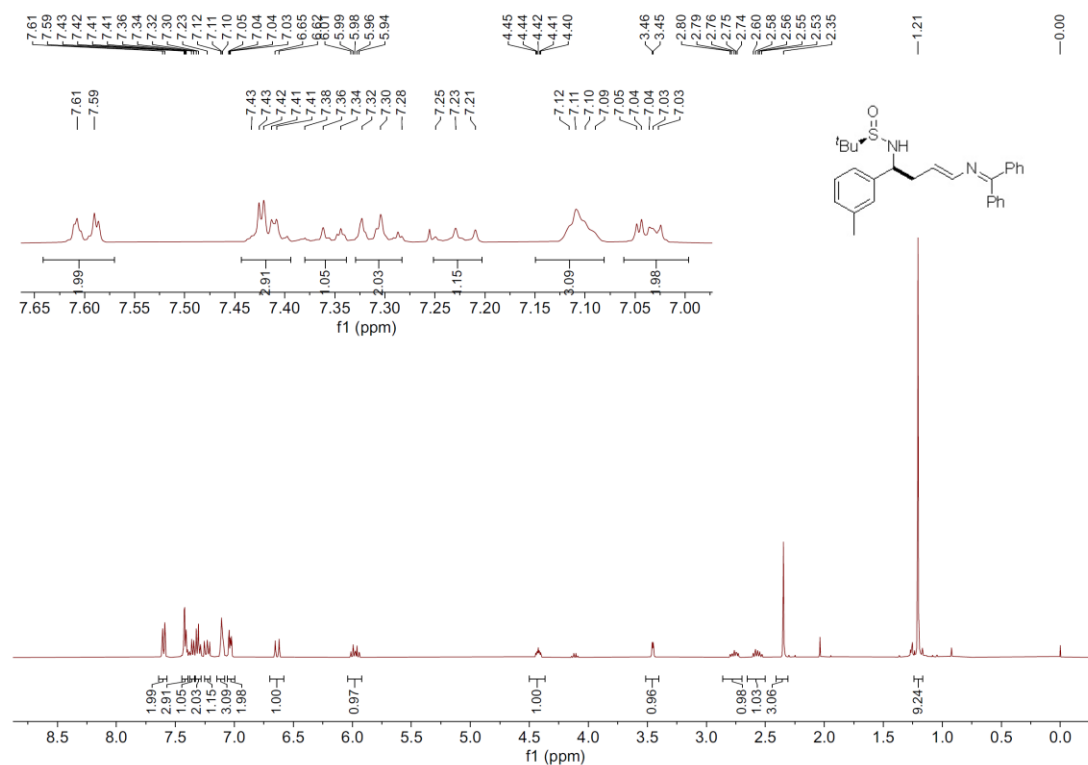
3ad ¹H NMR



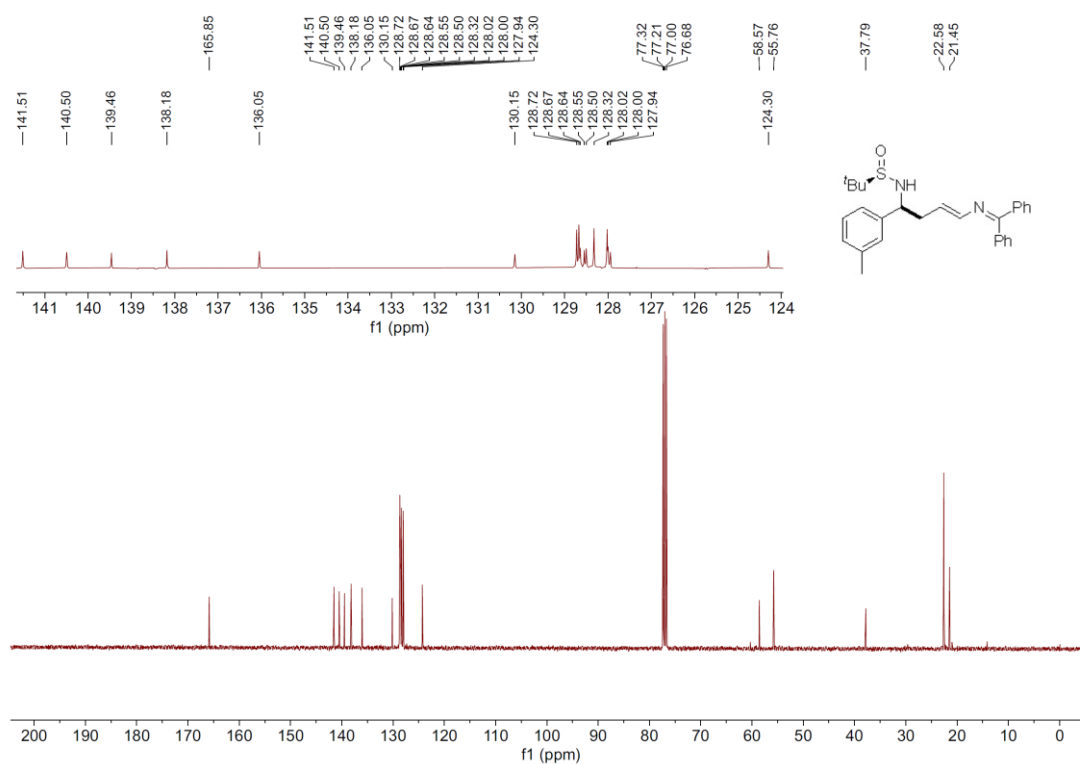
3ad ¹³CNMR



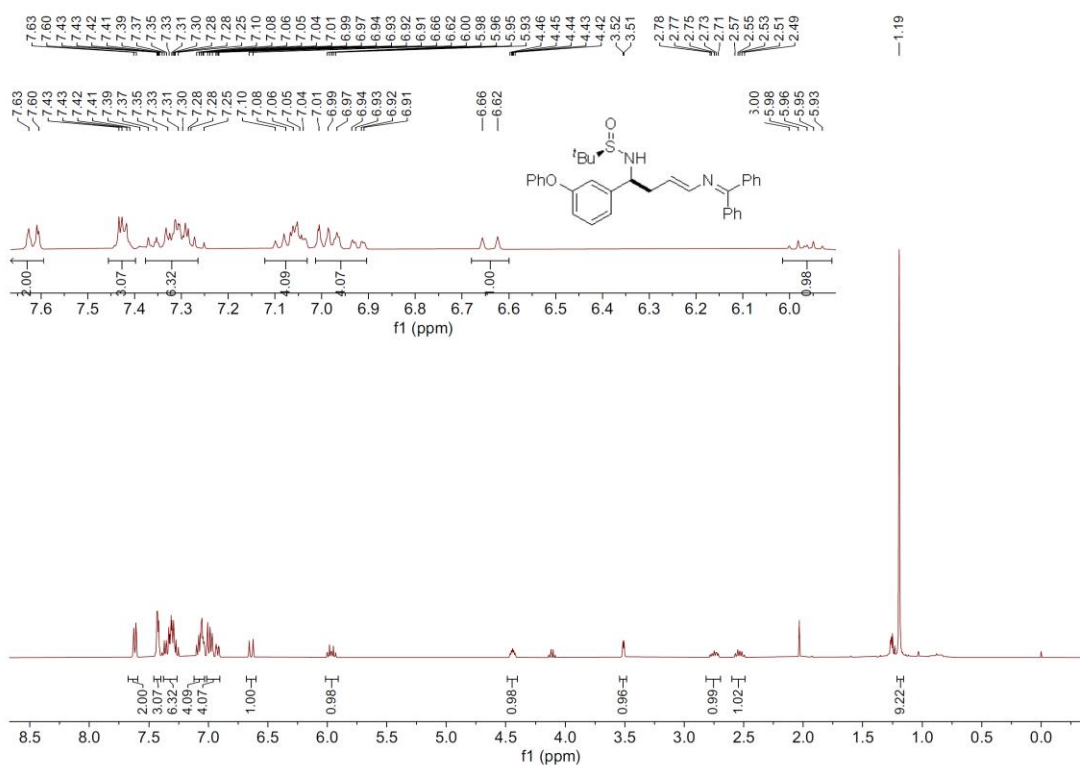
3ae ¹H NMR



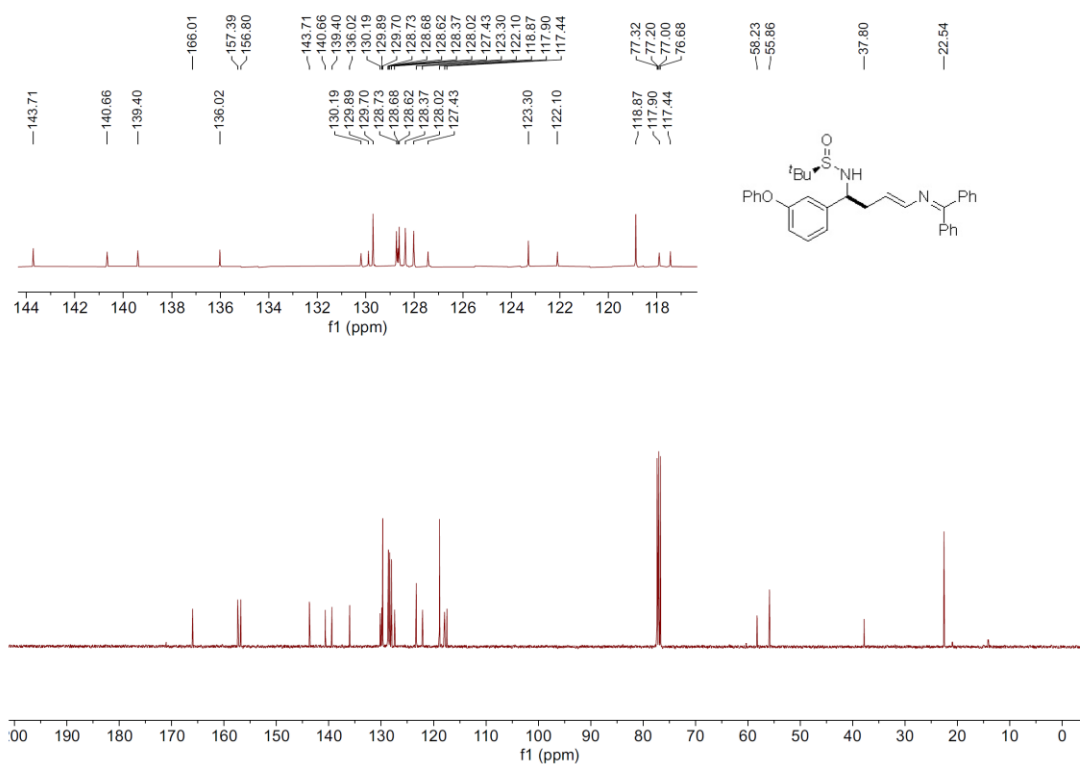
3ae ¹³CNMR



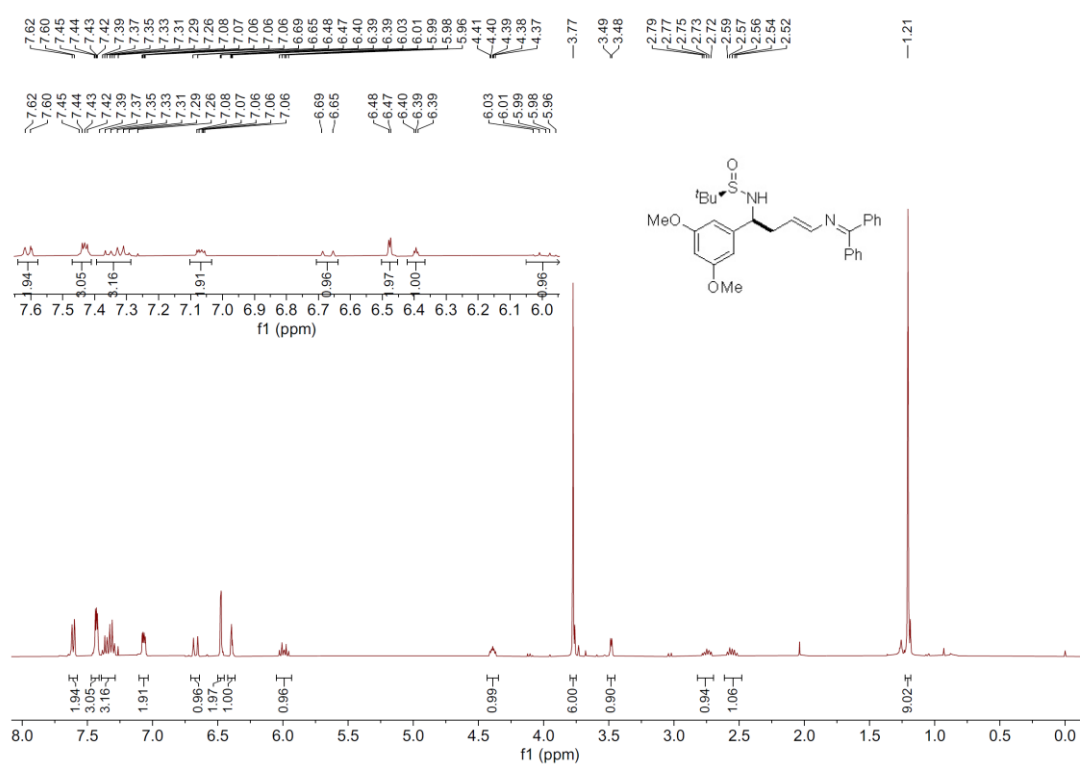
3af ¹H NMR



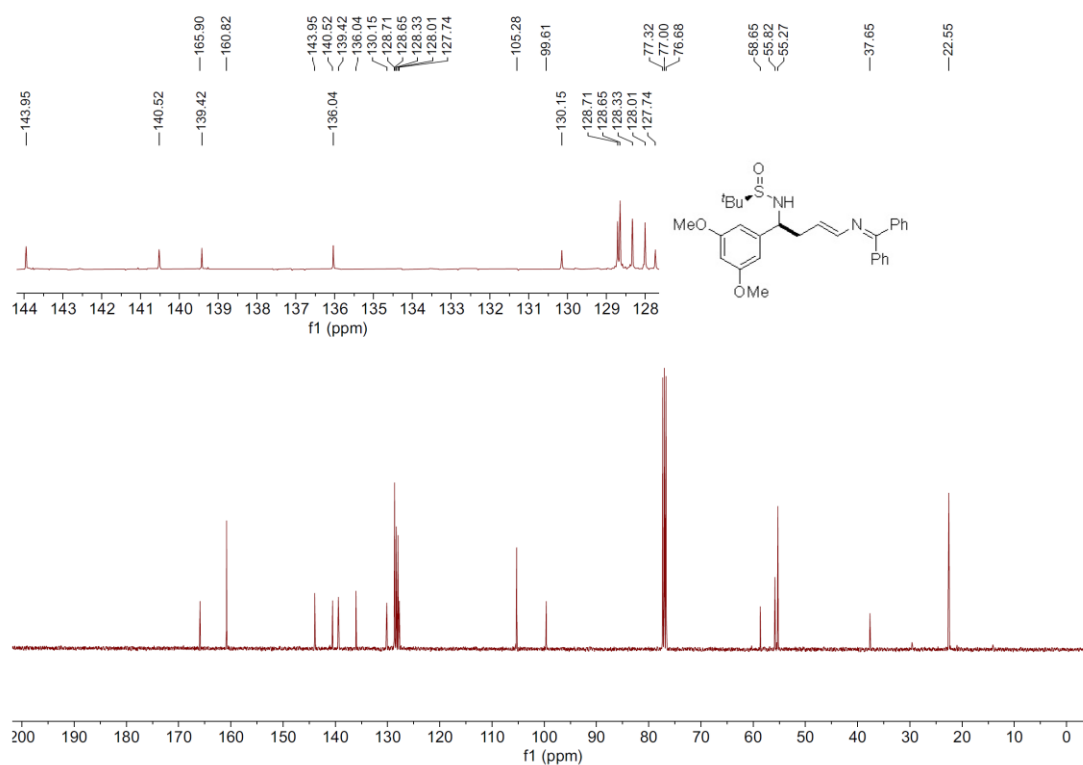
3af ¹³CNMR



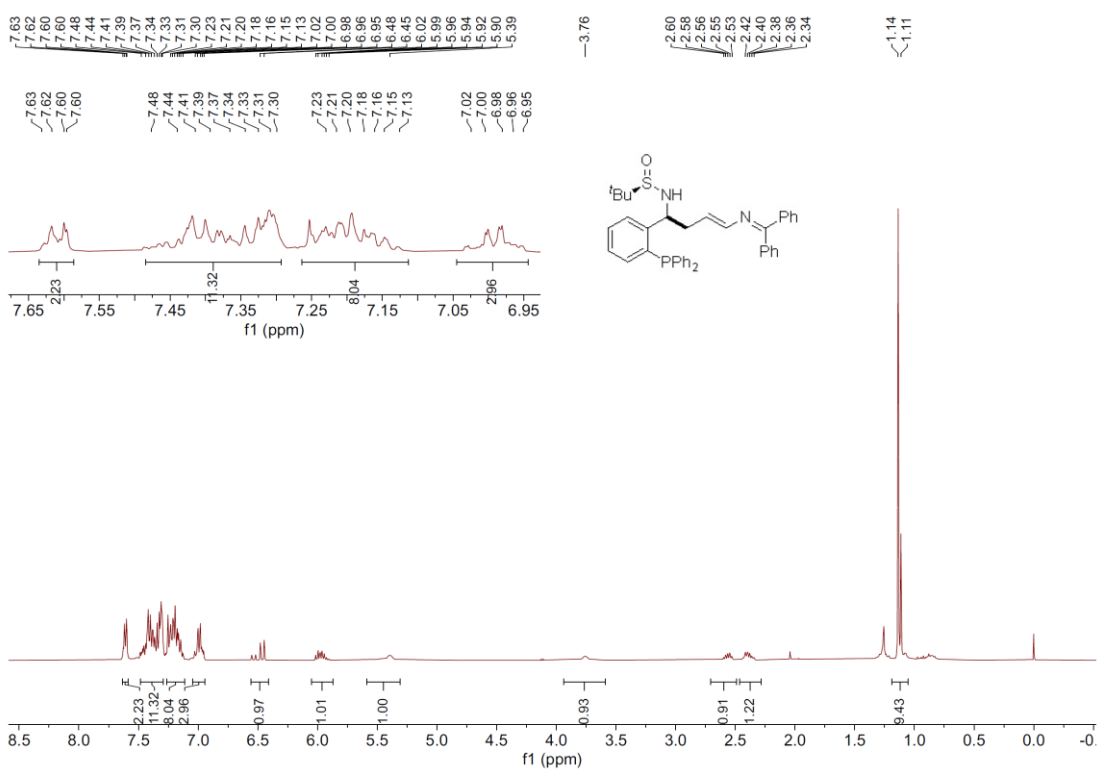
3ag ¹H NMR



3ag ¹³C NMR



3ah ¹H NMR

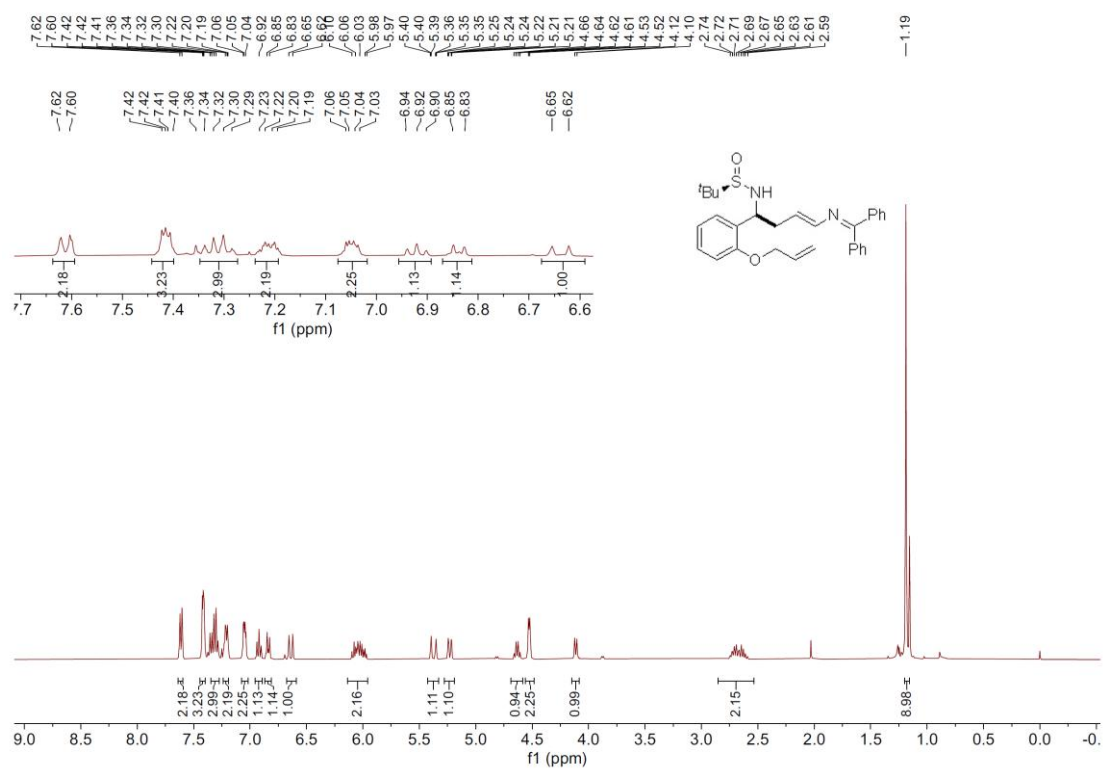


[illegible]

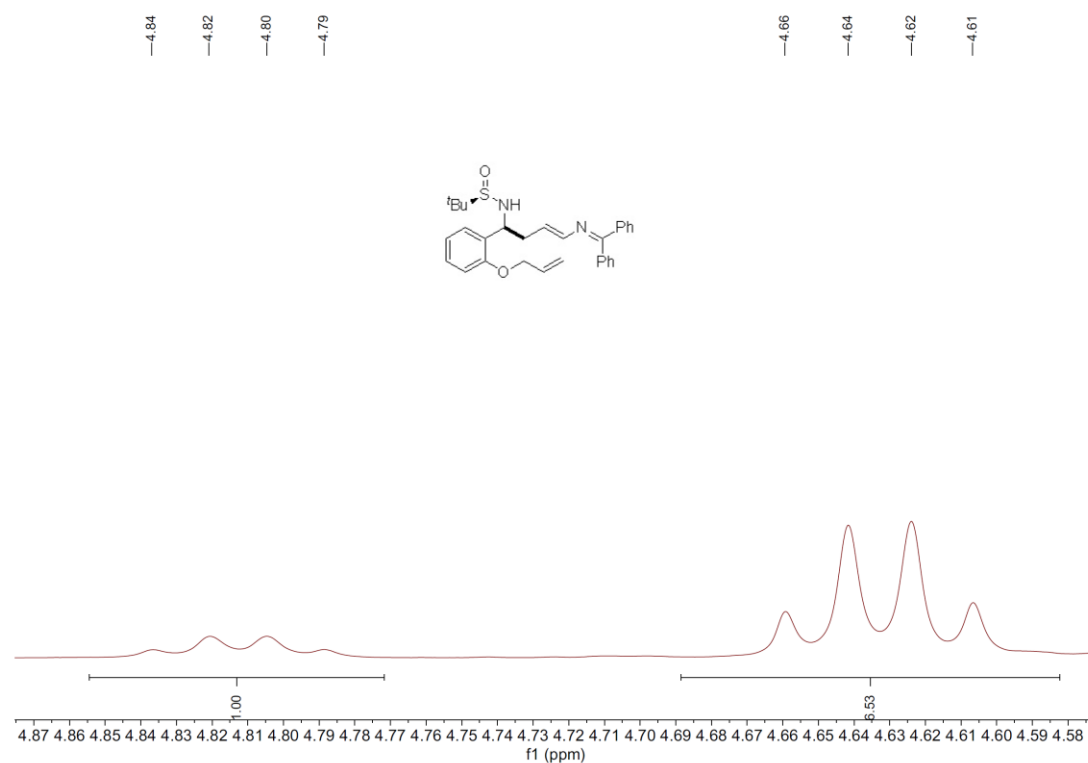
136.65, 136.55, 136.31, 136.21, 136.06, 135.31, 135.17, 134.50, 134.03, 133.83, 133.64, 146.71, 146.48, 140.75, 139.54, 136.65, 136.55, 136.31, 136.21, 136.06, 135.31, 135.17, 134.50, 134.03, 133.64, 130.18, 129.31, 128.79, 130.18, 128.78, 128.70, 128.79, 128.67, 128.78, 128.60, 128.52, 128.67, 128.45, 128.52, 128.35, 128.04, 127.73, 127.60, 127.43, 165.77, 56.02, 55.66, 37.80, 22.50

Chemical structure of compound 10: CC(C)(=O)N[C@@H](Cc1ccc(cc1)P(c2ccccc2)c3ccccc3)[C@@H](O)c4ccccc4

