Electronic Supplementary Information

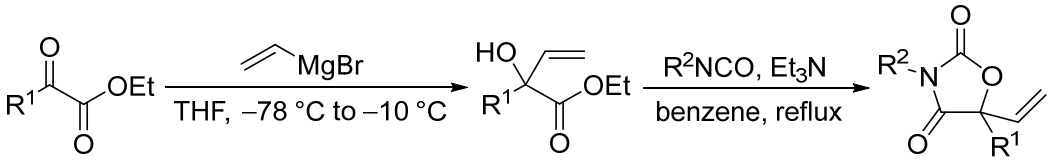
A fungicide-inspired precursors of π-allylpalladium intermediates for palladium-catalyzed decarboxylative cycloadditions

CONTENTS

General Information

All reactions were performed in Schlenk tubes under an atmosphere of argon using oven-dried glassware. Commercially obtained reagents were used without further purification, unless otherwise noted. Trichloromethane ($CHCl_3$) was distilled over P_2O_5 and stored over 3Å type molecular sieves. Tetrahydrofuran (THF) and toluene were distilled freshly before use over sodium and benzophenone. Acetonitrile (MeCN), Dichloromethane (DCM) and 1,2-dichloroethane (DCE) were distilled from CaH_2. Reactions were checked for completion by TLC analysis and plates were visualized with short-wave UV light (254 nm). The ^1H, ^{13}C and ^{19}F NMR spectra were obtained in $CDCl_3$ using a Bruker-BioSpin AVANCE III HD NMR spectrometer at 500, 125 and 470 MHz, respectively. Chemical shifts are reported in parts per million (δ value) calibrated against the residual solvent peak. Signal patterns are indicated as follows: s, singlet; d, doublet; t, triplet; q, quartet; m, multiplet. Coupling constants (*J*) are given in hertz (Hz). The infrared spectra were recorded on a Bruker VERTEX 70 IR spectrometer as KBr pellets, with absorption reported in cm^{-1}. High-resolution mass spectra were recorded on a Bruker Impact II UHR TOF LC/MS Mass Spectrometry. Melting points were determined on a Stuard SMP3 melting point apparatus. X-ray crystallographic data were collected using a MM007HF Saturn724+. HPLC analysis was performed on Agilent 1220 series, UV detection monitored at 254 nm, using a Chiralpak AD-H column, a Chiralcel OD-H column, Chiralpak IA column, Chiralpak IC column, Chiralpak ID column and Chiralpak IH column with hexane and i-PrOH as the eluent.

Preparation of Substrates: Synthesis of 5-Vinyloxazolidine-2,4-diones 1 or 4



The required Grignard reagent (1.2 equiv.) was added dropwise to a solution of the ethyl benzoylformate **S1** (1.0 equiv.) in anhydrous THF at –78 °C under argon atmosphere. The resulting mixture was stirred at –78 °C for 2 h. Then the resulting mixture was stirred at –10 °C for 2 h The reaction was quenched with aq. NH_4Cl and the organic layer was separated. The aqueous layer was extracted with EtOAc (3×100 mL). The combined organic layers were washed with brine (1×100 mL), dried over $MgSO_4$, and concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (Ethyl acetate/Petroleum ether = 1:15) to obtain the product **S2**.

A solution of **S2** (5.0 mmol, 1.0 equiv.), phenyl isocyanate (2.0 equiv.) and Et_3N (5.0 equiv.) in benzene was stirred at 80 °C for 12 h. The reaction was concentrated under reduced pressure. The residue was purified by flash chromatography on silica gel (Ethyl acetate/Petroleum ether = 1:10) to give the desired 5-vinyloxazolidine-2,4-diones **1** or **4**.

General Procedure for Palladium-Catalyzed Asymmetric (5 + 3) Cycloaddition

To an oven-dried 25 mL of Schlenk tube equipped with a stir bar, $Pd_2dba_3 \cdot CHCl_3$ (5 mol%) and (S, S, S)-(3, 5-dioxa-4-phosphacyclohepta[2, 1-a:3, 4-a']dinaphthalen-4-yl)bis(1-phenylethyl) amine **L3** (20 mol%) was added along with 5-vinyloxazolidine-2,4-diones **1** (0.12 mmol), azomethine imines **2** (0.1 mmol) and DCM (1.0 mL). The reaction was stirred at 25 ℃ under argon atmosphere until complete consumption of azomethine imines **2** as monitored by thin layer chromatography. The reaction mixture was directly purified by silica gel column chromatography (Ethyl acetate/Petroleum ether = 1:1) to afford the desired cycloadducts.

General Procedure for Scaled-up (5 + 3) Cycloaddition

To an oven-dried 100 mL of Schlenk tube equipped with a stir bar, $Pd_2dba_3 \cdot CHCl_3$ (5 mol%) and (S, S, S)-(3, 5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']dinaphthalen-4-yl)bis(1-phenylethyl)amine (20 mol%) was added along with 5-vinyloxazolidine-2,4-diones **1** (1.2 mmol), azomethine imines **2** (1.0 mmol) and DCM (10.0 mL). The reaction was stirred at 25 ℃ under argon atmosphere until complete consumption of azomethine imines **2** as monitored by thin layer chromatography. The reaction mixture was directly purified by silica gel column chromatography (Ethyl acetate/Petroleum ether = 1:1) to afford the desired cycloadducts.

General Procedure for Palladium-Catalyzed Asymmetric (3 + 2) Cycloaddition

To an oven-dried 25 mL of Schlenk tube equipped with a stir bar, $Pd_2dba_3 \cdot CHCl_3$ (2.5 mol%) and (S, S, S)-(3, 5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']dinaphthalen-4-yl)bis(1-phenylethyl)amine **L3** (10 mol%) was added along with 5-vinyloxazolidine-2,4-diones **4** (0.15 mmol), 1,1-dicyanoalkenes **5** (0.1 mmol) and DCM (1.0 mL). The reaction was stirred at 0 ℃ under argon atmosphere until complete consumption of 1,1-dicyanoalkenes **5** as monitored by thin layer chromatography. The reaction mixture was directly purified by silica gel column chromatography (Ethyl acetate/Petroleum ether = 10:1) to afford the desired cycloadducts.

General Procedure for Scaled-up (3 + 2) Cycloaddition

To an oven-dried 100 mL of Schlenk tube equipped with a stir bar, $Pd_2dba_3 \cdot CHCl_3$ (2.5 mol%) and (S, S, S)-(3, 5-dioxa-4-phosphacyclohepta[2,1-a:3,4-a']dinaphthalen-4-yl)bis(1-phenylethyl)amine (10 mol%) was added along with 5-vinyloxazolidine-2,4-diones **4** (1.5 mmol), 1,1-dicyanoalkenes **5** (1.0 mmol) and DCM (10.0 mL). The reaction was stirred at 0 ℃

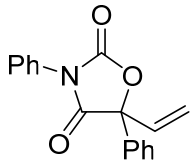
under argon atmosphere until complete consumption of 1,1-dicyanoalkenes **5** as monitored by thin layer chromatography. The reaction mixture was directly purified by silica gel column chromatography (Ethyl acetate/Petroleum ether = 10:1) to afford desired the cycloadducts.

General Procedure for Further Transformation

The $NaBH_4$ (2.0 mmol) was added to a solution of **6aa** (0.20 mmol) in DCM/MeOH (1:1, 4.0 mL) at 0 ℃. The reaction was stirred at 0 ℃ for 12 h, and the reaction was concentrated under reduced pressure. The residue purified by silica gel column chromatography (Ethyl acetate/Petroleum ether = 1:1) to afford the desired product **7**.

Characterization Data of Substrates and Products

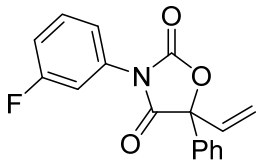
3,5-diphenyl-5-vinyloxazolidine-2,4-dione



1a

white solid, 499.7 mg, 36%, Mp: 98 – 100 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.58 – 7.47 (m, 2H), 7.42 – 7.22 (m, 8H), 6.23 – 6.11 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.65 – 5.56 (d, *J* = 17.0 Hz, 1H), 5.43 – 5.34 (d, *J* = 10.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.7, 153.1, 134.9, 133.4, 130.8, 129.5, 129.4, 129.1, 125.7, 125. 5, 118.4, 87.3. HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{14}NO_3$ $[M+H]^+$: 280.0968, found: 280.0968.

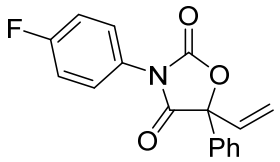
3-(3-fluorophenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1b

white solid, 808.7 mg, 54%, Mp: 78 – 80 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.70 – 7.57 (m, 2H), 7.52 – 7.36 (m, 4H), 7.32 – 7.19 (m, 2H), 7.16 – 7.05 (m, 1H), 6.34 – 6.19 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.76 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.56 – 5.45 (d, *J* = 10.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.3, 162.6 (d, *J* = 246.6 Hz), 152.5, 134.6, 133.1, 132.1 (d, *J* = 10.1 Hz), 130.6 (d, *J* = 8.8 Hz), 129.6, 129.1, 125.4, 121.1 (d, *J* = 3.4 Hz), 118.5, 116.1 (d, *J* = 20.9 Hz), 113.2 (d, *J* = 24.9 Hz), 87.3. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = –110.2. HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{13}FNO_3$ $[M+H]^+$: 298.0874, found: 298.0873.

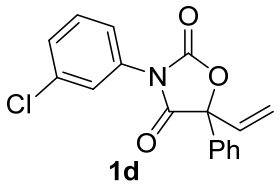
3-(4-fluorophenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1c

white solid, 992.8 mg, 67%, Mp: 108 – 110 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.71 – 7.55 (m, 2H), 7.52 – 7.29 (m, 5H), 7.19 – 7.03 (m, 2H), 6.36 – 6.17 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.78 – 5.62 (d, *J* = 17.0 Hz, 1H), 5.57 – 5.43 (d, *J* = 10.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.6, 162.4 (d, *J* = 248.1 Hz), 152.9, 134.7, 133.3, 129.6, 129.1, 127.7 (d, *J* = 8.6 Hz), 126.7 (d, *J* = 3.3 Hz), 125.4, 118.5, 116.4 (d, *J* = 23.0 Hz), 87.4. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = –111.3. HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{13}FNO_3$ $[M+H]^+$: 298.0874, found: 298.0871.

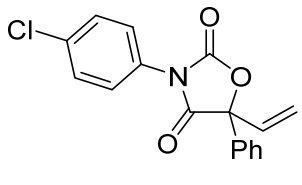
3-(3-chlorophenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1d

yellow oil, 869.6 mg, 55%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.65 – 7.57 (m, 2H), 7.51 – 7.33 (m, 7H), 6.31 – 6.21 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.77 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.57 – 5.47 (d, *J* = 10.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.3, 152.5, 135.0, 134.6, 133.1, 131.9, 130.3, 129.6, 129.2, 129.1, 125.8, 125.4, 123.7, 118.5, 87.4. HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{13}{}^{35}ClNO_3$ $[M+H]^+$: 314.0578, found: 314.0578.

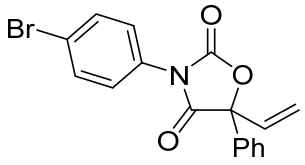
3-(4-chlorophenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1e

white solid, 753.4 mg, 48%, Mp: 82 – 84 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ =7.67 – 7.56 (m, 2H), 7.52 – 7.34 (m, 7H), 6.34 – 6.17 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.77 – 5.65 (d, *J* = 17.5 Hz, 1H), 5.57 – 5.43 (d, *J* = 11.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.4, 152.7, 134.8, 134.6, 133.2, 129.6, 129.6, 129.3, 129.1, 126.8, 125.4, 118.5, 87.4. HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{13}{}^{35}ClNO_3$ $[M+H]^+$: 314.0578, found: 314.0580.

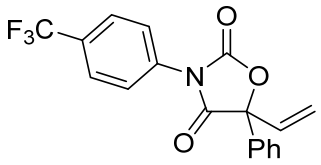
3-(4-bromophenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1f

white solid, 768.8 mg, 43%, Mp: 88 – 90 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.67 – 7.56 (m, 4H), 7.50 – 7.39 (m, 3H), 7.38 – 7.29 (m, 2H), 6.33 – 6.20 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.76 – 5.64 (d, *J* = 17.0 Hz, 1H), 5.55 – 5.45 (d, *J* = 10.5 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.4, 152.6, 134.6, 133.2, 132.5, 129.9, 129.6, 129.1, 127.1, 125.4, 122.9, 118.5, 87.4. HRMS (ESI, *m*/*z*) calcd for $C_{17}H_{13}{}^{79}BrNO_3$ $[M+H]^+$: 358.0073, found: 358.0074.

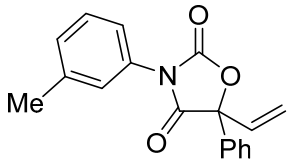
5-phenyl-3-(4-(trifluoromethyl)phenyl)-5-vinyloxazolidine-2,4-dione



1g

yellow oil, 979.8 mg, 56%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.78 – 7.70 (m, 2H), 7.67 – 7.57 (m, 4H), 7.50 – 7.36 (m, 3H), 6.33 – 6.19 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.78 – 5.66 (d, *J* = 17.5 Hz, 1H), 5.59 – 5.43 (d, *J* = 11.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.3, 152.4, 134.5, 134.0, 133.1, 130.9 (q, *J* = 32.9 Hz), 129.7, 129.1, 126.5 (q, *J* = 3.6 Hz), 125.7, 125.4, 123.6 (q, *J* = 270.8 Hz), 118.6, 87.4. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = –62.8. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{13}F_3NO_3$ $[M+H]^+$: 348.0842 , found: 348.0837.

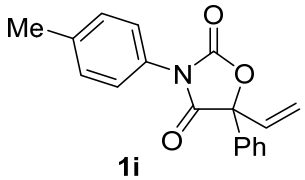
5-phenyl-3-(*m*-tolyl)-5-vinyloxazolidine-2,4-dione



1h

yellow oil, 988.3 mg, 67%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.68 – 7.56 (m, 2H), 7.48 – 7.37 (m, 3H), 7.36 – 7.29 (m, 1H), 7.24 – 7.14 (m, 3H), 6.33 – 6.20 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.76 – 5.67 (d, *J* = 17.0 Hz, 1H), 5.52 – 5.42 (d, *J* = 10.5 Hz, 1H), 2.37 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.8, 153.2, 139.6, 134.9, 133.4, 130.7, 130.0, 129.5, 129.2, 129.0, 129.0, 126.4, 125.4, 122.9, 118.3, 87.3, 21.3. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{16}NO_3$ $[M+H]^+$: 294.1125, found: 294.1120 .

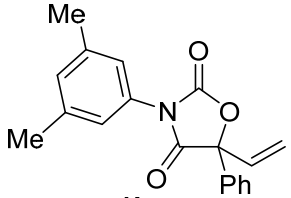
5-phenyl-3-(p-tolyl)-5-vinyloxazolidine-2,4-dione



1i

white solid, 788.3 mg, 54%, Mp: 92 – 94 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 – 7.47 (m, 2H), 7.40 – 7.24 (m, 3H), 7.21 – 7.12 (m, 4H), 6.27 – 6.09 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.66 – 5.55 (d, *J* = 17.5 Hz, 1H), 5.45 – 5.32 (d, *J* = 11.0 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.7, 152.1, 138.1, 133.8, 132.3, 128.9, 128.4, 127.9, 127.1, 124.5, 124.4, 117.2, 86.2, 20.1. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{16}NO_3$ $[M+H]^+$: 294.1125, found: 294.1120.

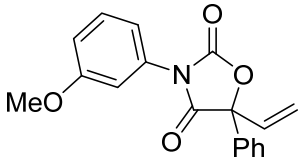
3-(3,5-dimethylphenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1j

yellow oil, 998.1 mg, 65%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.67 – 7.59 (m, 2H), 7.49 – 7.36 (m, 3H), 7.08 – 7.01 (m, 1H), 7.01 – 6.94 (d, *J* = 1.5 Hz, 2H), 6.33 – 6.22 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.76 – 5.66 (d, *J* = 17.0 Hz, 1H), 5.56 – 5.44 (d, *J* = 10.5 Hz, 1H), 2.34 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.9, 153.3, 139.3, 134.9, 133.4, 131.0, 130.4, 129. 5, 129.0, 125.4, 123.6, 118.3, 87.3, 21.2. HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{18}NO_3$ $[M+H]^+$: 308.1281, found: 308.1277.

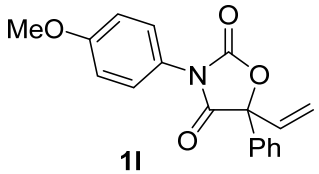
3-(3-methoxyphenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1k

yellow oil, 810.2 mg, 52%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.71 – 7.58 (m, 2H), 7.50 – 7.32 (m, 4H), 7.03 – 6.98 (m, 1H), 6.98 – 6.91 (m, 2H), 6.35 – 6.22 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.78 – 5.67 (d, *J* = 17.0 Hz, 1H), 5.55 – 5.46 (d, *J* = 10.5 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.6, 160.2, 153.0, 134.8, 133.3, 131.7, 130.1, 129.5, 129.0, 125.4, 118.4, 117.9, 115.0, 111.5, 87.2, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{16}NO_4$ $[M+H]^+$: 310.1074, found: 310.1072.

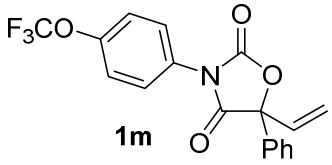
3-(4-methoxyphenyl)-5-phenyl-5-vinyloxazolidine-2,4-dione



1l

white solid, 977.8 mg, 63%, Mp: 93 – 95 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.69 – 7.57 (m, 2H), 7.49 – 7.37 (m, 3H), 7.34 – 7.27 (m, 2H), 7.02 – 6.91 (m, 2H), 6.33 – 6.20 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.77 – 5.63 (d, *J* = 17.5 Hz, 1H), 5.55 – 5.45 (d, *J* = 11.0 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.9, 159.9, 153.4, 134.9, 133.4, 129.5, 129.0, 127.2, 125.4, 123.3, 118.3, 114.7, 87.3, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{16}NO_4$ $[M+H]^+$: 310.1074, found: 310.1071.

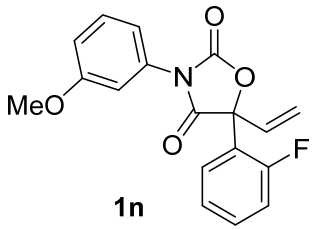
5-phenyl-3-(4-(trifluoromethoxy)phenyl)-5-vinyloxazolidine-2,4-dione



1m

yellow oil, 978.4 mg, 54%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.68 – 7.58 (m, 2H), 7.56 – 7.48 (m, 2H), 7.48 – 7.39 (m, 3H), 7.36 – 7.27 (m, 2H), 6.33 – 6.22 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.78 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.55 – 5.49 (d, *J* = 11.0 Hz, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.4, 152.7, 149.0, 134.6, 133.1, 129.6, 129.2, 129.1, 127.1, 125.4, 121.8, 120.4 (q, *J* = 256.8 Hz), 118.5, 87.4. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = –57.9. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{13}F_3NO_4$ $[M+H]^+$: 364.0791, found: 364.0785.

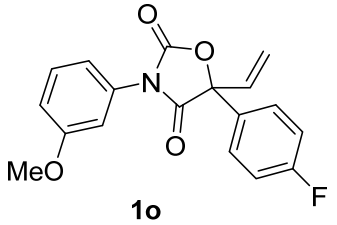
5-(2-fluorophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1n

yellow oil, 763.4 mg, 47%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.57 – 7.36 (m, 3H), 7.27 – 7.10 (m, 2H), 7.09 – 7.02 (dd, *J* = 8.0, 1.5 Hz, 1H), 7.01– 6.92 (m, 2H), 6.43 – 6.30 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.95 – 5.85 (d, *J* = 17.0 Hz, 1H), 5.77 – 5.66 (d, *J* = 11.0 Hz, 1H), 3.83 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.9, 161.2 (d, *J* = 248.8 Hz), 160.3, 153.2, 132.6 (d, *J* = 8.9 Hz), 132.0, 130.9, 130.3 (d, *J* = 2.6 Hz), 130.2, 124.6 (d, *J* = 3.4 Hz), 122.2 (d, *J* = 11.9 Hz), 120.0, 118.1, 116.5 (d, *J* = 21.4 Hz), 115.1, 111.7, 85.0, 55.5. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = –112.1. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}FNO_4$ $[M+H]^+$: 328.0980, found: 328.0977.

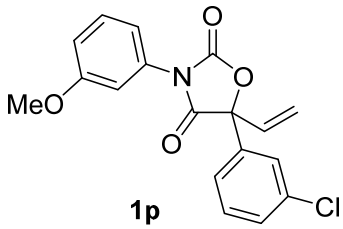
5-(4-fluorophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1o

yellow oil, 988.2 mg, 60%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.68 – 7.57 (m, 2H), 7.44 – 7.32 (m, 1H), 7.19 – 7.07 (m, 2H), 7.04– 6.90 (m, 3H), 6.30 – 6.17 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.75 – 5.62 (d, *J* = 17.0 Hz, 1H), 5.57 – 5.46 (d, *J* = 10.5 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.5, 163.3 (d, *J* = 248.1 Hz), 160.2, 152.8, 133.2, 131.6, 130.6 (d, *J* = 3.1 Hz), 130.1, 127.6 (d, *J* = 8.5 Hz), 118.6, 117.8, 116.0 (d, *J* = 21.8 Hz), 115.0, 111.5, 86.7, 55.5. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = –111.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}FNO_4$ $[M+H]^+$: 328.0980, found: 328.0975.

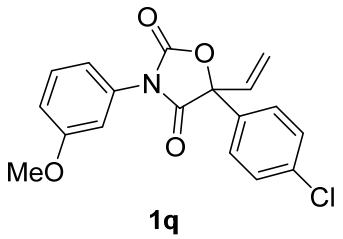
5-(3-chlorophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1p

yellow oil, 949.6 mg, 55%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.70 – 7.61 (m, 1H), 7.59 – 7.48 (m, 1H), 7.44 – 7.32 (m, 3H), 7.04– 6.88 (m, 3H), 6.29 – 6.17 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.77 – 5.67 (d, *J* = 17.0 Hz, 1H), 5.58 – 5.46 (d, *J* = 10.5 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.1, 160.2, 152.6, 136.7, 135.1, 133.0, 131.5, 130.3, 130.1, 129.7, 125.7, 123.5, 118.8, 117.8, 115.1, 111.4, 86.4, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}{}^{35}ClNO_4$ $[M+H]^+$: 344.0684, found: 344.0685.

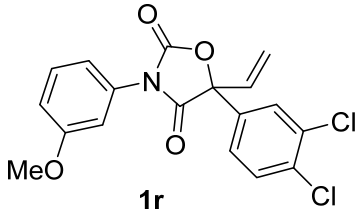
5-(4-chlorophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1q

white solid, 866.7 mg, 50%, Mp: 100 – 102 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.63 – 7.52 (m, 2H), 7.46 – 7.32 (m, 3H), 7.02 – 6.90 (m, 3H), 6.30 – 6.17 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.75 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.57 – 5.47 (d, *J* = 10.5 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.3, 160.2, 152.7, 135.7, 133.3, 133.1, 131.6, 130.1, 129.2, 126.9, 118.7, 117.8, 115.1, 111.4, 86.6, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}{}^{35}ClNO_4$ $[M+H]^+$: 344.0684, found: 344.0682.

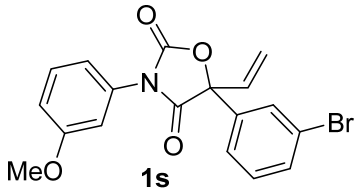
5-(3,4-dichlorophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1r

yellow oil, 958.6 mg, 51%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.80 – 7.73 (d, *J* = 2.0 Hz, 1H), 7.55 – 7.45 (m, 2H), 7.42 – 7.34 (t, *J* = 8.0 Hz, 1H), 7.03– 6.89 (m, 3H), 6.27 – 6.15 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.76 – 5.66 (d, *J* = 17.0 Hz, 1H), 5.58 – 5.48 (d, *J* = 11.0 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.9, 160.3, 152.4, 134.8, 134.0, 133.5, 132.7, 131.4, 131.0, 130.2, 127.5, 124.7, 119.1, 117.7, 115.2, 111.4, 85.9, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{14}{}^{35}Cl_2NO_4$ $[M+H]^+$: 378.0294, found: 378.0293.

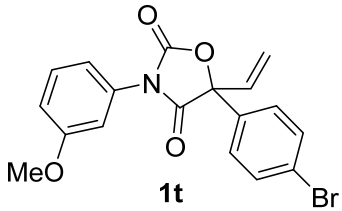
5-(3-bromophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1s

yellow oil, 896.0 mg, 46%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.84 – 7.76 (m, 1H), 7.62 – 7.51 (m, 2H), 7.41 – 7.35 (t, *J* = 8.0 Hz, 1H), 7.35– 7.28 (t, *J* = 8.0 Hz, 1H), 7.06 – 6.91 (m, 3H), 6.28 – 6.16 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.76 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.57 – 5.48 (d, *J* = 11.0 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.1, 160.2, 152.6, 136.9, 133.0, 132.6, 130.6, 130.1, 128.5, 124.0, 123.1, 118.8, 117.8, 115.1, 111.4, 86.3, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}{}^{79}BrNO_4$ $[M+H]^+$: 388.0179, found: 388.0178.

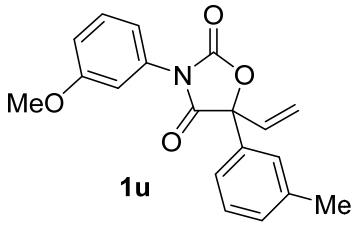
5-(4-bromophenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1t

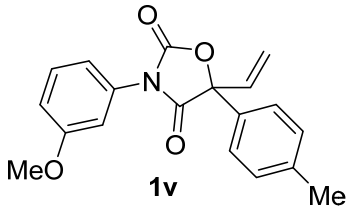
yellow oil, 993.9 mg, 51%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 – 7.55 (d, *J* = 8.5 Hz, 2H), 7.55 – 7.48 (d, *J* = 7.5 Hz, 2H), 7.43 – 7.32 (t, *J* = 8.0 Hz, 1H), 7.02– 6.89 (m, 3H), 6.29 – 6.16 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.74 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.56 – 5.47 (d, *J* = 11.0 Hz, 1H), 3.80 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.3, 160.2, 152.7, 133.8, 133.0, 132.2, 131.6, 130.1, 127.1, 123.9, 118.8, 117.8, 115.1, 111.4, 86.6, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}{}^{79}BrNO_4$ $[M+H]^+$: 388.0179, found: 388.0178.

3-(3-methoxyphenyl)-5-(*m*-tolyl)-5-vinyloxazolidine-2,4-dione



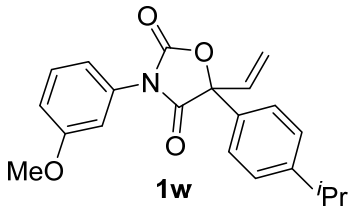
yellow oil, 613.9 mg, 38%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.47 – 7.40 (m, 2H), 7.40 – 7.29 (m, 2H), 7.29 – 7.19 (t, *J* = 6.5 Hz, 1H), 7.04 – 6.98 (dd, *J* = 8.5, 2.0 Hz, 1H), 6.98 – 6.91 (m, 2H), 6.32 – 6.21 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.75 – 5.64 (d, *J* = 17.0 Hz, 1H), 5.54 – 5.44 (d, *J* = 10.5 Hz, 1H), 3.80 (s, 3H), 2.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.7, 160.2, 153.0, 138.9, 134.8, 133.4, 131.8, 130.2, 130.1, 128.9, 125.9, 122.5, 118.2, 117.9, 115.0, 111.5, 87.3, 55.6, 21.6. HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{18}NO_4$ $[M+H]^+$: 324.1230, found: 324.1227.

3-(3-methoxyphenyl)-5-(*p*-tolyl)-5-vinyloxazolidine-2,4-dione



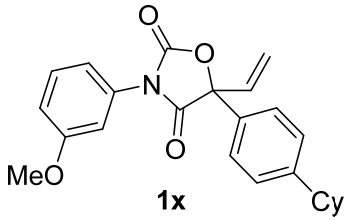
yellow oil, 982.7 mg, 61%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.55 – 7.45 (d, *J* = 8.0 Hz, 2H), 7.42 – 7.30 (t, *J* = 9.5 Hz, 1H), 7.28 – 7.18 (d, *J* = 8.0 Hz, 2H), 7.05 – 6.98 (d, *J* = 7.5 Hz, 1H), 6.98 – 6.87 (m, 2H), 6.35 – 6.18 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.76 – 5.64 (d, *J* = 17.5 Hz, 1H), 5.54 – 5.42 (d, *J* = 11.0 Hz, 1H), 3.79 (s, 3H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.8, 160.2, 153.1, 139.6, 133.4, 131.9, 131.8, 130.1, 129.7, 125.4, 118.2, 117.9, 115.0, 111.5, 87.3, 55.5, 21.2. HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{18}NO_4$ $[M+H]^+$: 324.1230, found: 324.1229.

5-(4-isopropylphenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



yellow oil, 822.6 mg, 47%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.58 – 7.51 (d, *J* = 8.0 Hz, 2H), 7.40 – 7.33 (t, *J* = 8.0 Hz, 1H), 7.33 – 7.26 (d, *J* = 8.0 Hz, 2H), 7.04 – 6.98 (m, 1H), 6.97 – 6.90 (m, 2H), 6.32 – 6.21 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.75 – 5.66 (d, *J* = 17.5 Hz, 1H), 5.52 – 5.43 (d, *J* = 11.0 Hz, 1H), 3.80 (s, 3H), 2.99 – 2.72 (m, 1H), 1.32 – 1.12 (d, *J* = 8.0 Hz, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.8, 160.2, 153.1, 150.4, 133.4, 132.2, 131.8, 130.1, 127.1, 125.5, 118.1, 117.9, 115.0, 111.5, 87.3, 55.5, 33.9, 23.9, 23.9. HRMS (ESI, *m*/*z*) calcd for $C_{21}H_{22}NO_4$ $[M+H]^+$: 352.1543, found: 352.1542.

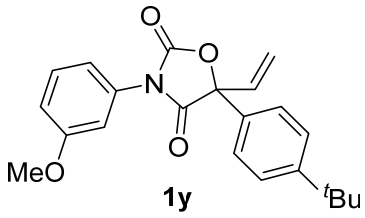
5-(4-cyclohexylphenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1x

white solid, 991.2 mg, 51%, Mp: 105 – 107 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.49 (d, *J* = 8.5 Hz, 2H), 7.42 – 7.31 (m, 1H), 7.31 – 7.25 (d, *J* = 8.0 Hz, 2H), 7.06 – 6.98 (d, *J* = 7.5 Hz, 1H), 6.97 – 6.89 (m, 2H), 6.35 – 6.21 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.75 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.53 – 5.44 (d, *J* = 10.5 Hz, 1H), 3.80 (s, 3H), 2.59 – 2.40 (m, 1H), 1.94 – 1.78 (m, 4H), 1.78 – 1.66 (m, 1H), 1.48 – 1.32 (m, 4H), 1.32 – 1.15 (m, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.8, 160.2, 153.1, 149.6, 133.4, 132.2, 131.8, 130.1, 127.5, 125.4, 118.1, 117.9, 115.0, 111.5, 87.3, 55.5, 44.3, 34.3, 34.3, 26.8, 26.1. HRMS (ESI, *m*/*z*) calcd for $C_{24}H_{26}NO_4$ $[M+H]^+$: 392.1856, found: 392.1855.

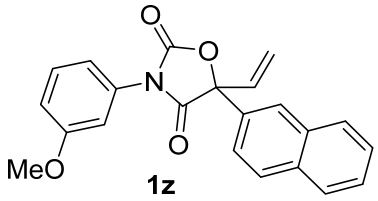
5-(4-(*tert*-butyl)phenyl)-3-(3-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



1y

yellow oil, 820.7 mg, 45%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.51 (d, *J* = 8.5 Hz, 2H), 7.51 – 7.43 (d, *J* = 8.5 Hz, 2H), 7.42 – 7.30 (m, 1H), 7.05 – 6.98 (m, 1H), 6.98 – 6.90 (m, 2H), 6.33 – 6.22 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.77 – 5.67 (d, *J* = 17.0 Hz, 1H), 5.53 – 5.45 (d, *J* = 11.0 Hz, 1H), 3.80 (s, 3H), 1.32 (s, 9H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.8, 160.2, 153.1, 152.7, 133.4, 131.8, 131.8, 130.1, 126.0, 125.2, 118.1, 117.9, 115.0, 111.5, 87.3, 55.5, 34.7, 31.2. HRMS (ESI, *m*/*z*) calcd for $C_{22}H_{24}NO_4$ $[M+H]^+$: 366.1700, found: 366.1699.

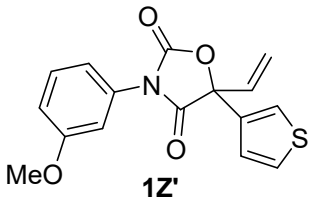
3-(3-methoxyphenyl)-5-(naphthalen-2-yl)-5-vinyloxazolidine-2,4-dione



1z

yellow oil, 980.2 mg, 54%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.20 – 8.09 (d, *J* = 2.5 Hz, 1H), 7.97 – 7.80 (m, 3H), 7.75 – 7.66 (m, 1H), 7.57 – 7.48 (m, 2H), 7.41 – 7.32 (t, *J* = 8.0 Hz, 1H), 7.06 – 6.99 (d, *J* = 8.0 Hz, 1H), 6.99 – 6.89 (m, 2H), 6.43 – 6.30 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.83 – 5.72 (d, *J* = 17.0 Hz, 1H), 5.59 – 5.49 (d, *J* = 10.5 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.7, 160.3, 153.0, 133.5, 133.3, 132.9, 132.0, 131.8, 130.1, 129.1, 128.6, 127.8, 127.3, 126.9, 124.8, 122.7, 118.7, 117.9, 115.1, 111.5, 87.4, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{22}H_{18}NO_4$ $[M+H]^+$: 360.1230, found: 360.1229.

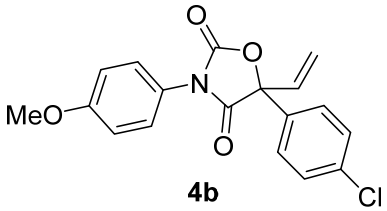
3-(3-methoxyphenyl)-5-(thiophen-3-yl)-5-vinyloxazolidine-2,4-dione



1Z'

yellow oil, 570.3 mg, 36%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.57 – 7.50 (m, 1H), 7.45 – 7.33 (m, 2H), 7.27 – 7.19 (m, 1H), 7.04 – 6.98 (m, 1H), 6.98 – 6.91 (m, 2H), 6.32 – 6.19 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.74 – 5.64 (d, *J* = 17.0 Hz, 1H), 5.54 – 5.45 (d, *J* = 11.0 Hz, 1H), 3.81 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.3, 160.2, 152.9, 135.3, 132.8, 131.7, 130.1, 127.5, 125.2, 123.5, 118.5, 117.8, 115.0, 111.5, 85.9, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{14}NO_4S$ $[M+H]^+$: 316.0638, found: 316.0636.

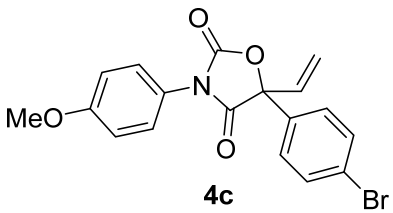
5-(4-chlorophenyl)-3-(4-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



4b

white solid, 770.6 mg, 45%, Mp: 110 – 112 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.63 – 7.53 (m, 2H), 7.45 – 7.39 (m, 2H), 7.33 – 7.27 (m, 2H), 7.01 – 6.93 (m, 2H), 6.30 – 6.16 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.73 – 5.66 (d, *J* = 17.0 Hz, 1H), 5.55 – 5.45 (d, *J* = 10.5 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.6, 159.9, 153.1, 135.7, 133.3, 133.1, 129.2, 127.1, 126.9, 123.1, 118.6, 114.7, 86.7, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}{}^{35}ClNO_4$ $[M+H]^+$: 344.0684, found: 344.0682.

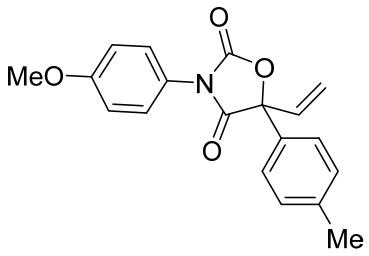
5-(4-bromophenyl)-3-(4-methoxyphenyl)-5-vinyloxazolidine-2,4-dione



4c

yellow oil, 847.3 mg, 44%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 – 7.55 (m, 2H), 7.53 – 7.49 (m, 2H), 7.32 – 7.27 (m, 2H), 7.01 – 6.92 (m, 2H), 6.28 – 6.18 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.73 – 5.65 (d, *J* = 17.0 Hz, 1H), 5.54 – 5.48 (d, *J* = 10.5 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.5, 159.9, 153.1, 133.9, 133.1, 132.2, 127.1, 123.9, 123.1, 118.7, 114.7, 86.7, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{18}H_{15}{}^{79}BrNO_4$ $[M+H]^+$: 388.0179, found: 388.0172.

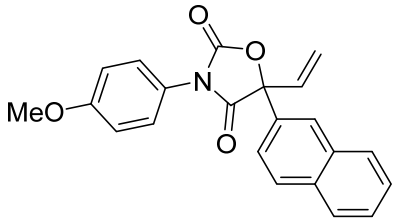
3-(4-methoxyphenyl)-5-(*p*-tolyl)-5-vinyloxazolidine-2,4-dione



4d

white solid, 814.1 mg, 50%, Mp: 100 – 102 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.54 – 7.45 (m, 2H), 7.36 – 7.29 (m, 2H), 7.29 – 7.19 (m, 2H), 7.02 – 6.93 (m, 2H), 6.32 – 6.21 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.74 – 5.65 (d, *J* = 17.5 Hz, 1H), 5.53 – 5.44 (d, *J* = 11.0 Hz, 1H), 3.81 (s, 3H), 2.37 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 171.1, 159.8, 153.5, 139.5, 133.4, 132.0, 129.7, 127.2, 125.4, 123.4, 118.2, 114.6, 87.4, 55.6, 21.2. HRMS (ESI, *m*/*z*) calcd for $C_{19}H_{18}NO_4$ $[M+H]^+$: 324.123, found: 324.1229.

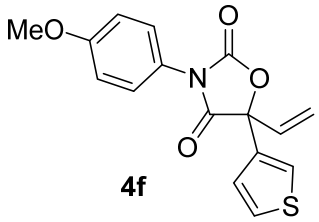
3-(4-methoxyphenyl)-5-(naphthalen-2-yl)-5-vinyloxazolidine-2,4-dione



4e

white solid, 832.8 mg, 46%, Mp: 142 – 144 °C. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.17 – 8.09 (d, *J* = 2.0 Hz, 1H), 7.93 – 7.80 (m, 3H), 7.73 – 7.66 (m, 1H), 7.55 – 7.46 (m, 2H), 7.35 – 7.29 (m, 2H), 7.02 – 6.91 (m, 2H), 6.40 – 6.30 (dd, *J* = 17.0, 11.0 Hz, 1H), 5.82 – 5.72 (d, *J* = 17.0 Hz, 1H), 5.59 – 5.49 (d, *J* = 11.0 Hz, 1H), 3.79 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 171.0, 159.9, 153.5, 133.4, 133.4, 132.9, 132.1, 129.1, 128.6, 127.8, 127.2, 126.9, 124.8, 123.3, 122.8, 118.6, 114.68, 87.5, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{22}H_{18}NO_4$ $[M+H]^+$: 360.123, found: 360.1228.

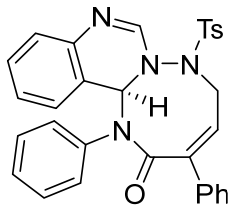
3-(4-methoxyphenyl)-5-(thiophen-3-yl)-5-vinyloxazolidine-2,4-dione



4f

yellow oil, 802.4 mg, 51%. ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.56 – 7.51 (m, 1H), 7.44 – 7.38 (m, 1H), 7.35 – 7.28 (m, 2H), 7.25 – 7.20 (m, 1H), 7.02 – 6.94 (m, 2H), 6.29 – 6.19 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.73 – 5.64 (d, *J* = 17.0 Hz, 1H), 5.53 – 5.46 (d, *J* = 10.5 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.6, 159.9, 153.3, 135.3, 132.9, 127.5, 127.1, 125.2, 123.4, 123.2, 118.4, 114.7, 86.0, 55.6. HRMS (ESI, *m*/*z*) calcd for $C_{16}H_{14}NO_4S$ $[M+H]^+$: 316.0638, found: 316.0635.

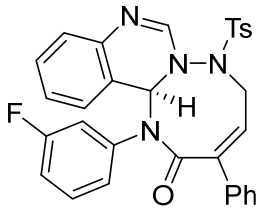
(*R*, *Z*)-1,3-diphenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3aa

colorless oil, 51.4 mg, 96%, 90% *ee*, $[\alpha]^{25}_{D}$ = 64.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.64 – 7.54 (m, 2H), 7.52 – 7.40 (m, 5H), 7.28 – 7.19 (m, 2H), 7.16 – 7.01 (m, 5H), 6.97 – 6.86 (m, 3H), 6.82 – 6.75 (m, 2H), 6.73 – 6.58 (d, *J* = 7.5 Hz, 2H), 5.14 – 5.03 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.43 – 4.32 (dd, *J* = 15.5, 10.5 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 146.5, 145.8, 141.7, 141.0, 136.2, 134.9, 133.0, 123.0, 129.9, 129.5, 129.4, 129.0, 128.9, 128.6, 128.5, 127.1, 126.6, 126.2, 126.0, 123.8, 119.9, 69.7, 49.1, 21.7. IR (film) ν_{max} = 2923, 1661, 1650, 1614, 1598, 1275, 1261, 1165, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{27}N_4O_3S$ $[M+H]^+$: 535.1798, found: 535.1799. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.7 min, t_{minor} = 17.3 min).

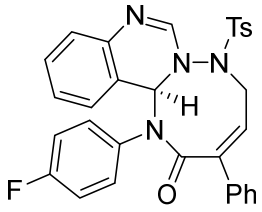
(*R*, *Z*)-1-(3-fluorophenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino [2,3-*c*]quinazolin-2-one



3ba

colorless oil, 44.2 mg, 80%, 90% *ee*, $[\alpha]^{25}_{D}$ = 80.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 – 7.55 (m, 2H), 7.52 – 7.41 (m, 5H), 7.30 – 7.22 (m, 2H), 7.12 – 7.07 (d, *J* = 8.0 Hz, 2H), 7.07 – 7.01 (m, 1H), 6.98 – 6.93 (m, 2H), 6.89 – 6.77 (m, 4H), 6.55 – 6.48 (d, *J* = 8.0 Hz, 1H), 6.39 – 6.30 (d, *J* = 9.5 Hz, 1H), 5.13 – 5.03 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.36 – 4.26 (dd, *J* = 15.5, 10.0 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.9, 162.1 (d, *J* = 246.5 Hz), 146.4, 145.9, 141.5, 140.9, 137.7 (d, *J* = 9.6 Hz), 134.8, 132.9, 130.2, 130.0, 129.7 (d, *J* = 8.9 Hz), 129.5, 129.1, 128.9, 127.0, 126.6, 126.5, 126.1, 125.3, 124.1, 119.5, 117.3 (d, *J* = 22.8 Hz), 115.7 (d, *J* = 20.8 Hz), 69.8, 49.1, 21.7. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 112.0. IR (film) ν_{max} = 2921, 1667, 1614, 1597, 1488, 1387, 1164, 1087, 765, 706. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{26}FN_4O_3S$ $[M+H]^+$: 553.1704, found: 553.1706. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.8 min, t_{minor} = 15.4 min).

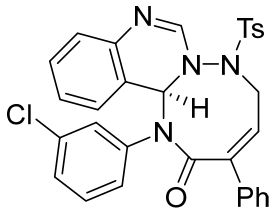
(*R*, *Z*)-1-(4-fluorophenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino [2,3-*c*]quinazolin-2-one



3ca

yellow oil, 49.2 mg, 89%, 91% *ee*, $[\alpha]^{25}_{D}$ = 72.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 – 7.53 (m, 2H), 7.51 – 7.48 (d, *J* = 2.0 Hz, 2H), 7.48 – 7.40 (m, 3H), 7.30 – 7.21 (m, 2H), 7.11 – 7.05 (d, *J* = 8.0 Hz, 2H), 6.99 – 6.90 (dd, *J* = 14.0, 8.0 Hz, 2H), 6.90– 6.86 (d, *J* = 1.5 Hz, 1H), 6.85 – 6.69 (m, 4H), 6.69 – 6.52 (m, 2H), 5.12 – 5.03 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.36 – 4.24 (dd, *J* = 15.5, 10.0 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 162.2 (d, *J* = 247.3 Hz), 146.4, 145.9, 141.6, 141.0, 134.8, 132.9, 132.1 (d, *J* = 3.3 Hz), 131.2, 130.1, 130.0, 129.4, 129.0, 128.8, 126.9, 126.6, 126.4, 126.1, 124.0, 119.8, 115.7 (d, *J* = 22.5 Hz), 69.7, 49.1, 21.7. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 112.5. IR (film) ν_{max} = 2922, 2851, 1662, 1615, 1598, 1508, 1389, 1165, 814, 764. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{26}FN_4O_3S$ $[M+H]^+$: 553.1704, found: 553.1702. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 12.1 min, t_{minor} = 25.8 min).

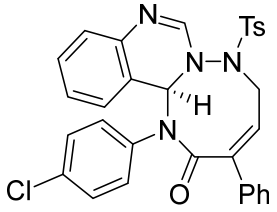
(*R*, *Z*)-1-(3-chlorophenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino [2,3-*c*]quinazolin-2-one



3da

colorless oil, 43.6 mg, 77%, 91% *ee*, $[\alpha]^{25}_{D}$ = 80.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 – 7.54 (m, 2H), 7.53 – 7.39 (m, 5H), 7.31 – 7.23 (m, 2H), 7.14 – 7.07 (m, 3H), 7.04 – 6.93 (m, 3H), 6.89 – 6.84 (m, 2H), 6.83– 6.77 (dd, *J* = 10.5, 7.0 Hz, 1H), 6.60 (s, 2H), 5.14 – 5.03 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.36 – 4.27 (dd, *J* = 15.5, 10.5 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.9, 146.3, 145.9, 141.4, 140.9, 137.4, 134.8, 133.9, 132.9, 130.3, 130.0, 129.5, 129.1, 128.9, 128.8, 127.8, 127.0, 126.6, 126.5, 126.1, 124.1, 119.5, 69.8, 49.1, 21.7. IR (film) ν_{max} = 2921, 2851, 1661, 1614, 1597, 1387, 1165, 765, 751, 729. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{26}{}^{35}ClN_4O_3S$ $[M+H]^+$: 569.1409, found: 569.1410. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.6 min, t_{minor} = 15.8 min).

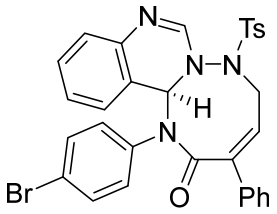
(*R*, *Z*)-1-(4-chlorophenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino [2,3-*c*]quinazolin-2-one



3ea

white solid, 52.3 mg, 91%, Mp: 195 – 197 °C, 92% *ee*, $[\alpha]^{25}_{D}$ = 72.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 – 7.51 (m, 2H), 7.51 – 7.37 (m, 5H), 7.31 – 7.18 (m, 2H), 7.12 – 7.05 (d, *J* = 8.0 Hz, 2H), 7.05 – 6.99 (d, *J* = 8.0 Hz, 2H), 6.99 – 6.94 (dd, *J* = 7.5, 1.0 Hz, 1H), 6.94 – 6.85 (m, 2H), 6.82 – 6.73 (m, 2H), 6.66 – 6.48 (m, 2H), 5.13 – 4.99 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.36 – 4.25 (dd, *J* = 15.0, 10.0 Hz, 1H), 2.31 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 146.4, 145.9, 141.5, 141.0, 134.8, 134.8, 134.5, 132.9, 130.8, 130.2, 130.0, 129.5, 129.1, 128.9, 128.8, 126.9, 126.6, 126.5, 126.2, 124.03, 119.6, 69.7, 49.1, 21.7. IR (film) ν_{max} = 2923, 2852, 1662, 1615, 1598, 1491, 1388, 1165, 1087, 764. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{26}{}^{35}ClN_4O_3S$ $[M+H]^+$: 569.1409, found: 569.1409. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 15.0 min, t_{minor} = 24.8 min).

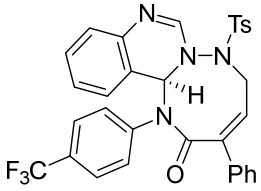
(*R*, *Z*)-1-(4-bromophenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino [2,3-*c*]quinazolin-2-one



3fa

yellow oil, 46.8 mg, 76%, 91% *ee*, $[\alpha]^{25}_{D}$ = 56.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.58 – 7.53 (m, 2H), 7.51 – 7.40 (m, 5H), 7.31 – 7.21 (m, 2H), 7.20 – 7.14 (d, *J* = 8.5 Hz, 2H), 7.11 – 7.05 (d, *J* = 8.0 Hz, 2H), 6.99 – 6.94 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.94 – 6.90 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.90 – 6.86 (d, *J* = 1.5 Hz, 1H), 6.82 – 6.75 (m, 2H), 6.58 – 6.49 (m, 2H), 5.17 – 4.93 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.38 – 4.19 (dd, *J* = 15.5, 10.0 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 146.4, 145.9, 141.5, 141.0, 135.3, 134.8, 132.9, 131.9, 131.1, 130.2, 130.0, 129.5, 129.1, 128.8, 126.9, 126.6, 126.4, 126.2, 124.0, 122.7, 119.6, 69.7, 49.1, 21.7. IR (film) ν_{max} = 2924, 1662, 1615, 1598, 1487, 1388, 1165, 1087, 764, 751. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{26}{}^{79}BrN_4O_3S$ $[M+H]^+$: 613.0903, found: 613.0897. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.6 min, t_{minor} = 25.4 min).

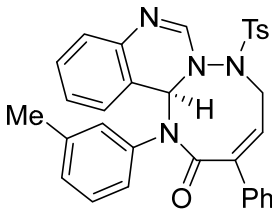
(*R*, *Z*)-3-phenyl-6-tosyl-1-(4-(trifluoromethyl)phenyl)-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ga

yellow oil, 42.5 mg, 71%, 90% *ee*, $[\alpha]^{25}_{D}$ = 56.0 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.61 – 7.54 (m, 2H), 7.52 – 7.41 (m, 5H), 7.35 – 7.20 (m, 4H), 7.13 – 7.04 (d, *J* = 8.5 Hz, 2H), 6.99 – 6.90 (dd, *J* = 16.5, 6.0 Hz, 2H), 6.88 (s, 2H), 6.85 – 6.75 (m, 3H), 5.12 – 5.04 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.37 – 4.27 (dd, *J* = 15.0, 10.0 Hz, 1H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 146.3, 146.0, 141.3, 140.9, 139.8, 134.7, 132.8, 130.4, 130.1, 130.0, 129.5, 129.1, 128.8, 126.9, 126.6, 126.5, 126.2, 125.7,125.7, 124.2, 123.6 (q, *J* = 270.9 Hz), 119.4, 69.8, 49.1, 21.6. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 62.8. IR (film) ν_{max} = 2922, 1665, 1615, 1598, 1388, 1324, 1165, 1064, 818, 765. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{26}F_3N_4O_3S$ $[M+H]^+$: 603.1672, found: 603.1670. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 21.3 min, t_{minor} = 26.4 min).

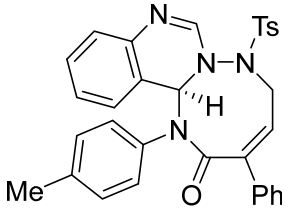
(*R*, *Z*)-3-phenyl-1-(*m*-tolyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ha

colorless oil, 51.4 mg, 94%, 92% *ee*, $[\alpha]^{25}_{D}$ = 72.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 – 7.55 (m, 2H), 7.54 – 7.48 (d, *J* = 8.5 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.28 – 7.20 (m, 2H), 7.11 – 7.05 (d, *J* = 8.0 Hz, 2H), 6.98 – 6.89 (m, 4H), 6.89 – 6.84 (d, *J* = 1.5 Hz, 1H), 6.82 – 6.75 (m, 2H), 6.55 – 6.30 (m, 2H), 5.12 – 5.01 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.42 – 4.34 (dd, *J* = 15.0, 10.5 Hz, 1H), 2.32 (s, 3H), 2.08 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 146.4, 145.8, 141.8, 141.1, 138.4, 136.0, 134.9, 133.0, 123.0, 129.9, 129.3, 129.2, 129.0, 128.9, 128.4, 127.1, 126.7, 126.5, 126.2, 125.9, 123.7, 112.0, 69.7, 49.1, 21.6, 21.0. IR (film) ν_{max} = 2961, 2923, 2853, 1660, 1597, 1388, 1260, 1161, 1087, 1017, 801. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{29}N_4O_3S$ $[M+H]^+$: 549.1955, found: 549.1950. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 7.0 min, t_{minor} = 15.2 min).

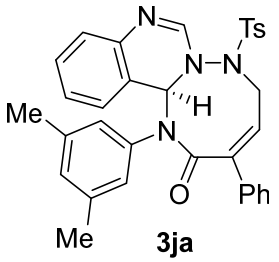
(*R*, *Z*)-3-phenyl-1-(*p*-tolyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ia

colorless oil, 51.3 mg, 94%, 90% *ee*, $[\alpha]^{25}_{D}$ = 53.3 (*c* 0.75, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.53 (m, 2H), 7.51 – 7.47 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.38 (m, 3H), 7.28 – 7.19 (m, 2H), 7.09 – 7.04 (d, *J* = 8.0 Hz, 2H), 6.96 – 6.88 (m, 3H), 6.87 – 6.80 (d, *J* = 8.0 Hz, 2H), 6.79 – 6.70 (m, 2H), 6.60 – 6.41 (m, 2H), 5.17 – 4.94 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.48 – 4.28 (dd, *J* = 15.5, 10.0 Hz, 1H), 2.31 (s, 3H), 2.17 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 146.5, 145.7, 141.8, 141.1, 138.3, 134.9, 133.4, 133.1, 123.0, 129.9, 129.4, 129.3, 129.1, 129.0, 128.9, 127.0, 126.6, 126.2, 126.0, 123.7, 120.1, 69.7, 49.0, 21.6, 21.1. IR (film) ν_{max} = 2922, 1661, 1615, 1598, 1510, 1387, 1275, 1261, 1165, 1087, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{29}N_4O_3S$ $[M+H]^+$: 549.1955, found: 549.1953. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 12.8 min, t_{minor} = 22.8 min).

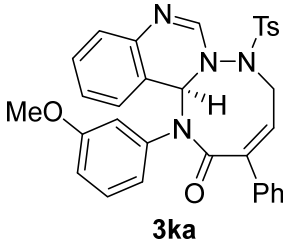
(*R*, *Z*)-1-(3,5-dimethylphenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ja

white solid, 53.3 mg, 95%, Mp: 214 – 216 °C, 91% *ee*, $[\alpha]^{25}_{D}$ = 56.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.61 – 7.55 (d, *J* = 7.0 Hz, 2H), 7.53 – 7.47 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.38 (m, 3H), 7.27 – 7.19 (m, 2H), 7.10 – 7.03 (d, *J* = 8.0 Hz, 2H), 6.96 – 6.89 (d, *J* = 8.0 Hz, 2H), 6.88 – 6.83 (d, *J* = 1.5 Hz, 1H), 6.80 – 6.70 (m, 3H), 6.38 – 6.05 (m, 2H), 5.16 – 4.95 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.48 – 4.27 (dd, *J* = 15.0, 10.0 Hz, 1H), 2.30 (s, 3H), 2.04 (s, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.9, 146.4, 145.7, 141.8, 141.1, 138.1, 135.7, 135.0, 133.1, 130.1, 130.0, 129.8, 129.3, 129.0, 128.9, 127.1, 126.7, 126.1, 125.9, 123.7, 120.0, 69.8, 49.0, 21.6, 20.9. IR (film) ν_{max} = 2922, 2852, 1662, 1597, 1389, 1358, 1164, 1089, 815, 765. HRMS (ESI, *m*/*z*) calcd for $C_{33}H_{31}N_4O_3S$ $[M+H]^+$: 563.2111, found: 563.2114. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 5.7 min, t_{minor} = 12.8 min).

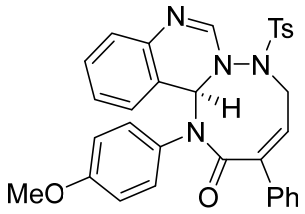
(*R*, *Z*)-1-(3-methoxyphenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ka

colorless oil, 49.9 mg, 88%, 93% *ee*, $[\alpha]^{25}_{D}$ = 88.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.61 – 7.55 (m, 2H), 7.52 – 7.48 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.40 (m, 3H), 7.29 – 7.20 (m, 2H), 7.11 – 7.06 (d, *J* = 8.0 Hz, 2H), 7.02 – 6.92 (m, 3H), 6.87 (s, 1H), 6.83 – 6.80 (d, *J* = 1.5 Hz, 1H), 6.80 – 6.74 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.70 – 6.64 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.35 (s, 1H), 6.07 (s, 1H), 5.18 – 4.93 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.44 – 4.24 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.9, 159.4, 146.5, 145.8, 141.7, 141.2, 137.1, 134.9, 133.0, 130.0, 129.4, 129.3, 129.0, 128.9, 127.1, 126.7, 126.2, 126.1, 123.9, 121.8, 119.9, 115.2, 114.6, 69.8, 55.2, 49.0, 21.7. IR (film) ν_{max} = 2923, 1662, 1614, 1598, 1490, 1389, 1229, 1163, 1088, 1037, 765, 706. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{29}N_4O_4S$ $[M+H]^+$: 565.1904, found: 565.1906. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.9 min, t_{minor} = 18.2 min).

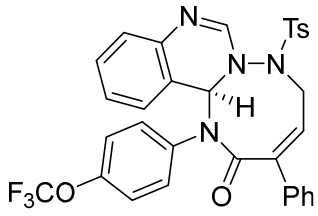
(*R*, *Z*)-1-(4-methoxyphenyl)-3-phenyl-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino [2,3-*c*]quinazolin-2-one



3la

yellow oil, 48.6 mg, 86%, 90% *ee*, $[\alpha]^{25}_{D}$ = 40.0 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.53 (m, 2H), 7.52 – 7.47 (d, *J* = 8.0 Hz, 2H), 7.47 – 7.39 (m, 3H), 7.28 – 7.19 (m, 2H), 7.09 – 7.04 (d, *J* = 8.5 Hz, 2H), 6.98 – 6.93 (dd, *J* = 7.5, 1.5 Hz, 1H), 6.92 – 6.87 (m, 2H), 6.78 – 6.71 (m, 2H), 6.56 (s, 4H), 5.15 – 4.96 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.39 – 4.29 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.65 (s, 3H), 2.31 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.2, 159.2, 146.5, 145.7, 141.9, 141.0, 134.9, 133.1, 130.4, 130.0, 129.9, 129.3, 129.0, 128.9, 128.5, 126.9, 126.6, 126.2, 126.0, 123.7, 120.0, 114.0, 69.7, 55.2, 49.1, 21.6. IR (film) ν_{max} = 2924, 1661, 1614, 1598, 1510, 1389, 1357, 1243, 1164, 1087, 809, 764. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{29}N_4O_4S$ $[M+H]^+$: 565.1904, found: 565.1902. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 18.7 min, t_{minor} = 35.1 min).

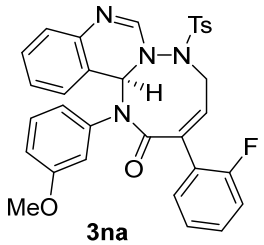
(*R*, *Z*)-3-phenyl-6-tosyl-1-(4-(trifluoromethoxy)phenyl)-1,5,6,13b-tetrahydro-2*H*-[1,2,4] triazocino[2,3-*c*]quinazolin-2-one



3ma

colorless oil, 40.2 mg, 65%, 90% *ee*, $[\alpha]^{25}_{D}$ = 160.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 – 7.55 (m, 2H), 7.52 – 7.41 (m, 5H), 7.29 – 7.21 (m, 2H), 7.12 – 7.06 (d, *J* = 8.0 Hz, 2H), 6.97 – 6.91 (m, 2H), 6.91 – 6.84 (m, 4H), 6.83 – 6.78 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.75 – 6.62 (m, 2H), 5.13 – 5.04 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.36 – 4.26 (dd, *J* = 15.0, 10.0 Hz, 1H), 2.33 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 148.8, 146.3, 145.9, 141.4, 140.9, 134.7, 132.8, 131.0, 130.2, 130.0, 129.5, 129.1, 128.8, 126.9, 126.6, 126.5, 126.1, 124.1, 120.9, 120.2 (q, *J* = 256.5 Hz), 119.6, 69.8, 49.1, 21.7. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 57.9. IR (film) ν_{max} = 2924, 1666, 1615, 1598, 1507, 1260, 1165, 1087, 764, 704. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{26}F_3N_4O_4S$ $[M+H]^+$: 619.1621, found: 619.1619. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.1 min, t_{minor} = 11.1 min).

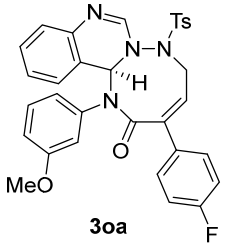
(*R*, *Z*)-3-(2-fluorophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4] triazocino[2,3-*c*]quinazolin-2-one



3na

yellow oil, 35.2 mg, 60%, 96% *ee*, $[\alpha]^{25}_{D}$ = - 32.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.36 (m, 4H), 7.30 – 7.20 (m, 3H), 7.18 – 7.10 (m, 2H), 7.03 – 6.92 (m, 5H), 6.82 – 6.77 (d, *J* = 2.0 Hz, 1H), 6.76 – 6.69 (dd, *J* = 9.5, 7.0 Hz, 1H), 6.67 – 6.60 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.41 – 6.33 (d, *J* = 7.5 Hz, 1H), 6.14 (s, 1H), 5.08 – 4.99 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.43 – 4.30 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.52 (s, 3H), 2.31 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.0, 159.9 (d, *J* = 245.1 Hz), 159.2, 146.5, 145.8, 141.0, 138.2, 137.5, 132.9, 131.1 (d, *J* = 8.5 Hz), 130.3 (d, *J* = 3.3 Hz), 129.9, 129.9, 129.1, 128.9, 127.9, 127.3 (d, *J* = 5.4 Hz), 126.2, 126.0, 125.1 (d, *J* = 3.1 Hz), 124.8 (d, *J* = 13.1 Hz), 121.6, 120.1, 115.5 (d, *J* = 21.1 Hz), 115.0, 114.6, 69.4, 55.2, 48.6, 21.6. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 114.3. IR (film) ν_{max} = 2922, 1661, 1599, 1574, 1488, 1394, 1261, 1165, 764, 750. HRMS (ESI, *m*/z) calcd for $C_{32}H_{28}FN_4O_4S$ $[M+H]^+$: 583.181, found: 583.1813. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.3 min, t_{minor} = 19.7 min).

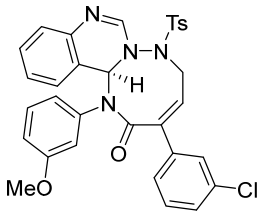
(*R*, *Z*)-3-(4-fluorophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4] triazocino[2,3-*c*]quinazolin-2-one



3oa

yellow oil, 55.1 mg, 95%, 93% *ee*, $[\alpha]^{25}_{D}$ = 96.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.64 – 7.57 (m, 2H), 7.53 – 7.46 (d, *J* = 8.0 Hz, 2H), 7.29 – 7.20 (m, 2H), 7.17 – 7.07 (m, 4H), 7.01 – 6.91 (m, 3H), 6.89 – 6.85 (d, *J* = 1.5 Hz, 1H), 6.85 – 6.78 (d, *J* = 2.0 Hz, 1H), 6.76 – 6.70 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.69 – 6.64 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.34 (s, 1H), 6.06 (s, 1H), 5.08 – 5.01 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.39 – 4.29 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.50 (s, 3H), 2.33 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.7, 163.4 (d, *J* = 248.3 Hz), 159.4, 146.4, 145.9, 141.1, 140.5, 137.0, 132.9, 131.1 (d, *J* = 3.3 Hz), 130.0, 130.0, 129.3, 128.9, 128.7, 128.6, 127.1, 126.2, 126.1, 124.0, 121.7, 119.8, 116.1, 115.9, 115.2, 114.6, 69.8, 55.2, 48.9, 21.7. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 111.6. IR (film) ν_{max} = 2922, 1661, 1599, 1508, 1387, 1231, 1163, 1088, 764, 750. HRMS (ESI, *m*/z) calcd for $C_{32}H_{28}FN_4O_4S$ $[M+H]^+$: 583.181, found: 583.1808. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 9.9 min, t_{minor} = 19.0 min).

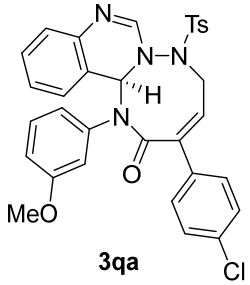
(*R*, *Z*)-3-(3-chlorophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4] triazocino[2,3-*c*]quinazolin-2-one



3pa

yellow oil, 54.2 mg, 91%, 92% *ee*, $[\alpha]^{25}_{D}$ = 96.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.58 – 7.55 (m, 1H), 7.54 – 7.48 (m, 3H), 7.42 – 7.34 (m, 2H), 7.30 – 7.23 (m, 2H), 7.16 – 7.11 (d, *J* = 8.0 Hz, 2H), 7.03 – 6.92 (m, 3H), 6.90 – 6.86 (d, *J* = 1.5 Hz, 1H), 6.82 – 6.74 (m, 2H), 6.71 – 6.65 (dd, *J* = 8.0, 2.5 Hz, 1H), 6.33 (s, 1H), 6.06 (s, 1H), 5.12 – 5.03 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.40 – 4.29 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.52 (s, 3H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.2, 159.4, 146.4, 146.0, 141.1, 140.4, 136.9, 136.7, 135.0, 133.0, 130.3, 130.1, 129.4, 129.3, 128.9, 127.1, 126.6, 126.3, 126.1, 125.4, 125.0, 121.7, 119.8, 115.2, 114.7, 69.76, 55.2, 48.8, 21.7. IR (film) ν_{max} = 2921, 2851, 1661, 1615, 1598, 1387, 1276, 1261, 1164, 764, 751. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{28}{}^{35}ClN_4O_4S$ $[M+H]^+$: 599.1514, found: 599.1518. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 8.8 min, t_{minor} = 15.5 min).

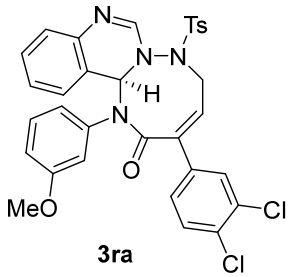
(*R*, *Z*)-3-(4-chlorophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4] triazocino[2,3-*c*]quinazolin-2-one



3qa

yellow solid, 51.5 mg, 86%, Mp: 115 – 117 °C, 96% *ee*, $[\alpha]^{25}_{D}$ = 112.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.54 (m, 2H), 7.52 – 7.48 (m, 2H), 7.45 – 7.39 (m, 2H), 7.29 – 7.21 (m, 2H), 7.14 – 7.09 (d, *J* = 8.0 Hz, 2H), 7.02 – 6.92 (m, 3H), 6.89 – 6.86 (d, *J* = 1.5 Hz, 1H), 6.83 – 6.75 (m, 2H), 6.70 – 6.65 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.33 (s, 1H), 6.05 (s, 1H), 5.10 – 5.02 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.39 – 4.31 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 159.4, 146.4, 145.9, 141.1, 140.5, 137.0, 135.5, 133.3, 132.8, 130.0, 129.3, 129.2, 128.9, 128.04, 127.1, 126.3, 126.1, 124.6, 121.7, 119.8, 115.2, 114.6, 69.8, 55.2, 48.9, 21.7. IR (film) ν_{max} = 2922, 2851, 1662, 1615, 1598, 1491, 1387, 1356, 1231, 1163, 763. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{28}{}^{35}ClN_4O_4S$ $[M+H]^+$: 599.1514, found: 599.1509. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 13.6 min, t_{minor} = 26.2 min).

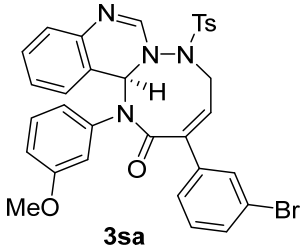
(*R*, *Z*)-3-(3,4-dichlorophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ra

yellow oil, 57.3 mg, 91%, 95% *ee*, $[\alpha]^{25}_{D}$ = 160.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.75 – 7.66 (d, *J* = 1.5 Hz, 1H), 7.56 – 7.45 (m, 4H), 7.31 – 7.22 (m, 2H), 7.20 – 7.11 (d, *J* = 8.0 Hz, 2H), 7.05 – 6.91 (m, 3H), 6.88 – 6.81 (m, 2H), 6.80 – 6.74 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.72 – 6.62 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.32 (s, 1H), 6.04 (s, 1H), 5.11 – 5.02 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.40 – 4.29 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H), 2.37 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 166.9, 159.4, 146.4, 146.1, 141.1, 139.5, 136.8, 134.9, 133.6, 133.2, 132.8, 130.9, 130.1, 129.3, 128.8, 128.5, 127.1, 126.3, 126.2, 125.9, 121.6, 119.6, 115.1, 114.7, 69.8, 55.2, 48.7, 21.7. IR (film) ν_{max} = 2920, 1661, 1599, 1574, 1489, 1375, 1275, 1261, 1164, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{27}{}^{35}Cl_2N_4O_4S$ $[M+H]^+$: 633.1125, found: 633.1123. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 70 : 30, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 23.8 min, t_{minor} = 28.6 min).

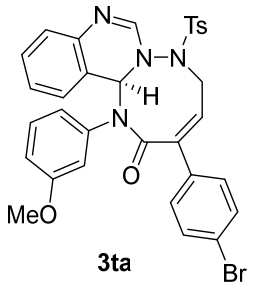
(*R*, *Z*)-3-(3-bromophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3sa

yellow oil, 53.4 mg, 83%, 94% *ee*, $[\alpha]^{25}_{D}$ = 104.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.75 – 7.70 (m, 1H), 7.58 – 7.54 (dd, *J* = 8.0, 2.0 Hz, 2H), 7.53 – 7.49 (d, *J* = 8.5 Hz, 2H), 7.34 – 7.22 (m, 3H), 7.17 – 7.10 (d, *J* = 8.5 Hz, 2H), 7.03 – 6.92 (m, 3H), 6.91 – 6.87 (d, *J* = 1.5 Hz, 1H), 6.80 – 6.73 (m, 2H), 6.71 – 6.66 (dd, *J* = 8.5, 3.0 Hz, 1H), 6.33 (s, 1H), 6.05 (s, 1H), 5.11 – 5.03 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.39 – 4.29 (dd, *J* = 15.5, 10.0 Hz, 1H), 3.52 (s, 3H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.2, 159.4, 146.4, 146.0, 141.1, 140.3, 137.0, 136.9, 132.9, 132.3, 130.5, 130.1, 129.5, 129.3, 128.9, 127.1, 126.3, 126.1, 125.5, 125.5, 123.1, 121.7, 119.7, 115.2, 114.7, 69.8, 55.2, 48.8, 21.7. IR (film) ν_{max} = 2920, 1661, 1598, 1489, 1387, 1276, 1261, 1164, 1088, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{28}{}^{79}BrN_4O_4S$ $[M+H]^+$: 643.1009, found: 643.1004. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 9.4 min, t_{minor} = 17.1 min).

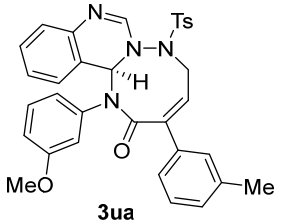
(*R*, *Z*)-3-(4-bromophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ta

yellow oil, 59.9 mg, 93%, 94% *ee*, $[\alpha]^{25}_{D}$ = 152.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 – 7.55 (m, 2H), 7.54 – 7.45 (m, 4H), 7.30 – 7.21 (m, 2H), 7.15 – 7.08 (d, *J* = 8.0 Hz, 2H), 7.02 – 6.92 (m, 3H), 6.89 – 6.85 (d, *J* = 2.0 Hz, 1H), 6.83 – 6.76 (m, 2H), 6.70 – 6.64 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.32 (s, 1H), 6.05 (s, 1H), 5.10 – 5.01 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.39 – 4.30 (dd, *J* = 15.5, 10.0 Hz, 1H), 3.51 (s, 3H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 159.4, 146.4, 145.9, 141.1, 140.6, 137.0, 133.8, 132.8, 132.2, 130.0, 129.3, 128.9, 128.3, 127.1, 126.3, 126.1, 124.7, 123.7, 121.7, 119.8, 115.2, 114.6, 69.8, 55.2, 48.9, 21.7. IR (film) ν_{max} = 2923, 1660, 1598, 1573, 1489, 1386, 1260, 1163, 1087, 764. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{28}{}^{79}BrN_4O_4S$ $[M+H]^+$: 643.1009, found: 643.1004. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 15.3 min, t_{minor} = 28.3 min).

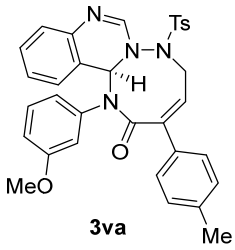
(*R*, *Z*)-1-(3-methoxyphenyl)-3-(*m*-tolyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ua

yellow oil, 51.6 mg, 89%, 92% *ee*, $[\alpha]^{25}_{D}$ = 72.0 (*c* 1.0, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.48 (d, *J* = 8.5 Hz, 2H), 7.43 – 7.40 (d, *J* = 1.0 Hz, 1H), 7.38 – 7.31 (m, 2H), 7.29 – 7.21 (m, 3H), 7.11 – 7.06 (d, *J* = 8.0 Hz, 2H), 7.01 – 6.93 (m, 3H), 6.88 – 6.85 (d, *J* = 1.5 Hz, 1H), 6.85 – 6.81 (d, *J* = 2.0 Hz, 1H), 6.79 – 6.72 (dd, *J* = 10.5, 7.0 Hz, 1H), 6.70 – 6.65 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.35 (s, 1H), 6.07 (s, 1H), 5.10 – 5.03 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.41 – 4.30 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.52 (s, 3H), 2.43 (s, 3H), 2.33 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 159.4, 146.5, 145.7, 141.8, 141.2, 138.7, 137.1, 134.8, 133.0, 130.2, 130.0, 130.0, 129.3, 128.9, 127.2, 127.1, 126.2, 126.0, 123.9, 123.7, 121.8, 120.0, 115.2, 114.5, 69.8, 55.2, 49.0, 21.7, 21.6. IR (film) ν_{max} = 2922, 1663, 1614, 1598, 1490, 1387, 1235, 1163, 1088, 765, 707. HRMS (ESI, *m*/*z*) calcd for $C_{33}H_{31}N_4O_4S$ $[M+H]^+$: 579.2061, found: 579.2065. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 7.9 min, t_{minor} = 16.2 min).

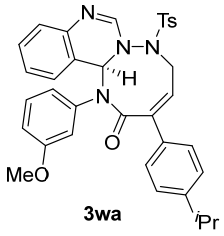
(*R*, *Z*)-1-(3-methoxyphenyl)-3-(*p*-tolyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3va

yellow oil, 53.5 mg, 93%, 93% *ee*, $[\alpha]^{25}_{D}$ = 104.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.44 (dd, *J* = 11.5, 8.5 Hz, 4H), 7.29 – 7.20 (m, 4H), 7.11 – 7.05 (d, *J* = 8.0 Hz, 2H), 7.02 – 6.90 (m, 3H), 6.88 – 6.85 (d, *J* = 1.5 Hz, 1H), 6.83 – 6.79 (d, *J* = 2.0 Hz, 1H), 6.76 – 6.70 (dd, *J* = 10.5, 7.0 Hz, 1H), 6.70 – 6.64 (m, 1H), 6.34 (s, 1H), 6.06 (s, 1H), 5.11 – 5.01 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.40 – 4.30 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H), 2.41 (s, 3H), 2.32 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 159.4, 146.6, 145.7, 141.6, 141.2, 139.5, 137.2, 133.1, 132.0, 130.0, 129.9, 129.7, 129.3, 128.9, 127.1, 126.5, 126.1, 126.0, 122.8, 121.8, 120.0, 115.2, 114.6, 69.7, 55.2, 49.1, 21.6, 21.3. IR (film) ν_{max} = 2922, 1663, 1614, 1598, 1387, 1231, 1163, 1088, 764, 706. HRMS (ESI, *m*/*z*) calcd for $C_{33}H_{31}N_4O_4S$ $[M+H]^+$: 579.2061, found: 579.2063. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 13.5 min, t_{minor} = 42.9 min).

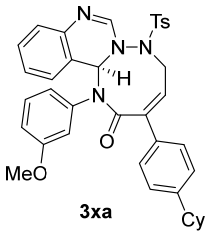
(*R*, *Z*)-3-(4-isopropylphenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3wa

white solid, 51.4 mg, 85%, Mp: 212 – 214 °C, 90% *ee*, $[\alpha]^{25}_{D}$ = 96.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.54 – 7.45 (m, 4H), 7.34 – 7.29 (d, *J* = 8.5 Hz, 2H), 7.29 – 7.21 (m, 2H), 7.10 – 7.03 (d, *J* = 8.5 Hz, 2H), 7.01 – 6.92 (m, 3H), 6.89 – 6.84 (d, *J* = 2.0 Hz, 1H), 6.82 – 6.78 (d, *J* = 2.0 Hz, 1H), 6.78 – 6.71 (dd, *J* = 10.0, 6.5 Hz, 1H), 6.70 – 6.64 (m, 1H), 6.35 (s, 1H), 6.07 (s, 1H), 5.10 – 5.00 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.40 – 4.30 (dd, *J* = 15.5, 10.0 Hz, 1H), 3.51 (s, 3H), 3.02 – 2.92 (m, 1H), 2.31 (s, 3H), 1.34 – 1.26 (dd, *J* = 6.5, 1.5 Hz, 6H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 159.4, 150.3, 146.6, 145.7, 141.6, 141.2, 137.2, 133.1, 132.4, 130.0, 129.9, 129.2, 128.9, 127.1, 127.1, 126.6, 126.1, 126.0, 122.8, 121.8, 120.0, 115.2, 114.6, 69.8, 55.2, 49.1, 34.0, 23.9, 21.6. IR (film) ν_{max} = 2960, 1667, 1598, 1387, 1362, 1275, 1261, 1164, 1088, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{35}H_{35}N_4O_4S$ $[M+H]^+$: 607.2374, found: 607.2375. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.2 min, t_{minor} = 32.4 min).

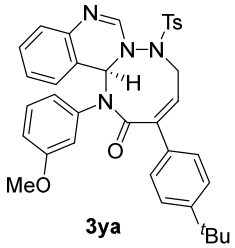
(*R*, *Z*)-3-(4-cyclohexylphenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3xa

yellow oil, 61.1 mg, 95%, 88% *ee*, $[\alpha]^{25}_{D}$ = 112.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.43 (m, 4H), 7.31 – 7.20 (m, 4H), 7.09 – 7.03 (d, *J* = 8.5 Hz, 2H), 7.02 – 6.92 (m, 3H), 6.89 – 6.85 (d, *J* = 1.5 Hz, 1H), 6.80 – 6.76 (d, *J* = 2.0 Hz, 1H), 6.76 – 6.71 (dd, *J* = 10.5, 7.0 Hz, 1H), 6.70 – 6.63 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.35 (s, 1H), 6.07 (s, 1H), 5.11 – 5.00 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.42 – 4.29 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H), 2.63 – 2.50 (m, 1H), 2.30 (s, 3H), 1.96 – 1.83 (m, 4H), 1.81 – 1.74 (m, 1H), 1.52 – 1.38 (m, 4H), 1.33 – 1.25 (m, 1H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 159.4, 149.5, 146.6, 145.7, 141.6, 141.2, 137.2, 133.1, 132.3, 130.0, 129.9, 129.2, 128.9, 127.5, 127.1, 126.6, 126.1, 126.0, 122.8, 121.8, 120.0, 115.2, 114.6, 69.7, 55.2, 49.1, 44.4, 34.4, 26.9, 26.1, 21.7. IR (film) ν_{max} = 2923, 2851, 1667, 1614, 1598, 1387, 1276, 1261, 1164, 1088, 764, 750. HRMS (ESI, *m*/z) calcd for $C_{38}H_{39}N_4O_4S$ $[M+H]^+$: 647.2687, found: 647.2691. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 27.2 min, t_{minor} = 66.9 min).

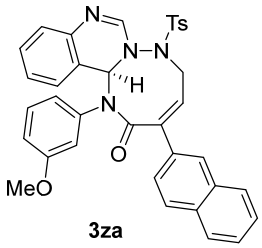
(*R*, *Z*)-3-(4-(tert-butyl)phenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3ya

white solid, 51.1 mg, 82%, Mp: 218 – 220 °C, 90% *ee*, $[\alpha]^{25}_{D}$ = 96.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.44 (m, 6H), 7.29 – 7.21 (m, 2H), 7.09 – 7.04 (d, *J* = 8.0 Hz, 2H), 7.01 – 6.93 (m, 3H), 6.88 – 6.84 (m, 1H), 6.83 – 6.79 (d, *J* = 1.5 Hz, 1H), 6.79 – 6.73 (dd, *J* = 10.5, 7.0 Hz, 1H), 6.71 – 6.65 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.36 (s, 1H), 6.07 (s, 1H), 5.10 – 5.01 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.40 – 4.32 (dd, *J* = 15.0, 10.5 Hz, 1H), 3.52 (s, 3H), 2.31 (s, 3H), 1.37 (s, 9H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.1, 159.4, 152.6, 146.6, 145.7, 141.5, 141.2, 137.2, 133.1, 132.0, 130.0, 129.9, 129.2, 128.9, 127.1, 126.3, 126.1, 126.0, 126.0, 122.9, 121.8, 120.0, 115.2, 114.6, 69.8, 55.2, 49.1, 34.8, 31.3, 21.6. IR (film) ν_{max} = 2961, 1666, 1598, 1387, 1275, 1262, 1232, 1164, 764, 750. HRMS (ESI, *m*/z) calcd for $C_{36}H_{37}N_4O_4S$ $[M+H]^+$: 621.253, found: 621.2533. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 15.1 min, t_{minor} = 28.9 min).

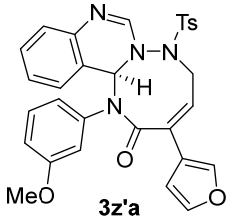
(*R*, *Z*)-1-(3-methoxyphenyl)-3-(naphthalen-2-yl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]-triazocino[2,3-*c*]quinazolin-2-one



3za

yellow oil, 58.8 mg, 96%, 94% *ee*, $[\alpha]^{25}_{D}$ = 128.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 8.11 – 8.01 (d, *J* = 2.0 Hz, 1H), 7.97 – 7.83 (m, 3H), 7.76 – 7.68 (dd, *J* = 8.5, 1.5 Hz, 1H), 7.58 – 7.44 (m, 4H), 7.28 – 7.23 (m, 1H), 7.23 – 7.17 (m, 1H), 7.10 – 7.04 (d, *J* = 8.0 Hz, 2H), 7.04 – 6.98 (t, *J* = 8.0 Hz, 1H), 6.98 – 6.86 (m, 5H), 6.71 – 6.66 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.39 (s, 1H), 6.10 (s, 1H), 5.17 – 5.07 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.47 – 4.37 (dd, *J* = 15.0, 10.5 Hz, 1H), 3.52 (s, 3H), 2.25 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.0, 159.4, 146.6, 145.8, 141.6, 141.1, 137.1, 133.6, 133.4, 133.0, 131.9, 130.0, 129.3, 128.9, 128.8, 128.7, 127.7, 127.1, 127.0, 126.7, 126.6, 126.2, 126.0, 124.1, 123.7, 121.8, 119.9, 115.3, 114.6, 69.8, 55.2, 49.1, 21.6. IR (film) ν_{max} = 3055, 2923, 1661, 1614, 1598, 1391, 1237, 1087, 764, 724. HRMS (ESI, *m*/*z*) calcd for $C_{36}H_{31}N_4O_4S$ $[M+H]^+$: 615.2061, found: 615.2058. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 15.0 min, t_{minor} = 46.8 min).

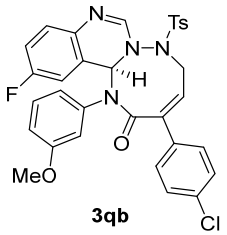
(*R*, *Z*)-1-(3-methoxyphenyl)-3-(thiophen-3-yl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]-triazocino[2,3-*c*]quinazolin-2-one



3z'a

white solid, 51.8 mg, 91%, Mp: 117 – 119 °C, 90% *ee*, $[\alpha]^{25}_{D}$ = 88.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.57 – 7.53 (dd, *J* = 3.0, 1.5 Hz, 1H), 7.53 – 7.48 (m, 2H), 7.42 – 7.38 (dd, *J* = 5.0, 3.0 Hz, 1H), 7.38 – 7.34 (dd, *J* = 5.0, 1.0 Hz, 1H), 7.28 – 7.19 (m, 2H), 7.13 – 7.08 (d, *J* = 8.0 Hz, 2H), 7.01 – 6.93 (m, 2H), 6.93 – 6.89 (dd, *J* = 7.5, 2.0 Hz, 1H), 6.88 – 6.86 (d, *J* = 1.5 Hz, 1H), 6.78 – 6.75 (d, *J* = 1.5 Hz, 1H), 6.75 – 6.70 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.70 – 6.65 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.33 (s, 1H), 6.05 (s, 1H), 5.09 – 5.01 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.38 – 4.30 (dd, *J* = 15.5, 10.0 Hz, 1H), 3.51 (s, 3H), 2.34 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 159.4, 146.5, 145.8, 141.2, 137.1, 136.9, 136.0, 133.0, 130.1, 130.0, 129.3, 128.8, 127.1, 126.8, 126.1, 126.0, 125.3, 124.6, 122.5, 121.7, 119.9, 115.2, 114.6, 69.7, 55.2, 48.9, 21.7. IR (film) ν_{max} = 2921, 1661, 1598, 1489, 1355, 1276, 1261, 1088, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{30}H_{27}N_4O_4S_2$ $[M+H]^+$: 571.1468, found: 571.1467. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 11.7 min, t_{minor} = 24.9 min).

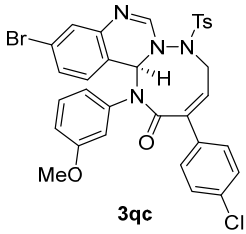
(*R*, *Z*)-3-(4-chlorophenyl)-12-fluoro-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qb

yellow oil, 52.0 mg, 84%, 96% *ee*, $[\alpha]^{25}_{D}$ = 104.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.54 (m, 2H), 7.53 – 7.49 (m, 2H), 7.46 – 7.41 (m, 2H), 7.17 – 7.12 (d, *J* = 8.0 Hz, 2H), 7.03 – 6.89 (m, 3H), 6.88 – 6.83 (d, *J* = 1.5 Hz, 1H), 6.81 – 6.76 (m, 2H), 6.72 – 6.68 (dd, *J* = 8.5, 3.0 Hz, 1H), 6.68 – 6.63 (dd, *J* = 8.0, 2.5 Hz, 1H), 6.34 (s, 1H), 6.15 (s, 1H), 5.09 – 4.99 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.36 – 4.27 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.56 (s, 3H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 160.6 (d, *J* = 245.9 Hz), 159.5, 146.1, 145.8, 140.3, 137.6 (d, *J* = 2.8 Hz), 136.9, 135.6, 133.1, 132.7, 130.1, 129.4, 129.3, 128.8, 128.0, 127.9, 124.6, 121.7, 120.9 (d, *J* = 7.8 Hz), 117.4 (d, *J* = 22.4 Hz), 115.2, 114.6, 113.1 (d, *J* = 23.1 Hz), 69.4, 55.2, 48.9, 21.7. ^{19}F NMR ($CDCl_3$, 470 MHz): δ = – 114.6. IR (film) ν_{max} = 2961, 2922, 2852, 1661, 1604, 1490, 1385, 1260, 1162, 1088, 1014, 800, 762. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{27}{}^{35}ClFN_4O_4S$ $[M+H]^+$: 617.142, found: 617.1418. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 13.0 min, t_{minor} = 33.4 min).

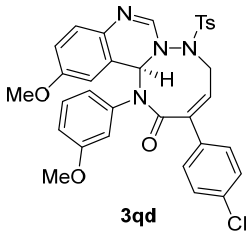
(*R*, *Z*)-11-bromo-3-(4-chlorophenyl)-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qc

yellow oil, 44.4 mg, 66%, 93% *ee*, $[\alpha]^{25}_{D}$ = 96.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.59 – 7.54 (m, 2H), 7.53 – 7.48 (d, *J* = 8.5 Hz, 2H), 7.44 – 7.39 (m, 2H), 7.38 – 7.32 (dd, *J* = 8.0, 2.0 Hz, 1H), 7.18 – 7.12 (d, *J* = 8.0 Hz, 2H), 7.12 – 7.08 (d, *J* = 2.0 Hz, 1H), 7.05 – 6.97 (t, *J* = 8.0 Hz, 1H), 6.91 – 6.88 (d, *J* = 1.5 Hz, 1H), 6.86 – 6.82 (d, *J* = 8.5 Hz, 1H), 6.81 – 6.75 (m, 2H), 6.74 – 6.68 (dd, *J* = 8.0, 7.0 Hz, 1H), 6.31 (s, 1H), 6.07 (s, 1H), 5.08 – 5.00 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.36 – 4.27 (dd, *J* = 15.5, 10.0 Hz, 1H), 3.55 (s, 3H), 2.36 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 159.6, 147.3, 146.2, 142.4, 140.4, 136.8, 135.6, 133.2, 132.6, 130.1 129.5, 129.3, 129.2, 128.9, 128.9, 128.5, 128.0, 124.7, 123.5, 121.7, 118.8, 115.2, 114.7, 69.4, 55.2, 48.9, 21.7. IR (film) ν_{max} = 2922, 1667, 1606, 1589, 1490, 1386, 1275, 1261, 1163, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{27}{}^{79}Br^{35}ClN_4O_4S$ $[M+H]^+$: 677.0619, found: 677.0618. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 60 : 40, *v* = 1.0 mL/min, λ = 254.0 nm; t_{minor} = 14.7 min, t_{major} = 21.7 min).

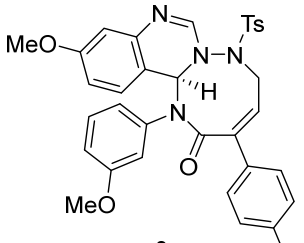
(*R*, *Z*)-3-(4-chlorophenyl)-12-methoxy-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qd

yellow oil, 57.3 mg, 91%, 92% *ee*, $[\alpha]^{25}_{D}$ = 72.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.60 – 7.54 (m, 2H), 7.54 – 7.48 (d, *J* = 8.0 Hz, 2H), 7.46 – 7.39 (m, 2H), 7.16 – 7.09 (d, *J* = 8.5 Hz, 2H), 7.03 – 6.95 (t, *J* = 8.0 Hz, 1H), 6.90 – 6.86 (m, 1H), 6.86 – 6.81 (m, 2H), 6.81 – 6.76 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.71 – 6.65 (m, 2H), 6.45 – 6.40 (d, *J* = 2.5 Hz, 1H), 6.35 (s, 1H), 6.15 (s, 1H), 5.08 – 5.01 (dd, *J* = 15.5, 6.5 Hz, 1H), 4.36 – 4.28 (dd, *J* = 15.5, 10.5 Hz, 1H), 3.80 (s, 3H), 3.54 (s, 3H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.6, 159.4, 158.0, 145.9, 144.6, 140.4, 137.0, 135.4, 135.0, 133.4, 132.8, 130.0, 129.3, 129.2, 128.9, 128.0, 127.3, 124.7, 121.7, 120.7, 115.7, 115.1, 114.6, 111.7, 69.8, 55.8, 55.1, 48.9, 21.7. IR (film) ν_{max} = 2922, 2850, 1661, 1619, 1603, 1494, 1386, 1228, 1163, 1089, 836. HRMS (ESI, *m*/*z*) calcd for $C_{33}H_{30}{}^{35}ClN_4O_5S$ $[M+H]^+$: 629.1620, found: 629.1621. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 12.2 min, t_{minor} = 55.7 min).

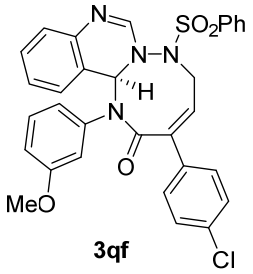
(*R*, *Z*)-3-(4-chlorophenyl)-11-methoxy-1-(3-methoxyphenyl)-6-tosyl-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qe

yellow oil, 43.3 mg, 69%, 94% *ee*, $[\alpha]^{25}_{D}$ = 80.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.58 – 7.48 (m, 4H), 7.45 – 7.37 (m, 2H), 7.17 – 7.08 (d, *J* = 8.0 Hz, 2H), 7.05 – 6.96 (t, *J* = 8.0 Hz, 1H), 6.85 – 6.72 (m, 5H), 6.72 – 6.67 (m, 1H), 6.48 – 6.44 (d, *J* = 2.0 Hz, 1H), 6.33 (s, 1H), 6.09 (s, 1H), 5.09 – 5.00 (dd, *J* = 15.5, 7.0 Hz, 1H), 4.38 – 4.30 (dd, *J* = 15.5, 10.0 Hz, 1H), 3.74 (s, 3H), 3.54 (s, 3H), 2.35 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 160.8, 159.4, 146.7, 145.9, 142.4, 140.6, 137.1, 135.4, 133.3, 132.9, 130.0, 129.3, 129.2, 128.9, 128.0, 127.9, 124.5, 121.7, 115.1, 114.7, 113.9, 112.3, 109.2, 69.7, 55.4, 55.2, 48.9, 21.7. IR (film) ν_{max} = 2921, 2851, 1660, 1603, 1570, 1493, 1387, 1231, 1163, 1088, 761. HRMS (ESI, *m*/*z*) calcd for $C_{33}H_{30}{}^{35}ClN_4O_5S$ $[M+H]^+$: 629.1620, found: 629.1618. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.9 min, t_{minor} = 25.6 min).

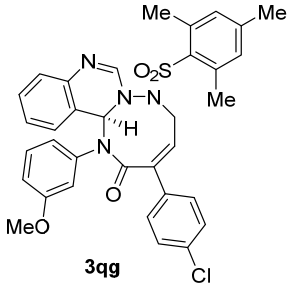
(*R*, *Z*)-3-(4-chlorophenyl)-1-(3-methoxyphenyl)-6-(phenylsulfonyl)-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qf

yellow oil, 56.9 mg, 97%, 94% *ee*, $[\alpha]^{25}_{D}$ = 128.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.67 – 7.61 (m, 2H), 7.59 – 7.52 (m, 3H), 7.46 – 7.40 (m, 2H), 7.37 – 7.30 (m, 2H), 7.30 – 7.20 (m, 2H), 7.02 – 6.89 (m, 3H), 6.86 – 6.82 (d, *J* = 1.5 Hz, 1H), 6.82 – 6.76 (m, 2H), 6.73 – 6.65 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.32 (s, 1H), 6.05 (s, 1H), 5.13 – 5.04 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.42 – 4.31 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.5, 159.4, 146.3, 141.0, 140.6, 136.9, 135.9, 135.5, 134.6, 133.2, 130.1, 129.4, 129.3, 129.3, 128.8, 128.0, 127.1, 126.3, 126.1, 124.3, 121.7, 119.8, 115.2, 114.6, 69.8, 55.2, 48.9. IR (film) ν_{max} = 2923, 1661, 1614, 1598, 1490, 1387, 1261, 1164, 1087, 764, 752. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{26}{}^{35}ClN_4O_4S$ $[M+H]^+$: 585.1358, found: 585.1355. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.4 min, t_{minor} = 40.3 min).

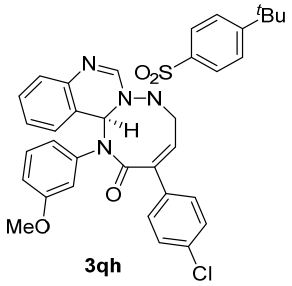
(*R*, *Z*)-3-(4-chlorophenyl)-6-(mesitylsulfonyl)-1-(3-methoxyphenyl)-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qg

yellow oil, 56.7 mg, 91%, 96% *ee*, $[\alpha]^{25}_{D}$ = 200.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.75 – 7.65 (m, 2H), 7.50 – 7.41 (m, 2H), 7.40 – 7.34 (d, *J* = 1.5 Hz, 1H), 7.25 – 7.18 (m, 2H), 7.12 – 7.05 (m, 1H), 7.02 – 6.94 (t, *J* = 8.5 Hz, 1H), 6.92 – 6.81 (m, 4H), 6.70 – 6.62 (dd, *J* = 8.5, 2.5 Hz, 1H), 6.44 – 6.41 (d, *J* = 1.5 Hz, 1H), 6.36 (s, 1H), 6.09 (s, 1H), 5.09 – 5.00 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.46 – 4.34 (dd, *J* = 15.0, 10.5 Hz, 1H), 3.51 (s, 3H), 2.45 – 2.07 (m, 9H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.8, 159.4, 145.9, 144.7, 141.4, 141.0, 140.2, 137.2, 135.4, 133.5, 132.3, 130.0, 129.3, 129.0, 128.3, 127.2, 126.3, 125.8, 125.2, 121.8, 120.1, 115.3, 114.5, 70.0, 55.2, 48.6, 22.5, 21.2. IR (film) ν_{max} = 2922, 2851, 1662, 1599, 1490, 1276, 1261, 1160, 764, 750. HRMS (ESI, *m*/*z*) calcd for $C_{34}H_{32}{}^{35}ClN_4O_4S$ $[M+H]^+$: 627.1827, found: 627.1826. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ID, *n*-hexane/2-propanol = 50 : 50, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 18.9 min, t_{minor} = 30.6 min).

