Supporting Information

Direct Synthesis of Benzo[*f*]indazoles from Sulfonyl Hydrazines and 1,3-Enynes by Copper-Catalyzed Annulation

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1. General considerations

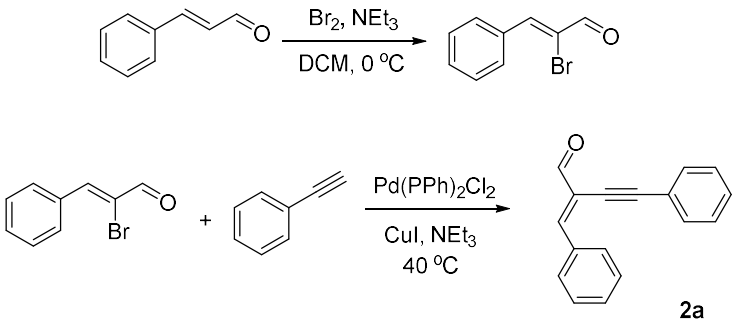
The reactions were carried out under air or nitrogen atmosphere. ^{1}H NMR and ^{13}C NMR spectra were measured on a Bruker Avance NMR spectrometer (400 MHz or 100 MHz, respectively) in $CDCl_3$ or DMSO-d_6 as solvent and recorded in ppm relative to internal standard tetramethylsilane. ^{1}H NMR data are reported as follows: δ, chemical shift; coupling constants (*J* are given in Hertz, Hz) and integration. Abbreviations to denote the multiplicity of a particular signal were s (singlet), d (doublet), t (triplet), q (quartet), m (multiplet), and br (broad singlet). High resolution mass spectroscopic data of the products were collected on an Agilent Technologies 6540 UHD Accurate-Mass Q-TOF LC/MS using ESI.

The chemicals and solvents were purchased from commercial suppliers either from Aldrich (USA) or Shanghai Chemical Company (China) without further purification unless otherwise specified. Products were purified by flash chromatography on 100–200 mesh silica gels, SiO_2.

2. Representative experiment procedures

2.1 Representative procedure for the synthesis of 2a

All compounds **2** were prepared according to reported method (See: Du, Q.; Neudörfl, J.-M.; Schmalz, H.-G. *Chem. Eur. J.* **2018**, *24*, 2379). A representative procedure for the synthesis of **2a** is shown as following route.



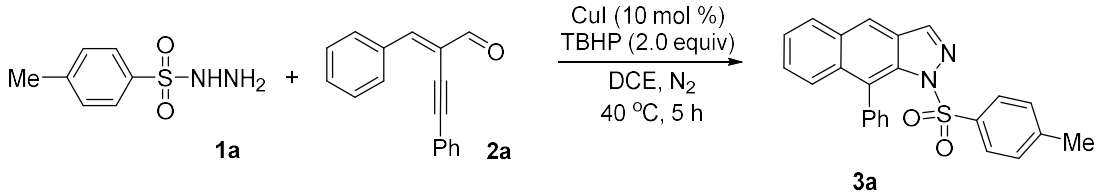
To a solution of cinnamaldehyde (1.32g, 10 mmol) in 15 mL DCM, was added Br_2 (1.92 g, 12 mmol, 1.2 equiv) at 0 ºC. The reaction mixture was stirred for 15 min, followed by the addition of Et_3N (2.4 mL, 17 mmol, 1.7 equiv). The resulting mixture was stirred 15 min at 0 ºC, then was diluted with DCM and washed with a 10 % Na_2SO_3 solution, H_2O and brine. The organic layer was dried over Na_2SO_4, filtered, and concentrated to yield orange oil. The crude residue was purified by flash

chromatography (PE/EA 10:1) to afford desired product 1:1 mixture of *Z*/*E* isomers. After 3 days at room temperature, the mixture crystallized completely as the *Z*-isomer to give (*Z*)-2-bromo-3-phenylacrylaldehyde in 86% yield (1.82 g).

A flame-dried 100 mL round bottom flask was charged with $Pd(PPh_2)_2Cl_2$ (70 mg, 0.10 mmol, 2.0 mol %), (*Z*)-2-bromo-3-phenylacrylaldehyde (1.05 g, 5.0 mmol) and alkyne (612 mg, 6.0 mmol, 1.2 equiv) and Et_3N (20 mL). After stirring 5 min, CuI (11.9 mg, 0.0625 mmol, 1.25 mol %) was added, then the mixture was stirred overnight at 40 °C. After the starting material was consumed, the mixture was quenched with NH_4Cl aqueous solution. Aqueous layer was extracted with ether (10 mL) twice. Combined organic layer was dried over sodium sulfate, and solvent was removed by evaporation. The crude residue was purified by flash chromatography (PE/EA 10:1) to afford (*E*)-2-benzylidene-4-phenylbut-3-ynal **2a** in 92% yield (1.07 g) as yellow oil.

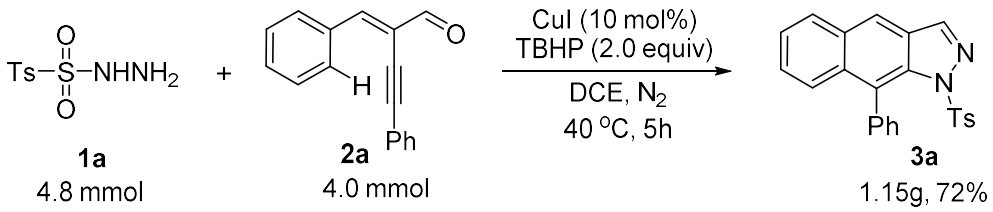
2.2 Representative procedure for the synthesis of 3a

2.2.1 Synthesis of 3a in 0.25 mmol scale



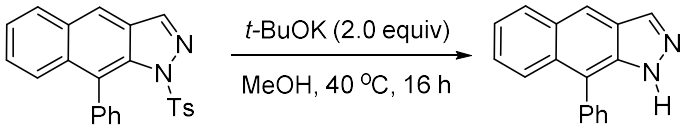
4-Methylbenzenesulfonohydrazide (**1a**, 0.30 mmol), (*E*)-2-benzylidene-4-phenylbut-3-ynal (**2a**, 0.25 mmol) and CuI (10 mol %) were added into a reaction tube (10 mL) with 2.0 mL of DCE. After stirring 5 min, TBHP (0.50 mmol) was added. The solvent was evacuated by pump and back-filled with high-purified nitrogen (>99.99%). The reaction was stirred in N_2 at 40 °C for 5 h. After the reaction was completed, the resulting crude mixture was purified by flash chromatography on silica gel (PE/EA = 5:1) to provide the desired product **3a** in 79% yield (78.7 mg).

2.2.2 Synthesis of 3a in 4.0 mmol scale



4-Methylbenzenesulfonohydrazide (**1a**, 4.8 mmol), (*E*)-2-benzylidene -4-phenylbut-3-ynal (**2a**, 4.0 mmol) and CuI (10 mol %) were added into a reaction tube (50 mL) with 32 mL of DCE. The mixture was set stirring 5 min. Finally, TBHP (8.0 mmol) was added. The reaction was stirred in N_2 at 40 ºC for 5 h. After the reaction was completed, the resulting crude mixture was purified by flash chromatography on silica gel (PE/EA = 5:1) to provide the desired product **3a** in 72% yield (1.15 g).

2.3 General procedure for the synthesis of 4 from 3a



3a, 0.25 mmol **4**, 84%

9-Phenyl-1-tosyl-1*H*-benzo[*f*]indazole (**3a**, 0.25 mmol) and *t*-BuOK (0.50 mmol), were added into a reaction tube (10 mL) with 2 mL of MeOH. The reaction was stirred in N_2 at 40 ºC for 16 h. After the reaction was completed, the resulting crude mixture was purified by flash chromatography on silica gel (PE/EA = 7:1) to provide the product 9-phenyl-1*H*-benzo[*f*]indazole **4** in 84% yield.

3. The radical trapping experiment

A radical scavenger BHT (butylated hydroxytoluene, 2.0 equiv) was added to the reaction solution of **1a** with **2a** under the standard reaction conditions. After 4 h, the crude reaction mixture was detected by HRMS (ESI) and vinyl radical adduct **5** with BHT was detected, as shown in Figure S1.

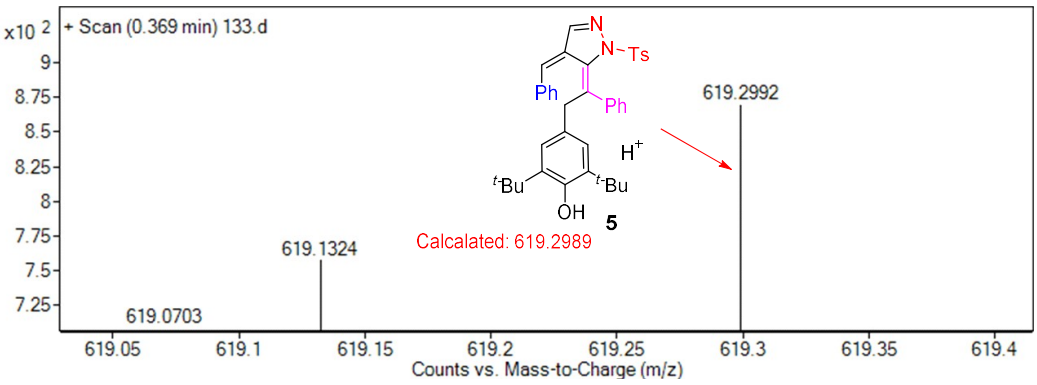
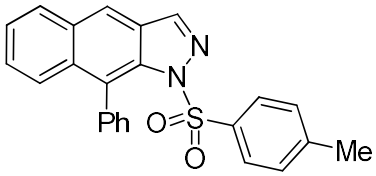
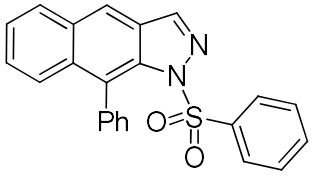


Figure S1. HRMS Analysis of the reaction solution of **1a** and **2a** with BHT

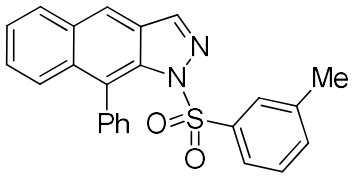
4. Characterization data for all products



9-Phenyl-1-tosyl-1*H*-benzo[*f*]indazole (3a). White solid, 78.7 mg, 79% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.30 (s, 3H), 7.11 (d, *J* = 8.0 Hz, 2H), 7.39–7.48 (m, 6H), 7.54 (t, *J* = 3.2 Hz, 3H), 7.68 (d, *J* = 8.4 Hz, 1H), 7.97 (d, *J* = 8.0 Hz, 1H), 8.23 (s, 1H), 8.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 120.6, 125.1, 125.3, 126.8, 127.3, 127.4, 127.6, 127.8, 128.0, 128.8, 129.2, 130.8, 130.9, 133.6, 134.6, 136.9, 137.5, 143.3, 144.5. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{19}N_2O_2S$: 399.1162, found: 399.1162.

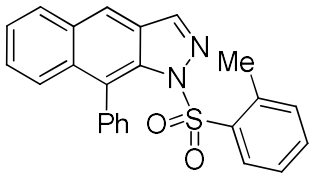


9-Phenyl-1-(phenylsulfonyl)-1*H*-benzo[*f*]indazole (3b). White solid, 72.1 mg, 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.31 (t, *J* = 7.8 Hz, 2H), 7.36–7.39 (m, 2H), 7.41–7.43 (m, 1H), 7.44–7.48 (m, 2H), 7.51 (dd, *J* = 4.8, 1.7 Hz, 3H), 7.58 (dd, *J* = 8.4, 1.2 Hz, 2H), 7.66 (d, *J* = 8.4 Hz, 1H), 7.97 (dd, *J* = 8.0, 1.0 Hz, 1H), 8.23 (s, 1H), 8.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.7, 125.1, 125.4, 126.9, 127.3, 127.4, 127.5, 127.8, 128.1, 128.6, 128.8, 130.8, 130.9, 133.4, 133.7, 136.9, 137.4, 137.6, 143.5. HRMS (ESI) ($[M+H]^+$) calculated for $C_{23}H_{17}N_2O_2S$: 385.1005, found: 385.1002.

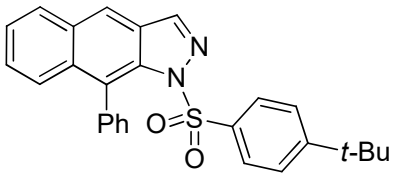


9-Phenyl-1-(*m*-tolylsulfonyl)-1*H*-benzo[*f*]indazole (3c). White solid, 72.7 mg, 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.28 (s, 3H), 7.18 (t, *J* = 7.6 Hz, 1H), 7.24 (d, *J* = 8.4 Hz, 1H), 7.35 (dd, *J* = 7.4, 2.2 Hz, 3H), 7.39–7.42 (m, 2H), 7.43–7.45 (m, 1H), 7.46–7.51 (m, 3H), 7.62 (d, *J* = 8.8 Hz, 1H), 7.96 (d, *J* = 8.0 Hz, 1H), 8.23 (s, 1H),

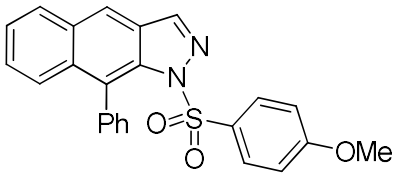
8.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.1, 120.7, 124.5, 124.8, 125.2, 126.7, 127.2, 127.3, 127.7, 127.8, 127.9, 128.4, 128.8, 130.7, 131.0, 133.6, 134.2, 136.6, 137.3, 137.5, 138.7, 143.1. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{19}N_2O_2S$: 399.1162, found: 399.1157.



9-Phenyl-1-(*o*-tolylsulfonyl)-1*H*-benzo[*f*]indazole (3d). White solid, 64.8 mg, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.32 (s, 3H), 7.15 (q, J = 7.7 Hz, 2H), 7.27 (dd, J = 8.0, 1.2 Hz, 2H), 7.37–7.42 (m, 4H), 7.44–7.49 (m, 3H), 7.57 (d, J = 8.8 Hz, 1H), 8.01 (d, J = 8.4 Hz, 1H), 8.32 (s, 1H), 8.44 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 20.2, 120.6, 124.2, 125.2, 126.1, 126.7, 126.9, 127.2, 127.7, 127.8, 128.8, 129.0, 130.6, 131.1, 132.2, 133.3, 133.7, 136.6, 137.2, 137.7, 138.0, 141.4. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{19}N_2O_2S$: 399.1162, found: 399.1160.

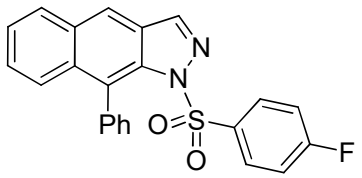


1-((4-(*tert*-Butyl)phenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3e). White solid, 80.4 mg, 73% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 1.24 (s, 9H), 7.33 (d, J = 8.4 Hz, 2H), 7.27 (dd, J = 6.4, 3.2 Hz, 2H), 7.40–7.43 (m, 1H), 7.44–7.48 (m, 1H), 7.50–7.53 (m, 5H), 7.64 (d, J = 8.8 Hz, 1H), 7.97 (d, J = 8.0 Hz, 1H), 8.25 (s, 1H), 8.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ; 30.9, 35.1, 120.6, 124.9, 125.2, 125.6, 126.8, 127.2, 127.4, 127.8, 128.0, 128.8, 130.7, 131.0, 133.7, 134.8, 136.8, 137.5, 143.1, 157.3. HRMS (ESI) ($[M+H]^+$) calculated for $C_{27}H_{25}N_2O_2S$: 441.1631, found: 441.1628.

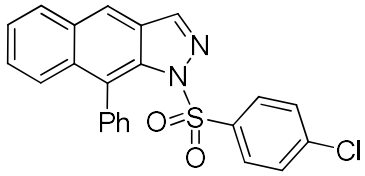


1-((4-Methoxyphenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3f). White solid, 86.0 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 3.74 (s, 3H), 6.75–6.78 (m, 2H),

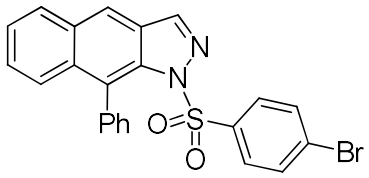
7.39–7.43 (m, 3H), 7.46 (dd, J = 6.6, 1.8 Hz, 1H), 7.52–7.55 (m, 5H), 7.69 (d, J = 8.8 Hz, 1H), 7.96 (d, J = 7.6 Hz, 1H), 8.22 (s, 1H), 8.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 55.5, 113.7, 120.6, 125.1, 125.2, 126.8, 127.2, 127.4, 127.7, 128.0, 128.8, 129.0, 129.9, 130.8, 130.9, 133.5, 136.9, 137.5, 143.3, 163.4. HRMS (ESI) ([M+H]$^+$) calculated for $C_{24}H_{18}N_2O_3S$: 415.1111, found: 415.1108.



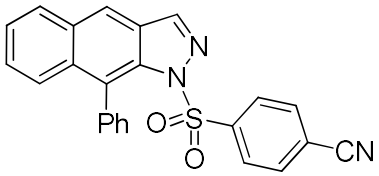
1-((4-Fluorophenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3g). White solid, 72.4 mg, 72% yield. ^{1}HN MR (400 MHz, $CDCl_3$) δ: 6.98–7.02 (m, 2H), 7.38–7.41 (m, 2H), 7.43–7.45 (m, 1H), 7.46–7.50 (m, 1H), 7.53 (t, J = 3.2 Hz, 3H), 7.59–7.63 (m, 2H), 7.67 (d, J = 8.8 Hz, 1H), 7.98 (dd, J = 8.0, 1.2 Hz, 1H), 8.25 (s, 1H), 8.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 115.9 (d, J = 22.6 Hz), 120.8, 125.1, 125.4, 126.8, 127.3, 127.4, 127.9, 128.1, 128.8, 130.5 (d, J = 9.5 Hz), 130.9, 133.5, 133.7, 136.8, 137.4, 143.7, 165.4 (d, J = 254.9 Hz). HRMS (ESI) ([M+H]$^+$) calculated for $C_{23}H_{16}FN_2O_2S$: 403.0911, found: 403.0907.



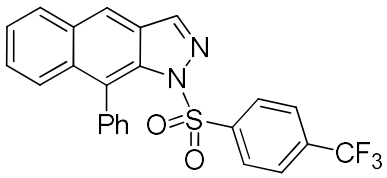
1-((4-Chlorophenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3h). White solid, 71.2 mg, 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.30 (dt, J = 8.8, 2.0 Hz, 2H),7.39 (dd, J = 6.6, 2.8 Hz, 2H), 7.42–7.50 (m, 2H), 7.52 (s, 1H), 7.53–7.55 (m, 4H), 7.67 (d, J = 8.4 Hz, 1H), 8.00 (d, J = 7.6 Hz, 1H), 8.26 (s, 1H), 8.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.8, 125.1, 125.4, 126.8, 127.3, 127.5, 127.9, 128.1, 128.8, 128.9, 129.0, 130.9, 133.6, 135.9, 136.7, 137.3, 140.0, 143.8. HRMS (ESI) ([M+H]$^+$) calculated for $C_{23}H_{16}ClN_2O_2S$: 419.0616, found: 419.0618.



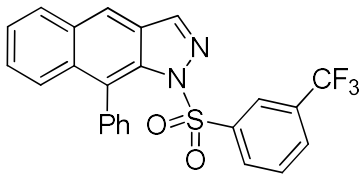
1-((4-Bromophenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3i). White solid, 79.9 mg, 69% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.39 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.43–7.50 (m, 6H), 7.51–7.54 (m, 3H), 7.67 (d, *J* = 8.4 Hz, 1H), 8.00 (d, *J* = 7.6 Hz, 1H), 8.26 (s, 1H), 8.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.9, 125.2, 125.5, 126.8, 127.3, 127.5, 127.9, 128.1, 128.7, 128.9, 129.1, 130.9, 131.9, 133.7, 136.5, 136.8, 137.3, 143.9. HRMS (ESI) ($[M+H]^+$) calculated for $C_{23}H_{16}BrN_2O_2S$: 463.0110, found: 463.0110.



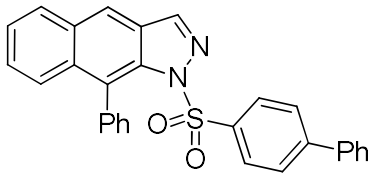
4-((9-Phenyl-1*H*-benzo[*f*]indazol-1-yl)sulfonyl)benzonitrile (3j). White solid, 66.5 mg, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36 (dd, *J* = 7.4, 1.8 Hz, 2H), 7.43–7.47 (m, 1H), 7.49–7.53 (m, 4H), 7.62–7.70 (m, 5H), 8.00 (d, *J* = 8.0 Hz, 1H), 8.28 (s, 1H), 8.49 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 117.0, 121.1, 125.1, 125.7, 126.8, 127.2, 127.7, 128.0, 128.1, 128.2, 128.9, 130.9, 131.0, 132.4, 133.7, 136.6, 137.1, 141.4, 144.3. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{16}N_3O_2S$: 410.958, found: 410.0953.



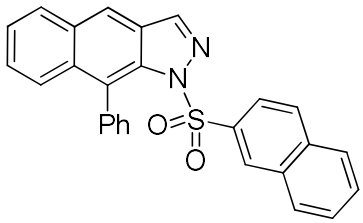
9-Phenyl-1-((4-(trifluoromethyl)phenyl)sulfonyl)-1*H*-benzo[*f*]indazole (3k). White solid, 72.4 mg, 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.40 (dd, *J* = 9.0, 3.0 Hz, 2H), 7.45–7.51 (m, 2H), 7.52–7.56 (m, 3H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.69 (d, *J* = 8.8 Hz, 1H), 7.76 (d, *J* = 8.4 Hz, 2H), 8.02 (d, *J* = 8.0 Hz, 1H), 8.30 (s, 1H), 8.53 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 121.0, 122.9 (q, *J* = 271.5 Hz), 125.1, 125.6, 125.8 (q, *J* = 3.7 Hz), 126.8, 127.3, 127.6, 128.0, 128.1, 128.1, 129.0 (q, *J* = 43.5 Hz), 130.9, 131.0, 133.8, 134.8 (q, *J* = 32.9 Hz), 136.3, 137.2, 141.0, 144.0. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{16}F_3N_2O_2S$: 453.0879, found: 453.0880.



9-Phenyl-1-((3-(trifluoromethyl)phenyl)sulfonyl)-1*H*-benzo[*f*]indazole (3l). White solid, 69.0 mg, 61% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35 (dd, *J* = 7.6, 1.6 Hz, 2H), 7.41–7.45 (m, 1H), 7.47–7.50 (m, 2H), 7.52 (d, *J* = 6.8 Hz, 3H), 7.63 (d, *J* = 8.8 Hz, 1H), 7.74 (d, *J* = 7.6 Hz, 1H), 7.81 (d, *J* = 8.0 Hz, 1H), 7.91 (s, 1H), 7.99 (d, *J* = 8.4 Hz, 1H), 8.28 (s, 1H), 8.52 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 121.0, 122.9 (q, *J* = 271.3 Hz), 124.8 (q, *J* = 3.7 Hz), 124.9, 125.6, 126.8, 127.2, 127.6, 128.1, 128.8, 129.6, 130.1 (q, *J* = 3.2 Hz), 130.7, 130.9, 131.3 (q, *J* = 72.3 Hz), 133.8, 136.5, 137.1, 138.8, 143.8. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{16}F_3N_2O_2S$: 453.0879, found: 453.0880.

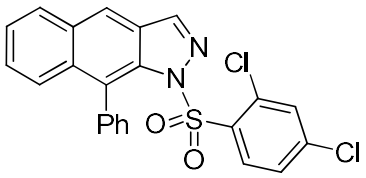


1-([1,1'-Biphenyl]-4-ylsulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3m). White solid, 89.8 mg, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35–7.38 (m, 2H), 7.39–7.45 (m, 5H), 7.47 (d, *J* = 1.2 Hz, 1H), 7.48–7.51 (m, 2H), 7.52–7.54 (m, 4H), 7.64 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 9.2 Hz, 1H), 7.97 (d, *J* = 7.6 Hz, 1H), 8.24 (s, 1H), 8.49 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.7, 125.1, 125.3, 126.8, 127.2, 127.3, 127.4, 127.8, 128.0, 128.5, 128.8, 128.9, 130.8, 131.0, 133.6, 136.1, 136.8, 137.4, 138.8, 143.5, 146.2. HRMS (ESI) ($[M+H]^+$) calculated for $C_{29}H_{21}N_2O_2S$: 464.1318, found: 461.1315.

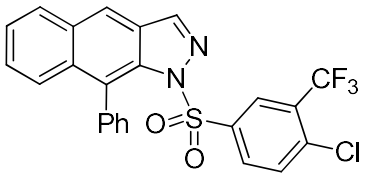


1-(Naphthalen-2-ylsulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3n). White solid, 86.9 mg, 80% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.35–7.39 (m, 3H), 7.41 (dd, *J* = 5.0, 1.4 Hz, 1H), 7.43–7.46 (m, 1H), 7.48 (s, 1H), 7.51 (d, *J* = 4.8 Hz, 1H), 7.53–7.57 (m,

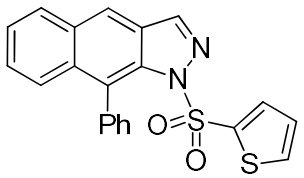
2H), 7.61 (t, J = 8.2Hz, 2H), 7.73 (d, J = 8.8 Hz, 1H), 7.76 (d, J = 7.6 Hz, 1H), 7.83 (dd, J = 8.4, 1.2 Hz, 1H), 7.94 (d, J = 8.4 Hz, 1H), 8.09 (s, 1H), 8.21 (s, 1H), 8.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.7, 122.2, 124.8, 125.2, 126.7, 127.3, 127.4, 127.8, 127.9, 127.9, 128.8, 128.9, 129.1, 129.4, 130.7, 131.0, 131.4, 133.6, 134.6, 134.9, 136.7, 137.4, 143.2. HRMS (ESI) ($[M+H]^+$) calculated for $C_{27}H_{19}N_2O_2S$: 435.1162, found: 435.1160.



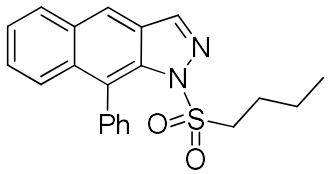
1-((2,4-Dichlorophenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3o). White solid, 79.3 mg, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.26 (dd, J = 8.0 Hz, 1H), 7.35 (d, J = 2.0 Hz, 1H), 7.37 (dd, J = 7.4, 1.7 Hz, 2H), 7.42–7.44 (m, 1H), 7.46–7.47 (m, 3H), 7.49–7.52 (m, 1H), 7.63 (d, J = 8.8 Hz, 1H), 7.72 (d, J = 8.8 Hz, 1H), 8.03 (d, J = 8.0 Hz, 1H), 8.33 (s, 1H), 8.43 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.9, 124.2, 125.3, 126.6, 126.7, 127.4, 127.4, 127.9, 128.0, 128.9, 130.8, 131.2, 131.2, 132.0, 133.5, 133.7, 135.8, 136.9, 137.2, 140.1, 142.1. HRMS (ESI) ($[M+H]^+$) calculated for $C_{23}H_{15}Cl_2N_2O_2S$: 453.0226, found: 453.0228.



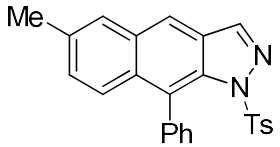
1-((4-Chloro-3-(trifluoromethyl)phenyl)sulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3p). White solid, 102.2 mg, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.34 (dd, J = 7.4, 1.4 Hz, 2H), 7.41–7.45 (m, 1H), 7.48 (dd, J = 6.6 Hz, 1H), 7.50–7.56 (m, 4H), 7.62 (d, J = 8.8 Hz, 1H), 7.73 (dd, J = 8.4, 2.6 Hz, 1H), 7.93 (d, J = 1.6 Hz, 1H), 7.99 (d, J = 8.4 Hz, 1H), 8.28 (s, 1H), 8.52 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.4, 121.7 (q, J = 272.4 Hz), 124.9, 125.6, 126.7, 127.0 (q, J = 5.8 Hz), 127.7, 128.1, 128.1, 129.0 (q, J = 32.5 Hz), 130.9, 130.9, 131.7, 132.1, 133.8, 136.3, 136.8, 137.1, 138.1, 144.0. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{15}ClF_3N_2O_2S$: 487.0489, found: 487.0491.



9-Phenyl-1-(thiophen-2-ylsulfonyl)-1*H*-benzo[*f*]indazole (3q). White solid, 56.6 mg, 58% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ 7.02–7.04 (m, 1H), 7.37 (dd, J = 3.8, 1.4 Hz, 1H), 7.43 (dt, J = 6.4, 1.6 Hz, 2H), 7.51–7.54 (m, 2H), 7.55–7.59 (m, 3H), 7.64 (dd, J = 4.8, 1.8 Hz, 1H), 7.91 (dd, J = 5.0, 1.4 Hz, 1H), 8.18 (dd, J = 6.8, 2.4 Hz, 1H), 8.54 (s, 1H), 8.95 (s, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 121.8, 125.7, 125.7, 126.1, 127.5, 127.7, 127.7, 127.9, 128.1, 129.3, 130.5, 130.9, 132.8, 134.4, 135.2, 135.8, 136.7, 137.0, 146.7. HRMS (ESI) ([M+H]$^+$) calculatedfor$C_{21}H_{15}N_2O_2S_2$: 391.0569, found: 391.0568.

