Electronic Supplementary Material (ESI) for ChemComm.

Supporting Information

Yannan Zhu, [a] Hongxing Jin [a] and You Huang* [a]

[a] State Key Laboratory and Institute of Elemento-Organic Chemistry, College of Chemistry, Nankai University, Tianjin 300071, China

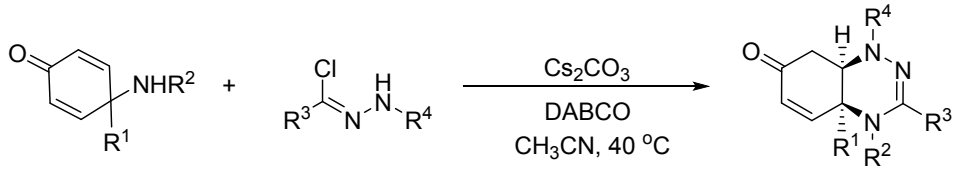
E-mail: hyou@nankai.edu.cn

1. General information S2
2. General procedure for the synthesis of tetrahydrobenzo[e][1,2,4]triazinones.....S2
3. General procedure for the synthetic transformations.....S2
4. Characterization data of products S3
5. References S17
6. NMR spectra of products S18
7. X-ray crystal structure of **3da**.....S50

1. General information

All the starting materials were obtained from commercial sources and used without further purification unless otherwise stated. Yields referred to isolated compounds through preparative TLC followed by recrystallization from the mixed solvents of ethyl acetate and petroleum ether. NMR spectra were recorded on Varian Brucker ARX 400 spectrometer in $CDCl_3$ solution and the chemical shifts were reported in parts per million (ppm) relative to internal standard TMS (0 ppm) for ^1H NMR and chloroform-d (77.0 ppm) for ^{13}C NMR. Coupling constants were given in Hertz (Hz). Multiplicity was indicated as follows: s (singlet), d (doublet), t (triplet), q (quartet), dd (doublet of doublet), brs (broad singlet) and m (multiplet). Infrared spectra (IR) spectra were recorded on a Perkin-Elmer 983G instrument. High resolution mass spectrometry (HRMS) were obtained on an IonSpec FT-ICR mass spectrometer with ESI or MALDI resource. Melting points were measured on a RY"I apparatus and are reported uncorrected. The N-protected amino cyclohexadienones **1** and hydrazonyl chlorides **2** were prepared according to the known methods. [1] [2]

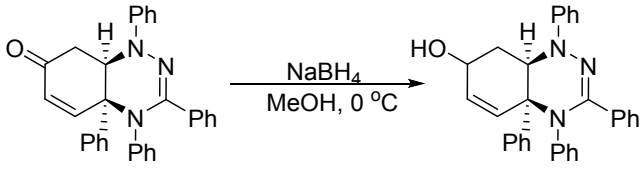
2. General procedure for the synthesis of tetrahydrobenzo[e][1,2,4]triazinones



1 **2** **3**

Cs_2CO_3 (0.04 mmol) and DABCO (0.4 mmol) were added to a mixture of *para*-quinamines **1** (1.0 eq, 0.2 mmol) and hydrazonyl chlorides **2** (2.0 eq, 0.4 mmol) in CH_3CN (4 mL). The resulting suspension was stirred at 40 °C for 5 hours. After the removal of the solvent, the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 5:1) to afford products **3**.

3. General procedure for the synthetic transformations

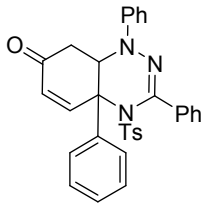


3aa (0.2 mmol) **4**

To a stirred solution of **3aa** (0.2 mmol, 1.0 equiv) in CH_3CN (2 mL) at 0 ºC, $NaBH_4$ (0.3 mmol, 1.5 equiv) was added in portions. After completion of the reaction (monitored by TLC, about 20 min), the reaction mixture was washed sequentially with diluted hydrochloric acid and brine. After that, the organic layer was dried over anhydrous magnesium sulphate ($MgSO_4$) and the solvent was removed via rotaryevaporation. Then the residue was purified by flash column chromatography (petroleum ether: ethyl acetate = 2:1) followed by recrystallization (ethyl acetate /petroleum ether) to give **4** as white solid (91 mg, 85% yield).

4. Characterization data of products

1,3,4a-triphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3aa**)



White solid, 76 mg, 69% yield

mp: 182-184 ℃

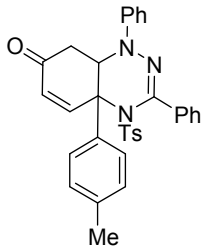
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 10.2 Hz, 1H), 7.56 – 7.52 (m, 2H), 7.41 – 7.31 (m, 6H), 7.30 – 7.27 (m, 1H), 7.23 (tdd, *J* = 8.6, 6.1, 3.1 Hz, 5H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.10 – 7.05 (m, 2H), 6.96 – 6.87 (m, 1H), 6.27 (d, *J* = 10.2 Hz, 1H), 5.02 (dd, *J* = 11.8, 4.1 Hz, 1H), 2.73 – 2.64 (m, 1H), 2.44 (dd, *J* = 17.2, 11.8 Hz, 1H), 2.38 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.45, 148.89, 144.60, 144.39, 141.17, 137.91, 136.02, 134.82, 129.83, 129.76, 129.32, 128.99, 128.84, 128.64, 128.33, 127.65, 127.45, 126.36, 121.55, 114.18, 62.89, 58.06, 36.50, 21.63.

IR (KBr, cm^{-1}): 3444, 1687, 1639, 1598, 1494, 1357, 1267, 1168, 1027, 752, 687, 578, 542.

HRMS (ESI): m/z calcd for $C_{32}H_{28}N_3O_3S$ ($[M+H]^+$): 534.1846; found: 534.1849.

1,3-diphenyl-4a-(p-tolyl)-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ba**)



White solid, 75 mg, 69% yield

mp: 136-138 ℃

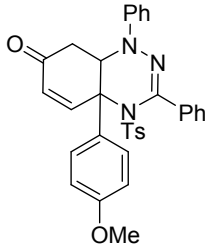
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.56 (d, *J* = 10.2 Hz, 1H), 7.41 (d, *J* = 8.3 Hz, 2H), 7.39 – 7.34 (m, 4H), 7.32 – 7.21 (m, 5H), 7.16 (dd, *J* = 8.3, 3.1 Hz, 4H), 7.13 – 7.10 (m, 2H), 6.93 (t, *J* = 7.3 Hz, 1H), 6.24 (d, *J* = 10.2 Hz, 1H), 5.05 (dd, *J* = 11.7, 4.0 Hz, 1H), 2.70 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.50 – 2.35 (m, 4H), 2.30 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.53, 149.01, 144.57, 144.38, 138.81, 137.95, 136.24, 134.29, 129.76, 129.69, 129.57, 129.33, 128.52, 128.28, 127.65, 127.46, 126.32, 121.47, 114.06, 62.42, 57.68, 36.68, 21.64, 21.07.

IR (KBr, cm^{-1}): 3478, 1689, 1648, 1494, 1359, 1266, 1168, 1026, 749, 705, 593, 564, 544.

HRMS (ESI): m/z calcd for $C_{33}H_{30}N_3O_3S$ ($[M+H]^+$): 548.2002; found: 548.1999.

4a-(4-methoxyphenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ca**)



White solid, 78 mg, 69% yield

mp: 196-198 ℃

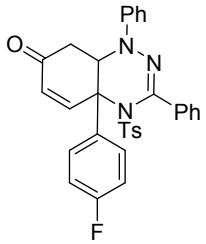
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.53 (d, J = 10.2 Hz, 1H), 7.47 – 7.41 (m, 2H), 7.41 – 7.36 (m, 4H), 7.32 – 7.20 (m, 5H), 7.14 (dd, J = 11.7, 8.2 Hz, 4H), 6.98 – 6.89 (m, 1H), 6.88 – 6.79 (m, 2H), 6.21 (d, J = 10.2 Hz, 1H), 5.05 (dd, J = 11.6, 3.9 Hz, 1H), 3.72 (s, 3H), 2.69 (dd, J = 17.2, 4.0 Hz, 1H), 2.38 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.42, 159.68, 148.84, 144.59, 144.32, 137.98, 136.38, 134.02, 132.62, 129.79, 129.43, 129.38, 128.40, 128.28, 127.87, 127.66, 127.51, 121.52, 114.29, 114.08, 62.01, 57.62, 55.30, 36.81, 21.65.

IR (KBr, cm-1): 3459, 1690, 1647, 1494, 1360, 1266, 1168, 1028, 748, 705, 687, 597, 566.

HRMS (ESI): m/z calcd for $C_{33}H_{30}N_3O_4S$ ($[M+H]^+$): 564.1952; found: 564.1955.

4a-(4-fluorophenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3da**)



White solid, 84 mg, 76% yield

mp: 188-190 ℃

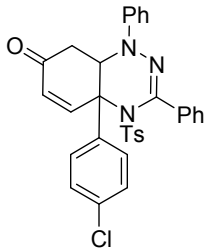
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (d, *J* = 10.3 Hz, 1H), 7.54 (dd, *J* = 8.9, 5.0 Hz, 2H), 7.38 – 7.28 (m, 5H), 7.28 – 7.19 (m, 4H), 7.15 (d, *J* = 8.1 Hz, 2H), 7.07 (d, *J* = 8.5 Hz, 4H), 6.92 (t, *J* = 7.3 Hz, 1H), 6.30 (d, *J* = 10.2 Hz, 1H), 4.93 (dd, *J* = 11.7, 4.1 Hz, 1H), 2.67 (dd, *J* = 17.2, 4.1 Hz, 1H), 2.47 (dd, *J* = 17.3, 11.7 Hz, 1H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.26, 162.51 (d, J = 249.3 Hz), 148.53, 144.73, 144.36, 137.77, 137.37 (d, J = 3.1 Hz), 135.70, 135.39, 130.06, 129.79, 129.38, 128.72, 128.46, 128.26 (d, J = 8.4 Hz), 127.61, 127.50, 121.74, 115.93 (d, J = 21.8 Hz), 114.27, 62.73, 58.59, 36.26, 21.64.

IR (KBr, cm^{-1}): 3745, 3461, 2923, 1693, 1597, 1495, 1358, 1267, 1168, 1027, 765, 686, 563.

HRMS (ESI): m/z calcd for $C_{32}H_{27}FN_3O_3S$ ($[M+H]^+$): 552.1752; found: 552.1756.

4a-(4-chlorophenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ea**)



White solid, 74 mg, 65% yield

mp: 161-163 ℃

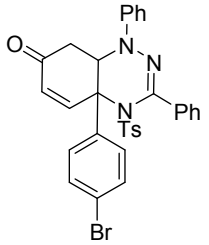
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 (d, *J* = 10.2 Hz, 1H), 7.44 (d, *J* = 8.4 Hz, 2H), 7.35 – 7.21 (m, 7H), 7.17 (td, *J* = 7.5, 3.7 Hz, 4H), 7.09 (d, *J* = 8.1 Hz, 2H), 7.00 (d, *J* = 8.2 Hz, 2H), 6.87 (t, *J* = 7.2 Hz, 1H), 6.26 (d, *J* = 10.2 Hz, 1H), 4.85 (dd, *J* = 11.7, 4.2 Hz, 1H), 2.61 (dd, *J* = 17.2, 4.2 Hz, 1H), 2.46 (dd, *J* = 17.2, 11.6 Hz, 1H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.19, 148.29, 144.74, 144.41, 140.22, 137.71, 135.76, 135.51, 134.75, 130.27, 129.76, 129.37, 129.12, 128.82, 128.49, 127.70, 127.61, 127.50, 121.80, 114.38, 63.02, 58.74, 36.12, 21.64.

IR (KBr, cm^{-1}): 3441, 1691, 1649, 1598, 1493, 1358, 1266, 1167, 1093, 1026, 764, 750, 688, 584, 544.

HRMS (ESI): m/z calcd for $C_{32}H_{27}ClN_3O_3S$ ($[M+H]^+$): 568.1456; found: 568.1461.

4a-(4-bromophenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3fa**)



White solid, 88 mg, 72% yield

mp: 158-160 ℃

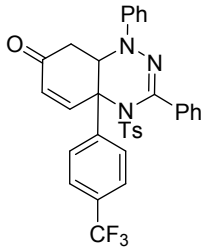
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 (d, *J* = 10.3 Hz, 1H), 7.54 (d, *J* = 8.6 Hz, 2H), 7.47 (d, *J* = 8.8 Hz, 2H), 7.34 (dt, *J* = 8.4, 2.7 Hz, 5H), 7.30 – 7.22 (m, 4H), 7.18 (d, *J* = 8.1 Hz, 2H), 7.13 – 7.06 (m, 2H), 7.01 – 6.89 (m, 1H), 6.36 (d, *J* = 10.3 Hz, 1H), 4.94 (dd, *J* = 11.6, 4.2 Hz, 1H), 2.71 (dd, *J* = 17.2, 4.2 Hz, 1H), 2.55 (dd, *J* = 17.2, 11.6 Hz, 1H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.20, 148.23, 144.75, 144.40, 140.76, 137.67, 135.78, 135.49, 132.07, 130.30, 129.77, 129.38, 128.82, 128.51, 127.98, 127.61, 127.52, 123.00, 121.82, 114.39, 63.09, 58.68, 36.10, 21.66.

IR (KBr, cm^{-1}): 3459, 1691, 1597, 1492, 1358, 1266, 1168, 997, 764, 685, 582, 543.

HRMS (ESI): m/z calcd for $C_{32}H_{25}BrN_3O_3S$ ($[M-H]^-$): 610.0805; found: 610.0803.

1,3-diphenyl-4-tosyl-4a-(4-(trifluoromethyl)phenyl)-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ga**)



White solid, 57 mg, 47% yield

mp: 183-186 ℃

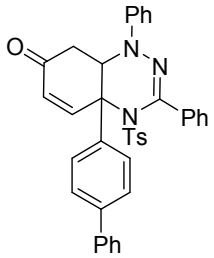
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.71 (d, *J* = 8.4 Hz, 2H), 7.69 – 7.63 (m, 3H), 7.35 – 7.24 (m, 6H), 7.24 – 7.18 (m, 3H), 7.14 (d, *J* = 8.2 Hz, 2H), 7.08 – 7.00 (m, 2H), 6.93 (td, *J* = 7.3, 1.2 Hz, 1H), 6.39 (d, *J* = 10.2 Hz, 1H), 4.89 (dd, *J* = 11.1, 4.8 Hz, 1H), 2.76 – 2.53 (m, 2H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.11, 147.99, 144.81, 144.46, 137.57, 136.69, 135.08, 130.68, 129.76, 129.38, 129.03, 128.61, 127.60, 127.54, 126.64, 125.95 (q), 121.96, 114.60, 63.72, 59.31, 35.75, 21.64.

IR (KBr, cm^{-1}): 3055, 2924, 1692, 1598, 1494, 1357, 1327, 1266, 1169, 1124, 1092, 1016, 910, 749, 705, 684, 582, 543.

HRMS (ESI): m/z calcd for $C_{33}H_{27}F_3N_3O_3S$ ($[M+H]^+$): 602.1720; found: 602.1722.

4a-([1,1'-biphenyl]-4-yl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ha**)



White solid, 59 mg, 49% yield

mp: 125-127 ℃

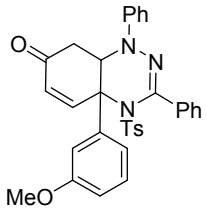
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.73 – 7.57 (m, 5H), 7.56 – 7.51 (m, 2H), 7.48 – 7.36 (m, 6H), 7.37 – 7.31 (m, 1H), 7.31 – 7.21 (m, 5H), 7.15 (dd, *J* = 10.8, 8.2 Hz, 4H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.28 (d, *J* = 10.2 Hz, 1H), 5.11 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.73 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.46 (dd, *J* = 17.2, 11.7 Hz, 1H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.40, 148.69, 144.65, 144.34, 141.63, 139.91, 137.89, 136.14, 134.50, 129.85, 129.81, 129.39, 128.87, 128.56, 128.39, 127.75, 127.68, 127.64, 127.53, 127.12, 126.94, 121.64, 114.25, 62.55, 57.83, 36.60, 21.67.

IR (KBr, cm^{-1}): 3455, 3055, 2987, 2306, 1691, 1598, 1491, 1422, 1266, 1169, 896, 749, 704.

HRMS (ESI): m/z calcd for $C_{38}H_{32}N_3O_3S$ ($[M+H]^+$): 610.2159; found: 610.2162.

4a-(3-methoxyphenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ia**)



White solid, 77 mg, 68% yield

mp: 190-192 ℃

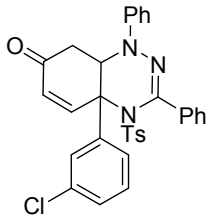
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 10.3 Hz, 1H), 7.40 – 7.33 (m, 4H), 7.30 (t, *J* = 8.0 Hz, 2H), 7.27 – 7.20 (m, 4H), 7.17 (dd, *J* = 8.2, 2.2 Hz, 3H), 7.13 – 7.07 (m, 2H), 7.00 (t, *J* = 2.2 Hz, 1H), 6.95 – 6.88 (m, 1H), 6.83 (ddd, *J* = 8.2, 2.5, 0.9 Hz, 1H), 6.28 (dd, *J* = 10.2, 0.8 Hz, 1H), 5.01 (dd, *J* = 11.8, 4.1 Hz, 1H), 3.62 (s, 3H), 2.70 (ddd, *J* = 17.3, 4.1, 1.0 Hz, 1H), 2.48 (dd, *J* = 17.2, 11.8 Hz, 1H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.51, 159.72, 148.78, 144.60, 144.56, 142.72, 137.91, 136.01, 134.78, 130.02, 129.90, 129.75, 129.34, 128.69, 128.34, 127.67, 127.44, 121.52, 118.62, 114.52, 114.06, 112.00, 62.82, 58.23, 55.07, 36.62, 21.63.

IR (KBr, cm^{-1}): 3459, 1681, 1647, 1494, 1360, 1266, 1168, 1028, 748, 705, 687, 577, 544.

HRMS (ESI): m/z calcd for $C_{33}H_{30}N_3O_4S$ ($[M+H]^+$): 564.1952; found: 564.1955.

4a-(3-chlorophenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ja**)



White solid, 82 mg, 73% yield

mp: 188-190 ℃

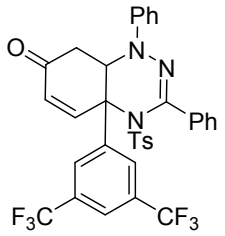
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.62 – 7.45 (m, 2H), 7.42 – 7.12 (m, 12H), 7.09 (d, *J* = 7.8 Hz, 2H), 7.00 (d, *J* = 8.0 Hz, 2H), 6.87 (t, *J* = 7.3 Hz, 1H), 6.28 (d, *J* = 10.3 Hz, 1H), 5.05 – 4.70 (m, 1H), 2.58 (qd, *J* = 17.2, 8.0 Hz, 2H), 2.33 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.10, 148.09, 144.75, 144.51, 143.65, 137.62, 136.08, 135.39, 134.85, 130.44, 130.12, 129.74, 129.33, 128.99, 128.90, 128.53, 127.65, 127.54, 126.71, 124.43, 121.88, 114.70, 63.33, 59.08, 36.06, 21.63.

IR (KBr, cm^{-1}): 3455, 1640, 1499, 1316, 1267, 1185, 1166, 751, 738, 712, 575.

HRMS (ESI): m/z calcd for $C_{32}H_{27}ClN_3O_3S$ ($[M+H]^+$): 568.1456; found: 568.1461.

4a-(3,5-bis(trifluoromethyl)phenyl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ka**)



3ka

White solid, 82 mg, 62% yield

mp: 170-173 ℃

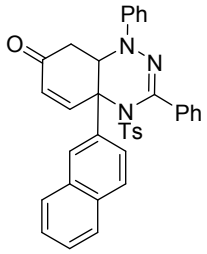
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.01 (s, 2H), 7.87 (s, 1H), 7.69 (d, *J* = 10.2 Hz, 1H), 7.43 – 7.16 (m, 9H), 7.13 (d, *J* = 8.1 Hz, 2H), 7.04 – 6.87 (m, 3H), 6.49 (d, *J* = 10.3 Hz, 1H), 4.78 (dd, *J* = 11.6, 4.4 Hz, 1H), 2.84 (dd, *J* = 17.3, 11.6 Hz, 1H), 2.72 (dd, *J* = 17.4, 4.4 Hz, 1H), 2.40 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.63, 146.67, 145.26, 145.06, 144.66, 138.01, 137.15, 134.41, 132.30, 131.96, 131.66, 129.74, 129.36, 129.22, 128.81, 127.68, 127.60, 126.41, 124.33, 122.74, 122.38, 121.62, 114.97, 764.10, 60.27, 35.63, 21.62.

IR (KBr, cm^{-1}): 3055, 2924, 1692, 1624, 1494, 1357, 1327, 1266, 1169, 1112, 1090, 1016, 910, 749, 705, 559, 543.

HRMS (ESI): m/z calcd for $C_{33}H_{27}F_3N_3O_3S$ ($[M+H]^+$): 670.1594; found: 670.1596.

4a-(naphthalen-2-yl)-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3la**)



White solid, 40 mg, 34% yield

mp: 105-108 ℃ ℃

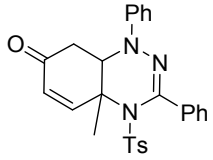
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (d, *J* = 8.8 Hz, 1H), 7.87 (dd, *J* = 8.8, 2.1 Hz, 1H), 7.80 (d, *J* = 8.0 Hz, 1H), 7.71 (d, *J* = 2.0 Hz, 1H), 7.68 (d, *J* = 10.2 Hz, 1H), 7.61 – 7.56 (m, 1H), 7.51 – 7.34 (m, 6H), 7.31 – 7.20 (m, 6H), 7.14 (td, *J* = 5.9, 2.7 Hz, 4H), 6.95 (t, *J* = 7.3 Hz, 1H), 6.29 (d, *J* = 10.2 Hz, 1H), 5.22 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.76 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.49 (dd, *J* = 17.2, 11.6 Hz, 1H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.34, 148.38, 144.65, 144.61, 137.94, 137.83, 136.21, 134.43, 133.05, 132.78, 129.86, 129.74, 129.48, 129.32, 129.08, 128.53, 128.49, 128.28, 127.70, 127.51, 127.45, 127.00, 126.65, 125.71, 124.22, 121.70, 114.44, 62.78, 58.29, 36.93, 21.59.

IR (KBr, cm^{-1}): 3458, 1634, 1503, 1316, 1267, 1185, 1166, 791, 762, 751, 738, 712, 689, 575.

HRMS (ESI): m/z calcd for $C_{36}H_{31}N_3O_3S$ ($[M+H]^+$): 584.2002; found: 584.2006.

4a-methyl-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ma**)



White solid, 77 mg, 82% yield

mp: 122-125 ℃

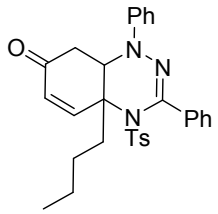
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.65 – 7.57 (m, 2H), 7.49 (d, *J* = 7.9 Hz, 2H), 7.42 – 7.28 (m, 3H), 7.23 (d, *J* = 7.6 Hz, 2H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.09 – 7.00 (m, 3H), 6.93 (t, *J* = 7.4 Hz, 1H), 6.07 (d, *J* = 10.2 Hz, 1H), 4.24 (dd, *J* = 9.3, 4.0 Hz, 1H), 2.56 (dd, *J* = 17.5, 4.0 Hz, 1H), 2.43 (dd, *J* = 17.5, 9.3 Hz, 1H), 2.37 (s, 3H), 1.78 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.63, 148.82, 144.64, 144.16, 138.05, 136.75, 133.25, 130.14, 129.82, 129.10, 128.35, 127.78, 127.74, 127.49, 121.75, 115.18, 59.46, 56.70, 37.28, 26.31, 21.58.

IR (KBr, cm^{-1}): 3465, 1643, 1502, 1362, 1321, 1185, 1169, 764, 690.

HRMS (ESI): m/z calcd for $C_{36}H_{31}N_3O_3S$ ($[M+H]^+$): 472.1689; found: 472.1695.

4a-butyl-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3na**)



White solid, 70 mg, 69% yield

mp: 94-96 ℃

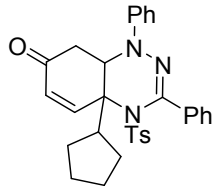
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.58 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.49 – 7.41 (m, 2H), 7.39 – 7.34 (m, 3H), 7.32 – 7.22 (m, 3H), 7.16 (d, *J* = 8.1 Hz, 2H), 7.11 (d, *J* = 8.2 Hz, 2H), 6.91 (t, *J* = 7.3 Hz, 1H), 6.22 (d, *J* = 10.2 Hz, 1H), 4.41 (dd, *J* = 11.8, 4.1 Hz, 1H), 2.54 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.36 (s, 3H), 2.04 (tt, *J* = 11.6, 5.1 Hz, 2H), 1.80 (ddd, *J* = 13.9, 11.9, 4.4 Hz, 1H), 1.58 (dtd, *J* = 15.1, 8.9, 8.1, 3.6 Hz, 1H), 1.43 – 1.18 (m, 3H), 0.88 (t, *J* = 7.0 Hz, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.68, 147.58, 144.61, 144.22, 137.97, 137.35, 132.26, 131.31, 129.87, 129.30, 128.26, 128.07, 127.62, 121.23, 113.52, 58.91, 55.91, 38.20, 36.81, 26.02, 22.83, 21.62, 13.97.

IR (KBr, cm^{-1}): 3459, 1648, 1495, 1362, 1267, 1185, 1169, 799, 764, 689.

HRMS (ESI): m/z calcd for $C_{30}H_{32}N_3O_3S$ ($[M+H]^+$): 514.2159; found: 514.2162.

4a-cyclopentyl-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3oa**)



White solid, 55 mg, 57% yield

mp: 112-114 ℃

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (dd, J = 7.3, 2.0 Hz, 2H), 7.40 (d, J = 8.1 Hz, 2H), 7.33 (d, J = 7.1 Hz, 3H), 7.26 (d, J = 10.4 Hz, 1H), 7.21 – 7.14 (m, 2H), 7.11 (d, J = 8.1 Hz, 2H), 7.05 (d, J = 8.2 Hz,

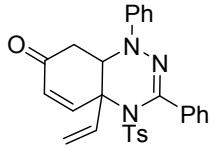
2H), 6.83 (t, J = 7.3 Hz, 1H), 6.28 (d, J = 10.3 Hz, 1H), 4.37 (dd, J = 12.9, 4.3 Hz, 1H), 2.43 – 2.33 (m, 2H), 2.29 (s, 3H), 2.17 (h, J = 6.8, 6.1 Hz, 1H), 2.11 – 1.99 (m, 1H), 1.75 – 1.49 (m, 4H), 1.47 – 1.27 (m, 2H), 1.16 – 1.01 (m, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.00, 145.15, 144.66, 144.29, 138.13, 137.98, 132.78, 131.15, 130.01, 129.41, 128.16, 127.60, 127.51, 121.03, 112.72, 60.87, 55.67, 44.16, 36.97, 28.74, 26.96, 26.86, 26.58, 21.62.

IR (KBr, cm^{-1}): 3459, 1648, 1556, 1495, 1362, 1277, 1185, 1169, 787, 684.

HRMS (ESI): m/z calcd for $C_{30}H_{32}N_3O_3S$ ($[M+H]^+$): 516.2159; found: 526.2162.

1,3-diphenyl-4-tosyl-4a-vinyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3pa**)



White solid, 94 mg, 97% yield

mp: 135-137 ℃

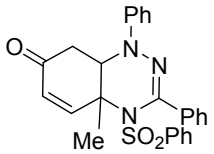
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.49 (dd, *J* = 6.6, 2.9 Hz, 2H), 7.40 (d, *J* = 8.0 Hz, 2H), 7.31 – 7.20 (m, 3H), 7.19 – 7.12 (m, 2H), 7.08 (d, *J* = 8.1 Hz, 2H), 7.03 – 6.96 (m, 3H), 6.86 (t, *J* = 7.3 Hz, 1H), 6.16 (dd, *J* = 17.4, 10.8 Hz, 1H), 6.08 (d, *J* = 10.2 Hz, 1H), 5.41 – 5.22 (m, 2H), 4.48 (dd, *J* = 9.1, 4.2 Hz, 1H), 2.60 – 2.39 (m, 2H), 2.28 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.63, 146.00, 144.72, 144.28, 138.00, 137.18, 136.46, 133.42, 130.96, 129.77, 129.19, 128.44, 127.89, 127.80, 127.70, 121.93, 119.33, 115.35, 77.47, 77.16, 76.84, 60.29, 58.54, 37.13, 21.64.

IR (KBr, cm^{-1}): 3459, 1648, 1556, 1495, 1362, 1277, 1185, 1169, 787, 684.

HRMS (ESI): m/z calcd for $C_{30}H_{32}N_3O_3S$ ($[M+H]^+$): 484.1689; found: 484.1694.

4a-methyl-1,3-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3qa**)



Light yellow oil, 77 mg, 91% yield

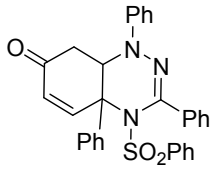
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (td, *J* = 7.8, 2.4 Hz, 4H), 7.56 – 7.49 (m, 1H), 7.38 (t, *J* = 7.9 Hz, 2H), 7.35 – 7.28 (m, 3H), 7.29 – 7.20 (m, 2H), 7.08 (dd, *J* = 14.5, 9.1 Hz, 3H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.10 (d, *J* = 10.1 Hz, 1H), 4.26 (dd, *J* = 9.6, 3.9 Hz, 1H), 2.56 (dd, *J* = 17.5, 3.9 Hz, 1H), 2.40 (dd, *J* = 17.5, 9.6 Hz, 1H), 1.79 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.70, 148.73, 144.18, 141.01, 136.62, 133.53, 133.03, 130.23, 129.29, 129.17, 128.41, 127.83, 127.67, 127.59, 121.85, 115.17, 59.49, 56.72, 37.21, 26.38.