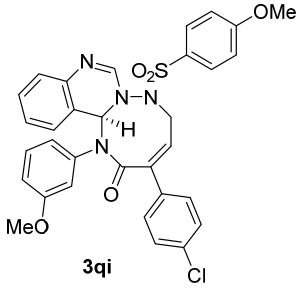
(*R*, *Z*)-6-((4-(tert-butyl)phenyl)sulfonyl)-3-(4-chlorophenyl)-1-(3-methoxyphenyl)-1,5,6, 13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qh

yellow oil, 61.5 mg, 96%, 97% *ee*, $[\alpha]^{25}_D$ = 80.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.52 – 7.46 (m, 4H), 7.45 – 7.38 (m, 2H), 7.31 – 7.27 (m, 1H), 7.25 – 7.19 (m, 3H), 7.06 – 7.02 (d, *J* = 2.0 Hz, 1H), 7.02 – 6.96 (m, 2H), 6.81 – 6.74 (m, 2H), 6.71 – 6.65 (dd, *J* = 8.5, 3.0 Hz, 1H), 6.43 – 6.39 (d, *J* = 2.0 Hz, 1H), 6.33 (s, 1H), 6.05 (s, 1H), 5.13 – 5.05 (dd, *J* = 15.0, 6.5 Hz, 1H), 4.39 – 4.31 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.51 (s, 3H), 1.21 (s, 9H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.4, 159.4, 158.7, 146.5, 141.2, 140.5, 136.9, 135.5, 133.2, 132.6, 130.1, 129.4, 129.3, 128.7, 127.8, 126.9, 126.4, 126.2, 126.1, 124.1, 121.6, 119.7, 115.2, 114.6, 69.8, 55.2, 48.9, 35.2, 30.9. HRMS (ESI, *m*/*z*) calcd for $C_{35}H_{34}{}^{35}ClN_4O_4S$ $[M+H]^+$: 641.1984, found: 641.1976. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK IA, *n*-hexane/2-propanol = 85 : 15, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 45.2 min, t_{minor} = 55.3 min).

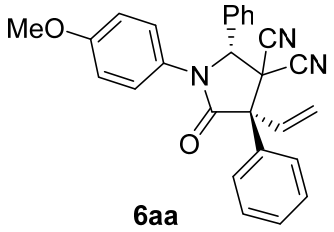
(*R*, *Z*)-3-(4-chlorophenyl)-1-(3-methoxyphenyl)-6-((4-methoxyphenyl)sulfonyl)-1,5,6,13b-tetrahydro-2*H*-[1,2,4]triazocino[2,3-*c*]quinazolin-2-one



3qi

yellow oil, 57.2 mg, 93%, 96% *ee*, $[\alpha]^{25}_D$ = 160.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.62 – 7.55 (m, 2H), 7.55 – 7.49 (m, 2H), 7.47 – 7.39 (m, 2H), 7.30 – 7.20 (m, 2H), 7.02 – 6.92 (m, 3H), 6.90 – 6.86 (d, *J* = 1.5 Hz, 1H), 6.84 – 6.82 (d, *J* = 2.0 Hz, 1H), 6.82 – 6.77 (dd, *J* = 10.0, 7.0 Hz, 1H), 6.76 – 6.72 (m, 2H), 6.70 – 6.65 (dd, *J* = 8.5, 2.5 Hz, 1H) 6.33 (s, 1H), 6.06 (s, 1H), 5.09 – 5.01 (dd, *J* = 15.0, 7.0 Hz, 1H), 4.39 – 4.30 (dd, *J* = 15.0, 10.0 Hz, 1H), 3.77 (s, 3H), 3.51 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 167.6, 164.4, 159.4, 146.5, 141.1, 140.5, 137.0, 135.5, 133.4, 131.1, 130.0, 129.3, 129.2, 128.1, 127.2, 126.6, 126.2, 126.1, 124.7, 121.7, 119.8, 115.1, 114.6, 69.7, 55.7, 55.2, 48.9. IR (film) ν_{max} = 2924, 2852, 1661, 1614, 1597, 1492, 1387, 1264, 1231, 1157, 1090, 764. HRMS (ESI, *m*/*z*) calcd for $C_{32}H_{28}{}^{35}ClN_4O_5S$ $[M+H]^+$: 615.1463, found: 615.1462. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK AD-H, *n*-hexane/2-propanol = 70 : 30, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 30.5 min, t_{minor} = 39.2 min).

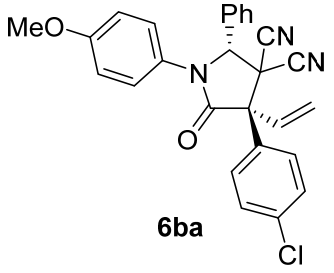
(2*R*, 4*R*)-1-(4-methoxyphenyl)-5-oxo-2,4-diphenyl-4-vinylpyrrolidine-3,3-dicarbo nitrile



6aa

white solid, 39.6 mg, 95%, Mp: 77 – 79 °C, 95% *ee*, $[\alpha]^{25}_{D}$ = 80.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.50 – 7.40 (m, 5H), 7.38 – 7.27 (m, 5H), 7.24 – 7.18 (m, 2H), 6.88 – 6.81 (m, 2H), 6.58 – 6.49 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.79 – 5.69 (dd, *J* = 17.5, 11.0 Hz, 2H), 5.27 (s, 1H), 3.76 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.8, 158.1, 133.7, 133.1, 130.3, 130.1, 129.8, 129.3, 129.0, 128.9, 128.7, 128.4, 125.1, 122.1, 114.5, 112.0, 111.8, 65.8, 62.8, 55.4, 50.5. IR (film) ν_{max} = 2923, 1721, 1511, 1457, 1363, 1251, 1031, 836, 736, 700. HRMS (ESI, *m*/z) calcd for $C_{27}H_{22}N_3O_2$ $[M+H]^+$: 420.1707, found: 420.1706. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 10.3 min, t_{minor} = 16.3 min).

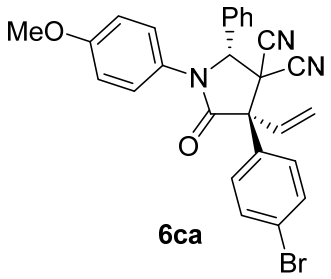
(2*R*, 4*R*)-4-(4-chlorophenyl)-1-(4-methoxyphenyl)-5-oxo-2-phenyl-4-vinylpyrrolidine-3,3-dicarbonitrile



6ba

white solid, 41.4 mg, 91%, Mp: 227 – 229 °C, 91% *ee*, $[\alpha]^{25}_{D}$ = 56.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.47 – 7.42 (m, 2H), 7.40 – 7.32 (m, 5H), 7.32 – 7.27 (m, 2H), 7.23 – 7.18 (m, 2H), 6.88 – 6.83 (m, 2H), 6.53 – 6.44 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.78 – 5.67 (dd, *J* = 17.5, 11.0 Hz, 2H), 5.28 (s, 1H), 3.76 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.2, 158.2, 136.1, 133.5, 132.0, 130.5, 130.3, 130.0, 129.5, 129.0, 128.6, 128.3, 125.0, 122.5, 114.5, 112.1, 111.5, 65.9, 62.3, 55.5, 50.3. IR (film) ν_{max} = 2916, 1724, 1610, 1512, 1494, 1252, 1097, 1031, 809, 704. HRMS (ESI, *m*/z) calcd for $C_{27}H_{21}{}^{35}ClN_3O_2$ $[M+H]^+$: 454.1317, found: 454.1312. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 13.4 min, t_{minor} = 25.3 min).

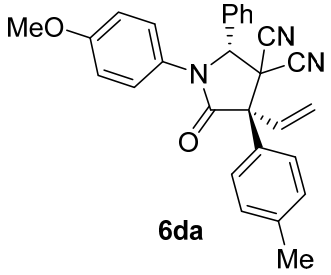
(2*R*, 4*R*)-4-(4-bromophenyl)-1-(4-methoxyphenyl)-5-oxo-2-phenyl-4-vinylpyrrolidine-3,3-dicarbonitrile



6ca

white solid, 44.4 mg, 89%, Mp: 208 – 210 °C, 91% *ee*, $[\alpha]^{25}_{D}$ = 48.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.63 – 7.57 (m, 2H), 7.40 – 7.28 (m, 7H), 7.23 – 7.17 (m, 2H), 6.90 – 6.82 (m, 2H), 6.52 – 6.43 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.78 – 5.73 (d, *J* = 11.0 Hz, 1H), 5.73 – 5.66 (d, *J* = 17.5 Hz, 1H), 5.27 (s, 1H), 3.76 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.2, 158.2, 133.5, 132.5, 130.6, 130.5, 130.0, 129.0, 128.6, 128.2, 125.0, 124.4, 122.6, 114.5, 112.1, 111.5, 65.9, 62.3, 55.5, 50.2. IR (film) ν_{max} = 2925, 1721, 1610, 1511, 1489, 1364, 1253, 1078, 1027, 804. HRMS (ESI, *m*/*z*) calcd for $C_{27}H_{21}{}^{79}BrN_3O_2$ $[M+H]^+$: 498.0812, found: 498.0809. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.2 min, t_{minor} = 30.2 min).

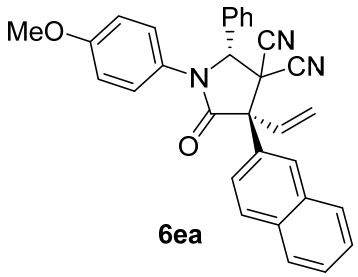
(2*R*, 4*R*)-1-(4-methoxyphenyl)-5-oxo-2-phenyl-4-(*p*-tolyl)-4-vinylpyrrolidine-3,3-dicarbonitrile



6da

white solid, 34.1 mg, 79%, Mp: 229 – 231 °C, 95% *ee*, $[\alpha]^{25}_{D}$ = 64.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.37 – 7.23 (m, 9H), 7.22 – 7.17 (m, 2H), 6.88 – 6.82 (m, 2H), 6.57 – 6.48 (dd, *J* = 18.0, 11.0 Hz, 1H), 5.77 – 5.69 (dd, *J* = 18.0, 11.0 Hz, 2H), 5.26 (s, 1H), 3.75 (s, 3H), 2.39 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.9, 158.1, 140.0, 133.8, 130.3, 130.2, 130.0, 129.9, 128.9, 128.7, 128.6, 128.4, 125.1, 121.8, 114.4, 112.1, 111.9, 65.8, 62.7, 55.4, 50.6, 21.2. IR (film) ν_{max} = 2923, 2853, 1722, 1511, 1457, 1363, 1252, 1029, 806, 704. HRMS (ESI, *m*/*z*) calcd for $C_{28}H_{24}N_3O_2$ $[M+H]^+$: 434.1863, found: 434.1859. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 17.8 min, t_{minor} = 30.2 min).

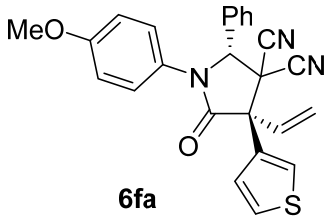
(2*R*, 4*R*)-1-(4-methoxyphenyl)-4-(naphthalen-2-yl)-5-oxo-2-phenyl-4-vinylpyrrolidine-3,3-dicarbonitrile



6ea

white solid, 44.5 mg, 95%, Mp: 238 – 240 °C, 92% *ee*, $[\alpha]^{25}_{D}$ = 64.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.99 – 7.94 (d, *J* = 9.0 Hz, 1H), 7.91 – 7.86 (d, *J* = 8.0 Hz, 1H), 7.85 – 7.81 (d, *J* = 2.0 Hz, 1H), 7.81 – 7.77 (d, *J* = 8.0 Hz, 1H), 7.62 – 7.49 (m, 3H), 7.35 – 7.23 (m, 7H), 6.90 – 6.85 (m, 2H), 6.65 – 6.57 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.83 – 5.73 (dd, *J* = 17.5, 11.0 Hz, 2H), 5.33 (s, 1H), 3.76 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.8, 158.2, 133.7, 133.4, 133.0, 130.4, 130.3, 130.1, 129.2, 129.0, 128.7, 128.7, 128.6, 128.5, 127.7, 127., 127.01, 125.8, 125.2, 122.5, 114.6, 112.1, 111.9, 66.0, 63.1, 55.5, 50.5. IR (film) ν_{max} = 2925, 1722, 1512, 1457, 1363, 1300, 1250, 1180, 837. HRMS (ESI, *m*/*z*) calcd for $C_{31}H_{24}N_3O_2$ $[M+H]^+$: 470.1863, found: 470.1857. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.4 min, t_{minor} = 48.7 min).

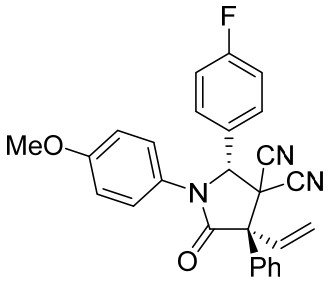
(2*R*, 4*S*)-1-(4-methoxyphenyl)-5-oxo-2-phenyl-4-(thiophen-3-yl)-4-vinylpyrrolidine-3,3-dicarbonitrile



6fa

white solid, 41.4 mg, 97%, Mp: 143 – 145 °C, 92% *ee*, $[\alpha]^{25}_{D}$ = 72.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.49 – 7.44 (m, 1H), 7.39 – 7.29 (m, 6H), 7.22 – 7.17 (m, 3H), 6.87 – 6.81 (m, 2H), 6.52 – 6.44 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.74 – 5.67 (dd, *J* = 17.5, 11.0 Hz, 2H), 5.34 (s, 1H), 3.75 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.5, 158.1, 133.3, 133.1, 130.4, 130.2, 129.0, 128.6, 128.5, 127.5, 127.3, 126.4, 125.0, 122.1, 114.5, 112.2, 111.6, 66.0, 60.2, 55.4, 50.2. IR (film) ν_{max} = 2923, 1723, 1511, 1457, 1362, 1252, 1029, 835, 737, 702. HRMS (ESI, *m*/*z*) calcd for $C_{25}H_{20}N_3O_2S$ $[M+H]^+$: 426.1271, found: 426.1270. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.5 min, t_{minor} = 25.8 min).

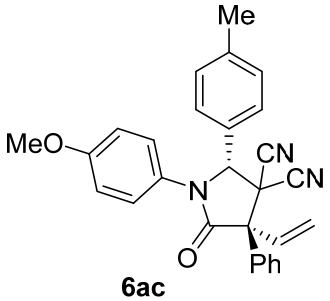
(2*R*, 4*R*)-2-(4-fluorophenyl)-1-(4-methoxyphenyl)-5-oxo-4-phenyl-4-vinylpyrrolidine-3,3-dicarbonitrile



6ab

white solid, 35.7 mg, 82%, Mp: 76 – 78 °C, 94% *ee*, $[\alpha]^{25}_{D}$ = 56.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.50 – 7.44 (m, 3H), 7.44 – 7.40 (m, 2H), 7.32 – 7.26 (m, 2H), 7.21 – 7.14 (m, 2H), 7.06 – 6.98 (m, 2H), 6.90 – 6.83 (m, 2H), 6.59 – 6.48 (dd, *J* = 18.0, 11.0 Hz, 1H), 5.82 – 5.70 (dd, *J* = 18.0, 11.0 Hz, 2H), 5.25 (s, 1H), 3.77 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.7, 163.7 (d, *J* = 249.4 Hz), 158.3, 133.6, 132.8, 130.6 (d, *J* = 8.5 Hz), 129.9, 129.4, 128.8, 128.1, 125.9 (d, *J* = 3.0 Hz), 125.1, 122.0, 116.4, 116.2, 114.6, 111.8 (d, *J* = 5.0 Hz), 65.2, 62.8, 55.5, 50.5. ^{19}F NMR ($CDCl_3$, 470 MHz): – 109.6. δ =IR (film) ν_{max} = 2923, 1720, 1511, 1447, 1363, 1274, 1254, 1179, 1030, 837, 750. HRMS (ESI, *m*/*z*) calcd for $C_{27}H_{21}FN_3O_2$ $[M+H]^+$: 438.1612, found: 438.1610. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 10.7 min, t_{minor} = 21.9 min).

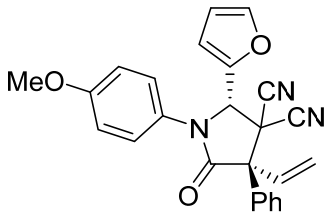
(2*R*, 4*R*)-1-(4-methoxyphenyl)-5-oxo-4-phenyl-2-(*p*-tolyl)-4-vinylpyrrolidine-3,3-dicarbonitrile



6ac

white solid, 37.3 mg, 86%, Mp: 216 – 218 °C, 95% *ee*, $[\alpha]^{25}_{D}$ = 40.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.50 – 7.39 (m, 5H), 7.23 – 7.15 (m, 4H), 7.15 – 7.09 (d, *J* = 2.0 Hz, 2H), 6.89 – 6.80 (m, 2H), 6.58 – 6.47 (dd, *J* = 17.5, 11.0 Hz, 1H), 5.78 – 5.68 (dd, *J* = 17.5, 11.0 Hz, 2H), 5.24 (s, 1H), 3.75 (s, 3H), 2.29 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 169.7, 158.1, 140.5, 133.8, 133.2, 129.8, 129.7, 129.3, 128.9, 128.5, 128.5, 127.1, 125.1, 122.0, 114.4, 112.1, 111.3, 65.74, 62.80, 55.4, 50.6, 21.3. δ =IR (film) ν_{max} = 2923, 1724, 1512, 1457, 1364, 1252, 1179, 1032, 754, 699. HRMS (ESI, *m*/*z*) calcd for $C_{28}H_{24}N_3O_2$ $[M+H]^+$: 434.1863, found: 434.1864. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 10.6 min, t_{minor} = 16.5 min).

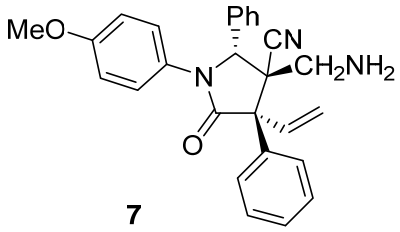
(2*S*, 4*R*)-2-(furan-2-yl)-1-(4-methoxyphenyl)-5-oxo-4-phenyl-4-vinylpyrrolidine-3,3-dicarbonitrile



6ad

white solid, 30.7 mg, 75%, Mp: 170 – 172 °C, 97% *ee*, $[\alpha]^{25}_{D}$ = 24.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.54 – 7.42 (m, 6H), 7.24 – 7.18 (m, 2H), 6.93 – 6.87 (m, 2H), 6.61 – 6.52 (dd, *J* = 17.0, 10.5 Hz, 1H), 6.48 – 6.45 (d, *J* = 3.5 Hz, 1H), 6.38 – 6.34 (dd, *J* = 3.5, 2.0 Hz, 1H), 5.75 – 5.69 (d, *J* = 10.5 Hz, 1H), 5.69 – 5.64 (d, *J* = 17.0 Hz, 1H), 5.46 (s, 1H), 3.79 (s, 3H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 168.6, 158.8, 144.8, 144.0, 134.1, 133.6, 129.7, 129.3, 128., 128.21, 126.0, 122.5, 114.6, 113.8, 112.3, 111.6, 111.3, 62.2, 61.6, 55.5, 48.5. δ =IR (film) ν_{max} = 2923, 1719, 1512, 1457, 1367, 1250, 1180, 836, 733. HRMS (ESI, *m*/*z*) calcd for $C_{25}H_{20}N_3O_3$ $[M+H]^+$: 410.1499, found: 410.1501. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 80 : 20, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 21.7 min, t_{minor} = 27.7 min).

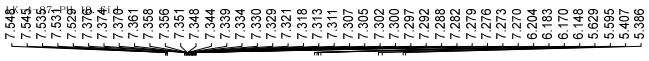
(2*R*, 3*S*, 4*R*)-3-(aminomethyl)-1-(4-methoxyphenyl)-5-oxo-2,4-diphenyl-4-vinylpyrrolidine-3-carbonitrile

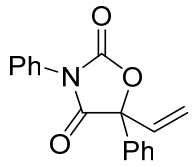


7

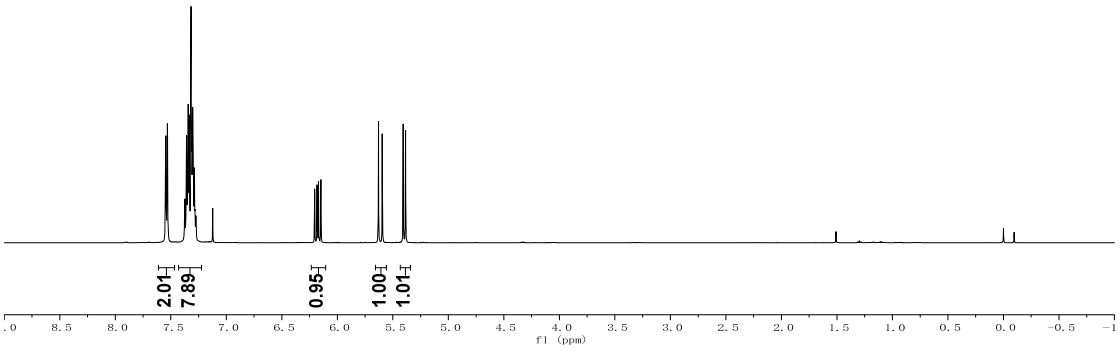
white solid, 63.3 mg, 75%, Mp: 235 – 237 °C, 95% *ee*, $[\alpha]^{25}_{D}$ = 96.0 (*c* 0.5, CH_2Cl_2). ^{1}H NMR (500 MHz, $CDCl_3$): δ = 7.53 – 7.43 (m, 4H), 7.41 – 7.27 (m, 8H), 6.88 – 6.78 (m, 2H), 6.56 – 6.45 (dd, *J* = 17.0, 10.5 Hz, 1H), 5.61 (s, 1H), 5.54 – 5.48 (d, *J* = 17.0 Hz, 1H), 5.48 – 5.42 (d, *J* = 10.5 Hz, 1H), 3.74 (s, 3H), 2.62 – 2.52 (d, *J* = 13.5 Hz, 1H), 2.52 – 2.44 (d, *J* = 13.5 Hz, 1H), 1.34 (s, 2H). ^{13}C NMR ($CDCl_3$, 125 MHz): δ = 170.9, 157.3, 138.3, 137.8, 135.7, 130.5, 129.1, 128.7, 128.5, 128.5, 127.9, 124.0, 121.2, 118.9, 114.2, 64.5, 60.7, 55.6, 55.4, 47.0. HRMS (ESI, *m*/*z*) calcd for $C_{27}H_{26}N_3O_2$ $[M+H]^+$: 424.2020, found: 424.2015. The *ee* value was determined by the chiral HPLC analysis (CHIRALPAK ADH, *n*-hexane/2-propanol = 75 : 25, *v* = 1.0 mL/min, λ = 254.0 nm; t_{major} = 14.3 min, t_{minor} = 51.5 min).

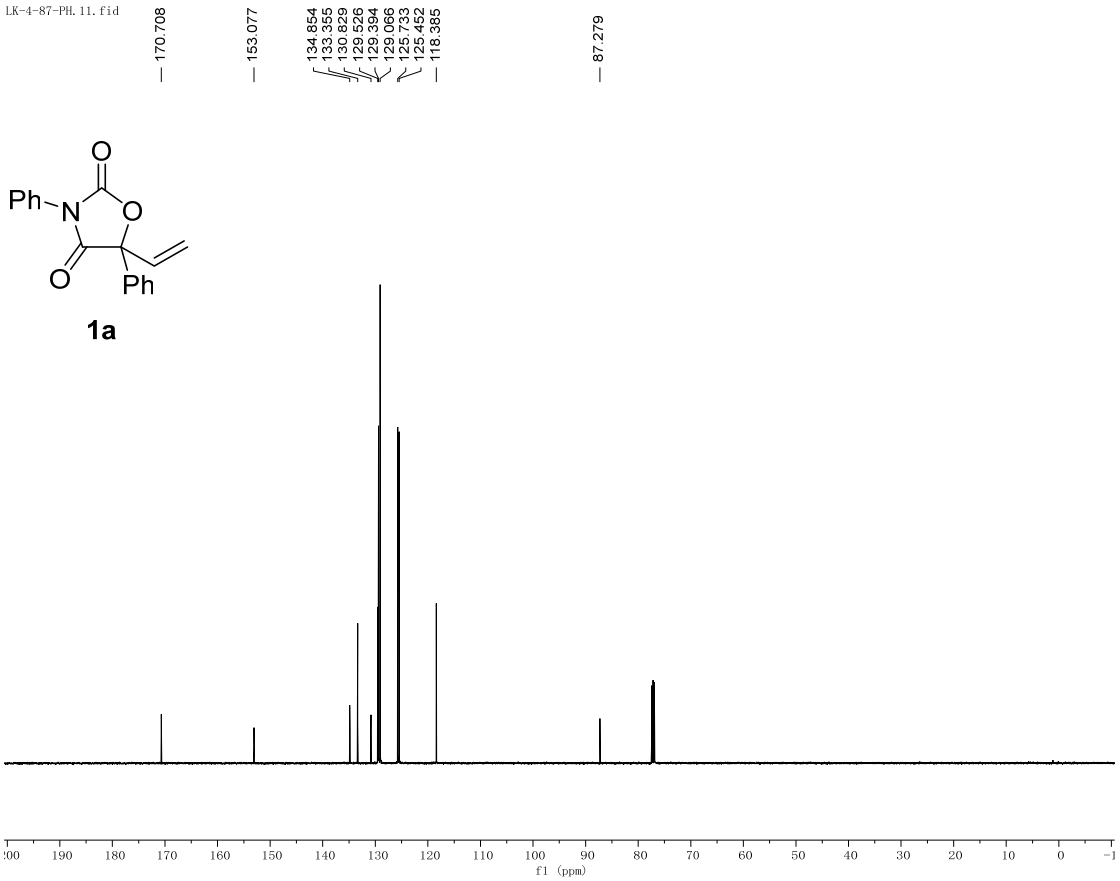
NMR Spectra of Substrates and Products





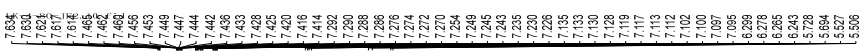
1a

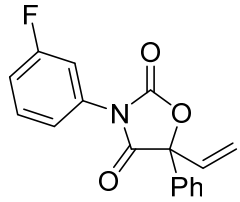




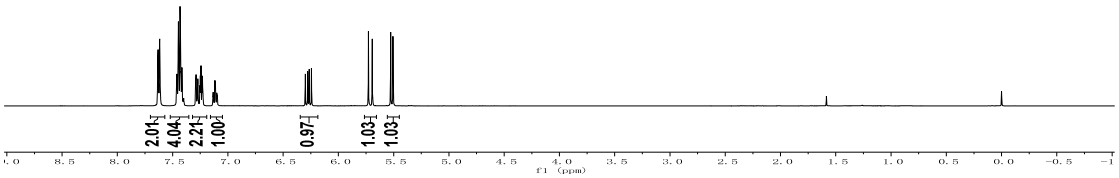
1a

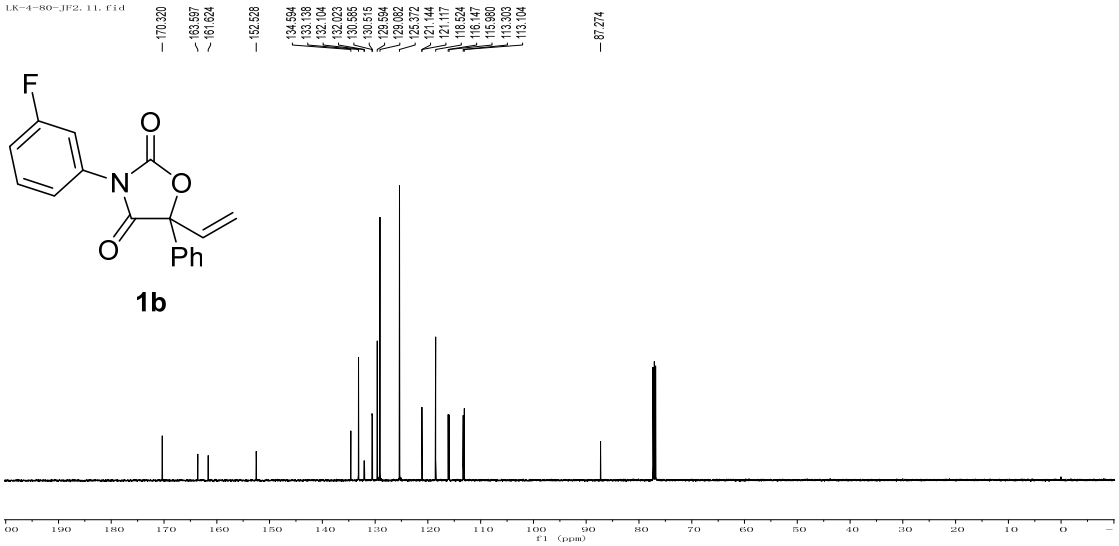
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1a**



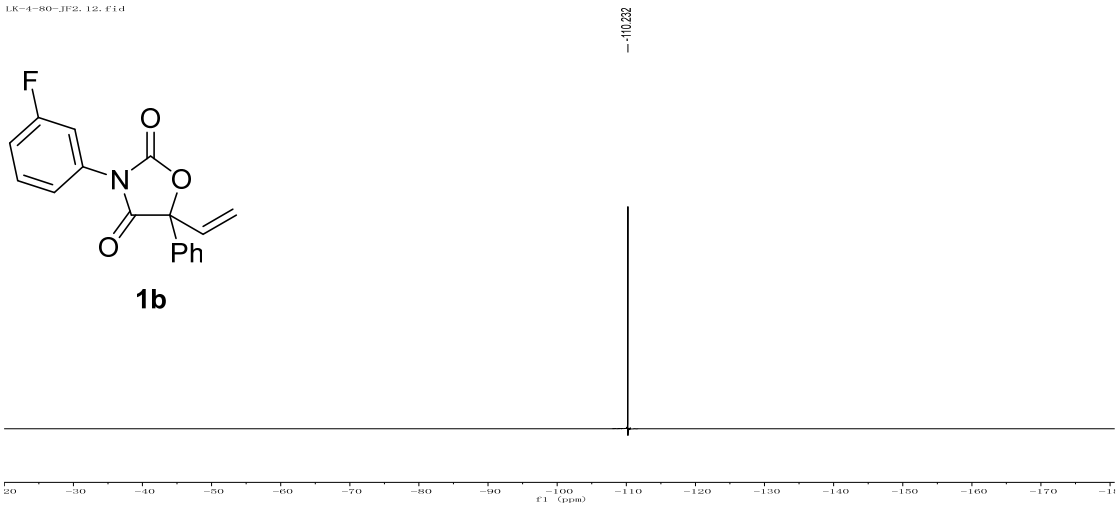


1b



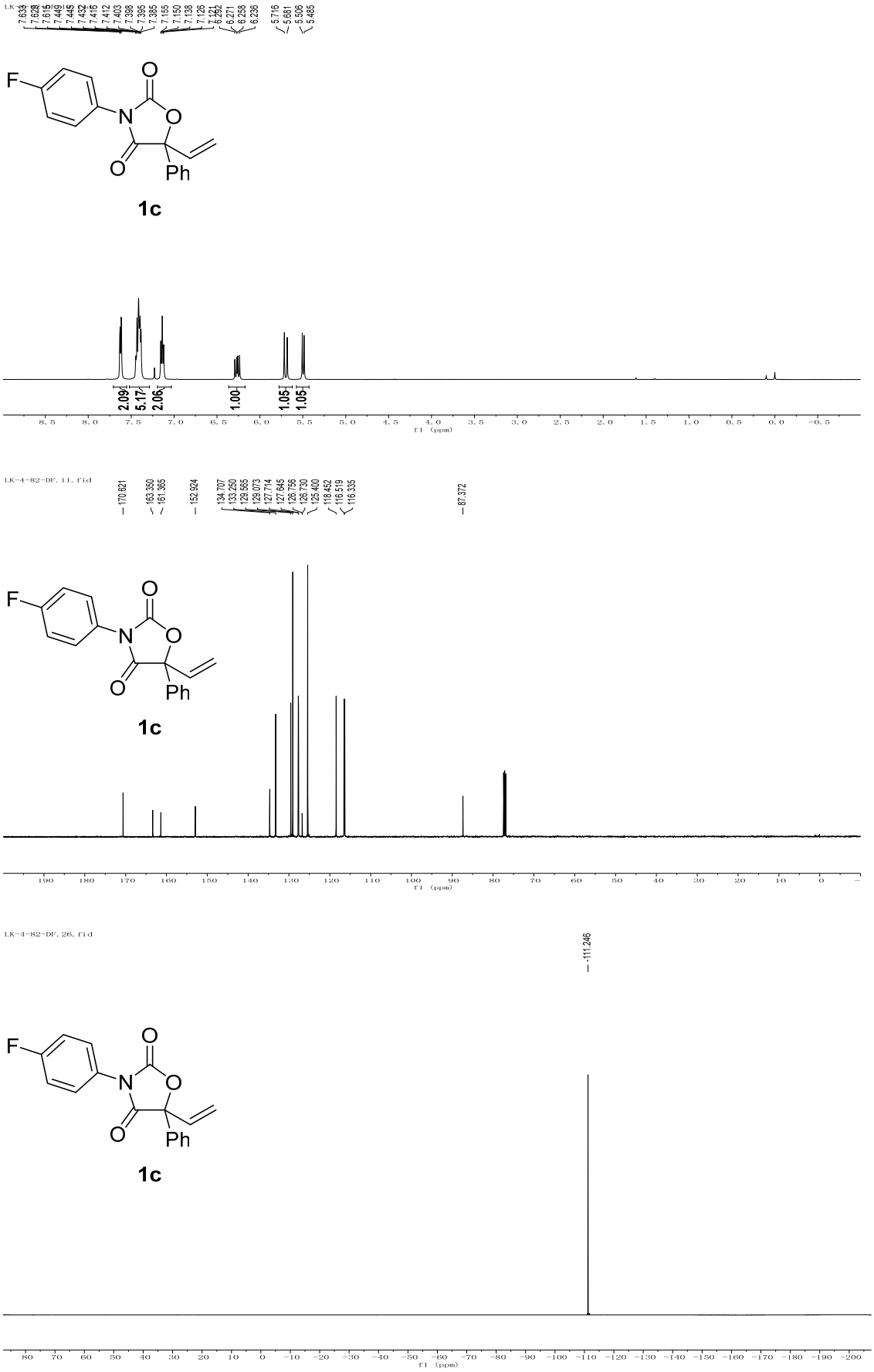


1b

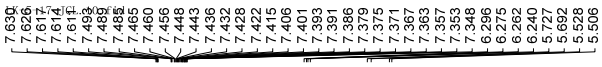


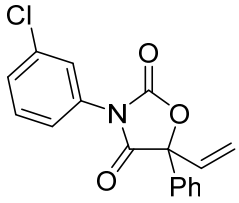
1b

^{1}H NMR (500 MHz) ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **1b**

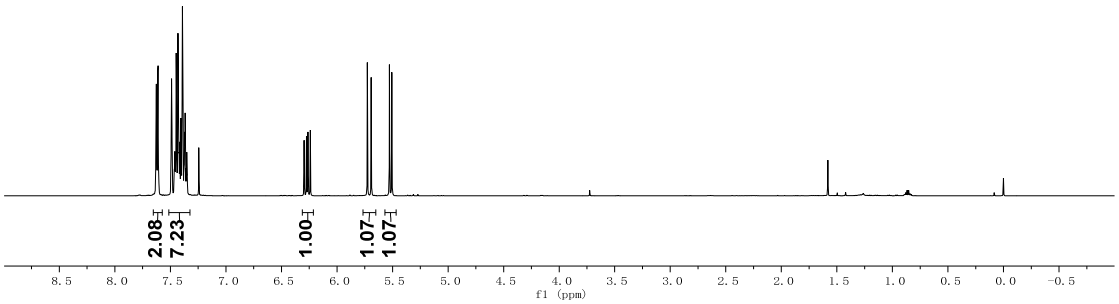


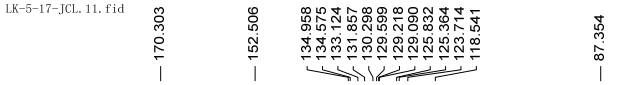
^{1}H NMR (500 MHz) ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **1c**

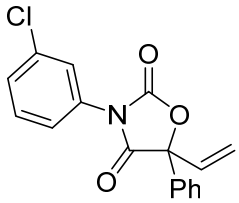




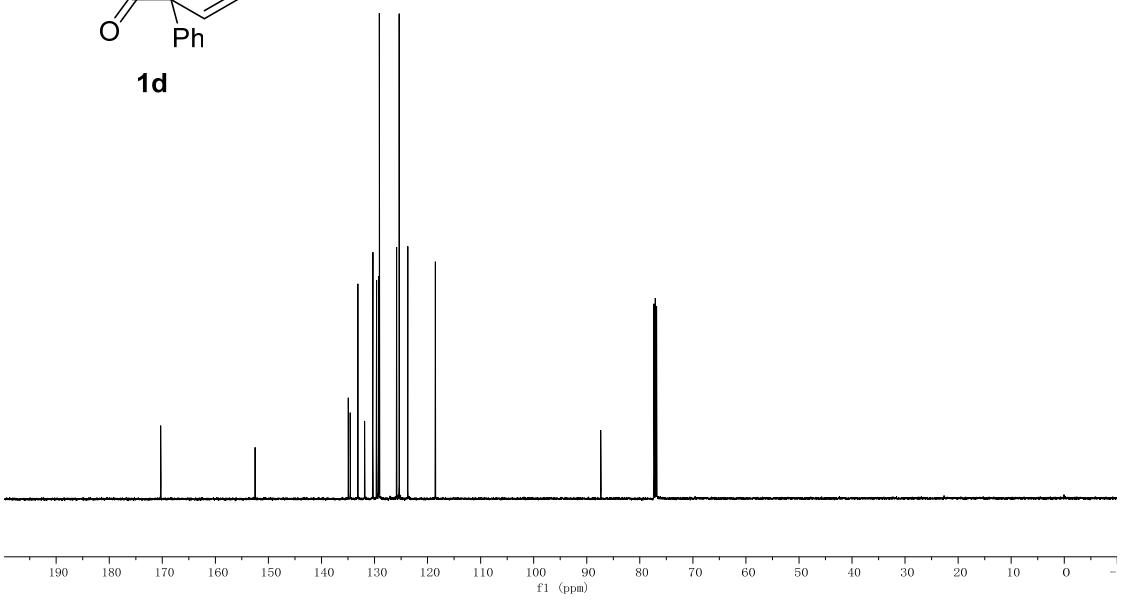
1d



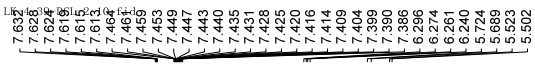


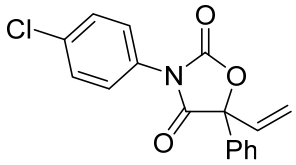


1d

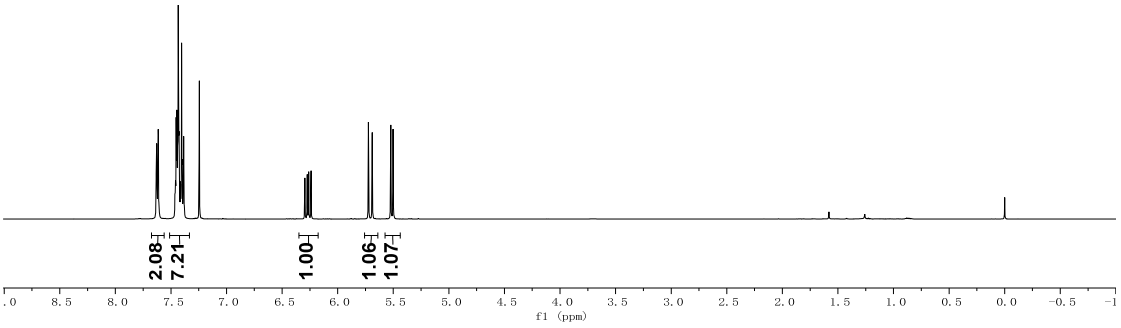


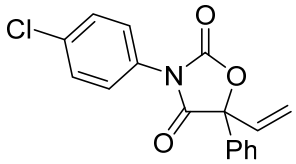
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1d**



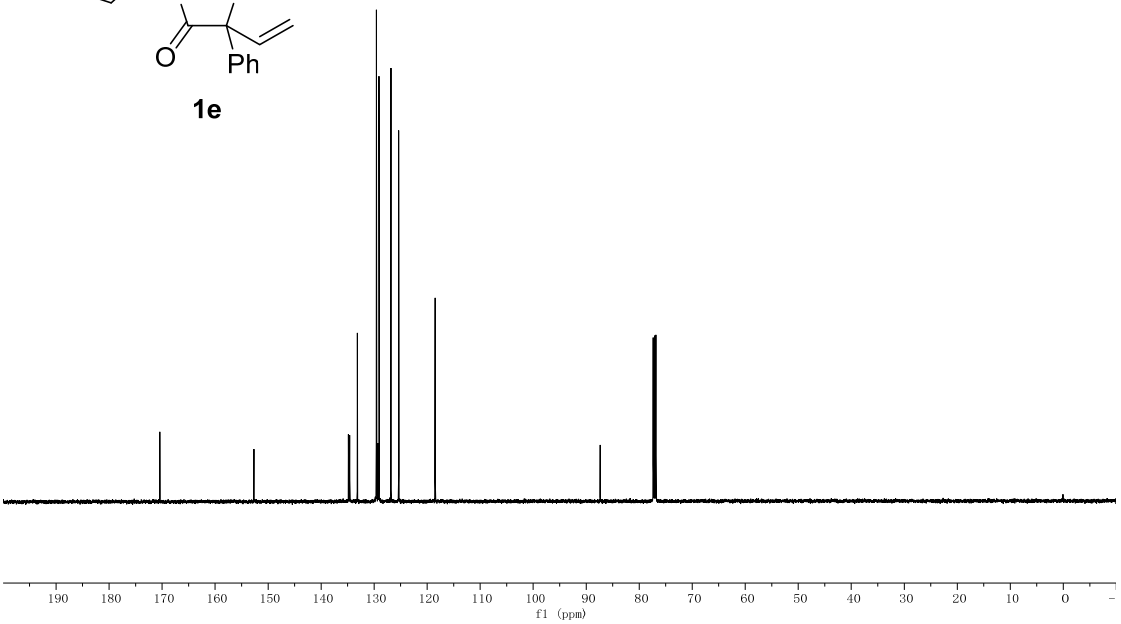


1e

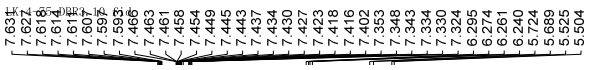


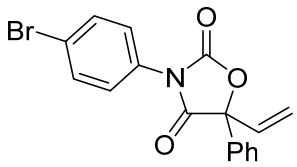


1e

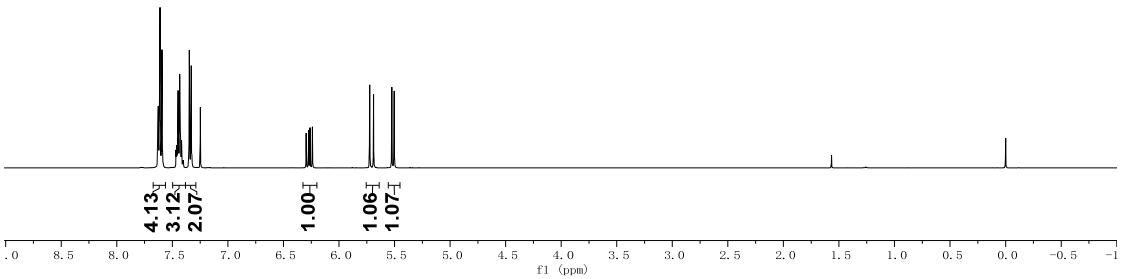


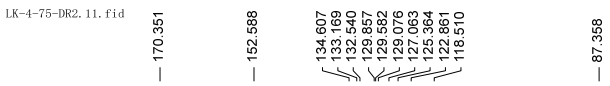
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1e**

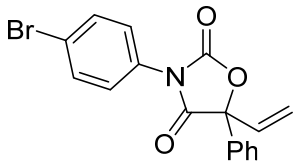




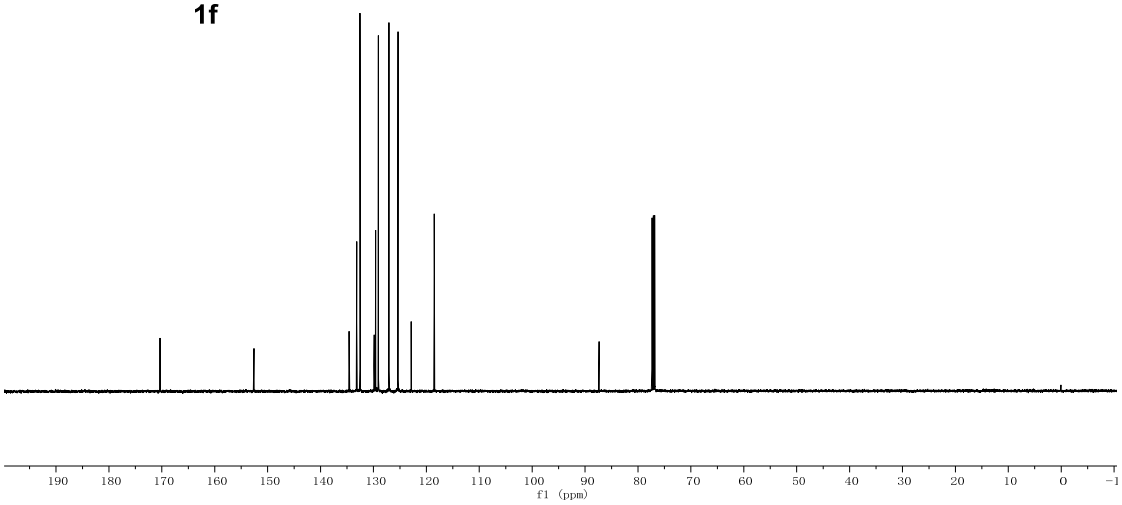
1f



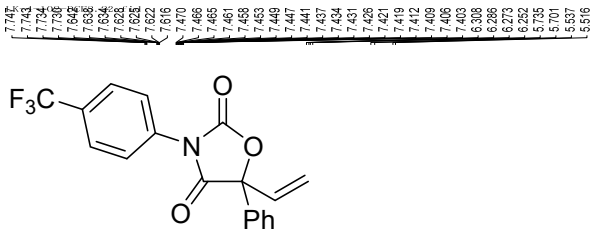




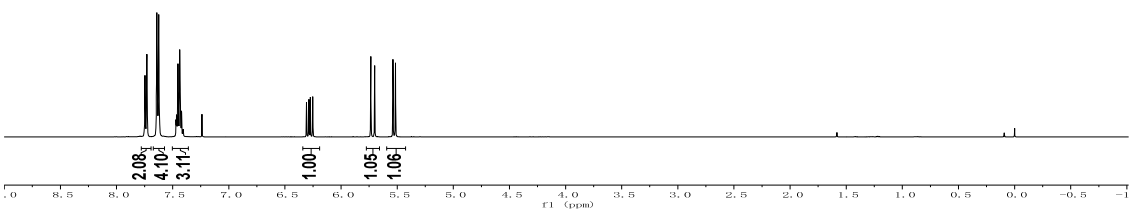
1f

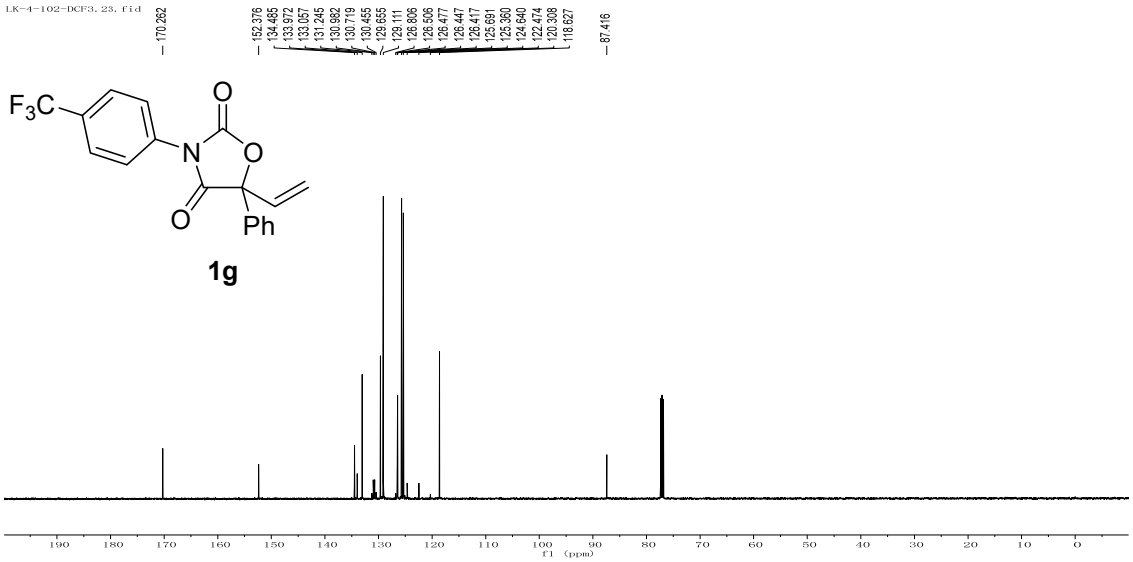


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1f**

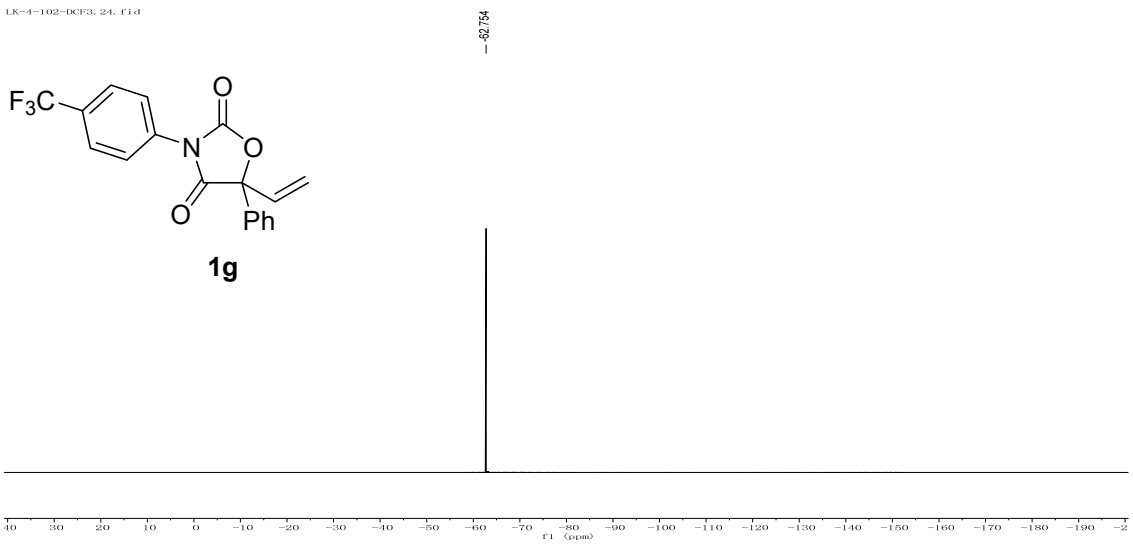


1g



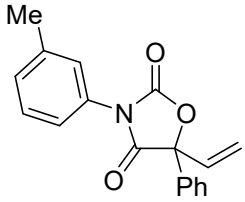


1g

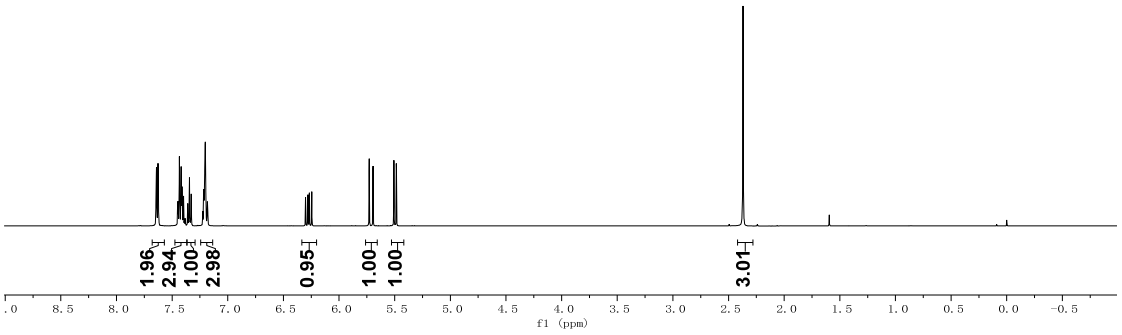


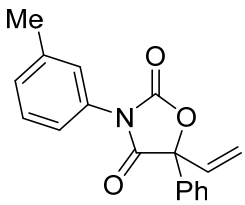
1g

^{1}H NMR (500 MHz) ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **1g**

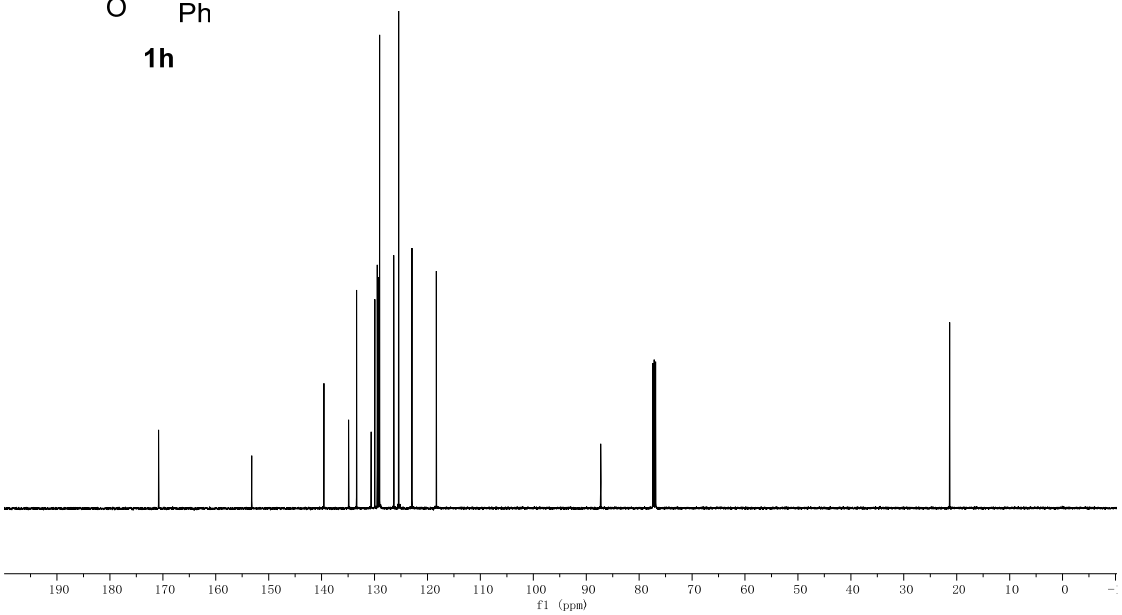


1h

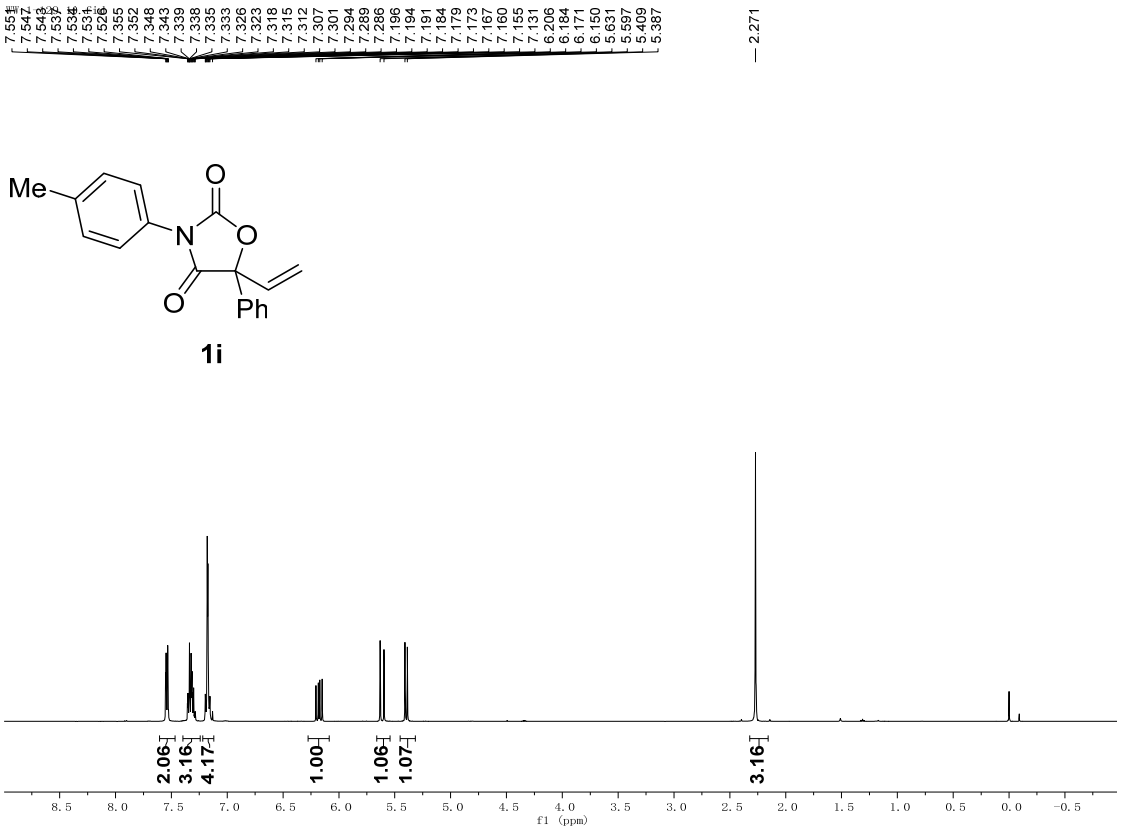


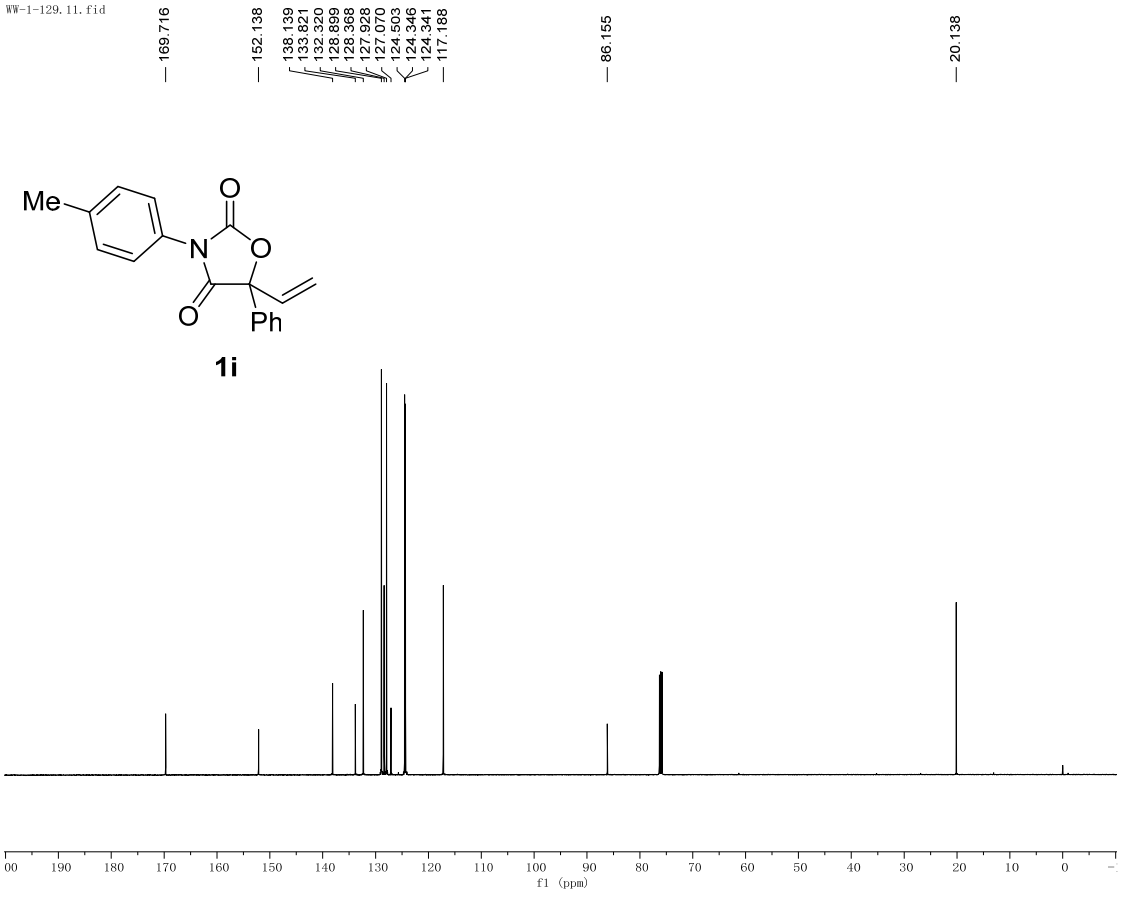


1h

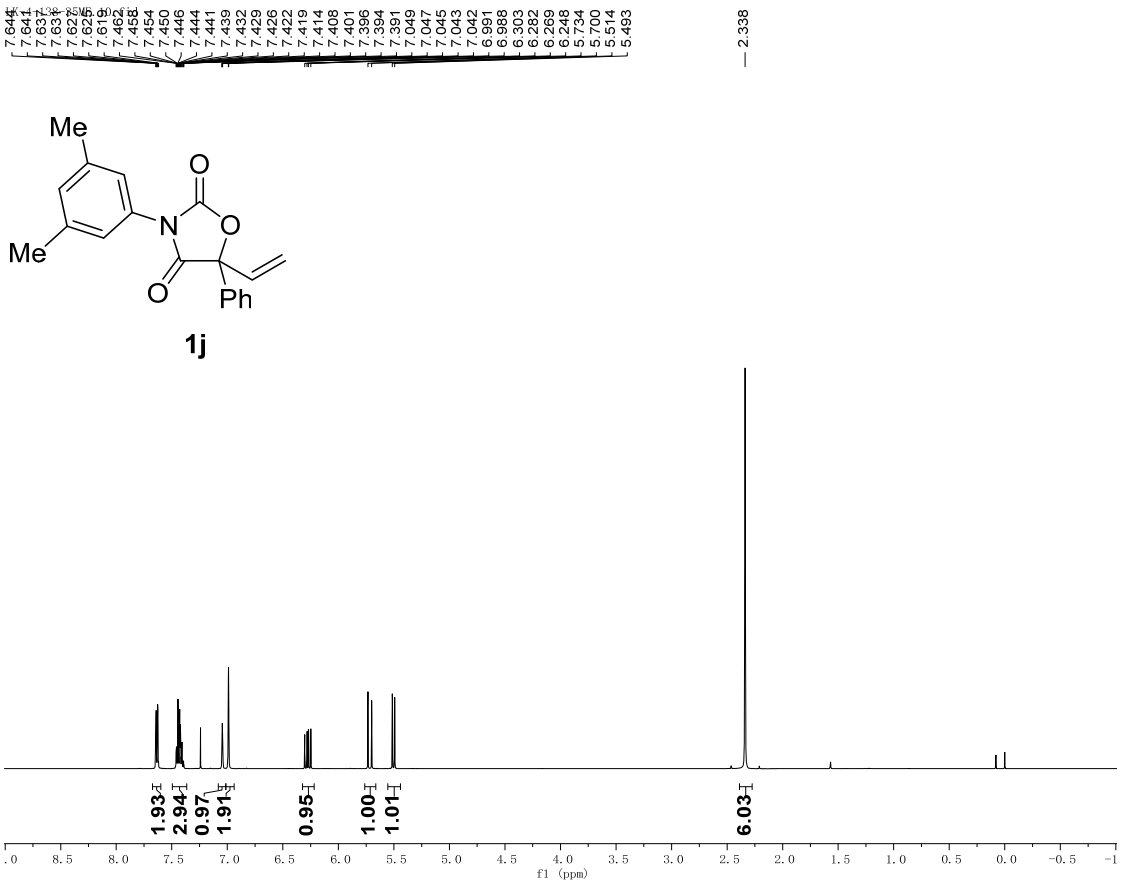


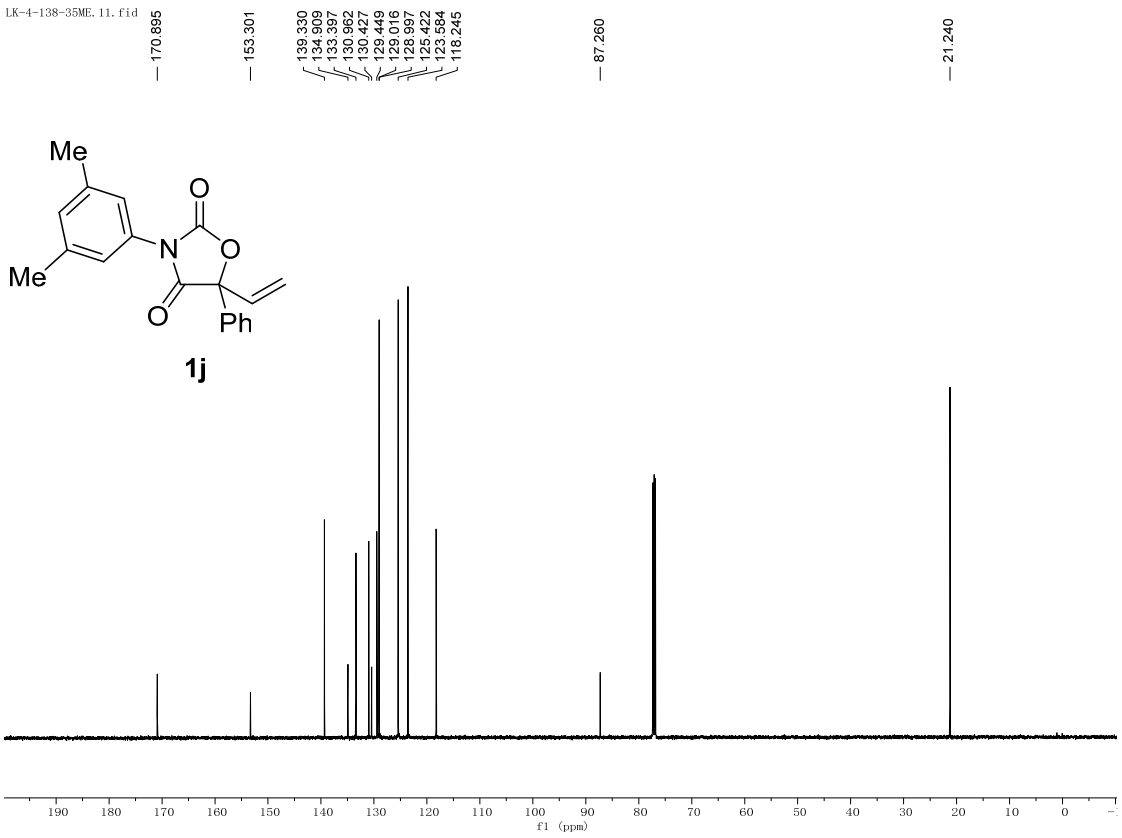
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1h**



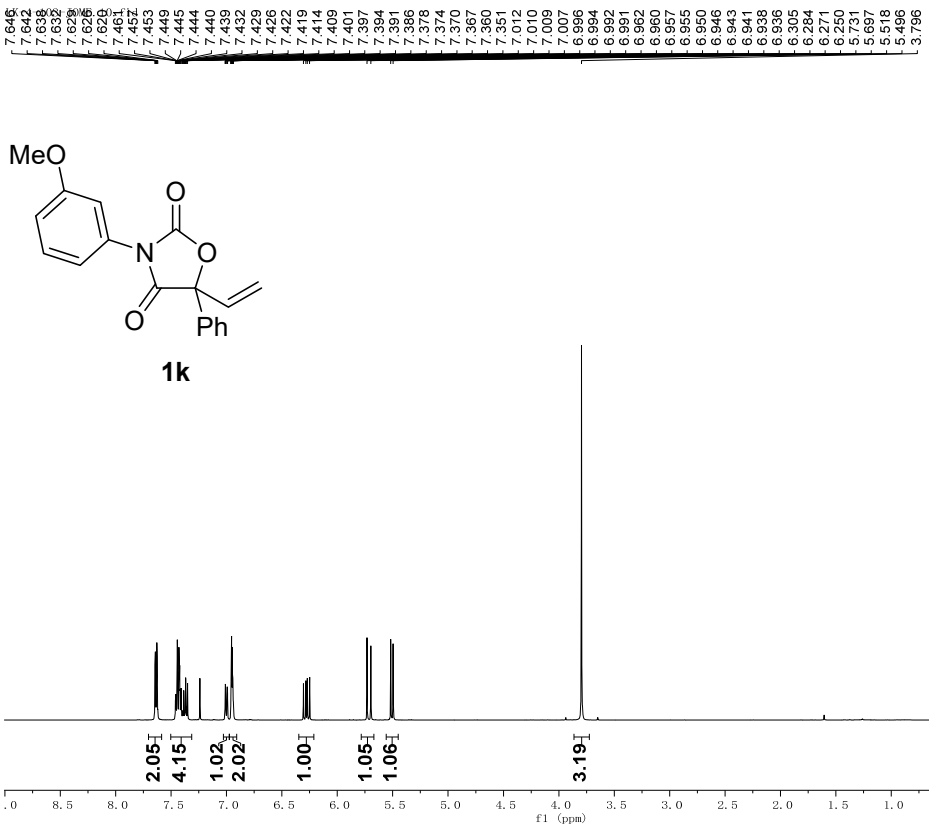


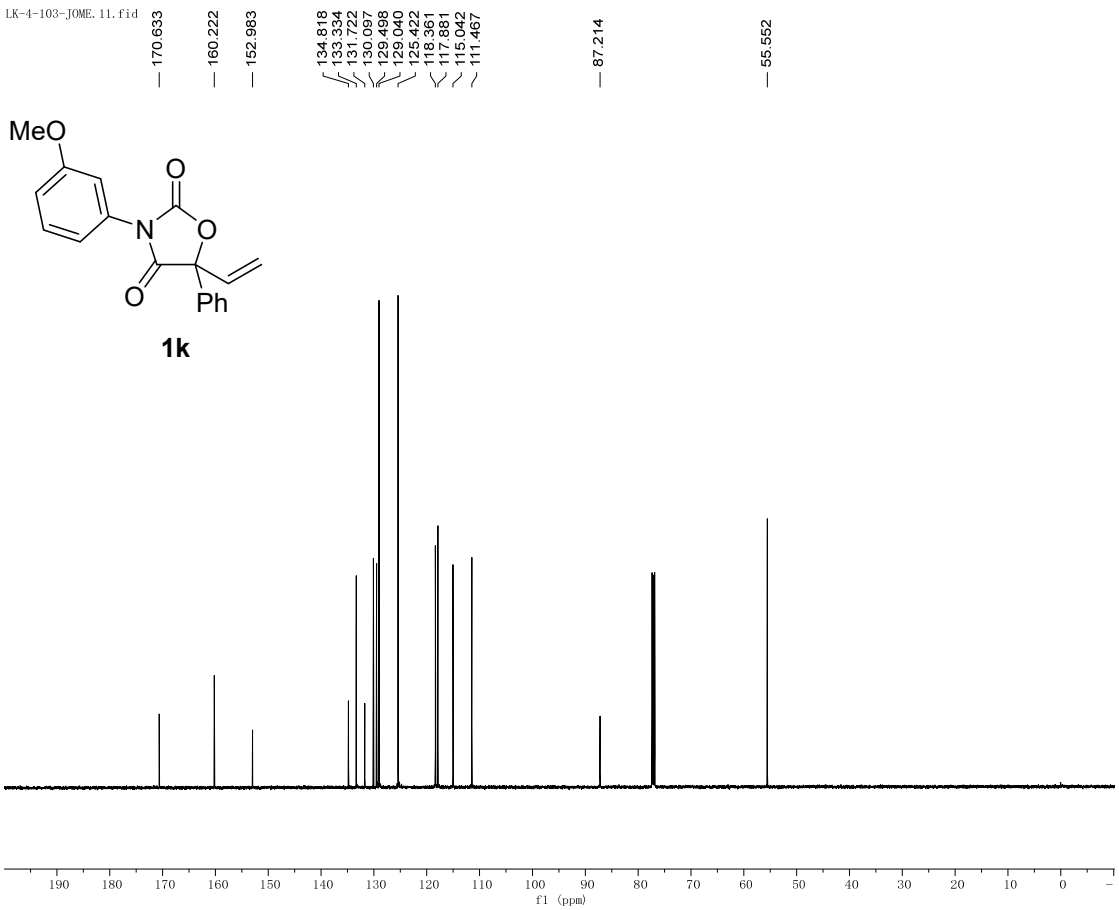
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1i**



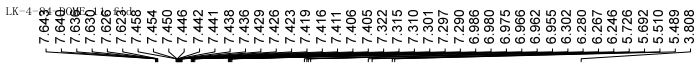


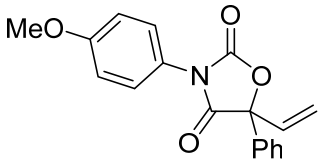
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1j**



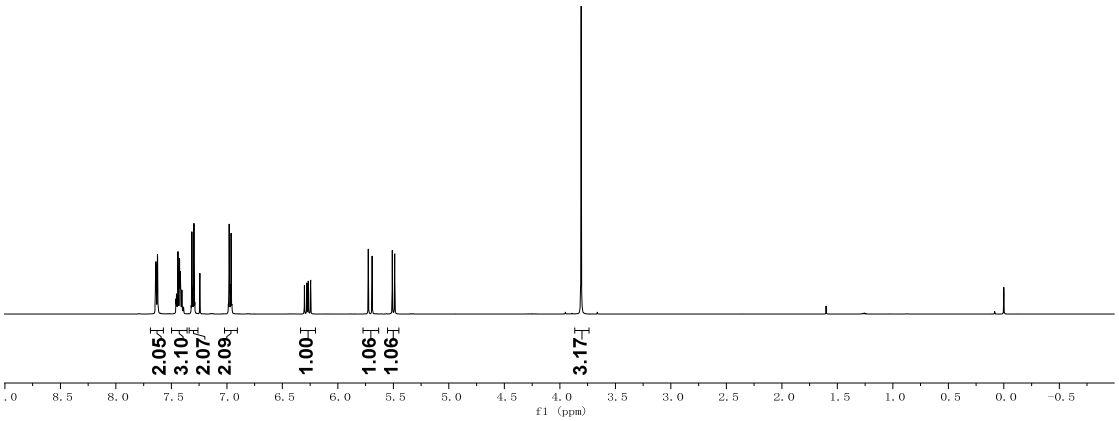


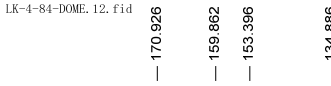
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1k**

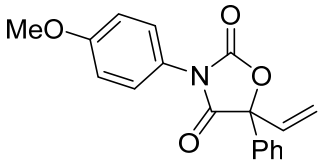




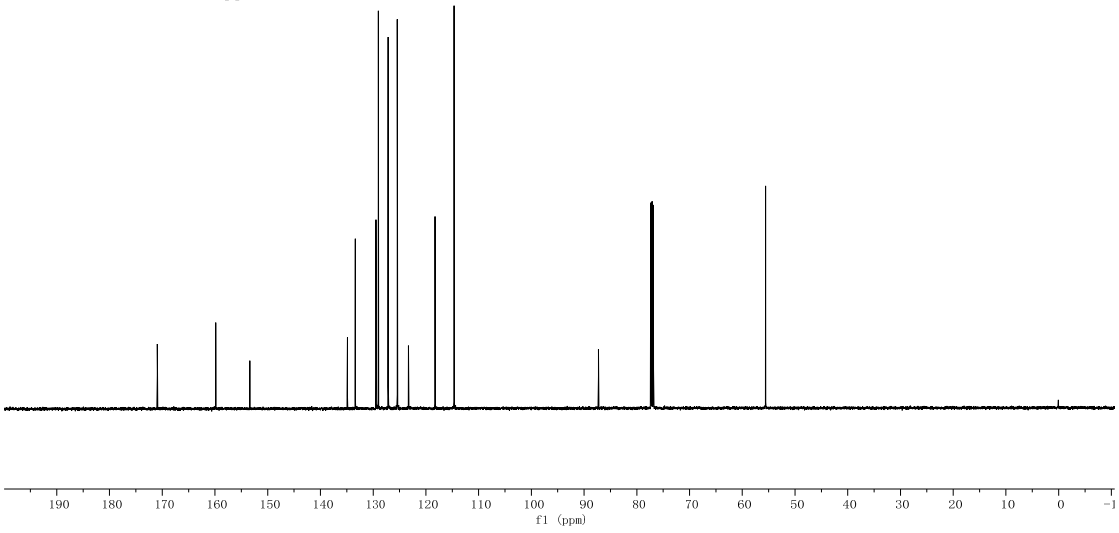
1l



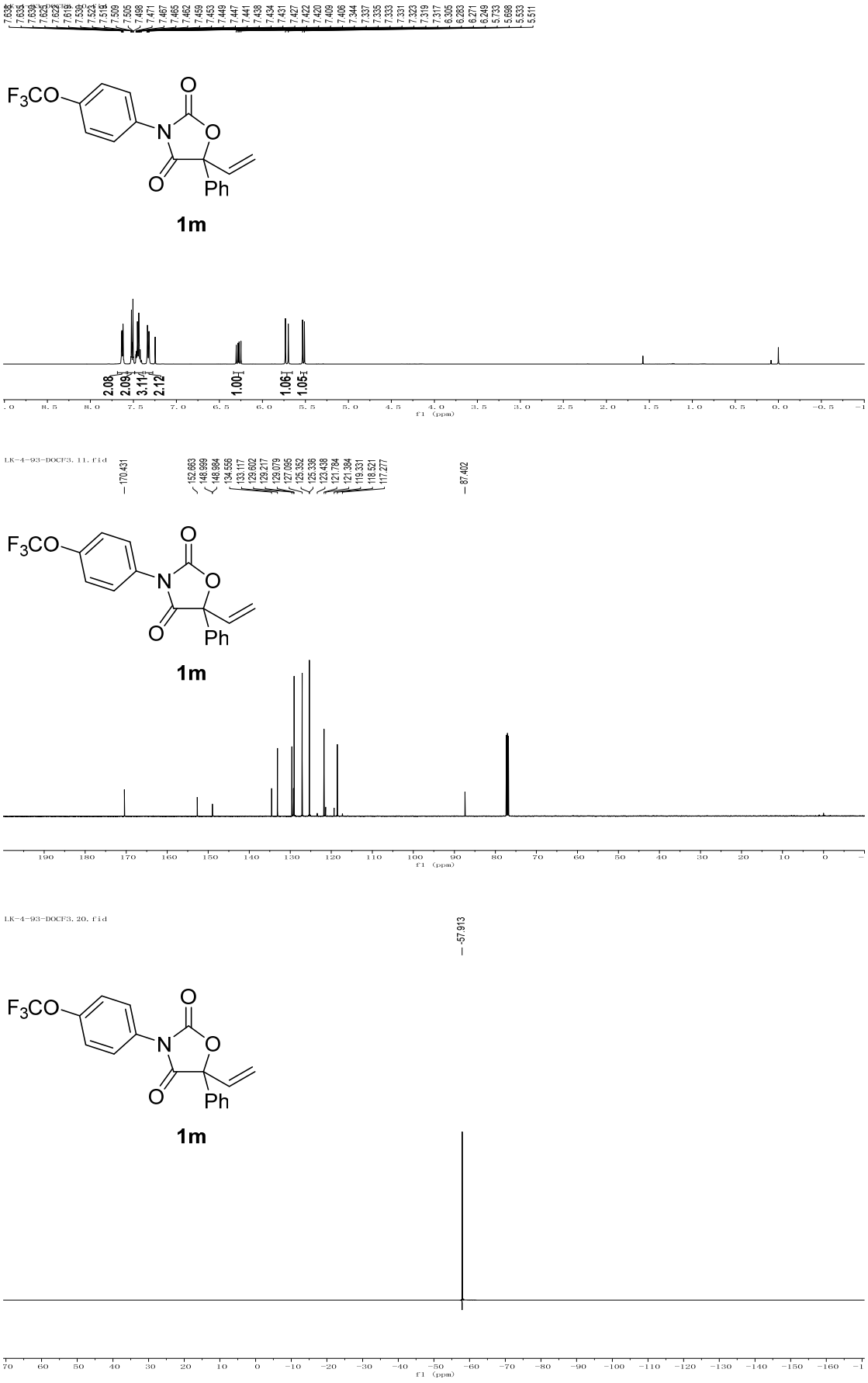




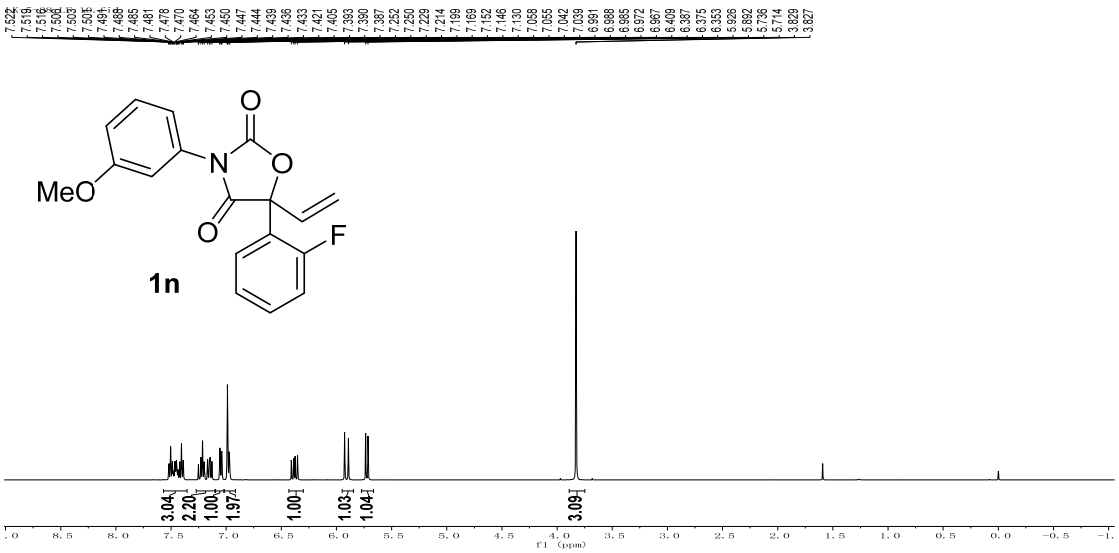
1l

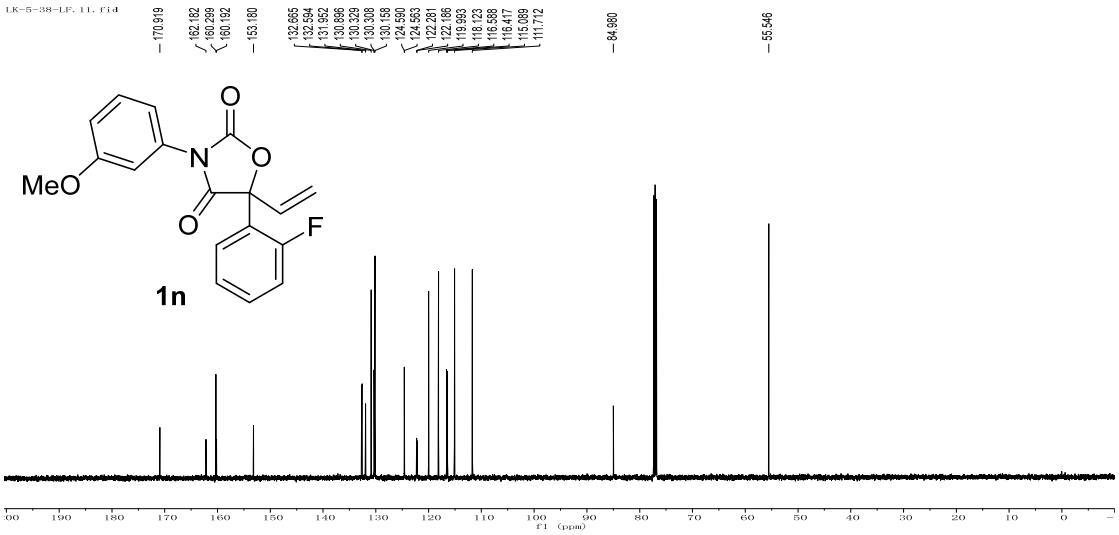


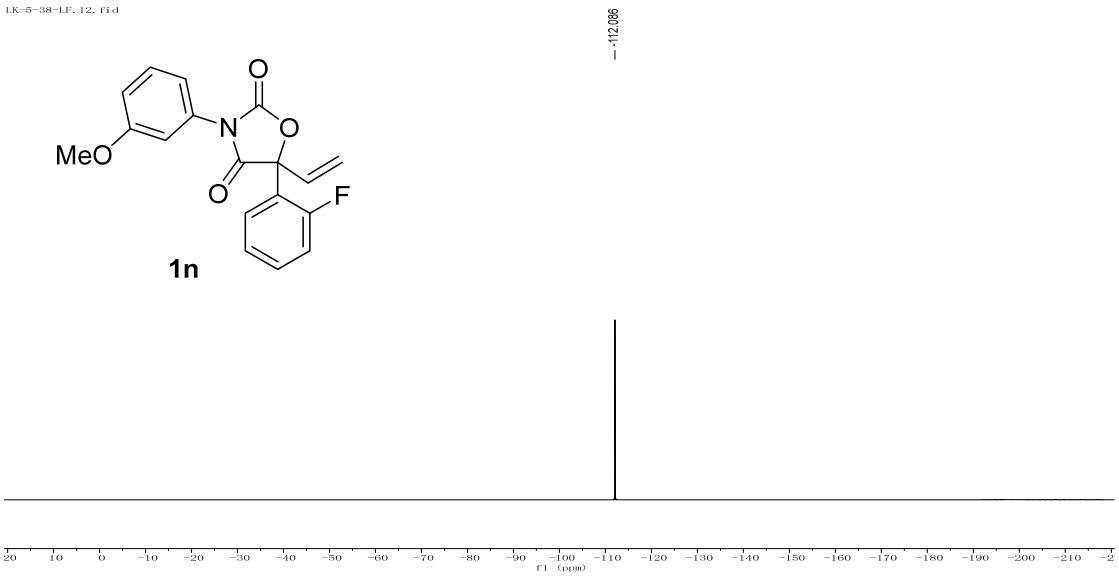
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1l**



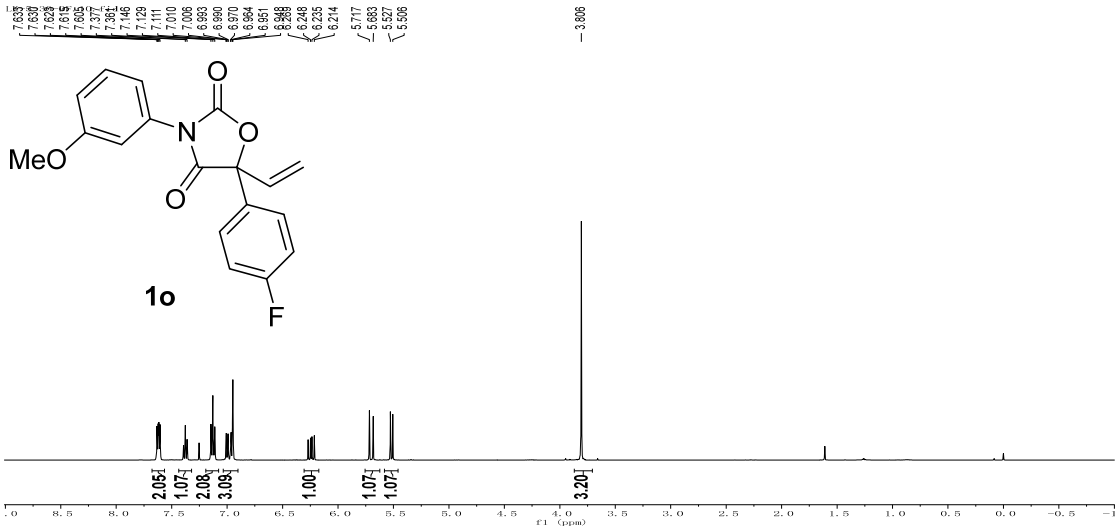
^{1}H NMR (500 MHz) ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **1m**

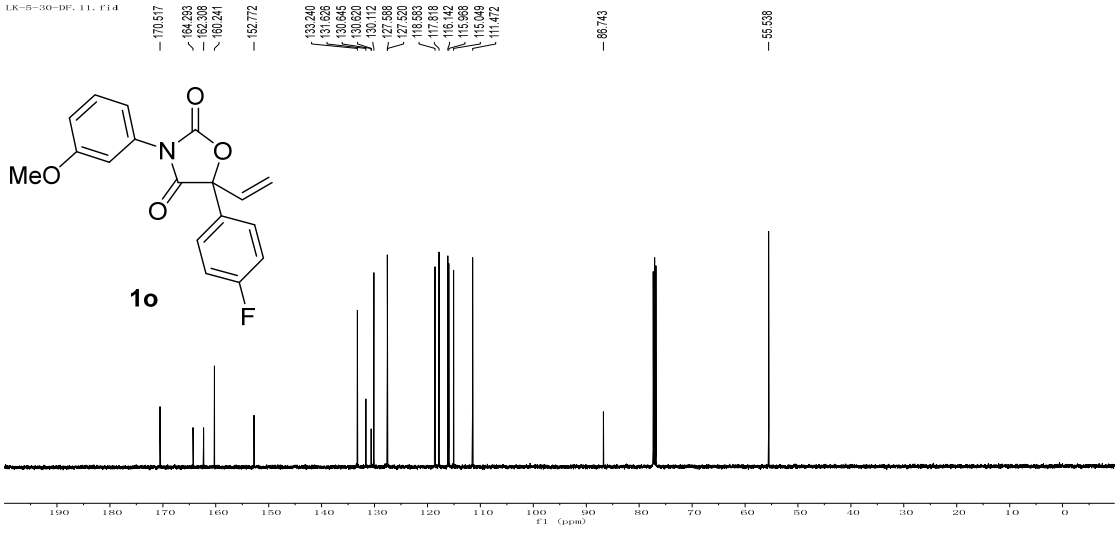


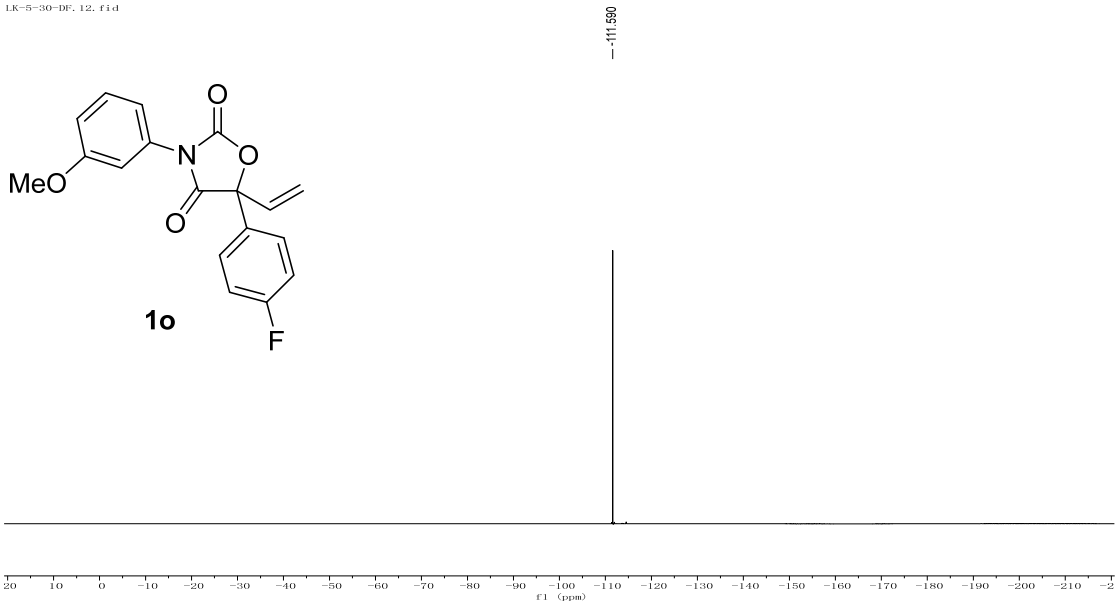




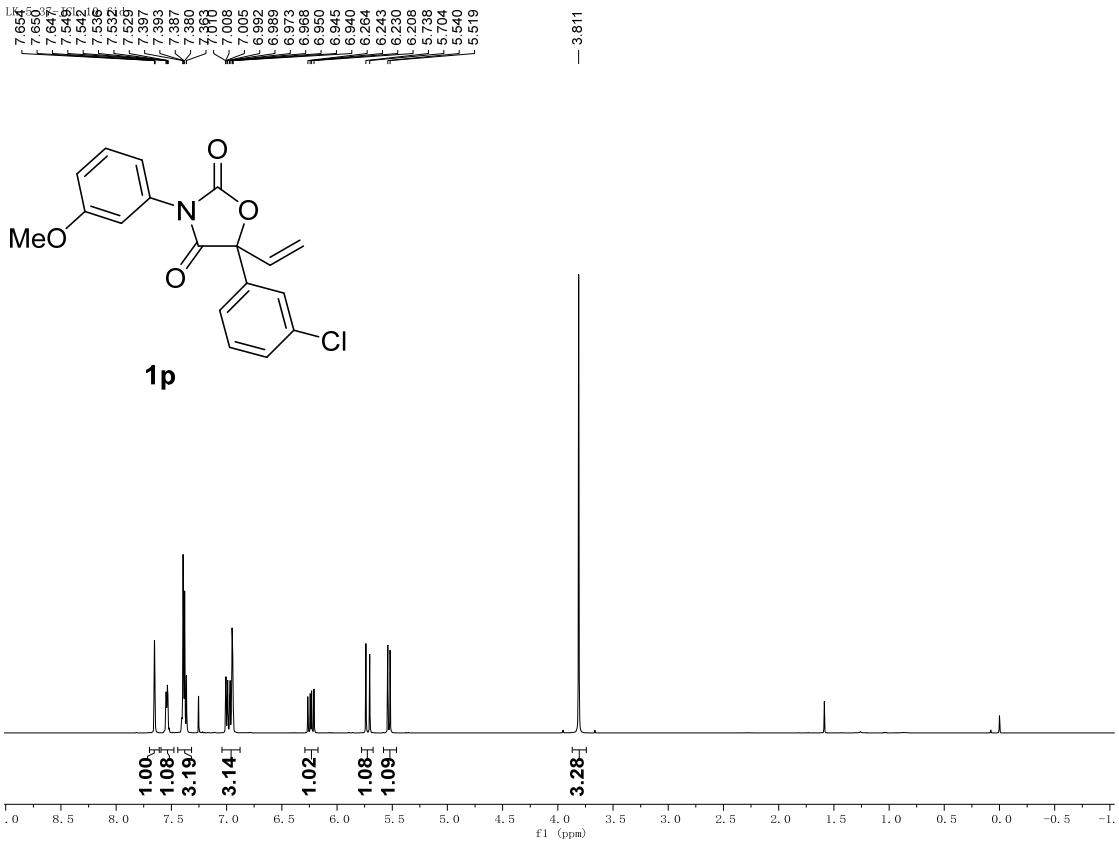
^{1}H NMR (500 MHz) ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **1n**