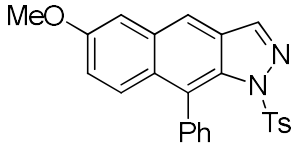


1-(Butylsulfonyl)-9-phenyl-1*H*-benzo[*f*]indazole (3r). Colorless oil, 59.2 mg, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.83 (t, J = 7.4 Hz, 3H), 1.26–1.31 (m, 2H), 1.56–1.63 (m, 2H), 3.07–3.11 (m, 2H), 7.40–7.44 (m, 3H), 7.48 (td, J = 7.4 Hz, 1H), 7.53–7.56 (m, 3H), 7.60 (d, J = 8.8, 1.2 Hz, 1H), 8.01 (d, J = 8.4 Hz, 1H), 8.33 (s, 1H), 8.51 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 13.3, 21.1, 24.7, 53.8, 120.7, 123.8, 125.1, 126.6, 126.9, 127.2, 128.0, 128.0, 128.8, 130.6, 131.2, 133.6, 136.7, 137.4, 141.7. HRMS (ESI) ([M+H]$^+$) calculated for $C_{21}H_{21}N_2O_2S$: 365.1318, found: 365.1314.

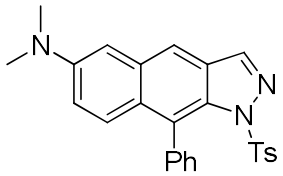


7-Methyl-9-phenyl-1-tosyl-1*H*-benzo[*f*]indazole (3s). White solid, 79.4 mg, 77% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.30 (s, 3H), 2.39 (s, 3H), 7.10 (d, J = 8.4 Hz, 2H), 7.30 (dd, J = 8.4, 1.6 Hz, 1H), 7.40 (dd, J = 6.6, 3.0 Hz, 2H), 7.43 (s, 1H), 7.47 (d, J = 8.0 Hz, 2H), 7.53–7.55 (m, 3H), 7.87 (d, J = 8.4, 1H), 8.16 (s, 1H), 8.41 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 22.3, 120.3, 124.4, 125.3, 126.9, 127.6,

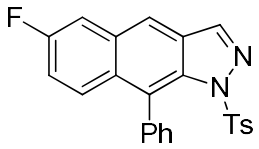
127.7, 127.9, 128.0, 128.6, 129.2, 129.3, 131.0, 133.9, 134.7, 137.3, 137.4, 137.6, 143.5, 144.4. HRMS (ESI) ([M+H]$^+$) calculated for $C_{25}H_{21}N_2O_2S$: 413.1318, found: 413.1316.



7-Methoxy-9-phenyl-1-tosyl-1*H*-benzo[*f*]indazole (3t). White solid, 66.4 mg, 62% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.30 (s, 3H), 3.65 (s, 3H), 6.90 (d, *J* = 2.4 Hz, 1H), 7.10–7.15 (m, 3H), 7.39–7.41 (m, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.51–7.55 (m, 3H), 7.85 (d, *J* = 9.2 Hz, 1H), 8.13 (s, 1H), 8.39 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 54.9, 104.1, 119.1, 120.4, 123.4, 125.8, 126.8, 127.6, 127.7, 128.1, 129.2, 130.3, 130.8, 134.7, 135.3, 137.6, 137.8, 143.4, 144.4, 158.6. HRMS (ESI) ([M+H]$^+$) calculated for $C_{25}H_{21}N_2O_3S$: 429.1267, found: 429.1264.

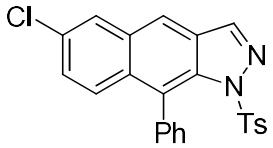


***N,N*-Dimethyl-9-phenyl-1-tosyl-1*H*-benzo[*f*]indazol-7-amine (3u).** White solid, 64.0 mg, 58% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.32 (s, 3H), 2.71 (s, 6H), 7.11 (s, 1H), 7.13 (s, 2H), 7.39 (dd, *J* = 7.0, 2.5 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.53–7.57 (m, 4H), 8.03 (s, 1H), 8.19 (s, 1H), 8.40 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 44.0, 115.2, 119.2, 119.6, 123.9, 126.8, 127.7, 127.9, 128.2, 128.3, 129.2, 130.8, 133.3, 133.7, 134.7, 137.4, 137.5, 143.3, 144.5, 150.4. HRMS (ESI) ([M+H]$^+$) calculated for $C_{26}H_{24}N_3O_2S$: 442.1584, found: 442.1582.

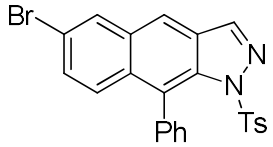


7-Fluoro-9-phenyl-1-tosyl-1*H*-benzo[*f*]indazole (3v). White solid, 72.9 mg, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.31 (s, 3H), 7.13 (d, *J* = 8.0 Hz, 2H), 7.23–7.28 (m, 2H), 7.35 (dd, *J* = 6.6, 3.0 Hz, 2H), 7.48 (d, *J* = 8.4 Hz, 2H), 7.53 (t, *J* = 3.2 Hz, 3H), 7.95–7.99 (m, 1H), 8.23 (s, 1H), 8.44 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:

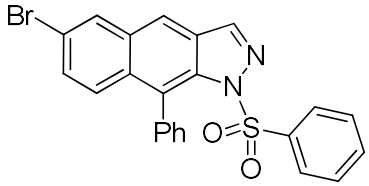
21.5, 109.8 (d, J = 23.2 Hz), 116.5 (d, J = 26.6 Hz), 120.8, 124.3 (d, J = 6.7 Hz), 127.0 (d, J = 2.3 Hz), 127.6, 127.9, 128.0, 128.2, 129.3, 130.8, 131.4 (d, J = 9.4 Hz), 134.7, 134.8 (d, J = 9.4 Hz), 137.2, 137.4, 142.9, 144.6, 161.3 (d, J = 246.8 Hz). HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{18}FN_2O_2S$: 417.1068, found: 417.1067.



7-Chloro-9-phenyl-1-tosyl-1*H*-benzo[*f*]indazole (3w). White solid, 81.2 mg, 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ; 2.32 (s, 3H), 7.13 (d, J = 8.4 Hz, 2H), 7.36 (dd, J = 6.4, 3.2 Hz, 2H), 7.40 (dd, J = 8.8, 2.0 Hz, 1H), 7.48 (d, J = 8.4 Hz, 2H), 7.52–7.55 (m, 3H), 7.62 (dd, J = 1.0, 0.6 Hz, 1H), 7.91 (d, J = 8.8 Hz, 1H), 8.22 (s, 1H), 8.44 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 120.6, 124.4, 125.5, 126.5, 127.6, 127.7, 128.1, 128.2, 129.0, 129.3, 130.4, 130.9, 133.4, 134.3, 134.8, 136.9, 137.5, 142.8, 144.7. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{18}ClN_2O_2S$: 433.0772, found: 433.0768.

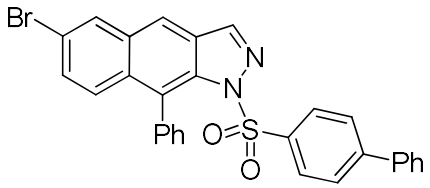


7-Bromo-9-phenyl-1-tosyl-1*H*-benzo[*f*]indazole (3x). White solid, 100.3 mg, 84% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.33 (s, 3H), 7.14 (d, J = 8.0 Hz, 2H), 7.37 (dd, J = 6.4, 3.1 Hz, 2H), 7.48 (d, J = 8.4 Hz, 2H), 7.52–7.55 (m, 4H), 7.81 (d, J = 1.2 Hz, 1H), 7.84 (d, J = 8.8 Hz, 1H), 8.21 (s, 1H), 8.44 (s, 1H); ^{13}CNMR (100 MHz, $CDCl_3$) δ: 21.5, 120.7, 122.0, 124.4, 127.7, 127.8, 128.2, 128.3, 128.9, 128.9, 129.1, 129.3, 130.3, 130.9, 134.7, 134.8, 136.8, 137.5, 142.8, 144.7. HRMS (ESI) ($[M+H]^+$) calculated for $C_{24}H_{18}BrN_2O_2S$: 477.0267, found: 477.0265.

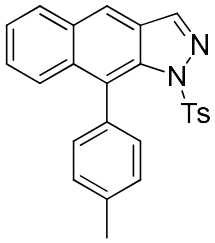


6-Bromo-9-phenyl-1-(phenylsulfonyl)-1*H*-benzo[*f*]indazole (3y). White solid, 93.8 mg, 81% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.33–7.37 (m,4H), 7.47–7.49 (m,

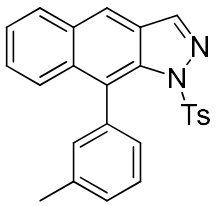
1H), 7.51–7.55 (m, 4H), 7.58 (dd, J = 8.4, 1.2 Hz, 2H), 7.80 (t, J = 0.8 Hz, 1H), 7.85 (d, J = 8.8 Hz, 1H), 8.22 (s, 1H), 8.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.8, 122.1, 124.3, 127.6, 128.3, 128.7, 128.8, 129.0, 129.1, 130.3, 130.9, 133.5, 134.7, 136.7, 137.4, 137.7, 143.0. HRMS (ESI) ([M+H]$^+$) calculated for $C_{23}H_{16}BrN_2O_2S$: 463.0110, found: 463.0107.



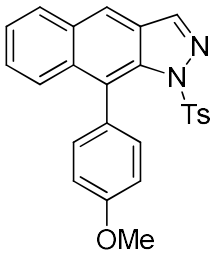
1-([1,1'-Biphenyl]-4-ylsulfonyl)-7-bromo-9-phenyl-1*H*-benzo[*f*]indazole (3z). White solid, 111.9 mg, 83% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 7.36–7.39 (m, 3H), 7.40–7.44 (m, 2H), 7.48–7.51 (m, 3H), 7.53–7.55 (m, 5H), 7.64 (dd, J = 7.6, 1.6 Hz, 2H), 7.80 (s, 1H), 7.83 (d, J = 8.8 Hz, 1H), 8.22 (s, 1H), 8.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 120.8, 122.0, 124.3, 127.2, 127.2, 127.6, 128.1, 128.2, 128.3, 128.6, 128.8, 128.9, 129.0, 129.1, 130.3, 130.9, 134.7, 136.2, 136.7, 137.4, 138.9, 143.0, 146.4. HRMS (ESI) ([M+H]$^+$) calculated for $C_{29}H_{20}BrN_2O_2S$: 539.0423, found: 539.0425



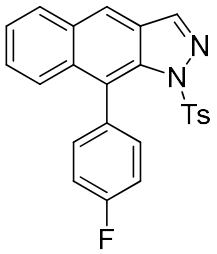
9-(*p*-Tolyl)-1-tosyl-1*H*-benzo[*f*]indazole (3aa). White solid, 77.3 mg, 75% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.29 (s, 3H), 2.50 (s, 3H), 7.09 (d, J = 8.0 Hz, 2H), 7.30 (q, J = 8.8 Hz, 4H), 7.38–7.44 (m, 2H), 7.47 (d, J = 8.4 Hz, 2H), 7.70 (d, J = 8.8 Hz, 1H), 7.94 (dd, J = 8.0, 1.2 Hz, 1H), 8.19 (s, 1H), 8.43 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.4, 120.4, 125.2, 125.3, 126.9, 127.1, 127.4, 127.5, 128.7, 128.7, 129.1, 130.7, 130.8, 133.7, 134.4, 134.6, 137.0, 137.3, 143.4, 144.4. HRMS (ESI) ([M+H]$^+$) calculated for $C_{25}H_{21}N_2O_2S$: 413.1318, found: 413.1315.



9-(*m*-Tolyl)-1-tosyl-1*H*-benzo[*f*]indazole (3ab). White solid, 80.4 mg, 78% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.29 (s, 3H), 2.41 (s, 3H), 7.10 (d, *J* = 8.0 Hz, 3H), 7.24 (dd, *J* = 8.4, 1.7 Hz, 1H), 7.33 (d, *J* = 7.6 Hz, 1H), 7.37–7.44 (m, 3H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.67 (d, *J* = 8.4 Hz, 1H), 7.94 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.21 (s, 1H), 8.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.4, 120.4, 125.1, 125.2, 126.9, 127.1, 127.3, 127.5, 127.7, 128.2, 128.4, 128.7, 129.2, 130.7, 131.5, 133.6, 134.8, 136.7, 137.2, 137.3, 143.1, 144.3. HRMS (ESI) ($[M+H]^+$) calculated for $C_{25}H_{21}N_2O_2S$: 413.1318, found: 413.1317.

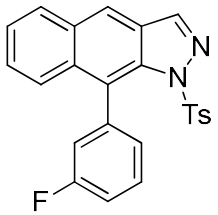


9-(4-Methoxyphenyl)-1-tosyl-1*H*-benzo[*f*]indazole (3ac). White solid, 70.7 mg, 66% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.30 (s, 3H), 3.92 (s, 3H), 7.04 (d, *J* = 8.4 Hz, 2H), 7.10 (d, *J* = 8.4 Hz, 2H), 7.28 (d, *J* = 8.4 Hz, 2H), 7.39–7.44 (m, 2H), 7.47 (d, *J* = 8.4 Hz, 2H), 7.70 (d, *J* = 8.8 Hz, 1H), 7.96 (d, *J* = 7.6 Hz, 1H), 8.21 (s, 1H), 8.45 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 55.2, 113.4, 120.4, 125.0, 125.2, 126.9, 127.2, 127.4, 127.5, 128.8, 129.2, 129.5, 130.9, 132.0, 134.0, 134.7, 137.3, 143.3, 144.4, 159.2. HRMS (ESI) ($[M+H]^+$) calculated for $C_{25}H_{21}N_2O_3S$: 429.1267, found: 429.1264.

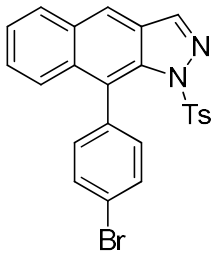


9-(4-Fluorophenyl)-1-tosyl-1*H*-benzo[*f*]indazole (3ad). White solid, 72.9 mg, 70% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.34 (s, 3H), 7.14 (d, *J* = 8.4 Hz, 2H), 7.12–7.23

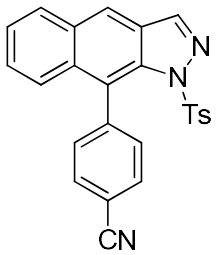
(m, 2H), 7.35 (td, J = 8.0, 2.1 Hz, 2H), 7.43–7.47 (m, 2H), 7.48–7.52 (m, 2H), 7.64 (d, J = 8.8 Hz, 1H), 8.00 (d, J = 7.6 Hz, 1H), 8.27 (s, 1H), 8.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 115.1 (d, J = 21.4 Hz), 120.9, 123.9, 125.4, 126.6, 127.5 (d, J = 7.3 Hz), 128.9, 129.3, 130.8, 132.5, 132.6, 133.3 (d, J = 3.5 Hz), 133.7, 134.7, 137.1, 143.3, 144.6, 162.6 (d, J = 245.1 Hz). HRMS (ESI) ([M+H]$^+$) calculated for $C_{24}H_{18}FN_2O_2S$: 417.1068, found: 417.1073.



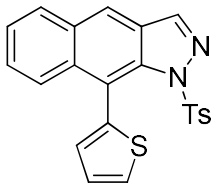
9-(3-Fluorophenyl)-1-tosyl-1*H*-benzo[*f*]indazole (3ae). White solid, 70.8 mg, 68% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.31 (s, 3H), 7.02–7.05 (m, 1H), 7.14 (d, J = 8.4 Hz, 2H), 7.20–7.25 (m, 2H), 7.42–7.46 (m, 1H), 7.46–7.52 (m, 4H), 7.64 (dd, J = 8.8, 0.9 Hz, 1H), 7.98 (dd, J = 8.4, 1.5 Hz, 1H), 8.26 (s, 1H), 8.47 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 21.5, 114.8 (d, J = 20.7 Hz), 118.1 (d, J = 21.6 Hz), 121.1, 123.4, 125.4, 126.5, 127.0 (d, J = 2.9 Hz), 127.4, 127.5, 127.6, 128.9, 129.3, 129.6 (d, J = 8.4 Hz), 130.7, 133.3, 134.6, 136.6, 139.5 (d, J = 8.0 Hz), 143.2, 144.7, 162.6 (d, J = 244.7 Hz). HRMS (ESI) ([M+H]$^+$) calculated for $C_{24}H_{18}FN_2O_2S$: 417.1068, found: 417.1066.



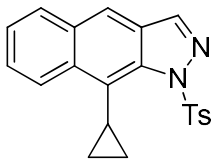
9-(4-Bromophenyl)-1-tosyl-1*H*-benzo[*f*]indazole (3af). White solid, 77.8 mg, 65% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.33 (s, 3H), 7.14 (d, J = 8.0 Hz, 2H), 7.23 (dt, J = 8.4, 1.8 Hz, 2H), 7.42–7.50 (m, 4H), 7.60 (dt, J = 8.4, 1.9 Hz, 3H), 7.98 (dd, J = 8.0, 1.2 Hz, 1H), 8.26 (s, 1H), 8.46 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 121.1, 122.0, 123.5, 125.4, 126.4, 127.4, 127.5, 128.9, 129.3, 130.8, 131.2, 132.6, 133.3, 134.7, 136.3, 136.7, 143.3, 144.6. HRMS (ESI) ([M+H]$^+$) calculated for $C_{24}H_{18}BrN_2O_2S$: 477.0267, found: 477.0271.



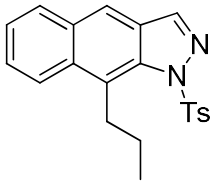
4-(1-Tosyl-1*H*-benzo[*f*]indazol-9-yl)benzonitrile (3ag). White solid, 78.3 mg, 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 2.34 (s, 3H), 7.16 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.50 (dt, *J* = 8.4, 1.7 Hz, 1H), 7.53–7.58 (m, 4H), 7.83 (d, *J* = 8.4 Hz, 2H), 8.03 (dd, *J* = 8.0, 1.2 Hz, 1H), 8.32 (s, 1H), 8.48 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 111.7, 118.9, 121.7, 122.8, 125.6, 125.9, 127.4, 127.5, 128.0, 129.2, 129.4, 130.8, 131.8, 131.9, 132.7, 134.3, 136.7, 142.7, 143.6, 145.0. HRMS (ESI) ($[M+H]^+$) calculated for $C_{25}H_{18}N_3O_2S$: 424.1114, found: 424.1114.



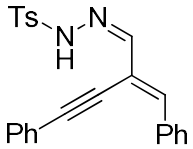
9-(Thiophen-2-yl)-1-tosyl-1*H*-benzo[*f*]indazole (3ah). White solid, 76.9 mg, 76% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 2.29 (s, 3H), 7.12 (d, *J* = 8.4 Hz, 2H), 7.16 (dd, *J* = 3.4, 0.9 Hz, 1H), 7.25–7.27 (m, 1H), 7.44–7.50 (m, 2H), 7.57–7.59 (m, 3H), 7.89–7.95 (m, 2H), 8.23 (s, 1H), 8.42 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 21.5, 117.3, 121.8, 125.4, 126.5, 126.8, 126.8, 127.4, 127.7, 127.7, 128.7, 129.2, 129.7, 130.6, 134.6, 134.7, 137.5, 138.5, 143.1, 144.6. HRMS (ESI) ($[M+H]^+$) calculated for $C_{22}H_{17}N_2O_2S_2$: 405.0726, found: 405.0723.



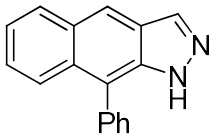
9-Cyclopropyl-1-tosyl-1*H*-benzo[*f*]indazole (3ai). Colorless oil, 67.0 mg, 74% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ: 0.67–0.71 (m, 2H), 1.40–1.45 (m, 2H), 2.27 (s, 3H), 7.04 (d, *J* = 8.0 Hz, 2H), 7.46 (d, *J* = 8.4 Hz, 2H), 7.48–7.52 (m, 1H), 7.63–7.67 (m, 1H), 7.91 (d, *J* = 8.0 Hz, 1H), 7.98, (s, 1H), 8.28 (s, 1H), 8.83 (d, *J* = 8.8 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 10.3, 13.4, 21.4, 119.7, 125.4, 126.6, 127.1, 127.7, 127.9, 128.0, 129.0, 129.2, 131.5, 133.7, 135.1, 139.7, 144.4, 146.9. HRMS (ESI) ($[M+H]^+$) calculated for $C_{21}H_{19}N_2O_2S$: 363.1162, found:363.1157.



9-Propyl-1-tosyl-1*H*-benzo[*f*]indazole (3aj). Colorless oil, 58.3 mg, 64% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 1.13 (t, *J* = 7.2 Hz, 3H), 1.85–1.94 (m, 2H), 2.30 (s, 3H), 3.74–3.78 (m, 2H), 7.12 (d, *J* = 8.0 Hz, 2H), 7.49 (td, *J* = 7.4, 0.7 Hz, 1H), 7.60–7.63 (m, 3H), 7.92 (d, *J* = 8.0 Hz, 1H), 8.23 (s, 1H), 8.28 (d, *J* = 8.8 Hz, 1H), 8.33 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ: 14.4. 21.5, 24.3, 31.6, 119.1, 125.1, 125.2, 126.7, 127.1, 127.7, 128.0, 129.3, 129.6, 131.5, 133.1, 134.2, 138.3, 144.7, 145.2. HRMS (ESI) ([M+H]$^+$) calculated for $C_{21}H_{21}N_2O_2S$: 365.1318, found: 365.1322.

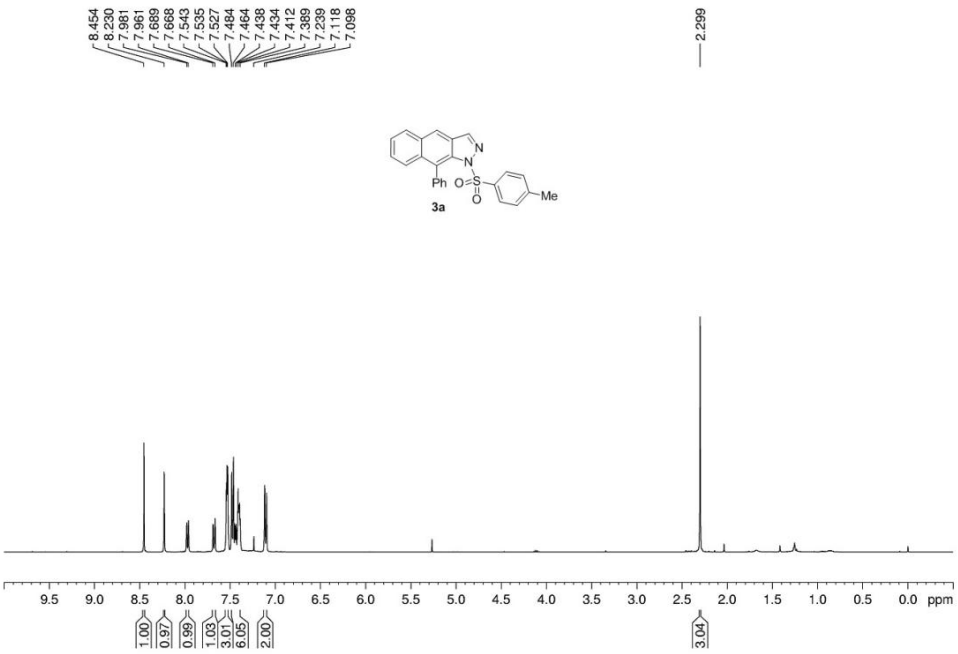


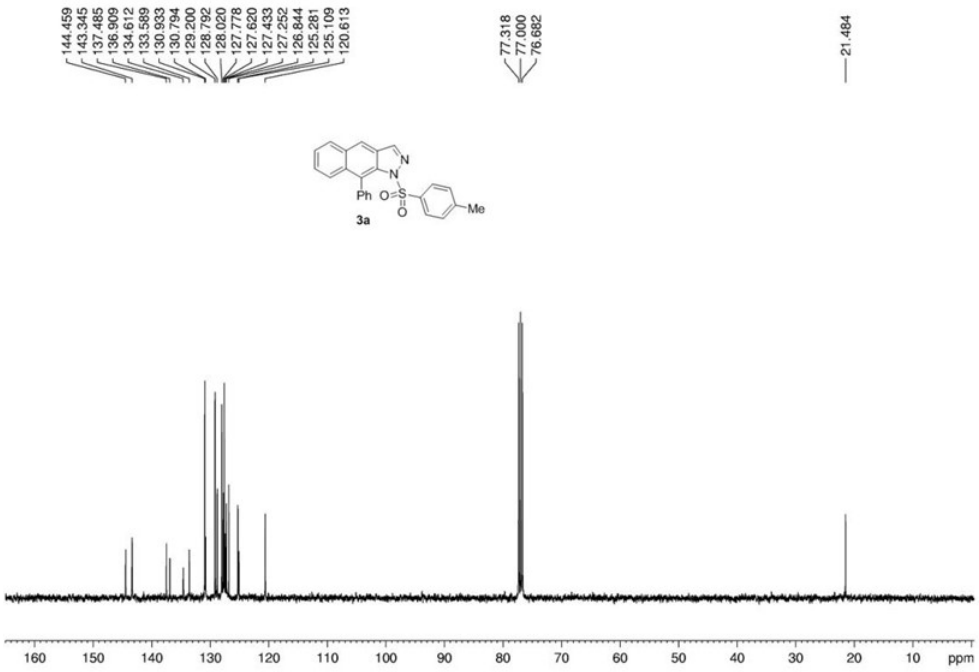
(*E*)-2-Benzylidene-4-phenylbut-3-yn-1-ylidene-4-methylbenzenesulfonohydrazide (A). White solid, 92.0 mg, 92% yield. ^{1}H NMR (400 MHz, DMSO-d_6) δ: 2.34 (s, 3H), 7.20 (s, 1H), 7.35 (d, *J* = 8.4 Hz, 2H), 7.40 (d, *J* = 7.2 Hz, 1H), 7.45–7.53 (m, 7H), 7.79 (t, *J* = 7.8 Hz, 3H), 8.00 (d, *J* = 8.0 Hz, 2H), 11.51 (brs, 1H); ^{13}C NMR (100 MHz, DMSO-d_6) δ: 21.4, 85.0, 98.6, 118.0, 122.6, 127.8, 129.1, 129.4, 129.7, 129.9, 130.1, 131.7, 135.6, 136.5, 142.1, 143.9, 149.2. HRMS (ESI) ([M+H]$^+$) calculated for $C_{24}H_{21}N_2O_2S_2$: 401.1318, found: 401.1315.

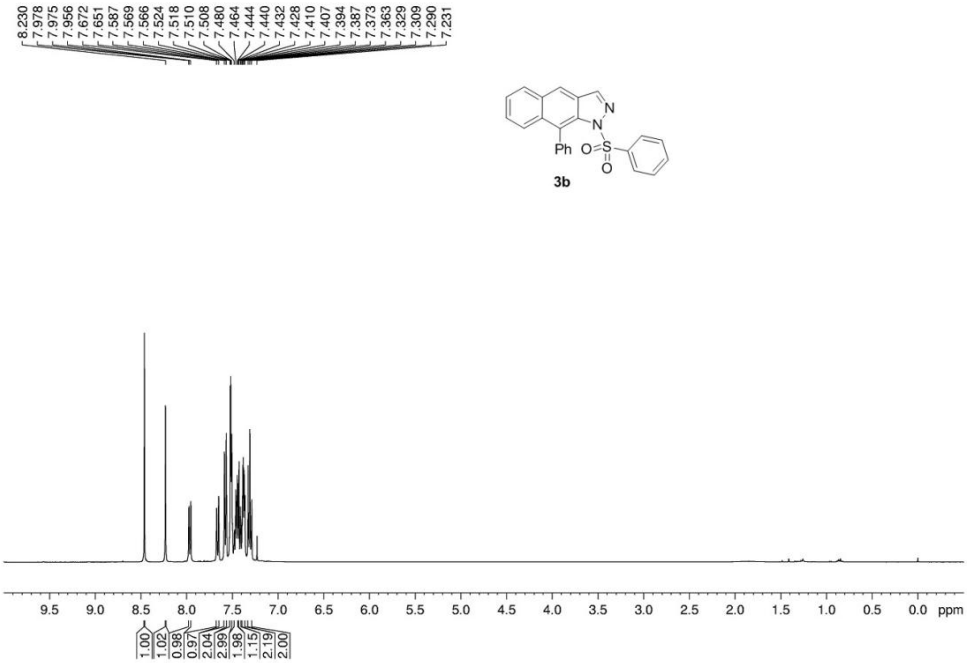


9-Phenyl-1*H*-benzo[*f*]indazole (4). White solid, 52.5 mg, 86% yield. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.34–7.41 (m, 2H), 7.46–7.52 (m, 1H), 7.58 (d, *J* = 4.4 Hz, 4H), 7.86–7.90 (m, 1H), 7.99–8.03 (m, 1H), 8.23 (s, 1H), 8.33 (s, 1H), 10.15 (brs, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ:118.0, 119.1, 123.2, 123.8, 124.8, 126.1, 128.1, 129.2, 129.4, 129.5, 130.3, 130.4, 135.5, 136.1, 137.8. HRMS (ESI) ([M+H]$^+$) calculated for $C_{17}H_{13}N_2$: 245.1073, found: 245.1068.