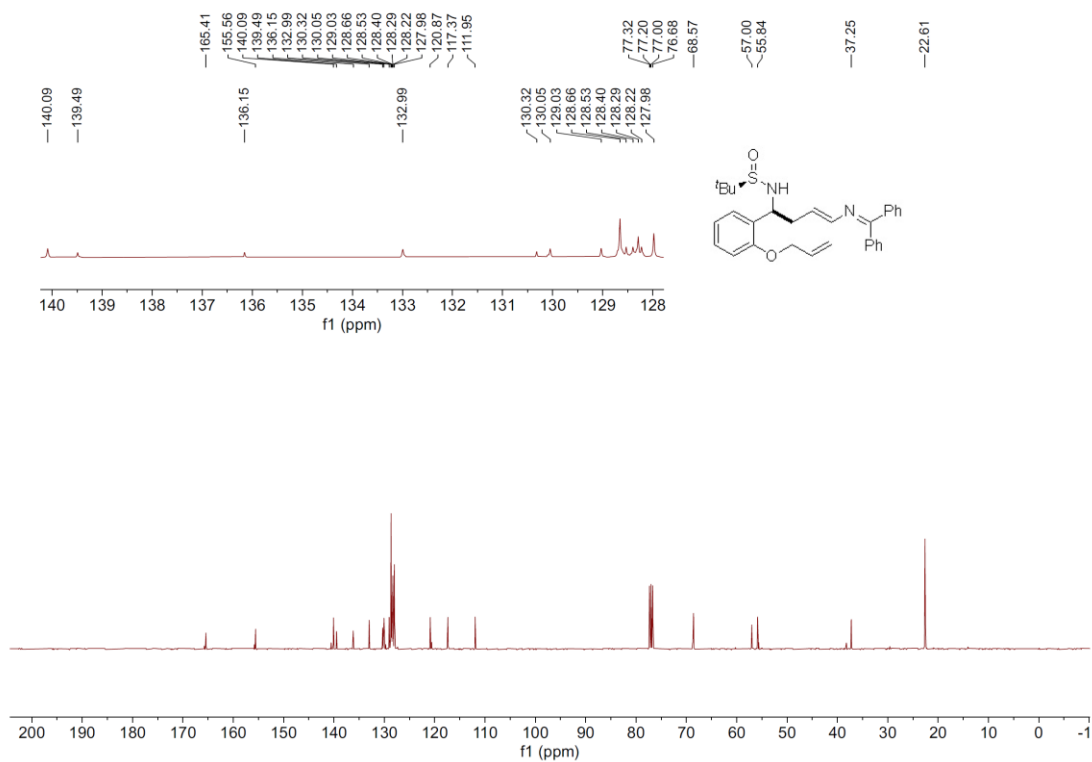
3ai ¹H NMR



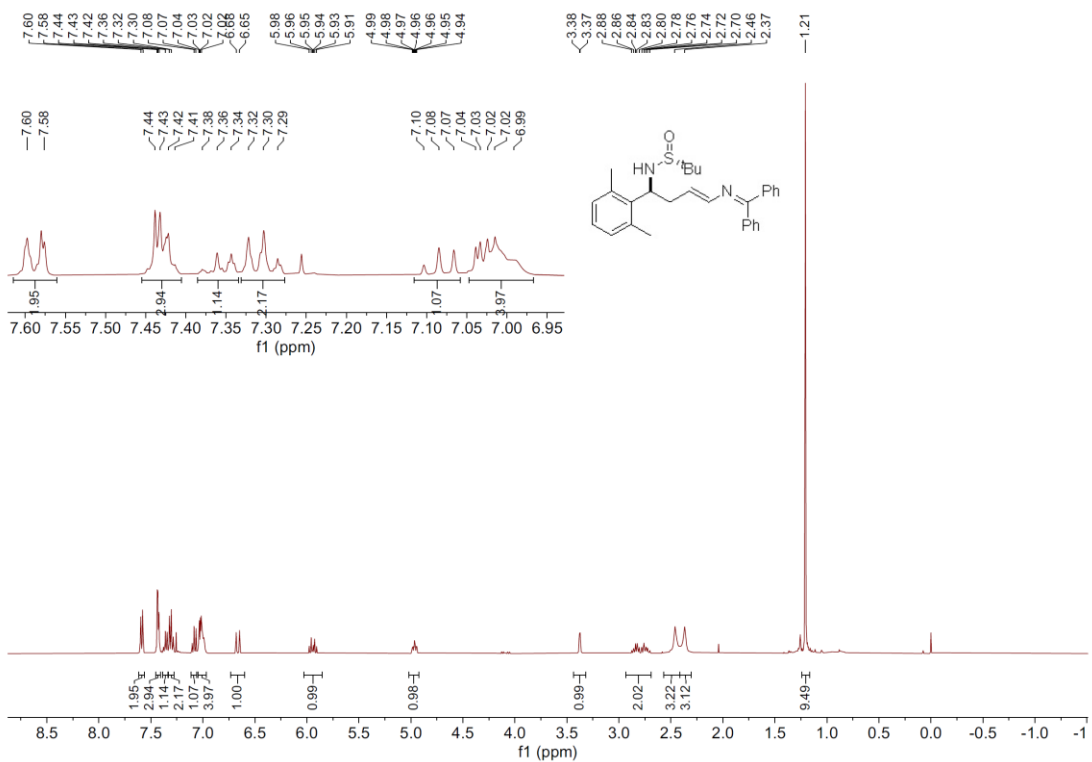
3ai dr



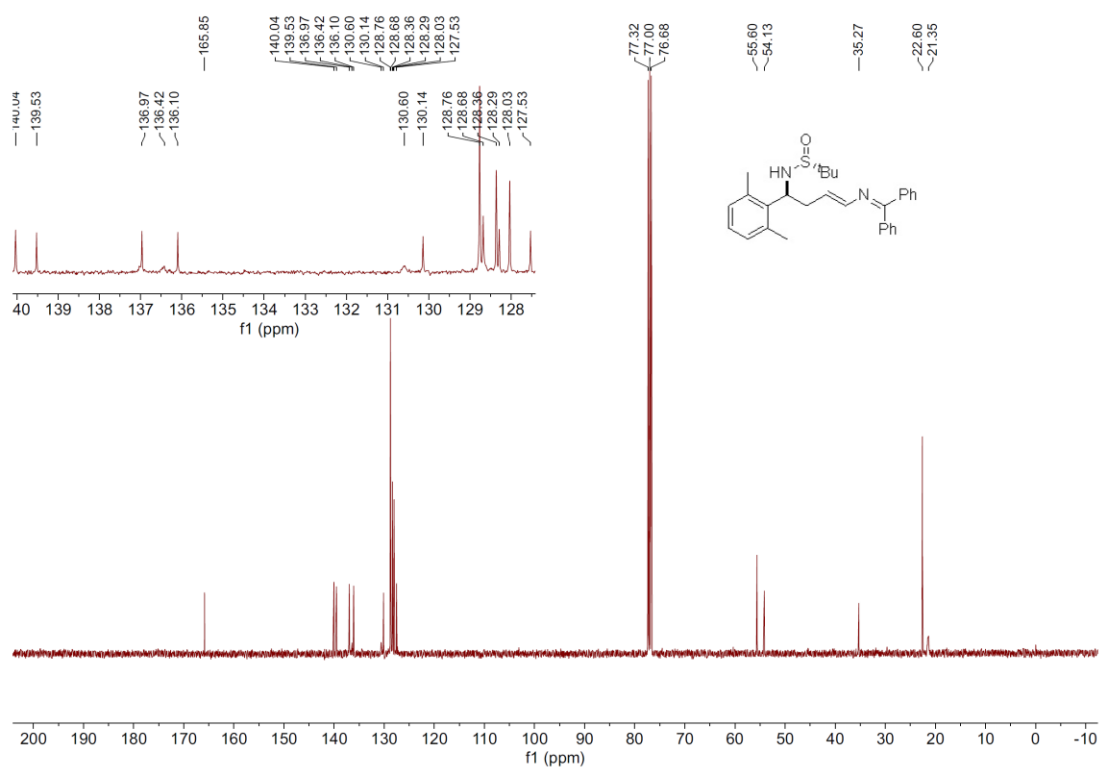
3ai ¹³C NMR



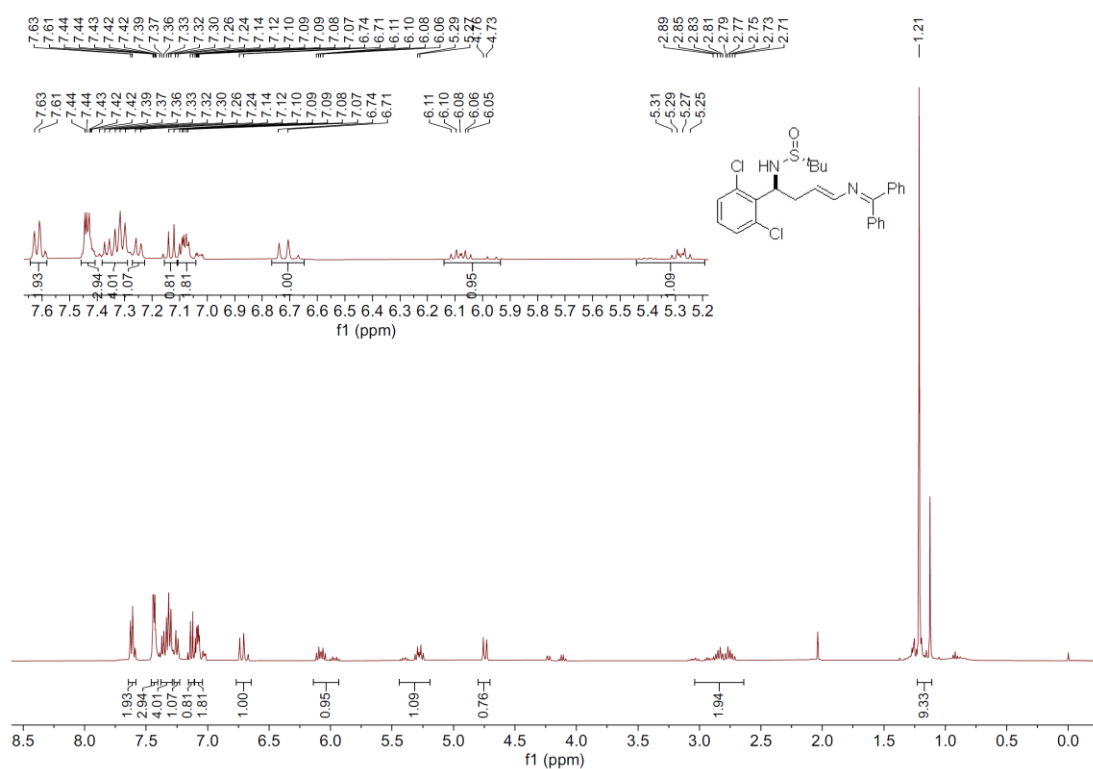
3aj ¹H NMR



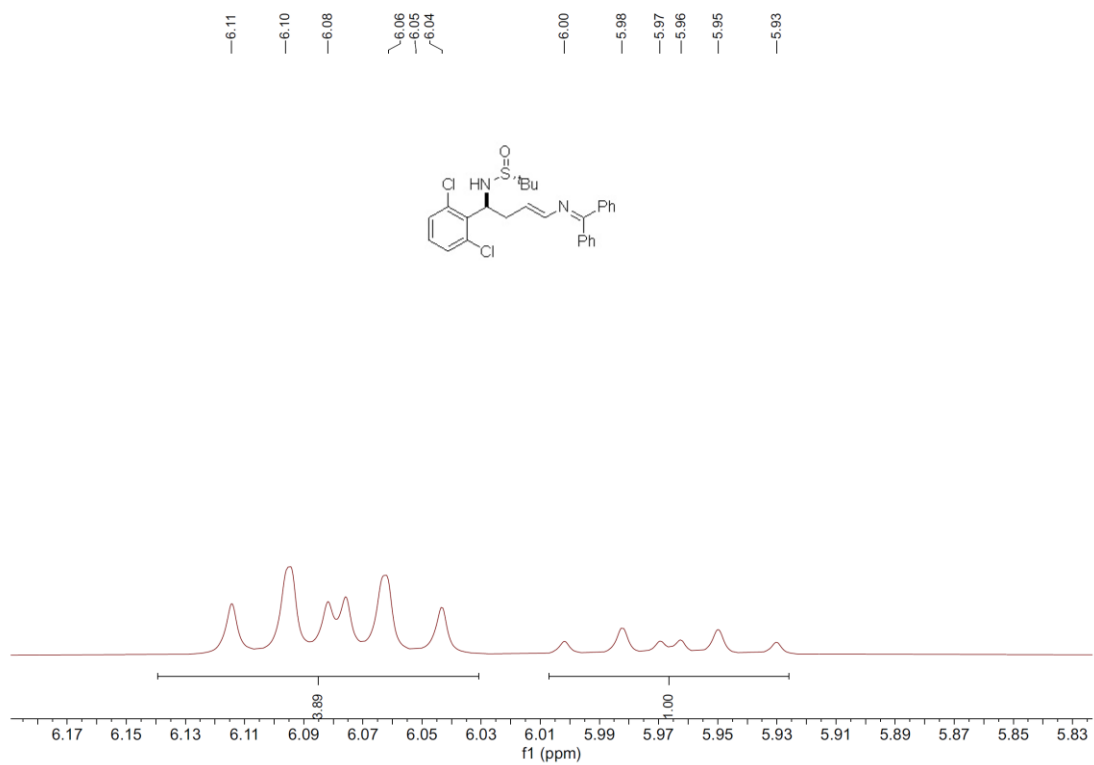
3aj ¹³C NMR



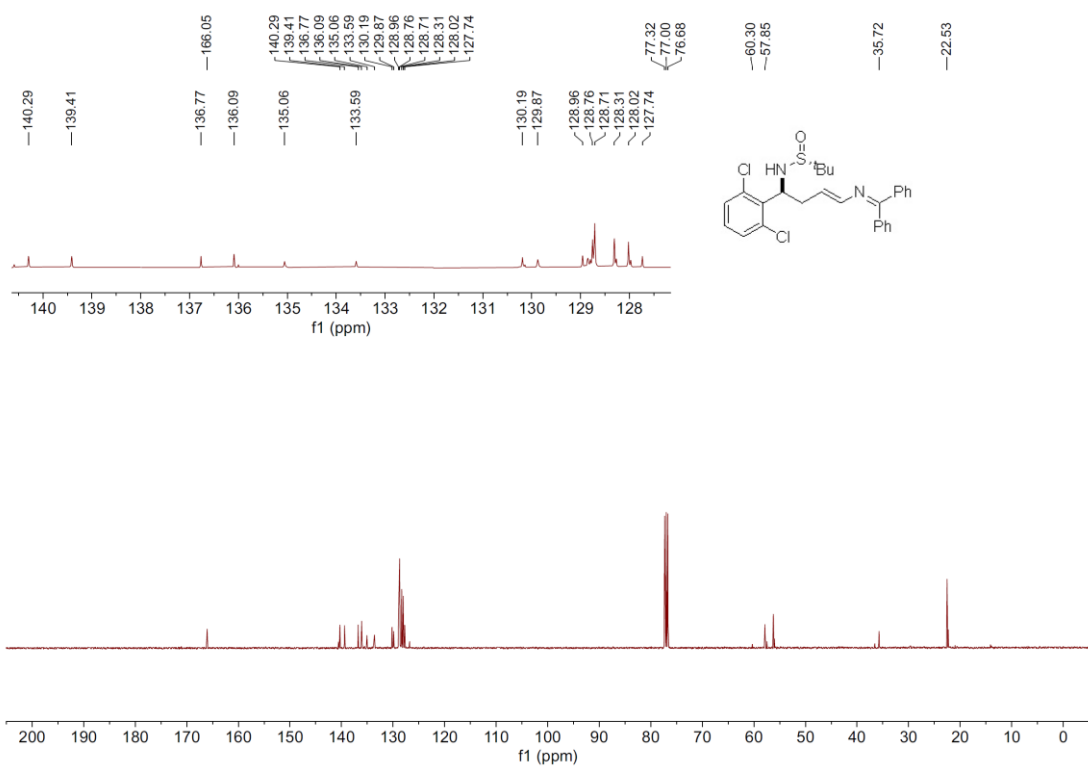
3ak ¹H NMR



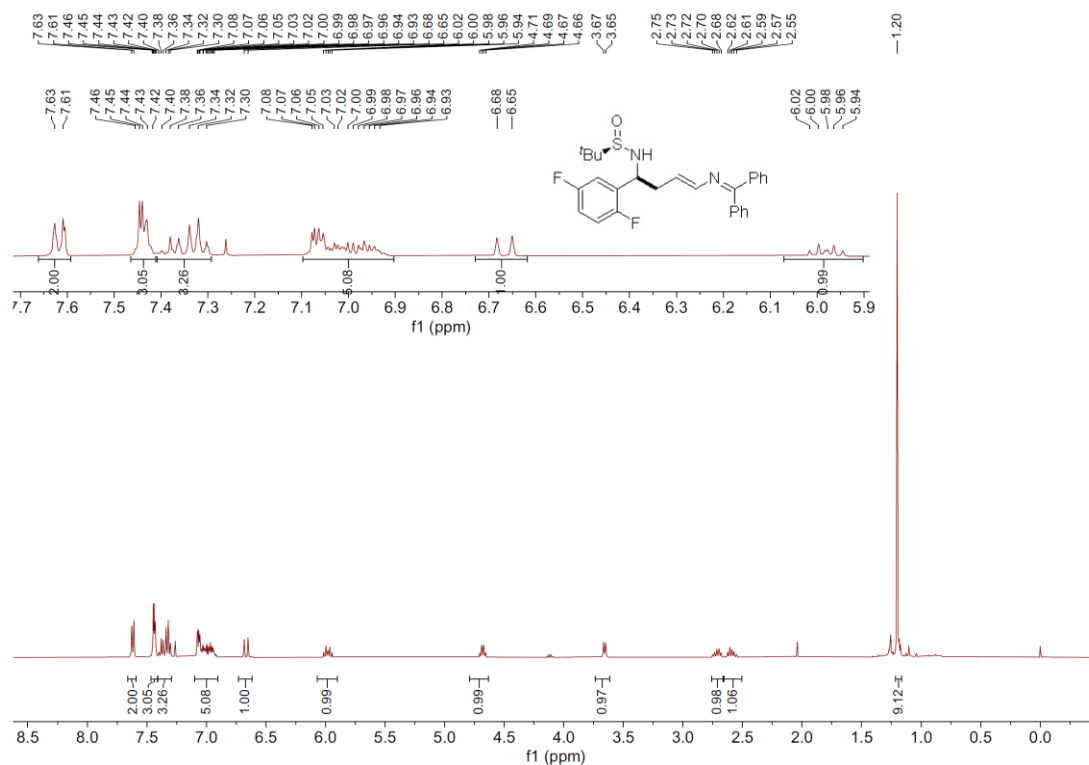
3ak dr



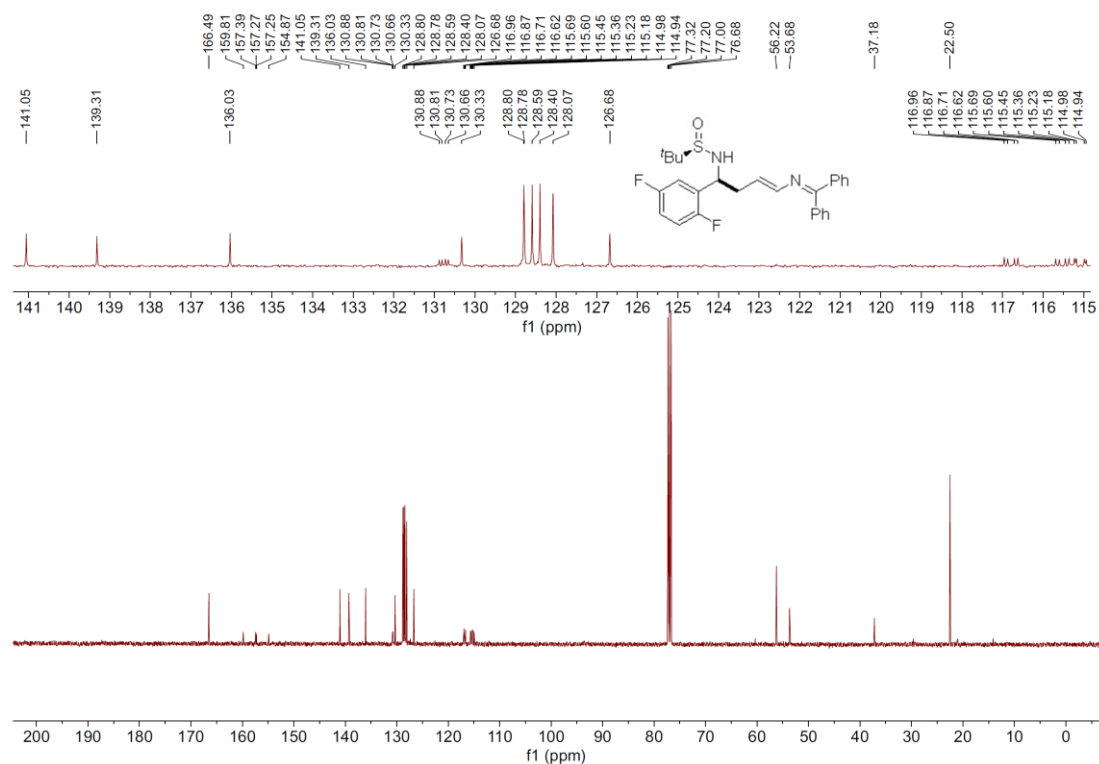
3ak ¹³CNMR



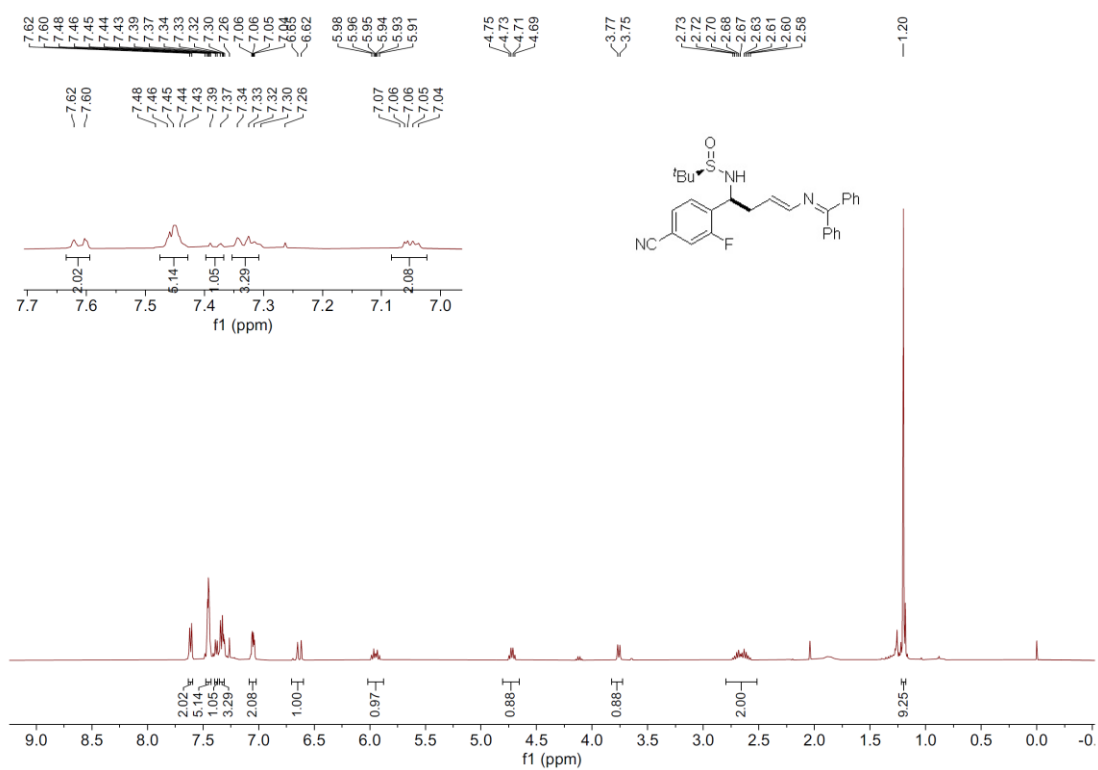
3aI ¹H NMR



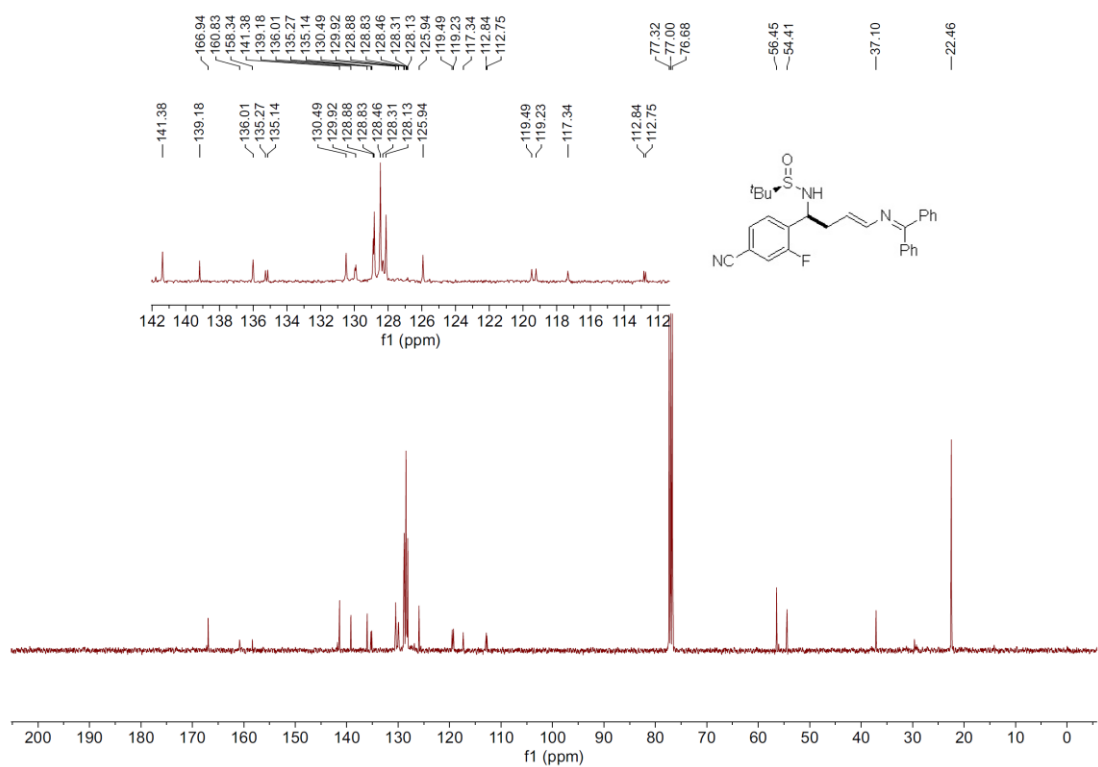
3aI ¹³C NMR



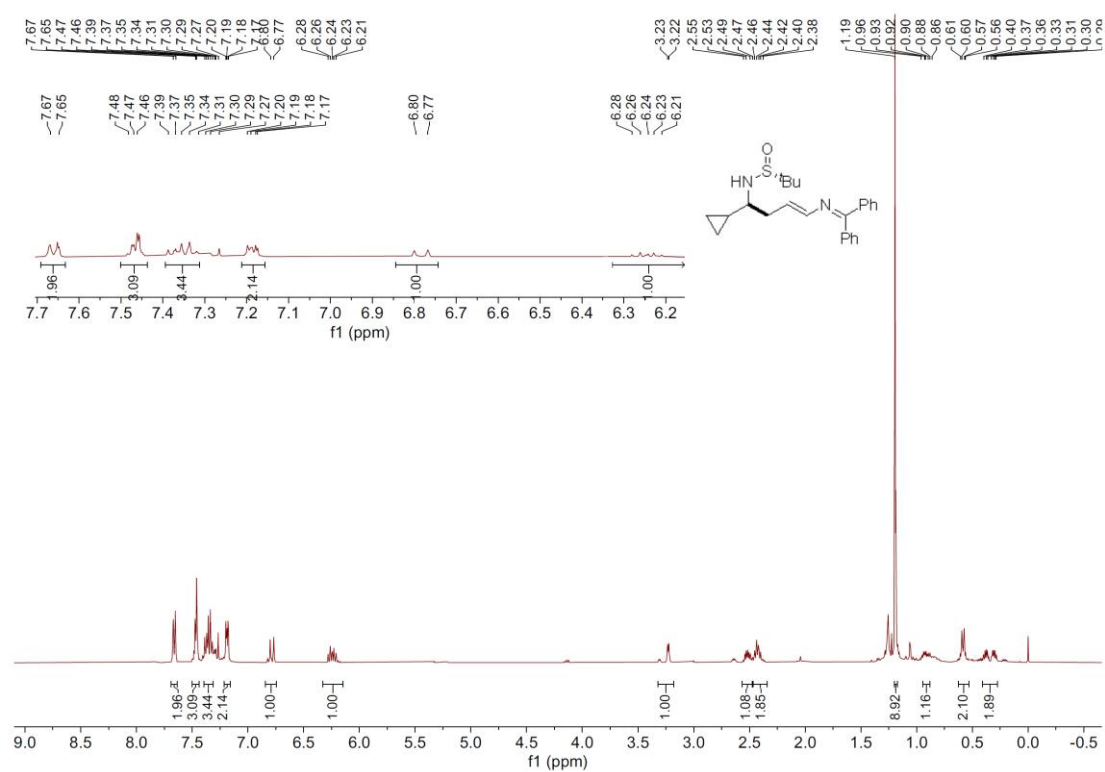
3am ¹H NMR



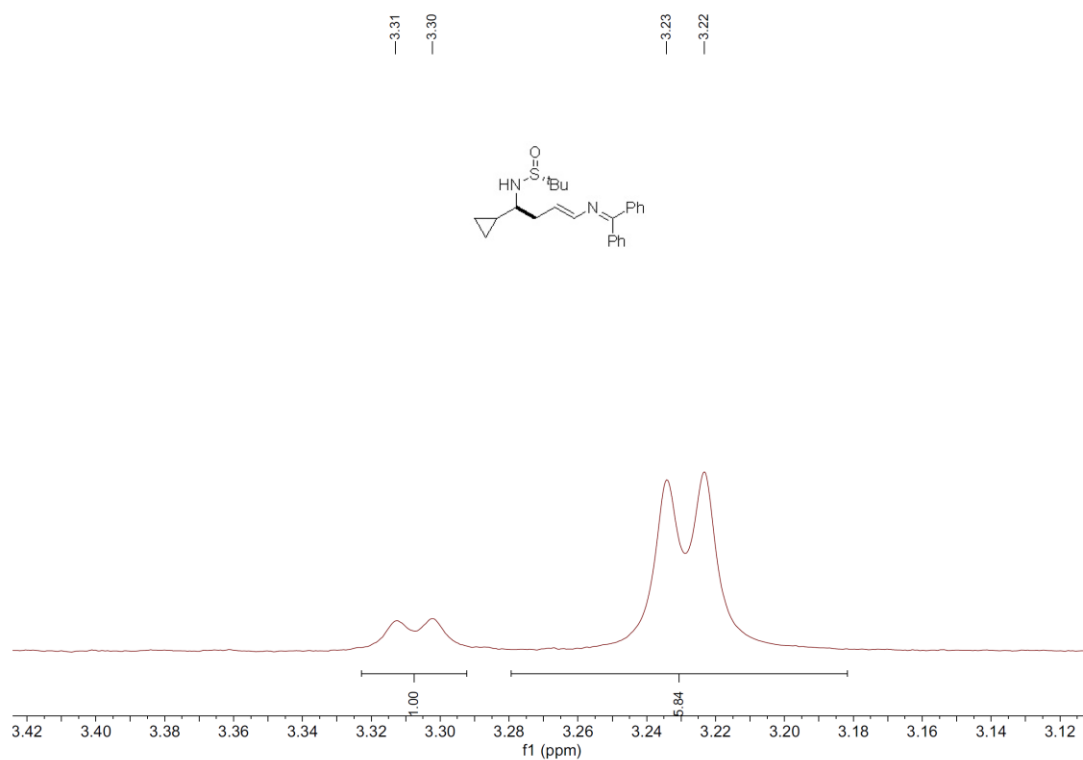
3am ¹³C NMR



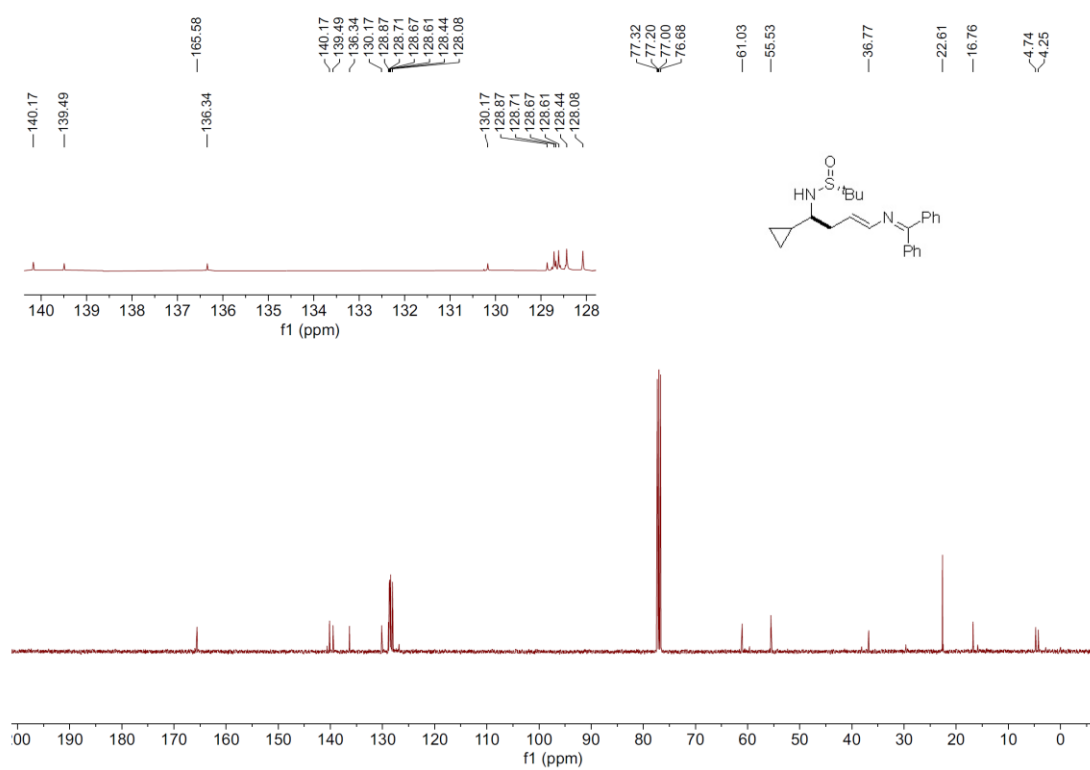
3an ¹H NMR



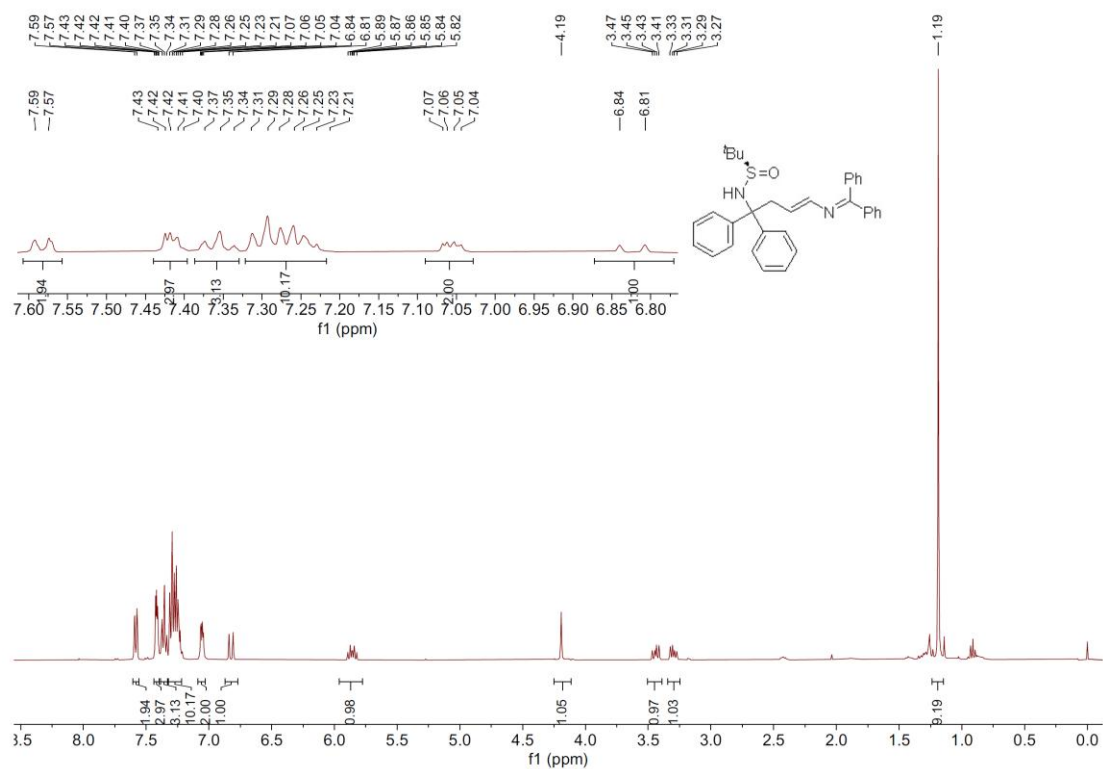
3an *dr*



3an ¹³CNMR



3ao ¹H NMR



The figure displays two ¹³C NMR spectra and the chemical structure of compound 10. The top spectrum is the ¹³C NMR spectrum of compound 10 in CDCl₃, showing peaks from 127 to 146 ppm. The bottom spectrum is the ¹³C NMR spectrum of compound 10 in DMSO-d₆, showing peaks from 22 to 80 ppm. The chemical structure of compound 10 is shown to the right of the top spectrum.

Chemical Structure of Compound 10:

CC(C)(C)OC(=O)N(C1=CC=CC=C1)C2=CC=CC=C2C/C=C/N=C(C3=CC=CC=C3)C4=CC=CC=C4

¹³C NMR Spectrum in CDCl₃ (Top):

Chemical Shift (ppm)
145.52
143.76
142.90
139.60
135.85
130.19
128.87
128.82
128.79
128.46
128.31
128.23
128.04
128.00
127.31
126.89
126.85

¹³C NMR Spectrum in DMSO-d₆ (Bottom):

Chemical Shift (ppm)
166.25
139.60
135.85
130.19
128.87
128.82
128.79
128.46
128.31
128.23
128.04
128.00
127.31
126.89
126.85

Chemical structure of compound 10 is shown above the spectra. The structure is a complex molecule featuring a central benzene ring substituted with a *tert*-butyl sulfonamide group, a 2-phenyl-2-propenyl group, and a 2,2,6,6-tetramethyl-1,3-dioxane-4-carboxylate group.

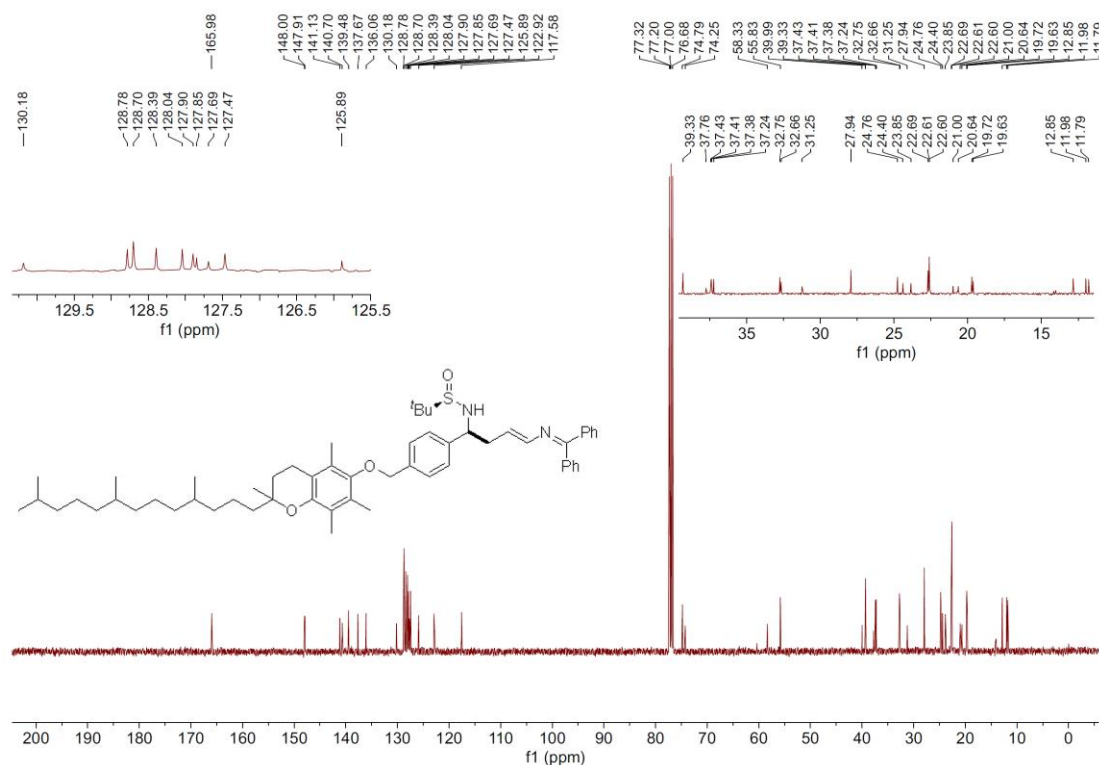
¹³C NMR (CDCl₃) peaks (ppm): 166.38, 165.59, 146.97, 141.02, 139.33, 135.96, 130.30, 130.11, 129.34, 128.79, 128.58, 128.40, 128.06, 127.38, 126.78, 129.34, 128.79, 128.58, 128.40, 128.06, 127.38, 126.78, 109.13, 108.82, 101.57.

¹H NMR (CDCl₃) peaks (ppm): 7.77, 7.73, 7.70, 7.68, 7.07, 7.05, 7.04, 7.02, 7.00, 6.53, 6.31, 6.13, 5.82, 5.63, 3.78, 2.64, 2.55, 2.53, 2.51, 2.27, 2.25, 2.23, 2.21, 2.19, 2.17, 2.15, 2.13, 2.11, 2.09, 2.07, 2.05, 2.03, 2.01, 1.99, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01.

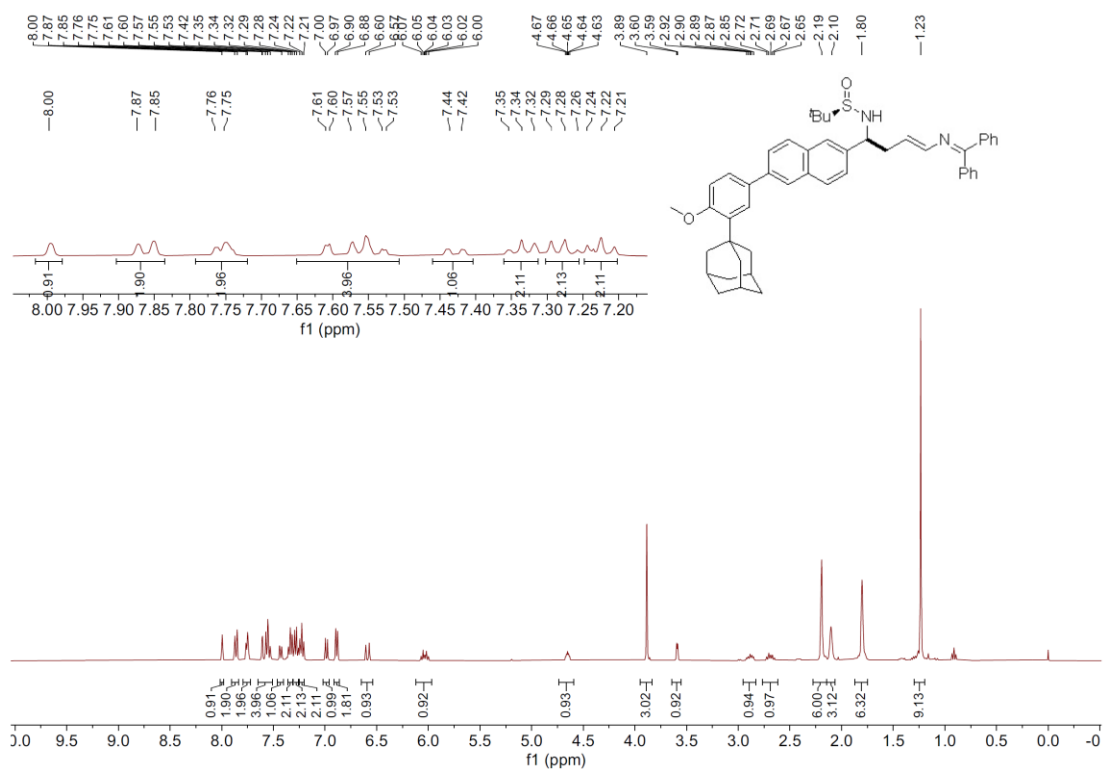
2D COSY peaks (ppm): 7.77, 7.73, 7.70, 7.68, 7.07, 7.05, 7.04, 7.02, 7.00, 6.53, 6.31, 6.13, 5.82, 5.63, 3.78, 2.64, 2.55, 2.53, 2.51, 2.27, 2.25, 2.23, 2.21, 2.19, 2.17, 2.15, 2.13, 2.11, 2.09, 2.07, 2.05, 2.03, 2.01, 1.99, 1.97, 1.95, 1.93, 1.91, 1.89, 1.87, 1.85, 1.83, 1.81, 1.79, 1.77, 1.75, 1.73, 1.71, 1.69, 1.67, 1.65, 1.63, 1.61, 1.59, 1.57, 1.55, 1.53, 1.51, 1.49, 1.47, 1.45, 1.43, 1.41, 1.39, 1.37, 1.35, 1.33, 1.31, 1.29, 1.27, 1.25, 1.23, 1.21, 1.19, 1.17, 1.15, 1.13, 1.11, 1.09, 1.07, 1.05, 1.03, 1.01, 0.99, 0.97, 0.95, 0.93, 0.91, 0.89, 0.87, 0.85, 0.83, 0.81, 0.79, 0.77, 0.75, 0.73, 0.71, 0.69, 0.67, 0.65, 0.63, 0.61, 0.59, 0.57, 0.55, 0.53, 0.51, 0.49, 0.47, 0.45, 0.43, 0.41, 0.39, 0.37, 0.35, 0.33, 0.31, 0.29, 0.27, 0.25, 0.23, 0.21, 0.19, 0.17, 0.15, 0.13, 0.11, 0.09, 0.07, 0.05, 0.03, 0.01.

Figure 1 displays the ^1H NMR spectra of compound **1**. The top spectrum shows the ^1H NMR of compound **1** in CDCl_3 , with peaks labeled from 7.62 to 0.84 ppm. The bottom spectrum shows the ^1H NMR of compound **1** in CDCl_3 , with peaks labeled from 7.62 to 0.84 ppm. The chemical structure of compound **1** is shown in the center, featuring a complex molecule with a long alkyl chain, a phenyl ring, and a chiral center.