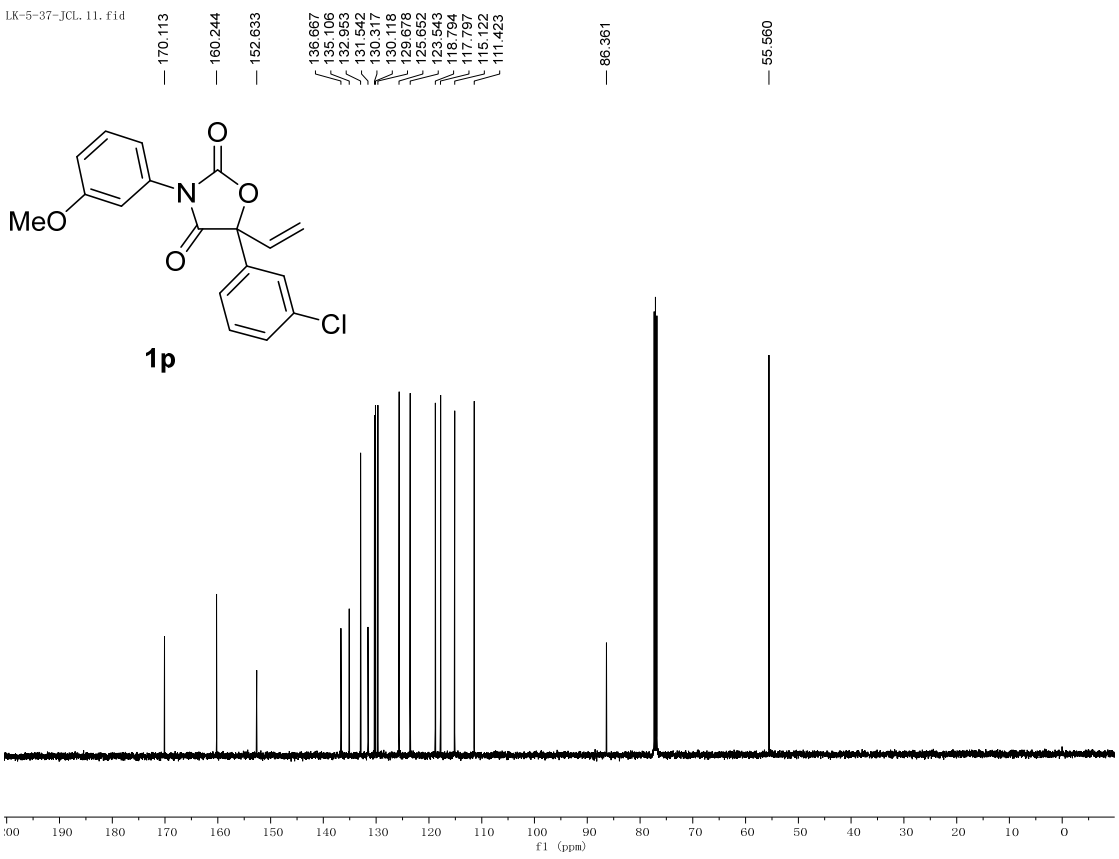




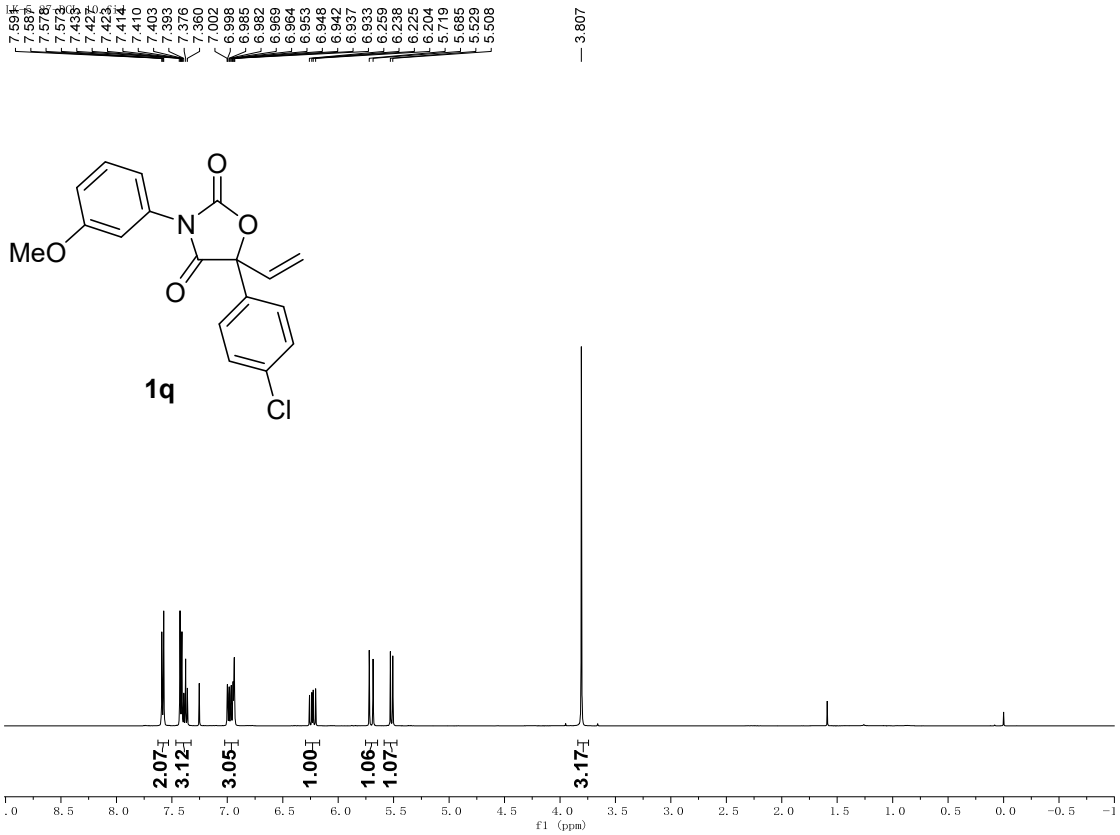


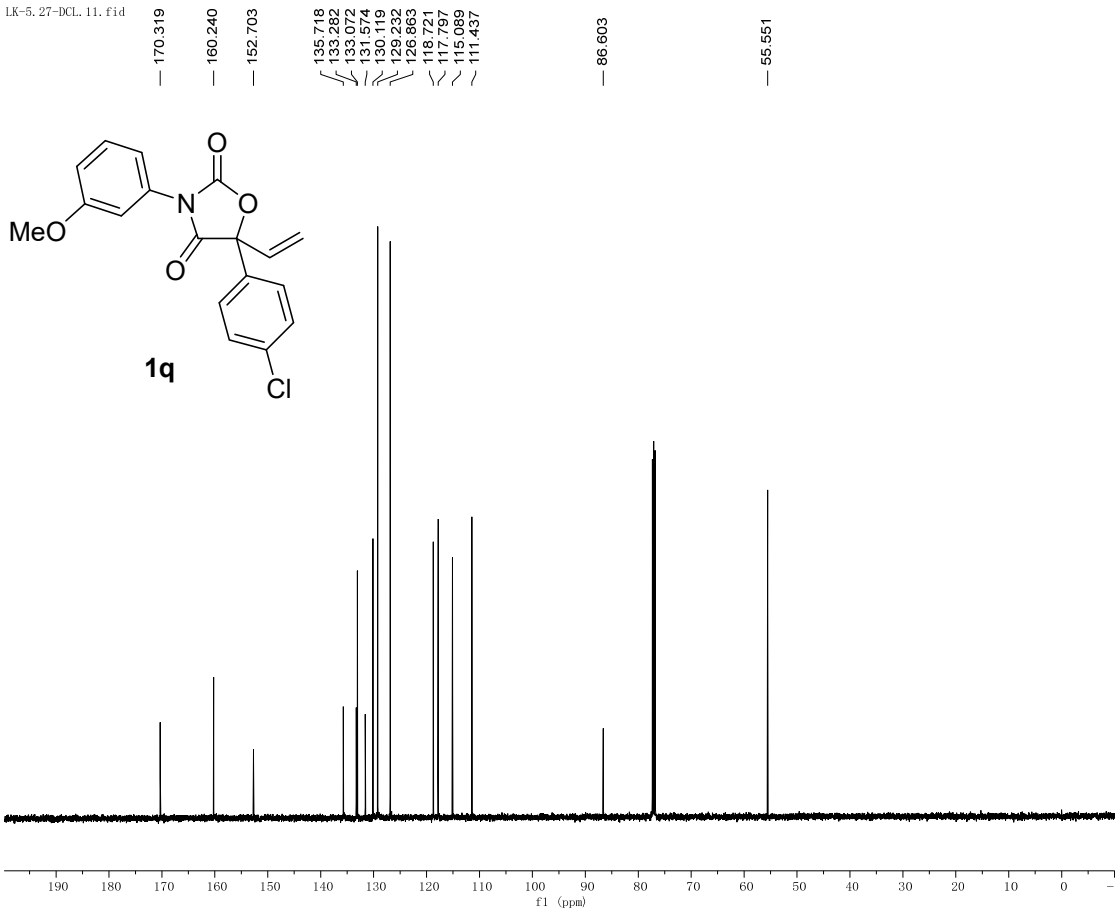
^{1}H NMR (500 MHz) ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **1o**



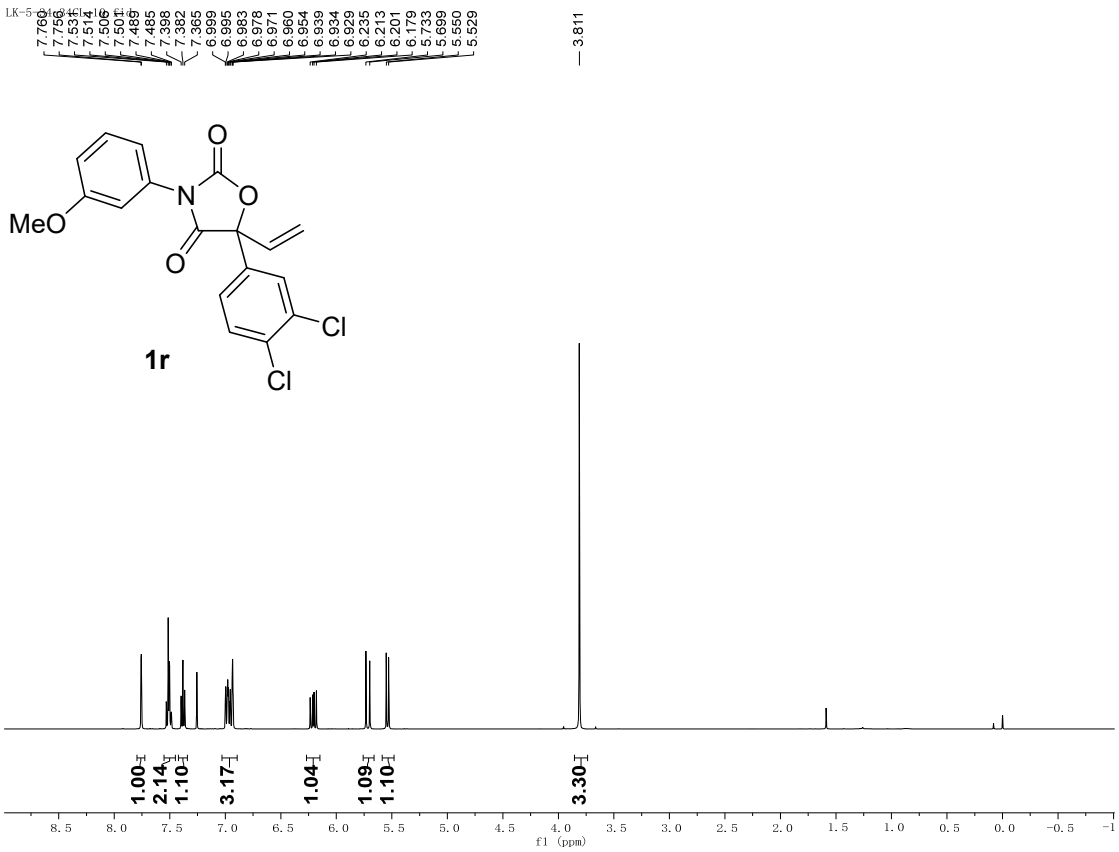


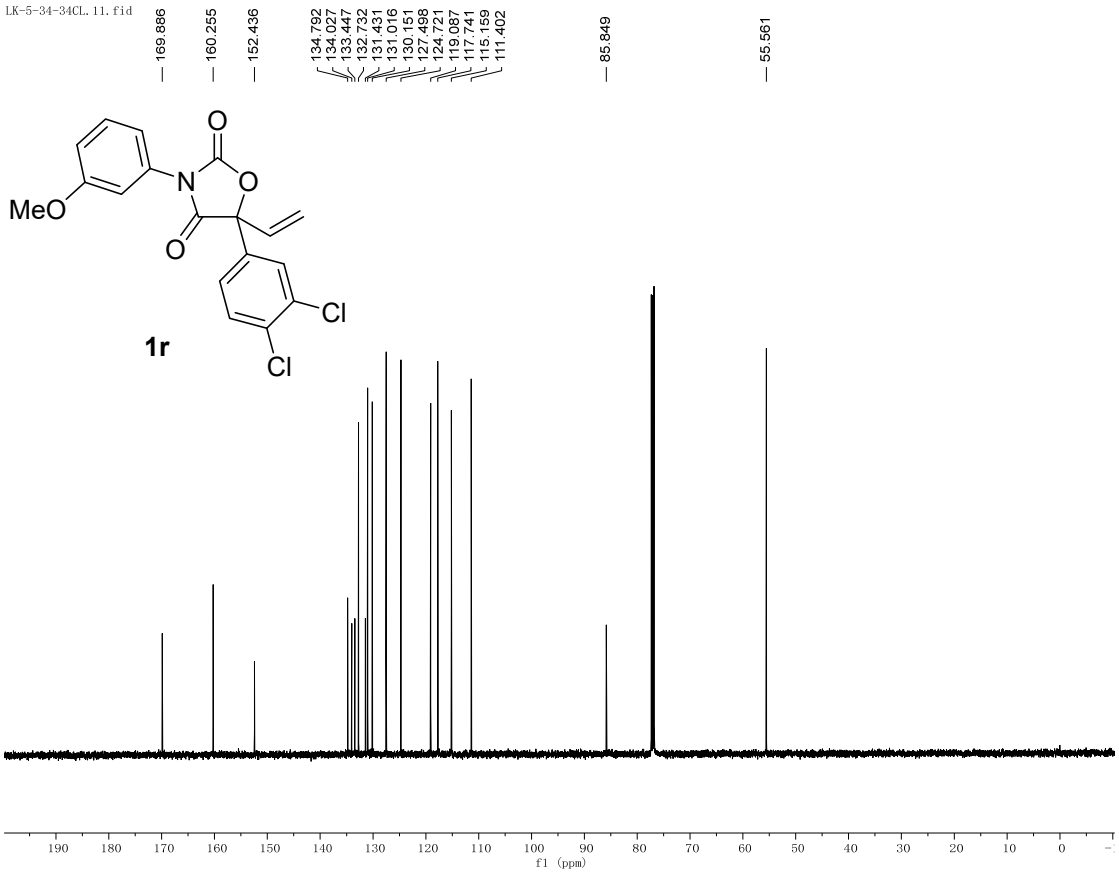
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1p**



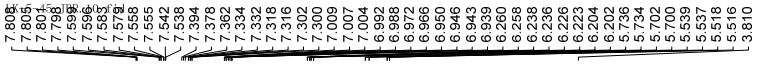


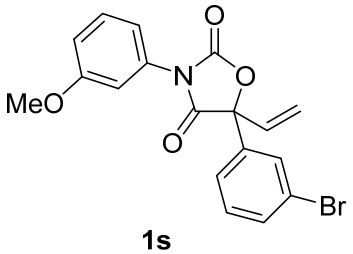
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1q**



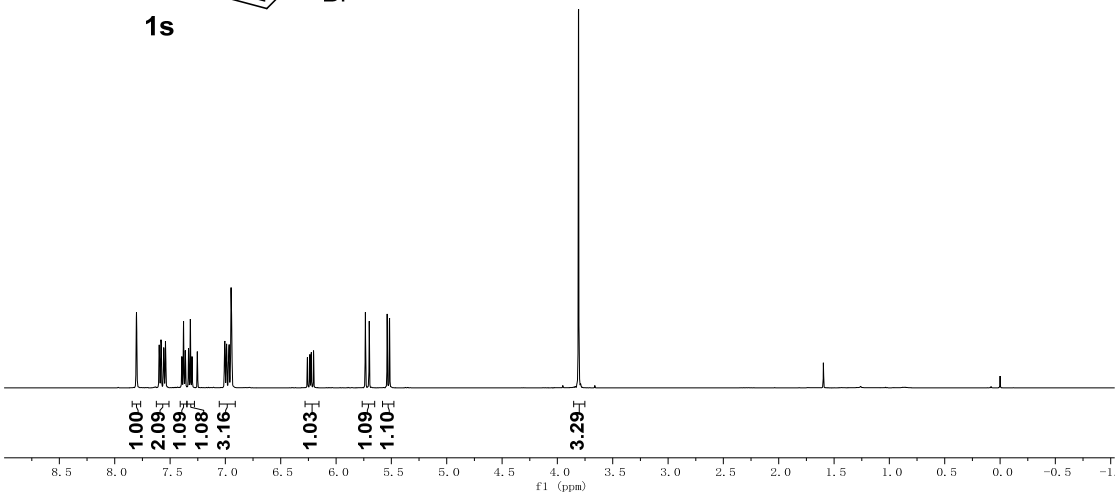


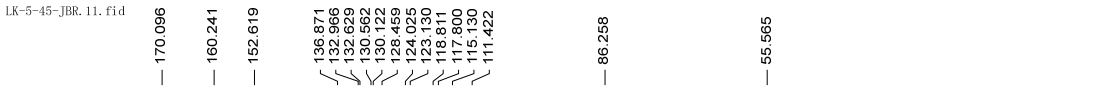
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1r**

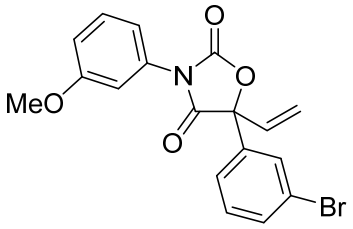




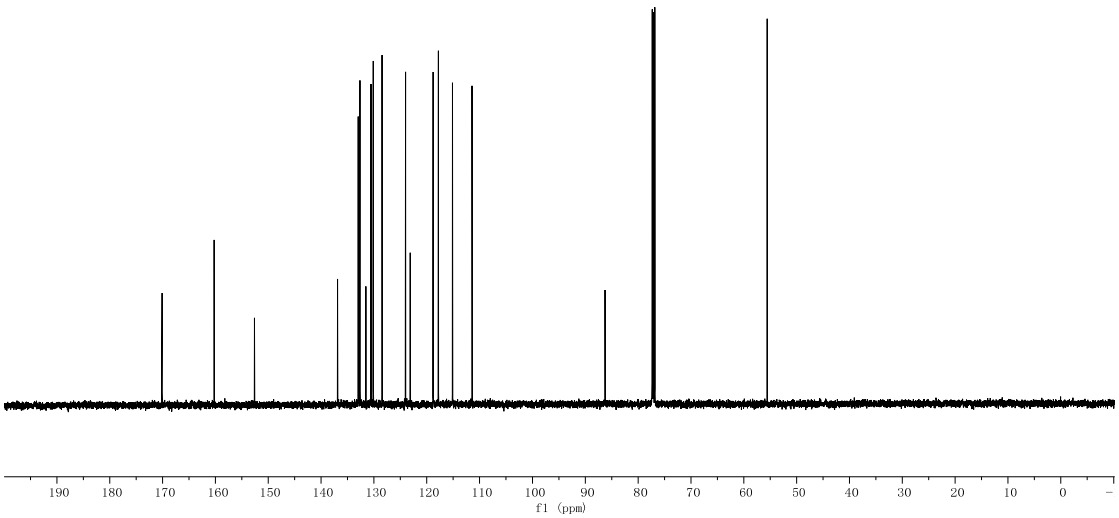
1s



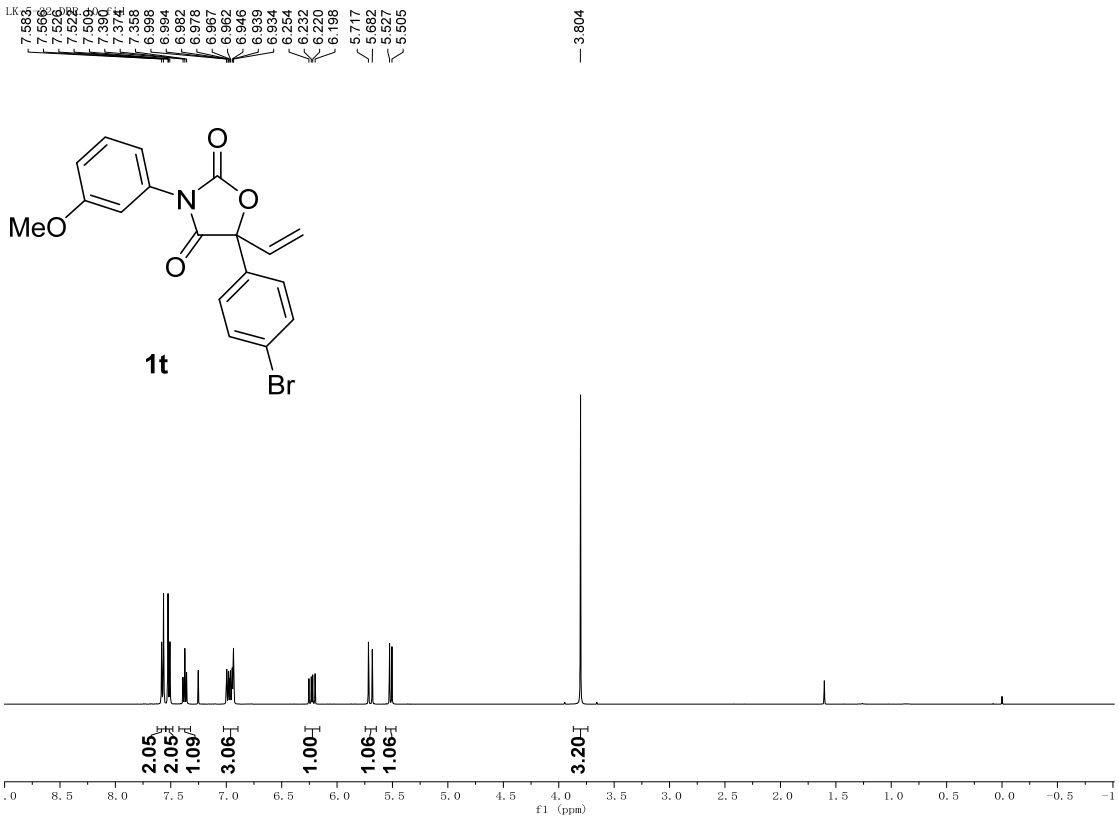


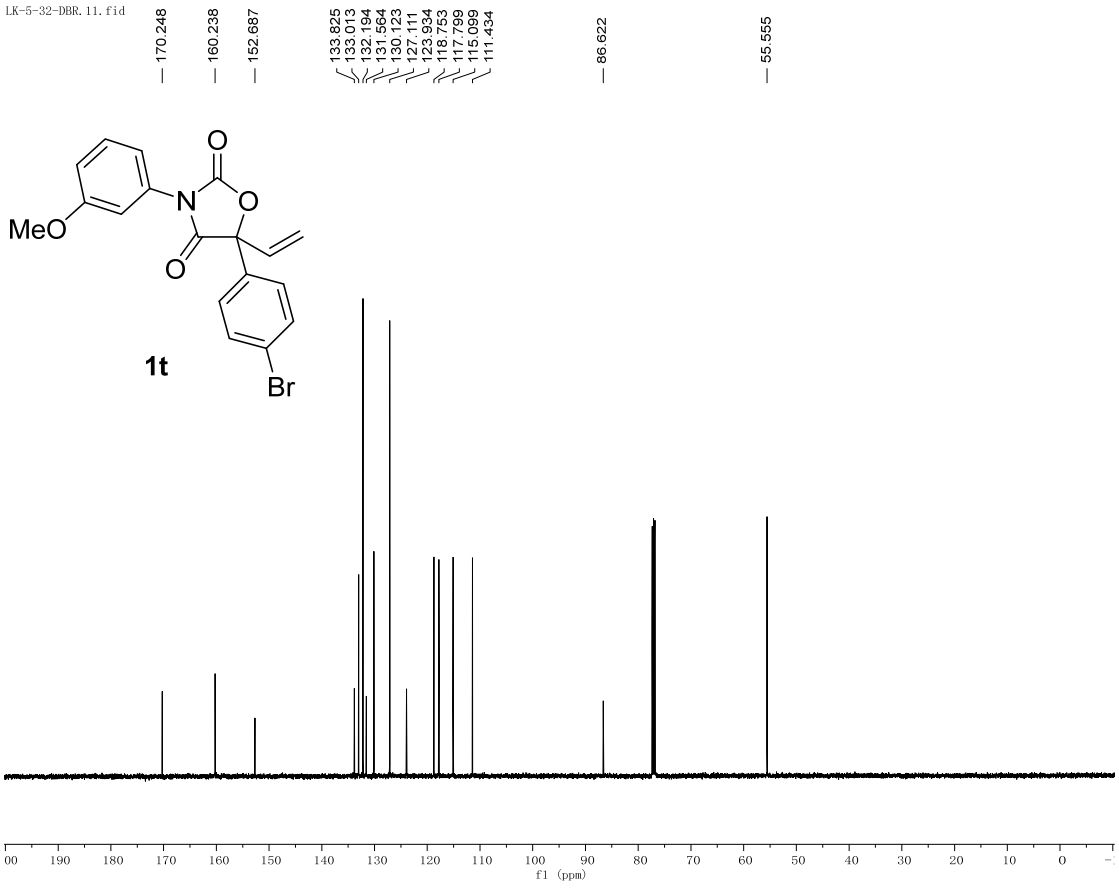


1s

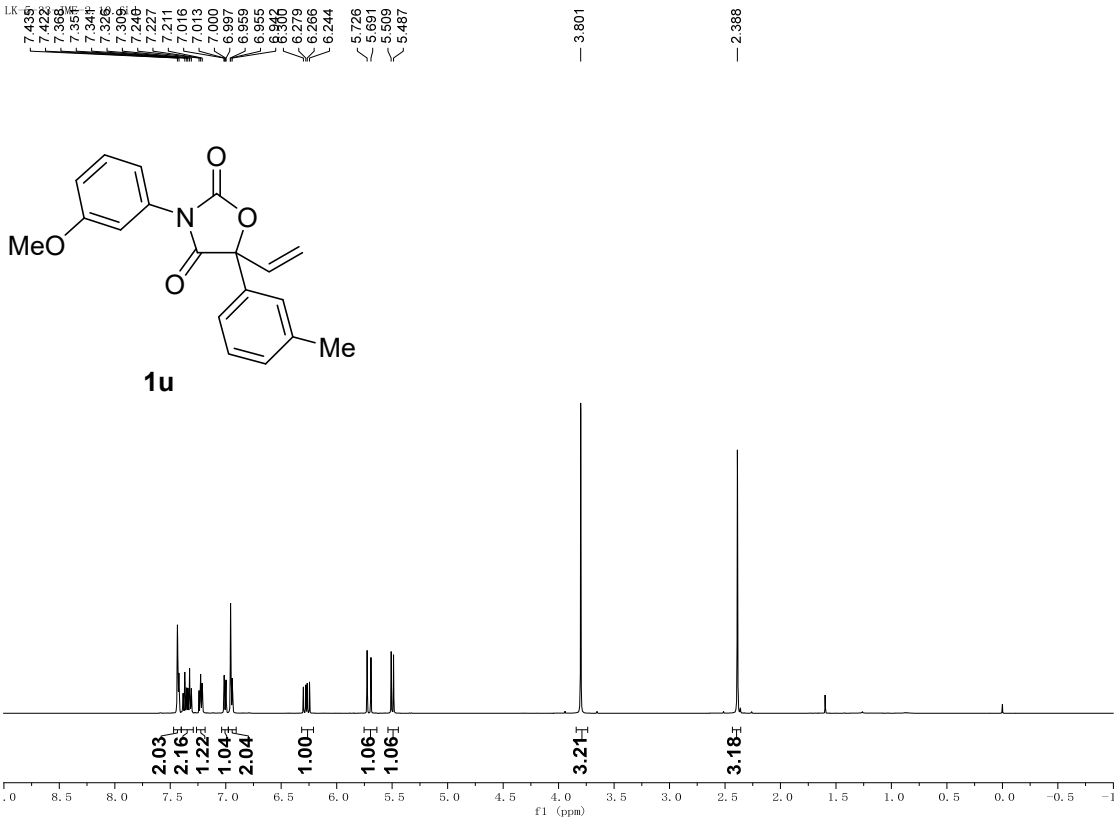


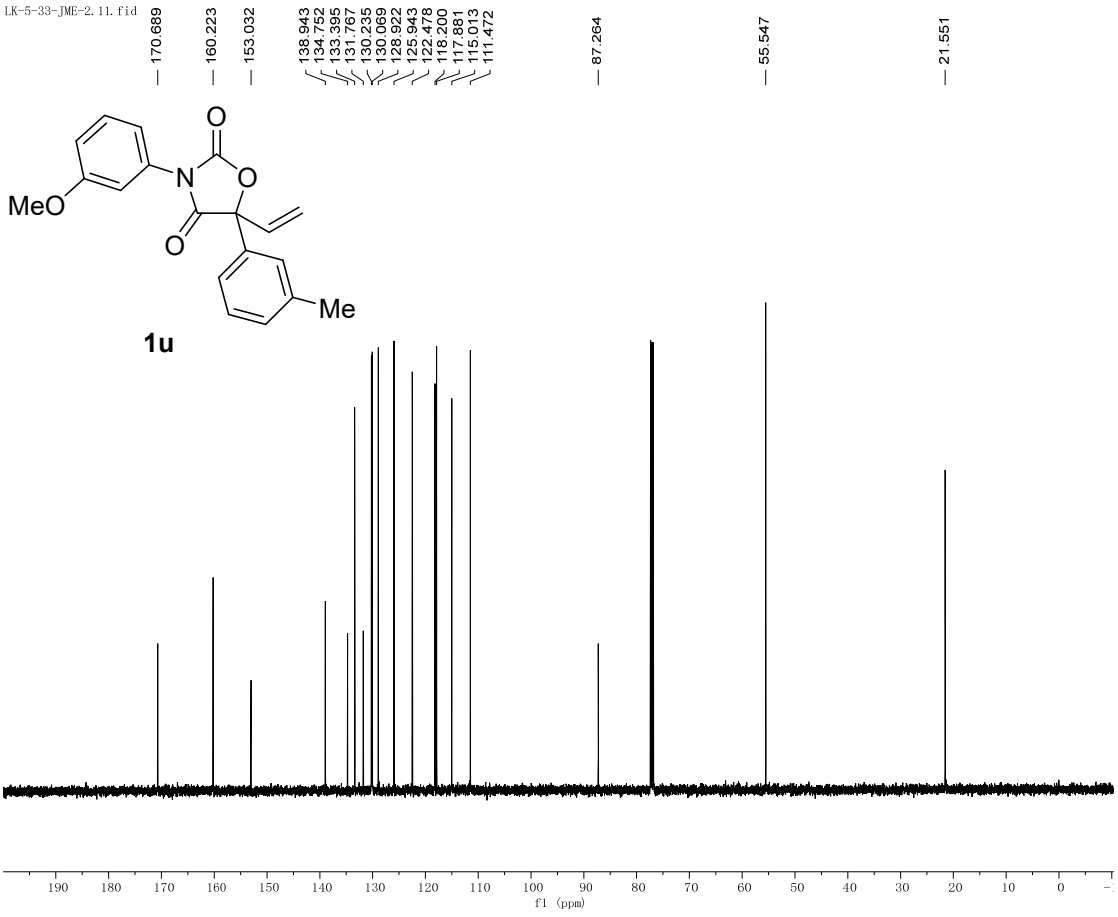
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1s**



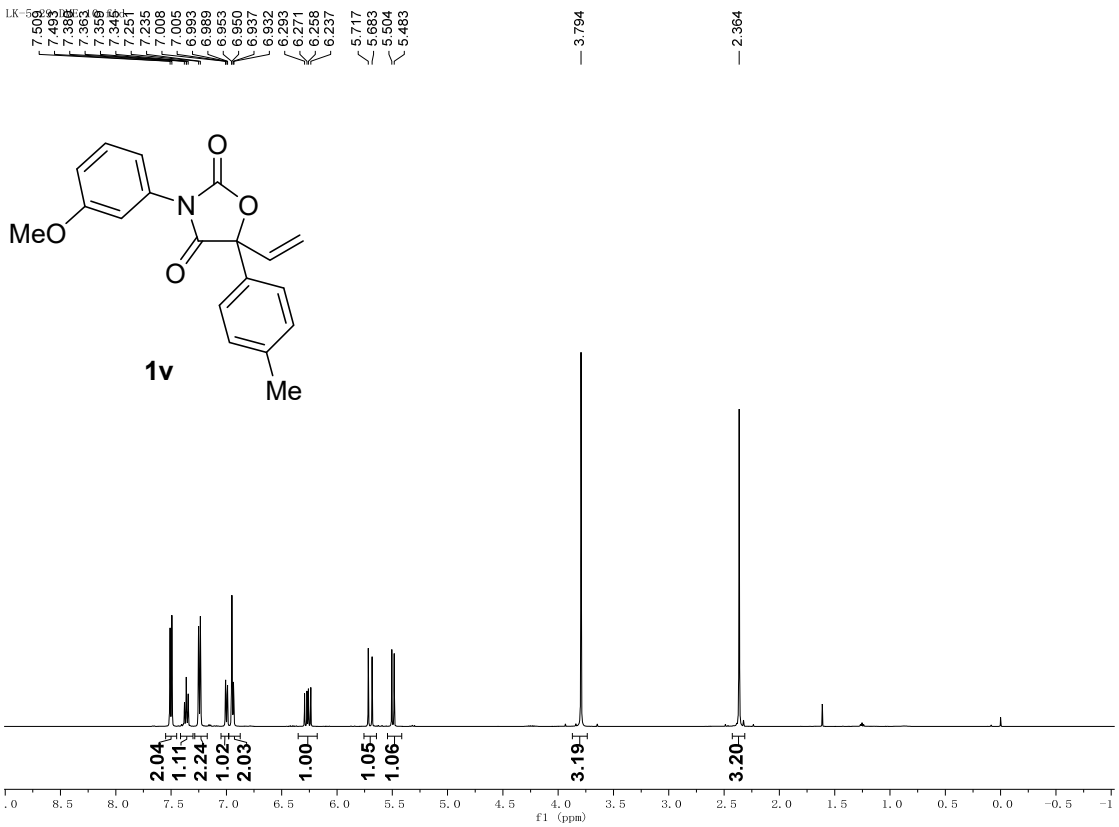


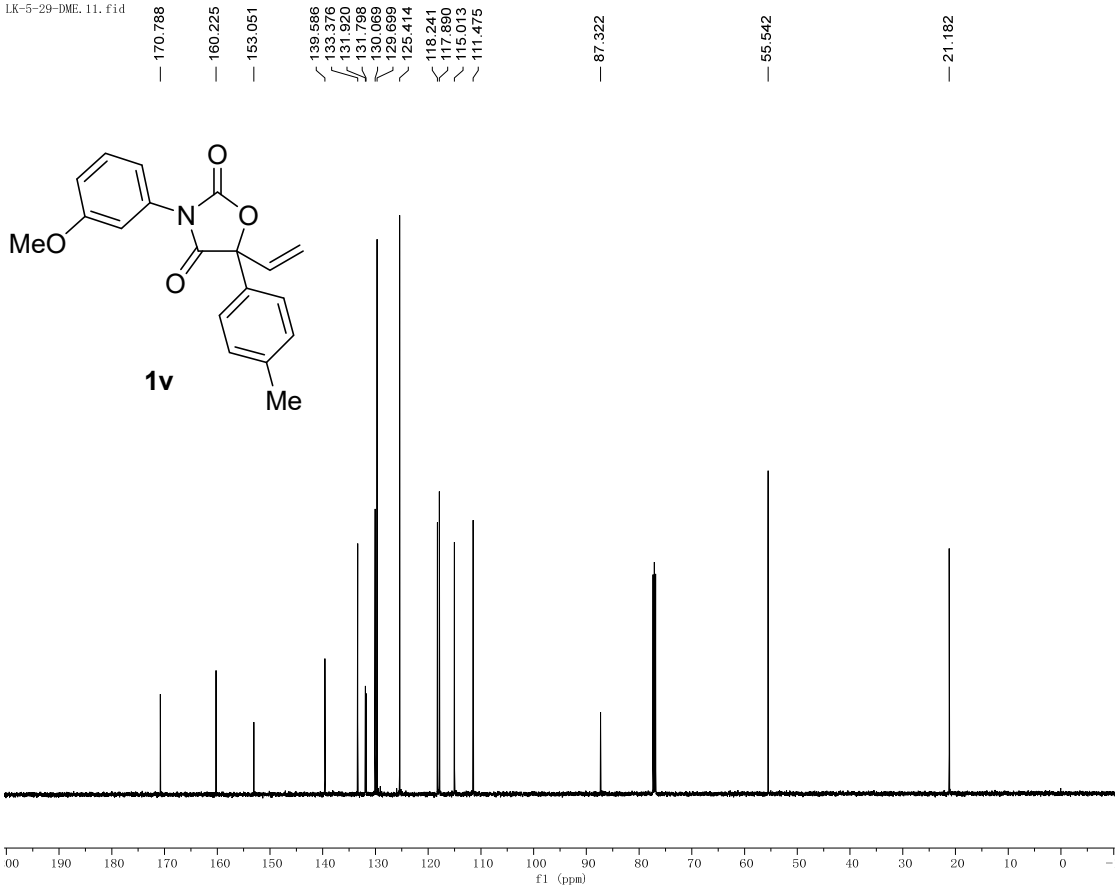
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1t**



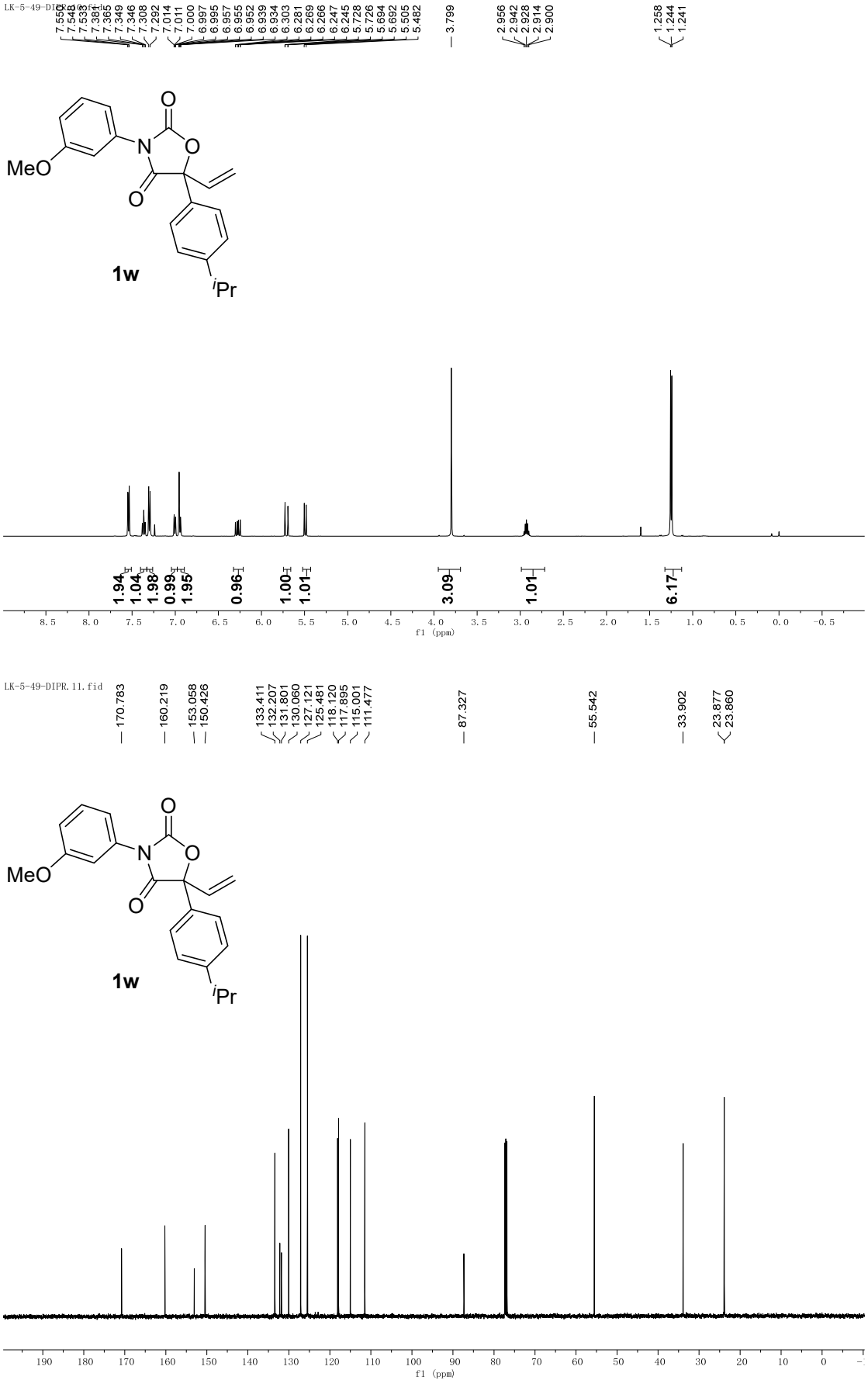


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1u**

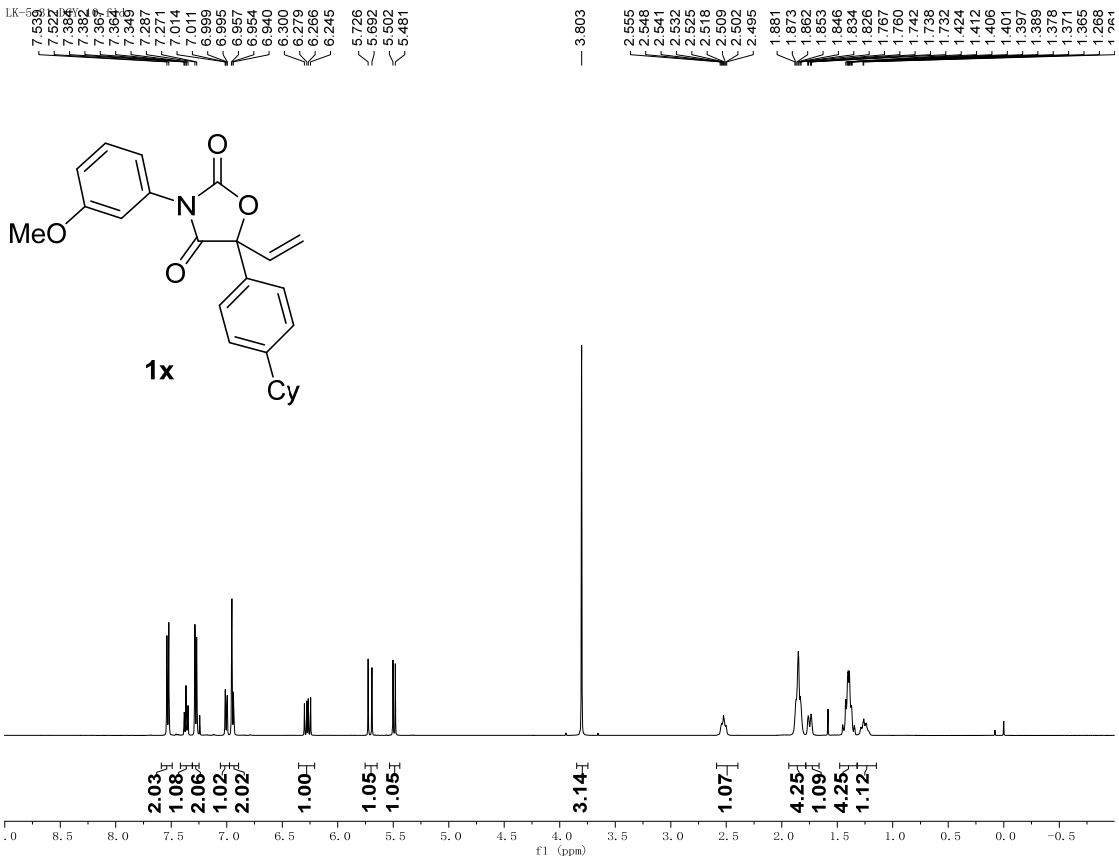


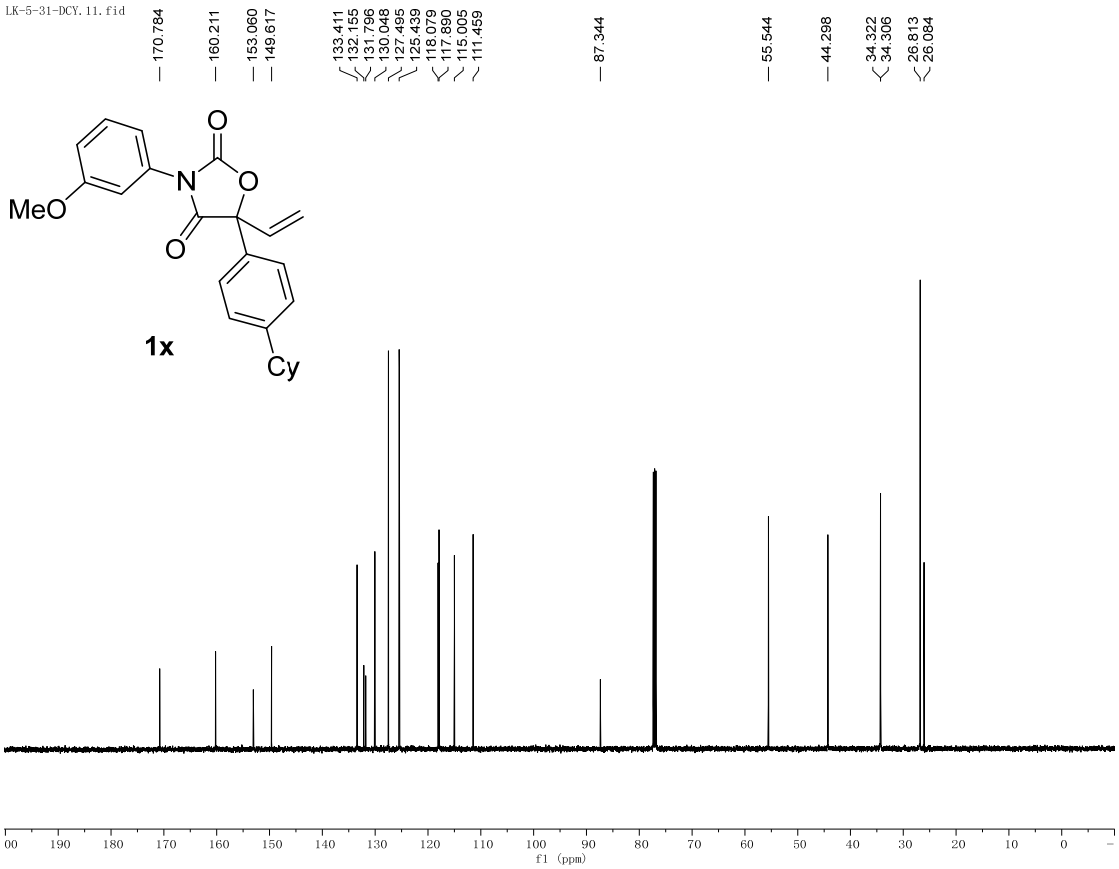


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1v**

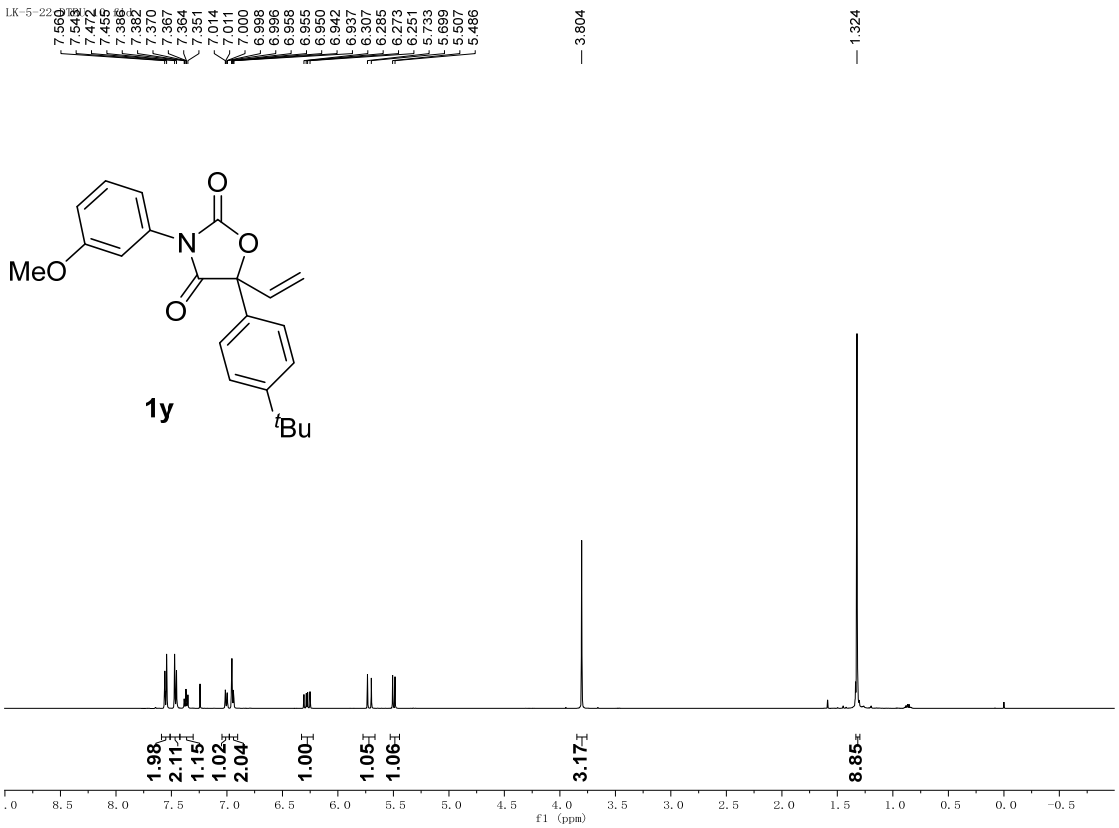


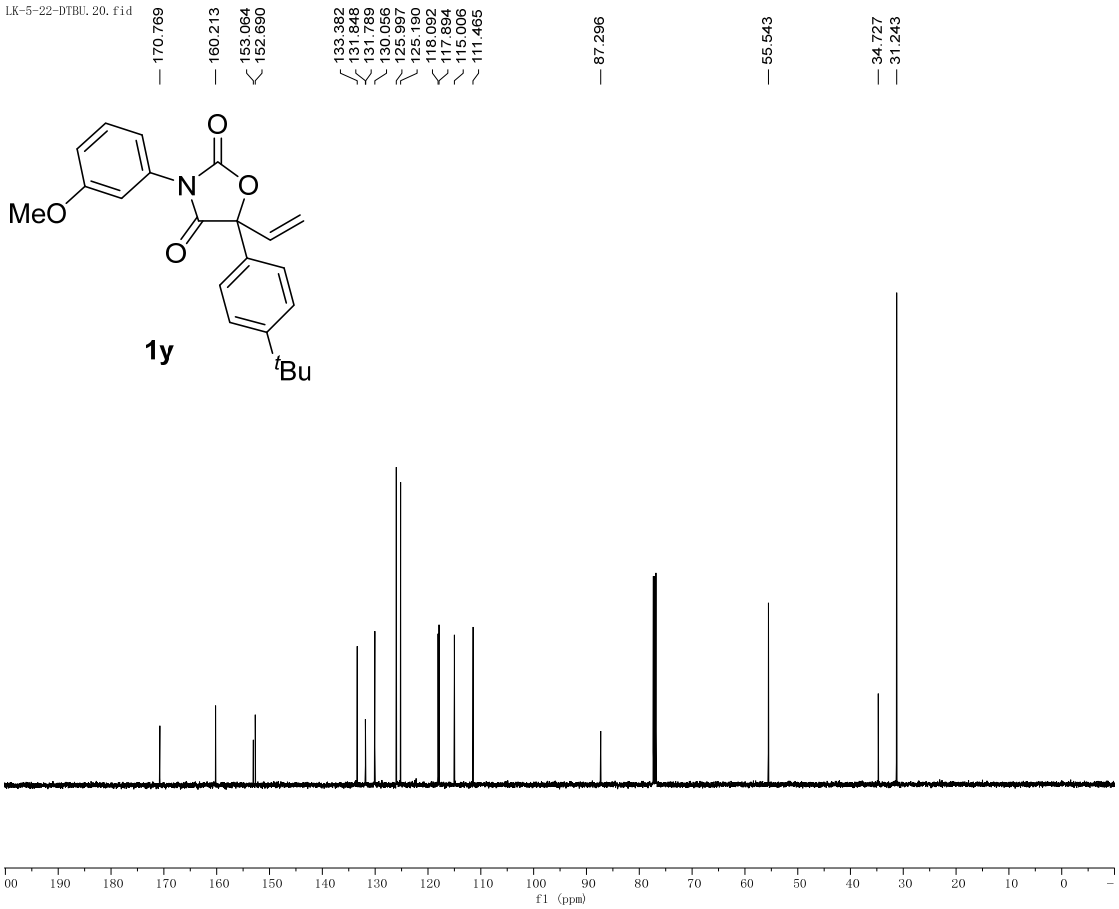
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1w**



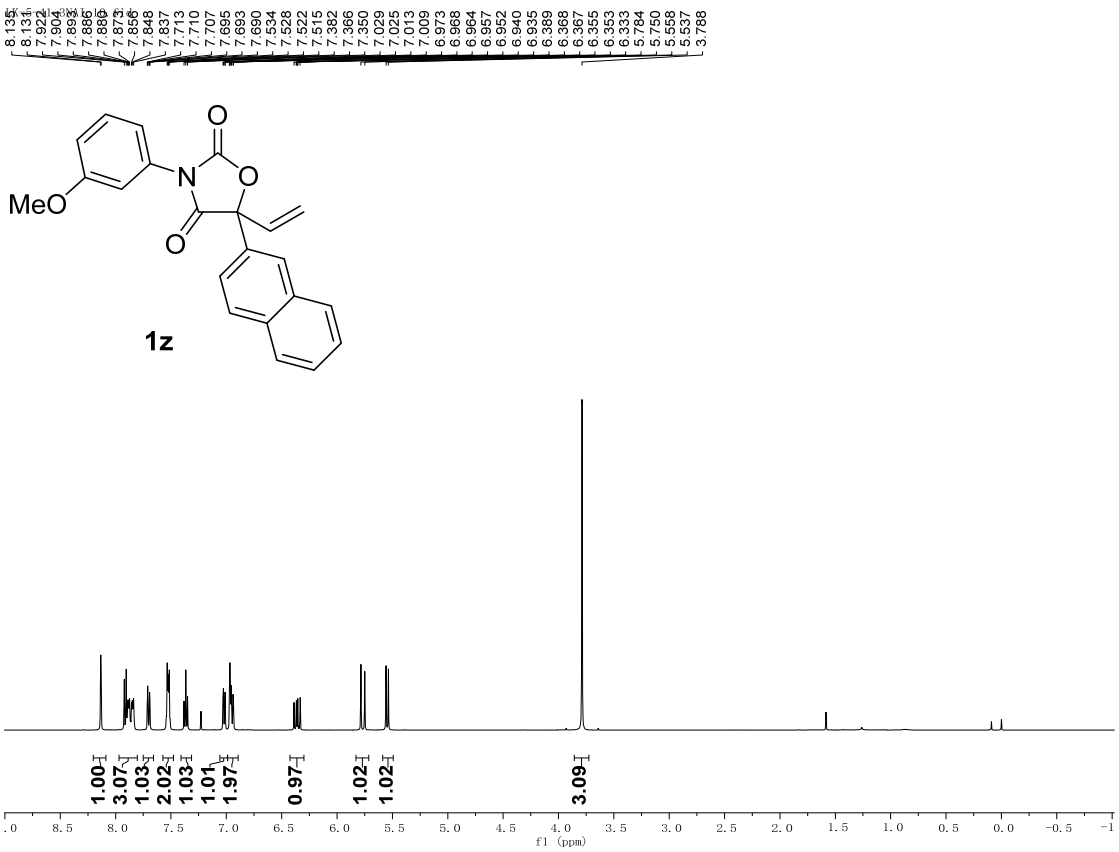


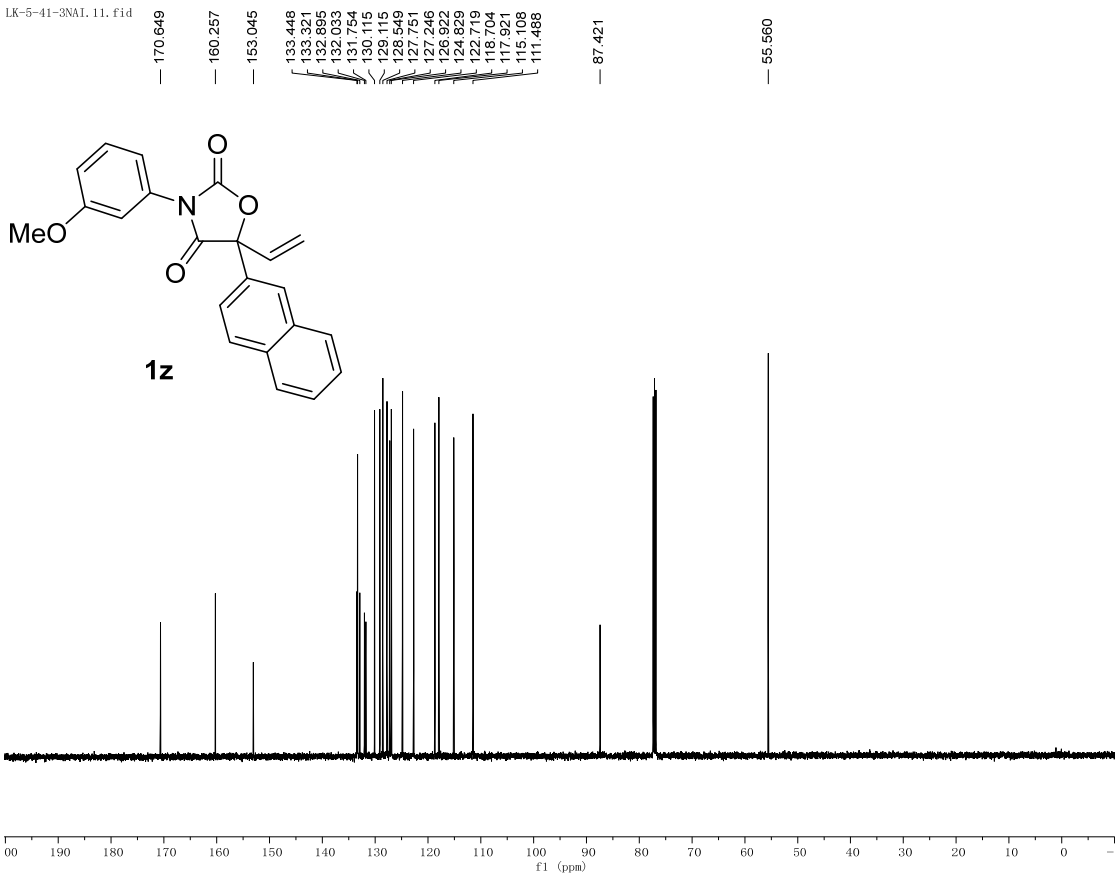
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1x**



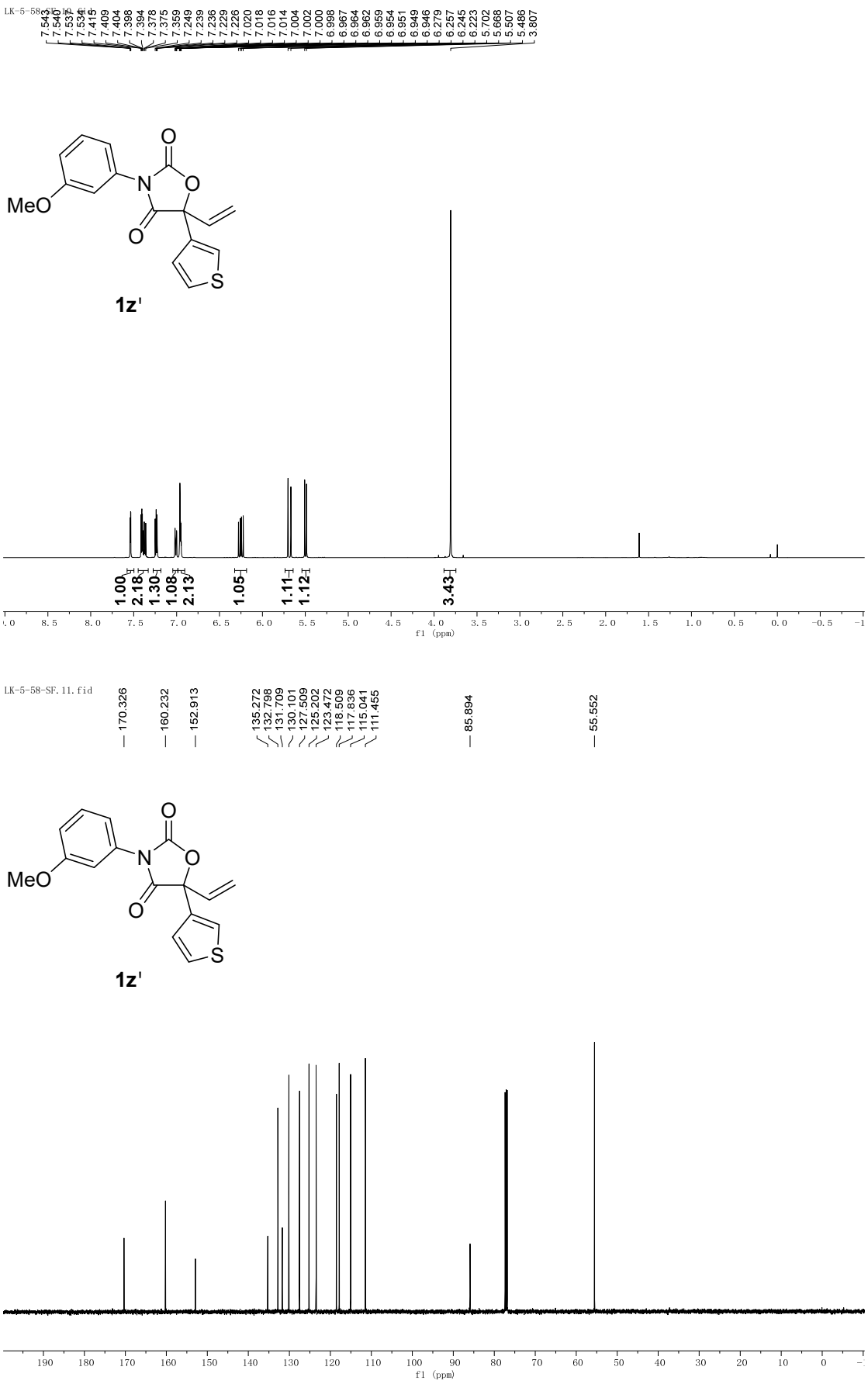


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1y**

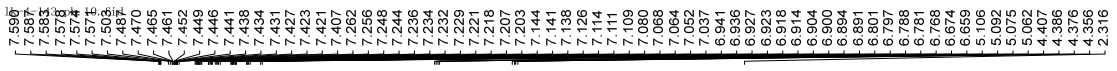


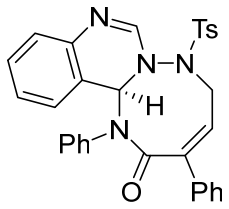


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1z**

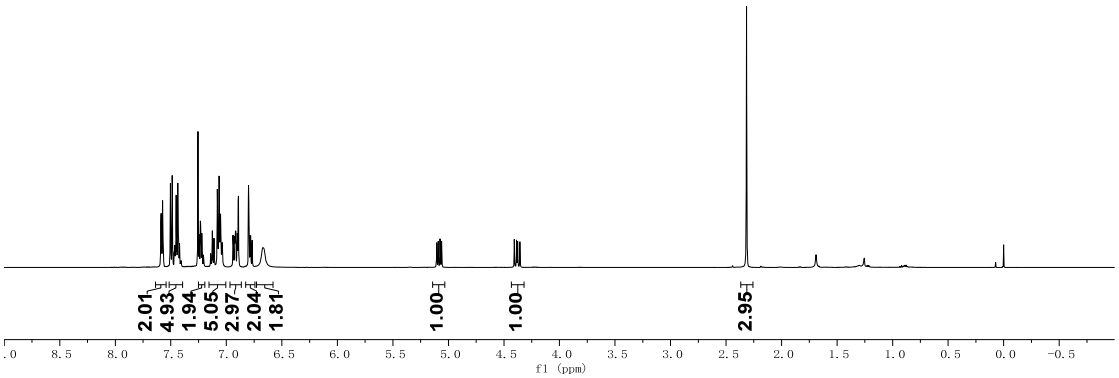


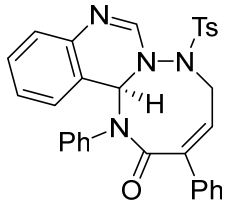
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **1z'**



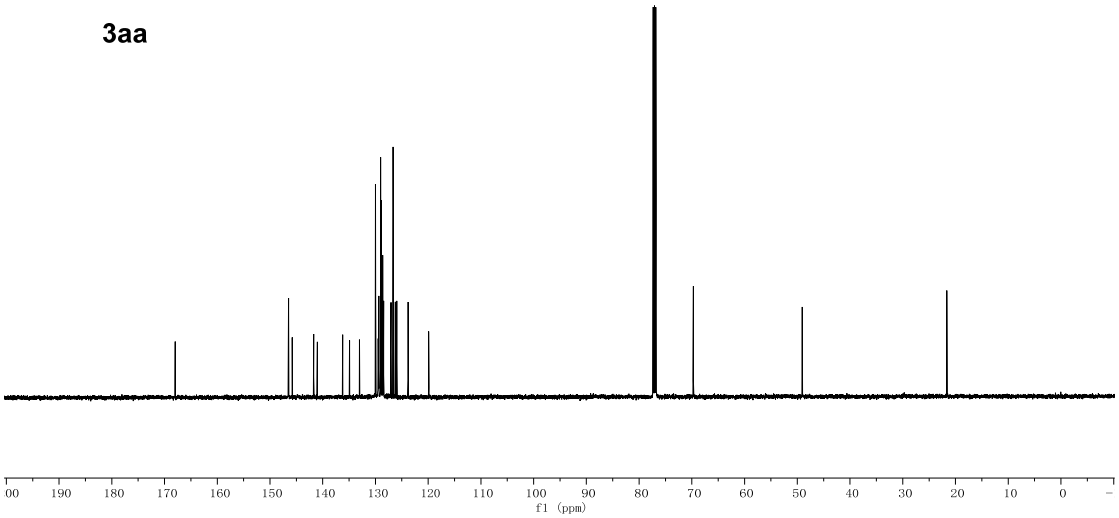


3aa

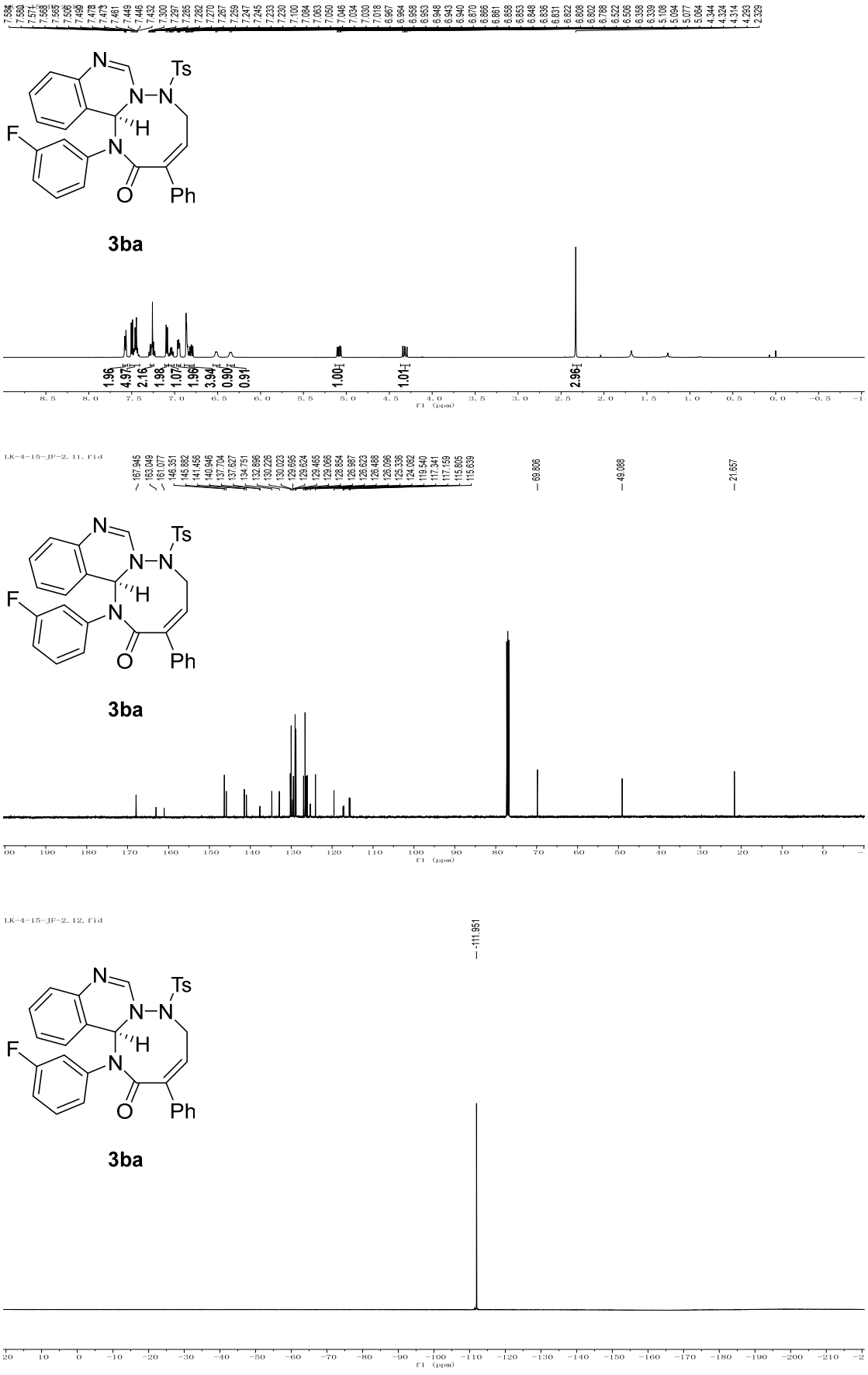




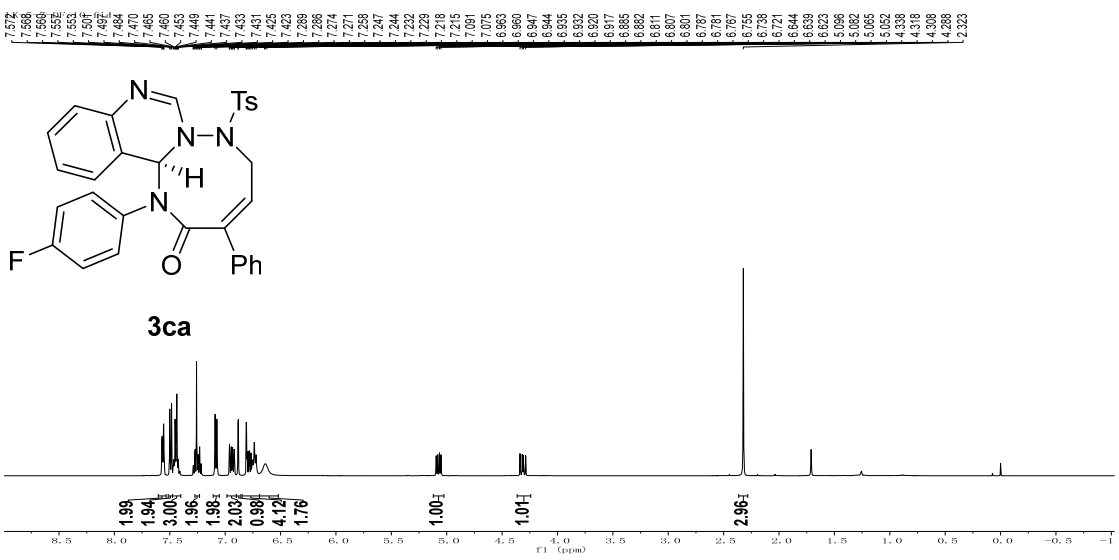
3aa

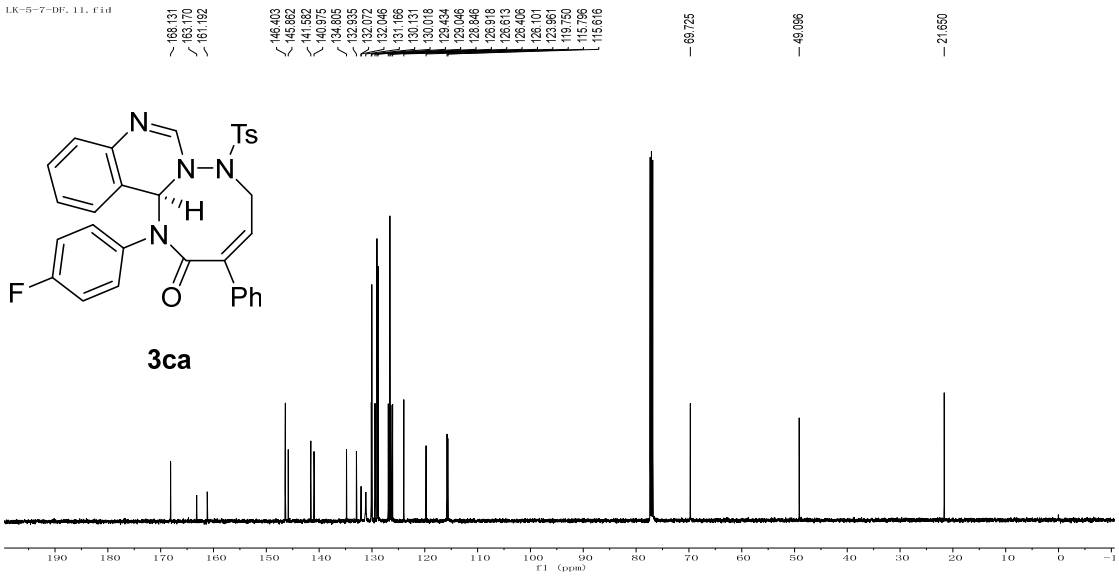


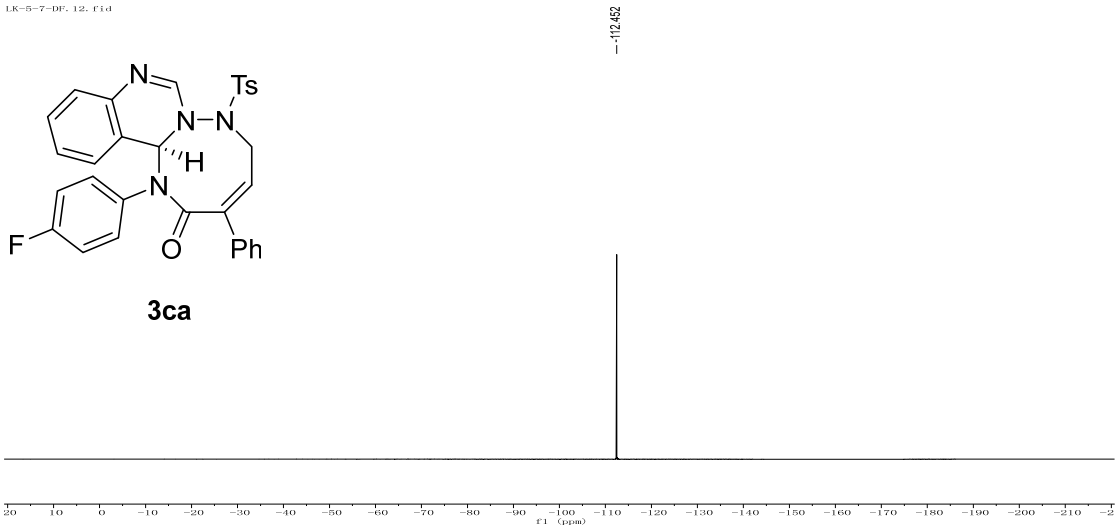
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3aa**



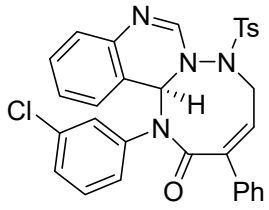
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3ba**



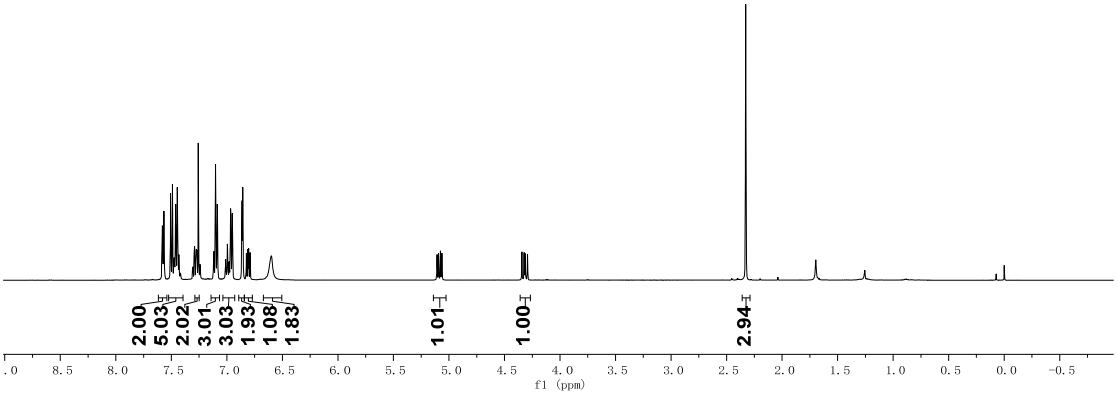


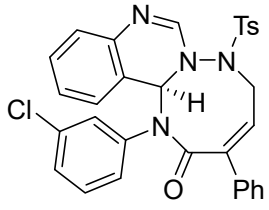


^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3ca**



3da





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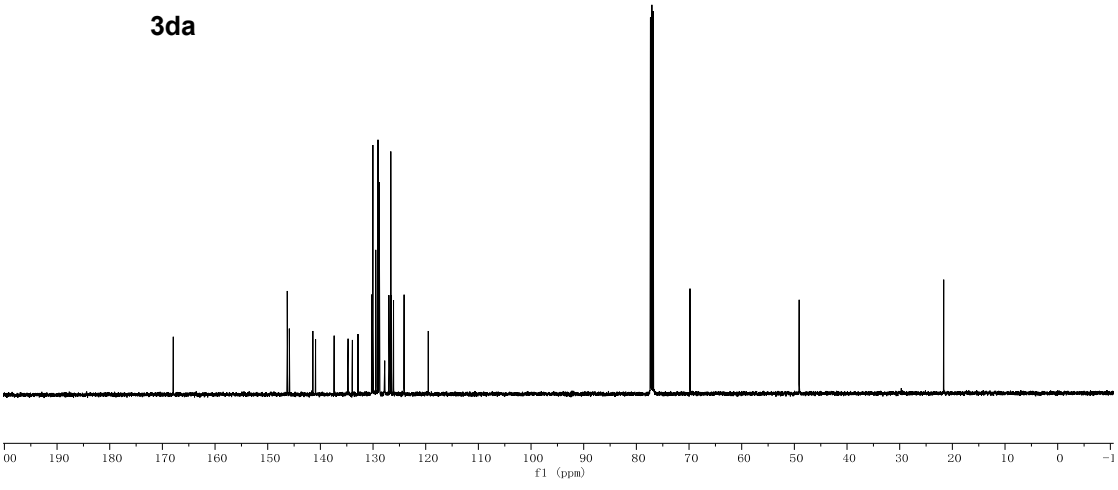
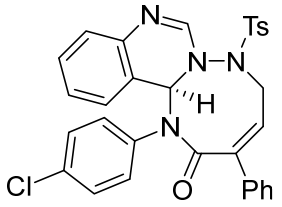
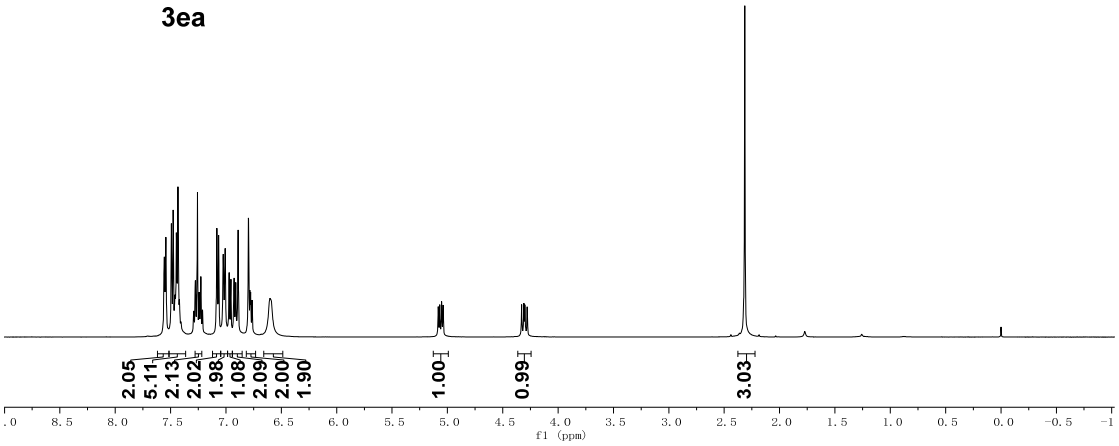
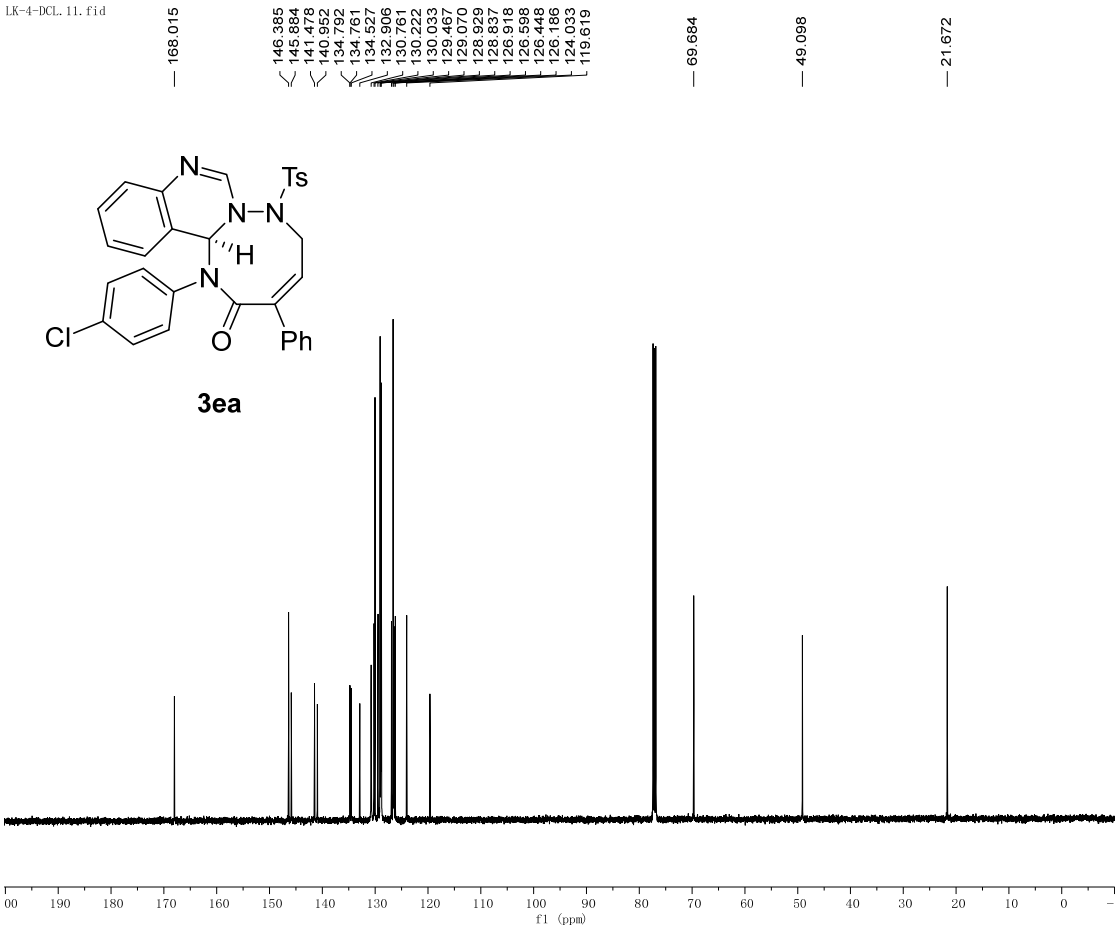


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3da**



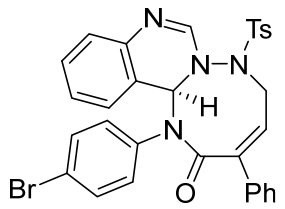
3ea





3ea

^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ea**



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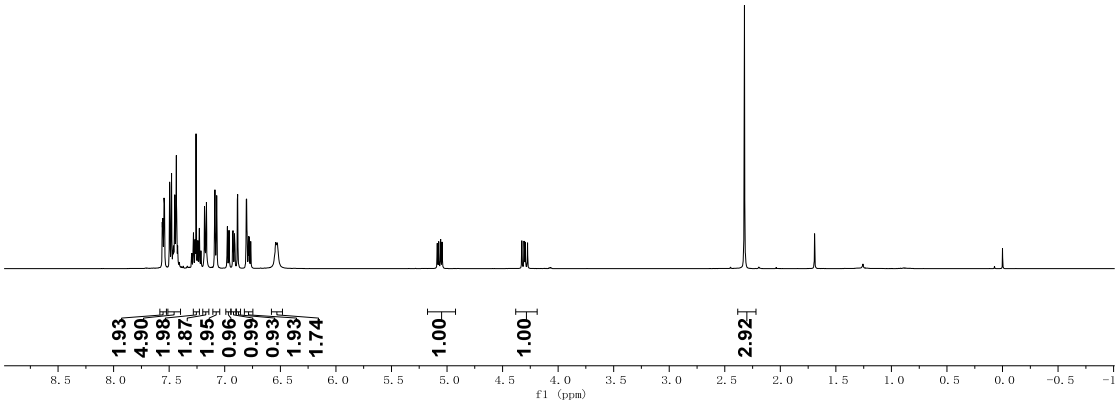
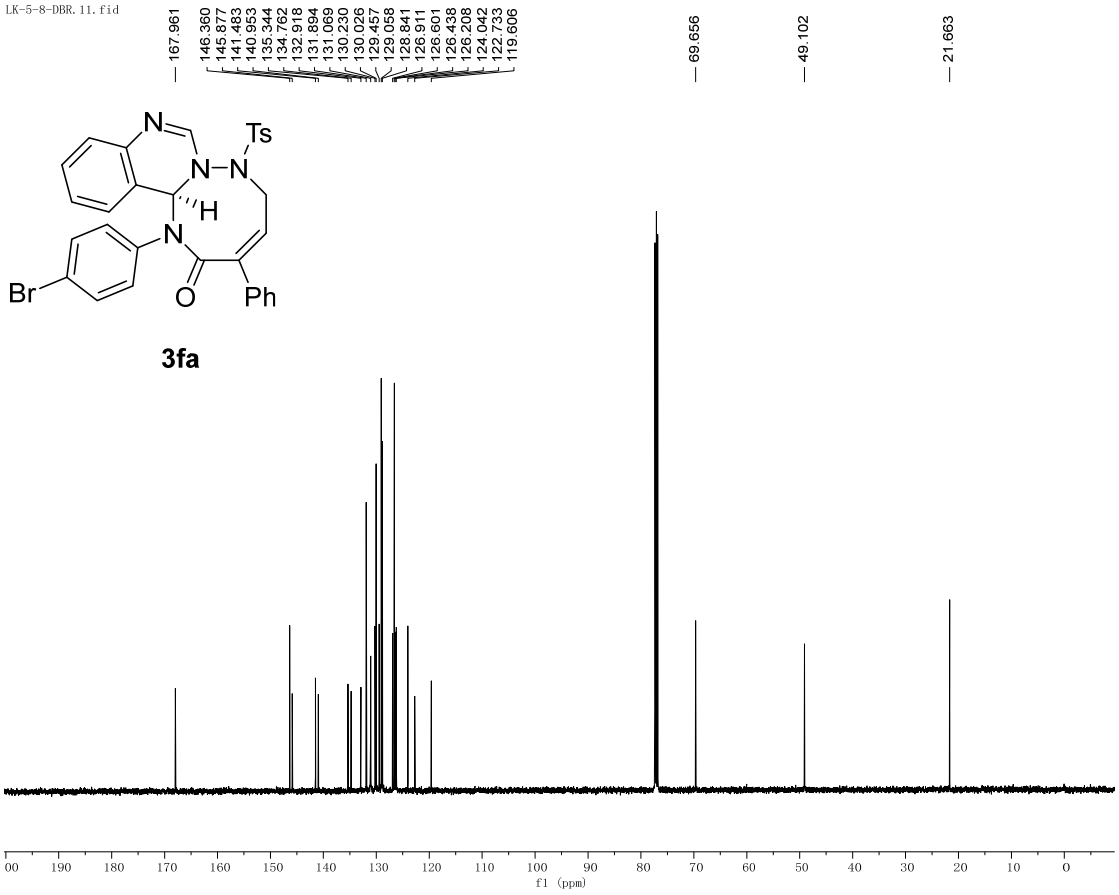
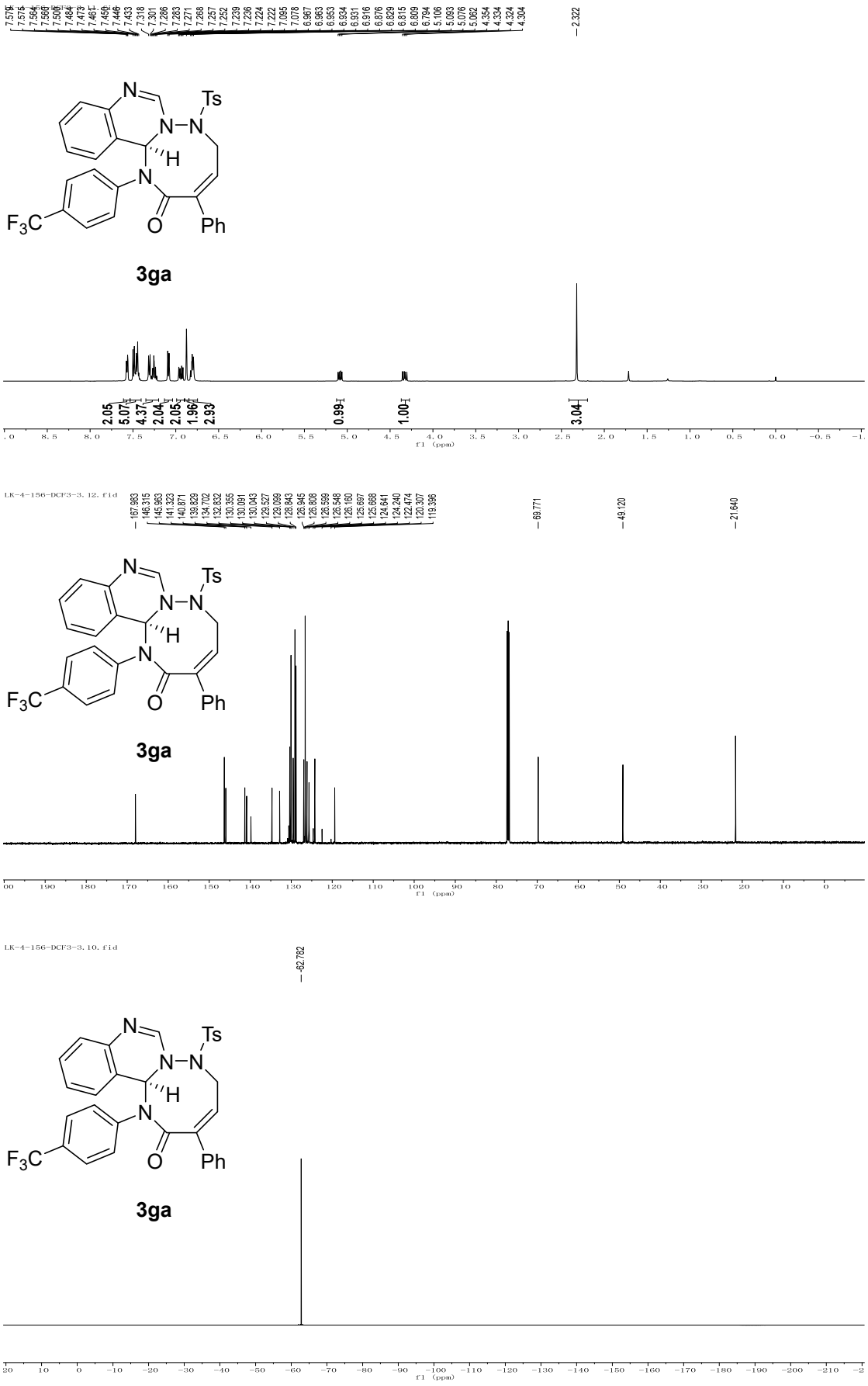


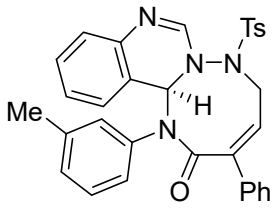


3fa

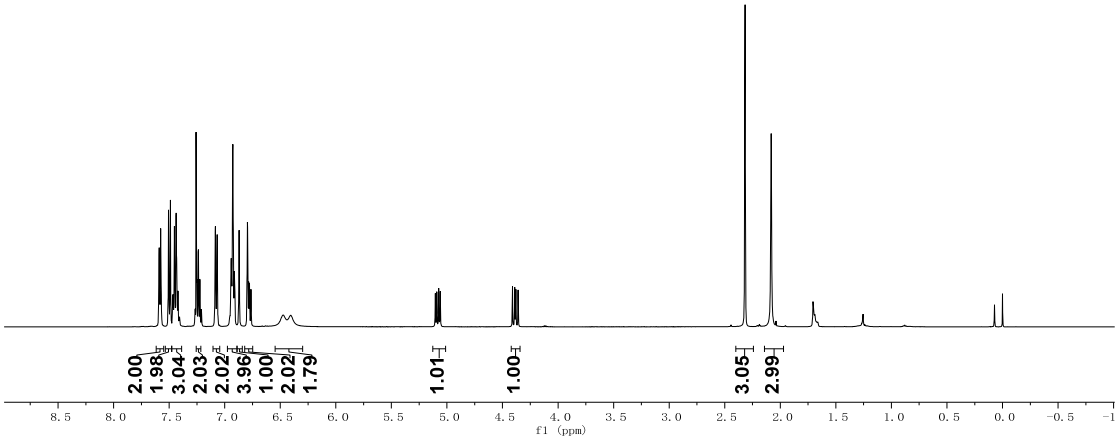
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3fa**

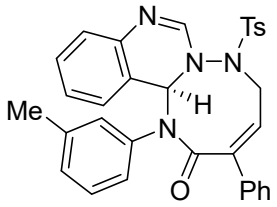


^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3ga**

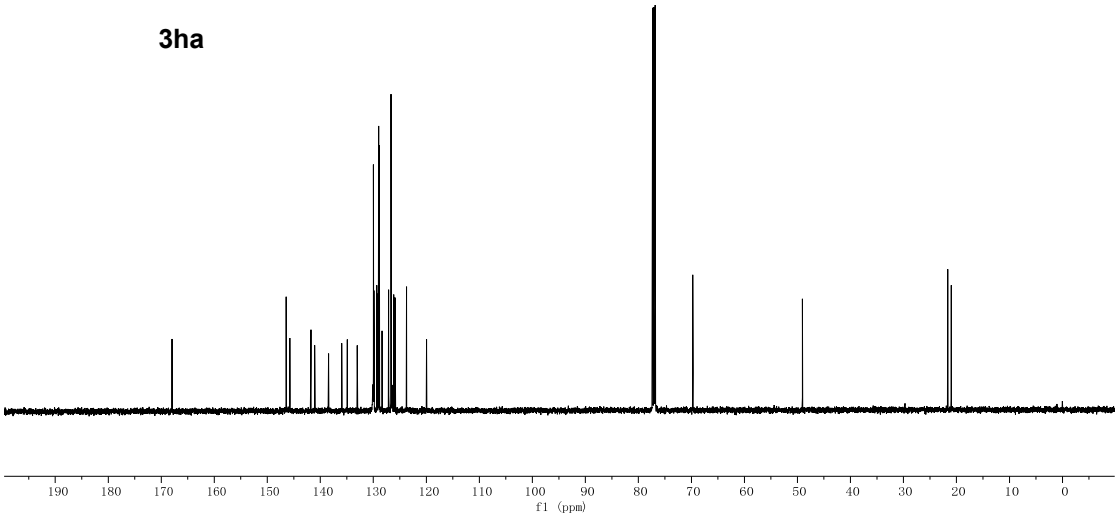


3ha

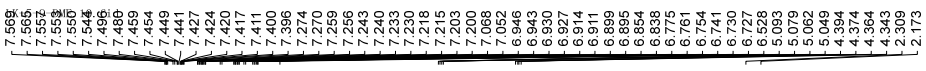


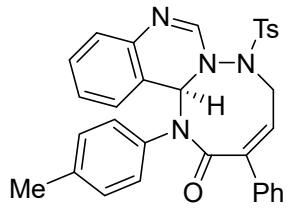


3ha

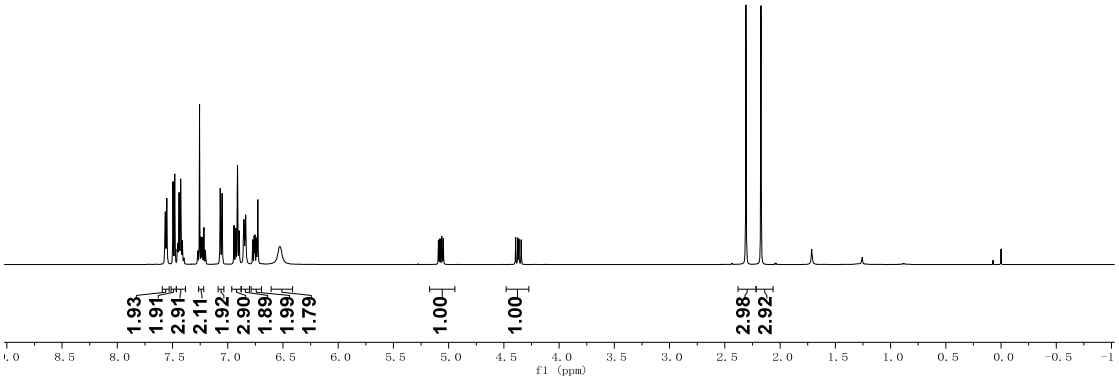


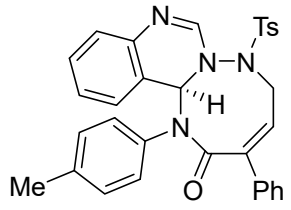
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ha**