5. ^{1}H and ^{13}C NMR spectra of all products



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Ph
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S
O
3b
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 ppm
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1.02
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2.09
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1.15
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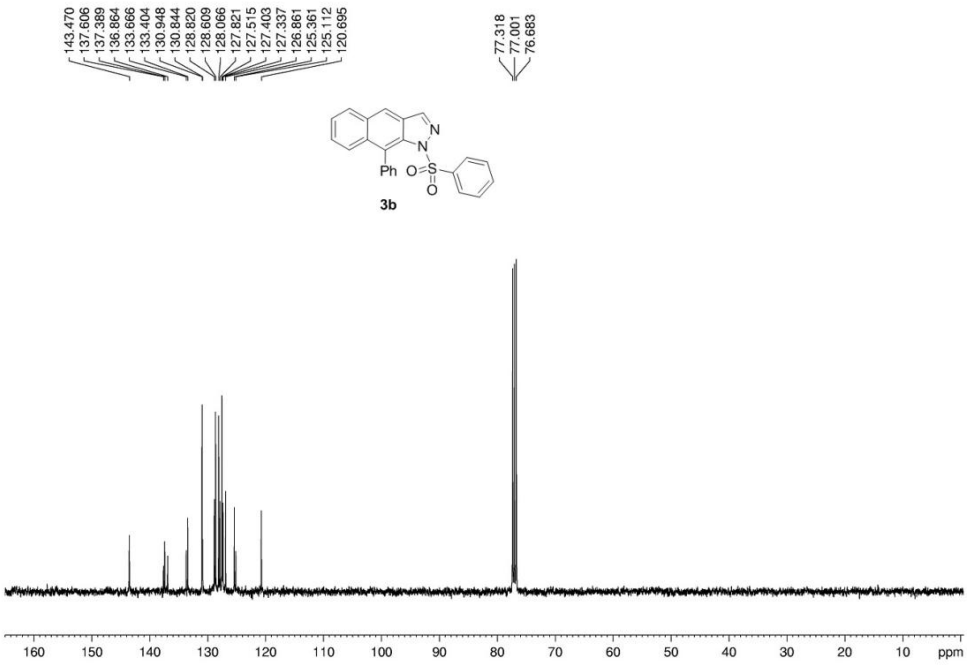
2.00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127.337
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O
3b
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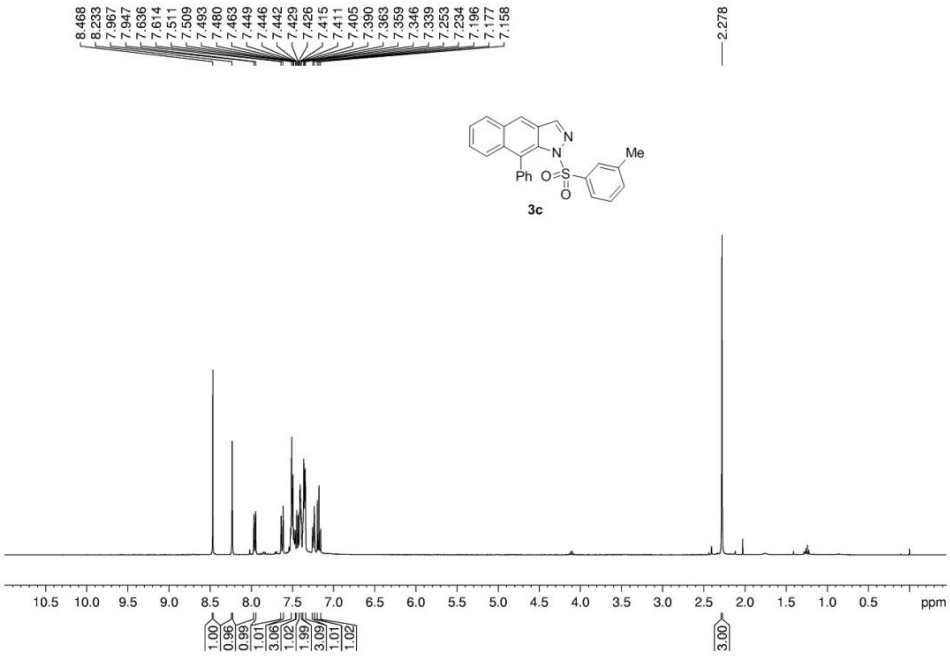
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1.99
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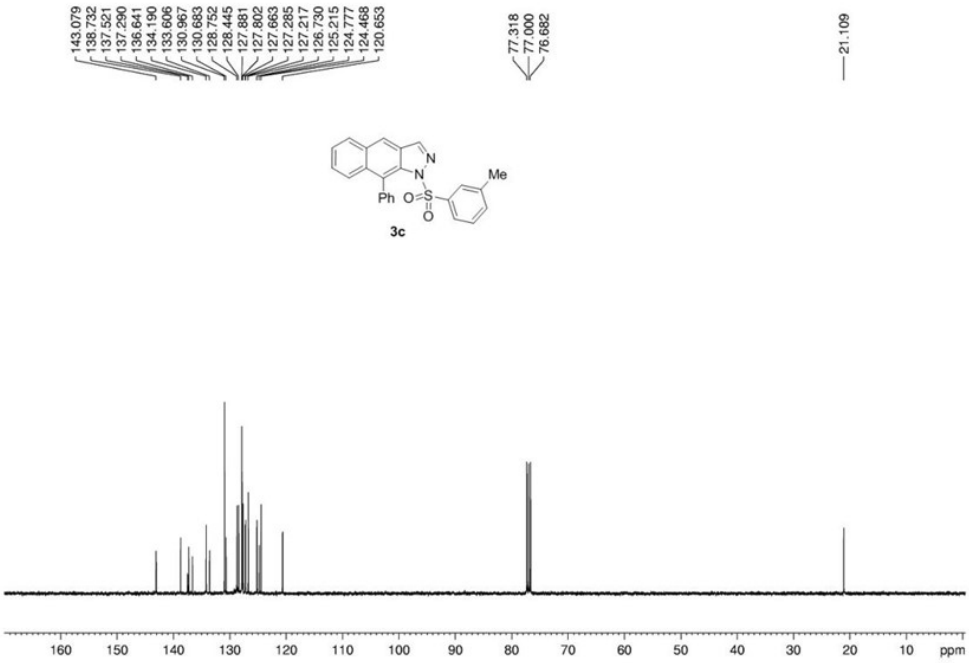
3.00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Me
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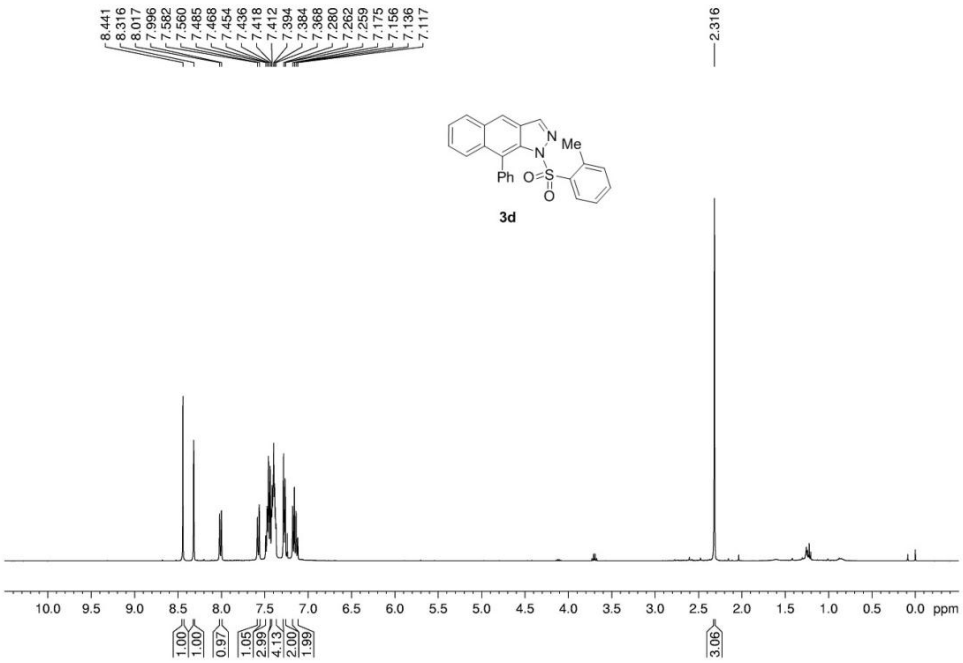
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Ph
Me
3d
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
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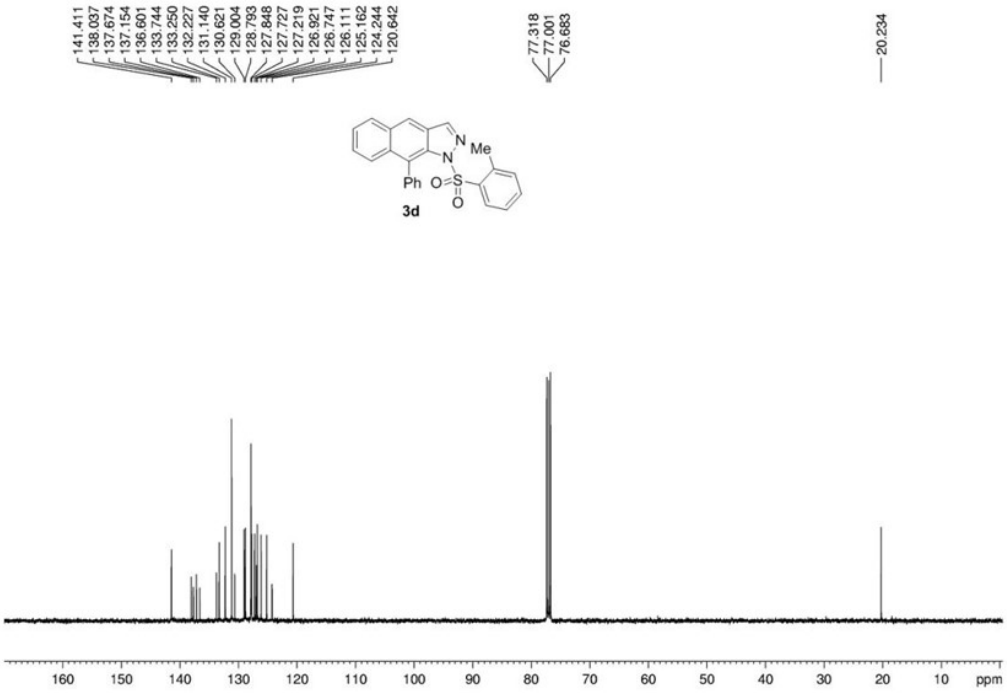
1.00
0.97
1.05
2.99
4.13
2.00
1.99
3.06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137.154
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133.744
133.250
132.227
131.140
130.621
129.004
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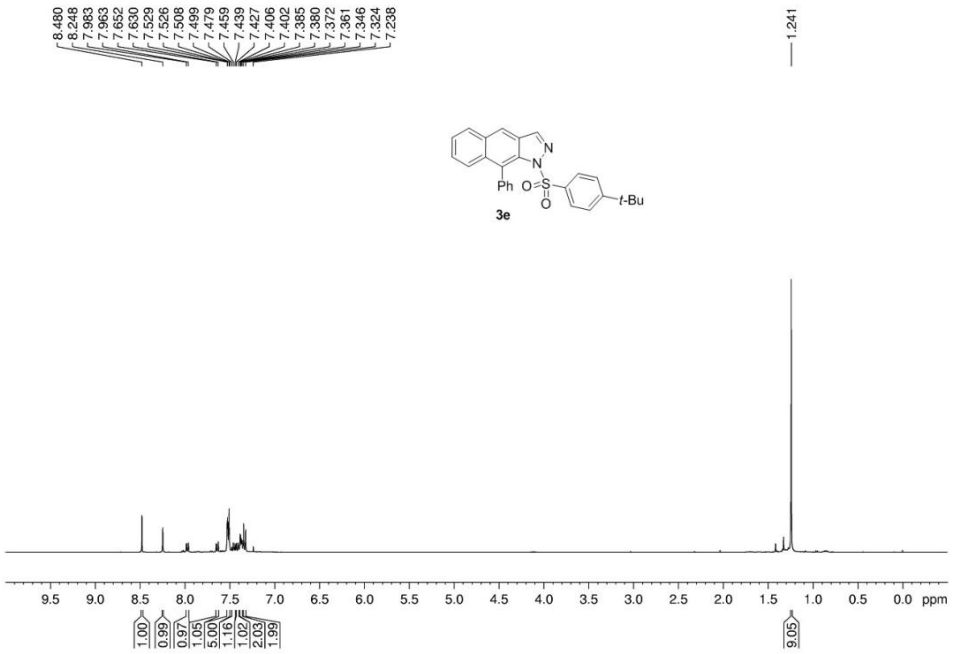
127.848
127.727
127.219
126.921
126.747
126.111
125.162
124.244
120.642
77.318
77.001
76.683
20.234
Ph
Me
3d
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.963
7.652
7.630
7.529
7.526
7.508
7.499
7.479
7.459
7.439
7.427
7.406
7.402
7.385
7.380
7.372
7.361
7.346
7.324
7.238
1.241
Ph
t-Bu
3e
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 ppm
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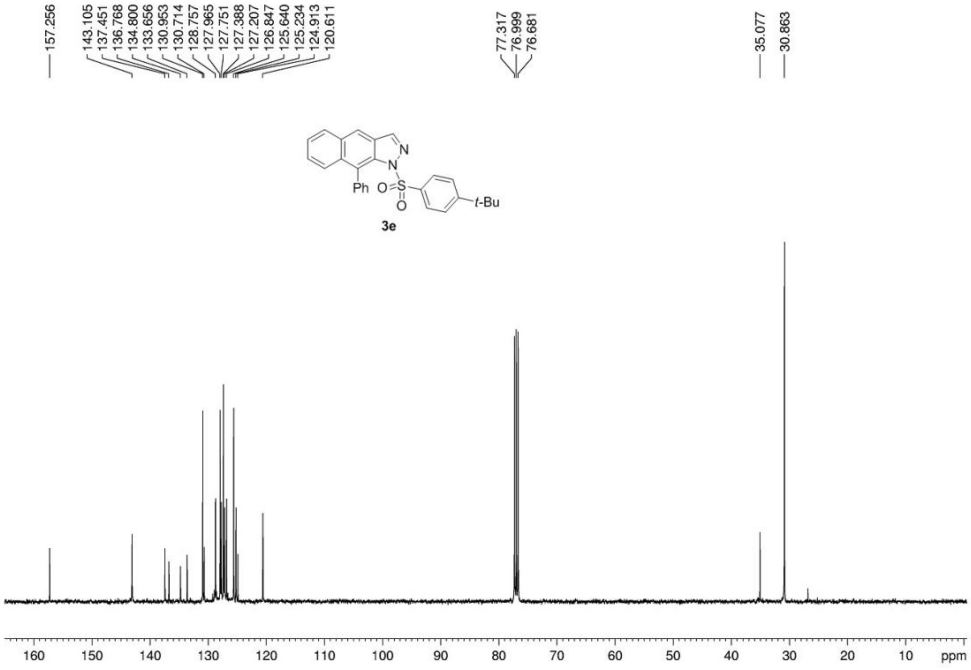
0.99
0.97
1.05
5.00
1.16
1.02
2.03
1.99
9.05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137.451
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133.656
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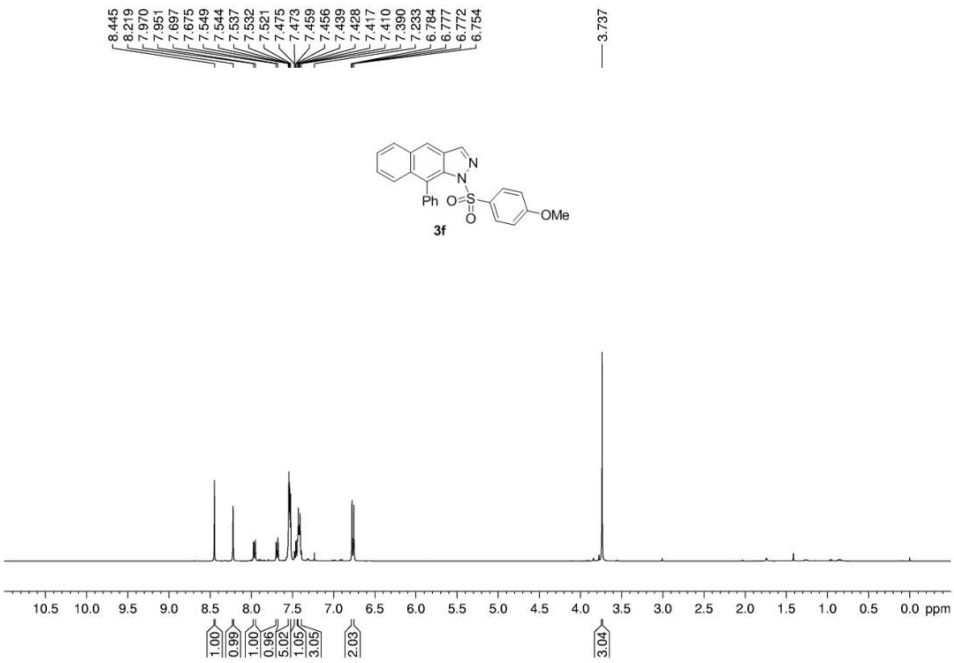
130.714
128.757
127.965
127.751
127.388
127.207
126.847
125.640
125.234
124.913
120.611
77.317
76.999
76.681
35.077
30.863
Ph
t-Bu
3e
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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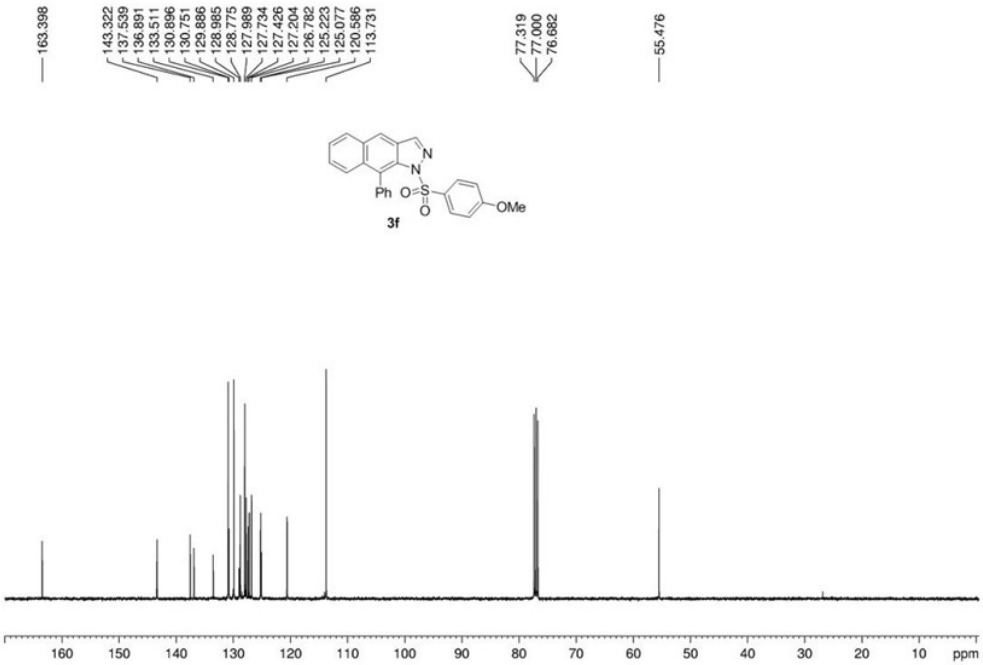
8.219
7.970
7.951
7.697
7.675
7.549
7.544
7.537
7.532
7.521
7.475
7.473
7.459
7.456
7.439
7.428
7.417
7.410
7.390
7.233
6.784
6.777
6.772
6.754
3.737
Ph
OMe
3f
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.99
1.00
0.96
5.02
1.05
3.05
2.03
3.04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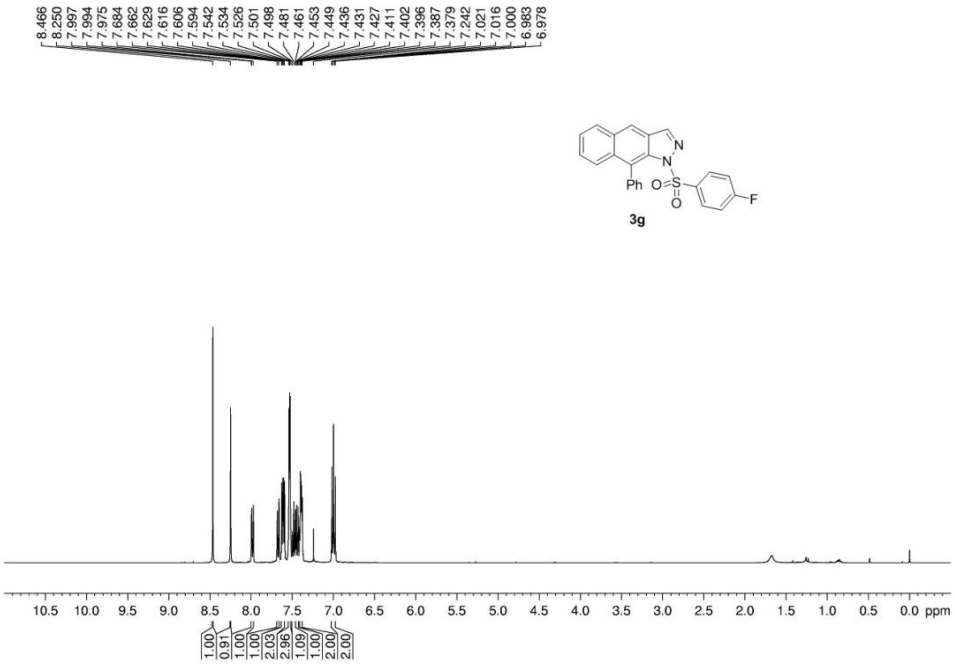
143.322
137.539
136.891
133.511
130.896
130.751
129.886
128.985
128.775
127.989
127.734
127.426
127.204
126.782
125.223
125.077
120.586
113.731
77.319
77.000
76.682
55.476
Ph
OMe
3f
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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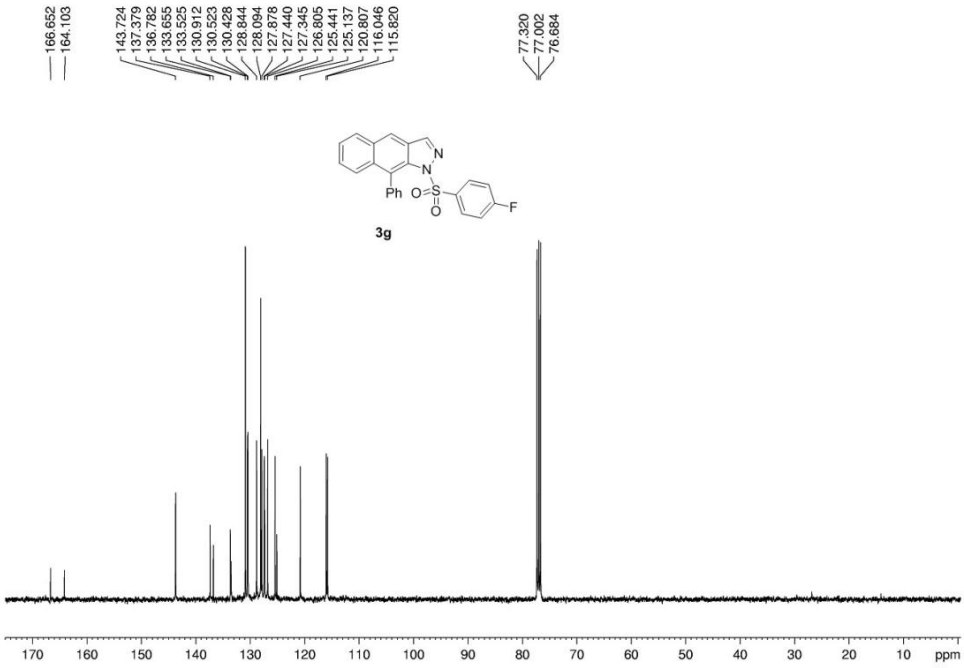
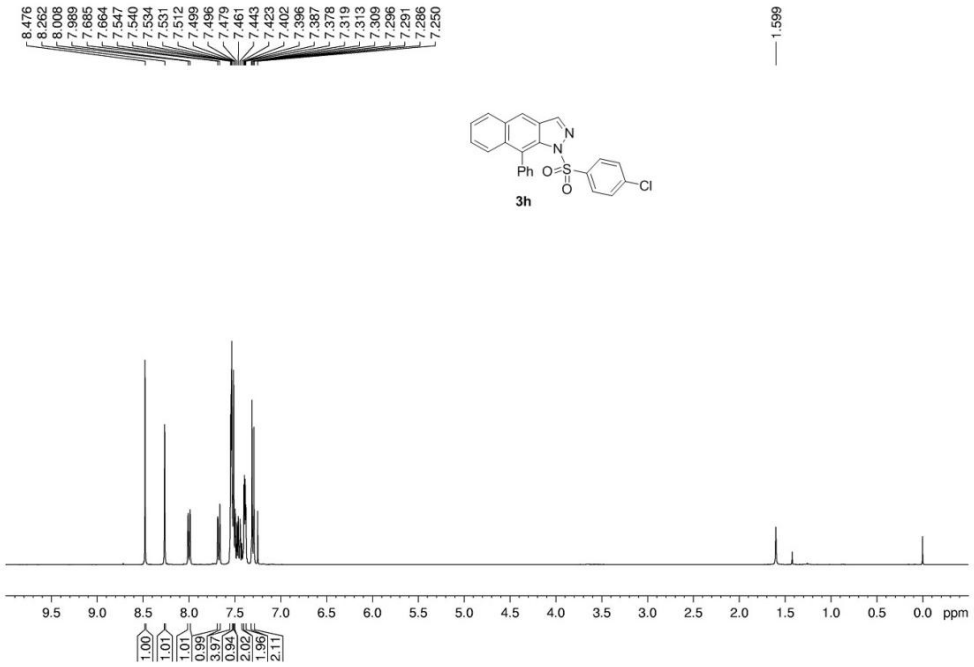
8.250
7.997
7.994
7.975
7.684
7.662
7.629
7.616
7.606
7.594
7.542
7.534
7.526
7.501
7.498
7.481
7.461
7.453
7.449
7.436
7.431
7.427
7.411
7.402
7.396
7.387
7.379
7.242
7.021
7.016
7.000
6.983
6.978
N
N
Ph
O
S
O
F
3g
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.91
1.00
1.00
2.03
2.96
1.08
1.00
2.00
2.00