3aq ¹³CNMR

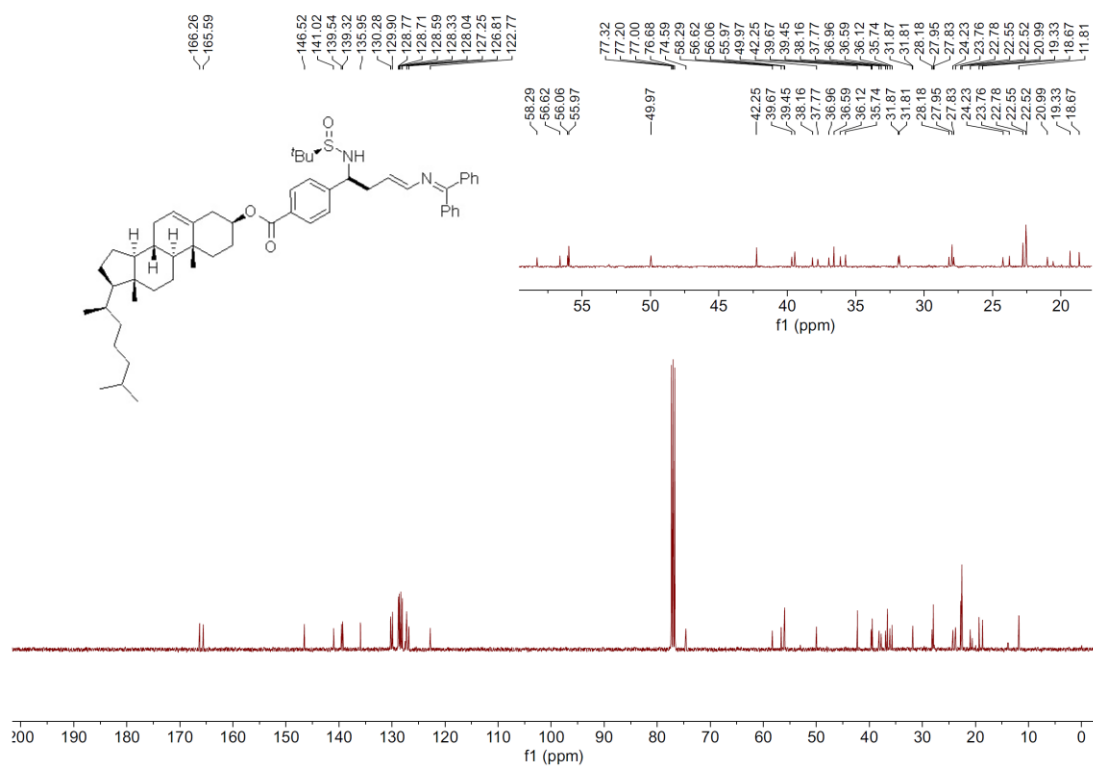


3ar ¹H NMR

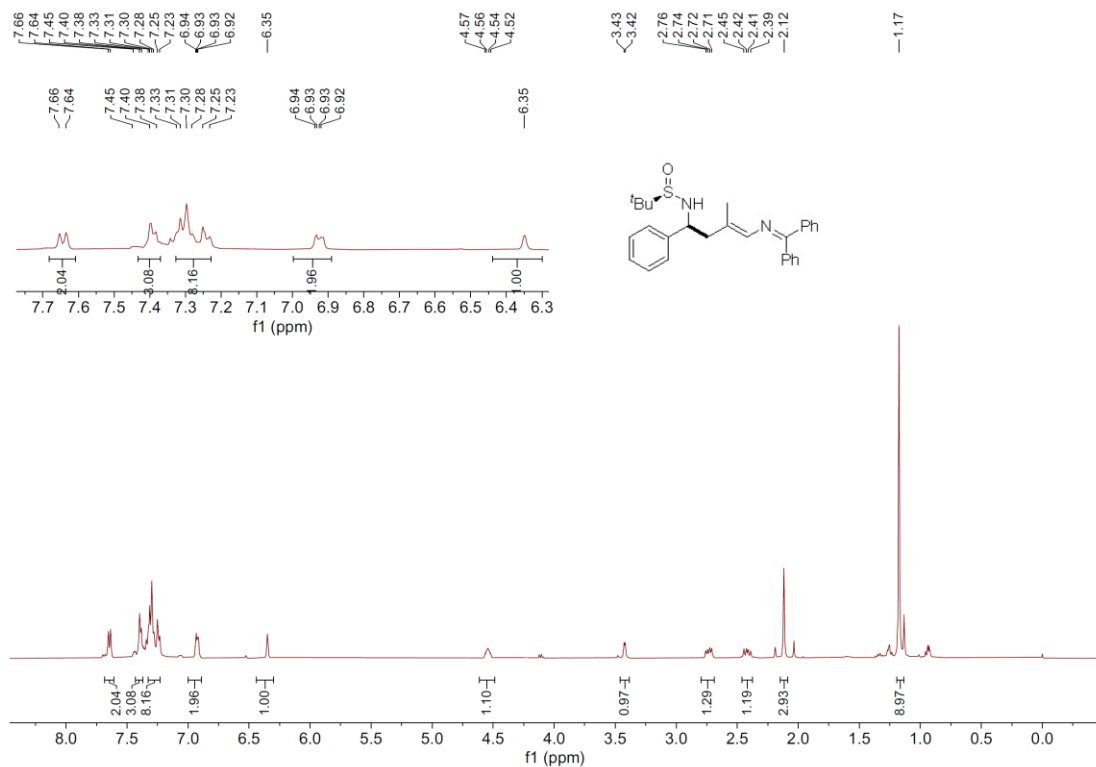


[illegible][illegible]

