

Supporting Information

Cu(I)-Catalyzed Enantioselective [5 + 1] Cycloaddition of N-Aromatic Compounds and Alkynes via Chelating Assisted 1,2-Dearomatic Addition

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Acknowledgment We acknowledge the Korea Basic Science Institute (KBSI) for the HRMS and X-ray analysis.

I. General Methods

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. The quinolinium zwitterions (**1**) were prepared according to the reported procedure.^{S1} Analytical thin layer chromatography (TLC) was performed on Merck pre-coated silica gel 60 F254 plates. Visualization on TLC was achieved by use of UV light (254 nm). Flash column chromatography was undertaken on silica gel (Merck Kiesel gel 60 F254 230-400 mesh). ¹H NMR were recorded on Bruker DPX FT (400 MHz) and JEOL (300 MHz). Chemical shifts were quoted in parts per million (ppm) referenced to the appropriate solvent peak or 0.0 ppm for tetramethylsilane. The following abbreviations were used to describe peak splitting patterns when appropriate: br = broad, s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Coupling constants, *J*, were reported in hertz unit (Hz). ¹³C NMR were recorded on Bruker DPX FT (100 MHz) and JEOL (75MHz). There were fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm referenced to the center line of a triplet at 77.0 ppm of chloroform-*d*. Infrared spectra were recorded on JASCO FT/IR-4700 and FT/IR-4200 FT-IR spectrometer. Analytical normal-phase high-performance liquid chromatography (HPLC) was using an Agilent 1260 Infinity II series instrument equipped with a photodiode array detector (254 nm) and columns (chiral supports, 5 μm particle size, 4.6 x 250 mm) from Daicel Chemical Industries. Frequencies are given in reciprocal centimeters (cm-1) and only selected absorbance is reported. High resolution mass spectra were obtained from the Korea Basic Science Institute (Daegu) by EI and FAB method and Organic Chemistry Research Center in Sogang University by ESI.

II. Experimental Procedure

II-1. Experimental Procedure for the Synthesis of N-Aromatic Zwitterions (S1)

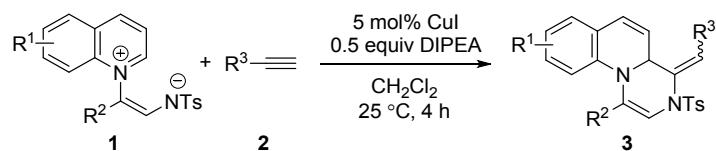
To a test tube with a triangular-shaped stir bar were added 4-phenyl-1-toluenesulfonyl-1,2,3-triazole (2.0 equiv), and Rh₂(OPiv)₄ (4.0 mol %), and *p*-xylene (2.0 mL) under N₂ atmosphere. To this stirred reaction mixture was added N-heteroaromatic compound (0.2 mmol) and the reaction mixture was stirred at 110 °C for the indicated time. The reaction mixture was then cooled to room temperature and concentrated under reduced pressure to remove the solvent and the residue was purified by chromatography on silica gel to give the desired N-aromatic zwitterion **1**.

II-2 Procedure for the Cu-Catalyzed Cycloaddition of Quinolinium Zwitterions (**1**) and Alkynes (**2**)

A. [5 + 1] Cycloaddition of Quinolinium Zwitterions (**1**) and Alkynes (**2**)

To a test tube with a triangular-shaped stir bar were added quinolinium zwitterion (**1**, 0.2 mmol), terminal alkyne (**2**, 1.2 equiv), Cul (5 mol%), and CH₂Cl₂ (2 mL) under N₂ atmospheric conditions. After confirming the completion of the reaction using TLC, the reaction mixture was filtered through a pad of celite and then washed with EtOAc (10 mL x 3). The organic solvent was removed under reduced pressure. The organic residue was purified by chromatography on silica gel to give the desired product **3**.

Scheme S1. [5 + 1] Cycloaddition of Quinolinium Zwitterions and Alkynes



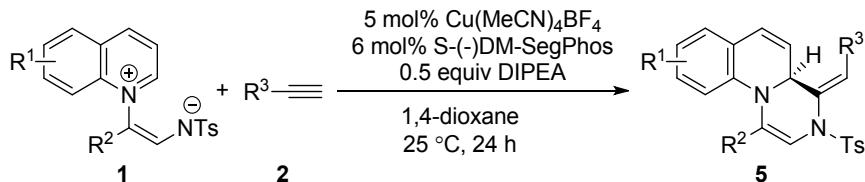
B. Control experiment (Isotope experiment)

To a test tube with a triangular-shaped stir bar were added quinolinium zwitterion (**1a**, 0.2 mmol), ethyl propiolate (**2a**, 1.2 equiv), CuI (5 mol%), and CH₂Cl₂ (2 mL), deuterium oxide (0.5mL) under N₂ atmospheric conditions. After 4 h, the reaction mixture was filtered through a pad of celite and then washed with EtOAc (10 mL x 3). The organic solvent was removed under reduced pressure. The ratio of deuterium incorporation was determined by ¹H NMR.

C. Asymmetric [5 + 1] Cycloaddition of Quinolinium Zwitterions (1) and Alkyne (2)

To a test tube with a triangular-shaped stir bar were added quinolinium zwitterion (**1**, 0.2 mmol), DIPEA (0.5 equiv), and 1,4-dioxane (1 mL) under N₂ atmospheric conditions. To this stirred reaction mixture was added a catalytic mixture of Cu(MeCN)₄BF₄ (5 mol%) and S-(-)-DM-SegPhos (6 mol%) in 1,4-dioxane (1mL). Afterwards, dropwise terminal alkyne (**2**, 1.2 equiv) in 1,4-dioxane (1mL) for 4 h at room temperature to the stirred reaction mixture. After 24 h, the reaction mixture was filtered through a pad of celite and then washed with EtOAc (10 mL x 3). The organic solvent was removed under reduced pressure. The organic residue was purified by chromatography on silica gel to give the desired product **5**.

Scheme S2. Asymmetric [5 + 1] Cycloaddition of Quinolinium Zwitterions and Alkyne



III. Spectroscopic Data

A. Unpublished N-Aromatic Zwitterions

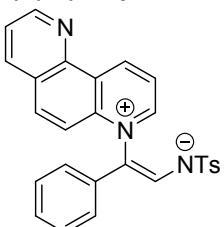
(Z)-(2-(4-methoxyphenyl)-2-(quinolin-1-iun-1-yl)vinyl)(tosyl)amide:

Purple Solid; R_f = 0.5 (DCM/MeOH = 10:1); m.p. 285-286 °C; ¹H NMR (300 MHz, CDCl₃) δ 8.90 (d, J = 8.29 Hz, 1H), 8.79 (d, J = 5.50 Hz, 1H), 8.15-8.12 (m, 1H), 8.09 (s, 1H), 8.06-8.03 (m, 1H), 7.85-7.80 (m, 1H), 7.79-7.73 (m, 2H), 7.64 (d, J = 8.14 Hz, 2H), 7.14 (d, J = 8.05 Hz, 2H), 6.70 (s, 4H), 3.73 (s, 3H), 2.36 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 157.3, 152.2, 146.1, 143.4, 140.3, 140.0, 139.4, 135.3, 130.5, 129.9, 129.8, 128.8, 126.0, 122.1, 121.9, 121.3, 114.5, 114.3, 55.3, 21.3; IR (liquid) ν 1604.0, 1510.95, 1249.16, 1130.08, 1083.8 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₅H₂₃N₂O₃S [M+H]⁺: 431.1429, found: 431.1431

(Z)-(2-(4,7-phenanthrolin-4-iun-4-yl)-2-phenylvinyl)(tosyl)amide:

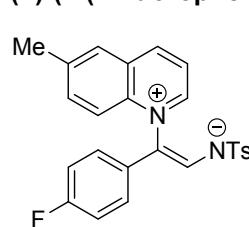
Purple Solid; R_f = 0.4 (DCM/MeOH = 10:1); m.p. 171-172 °C; ¹H NMR (300 MHz, CDCl₃) δ 9.72 (d, J = 8.36 Hz, 1H), 8.84-8.82 (m, 1H), 8.64-8.53 (m, 2H), 8.43 (s, 1H), 8.14-7.98 (m, 2H), 7.80 (d, J = 8.03 Hz, 3H), 7.34-7.24 (m, 3H), 7.18-7.11 (m, 2H), 7.06-7.02 (m, 1H), 6.73-6.71 (m, 2H), 2.41-2.40 (m, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 152.5, 149.8, 146.4, 143.1, 142.8, 140.8, 140.6, 140.1, 139.0, 136.1, 132.1, 129.2, 129.1, 128.5, 125.9, 125.0, 123.9, 123.6, 123.4, 121.2, 120.2, 114.7, 21.4; IR (liquid) ν 1591.95, 1496.01, 1242.41, 1131.05, 1083.8 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₇H₂₂N₃O₂S [M+H]⁺: 452.1433, found: 452.1434.

(Z)-(2-(1,7-phenanthrolin-7-iium-7-yl)-2-phenylvinyl)(tosyl)amide:



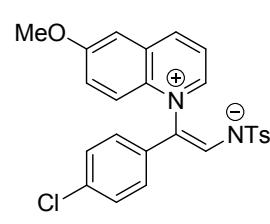
Purple Solid; $R_f = 0.4$ (DCM/MeOH = 10:1); m.p. 166-168 °C; ^1H NMR (300 MHz, CDCl₃) δ 10.25 (d, $J = 7.45$ Hz, 1H), 9.14 (s, 1H), 8.86 (d, $J = 5.75$ Hz, 1H), 8.33-8.29 (m, 2H), 8.14 (q, $J = 4.73$ Hz, 1H), 8.01 (s, 2H), 7.77-7.73 (m, 1H), 7.65 (d, $J = 8.06$ Hz, 2H), 7.18-7.11 (m, 4H), 7.04-6.99 (m, 1H), 6.74 (d, $J = 7.66$ Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (75 MHz, CDCl₃) δ 151.7, 151.6, 144.1, 143.2, 143.1, 142.0, 141.2, 140.0, 137.0, 136.6, 136.1, 130.5, 129.1, 128.8, 126.6, 126.0, 124.7, 124.5, 123.3, 120.2, 119.2, 114.0, 21.3; IR (liquid) ν 1591.95, 1506.61, 1241.93, 1131.05, 1083.8 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₇H₂₂N₃O₂S [M+H]⁺: 452.1433, found: 452.1431.

(Z)-(2-(4-fluorophenyl)-2-(6-methylquinolin-1-iium-1-yl)vinyl)(tosyl)amide:



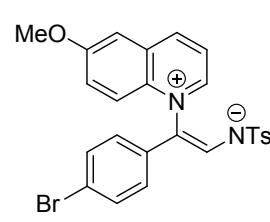
Purple Solid; $R_f = 0.5$ (DCM/MeOH = 10:1); m.p. 205-206 °C; ^1H NMR (300 MHz, CDCl₃) δ 8.81 (d, $J = 8.28$ Hz, 1H), 8.68 (d, $J = 5.24$ Hz, 1H), 8.14 (s, 1H), 7.91-7.78 (m, 3H), 7.65-7.57 (m, 3H), 7.14 (d, $J = 7.94$ Hz, 2H), 6.84 (t, $J = 8.58$ Hz, 2H), 6.70-6.66 (m, 2H), 2.52 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (75 MHz, CDCl₃) δ 162.0, 158.8, 151.0, 145.8, 145.8, 143.1, 143.0, 140.9, 140.9, 140.3, 140.2, 140.2, 140.1, 140.1, 138.7, 137.8, 133.1, 133.0, 130.8, 128.9, 128.9, 128.8, 128.5, 128.5, 126.4, 126.2, 126.0, 122.2, 122.1, 122.0, 120.7, 120.6, 116.1, 116.1, 115.8, 115.8, 113.5, 21.4, 21.3; IR (liquid) ν 1590.02, 1519.63, 1263.15, 1130.56, 1083.32 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₅H₂₂FN₂O₂S [M+H]⁺: 433.1386, found: 433.1383.

(Z)-(2-(4-chlorophenyl)-2-(6-methoxyquinolin-1-iium-1-yl)vinyl)(tosyl)amide:



Purple Solid; $R_f = 0.5$ (DCM/MeOH = 10:1); m.p. 195-196 °C; ^1H NMR (300 MHz, CDCl₃) δ 8.78 (d, $J = 8.30$ Hz, 1H), 8.44-8.42 (m, 1H), 8.26 (s, 1H), 7.87-7.83 (m, 1H), 7.67 (d, $J = 8.13$ Hz, 2H), 7.59 (dd, $J = 4.70$ Hz, 1H), 7.35-7.32 (m, 2H), 7.17 (d, $J = 8.00$ Hz, 2H), 7.09 (d, $J = 8.72$ Hz, 2H), 6.61 (d, $J = 8.73$ Hz, 2H), 3.79 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, CDCl₃) δ 159.8, 148.2, 145.4, 143.0, 140.9, 140.5, 135.8, 135.2, 132.4, 129.8, 129.1, 129.0, 128.6, 125.9, 122.2, 121.8, 121.2, 113.3, 107.1, 56.2, 21.3; IR (liquid) ν 1586.16, 1262.66, 1131.05, 1082.83, 858.65 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₅H₂₂CIN₂O₃S [M+H]⁺: 465.1040, found: 465.1041.

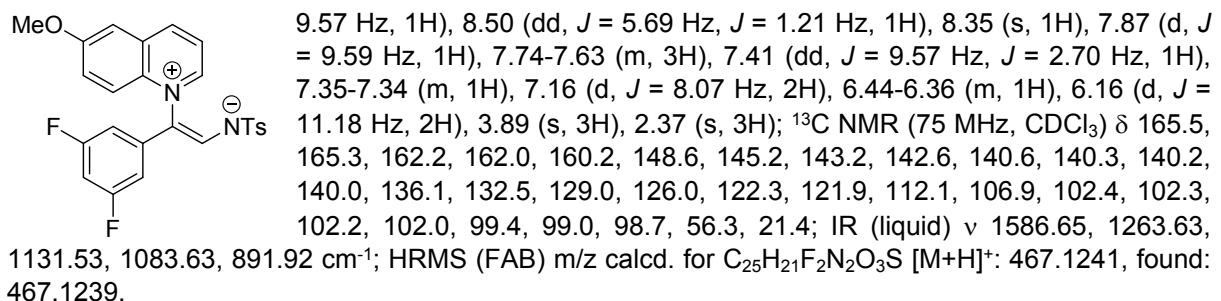
(Z)-(2-(4-bromophenyl)-2-(6-methoxyquinolin-1-iium-1-yl)vinyl)(tosyl)amide:



Purple Solid; $R_f = 0.5$ (DCM/MeOH = 10:1); m.p. 165-166 °C; ^1H NMR (300 MHz, CDCl₃) δ 8.79 (d, $J = 8.36$ Hz, 1H), 8.51-8.45 (m, 2H), 7.87 (d, $J = 9.35$ Hz, 1H), 7.72-7.64 (m, 3H), 7.41-7.34 (m, 4H), 7.17 (d, $J = 7.90$ Hz, 2H), 6.75 (d, $J = 8.28$, 2H), 3.87 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (75 MHz, CDCl₃) δ 159.9, 148.3, 145.3, 143.0, 141.1, 140.5, 135.8, 135.7, 132.4, 132.0, 129.0, 128.7, 125.9, 122.2, 121.9, 121.5, 117.5, 113.2, 107.1, 56.2, 21.3; IR (liquid) ν 1592.43, 1262.18, 1131.05, 1082.83, 857.686 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₅H₂₂BrN₂O₃S [M+H]⁺: 509.0535, found: 509.0539.

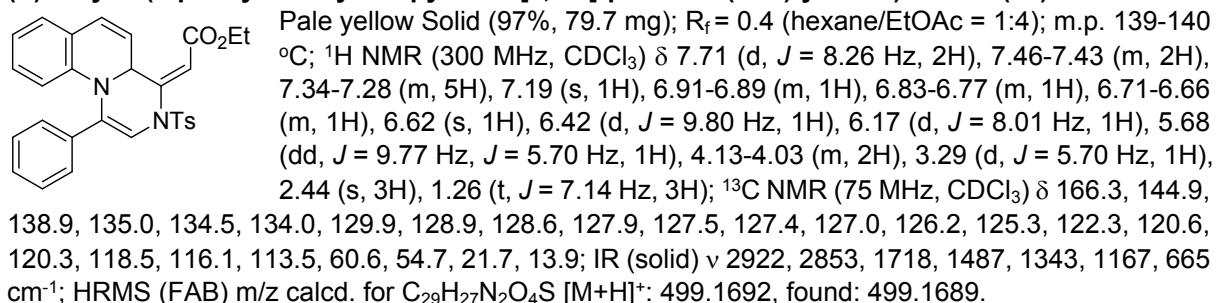
(Z)-(2-(3,5-difluorophenyl)-2-(6-methoxyquinolin-1-iium-1-yl)vinyl)(tosyl)amide:

Purple Solid; $R_f = 0.5$ (DCM/MeOH = 10:1); m.p. 224-225 °C; ^1H NMR (300 MHz, CDCl₃) δ 8.77 (d, $J =$

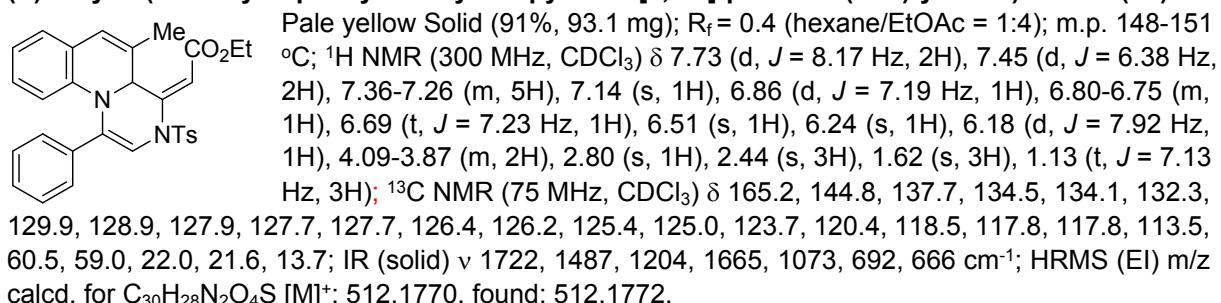


B. [5+1] Cycloadducts

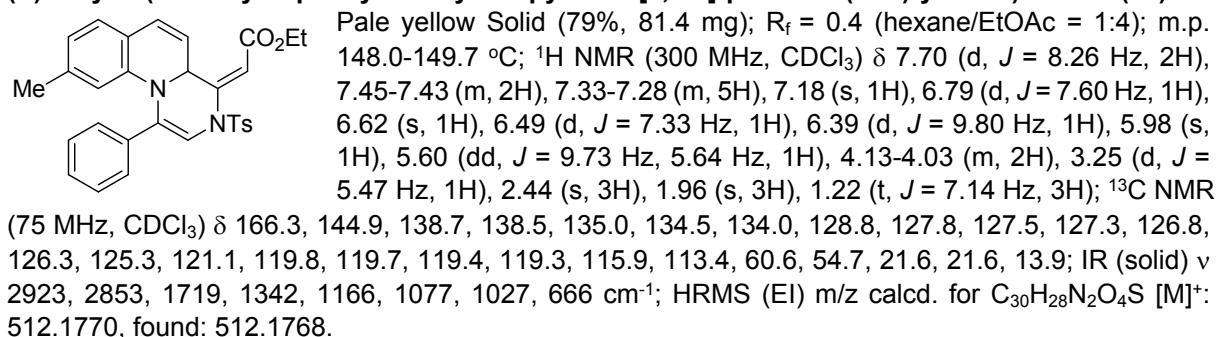
(E)-ethyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3a):



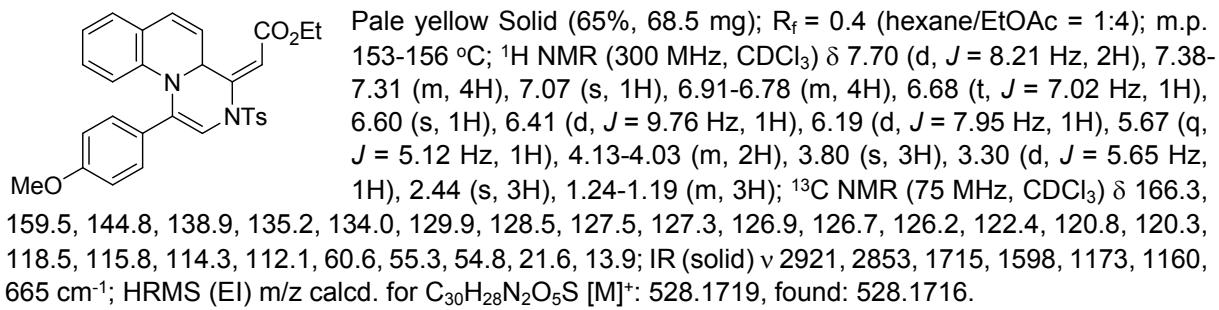
(E)-ethyl 2-(5-methyl-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3b):



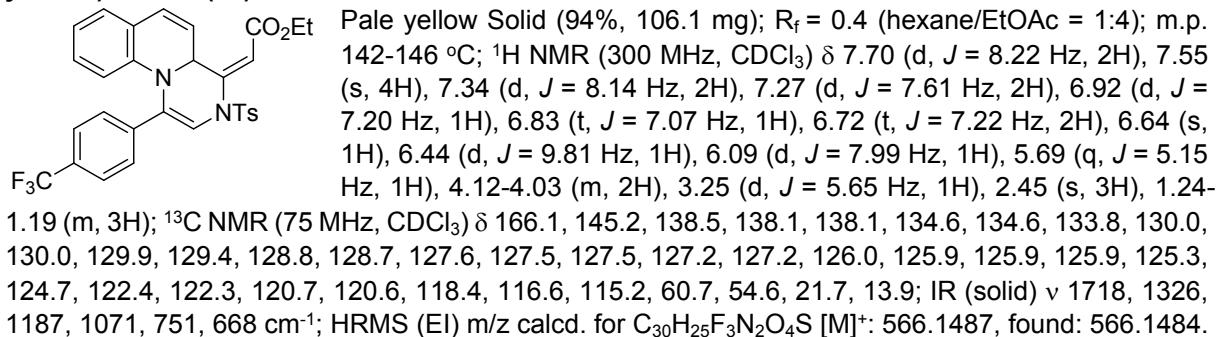
(E)-ethyl 2-(9-methyl-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3c):



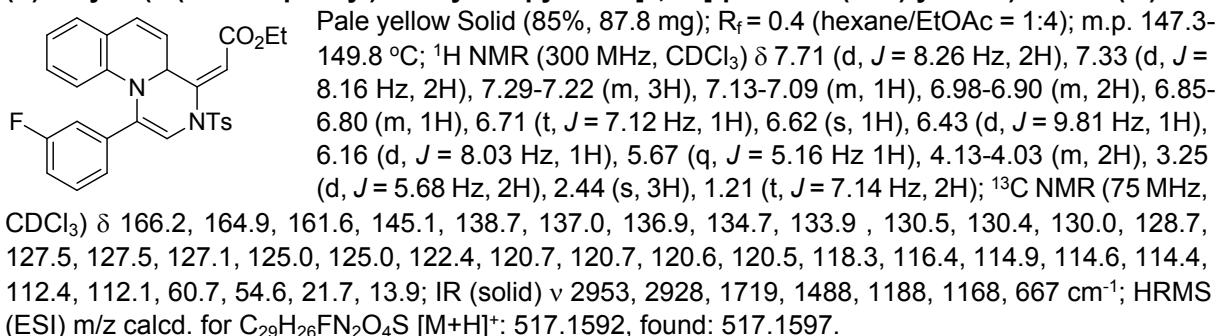
(E)-ethyl 2-(1-(4-methoxyphenyl)-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3d):



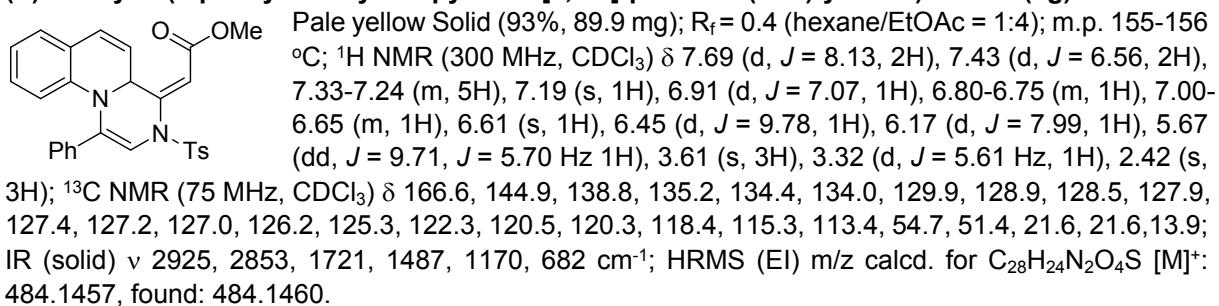
(E)-ethyl 2-(3-tosyl-1-(4-(trifluoromethyl)phenyl)-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3e):



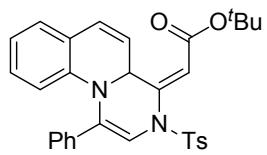
(E)-ethyl 2-(1-(3-fluorophenyl)-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3f):



(E)-methyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3g):

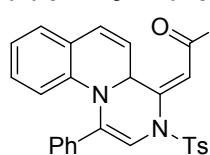


(E)-tert-butyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3h):



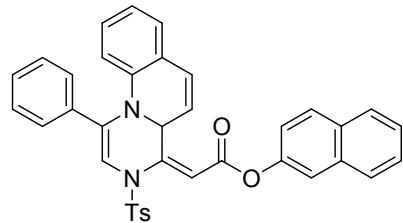
Pale yellow Solid (96%, 101.6 mg.); R_f = 0.5 (hexane/EtOAc = 1:4); m.p. 112-116 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.70 (d, J = 8.14 Hz, 2H), 7.45-7.43 (m, 2H), 7.33-7.25 (m, 5H), 7.17 (s, 1H), 6.92 (d, J = 6.70 Hz, 1H), 6.81-6.79 (m, 1H), 6.71-6.66 (m, 1H), 6.60 (s, 1H), 6.41 (d, J = 9.77 Hz, 1H), 6.17 (d, J = 7.96 Hz, 1H), 5.74 (dd, J = 9.71 Hz, 5.68 Hz, 1H), 3.19 (d, J = 5.59 Hz, 1H), 2.43 (s, 3H), 1.43 (s, 9H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.2, 144.9, 138.8, 134.6, 134.2, 133.9, 129.9, 128.9, 128.5, 127.8, 127.8, 127.6, 126.8, 126.2, 125.3, 122.3, 121.1, 120.2, 118.6, 118.4, 113.6, 81.7, 54.7, 28.0, 21.7; IR (solid) ν 2926, 2854, 1715, 1457, 1016, 668 cm^{-1} ; HRMS (EI) m/z calcd. for $\text{C}_{31}\text{H}_{30}\text{N}_2\text{O}_4\text{S}$ [M] $^+$: 526.1926, found: 526.1929.

(E)-phenyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3i):



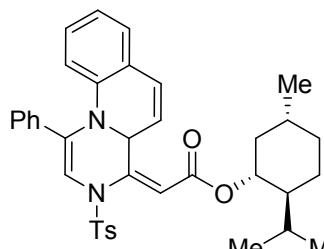
Pale yellow Solid (79%, 86.4 mg); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 118-119 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.73 (d, J = 8.23 Hz, 2H), 7.48-7.46 (m, 2H), 7.40-7.20 (m, 9H), 7.03-6.96 (m, 3H), 6.85-6.79 (m, 2H), 6.74-6.72 (m, 1H), 6.50 (d, J = 9.83 Hz, 1H), 6.22 (d, J = 7.96 Hz, 1H), 5.80 (dd, J = 9.77 Hz, 5.68 Hz, 1H), 3.43 (d, J = 5.65 Hz, 1H), 2.42 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 164.50, 150.41, 145.12, 138.73, 137.24, 134.19, 134.02, 129.99, 129.41, 128.93, 128.60, 128.03, 127.48, 127.34, 127.02, 126.38, 125.84, 125.36, 122.39, 121.32, 121.21, 120.59, 118.69, 114.26, 113.40, 55.01, 21.65; IR (solid) ν 3058, 2920, 1733, 1487, 1167, 1079, 665 cm^{-1} ; HRMS (FAB) m/z calcd. for $\text{C}_{33}\text{H}_{27}\text{N}_2\text{O}_4\text{S}$ [M+H] $^+$: 547.1692, found: 547.1694.

(E)-naphthalen-2-yl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3j):



Pale yellow Solid (77%, 91.7 mg); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 108-110 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.87-7.80 (m, 3H), 7.76-7.73 (m, 2H), 7.52-7.47 (m, 6H), 7.35-7.31 (m, 5H), 7.18-7.14 (m, 1H), 7.02-7.00 (m, 1H), 6.88-6.84 (m, 2H), 6.78-6.73 (m, 1H); 6.53 (d, J = 9.92 Hz, 1H), 6.24 (d, J = 8.05 Hz, 1H), 5.83 (q, J = 5.17, 1H), 3.46 (d, J = 5.47 Hz, 1H), 2.44 (s, 3H); ^{13}C NMR (75 MHz, CDCl_3) δ 164.7, 148.1, 145.1, 138.8, 137.4, 134.2, 134.1, 133.7, 131.4, 130.0, 129.4, 128.9, 128.7, 128.1, 127.8, 127.7, 127.5, 127.4, 127.1, 126.6, 126.4, 125.8, 125.4, 122.4, 121.3, 120.8, 120.6, 118.8, 118.3, 114.2, 113.4, 55.1, 21.7; IR (solid) ν 2920, 2852, 1738, 1487, 1149, 663 cm^{-1} ; HRMS (ESI) m/z calcd. for $\text{C}_{37}\text{H}_{28}\text{N}_2\text{NaO}_4\text{S}$ [M+Na] $^+$: 619.1667, found: 619.1665.

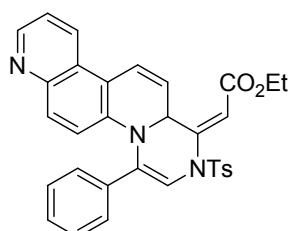
(E)-(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3k):



Pale yellow Solid (80%, 97.5 mg); R_f = 0.6 (hexane/EtOAc = 1:4); d.r.: 1:1; m.p. 104-107 °C; ^1H NMR (300 MHz, CDCl_3) δ 7.72-7.68 (m, 2H), 7.45-7.42 (m, 2H), 7.34-7.28 (m, 5H), 7.21 (s, 0.5H), 7.17 (s, 0.5H), 6.89-6.85 (m, 1H), 6.82-6.74 (m, 1H), 6.70-6.60 (m, 2H), 6.39 (d, J = 4.43 Hz, 0.5H), 6.36 (d, J = 4.43 Hz, 0.5H), 6.16 (d, J = 8.00 Hz, 1H), 5.82-5.77 (m, 0.5H), 5.76-5.72 (m, 0.5H), 4.71-4.59 (m, 1H), 3.32 (d, J = 5.62 Hz, 0.5H), 3.27 (d, J = 5.52 Hz, 0.5H), 2.44 (s, 3H), 2.03-1.99 (m, 1H), 1.67-1.65 (m, 3H), 1.48 (m, 1H), 1.32-1.28 (m, 1H), 0.97-0.92 (m, 4H), 0.88-0.75 (m, 8H); ^{13}C NMR (75 MHz, CDCl_3) δ 165.6, 165.4, 144.9, 138.6, 138.5, 136.5, 135.5, 134.4, 134.4, 133.9, 133.9, 129.9, 128.9, 128.4, 128.3, 127.9, 127.6, 127.5, 126.9, 126.9, 126.6, 126.2, 125.3, 125.3, 122.3, 121.2, 121.1, 120.2, 120.1, 118.5, 118.5, 116.6, 115.9, 113.5, 113.4, 75.1, 74.9, 54.9, 54.8, 46.6, 46.6, 40.7, 40.5, 34.1, 34.0, 31.4, 31.3, 26.0, 25.5, 23.2, 23.2, 22.1, 22.0, 21.7, 20.8, 20.7, 16.4,

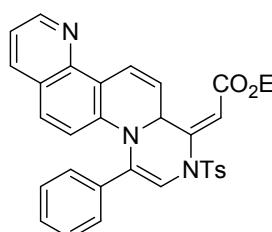
16.2; IR (solid) ν 2952, 2869, 1713, 1487, 1366, 1170, 665 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₇H₄₁N₂O₄S [M+H]⁺: 609.2782, found: 609.2787.

(E)-ethyl 2-(10-phenyl-8-tosyl-6aH-pyrazino[2,1-c][4,7]phenanthrolin-7(8H)-ylidene)acetate (3l):



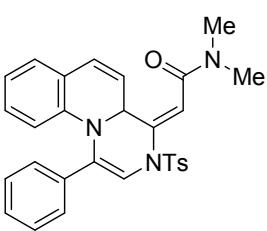
Yellow Solid (95%, 104.6 mg); R_f = 0.5 (hexane/EtOAc = 2:1); m.p. 108-112; ¹H NMR (300 MHz, CDCl₃) δ 8.69-8.68 (m, 1H), 8.20 (d, J = 8.51 Hz, 1H), 7.73 (d, J = 8.26 Hz, 2H), 7.58 (d, J = 9.24 Hz, 1H), 7.49-7.46 (m, 2H), 7.36-7.30 (m, 7H), 7.13 (d, J = 10.06 Hz, 1H), 6.78 (d, J = 9.23 Hz, 1H), 6.65 (s, 1H), 5.89 (dd, J = 9.98 Hz, J = 5.86 Hz, 1H), 4.11-3.98 (m, 2H), 3.52 (d, J = 5.86 Hz, 1H), 2.44 (s, 3H), 1.06 (t, J = 7.13 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.1, 147.9, 145.1, 143.7, 137.4, 135.4, 134.2, 134.0, 130.1, 130.0, 129.6, 129.2, 129.1, 129.1, 128.2, 127.5, 125.8, 125.3, 125.0, 115.8, 114.7, 114.0, 60.7, 54.7, 21.7, 13.8; IR (solid) ν 1717.78, 1374.03, 1186.97, 1172.03, 668.21 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₂H₂₇N₃O₄S [M+H]⁺: 550.1801, found: 550.1804.

(E)-ethyl 2-(4-phenyl-2-tosyl-2,13a-dihydro-1H-pyrazino[1,2-i][1,7]phenanthrolin-1-ylidene)acetate (3m):



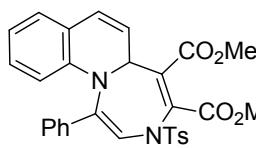
Yellow Solid (78%, 85.5 mg); R_f = 0.2 (hexane/EtOAc = 1:3); m.p. 165-166; ¹H NMR (300 MHz, CDCl₃) δ 8.76-8.74 (m, 1H), 7.86-7.72 (m, 4H), 7.50-7.47 (m, 2H), 7.36-7.23 (m, 7H), 7.15 (dd, J = 8.12 Hz, J = 4.22 Hz, 1H), 6.71 (s, 1H), 6.60 (d, J = 8.96 Hz, 1H), 5.78 (dd, J = 10.01 Hz, J = 5.70 Hz, 1H), 4.11-3.99 (m, 2H), 3.39 (d, J = 5.71 Hz, 1H), 2.44 (s, 3H), 0.94 (t, J = 7.13 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.3, 150.0, 145.1, 144.6, 139.7, 135.8, 134.5, 133.8, 130.0, 129.1, 128.1, 127.6, 127.5, 125.6, 125.2, 123.3, 122.8, 119.7, 119.1, 118.9, 117.1, 116.5, 114.2, 60.9, 54.8, 21.7, 13.5; IR (solid) ν 1718.75, 1500.83, 1365.84, 1172.51, 735.23 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₂H₂₇N₃O₄S [M+H]⁺: 550.1801, found: 550.1800.

(E)-N,N-dimethyl-2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetamide (3n):



Pale yellow Solid (79%, 78.6 mg); R_f = 0.5 (hexane/EtOAc = 2:1); m.p. 166-167 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.77 (d, J = 8.05 Hz, 2H), 7.44 (d, J = 6.94 Hz, 2H), 7.35-7.26 (m, 5H), 7.17 (s, 1H), 6.89 (d, J = 7.06 Hz, 1H), 6.79-6.74 (m, 2H), 6.66 (t, J = 7.23 Hz, 1H), 6.40 (d, J = 9.78 Hz, 1H), 6.18 (d, J = 7.96 Hz, 1H), 5.77 (q, J = 5.11 Hz, 1H), 3.11 (d, J = 5.55 Hz, 2H), 2.81 (s, 3H), 2.42 (s, 3H), 2.27 (s, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.3, 144.8, 139.1, 134.6, 133.7, 133.7, 132.3, 129.9, 128.9, 128.5, 127.8, 126.6, 126.0, 125.9, 125.2, 122.9, 121.4, 121.2, 120.1, 118.3, 113.9, 54.8, 37.8, 33.8, 21.6; IR (solid) ν 2921, 2853, 1646, 1358, 1341, 1174, 666 cm⁻¹; HRMS (ESI) m/z calcd. for C₂₉H₂₇N₃NaO₃S [M+Na]⁺: 520.1665, found: 520.1668.

Dimethyl 1-phenyl-3-tosyl-3,5a-dihydro-[1,4]diazepino[1,7-a]quinoline-4,5-dicarboxylate (4):

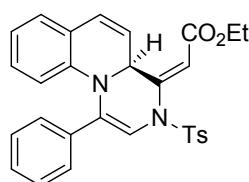


Yellow Solid (97%, 105.3 mg); R_f = 0.3 (hexane/EtOAc = 4:1); m.p. 178-179 °C; ¹H NMR (400 MHz, CDCl₃) δ 7.75 (d, J = 8.3 Hz, 2H), 7.41 (d, J = 8.0 Hz, 2H), 7.27-7.21 (m, 5H), 6.87 (dd, J = 7.4, 1.4 Hz, 1H), 6.78-6.73 (m, 1H), 6.68-6.64 (m, 1H), 6.50 (d, J = 9.6 Hz, 1H), 6.47 (s, 1H), 6.12 (d, J = 8.1 Hz, 1H), 5.49 (dd, J = 9.6, 6.3 Hz, 1H), 4.03 (d, J = 6.4 Hz, 1H), 3.82 (s, 3H), 3.42 (s, 3H), 2.51 (s, 3H); ¹³C NMR (100 MHz, CDCl₃) δ 165.6, 163.2, 147.5, 145.1, 138.9, 136.5, 133.2, 132.9, 130.7, 130.1, 128.6, 128.3, 128.2, 127.8, 127.8, 126.4, 124.0, 120.6, 120.5, 118.8, 114.6, 54.7, 53.0, 52.1, 21.8; IR (liquid) ν 3027, 2951, 1736, 1598, 1487, 1368, 1233, 1170, 1058 cm⁻¹; HRMS (EI) m/z

calcd. for $C_{30}H_{26}N_2O_6S$ [M]⁺: 542.1512, found: 542.1516.

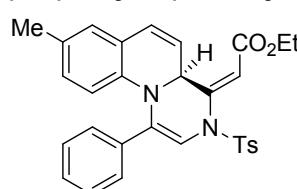
C. Chiral [5+1] cycloadducts

(S,E)-ethyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5a):



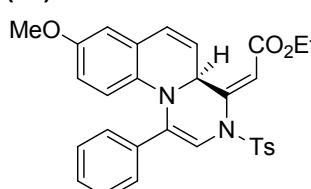
Pale yellow Solid (96%, 95.4 mg); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 139-140 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.71 (d, J = 8.26 Hz, 2H), 7.46-7.43 (m, 2H), 7.34-7.28 (m, 5H), 7.19 (s, 1H), 6.91-6.89 (m, 1H), 6.83-6.77 (m, 1H), 6.71-6.66 (m, 1H), 6.62 (s, 1H), 6.42 (d, J = 9.80 Hz, 1H), 6.17 (d, J = 8.01 Hz, 1H), 5.68 (dd, J = 9.77 Hz, J = 5.70 Hz, 1H), 4.13-4.03 (m, 2H), 3.29 (d, J = 5.70 Hz, 1H), 2.44 (s, 3H), 1.26 (t, J = 7.14 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 144.9, 138.9, 135.0, 134.5, 134.0, 129.9, 128.9, 128.6, 127.9, 127.5, 127.4, 127.0, 126.2, 125.3, 122.3, 120.6, 120.3, 118.5, 116.1, 113.5, 60.6, 54.7, 21.7, 13.9; IR (solid) ν 2922, 2853, 1718, 1487, 1343, 1167, 665 cm⁻¹; HRMS (FAB) m/z calcd. for C₂₉H₂₇N₂O₄S [M+H]⁺: 499.1692, found: 499.1689; HPLC analysis: 80% ee (CHIRALPAK AD-H, hexane/i-PrOH = 90/10, flow rate: 1.0 mL/min, T = 25 °C, 254 nm), tR (minor) = 7.840 min, tR (major) = 15.394 min.