166.652
164.103
143.724
137.379
136.782
133.655
133.525
130.912
130.523
130.428
128.844
128.094
127.878
127.440
127.345
126.805
125.441
125.137
120.807
116.046
115.820
77.320
77.002
76.684
N
N
Ph
O
S
O
F
3g
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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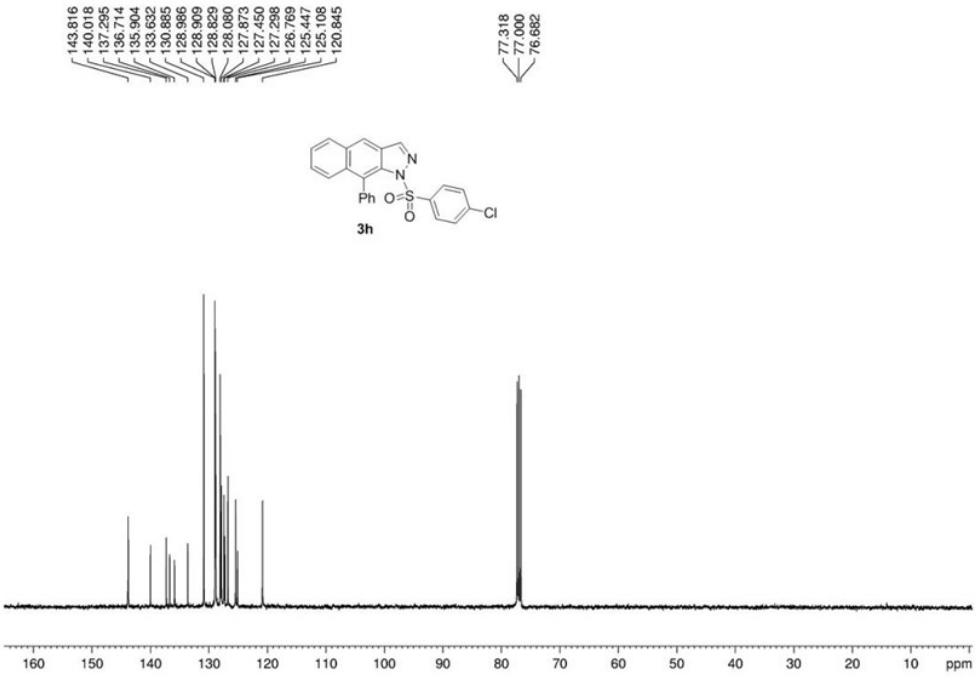
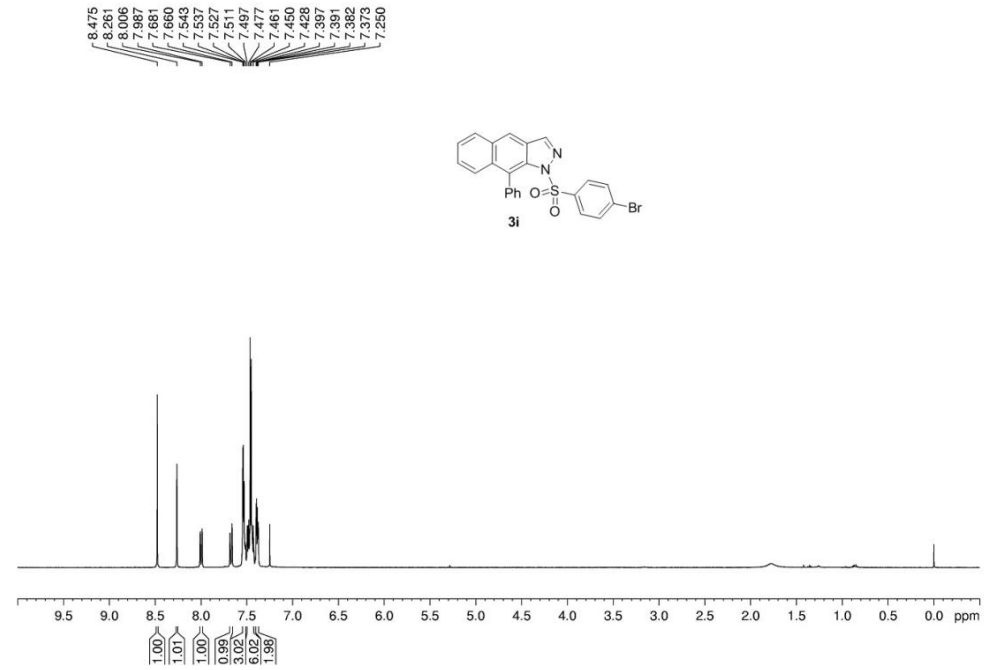
8.262
8.008
7.989
7.685
7.664
7.547
7.540
7.534
7.531
7.512
7.499
7.496
7.479
7.461
7.443
7.423
7.402
7.396
7.387
7.378
7.319
7.313
7.309
7.296
7.291
7.286
7.250
1.599
N
N
Ph
O
S
O
Cl
3h
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.01
1.01
0.99
3.97
0.94
2.02
1.96
2.11


143.816
140.018
137.295
136.714
135.904
133.632
130.885
128.986
128.909
128.829
128.060
127.873
127.450
127.298
126.769
125.447
125.108
120.845
77.318
77.000
76.682
N
N
Ph
O
S
O
Cl
3h
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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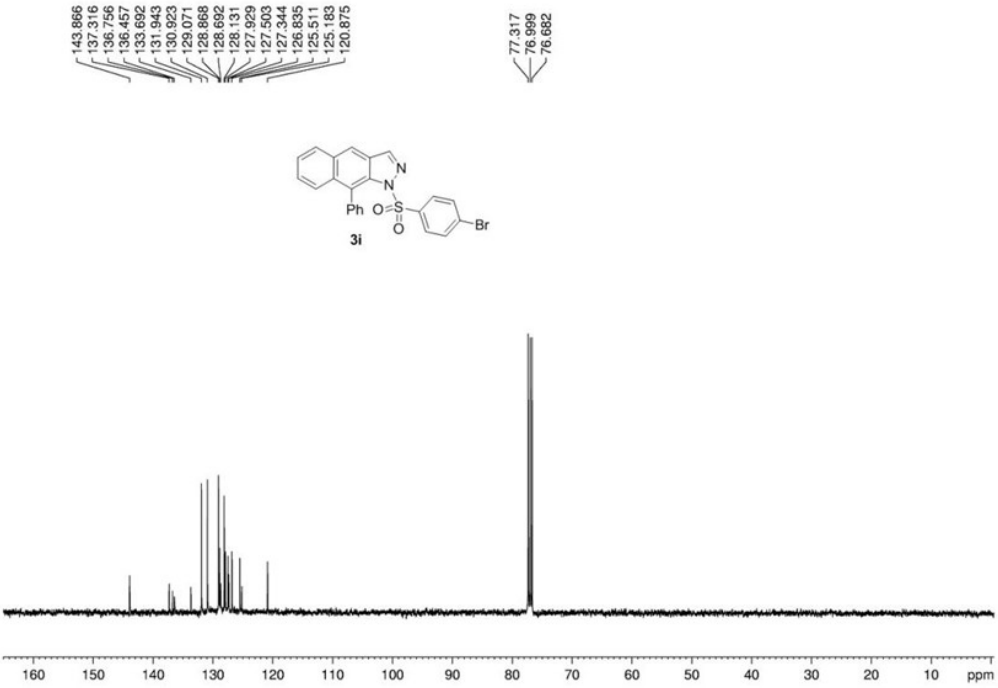
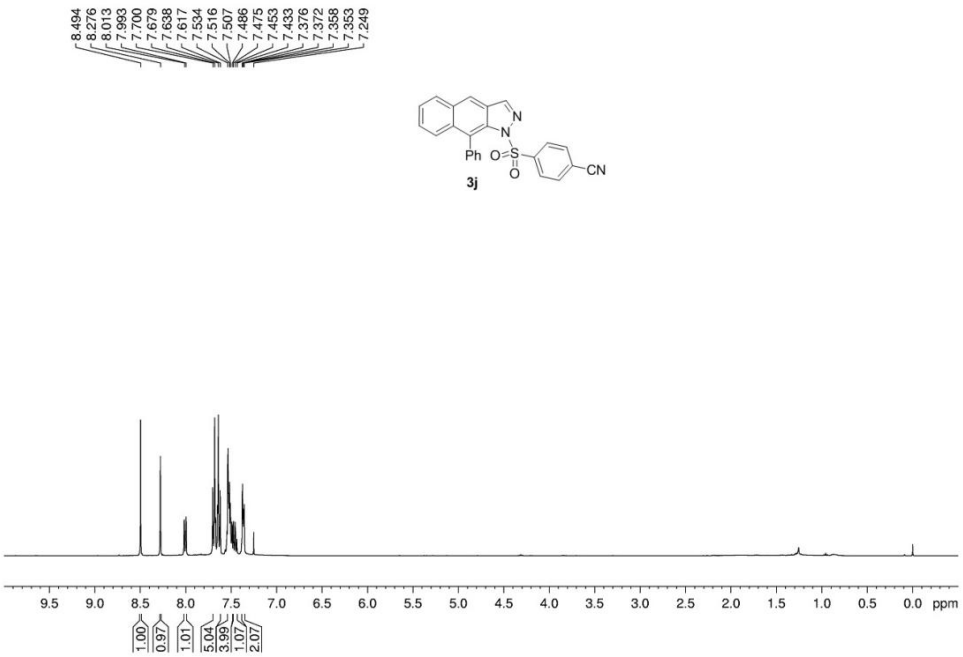
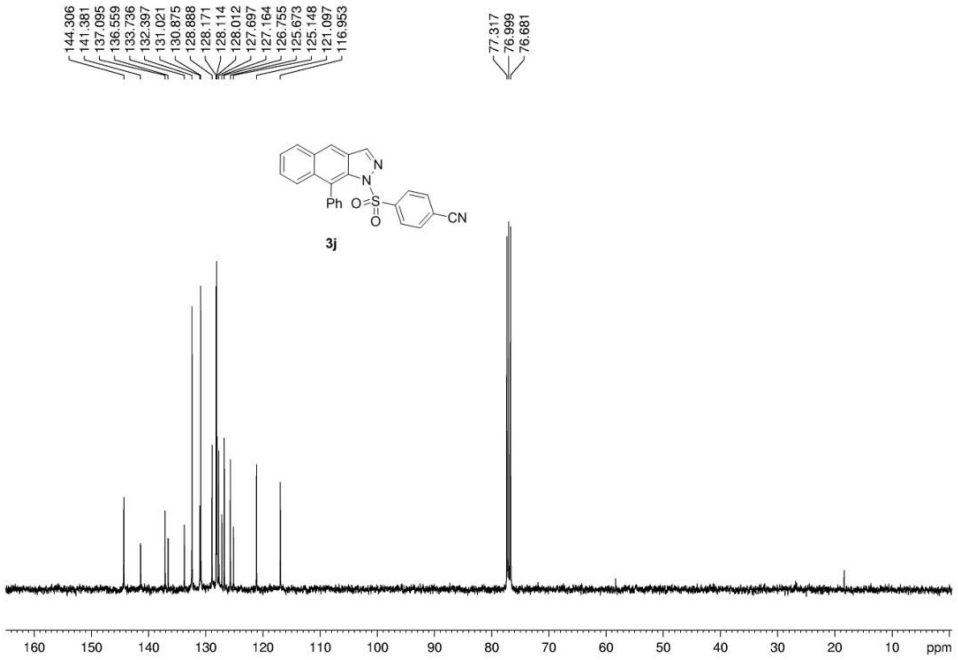
8.261
8.006
7.987
7.681
7.660
7.543
7.537
7.527
7.511
7.497
7.477
7.461
7.450
7.428
7.397
7.391
7.382
7.373
7.250
Ph
Br
3i
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.01
1.00
0.99
3.02
6.02
1.98


143.866
137.316
136.756
136.457
133.692
131.943
130.923
129.071
128.868
128.692
128.131
127.929
127.503
127.344
126.835
125.511
125.183
120.875
77.317
76.999
76.682
Ph
Br
3i
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.494
8.276
8.013
7.993
7.700
7.679
7.638
7.617
7.534
7.516
7.507
7.486
7.475
7.453
7.433
7.376
7.372
7.358
7.353
7.249
N
N
Ph
O
S
O
CN
3j
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 ppm
1.00
0.97
1.01
5.04
3.99
1.07
2.07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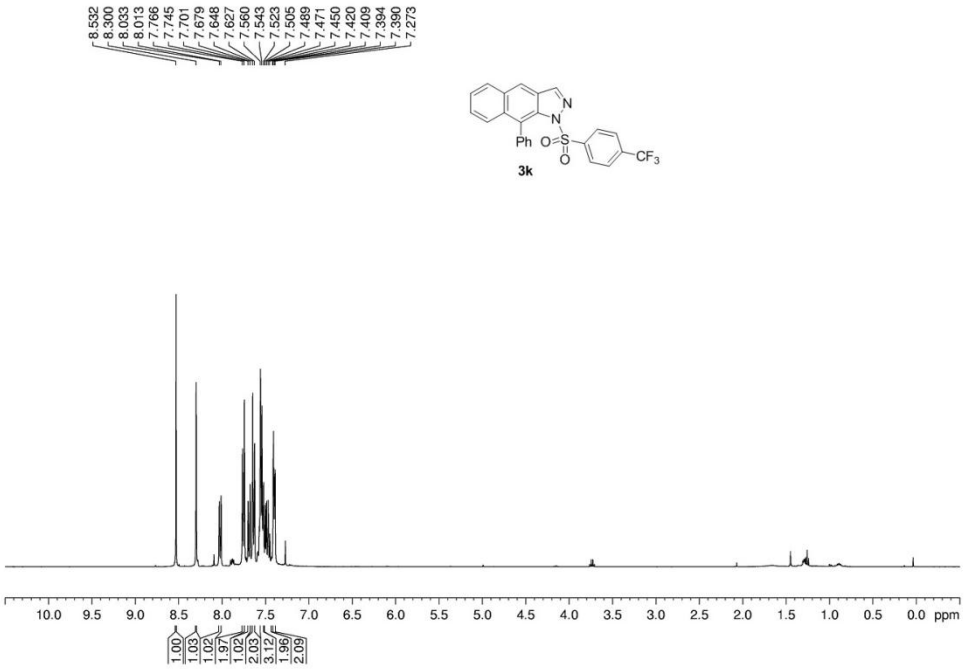
141.381
137.095
136.559
133.736
132.397
131.021
130.875
128.888
128.171
128.114
128.012
127.697
127.164
126.755
125.673
125.148
121.097
116.953
77.317
76.999
76.681
N
N
Ph
O
S
O
CN
3j
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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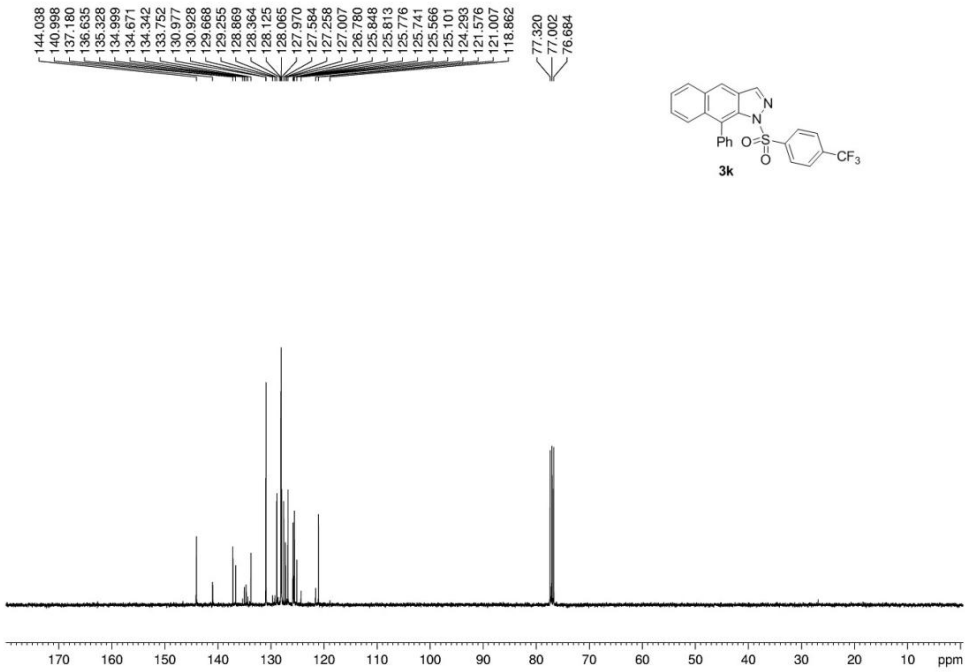
8.300
8.033
8.013
7.766
7.745
7.701
7.679
7.648
7.627
7.560
7.543
7.523
7.505
7.489
7.471
7.450
7.420
7.409
7.394
7.390
7.273
N
N
Ph
O
S
O
CF3
3k
10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.03
1.02
1.97
1.02
2.03
3.12
1.96
2.09


144.038
140.998
137.180
136.635
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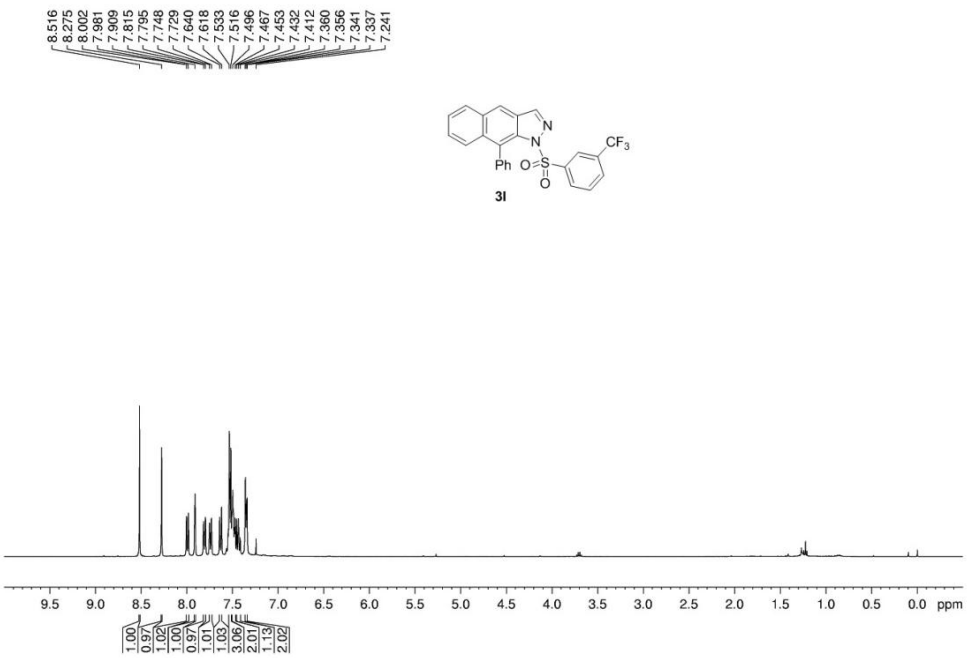
134.999
134.671
134.342
133.752
130.977
130.928
129.668
129.255
128.869
128.364
128.125
128.065
127.970
127.584
127.258
127.007
126.780
125.848
125.813
125.776
125.741
125.566
125.101
124.293
121.576
121.007
118.862
77.320
77.002
76.684
N
N
Ph
O
S
O
CF3
3k
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.002
7.981
7.909
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7.748
7.729
7.640
7.618
7.533
7.516
7.496
7.467
7.453
7.432
7.412
7.360
7.356
7.341
7.337
7.241
N
N
CF3
Ph
O
S
O
3l
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 ppm
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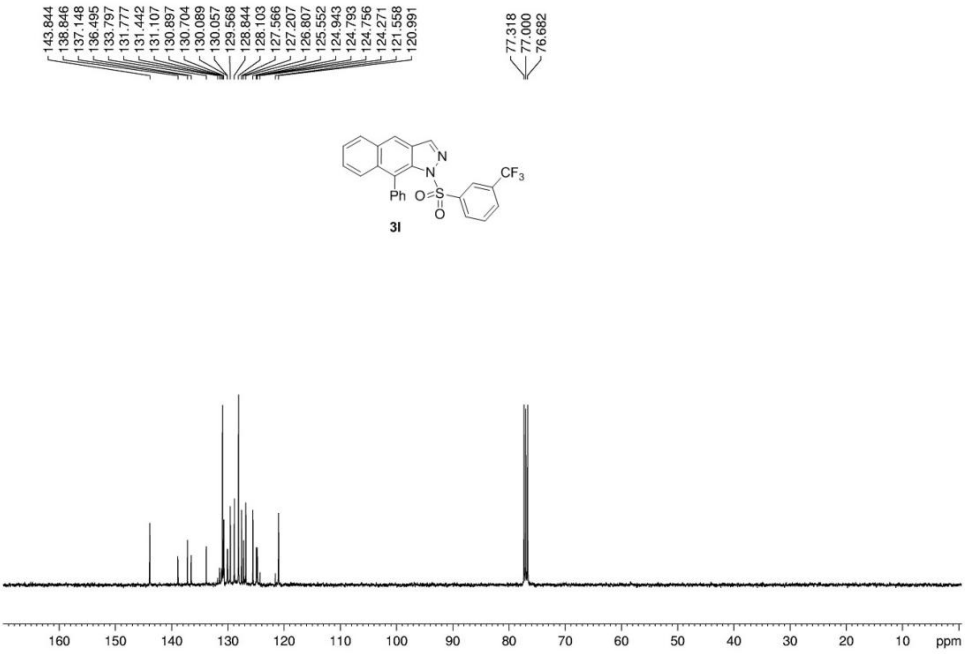
0.97
1.02
1.00
0.97
1.01
1.03
3.06
2.01
1.13
2.02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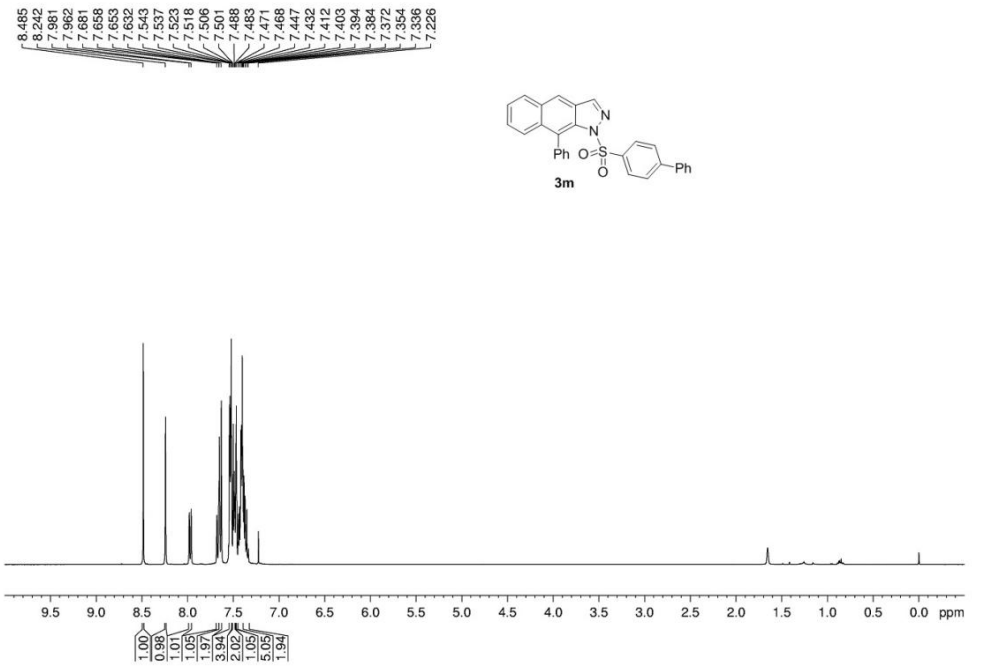
136.495
133.797
131.777
131.442
131.107
130.897
130.704
130.089
130.057
129.568
128.844
128.103
127.566
127.207
126.807
125.552
124.943
124.793
124.756
124.271
121.558
120.991
77.318
77.000
76.682
N
N
CF3
Ph
O
S
O
3l
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.981
7.962
7.681
7.658
7.653
7.632
7.543
7.537
7.523
7.518
7.506
7.501
7.488
7.483
7.471
7.468
7.447
7.432
7.412
7.403
7.394
7.384
7.372
7.354
7.336
7.226
N
N
Ph
O
S
O
Ph
3m
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 ppm
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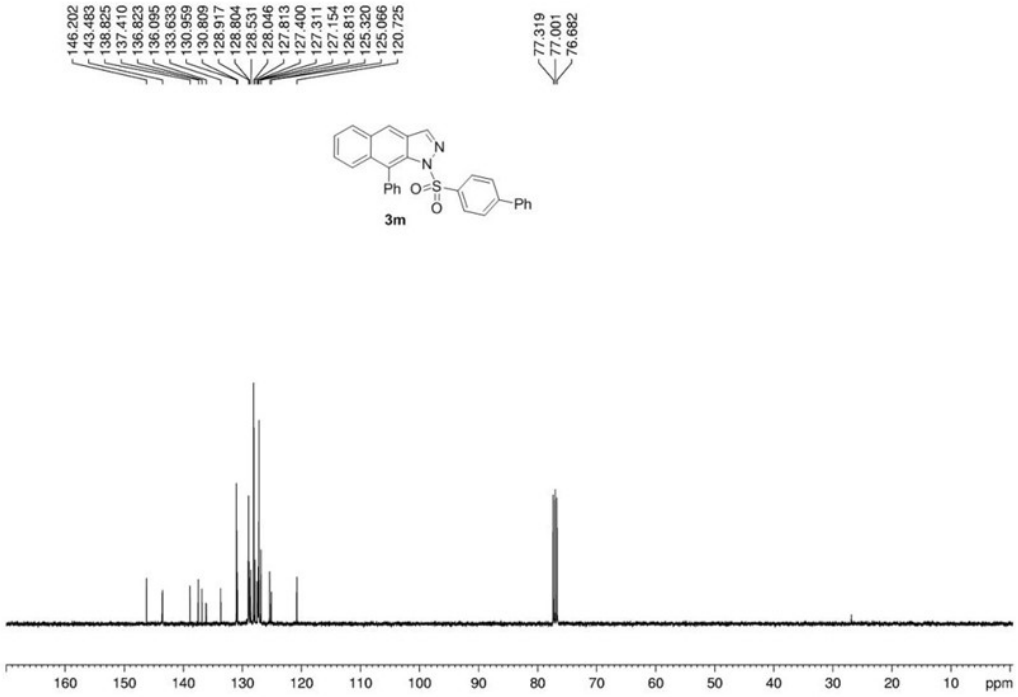
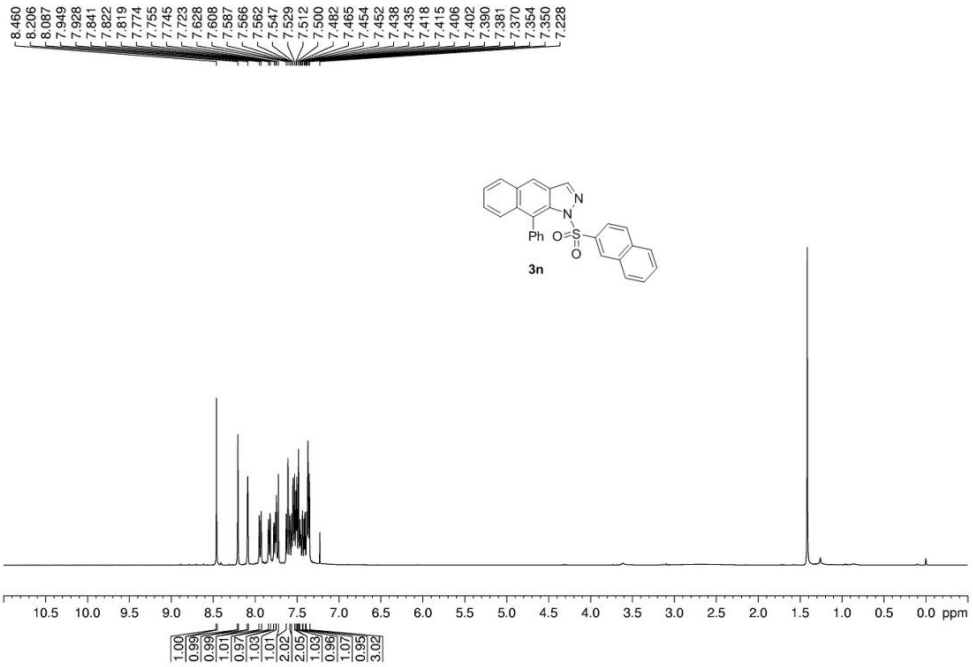
0.98
1.01
1.05
1.97
3.94
2.02
1.05
5.05
1.94