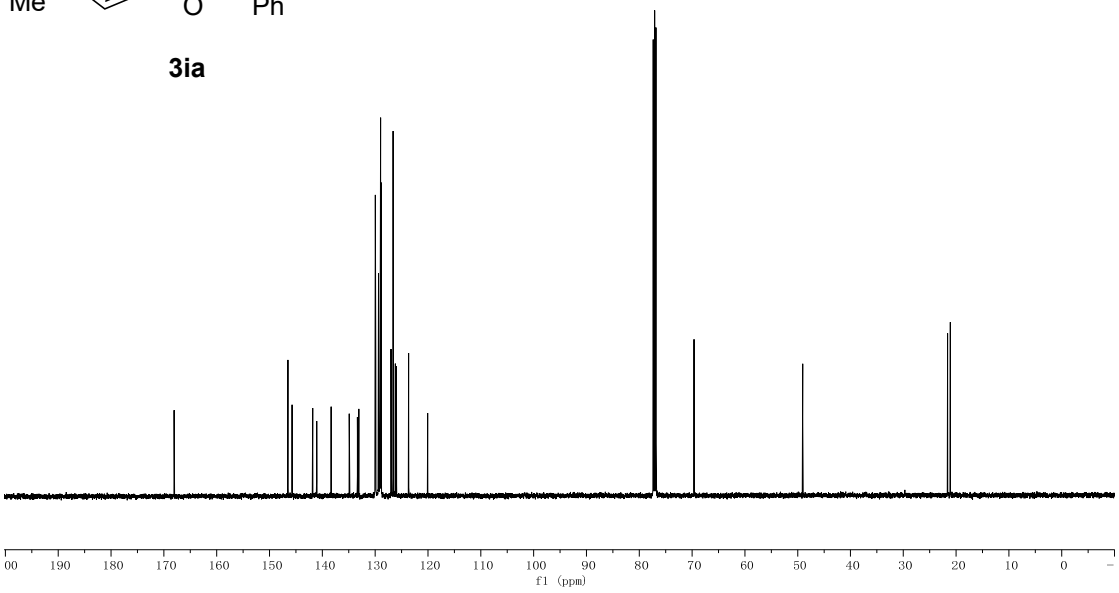


3ia

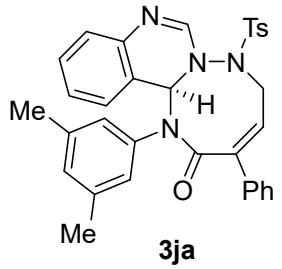




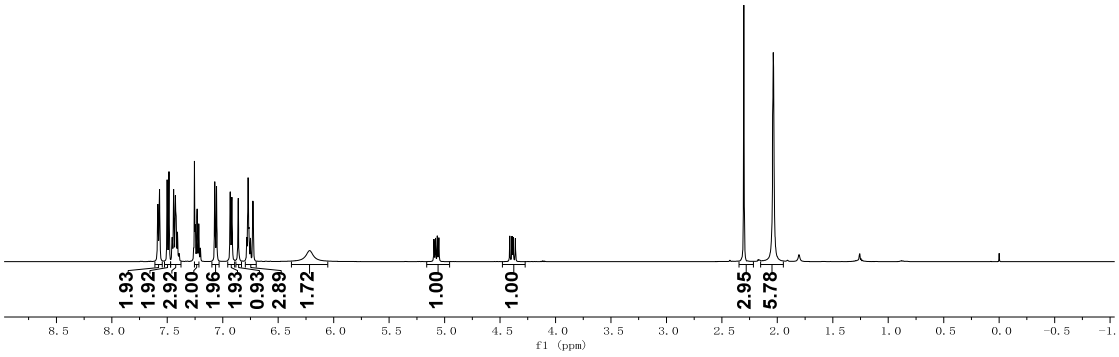
3ia

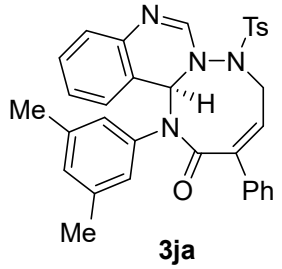


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ia**



3ja





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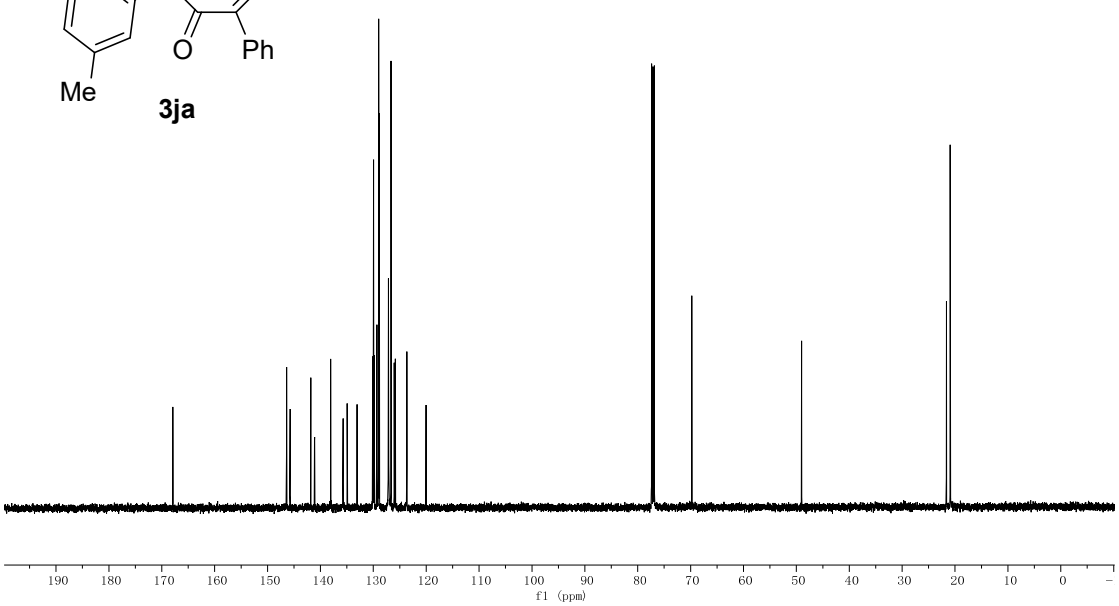
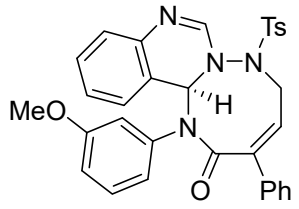
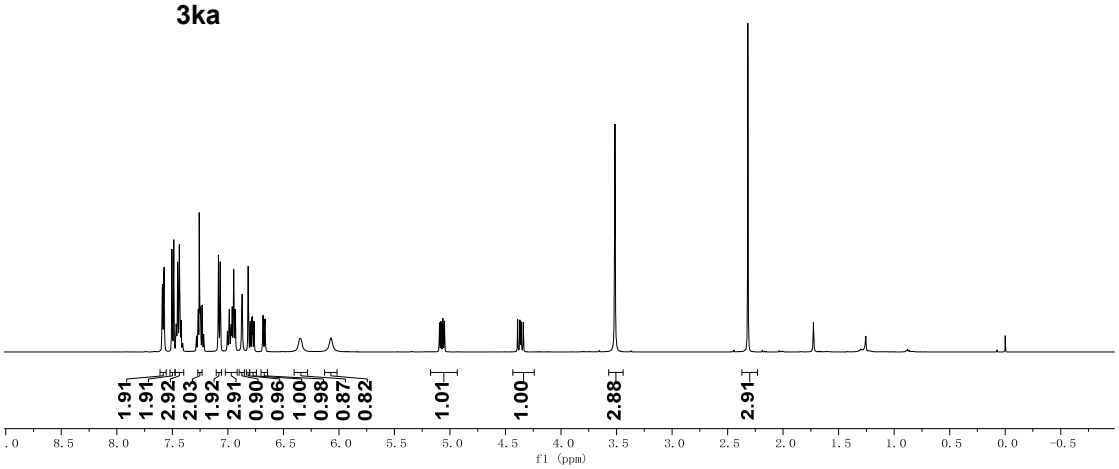
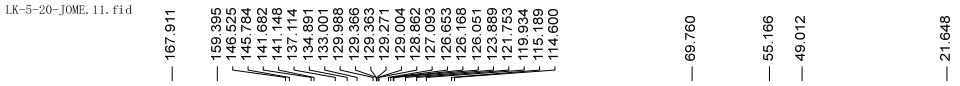


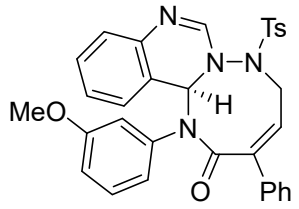
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ja**



3ka







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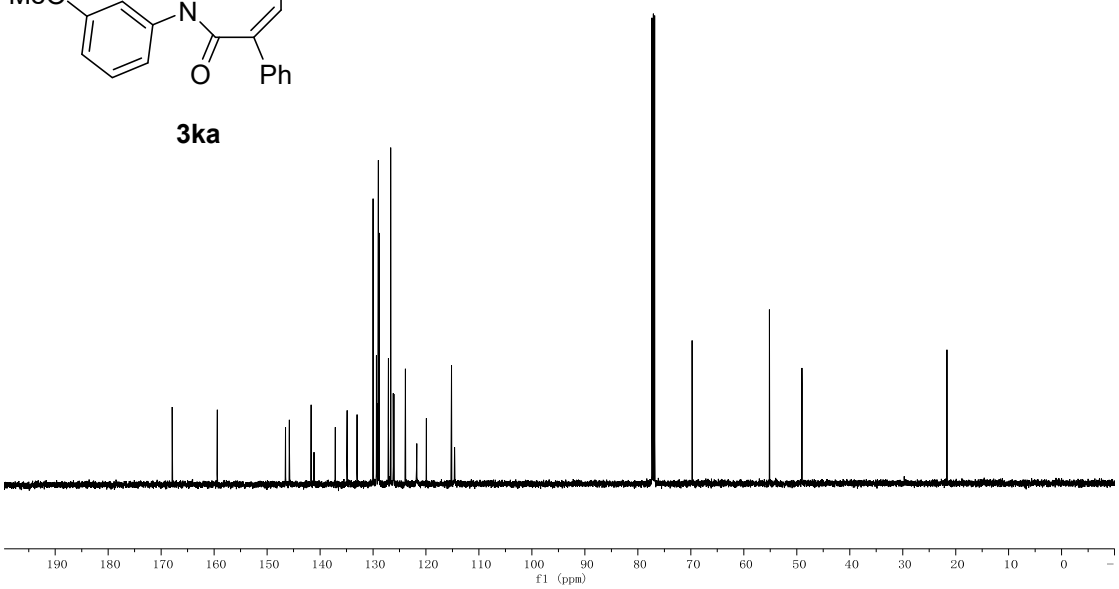
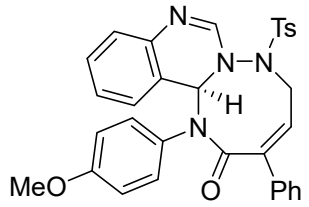
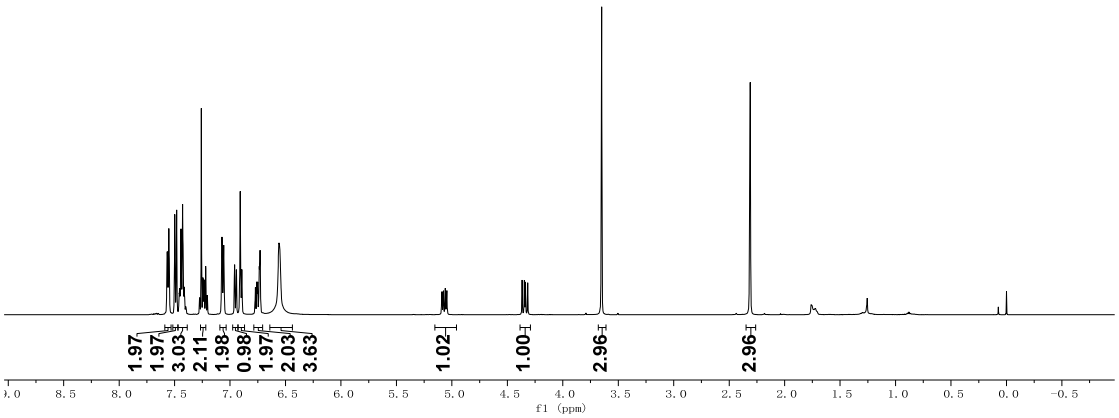
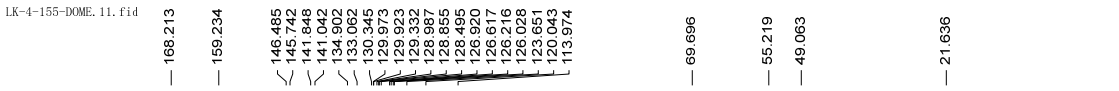


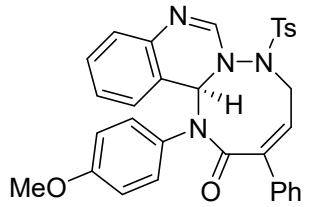
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ka**



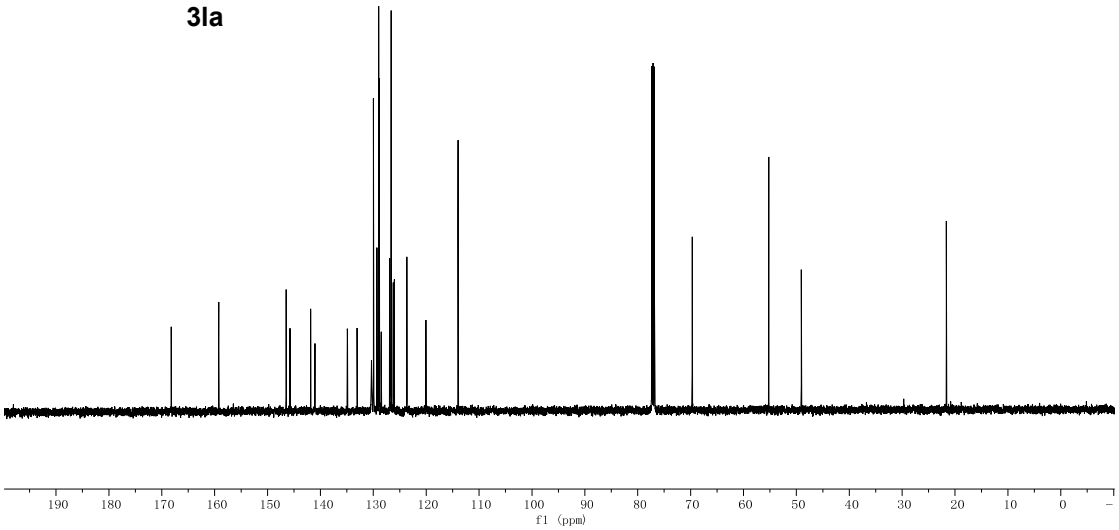
3la



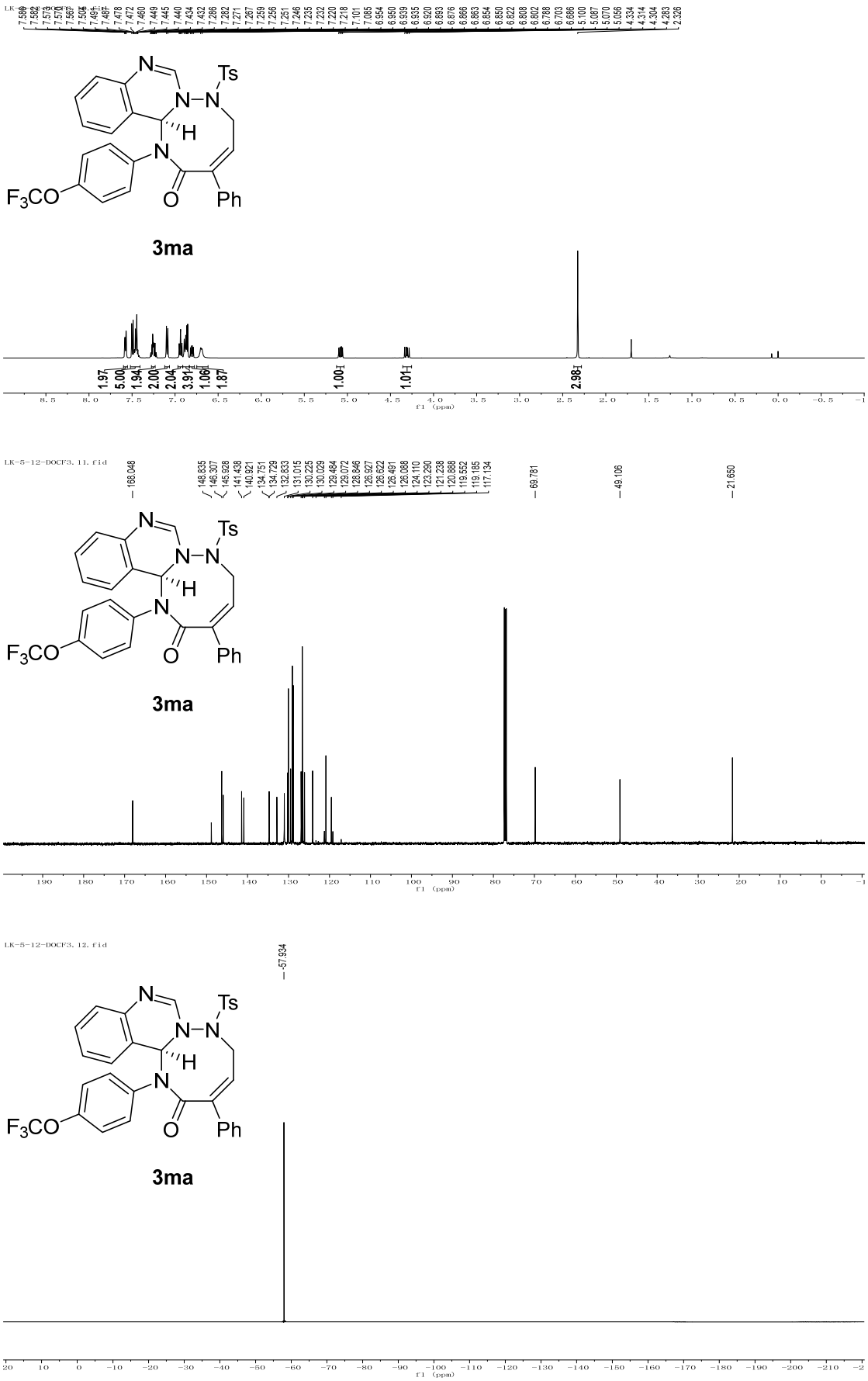




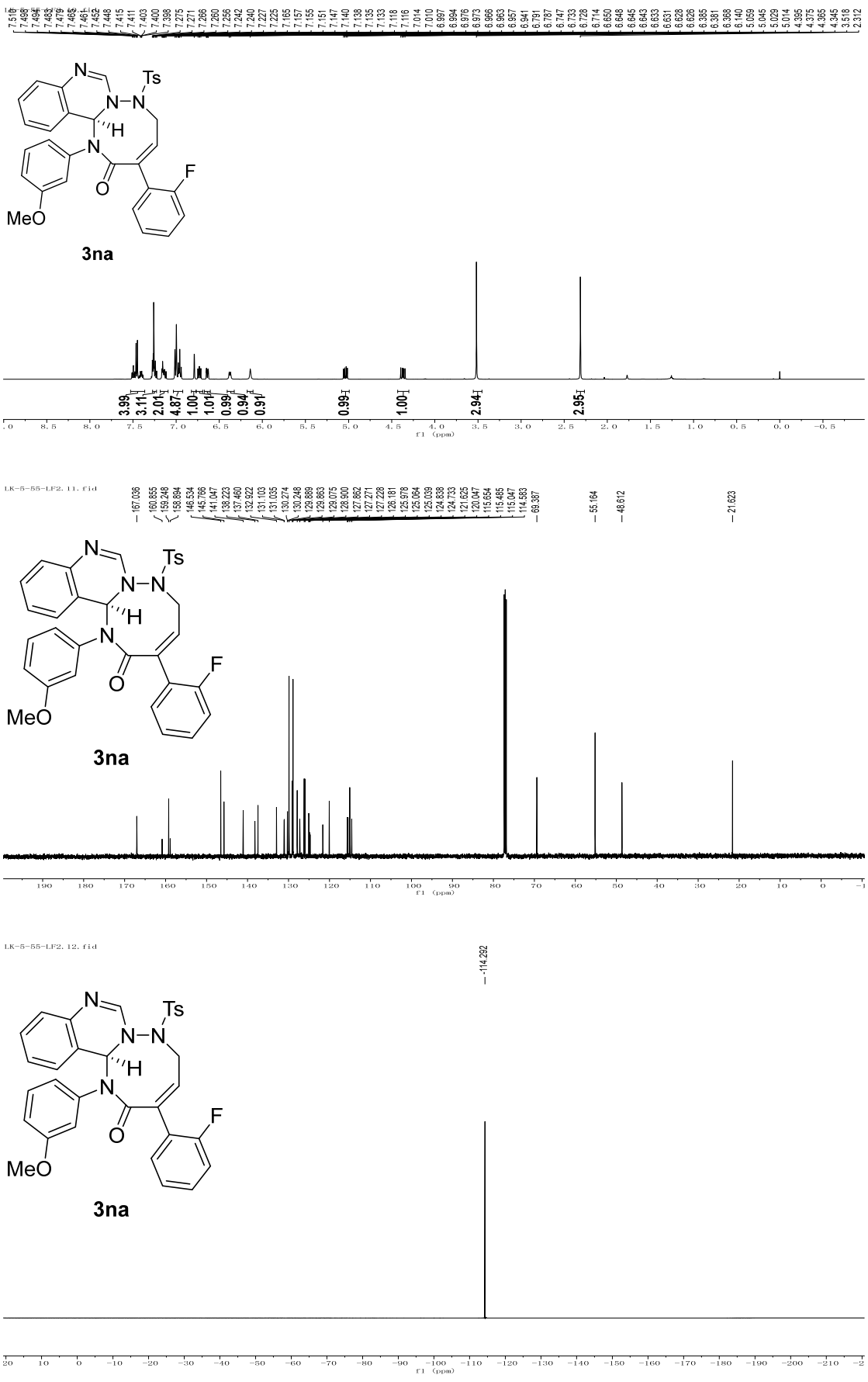
3la



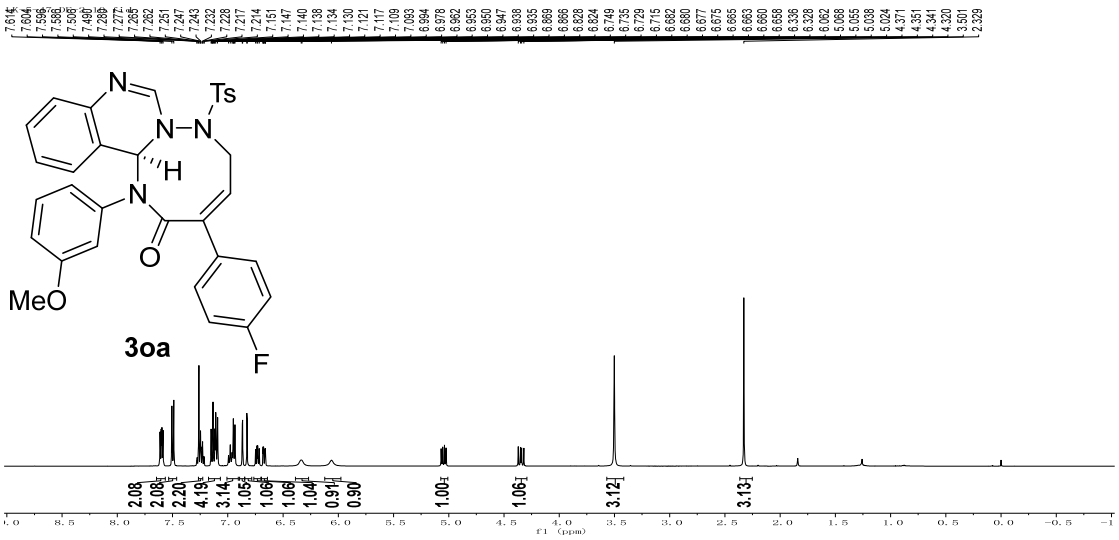
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3la**

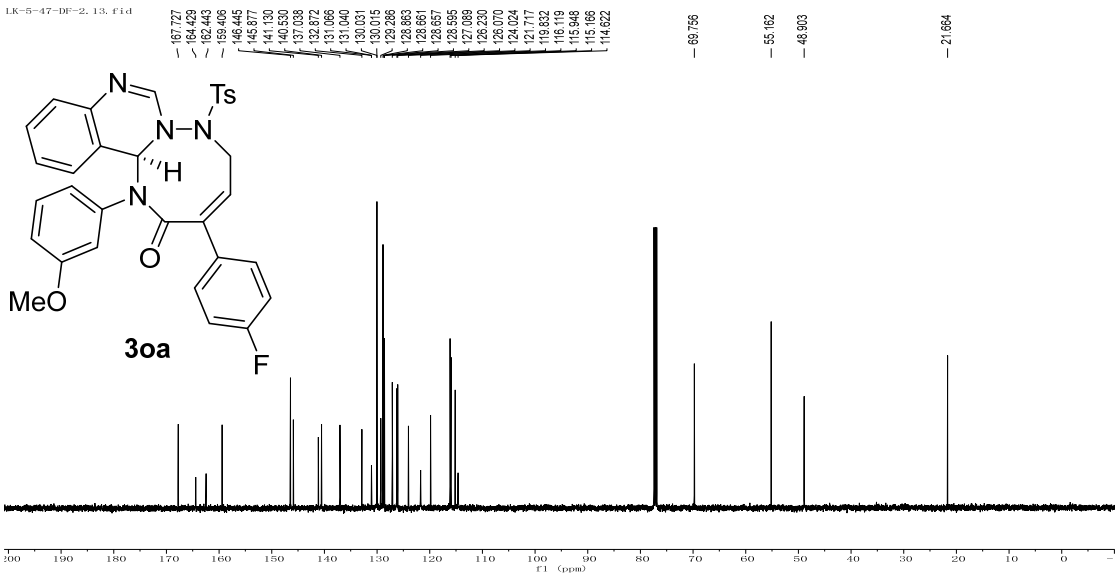


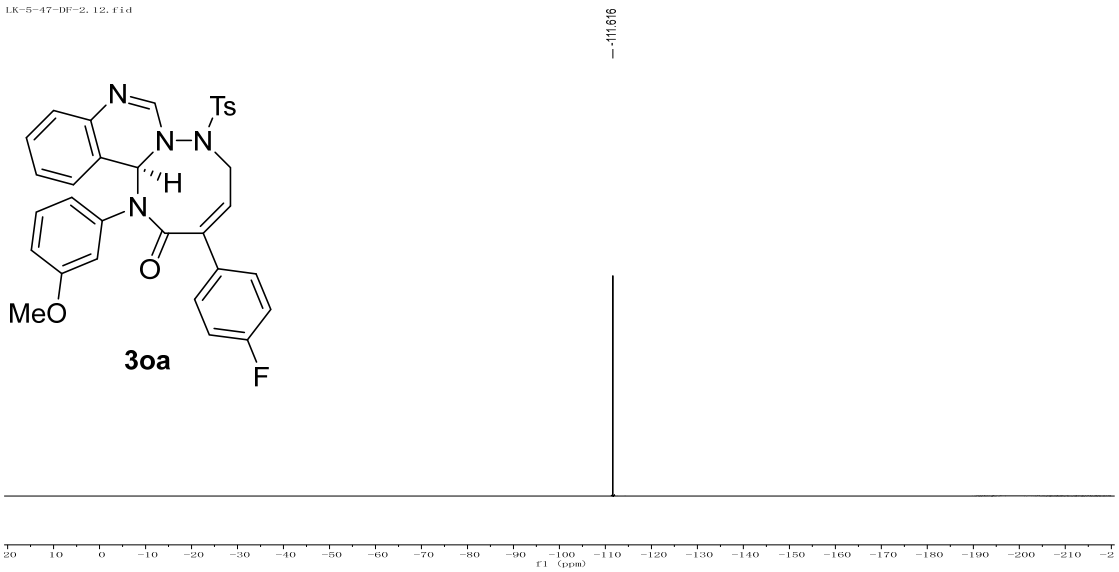
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3ma**



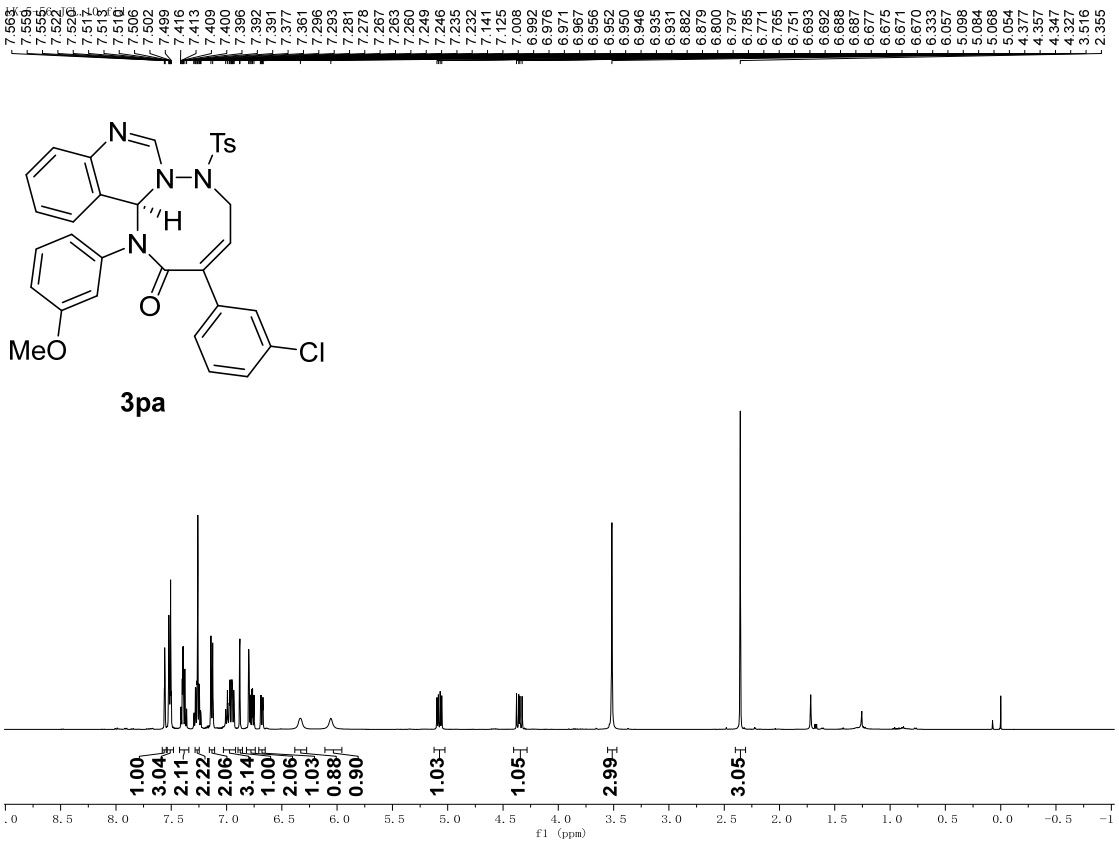
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3na**

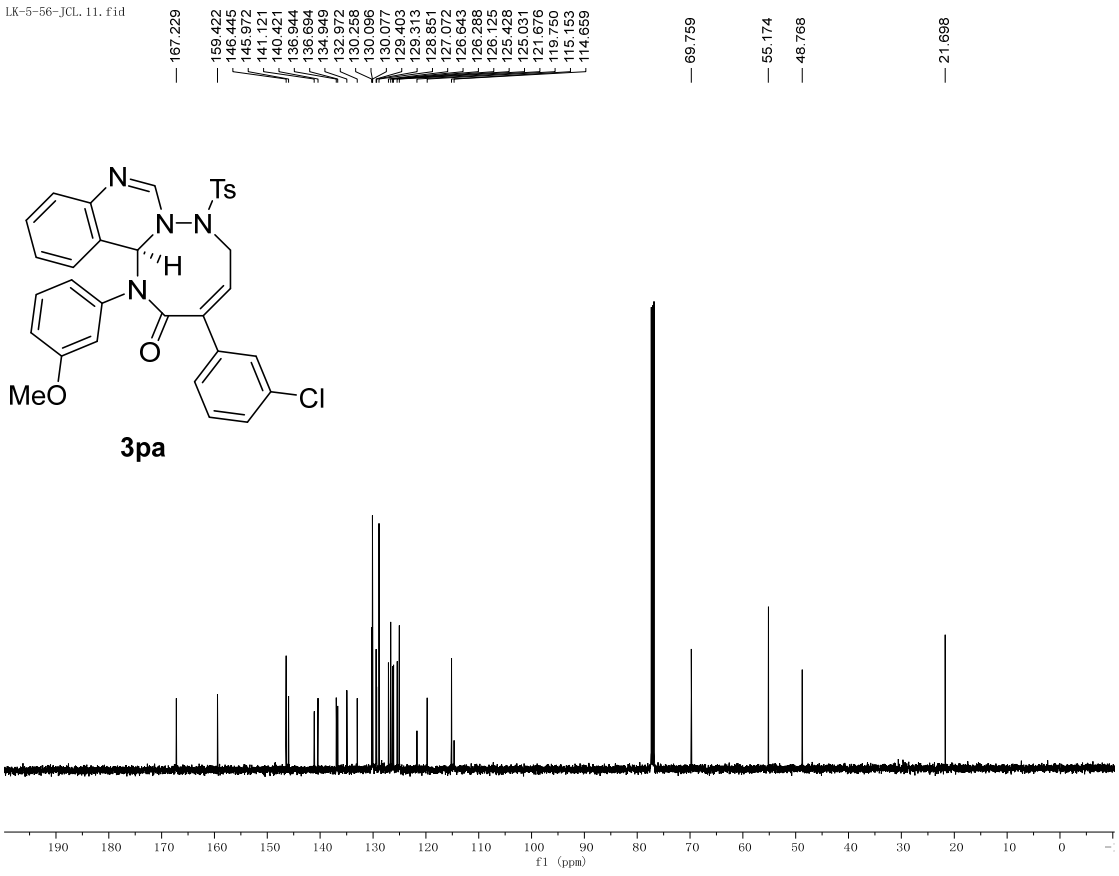




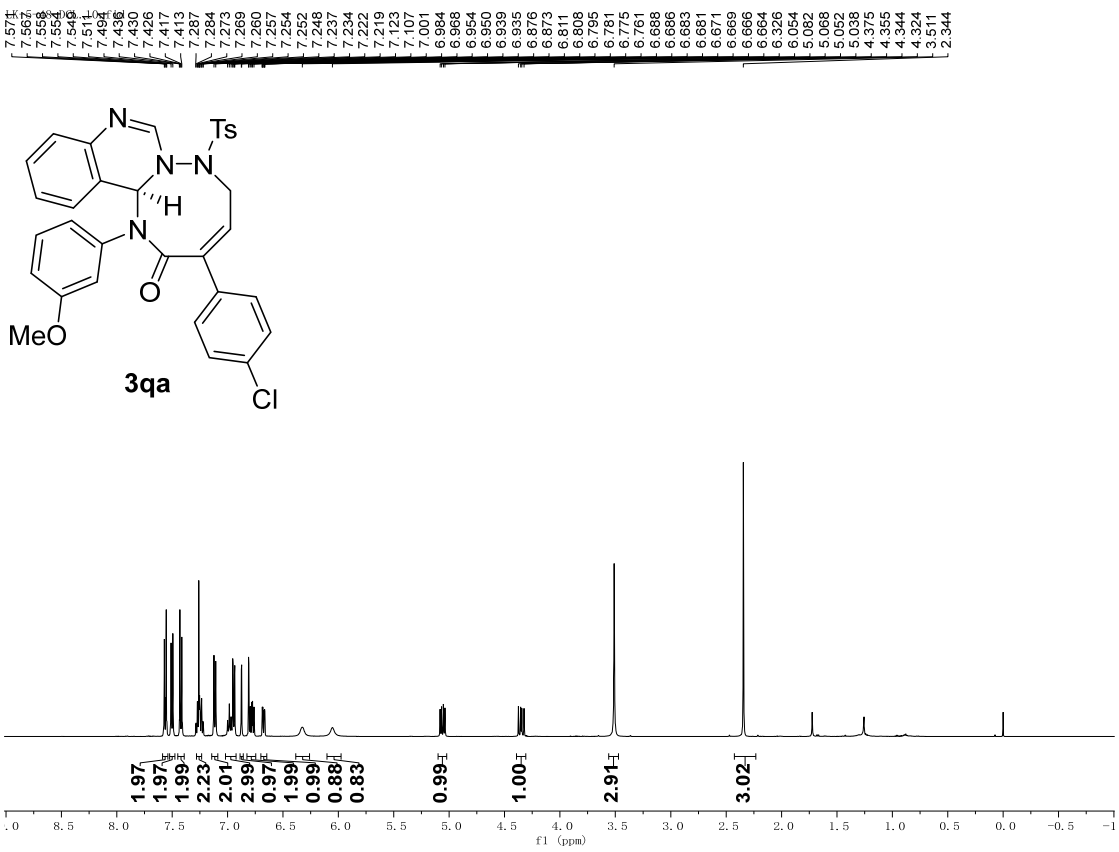


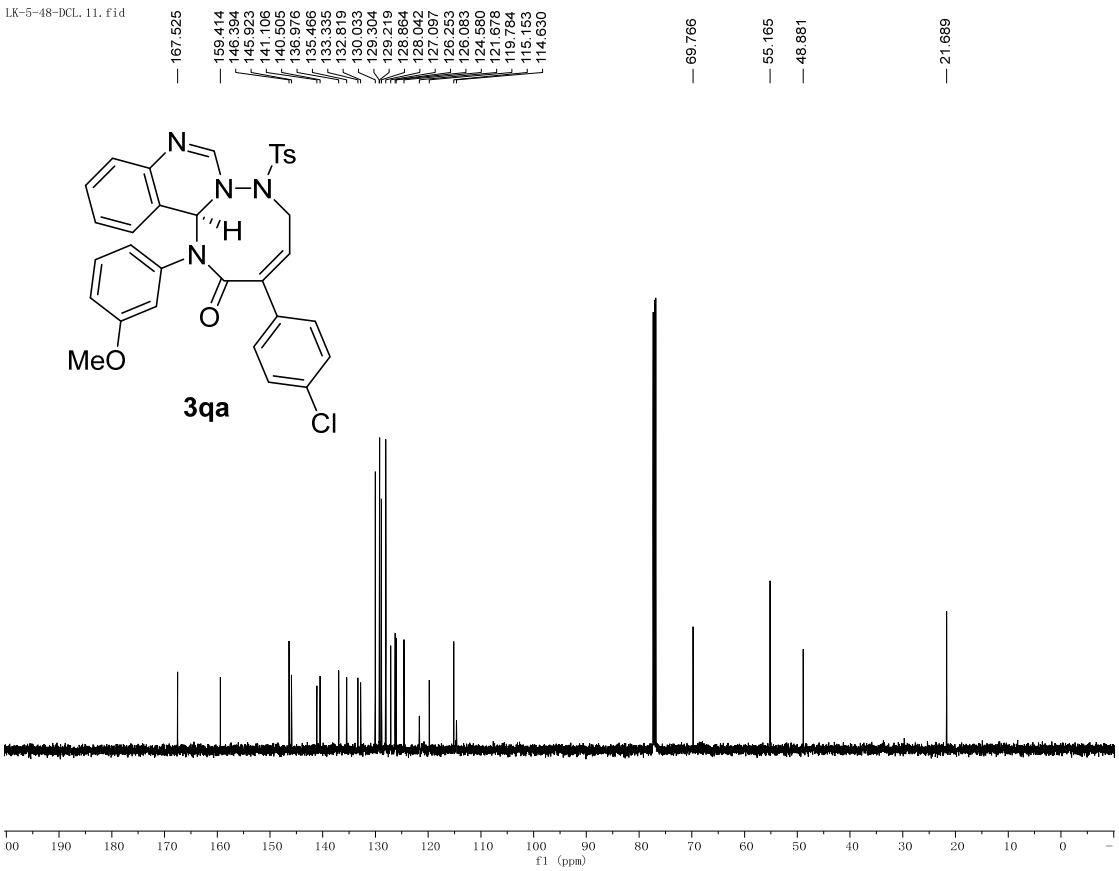
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3oa**



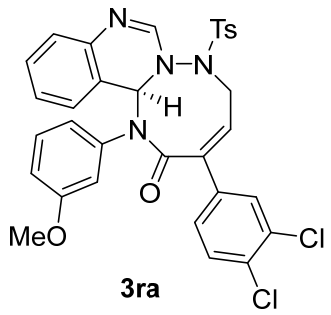


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3pa**

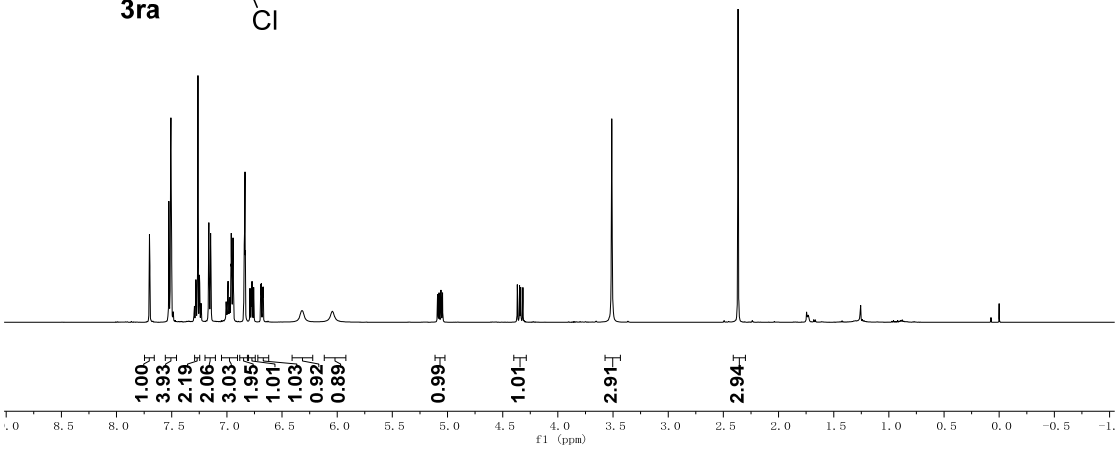


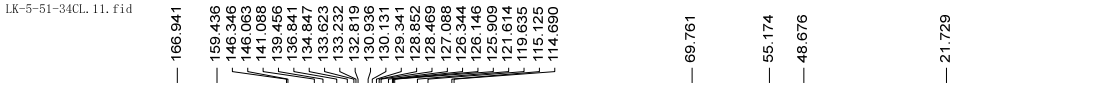


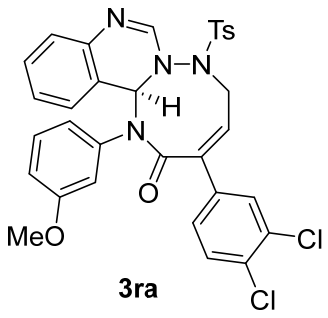
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qa**



3ra







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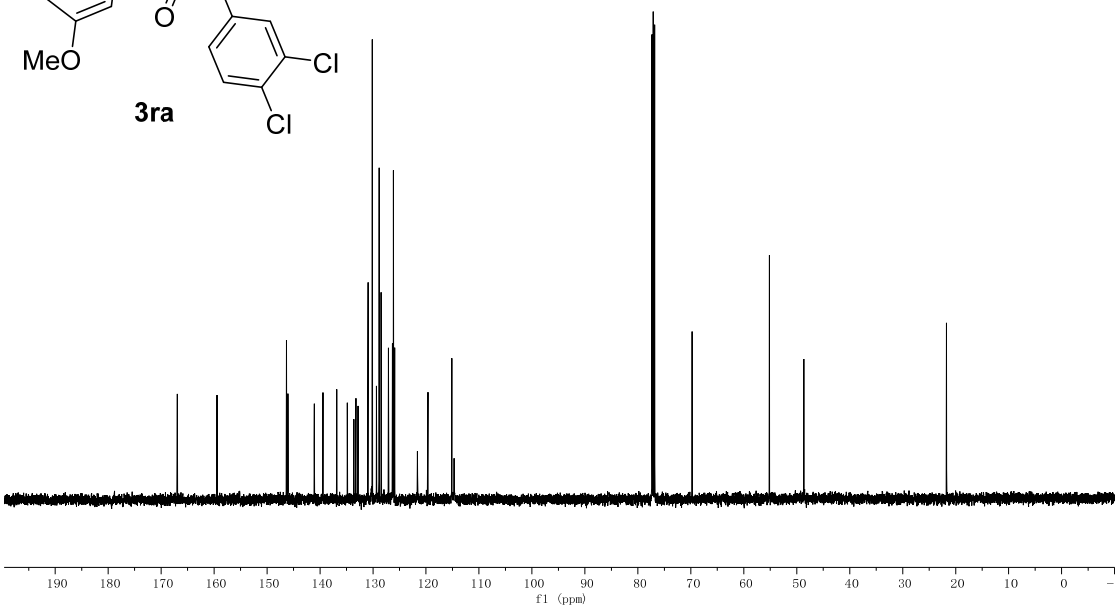
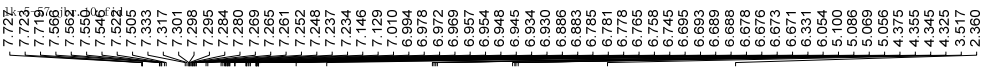
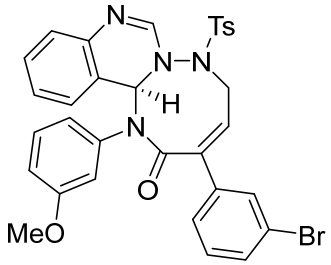
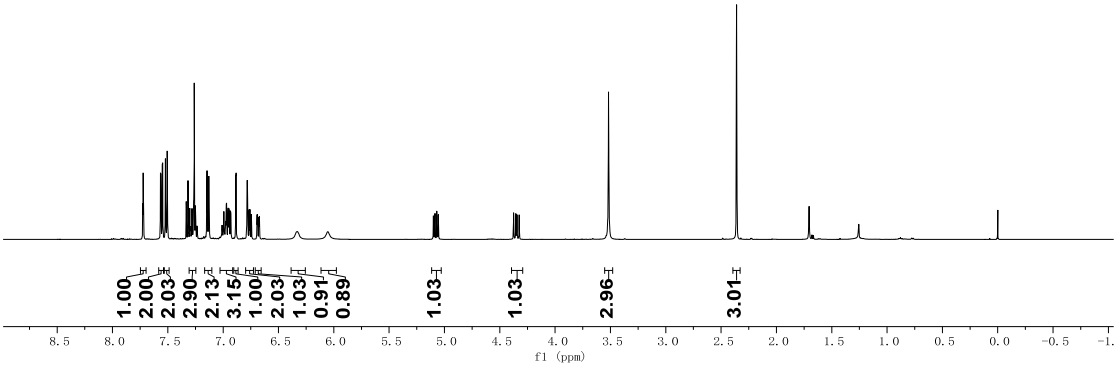


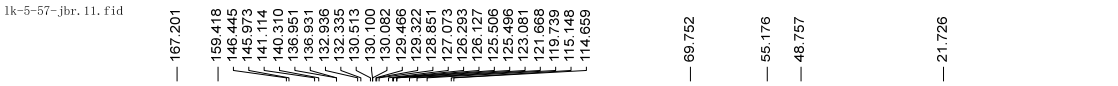
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ra**

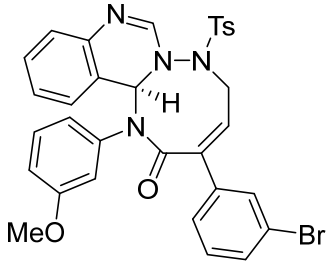




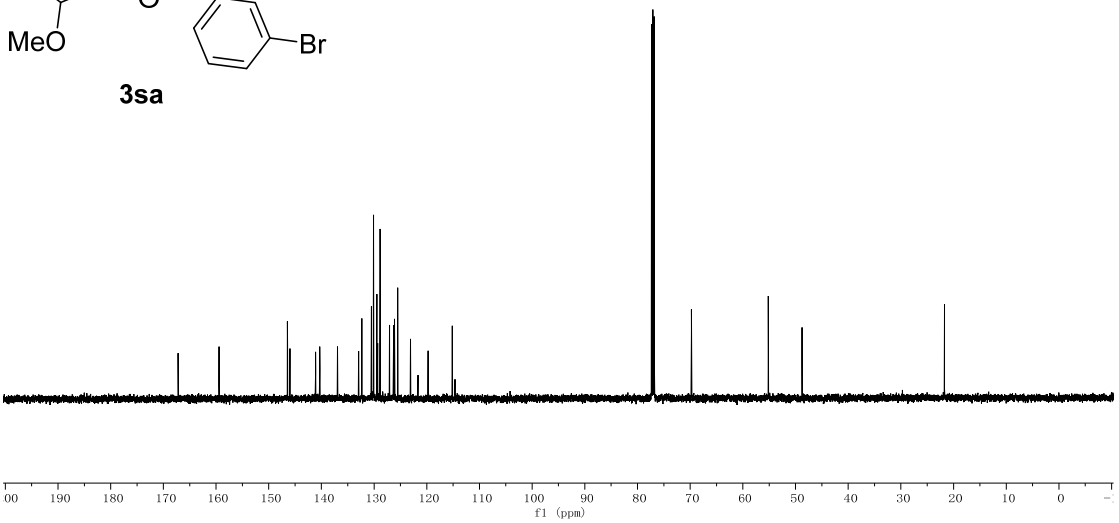
3sa



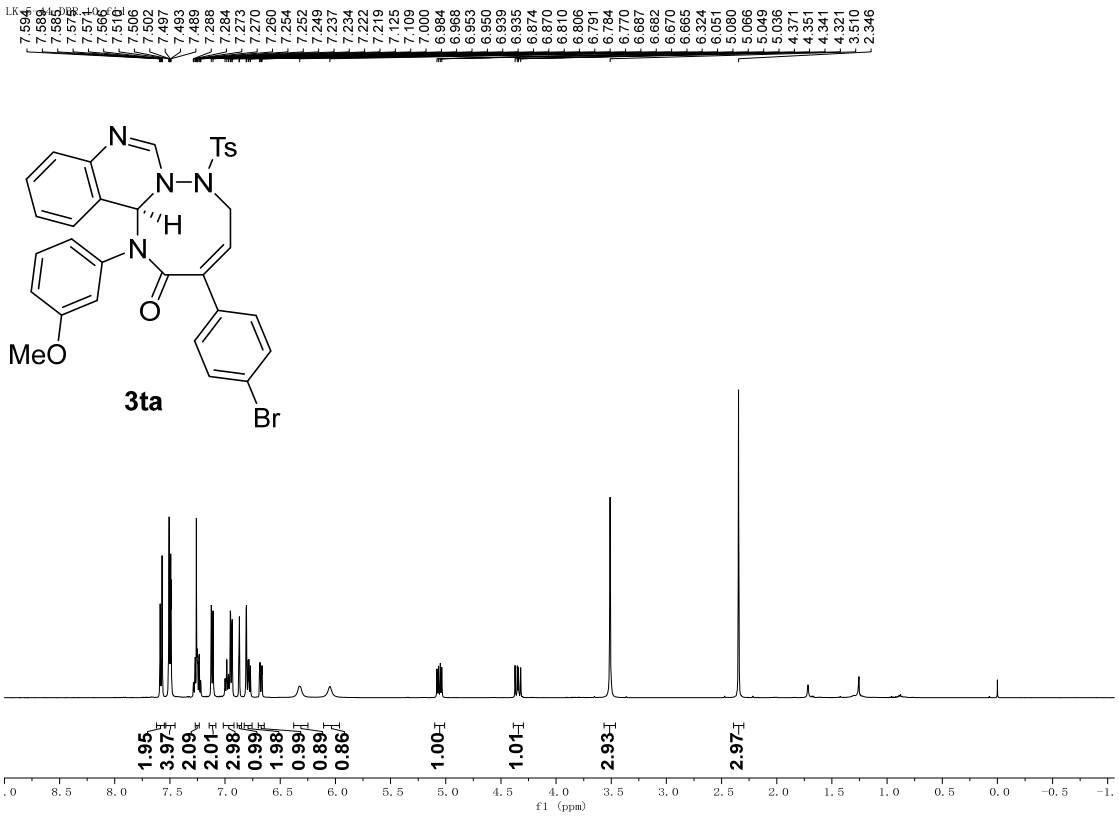


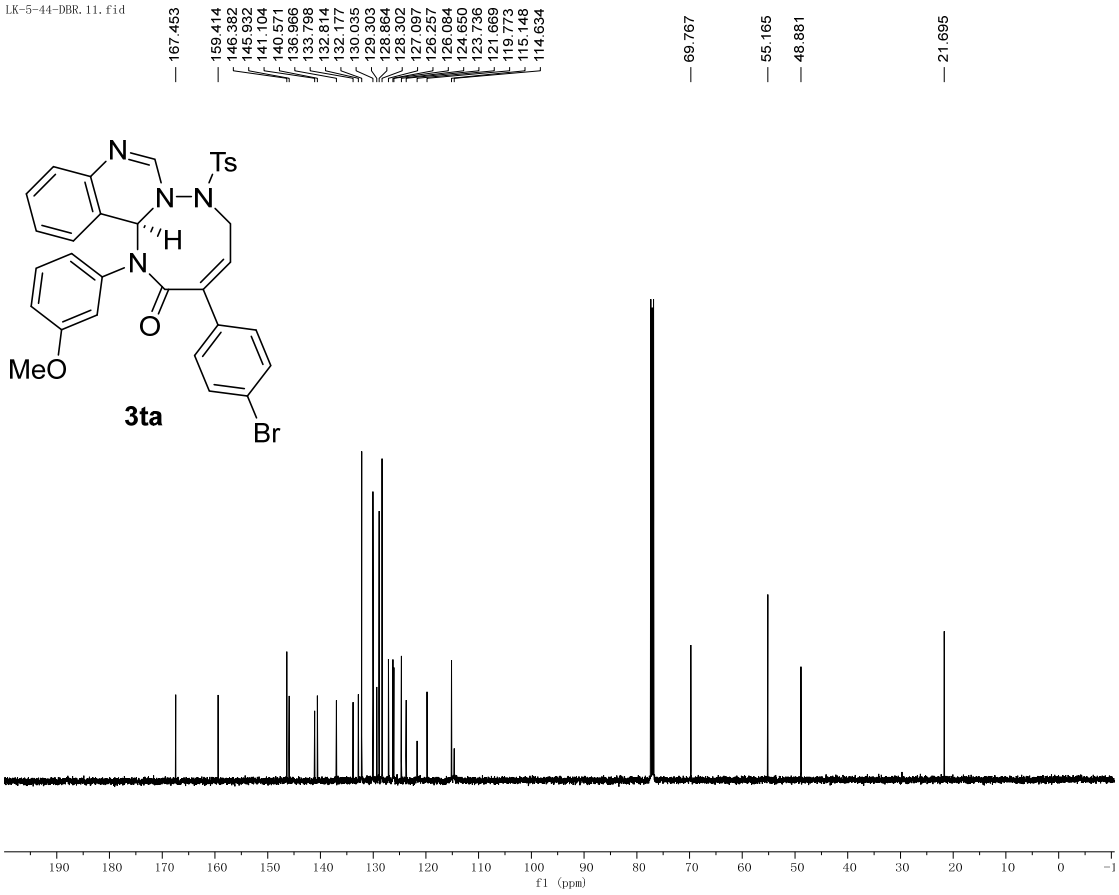


3sa

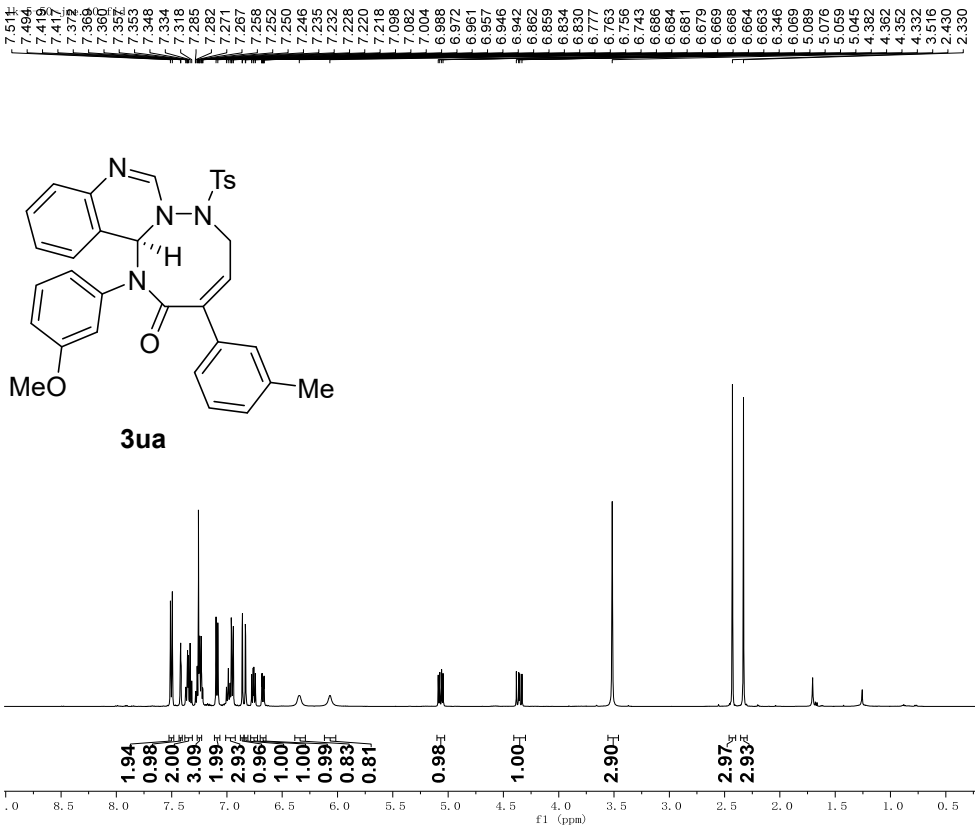


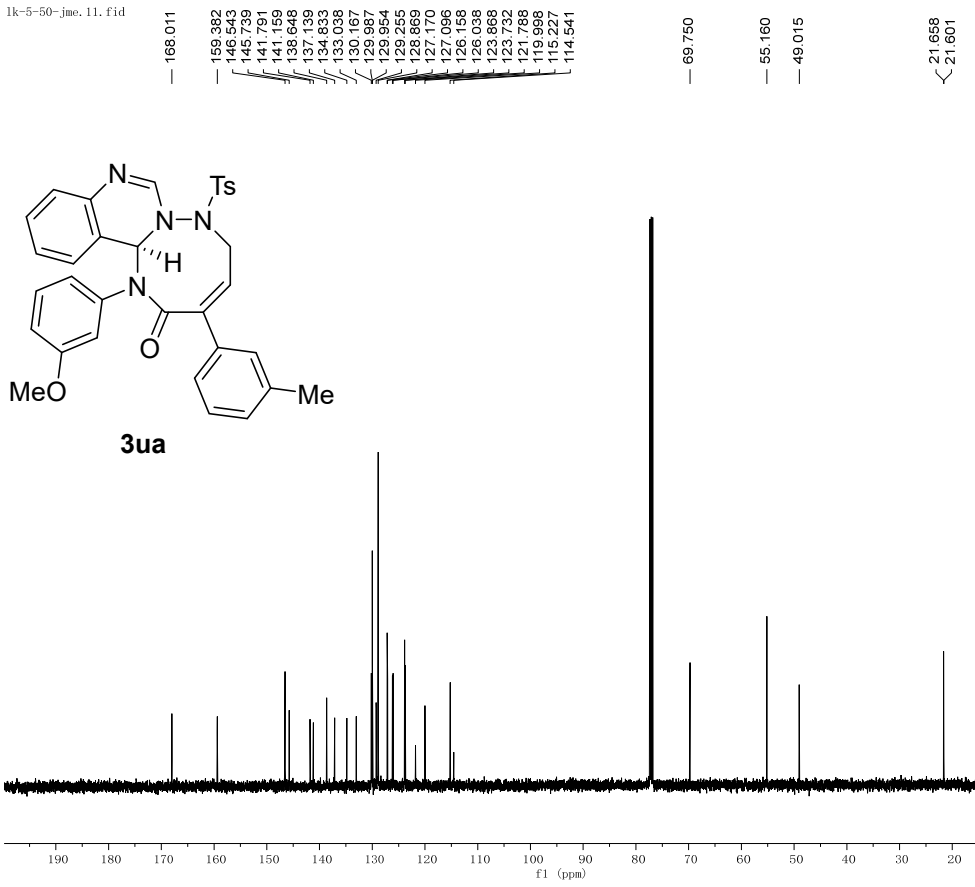
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3sa**



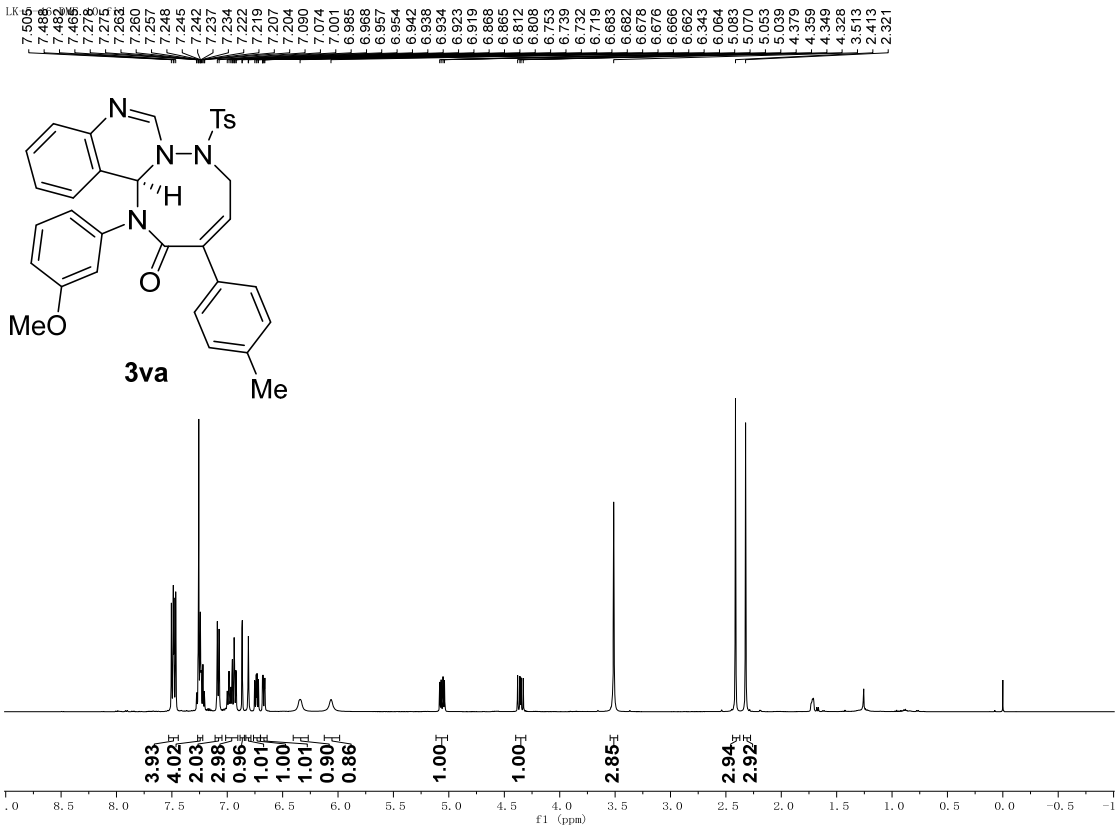


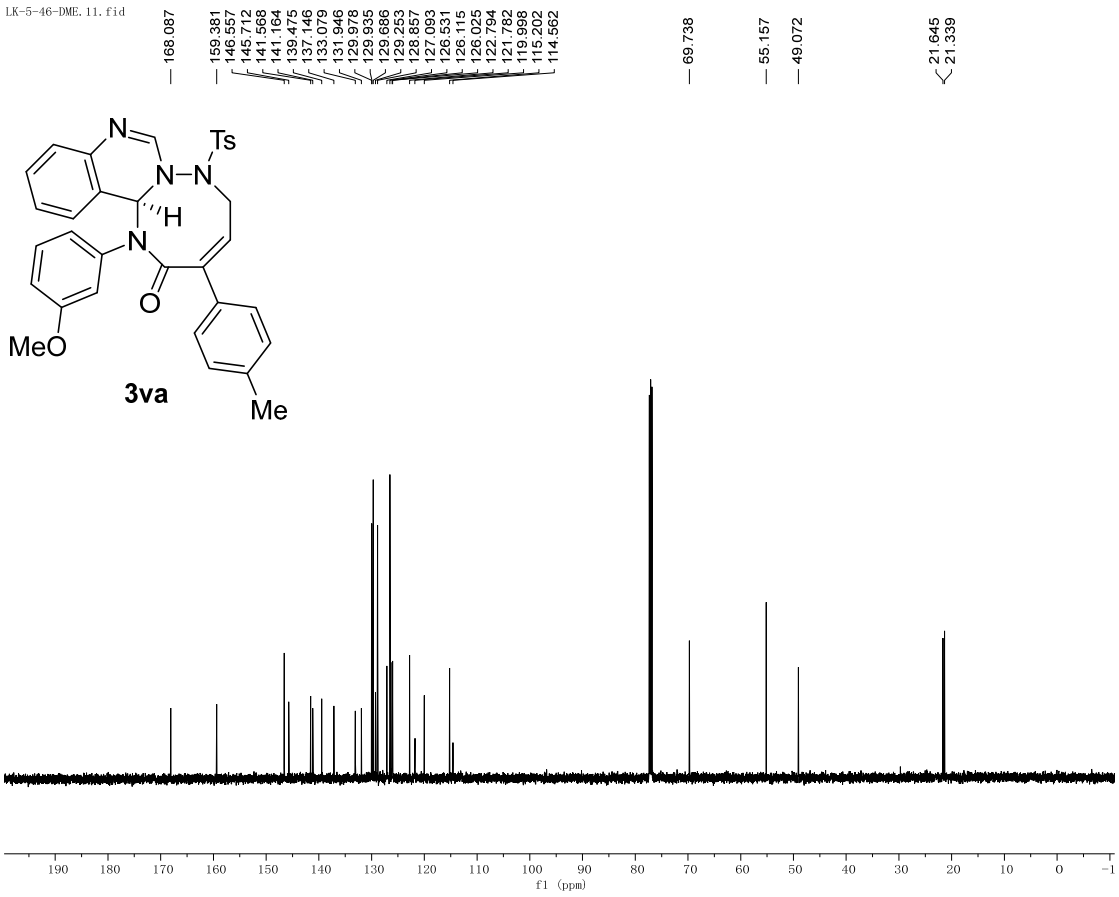
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ta**



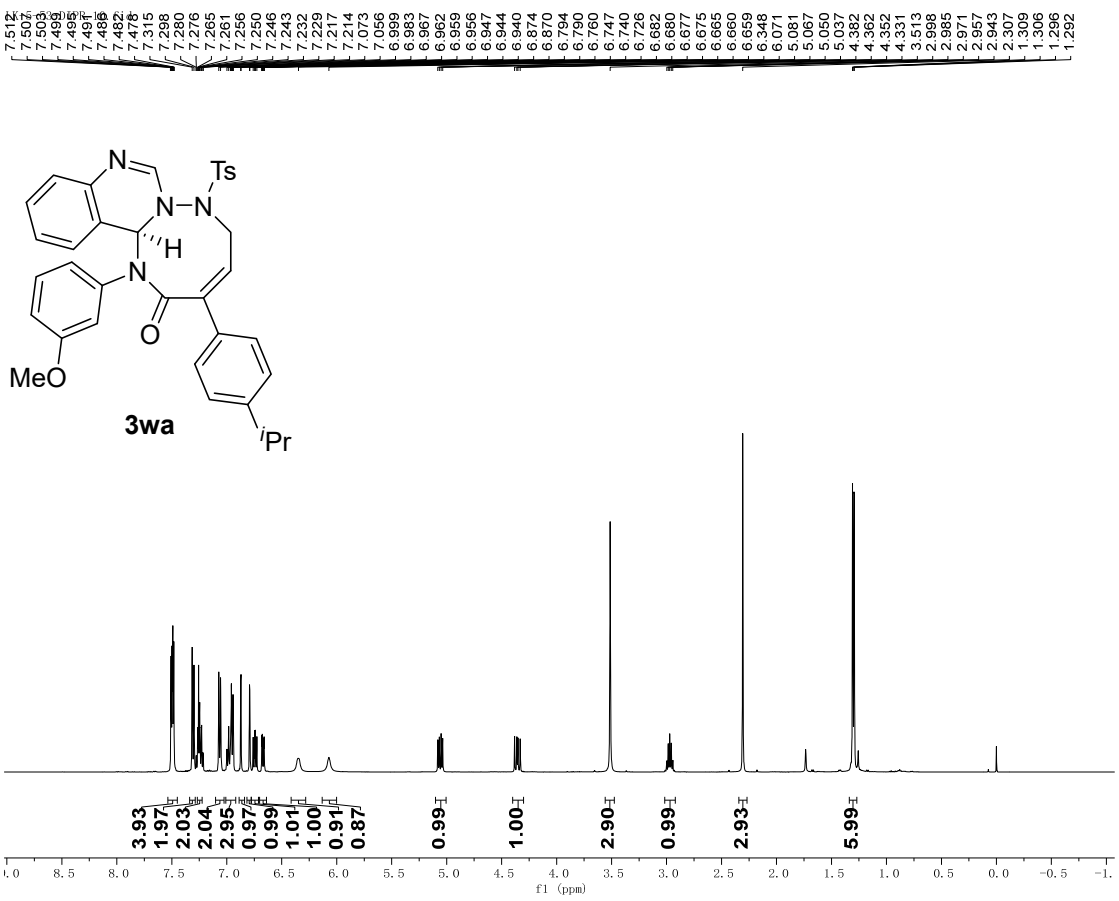


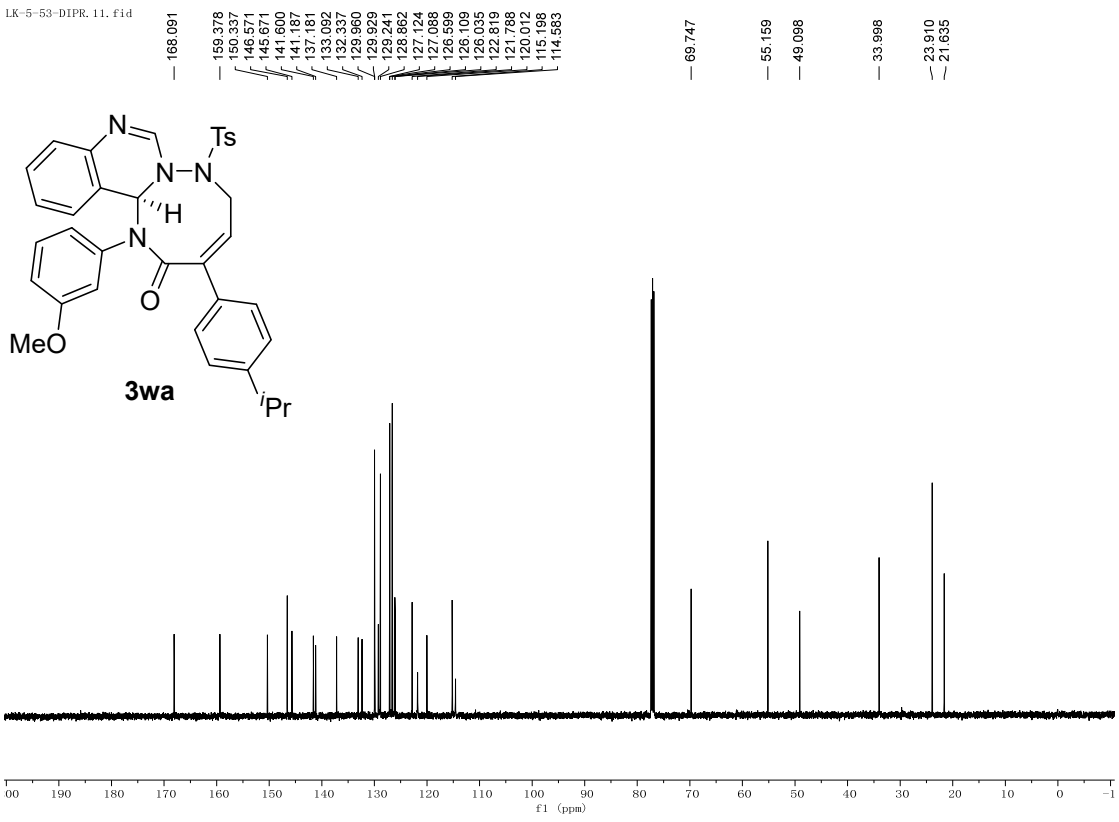
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ua**



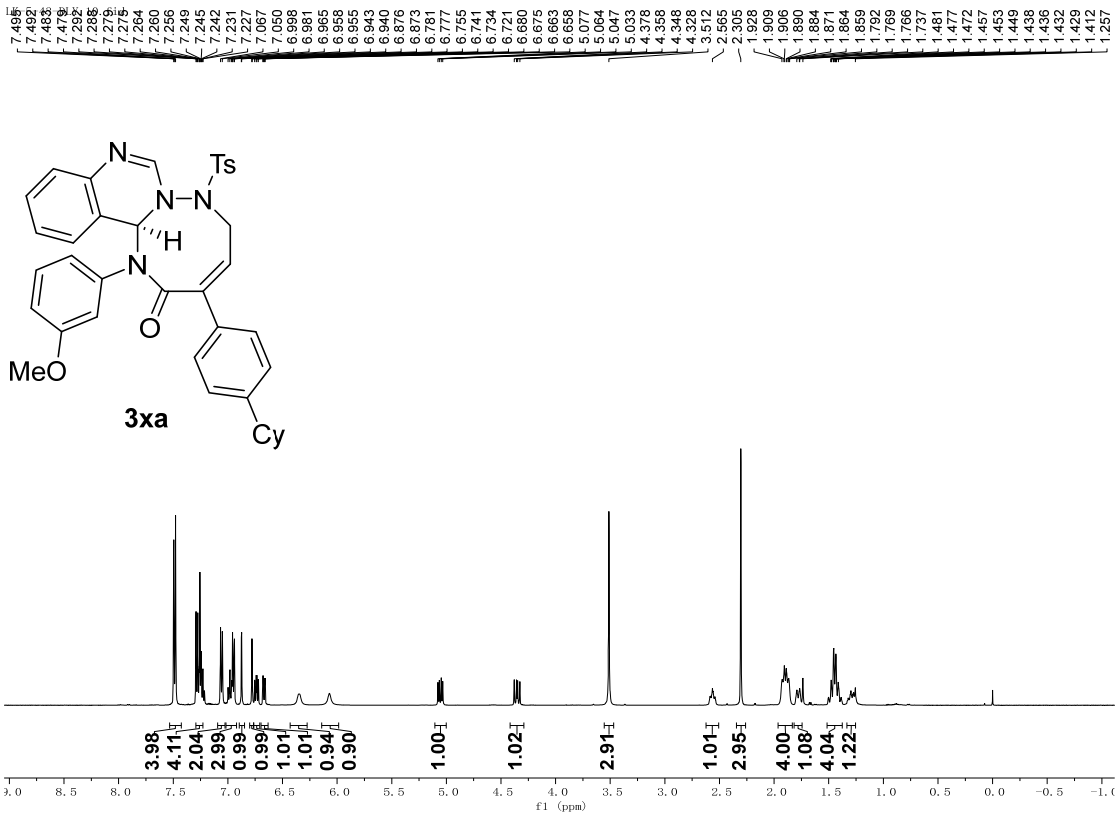


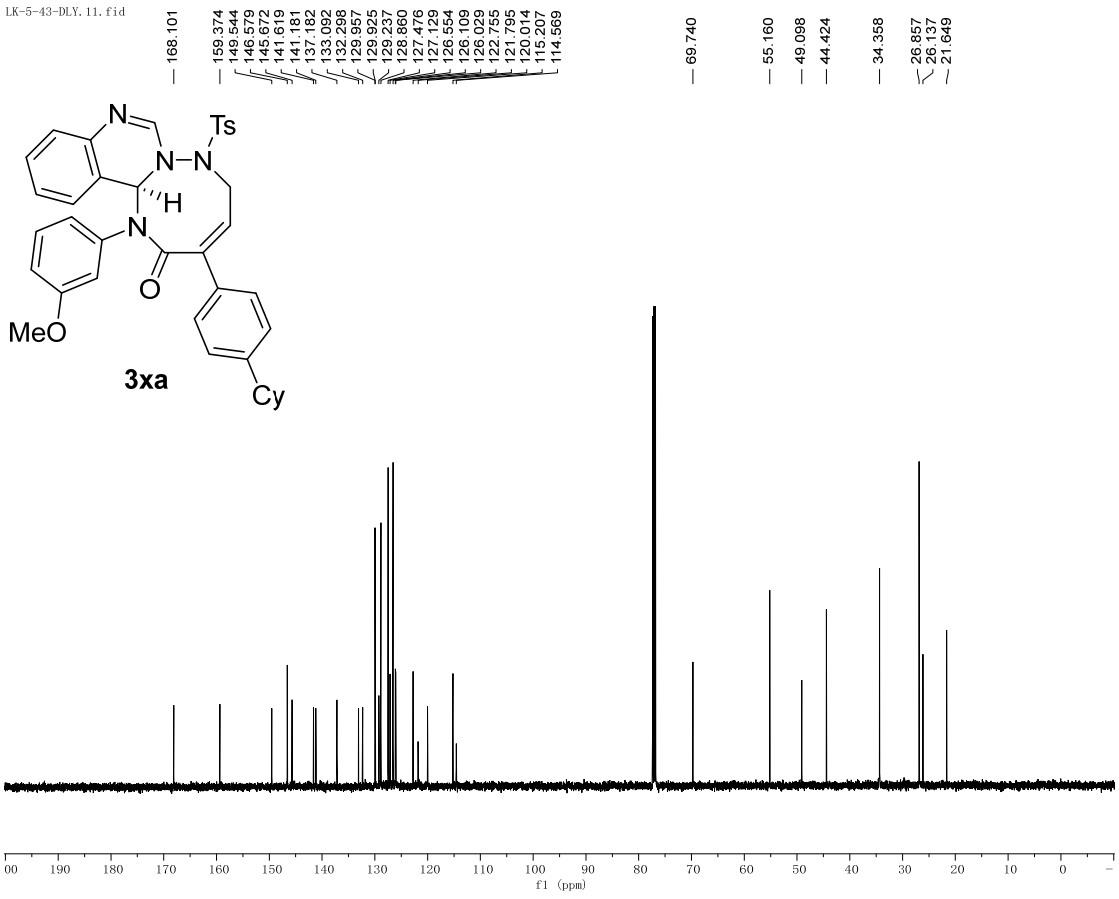
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3va**



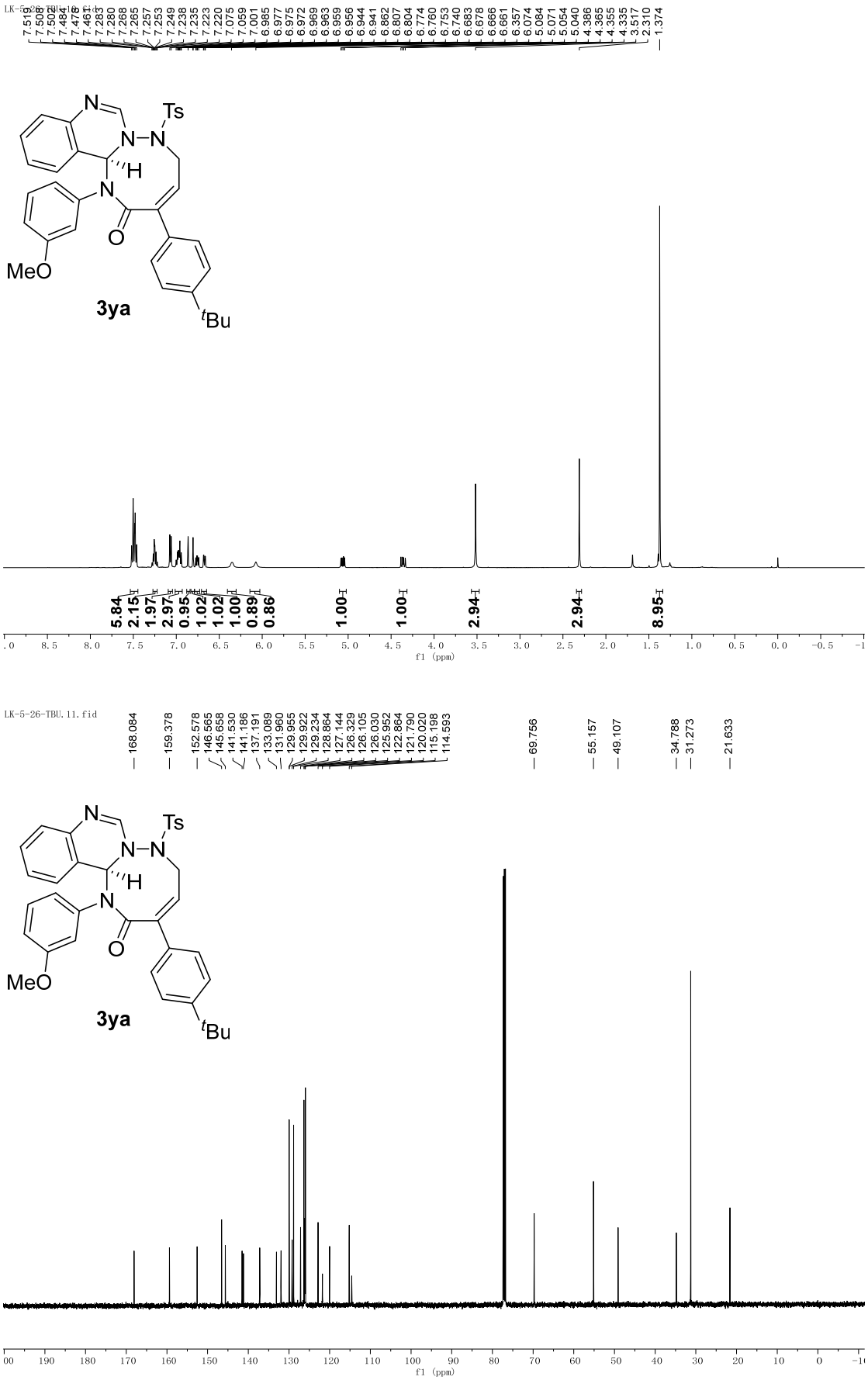


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3wa**

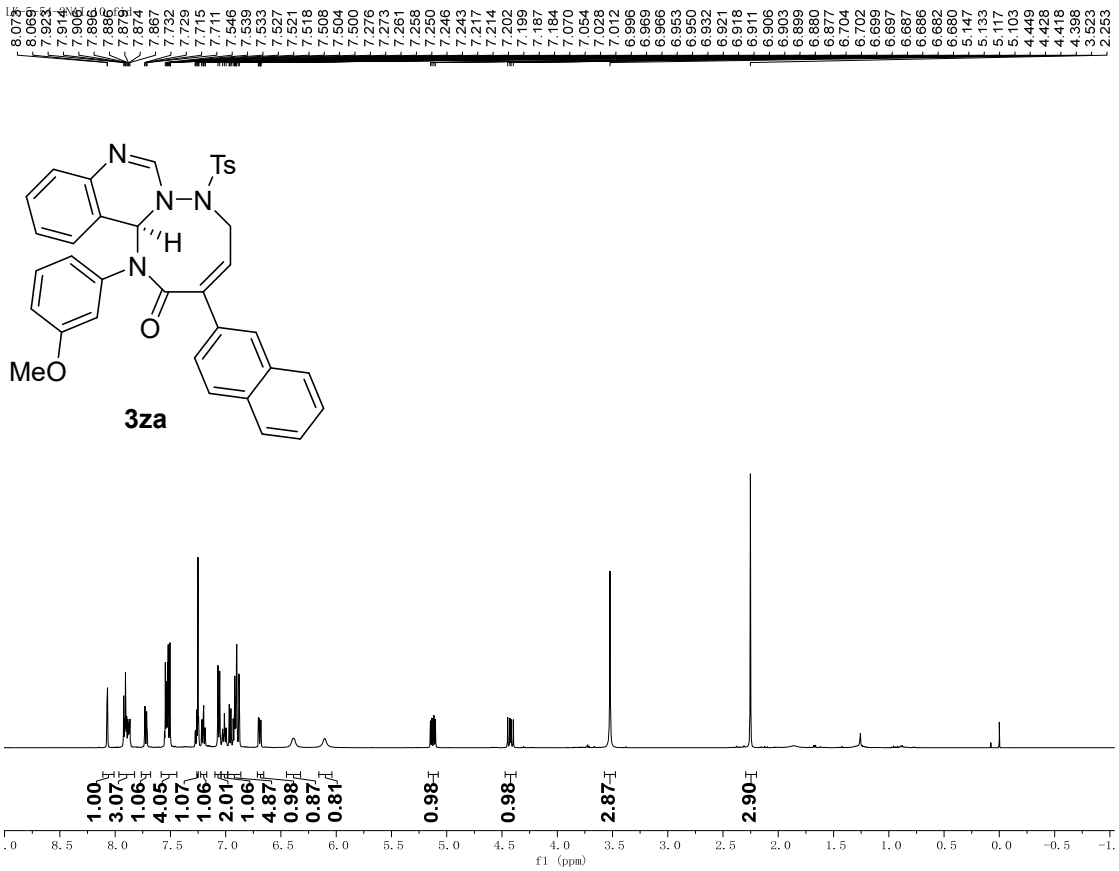


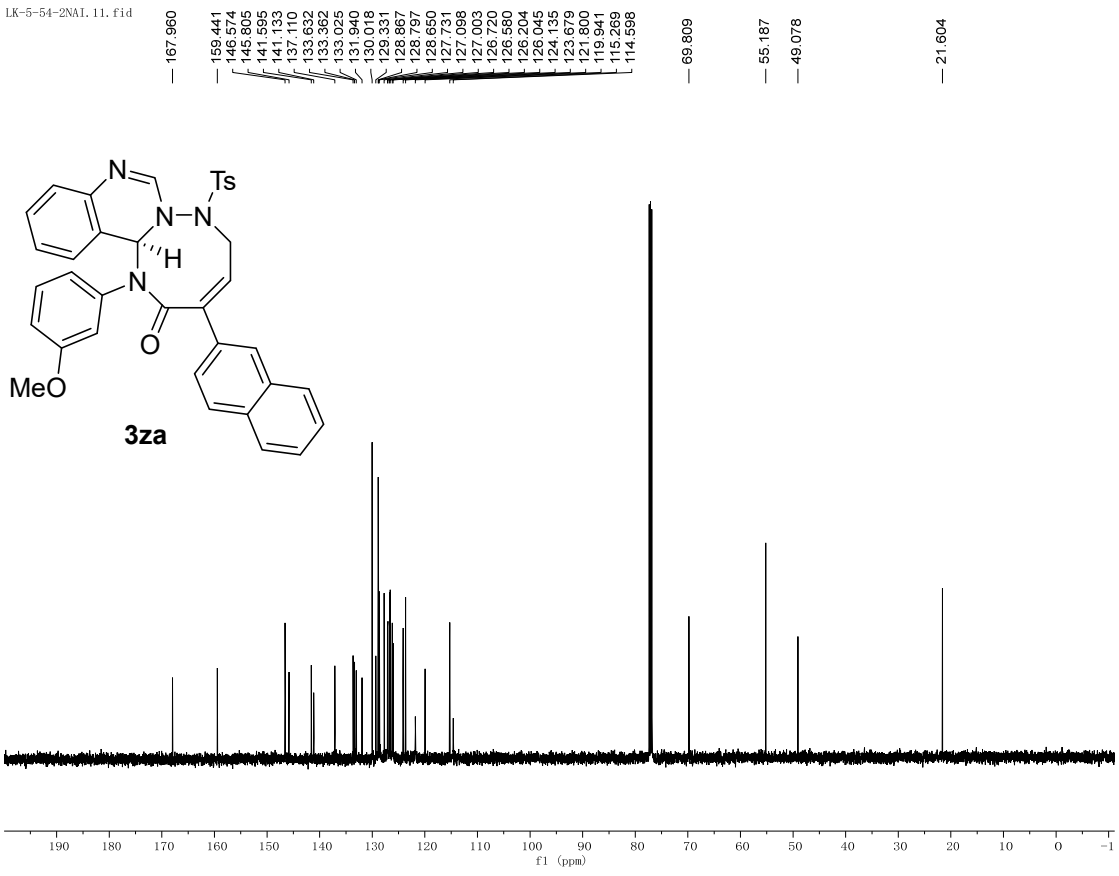


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3xa**

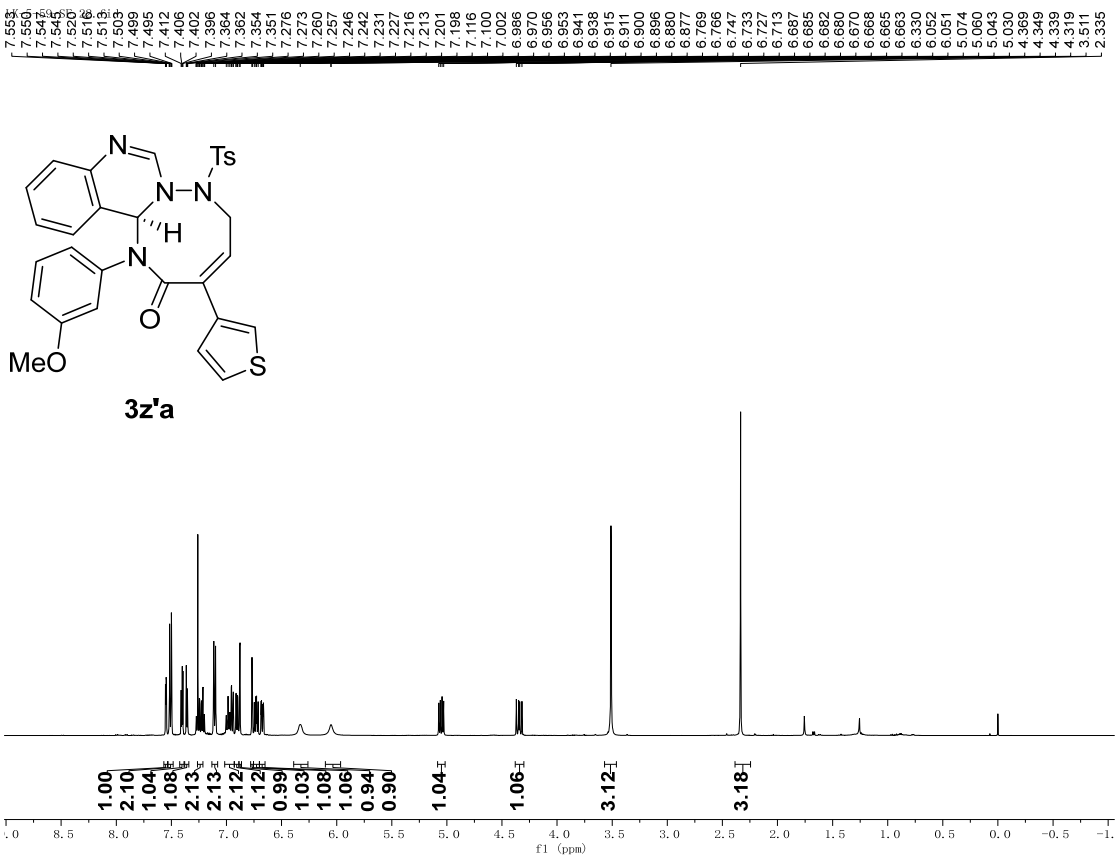


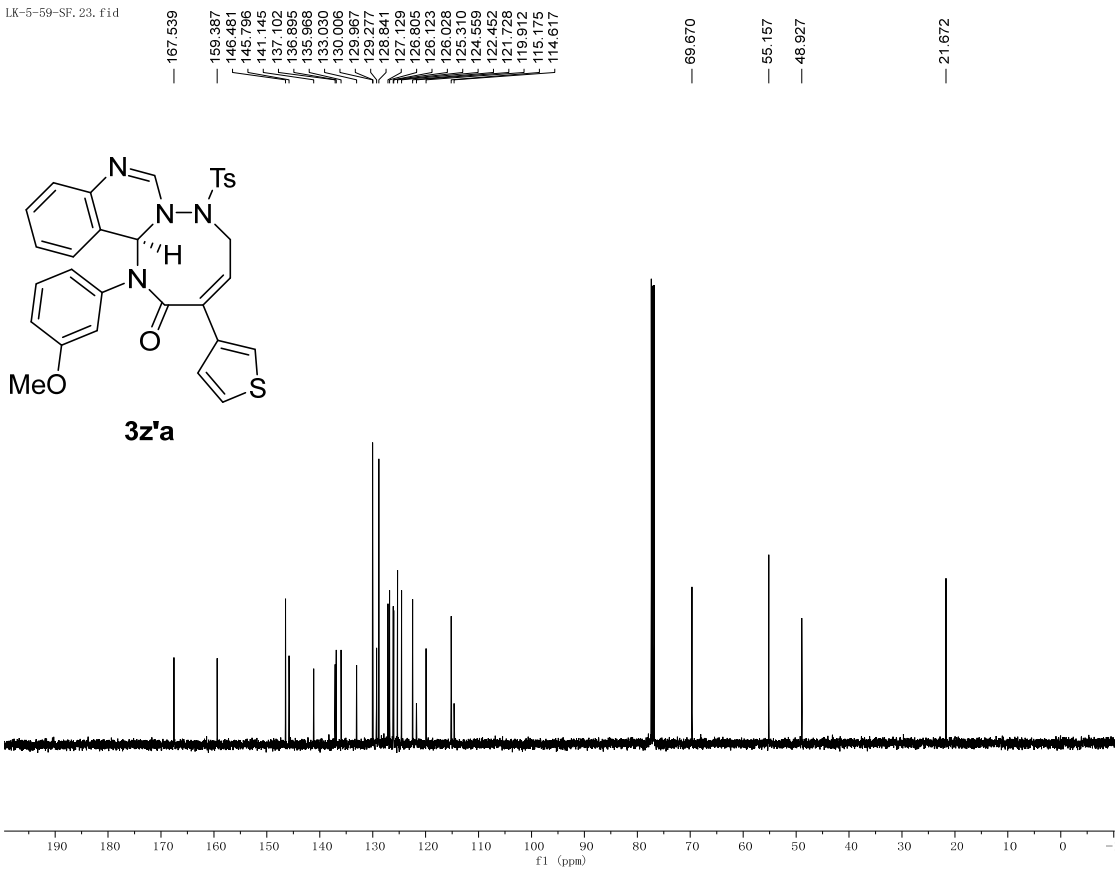
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3ya**