IR (KBr, cm^{-1}): 3461, 1687, 1649, 1493, 1359, 1270, 1173, 1072, 751, 727, 690, 598.

HRMS (ESI): m/z calcd for $C_{27}H_{26}N_3O_3S$ ($[M+H]^+$): 458.1533; found: 458.1535.

1,3,4a-triphenyl-4-(phenylsulfonyl)-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ra**)



White solid, 83 mg, 76% yield

mp: 97-99 ℃

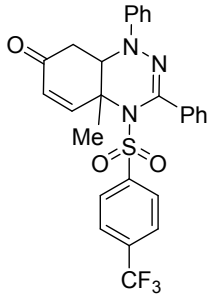
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 10.2 Hz, 1H), 7.64 – 7.54 (m, 3H), 7.51 (d, *J* = 7.8 Hz, 2H), 7.46 – 7.23 (m, 12H), 7.13 (d, *J* = 8.2 Hz, 2H), 6.97 (t, *J* = 7.3 Hz, 1H), 6.34 (d, *J* = 10.2 Hz, 1H), 5.08 (dd, *J* = 11.6, 4.1 Hz, 1H), 2.73 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.49 (dd, *J* = 17.2, 11.6 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.38, 148.84, 144.40, 141.11, 140.81, 135.83, 134.82, 133.46, 129.96, 129.36, 129.22, 129.01, 128.91, 128.70, 128.41, 127.55, 127.53, 126.36, 121.67, 114.33, 63.09, 58.25, 36.42.

IR (KBr, cm^{-1}): 3458, 1669, 1485, 1357, 1267, 1175, 1045, 752, 687, 578, 542.

HRMS (ESI): m/z calcd for $C_{31}H_{26}N_3O_3S$ ($[M+H]^+$): 520.1689; found: 520.1693.

4a-methyl-1,3-diphenyl-4-((4-(trifluoromethyl)phenyl)sulfonyl)-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3sa**)



White solid, 97 mg, 93% yield

mp: 125-127 ℃

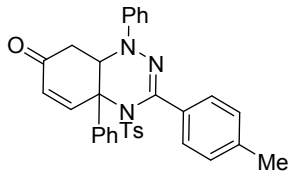
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.89 (d, *J* = 8.3 Hz, 2H), 7.82 (d, *J* = 8.4 Hz, 2H), 7.75 – 7.68 (m, 2H), 7.57 – 7.34 (m, 5H), 7.30 – 7.20 (m, 3H), 7.17 (tt, *J* = 7.2, 1.1 Hz, 1H), 6.31 (d, *J* = 10.2 Hz, 1H), 4.51 (dd, *J* = 7.7, 5.0 Hz, 1H), 2.86 (dd, *J* = 6.5, 3.1 Hz, 2H), 2.07 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 195.16, 148.45, 144.20, 143.92, 135.70, 135.09, 134.75, 133.11, 130.36, 129.22, 128.70, 128.22, 128.11, 127.94, 127.70, 126.24(q), 122.20, 115.46, 59.82, 57.86, 37.20, 26.25.

IR (KBr, cm^{-1}): 3745, 1692, 1495, 1365, 1323, 1174, 1135, 1062, 766, 716.

HRMS (ESI): m/z calcd for $C_{27}H_{23}F_3N_3O_3S$ ($[M+H]^+$): 526.1407; found: 526.1411.

1,4a-diphenyl-3-(p-tolyl)-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ab**)



White solid, 67 mg, 61% yield

mp: 191-193 ℃

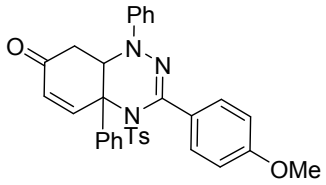
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.46 (dd, *J* = 16.6, 8.9 Hz, 3H), 7.24 (t, *J* = 7.7 Hz, 4H), 7.14 (dt, *J* = 15.7, 6.0 Hz, 5H), 7.04 (d, *J* = 8.0 Hz, 2H), 6.98 (d, *J* = 8.2 Hz, 2H), 6.94 (d, *J* = 7.8 Hz, 2H), 6.80 (t, *J* = 7.3 Hz, 1H), 6.16 (d, *J* = 10.2 Hz, 1H), 4.92 (dd, *J* = 11.7, 4.0 Hz, 1H), 2.58 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.41 – 2.30 (m, 1H), 2.27 (s, 3H), 2.23 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.51, 148.97, 144.57, 144.49, 141.21, 138.35, 138.00, 134.97, 133.25, 129.81, 129.71, 129.32, 128.97, 128.82, 128.58, 128.19, 127.67, 126.41, 121.46, 114.20, 62.95, 58.14, 36.51, 21.66, 21.42.

IR (KBr, cm^{-1}): 3460, 1690, 1650, 1598, 1496, 1359, 1266, 1168, 749, 704, 570, 517.

HRMS (ESI): m/z calcd for $C_{33}H_{30}N_3O_3S$ ($[M+H]^+$): 548.2002; found: 548.2006.

3-(4-methoxyphenyl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ac**)



White solid, 80 mg, 71% yield

mp: 166-168 ℃

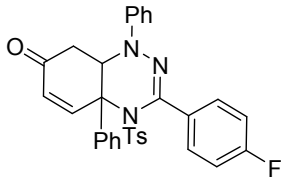
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.61 (d, *J* = 10.3 Hz, 1H), 7.54 (d, *J* = 7.7 Hz, 2H), 7.39 – 7.30 (m, 4H), 7.30 – 7.18 (m, 5), 7.14 (d, *J* = 8.1 Hz, 2H), 7.06 (d, *J* = 8.2 Hz, 2H), 6.89 (t, *J* = 7.3 Hz, 1H), 6.74 (d, *J* = 8.4 Hz, 2H), 6.28 (d, *J* = 10.2 Hz, 1H), 4.98 (dd, *J* = 11.8, 4.1 Hz, 1H), 3.78 (s, 3H), 2.68 (dd, *J* = 17.3, 4.0 Hz, 1H), 2.49 (dd, *J* = 17.2, 11.8 Hz, 1H), 2.37 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.61, 159.77, 149.11, 144.55, 144.51, 141.43, 138.02, 135.30, 130.19, 129.79, 129.72, 129.31, 129.09, 128.95, 128.78, 128.27, 127.58, 126.29, 121.40, 114.20, 112.91, 63.33, 58.49, 55.34, 36.37, 21.64.

IR (KBr, cm^{-1}): 3481, 1691, 1598, 1495, 1358, 1251, 1168, 1029, 834, 751, 690, 573, 542.

HRMS (ESI): m/z calcd for $C_{33}H_{30}N_3O_4S$ ($[M+H]^+$): 564.1952; found: 564.1956.

3-(4-fluorophenyl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ad**)



White solid, 55 mg, 50% yield

mp: 191-193 ℃

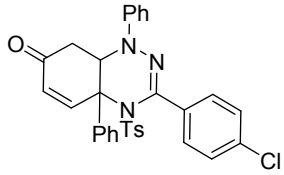
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.60 (dd, *J* = 18.7, 8.9 Hz, 3H), 7.47 – 7.33 (m, 7H), 7.29 (t, *J* = 7.7 Hz, 2H), 7.22 (d, *J* = 7.9 Hz, 2H), 7.13 (d, *J* = 8.1 Hz, 2H), 6.96 (t, *J* = 8.6 Hz, 3H), 6.32 (d, *J* = 10.2 Hz, 1H), 5.08 (dd, *J* = 11.7, 4.1 Hz, 1H), 2.74 (dd, *J* = 17.1, 4.0 Hz, 1H), 2.43 (s, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.33, 162.70 (d, J = 248.2 Hz), 148.72, 144.85, 144.29, 141.08, 137.87, 133.70, 132.19 (d, J = 3.3 Hz), 130.42 (d, J = 8.5 Hz), 129.89, 129.41, 129.06, 128.94, 127.58, 126.32, 121.67, 114.52 (d, J = 21.8 Hz), 114.08, 62.83, 57.89, 36.54, 21.66.

IR (KBr, cm^{-1}): 3745, 1696, 1497, 1360, 1268, 1169, 1016, 751, 702, 570.

HRMS (ESI): m/z calcd for $C_{32}H_{27}FN_3O_3S$ ($[M+H]^+$): 552.1752; found: 552.1756.

3-(4-chlorophenyl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ae**)



White solid, 78 mg, 69% yield

mp: 189-191 ℃

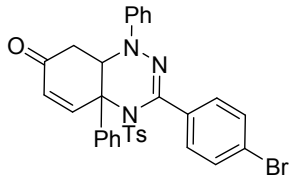
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.45 (t, *J* = 8.5 Hz, 3H), 7.32 (d, *J* = 7.9 Hz, 3H), 7.29 – 7.20 (m, 4H), 7.17 (d, *J* = 7.5 Hz, 2H), 7.15 – 7.08 (m, 4H), 7.03 (d, *J* = 8.2 Hz, 2H), 6.87 (t, *J* = 7.4 Hz, 1H), 6.17 (d, *J* = 10.2 Hz, 1H), 5.15 – 4.90 (m, 1H), 2.62 (dd, *J* = 17.5, 4.0 Hz, 1H), 2.39 – 2.15 (m, 4H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.14, 148.47, 144.94, 144.15, 140.70, 137.80, 134.85, 134.23, 132.91, 129.92, 129.89, 129.61, 129.43, 129.09, 129.00, 127.72, 127.64, 126.43, 121.79, 114.08, 62.37, 57.48, 36.73, 21.67.

IR (KBr, cm^{-1}): 3459, 1692, 1649, 1598, 1493, 1360, 1266, 1168, 1092, 1030, 749, 704, 543.

HRMS (ESI): m/z calcd for $C_{32}H_{27}ClN_3O_3S$ ($[M+H]^+$): 568.1456; found: 568.1460.

3-(4-bromophenyl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3af**)



White solid, 76 mg, 62% yield

mp: 184-186 ℃

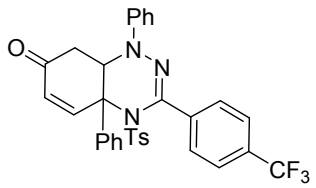
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.57 – 7.46 (m, 1H), 7.43 – 7.29 (m, 2H), 7.29 – 7.20 (m, 1H), 7.17 (d, *J* = 7.9 Hz, 1H), 7.10 (d, *J* = 8.2 Hz, 1H), 6.93 (t, *J* = 7.3 Hz, 0H), 6.22 (d, *J* = 10.2 Hz, 0H), 5.09 (d, *J* = 11.4 Hz, 0H), 2.69 (dd, *J* = 17.3, 4.0 Hz, 0H), 2.37 (s, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.11, 148.38, 144.98, 144.16, 140.65, 137.78, 135.40, 132.88, 130.69, 129.96, 129.87, 129.46, 129.10, 129.02, 127.68, 126.47, 122.47, 121.84, 114.13, 62.34, 57.43, 36.76, 21.70.

IR (KBr, cm^{-1}): 3459, 1693, 1649, 1600, 1495, 1327, 1247, 1168, 1116, 1030, 749, 689.

HRMS (ESI): m/z calcd for $C_{32}H_{27}BrN_3O_3S$ ($[M+H]^+$): 612.0951; found: 612.0954.

1,4a-diphenyl-4-tosyl-3-(4-(trifluoromethyl)phenyl)-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ag**)

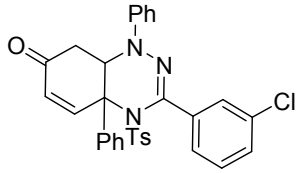


White solid, 56 mg, 47% yield

mp: 192-194 ℃

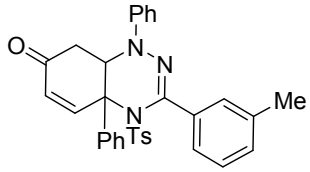
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 – 7.42 (m, 7H), 7.38 (d, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 7.5 Hz, 2H), 7.28 – 7.20 (m, 3H), 7.15 (d, *J* = 8.0 Hz, 2H), 7.10 (d, *J* = 8.2 Hz, 2H), 6.93 (t, *J* = 7.3 Hz, 1H), 6.19 (d, *J* = 10.2 Hz, 1H), 5.12 (dd, *J* = 11.8, 4.1 Hz, 1H), 2.68 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.47 – 2.16 (m, 4H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 195.93, 148.10, 145.13, 143.98, 140.37, 140.16, 137.67, 131.94, 130.03, 129.52, 129.16, 129.13, 128.30, 127.70, 126.55, 124.52(q), 122.07, 114.11, 61.91, 57.03, 36.91, 21.63.
IR (KBr, cm^{-1}): 3745, 1694, 1597, 1495, 1362, 1323, 1268, 1167, 1122, 1077, 1017, 845, 751, 689, 543.
HRMS (ESI): m/z calcd for $C_{33}H_{27}F_3N_3O_3S$ ($[M+H]^+$): 602.1720; found: 602.1722.

3-(3-chlorophenyl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ah**)



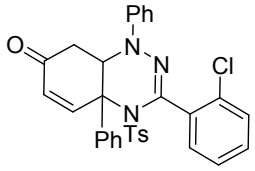
White solid, 69 mg, 61% yield
mp: 163-165 ℃
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.59 (d, *J* = 10.2 Hz, 1H), 7.55 (d, *J* = 7.3 Hz, 2H), 7.47 – 7.26 (m, 10H), 7.25 – 7.20 (m, 3H), 7.15 (d, *J* = 8.2 Hz, 2H), 6.99 (t, *J* = 7.3 Hz, 1H), 6.32 (d, *J* = 10.2 Hz, 1H), 5.12 (dd, *J* = 11.6, 4.0 Hz, 1H), 2.77 (dd, *J* = 17.2, 4.1 Hz, 1H), 2.53 (dd, *J* = 17.2, 11.6 Hz, 1H), 2.45 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.20, 148.37, 145.03, 144.19, 140.76, 137.75, 137.59, 133.37, 133.12, 130.13, 129.95, 129.43, 129.07, 129.01, 128.88, 128.34, 128.28, 127.65, 126.83, 126.39, 121.94, 114.39, 62.72, 57.92, 36.64, 21.68.
IR (KBr, cm^{-1}): 3442, 1692, 1649, 1597, 1495, 1359, 1265, 1184, 1080, 1030, 750, 681, 692, 592, 540.
HRMS (ESI): m/z calcd for $C_{32}H_{28}ClN_3O_3S$ ($[M+H]^+$): 568.1456; found: 568.1460.

1,4a-diphenyl-3-(m-tolyl)-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ai**)



White solid, 82 mg, 75% yield
mp: 165-167 ℃
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.66 (d, *J* = 10.2 Hz, 1H), 7.55 (d, *J* = 7.7 Hz, 2H), 7.37 (t, *J* = 7.5 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 3H), 7.22 (t, *J* = 8.4 Hz, 3H), 7.14 (d, *J* = 7.9 Hz, 3H), 7.07 (dd, *J* = 13.6, 7.8 Hz, 3H), 6.98 (s, 1H), 6.90 (t, *J* = 7.3 Hz, 1H), 6.33 (d, *J* = 10.2 Hz, 1H), 4.95 (dd, *J* = 11.2, 4.6 Hz, 1H), 2.80 – 2.53 (m, 2H), 2.39 (s, 3H), 2.21 (s, 3H).
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.67, 149.09, 144.62, 144.43, 141.62, 137.92, 136.89, 136.29, 135.34, 130.05, 129.61, 129.49, 129.27, 128.88, 128.74, 127.67, 127.48, 126.29, 126.22, 121.57, 114.54, 63.68, 59.10, 36.18, 21.60, 21.32.
IR (KBr, cm^{-1}): 3461, 3055, 2987, 1689, 1598, 1494, 1422, 1356, 1266, 1168, 896, 748, 704.
HRMS (ESI): m/z calcd for $C_{33}H_{31}N_3O_3S$ ($[M+H]^+$): 548.2002; found: 548.2006.

3-(2-chlorophenyl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3aj**)



Light yellow oil, 49 mg, 43% yield

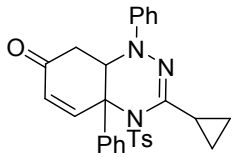
^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 10.3 Hz, 1H), 7.76 (d, *J* = 7.7 Hz, 2H), 7.54 (t, *J* = 7.6 Hz, 2H), 7.44 (t, *J* = 7.4 Hz, 1H), 7.34 (d, *J* = 8.9 Hz, 2H), 7.28 – 7.20 (m, 4H), 7.15 (d, *J* = 8.1 Hz, 3H), 7.00 (d, *J* = 8.2 Hz, 2H), 6.94 (t, *J* = 7.3 Hz, 1H), 6.55 (d, *J* = 10.4 Hz, 1H), 4.73 (dd, *J* = 12.1, 4.3 Hz, 1H), 3.20 (s, 1H), 2.66 (dd, *J* = 17.5, 4.4 Hz, 1H), 2.46 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.12, 149.78, 144.92, 144.64, 135.25, 134.11, 130.48, 130.10, 129.30, 129.16, 128.76, 128.48, 128.00, 125.53, 121.76, 115.16, 65.65, 61.87, 35.24, 21.62.

IR (KBr, cm^{-1}): 3486, 3055, 2987, 1690, 1598, 1495, 1423, 1357, 1266, 1170, 1032, 896, 750, 705, 579, 542.

HRMS (ESI): m/z calcd for $C_{32}H_{28}ClN_3O_3S$ ($[M+H]^+$): 568.1456; found: 568.1460.

3-cyclopropyl-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3ak**)



White solid, 41 mg, 41% yield

mp: 203-205 ℃

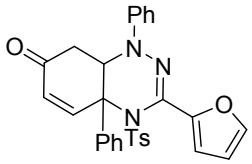
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.78 (d, *J* = 10.3 Hz, 1H), 7.75 – 7.67 (m, 2H), 7.55 – 7.44 (m, 2H), 7.40 (dd, *J* = 8.7, 6.8 Hz, 2H), 7.32 (dd, *J* = 7.7, 3.4 Hz, 3H), 7.19 – 7.06 (m, 2H), 6.89 – 6.84 (m, 2H), 6.82 (t, *J* = 7.4 Hz, 1H), 6.38 (d, *J* = 10.3 Hz, 1H), 4.57 (dd, *J* = 9.7, 6.4 Hz, 1H), 2.51 – 2.41 (m, 5H), 2.37 (tt, *J* = 8.1, 5.1 Hz, 1H), 0.97 – 0.74 (m, 2H), 0.44 (ddt, *J* = 9.6, 6.5, 4.5 Hz, 1H), 0.31 (tdd, *J* = 8.6, 6.5, 4.1 Hz, 1H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 197.36, 151.47, 145.26, 144.51, 142.70, 139.70, 138.86, 129.94, 129.65, 129.07, 128.77, 128.35, 127.18, 125.22, 120.98, 114.28, 66.20, 61.69, 34.53, 21.60, 14.57, 9.93, 7.34.

IR (KBr, cm^{-1}): 3449, 1720, 1655, 1495, 1407, 1268, 1165, 1139, 734, 673.

HRMS (ESI): m/z calcd for $C_{29}H_{29}N_3O_3S$ ($[M+H]^+$): 498.1846; found: 498.1849.

3-(furan-2-yl)-1,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3al**)



Light yellow oil, 59 mg, 56% yield

^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 7.9 Hz, 2H), 7.41 (d, *J* = 7.7 Hz, 2H), 7.19 (dq, *J* = 15.6, 7.3 Hz, 8H), 7.01 (d, *J* = 7.4 Hz, 3H), 6.84 (t, *J* = 7.3 Hz, 1H), 6.61 – 6.49 (m, 1H), 6.37 (s, 1H), 6.13 (d, *J* = 10.1 Hz, 1H), 5.05 (dd, *J* = 11.2, 5.1 Hz, 1H), 2.73 – 2.55 (m, 2H), 2.33 (s, 3H).

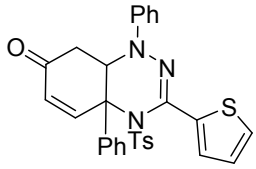
^{13}C NMR (101 MHz, $CDCl_3$) δ 196.47, 148.46, 147.44, 144.78, 144.18, 141.96, 140.27, 137.76, 130.37, 129.83, 129.32, 129.16, 128.73, 128.02, 126.03, 125.14, 121.79, 113.99, 111.25, 109.79, 62.40, 58.34,

37.03, 21.69.

IR (KBr, cm^{-1}): 3442, 1649, 1503, 1479, 1266, 1232, 747, 705.

HRMS (ESI): m/z calcd for $C_{30}H_{25}N_3O_4SNa$ ($[M+Na]^+$): 546.1462; found: 546.1458.

1,4a-diphenyl-3-(thiophen-2-yl)-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3am**)



White solid, 32 mg, 30% yield

mp: 172-174 ℃

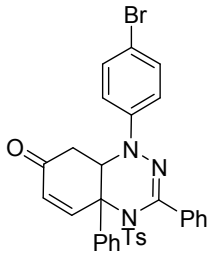
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.54 – 7.45 (m, 2H), 7.45 – 7.37 (m, 3H), 7.36 – 7.20 (m, 7H), 7.17 (d, *J* = 8.1 Hz, 2H), 7.14 – 7.08 (m, 2H), 7.07 (dd, *J* = 3.7, 1.2 Hz, 1H), 6.93 (td, *J* = 7.2, 1.1 Hz, 1H), 6.89 (dd, *J* = 5.1, 3.7 Hz, 1H), 6.21 (d, *J* = 10.2 Hz, 1H), 5.13 (dd, *J* = 11.0, 4.1 Hz, 1H), 2.76 (dd, *J* = 17.2, 4.0 Hz, 1H), 2.61 (dd, *J* = 17.2, 11.1 Hz, 1H), 2.39 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.12, 148.32, 144.61, 144.14, 138.02, 137.79, 129.73, 129.30, 129.05, 128.90, 128.08, 127.75, 126.45, 126.22, 126.18, 121.88, 114.61, 63.11, 58.05, 37.08, 21.64.

IR (KBr, cm^{-1}): 3442, 1675, 1649, 1530, 1265, 748, 705.

HRMS (ESI): m/z calcd for $C_{29}H_{29}N_3O_3S$ ($[M+H]^+$): 540.1410; found: 540.1414.

1-(4-bromophenyl)-3,4a-diphenyl-4-tosyl-4,4a,8,8a-tetrahydrobenzo[e][1,2,4]triazin-7(1H)-one (**3an**)



White solid, 72 mg, 58% yield

mp: 141-143 ℃

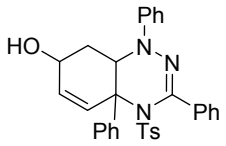
^{1}H NMR (400 MHz, $CDCl_3$) δ 7.63 (d, *J* = 10.2 Hz, 1H), 7.55 (d, *J* = 7.6 Hz, 2H), 7.38 (dt, *J* = 21.0, 7.7 Hz, 10H), 7.30 – 7.23 (m, 2H), 7.19 (d, *J* = 8.0 Hz, 2H), 7.00 (d, *J* = 8.7 Hz, 2H), 6.32 (d, *J* = 10.2 Hz, 1H), 5.00 (dd, *J* = 11.7, 4.2 Hz, 1H), 2.69 (dd, *J* = 17.2, 4.1 Hz, 1H), 2.53 (dd, *J* = 17.2, 11.7 Hz, 1H), 2.43 (s, 3H).

^{13}C NMR (101 MHz, $CDCl_3$) δ 196.13, 148.72, 144.74, 143.55, 141.07, 137.74, 135.85, 135.69, 132.13, 129.97, 129.80, 129.05, 128.95, 128.72, 128.56, 127.67, 127.52, 126.22, 115.69, 113.86, 63.01, 58.18, 36.34, 21.67.

IR (KBr, cm^{-1}): 3463, 1690, 1566, 1430, 1365, 1198, 1165, 878, 793, 695, 582, 544.

HRMS (ESI): m/z calcd for $C_{29}H_{29}N_3O_3S$ ($[M+H]^+$): 612.0951; found: 612.0955.

1,3,4a-triphenyl-4-tosyl-1,4,4a,7,8,8a-hexahydrobenzo[e][1,2,4]triazin-7-ol (**4**)



White solid, 91 mg, 85% yield

mp: 96-99 ℃

^{1}H NMR (400 MHz, DMSO-d_6) δ 7.49 (d, J = 7.8 Hz, 2H), 7.42 – 7.32 (m, 4H), 7.32 – 7.18 (m, 6H), 7.12 (dt, J = 9.0, 4.4 Hz, 6H), 6.84 (t, J = 7.2 Hz, 1H), 6.49 (dd, J = 10.2, 1.8 Hz, 1H), 6.26 (d, J = 10.3 Hz, 1H), 5.21 (s, 1H), 4.76 – 4.37 (m, 2H), 2.38 (s, 3H), 2.01 – 1.88 (m, 1H), 1.88 – 1.69 (m, 1H).

^{13}C NMR (101 MHz, DMSO) δ 145.60, 145.08, 144.28, 138.75, 137.59, 135.63, 129.92, 129.46, 129.25, 128.56, 128.38, 128.22, 127.90, 127.69, 127.53, 126.08, 120.68, 114.18, 66.75, 65.09, 58.78, 30.14, 21.52.

IR (KBr, cm-1): 3463, 3298, 1746, 1675, 1566, 1430, 1365, 1198, 1165, 878, 793, 695, 582, 544.

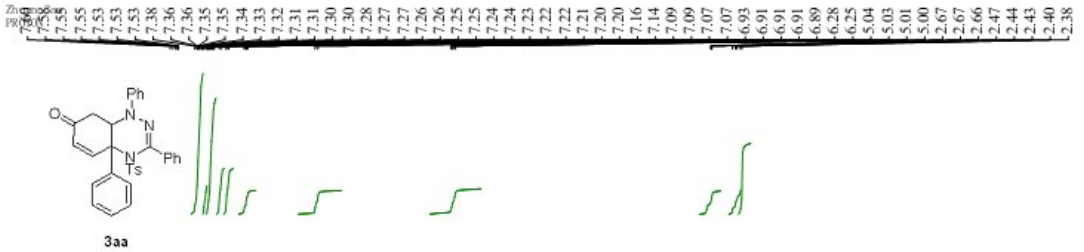
HRMS (ESI): m/z calcd for C29H29N3O3S ([M+H]+): 536.2002; found: 536.2007.

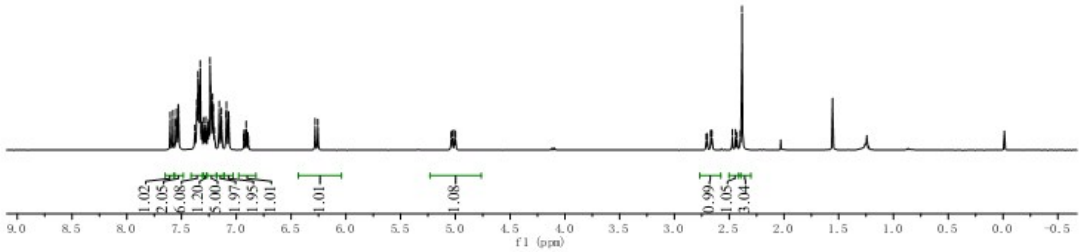
5. References

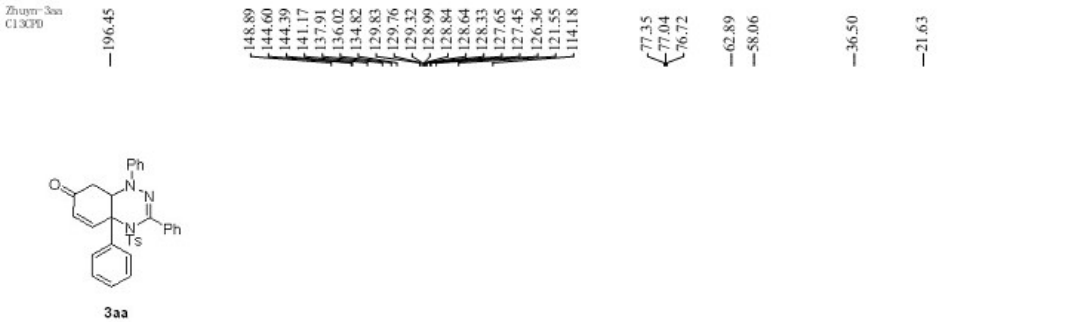
[1] Jin, H.; Zhang, Q.; Li, E.; Jia, P.; Li, N. and Huang, Y. *Org. Biomol. Chem.* **2017**, *15*, 7097-7101. General Procedure and Spectroscopic Data

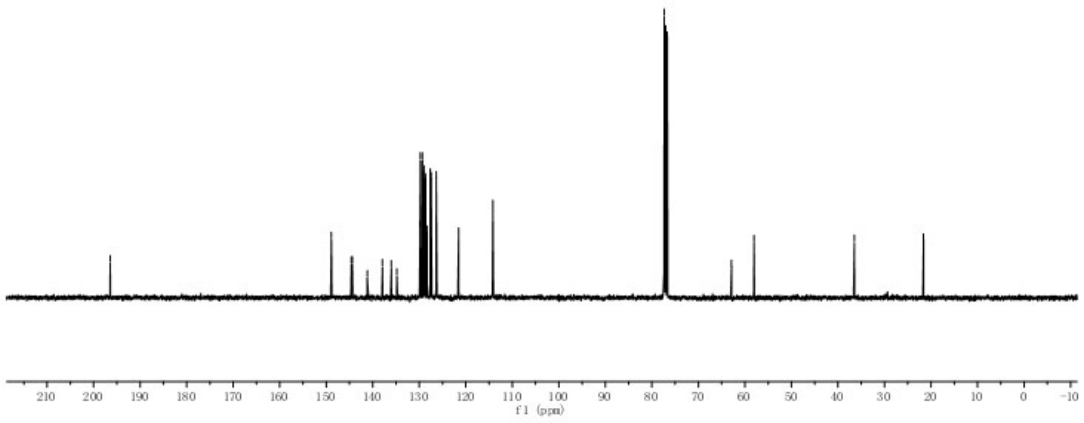
[2] Garve, L. K. B.; Petzold, M.; Jones, P. G.; Werz, D.B. *Org. Lett.* **2016**, *18*, 564.