146.202
143.483
138.825
137.410
136.823
136.095
133.633
130.959
130.809
128.917
128.804
128.531
128.046
127.813
127.400
127.311
127.154
126.813
125.320
125.066
120.725
77.319
77.001
76.682
N
N
Ph
O
S
O
Ph
3m
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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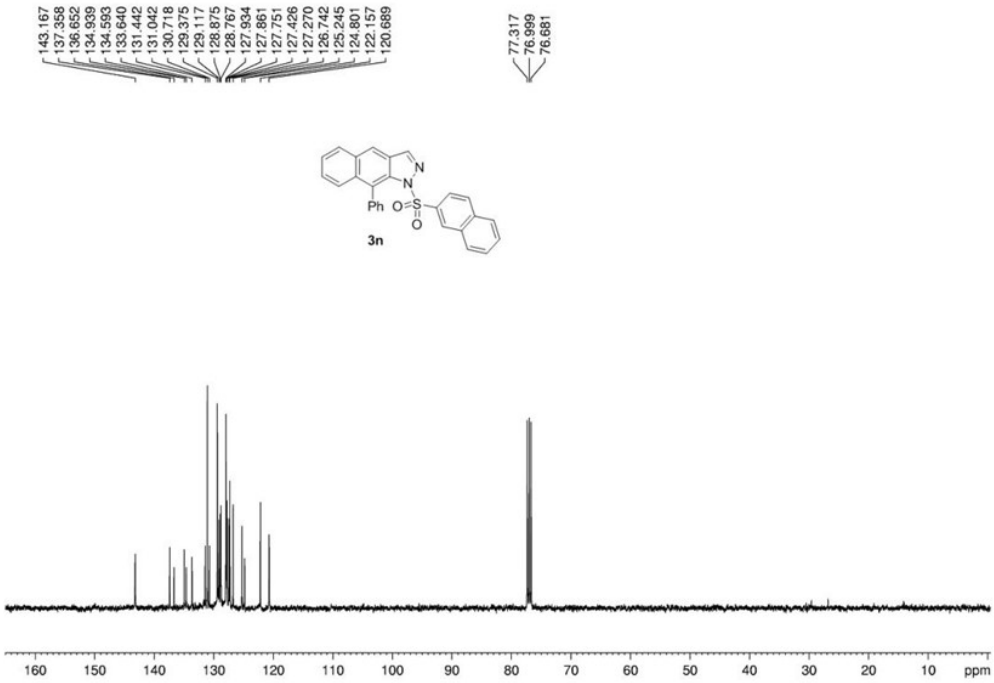
7.949
7.928
7.841
7.822
7.819
7.774
7.755
7.745
7.723
7.628
7.608
7.587
7.566
7.562
7.547
7.529
7.512
7.500
7.482
7.465
7.454
7.452
7.438
7.435
7.418
7.415
7.406
7.402
7.390
7.381
7.370
7.354
7.350
7.228
N
N
Ph
O
S
O
3n
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.99
0.99
1.01
0.97
1.03
1.01
2.02
2.05
1.03
0.96
1.07
0.95
3.02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134.939
134.593
133.640
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131.042
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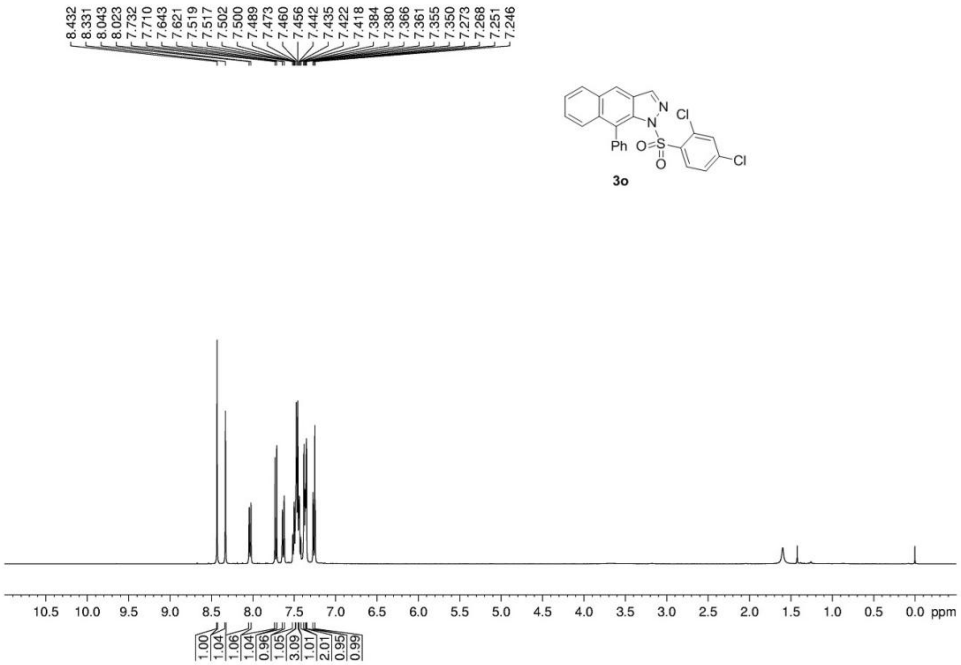
129.375
129.117
128.875
128.767
127.934
127.861
127.751
127.426
127.270
126.742
125.245
124.801
122.157
120.689
77.317
76.999
76.681
N
N
Ph
O
S
O
3n
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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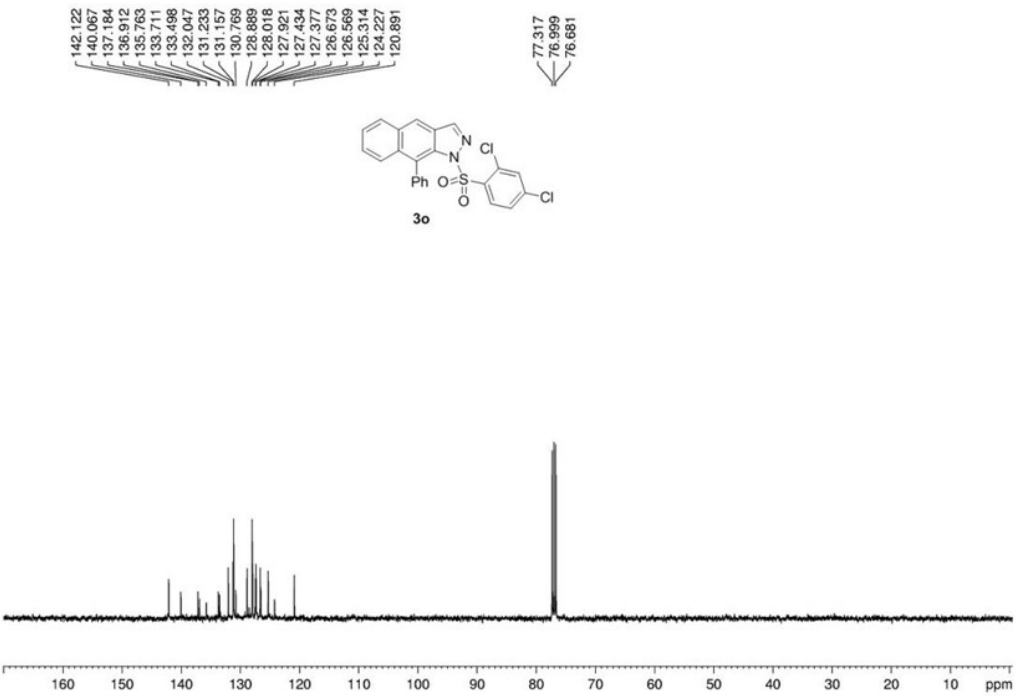
8.023
7.732
7.710
7.643
7.621
7.519
7.517
7.502
7.500
7.489
7.473
7.460
7.456
7.442
7.435
7.422
7.418
7.384
7.380
7.366
7.361
7.355
7.350
7.273
7.268
7.251
7.246
N
N
Cl
Ph
O
S
O
Cl
3o
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.04
1.06
1.04
0.96
1.05
3.09
1.01
2.01
0.95
0.99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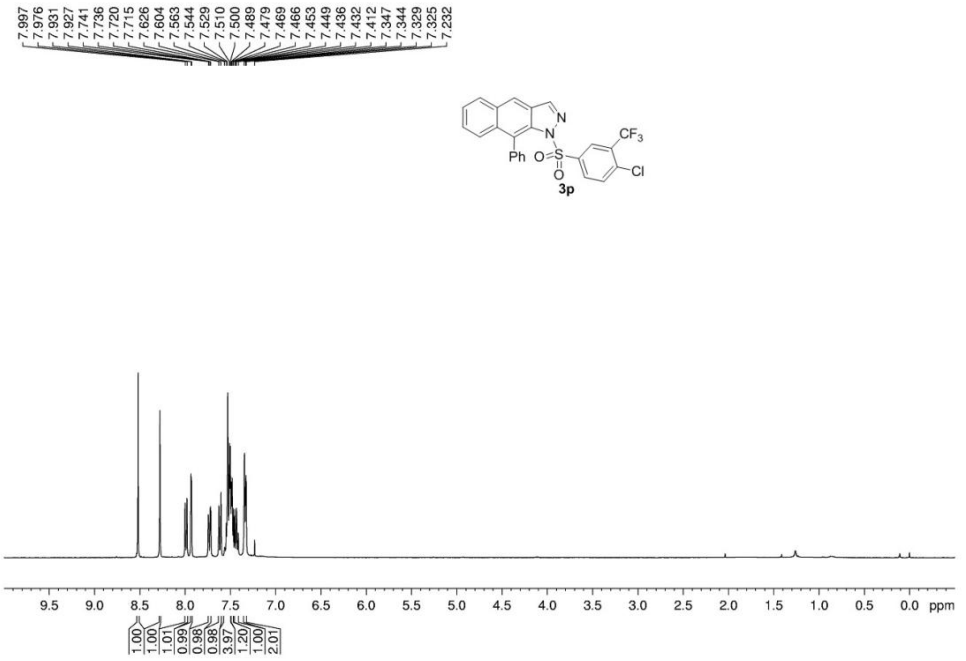
137.184
136.912
135.763
133.711
133.498
132.047
131.233
131.157
130.769
128.889
128.018
127.921
127.434
127.377
126.673
126.569
125.314
124.227
120.891
77.317
76.999
76.681
N
N
Cl
Ph
O
S
O
Cl
3o
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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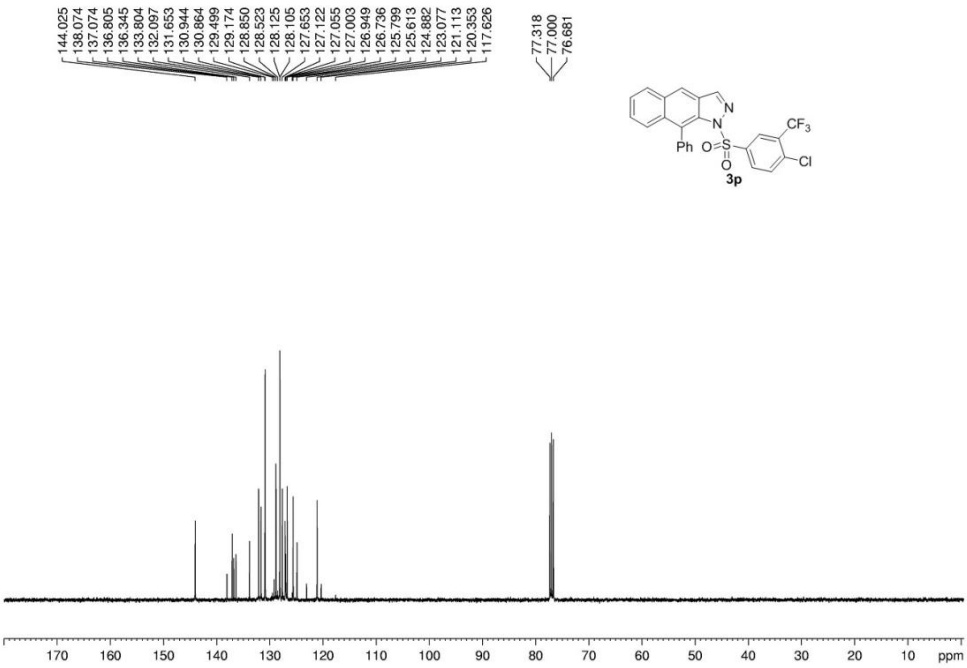
7.976
7.931
7.927
7.741
7.736
7.720
7.715
7.626
7.604
7.563
7.544
7.529
7.510
7.500
7.489
7.479
7.469
7.466
7.453
7.449
7.436
7.432
7.412
7.347
7.344
7.329
7.325
7.232
N
N
CF3
Ph
O
S
O
Cl
3p
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.00
1.01
0.99
0.98
0.98
3.97
1.20
1.00
2.01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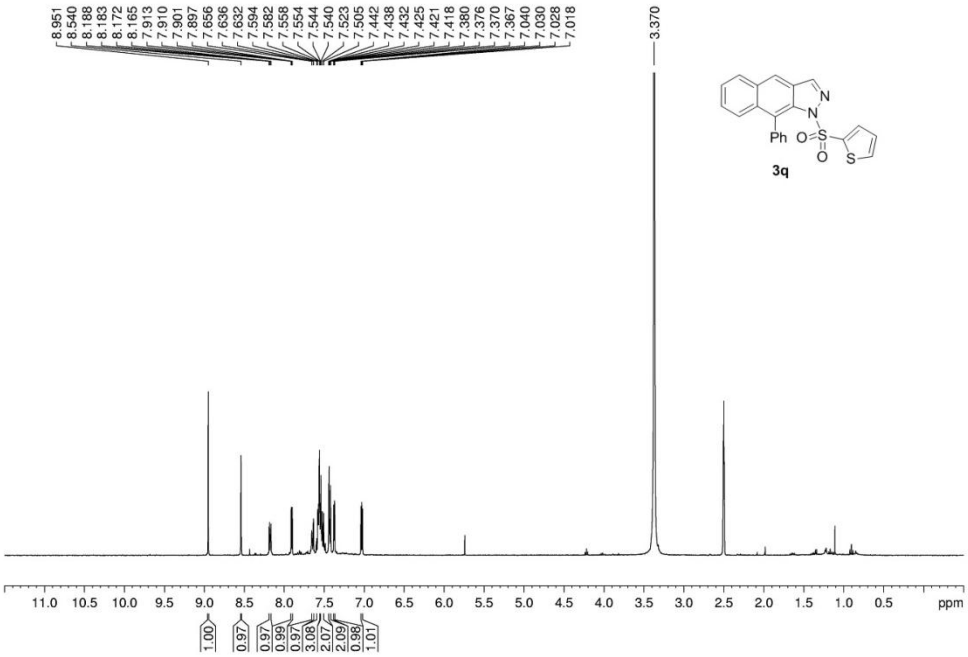
138.074
137.074
136.805
136.345
133.804
132.097
131.653
130.944
130.864
129.499
129.174
128.850
128.523
128.125
128.105
127.653
127.122
127.055
127.003
126.949
126.736
125.799
125.613
124.882
123.077
121.113
120.353
117.626
77.318
77.000
76.681
N
N
CF3
Ph
O
S
O
Cl
3p
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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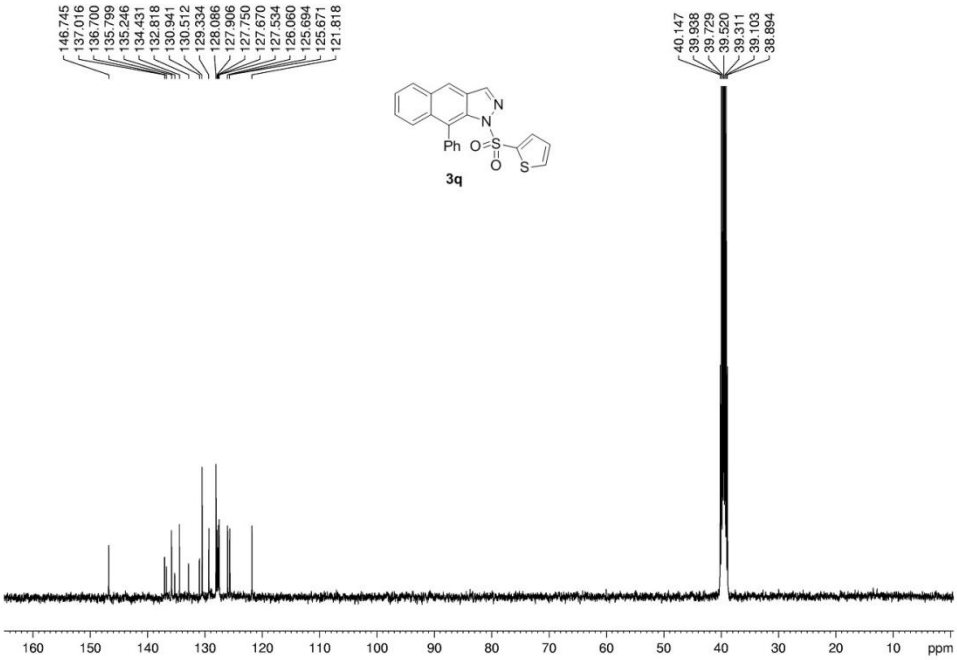
8.540
8.188
8.183
8.172
8.165
7.913
7.910
7.901
7.897
7.656
7.636
7.632
7.594
7.582
7.558
7.554
7.544
7.540
7.523
7.505
7.442
7.438
7.432
7.425
7.421
7.418
7.380
7.376
7.370
7.367
7.040
7.030
7.028
7.018
3.370
N
N
Ph
O
S
O
S
3q
11.0 10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 ppm
1.00
0.97
0.97
0.99
0.97
3.08
2.07
2.09
0.98
1.01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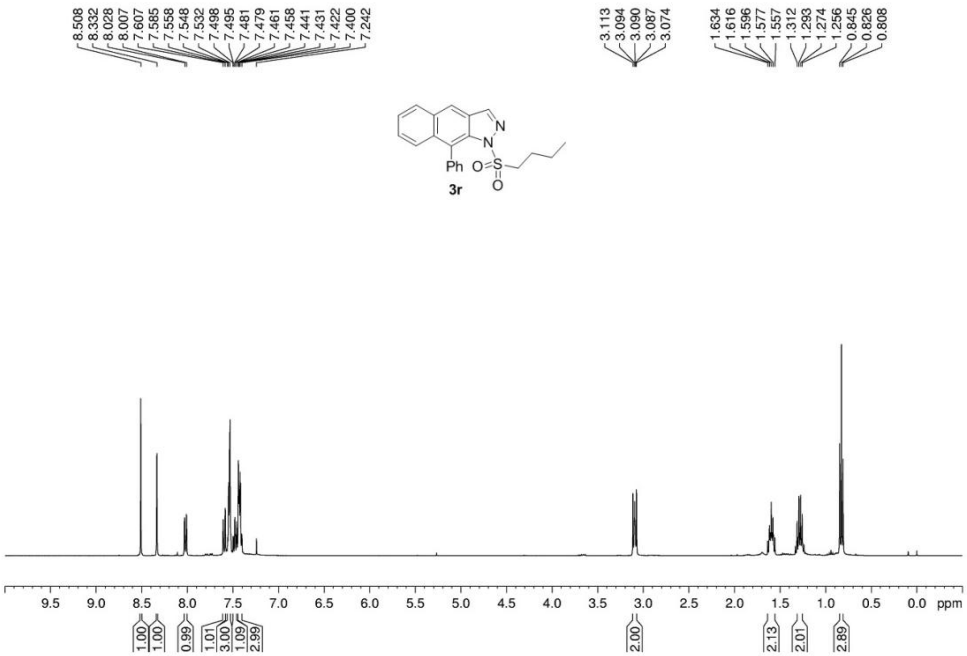
137.016
136.700
135.799
135.246
134.431
132.818
130.941
130.512
129.334
128.086
127.906
127.750
127.670
127.534
126.060
125.694
125.671
121.818
40.147
39.938
39.729
39.520
39.311
39.103
38.894
N
N
Ph
O
S
O
S
3q
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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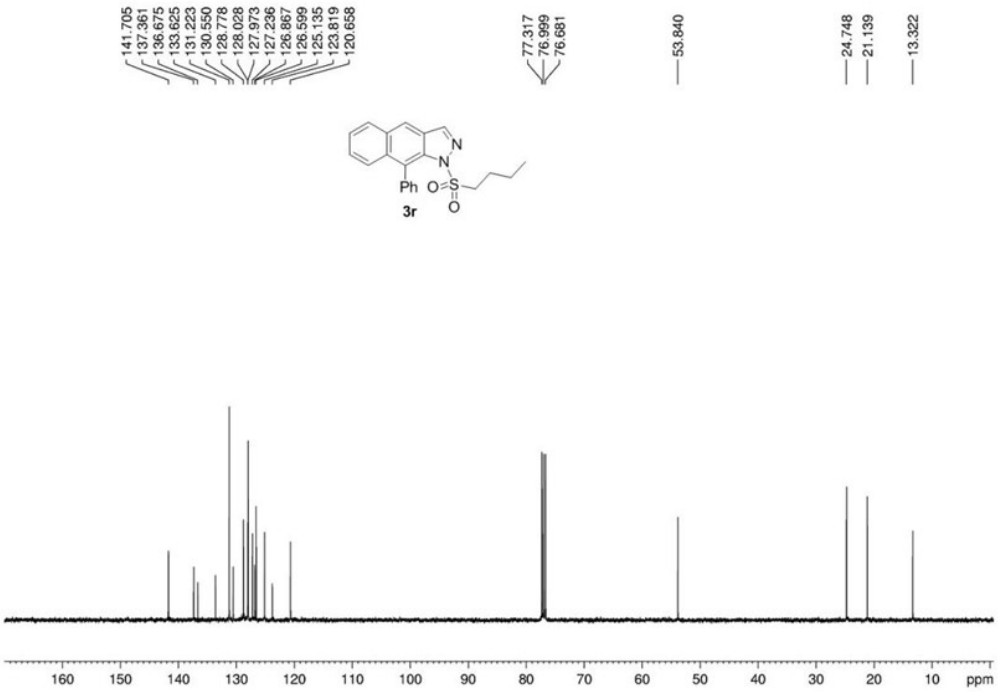
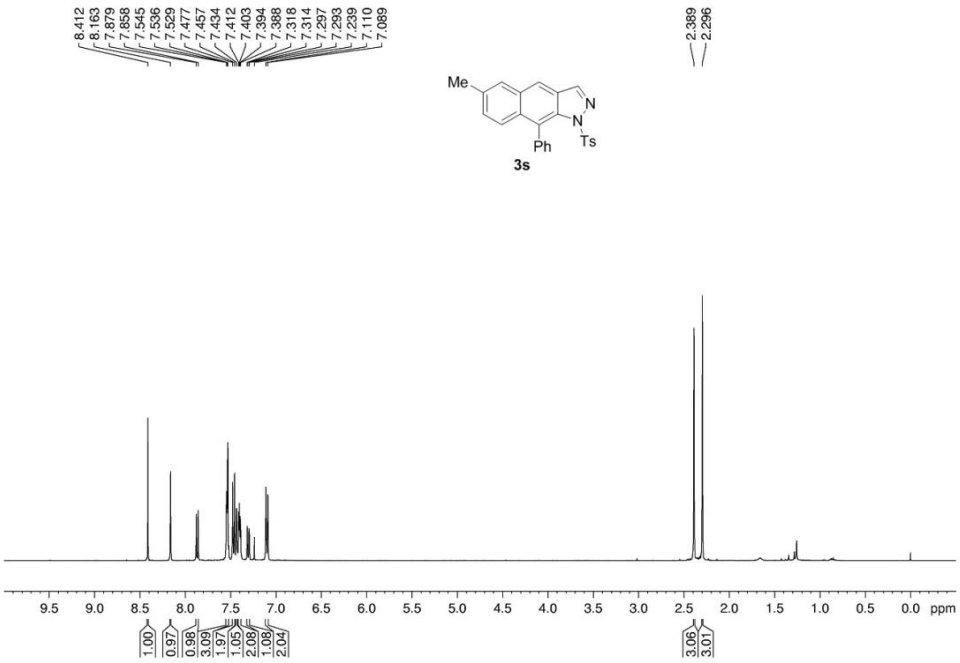
8.332
8.028
8.007
7.607
7.585
7.558
7.548
7.532
7.498
7.495
7.481
7.479
7.461
7.458
7.441
7.431
7.422
7.400
7.242
3.113
3.094
3.090
3.087
3.074
1.634
1.616
1.596
1.577
1.557
1.312
1.293
1.274
1.256
0.845
0.826
0.808
Ph
3r
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
1.00
0.99
1.01
3.00
1.09
2.99
2.00
2.13
2.01
2.89


141.705
137.361
136.675
133.625
131.223
130.550
128.778
128.028
127.973
127.236
126.867
126.599
125.135
123.819
120.658
77.317
76.999
76.681
53.840
24.748
21.139
13.322
Ph
3r
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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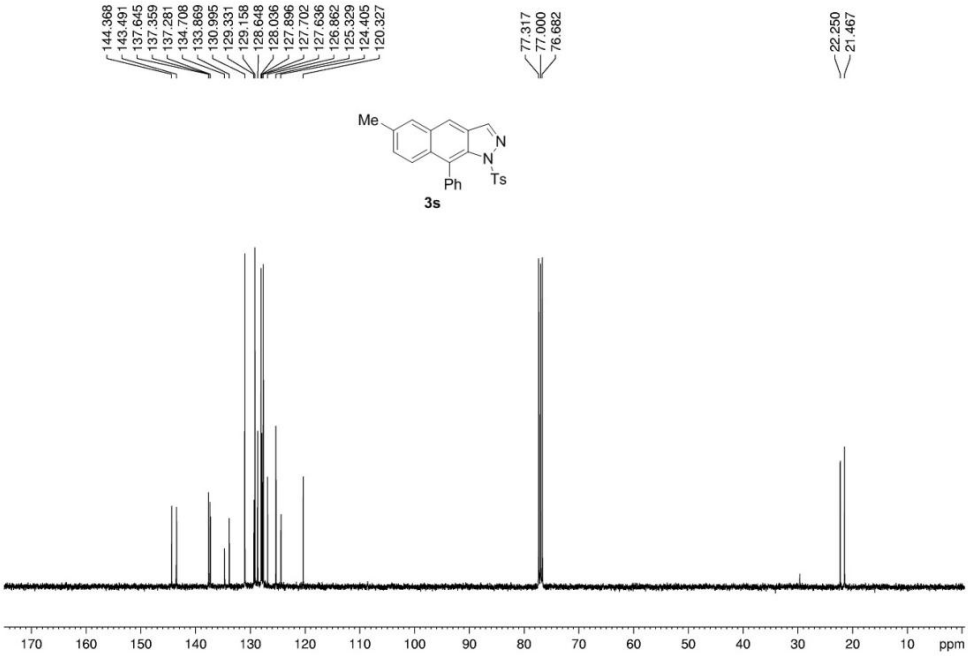
8.163
7.879
7.858
7.545
7.536
7.529
7.477
7.457
7.434
7.412
7.403
7.394
7.388
7.318
7.314
7.297
7.293
7.239
7.110
7.089
2.389
2.296
Me
N
N
Ts
Ph
3s
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.97
0.98
3.09
1.97
1.05
2.08
1.08
2.04
3.06
3.01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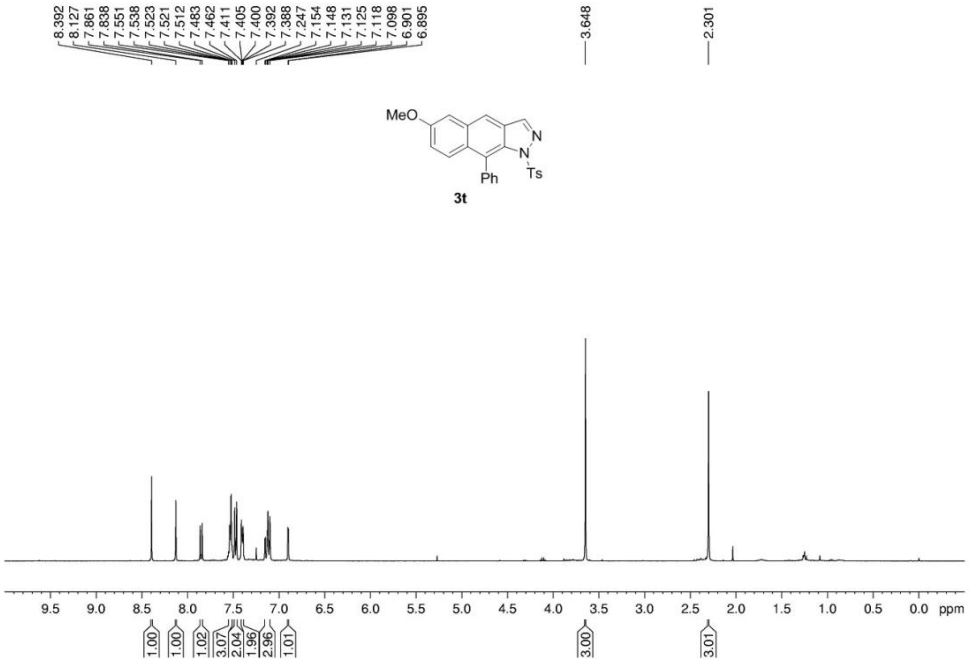
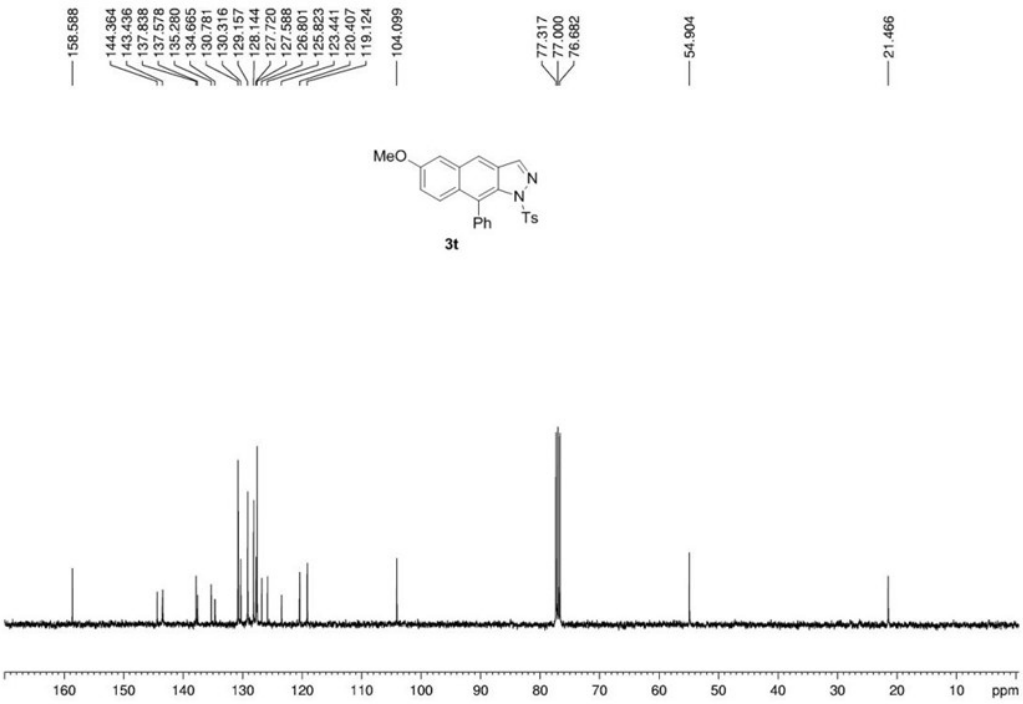
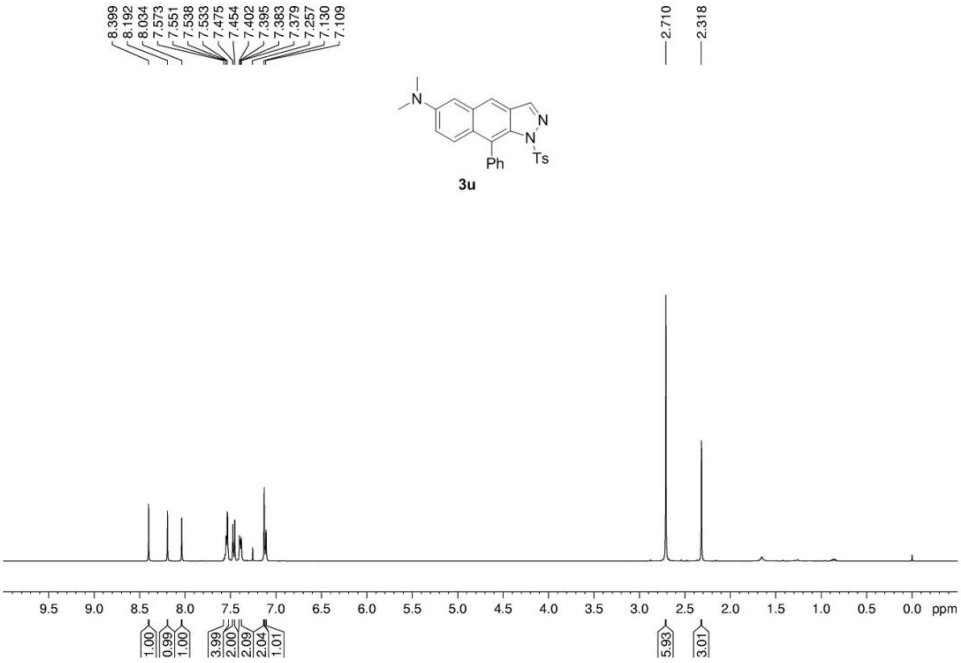
143.491
137.645
137.359
137.281
134.708
133.869
130.995
129.331
129.158
128.648
128.036
127.896
127.702
127.638
126.862
125.329
124.405
120.327
77.317
77.000
76.682
22.250
21.467
Me
N
N
Ts
Ph
3s
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.392
8.127
7.861
7.838
7.551
7.538
7.523
7.521
7.512
7.483
7.462
7.411
7.405
7.400
7.392
7.388
7.247
7.154
7.148
7.131
7.125
7.118
7.098
6.901
6.895
3.648
2.301
MeO
N
N
Ph
Ts
3t
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 ppm
1.00
1.00
1.02
3.07
2.04
1.96
2.96
1.01
3.00
3.01