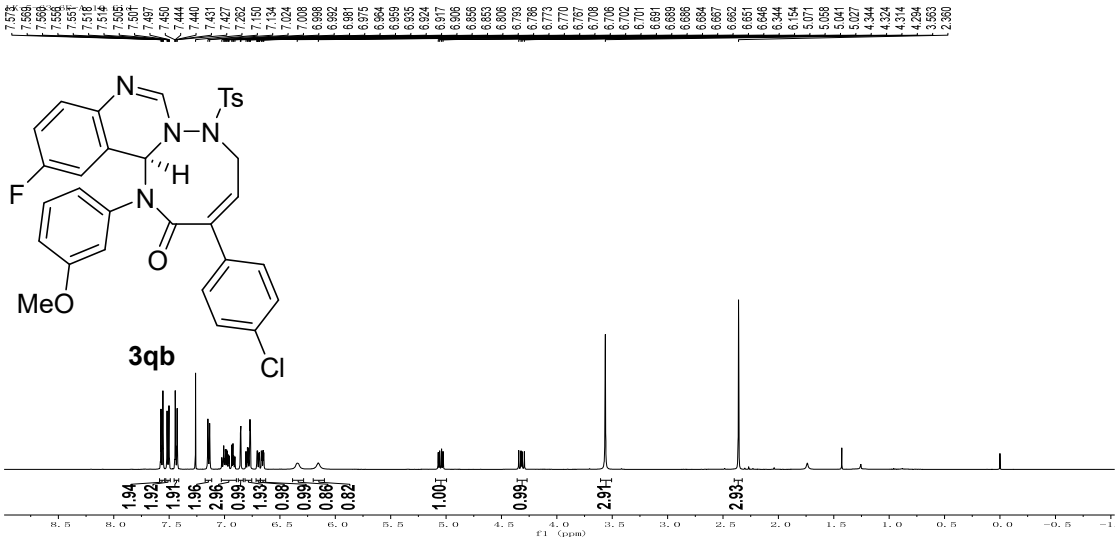


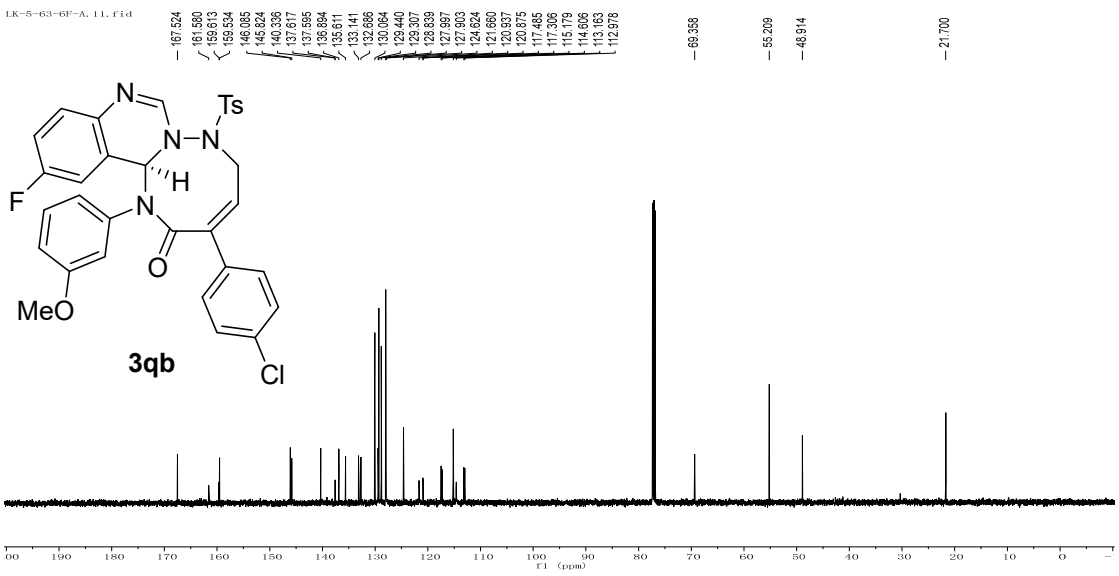
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3za**

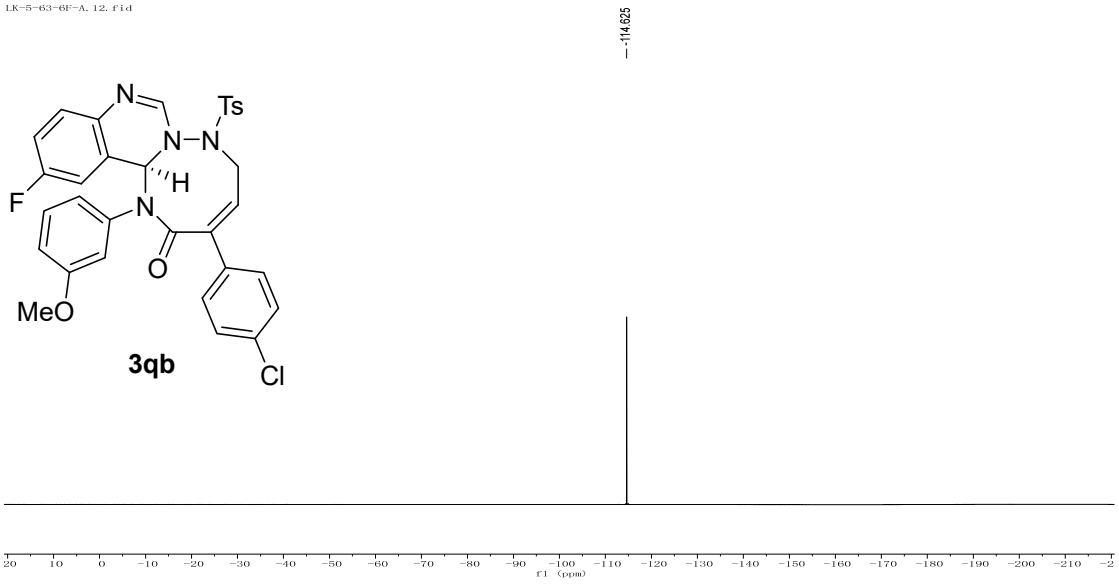




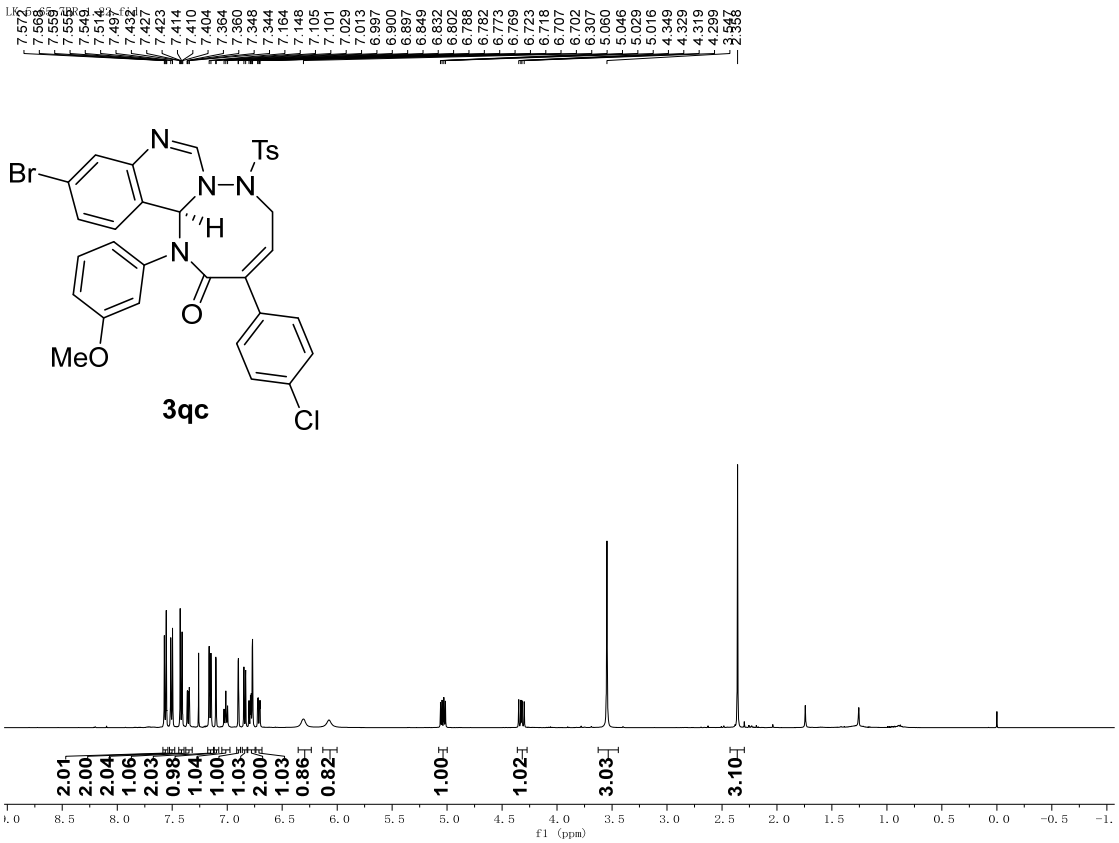
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3z'a**

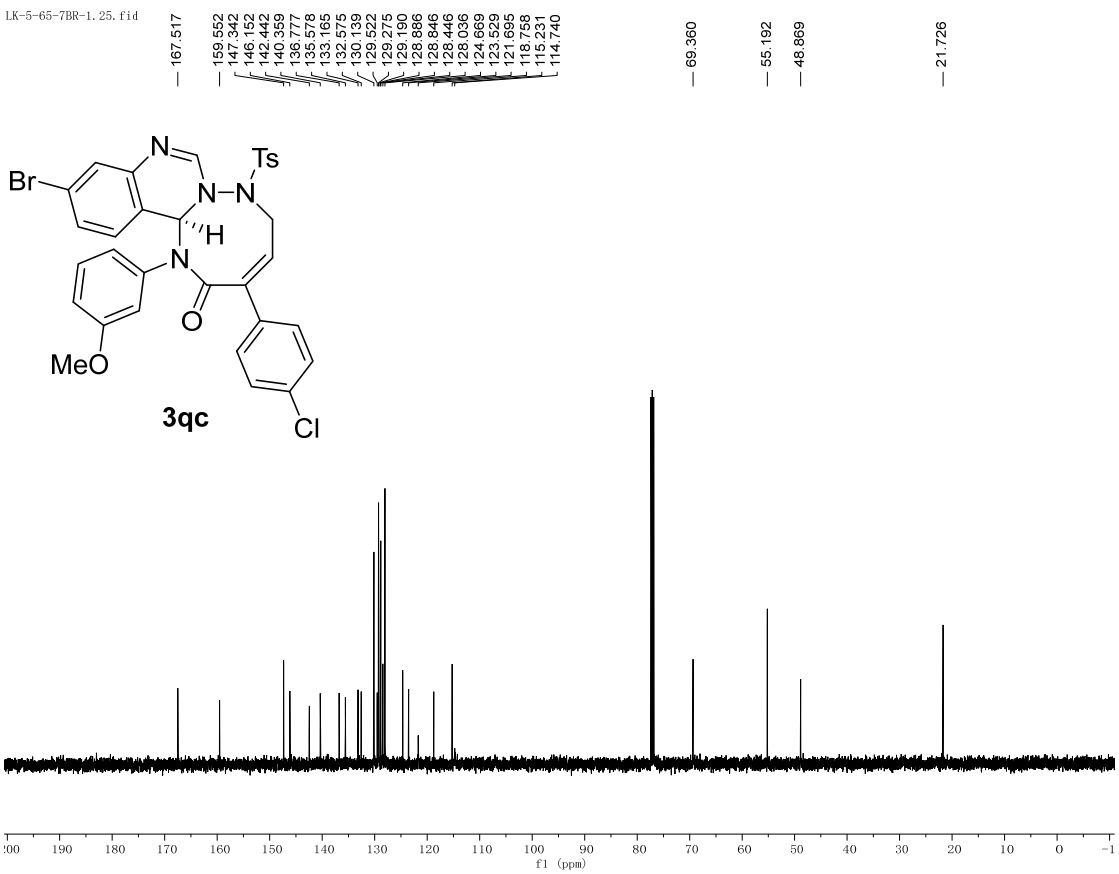




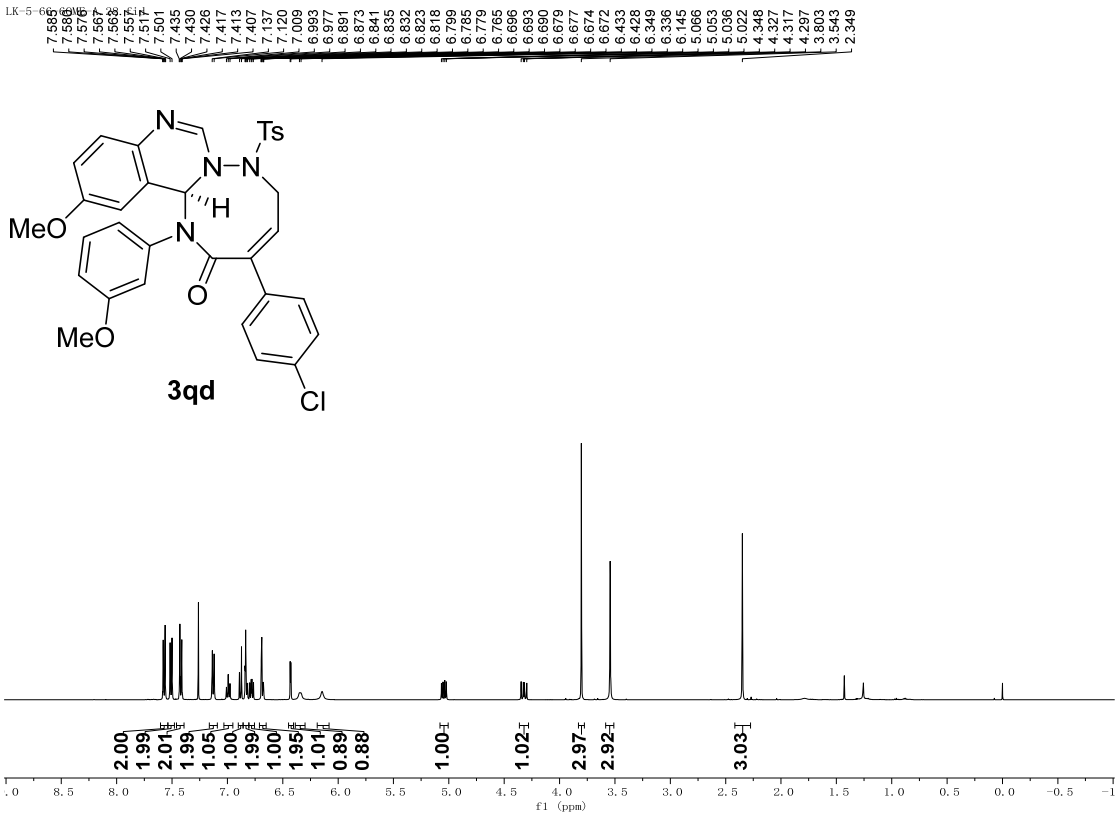


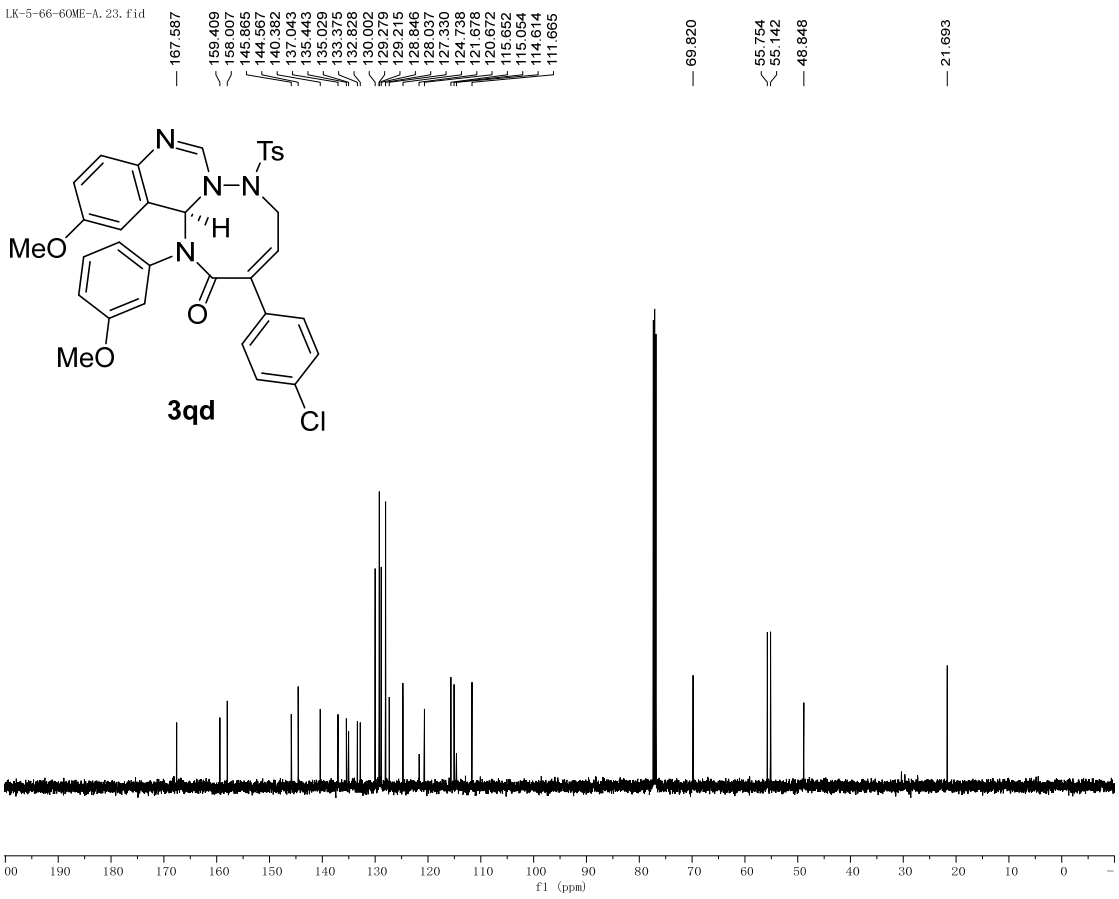
^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **3qb**



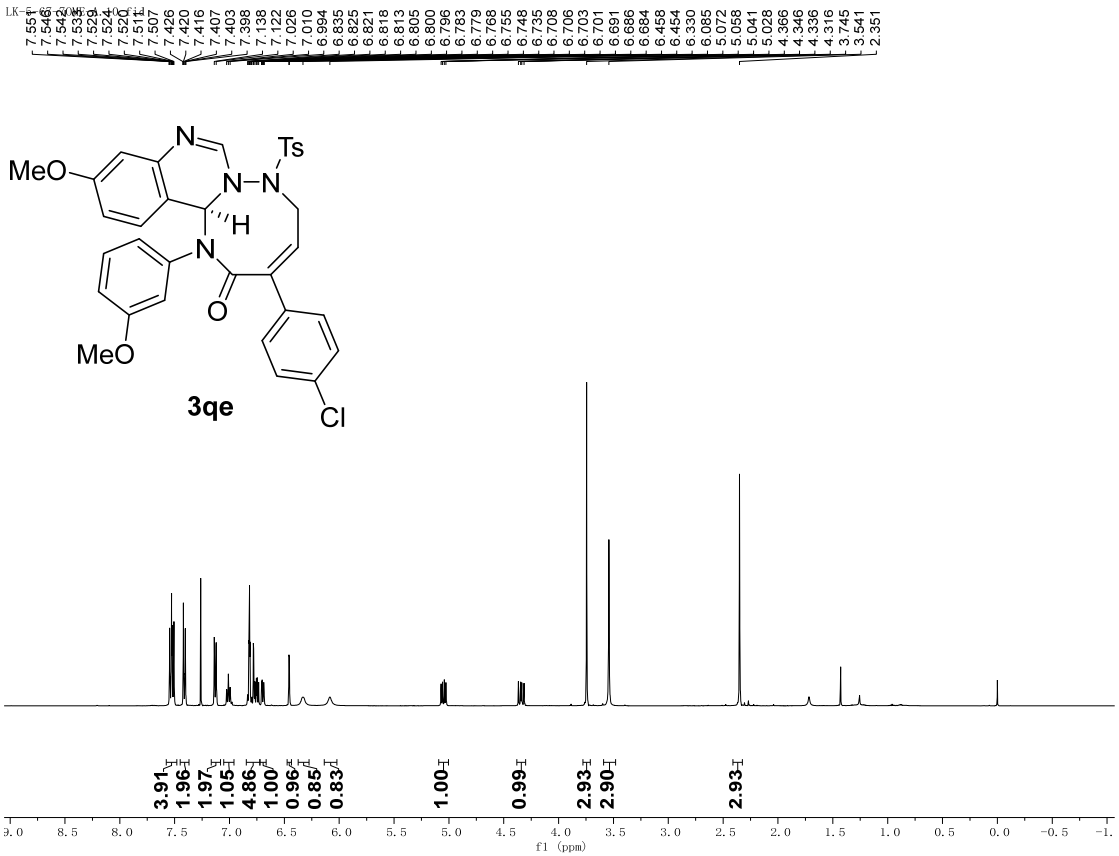


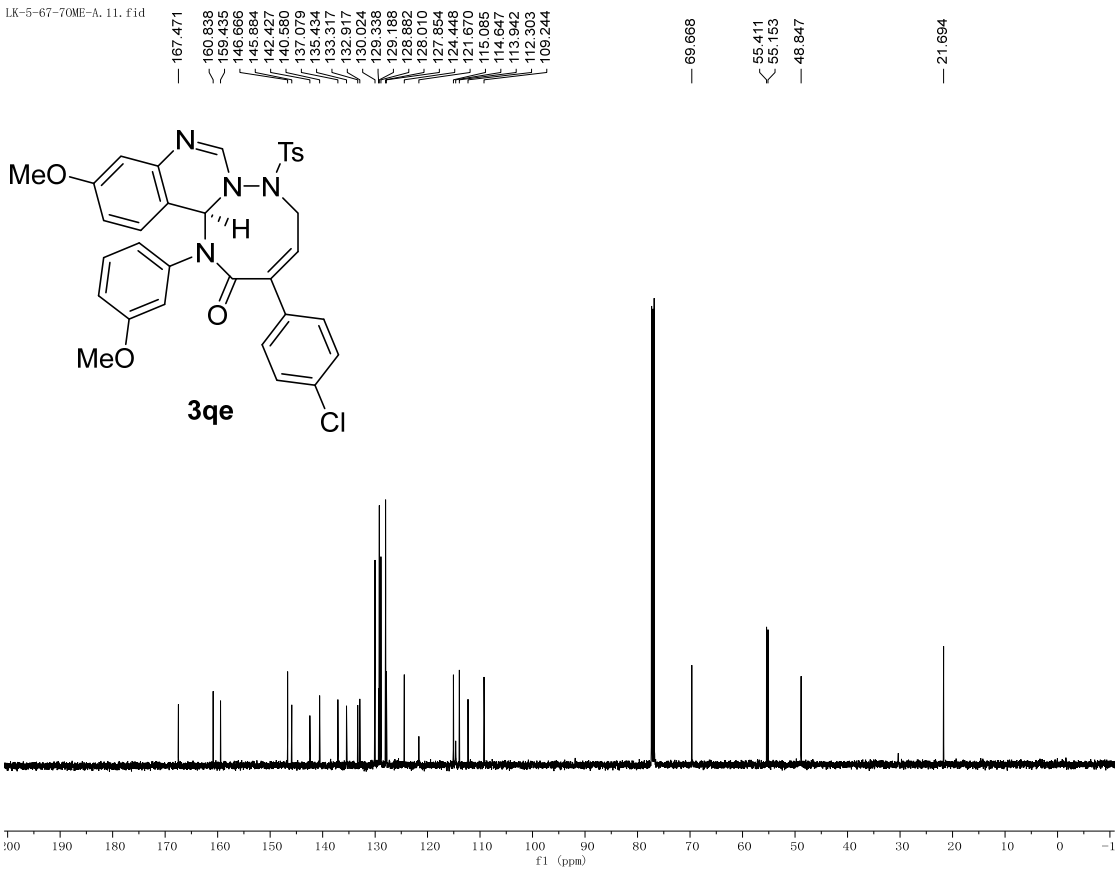
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qc**



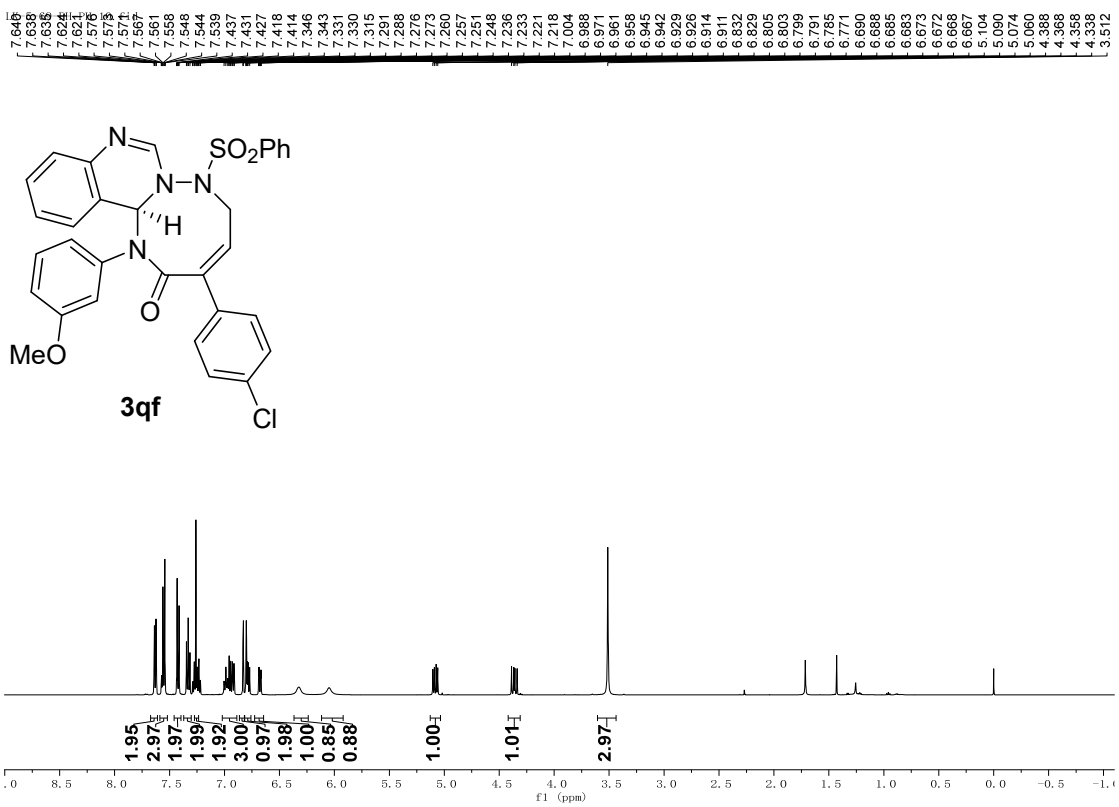


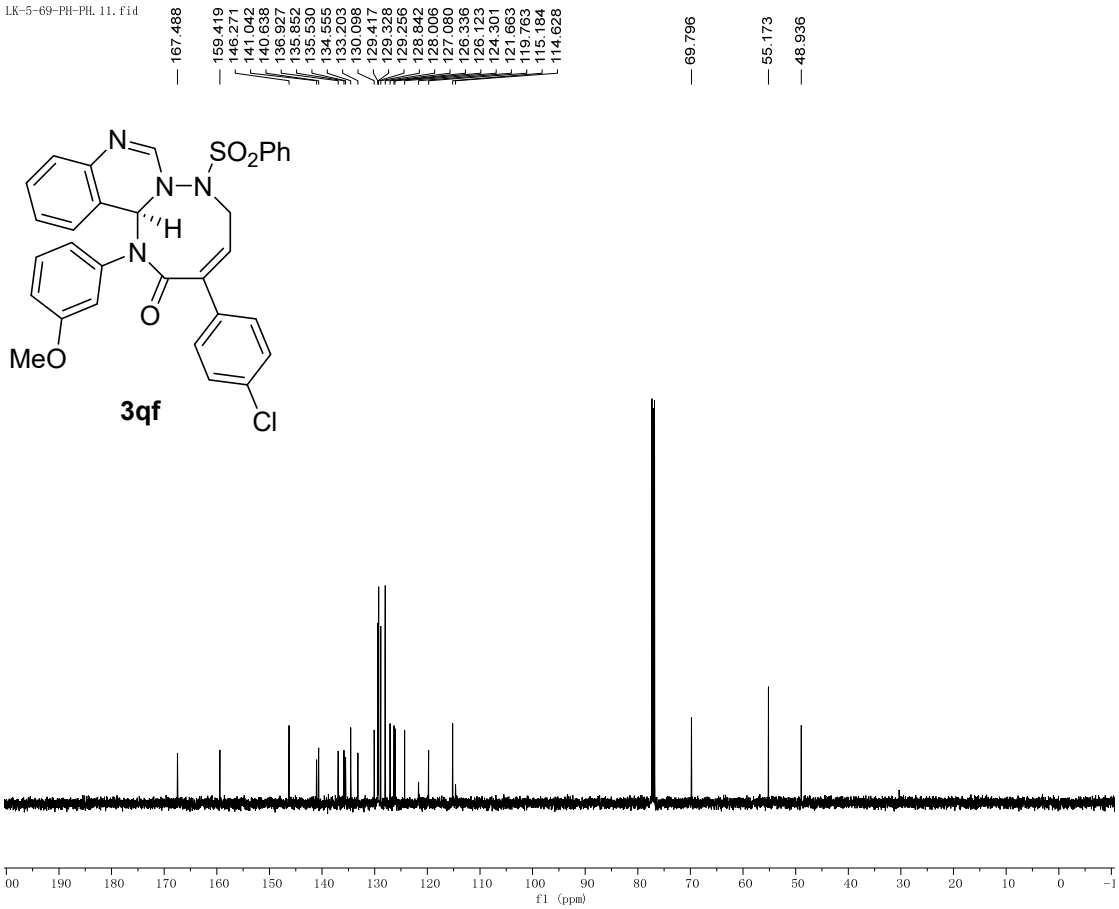
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qd**



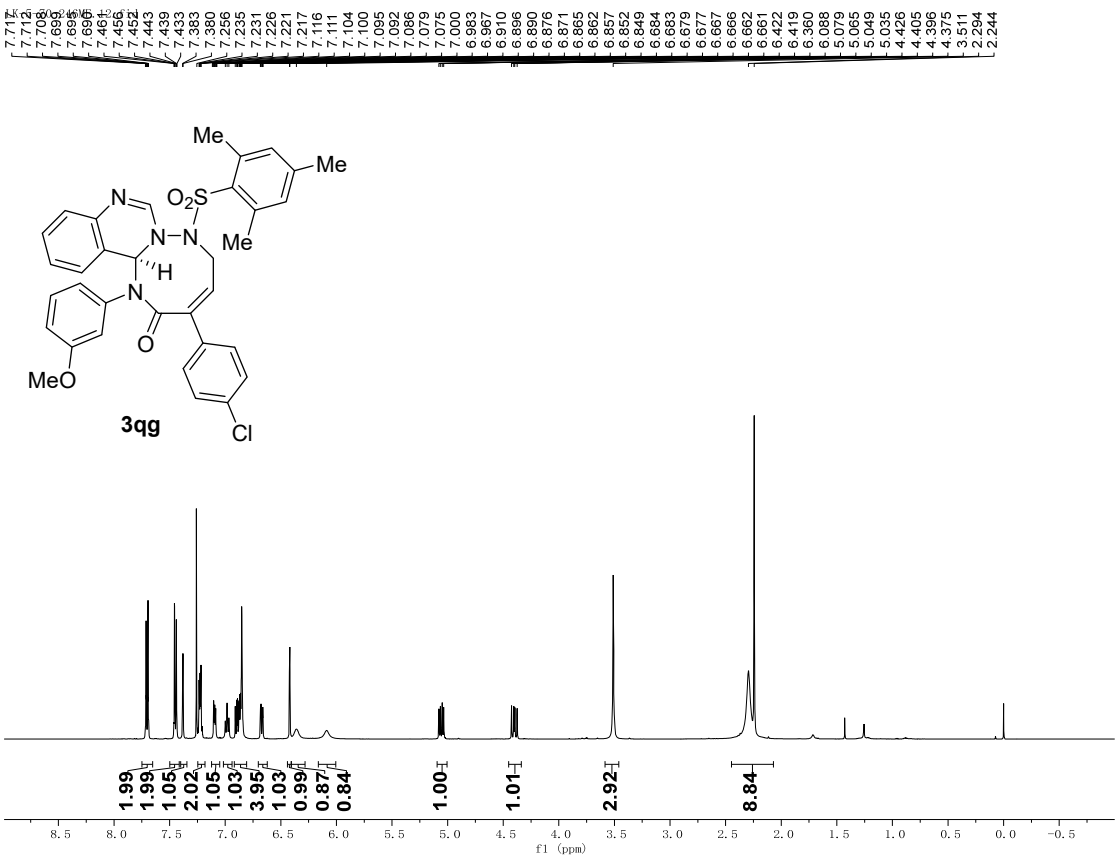


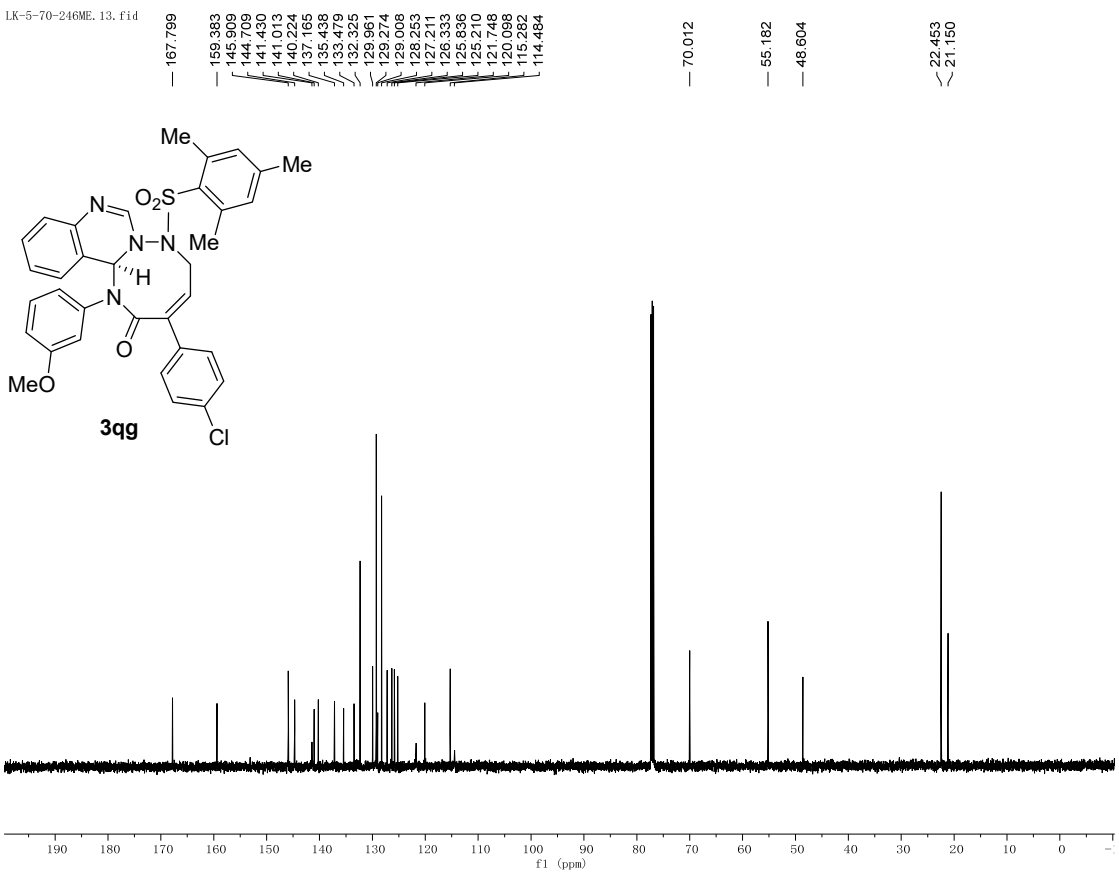
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qe**



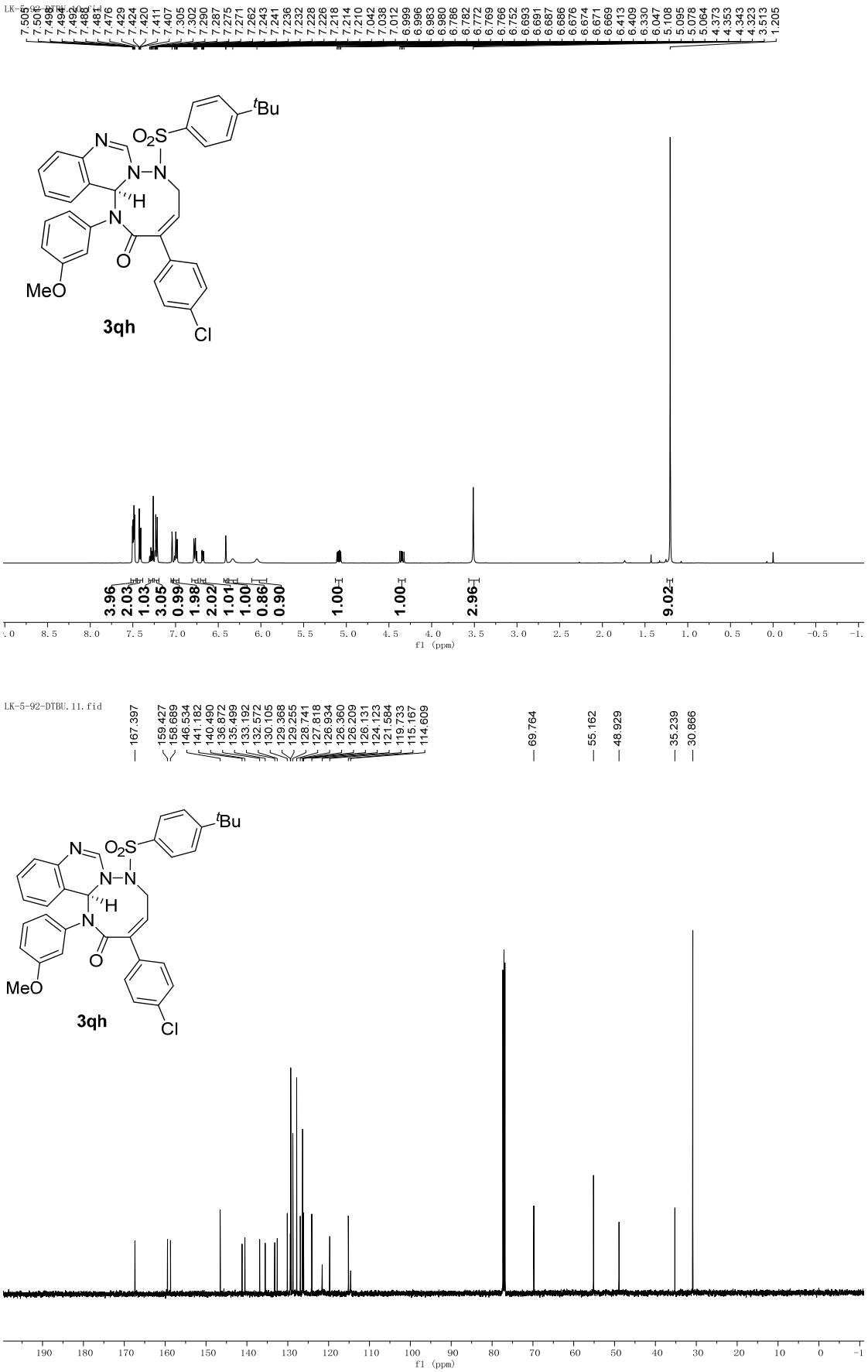


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qf**

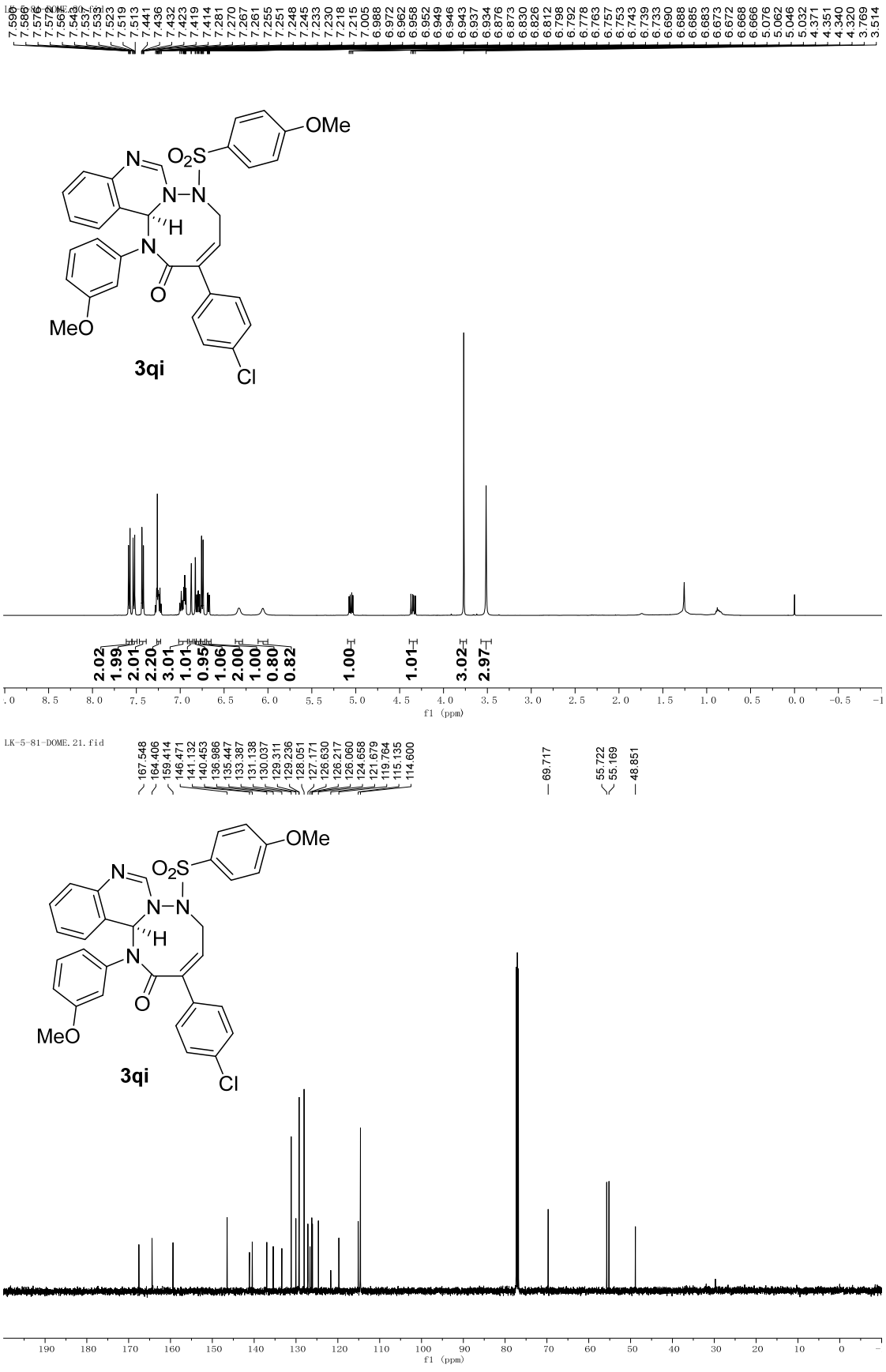




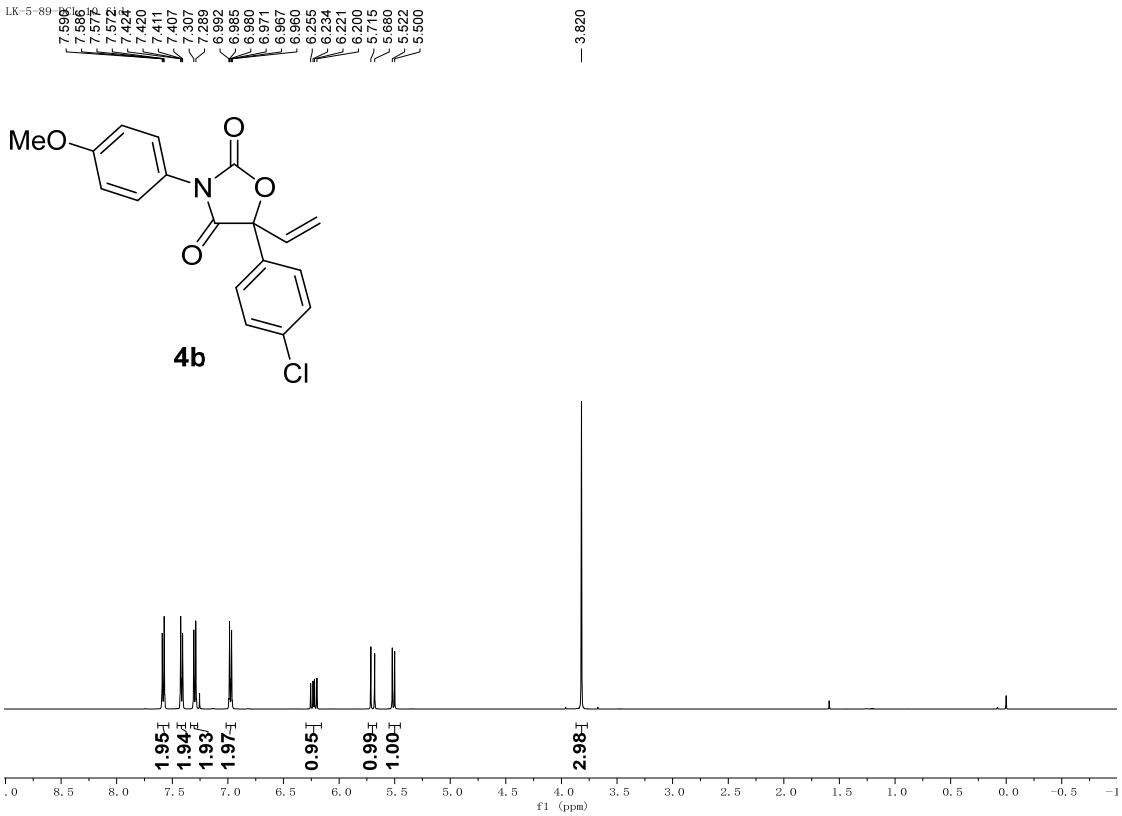
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qg**

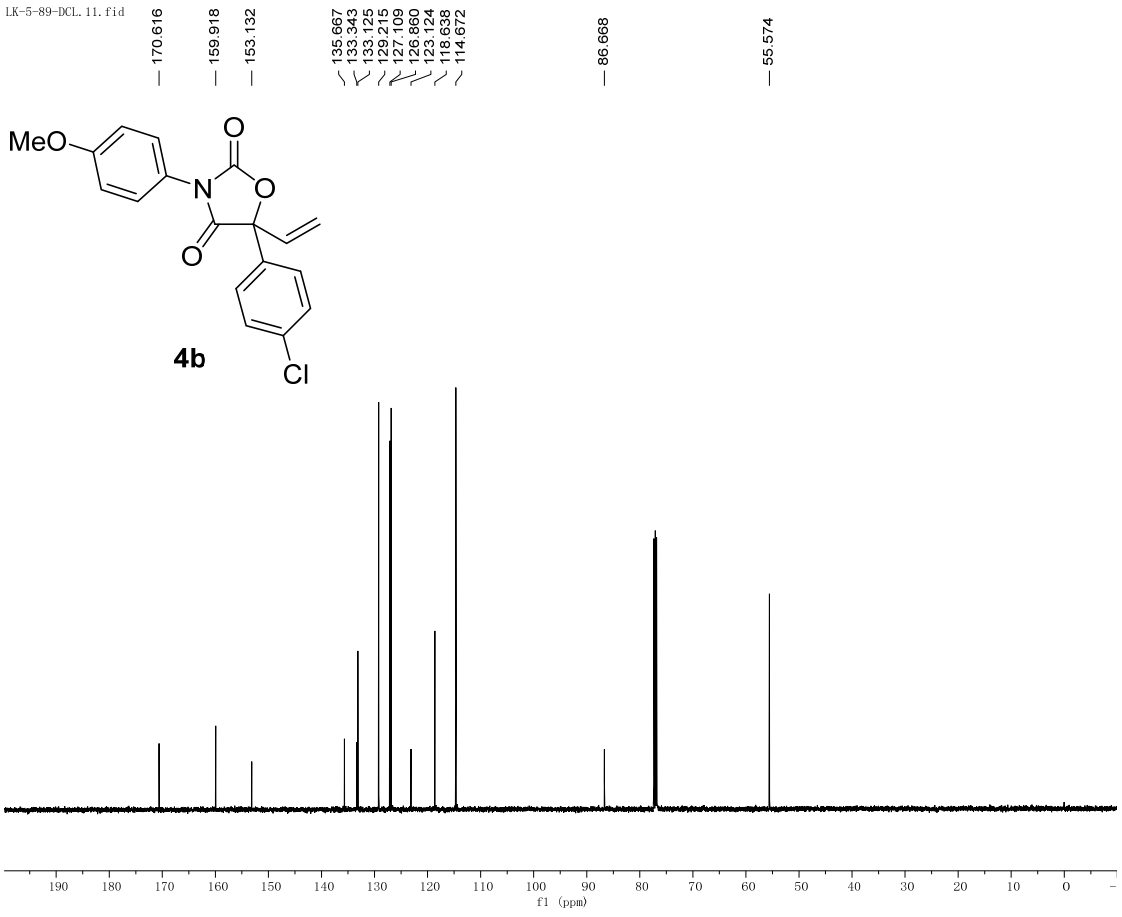


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qh**

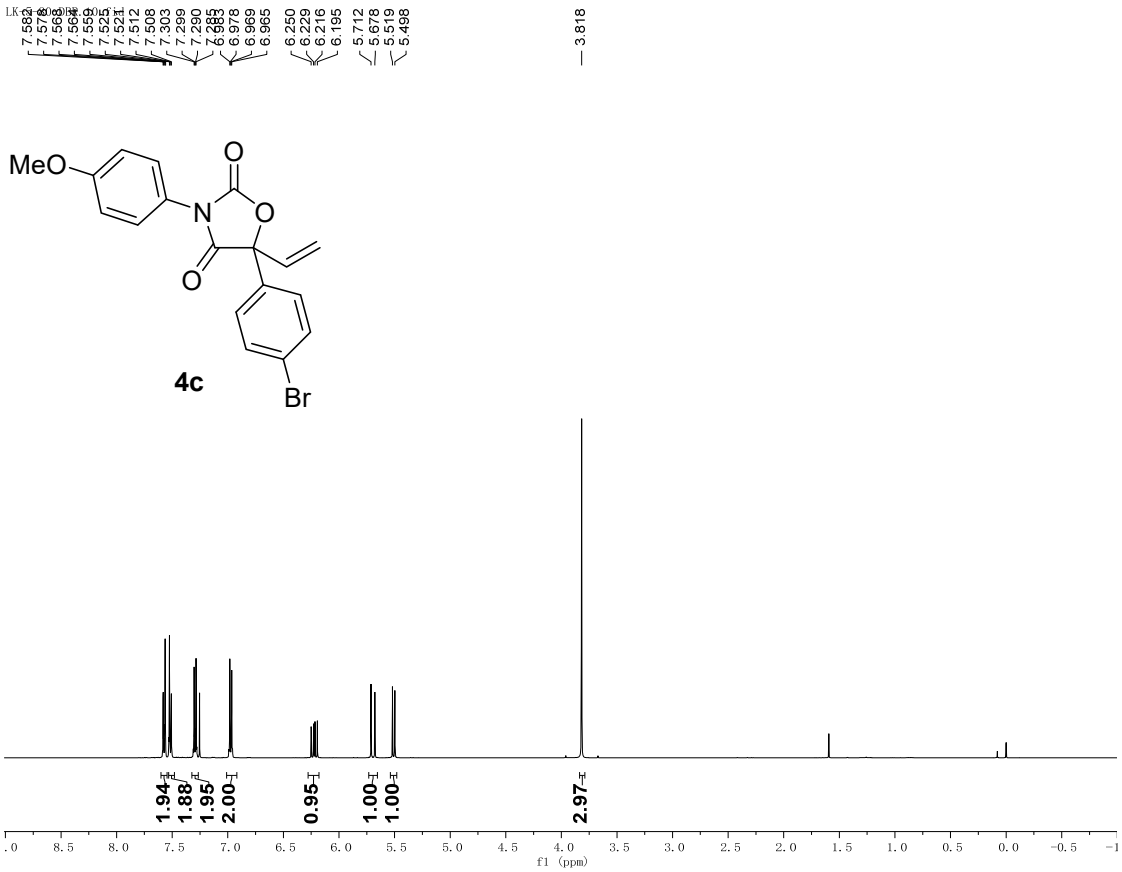


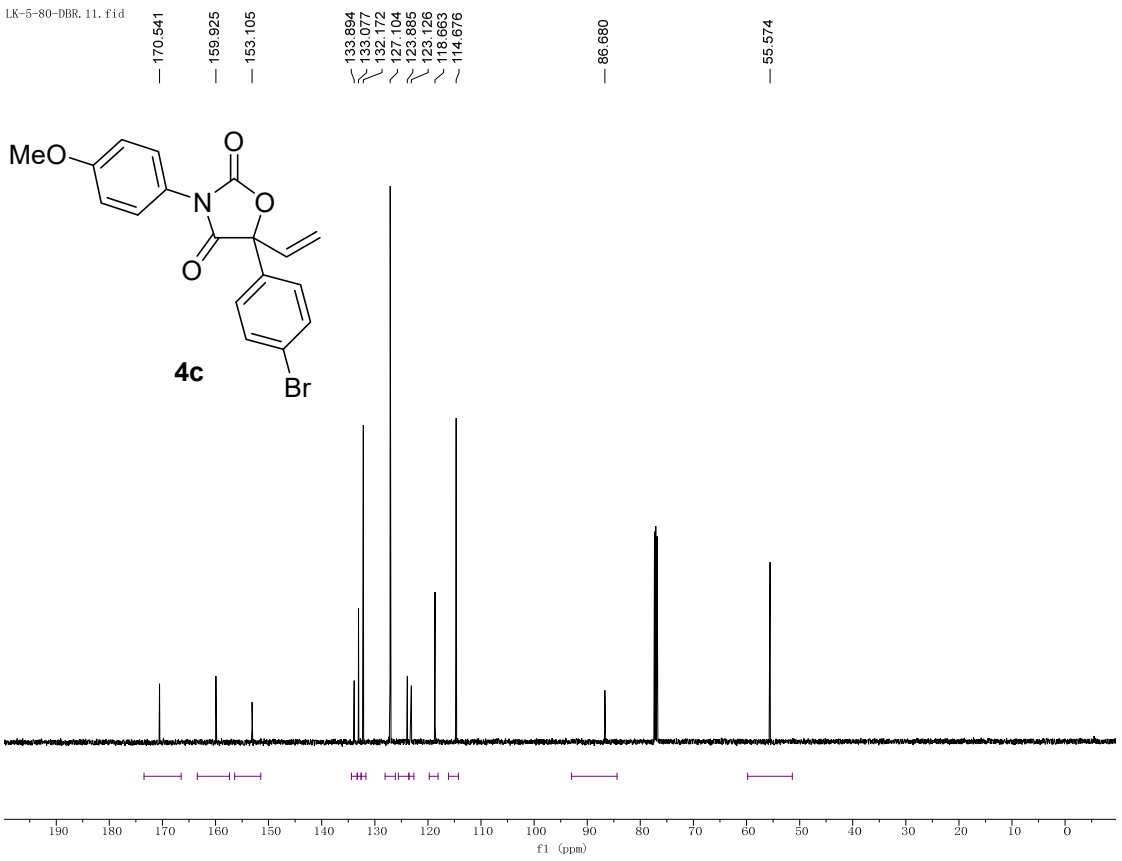
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **3qi**



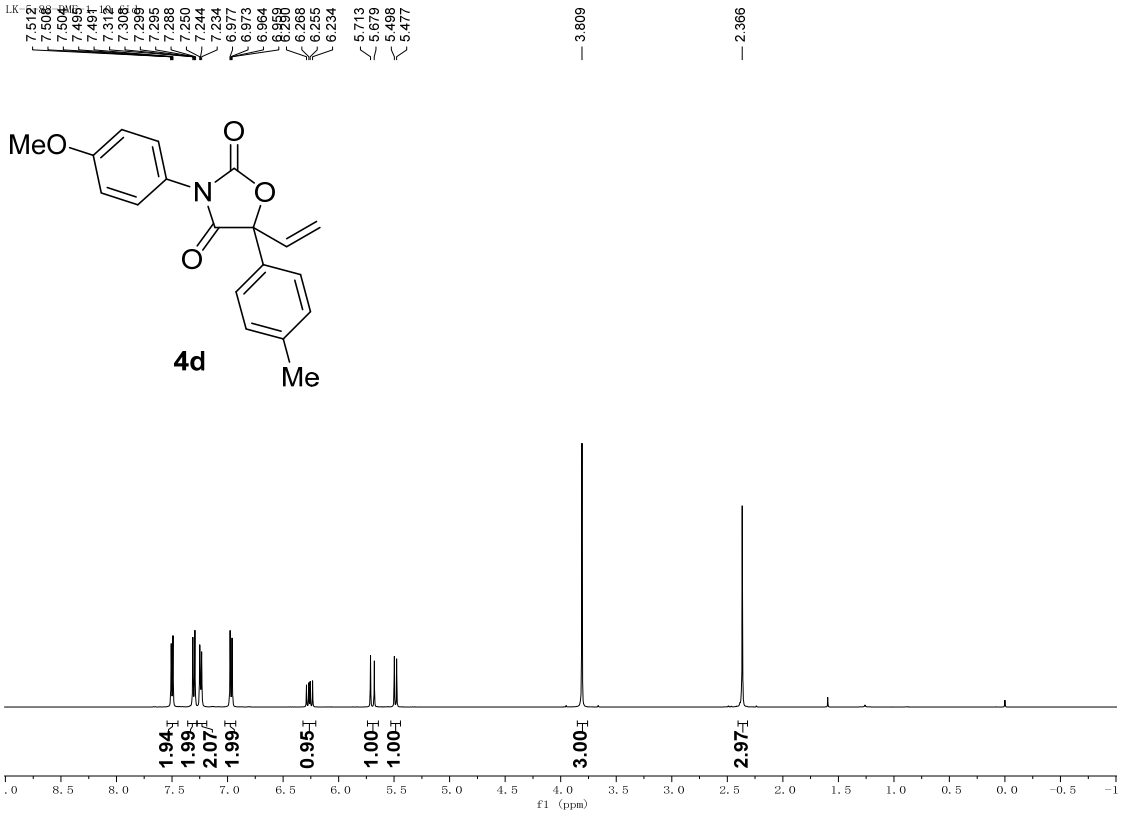


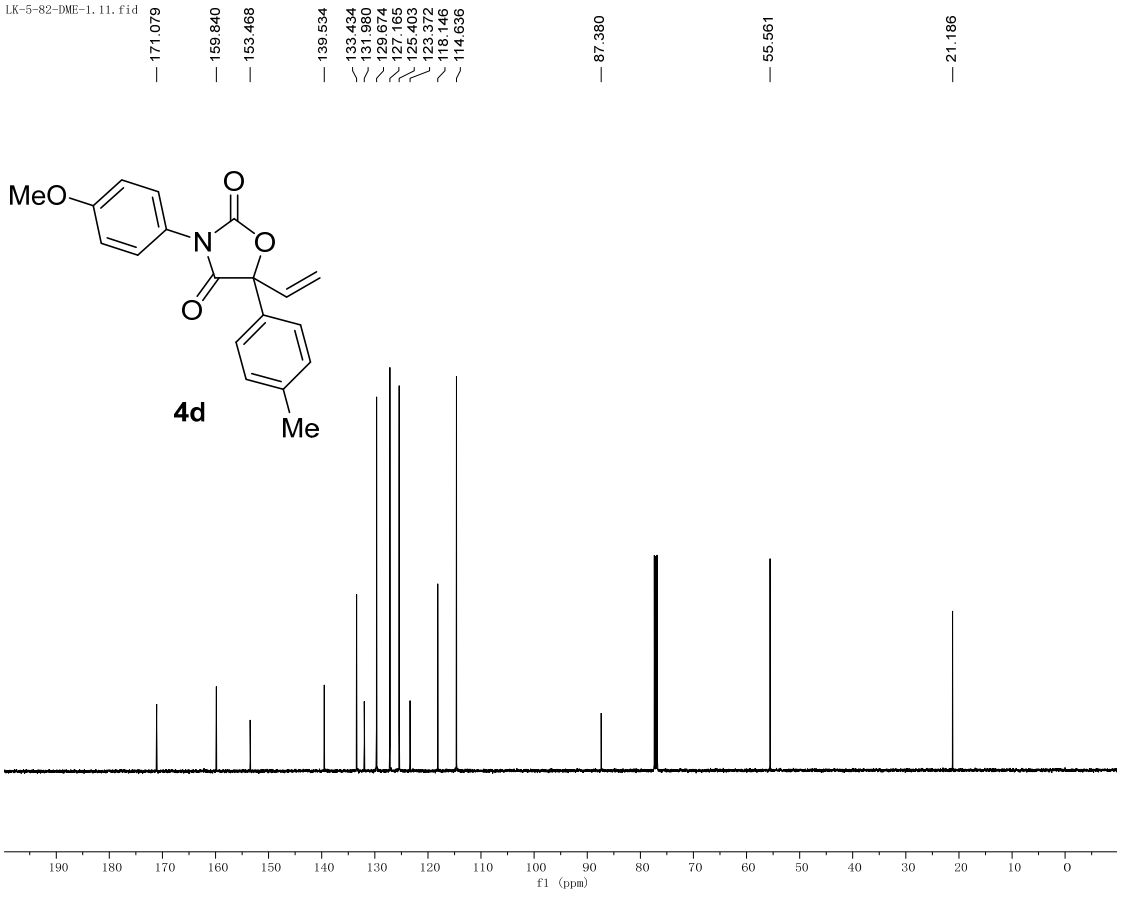
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **4b**



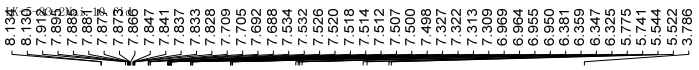


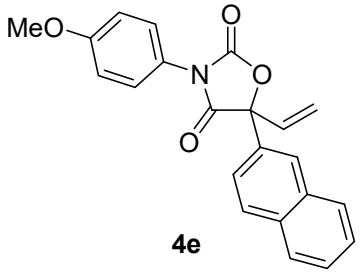
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **4c**



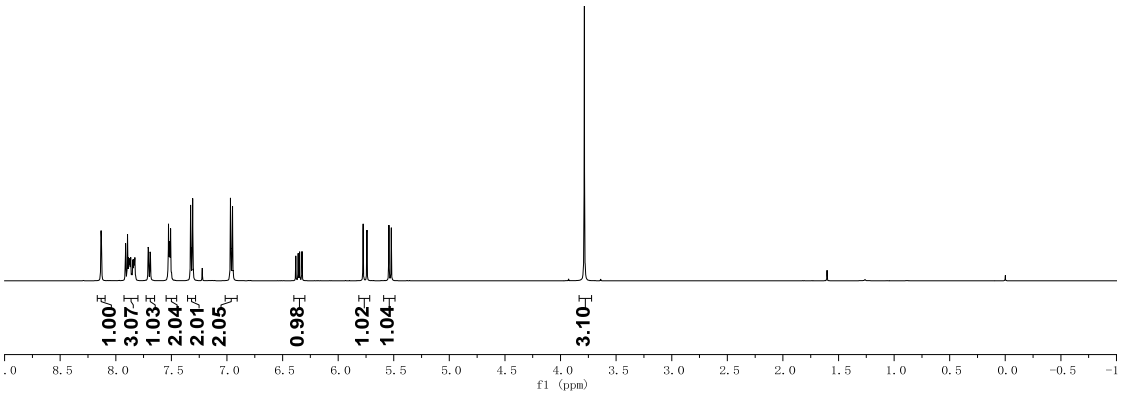


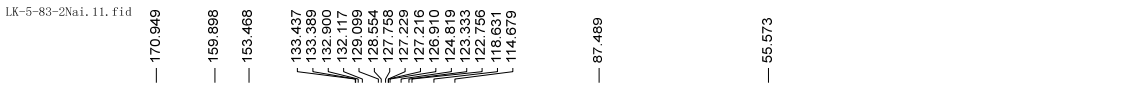
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **4d**

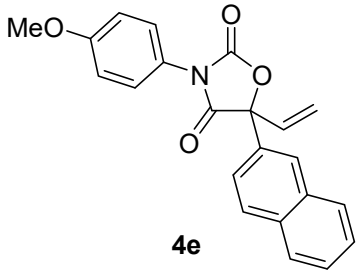




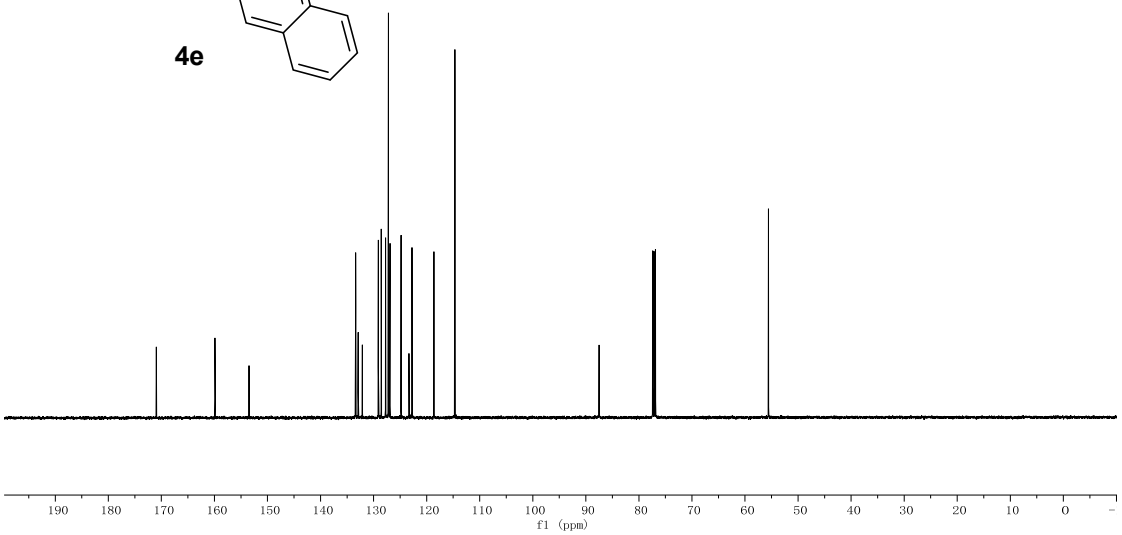
4e



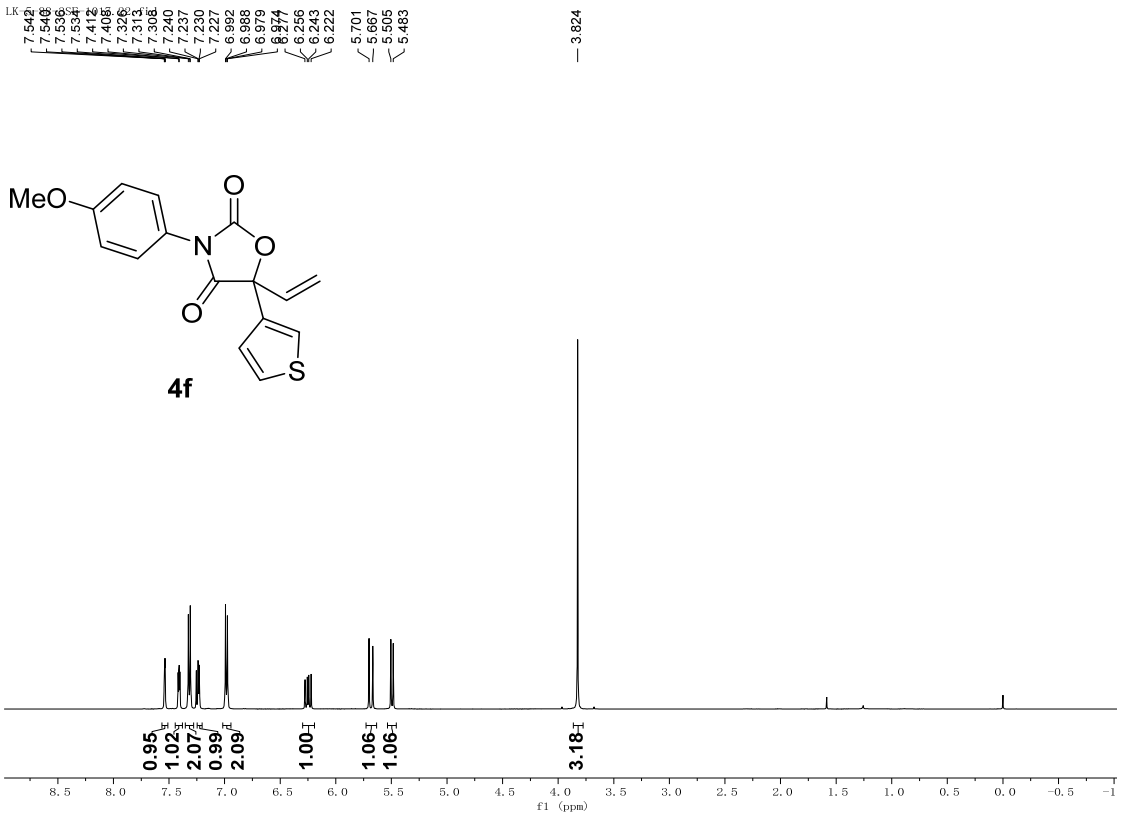


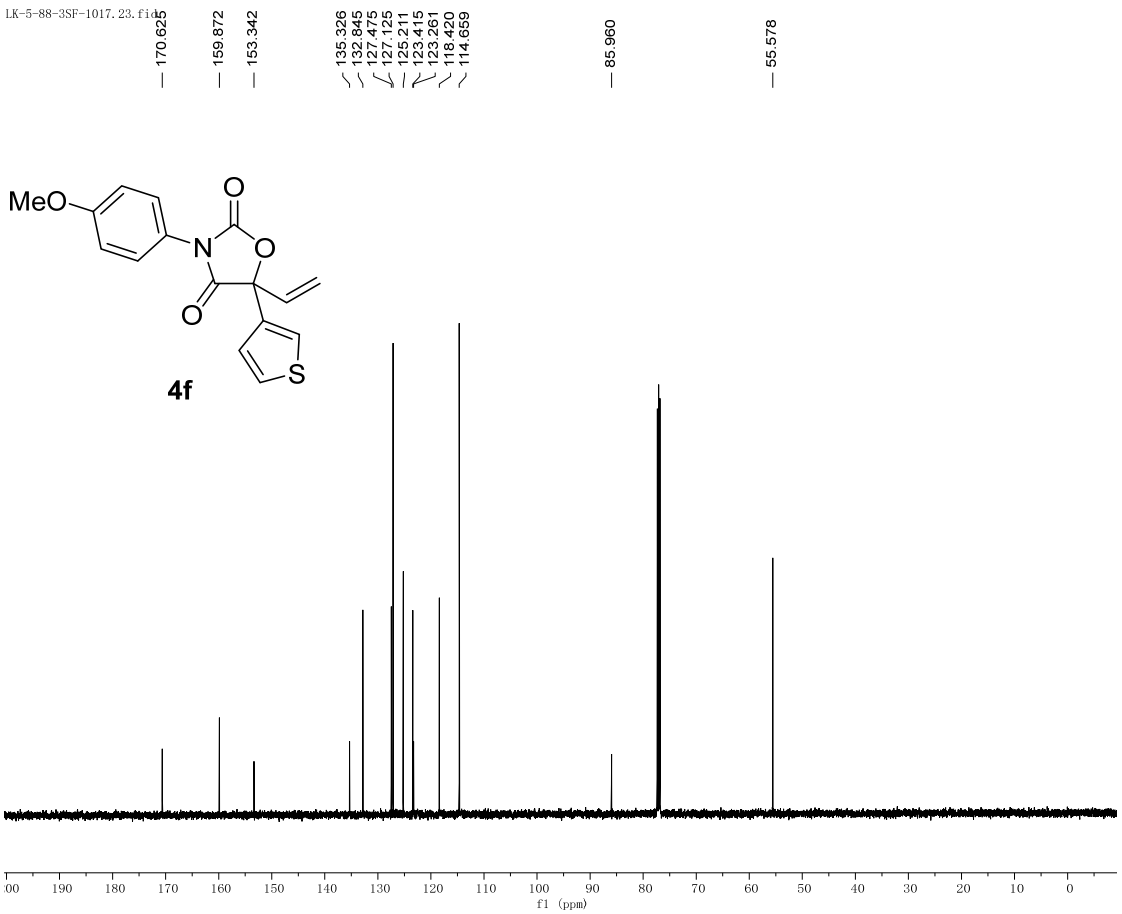


4e

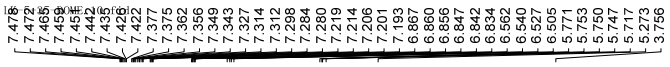


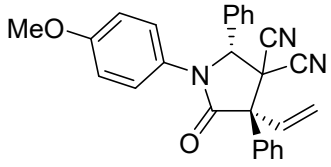
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **4e**



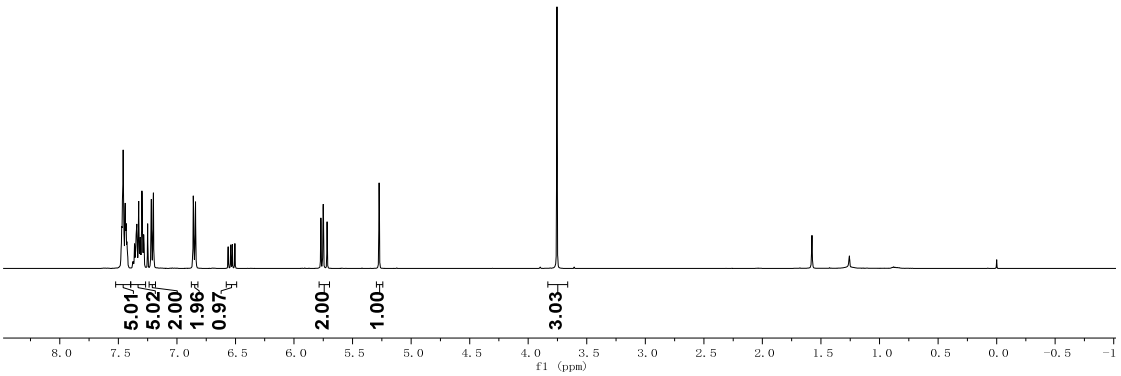


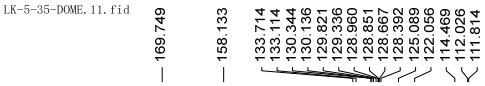
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **4f**

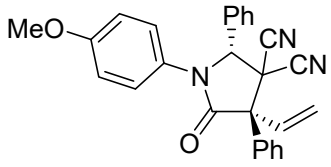




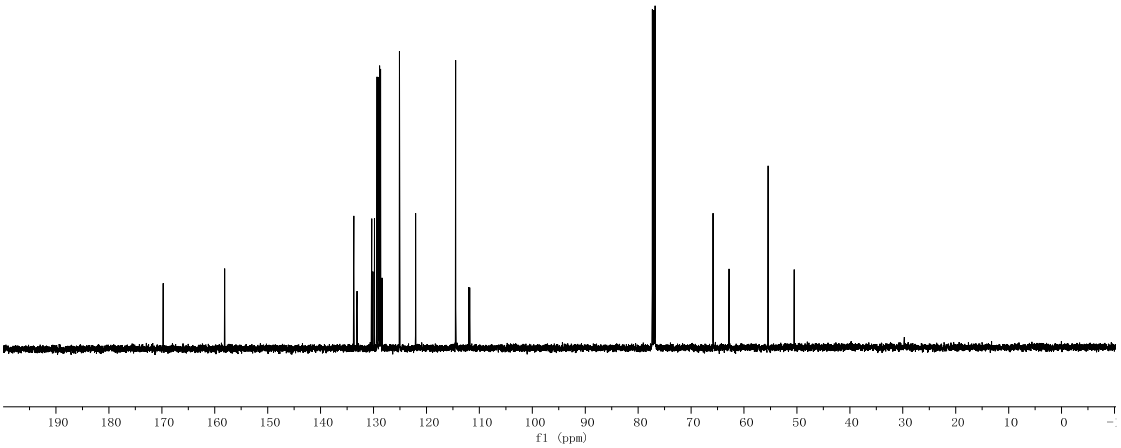
6aa



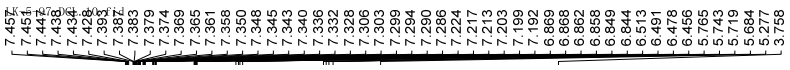


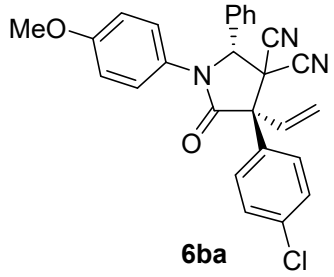


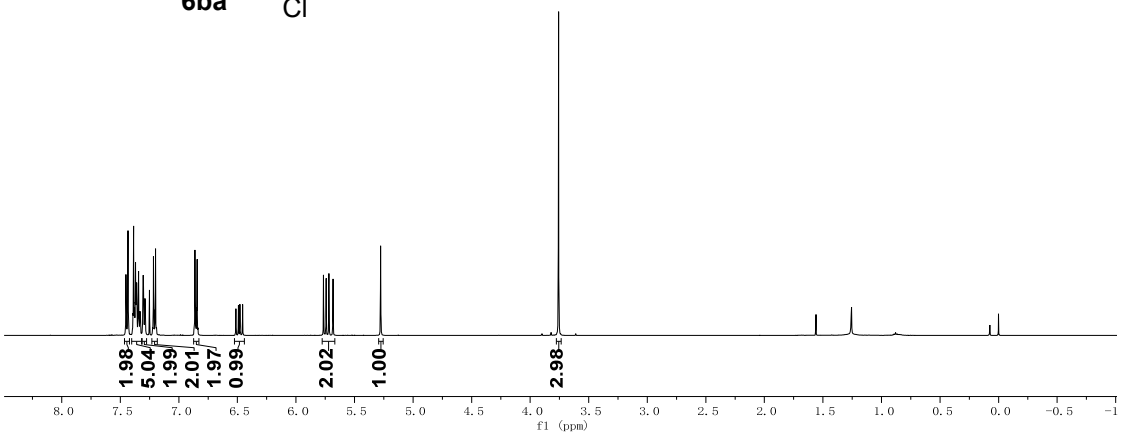
6aa

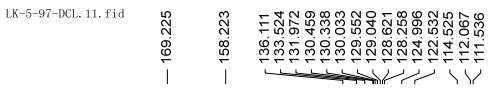


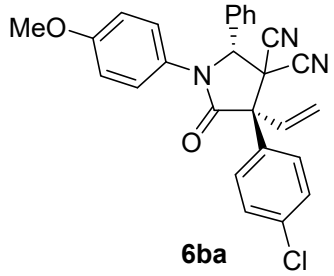
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6aa**

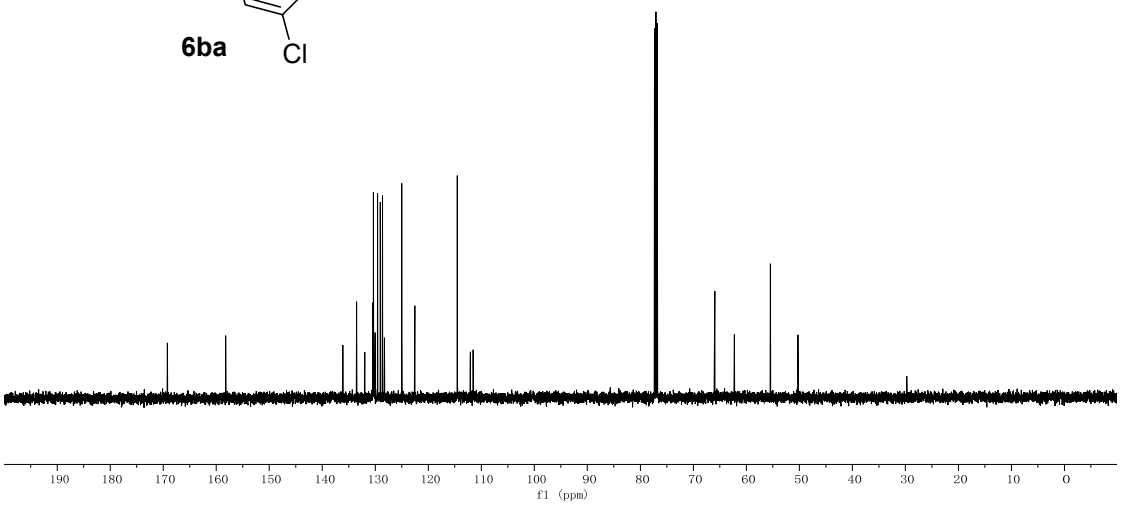




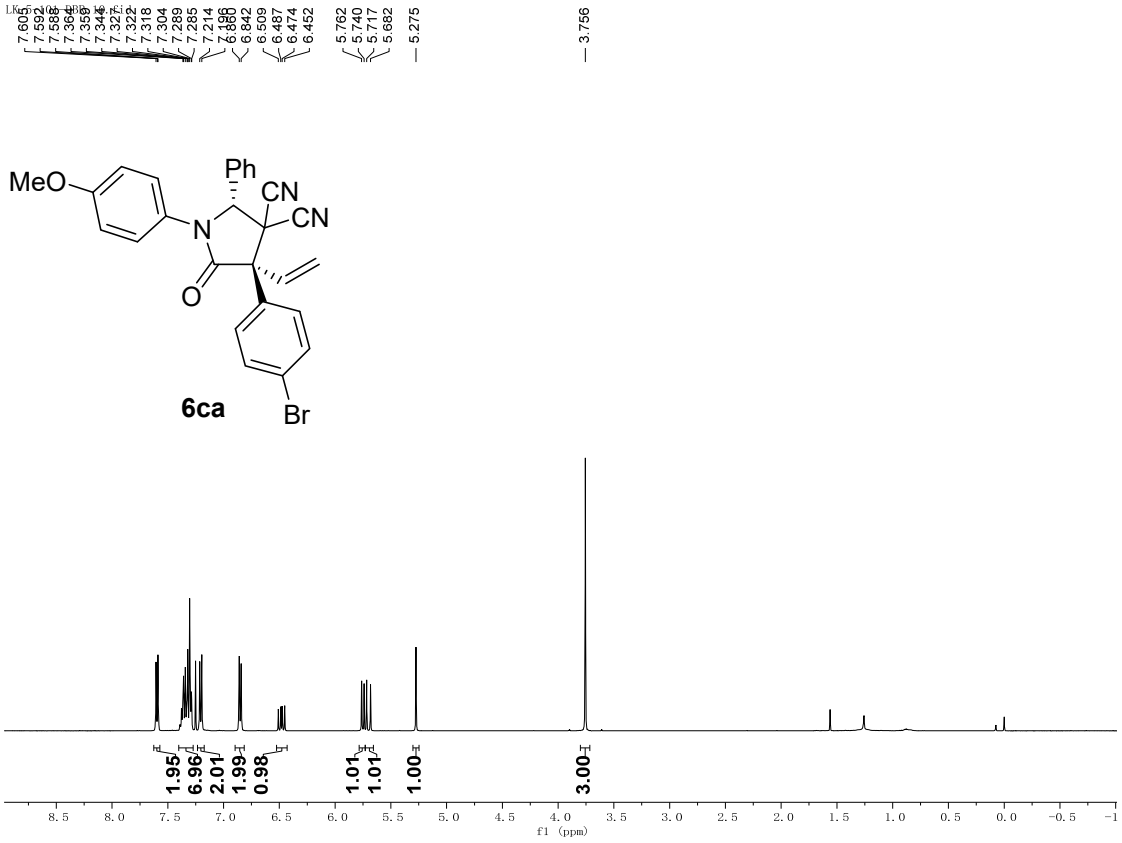


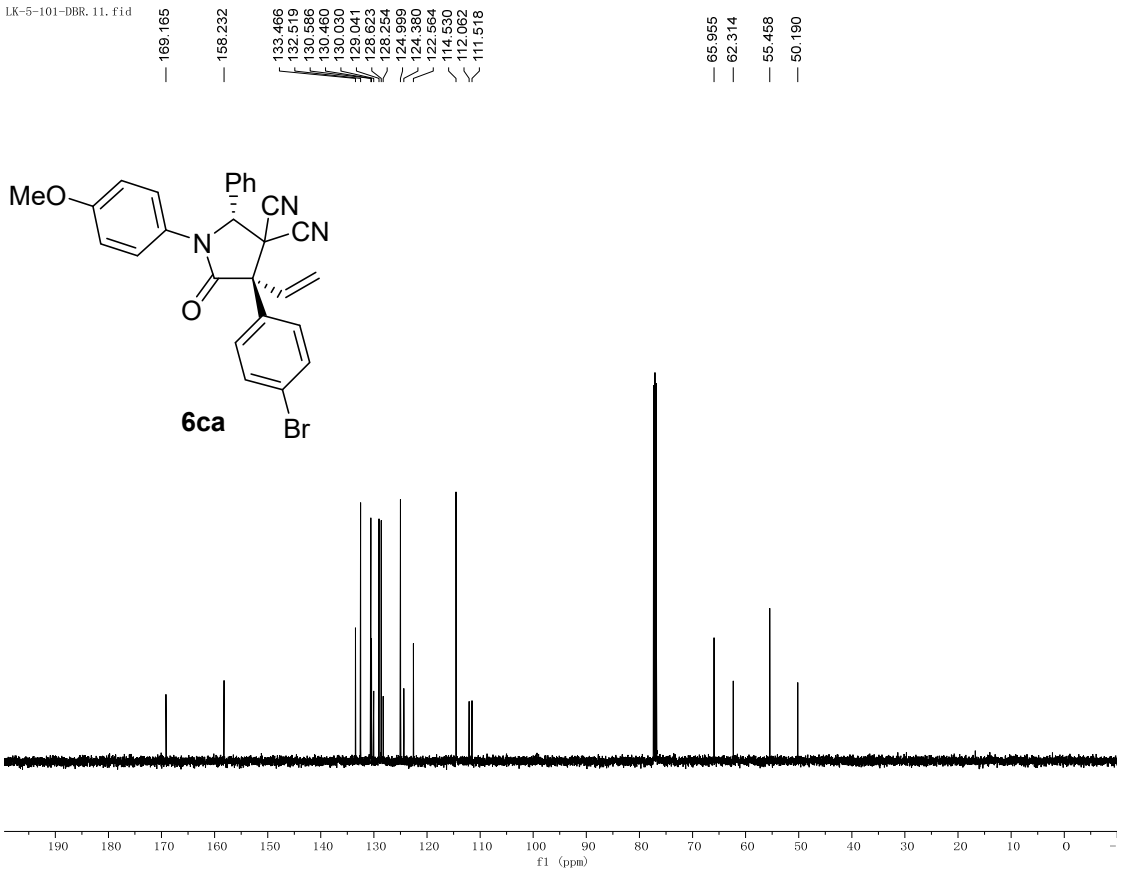




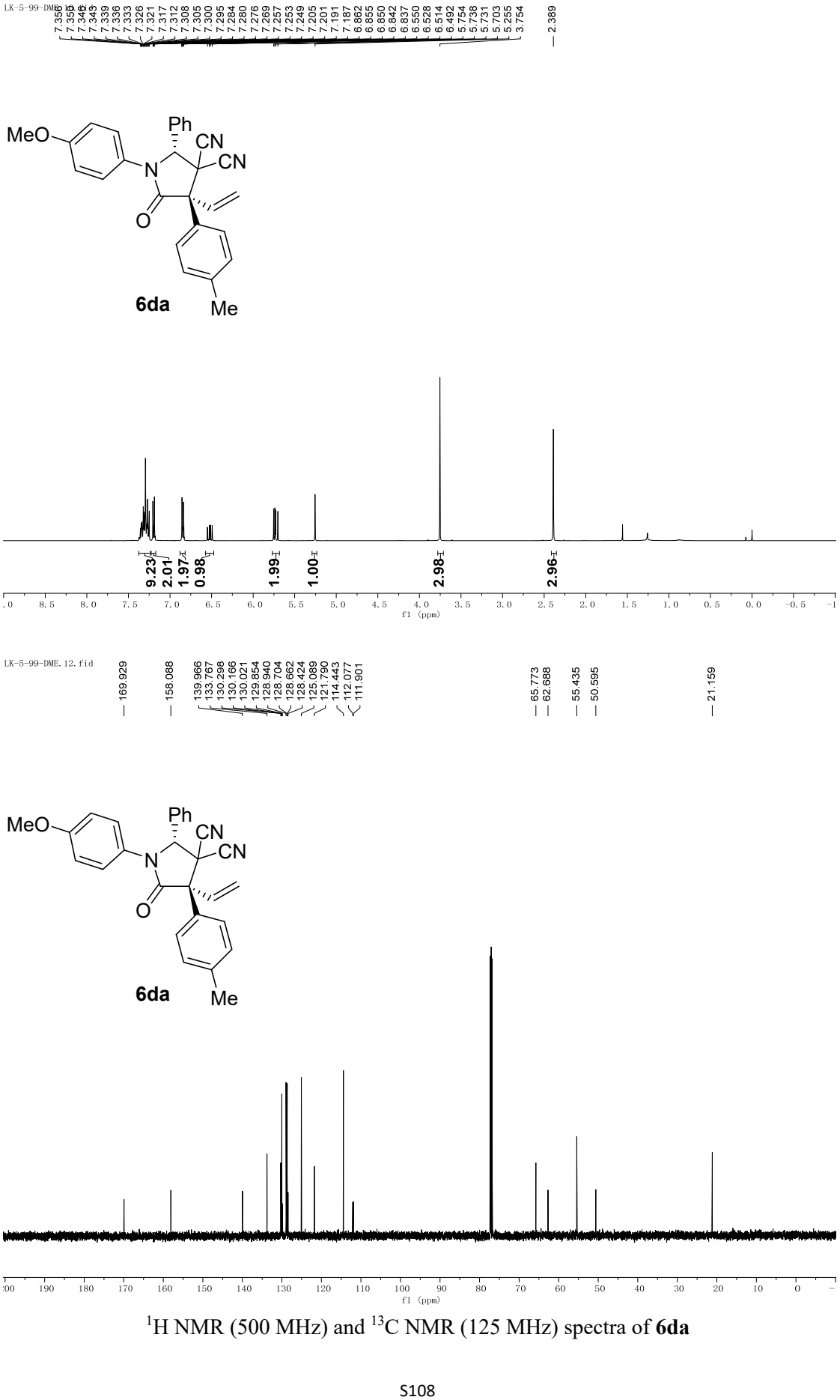


^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6ba**

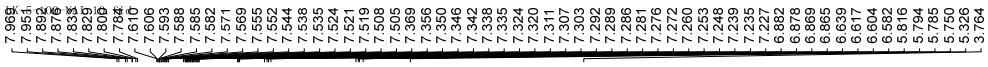


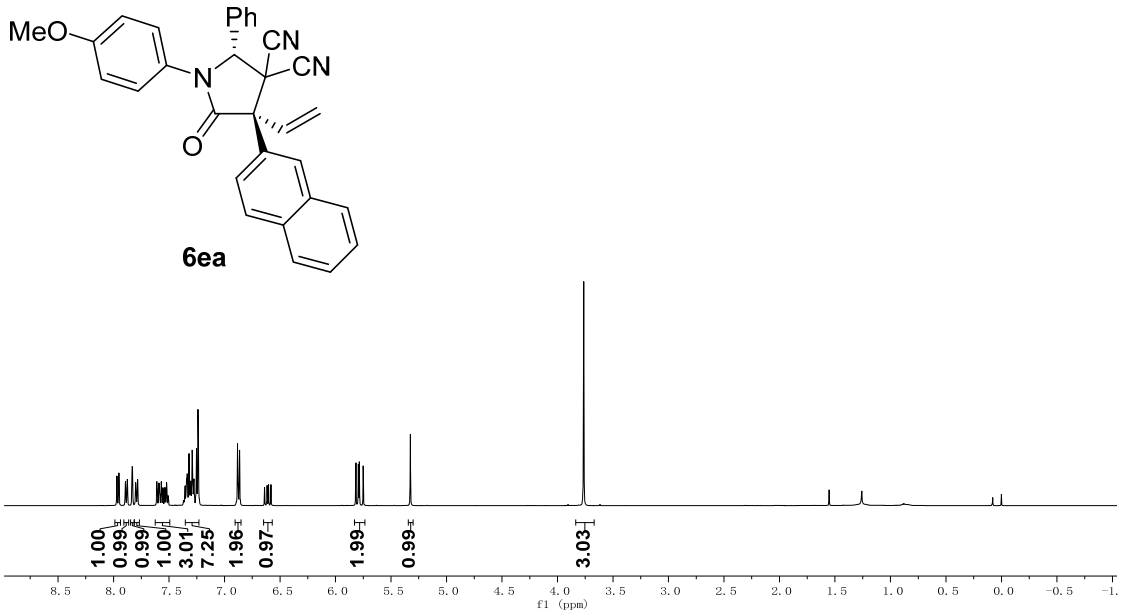


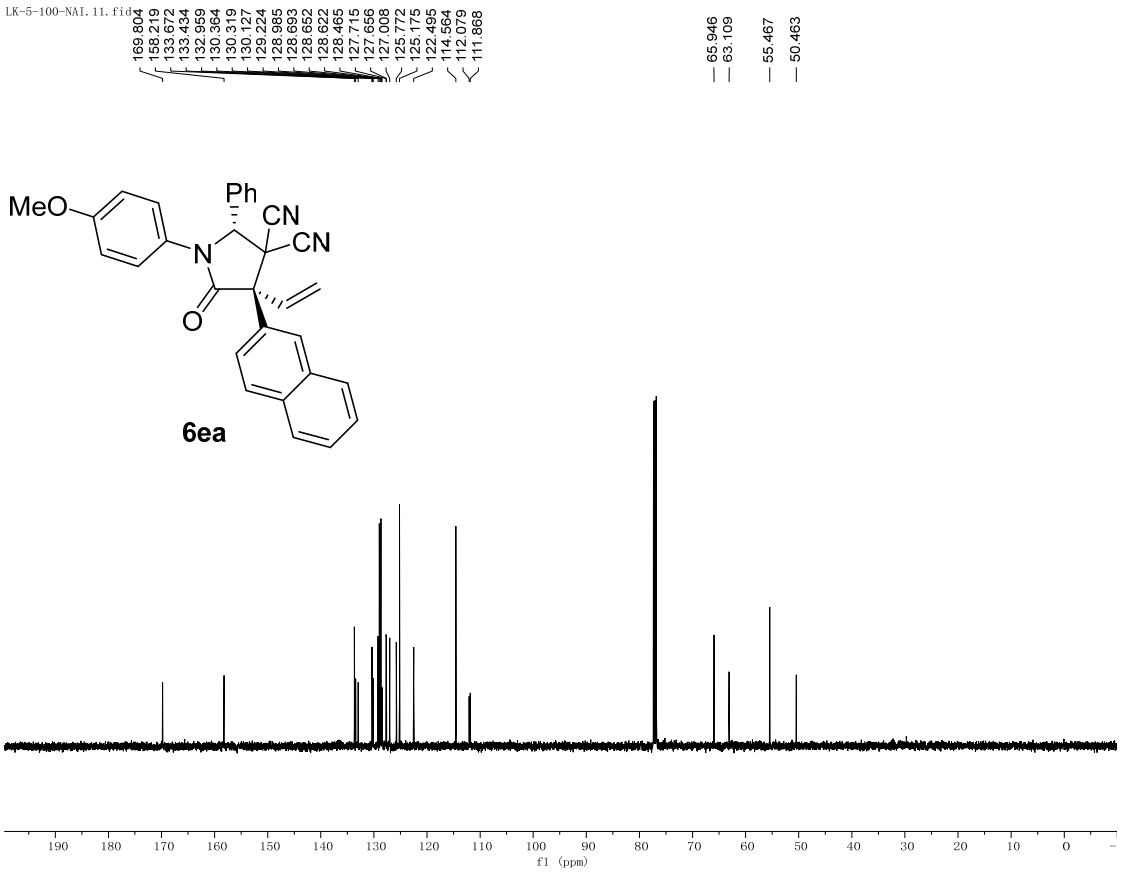
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6ca**



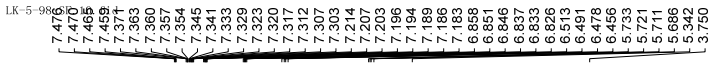
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6da**

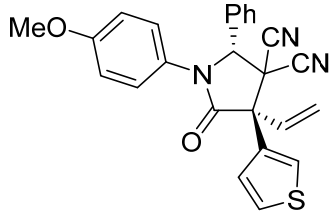




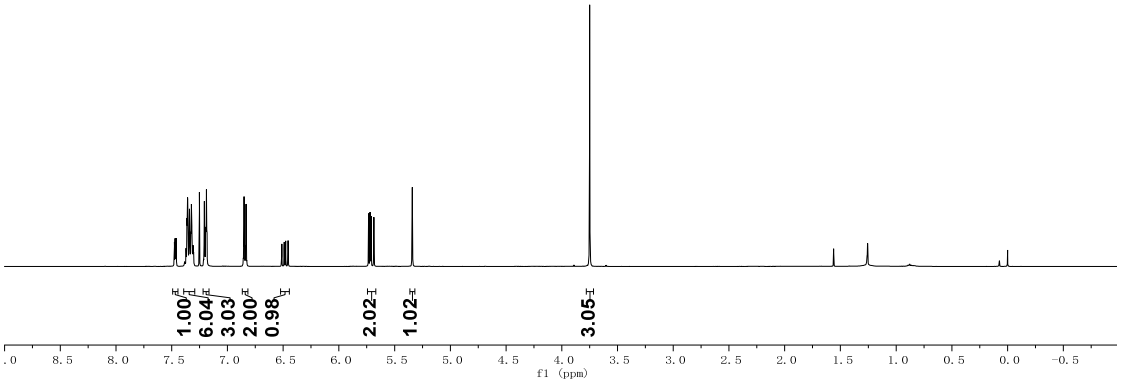


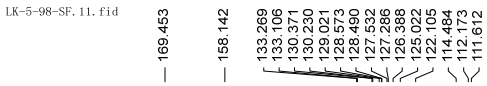
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6ea**

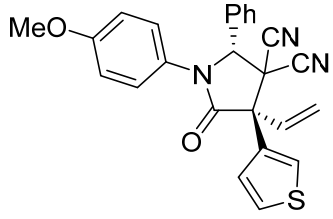




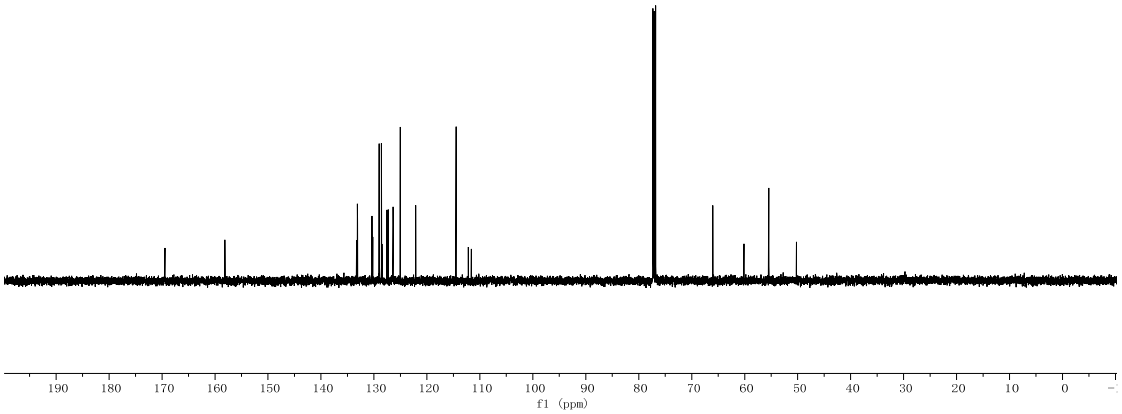
6fa



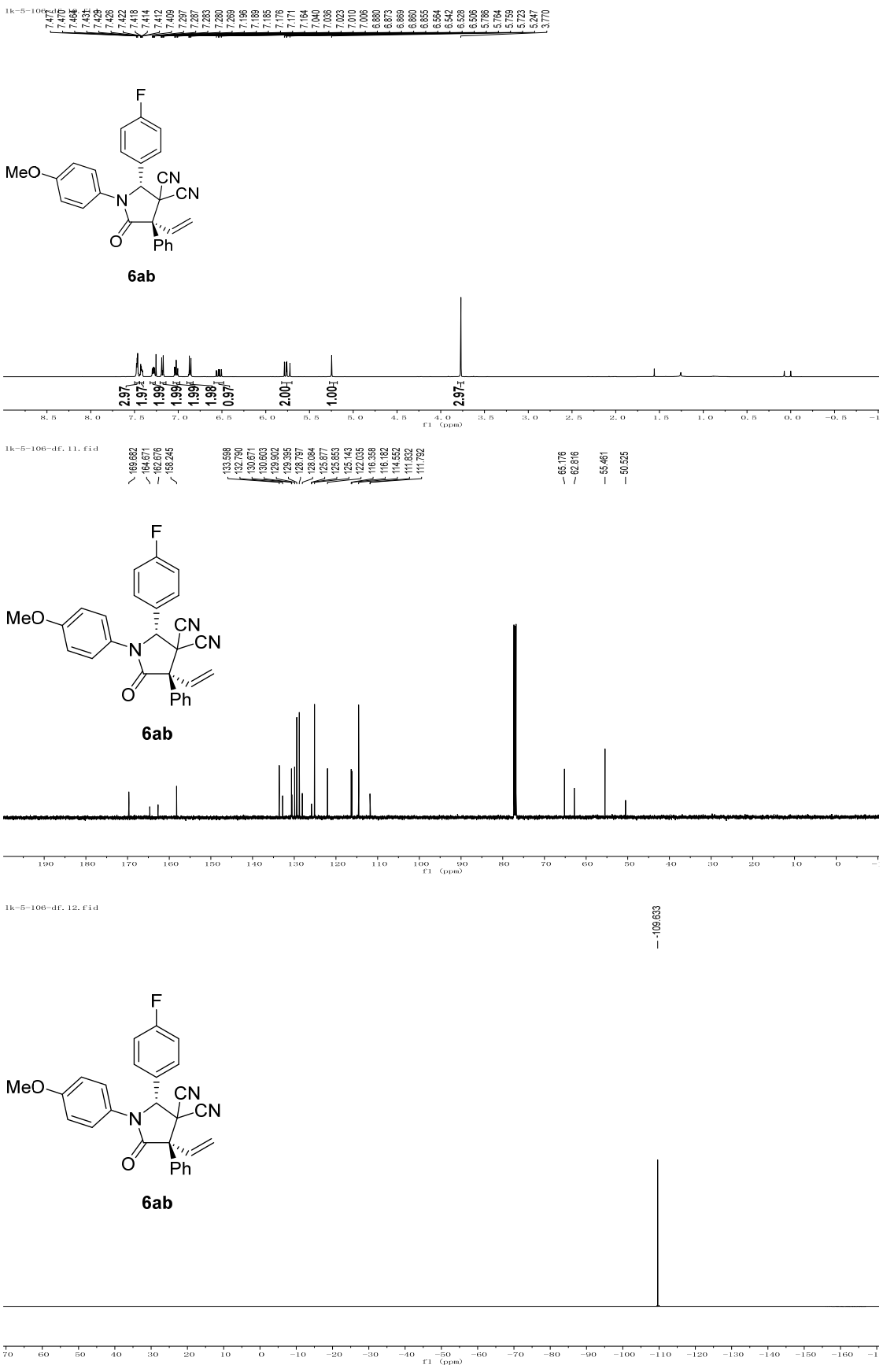




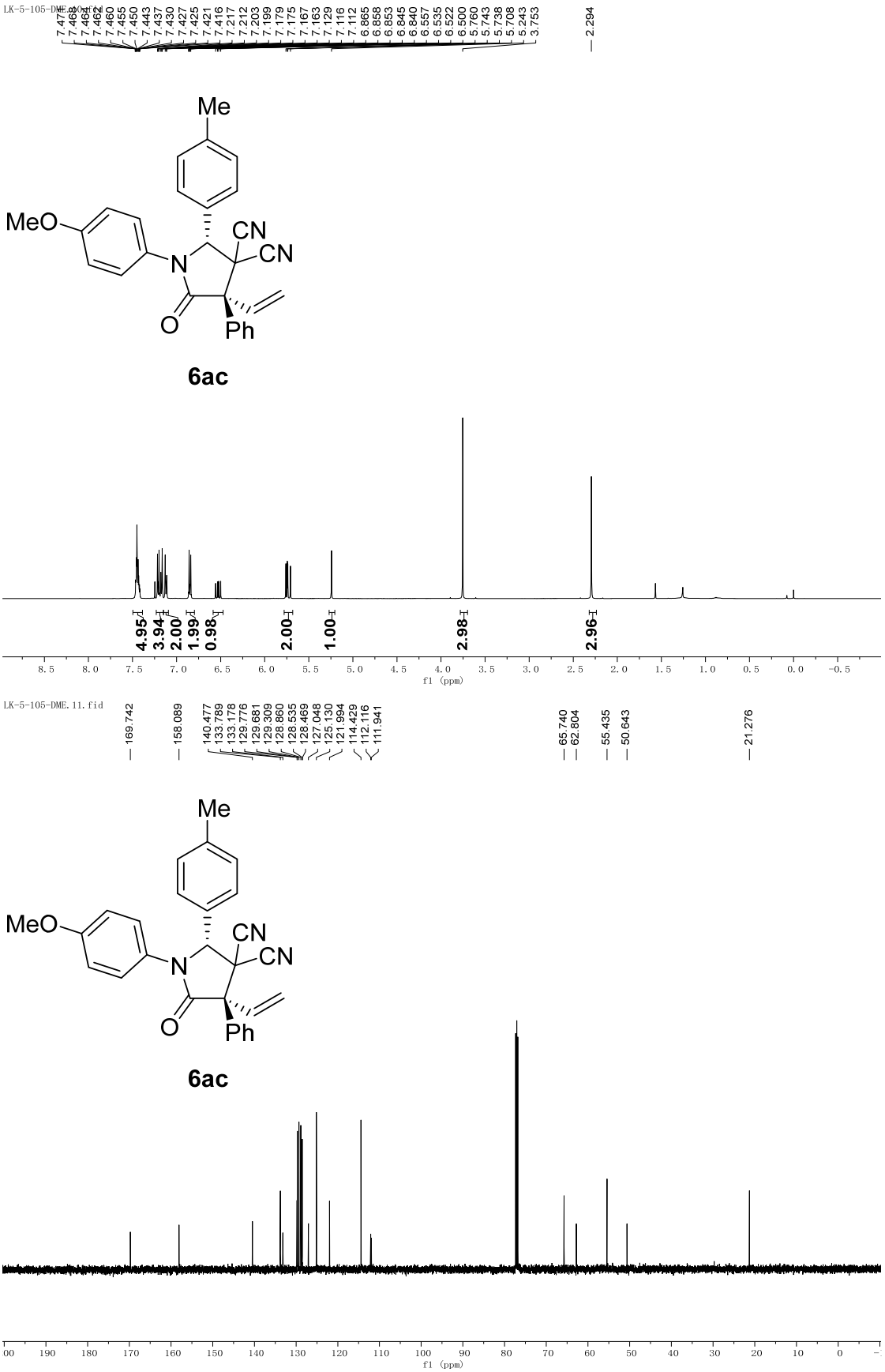
6fa



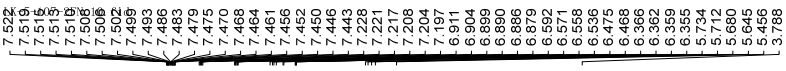
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6fa**

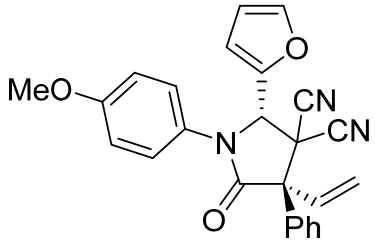


^{1}H NMR (500 MHz), ^{13}C NMR (125 MHz) and ^{19}F NMR (470 MHz) spectra of **6ab**

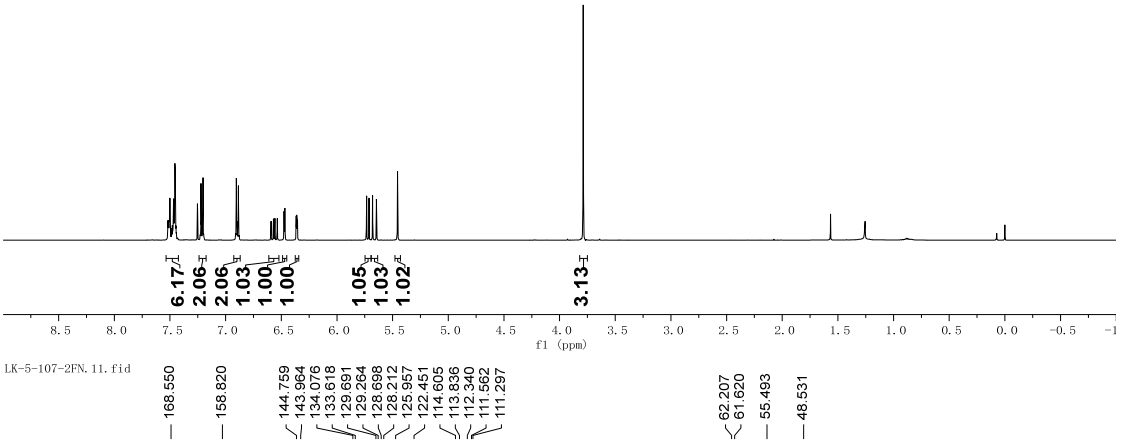


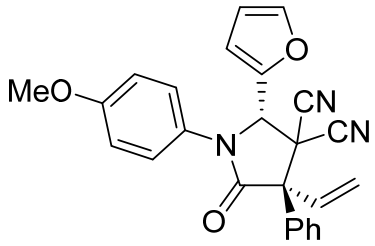
^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6ac**



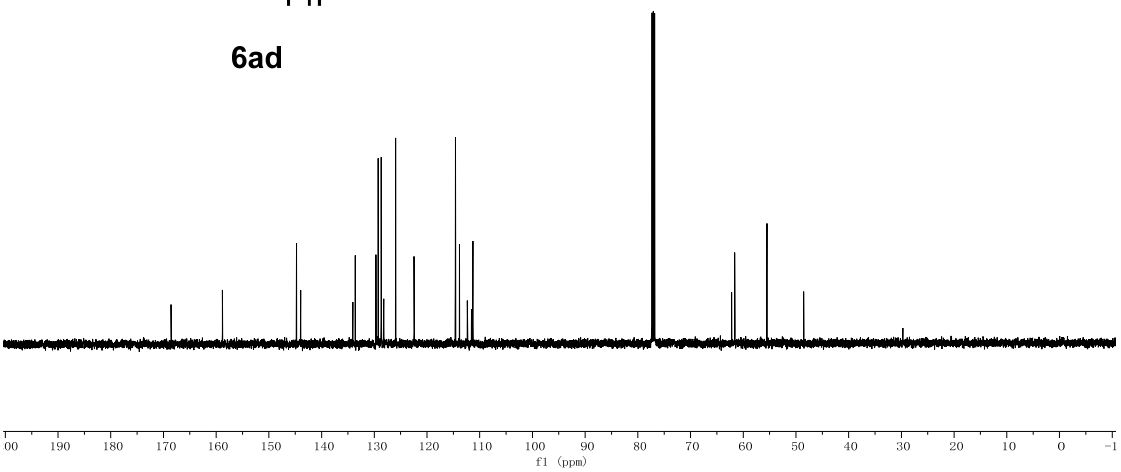


6ad

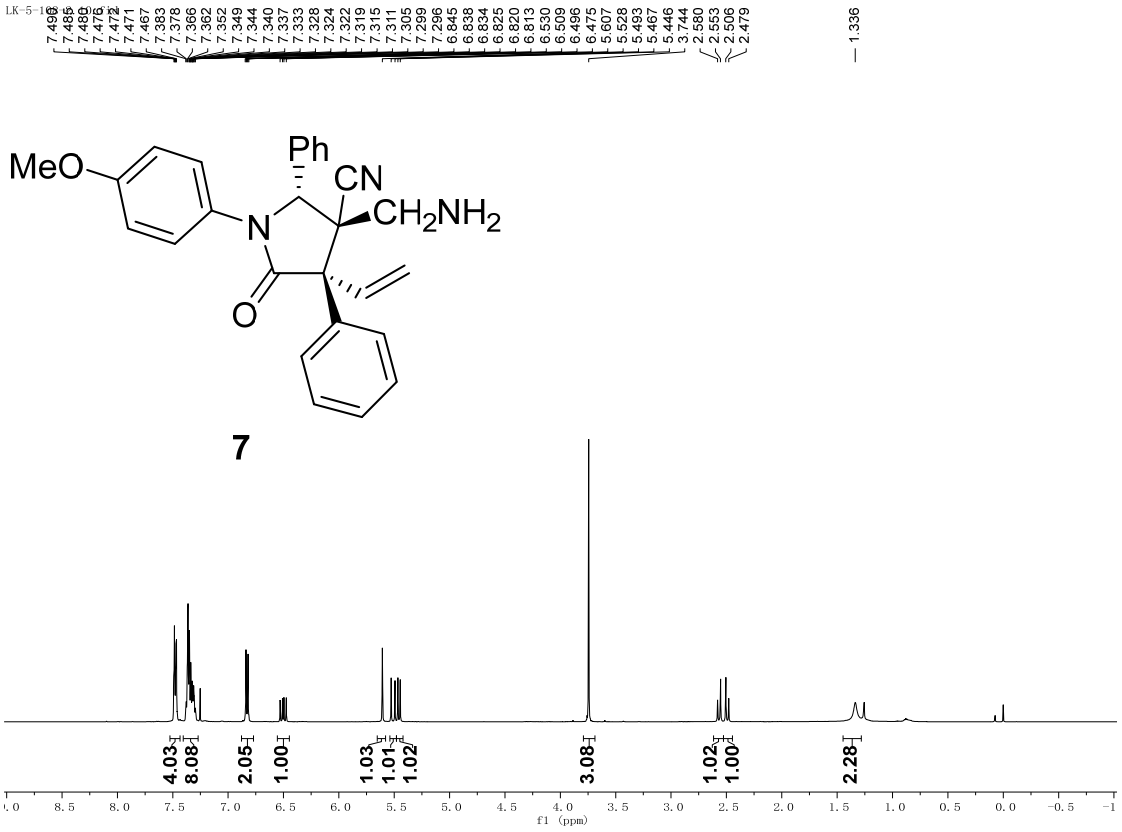


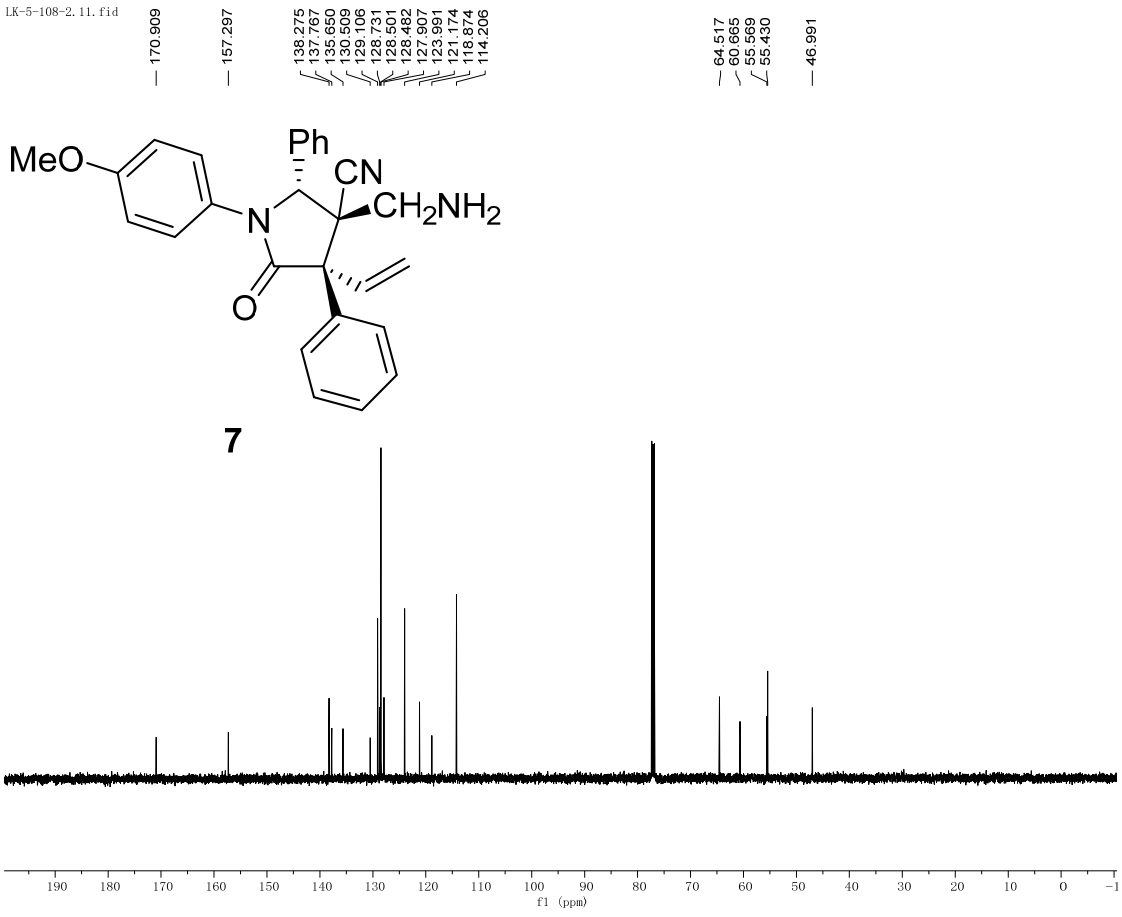


6ad



^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **6ad**

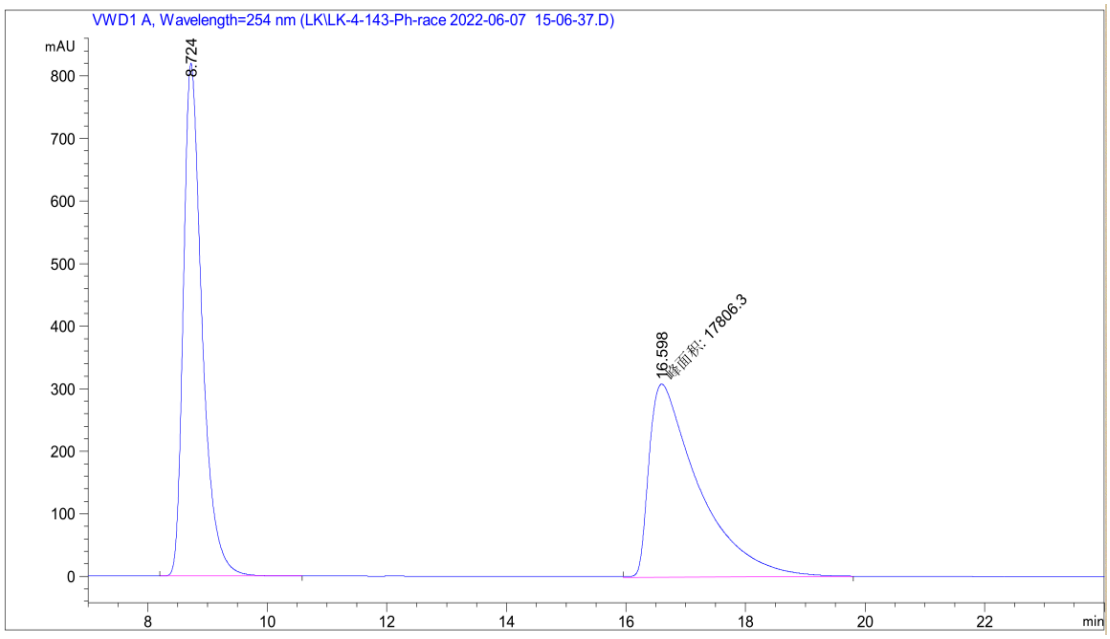




^{1}H NMR (500 MHz) and ^{13}C NMR (125 MHz) spectra of **7**

HPLC Chromatograms of All Products

HPLC chromatogram of racemic 3aa



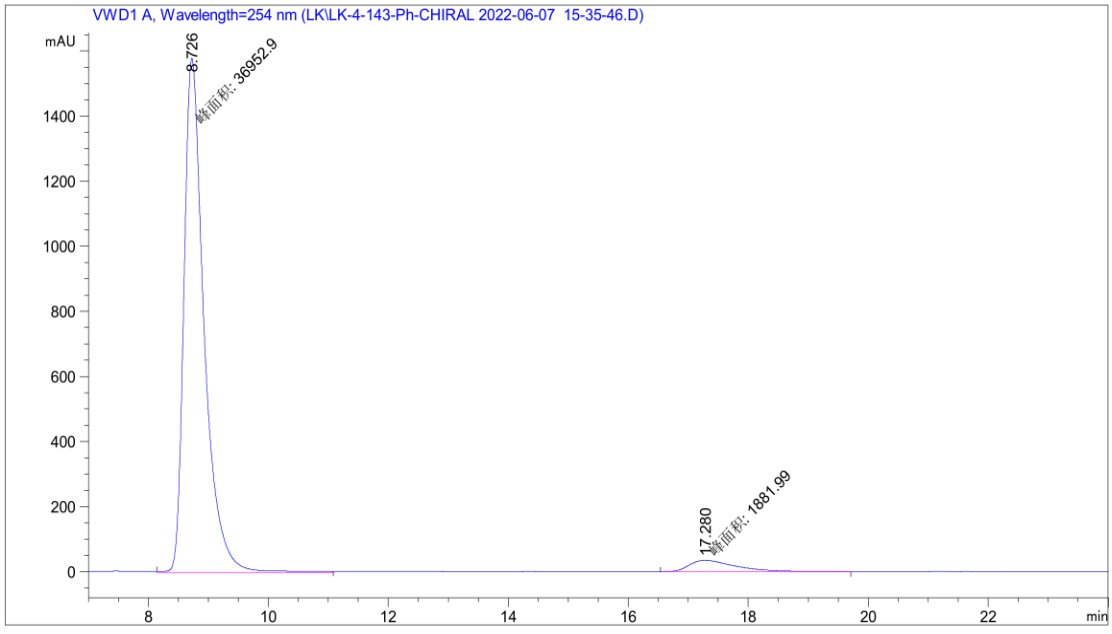
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.724 BB 0.3282 1.77930e4 819.70538 49.9814

2 16.598 MM 0.9627 1.78062e4 308.27737 50.0186

HPLC chromatogram of chiral 3aa



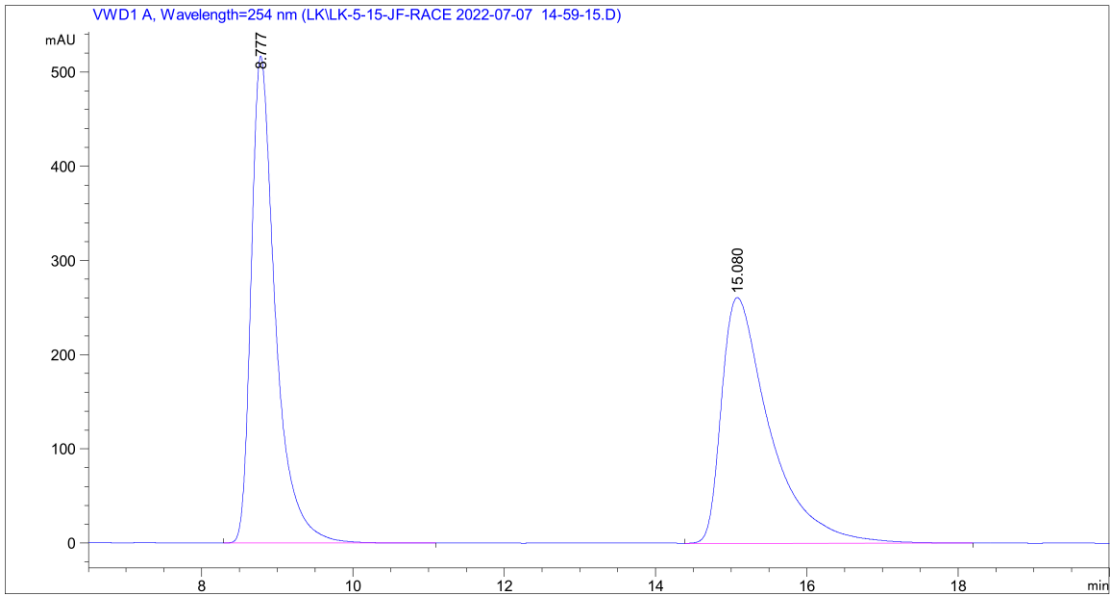
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.726 MM 0.3897 3.69529e4 1580.50281 95.1539

2 17.280 MM 0.8985 1881.99304 34.91178 4.8461

HPLC chromatogram of racemic 3ba



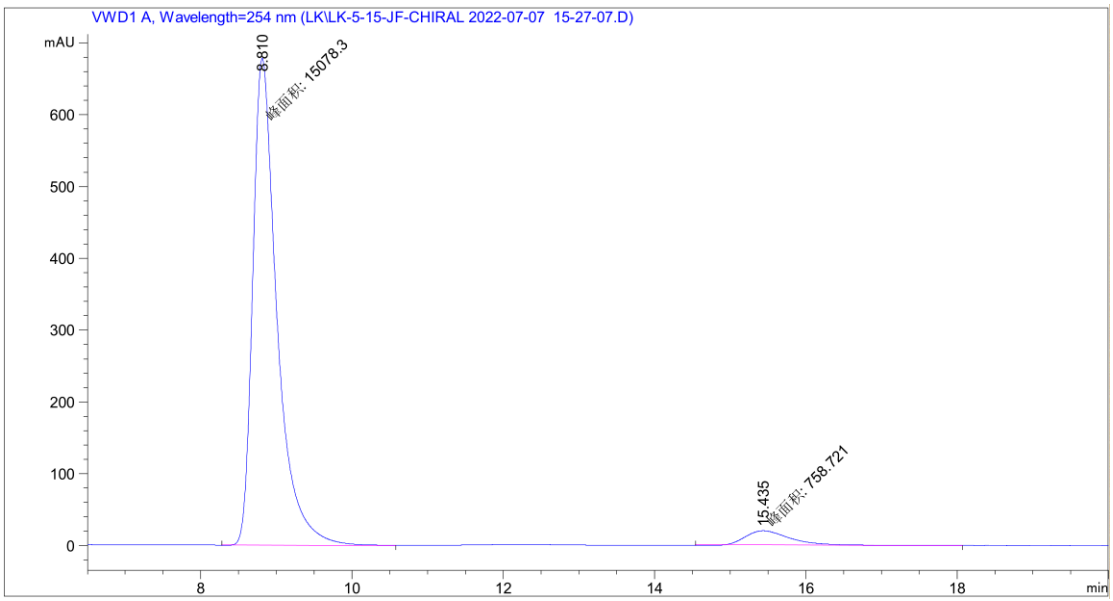
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.777 BB 0.3337 1.15038e4 516.84399 49.8798

2 15.080 BB 0.6532 1.15592e4 260.73074 50.1202

HPLC chromatogram of chiral 3ba



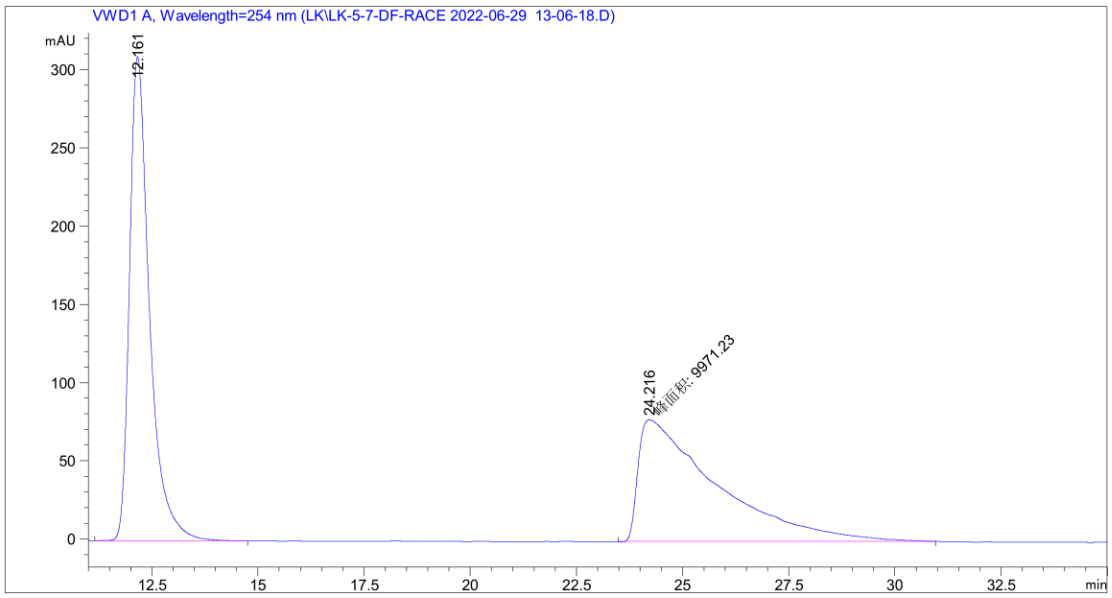
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.810 MM 0.3707 1.50783e4 677.91364 95.2092

2 15.435 MM 0.6509 758.72125 19.42758 4.7908

HPLC chromatogram of racemic 3ca



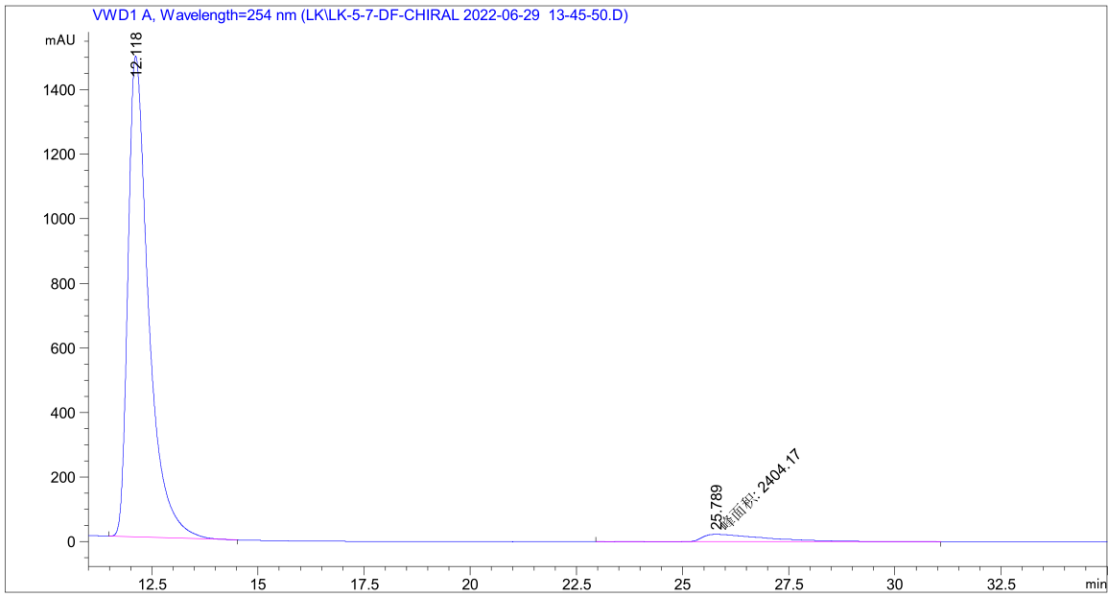
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 12.161 BB 0.4908 1.01460e4 309.18802 50.4343

2 24.216 MM 2.1396 9971.23145 77.67324 49.5657

HPLC chromatogram of chiral 3ca



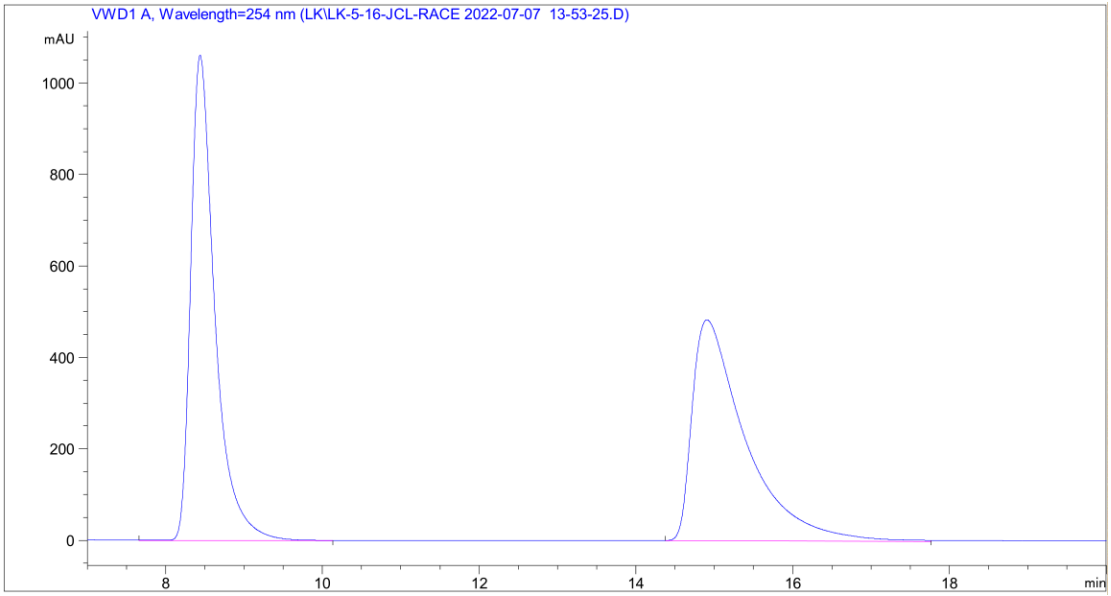
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 12.118 BB 0.5046 5.02312e4 1489.04077 95.4324

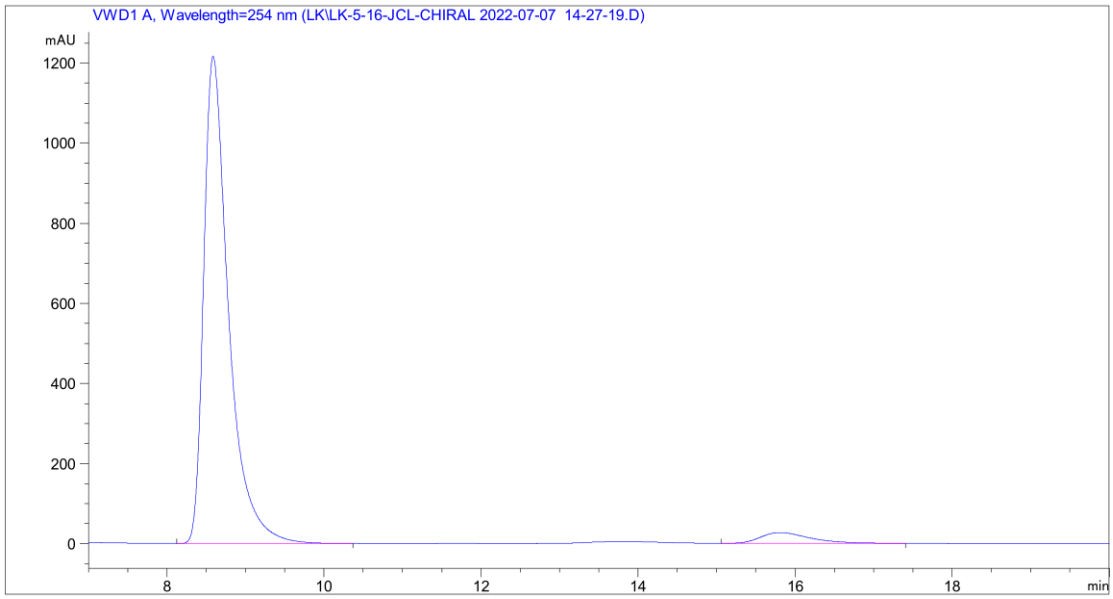
2 25.789 MM 1.7498 2404.16504 22.89896 4.5676

HPLC chromatogram of racemic 3da



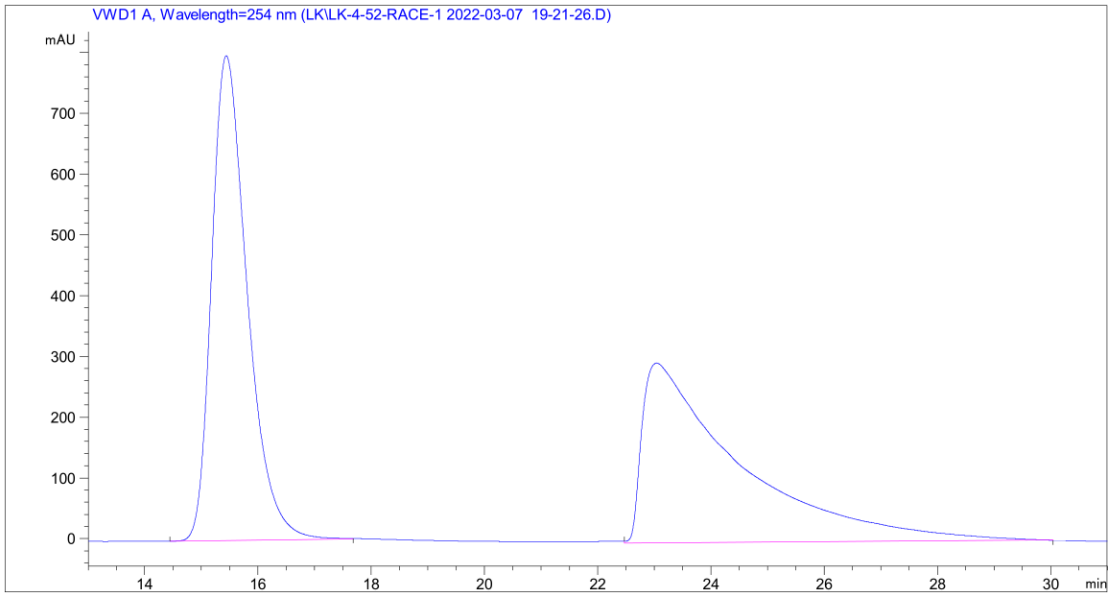
#	[min]	[min]	[mAU*s]	%
1	8.440	VB	0.3221	2.27468e4	49.8292
2	14.905	MM	0.7899	2.29027e4	50.1708

HPLC chromatogram of chiral 3da



#	[min]	[min]	[mAU*s]	%
1	8.587	VB	0.3300	2.68112e4	95.6306
2	15.809	VB	0.6739	1225.02551	4.3694

HPLC chromatogram of racemic 3ea



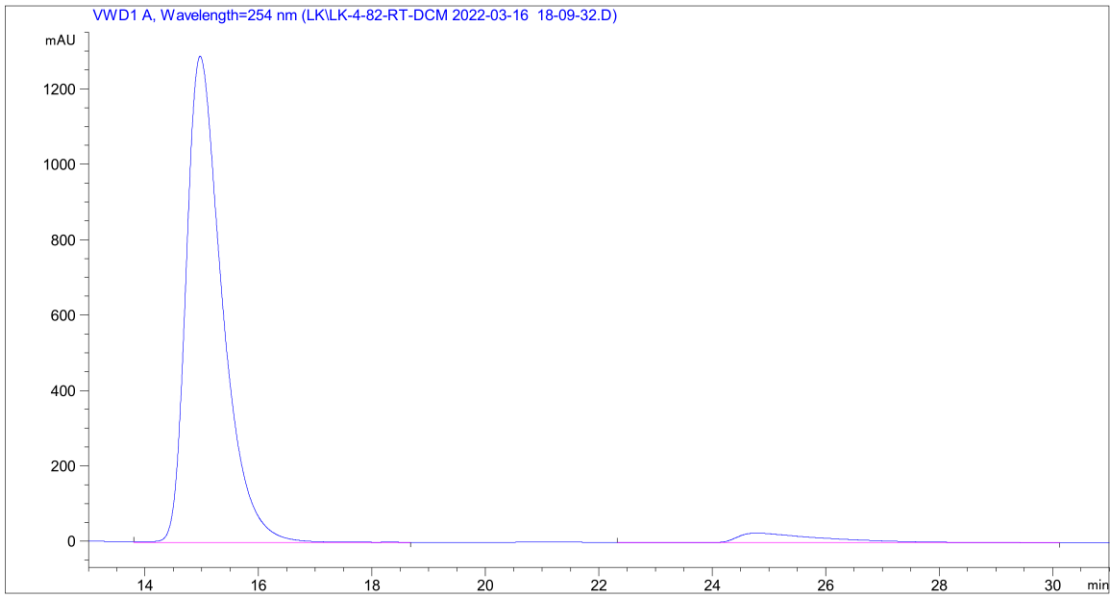
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 15.439 MM 0.7295 3.49062e4 49.7790

2 23.041 MM 1.9846 3.52162e4 50.2210

HPLC chromatogram of chiral 3ea



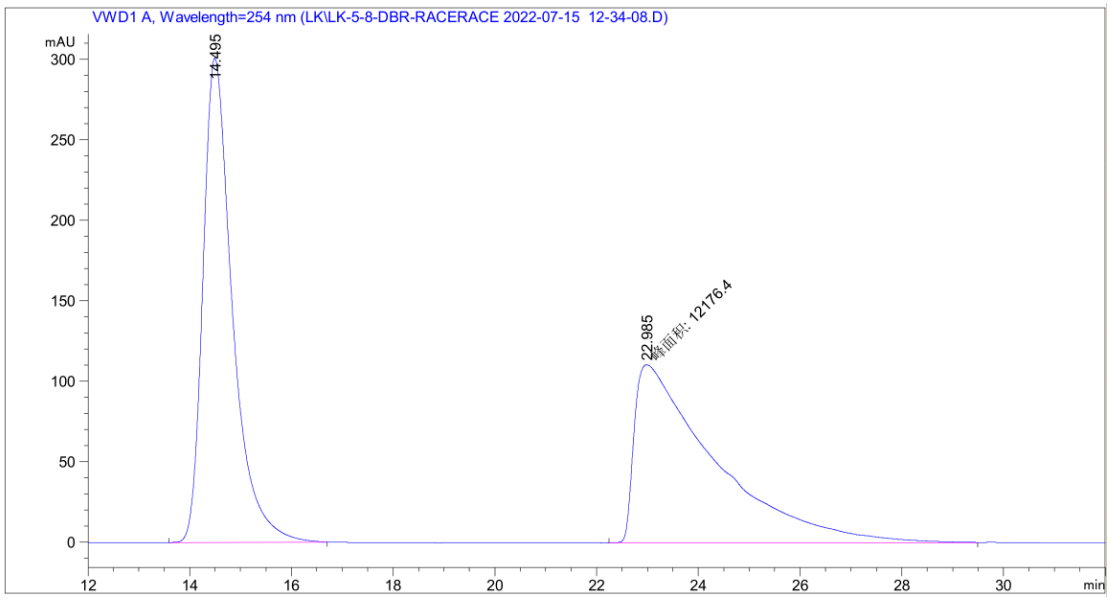
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 14.971 MM 0.7356 5.69326e4 95.9517

2 24.789 MM 1.6323 2402.05786 4.0483

HPLC chromatogram of racemic 3fa



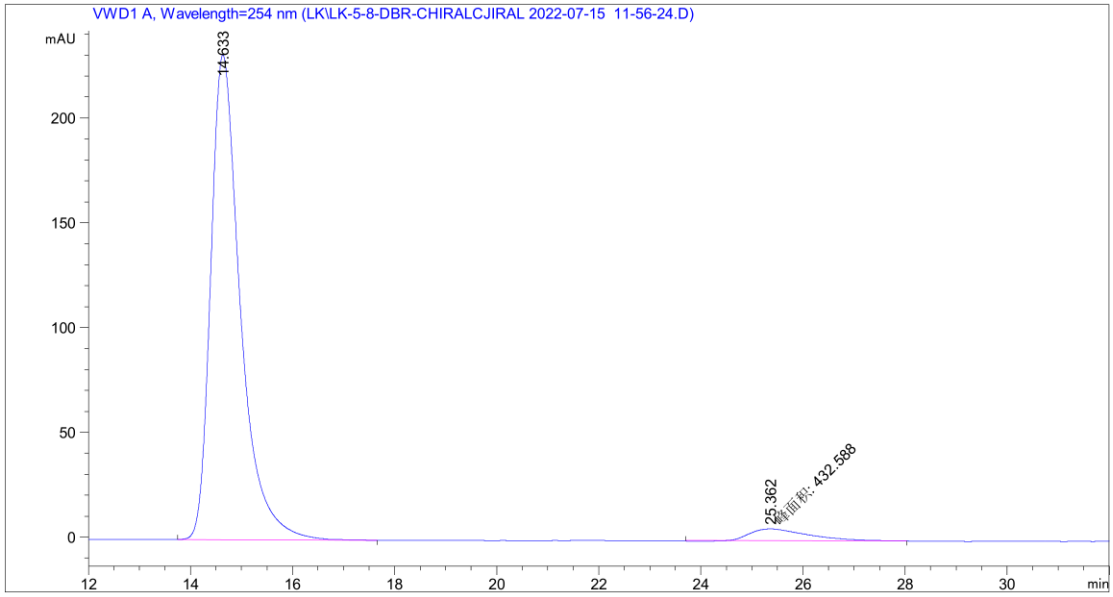
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.495 BB 0.6062 1.21084e4 301.09158 49.8601

2 22.985 MM 1.8310 1.21764e4 110.83334 50.1399

HPLC chromatogram of chiral 3fa



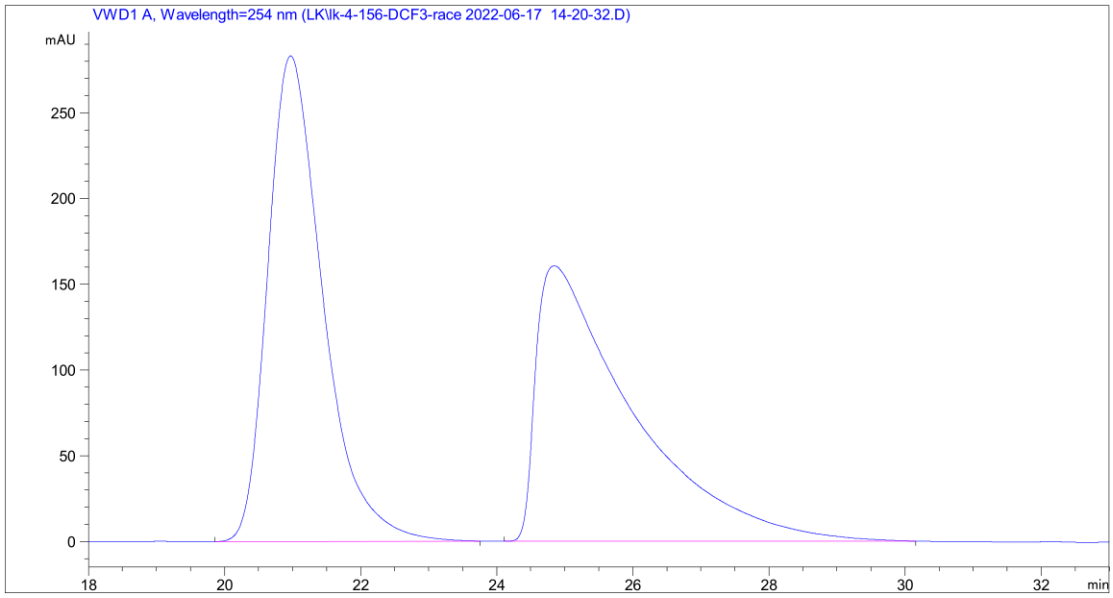
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.633 BB 0.6075 9326.43750 231.26280 95.5673

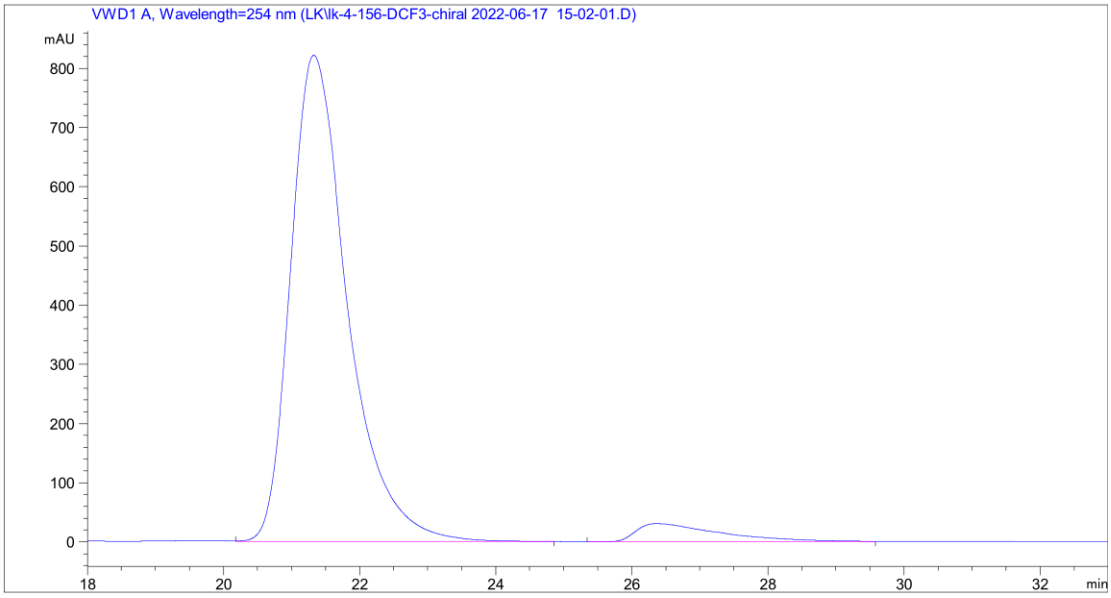
2 25.362 MM 1.3008 432.58820 5.54270 4.4327

HPLC chromatogram of racemic 3ga



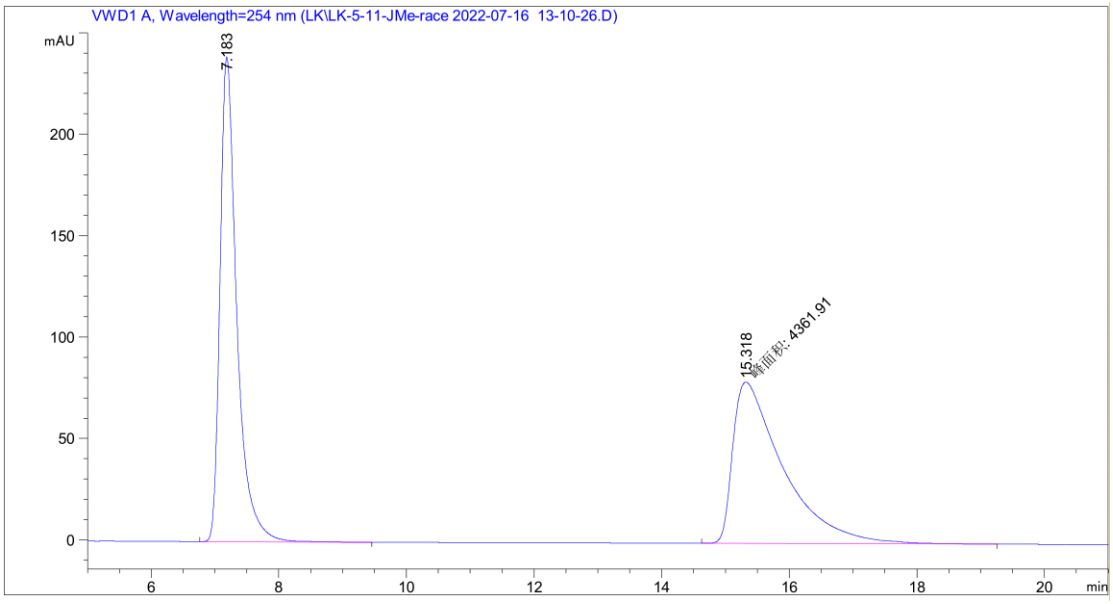
#	[min]	[min]	[mAU*s]	%
1	20.972	BB	0.8731	1.59504e4	50.1490
2	24.845	BB	1.3688	1.58556e4	49.8510

HPLC chromatogram of chiral 3ga



#	[min]	[min]	[mAU*s]	%
1	21.327	VB	0.8852	4.77424e4	94.8509
2	26.364	MM	1.4100	2591.74219	5.1491

HPLC chromatogram of racemic 3ha



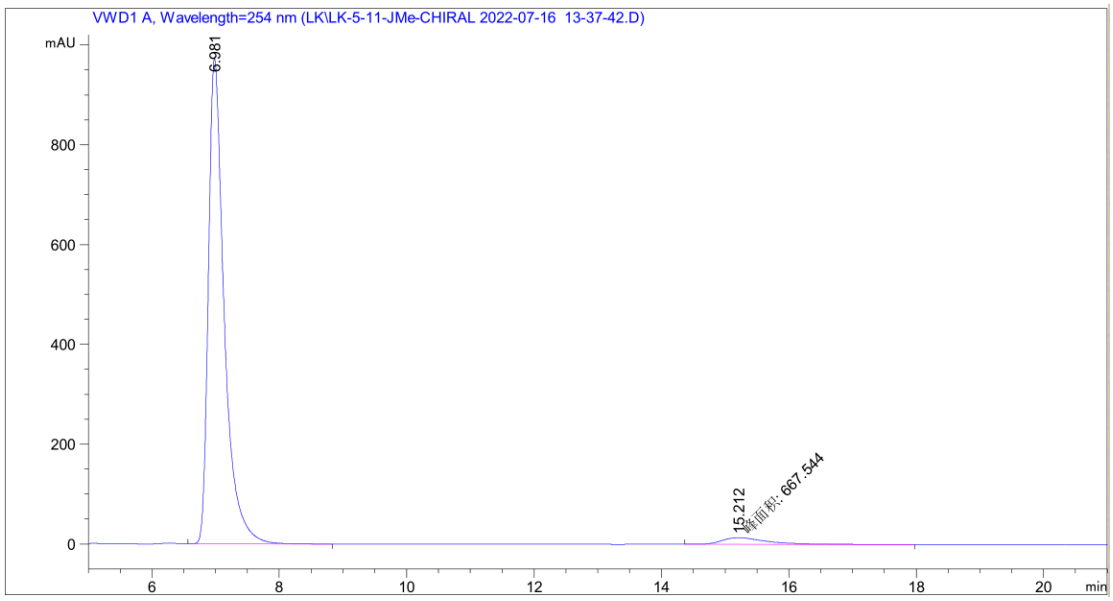
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 7.183 BB 0.2732 4367.15967 238.93665 50.0301

2 15.318 MM 0.9143 4361.90723 79.51097 49.9699

HPLC chromatogram of chiral 3ha



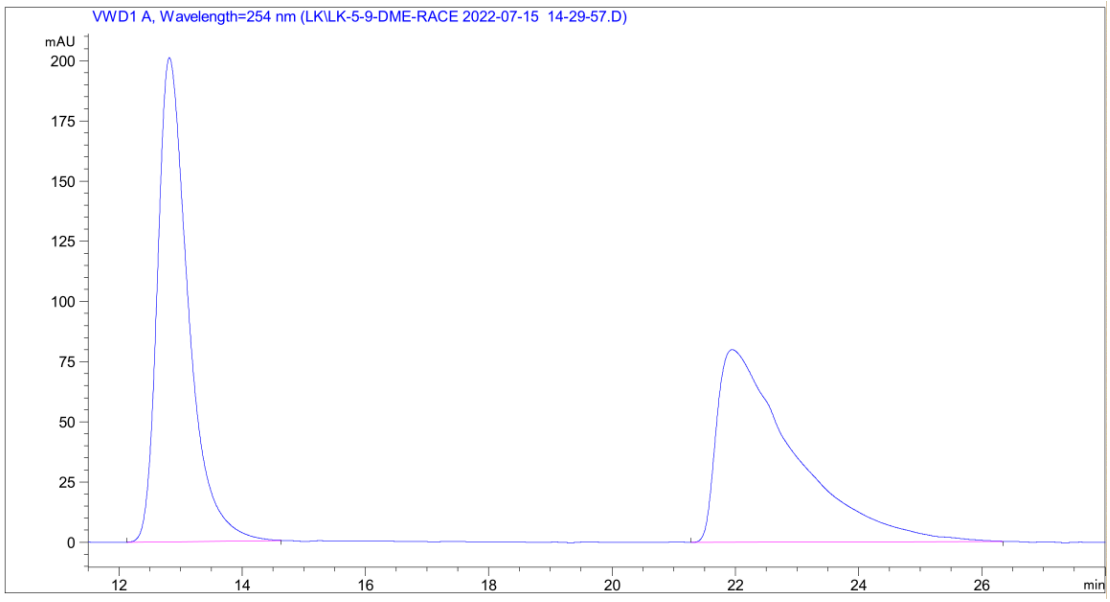
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 6.981 BB 0.2573 1.67711e4 972.10944 96.1720

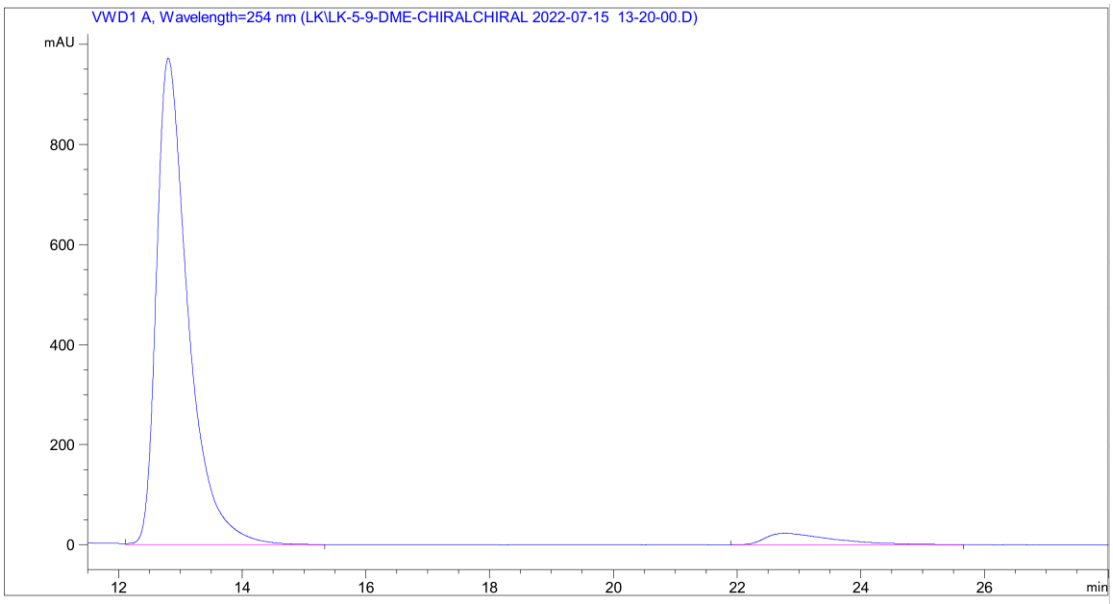
2 15.212 MM 0.8474 667.54431 13.12926 3.8280

HPLC chromatogram of racemic 3ia



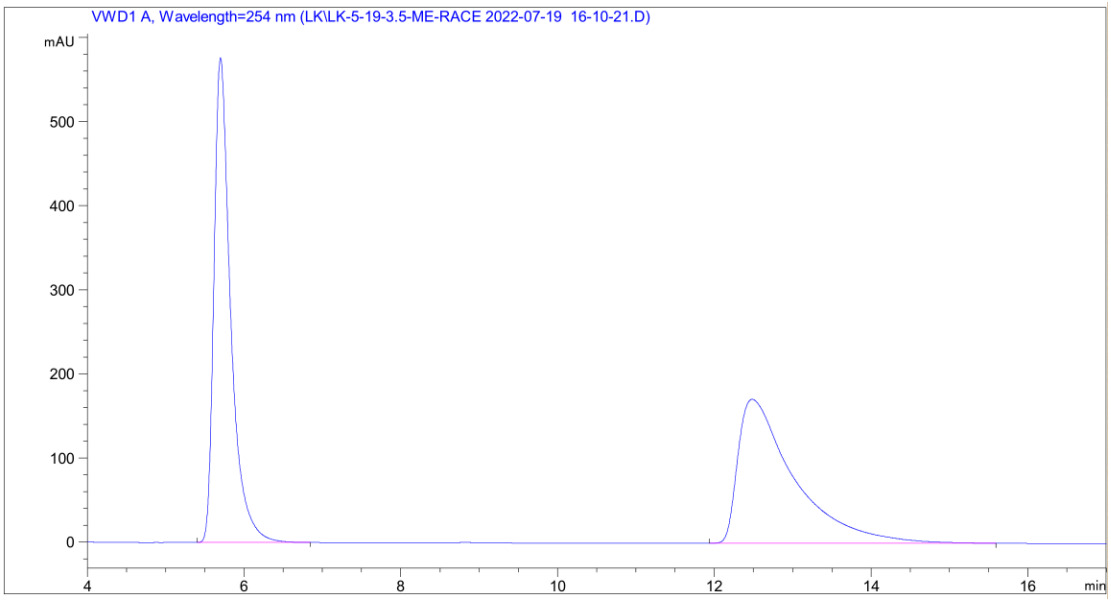
#	[min]	[min]	[mAU*s]	%
1	12.822	BB	0.5243	6986.02930	50.1784
2	21.951	BB	1.2013	6936.34082	49.8216

HPLC chromatogram of chiral 3ia



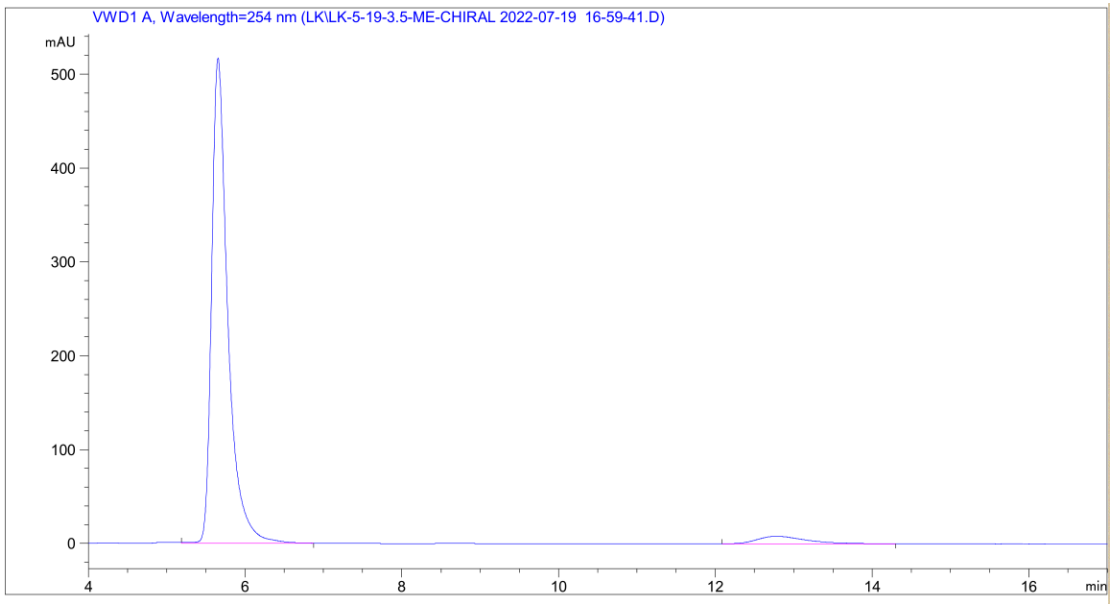
#	[min]	[min]	[mAU*s]	%
1	12.808	VB	0.5339	3.44819e4	95.1610
2	22.778	BB	1.1110	1753.44043	4.8390

HPLC chromatogram of racemic 3ja



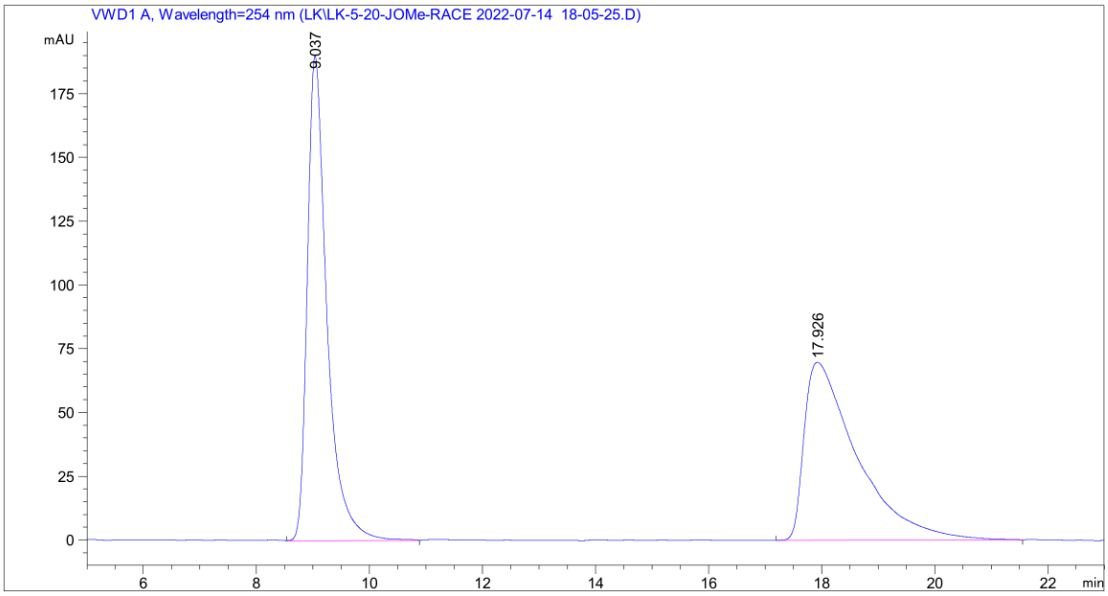
#	[min]	[min]	[mAU*s]	%
1	5.702	BB	0.2218	8538.40723	50.0256
2	12.484	BB	0.7202	8529.68164	49.9744

HPLC chromatogram of chiral 3ja



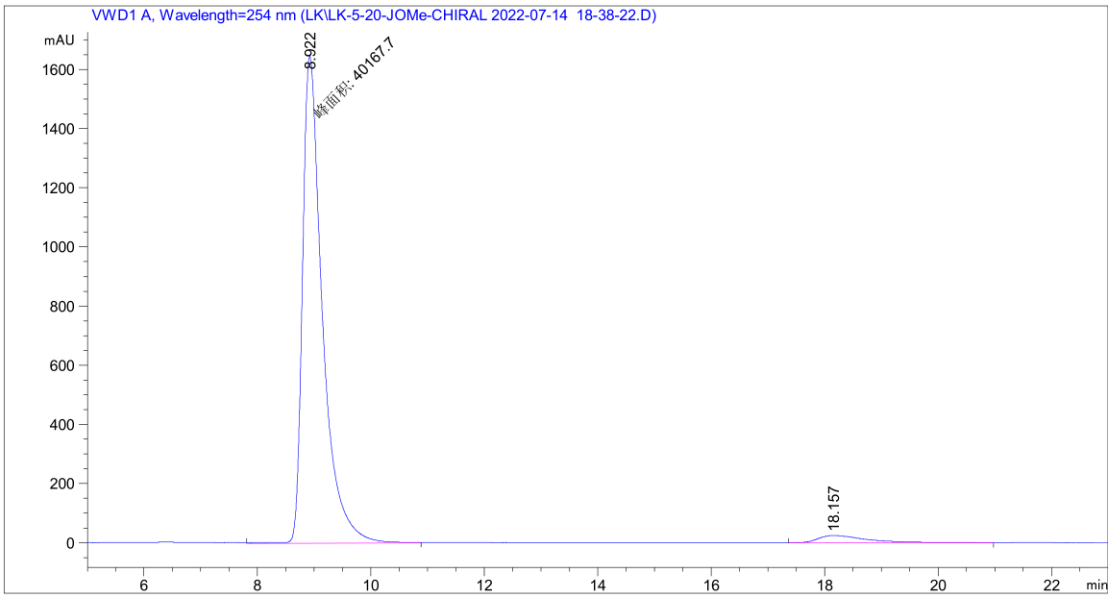
#	[min]	[min]	[mAU*s]	%
1	5.657	VB	0.2133	7408.94873	95.4209
2	12.785	MM	0.7482	355.54395	4.5791

HPLC chromatogram of racemic 3ka



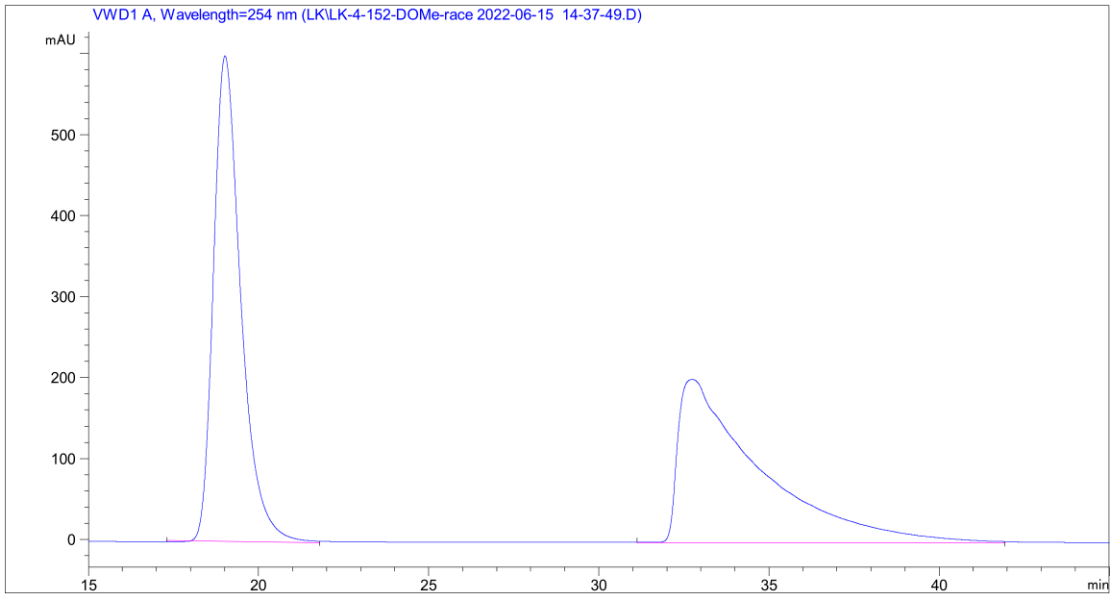
#	[min]	[min]	[mAU*s]	[mAU]	%
1	9.037	BB	0.3603	4583.00537	190.09694	50.2988
2	17.926	BB	0.9254	4528.54688	69.75281	49.7012

HPLC chromatogram of chiral 3ka



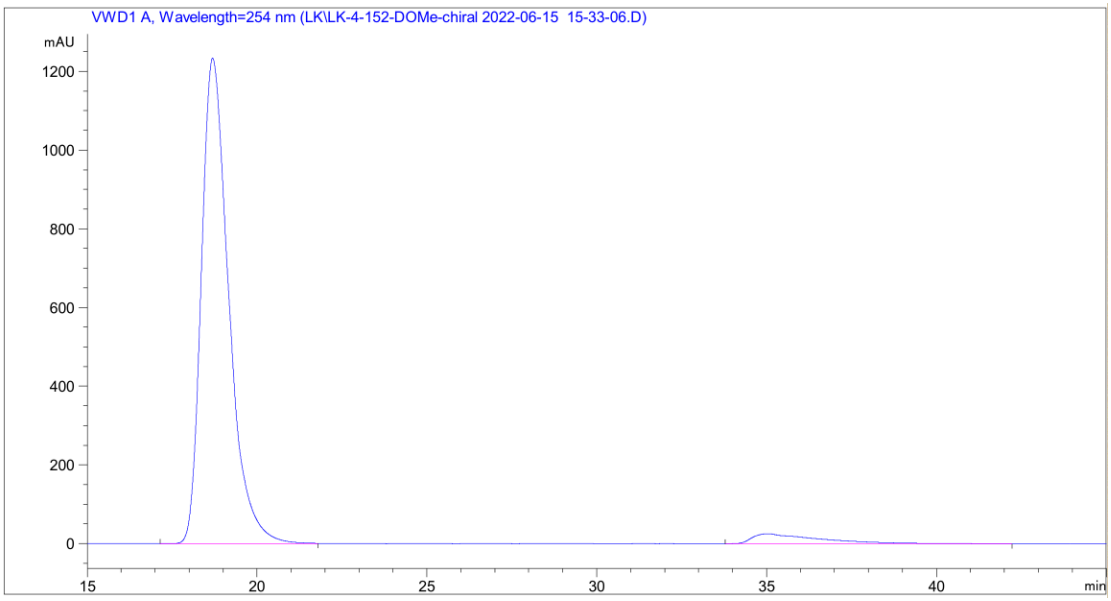
#	[min]	[min]	[mAU*s]	[mAU]	%
1	8.922	MM	0.4068	4.01677e4	1645.86377	96.5148
2	18.157	BB	0.8887	1450.47156	24.32479	3.4852

HPLC chromatogram of racemic 3la



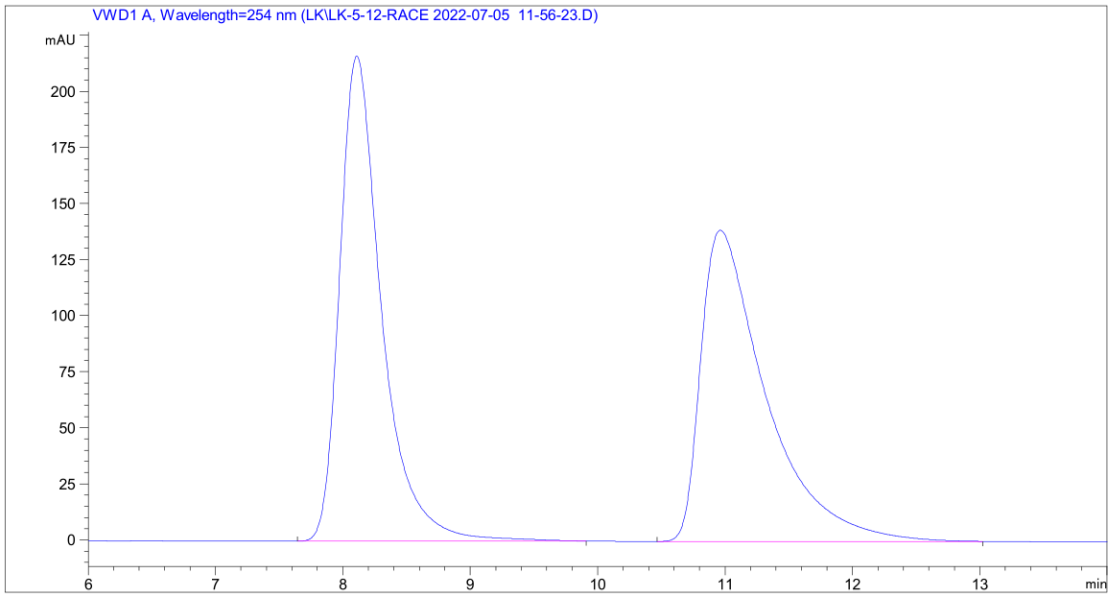
#	[min]	[min]	[mAU*s]	%
1	19.017	MM	0.9332	3.35479e4	49.9348
2	32.754	MM	2.7830	3.36355e4	50.0652

HPLC chromatogram of chiral 3la



#	[min]	[min]	[mAU*s]	%
1	18.693	MM	0.9354	6.92964e4	95.1047
2	35.055	MM	2.2887	3566.83887	4.8953

HPLC chromatogram of racemic 3ma



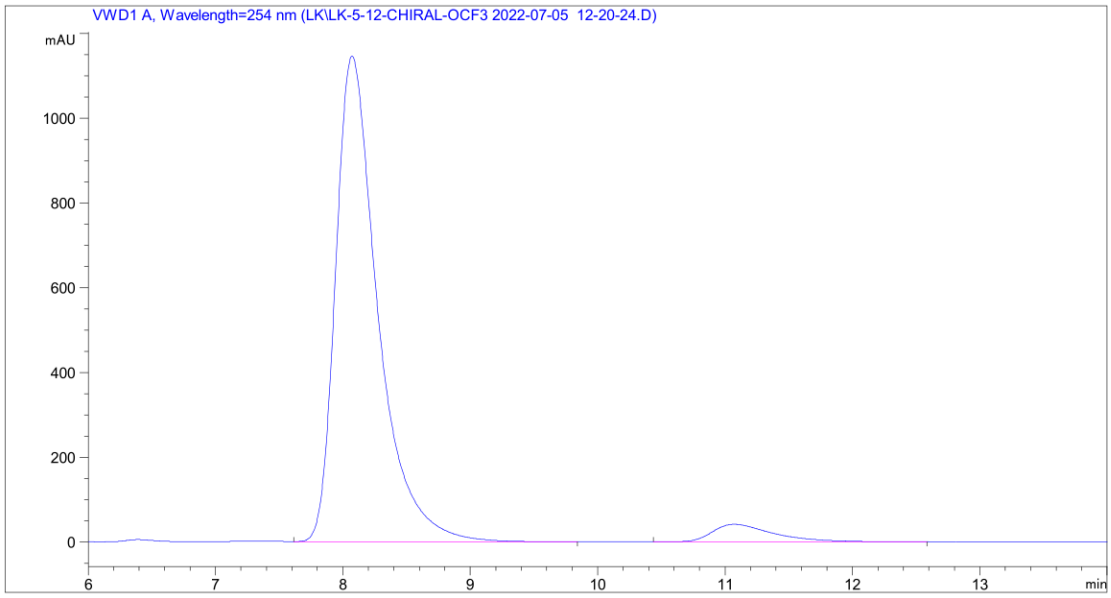
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 8.109 BB 0.3446 4959.45898 50.1475

2 10.964 BB 0.5214 4930.29053 49.8525

HPLC chromatogram of chiral 3ma



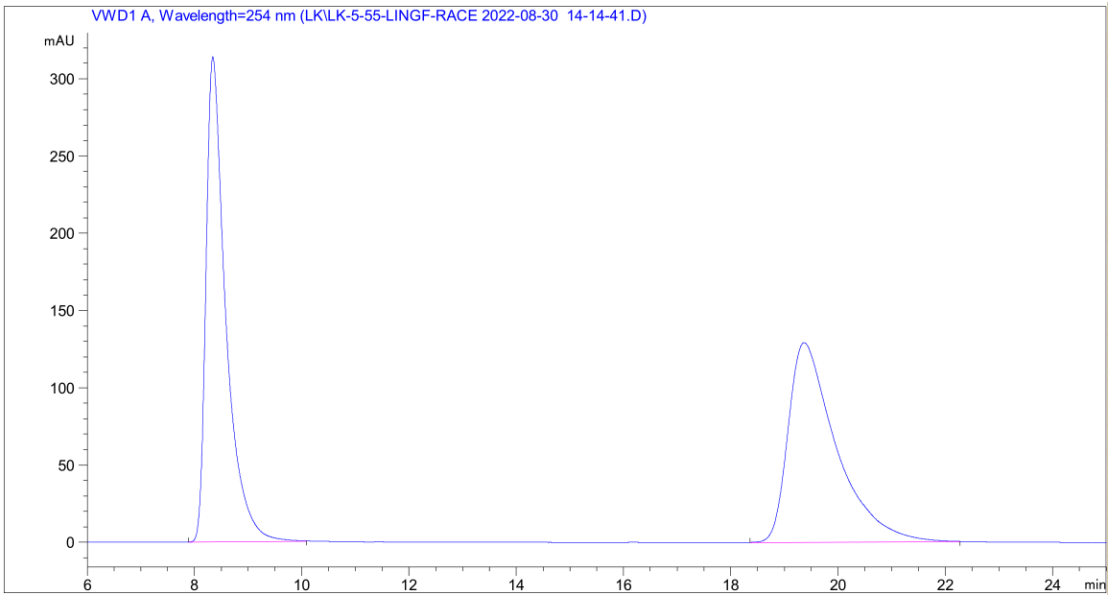
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 8.071 VB 0.3460 2.64389e4 94.9095

2 11.072 VB 0.5076 1418.06592 5.0905

HPLC chromatogram of racemic 3na



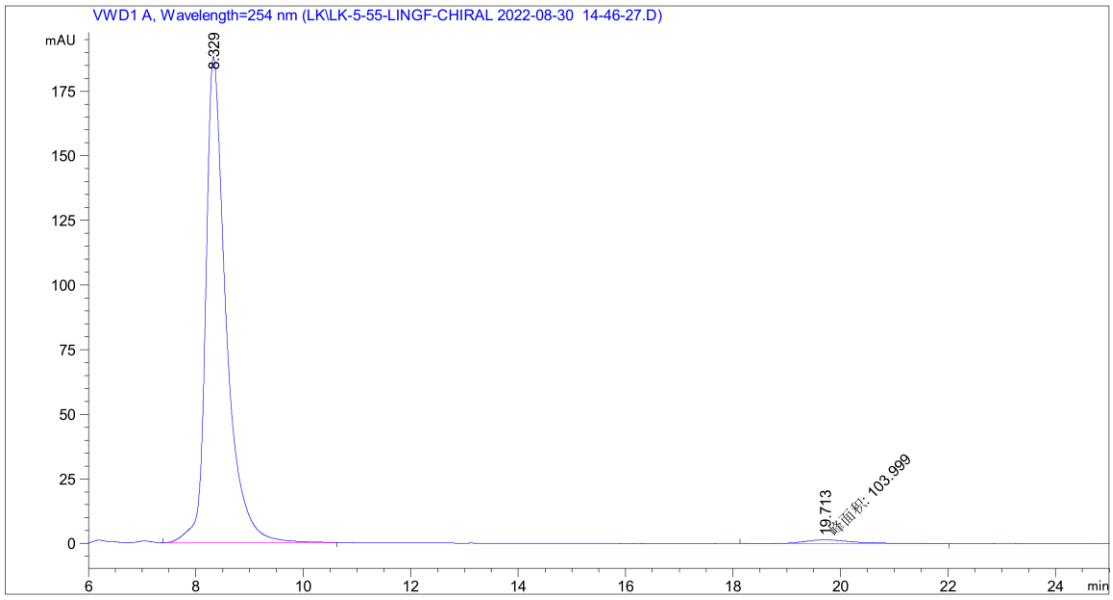
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 8.343 BB 0.3746 8036.51709 49.9966

2 19.368 BB 0.9140 8037.61084 50.0034

HPLC chromatogram of chiral 3na



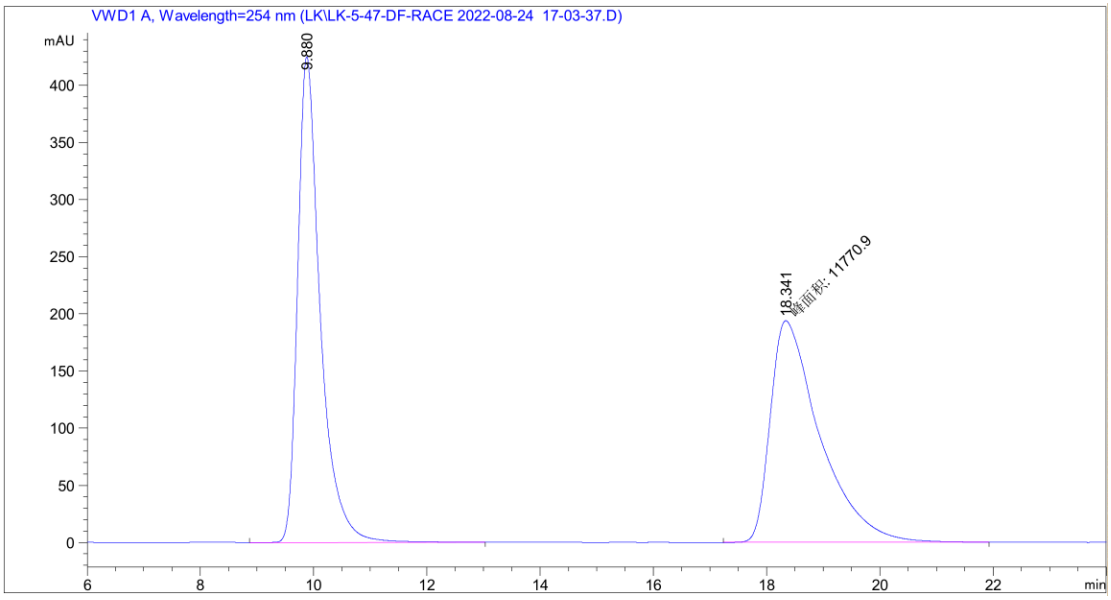
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.329 BB 0.3863 4939.54346 188.13016 97.9380

2 19.713 MM 1.1251 103.99916 1.54053 2.0620

HPLC chromatogram of racemic 3oa



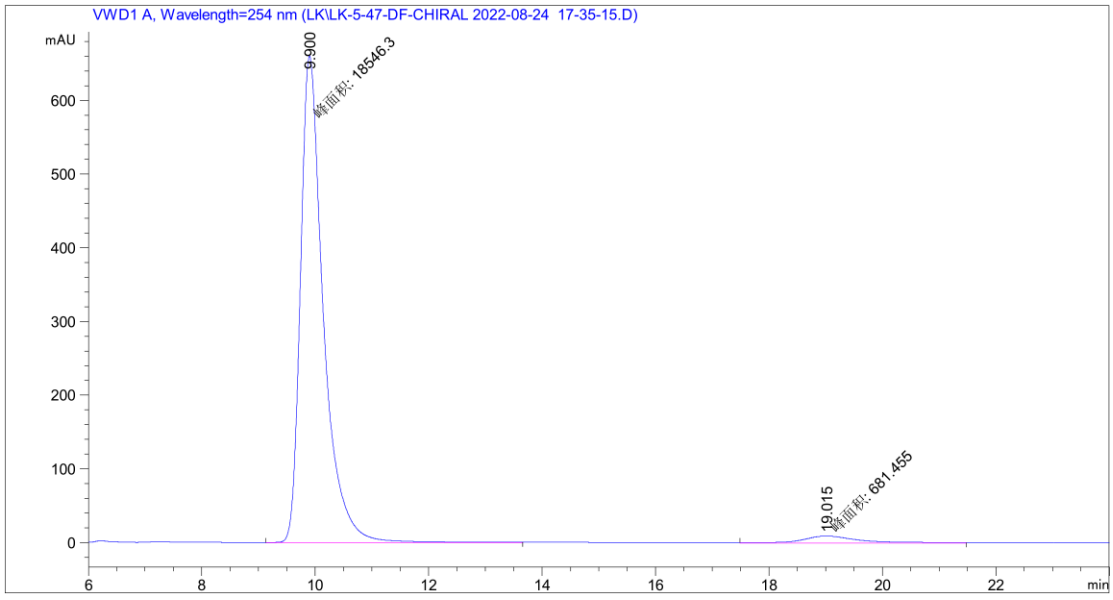
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 9.880 BB 0.4144 1.18162e4 424.94348 50.0960

2 18.341 MM 1.0121 1.17709e4 193.84132 49.9040

HPLC chromatogram of chiral 3oa



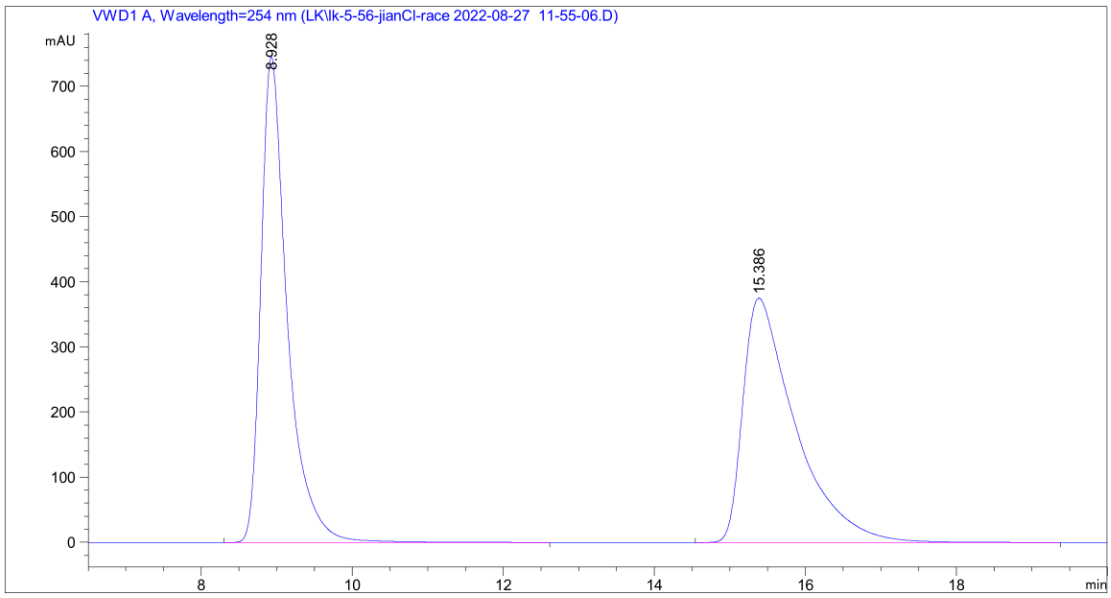
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 9.900 MM 0.4680 1.85463e4 660.43506 96.4559

2 19.015 MM 1.1973 681.45453 9.48579 3.5441

HPLC chromatogram of racemic 3pa



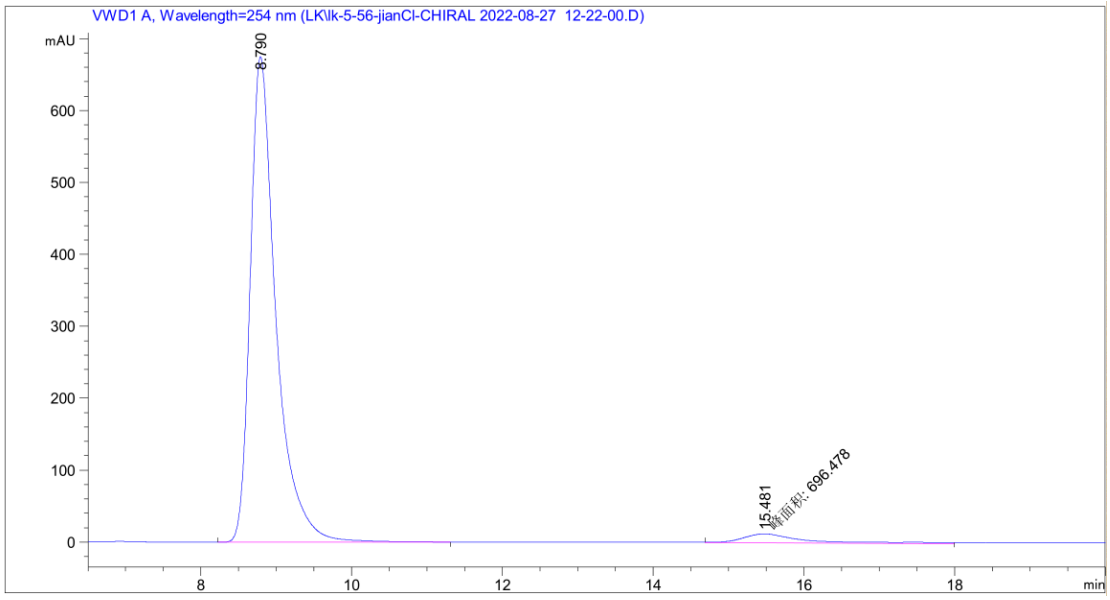
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.928 BB 0.3619 1.82076e4 745.71851 50.1274

2 15.386 BB 0.6963 1.81150e4 375.16321 49.8726

HPLC chromatogram of chiral 3pa



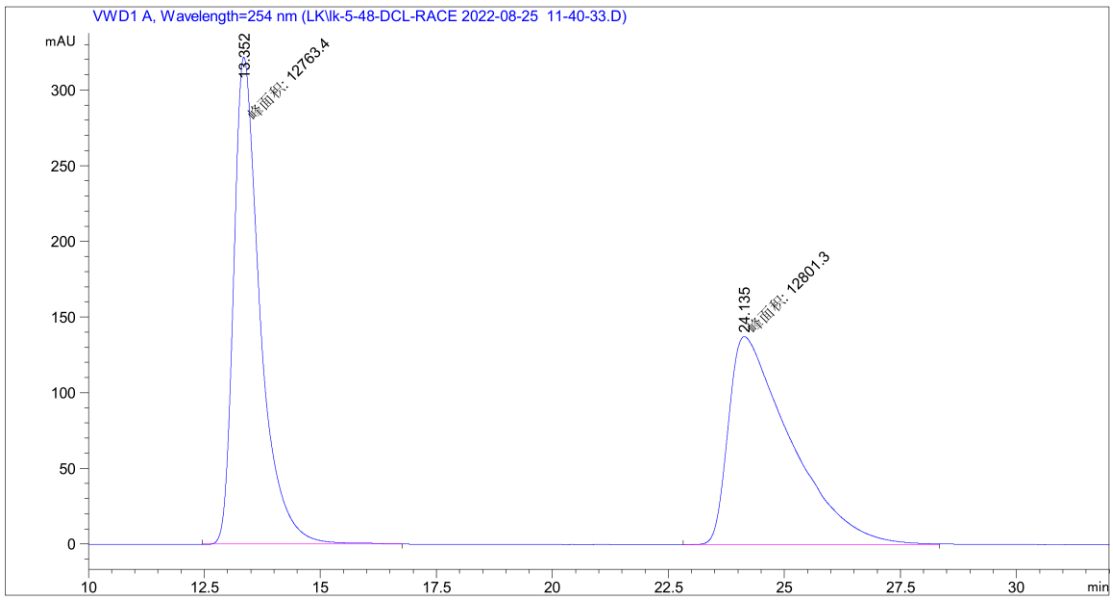
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 8.790 BB 0.3517 1.60045e4 674.81464 95.8297

2 15.481 MM 0.9177 696.47778 12.64919 4.1703

HPLC chromatogram of racemic 3qa



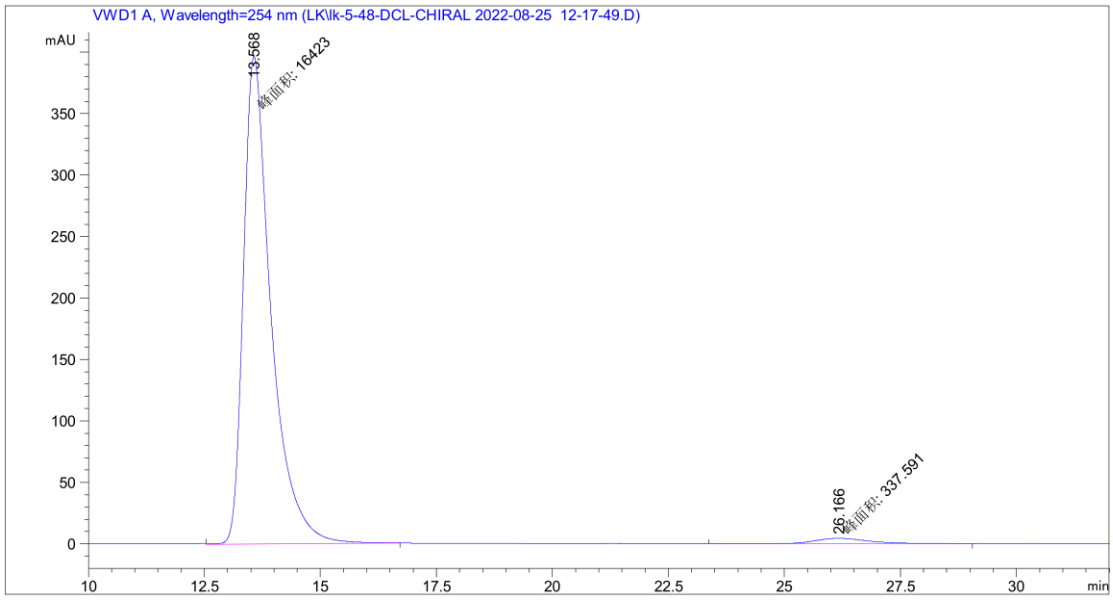
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 13.352 MM 0.6615 1.27634e4 321.59570 49.9258

2 24.135 MM 1.5518 1.28013e4 137.48785 50.0742

HPLC chromatogram of chiral 3qa



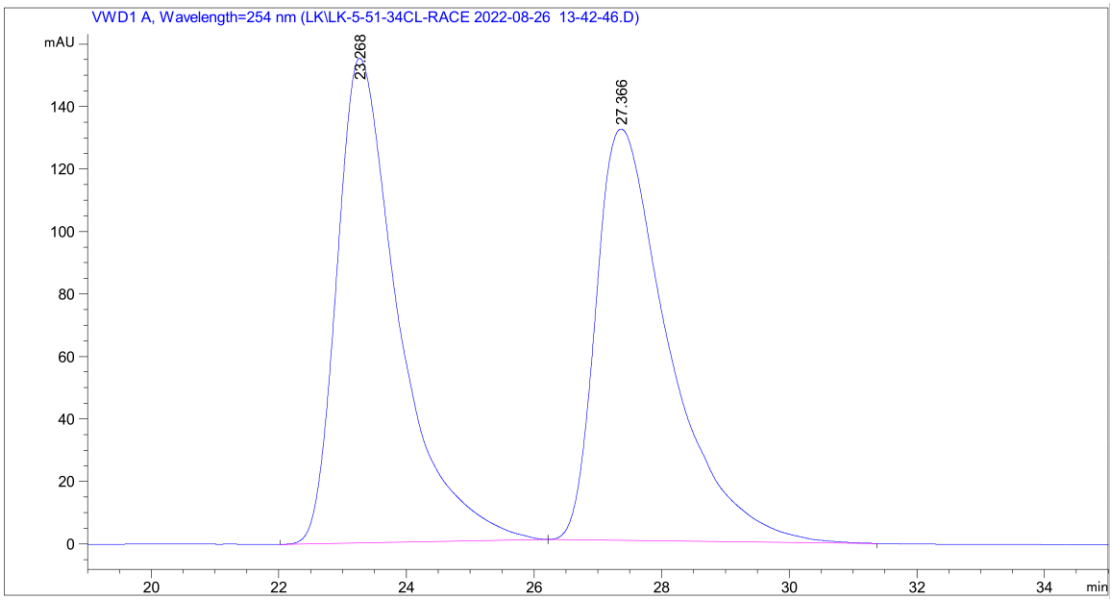
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 13.568 MM 0.6899 1.64230e4 396.73520 97.9858

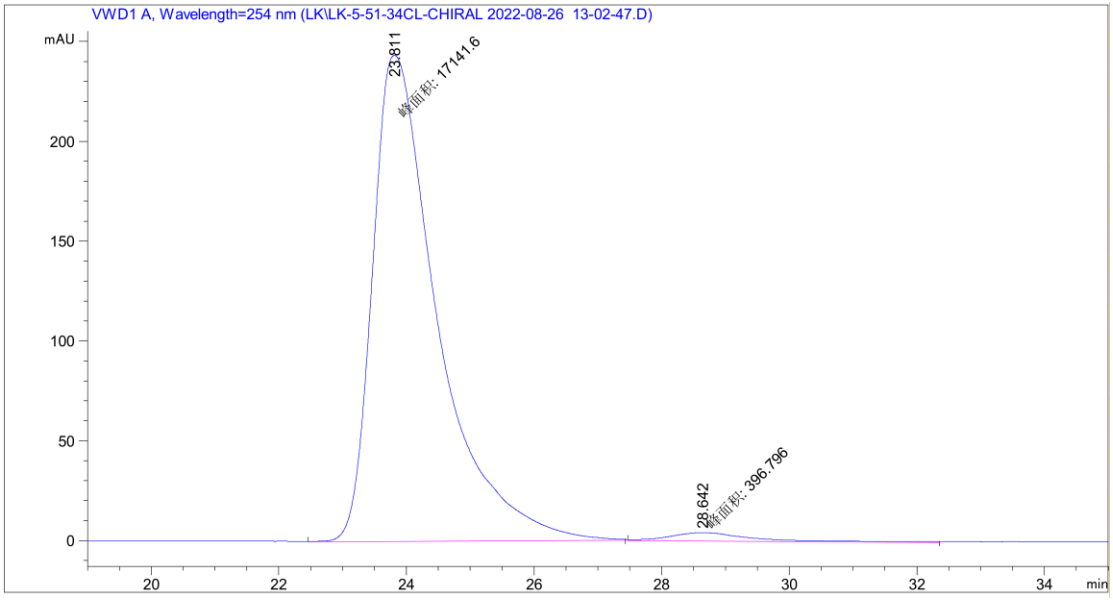
2 26.166 MM 1.3021 337.59055 4.32118 2.0142

HPLC chromatogram of racemic 3ra



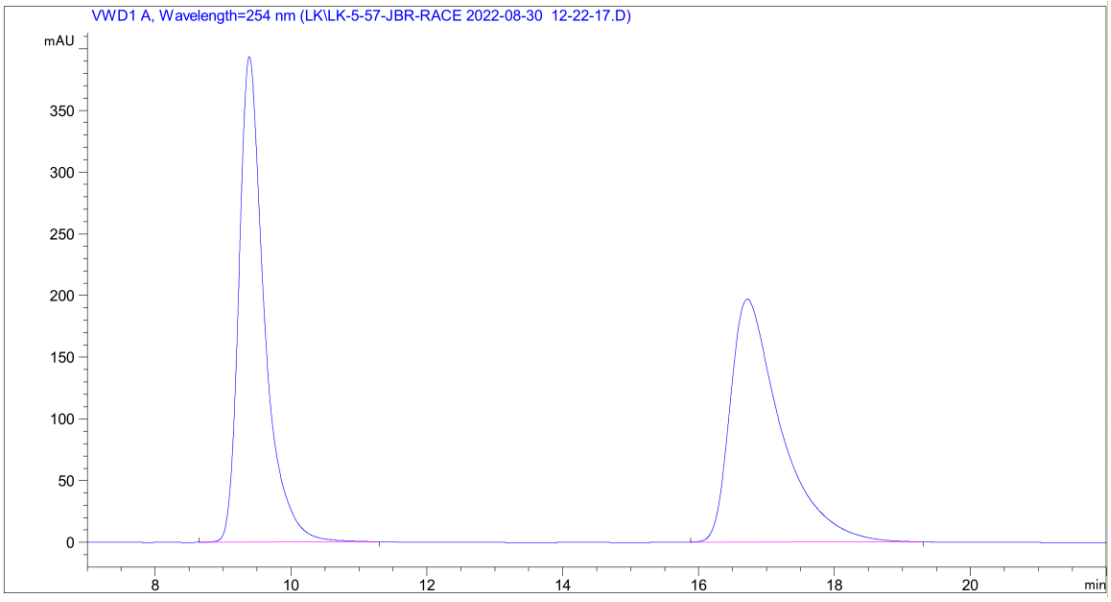
#	[min]		[min]	[mAU*s]	[mAU]	%
1	23.268	BB	1.0026	1.04235e4	155.19463	50.0391
2	27.366	BB	1.1553	1.04072e4	131.64528	49.9609

HPLC chromatogram of chiral 3ra



#	[min]		[min]	[mAU*s]	[mAU]	%
1	23.811	MM	1.1735	1.71416e4	243.45654	97.7376
2	28.642	MM	1.5680	396.79575	4.21756	2.2624

HPLC chromatogram of racemic 3sa



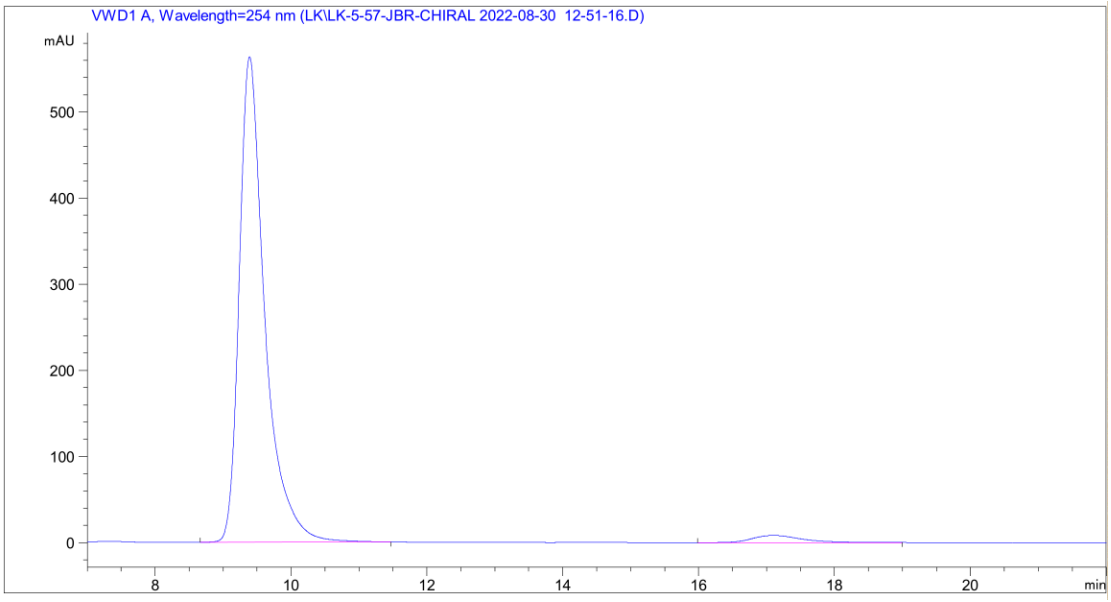
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 9.387 BB 0.3873 1.02630e4 50.2641

2 16.718 BB 0.7589 1.01552e4 49.7359

HPLC chromatogram of chiral 3sa



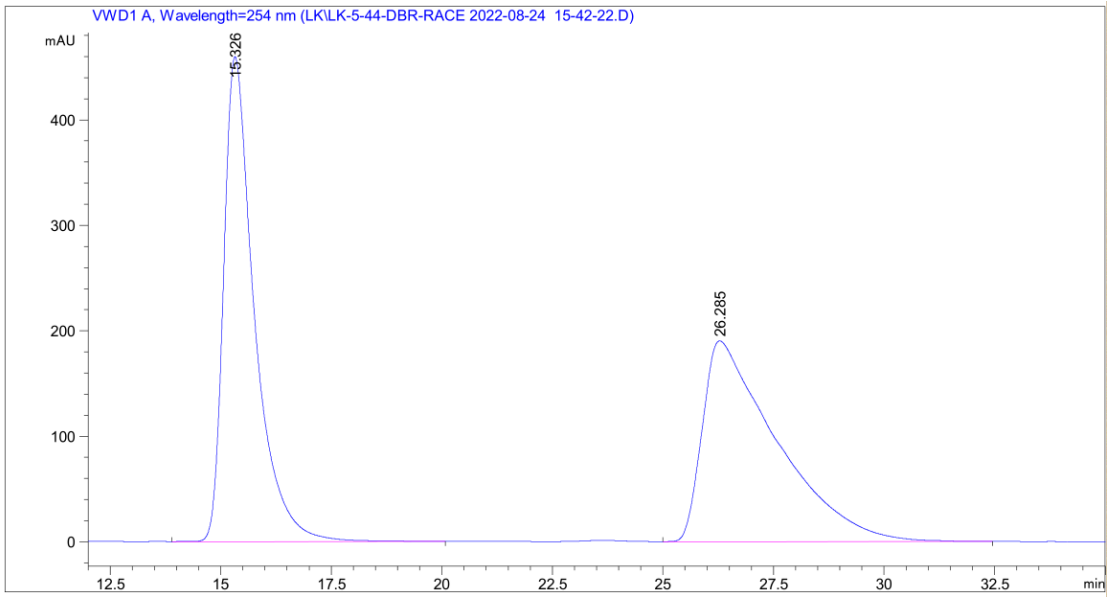
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 9.391 BB 0.3884 1.47613e4 96.8764

2 17.103 MM 0.9183 475.95520 3.1236

HPLC chromatogram of racemic 3ta



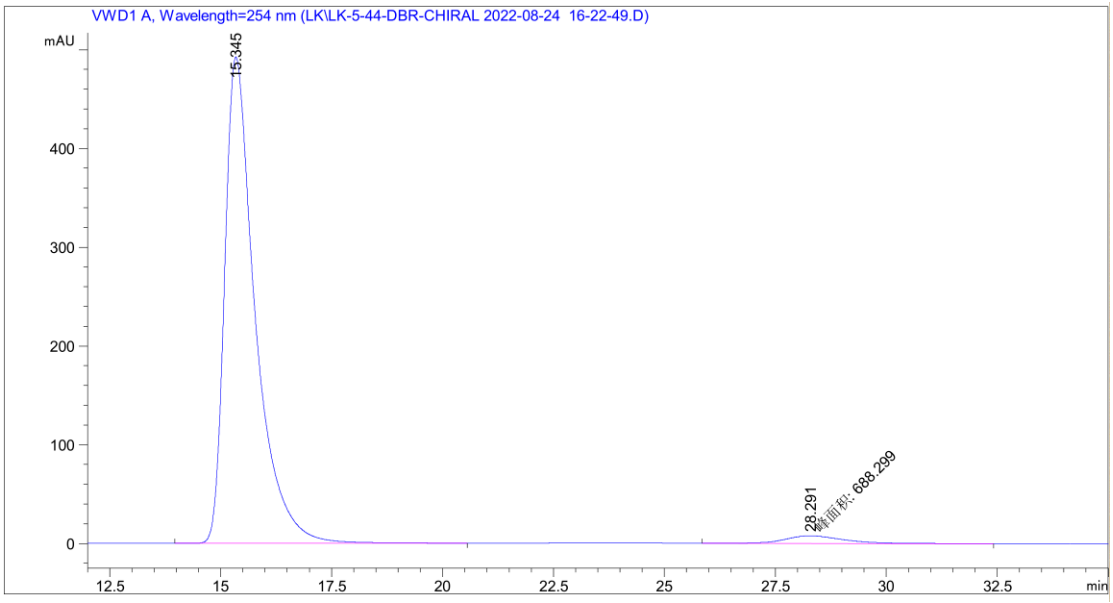
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 15.326 BB 0.7129 2.21786e4 459.67737 50.0358

2 26.285 BB 1.5522 2.21469e4 190.23903 49.9642

HPLC chromatogram of chiral 3ta



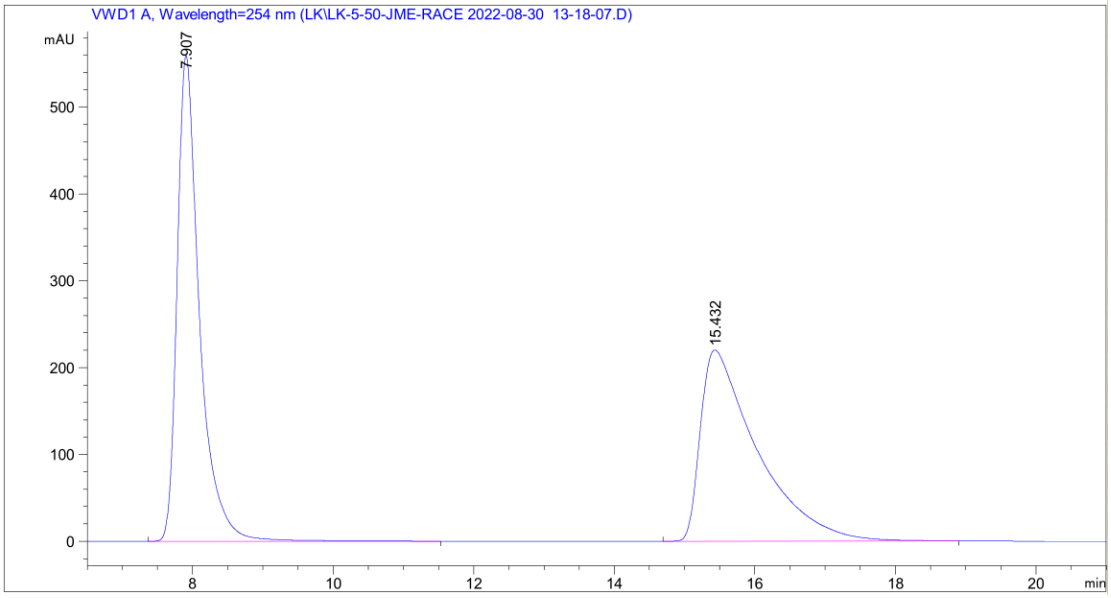
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 15.345 BB 0.7076 2.35413e4 492.54547 97.1593

2 28.291 MM 1.4994 688.29889 7.65094 2.8407

HPLC chromatogram of racemic 3ua



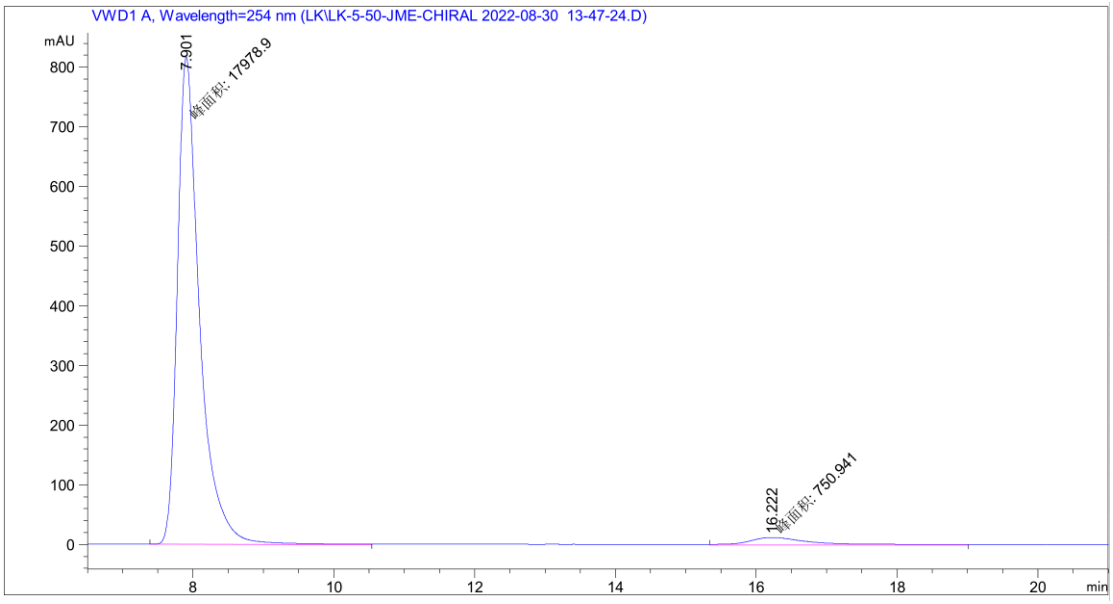
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 7.907 BB 0.3277 1.23604e4 559.49518 50.0558

2 15.432 BB 0.7984 1.23329e4 220.21907 49.9442

HPLC chromatogram of chiral 3ua



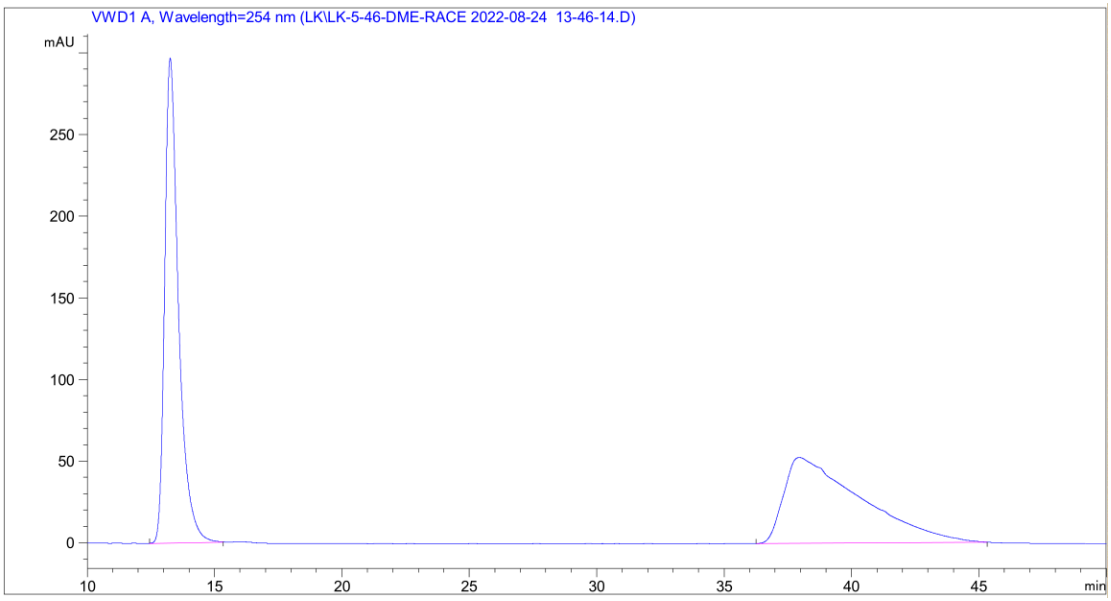
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 7.901 MM 0.3669 1.79789e4 816.79956 95.9907

2 16.222 MM 1.0085 750.94104 12.41005 4.0093

HPLC chromatogram of racemic 3va



[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 13.259 BB 0.5638 1.12174e4 50.3572

2 37.952 BB 2.6629 1.10582e4 49.6428

HPLC chromatogram of chiral 3va

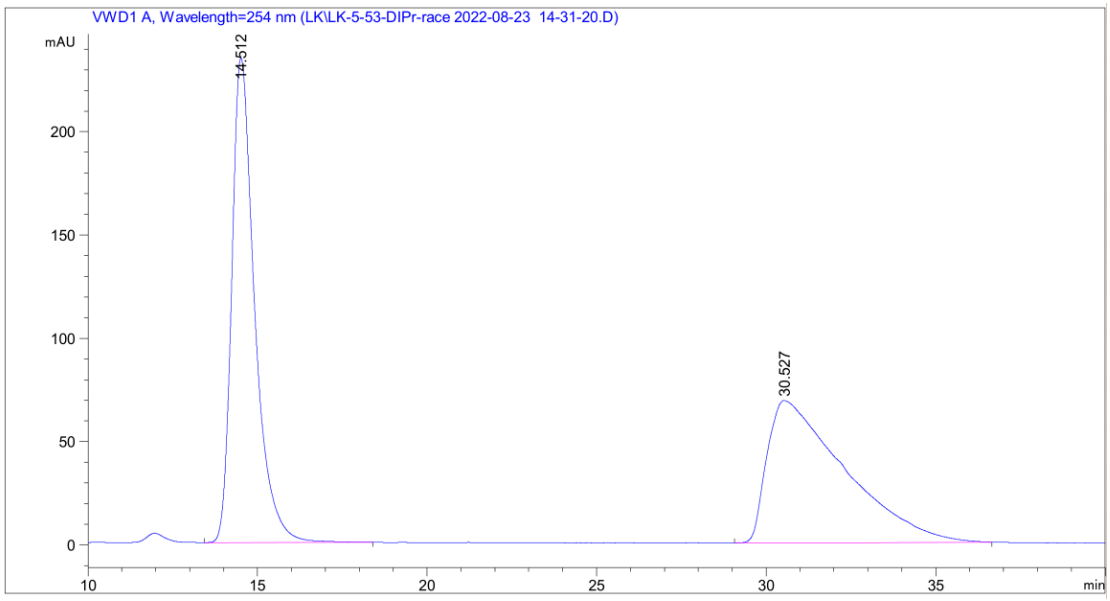
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 13.468 BB 0.5889 1.36397e4 96.4101

2 42.881 MM 2.1820 507.88211 3.5899

HPLC chromatogram of racemic 3wa



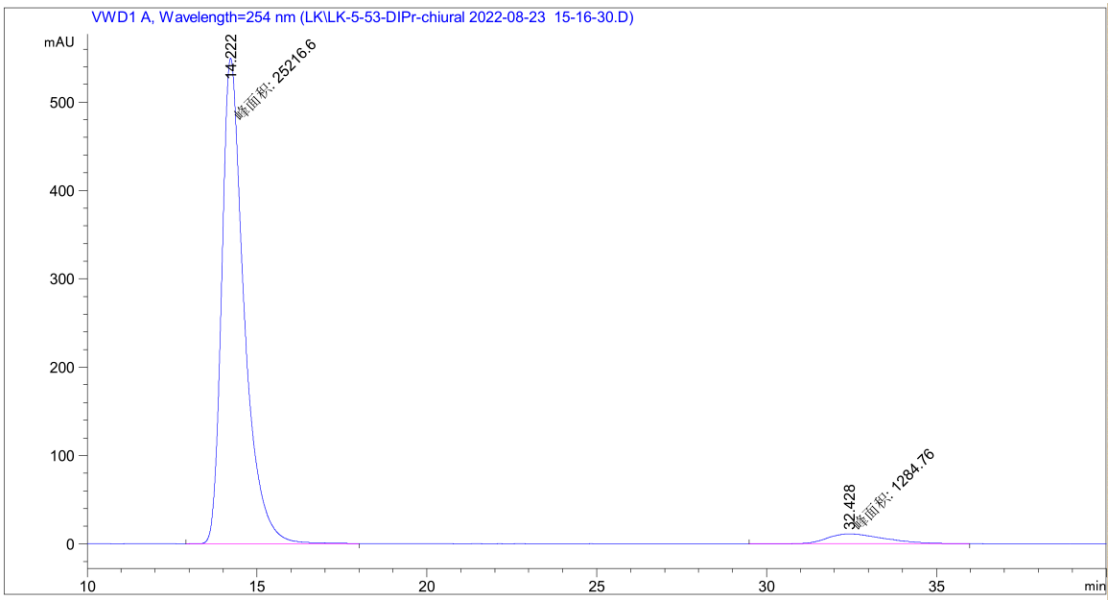
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.512 BB 0.7007 1.10077e4 234.48201 50.2284

2 30.527 BB 2.1645 1.09076e4 68.80553 49.7716

HPLC chromatogram of chiral 3wa



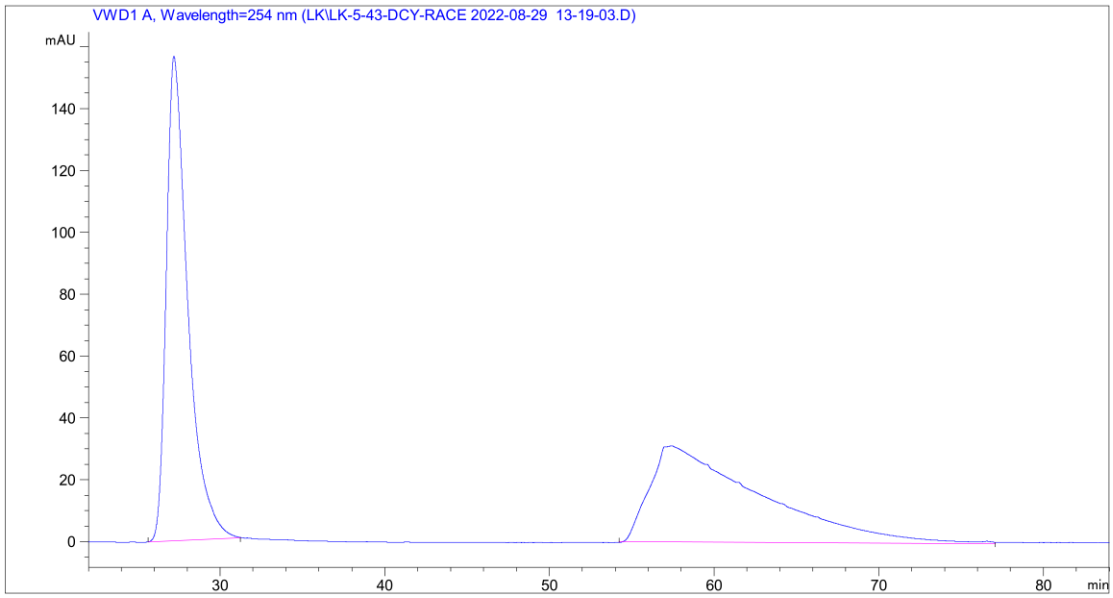
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.222 MM 0.7645 2.52166e4 549.77490 95.1521

2 32.428 MM 1.9339 1284.76306 11.07205 4.8479

HPLC chromatogram of racemic 3xa



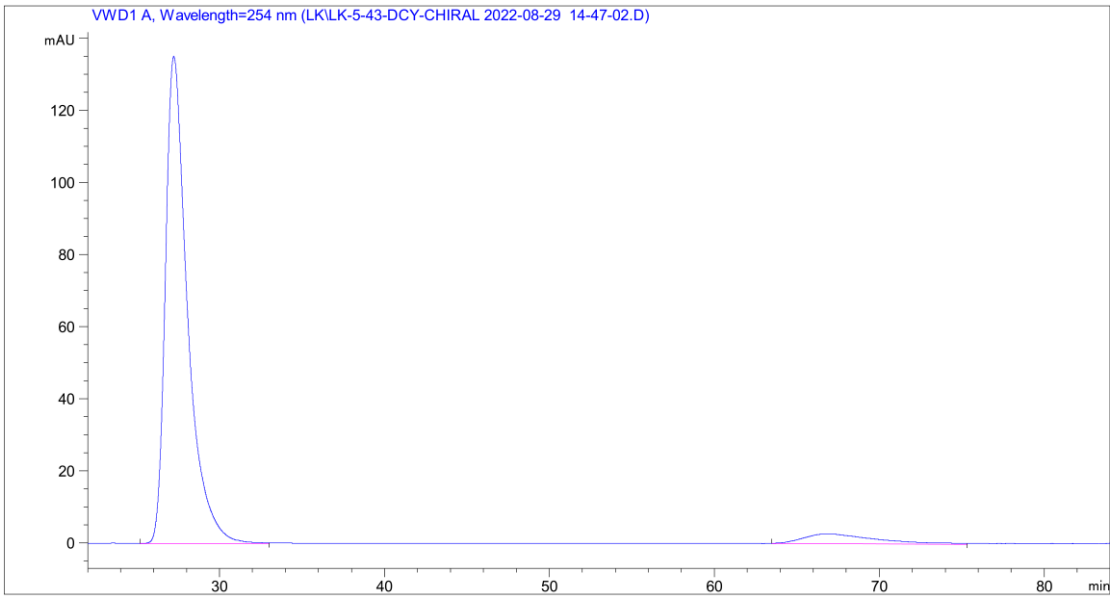
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 27.193 BB 1.3514 1.42704e4 49.7911

2 57.432 MM 7.7491 1.43901e4 50.2089

HPLC chromatogram of chiral 3xa



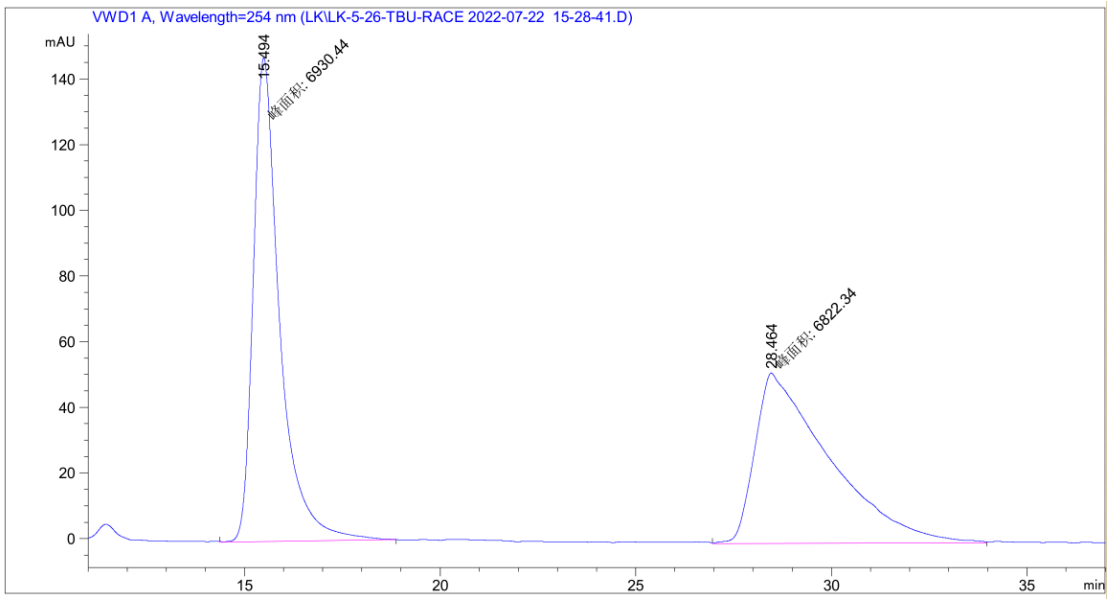
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 27.226 MM 1.5546 1.26123e4 93.8706

2 66.873 MM 5.1071 823.53241 6.1294

HPLC chromatogram of racemic 3ya



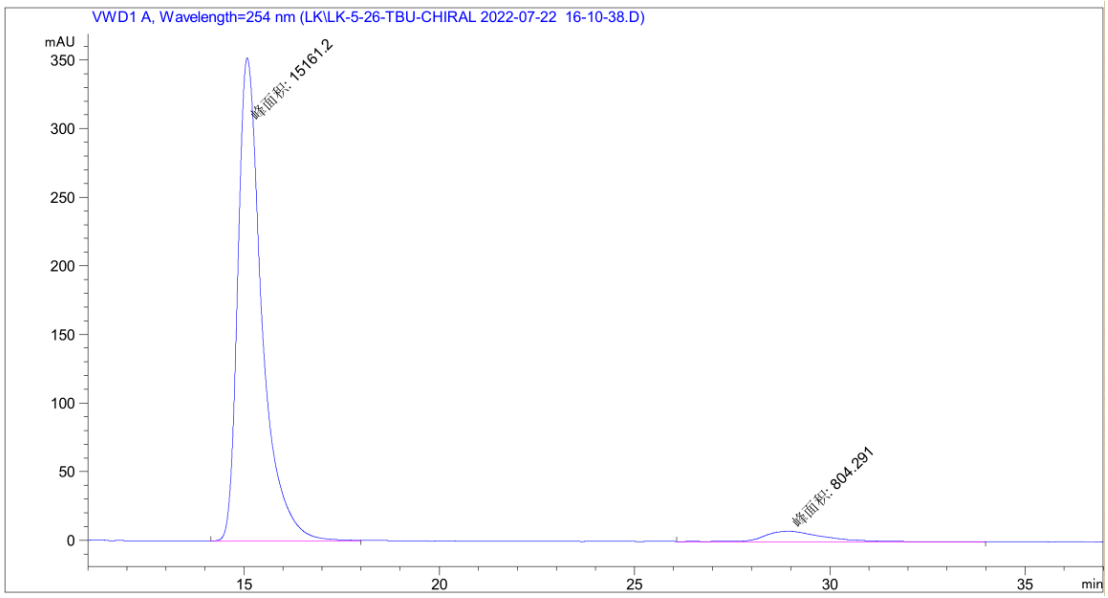
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 15.494 MM 0.7844 6930.44287 147.25853 50.3930

2 28.464 MM 2.1938 6822.34375 51.83133 49.6070

HPLC chromatogram of chiral 3ya



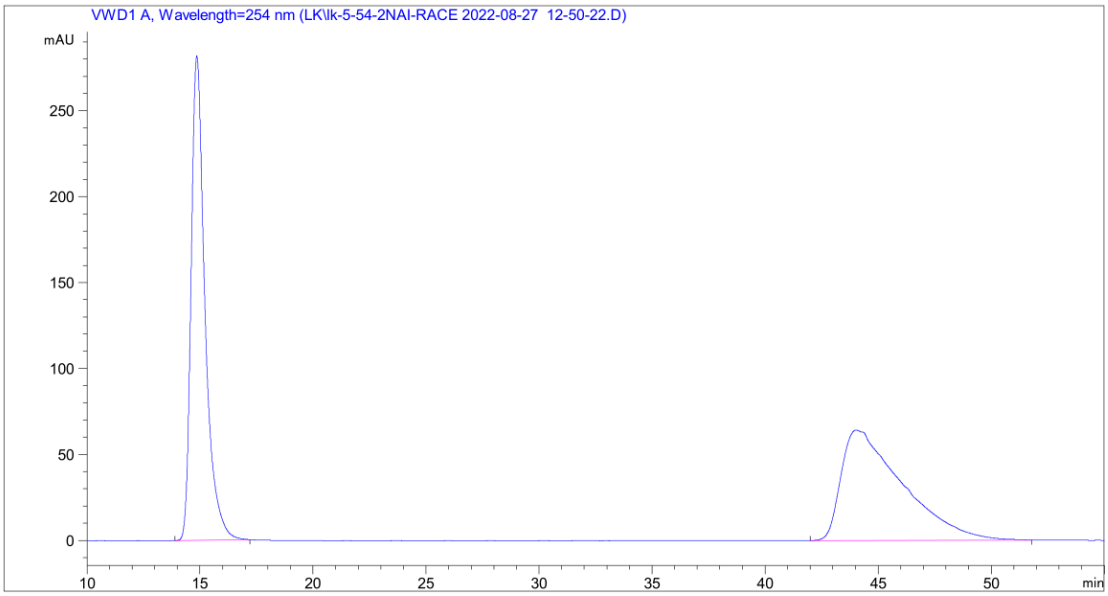
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 15.084 MM 0.7173 1.51612e4 352.28564 94.9623

2 28.945 MM 1.7540 804.29095 7.64239 5.0377

HPLC chromatogram of racemic 3za



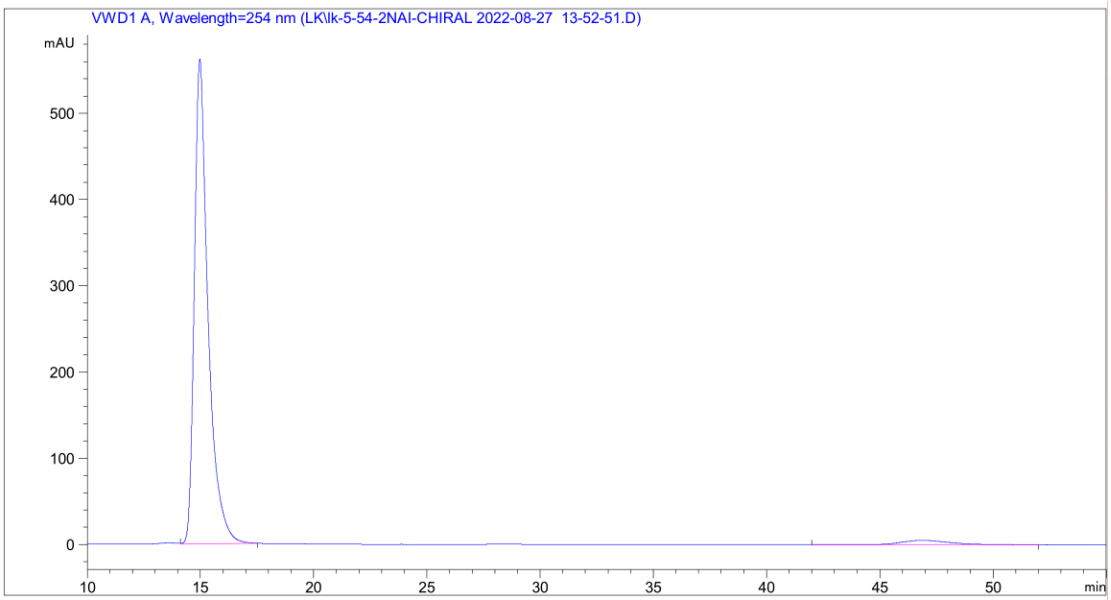
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 14.861 BB 0.6409 1.20314e4 49.8891

2 44.034 MM 3.1363 1.20849e4 50.1109

HPLC chromatogram of chiral 3za



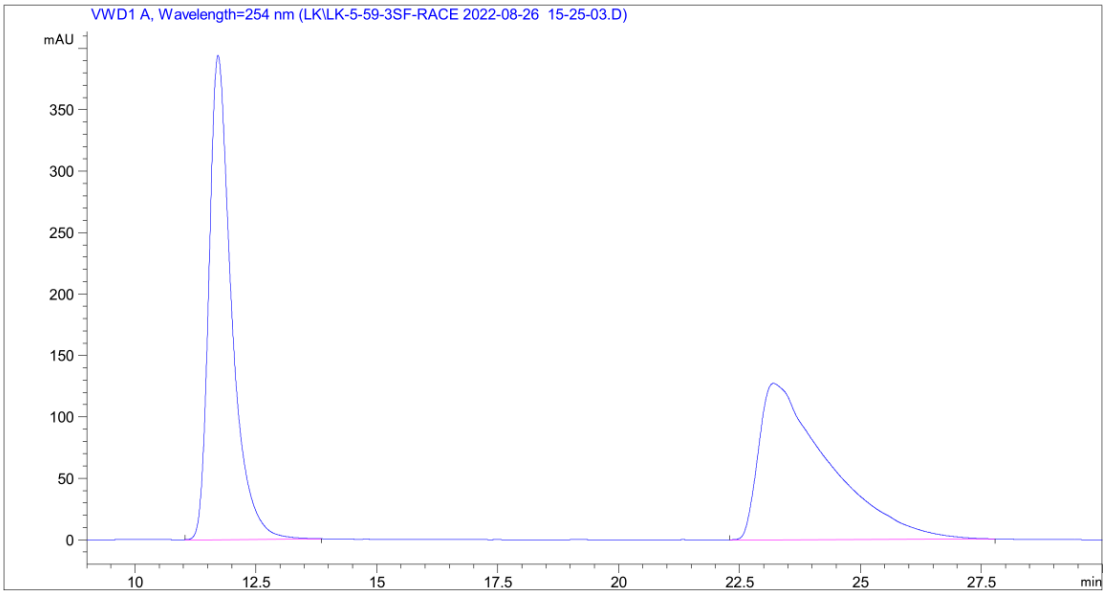
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 14.975 VB 0.6170 2.36603e4 97.0652

2 46.770 MM 2.4189 715.37592 2.9348

HPLC chromatogram of racemic 3z'a



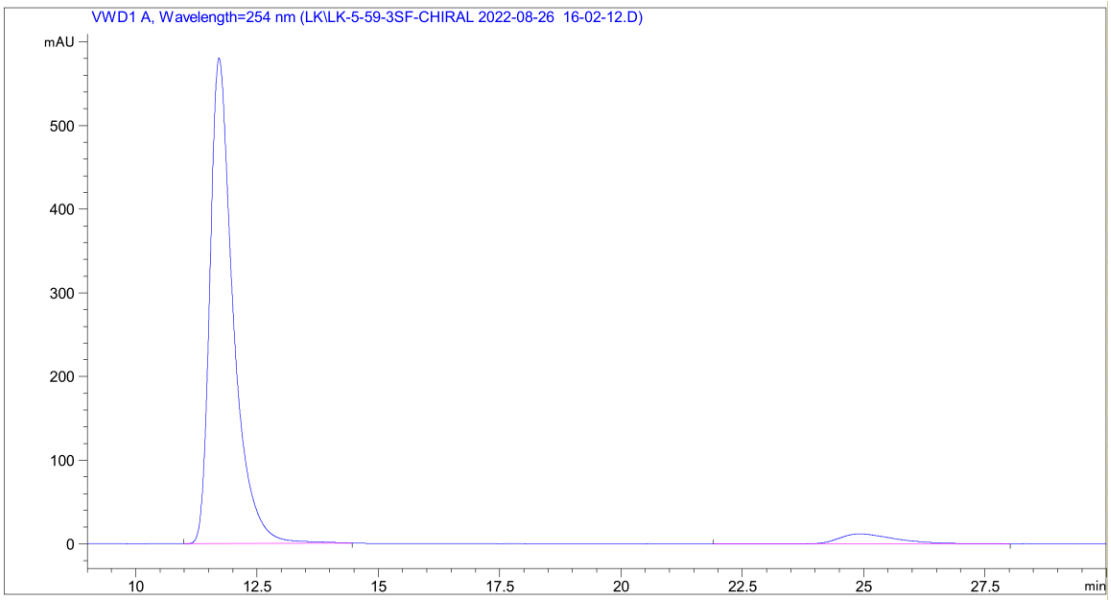
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 11.717 BB 0.4856 1.28185e4 50.0608

2 23.204 BB 1.3798 1.27874e4 49.9392

HPLC chromatogram of chiral 3z'a



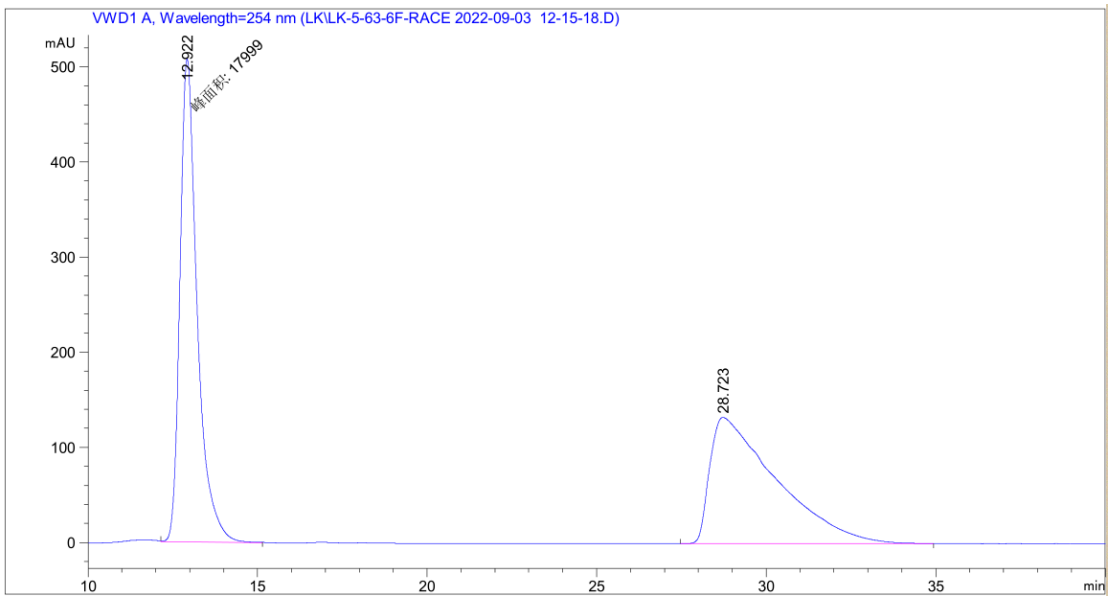
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 11.718 MM 0.5561 1.93661e4 95.1845

2 24.921 MM 1.3796 979.75549 4.8155

HPLC chromatogram of racemic 3qb



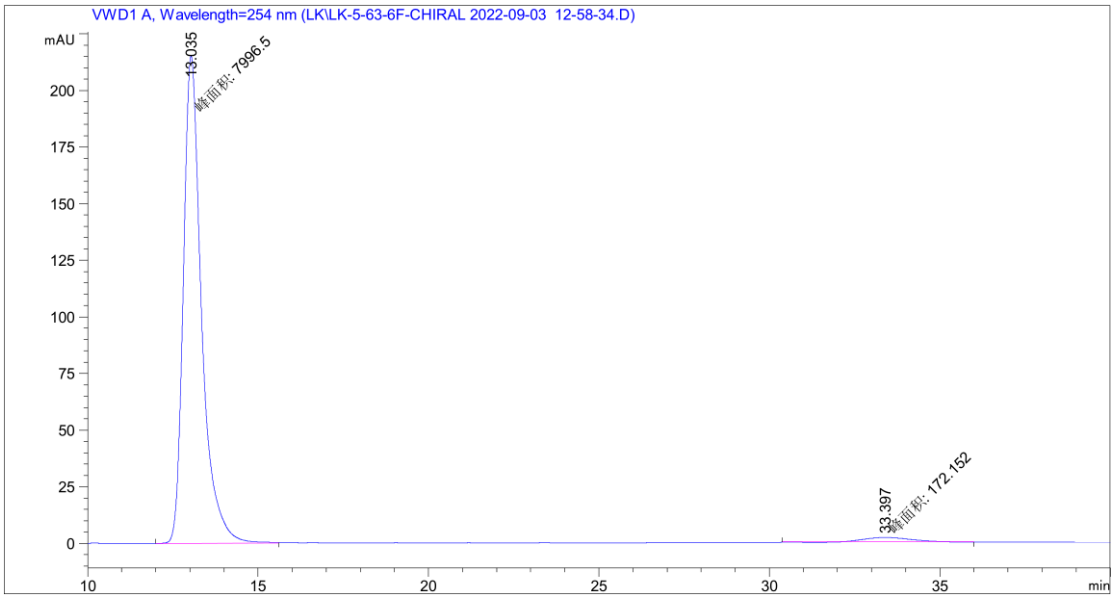
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 12.922 MM 0.5909 1.79990e4 507.67300 49.9228

2 28.723 BB 1.8281 1.80547e4 132.71982 50.0772

HPLC chromatogram of chiral 3qb



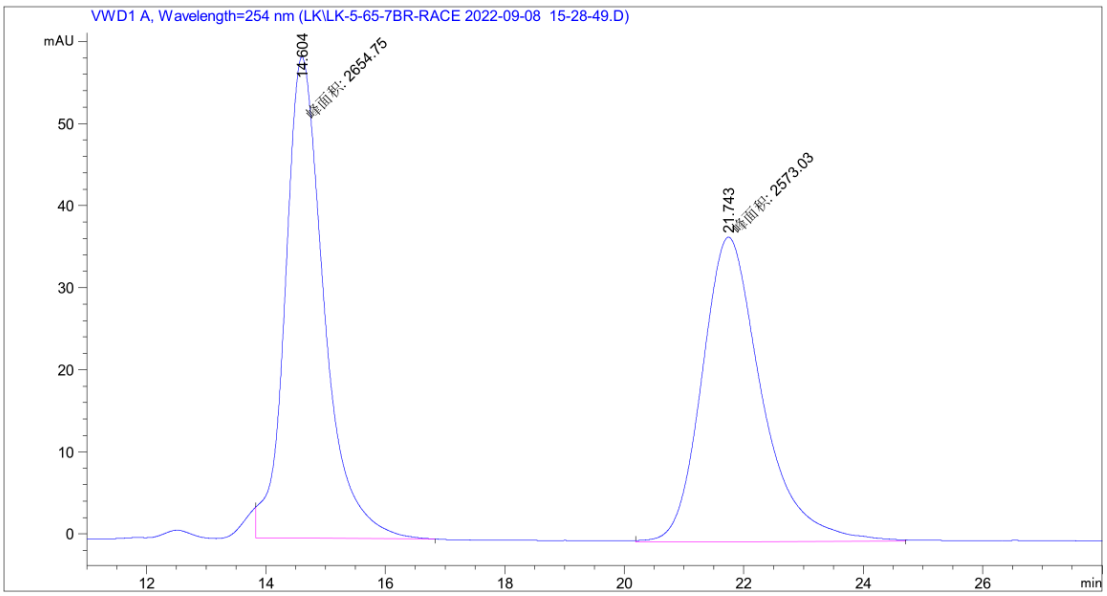
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 13.035 MM 0.6189 7996.50488 215.35405 97.8925

2 33.397 MM 1.5323 172.15236 1.87247 2.1075

HPLC chromatogram of racemic 3qc



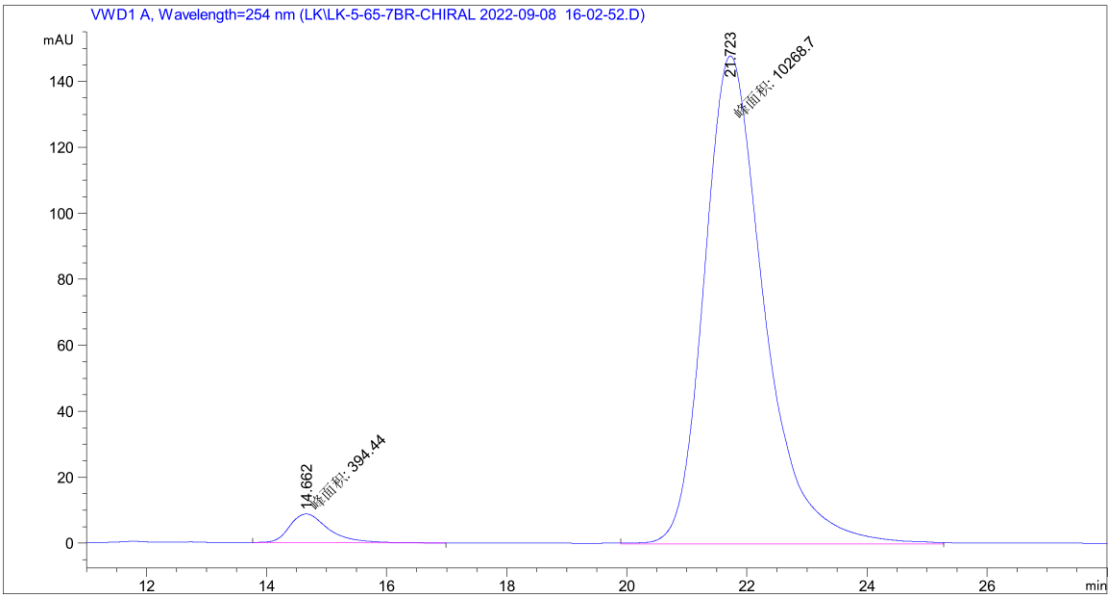
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.604 MM 0.7544 2654.74976 58.64896 50.7816

2 21.743 MM 1.1562 2573.02856 37.09153 49.2184

HPLC chromatogram of chiral 3qc



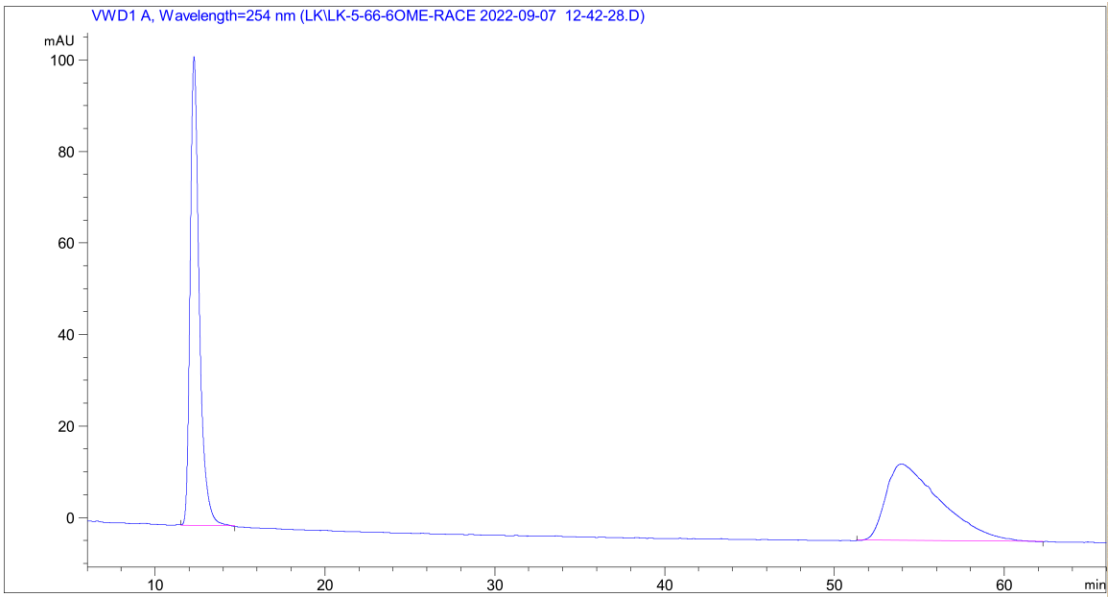
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.662 MM 0.7575 394.44040 8.67807 3.6991

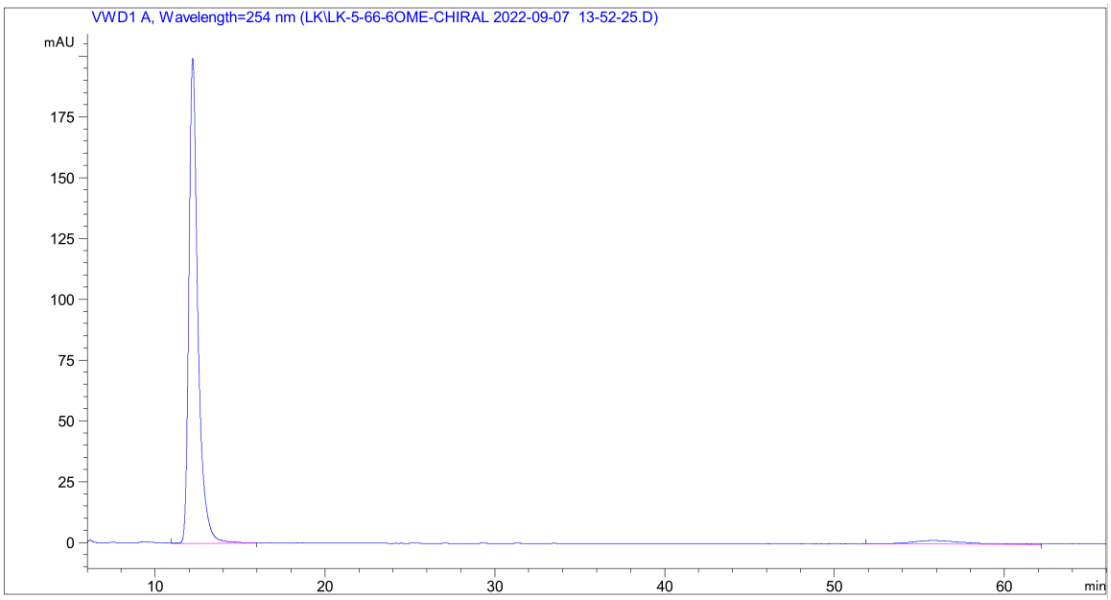
2 21.723 MM 1.1570 1.02687e4 147.91916 96.3009

HPLC chromatogram of racemic 3qd



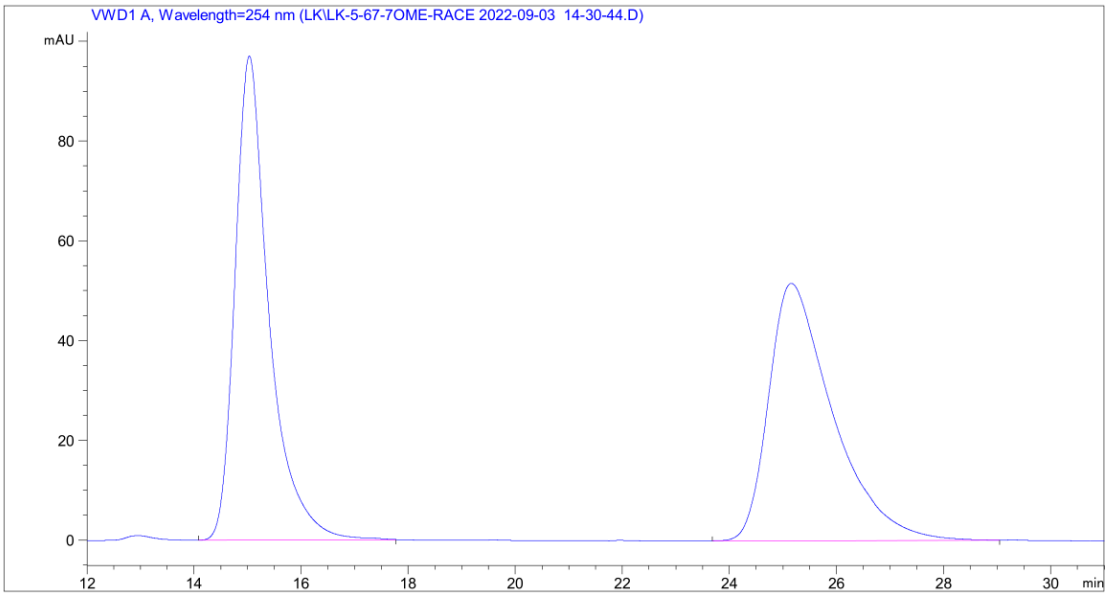
#	[min]	[min]	[mAU*s]	%
1	12.292	MM	0.6190	3800.56201	50.6241
2	53.978	MM	3.7083	3706.85840	49.3759

HPLC chromatogram of chiral 3qd



#	[min]	[min]	[mAU*s]	%
1	12.217	MM	0.6147	7357.34717	96.2331
2	55.734	MM	3.3545	287.99057	3.7669

HPLC chromatogram of racemic 3qe



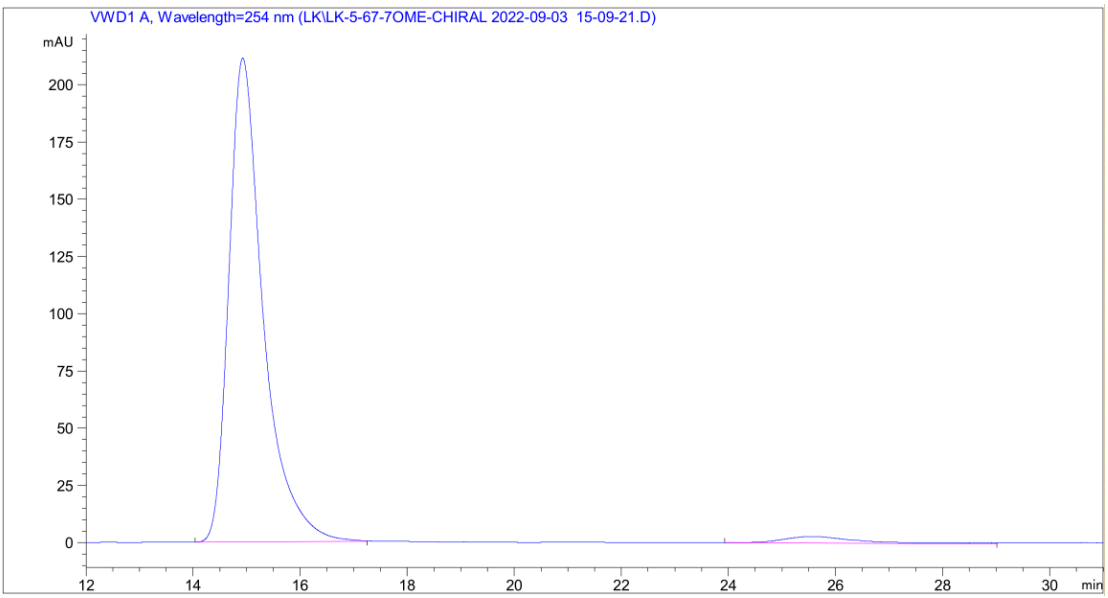
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 15.033 MM 0.7379 4298.45361 50.0238

2 25.154 MM 1.3865 4294.36523 49.9762

HPLC chromatogram of chiral 3qe



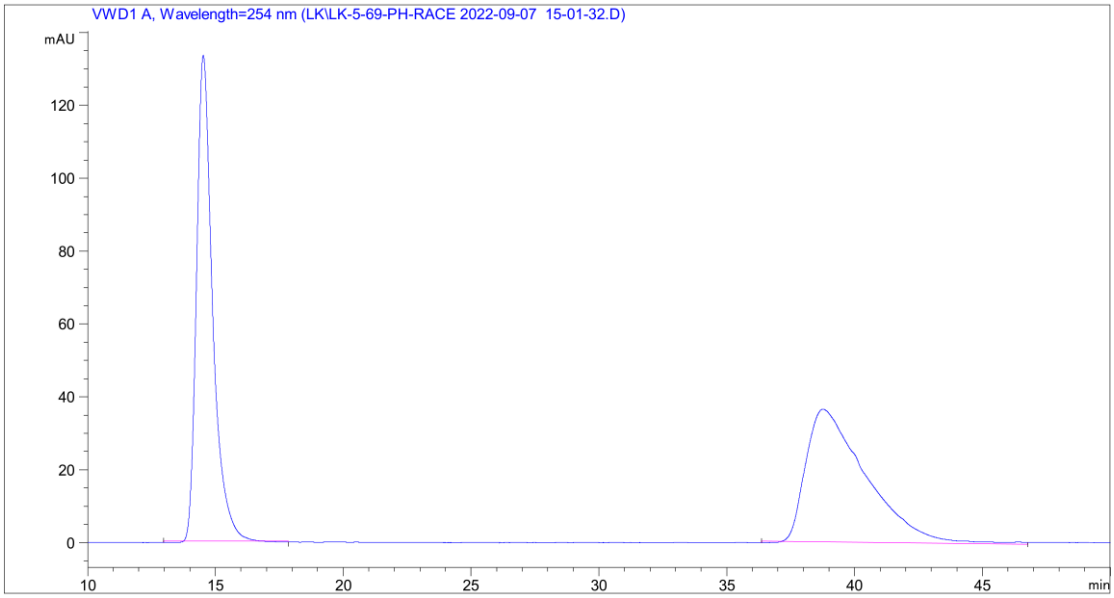
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 14.927 BB 0.6656 9411.11230 97.0361

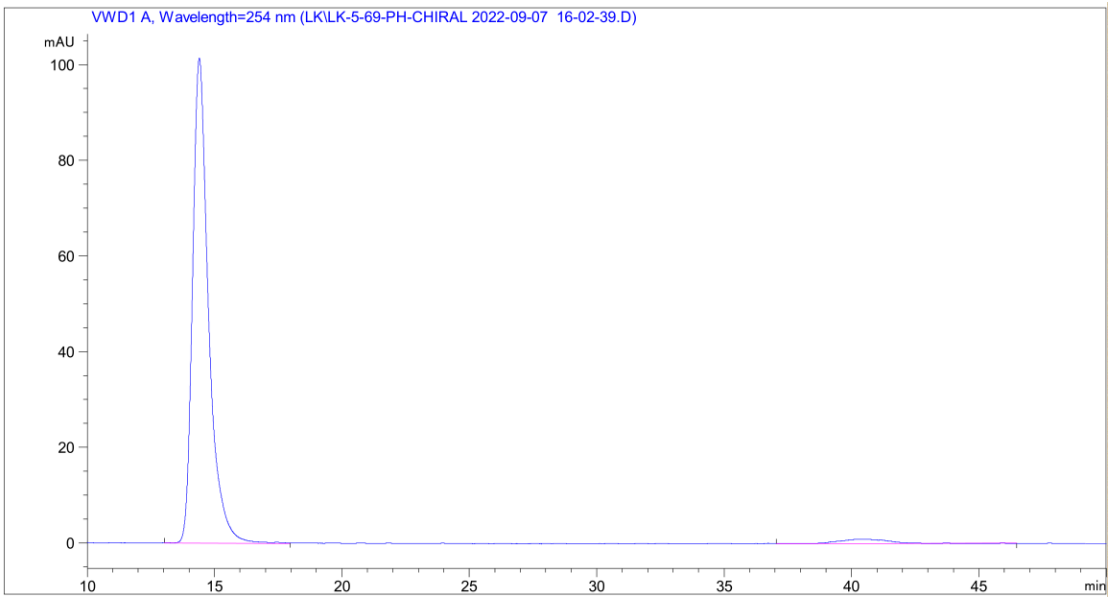
2 25.568 MM 1.6596 287.45319 2.9639

HPLC chromatogram of racemic 3qf



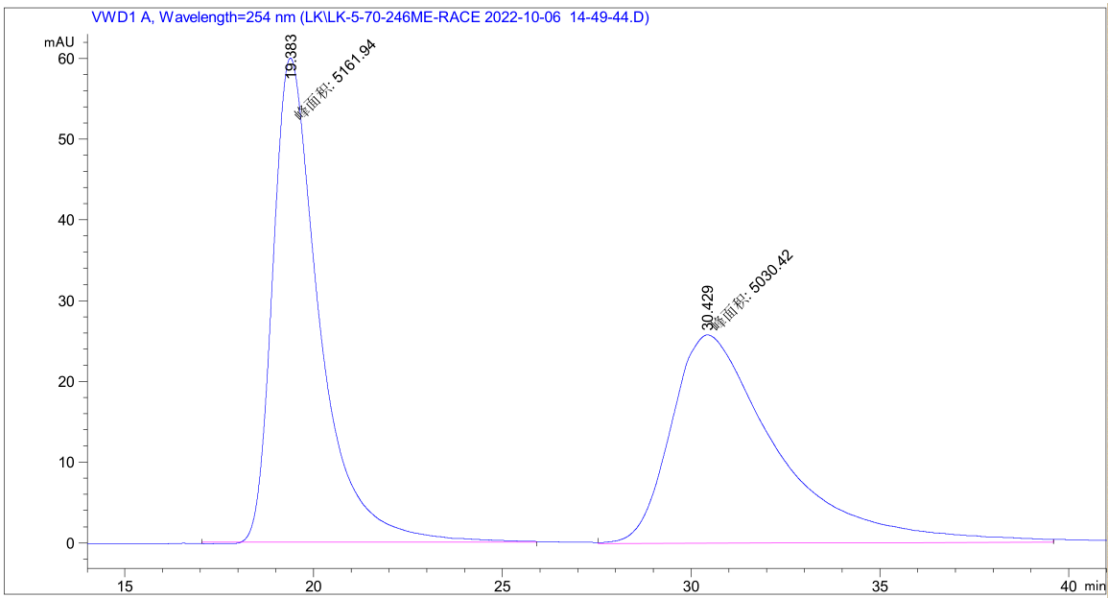
#	[min]	[min]	[mAU*s]	%
1	14.526	MM	0.7261	5803.68066	49.5605
2	38.768	MM	2.7109	5906.61914	50.4395

HPLC chromatogram of chiral 3qf



#	[min]	[min]	[mAU*s]	%
1	14.402	MM	0.7270	4421.93359	97.1068
2	40.346	MM	2.3291	131.74649	2.8932

HPLC chromatogram of racemic 3qg



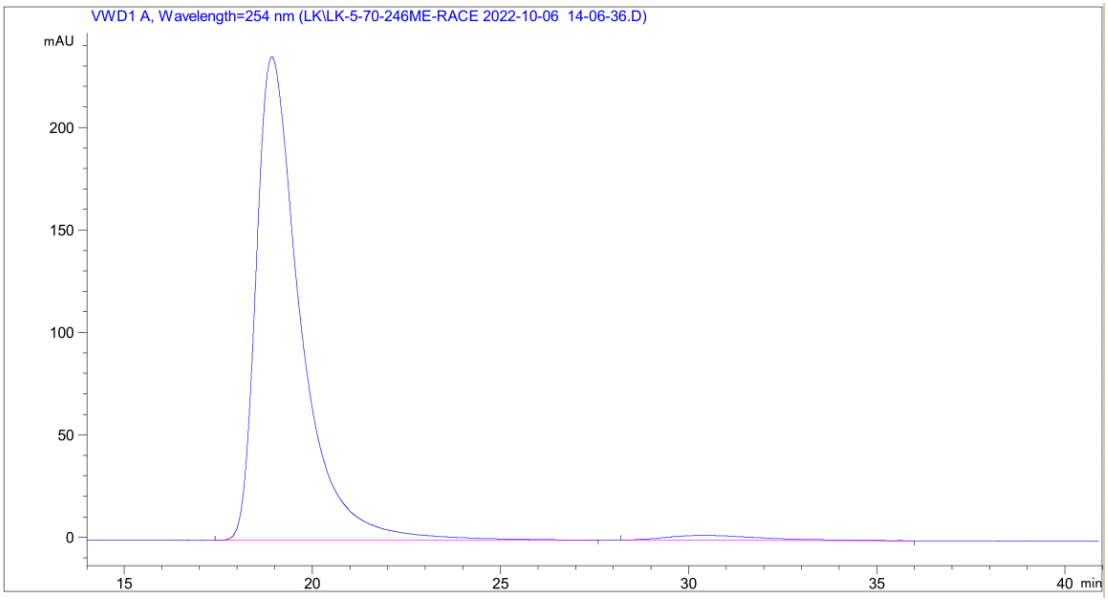
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 19.383 MM 1.4354 5161.94287 59.93750 50.6452

2 30.429 MM 3.2496 5030.42432 25.80011 49.3548

HPLC chromatogram of chiral 3qg



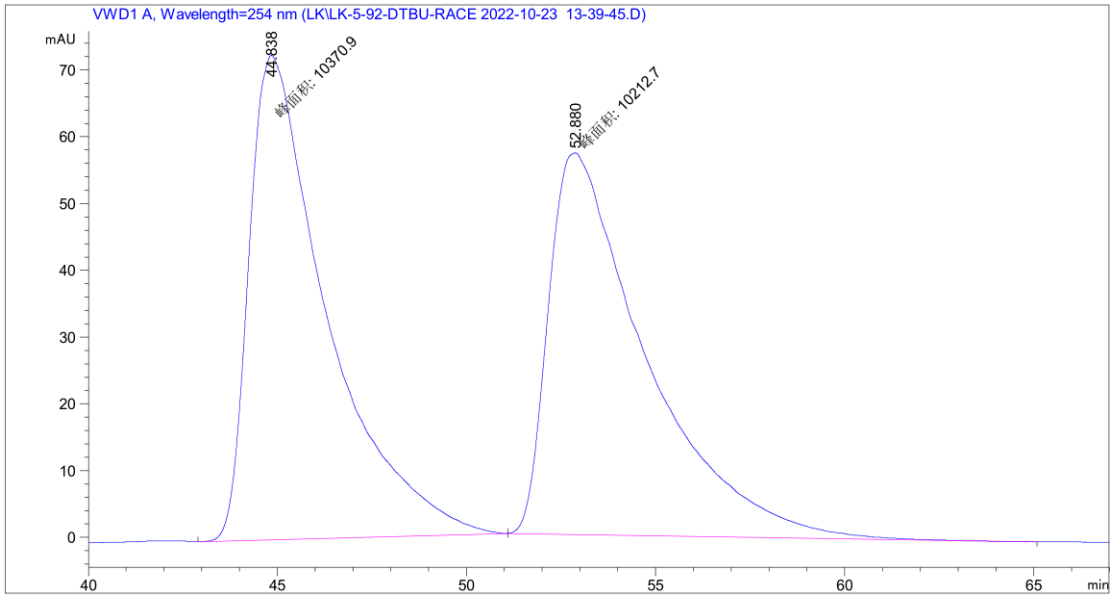
[min] [min] [mAU*s] %

----|-------|------|-------|----------|--------|

1 18.923 MM 1.3653 1.93155e4 97.7685

2 30.552 MM 3.1344 440.87170 2.2315

HPLC chromatogram of racemic 3qh



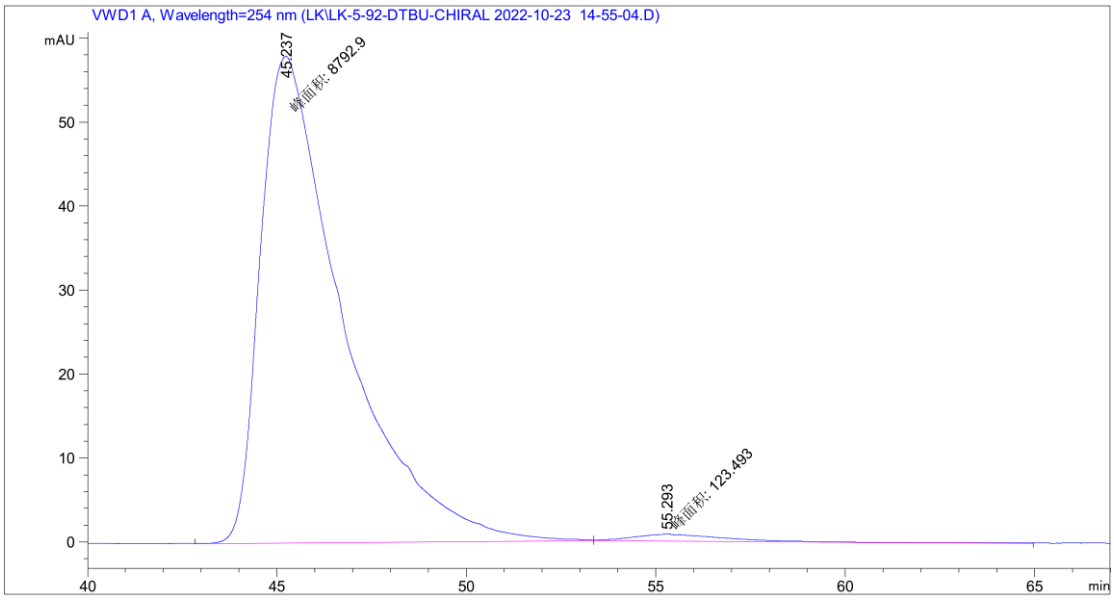
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 44.838 MM 2.3825 1.03709e4 72.55044 50.3843

2 52.880 MM 2.9784 1.02127e4 57.14888 49.6157

HPLC chromatogram of chiral 3qh



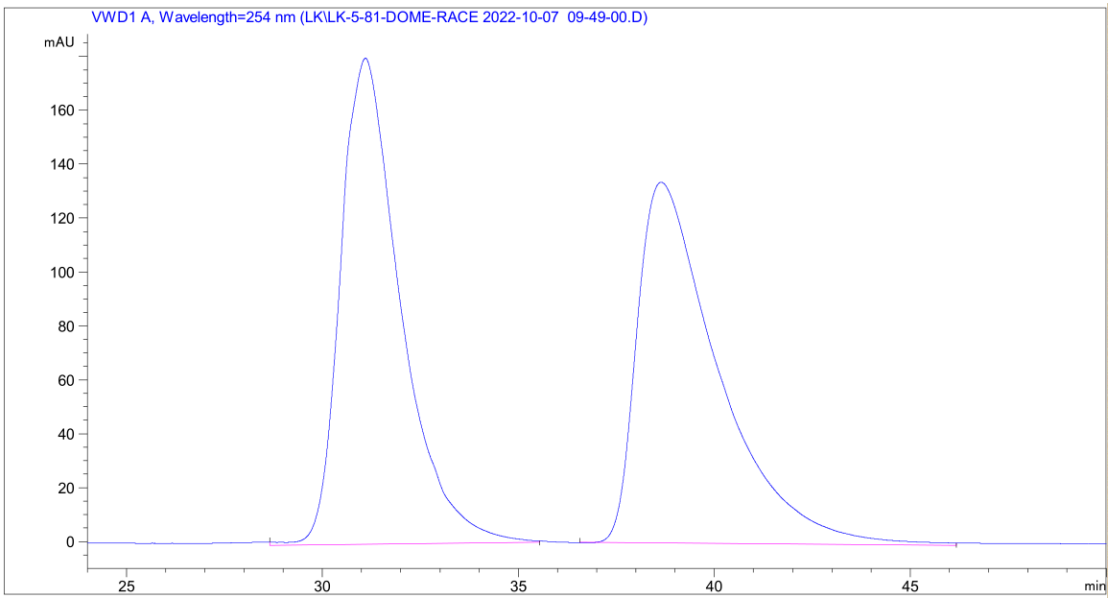
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 45.237 MM 2.5289 8792.89746 57.95037 98.6150

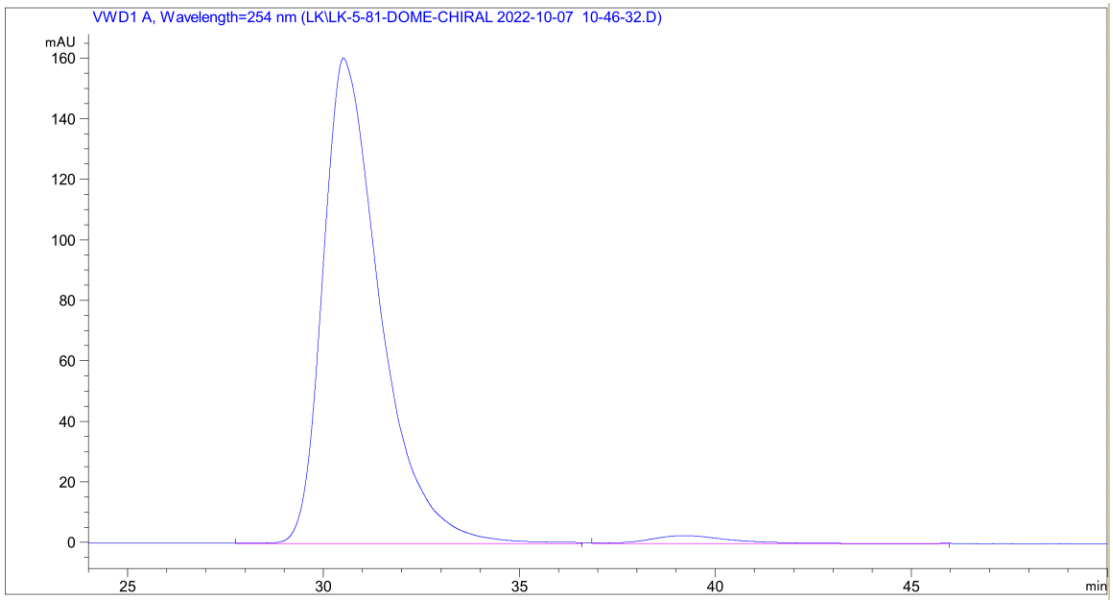
2 55.293 MM 2.4472 123.49287 8.41044e-1 1.3850

HPLC chromatogram of racemic 3qi



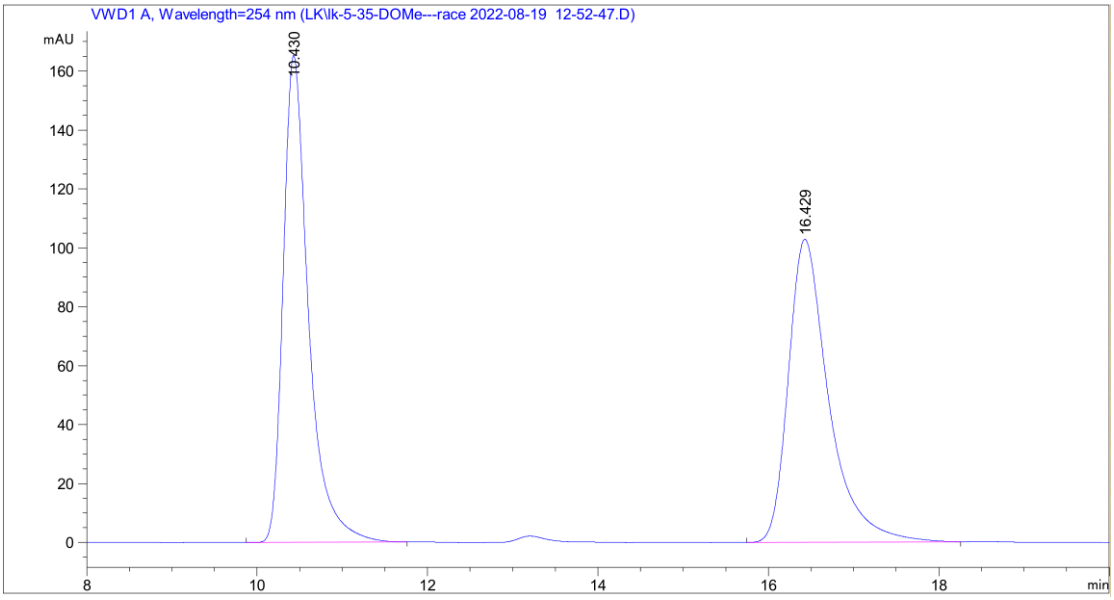
#	[min]	[min]	[mAU*s]		%
1	31.099	MM	1.7772	1.92344e4	49.9328
2	38.643	MM	2.4022	1.92861e4	50.0672

HPLC chromatogram of chiral 3qi



#	[min]	[min]	[mAU*s]		%
1	30.510	MM	1.6962	1.63254e4	97.7763
2	39.167	MM	2.3891	371.28946	2.2237

HPLC chromatogram of racemic 6aa



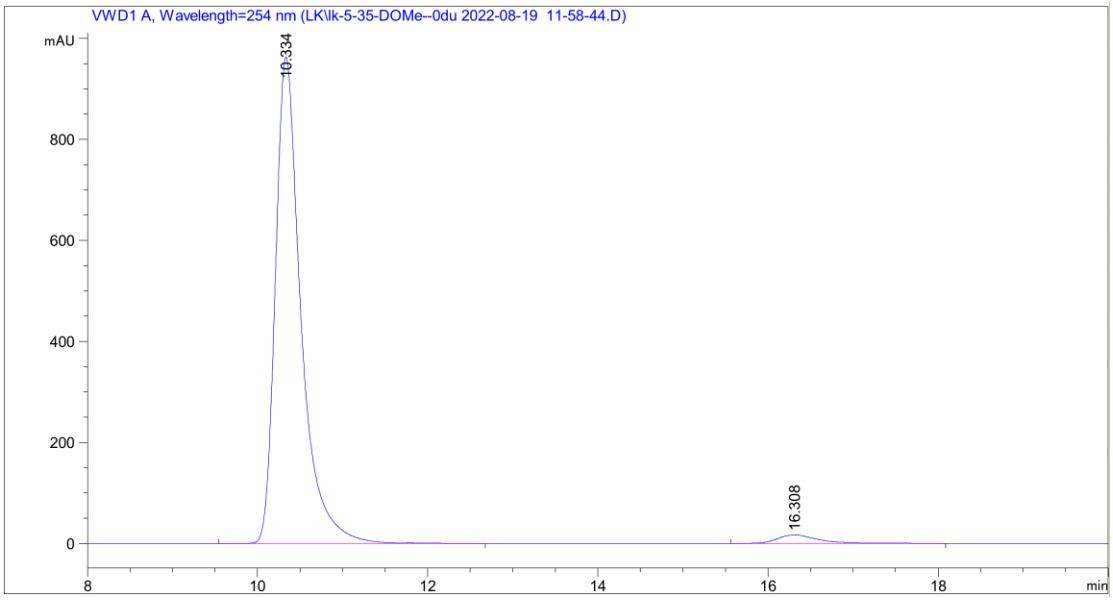
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 10.430 BB 0.3099 3412.05347 165.27567 50.2034

2 16.429 BB 0.4940 3384.41138 102.83238 49.7966

HPLC chromatogram of chiral 6aa



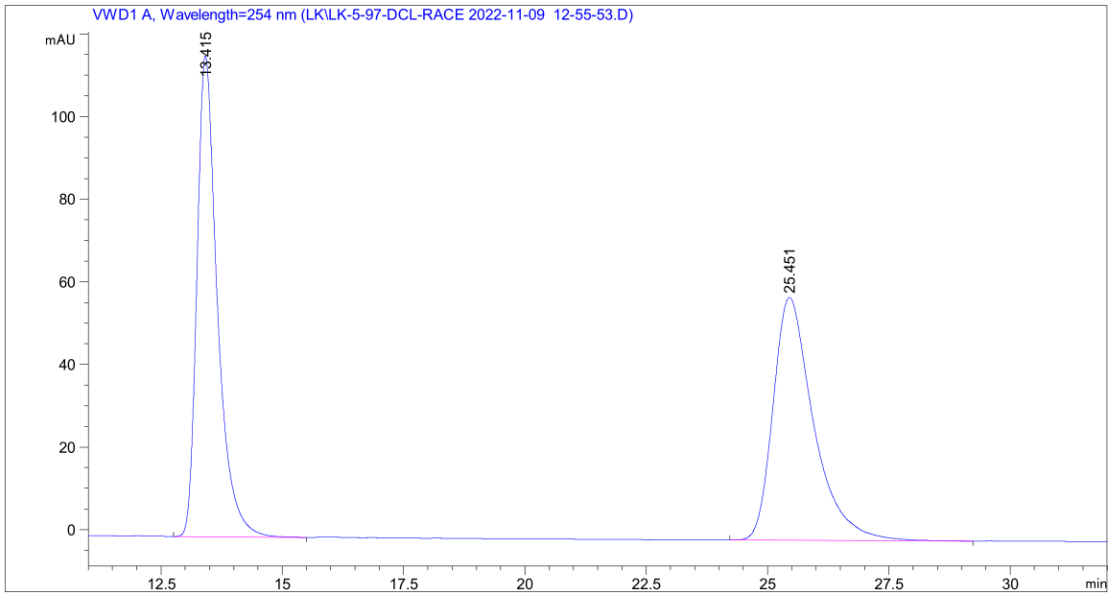
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 10.334 BV R 0.3126 2.01078e4 963.15576 97.3010

2 16.308 BB 0.4970 557.75970 16.77070 2.6990

HPLC chromatogram of racemic 6ba



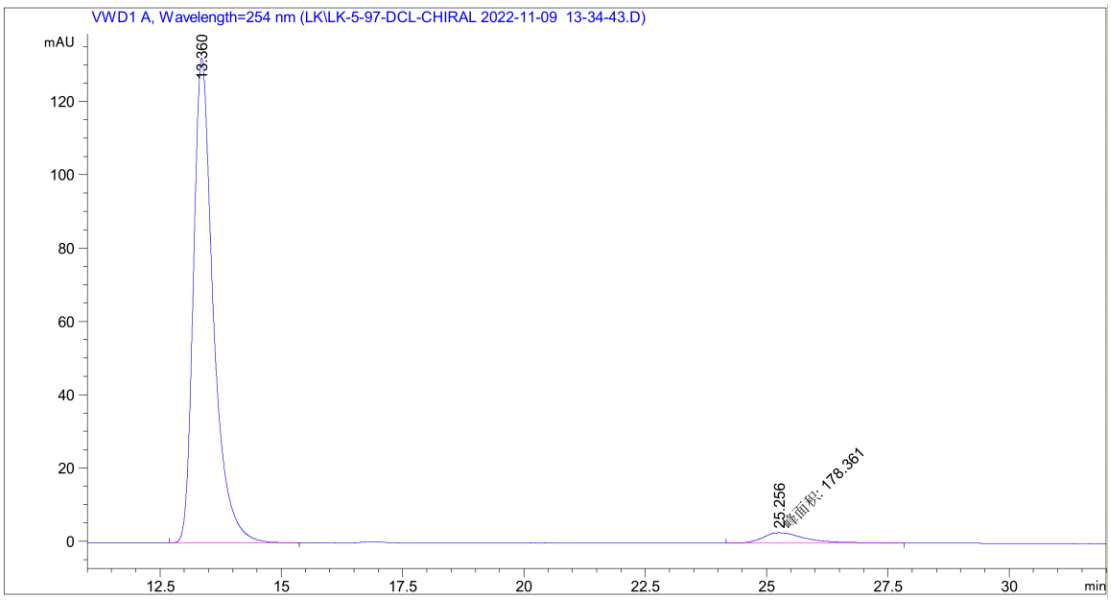
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 13.415 BB 0.4378 3409.54370 116.38366 50.0047

2 25.451 BB 0.8644 3408.90674 58.80105 49.9953

HPLC chromatogram of chiral 6ba



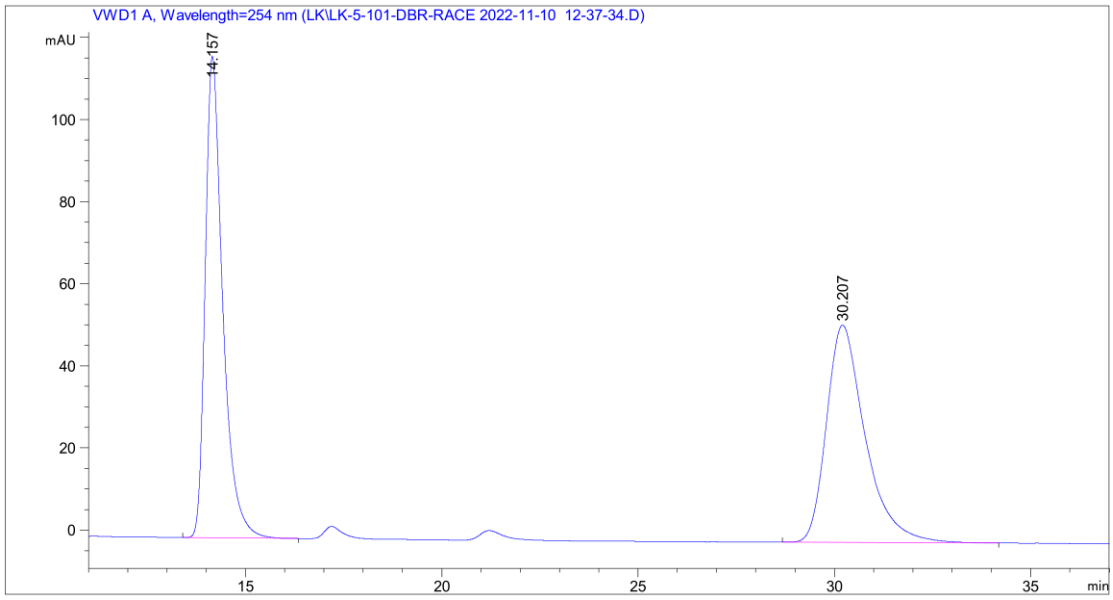
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 13.360 BB 0.4251 3763.02344 132.20900 95.4747

2 25.256 MM 1.0438 178.36073 2.84792 4.5253

HPLC chromatogram of racemic 6ca



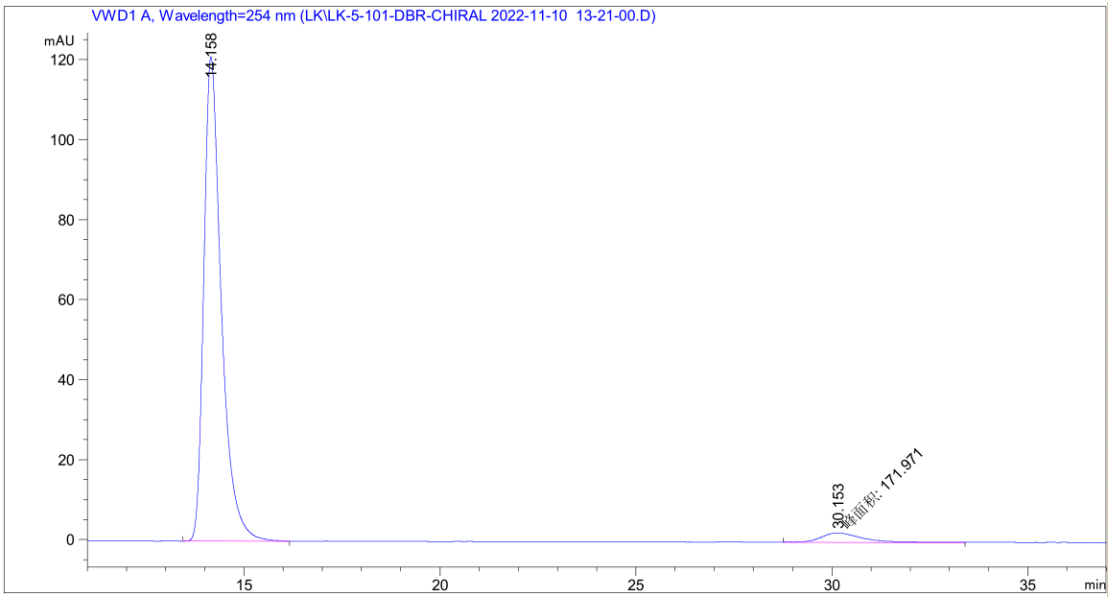
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.157 BB 0.4642 3640.86011 117.27529 50.0305

2 30.207 BB 1.0323 3636.42603 52.94779 49.9695

HPLC chromatogram of chiral 6ca



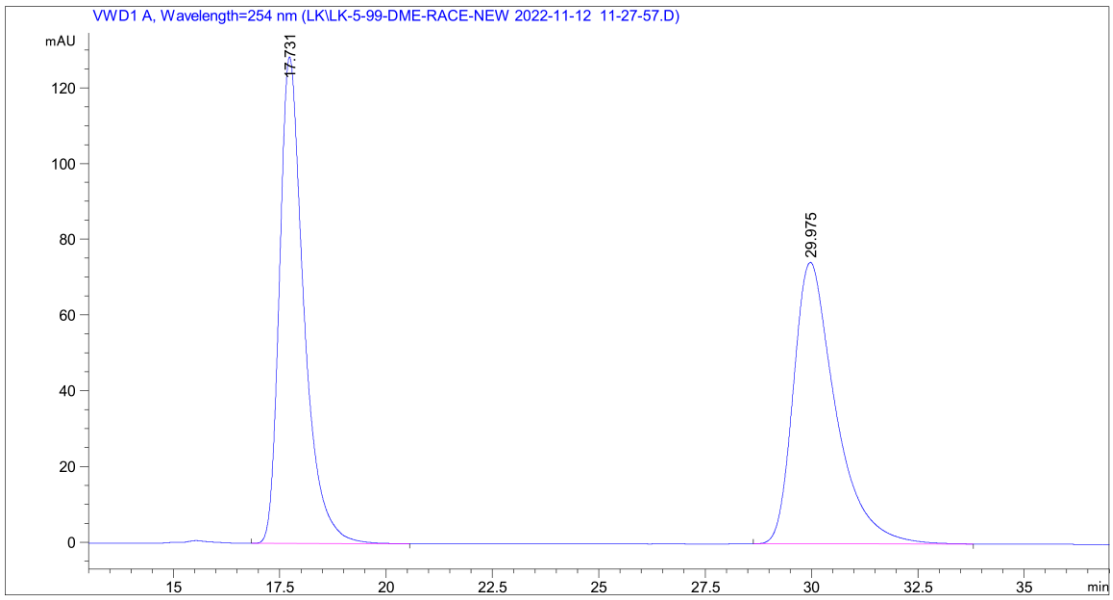
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.158 BB 0.4668 3764.79956 121.05619 95.6317

2 30.153 MM 1.2085 171.97060 2.37162 4.3683

HPLC chromatogram of racemic 6da



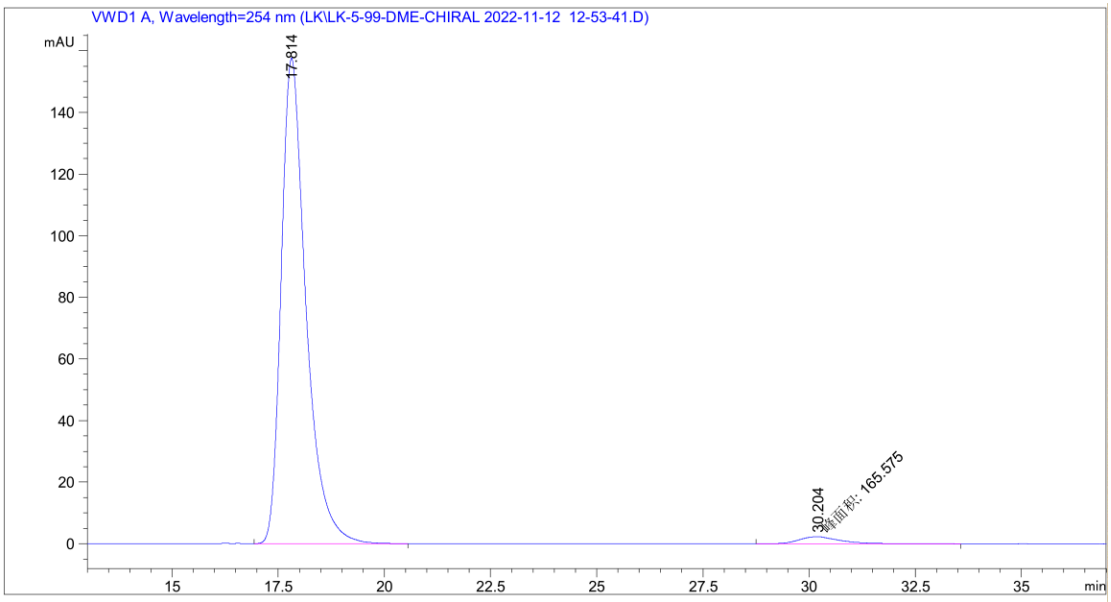
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 17.731 BB 0.5955 5110.96631 128.36464 50.0586

2 29.975 BB 1.0157 5099.00293 74.29411 49.9414

HPLC chromatogram of chiral 6da



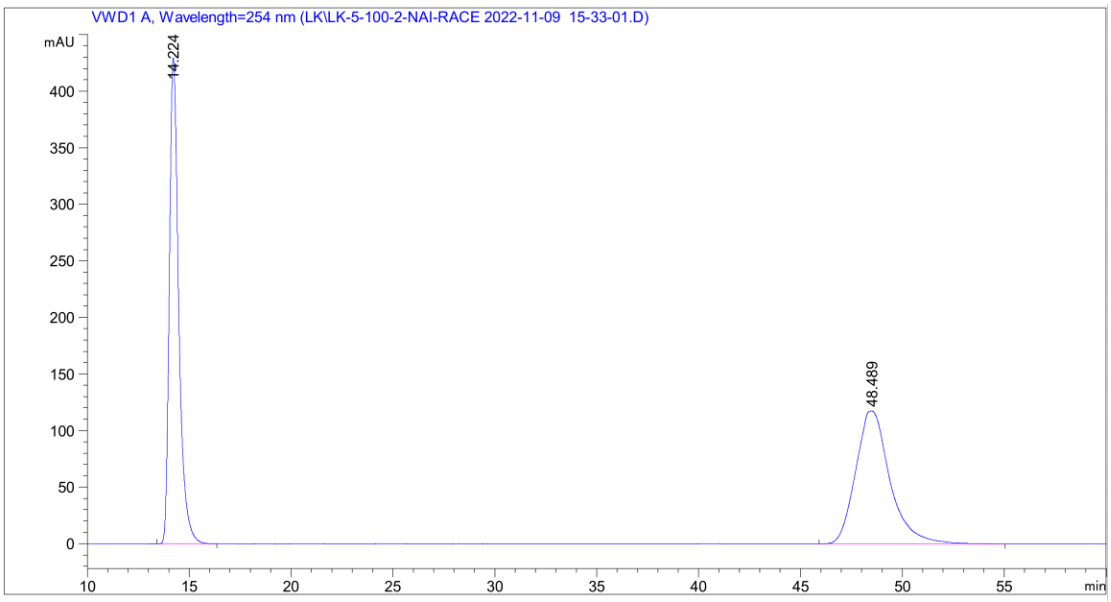
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 17.814 BB 0.6083 6394.06592 157.60391 97.4758

2 30.204 MM 1.1956 165.57541 2.30816 2.5242

HPLC chromatogram of racemic 6ea



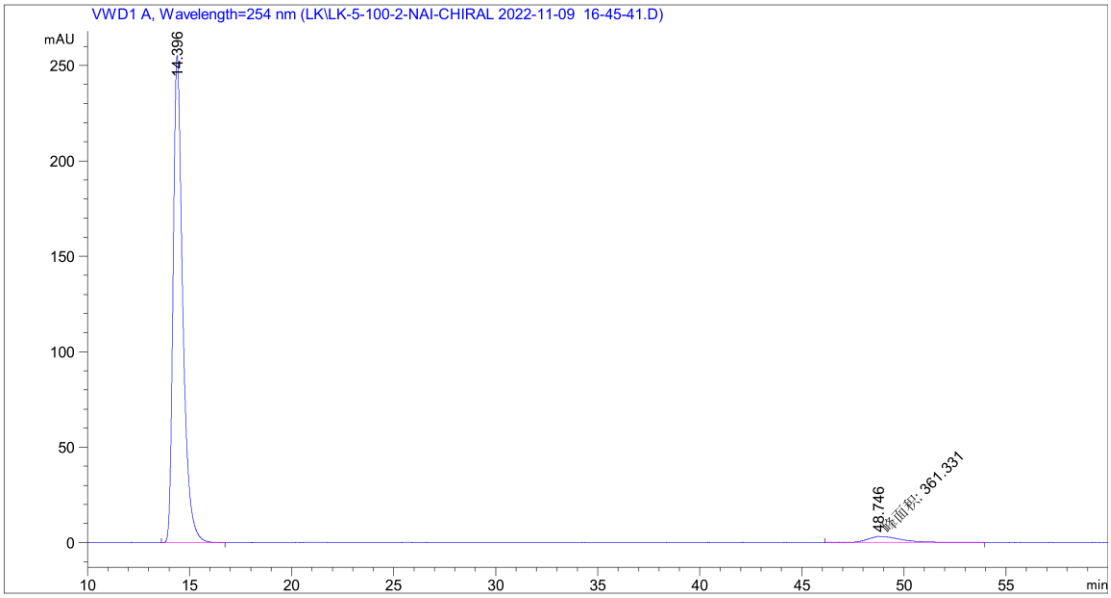
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.224 BB 0.4838 1.36801e4 429.24008 49.8732

2 48.489 BB 1.6573 1.37497e4 117.48980 50.1268

HPLC chromatogram of chiral 6ea



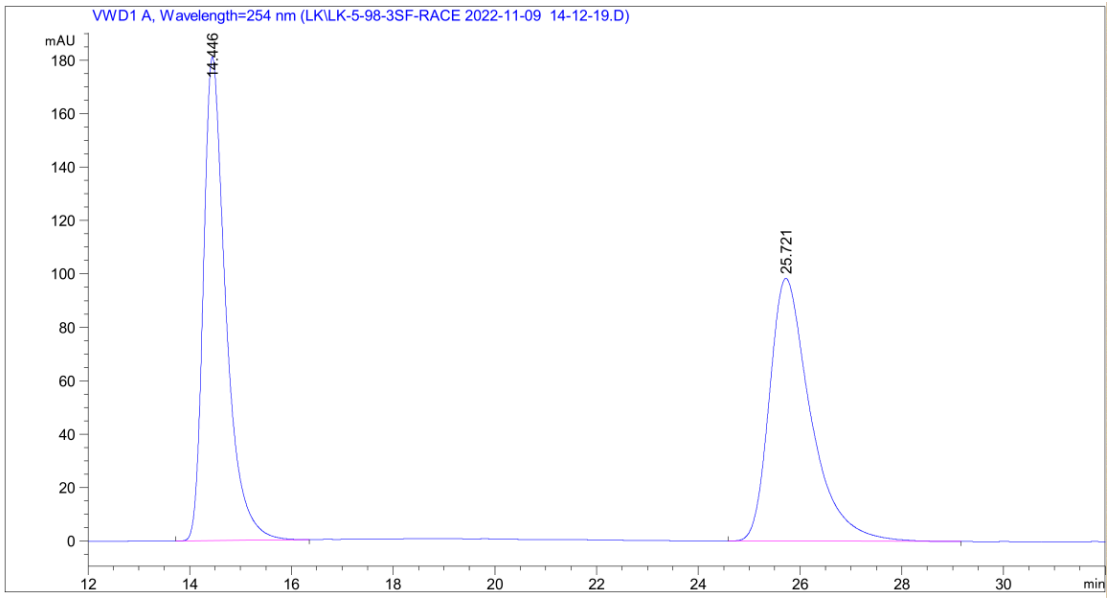
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.396 BB 0.4946 8349.77441 255.28419 95.8521

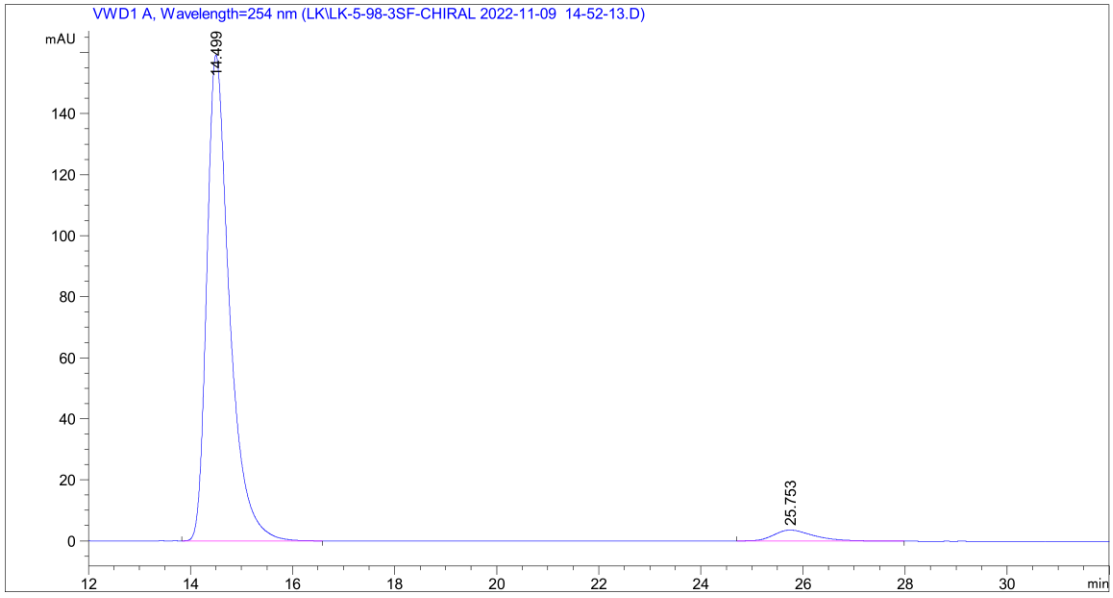
2 48.746 MM 1.9113 361.33124 3.15085 4.1479

HPLC chromatogram of racemic 6fa



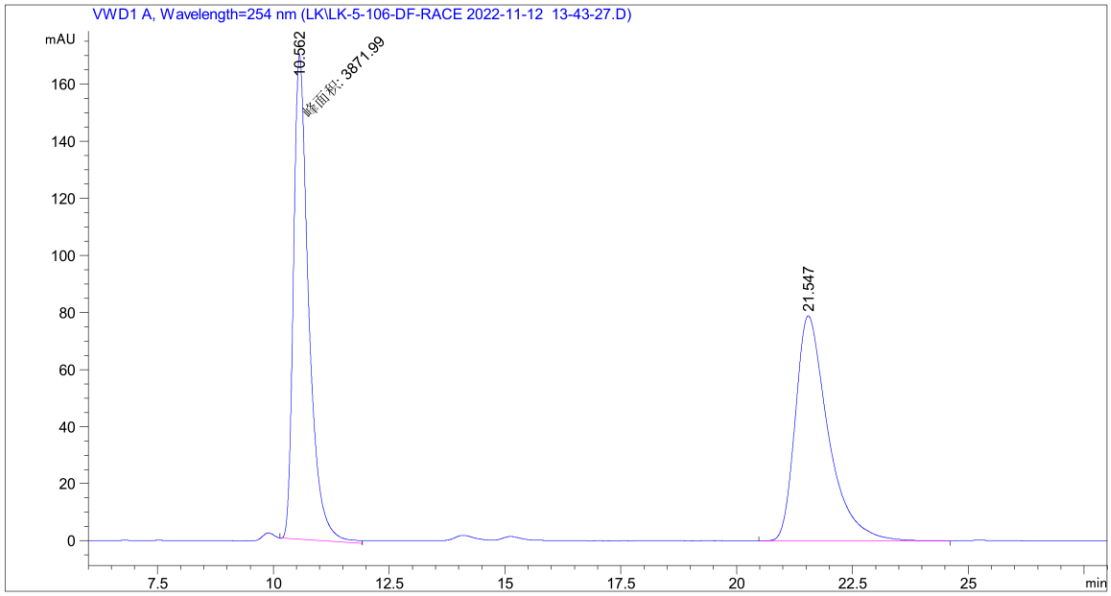
#	[min]	[min]	[mAU*s]	[mAU]	%
1	14.446	BB	0.4529	5527.47705	181.18355	50.0001
2	25.721	BB	0.8364	5527.46338	98.39390	49.9999

HPLC chromatogram of chiral 6fa



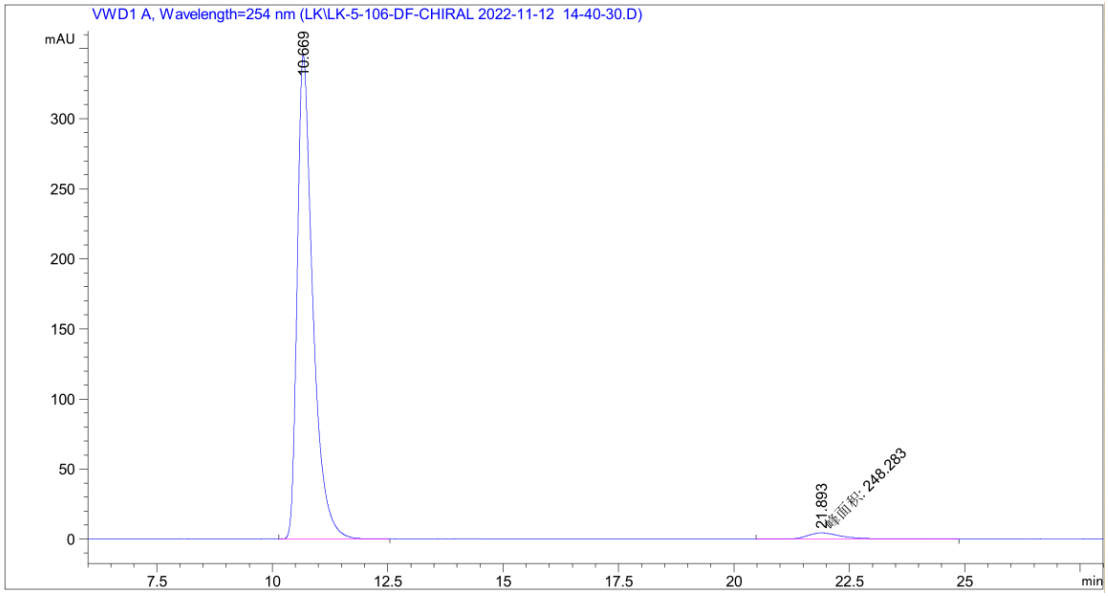
#	[min]	[min]	[mAU*s]	[mAU]	%
1	14.499	BB	0.4592	4917.06787	159.24268	96.1186
2	25.753	BB	0.7739	198.55565	3.61418	3.8814

HPLC chromatogram of racemic 6ab



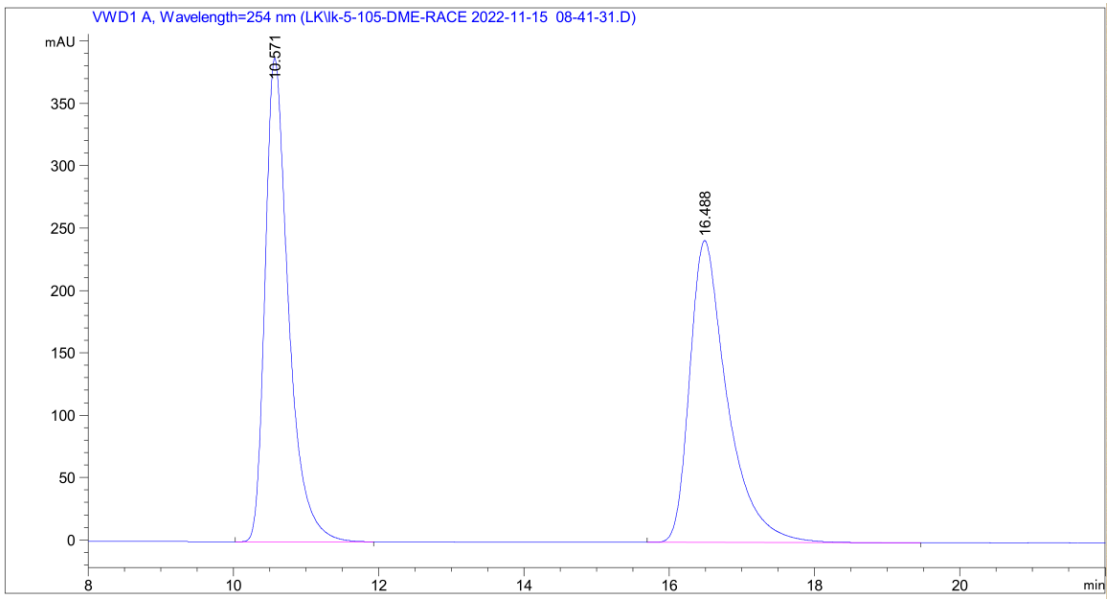
#	[min]	[min]	[mAU*s]	[mAU]	%
1	10.562	MM	0.3804	3871.99121	169.63054	49.9591
2	21.547	BB	0.7329	3878.33789	78.84607	50.0409

HPLC chromatogram of chiral 6ab



#	[min]	[min]	[mAU*s]	[mAU]	%
1	10.669	BB	0.3500	8109.33301	345.31799	97.0293
2	21.893	MM	0.9230	248.28287	4.48323	2.9707

HPLC chromatogram of racemic 6ac



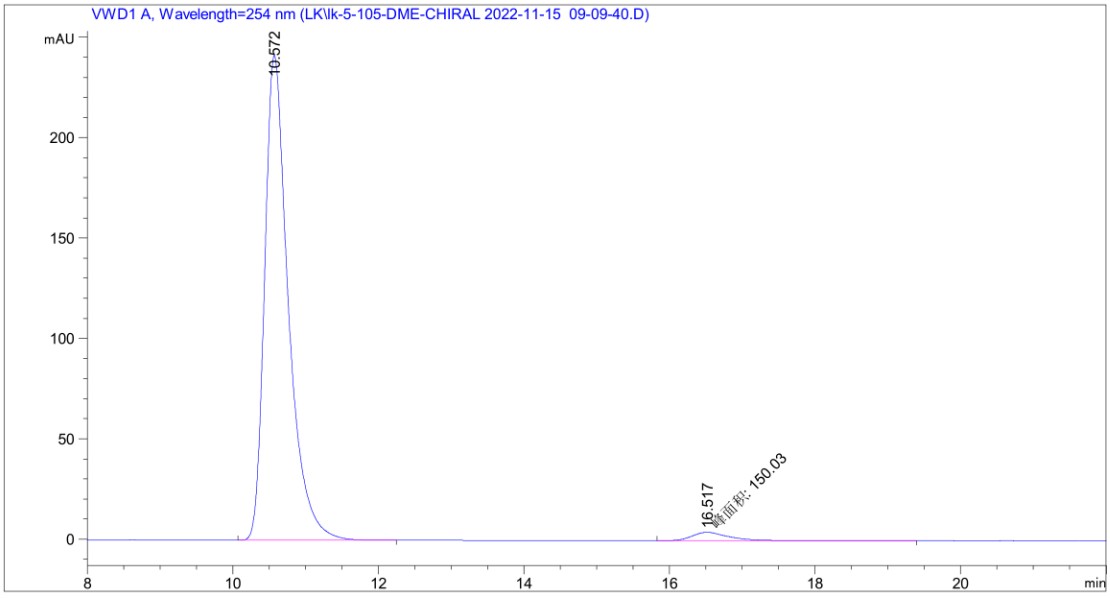
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 10.571 BB 0.3360 8675.61914 387.80081 49.9306

2 16.488 BB 0.5284 8699.72949 242.01027 50.0694

HPLC chromatogram of chiral 6ac



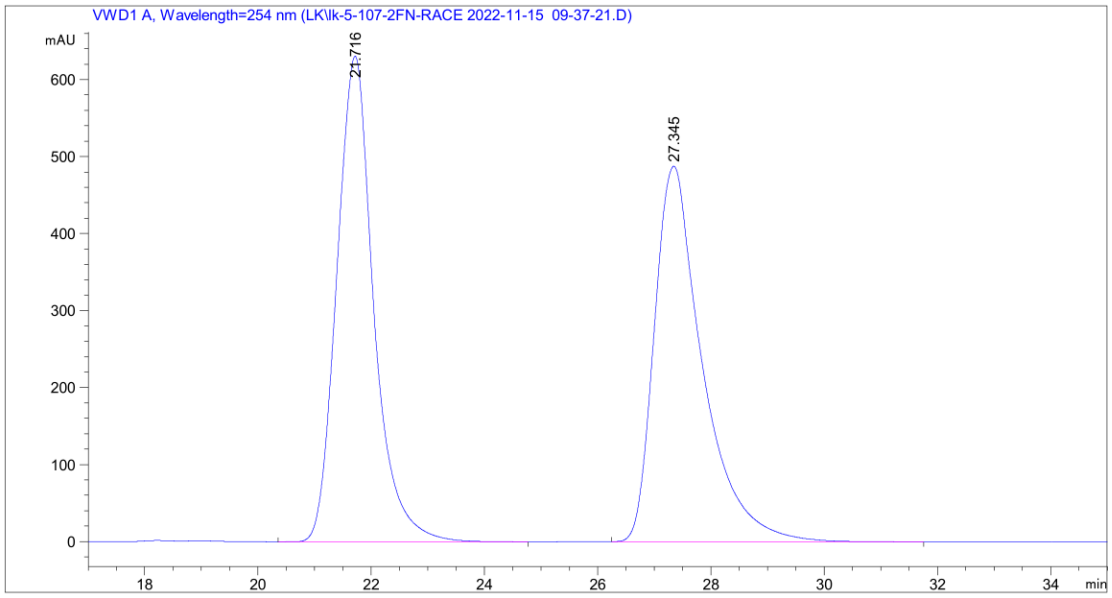
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 10.572 BB 0.3366 5458.12207 241.57108 97.3248

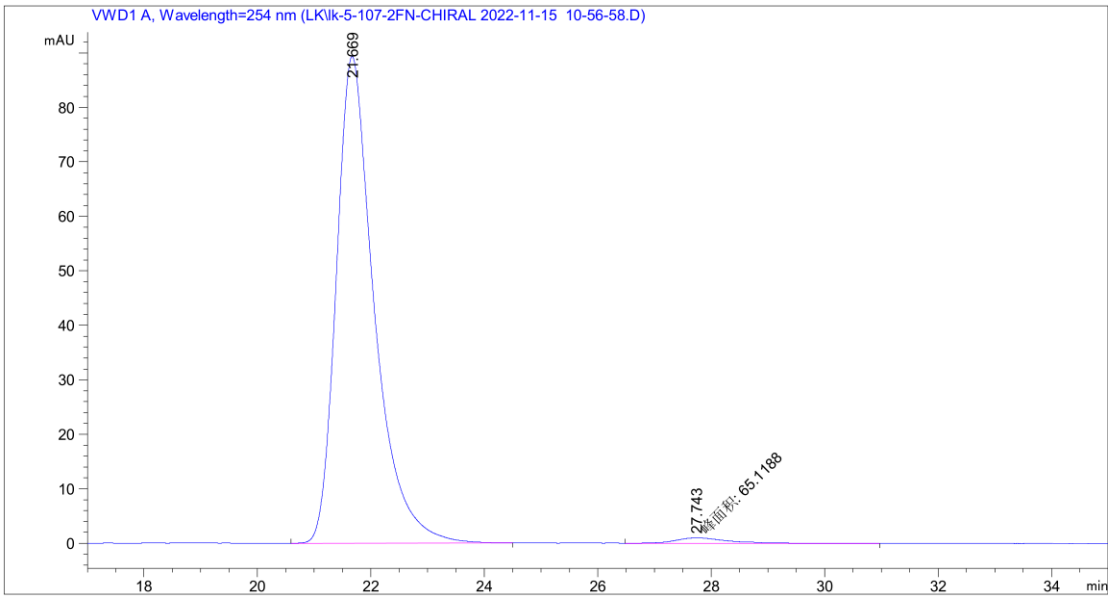
2 16.517 MM 0.5957 150.02959 4.19725 2.6752

HPLC chromatogram of racemic 6ad



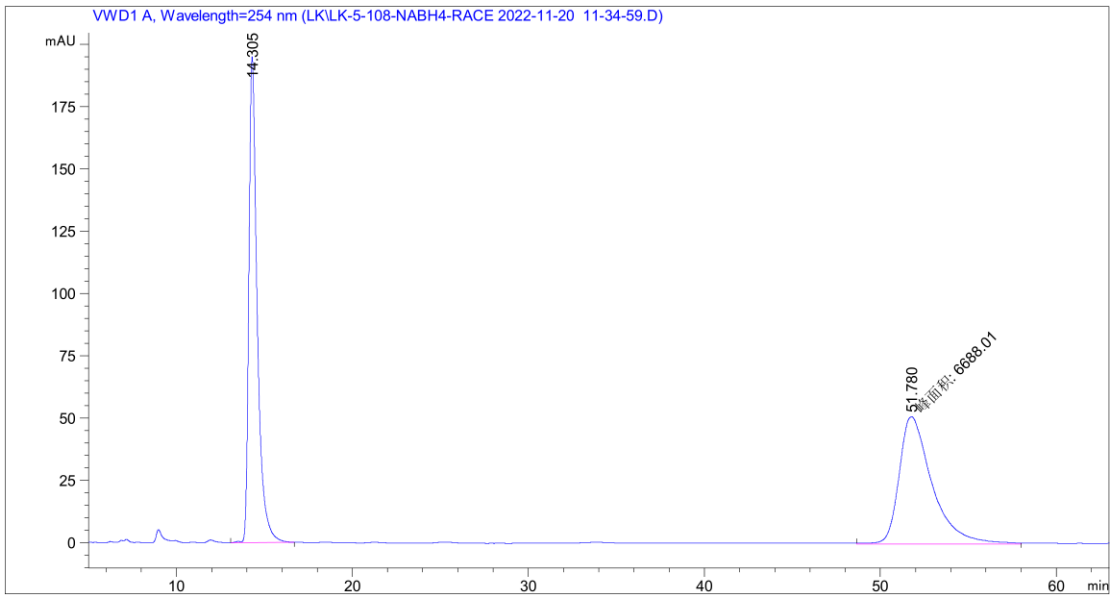
#	[min]		[min]	[mAU*s]	[mAU]	%
1	21.716	BB	0.6955	2.85825e4	630.91125	49.8678
2	27.345	BB	0.8564	2.87340e4	487.67487	50.1322

HPLC chromatogram of chiral 6ad



#	[min]		[min]	[mAU*s]	[mAU]	%
1	21.669	BB	0.6895	4154.13623	89.33522	98.4566
2	27.743	MM	1.0746	65.11877	1.00998	1.5434

HPLC chromatogram of racemic 7



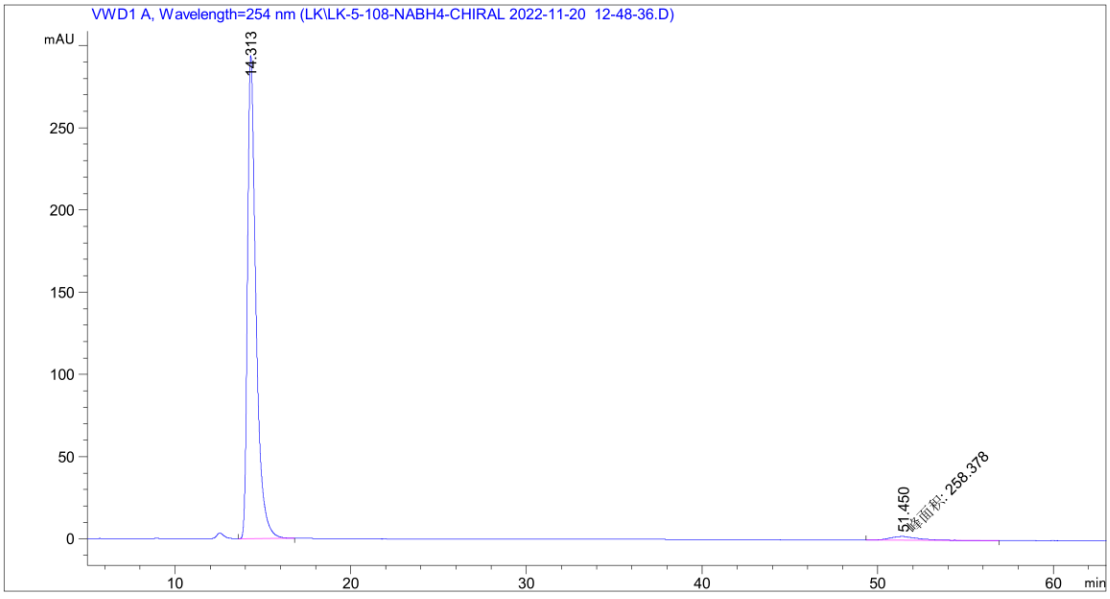
[min] [min] [mAU*s] [mAU] %

----|-------|----|-------|----------|----------|--------|

1 14.305 BB 0.4858 6426.32715 194.83614 49.0023

2 51.780 MM 2.1814 6688.00684 51.09893 50.9977

HPLC chromatogram of chiral 7



[min] [min] [mAU*s] [mAU] %

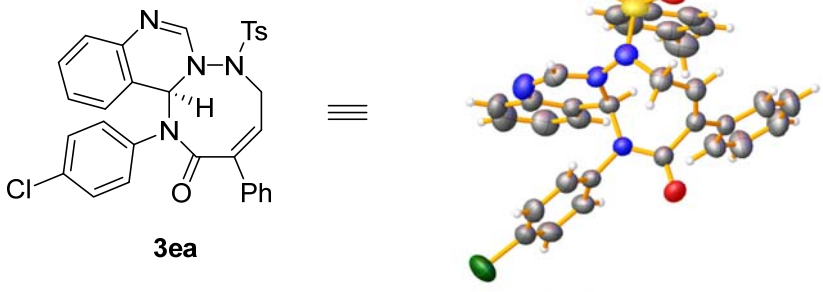
----|-------|----|-------|----------|----------|--------|

1 14.313 BB 0.4939 9851.08496 293.98166 97.4442

2 51.450 MM 1.9238 258.37796 2.23840 2.5558

X-Ray Crystallographic Data of 3ea, 6aa and 7

Crystallographic data for **3ea** have been deposited with the Cam-bridge Crystallographic Data Centre as deposition number 2208234. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.



3ea

Table S1. Crystal data and structure refinement for 3ea

Identification code	**3ea**
Empirical formula	$C_{31}H_{25}ClN_4O_3S$
Formula weight	569.06
Temperature	297.0 K
Wavelength	1.54178 Å
Crystal system	Monoclinic
Space group	P 1 21 1
Unit cell dimensions	a = 11.6897(6) Å α = 90°
	b = 8.7462(4) Å β = 97.984(3)°
	c = 27.9426(14) Å γ = 90°
Volume	2829.2(2) $Å^3$
Z	4
Density (calculated)	1.336 Mg/m^3
Absorption coefficient	2.208 mm^{-1}
F(000)	1184
Crystal size	0.19 x 0.12 x 0.1 mm^3
Theta range for data collection	3.194 to 68.397°.
Index ranges	-13<=h<=13, -10<=k<=9, -33<=l<=33
Reflections collected	71651
Independent reflections	9849 [R(int) = 0.0686]
Completeness to theta = 67.679°	98.9 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7362 and 0.5944
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	9849 / 1 / 723

Goodness-of-fit on F^2	1.118
Final R indices [I>2sigma(I)]	R1 = 0.0471, wR2 = 0.1158
R indices (all data)	R1 = 0.0620, wR2 = 0.1270
Absolute structure parameter	0.077(7)
Extinction coefficient	n/a
Largest diff. peak and hole	0.274 and -0.425 e.$Å^{-3}$

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for 3ea. U(eq) is defined as one third of the trace of the orthogonalized Uij tensor.

	x	y	z	U (eq)
S(01)	1814(1)	6120(2)	4804(1)	68(1)
S(02)	4987(1)	6834(1)	8175(1)	65(1)
Cl(03)	388(1)	2012(2)	10337(1)	96(1)
Cl(04)	-1476(1)	8051(2)	7739(1)	102(1)
N(005)	1917(3)	7732(4)	6358(1)	44(1)
O(006)	2989(3)	9790(4)	6638(1)	65(1)
O(007)	5670(3)	2601(5)	9904(1)	75(1)
N(008)	3774(3)	5318(4)	8708(1)	54(1)
N(009)	4332(3)	3231(4)	9269(1)	50(1)
N(00A)	1396(3)	7380(4)	5197(1)	55(1)
N(00B)	4648(3)	6426(4)	8724(1)	57(1)
O(00C)	813(4)	5225(5)	4641(1)	89(1)
N(00D)	996(3)	6678(4)	5589(1)	49(1)
O(00E)	3947(3)	7368(4)	7902(1)	82(1)
O(00F)	2363(3)	7019(5)	4476(1)	87(1)
C(00G)	2821(3)	8712(5)	6359(1)	47(1)
O(00H)	5974(4)	7795(5)	8266(1)	94(1)
C(00I)	3626(3)	8450(4)	5988(1)	46(1)
N(00J)	1763(4)	5020(5)	8535(2)	71(1)
C(00K)	1130(3)	7943(4)	6708(1)	45(1)
C(00L)	3048(4)	2820(5)	8503(1)	51(1)
C(00M)	3390(4)	2927(5)	9541(1)	51(1)
C(00N)	1752(3)	6376(4)	6040(1)	43(1)
C(00O)	3259(4)	8644(5)	5520(2)	52(1)
C(00P)	1237(4)	5056(5)	6282(1)	48(1)
C(00Q)	7293(4)	2590(6)	9138(2)	57(1)
N(00R)	-677(3)	5594(5)	5828(2)	66(1)
C(00S)	5442(4)	3116(5)	9498(2)	55(1)
C(00T)	4805(3)	7933(5)	6176(1)	46(1)
C(00U)	58(4)	4788(5)	6186(2)	56(1)

C(00V)	91(4)	8681(5)	6577(2)	54(1)
C(00W)	6397(4)	3706(6)	9237(1)	54(1)
C(00X)	4047(4)	3706(5)	8759(1)	48(1)
C(00Y)	1387(4)	7308(5)	7161(2)	54(1)
C(00Z)	-709(4)	8738(6)	6901(2)	62(1)
C(010)	2024(4)	8850(5)	5292(2)	58(1)
C(011)	2658(5)	5841(6)	8663(2)	66(1)
C(012)	-431(5)	3627(6)	6437(2)	69(1)
C(013)	5018(4)	7107(6)	6601(2)	60(1)
C(014)	4781(5)	4403(6)	5490(2)	66(1)
C(015)	6457(4)	5173(6)	9117(2)	59(1)
C(016)	1966(4)	3498(6)	8414(2)	59(1)
C(017)	-457(4)	8057(6)	7343(2)	62(1)
C(018)	3195(4)	1344(6)	8346(2)	62(1)
C(019)	2889(4)	4107(6)	9759(2)	61(1)
C(01A)	8446(4)	3018(7)	9173(2)	72(1)
C(01B)	593(4)	7346(6)	7481(2)	63(1)
C(01C)	1947(4)	3837(6)	9999(2)	69(1)
C(01D)	5566(4)	6364(6)	9153(2)	64(1)
C(01E)	2835(4)	4896(6)	5130(2)	62(1)
C(01F)	4408(5)	3191(6)	5753(2)	68(1)
C(01G)	-178(4)	6449(5)	5554(2)	59(1)
C(01H)	4487(5)	4262(6)	7645(2)	64(1)
C(01I)	5722(4)	8130(6)	5914(2)	64(1)
C(01J)	6988(4)	1139(6)	8965(2)	66(1)
C(01K)	2987(4)	1449(5)	9574(2)	58(1)
C(01L)	4005(5)	5271(6)	5184(2)	65(1)
C(01M)	1924(4)	4149(5)	6609(2)	57(1)
C(01N)	259(5)	2760(6)	6768(2)	78(2)
C(01O)	6969(4)	6623(7)	6474(2)	71(1)
C(01P)	6087(4)	6454(7)	6745(2)	72(1)
C(01Q)	5360(4)	5128(6)	7906(2)	60(1)
C(01R)	1445(5)	2999(6)	6851(2)	75(1)
C(01S)	1548(4)	2371(6)	10027(2)	63(1)
C(01T)	4744(6)	2860(7)	7459(2)	77(2)
C(01U)	9255(5)	2018(9)	9035(2)	83(2)
C(01V)	3245(5)	2819(6)	5679(2)	72(1)
C(01W)	1035(5)	2658(7)	8173(2)	75(2)
C(01X)	2054(4)	1167(6)	9817(2)	66(1)
C(01Y)	6483(5)	4605(8)	7964(2)	80(2)
C(01Z)	6780(4)	7467(7)	6061(2)	72(1)
C(020)	1208(5)	1191(8)	8029(2)	82(2)

C(021)	2273(5)	543(7)	8108(2)	77(2)
C(022)	2458(5)	3658(6)	5373(2)	69(1)
C(023)	6725(6)	3193(9)	7772(2)	93(2)
C(024)	5238(6)	2344(7)	6115(2)	91(2)
C(025)	7799(5)	165(7)	8827(2)	79(2)
C(026)	5853(7)	2298(8)	7526(2)	93(2)
C(027)	8936(5)	605(9)	8859(2)	87(2)
C(028)	6137(10)	752(10)	7338(3)	151(4)
S(01)	1814(1)	6120(2)	4804(1)	68(1)
S(02)	4987(1)	6834(1)	8175(1)	65(1)
Cl(03)	388(1)	2012(2)	10337(1)	96(1)
Cl(04)	-1476(1)	8051(2)	7739(1)	102(1)
N(005)	1917(3)	7732(4)	6358(1)	44(1)
O(006)	2989(3)	9790(4)	6638(1)	65(1)
O(007)	5670(3)	2601(5)	9904(1)	75(1)
N(008)	3774(3)	5318(4)	8708(1)	54(1)
N(009)	4332(3)	3231(4)	9269(1)	50(1)
N(00A)	1396(3)	7380(4)	5197(1)	55(1)
N(00B)	4648(3)	6426(4)	8724(1)	57(1)
O(00C)	813(4)	5225(5)	4641(1)	89(1)
N(00D)	996(3)	6678(4)	5589(1)	49(1)
O(00E)	3947(3)	7368(4)	7902(1)	82(1)
O(00F)	2363(3)	7019(5)	4476(1)	87(1)
C(00G)	2821(3)	8712(5)	6359(1)	47(1)
O(00H)	5974(4)	7795(5)	8266(1)	94(1)
C(00I)	3626(3)	8450(4)	5988(1)	46(1)
N(00J)	1763(4)	5020(5)	8535(2)	71(1)
C(00K)	1130(3)	7943(4)	6708(1)	45(1)
C(00L)	3048(4)	2820(5)	8503(1)	51(1)
C(00M)	3390(4)	2927(5)	9541(1)	51(1)
C(00N)	1752(3)	6376(4)	6040(1)	43(1)
C(00O)	3259(4)	8644(5)	5520(2)	52(1)
C(00P)	1237(4)	5056(5)	6282(1)	48(1)
C(00Q)	7293(4)	2590(6)	9138(2)	57(1)
N(00R)	-677(3)	5594(5)	5828(2)	66(1)
C(00S)	5442(4)	3116(5)	9498(2)	55(1)
C(00T)	4805(3)	7933(5)	6176(1)	46(1)
C(00U)	58(4)	4788(5)	6186(2)	56(1)
C(00V)	91(4)	8681(5)	6577(2)	54(1)
C(00W)	6397(4)	3706(6)	9237(1)	54(1)
C(00X)	4047(4)	3706(5)	8759(1)	48(1)
C(00Y)	1387(4)	7308(5)	7161(2)	54(1)

C(00Z)	-709(4)	8738(6)	6901(2)	62(1)
C(010)	2024(4)	8850(5)	5292(2)	58(1)
C(011)	2658(5)	5841(6)	8663(2)	66(1)
C(012)	-431(5)	3627(6)	6437(2)	69(1)
C(013)	5018(4)	7107(6)	6601(2)	60(1)
C(014)	4781(5)	4403(6)	5490(2)	66(1)
C(015)	6457(4)	5173(6)	9117(2)	59(1)
C(016)	1966(4)	3498(6)	8414(2)	59(1)
C(017)	-457(4)	8057(6)	7343(2)	62(1)
C(018)	3195(4)	1344(6)	8346(2)	62(1)
C(019)	2889(4)	4107(6)	9759(2)	61(1)
C(01A)	8446(4)	3018(7)	9173(2)	72(1)
C(01B)	593(4)	7346(6)	7481(2)	63(1)
C(01C)	1947(4)	3837(6)	9999(2)	69(1)
C(01D)	5566(4)	6364(6)	9153(2)	64(1)
C(01E)	2835(4)	4896(6)	5130(2)	62(1)
C(01F)	4408(5)	3191(6)	5753(2)	68(1)
C(01G)	-178(4)	6449(5)	5554(2)	59(1)
C(01H)	4487(5)	4262(6)	7645(2)	64(1)
C(01I)	5722(4)	8130(6)	5914(2)	64(1)
C(01J)	6988(4)	1139(6)	8965(2)	66(1)
C(01K)	2987(4)	1449(5)	9574(2)	58(1)
C(01L)	4005(5)	5271(6)	5184(2)	65(1)
C(01M)	1924(4)	4149(5)	6609(2)	57(1)
C(01N)	259(5)	2760(6)	6768(2)	78(2)
C(01O)	6969(4)	6623(7)	6474(2)	71(1)
C(01P)	6087(4)	6454(7)	6745(2)	72(1)
C(01Q)	5360(4)	5128(6)	7906(2)	60(1)
C(01R)	1445(5)	2999(6)	6851(2)	75(1)
C(01S)	1548(4)	2371(6)	10027(2)	63(1)
C(01T)	4744(6)	2860(7)	7459(2)	77(2)
C(01U)	9255(5)	2018(9)	9035(2)	83(2)
C(01V)	3245(5)	2819(6)	5679(2)	72(1)
C(01W)	1035(5)	2658(7)	8173(2)	75(2)
C(01X)	2054(4)	1167(6)	9817(2)	66(1)
C(01Y)	6483(5)	4605(8)	7964(2)	80(2)
C(01Z)	6780(4)	7467(7)	6061(2)	72(1)
C(020)	1208(5)	1191(8)	8029(2)	82(2)
C(021)	2273(5)	543(7)	8108(2)	77(2)
C(022)	2458(5)	3658(6)	5373(2)	69(1)
C(023)	6725(6)	3193(9)	7772(2)	93(2)
C(024)	5238(6)	2344(7)	6115(2)	91(2)

C(025)	7799(5)	165(7)	8827(2)	79(2)
C(026)	5853(7)	2298(8)	7526(2)	93(2)
C(027)	8936(5)	605(9)	8859(2)	87(2)
C(028)	6137(10)	752(10)	7338(3)	151(4)

Table S3. Bond lengths [Å] and angles [°] for 3ea

S(01)-N(00A)	1.675(4)
S(01)-O(00C)	1.429(4)
S(01)-O(00F)	1.426(4)
S(01)-C(01E)	1.760(5)
S(02)-N(00B)	1.676(4)
S(02)-O(00E)	1.422(4)
S(02)-O(00H)	1.421(4)
S(02)-C(01Q)	1.753(5)
Cl(03)-C(01S)	1.736(5)
Cl(04)-C(017)	1.734(4)
N(005)-C(00G)	1.360(5)
N(005)-C(00K)	1.443(5)
N(005)-C(00N)	1.478(5)
O(006)-C(00G)	1.223(5)
O(007)-C(00S)	1.216(5)
N(008)-N(00B)	1.404(5)
N(008)-C(00X)	1.448(6)
N(008)-C(011)	1.372(6)
N(009)-C(00M)	1.446(5)
N(009)-C(00S)	1.369(5)
N(009)-C(00X)	1.477(5)
N(00A)-N(00D)	1.393(5)
N(00A)-C(010)	1.486(6)
N(00B)-C(01D)	1.494(6)
N(00D)-C(00N)	1.460(5)
N(00D)-C(01G)	1.377(5)
C(00G)-C(00I)	1.511(5)
C(00I)-C(00O)	1.329(6)
C(00I)-C(00T)	1.477(6)
N(00J)-C(011)	1.278(6)
N(00J)-C(016)	1.402(7)
C(00K)-C(00V)	1.380(6)
C(00K)-C(00Y)	1.377(6)
C(00L)-C(00X)	1.499(6)
C(00L)-C(016)	1.388(6)

C(00L)-C(018)	1.382(7)
C(00M)-C(019)	1.371(6)
C(00M)-C(01K)	1.384(7)
C(00N)-C(00P)	1.504(6)
C(00O)-C(010)	1.506(6)
C(00P)-C(00U)	1.387(6)
C(00P)-C(01M)	1.381(6)
C(00Q)-C(00W)	1.485(6)
C(00Q)-C(01A)	1.390(6)
C(00Q)-C(01J)	1.387(7)
N(00R)-C(00U)	1.412(6)
N(00R)-C(01G)	1.269(6)
C(00S)-C(00W)	1.507(6)
C(00T)-C(013)	1.382(6)
C(00T)-C(01I)	1.390(6)
C(00U)-C(012)	1.400(7)
C(00V)-C(00Z)	1.390(6)
C(00W)-C(015)	1.330(7)
C(00Y)-C(01B)	1.375(6)
C(00Z)-C(017)	1.367(7)
C(012)-C(01N)	1.370(8)
C(013)-C(01P)	1.382(7)
C(014)-C(01F)	1.394(7)
C(014)-C(01L)	1.383(7)
C(015)-C(01D)	1.487(7)
C(016)-C(01W)	1.405(7)
C(017)-C(01B)	1.383(7)
C(018)-C(021)	1.377(7)
C(019)-C(01C)	1.387(7)
C(01A)-C(01U)	1.381(8)
C(01C)-C(01S)	1.371(7)
C(01E)-C(01L)	1.394(7)
C(01E)-C(022)	1.383(7)
C(01F)-C(01V)	1.385(8)
C(01F)-C(024)	1.497(7)
C(01H)-C(01Q)	1.393(7)
C(01H)-C(01T)	1.381(8)
C(01I)-C(01Z)	1.375(7)
C(01J)-C(025)	1.369(7)
C(01K)-C(01X)	1.384(6)
C(01M)-C(01R)	1.373(7)
C(01N)-C(01R)	1.389(8)

C(01O)-C(01P)	1.369(7)
C(01O)-C(01Z)	1.364(7)
C(01Q)-C(01Y)	1.378(7)
C(01S)-C(01X)	1.378(7)
C(01T)-C(026)	1.375(9)
C(01U)-C(027)	1.363(10)
C(01V)-C(022)	1.377(7)
C(01W)-C(020)	1.368(9)
C(01Y)-C(023)	1.390(9)
C(020)-C(021)	1.358(8)
C(023)-C(026)	1.389(10)
C(025)-C(027)	1.374(8)
C(026)-C(028)	1.504(11)
N(00A)-S(01)-C(01E)	107.46(18)
O(00C)-S(01)-N(00A)	105.6(2)
O(00C)-S(01)-C(01E)	107.4(3)
O(00F)-S(01)-N(00A)	104.9(2)
O(00F)-S(01)-O(00C)	121.2(2)
O(00F)-S(01)-C(01E)	109.6(2)
N(00B)-S(02)-C(01Q)	108.45(19)
O(00E)-S(02)-N(00B)	105.6(2)
O(00E)-S(02)-C(01Q)	107.1(2)
O(00H)-S(02)-N(00B)	104.5(2)
O(00H)-S(02)-O(00E)	120.9(3)
O(00H)-S(02)-C(01Q)	109.7(3)
C(00G)-N(005)-C(00K)	119.1(3)
C(00G)-N(005)-C(00N)	122.9(3)
C(00K)-N(005)-C(00N)	117.8(3)
N(00B)-N(008)-C(00X)	121.3(3)
C(011)-N(008)-N(00B)	116.8(4)
C(011)-N(008)-C(00X)	121.9(4)
C(00M)-N(009)-C(00X)	118.2(3)
C(00S)-N(009)-C(00M)	118.8(3)
C(00S)-N(009)-C(00X)	122.9(3)
N(00D)-N(00A)-S(01)	112.7(3)
N(00D)-N(00A)-C(010)	116.8(3)
C(010)-N(00A)-S(01)	120.4(3)
N(008)-N(00B)-S(02)	112.3(3)
N(008)-N(00B)-C(01D)	116.1(3)
C(01D)-N(00B)-S(02)	120.4(3)
N(00A)-N(00D)-C(00N)	122.1(3)

C(01G)-N(00D)-N(00A)	116.7(3)
C(01G)-N(00D)-C(00N)	120.8(3)
N(005)-C(00G)-C(00I)	117.5(3)
O(006)-C(00G)-N(005)	122.9(4)
O(006)-C(00G)-C(00I)	119.6(4)
C(00O)-C(00I)-C(00G)	120.5(4)
C(00O)-C(00I)-C(00T)	123.2(4)
C(00T)-C(00I)-C(00G)	116.3(3)
C(011)-N(00J)-C(016)	116.2(4)
C(00V)-C(00K)-N(005)	120.0(4)
C(00Y)-C(00K)-N(005)	119.5(3)
C(00Y)-C(00K)-C(00V)	120.3(4)
C(016)-C(00L)-C(00X)	119.7(4)
C(018)-C(00L)-C(00X)	120.8(4)
C(018)-C(00L)-C(016)	119.6(4)
C(019)-C(00M)-N(009)	119.9(4)
C(019)-C(00M)-C(01K)	120.2(4)
C(01K)-C(00M)-N(009)	119.9(4)
N(005)-C(00N)-C(00P)	111.9(3)
N(00D)-C(00N)-N(005)	112.8(3)
N(00D)-C(00N)-C(00P)	107.1(3)
C(00I)-C(00O)-C(010)	126.2(4)
C(00U)-C(00P)-C(00N)	119.4(4)
C(01M)-C(00P)-C(00N)	120.4(4)
C(01M)-C(00P)-C(00U)	120.1(4)
C(01A)-C(00Q)-C(00W)	120.8(5)
C(01J)-C(00Q)-C(00W)	120.9(4)
C(01J)-C(00Q)-C(01A)	118.0(5)
C(01G)-N(00R)-C(00U)	115.8(4)
O(007)-C(00S)-N(009)	122.3(4)
O(007)-C(00S)-C(00W)	119.8(4)
N(009)-C(00S)-C(00W)	117.8(3)
C(013)-C(00T)-C(00I)	120.9(4)
C(013)-C(00T)-C(01I)	117.2(4)
C(01I)-C(00T)-C(00I)	121.6(4)
C(00P)-C(00U)-N(00R)	122.9(4)
C(00P)-C(00U)-C(012)	119.3(5)
C(012)-C(00U)-N(00R)	117.8(4)
C(00K)-C(00V)-C(00Z)	119.4(4)
C(00Q)-C(00W)-C(00S)	117.0(4)
C(015)-C(00W)-C(00Q)	121.6(4)
C(015)-C(00W)-C(00S)	121.4(4)

N(008)-C(00X)-N(009)	112.7(3)
N(008)-C(00X)-C(00L)	108.0(4)
N(009)-C(00X)-C(00L)	111.8(3)
C(01B)-C(00Y)-C(00K)	120.5(4)
C(017)-C(00Z)-C(00V)	119.6(4)
N(00A)-C(010)-C(00O)	113.1(4)
N(00J)-C(011)-N(008)	124.7(5)
C(01N)-C(012)-C(00U)	119.8(5)
C(00T)-C(013)-C(01P)	121.0(4)
C(01L)-C(014)-C(01F)	121.1(5)
C(00W)-C(015)-C(01D)	126.6(5)
N(00J)-C(016)-C(01W)	117.8(5)
C(00L)-C(016)-N(00J)	122.9(4)
C(00L)-C(016)-C(01W)	119.2(5)
C(00Z)-C(017)-Cl(04)	119.8(4)
C(00Z)-C(017)-C(01B)	121.3(4)
C(01B)-C(017)-Cl(04)	118.9(4)
C(021)-C(018)-C(00L)	120.3(5)
C(00M)-C(019)-C(01C)	120.3(5)
C(01U)-C(01A)-C(00Q)	120.4(6)
C(00Y)-C(01B)-C(017)	118.9(5)
C(01S)-C(01C)-C(019)	119.1(5)
C(015)-C(01D)-N(00B)	113.8(4)
C(01L)-C(01E)-S(01)	119.8(4)
C(022)-C(01E)-S(01)	119.4(4)
C(022)-C(01E)-C(01L)	120.4(5)
C(014)-C(01F)-C(024)	120.8(6)
C(01V)-C(01F)-C(014)	118.1(5)
C(01V)-C(01F)-C(024)	121.0(5)
N(00R)-C(01G)-N(00D)	125.5(4)
C(01T)-C(01H)-C(01Q)	119.9(5)
C(01Z)-C(01I)-C(00T)	121.2(4)
C(025)-C(01J)-C(00Q)	120.9(5)
C(00M)-C(01K)-C(01X)	119.9(5)
C(014)-C(01L)-C(01E)	119.1(5)
C(01R)-C(01M)-C(00P)	120.5(5)
C(012)-C(01N)-C(01R)	120.6(5)
C(01Z)-C(01O)-C(01P)	118.8(5)
C(01O)-C(01P)-C(013)	120.9(4)
C(01H)-C(01Q)-S(02)	118.7(4)
C(01Y)-C(01Q)-S(02)	121.5(4)
C(01Y)-C(01Q)-C(01H)	119.8(5)

C(01M)-C(01R)-C(01N)	119.6(5)
C(01C)-C(01S)-Cl(03)	119.5(4)
C(01C)-C(01S)-C(01X)	121.4(4)
C(01X)-C(01S)-Cl(03)	119.1(4)
C(026)-C(01T)-C(01H)	121.1(6)
C(027)-C(01U)-C(01A)	120.7(5)
C(022)-C(01V)-C(01F)	121.7(5)
C(020)-C(01W)-C(016)	119.7(5)
C(01S)-C(01X)-C(01K)	119.1(5)
C(01Q)-C(01Y)-C(023)	119.4(6)
C(01O)-C(01Z)-C(01I)	120.9(4)
C(021)-C(020)-C(01W)	120.9(5)
C(020)-C(021)-C(018)	120.3(6)
C(01V)-C(022)-C(01E)	119.4(5)
C(026)-C(023)-C(01Y)	121.1(6)
C(01J)-C(025)-C(027)	120.6(6)
C(01T)-C(026)-C(023)	118.6(6)
C(01T)-C(026)-C(028)	121.6(8)
C(023)-C(026)-C(028)	119.8(8)
C(01U)-C(027)-C(025)	119.4(6)

Table S4. Anisotropic displacement parameters ($Å^2x10^3$) for 3ea. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2}U_{11} + ... + 2 h k a^* b^* U_{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
S(01)	79(1)	82(1)	40(1)	-4(1)	-2(1)	6(1)
S(02)	82(1)	56(1)	55(1)	11(1)	1(1)	-13(1)
Cl(03)	70(1)	127(1)	96(1)	15(1)	34(1)	-4(1)
Cl(04)	84(1)	141(1)	90(1)	-19(1)	46(1)	-4(1)
N(005)	43(2)	44(2)	47(2)	-7(1)	7(1)	0(1)
O(006)	62(2)	56(2)	80(2)	-24(2)	16(2)	-10(2)
O(007)	67(2)	108(3)	48(2)	25(2)	7(2)	5(2)
N(008)	57(2)	49(2)	53(2)	1(2)	4(2)	-1(2)
N(009)	50(2)	62(2)	39(2)	6(2)	6(2)	-2(2)
N(00A)	58(2)	60(2)	44(2)	6(2)	-3(2)	3(2)
N(00B)	68(2)	52(2)	49(2)	-1(2)	-2(2)	-8(2)
O(00C)	94(3)	105(3)	60(2)	-27(2)	-18(2)	-9(2)
N(00D)	45(2)	54(2)	46(2)	1(2)	-3(1)	2(2)
O(00E)	101(3)	71(2)	67(2)	18(2)	-8(2)	16(2)
O(00F)	103(3)	112(3)	47(2)	18(2)	12(2)	18(2)
C(00G)	44(2)	45(2)	50(2)	-4(2)	5(2)	-1(2)
O(00H)	111(3)	83(3)	86(3)	12(2)	3(2)	-51(2)

C(00I)	43(2)	44(2)	49(2)	0(2)	5(2)	-1(2)
N(00J)	56(3)	81(3)	74(3)	5(2)	7(2)	3(2)
C(00K)	41(2)	46(2)	48(2)	-12(2)	7(2)	2(2)
C(00L)	54(3)	58(3)	40(2)	6(2)	4(2)	-8(2)
C(00M)	53(2)	59(3)	39(2)	7(2)	3(2)	-2(2)
C(00N)	43(2)	47(2)	39(2)	-5(2)	3(2)	4(2)
C(00O)	50(2)	52(2)	53(2)	7(2)	6(2)	0(2)
C(00P)	51(3)	44(2)	47(2)	-7(2)	6(2)	1(2)
C(00Q)	53(3)	75(3)	42(2)	3(2)	1(2)	-3(2)
N(00R)	50(2)	67(2)	78(3)	0(2)	1(2)	-2(2)
C(00S)	54(3)	65(3)	43(2)	4(2)	3(2)	0(2)
C(00T)	41(2)	50(2)	46(2)	-1(2)	6(2)	-6(2)
C(00U)	54(3)	51(2)	63(3)	-8(2)	5(2)	-6(2)
C(00V)	51(3)	48(2)	63(3)	-5(2)	7(2)	3(2)
C(00W)	51(3)	71(3)	39(2)	5(2)	1(2)	-6(2)
C(00X)	56(3)	48(2)	39(2)	4(2)	6(2)	-4(2)
C(00Y)	51(2)	64(3)	47(2)	-9(2)	4(2)	6(2)
C(00Z)	42(2)	64(3)	80(3)	-14(2)	12(2)	5(2)
C(010)	59(3)	58(3)	56(3)	14(2)	-2(2)	3(2)
C(011)	72(4)	64(3)	60(3)	0(2)	6(2)	12(3)
C(012)	64(3)	61(3)	82(3)	-7(3)	14(3)	-19(2)
C(013)	53(3)	76(3)	50(2)	9(2)	8(2)	2(2)
C(014)	77(3)	67(3)	56(3)	-10(2)	16(2)	11(3)
C(015)	61(3)	73(3)	41(2)	4(2)	-2(2)	-13(2)
C(016)	58(3)	65(3)	52(2)	5(2)	7(2)	-5(2)
C(017)	52(3)	70(3)	67(3)	-22(2)	18(2)	-6(2)
C(018)	70(3)	61(3)	55(2)	0(2)	5(2)	-11(2)
C(019)	74(3)	59(3)	54(3)	-3(2)	19(2)	-5(2)
C(01A)	51(3)	107(4)	59(3)	-13(3)	5(2)	-18(3)
C(01B)	75(3)	69(3)	48(2)	-8(2)	13(2)	-1(2)
C(01C)	71(3)	77(3)	60(3)	1(2)	16(2)	7(3)
C(01D)	80(3)	62(3)	47(2)	-6(2)	0(2)	-16(2)
C(01E)	73(3)	65(3)	48(2)	-14(2)	9(2)	7(2)
C(01F)	97(4)	53(3)	54(3)	-8(2)	13(3)	18(3)
C(01G)	51(3)	57(3)	64(3)	-6(2)	-8(2)	7(2)
C(01H)	75(3)	73(3)	45(2)	7(2)	10(2)	-1(3)
C(01I)	52(3)	83(3)	61(3)	19(2)	16(2)	2(2)
C(01J)	54(3)	78(3)	67(3)	-1(3)	11(2)	-6(2)
C(01K)	64(3)	60(3)	52(2)	6(2)	11(2)	-1(2)
C(01L)	91(4)	60(3)	45(2)	-4(2)	19(2)	11(3)
C(01M)	66(3)	54(3)	52(2)	1(2)	7(2)	4(2)
C(01N)	95(4)	54(3)	88(4)	10(3)	21(3)	-14(3)

C(01O)	46(3)	86(4)	79(3)	7(3)	0(2)	3(2)
C(01P)	58(3)	97(4)	60(3)	23(3)	3(2)	3(3)
C(01Q)	68(3)	71(3)	41(2)	16(2)	5(2)	-2(2)
C(01R)	97(4)	57(3)	71(3)	13(2)	14(3)	8(3)
C(01S)	51(3)	87(4)	51(3)	9(2)	8(2)	1(2)
C(01T)	108(5)	71(3)	52(3)	2(2)	14(3)	-1(3)
C(01U)	53(3)	128(5)	70(3)	-11(4)	9(3)	-6(3)
C(01V)	103(4)	48(3)	67(3)	-5(2)	17(3)	6(3)
C(01W)	57(3)	96(4)	71(3)	10(3)	3(2)	-12(3)
C(01X)	65(3)	76(3)	58(3)	13(2)	9(2)	-9(3)
C(01Y)	69(4)	118(5)	53(3)	19(3)	3(3)	1(3)
C(01Z)	46(3)	96(4)	77(3)	11(3)	16(2)	3(3)
C(020)	74(4)	92(4)	77(3)	2(3)	-2(3)	-31(3)
C(021)	89(4)	69(3)	72(3)	-8(3)	3(3)	-21(3)
C(022)	87(4)	59(3)	61(3)	-17(2)	12(3)	-1(3)
C(023)	90(4)	127(6)	64(3)	15(4)	11(3)	43(4)
C(024)	112(5)	87(4)	73(4)	4(3)	7(3)	37(3)
C(025)	77(4)	82(4)	77(3)	-11(3)	11(3)	-1(3)
C(026)	132(6)	94(4)	54(3)	15(3)	16(4)	39(4)
C(027)	66(4)	123(5)	74(4)	-13(4)	14(3)	12(3)
C(028)	255(11)	105(6)	97(5)	16(4)	38(6)	79(7)

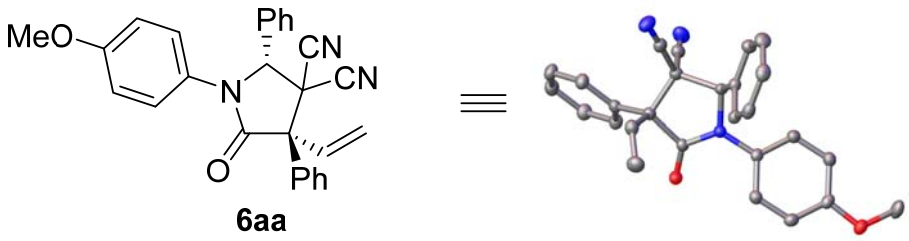
Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 3ea.

	x	y	z	U(eq)
H(00N)	2508	6060	5962	52
H(00O)	3819	8654	5314	62
H(00V)	-73	9137	6274	65
H(00X)	4722	3505	8596	57
H(00Y)	2102	6850	7252	65
H(00Z)	-1411	9237	6817	74
H(01A)	1623	9469	5504	70
H(01B)	2012	9399	4990	70
H(011)	2545	6867	8731	79
H(012)	-1222	3445	6379	83
H(013)	4434	6988	6792	72
H(014)	5564	4633	5521	79
H(015)	7125	5485	8998	71
H(018)	3921	889	8401	75

H(019)	3181	5093	9746	73
H(01D)	8675	3982	9289	87
H(01C)	760	6901	7785	76
H(01E)	1591	4640	10139	82
H(01F)	5942	7354	9192	77
H(01H)	5206	6171	9440	77
H(01G)	-644	6966	5309	71
H(01J)	3733	4627	7596	77
H(01I)	5618	8721	5635	77
H(01K)	6223	823	8942	79
H(01Q)	3341	646	9433	70
H(01L)	4261	6094	5017	77
H(01M)	2716	4318	6666	69
H(01N)	-69	2005	6940	94
H(01O)	7684	6171	6571	85
H(01P)	6209	5892	7030	86
H(01R)	1912	2383	7068	90
H(01T)	4157	2286	7286	92
H(01U)	10026	2313	9062	100
H(01V)	2990	1981	5839	86
H(01W)	305	3097	8111	90
H(01X)	1774	178	9839	80
H(01Y)	7073	5191	8130	96
H(01Z)	7374	7597	5875	87
H(020)	587	630	7875	98
H(021)	2380	-447	8001	93
H(022)	1680	3395	5331	82
H(023)	7483	2842	7810	112
H(02A)	5957	2211	5991	137
H(02B)	4922	1361	6176	137
H(02C)	5368	2916	6411	137
H(025)	7579	-802	8710	95
H(027)	9482	-56	8761	105
H(02D)	5521	52	7372	227
H(02E)	6841	383	7519	227
H(02F)	6231	834	7003	227

X-Ray Crystallographic Data of 6aa

Crystallographic data for **6aa** have been deposited with the Cam-bridge Crystallographic Data Centre as deposition number 2219264. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.



6aa

Table S6. Crystal data and structure refinement for 6aa.

Identification code	**6aa**
Empirical formula	$C_{27}H_{21}N_3O_2$
Formula weight	419.47
Temperature/K	100.01(10)
Crystal system	monoclinic
Space group	$P2_1$
a/Å	8.30066(14)
b/Å	8.18447(13)
c/Å	16.4485(3)
α/°	90
β/°	104.3873(18)
γ/°	90
Volume/Å^3	1082.41(3)
Z	2
ρ_{calc}g/cm^3	1.287
μ/mm^{-1}	0.659
F(000)	440.0
Crystal size/mm^3	0.15 × 0.08 × 0.08
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.546 to 153.332
Index ranges	-10≤h≤9, -9≤k≤10, -20≤l≤20
Reflections collected	20288
Independent reflections	4370 [R_{int} = 0.0414, R_{sigma} = 0.0282]
Data/restraints/parameters	4370/1/290
Goodness-of-fit on F^2	1.090
Final R indexes [I>=2σ (I)]	R_1 = 0.0327, wR_2 = 0.0856
Final R indexes [all data]	R_1 = 0.0338, wR_2 = 0.0864
Largest diff. peak/hole / e Å^{-3}	0.13/-0.20
Flack parameter	-0.12(10)

Table S7. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 6aa. Ueq is defined as 1/3 of the trace of the orthogonalised UIJ tensor.

Atom	x	y	z	U(eq)
O24	3969.0(18)	2883.9(18)	3739.0(9)	25.0(3)
O31	1788.9(18)	9428.3(19)	5104.2(9)	27.4(3)
N7	3787(2)	5154(2)	2898.4(10)	20.2(3)
N26	4298(2)	3689(3)	226.4(12)	33.5(4)
N28	8232(2)	4574(2)	2407.5(14)	34.4(5)
C12	2690(2)	6369(2)	1469.8(12)	21.1(4)
C17	1045(2)	6068(3)	1483.6(13)	22.7(4)
C4	2292(2)	8473(3)	4530.5(12)	22.3(4)
C23	6817(3)	1115(3)	3328.9(13)	24.9(4)
C8	4074(2)	3542(2)	3087.9(12)	19.7(4)
C13	3023(3)	7359(3)	841.1(13)	25.2(4)
C11	4158(2)	5698(2)	2122.0(12)	20.2(4)
C6	3828(3)	7883(3)	3507.2(13)	24.3(4)
C10	5012(2)	4123(3)	1852.9(12)	21.2(4)
C5	3359(3)	8985(3)	4052.1(13)	25.2(4)
C27	6836(2)	4345(3)	2156.9(13)	24.4(4)
C18	5783(2)	1335(2)	2532.0(13)	21.6(4)
C1	3240(2)	6298(2)	3435.5(12)	20.2(4)
C21	8331(3)	-994(3)	2805.9(14)	29.4(5)
C3	1652(3)	6898(3)	4435.2(13)	24.0(4)
C9	4426(2)	2650(2)	2330.7(12)	21.0(4)
C19	6046(3)	383(3)	1871.7(13)	26.3(4)
C29	2801(3)	1915(3)	1818.4(14)	24.8(4)
C2	2105(2)	5805(3)	3888.4(12)	22.3(4)
C25	4616(2)	3899(3)	936.0(13)	24.5(4)
C16	-234(3)	6771(3)	879.9(14)	26.1(4)
C14	1737(3)	8046(3)	234.5(14)	30.8(5)
C22	8076(3)	-53(3)	3462.4(14)	28.0(5)
C20	7314(3)	-769(3)	2010.1(14)	29.4(5)
C15	106(3)	7771(3)	259.8(13)	30.2(5)
C30	1431(3)	1701(3)	2069.9(16)	33.7(5)
C32	2566(3)	10983(3)	5278.0(16)	33.8(5)

Table S8. Anisotropic Displacement Parameters ($Å^2×10^3$) for 6aa. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
O24	31.6(8)	20.6(7)	25.0(7)	2.8(6)	10.9(6)	3.8(6)
O31	31.1(7)	26.3(8)	26.8(8)	-4.8(6)	10.6(6)	2.1(6)
N7	22.3(8)	18.6(8)	20.5(8)	1.2(6)	6.9(6)	0.6(6)
N26	37.5(10)	38.2(11)	26.2(10)	0.6(8)	10.4(8)	9.7(9)
N28	25.7(9)	30.9(10)	48.0(12)	4.3(9)	11.8(8)	-0.8(8)
C12	22.3(9)	19.0(9)	22.3(9)	-0.7(8)	6.3(8)	0.5(8)
C17	24.0(10)	21.3(10)	24.1(10)	-2.5(8)	8.2(8)	-0.2(8)
C4	22.1(9)	24.6(10)	19.1(9)	-1.4(8)	3.0(7)	5.7(8)
C23	25.4(10)	23.9(11)	25.1(10)	-1.4(8)	5.5(8)	1.7(8)
C8	18.9(9)	18.0(9)	22.4(9)	1.1(8)	5.3(7)	0.9(7)
C13	25.1(10)	25.6(10)	25.6(10)	3.6(8)	7.6(8)	1.3(8)
C11	20.5(9)	20.7(10)	21.3(9)	0.4(8)	9.1(7)	-1.5(7)
C6	27.1(10)	21.7(10)	26.0(10)	1.5(9)	10.3(8)	0.4(8)
C10	19.7(9)	22.3(10)	22.0(9)	1.7(8)	5.8(7)	1.4(8)
C5	27.8(10)	20.0(10)	28.2(10)	-0.6(8)	8.0(8)	-0.5(8)
C27	24.3(10)	22.6(10)	27.8(10)	3.4(8)	9.3(8)	1.8(8)
C18	21.3(9)	17.7(9)	26.5(10)	0.0(8)	7.4(8)	-1.2(7)
C1	21.1(9)	20.2(9)	18.8(9)	0.7(8)	3.9(7)	2.4(8)
C21	27.2(10)	24.7(11)	35.7(12)	1.4(9)	6.6(9)	5.0(9)
C3	23.3(10)	27.6(10)	22.3(10)	1.4(8)	7.8(8)	1.4(8)
C9	20.1(9)	20.2(10)	22.8(9)	1.1(8)	5.4(8)	0.4(8)
C19	28.0(10)	25.1(11)	24.8(10)	-2.1(8)	4.5(8)	2.0(9)
C29	23.5(10)	22.6(10)	27.2(10)	-0.7(8)	4.1(8)	0.5(8)
C2	22.3(10)	20.4(10)	24.0(10)	0.3(8)	5.3(8)	-0.6(8)
C25	25.2(9)	22.6(10)	27.0(11)	1.4(8)	9.0(8)	4.8(8)
C16	21.3(10)	25.3(11)	30.5(11)	-6.3(9)	4.3(8)	3.2(8)
C14	36.3(12)	29.9(12)	25.5(10)	7.2(9)	6.5(9)	4.4(9)
C22	25.7(10)	28.1(11)	28.2(11)	1.1(9)	2.8(8)	4.0(9)
C20	32.3(11)	26.7(11)	29.7(11)	-5.2(9)	9.0(9)	5.7(9)
C15	29.5(11)	29.4(11)	27.6(11)	0.2(9)	-0.5(9)	7.1(9)
C30	27.8(11)	37.3(13)	35.8(12)	-1.8(10)	7.7(9)	-6.5(10)
C32	31.8(11)	30.3(12)	40.3(13)	-15.5(10)	10.5(9)	-1.6(10)

Table S9. Bond Lengths for 6aa.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O24	C8	1.221(2)		C11	C10	1.586(3)
O31	C4	1.368(2)		C6	C5	1.393(3)
O31	C32	1.423(3)		C6	C1	1.381(3)
N7	C8	1.363(3)		C10	C27	1.483(3)
N7	C11	1.456(2)		C10	C9	1.581(3)
N7	C1	1.436(2)		C10	C25	1.473(3)
N26	C25	1.144(3)		C18	C9	1.533(3)
N28	C27	1.144(3)		C18	C19	1.397(3)
C12	C17	1.393(3)		C1	C2	1.398(3)
C12	C13	1.394(3)		C21	C22	1.385(3)
C12	C11	1.512(3)		C21	C20	1.382(3)
C17	C16	1.386(3)		C3	C2	1.385(3)
C4	C5	1.388(3)		C9	C29	1.526(3)
C4	C3	1.388(3)		C19	C20	1.389(3)
C23	C18	1.389(3)		C29	C30	1.315(3)
C23	C22	1.393(3)		C16	C15	1.390(3)
C8	C9	1.533(3)		C14	C15	1.384(3)
C13	C14	1.386(3)				

Table S10. Bond Angles for 6aa.

Atom	Atom	Atom	Angle/°		Atom	Atom	Atom	Angle/°
C4	O31	C32	116.67(16)		C4	C5	C6	119.30(19)
C8	N7	C11	115.70(16)		N28	C27	C10	177.2(2)
C8	N7	C1	123.67(16)		C23	C18	C9	122.94(18)
C1	N7	C11	120.54(16)		C23	C18	C19	118.79(18)
C17	C12	C13	119.38(19)		C19	C18	C9	118.16(17)
C17	C12	C11	122.98(18)		C6	C1	N7	120.41(17)
C13	C12	C11	117.63(17)		C6	C1	C2	119.76(18)
C16	C17	C12	119.62(19)		C2	C1	N7	119.84(18)
O31	C4	C5	124.45(19)		C20	C21	C22	119.3(2)
O31	C4	C3	115.78(18)		C2	C3	C4	120.98(19)
C5	C4	C3	119.77(19)		C8	C9	C10	100.66(15)
C18	C23	C22	120.1(2)		C18	C9	C8	115.91(16)
O24	C8	N7	125.51(18)		C18	C9	C10	110.06(15)
O24	C8	C9	124.91(18)		C29	C9	C8	108.36(15)
N7	C8	C9	109.44(16)		C29	C9	C10	111.41(16)
C14	C13	C12	120.7(2)		C29	C9	C18	110.12(16)
N7	C11	C12	115.13(16)		C20	C19	C18	120.65(19)
N7	C11	C10	101.70(15)		C30	C29	C9	126.5(2)

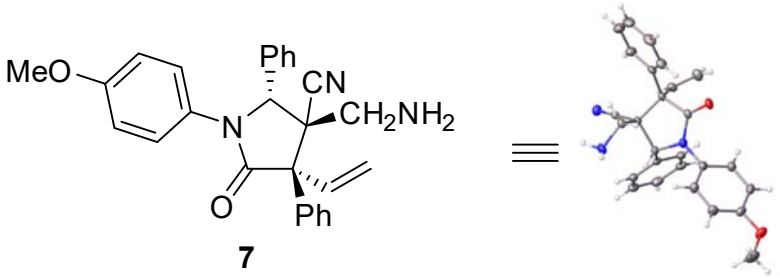
C12	C11	C10	115.74(16)		C3	C2	C1	119.18(19)
C1	C6	C5	120.91(18)		N26	C25	C10	178.4(2)
C27	C10	C11	107.24(17)		C17	C16	C15	120.76(19)
C27	C10	C9	109.87(16)		C15	C14	C13	119.8(2)
C9	C10	C11	105.50(14)		C21	C22	C23	120.9(2)
C25	C10	C11	112.67(17)		C21	C20	C19	120.3(2)
C25	C10	C27	108.05(16)		C14	C15	C16	119.8(2)
C25	C10	C9	113.33(17)					

Table S11. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 6aa.

Atom	x	y	z	U(eq)
H17	801.66	5384.91	1904.54	27
H23	6666.52	1762.63	3783.69	30
H13	4142.46	7564.94	828.43	30
H11	5017.84	6577.7	2265.01	24
H6	4562.03	8227.51	3180.43	29
H5	3765.82	10074.2	4095.81	30
H21	9194.98	-1785.2	2901.45	35
H3	891.69	6564.25	4749.82	29
H19	5351.31	525.31	1322.82	32
H29	2775.84	1579.36	1262.52	30
H2	1650.16	4734.15	3821.96	27
H16	-1355.33	6567.85	889.93	31
H14	1975.32	8703.47	-197.16	37
H22	8768.54	-205.87	4010.94	34
H20	7483.12	-1405.58	1555.45	35
H15	-779.31	8263.51	-145.08	36
H30A	1393.16	2016.62	2620.6	40
H30B	479.62	1229.75	1701.05	40
H32A	2205.17	11692.3	4786.38	51
H32B	3776.79	10849.49	5408.36	51
H32C	2252.36	11477.68	5759.08	51

X-Ray Crystallographic Data of 7

Crystallographic data for **7** have been deposited with the Cam-bridge Crystallographic Data Centre as deposition number 2221630. These data can be obtained free of charge via www.ccdc.cam.ac.uk/data_request/cif, or by emailing data_request@ccdc.cam.ac.uk, or by contacting The Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge CB2 1EZ, UK; fax: +44 1223 336033.



7

Table S12. Crystal data and structure refinement for 7.

Identification code	**7**
Empirical formula	$C_{27}H_{25}N_3O_2$
Formula weight	423.50
Temperature/K	173.00
Crystal system	orthorhombic
Space group	P212121
a/Å	9.76060(10)
b/Å	10.33100(10)
c/Å	21.9651(3)
α/°	90
β/°	90
γ/°	90
Volume/Å^3	2214.89(4)
Z	4
ρ_{calc}g/cm^3	1.270
μ/mm^{-1}	0.645
F(000)	896.0
Crystal size/mm^3	0.13 × 0.12 × 0.1
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	8.05 to 151.714
Index ranges	-8≤h≤12, -12≤k≤12, -26≤l≤27
Reflections collected	15467
Independent reflections	4549 [Rint = 0.0316, Rsigma = 0.0287]
Data/restraints/parameters	4549/0/306
Goodness-of-fit on F^2	1.040
Final R indexes [I>=2σ (I)]	R1 = 0.0309, wR2 = 0.0739
Final R indexes [all data]	R1 = 0.0344, wR2 = 0.0755
Largest diff. peak/hole / e Å^{-3}	0.17/-0.16
Flack parameter	0.02(10)

Table S13. Fractional Atomic Coordinates ($\times 10^4$) and Equivalent Isotropic Displacement Parameters ($Å^2 \times 10^3$) for 7. U_{eq} is defined as 1/3 of the trace of the orthogonalised U_{IJ} tensor.

Atom	x	y	z	U(eq)
O(2)	4712.9(12)	6137.7(12)	2596.1(6)	28.3(3)
O(1)	3637.7(16)	4722.7(16)	5375.2(6)	39.6(3)
N(1)	6394.0(14)	5165.9(14)	3162.1(6)	21.7(3)
N(3)	8219.3(16)	2237.2(15)	2468.5(7)	27.3(3)
N(2)	10468.4(15)	4802.6(15)	2012.9(7)	26.8(3)
C(16)	9372.2(16)	4741.6(15)	2194.8(7)	19.7(3)
C(18)	5867.0(16)	5702.4(15)	2648.4(8)	20.6(3)
C(5)	5648.0(16)	5027.4(17)	3718.2(8)	22.7(3)
C(8)	7781.9(15)	4649.2(16)	3103.3(7)	19.6(3)
C(15)	7942.9(15)	4604.2(15)	2394.7(7)	18.1(3)
C(19)	6994.2(15)	5722.1(15)	2159.7(7)	19.1(3)
C(17)	7432.6(16)	3255.0(15)	2174.2(8)	21.3(3)
C(9)	8871.6(16)	5383.6(16)	3454.1(7)	21.2(3)
C(6)	5171.1(18)	6115.1(17)	4028.7(8)	25.4(3)
C(14)	8728.0(18)	6669.2(17)	3637.0(8)	24.6(3)
C(7)	4492.8(18)	5976.0(18)	4575.6(9)	27.9(4)
C(20)	7675.4(17)	7056.1(16)	2208.1(8)	23.5(3)
C(22)	6525.0(17)	5481.4(16)	1506.4(8)	22.6(3)
C(10)	10085.9(17)	4729.8(18)	3591.7(7)	25.7(3)
C(2)	4281.4(18)	4748(2)	4823.4(8)	28.4(4)
C(13)	9788(2)	7289.6(18)	3947.3(8)	29.4(4)
C(4)	5409.3(19)	3806.7(17)	3957.1(9)	28.2(4)
C(23)	5212.8(19)	5049.5(17)	1355.0(9)	29.6(4)
C(27)	7481(2)	5631(2)	1041.7(9)	31.6(4)
C(11)	11145.4(18)	5351(2)	3894.7(8)	31.7(4)
C(12)	10993(2)	6634(2)	4075.1(8)	32.8(4)

C(21)	7018(2)	8152.8(18)	2229.6(10)	32.6(4)
C(3)	4726(2)	3656.9(18)	4508.9(9)	30.8(4)
C(25)	5856(2)	4909(2)	296.0(9)	39.8(5)
C(24)	4888(2)	4771(2)	748.5(10)	39.1(5)
C(26)	7159(2)	5335(2)	441.0(9)	39.6(5)
C(1)	3454(3)	3499(3)	5661.6(11)	50.4(6)

Table S14. Anisotropic Displacement Parameters ($Å^2×10^3$) for 7. The Anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11}+2hka^*b^*U_{12}+\ldots]$.

Atom	U11	U22	U33	U23	U13	U12
O(2)	18.4(5)	29.1(6)	37.4(7)	0.1(5)	0.2(5)	6.3(5)
O(1)	41.3(7)	47.2(8)	30.3(6)	-0.9(6)	13.5(6)	-6.1(7)
N(1)	17.4(6)	23.2(6)	24.5(6)	0.1(5)	1.4(5)	1.4(5)
N(3)	29.0(7)	18.7(7)	34.1(8)	0.2(6)	-2.6(7)	3.6(6)
N(2)	20.6(7)	29.1(7)	30.7(7)	-3.2(6)	1.5(6)	-2.5(6)
C(16)	21.0(8)	18.6(7)	19.7(7)	-1.4(6)	-4.3(6)	0.4(6)
C(18)	18.6(7)	16.7(7)	26.6(8)	-1.9(6)	-1.4(6)	0.4(5)
C(5)	17.2(7)	26.7(8)	24.3(7)	-0.9(6)	0.7(6)	-0.2(6)
C(8)	17.5(7)	21.0(7)	20.4(7)	1.2(6)	0.7(6)	1.4(6)
C(15)	15.7(6)	18.2(7)	20.4(7)	-0.2(6)	-1.8(5)	1.0(5)
C(19)	15.3(7)	18.3(7)	23.6(8)	0.2(6)	-1.6(6)	1.3(6)
C(17)	17.8(7)	18.3(7)	27.7(8)	-2.3(6)	-2.7(6)	-0.4(6)
C(9)	19.8(7)	27.6(8)	16.2(6)	0.5(6)	1.6(6)	-0.8(6)
C(6)	23.2(8)	24.1(8)	28.7(8)	-1.1(7)	1.4(7)	0.9(6)
C(14)	26.5(8)	27.2(8)	20.2(7)	0.3(6)	-0.1(6)	1.0(7)
C(7)	24.6(8)	30.9(9)	28.2(9)	-6.0(7)	2.6(7)	2.0(7)
C(20)	20.9(7)	22.0(8)	27.7(8)	2.1(6)	-3.7(6)	-2.4(6)
C(22)	23.6(8)	19.6(7)	24.6(8)	0.9(6)	-6.6(6)	3.6(6)
C(10)	23.6(8)	33.4(8)	20.1(7)	0.3(7)	-0.2(6)	3.7(7)

C(2)	21.2(7)	39.3(10)	24.8(8)	-1.3(7)	3.3(6)	-3.9(7)
C(13)	38.2(9)	31.1(9)	18.8(7)	-1.2(7)	0.3(7)	-7.6(7)
C(4)	26.0(8)	25.2(8)	33.4(9)	-2.2(7)	5.0(7)	-0.3(7)
C(23)	25.2(8)	29.2(9)	34.3(9)	-1.6(7)	-6.6(7)	-0.6(7)
C(27)	28.3(9)	40.5(10)	26.1(9)	3.4(7)	-3.1(7)	0.0(7)
C(11)	22.7(8)	48.8(11)	23.7(8)	1.9(8)	-3.7(7)	2.7(8)
C(12)	30.3(9)	47.5(11)	20.7(8)	0.3(7)	-4.1(7)	-11.4(8)
C(21)	31.0(9)	21.4(8)	45.6(11)	-0.1(8)	-1.9(8)	-2.0(7)
C(3)	29.4(9)	28.5(9)	34.6(10)	4.5(7)	4.1(8)	-4.4(7)
C(25)	52.4(12)	39.6(11)	27.6(9)	-4.8(8)	-15.2(9)	6.5(9)
C(24)	38.4(10)	34.6(10)	44.3(11)	-4.9(9)	-19.7(9)	-1.3(9)
C(26)	44.4(11)	48.7(12)	25.6(9)	0.5(9)	-1.2(8)	5.1(10)
C(1)	59.3(15)	55.1(14)	36.9(11)	7.2(10)	17.2(11)	-13.9(12)

Table S15. Bond Lengths for 7.

Atom	Atom	Length/Å		Atom	Atom	Length/Å
O(2)	C(18)	1.218(2)		C(9)	C(14)	1.395(2)
O(1)	C(2)	1.366(2)		C(9)	C(10)	1.397(2)
O(1)	C(1)	1.424(3)		C(6)	C(7)	1.379(3)
N(1)	C(18)	1.358(2)		C(14)	C(13)	1.395(3)
N(1)	C(5)	1.429(2)		C(7)	C(2)	1.396(3)
N(1)	C(8)	1.462(2)		C(20)	C(21)	1.303(3)
N(3)	C(17)	1.454(2)		C(22)	C(23)	1.397(2)
N(2)	C(16)	1.144(2)		C(22)	C(27)	1.391(3)
C(16)	C(15)	1.469(2)		C(10)	C(11)	1.387(3)
C(18)	C(19)	1.537(2)		C(2)	C(3)	1.391(3)
C(5)	C(6)	1.395(2)		C(13)	C(12)	1.386(3)
C(5)	C(4)	1.386(2)		C(4)	C(3)	1.392(3)
C(8)	C(15)	1.565(2)		C(23)	C(24)	1.399(3)

C(8)	C(9)	1.517(2)		C(27)	C(26)	1.390(3)
C(15)	C(19)	1.568(2)		C(11)	C(12)	1.391(3)
C(15)	C(17)	1.557(2)		C(25)	C(24)	1.378(3)
C(19)	C(20)	1.534(2)		C(25)	C(26)	1.384(3)
C(19)	C(22)	1.527(2)				

Table S16. Bond Angles for 7.

Atom	Atom	Atom	Angle/˚		Atom	Atom	Atom	Angle/˚
C(2)	O(1)	C(1)	117.85(17)		N(3)	C(17)	C(15)	109.89(13)
C(18)	N(1)	C(5)	123.91(14)		C(14)	C(9)	C(8)	123.52(15)
C(18)	N(1)	C(8)	115.24(13)		C(14)	C(9)	C(10)	118.90(16)
C(5)	N(1)	C(8)	120.74(13)		C(10)	C(9)	C(8)	117.57(15)
N(2)	C(16)	C(15)	176.16(17)		C(7)	C(6)	C(5)	120.15(16)
O(2)	C(18)	N(1)	125.38(16)		C(13)	C(14)	C(9)	120.26(16)
O(2)	C(18)	C(19)	126.24(15)		C(6)	C(7)	C(2)	120.35(16)
N(1)	C(18)	C(19)	108.33(13)		C(21)	C(20)	C(19)	124.78(16)
C(6)	C(5)	N(1)	120.49(15)		C(23)	C(22)	C(19)	123.44(16)
C(4)	C(5)	N(1)	120.03(15)		C(27)	C(22)	C(19)	118.06(15)
C(4)	C(5)	C(6)	119.48(15)		C(27)	C(22)	C(23)	118.40(16)
N(1)	C(8)	C(15)	101.06(12)		C(11)	C(10)	C(9)	120.81(17)
N(1)	C(8)	C(9)	114.98(13)		O(1)	C(2)	C(7)	115.56(17)
C(9)	C(8)	C(15)	116.72(13)		O(1)	C(2)	C(3)	124.66(18)
C(16)	C(15)	C(8)	112.92(12)		C(3)	C(2)	C(7)	119.78(16)
C(16)	C(15)	C(19)	113.04(13)		C(12)	C(13)	C(14)	120.26(17)
C(16)	C(15)	C(17)	107.29(13)		C(5)	C(4)	C(3)	120.76(17)
C(8)	C(15)	C(19)	104.25(12)		C(22)	C(23)	C(24)	120.01(18)
C(17)	C(15)	C(8)	107.68(13)		C(26)	C(27)	C(22)	121.38(18)
C(17)	C(15)	C(19)	111.60(12)		C(10)	C(11)	C(12)	119.86(17)
C(18)	C(19)	C(15)	100.55(12)		C(13)	C(12)	C(11)	119.90(17)

C(20)	C(19)	C(18)	105.89(13)		C(2)	C(3)	C(4)	119.45(17)
C(20)	C(19)	C(15)	112.52(13)		C(24)	C(25)	C(26)	119.80(18)
C(22)	C(19)	C(18)	116.07(13)		C(25)	C(24)	C(23)	120.67(18)
C(22)	C(19)	C(15)	111.51(13)		C(25)	C(26)	C(27)	119.7(2)
C(22)	C(19)	C(20)	109.97(13)					

Table S17. Torsion Angles for 7.

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O(2)	C(18)	C(19)	C(15)	-159.11(16)	C(8)	C(9)	C(14)	C(13)	-178.62(15)
O(2)	C(18)	C(19)	C(20)	83.62(19)	C(8)	C(9)	C(10)	C(11)	177.99(15)
O(2)	C(18)	C(19)	C(22)	-38.7(2)	C(15)	C(8)	C(9)	C(14)	95.90(18)
O(1)	C(2)	C(3)	C(4)	-178.02(18)	C(15)	C(8)	C(9)	C(10)	-83.29(18)
N(1)	C(18)	C(19)	C(15)	23.58(16)	C(15)	C(19)	C(20)	C(21)	-157.52(19)
N(1)	C(18)	C(19)	C(20)	-93.69(15)	C(15)	C(19)	C(22)	C(23)	103.61(18)
N(1)	C(18)	C(19)	C(22)	143.99(14)	C(15)	C(19)	C(22)	C(27)	-72.61(19)
N(1)	C(5)	C(6)	C(7)	-177.78(16)	C(19)	C(15)	C(17)	N(3)	-172.11(13)
N(1)	C(5)	C(4)	C(3)	177.75(17)	C(19)	C(22)	C(23)	C(24)	-175.85(16)
N(1)	C(8)	C(15)	C(16)	151.76(13)	C(19)	C(22)	C(27)	C(26)	175.12(18)
N(1)	C(8)	C(15)	C(19)	28.68(15)	C(17)	C(15)	C(19)	C(18)	84.28(15)
N(1)	C(8)	C(15)	C(17)	-89.98(14)	C(17)	C(15)	C(19)	C(20)	-163.46(13)
N(1)	C(8)	C(9)	C(14)	-22.2(2)	C(17)	C(15)	C(19)	C(22)	-39.35(18)
N(1)	C(8)	C(9)	C(10)	158.58(14)	C(9)	C(8)	C(15)	C(16)	26.30(19)
C(16)	C(15)	C(19)	C(18)	-154.68(13)	C(9)	C(8)	C(15)	C(19)	-96.78(15)
C(16)	C(15)	C(19)	C(20)	-42.42(18)	C(9)	C(8)	C(15)	C(17)	144.56(14)
C(16)	C(15)	C(19)	C(22)	81.70(16)	C(9)	C(14)	C(13)	C(12)	0.1(3)
C(16)	C(15)	C(17)	N(3)	63.55(17)	C(9)	C(10)	C(11)	C(12)	1.2(3)
C(18)	N(1)	C(5)	C(6)	-62.3(2)	C(6)	C(5)	C(4)	C(3)	-1.4(3)
C(18)	N(1)	C(5)	C(4)	118.52(19)	C(6)	C(7)	C(2)	O(1)	178.01(17)
C(18)	N(1)	C(8)	C(15)	-14.90(17)	C(6)	C(7)	C(2)	C(3)	-1.7(3)

C(18)	N(1)	C(8)	C(9)	111.72(16)	C(14)	C(9)	C(10)	C(11)	-1.2(2)
C(18)	C(19)	C(20)	C(21)	-48.6(2)	C(14)	C(13)	C(12)	C(11)	-0.2(3)
C(18)	C(19)	C(22)	C(23)	-10.7(2)	C(7)	C(2)	C(3)	C(4)	1.6(3)
C(18)	C(19)	C(22)	C(27)	173.07(15)	C(20)	C(19)	C(22)	C(23)	-130.85(17)
C(5)	N(1)	C(18)	O(2)	0.6(3)	C(20)	C(19)	C(22)	C(27)	52.9(2)
C(5)	N(1)	C(18)	C(19)	177.94(14)	C(22)	C(19)	C(20)	C(21)	77.5(2)
C(5)	N(1)	C(8)	C(15)	161.53(14)	C(22)	C(23)	C(24)	C(25)	0.5(3)
C(5)	N(1)	C(8)	C(9)	-71.85(19)	C(22)	C(27)	C(26)	C(25)	1.4(3)
C(5)	C(6)	C(7)	C(2)	0.2(3)	C(10)	C(9)	C(14)	C(13)	0.6(2)
C(5)	C(4)	C(3)	C(2)	-0.1(3)	C(10)	C(11)	C(12)	C(13)	-0.5(3)
C(8)	N(1)	C(18)	O(2)	176.90(15)	C(4)	C(5)	C(6)	C(7)	1.4(3)
C(8)	N(1)	C(18)	C(19)	-5.76(18)	C(23)	C(22)	C(27)	C(26)	-1.3(3)
C(8)	N(1)	C(5)	C(6)	121.54(17)	C(27)	C(22)	C(23)	C(24)	0.4(3)
C(8)	N(1)	C(5)	C(4)	-57.6(2)	C(24)	C(25)	C(26)	C(27)	-0.4(3)
C(8)	C(15)	C(19)	C(18)	-31.67(14)	C(26)	C(25)	C(24)	C(23)	-0.5(3)
C(8)	C(15)	C(19)	C(20)	80.59(15)	C(1)	O(1)	C(2)	C(7)	-177.1(2)
C(8)	C(15)	C(19)	C(22)	-155.30(13)	C(1)	O(1)	C(2)	C(3)	2.6(3)
C(8)	C(15)	C(17)	N(3)	-58.27(17)					

Table S18. Hydrogen Atom Coordinates (Å×10^4) and Isotropic Displacement Parameters (Å^2×10^3) for 7.

Atom	x	y	z	U(eq)
H(8)	7773.4	3737.39	3256.05	24
H(17A)	6449.27	3152.81	2273.57	26
H(17B)	7537.78	3189.13	1726.95	26
H(6)	5313.87	6953.87	3863.16	30
H(14)	7905.19	7124.03	3549.89	30
H(7)	4167.78	6719.92	4784.86	33
H(20)	8647.59	7084.79	2223.54	28

H(10)	10187.34	3848.75	3476.32	31
H(13)	9683.01	8164.88	4071.47	35
H(4)	5715.44	3063.46	3741.77	34
H(23)	4540.46	4944.62	1663.87	35
H(27)	8371.54	5940.76	1136.89	38
H(11)	11973.21	4902.2	3978.81	38
H(12)	11713.56	7060.52	4285.55	39
H(3)	4564.61	2816.78	4669.45	37
H(25)	5628.4	4711.08	-114.12	48
H(24)	3991.6	4484.35	647.48	47
H(26)	7831.85	5425.76	131.35	47
H(1A)	2822.85	2970.73	5419.05	76
H(1B)	3072.42	3625.6	6069.94	76
H(1C)	4339.54	3056.85	5692.82	76
H(21A)	7500(20)	8980(20)	2256(10)	25(5)
H(3A)	7670(30)	1560(30)	2543(13)	46(7)
H(3B)	8940(30)	2000(20)	2221(11)	38(6)
H(21B)	6050(40)	8120(30)	2222(15)	73(10)