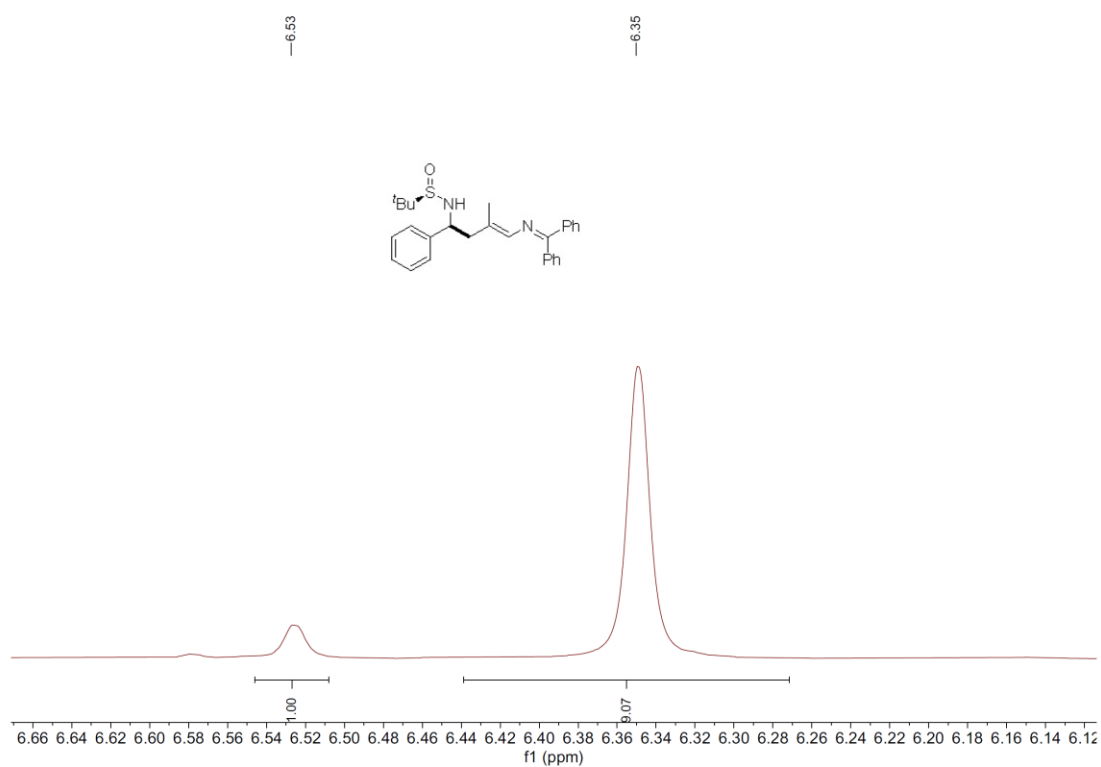
3as ¹³C NMR



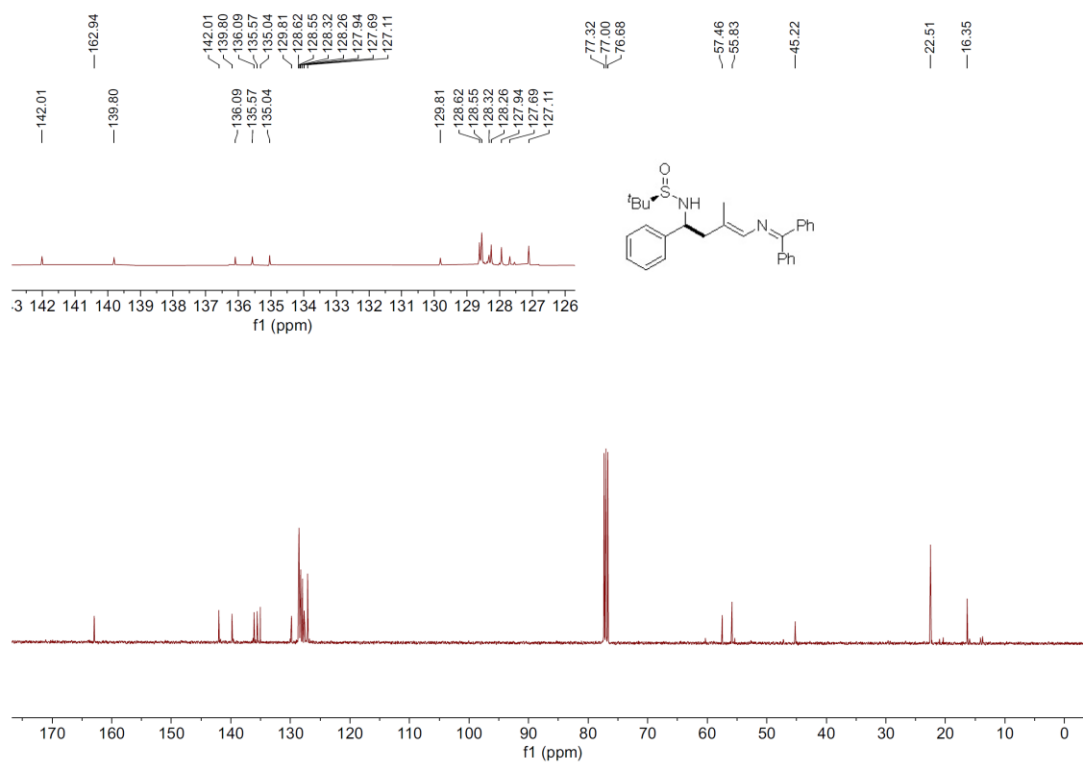
3at ¹H NMR



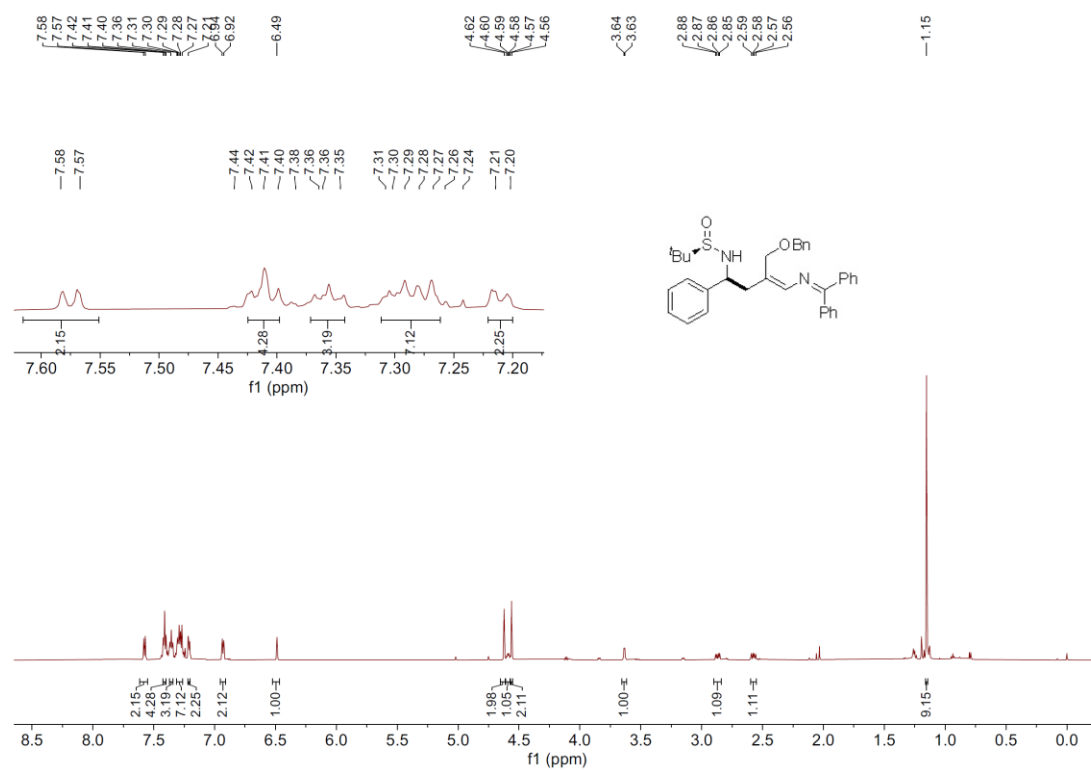
3at *E/Z*



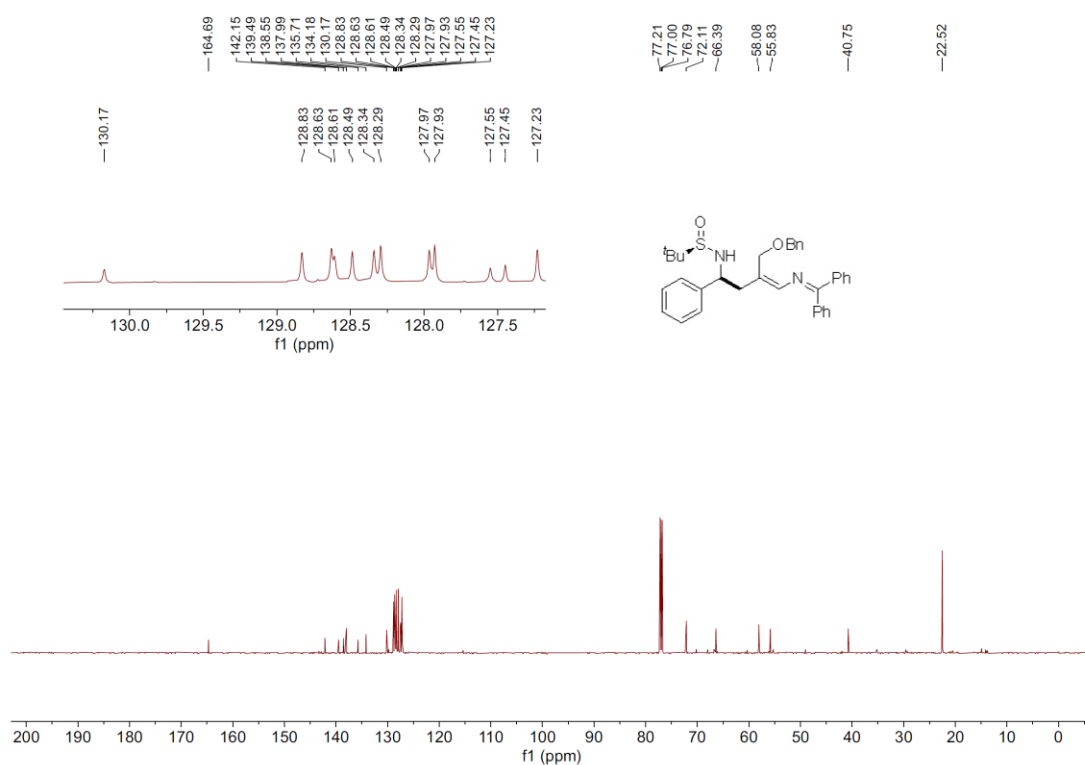
3at ¹³C NMR



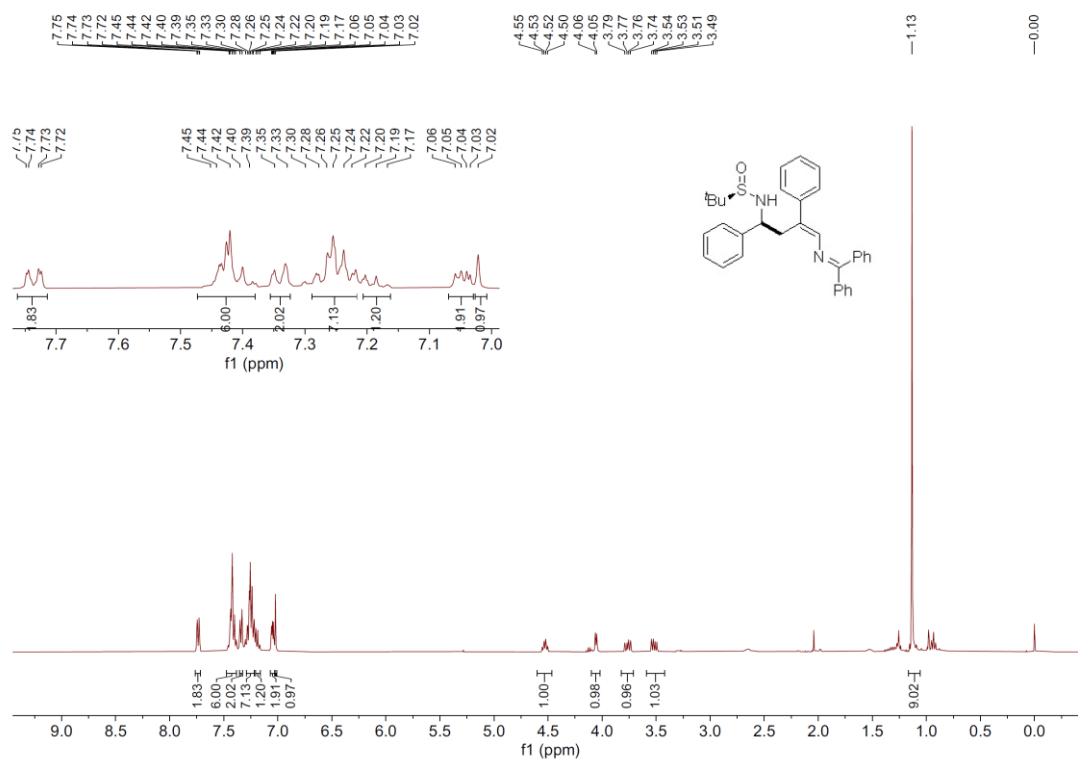
3au ¹H NMR



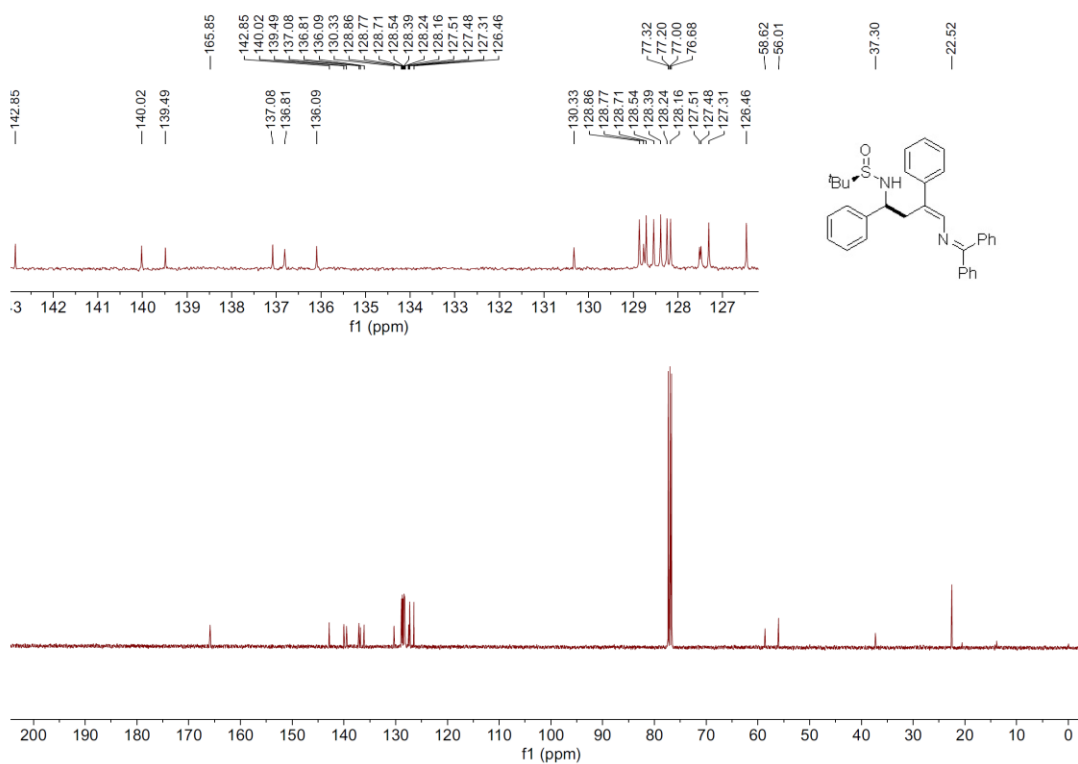
3au ¹³C NMR



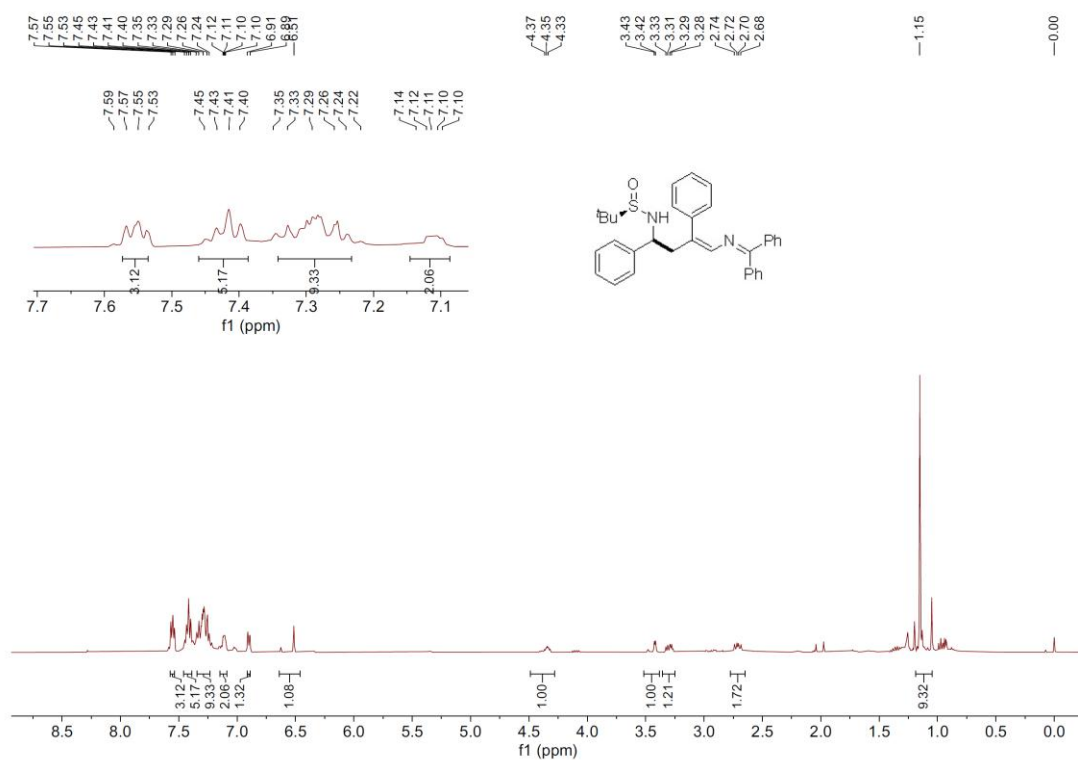
3av *E*-isomer ^1H NMR



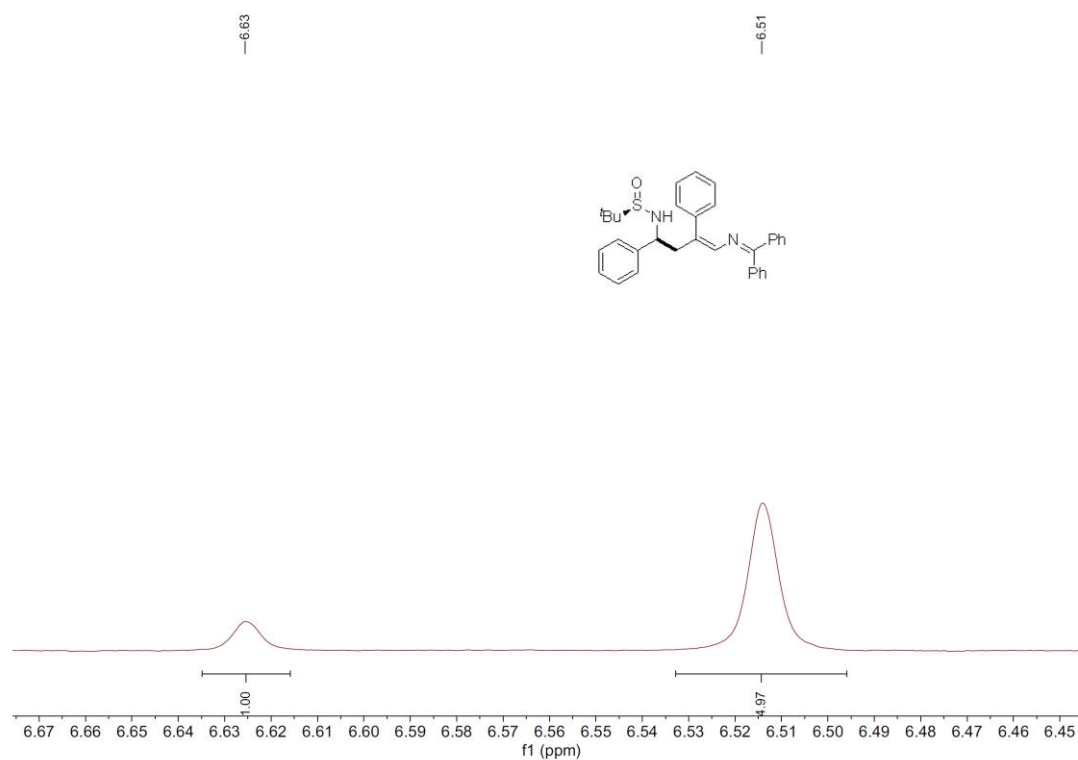
3av *E*-isomer ^{13}C NMR



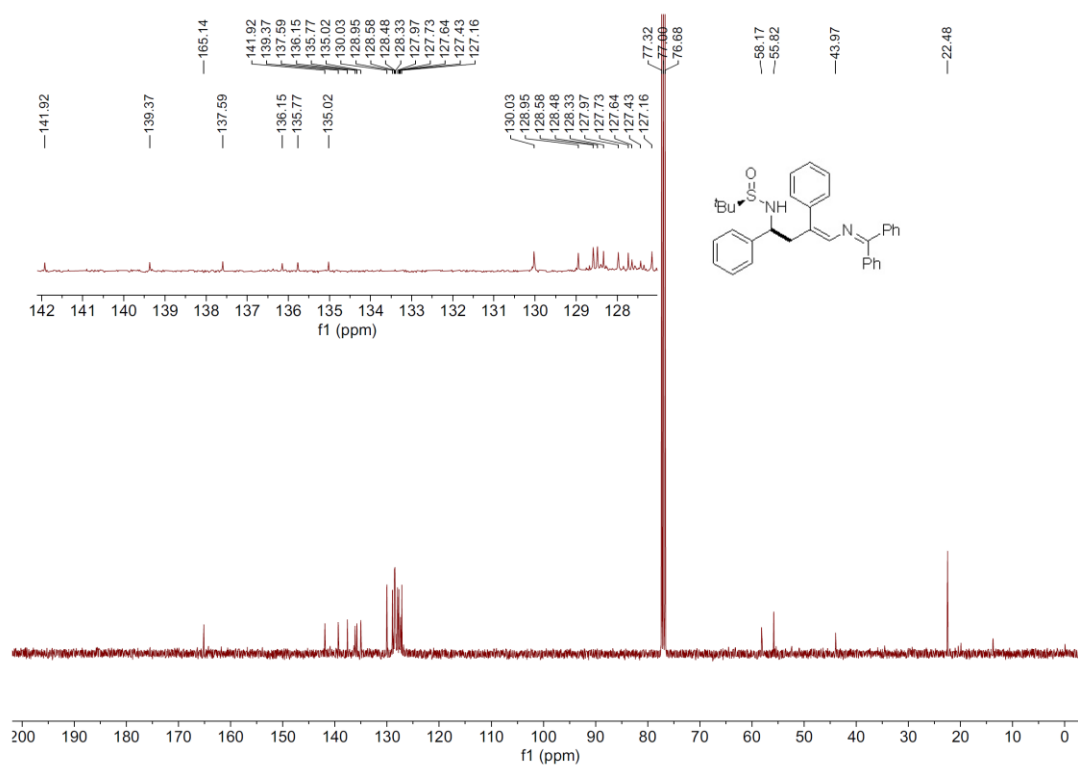
3av Z-isomer ^1H NMR



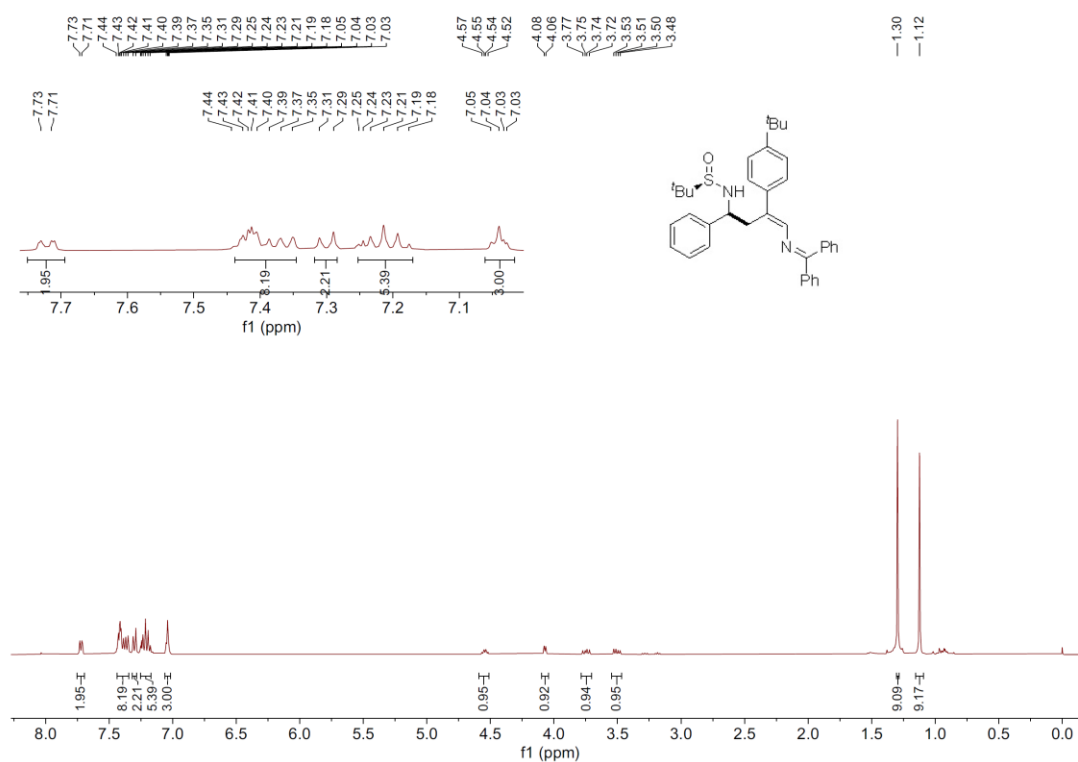
3av Z-isomer *dr*



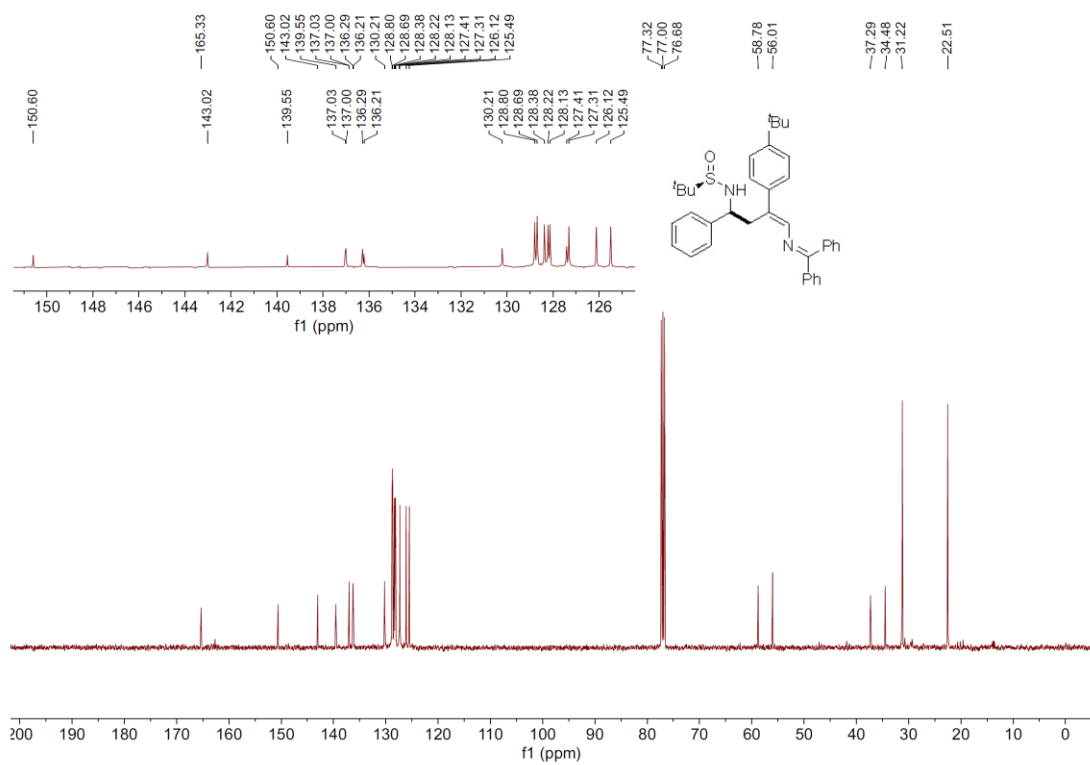
3av Z-isomer ^{13}C NMR



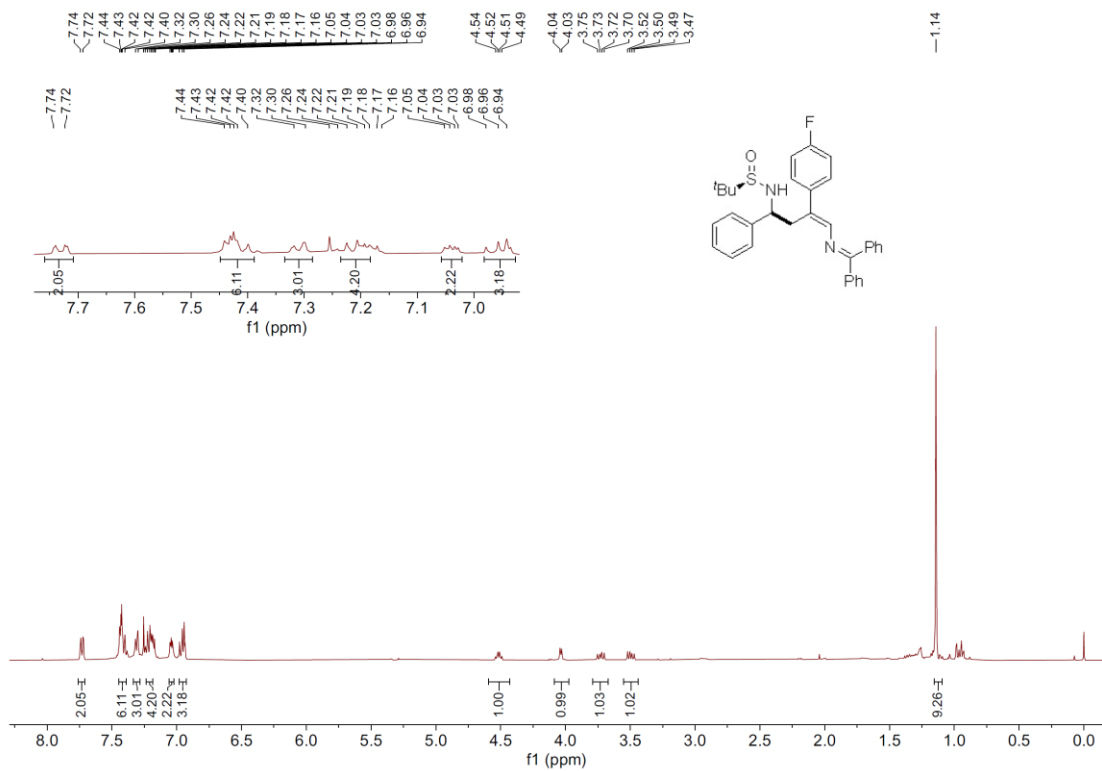
3aw ^1H NMR



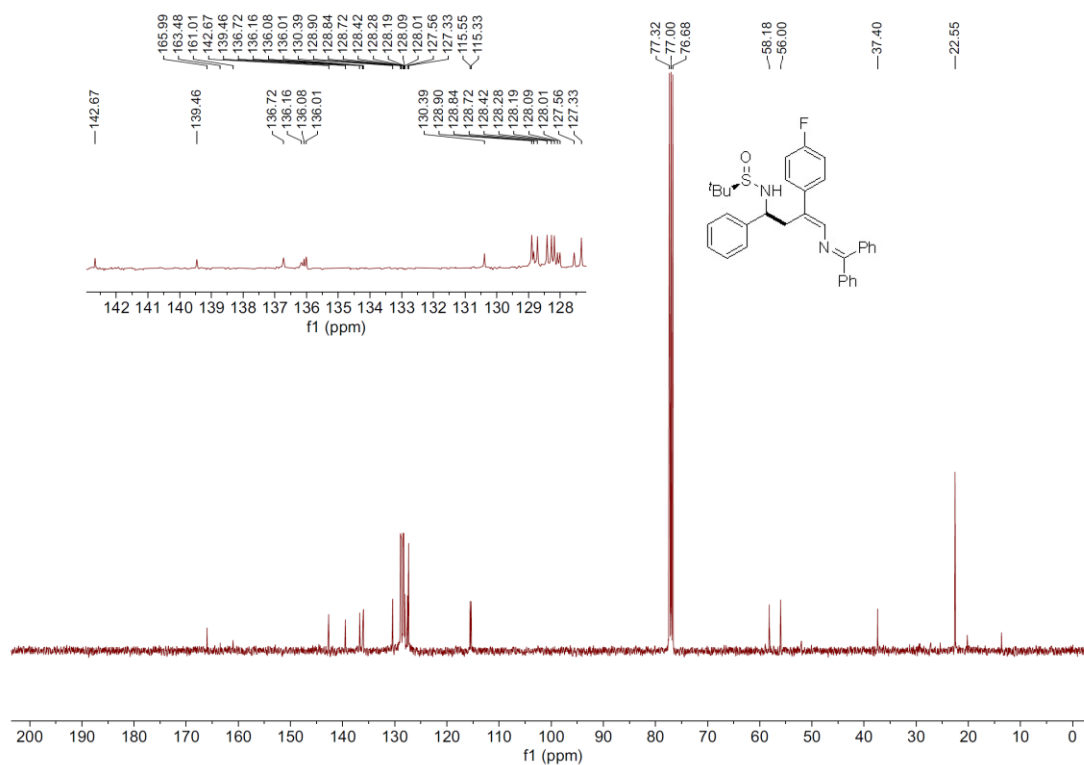
3aw ^{13}C NMR



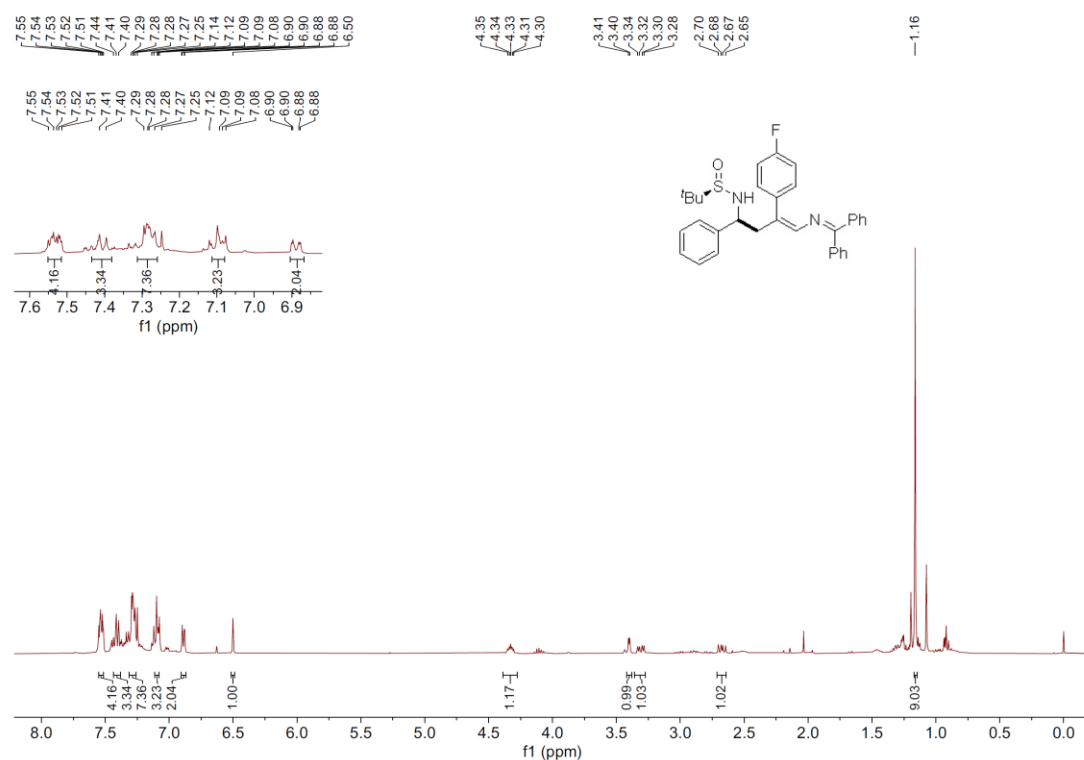
3ax *E*-isomer ¹H NMR



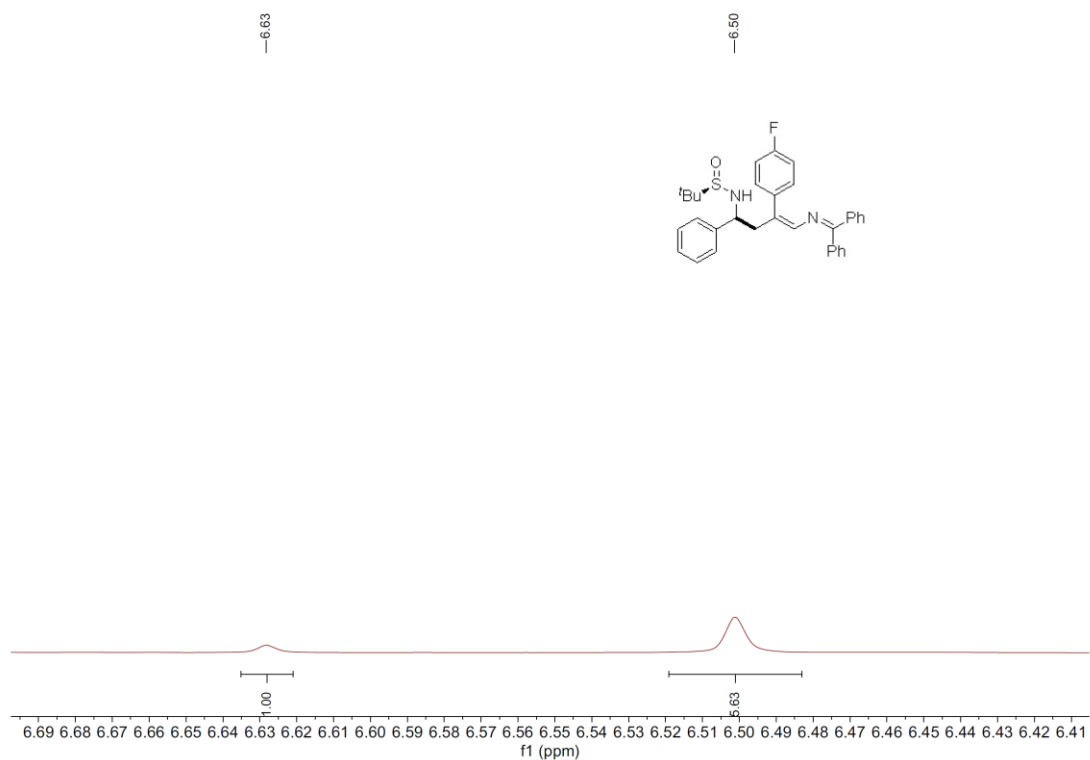
3ax *E*-isomer ^{13}C NMR



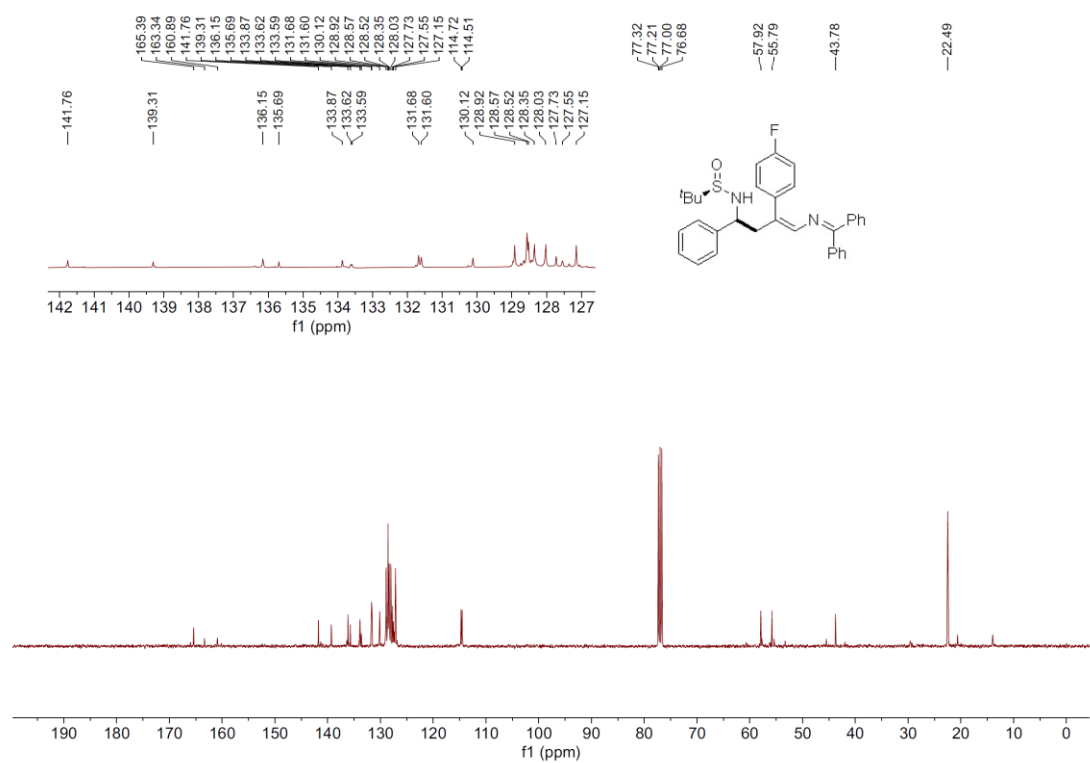
3ax *Z*-isomer ^1H NMR



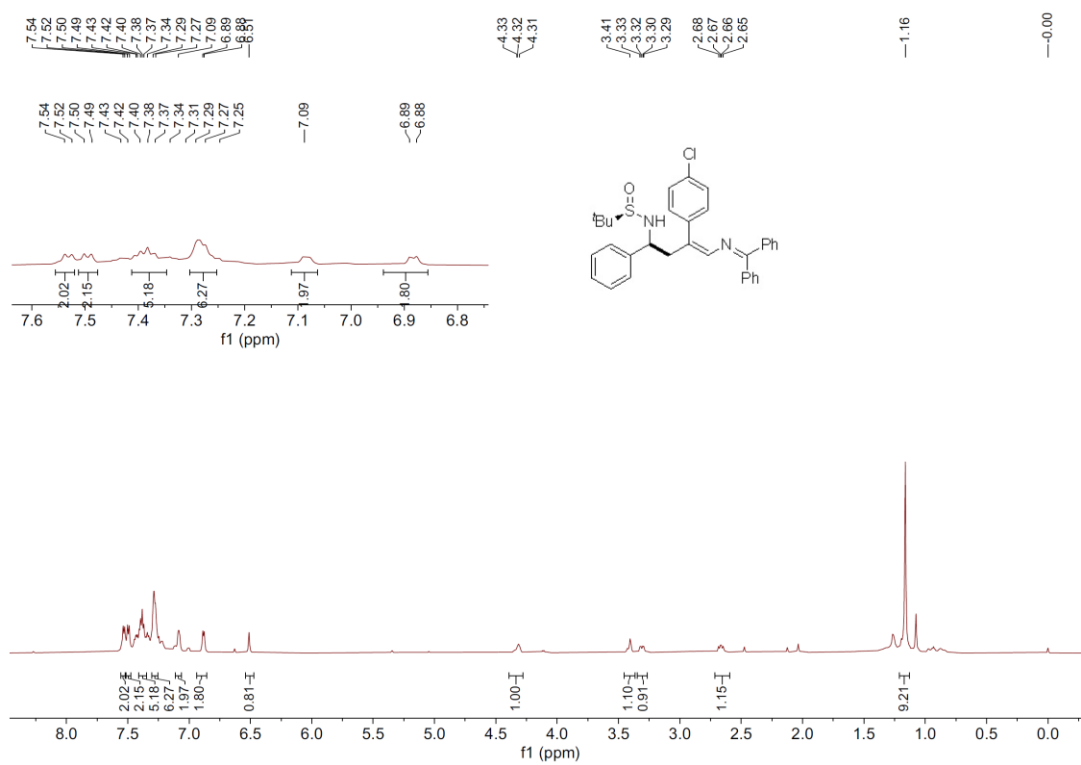
3ax Z-isomer *dr*



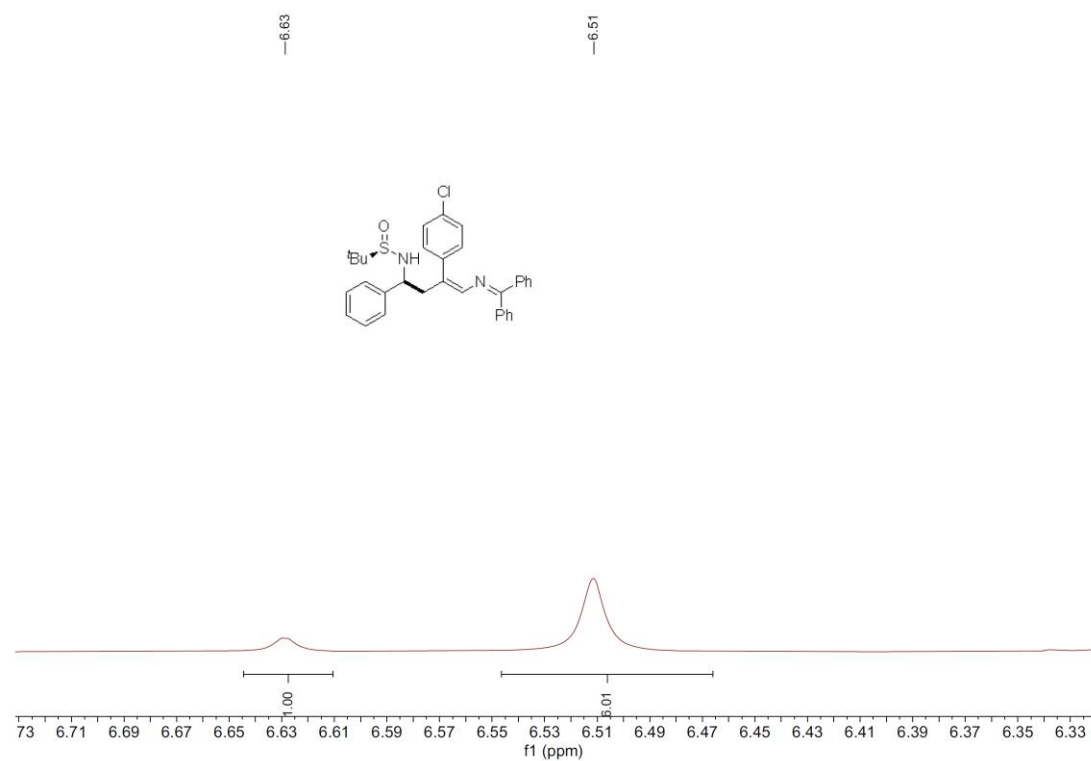
3ax Z-isomer ¹³CNMR

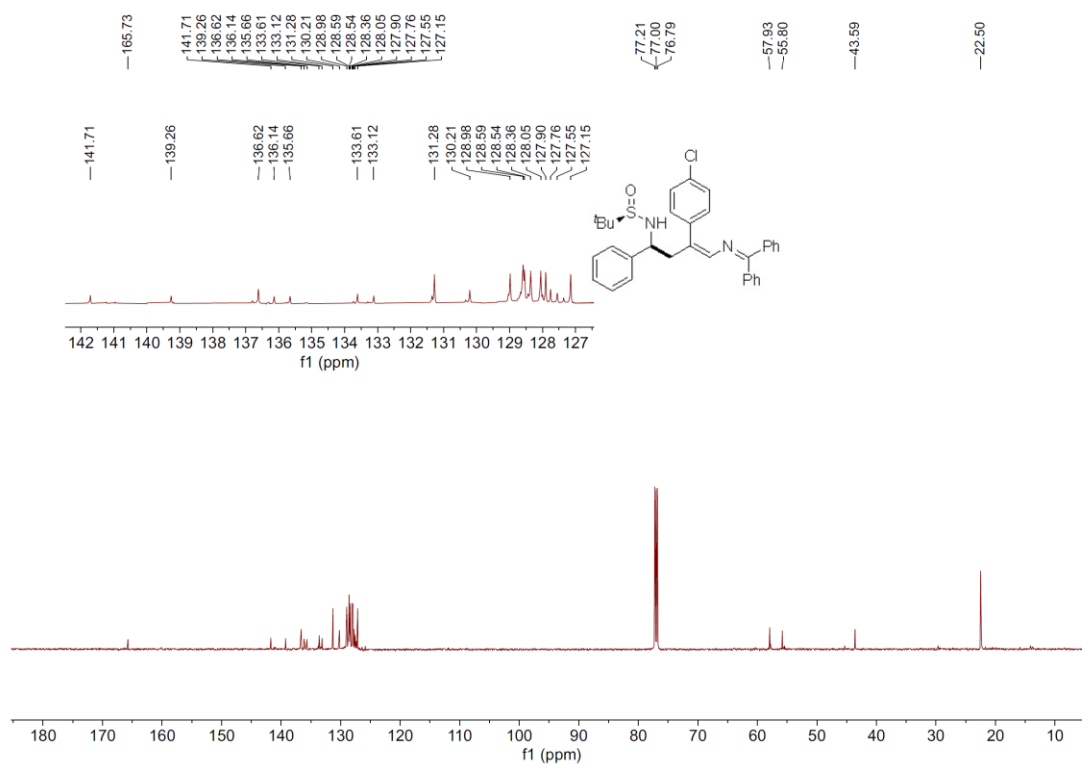


3ay ¹H NMR

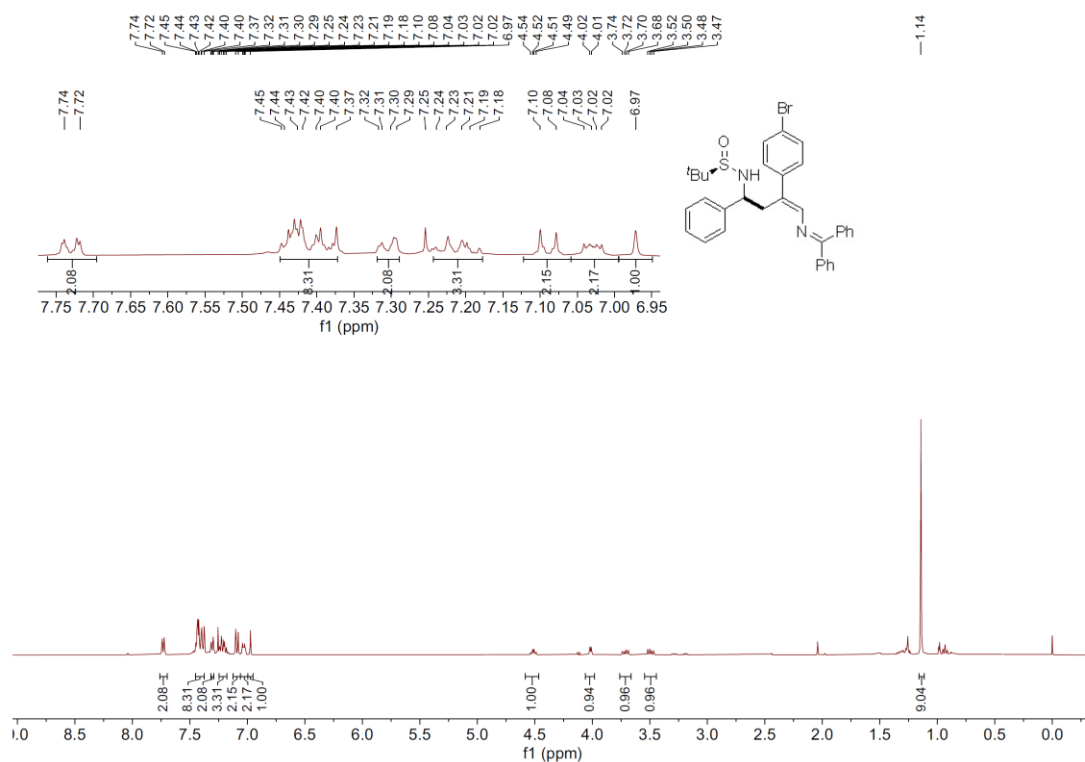


3ay E/Z

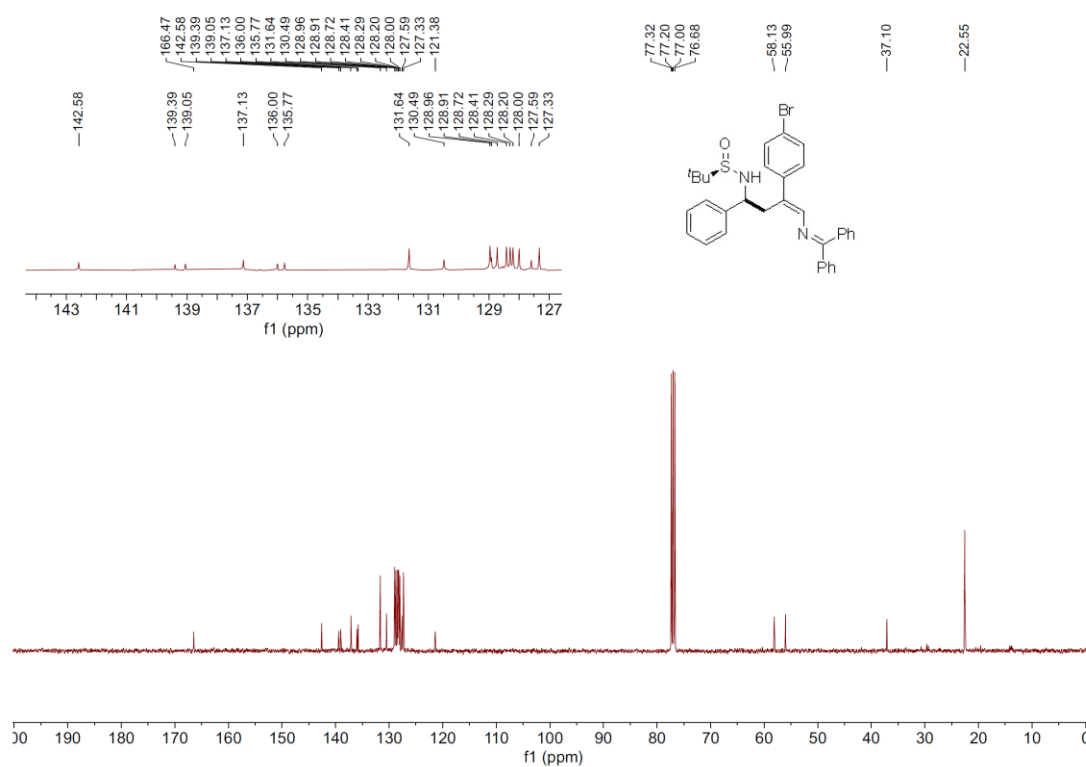


¹³CNMR

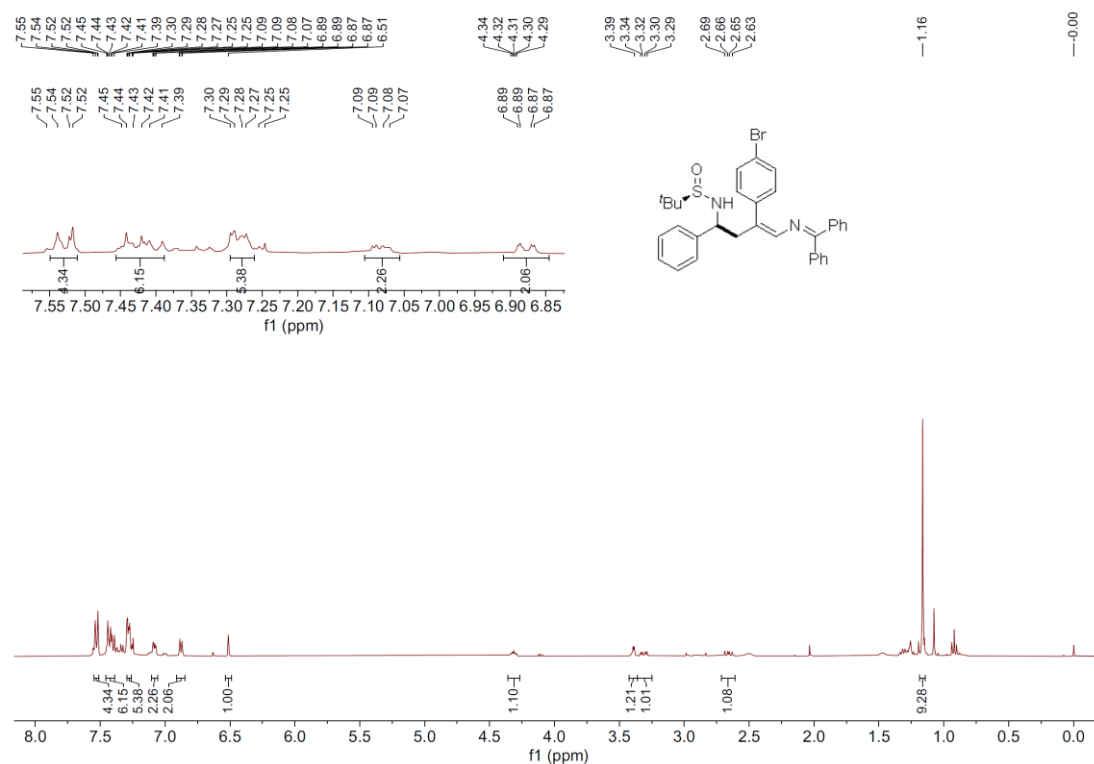
3az *E*-isomer ¹H NMR



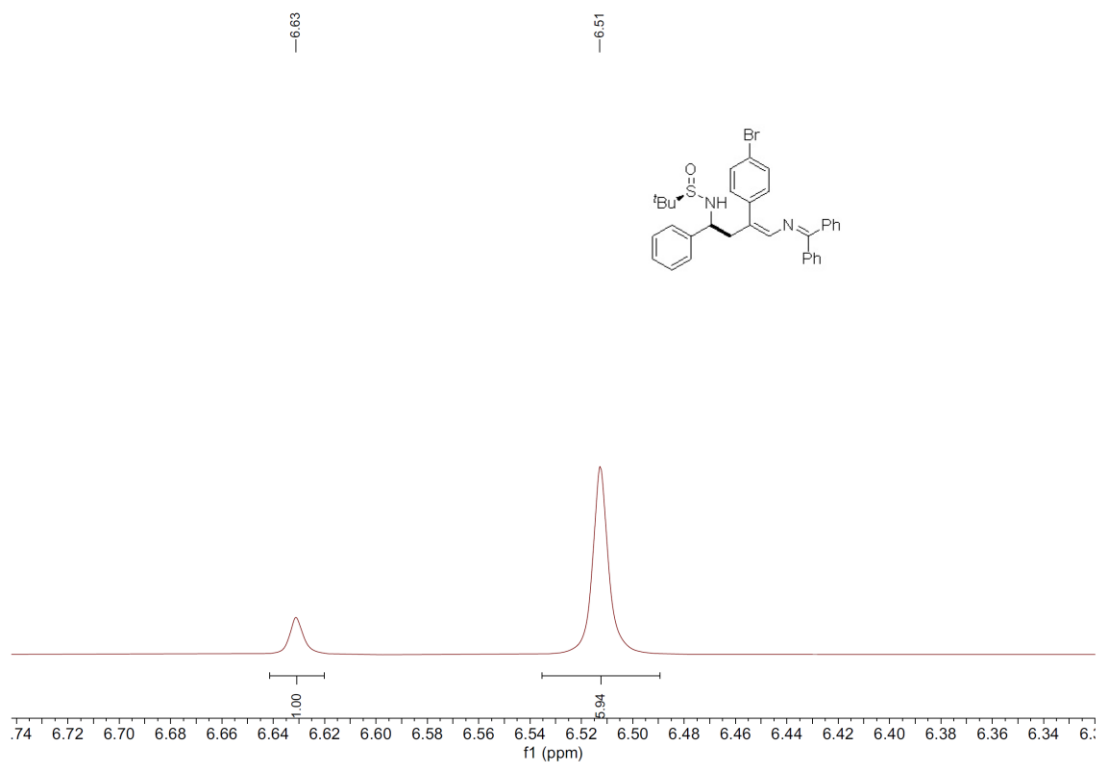
3az *E*-isomer ^{13}C NMR



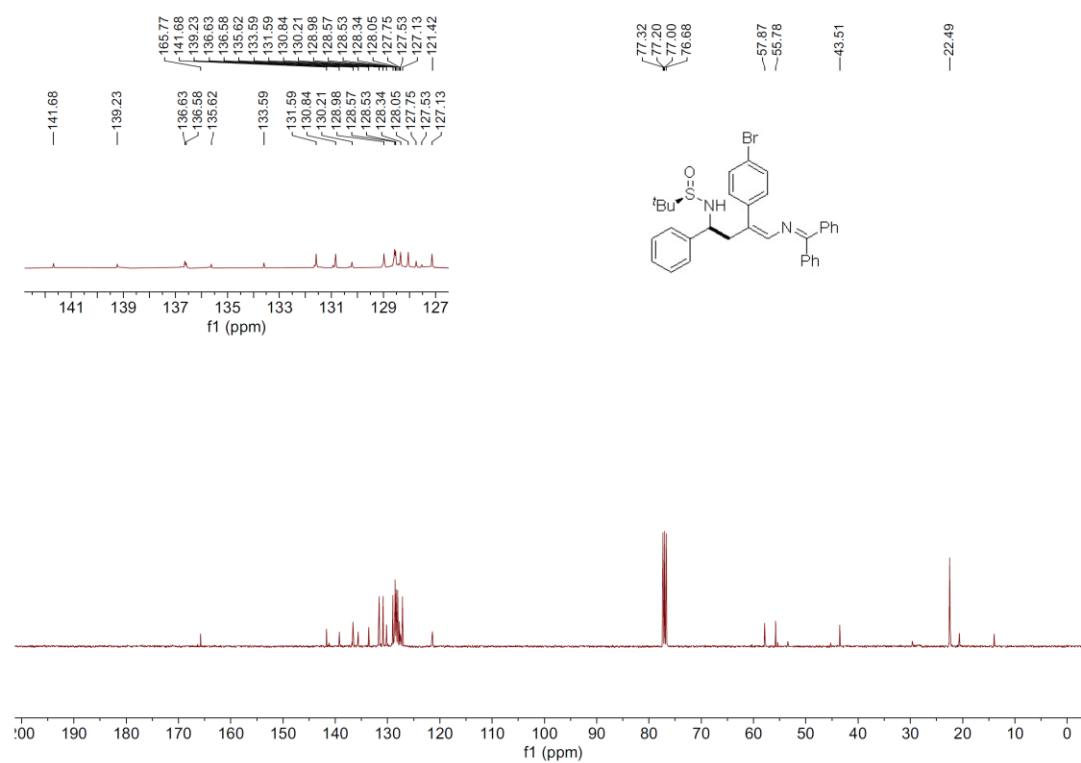
3az *Z*-isomer ^1H NMR



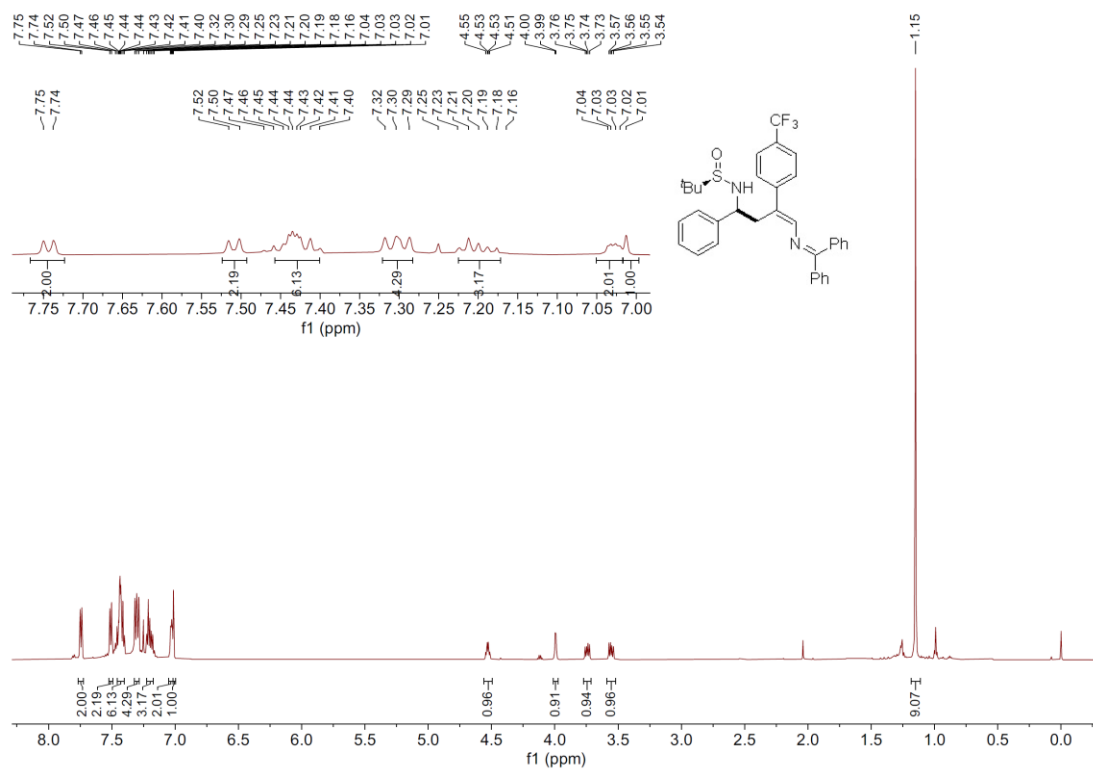
3az Z-isomer *dr*



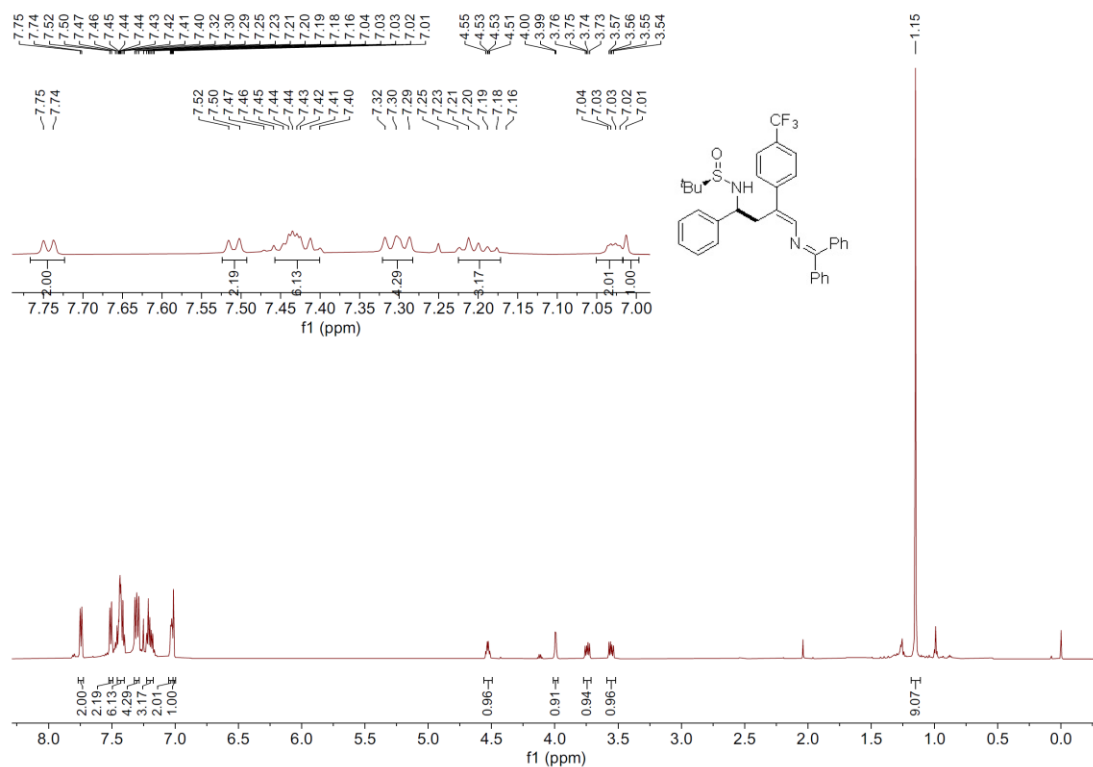
3az Z-isomer ¹³CNMR



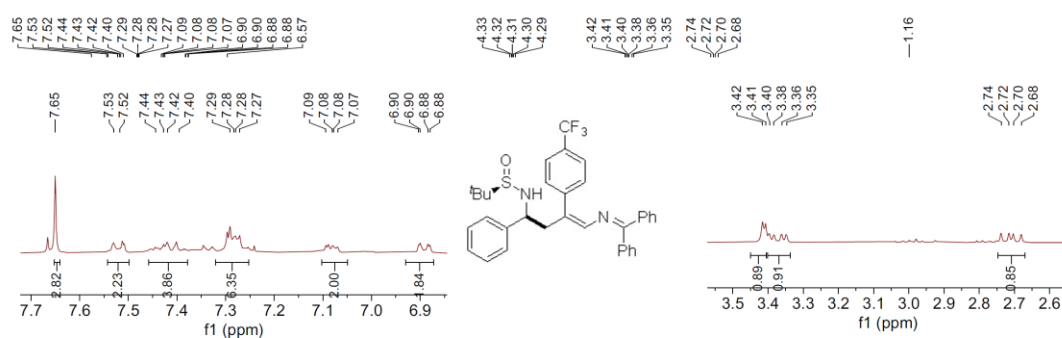
3ba *E*-isomer ^1H NMR



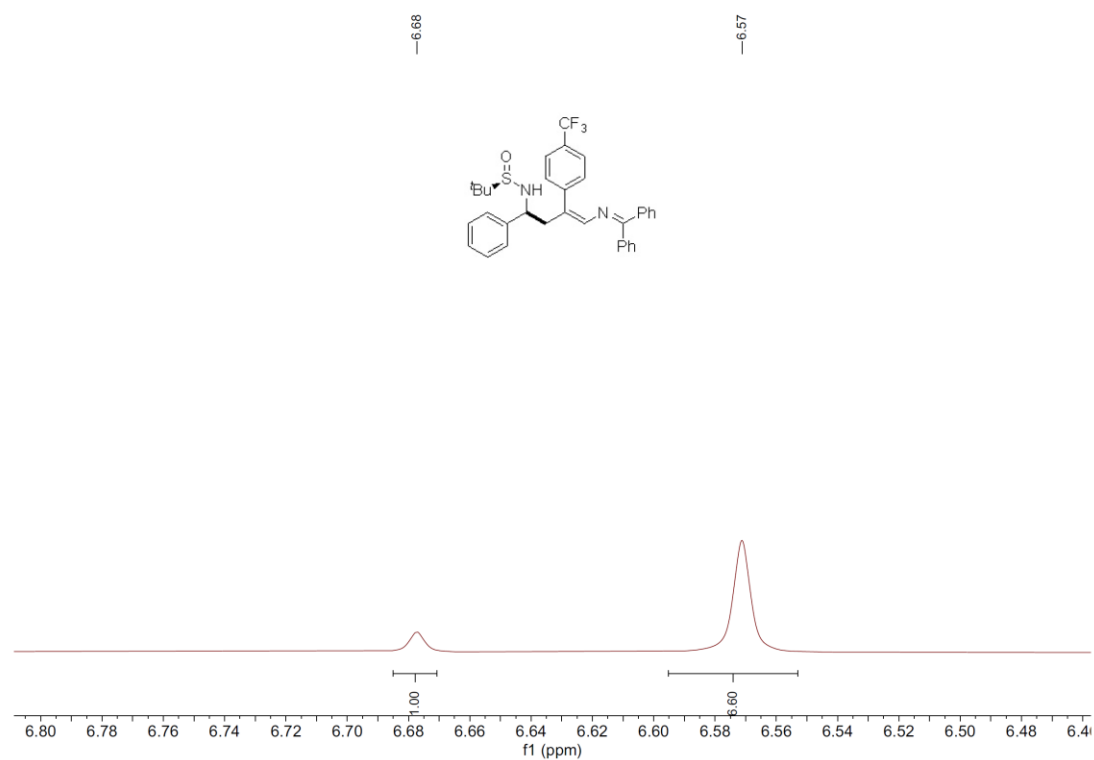
3ba *E*-isomer ^{13}C NMR



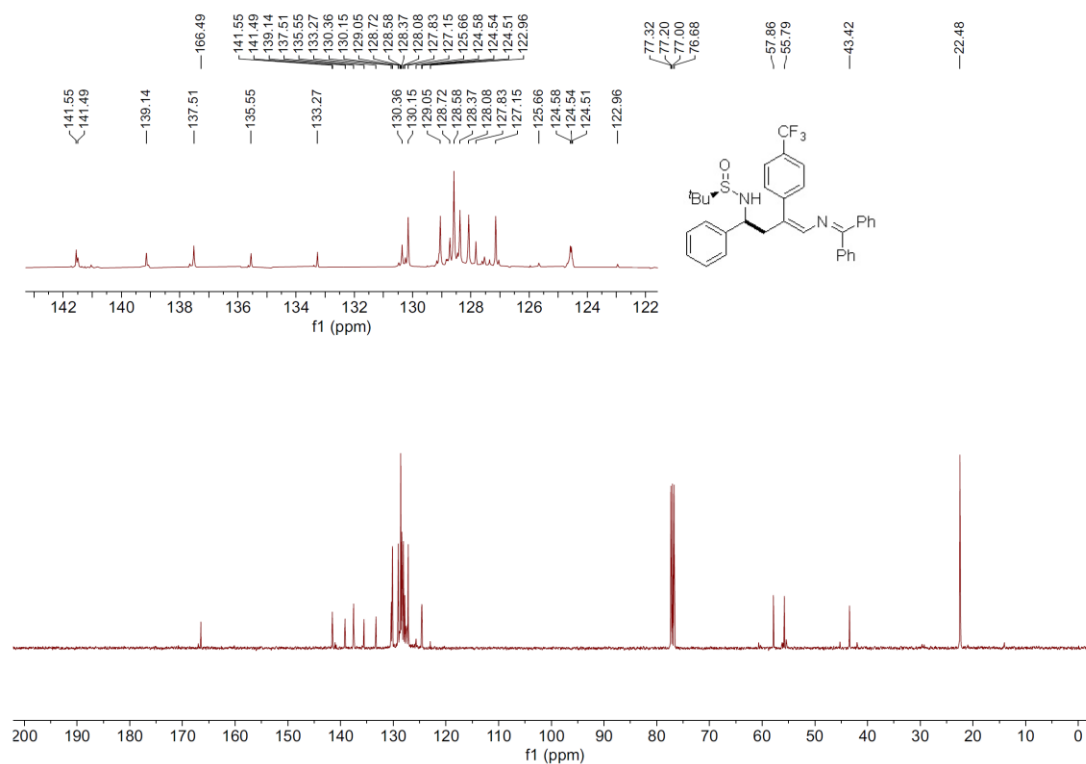
3ba Z-isomer ¹H NMR



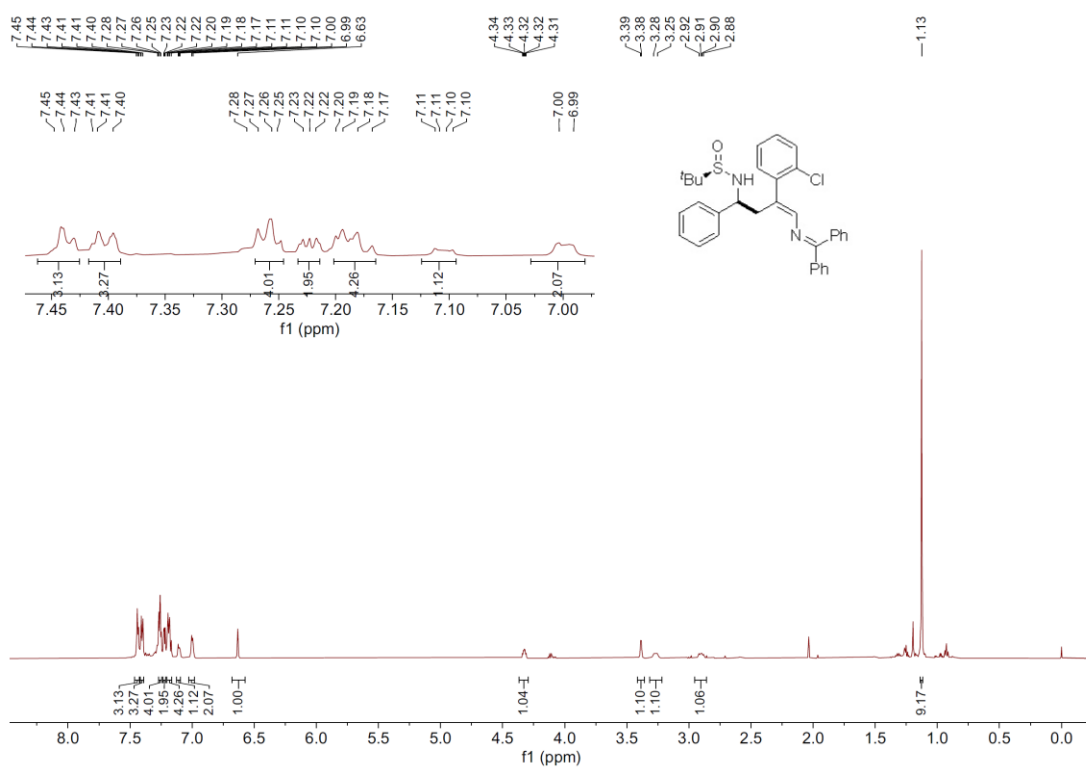
3ba Z-isomer *dr*



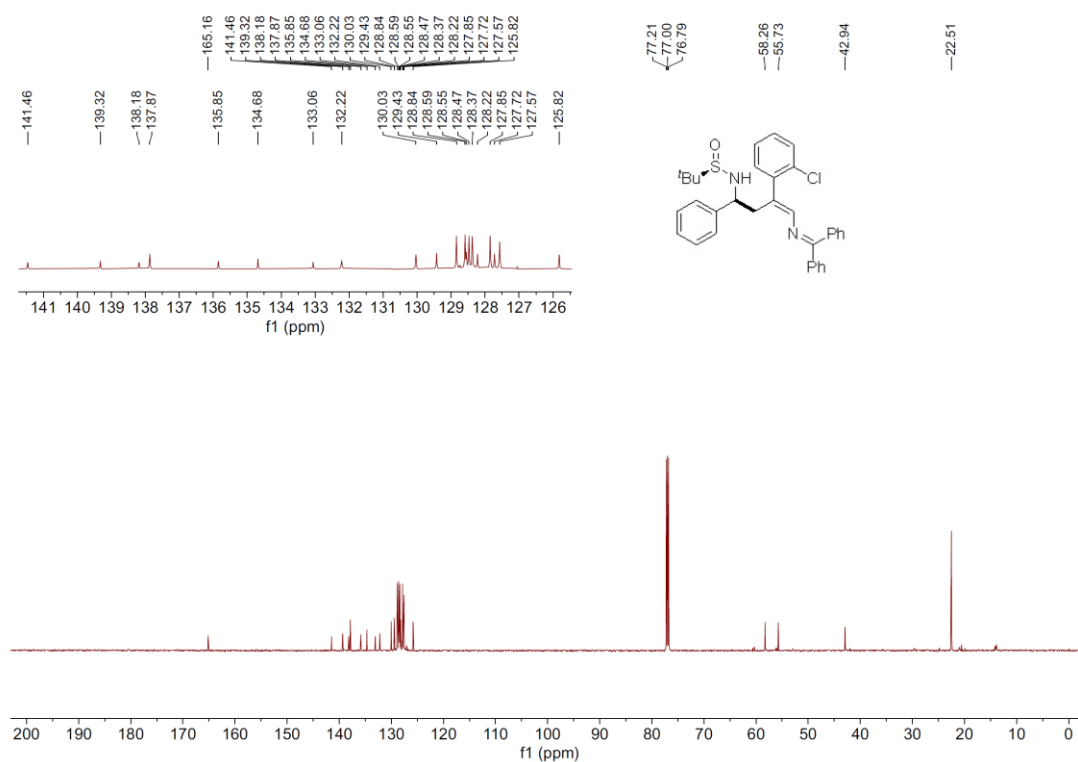
3ba Z-isomer ^{13}C NMR



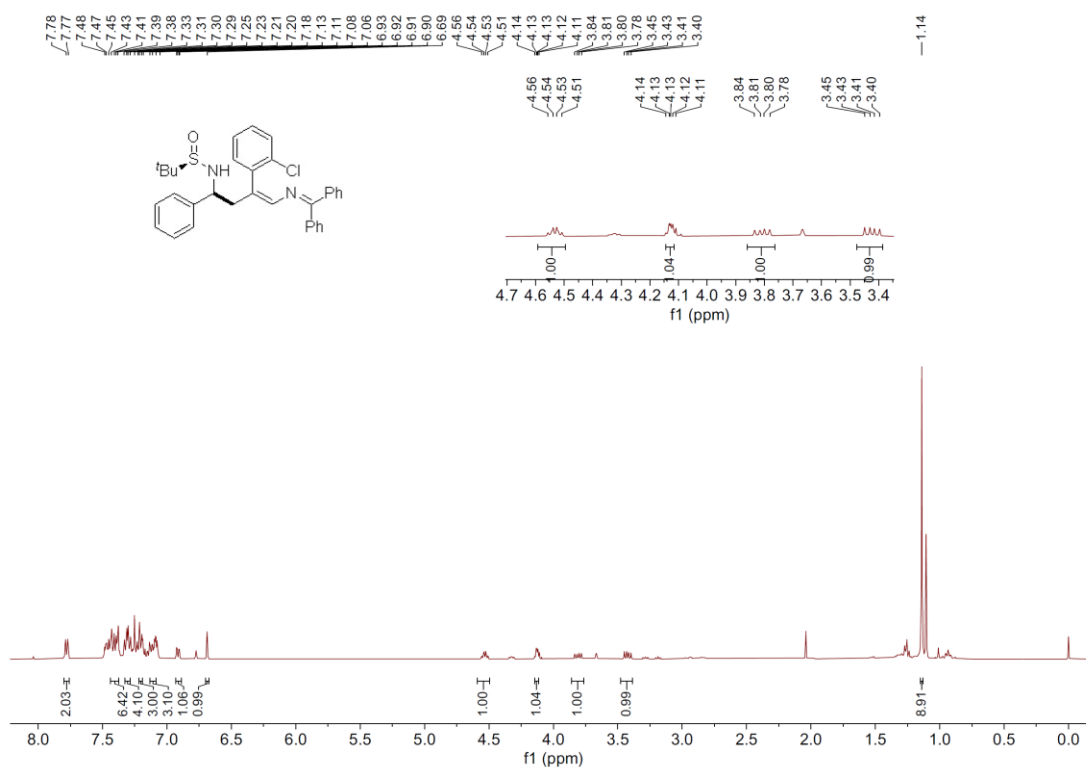
3bb E-isomer ^1H NMR



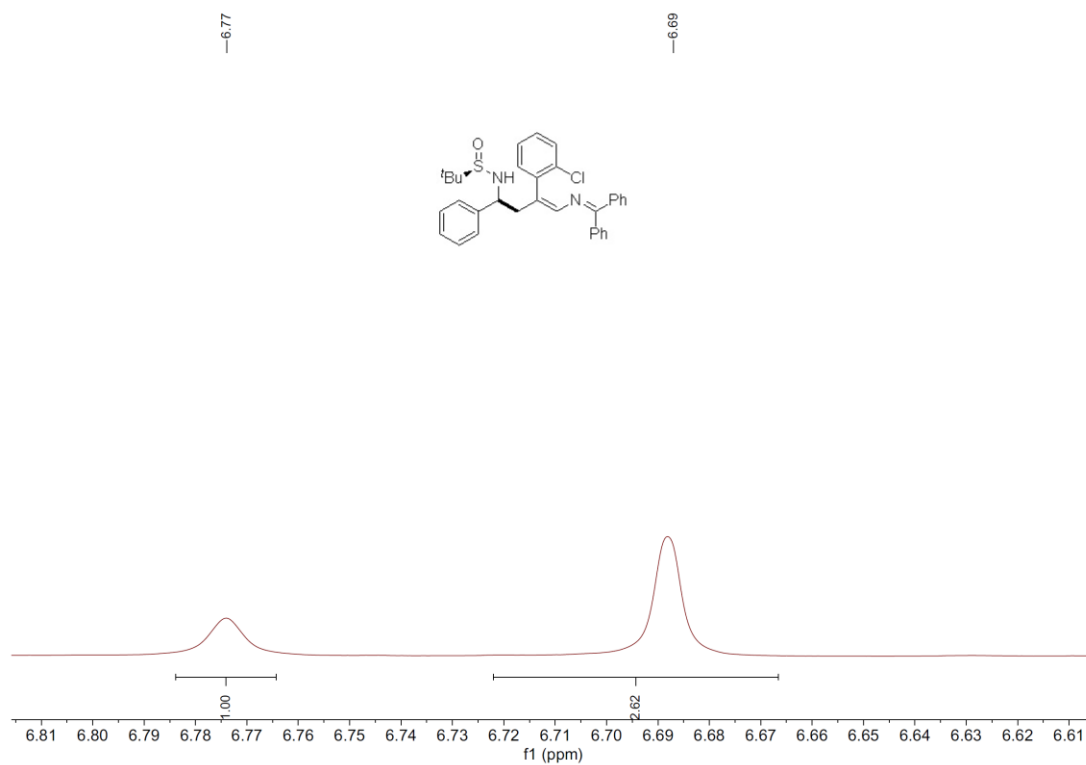
3bb *E*-isomer ^{13}C NMR



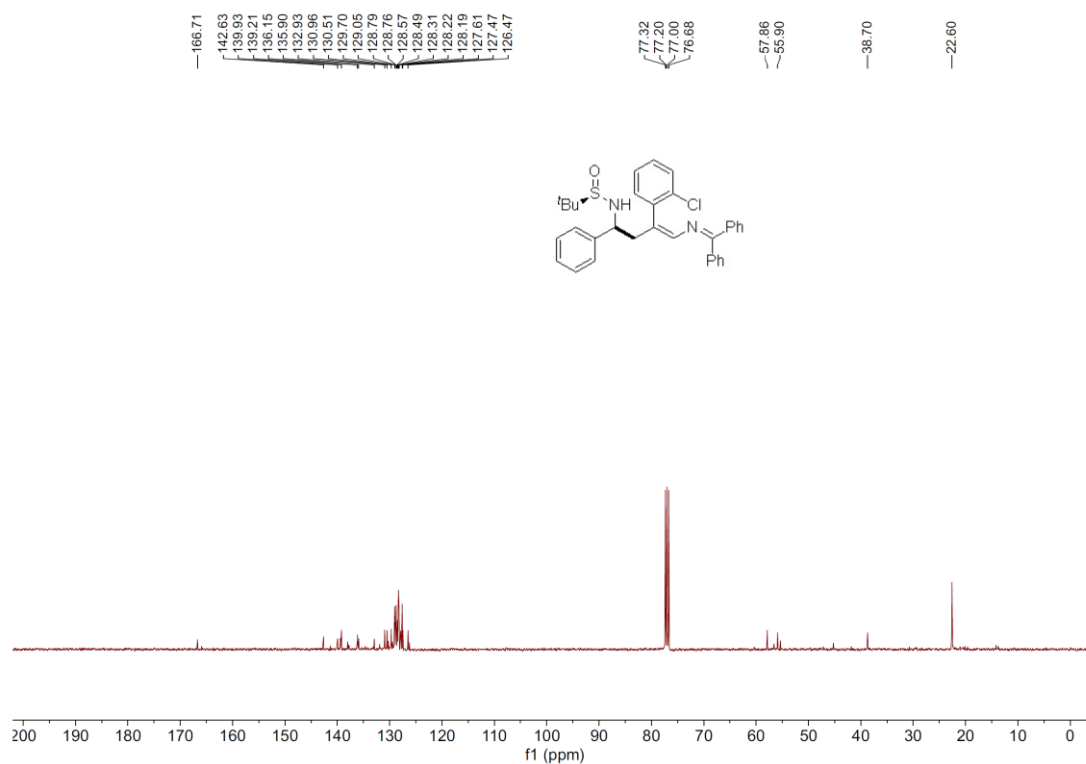
3bb *Z*-isomer ^1H NMR



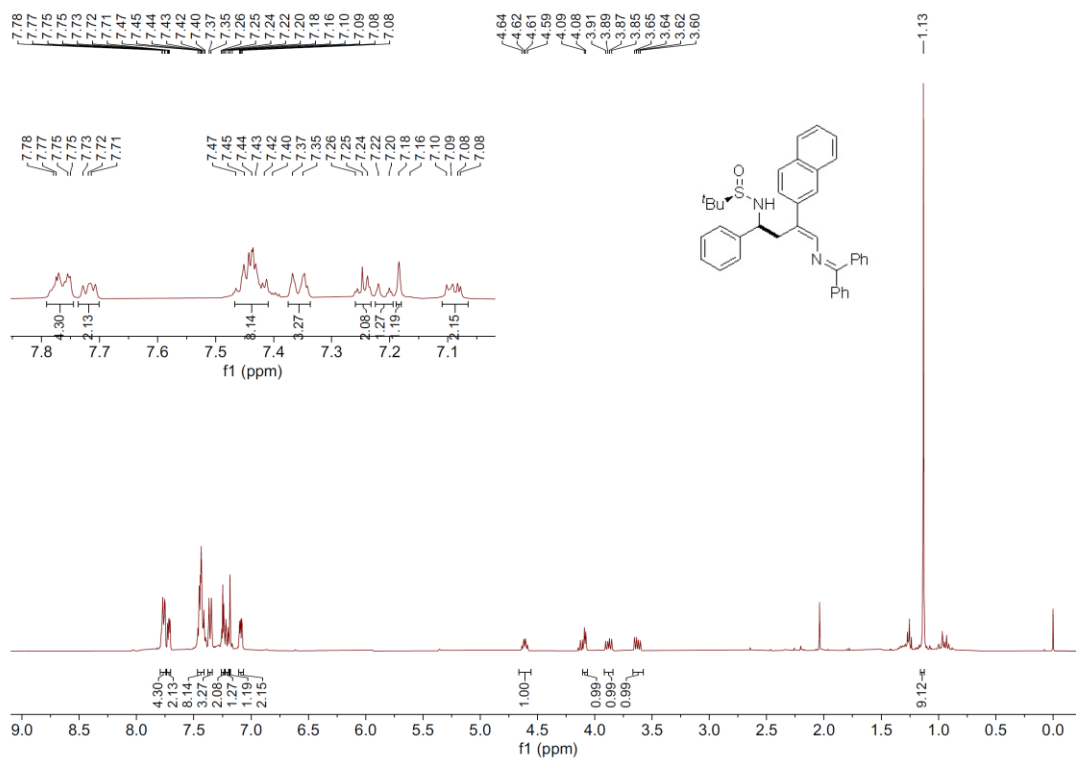
3bb Z-isomer *dr*



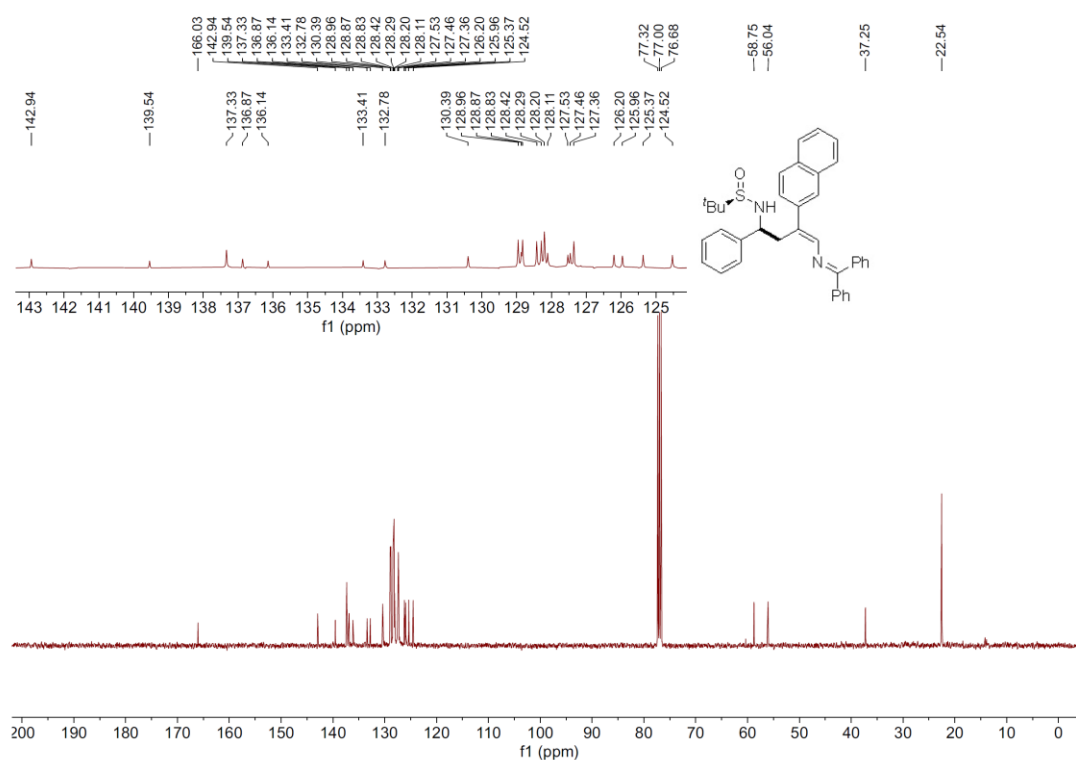
3bb Z-isomer ¹³CNMR



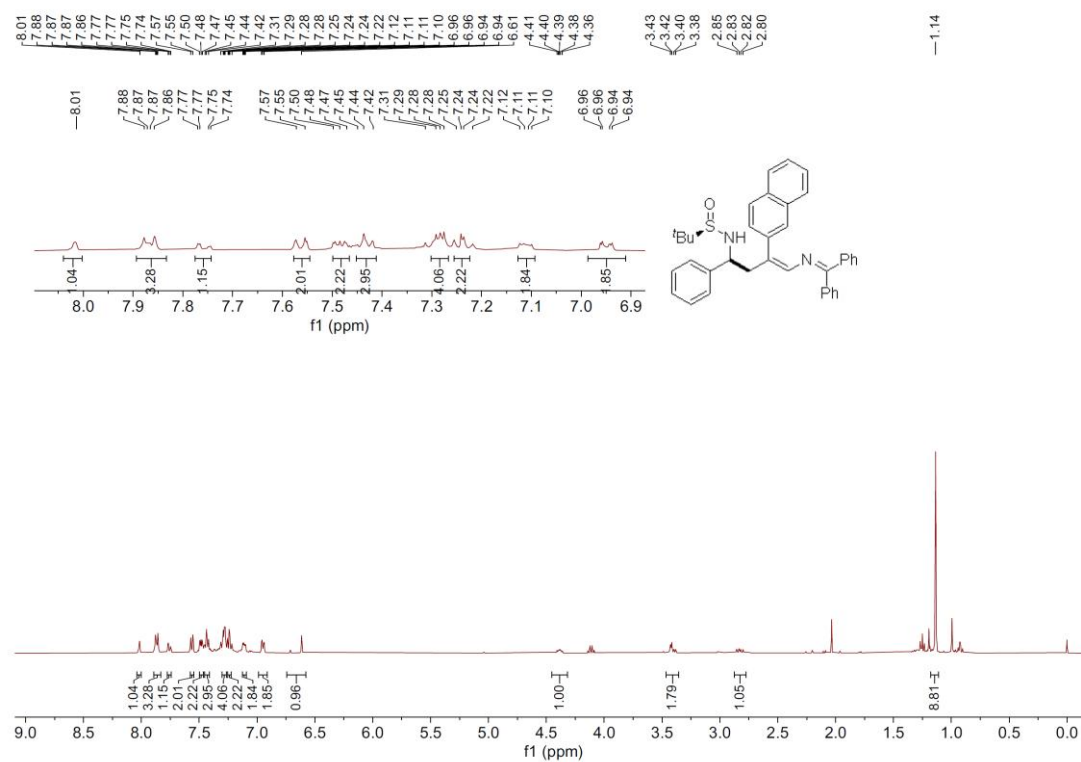
3bc *E*-isomer ¹H NMR



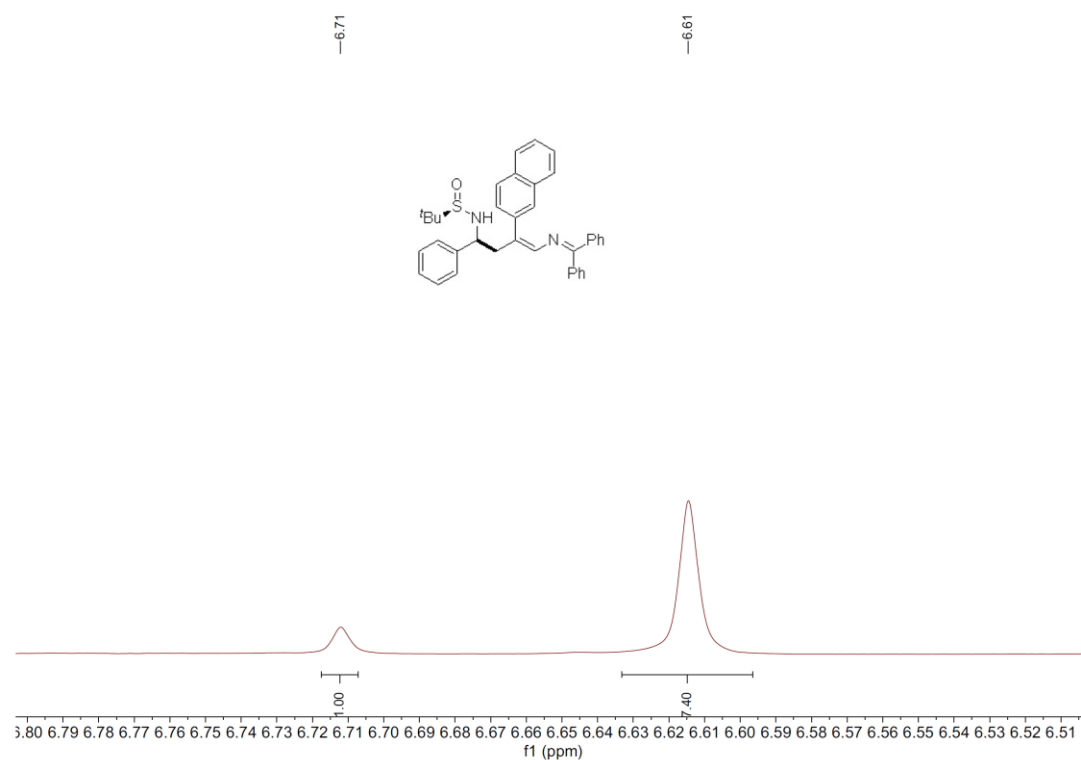
3bc *E*-isomer ¹³C NMR



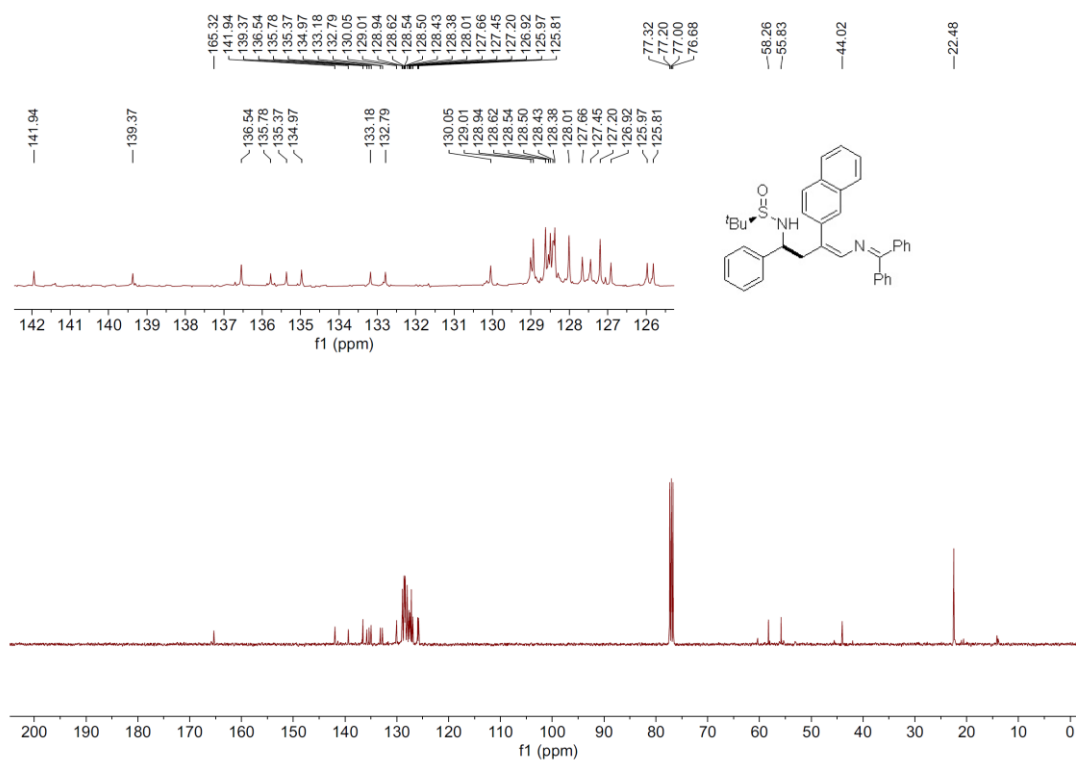
3bc Z-isomer ¹H NMR



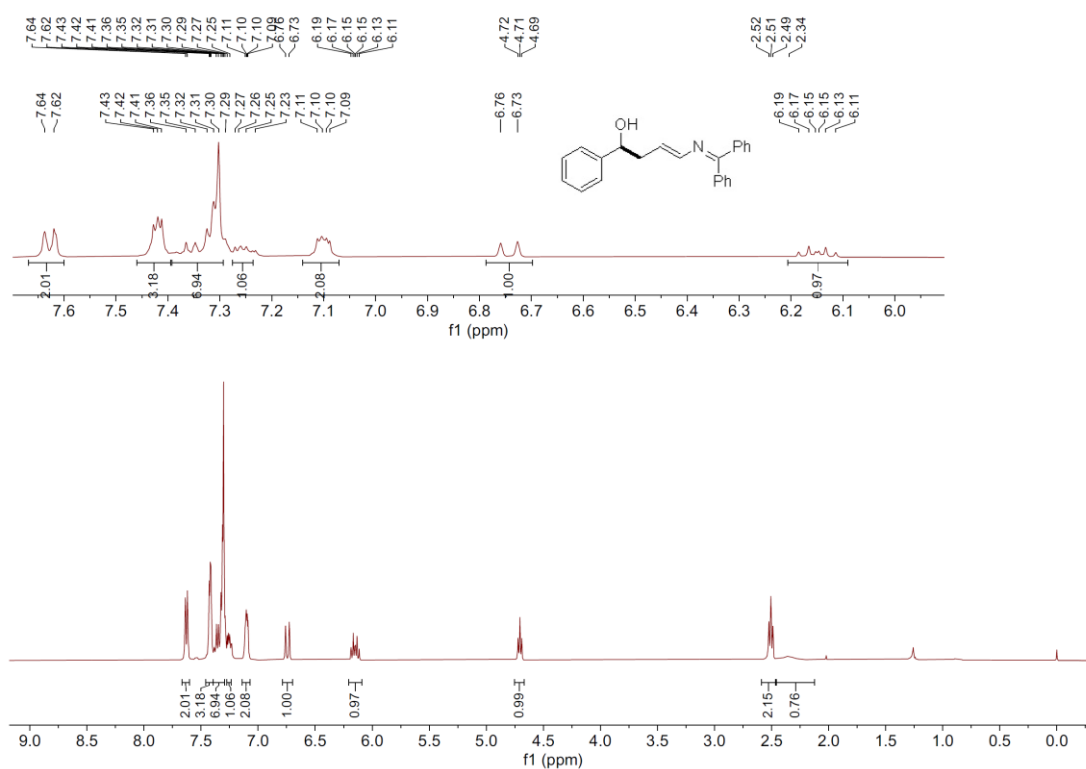
3bc Z-isomer *dr*



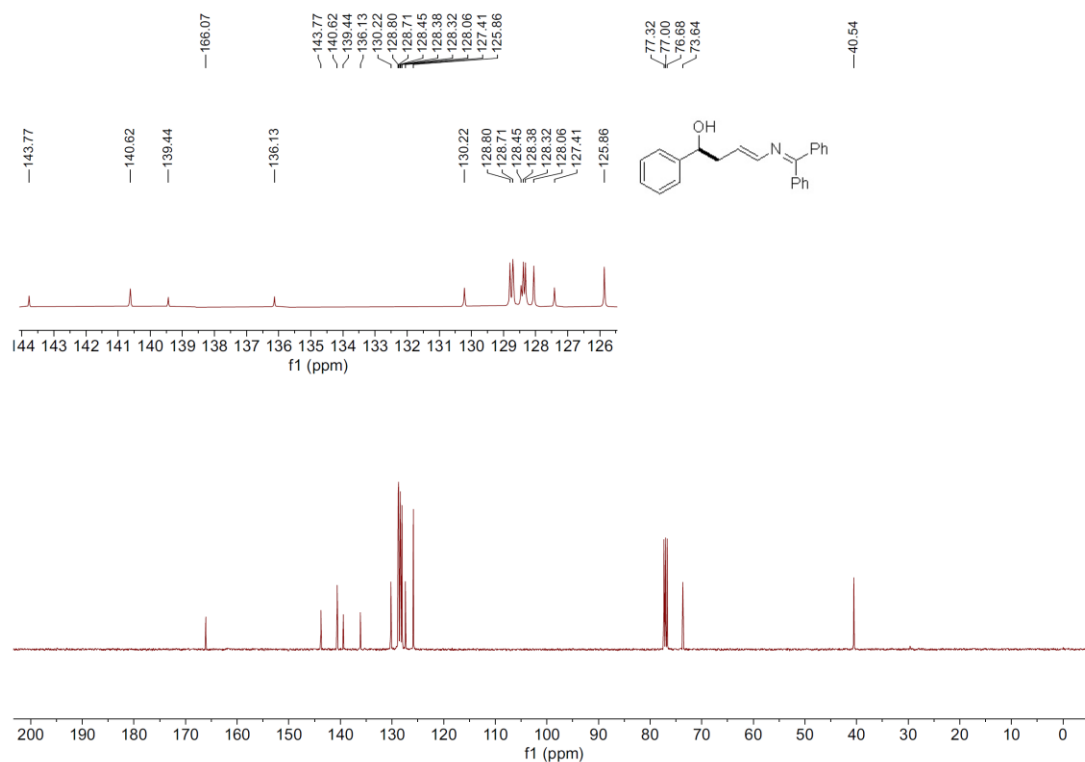
3bc Z-isomer ¹³C NMR



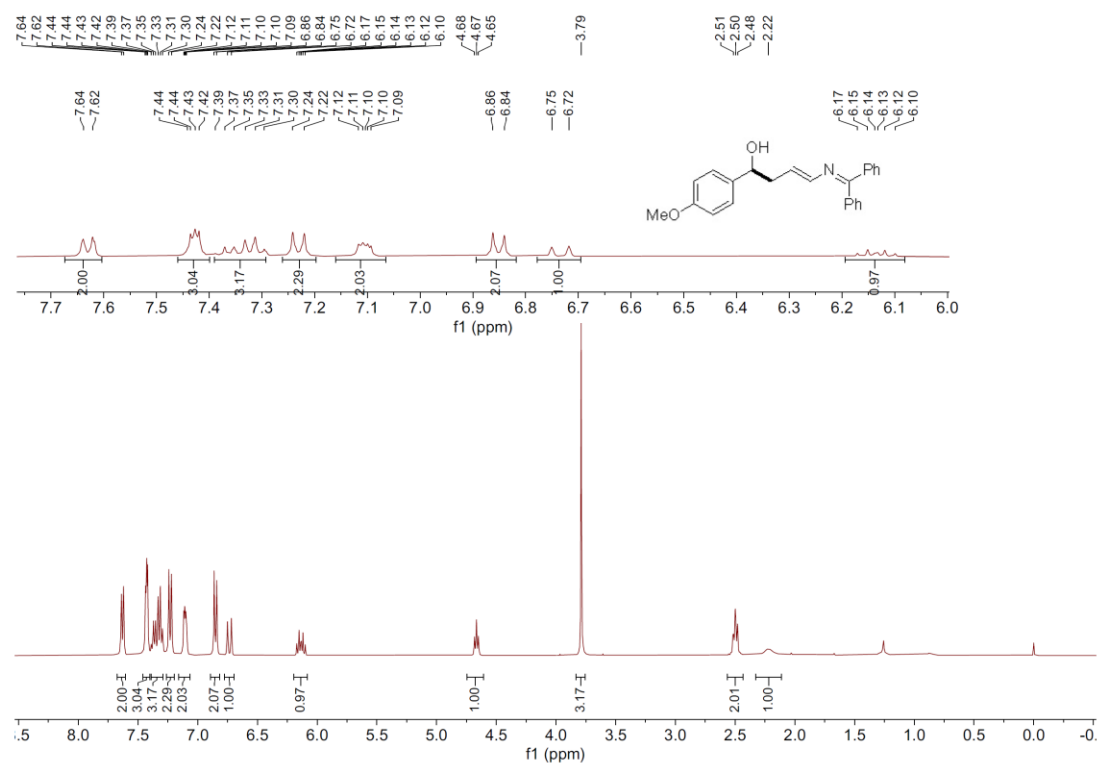
4a ¹H NMR



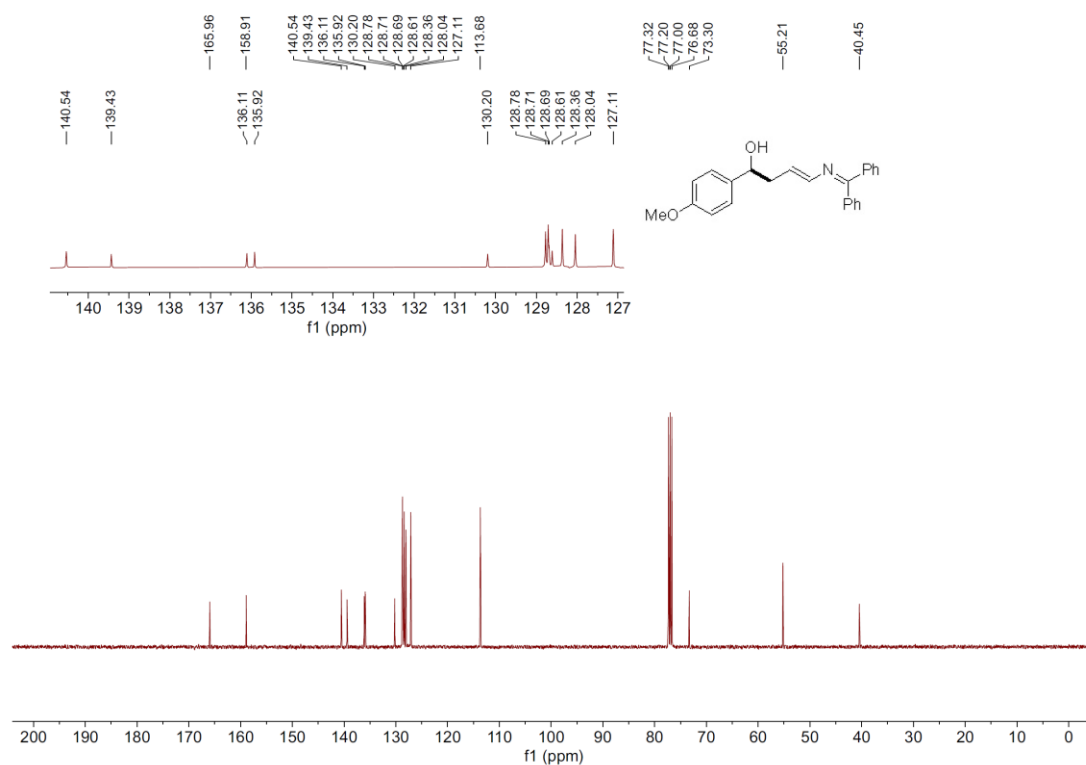
4a ¹³C NMR



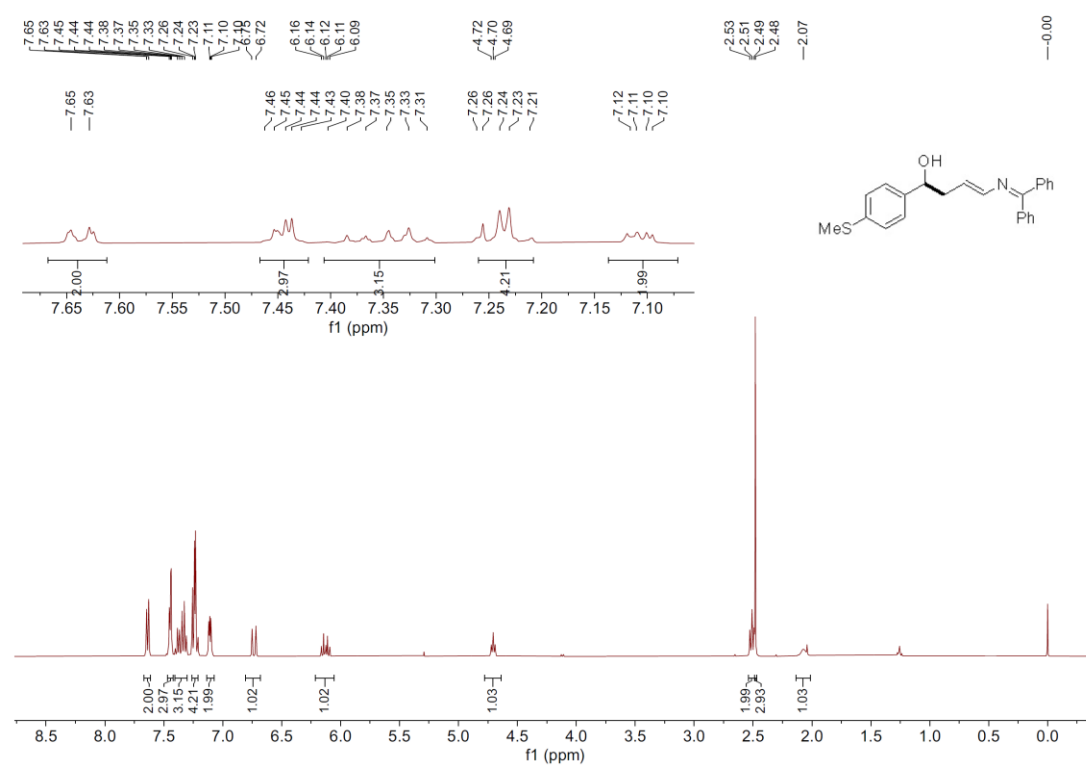
4b ¹H NMR



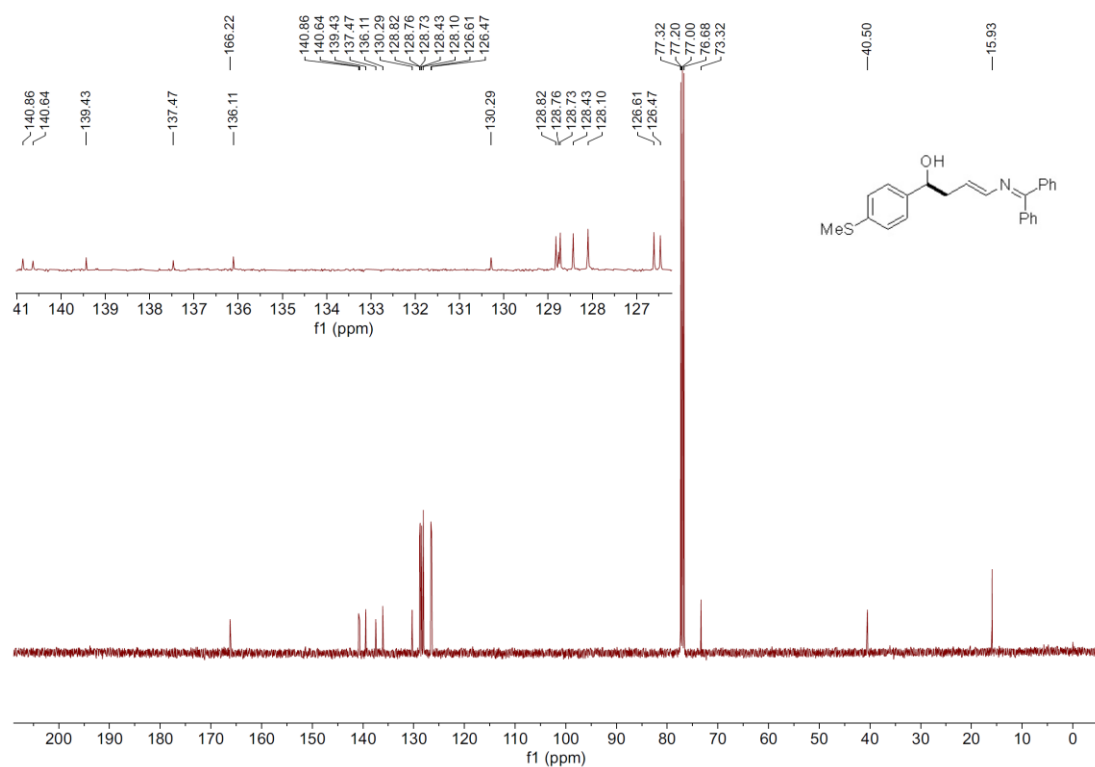
4b ¹³CNMR



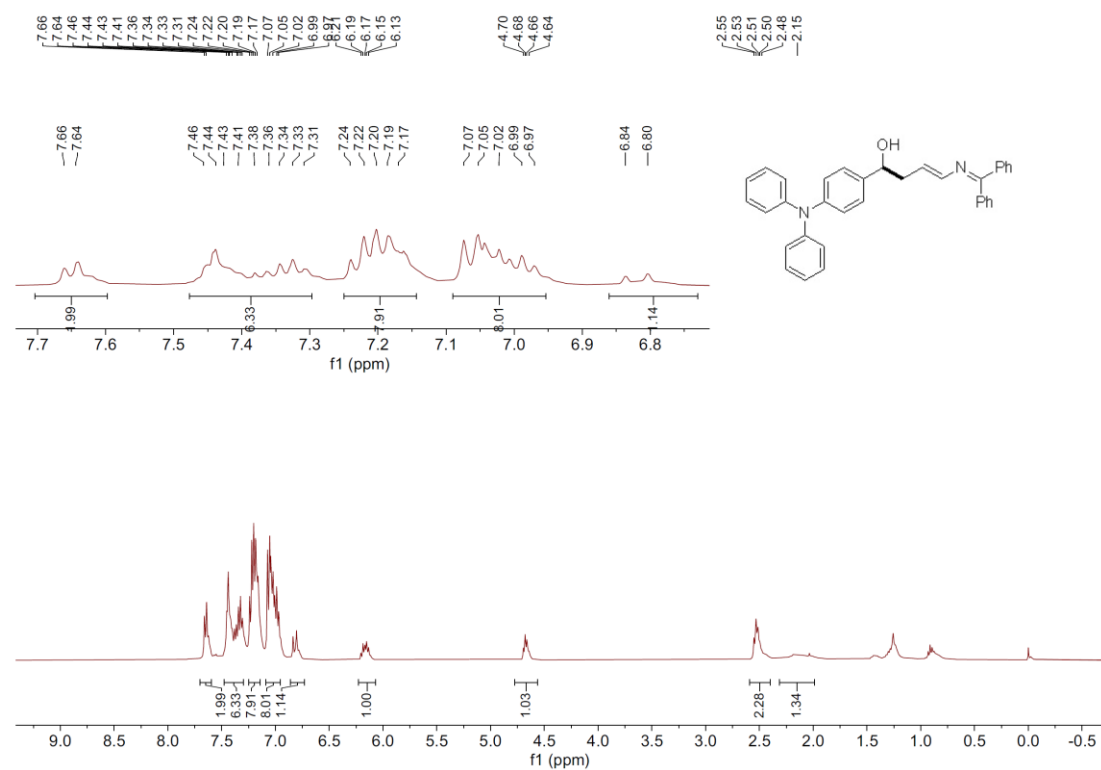
4c ¹H NMR



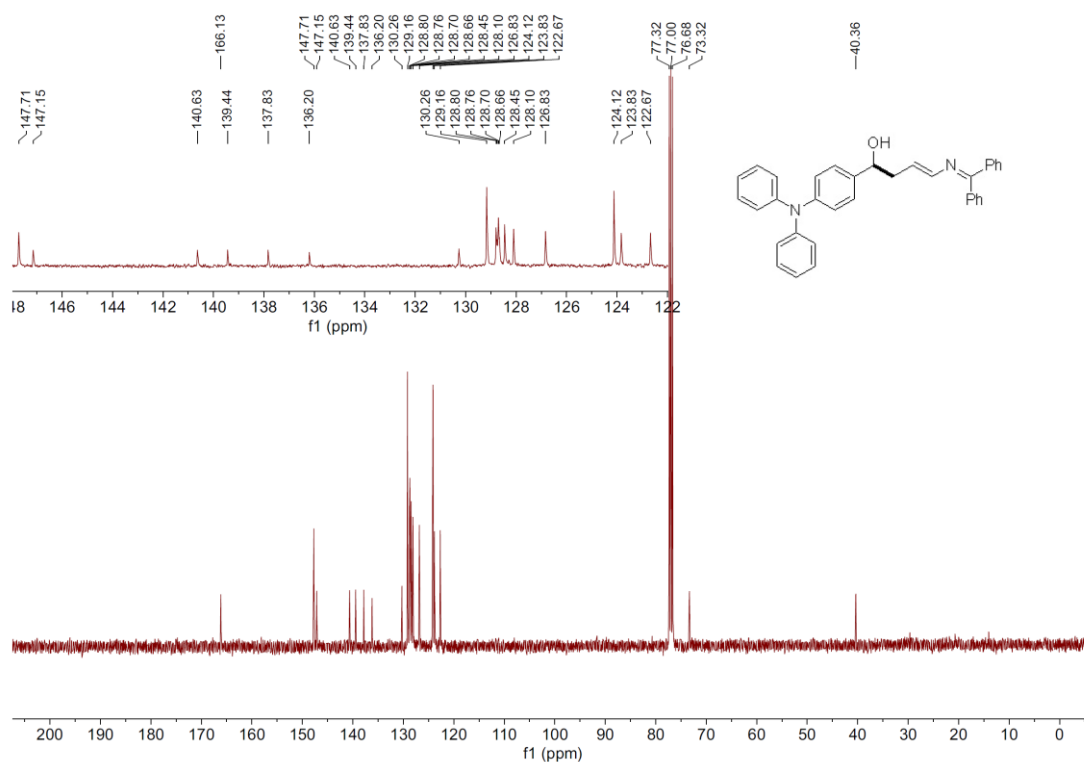
4c ¹³C NMR



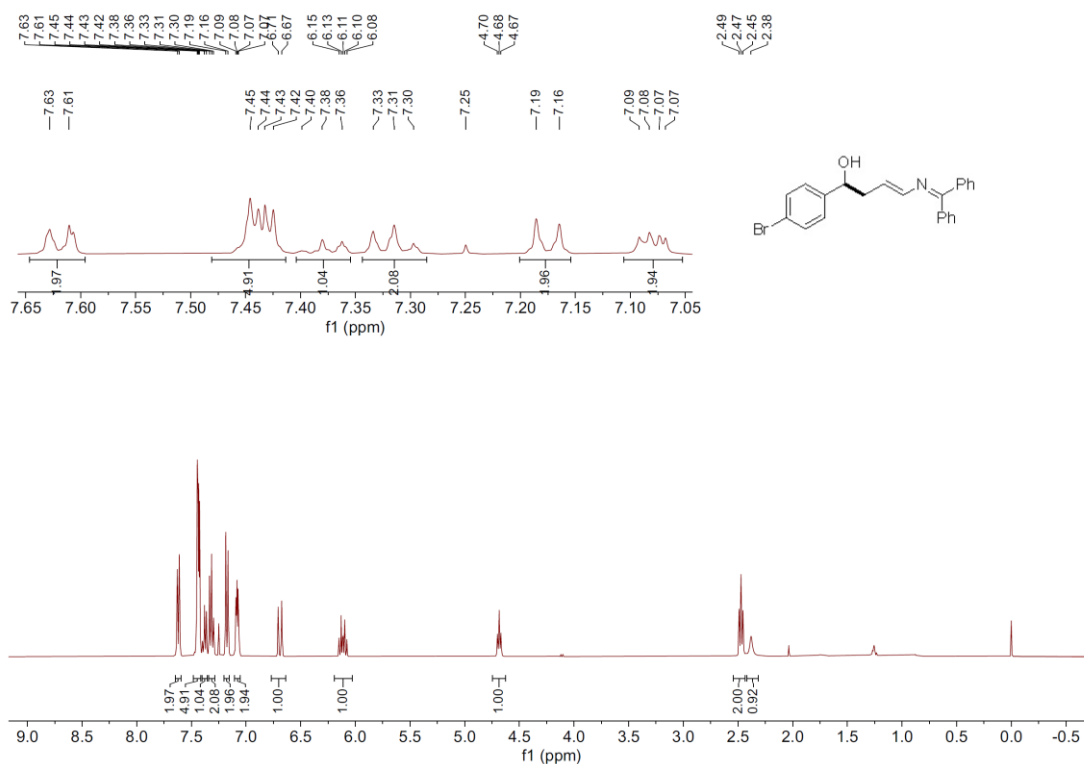
4d ¹H NMR



4d ^{13}C NMR



4e ^1H NMR



Chemical structure: OCC(O)C=C/N=C/c1ccccc1 (E)-1-(4-bromophenyl)-2-hydroxy-3-phenylprop-2-en-1-ol

¹³C NMR spectrum (ppm):

- 142.74
- 140.95
- 139.33
- 136.05
- 131.36
- 130.34
- 128.83
- 128.79
- 128.66
- 128.44
- 128.09
- 127.66
- 127.68
- 127.66
- 121.15
- 121.15
- 77.32
- 77.21
- 77.00
- 76.68
- 72.99
- 40.54

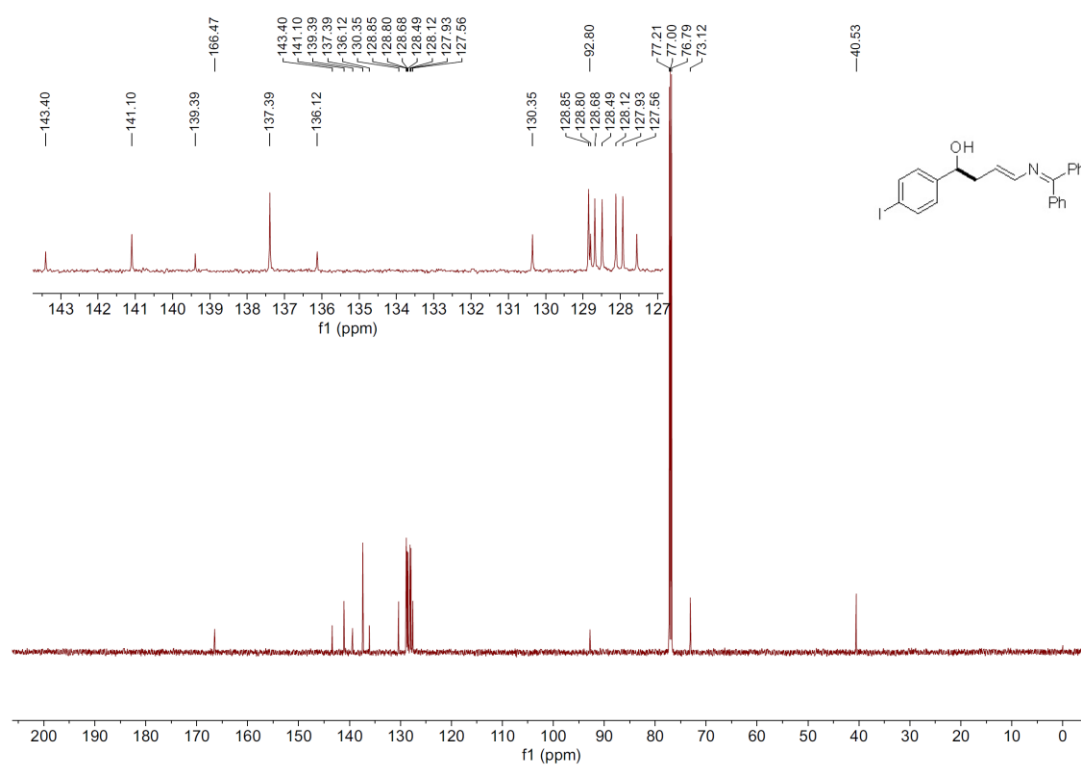
O[C@H](c1ccc(I)cc1)C=Cc2ccccc2N=Cc3ccccc3

Chemical structure: (S)-1-(4-iodophenyl)-2-(benzylideneamino)ethan-1-ol

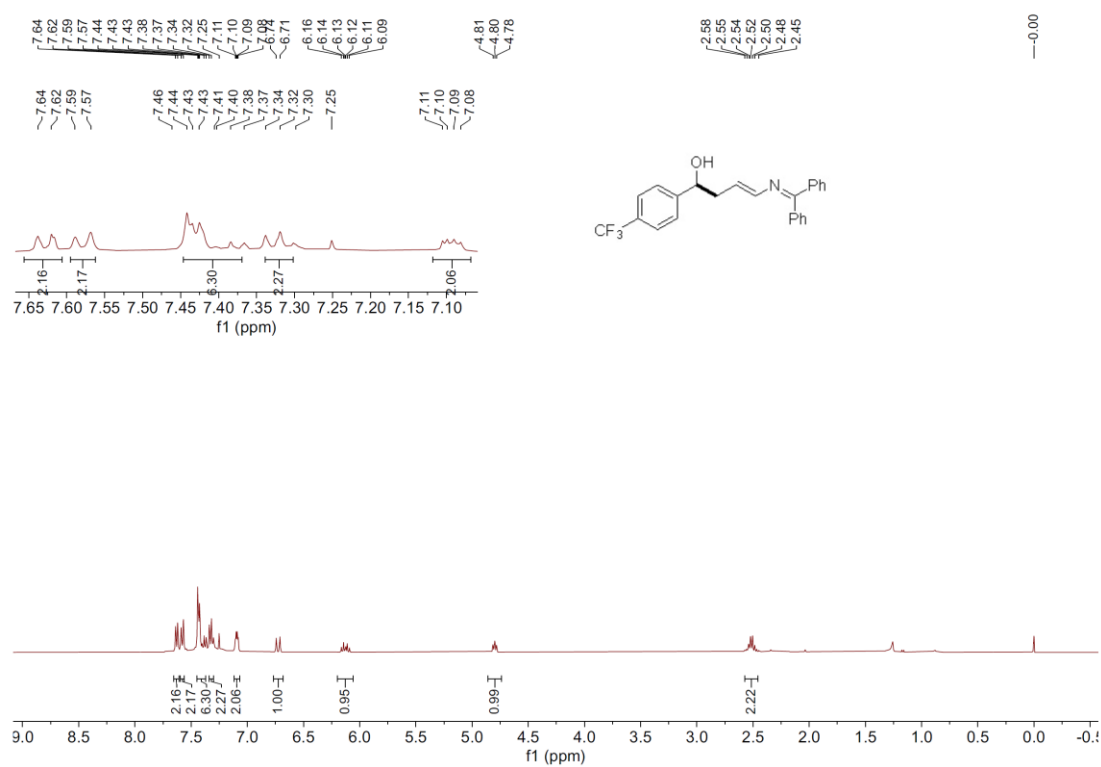
¹H NMR spectrum (CDCl₃) showing peaks and integration values:

Chemical Shift (ppm)	Integration
7.66, 7.65, 7.64, 7.63, 7.47, 7.46, 7.45, 7.44, 7.45, 7.40, 7.37, 7.34, 7.33, 7.31, 7.28, 7.33, 7.31, 7.26, 7.10, 7.10, 7.09, 7.09, 7.08, 7.08, 7.06, 7.06, 6.72, 6.89, 6.13, 6.11, 6.10, 6.09, 6.08, 4.70, 4.69, 4.68	2.12, 1.80, 3.17, 1.10, 1.24, 1.97, 2.02, 1.00, 0.98, 1.02
2.50, 2.49, 2.48, 2.48, 2.47, 2.46, 2.14	2.11, 0.97
6.13, 6.11, 6.10, 6.09, 6.08	0.98

4f ^{13}C NMR



4g ^1H NMR



Chemical structure: O=C1C(=C/C(O)C2=CC=C(C=C2)C(F)(F)F)N1C3=CC=CC=C3

¹³C NMR spectrum (ppm):

- 130.41
- 129.76
- 129.44
- 128.86
- 128.63
- 128.45
- 128.13
- 127.37
- 126.68
- 126.18
- 125.52
- 125.32
- 125.28
- 125.24
- 125.20
- 122.81
- 77.32
- 77.00
- 76.68
- 72.96
- 40.62

Chemical structure of (S)-1-(4-cyanophenyl)-2-(dimethylamino)ethanol (1): CN(C)[C@H](O)c1ccc(C#N)cc1

¹H NMR spectrum (CDCl₃) of compound 1. The spectrum shows peaks from 0 to 8 ppm. Aromatic protons appear between 7.0 and 7.6 ppm, the hydroxyl proton at ~5.2 ppm, the dimethylamino protons at ~2.8 ppm, and the solvent peak at ~7.26 ppm. Integration values are provided below the peaks.

Chemical Shift (ppm)	Integration
7.55 - 7.61	4.06
7.36 - 7.45	6.14
7.26 (solvent)	1.98
7.08 - 7.32	2.27
6.92	1.98
5.18	1.00
4.77 - 4.79	0.95
2.82	0.96
2.42 - 2.52	0.72
2.27	2.00

Chemical structure of compound 10: O[C@H](c1ccc(C#N)cc1)/C=C/N=C(c2ccccc2)c3ccccc3

¹³C NMR spectrum (top): CDCl₃. Peaks (ppm): 132.07, 130.43, 128.86, 128.81, 128.56, 128.44, 128.09, 127.21, 126.53, 118.81, 110.94.

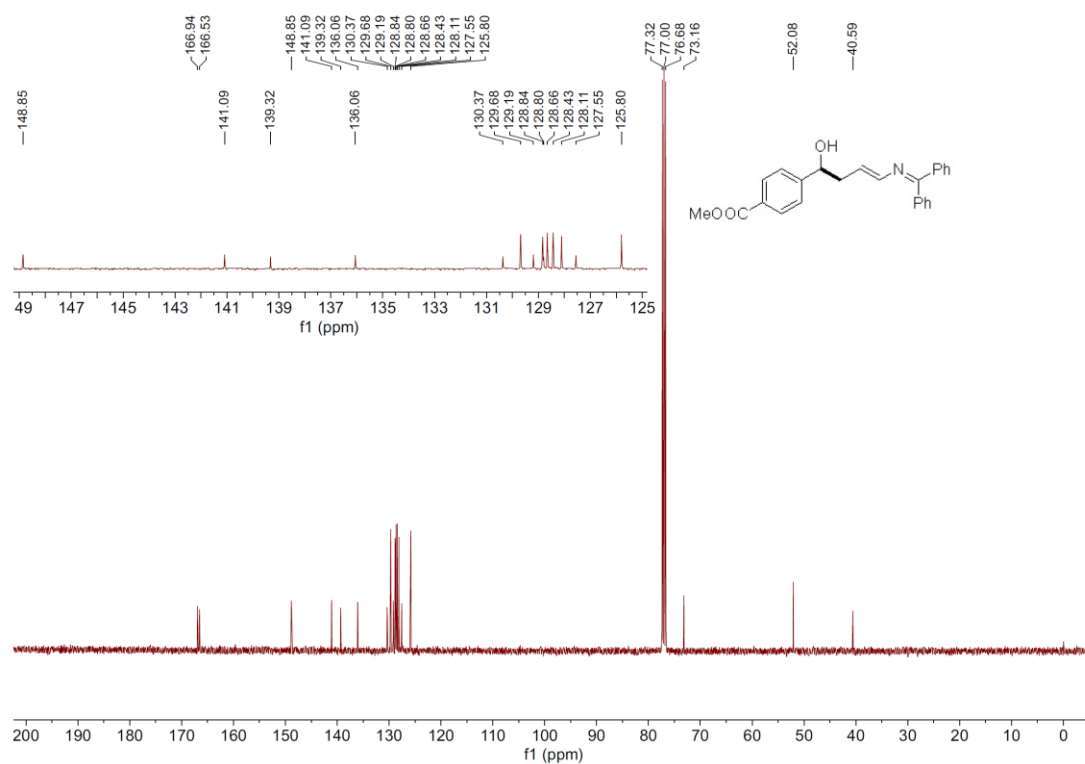
¹³C NMR spectrum (bottom): DMSO-d₆. Peaks (ppm): 166.81, 149.24, 147.15, 139.18, 135.98, 132.07, 130.43, 128.86, 128.81, 128.56, 128.44, 128.09, 127.21, 126.53, 118.81, 110.94, 77.32, 77.20, 77.00, 76.68, 72.73, 40.52.

Chemical structure of compound 10: COC(=O)c1ccc(cc1)[C@H](O)/C=C/N=C(c2ccccc2)c3ccccc3

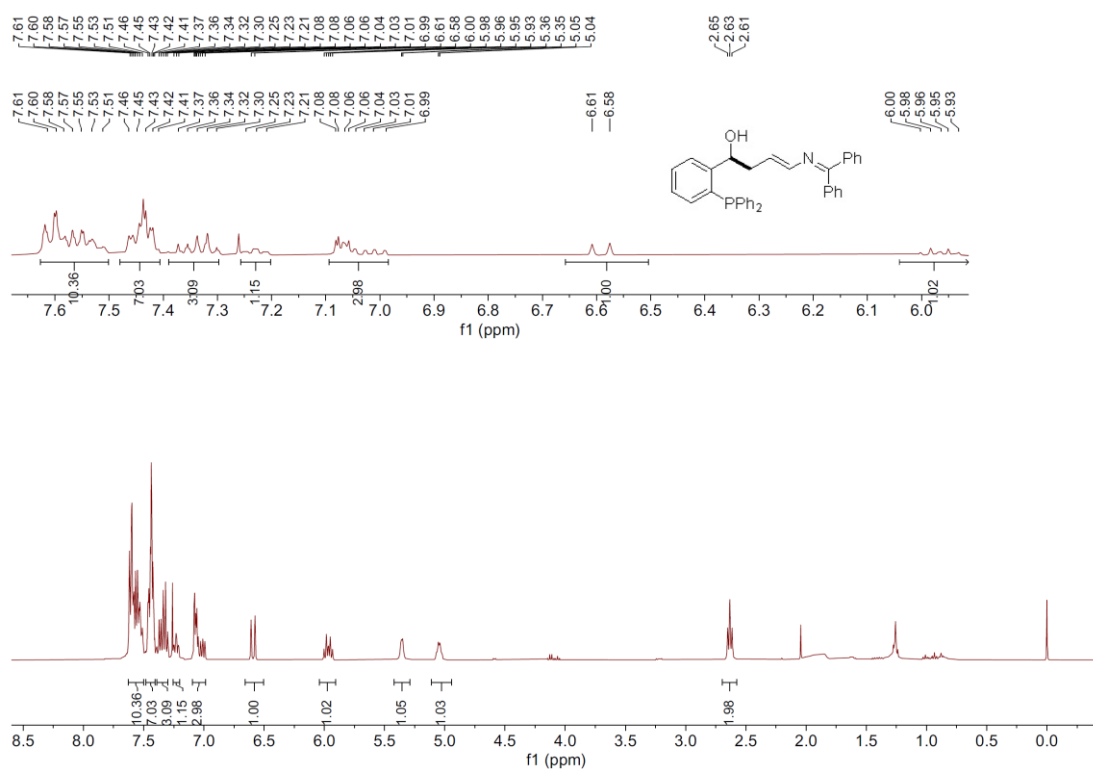
¹H NMR spectrum (top): CDCl₃, 400 MHz. Peaks (ppm): 7.45, 7.44, 7.43, 7.42, 7.41, 7.39, 7.37, 7.36, 7.35, 7.34, 7.33, 7.26, 7.11, 7.10, 7.09, 7.08, 6.75, 6.72, 6.17, 6.15, 6.13, 6.12, 6.10, 6.09, 6.08, 6.07, 6.06, 6.05, 6.04, 6.03, 6.02, 6.01, 5.99, 5.98, 5.97, 5.96, 5.95, 5.94, 5.93, 5.92, 5.91, 5.90, 5.89, 5.88, 5.87, 5.86, 5.85, 5.84, 5.83, 5.82, 5.81, 5.80, 5.79, 5.78, 5.77, 5.76, 5.75, 5.74, 5.73, 5.72, 5.71, 5.70, 5.69, 5.68, 5.67, 5.66, 5.65, 5.64, 5.63, 5.62, 5.61, 5.60, 5.59, 5.58, 5.57, 5.56, 5.55, 5.54, 5.53, 5.52, 5.51, 5.50, 5.49, 5.48, 5.47, 5.46, 5.45, 5.44, 5.43, 5.42, 5.41, 5.40, 5.39, 5.38, 5.37, 5.36, 5.35, 5.34, 5.33, 5.32, 5.31, 5.30, 5.29, 5.28, 5.27, 5.26, 5.25, 5.24, 5.23, 5.22, 5.21, 5.20, 5.19, 5.18, 5.17, 5.16, 5.15, 5.14, 5.13, 5.12, 5.11, 5.10, 5.09, 5.08, 5.07, 5.06, 5.05, 5.04, 5.03, 5.02, 5.01, 5.00, 4.99, 4.98, 4.97, 4.96, 4.95, 4.94, 4.93, 4.92, 4.91, 4.90, 4.89, 4.88, 4.87, 4.86, 4.85, 4.84, 4.83, 4.82, 4.81, 4.80, 4.79, 4.78, 4.77, 4.76, 4.75, 4.74, 4.73, 4.72, 4.71, 4.70, 4.69, 4.68, 4.67, 4.66, 4.65, 4.64, 4.63, 4.62, 4.61, 4.60, 4.59, 4.58, 4.57, 4.56, 4.55, 4.54, 4.53, 4.52, 4.51, 4.50, 4.49, 4.48, 4.47, 4.46, 4.45, 4.44, 4.43, 4.42, 4.41, 4.40, 4.39, 4.38, 4.37, 4.36, 4.35, 4.34, 4.33, 4.32, 4.31, 4.30, 4.29, 4.28, 4.27, 4.26, 4.25, 4.24, 4.23, 4.22, 4.21, 4.20, 4.19, 4.18, 4.17, 4.16, 4.15, 4.14, 4.13, 4.12, 4.11, 4.10, 4.09, 4.08, 4.07, 4.06, 4.05, 4.04, 4.03, 4.02, 4.01, 4.00, 3.99, 3.98, 3.97, 3.96, 3.95, 3.94, 3.93, 3.92, 3.91, 3.90, 3.89, 3.88, 3.87, 3.86, 3.85, 3.84, 3.83, 3.82, 3.81, 3.80, 3.79, 3.78, 3.77, 3.76, 3.75, 3.74, 3.73, 3.72, 3.71, 3.70, 3.69, 3.68, 3.67, 3.66, 3.65, 3.64, 3.63, 3.62, 3.61, 3.60, 3.59, 3.58, 3.57, 3.56, 3.55, 3.54, 3.53, 3.52, 3.51, 3.50, 3.49, 3.48, 3.47, 3.46, 3.45, 3.44, 3.43, 3.42, 3.41, 3.40, 3.39, 3.38, 3.37, 3.36, 3.35, 3.34, 3.33, 3.32, 3.31, 3.30, 3.29, 3.28, 3.27, 3.26, 3.25, 3.24, 3.23, 3.22, 3.21, 3.20, 3.19, 3.18, 3.17, 3.16, 3.15, 3.14, 3.13, 3.12, 3.11, 3.10, 3.09, 3.08, 3.07, 3.06, 3.05, 3.04, 3.03, 3.02, 3.01, 3.00, 2.99, 2.98, 2.97, 2.96, 2.95, 2.94, 2.93, 2.92, 2.91, 2.90, 2.89, 2.88, 2.87, 2.86, 2.85, 2.84, 2.83, 2.82, 2.81, 2.80, 2.79, 2.78, 2.77, 2.76, 2.75, 2.74, 2.73, 2.72, 2.71, 2.70, 2.69, 2.68, 2.67, 2.66, 2.65, 2.64, 2.63, 2.62, 2.61, 2.60, 2.59, 2.58, 2.57, 2.56, 2.55, 2.54, 2.53, 2.52, 2.51, 2.50, 2.49, 2.48, 2.47, 2.46, 2.45, 2.44, 2.43, 2.42, 2.41, 2.40, 2.39, 2.38, 2.37, 2.36, 2.35, 2.34, 2.33, 2.32, 2.31, 2.30, 2.29, 2.28, 2.27, 2.26, 2.25, 2.24, 2.23, 2.22, 2.21, 2.20, 2.19, 2.18, 2.17, 2.16, 2.15, 2.14, 2.13, 2.12, 2.11, 2.10, 2.09, 2.08, 2.07, 2.06, 2.05, 2.04, 2.03, 2.02, 2.01, 2.00, 1.99, 1.98, 1.97, 1.96, 1.95, 1.94, 1.93, 1.92, 1.91, 1.90, 1.89, 1.88, 1.87, 1.86, 1.85, 1.84, 1.83, 1.82, 1.81, 1.80, 1.79, 1.78, 1.77, 1.76, 1.75, 1.74, 1.73, 1.72, 1.71, 1.70, 1.69, 1.68, 1.67, 1.66, 1.65, 1.64, 1.63, 1.62, 1.61, 1.60, 1.59, 1.58, 1.57, 1.56, 1.55, 1.54, 1.53, 1.52, 1.51, 1.50, 1.49, 1.48, 1.47, 1.46, 1.45, 1.44, 1.43, 1.42, 1.41, 1.40, 1.39, 1.38, 1.37, 1.36, 1.35, 1.34, 1.33, 1.32, 1.31, 1.30, 1.29, 1.28, 1.27, 1.26, 1.25, 1.24, 1.23, 1.22, 1.21, 1.20, 1.19, 1.18, 1.17, 1.16, 1.15, 1.14, 1.13, 1.12, 1.11, 1.10, 1.09, 1.08, 1.07, 1.06, 1.05, 1.04, 1.03, 1.02, 1.01, 1.00, 0.99, 0.98, 0.97, 0.96, 0.95, 0.94, 0.93, 0.92, 0.91, 0.90, 0.89, 0.88, 0.87, 0.86, 0.85, 0.84, 0.83, 0.82, 0.81, 0.80, 0.79, 0.78, 0.77, 0.76, 0.75, 0.74, 0.73, 0.72, 0.71, 0.70, 0.69, 0.68, 0.67, 0.66, 0.65, 0.64, 0.63, 0.62, 0.61, 0.60, 0.59, 0.58, 0.57, 0.56, 0.55, 0.54, 0.53, 0.52, 0.51, 0.50, 0.49, 0.48, 0.47, 0.46, 0.45, 0.44, 0.43, 0.42, 0.41, 0.40, 0.39, 0.38, 0.37, 0.36, 0.35, 0.34, 0.33, 0.32, 0.31, 0.30, 0.29, 0.28, 0.27, 0.26, 0.25, 0.24, 0.23, 0.22, 0.21, 0.20, 0.19, 0.18, 0.17, 0.16, 0.15, 0.14, 0.13, 0.12, 0.11, 0.10, 0.09, 0.08, 0.07, 0.06, 0.05, 0.04, 0.03, 0.02, 0.01, 0.00.

¹H NMR spectrum (bottom): DMSO-d₆, 400 MHz. Peaks (ppm): 8.01, 7.99, 7.64, 7.62, 7.45, 7.44, 7.43, 7.42, 7.41, 7.39, 7.37, 7.36, 7.35, 7.34, 7.33, 7.26,

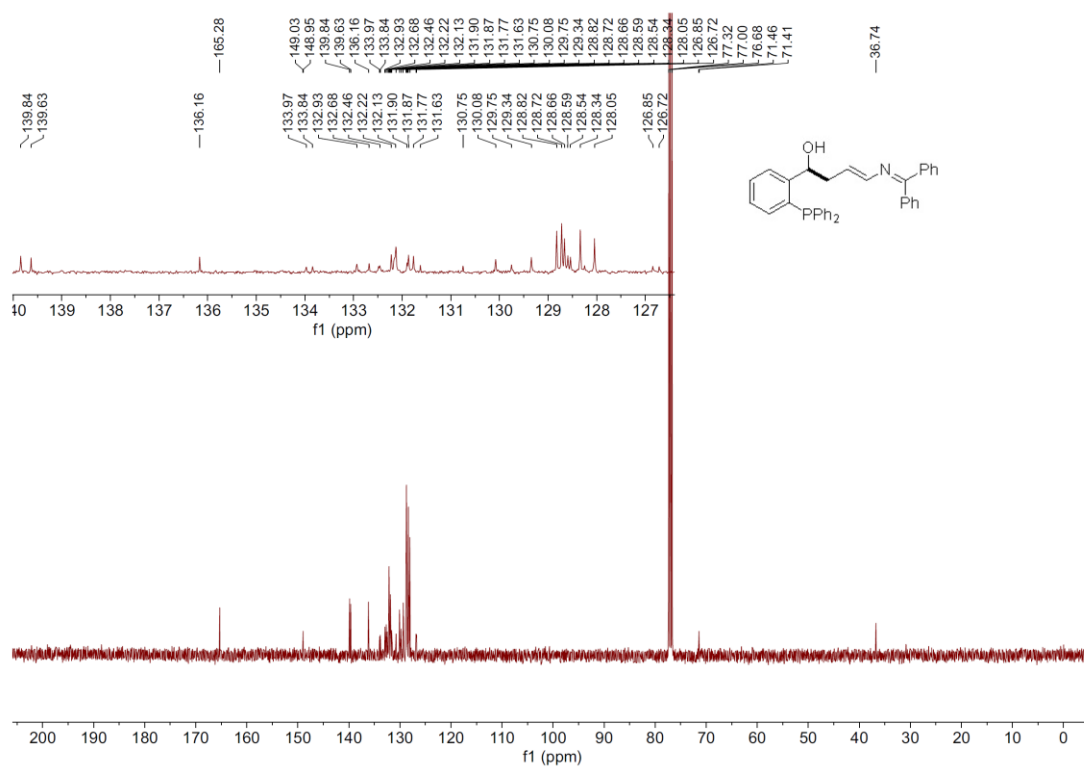
4i ¹³CNMR



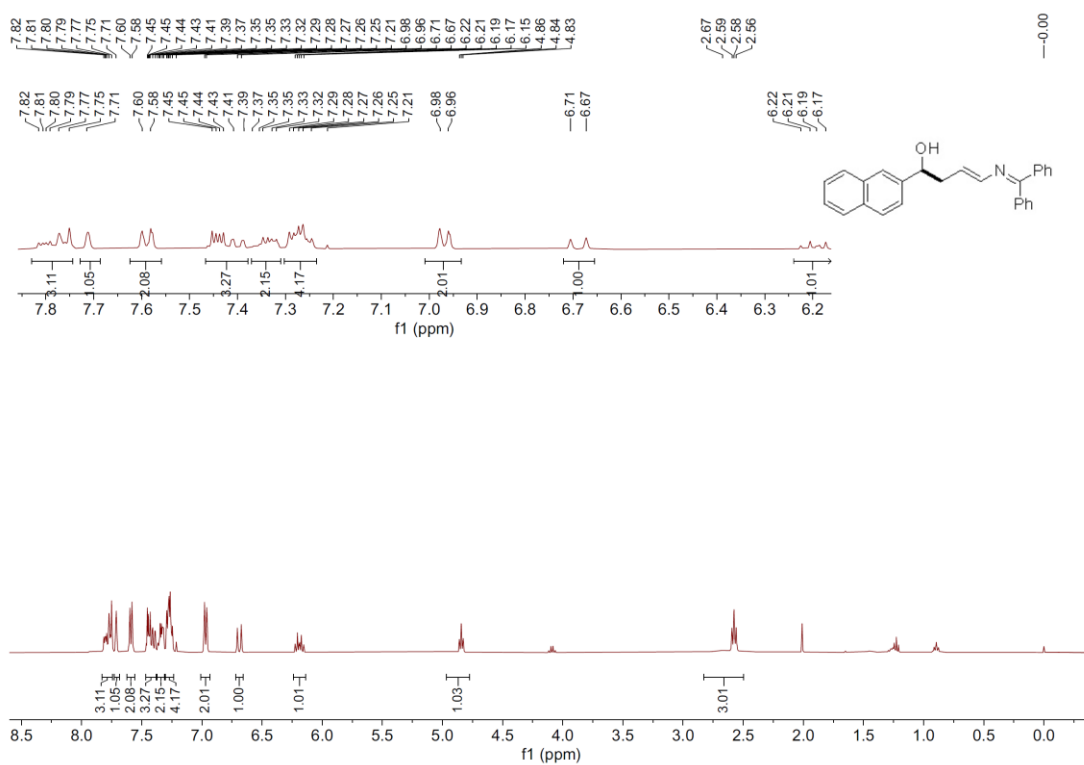
4j ¹H NMR



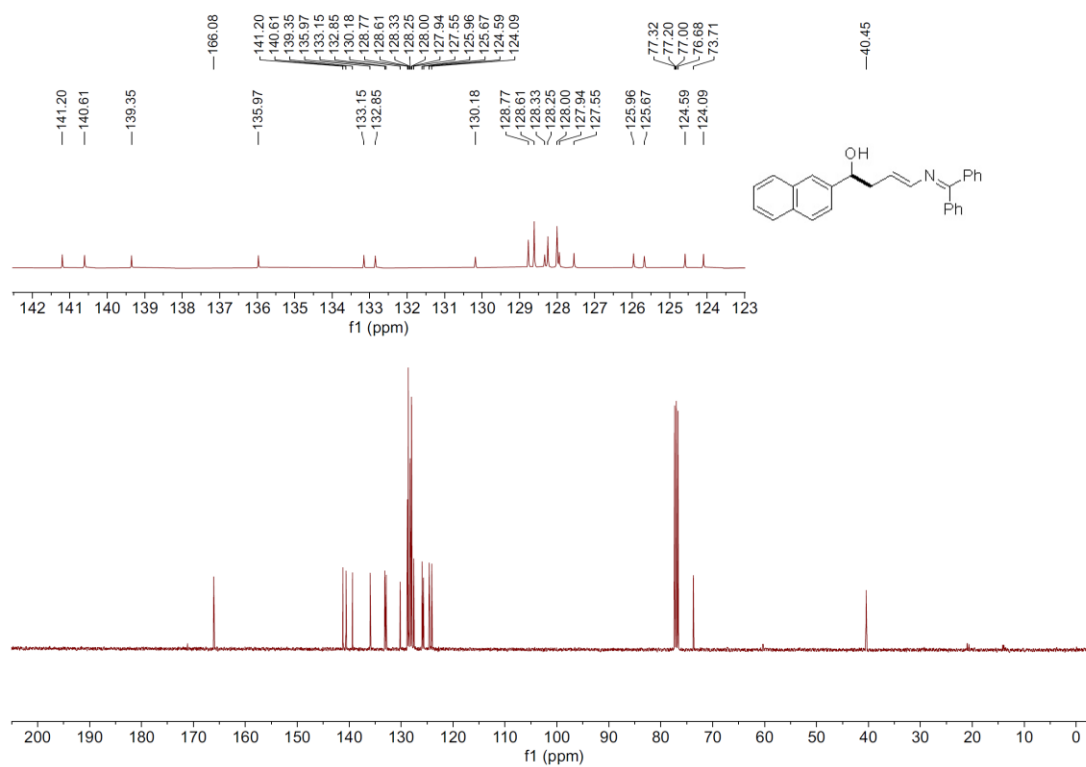
4j ¹³C NMR



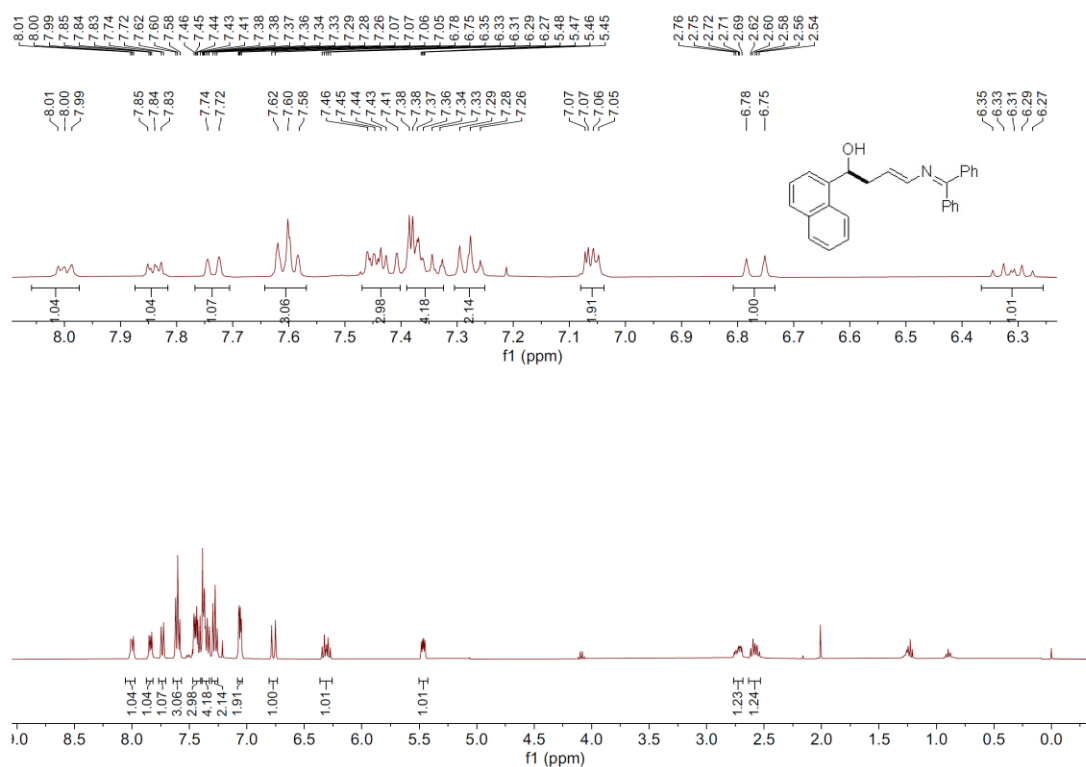
4k ¹H NMR



4k ¹³CNMR



4l ¹H NMR



Chemical structure: O[C@H](c1ccc2ccccc2c1)/C=C/N=C(c3ccccc3)c4ccccc4

¹³C NMR (CDCl₃) peaks (ppm): 140.40, 139.40, 139.36, 136.07, 133.67, 130.18, 128.94, 128.79, 128.67, 128.32, 128.01, 127.77, 126.88, 125.88, 125.38, 125.35, 123.00, 122.96, 77.77, 77.20, 76.68, 70.35, 39.60.

¹H NMR (CDCl₃) peaks (ppm): 7.77, 7.72, 7.70, 7.68, 7.35, 7.33, 7.31, 7.29, 7.27, 7.25, 7.23, 7.21, 7.19, 7.17, 7.15, 7.13, 7.11, 7.09, 7.07, 7.05, 7.03.

Chemical structure: O[C@H](c1ccc(NC(=O)c2ccccc2)c(c1)c3ccccc3)c4ccccc4

¹H NMR spectrum (CDCl₃) showing peaks from 0.00 to 7.70 ppm. Integration values are provided below the peaks: 2.04, 2.99, 3.17, 0.99, 1.98, 1.96, 1.00, 0.98, 0.99, 2.16.

Chemical structure of (S)-1-(4-phenyl-1,3-bisoxazol-5-yl)ethanol:

O[C@H](c1ccc2oc3ccccc3no2)c1

¹³C NMR spectrum (CDCl₃) peaks (ppm):

- 130.24
- 128.79
- 128.71
- 128.67
- 128.38
- 128.03
- 127.91
- 126.49
- 124.42
- 123.71

¹³C NMR spectrum (DMSO-d₆) peaks (ppm):

- 166.27
- 147.76
- 140.73
- 138.33
- 136.06
- 130.24
- 128.79
- 128.71
- 128.67
- 128.38
- 128.03
- 127.91
- 126.49
- 124.42
- 123.71
- 77.32
- 77.20
- 77.00
- 76.68
- 69.58
- 40.54

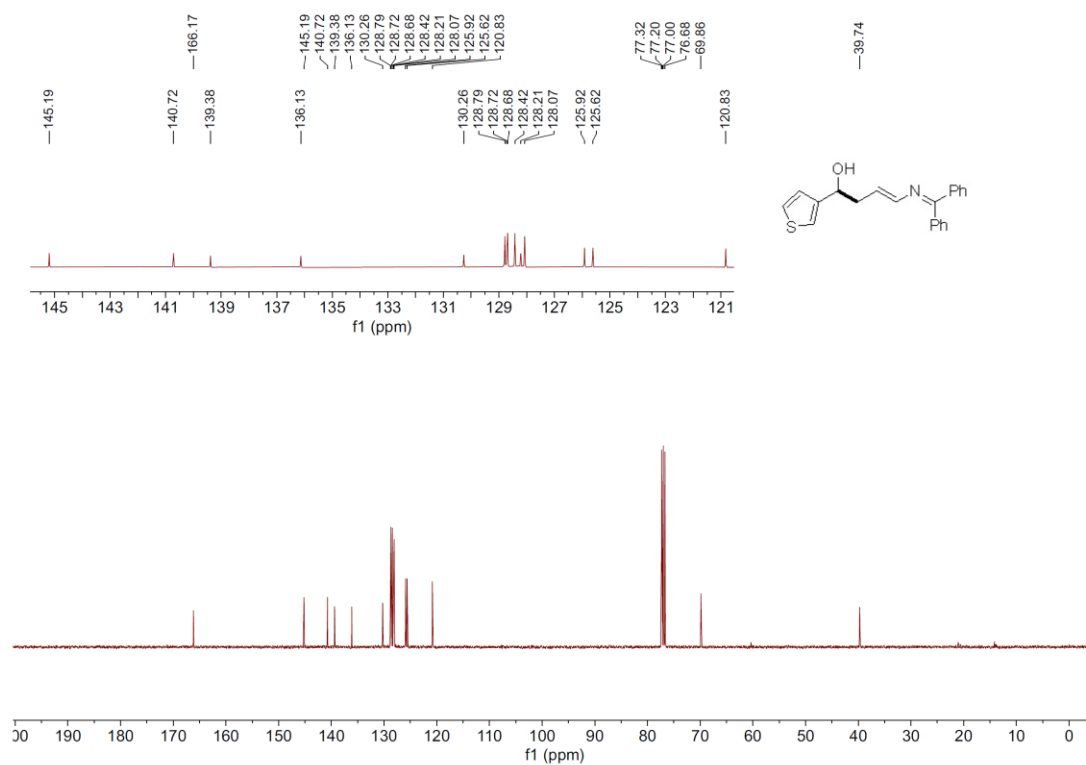
Chemical structure: C=C(C)C(O)c1ccc(O)cc1

¹H NMR spectrum (400 MHz, CDCl₃) showing peaks from 0.00 to 7.65 ppm. Integration values are provided below the peaks.

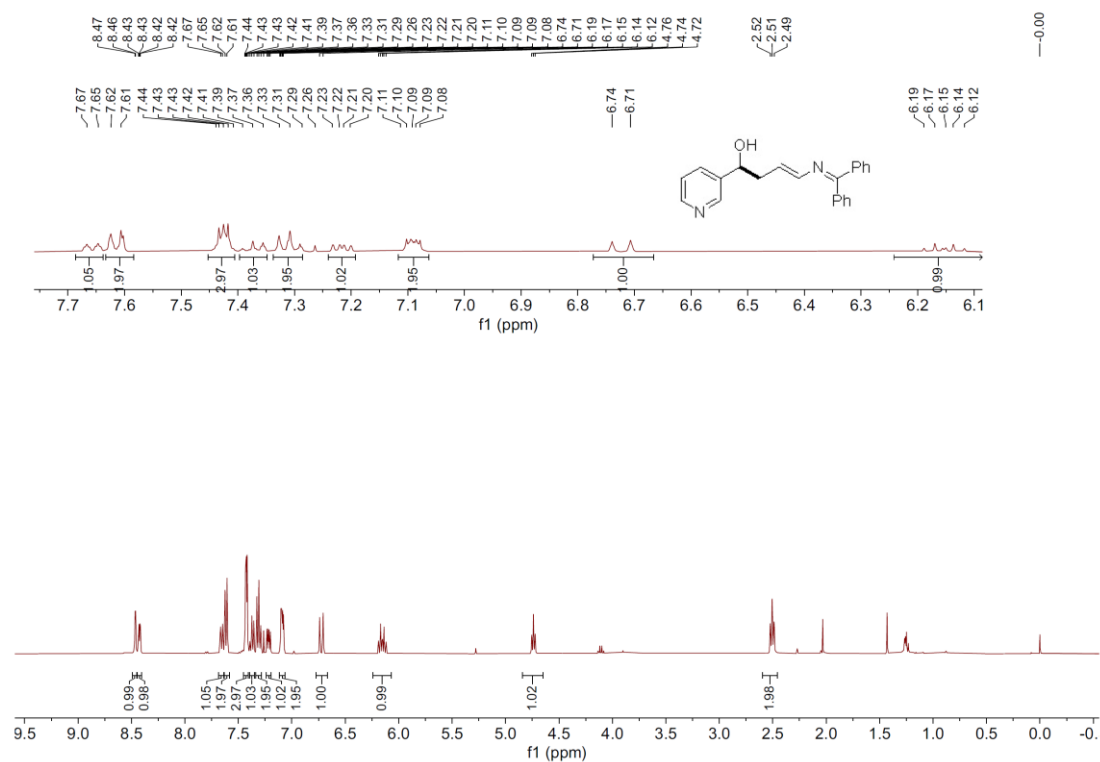
Peak list (ppm): 7.65, 7.63, 7.45, 7.44, 7.38, 7.36, 7.34, 7.32, 7.27, 7.26, 7.15, 7.14, 7.13, 7.04, 7.03, 6.80, 6.78, 6.77, 6.37, 6.15, 6.13, 6.11, 4.83, 4.81, 4.79, 7.15, 7.15, 7.14, 7.13, 7.04, 7.03, 2.58, 2.57, 2.55, 2.54, 2.52, 2.51, 2.50, 2.27, 0.00.

Integration values: 2.06, 3.10, 3.24, 1.18, 2.99, 1.00, 1.02, 1.00, 1.03, 2.23, 1.12.

4n ¹³C NMR

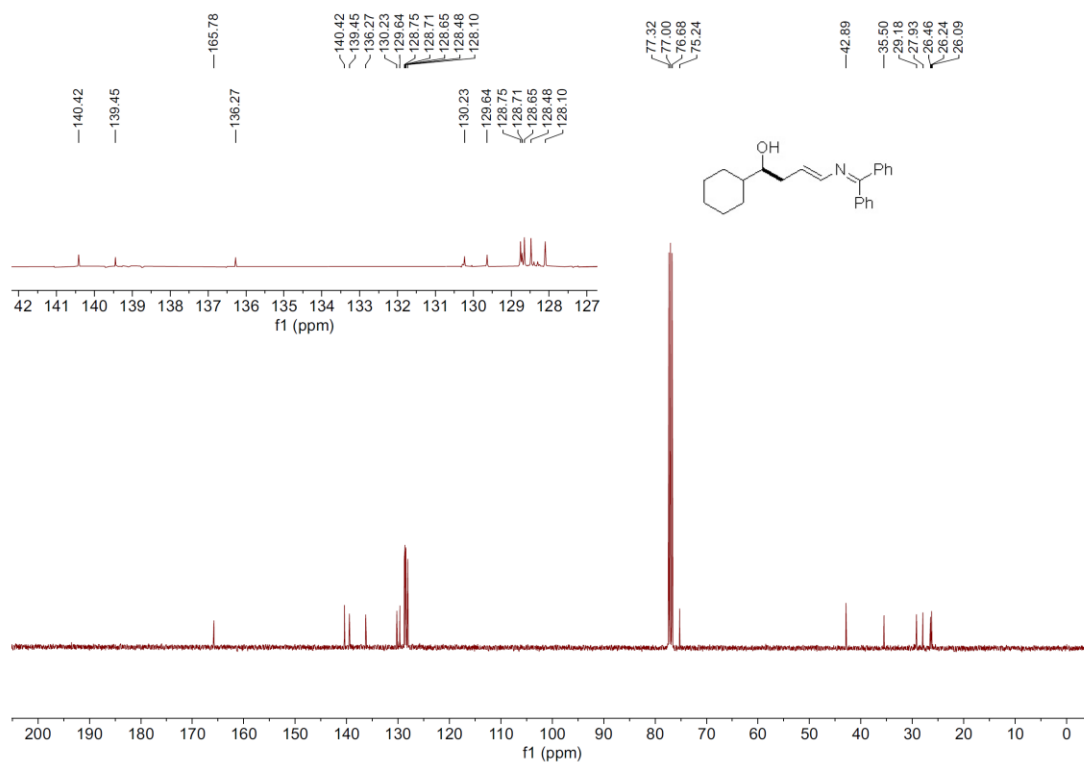


4o ¹H NMR

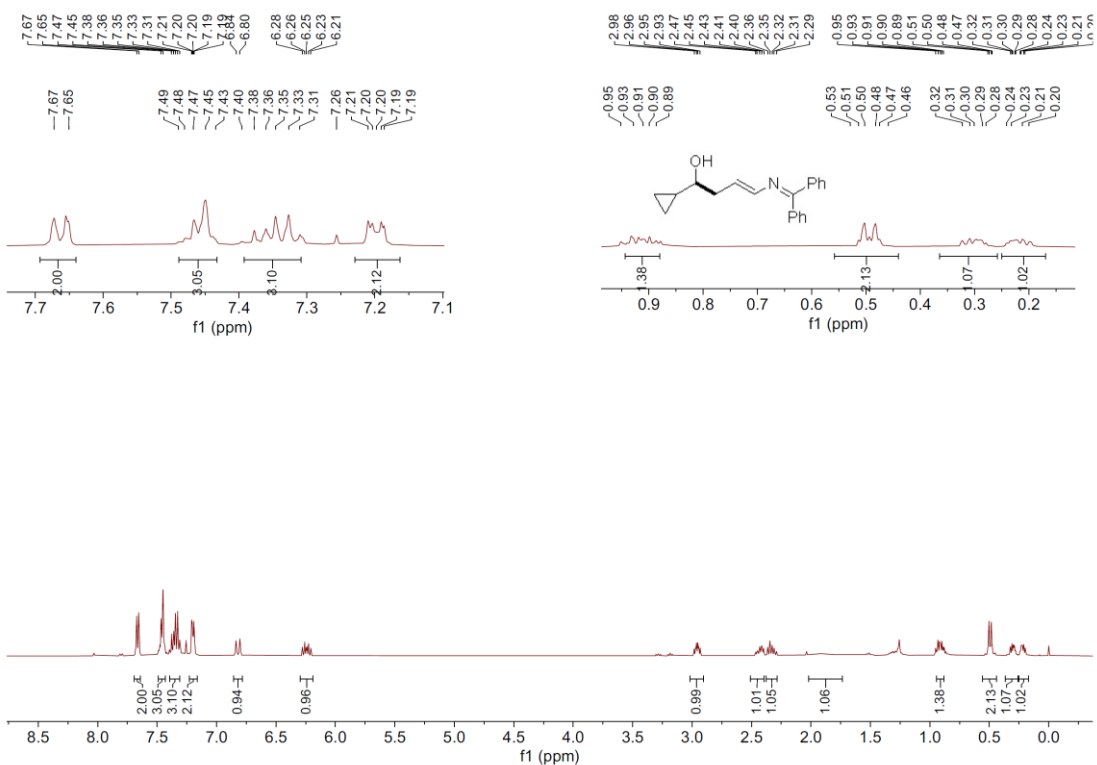


[illegible]

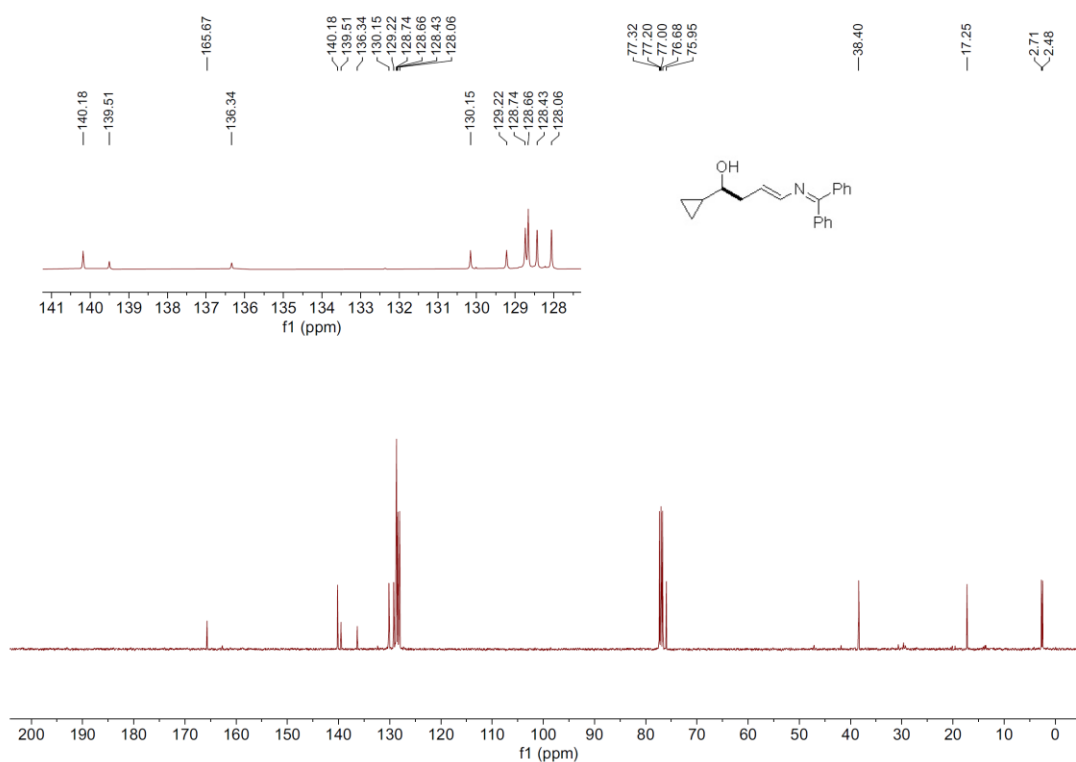
4p ¹³C NMR



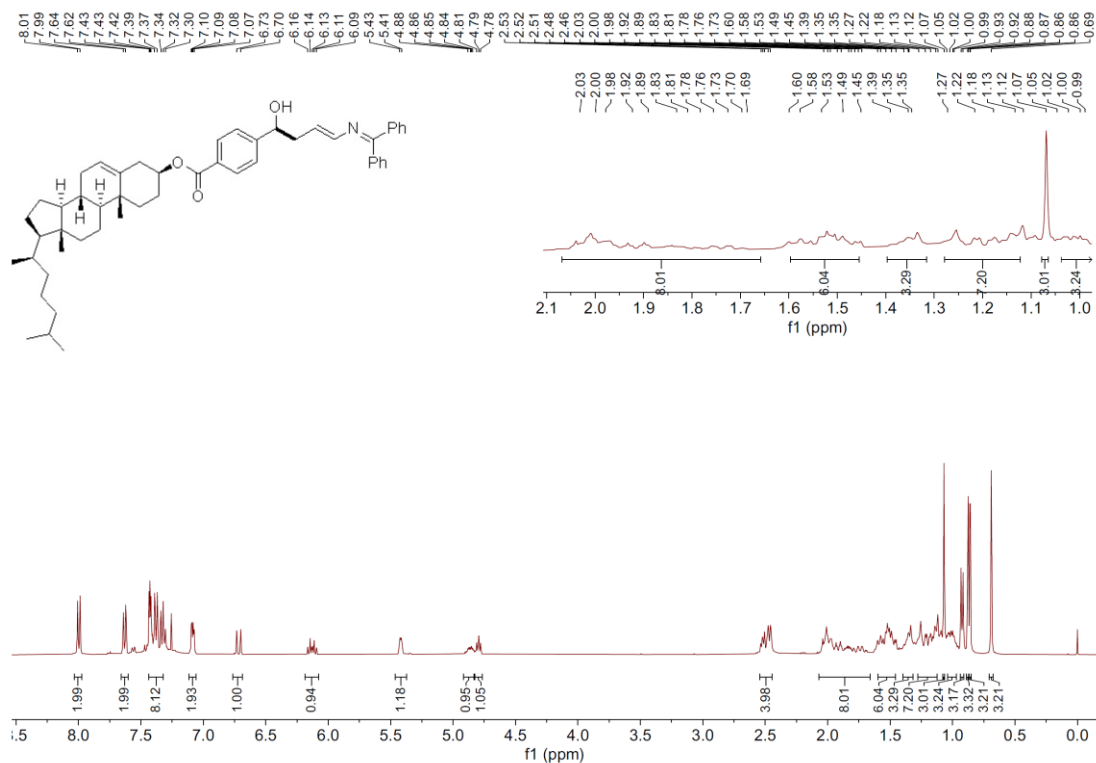
4q ¹H NMR



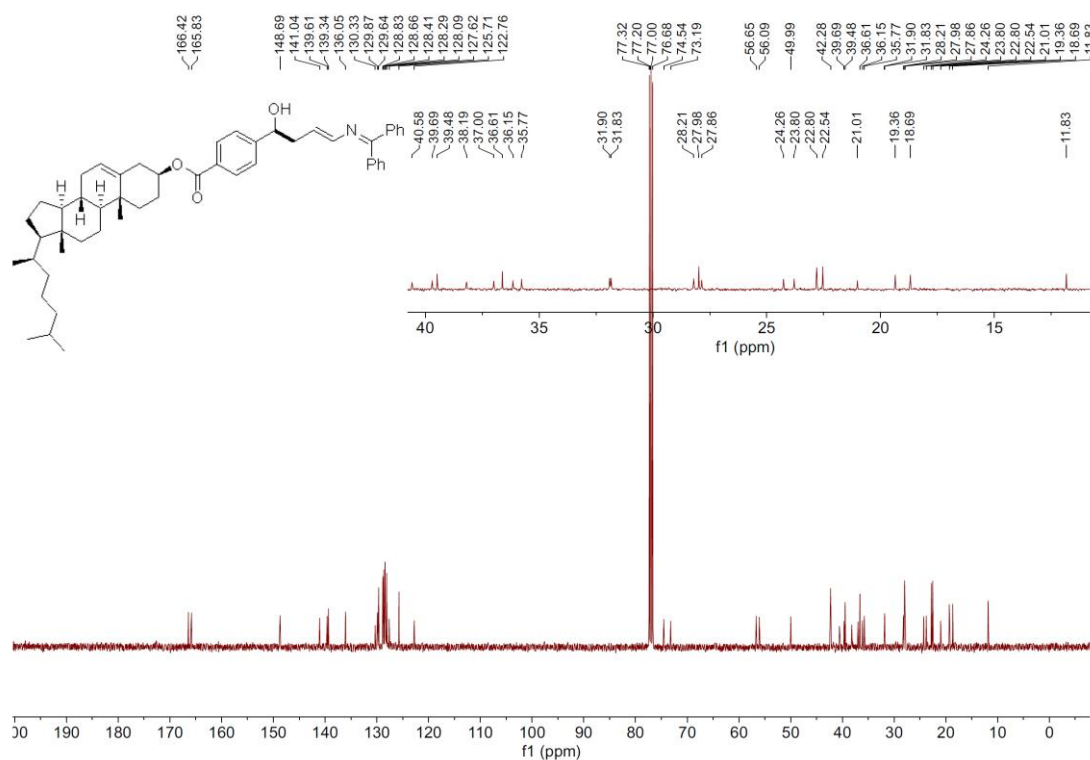
4q ¹³CNMR



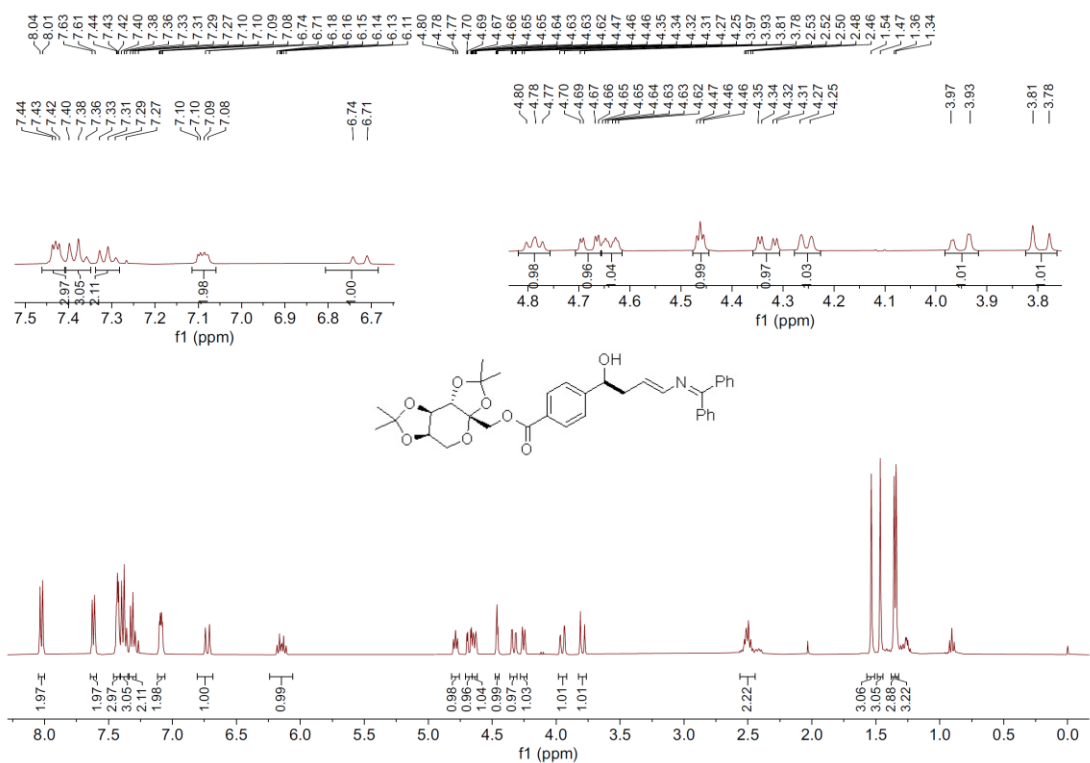
4r ¹H NMR



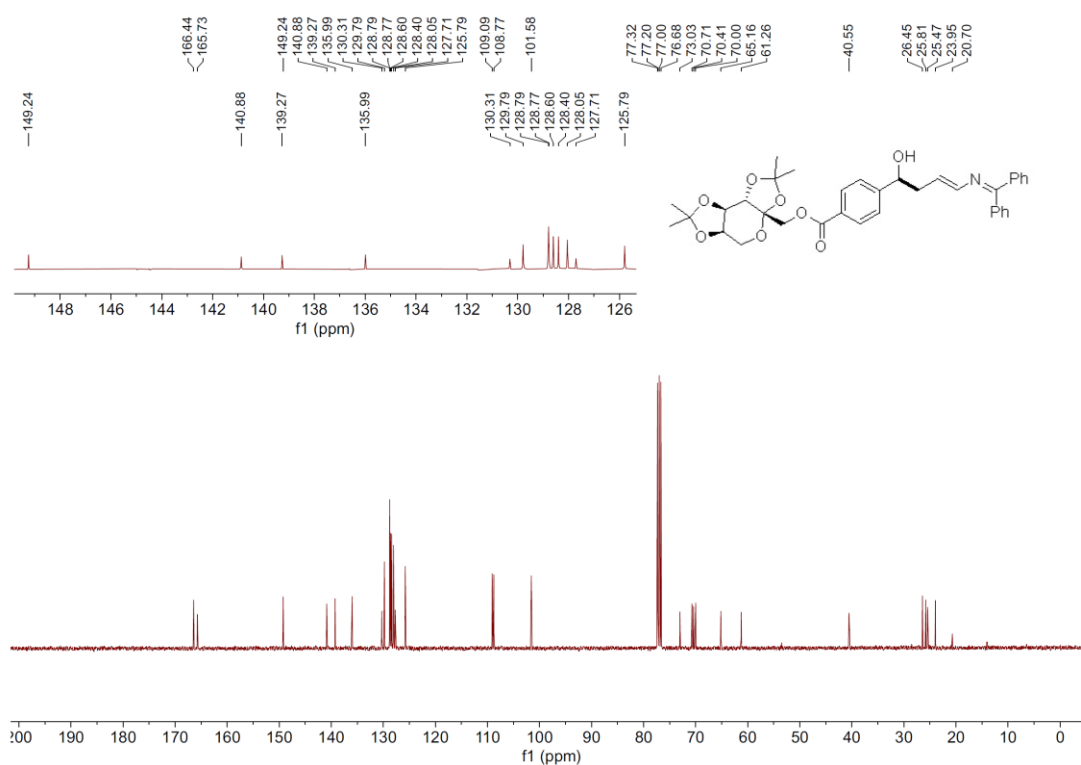
4r ¹³CNMR



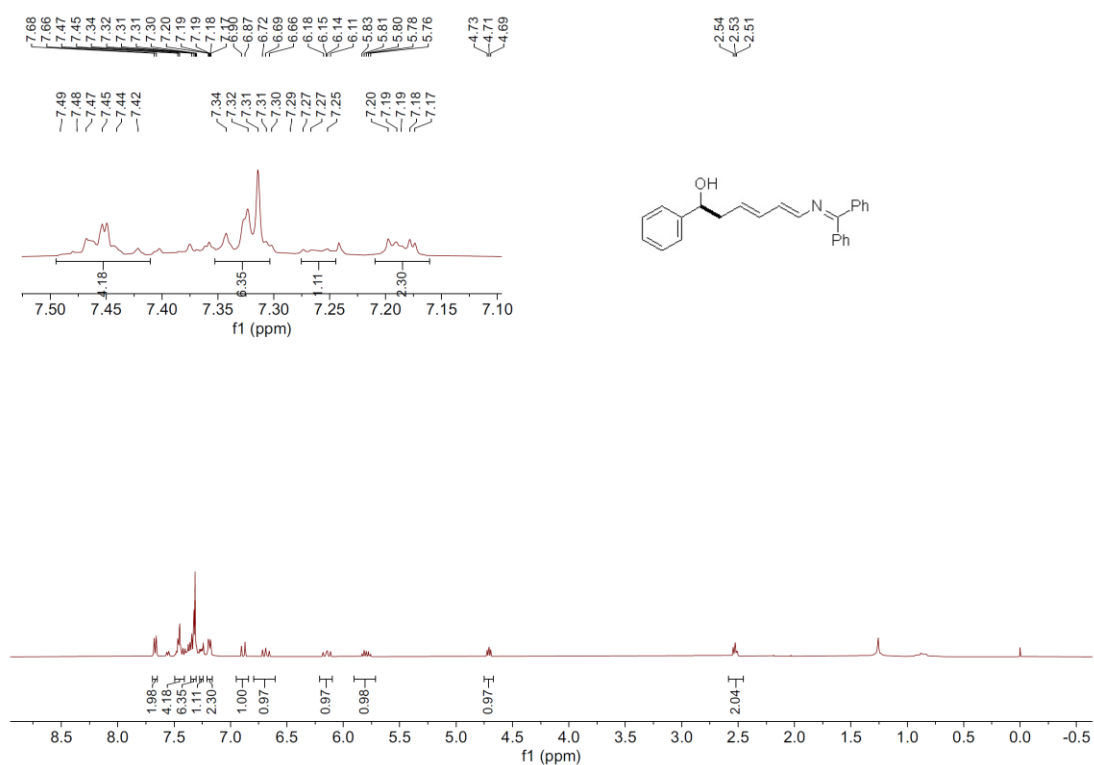
4s ¹H NMR



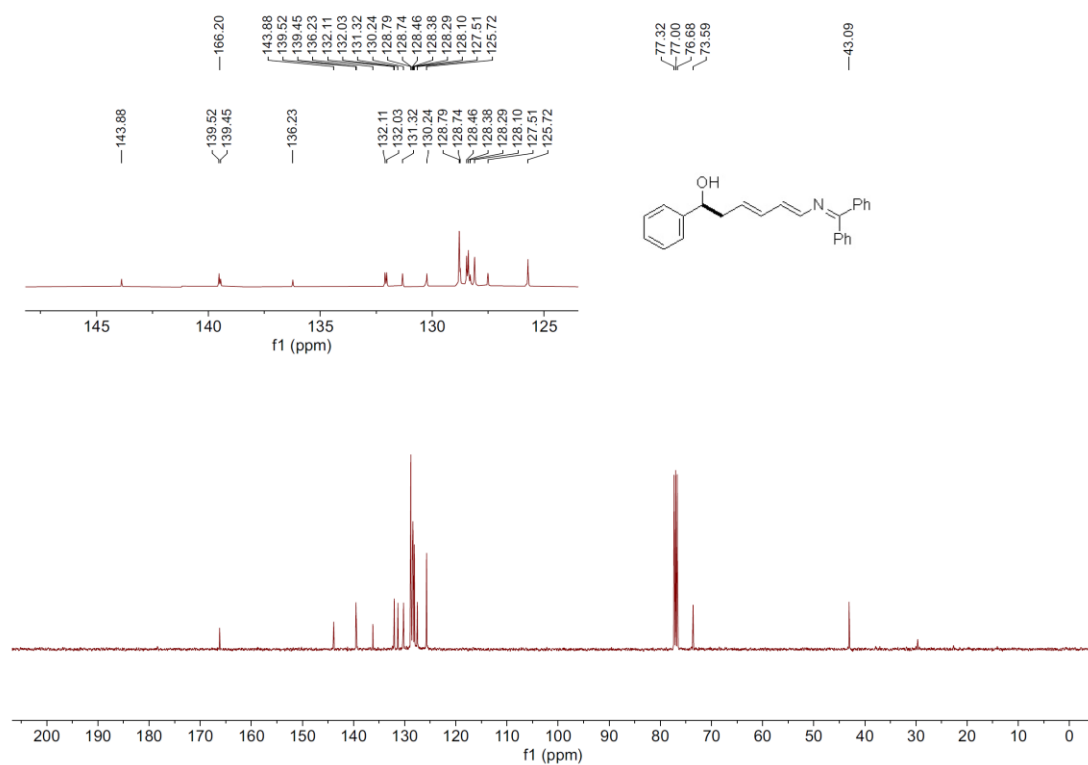
4s ¹³C NMR



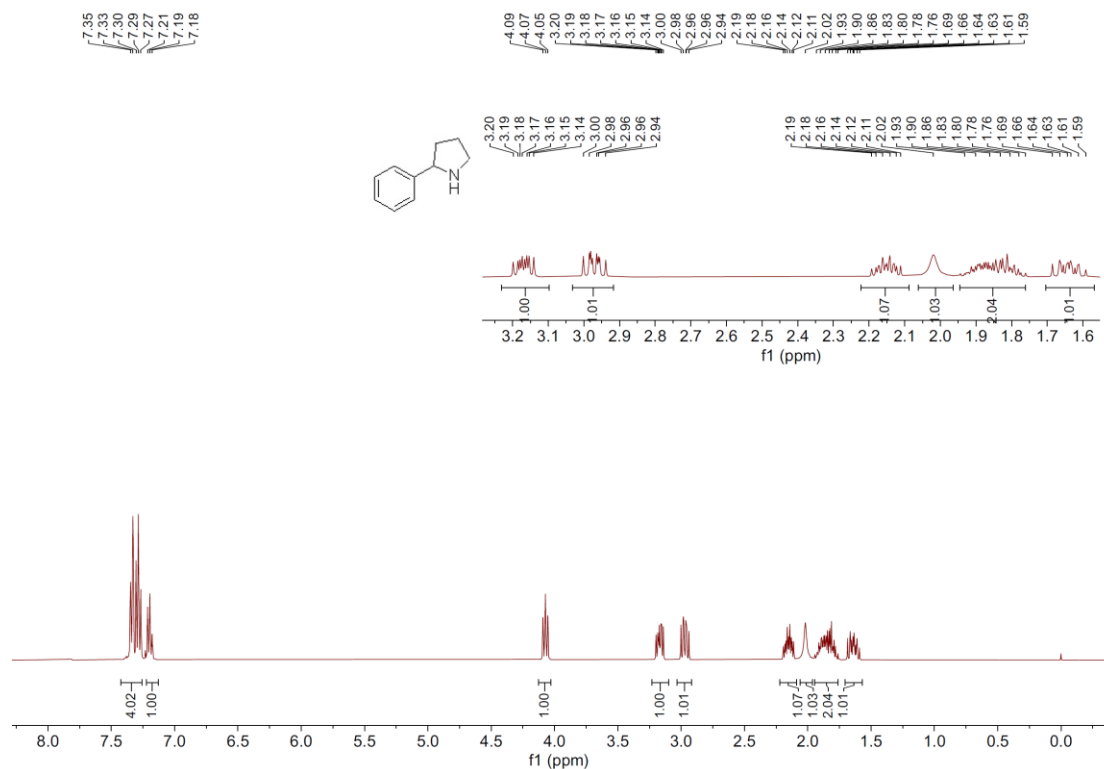
4t ¹H NMR



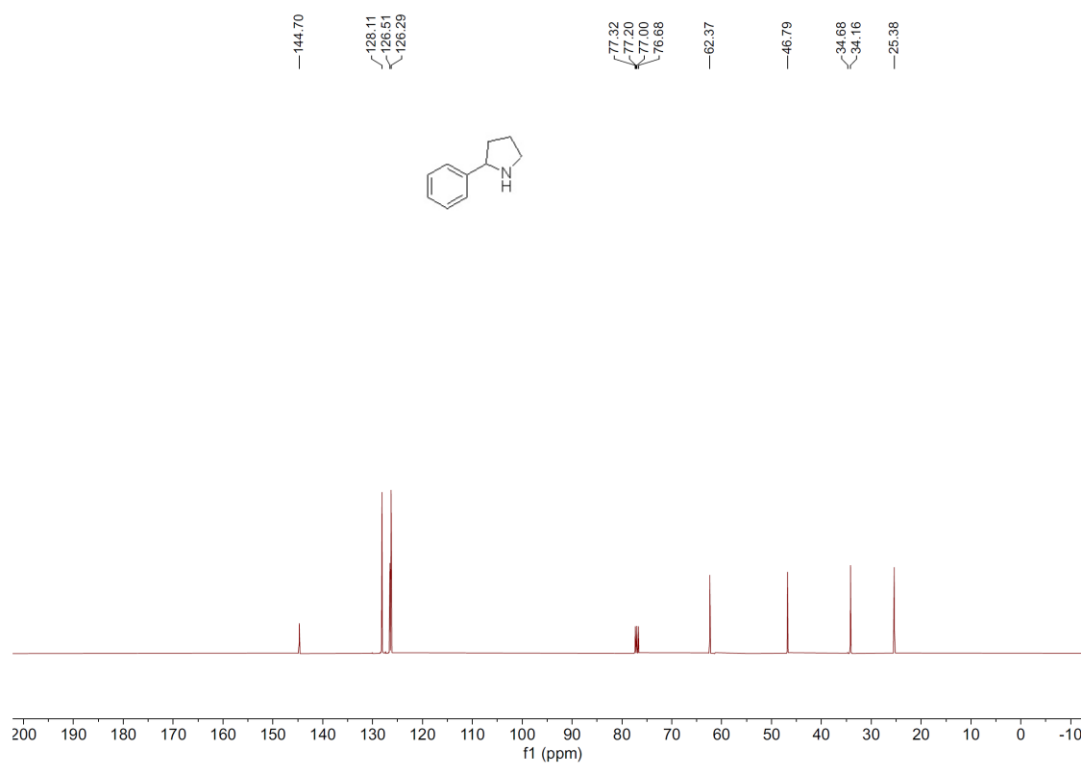
4t ¹³CNMR



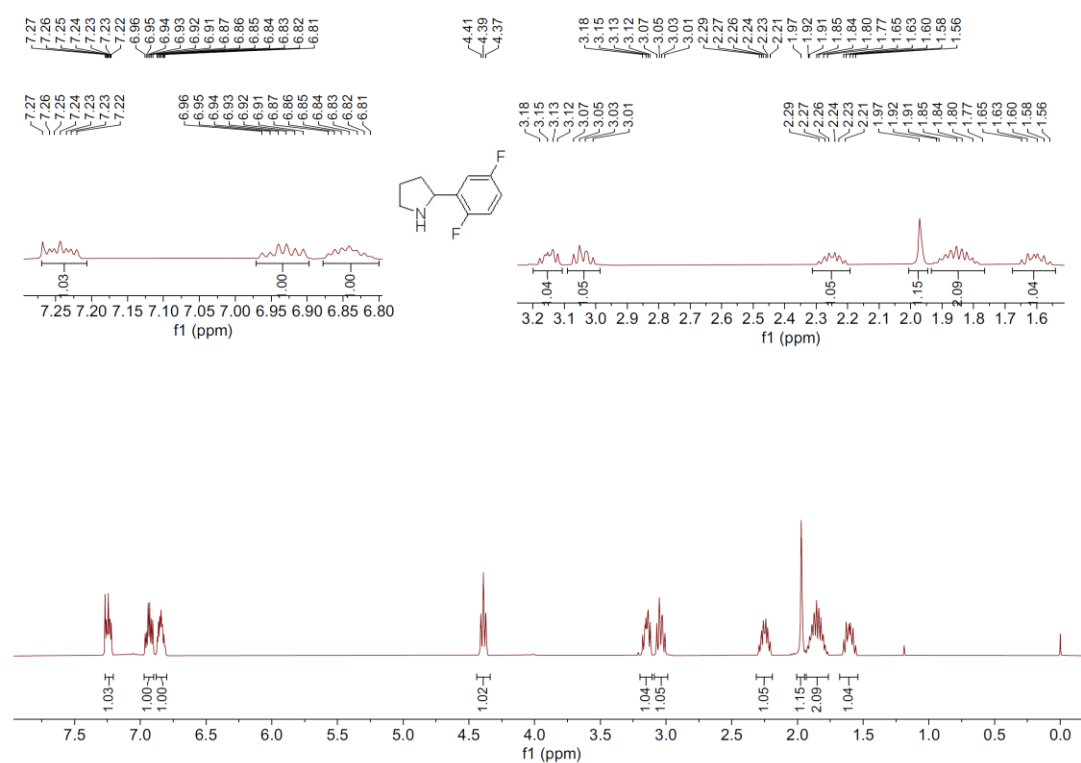
5 ¹H NMR



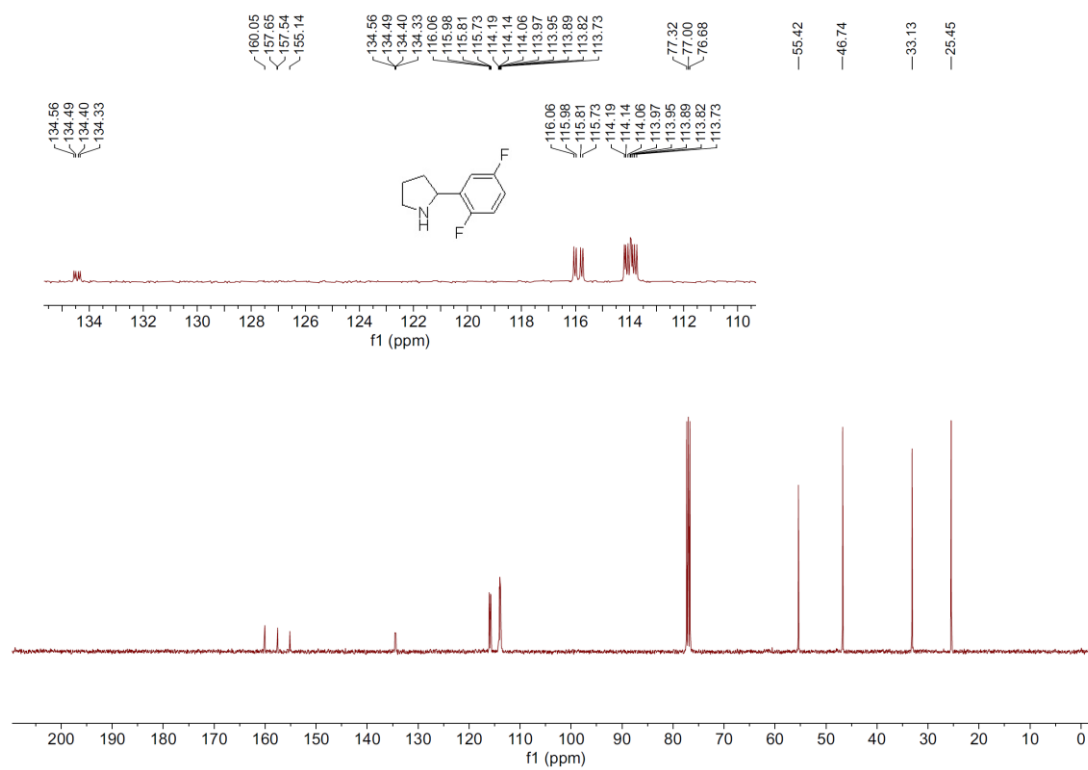
5 ^{13}C NMR



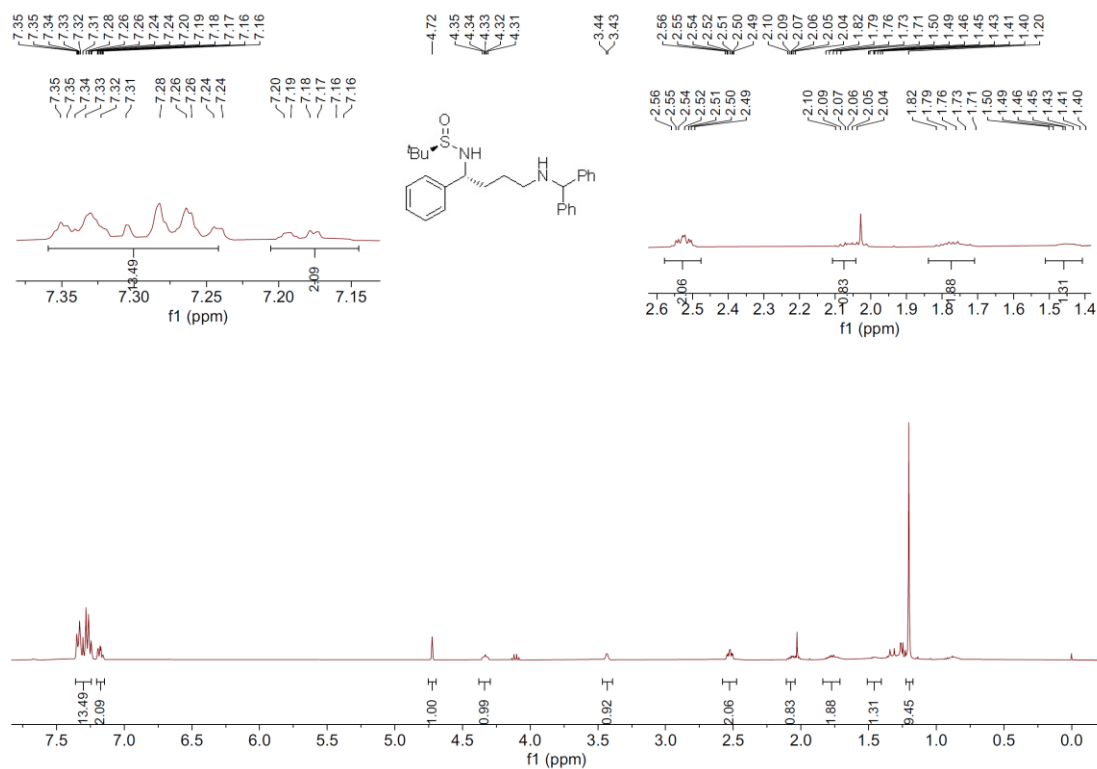
6 ^1H NMR



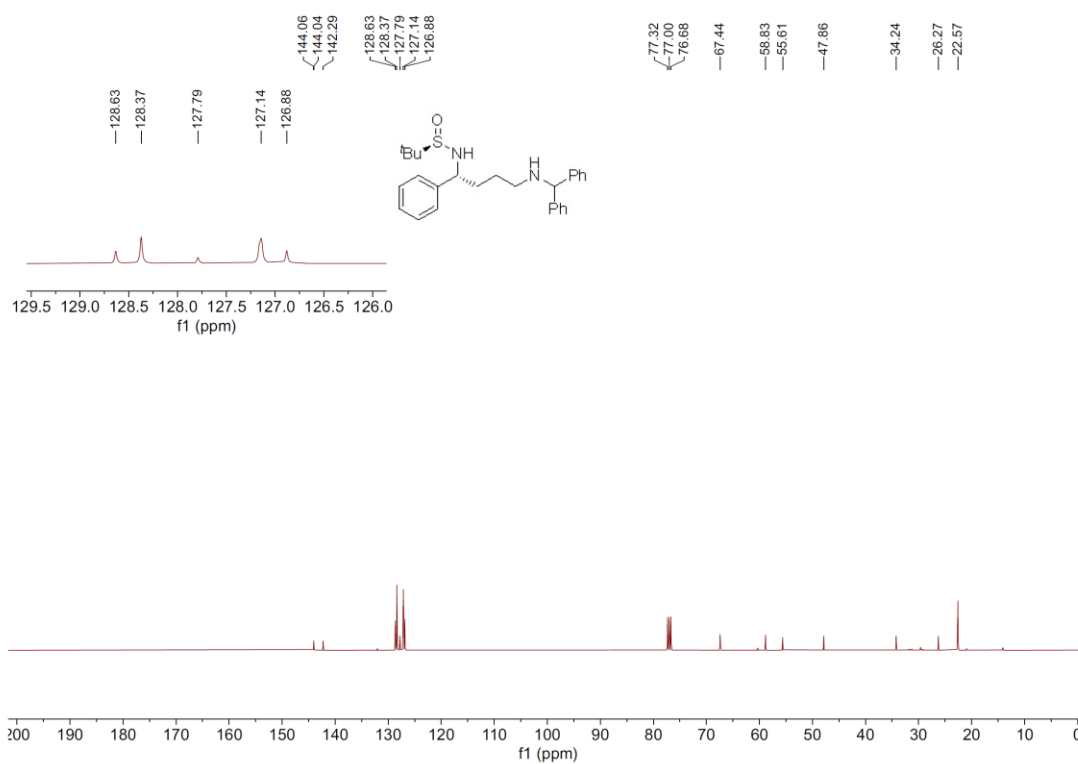
6 ^{13}C NMR



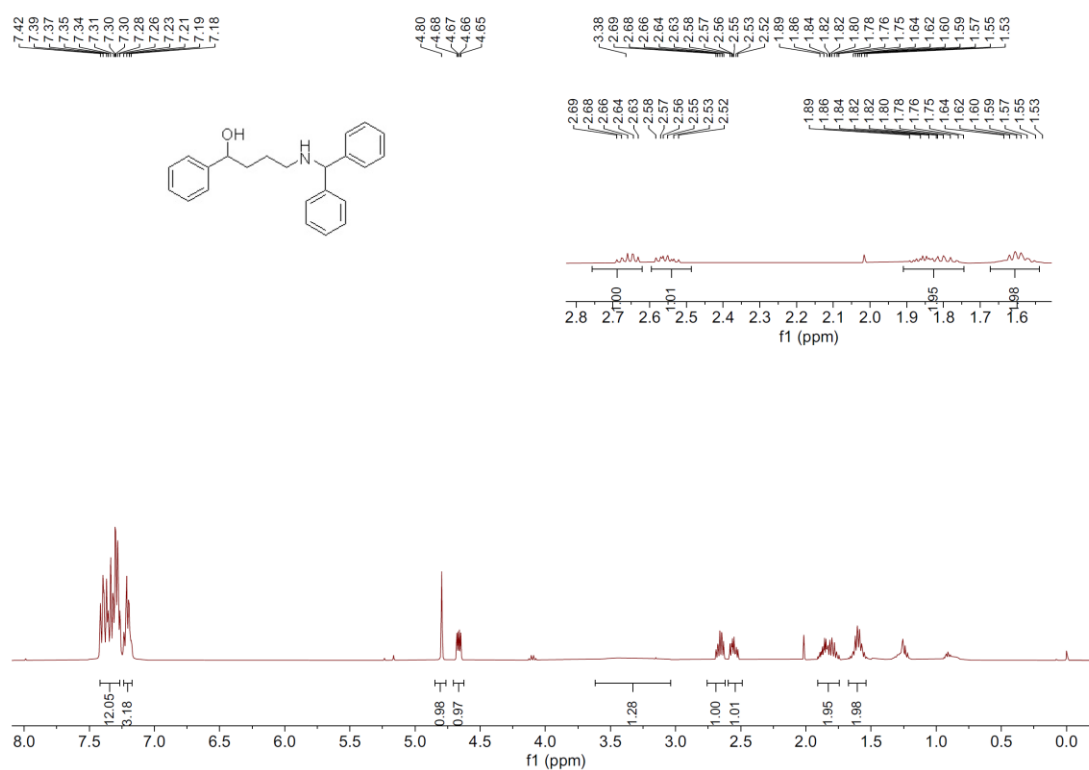
7 ^1H NMR



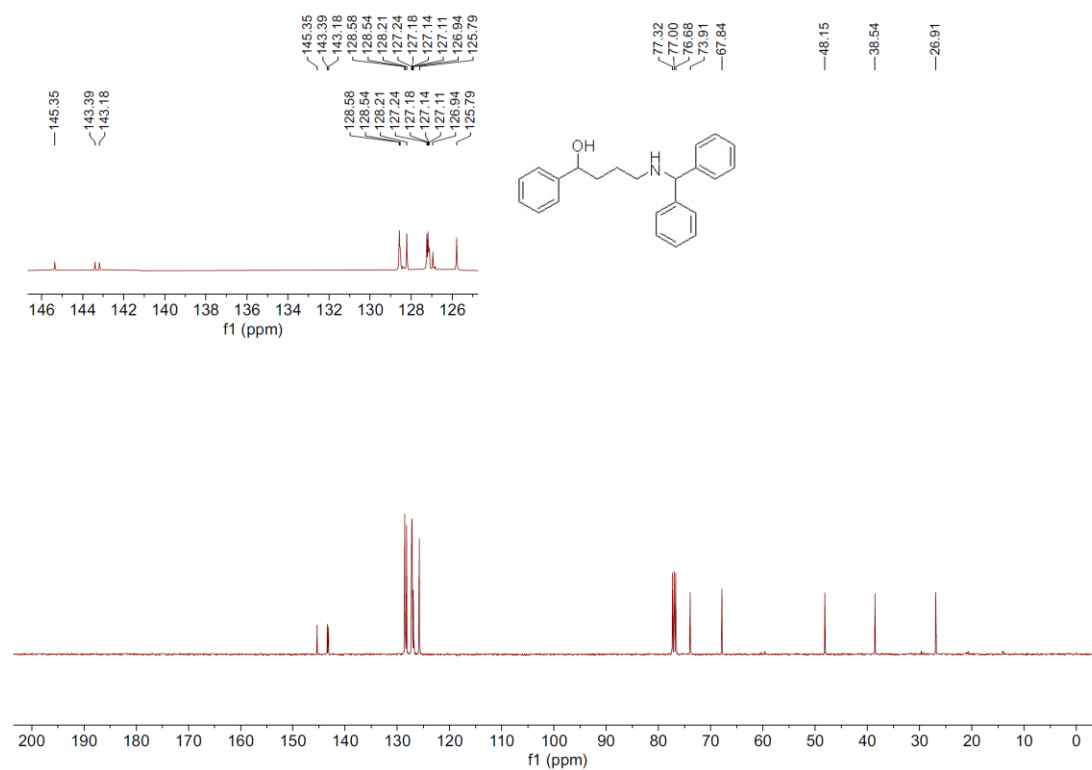
7 ^{13}C NMR



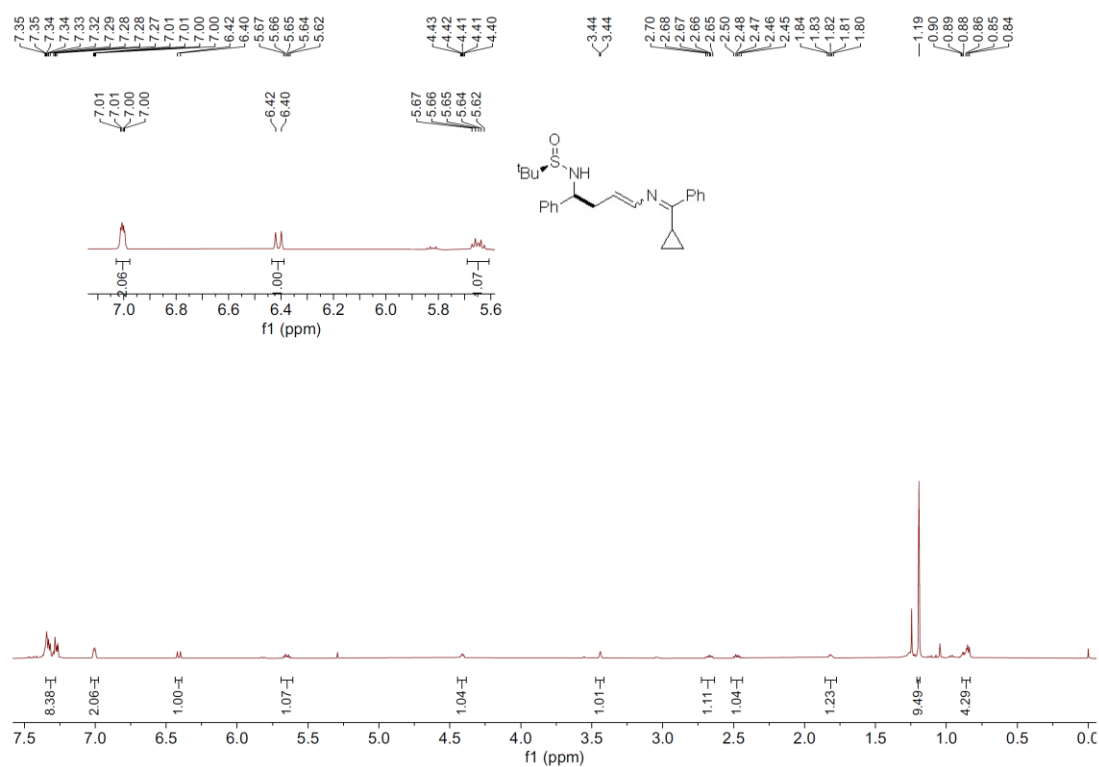
8 ^1H NMR



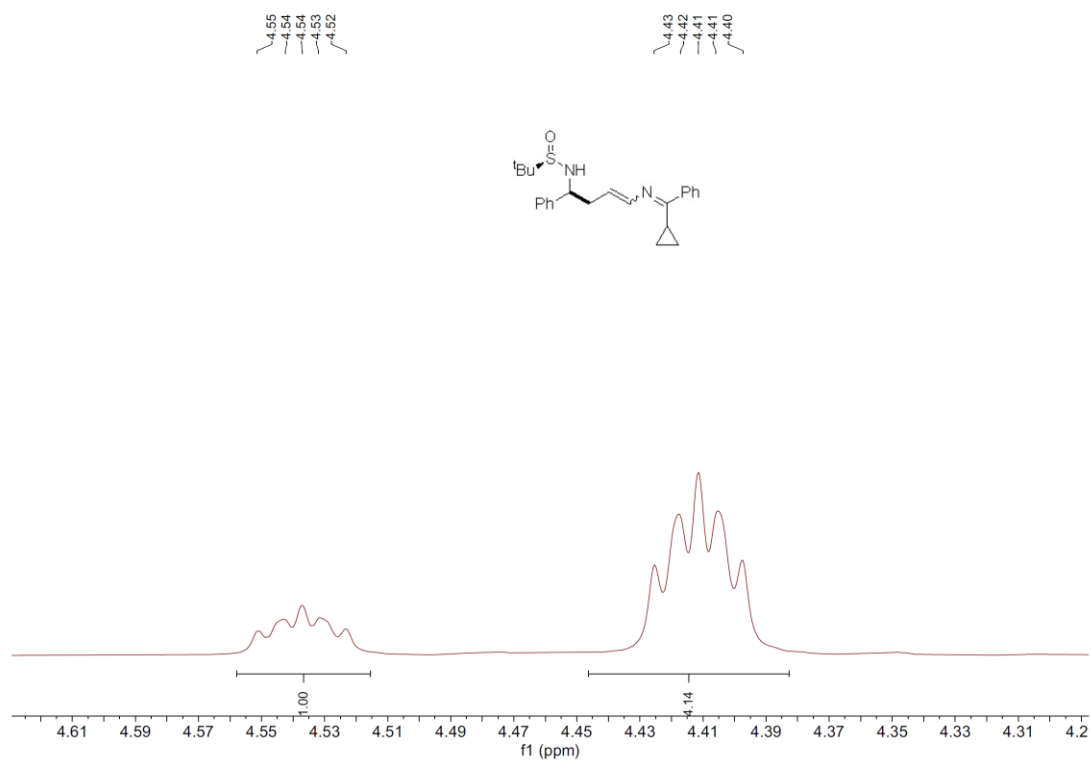
8 ¹³CNMR



3be ¹H NMR



3be *E/Z*



3be ¹³CNMR