158.588
144.364
143.436
137.838
137.578
135.280
134.665
130.781
130.316
129.157
128.144
127.720
127.588
126.801
125.823
123.441
120.407
119.124
104.099
77.317
77.000
76.682
54.904
21.466
MeO
N
N
Ph
Ts
3t
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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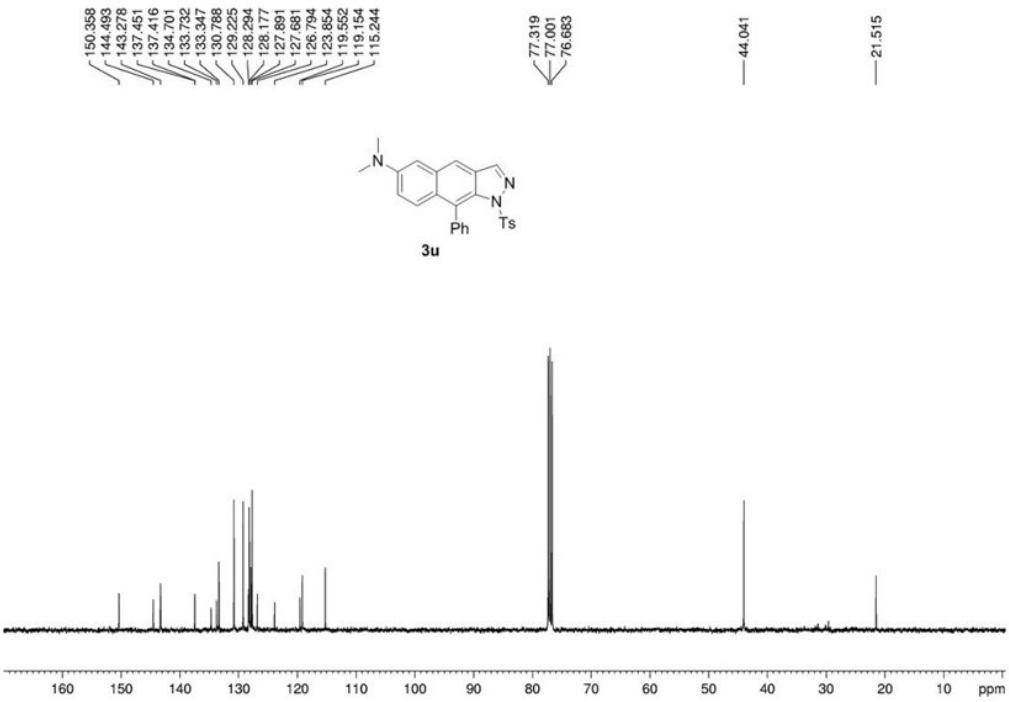
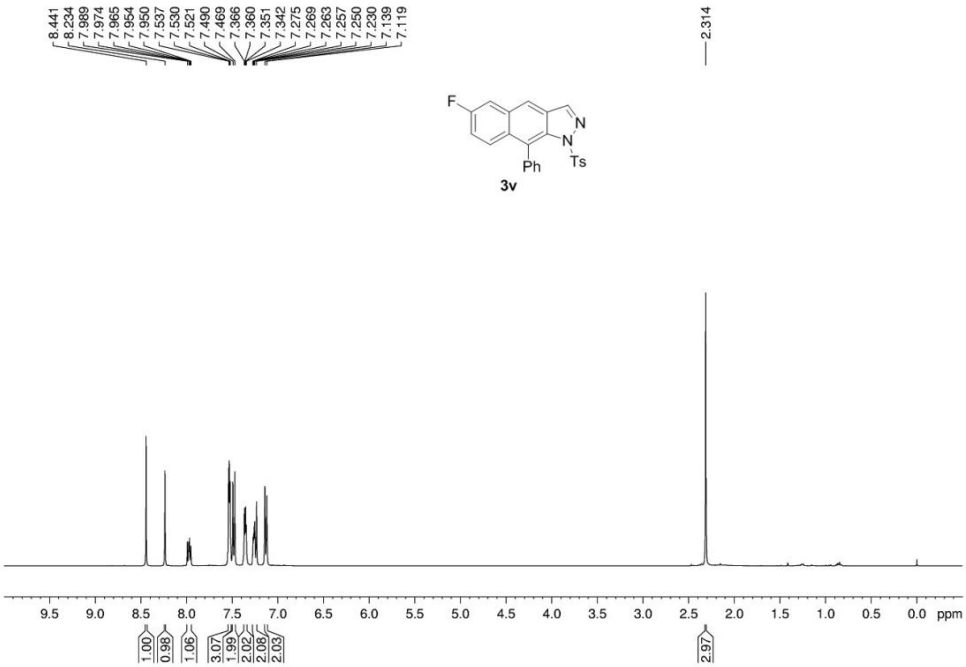
8.192
8.034
7.573
7.551
7.538
7.533
7.475
7.454
7.402
7.395
7.383
7.379
7.257
7.130
7.109
2.710
2.318
N
N
N
Ph
Ts
3u
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.99
1.00
3.99
2.00
2.09
2.04
1.01
5.93
3.01


150.358
144.493
143.278
137.451
137.416
134.701
133.732
133.347
130.788
129.225
128.294
128.177
127.891
127.681
126.794
123.654
119.552
119.154
115.244
77.319
77.001
76.683
44.041
21.515
N
N
N
Ph
Ts
3u
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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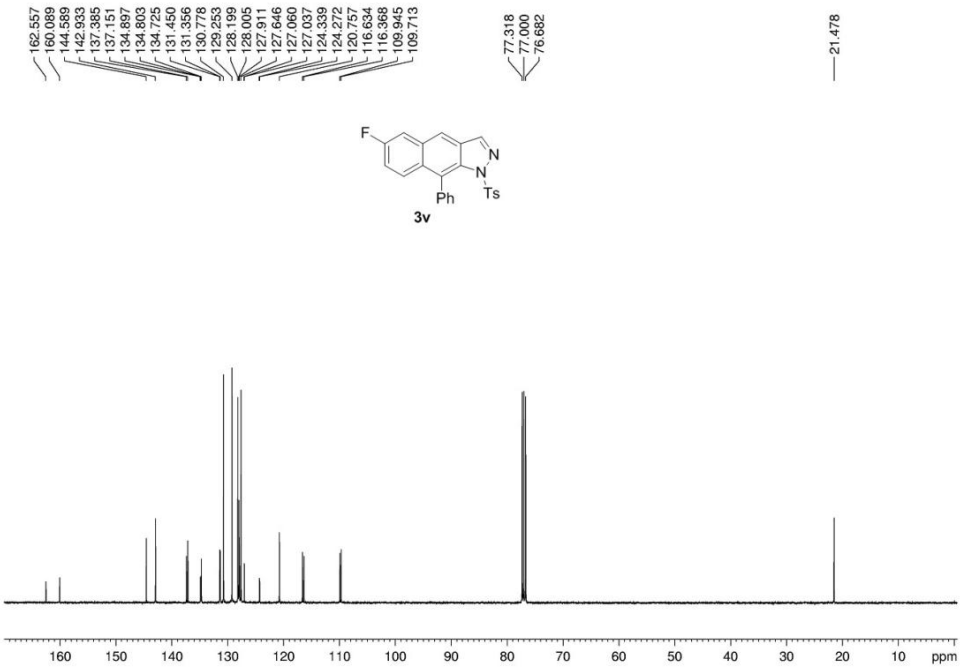
8.234
7.989
7.974
7.965
7.954
7.950
7.537
7.530
7.521
7.490
7.469
7.366
7.360
7.351
7.342
7.275
7.269
7.263
7.257
7.250
7.230
7.139
7.119
2.314
F
N
N
Ts
Ph
3v
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.99
1.06
3.07
1.99
2.02
2.08
2.03
2.97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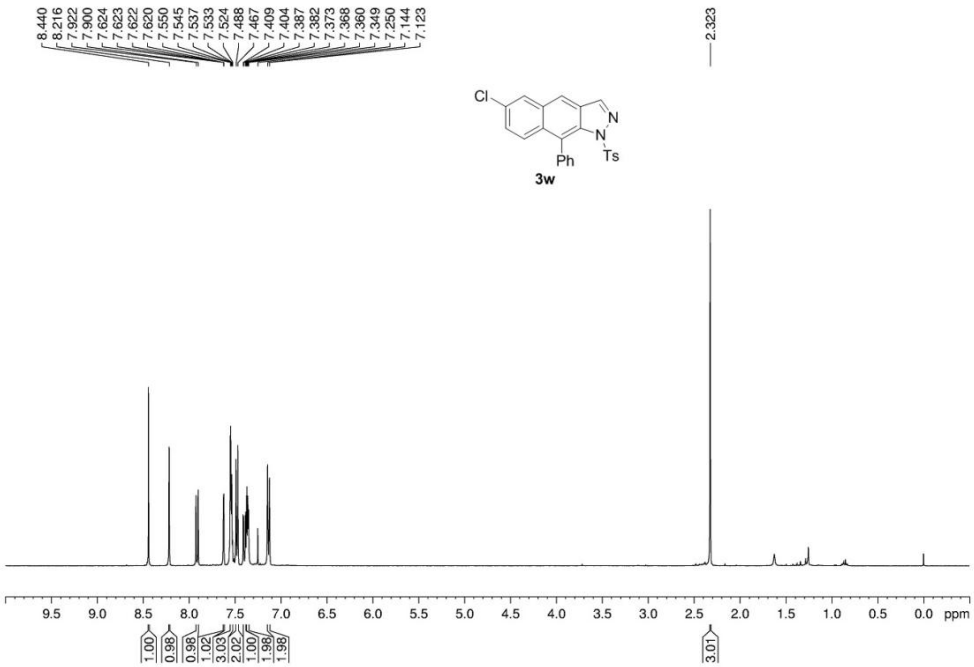
144.589
142.933
137.385
137.151
134.897
134.803
134.725
131.450
131.356
130.778
129.253
128.199
128.005
127.911
127.646
127.060
127.037
124.339
124.272
120.757
116.634
116.368
109.945
109.713
77.318
77.000
76.682
21.478
F
N
N
Ts
Ph
3v
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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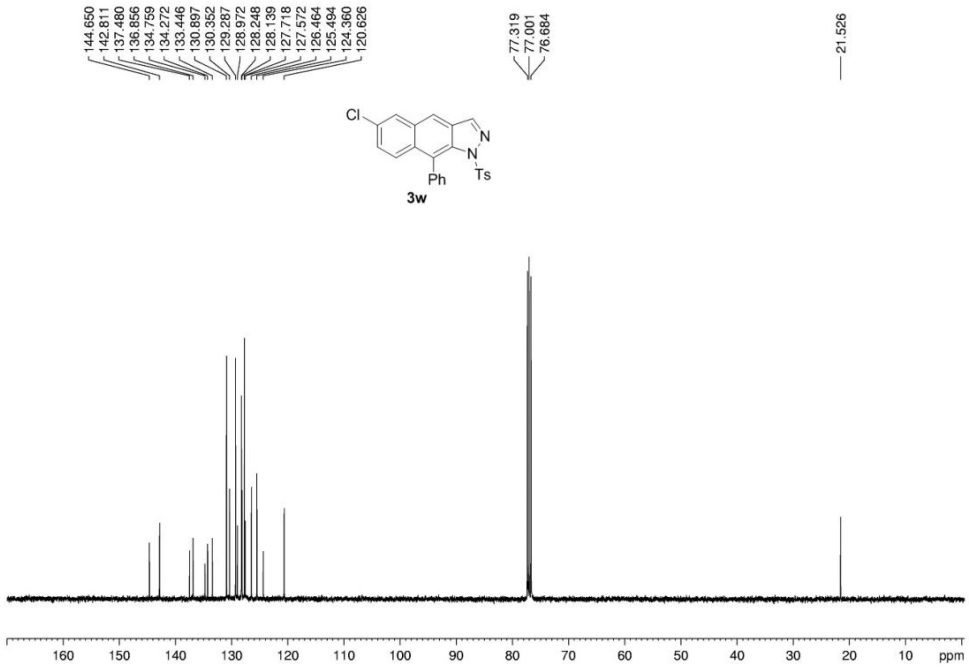
7.900
7.624
7.623
7.622
7.620
7.550
7.545
7.537
7.533
7.524
7.488
7.467
7.409
7.404
7.387
7.382
7.373
7.368
7.360
7.349
7.250
7.144
7.123
2.323
Cl
N
N
Ts
Ph
3w
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.98
0.98
1.02
3.03
2.02
1.00
1.98
1.98
3.01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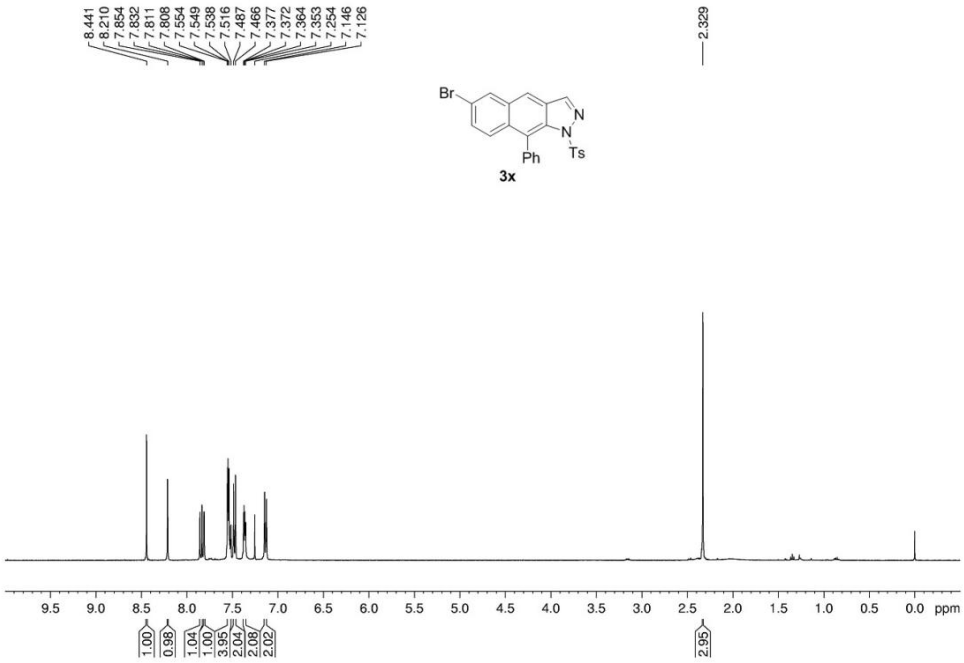
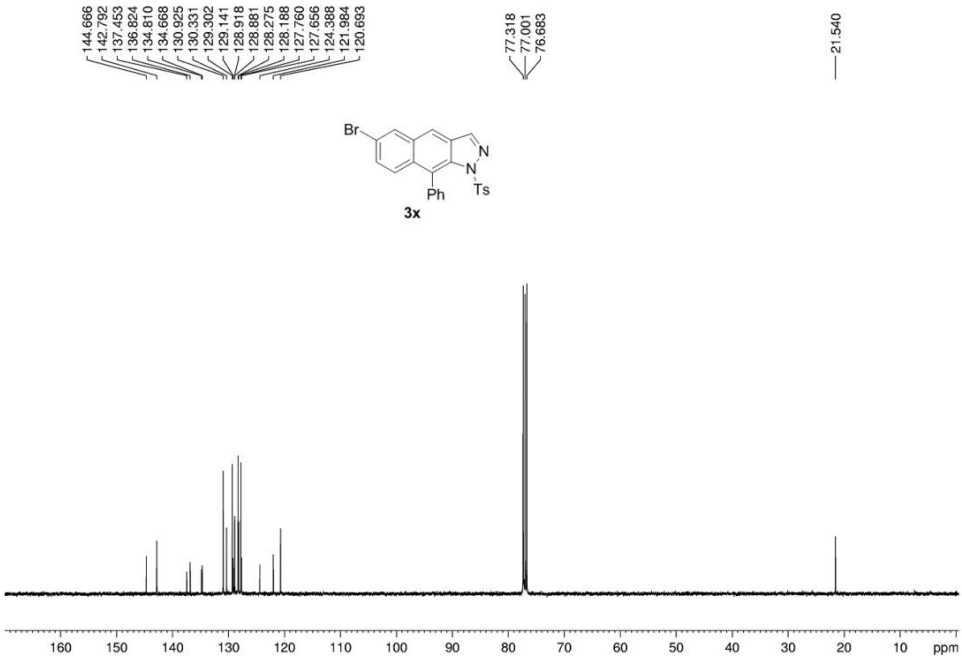
142.811
137.480
136.856
134.759
134.272
133.446
130.897
130.352
129.287
128.972
128.248
128.139
127.718
127.572
126.464
125.494
124.360
120.626
77.319
77.001
76.684
21.526
Cl
N
N
Ts
Ph
3w
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