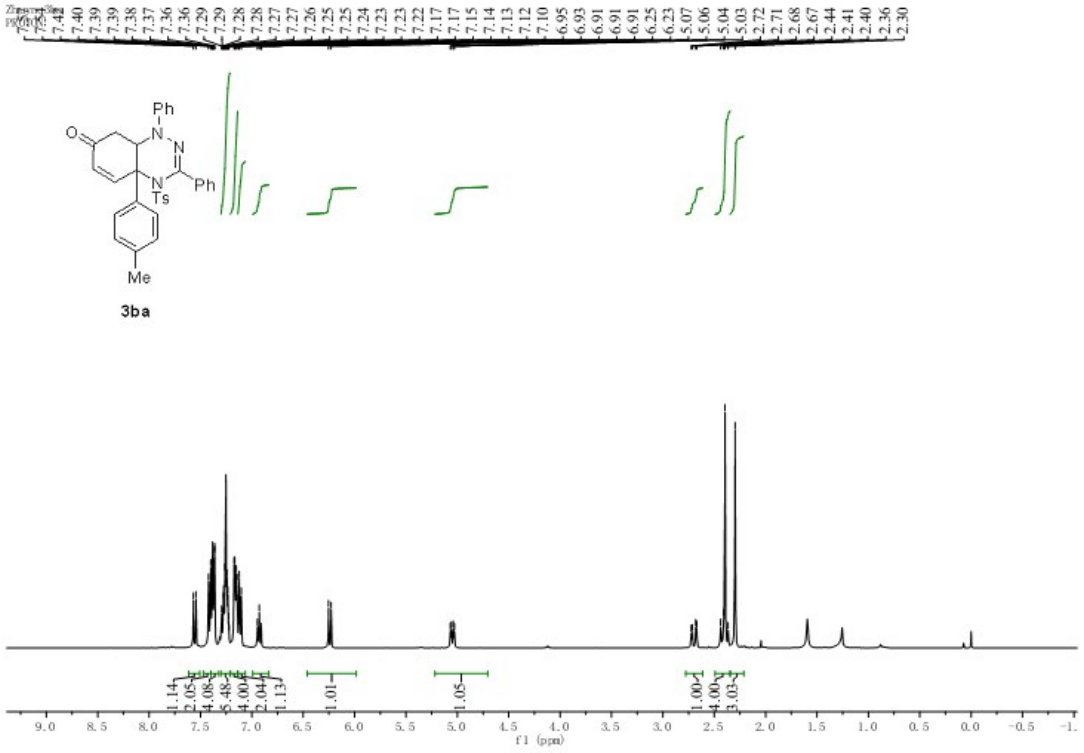
6. NMR spectra of products

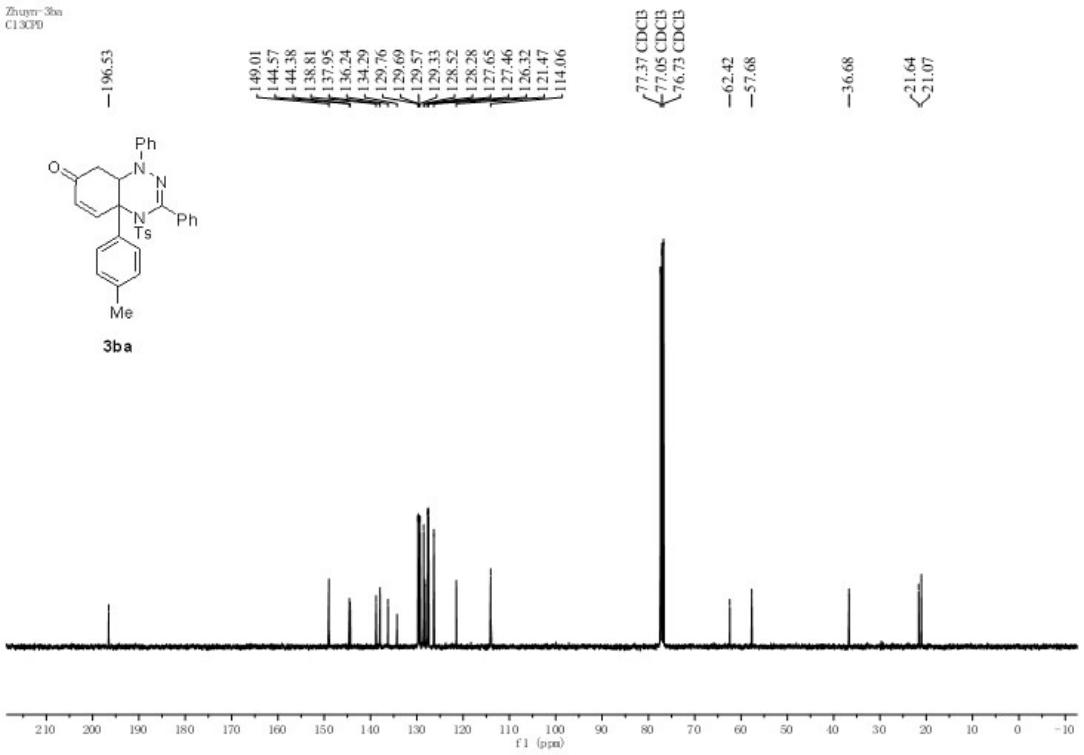


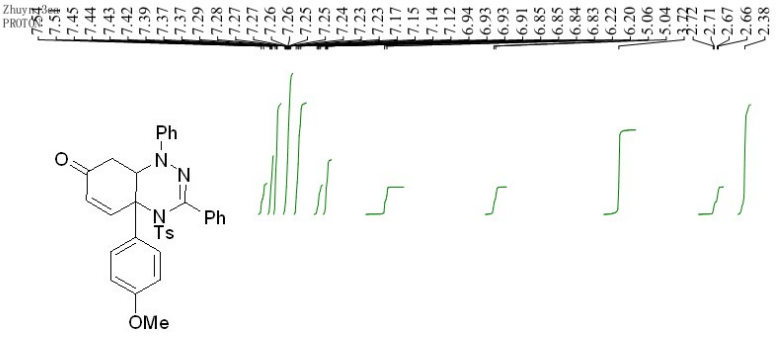




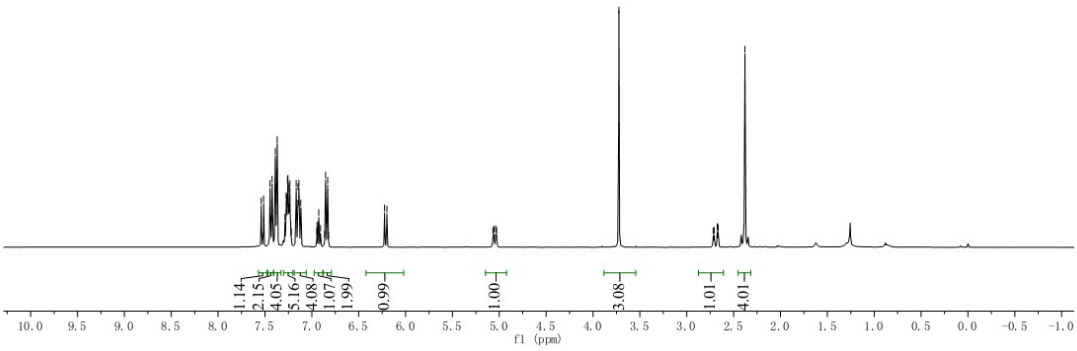


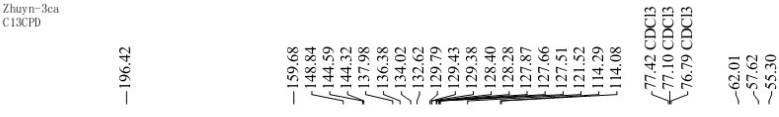

Ph
N
N
O
Ph
N
Ts
Me
3ba
1.14
2.05
4.08
5.48
4.00
2.04
1.13
1.01
1.05
1.00
4.00
3.03
f1 (ppm)


196.53
149.01
144.57
144.38
138.81
137.95
136.24
134.29
129.76
129.69
129.57
129.33
128.52
128.28
127.65
127.46
126.32
121.47
114.06
77.37 CDCl3
77.05 CDCl3
76.73 CDCl3
62.42
57.68
36.68
21.64
21.07
Ph
N
N
O
Ph
N
Ts
Me
3ba
f1 (ppm)


Ph
N
N
O
N
Ts
Ph
OMe

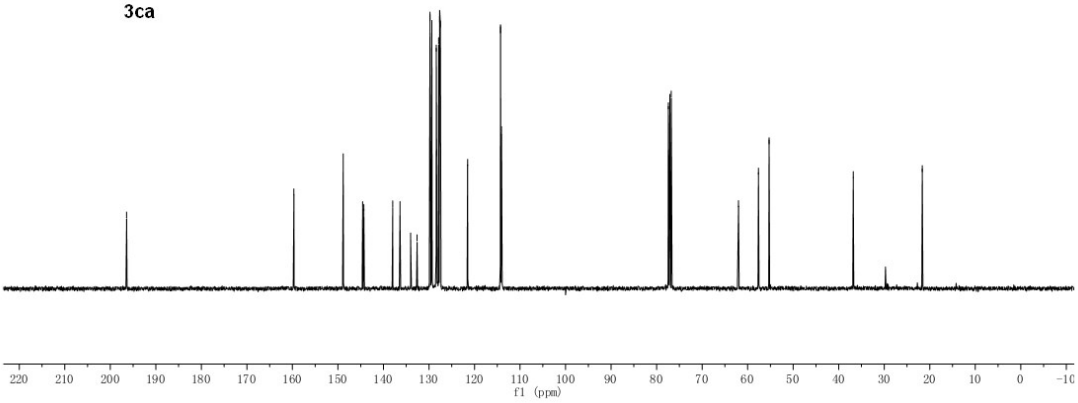
3ca

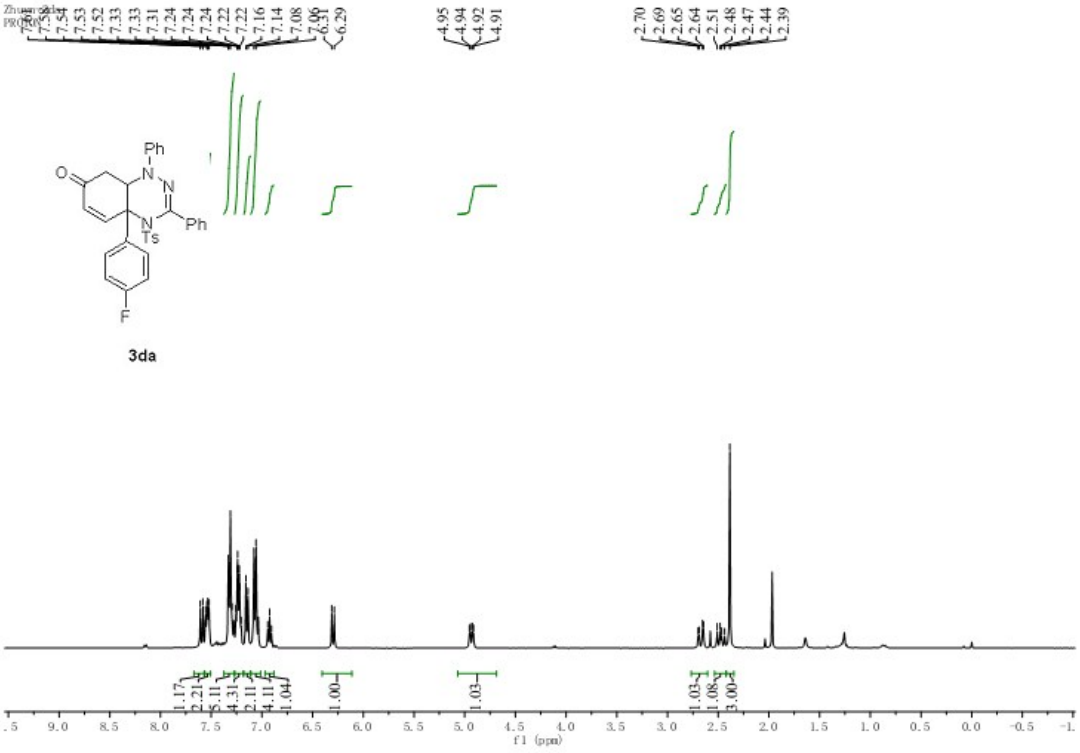

1.14
2.15
4.05
5.16
4.08
1.07
1.99
0.99
1.00
3.08
1.01
4.01
f1 (ppm)


196.42
159.68
148.84
144.59
144.32
137.98
136.38
134.02
132.62
129.79
129.43
129.38
128.40
128.28
127.87
127.66
127.51
121.52
114.29
114.08
77.42 CDCl3
77.10 CDCl3
76.79 CDCl3
62.01
57.62
55.30
36.81
21.65

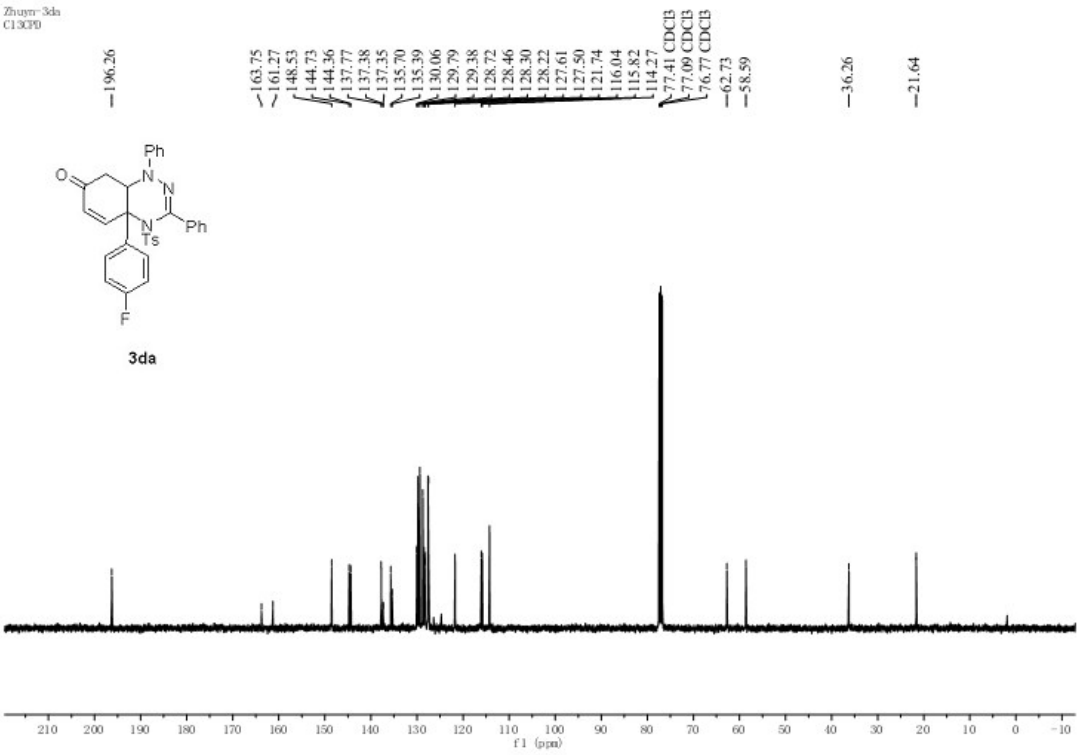

Ph
N
N
O
N
Ts
Ph
OMe

3ca

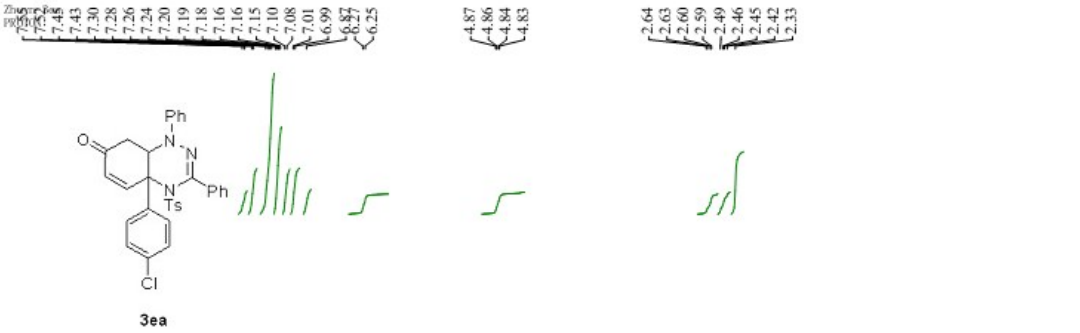

f1 (ppm)


7.58
7.54
7.53
7.52
7.33
7.31
7.24
7.24
7.24
7.22
7.22
7.16
7.14
7.08
7.06
6.31
6.29
4.95
4.94
4.92
4.91
2.70
2.69
2.65
2.64
2.51
2.48
2.47
2.44
2.39
Ph
N
N
O
Ph
N
Ts
F
1.17
2.21
5.11
4.31
2.11
4.11
1.04
1.00
1.03
1.03
1.08
3.00
f1 (ppm)

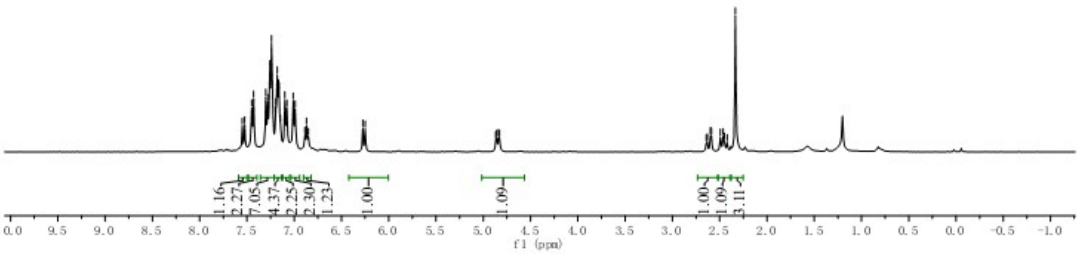
3da

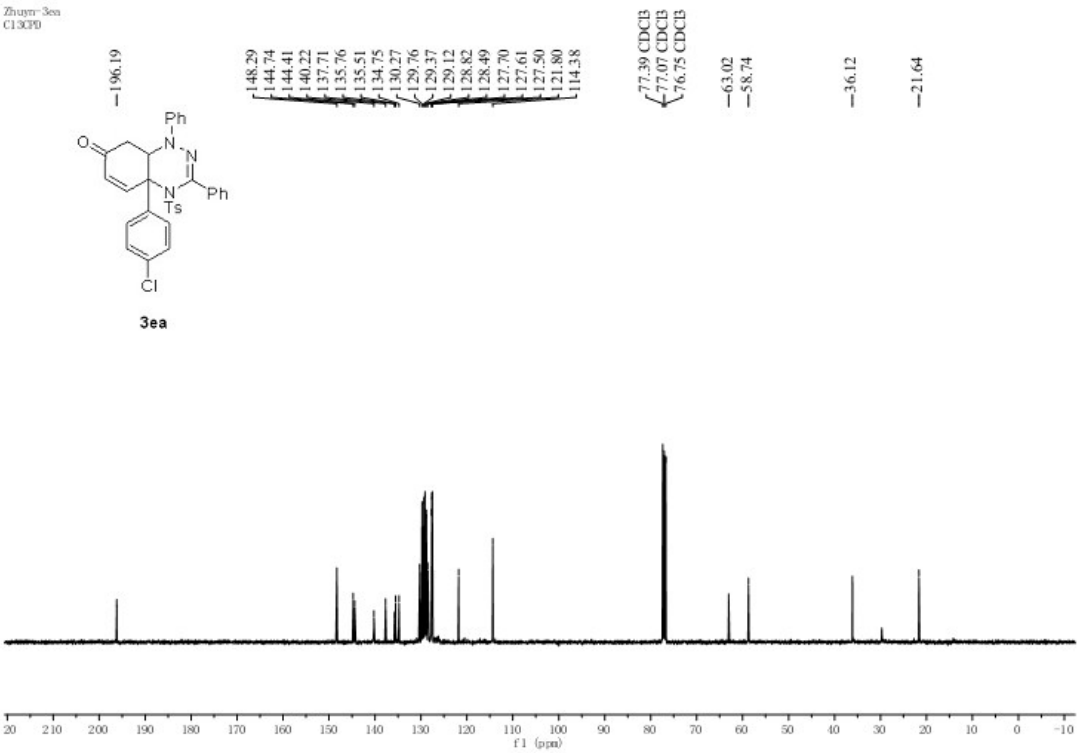

Zhuym-3da
C13CPD
196.26
163.75
161.27
148.53
144.73
144.36
137.77
137.38
137.35
135.70
135.39
130.06
129.79
129.38
128.72
128.46
128.30
128.22
127.61
127.50
121.74
116.04
115.82
114.27
77.41 CDCl3
77.09 CDCl3
76.77 CDCl3
62.73
58.59
36.26
21.64
Ph
N
N
O
Ph
N
Ts
F
f1 (ppm)

3da

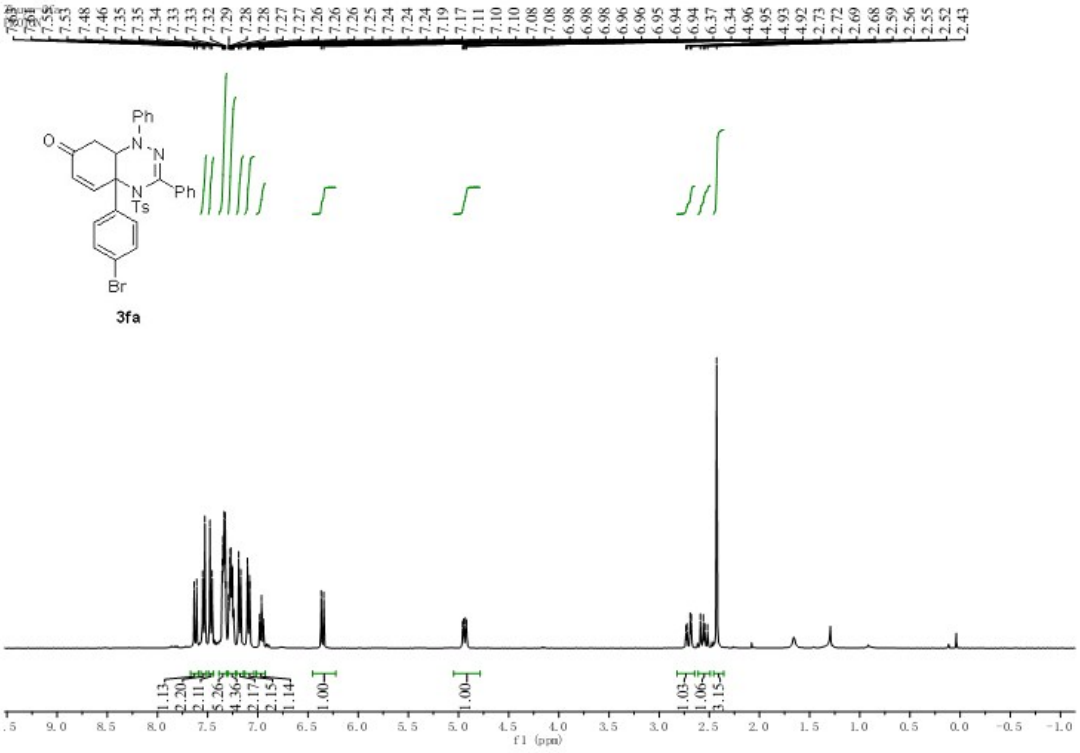

7.45
7.43
7.30
7.28
7.26
7.24
7.20
7.19
7.18
7.16
7.16
7.15
7.10
7.08
7.01
6.99
6.87
6.27
6.25
4.87
4.86
4.84
4.83
2.64
2.63
2.60
2.59
2.49
2.46
2.45
2.42
2.33
Ph
N
N
O
Ph
N
Ts
Cl

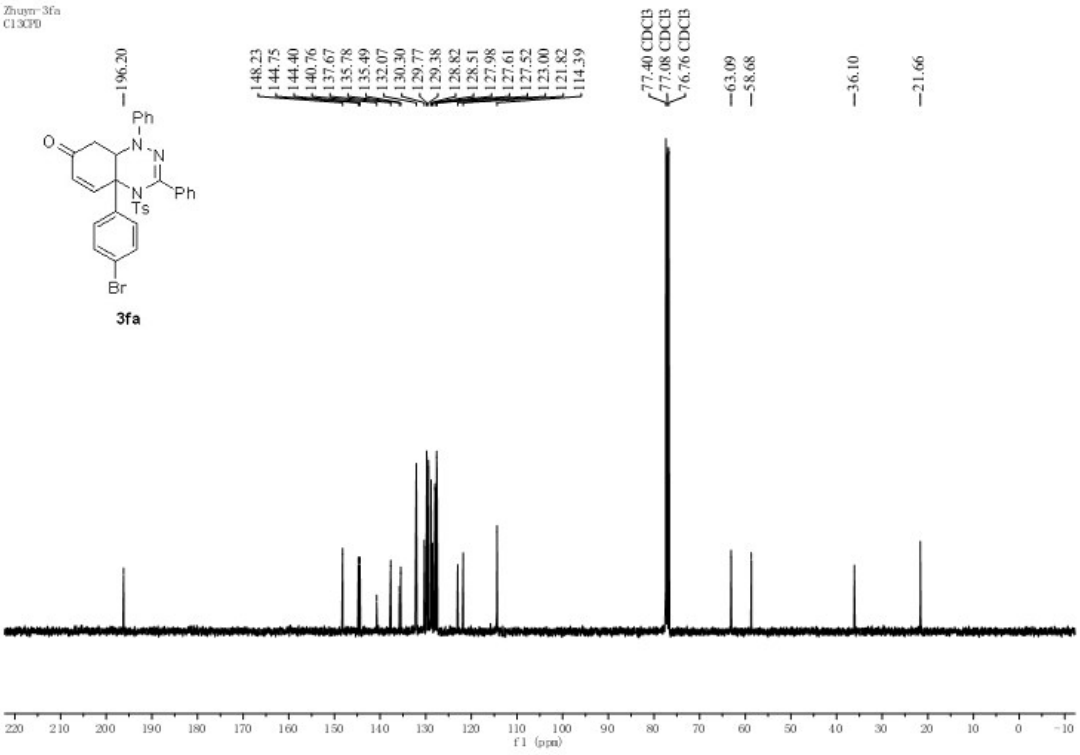
3ea

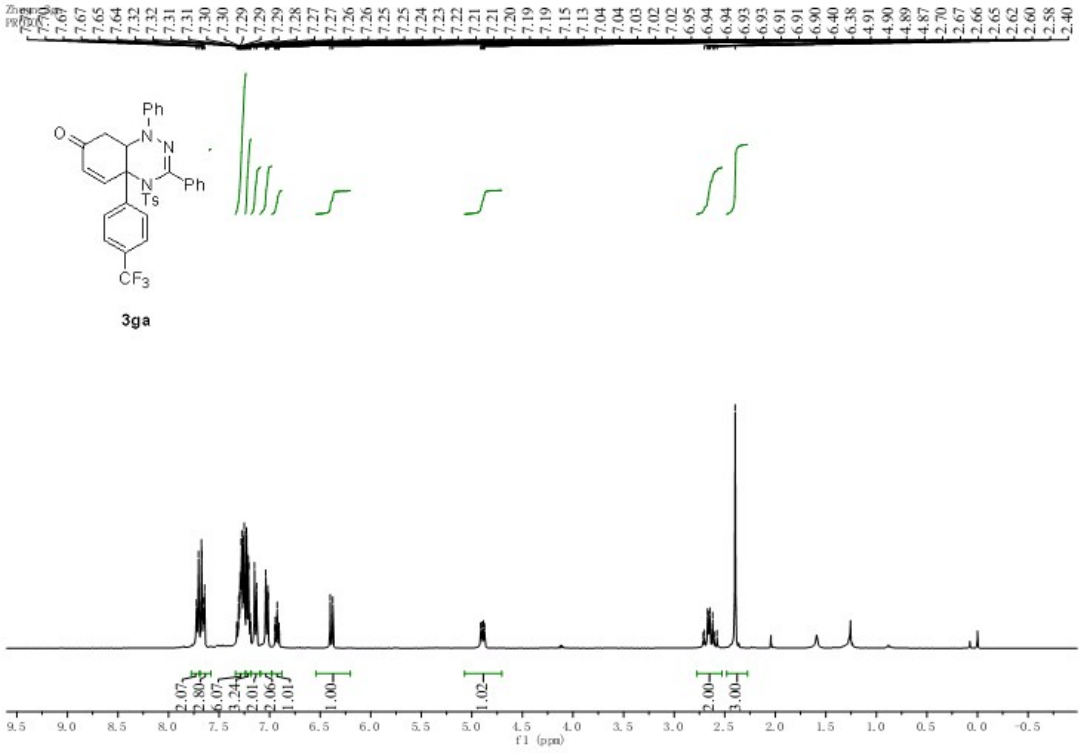

1.16
2.27
7.05
4.37
2.25
2.30
1.23
1.00
1.09
1.00
1.09
3.11
f1 (ppm)

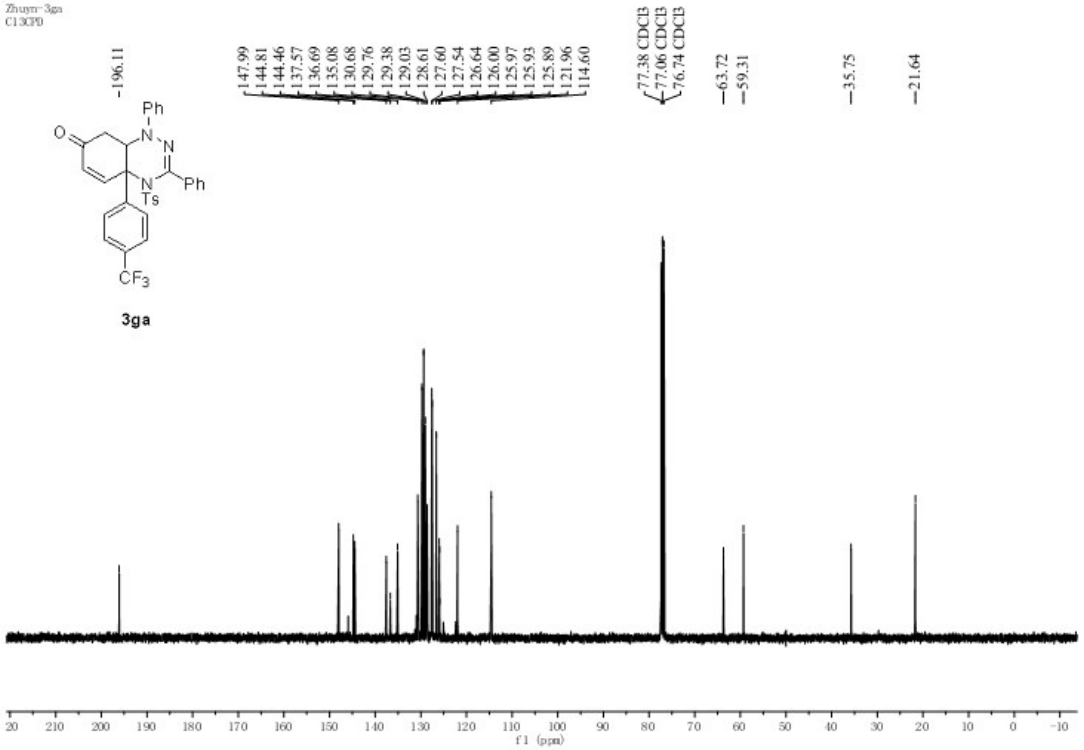

Zhuym-3ea
C13CPD
196.19
148.29
144.74
144.41
140.22
137.71
135.76
135.51
134.75
130.27
129.76
129.37
129.12
128.82
128.49
127.70
127.61
127.50
121.80
114.38
77.39 CDCl3
77.07 CDCl3
76.75 CDCl3
63.02
58.74
36.12
21.64
Ph
N
N
O
Ph
N
Ts
Cl
f1 (ppm)

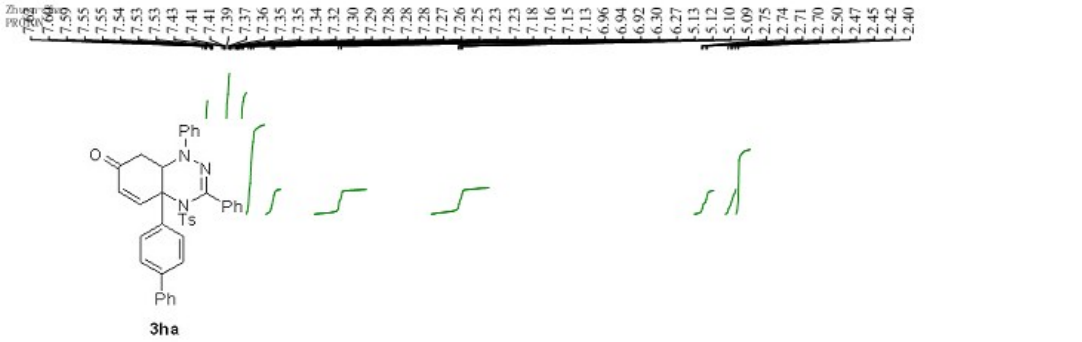
3ea


Ph
N
N
O
Ph
N
Ts
Br
3fa
1.13
2.20
2.11
5.26
4.36
2.17
2.15
1.14
1.00
1.00
1.03
1.06
3.15
f1 (ppm)

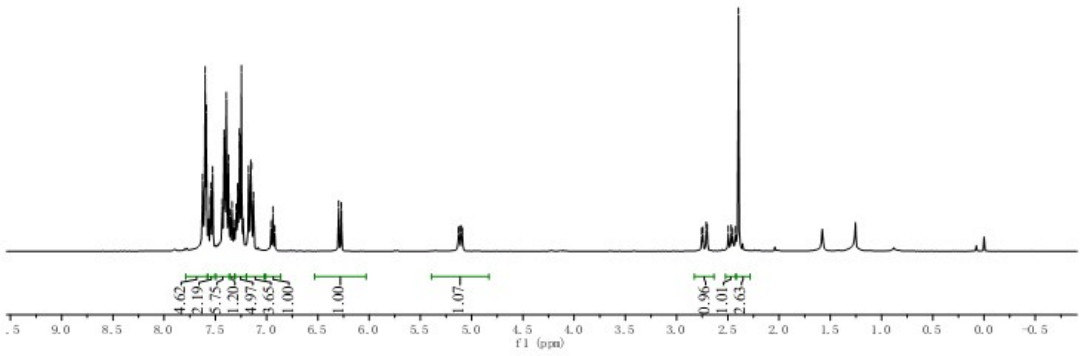

Zhuym-3fa
C13CPD
196.20
148.23
144.75
144.40
140.76
137.67
135.78
135.49
132.07
130.30
129.77
129.38
128.82
128.51
127.98
127.61
127.52
123.00
121.82
114.39
77.40 CDCl3
77.08 CDCl3
76.76 CDCl3
63.09
58.68
36.10
21.66
Ph
N
N
O
Ph
N
Ts
Br
3fa
f1 (ppm)

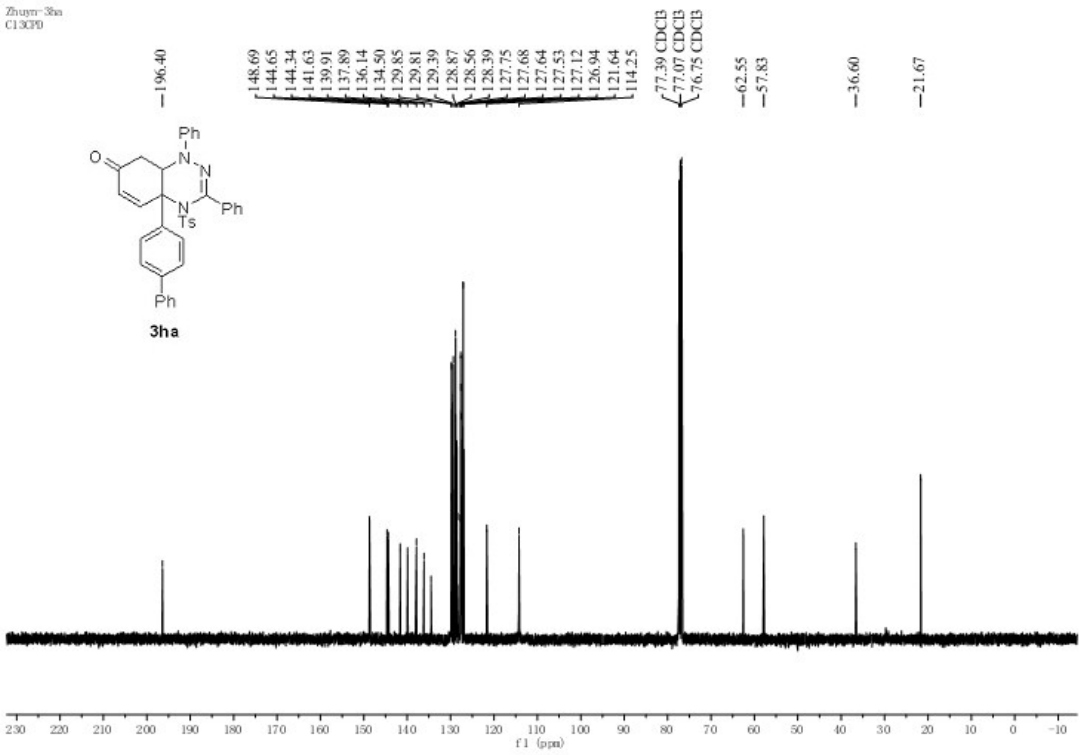

Ph
N
N
O
Ph
N
Ts
CF3
3ga
2.07
2.80
6.07
3.24
2.01
2.06
1.01
1.00
1.02
2.00
3.00
f1 (ppm)


Zhuym-3ga
C13CPD
196.11
147.99
144.81
144.46
137.57
136.69
135.08
130.68
129.76
129.38
129.03
128.61
127.60
127.54
126.64
126.00
125.97
125.93
125.89
121.96
114.60
77.38 CDCl3
77.06 CDCl3
76.74 CDCl3
63.72
59.31
35.75
21.64
Ph
N
N
O
Ph
N
Ts
CF3
3ga
f1 (ppm)

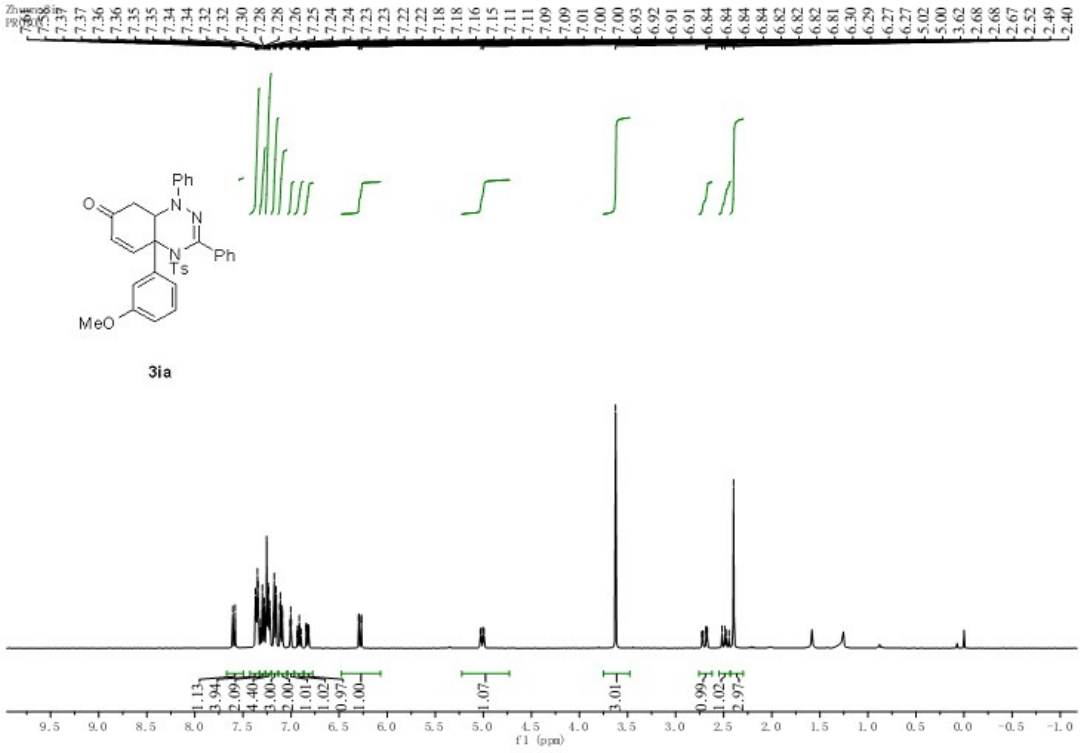

Ph
N
N
Ph
Ts
Ph
O

3ha

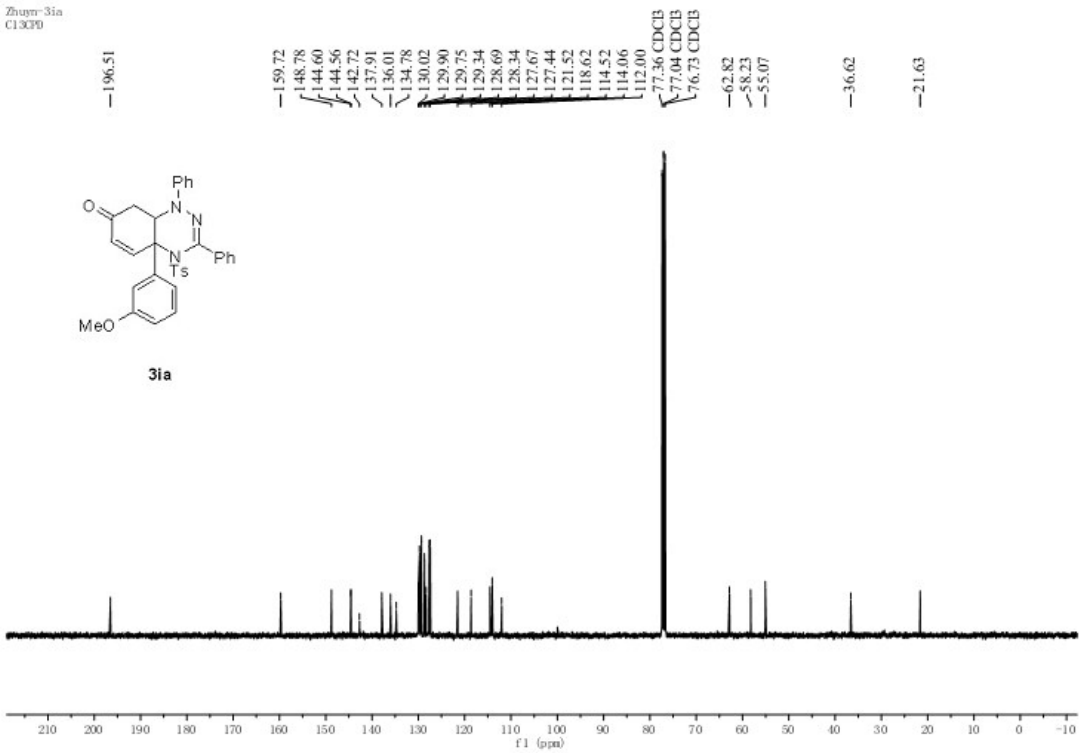

4.62
2.19
5.75
1.20
4.97
3.65
1.00
1.00
1.07
0.96
1.01
2.63
f1 (ppm)


196.40
148.69
144.65
144.34
141.63
139.91
137.89
136.14
134.50
129.85
129.81
129.39
128.87
128.56
128.39
127.75
127.68
127.64
127.53
127.12
126.94
121.64
114.25
77.39 CDCl3
77.07 CDCl3
76.75 CDCl3
62.55
57.83
36.60
21.67
Ph
N
N
Ph
Ts
Ph
O
f1 (ppm)

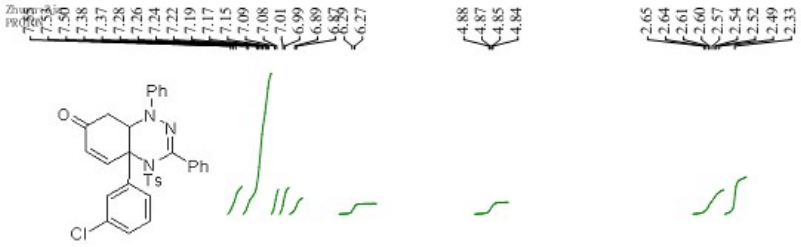
3ha


Ph
N
N
O
Ph
N
Ts
MeO
1.13
3.94
2.09
4.40
3.00
2.00
1.01
1.02
0.97
1.00
1.07
3.01
0.99
1.02
2.97
f1 (ppm)

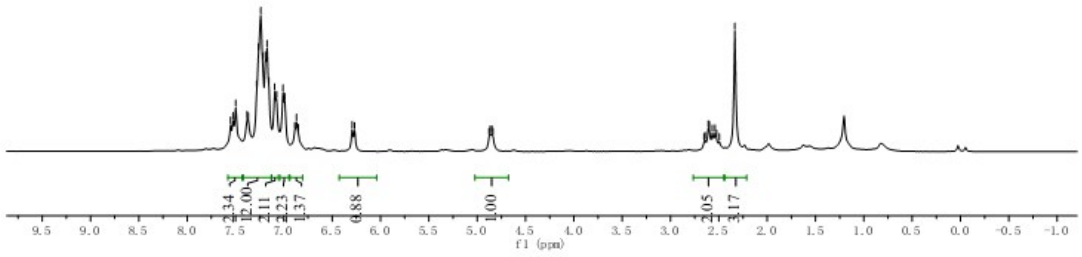
3ia

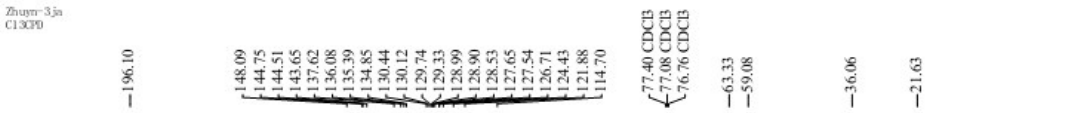

Zhuym-3ia
C13CPD
196.51
159.72
148.78
144.60
144.56
142.72
137.91
136.01
134.78
130.02
129.90
129.75
129.34
128.69
128.34
127.67
127.44
121.52
118.62
114.52
114.06
112.00
77.36 CDCl3
77.04 CDCl3
76.73 CDCl3
62.82
58.23
55.07
36.62
21.63
Ph
N
N
O
Ph
N
Ts
MeO
f1 (ppm)

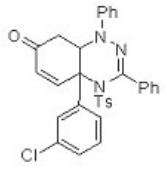
3ia



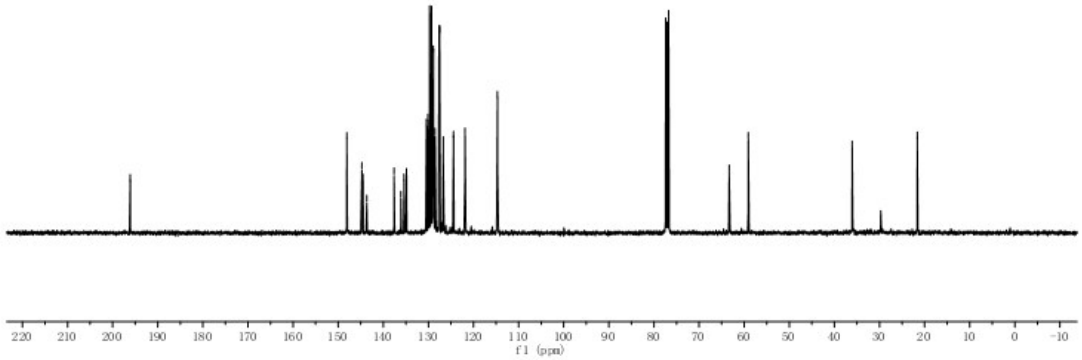
3ja

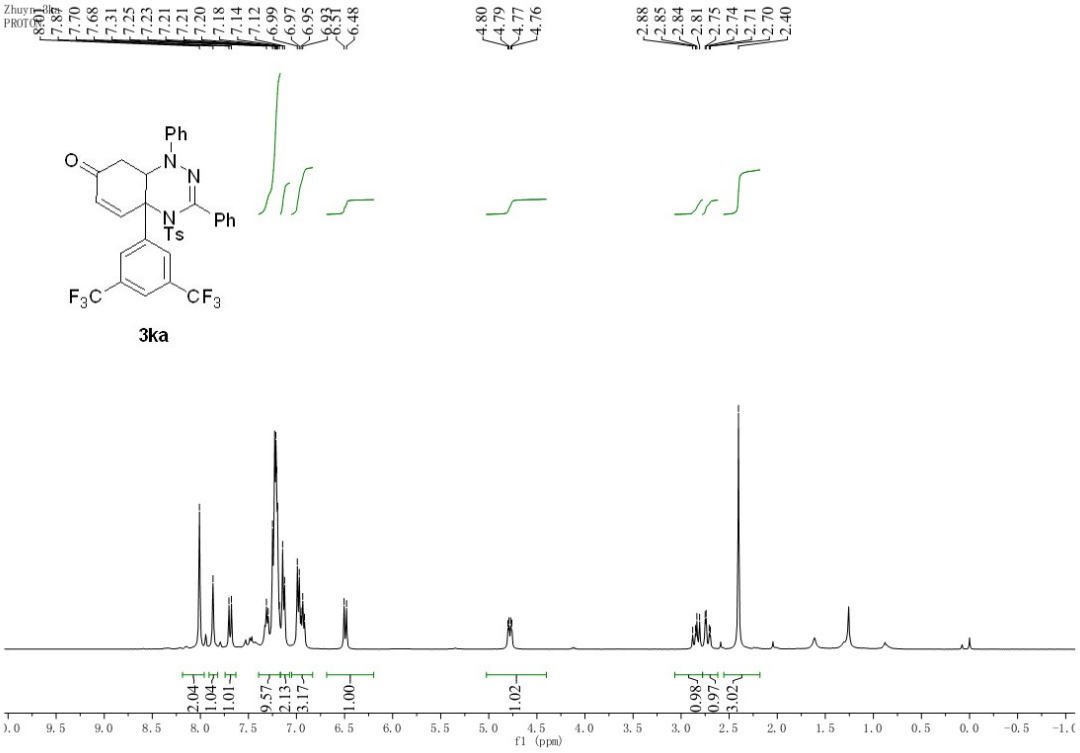




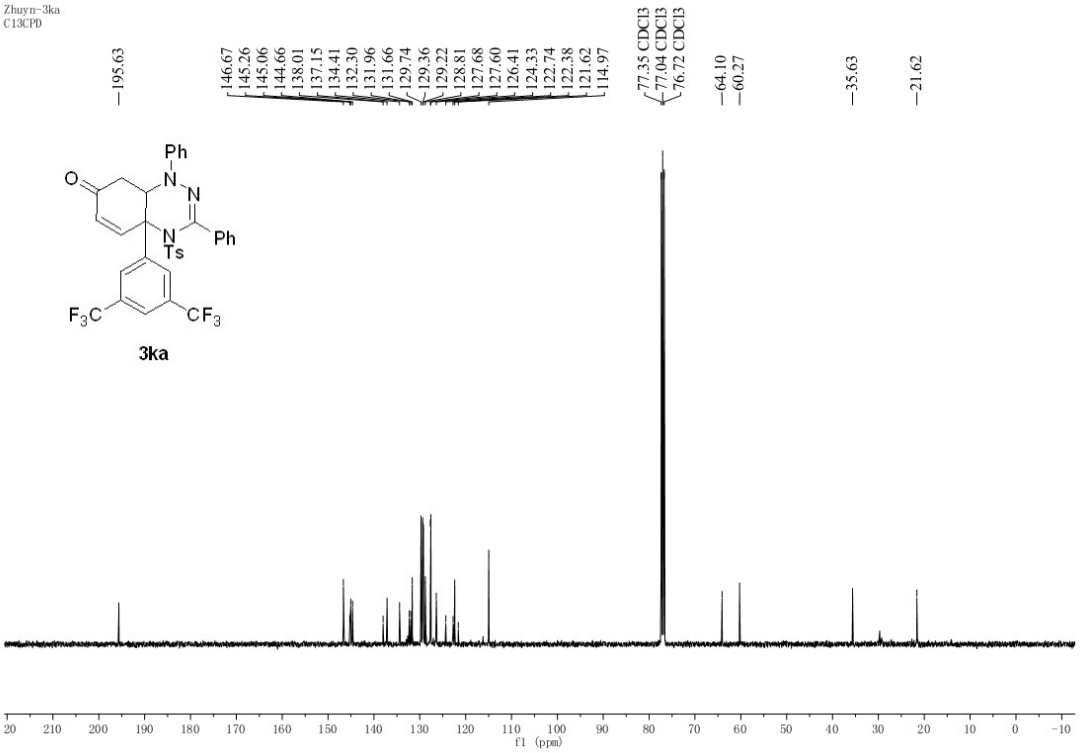


3ja

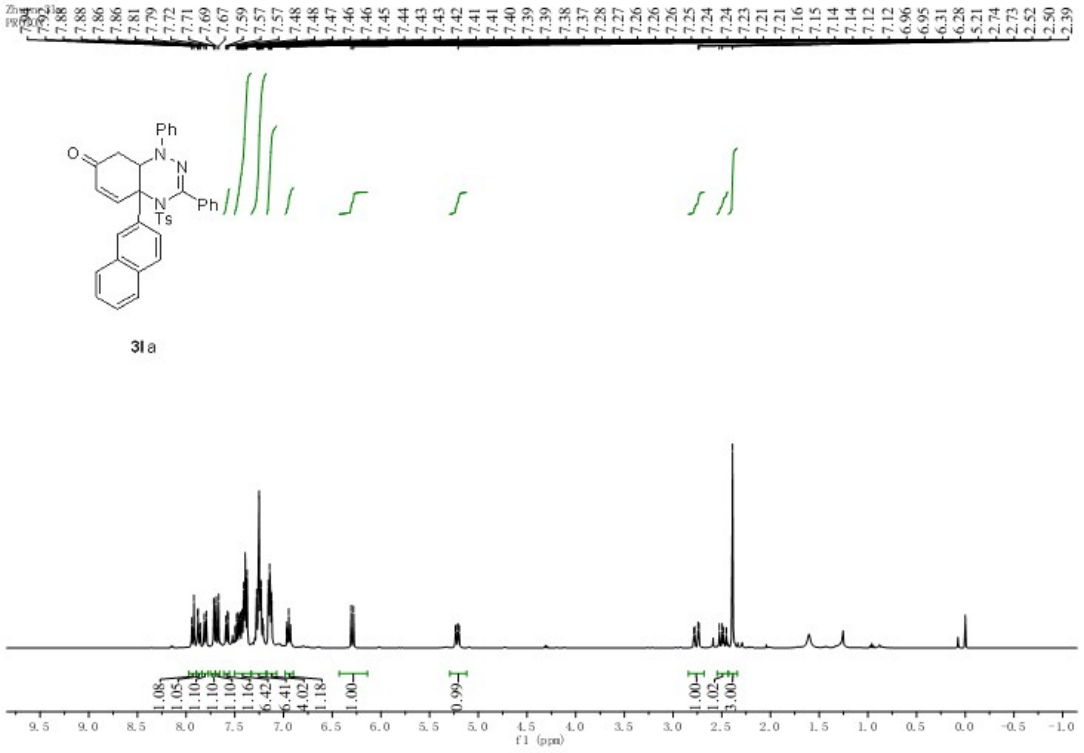



Zhuyn-3ka
PROTON
8.01
7.89
7.87
7.70
7.68
7.31
7.25
7.23
7.21
7.21
7.20
7.18
7.14
7.12
6.99
6.97
6.95
6.93
6.51
6.48
4.80
4.79
4.77
4.76
2.88
2.85
2.84
2.81
2.75
2.74
2.71
2.70
2.40
Ph
N
N
O
Ph
N
Ts
F3C
CF3
2.04
1.04
1.01
9.57
2.13
3.17
1.00
1.02
0.98
0.97
3.02
f1 (ppm)

3ka

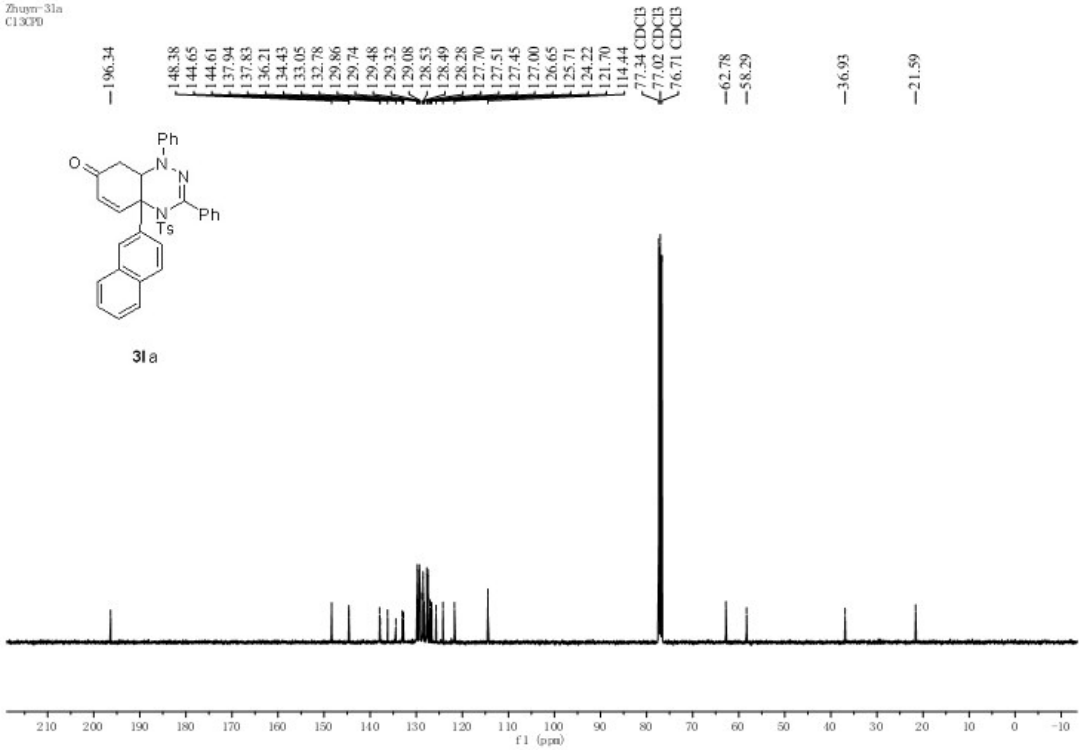

Zhuyn-3ka
C13CPD
195.63
146.67
145.26
145.06
144.66
138.01
137.15
134.41
132.30
131.96
131.66
129.74
129.36
129.22
128.81
127.68
127.60
126.41
124.33
122.74
122.38
121.62
114.97
77.35 CDCl3
77.04 CDCl3
76.72 CDCl3
64.10
60.27
35.63
21.62
Ph
N
N
O
Ph
N
Ts
F3C
CF3
f1 (ppm)

3ka


Ph
N
N
O
N
Ph
Ts

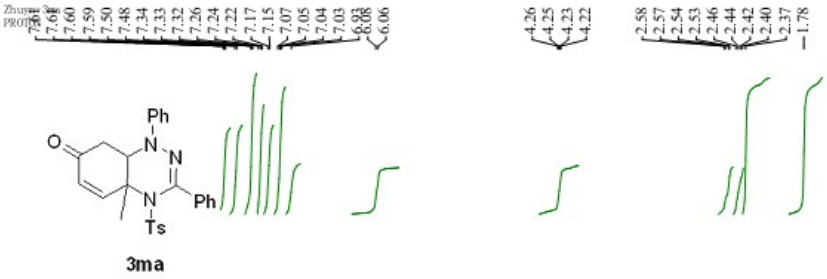
3l a

1.08
1.05
1.10
1.10
1.10
1.16
6.42
6.41
4.02
1.18
1.00
10.99
1.00
1.02
3.00
f1 (ppm)

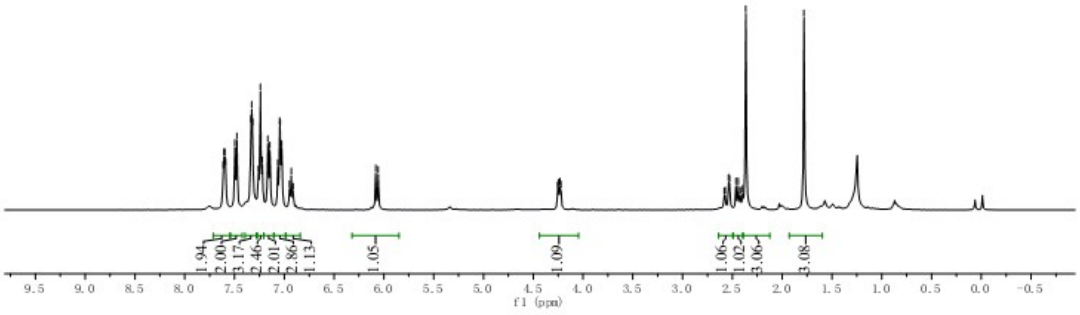

Zhuym-31a
C13CPD
196.34
148.38
144.65
144.61
137.94
137.83
136.21
134.43
133.05
132.78
129.86
129.74
129.48
129.32
129.08
128.53
128.49
128.28
127.70
127.51
127.45
127.00
126.65
125.71
124.22
121.70
114.44
77.34 CDCl3
77.02 CDCl3
76.71 CDCl3
62.78
58.29
36.93
21.59
f1 (ppm)

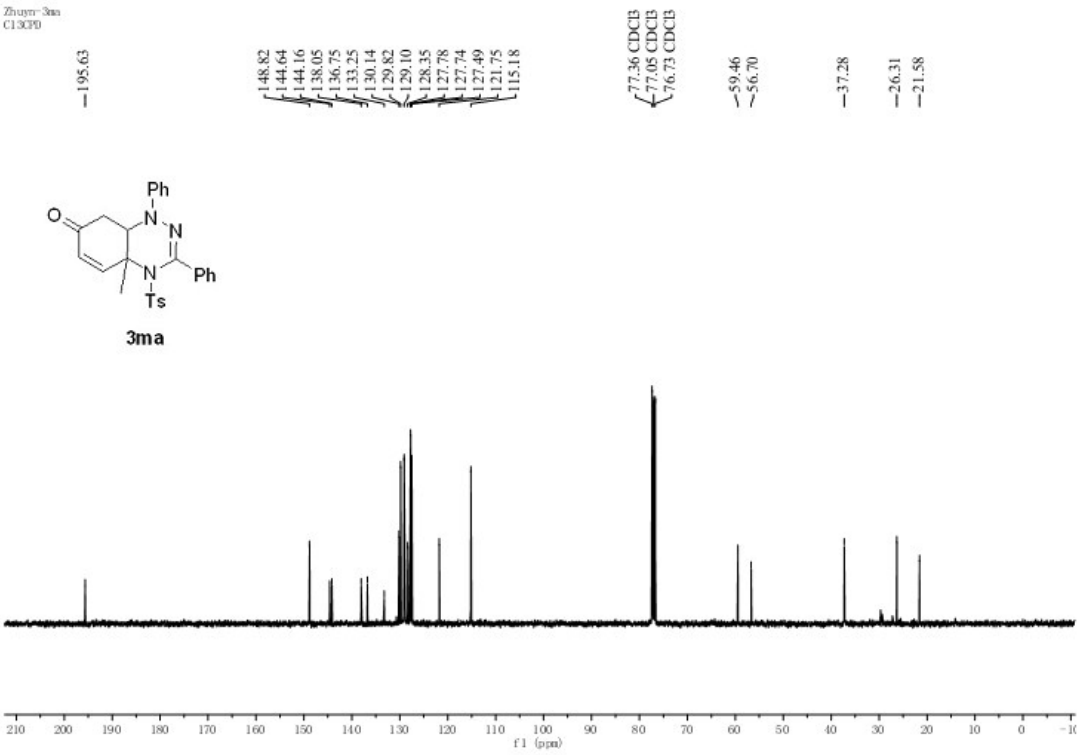
Ph
N
N
O
N
Ph
Ts

3l a

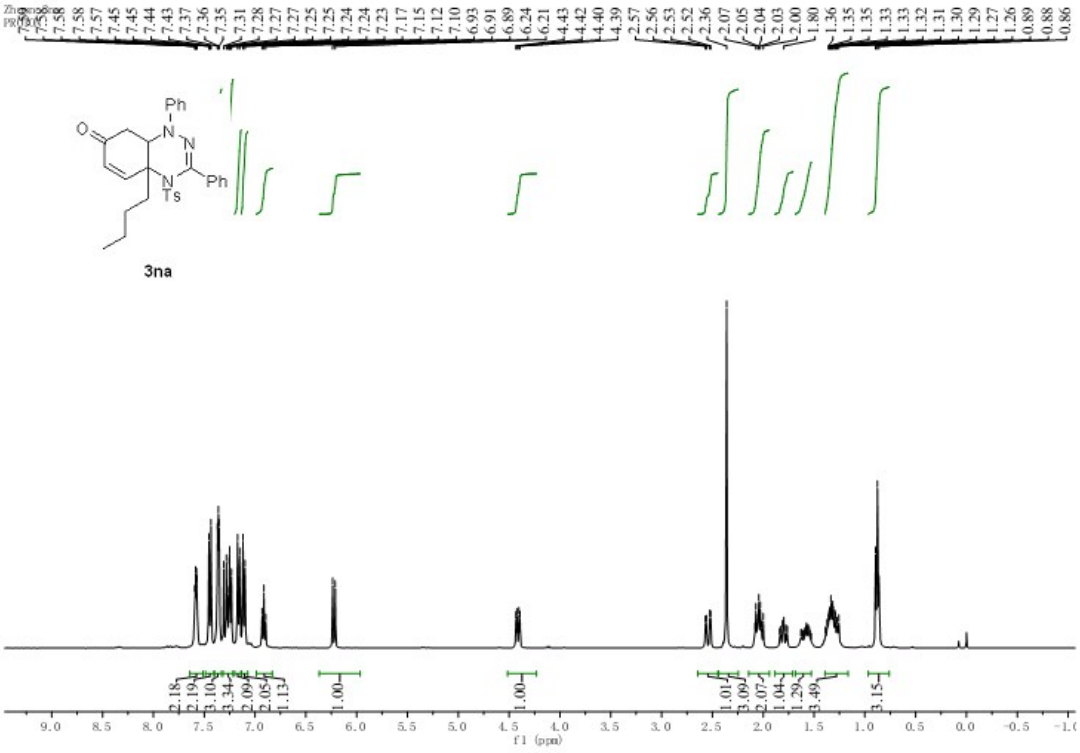

7.61
7.60
7.59
7.50
7.48
7.34
7.33
7.32
7.26
7.24
7.22
7.17
7.15
7.07
7.05
7.04
7.03
6.08
6.06
4.26
4.25
4.23
4.22
2.58
2.57
2.54
2.53
2.46
2.44
2.42
2.40
2.37
1.78
Ph
N
N
O
Ph
N
Ts

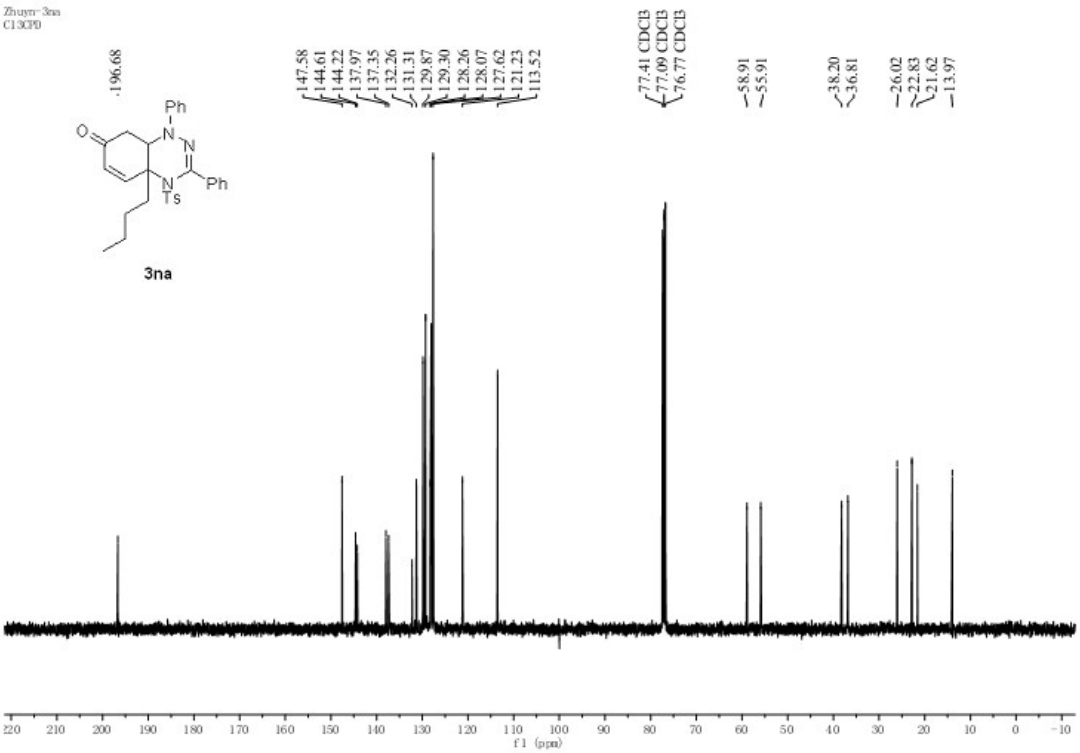
3ma

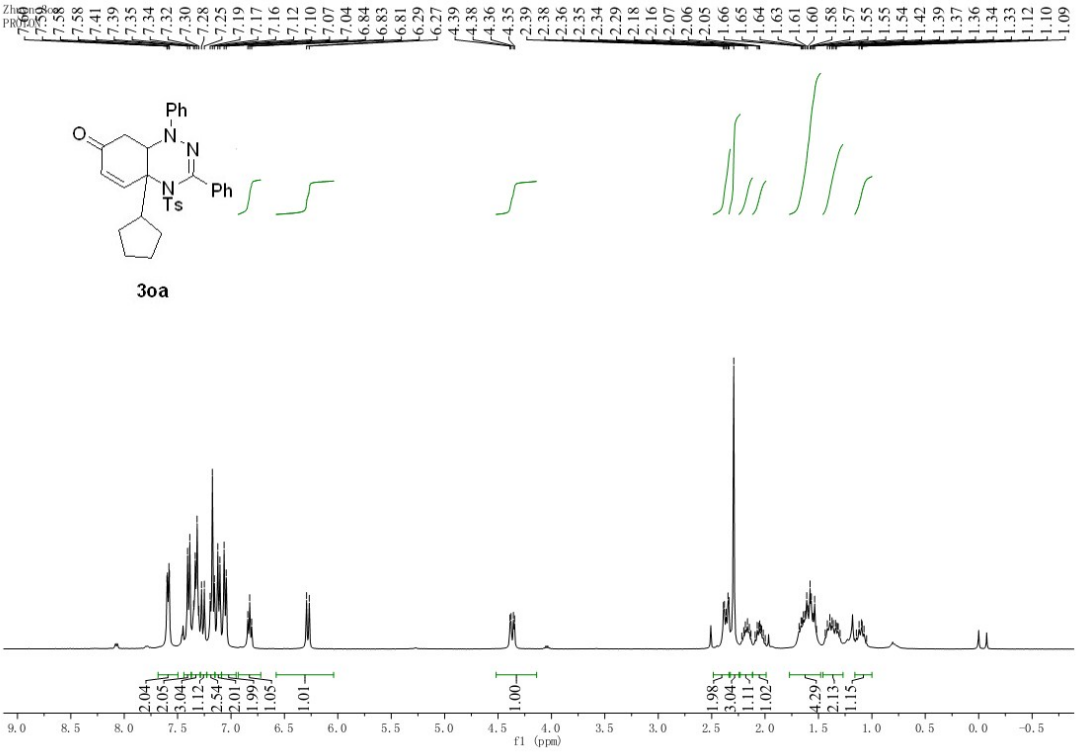

1.94
2.00
3.17
2.46
2.01
2.86
1.13
1.05
1.09
1.06
1.02
3.06
3.08
f1 (ppm)

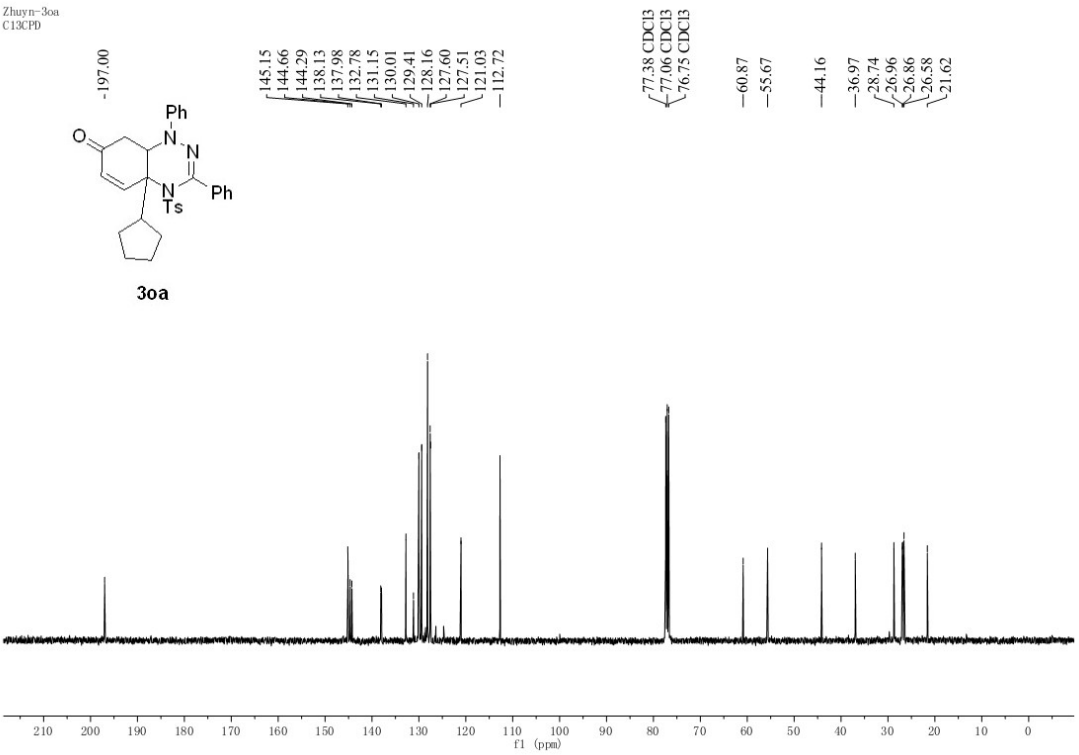

195.63
148.82
144.64
144.16
138.05
136.75
133.25
130.14
129.82
129.10
128.35
127.78
127.74
127.49
121.75
115.18
77.36 CDCl3
77.05 CDCl3
76.73 CDCl3
59.46
56.70
37.28
26.31
21.58
Ph
N
N
O
Ph
N
Ts
f1 (ppm)

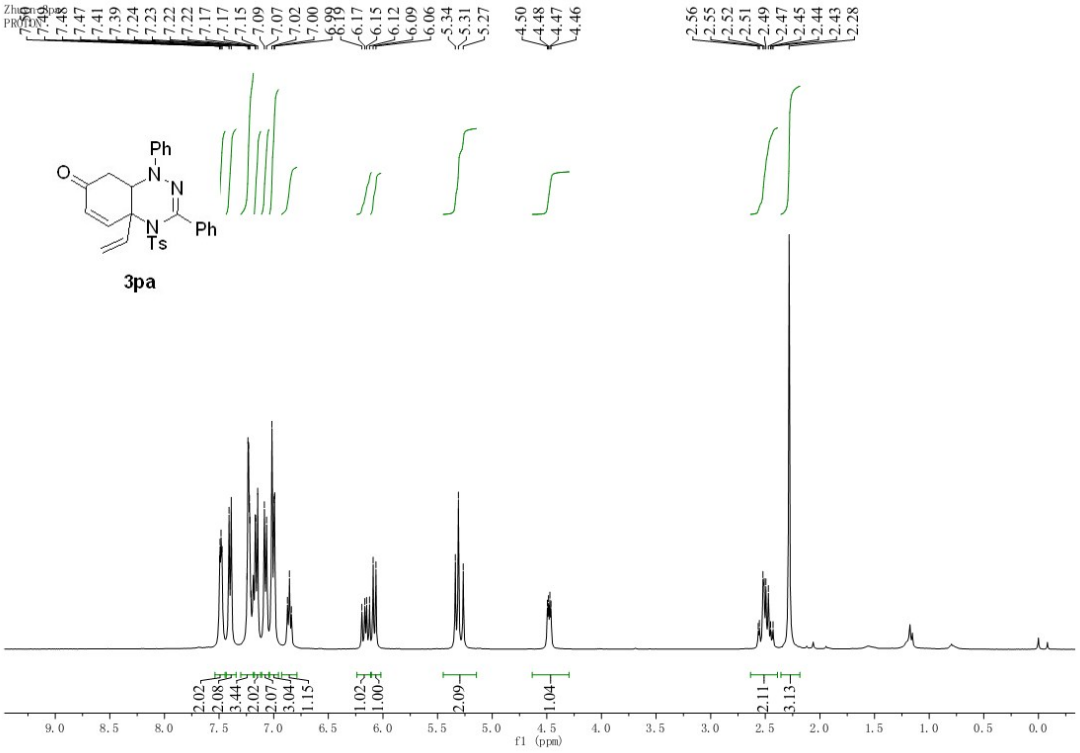
3ma

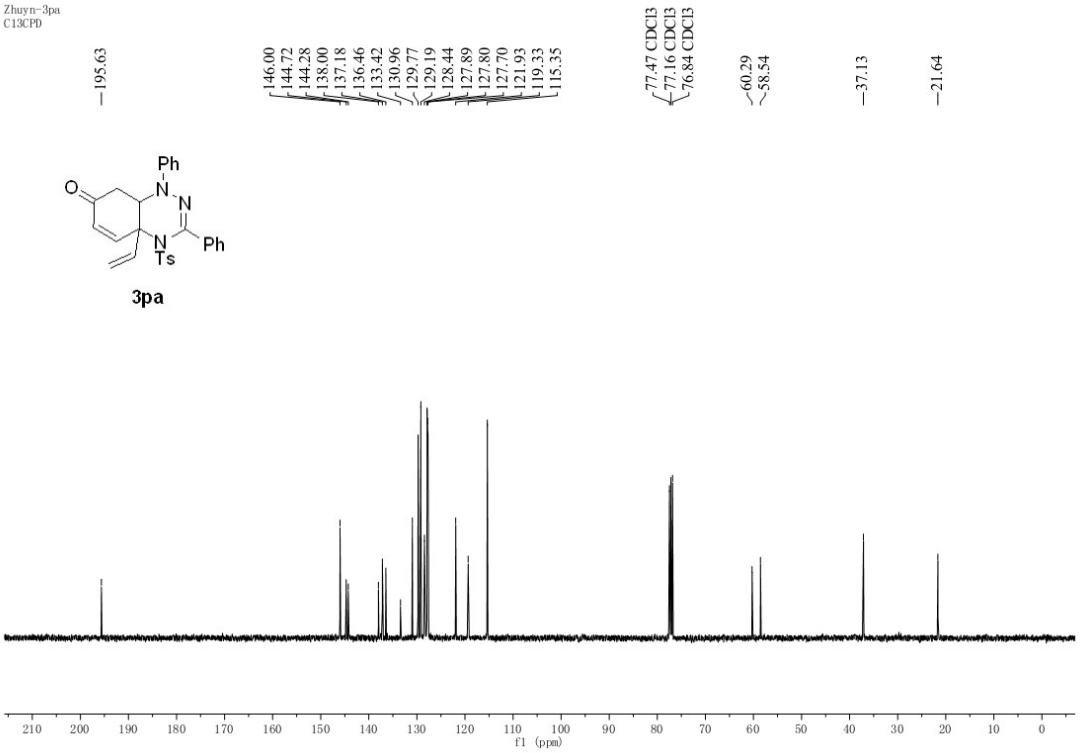

Ph
N
N
O
Ph
N
Ts
3na
2.18
2.19
3.10
3.34
2.09
2.05
1.13
1.00
1.00
1.01
3.09
2.07
1.04
1.29
3.49
3.15
f1 (ppm)

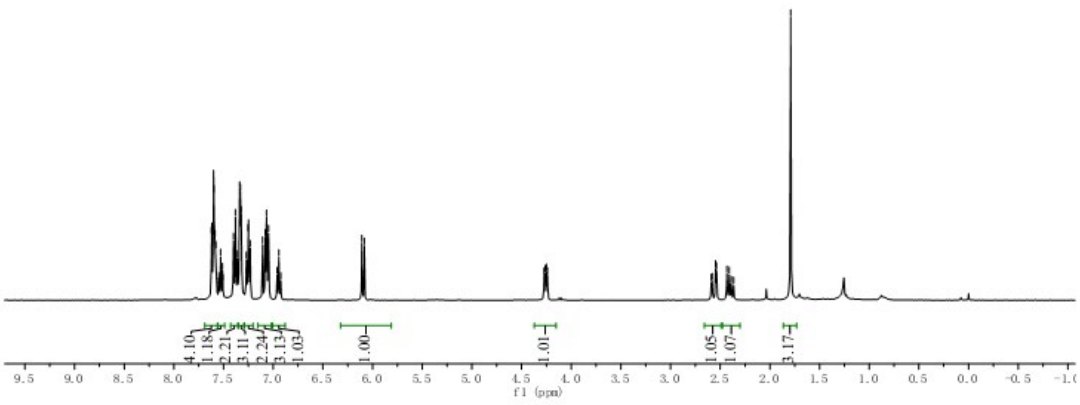

196.68
147.58
144.61
144.22
137.97
137.35
132.26
131.31
129.87
129.30
128.26
128.07
127.62
121.23
113.52
77.41 CDCl3
77.09 CDCl3
76.77 CDCl3
58.91
55.91
38.20
36.81
26.02
22.83
21.62
13.97
Ph
N
N
O
Ph
N
Ts
3na
f1 (ppm)

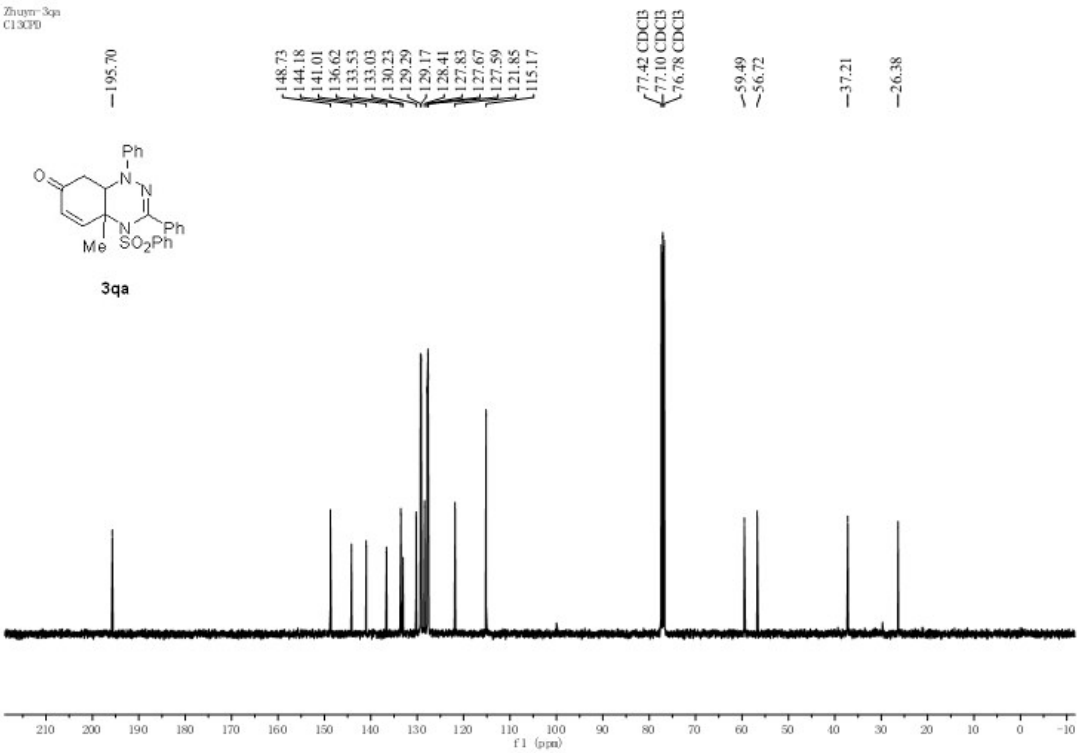

Ph
N
N
O
N
Ts
Ph
3oa
f1 (ppm)

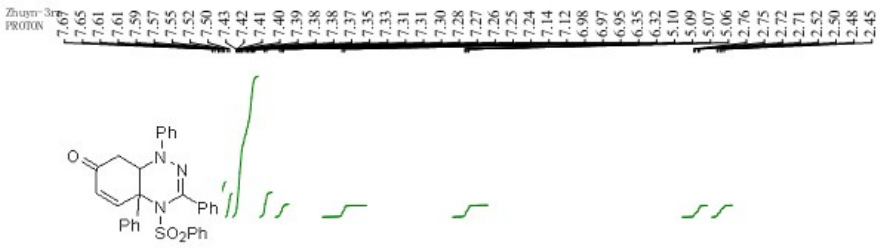

Zhuyn-3oa
C13CPD
197.00
145.15
144.66
144.29
138.13
137.98
132.78
131.15
130.01
129.41
128.16
127.60
127.51
121.03
112.72
77.38 CDCl3
77.06 CDCl3
76.75 CDCl3
60.87
55.67
44.16
36.97
28.74
26.96
26.86
26.58
21.62
Ph
N
N
O
N
Ts
Ph
3oa
f1 (ppm)


Ph
N
N
O
N
Ts
Ph
3pa
f1 (ppm)

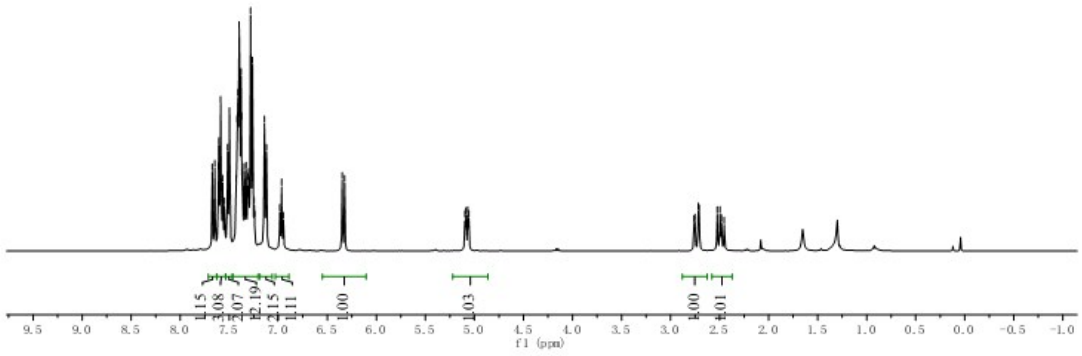

Ph
N
N
O
N
Ts
Ph
3pa
f1 (ppm)

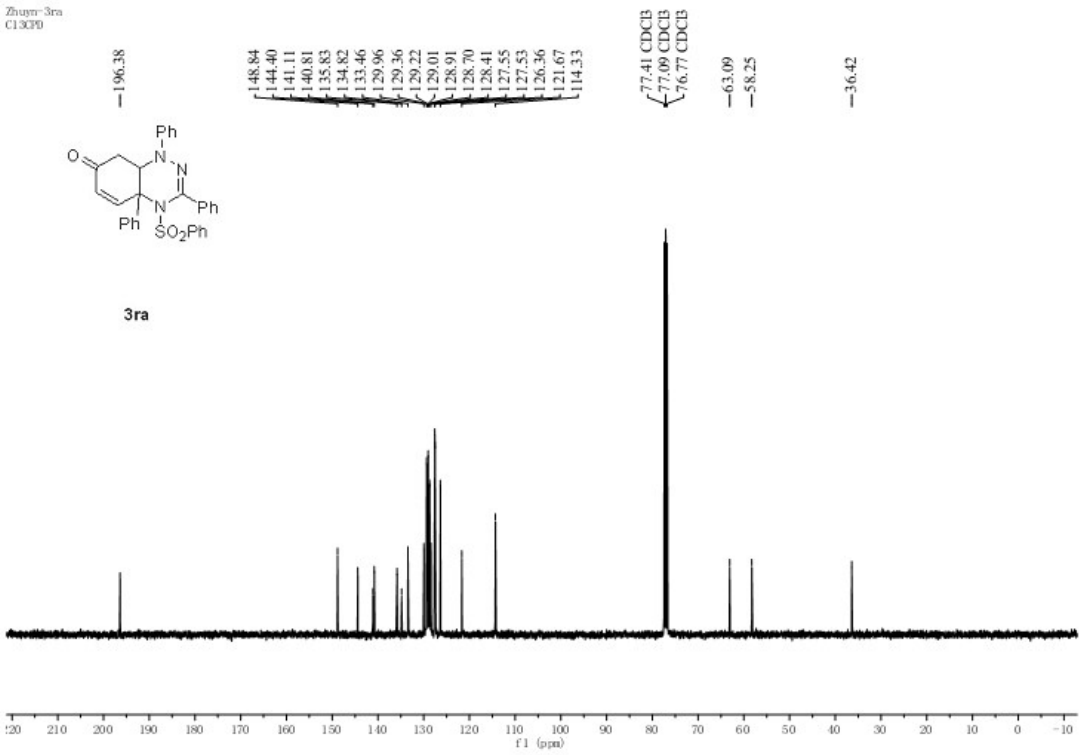




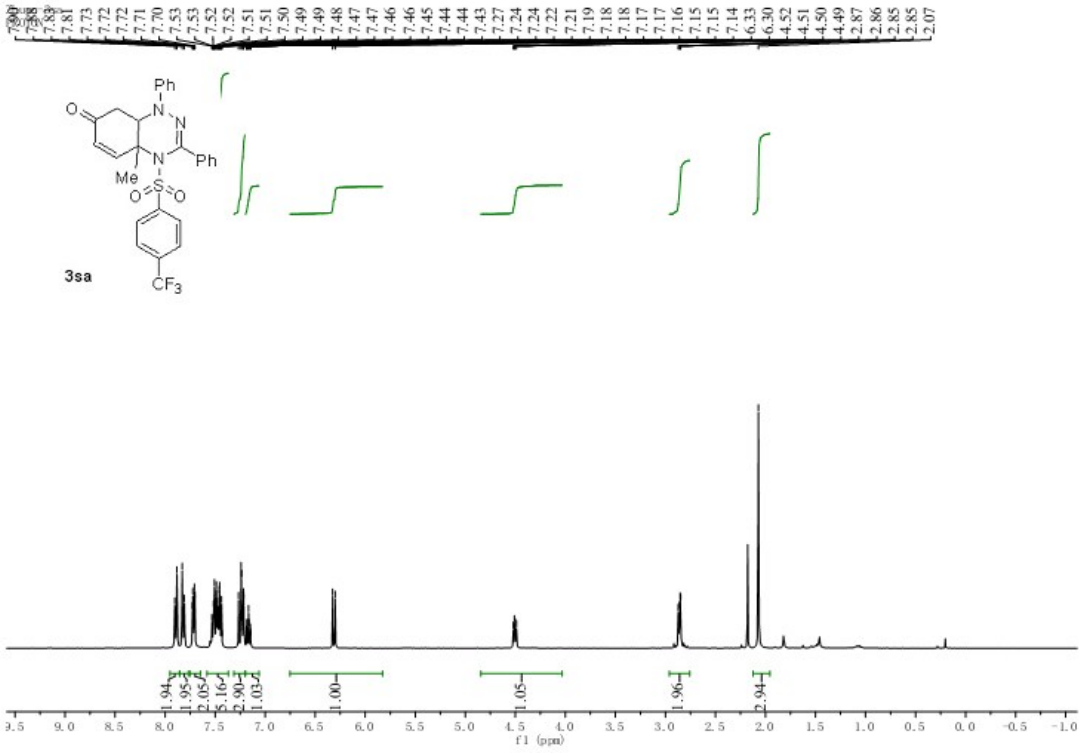

Zhuyn-3ra
PROTON
7.67
7.65
7.61
7.61
7.59
7.57
7.55
7.52
7.50
7.43
7.42
7.41
7.40
7.39
7.38
7.38
7.37
7.35
7.33
7.31
7.31
7.30
7.28
7.27
7.26
7.25
7.24
7.14
7.12
6.98
6.97
6.95
6.35
6.32
5.10
5.09
5.07
5.06
2.76
2.75
2.72
2.71
2.52
2.50
2.48
2.45
Ph
N
N
O
Ph
N
Ph
Ph
SO2Ph

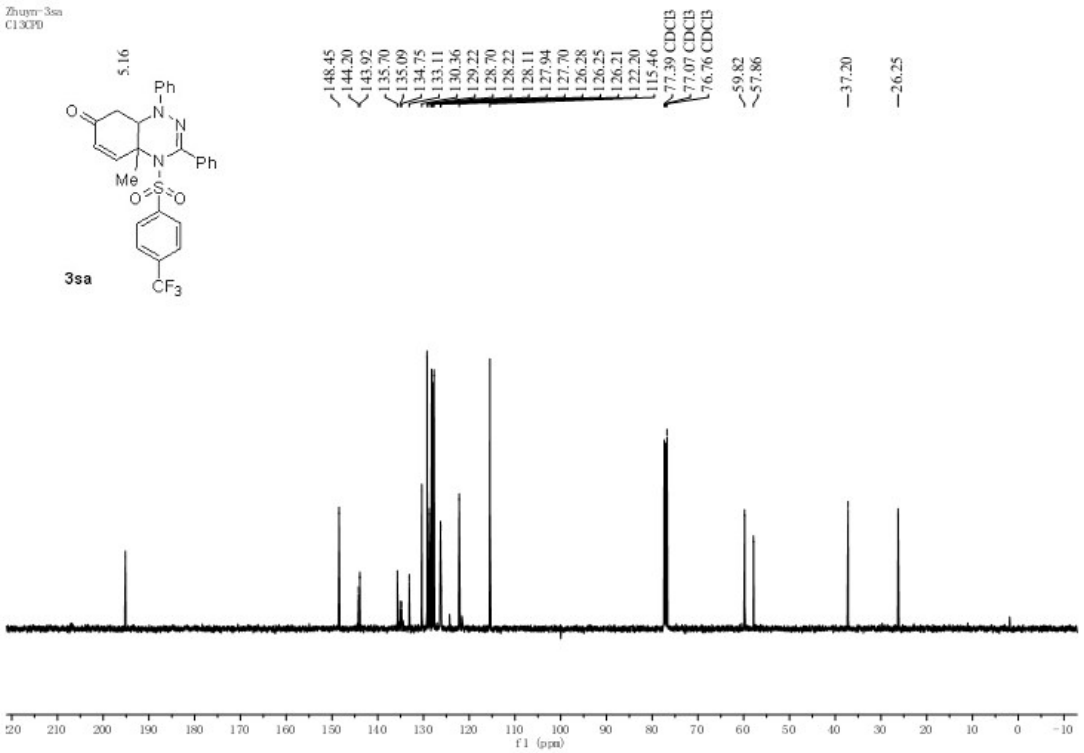
3ra

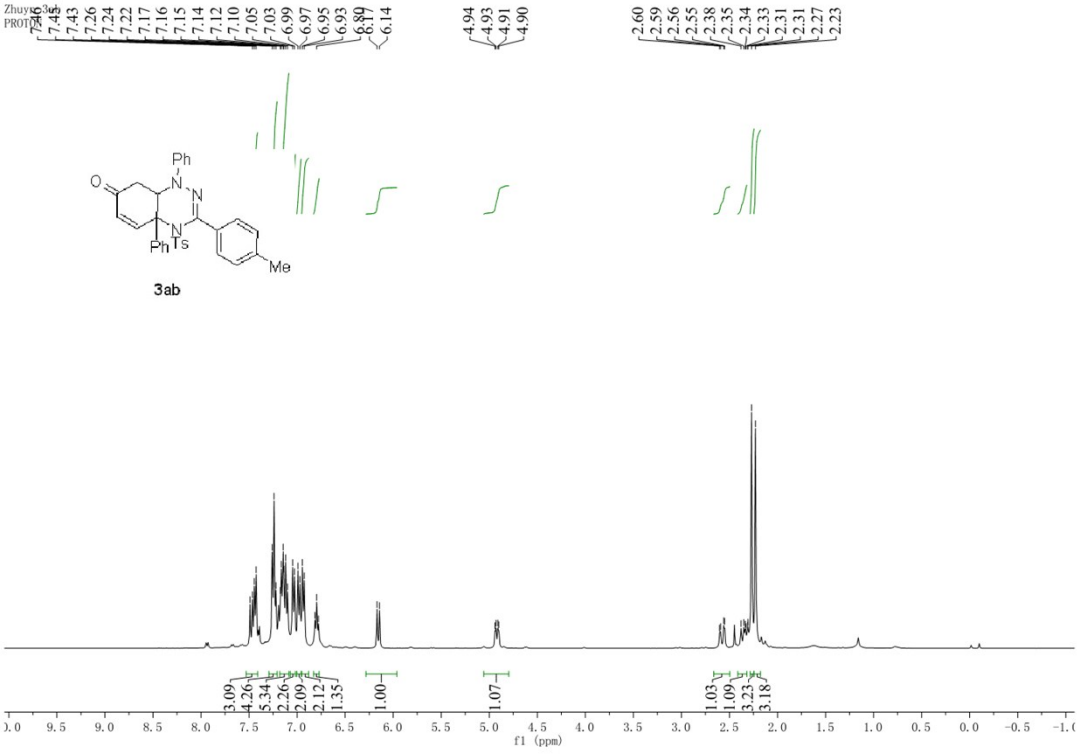

1.15
3.08
1.07
2.19
2.15
1.11
1.00
1.03
4.00
1.01
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
-1.0
f1 (ppm)

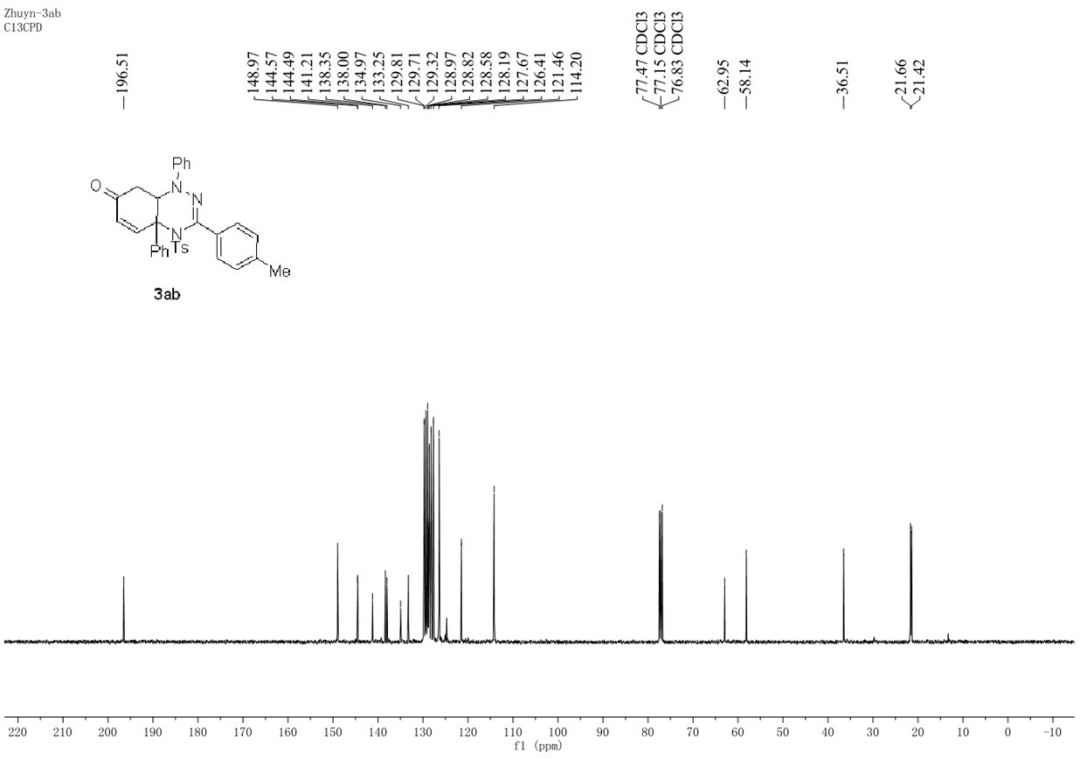

Zhuyn-3ra
C13CPD
196.38
148.84
144.40
141.11
140.81
135.83
134.82
133.46
129.96
129.36
129.22
129.01
128.91
128.70
128.41
127.55
127.53
126.36
121.67
114.33
77.41 CDCl3
77.09 CDCl3
76.77 CDCl3
63.09
58.25
36.42
Ph
N
N
O
Ph
N
Ph
Ph
SO2Ph
220
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
-10
f1 (ppm)

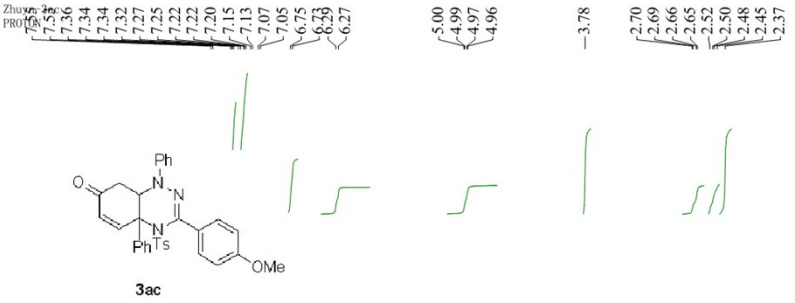
3ra


3sa
f1 (ppm)

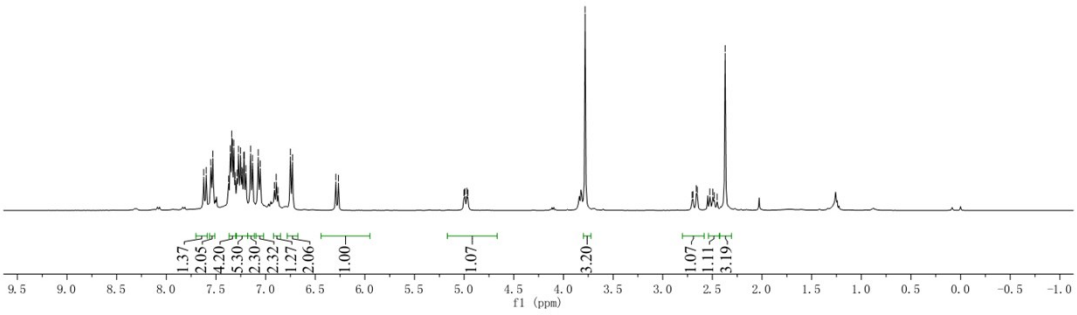

Zhuym-3sa
C13CPD
3sa
f1 (ppm)

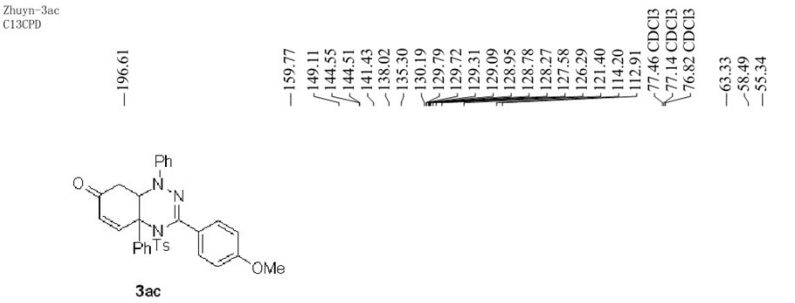

Zhuyn-3ab
PROTON
7.46
7.45
7.43
7.26
7.24
7.22
7.17
7.16
7.15
7.14
7.12
7.10
7.05
7.03
6.99
6.97
6.95
6.93
6.80
6.77
6.14
4.94
4.93
4.91
4.90
2.60
2.59
2.56
2.55
2.38
2.35
2.34
2.33
2.31
2.31
2.27
2.23
Ph
N
N
O
Ph
Ts
Me
3ab
3.09
4.26
5.34
2.26
2.09
2.12
1.35
1.00
1.07
1.03
1.09
3.23
3.18
f1 (ppm)


Zhuyn-3ab
C13CPD
196.51
148.97
144.57
144.49
141.21
138.35
138.00
134.97
133.25
129.81
129.71
129.32
128.97
128.82
128.58
128.19
127.67
126.41
121.46
114.20
77.47 CDCl3
77.15 CDCl3
76.83 CDCl3
62.95
58.14
36.51
21.66
21.42
Ph
N
N
O
Ph
Ts
Me
3ab
f1 (ppm)

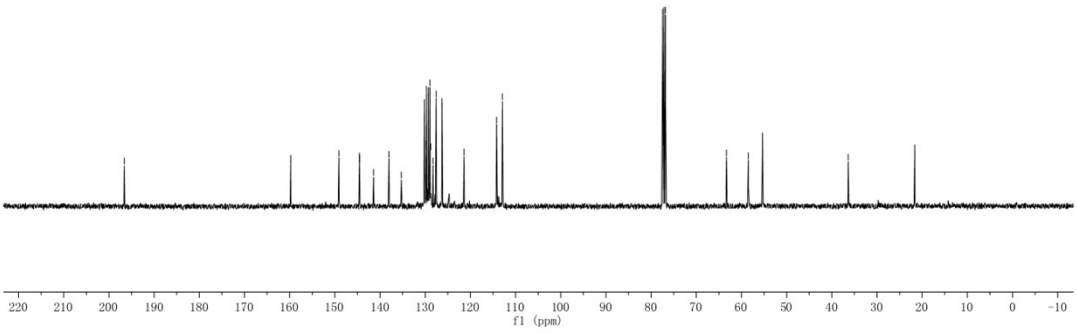

7.57
7.36
7.34
7.34
7.32
7.27
7.25
7.22
7.22
7.20
7.15
7.13
7.07
7.05
6.75
6.73
6.29
6.27
5.00
4.99
4.97
4.96
3.78
2.70
2.69
2.66
2.65
2.52
2.50
2.48
2.45
2.37
Ph
N
N
O
N
Ph
Ts
OMe

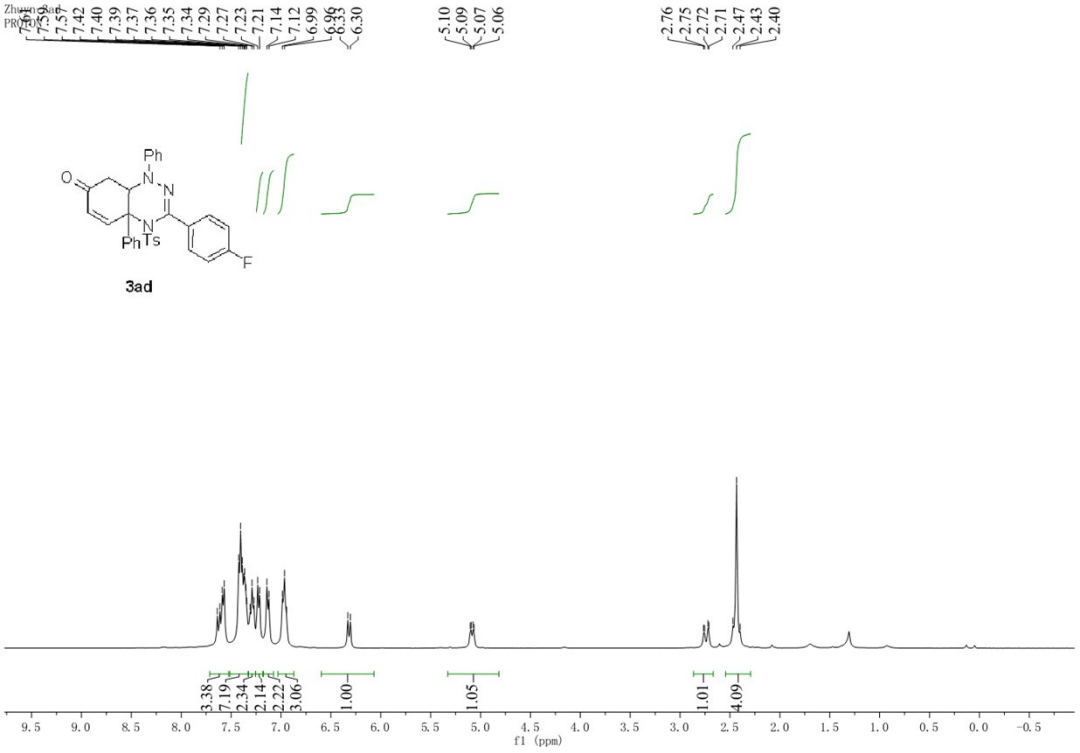
3ac

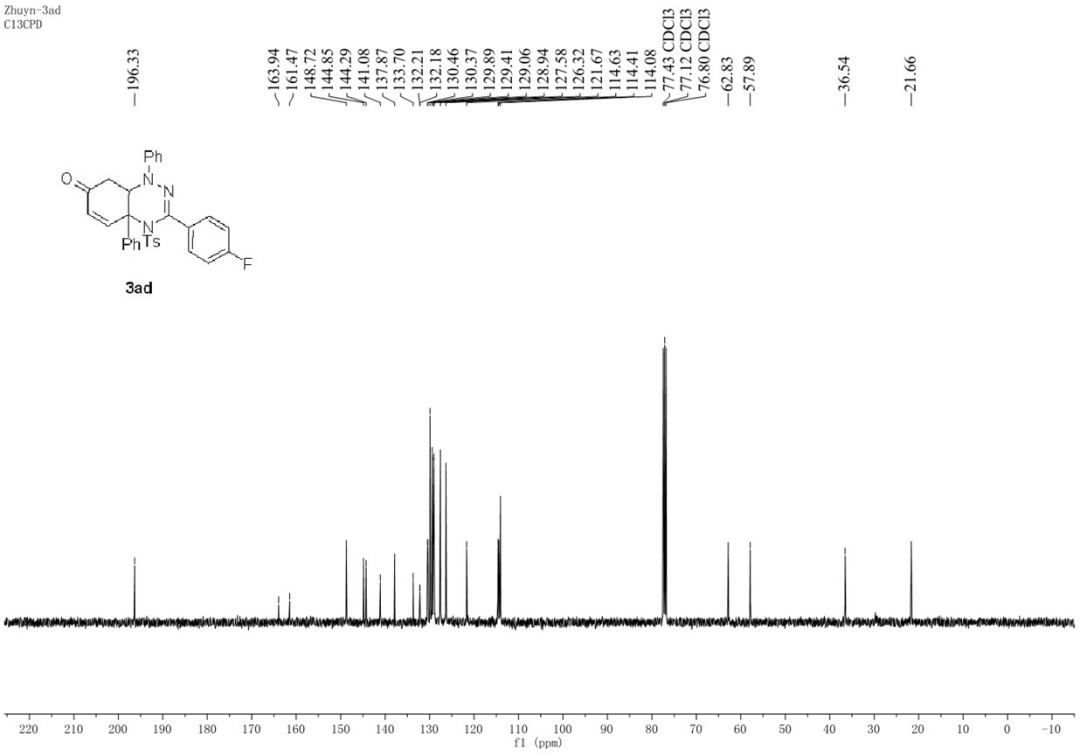

1.37
2.05
4.20
5.30
2.30
2.32
1.27
2.06
1.00
1.07
3.20
1.07
1.11
3.19
f1 (ppm)

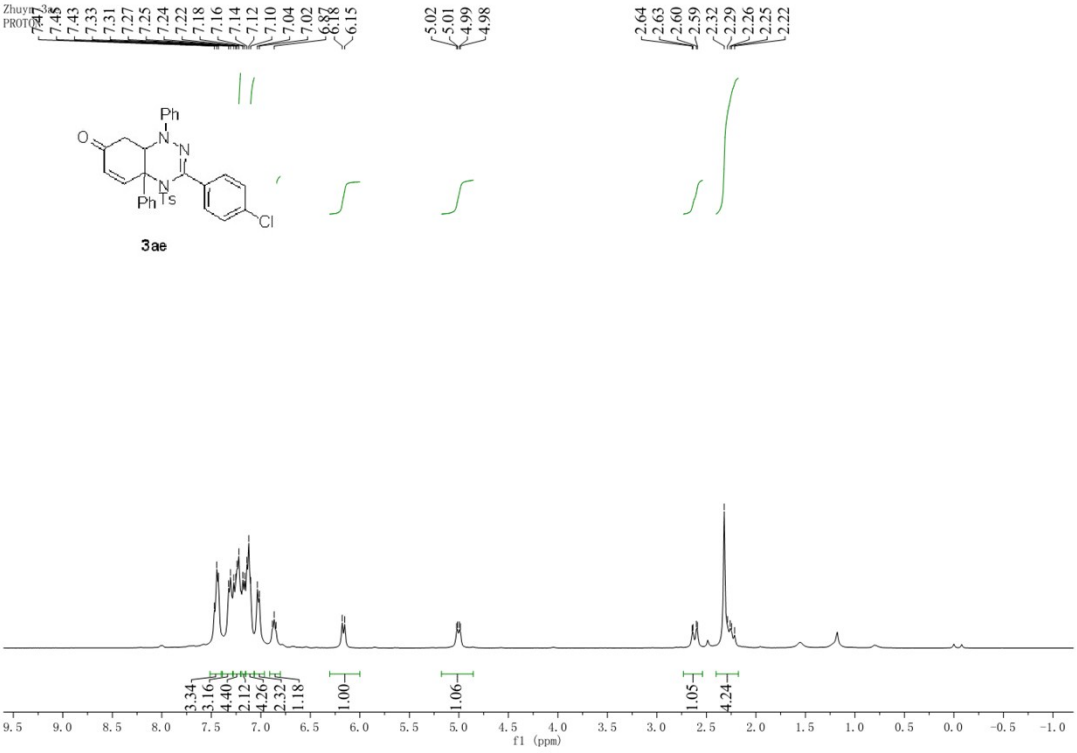

Zhuyn-3ac
C13CPD
196.61
159.77
149.11
144.55
144.51
141.43
138.02
135.30
130.19
129.79
129.72
129.31
129.09
128.95
128.78
128.27
127.58
126.29
121.40
114.20
112.91
77.46 CDCl3
77.14 CDCl3
76.82 CDCl3
63.33
58.49
55.34
36.37
21.64
Ph
N
N
O
N
Ph
Ts
OMe

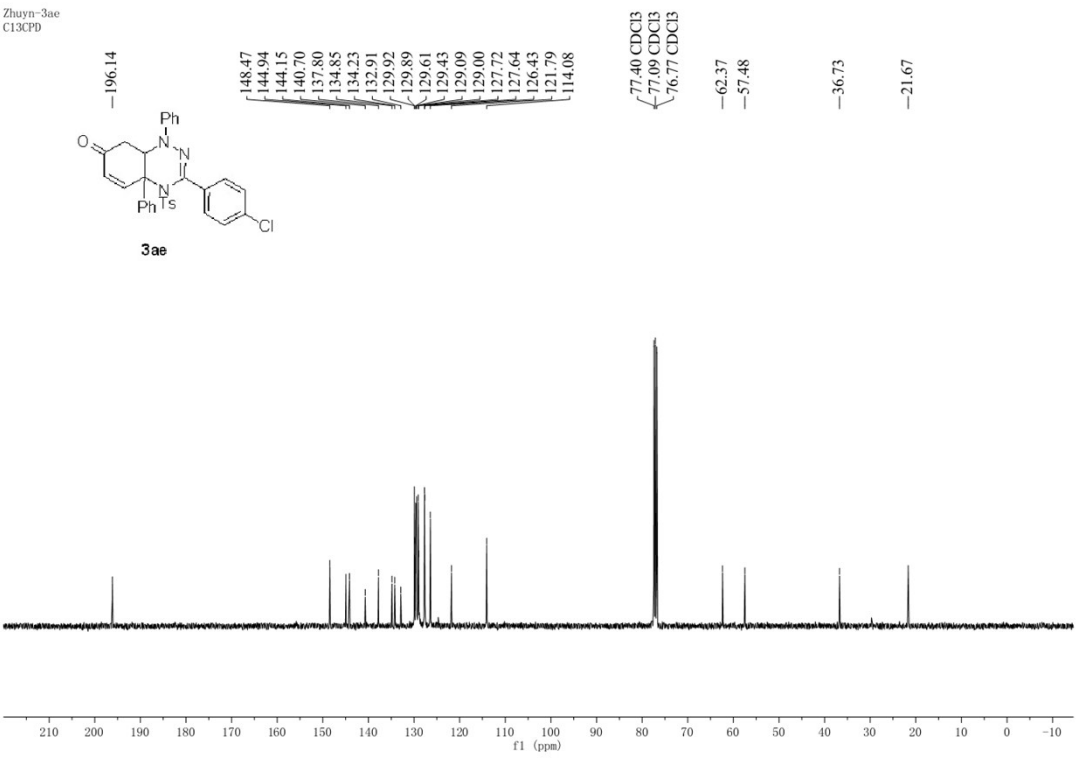
3ac

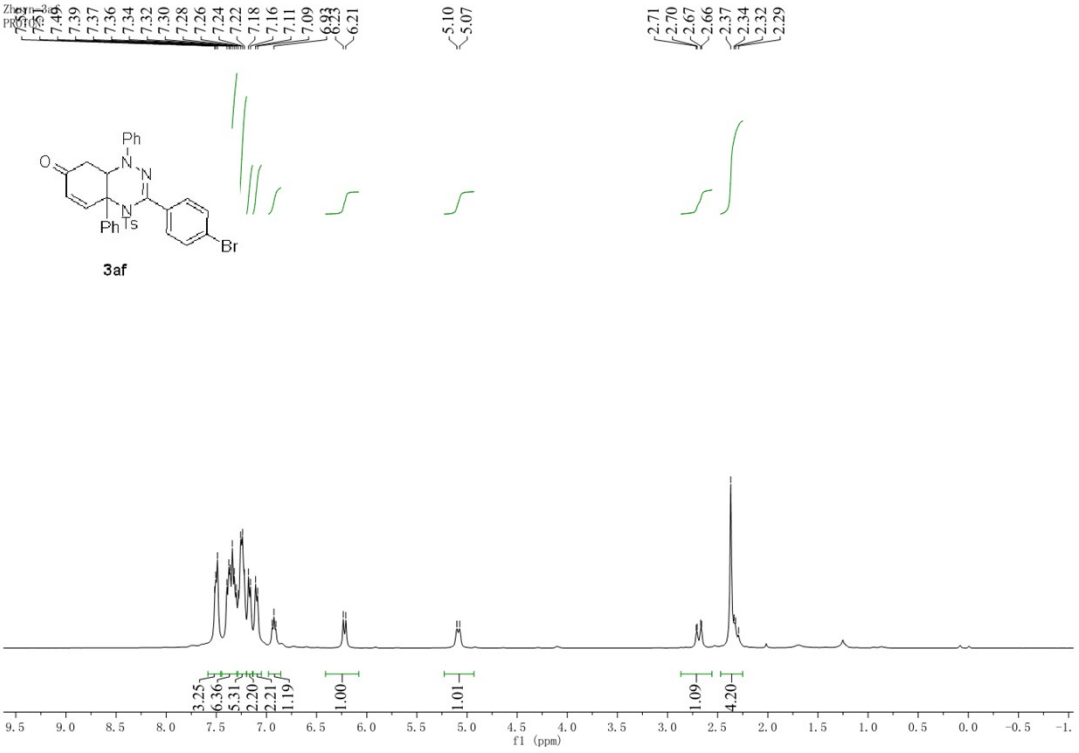

f1 (ppm)

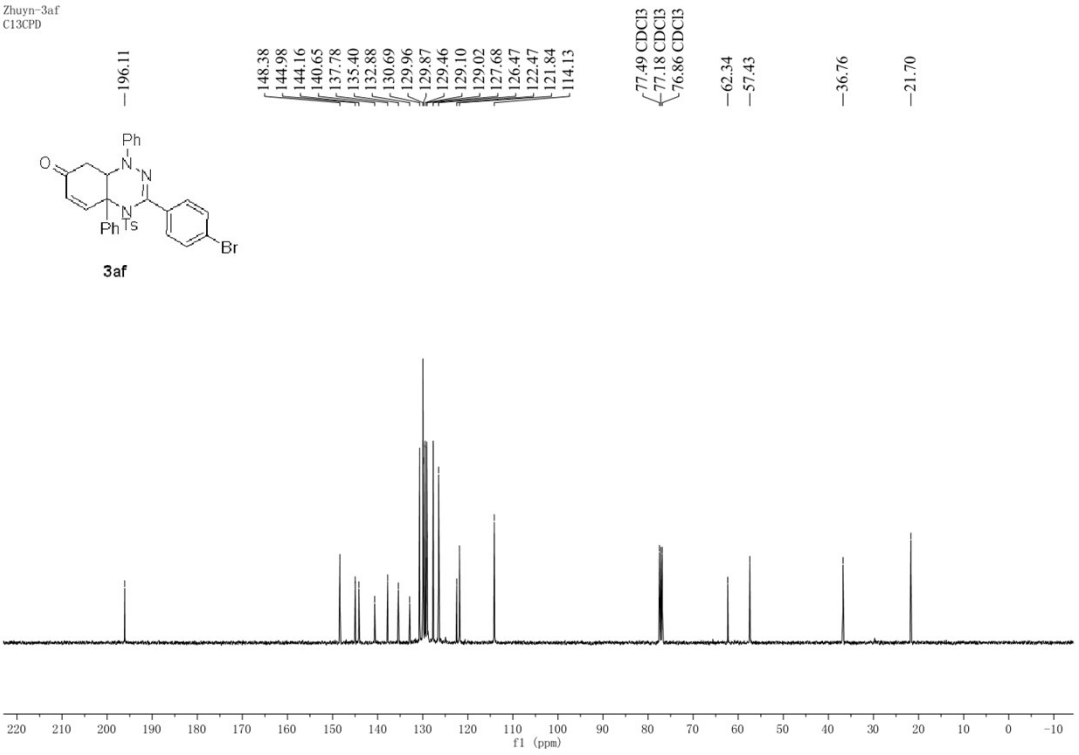

7.61
7.59
7.57
7.42
7.40
7.39
7.37
7.36
7.35
7.34
7.29
7.27
7.23
7.21
7.14
7.12
6.99
6.96
6.33
6.30
5.10
5.09
5.07
5.06
2.76
2.75
2.72
2.71
2.47
2.43
2.40
Ph
N
N
O
N
Ph
Ts
F
3ad
3.38
7.19
2.34
2.14
2.22
3.06
1.00
1.05
1.01
4.09
f1 (ppm)

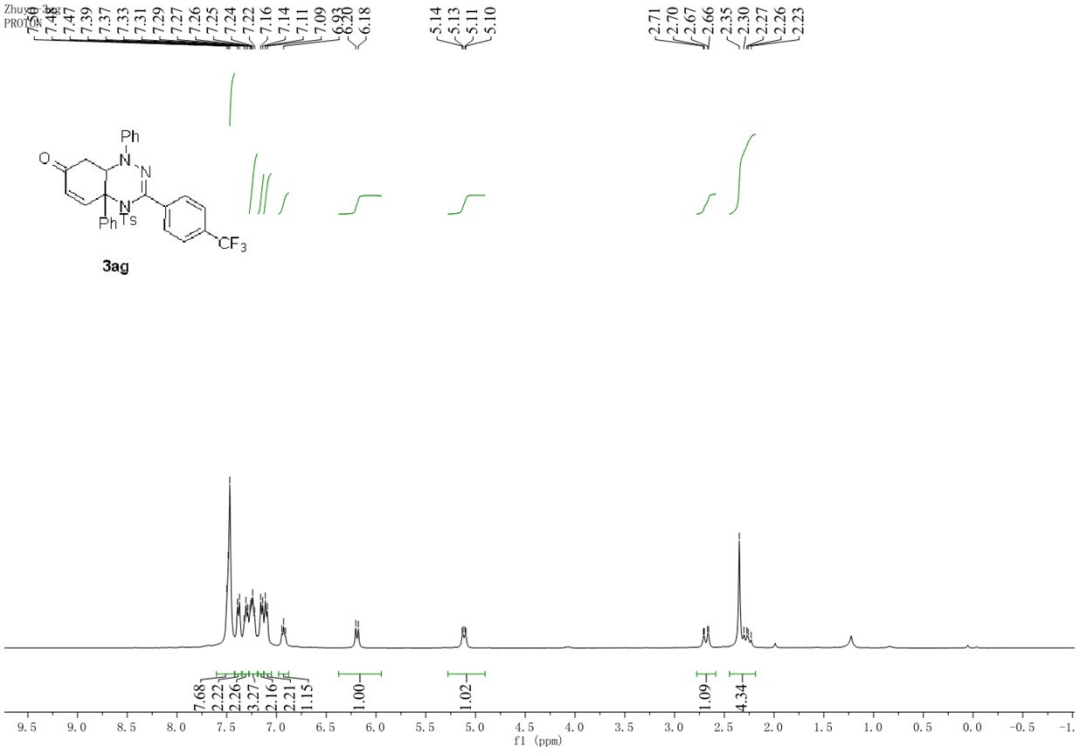

Zhuyn-3ad
C13CPD
196.33
163.94
161.47
148.72
144.85
144.29
141.08
137.87
133.70
132.21
132.18
130.46
130.37
129.89
129.41
129.06
128.94
127.58
126.32
121.67
114.63
114.41
114.08
77.43 CDCl3
77.12 CDCl3
76.80 CDCl3
62.83
57.89
36.54
21.66
Ph
N
N
O
N
Ph
Ts
F
3ad
f1 (ppm)

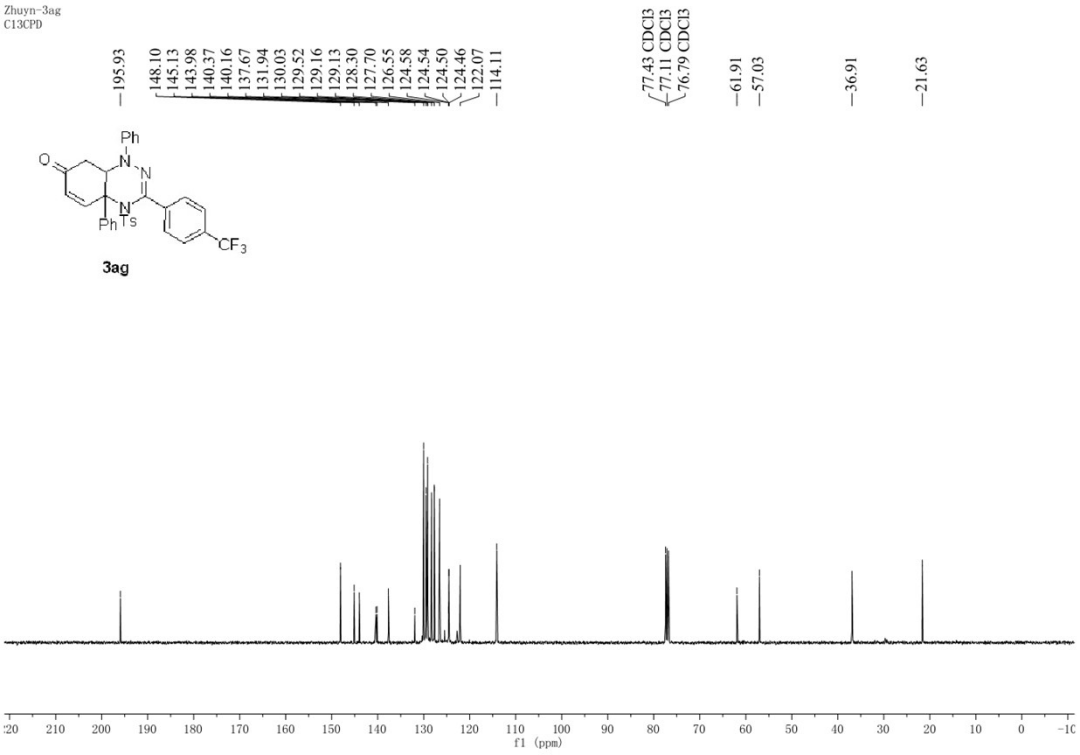

Zhuyn-3ae
PROTON
7.47
7.45
7.43
7.33
7.31
7.27
7.25
7.24
7.22
7.18
7.16
7.14
7.12
7.10
7.04
7.02
6.87
6.18
6.15
5.02
5.01
4.99
4.98
2.64
2.63
2.60
2.59
2.32
2.29
2.26
2.25
2.22
Ph
O
N
N
Ph
Ts
Cl
3ae
3.34
3.16
4.40
2.12
4.26
2.32
1.18
1.00
1.06
1.05
4.24
f1 (ppm)

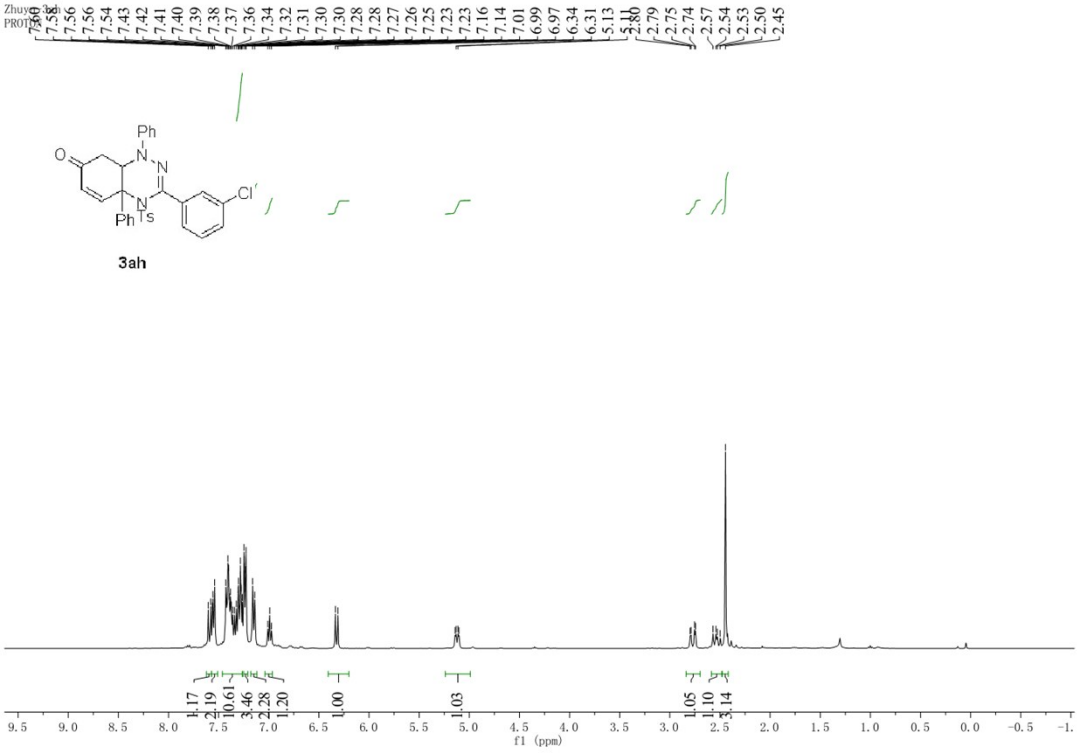

Zhuyn-3ae
C13CPD
196.14
148.47
144.94
144.15
140.70
137.80
134.85
134.23
132.91
129.92
129.89
129.61
129.43
129.09
129.00
127.72
127.64
126.43
121.79
114.08
77.40 CDCl3
77.09 CDCl3
76.77 CDCl3
62.37
57.48
36.73
21.67
Ph
O
N
N
Ph
Ts
Cl
3ae
f1 (ppm)

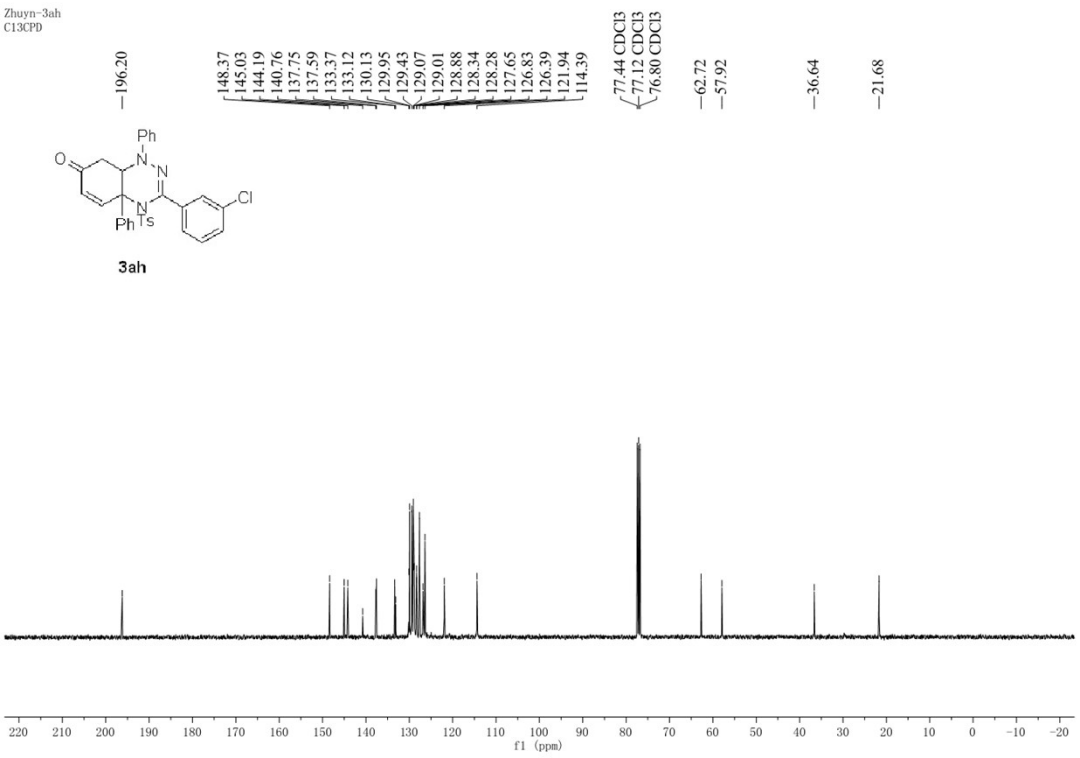

7.49
7.39
7.37
7.36
7.34
7.32
7.30
7.28
7.26
7.24
7.22
7.18
7.16
7.11
7.09
6.23
6.21
5.10
5.07
2.71
2.70
2.67
2.66
2.37
2.34
2.32
2.29
Ph
N
N
O
Ph
Ts
Br
3af
3.25
6.36
5.31
2.20
2.21
1.19
1.00
1.01
1.09
4.20
f1 (ppm)

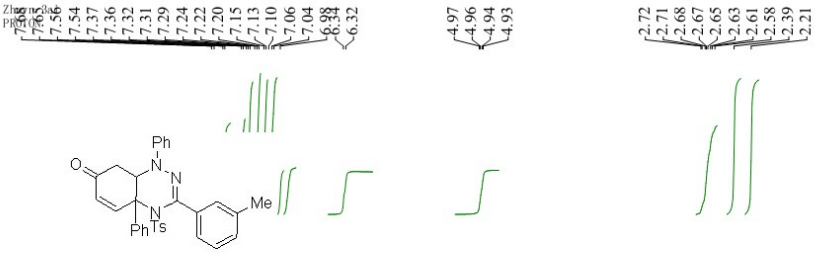

Zhuyn-3af
C13CPD
196.11
148.38
144.98
144.16
140.65
137.78
135.40
132.88
130.69
129.96
129.87
129.46
129.10
129.02
127.68
126.47
122.47
121.84
114.13
77.49 CDCl3
77.18 CDCl3
76.86 CDCl3
62.34
57.43
36.76
21.70
Ph
N
N
O
Ph
Ts
Br
3af
f1 (ppm)


7.48
7.47
7.39
7.37
7.33
7.31
7.29
7.27
7.26
7.25
7.24
7.22
7.16
7.14
7.11
7.09
6.93
6.20
6.18
5.14
5.13
5.11
5.10
2.71
2.70
2.67
2.66
2.35
2.30
2.27
2.26
2.23
Ph
N
N
O
Ph
Ts
CF3
3ag
7.68
2.22
2.26
3.27
2.16
2.21
1.15
1.00
1.02
1.09
4.34
f1 (ppm)

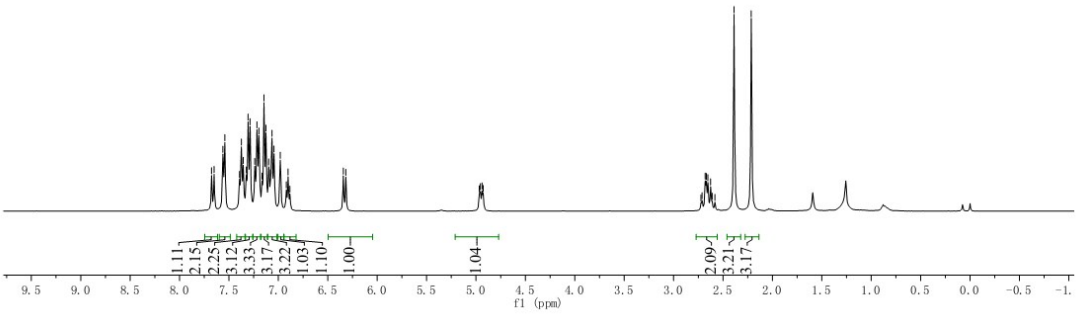

Zhuyn-3ag
C13CPD
195.93
148.10
145.13
143.98
140.37
140.16
137.67
131.94
130.03
129.52
129.16
129.13
128.30
127.70
126.55
124.58
124.54
124.50
124.46
122.07
114.11
77.43 CDCl3
77.11 CDCl3
76.79 CDCl3
61.91
57.03
36.91
21.63
Ph
N
N
O
Ph
Ts
CF3
3ag
f1 (ppm)

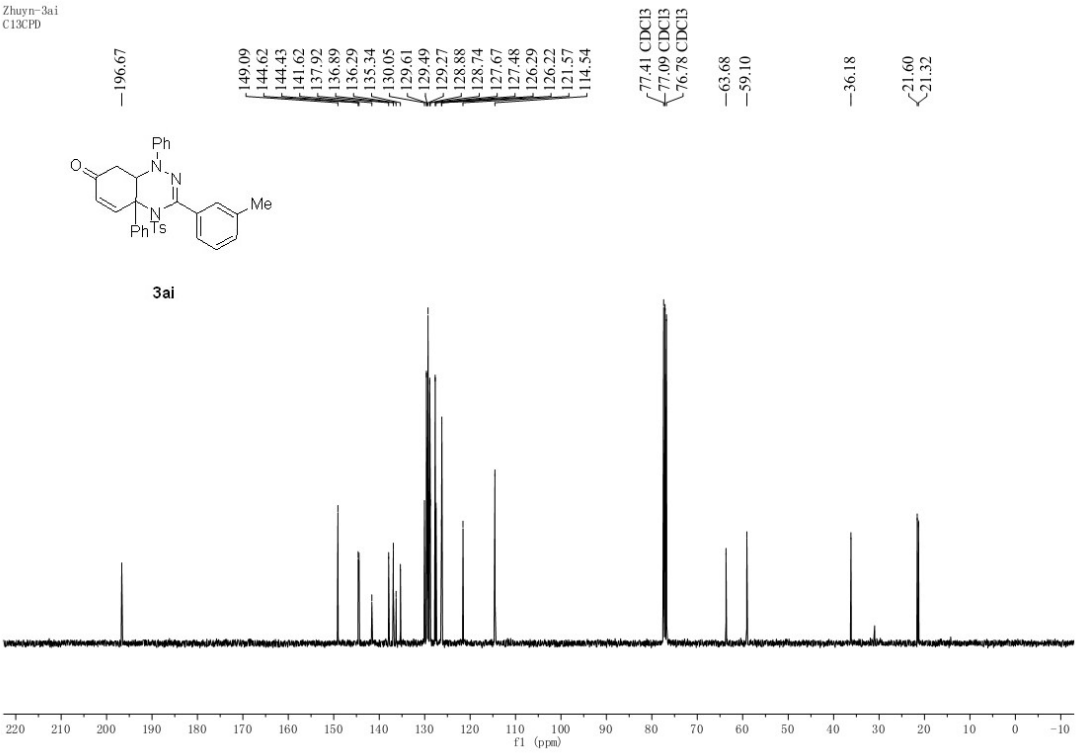

Ph
N
N
O
Cl
Ph
Ts
3ah
1.17
2.19
10.61
3.46
2.28
1.20
1.00
1.03
1.05
1.10
3.14
f1 (ppm)


Zhuyn-3ah
C13CPD
196.20
148.37
145.03
144.19
140.76
137.75
137.59
133.37
133.12
130.13
129.95
129.43
129.07
129.01
128.88
128.34
128.28
127.65
126.83
126.39
121.94
114.39
77.44 CDCl3
77.12 CDCl3
76.80 CDCl3
62.72
57.92
36.64
21.68
Ph
N
N
O
Cl
Ph
Ts
3ah
f1 (ppm)

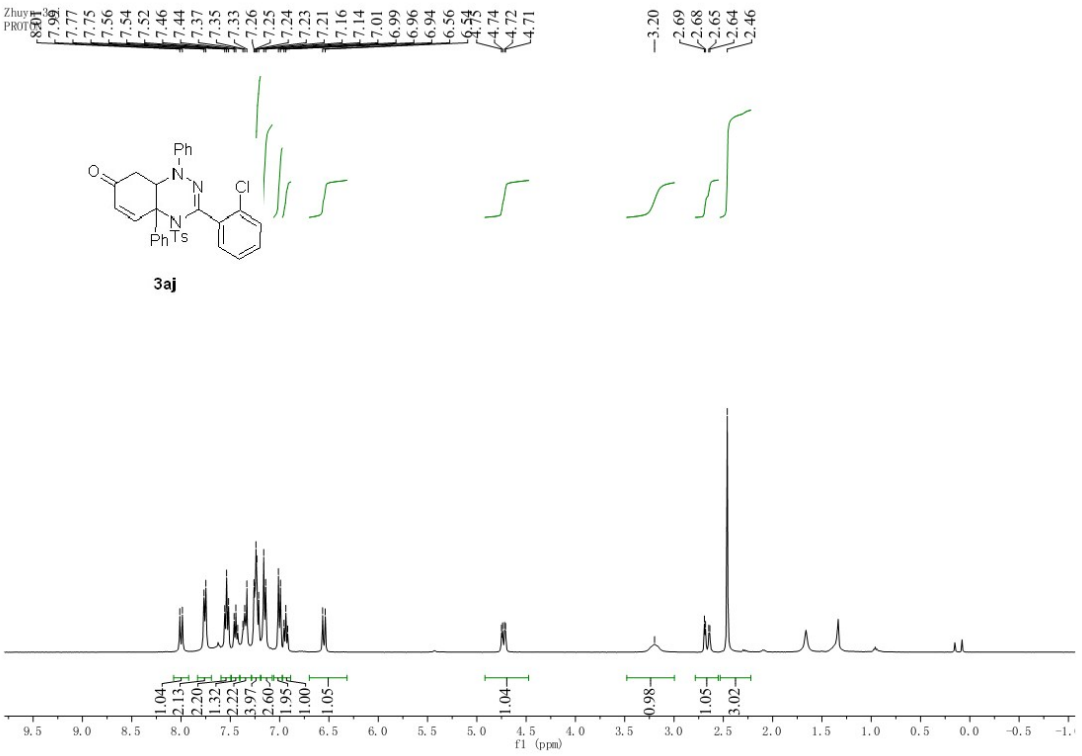

7.56
7.54
7.37
7.36
7.32
7.31
7.29
7.24
7.22
7.20
7.15
7.13
7.10
7.06
7.04
6.98
6.34
6.32
4.97
4.96
4.94
4.93
2.72
2.71
2.68
2.67
2.65
2.63
2.61
2.58
2.39
2.21
Ph
N
N
O
Me
Ph
Ts

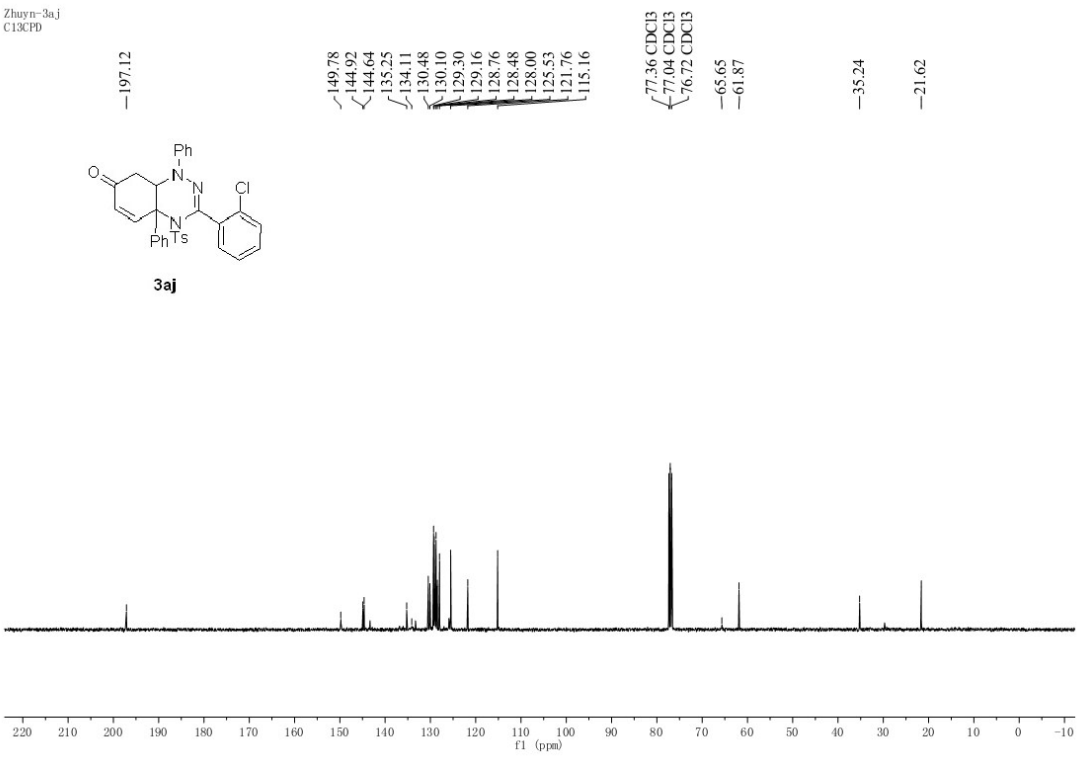
3ai

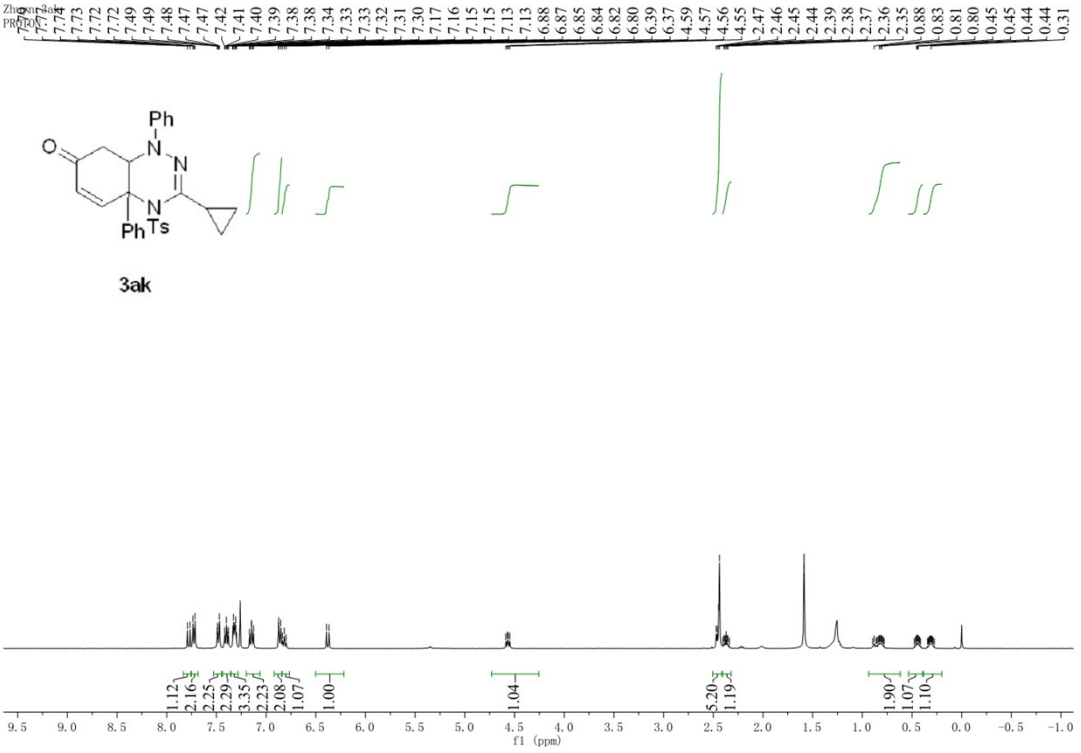

1.11
2.15
2.25
3.12
3.33
3.17
3.22
1.03
1.10
1.00
1.04
2.09
3.21
3.17
f1 (ppm)

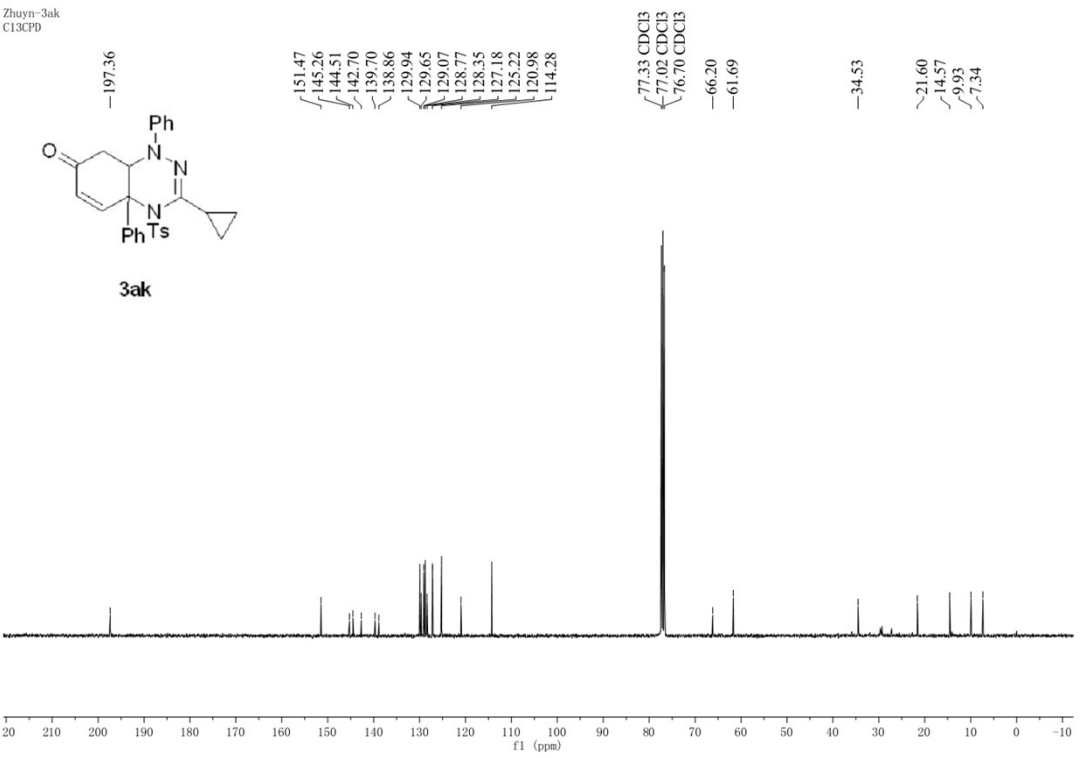

Zhuyn-3ai
C13CPD
196.67
149.09
144.62
144.43
141.62
137.92
136.89
136.29
135.34
130.05
129.61
129.49
129.27
128.88
128.74
127.67
127.48
126.29
126.22
121.57
114.54
77.41 CDCl3
77.09 CDCl3
76.78 CDCl3
63.68
59.10
36.18
21.60
21.32
Ph
N
N
O
Me
Ph
Ts
f1 (ppm)

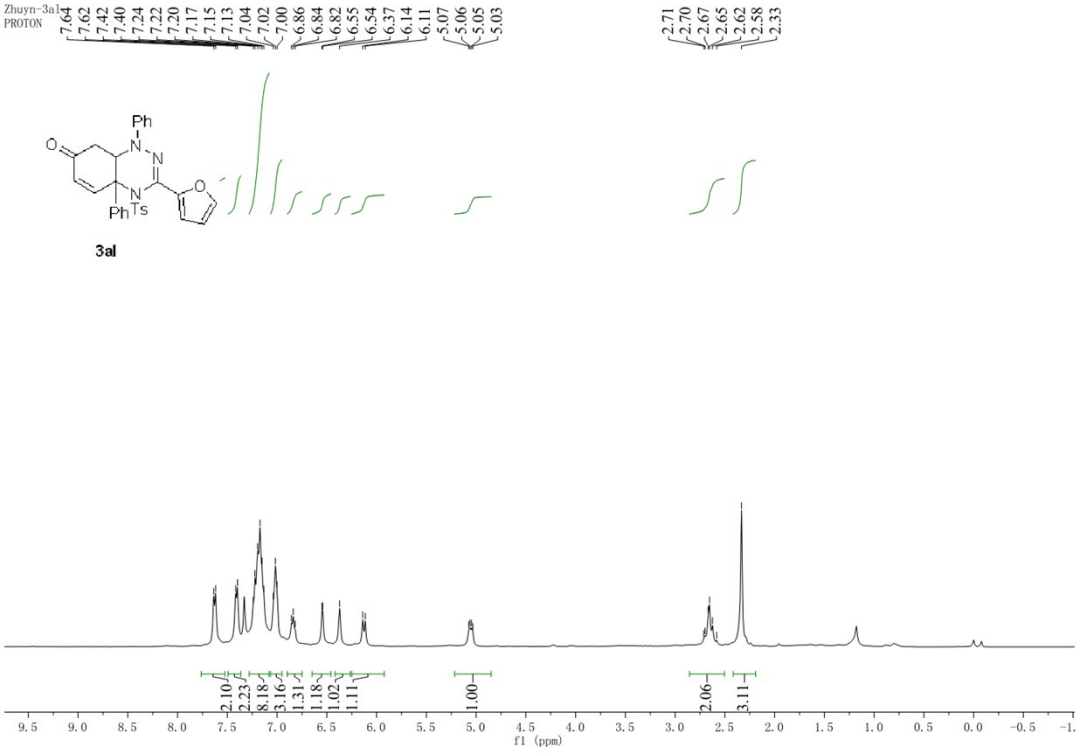
3ai

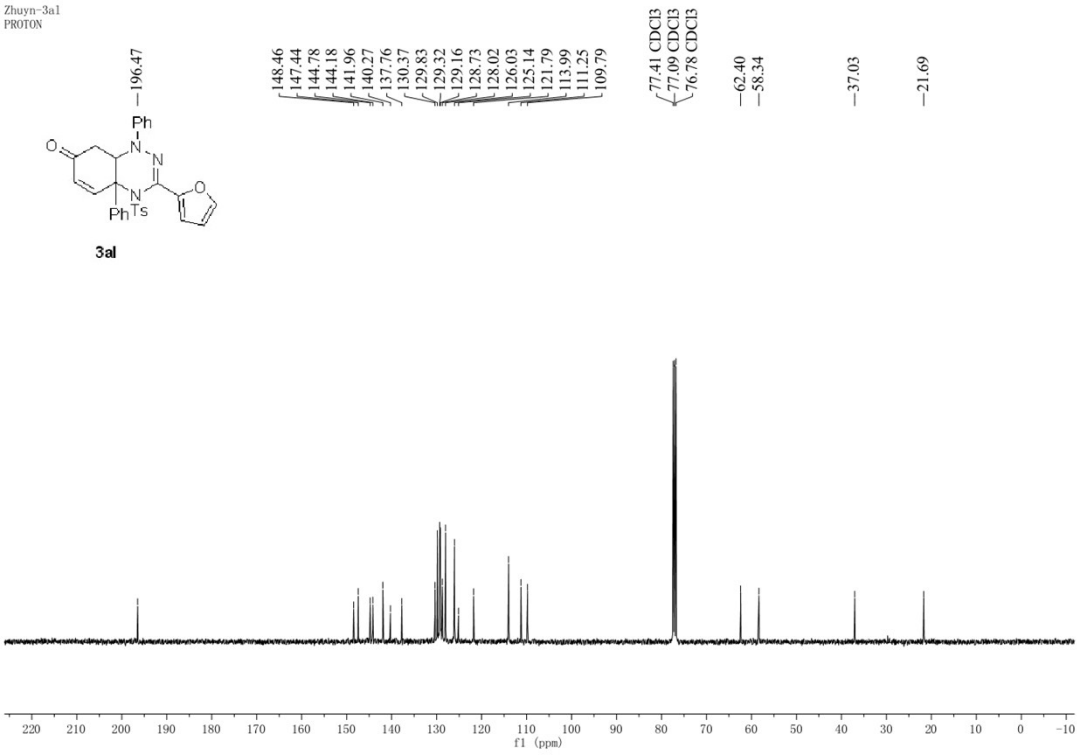

Zhuyn-3aj
PROTON
8.01
7.99
7.77
7.75
7.56
7.54
7.52
7.46
7.44
7.37
7.35
7.33
7.26
7.25
7.24
7.23
7.21
7.16
7.14
7.01
6.99
6.96
6.94
6.56
6.54
4.75
4.74
4.72
4.71
3.20
2.69
2.68
2.65
2.64
2.46
Ph
N
N
O
Cl
N
Ph
Ts
3aj
1.04
2.13
2.20
1.32
2.22
3.97
2.60
1.95
1.00
1.05
1.04
0.98
1.05
3.02
f1 (ppm)

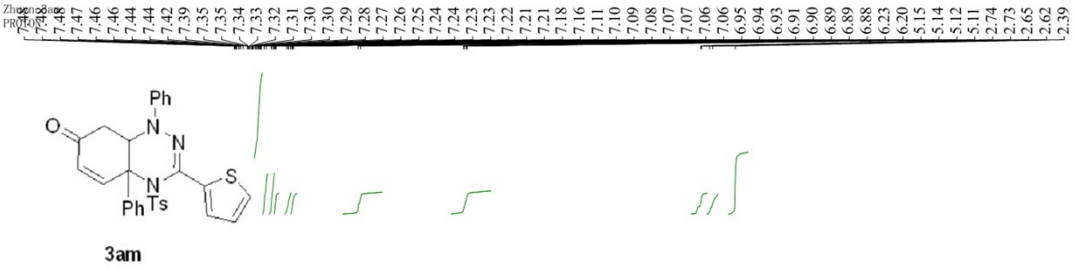

Zhuyn-3aj
C13CPD
197.12
149.78
144.92
144.64
135.25
134.11
130.48
130.10
129.30
129.16
128.76
128.48
128.00
125.53
121.76
115.16
77.36 CDCl3
77.04 CDCl3
76.72 CDCl3
65.65
61.87
35.24
21.62
Ph
N
N
O
Cl
N
Ph
Ts
3aj
f1 (ppm)


Ph
N
N
O
N
Ph
Ts
3ak
1.12
2.16
2.25
2.29
3.35
2.23
2.08
1.07
1.00
1.04
5.20
1.19
1.90
1.07
1.10
f1 (ppm)

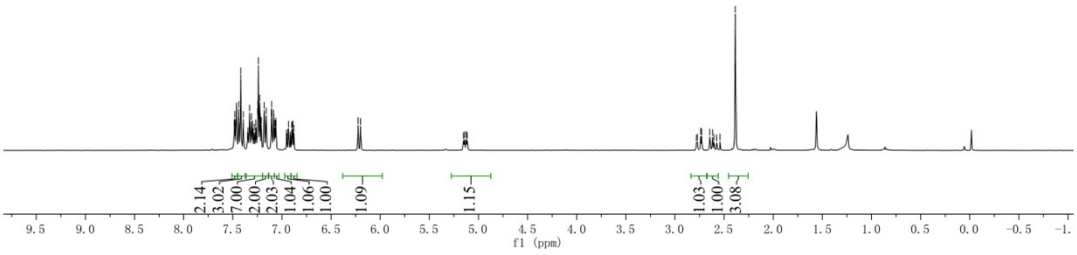

Zhuyn-3ak
C13CPD
197.36
151.47
145.26
144.51
142.70
139.70
138.86
129.94
129.65
129.07
128.77
128.35
127.18
125.22
120.98
114.28
77.33 CDCl3
77.02 CDCl3
76.70 CDCl3
66.20
61.69
34.53
21.60
14.57
9.93
7.34
Ph
N
N
O
N
Ph
Ts
3ak
f1 (ppm)

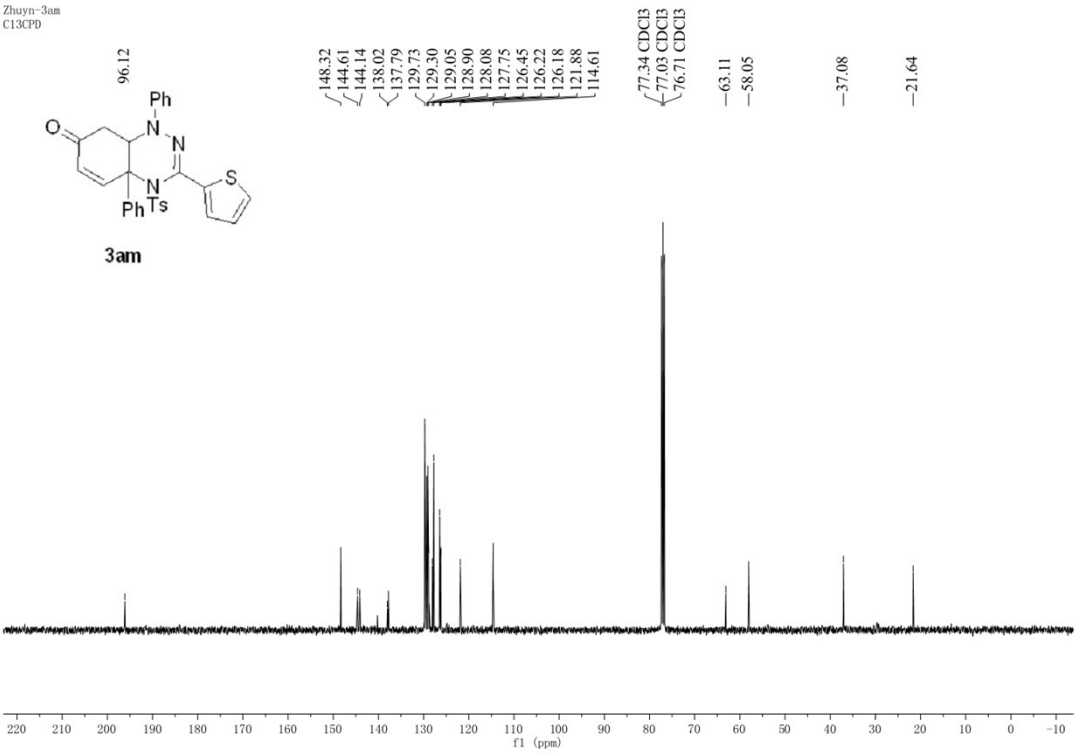

Zhuyn-3a1
PROTON
7.64
7.62
7.42
7.40
7.24
7.22
7.20
7.17
7.15
7.13
7.04
7.02
7.00
6.86
6.84
6.82
6.55
6.54
6.37
6.14
6.11
5.07
5.06
5.05
5.03
2.71
2.70
2.67
2.65
2.62
2.58
2.33
Ph
N
N
O
O
N
Ph
Ts
3al
2.10
2.23
8.18
3.16
1.31
1.18
1.02
1.11
1.00
2.06
3.11
f1 (ppm)


Zhuyn-3a1
PROTON
196.47
148.46
147.44
144.78
144.18
141.96
140.27
137.76
130.37
129.83
129.32
129.16
128.73
128.02
126.03
125.14
121.79
113.99
111.25
109.79
77.41 CDCl3
77.09 CDCl3
76.78 CDCl3
62.40
58.34
37.03
21.69
Ph
N
N
O
O
N
Ph
Ts
3al
f1 (ppm)

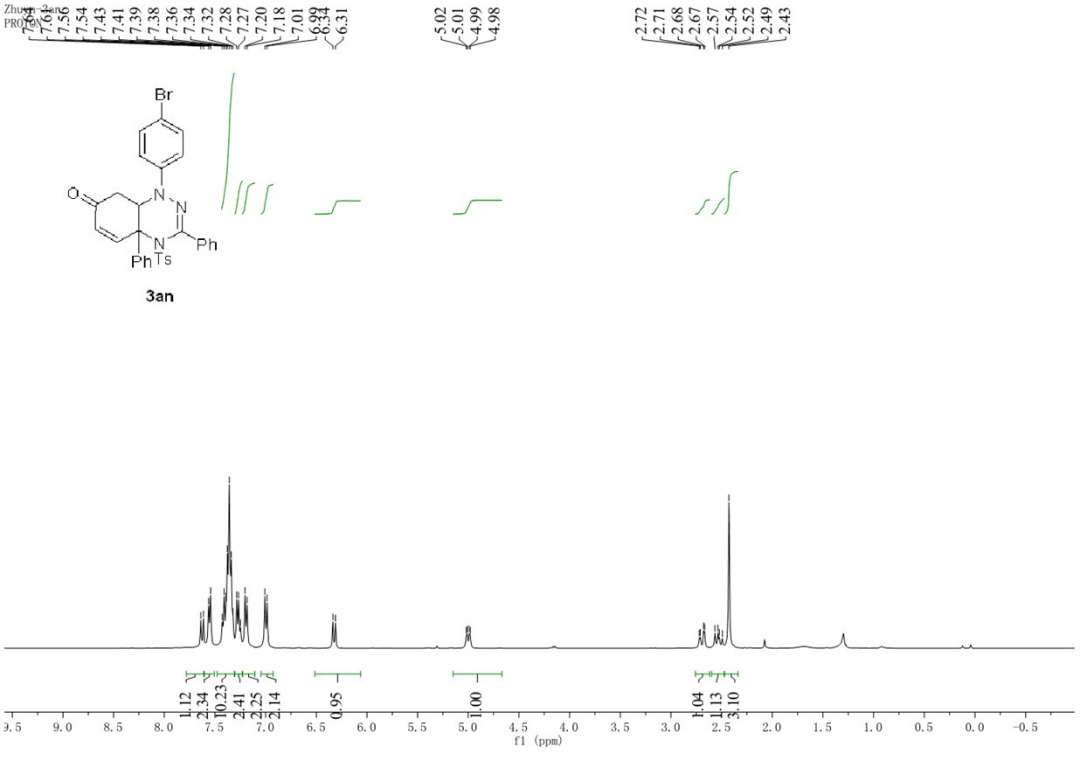


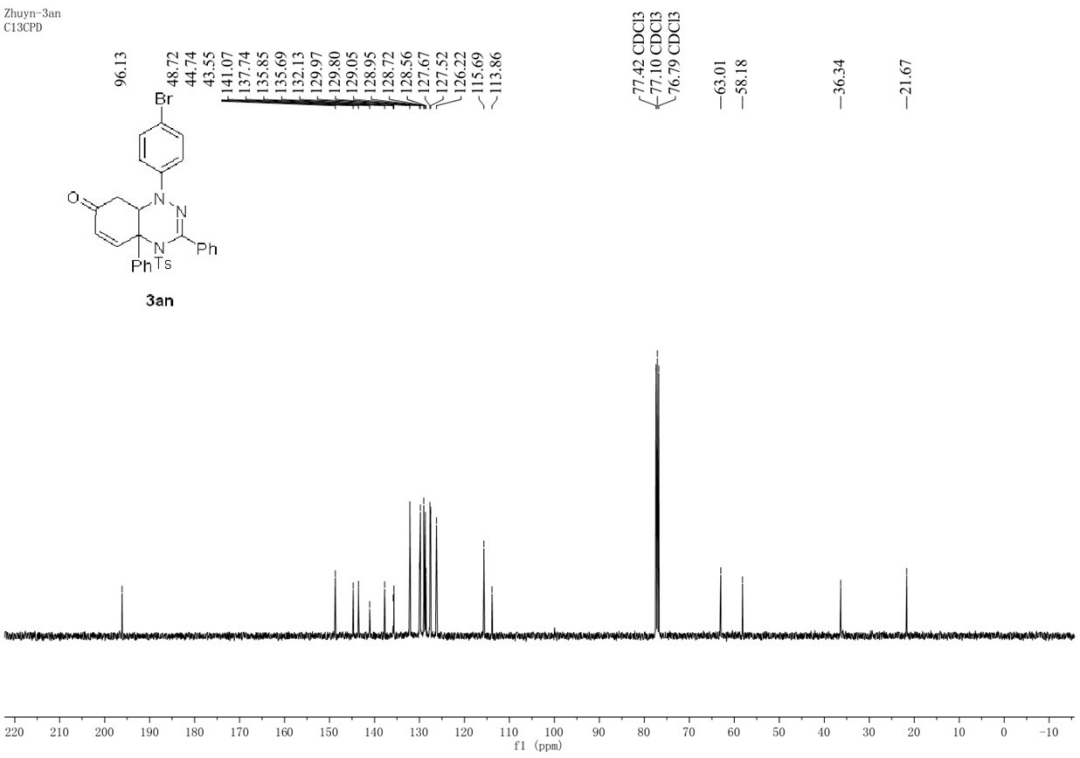
3am

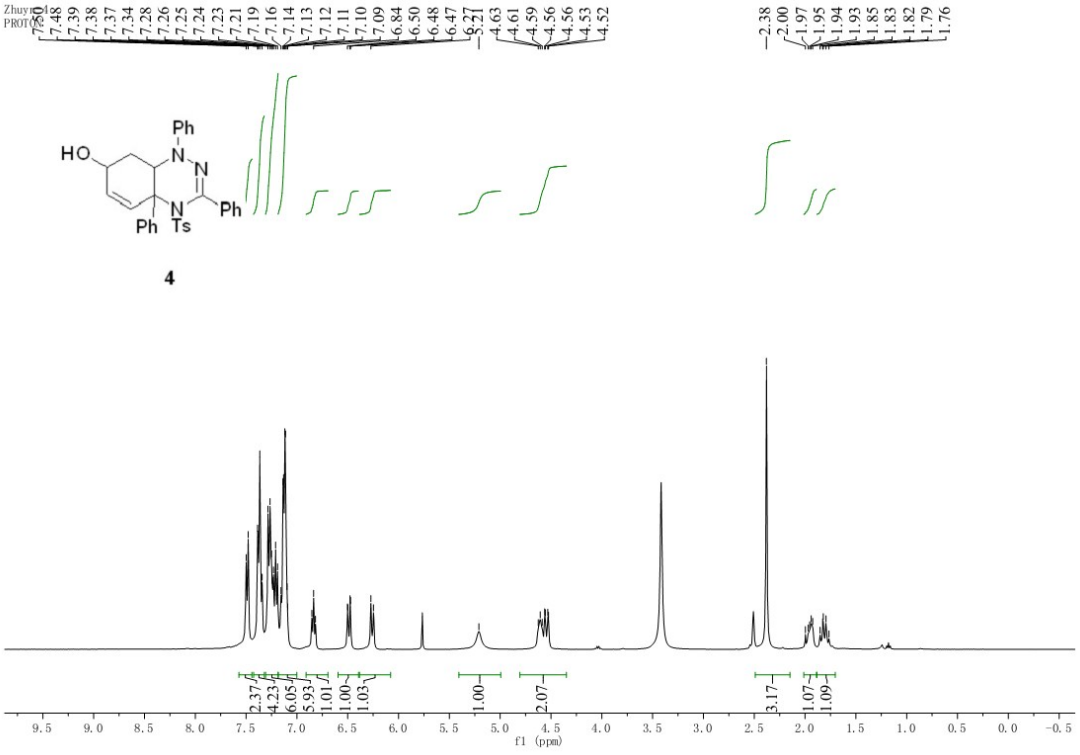


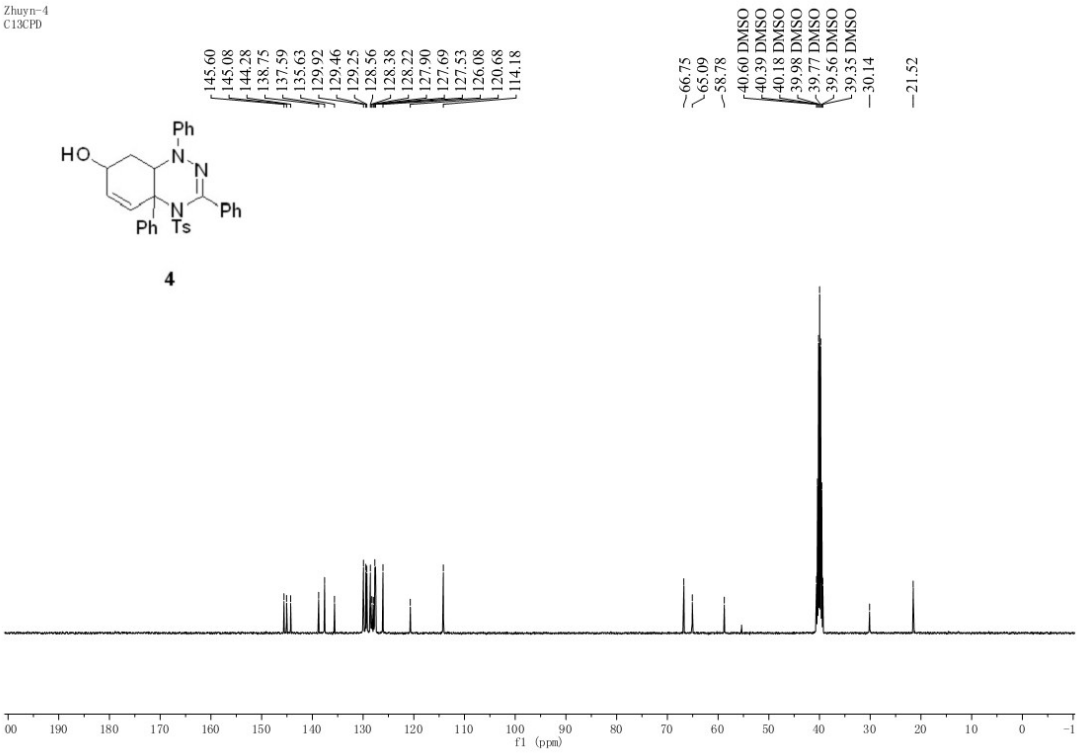


3am


7.64
7.56
7.54
7.43
7.41
7.39
7.38
7.36
7.34
7.32
7.28
7.27
7.20
7.18
7.01
6.99
6.34
6.31
5.02
5.01
4.99
4.98
2.72
2.71
2.68
2.67
2.57
2.54
2.52
2.49
2.43
Br
O
N
N
Ph
N
Ph
Ts
3an
1.12
2.34
10.23
2.41
2.25
2.14
0.95
1.00
1.04
1.13
3.10
f1 (ppm)

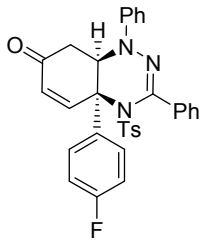

Zhuyn-3an
C13CPD
96.13
48.72
44.74
43.55
141.07
137.74
135.85
135.69
132.13
129.97
129.80
129.05
128.95
128.72
128.56
127.67
127.52
126.22
115.69
113.86
77.42 CDCl3
77.10 CDCl3
76.79 CDCl3
63.01
58.18
36.34
21.67
Br
O
N
N
Ph
N
Ph
Ts
3an
f1 (ppm)





7. X-ray crystal structure of 3da

3da (CCDC 1879117)



3da