Supporting Information

Gold-catalyzed [5+2] cycloaddition of quinolinium zwitterions and allenamides as an efficient route to fused 1,4-diazepines

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I. General Information

Unless otherwise stated, all commercial reagents and solvents were used without additional purification. Allenamides were prepared following literature reported procedures by base catalyzed isomerization of the corresponding propargyl precursors.[S1] Analytical data are in agreement with the literature. 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 400-630 mesh). ^{1}H NMR was recorded on Bruker DPX FT (400 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). ^{13}C NMR was recorded on Bruker FT AM 400 (100 MHz) and was fully decoupled by broad band proton decoupling. Chemical shifts were reported in ppm either in referenced to the center line of a triplet at 77.0 ppm of chloroform-d or in referenced to the center line of a septet at 39.5 ppm of dimethylsulfoxide-d_6. Infrared spectra were recorded on a Nicolet 6700 FT/IR spectrometer (Thermo Electron Corporation, WI, USA). 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/FAB method.

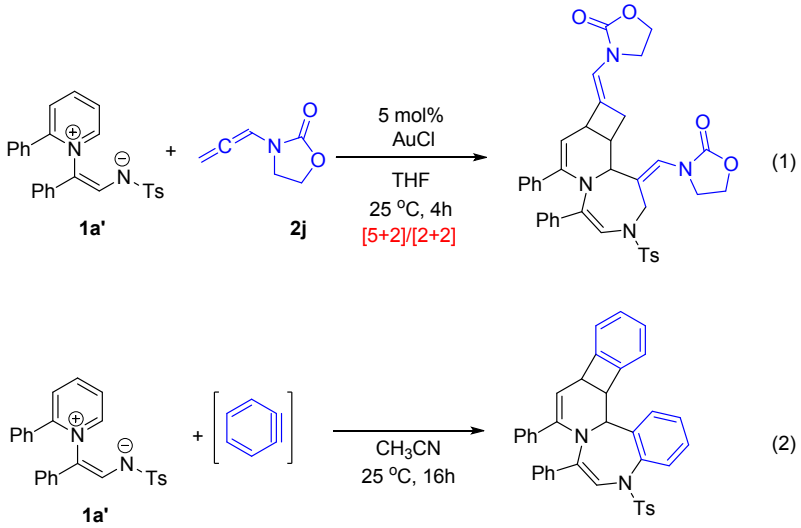
II. Experimental Procedures

II-1. General experimental procedure for the synthesis of quinolinium zwitterions:
To a test tube with a triangular-shaped stir bar were added 4-phenyl-1-toluenesulfonyl-1,2,3-triazole (2.0 equiv), and $Rh_2(OPiv)_4$ (4.0 mol %), and *p*-xylene (2.0 mL) under N_2 atmosphere. To this stirred reaction mixture was added respective quinoline derivative (0.2 mmol) and the reaction mixture was stirred at 110 °C (TLC). 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 product **1a-v**.

II-2. General experimental procedure for the optimization studies for [5+2] cycloaddition reactions (Table 1): To a flame dried test tube with a triangular-shaped stir bar were added quinolinium zwitterion (**1a**, 0.1 mmol), allenamide (**2a**, 1.3 equiv), catalyst and solvent (2.0 mL). The reaction mixture was stirred at indicated temperature and monitored by TLC. Reaction mixture was then cooled to room temperature, filtered through a pad of celite and then washed with CH_2Cl_2 (5 mL x 3). The combined filtrates were concentrated under reduced pressure. The NMR yield of desired product **3aa** was determined by integration using CH_2Br_2 as internal standard.

■ Gold(I)-Catalyzed cycloaddition between pyridinium zwitterion and allenamide (Scheme S1)

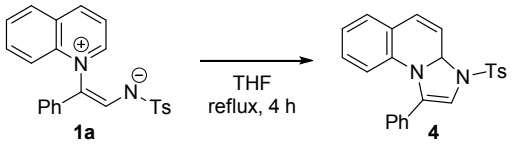
A similar reaction profile using pyridinium zwitterion (**1a'**) and allenamide **2j** formed a cascade [5+2]/[2+2]-cycloadduct in low yield (Eq. 1, Scheme S1) following a similar sequence as observed for the reaction between pyridinium zwitterion (**1a'**) and benzyne (Eq. 2).[S2]



Scheme S1. Cascade [5+2]/[2+2] cycloaddition of pyridinium zwitterion and allenamide

■ Intramolecular cyclization of quinolinium zwitterion at high temperature (Scheme S2)

During optimization studies, a control experiment under catalyst-free conditions (Table 1, entry 11) afforded an intramolecular cyclized product (**4**) under refluxing condition (Scheme S2).



Scheme S2. Thermal cyclization of quinolinium zwitterion under catalyst-free condition

II-3. General procedure for the [5+2] cycloadditions of quinolinium zwitterions (1) and allenamides (2) (Table 2, Table 3):

To a flame dried test tube with a triangular-shaped stir bar were added quinolinium zwitterion (**1**, 0.1 mmol), allenamides (**2**, 1.3 equiv), AuCl (5 mol%) and THF (2.0 mL). The reaction mixture was stirred at room temperature and monitored by TLC. After completion, the reaction, mixture was filtered through a pad of celite and then washed with CH_2Cl_2 (5 mL x 3). The combined filtrates were concentrated under reduced pressure. The organic residue was purified by chromatography on silica gel to give the desired product **3** (eluent; EtOAc:Hexane = 1:4).

II-4. Experimental procedure for selective reduction of cycloadduct 3aa:

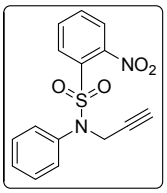
To a flame dried two-neck round bottom flask, equipped with a stir bar, were added cycloadduct **3aa** (0.2 mmol), Pd/C (20 mol%) and EtOAc (10 mL). The reaction vessel was closed, evacuated three times and backfilled by H_2-balloon. The reaction mixture was stirred at room temperature under H_2-balloon pressure for 8 h (TLC). After completion, the reaction mixture was filtered through a pad of celite, washed with EtOAc (5 mL x 3). The combined filtrates were concentrated under reduced pressure and the resulting residue was purified by chromatography on silica gel (eluent; EtOAc:Hexane = 1:4) to afford the desired product **4aa** (96%).

II-5. Experimental procedure for Suzuki coupling reaction of cycloadduct 3ea:

To a flame dried test tube with a triangular-shaped stir bar were added cycloadduct **3ea** (0.1 mmol), Phenylboronic acid (1.5 equiv) in 1,4-dioxane (5 mL). To this stirred solution was added K_2CO_3 (2.5 equiv, dissolved in 1.0 mL H_2O). The reaction mixture was then degassed (N_2) for 10 minutes prior to add
ition of $Pd(PPh_3)_4$ (5 mol%) and the reaction mixture was heated for 6 h at 100 °C. Reaction mixture was then cooled to room temperature, filtered through a pad of celite and concentrated in vacuo. The crude mixture was purified by silica gel column chromatography to afford compound **5ea** (56%).

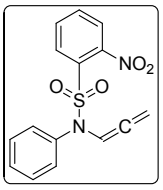
III. Spectroscopic data

2-nitro-*N*-phenyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide:



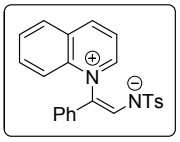
Yellow viscous oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70-7.62 (m, 3H), 7.53-7.49 (m, 1H), 7.36-7.33 (m, 3H), 7.30-7.28 (m, 2H), 4.59 (d, *J* = 2.4 Hz, 2H), 2.26 (t, *J* = 2.4 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.0, 137.7, 133.9, 132.2, 132.0, 131.3, 129.6, 129.4, 129.0, 124.1, 78.2, 73.8, 42.4; IR (KBr) ν 3292, 3098, 2978, 2123, 1655, 1593, 1484, 1373, 1171 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{15}H_{12}N_2O_4S$ $[M+H]^+$: 317.0591, found: 317.0593.

(2-nitro-*N*-phenyl-*N*-(propa-1,2-dien-1-yl)benzenesulfonamide (2h):



Light yellow viscous oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71-7.64 (m, 2H), 7.62-7.60 (m, 1H), 7.54-7.50 (m, 1H), 7.35-7.29 (m, 3H), 7.21-7.14 (m, 3H), 5.09 (d, *J* = 6.4 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 200.4, 148.1, 136.1, 134.1, 131.9, 131.5, 131.3, 130.0, 129.2, 129.1, 124.1, 103.1, 88.2; IR (KBr) ν 3098, 3067, 2905, 1965, 1543, 1373, 1252, 1171, 1063 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{15}H_{12}N_2O_4S$ $[M+H]^+$: 317.0591, found: 317.0598.

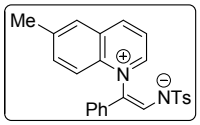
(Z)-(2-Phenyl-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1a):



Purple solid; m.p. 207.4-208.6 °C; ^{1}H NMR (400 MHz, DMSO d_6) δ 9.41-9.34 (m, 2H), 8.53 (d, *J* = 7.1 Hz, 1H), 8.28-8.24 (m, 1H), 8.09 (s, 1H), 8.01-7.94 (m, 3H), 7.41 (d, *J* = 7.7 Hz, 2H), 7.19-7.17 (m, 4H), 7.03-7.00 (m, 1H), 6.81 (d, *J* = 7.5 Hz, 2H), 2.32 (s, 3H);

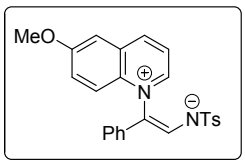
^{13}C NMR (100 MHz, DMSO d_6) δ 153.6, 147.7, 139.3, 135.7, 130.4, 130.2, 129.9, 129.0, 128.7, 125.3, 124.1, 123.0, 119.8, 119.7, 20.8; IR (KBr) ν 3054.7, 2986.2, 1591.9, 1421.3, 1264.1, 1130.1, 1082.8, 964.2cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{20}N_2S_2O$ [M+H]$^+$: 401.1324, found: 401.1322.

(*Z*)-(2-(6-methylquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1b):



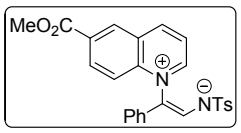
Purple solid; m.p. 214.2-215.9℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.82 (d, J = 8.4 Hz, 1H), 8.64 (dd, *J* = 5.8 Hz, 1.4 Hz, 1H), 8.27 (s, 1H), 7.92 (d, *J* = 9.2 Hz, 1H), 7.83 (s, 1H), 7.76 (dd, *J* = 8.6 Hz, 5.8 Hz, 1H), 7.65 (d, *J* = 8.24 Hz, 2H), 7.56 (dd, *J* = 9.02 Hz, 1.76 Hz, 1H), 7.15-7.11 (m, 4H), 7.00 (t, *J* = 7.32 Hz, 1H), 6.72 (dd, *J* = 8.68 Hz, 1.2 Hz, 2H), 2.49 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 150.9, 145.8, 143.3, 140.8, 140.6, 140.1, 138.9, 137.5, 136.8, 130.7, 129.0, 128.8, 128.4, 126.0, 124.5, 122.0, 120.8, 120.2, 114.2, 21.4, 21.3; IR (KBr) ν 3054, 2984, 1589, 1516, 1444, 1246, 1130, 1084 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{22}N_2O_2S$ [M+H]$^+$: 415.1475, found: 415.1477.

(*Z*)-(2-(6-Methoxyquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1c):



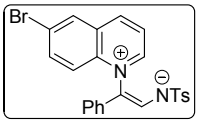
Red solid; m.p. 195.4-196.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.78 (d, J = 8.4 Hz, 1H), 8.47 (dd, *J* = 5.6, 1.3 Hz, 1H), 8.28 (s, 1H), 7.91 (d, *J* = 9.2 Hz, 1H), 7.69 (d, *J* = 8.2 Hz, 2H), 7.60 (dd, *J* = 8.4, 5.6 Hz, 1H), 7.36-7.32 (m, 2H), 7.18-7.12 (m, 4H), 7.00 (t, *J* = 7.2 Hz, 1H), 6.73-6.70 (m, 2H), 3.83 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 159.7, 148.0, 145.4, 143.2, 140.3, 140.3, 136.6, 135.9, 132.4, 129.0, 128.4, 125.9, 124.6, 122.1, 121.9, 120.2, 114.4, 107.1, 56.2, 21.3; IR (KBr) ν 3055, 2978, 1591, 1514, 1394, 1266, 1127, 1084 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{22}N_2O_3S$ [M+H]$^+$: 431.1424, found: 431.1431.

(*Z*)-(2-(6-(methoxycarbonyl)quinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1d):



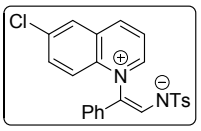
Purple solid; m.p. 122.6-124.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.03 (d, *J* = 8.2 Hz, 1H), 8.86 (d, *J* = 5.5 Hz, 1H), 8.72 (s, 1H), 8.26 (s, 1H), 8.24 (dd, *J* = 9.2 Hz, 1.6 Hz, 1H), 8.04 (d, *J* = 9.2 Hz, 1H), 7.95 (dd, *J* = 8.2 Hz, 5.6 Hz, 1H), 7.63 (d, *J* = 8.2 Hz, 2H), 7.17-7.13 (m, 4H), 7.02 (t, *J* = 7.2 Hz, 1H), 6.73 (d, *J* = 7.4 Hz, 2H), 4.00 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.4, 153.9, 148.3, 142.8, 141.8, 140.5, 136.3, 134.5, 132.1, 131.1, 129.7, 129.5, 129.1, 129.0, 125.9, 124.9, 123.4, 121.4, 120.4, 114.4, 53.0, 21.3; IR (KBr) ν 3064, 2950, 1724, 1594, 1516, 1442, 1275, 1134, 1084 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{26}H_{22}N_2O_4S$ [M+H]$^+$: 459.1374, found: 459.1380.

(*Z*)-(2-(6-bromoquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1e):



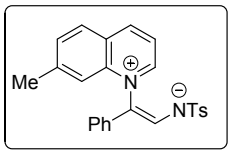
Brown solid; m.p. 155.3-157.0℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, *J* = 8.4 Hz, 1H), 8. 47 (dd, *J* = 5.6 Hz, 1.2 Hz, 1H), 8.27 (s, 1H), 8.24 (d, *J* = 2.0 Hz, 1H), 7.88 (d, *J* = 9.4 Hz, 1H), 7.80-7.73 (m, 2H), 7.67 (d, *J* = 8.2 Hz, 2H), 7.18-7.13 (m, 4H), 7.03 (t, *J* = 7.2 Hz 1H), 6.73-6.70 (m, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 146.3, 143.0, 140.6, 140.5, 138.7, 138.5, 136.3, 131.9, 131.2, 129.1, 125.9, 124.8, 124.2, 123.2, 122.3, 120.2, 114.1, 21.3; IR (KBr) ν 3059, 2919, 1590, 1504, 1445, 1244, 1130, 1085 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{19}BrN_2O_2S$ [M+H]$^+$: 479.0424, found: 479.0430.

(*Z*)-(2-(6-chloroquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1f):



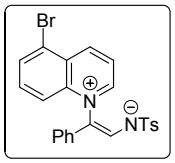
Purple solid; m.p. 149.9-151.6℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.91 (d, *J* = 8.0 Hz, 1H), 8.76-8.74 (m, 1H), 8.27 (s, 1H), 8.06 (d, *J* = 2.0 Hz, 1H), 7.97 (d, *J* = 9.2 Hz, 1H), 7.83-7.80 (m, 1H), 7.66 (d, *J* = 8.0 Hz, 2H), 7.62 (dd, *J* = 9.2 Hz, *J* = 2.2 Hz, 1H), 7.18-7.14 (m, 4H), 7.03 (d, *J* = 7.4 Hz, 1H), 6.72 (d, *J* = 7.4 Hz, 2H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 146.4, 143.0, 140.6, 140.5, 138.6, 136.4, 136.1, 136.0, 131.0, 129.14, 129.09, 128.5, 125.9, 124.9, 123.3, 122.5, 120.3, 114.2, 21.4; IR (KBr) ν 3060, 2918, 1589, 1510, 1445, 1244, 1129, 1086 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{19}ClN_2O_2S$ $[M+H]^+$: 435.0929, found: 435.0937.

(*Z*)-(2-(7-Methylquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1g):



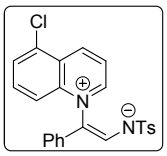
Violet solid; m.p. 204.3-205.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.86 (d, *J* = 8.0 Hz, 1H), 8.61 (dd, *J* = 5.8, 1.6 Hz, 1H), 8.29 (s, 1H), 8.00 (d, *J* = 8.4 Hz, 1H), 7.79 (s, 1H), 7.70 (dd, *J* = 8.0, 5.8 Hz, 1H), 7.64 (d, *J* = 7.8 Hz, 2H), 7.55 (dd, *J* = 8.4, 1.2 Hz, 1H), 7.16-7.12 (m, 4H), 7.00 (t, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 7.8 Hz, 2H), 2.41 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.5, 147.9, 146.2, 143.4, 140.7, 140.1, 136.8, 132.2, 129.6, 129.0, 128.90, 128.87, 125.9, 124.5, 121.1, 120.2, 119.7, 114.0, 21.7, 21.3; IR (KBr) ν 3060, 2920, 1590, 1510, 1443, 1245, 1130, 1085 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{22}N_2O_2S$ $[M+H]^+$: 415.1475, found: 415.1479.

(*Z*)-(2-(5-bromoquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1h):



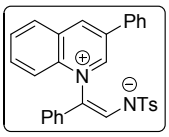
Purple solid; m.p. 156.5-158.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.22 (d, *J* = 8.2 Hz, 1H), 8.87 (d, *J* = 4.4 Hz, 1H), 8.27 (s, 1H), 8.07-8.04 (m, 3H), 7.63-7.58 (m, 3H), 7.17-7.11 (m, 4H), 7.02 (t, *J* = 7.2 Hz, 1H), 6.72 (d, *J* = 7.8 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.4, 145.7, 142.8, 141.4, 140.6, 140.3, 136.5, 135.3, 133.9, 129.7, 129.0, 128.9, 126.0, 124.8, 124.0, 123.6, 120.9, 120.3, 114.3, 21.3; IR (KBr) ν 3069, 2921, 1591, 1515, 1444, 1246, 1132, 1084 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{19}BrN_2O_2S$ $[M+H]^+$: 479.0424, found: 479.0431.

(*Z*)-(2-(5-chloroquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1i):



Blue solid; m.p. 141.1-142.8℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.25 (d, *J* = 8.4 Hz, 1H), 8.89 (d, *J* = 5.0 Hz, 1H), 8.26 (s, 1H), 8.07-8.03 (m, 1H), 8.00 (d, *J* = 9.0 Hz, 1H), 7.87 (d, *J* = 7.6 Hz, 1H), 7.70-7.66 (m, 1H), 7.62 (d, *J* = 8.2 Hz, 2H), 7.17-7.11 (m, 4H), 7.02 (t, *J* = 7.4 Hz, 1H), 6.72 (d, *J* = 8.2 Hz, 2H), 2.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 153.5, 143.0, 142.9, 141.3, 140.8, 140.2, 136.6, 134.9, 133.8, 130.1, 129.0, 128.8, 128.7, 126.0, 124.7, 123.3, 120.3, 114.3, 53.4, 21.3; IR (KBr) ν 3075, 2919, 1590, 1515, 1444, 1246, 1129, 1086 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{19}ClN_2O_2S$ $[M+H]^+$: 435.0929, found: 435.0931.

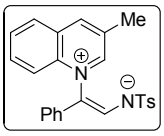
(*Z*)-(2-phenyl-2-(3-phenylquinolin-1-ium-1-yl)vinyl)(tosyl)amide (1j):



Purple solid; m.p. 156.3-157.9℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 9.09 (d, *J* = 1.6 Hz, 1H), 8.93 (d, *J* = 2.0 Hz, 1H), 8.38 (s, 1H), 8.22-8.18 (m, 1H), 7.97-7.95 (m, 1H), 7.74 (d, *J* = 8.2 Hz, 2H), 7.65-7.50 (m, 2H), 7.47-7.37 (m, 5H), 7.17-7.14 (m, 4H), 7.02 (t, *J* = 7.4 Hz, 1H), 6. 80 (d, *J* = 8.6 Hz, 2H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.0, 143.3, 142.8, 141.0, 140.1, 138.6, 136.6, 135.0, 134.7, 132.9, 130.6, 130.4, 129.9, 129.8, 129.5, 129.0, 128.9,

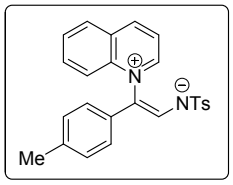
127.1, 126.0, 124.6, 120.5, 120.3, 114.9, 21.4; IR (KBr) ν 3055, 2920, 1591, 1516, 1447, 1343, 1244, 1134, 1085 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{30}H_{24}N_2O_2S$ $[M+H]^+$: 477.1632, found: 477.1639..

(*Z*)-(2-(3-methylquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1k):



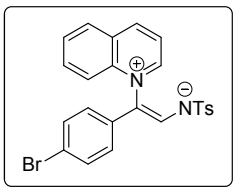
Brown solid; m.p. 204.2-206.0°C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (s, 1H), 8.58 (d, *J* = 2.0 Hz, 1H), 8.28 (s, 1H), 8.08-8.06 (m, 1H), 7.98-7.96 (m, 1H), 7.70-7.65 (m, 4H), 7.16-7.12 (m, 4H), 7.00 (t, *J* = 7.4 Hz, 1H), 6.72 (dd, *J* = 8.4 Hz, 1.2Hz, 2H), 2.46 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.9, 145.5, 143.3, 141.1, 140.0, 138.9, 136.9, 134.4, 132.6, 130.4, 129.9, 129.0, 128.8, 126.0, 124.5, 121.0, 120.2, 114.1, 53.4, 21.3, 18.5; IR (KBr) ν 3043, 2920, 1585, 1513, 1445, 1243, 1130, 1085 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{22}N_2O_2S$ $[M+H]^+$: 415.1475, found: 415.1483.

(*Z*)-(2-(quinolin-1-ium-1-yl)-2-(p-tolyl)vinyl)(tosyl)amide (1l):



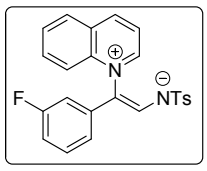
Grey solid; m.p. 165.9-168.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, *J* = 8.2 Hz, 1H), 8.68 (d, *J* = 5.2 Hz, 1H), 8.20 (s, 1H), 8.09 (d, *J* = 8.0 Hz, 1H), 8.01 (d, *J* = 8.7 Hz, 1H), 7.78-7.64 (m, 5H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.95 (d, *J* = 8.0 Hz, 2H), 6.63 (d, *J* = 8.2 Hz, 2H), 2.35 (s, 3H), 2.24 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.0, 146.8, 143.3, 140.1, 139.8, 135.2, 134.5, 133.9, 130.4, 130.0, 129.7, 129.6, 128.9, 125.9, 122.0, 120.9, 120.4, 114.6, 21.3, 20.8; IR (KBr) ν 3023, 2981, 2860, 1600, 1518, 1382 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{22}N_2O_2S$ $[M+H]^+$: 415.1480, found: 415.1478.

(*Z*)-(2-(4-Bromophenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1m):



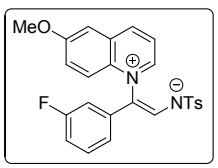
Brown solid; m.p. 185.6-186.3 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.93 (d, *J* = 8.2 Hz, 1H), 8.76 (d, *J* = 4.7 Hz, 1H), 8.28 (s, 1H), 8.15 (d, *J* = 9.2 Hz, 1H), 8.0 (d, *J* = 8.2 Hz, 1H), 7.87-7.76 (m, 3H), 7.26 (d, *J* = 8.1 Hz, 2H), 7.24 (d, *J* = 8.7 Hz, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.58 (d, *J* = 8.7 Hz, 2H), 2.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 146.7, 142.9, 141.6, 140.3, 140.2, 135.8, 135.6, 132.0, 130.5, 130.0, 130.0, 128.9, 125.9, 122.2, 121.6, 120.9, 117.5, 113.0, 21.3; IR (KBr) ν 3060, 2978, 1592, 1580, 1518, 1399, 1240, 1129, 1080 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{19}BrN_2O_2S$ $[M+H]^+$: 479.0423, found: 479.0427.

(*Z*)-(2-(3-Fluorophenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1n):



Red solid; m.p. 220.1-222.7 °C; ^{1}H NMR (400 MHz, DMSO-D_6) δ 9.39 (d, *J* = 8.3 Hz, 1H), 9.34 (d, *J* = 5.4 Hz, 1H), 8.53-8.51 (m, 1H), 8.27-8.24 (m, 1H), 8.16 (s, 1H), 8.04-7.92 (m, 3H), 7.42 (d, *J* = 7.4 Hz, 2H), 7.23-7.17 (m, 3H), 6.82-6.78 (m, 1H), 6.65-6.61 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, DMSO-D_6) δ 164.1, 161.7, 153.7, 147.9, 143.4, 141.4, 139.7, 139.2, 135.8, 130.9, 130.8, 130.4, 130.2, 129.9, 128.8, 125.3, 123.1, 119.5, 115.7, 112.3, 110.3, 110.1, 106.4, 106.1, 20.8; IR (KBr) ν 3069, 2979, 2921, 1594, 1513, 1437, 1245, 1130, 1086 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{19}FN_2O_2S$ $[M+H]^+$: 419.1225, found: 419.1233.

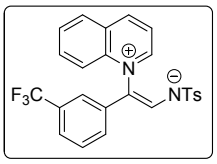
(*Z*)-(2-(3-Fluorophenyl)-2-(6-methoxyquinolin-1-ium-1-yl)vinyl)(tosyl)amide (1o):



Violet solid; m.p. 208.1-208.9 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.77 (d, *J* = 8.3 Hz, 1H), 8.49 (d, *J* = 4.5 Hz, 1H), 8.32 (s, 1H), 7.89 (d, *J* = 9.3 Hz, 1H), 7.67 (d, *J* = 8.2 Hz,

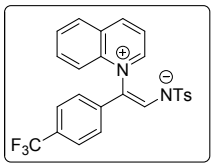
3H), 7.39-7.35 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.12-7.07 (m, 1H), 6.67 (td, *J* = 1.9, 8.3 Hz, 1H), 6.52 (d, *J* = 8.0 Hz, 1H), 6.31 (d, *J* = 10.9 Hz, 1H), 3.85 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.7, 162.2, 159.9, 148.3, 145.3, 142.9, 141.8, 140.5, 139.1, 139.0, 136.0, 132.4, 130.6, 130.5, 129.0, 128.7, 126.0, 122.2, 122.0, 115.5, 113.1, 111.1, 110.8, 107.0, 106.8, 106.6, 56.2, 21.3; IR (KBr) ν 3062, 2979, 1586, 1519, 1437, 1396, 1259, 1128, 1082 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{21}FN_2O_3S$ $[M+H]^+$: 449.1330, found: 449.1334.

(*Z*)-(2-(quinolin-1-ium-1-yl)-2-(3-(trifluoromethyl)phenyl)vinyl)(tosyl)amide (1p):



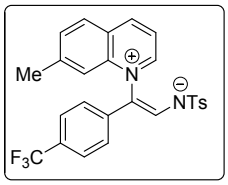
Red solid; m.p. 201.7-203.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.96 (d, *J* = 8.4 Hz, 1H), 8.77 (dd, *J* = 5.8 Hz, 1.4 Hz, 1H), 8.40 (s, 1H), 8.18-8.16 (m, 1H), 8.02-8.00 (m, 1H), 7.88 (dd, *J* = 8.4 Hz, 5.8 Hz, 1H), 7.84-7.77 (m, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.24-7.21 (m, 2H), 7.14 (d, *J* = 8.0 Hz, 2H), 6.93 (s, 1H), 6.86-8.83 (m, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 147.2, 142.8, 142.4, 140.5, 140.0, 137.5, 135.7, 131.9, 131.6, 131.3, 130.9, 130.5, 130.1, 130.0, 129.5, 128.9, 125.9, 125.2, 122.9, 122.3, 120.6, 120.5, 116.1, 112.6, 21.3; IR (KBr) ν 3074, 2979, 1586, 1514, 1347, 1263, 1129, 1085 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{19}F_3N_2O_2S$ $[M+H]^+$: 469.1193, found: 469.1198.

(*Z*)-(2-(Quinolin-1-ium-1-yl)-2-(4-(trifluoromethyl)phenyl)vinyl)(tosyl)amide (1q):



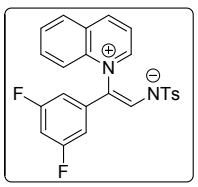
Brown solid; m.p. 207.6-208.2 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8. 95 (d, *J* = 8.4 Hz, 1H), 8.78-8.76 (m, 1H), 8.45 (s, 1H), 8.18-8.16 (m, 1H), 8.00 (d, *J* = 7.8 Hz, 1H), 7.89 (dd, *J* = 8.2, 5.8 Hz, 1H), 7.84-7.78 (m, 2H), 7.61 (d, *J* = 8.2 Hz, 2H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.14 (d, *J* = 8.2 Hz, 2H), 6.76 (d, *J* =8.4 Hz, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 147.0, 143.2, 142.6, 140.6, 140.1, 135.7, 130.5, 130.1, 129.0, 126.01, 125.98, 125.9, 125.8, 125.54, 125.47, 122.9, 122.4, 120.6, 119.4, 112.6, 21.3; IR (KBr) ν 3075, 2925, 1586, 1323, 1245, 1139, 1112, 1084, 1063 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{25}H_{19}F_3N_2O_2S$ $[M+H]^+$: 469.1193, found: 469.1202.

(*Z*)-(2-(7-Methylquinolin-1-ium-1-yl)-2-(4-(trifluoromethyl)phenyl)vinyl)(tosyl)amide (1r):



Red solid; m.p. 213.5-214.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.87 (d, *J* = 8.4 Hz, 1H), 8.67-8.65 (m, 1H), 8.46 (s, 1H), 8.06 (d, *J* = 8.4 Hz, 1H), 7.82-7.78 (m, 1H), 7.75 (s, 1H), 7.64-7.60 (m, 3H), 7.36 (d, *J* = 8.4 Hz, 2H), 7.13 (d, *J* = 8.0 Hz, 2H), 6.76 (d, *J* = 8.4 Hz, 2H), 2.44, (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 151.7, 148.4, 146.3, 143.3, 142.8, 140.7, 140.4, 140.3, 132.5, 129.6, 129.0, 128.9, 126.05, 126.01, 125.9, 125.7, 125.3, 122.9, 121.3, 119.5, 119.3, 112.4, 22.7, 21.3; IR (KBr) ν 3064, 2925, 1585, 1324, 1250, 1134, 1115, 1084, 1062 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{26}H_{21}F_3N_2O_2S$ $[M+H]^+$: 483.1349, found: 483.1352.

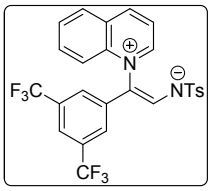
(*Z*)-(2-(3,5-Difluorophenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1s):



Red solid; m.p. 231.2-233.2 °C; ^{1}H NMR (400 MHz, DMSO-D_6) δ 9.39 (d, *J* = 8.2 Hz, 1H), 9.31 (dd, *J* = 5.8, 1.4 Hz, 1H), 8.53-8.50 (m, 1H), 8.26-8.23 (m, 2H), 8.05-7.97 (m, 2H), 7.94-7.92 (m, 1H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 6.80-6.74 (m, 1H), 6.54-6.51 (m, 2H), 2.31 (s, 3H); ^{13}C NMR (100 MHz, DMSO-D_6) δ 164.4, 164.3, 162.0, 161.8, 153.8, 148.1, 143.1, 143.0, 140.7, 139.8, 139.3, 135.8, 130.5,

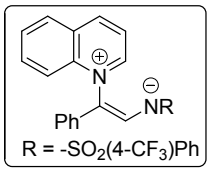
130.3, 129.9, 128.8, 125.3, 123.2, 119.4, 111.5, 102.4, 102.2, 102.1, 98.5, 98.2, 20.8; IR (KBr) ν 3085, 2976, 1585, 1448, 1265, 1128, 1084 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{18}F_2N_2O_2S$ $[M+H]^+$: 437.1130, found: 437.1137.

(*Z*)-(2-(3,5-bis(trifluoromethyl)phenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1t):



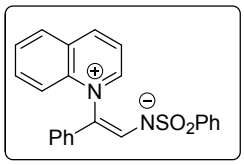
Red solid; m.p. 212.3-213.9℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.99 (d, *J* = 8.4 Hz, 1H), 8.81 (dd, *J* = 5.8 Hz, 1.6 Hz, 1H), 8.53 (s, 1H), 8.22 (dd, *J* = 6.2 Hz, 3.4 Hz, 1H), 8.00-7.94 (m, 2H), 7.89-7.85 (m, 2H), 7.59 (d, *J* = 8.2 Hz, 2H), 7.42 (s, 1H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.06-7.03 (m, 2H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.6, 147.4, 144.3, 142.3, 140.8, 140.0, 138.9, 136.1, 134.6, 132.9, 132.5, 132.2, 131.9, 130.6, 129.0, 128.9, 127.2, 125.9, 124.4, 122.5, 121.7, 120.2, 118.6, 116.8, 111.1, 21.3; IR (KBr) ν 3084, 3030, 2926, 1574, 1392, 1276, 1133, 1084 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{26}H_{18}F_6N_2O_2S$ $[M+H]^+$: 537.1066, found: 537.1068.

(*Z*)-(2-Phenyl-2-(quinolin-1-ium-1-yl)vinyl)((4-(trifluoromethyl)phenyl)sulfonyl)amide (1u):



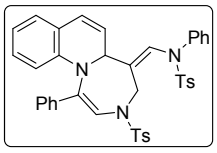
Red solid; m.p. 218.2-219.5 °C; ^{1}H NMR (400 MHz, DMSO-D_6) δ 9.40 (d, *J* = 8.4 Hz, 1H), 9.36 (dd, *J* = 5.8 Hz, 1.4 Hz, 1H), 8.52-8.50 (m, 1H), 8.26 (dd, *J* = 8.4 Hz, 5.6 Hz, 1H), 8.08 (s, 1H), 7.98-7.91 (m, 3H), 7.75-7.70 (m, 4H), 7.20 (t, *J* = 8.0 Hz, 2H), 7.04 (t, *J* = 7.2 Hz, 1H), 6.86 (d, *J* = 8.8 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-D_6) δ 153.4, 150.3, 147.9, 139.2, 139.0, 136.3, 135.7, 130.4, 130.1, 130.0, 129.6, 129.0, 126.0, 125.6, 125.5, 124.6, 123.1, 120.2, 119.6, 114.7, 54.9; IR (KBr) ν 3070, 3023, 1598, 1513, 1326, 1269, 1127, 1085 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{24}H_{17}F_3N_2O_2S$ $[M+H]^+$: 455.1036, found: 455.1039.

(*Z*)-(2-Phenyl-2-(quinolin-1-ium-1-yl)vinyl)(phenylsulfonyl)amide (1v):



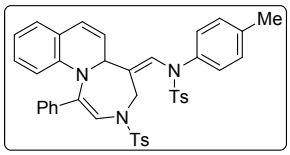
Brown solid; m.p. 206.6-207.1 °C; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.90 (d, *J* = 8.3 Hz, 1H), 8.77 (d, *J* = 5.2 Hz, 1H), 8.27 (s, 1H), 8.16-8.13 (m, 1H), 8.04-8.02 (m, 1H), 7.87-7.84 (m, 1H), 7.80-7.73 (m, 4H), 7.39-7.31 (m, 3H), 7.18-7.14 (m, 2H), 7.05-7.01 (m, 1H), 6.75 (d, *J* = 7.6 Hz, 2H); ^{13}C NMR (100 MHz, DMSO-D_6) δ 153.5, 147.7, 139.2, 136.5, 135.7, 130.4, 130.1, 129.9, 129.0, 128.3, 127.8, 126.9, 126.6, 125.2, 124.3, 123.0, 120.0, 119.7, 113.7; IR (KBr) ν 3059, 2985, 1593, 1518, 1445, 1244, 1133, 1086 cm^{-1}; HRMS (FAB) m/z calcd. for $C_{23}H_{18}N_2O_2S$ $[M+H]^+$: 387.1162, found: 387.1169.

(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3aa):



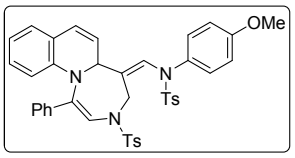
Off-white solid (96%); m.p. 177.8-179.5℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.24 (m, 2H), 7.19-7.15 (m, 7H), 7.09-7.07 (m, 3H), 6.93-6.91 (m, 3H), 6.70 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.54 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.42 (td, *J* = 7.4 Hz, 1.2 Hz, 1H), 6.25 (d, *J* = 9.6 Hz, 1H), 6.22 (d, *J* = 1.8 Hz, 1H), 5.84 (d, *J* = 8.0 Hz, 1H), 5.74 (dd, *J* = 9.6 Hz, 5.2 Hz, 1H), 4.86 (d, *J* = 5.2 Hz, 1H), 4.41-4.32 (m, 2H), 2.42 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 144.1, 142.1, 139.6, 135.6, 135.1, 134.5, 133.8, 129.9, 129.6, 129.0, 128.7, 128.6, 127.8, 127.7, 127.52, 127.5, 126.9, 126.8, 126.7, 125.6, 125.3, 124.9, 122.6, 121.6, 120.7, 117.8, 113.3, 59.3, 50.4, 21.6, 21.5; IR (KBr) ν 3064, 2925, 1637, 1594, 1490, 1450, 1350, 1166 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{35}N_3O_4S_2$ $[M]^+$: 685.2069, found: 685.2072.

(*E*)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-(p-tolyl)benzenesulfonamide (3ab):



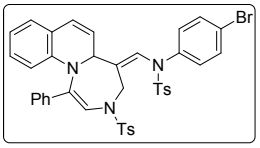
Light yellow solid (89%); m.p. 135.6-137.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.24 (m, 2H), 7.17-7.15 (m, 7H), 6.97 (s, 1H), 6.84-6.82 (m, 2H), 6.79-6.77 (m, 2H), 6.69 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.52-6.47 (m, 1H), 6.42-6.38 (m, 1H), 6.25-6.23 (m, 2H), 5.77 (d, *J* = 8.0 Hz, 1H), 5.65 (dd, *J* = 9.6 Hz, 5.0 Hz, 1H), 4.82-4.80 (m, 1H) 4.36 (s, 2H), 2.43 (s, 3H), 2.36 (s, 3H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 144.1, 142.4, 137.7, 136.7, 135.6, 135.1, 134.0, 132.6, 129.9, 129.8, 129.6, 128.9, 128.6, 127.9, 127.6, 127.4, 126.93, 126.9, 126.8, 126.0, 125.3, 124.8, 123.1, 121.6, 120.1, 117.5, 112.7, 59.1, 50.2, 21.6, 21.56, 21.0; IR (KBr) ν 3057, 3028, 2920, 1638, 1600, 1490, 1347, 1164 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_4S_2$ $[M]^+$: 699.2225, found: 699.2229.

(*E*)-*N*-(4-methoxyphenyl)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ac):



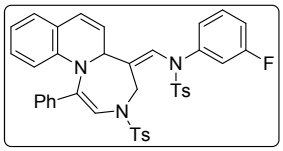
Off-white solid (83%); m.p. 136.5-138.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.24 (m, 2H), 7.17-7.15 (m, 7H), 6.96 (s, 1H), 6.79 (d, *J* = 9.0 Hz, 2H), 6.69 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.56-6.53 (m, 2H), 6.50 (td, *J* = 7.6 Hz, 1.4 Hz, 1H), 6.40 (td, *J* = 7.4 Hz, 1.2 Hz, 1H), 6.26-6.24 (m, 2H), 5.77 (d, *J* = 8.0 Hz, 1H), 5.66 (dd, *J* = 9.8 Hz, 5.0 Hz, 1H), 4.87-4.85 (m, 1H) 4.36 (s, 2H), 3.64 (s, 3H), 2.43 (s, 3H), 2.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.9, 144.2, 144.1, 142.5, 135.6, 135.1, 133.9, 132.0, 131.8, 129.9, 129.7, 128.9, 128.6, 128.57, 127.9, 127.6, 127.5, 126.9, 126.8, 126.1, 125.3, 124.8, 123.2, 121.7, 120.0, 117.5, 114.3, 112.6, 59.1, 55.3, 50.2, 21.6, 21.56, IR (KBr) ν 3060, 2924, 1640, 1599, 1510, 1443, 1351, 1165 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_5S_2$ $[M]^+$: 715.2175, found: 715.2175.

(*E*)-*N*-(4-bromophenyl)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ad):



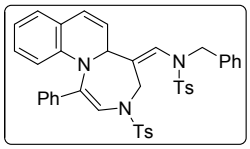
Light yellow solid (76%); m.p. 147.6-149.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.28-7.26 (m, 2H), 7.21-7.16 (m, 9H), 6.90 (s, 1H), 6.81 (d, *J* = 8.8 Hz, 2H), 6.70 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.55 (td, *J* = 7.6 Hz, 1.6 Hz, 1H), 6.44 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.25 (d, *J* = 9.8 Hz, 1H), 6.14 (d, *J* = 1.8 Hz, 1H), 5.85 (d, *J* = 8.0 Hz, 1H), 5.75 (dd, *J* = 9.8 Hz, 5.4 Hz, 1H), 4.90 (d, *J* = 5.2 Hz, 1H) 4.41-4.30 (m, 2H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 144.2, 142.0, 138.9, 135.8, 135.5, 134.9, 133.5, 132.2, 130.0, 129.8, 128.8, 128.7, 128.1, 128.0, 127.8, 127.2, 127.0, 126.8, 125.6, 125.1, 124.9, 122.4, 121.4, 121.3, 120.7, 118.0, 113.5, 59.3, 50.3, 21.64, 21.58, IR (KBr) ν 3060, 2924, 1639, 1599, 1491, 1348, 1267, 1168 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}BrN_3O_4S_2$ $[M]^+$: 763.1174, found: 763.1173.

(*E*)-*N*-(3-fluorophenyl)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ae):



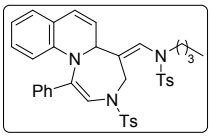
Light yellow solid (85%); m.p. 179.7-180.8℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.69 (d, *J* = 8.4 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.28-7.25 (m, 2H), 7.22-7.17 (m, 7H), 7.07-7.00 (m, 1H), 6.91 (s, 1H), 6.80-6.70 (m, 4H), 6.58 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.45 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.26 (d, *J* = 9.8 Hz, 1H), 6.09 (d, *J* = 1.8 Hz, 1H), 5.89 (d, *J* = 8.0 Hz, 1H), 5.82 (dd, *J* = 9.8 Hz, 5.4 Hz, 1H), 4.96 (d, *J* = 5.2 Hz, 1H) 4.42-4.30 (m, 2H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 163.6, 161.2, 144.6, 144.2, 141.9, 137.4, 135.5, 135.0, 133.6, 130.0, 129.8, 128.7, 128.6, 127.9, 127.8, 127.6, 127.0, 126.7, 125.5, 125.0, 124.9, 122.2, 121.6, 121.5, 121.1, 118.1, 114.3, 114.1, 113.8, 113.7, 113.5, 59.5, 50.3, 21.64, 21.5, IR (KBr) ν 3063, 2925, 1638, 1597, 1488, 1447, 1360, 1341, 1166 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}FN_3O_4S_2$ [M]$^+$: 703.1975, found: 703.1973.

(*E*)-*N*-benzyl-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3af):



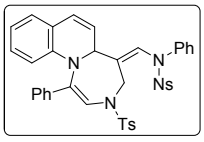
White solid (95%); m.p. 199.8-201.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.74 (t, *J* = 8.3 Hz, 4H), 7.37 (d, *J* = 8.0 Hz, 2H), 7.28-7.26 (m, 2H), 7.25-7.23 (m, 2H), 7.20-7.18 (m, 3H), 7.11-7.07 (m, 5H), 6.76 (s, 1H), 6.70 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.60 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.47 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.19 (dd, *J* = 9.8 Hz, 5.6 Hz, 1H), 6.07-6.04 (m, 1H), 5.90 (d, *J* = 8.0 Hz, 1H), 5.44 (d, *J* = 5.6 Hz, 1H), 5.21 (d, *J* = 1.8 Hz, 1H), 4.29-4.19 (m, 2H), 4.09-4.05 (m, 1H), 3.78 (m, 1H), 2.46 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 143.8, 141.6, 135.7, 135.6, 134.2, 134.0, 130.1, 130.0, 129.4, 128.6, 128.4, 128.1, 128.0, 127.9, 127.6, 127.0, 126.6, 125.3, 125.0, 124.5, 123.0, 122.5, 121.8, 118.3, 114.8, 60.4, 55.8, 50.8, 21.62, 21.58; IR (KBr) ν 3059, 3029, 2920, 1633, 1596, 1485, 1450, 1344, 1165 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_4S_2$ [M]$^+$: 699.2225, found: 699.2222.

(*E*)-*N*-butyl-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ag):



Light yellow solid (95%); m.p. 132.3-133.8℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 8.4 Hz, 2H), 7.68 (d, *J* = 8.2 Hz, 2H), 7.35-7.32 (m, 4H), 7.28 (d, *J* = 8.0 Hz, 2H), 7.24-7.18 (m, 3H), 6.88-6.86 (m, 2H), 6.70 (dd, *J* = 7.6 Hz, 1.6 Hz, 1H), 6.59-6.55 (m, 1H), 6.51-6.47 (m, 1H), 6.41-6.38 (m, 1H), 6.09-6.07 (m, 1H), 5.60 (d, *J* = 5.5 Hz, 1H), 5.09 (d, *J* = 1.6 Hz, 1H), 4.37-4.35 (m, 1H), 4.25-4.22 (m, 1H), 3.12-3.05 (m, 1H), 2.54-2.47 (m, 1H), 2.43 (s, 3H), 2.38 (s, 3H), 1.33-1.27 (m, 2H), 1.19-1.10 (m, 2H), 0.74 (t, *J* = 7.0 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 143.8, 142.8, 141.5, 135.7, 135.5, 133.9, 130.1, 129.8, 128.6, 128.2, 128.1, 127.7, 127.68, 127.1, 126.5, 125.5, 125.4, 124.6, 123.7, 123.0, 121.6, 118.6, 115.4, 60.2, 51.2, 50.9, 29.78, 21.5, 20.1, 13.6; IR (KBr) ν 3057, 2954, 2929, 2868, 1635, 1596, 1482, 1346, 1162 cm^{-1}; HRMS (EI) m/z calcd. for $C_{38}H_{39}N_3O_4S_2$ [M]$^+$: 665.2382, found: 665.2382.

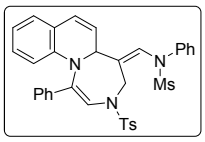
(*E*)-2-nitro-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ah):



Yellow solid (43%); m.p. 200.6-202.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.64-7.60 (m, 2H), 7.54-7.49 (m, 2H), 7.20-7.18 (m, 7H), 7.13-7.10 (m, 5H), 6.95 (s, 1H), 6.69 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.56 (td, *J* = 7.7 Hz, 1.5 Hz, 1H), 6.49

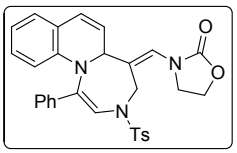
(d, *J* = 1.7 Hz, 1H), 6.42 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.25 (d, *J* = 9.8 Hz, 1H), 5.86 (d, *J* = 8.0 Hz, 1H), 5.57 (q, *J* = 5.0 Hz, 1H), 4.94 (d, *J* = 5.0 Hz, 1H) 4.46-4.36 (m, 2H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 148.1, 144.1, 142.2, 138.6, 135.5, 135.4, 135.1, 134.4, 132.1, 131.2, 130.05, 129.96, 129.4, 128.9, 128.6, 128.0, 127.5, 127.3, 126.94, 126.87, 126.8, 125.8, 125.1, 124.8, 124.0, 122.9, 121.1, 120.1, 117.7, 113.0, 59.2, 49.9, 21.5, IR (KBr) ν 3063, 2926, 1640, 1597, 1546, 1491, 1362, 1166 cm^{-1}; HRMS (EI) m/z calcd. for $C_{39}H_{32}N_4O_6S_2$ [M]$^+$: 716.1763, found: 716.1767.

(*E*)-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)methanesulfonamide (3ai):



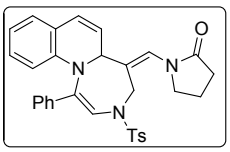
Yellow Off-white solid (92%); m.p. 102.2-104.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.25-17 (m, 11H), 7.11-7.15 (m, 1H), 7.05 (s, 1H), 6.71 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.57 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.44 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.37 (d, *J* = 2.0 Hz, 1H), 6.23 (d, *J* = 9.8 Hz, 1H), 5.88 (d, *J* = 8.0 Hz, 1H), 5.59 (dd, *J* = 9.8 Hz, 5.4 Hz, 1H), 4.73-4.75 (m, 1H) 4.38 (s, 2H), 2.87 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.1, 142.1, 139.1, 135.5, 135.0, 133.3, 129.9, 129.5, 128.8, 128.5, 127.55, 127.49, 127.4, 126.9, 126.7, 126.0, 125.4, 124.9, 124.7, 122.7, 121.2, 120.4, 117.8, 113.2, 59.0, 50.3, 36.9, 21.5, IR (KBr) ν 3061, 2925, 1637, 1593, 1488, 1451, 1346, 1160 cm^{-1}; HRMS (EI) m/z calcd. for $C_{34}H_{31}N_3O_4S_2$ [M]$^+$: 609.1756, found: 609.1755.

(*E*)-3-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)oxazolidin-2-one (3aj):



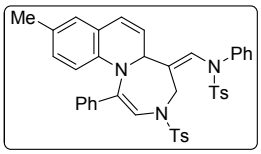
Off-white solid (89%); m.p. 163.7-165.4℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.38-7.36 (m, 2H), 7.28-7.26 (m, 2H), 7.24-7.20 (m, 3H), 7.03 (s, 1H), 6.87 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.74 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.57 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.37 (d, *J* = 9.8 Hz, 1H), 6.13 (d, *J* = 8.0 Hz, 1H), 5.88 (d, *J* = 1.8 Hz, 1H), 5.67 (dd, *J* = 9.8 Hz, 5.6 Hz, 1H), 5.23 (d, *J* = 5.6 Hz, 1H) 4.41 (s, 2H), 4.40-4.35 (m, 2H), 3.73-3.67 (m, 1H), 3.54-3.48 (m, 1H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 156.0, 144.1, 142.0, 135.6, 135.4, 130.3, 130.0, 129.0, 128.7, 127.6, 127.2, 127.1, 126.7, 125.4, 125.1, 122.5, 121.8, 121.4, 118.4, 114.6, 62.0, 59.7, 51.1, 45.7, 21.5, IR (KBr) ν 3058, 2988, 2918, 1760, 1667, 1599, 1490, 1450, 1160 cm^{-1}; HRMS (EI) m/z calcd. for $C_{30}H_{27}N_3O_4S$ [M]$^+$: 525.1722, found: 525.1722.

(*E*)-1-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)pyrrolidin-2-one (3ak):



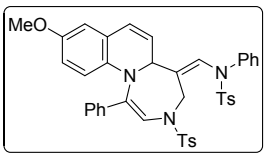
Yellow solid (40%); m.p. 185.6-187.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 (d, *J* = 8.4 Hz, 2H), 7.40-7.38 (m, 2H), 7.20-7.25 (m, 5H), 7.07 (s, 1H), 6.84 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.70 (td, *J* = 7.8 Hz, 1.4 Hz, 1H), 6.54 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.32 (d, *J* = 9.8 Hz, 1H), 6.09 (d, *J* = 8.0 Hz, 1H), 5.98 (d, *J* = 1.4 Hz, 1H), 5.57 (dd, *J* = 5.0 Hz, 5.4 Hz, 1H), 5.36 (d, *J* = 5.4 Hz, 1H) 4.46-4.38 (m, 2H), 3.53-3.47 (m, 1H), 3.34-3.29 (m, 1H), 2.44-2.41 (m, 2H), 2.39 (s, 3H), 2.10-2.02 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 174.4, 143.9, 142.3, 135.8, 135.5, 129.9, 129.5, 129.0, 128.7, 127.5, 127.2, 126.8, 126.7, 125.3, 125.0, 122.9, 122.3, 121.7, 121.1, 118.1, 114.2, 60.0, 51.3, 48.4, 30.5, 21.5, 18.4; IR (KBr) ν 3061, 2923, 1707, 1649, 1598, 1491, 1449, 1339, 1157 cm^{-1}; HRMS (EI) m/z calcd. for $C_{31}H_{29}N_3O_3S$ [M]$^+$: 523.1930, found: 523.1932.

(*E*)-4-methyl-*N*-((9-methyl-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ba):



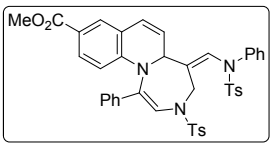
Off-white solid (91%); m.p. 192.6-194.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.2 Hz, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.25-7.23 (m, 2H), 7.21-7.15 (m, 7H), 7.12-7.09 (m, 3H), 6.93-6.91 (m, 2H), 6.88 (s, 1H), 6.54 (d, *J* = 1.8 Hz, 1H), 6.37 (dd, *J* = 8.2 Hz, 1.6 Hz, 1H), 6.23 (d, *J* = 9.8 Hz, 1H), 6.18 (d, *J* = 1.8 Hz, 1H), 5.84 (dd, *J* = 9.8 Hz, 5.6 Hz, 1H), 5.79 (d, *J* = 8.0 Hz, 1H), 4.84 (d, *J* = 5.4 Hz, 1H), 4.40-4.28 (m, 2H), 2.42 (s, 3H), 2.38 (s, 3H), 2.05 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 144.1, 139.8, 139.7, 135.7, 135.51, 135.5, 133.9, 129.9, 129.6, 129.1, 129.0, 128.5, 128.0, 127.9, 127.5, 127.4, 127.3, 127.1, 127.0, 126.7, 125.5, 125.2, 125.1, 122.1, 122.0, 121.2, 113.8, 59.4, 50.7, 21.62, 21.57, 20.2; IR (KBr) ν 3059, 2924, 1638, 1594, 1494, 1349, 1264, 1164 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_4S_2$ $[M]^+$: 699.2225, found: 699.2224.

(*E*)-*N*-((9-methoxy-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ca):



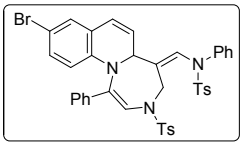
Light yellow solid (87%); m.p. 203.5-205.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.24-7.13 (m, 12H), 6.95-6.92 (m, 2H), 6.81 (s, 1H), 6.34 (d, *J* = 2.8 Hz, 1H), 6.25 (d, *J* = 9.8 Hz, 1H), 6.21 (dd, *J* = 8.8 Hz, 2.8 Hz, 1H), 6.14 (d, *J* = 1.8 Hz, 1H), 6.03 (dd, *J* = 9.8 Hz, 5.8 Hz, 1H), 5.88 (d, *J* = 8.8 Hz, 1H), 4.80 (d, *J* = 5.6 Hz, 1H), 4.43-4.39 (m, 1H), 4.29-4.25 (m, 1H), 3.60 (s, 3H), 2.42 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.4, 144.2, 144.1, 140.0, 136.6, 135.8, 135.64, 135.56, 133.8, 130.0, 129.6, 129.0, 128.5, 128.4, 127.9, 127.6, 127.3, 127.1, 126.5, 125.4, 124.9, 123.4, 123.1, 121.2, 115.5, 113.9, 112.2, 60.4, 59.5, 55.5, 51.3, 21.63, 21.58; IR (KBr) ν 3057, 2930, 1635, 1596, 1491, 1448, 1354, 1166 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_5S_2$ $[M]^+$: 715.2175, found: 715.2175.

(*E*)-methyl 5-((4-methyl-*N*-phenylphenylsulfonamido)methylene)-1-phenyl-3-tosyl-3,4,5,5a-tetrahydro-[1,4]diazepino[1,7-*a*]quinoline-9-carboxylate (3da):



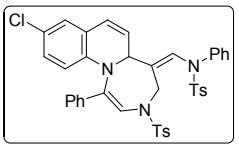
Off-white solid (91%); m.p. 130.1-131.8℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 (d, *J* = 8.4 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.33 (d, *J* = 2.0 Hz, 1H), 7.24 (m, 2H), 7.19-7.16 (m, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.11-7.08 (m, 3H), 7.05 (s, 1H), 7.01-6.98 (m, 3H), 6.91-6.89 (m, 2H), 6.38 (d, *J* = 1.6 Hz, 1H), 6.23 (dd, *J* = 10.0 Hz, 0.8 Hz, 1H), 5.63 (d, *J* = 8.6 Hz, 1H), 5.46 (dd, *J* = 10.0 Hz, 4.6 Hz, 1H), 4.85 (d, *J* = 4.6 Hz, 1H), 4.42-4.39 (m, 1H), 4.31-4.28 (m, 1H), 3.79 (s, 3H), 2.43 (s, 3H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 166.8, 147.0, 144.6, 144.5, 139.1, 135.1, 133.9, 133.7, 131.3, 130.3, 129.9, 129.7, 129.2, 128.8, 128.4, 127.9, 127.8, 127.3, 127.2, 126.8, 126.7, 125.2, 124.3, 124.0, 121.6, 118.5, 118.1, 110.8, 58.9, 51.5, 49.3, 21.6; 21.4 IR (KBr) ν 3060, 2949, 1710, 1645, 1599, 1495, 1446, 1359, 1279, 1166 cm^{-1}; HRMS (EI) m/z calcd. for $C_{42}H_{37}N_3O_6S_2$ $[M]^+$: 743.2124, found: 743.2126.

(*E*)-*N*-((9-bromo-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ea)



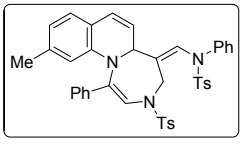
Off-white solid (91%); m.p. 122.9-124.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.23-7.25 (m, 2H), 7.20-7.17 (m, 5H), 7.13-7.11 (m, 2H), 7.06-7.04 (m, 3H), 6.96 (s, 1H), 6.92-6.90 (m, 2H), 6.77 (d, *J* = 2.4 Hz, 1H), 6.52 (dd, *J* = 8.6 Hz, 2.4 Hz, 1H), 6.28 (d, *J* = 1.8 Hz, 1H), 6.16 (d, *J* = 9.8 Hz, 1H), 5.67 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 5.62 (d, *J* = 8.8 Hz, 1H), 4.84 (d, *J* = 5.0 Hz, 1H), 4.43-4.40 (m, 1H), 4.29-4.26 (m, 1H), 2.43 (s, 3H), 2.41 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.44, 144.39, 141.6, 139.4, 135.4, 134.5, 133.7, 132.8, 131.2, 129.9, 129.7, 129.1, 128.9, 128.7, 127.8, 127.74, 127.67, 127.5, 126.9, 126.8, 126.2, 124.7, 124.3, 123.2, 122.9, 121.8, 114.2, 109.5, 58.9, 50.0, 21.62, 21.60; IR (KBr) ν 3060, 2925, 1641, 1596, 1486, 1353, 1264, 1165 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}BrN_3O_4S_2$ $[M]^+$: 763.1174, found: 763.1177.

(*E*)-*N*-((9-chloro-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3fa)



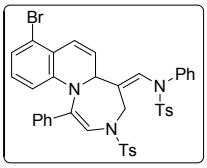
Off-white solid (93%); m.p. 188.5-190.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.23-7.25 (m, 2H), 7.19-7.17 (m, 5H), 7.14-7.11 (m, 2H), 7.07-7.05 (m, 3H), 6.95 (s, 1H), 6.92-6.90 (m, 2H), 6.64 (d, *J* = 2.4 Hz, 1H), 6.39 (dd, *J* = 8.6 Hz, J_2 = 2.6 Hz, 1H), 6.27 (d, *J* = 1.8 Hz, 1H), 6.16 (d, *J* = 9.8 Hz, 1H), 5.72-5.67 (m, 2H), 4.84 (d, *J* = 5.2 Hz, 1H) 4.43-4.40 (m, 1H), 4.30-4.26 (m, 1H), 2.43 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 141.0, 139.4, 135.4, 134.6, 133.7, 133.0, 129.9, 129.7, 129.1, 128.6, 128.2, 127.8, 127.7, 127.6, 126.8, 126.13, 126.11, 124.7, 124.4, 123.05, 123.01, 122.4, 121.5, 113.8, 58.9, 50.1, 21.6, 21.5; IR (KBr) ν 3060, 2925, 1639, 1596, 1487, 1350, 1265, 1164 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}ClN_3O_4S_2$ $[M]^+$: 719.1679, found: 719.1682.

(*E*)-4-methyl-*N*-((10-methyl-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ga):



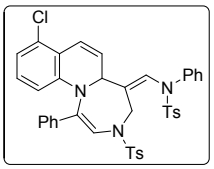
Off-white solid (87%); m.p. 122.3-124.0℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.25-7.23 (m, 2H), 7.20-7.15 (m, 7H), 7.08-7.06 (m, 3H), 6.95 (s, 1H), 6.90-6.88 (m, 2H), 6.61 (d, *J* = 7.6 Hz, 1H), 6.27-6.25 (m, 1H), 6.22 (d, *J* = 9.8 Hz, 1H), 6.19 (d, *J* = 1.8 Hz, 1H), 5.75 (s, 1H), 5.68 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.84 (d, *J* = 5.2 Hz, 1H) 4.38 (s, 2H), 2.42 (s, 3H), 2.36 (s, 3H), 1.91 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 144.0, 142.2, 139.6, 138.6, 135.8, 135.4, 134.8, 134.0, 129.9, 129.7, 129.0, 128.6, 127.8, 127.5, 127.4, 127.0, 126.8, 126.7, 125.6, 125.2, 124.9, 122.6, 121.7, 120.6, 118.9, 118.4, 114.1, 59.5, 50.4, 21.63, 21.56, 21.1; IR (KBr) ν 3046, 2923, 1634, 1595, 1497, 1445, 1352, 1266, 1164 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_4S_2$ $[M]^+$: 699.2225, found: 699.2226.

(*E*)-*N*-((8-bromo-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ha):



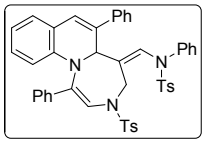
Light-yellow solid (88%); m.p. 177.9-179.5℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.27 (m, 1H), 7.25-7.22 (m, 3H), 7.18-7.16 (m, 5H), 7.12-7.10 (m, 3H), 6.93-6.90 (m, 3H), 6.71-6.66 (m,2H), 6.40 (t, *J* = 8.0 Hz, 1H), 6.20 (d, *J* = 1.8 Hz, 1H), 5.97 (dd, *J* =10.0 Hz, 5.6 Hz, 1H), 5.87 (d, *J* = 8.2 Hz, 1H), 4.92 (d, *J* = 5.4 Hz, 1H) 4.43-4.40 (m, 1H), 4.29-4.25 (m, 1H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.34, 144.27, 143.4, 139.5, 135.7, 134.8, 135.7, 134.1, 130.1, 129.7, 129.2, 129.1, 128.7, 127.9, 127.8, 127.7, 127.3, 127.0, 126.8, 126.1, 124.9, 123.8, 123.6, 122.6, 122.15, 122.1, 120.4, 113.3, 59.3, 50.6, 21.63, 21.58; IR (KBr) ν 3059, 2926, 1636, 1591, 1554, 1496, 1445, 1352, 1163 cm-1; HRMS (EI) m/z calcd. for $C_{40}H_{34}BrN_3O_4S_2$ [M]$^+$: 763.1174, found: 763.1176.

(*E*)-*N*-((8-chloro-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ia):



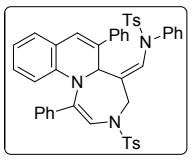
Off-white solid (90%); m.p. 103.6-105.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.70 (d, *J* = 8.4 Hz, 2H), 7.45 (d, *J* = 8.4 Hz, 2H), 7.27 (m, 1H), 7.25-7.23 (m, 2H), 7.21 (m, 1H), 7.18-7.15 (m, 5H), 7.11-7.10 (m, 3H), 6.93-6.90 (m, 3H), 6.71 (d, *J* = 10.4 Hz, 1H), 6.50-6.44 (m, 2H), 6.22 (d, *J* = 1.6 Hz, 1H), 5.92 (dd, *J* = 10.0 Hz, 5.6 Hz, 1H), 5.82-5.80 (m, 1H), 4.90 (d, *J* = 5.4 Hz, 1H), 4.42-4.39 (m, 1H), 4.30-4.26 (m, 1H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 144.2, 143.3, 139.5, 135.6, 134.8, 134.4, 134.0, 130.4, 130.0, 129.7, 129.1, 128.70, 128.66, 127.8, 127.72, 127.68, 127.4, 127.0, 126.8, 126.1, 124.9, 123.2, 122.6, 121.2, 118.8, 118.7, 112.4, 59.2, 50.5, 21.6, 21.5; IR (KBr) ν 3060, 2925, 1634, 1589, 1496, 1448, 1349, 1266, 1163 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}ClN_3O_4S_2$ [M]$^+$: 719.1679, found: 719.1679.

(*E*)-*N*-((1,6-diphenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ja, *E*-isomer):



Yellow solid (38%); m.p. 169.3-171.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (d, *J* = 8.2 Hz, 2H), 7.31-7.27 (m, 3H), 7.25-7.23 (m, 2H), 7.20-7.18 (m, 5H), 7.15-7.08 (m, 8H), 6.96-6.92 (m, 3H), 7.90-7.87 (m, 2H), 6.79-6.76 (m, 1H), 6.72 (d, *J* = 7.6 Hz, 2H), 6.21 (d, *J* = 8.0 Hz, 1H), 5.88 (s, 1H), 4.93 (d, *J* = 17.2 Hz, 1H), 4.73 (s, 1H), 3.43 (d, *J* = 17.2 Hz, 1H), 2.43 (s, 3H), 2.40 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 143.9, 143.6, 141.0, 139.6, 137.5, 136.2, 135.5, 134.0, 132.7, 131.5, 130.1, 129.4, 129.3, 129.1, 128.6, 128.5, 128.0, 127.8, 127.7, 127.6, 127.1, 127.0, 126.8, 126.2, 125.4, 125.0, 123.1, 120.0, 119.2, 118.0, 61.7, 48.2, 21.9, 21.6; IR (KBr) ν 3059, 3029, 2922, 1650, 1593, 1485, 1354, 1266, 1165 cm^{-1}; HRMS (EI) m/z calcd. for $C_{46}H_{39}N_3O_4S_2$ [M]$^+$: 761.2382, found: 761.2384.

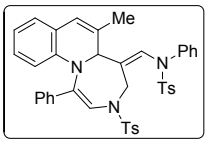
(*Z*)-*N*-((1,6-diphenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ja, *Z*-isomer):



Off-white solid (54%); m.p. 224.7-226.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.96 (d, *J* = 8.2 Hz, 2H), 7.48 (d, *J* = 8.0 Hz, 2H), 7.38-7.36 (m, 3H), 7.20-7.18 (m, 2H), 7.15-7.08 (m, 10H), 7.01-6.97 (m, 2H), 6.95 (s, 1H), 6.73 (td, *J* = 7.8 Hz, 1.2 Hz, 1H), 6.50 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.33 (d, *J* = 7.6 Hz, 2H), 6.28 (d, *J* = 6.6 Hz, 1H), 6.19 (d, *J* = 8.0

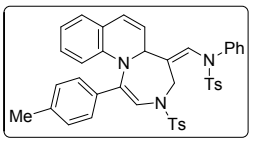
Hz, 1H), 6.06 (s, 1H), 6.03 (s, 1H), 4.76-4.72 (m, 2H), 4.24-4.21 (m, 1H), 2.53 (s, 3H), 2.33 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.0, 143.9, 142.7, 139.5, 136.9, 136.1, 135.7, 135.1, 132.0, 130.5, 129.9, 129.2, 128.6, 128.5, 128.1, 128.0, 127.8, 127.59, 127.56, 126.6, 126.1, 125.9, 125.8, 125.3, 124.5, 122.3, 119.5, 119.3, 116.6, 61.0, 54.0, 21.9, 21.5; IR (KBr) ν 3054, 3029, 2921, 1625, 1595, 1485, 1445, 1353, 1164 cm^{-1}; HRMS (EI) m/z calcd. for $C_{46}H_{39}N_3O_4S_2$ $[M]^+$: 761.2382, found: 761.2383.

(*E*)-4-methyl-*N*-((6-methyl-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ka):



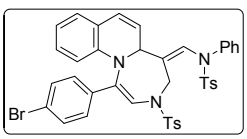
White solid (96%); m.p. 243.2-245.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 8.4 Hz, 2H), 7.33 (d, *J* = 8.4 Hz, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.16-7.10 (m, 5H), 7.07-7.05 (m, 2H), 7.00 (s, 1H), 6.89-6.86 (m, 2H), 6.84-6.81 (m, 3H), 6.41-6.37 (m, 2H), 6.34-6.25 (m, 2H), 5.89 (s, 1H), 5.62 (d, *J* = 7.8 Hz, 1H), 4.45-4.42 (m, 2H), 4.25-4.22 (m, 1H), 2.41 (s, 3H), 2.36 (s, 3H), 1.85 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 143.9, 141.3, 139.9, 135.3, 134.4, 133.0, 129.9, 129.6, 129.5, 128.9, 128.8, 128.6, 128.5, 127.9, 127.8, 127.5, 127.4, 127.1, 126.8, 126.7, 125.8, 124.4, 123.3, 122.4, 119.9, 117.0, 111.6, 61.4, 50.2, 21.6, 21.5, 21.0; IR (KBr) ν 3059, 3029, 2919, 1594, 1485, 1444, 1349, 1264, 1163 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_4S_2$ $[M]^+$: 699.2225, found: 699.2226.

(*E*)-4-methyl-*N*-phenyl-*N*-((1-(p-tolyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3la):



Yellow solid (96%); m.p. 108.0-109.6℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.25-7.23 (m, 2H), 7.17 (d, *J* = 8.0 Hz, 2H), 7.11-7.06 (m, 5H), 6.98-6.96 (m, 2H), 6.93-6.91 (m, 2H), 6.87 (s, 1H), 6.69 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.54 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.42 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.24 (d, *J* = 9.8 Hz, 1H), 6.20 (d, *J* = 1.8 Hz, 1H), 5.83 (d, *J* = 8.0 Hz, 1H), 5.75 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.86 (d, *J* = 5.2 Hz, 1H), 4.40-4.30 (m, 2H), 2.42 (s, 3H), 2.36 (s, 3H), 2.27 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.2, 144.0, 142.1, 139.7, 137.4, 135.5, 134.9, 133.8, 132.3, 129.9, 129.6, 129.2, 129.0, 128.7, 127.9, 127.8, 127.4, 126.9, 126.7, 126.6, 125.5, 125.2, 124.9, 121.7, 121.6, 120.8, 117.8, 113.5, 59.4, 50.4, 21.6, 21.5, 21.1; IR (KBr) ν 3045, 2922, 1639, 1593, 1490, 1350, 1165 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{37}N_3O_4S_2$ $[M]^+$: 699.2225, found: 699.2226.

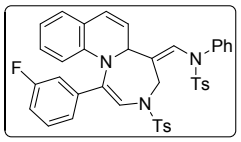
(*E*)-*N*-((1-(4-bromophenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ma):



Off-white solid (98%); m.p. 121.3-123.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.29-7.26 (m, 2H), 7.25-7.23 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.12-7.10 (m, 3H), 7.05-7.03 (m, 2H), 6.93-6.90 (m, 3H), 6.71 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.56 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.45 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.25 (d, *J* = 10.0 Hz, 1H), 6.21 (d, *J* = 1.8 Hz, 1H), 5.81 (d, *J* = 8.0 Hz, 1H), 5.76 (dd, *J* = 9.8 Hz, 5.3 Hz, 1H), 4.86 (d, *J* = 5.2 Hz, 1H), 4.39-4.29 (m, 2H), 2.43 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 144.2, 141.8, 139.6, 135.5, 134.5, 134.3, 133.8, 131.7, 130.0, 129.7, 129.1, 128.8,

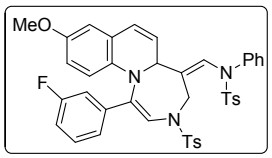
127.8, 127.6, 126.9, 126.8, 126.7, 126.6, 126.4, 125.8, 125.2, 123.0, 121.7, 121.2, 120.8, 118.1, 113.2, 59.3, 50.3, 21.6, 21.5; IR (KBr) ν 3063, 2923, 1487, 1356, 1343, 1263, 1164, 1089 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}BrN_3O_4S_2$ $[M]^+$: 703.1975, found: 703.1979.

(*E*)-*N*-((1-(3-fluorophenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3na):



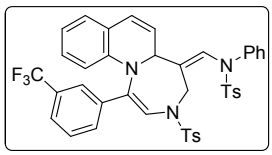
Light-yellow solid (93%); m.p. 188.5-190.2℃; ^1H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.4 Hz, 2H), 7.24 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.16-7.13 (m, 1H), 7.11-7.08 (m, 3H), 6.99-6.97 (m, 2H), 6.93-6.90 (m, 2H), 6.86-6.81 (m, 2H), 6.71 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.56 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.45 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.25 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 1.8 Hz, 1H), 5.82 (d, *J* = 8.0 Hz, 1H), 5.72 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.86 (d, *J* = 5.2 Hz, 1H), 4.39-4.30 (m, 2H), 2.43 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.3, 161.9, 144.4, 144.3, 142.1, 139.6, 137.95, 137.88, 135.5, 134.1, 133.8, 130.0, 129.7, 129.1, 128.8, 127.9, 127.6, 126.93, 126.87, 127.4, 125.9, 125.4, 123.9, 121.6, 120.6, 120.4, 118.1, 114.4, 114.2, 113.0, 111.7, 111.5, 59.3, 50.3, 21.63, 21.57; IR (KBr) ν 3064, 2924, 1637, 1597, 1454, 1351, 1163 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{34}FN_3O_4S_2$ $[M]^+$: 703.1975, found: 703.1979.

(*E*)-*N*-((1-(3-fluorophenyl)-9-methoxy-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3oa):



Light-yellow solid (91%); m.p. 165.6-167.2℃; ^1H NMR (400 MHz, $CDCl_3$) δ 7.72 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.4 Hz, 2H), 7.25-7.23 (m, 4H), 7.17-7.11 (m, 4H), 7.00 (d, *J* = 7.8 Hz, 1H), 6.94-6.92 (m, 2H), 6.87-6.82 (m, 3H), 6.35 (d, *J* = 2.8 Hz, 1H), 6.27-6.21 (m, 2H), 6.14 (d, *J* = 1.4 Hz, 1H), 6.02 (dd, *J* = 9.8 Hz, 5.7 Hz, 1H), 5.87 (d, *J* = 8.8 Hz, 1H), 4.80 (d, *J* = 5.4 Hz, 1H), 4.41-4.24 (m, 2H), 3.62 (s, 3H), 2.42 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.2, 161.8, 152.5, 144.3, 139.9, 138.4, 138.3, 136.1, 135.6, 135.4, 133.8, 130.1, 130.0, 129.9, 129.6, 129.0, 127.8, 127.4, 127.0, 126.5, 125.6, 124.9, 123.3, 123.0, 122.4, 120.8, 120.7, 115.1, 114.4, 114.2, 113.9, 112.3, 112.1, 111.9, 59.4, 55.5, 51.1, 21.6, 21.5; IR (KBr) ν 3062, 2929, 1493, 1356, 1269, 1242, 1165, 1090 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{36}FN_3O_5S_2$ $[M]^+$: 721.1881, found: 721.1880.

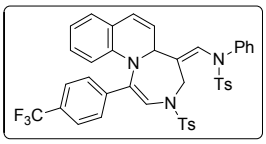
(*E*)-4-methyl-*N*-phenyl-*N*-((3-tosyl-1-(3-(trifluoromethyl)phenyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3pa):



Yellow solid (81%); m.p. 121.1-123.0℃; ^1H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H), 7.43-7.40 (m, 5H), 7.29-7.28 (m, 1H), 7.24-7.18 (m, 4H), 7.05-7.03 (m, 4H), 6.92-6.90 (m, 2H), 6.71 (d, *J* = 6.4 Hz, 1H), 6.56-6.52 (m, 1H), 6.46-6.43 (m, 1H), 6.28-6.23 (m, 2H), 5.79 (d, *J* = 8.0 Hz, 1H), 5.72 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.85 (d, *J* = 5.0 Hz, 1H), 4.41-4.32 (m, 2H), 2.43 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.42, 144.38, 142.1, 139.6, 136.3, 135.5, 133.8, 133.7, 130.1, 129.7, 129.2, 129.1, 128.9, 128.0, 127.8, 127.6, 127.0, 126.93, 126.89, 126.1, 125.4, 124.5, 124.11, 124.07, 122.6, 121.6, 121.3,

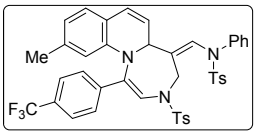
120.5, 118.1, 112.7, 59.1, 50.2, 21.61, 21.56; IR (KBr) ν 3065, 2925, 1638, 1594, 1489, 1333, 1258, 1165, 1126 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{34}F_3N_3O_4S_2$ $[M]^+$: 753.1943, found: 753.1945.

(*E*)-4-methyl-*N*-phenyl-*N*-((3-tosyl-1-(4-(trifluoromethyl)phenyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3qa):



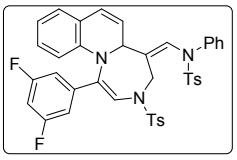
Off-white solid (95%); m.p. 184.7-186.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.4 Hz, 2H), 7.43-7.40 (m, 4H), 7.28 (m, 2H), 7.24 (m, 2H), 7.20 (d, *J* = 8.0 Hz, 2H), 7.10-7.06 (m, 4H), 6.91-6.89 (m, 2H), 6.73 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.57 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.46 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.26 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 1.8 Hz, 1H), 5.81 (d, *J* = 8.0 Hz, 1H), 5.74 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.89 (d, *J* = 5.2 Hz, 1H) 4.41-4.33 (m, 2H), 2.43 (s, 3H), 2.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 141.9, 139.6, 139.0, 135.5, 134.1, 133.8, 130.1, 129.7, 129.4, 129.1, 128.9, 127.8, 127.6, 127.0, 126.9, 126.8, 126.0, 125.9, 125.63, 125.59, 125.5, 125.4, 124.9, 124.8, 121.7, 120.7, 118.2, 112.9, 59.3, 50.3, 21.62, 21.58; IR (KBr) ν 3064, 2924, 1639, 1599, 1490, 1451, 1359, 1321, 1166 cm^{-1}; HRMS (EI) m/z calcd. for $C_{41}H_{34}F_3N_3O_4S_2$ $[M]^+$: 753.1943, found: 753.1941.

(*E*)-4-methyl-*N*-((10-methyl-3-tosyl-1-(4-(trifluoromethyl)phenyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ra):



Off-white solid (91%); m.p. 220.4-222.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.68 (d, *J* = 8.4 Hz, 2H), 7.43-7.40 (m, 4H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.23 (m, 2H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.09 (s, 1H), 7.08-7.06 (m, 3H), 6.89-6.86 (m, 2H), 6.63 (d, *J* = 7.4 Hz, 1H), 6.30 (dd, *J* = 7.6 Hz, 0.8 Hz, 1H), 6.24 (d, *J* = 9.8 Hz, 1H), 6.20 (d, *J* = 1.8 Hz, 1H), 5.71 (s, 1H), 5.67 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.86 (d, *J* = 5.2 Hz, 1H) 4.39 (s, 2H), 2.43 (s, 3H), 2.36 (s, 3H), 1.92 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.35, 144.30, 141.9, 139.6, 139.1, 138.8, 135.7, 134.4, 133.9, 130.0, 129.7, 129.05, 128.96, 127.8, 127.5, 127.0, 126.9, 126.8, 125.9, 125.62, 125.58, 125.5, 125.3, 124.9, 124.8, 120.6, 119.2, 118.3, 113.7, 59.5, 50.2, 21.64, 21.62, 21.58; IR (KBr) ν 3045, 2924, 1605, 1496, 1354, 1325, 1167, 1113 cm^{-1}; HRMS (EI) m/z calcd. for $C_{42}H_{36}F_3N_3O_4S_2$ $[M]^+$: 767.2099, found: 767.2097.

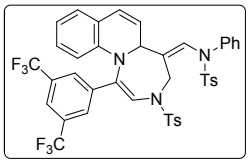
(*E*)-*N*-((1-(3,5-difluorophenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3sa):



Off-white solid (96%); m.p. 178.6-180.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.2 Hz, 2H), 7.27 (m, 1H), 7.24 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.13-7.11 (m, 3H), 7.00 (s, 1H), 6.93-6.90 (m, 2H), 6.73 (dd, *J* = 7.4 Hz, 1.4 Hz, 1H), 6.69-6.66 (m, 2H), 6.61-6.56 (m, 2H), 6.47 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.25 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 1.8 Hz, 1H), 5.81 (d, *J* = 8.0 Hz, 1H), 5.71 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.85 (d, *J* = 5.2 Hz, 1H), 4.38-4.29 (m, 2H), 2.43 (s, 3H), 2.38 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 164.5, 164.4, 162.1, 162.0, 144.44, 144.41, 141.9, 139.6, 139.4, 135.5, 133.8, 133.7, 130.1, 129.7, 129.1, 128.9, 127.8, 127.6, 127.0, 126.9, 126.1, 125.4, 125.1, 121.6, 120.6, 118.3, 112.7, 107.5, 107.2, 102.9,

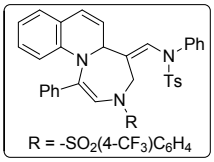
102.6, 102.4, 59.2, 50.2, 21.62, 21.58; IR (KBr) ν 3065, 2924, 1613, 1594, 1484, 1444, 1345, 1164 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{33}F_2N_3O_4S_2$ $[M]^+$: 721.1881, found: 721.1880.

(*E*)-*N*-((1-(3,5-bis(trifluoromethyl)phenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ta):



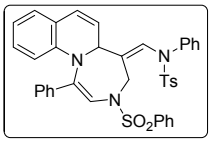
Yellow solid (85%); m.p. 125.4-127.1℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66-7.64 (m, 3H), 7.51 (m, 2H), 7.41 (d, *J* = 8.4 Hz, 2H), 7.27 (m, 1H), 7.24 (m, 1H), 7.21 (d, *J* = 8.0 Hz, 2H), 7.14 (s, 1H), 7.05-7.03 (m, 3H), 6.91-6.89 (m, 2H), 6.74 (dd, *J* = 7.4 Hz, 1.6 Hz, 1H), 6.55 (td, *J* = 7.6 Hz, 1.6 Hz, 1H), 6.47 (td, *J* = 7.4 Hz, 1.0 Hz, 1H), 6.28 (d, *J* = 10.0 Hz, 1H), 6.24 (d, *J* = 1.8 Hz, 1H), 5.77 (d, *J* = 8.0 Hz, 1H), 5.72 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.83 (d, *J* = 5.2 Hz, 1H) 4.42-4.32 (m, 2H), 2.43 (s, 3H), 2.39 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.6, 144.5, 141.9, 139.6, 138.1, 135.4, 133.7, 133.0, 132.2, 131.9, 130.1, 129.7, 129.6, 129.3, 129.1, 129.0, 127.8, 127.6, 127.3, 127.0, 126.9, 126.4, 126.3, 125.5, 124.5, 124.3, 121.8, 121.7, 121.6, 120.8, 120.5, 118.6, 112.2, 58.9, 50.1, 21.62, 21.58; IR (KBr) ν 3064, 2925, 1635, 1595, 1484, 1354, 1276, 1164, 1135 cm^{-1}; HRMS (EI) m/z calcd. for $C_{42}H_{33}F_6N_3O_4S_2$ $[M]^+$: 821.1817, found: 821.1821.

(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-((4-(trifluoromethyl)phenyl)sulfonyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ua):



Light-yellow solid (94%); m.p. 104.5-106.5℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.88 (d, *J* = 8.2 Hz, 2H), 7.63 (d, *J* = 8.4 Hz, 2H), 7.42 (d, *J* = 8.2 Hz, 2H), 7.24 (m, 2H), 7.20-7.16 (m, 5H), 7.07-7.05 (m, 3H), 6.93-6.91 (m, 3H), 6.67 (dd, *J* = 7.2 Hz, 1.6 Hz, 1H), 6.45 (td, *J* = 7.8 Hz, 1.6 Hz, 1H), 6.39 (td, *J* = 7.2 Hz, 1.0 Hz, 1H), 6.31 (d, *J* = 1.6 Hz, 1H), 6.23 (d, *J* = 10.0 Hz, 1H), 5.72 (d, *J* = 8.0 Hz, 1H), 5.64 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.81 (d, *J* = 5.0 Hz, 1H), 4.48-4.45 (m, 1H), 4.39-4.35 (m, 1H), 2.43 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 142.1, 141.9, 139.4, 134.9, 134.5, 133.8, 132.9, 129.7, 129.6, 129.1, 128.8, 128.6, 127.9, 127.8, 127.7, 127.4, 126.9, 126.8, 126.5, 126.4, 126.2, 125.5, 125.0, 121.9, 121.3, 120.1, 118.0, 112.6, 58.8, 50.6, 21.6; IR (KBr) ν 3068, 2925, 1640, 1597, 1490, 1449, 1358, 1321, 1171 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{32}F_3N_3O_4S_2$ $[M]^+$: 739.1786, found: 739.1789.

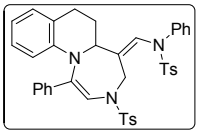
(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-(phenylsulfonyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3va):



Light-yellow solid (83%); m.p. 100.8-102.3℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.79 (d, *J* = 7.4 Hz, 2H), 7.54-7.51 (m, 1H), 7.43-7.40 (m, 4H), 7.23-7.25 (m, 2H), 7.19-7.15 (m, 5H), 7.10-7.08 (m, 3H), 6.96-6.93 (m, 3H), 6.70 (dd, *J* = 7.4 Hz, 1.2 Hz, 1H), 6.58-6.53 (m, 1H), 6.44-6.40 (m, 1H), 6.24 (d, *J* = 10.0 Hz, 1H), 6.22 (d, *J* = 1.6 Hz, 1H), 5.85 (d, *J* = 8.0 Hz, 1H), 5.74 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.86 (d, *J* = 5.2 Hz, 1H), 4.41-4.32 (m, 2H), 2.42 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 142.1, 139.7, 138.6, 135.1, 134.6, 133.9, 133.2, 129.7, 129.4, 129.1, 128.8, 128.6, 128.0, 127.9, 127.6, 127.5, 126.9, 126.82, 126.78, 125.8, 125.3, 125.0,

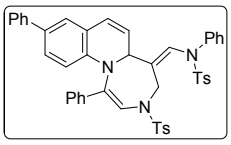
122.5, 121.7, 120.8, 118.1, 113.4, 59.4, 50.5, 21.6; IR (KBr) ν 3065, 2924, 1639, 1595, 1489, 1446, 1347, 1163 cm^{-1}; HRMS (EI) m/z calcd. for $C_{39}H_{33}N_3O_4S_2$ $[M]^+$: 671.1912, found: 671.1910.

(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4,6,7-tetrahydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (4aa):



White solid (96%); m.p. 119.6-121.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 8.2 Hz, 2H), 7.41 (d, *J* = 8.2 Hz, 2H), 7.23 (d, *J* = 8.2 Hz, 2H), 7.20 (d, *J* = 8.4 Hz, 2H), 7.10-7.06 (m, 6H), 6.96-6.92 (m, 4H), 6.81(d, *J* = 7.2 Hz, 1H), 6.76 (s, 1H), 6.57-6.53 (m, 2H), 6.44 (t, *J* = 7.2 Hz, 1H), 5.78 (d, *J* = 8.0 Hz, 1H), 4.23-4.20 (m, 1H), 4.12-4.05 (m, 2H), 2.69-2.62 (m, 1H), 2.60-2.52 (m, 1H), 2.42 (s, 3H), 2.35 (s, 3H), 2.04-2.00 (m, 1H), 1.96-1.88 (m, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.3, 144.0, 143.1, 139.3, 136.2, 135.3, 133.7, 130.9, 129.9, 129.6, 129.5, 129.1, 128.7, 128.4, 128.2, 127.8, 127.7, 127.3, 127.1, 126.9, 126.7, 124.9, 122.7, 121.9, 117.3, 114.7, 58.9, 49.0, 27.0, 25.8, 21.6, 21.5; IR (KBr) ν 3060, 2925, 1639, 1600, 1489, 1349, 1165 cm^{-1}; HRMS (EI) m/z calcd. for $C_{40}H_{37}N_3O_4S_2$ [M+]: 687.2225, found: 687.2226.

(*E*)-*N*-((1,9-diphenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (5ea):



Off-white solid (56%); m.p. 207.8-209.2℃; ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 (d, *J* = 8.4 Hz, 2H), 7.43 (d, *J* = 8.2 Hz, 2H), 7.38-7.31 (m, 5H), 7.23-7.22 (m, 2H), 7.21-7.18 (m, 5H), 7.15 (d, *J* = 8.2 Hz, 2H), 7.08-7.07 (m, 3H), 6.99 (s, 1H), 6.95-6.92 (m, 3H), 6.76 (dd, *J* = 8.2 Hz, 2.0 Hz, 1H), 6.31 (d, *J* = 9.8 Hz, 1H), 6.27 (d, *J* = 1.6 Hz, 1H), 5.89 (d, *J* = 8.4 Hz, 1H), 5.74 (dd, *J* = 9.8 Hz, 5.2 Hz, 1H), 4.89 (d, *J* = 5.0 Hz, 1H), 4.44-4.35 (m, 2H), 2.43 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 144.4, 144.2, 142.0, 140.7, 139.6, 135.6, 135.1, 133.9, 133.8, 130.6, 129.9, 129.7, 129.1, 128.7, 128.6, 127.9, 127.7, 127.6, 127.4, 127.3, 126.95, 126.92, 126.2, 126.0, 125.9, 125.4, 125.3, 124.9, 123.0, 122.0, 120.6, 113.3, 59.3, 50.2, 21.6, 21.4; IR (KBr) ν 3059, 2983, 1650, 1560, 1456, 1341, 1162 cm^{-1}; HRMS (EI) m/z calcd. for $C_{46}H_{39}N_3O_4S_2$ [M+]: 761.2382, found: 761.2379.

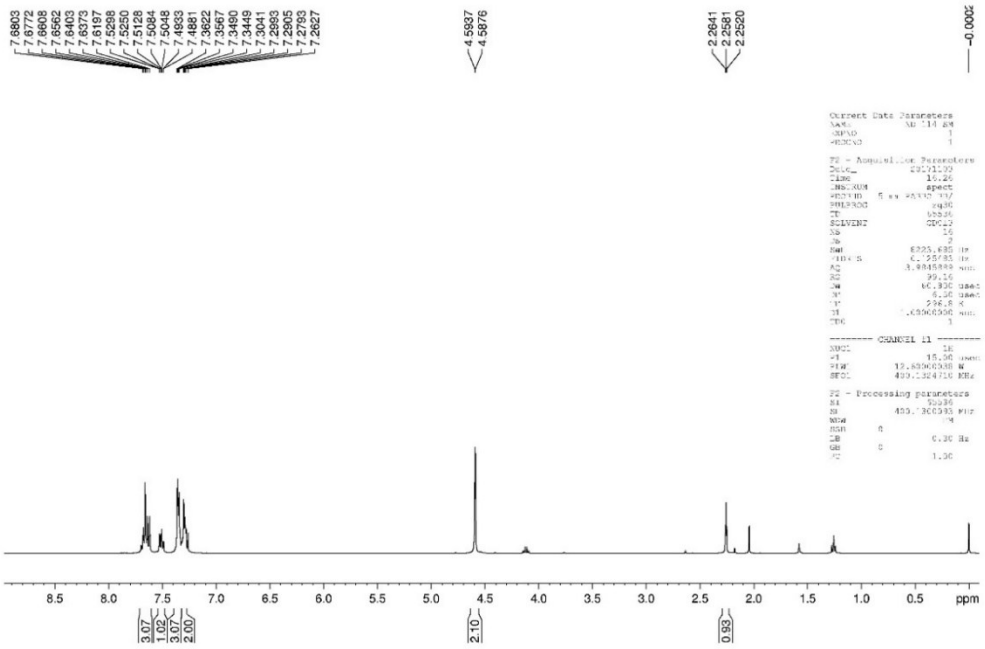
V. References

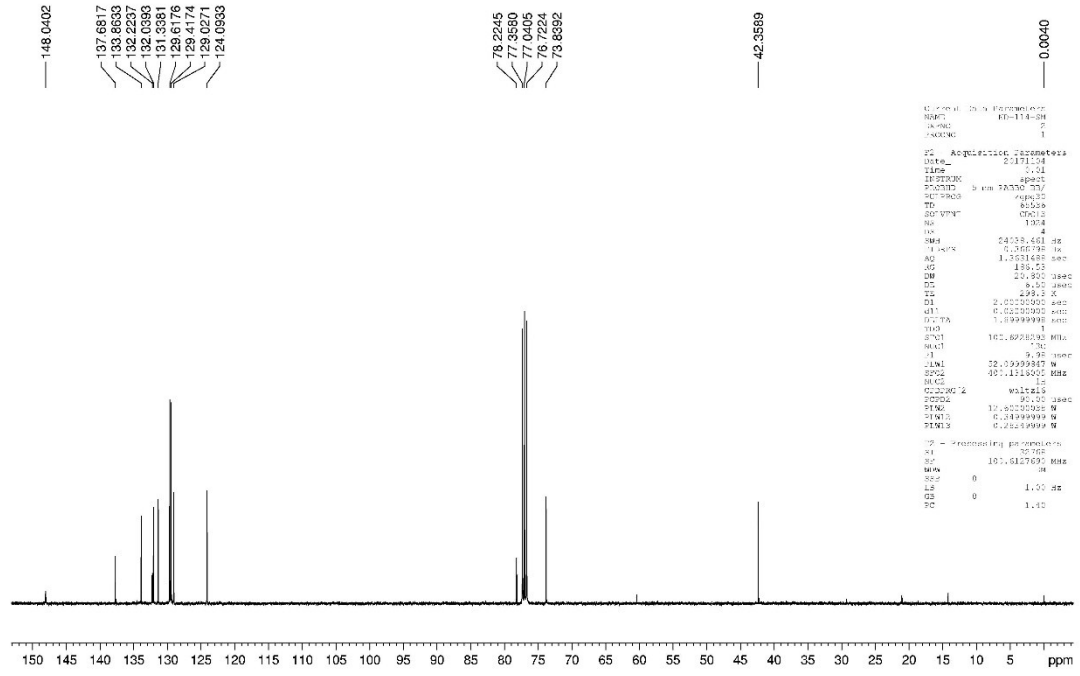
S1. (a) L.-L. Wei, J. A. Mulder, H. Xiong, C. A. Zificsak, C. J. Douglas and R. P. Hsung, *Tetrahedron* 2001, **57**, 459; (b) A. Ballesteros, P. Morán-Poladura and J. M. González, *Chem. Commun.*, 2016, **52**, 2905; (c) H.-H. Li, X.-X. Li, Z.-G. Zhao, X. Yuan and C.-Y. Sun, *Org. Biomol. Chem.*, 2017, **15**, 4005.

S2. J. Shin, J. Lee, D. Ko, N. De and E. J. Yoo, *Org. Lett.* 2017, **19**, 2901.

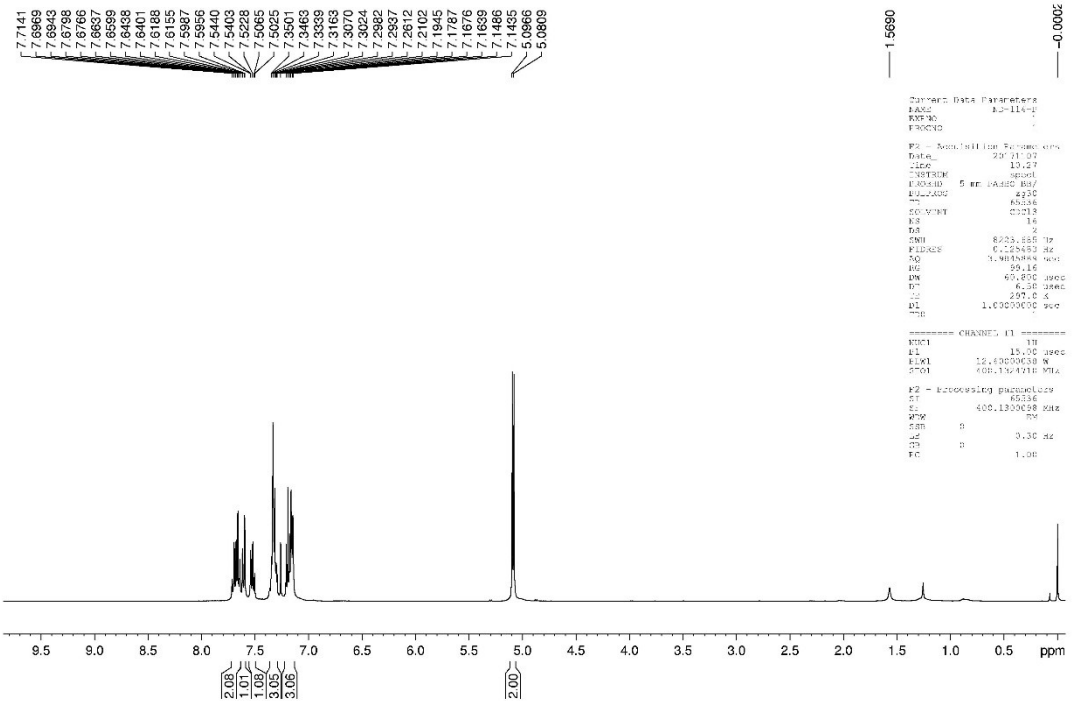
VI. Copies of Spectral Data of Compounds Obtained in this Study

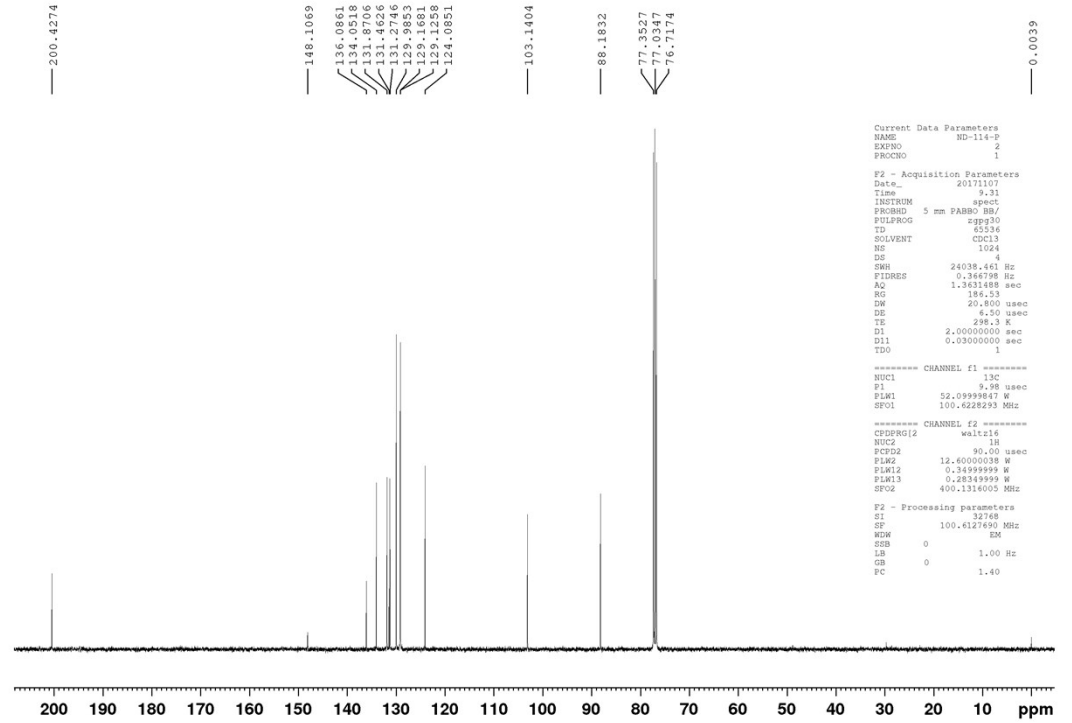
2-nitro-*N*-phenyl-*N*-(prop-2-yn-1-yl)benzenesulfonamide:



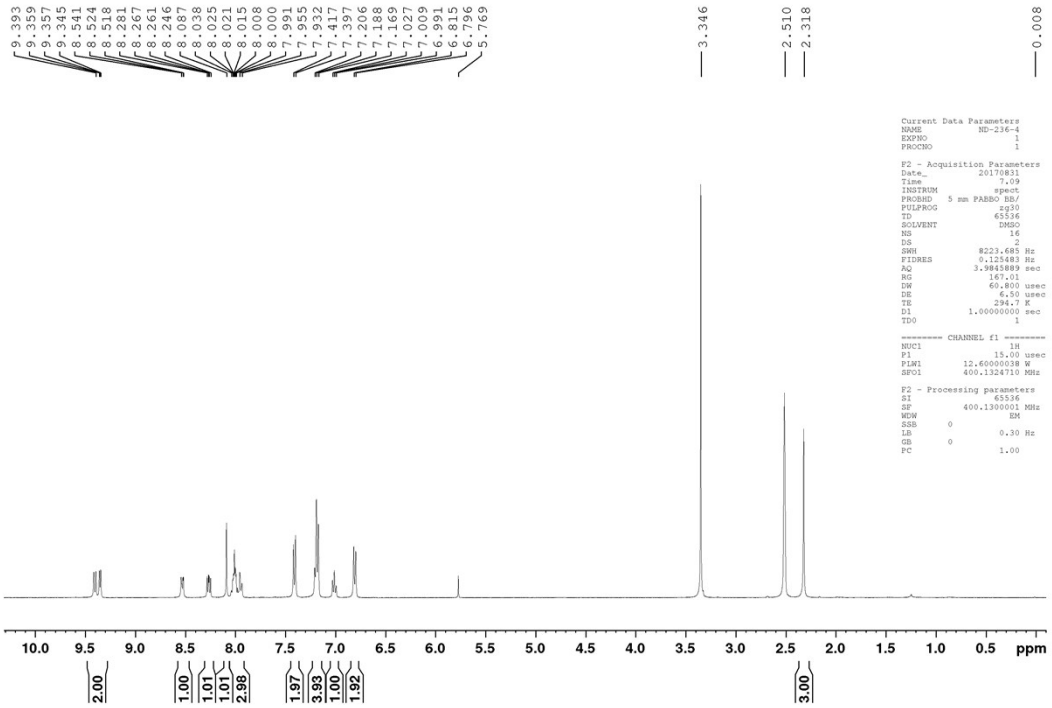


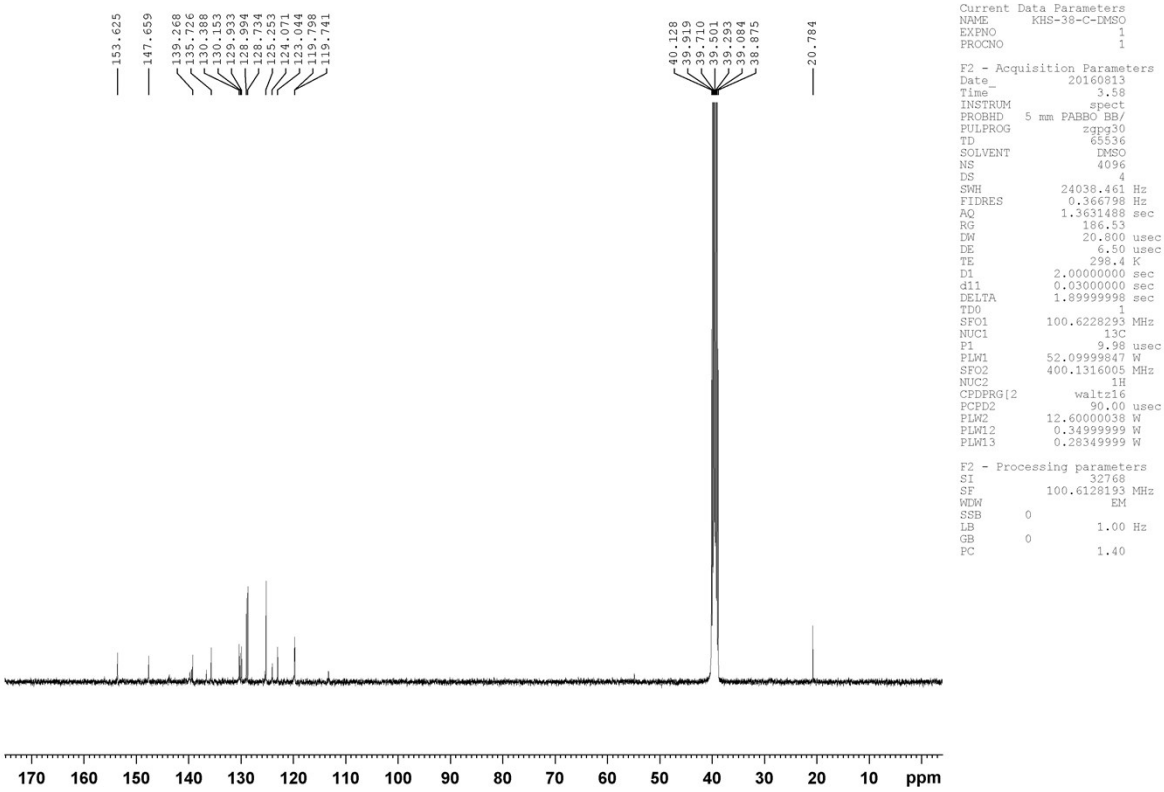
2-nitro-*N*-phenyl-*N*-(propa-1,2-dien-1-yl)benzenesulfonamide (2h):



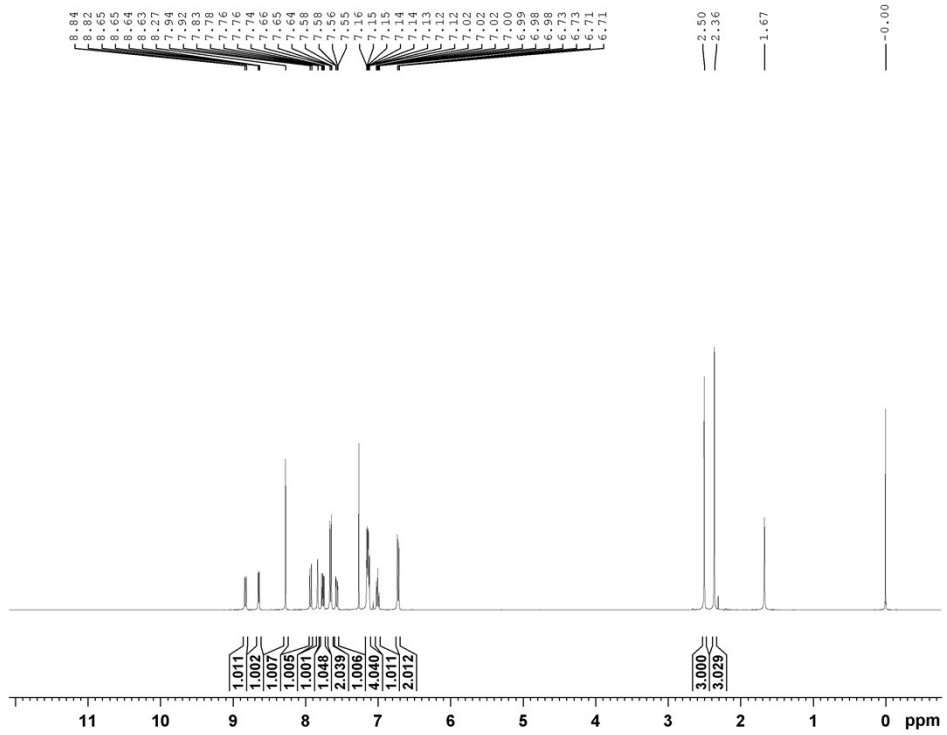


(Z)-(2-phenyl-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1a):





(*Z*)-(2-(6-methylquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1b):

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Current Data Parameters
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EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
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Time                  15.13
INSTRUM               spect
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PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                   140.47
DW                   60.800 usec
DE                    6.50 usec
TE                   297.4 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300093 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
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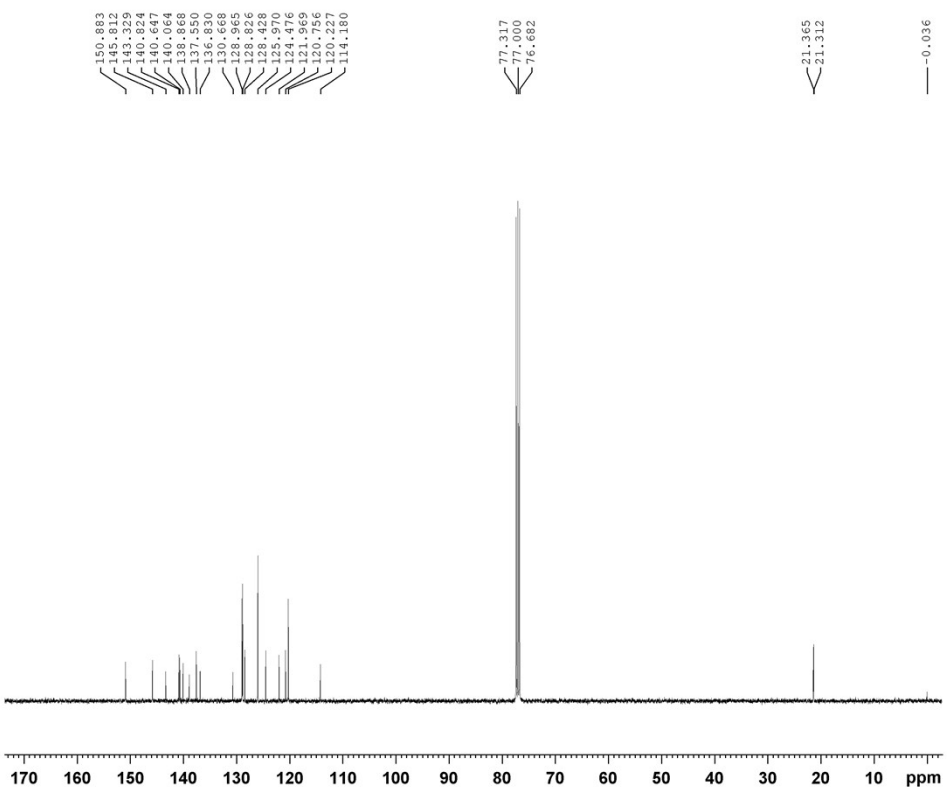


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Current Data Parameters
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EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
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Time                  19.02
INSTRUM               spect
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PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                   186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   298.9 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1
SFO1            100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                    32768
SF              100.6127723 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
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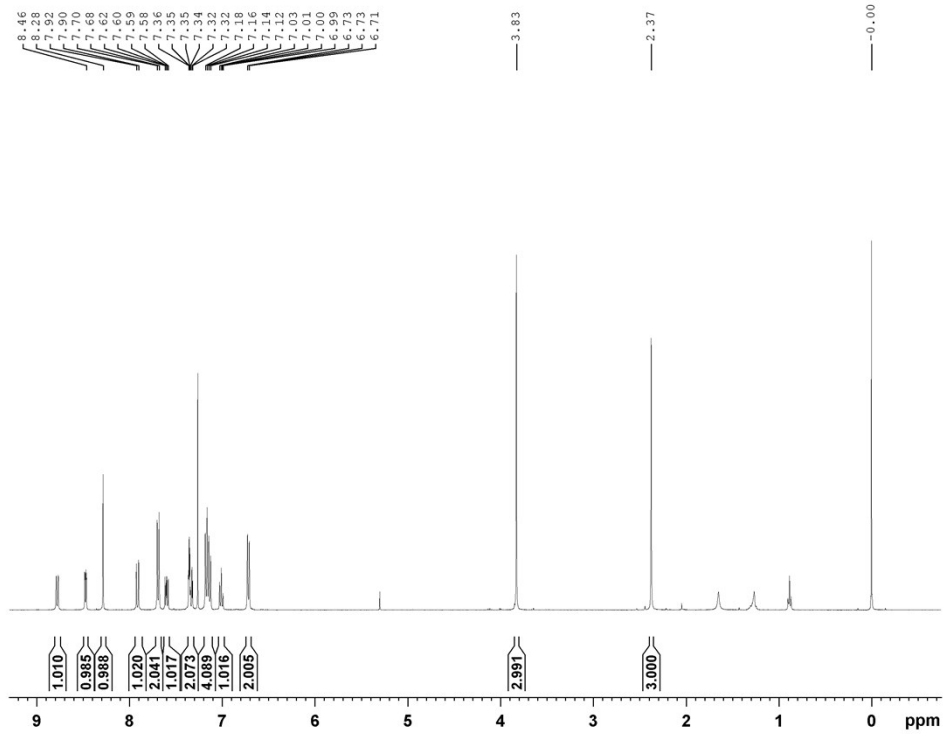
(Z)-(2-(6-methoxyquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1c):

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Current Data Parameters
NAME                  ND-119-P
EXPNO                        1
PROCNO                       1

F2 - Acquisition Parameters
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Time                    19.47
INSTRUM                 spect
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PULPROG                 zg30
TD                     65536
SOLVENT                CDC13
NS                        16
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     140.47
DW                     60.800 usec
DE                      6.50 usec
TE                     296.4 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1               12.60000038 W
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                         65536
SF                400.1300095 MHz
WDW                           EM
SSB                        0
LB                      0.30 Hz
GB                         0
PC                      1.00
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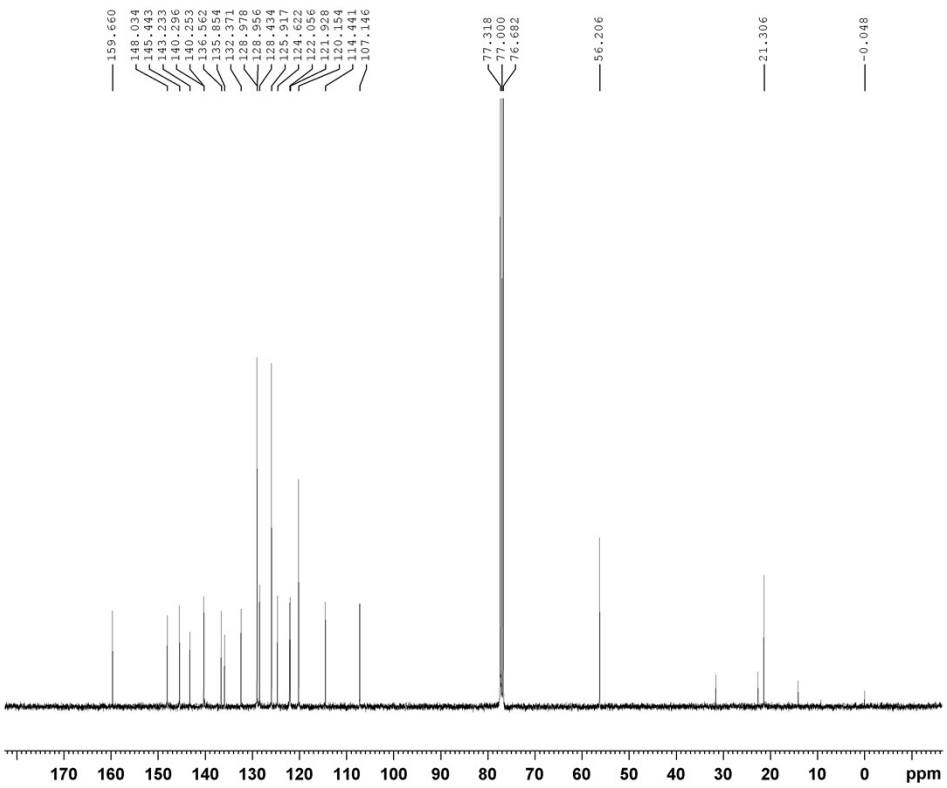


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Current Data Parameters
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EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
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INSTRUM                 spect
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PULPROG                 zgpg30
TD                     65536
SOLVENT                CDC13
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                     20.800 usec
DE                      6.50 usec
TE                     297.8 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                          1
SFO1              100.6228293 MHz
NUC1                       13C
P1                       9.98 usec
PLW1               52.09999847 W
SFO2              400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                   90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

F2 - Processing parameters
SI                         32768
SF                100.6127746 MHz
WDW                           EM
SSB                        0
LB                      1.00 Hz
GB                         0
PC                      1.40
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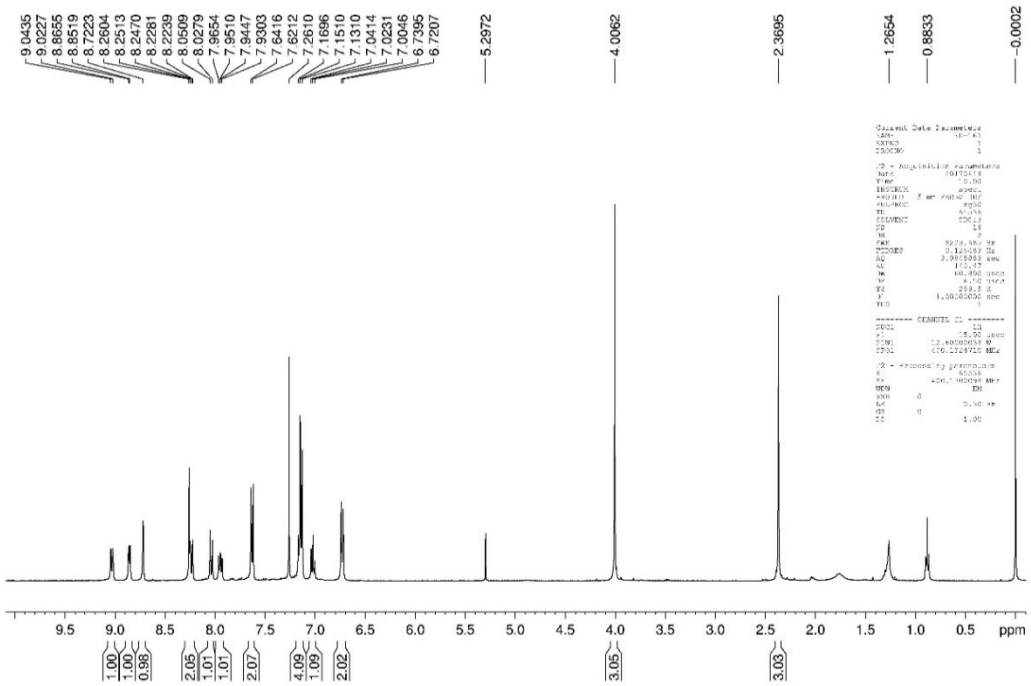
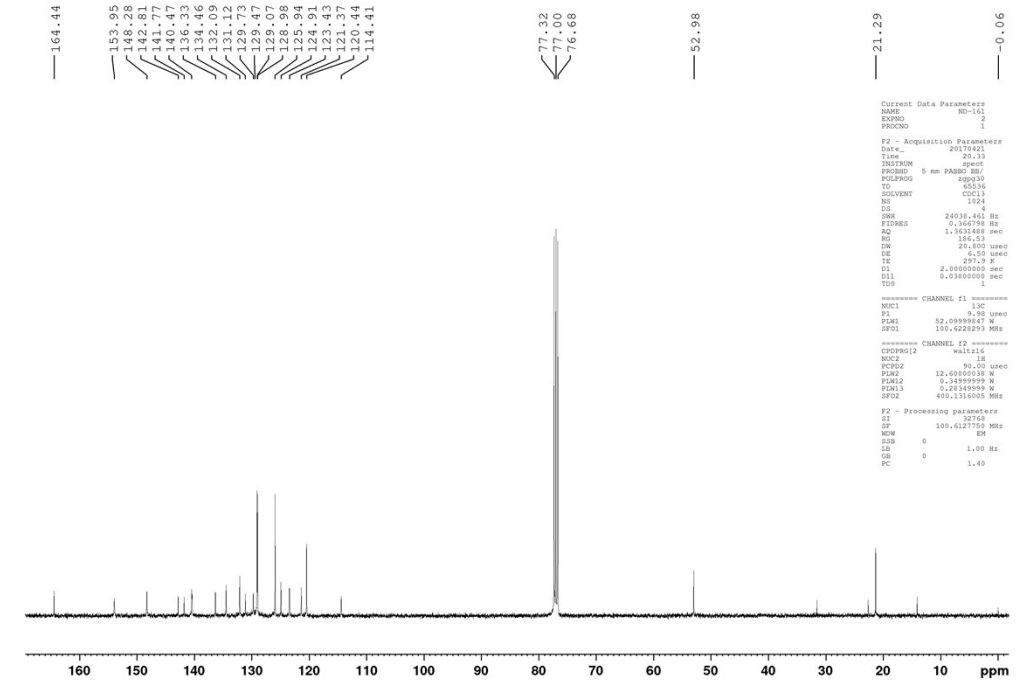
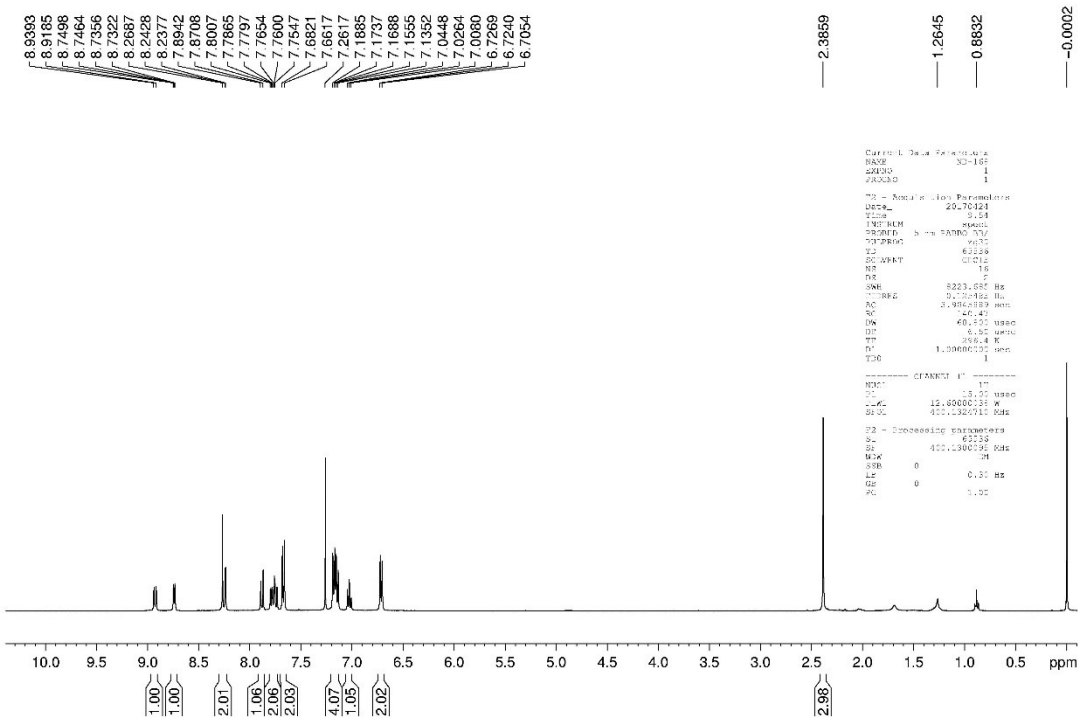
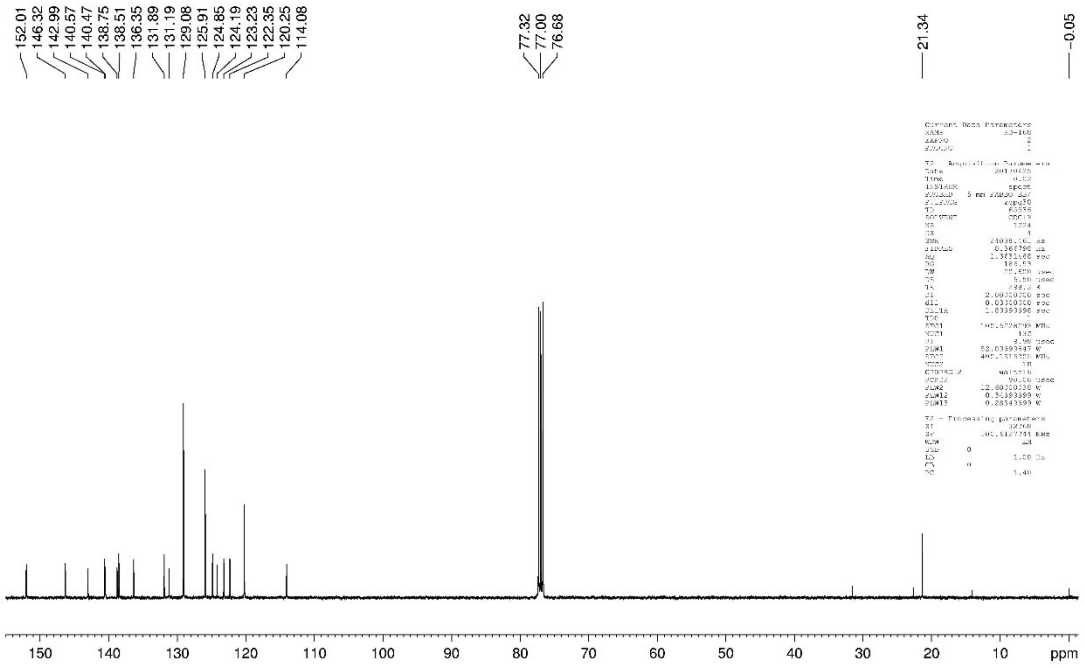
(*Z*)-(2-(6-(methoxycarbonyl)quinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1d):



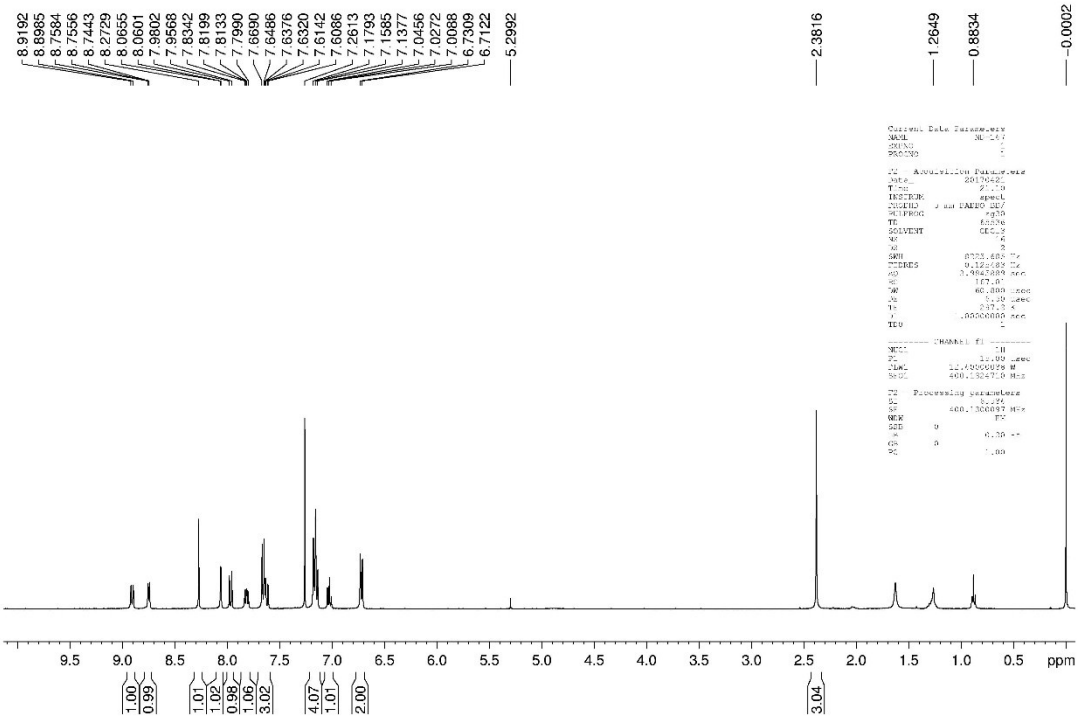


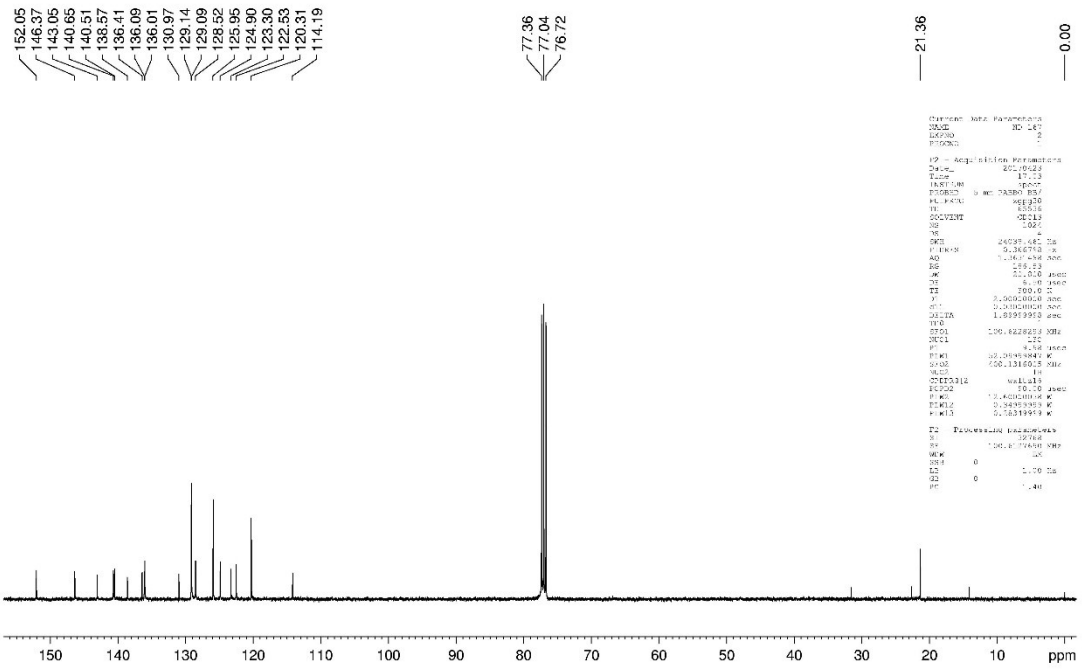
(*Z*)-(2-(6-bromoquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1e):



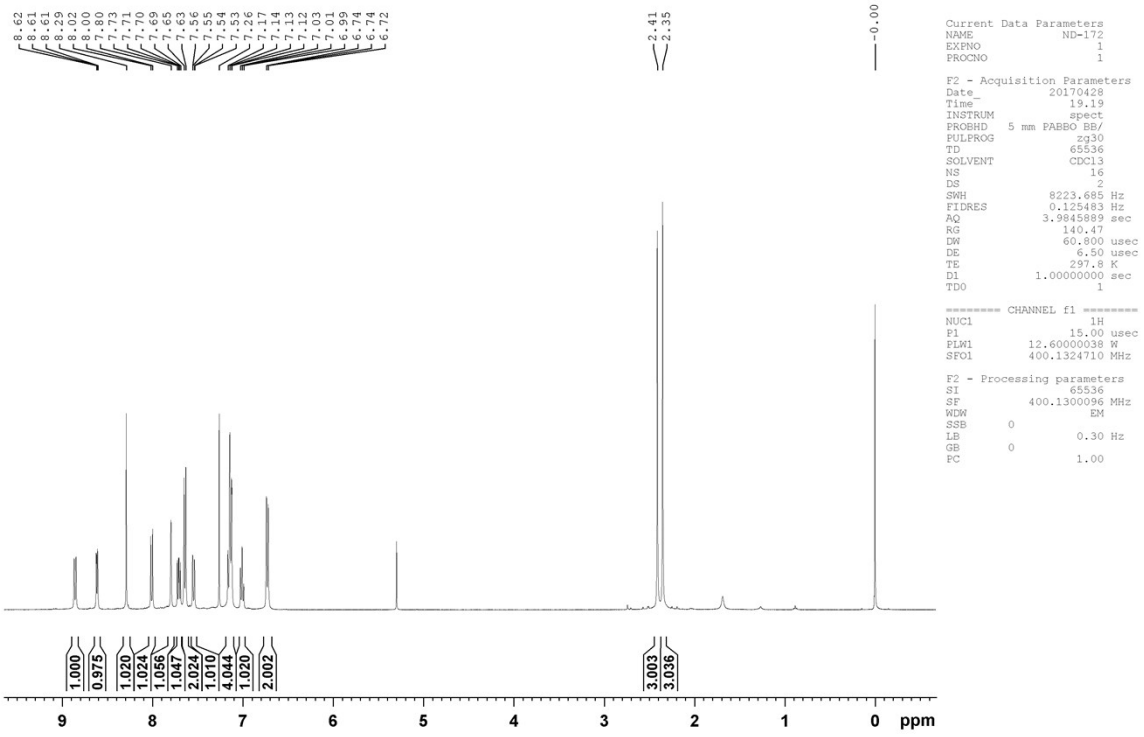


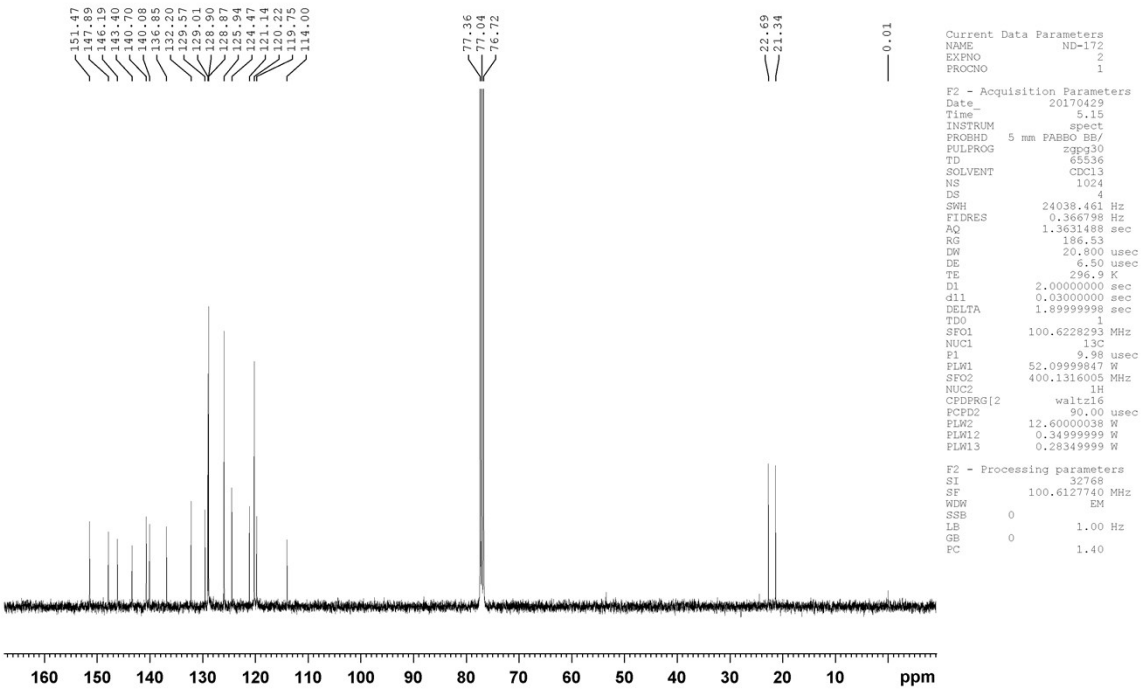
(*Z*)-(2-(6-chloroquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1f):



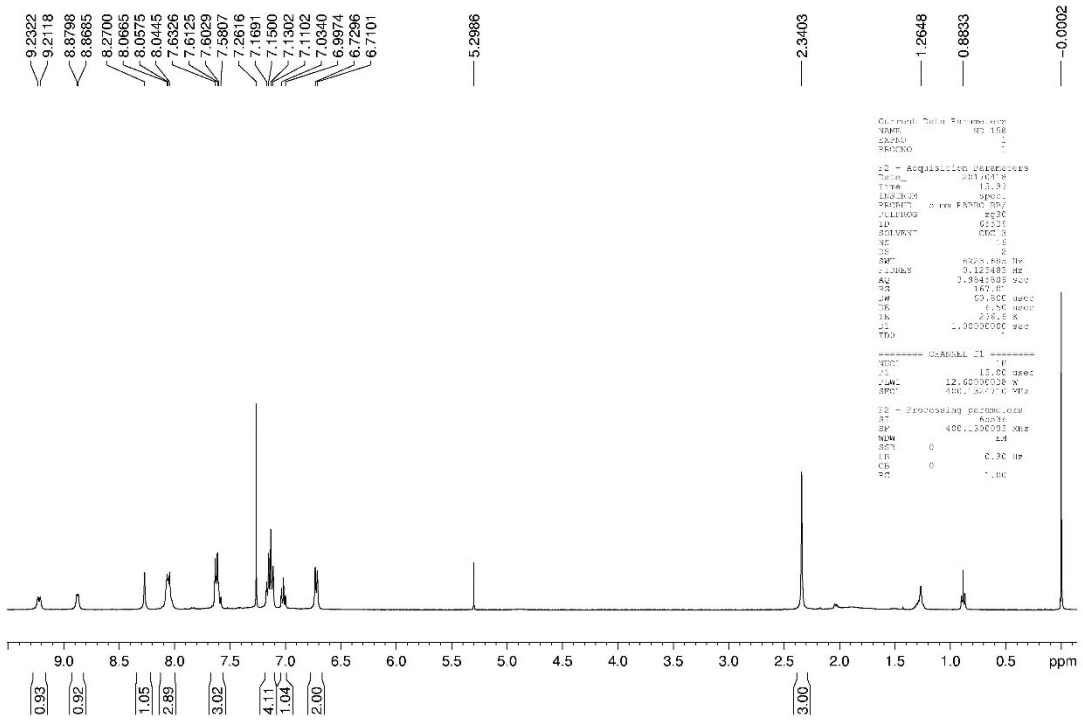


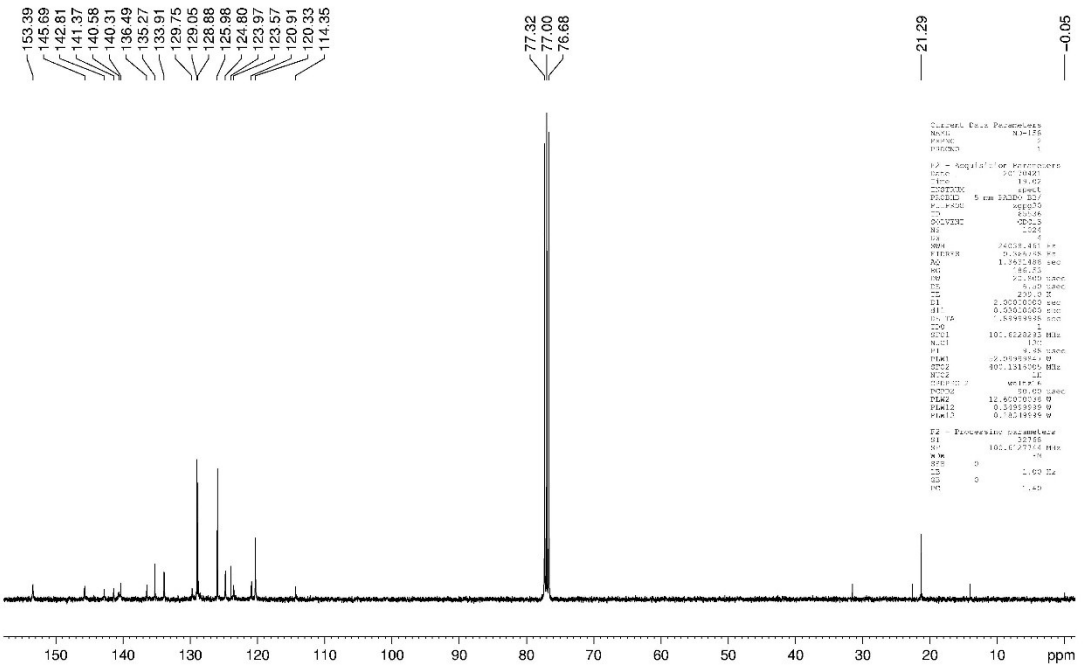
(Z)-(2-(7-methylquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1g):



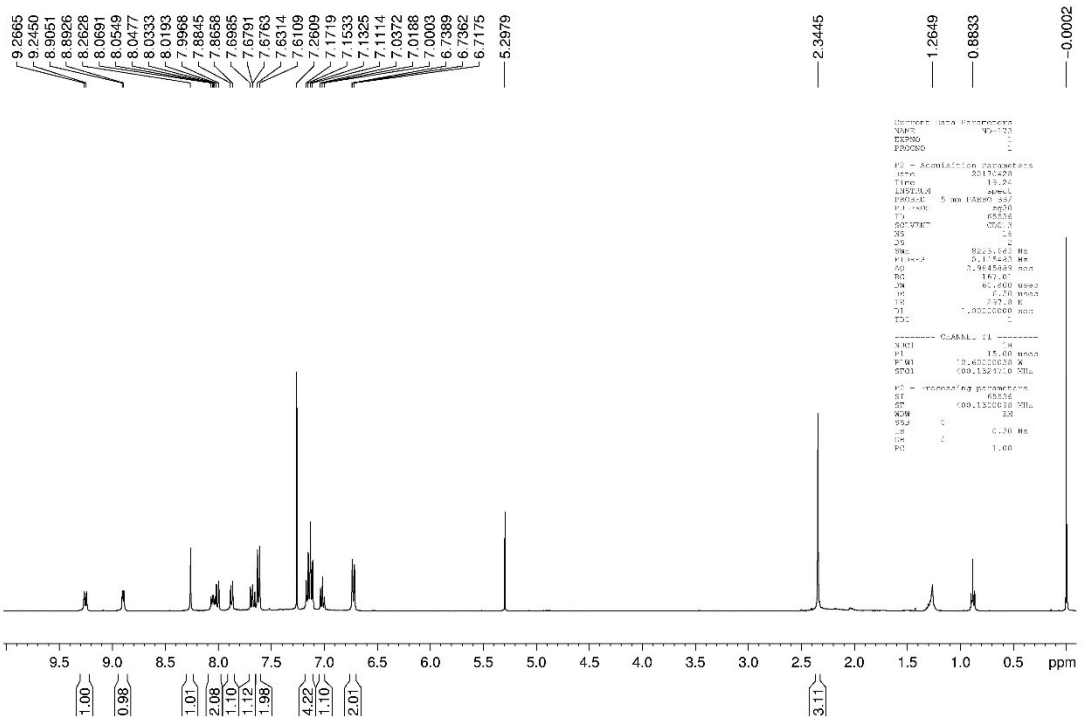


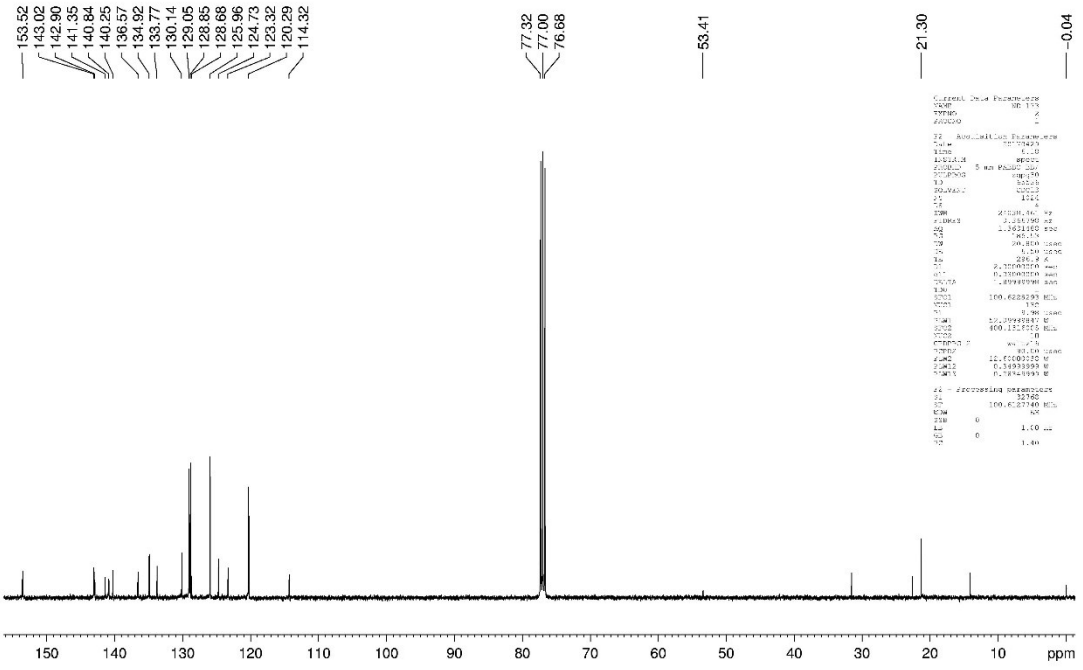
(*Z*)-(2-(5-bromoquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1h):



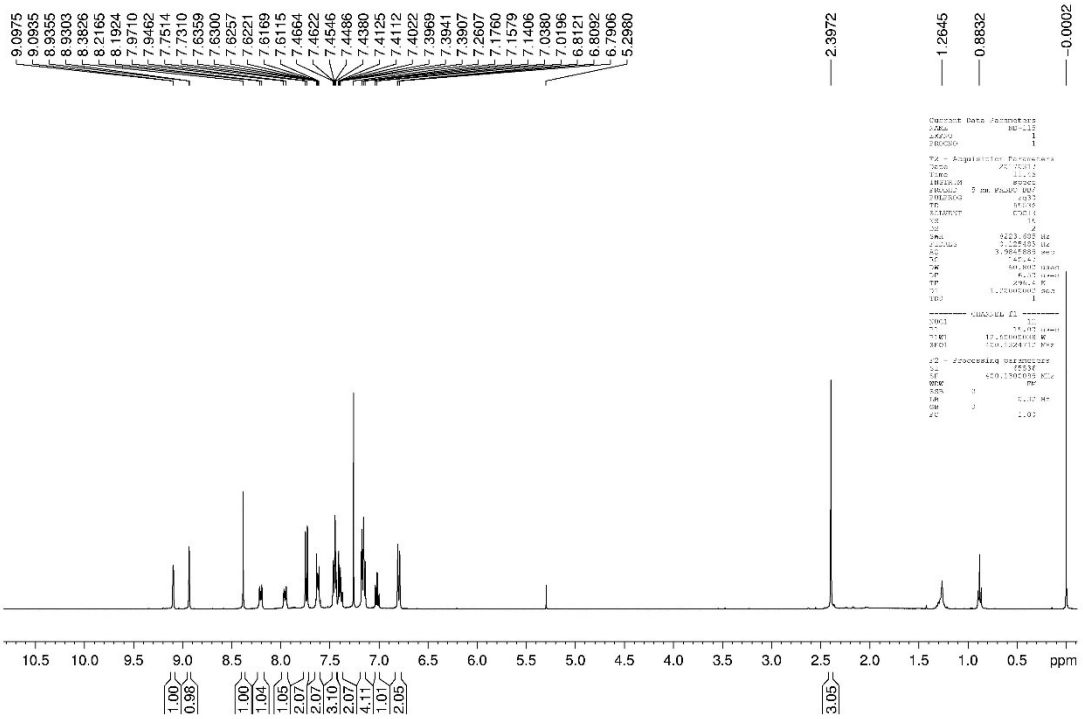


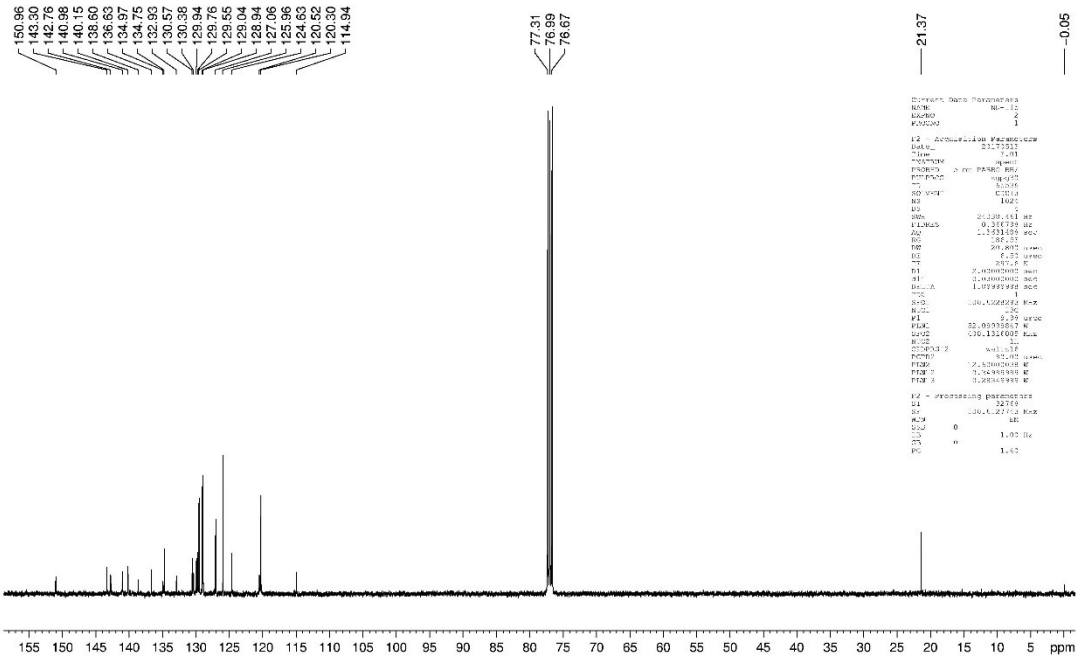
(*Z*)-(2-(5-chloroquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1i):



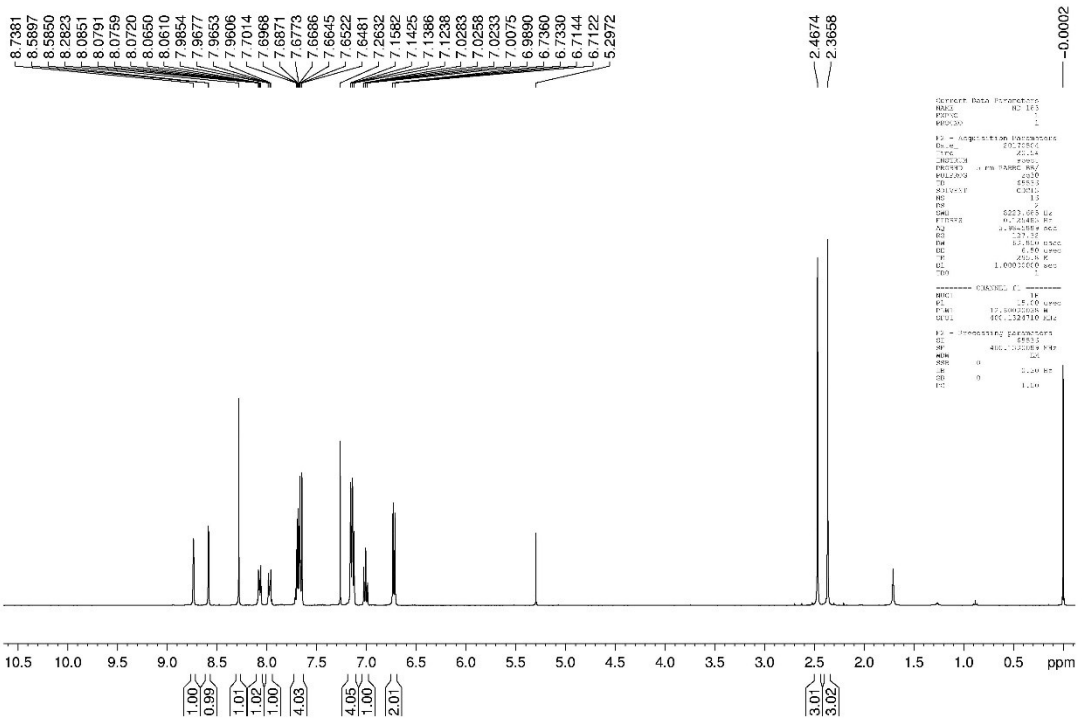


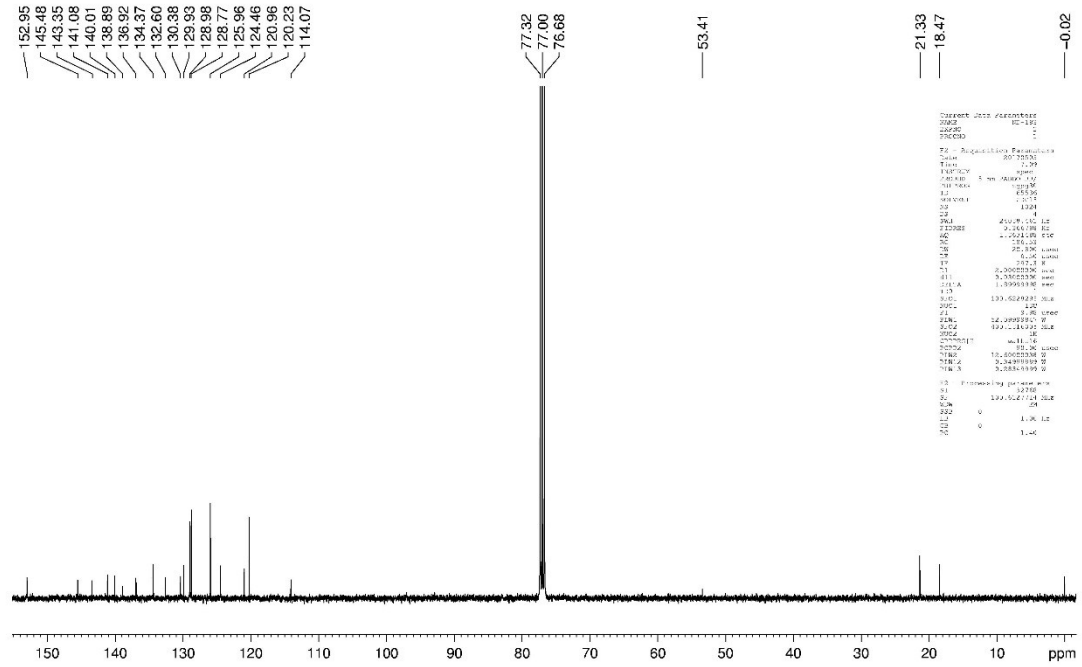
(*Z*)-(2-phenyl-2-(3-phenylquinolin-1-ium-1-yl)vinyl)(tosyl)amide (1j):



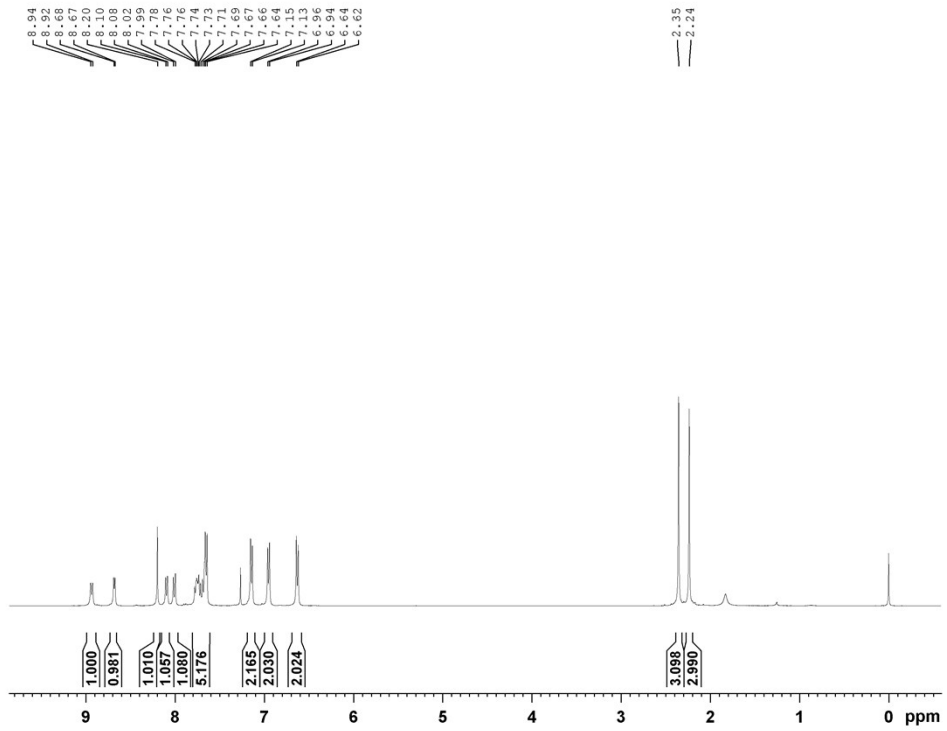


(*Z*)-(2-(3-methylquinolin-1-ium-1-yl)-2-phenylvinyl)(tosyl)amide (1k):





(*Z*)-(2-(quinolin-1-ium-1-yl)-2-(p-tolyl)vinyl)(tosyl)amide (1l):

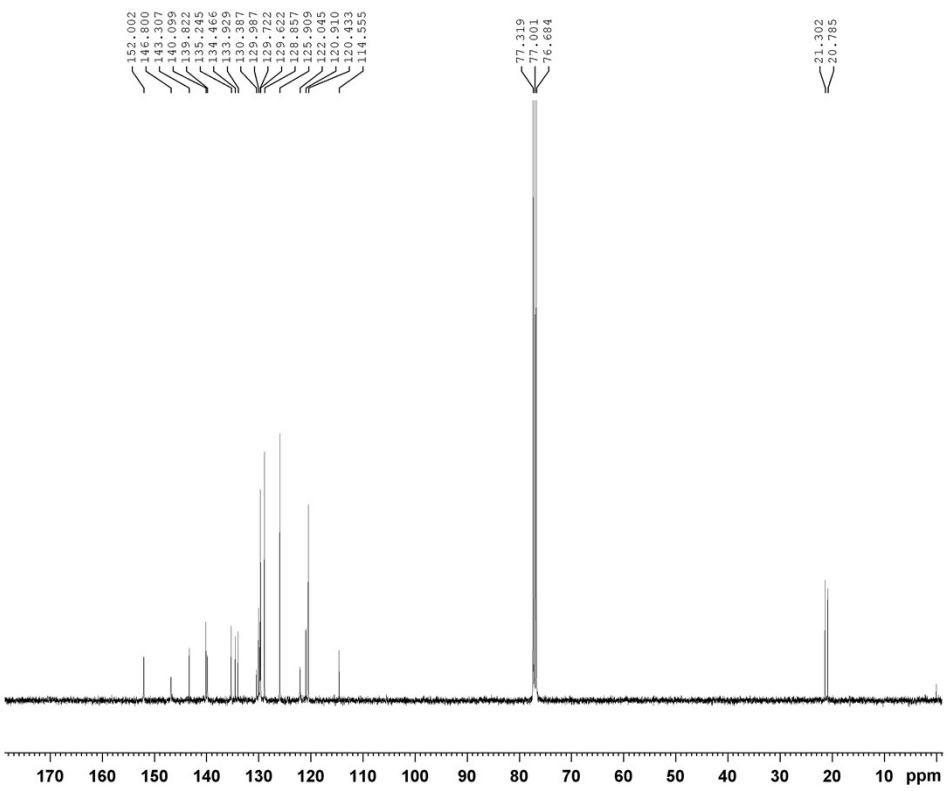



```
Current Data Parameters
NAME                  KDW-401-C
EXPNO                         2
PROCNO                        1

F2 - Acquisition Parameters
Date_               20160720
Time                   21.59
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                     99.16
DW                    60.800 usec
DE                     6.50 usec
TE                    296.0 K
D1                 1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF                400.1300077 MHz
WDW                      EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

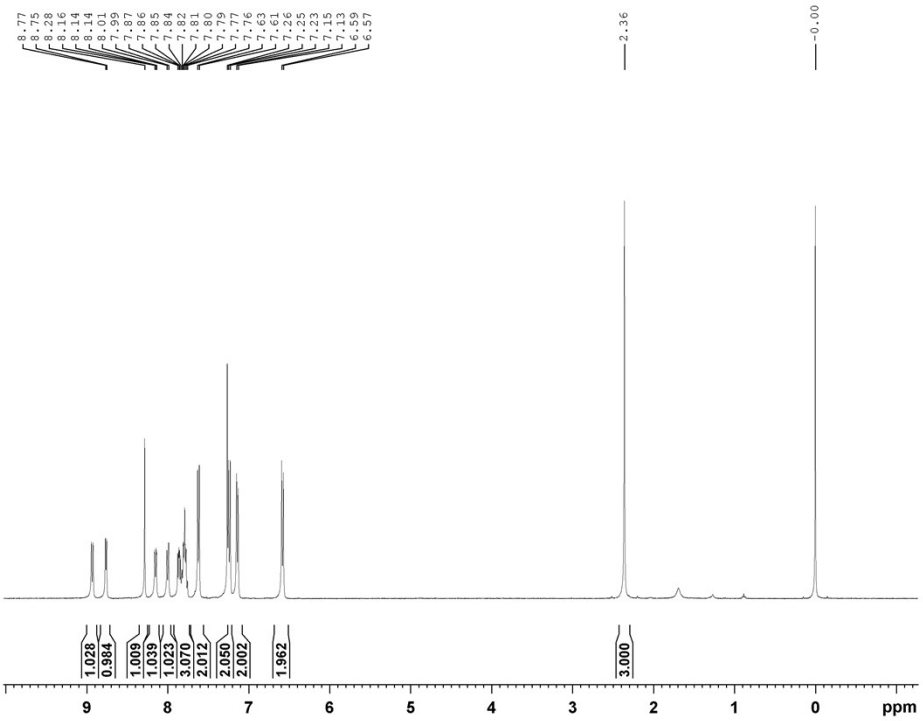



```
Current Data Parameters
NAME                  KDW-401-C
EXPNO                         3
PROCNO                        1

F2 - Acquisition Parameters
Date_               20160721
Time                    5.14
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    296.3 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                       1
SFO1             100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1              52.09999847 W
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

F2 - Processing parameters
SI                    32768
SF                100.6127746 MHz
WDW                      EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

(*Z*)-(2-(4-bromophenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1m):

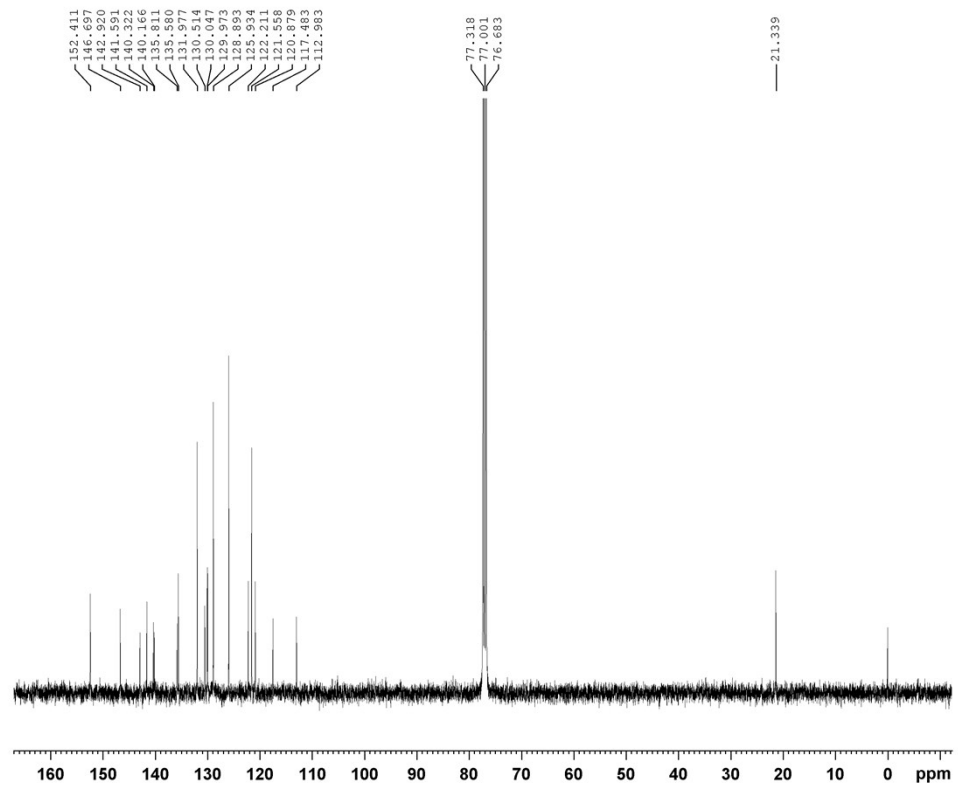



```
Current Data Parameters
NAME          LJY-1385-C
EXPNO                  2
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180112
Time              17.28
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG            zg30
TD                65536
SOLVENT           CDCl3
NS                   16
DS                    2
SWH            8223.685 Hz
FIDRES        0.125483 Hz
AQ             3.9845889 sec
RG                140.47
DW                60.800 usec
DE                 6.50 usec
TE                0 K
D1             1.00000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                  1H
P1                15.00 usec
PLW1        12.60000038 W
SFO1        400.1324710 MHz

F2 - Processing parameters
SI                65536
SF          400.1300091 MHz
WDW                  EM
SSB               0
LB                0.30 Hz
GB                0
PC                1.00
```

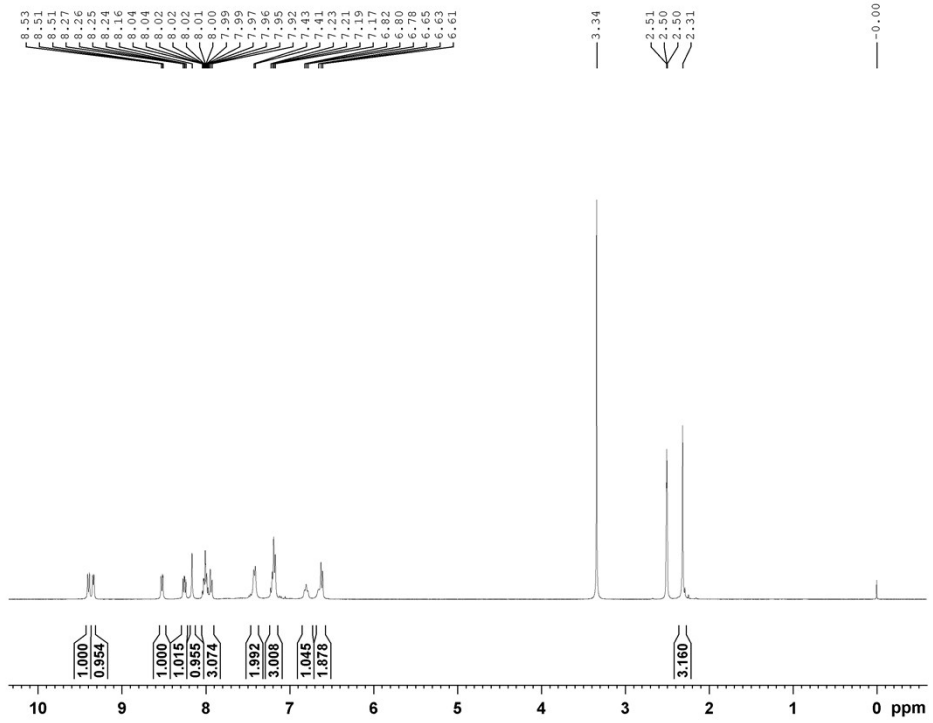



```
Current Data Parameters
NAME          LJY-1385-C
EXPNO                  4
PROCNO                 1

F2 - Acquisition Parameters
Date_           20180113
Time              1.01
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 1024
DS                    4
SWH           24038.461 Hz
FIDRES        0.366798 Hz
AQ             1.3631488 sec
RG                186.53
DW                20.800 usec
DE                 6.50 usec
TE                619.1 K
D1             2.00000000 sec
d11            0.03000000 sec
DELTA          1.89999998 sec
TD0                   1
SFO1        100.6228293 MHz
NUC1                 13C
P1                 9.98 usec
PLW1        52.09999847 W
SFO2        400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2             90.00 usec
PLW2        12.60000038 W
PLW12        0.34999999 W
PLW13        0.28349999 W

F2 - Processing parameters
SI                32768
SF          100.6127721 MHz
WDW                  EM
SSB               0
LB                1.00 Hz
GB                0
PC                1.40
```

(*Z*)-(2-(3-fluorophenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1n):

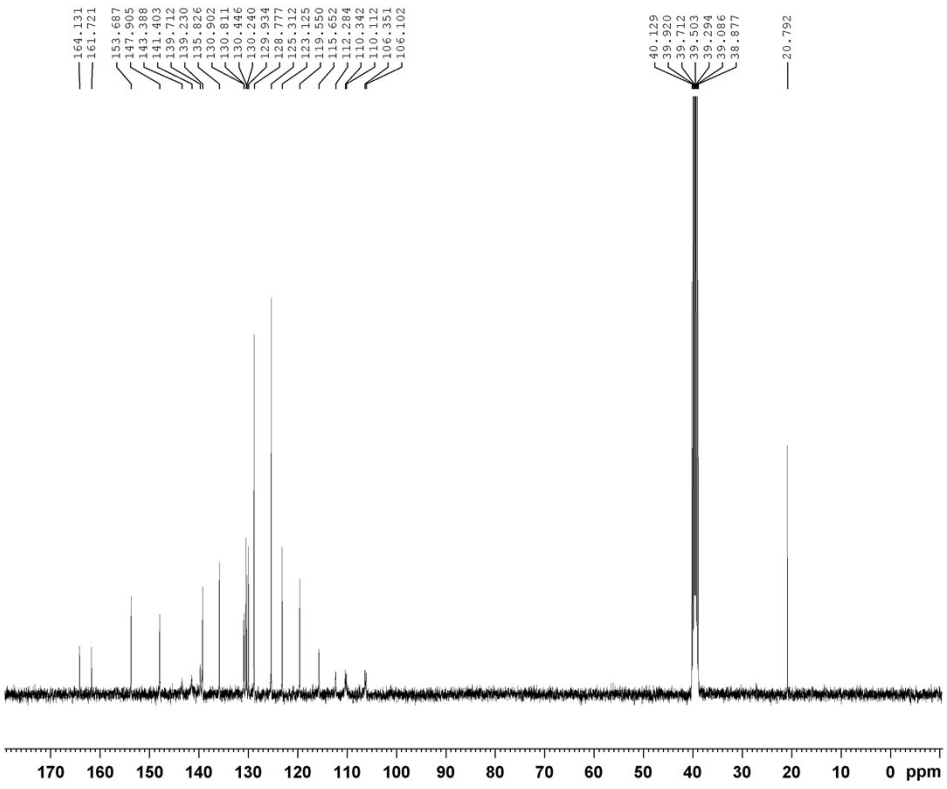



```
Current Data Parameters
NAME                  ND-93
EXPNO                     4
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170511
Time                 20.23
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT              DMSO
NS                     16
DS                      2
SWH              8223.685 Hz
FIDRES           0.125483 Hz
AQ               3.9845889 sec
RG                  127.32
DW                 60.800 usec
DE                  6.50 usec
TE                 295.8 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                   1H
P1                  15.00 usec
PLW1          12.60000038 W
SFO1         400.1324710 MHz

F2 - Processing parameters
SI                  65536
SF            400.1300032 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

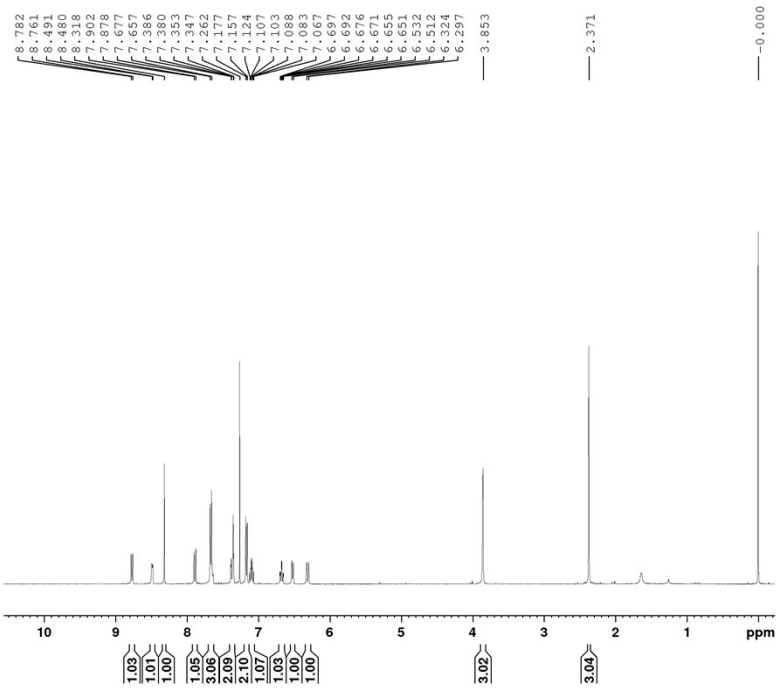



```
Current Data Parameters
NAME                  ND-93
EXPNO                     6
PROCNO                    1

F2 - Acquisition Parameters
Date_              20170513
Time                 13.09
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG           zgpg30
TD                  65536
SOLVENT              DMSO
NS                   1024
DS                      4
SWH             24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                  186.53
DW                 20.800 usec
DE                  6.50 usec
TE                 297.9 K
D1              2.00000000 sec
d11             0.03000000 sec
DELTA           1.89999998 sec
TD0                     1
SFO1         100.6228293 MHz
NUC1                   13C
P1                   9.98 usec
PLW1          52.09999847 W
SFO2         400.1316005 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               90.00 usec
PLW2          12.60000038 W
PLW12          0.34999999 W
PLW13          0.28349999 W

F2 - Processing parameters
SI                  32768
SF           100.6128193 MHz
WDW                    EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```

(*Z*)-(2-(3-fluorophenyl)-2-(6-methoxyquinolin-1-ium-1-yl)vinyl)(tosyl)amide (1o):

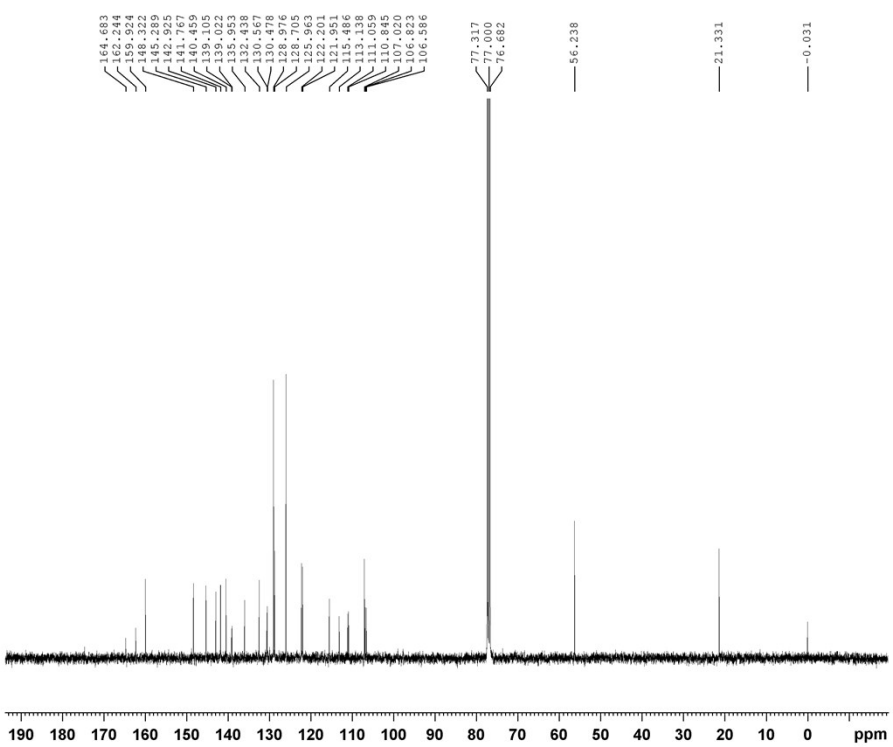



```
Current Data Parameters
NAME                  ND-305
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180111
Time                  17.18
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    140.47
DW                   60.800 usec
DE                    6.50 usec
TE                   296.7 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                    15.00 usec
PLW1           12.60000038 W
SFO1           400.1324710 MHz

F2 - Processing parameters
SI                    65536
SF               400.1300093 MHz
WDW                      EM
SSB          0
LB                    0.30 Hz
GB           0
PC                    1.00
```

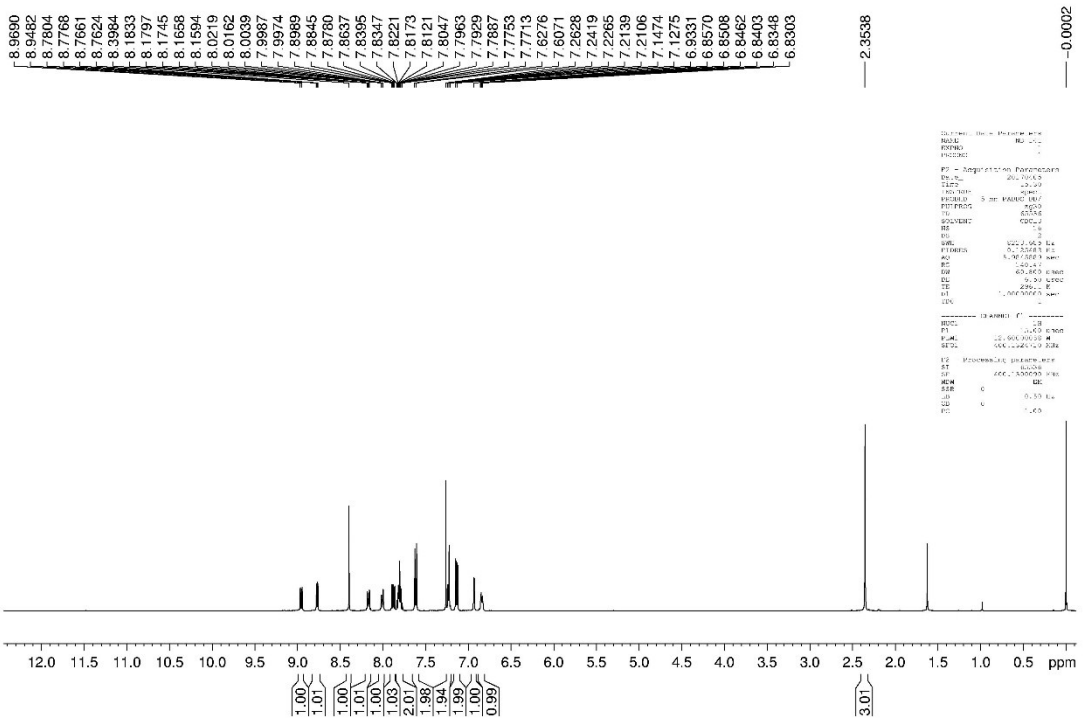


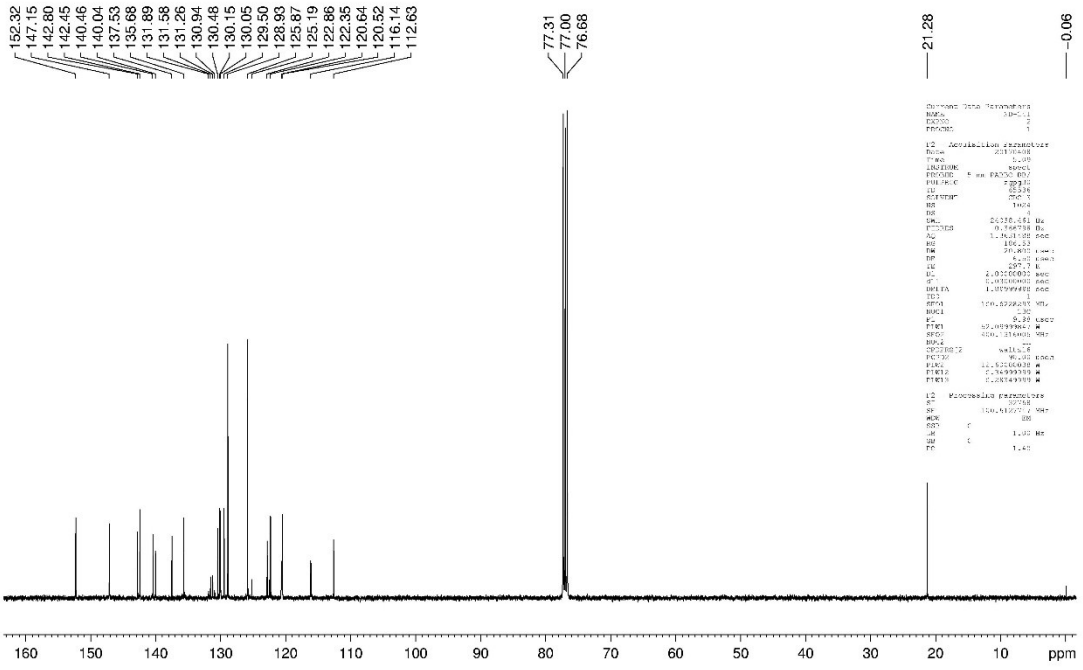

```
Current Data Parameters
NAME                  ND-305
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20180112
Time                   2.02
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   298.2 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1           100.6228293 MHz
NUC1                     13C
P1                    9.98 usec
PLW1           52.09999847 W
SFO2           400.1316005 MHz
NUC2                      1H
CPDPRG[2             waltz16
PCPD2                90.00 usec
PLW2           12.60000038 W
PLW12           0.34999999 W
PLW13           0.28349999 W

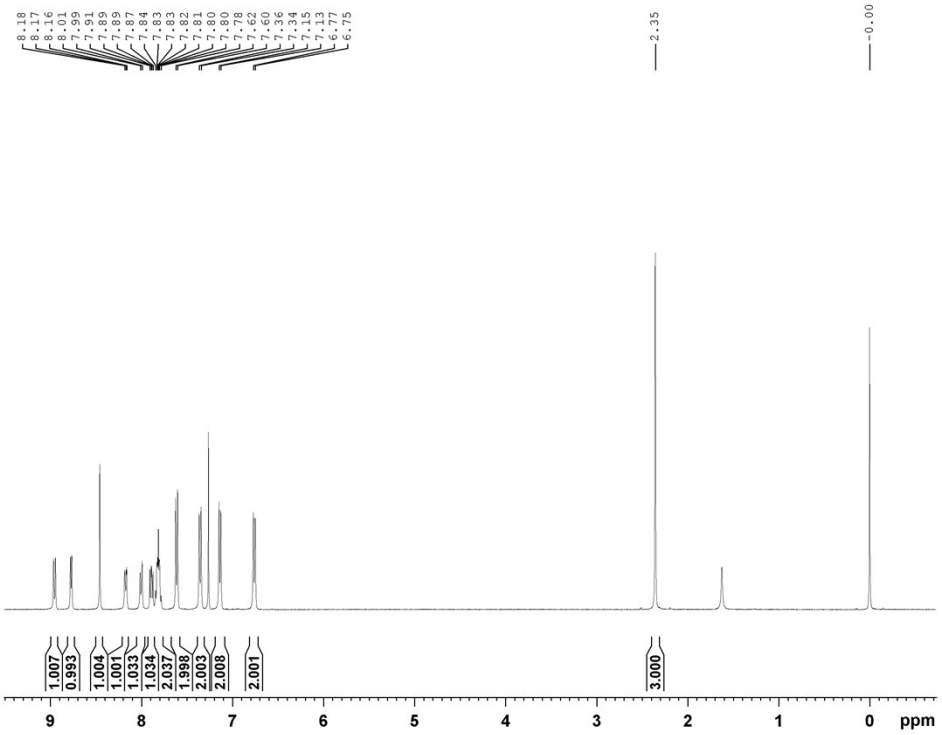
F2 - Processing parameters
SI                    32768
SF               100.6127721 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

(*Z*)-(2-(quinolin-1-ium-1-yl)-2-(3-(trifluoromethyl)phenyl)vinyl)(tosyl)amide (1p):





(*Z*)-(2-(quinolin-1-ium-1-yl)-2-(4-(trifluoromethyl)phenyl)vinyl)(tosyl)amide (1q):

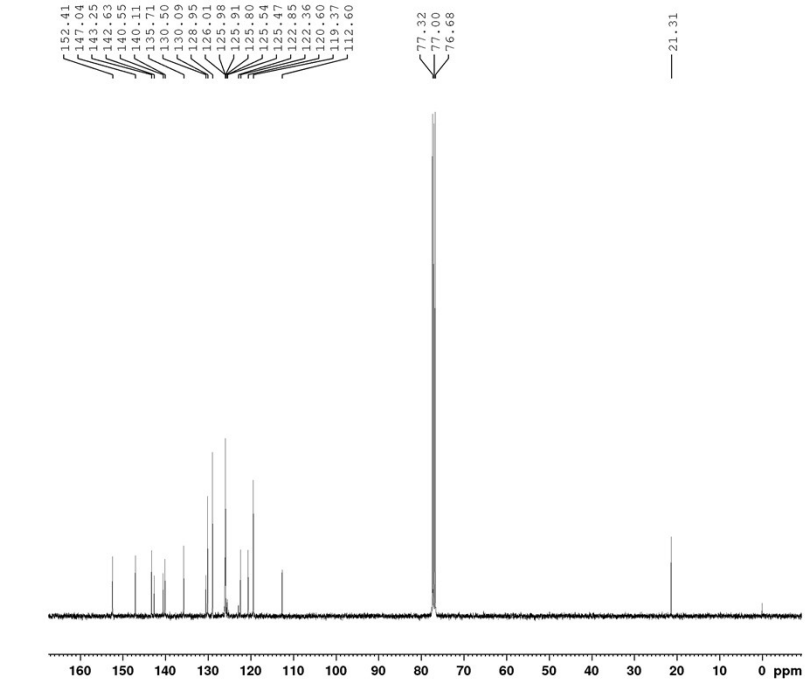



```
Current Data Parameters
NAME                  ND-187
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170526
Time                  16.12
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    167.01
DW                   60.800 usec
DE                    6.50 usec
TE                   296.6 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300094 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```



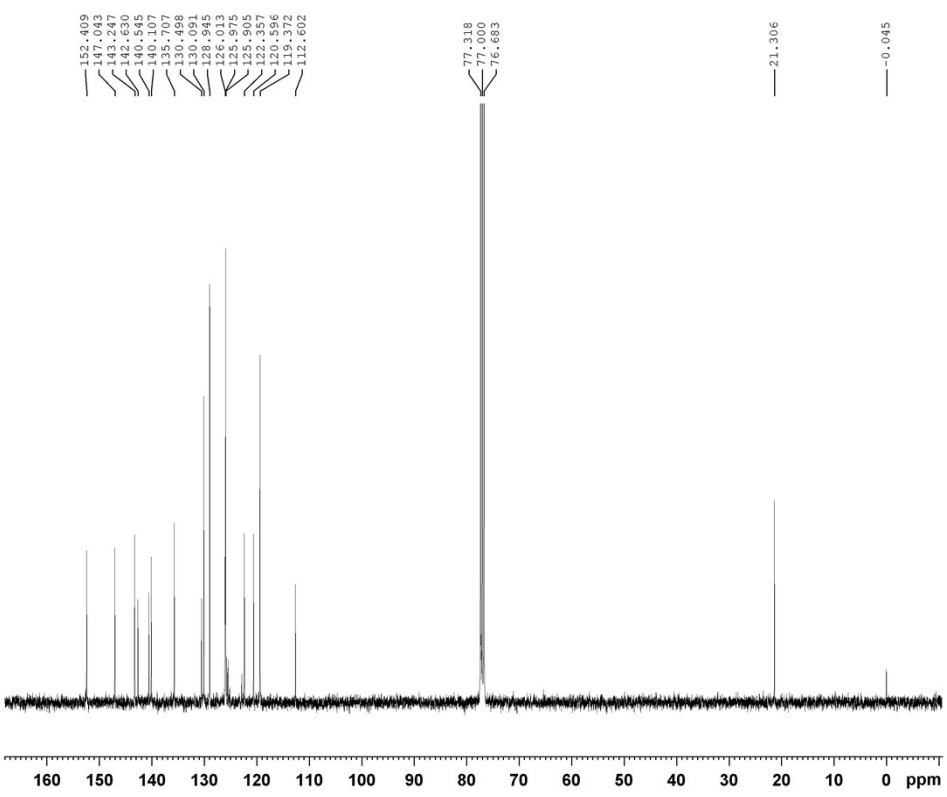

```
Current Data Parameters
NAME                  ND-187
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170526
Time                  20.32
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG               zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   297.7 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO1            100.6228293 MHz

======== CHANNEL f2 ========
CPDPRG[2              waltz16
NUC2                      1H
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W
SFO2            400.1316005 MHz

F2 - Processing parameters
SI                        32768
SF               100.6127733 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

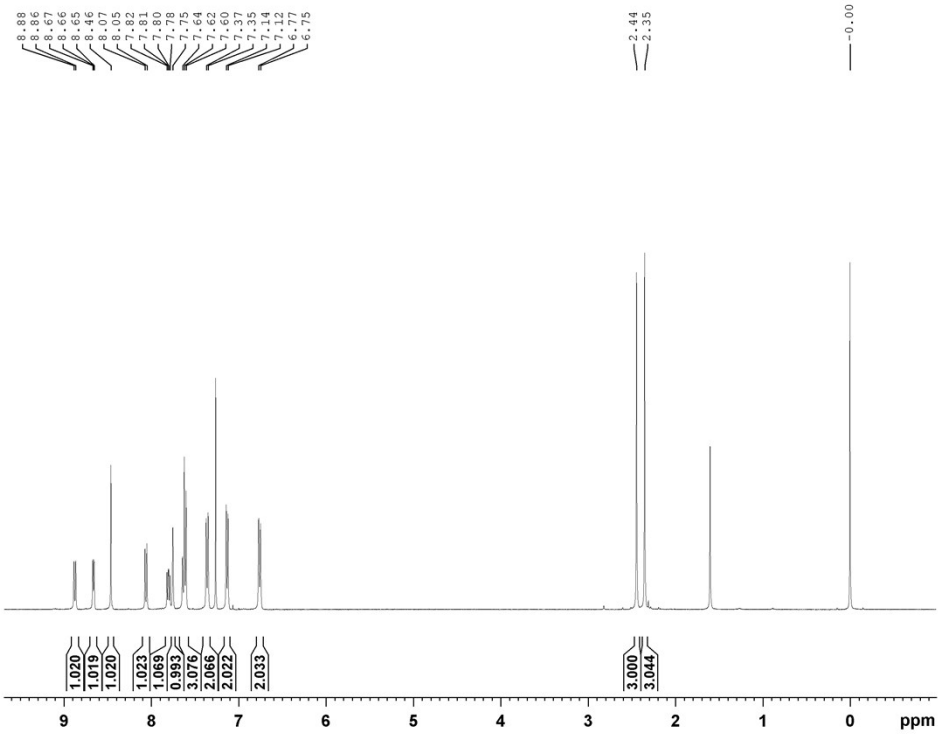



```
Current Data Parameters
NAME                  ND-187
EXPNO                      3
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170527
Time                   0.02
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                    1024
DS                       4
SWH              24038.461 Hz
FIDRES           0.366798 Hz
AQ               1.3631488 sec
RG                  186.53
DW                  20.800 usec
DE                   6.50 usec
TE                  297.7 K
D1               2.00000000 sec
d11              0.03000000 sec
DELTA            1.89999998 sec
TD0                        1
SFO1           100.6228293 MHz
NUC1                    13C
P1                     9.98 usec
PLW1           52.09999847 W
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                90.00 usec
PLW2           12.60000038 W
PLW12           0.34999999 W
PLW13           0.28349999 W

F2 - Processing parameters
SI                     32768
SF             100.6127735 MHz
WDW                       EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

(*Z*)-(2-(7-methylquinolin-1-ium-1-yl)-2-(4-(trifluoromethyl)phenyl)vinyl)(tosyl)amide (1r):

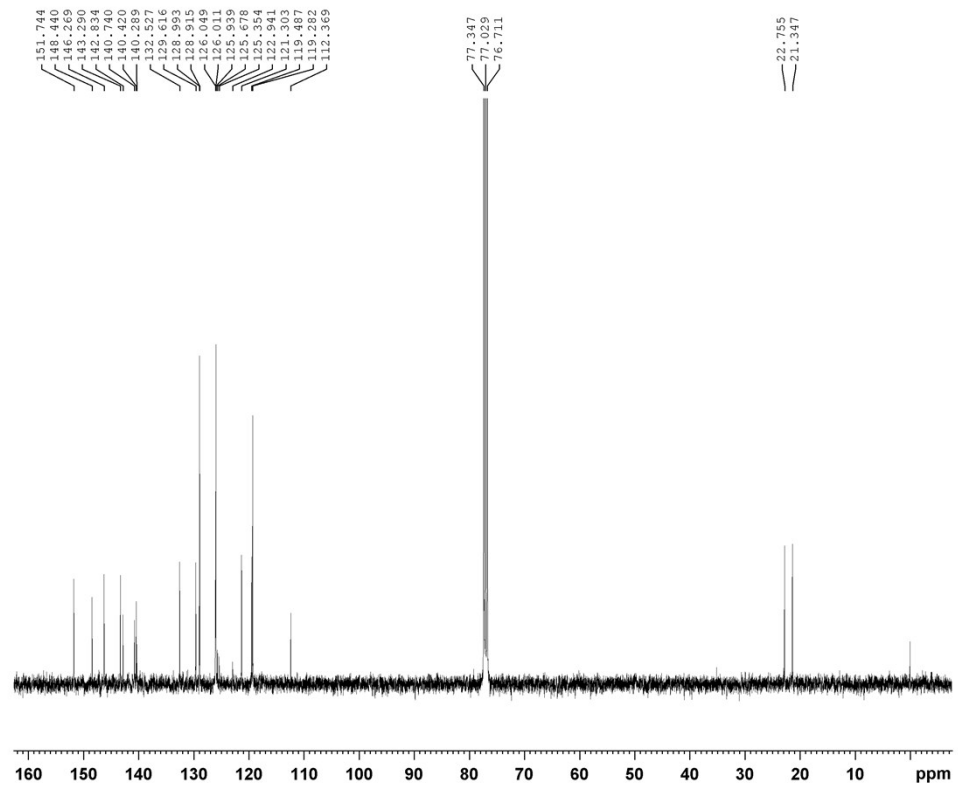



```
Current Data Parameters
NAME                  ND-188
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170526
Time                  16.16
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES            0.125483 Hz
AQ                3.9845889 sec
RG                    167.01
DW                   60.800 usec
DE                    6.50 usec
TE                   296.5 K
D1                1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1             12.60000038 W
SFO1            400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF               400.1300093 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

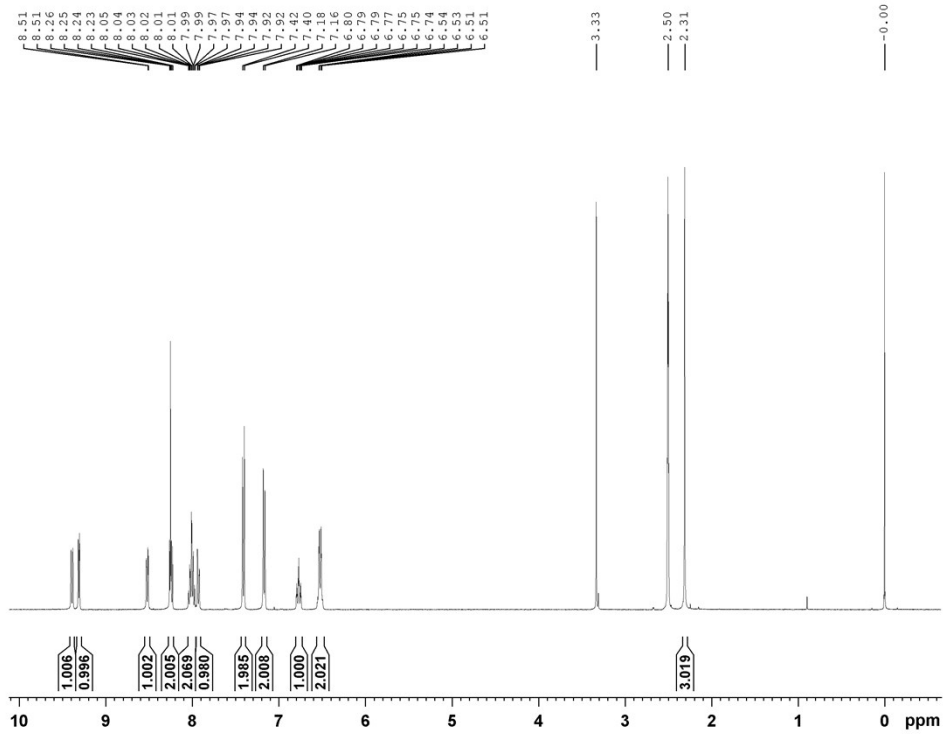



```
Current Data Parameters
NAME                  ND-188
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170531
Time                   0.02
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG             zgpg30
TD                    65536
SOLVENT               CDCl3
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES            0.366798 Hz
AQ                1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   298.4 K
D1                2.00000000 sec
d11               0.03000000 sec
DELTA             1.89999998 sec
TD0                        1
SFO1            100.6228293 MHz
NUC1                     13C
P1                     9.98 usec
PLW1             52.09999847 W
SFO2            400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                 90.00 usec
PLW2             12.60000038 W
PLW12             0.34999999 W
PLW13             0.28349999 W

F2 - Processing parameters
SI                        32768
SF              100.6127686 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

(Z)-(2-(3,5-difluorophenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1s):

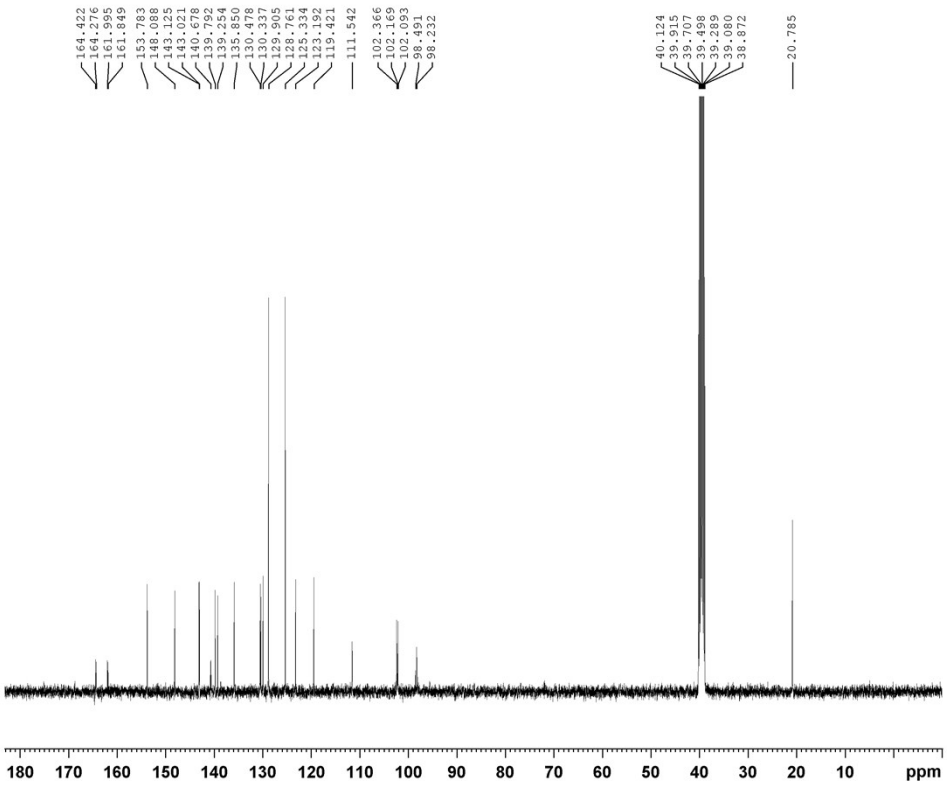



```
Current Data Parameters
NAME                  ND-110
EXPNO                      1
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170314
Time                  10.34
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT                DMSO
NS                       16
DS                        2
SWH                8223.685 Hz
FIDRES             0.125483 Hz
AQ                 3.9845889 sec
RG                    167.01
DW                   60.800 usec
DE                    6.50 usec
TE                   296.1 K
D1                 1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1              12.60000038 W
SFO1             400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                400.1300030 MHz
WDW                        EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

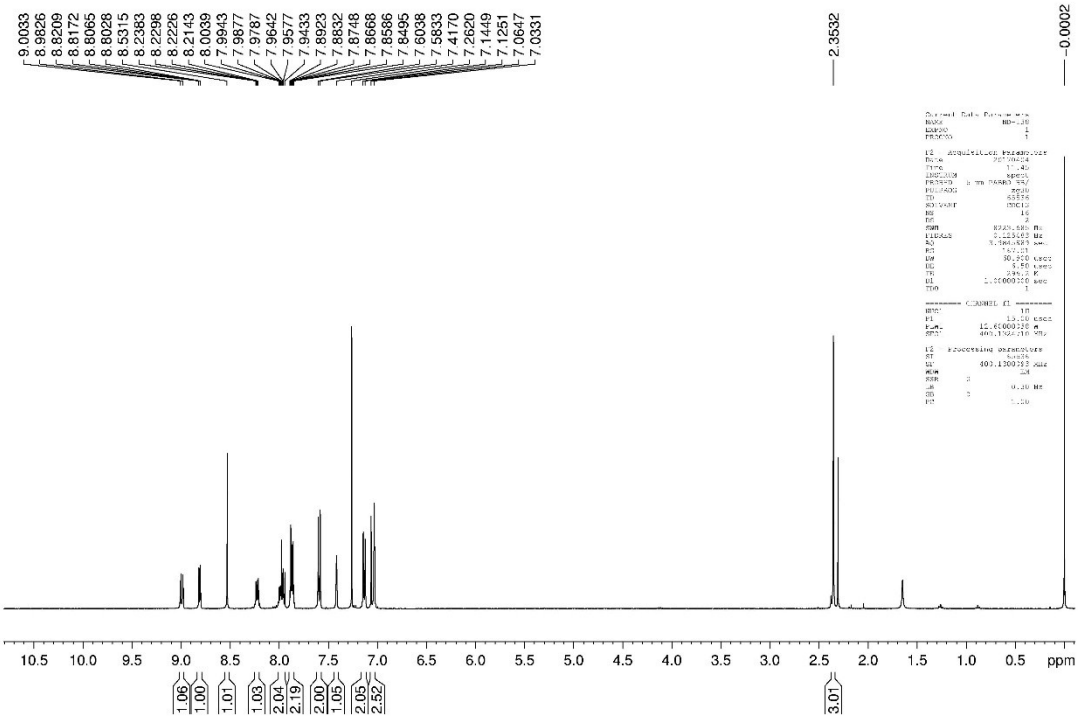


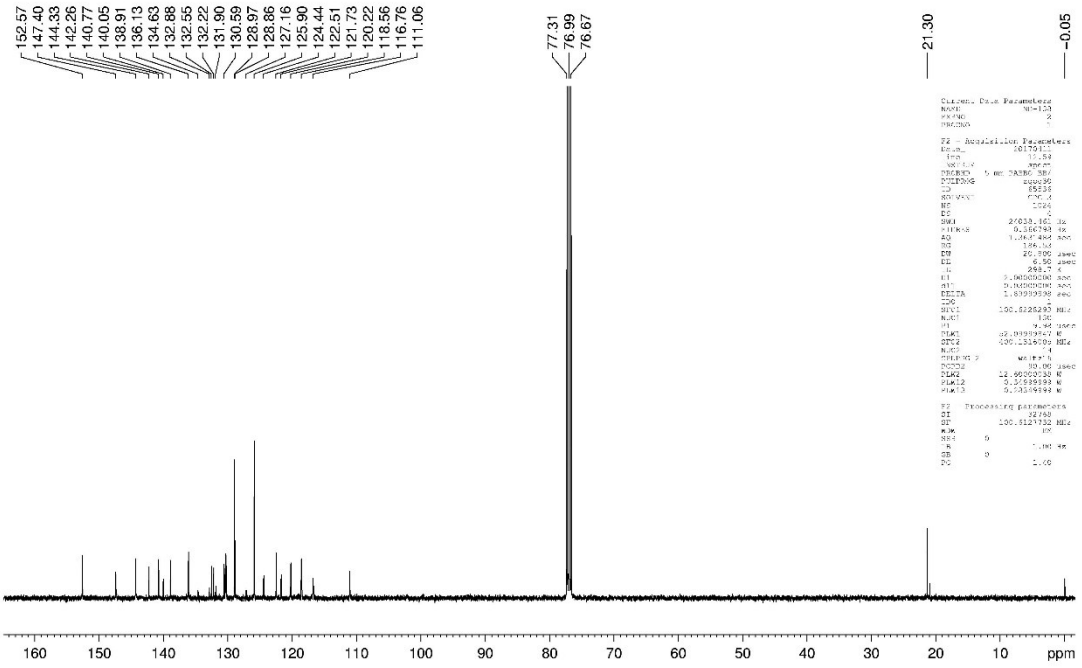

```
Current Data Parameters
NAME                  ND-110
EXPNO                      2
PROCNO                     1

F2 - Acquisition Parameters
Date_              20170314
Time                  13.01
INSTRUM                spect
PROBHD   5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT                DMSO
NS                     1024
DS                        4
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                    186.53
DW                   20.800 usec
DE                    6.50 usec
TE                   297.7 K
D1                 2.00000000 sec
d11                0.03000000 sec
DELTA              1.89999998 sec
TD0                        1
SFO1             100.6228293 MHz
NUC1                      13C
P1                     9.98 usec
PLW1              52.09999847 W
SFO2             400.1316005 MHz
NUC2                      1H
CPDPRG[2              waltz16
PCPD2                  90.00 usec
PLW2              12.60000038 W
PLW12              0.34999999 W
PLW13              0.28349999 W

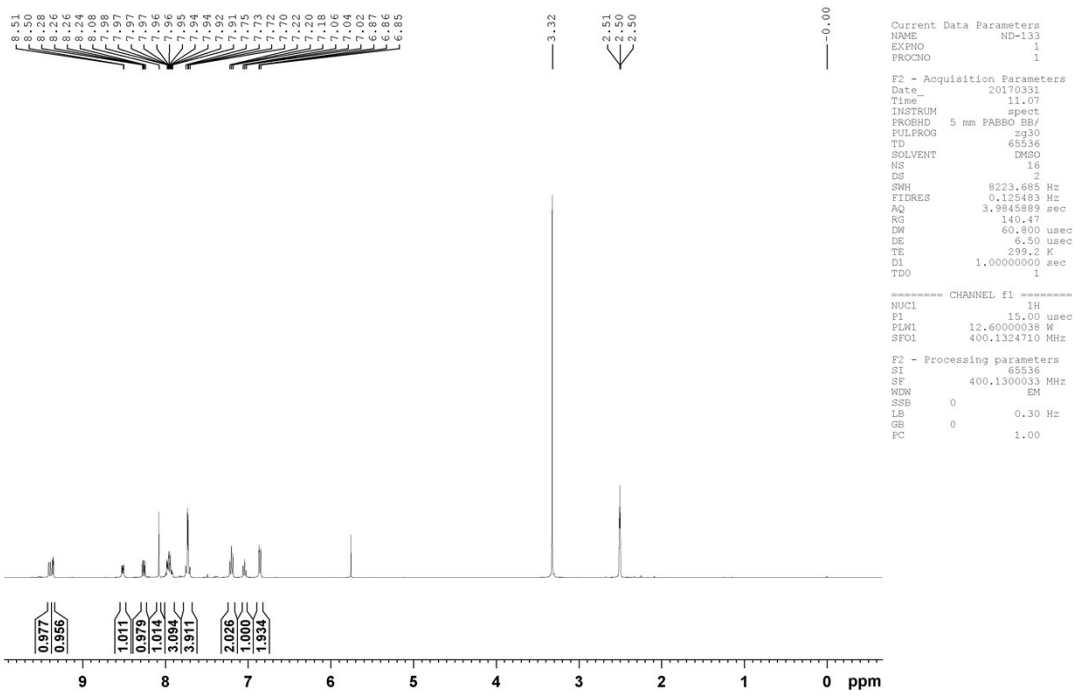
F2 - Processing parameters
SI                        32768
SF               100.6128193 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

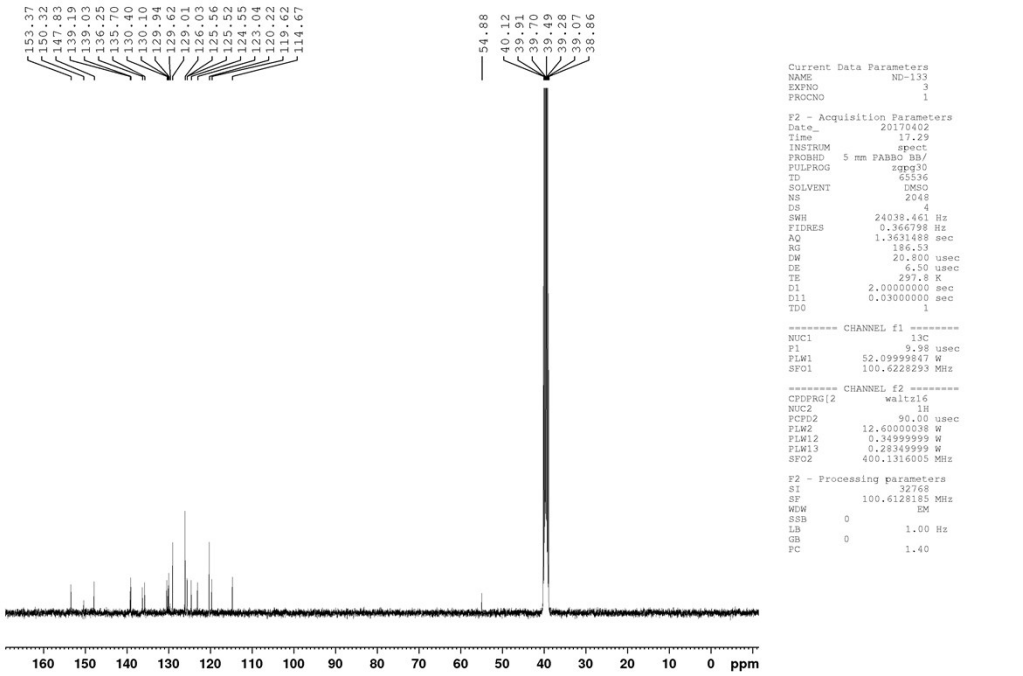
(*Z*)-(2-(3,5-bis(trifluoromethyl)phenyl)-2-(quinolin-1-ium-1-yl)vinyl)(tosyl)amide (1t):



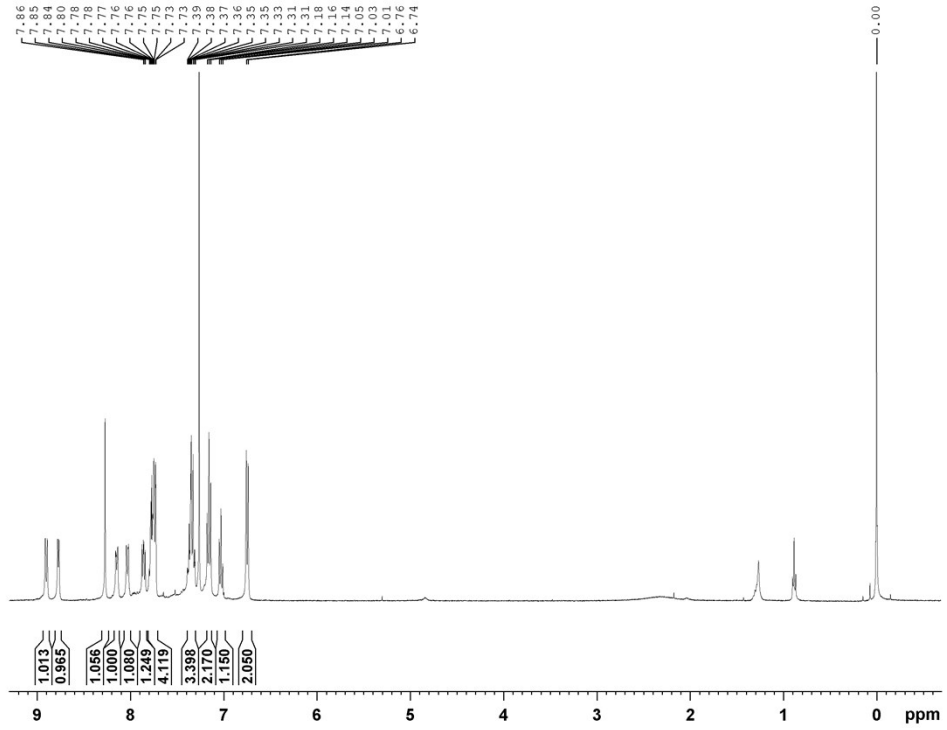


(Z)-(2-phenyl-2-(quinolin-1-ium-1-yl)vinyl)((4-(trifluoromethyl)phenyl)sulfonyl)amide (1u):





(Z)-(2-phenyl-2-(quinolin-1-ium-1-yl)vinyl)(phenylsulfonyl)amide (1v):

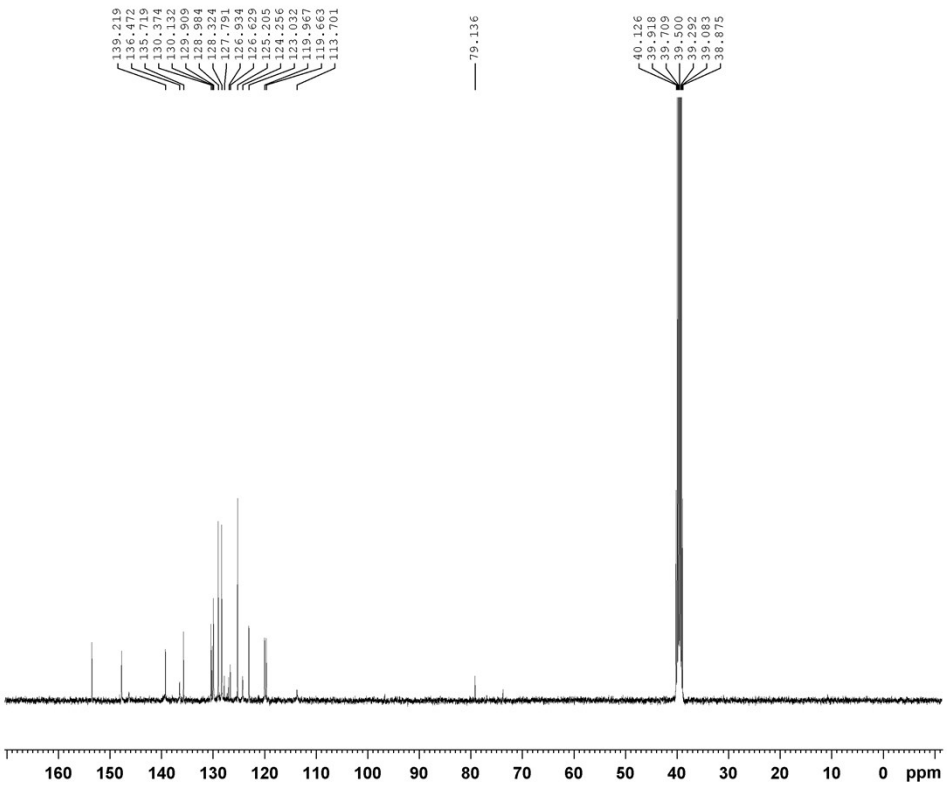



```
Current Data Parameters
NAME                  ND-146
EXPNO                      5
PROCNO                     1

F2 - Acquisition Parameters
Date_                20180120
Time                    22.53
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG                 zg30
TD                     65536
SOLVENT                CDCl3
NS                        32
DS                         2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     167.01
DW                     60.800 usec
DE                      6.50 usec
TE                     297.4 K
D1                  1.00000000 sec
TD0                        1

======== CHANNEL f1 ========
NUC1                      1H
P1                     15.00 usec
PLW1               12.60000038 W
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                     65536
SF                400.1300097 MHz
WDW                       EM
SSB          0
LB                     0.30 Hz
GB           0
PC                     1.00
```

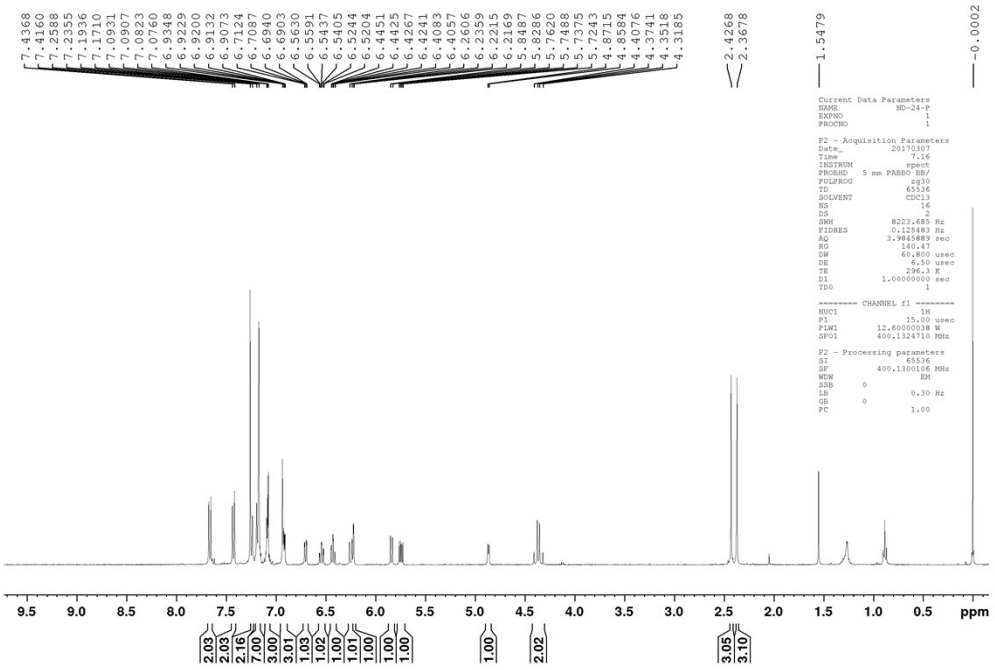


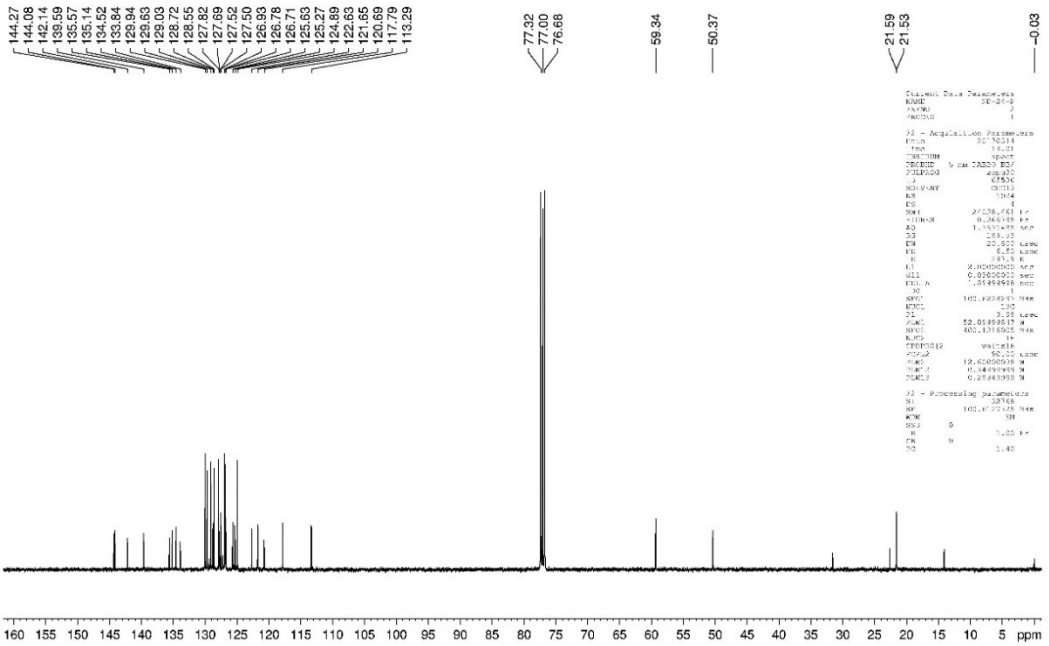

```
Current Data Parameters
NAME                  ND-146
EXPNO                      8
PROCNO                     1

F2 - Acquisition Parameters
Date_                20180121
Time                    19.26
INSTRUM                 spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                     65536
SOLVENT                DMSO
NS                      1024
DS                         4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                     20.800 usec
DE                      6.50 usec
TE                     298.8 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                        1
SFO1              100.6228293 MHz
NUC1                      13C
P1                      9.98 usec
PLW1               52.09999847 W
SFO2              400.1316005 MHz
NUC2                      1H
CPDPRG[2               waltz16
PCPD2                  90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

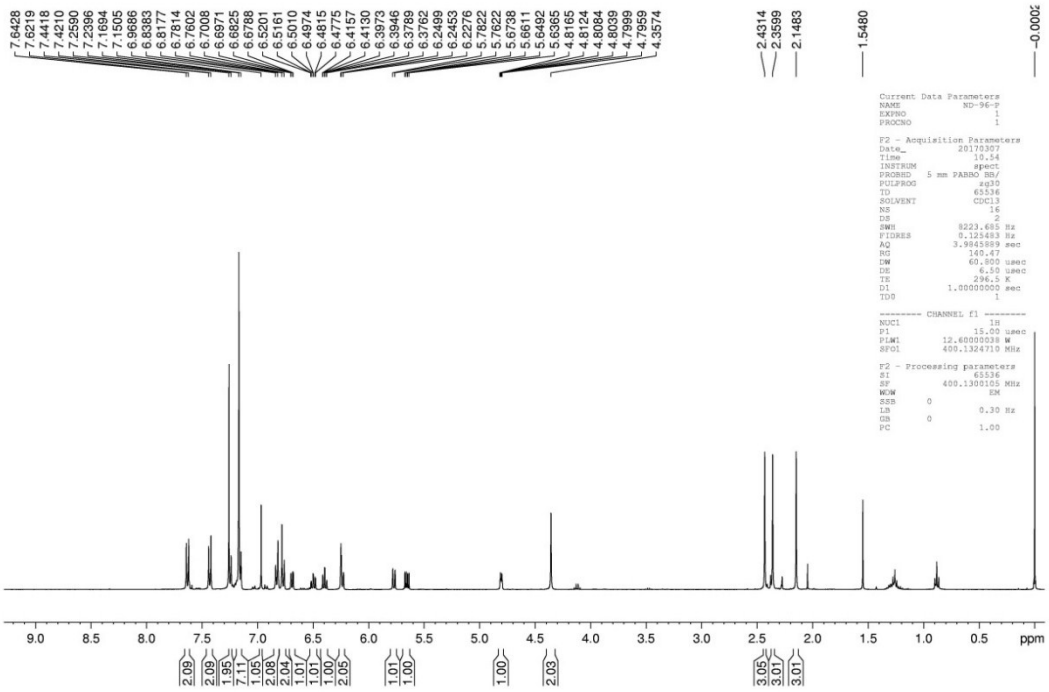
F2 - Processing parameters
SI                     32768
SF                100.6128211 MHz
WDW                       EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

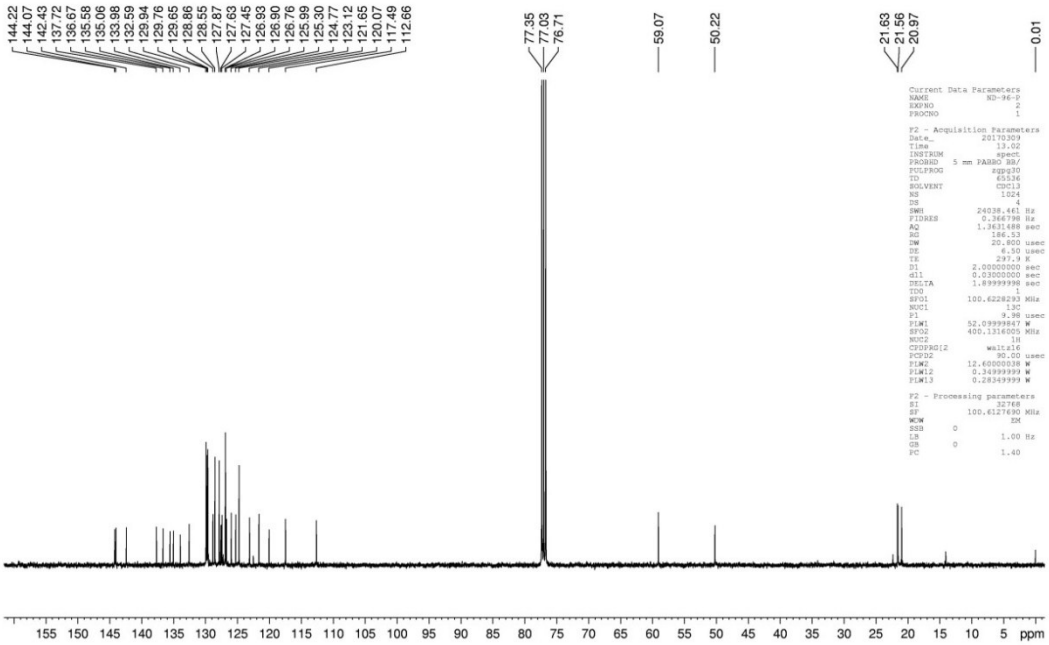
(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3aa):



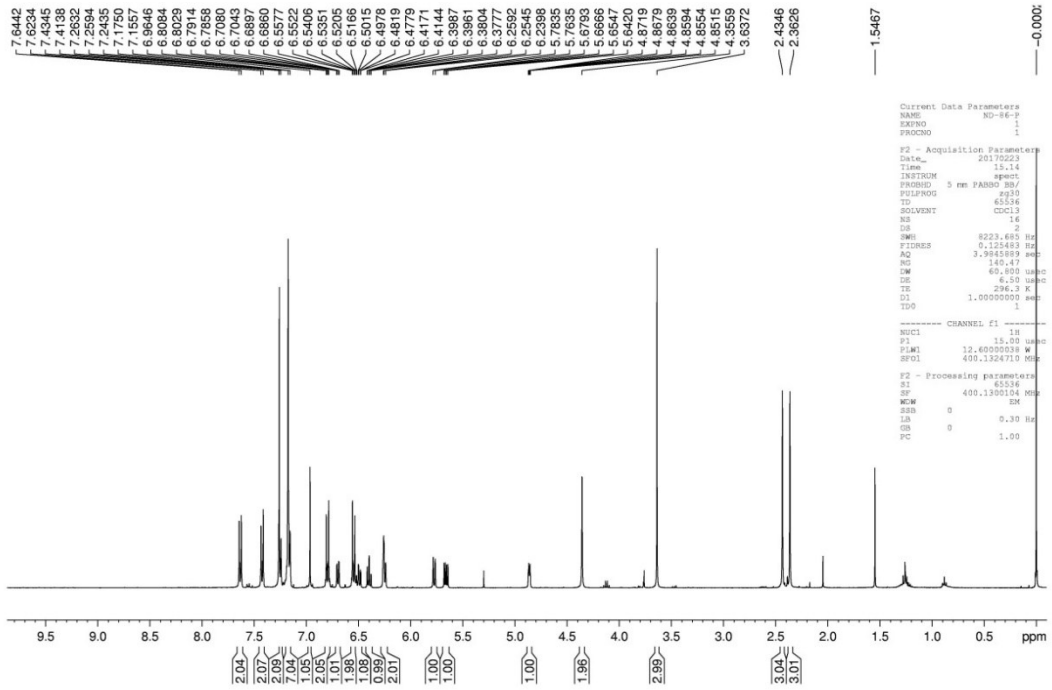


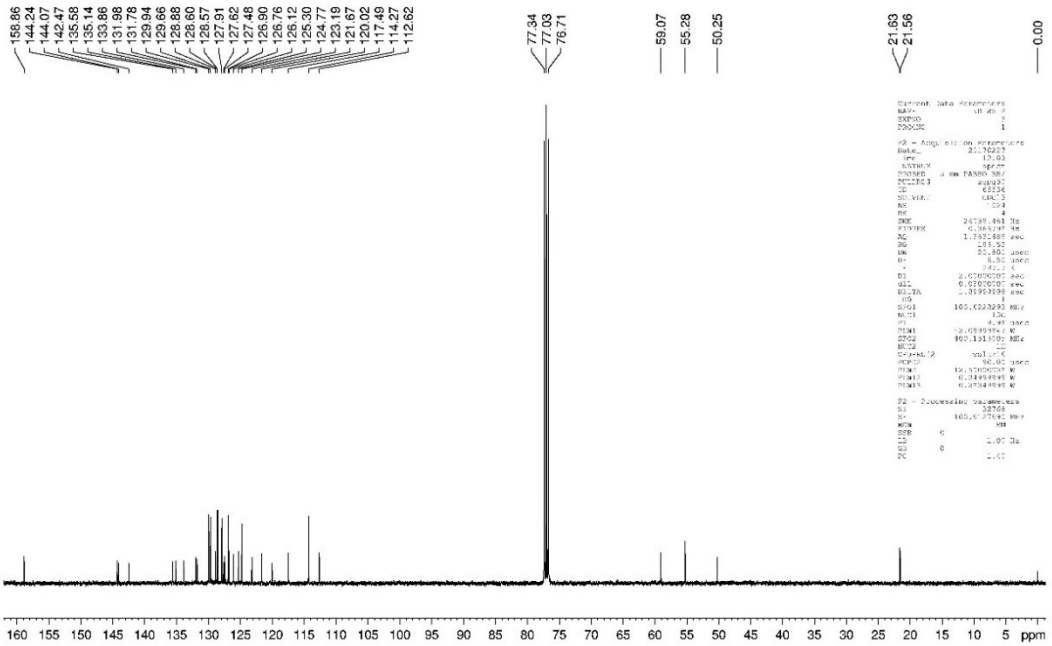
(*E*)-4-methyl-N-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-(p-tolyl)benzenesulfonamide (3ab):



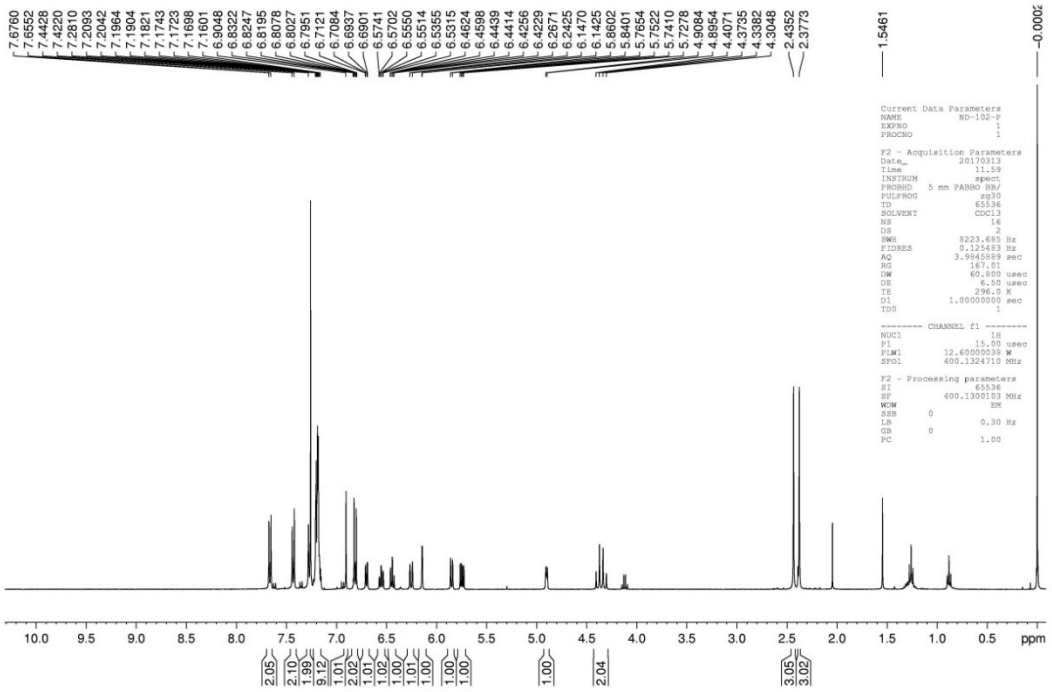


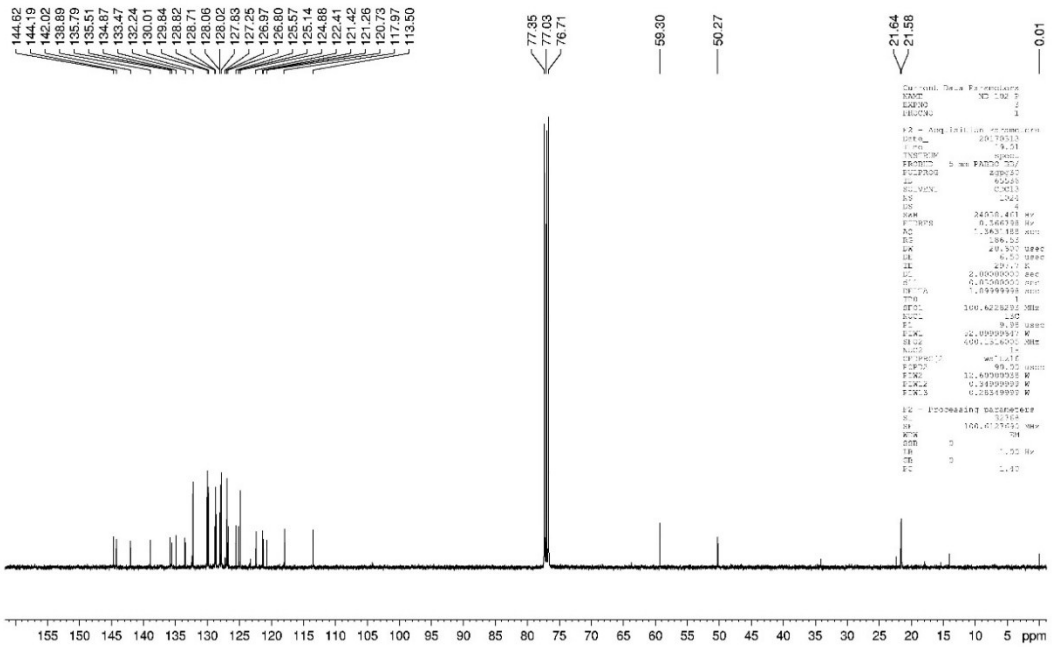
(*E*)-N-(4-methoxyphenyl)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ac):



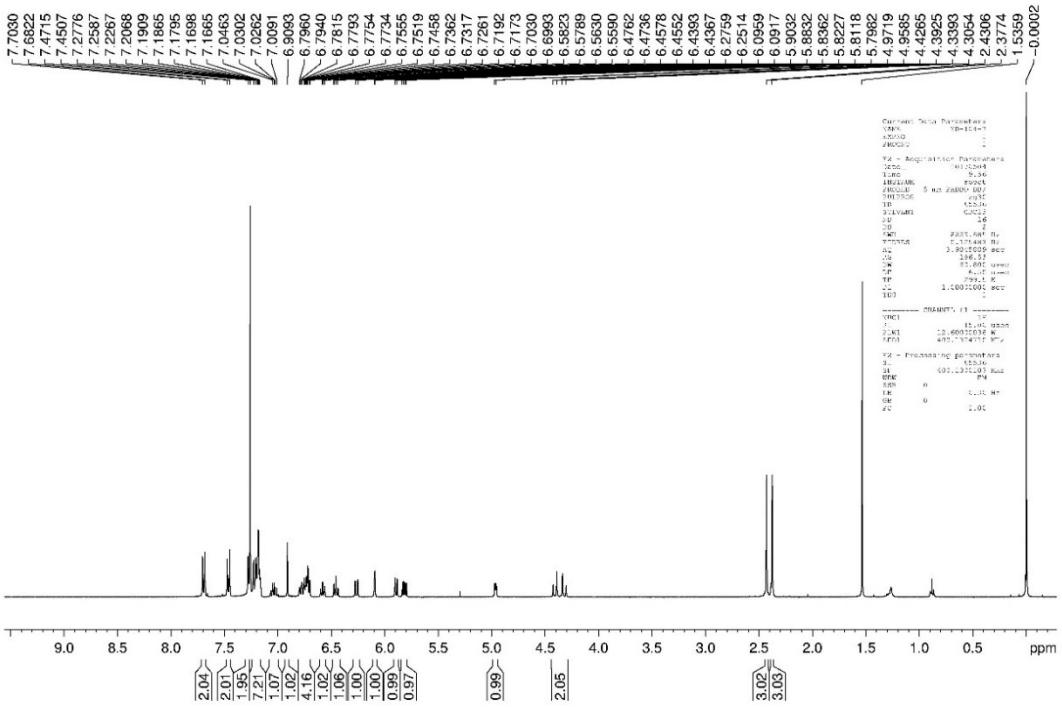


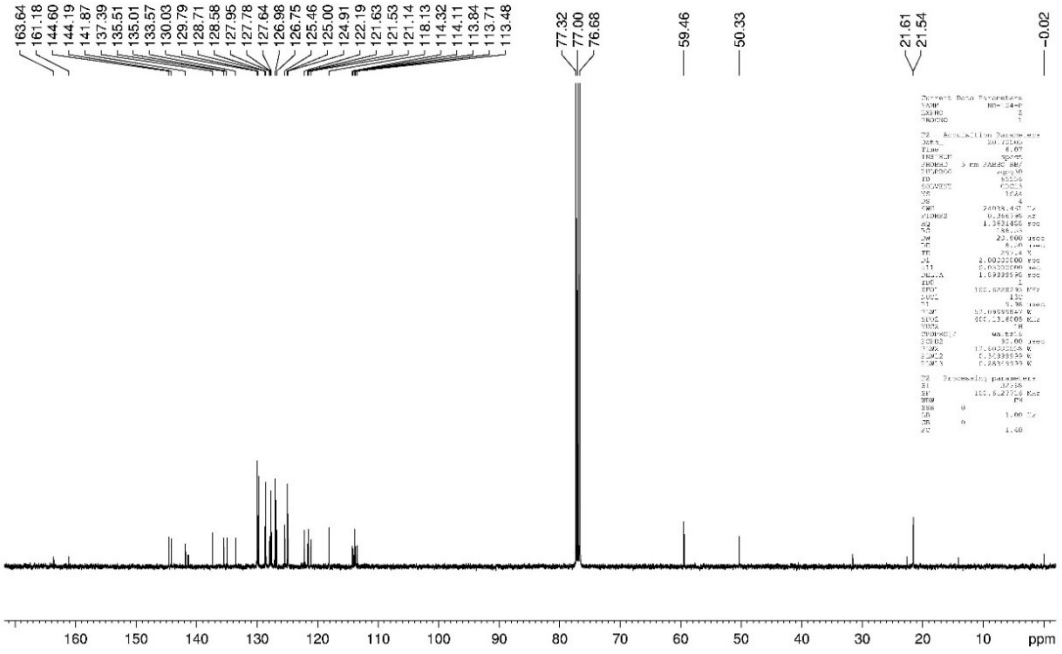
(*E*)-*N*-(4-bromophenyl)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ad):



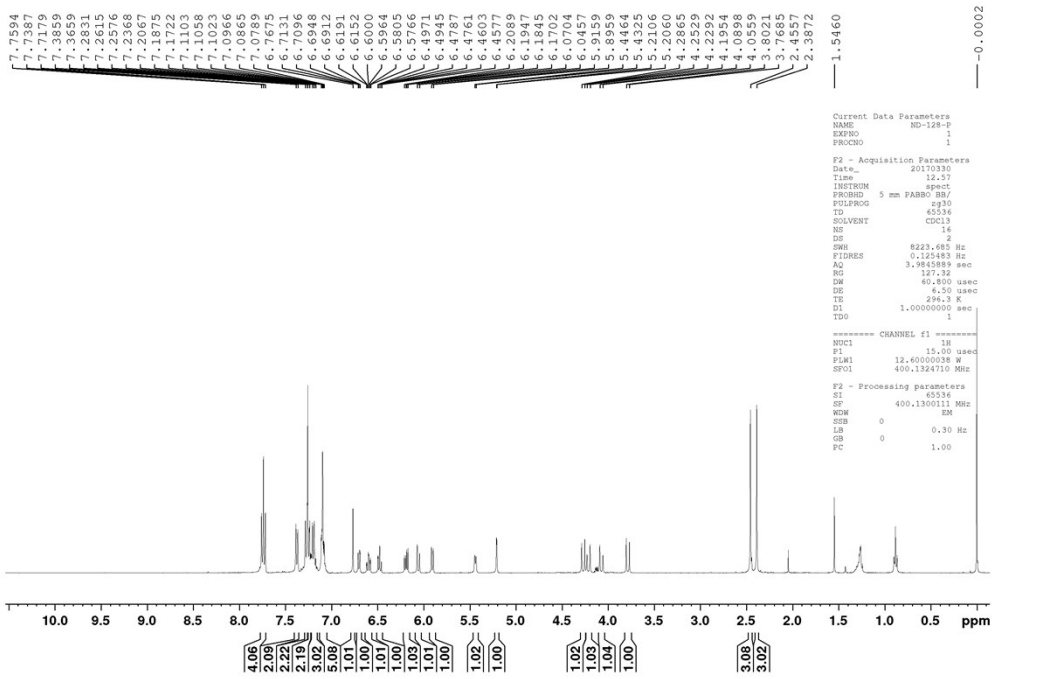


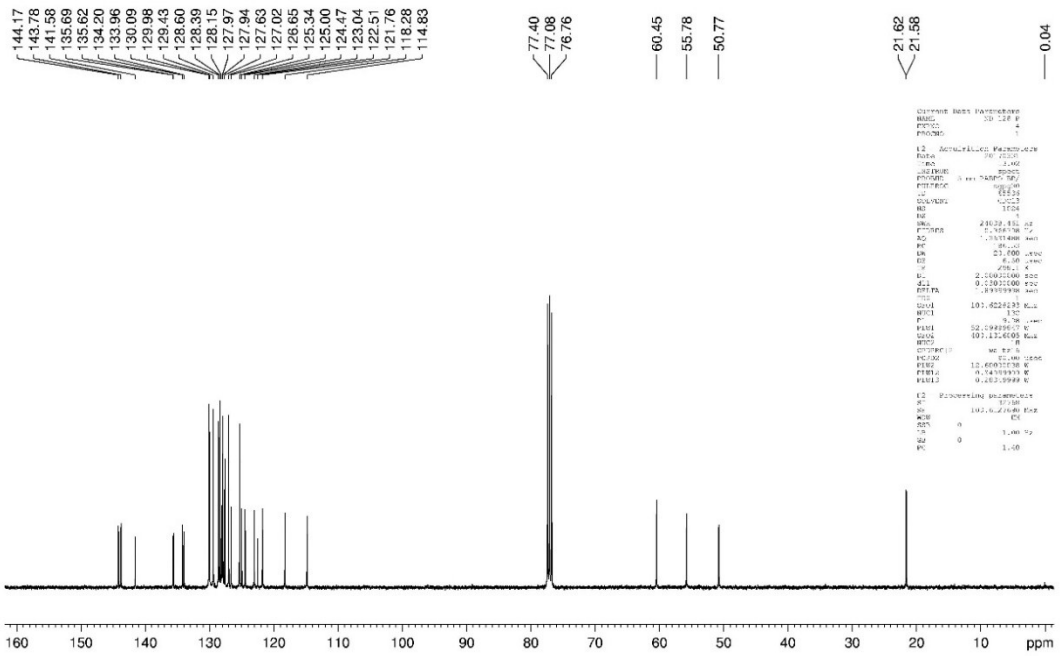
(*E*)-*N*-(3-fluorophenyl)-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ae):



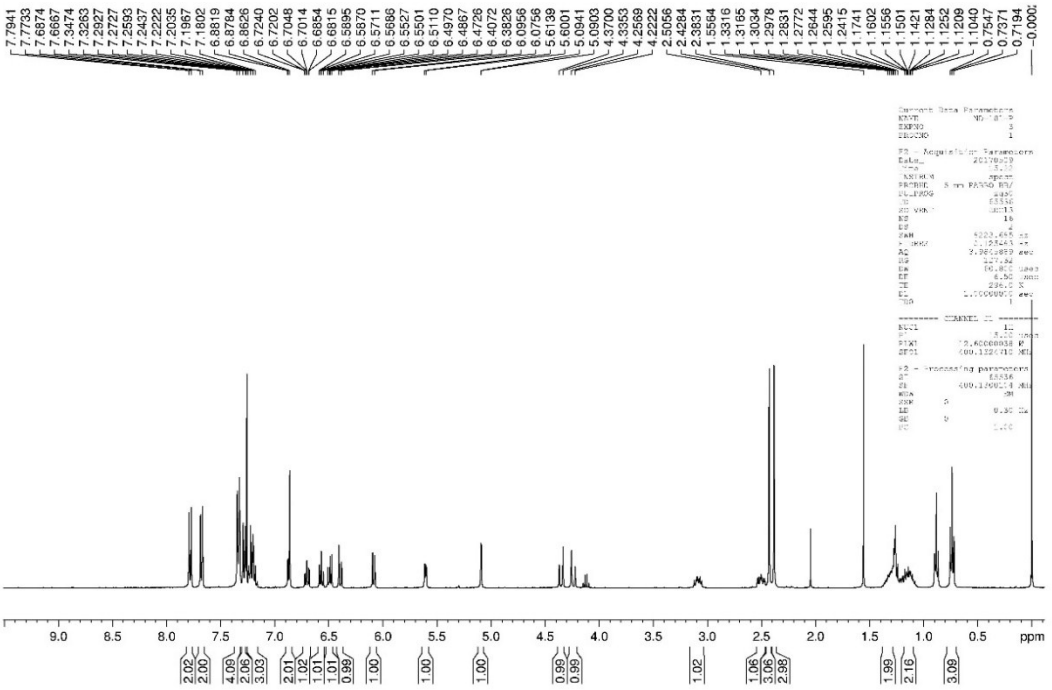


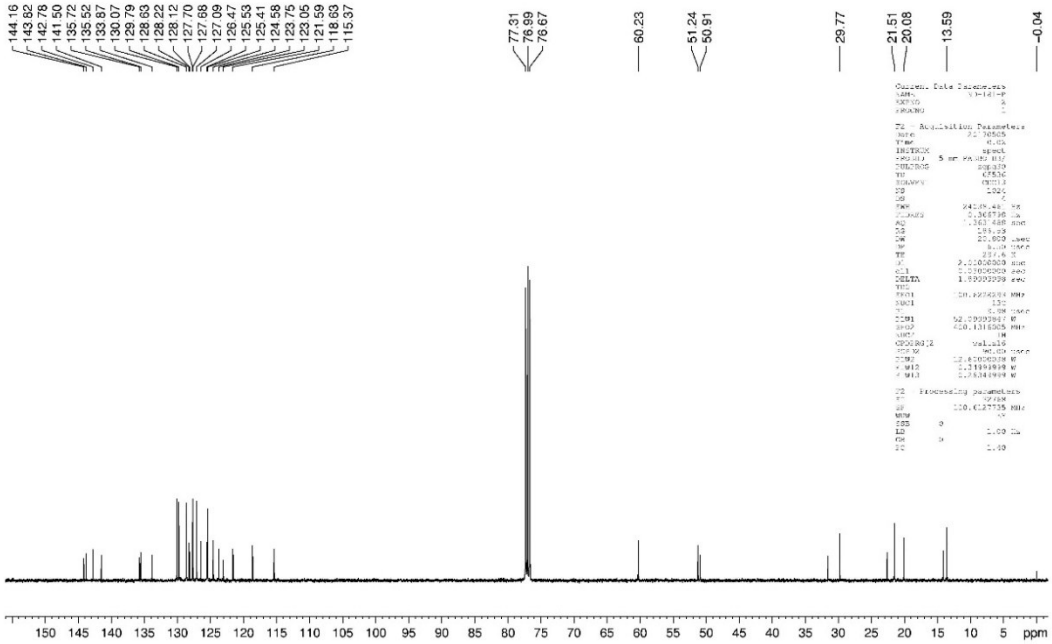
(*E*)-*N*-benzyl-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3af):



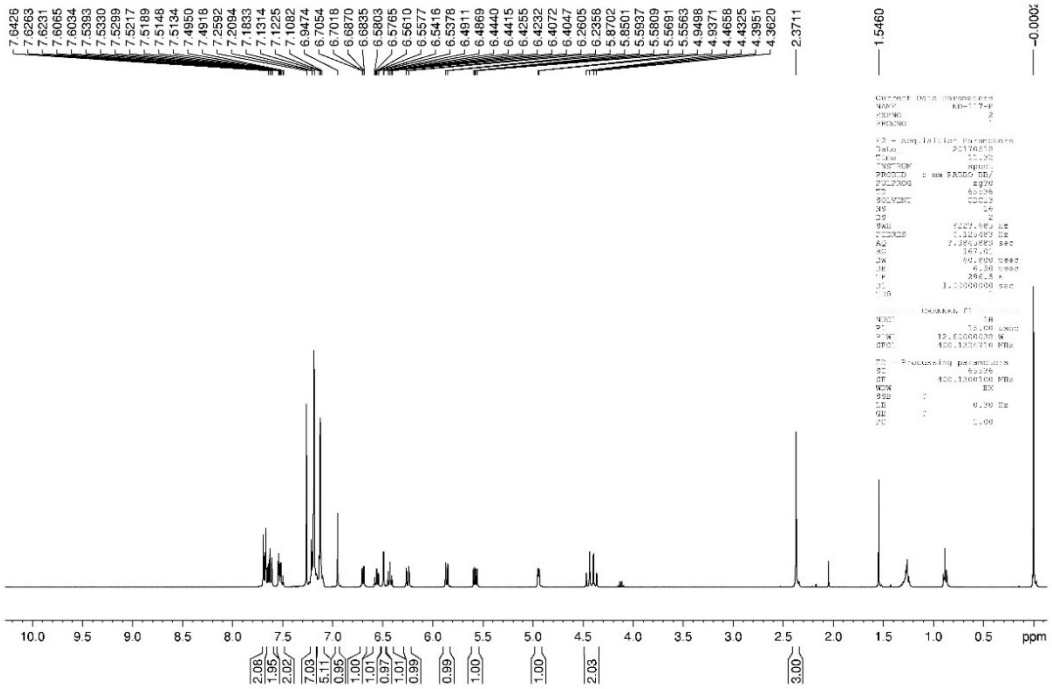


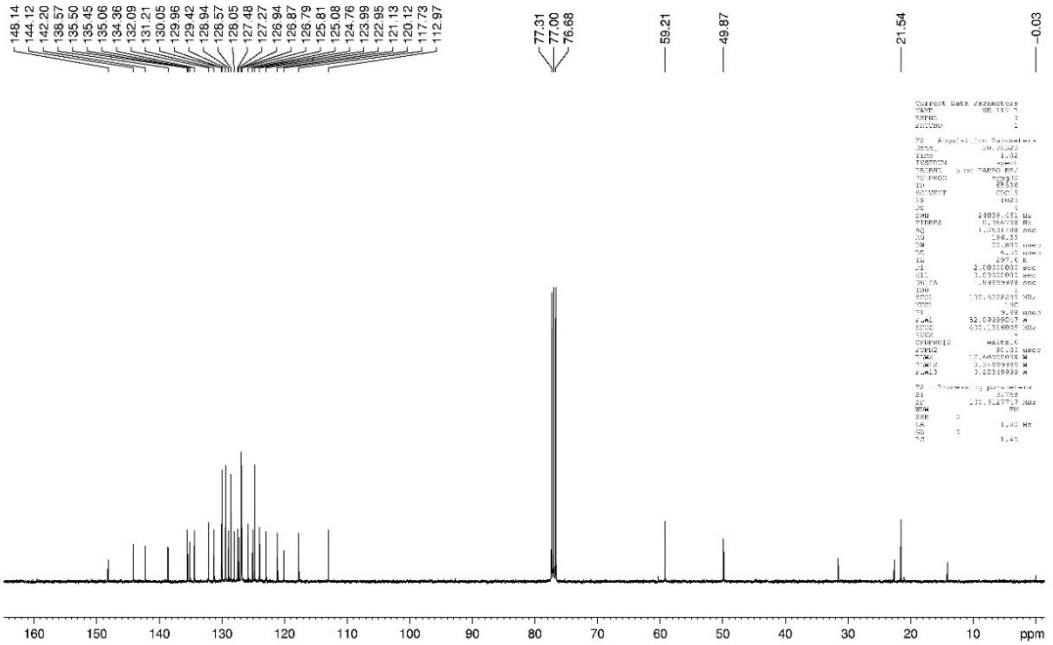
(*E*)-*N*-butyl-4-methyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ag):



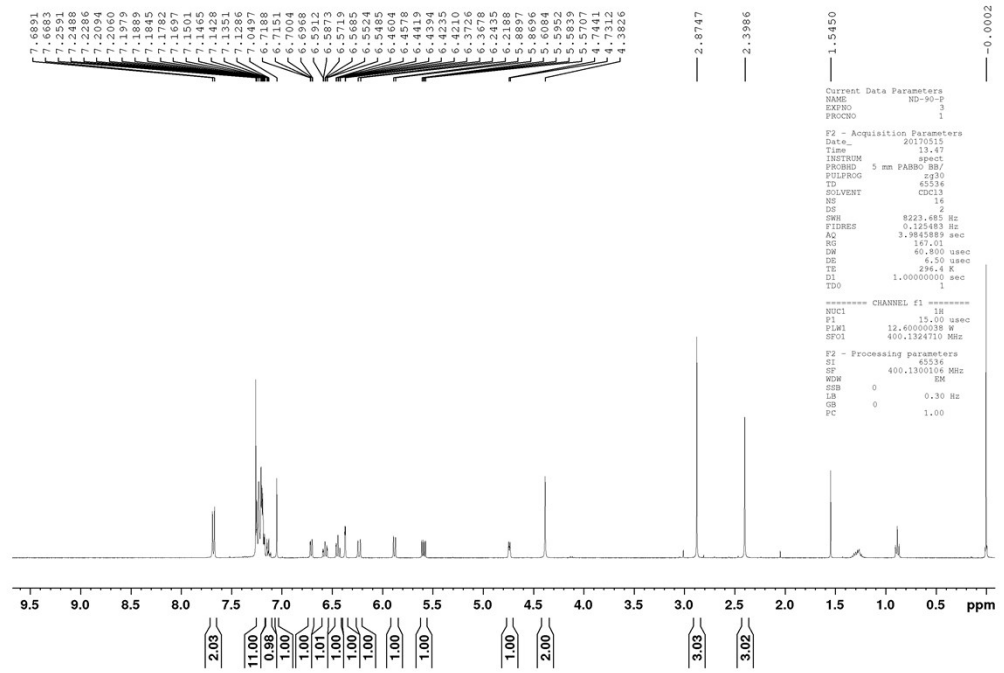


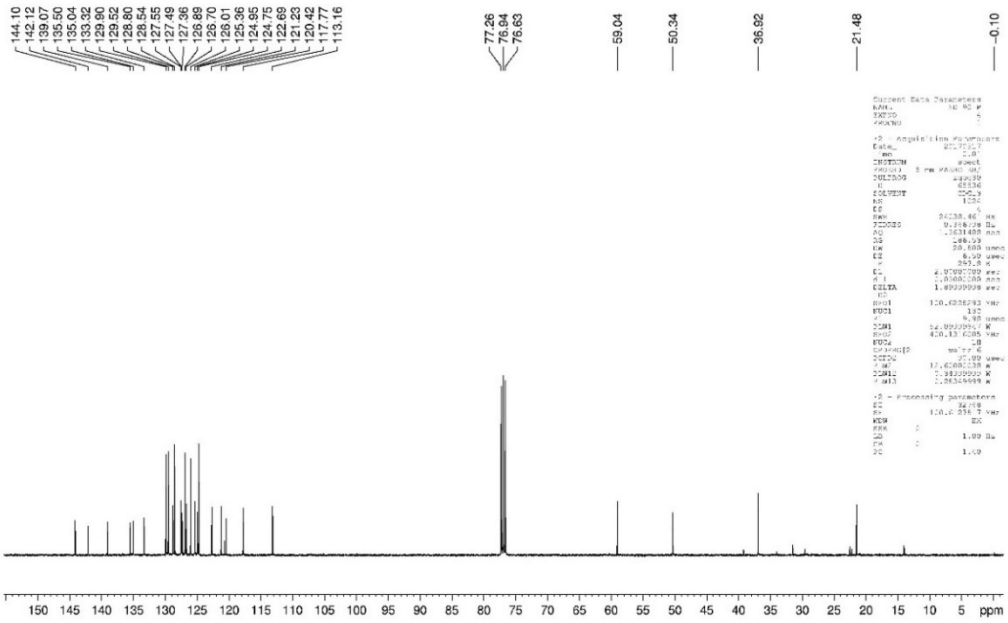
(*E*)-2-nitro-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ah):



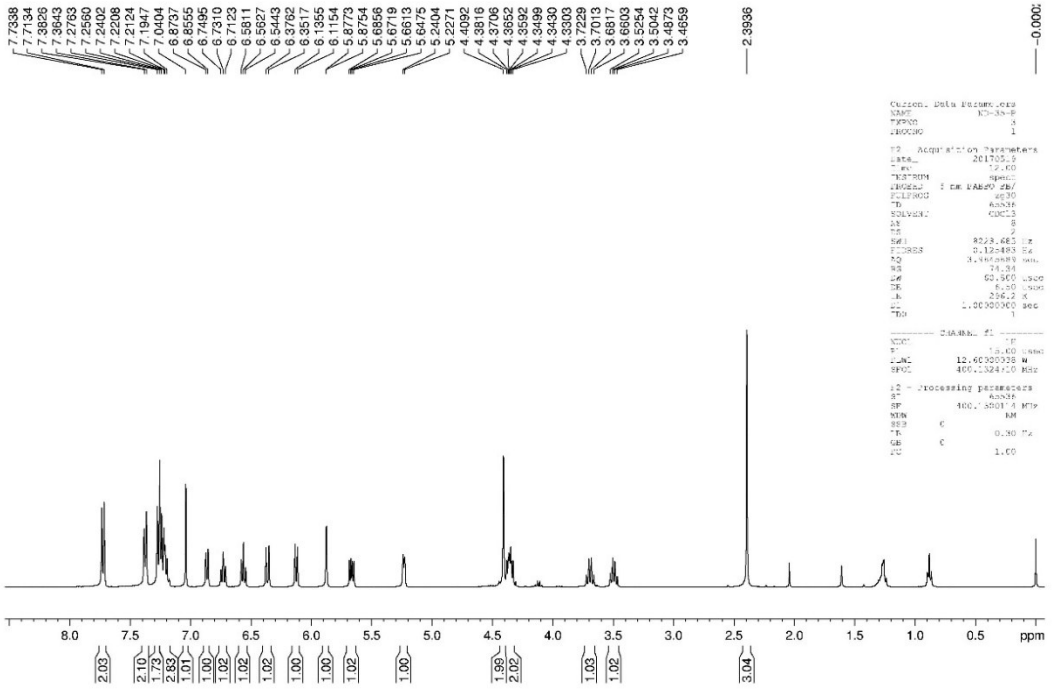


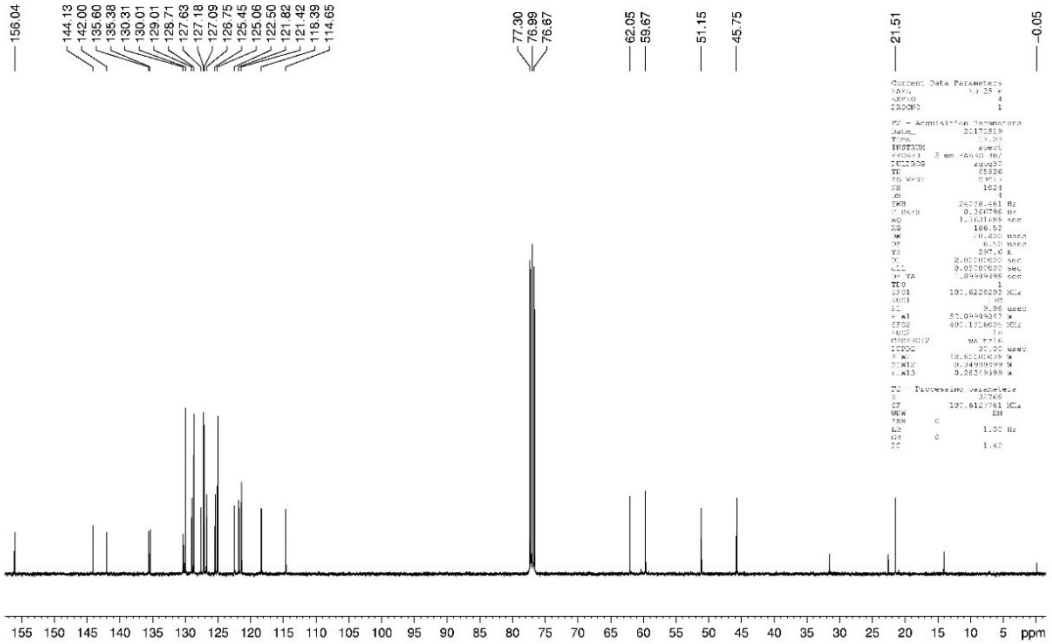
(*E*)-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)methanesulfonamide (3ai):



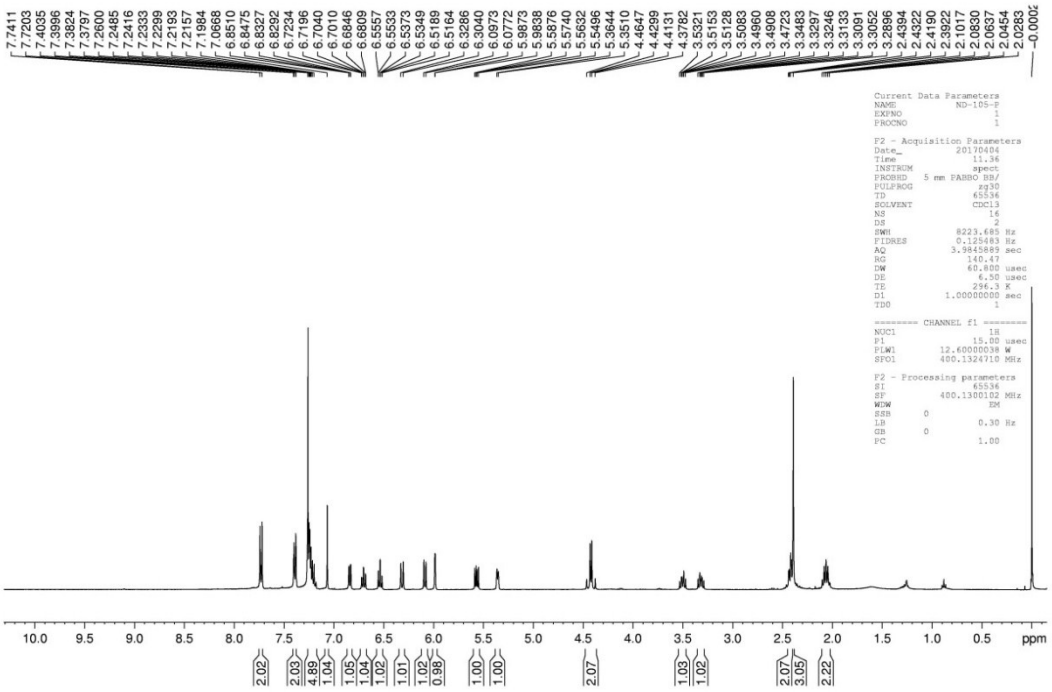


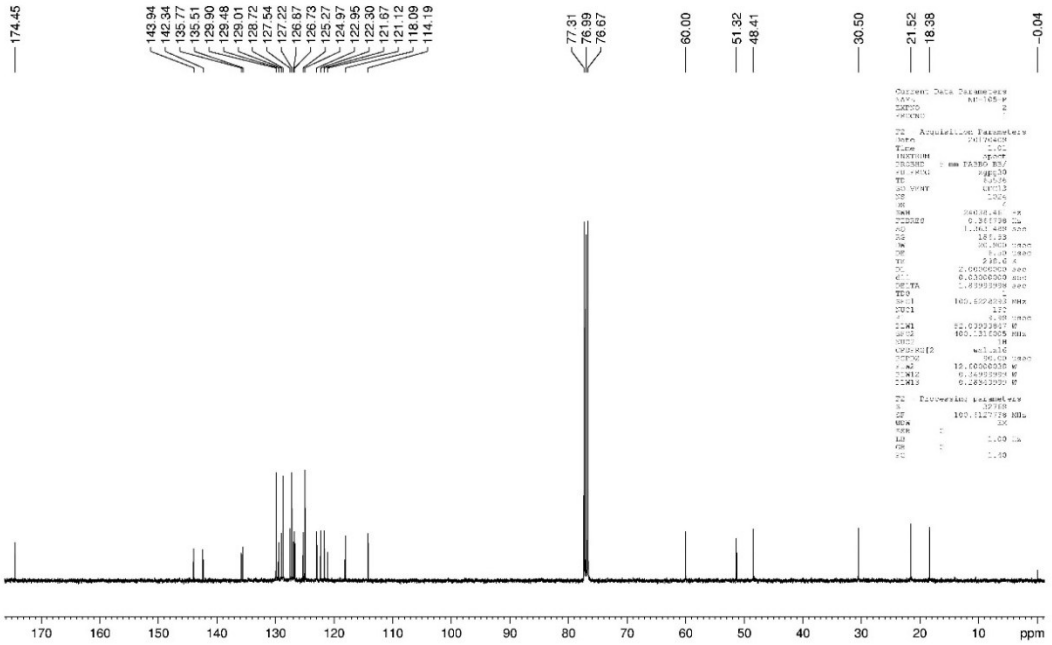
(*E*)-3-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)oxazolidin-2-one (3aj):



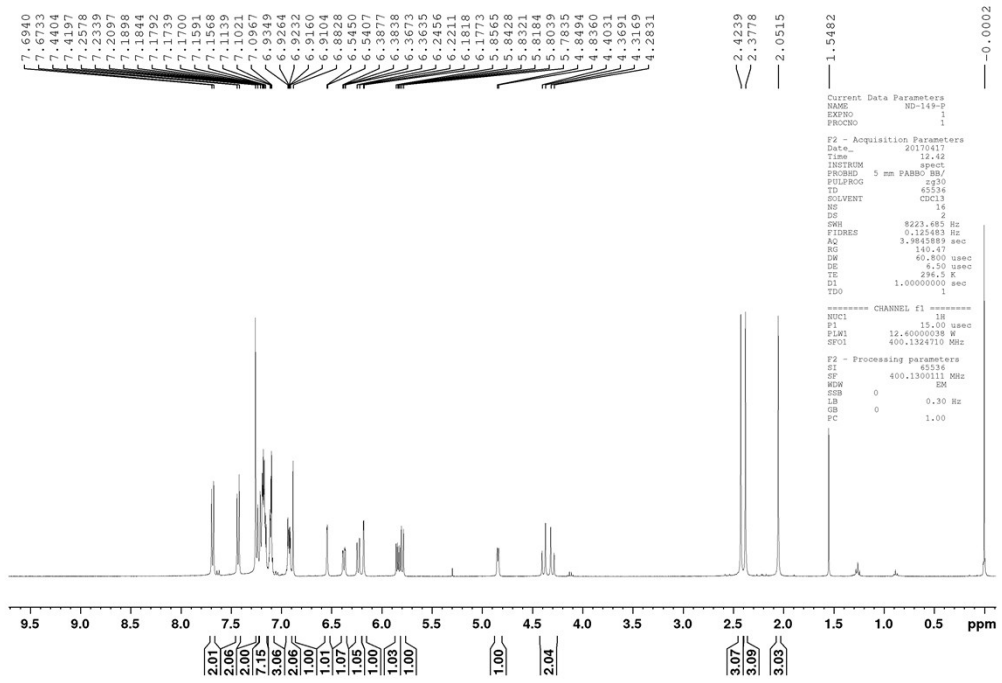


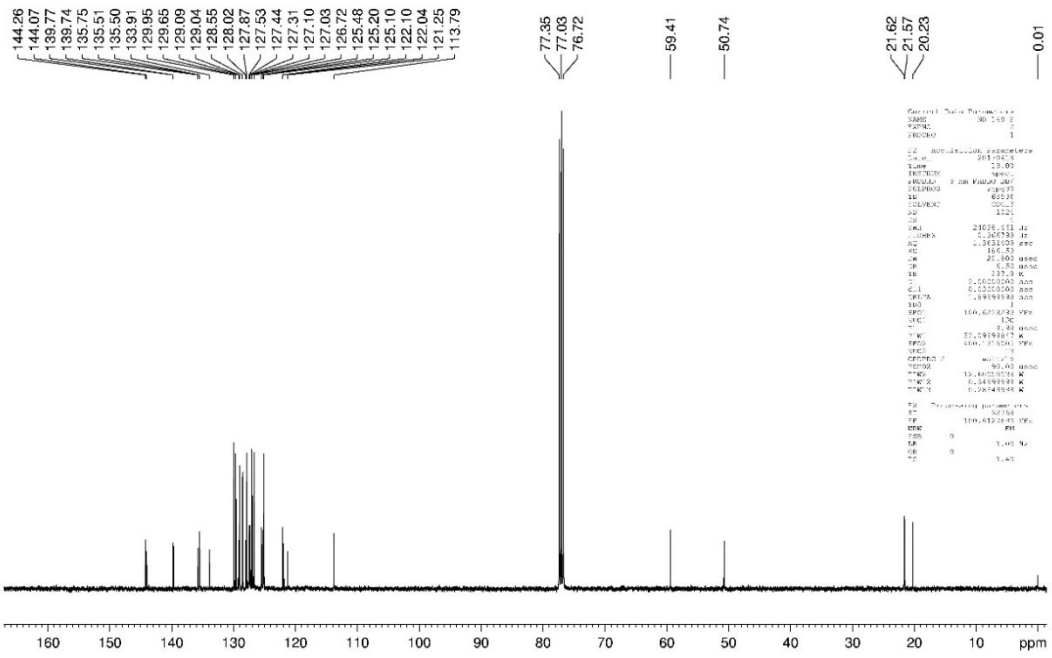
(*E*)-1-((1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)pyrrolidin-2-one (3ak):



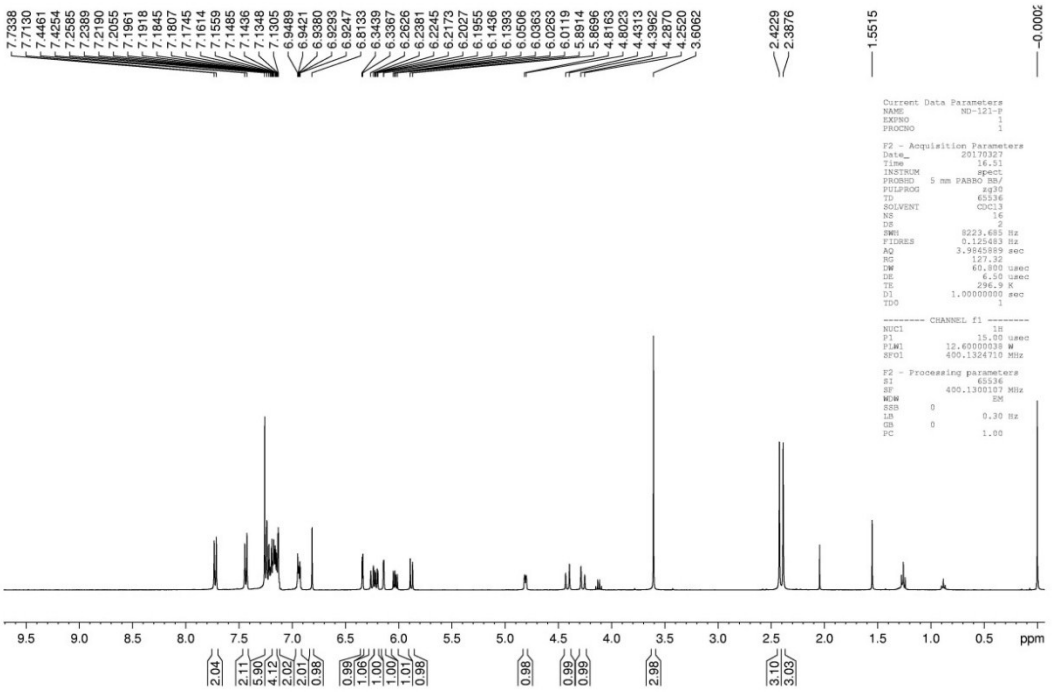


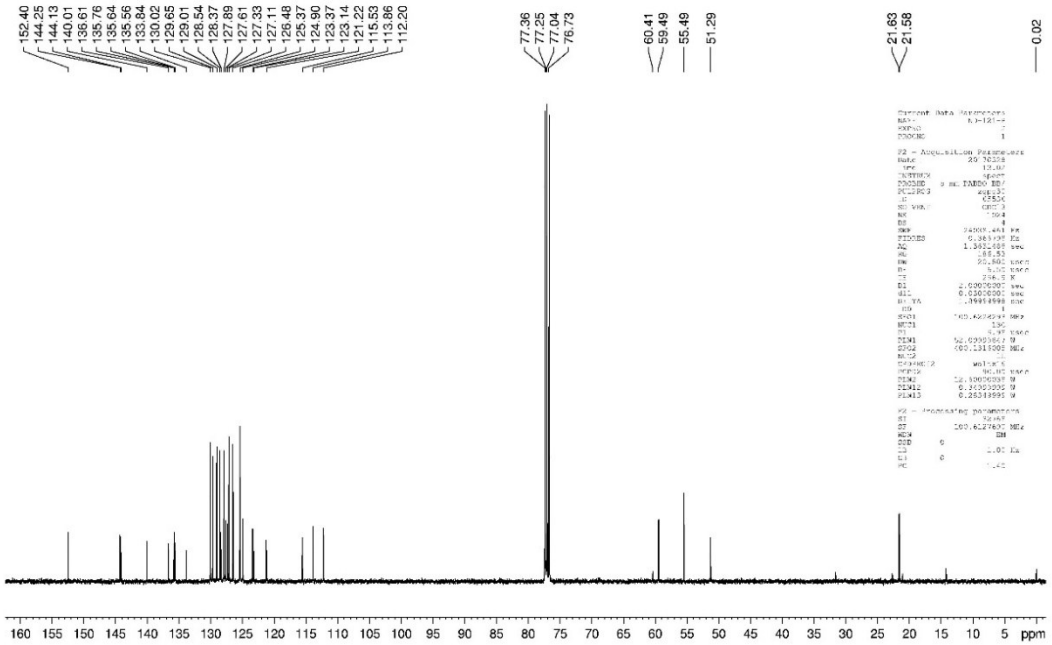
(*E*)-4-methyl-*N*-((9-methyl-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ba):



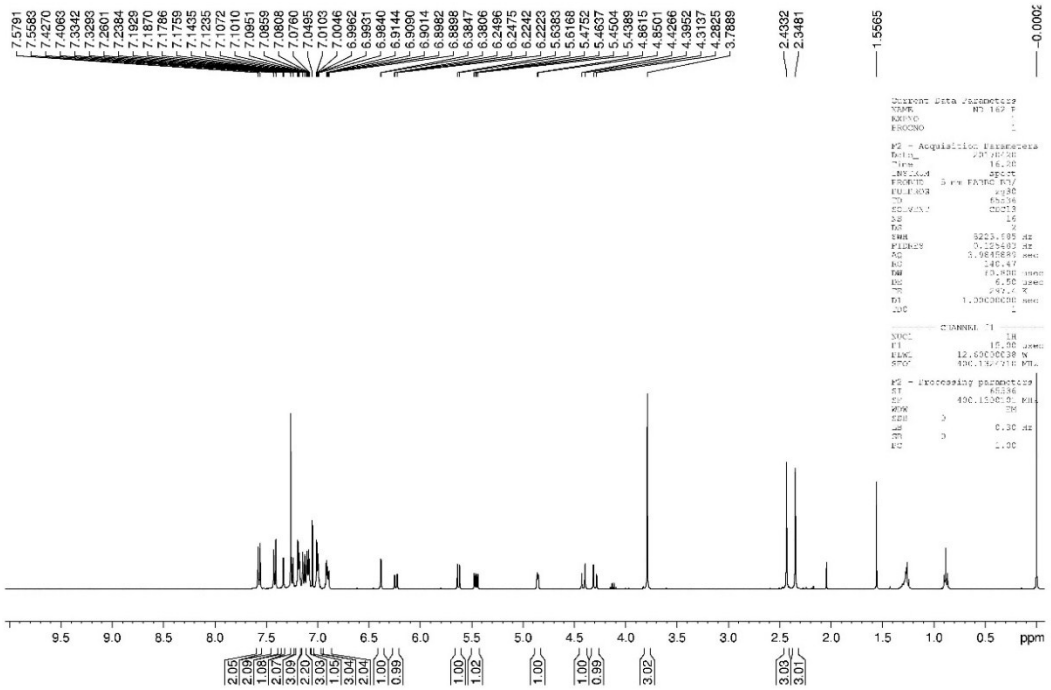


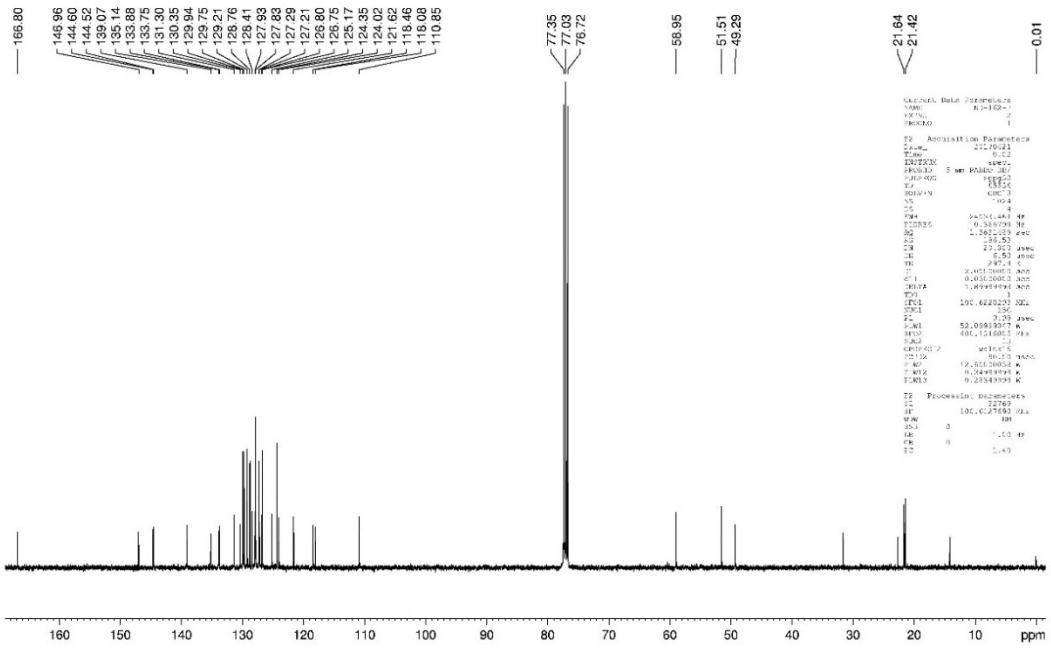
(*E*)-*N*-((9-methoxy-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ca):



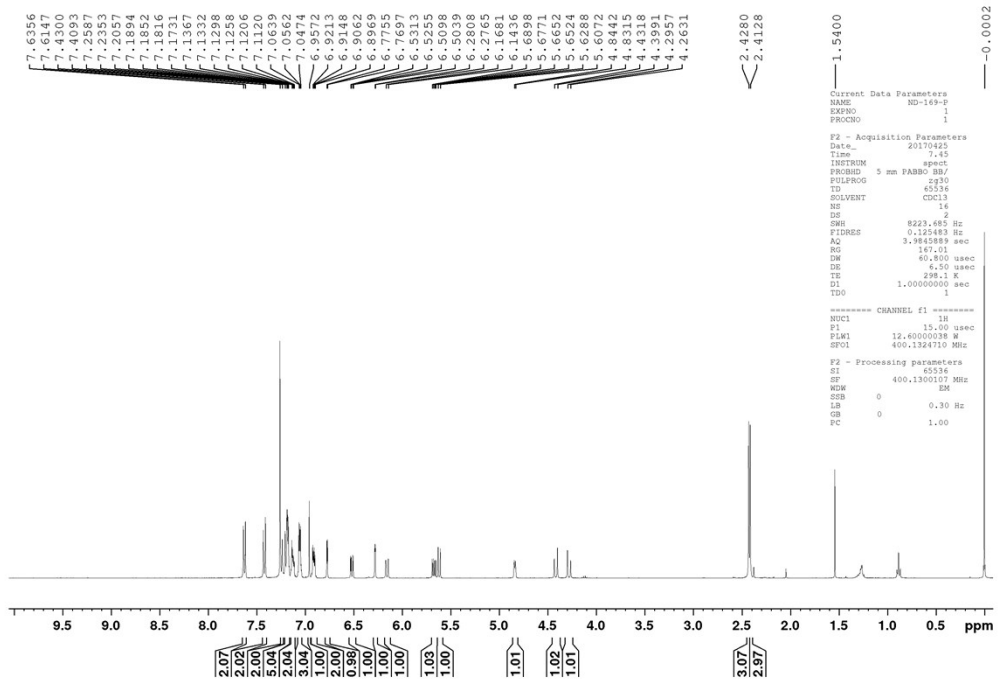


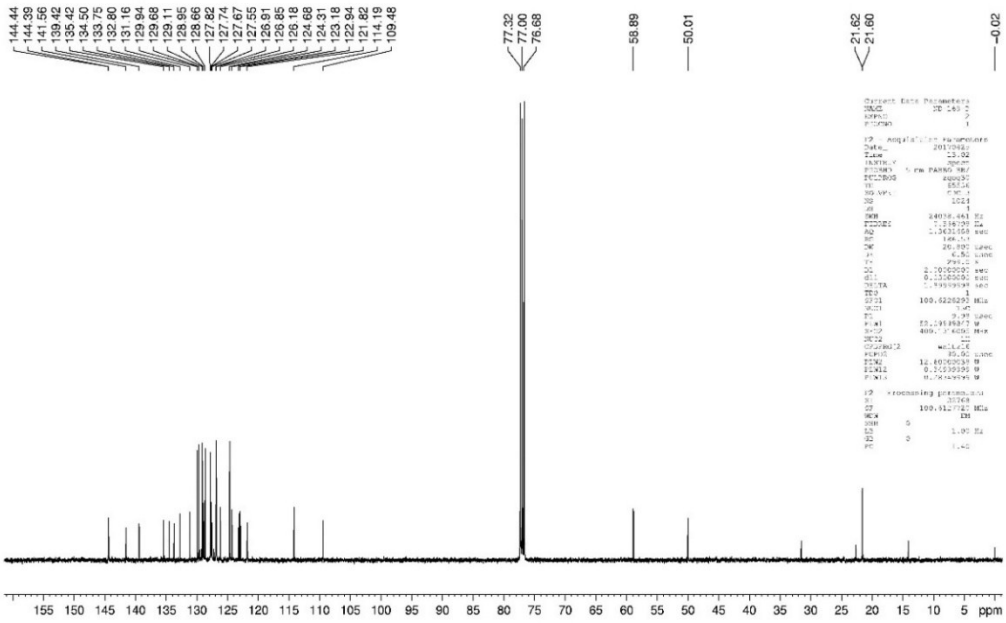
(*E*)-methyl 5-((4-methyl-*N*-phenylphenylsulfonamido)methylene)-1-phenyl-3-tosyl-3,4,5,5a-tetrahydro-[1,4]diazepino[1,7-*a*]quinoline-9-carboxylate (3da):



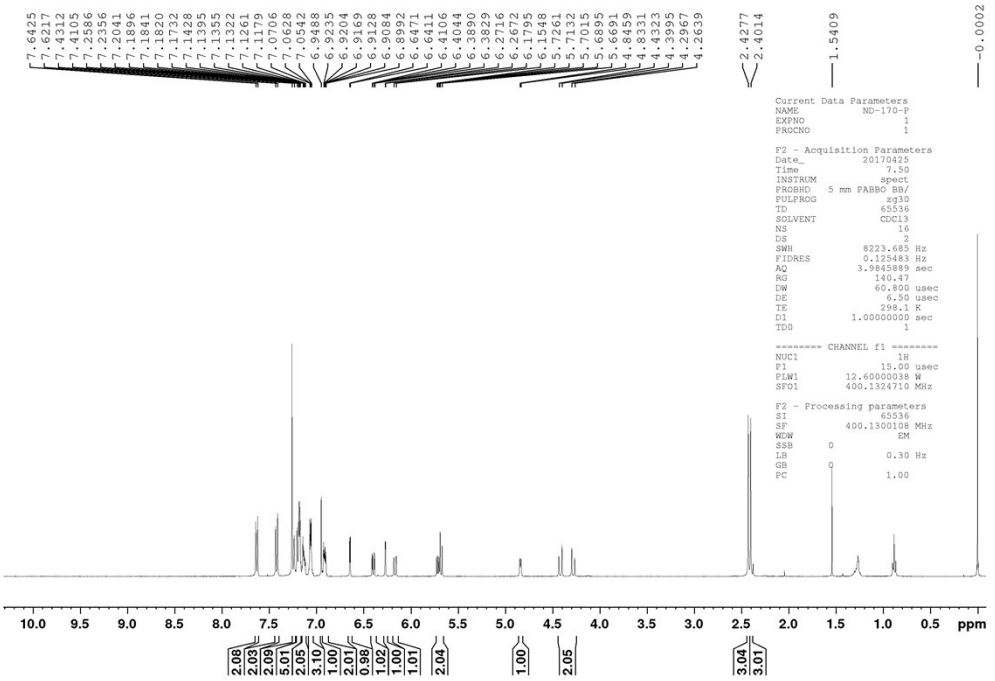


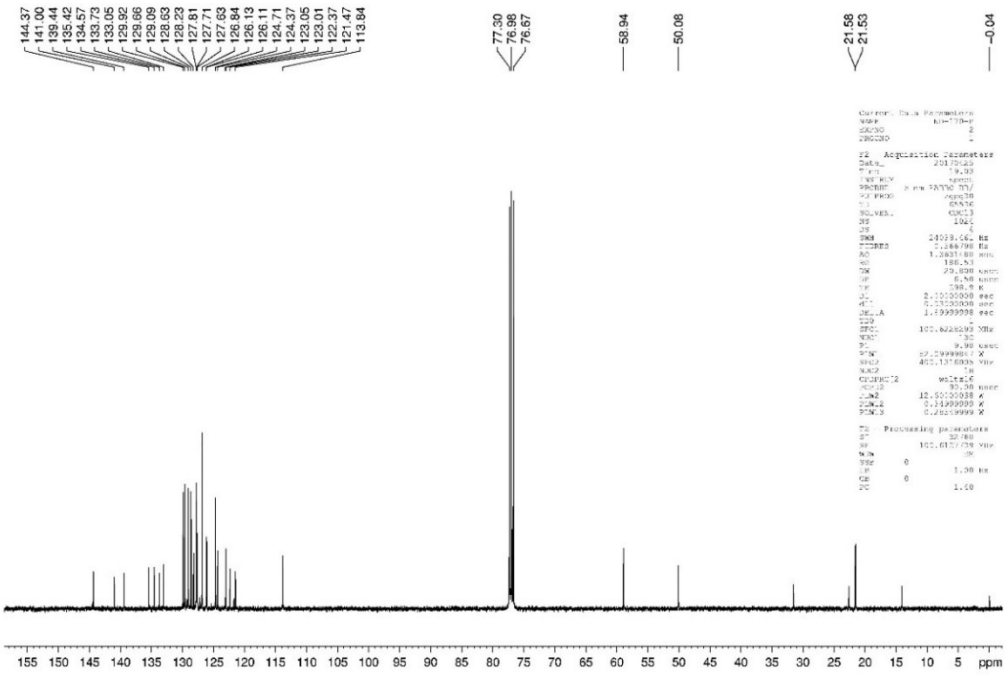
(*E*)-*N*-((9-bromo-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ea):



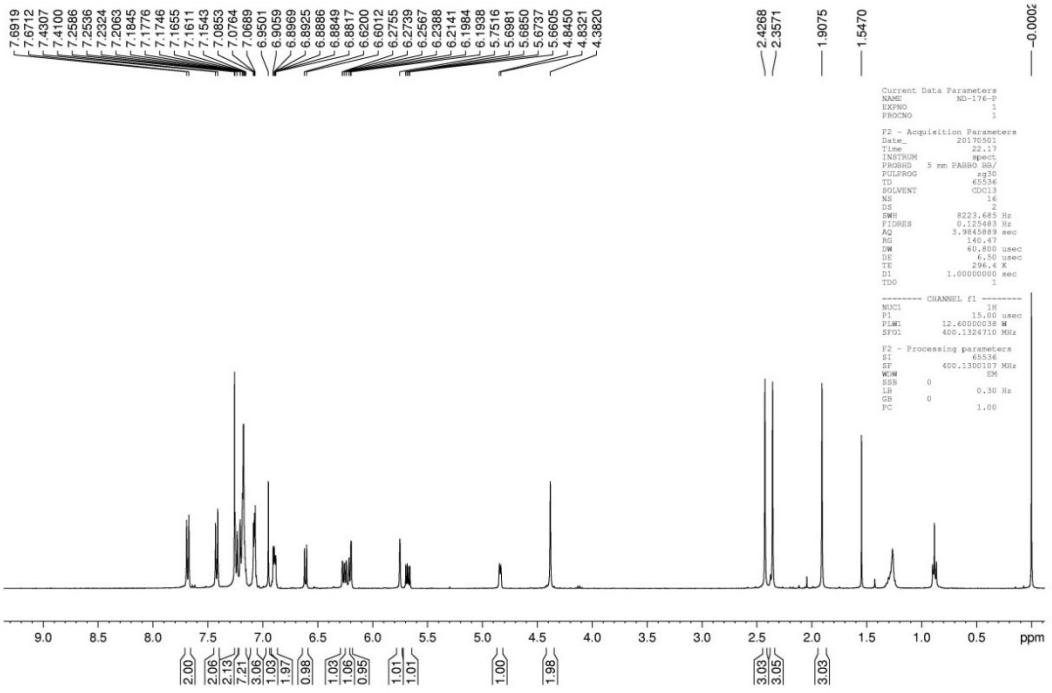


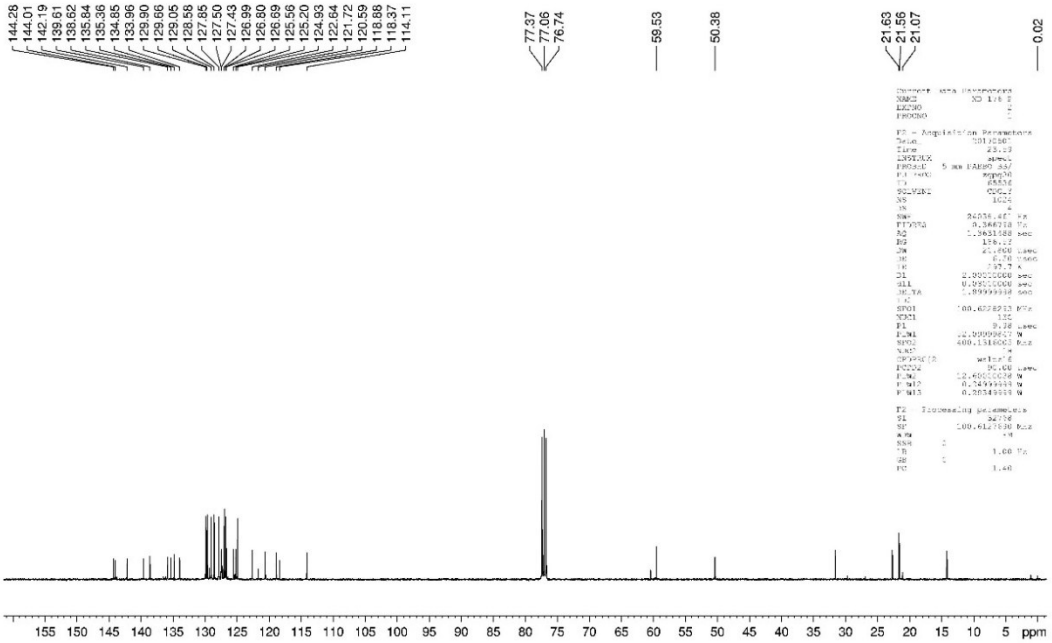
(*E*)-*N*-((9-chloro-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3fa):



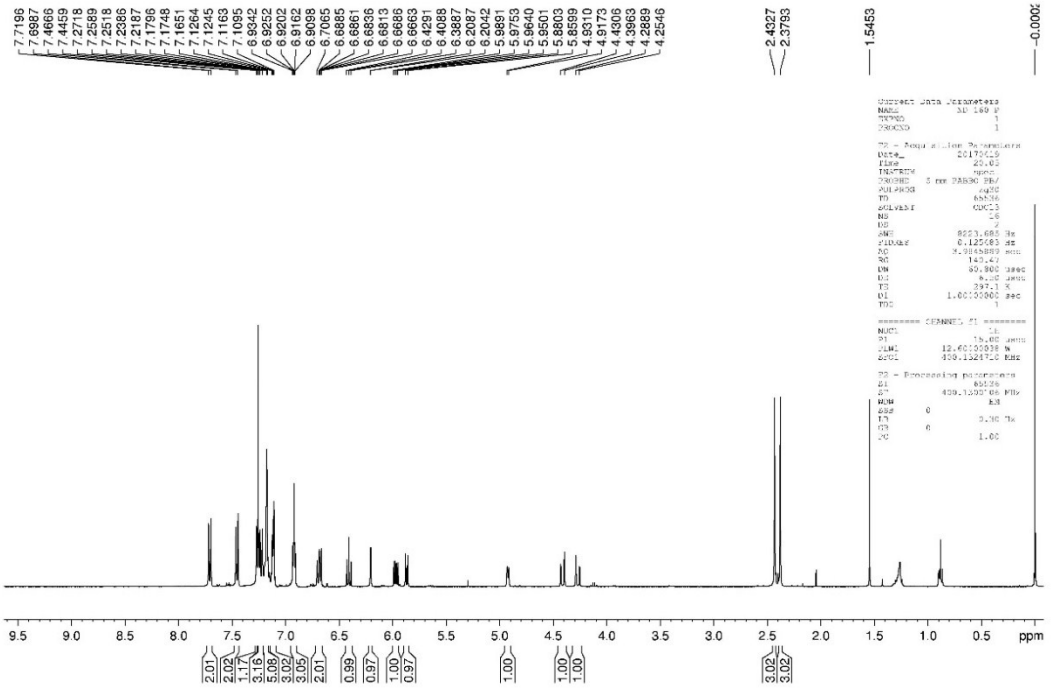


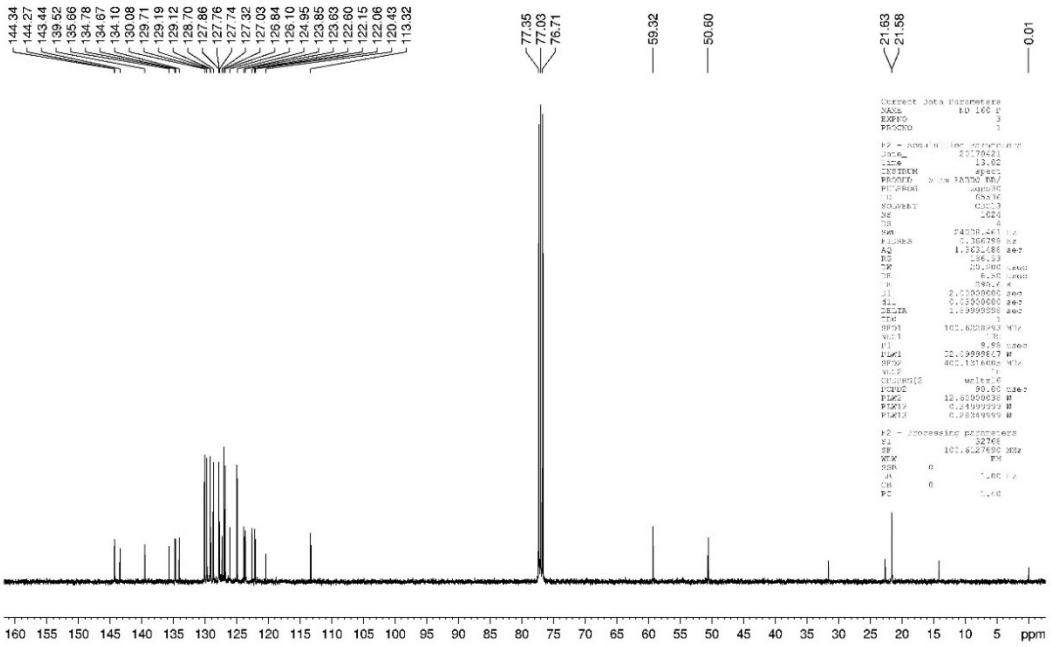
(*E*)-4-methyl-*N*-((10-methyl-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ga):



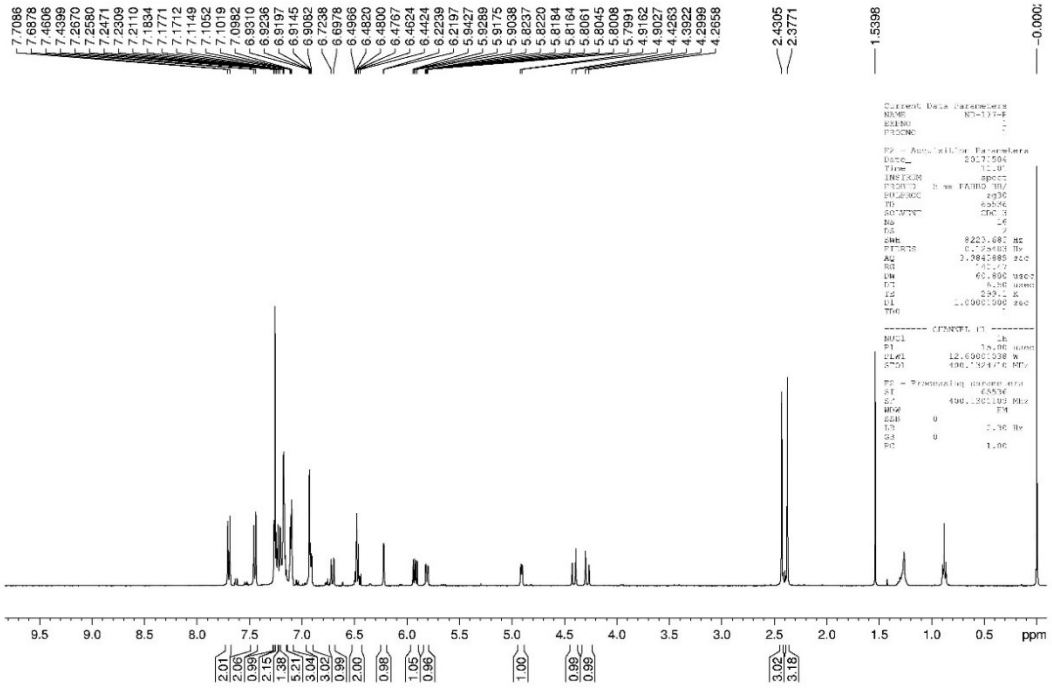


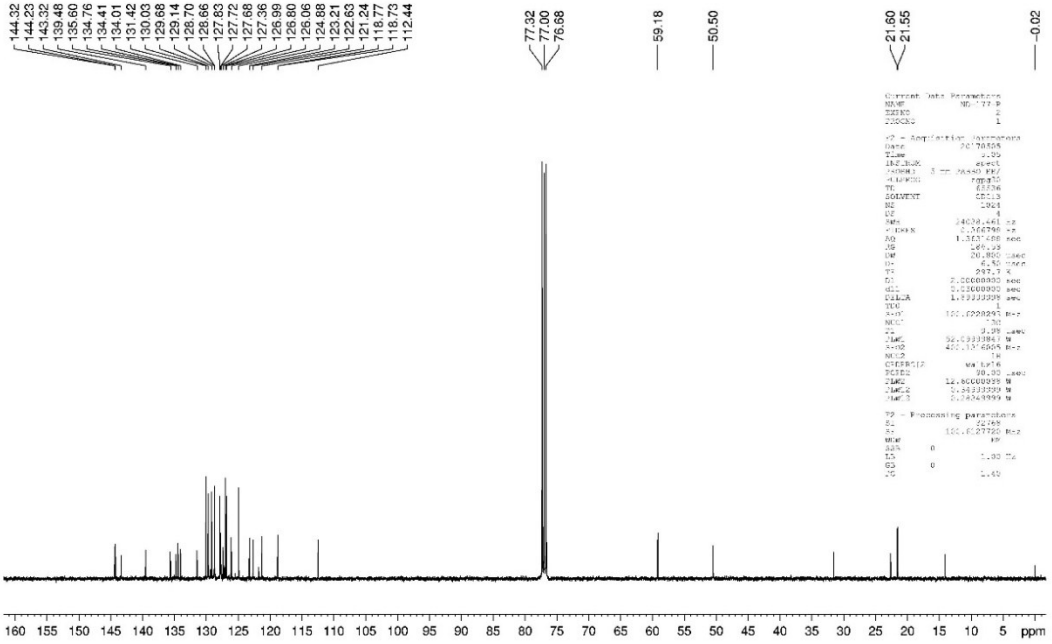
(*E*)-*N*-((8-bromo-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ha):



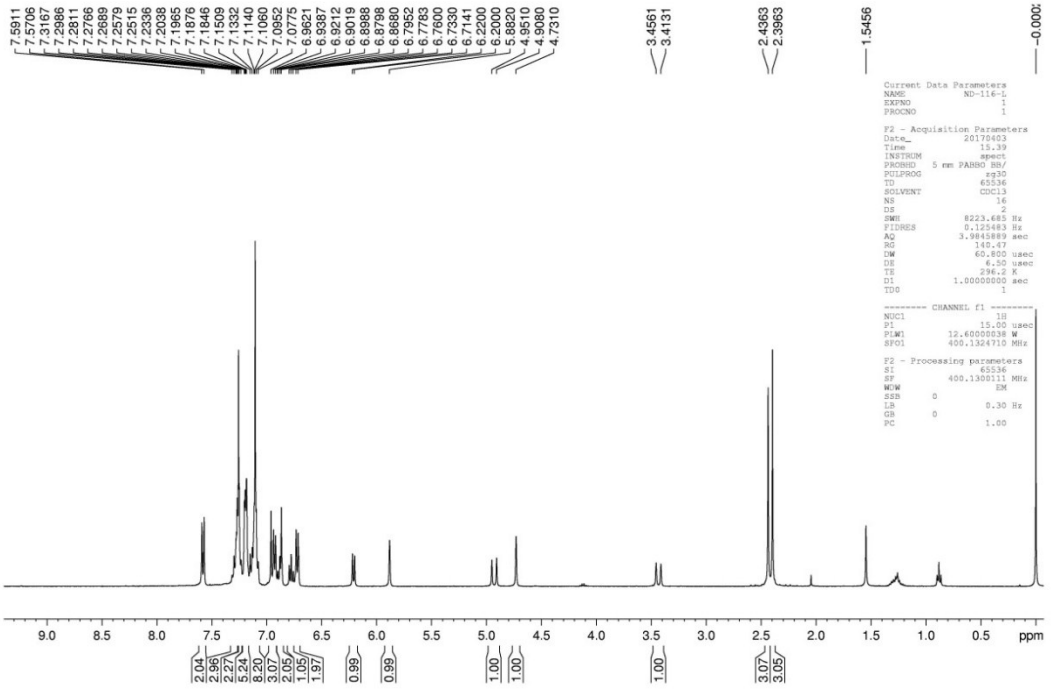


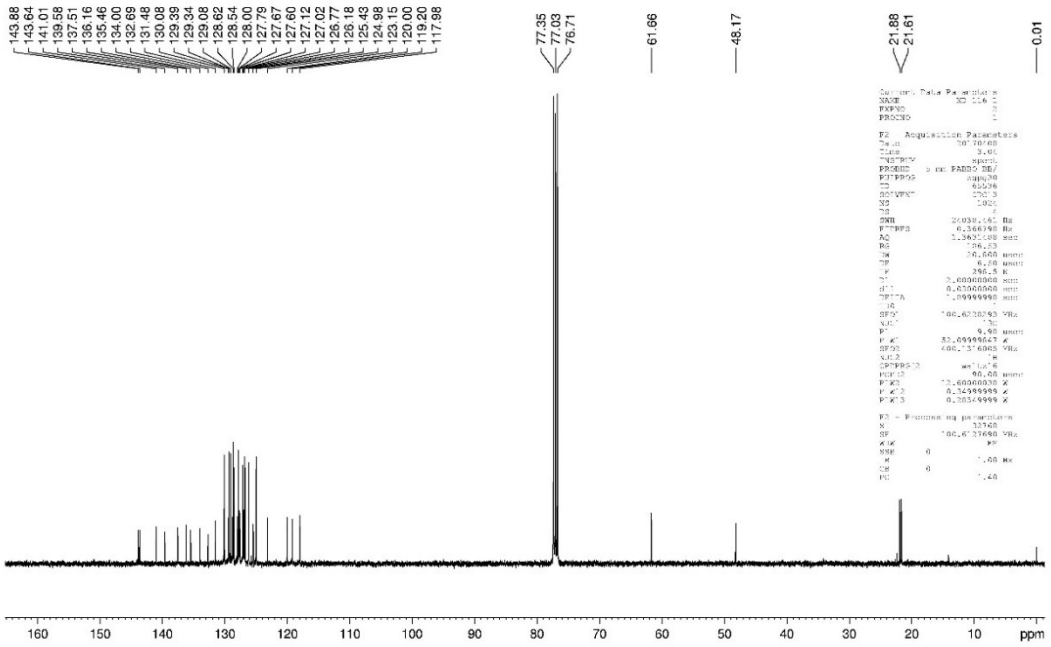
(*E*)-*N*-((8-chloro-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ia):



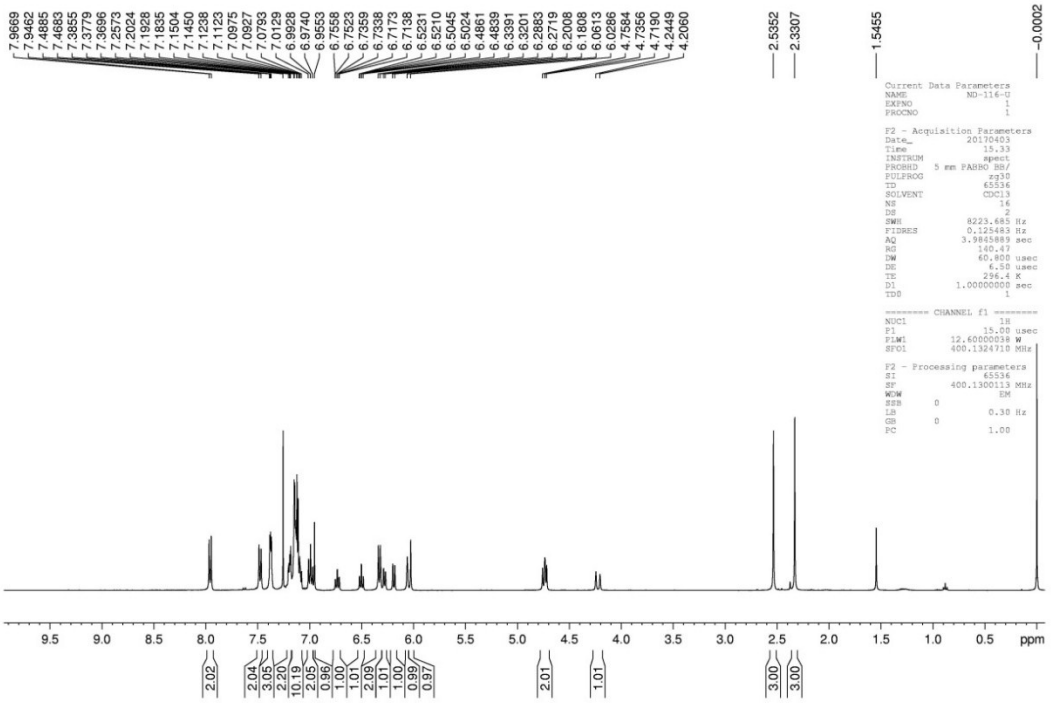


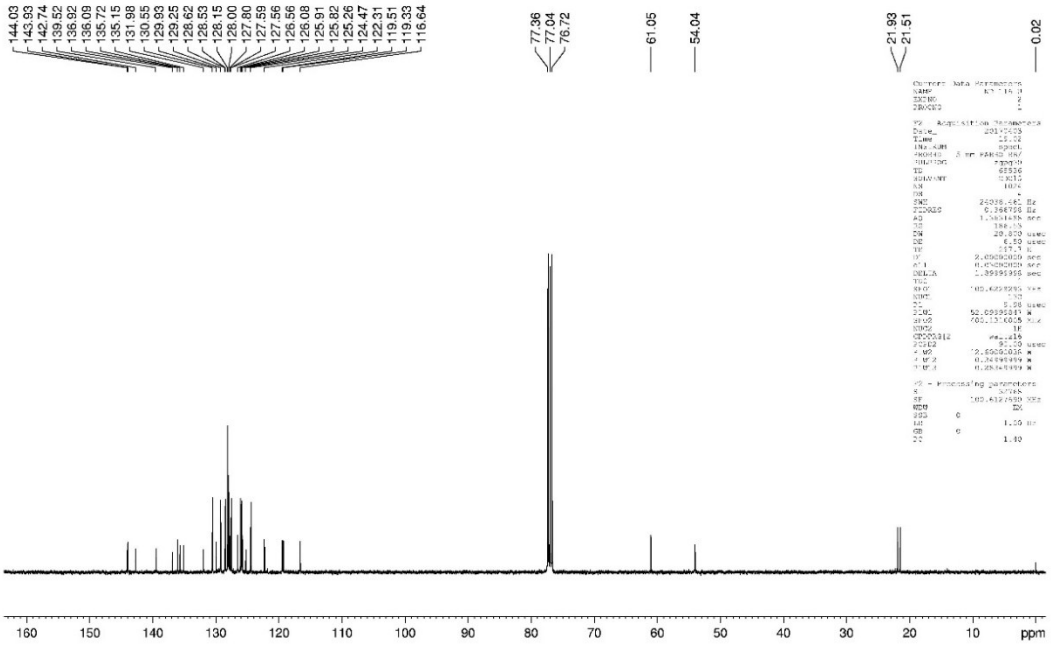
(*E*)-*N*-((1,6-diphenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ja, *E*-isomer):



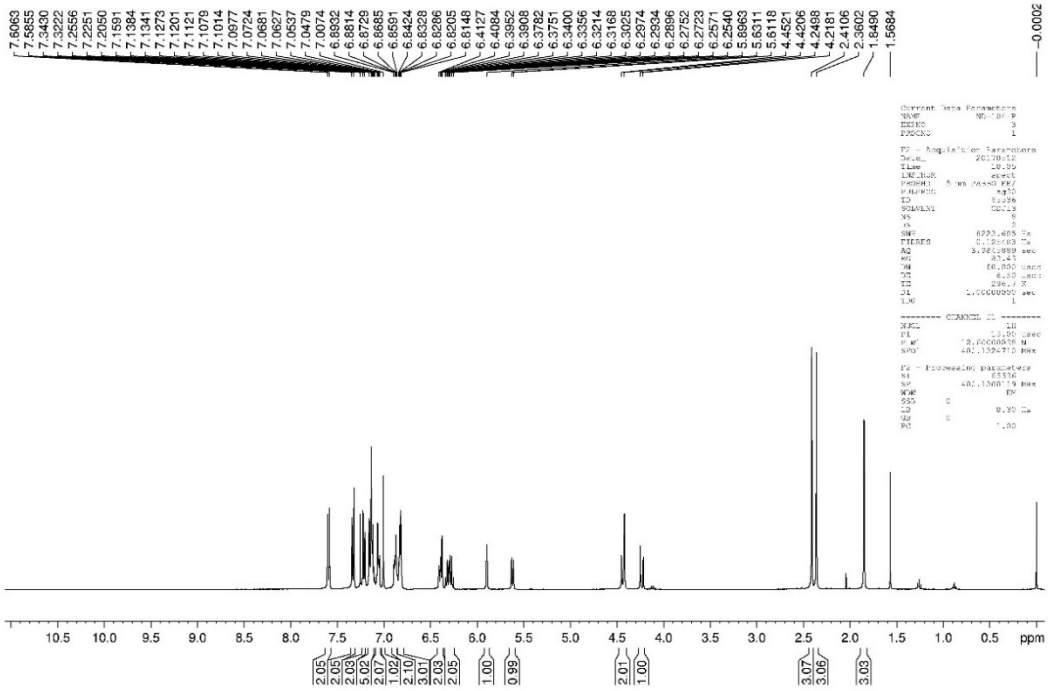


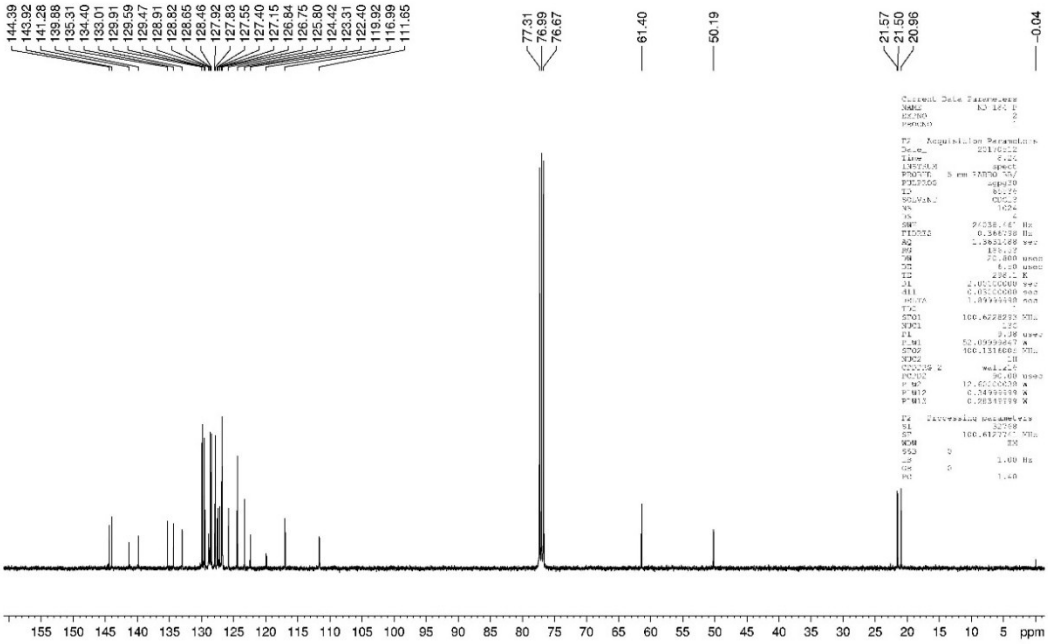
(*Z*)-*N*-((1,6-diphenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ja, *Z*-isomer):



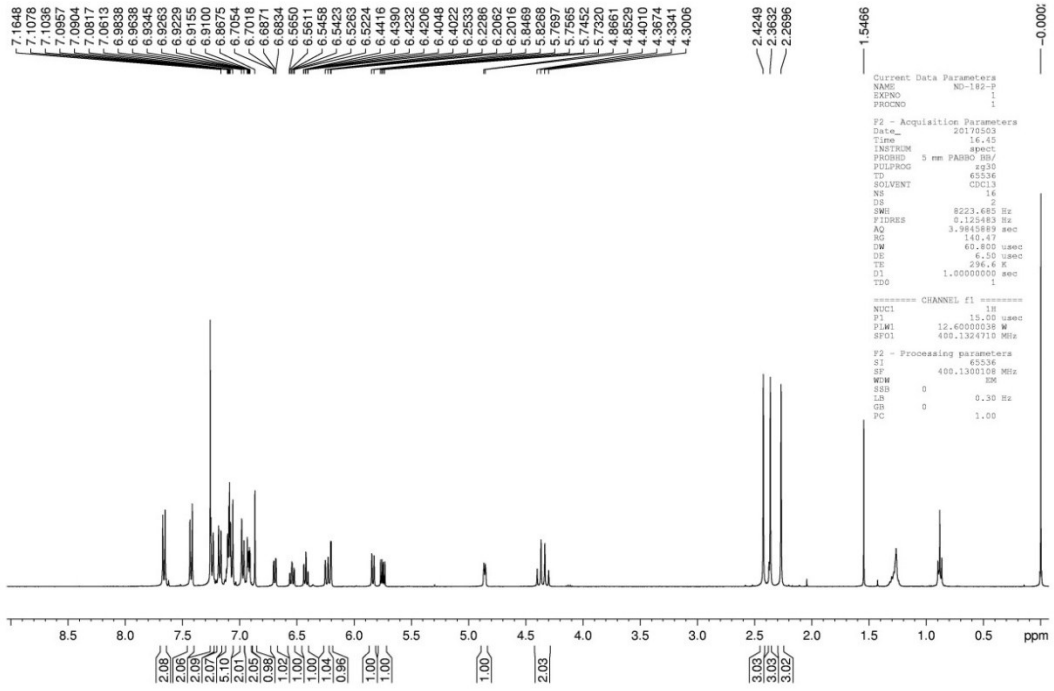


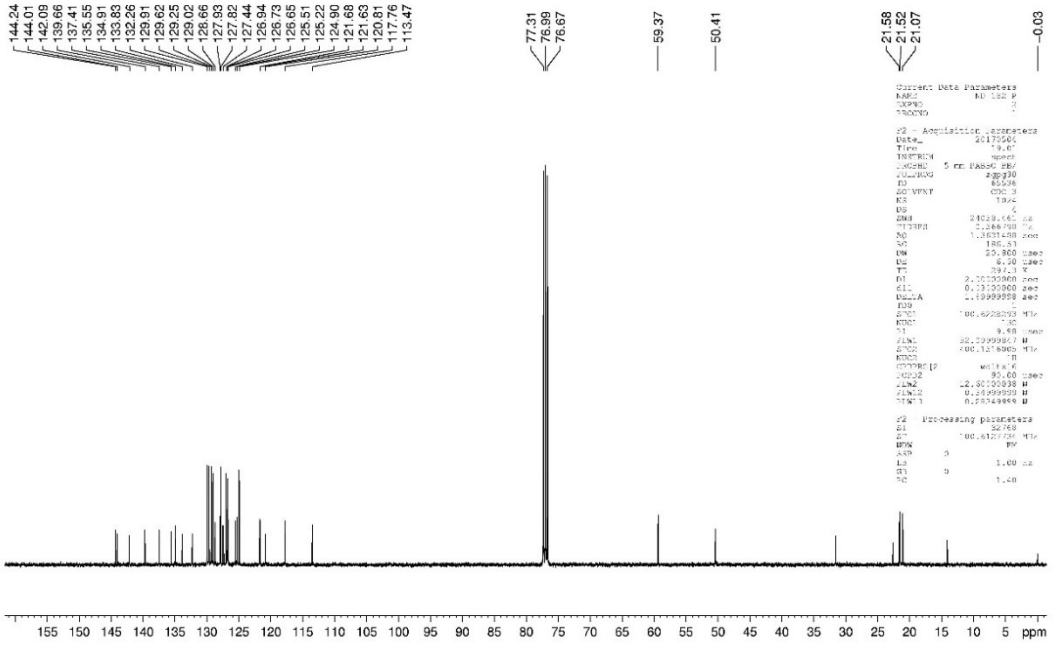
(*E*)-4-methyl-*N*-((6-methyl-1-phenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ka):



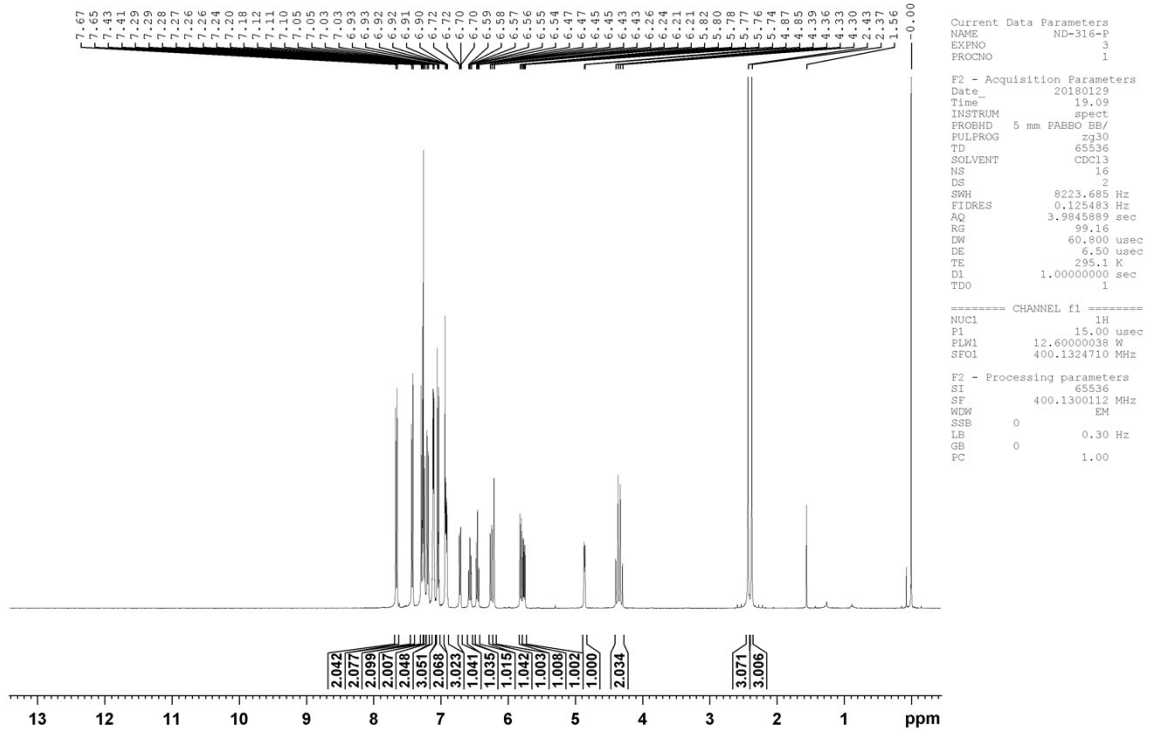


(*E*)-4-methyl-*N*-phenyl-*N*-((1-(p-tolyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3la):





(*E*)-*N*-((1-(4-bromophenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ma):

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Current Data Parameters
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EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180129
Time                     19.09
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                  zg30
TD                      65536
SOLVENT                 CDCl3
NS                         16
DS                          2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                      99.16
DW                     60.800 usec
DE                      6.50 usec
TE                     295.1 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                        1H
P1                      15.00 usec
PLW1               12.60000038 W
SFO1               400.1324710 MHz

F2 - Processing parameters
SI                          65536
SF                 400.1300112 MHz
WDW                            EM
SSB           0
LB                       0.30 Hz
GB            0
PC                       1.00
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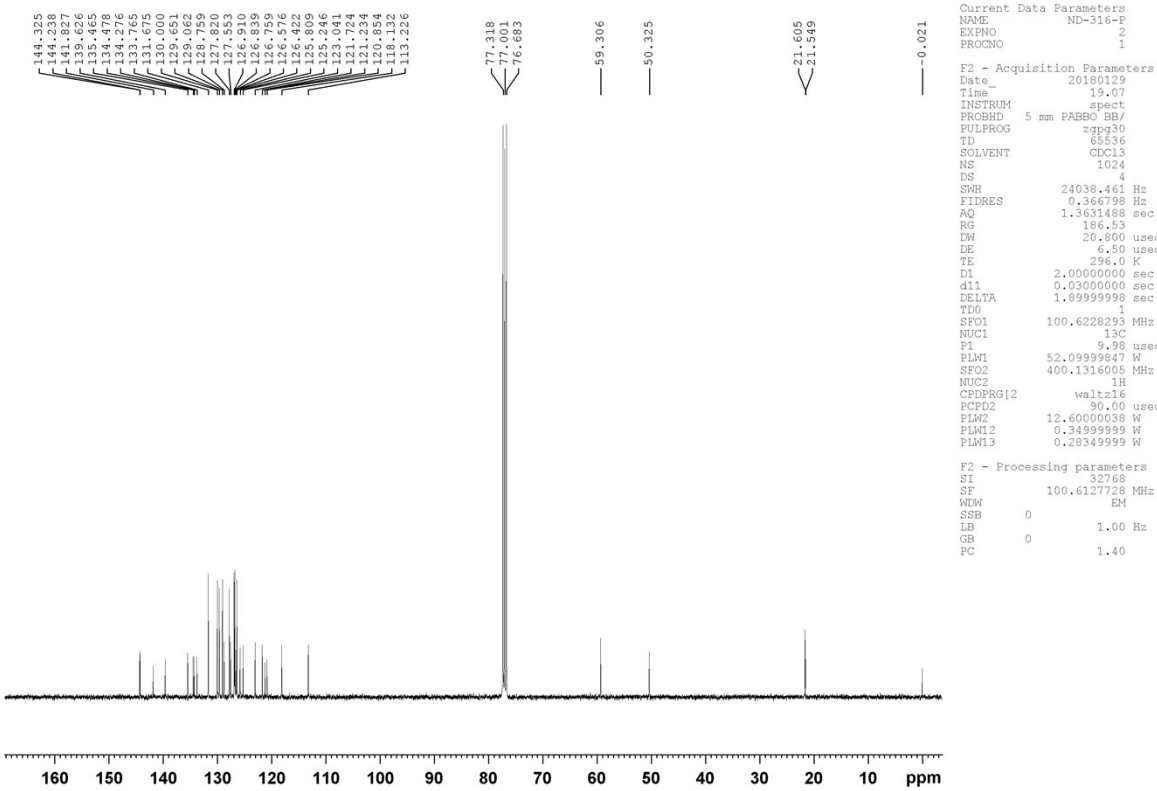


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Current Data Parameters
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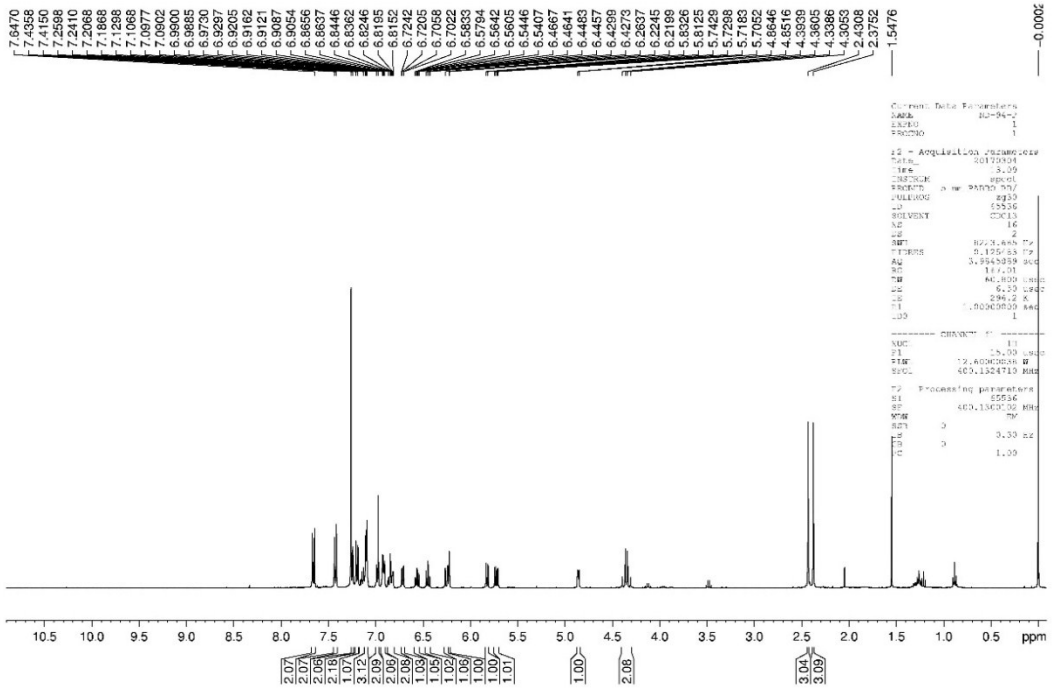
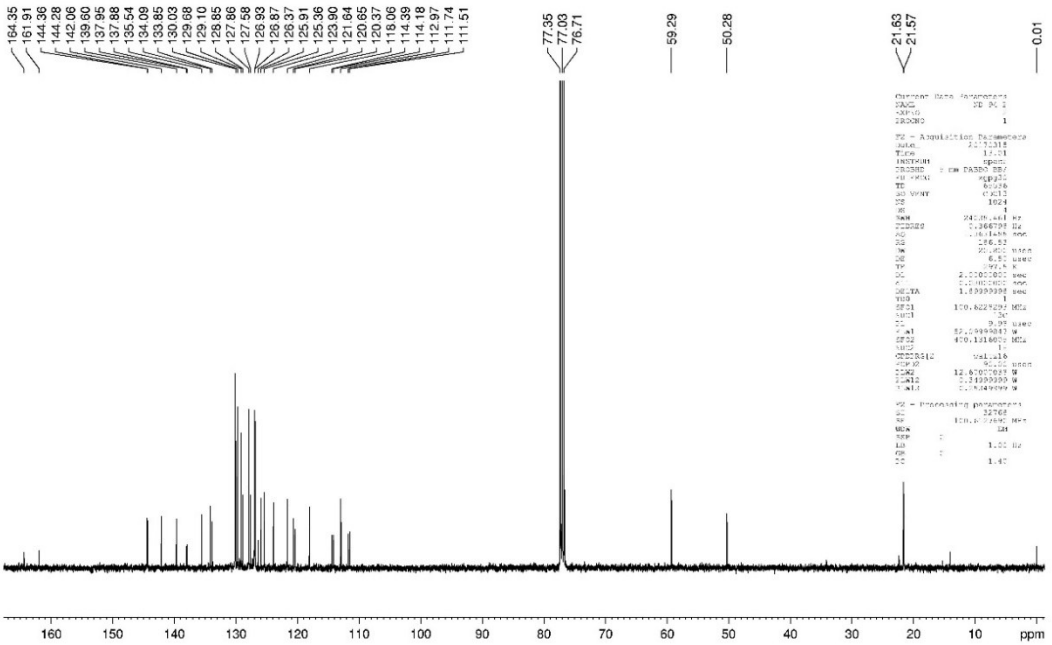
EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_                 20180129
Time                     19.07
INSTRUM                  spect
PROBHD    5 mm PABBO BB/
PULPROG                zgpg30
TD                      65536
SOLVENT                 CDCl3
NS                       1024
DS                          4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                     20.800 usec
DE                      6.50 usec
TE                     296.0 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                          1
SFO1               100.6228293 MHz
NUC1                        13C
P1                       9.98 usec
PLW1               52.09999847 W
SFO2               400.1316005 MHz
NUC2                        1H
CPDPRG[2                waltz16
PCPD2                   90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

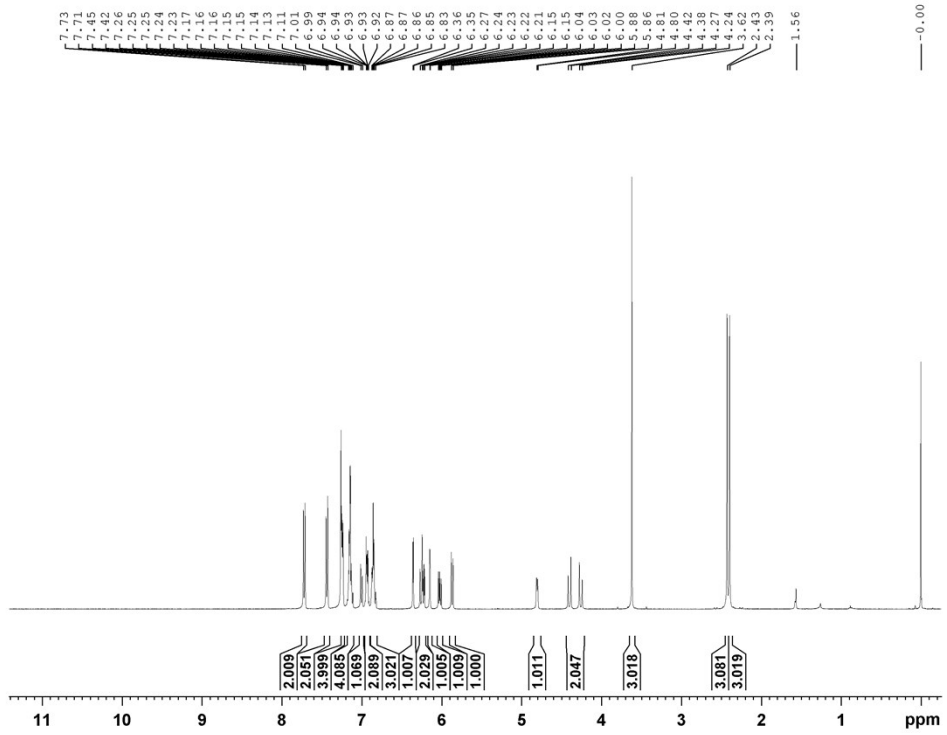
F2 - Processing parameters
SI                          32768
SF                 100.6127728 MHz
WDW                            EM
SSB           0
LB                       1.00 Hz
GB            0
PC                       1.40
```

(*E*)-*N*-((1-(3-fluorophenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3na):





(*E*)-*N*-((1-(3-fluorophenyl)-9-methoxy-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3oa):

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EXPNO                        2
PROCNO                       1

F2 - Acquisition Parameters
Date_               20180129
Time                   12.01
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                           4
DS                           2
SWH                 8223.685 Hz
FIDRES              0.125483 Hz
AQ                  3.9845889 sec
RG                     99.16
DW                    60.800 usec
DE                     6.50 usec
TE                    293.9 K
D1                  1.00000000 sec
TD0                          1

======== CHANNEL f1 ========
NUC1                       1H
P1                      15.00 usec
PLW1               12.60000038 W
SFO1              400.1324710 MHz

F2 - Processing parameters
SI                        65536
SF                  400.1300105 MHz
WDW                          EM
SSB             0
LB                      0.30 Hz
GB              0
PC                      1.00
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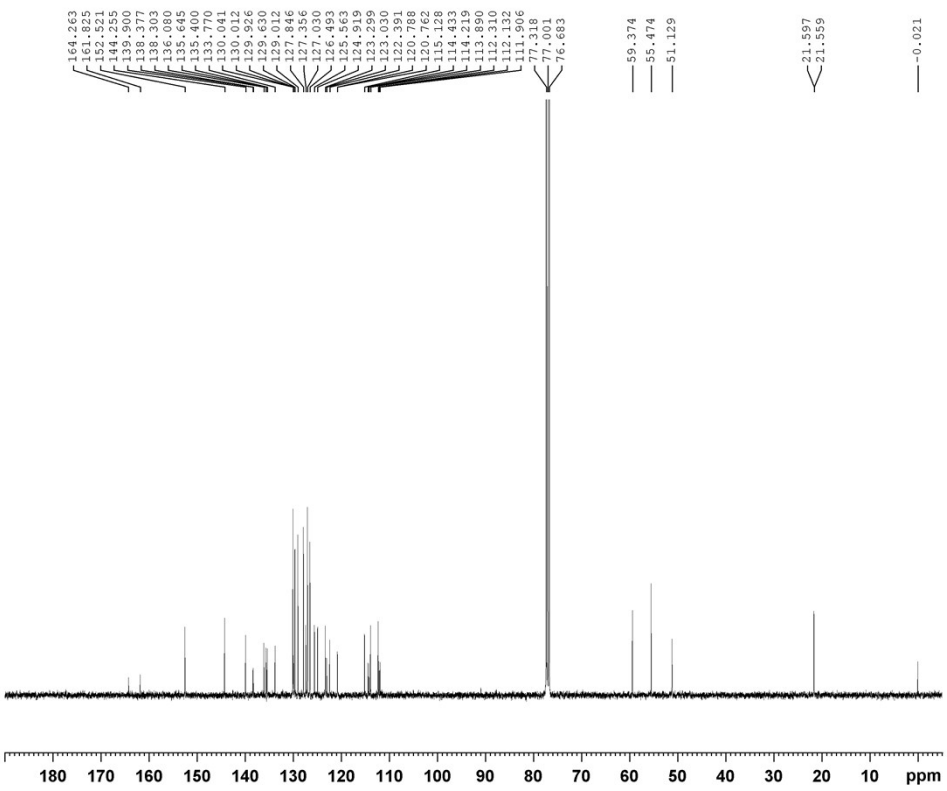
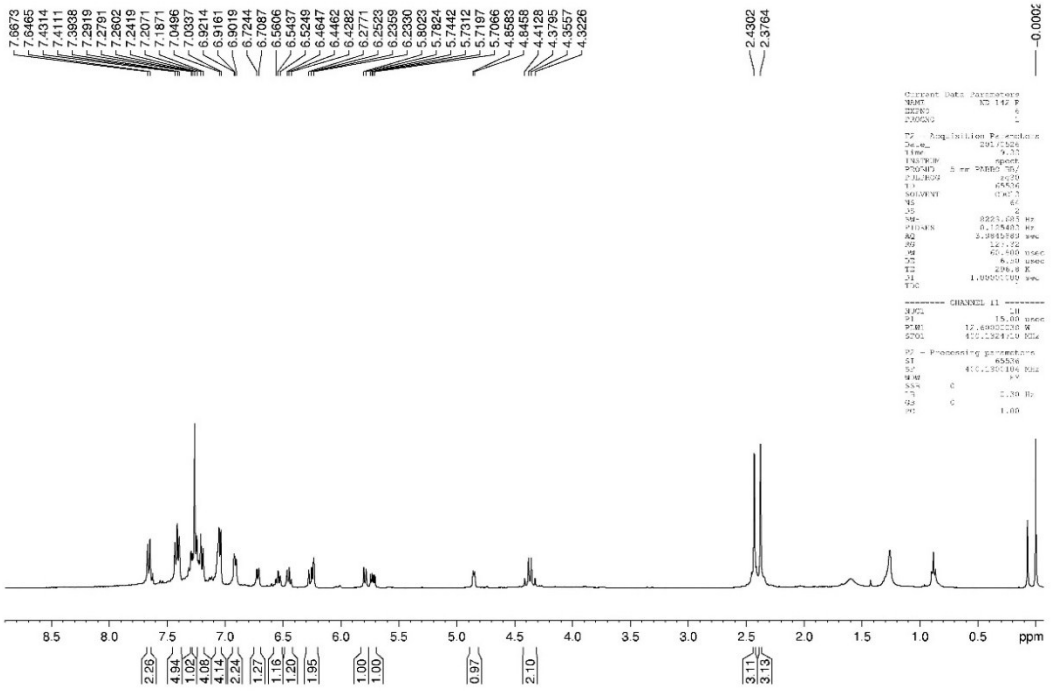


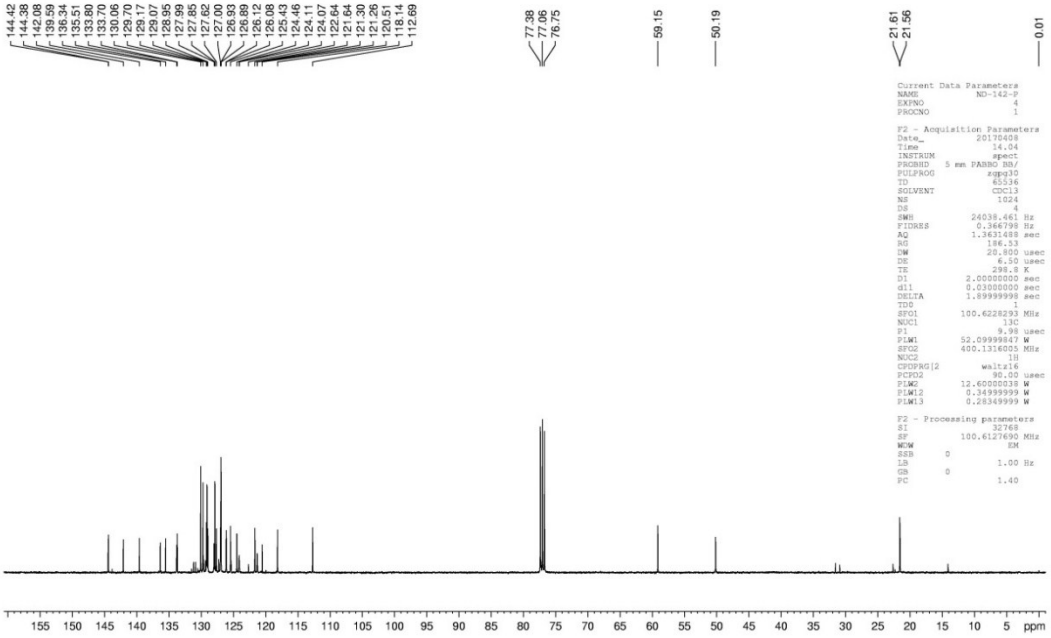

```
Current Data Parameters
NAME                  ND-317-P
EXPNO                        3
PROCNO                       1

F2 - Acquisition Parameters
Date_               20180129
Time                   13.04
INSTRUM                spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                        1024
DS                           4
SWH                24038.461 Hz
FIDRES              0.366798 Hz
AQ                  1.3631488 sec
RG                     186.53
DW                    20.800 usec
DE                     6.50 usec
TE                    295.5 K
D1                  2.00000000 sec
d11                 0.03000000 sec
DELTA               1.89999998 sec
TD0                          1
SFO1               100.6228293 MHz
NUC1                       13C
P1                      9.98 usec
PLW1               52.09999847 W
SFO2              400.1316005 MHz
NUC2                       1H
CPDPRG[2                waltz16
PCPD2                  90.00 usec
PLW2               12.60000038 W
PLW12               0.34999999 W
PLW13               0.28349999 W

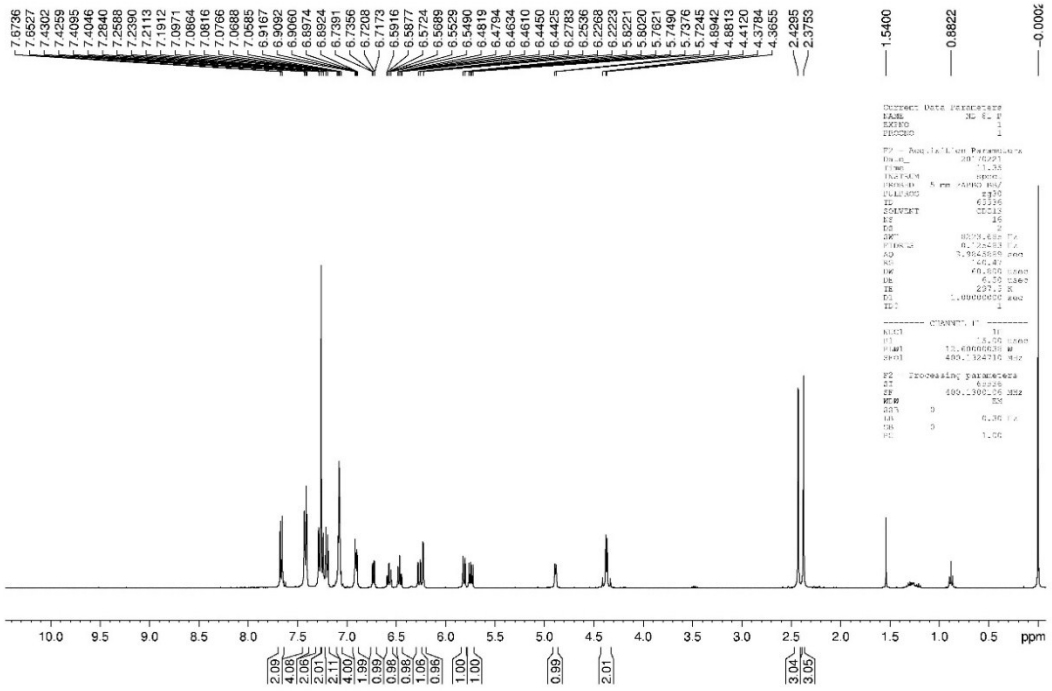
F2 - Processing parameters
SI                        32768
SF                  100.6127727 MHz
WDW                          EM
SSB             0
LB                      1.00 Hz
GB              0
PC                      1.40
```

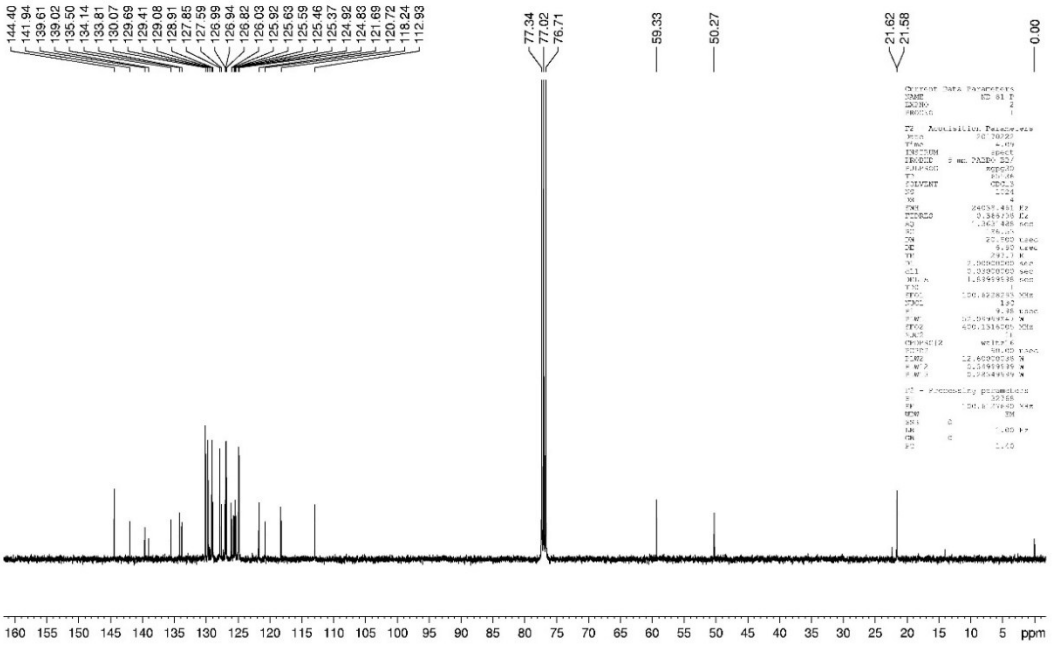
(*E*)-4-methyl-*N*-phenyl-*N*-((3-tosyl-1-(3-(trifluoromethyl)phenyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3pa):



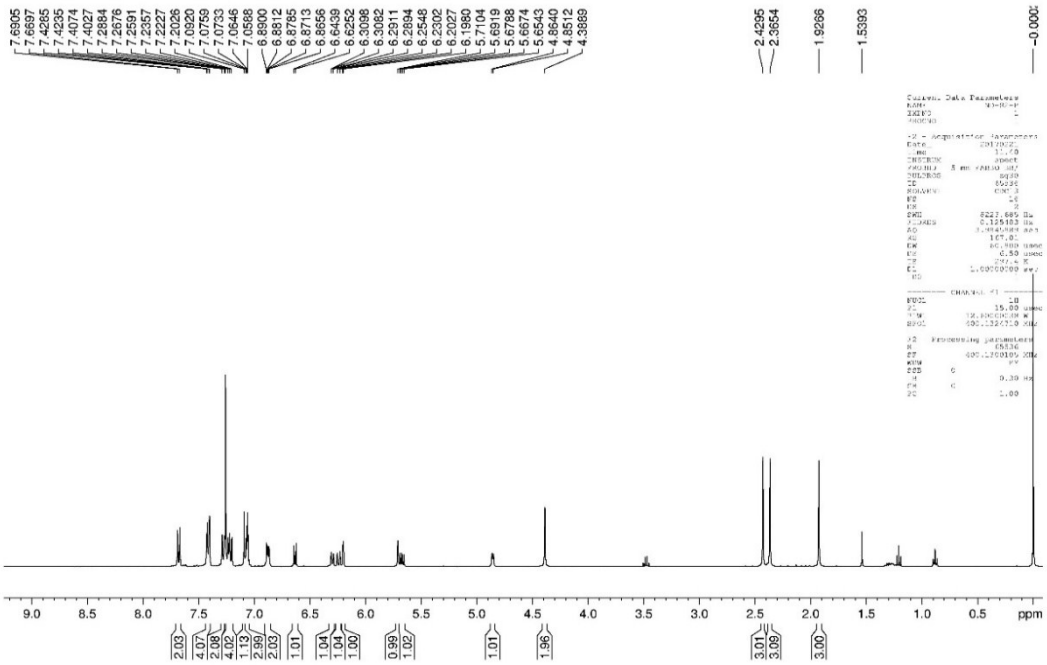


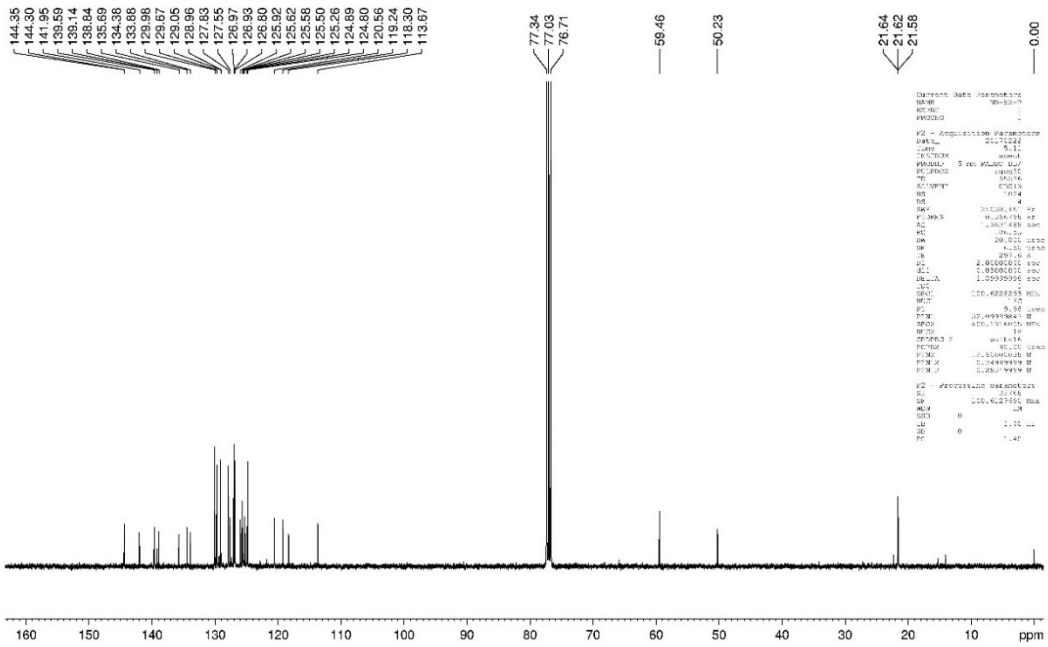
(*E*)-4-methyl-*N*-phenyl-*N*-((3-tosyl-1-(4-(trifluoromethyl)phenyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3qa):



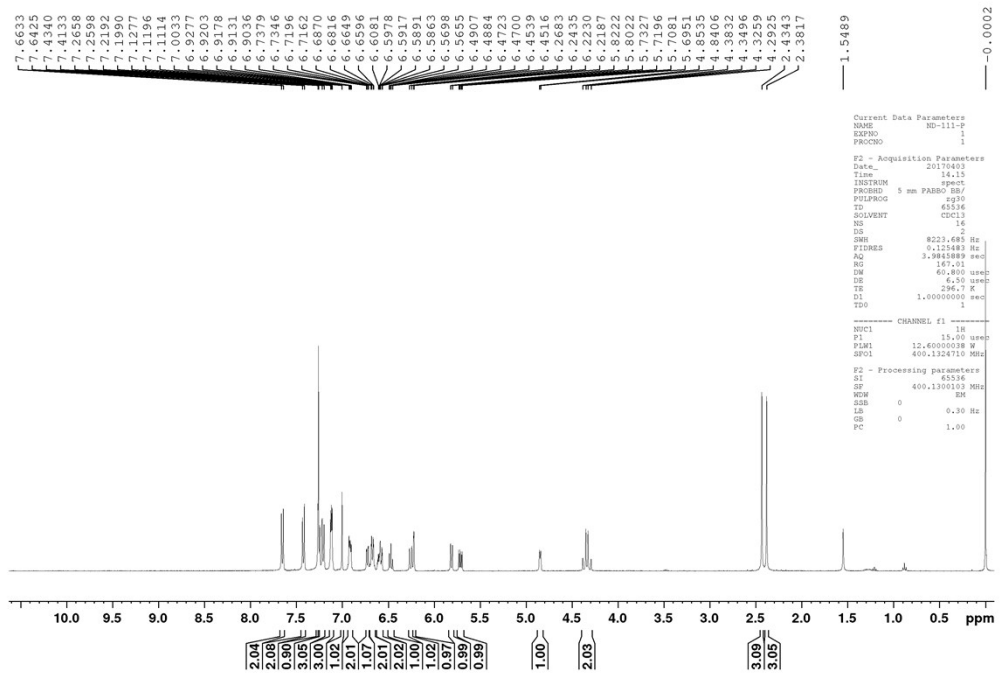


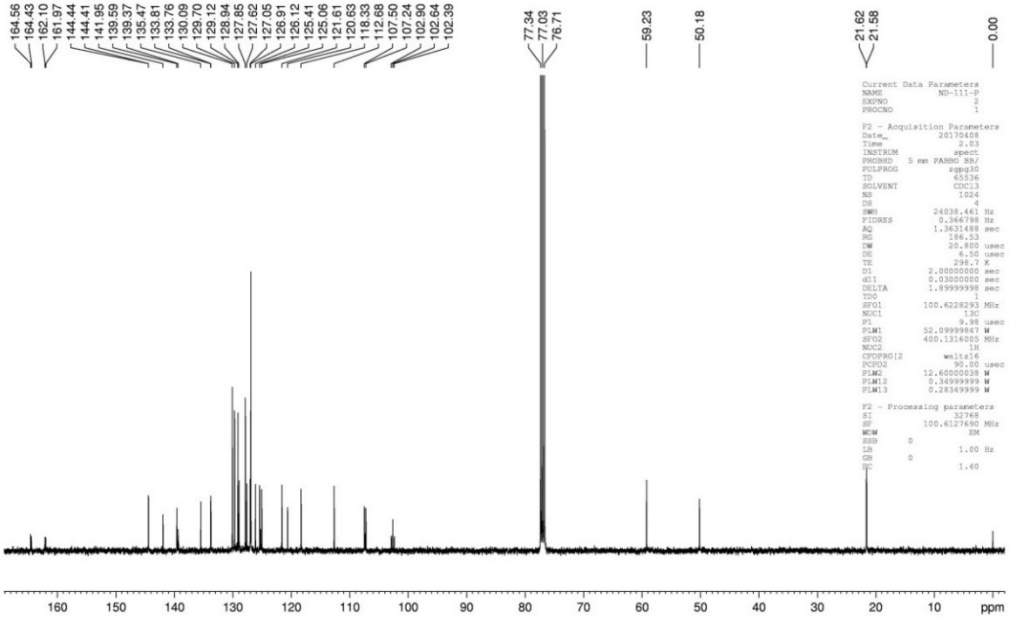
(*E*)-4-methyl-*N*-((10-methyl-3-tosyl-1-(4-(trifluoromethyl)phenyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-*N*-phenylbenzenesulfonamide (3ra):



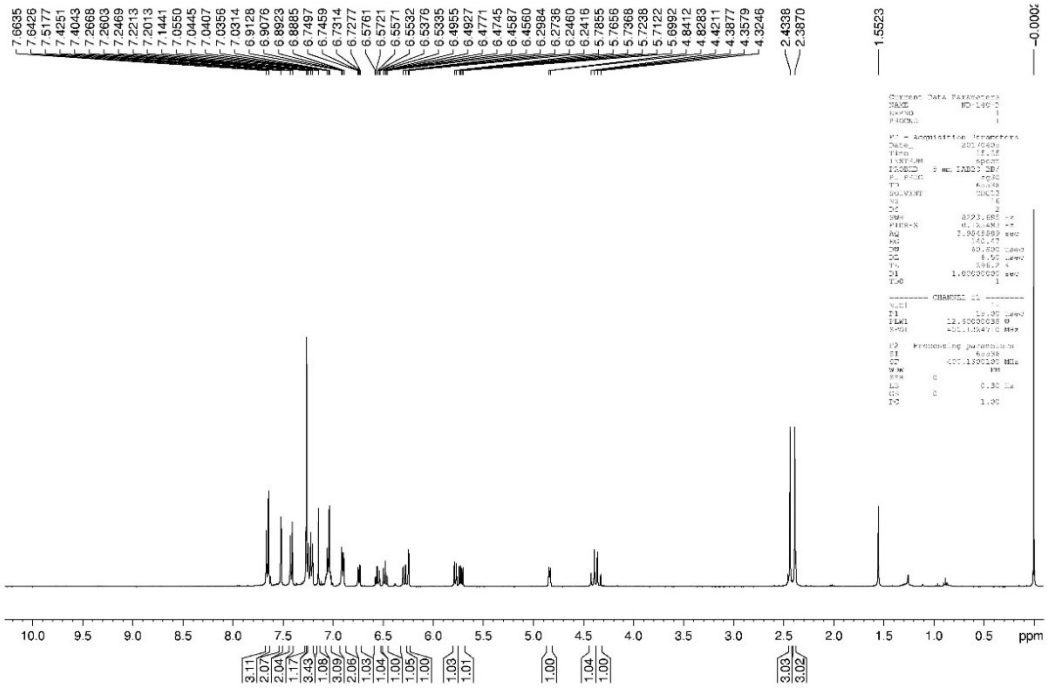


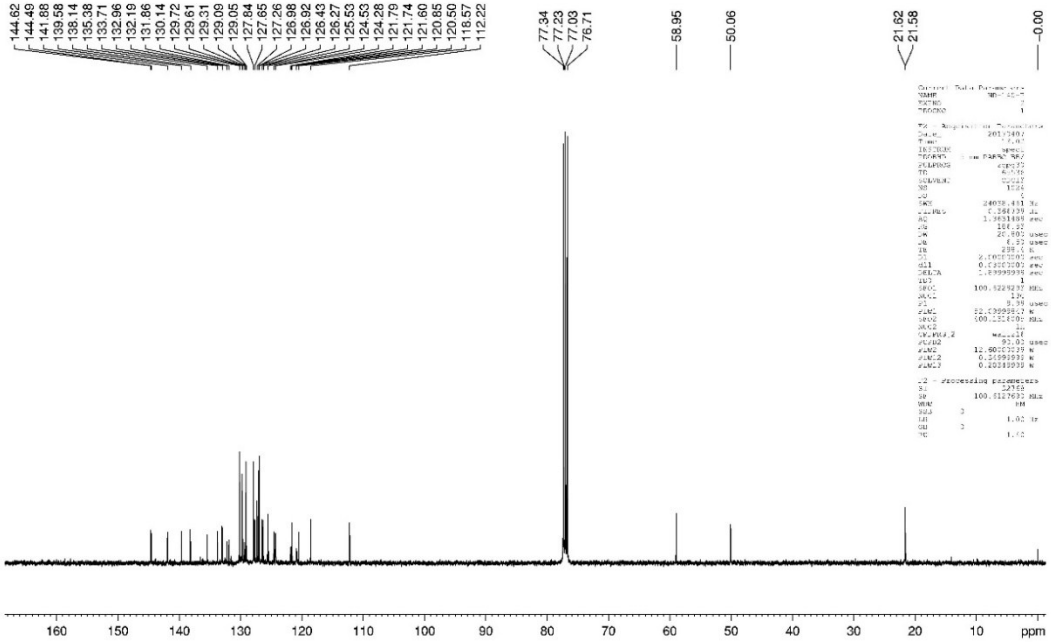
(*E*)-*N*-((1-(3,5-difluorophenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3sa):



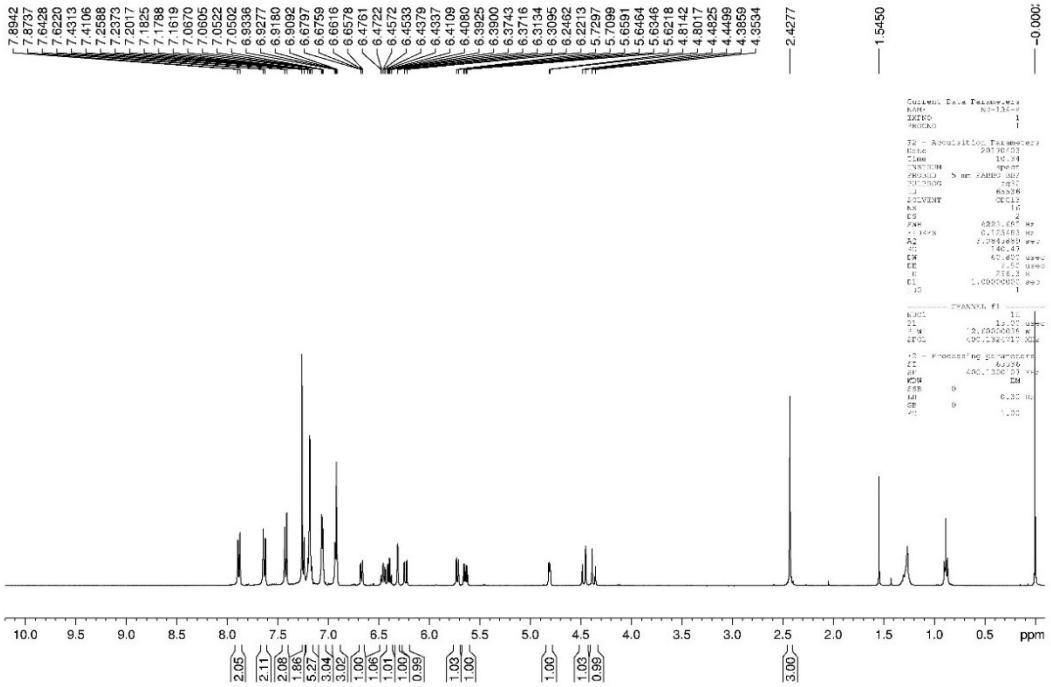


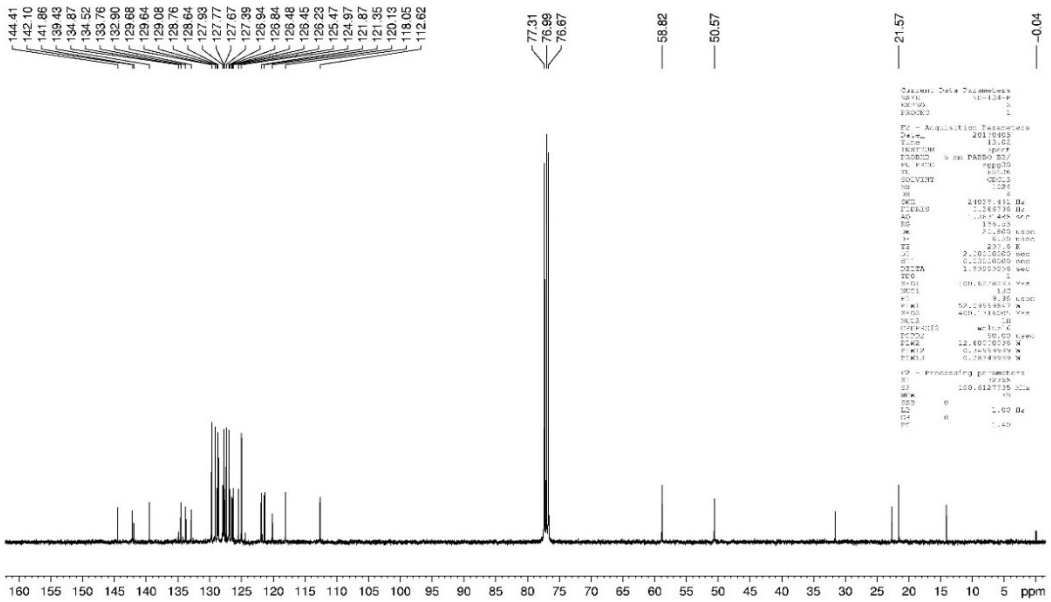
(*E*)-*N*-((1-(3,5-bis(trifluoromethyl)phenyl)-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (3ta):



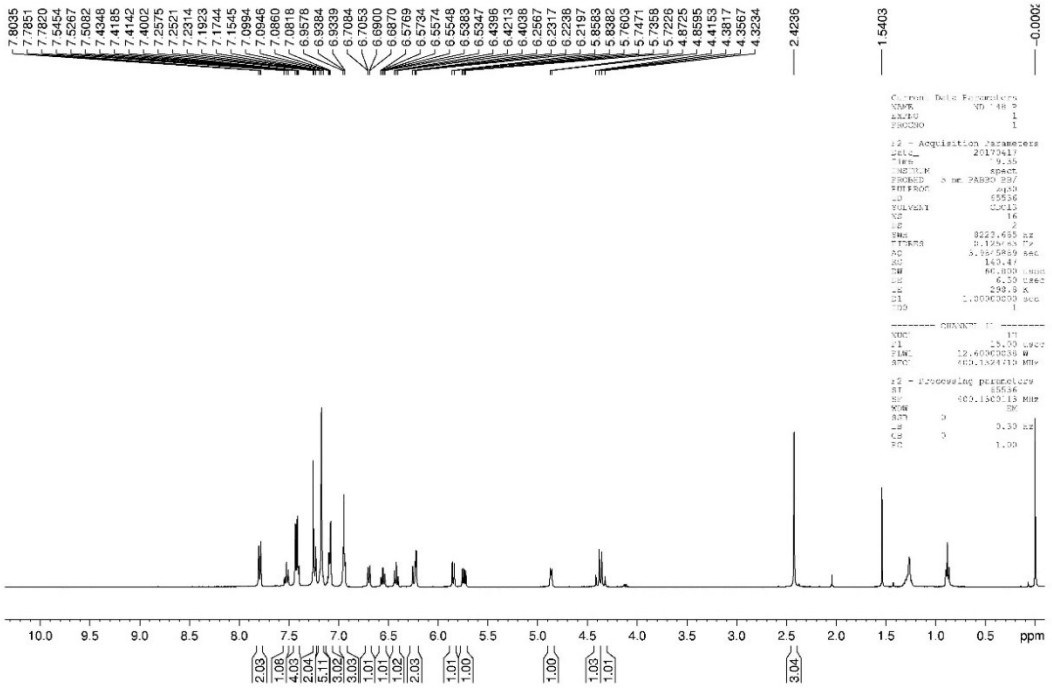


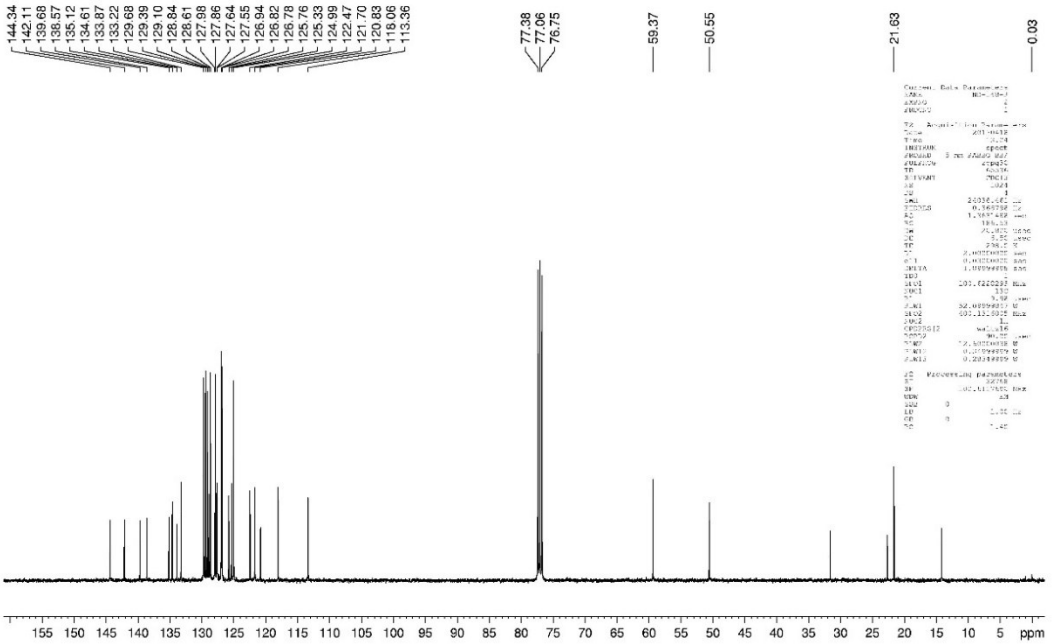
(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-((4-(trifluoromethyl)phenyl)sulfonyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3ua):



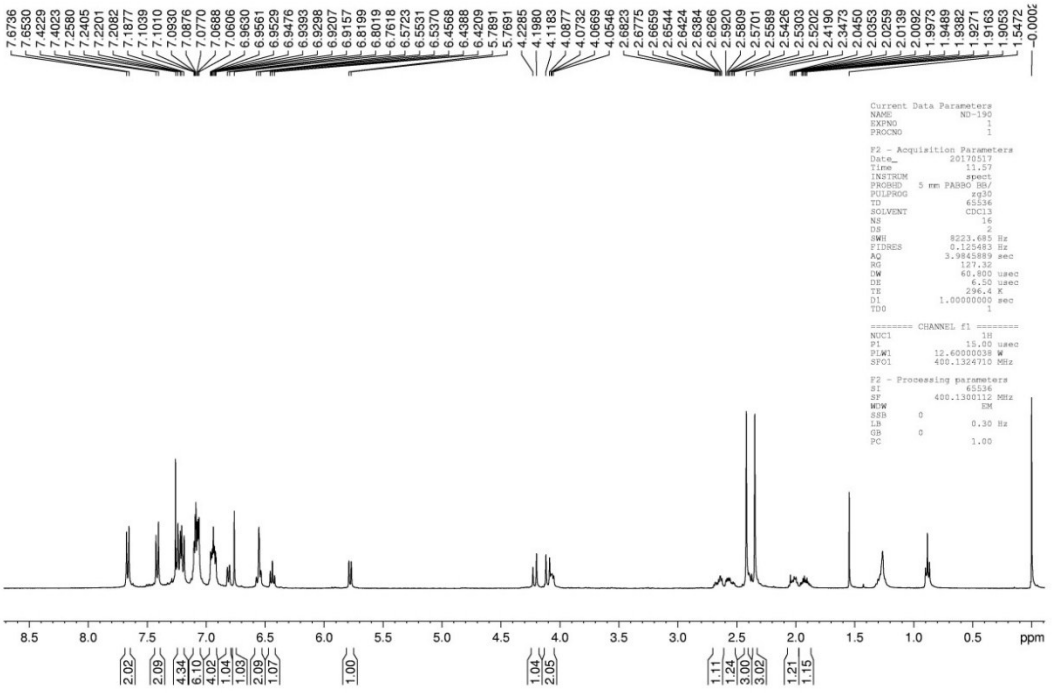


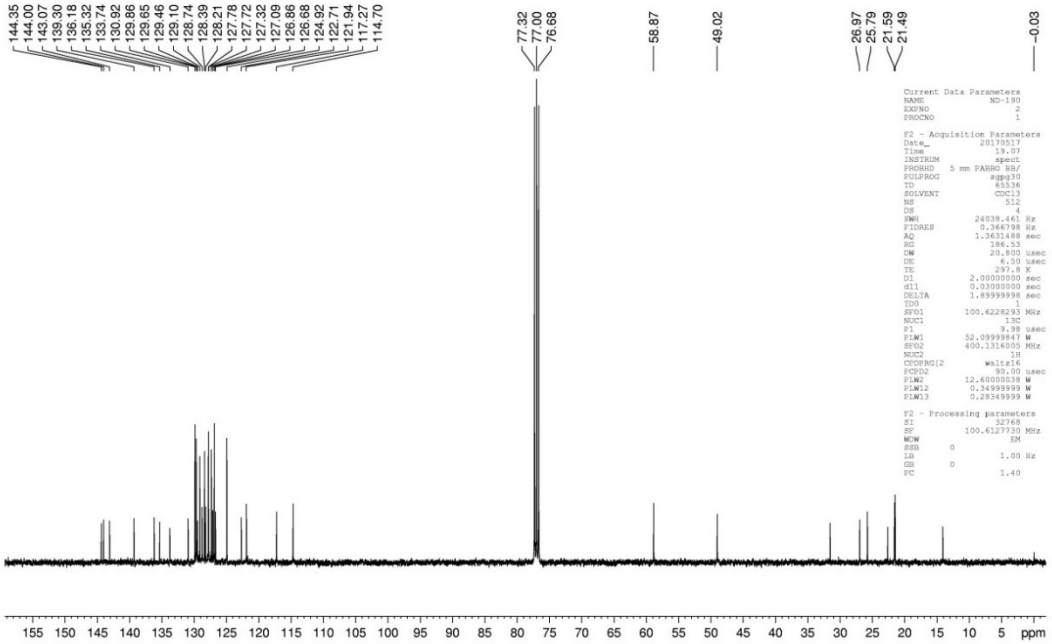
(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-(phenylsulfonyl)-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (3va):



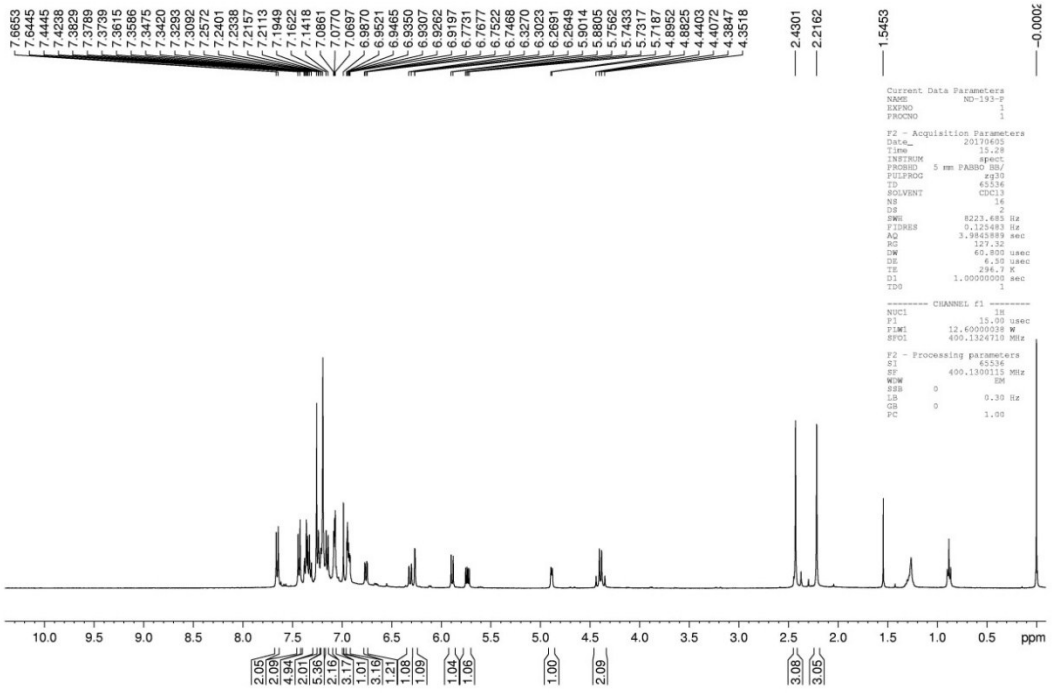


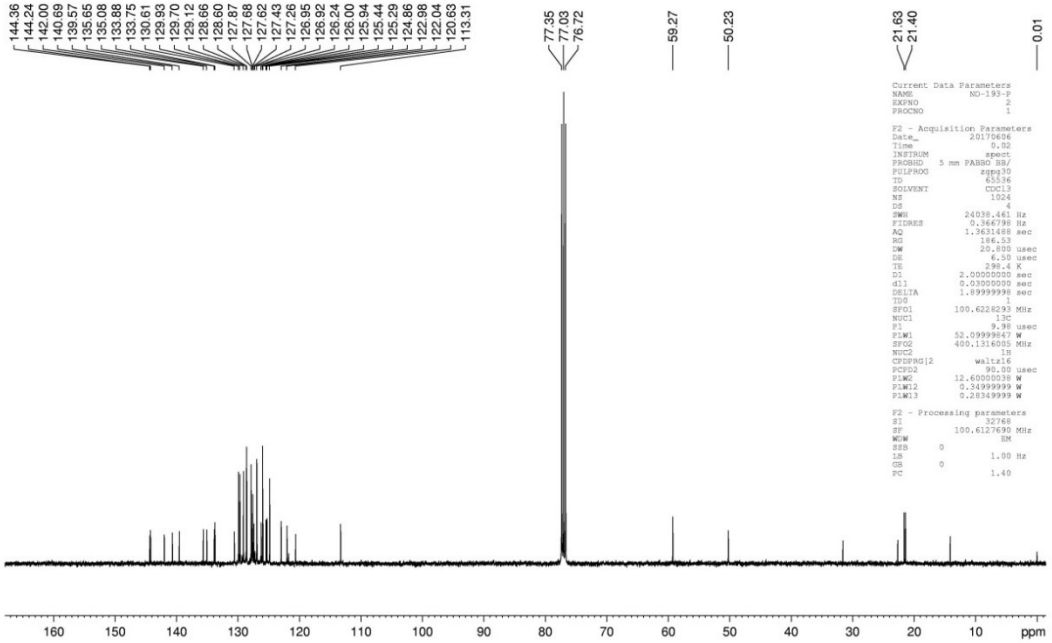
(*E*)-4-methyl-*N*-phenyl-*N*-((1-phenyl-3-tosyl-3,4,6,7-tetrahydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)benzenesulfonamide (4aa):





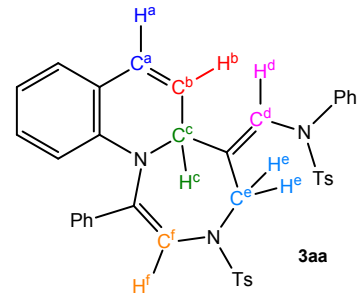
(*E*)-*N*-((1,9-diphenyl-3-tosyl-3,4-dihydro-[1,4]diazepino[1,7-*a*]quinolin-5(5a*H*)-ylidene)methyl)-4-methyl-*N*-phenylbenzenesulfonamide (5ea):



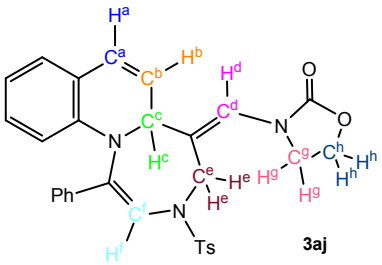


VII. Stereochemistry assignment:

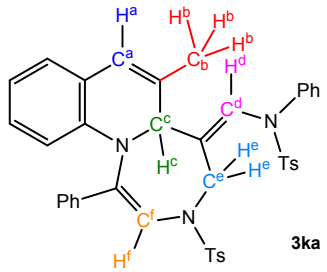
First, the labelled protons and carbons in following structures of compounds **3aa**, **3aj** and **3ka** have been assigned from ^{1}H NMR, ^{13}C NMR in combination with 2D NMR (HSQC-GP and HMBC-GP) analysis (Figure S1).



Proton	ppm (mult)	Carbon	ppm
H^a	6.25 (d)	C^a	125.31
H^b	5.74 (dd)	C^b	121.68
H^c	4.86 (d)	C^c	59.37
H^d	6.22(d)	C^d	125.67
H^e	4.36 (d)	C^e	50.41
H^f	6.93 (s)	C^f	122.61



Proton	ppm (mult)	Carbon	ppm
H^a	6.25 (d)	C^a	125.31
H^b	5.66 (dd)	C^b	121.46
H^c	5.24 (d)	C^c	59.68
H^d	5.87(d)	C^d	121.78
H^e	4.40 (s)	C^e	51.1
H^f	7.04 (s)	C^f	122.51
H^g	3.49 (dd), 3.69 (dd)	C^g	45.79
H^h	4.35 (m)	C^h	61.97



Proton	ppm (mult)	Carbon	ppm
H^a	5.89 (s)	C^a	123.2
H^b	1.85 (s)	C^b	20.9
H^c	4.4(s)	C^c	61.2
H^d	6.37(d)	C^d	127.5
H^e	4.23/4.4 (d)	C^e	50.1
H^f	7.0 (s)	C^f	122.3

Figure S1: Assignment of relevant protons by 2D NMR studies

Significant nOe has observed between H^e and H^g protons in compound **3aj** which confirms its *E*-stereochemistry (Figure S2). Only one case we have isolated both the isomers (*E*- and *Z*-isomers of **3ja**). Comparing the ^{1}H NMR and ^{13}C NMR of all other compounds with that of **3aj**, *E*-stereochemistry has been determined for all the compounds as nOe experiments were found insignificant due to presence of overlapping aromatic protons.

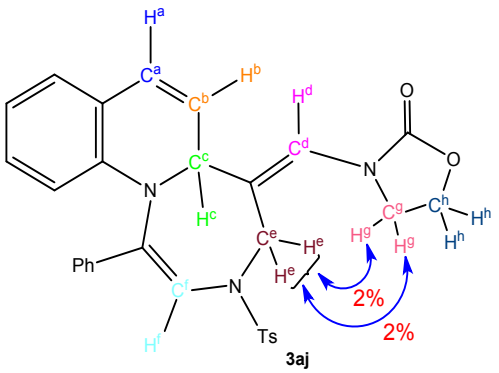
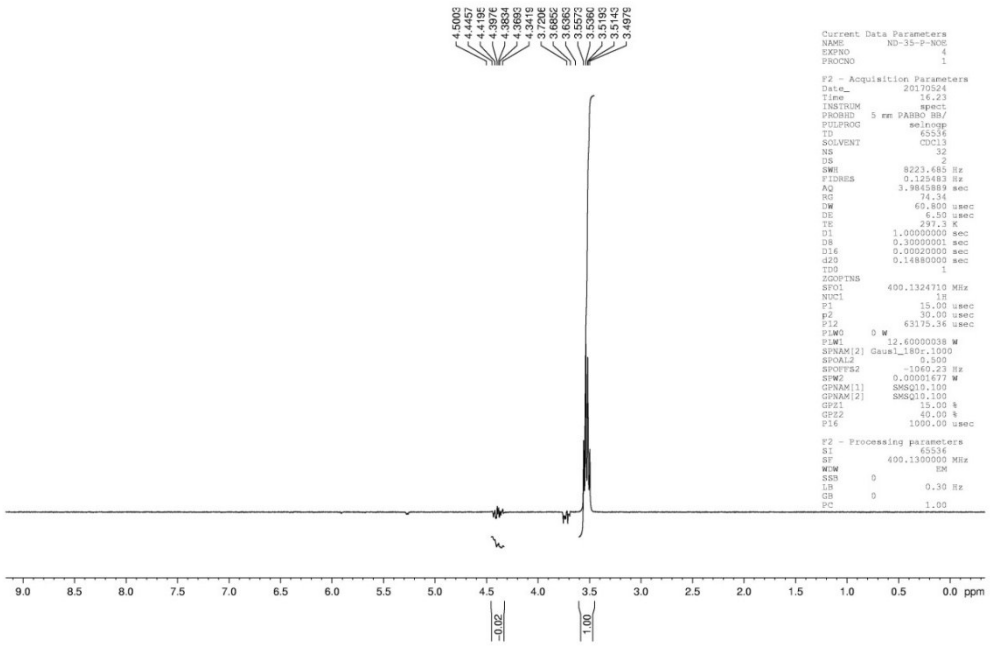


Figure S2: Significant nOe between H^e and H^g proton of compound **3aj**

NOE of **3aj** (irradiation of up-fielded H^{g}-proton):



NOE of **3aj** (irradiation of down-fielded H^{g}-proton):