8.441
8.210
7.854
7.832
7.811
7.808
7.554
7.549
7.538
7.516
7.487
7.466
7.377
7.372
7.364
7.353
7.254
7.146
7.126
2.329
Br
N
N
Ts
Ph
3x
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 ppm
1.00
0.98
1.04
1.00
3.95
2.04
2.08
2.02
2.95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137.453
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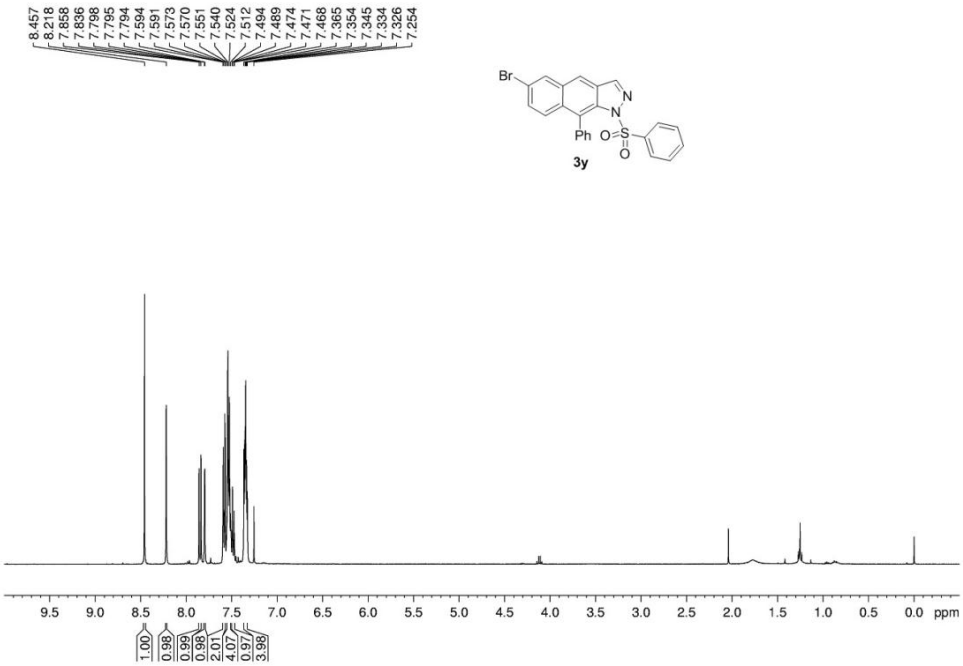
134.810
134.668
130.925
130.331
129.302
129.141
128.918
128.881
128.275
128.188
127.760
127.656
124.388
121.984
120.693
77.318
77.001
76.683
21.540
Br
N
N
Ts
Ph
3x
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.218
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7.836
7.798
7.795
7.794
7.594
7.591
7.573
7.570
7.551
7.540
7.524
7.512
7.494
7.489
7.474
7.471
7.468
7.365
7.354
7.345
7.334
7.326
7.254
Br
N
N
Ph
O
S
O
3y
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 ppm
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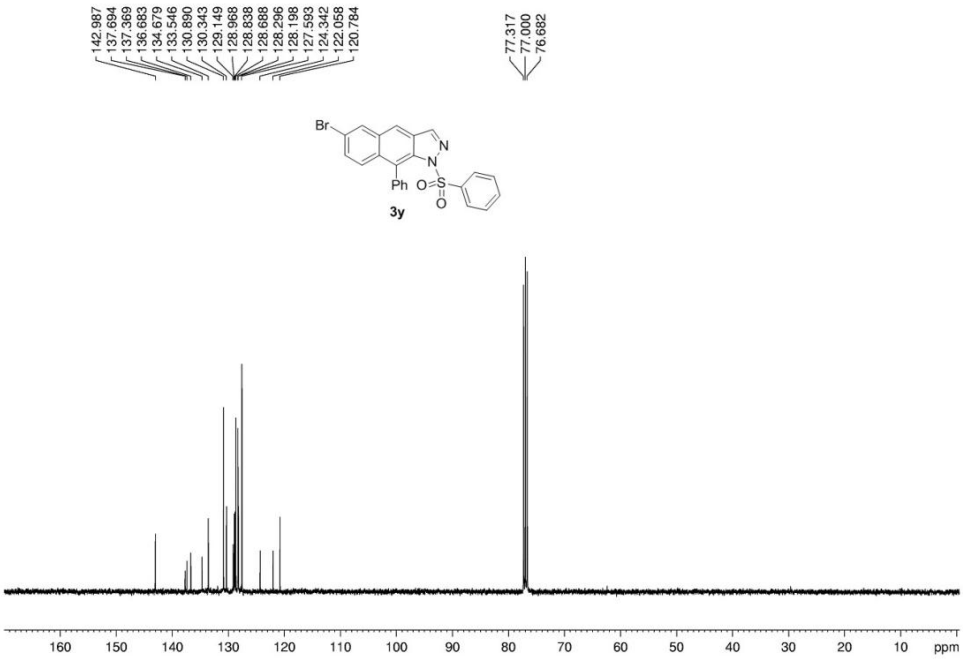
0.98
0.99
0.98
2.01
4.07
0.97
3.98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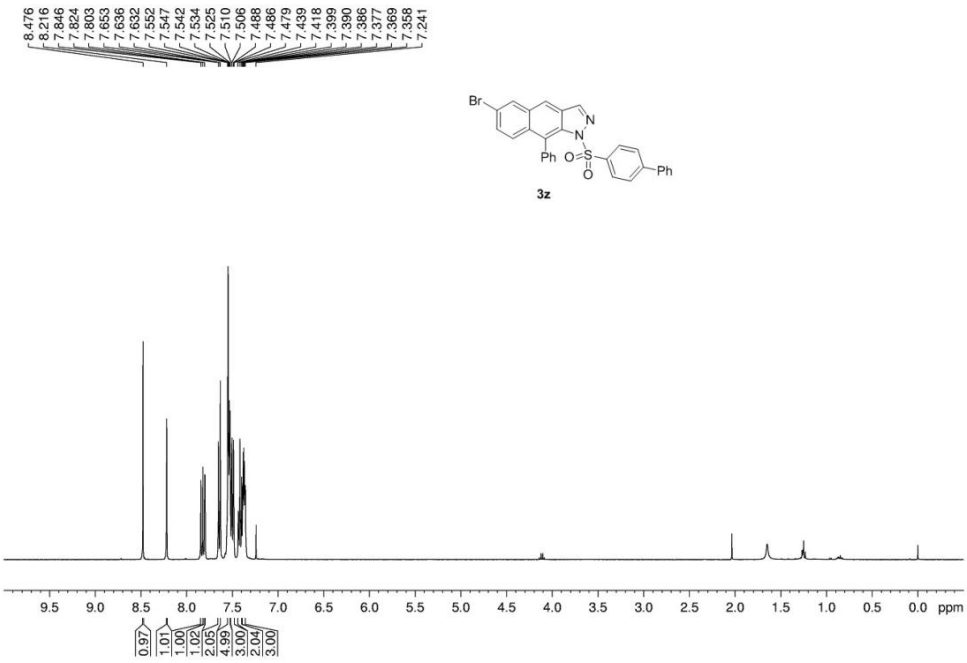
137.369
136.683
134.679
133.546
130.890
130.343
129.149
128.968
128.838
128.688
128.296
128.198
127.593
124.342
122.058
120.784
77.317
77.000
76.682
Br
N
N
Ph
O
S
O
3y
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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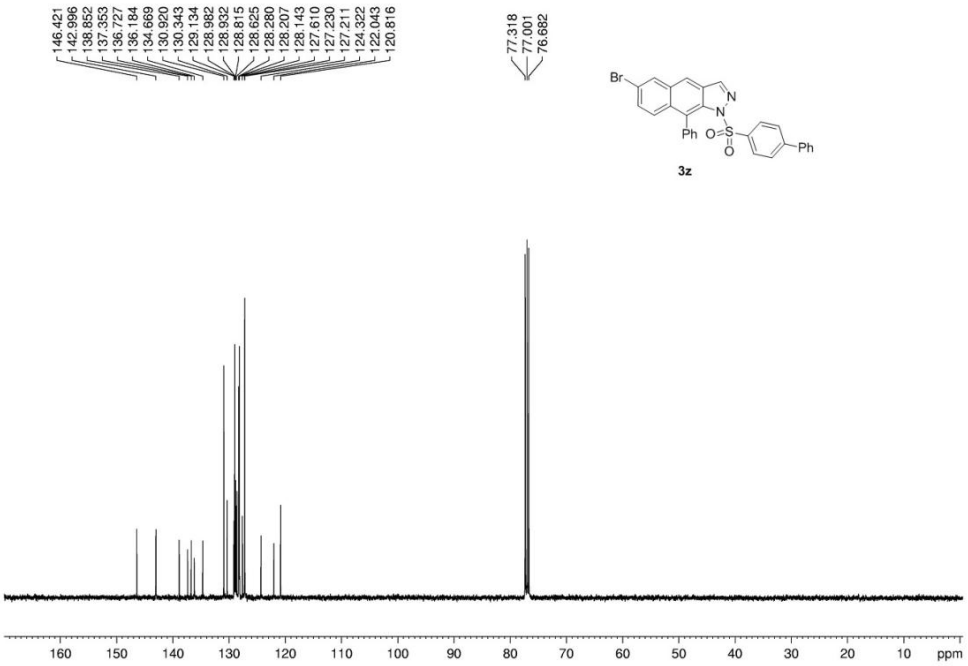
7.846
7.824
7.803
7.653
7.636
7.632
7.552
7.547
7.542
7.534
7.525
7.510
7.506
7.488
7.486
7.479
7.439
7.418
7.399
7.390
7.386
7.377
7.369
7.358
7.241
Br
N
N
Ph
O
S
O
Ph
3z
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
0.97
1.01
1.00
1.02
2.05
4.99
3.00
2.04
3.00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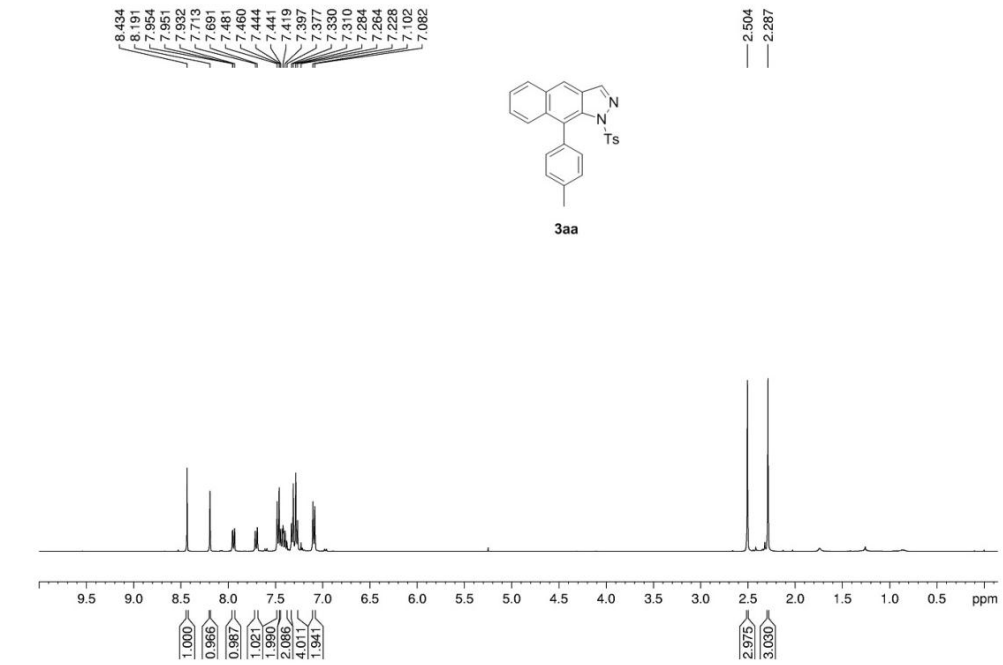
142.996
138.852
137.353
136.727
136.184
134.669
130.920
130.343
129.134
128.982
128.932
128.815
128.625
128.280
128.207
128.143
127.610
127.230
127.211
124.322
122.043
120.816
77.318
77.001
76.682
Br
N
N
Ph
O
S
O
Ph
3z
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.191
7.954
7.951
7.932
7.713
7.691
7.481
7.460
7.444
7.441
7.419
7.397
7.377
7.330
7.310
7.284
7.264
7.228
7.102
7.082
2.504
2.287
N
N
Ts
3aa
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 ppm
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0.966
0.987
1.021
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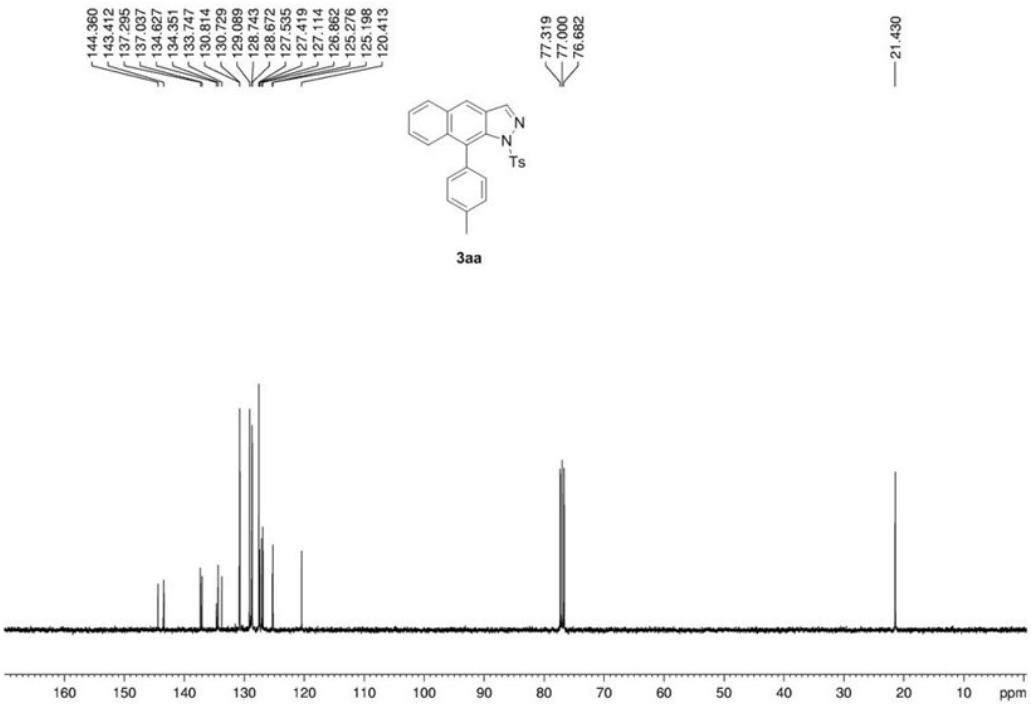
2.086
4.011
1.941
2.975
3.030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143.412
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137.037
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134.351
133.747
130.814
130.729
129.089
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128.672
127.535
127.419
127.114
126.862
125.276
125.198
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77.319
77.000
76.682
21.430
N
N
Ts
3aa
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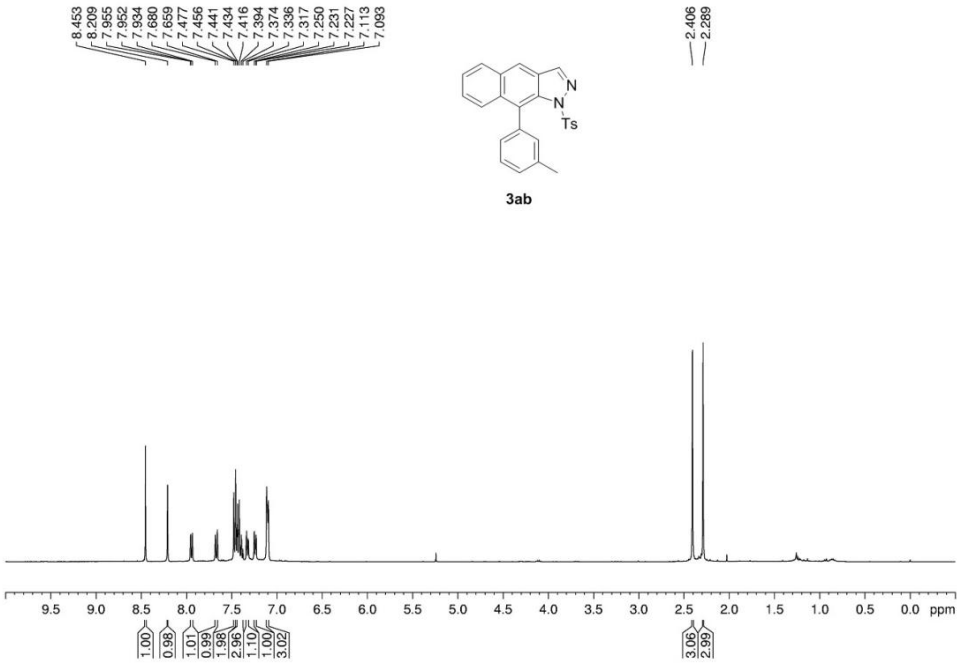
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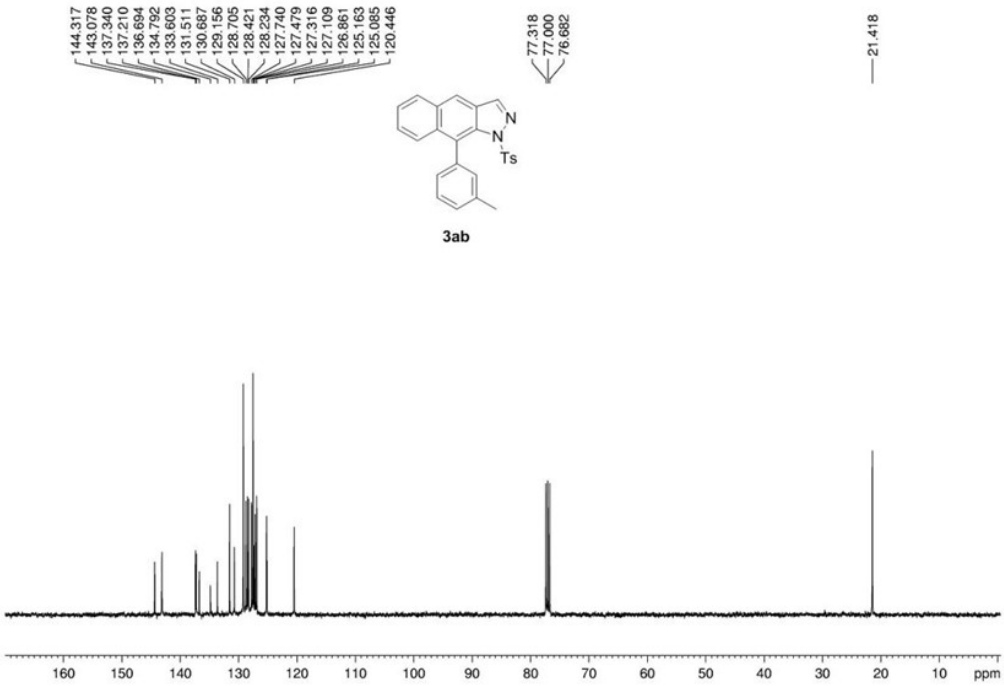
8.209
7.955
7.952
7.934
7.680
7.659
7.477
7.456
7.441
7.434
7.416
7.394
7.374
7.336
7.317
7.250
7.231
7.227
7.113
7.093
2.406
2.289
N
N
Ts
3ab
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.98
1.01
0.99
1.98
2.96
1.10
1.00
3.02
3.06
2.99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134.792
133.603
131.511
130.687
129.156
128.705
128.421
128.234
127.740
127.479
127.316
127.109
126.861
125.163
125.085
120.446
77.318
77.000
76.682
21.418
N
N
Ts
3ab
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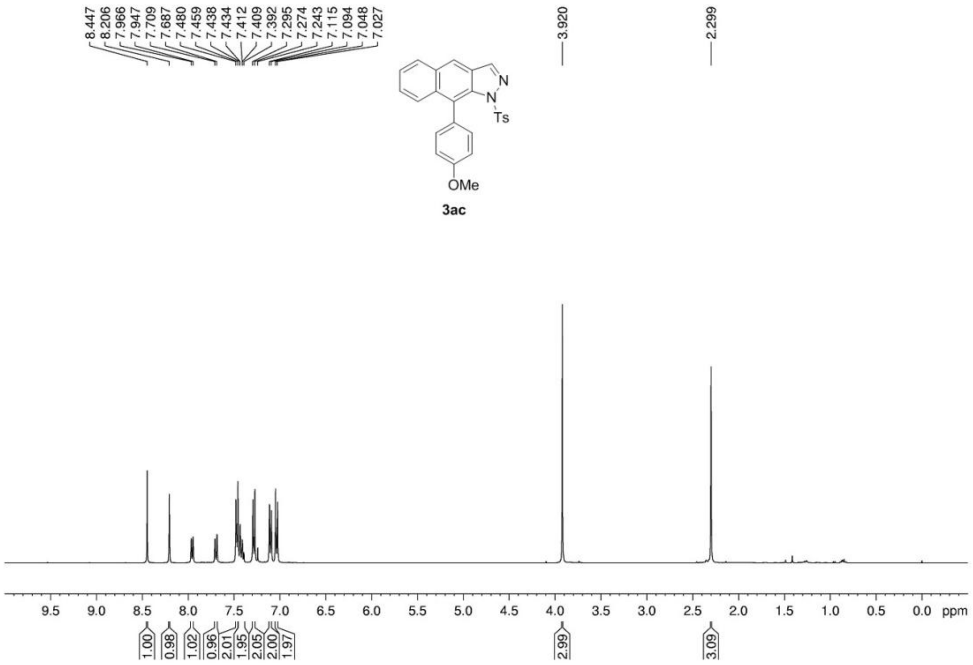
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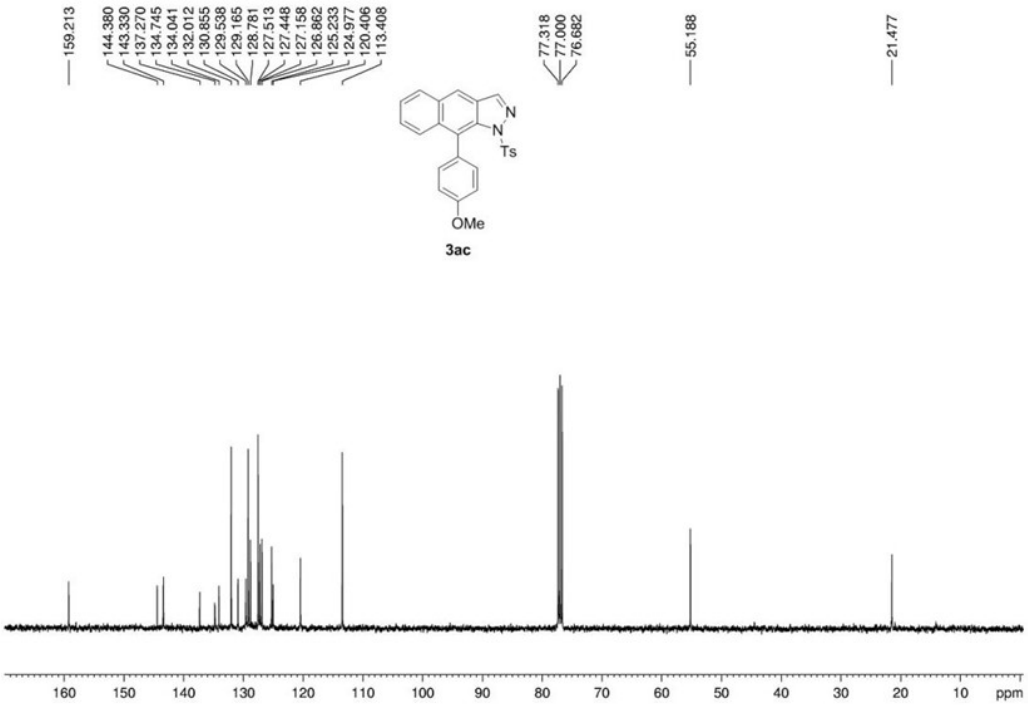
8.206
7.966
7.947
7.709
7.687
7.480
7.459
7.438
7.434
7.412
7.409
7.392
7.295
7.274
7.243
7.115
7.094
7.048
7.027
3.920
2.299
N
N
Ts
OMe
3ac
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.98
1.02
0.96
2.01
1.95
2.05
2.00
1.97
2.99
3.09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144.380
143.330
137.270
134.745
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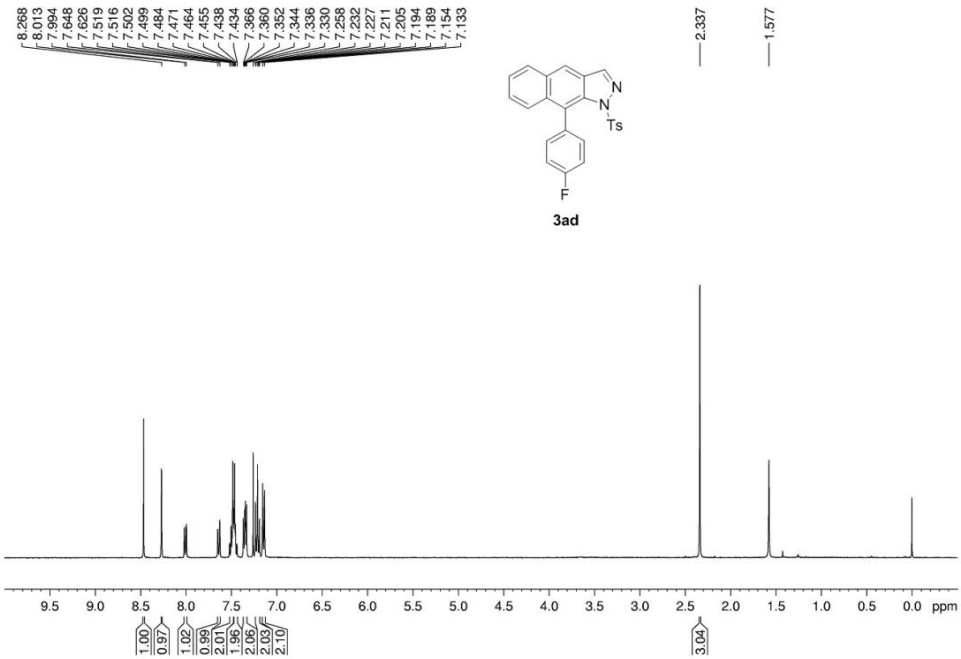
132.012
130.855
129.538
129.165
128.781
127.513
127.448
127.158
126.862
125.233
124.977
120.406
113.408
77.318
77.000
76.682
55.188
21.477
N
N
Ts
OMe
3ac
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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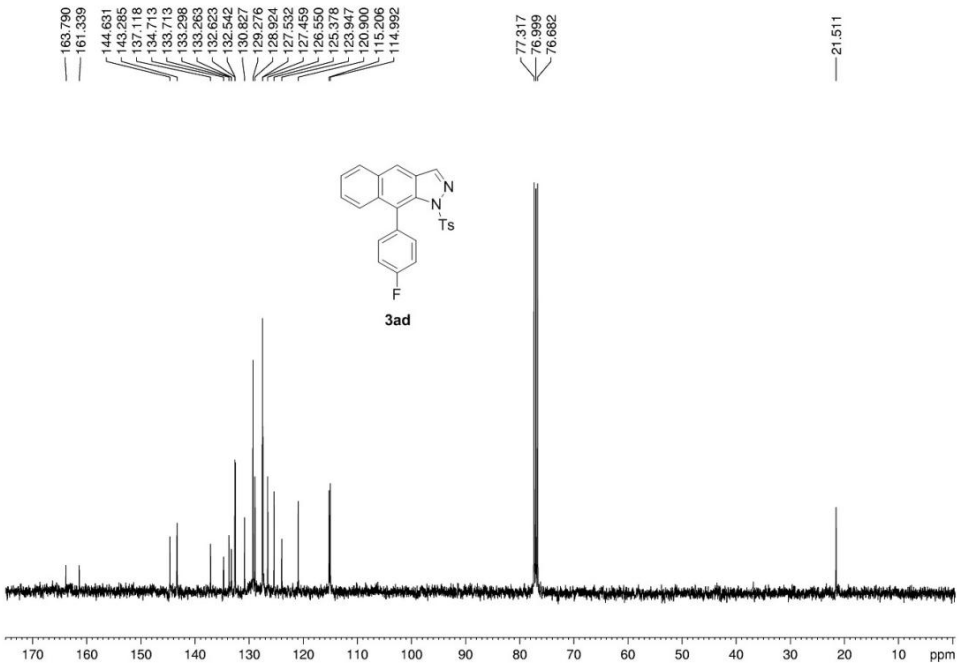
8.013
7.994
7.648
7.626
7.519
7.516
7.502
7.499
7.484
7.471
7.464
7.455
7.438
7.434
7.366
7.360
7.352
7.344
7.336
7.330
7.258
7.232
7.227
7.211
7.205
7.194
7.189
7.154
7.133
2.337
1.577
N
N
Ts
F
3ad
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.97
1.02
0.99
2.01
1.96
2.06
2.03
2.10
3.04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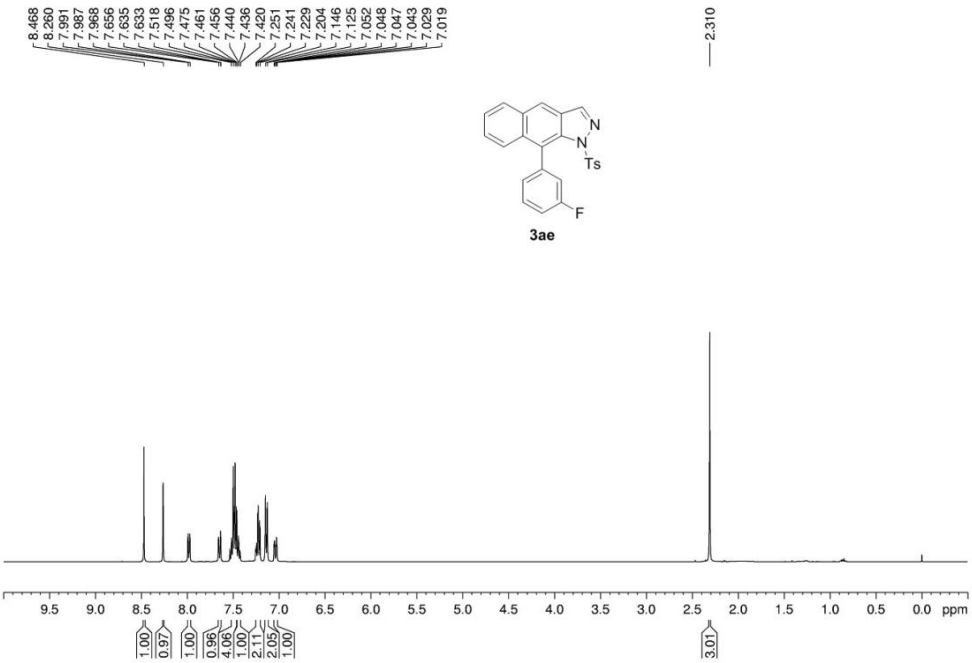
161.339
144.631
143.285
137.118
134.713
133.713
133.298
133.263
132.623
132.542
130.827
129.276
128.924
127.532
127.459
126.550
125.378
123.947
120.900
115.206
114.992
77.317
76.999
76.682
21.511
N
N
Ts
F
3ad
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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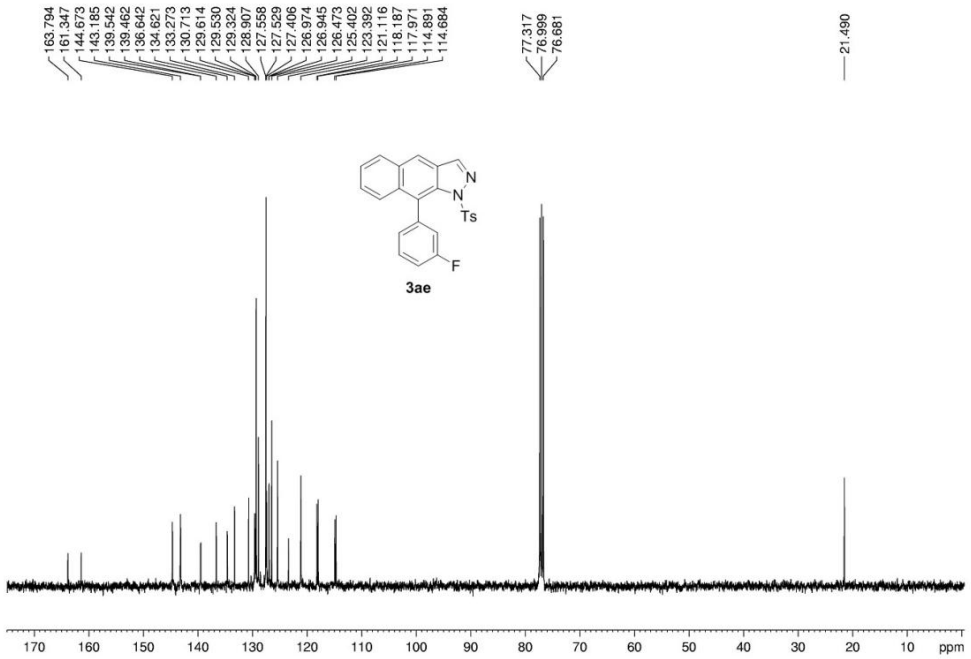
8.260
7.991
7.987
7.968
7.656
7.635
7.633
7.518
7.496
7.475
7.461
7.456
7.440
7.436
7.420
7.251
7.241
7.229
7.204
7.146
7.125
7.052
7.048
7.047
7.043
7.029
7.019
2.310
N
N
Ts
F
3ae
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.00