(S,E)-ethyl 2-(8-methyl-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5b):



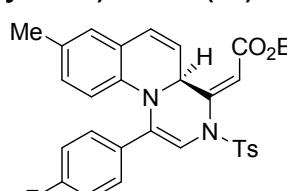
Pale yellow oil (96%); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 136-137 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.70 (d, J = 8.29 Hz, 2H), 7.46-7.43 (m, 2H), 7.34-7.28 (m, 5H), 7.16 (s, 1H), 6.72 (s, 1H), 6.61-6.59 (m, 2H), 6.39 (d, J = 9.79 Hz, 1H), 6.06 (d, J = 8.21 Hz, 1H), 5.66 (dd, J = 9.74 Hz, 5.70 Hz, 1H), 4.14-4.03 (m, 2H), 3.24 (d, J = 5.68 Hz, 1H), 2.44 (s, 3H), 2.13 (s, 3H), 1.23 (t, J = 7.15 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.4, 144.9, 136.5, 135.0, 134.0, 129.9, 129.5, 129.2, 128.9, 127.9, 127.6, 127.5, 127.5, 126.4, 125.3, 122.2, 120.7, 118.4, 116.0, 113.2, 60.6, 54.7, 21.7, 20.3, 13.9; IR (solid) ν 2981, 2912, 1715, 1492, 1186, 969, 665 cm⁻¹; HRMS (FAB) m/z calcd. For C₃₀H₂₉N₂O₄S [M+H]⁺ 513.1848, found: 513.1844; HPLC analysis: 92% ee (CHIRALPAK AD-H, hexane/i-PrOH = 90/10, flow rate: 0.15 mL/min, T = 25 °C, 254 nm), tR (major) = 66.350 min, tR (minor) = 75.923 min.

(S,E)-ethyl 2-(8-methoxy-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5c):



Pale yellow Solid (86%, 91.1 mg); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 147-148; ¹H NMR (300 MHz, CDCl₃) δ 7.72 (d, J = 8.22, 2H), 7.44-7.42 (m, 2H), 7.34-7.28 (m, 5H), 7.13 (s, 1H), 6.60 (s, 1H), 6.50 (d, J = 2.81, 1H), 6.40-6.35 (m, 2H), 6.10 (d, J = 8.80 Hz, 1H), 5.71 (dd, J = 9.73 Hz, 5.65 Hz, 1H), 4.14-4.03 (m, 2H), 3.65 (s, 3H), 3.30 (d, J = 5.62 Hz, 1H), 2.44 (m, 3H), 1.23 (t, J = 7.14 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.3, 153.6, 144.9, 135.2, 134.6, 134.0, 132.7, 129.9, 128.8, 127.9, 127.5, 127.2, 126.6, 125.5, 123.6, 122.1, 119.6, 115.7, 113.4, 112.7, 112.7, 60.6, 55.4, 54.8, 21.7, 14.0; IR (solid) ν 2963, 2921, 1721, 1488, 1166, 1079, 664 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₀H₂₉N₂O₅S [M+H]⁺: 529.1797, found: 529.1796; HPLC analysis: 98% ee (CHIRALPAK AD-H, hexane/i-PrOH = 90/10, flow rate: 1.0 mL/min, T = 25 °C, 254 nm), tR (minor) = 12.446 min, tR (major) = 33.910 min.

(S,E)-ethyl 2-(1-(4-fluorophenyl)-8-methyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5d):



Pale yellow oil (98%, 103.5 mg); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 133-134 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.70 (d, J = 8.28 Hz, 2H), 7.42-7.32 (m, 4H), 7.09 (s, 1H), 6.99 (t, J = 8.65 Hz, 2H), 6.72 (s, 1H), 6.63-6.59 (m, 2H), 6.38 (d, J = 9.79 Hz, 1H), 6.03 (d, J = 8.20 Hz, 1H), 5.66 (dd, J = 9.74 Hz, 5.68 Hz, 1H), 4.13-4.03 (m, 2H), 3.26 (d, J = 5.63 Hz, 1H), 2.44 (s, 3H), 2.14 (s, 3H), 1.22 (t, J = 7.14 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.3,

164.1, 160.8, 145.0, 136.4, 135.0, 134.0, 130.7, 130.6, 129.9, 129.8, 129.1, 127.7, 127.5, 127.5, 127.1, 127.0, 125.6, 122.4, 120.8, 118.4, 116.0, 115.9, 115.7, 112.8, 60.7, 54.8, 21.7, 20.3, 13.9; IR (solid) ν 2975, 2924, 1716, 1492, 1168, 662 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₀H₂₈FN₂O₄S [M+H]⁺: 531.1754, found: 531.1756; HPLC analysis: 80% ee (CHIRALPAK AD-H, hexane/i-PrOH = 30/70, flow rate: 0.2 mL/min, T = 25 °C, 254 nm), tR (major) = 35.841 min, tR (minor) = 42.194 min.

(S,E)-ethyl 2-(1-(4-chlorophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5e):

Pale yellow Solid (94%, 106.2 mg); R_f = 0.5 (hexane/EtOAc = 1:4); m.p. 133-134 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.70 (d, J = 8.16 Hz, 2H), 7.37-7.24 (m, 6H), 7.11 (s, 1H), 6.59 (s, 1H), 6.51-6.50 (m, 1H), 6.40-6.37 (m, 2H), 6.05 (d, J = 8.78 Hz, 1H), 5.70 (dd, J = 9.72 Hz, 5.65 Hz, 1H), 4.13-4.03 (m, 2H), 3.66 (s, 3H), 3.27 (d, J = 5.55 Hz, 1H), 2.44 (s, 3H), 1.25-1.20 (m, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.2, 153.8, 145.0, 135.0, 133.9, 133.5, 133.1, 132.4, 129.9, 129.0, 127.5, 127.2, 126.7, 125.5, 123.7, 122.1, 119.5, 115.8, 113.3, 112.9, 112.9, 60.7, 55.4, 54.7, 21.7, 14.0; IR (solid) ν 2920, 2852, 1716, 1488, 1363, 1167, 1077, 658 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₀H₂₈ClN₂O₅S [M+H]⁺: 563.1407, found: 563.1404; HPLC analysis: 99% ee (CHIRALPAK AD-H, hexane/i-PrOH = 70/30, flow rate: 1.0 mL/min, T = 25 °C, 254 nm), tR (minor) = 11.587 min, tR (major) = 29.693 min.

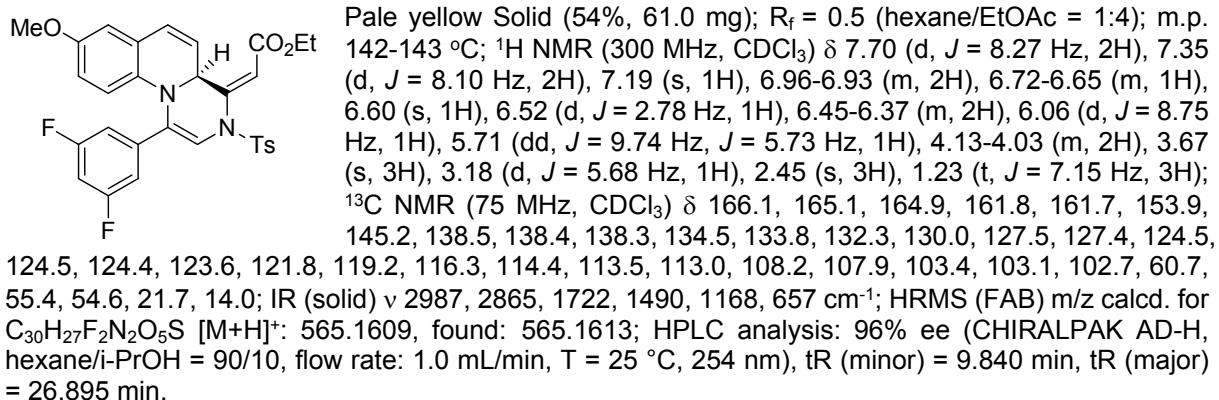
(S,E)-ethyl 2-(1-(4-bromophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5f):

Pale yellow Solid (64%, 77.2 mg); R_f = 0.5 (hexane/EtOAc = 1:4); m.p. 142-143 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.70 (d, J = 8.09 Hz, 2H), 7.43-7.40 (m, 2H), 7.34-7.27 (m, 4H), 7.12 (s, 1H), 6.59 (s, 1H), 6.50 (d, J = 2.59 Hz, 1H), 6.41-6.37 (m, 2H), 6.05 (d, J = 8.77 Hz, 1H), 5.70 (dd, J = 9.70 Hz, 5.65 Hz, 1H), 4.15-4.03 (m, 2H), 3.66 (s, 3H), 3.26 (d, J = 5.58 Hz, 1H), 2.44 (s, 3H), 1.22 (t, J = 7.13 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.2, 153.8, 145.0, 135.0, 133.9, 133.6, 132.4, 132.0, 129.9, 127.5, 127.2, 127.0, 125.5, 123.7, 122.1, 121.7, 119.5, 115.9, 113.3, 113.0, 112.9, 60.7, 55.4, 54.7, 21.7, 14.0; IR (solid) ν 2983, 1717, 1488, 1167, 1078, 667 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₀H₂₇BrN₂O₅S [M+H]⁺: 607.0902, found: 607.0900; HPLC analysis: 94% ee (CHIRALPAK AD-H, hexane/i-PrOH = 80/20, flow rate: 1.0 mL/min, T = 25 °C, 254 nm), tR (minor) = 17.033 min, tR (major) = 42.194 min.

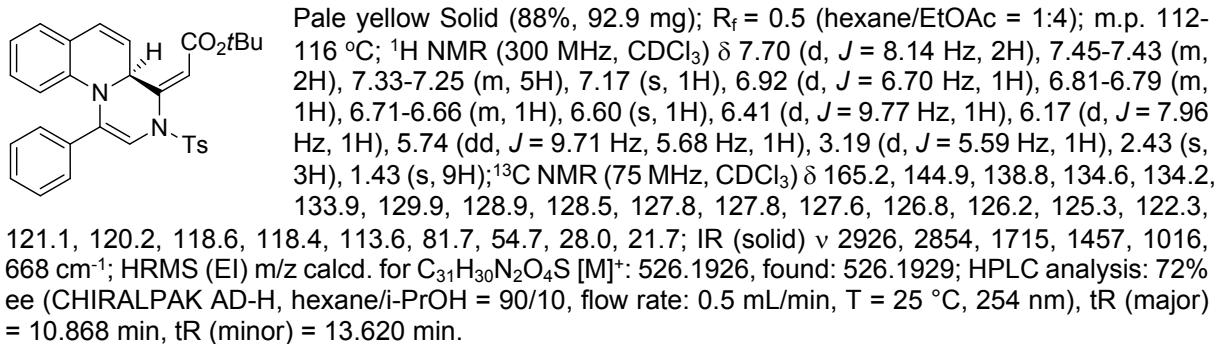
(S,E)-ethyl 2-(1-(3-fluorophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5g):

Pale yellow Solid (77%, 84.2 mg); R_f = 0.4 (hexane/EtOAc = 1:4); m.p. 145-146 °C; ¹H NMR (300 MHz, CDCl₃) δ 7.70 (d, J = 8.29 Hz, 2H), 7.34 (d, J = 8.06 Hz, 2H), 7.28-7.22 (m, 2H), 7.16 (s, 1H), 7.10 (d, J = 9.84 Hz, 1H), 6.97-6.91 (m, 1H), 6.60 (s, 1H), 6.51-6.50 (m, 1H), 6.42-6.37 (m, 2H), 6.08 (d, J = 8.78 Hz, 1H), 5.71 (dd, J = 9.72 Hz, 5.70 Hz, 1H), 4.14-4.03 (m, 2H), 3.66 (s, 3H), 3.24 (d, J = 5.55 Hz, 1H), 2.44 (s, 3H), 1.23 (t, J = 7.14 Hz, 3H); ¹³C NMR (75 MHz, CDCl₃) δ 166.2, 164.8, 161.6, 153.8, 145.1, 137.2, 137.1, 134.9, 134.0, 132.5, 130.4, 130.3, 130.0, 127.5, 127.3, 125.4, 125.4, 123.7, 122.0, 120.9, 120.9, 119.4, 116.0, 114.8, 114.6, 113.5, 113.4, 112.8, 112.6, 112.2, 60.7, 55.4, 54.7, 21.7, 14.0; IR (solid) ν 2986, 2901, 1721, 1226, 1049, 664 cm⁻¹; HRMS (FAB) m/z calcd. for C₃₀H₂₈FN₂O₅S [M+H]⁺: 547.1707, found: 547.1707; HPLC analysis: 98% ee (CHIRALPAK AD-H, hexane/i-PrOH = 90/10, flow rate: 1.0 mL/min, T = 25 °C, 254 nm), tR (minor) = 13.012 min, tR (major) = 34.082 min.

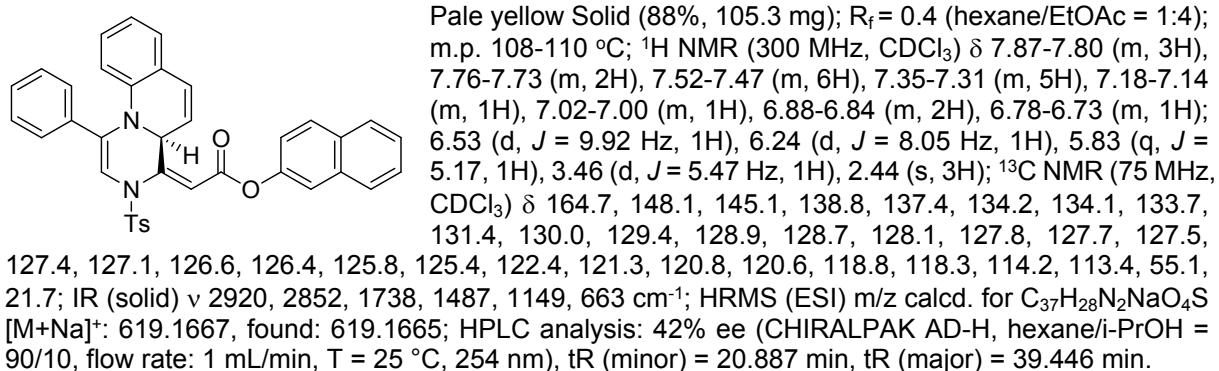
(S,E)-ethyl 2-(1-(3,5-difluorophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5h):



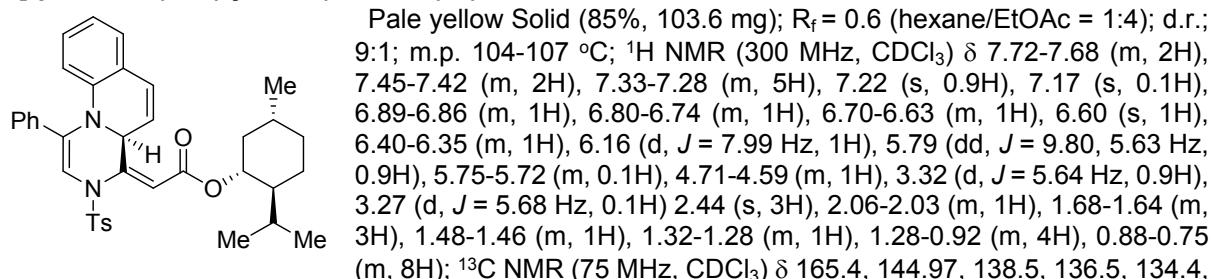
(S,E)-tert-butyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5i):



(S,E)-naphthalen-2-yl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5j):



**(E)-(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl
a]quinolin-4(4aH)-ylidene)acetate (5k):**



134.0, 129.9, 128.9, 128.3, 127.9, 127.6, 126.9, 126.6, 126.2, 125.3, 122.3, 121.2, 120.1, 118..5, 116.0, 113.5, 75.0, 54.9, 46.6, 40.7, 34.1, 31.4, 25.5, 23.2, 22.0, 21.7, 20.9, 16.4; IR (solid) ν 2952, 2869, 1713, 1487, 1366, 1170, 665 cm^{-1} ; HRMS (FAB) m/z calcd. for $\text{C}_{37}\text{H}_{41}\text{N}_2\text{O}_4\text{S} [\text{M}+\text{H}]^+$: 609.2782, found: 609.2787; HPLC analysis: 80% ee (CHIRALPAK OD-H, hexane/i-PrOH = 90/10, flow rate: 0.5 mL/min, $T = 25^\circ\text{C}$, 254 nm), tR (major) = 9.500 min, tR (minor) = 10.380 min.

IV. Computational details

All calculations were carried out using density functional theory (DFT)^{S2} implemented in Jaguar 9.1 suite of program.^{S3} Geometry optimizations were carried out with B3LYP-D3^{S4} levels of theory and 6-31G** basis set.^{S5} For the Cu and I atom, Los Alamos LACVP**^{S6} basis set was applied, which includes effective core potentials. With the optimized geometries, single point energies were re-evaluated using triple- ζ quality of basis set, cc-pVTZ(-f),^{S7} where Cu and I atoms were computed with LACV3P** basis set. Frequency calculations were performed at the same level as the geometry optimizations, and zero-point energies and entropy correction terms were derived. Solvation correction energies were evaluated from the self-consistent reaction field (SCRF) approximations,^{S8} which is the solution for the linearized Poisson-Boltzmann equations with a proper dielectric constant ($\epsilon = 8.93$ for DCM solvents). Several transition states were found by using the quadratic synchronous transit search method (QST).^{S9} Final solution phase Gibbs free energies were computed as follows:

$$G(\text{Sol}) = G(\text{gas}) + G^{\text{solv}} \quad (\text{eq } 1)$$

$$G(\text{gas}) = H(\text{gas}) - TS(\text{gas}) \quad (\text{eq } 2)$$

$$H(\text{Gas}) = E(\text{SCF}) + ZPE \quad (\text{eq } 3)$$

$$\Delta G(\text{Sol}) = \sum G(\text{Sol}) \text{ for products} - \sum G(\text{Sol}) \text{ for reactants} \quad (\text{eq } 4)$$

$G(\text{Sol})$ is the solvation corrected Gibbs free energy; $G(\text{gas})$ is the gas phase free energy; $H(\text{gas})$ is the enthalpy in the gas phase; T is the temperature (120°C , 393.15 K); $S(\text{gas})$ is the entropy in the gas phase; $E(\text{SCF})$ is the electronic energy converged from the self-consistent field method; ZPE is the vibrational zero-point energy; and S for the vibrational entropy correction. Note that here entropy refers specifically to the vibrational/rotational/translational entropy of the solute(s). The solvent entropies are implicitly included in the continuum model.

IV-1. Full Energy profile of the [5 + 1] cycloaddition process

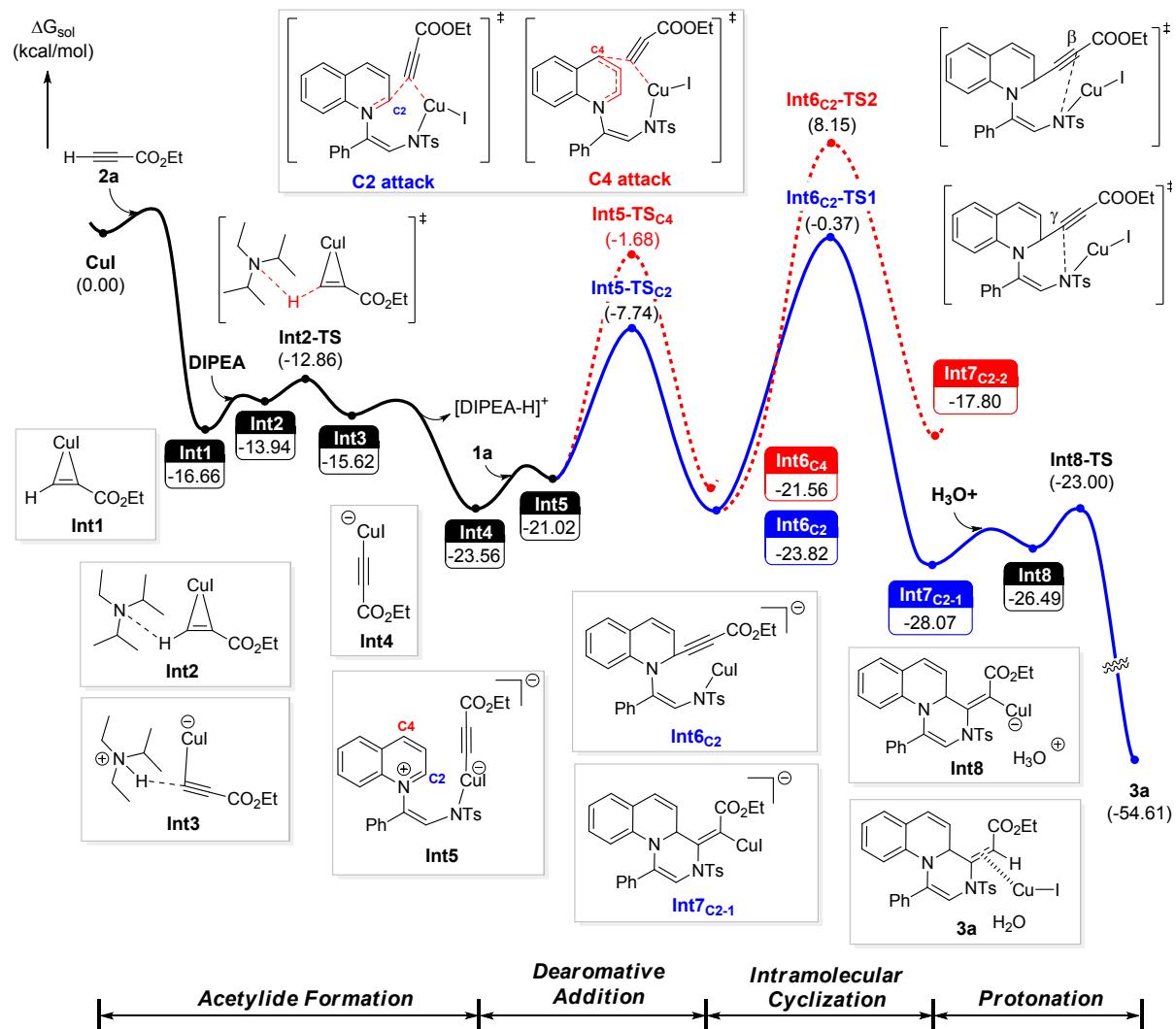


Figure S1. Full energy profile of overall catalysis

IV-2. DFT-optimized structure's energy components

Table S1. Computed energy components for DFT-optimized structures.

	E(SCF)/(eV)	ZPE/(kcal/mol)	S(gas)/(cal/mol)	G(solv)/(kcal/mol)
	cc-pVTZ(-f)/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**	6-31G**/LACVP**
CuI	-5648.89	0.345	61.362	-12.08
1a	-43133.117	242.104	168.103	-20.8
2a	-9378.444	62.757	84.944	-6.15
DPEA	-10100.601	165.176	101.928	-1.3
[DPEA-H]⁺	-10111.292	175.331	100.396	-47.17
H₂O	-2080.542	13.447	46.482	-7.63
H₃O⁺	-2088.092	21.634	48.409	-89.54
Int1	-15028.676	63.539	117.177	-13.06
Int2	-25129.922	230.213	178.792	-10.29
Int2-TS	-25129.762	228.942	174.375	-12.94
Int3	-25129.848	231.816	175.764	-16.18
Int4	-15015.106	57.064	113.05	-45.85
Int5	-58149.125	299.568	233.322	-58.42
Int5-TS_{C2}	-58148.621	298.826	239.558	-54.17
Int6_{C2}	-58149.652	300.188	238.665	-48.1
Int5-TS_{C4}	-58148.422	298.875	237.188	-53.45
Int6_{C4}	-58149.559	300.481	238.135	-48.43
Int6_{C2}-TS1	-58148.641	299.9	230.826	-50.01
Int6_{C2}-TS2	-58148.566	299.898	224.265	-45.08
Int7_{C2}-1	-58149.871	301.752	231.687	-50.94
Int7_{C2}-2	-58149.758	301.535	214.367	-48.23
Int8	-60243.605	323.955	240.731	-21.1
Int8-TS	-60243.48	322.895	238.132	-20.21
3a	-60244.953	325.011	239	-21.01

IV-3. Cartesian coordinates of the optimized geometries

Table S2. Cartesian Coordinates of the Optimized Geometries.

Cu	-0.412104398	-0.004865270	-1.710399270	C	-3.612285137	0.138540044	-0.136312813
I	-0.412104398	-0.004865270	-4.146350861	O	-3.877204418	1.166050553	0.452548087
1a				O	-3.302041292	-1.035730720	0.445861548
S	11.500761986	9.006990433	17.362535477	C	-3.269607544	-1.036883473	1.897781968
O	11.973649979	7.652774811	17.677822113	H	-4.131026268	-0.476852536	2.271574497
O	10.613439560	9.712651253	18.311840057	H	-3.378446102	-2.090986013	2.161948681
C	12.947298050	10.046744347	17.126338959	C	-1.964202166	-0.454300314	2.417387486
C	14.109297752	9.496315956	16.581996918	H	-1.935136437	-0.529062808	3.509517908
H	14.144269943	8.434886932	16.359560013	H	-1.108292460	-0.998899341	2.009004354
C	15.206830025	10.319381714	16.349010468	H	-1.882485747	0.599452615	2.141132355
H	16.114816666	9.895013809	15.926396370				
C	15.164545059	11.689129829	16.653600693				
C	13.990452766	12.213978767	17.206785202				
H	13.943722725	13.270974159	17.457748413				
C	12.881507874	11.401700020	17.445968628				
H	11.974184990	11.801660538	17.886146545				
N	10.867301941	8.961616516	15.825542450				
C	9.793774605	9.706750870	15.605989456				
H	9.342392921	10.271635056	16.425586700				
C	9.168543816	9.823209763	14.365386963				
C	7.971968174	10.620610237	14.106476784				
C	7.667078972	11.754991531	14.889806747				
H	8.349890709	12.064314842	15.674986839				
C	6.514533997	12.499197006	14.653619766				
H	6.305634499	13.366142273	15.274548531				
C	5.644230366	12.157927513	13.615035057				
H	4.754250050	12.749966621	13.424356461				
C	5.940220356	11.048456192	12.820807457				
H	5.273398399	10.764410019	12.010869980				
C	7.079387665	10.287551880	13.065858841				
H	7.277441502	9.415708542	12.449009895				
N	9.712850571	9.042119026	13.285727501				
C	10.140007973	9.633846283	12.091400146				
C	10.662698746	8.802744865	11.056351662				
C	10.820591927	7.416484356	11.293539047				
H	11.232925415	6.786441326	10.511829376				
C	10.465811729	6.892512798	12.516285896				
H	10.584405899	5.839828014	12.743833542				
C	9.897656441	7.723577499	13.483036995				
C	16.370979309	12.563588142	16.405855179				
H	17.180303574	12.325853348	17.106821060				
H	16.767972946	12.417006493	15.395000458				
H	16.130994797	13.624247551	16.524120331				
H	9.562524796	7.346113205	14.437938690				
C	11.056143761	9.402522087	9.831327438				
H	11.441815376	8.763105392	9.042511940				
C	10.090106964	11.031597137	11.909139633				
H	9.734464645	11.663758278	12.710268974				
C	10.498306274	11.578534126	10.710533142				
H	10.462533951	12.655669212	10.580966949				
C	10.969242096	10.763467789	9.656580925				
H	11.276865959	11.215989113	8.719141960				
2a							
H	-3.572149038	-0.069772825	-3.852398634				
C	-3.579743624	-0.033312812	-2.786874056				
C	-3.590519190	0.017917665	-1.580904245				

H	-4.633897305	0.265839815	-4.582134724	H	-6.540258408	-1.483180165	-7.247339249
H	-2.386822939	1.899728417	-1.224757314	H	-5.370159149	-2.430398464	-6.320995331
H	-4.087001324	2.275995970	-1.453346848	H	-5.636474609	2.793981314	-6.291402817
H	-3.627748728	0.679297030	-0.868987083	C	-3.888095617	1.586044908	-6.444665432
H	0.711864233	0.482611030	-1.522723675	C	-5.822257519	1.640326381	-8.077309608
H	-0.903234243	0.311628640	-0.842371821	H	-3.546918154	0.619154811	-6.825403214
H	-0.109332874	-1.069397449	-1.635913014	H	-3.371481657	2.363274813	-7.015320301
H	0.209829926	-1.056545496	-4.238019943	H	-3.567251444	1.668863416	-5.402054787
H	-0.229684815	0.412844032	-5.146157265	H	-6.881035328	1.873911262	-8.217298508
H	1.120450616	0.435608923	-4.014778614	H	-5.247791290	2.350639820	-8.682176590
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H ₂ O							
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H	-1.584139466	0.029185895	-4.309783459	H	-7.750090599	2.173318148	-5.992175102
O	-1.572526336	0.006211828	-5.273819923	C	-8.480875969	0.207272530	-6.441217899
H	-1.148426414	-0.833086252	-5.483215332	C	-8.132694244	1.170851469	-4.143980026
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H ₃ O+							
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H	-1.439064145	0.237803861	-4.333605766	H	-5.691183090	1.069013834	-4.625118256
O	-1.606095433	-0.021068072	-5.266177177	C	-5.147783756	1.238115072	-3.382566452
H	-0.969501019	-0.691472590	-5.597656727	C	-4.694851398	1.351420760	-2.231908321
H	-1.697879791	0.750199676	-5.867311954	C	-4.050462723	1.731834173	-0.981965959
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Int1							
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H	-4.514518261	2.143702269	-3.724833488	H	-3.350543737	2.713120699	-0.849657953
C	-4.431240559	1.834008336	-2.702206135	O	-4.346377850	0.841892123	-0.014603788
C	-4.177646160	1.678278685	-1.510039687	C	-3.732468605	1.062424302	1.283774257
C	-3.741186619	1.748944521	-0.106501281	H	-3.759596825	2.132029533	1.508817673
O	-2.954156160	2.579530716	0.282870829	H	-4.382849693	0.525745749	1.977216840
O	-4.339341640	0.797537029	0.610915303	C	-2.311006069	0.522581220	1.304280281
C	-3.996552944	0.723632991	2.030118942	H	-1.887298107	0.627373099	2.308549881
H	-3.950689793	1.741428494	2.425898790	H	-2.299082756	-0.536905885	1.031883121
H	-4.843152046	0.194274336	2.469025373	H	-1.682938099	1.07948498	0.604052663
C	-2.686925888	-0.021310335	2.225899935	Cu	-5.755667686	-0.521072149	-2.441339731
H	-2.481001377	-0.124080122	3.296094418	I	-6.893315315	-2.728375673	-2.391909599
H	-2.743328094	-1.021122217	1.786658287	N	-6.151451588	0.772317588	-5.818737507
H	-1.860375404	0.527572632	1.767969251	C	-5.835749626	-0.688854218	-5.842511654
Cu	-5.489286423	0.113189504	-2.109960318	C	-5.313005924	1.688775897	-6.672486305
I	-6.953001499	-1.858584166	-2.154719353	C	-7.623710155	1.121730089	-5.812602520
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Int2							
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H	-5.412692547	1.487176299	-4.010047436	H	-4.889014721	-0.805146694	-5.302953720
C	-5.001444340	1.505541801	-2.975527287	H	-6.579095840	-1.173679233	-5.205496788
C	-4.562833786	1.543895364	-1.827366233	C	-5.739256859	-1.425210714	-7.181012630
C	-3.920972586	1.835506916	-0.542443514	H	-4.904396057	-1.075229049	-7.791975498
O	-3.155374765	2.757423162	-0.376993626	H	-6.650994778	-1.352666020	-7.774718285
O	-4.312249184	0.942381442	0.376340419	H	-5.565672398	-2.484551907	-6.966044903
C	-3.724067688	1.060459614	1.705179572	H	-5.466055870	2.673964024	-6.210289955
H	-3.664490938	2.120120287	1.966503143	C	-3.820544958	1.359360576	-6.537015438
H	-4.446173191	0.561269403	2.353357077	C	-5.735455513	1.802206159	-8.143261909
C	-2.360501289	0.390421242	1.744712114	H	-3.554922342	0.427740961	-7.043027401
H	-1.963499427	0.421991944	2.764538765	H	-3.239812851	2.162353039	-7.000027180
H	-2.437570095	-0.655818701	1.435197592	H	-3.515060425	1.286724329	-5.490597725
H	-1.659411788	0.908975482	1.085789800	H	-6.758870602	2.168914557	-8.251438141
Cu	-5.641353130	-0.300963789	-2.072175026	H	-5.078276634	2.521351337	-8.642772675
I	-6.746649265	-2.501758337	-1.868583918	H	-5.651553631	0.850630999	-8.671847343
N	-6.149561405	0.910814762	-5.637733936	H	-7.655741215	2.186810732	-6.068045616
C	-5.723911285	-0.489405632	-5.461435795	C	-8.473124504	0.351847619	-6.832281113
C	-5.405332565	1.762979150	-6.598134518	C	-8.219310760	0.959581792	-4.405883312
C	-7.617871284	1.160070419	-5.593381405	H	-9.485562325	0.767277181	-6.832238674
H	-4.748957634	-0.486023247	-4.952908039	H	-8.083244324	0.419302106	-7.848970890
H	-6.410271645	-0.941548944	-4.739758492	H	-8.556298256	-0.704253137	-6.559188843
C	-5.611168385	-1.423298717	-6.678277493	H	-8.138733864	-0.070262954	-4.042335987
H	-4.814319134	-1.117898941	-7.361166954	H	-7.732660294	1.611392617	-3.677279711
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Int3							
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H	-5.834667206	0.967998505	-4.878380775	H	-6.060727119	1.939709783	10.217313766	
C	-5.124508381	1.201382875	-3.376054764	H	-6.714450836	0.506666839	11.055256844	
C	-4.678544998	1.317632318	-2.216357231	C	-4.882508755	1.301669240	11.918548584	
C	-4.065066338	1.715490818	-0.963163555	H	-5.389751434	1.943241477	12.648912430	
O	-3.391659021	2.716134787	-0.817757905	H	-4.588481903	0.371761501	12.416379929	
O	-4.349518776	0.824679971	0.012545847	H	-3.982230902	1.811833501	11.569114685	
C	-3.763958454	1.086647153	1.312631488	Cu	-2.172201157	-2.657597780	6.652767181	
H	-3.837764502	2.156742573	1.525866270	S	-1.899662614	-3.816845179	3.602802992	
H	-4.398260117	0.531596422	2.007061958	O	-2.877159119	-3.055118561	2.804049492	
C	-2.319852114	0.610613108	1.360751510	O	-1.316041350	-5.043632030	3.017521620	
H	-1.914350152	0.744998693	2.369118214	C	-0.566819429	-2.701918364	4.031260014	
H	-2.257015944	-0.450139672	1.100080013	N	-2.583526611	-4.112500668	5.102006912	
H	-1.70866954	1.186763406	0.661591291	C	-0.878197610	-1.393723845	4.416769028	
Cu	-5.768301487	-0.562900722	-2.557482481	C	0.741223693	-3.172683954	4.081079960	
I	-6.971524715	-2.752318144	-2.615356684	H	-1.901539445	-1.038404465	4.363153458	
N	-6.215029716	0.739968836	-5.892019272	C	0.141255200	-0.564440310	4.877542496	
C	-5.930918217	-0.741548955	-5.977842331	H	-0.103741057	0.440247267	5.212011814	
C	-5.353491783	1.676806331	-6.730430126	C	1.464933991	-1.018263340	4.950635910	
C	-7.694424629	1.127623200	-5.864355087	C	1.750334620	-2.321132660	4.526419163	
H	-4.987984657	-0.883662879	-5.443303108	C	2.541975260	-0.140665099	5.540976524	
H	-6.684329987	-1.227821827	-5.355668068	H	2.771146774	-2.690554380	4.585494518	
C	-5.856203556	-1.403889537	-7.350640297	H	0.949730515	-4.198022842	3.798040628	
H	-5.010293007	-1.050245047	-7.943411827	C	-2.766289711	-5.401069164	5.431294441	
H	-6.765504360	-1.280691147	-7.939274311	H	-2.297982931	-6.171095848	4.816769123	
H	-5.712767124	-2.476120234	-7.184472561	C	-3.529162884	-5.830478668	6.499671459	
H	-5.491367340	2.640040874	-6.223750591	C	-3.645432472	-7.210012436	6.949705601	
C	-3.872267723	1.307519317	-6.604329109	N	-4.309440136	-4.828204155	7.199426651	
C	-5.797001362	1.839485645	-8.185751915	C	-2.609471083	-8.139503479	6.710875034	
H	-3.624541044	0.391039073	-7.145503998	C	-4.778970718	-7.663522720	7.657997131	
H	-3.276030064	2.116800785	-7.035377026	H	-1.694502234	-7.801383972	6.234962940	
H	-3.581653118	1.194586635	-5.557414055	C	-2.725244045	-9.462145805	7.127071857	
H	-6.812064171	2.233953953	-8.270895958	H	-1.908095241	-10.152592659	6.932269573	
H	-5.128482819	2.560057163	-8.666876793	C	-3.856557608	-9.897291183	7.823446751	
H	-5.737433434	0.905738711	-8.747241974	H	-3.932886124	-10.925748825	8.165802956	
H	-7.693948746	2.200148582	-6.085210800	C	-4.877299786	-8.982430458	8.091672897	
C	-8.550918579	0.405567348	-6.906627178	H	-5.761687279	-9.298570633	8.640432358	
C	-8.269933701	0.927136183	-4.457904816	H	-5.588646889	-6.97024586	7.868833065	
H	-9.555685997	0.837423563	-6.882085800	C	-4.085295200	-4.527226448	8.542984009	
H	-8.169076920	0.507008970	-7.923404694	C	-5.191764832	-4.112909317	6.479850292	
H	-8.649618149	-0.657498121	-6.670343399	C	-4.831351280	-3.468146086	9.138739586	
H	-8.229241371	-0.120401546	-4.142555714	C	-3.095055103	-5.199647427	9.286566734	
H	-7.736301422	1.520493269	-3.713459969	C	-5.740513802	-2.729755878	8.349665642	
H	-9.319440842	1.235864043	-4.4605455540	C	-4.577291965	-3.127028465	10.490275383	
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Int4				H	-6.238430500	-1.874577761	8.791758537	
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C	-2.700005054	-1.087309957	8.563749313	C	-5.923947334	-3.062846422	7.024960518	
C	-3.369582415	-0.216331765	9.120898247	H	-6.588897228	-2.500290632	6.380941391	
C	-4.137498856	0.807126820	9.744308472	H	-5.269426823	-4.396858692	5.439546585	
O	-4.027868748	2.014169216	9.577053070	H	2.404412270	0.911047697	5.266087055	
O	-5.071971893	0.278332651	10.606404305	H	2.514348984	-0.199968562	6.636059761	
C	-5.881657600	1.234000802	11.304340363	H	3.540850878	-0.452029139	5.218191624	
H	-6.185415745	2.0327666342	10.619507790	H	-5.108764648	-2.280799866	10.910445213	
H	-6.768444538	0.673529088	11.617789268	C	-3.628754377	-3.811811447	11.211820602	
C	-5.144186497	1.815459847	12.505846024	H	-2.472164154	-5.940690041	8.809638023	
H	-5.800510406	2.486071587	13.073149681	C	-2.884639025	-4.844282150	10.601500511	
H	-4.804837704	1.014355302	13.170188904	H	-2.095366955	-5.340662479	11.156929970	
H	-4.275117874	2.380993843	12.162494659	H	-3.421060085	-3.534628868	12.241329193	
Cu	-1.675739169	-2.436619997	7.731857777	I	-0.029517740	-3.994134665	7.744849205	
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Int5				<hr/>				
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C	-3.064755678	-1.184845924	7.463758945	C	-4.592882633	-2.591834068	7.132783890	
C	-3.632411957	-0.308942437	8.126902580	C	-5.671896935	-1.989696622	7.232582092	
C	-4.243440151	0.671234906	8.944450378	C	-6.859876156	-1.221808910	7.409618378	
O	-4.037826061	1.875882149	8.961069107	O	-7.372366905	-0.463304877	6.603885174	
O	-5.182324886	0.100760974	9.806852341	O	-7.395478725	-1.448698521	8.656668663	
C	-5.796809196	1.010871649	10.733160973	C	-8.582190514	-0.695356548	8.967459679	
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H	-7.541970730	0.722415388	10.232118607	O	-2.899425507	-1.462031722	4.238188744
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Cu	-2.680474281	-2.398050070	6.521539688	C	-0.556172311	-2.615020514	4.585879803
S	-1.269893885	-3.661099195	3.959587097	N	-2.846837044	-3.638634443	5.543009758
O	-1.576382637	-2.296246290	3.508098364	C	-0.161229238	-1.608651876	5.470125675
O	-1.289808989	-4.776911736	2.987578869	C	0.361382902	-3.549568653	4.109778404
C	0.366625905	-3.618884802	4.700393677	H	-0.889144063	-0.897578180	5.844190598
N	-2.220086813	-3.984098434	5.284929752	C	1.161642790	-1.560099483	5.897649765
C	0.723074734	-2.514776230	5.477152824	H	1.456144452	-0.797731221	6.614145756
C	1.226357102	-4.706598759	4.564473152	C	2.101950407	-2.497010946	5.448019505
H	0.043036181	-1.677469850	5.583663464	C	1.687237501	-3.480161428	4.539775372
C	1.942794442	-2.520361423	6.145359039	C	3.515958309	-2.470694780	5.978600025
H	2.198036909	-1.672750592	6.776391983	H	2.407736540	-4.208450794	4.173588753
C	2.824991226	-3.604743481	6.035524845	H	0.031197913	-4.315679550	3.415628672
C	2.455234051	-4.688522339	5.227757931	C	-3.092329264	-4.971077442	5.383937836
C	4.124372005	-3.607996702	6.805225849	H	-3.116538525	-5.341122150	4.361106873
H	3.133893728	-5.532331467	5.120352745	C	-3.265413523	-5.874262333	6.396681309
H	0.929592371	-5.545573235	3.943438053	C	-3.621001482	-7.280573368	6.166481972
C	-2.770863771	-5.220118523	5.364573002	N	-3.129015684	-5.494567871	7.771142483
H	-2.765746593	-5.834259033	4.464114666	C	-4.219289303	-7.734980583	4.971240997
C	-3.281650305	-5.771018505	6.512380600	C	-3.395663500	-8.237420082	7.179745197
C	-3.968395948	-7.056479931	6.604850769	H	-4.462844849	-7.021404266	4.190460682
N	-3.134229422	-5.046853065	7.759816170	C	-4.535796165	-9.077465057	4.788739204
C	-4.499819756	-7.710495472	5.470160007	H	-4.996971607	-9.392639160	3.855423450
C	-4.150827885	-7.688782215	7.855044365	C	-4.296520710	-10.013204575	5.799989223
H	-4.429763794	-7.234862804	4.497212410	H	-4.560874462	-11.058153152	5.660221577
C	-5.142626286	-8.938876152	5.580312729	C	-3.728959084	-9.577371597	6.998728752
H	-5.541294098	-9.409600258	4.684558868	H	-3.540062428	-10.286285400	7.802151680
C	-5.307026386	-9.554996490	6.825334072	H	-2.947121382	-7.910217285	8.112929344
H	-5.825271606	-10.506230354	6.909011841	C	-1.902786374	-5.126204967	8.332162857
C	-4.807622910	-8.912608147	7.959869385	C	-4.400795937	-5.360965252	8.502690315
H	-4.928613186	-9.366996765	8.940855026	C	-1.811923385	-4.899314404	9.730302811
H	-3.764521837	-7.211017132	8.749982834	C	-0.735684395	-5.012012959	7.554987431
C	-1.877114773	-4.889872074	8.359914780	C	-3.006556034	-5.059920311	10.540118217
C	-4.229607582	-4.367468357	8.218385696	C	-0.585564852	-4.535663128	10.293875694
C	-1.799899101	-4.203812122	9.599984169	H	-2.900800467	-4.979364395	11.620058060
C	-0.706811786	-5.391635418	7.768058300	C	-4.206302166	-5.303798676	9.999767303
C	-3.007435083	-3.697533131	10.189150810	H	-5.100135326	-5.413907051	10.606485367
C	-0.541973531	-4.025307178	10.204380989	H	-5.007694244	-6.243892193	8.249511719
H	-2.947679520	-3.209996939	11.158051491	H	3.896064281	-1.446350336	6.057714462
C	-4.191107750	-3.799504757	9.537748337	H	3.558615208	-2.907382488	6.984875202
H	-5.107819080	-3.364289761	9.917438507	H	4.199749947	-3.040339231	5.341265202
H	-5.162870407	-4.732064724	7.814729214	H	-0.547104478	-4.343118668	11.363755226
H	4.631886959	-2.639329433	6.737411976	C	0.559738338	-4.400773525	9.515146255
H	3.943632364	-3.800033092	7.870667934	H	-0.786050916	-5.178178310	6.487926960
H	4.811285973	-4.378315926	6.440505981	C	0.472277790	-4.647198200	8.144316673
H	-0.492451549	-3.474186420	11.139560699	H	1.344194889	-4.531259060	7.506370544
C	0.609405816	-4.504622936	9.604770660	H	1.498502970	-4.092352390	9.965654373
H	-0.765863001	-5.899529457	6.815864563	I	-1.934105039	-0.946590602	8.971997261

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Int5-TSV

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C	-3.587924242	-1.903615475	8.010841370
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O	-3.592478514	1.403333426	6.915669918
O	-4.843957424	1.220396161	8.806703568
C	-5.065693378	2.642619371	8.758063316
C	-5.261033535	2.946783304	7.724936008
H	-5.968020916	2.800591946	9.356688499
C	-3.878296852	3.407237768	9.329777718
H	-4.092764378	4.481871605	9.354850769
H	-3.659857035	3.070850849	10.348060608
H	-2.996839523	3.240238190	8.706757545
Cu	-2.227208614	-3.099596024	7.141728878
S	-2.086081982	-3.662577629	3.983821392
O	-3.227574825	-3.064989567	3.264271975
O	-1.236221790	-4.625476360	3.248499155
C	-1.059454560	-2.329050303	4.586249828
N	-2.617726326	-4.302696705	5.443394184

C	-1.672499657	-1.188299537	5.113615036	H	-1.820482612	0.924450934	5.329008579
C	0.326169580	-2.469898939	4.587746620	C	0.201304644	0.290096074	4.896140099
H	-2.751359940	-1.085924029	5.095132351	C	0.994414330	-0.795330405	4.503985882
C	-0.879745066	-0.192826942	5.680482388	C	0.824095786	1.627557755	5.218639374
H	-1.370569587	0.668414652	6.124049187	H	2.069795132	-0.665248215	4.403656960
C	0.513356745	-0.324645728	5.719484329	H	1.028293729	-2.883399963	3.917544842
C	1.102605343	-1.460028172	5.148392677	C	-2.386178017	-5.729935169	5.364567757
C	1.361023426	0.697281003	6.435754299	H	-1.913850188	-6.284455776	4.552841187
H	2.183729172	-1.572341919	5.178300381	C	-3.183901787	-6.417747498	6.232720852
H	0.771316826	-3.369683743	4.177957058	C	-3.345489740	-7.874674797	6.211750507
C	-2.885586739	-5.627462864	5.406208038	N	-4.002693176	-5.661063671	7.136018753
H	-2.516962051	-6.189967632	4.547668457	C	-2.440056801	-8.726942062	5.540440559
C	-3.601014614	-6.319417477	6.356460094	C	-4.430471897	-8.482171059	6.878087521
C	-3.870169163	-7.751615047	6.357927799	H	-1.560150385	-8.307226181	5.062666893
N	-4.185009003	-5.516910076	7.410515308	C	-2.640681744	-10.102912903	5.498762608
C	-3.192831039	-8.651750565	5.501332760	H	-1.926822186	-10.727992058	4.966720104
C	-4.822451115	-8.307135582	7.242501736	C	-3.731233120	-10.686444283	6.150290966
H	-2.420323849	-8.282064438	4.835011005	H	-3.877862453	-11.763203621	6.126759052
C	-3.477382421	-10.012488365	5.511865616	C	-4.617291451	-9.861901283	6.846357346
H	-2.933626413	-10.670449257	4.837561607	H	-5.465909481	-10.296065331	7.370478153
C	-4.430848122	-10.543231010	6.387400627	H	-5.130720615	-7.855162621	7.420333385
H	-4.640055656	-11.609292030	6.400561333	C	-3.705787182	-5.529427528	8.499107361
C	-5.093726158	-9.673447609	7.255046844	C	-5.159036160	-5.079257011	6.634727478
H	-5.832555294	-10.059963226	7.953891277	C	-4.455806732	-4.645203114	9.303318024
H	-5.350944996	-7.652330399	7.928402901	C	-2.678049088	-6.289219379	9.083197594
C	-3.581899881	-5.410381317	8.668547630	C	-5.498639584	-3.715924263	8.676837921
C	-5.272019386	-4.751066208	7.105414867	C	-4.175155640	-4.564672947	10.667049408
C	-3.949187756	-4.327326775	9.504281998	H	-6.350905895	-3.630894899	9.368396759
C	-2.635910749	-6.351382256	9.106659889	C	-5.948405266	-4.251564503	7.334558010
C	-4.832878590	-3.311339617	8.969060898	H	-6.844043732	-3.842651367	6.882018566
C	-3.361917019	-4.220359325	10.776526451	H	-5.389723778	-5.376430988	5.617899418
H	-5.182794094	-2.555558205	9.661287308	H	0.168521523	2.454314232	4.924953938
C	-5.680399418	-3.712412357	7.894699574	H	1.000971437	1.721734166	6.297134399
H	-6.515923977	-3.096971035	7.585620880	H	1.786205411	1.757427573	4.712281227
H	-5.746221542	-5.003414154	6.165235043	H	-4.742506027	-3.861126661	11.272425652
H	0.889619827	1.685367346	6.436681747	C	-3.163807392	-5.325240135	11.247859955
H	1.496068120	0.391362458	7.480660439	H	-2.092731237	-6.952061176	8.457175255
H	2.356267452	0.788678348	5.986602306	C	-2.410520554	-6.180308819	10.441302299
H	-3.613341570	-3.362945318	11.394725800	H	-1.600561619	-6.764176846	10.870116234
C	-2.456493139	-5.168421268	11.218525887	H	-2.946180105	-5.230313778	12.307486534
H	-2.336922884	-7.156212330	8.448116302	I	-0.823426187	-2.420598269	9.183109283
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C	-4.821478367	-3.234471560	7.400520325				
C	-5.233264923	-2.185320377	8.014763832				
C	-4.772572517	-0.843588531	8.058764458				
O	-5.361106396	0.186915681	7.789143562				
O	-3.445422888	-0.785341382	8.583147049				
C	-2.919785500	0.544787645	8.803588867				
H	-3.717605352	1.164585710	9.221829414				
H	-2.126377344	0.404990137	9.542743683				
C	-2.378772974	1.144892097	7.512493134				
H	-2.025761366	2.168411732	7.688045979				
H	-1.534393072	0.549404740	7.147760391				
H	-3.165636301	1.158121467	6.755607605				
Cu	-2.044036865	-2.134466171	7.593154430				
S	-3.787340641	-2.521764278	4.830704212				
O	-4.097352982	-1.109436154	5.067920685				
O	-4.763666153	-3.400625944	4.162869453				
C	-2.250493765	-2.623945475	3.907355070				
N	-3.356062651	-3.190722704	6.357001305				
C	-1.171246409	-1.823506236	4.287822247				
C	-2.121867180	-3.568340540	2.889782667				
H	-1.277890325	-1.106756330	5.094556332				
C	0.052627075	-1.989128828	3.647514582				
H	0.901314080	-1.392327189	3.970055819				
C	0.212896466	-2.934630394	2.623520374				
C	-0.892407477	-3.708949327	2.246353388				
C	1.562925220	-3.138782978	1.978625774				

H	-0.785446346	-4.445038795	1.452768564	C	-2.408386707	-5.810786247	6.022752285
H	-2.976199865	-4.181749344	2.623847485	C	-2.739942789	-7.234930992	5.917011738
C	-2.669408798	-4.431712151	6.265500546	N	-1.960951328	-5.368016720	7.316122532
H	-1.898735166	-4.507696152	5.507040977	C	-3.498095989	-7.761528015	4.848560810
C	-2.875128269	-5.467810631	7.111510754	C	-2.320297956	-8.134575844	6.919639111
C	-1.983839393	-6.644415379	7.099977016	H	-3.889965773	-7.092098713	4.089031219
N	-4.013160706	-5.484228611	7.940098763	C	-3.780078173	-9.121599197	4.768982887
C	-0.607024848	-6.499007225	6.855360031	H	-4.366269588	-9.495868683	3.932816029
C	-2.495927811	-7.930359840	7.341961384	C	-3.344235182	-10.001295090	5.764643192
H	-0.188186377	-5.501880169	6.746068954	H	-3.581634998	-11.060427666	5.707693577
C	0.223362297	-7.618217468	6.813295841	C	-2.618060827	-9.492682457	6.842915535
H	1.286757469	-7.487878799	6.628449440	H	-2.278722763	-10.158164978	7.633739948
C	-0.296644002	-8.894286156	7.040702343	H	-1.752120018	-7.749214649	7.759666443
H	0.356240422	-9.763535500	7.023668766	C	-0.634234071	-5.016340733	7.533741474
C	-1.659965634	-9.043159485	7.311482430	C	-3.025525570	-4.950706959	8.217948914
H	-2.072923183	-10.031322479	7.500636101	C	-0.231198624	-4.604737759	8.833559990
H	-3.555092335	-8.038895607	7.554922581	C	0.343331754	-5.126571178	6.528967857
C	-3.913489103	-5.658746243	9.329459190	C	-1.231985211	-4.563540936	9.887529373
C	-5.145409584	-4.701261520	7.394339561	C	1.113412976	-4.298830986	9.075213432
C	-5.117871761	-5.769931793	10.070492744	H	-0.894819558	-4.376892567	10.905359268
C	-2.684757471	-5.762510300	9.997210503	C	-2.531974316	-4.762556076	9.632823944
C	-6.378509998	-5.529669762	9.383031845	H	-3.291306257	-4.715509415	10.408514023
C	-5.054639816	-6.059685230	11.437329292	H	-3.794217110	-5.734910011	8.200723648
H	-7.301537991	-5.729417324	9.923600197	H	3.970916510	-0.421289802	6.223397255
C	-6.408432484	-5.011588573	8.147917747	H	4.119399071	-2.126395941	6.649861813
H	-7.340280056	-4.756632805	7.654173851	H	4.643971920	-1.569546342	5.051998615
H	-5.252021313	-5.022757053	6.349850178	H	1.398237705	-3.982864141	10.076857567
H	2.062817812	-2.183794498	1.784857392	C	2.073177576	-4.399379253	8.071622849
H	2.221155405	-3.719042063	2.637259007	H	0.048916556	-5.436670303	5.534793854
H	1.480469584	-3.680345774	1.031193733	C	1.672921896	-4.822349072	6.800405025
H	-5.986376762	-6.149434090	11.992519379	H	2.399472475	-4.891463280	5.995630741
C	-3.831488371	-6.212744713	12.088862419	H	3.112541676	-4.155440331	8.274149895
H	-1.759724975	-5.613793373	9.453906059	I	-6.593009949	-2.114363432	10.750028610

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Int7_{C₂}-1

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===== Int6 _{C₂} -TS2 =====	C	-3.692598104	-3.674438477	7.744444370	C	-5.391119003	-3.658762217	8.049081802
	C	-3.625785828	-2.826697588	6.817229748	C	-5.539628029	-2.521217585	8.737656593
	C	-4.037910461	-1.551985502	6.213871002	C	-6.131400936	-2.372460365	9.728899002
	O	-5.135102749	-1.359878063	5.734241486	O	-7.768302917	-2.040154934	9.514405251
	O	-3.070680857	-0.631369948	6.331506729	O	-6.130521774	-2.578624964	10.995078087
	C	-3.316118717	0.620608032	5.643231392	C	-7.076682091	-2.420126915	12.061581612
	H	-3.750177860	0.393818915	4.668507576	H	-8.028678894	-2.881520271	11.776393890
	H	-4.039260864	1.197515368	6.231857777	H	-6.645077229	-2.980168104	12.896595955
	C	-1.979596972	1.323265553	5.511104107	C	-7.274747372	-0.949255049	12.408729553
	H	-2.119729042	2.297507524	5.029847622	H	-7.944240093	-0.840634108	13.270773888
	H	-1.517915606	1.484714508	6.490880489	H	-6.314678669	-0.481890202	12.649291039
	H	-1.308029175	0.719381392	4.896894932	H	-7.713690281	-0.428979874	11.554313660
	Cu	-5.062669277	-2.804978848	8.902579308	Cu	-4.295059681	-1.039511323	8.550072670
	S	-1.749448419	-2.738204718	3.855903387	S	-4.811170578	-3.280181885	5.455057621
	O	-2.479041576	-1.464436293	3.706589937	O	-5.505682468	-2.002504110	5.592834949
	O	-1.595626116	-3.587373734	2.653428078	O	-5.448134422	-4.404547215	4.743340015
	C	-0.089372709	-2.315196514	4.408663273	C	-3.204835653	-3.001706600	4.723174095
	N	-2.336811781	-3.569294214	5.144714355	N	-4.327646732	-3.778446198	7.062716961
	C	0.084999934	-1.696496248	5.651068687	C	-2.426949739	-1.943810940	5.199575901
	C	1.004313827	-2.629569530	3.609030008	C	-2.767428875	-3.828530073	3.691475868
	H	-0.7766670516	-1.477994800	6.271491051	H	-2.781884193	-1.310149670	6.008471489
	C	1.370631099	-1.396870375	6.083203793	C	-1.182674766	-1.723210692	4.619745255
	H	1.512302041	-0.937929213	7.058895111	H	-0.569825768	-0.904251099	4.988148689
	C	2.493368864	-1.710474133	5.300055027	C	-0.710090220	-2.537433147	3.577187061
	C	2.291310787	-2.322289705	4.059593678	C	-1.516870856	-3.587549448	3.122168779
	C	3.882089138	-1.439540386	5.827126503	C	0.653680563	-2.292772532	2.975266457
	H	3.149951696	-2.574735641	3.440551519	H	-1.164948463	-4.224908352	2.314209938
	H	0.839217842	-3.121246576	2.656048298	H	-3.403978825	-4.636813164	3.347359180
	C	-2.481637001	-4.923161030	4.988623142	C	-3.620717525	-4.992210388	7.079955578
	H	-2.638223171	-5.309297562	3.981132269	H	-2.874022961	-5.115273476	6.304669857
					C	-3.831509352	-5.970636845	7.998592854
					C	-2.976638317	-7.171371937	8.049091339
					N	-4.976098061	-5.912061214	8.828408241
					C	-1.615057588	-7.117149830	7.701971054

C	-3.512584448	-8.408456802	8.449981689	C	-3.145989418	-10.224246979	6.119248867
H	-1.170288801	-6.160453796	7.443828106	H	-3.230170727	-11.307497978	6.148589134
C	-0.825865865	-8.265693665	7.726133823	C	-3.044333935	-9.493978500	7.304535389
H	0.225466371	-8.198826790	7.456746578	H	-3.051560163	-10.005839348	8.263420105
C	-1.370641947	-9.489209175	8.120688438	H	-2.836931705	-7.540357590	8.187664032
H	-0.750079334	-10.380824089	8.155924797	C	-0.841354907	-5.599191666	7.410240650
C	-2.717983484	-9.550705910	8.486516953	C	-3.066778898	-4.499673367	8.014544487
H	-3.153019428	-10.495974541	8.802121162	C	-0.287680894	-5.246729374	8.667833328
H	-4.559288979	-8.455229759	8.732431412	C	-0.019766361	-6.241217613	6.468856335
C	-4.878053665	-5.972168922	10.232392311	C	-1.150080562	-4.596196175	9.640295029
C	-6.028369904	-5.041942596	8.237252235	C	1.046736121	-5.556355953	8.944923401
C	-6.076687813	-5.873120308	10.985670090	H	-0.737815440	-4.381670475	10.623874664
C	-3.665426254	-6.150434971	10.911555290	C	-2.417318344	-4.273326874	9.358056068
C	-7.312317848	-5.539592743	10.293137550	H	-3.052453279	-3.793088436	10.096350670
C	-6.030342579	-6.023187160	12.374638557	H	-3.967712879	-5.115179539	8.195765495
H	-8.240567207	-5.569442749	10.858765602	H	3.725148916	-2.235907793	6.729327679
C	-7.297181606	-5.113169670	9.024130821	H	3.226963520	-3.709643602	7.574340820
H	-8.194436073	-4.760015965	8.527700424	H	4.040806293	-3.824160337	6.007733345
H	-6.216178417	-5.451707840	7.235078812	H	1.448139787	-5.279244900	9.917685509
H	0.808406830	-1.229883552	2.760699749	C	1.851415753	-6.214401245	8.013936996
H	1.448611379	-2.600213528	3.666169643	H	-0.413672775	-6.480498791	5.488939762
H	0.788820386	-2.851249218	2.043890953	C	1.304033160	-6.551425457	6.775779724
H	-6.959774971	-5.943789482	12.934824944	H	1.915007472	-7.047730446	6.026082516
C	-4.825150967	-6.240229607	13.040695190	H	2.885271549	-6.452474117	8.248429298
H	-2.736072540	-6.172269344	10.357792854	I	-5.323737144	-0.477179974	10.611895561
C	-3.644568443	-6.290229321	12.299563408	=====	=====	=====	=====
H	-2.689474821	-6.424552917	12.800796509	Int8	=====	=====	=====
H	-4.804989338	-6.346524715	14.121782303	=====	=====	=====	=====
I	-2.489971399	0.721086502	8.269701958	=====	=====	=====	=====

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Int7_{C2}-2

C	-3.640337467	-3.204664707	7.463829517	C	-5.516237259	-3.409469128	8.012941360
C	-3.728305101	-2.940297127	6.141867638	C	-5.745001793	-2.323819399	8.784767151
C	-4.606181622	-1.829761505	5.651688099	C	-6.997488022	-2.256377220	9.567074776
O	-5.388844013	-1.922909260	4.727672100	O	-8.114917755	-2.089229107	9.115379333
O	-4.472201824	-0.705650687	6.400285244	O	-6.737741947	-2.361250639	10.901868820
C	-5.410101891	0.351787388	6.120781898	C	-7.890379429	-2.397448301	11.772796631
H	-5.416819572	0.543427765	5.042948723	H	-8.644207954	-3.055947542	11.328989029
H	-6.412762165	0.015039838	6.410466671	H	-7.515675545	-2.851839304	12.694197655
C	-4.970552444	1.557570100	6.929403782	C	-8.461169243	-1.009414673	12.019388199
H	-5.663726330	2.390811920	6.767248154	H	-9.282692909	-1.065405250	12.742210388
H	-4.956326962	1.312035561	7.995043755	H	-7.692144871	-0.341584116	12.418992996
H	-3.967052221	1.874686599	6.627667427	H	-8.844683647	-0.594115019	11.085432053
Cu	-4.398562908	-1.939851999	8.759522438	Cu	-4.407651901	-0.837795675	8.529880524
S	-2.175932646	-3.095311165	3.934520721	S	-4.819008827	-2.536248684	5.611605644
O	-2.518811464	-1.680226445	3.786133528	O	-5.049017906	-1.144135594	6.013234138
O	-2.150740147	-4.004462242	2.780667305	O	-5.861252308	-3.299505234	4.916081905
C	-0.559264898	-3.152532816	4.713613510	C	-3.296945095	-2.640534163	4.700836182
N	-3.254093409	-3.766431332	5.054369450	N	-4.388473511	-3.398012400	7.107571602
C	-0.367723525	-2.509243011	5.942070007	C	-2.200590611	-1.890429974	5.134692669
C	0.490806401	-3.804379225	4.073394775	C	-3.226593256	-3.484437227	3.593743324
H	-1.194837689	-2.009818077	6.434502125	H	-2.282189846	-1.247140527	6.006087780
C	0.889133990	-2.553795099	6.534244061	C	-1.004690409	-2.008702517	4.435042858
H	1.034834266	-2.088022232	7.505511284	H	-0.140585467	-1.437011838	4.762683392
C	1.967903614	-3.199671745	5.909346581	C	-0.894095659	-2.851691723	3.315873861
C	1.752119780	-3.810332537	4.670523167	C	-2.018669844	-3.579376936	2.904755116
C	3.316049099	-3.243908882	6.587230206	C	0.420628488	-2.972018242	2.584603786
H	2.574774265	-4.323046684	4.177387714	H	-1.948898435	-4.231907368	2.038664818
H	0.310639322	-4.300096512	3.125597239	H	-4.100400448	-4.050469398	3.289077759
C	-3.344838381	-5.179307938	5.057263851	C	-3.694650650	-4.609650612	6.929998875
H	-3.896727085	-5.619540691	4.233616352	H	-2.940263033	-4.616686344	6.156136036
C	-2.803643703	-5.938311577	6.028004169	C	-3.905105114	-5.691373825	7.715496540
C	-2.918056488	-7.419589043	6.041740417	C	-3.051987648	-6.893772125	7.685942173
N	-2.179722786	-5.322472572	7.139869690	N	-5.041881561	-5.687035561	8.564893723
C	-3.003691673	-8.165458679	4.854583263	C	-1.688343406	-6.810498714	7.353858471
C	-2.928722382	-8.106470108	7.266388416	C	-3.588325739	-8.149168015	8.019571304
H	-2.946977377	-7.655050755	3.897998810	H	-1.245408773	-5.841103554	7.142927170
C	-3.122492552	-9.552859306	4.894404888	C	-0.891918898	-7.953553200	7.333286762
H	-3.181300402	-10.113665581	3.965041876	H	0.161183387	-7.869615078	7.079339981
C	0.809385300	-10.084179878	H	-1.435332894	-9.196441650	7.664855003	
C	-2.785648823	-9.287139893	H	-0.809385300	-10.084179878	7.665339947	
C	-3.215905666	-10.249344826	H	-2.785648823	-9.287139893	8.010501862	

H	-4.638251781	-8.219063759	8.285524368	H	-4.091094494	-8.557023048	8.814475060
C	-4.877510071	-5.726061344	9.957560539	C	-4.450610161	-6.232564449	10.580345154
C	-6.130498409	-4.820113182	8.043244362	C	-5.487707138	-5.110438824	8.602960587
C	-6.043609142	-5.654150486	10.764609337	C	-5.694216251	-6.205173492	11.258503914
C	-3.616142750	-5.819581032	10.579902649	C	-3.285756350	-6.524915695	11.300273895
C	-7.328188896	-5.442893505	10.109336853	C	-6.880236626	-5.756052971	10.543727875
C	-5.918462276	-5.742451191	12.152627945	C	-5.740458488	-6.532341957	12.617813110
H	-8.233630180	-5.576475620	10.695051193	H	-7.838552475	-5.820406914	11.052192688
C	-7.383897305	-5.019447327	8.839644432	C	-6.791395664	-5.197412968	9.331082344
H	-8.321266174	-4.769643784	8.356986046	H	-7.654184341	-4.777192593	8.825307846
H	-6.299915314	-5.131255627	7.006350040	H	-5.638510227	-5.475157738	7.575976372
H	0.790897548	-1.988126993	2.276793718	H	1.476271033	-1.710209370	3.008467674
H	1.186468482	-3.416105032	3.231306076	H	2.089197159	-2.222565889	4.579454422
H	0.331732482	-3.596296549	1.691513300	H	1.805565357	-3.423128366	3.306721449
H	-6.820437908	-5.691280365	12.757523537	H	-6.702826500	-6.509232521	13.123739243
C	-4.671441078	-5.871739388	12.768300056	C	-4.583559990	-6.856100559	13.323587418
H	-2.719334602	-5.905810833	9.977104187	H	-2.322046995	-6.508023739	10.807929993
C	-3.525406837	-5.910338879	11.979155540	C	-3.358340740	-6.843422413	12.656842232
H	-2.545518637	-6.002341747	12.438550949	H	-2.441961765	-7.069805622	13.194585800
H	-4.598635197	-5.933257103	13.849318504	H	-4.635352612	-7.103439808	14.379411697
I	-1.931646347	-0.338678032	9.004595757	I	-3.045170069	1.094745517	8.152381897
O	-3.691172123	-2.805207729	10.660043716	O	-2.451383114	-2.014280319	9.385800362
H	-4.465490818	-2.562001467	9.994139671	H	-3.524014950	-2.233850241	9.462457657
H	-3.552726746	-3.792798519	10.661175728	H	-2.271100760	-2.488603830	8.543945313
H	-2.902699471	-2.291490555	10.311347961	H	-2.427207232	-1.025542974	9.168736458

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C	-4.869463921	-3.715085506	8.458010674
C	-5.114939690	-2.555400848	9.099085808
C	-6.123346329	-2.468819857	10.176261902
O	-7.226051807	-1.960770488	10.084046364
O	-5.596337795	-2.946518898	11.333147049
C	-6.440426826	-2.883079529	12.505650520
H	-7.471734524	-3.099495649	12.212721825
H	-6.068840504	-3.685761213	13.147235870
C	-6.333137035	-1.519689798	13.171662331
H	-6.922566891	-1.499551535	14.094784737
H	-5.291683197	-1.293773532	13.420858383
H	-6.712039471	-0.744601727	12.500569344
Cu	-4.785738945	-0.847693920	8.039097786
S	-4.217959404	-3.246624231	5.872249603
O	-4.882325649	-1.941846132	6.055721760
O	-4.902748585	-4.335628986	5.170222282
C	-2.608060360	-2.984354019	5.166245461
N	-3.749974966	-3.771936655	7.519375324
C	-1.896523118	-1.834040642	5.519837856
C	-2.055890799	-3.973406553	4.352837563
H	-2.357893467	-1.058745027	6.126762390
C	-0.592995703	-1.695186496	5.055593967
H	-0.029210269	-0.804559827	5.320760727
C	0.003691592	-2.680194616	4.249761581
C	-0.748289347	-3.808992624	3.897966385
C	1.420191884	-2.506289721	3.760087729
H	-0.304910660	-4.573631287	3.266114235
H	-2.641465425	-4.848021507	4.089684486
C	-3.055673599	-5.020222264	7.511574745
H	-2.278513908	-5.115191460	6.766241074
C	-3.296848774	-6.023997784	8.392290115
C	-2.443541288	-7.232871056	8.410400391
N	-4.451214790	-5.982304573	9.189220428
C	-1.060368896	-7.151840687	8.189406395
C	-3.022757530	-8.492583275	8.634663582
H	-0.595658720	-6.178516865	8.059329033
C	-0.278080612	-8.306017876	8.170551300
H	0.792397857	-8.228363991	8.001832008
C	-0.862837076	-9.553898811	8.391132355
H	-0.251060873	-10.451508522	8.390102386
C	-2.237573624	-9.641705513	8.625885963
H	-2.699558496	-10.609175682	8.801632881

H	-4.091094494	-8.557023048	8.814475060
C	-4.450610161	-6.232564449	10.580345154
C	-5.487707138	-5.110438824	8.602960587
C	-5.694216251	-6.205173492	11.258503914
C	-3.285756350	-6.524915695	11.300273895
C	-6.880236626	-5.756052971	10.543727875
C	-5.740458488	-6.532341957	12.617813110
H	-7.838552475	-5.820406914	11.052192688
C	-6.791395664	-5.197412968	9.331082344
H	-7.654184341	-4.777192593	8.825307846
H	-5.638510227	-5.475157738	7.575976372
H	1.476271033	-1.710209370	3.008467674
H	2.089197159	-2.222565889	4.579454422
H	1.805565357	-3.423128366	3.306721449
H	-6.702826500	-6.509232521	13.123739243
C	-4.583559990	-6.856100559	13.323587418
H	-2.322046995	-6.508023739	10.807929993
C	-3.358340740	-6.843422413	12.656842232
H	-2.441961765	-7.069805622	13.194585800
H	-4.635352612	-7.103439808	14.379411697
I	-3.045170069	1.094745517	8.152381897
O	-2.451383114	-2.014280319	9.385800362
H	-3.524014950	-2.233850241	9.462457657
H	-2.271100760	-2.488603830	8.543945313
H	-2.427207232	-1.025542974	9.168736458

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C	-4.230327606	-4.121068001	8.477366447
C	-4.034122944	-2.874767303	8.996268272
C	-4.824893951	-2.289507627	10.128927231
O	-6.026213646	-2.062058687	10.096913338
O	-4.016378880	-1.981637239	11.143392563
C	-4.583386421	-1.158832669	12.203019142
H	-5.557523251	-1.568287253	12.488271713
H	-3.879542112	-1.281083226	13.030515671
C	-4.687387943	0.290246844	11.748199463
H	-4.973118305	0.925805926	12.593909264
H	-3.727806568	0.628061235	11.346430779
H	-5.444910526	0.392260760	10.965458870
Cu	-5.380921364	-1.951406121	7.449536324
S	-3.263516665	-3.745666504	5.931447983
O	-4.555425644	-3.068546057	5.694542885
O	-2.743709326	-4.693694592	4.951220989
C	-2.036449026	-2.501821518	6.273779869
N	-3.424919605	-4.624091148	7.415974140
C	-2.285999060	-1.188008070	5.877726555
C	-0.820400059	-2.879572392	6.850465298
H	-3.253588915	-0.907982647	5.473361969
C	-1.276313305	-0.239466026	6.050429821
H	-1.460480332	0.785879970	5.741156101
C	-0.042243071	-0.583010435	6.622427940
C	0.162306532	-1.912729621	7.030062675
C	1.055442572	0.440977424	6.772428513
H	1.105692506	-2.191433430	7.491375446
H	-0.654729784	-3.904619217	7.167504787
C	-3.134020567	-6.011593819	7.366993427
H	-2.736450195	-6.370604515	6.430873394
C	-3.366701603	-6.817664146	8.426368713
C	-2.999306440	-8.247252464	8.449746132
N	-4.125213146	-6.291160107	9.494535446
C	-1.865378141	-8.722550392	7.771732330
C	-3.792478085	-9.159969330	9.164433479
H	-1.218492746	-8.022024155	7.251676083
C	-1.547804952	-10.079202652	7.788004875
H	-0.666507781	-10.431537628	7.259426117
C	-2.344800472	-10.979733467	8.497883797
H	-2.089703321	-12.035324097	8.520038605
C	-3.465299368	-10.512942314	9.188786507
H	-4.088936806	-11.205806732	9.746814728

H	-4.664974689	-8.795399666	9.697146416	H	-4.683199883	-5.311537743	13.916954041
C	-3.626302958	-6.251799107	10.817268372	C	-2.778028011	-6.231112480	13.495804787
C	-5.085626125	-5.267917156	9.053550720	H	-1.699815631	-7.124807358	10.392527580
C	-4.466582775	-5.720532417	11.823808670	C	-1.948007584	-6.734394073	12.492764473
C	-2.360047579	-6.739400864	11.159749031	H	-0.963227808	-7.119007587	12.742545128
C	-5.751421928	-5.160645485	11.431457520	H	-2.450317383	-6.226148129	14.530773163
C	-4.028971195	-5.723639011	13.152459145	I	-5.887428761	0.474811554	6.920762062
H	-6.457675457	-4.897422314	12.214616776	O	-2.853074312	-0.006382370	8.991866112
C	-6.053407192	-4.930770874	10.147130966	H	-3.150022507	-2.291429520	8.747540474
H	-6.983585835	-4.460778713	9.853160858	H	-2.247539282	0.178658694	8.262848854
H	-5.630333900	-5.703505039	8.205722809	H	-3.717717171	0.262022883	8.635411263
H	1.692619562	0.450418741	5.879142761				
H	0.651275098	1.449682832	6.895466805				
H	1.696464658	0.219511703	7.630654812				

IV-4. Vibrational frequencies of the optimized geometries

Table S3. Vibrational Frequencies (in cm⁻¹) of the Optimized Geometries

Cul							
241.66							
1a							
1.56	18.27	27.44	32.28	42.27	48.73		
58.55	64.64	67.68	110.07	133.44	162.34		
179.93	194.27	204.04	212.84	252.13	276.60		
278.63	289.40	321.96	325.97	351.70	397.23		
407.66	416.27	416.51	420.85	475.81	478.21		
482.64	489.42	516.50	523.62	541.24	546.26		
559.37	600.06	611.68	631.59	636.70	648.57		
655.45	681.28	709.39	715.22	719.70	745.33		
769.44	781.30	796.23	815.36	818.40	823.35		
832.11	848.62	858.19	869.93	881.83	906.68		
938.57	964.43	969.38	972.64	975.87	980.72		
991.17	991.45	1001.59	1007.90	1009.69	1016.25		
1036.79	1045.72	1059.97	1064.93	1068.77	1084.82		
1118.66	1128.97	1137.73	1149.23	1180.28	1184.43		
1196.64	1199.18	1218.88	1225.66	1235.08	1242.15		
1262.39	1279.57	1295.62	1317.27	1329.96	1335.26		
1339.05	1352.65	1357.42	1371.95	1404.41	1412.37		
1427.09	1440.32	1442.57	1489.26	1494.26	1498.88		
1502.04	1508.32	1539.11	1539.34	1567.32	1586.29		
1620.79	1630.00	1632.97	1639.21	1658.69	1658.92		
1675.50	3035.80	3092.99	3112.46	3121.05	3171.42		
3171.53	3175.35	3179.30	3188.72	3190.02	3197.93		
3200.94	3205.45	3207.11	3214.62	3214.67	3216.39		
3232.55	3260.09	3278.28					
2a							
78.93	113.99	160.57	241.80	283.32	337.20		
419.05	558.70	595.29	645.14	686.40	767.04		
805.99	873.35	919.33	1045.46	1125.02	1201.89		
1261.39	1333.73	1404.51	1433.70	1498.80	1506.62		
1522.99	1795.79	2238.32	3055.93	3081.57	3128.07		
3134.65	3156.53	3488.01					
DIPEA							
82.00	104.44	144.95	162.13	228.09	239.15		
243.62	256.42	294.80	309.88	326.15	333.30		
365.10	376.93	406.39	497.05	523.28	564.52		
706.56	792.95	840.05	887.54	924.76	928.22		
939.52	944.21	959.16	1035.45	1061.83	1119.40		
1131.89	1139.86	1147.32	1168.34	1208.34	1243.19		
1285.95	1346.56	1352.62	1371.21	1395.04	1409.23		
1412.47	1414.52	1423.08	1429.55	1432.43	1450.48		
1494.83	1496.65	1500.22	1505.87	1506.40	1508.06		
1516.36	1521.68	1526.12	1528.33	1534.85	2989.72		
3025.88	3036.15	3038.09	3039.99	3041.83	3043.40		
3049.23	3076.10	3101.24	3107.35	3110.36	3112.23		
3118.68	3124.74	3125.35	3127.66	3133.45	3141.44		
[DIPEA-H]+							
97.28	124.35	181.17	215.92	236.77	245.73		
253.22	259.97	277.06	303.74	329.54	335.28		
342.33	364.24	410.92	476.33	537.89	638.25		
711.03	771.20	843.19	861.61	919.15	923.94		
956.70	960.39	967.69	973.27	1035.80	1086.92		
1112.70	1117.22	1167.66	1172.30	1197.14	1212.10		
1217.37	1334.49	1354.18	1361.36	1388.23	1390.79		
1423.43	1428.66	1437.98	1440.31	1446.12	1456.38		
1461.13	1476.00	1492.43	1495.56	1503.12	1505.49		
1508.92	1514.66	1523.68	1527.06	1529.15	1531.77		
1535.04	3048.42	3058.32	3063.33	3074.07	3081.70		
3083.83	3093.42	3101.48	3123.48	3133.70	3141.42		
3145.06	3146.95	3148.82	3153.17	3157.33	3170.60		
3183.65	3192.47	3441.62					
H2O							
1658.58	3815.05	3932.74					
H3O+							
814.41	1671.47	1671.51	3582.62	3696.68	3696.83		
Int1							
20.02	27.54	63.69	78.91	87.96	99.96		
157.66	222.64	248.49	274.71	324.18	329.85		
413.92	538.16	576.09	696.61	704.68	751.82		
807.48	868.00	910.99	1028.38	1121.93	1200.41		
1259.86	1333.34	1405.29	1434.13	1499.22	1506.79		
1519.78	1817.92	2099.13	3058.90	3091.71	3135.11		
3140.98	3165.04	3424.68					
Int2							
17.27	21.02	27.78	32.72	36.96	56.21		
68.17	70.87	84.89	91.02	95.76	118.05		
129.73	153.49	173.87	179.60	224.69	226.68		
235.23	248.23	249.84	254.29	276.67	287.91		
303.43	325.61	328.64	330.44	331.89	357.69		
364.68	380.94	417.75	424.65	500.83	545.45		
555.68	582.56	609.33	694.57	751.27	803.52		
806.17	848.60	869.44	889.33	910.09	930.96		
938.40	942.99	953.98	962.19	1006.01	1009.32		
1034.30	1057.65	1074.28	1116.45	1122.17	1133.71		
1145.36	1154.04	1172.41	1200.68	1208.13	1232.17		
1252.92	1256.58	1333.13	1351.50	1360.63	1379.06		
1404.47	1408.22	1412.84	1418.98	1422.75	1431.59		
1433.35	1440.63	1442.27	1448.66	1498.55	1499.08		
1500.78	1501.95	1506.40	1506.86	1513.28	1515.05		
1519.55	1522.39	1525.46	1530.84	1532.56	1537.02		
1811.87	2034.76	2803.06	3000.15	3012.09	3041.19		
3044.29	3050.83	3052.33	3056.37	3056.56	3059.59		

3089.11	3096.51	3110.08	3118.28	3119.06	3121.47		1151.49	1170.52	1183.02	1185.86	1193.22	1197.63											
3124.47	3128.55	3131.43	3132.05	3136.96	3143.49		1202.16	1221.24	1223.73	1235.75	1245.62	1269.47											
3148.68	3157.09	3160.09					1274.50	1293.46	1319.96	1331.11	1332.04	1338.27											
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Int2-TS																							
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-1027.20	19.13	22.53	31.06	35.89	42.32		1495.16	1497.09	1500.86	1500.91	1502.93	1507.01											
64.96	72.23	81.13	98.75	98.87	119.80		1524.98	1539.76	1539.79	1570.25	1598.04	1619.25											
136.70	140.73	171.45	187.76	189.47	224.46		1629.78	1634.08	1640.42	1657.81	1659.58	1676.96											
234.75	246.79	248.95	257.26	269.08	277.98		1754.46	2163.37	3031.89	3040.90	3051.34	3093.07											
287.25	308.37	325.78	335.52	337.32	350.68		3098.70	3110.20	3113.62	3135.34	3150.37	3160.10											
360.23	364.31	380.10	424.00	429.29	496.16		3170.71	3175.01	3181.29	3183.10	3186.93	3193.13											
551.78	562.03	606.97	682.16	755.05	757.58		3206.04	3208.73	3219.41	3222.65	3224.52	3225.88											
796.51	811.26	851.86	872.68	891.06	927.08		3236.91	3264.85	3278.97														
940.69	949.94	953.29	963.45	968.21	987.25		<hr/>																
1043.89	1065.00	1111.02	1123.73	1134.06	1135.75		Int5-TSC2																
1167.93	1180.52	1201.75	1212.76	1220.20	1233.78		-269.18	11.50	14.42	19.16	21.47	30.07											
1248.80	1333.25	1353.61	1362.54	1379.24	1403.60		31.96	36.90	46.46	49.92	54.42	55.38											
1407.59	1411.34	1425.34	1428.77	1432.79	1436.09		59.71	62.07	74.44	75.25	82.48	108.74											
1446.20	1451.72	1458.10	1498.56	1498.87	1499.47		116.25	120.16	128.19	136.49	153.14	163.66											
1503.60	1506.10	1508.18	1513.54	1514.86	1520.62		176.93	181.67	198.56	204.32	212.81	224.92											
1520.99	1528.75	1532.46	1534.39	1538.67	1564.95		228.21	243.70	258.76	279.15	288.71	305.66											
1579.26	1798.73	2129.86	3024.11	3052.45	3054.47		329.60	333.56	345.32	354.66	361.66	400.25											
3058.66	3061.28	3061.60	3062.66	3065.07	3068.96		411.52	415.65	418.74	420.67	422.10	471.79											
3083.89	3117.45	3121.08	3127.78	3128.13	3128.73		485.96	492.58	501.49	518.38	523.11	537.25											
3133.56	3134.32	3136.98	3142.99	3147.94	3155.09		539.12	564.94	572.38	602.76	622.48	624.47											
3155.51	3156.95	3166.26					628.82	639.06	643.15	655.87	674.37	705.80											
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Int3																							
<hr/>																							
16.72	22.56	30.97	36.07	44.55	63.96		919.54	942.43	950.39	959.28	963.76	968.32											
69.76	82.34	92.68	104.62	113.93	126.63		979.11	980.27	984.04	990.95	999.08	1003.77											
141.35	143.63	177.02	190.44	215.91	231.74		1015.60	1035.42	1046.36	1054.65	1059.80	1063.31											
242.03	247.41	256.85	266.38	270.51	284.25		1067.98	1076.36	1081.46	1116.32	1128.38	1136.05											
297.42	319.37	336.97	338.25	348.95	354.41		1150.41	1172.55	1185.49	1192.60	1195.81	1198.88											
376.81	386.13	420.98	424.59	486.77	547.94		1199.48	1221.08	1223.77	1234.98	1236.71	1251.54											
557.03	604.22	650.54	726.23	758.30	799.53		1278.61	1288.95	1308.40	1331.42	1332.12	1339.22											
806.88	849.31	873.28	884.05	919.48	934.08		1343.81	1355.24	1363.94	1370.33	1378.08	1387.66											
948.98	955.60	965.04	969.54	980.46	1046.72		1399.70	1422.54	1426.14	1430.38	1440.68	1472.20											
1056.64	1103.28	1124.85	1130.33	1135.28	1168.64		1486.85	1494.95	1496.31	1498.34	1502.45	1508.39											
1177.18	1201.55	1209.27	1216.50	1224.49	1239.47		1524.59	1538.03	1539.20	1551.18	1608.18	1615.98											
1333.34	1353.15	1363.20	1376.78	1401.32	1402.85		1624.68	1627.26	1656.51	1659.80	1663.20	1669.54											
1409.30	1427.80	1430.85	1432.41	1437.43	1446.08		1761.21	2103.90	3028.31	3044.39	3058.19	3086.34											
1453.56	1457.52	1497.52	1498.60	1499.19	1502.30		3105.48	3112.98	3118.35	3143.01	3152.38	3160.84											
1505.72	1508.86	1512.18	1514.38	1520.05	1521.65		3162.43	3169.02	3176.28	3182.95	3190.01	3190.15											
1528.95	1532.28	1534.36	1540.00	1611.46	1635.18		3193.01	3199.61	3203.41	3205.97	3211.14	3224.83											
1786.40	2063.97	2111.84	3049.58	3053.33	3056.02		3230.05	3252.44	3254.55														
3063.85	3065.32	3068.53	3071.60	3072.86	3079.88		<hr/>																
3093.81	3125.46	3126.05	3131.21	3132.11	3132.33		Int4																
3134.57	3137.67	3143.51	3152.75	3153.24	3153.35		<hr/>																
3158.95	3162.70	3170.79					11.99	16.53	22.32	28.92	31.98	38.44											
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Int5																							
<hr/>																							
9.57	15.68	19.26	25.01	30.50	35.09		853.53	858.47	860.65	866.91	888.04	906.31											
39.57	49.34	51.96	59.64	61.83	63.64		922.65	952.19	953.16	962.20	963.48	964.92											
69.20	71.51	80.10	85.88	91.73	103.96		974.51	982.09	986.10	988.07	1006.90	1017.64											
114.16	121.00	132.26	137.17	139.36	156.92		1018.88	1036.02	1047.45	1063.63	1063.88	1078.14											
159.74	185.28	190.21	203.56	207.93	233.20		1082.07	1084.84	1114.91	1126.59	1130.18	1134.67											
259.04	264.08	277.04	282.99	287.40	315.22		1151.19	1163.80	1191.23	1197.68	1203.09	1207.83											
321.84	334.42	350.77	369.39	377.74	399.01		1219.16	1221.49	1235.10	1247.22	1259.95	1274.57											
404.35	412.71	416.11	421.39	435.86	470.63		1288.70	1296.33	1317.07	1325.63	1327.14	1331.62											

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Int5-TSC4						
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-301.83	10.56	15.97	17.51	22.30	35.05	646.47
42.45	44.66	47.53	56.42	56.82	60.50	647.56
65.81	71.48	77.39	87.40	95.73	102.98	662.10
114.43	122.59	130.25	138.43	146.49	148.01	680.70
164.25	172.07	175.25	190.16	215.18	225.46	709.04
232.65	254.40	271.39	284.19	296.66	308.50	714.40
320.66	330.48	343.99	368.72	381.84	395.20	756.90
403.28	411.17	416.49	418.71	422.31	478.93	769.40
485.46	487.08	501.02	511.47	523.22	533.43	827.85
548.30	562.99	571.50	600.22	607.83	628.96	837.84
634.31	640.17	646.84	653.63	682.31	706.32	859.14
710.78	729.25	749.45	760.25	762.73	766.45	966.69
771.10	787.22	803.93	820.48	822.09	831.91	969.75
841.01	864.29	864.89	866.93	870.51	889.32	1014.12
921.02	940.56	942.07	953.75	958.58	967.53	1017.92
969.10	975.98	979.12	991.94	1001.86	1021.20	1064.36
1023.94	1034.18	1049.03	1059.07	1060.96	1062.99	1123.21
1071.13	1079.86	1091.34	1115.38	1128.61	1140.05	1128.23
1152.82	1168.47	1179.47	1192.17	1199.38	1200.58	1133.28
1219.49	1221.66	1224.80	1237.10	1237.48	1243.95	1338.06
1268.73	1286.83	1309.79	1332.70	1334.04	1336.30	1368.01
1349.56	1358.61	1360.05	1372.29	1377.06	1386.96	1394.75
1400.33	1416.72	1417.46	1431.02	1444.04	1474.19	1402.03
1488.54	1496.78	1500.95	1503.73	1507.14	1511.09	1489.66
1524.86	1538.31	1539.43	1547.26	1597.01	1609.40	1516.32
1618.30	1630.03	1645.28	1657.44	1659.91	1669.44	1532.87
1733.49	2078.81	3030.93	3045.92	3061.41	3093.04	1536.96
3108.59	3111.57	3119.83	3135.05	3151.55	3159.21	1538.96
3167.03	3173.01	3179.01	3189.22	3189.67	3198.57	1619.16
3201.35	3203.31	3205.55	3216.57	3221.42	3227.45	1626.89
3229.02	3243.42	3243.84				1656.99
=====						
Int6C4						
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10.76	12.11	24.16	29.04	32.27	36.93	-213.29
43.40	44.52	48.99	55.58	59.47	59.94	3.00
73.91	78.96	81.40	89.15	97.85	100.22	44.87
107.88	124.06	135.92	143.19	151.12	155.64	51.31
174.70	186.51	197.28	203.97	232.93	248.87	52.92
265.94	269.87	283.65	304.05	324.70	330.20	24.94
340.48	346.26	361.36	379.64	394.80	408.54	36.25
418.35	418.81	430.74	444.49	453.91	479.10	40.40
484.02	495.01	507.81	522.57	534.52	552.46	44.77
558.14	567.59	593.76	614.91	631.91	633.82	51.31
646.12	648.71	662.69	685.18	707.94	715.35	52.92
719.49	732.92	742.90	754.06	755.29	771.26	97.15
793.72	799.31	812.52	824.63	834.33	846.84	106.62
850.03	861.49	864.81	867.55	891.05	900.05	114.78
929.20	938.86	953.43	958.60	966.09	967.12	112.44
973.30	978.73	993.39	994.07	1006.96	1018.60	1128.21
1020.30	1036.26	1049.59	1064.67	1066.23	1079.34	1005.55
1081.43	1088.96	1117.05	1129.73	1139.17	1153.23	1015.12
1155.61	1176.16	1192.47	1196.84	1201.42	1203.26	1064.81
1221.27	1222.45	1236.11	1236.95	1264.32	1267.17	1070.27
1278.43	1287.59	1306.39	1324.21	1331.55	1334.57	1132.82
1336.41	1340.25	1356.01	1360.81	1370.30	1378.50	1143.97
1398.93	1407.93	1422.73	1429.37	1439.26	1442.54	1145.95
1488.77	1491.86	1501.28	1502.62	1503.02	1507.91	1152.00
1515.66	1534.18	1538.51	1539.33	1618.61	1629.89	1223.39
1630.95	1639.43	1657.89	1661.58	1666.85	1722.94	1235.62
1764.43	2345.00	2985.36	3033.32	3044.53	3064.85	1244.05
3093.86	3112.38	3114.03	3131.75	3133.76	3158.10	1252.11
3163.93	3164.58	3167.11	3167.88	3177.96	3186.09	1258.47
3197.67	3198.48	3206.43	3207.00	3211.31	3219.78	1314.90
3224.25	3226.88	3233.07				1325.65
=====						
Int6C2-1						
=====						
12.55	16.65	20.45	27.53	35.12	40.53	12.55
40.99	49.78	50.35	54.58	58.18	63.07	49.78
76.19	78.41	90.59	97.17	104.21	114.44	78.41
126.07	137.48	140.38	156.90	164.84	179.80	137.48
191.27	209.02	232.89	238.85	250.22	265.34	209.02
271.19	283.86	309.64	330.41	337.76	345.26	283.86
347.60	384.40	397.40	406.76	416.24	422.08	384.40
426.18	442.03	464.98	485.98	489.28	501.50	442.03
509.54	528.86	542.39	554.67	567.70	581.51	528.86
588.61	604.52	632.35	632.96	646.78	653.25	604.52
657.60	683.20	694.08	707.47	713.60	717.82	683.20
733.34	751.09	756.53	776.59	786.10	803.06	751.09
816.35	821.03	824.51	834.22	853.61	861.51	821.03
864.21	870.11	872.29	882.71	910.33	920.99	870.11
923.93	940.80	952.25	958.19	971.55	972.75	940.80
974.79	990.13	1005.19	1013.04	1016.15	1031.08	990.13
1034.52	1041.56	1058.86	1065.01	1076.85	1081.11	1041.56
1088.15	1103.68	1114.44	1128.67	1132.64	1143.07	1103.68
1153.83	1161.90	1192.69	1198.63	1200.64	1209.84	1161.90
1212.71	1216.53	1219.49	1235.42	1245.03	1249.76	1216.53
1280.38	1313.56	1314.89	1328.05	1335.49	1339.12	1313.56
1340.43	1349.73	1357.41	1365.29	1367.86	1396.92	1349.73
1399.46	1415.53	1425.11	1427.96	1441.65	1441.97	1415.53

1488.09	1495.40	1497.60	1498.34	1503.69	1508.11	-291.60	16.59	18.52	27.16	28.35	31.99
1524.81	1532.57	1537.87	1538.67	1621.61	1625.64	39.45	47.32	51.47	55.81	58.07	64.65
1629.79	1652.60	1655.33	1655.39	1666.75	1674.79	66.05	67.61	79.59	85.25	98.59	104.99
1717.77	1768.15	3017.46	3034.12	3039.26	3054.12	106.65	113.83	127.13	142.58	147.06	149.11
3093.44	3103.24	3113.33	3117.92	3148.35	3159.78	155.93	172.49	189.70	206.46	219.36	225.56
3163.99	3169.76	3172.06	3173.79	3174.36	3182.24	235.31	241.35	265.03	283.39	287.02	298.42
3188.34	3191.02	3193.43	3197.43	3209.64	3217.14	313.00	329.76	339.04	344.43	370.80	387.14
3217.56	3219.06	3237.06				399.49	413.31	418.26	421.19	430.44	444.01
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5.28	9.30	18.85	28.13	35.01	49.56	604.71	624.33	629.02	632.46	645.25	654.59
52.57	55.88	58.70	64.21	67.40	76.21	665.43	679.55	694.72	710.22	713.63	715.95
83.38	91.08	100.17	105.04	105.40	110.70	733.65	748.56	764.17	780.19	789.68	800.49
118.67	138.37	154.59	162.99	183.02	189.38	817.38	817.95	821.67	826.53	839.31	865.70
196.97	211.79	231.07	243.99	260.10	264.50	869.64	870.96	874.89	877.75	906.28	933.41
271.40	287.89	295.09	298.64	323.85	335.64	938.17	939.34	951.42	975.63	978.64	983.81
349.86	365.45	377.54	387.32	404.20	415.54	986.21	1001.65	1003.50	1015.35	1018.88	1030.43
417.42	418.92	433.87	462.95	481.82	496.53	1031.55	1041.79	1057.51	1065.86	1077.12	1080.22
511.94	519.42	531.84	546.10	556.74	562.98	1084.04	1110.24	1116.87	1125.65	1133.68	1140.67
588.10	602.04	631.56	643.58	647.81	657.65	1157.46	1159.85	1169.66	1197.89	1200.01	1204.18
668.14	675.02	694.60	711.73	712.90	730.38	1205.44	1218.93	1219.40	1224.64	1237.47	1247.27
741.96	752.11	777.05	782.51	792.39	808.59	1271.44	1288.91	1301.51	1317.29	1331.20	1337.56
820.09	825.71	827.35	832.79	847.10	852.65	1341.61	1343.54	1356.98	1360.66	1364.81	1366.46
856.63	859.76	864.12	892.67	914.72	917.95	1401.41	1420.04	1428.58	1431.67	1441.58	
934.11	950.91	963.35	966.73	975.29	976.40	1444.92	1489.15	1497.17	1498.35	1498.99	1506.77
984.70	994.98	997.79	1014.72	1017.92	1029.45	1508.45	1522.02	1533.94	1537.08	1539.29	1600.80
1037.78	1049.39	1053.94	1062.47	1066.72	1080.02	1611.65	1623.77	1626.88	1629.15	1632.78	1651.13
1088.11	1100.28	1116.92	1134.55	1142.51	1146.65	1657.07	1659.42	1667.15	1722.53	1752.86	1786.45
1155.93	1166.92	1188.69	1194.52	1198.40	1217.54	3002.93	3010.42	3044.36	3049.61	3075.44	3104.26
1220.27	1225.25	1237.06	1248.89	1255.86	1269.72	3120.01	3127.75	3133.35	3148.71	3172.53	3176.94
1279.35	1288.35	1300.21	1312.04	1323.69	1329.94	3178.74	3182.28	3184.91	3186.40	3189.85	3192.19
1340.87	1343.06	1357.14	1367.02	1371.88	1387.26	3193.99	3203.98	3205.78	3211.83	3216.43	3219.69
3235.16	3235.72					3235.16	3247.81	3593.44			
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3a											
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13.45	20.57	23.01	24.35	30.04	35.35	6.85	12.37	20.70	25.68	28.39	36.13
43.21	48.57	51.13	58.71	60.56	61.36	42.73	52.18	54.23	57.46	60.96	64.85
70.98	77.37	80.80	91.65	106.77	115.16	71.21	74.74	76.75	91.87	103.23	114.33
125.60	132.24	141.77	146.73	154.98	167.62	118.43	119.16	127.45	139.77	147.98	158.75
175.58	181.52	196.01	212.88	228.12	228.94	169.39	182.93	194.52	201.77	202.97	210.70
242.71	246.03	268.55	275.40	284.72	302.93	229.35	237.79	253.30	256.94	262.23	284.51
323.08	328.06	339.09	347.73	393.17	398.59	290.59	295.43	307.83	330.07	335.77	359.12
403.00	419.48	419.64	425.98	440.11	461.83	370.06	397.59	402.58	412.17	418.29	421.77
466.74	481.22	490.04	501.88	505.98	524.25	427.92	445.02	469.10	481.33	493.94	502.52
536.85	548.47	555.66	556.46	576.32	583.76	505.39	512.18	523.96	529.30	550.60	560.47
591.78	607.89	629.73	632.52	642.10	658.28	574.39	605.93	631.14	635.65	644.73	647.58
661.04	684.87	695.44	711.39	715.09	717.12	660.55	666.09	683.61	708.74	711.18	714.64
735.06	752.40	766.67	781.98	795.81	806.90	725.27	762.48	765.32	780.26	792.47	809.21
811.04	818.60	825.65	837.21	861.67	865.24	814.06	820.41	827.93	835.70	838.44	861.19
867.46	870.66	876.85	884.34	906.20	934.58	864.03	870.45	871.87	878.44	891.43	916.83
944.84	946.94	956.14	978.62	979.31	983.08	934.92	940.50	952.82	971.05	971.88	977.72
988.39	1000.44	1003.01	1013.92	1017.08	1029.64	978.08	989.87	991.91	1002.89	1014.57	1022.20
1033.56	1045.20	1059.27	1066.28	1074.95	1079.32	1029.86	1034.45	1042.20	1054.60	1064.19	1078.52
1084.43	1103.09	1107.92	1117.71	1126.46	1128.62	1079.48	1082.15	1104.18	1118.55	1128.39	1128.68
1139.62	1157.16	1160.86	1197.81	1201.14	1203.95	1145.89	1163.13	1170.83	1197.82	1202.42	1203.61
1209.78	1218.56	1221.80	1224.63	1235.89	1243.07	1218.27	1219.66	1227.91	1235.07	1237.65	1247.28
1253.43	1276.98	1306.52	1310.18	1332.69	1333.33	1260.34	1279.50	1311.83	1317.36	1324.88	1333.74
1336.54	1339.59	1344.80	1358.79	1367.42	1368.34	1338.23	1346.76	1348.34	1352.02	1364.17	1365.94
1392.00	1402.75	1408.93	1427.88	1432.31	1436.56	1367.08	1390.92	1410.99	1413.98	1429.07	1437.97
1445.24	1488.33	1491.20	1496.60	1496.60	1505.81	1439.16	1444.22	1489.75	1498.07	1499.14	1500.77
1507.23	1524.91	1528.29	1537.13	1538.86	1555.03	1503.65	1510.53	1529.15	1534.57	1537.50	1539.63
1610.82	1617.83	1628.57	1629.31	1637.91	1645.39	1619.33	1623.88	1626.61	1631.64	1649.30	1658.11
1652.86	1658.68	1675.51	1711.37	1779.28	2329.98	1659.89	1662.49	1686.11	1716.89	1747.34	3029.26
3042.43	3051.42	3063.14	3063.67	3101.88	3113.32	3041.24	3048.66	3071.31	3105.56	3121.32	3128.35
3124.31	3130.59	3157.86	3167.30	3176.42	3178.54	3134.39	3147.99	3175.32	3178.11	3182.45	3183.83
3183.75	3185.73	3187.92	3188.84	3191.32	3193.30	3185.50	3187.29	3188.96	3190.54	3195.12	3204.53
3203.40	3204.62	3210.50	3210.89	3221.64	3221.66	3206.34	3208.45	3211.16	3214.54	3228.66	3235.59
3232.31	3246.30	3254.06				3283.89	3697.75	3859.55			
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V. X-ray Crystal Data (3a and 5e)

Compound 3a

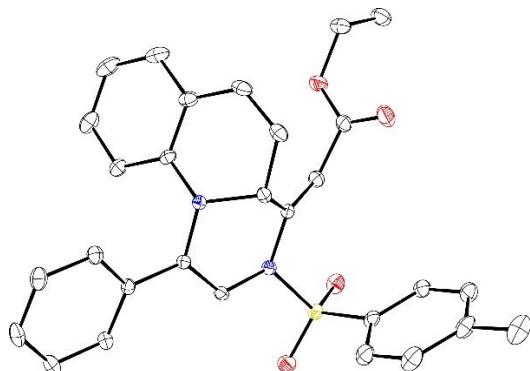


Table S4. Crystal data and structure refinement for compound 3a.

Identification code	3a
Empirical formula	C ₂₉ H ₂₆ N ₂ O ₄ S
Formula weight	498.58
Temperature	140(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 16.6324(8) Å α = 90°. b = 12.5786(5) Å β = 90.5504(18)°. c = 23.5913(12) Å γ = 90°.
Volume	4935.4(4) Å ³
Z	8
Density (calculated)	1.342 Mg/m ³
Absorption coefficient	0.170 mm ⁻¹
F(000)	2096
Crystal size	0.423 x 0.384 x 0.287 mm ³
Theta range for data collection	2.936 to 27.999°.
Index ranges	-21<=h<=21, -16<=k<=16, -31<=l<=31
Reflections collected	131978
Independent reflections	11907 [R(int) = 0.0411]
Completeness to theta = 25.242°	99.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7461 and 0.7251
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	11907 / 0 / 659
Goodness-of-fit on F ²	1.041
Final R indices [I>2sigma(I)]	R1 = 0.0411, wR2 = 0.0952
R indices (all data)	R1 = 0.0579, wR2 = 0.1070
Largest diff. peak and hole	0.406 and -0.517 e·Å ⁻³

Compound 5e

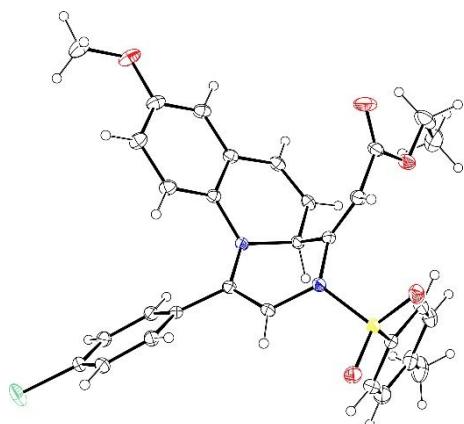


Table S5. Crystal data and structure refinement for compound 5e.

Identification code	5e
Empirical formula	C ₃₀ H ₂₇ N ₂ O ₅ ClS
Formula weight	563.04
Temperature	173(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	P2 ₁ /c
Unit cell dimensions	a = 9.7732(3) Å α = 90° b = 22.9861(8) Å β = 107.7771(11)° c = 12.4889(4) Å γ = 90°
Volume	2671.64(15) Å ³
Z	4
Density (calculated)	1.400 Mg/m ³
Absorption coefficient	0.266 mm ⁻¹
F(000)	1176
Crystal size	0.157 x 0.142 x 0.087 mm ³
Theta range for data collection	2.929 to 28.318°.
Index ranges	-13<=h<=12, -30<=k<=30, -15<=l<=16
Reflections collected	30954
Independent reflections	6574 [R(int) = 0.0355]
Completeness to theta = 25.242°	98.8 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.7457 and 0.6840
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	6574 / 0 / 364
Goodness-of-fit on F ²	1.061
Final R indices [I>2sigma(I)]	R1 = 0.0446, wR2 = 0.1047
R indices (all data)	R1 = 0.0545, wR2 = 0.1097
Largest diff. peak and hole	0.368 and -0.430 e·Å ⁻³

VI. Reference

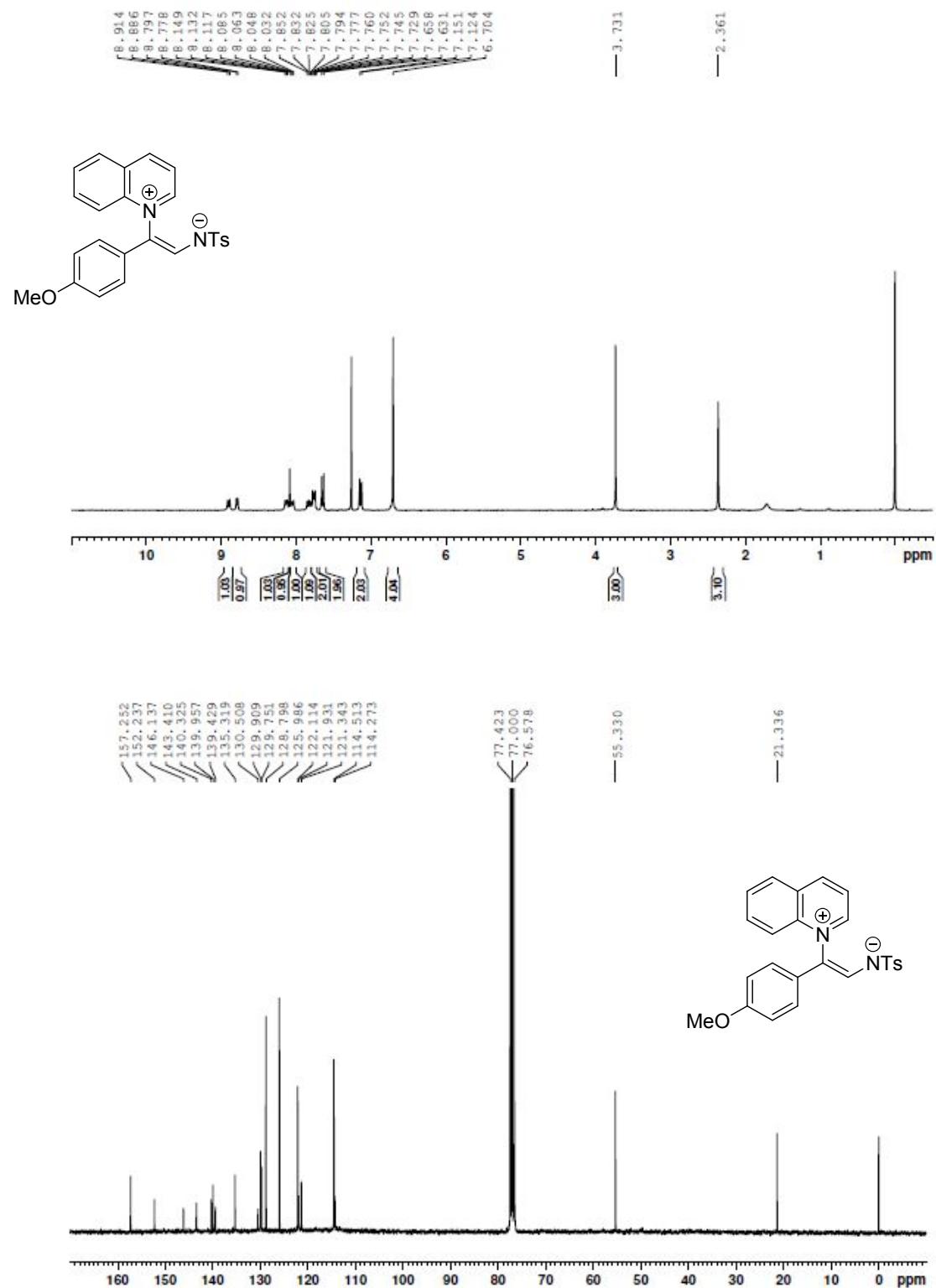
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S8. (a) Marten, B.; Kim, K.; Cortis, C.; Friesner, R. A.; Murphy, R. B.; Ringnalda, M. N.; Sitkoff, D.; Honig, B., New Model for Calculation of Solvation Free Energies: Correction of Self-Consistent Reaction Field Continuum Dielectric Theory for Short-Range Hydrogen-Bonding Effects. *J. Phys. Chem.* **1996**, *100*, 11775–11788. (b) Friedrichs, M.; Zhou, R.; Edinger, S. R.; Friesner, R. A., Poisson–Boltzmann Analytical Gradients for Molecular Modeling Calculations. *J. Phys. Chem. B* **1999**, *103*, 3057–3061. (c) Edinger, S. R.; Cortis, C.; Shenkin, P. S.; Friesner, R. A., Solvation Free Energies of Peptides: Comparison of Approximate Continuum Solvation Models with Accurate Solution of the Poisson–Boltzmann Equation. *J. Phys. Chem. B* **1997**, *101*, 1190–1197.

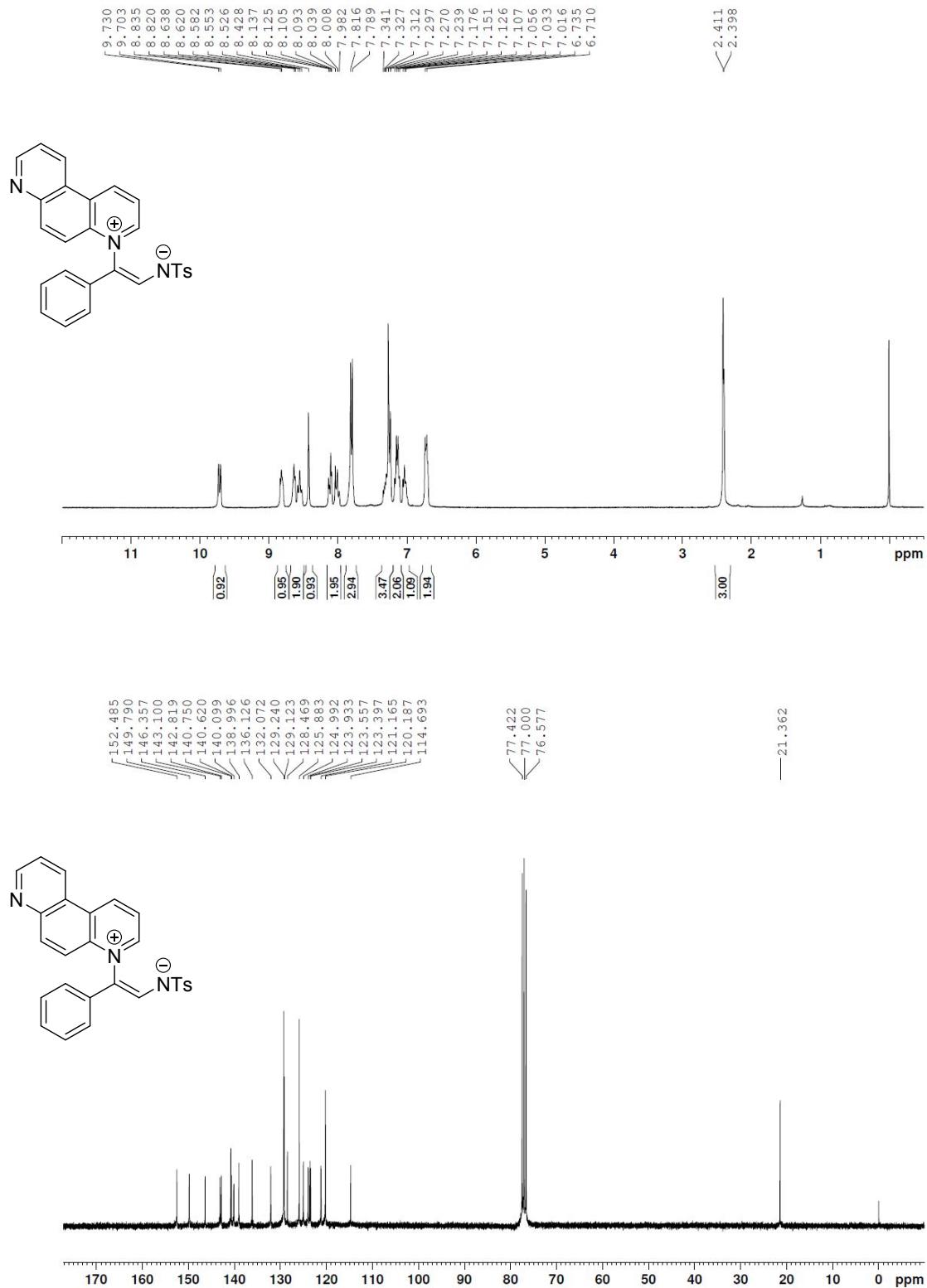
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VII. Copies of Spectral Data of Compounds Obtained in this Study

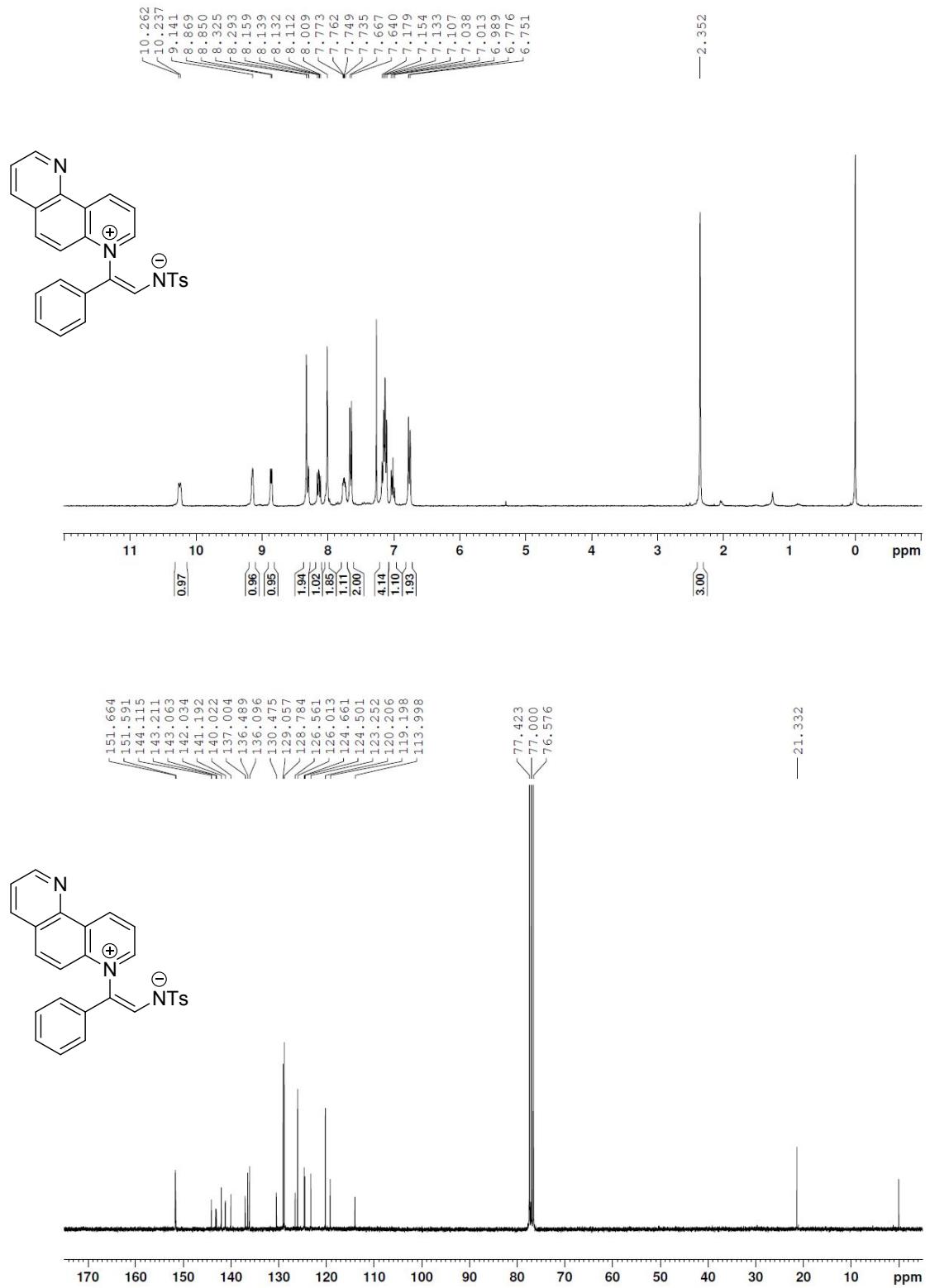
(Z)-(2-(4-methoxyphenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide:



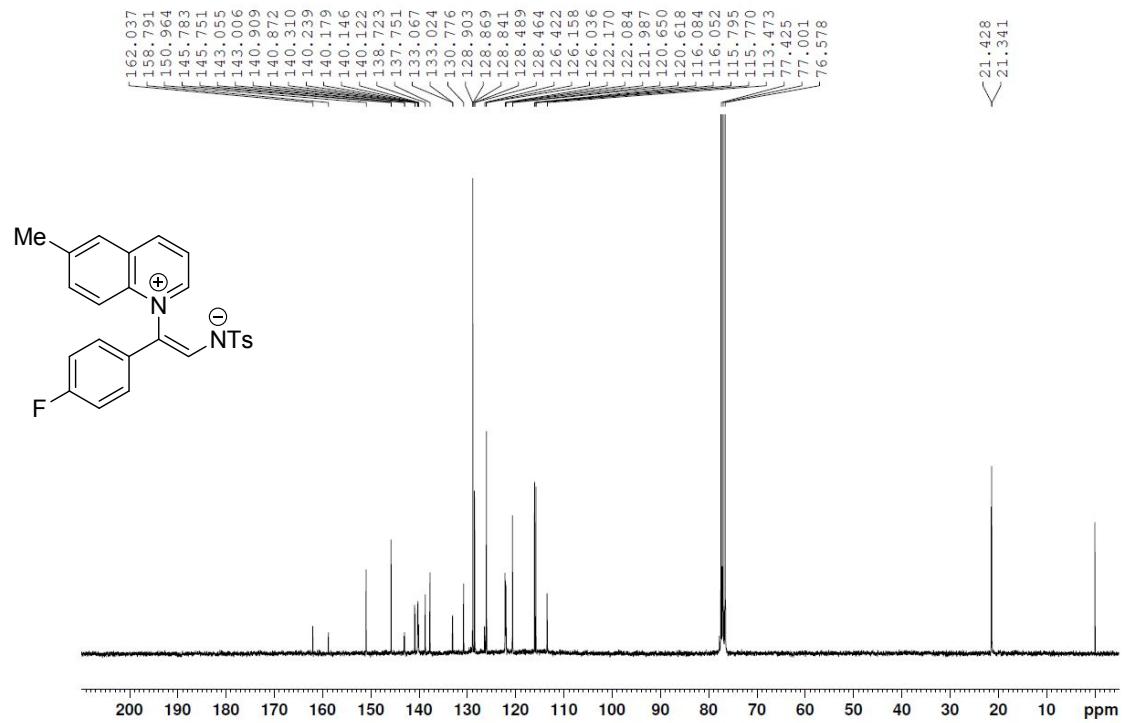
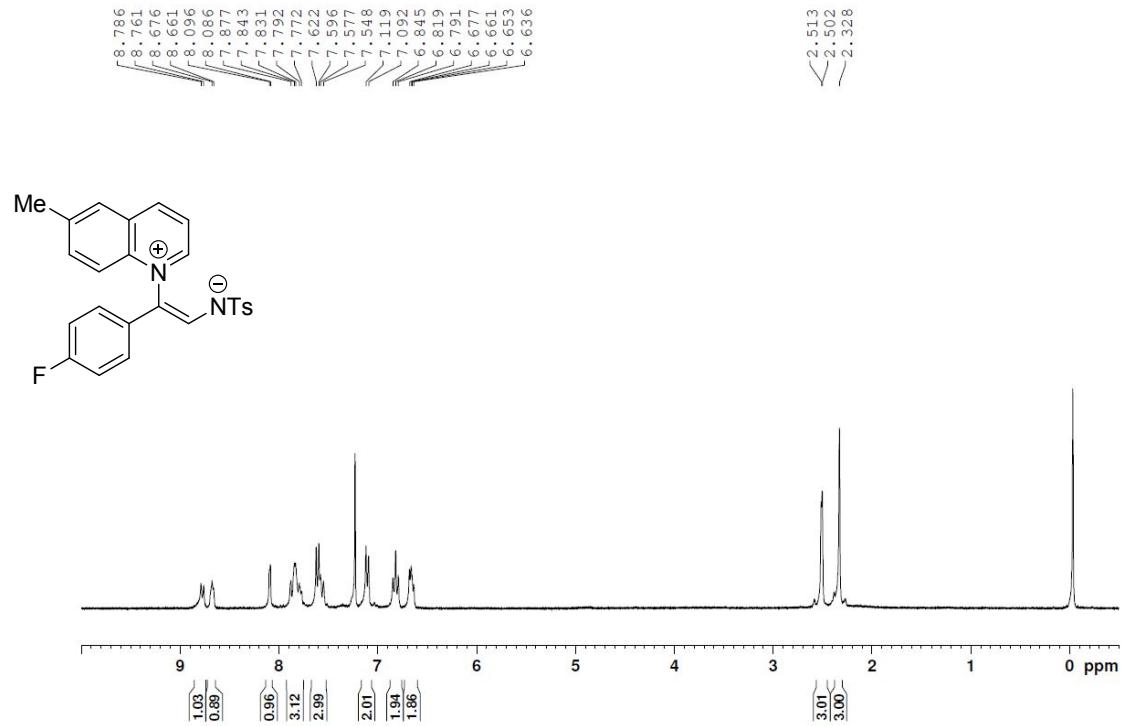
(Z)-(2-(4,7-phenanthrolin-4-i um-4-yl)-2-phenylvinyl)(tosyl)amide:



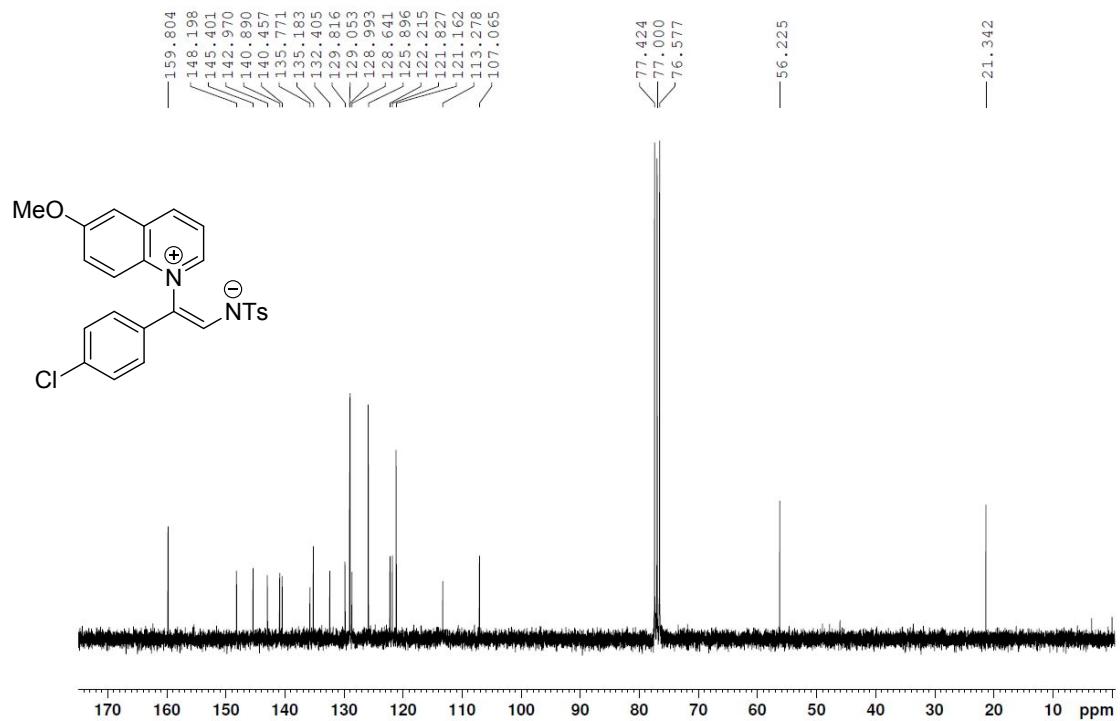
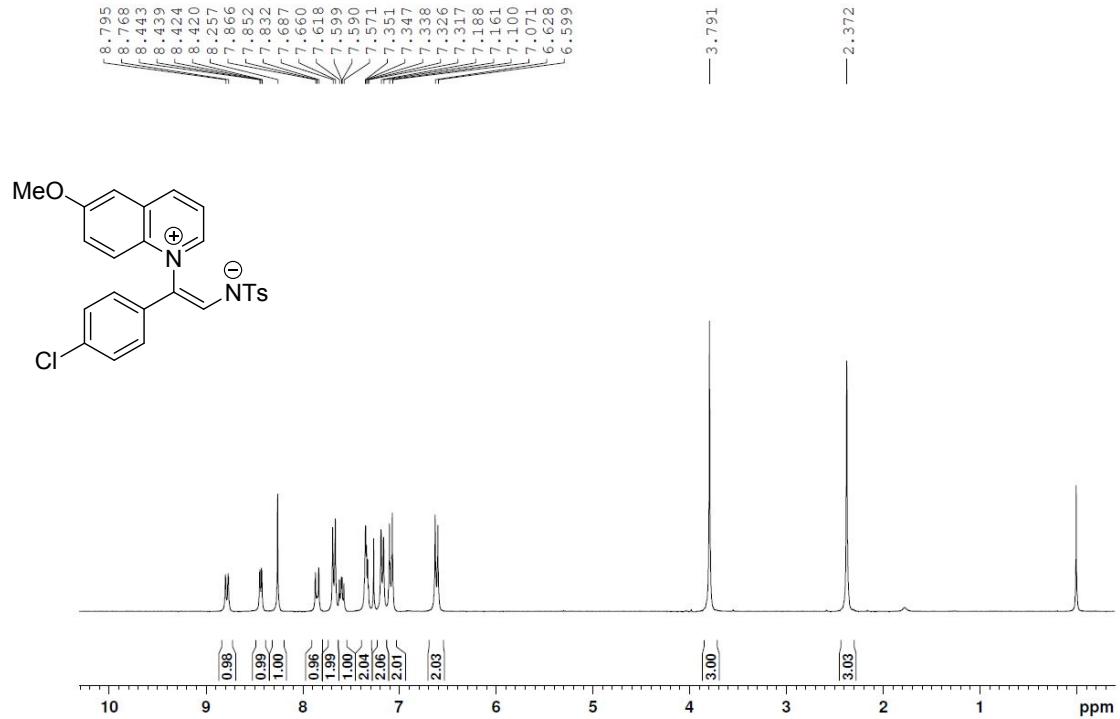
(Z)-(2-(1,7-phenanthrolin-7-ium-7-yl)-2-phenylvinyl)(tosyl)amide:



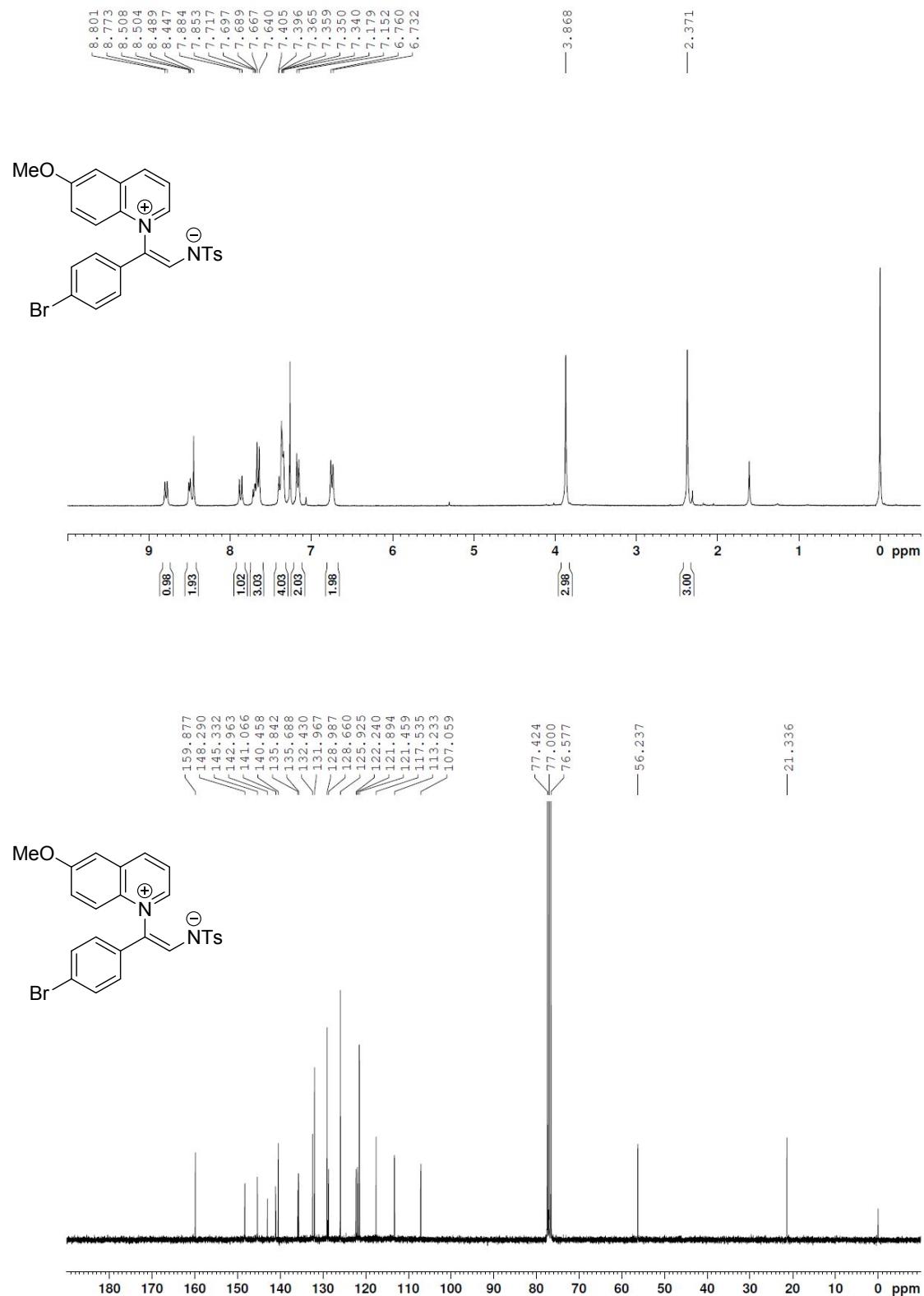
(Z)-(2-(4-fluorophenyl)-2-(6-methylquinolin-1-ium-1-yl)vinyl)(tosyl)amide:



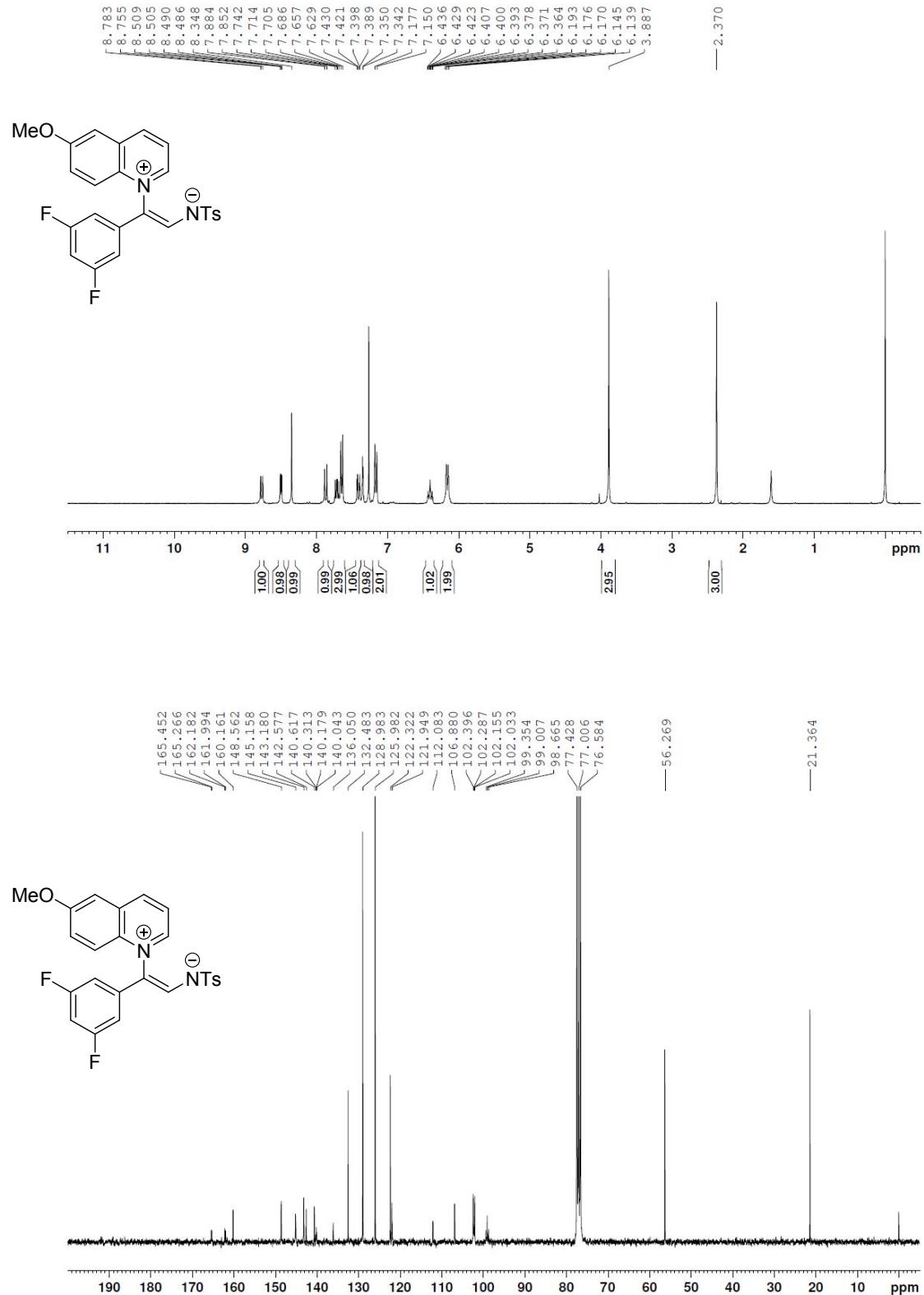
(Z)-(2-(4-chlorophenyl)-2-(6-methoxyquinolin-1-ium-1-yl)vinyl)(tosyl)amide:



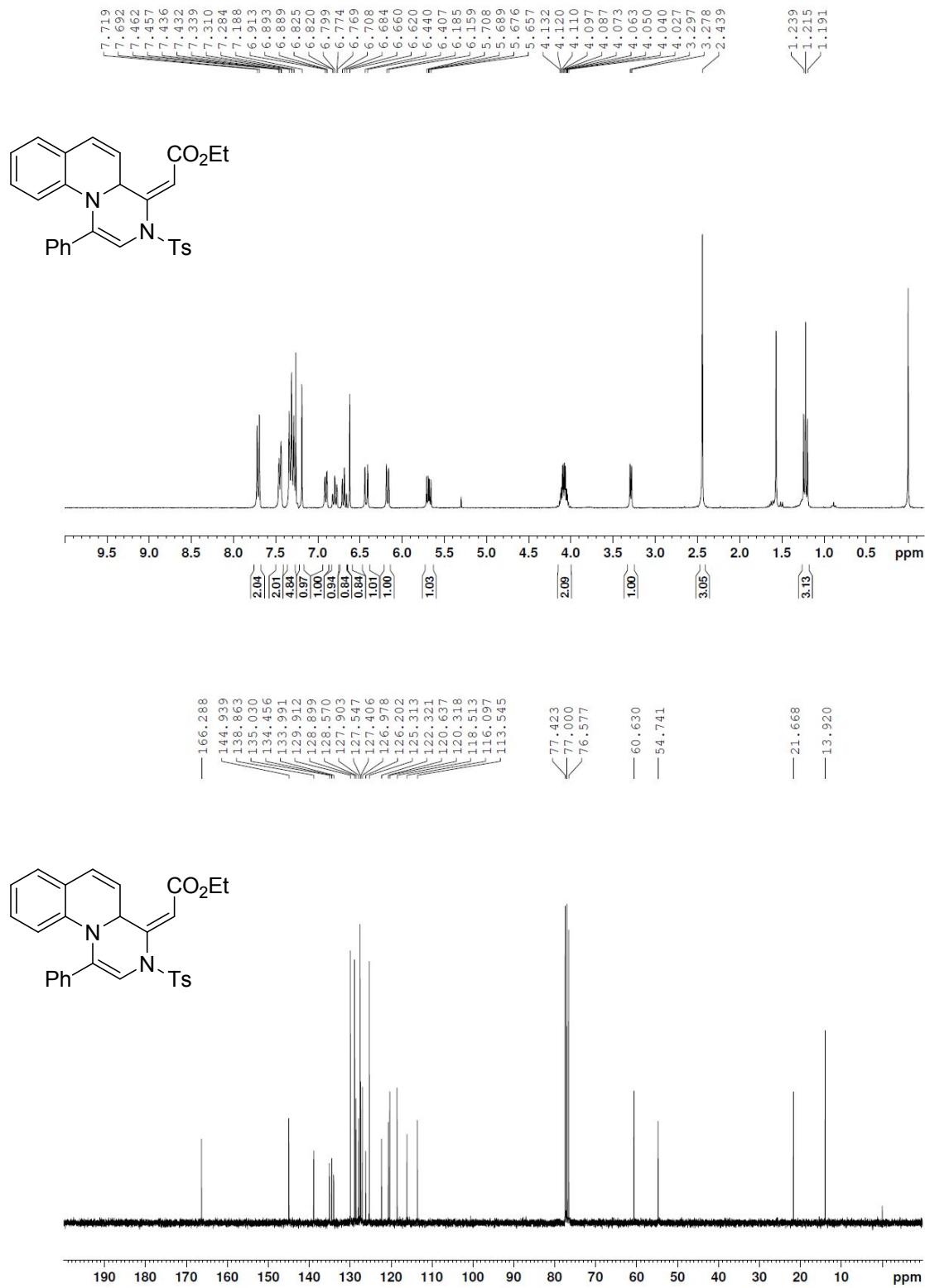
(Z)-(2-(4-bromophenyl)-2-(6-methoxyquinolin-1-i^{um}-1-yl)vinyl)(tosyl)amide:



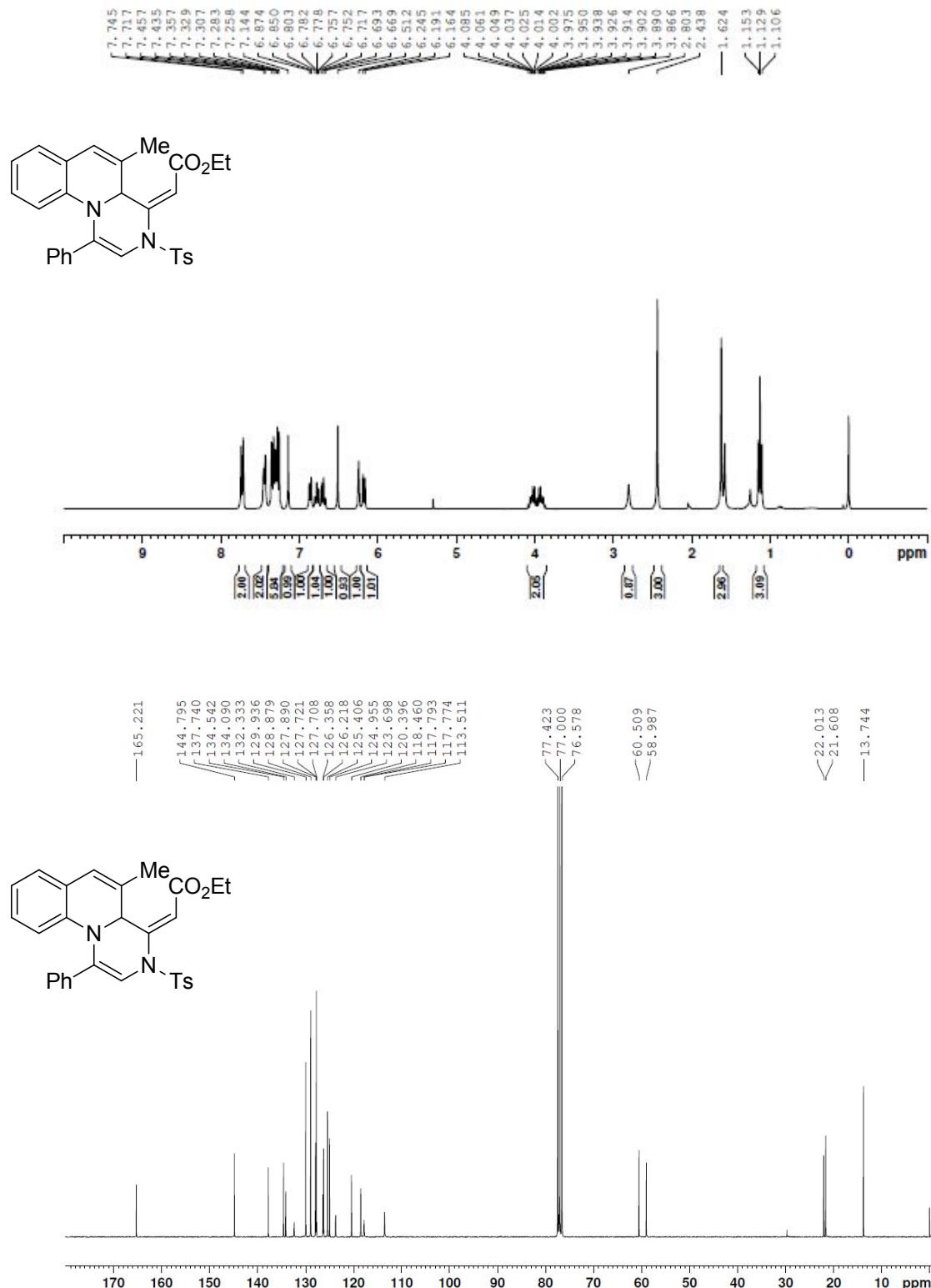
(Z)-(2-(3,5-difluorophenyl)-2-(6-methoxyquinolin-1-i^{um}-1-yl)vinyl)(tosyl)amide:



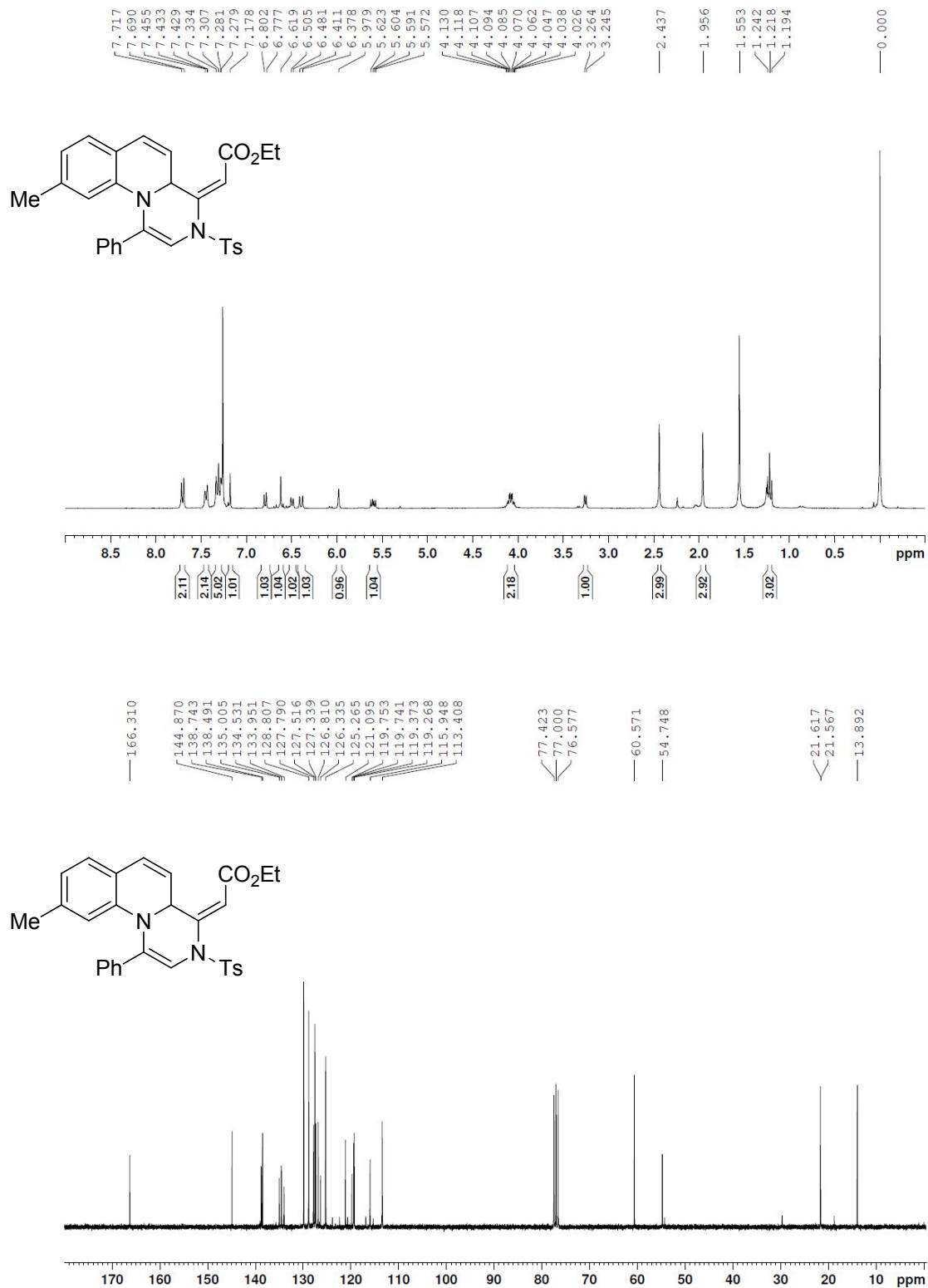
(E)-ethyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3a):



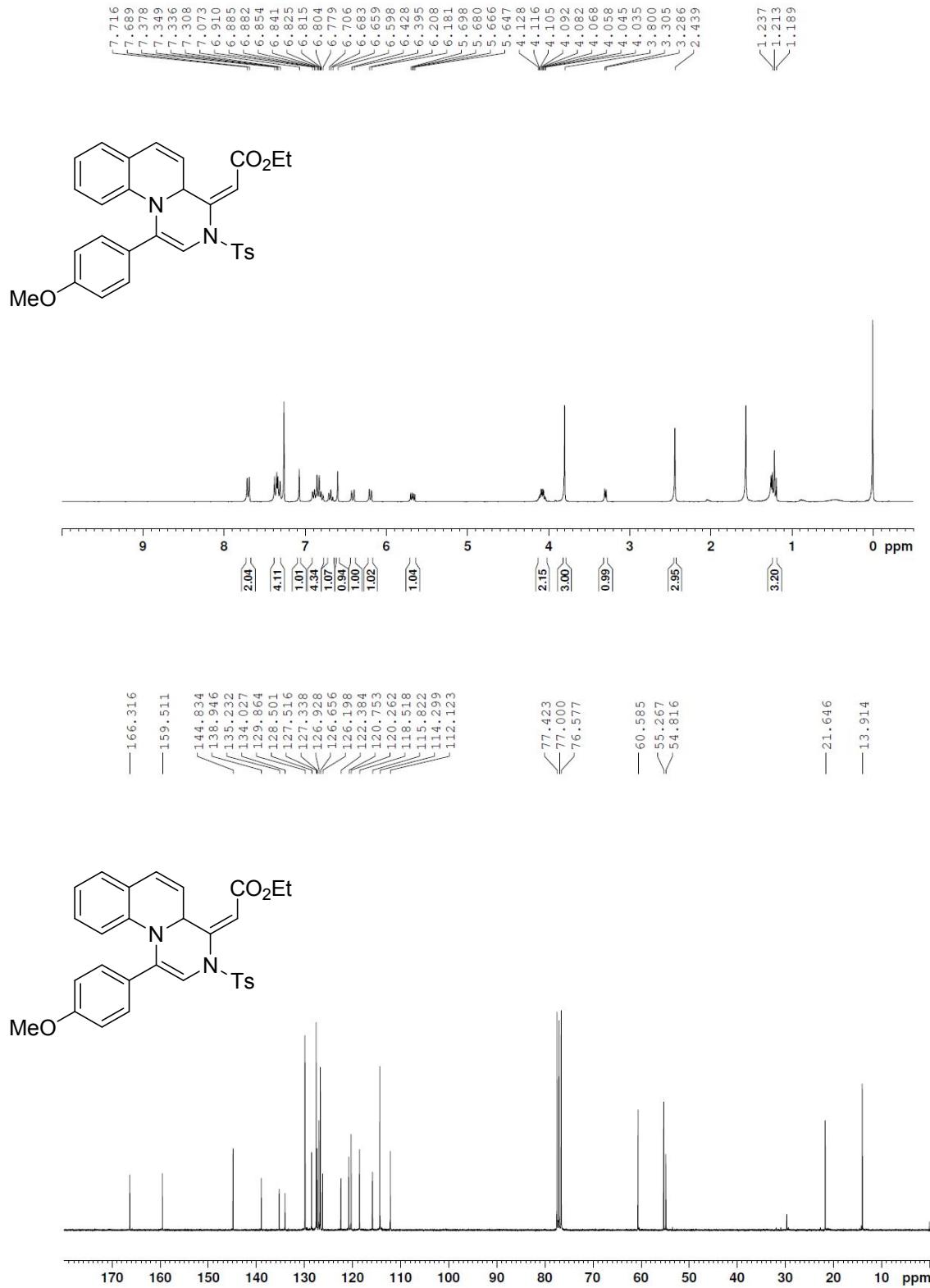
(E)-ethyl 2-(5-methyl-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3b):



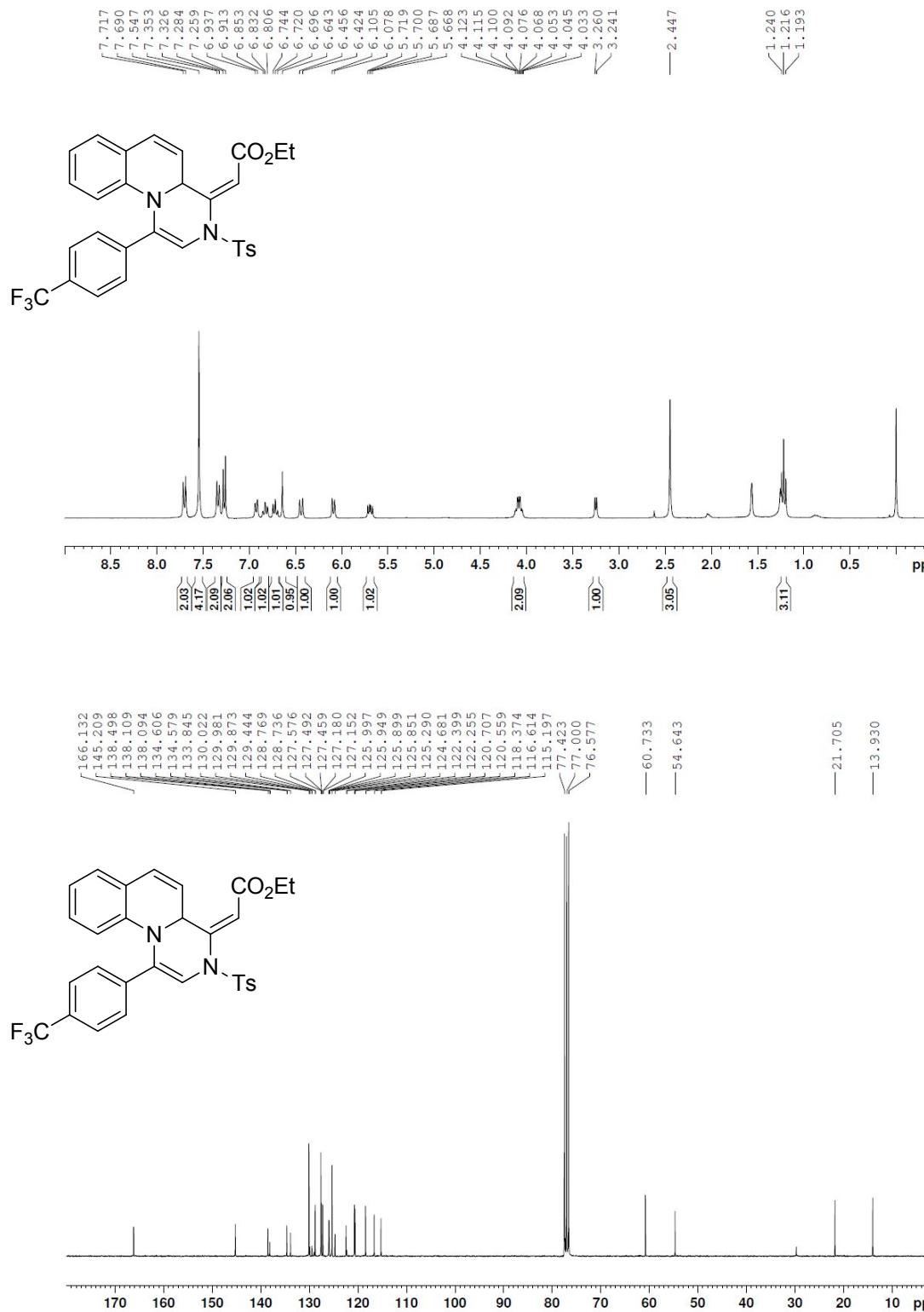
(E)-ethyl 2-(9-methyl-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3c):



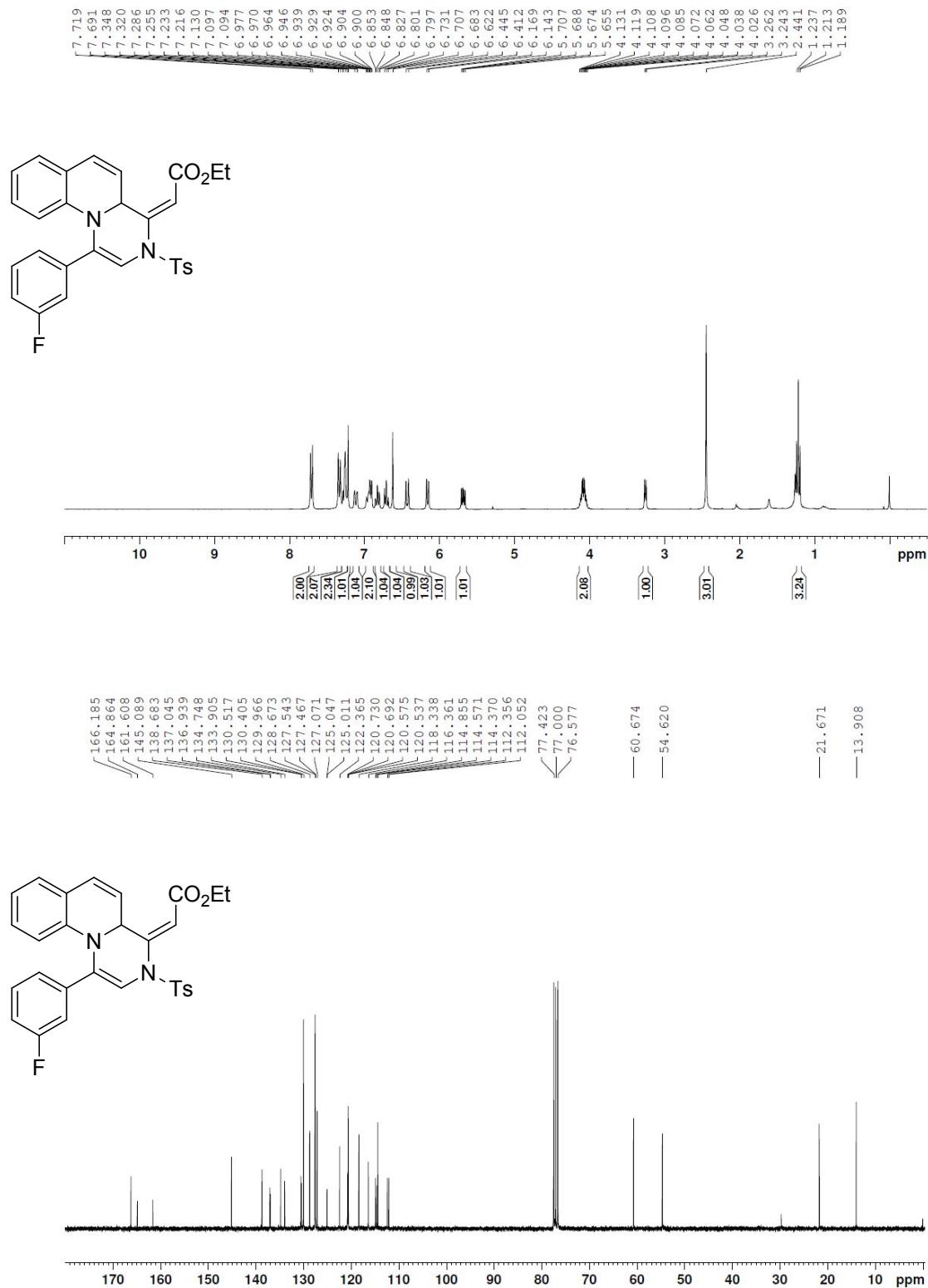
(E)-ethyl 2-(1-(4-methoxyphenyl)-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3d):



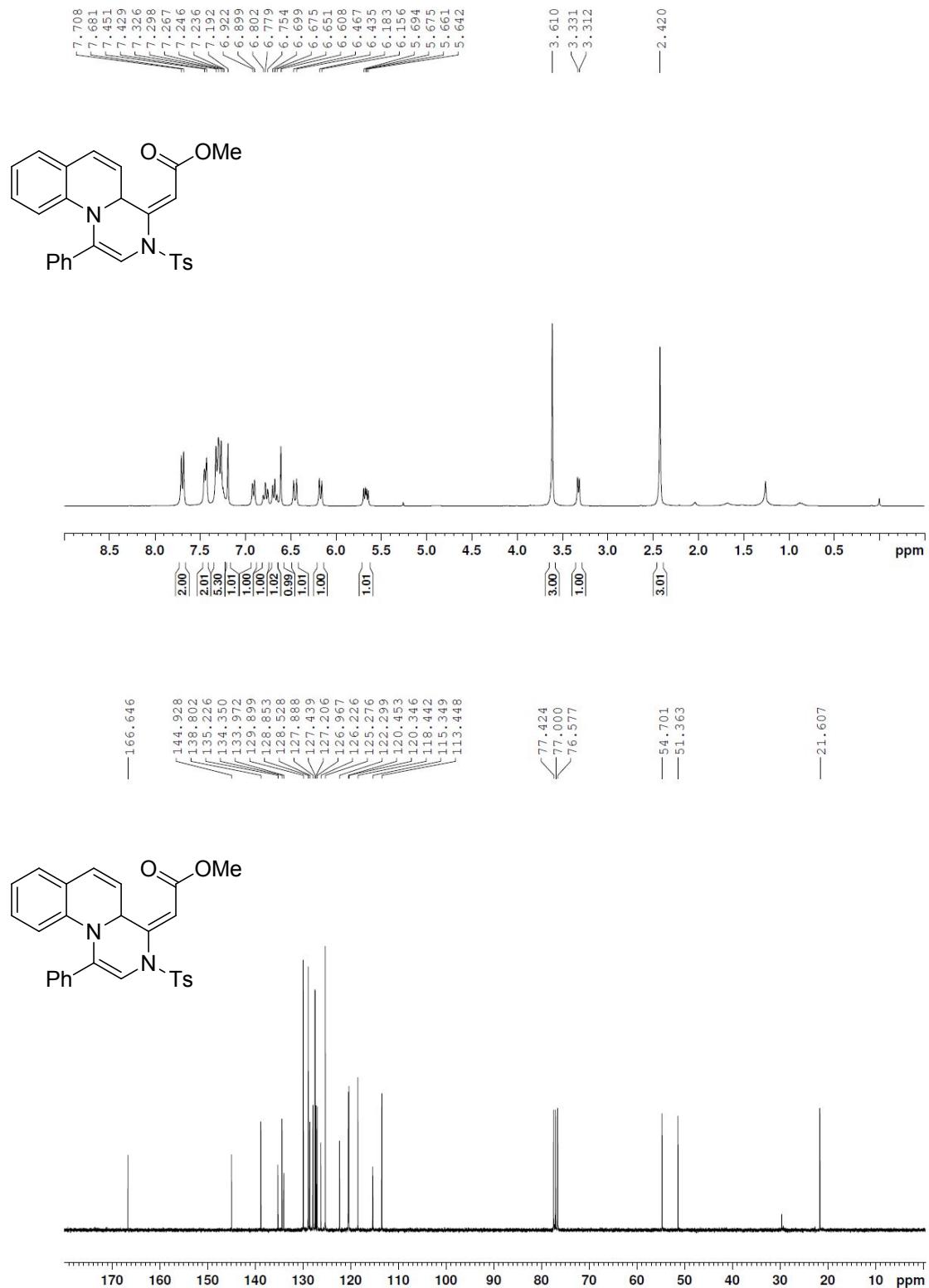
**(E)-ethyl
2-(3-tosyl-1-(4-(trifluoromethyl)phenyl)-3H-pyrazino[1,2-a]quinolin-4(4aH)-
ylidene)acetate (3e):**



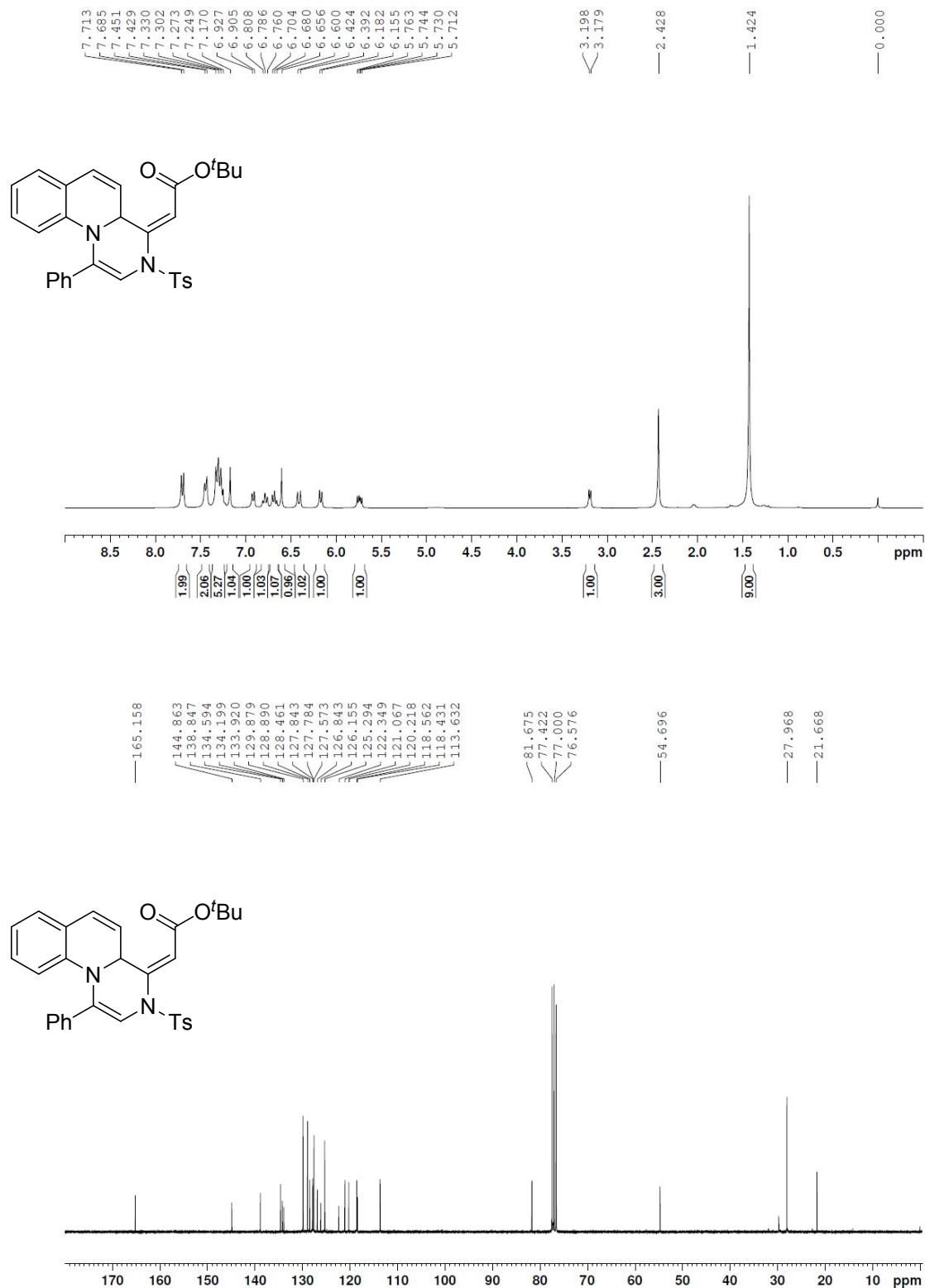
(E)-ethyl 2-(1-(3-fluorophenyl)-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3f):



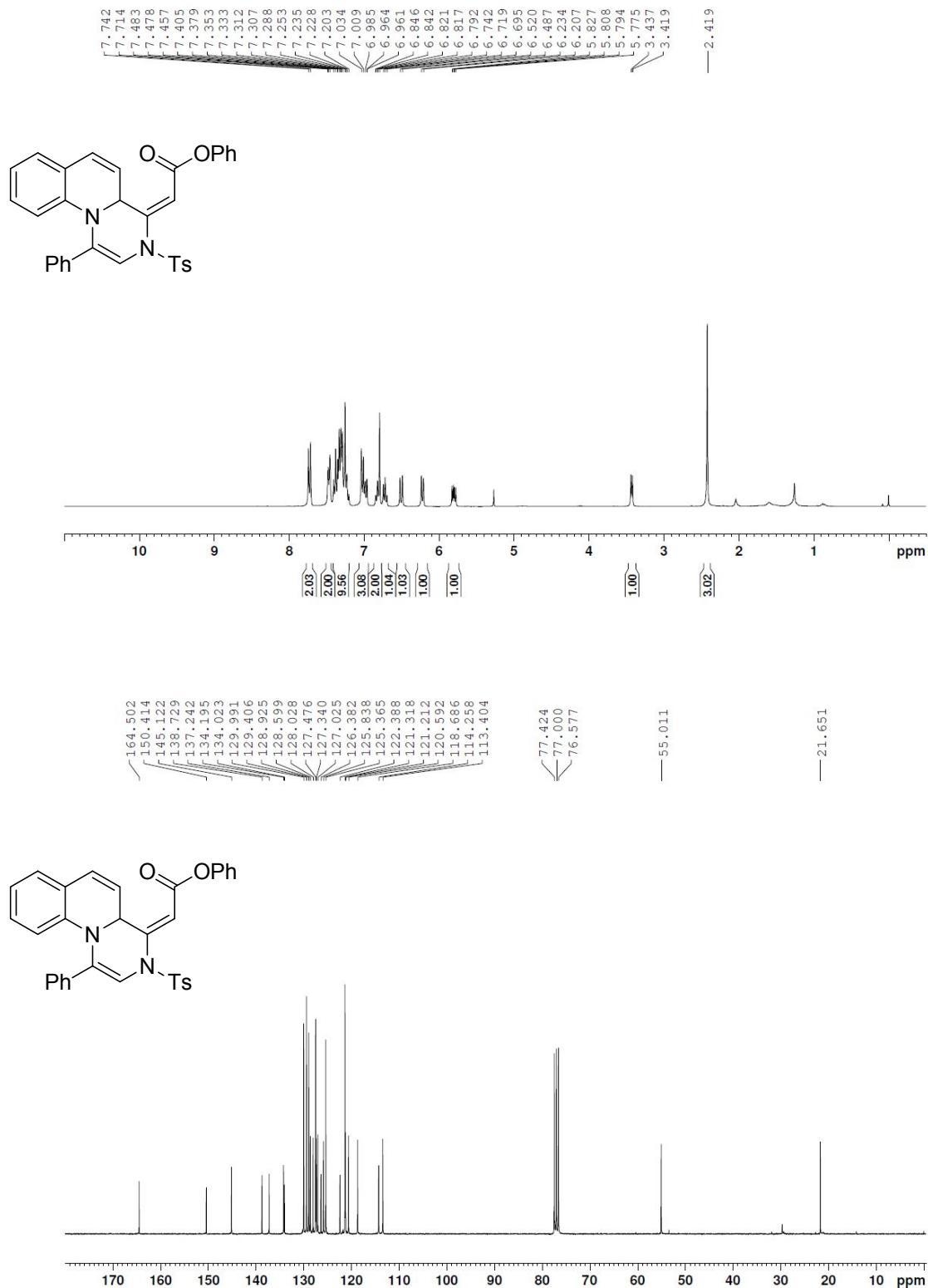
(E)-methyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3g):



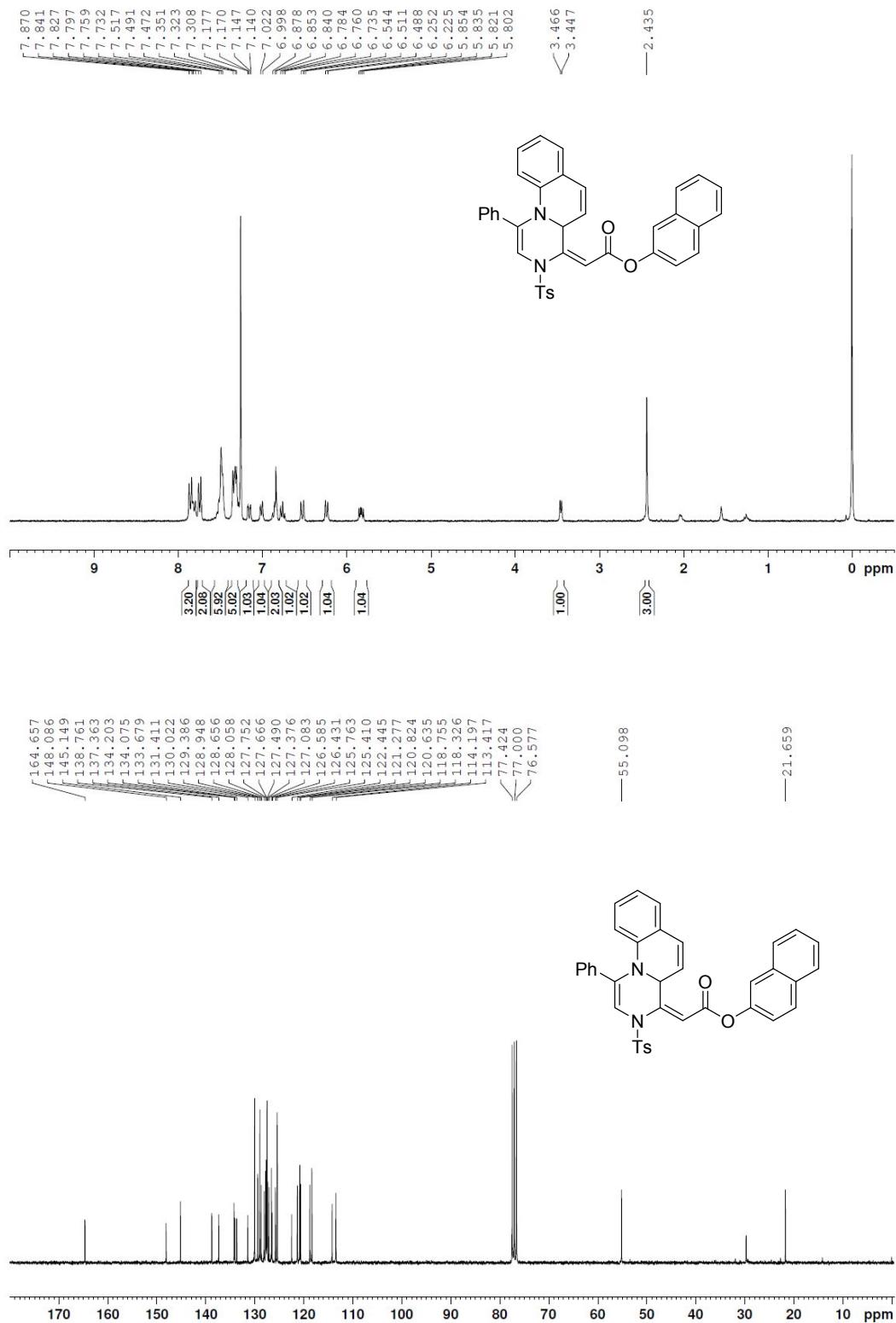
(E)-tert-butyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3h):



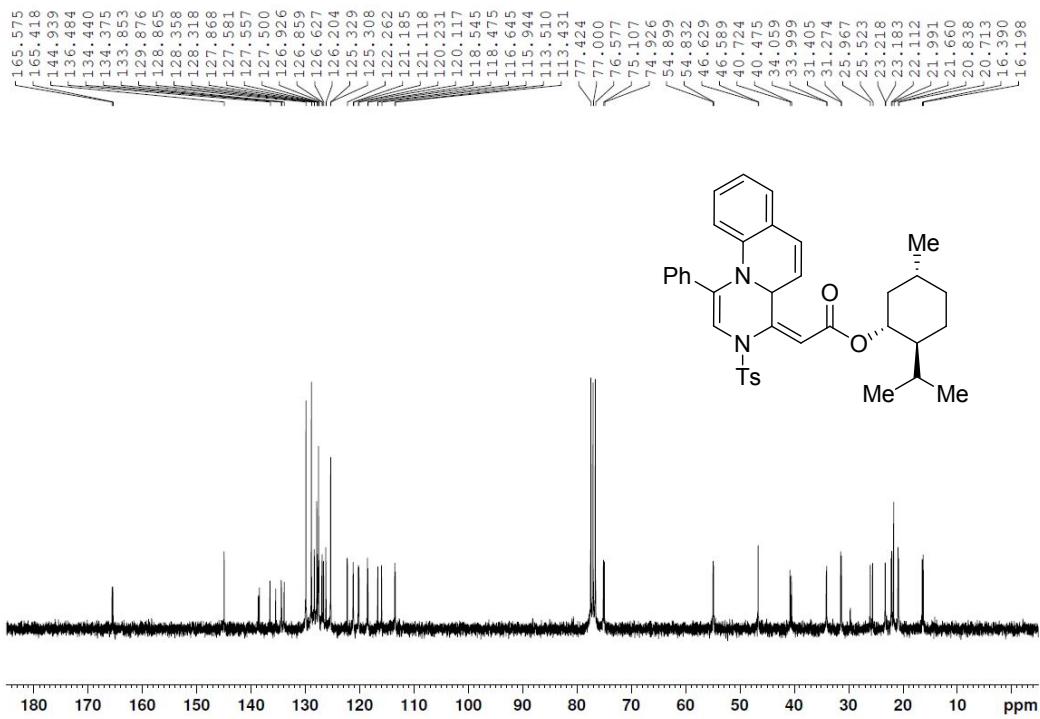
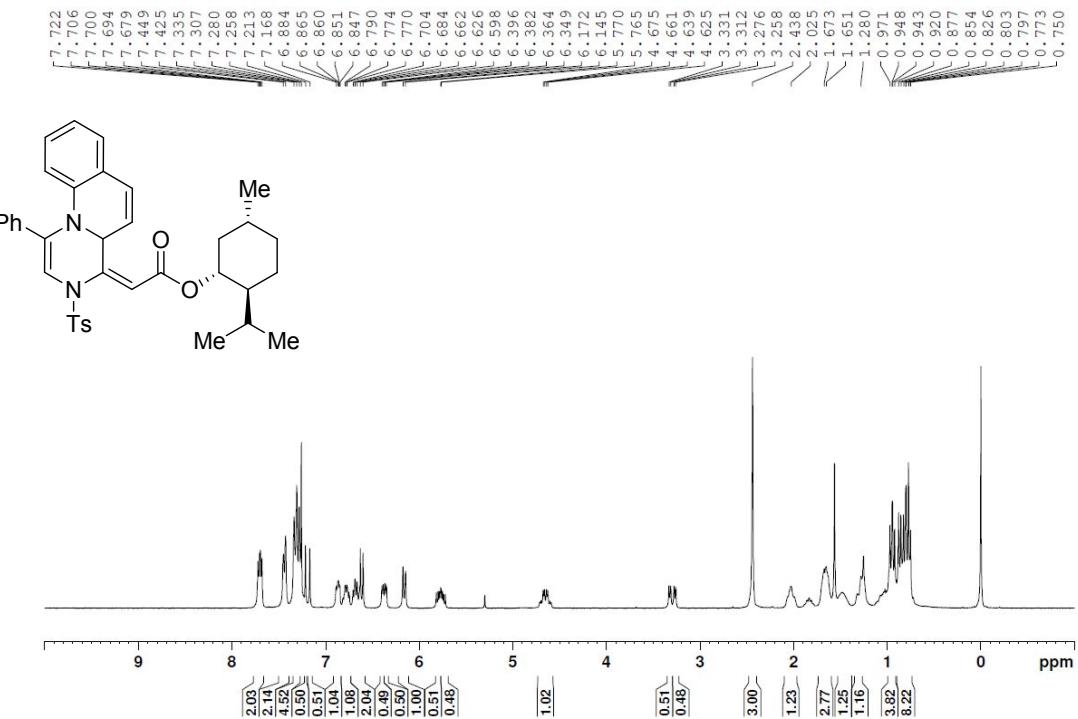
(E)-phenyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3i):



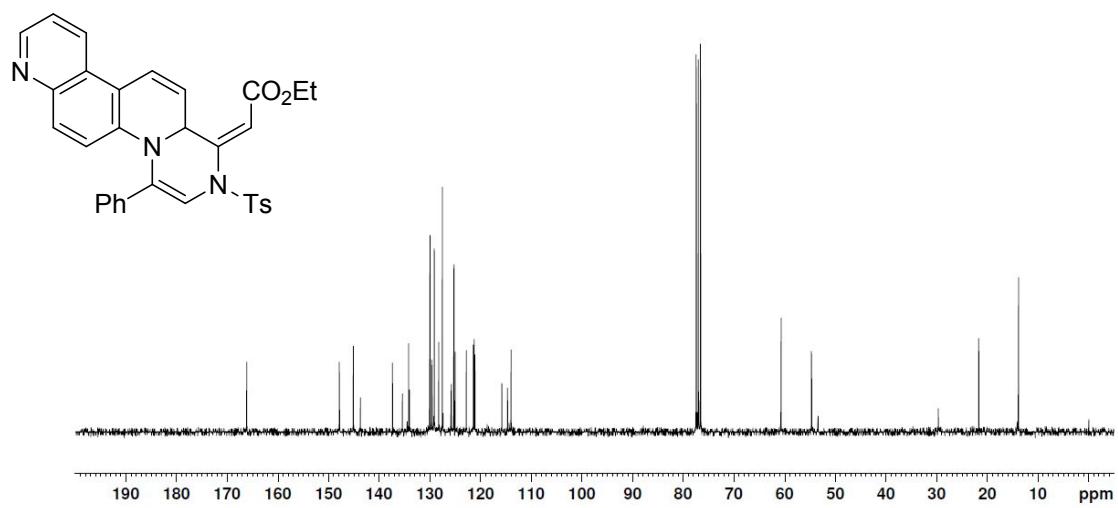
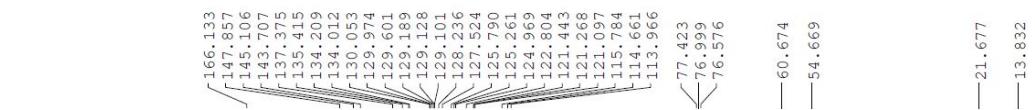
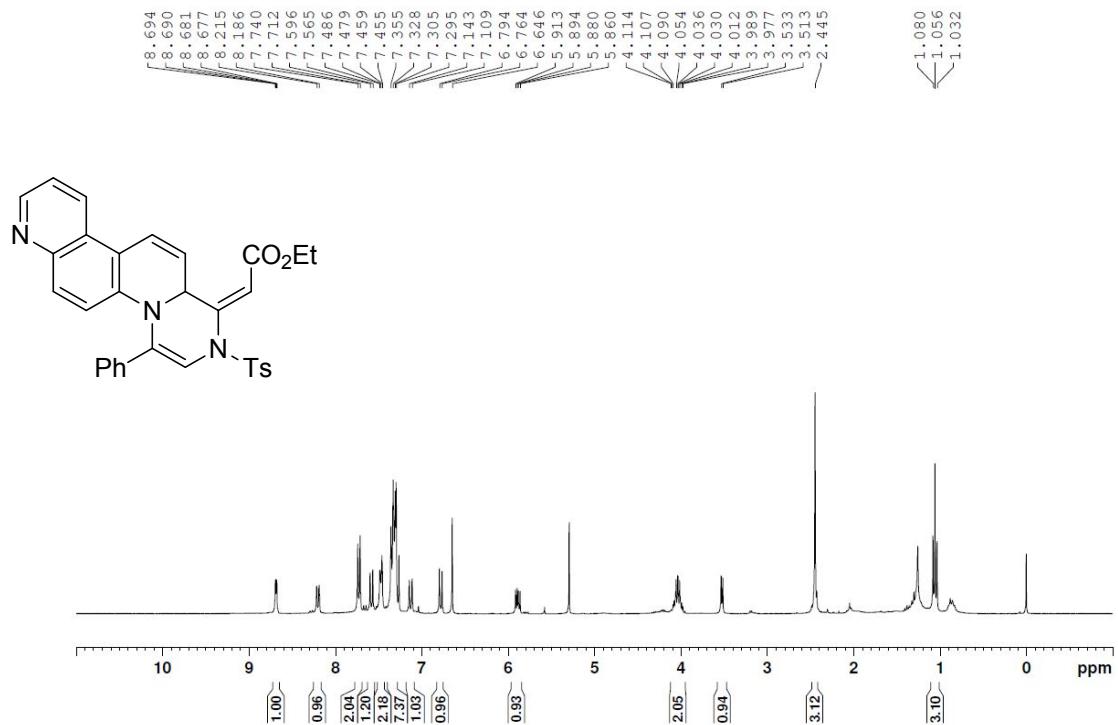
(E)-naphthalen-2-yl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3j):



(E)-(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (3k):

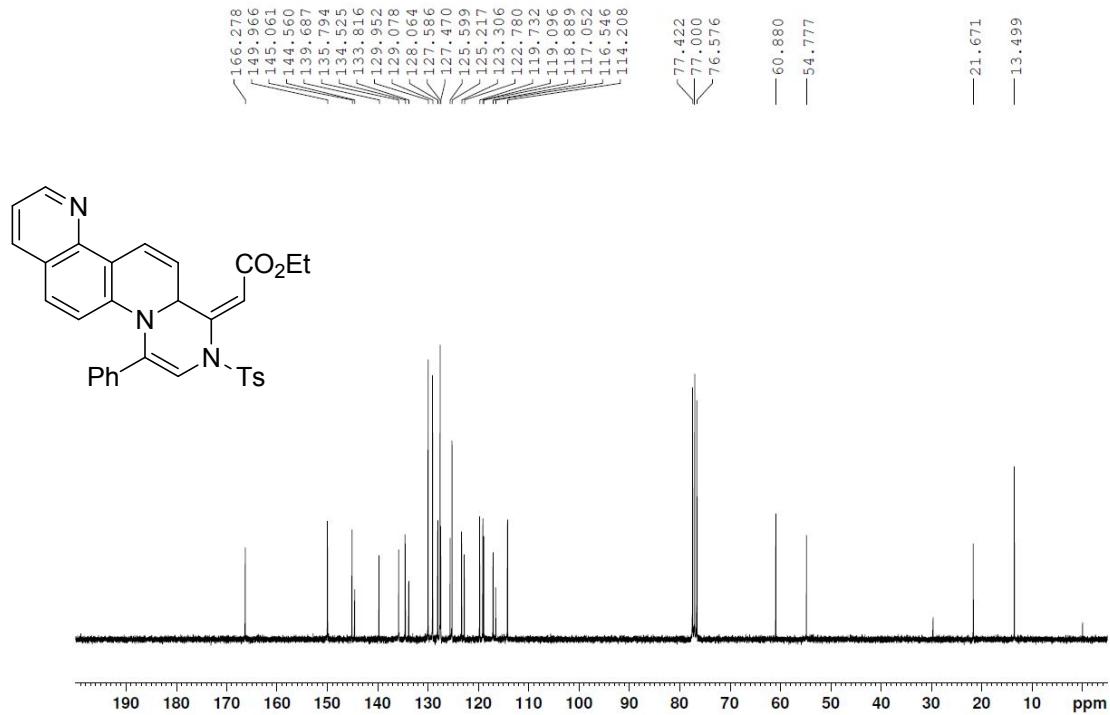
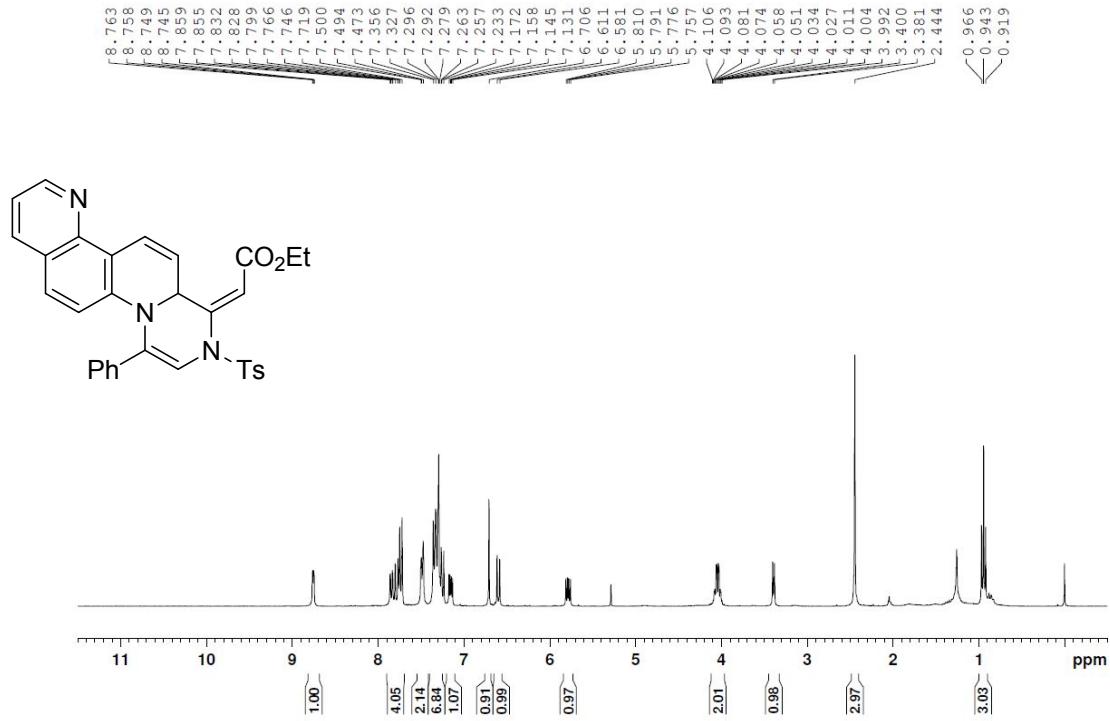


(E)-ethyl 2-(10-phenyl-8-tosyl-6aH-pyrazino[2,1-c][4,7]phenanthrolin-7(8H)-ylidene)acetate (3l):

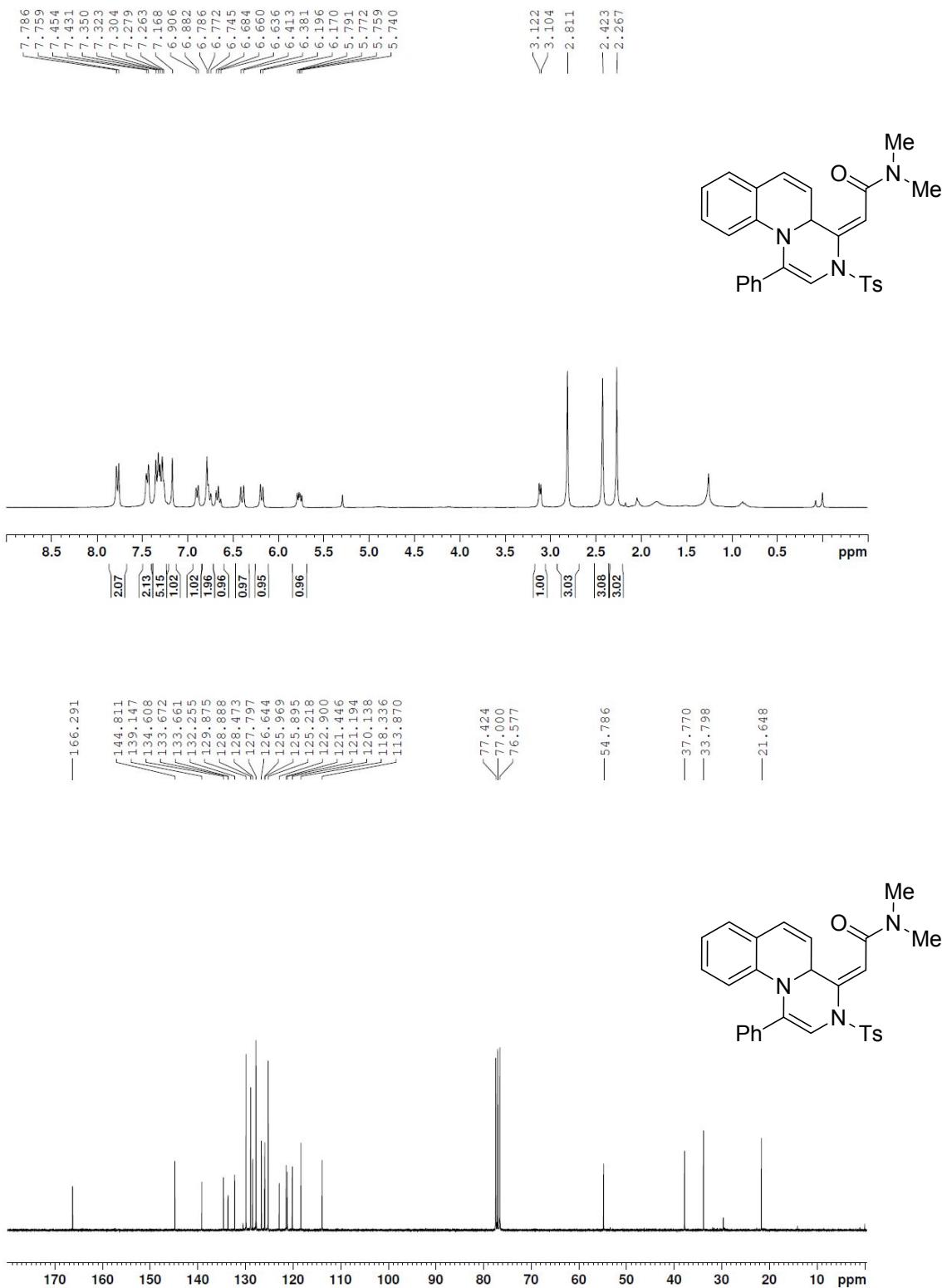


(E)-ethyl ylidene)acetate (3m):

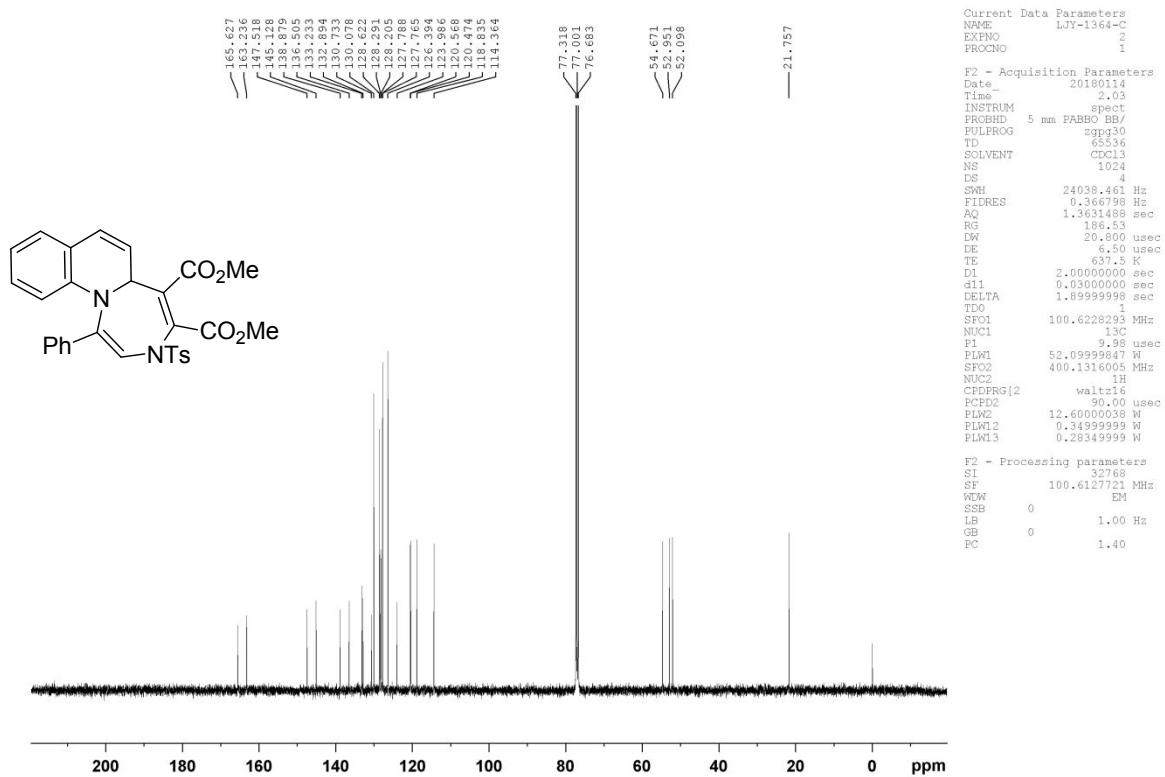
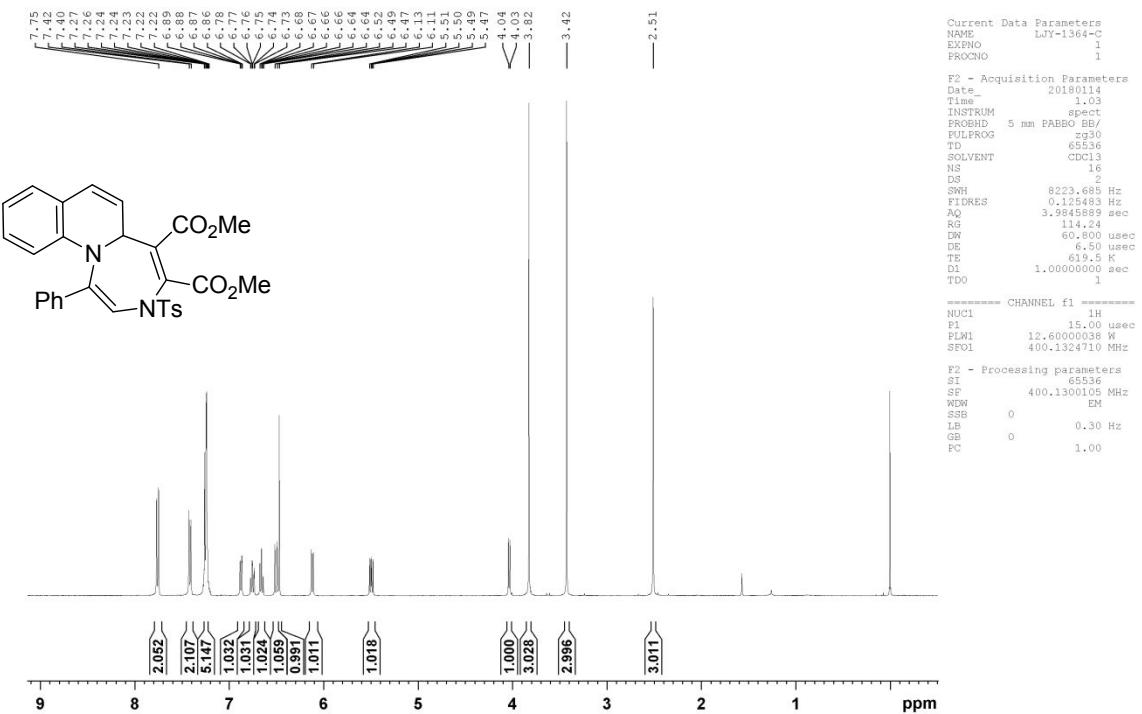
2-(4-phenyl-2-tosyl-2,13a-dihydro-1H-pyrazino[1,2-i][1,7]phenanthrolin-1-



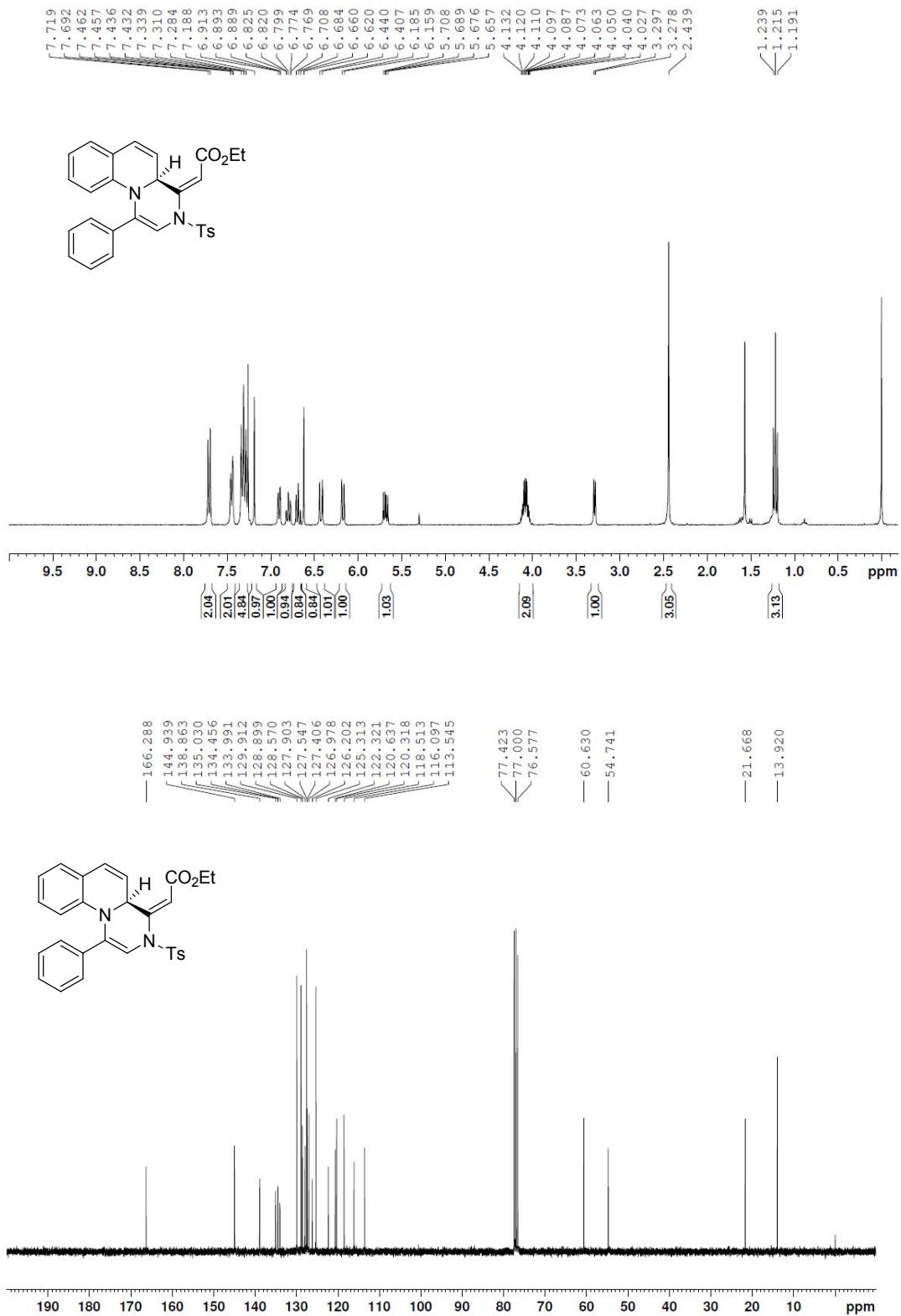
(E)-N,N-dimethyl-2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetamide (3n):



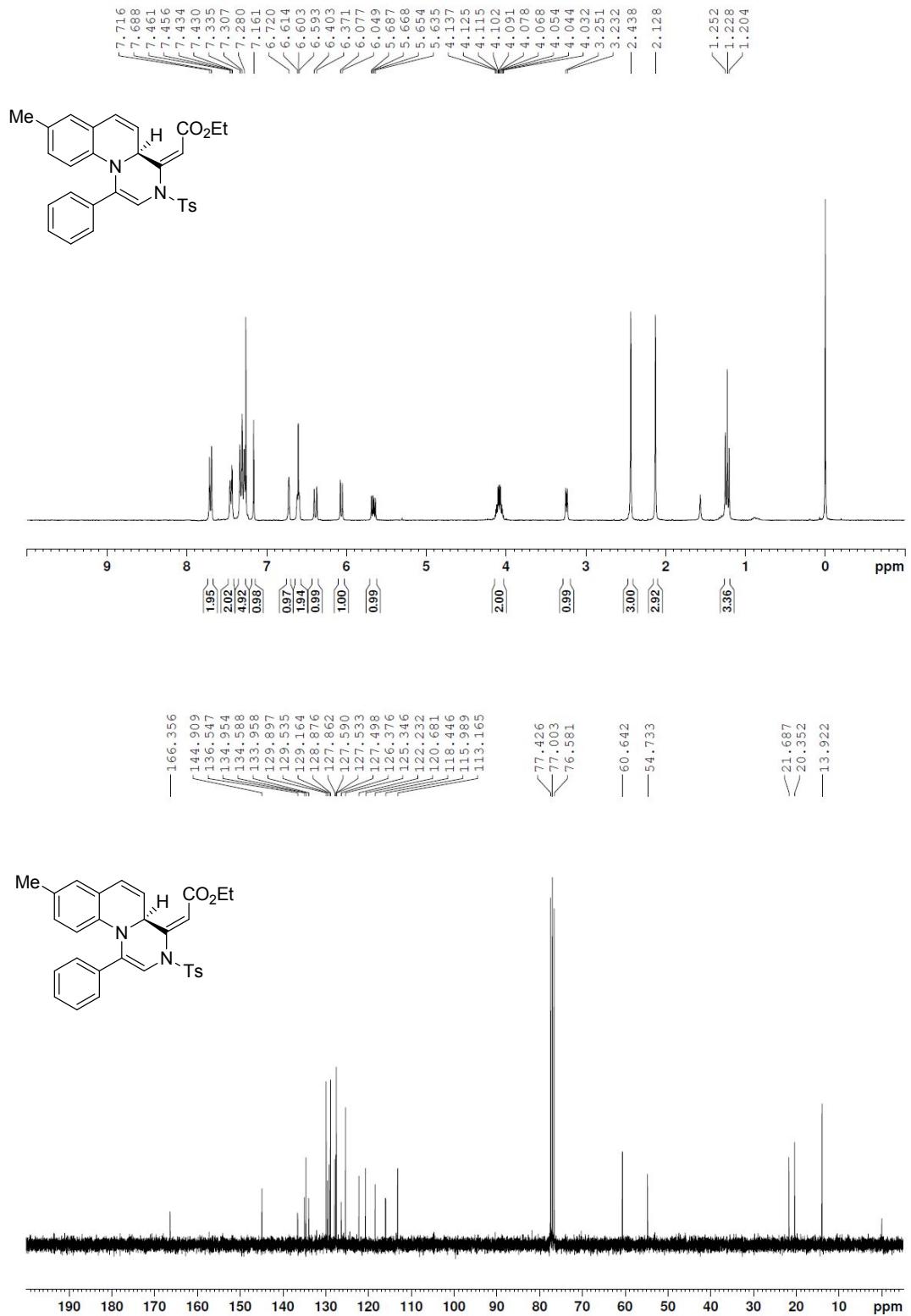
Dimethyl 1-phenyl-3-tosyl-3,5a-dihydro-[1,4]diazepino[1,7-a]quinoline-4,5-dicarboxylate (4):



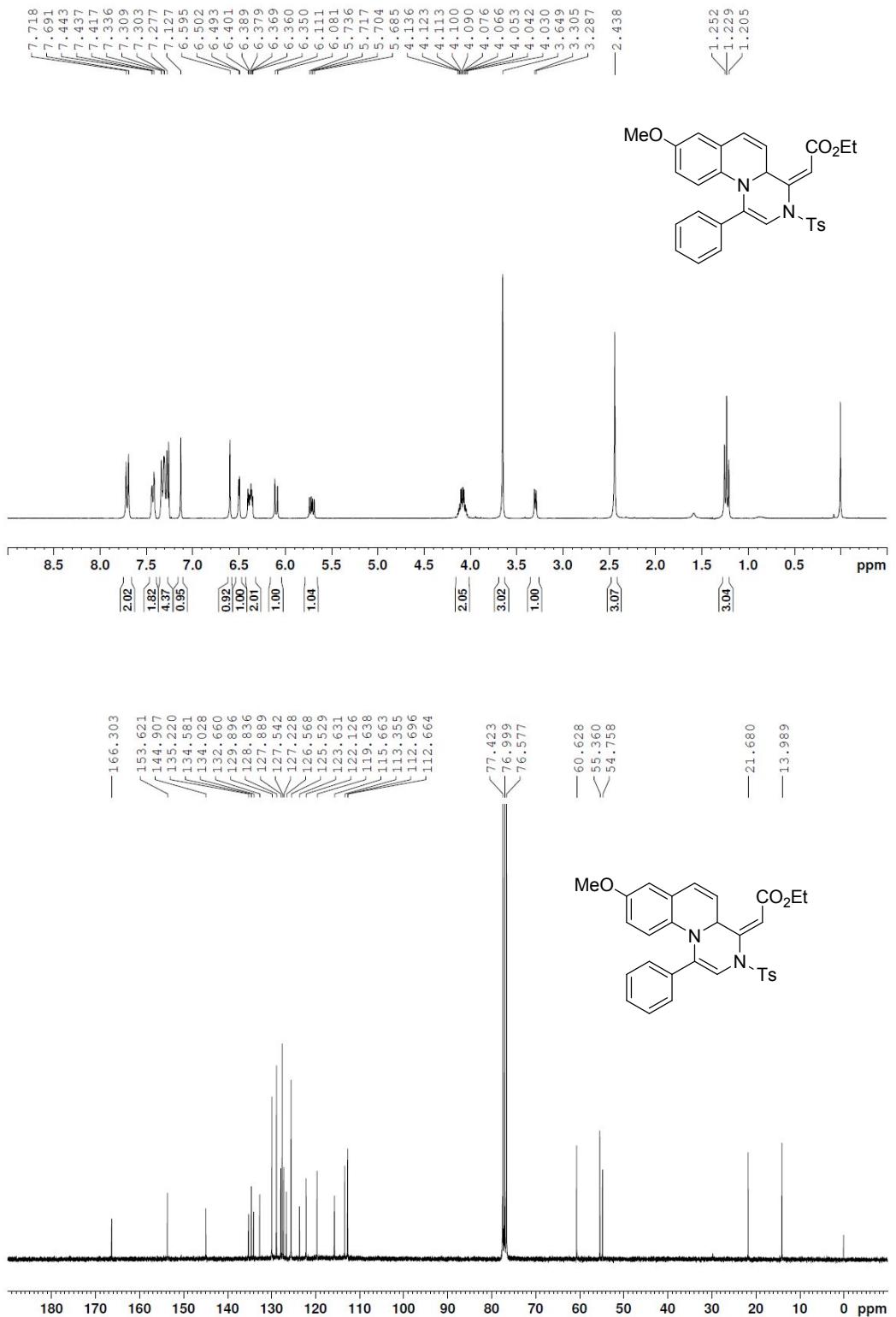
(S,E)-ethyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5a):



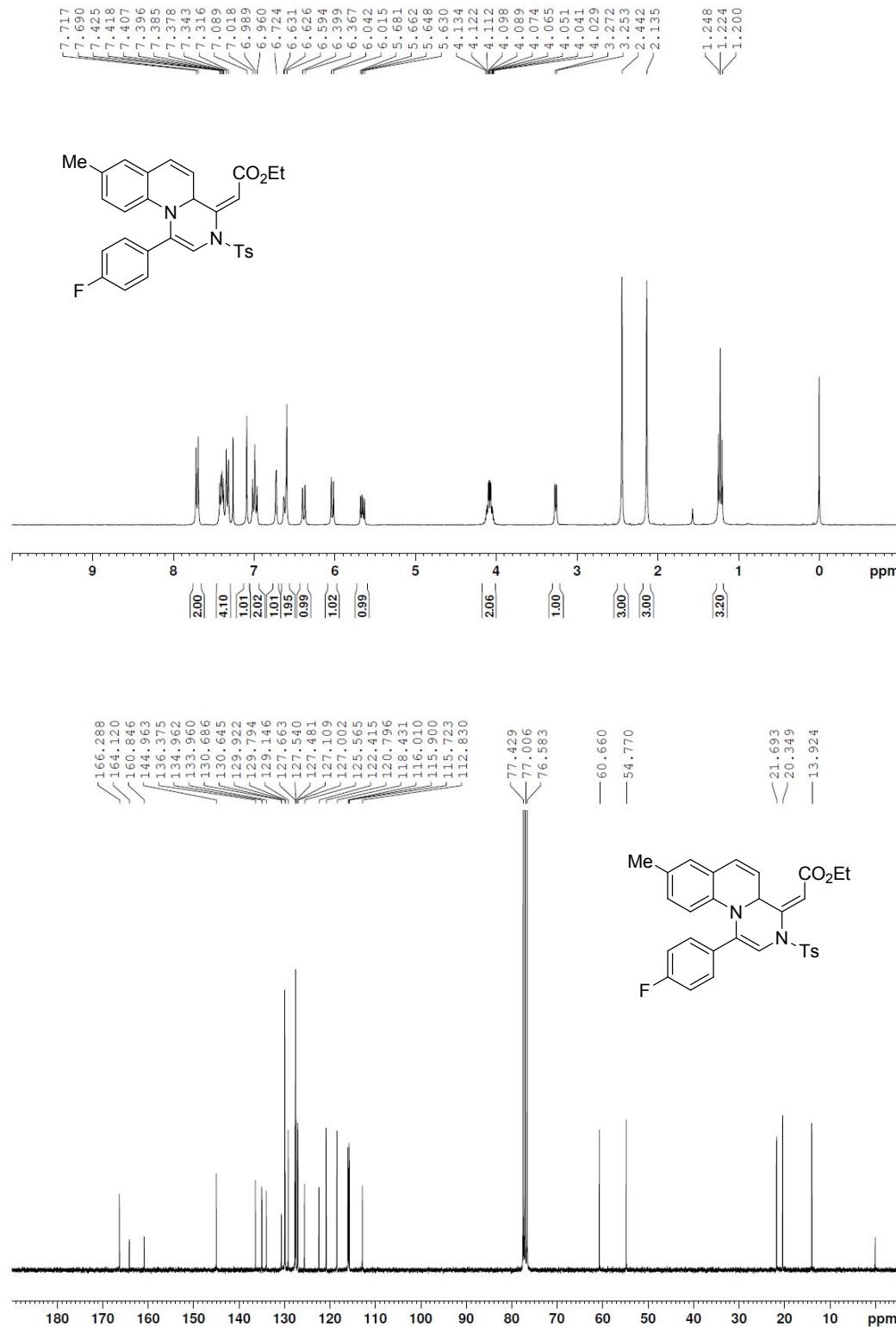
(S,E)-ethyl 2-(8-methyl-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5b):



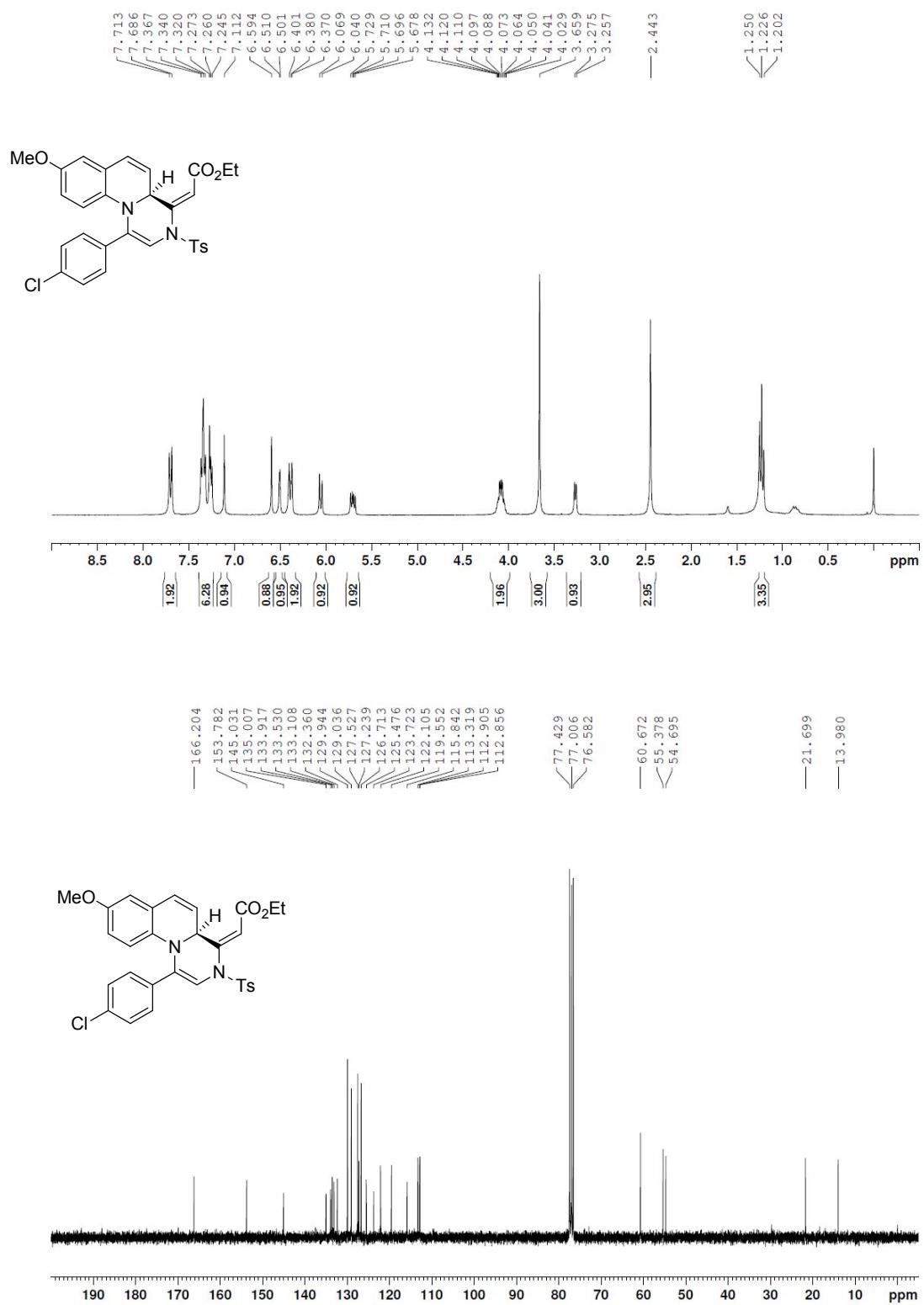
(S,E)-ethyl 2-(8-methoxy-1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5c):



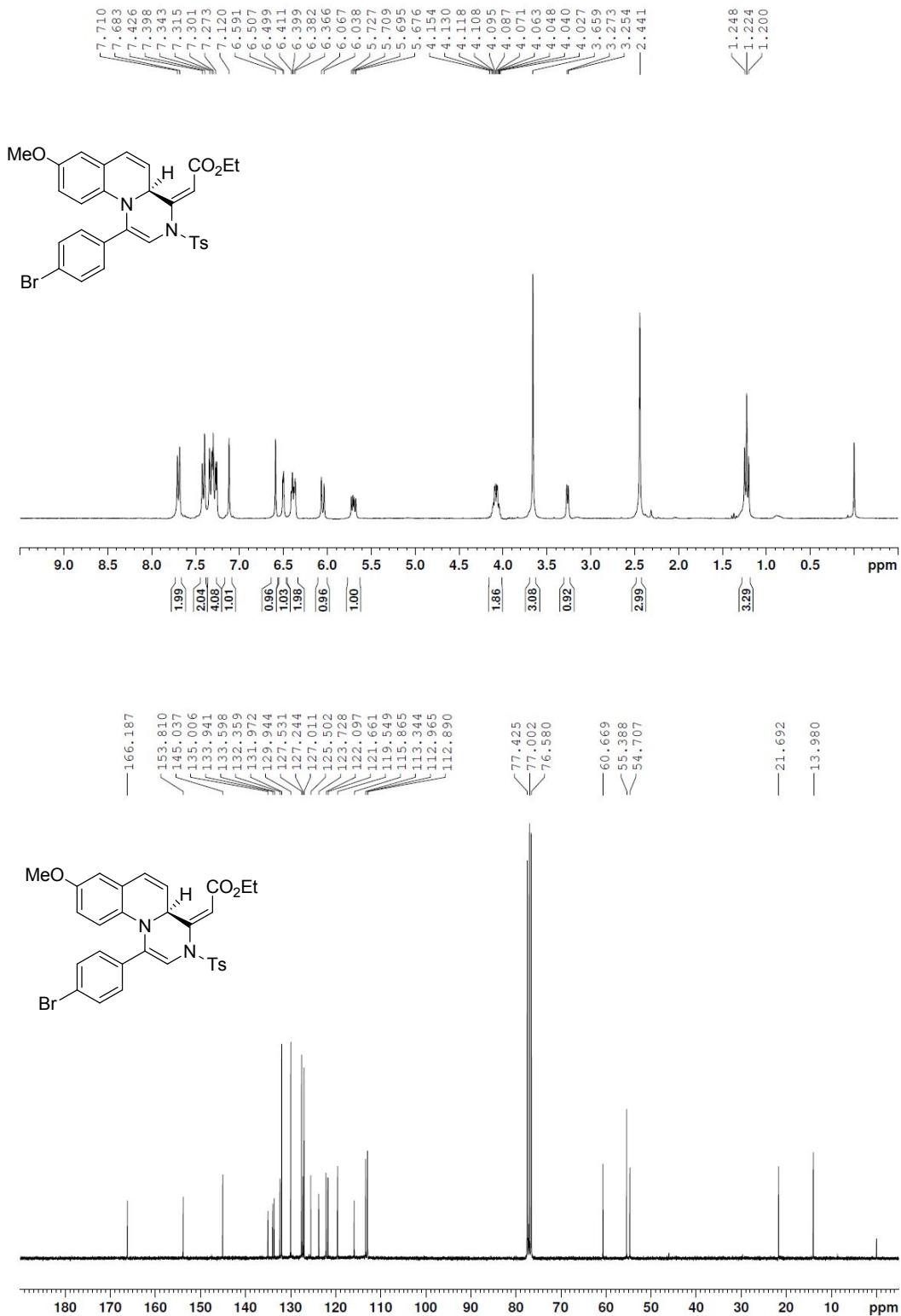
**(S,E)-ethyl
ylidene)acetate (5d):**



(S,E)-ethyl 2-(1-(4-chlorophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5e):

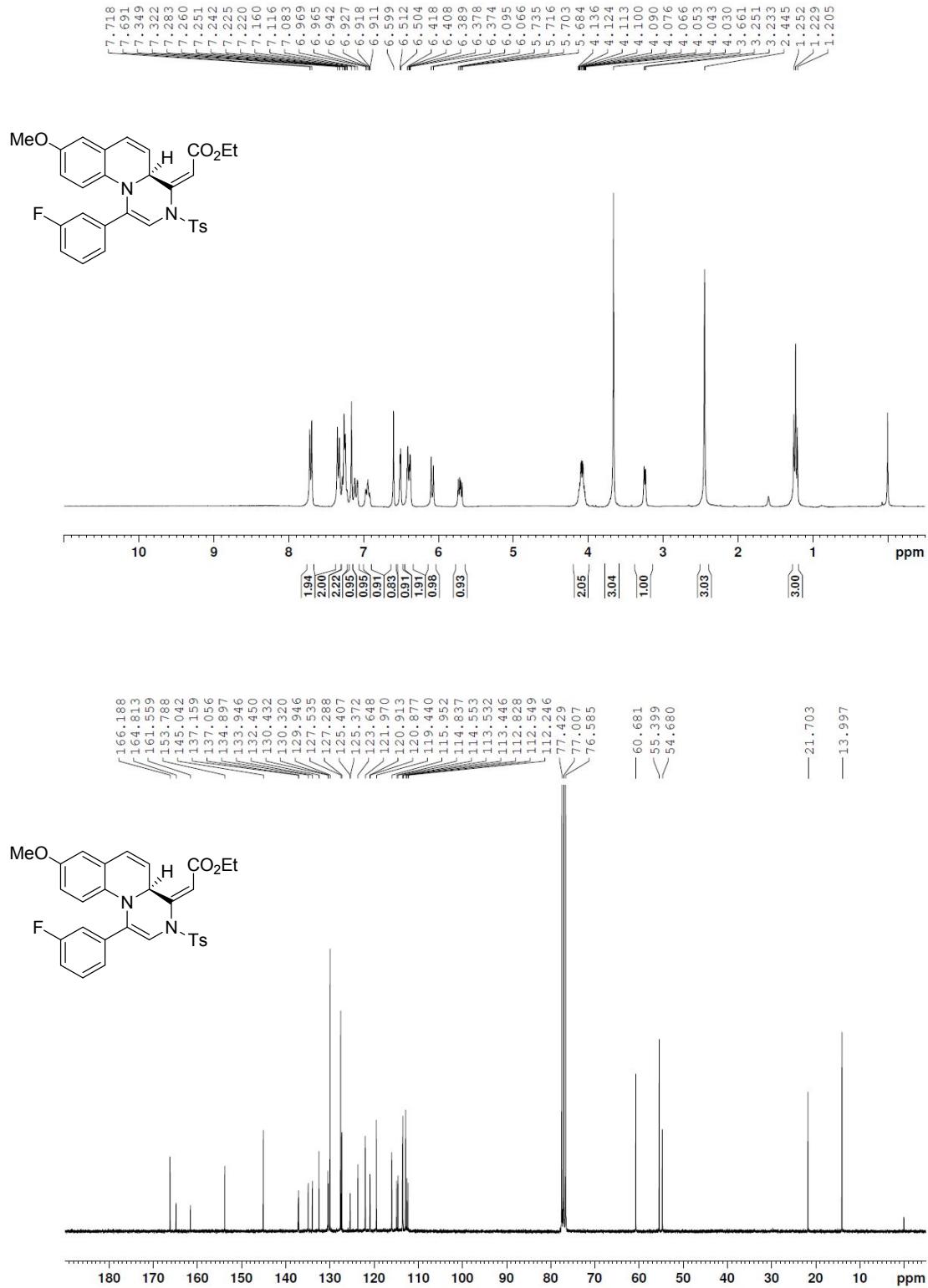


(S,E)-ethyl 2-(1-(4-bromophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5f):

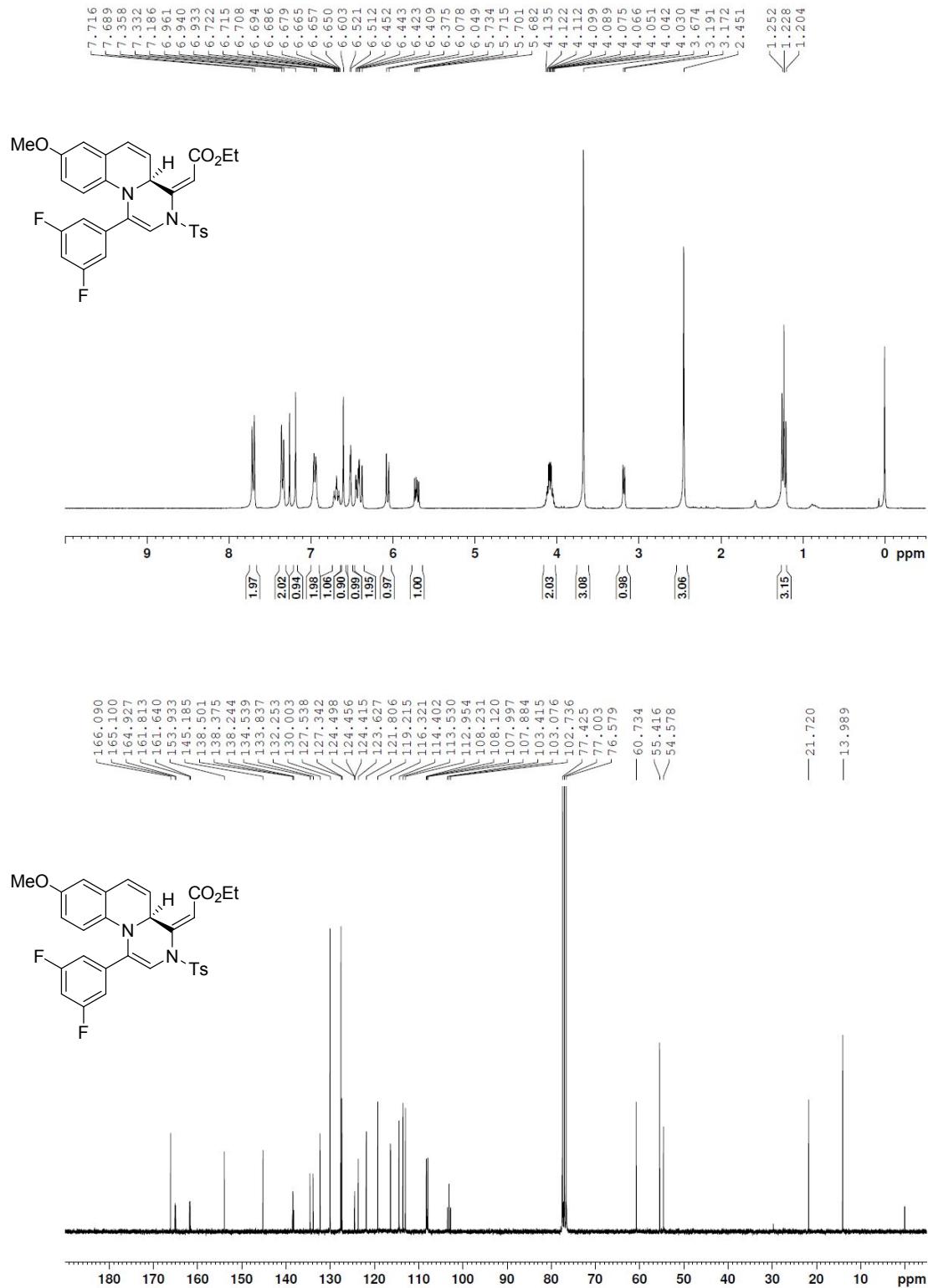


(S,E)-ethyl
ylidene)acetate (5g):

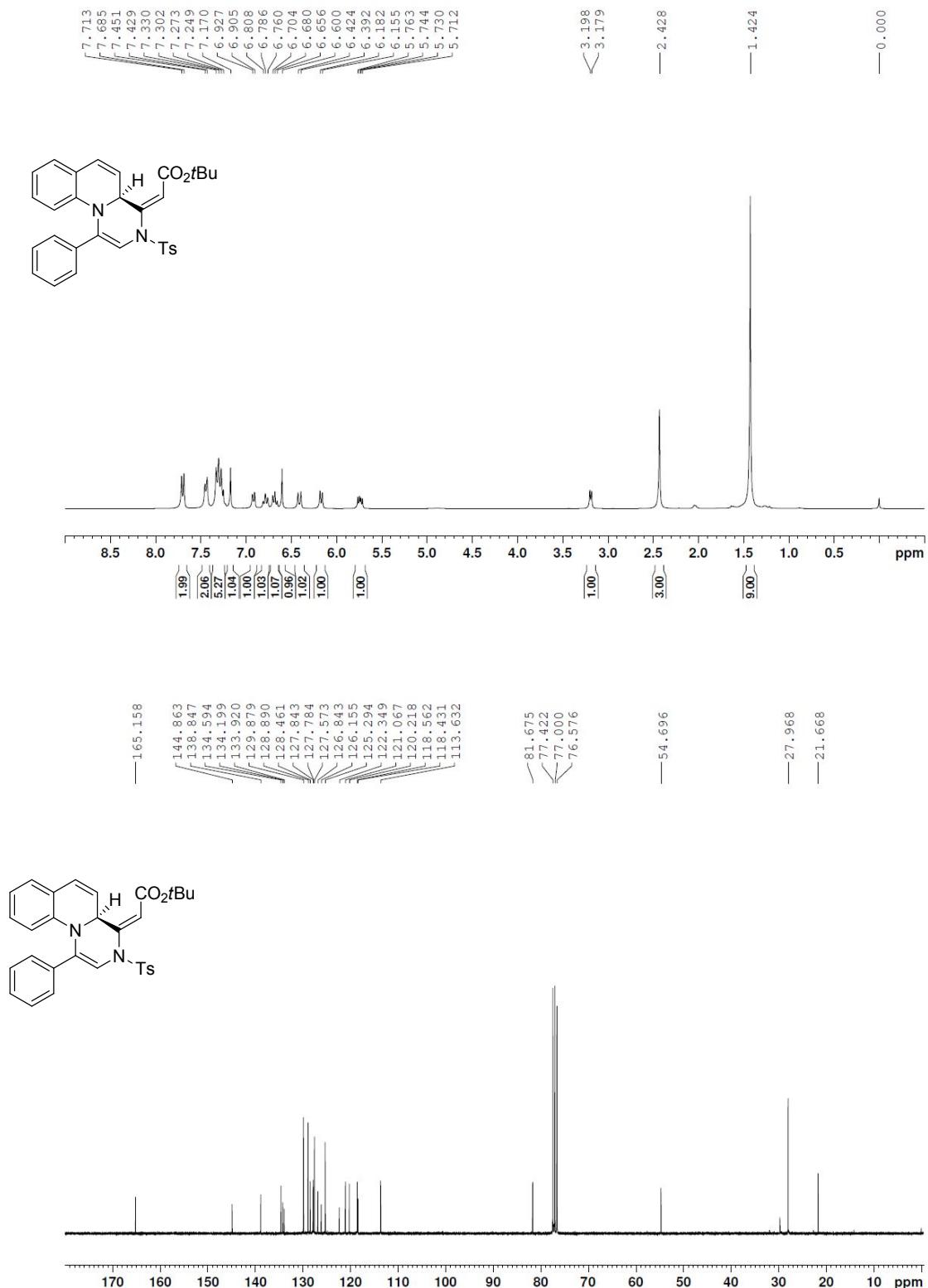
2-(1-(3-fluorophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-



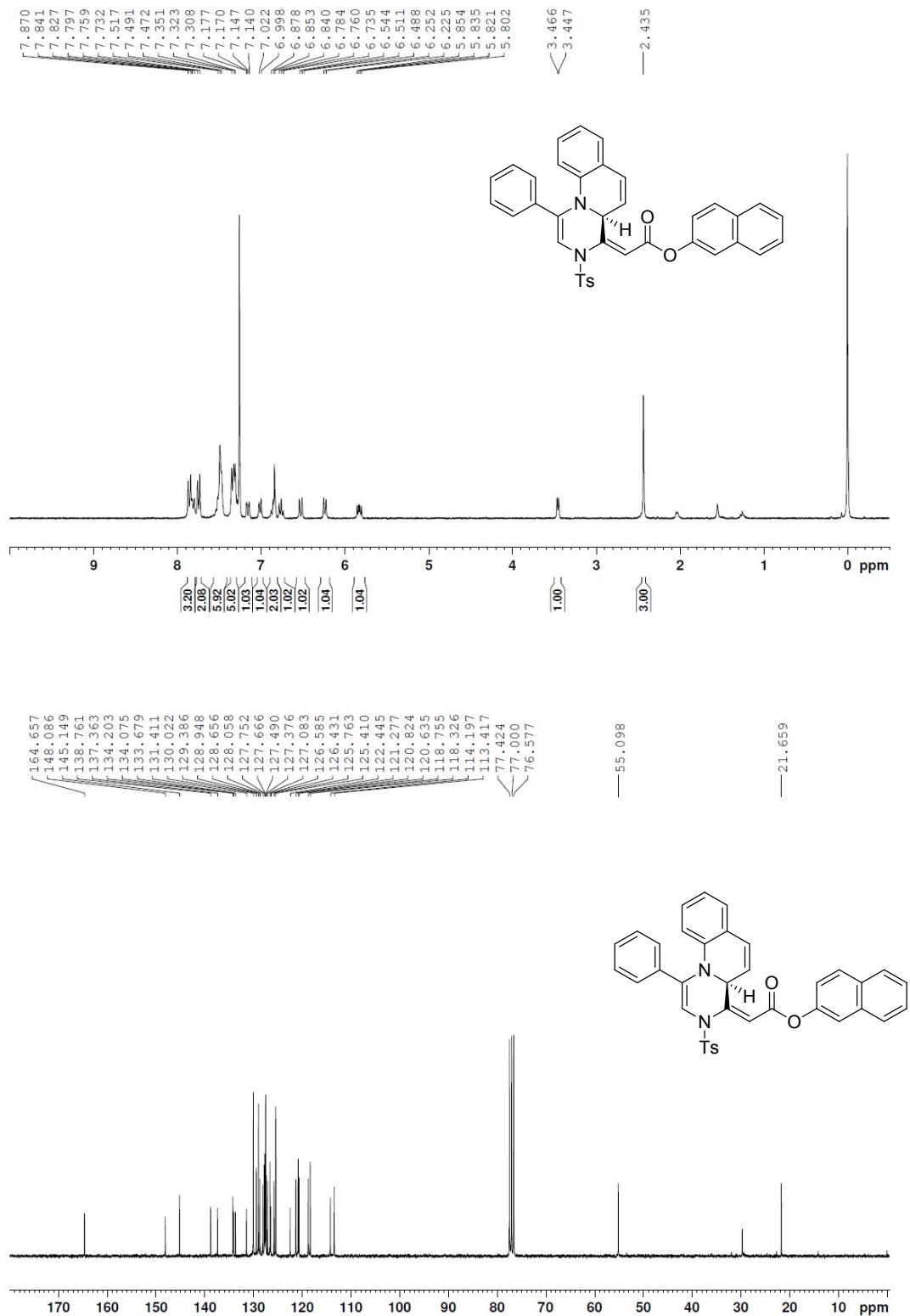
(S,E)-ethyl 2-(1-(3,5-difluorophenyl)-8-methoxy-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5h):



(S,E)-tert-butyl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5i):

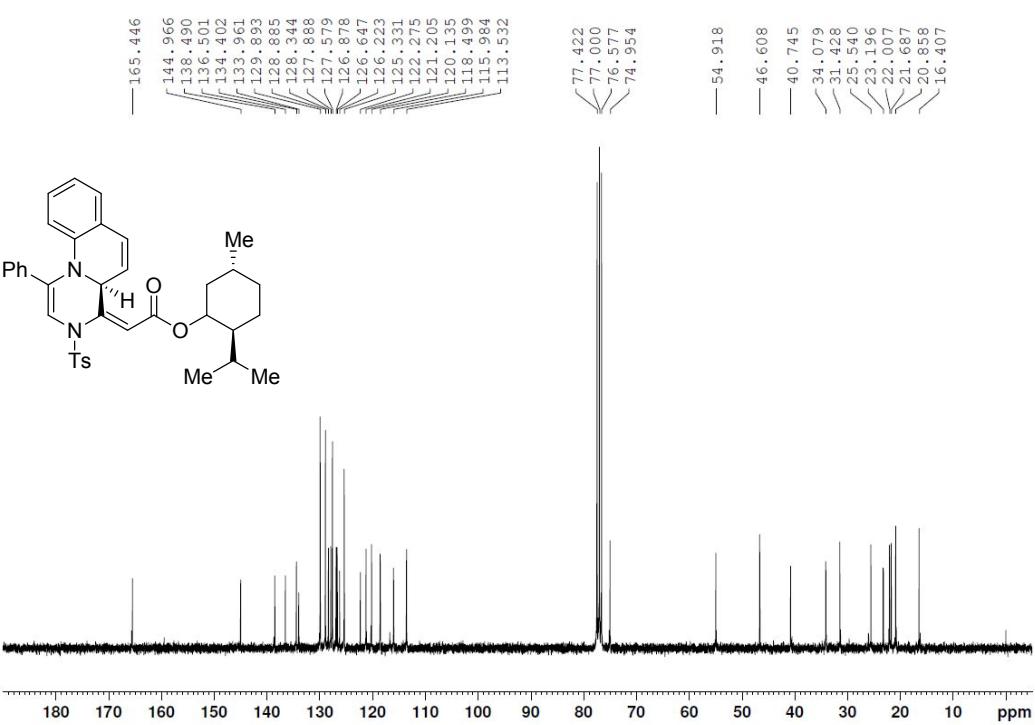
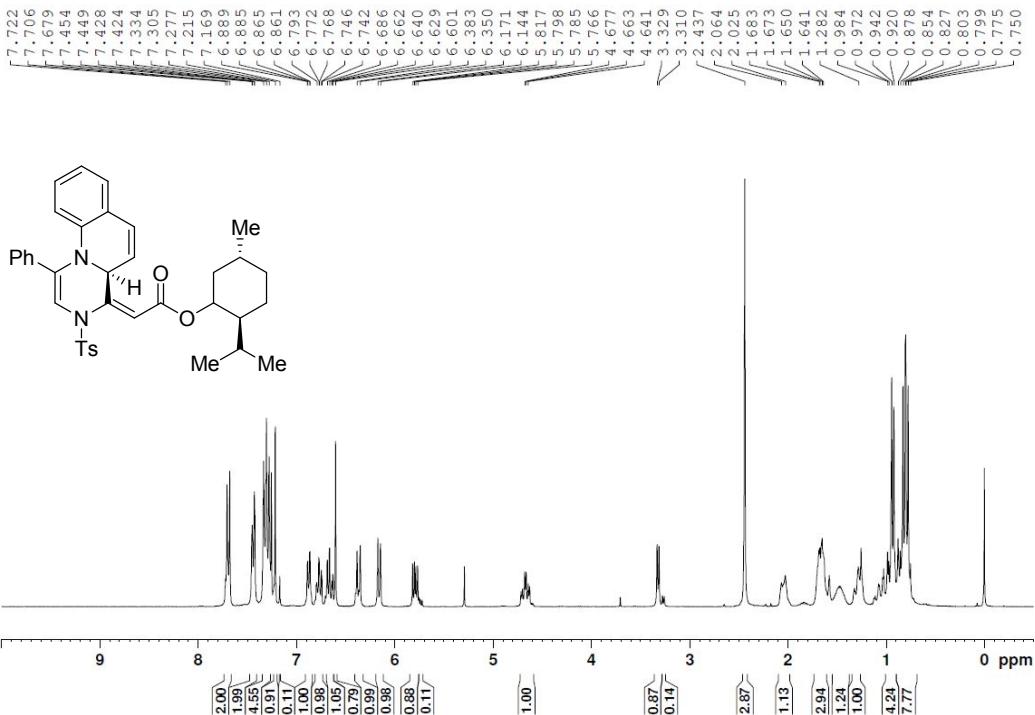


(S,E)-naphthalen-2-yl 2-(1-phenyl-3-tosyl-3H-pyrazino[1,2-a]quinolin-4(4aH)-ylidene)acetate (5j):



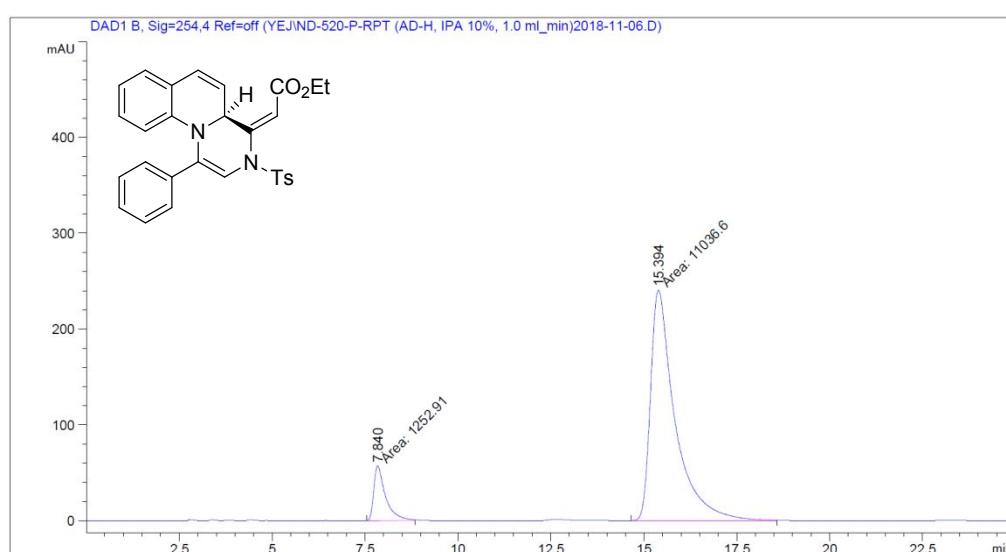
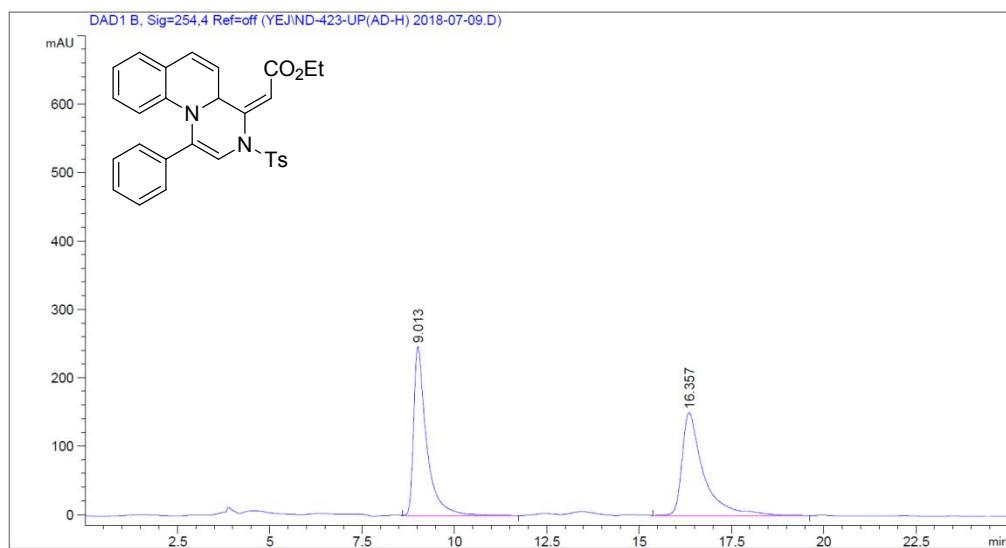
**(E)-(1R,2S,5R)-2-isopropyl-5-methylcyclohexyl
a]quinolin-4(4aH)-ylidene)acetate**

2-((S)-1-phenyl-3-tosyl-3H-pyrazino[1,2- (5k):

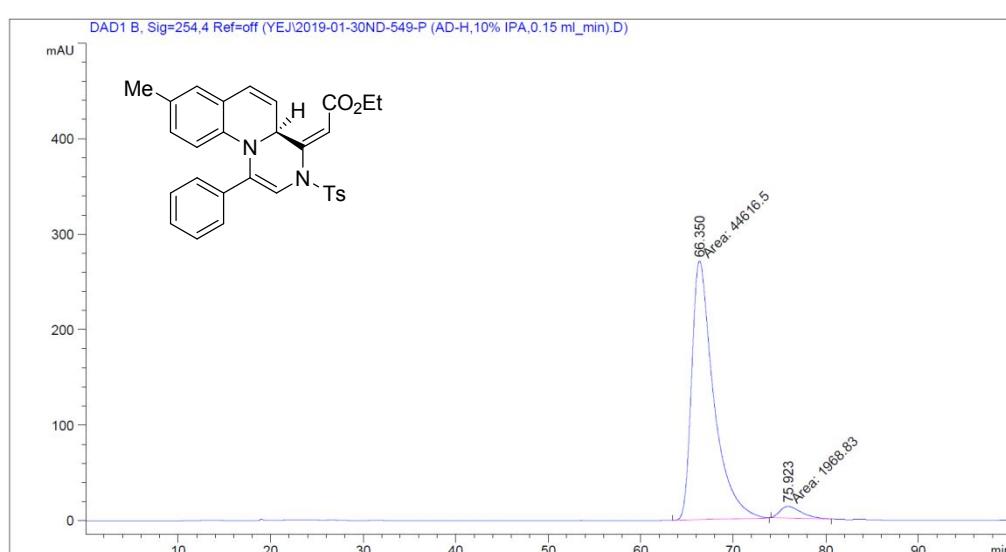
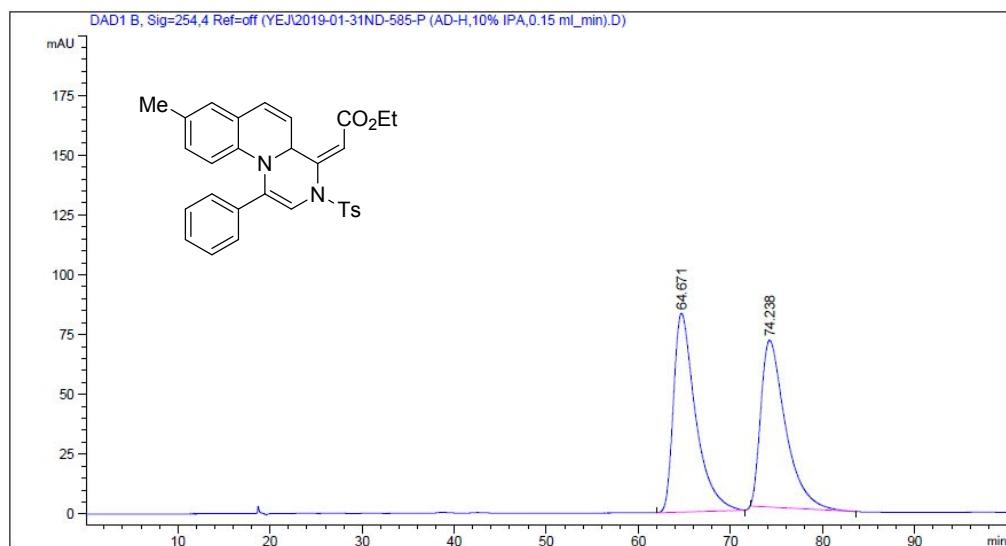


VIII. Copies of HPLC Data of Compound 5

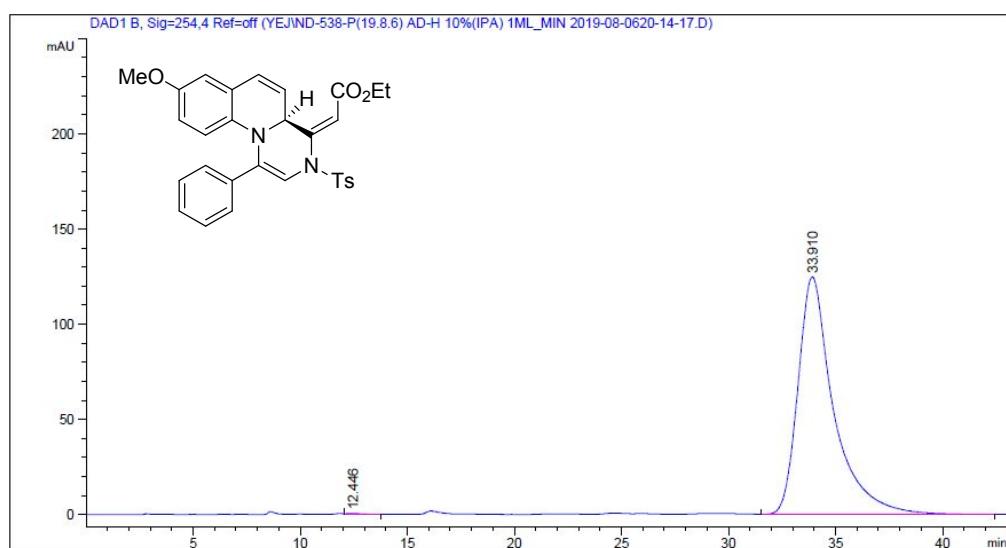
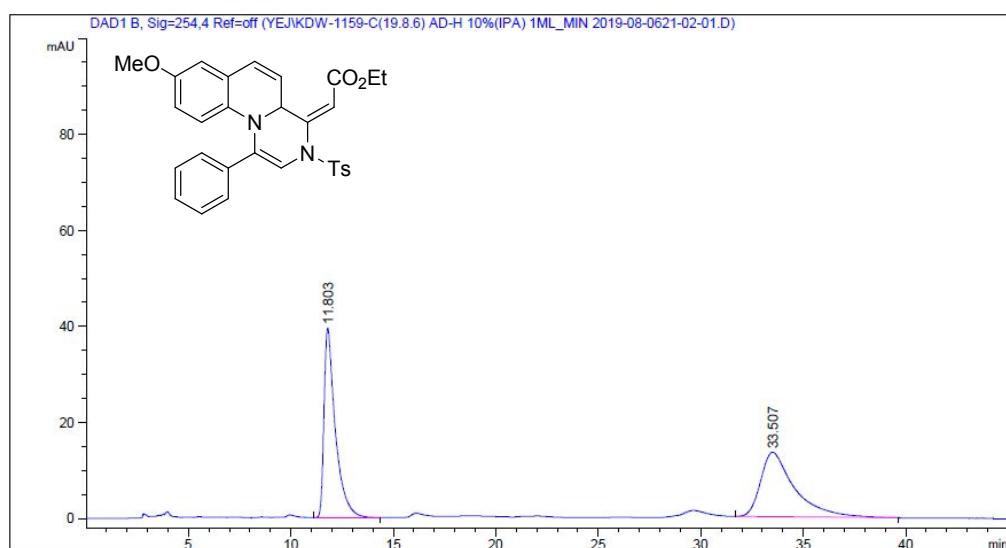
5a



Totals : 1.22895e4 297.87621

5b

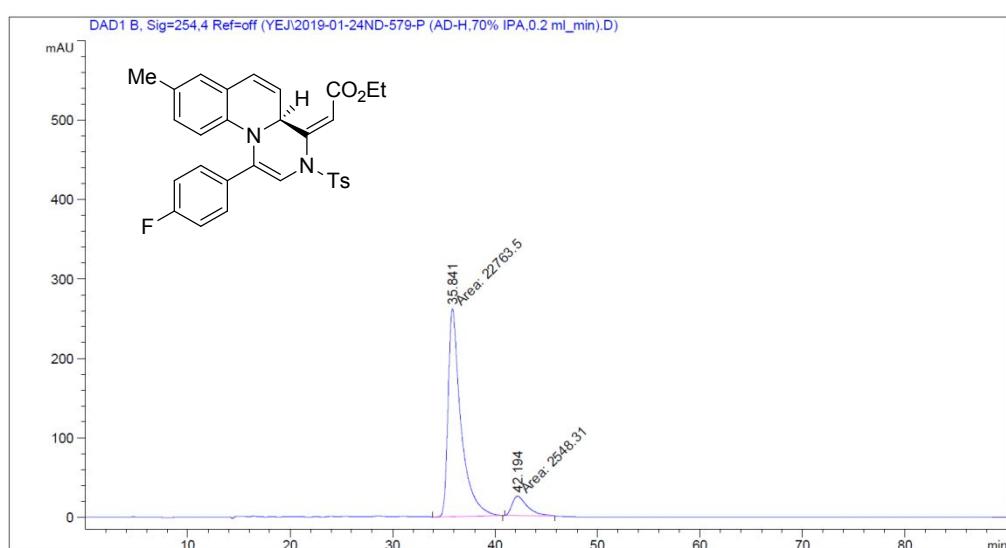
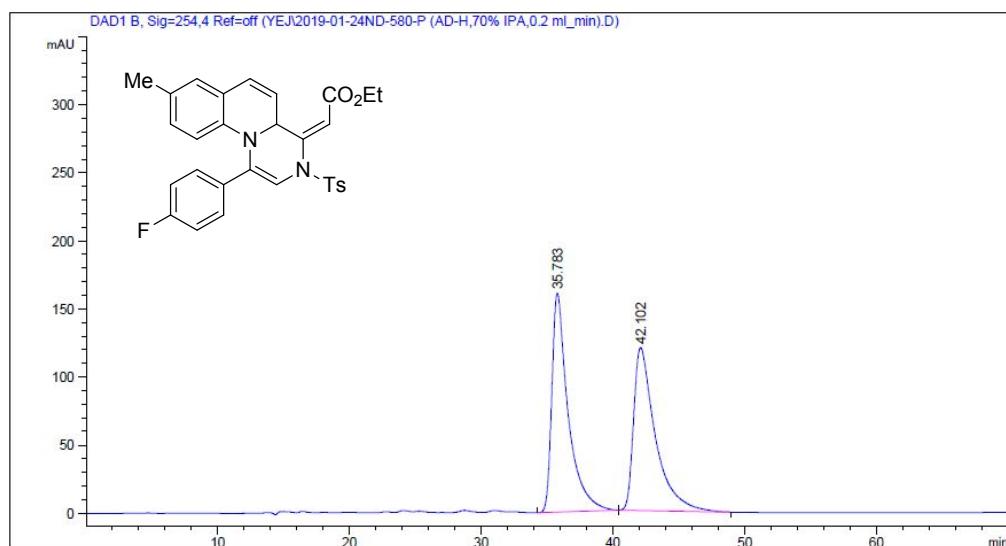
Totals : 4.65853e4 282.86641

5c

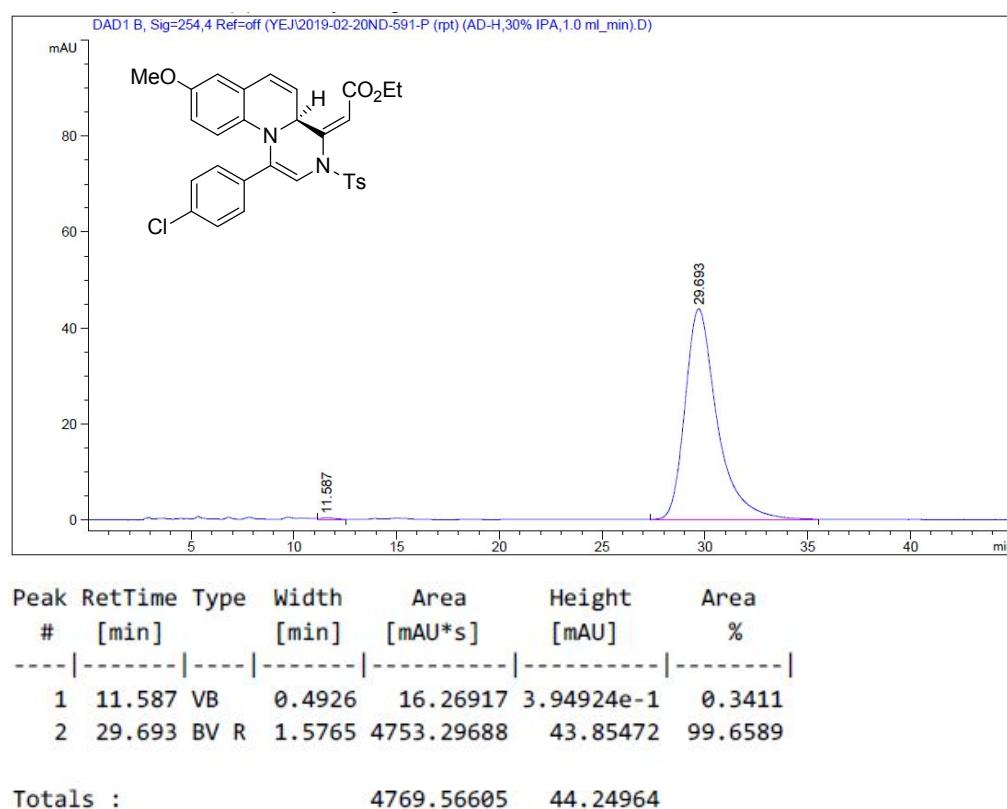
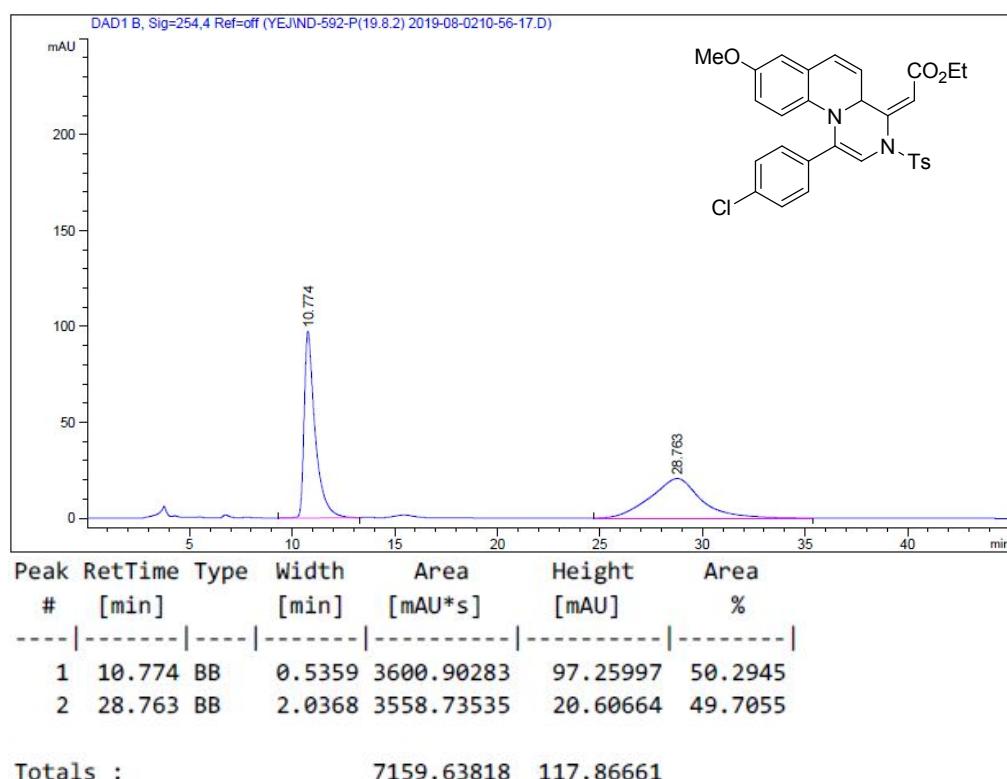
Peak RetTime Type Width Area Height Area

#	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.446	VB	0.5346	25.35058	5.61651e-1	0.1766
2	33.910	BV R	1.6606	1.43317e4	124.54022	99.8234

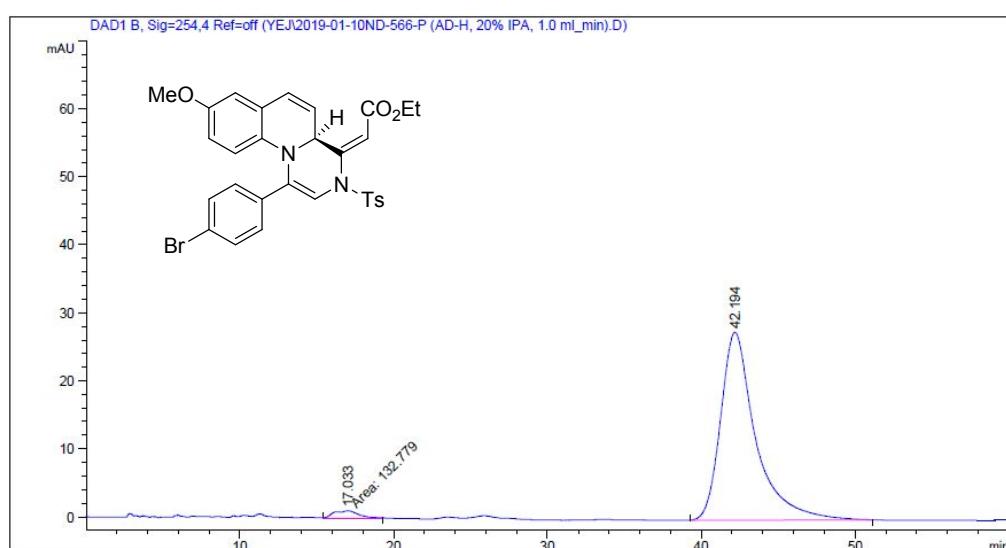
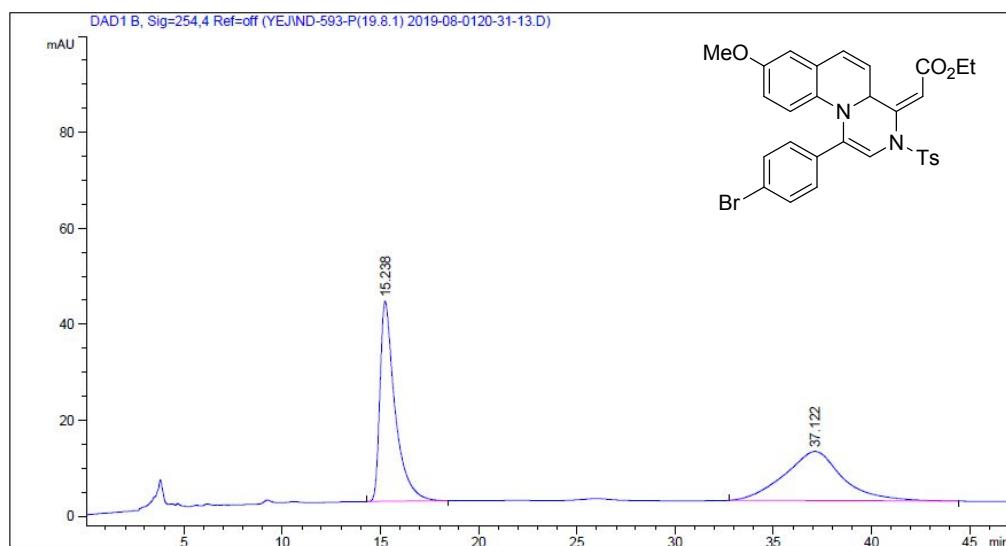
Totals : 1.43570e4 125.10187

5d

Totals : 2.53118e4 286.43693

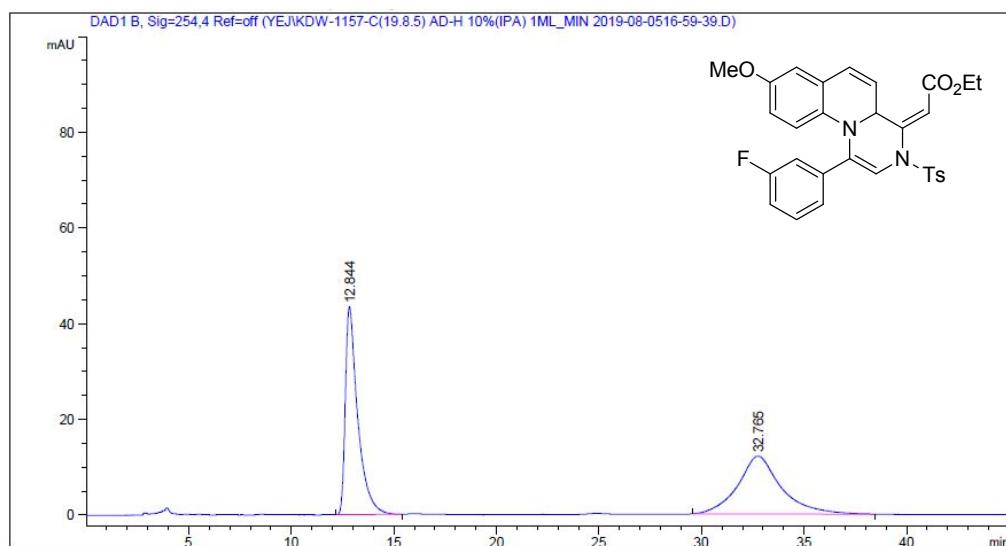
5e

5f

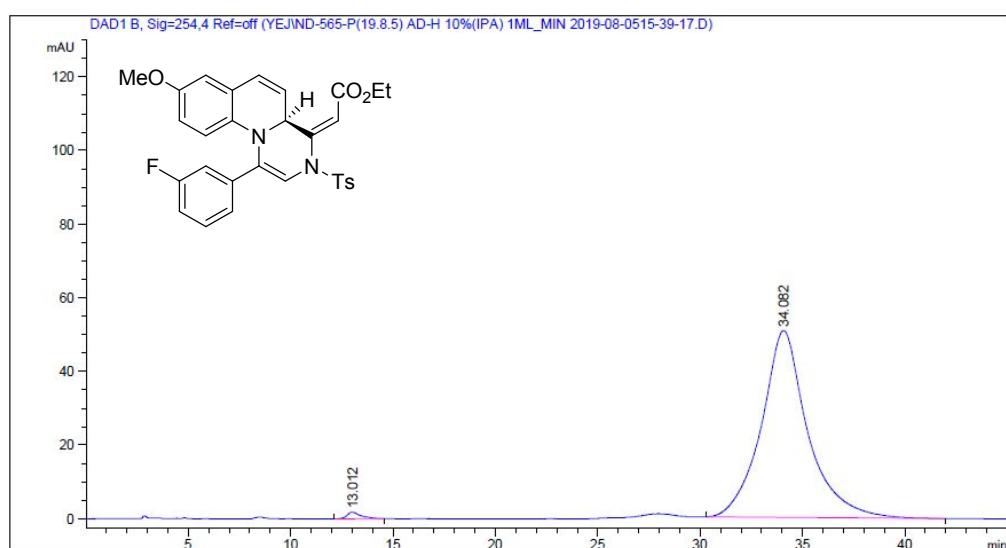


Totals : 4497.21159 28.73869

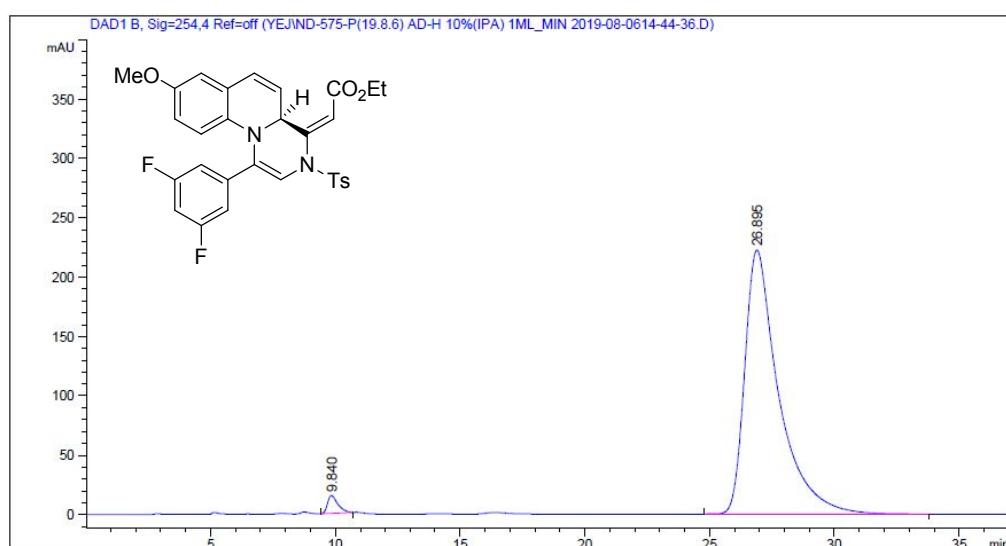
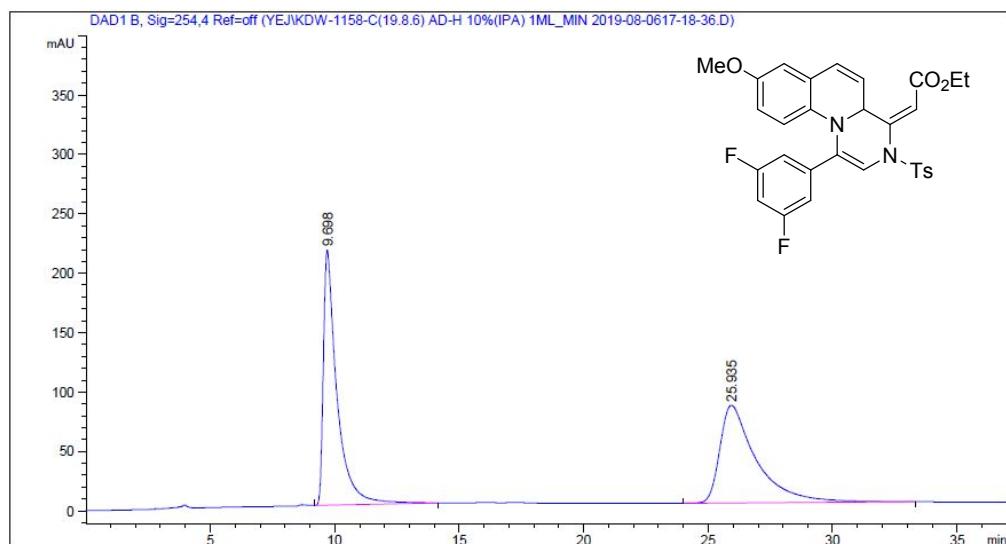
5g



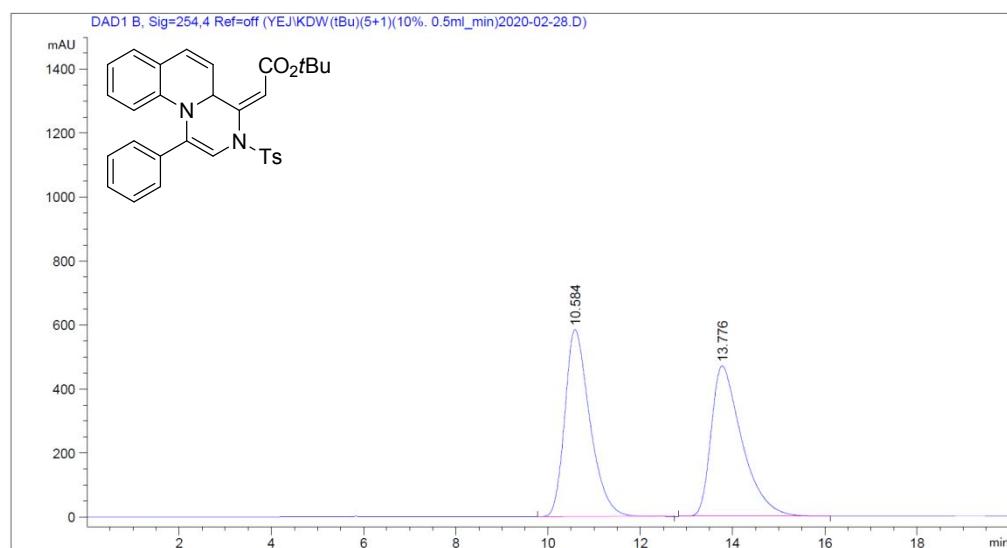
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.844	BB	0.6079	1824.76941	43.45620	50.5835
2	32.765	BB	1.7647	1782.67175	12.10078	49.4165
Totals :				3607.44116	55.55698	



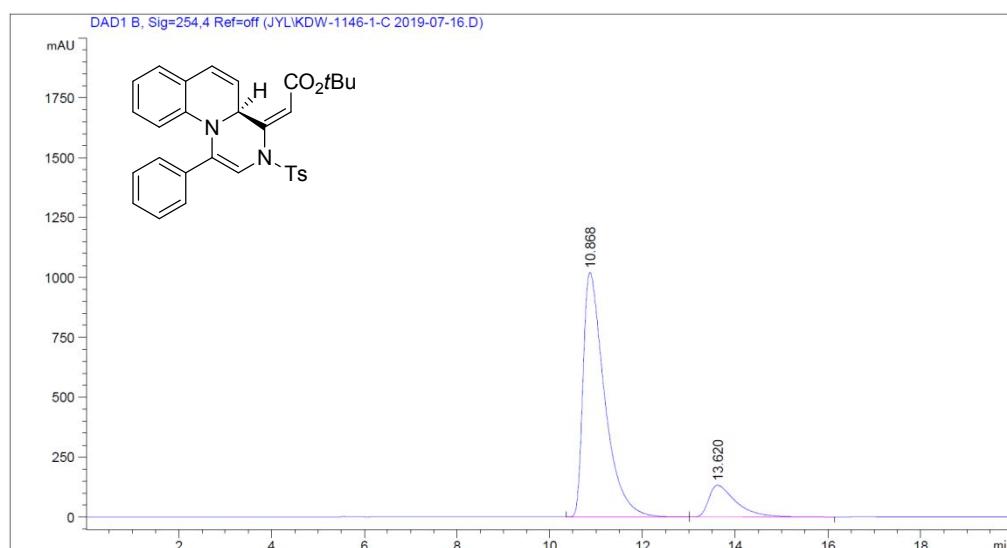
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.012	BB	0.5695	83.24937	1.81378	1.0327
2	34.082	BB	2.1549	7978.08301	50.72492	98.9673
Totals :				8061.33238	52.53869	

5h

Totals : 2.13643e4 237.34493

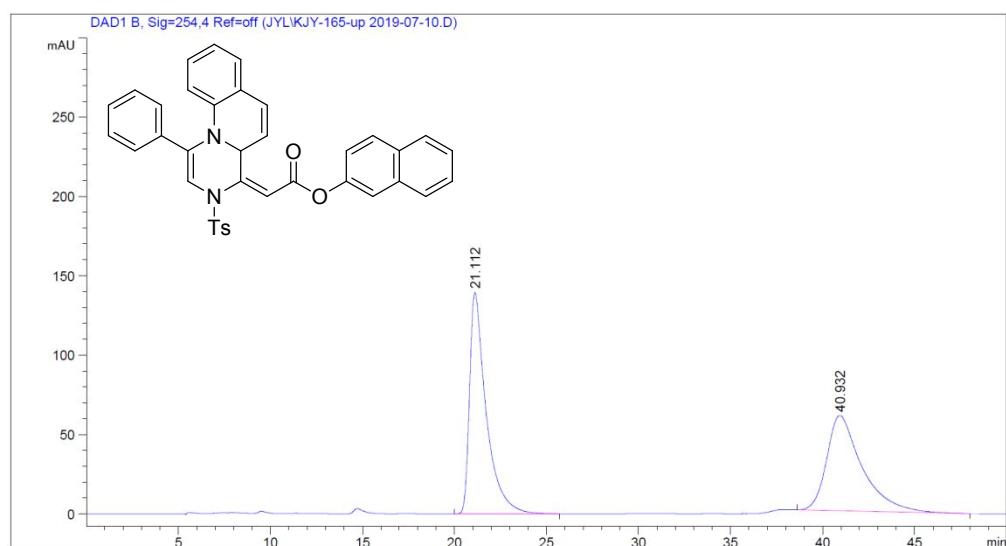
5i

Totals : 4.37752e4 1053.86191



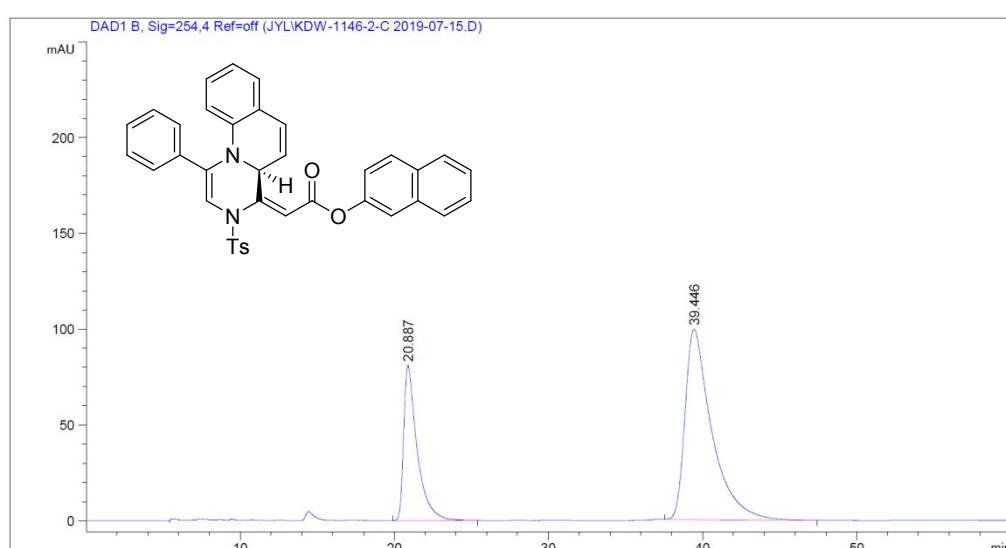
Totals : 3.82257e4 1153.61644

5j



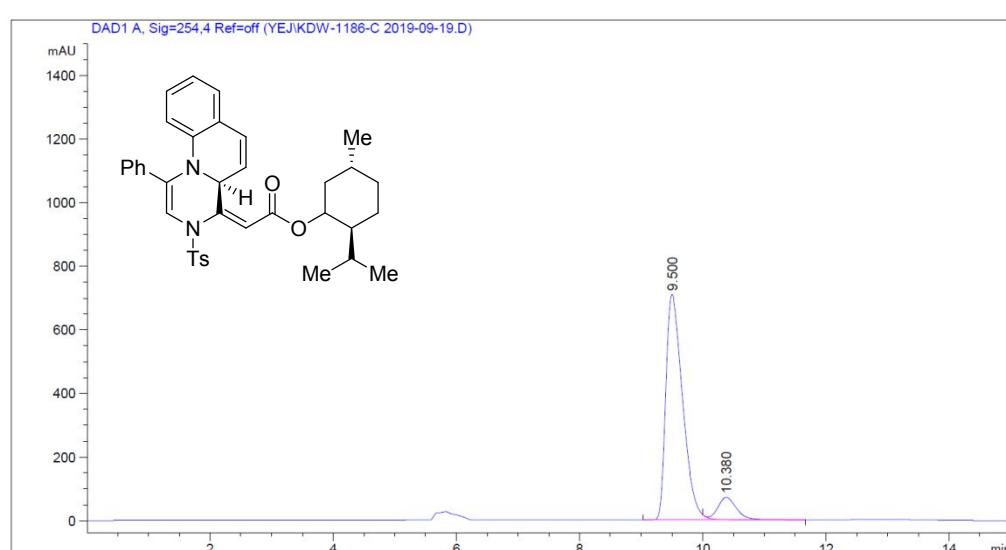
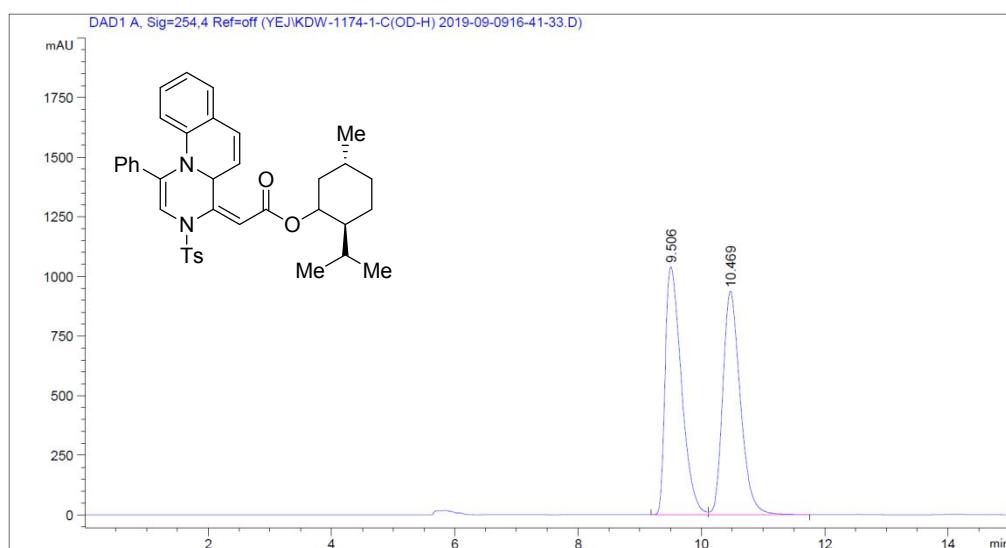
Peak	RetTime	Type	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	21.112	BB	0.9009	8737.45313	139.46373	52.2306
2	40.932	BB	1.8718	7991.16016	60.07763	47.7694

Totals : 1.67286e4 199.54136



Peak	RetTime	Type	Width	Area	Height	Area
#	[min]		[min]	[mAU*s]	[mAU]	%
1	20.887	BB	0.8700	4902.65332	81.01916	29.0484
2	39.446	BB	1.6903	1.19749e4	99.34174	70.9516

Totals : 1.68775e4 180.36090

5k

Totals : 1.48610e4 779.43784