0.97
1.00
0.96
4.06
1.00
2.11
2.05
1.00
3.01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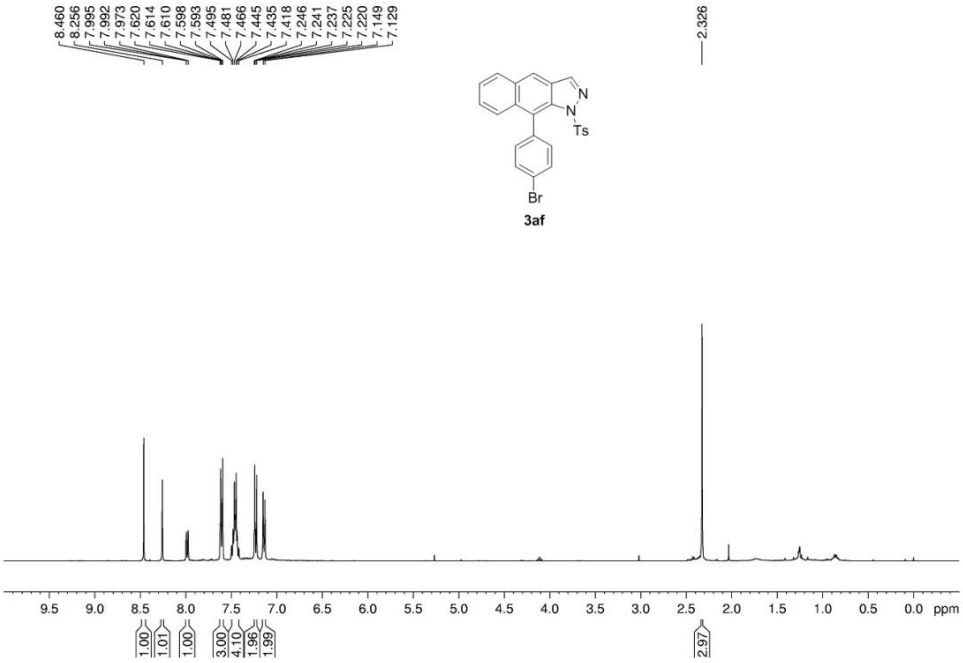
144.673
143.185
139.542
138.462
136.642
134.621
133.273
130.713
129.614
129.530
129.324
128.907
127.558
127.529
127.406
126.974
126.945
126.473
125.402
123.392
121.116
118.187
117.971
114.891
114.684
77.317
76.999
76.681
21.490
N
N
Ts
F
3ae
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.256
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7.992
7.973
7.620
7.614
7.610
7.598
7.593
7.495
7.481
7.466
7.445
7.435
7.418
7.246
7.241
7.237
7.225
7.220
7.149
7.129
2.326
N
N
Ts
Br
3af
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 ppm
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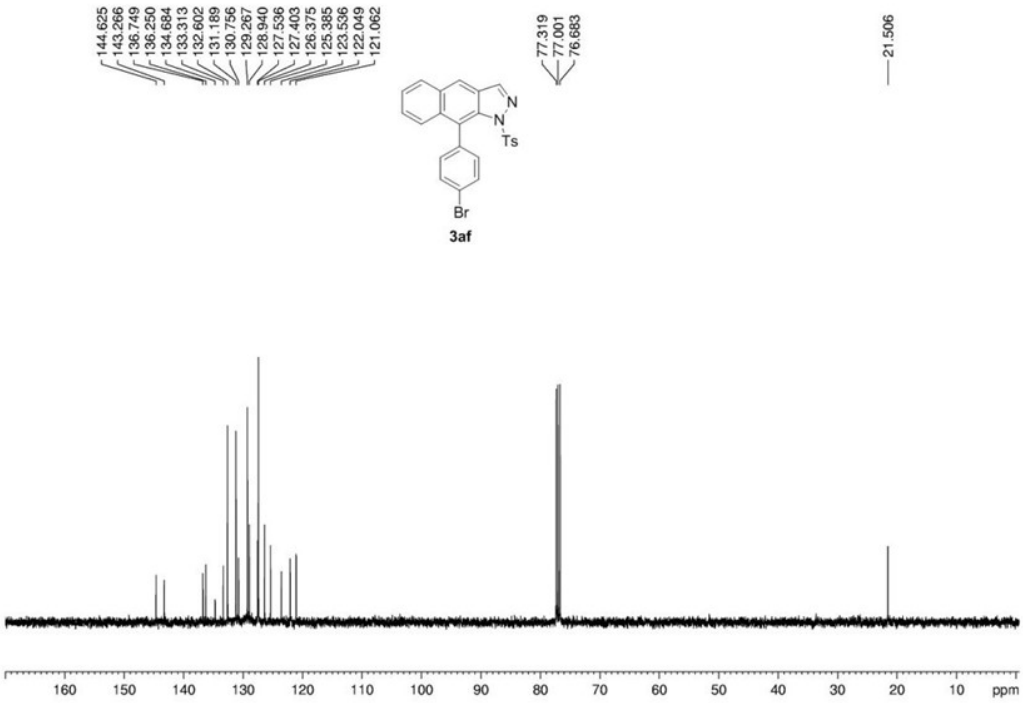
1.01
1.00
3.00
4.10
1.96
1.99
2.97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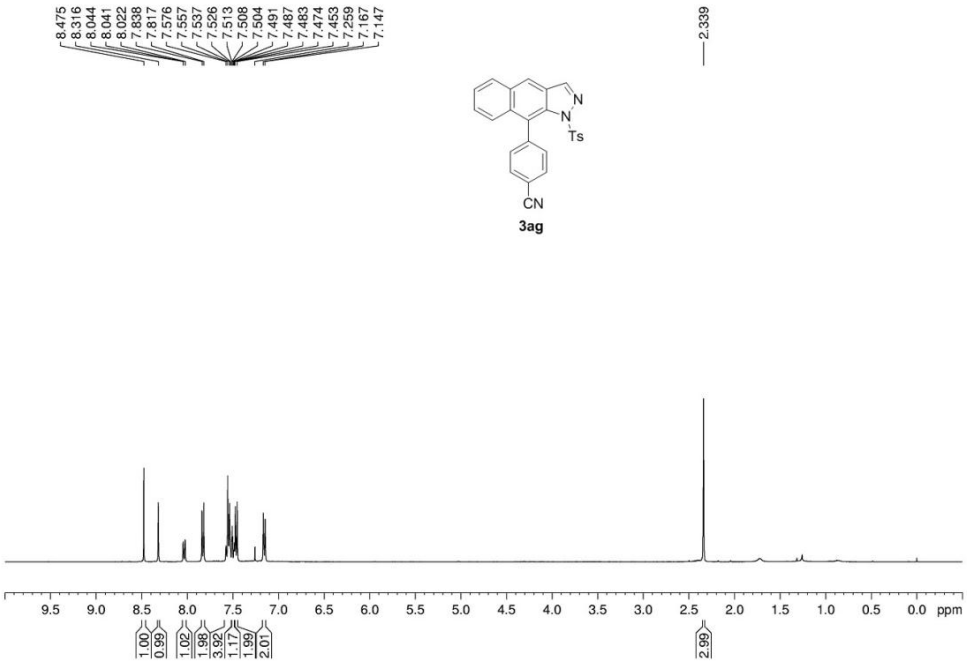
143.266
136.749
136.250
134.684
133.313
132.602
131.189
130.756
129.267
128.940
127.536
127.403
126.375
125.385
123.536
122.049
121.062
77.319
77.001
76.683
21.506
N
N
Ts
Br
3af
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.041
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7.817
7.576
7.557
7.537
7.526
7.513
7.508
7.504
7.491
7.487
7.483
7.474
7.453
7.259
7.167
7.147
2.339
N
N
Ts
CN
3ag
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 ppm
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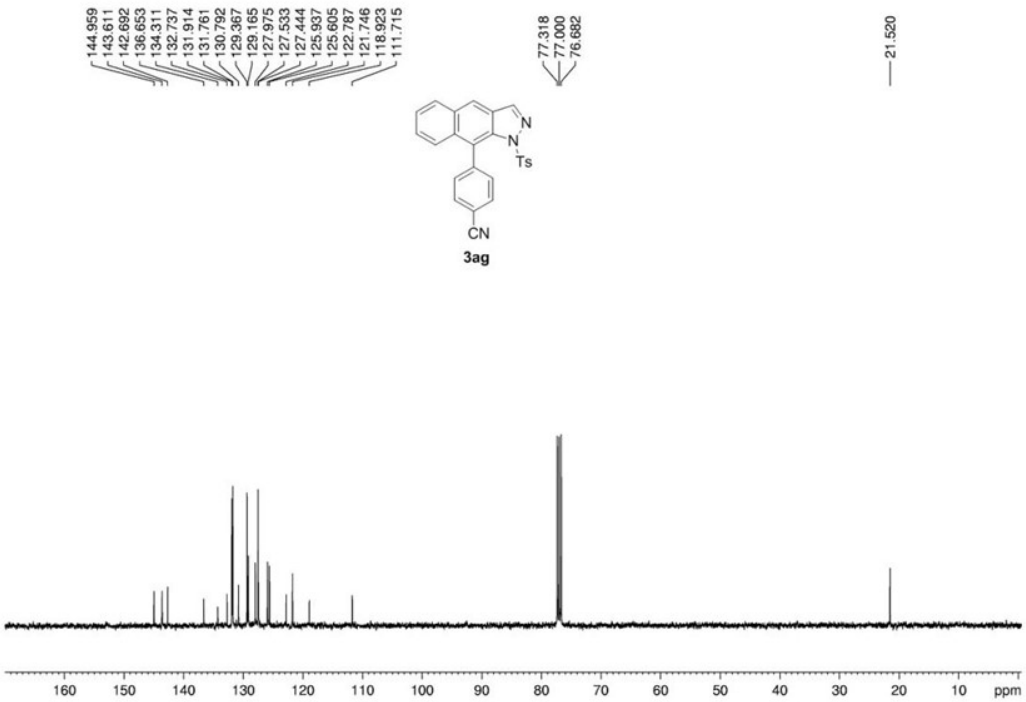
0.99
1.02
1.98
3.92
1.17
1.99
2.01
2.99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142.692
136.653
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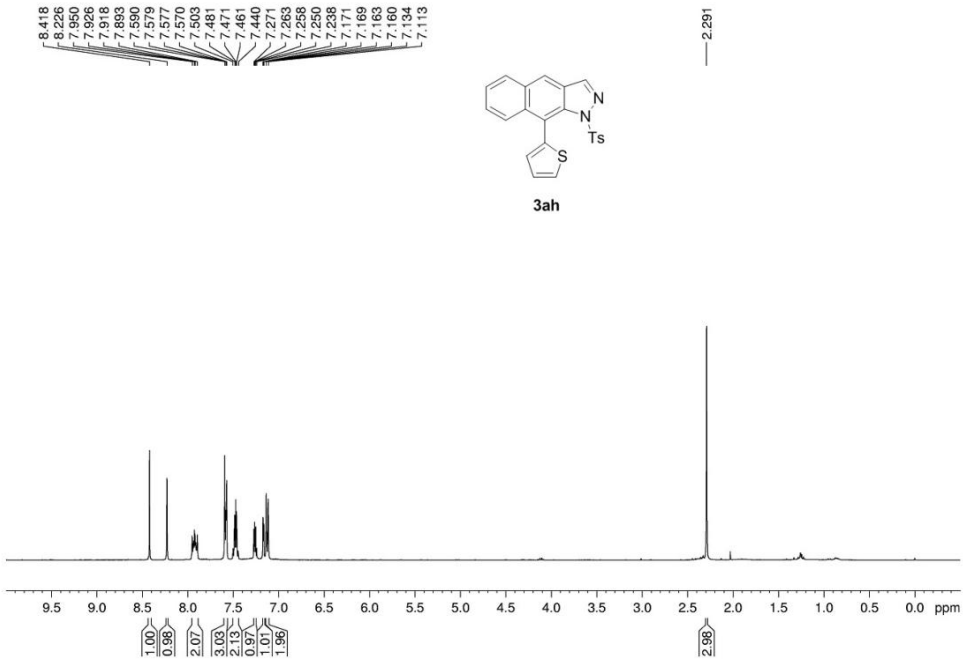
132.737
131.914
131.761
130.792
129.387
129.165
127.975
127.533
127.444
125.937
125.605
122.787
121.746
118.923
111.715
77.318
77.000
76.682
21.520
N
N
Ts
CN
3ag
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.579
7.577
7.570
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7.481
7.471
7.461
7.440
7.271
7.263
7.258
7.250
7.238
7.171
7.169
7.163
7.160
7.134
7.113
2.291
N
N
Ts
S
3ah
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 ppm
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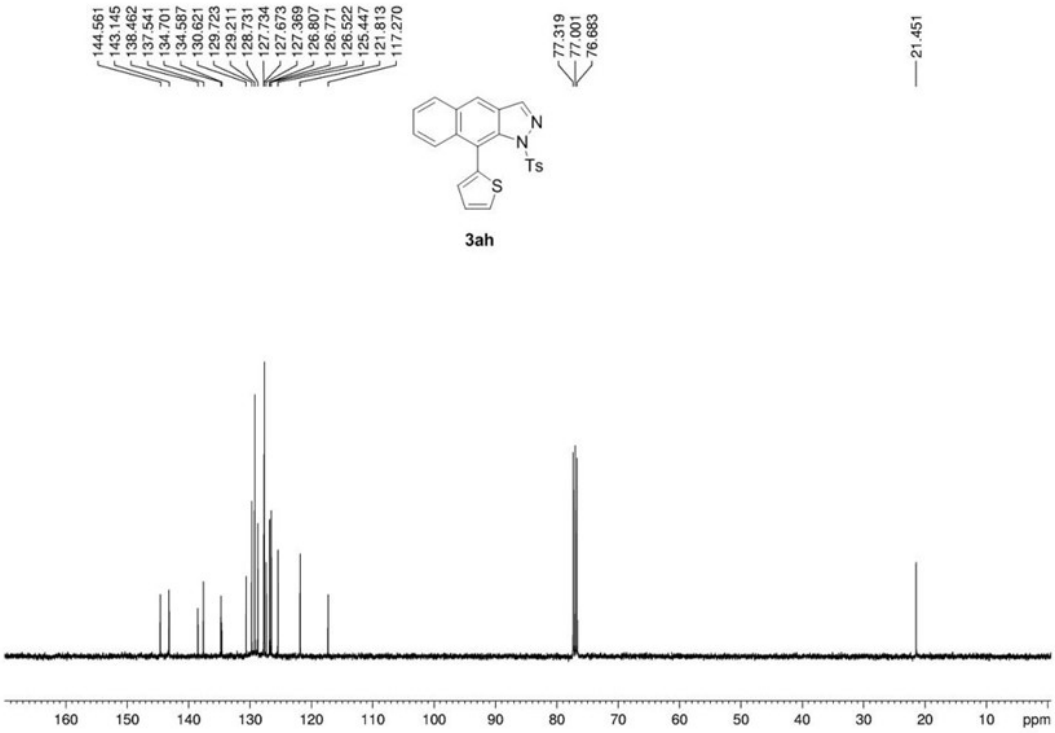
0.98
2.07
3.03
2.13
0.97
1.01
1.96
2.98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138.462
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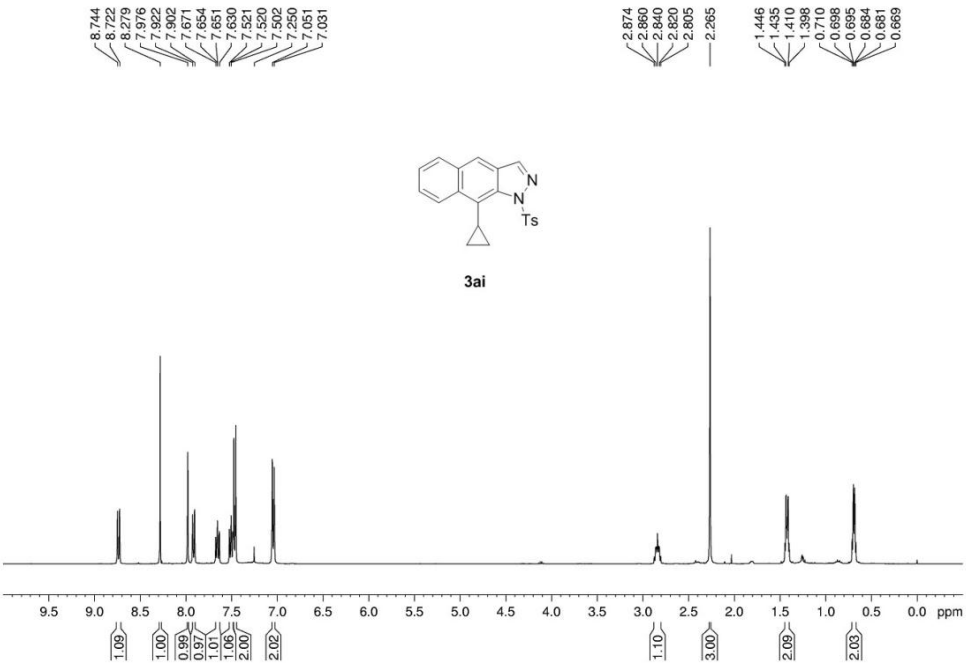
129.723
129.211
128.731
127.734
127.673
127.369
126.807
126.771
126.522
125.447
121.813
117.270
77.319
77.001
76.683
21.451
N
N
Ts
S
3ah
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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8.279
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7.922
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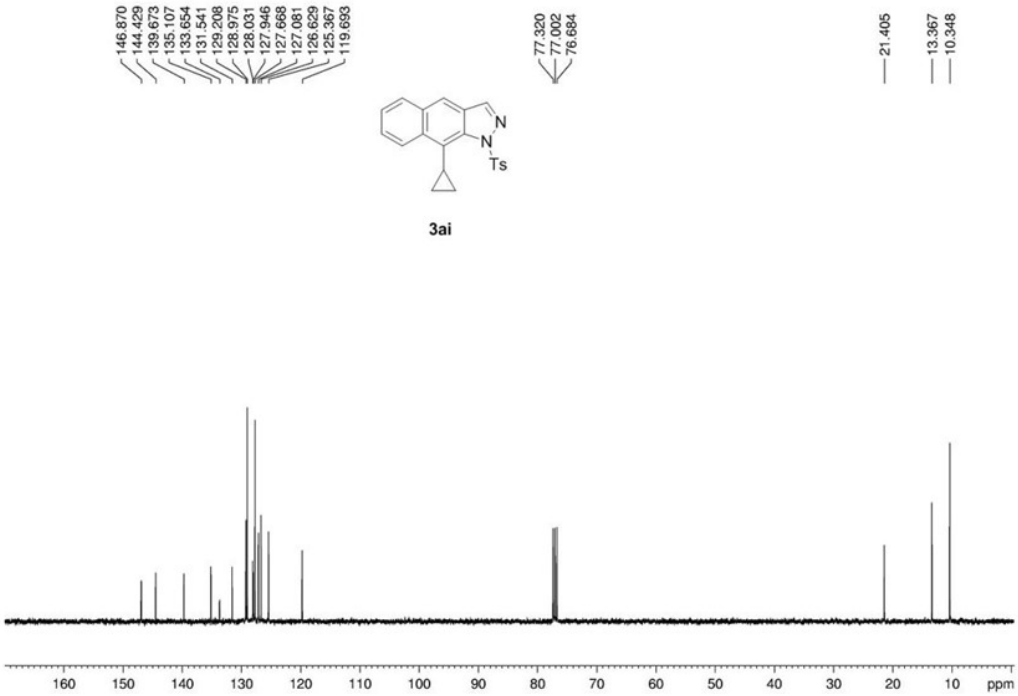
7.671
7.654
7.651
7.630
7.521
7.520
7.502
7.250
7.051
7.031
2.874
2.860
2.840
2.820
2.805
2.265
1.446
1.435
1.410
1.398
0.710
0.698
0.695
0.684
0.681
0.669
N
N
Ts
3ai
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.09
1.00
0.99
0.97
1.01
1.06
2.00
2.02
1.10
3.00
2.09
2.03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128.975
128.031
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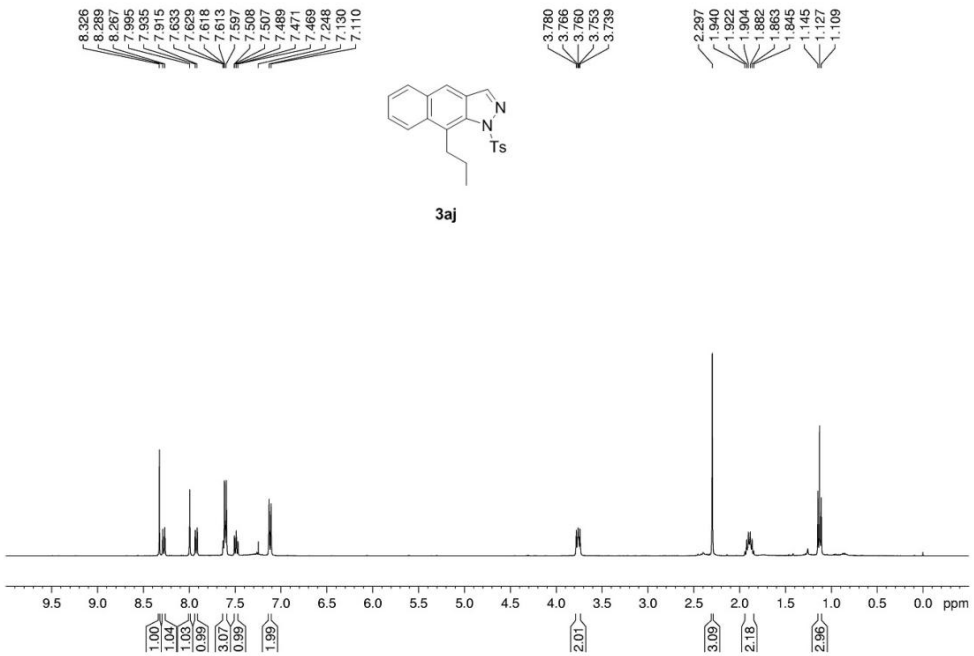
127.081
126.629
125.367
119.693
77.320
77.002
76.684
21.405
13.367
10.348
N
N
Ts
3ai
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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7.935
7.915
7.633
7.629
7.618
7.613
7.597
7.508
7.507
7.489
7.471
7.469
7.248
7.130
7.110
3.780
3.766
3.760
3.753
3.739
2.297
1.940
1.922
1.904
1.882
1.863
1.845
1.145
1.127
1.109
N
N
Ts
3aj
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 ppm
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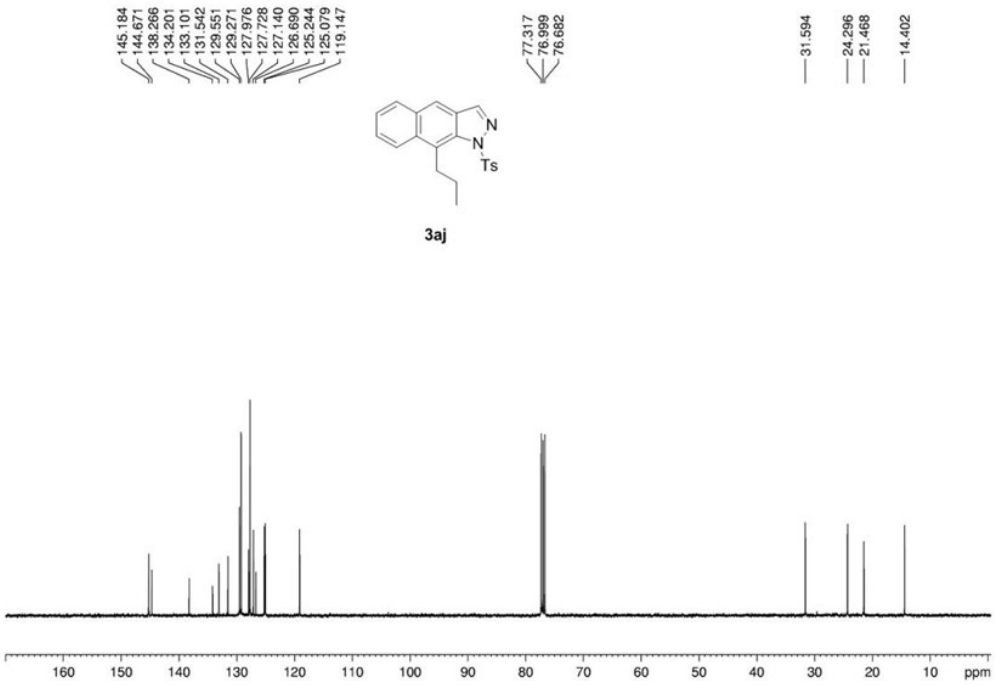
1.04
1.03
0.99
3.07
0.99
1.99
2.01
3.09
2.18
2.96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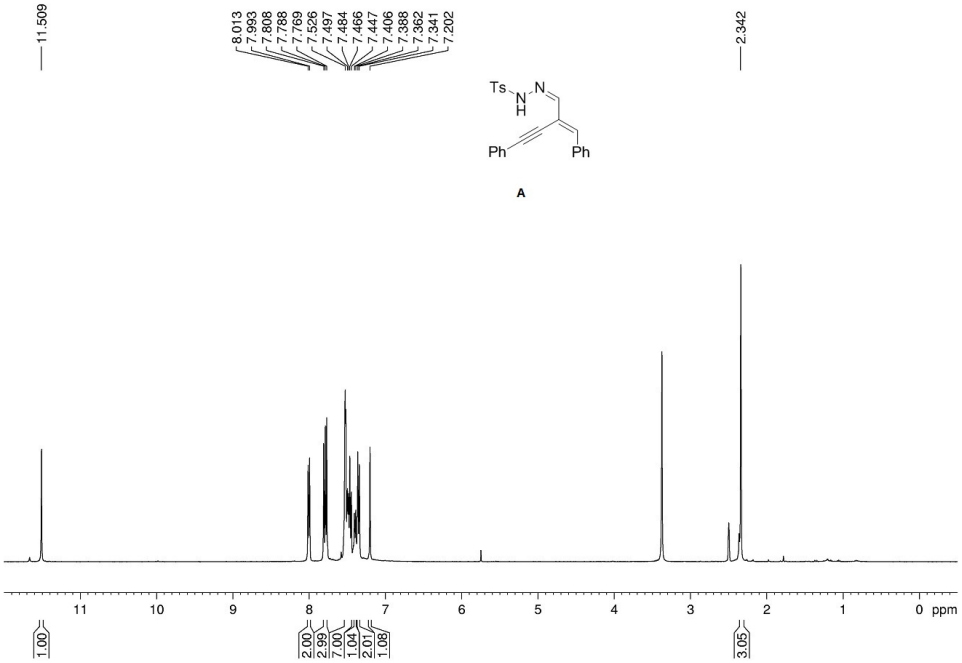
131.542
129.551
129.271
127.976
127.728
127.140
126.690
125.244
125.079
119.147
77.317
76.999
76.682
31.594
24.296
21.468
14.402
N
N
Ts
3aj
160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm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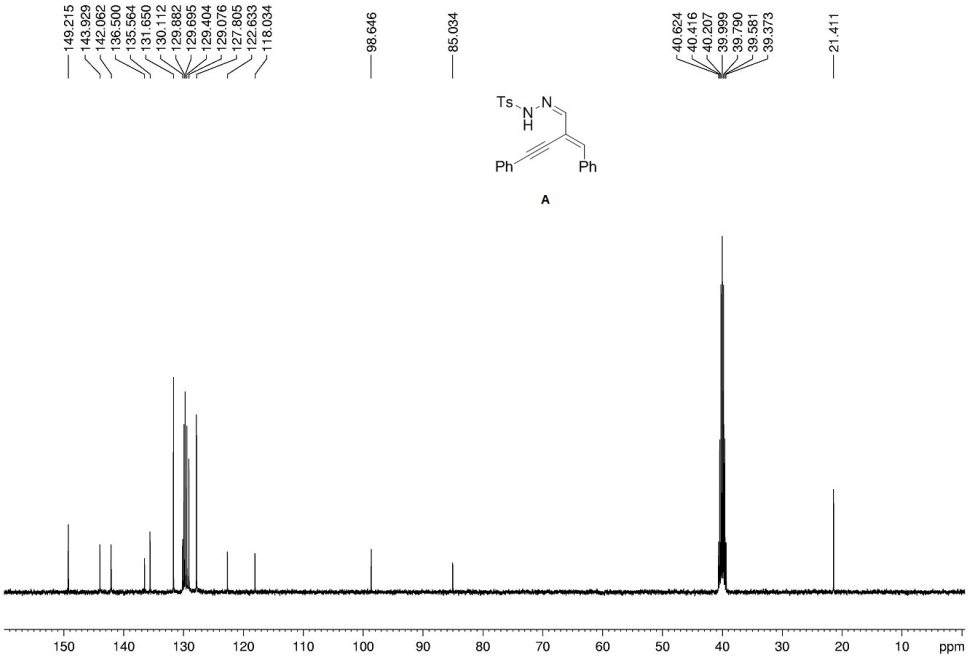
7.526
7.497
7.484
7.466
7.447
7.406
7.388
7.362
7.341
7.202
2.342
Ts
N
H
N
Ph
Ph
A
11
10
9
8
7
6
5
4
3
2
1
0 ppm
1.00
2.00
2.99
7.00
1.04
2.01
1.08
3.05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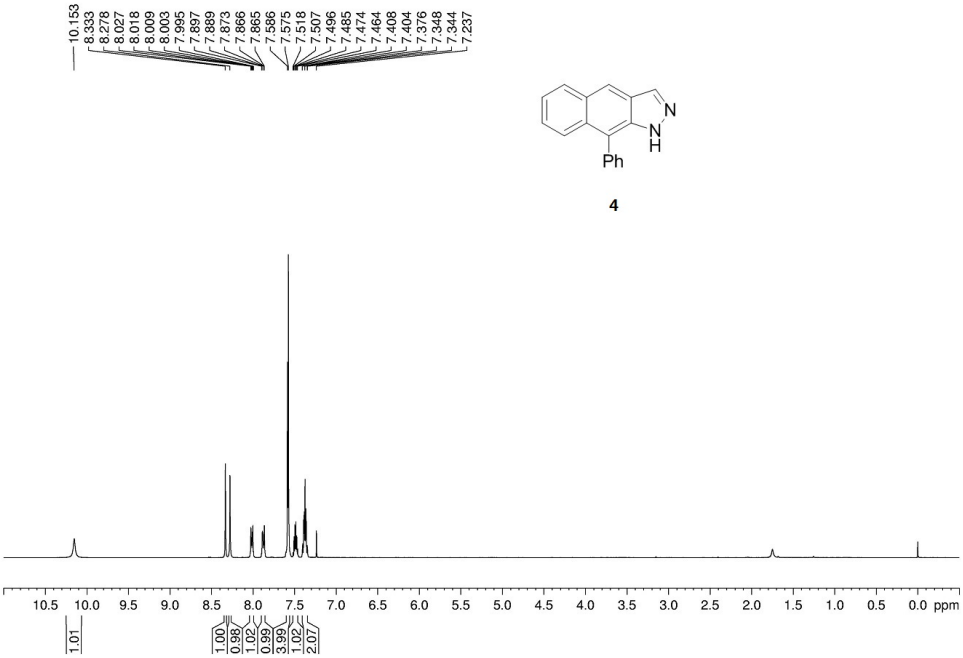
136.500
135.564
131.650
130.112
129.882
129.695
129.404
129.076
127.805
122.633
118.034
98.646
85.034
40.624
40.416
40.207
39.999
39.790
39.581
39.373
21.411
Ts
N
H
N
Ph
Ph
A
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
ppm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8.018
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8.003
7.995
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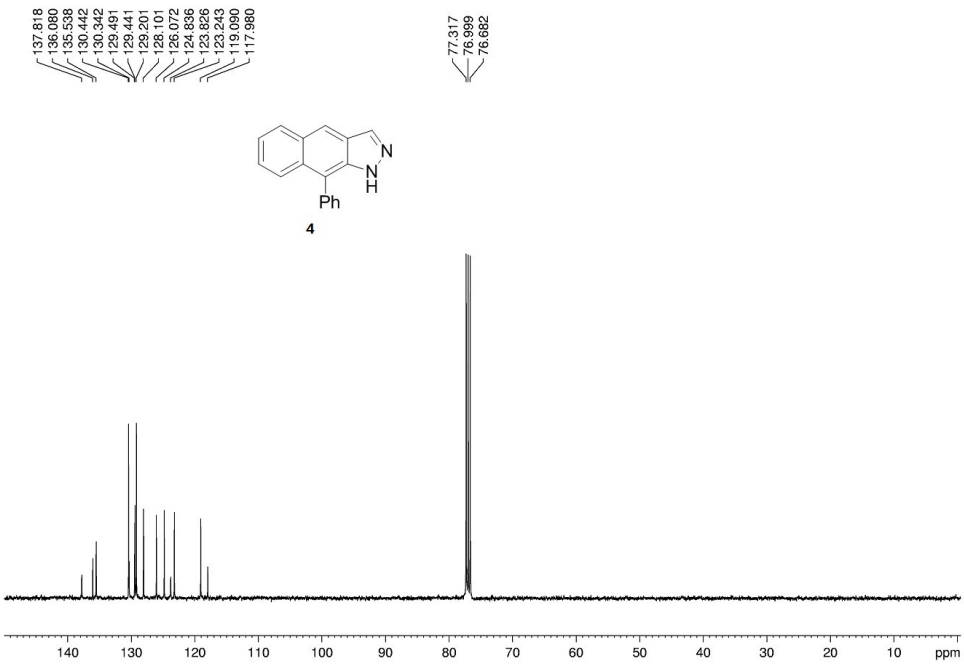
7.889
7.873
7.866
7.865
7.586
7.575
7.518
7.507
7.496
7.485
7.474
7.464
7.408
7.404
7.376
7.348
7.344
7.237
N
N
H
Ph
4
10.5 10.0 9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0 ppm
1.01
1.00
0.98
1.02
0.99
3.99
1.02
2.07


137.818
136.080
135.538
130.442
130.342
129.491
129.441
129.201
128.101
126.072
124.836
123.826
123.243
119.090
117.980
77.317
76.999
76.682
N
N
H
Ph
4
140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm