Supporting Information

Stereoselective Rhodium-Catalyzed 2-C-H 1,3-Dienylation of Indoles-Dual Functions of the Directing Group

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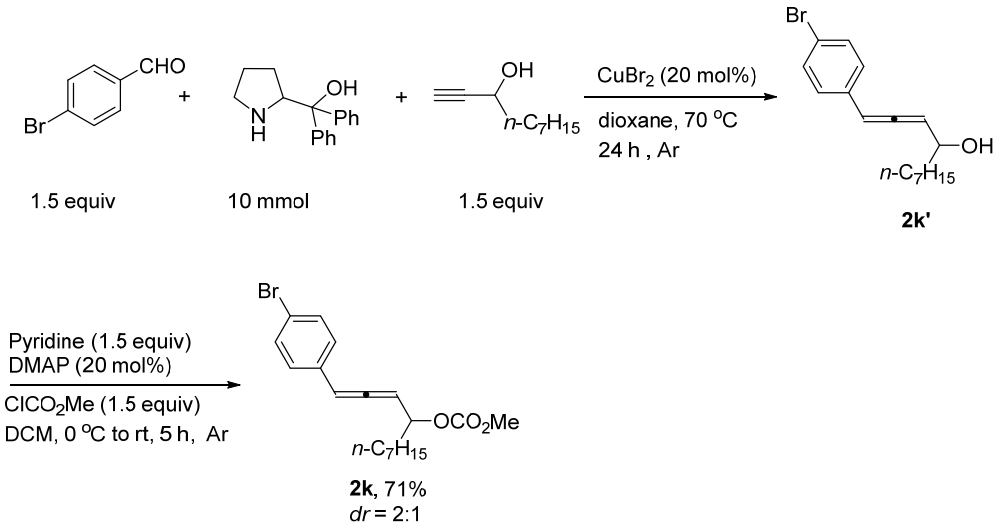
General Information. NMR spectra were recorded on Agilent 400 MHz, Varian Mercury 400 MHz, Bruker 400 MHz, or Bruker 600 MHz (400 MHz or 600 MHz for ^{1}H NMR in $CDCl_3$ or C_6D_6, 100 MHz for ^{13}C NMR, and 376 MHz for ^{19}F NMR in $CDCl_3$). ^{1}H NMR experiments were measured using tetramethylsilane (TMS) as the internal standard in $CDCl_3$ or in relative to the signal of C_6D_6 (7.16 ppm). ^{13}C NMR experiments were measured in relative to the signal of $CDCl_3$ (77.00 ppm). ^{19}F NMR experiments were measured in relative to the signal of $CFCl_3$ (0 ppm) in $CDCl_3$. All reactions were carried out under argon atmosphere in oven-dried Schlenk tubes or flasks. Indoles **1a-1g**[1] and 2,3-dienol derivatives **2a-2p**[2,3] were prepared according to the reported method. $[Cp^*RhCl_2]_2$ and PivOH were purchased from TCI. $AgSbF_6$ was purchased from Alfa Asear and stored in the glove box. Toluene and dioxane was dried over sodium wire with benzophenone as the indicator and distilled before use. CH_2Cl_2 was dried over calcium hydride and distilled before use. Other reagents were used without further treatment. Petroleum ether (60 - 90 ^{o}C) was used for chromatography on silica gel.

1. Synthesis of 4-aryl-2,3-allenyl carbonates and 4-alkyl-2,3-allenyl carbonates.

(1) Synthesis of 1-(4-bromophenyl)undeca-1,2-dien-4-yl methyl carbonate 2k[2c, 3] (zyz-6-34, zyz-6-92)

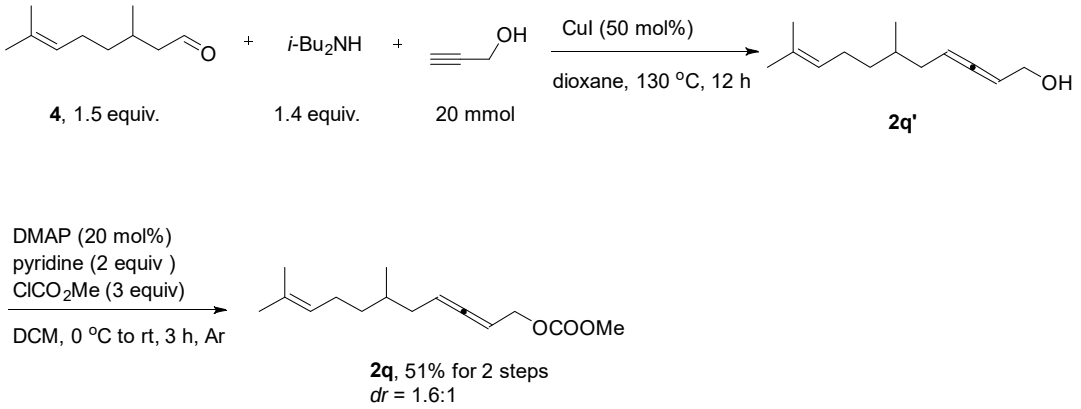


To an oven-dried Schlenk flask were added $CuBr_2$ (449.0 mg, 2 mmol), 2-diphenylhydroxymethylpyrrolidine (2.5332 g, 10 mmol), dec-1-yn-3-ol (2.3169 g, 15 mmol), 4-bromobenzaldehyde (2.7796 g, 15 mmol), and dioxane (30 mL) sequentially under argon atmosphere. The resulting mixture was stirred in an oil bath preheated at 70 °C for 24 h. Then the resulting mixture was diluted by 30 mL of Et_2O and washed with an aqueous solution of hydrochloric acid (3 M, 30 mL). The aqueous layer was extracted with Et_2O (30 mL × 2). The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified by flash column chromatography on silica gel to afford **2k'** (1.3573 g) (eluent: petroleum ether /ethyl acetate = 30/1) as a liquid, which was then submitted to the next step without further treatment.

Typical Procedure I: **2k'** (973.2 mg, 3 mmol), DMAP (73.9 mg, 0.6 mmol), pyridine (0.36 mL, d = 0.9819 g/cm^3, 353.5 mg, 4.5 mmol), and DCM (10 mL) were added sequentially into a flask under argon at room temperature. Then methyl chloroformate (0.35 mL, d = 1.223 g/cm^3, 428.1 mg, 4.5 mmol) was added dropwise at 0 °C. The resulting mixture was allowed to stir at room temperature for 5 h as monitored by TLC. Upon completion, the resulting mixture was sequentially washed with 3 M HCl (10

mL), a saturated aqueous solution of $NaHCO_3$ (10 mL), and brine (10 mL) and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified via column chromatography on silica gel to afford **2k** (813.3 mg, 71%, *dr* = 2:1) (eluent: petroleum ether / ethyl acetate = 30/1) as an oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.45-7.38 (m, 2 H, Ar-H), 7.19-7.10 (m, 2 H, Ar-H), [6.28 (dd, J_1 = 6.4 Hz, J_2 = 2.0 Hz, 0.34 H), 6.23 (dd, J_1 = 6.4 Hz, J_2 = 1.6 Hz, 0.66 H), 1 H, =CH], 5.66 (t, J = 6.4 Hz, 1 H, =CH), 5.23-5.10 (m, 1 H, CH), [3.79 (s, 2 H), 3.72 (s, 1 H), 3 H, CH_3], 1.86-1.68 (m, 2 H, CH_2), 1.52-1.13 (m, 10 H, 5xCH_2), 0.87 (t, J = 6.8 Hz, 3 H, CH_3); MS (ESI) *m/z* 400 $(M(^{81}Br)+NH_4)^+$, 398 $(M(^{79}Br)+NH_4)^+$; IR (neat, cm^{-1}): 2925, 2855, 1954, 1745, 1589, 1488, 1441, 1259, 1068, 1010; Anal. calcd for $C_{19}H_{25}O_3Br$ (%): C 59.85, H 6.61, Found: C 59.63, H 6.39.

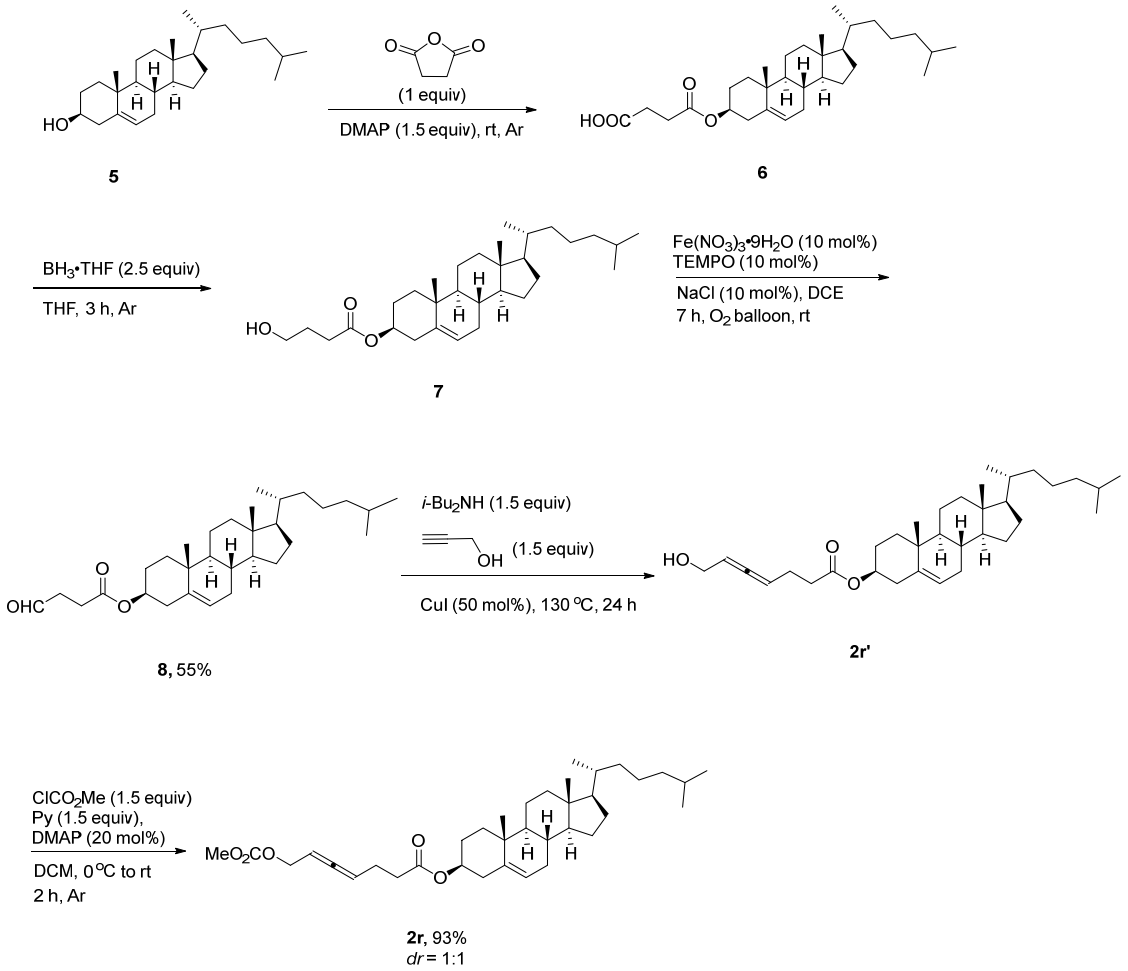
(2) Synthesis of 2q[2a,3] (cyf-4-49, cyf-4-51)



To a flame-dried round bottle flask with a reflux condenser were added CuI (1.9265 g, 10.0 mmol), (±)-citronellal **4** (4.6305 g, 30.0 mmol)/dioxane (10 mL), *i*-Bu_2NH (4.86 mL**,** d = 0.745 g/mL, 3.6207 g, 28 mmol**),** and propargyl alcohol (1.17 mL, d = 0.963 g/mL, 1.1267 g, 20 mmol) sequentially under argon atmosphere. The reaction was complete after being stirred in an oil bath preheated at 130 ºC for 12 h as monitored by TLC. After cooling to room temperature, the resulting mixture was filtrated through a short column of silica gel eluted with diethyl ether (20 mL) and washed with an aqueous solution of hydrochloric acid (2 M, 10 mL × 3) and brine and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified by chromatography on silica gel to afford **2q'** (2.1486 g) (eluent: petroleum ether (60-90 ºC)/ethyl acetate = 30/1) as a liquid, which was used in the next step without further purification.

To a flame-dried round bottle flask were added DMAP (274.1 mg, 2.2 mmol), **2q'** (2.1486 g, 11.1 mmol), pyridine (1.79 mL, d = 0.9819 g/mL, 1.7576 g, 22.2 mmol), and DCM (22 mL) sequentially. The resulting mixture was stirred at 0 ºC for 10 min followed by the dropwise addition of a solution of methyl chloroformate (2.56 mL, d = 1.223 g/mL, 3.1309 g, 33.1 mmol) within 5 min at 0 ºC. After the addition, the resulting mixture was stirred at this temperature for 10 min, removed from the cooling bath, allowed to warm up to room temperature gradually, and reacted at room temperature for 3 h. After the reaction was complete as monitored by TLC, it was quenched with an aqueous solution of hydrochloric acid (2 M, 22 mL). The aqueous layer was separated and extracted with DCM (22 mL × 3). The organic layer was combined, washed with brine, and dried over anhydrous Na_2SO_4. After filtration, evaporation of the solvent and chromatography on silica gel (eluent: petroleum ether (30-60 ºC)/ethyl acetate = 100/1) afforded **2q** (2.5994 g, 51% for 2 steps, *dr* = 1.6:1) as an oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.29-5.19 (m, 2 H, HC=C=CH), 5.09 (t, J = 7.0 Hz, 1 H, =CH), 4.60 (dd, J_1 = 6.4 Hz, J_2 = 2.0 Hz, 2 H, OCH_2), 3.79 (s, 3 H, OCH_3), 2.10-1.83 (m, 4 H, 2 × CH_2), 1.68 (s, 3 H, CH_3), 1.60 (s, 3 H, CH_3), 1.57-1.48 (m, 1 H, CH), 1.42-1.32 (m, 1 H, one proton of CH_2), 1.23-1.12 (m, 1 H, one proton of CH_2), 0.91 (dd, J_1 = 6.8 Hz, J_2 = 1.2 Hz, 3 H, CH_3); MS (DART) *m/z* 270 $(M+NH_4)^+$, 253$(M+H)^+$; IR (neat, cm^{-1}): 2958, 2917, 1966, 1748, 1445, 1371, 1253, 1110; HRMS calcd for $C_{15}H_{24}O_3Na$ $(M+Na)^+$: 275.1618. Found: 275.1618.

(3) Synthesis of 2r^3 (zyz-6-107, zyz-6-108, zyz-6-109, zyz-6-110, zyz-6-111)



Compound **6**[4], **7**[5], **8**[6], and **2r'**[2a] were synthetized according to literature.

To a three-necked flask were added cholesterol **5** (23.2102 g, 60 mmol), succinic anhydride (6.0174 g, 60 mmol), DMAP (7.3796 g, 60 mmol), and DCM (200 mL) under argon atmosphere. The resulting mixture was allowed to stir at room temperature for 22 h as monitored by TLC. Then extra DMAP (3.6721 g, 30 mmol) was added. The mixture was stirred 24 h at room temperature as monitored by TLC. Upon completion, the mixture was washed with 3M HCl (100 mL × 3), H_2O (100 mL × 2) and brine (100 mL) sequentially. The organic layer was dried over anhydrous Na_2SO_4, filtrated and evaporated to afford **6** (26.2839 g) without further purification.

To a three-necked flask were added **6** (19.4650 g, 40 mmol) and 200 mL of THF under argon atmosphere at room temperature. BH_3•THF (100 mL, 1 M in THF, 100 mmol) was added dropwise over 20 min at 0 ºC. The resulting mixture was allowed to stir at room temperature for 3 h as monitored by TLC. Upon completion, the mixture was

quenched with water (100 mL) at 0 ºC. The resulting mixture was extracted with EtOAc (100 mL × 3). The combined organic layer was washed with brine (100 mL) and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified by column chromatography to afford **7** (11.6000 g) (eluent: petroleum ether/ethyl acetate = 5/1), which was then used in the next step without further characterization.

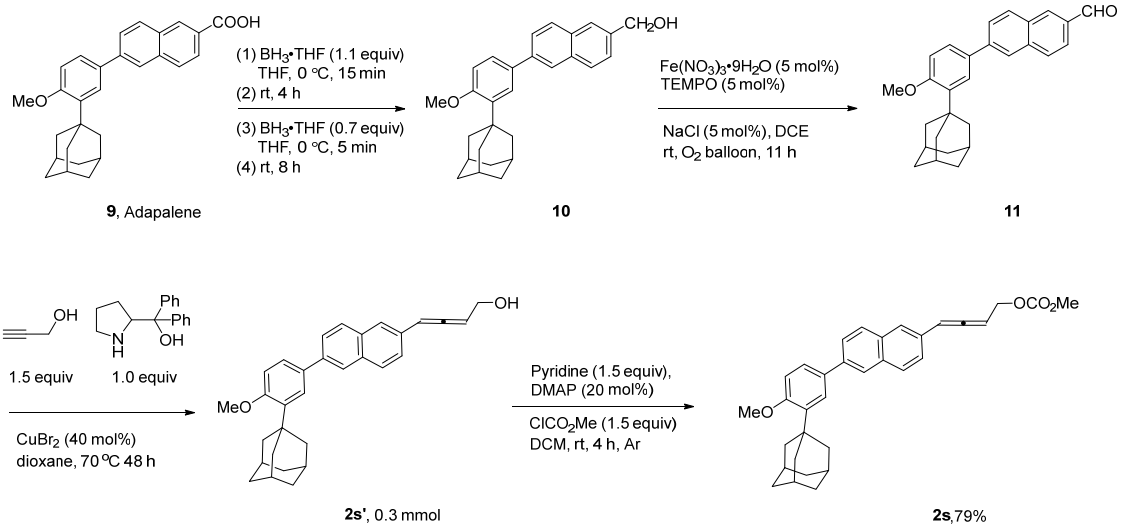
To a three-necked flask were added $Fe(NO_3)_3 \cdot 9H_2O$ (987.2 mg, 2.44 mmol), TEMPO (384.1 mg, 2.46 mmol), NaCl (146.3 mg, 2.50 mmol), **7** (11.6000 g, 24.5 mmol), and DCE (100 mL) sequentially under the atmosphere of oxygen from a gas bag (4 L). The flask was then stirred at room temperature until completion of the reaction as monitored by TLC. The crude reaction mixture was filtrated through a short column of silica gel eluted with DCM (50 mL × 3). After evaporation, the residue was purified by column chromatography to afford **8 (**6.3334 g, 55%) (eluent: petroleum ether/ethyl acetate = 8/1), which was then used in the next step without further characterization.

To a flame-dried three-necked flask with a reflux condenser were added **8** (3.7694, 8 mmol), CuI (764.7 mg, 4 mmol), dioxane (20 mL), *i*-Bu_2NH (2.1 mL, d = 0.745 g/mL, 1.5645 g, 12 mmol), and propargyl alcohol (0.69 mL, d = 0.9715 g/mL, 670.3 mg, 12 mmol) sequentially. The resulting mixture was stirred at 130 ºC for 24 h as monitored by TLC, diluted with ether (20 mL), and washed with an aqueous solution of hydrochloric acid (3 M, 20 mL). The organic layer was separated and the aqueous layer was extracted with ether (20 mL × 2). The combined organic layer was washed with brine and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified by chromatography to afford **2r'** (1.2624 g) (eluent: petroleum ether/ethyl acetate = 5/1), which was then used in the next step without further characterization.

Following Procedure I, the reaction of **2r'** (1.2624 g, 2.5 mmol), DMAP (61.7 mg, 0.5 mmol), pyridine (0.3 mL, d = 0.9819 g/cm^3, 294.6 mg, 3.72 mmol), DCM (5 mL), and methyl chloroformate (0.29 mL, d = 1.223 g/cm^3, 354.7 mg, 3.75 mmol) afforded **2r** (1.3097 g, 93%, *dr* = 1:1) (eluent: petroleum ether/ethyl acetate = 50/1) as an oil. The *dr* ratio of **2r** was determined to be 1:1 by HPLC (HPLC conditions: Chiralcel OD-H column, hexane/*i*-PrOH = 200/1, 1.0 mL/min, λ = 214 nm, t_{R1} = 20.461 min, t_{R2} = 22.989 min); ^{1}H NMR (400 MHz, $CDCl_3$) δ 5.43-5.25 (m, 3 H, =CH and HC=C=CH), 4.66-4.52 (m, 3 H, OCH and OCH_2), 3.79 (s, 3 H, CH_3), 2.44-2.28 (m, 6 H), 2.07-1.92 (m, 2 H),

1.89-1.81 (m, 3 H), 1.62-0.84 (m, 33 H), 0.68 (s, 3 H, CH_3); MS (DART) *m/z* 586 $(M+NH_4)^+$, 569 $(M+H)^+$; IR (neat, cm^{-1}): 2934, 2865, 2817, 1965, 1732, 1556, 1449, 1420, 1366, 1249, 1161, 1082, 1054; HRMS (ESI) Calcd for $C_{36}H_{56}O_5Na$ $(M+Na)^+$: 591.4020, Found: 591.4003.

(4) Synthesis of 2s[3] (wwy-2-198, wwy-2-200, wwy-3-003, zyz-6-95)

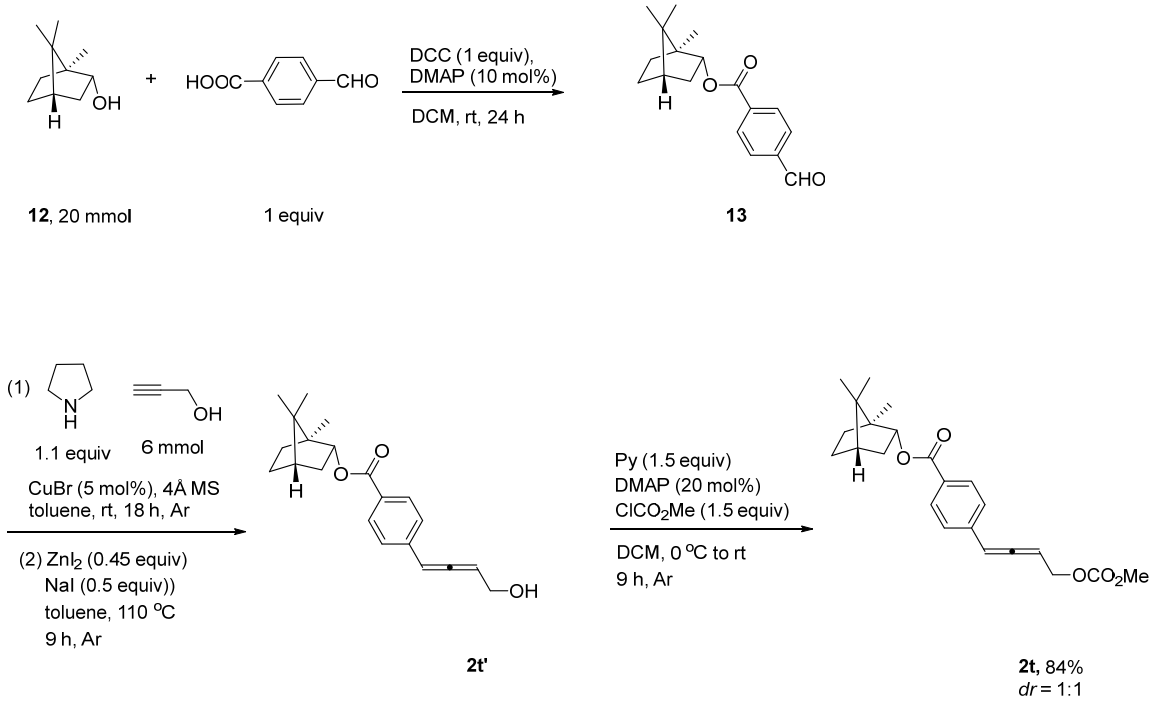


Compound **10**[5], **11**[6], and **2s'**[2c] were synthetized according to literature.

Following Procedure I, the reaction of **2s'** (132.1 mg, 0.3 mmol), DCM (1 mL), DMAP (8.7 mg, 0.07 mmol), pyridine (36 μL, d = 0.9819 g/cm^3, 35.3 mg, 0.45 mmol), and methyl chloroformate (35 μL, d = 1.223 g/cm^3, 42.8 mg, 0.45 mmol) afforded **2s** (118.4 mg, 79%) (eluent: petroleum ether / ethyl acetate = 20/1) as an oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.93 (s, 1 H, Ar-H), 7.81 (d, *J* = 8.8 Hz, 2 H, Ar-H), 7.70 (dd, J_1 = 8.6 Hz, J_2 = 1.4 Hz, 1 H, Ar-H), 7.66 (s, 1 H, Ar-H), 7.58 (d, *J* = 2.0 Hz, 1 H, Ar-H), 7.53-7.44 (m, 2 H, Ar-H), 6.97 (d, *J* = 8.8 Hz, 1 H, Ar-H), 6.53-6.46 (m, 1 H, =CH), 5.82 (q, *J* = 6.5 Hz, 1 H, =CH), 4.83-4.70 (m, 2 H, CH_2), 3.88 (s, 3 H, OCH_3), 3.78 (s, 3 H, OCH_3), 2.18 (s, 6 H, 3 × CH_2), 2.10 (s, 3 H, 3 × CH), 1.80 (s, 6 H, 3 × CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.1, 158.5, 155.5, 139.0, 138.8, 133.2, 133.0, 132.3, 130.2, 128.5, 128.1, 126.0, 125.8, 125.5, 125.0, 124.8, 112.0, 97.2, 90.9, 65.3, 55.1, 54.9, 40.6, 37.1, 29.1; MS (ESI) *m/z* 517 $(M+Na)^+$, 495 $(M+H)^+$; IR (neat, cm^{-1}): 2901, 2852, 1949, 1744, 1602,

1493, 1444, 1372, 1235, 1182, 1138, 1104, 1061, 1026; HRMS (ESI) Calcd for $C_{33}H_{34}O_4Na$ $(M+Na)^+$: 517.2349, Found: 517.2354.

(5) Synthesis of 2t[2b] (zyz-6-90, zyz-6-142, zyz-6-143)



To a round-bottomed flasks were added 4-formylbenzoic acid (3.0072 g, 20 mmol), (L)-(-)-borneol **12** (3.0720 g, 20 mmol), DCC (4.1276 g, 20 mmol), DMAP (247.9 mg, 2 mmol), and DCM (100 mL). The resulting mixture was stirred at room temperature for 24 h as monitored by TLC, washed sequentially with 3 M HCl (40 mL) and brine (30 mL) and dried over anhydrous Na_2SO_4. After filtration and evaporation, the residue was purified by column chromatography to afford **13** (4.0239 g) (eluent: petroleum ether/ethyl acetate = 8/1), which was then used in the next step without further characterization.

To an oven-dried Schlenk flask were added CuBr (41.2 mg, 0.3 mmol), 4 Å molecular sieve (1.8376 g), **13** (1.8976 g, 6.6 mmol), pyrrolidine (478.7 mg, 6.7 mmol), propargyl alcohol (339.9 mg, 6 mmol), and toluene (24 mL) sequentially under argon atmosphere. The resulting mixture was stirred for 18 h. After the reaction was complete as monitored by TLC, the resulting mixture was filtrated through a short column of celite

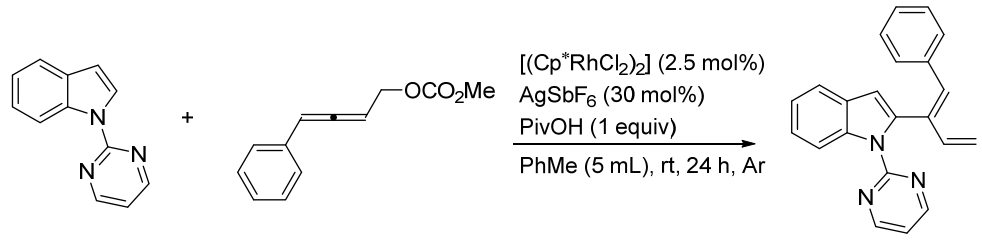
eluted with Et_2O (30 mL × 3). After evaporation, the crude product was used in the next step.

To another three-necked flask were added ZnI_2 (867.2 mg, 2.7 mmol) and NaI (454.2 mg, 3 mmol). Then the loaded flask was dried under vacuum with a heating gun. The crude product prepared above and toluene (30 mL) were added to the flask under argon atmosphere. The flask was placed in an oil bath pre-heated at 110 ºC with stirring for 9 h as monitored by TLC. The resulting mixture was cooled to room temperature and filtrated through a short column of celite eluted with Et_2O (20 mL × 3). After evaporation, the residue was purified by flash column chromatography on silica gel to afford **2t'** (165.7 mg) (eluent: petroleum ether/ethyl acetate = 6/1) as an oil, which was then submitted to the next step without further treatment.

Following Procedure I, the reaction of **2t'** (132.7 mg, 0.4 mmol), DCM (2 mL), pyridine (49.2 mg, 0.6 mmol), and $ClCO_2Me$ (57.1 mg, 0.6 mmol) afforded **2t** (131.8 mg, 84%) (eluent: petroleum ether/ethyl acetate = 20/1) as an oil. The *dr* ratio of **2t** was determined to be 1:1 by HPLC (HPLC conditions: Chiralcel AD-H column, *n*-hexane/*i*-PrOH = 100/1, 1.0 mL/min, λ = 214 nm, t_{R1} = 24.466 min, t_{R2} = 26.409 min): ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.00 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.36 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.40-6.33 (m, 1 H, =CH), 5.81 (q, *J* = 6.4 Hz, 1 H, =CH), 5.14-5.08 (m, 1 H, OCH), 4.82-4.68 (m, 2 H, OCH_2), 3.79 (s, 3 H, OCH_3), 2.53-2.42 (m, 1 H, one proton of CH_2), 2.16-2.08 (m, 1 H, one proton of CH_2), 1.86-1.76 (m, 1 H, one proton of CH_2), 1,74 (t, *J* = 4.6 Hz, 1 H, CH), 1.46-1.37 (m, 1 H, one proton of CH_2), 1.35-1.25 (m, 1 H, one proton of CH_2), 1.12 (dd, J_1 = 13.8 Hz, J_2 = 3.4 Hz, 1 H, one proton of CH_2), 0.97 (s, 3 H, CH_3), 0.93-0.90 (m, 6 H, 2 × CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 207.4, 166.5, 155.4, 137.9, 129.9, 129,6, 126.8, 96.3, 91.1, 80.4, 64.8, 54.9, 49.0, 47.8, 44.9, 36.8, 28.0, 27.3, 19.7, 18.9, 13.6; MS (ESI) *m/z* 385 $(M+H)^+$, 402 $(M+NH_4)^+$; IR (neat, cm^{-1}): 2953, 2878, 1953, 1748, 1711, 1607, 1444, 1375, 1256, 1175, 1106, 1045, 1017; HRMS (ESI) Calcd for $C_{23}H_{29}O_5$ $(M+H)^+$: 385.2010, Found: 385.2008.

Rhodium(III)-Catalyzed 2-C-H Functionalization of Indoles with Allenyl Carbonates

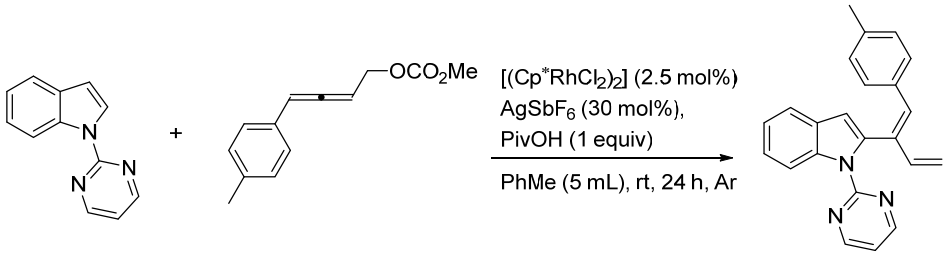
(1) 2-[(*Z*)-1-phenyl-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3aa (zyz-5-68)



Typical Procedure II: To an oven-dried Schlenk tube were added [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (102.7 mg, 0.3 mmol), **1a** (196.0 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2a** (224.9 mg, 1.1 mmol)/toluene (3 mL) sequentially under the argon atmosphere. The resulting mixture was stirred at room temperature for 24 h as monitored by TLC and filtrated through a short column of celite eluted with DCM (30 mL × 3). The crude product was purified by column chromatography to afford **3aa** (226.1 mg, 70%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.74 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.02 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.50 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.35-7.31 (m, 1 H, Ar-H), 7.21-7.16 (m, 3 H, Ar-H), 6.87-6.82 (m, 3 H, Ar-H), 6.71-6.65 (m, 2 H, =CH and Ar-H), 6.57 (s, 1 H, =CH), 5.97 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.10 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.96 (d, *J* = 10.2 Hz, 1 H, one proton of =CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 157.3, 140.4, 136.54, 136.49, 135.2, 133.9, 132.8, 129.4, 128.9, 127.9, 127.0, 123.3, 121.8, 120.6, 116.9, 115.5, 114.0, 108.5; MS (ESI) *m/z* 324 $(M+H)^+$; IR (neat, cm^{-1}): 1601, 1561, 1489, 1475, 1451, 1420, 1369, 1346, 1307, 1266, 1236, 1212, 1178, 1149, 1112, 1093, 1076, 1035, 1014; HRMS (ESI) Calcd for $C_{22}H_{18}N_3$ $(M+H)^+$: 324.1495, Found: 324.1499.

The following signals are discernible for (*E*-**3aa**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.68 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.62 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.40 (d, *J* = 7.8 Hz, 2 H, Ar-H), 7.36 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.27 (t, *J* = 7.5 Hz, 1 H, Ar-H), 7.05 (t, *J* = 7.5 Hz, 1 H, Ar-H), 7.00 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.91 (s, 1 H, Ar-H), 6.75 (s, 1 H, =CH), 5.19 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.88 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

(2) 2-[(*Z*)-1-(4-methylphenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ab (zyz-5-82)

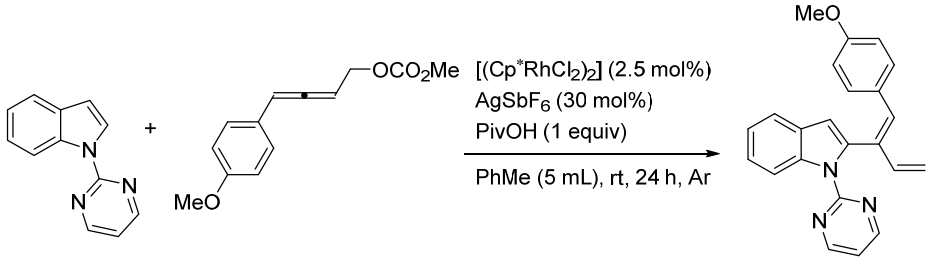


Typical Procedure III: To an oven-dried Schlenk tube were added $[(Cp^*RhCl_2)_2]$ (15.4 mg, 0.025 mmol), $AgSbF_6$ (102.7mg, 0.3 mmol), **1a** (195.7 mg, 1.0 mmol), PivOH (102.3 mg, 1 mmol)/toluene (2 mL), and **2b** (240.3 mg, 1.1 mmol)/toluene (3 mL) sequentially under argon atmosphere. The resulting mixture was stirred at room temperature for 24 h. After the reaction was complete as monitored by TLC, the mixture was diluted with 20 mL of DCM and washed with 20 mL of a saturated aqueous solution of $NaHCO_3$. The aqueous layer was extracted with DCM (10 mLx2) and the combined organic layer was washed with 20 mL of brine, dried over anhydrous Na_2SO_4, filtrated and concentrated. The crude product was purified by column chromatography to afford **3ab** (276.6 mg, 82%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.75 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.04 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.52 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.37-7.31 (m, 1 H, Ar-H), 7.21 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.10 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.74-6.64 (m, 4 H, Ar-H and =CH), 6.59 (s, 1 H, =CH), 5.99 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.10 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, *J* = 10.2 Hz, 1 H, one proton of $=CH_2$), 1.91 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 157.3, 140.6, 136.9, 136.5, 135.5, 133.7, 133.03, 129.99, 129.4, 128.9, 128.7, 123.2, 121.8, 120.6, 116.9, 114.9, 114.1, 108.2, 21.1; MS (ESI) *m/z* 338 $(M+H)^+$; IR (neat, cm^{-1}): 1600, 1561, 1507, 1475, 1451, 1421, 1383, 1346, 1305, 1266, 1237, 1211, 1180, 1149, 1112, 1093, 1078, 1036, 1016; HRMS (ESI) Calcd for $C_{23}H_{20}N_3$ $(M+H)^+$: 338.1652, Found: 338.1653.

The following signals are discernible for (*E*-**3ab**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.66 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.62 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.26 (t, *J* = 7.2 Hz, 1 H, Ar-H), 6.99 (d, *J* = 7.8 Hz, 2 H, Ar-H), 6.94 (s, 1 H, Ar-H), 6.76 (s, 1 H, =CH), 5.20 (d, *J* = 17.4

Hz, 1 H, one proton of =CH_2), 4.90 (d, J = 10.8 Hz, 1 H, one proton of =CH_2), 2.11 (s, 3 H, CH_3).

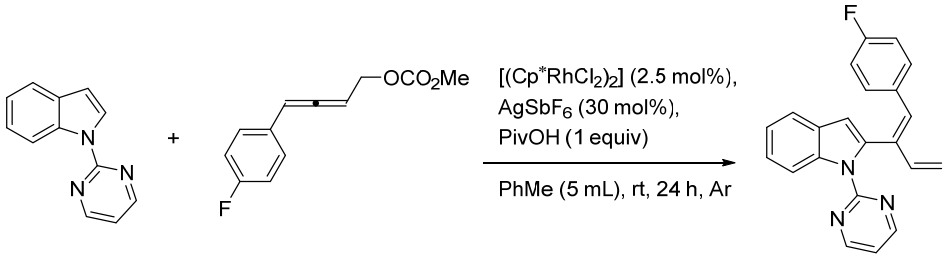
(3) 2-[(*Z*)-1-(4-methoxyphenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ac (zyz-6-171)



Following **Typical Procedrue II**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (102.5 mg, 0.3 mmol), **1a** (195.5 mg, 1.0 mmol), PivOH (102.4 mg, 1 mmol) /toluene (2 mL), and **2c** (259.0 mg, 1.1 mmol)/toluene (3 mL) afforded **3ac** (261.5 mg, 74%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 20/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.74 (d, J = 8.4 Hz, 1 H, Ar-H), 8.07 (d, J = 4.8 Hz, 2 H, Ar-H), 7.54 (d, J = 7.8 Hz, 1 H, Ar-H), 7.34 (t, J = 7.8 Hz, 1 H, Ar-H), 7.22 (t, J = 7.5 Hz, 1 H, Ar-H), 7.08 (d, J = 8.4 Hz, 2 H, Ar-H), 6.73 (dd, J_1 = 17.4 Hz, J_2 = 10.2 Hz, 1 H, =CH), 6.67 (s, 1 H, Ar-H), 6.62 (s, 1 H, =CH), 6.43 (d, J = 8.4 Hz, 2 H, Ar-H), 6.02 (t, J = 4.8 Hz, 1 H, Ar-H), 5.10 (d, J = 16.8 Hz, 1 H, one proton of =CH_2), 4.98 (d, J = 10.8 Hz, 1 H, one proton of =CH_2), 3.11 (s, 3 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.7, 157.8, 157.4, 140.7, 136.5, 135.7, 132.7, 132.0, 130.4, 129.5, 129.3, 123.1, 121.8, 120.6, 117.0, 114.5, 114.1, 113.5, 108.2, 55.1; MS (ESI) *m/z* 354 $(M+H)^+$; IR (neat, cm^{-1}): 1598, 1561, 1506, 1451, 1420, 1346, 1299, 1249, 1211, 1174, 1149, 1111, 1093, 1078, 1030; HRMS (ESI) Calcd for $C_{23}H_{20}N_3O$ $(M+H)^+$: 354.1601, Found: 354.1597.

The following signals are discernible for (*E*-**3ac**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.64 (d, J = 8.4 Hz, 1 H, Ar-H), 7.62 (d, J = 7.2 Hz, 1 H, Ar-H), 7.26 (t, J = 7.5 Hz, 1 H, Ar-H), 6.93 (s, 1 H, Ar-H), 6.77 (d, J = 5.4 Hz, 2 H, Ar-H), 5.20 (d, J = 17.4 Hz, 1 H, one proton of =CH_2), 4.91 (d, J = 10.8 Hz, 1 H, one proton of =CH_2), 3.31 (s, 3 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.0, 131.0.

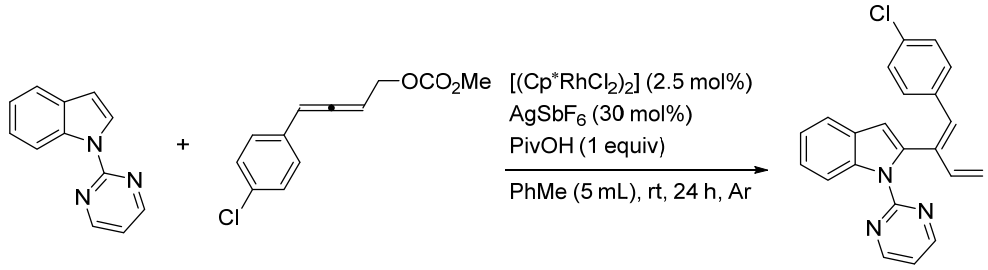
(4) 2-[(*Z*)-1-(4-fluorophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ad (zyz-5-81)



Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (15.7 mg, 0.025 mmol), $AgSbF_6$ (103.2mg, 0.3 mmol), **1a** (195.7 mg, 1.0 mmol), PivOH (103.5 mg, 1 mmol)/toluene (2 mL), and **2d** (244.9 mg, 1.1 mmol)/toluene (3 mL) afforded **3ad** (286.4 mg, 84%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.71 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.00 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.52 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.36-7.32 (m, 1 H, Ar-H), 7.24-7.20 (m, 1 H, Ar-H), 6.96-6.92 (m, 2 H, Ar-H), 6.64 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.54 (s, 1 H, Ar-H), 6.52 (s, 1 H, =CH), 6.45 (t, *J* = 8.7 Hz, 2 H, Ar-H), 5.97 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.11 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 161.7 (d, *J* = 245.9 Hz), 157.8, 157.3, 140.2 (d, *J* = 4.6 Hz), 136.5, 135.0, 133.7, 132.7 (d, *J* = 3.0 Hz), 131.5 (d, *J* = 6.8 Hz), 130.6 (d, *J* = 7.6 Hz), 129.3, 123.4, 121.9, 120.6, 117.0, 115.6, 114.9 (d, *J* = 21.3 Hz), 114.0, 108.5 (d, *J* = 8.4 Hz); ^{19}F NMR (376 MHz, $CDCl_3$) δ -114.6; MS (ESI) *m/z* 342 $(M+H)^+$; IR (neat, cm^{-1}): 1596, 1561, 1503, 1475, 1451, 1420, 1346, 1309, 1267, 1219, 1178, 1156, 1113, 1095, 1078, 1036, 1013; HRMS (ESI) Calcd for $C_{22}H_{17}FN_3$ $(M+H)^+$: 342.1401, Found: 342.1403.

The following signals are discernible for (*E*-**3ad**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.68 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.63 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.27 (t, *J* = 7.8 Hz, 1 H, Ar-H), 6.85 (dd, J_1 = 17.1 Hz, J_2 = 11.1 Hz, 1 H, =CH), 6.74 (s, 1 H, =CH), 6.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.16 (d, *J* = 16.8 Hz, 1 H, one proton of =CH), 4.87 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$).

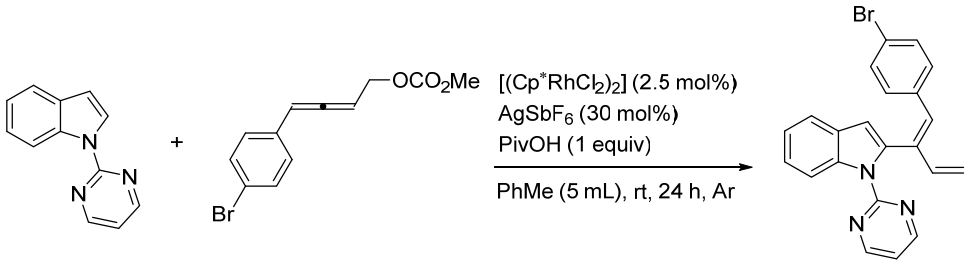
(5) 2-[(*Z*)-1-(4-chlorophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ae (zyz-5-76)



Following **Typical Procedrue II**, the reaction of $[(Cp^*RhCl_2)_2]$ (15.7 mg, 0.025 mmol), $AgSbF_6$ (103.5 mg, 0.3 mmol), **1a** (195.9 mg, 1.0 mmol), PivOH (104.3 mg, 1 mmol) /toluene (2 mL), and **2e** (264.2 mg, 1.1 mmol)/toluene (3 mL) afforded **3ae** (255.1 mg, 71%, *Z/E* = 97/3) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.70 (d, *J* = 7.8 Hz, 1 H, Ar-H), 8.01 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.51 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.35-7.32 (m, 1 H, Ar-H), 7.23-7.20 (m, 1 H, Ar-H), 6.88 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.75 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.61 (dd, J_1 = 16.8 Hz, J_2 = 10.2 Hz, 1 H, =CH), 6.51 (s, 1 H, Ar-H), 6.48 (s, 1 H, =CH), 6.00 (t, *J* = 4.5 Hz, 1 H, Ar-H), 5.08 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 4.97 (d, *J* = 10.2 Hz, 1 H, one proton of $=CH_2$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.3, 140.1, 136.5, 135.1, 134.9, 134.5, 132.7, 131.4, 130.2, 129.3, 128.1, 123.4, 122.0, 120.7, 117.0, 116.0, 114.1, 108.6; MS (ESI) *m/z* 360 $(M(^{37}Cl)+H)^+$, 358 $(M(^{35}Cl)+H)^+$; IR (neat, cm^{-1}): 1561, 1486, 1451, 1420, 1368, 346, 1310, 1301, 1266, 1236, 1211, 1177, 1149, 1112, 1088, 1036, 1010; HRMS (ESI) Calcd for $C_{22}H_{17}{}^{35}ClN_3$ $(M+H)^+$: 358.1106, Found: 358.1111.

The following signals are discernible for (*E*-**3ae**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.66 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.04 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.62 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.26 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.82 (dd, J_1 = 18.0 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.03 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.15 (d, *J* = 18.0 Hz, 1 H, one proton of =CH), 4.87 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$).

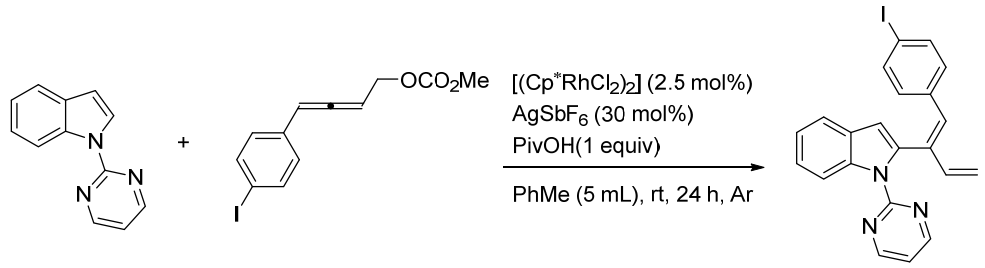
(6) 2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3af (zyz-5-83)



Following **Typical Procedrue III**, the reaction of [(Cp*RhCl$_2$)$_2$] (15.6 mg, 0.025 mmol), $AgSbF_6$ (104.0 mg, 0.3 mmol), **1a** (195.0 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2f** (314.2 mg, 1.1 mmol)/toluene (3 mL) afforded **3af** (342.8 mg, 85%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) 8.71 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.99 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.51 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.37-7.32 (m, 1 H, Ar-H), 7.23-7.20 (m, 1 H, Ar-H), 6.91-6.85 (m, 2 H, Ar-H), 6.82-6.78 (m, 2 H, Ar-H), 6.60 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.50 (s, 1 H, Ar-H), 6.44 (s, 1 H, =CH), 5.97 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.08 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.97 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.3, 140.1, 136.5, 135.5, 134.9, 134.7, 131.4, 131.1, 130.5, 129.3, 123.4, 122.0, 121.0, 120.7, 117.0, 116.1, 114.1, 108.6; MS (ESI) *m/z* 404 (M(^{81}Br)+H)$^+$, 402 (M(^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 1601, 1561, 1483, 1451, 1421, 1368, 1346, 1301, 1266, 1236, 1211, 1178, 1149, 1112, 1071, 1036, 1006; HRMS (ESI) Calcd for $C_{22}H_{17}{}^{79}BrN_3$ (M+H)$^+$: 402.0600, Found: 402.0599.

The following signals are discernible for (*E*-**3af**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.67 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.62 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.27 (t, *J* = 7.8 Hz, 1 H, Ar-H), 7.01 (d, *J* = 7.8 Hz, 2 H, Ar-H), 6.71 (s, 1 H, Ar-H), 6.67 (s, 1 H, =CH), 6.01 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.15 (d, *J* = 18.6 Hz, 1 H, one proton of =CH_2), 4.86 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

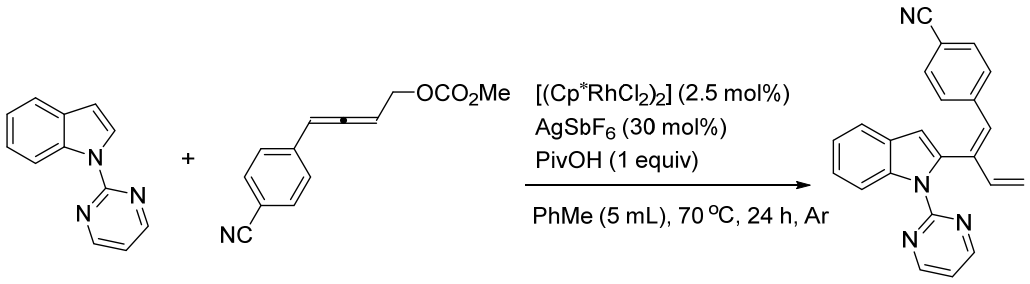
(7) 2-[(*Z*)-1-(4-iodophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ag (zyz-5-86)



Following **Typical Procedrue III**, the reaction of [(Cp*RhCl$_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (103.5 mg, 0.3 mmol), **1a** (195.9 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2g** (365.5 mg, 1.1 mmol)/toluene (3 mL) afforded **3ag** (363.6 mg, 81%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.72 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.99 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.51 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.36-7.32 (m, 1 H, Ar-H), 7.21 (t, *J* = 7.5 Hz, 1 H, Ar-H), 7.08 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.68 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.61 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.49 (s, 1 H, Ar-H), 6.43 (s, 1 H, =CH), 5.96 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.07 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.96 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.3, 140.1, 137.0, 136.5, 136.1, 134.84, 134.82, 131.5, 130.7, 129.3, 123.4, 122.0, 120.7, 117.0, 116.1, 114.1, 108.5, 92.7; MS (ESI) *m/z* 450 $(M+H)^+$; IR (neat, cm^{-1}): 1602, 1561, 1481, 1451, 1422, 1368, 1346, 1301, 1266, 1236, 1212, 1178, 1149, 1112, 1078, 1060, 1036, 1002; HRMS (ESI) Calcd for $C_{22}H_{17}IN_3$ $(M+H)^+$: 450.0462, Found: 450.0468.

The following signals are discernible for (*E*-**3ag**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.67 (d, *J* = 7.8 Hz, 1 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.62 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.44 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.27 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.88 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.80 (dd, J_1 = 17.7 Hz, J_2 = 10.5 Hz, 1 H, =CH); 6.71 (s, 1 H, Ar-H), 6.66 (s, 1 H, =CH), 6.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.15 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.86 (d, *J* = 9.6 Hz, 1 H, one proton of =CH_2).

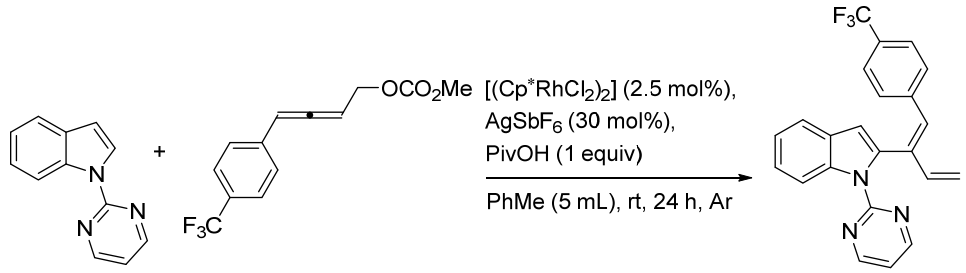
(8) 2-[(*Z*)-1-(4-cyanophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ah (zyz-5-122)



Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (102.1 mg, 0.3 mmol), **1a** (195.9 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol) /toluene (2 mL), and **2h** (254.5 mg, 1.1 mmol)/toluene (3 mL) at 70 °C afforded **3ah** (267.7 mg, 77%, *Z/E* = 73/27) (eluent: petroleum ether/ethyl acetate = 6/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.69 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.98 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.51 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.38-7.32 (m, 1 H, Ar-H), 7.21 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.77 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.65 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.55 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.42 (s, 1 H, Ar-H), 6.35 (s, 1 H, =CH), 6.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.08 (d, *J* = 16.8 Hz, 1 H, one proton of =CH_2), 4.98 (d, *J* = 10.2 Hz, 1 H, one proton of =CH_2); MS (ESI) *m/z* 349 $(M+H)^+$; IR (neat, cm^{-1}): 2223, 1600, 1561, 1498, 1451, 1420, 1346, 1306, 1237, 1212, 1176, 1149, 1112, 1078, 1036, 1015; Anal. calcd for $C_{23}H_{16}N_4$ (%): C 79.29, H 4.63, N 16.08, Found: C 79.18, H 4.96, N 16.00.

The following signals are discernible for (*E*-**3ah**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.67 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.62 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.26 (t, *J* = 7.5 Hz, 1 H, Ar-H), 7.01 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.65 (d, *J* = 7.8 Hz, 2 H, Ar-H), 6.59 (s, 1 H, =CH), 6.04 (t, *J* = 4.5 Hz, 1 H, Ar-H), 5.13 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.86 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

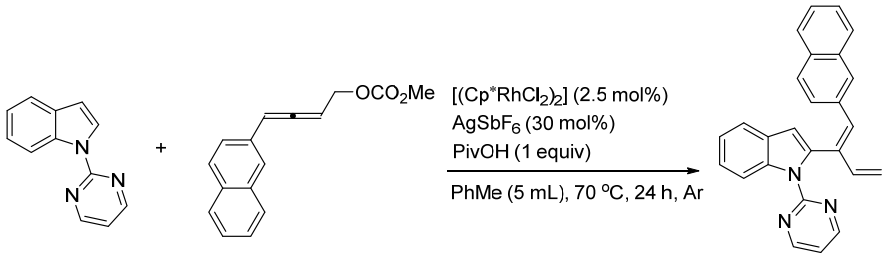
(9) 2-[(*Z*)-1-(4-(trifluoromethyl)phenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ai (zyz-5-96)



Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (102.1 mg, 0.3 mmol), **1a** (195.9 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2i** (301.1 mg, 1.1 mmol)/toluene (3 mL) afforded **3ai** (336.3 mg, 86%, *Z/E*= 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.73 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.99 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.50 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.37-7.33 (m, 1 H, Ar-H), 7.24-7.19 (m, 1 H, Ar-H), 7.01-6.95 (m, 4 H, Ar-H), 6.60 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.48 (s, 2 H, Ar-H and =CH), 5.97 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.09 (d, *J* = 16.8 Hz, 1 H, one proton of =CH_2), 4.98 (d, *J* = 10.2 Hz, 1 H, one proton of =CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.2, 140.2, 139.9, 136.5, 136.2, 134.6, 130.9, 129.2, 129.1, 128.4 (q, *J* = 32.2 Hz), 124.8 (q, *J* = 3.6 Hz), 124.1 (q, *J* = 270.3 Hz), 123.5, 122.0, 120.7, 117.0, 116.9, 114.2, 108.7; ^{19}F NMR (376 MHz, $CDCl_3$) δ -63.1; MS (ESI) *m/z* 392 $(M+H)^+$; IR (neat, cm^{-1}): 1611, 1561, 1475, 1452, 1422, 1347, 1320, 1238, 1213, 1162, 1108, 1065, 1037, 1014; HRMS (ESI) Calcd for $C_{25}H_{17}N_3F_3$ $(M+H)^+$: 392.13691, Found: 392.13745.

The following signals are discernible for (*E*-**3ai**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.69 (d, *J* = 9.0 Hz, 1 H, Ar-H), 8.04 (d, *J* = 4.2 Hz, 2 H, Ar-H), 7.64 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.28 (t, *J* = 7.8 Hz, 1 H, Ar-H), 6.78 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.73 (s, 1 H, Ar-H), 6.70 (s, 1 H, =CH), 6.01 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.17 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.89 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

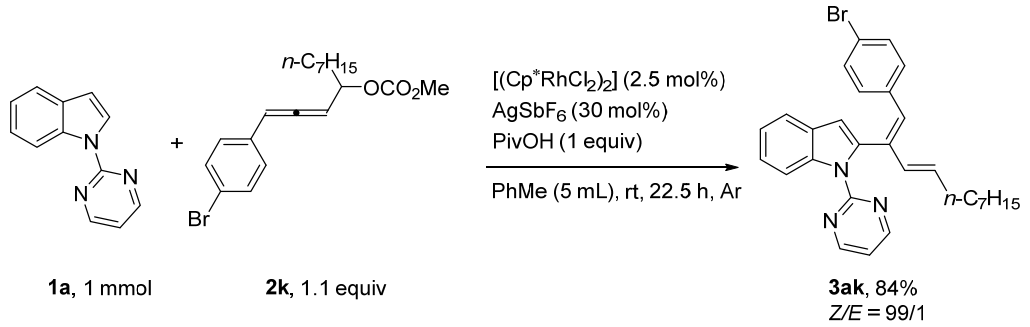
(10) 2-[(*Z*)-1-(2-naphthalenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3aj (zyz-5-123)



Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (15.5 mg, 0.025 mmol), $AgSbF_6$ (103.5 mg, 0.3 mmol), **1a** (195.1 mg, 1.0 mmol), PivOH (102.5 mg, 1 mmol)/toluene (2 mL), and **2j** (281.3 mg, 1.1 mmol)/toluene (3 mL) at 70 °C afforded **3aj** (299.9 mg, 80%, *Z/E* = 95/5) (eluent: petroleum ether/ethyl acetate = 15/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.74 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.98 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.55-7.50 (m, 2 H, Ar-H), 7.44-7.41 (m, 1 H, Ar-H), 7.40-7.33 (m, 3 H, Ar-H), 7.25-7.21 (m, 1 H, Ar-H), 7.18-7.16 (m, 1 H, Ar-H), 7.12-7.05 (m, 2 H, Ar-H), 6.83 (s, 1 H, Ar-H), 6.76 (dd, J_1 = 16.8 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.61 (s, 1 H, =CH), 5.93 (t, *J* = 4.5 Hz, 1 H, Ar-H), 5.17 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 5.02 (d, *J* = 10.2 Hz, 1 H, one proton of $=CH_2$); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.4, 140.5, 136.6, 135.4, 134.4, 134.3, 133.1, 132.9, 132.4, 129.4, 128.7, 128.0, 127.5, 127.3, 126.4, 125.8, 123.3, 121.9, 120.7, 116.9, 115.6, 114.1, 108.8; MS (ESI) *m/z* 374 $(M+H)^+$; IR (neat, cm^{-1}): 1603, 1561, 1505, 1451, 1421, 1347, 1306, 1268, 1238, 1210, 1179, 1149, 1125, 1078, 1036, 1016; Anal. calcd for $C_{26}H_{19}N_3$ (%): C 83.62, H 5.13, N 11.25, Found: C 83.26, H 5.43, N 10.71.

The following signals are discernible for (*E*-**3aj**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.69 (d, *J* = 9.0 Hz, 1 H, Ar-H), 8.05 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.85 (s, 1 H, Ar-H), 7.65 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.29 (t, *J* = 6.9 Hz, 1 H, Ar-H), 7.05 (s, 1 H, Ar-H), 5.99 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.25 (d, *J* = 18.0 Hz, 1 H, one proton of $=CH_2$), 4.93 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$).

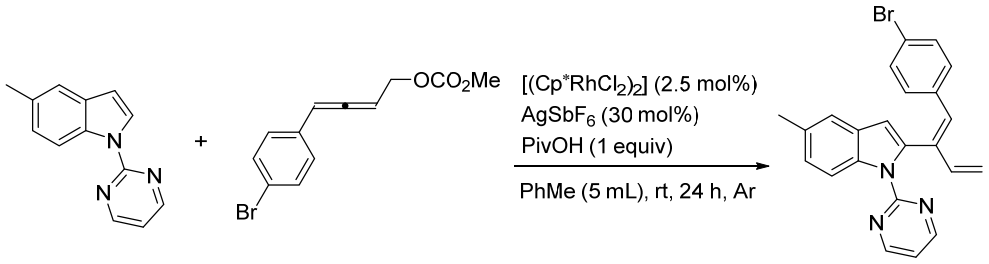
(11) 2-[(1*Z*,3*E*)-1-(4-bromophenyl)-1,3-undecadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ak (wj-2-45)



Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.6 mg, 0.025 mmol), $AgSbF_6$ (103.4 mg, 0.3 mmol), **1a** (195.2 mg, 1.0 mmol), PivOH (102.4 mg, 1 mmol)/toluene (2 mL), and **2k** (419.3 mg, 1.1 mmol)/toluene (3 mL) afforded **3ak** (420.9 mg, 84%, *Z/E*= 99/1) (eluent: petroleum ether/ethyl acetate = 40/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.70 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.05 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.52 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.36-7.31 (m, 1 H, Ar-H), 7.23-7.19 (m, 1 H, Ar-H), 6.94 (d, *J* = 9.0 Hz, 2 H, Ar-H), 6.89 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.55 (s, 1 H, Ar-H), 6.47 (s, 1 H, =CH), 6.38 (d, *J* = 15.0 Hz, 1 H, =CH), 6.02 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.62-5.54 (m, 1 H, =CH), 1.94-1.85 (m, 2 H, CH_2), 1.28-1.21 (m, 2 H, CH_2), 1.17-1.02 (m, 8 H, 4xCH_2), 0.88 (t, *J* = 7.2 Hz, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) 157.8, 157.4, 136.5, 136.2, 136.0, 134.7, 134.0, 133.4, 131.0, 130.4, 129.3, 129.0, 123.3, 121.9, 120.7, 120.4, 117.0, 113.9, 108.2, 32.8, 31.7, 29.2, 29.0, 28.9, 22.6, 14.1; MS (ESI) *m/z* 502 (M(^{81}Br)+H)$^+$, 500 (M(^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 3022, 2924, 2853, 1563, 1484, 1452, 1425, 1374, 1347, 1304, 1264, 1236, 1213, 1179, 1150, 1072, 1008; HRMS (ESI) Calcd for $C_{29}H_{31}N_3{}^{79}Br$ (M+H)$^+$: 500.1696, Found: 500.1703

The following signals are discernible for (*E*-**3ak**): ^{1}H NMR (400 MHz, C_6D_6) δ 8.65 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.08 (d, *J* = 4.8 Hz, 2 H, Ar-H), 6.68 (s, 1 H, Ar-H), 6.60 (d, *J* = 16.8 Hz, 1 H, =CH), 6.52 (s, 1 H, =CH), 6.06 (t, *J* = 4.8 Hz, 1 H, Ar-H).

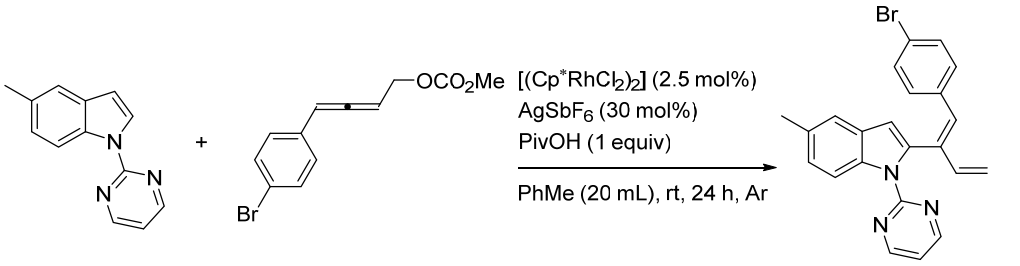
(12) 2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-5-methyl-1-(2-pyrimidinyl)-1*H*-indole 3bf (zyz-5-90)



Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (15.7 mg, 0.025 mmol), $AgSbF_6$ (102.1 mg, 0.3 mmol), **1b** (209.9 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2f** (313.2 mg, 1.1 mmol)/toluene (3 mL) afforded **3bf** (369.6 mg, 89%, *Z/E* = 95/5) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) 8.69 (d, *J* = 9.0 Hz, 1 H, Ar-H), 8.00 (d, *J* = 4.8 Hz, 1 H, Ar-H), 7.27 (s, 1 H, Ar-H), 7.21 (d, *J* = 8.4 Hz, 1 H, Ar-H), 6.92 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.83 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.63 (dd, J_1 = 17.4 Hz, J_2 = 10.2 Hz, 1 H, =CH), 6.48 (s, 1 H, Ar-H), 6.46 (s, 1 H, =CH), 5.96 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.12 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 4.98 (d, *J* = 10.8 Hz, 1 H, $=CH_2$), 2.34 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.3, 140.2, 135.6, 134.92, 134.84, 131.4, 131.2, 131.1, 130.5, 129.5, 124.9, 120.9, 120.4, 116.8, 116.0, 114.0, 108.4, 21.3; MS (ESI) *m/z* 418 $(M(^{81}Br)+H)^+$, 416 $(M(^{79}Br)+H)^+$; IR (neat, cm^{-1}): 1570, 1559, 1484, 1423, 1339, 1316, 1294, 1266, 1240, 1217, 1183, 1149, 1071, 1036, 1007; HRMS (ESI) Calcd for $C_{23}H_{19}N_3{}^{79}Br$ $(M+H)^+$: 416.07569, Found: 416.07588.

The following signals are discernible for (*E*-**3bf**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.66 (d, *J* = 8.4 Hz, 2 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.41 (s, 1 H, Ar-H), 7.02 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.72 (s, 1 H, Ar-H), 6.69 (s, 1 H, =CH), 5.99 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.18 (d, *J* = 16.8 Hz, 1 H, one proton of CH_2), 4.87 (d, *J* = 10.8 Hz, 1 H, one proton of CH_2), 2.39 (s, 3 H, CH_3).

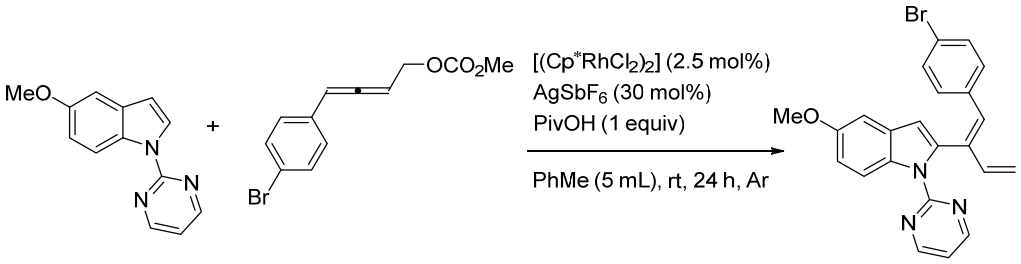
(13) Gram-scale synthesis of 3bf (zyz-5-142)



Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (61.5 mg, 0.1 mmol), $AgSbF_6$ (413.0 mg, 1.2 mmol), **1b** (837.7 mg, 4.0 mmol), PivOH (402.7 mg, 4 mmol)/toluene (8 mL), and **2f** (1.2470 g, 4.4 mmol)/toluene (12 mL) afforded **3bf** (1.4149 g, 85%, *Z/E* = 95/5) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, $CDCl_3$) 8.69 (d, *J* = 9.0 Hz, 1 H, Ar-H), 8.00 (d, *J* = 4.2 Hz, 2 H, Ar-H), 7.27 (s, 1 H, Ar-H), 7.21 (m, 1 H, Ar-H), 6.92 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.83 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.63 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.48 (s, 1 H, Ar-H), 6.46 (s, 1 H, =CH), 5.93 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.12 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 4.98 (d, *J* = 10.2 Hz, 1 H, $=CH_2$), 2.34 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 157.3, 140.2, 135.6, 134.9, 134.8, 131.3, 131.2, 131.0, 130.4, 129.5, 124.9, 120.9, 120.4, 116.7, 116.0, 114.0, 108.3, 21.3.

The following signals are discernible for (*E*-**3bf**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.66 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.41 (s, 1 H, Ar-H), 7.02 (d, *J* = 7.8 Hz, 2 H, Ar-H), 6.72 (s, 1 H, Ar-H), 6.69 (s, 1 H, =CH), 6.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.18 (d, *J* = 16.8 Hz, 1 H, one proton of CH_2), 4.87 (d, *J* = 10.8 Hz, 1 H, one proton of CH_2), 2.39 (s, 3 H, CH_3).

(14) 2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-5-methoxy-1-(2-pyrimidinyl)-1*H*-indole 3cf (zyz-5-94)

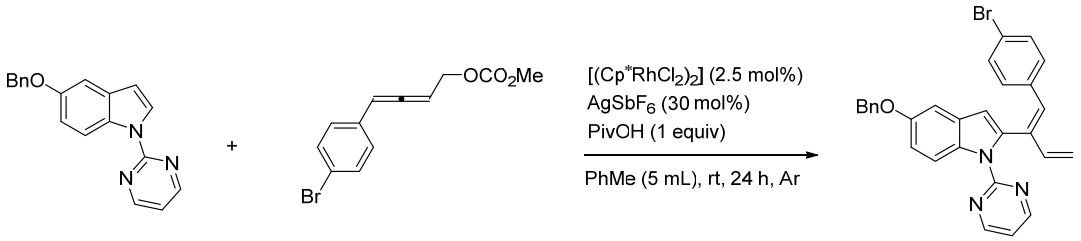


1c, 0.2 mmol **2f**, 1.1 equiv **3cf**, 85%, *Z/E* = 96/4

Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.9 mg, 0.025 mmol), $AgSbF_6$ (103.5 mg, 0.3 mmol), **1c** (225.9 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (3 mL), and **2f** (316.2 mg, 1.1 mmol)/toluene (3 mL) afforded **3cf** (367.9 mg, 85%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 20/1) as white solid: mp. 185.7-186.7 ºC (petroleum ether/ethyl acetate); ^{1}H NMR (600 MHz, $CDCl_3$) 8.60 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.28 (d, *J* = 9.0 Hz, 1 H, Ar-H), 7.19 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.03 (d, *J* = 3.0 Hz, 1 H, Ar-H), 7.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.95 (dd, J_1 = 9.3 Hz, J_2 = 2.7 Hz, 1 H, Ar-H), 6.88 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.64 (dd, J_1 = 17.1 Hz, J_2 = 11.1 Hz, 1 H, =CH), 6.58 (s, 1 H, Ar-H), 6.42 (s, 1 H, =CH), 5.04 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2), 4.96 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 3.87 (s, 3 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.2, 155.5, 140.2, 135.6, 135.4, 134.9, 131.5, 131.2, 131.1, 130.5, 130.0, 121.0, 116.8, 116.0, 115.3, 112.9, 108.5, 102.6, 55.7; MS (ESI) *m/z* 434 (M(^{81}Br)+H)$^+$, 432 (M(^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 1609, 1575, 1561, 1478, 1466, 1447, 1419, 1327, 1297, 1245, 1209, 1185, 1153, 1121, 1084, 1075, 1036, 1008; Anal. calcd for $C_{23}H_{18}N_3OBr$ (%):C 63.90, H 4.20, N 9.72, Found: C 63.93, H 4.30, N 9.56.

The following signals are discernible for (*E*-**3cf**): ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.67 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.19 (d, *J* = 9.0 Hz, 1 H, Ar-H), 7.49 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.28 (d, *J* = 7.8 Hz, 2 H, Ar-H), 7.09 (d, *J* = 2.4 Hz, 1 H, Ar-H), 6.75-6.60 (m, 3 H, 2x=CH and Ar-H), 4.99 (d, *J* = 9.6 Hz, 1 H, one proton of =CH_2), 3.89 (s, 3 H, OCH_3).

(15) 5-Benzyloxy-2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole 3df (zyz-6-172)

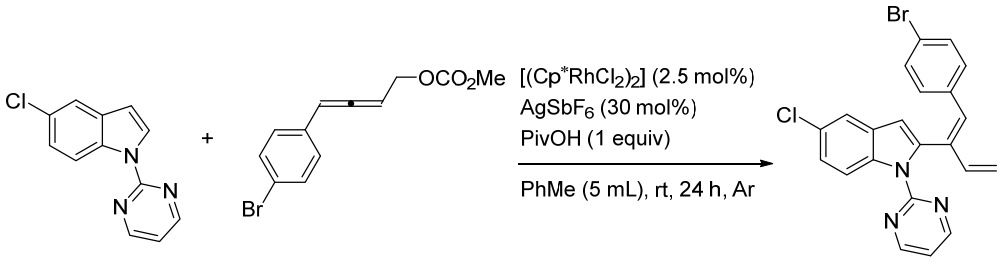


1d, 1 mmol **2f**, 1.1 equiv **3df**, 84% *Z*/*E* = 96/4

Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (103.2 mg, 0.3 mmol), **1d** (302.7 mg, 1.0 mmol), PivOH (103.1 mg, 1 mmol)/toluene (2 mL), and **2f** (310.2 mg, 1.1 mmol)/toluene (3 mL) afforded **3df** (427.3 mg, 84%, *Z*/*E* = 96/4) (eluent: petroleum ether/ethyl acetate = 20/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.68 (d, *J* = 9.0 Hz, 1 H, Ar-H), 8.00 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.35 (d, *J* = 7.2 Hz, 2 H, Ar-H), 7.25 (dd, J_1 = 9.0 Hz, J_2 = 2.4 Hz, 1 H, Ar-H), 7.19-7.15 (m, 1 H, Ar-H), 7.10 (t, *J* = 7.2 Hz, 1 H, Ar-H), 7.05 (d, *J* = 2.4 Hz, 1 H, Ar-H), 6.94 (d, *J* = 9.0 Hz, 2 H, Ar-H), 6.84 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.64 (dd, J_1 = 17.1 Hz, J_2 = 11.1 Hz, 1 H, =CH), 6.47 (s, 1 H, Ar-H), 6.44 (s, 1 H, =CH), 5.98 (t, *J* = 4.5 Hz, 1 H, Ar-H), 5.11 (d, *J* = 16.8 Hz, 1 H, one proton of =CH_2), 4.99 (d, *J* = 10.2 Hz, 1 H, one proton of =CH_2), 4.86 (s, 2 H, OCH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.8, 157.2, 154.7, 140.2, 137.4, 135.6, 135.4, 134.9, 131.6, 131.2, 131.1, 130.5, 130.0, 128.5, 127.8, 127.5, 121.0, 116.8, 116.0, 115.3, 113.5, 108.5, 104.0, 70.6; MS (ESI) *m/z* 510 (M(^{81}Br)+H)$^+$, 508 (M(^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 1610, 1571, 1561, 1474, 1447, 1424, 1381, 1327, 1289, 1248, 1193, 1156, 1117, 1072, 1023, 1007; HRMS (ESI) Calcd for $C_{29}H_{22}N_3O^{79}BrNa$ (M+Na)$^+$: 530.08385, Found: 530.08336.

The following signals are discernible for (*E*-**3df**): ^{1}H NMR (600 MHz, C_6D_6) 8.64 (d, *J* = 9.0 Hz, 1 H, Ar-H), 8.03 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.37 (d, *J* = 6.6 Hz, 1 H, Ar-H), 6.69 (s, 1 H, Ar-H), 6.68 (s, 1 H, =CH), 6.01 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.18 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.91 (s, 2 H, OCH_2), 4.88 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

(16) 2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-5-chloro-1-(2-pyrimidinyl)-1*H*-indole 3ef (zyz-5-92)

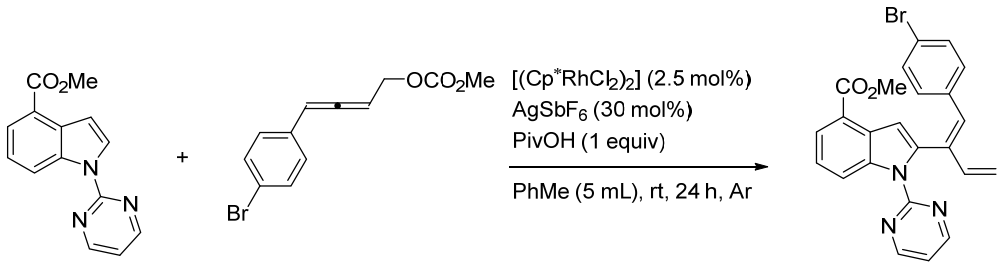


1e, 1 mmol **2f**, 1.1 equiv **3ef**, 85% *Z*/*E* = 96/4

Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (103.8 mg, 0.3 mmol), **1e** (229.0 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2f** (311.0 mg, 1.1 mmol)/toluene (3 mL) afforded **3ef** (369.1 mg, 85%, *Z*/*E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.44 (d, *J* = 9.0 Hz, 1 H, Ar-H), 7.94 (d, *J* = 4.8 Hz, 1 H, Ar-H), 7.44 (d, *J* = 1.8 Hz, 1 H, Ar-H), 7.33 (dd, J_1 = 8.7 Hz, J_2 = 2.1 Hz, 1 H, Ar-H), 6.94 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.75 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.56 (dd, J_1 = 17.1 Hz, J_2 = 10.5 Hz, 1 H, =CH), 6.42 (s, 1 H, Ar-H), 6.26 (s, 1 H, =CH), 5.96 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.00 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.95 (d, *J* = 10.2 Hz, 1 H, one proton of =CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 157.0, 139.9, 136.3, 135.4, 134.8, 134.3, 131.7, 131.1, 130.4, 130.3, 127.5, 123.6, 121.1, 120.0, 117.3, 116.1, 115.4, 107.8; MS (ESI) *m/z* 440 (M(^{37}Cl+^{81}Br)+H)$^+$, 438 [(M(^{37}Cl+^{79}Br)+H)$^+$ and (M(^{35}Cl+^{81}Br)+H)$^+$], 436 (M(^{35}Cl+^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 1603, 1560, 1484, 1441, 1421, 1338, 1311, 1280, 1264, 1233, 1208, 1175, 1127, 1068, 1032, 1007; HRMS (ESI) Calcd for $C_{22}H_{16}N_3{}^{35}Cl^{79}Br$ (M+H)$^+$: 436.02106, Found: 436.02055.

The following signals are discernible for (*E*-**3ef**): ^{1}H NMR (600 MHz, C_6D_6) δ 7.97 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.57 (d, *J* = 2.4 Hz, 1 H, Ar-H), 7.24 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.00 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.47 (s, 1 H, =CH), 6.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.05 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.83 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

(17) Methyl 2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole- 4-carboxylate 3ff (zyz-5-104)

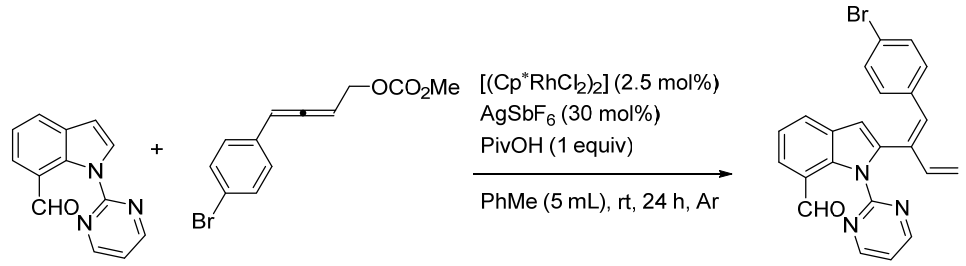


1f, 1 mmol **2f**, 1.1 equiv **3ff**, 85% *Z/E* = 97/3

Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.6 mg, 0.025 mmol), $AgSbF_6$ (102.7 mg, 0.3 mmol), **1f** (253.6 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2f** (314.7 mg, 1.1 mmol)/toluene (3 mL) afforded **3ff** (391.3 mg, 85%, *Z/E* = 97/3) (eluent: petroleum ether/ethyl acetate = 15/1) as an oil: ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.62 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.48 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.01 (dd, J_1 = 7.5 Hz, J_2 = 0.9 Hz, 1 H, Ar-H), 7.35 (t, *J* = 7.8 Hz, 1 H, Ar-H), 7.24 (s, 1 H, Ar-H), 7.16 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.05 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.81 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.65 (dd, J_1 = 16.8 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.60 (s, 1 H, =CH), 5.10 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2), 5.02 (d, *J* = 16.8 Hz, 1 H, one proton of =CH_2), 3.95 (s, 3 H, OCH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.6, 157.9, 156.9, 139.8, 137.1, 136.8, 135.2, 134.0, 131.9, 131.1, 130.3, 128.9, 125.2, 122.6, 121.5, 121.1, 118.6, 117.5, 116.5, 109.2, 51.8; MS (ESI) m/z 462 (M(^{81}Br)+H)$^+$, 460 (M(^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 1709, 1597, 1562, 1484, 1421, 1368, 1348, 1312, 1286, 1230, 1193, 1068, 1043, 1008; HRMS (ESI) Calcd for $C_{24}H_{18}N_3O_2Na^{79}Br$ (M+H)$^+$: 482.04746, Found: 482.04726.

The following signals are discernible for (*E*-**3ff**): ^{1}H NMR (600 MHz, $CDCl_3$) δ 8.71 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.43 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.29 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.11 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.85 (s, 1 H, =CH), 4.98 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2), 4.00 (s, 3 H, OCH_3).

(18) 2-[(*Z*)-1-(4-bromophenyl)-1,3-butadien-2-yl]-1-(2-pyrimidinyl)-1*H*-indole-7-carbaldehyde 3gf (zyz-5-119)

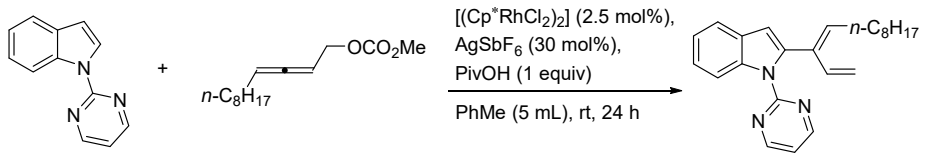


1g, 1 mmol **2f**, 1.1 equiv **3gf**, 78%
Z/E = 91/9

Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (15.7 mg, 0.025 mmol), $AgSbF_6$ (103.5 mg, 0.3 mmol), **1g** (223.9 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2f** (315.2 mg, 1.1 mmol)/toluene (3 mL) afforded **3gf** (338.2 mg, 78%, *Z/E* = 91/9) (eluent: petroleum ether/ethyl acetate = 5/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 9.71 (s, 1 H, CHO), 8.07 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.53 (dd, J_1 = 7.8 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.36 (dd, J_1 = 7.5 Hz, J_2 = 0.9 Hz, 1 H, Ar-H), 7.02 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.87 (s, 4 H, Ar-H), 6.44 (s, 1 H, =CH), 6.43-6.37 (m, 2 H, =CH and Ar-H), 6.16 (t, *J* = 4.8 Hz, 1 H, Ar-H), 4.97 (d, *J* = 17.4 Hz, 1 H, one proton of =CH_2), 4.91 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2); MS (ESI) *m/z* 432 (M(^{81}Br)+H)$^+$, 430 (M(^{79}Br)+H)$^+$; IR (neat, cm^{-1}): 1686, 1580, 1563, 1485, 1436, 1415, 1307, 1288, 1255, 1179, 1166, 1121, 1072, 1051, 1025, 1008; Anal. calcd for $C_{23}H_{16}BrN_3O$ (%): C 64.20, H 3.75, N 9.77, Found: C 64.29, H 3.99, N 9.58.

The following signals are discernible for (*E*-**3gf**): ^{1}H NMR (600 MHz, C_6D_6) δ 9.73 (s, 1 H, CHO), 8.11 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.60 (dd, J_1 = 7.5 Hz, J_2 = 0.9 Hz, 1 H, Ar-H), 7.41 (dd, J_1 = 7.2 Hz, J_2 = 1.2 Hz, 1 H, Ar-H), 7.20 (d, *J* = 9.0 Hz, 2 H, Ar-H), 6.89 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.63 (s, 1 H, =CH), 6.61-6.58 (m, 2 H, =CH and Ar-H), 6.19 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.08 (d, *J* = 18.0 Hz, 1 H, one proton of =CH_2), 4.85 (d, *J* = 10.8 Hz, 1 H, one proton of =CH_2).

(19) 2-[(*E*)-dodeca-1,3-dien-3-yl]-1-(2-pyrimidinyl)-1*H*-indole 3al (zyz-6-63)



1a, 1 mmol **2l**, 1.1 equiv **3al**, 50%
E/*Z* = 90/10

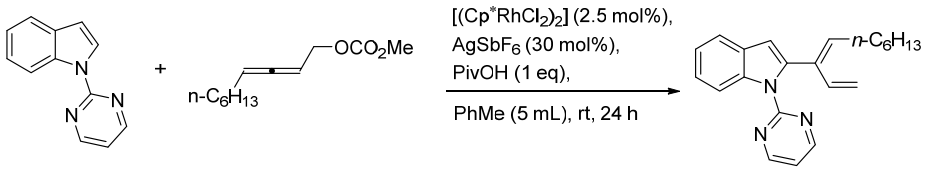
Following **Typical Procedrue III**, the reaction of [(Cp*RhCl$_2$)$_2$] (15.6 mg, 0.025 mmol), AgSbF$_6$ (102.0 mg, 0.3 mmol), **1a** (195.9 mg, 1.0 mmol), PivOH (103.7 mg, 1 mmol)/toluene (2 mL), and **2l** (266.1 mg, 1.1 mmol)/toluene (2 mL) afforded 54% NMR yield of **3al** with 91/9 *E*/*Z* ratio as determined by the ^{1}H NMR analysis of the crude product. The crude product was purified by column chromatography on silica gel to afford pure *E*-**3al** (154.6 mg, 43%) and a *Z*/*E* mixture of **3al** (25.0 mg, 7%, *Z*-**3al**/*E*-**3al** = 2.5/1). The yield and *Z*/*E* were calculated based on these data (179.6 mg, 50%, *E*/*Z* = 90/10) (eluent: petroleum ether/ethyl acetate = 30/1). Further purification of the *Z*/*E* mixture of **3al** via thin layer chromatography afforded *Z*-**3al** (12.3 mg, 3%) (eluent: petroleum ether/ethyl acetate = 40/1)

E-**3al** (major, the more polar isomer), oil: ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.70 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.17 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.60 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.30-7.16 (m, 2 H, Ar-H), 7.08 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.75-6.52 (m, 2 H, Ar-H and =CH), 5.86 (t, *J* = 7.4 Hz, 1 H, =CH), 4.90-4.78 (m, 2 H, =CH$_2$), 2.31 (q, *J* = 7.3 Hz, 2 H, CH$_2$), 1.51-1.42 (m, 2 H, CH$_2$), 1.40-1.22 (m, 10 H, 5xCH$_2$), 0.94-0.78 (m, 3 H, CH$_3$); ^{13}C NMR (100 MHz, CDCl$_3$) 157.93, 157.89, 140.3, 136.8, 134.5, 133.0, 132.7, 129.1, 123.1, 121.7, 120.3, 117.1, 115.5, 113.2, 108.1, 31.9, 29.5, 29.4, 29.3, 29.2, 28.1, 22.7, 14.1; MS (ESI) *m/z* 360 (M+H)$^+$; IR (neat, cm^{-1}): 3042, 2922, 2852, 1572, 1561, 1453, 1422, 1348, 1322, 1259, 1216, 1201, 1150, 1109, 1079, 1034, 1015; HRMS (ESI) Calcd for C$_{24}$H$_{30}$N$_3$ (M+H)$^+$: 360.2434, Found: 360.2434.

Z-**3al** (minor, the less polar isomer), oil: ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.70 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.26 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.62 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.32-7.21 (m, 2 H, Ar-H), 7.08 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.53 (s, 1 H, Ar-H), 6.46 (dd, J_1 = 17.2 Hz, J_2 = 10.4 Hz, 1 H, =CH), 5.79 (t, *J* = 7.4 Hz, 1 H, =CH), 4.87-4.70 (m, 2 H, =CH$_2$), 2.03 (q, *J* = 7.3 Hz, 2 H, CH$_2$), 1.27-1.16 (m, 12 H, 6xCH$_2$), 0.85 (t, *J* = 6.8 Hz, 3 H, CH$_3$); ^{13}C NMR (100 MHz, CDCl$_3$) 157.9, 157.7, 139.9, 136.6, 136.5, 135.5, 134.0, 129.3, 123.0, 121.7, 120.3, 117.1, 113.7, 113.2, 108.5, 31.8, 29.7, 29.5, 29.3, 29.2, 29.1,

22.6, 14.1; MS (ESI) *m/z* 360 $(M+H)^+$; IR (neat, cm^{-1}): 2923, 2853, 1740, 1635, 1605, 1573, 1561, 1454, 1427, 1368, 1347, 1307, 1265, 1206, 1150, 1079, 1035; HRMS (ESI) Calcd for $C_{24}H_{30}N_3$ $(M+H)^+$: 360.2434, Found: 360.2433.

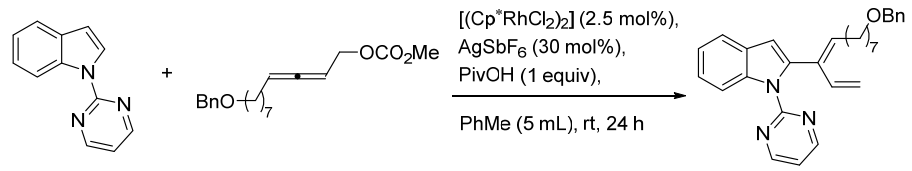
(20) 2-[(*E*)-deca-1,3-dien-3-yl]-1-(2-pyrimidinyl)-1*H*-indole 3am (zyz-6-79)



1a, **1** mmol **2m**, 1.1 equiv **3am**, 52% *E/Z* = 91/9

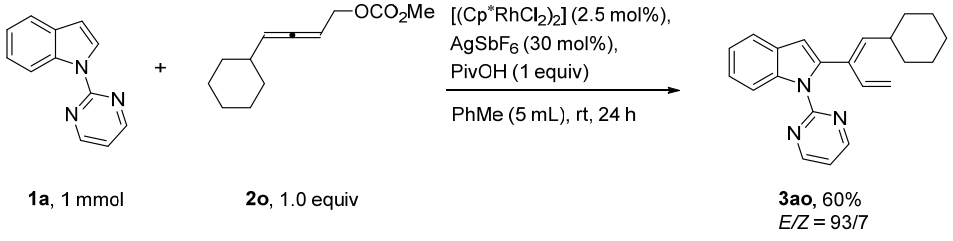
Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (15.4 mg, 0.025 mmol), $AgSbF_6$ (103.2 mg, 0.3 mmol), **1a** (195.7 mg, 1.0 mmol), PivOH (102.7 mg, 1 mmol)/toluene (2 mL), and **2m** (235.7 mg, 1.1 mmol)/toluene (3 mL) afforded 60% NMR yield of **3am** with 90/10 *E*/*Z* ratio as determined by the ^1H NMR analysis of the crude product. The crude product was purified by column chromatography on silica gel to afford pure *E*-**3am** (129.0 mg, 39%) and a *Z*/*E* mixture of **3am** (45.2 mg, 14%, *E*-**3am**/*Z*-**3am** = 2/1). The yield and *Z*/*E* were calculated based on these data (174.2 mg, 52 %, *E*/*Z* = 91/9) (eluent: petroleum ether/ethyl acetate = 60/1): Oil; ^1H NMR (400 MHz, $CDCl_3$) δ 8.70 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.17 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.60 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.31-7.16 (m, 2 H, Ar-H), 7.07 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.73-6.59 (m, 2 H, Ar-H and =CH), 5.86 (t, *J* = 7.8 Hz, 1 H, =CH), 4.91-4.80 (m, 2 H, $=CH_2$), 2.31 (q, *J* = 7.3 Hz, 2 H, CH_2), 1.52-1.43 (m, 2 H, CH_2), 1.41-1.27 (m, 6 H, 3xCH_2), 0.90 (t, *J* = 6.8 Hz, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) 157.92, 157.86, 140.3, 136.8, 134.4, 133.0, 132.7, 129.1, 123.1, 121.7, 120.3, 117.1, 115.5, 113.1, 108.1, 31.8, 29.3, 28.9, 28.1, 22.7, 14.1; MS (ESI) *m/z* 332 $(M+H)^+$; IR (neat, cm^{-1}): 3045, 2954, 2924, 2855, 1562, 1453, 1423, 1348, 1324, 1261, 1214, 1150, 1080, 1016; HRMS (ESI) Calcd for $C_{22}H_{26}N_3$ $(M+H)^+$: 332.2121, Found: 332.2119.

(21) 2-[(*E*)-11-(benzyloxy)-undeca-1,3-dien-3-yl]-1-(2-pyrimidinyl)-1*H*-indole 3an (zyz-6-68)



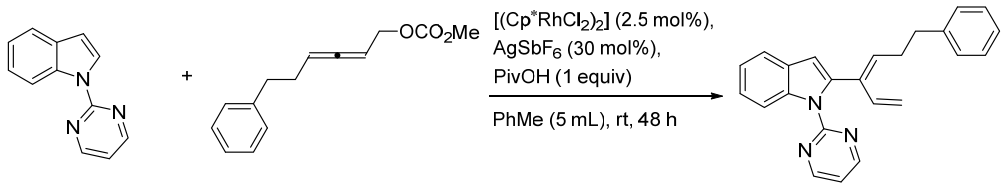
Following **Typical Procedrue III**, the reaction of [(Cp*RhCl$_2$)$_2$] (15.7 mg, 0.025 mmol), AgSbF$_6$ (103.7 mg, 0.3 mmol), **1a** (195.7 mg, 1.0 mmol), PivOH (102.7 mg, 1 mmol)/toluene (2 mL), and **2n** (333.5 mg, 1.0 mmol)/toluene (3 mL) afforded 59% NMR yield of **3an** with 90/10 *E*/*Z* ratio as determined by the ^{1}H NMR analysis of the crude product. The crude product was purified by column chromatography on silica gel to afford pure *E*-**3an** (151.6 mg, 33%) and a *Z*/*E* mixture of **3an** (69.7 mg, 15%, *E*-**3an**/*Z*-**3an** = 2.5/1). The yield and *Z*/*E* were calculated based on these data (221.3 mg, 49 %, *E*/*Z* = 91/9) (eluent: petroleum ether/ethyl acetate = 30/1): oil; ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.67 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.17 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.59 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.35-7.17 (m, 7 H, Ar-H), 7.01 (t, *J* = 9.6 Hz, 1 H, Ar-H); 6.71-6.60 (m, 2 H, Ar-H, and =CH), 5.85 (t, *J* = 15.6 Hz, 1 H, Ar-H), 4.91-4.81 (m, 2 H, =CH$_2$), 4.49 (s, 2 H, OCH$_2$), 3.47 (t, *J* = 6.6 Hz, 2 H, CH$_2$), 2.30 (q, *J* = 7.3 Hz, 2 H, CH$_2$), 1.70-1.55 (m, 2 H, CH$_2$), 1.52-1.25 (m, 8 H, 4xCH$_2$); ^{13}C NMR (100 MHz, CDCl$_3$) 157.9, 157.8, 140.3, 138.6, 136.8, 134.3, 132.9, 132.7, 129.0, 128.3, 127.5, 127.4, 123.0, 121.7, 120.2, 117.1, 115.5, 113.1, 108.0, 72.8, 70.4, 29.7, 29.3, 29.2, 29.1, 28.0, 26.1; MS (ESI) *m/z* 452 (M+H)$^+$; IR (neat, cm^{-1}): 3025, 2925, 2855, 1563, 1495, 1452, 1421, 1347, 1322, 1260, 1202, 1150, 1112, 1077, 1032; HRMS (ESI) Calcd for C$_{30}$H$_{34}$ON$_3$ (M+H)$^+$: 452.2696, Found: 452.2700.

(22) 2-[(*E*)-4-cyclohexylbuta-1,3-dien-3-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ao (zyz-6-64)



Following **Typical Procedrue III**, the reaction of [(Cp*RhCl$_2$)$_2$] (15.3 mg, 0.025 mmol), AgSbF$_6$ (102.0 mg, 0.3 mmol), **1a** (195.0 mg, 1.0 mmol), PivOH (102.9 mg, 1 mmol)/toluene (2 mL), and **2o** (212.7 mg, 1.0 mmol)/toluene (3 mL) afforded 65% NMR yield of **3ao** with 93/7 *E*/*Z* ratio as determined by the ^{1}H NMR analysis of the crude product. The crude product was purified by column chromatography on silica gel to afford pure *E*-**3ao** (142.2 mg, 43%) and a *Z*/*E* mixture of **3ao** (55.2 mg, 17%, *E*-**3ao**/*Z*-**3ao** = 3/1). The yield and *Z*/*E* were calculated based on these data (197.4 mg, 60 %, *E*/*Z* = 93/7) (eluent: petroleum ether/ethyl acetate = 30/1): oil: ^{1}H NMR (400 MHz, CDCl$_3$) δ 8.69 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.15 (d, *J* = 8.0 Hz, 1 H, Ar-H), 7.59 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.29-7.16 (m, 2 H, Ar-H), 7.06 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.70 (dd, J_1 = 17.4 Hz, J_2 = 11.0 Hz, 1 H, =CH), 6.61 (s, 1 H, Ar-H), 5.60 (d, *J* = 9.6 Hz, 1 H, =CH), 4.98-4.87 (m, 2 H, =CH$_2$), 2.62-2.41 (m, 1 H, CH), 1.82-1.51 (m, 5 H), 1.35-1.07 (m, 5 H); ^{13}C NMR (100 MHz, CDCl$_3$) δ 157.9, 157.8, 140.1, 139.8, 136.8, 133.1, 130.8, 129.0, 123.0, 121.7, 120.2, 117.1, 115.7, 113.0, 107.9, 36.9, 32.7, 25.9, 25.7; MS (ESI) *m/z* 330 (M+H)$^+$; IR (neat, cm^{-1}): 3043, 2921, 2848, 1631, 1563, 1452, 1421, 1347, 1258, 1213, 1189, 1150, 1109, 1078, 1034, 1015; HRMS (ESI) Calcd for C$_{22}$H$_{24}$N$_3$ (M+H)$^+$: 330.1965, Found: 330.1965.

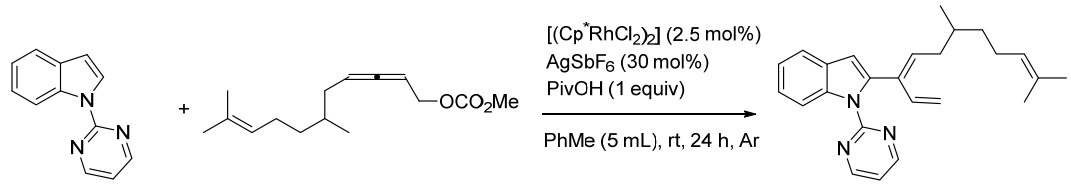
(23) 2-[(*E*)-6-phenylhexa-1,3-dien-3-yl]-1-(2-pyrimidinyl)-1*H*-indole 3ap (zyz-6-65)



Following **Typical Procedrue III**, the reaction of [(Cp*RhCl$_2$)$_2$] (15.7 mg, 0.025 mmol), AgSbF$_6$ (102.5 mg, 0.3 mmol), **1a** (195.7 mg, 1.0 mmol), PivOH (103.8 mg, 1 mmol)/toluene (2 mL), and **2p** (232.9 mg, 1.0 mmol)/toluene (2 mL) afforded 62% NMR yield of **3ap** with 90/10 *E*/*Z* ratio as determined by the ^{1}H NMR analysis of the crude product. The crude product was purified by column chromatography on silica gel to afford pure *E*-**3ap** (137.7 mg, 39%) and a *Z*/*E* mixture of **3ap** (71.1 mg, 20%, *E*-**3ap**/*Z*-**3ap** = 2.5/1). The yield and *Z*/*E* were calculated based on these data (208.8 mg, 59 %,

E/Z = 90/10) (eluent: petroleum ether/ethyl acetate = 30/1): oil; ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.65 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.18 (d, *J* = 8.8 Hz, 1 H, Ar-H), 7.59 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.32-7.15 (m, 7 H, Ar-H), 7.02 (t, *J* = 4.8 Hz, 1 H, Ar-H), 6.69-6.58 (m, 2 H, Ar-H and =CH), 5.90 (t, *J* = 7.4 Hz, 1 H, =CH), 4.92-4.78 (m, 2 H, $=CH_2$), 2.78 (t, *J* = 7.6 Hz, 2 H, CH_2), 2.64 (q, *J* = 7.6 Hz, 2 H, CH_2); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 157.7, 141.6, 140.0, 136.8, 133.2, 132.8, 132.7, 129.0, 128.4, 128.3, 125.9, 123.2, 121.7, 120.3, 117.1, 116.0, 113.2, 108.2, 35.5, 29.9; MS (ESI) *m/z* 352 $(M+H)^+$; IR (neat, cm^{-1}): 3025, 2925, 2855, 1563, 1495, 1452, 1421, 1347, 1322, 1260, 1202, 1150, 1112, 1077, 1032; HRMS (ESI) Calcd for $C_{24}H_{22}N_3$ $(M+H)^+$: 352.1808, Found: 352.1808.

(24) Synthesis of 3aq (zyz-6-106)

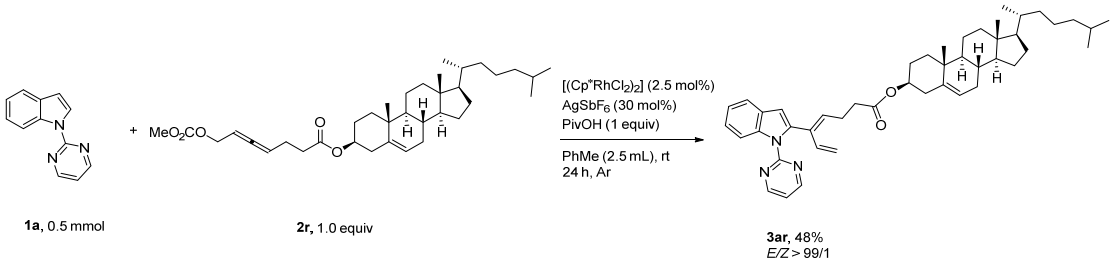


Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (15.7 mg, 0.025 mmol), $AgSbF_6$ (102.1 mg, 0.3 mmol), **1a** (195.0 mg, 1.0 mmol), PivOH (103.5 mg, 1 mmol)/toluene (2 mL), and **2q** (252.9 mg, 1.0 mmol)/toluene (3 mL) afforded **3aq** (252.2 mg, 68%, *E/Z* = 97/3) (eluent: petroleum ether/ethyl acetate = 25/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.67 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.13 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.62 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.35 (t, *J* = 7.8 Hz, 1 H, Ar-H), 7.26 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.77 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.68 (s, 1 H, Ar-H), 6.08 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.92 (t, *J* = 7.8 Hz, 1 H, Ar-H), 5.23 (t, *J* = 7.2 Hz, 1 H, =CH), 5.05 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.84 (d, *J* = 11.4 Hz, 1 H, one proton of $=CH_2$), 2.32-2.25 (m, 1 H, one proton of CH_2), 2.18-2.01 (m, 3 H, CH_2 and one proton of CH_2), 1.69 (s, 3 H, CH_3), 1.65-1.58 (m, 4 H, CH_3 and one proton of CH_2), 1.56-1.49 (m, 1 H, one proton of CH_2), 1.31-1.22 (m, 1 H, one proton of CH_2), 0.98 (d, *J* = 6.6 Hz, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.9, 157.8, 140.5, 136.7, 133.5, 133.2, 133.1, 131.1, 129.0, 124.8, 123.1, 121.7, 120.2, 117.0, 115.5, 113.2, 108.0, 36.7, 35.3, 33.4, 25.69,

25.66, 19.5, 17.6; MS (ESI) *m/z* 372 $(M+H)^+$; IR (neat, cm^{-1}): 3042, 2911, 2851, 1563, 1452, 1423, 1376, 1347, 1322, 1258, 1213, 1150, 1079, 1034; HRMS (ESI) Calcd for $C_{25}H_{30}N_3$ $(M+H)^+$: 372.2434, Found: 372.2427.

The following signals are discernible for (*Z*-**3aq**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.70 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.10 (d, *J* = 4.8 Hz, 2 H, Ar-H), 6.57 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 5.85 (t, *J* = 7.5 Hz, 1 H, Ar-H), 4.98 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$).

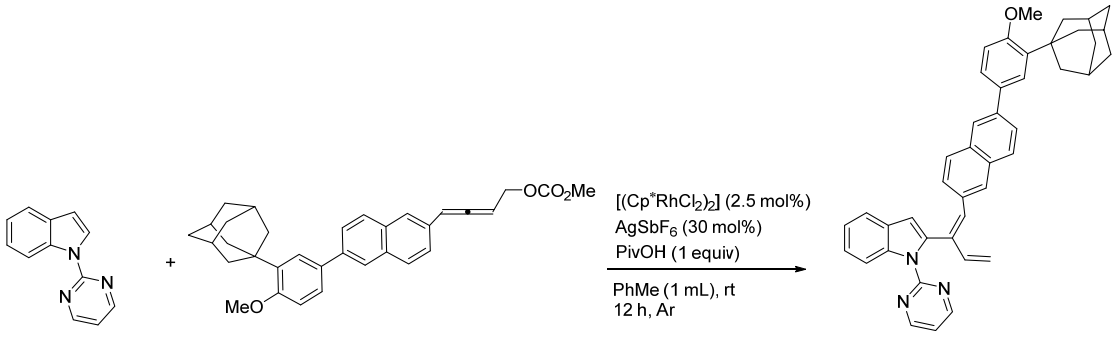
(25) Synthesis of 3ar (zyz-6-112)



Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (7.8 mg, 0.0125 mmol), $AgSbF_6$ (51.7 mg, 0.15 mmol), **1a** (97.9 mg, 0.5 mmol), PivOH (52.3 mg, 0.5 mmol)/toluene (1 mL), and **2r** (284.9 mg, 0.5 mmol)/toluene (1.5 mL) afforded **3ar** (165.3 mg, 48%, *E/Z* > 99/1) (eluent: petroleum ether/ethyl acetate = 20/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) 8.65 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.13 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.61 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.34 (t, *J* = 7.8 Hz, 1 H, Ar-H), 7.25 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.76 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.68 (s, 1 H, Ar-H), 6.08 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.84 (t, *J* = 7.8 Hz, 1 H, =CH), 5.39-5.34 (m, 1 H, =CH), 5.05 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.96-4.89 (m, 1 H, OCH), 4.85 (d, *J* = 11.4 Hz, 1 H, one proton of $=CH_2$), 2.64 (q, *J* = 7.6 Hz, 2 H, CH_2), 2.59-2.52 (m, 1 H), 2.45 (t, *J* = 12.3 Hz, 1 H), 2.34 (t, *J* = 7.8 Hz, 2 H), 2.07-1.97 (m, 1 H), 1.97-1.82 (m, 3 H), 1.64-0.84 (m, 34 H), 0.67 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) 172.2, 157.9, 157.8, 139.8, 139.6, 136.8, 133.9, 132.7, 131.2, 129.0, 123.3, 122.6, 121.8, 120.3, 117.1, 116.4, 113.3, 108.4, 74.0, 56.6, 56.1, 50.0, 42.3, 39.7, 39.5, 38.1, 37.0, 36.6, 36.1, 35.7, 34.2, 31.9, 31.8, 28.2, 28.0, 27.8, 24.2, 23.8, 23.7, 22.8, 22.5, 21.0, 19.3, 18.7, 11.8; MS (ESI) *m/z* 688 $(M+H)^+$;

IR (neat, cm^{-1}): 2936, 2866, 1728, 1563, 1453, 1425, 1348, 1255, 1169, 1080; HRMS (ESI) Calcd for $C_{46}H_{62}O_2N_3$ $(M+H)^+$: 688.4837, Found: 688.4820.

(26) Synthesis of 3as (zyz-7-2)

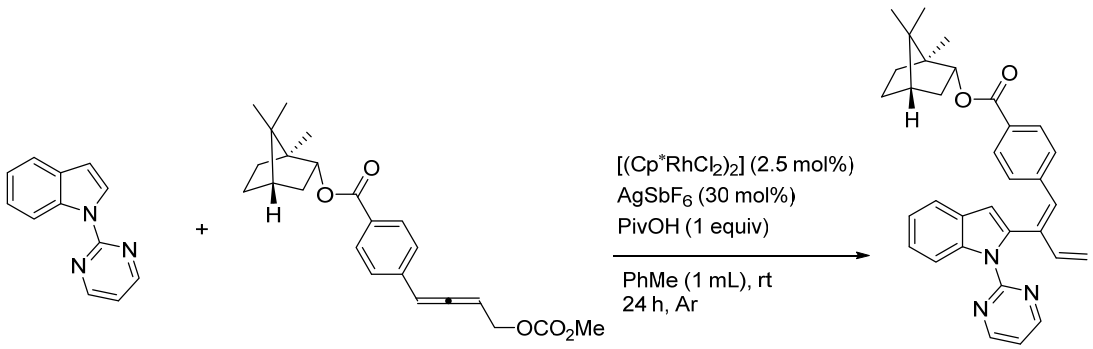


Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (6.2 mg, 0.01 mmol), $AgSbF_6$ (41.4 mg, 0.12 mmol), **1a** (78.7 mg, 0.4 mmol), PivOH (41.8 mg, 0.4 mmol)/toluene (1 mL), and **2s** (217.9 mg, 0.44 mmol)/toluene (1 mL) afforded **3as** (162.3 mg, 62%, purity 95%, *Z/E* = 98/2) (eluent: petroleum ether/ethyl acetate = 15/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.74 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.99 (d, *J* = 4.2 Hz, 2 H, Ar-H), 7.84 (s, 1 H, Ar-H), 7.66 (d, *J* = 2.4 Hz, 1 H, Ar-H), 7.63 (dd, J_1 = 8.4 Hz, J_2 = 1.8 Hz, 1 H, Ar-H), 7.58-7.52 (m, 3 H, Ar-H), 7.42-7.33 (m, 3 H, Ar-H), 7.29-7.22 (m, 2 H, Ar-H), 6.86 (s, 1 H, Ar-H), 6.80 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.67 (s, 1 H, =CH), 6.65 (d, *J* = 8.4 Hz, 1 H, Ar-H), 5.94 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.23 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 5.06 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 3.38 (s, 3 H, OCH_3), 2.27 (s, 6 H, 3xCH_2), 2.10 (s, 3 H, 3xCH), 1.87-1.76 (m, 6 H, 3xCH_2); ^{13}C NMR (100 MHz, $CDCl_3$) 158.5, 157.8, 157.4, 140.5, 138.9, 138.7, 136.5, 135.4, 134.02, 134.00, 133.05, 133.02, 132.8, 131.9, 129.4, 128.5, 128.3, 127.5, 126.7, 125.7, 125.6, 125.4, 124.6, 123.3, 121.9, 120.7, 116.9, 115.5, 114.1, 112.0, 108.8, 55.1, 40.5, 37.1, 29.0; MS (ESI) *m/z* 614 $(M+H)^+$; IR (neat, cm^{-1}): 2900, 2846, 1604, 1563, 1495, 1452, 1424, 1347, 1307, 1265, 1234, 1180, 1138, 1101, 1026; HRMS (ESI) Calcd for $C_{43}H_{40}ON_3$ $(M+H)^+$: 614.3166, Found: 614.3167.

The following signals are discernible for (*E*-**3as**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.70 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.06 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.93 (s, 1 H, Ar-H), 7.10 (s, 1 H,

Ar-H), 6.85 (s, 1 H, Ar-H), 6.72 (d, J = 7.8 Hz, 1 H, Ar-H), 6.00 (t, J = 4.5 Hz, 1 H, Ar-H), 5.27 (d, J = 18.0 Hz, 1 H, one proton of $=CH_2$), 4.96 (d, J = 10.8 Hz, 1 H, one proton of $=CH_2$), 3.41 (s, 3 H, OCH_3), 2.31 (s, 6 H, 3xCH_2).

(27) Synthesis of 3at (zyz-6-174)



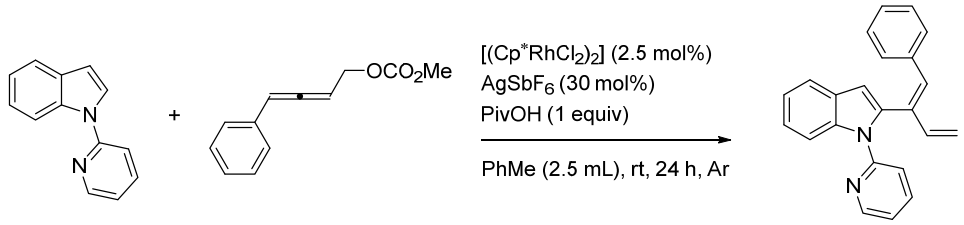
1a, 0.2 mmol **2t**, 1.1 equiv **3at**, 65% *Z/E* = 96/4

Following **Typical Procedrue III**, the reaction of [(Cp*$RhCl_2$)$_2$] (3.2 mg, 0.005 mmol), $AgSbF_6$ (20.5 mg, 0.06 mmol), **1a** (39.2 mg, 0.2 mmol), PivOH (20.9 mg, 0.2 mmol) /toluene (0.5 mL), and **2t** (84.0 mg, 0.22 mmol)/toluene (0.5 mL) afforded **3at** (65.5 mg, 65%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 20/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.69 (d, J = 8.4 Hz, 1 H. Ar-H), 8.07 (d, J = 4.8 Hz, 2 H, Ar-H), 7.94 (d, J = 8.4 Hz, 2 H, Ar-H), 7.47 (d, J = 7.2 Hz, 1 H, Ar-H), 7.30 (t, J = 7.8 Hz, 1 H, Ar-H), 7.23 (d, J = 8.4 Hz, 2 H, Ar-H), 7.19-7.17 (m, 1 H, Ar-H), 6.65-6.57 (m, 2 H, Ar-H and =CH), 6.52 (s, 1 H, =CH), 6.08 (t, J = 4.8 Hz, 1 H, Ar-H), 5.18 (d, J = 9.6 Hz, 1 H, OCH), 5.04 (d, J = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.96 (d, J = 10.2 Hz, 1 H, one proton of $=CH_2$), 2.39-2.32 (m, 1 H, one proton of CH_2), 2.04-1.94 (m, 1 H, one proton of CH_2), 1.63-1.53 (m, 1 H, one proton of CH_2), 1.48-1.43 (m, 1 H, one proton of CH_2), 1.18 (t, J = 12.6 Hz, 1 H, one proton of CH_2), 1.14-1.07 (m, 1 H, one proton of CH_2), 1.01 (dd, J_1 = 13.8 Hz, J_2 = 2.4 Hz, 1 H, one proton of CH_2), 0.76 (s, 3 H, CH_3), 0.72 (s, 3 H, CH_3), 0.69 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) 166.6, 157.9, 157.4, 141.2, 140.2, 136.6, 136.2, 134.9, 131.7, 129.4, 129.2, 129.0, 128.9, 123.5, 122.0, 120.8, 117.0, 116.7, 114.3, 106.8, 80.3, 49.0, 47.8, 44.9, 36.8, 28.0, 27.3, 19.7, 18.9, 13.5; MS (ESI) *m/z* 504 $(M+H)^+$; IR (neat, cm^{-1}): 2954, 2877, 1707, 1603, 1563, 1452, 1424, 1377, 1347,

1304, 1269, 1178, 1105, 1016; HRMS (ESI) Calcd for $C_{33}H_{34}O_2N_3$ $(M+H)^+$: 504.2646, Found:. 504.2641.

The following signals are discernible for (*E*-**3at**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.64 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.19 (d, *J* = 7.8 Hz, 2 H, Ar-H), 8.09 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.62 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.36 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.27 (d, *J* = 7.2 Hz, 1 H, Ar-H), 6.89 (dd, J_1 = 17.4 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.79 (s, 1 H, Ar-H), 6.72 (s, 1 H, Ar-H), 5.32 (d, *J* = 9.6 Hz, 1 H, OCH), 4.92 (d, *J* = 11.4 Hz, 1 H, one proton of $=CH_2$), 2.50-2.44 (m, 1 H, m, 1 H, one proton of CH_2), 2.29-2.22 (m, 1 H, one proton of CH_2), 1.74-1.67 (m, 1 H, one proton of CH_2), 1.35 (t, *J* = 12.3 Hz, 1 H, one proton of CH_2), 1.29-1.26 (m, 1 H, one proton of CH_2), 0.90 (s, 3 H, CH_3), 0.79 (s, 3 H, CH_3)

(28) 2-[(*Z*)-1-phenyl-1,3-butadien-2-yl]-1-(2-pyridinyl)-1*H*-indole 3ka (zyz-6-88)

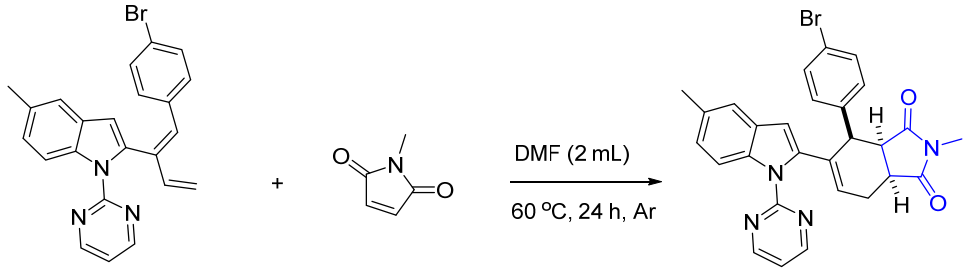


Following **Typical Procedrue III**, the reaction of $[(Cp^*RhCl_2)_2]$ (7.8 mg, 0.0125 mmol), $AgSbF_6$ (52.1 mg, 0.15 mmol), **1k** (97.9 mg, 0.5 mmol), PivOH (51.0 mg, 0.5 mmol)/toluene (1 mL), and **2a** (113.5 mg, 0.55 mmol)/toluene (1.5 mL) afforded **3ka** (83.8 mg, 52%, *Z/E* = 90/10) (eluent: petroleum ether/ethyl acetate = 15/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.17 (d, *J* = 4.8 Hz, 1 H, Ar-H), 7.95 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.63 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.25-7.20 (m, 2 H, Ar-H), 7.00 (d, *J* = 7.8 Hz, 1 H, Ar-H), 6.95 (d, *J* = 7.8 Hz, 2 H, Ar-H), 6.93-6.90 (m, 1 H, Ar-H), 6.83-6.77 (m, 3 H, Ar-H), 6.65 (s, 1 H, =CH), 6.56-6.50 (m, 2 H, Ar-H and =CH), 6.44-6.40 (m, 1 H, Ar-H), 5.28 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 5.06 (d, *J* = 10.2 Hz, 1 H, one proton of $=CH_2$); MS (ESI) *m/z* 323 $(M+H)^+$; IR (neat, cm^{-1}): 3053, 3018, 1585, 1550, 1467, 1450, 1434, 1385, 1340, 1312, 1279, 1235, 1205, 1180, 1149, 1113, 1096, 1076, 1051, 1026; Anal. calcd for $C_{23}H_{18}N_2$ (%): C 85.68, H 5.63, N 8.69, Found: C 85.49, H 5.30, N 8.35.

The following signals are discernible for (*E*-**3ka**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.31 (d, *J* = 4.2 Hz, 1 H, Ar-H), 8.07 (d, *J* = 7.2 Hz, 1 H, Ar-H), 7.69 (d, *J* = 7.8 Hz, 1 H, Ar-H), 7.09 (t, *J* = 7.5 Hz, 1 H, Ar-H), 6.74 (s, 1 H, =CH), 6.47-6.44 (m, 1 H, Ar-H), 5.36 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.99 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$).

3. Synthetic applications of 3bf

(1) Intermolecular Diels-Alder reaction with 3bf and *N*-methylmaleimide[7] (14, zyz-6-23)



3bf, 0.5 mmol
Z/*E* = 96:4

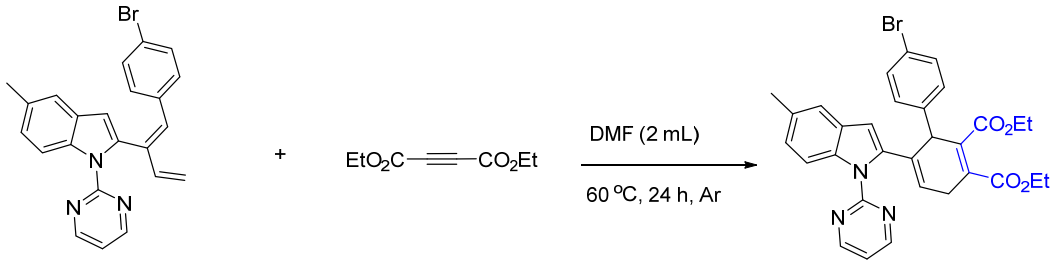
4 equiv

14, 80%, *dr* > 20:1

To an oven-dried Schlenk tube were added **3bf** (209.3 mg, 0.5 mmol), *N*-methylmaleimide (228.3 mg, 2 mmol) and DMF (2 mL) sequentially under argon atmosphere. The resulting mixture was stirred at 60 °C for 24 h. After the reaction was complete as monitored by TLC, the resulting mixture was quenched with 20 mL of H_2O and extracted with diethyl ether (20 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtrated and concentrated. The crude product was purified by column chromatography to afford **14** (211.2 mg, 80%, *dr* > 20:1) (eluent: petroleum ether/ethyl acetate = 2/1) as an oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.35 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.27 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.22 (s, 1 H, Ar-H), 7.12 (t, *J* = 4.8 Hz, 1 H, Ar-H), 7.07 (dd, J_1 = 8.6 Hz, J_2 = 1.4 Hz, 1 H, Ar-H), 6.86 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.23-6.18 (m, 2 H, Ar-H and =CH), 4.07 (d, *J* = 6.8 Hz, 1 H, CH), 3.53 (dd, J_1 = 8.6 Hz, J_2 = 7.0 Hz, 1 H, CH), 3.24-3.15 (m, 1 H, CH), 3.02-2.90 (m, 1 H, one proton of CH_2), 2.83-2.71 (m, 1 H, one proton of CH_2), 2,44 (s, 3 H, CH_3), 2.38 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 179.5, 177.7, 158.0, 157.9, 139.5, 135.3, 134.9, 131.7, 131.2, 130.7, 129.3, 125.7, 125.1, 121.4, 120.2, 116.7, 114.8, 109.3, 45.8, 45.0,

36.8, 23.9, 21.6, 21.2; MS (ESI) *m/z* 529 ($M(^{81}Br)+H)^+$, 527 ($M(^{79}Br)+H)^+$; IR (neat, cm^{-1}): 2915, 1776, 1698, 1575, 1560, 1485, 1421, 1380, 1337, 1317, 1296, 1188, 1130, 1072, 1009; HRMS (ESI) Calcd for $C_{28}H_{24}N_4O_2{}^{79}Br$ $(M+H)^+$: 527.1077, Found: 527.1072.

(2) Intermolecular Diels-Alder reaction with 3bf and diethyl acetylenedicarboxylate[7] (15, zyz-6-24)



3bf, 0.5 mmol
Z/E = 96:4

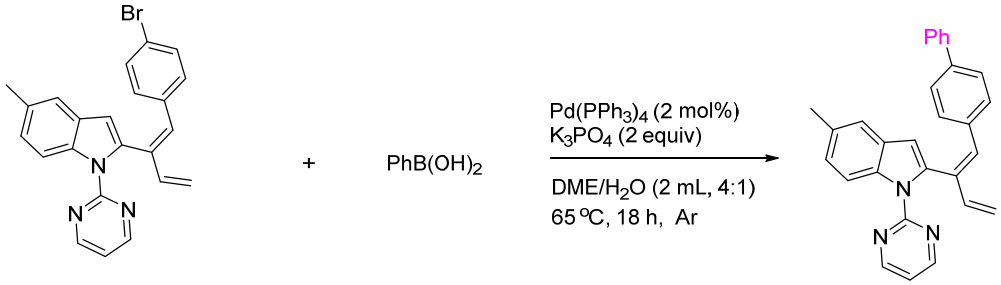
3 equiv

15, 77%

To an oven-dried Schlenk tube were added **3bf** (209.3 mg, 0.5 mmol), diethyl acetylenedicarboxylate (257.3 mg, 1.5 mmol) and 2 mL of DMF sequentially under the argon atmosphere. The resulting mixture was stirred at 60 °C for 24 h. After the reaction was complete as monitored by TLC, the resulting mixture was quenched with 20 mL of H_2O and extracted with diethyl ether (20 mL × 3). The combined organic layer was dried over anhydrous Na_2SO_4, filtrated and concentrated. The crude product was purified by column chromatography to afford **15** (226.1 mg, 77%) (eluent: petroleum ether/ethyl acetate = 3/1) as an oil: ^1H NMR (400 MHz, $CDCl_3$) δ 8.75 (d, *J* = 4.8 Hz, 2 H, Ar-H), 8.19 (d, *J* = 8.8 Hz, 1 H, Ar-H), 7.28-7.19 (m, 3 H, Ar-H), 7.12-7.02 (m, 2 H, Ar-H), 6.90 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.12 (s, 1 H, Ar-H), 5.98-5.90 (m, 1 H, =CH), 4.57 (t, *J* = 5.8 Hz, 1 H, CH), 4.24 (q, *J* = 7.1 Hz, 2 H, OCH_2), 4.08-3.92 (m, 2 H, OCH_2), 3.43-3.32 (m, 1 H, one proton of CH_2), 3.27-3.14 (m, 1 H, one proton of CH_2), 2.38 (s, 3 H, CH_3), 1.30 (t, *J* = 7.2 Hz, 3 H, CH_3), 1.02 (t, *J* = 7.0 Hz, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 158.1, 157.8, 139.2, 138.5, 136.9, 135.1, 133.2, 131.3, 131.2, 130.6, 130.2, 129.1, 124.9, 122.4, 120.8, 120.1, 116.9, 113.7, 109.1, 61.2, 60.8, 47.2, 28.6, 21.2, 13.9, 13.7; MS (ESI) *m/z* 588 ($M(^{81}Br)+H)^+$, 586 ($M(^{79}Br)+H)^+$; IR (neat, cm^{-1}): 2980, 2904, 1715, 1646, 1573, 1561, 1422, 1373, 1338, 1319, 1298, 1258, 1243, 1190, 1176, 1138, 1101,

1067, 1028, 1010; HRMS (ESI) Calcd for $C_{31}H_{29}N_3O_4{}^{81}Br$ $(M+H)^+$:588.1315, Found: 588.1305.

(3) Coupling reaction of 3bf with $PhB(OH)_2$[8] (16, zyz-6-144)



3bf, 0.5 mmol
Z/E = 96:4

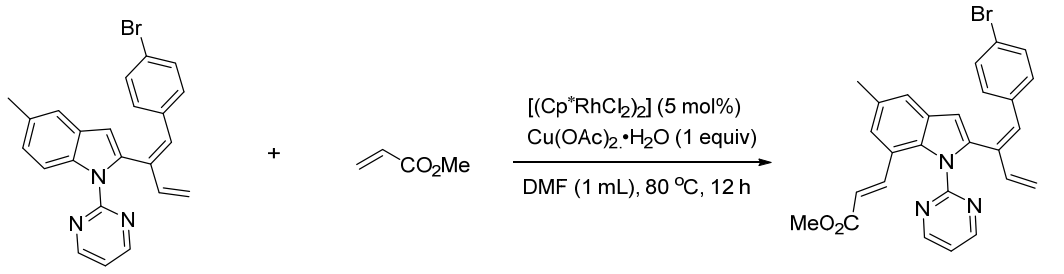
1.2 equiv

16, 89%
Z/E = 96/4

To an oven-dried Schlenk tube were added **3bf** (208.5 mg, 0.5 mmol), $Pd(PPh_3)_4$ (11.5 mg, 0.01 mmol), K_3PO_4 (213.5 mg, 1 mmol), $PhB(OH)_2$ (73.9 mg, 0.6 mmol), and 2 mL of mixed solvent of DME and H_2O (4/1) sequentially under the argon atmosphere. The resulting mixture was stirred at 65 °C for 18 h. After the reaction was complete as monitored by TLC, the reaction mixture was evaporated, diluted by 20 mL of ethyl acetate, washed sequentially with 10 mL of a saturated aqueous solution of $NaHCO_3$ and 10 mL of brine, dried over anhydrous Na_2SO_4, filtrated and concentrated. The crude product was purified by column chromatography to afford **16** (183.5 mg, 89%, *Z/E* = 96/4) (eluent: petroleum ether/ethyl acetate = 30/1) as an oil: ^1H NMR (600 MHz, C_6D_6) δ 8.75 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.04 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.31-7.27 (m, 3 H, Ar-H), 7.24-7.20 (m, 3 H, Ar-H), 7.16-7.13 (m, 2 H, Ar-H), 7.11 (t, *J* = 7.8 Hz, 2 H, Ar-H), 7.07-7.03 (m, 1 H, Ar-H), 6.79-6.72 (m, 2 H, Ar-H and =CH), 6.60 (s, 1 H, =CH), 5.97 (t, *J* = 4.5 Hz, 1 H, Ar-H), 5.17 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 5.02 (d, *J* = 10.2 Hz, 1 H, one proton of $=CH_2$), 2.35 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 157.7, 157.4, 140.6, 140.5, 139.4, 135.7, 135.3, 134.8, 134.2, 132.3, 131.2, 129.7, 129.4, 128.6, 127.1, 126.7, 126.5, 124.7, 120.4, 116.7, 115.4, 114.1, 108.2, 21.3; MS (ESI) *m/z* 414 (M+H)+; IR (neat, cm^{-1}): 3026, 2917, 1597, 1570, 1558, 1484, 1423, 1339, 1313, 1295, 1266, 1239, 1216, 1188, 1149, 1117, 1078, 1036, 1006; HRMS (ESI) Calcd for $C_{29}H_{24}N_3$ $(M+H)^+$: 414.1965, Found: 414.1963.

The following signals are discernible for (*E*-**16**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.67 (d, *J* = 8.4 Hz, 1 H, Ar-H), 8.07 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.49 (d, *J* = 7.2 Hz, 2 H, Ar-H), 7.42 (s, 1 H, Ar-H), 6.97 (s, 1 H, Ar-H), 6.80 (s, 1 H, =CH), 6.00 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.25 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 4.94 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 2.40 (s, 3 H, CH_3).

(4) C-H functionalization at C-7 of 3bf with methyl acrylate[9] (17, zyz-6-2)



3bf, 0.2 mmol
Z/*E* = 96:4

1.5 equiv

17, 65%, *Z*/*E* = 93/7

To an oven-dried Schlenk tube were added **3bf** (83.9 mg, 0.2 mmol), $Cu(OAc)_2 \cdot H_2O$ (40.7 mg, 0.2 mmol), $[(Cp^*RhCl_2)_2]$ (6.3 mg, 0.01 mmol), methyl acrylate (26.9 mg, 0.3 mmol), and DMF (1 mL) sequentially under argon atmosphere. The resulting mixture was stirred at 80 °C for 12 h as monitored by TLC, diluted by 10 mL of H_2O, and extracted with diethyl ether (10 mLx3). The combined organic layer was dried over anhydrous Na_2SO_4, filtrated and concentrated. The crude product was purified by column chromatography to afford **17** (65.3 mg, 65%, *Z*/*E* = 93/7) (eluent: petroleum ether/ethyl acetate = 3/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 8.10 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.75 (d, *J* = 15.6 Hz, 1 H, =CH), 7.24 (s, 1 H, Ar-H), 7.17-7.14 (m, 1 H, Ar-H), 6.94 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.88 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.44-6.38 (m, 3 H, 2 x =CH and Ar-H), 6.31 (d, *J* = 15.6 Hz, 1 H, =CH), 6.20 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.14 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 4.98 (d, *J* = 10.2 Hz, 1 H, one proton of $=CH_2$), 3.37 (s, 3 H, OCH_3), 2.23 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 167.2, 158.1, 157.9, 143.0, 139.6, 136.7, 135.0, 133.7, 133.3, 133.2, 131.2, 131.0, 130.6, 130.5, 124.3, 122.8, 121.5, 120.2, 118.8, 116.9, 116.7, 106.3, 51.3, 21.1; MS (ESI) *m/z* 502 $(M(^{81}Br)+H)^+$, 500 $(M(^{79}Br)+H)^+$; IR (neat, cm^{-1}): 3084, 3039, 2947, 1710, 1631, 1561, 1485, 1417, 1348,

1298, 1262, 1190, 1169, 1064, 1033, 1008; HRMS (ESI) Calcd for $C_{27}H_{23}O_2N_3{}^{79}Br$ $(M+H)^+$: 500.0968, Found: 500.0963.

The following signals are discernible for (*E*-**17**): ^{1}H NMR (600 MHz, C_6D_6) δ 8.19 (d, *J* = 4.8 Hz, 2 H, Ar-H), 7.85 (d, *J* = 15.0 Hz, 2 H, =CH), 7.35 (s, 1 H, Ar-H), 7.18 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.67 (s, 1 H, Ar-H), 6.64 (s, 1 H, Ar-H), 6.59 (dd, J_1 = 18.0 Hz, J_2 = 10.8 Hz, 1 H, =CH), 6.24 (t, *J* = 4.8 Hz, 1 H, Ar-H), 5.30 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 4.93 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 3.38 (s, 3 H, CH_3), 2.27 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 158.4, 131.3, 122.7, 107.1.

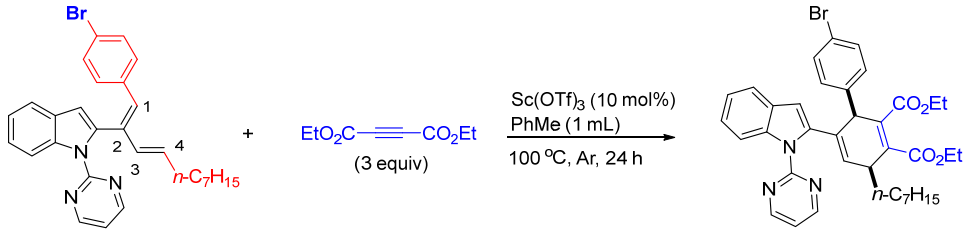
(5) Removing pyrimidinyl directing group of 3bf (18, zyz-7-66)

3bf, *Z*/*E* = 95/5 **18**, 66%, *Z*/*E* = 95/5

To an oven-dried Schlenk tube were added **3bf** (84.3 mg, 0.2 mmol), DMSO (2 mL), and NaOEt (54.9 mg, 0.8 mmol) sequentially under argon atmosphere. The resulting mixture was stirred at room temperature for 36 h as monitored by TLC, diluted by 10 mL of H_2O, and extracted with ethyl acetate (10 mL × 3). The combined organic layer was washed with 10 mL of brine, dried over anhydrous Na_2SO_4, filtrated, and concentrated. The crude product was purified by column chromatography to afford **18** (45.0 mg, 66%, *Z*/*E* = 95/5) (eluent: petroleum ether/ethyl acetate = 40/1) as an oil: ^{1}H NMR (600 MHz, C_6D_6) δ 7.38 (s, 1 H, Ar-H), 7.03 (d, *J* = 8.4 Hz, 1 H, Ar-H), 6.89-6.85 (m, 3 H, Ar-H), 6.71 (brs, 1 H, NH), 6.56-6.50 (m, 3 H, Ar-H), 6.39-6.36 (m, 1 H, =CH), 6.32 (s, 1 H, Ar-H), 5.29 (d, *J* = 16.8 Hz, 1 H, one proton of $=CH_2$), 5.13 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 2.38 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 139.6, 135.0, 134.3, 133.3, 132.4, 131.4, 131.3, 130.6, 129.3, 128.8, 123.9, 121.5, 120.3, 117.6, 110.7, 103.3, 21.4; MS (EI, 70 eV) *m/z* (%) 339 (M^+(^{81}Br), 56.89), 337 (M^+(^{79}Br), 56.2), 185 (100); IR (neat, cm^{-1}): 3390, 3012, 2916, 1581, 1483, 1453, 1401, 1327, 1309, 1071, 1007; HRMS Calcd for $C_{19}H_{16}N^{79}Br$ (M^+): 337.0461, Found: 337.0460.

The following signals are discernible for (*E*-**18**): ^{1}H NMR (600 MHz, C_6D_6) δ 7.43 (s, 1 H, Ar-H), 7.28 (d, *J* = 8.4 Hz, 2 H, Ar-H), 7.11 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.07 (d, *J* = 9.6 Hz, 1 H, Ar-H), 6.98 (d, *J* = 8.4 Hz, 1 H, Ar-H), 6.65 (brs, 1 H, NH), 5.57 (d, *J* = 17.4 Hz, 1 H, one proton of $=CH_2$), 5.21 (d, *J* = 10.8 Hz, 1 H, one proton of $=CH_2$), 2.42 (s, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 133.7, 131.1, 127.4, 124.2.

(6) Intermolecular Diels-Alder reaction with 3am and diethyl acetylenedicarboxylate (*cis*-19, zyz-7-71)



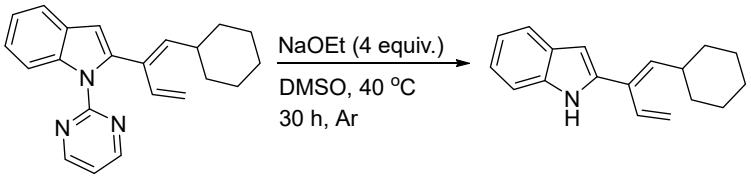
3am
Z/*E* of C^1=C^2 bond = 99/1
E/*Z* of C^3=C^4 bond = 100/0

cis-**19**, 55%

To an oven-dried Schlenk tube were added $Sc(OTf)_3$ (9.7 mg, 0.02 mmol), **3am** (101.3 mg, 0.2 mmol)/toluene (0.5 mL), and diethyl acetylenedicarboxylate (101.3 mg, 0.6 mmol)/toluene (0.5 mL) sequentially under argon atmosphere. The resulting mixture was stirred at 100 °C for 24 h. After the reaction was complete as monitored by TLC, the resulting mixture was allowed to cool to room temperature, transferred with 20 mL of DCM, and evaporated to remove the solvent. The crude product was purified by column chromatography to afford *cis*-**19** (74.7 mg, 55%) (eluent: petroleum ether/ethyl acetate = 10/1, 440 mL; petroleum ether/ethyl acetate = 5/1, 480 mL) as an oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.74 (d, *J* = 4.4 Hz, 2 H, Ar-H), 8.22 (d, *J* = 8.4 Hz, 1 H, Ar-H), 7.47 (d, *J* = 7.6 Hz, 1 H, Ar-H), 7.29-7.21 (m, 3 H, Ar-H), 7.19-7.09 (m, 2 H, Ar-H), 6.97 (d, *J* = 8.4 Hz, 2 H, Ar-H), 6.28 (s, 1 H, Ar-H), 5.92 (d, *J* = 4.4 Hz, 1 H, =CH), 4.62 (d, *J* = 4.8 Hz, 1 H, CH), 4.36-4.20 (m, 2 H, CH_2), 4.08-3.92 (m, 2 H, CH_2), 3.38-3.20 (m, 1 H, CH), 2.05-1.92 (m, 1 H, one proton of CH_2), 1.58-1.21 (m, 14 H, 5 × CH_2, CH_3, and one proton of CH_2), 1.05 (t, *J* = 7.2 Hz, 3 H, CH_3), 0.90 (t, *J* = 6.4 Hz, 3 H, CH_3); ^{13}C NMR (100 MHz, $CDCl_3$) δ 168.1, 166.7, 158.2, 158.0, 139.3, 138.8, 138.7, 137.1, 133.8, 131.9, 131.1, 130.6, 128.9, 127.8, 123.5, 122.1, 120.6, 120.4, 117.2, 113.7, 109.0, 61.2, 60.9, 46.9, 38.9, 35.7, 31.8, 29.5, 29.1, 27.2, 22.6, 14.05, 14.03, 13.8; Ms (EI, 70 eV) *m/z* (%) 671 (M^+

(^{81}Br), 3.55), 669 (M^+(^{79}Br), 3.77), 183 (100); IR (neat, cm^{-1}): 2927, 2854, 1717, 1563, 1452, 1422, 1347, 1256, 1242, 1176, 1069, 1012; HRMS calcd for $C_{37}H_{40}{}^{79}BrN_3O_4$ (M^+): 669.2197, found: 669.2199.

(7) Removing pyrimidinyl directing group of *E*-3an (*E*-20, zyz-7-68)



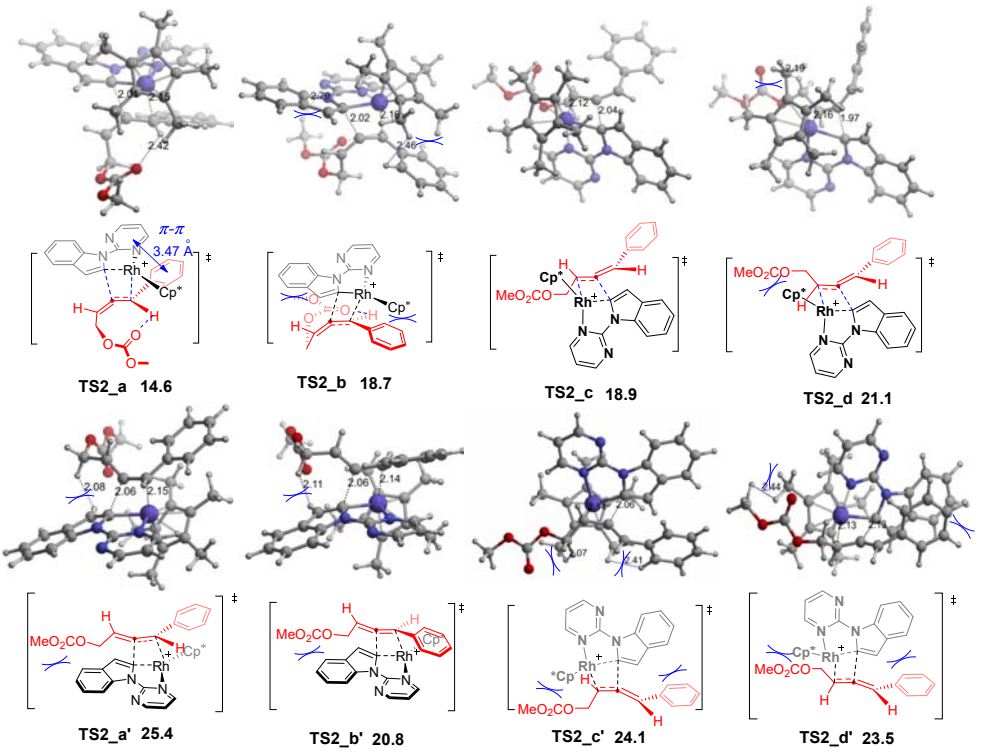
E-**3an** *E*-**20**, 58%

To an oven-dried Schlenk tube were added *E*-**3an** (66.3 mg, 0.2 mmol), DMSO (2 mL), and NaOEt (54.9 mg, 0.8 mmol) sequentially under argon atmosphere. The resulting mixture was stirred at 40 °C for 30 h as monitored by TLC, diluted by 10 mL of H_2O, and extracted with ethyl acetate (10 mL × 3). The combined organic layer was washed with 10 mL of brine, dried over anhydrous Na_2SO_4, filtrated, and concentrated. The crude product was purified by column chromatography to afford *E*-**20** (29.1 mg, 58%) (eluent: petroleum ether/ethyl acetate = 40/1) as an oil: ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.04 (brs, 1 H, NH), 7.56 (d, J = 7.6 Hz, 1 H, Ar-H), 7.32 (d, J = 8.0 Hz, 1 H, Ar-H), 7.14 (t, J = 7.4 Hz, 1 H, Ar-H), 7.07 (t, J = 7.4 Hz, 1 H, Ar-H), 6.79 (dd, J_1 = 17.6 Hz, J_2 = 11.2 Hz, 1 H, =CH), 6.49 (s, 1 H, Ar-H), 5.72 (d, J = 9.6 Hz, 1 H, =CH), 5.48 (d, J = 17.6 Hz, 1 H, one proton of $=CH_2$), 5.36 (d, J = 11.2 Hz, 1 H, one proton of $=CH_2$), 2.62-2.47 (m, 1 H, CH), 1.81-1.68 (m, 5 H), 1.36-1.15 (m, 5 H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 138.2, 138.0, 135.8, 132.4, 129.4, 128.7, 121.8, 120.3, 119.8, 118.3, 110.5, 101.4, 37.3, 33.1, 25.9, 25.8; Ms (EI, 70 eV) *m/z* (%) 251 (M^+, 100); IR (neat, cm^{-1}): 3416, 3052, 2922, 2848, 1829, 1709, 1449, 1401, 1344, 1303, 1259, 1224, 1090, 1018; HRMS calcd for $C_{18}H_{21}N$ (M^+): 251.1669, found: 251.1669.

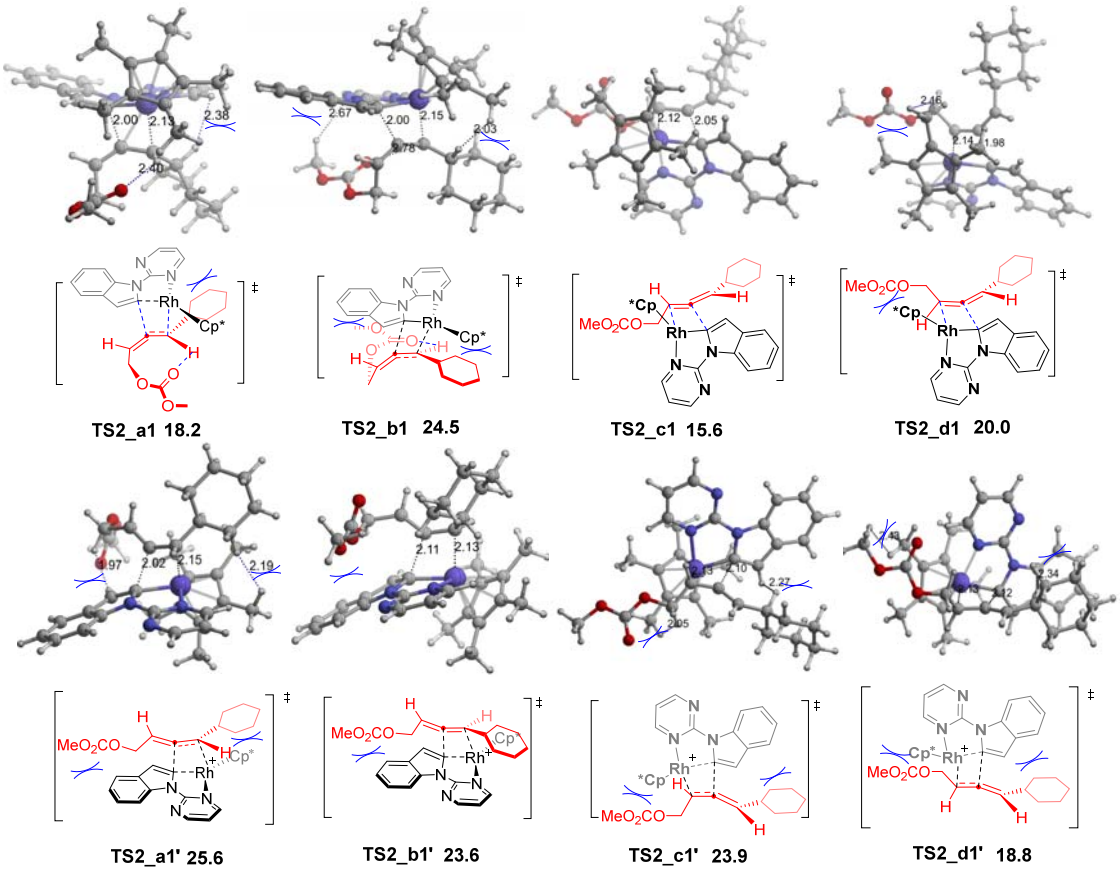
Computational Methodology.

All calculations were performed with the Gaussian 09 program.[10] Geometries have been fully optimized with the density functional theory of wB97XD method.[11] The standard 6-31G(d)[12] basis set was used for carbon, hydrogen and oxygen atoms and LANL2DZ basis set[13] with effective core potential (ECP) for rhodium. Harmonic vibration frequency calculations were carried out for all the stationary points to confirm each structure being either a minimum (no imaginary frequency) or a transition structure (one imaginary frequency). Intrinsic reaction coordinate (IRC)[14] calculations were performed to confirm the connection of the transition structures with their corresponding reactants and products. The single point energies and solvent effects in toluene (ε = 2.37) were computed with wB97XD/SDD[15]-6-311+G(d,p) basis sets by using IEFPCM[16] solvation model. The reported relative energies are the Gibbs free energies (ΔG_{sol}) in THF unless otherwise specified.

Scheme S1 Eight competing transition structures for the stereoselectivity of the carborhodation step of indole **1a** with 4-phenyl-2,3-allenyl carbonates **2a**. Free energies are given in kcal/mol and bond lengths are given in angstroms.



Scheme S2 Eight competing transition structures for the stereoselectivity of the carborhodation step of indole **1a** with cyclohexyl-substituted allenyl carbonate **2o**. Free energies are given in kcal/mol and bond lengths are given in angstroms.



Energies of intermediates and transition states

Table S1. Electronic energies (E_{elec}), Gibbs free energies (G_{298}), thermal correction to Gibbs free energy (*cor* G_{gas}), solvation energies (E_{sol}), solvation free energies (G_{sol}) in toluene (ε = 2.37) for all stationary points of the process.

species	E_{elec} (a.u.)	G_{298} (a.u.)	*cor* G_{gas} (a.u.)	E_{sol} (a.u.)	G_{sol} (a.u.)	*Imaginary frequencies*
INT1	-1472.433482	-1471.939579	0.493903	-1473.894219	-1473.400316	
TS1	-1472.406760	-1471.920152	0.487586	-1473.871666	-1473.384080	-707.78
INT2	-1472.434536	-1471.940463	0.494074	-1473.899144	-1473.405070	
2a	-689.9018057	-689.7270370	0.174769	-690.0854969	-689.9107279	
PivOH	-346.9220987	-346.8051200	0.116979	-347.0294536	-346.9124746	
INT3	-1815.421840	-1814.860685	0.561155	-1816.970670	-1816.409515	

TS2_a	-1815.401821	-1814.841295	0.560526	-1816.946880	-1816.386360	-350.78
INT4	-1815.446951	-1814.884534	0.562417	-1816.988689	-1816.426272	
INT5	-1815.447404	-1814.883984	0.563419	-1816.986069	-1816.422650	
TS3	-1815.420668	-1814.860434	0.560234	-1816.966152	-1816.405918	-323.57
INT6	-1815.443747	-1814.881714	0.562033	-1816.993147	-1816.431114	
TS2_b	-1815.394083	-1814.834159	0.559924	-1816.939597	-1816.379673	-291.91
TS2_c	-1815.394321	-1814.834420	0.559901	-1816.939229	-1816.379328	-329.30
TS2_d	-1815.389225	-1814.830073	0.559152	-1816.935117	-1816.375965	-321.07
TS2_a'	-1815.387477	-1814.824467	0.563009	-1816.931974	-1816.368965	-303.49
TS2_b'	-1815.390149	-1814.831305	0.558844	-1816.935195	-1816.376351	-341.13
TS2_c'	-1815.383971	-1814.824722	0.559249	-1816.930390	-1816.371141	-315.10
TS2_d'	-1815.388861	-1814.828382	0.560479	-1816.933257	-1816.372778	-283.19
INT3_1	-1819.061162	-1818.433041	0.628122	-1820.613607	-1819.985485	
TS2_a1	-1819.037999	-1818.408663	0.629336	-1820.585824	-1819.956488	-342.40
TS2_b1	-1819.029030	-1818.398183	0.630847	-1820.577242	-1819.946395	-306.57
TS2_c1	-1819.040343	-1818.413156	0.627187	-1820.587854	-1819.960667	-318.54
TS2_d1	-1819.034769	-1818.405490	0.629279	-1820.582805	-1819.953526	-318.80
TS2_a1'	-1819.026694	-1818.396612	0.630082	-1820.574825	-1819.944743	-338.35
TS2_b1'	-1819.024953	-1818.399197	0.625756	-1820.573579	-1819.947823	-297.53
TS2_c1'	-1819.028458	-1818.398024	0.630434	-1820.577821	-1819.947387	-282.73
TS2_d1'	-1819.038030	-1818.409312	0.628718	-1820.584188	-1819.955470	-280.02

Cartesian coordinates for the optimized structures

INT1

C	-1.66270900	2.51740400	0.97267200
C	-0.30469700	2.28350000	1.36434500
C	0.50878500	2.26524200	0.16508100
C	-0.35724800	2.44604000	-0.95704500
C	-1.71215000	2.56845100	-0.46922400
Rh	-0.97127100	0.66404200	0.11662800
C	1.99847000	2.19704600	0.12960800
H	2.36733500	1.75944500	-0.79952200
H	2.40267900	3.21292800	0.21190400
H	2.40175300	1.61367500	0.95962200
C	0.05559500	2.45530300	-2.38988500
H	0.25371400	3.48616200	-2.70579600
H	0.96197000	1.86541700	-2.54121900
H	-0.72920400	2.04716200	-3.03063000
C	-2.93603400	2.80440800	-1.29286200
H	-3.08345600	3.87877600	-1.45008900
H	-2.85141600	2.32496600	-2.27049700
H	-3.82460400	2.40656600	-0.79743500
C	-2.85998800	2.59840400	1.86044700
H	-3.29168600	3.60352800	1.80101800
H	-3.62485200	1.88260100	1.54428600
H	-2.60970300	2.39624900	2.90299900
C	0.21790600	2.14315700	2.75775400
H	0.58342600	3.10939100	3.12286600

H	-0.55447400	1.79031300	3.44471200
H	1.04995900	1.43496700	2.79453200
O	-1.63280100	-0.69114200	-1.44812100
O	-2.71728500	-0.55193500	0.42615300
C	-2.55568800	-1.13602300	-0.69752800
C	3.46103000	-0.76610300	-0.32004300
C	1.47614200	-0.92311100	-1.43128200
C	3.68330800	-0.51087600	-1.68711600
C	4.48970500	-0.69265900	0.61954800
C	2.41332800	-0.63411100	-2.36253400
H	0.42548100	-1.14222500	-1.55083000
C	4.96922900	-0.18986200	-2.13448600
C	5.75506600	-0.36648800	0.15107200
H	4.31829600	-0.90655400	1.66540300
H	2.23747100	-0.55479100	-3.42635300
C	5.99726200	-0.12051500	-1.20875100
H	5.15259900	0.00039600	-3.18736500
H	6.57743000	-0.31229000	0.85726200
H	7.00293100	0.12261900	-1.53599400
C	1.41900700	-1.30736800	1.00397500
N	0.10448600	-1.00469800	1.10650800
N	2.13077700	-1.89082100	1.96730400
C	-0.54346400	-1.48442600	2.18694300
C	1.48762400	-2.29048100	3.05621500
C	0.10806200	-2.16189500	3.19724800
H	-1.61018200	-1.28870000	2.21494400
H	2.09840100	-2.74214500	3.83365000
H	-0.42330800	-2.53710000	4.06229200
N	2.07879400	-0.99947000	-0.16560300
C	-3.35577600	-2.36422700	-1.07177000
C	-3.55908000	-2.41088200	-2.59171000
H	-2.60303600	-2.40222100	-3.12110800
H	-4.09592200	-3.32614000	-2.86033500
H	-4.15165900	-1.55766200	-2.93845800
C	-4.70174500	-2.36729700	-0.33851300
H	-5.25152700	-3.28019700	-0.58861700
H	-4.56685200	-2.33200200	0.74576300
H	-5.31680900	-1.51072900	-0.63365100
C	-2.50041800	-3.56796500	-0.61765900
H	-2.33461200	-3.54893700	0.46543200
H	-3.02098900	-4.49879000	-0.86351700
H	-1.52882500	-3.57502200	-1.12226000

TS1

C	0.46021900	-2.58591700	1.27138100
C	-0.51743500	-2.63172700	0.21140000
C	0.20524600	-2.62667400	-1.04368200
C	1.59171700	-2.47061200	-0.75325500
C	1.75750500	-2.44709900	0.68761600
Rh	0.53416000	-0.75819600	0.05387300

C	-1.00283600	0.43874200	-0.91404500
C	-1.82859300	0.19146300	-1.99016000
C	-3.17674200	0.50225200	-1.63861000
H	-1.48388300	-0.12415900	-2.96624800
C	-3.16677100	0.96448600	-0.30180300
C	-4.39050600	0.43097400	-2.34383400
C	-4.33661800	1.35320600	0.35653800
C	-5.54955600	0.80790900	-1.69646200
H	-4.40972200	0.08745700	-3.37335800
C	-5.51671000	1.26253200	-0.36220800
H	-4.31344800	1.72481100	1.37245100
H	-6.50011400	0.76187200	-2.21712100
H	-6.44515600	1.55983700	0.11486100
N	-1.84922500	0.91543700	0.13146500
N	-0.09884900	0.60395000	1.56239600
C	-1.31542200	1.15895600	1.36933200
C	0.55085900	0.90290700	2.69218000
N	-1.97189000	1.88298200	2.26682700
C	-0.03681900	1.69009100	3.66613300
H	1.54481100	0.48057000	2.79700900
C	-1.33440900	2.13044700	3.40906100
H	0.47781200	1.93119500	4.58715400
H	-1.88358700	2.71441200	4.14250900
C	-0.38380700	-2.81916100	-2.40371900
H	0.08033600	-2.16106100	-3.14236100
H	-0.21440000	-3.85387900	-2.72297700
H	-1.45938500	-2.63665700	-2.40571800
C	-1.99437800	-2.81368000	0.37204000
H	-2.34451100	-2.40206400	1.32188100
H	-2.54192100	-2.30650600	-0.42678300
H	-2.25629300	-3.87739200	0.34775800
C	0.14681400	-2.62374600	2.73145700
H	0.06171400	-3.66583000	3.05948700
H	0.92978600	-2.14994300	3.32788400
H	-0.80145600	-2.12703500	2.95083200
C	3.07709700	-2.32841800	1.37996400
H	2.95819200	-2.14687100	2.45051600
H	3.65375400	-3.25226300	1.25969200
H	3.65784600	-1.50442300	0.95416800
C	2.71460100	-2.36244300	-1.73201900
H	3.36468200	-1.52184100	-1.47211100
H	3.31490800	-3.27903600	-1.71714400
H	2.34827000	-2.21091700	-2.74917100
O	2.17607900	0.54133400	-0.24207100
C	2.07893700	1.65723800	-0.84940000
O	1.00383000	2.10052300	-1.32612800
H	-0.00708300	1.17971400	-1.14252000
C	3.34496700	2.50459100	-0.99775200
C	4.55368700	1.81359000	-0.36122800
H	4.76112500	0.85056500	-0.83857000

H	5.43994900	2.44629500	-0.47556600
H	4.39683700	1.63608000	0.70724500
C	3.58751200	2.72491600	-2.50118500
H	2.72969600	3.21513800	-2.96848900
H	4.47100800	3.35599800	-2.64269100
H	3.76757100	1.77376900	-3.01546100
C	3.08098400	3.85590900	-0.30946100
H	2.89860000	3.72406700	0.76368800
H	3.95527100	4.50503000	-0.42387600
H	2.21481400	4.35605400	-0.75015300

INT2

C	2.33772000	-2.30862800	0.15072600
C	1.20871000	-2.66742700	-0.71408200
C	1.29090900	-1.85546700	-1.90331800
C	2.29293700	-0.87366400	-1.66928200
C	2.98341500	-1.20551200	-0.41659500
Rh	0.78558000	-0.66837600	-0.12954800
C	-1.10039400	-0.24938600	-0.71570200
C	-1.77136600	0.09361200	-1.85155100
C	-3.17934600	0.23691200	-1.53518700
H	-1.32999200	0.22310700	-2.83093200
C	-3.33413500	-0.02908000	-0.16188100
C	-4.29858700	0.56548800	-2.30342100
C	-4.57113600	0.02243200	0.47485400
C	-5.53754300	0.61960700	-1.68137300
H	-4.19818800	0.77264800	-3.36434400
C	-5.66882300	0.35195900	-0.31147400
H	-4.66948600	-0.18293200	1.53232600
H	-6.41935800	0.87304100	-2.26102500
H	-6.64984000	0.40314200	0.14960100
N	-2.04994700	-0.32167100	0.32950700
N	-0.28279500	-0.76285400	1.70123200
C	-1.62061400	-0.56860900	1.59831700
C	0.22238900	-0.94831400	2.92519100
N	-2.47378500	-0.59566500	2.61754700
C	-0.58900700	-0.97927700	4.04450000
H	1.29835400	-1.07193300	2.98494400
C	-1.95441700	-0.80516800	3.82333200
H	-0.18128700	-1.13203000	5.03516200
H	-2.66294000	-0.82975900	4.64695900
C	0.48046500	-2.04183900	-3.14384000
H	0.46645600	-1.13839900	-3.75739600
H	0.92695100	-2.84400700	-3.74253700
H	-0.55140900	-2.31695500	-2.91750700
C	0.31482300	-3.85164500	-0.52589400
H	0.11867400	-4.03634900	0.53325400
H	-0.64575100	-3.70128200	-1.02391500
H	0.78106700	-4.75093100	-0.94486600
C	2.67869300	-3.02008400	1.42052900

H	3.21344500	-3.94932200	1.19364800
H	3.31786500	-2.41650200	2.06939800
H	1.77812300	-3.29369900	1.97817500
C	4.13562400	-0.42174300	0.12414600
H	4.49964400	-0.83170200	1.06835700
H	4.96698600	-0.42653200	-0.58886200
H	3.84363600	0.61964000	0.29585300
C	2.72193200	0.22220200	-2.59233600
H	3.03592500	1.10417200	-2.02682500
H	3.57192400	-0.10410200	-3.20272800
H	1.91562300	0.52026000	-3.26651600
O	1.27611500	1.42773100	0.41264100
C	0.86307600	2.51590600	-0.00375800
O	-0.18312900	2.63450800	-0.78392400
H	-0.59021400	1.75206000	-0.96316200
C	1.52557700	3.83180300	0.36295400
C	2.83031300	3.56650000	1.11835000
H	3.28934600	4.52058000	1.39406100
H	2.65769300	2.99200100	2.03265100
H	3.54568500	3.01726900	0.49719500
C	1.80686000	4.62219100	-0.92846500
H	0.88454500	4.84918700	-1.46836500
H	2.29807700	5.56567900	-0.67163800
H	2.47481300	4.06750900	-1.59720700
C	0.54043100	4.61533800	1.25484100
H	0.32482100	4.07216200	2.18143000
H	0.98989600	5.57596800	1.52442000
H	-0.40141400	4.80971000	0.73484300

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C	-0.98413400	-2.09569000	0.58907200
C	0.28295900	-1.98529800	0.29474700
H	-1.29629100	-2.30538000	1.61167700
C	1.55044100	-1.86480900	-0.01373800
C	2.31120000	-0.59930700	-0.00229000
C	1.66810300	0.64387000	0.03857900
C	3.70808100	-0.64032900	-0.04178100
C	2.41493500	1.81482600	0.05751500
H	0.58219900	0.68695000	0.02904900
C	4.45278400	0.53450200	-0.02335600
H	4.21428400	-1.60172200	-0.08359500
C	3.80800000	1.76618700	0.03004700
H	1.90550300	2.77369100	0.08401300
H	5.53745000	0.48574600	-0.05252300
H	4.38632000	2.68542300	0.04164300
H	2.09836100	-2.76458400	-0.29346600
C	-2.07920700	-1.94805300	-0.43211400
H	-2.64940100	-2.87419000	-0.53427400
H	-1.67282300	-1.65411300	-1.40179200
O	-3.05830400	-0.99115200	0.00252600

C	-2.73380100	0.28946100	-0.18094100
O	-1.74482000	0.70765600	-0.73591300
O	-3.70334000	1.03721200	0.34368800
C	-3.50646900	2.44387200	0.21101300
H	-4.38291800	2.90273700	0.66699300
H	-2.59755100	2.75561100	0.73151900
H	-3.43077400	2.72471700	-0.84215800

PivOH

O	1.52320800	1.24199900	0.00015800
C	0.94112200	0.18341200	0.00025500
O	1.60885800	-0.99116300	0.00018800
H	2.55147100	-0.76113500	0.00011800
C	-0.57061100	-0.00973800	0.00002900
C	-1.24536600	1.36382700	0.00113000
H	-2.33366600	1.23946100	0.00087300
H	-0.96142200	1.94249500	0.88473000
H	-0.96117200	1.94406300	-0.88138300
C	-0.96895800	-0.80023500	-1.25941000
H	-0.49678400	-1.78614500	-1.27635900
H	-2.05580300	-0.93639200	-1.27650100
H	-0.68214200	-0.26332900	-2.17021900
C	-0.96952600	-0.80248500	1.25781000
H	-0.68341800	-0.26718300	2.16977900
H	-2.05635400	-0.93886300	1.27401400
H	-0.49720700	-1.78834700	1.27330100

INT3

C	0.00775500	0.32025200	-3.09744300
C	0.63297100	1.48310800	-2.55115000
C	1.83619900	1.05988400	-1.89997300
C	2.03923700	-0.35132500	-2.20330600
C	0.91670500	-0.80681100	-2.92259300
Rh	0.16737200	-0.01410500	-0.92324800
C	1.07224600	-1.28014000	0.77957600
C	1.10870500	0.07138900	1.01503100
C	1.50517800	1.05676300	1.78955900
C	-1.11454800	1.28444500	-0.05229900
C	-1.13136000	2.58072200	0.34006500
C	-2.45586400	2.88918100	0.84260300
H	-0.30329800	3.27456500	0.29050400
C	-3.23601900	1.72230500	0.73751200
C	-3.02912800	4.04970200	1.36660900
C	-4.56807700	1.67063300	1.13661000
C	-4.35714800	4.01292200	1.76975300
H	-2.44722100	4.96188100	1.45705100
C	-5.11401800	2.83923000	1.65565100
H	-5.14780600	0.76189200	1.04647700
H	-4.81757500	4.90565100	2.18081200
H	-6.15014600	2.83902400	1.97863100

N	-2.39675100	0.74033900	0.18073200
N	-1.58299600	-1.18830300	-0.70954100
C	-2.64131500	-0.55248600	-0.14958700
C	-1.72796200	-2.48435300	-1.00614100
N	-3.82525200	-1.11055300	0.08783900
C	-2.91921700	-3.14680400	-0.78516400
H	-0.85748900	-2.98269000	-1.41577100
C	-3.95210800	-2.39355700	-0.22955100
H	-3.03439600	-4.19685100	-1.01845800
H	-4.92227200	-2.83989100	-0.02790000
C	2.85053900	1.94575800	-1.25149000
H	3.44196800	1.38687300	-0.52432200
H	3.52963500	2.35478000	-2.00866100
H	2.37956100	2.78386200	-0.73186400
C	0.13734000	2.88525400	-2.68537200
H	-0.94340700	2.95308700	-2.54751400
H	0.61039200	3.55078500	-1.96114900
H	0.38176800	3.25384400	-3.68850800
C	-1.27638300	0.29984500	-3.86450900
H	-1.08787000	0.47515500	-4.92984200
H	-1.78444000	-0.66305100	-3.76748000
H	-1.95838700	1.07573400	-3.50812600
C	0.72493700	-2.17346600	-3.50178500
H	-0.33227600	-2.39757800	-3.66479600
H	1.22455800	-2.24187800	-4.47470700
H	1.14922200	-2.95030500	-2.85882800
C	3.26748600	-1.12776100	-1.85452400
H	3.08544500	-2.20551600	-1.87792200
H	4.05207500	-0.91110800	-2.58964500
H	3.65781900	-0.86043300	-0.86707700
H	1.25720700	2.09153900	1.57774400
C	2.37335000	0.77519000	2.98770500
H	2.00079600	1.28652800	3.87647500
H	2.44129600	-0.29789900	3.17939500
O	3.68959800	1.31853600	2.80234600
C	4.47099900	0.66552000	1.94381900
O	4.17222200	-0.33843700	1.32879700
H	1.93188700	-1.72621400	0.28377100
C	0.15434700	-2.21761800	1.44535600
C	0.32810900	-3.59124800	1.24785200
C	-0.89292400	-1.77039400	2.26178700
C	-0.53132800	-4.50530000	1.85014900
H	1.14773000	-3.94422700	0.62590700
C	-1.75834100	-2.68253100	2.84927200
H	-1.03278100	-0.70390400	2.41838200
C	-1.58094500	-4.05222500	2.64384400
H	-0.37983400	-5.56955100	1.70016000
H	-2.57115900	-2.32666000	3.47440700
H	-2.25565900	-4.76270800	3.11088100
O	5.62966800	1.30187600	1.86797200

C	6.59220400	0.71700000	0.98855200
H	7.49147500	1.31956200	1.10285400
H	6.78714000	-0.32095500	1.26593300
H	6.23764900	0.75670700	-0.04528700

TS2_a

C	0.04100800	-0.61955700	3.17809300
C	-0.56491600	0.63913400	2.97821300
C	-1.77744300	0.42059100	2.21398700
C	-1.98575500	-1.00428900	2.09480700
C	-0.83895200	-1.64893100	2.61950800
Rh	-0.15397900	-0.34412900	0.96562600
C	-0.91269700	-0.91488300	-0.96277600
C	-0.68568100	0.47847500	-1.03516400
C	-1.15904900	1.46465200	-1.78791600
C	0.79805000	1.26036000	0.07184100
C	0.72527100	2.61359100	0.22451900
C	1.99445300	3.18273500	-0.14657700
H	-0.15865300	3.16603200	0.51203100
C	2.84608100	2.12252400	-0.51718500
C	2.46892000	4.49847100	-0.19633600
C	4.16027500	2.33043800	-0.92790900
C	3.77427000	4.71706800	-0.60627000
H	1.82518600	5.32742400	0.08141200
C	4.60659900	3.64541000	-0.96471600
H	4.79842200	1.50448800	-1.21119700
H	4.16131500	5.72975800	-0.65445900
H	5.62406000	3.84639600	-1.28421700
N	2.10562400	0.93755600	-0.36448400
N	1.70641400	-1.19651200	0.35828100
C	2.56393800	-0.34690200	-0.24811400
C	2.06118200	-2.48428200	0.42710600
N	3.75852200	-0.67788900	-0.72448100
C	3.28187400	-2.92274700	-0.04886300
H	1.33529500	-3.15902800	0.86505000
C	4.10994700	-1.95505500	-0.61270700
H	3.56941900	-3.96418600	0.00837400
H	5.09065100	-2.21389200	-1.00266700
C	-2.76455800	1.46675800	1.80240200
H	-3.29781900	1.15662800	0.90108800
H	-3.49670200	1.63353400	2.60124700
H	-2.27292700	2.41999800	1.59352800
C	-0.03684800	1.95581500	3.45069300
H	1.03702800	2.05045800	3.26958100
H	-0.53104800	2.78962000	2.94881800
H	-0.21379600	2.06382200	4.52657800
C	1.32462200	-0.88407700	3.89840600
H	1.12410100	-1.18202000	4.93401000
H	1.89149700	-1.69067600	3.42449200
H	1.95892100	0.00518700	3.91957600

C	-0.64597300	-3.12757400	2.75993400
H	0.39824700	-3.37751400	2.96469000
H	-1.23985800	-3.50928700	3.59815600
H	-0.95996600	-3.66350800	1.85902400
C	-3.20306000	-1.66558300	1.53368900
H	-2.97611000	-2.66242000	1.14582900
H	-3.95079600	-1.78216100	2.32750200
H	-3.65629100	-1.07817400	0.73056100
H	-0.90209000	2.50392100	-1.62467300
C	-2.08980800	1.16648000	-2.93305700
H	-1.73220300	1.62818700	-3.85497300
H	-2.21546200	0.09258900	-3.08515600
O	-3.36742100	1.78401800	-2.71356800
C	-4.16220300	1.18168600	-1.83215700
O	-3.90889700	0.15646700	-1.23025600
H	-1.94911900	-1.18074500	-0.76077500
C	-0.15193800	-1.91362100	-1.74121900
C	-0.44319200	-3.27236200	-1.57333600
C	0.86011400	-1.54361900	-2.63448000
C	0.27343700	-4.24238000	-2.26571000
H	-1.24036200	-3.56510900	-0.89320000
C	1.57986700	-2.51385200	-3.32308400
H	1.08193300	-0.49066400	-2.78874900
C	1.29312100	-3.86524900	-3.13723400
H	0.03418700	-5.29261900	-2.12970300
H	2.36092200	-2.21298100	-4.01449600
H	1.85179300	-4.62032900	-3.68117000
O	-5.27419900	1.88787100	-1.71964300
C	-6.25614100	1.35370000	-0.82831200
H	-7.08409000	2.05958000	-0.85796200
H	-6.58122100	0.36675800	-1.16470900
H	-5.85408700	1.28023900	0.18549000

INT4

C	-1.99967800	-2.40935200	1.31272800
C	-2.08985200	-1.17568300	1.97240300
C	-2.90762200	-0.30240100	1.13295000
C	-3.43172000	-1.07834600	0.04298200
C	-2.83469700	-2.35650400	0.10830900
C	-3.40696800	1.04933400	1.54043900
H	-4.37037000	0.93688300	2.05144600
H	-2.72063700	1.54116600	2.23344900
H	-3.56070200	1.71769100	0.68800200
C	-4.48787500	-0.65311300	-0.92705400
H	-5.46654400	-1.00763600	-0.58097400
H	-4.55012100	0.43343900	-1.01740400
H	-4.31683300	-1.07181800	-1.92247700
C	-3.24968800	-3.53945100	-0.71290200
H	-4.23616900	-3.88256500	-0.37836000
H	-3.33696300	-3.29699600	-1.77699100

H	-2.56581000	-4.38404800	-0.59760600
C	-1.26658800	-3.62608900	1.78225200
H	-1.96526500	-4.33308600	2.24463500
H	-0.77271700	-4.14599400	0.95547800
H	-0.50506000	-3.37158300	2.52253300
C	-1.52150300	-0.83022500	3.31131100
H	-2.21786500	-1.14299200	4.09831300
H	-0.56622800	-1.33130700	3.48625100
H	-1.35087300	0.24214000	3.42192200
Rh	-1.15222400	-0.84606500	-0.09568000
C	-0.37604300	1.28459900	0.48162900
H	-1.31124000	1.82335300	0.37649900
C	0.16209300	0.75065400	-0.69592400
C	-0.76091800	0.40762700	-1.76116400
H	-0.29037700	-0.07744800	-2.61446000
C	-1.92560500	1.28398100	-2.14998800
H	-2.58020300	1.52022500	-1.31329400
H	-2.51026100	0.79059200	-2.92816400
O	-1.46949800	2.51443800	-2.72974100
C	1.62333800	0.53258300	-0.75631700
C	2.51837700	1.54490500	-0.74757100
C	3.83398300	0.98876300	-0.59734200
H	2.26162300	2.59473900	-0.78491500
C	3.69549600	-0.40788300	-0.51640400
C	5.09194800	1.58611700	-0.48781100
C	4.80419500	-1.23117100	-0.31038700
C	6.19531000	0.77356600	-0.28884600
H	5.19446700	2.66460200	-0.55336000
C	6.04460000	-0.61658900	-0.19640400
H	4.70996100	-2.30350900	-0.24216100
H	7.18274800	1.21394400	-0.19737000
H	6.91979200	-1.23682500	-0.03118300
C	1.77670700	-1.94278400	-0.89132800
N	0.43426200	-2.08634900	-0.97460600
N	2.64289000	-2.93907000	-1.07937000
C	0.00377500	-3.24035000	-1.51826800
C	2.18335300	-4.10111400	-1.51360900
C	0.84079800	-4.29089900	-1.82814100
H	-1.05981400	-3.30406400	-1.69405500
H	2.91729900	-4.89431600	-1.63028800
H	0.46349100	-5.20842600	-2.26057700
C	0.31734600	1.53918500	1.75126300
C	1.30858800	0.70108500	2.28091500
C	-0.07534600	2.66990000	2.47961300
C	1.90180800	0.99852900	3.49875500
H	1.59597500	-0.20206500	1.75255500
C	0.52526000	2.96925600	3.69914400
H	-0.84064000	3.32665300	2.07250200
C	1.51388800	2.13397700	4.21057100
H	2.66674800	0.34035800	3.89836800

H	0.21891200	3.85361500	4.24859800
H	1.97908400	2.36157500	5.16436700
C	-1.53849200	3.59468000	-1.94606900
O	-1.98675500	3.63079400	-0.81762600
O	-1.03946100	4.62094400	-2.61205400
C	-1.07820500	5.87545000	-1.92373000
H	-0.64120900	6.59435600	-2.61440400
H	-2.10923300	6.14764200	-1.68825500
H	-0.49498900	5.82319200	-1.00151700
N	2.30934200	-0.70049500	-0.63490600

INT5

C	-3.15282300	0.99457100	-1.17931200
C	-3.36851200	1.63329500	0.12829000
C	-2.24043200	2.39509900	0.43454900
C	-1.30039300	2.26074000	-0.67899400
C	-1.92277100	1.48195600	-1.70945500
Rh	-1.55155200	0.23463000	0.05149500
C	-0.61672300	-1.32177500	-1.00141800
C	0.86749100	-1.35403500	-0.75867100
C	1.56082400	-2.47663300	-0.47532000
C	1.58204000	-0.06650000	-0.88938700
C	2.31891200	0.39665300	-1.92935300
C	3.04568600	1.55752400	-1.48418400
H	2.40756400	-0.09450600	-2.88845100
C	2.73037400	1.75594700	-0.12673500
C	3.92226800	2.43843200	-2.12742700
C	3.25805900	2.81840800	0.60747700
C	4.45606900	3.49206900	-1.40485000
H	4.17494400	2.29370700	-3.17317700
C	4.12452900	3.67741700	-0.05315200
H	3.02688100	2.95444500	1.65604400
H	5.14196700	4.18262400	-1.88468500
H	4.56279300	4.50658800	0.49301000
N	1.78427800	0.77761600	0.22416300
N	-0.01011300	0.10862200	1.58687200
C	1.25459100	0.56889500	1.48594100
C	-0.44463900	-0.20692800	2.81971600
N	2.04145800	0.84487800	2.52272000
C	0.32649200	0.00311500	3.94621800
H	-1.44730700	-0.61641000	2.87617500
C	1.57332300	0.58464100	3.73798300
H	-0.03763000	-0.24654900	4.93457800
H	2.22856000	0.83757400	4.56731700
C	-1.25027700	-2.66246300	-0.65933000
H	-0.95134300	-2.98843800	0.34057700
H	-0.98730200	-3.43562600	-1.38471100
O	-2.70100200	-2.67890700	-0.69693300
C	-3.29308600	-2.08042200	0.31000500

O	-2.71961200	-1.35601300	1.12674600
O	-4.58315600	-2.29419700	0.41042200
C	-5.21894600	-3.21769000	-0.49482900
H	-4.76681000	-4.20612200	-0.40254300
H	-6.26045200	-3.24212300	-0.18152200
H	-5.13364000	-2.85778400	-1.52172800
C	-1.96535100	3.19725200	1.66762000
H	-2.06706600	4.26864100	1.46128700
H	-2.65298300	2.94330900	2.47719800
H	-0.94568400	3.02742200	2.02804800
C	-4.58299200	1.40611200	0.96798200
H	-5.46494800	1.82841500	0.47347000
H	-4.76312400	0.33704500	1.11952300
H	-4.48923000	1.87464900	1.94945100
C	-4.18508800	0.20382900	-1.92281200
H	-4.87950900	-0.28481300	-1.23423000
H	-4.77467400	0.86366000	-2.56958700
H	-3.72544200	-0.56287400	-2.55281700
C	-1.37231500	1.26101700	-3.08010800
H	-1.56927800	2.14126100	-3.70257300
H	-0.29018000	1.10290300	-3.04814800
H	-1.83481200	0.39868700	-3.56698300
C	-0.08068200	3.10088200	-0.84981100
H	0.43605900	3.27687300	0.09529200
H	0.62879100	2.65872800	-1.55048000
H	-0.38413800	4.07767300	-1.24710900
H	-0.79876800	-1.09101500	-2.05758100
C	3.00296300	-2.68898100	-0.24621100
C	3.50125800	-3.97012400	-0.53013800
C	3.89944600	-1.72926800	0.24602500
C	4.84590000	-4.27637200	-0.36392500
H	2.82167200	-4.73542400	-0.89792900
C	5.24349000	-2.03802800	0.42017600
H	3.56181300	-0.73790800	0.51890000
C	5.72514200	-3.30705600	0.11061500
H	5.20594100	-5.27298300	-0.59973500
H	5.91767800	-1.27856000	0.80393700
H	6.77628100	-3.54063400	0.24760600
H	1.01104400	-3.41512300	-0.45692500

TS3

C	3.08553600	-1.69800900	0.72345200
C	2.12545000	-1.66127600	1.79849000
C	0.92025800	-2.29208500	1.32024600
C	1.10847900	-2.66479000	-0.04713500
C	2.46407100	-2.29630200	-0.41841400
Rh	1.36512900	-0.51456500	0.11696800
C	0.78949700	0.00085500	-2.04711700
C	-0.48515400	0.70189500	-1.74964000
C	-0.61507800	2.03247900	-1.60351700

C	-1.56565100	-0.25448800	-1.42463900
C	-2.25007000	-1.10828000	-2.22862500
C	-3.21091200	-1.81022400	-1.41712300
H	-2.11417900	-1.19950700	-3.29755200
C	-3.07700500	-1.32780000	-0.10037500
C	-4.15361100	-2.80899200	-1.69110800
C	-3.85263500	-1.81390800	0.95320900
C	-4.92878900	-3.29668200	-0.65224400
H	-4.27288300	-3.19125700	-2.70023100
C	-4.77797100	-2.80286600	0.65422200
H	-3.76012500	-1.41225600	1.95466800
H	-5.66797800	-4.06668200	-0.84783600
H	-5.40767400	-3.19384900	1.44701500
N	-2.02985400	-0.39975000	-0.10541700
N	-0.28545800	0.61343200	1.07986500
C	-1.60645100	0.37334000	0.96526600
C	0.08776300	1.49515700	2.02269500
N	-2.53766000	0.81939000	1.79895200
C	-0.82490500	2.05922500	2.89371700
H	1.14614800	1.72733400	2.05476300
C	-2.14599000	1.64298200	2.76459700
H	-0.51509800	2.76923900	3.64981800
H	-2.92017000	1.98816500	3.44419500
C	1.88337400	0.61339600	-2.67448800
H	1.84098600	1.65594500	-2.96958800
H	2.55937900	0.00170200	-3.25699600
O	3.50752000	1.10975000	-1.61609600
C	3.30441200	1.62067600	-0.48596200
O	2.35773300	1.33558500	0.30609100
O	4.13505800	2.54974400	-0.01784300
C	5.18899000	2.97876500	-0.88520700
H	4.78267400	3.38687300	-1.81310800
H	5.71860200	3.75253600	-0.33144000
H	5.86146500	2.14941100	-1.11604700
C	-0.31549100	-2.52797900	2.12371000
H	-0.20928800	-3.47111600	2.67222200
H	-0.48013800	-1.73328000	2.85585600
H	-1.20273800	-2.60676800	1.49172400
C	2.37080600	-1.15013700	3.18164600
H	2.83303600	-1.92784300	3.80022300
H	3.03998100	-0.28590000	3.17054600
H	1.43834800	-0.84901800	3.66545700
C	4.48224700	-1.17507500	0.78615100
H	4.56499400	-0.34650200	1.49325900
H	5.15905600	-1.97167700	1.11542100
H	4.81750600	-0.82415700	-0.19248800
C	3.13390000	-2.58665400	-1.72247300
H	3.66296300	-3.54445900	-1.66141900
H	2.40968900	-2.66046900	-2.53730400
H	3.85976500	-1.81033800	-1.97506700

C	0.13627500	-3.43150900	-0.88435000
H	-0.89803500	-3.17065900	-0.64833200
H	0.28669700	-3.25064500	-1.95099100
H	0.26858000	-4.50514100	-0.70703400
H	0.65908500	-1.04144000	-2.33055800
C	-1.78415300	2.75442200	-1.07611200
C	-1.54708400	3.84894400	-0.23167800
C	-3.11097400	2.36862200	-1.31408600
C	-2.59860900	4.51035900	0.39292700
H	-0.52376700	4.17185300	-0.05389700
C	-4.16094700	3.03257000	-0.69152800
H	-3.32267900	1.54959400	-1.99327100
C	-3.91007900	4.09760500	0.17093000
H	-2.39387900	5.35234000	1.04751600
H	-5.18187800	2.71899800	-0.88506400
H	-4.73462000	4.61318200	0.65349400
H	0.27671000	2.64367300	-1.73515900

INT6

C	3.07887300	-2.12542200	0.27287000
C	2.31199800	-1.85900700	1.47498800
C	0.97555400	-2.33136600	1.25749200
C	0.87539400	-2.80343300	-0.09272200
C	2.19353000	-2.70245500	-0.68805600
Rh	1.50591500	-0.69363500	-0.15025300
C	0.47459500	-0.33400300	-2.33026400
C	-0.70691000	0.46029200	-1.96751200
C	-0.69717300	1.80704100	-1.94425800
C	-1.78726100	-0.36775200	-1.39993000
C	-2.67964100	-1.19916700	-1.99660400
C	-3.51138600	-1.76588100	-0.96693500
H	-2.76388100	-1.36270900	-3.06229500
C	-3.08542700	-1.22108900	0.26032400
C	-4.56027200	-2.69423500	-0.98058100
C	-3.67736800	-1.57206200	1.47511800
C	-5.15115400	-3.05004800	0.22000100
H	-4.90229500	-3.12380400	-1.91704400
C	-4.71334400	-2.49281000	1.43339700
H	-3.36468500	-1.12049100	2.40902900
H	-5.96677600	-3.76567200	0.22709000
H	-5.20319500	-2.77919000	2.35850700
N	-1.98507200	-0.39960100	-0.00966100
N	-0.03457100	0.59345600	0.87815900
C	-1.37838400	0.46479000	0.89906900
C	0.48741400	1.48623900	1.73782000
N	-2.19227700	1.08446400	1.74353200
C	-0.29378700	2.21936900	2.60950500
H	1.56594400	1.56293700	1.73334000
C	-1.65726600	1.95577200	2.59099200
H	0.14804800	2.93781300	3.28806500

H	-2.34622500	2.45175500	3.26891700
C	1.77024700	0.10312400	-2.36606700
H	2.54700600	-0.53248900	-2.77880000
O	2.07894000	2.65118500	-0.69611300
C	2.97994900	2.03375700	-0.13605200
O	2.95453000	0.80133800	0.26549500
O	4.16077400	2.59935100	0.16894100
C	4.30174500	3.96947400	-0.20191900
H	3.58695700	4.59396800	0.34055100
H	5.32156700	4.24059100	0.06975500
H	4.14631300	4.10018400	-1.27532500
C	-0.11855100	-2.33602100	2.27077700
H	0.01138400	-3.20719700	2.92366100
H	-0.09069900	-1.44339100	2.90095700
H	-1.10410900	-2.40959700	1.80756900
C	2.87780800	-1.26000800	2.71870100
H	3.51867200	-1.98592300	3.23134300
H	3.48371800	-0.38442000	2.46520400
H	2.09182900	-0.95299600	3.41230600
C	4.52831800	-1.81464500	0.12182400
H	4.70139800	-0.75821600	0.35309400
H	5.11237800	-2.42660700	0.81790100
H	4.88631500	-2.01195900	-0.88997200
C	2.56205200	-3.21603500	-2.04025400
H	2.71593200	-4.29953200	-1.97767500
H	1.77165900	-3.04035400	-2.77448000
H	3.48543900	-2.76796400	-2.41141700
C	-0.30399500	-3.49416100	-0.69559200
H	-1.24569200	-3.13219300	-0.27894400
H	-0.34825400	-3.35863300	-1.77805100
H	-0.23357100	-4.57015400	-0.49656500
H	0.26269000	-1.35401100	-2.64375200
C	-1.69140400	2.68657000	-1.31697200
C	-1.19664900	3.81896600	-0.65214500
C	-3.06641900	2.41703900	-1.27622000
C	-2.05416000	4.64020800	0.07090800
H	-0.13019100	4.02583100	-0.68411100
C	-3.92040900	3.24934600	-0.56345900
H	-3.46875300	1.56038000	-1.80653200
C	-3.41715500	4.35532500	0.11890800
H	-1.65960000	5.51004100	0.58733700
H	-4.98387300	3.03405300	-0.54054600
H	-4.08867300	5.00099600	0.67656700
H	0.19736100	2.30867800	-2.30059200
H	2.01302000	1.14433800	-2.18742600

TS2_b

C	1.47876500	-2.76319300	1.09235300
C	1.56720900	-2.88052300	-0.31000300
C	2.54013700	-1.91012800	-0.77201900

C	3.17669800	-1.32818100	0.38648600
C	2.47482000	-1.78126800	1.52859200
Rh	0.96817000	-0.76282300	0.25947800
C	1.11729900	1.37214300	-0.01081200
C	0.09777800	0.98426300	-0.90326000
H	0.77769000	1.80221500	0.93020500
C	-0.71792600	1.62191300	-1.72909600
C	-0.77740700	-0.83020500	-0.83184500
C	-1.14439500	-1.34330600	-2.03815900
C	-2.56325900	-1.60237500	-2.00305300
H	-0.49188300	-1.46154000	-2.89196600
C	-3.03945600	-1.21765700	-0.73183100
C	-3.46063800	-2.11517800	-2.94578900
C	-4.37861200	-1.33501600	-0.36850600
C	-4.79701300	-2.23181300	-2.59660400
H	-3.11418700	-2.41354300	-3.93049700
C	-5.24691300	-1.84727500	-1.32432800
H	-4.72464100	-1.03243900	0.61074400
H	-5.50835400	-2.62369700	-3.31635200
H	-6.29937500	-1.94899700	-1.08019200
N	-1.92598800	-0.76139500	-0.01145600
N	-0.52985200	-0.21017600	1.70610100
C	-1.80699600	-0.34948500	1.28253400
C	-0.33905300	0.26825200	2.93963100
N	-2.88597300	-0.11906000	2.02408100
C	-1.40023900	0.54766400	3.77915600
H	0.69325100	0.41519900	3.24010400
C	-2.67277600	0.31598100	3.26130200
H	-1.24710200	0.92770000	4.78065200
H	-3.56111600	0.49486900	3.86149800
C	3.00592600	-1.75858800	-2.18562500
H	3.48676900	-0.79079000	-2.34127100
H	3.73397700	-2.54159300	-2.42786200
H	2.17652000	-1.84309600	-2.89282600
C	0.80394600	-3.83592100	-1.16756300
H	-0.21388300	-3.98930900	-0.80168300
H	0.73622400	-3.48577900	-2.19879100
H	1.31552300	-4.80527300	-1.17514200
C	0.58623700	-3.54936500	1.99932800
H	1.11749600	-4.42291400	2.39408700
H	0.25387500	-2.95003600	2.85166800
H	-0.30247200	-3.90465700	1.47233500
C	2.81088200	-1.47106200	2.95326200
H	1.94408000	-1.59330500	3.60822600
H	3.58764900	-2.15568800	3.31334200
H	3.19007700	-0.45118200	3.06405300
C	4.39759500	-0.47170200	0.38061500
H	4.42356100	0.21004700	1.23305300
H	5.28215600	-1.11778400	0.43670200
H	4.47598800	0.12680600	-0.52872200

H	-1.46452200	1.11933100	-2.33356800
C	-0.77186900	3.12667500	-1.70300400
H	-0.00896100	3.55055400	-1.04635700
H	-0.67598300	3.55680900	-2.70115600
O	-2.07767000	3.53101700	-1.27171300
C	-2.39034800	3.26665000	0.00007600
O	-1.64940900	2.79675000	0.83839800
C	2.39831500	1.91373800	-0.50925200
C	3.22740300	2.61893300	0.37034900
C	2.79189300	1.78680000	-1.84817200
C	4.42510200	3.17246400	-0.07110900
H	2.92570600	2.73954600	1.40832800
C	3.99116200	2.33475100	-2.28784500
H	2.14752400	1.26090800	-2.54702600
C	4.81473300	3.02668500	-1.39995800
H	5.05282800	3.72347600	0.62217500
H	4.28028600	2.23007500	-3.32918700
H	5.74755900	3.45958300	-1.74634000
O	-3.65473800	3.61180100	0.18585900
C	-4.18008500	3.34790400	1.48677000
H	-5.16305400	3.81570800	1.50158900
H	-4.26975900	2.26895500	1.63908300
H	-3.53735100	3.77930800	2.25740300

TS2_c

C	1.88481200	-2.39801400	-0.98809300
C	0.56447700	-2.94117800	-1.32146400
C	0.02516700	-2.17000900	-2.37176700
C	0.94435100	-1.07712400	-2.62953100
C	2.13971600	-1.30549500	-1.84836600
Rh	0.35197700	-0.84946700	-0.54938500
C	1.05235800	1.06008600	0.04120200
C	-0.28015900	1.34189600	-0.30538200
C	-1.05630600	2.41046200	-0.48774200
C	-1.60393000	-0.20441200	-0.41956000
C	-2.59359600	0.02291300	-1.32784000
C	-3.86402700	-0.15517900	-0.67114700
H	-2.44251300	0.35530000	-2.34548400
C	-3.60607800	-0.50338100	0.67056000
C	-5.18722900	-0.03795300	-1.11100100
C	-4.62573300	-0.74484700	1.58786900
C	-6.20980400	-0.27414700	-0.20577700
H	-5.40418300	0.23098100	-2.14016700
C	-5.92963700	-0.62303500	1.12412400
H	-4.40867700	-1.00529300	2.61477500
H	-7.24279300	-0.18542800	-0.52629200
H	-6.75004600	-0.79766600	1.81274700
N	-2.20915100	-0.54692500	0.81256500
N	-0.15704300	-1.29385000	1.49363500
C	-1.45535000	-1.08463400	1.81547900

C	0.64037800	-1.79714500	2.44521200
N	-2.00450600	-1.36006500	2.99442600
C	0.15189600	-2.12207800	3.69709700
H	1.68454700	-1.91119000	2.18220400
C	-1.20295200	-1.88314400	3.91722600
H	0.79624600	-2.53114800	4.46431900
H	-1.66522200	-2.10992300	4.87418300
C	-1.26455700	-2.42863000	-3.08112800
H	-1.60115600	-1.55214100	-3.63743100
H	-1.12906400	-3.24564900	-3.79878400
H	-2.06061700	-2.70972400	-2.38743900
C	-0.04732600	-4.15603900	-0.69902800
H	0.13351100	-4.18754700	0.37941200
H	-1.12767400	-4.18291400	-0.85919600
H	0.38265300	-5.06533300	-1.13450400
C	2.85715700	-3.01444100	-0.03090000
H	3.55214400	-3.66421300	-0.57553000
H	3.44584700	-2.25909400	0.49845000
H	2.34769100	-3.63737900	0.70872600
C	3.42610400	-0.55521700	-1.97465600
H	4.07892100	-0.74495300	-1.12068400
H	3.94975100	-0.88726400	-2.87874400
H	3.28174000	0.52493400	-2.05960200
C	0.80119500	-0.03797900	-3.69743700
H	1.34497800	0.87419600	-3.43817700
H	1.20127600	-0.41069800	-4.64757400
H	-0.24557700	0.23197500	-3.85513300
C	-0.61245900	3.80720500	-0.31860500
C	-1.61128700	4.78047600	-0.18015600
C	0.72899800	4.21478600	-0.29879700
C	-1.28352500	6.11993000	-0.00616300
H	-2.65609600	4.48153800	-0.20556800
C	1.05489100	5.55468100	-0.12899800
H	1.53114200	3.49604500	-0.42859900
C	0.05225600	6.51039400	0.02253600
H	-2.07107700	6.85861500	0.10346900
H	2.09831900	5.85388200	-0.11914000
H	0.31130500	7.55573100	0.15717000
H	-2.10444800	2.28165700	-0.72964100
C	1.53652900	1.24335400	1.45747200
H	1.86503900	2.27670400	1.60363600
H	0.76277200	1.01294400	2.18739100
O	2.62436000	0.36071600	1.76163400
C	3.79858000	0.70574200	1.22136700
O	4.01222700	1.69796400	0.56713100
O	4.68108200	-0.24513800	1.51765600
C	6.02296500	0.01751400	1.08544100
H	6.40650800	0.91701500	1.57056300
H	6.59822400	-0.85549100	1.38858800
H	6.05975900	0.14802000	0.00143100

H	1.80408300	1.31494600	-0.70507600

TS2_d

C	0.25861100	-2.37929000	-2.00243700
C	-0.51604600	-1.41662700	-2.69830200
C	0.28532400	-0.22448200	-2.78586800
C	1.59260500	-0.50078500	-2.23448500
C	1.57479800	-1.82292400	-1.72073100
Rh	-0.01266700	-0.62379800	-0.63640200
C	0.70646500	0.57226500	1.00621900
C	-0.06813300	1.38935200	0.16502900
H	0.23686500	0.21008100	1.91950200
C	0.02499000	2.60980000	-0.37502100
C	-1.75569500	0.43512100	-0.21025600
C	-2.66790500	1.15112600	-0.93024100
C	-3.94920400	1.05538200	-0.28675300
H	-2.44623000	1.77891800	-1.78185400
C	-3.79717600	0.23876400	0.84940000
C	-5.19881600	1.61400800	-0.57728600
C	-4.85741600	-0.05088000	1.70387200
C	-6.26102300	1.33276700	0.26669000
H	-5.32886300	2.25395500	-1.44441800
C	-6.08961000	0.50953100	1.38967400
H	-4.72503100	-0.67575400	2.57595800
H	-7.23799200	1.75849300	0.06252500
H	-6.93733000	0.30961500	2.03702400
N	-2.44583200	-0.16370500	0.88295700
N	-0.76594000	-1.72556700	1.00417300
C	-1.93696700	-1.27266900	1.50597000
C	-0.16877100	-2.74551100	1.63234000
N	-2.57651300	-1.81714700	2.53568500
C	-0.76496500	-3.37125800	2.70998300
H	0.80320400	-3.03770100	1.25238800
C	-1.99910900	-2.86547000	3.11426400
H	-0.29120400	-4.20357100	3.21373900
H	-2.54004000	-3.30722800	3.94672500
C	2.19477100	0.68392000	1.13393100
H	2.46385900	1.42902500	1.89099100
H	2.68369800	0.95983600	0.20221600
O	2.65147400	-0.59651400	1.59164000
C	3.91215400	-0.91806500	1.29120400
O	4.66857700	-0.26600600	0.60983400
O	4.17368700	-2.09627600	1.84632000
C	5.49633300	-2.59335400	1.61076000
H	5.55412300	-3.53109500	2.16070700
H	5.65510000	-2.76478000	0.54321400
H	6.24090100	-1.88493100	1.97849300
C	-0.07659200	1.00294700	-3.55899500
H	0.43474600	1.88833000	-3.17590400
H	0.22311300	0.87183000	-4.60553800

H	-1.15385300	1.18321700	-3.54656700
C	-1.89808300	-1.58107900	-3.24583600
H	-2.38020400	-2.47787400	-2.84997600
H	-2.52940700	-0.72420300	-2.98973600
H	-1.86824900	-1.66970100	-4.33758400
C	-0.14980100	-3.78247200	-1.68746100
H	0.06021400	-4.42704200	-2.54884600
H	0.40881300	-4.18350400	-0.83807900
H	-1.21693300	-3.85650900	-1.46459000
C	2.73655100	-2.60740500	-1.19286400
H	2.53048100	-3.06734400	-0.22203700
H	2.99176200	-3.41177700	-1.89227100
H	3.61906000	-1.97456400	-1.08085300
C	2.74025400	0.45523200	-2.28695500
H	3.56327900	0.15589400	-1.63459900
H	3.12290700	0.51698800	-3.31233900
H	2.42442200	1.46323000	-1.99490500
C	0.84213100	3.69220000	0.19104900
C	1.37780000	4.65404300	-0.67548900
C	1.10731500	3.79568800	1.56327000
C	2.19486600	5.66771300	-0.18854600
H	1.16114600	4.59817400	-1.73970100
C	1.91909000	4.81365100	2.04860900
H	0.64703900	3.09463800	2.25444000
C	2.47223800	5.74716700	1.17386300
H	2.61036400	6.40019300	-0.87338800
H	2.10818800	4.88979800	3.11482300
H	3.10564800	6.54168400	1.55495700
H	-0.54137000	2.84943500	-1.27009200

TS2_a'

C	0.16460500	-1.19781200	2.67345900
C	-0.45683100	0.06670500	2.56177000
C	-1.73042100	-0.11474200	1.89712900
C	-1.94978000	-1.52543200	1.72042100
C	-0.76771000	-2.18608200	2.14608200
Rh	-0.15330500	-0.82489500	0.49232100
C	-0.90406700	-0.78453000	-1.52711600
C	-0.29071300	0.47398000	-1.34186800
C	-0.38907600	1.61114100	-2.02718200
C	1.35247800	0.46151800	-0.09499900
C	1.79260000	1.66026700	0.37546900
C	3.19227400	1.79114200	0.05112400
H	1.17087600	2.40257500	0.85189200
C	3.58986300	0.62112700	-0.62302400
C	4.12363300	2.81177000	0.26746800
C	4.88884600	0.42832000	-1.08347300
C	5.42136400	2.63225900	-0.18722400
H	3.83367100	3.72307800	0.78140000
C	5.79616600	1.45551800	-0.85205600

H	5.17405700	-0.47678400	-1.60218000
H	6.15916300	3.41252500	-0.03046200
H	6.81746000	1.34321400	-1.20145900
N	2.45511000	-0.20976500	-0.68777700
N	1.27600000	-2.14877300	-0.41993200
C	2.40800900	-1.55921900	-0.86884400
C	1.13216900	-3.45986600	-0.65218800
N	3.41957200	-2.19814800	-1.45263000
C	2.12737200	-4.20230800	-1.25707700
H	0.19379700	-3.90004500	-0.33447500
C	3.27948200	-3.50692400	-1.62556400
H	2.01430600	-5.26409000	-1.43292800
H	4.11798400	-4.01765100	-2.09153400
C	-2.74846000	0.96196600	1.70734300
H	-3.51528800	0.66295000	0.99117800
H	-3.24128100	1.16614700	2.66596500
H	-2.27836900	1.88490400	1.36088700
C	0.04365700	1.35916700	3.11567700
H	1.13451100	1.39345200	3.14699600
H	-0.32015400	2.21342300	2.54110300
H	-0.32507400	1.46330700	4.14371500
C	1.49599000	-1.48346200	3.29427000
H	1.39689000	-1.63837400	4.37469300
H	1.95001300	-2.38237800	2.86850100
H	2.18882600	-0.65331000	3.13230600
C	-0.57173900	-3.66524400	2.23128500
H	0.47291100	-3.95003800	2.08053400
H	-0.85949300	-4.00720200	3.23247100
H	-1.19538200	-4.20351900	1.51239700
C	-3.21166800	-2.17545000	1.25708600
H	-3.01650000	-3.09475500	0.69950800
H	-3.83172700	-2.43209700	2.12439900
H	-3.79391200	-1.51712300	0.60976900
H	-0.97860300	1.48521000	-2.93775400
C	0.11726800	3.00899600	-1.85385000
H	0.86615900	3.11062000	-1.07530100
H	0.52964100	3.36284400	-2.79997700
O	-0.98493300	3.90085200	-1.60808600
C	-1.37385600	4.02305200	-0.34371500
O	-0.85189100	3.49139000	0.61720000
O	-2.42560300	4.82328600	-0.30467800
C	-2.94624000	5.09923900	0.99814400
H	-3.73172900	5.83669400	0.84290600
H	-3.36161400	4.19143600	1.44336700
H	-2.16583300	5.50094800	1.64759100
H	-0.32257700	-1.53107300	-2.06466100
C	-2.36186000	-0.95298700	-1.70662400
C	-2.84085700	-2.21860300	-2.07093300
C	-3.27988700	0.09508600	-1.56911500
C	-4.19735300	-2.43801700	-2.27609500

H	-2.13542400	-3.03704900	-2.19880700
C	-4.63883700	-0.12545400	-1.77062300
H	-2.92836300	1.08883700	-1.31074600
C	-5.10408800	-1.39176900	-2.11976900
H	-4.54820400	-3.42454900	-2.56279200
H	-5.33746900	0.69909300	-1.66588500
H	-6.16388800	-1.55849300	-2.28249700

TS2_b'

C	0.05531000	-1.45552500	2.76614700
C	-1.19318100	-1.62617900	2.12371200
C	-1.01881300	-2.57861800	1.04579400
C	0.32362500	-3.09964100	1.11976700
C	0.99764800	-2.36933100	2.13498600
Rh	0.32824800	-0.90903300	0.59551200
C	0.54959600	-1.14408800	-1.52315400
C	-0.49864300	-0.20146200	-1.38508600
C	-1.40378100	0.23649300	-2.25563600
C	-0.43846500	0.98677100	0.29430400
C	-1.60752200	1.58277800	0.65885800
C	-1.36585200	2.99507700	0.81680500
H	-2.55958500	1.08094000	0.74129900
C	-0.00480300	3.23163900	0.54443400
C	-2.19943100	4.06742000	1.15321300
C	0.55997700	4.50242600	0.61177800
C	-1.64900200	5.33772900	1.22149700
H	-3.25273400	3.90316100	1.35875700
C	-0.28724600	5.54845200	0.95679200
H	1.60843100	4.66392600	0.40083700
H	-2.27754800	6.18306500	1.48247000
H	0.11731500	6.55365900	1.01783600
N	0.56793600	1.98402200	0.23904500
N	2.09116700	0.30093700	0.51458900
C	1.88434000	1.62153900	0.32251300
C	3.35809200	-0.12954900	0.49564600
N	2.83934400	2.53662400	0.20016500
C	4.41715800	0.74743700	0.36469100
H	3.50315300	-1.19896800	0.58375800
C	4.09256700	2.09569100	0.23583600
H	5.44111600	0.39816400	0.35285500
H	4.86647100	2.85284300	0.14276200
C	-2.10813100	-3.08432100	0.15340900
H	-1.70710200	-3.46494200	-0.79020900
H	-2.64046300	-3.90854800	0.64308400
H	-2.82609800	-2.29347200	-0.07516300
C	-2.48899300	-1.00161900	2.52297700
H	-2.34138900	-0.01599700	2.96936400
H	-3.17251800	-0.90572000	1.67687900
H	-2.96864700	-1.64126100	3.27391600
C	0.34360600	-0.56763400	3.93582000

H	0.13507700	-1.08497500	4.87941700
H	1.39126700	-0.25587800	3.95119400
H	-0.27053100	0.33622400	3.90284200
C	2.39491700	-2.60283900	2.61211100
H	2.87953900	-1.67378400	2.92390200
H	2.37221600	-3.26761100	3.48347500
H	3.01436900	-3.08425900	1.85084000
C	0.88298900	-4.22587600	0.30865400
H	1.96155100	-4.12305800	0.16299900
H	0.70390400	-5.18153000	0.81462900
H	0.41388000	-4.28742700	-0.67701200
H	-1.25329200	-0.19401900	-3.24753500
C	-2.56702600	1.18006100	-2.22212200
H	-2.69673900	1.69194400	-1.27472000
H	-2.45021300	1.91951400	-3.01675900
O	-3.76979200	0.48200800	-2.58231300
C	-4.34769100	-0.22667800	-1.61630900
O	-3.96675000	-0.30162000	-0.46413700
O	-5.40853300	-0.83273700	-2.11904700
C	-6.16552100	-1.61893400	-1.19494100
H	-7.02199600	-1.98127000	-1.76041700
H	-5.56822500	-2.45852000	-0.83025500
H	-6.49312500	-1.00848300	-0.35080400
C	1.85252500	-0.82587000	-2.14543700
C	2.81680200	-1.83395600	-2.26335600
C	2.15616100	0.45686500	-2.61602500
C	4.06229400	-1.56480100	-2.82016700
H	2.58177200	-2.83794000	-1.91672300
C	3.40418800	0.72740000	-3.16629300
H	1.41001400	1.24397500	-2.55072300
C	4.36254200	-0.27953600	-3.26659700
H	4.79718300	-2.35871300	-2.91225400
H	3.62460800	1.72692200	-3.52843600
H	5.33219800	-0.06821600	-3.70599000
H	0.22500500	-2.17346500	-1.67450000

TS2_c'

C	0.05531000	-1.45552500	2.76614700
C	-1.19318100	-1.62617900	2.12371200
C	-1.01881300	-2.57861800	1.04579400
C	0.32362500	-3.09964100	1.11976700
C	0.99764800	-2.36933100	2.13498600
Rh	0.32824800	-0.90903300	0.59551200
C	0.54959600	-1.14408800	-1.52315400
C	-0.49864300	-0.20146200	-1.38508600
C	-1.40378100	0.23649300	-2.25563600
C	-0.43846500	0.98677100	0.29430400
C	-1.60752200	1.58277800	0.65885800
C	-1.36585200	2.99507700	0.81680500
H	-2.55958500	1.08094000	0.74129900

C	-0.00480300	3.23163900	0.54443400
C	-2.19943100	4.06742000	1.15321300
C	0.55997700	4.50242600	0.61177800
C	-1.64900200	5.33772900	1.22149700
H	-3.25273400	3.90316100	1.35875700
C	-0.28724600	5.54845200	0.95679200
H	1.60843100	4.66392600	0.40083700
H	-2.27754800	6.18306500	1.48247000
H	0.11731500	6.55365900	1.01783600
N	0.56793600	1.98402200	0.23904500
N	2.09116700	0.30093700	0.51458900
C	1.88434000	1.62153900	0.32251300
C	3.35809200	-0.12954900	0.49564600
N	2.83934400	2.53662400	0.20016500
C	4.41715800	0.74743700	0.36469100
H	3.50315300	-1.19896800	0.58375800
C	4.09256700	2.09569100	0.23583600
H	5.44111600	0.39816400	0.35285500
H	4.86647100	2.85284300	0.14276200
C	-2.10813100	-3.08432100	0.15340900
H	-1.70710200	-3.46494200	-0.79020900
H	-2.64046300	-3.90854800	0.64308400
H	-2.82609800	-2.29347200	-0.07516300
C	-2.48899300	-1.00161900	2.52297700
H	-2.34138900	-0.01599700	2.96936400
H	-3.17251800	-0.90572000	1.67687900
H	-2.96864700	-1.64126100	3.27391600
C	0.34360600	-0.56763400	3.93582000
H	0.13507700	-1.08497500	4.87941700
H	1.39126700	-0.25587800	3.95119400
H	-0.27053100	0.33622400	3.90284200
C	2.39491700	-2.60283900	2.61211100
H	2.87953900	-1.67378400	2.92390200
H	2.37221600	-3.26761100	3.48347500
H	3.01436900	-3.08425900	1.85084000
C	0.88298900	-4.22587600	0.30865400
H	1.96155100	-4.12305800	0.16299900
H	0.70390400	-5.18153000	0.81462900
H	0.41388000	-4.28742700	-0.67701200
H	-1.25329200	-0.19401900	-3.24753500
C	-2.56702600	1.18006100	-2.22212200
H	-2.69673900	1.69194400	-1.27472000
H	-2.45021300	1.91951400	-3.01675900
O	-3.76979200	0.48200800	-2.58231300
C	-4.34769100	-0.22667800	-1.61630900
O	-3.96675000	-0.30162000	-0.46413700
O	-5.40853300	-0.83273700	-2.11904700
C	-6.16552100	-1.61893400	-1.19494100
H	-7.02199600	-1.98127000	-1.76041700
H	-5.56822500	-2.45852000	-0.83025500

H	-6.49312500	-1.00848300	-0.35080400
C	1.85252500	-0.82587000	-2.14543700
C	2.81680200	-1.83395600	-2.26335600
C	2.15616100	0.45686500	-2.61602500
C	4.06229400	-1.56480100	-2.82016700
H	2.58177200	-2.83794000	-1.91672300
C	3.40418800	0.72740000	-3.16629300
H	1.41001400	1.24397500	-2.55072300
C	4.36254200	-0.27953600	-3.26659700
H	4.79718300	-2.35871300	-2.91225400
H	3.62460800	1.72692200	-3.52843600
H	5.33219800	-0.06821600	-3.70599000
H	0.22500500	-2.17346500	-1.67450000

TS2_d'

C	-2.74537500	1.41932100	0.89081100
C	-1.55480200	1.93062900	1.57339100
C	-0.85475900	2.77502700	0.68685500
C	-1.52304500	2.69701800	-0.59719400
C	-2.75201000	1.94671900	-0.41959300
Rh	-0.90022600	0.66343300	-0.13981800
C	-1.23798100	-0.41447600	-1.94880700
C	0.14646900	-0.55922500	-1.82058200
C	1.09406600	-1.37952600	-2.24978300
C	1.13463500	0.69892300	-0.42083600
C	2.02331300	1.54518100	-1.00778100
C	3.27127500	1.45060700	-0.29212500
H	1.82844900	2.15007200	-1.88270600
C	3.10635400	0.49687300	0.73304800
C	4.51372400	2.06726500	-0.46581800
C	4.14263900	0.13764300	1.59024300
C	5.55224300	1.71852600	0.38352400
H	4.66011000	2.80049700	-1.25314100
C	5.36579200	0.76624100	1.39687100
H	4.00000900	-0.60788800	2.36027700
H	6.52418000	2.18657400	0.26454200
H	6.19715600	0.50958900	2.04571900
N	1.77876500	0.05257100	0.65433700
N	-0.21417600	-0.98581600	1.09637300
C	1.10307700	-0.87477000	1.39668700
C	-0.91435500	-1.93049700	1.73619700
N	1.74005600	-1.58465800	2.32085300
C	-0.32370900	-2.73540000	2.69639400
H	-1.95526400	-2.03884400	1.44578100
C	1.02090400	-2.49925900	2.96698400
H	-0.88874800	-3.50085900	3.21233300
H	1.54935600	-3.06752600	3.72801000
C	0.36834600	3.57157700	1.01039800
H	0.92319800	3.84073000	0.11054600
H	0.08104200	4.49608500	1.52371800

H	1.04945200	3.01722900	1.66164700
C	-1.21966200	1.65683300	3.00494200
H	-1.48381800	0.63281000	3.28474600
H	-0.15432100	1.80115200	3.20130000
H	-1.77878600	2.33448900	3.66044500
C	-3.83520900	0.65267700	1.57128500
H	-4.29760100	1.27407500	2.34685900
H	-4.61406800	0.36614100	0.86310700
H	-3.46121900	-0.25526000	2.05302600
C	-3.83824900	1.83591900	-1.44100200
H	-4.50763300	0.99717600	-1.24876300
H	-4.42785300	2.76050900	-1.43307000
H	-3.43757900	1.71473200	-2.45047900
C	-1.16996700	3.48861100	-1.81729600
H	-1.47782400	2.97358500	-2.73103900
H	-1.67391600	4.46187000	-1.79781900
H	-0.09445900	3.66878200	-1.87785000
C	-2.06526100	-1.67338200	-1.86079900
H	-1.98335000	-2.22642400	-2.80429500
H	-1.73739000	-2.31718700	-1.04405500
O	-3.45082000	-1.35694500	-1.72002200
C	-4.09096500	-1.83606000	-0.65554700
O	-3.60917100	-2.49546200	0.23989900
O	-5.35975000	-1.45736800	-0.73742100
C	-6.22275100	-1.97126600	0.28555100
H	-5.85467600	-1.69324800	1.27562600
H	-7.19398400	-1.51887600	0.09447500
H	-6.28559900	-3.05864700	0.21126500
H	-1.60912800	0.32454100	-2.65940100
C	2.47604700	-1.64438400	-1.78652600
C	3.56333600	-0.99042200	-2.36591100
C	2.69834900	-2.60582400	-0.79710000
C	4.85644700	-1.26497400	-1.93064600
H	3.39406400	-0.25038300	-3.14227400
C	3.99073400	-2.87996200	-0.36423200
H	1.85340400	-3.13478100	-0.36292800
C	5.07094500	-2.20469700	-0.92721600
H	5.69607000	-0.73844500	-2.37220800
H	4.15330400	-3.61931300	0.41357200
H	6.07964200	-2.41158100	-0.58451800
H	0.75979600	-1.97112800	-3.10755200

INT3_1

C	-0.24693200	-2.66677400	1.70989300
C	0.38764800	-3.00008800	0.47398700
C	1.64613700	-2.32156400	0.44342700
C	1.86338100	-1.70472000	1.74871600
C	0.71094800	-1.92009200	2.52320400
Rh	0.06881600	-0.77253100	0.65004600
C	1.12201300	1.26629200	0.49862500

C	1.18845500	0.56478800	-0.66760800
C	1.59036500	0.41353800	-1.90907500
C	-1.28120300	-0.81616700	-0.85123800
C	-1.37741300	-1.27523600	-2.12074000
C	-2.73253300	-1.05581800	-2.58969200
H	-0.58610300	-1.73684900	-2.69492300
C	-3.45300800	-0.44552000	-1.54665600
C	-3.37653800	-1.32512300	-3.79859300
C	-4.79342300	-0.09285300	-1.66493800
C	-4.71456900	-0.97843700	-3.93216300
H	-2.84071300	-1.79422200	-4.61814400
C	-5.41119300	-0.37092500	-2.87940100
H	-5.32702900	0.37660900	-0.84952400
H	-5.22938900	-1.17893400	-4.86632600
H	-6.45669800	-0.11177700	-3.01138300
N	-2.54879600	-0.30753800	-0.47669500
N	-1.58336600	0.23939600	1.50852200
C	-2.70582200	0.25292600	0.74589500
C	-1.64730900	0.82140000	2.71145000
N	-3.87124100	0.77792100	1.12080500
C	-2.81360100	1.39582500	3.17783400
H	-0.73044100	0.82166200	3.29076000
C	-3.91547700	1.33746700	2.32330700
H	-2.86376300	1.86749900	4.15035200
H	-4.87225300	1.76229400	2.61527400
C	2.69208900	-2.46335200	-0.61391000
H	3.39428600	-1.62969100	-0.58224400
H	3.25108200	-3.39273100	-0.45321800
H	2.25489700	-2.50350900	-1.61429300
C	-0.14912800	-3.92448400	-0.56841000
H	-1.22835200	-3.81782800	-0.69160900
H	0.31881800	-3.75037200	-1.53922800
H	0.06528700	-4.95840100	-0.27332800
C	-1.57968800	-3.16788200	2.17039200
H	-1.47177500	-4.14028500	2.66425300
H	-2.04106300	-2.48004400	2.88383700
H	-2.26637900	-3.28927300	1.32888800
C	0.51024600	-1.54033800	3.95593800
H	-0.54636800	-1.38929100	4.19110800
H	0.87449600	-2.34347500	4.60671600
H	1.05914800	-0.63125400	4.21814100
C	3.12915900	-1.02702600	2.16459100
H	2.97142500	-0.36471300	3.01997100
H	3.86863000	-1.77995300	2.46236500
H	3.56547400	-0.44155500	1.34828300
H	1.26112700	-0.41826000	-2.52221300
C	2.57832800	1.37621600	-2.51137600
H	2.25926700	1.70309700	-3.50231700
H	2.72266300	2.24403100	-1.86426400
O	3.84056300	0.73477100	-2.74658000

C	4.58271300	0.50814200	-1.66319300
O	4.29622200	0.81905200	-0.52506200
H	1.91758000	1.10939600	1.22630600
O	5.68444200	-0.12399200	-2.03863700
C	6.60890700	-0.41612900	-0.98889400
H	7.45969200	-0.88801200	-1.47718000
H	6.91737400	0.50082600	-0.48252100
H	6.16079900	-1.09959400	-0.26224500
C	0.34643800	2.55630000	0.65999700
C	1.35806300	3.71701500	0.77085400
C	-0.65929800	2.84164900	-0.45815800
H	-0.19286900	2.52704300	1.61629800
C	0.63381800	5.04454100	1.01796800
H	1.93507700	3.77862900	-0.16213500
H	2.07809600	3.51972700	1.57426700
C	-1.40082800	4.15411900	-0.19388000
H	-0.12041800	2.91376700	-1.41240200
H	-1.36602600	2.01503900	-0.57439800
C	-0.41933100	5.32187300	-0.05838900
H	1.36418100	5.85939600	1.05757100
H	0.14703400	5.00816000	2.00284000
H	-2.11584800	4.34682400	-1.00035300
H	-1.98726500	4.05797600	0.73190100
H	-0.95741700	6.24759600	0.17121800
H	0.08252500	5.47989500	-1.02294100

TS2_a1

C	-0.35262300	-0.17421100	2.94495600
C	0.43795700	0.89683100	2.48382100
C	-0.42871500	1.78157900	1.72880000
C	-1.78715000	1.32963000	1.89154400
C	-1.74523000	0.09665800	2.57559000
Rh	-0.51526000	-0.17991300	0.70576900
C	-1.32123300	-0.18665000	-1.29264200
C	-0.05210700	0.41404900	-1.38224400
C	0.49958300	1.28920100	-2.22883900
C	1.24296100	-0.66303200	-0.25874200
C	2.52541000	-0.20720800	-0.17904700
C	3.41267300	-1.26746800	-0.58404000
H	2.82847400	0.79188700	0.09793500
C	2.63002000	-2.39677100	-0.88506500
C	4.80286000	-1.32890500	-0.72345500
C	3.18892000	-3.59568200	-1.31708500
C	5.37145900	-2.51790900	-1.15310600
H	5.41636200	-0.46189900	-0.49913900
C	4.57279500	-3.63362800	-1.44454200
H	2.57443600	-4.45483000	-1.54790500
H	6.44776000	-2.58924600	-1.27142500
H	5.04356500	-4.54995800	-1.78574500
N	1.28649500	-2.03465200	-0.64974100

N	-0.73794300	-2.28363000	0.40015800
C	0.27364300	-2.87339700	-0.27924200
C	-1.78992500	-3.04499300	0.72505000
N	0.32328900	-4.16488400	-0.59442100
C	-1.81996600	-4.39685200	0.44147800
H	-2.61259100	-2.53977000	1.21694800
C	-0.70707600	-4.91436200	-0.22005100
H	-2.66526300	-5.01430900	0.71623200
H	-0.64410900	-5.96976400	-0.47140900
C	-0.05852800	3.11259100	1.15547900
H	-0.32318300	3.19298200	0.09762300
H	-0.57953000	3.91113600	1.69586100
H	1.01186000	3.28882800	1.25450600
C	1.89694000	1.09293000	2.74498200
H	2.44843500	0.15152000	2.68144700
H	2.35015900	1.79337100	2.04040200
H	2.03153400	1.49699000	3.75510500
C	0.10869400	-1.34043500	3.76096400
H	-0.06970900	-1.15689100	4.82676900
H	-0.42249700	-2.25737000	3.48878100
H	1.17744300	-1.52036600	3.62364900
C	-2.92615400	-0.67632700	3.07372800
H	-2.66810000	-1.71293700	3.30533900
H	-3.29366500	-0.22341800	4.00213100
H	-3.75418300	-0.67152400	2.35896100
C	-2.99617300	2.13168200	1.53596200
H	-3.89159900	1.51613500	1.43343000
H	-3.18508900	2.86072900	2.33381900
H	-2.85407300	2.69537700	0.61094400
H	-0.11487100	1.44743800	-3.11277700
C	1.81097700	2.00349800	-2.26931400
H	2.59575300	1.46659800	-1.74097500
H	2.11040700	2.13237000	-3.31113900
O	1.69183500	3.34176700	-1.74892000
C	2.46179500	3.67687400	-0.71832800
O	3.19625500	2.93888700	-0.09280800
O	2.27327000	4.96388500	-0.46678600
C	3.04575900	5.49707500	0.61269000
H	2.80947100	6.55938600	0.63758100
H	2.76533600	5.02238400	1.55686000
H	4.11157900	5.34392300	0.43324900
H	-1.36619100	-1.23034300	-1.60708600
C	-2.62687200	0.53700500	-1.53642700
C	-2.90747700	0.66876200	-3.04790000
C	-3.78956900	-0.21383400	-0.87151100
H	-2.55647600	1.54889200	-1.11985900
C	-4.25137200	1.36111000	-3.30347600
H	-2.91730400	-0.33386100	-3.49864400
H	-2.10882600	1.23102500	-3.54191400
C	-5.13626100	0.46907300	-1.11730600

H	-3.82228600	-1.23421500	-1.28363800
H	-3.59359700	-0.31885300	0.20114400
C	-5.40497800	0.62841900	-2.61569300
H	-4.43005100	1.42860900	-4.38168200
H	-4.19915000	2.39249400	-2.92768300
H	-5.94058700	-0.10363500	-0.64222100
H	-5.13136700	1.46135900	-0.64455300
H	-6.34569400	1.16495100	-2.77694100
H	-5.52585300	-0.36508400	-3.06937900

TS2_b1

C	1.14957000	-2.98786800	0.94866300
C	1.00172900	-3.13562800	-0.44507800
C	2.05313800	-2.36153400	-1.07486500
C	2.95619800	-1.91303800	-0.04274900
C	2.36294400	-2.20680600	1.20572100
Rh	0.87583900	-0.93920000	0.12428100
C	1.23789300	1.16979100	-0.09815800
C	0.14675000	0.96912700	-0.96594000
H	0.96300700	1.61903600	0.85814300
C	-0.67495000	1.71207700	-1.69550800
C	-0.91509600	-0.72019200	-0.86698200
C	-1.41649600	-1.15367900	-2.05730700
C	-2.84746300	-1.27168100	-1.92731700
H	-0.84272200	-1.30238900	-2.96142300
C	-3.19251600	-0.89313900	-0.61253900
C	-3.85521900	-1.65623900	-2.81865700
C	-4.50808500	-0.89774300	-0.15478700
C	-5.16848800	-1.65771900	-2.37557600
H	-3.61105500	-1.94455500	-3.83640400
C	-5.48718600	-1.28564500	-1.06052000
H	-4.75081800	-0.60789400	0.85871500
H	-5.96350000	-1.95041500	-3.05362400
H	-6.52459900	-1.29650700	-0.74196000
N	-1.99284500	-0.57353300	0.03810700
N	-0.43824700	-0.25680300	1.67716500
C	-1.74724700	-0.24961500	1.34059000
C	-0.11508800	0.13319000	2.91428100
N	-2.74549200	0.03346900	2.17106600
C	-1.08459700	0.46632400	3.84055100
H	0.94565400	0.16512100	3.14227300
C	-2.40653700	0.37930800	3.40820400
H	-0.82838500	0.77377100	4.84595300
H	-3.22907100	0.60395700	4.08216300
C	2.33004500	-2.27829500	-2.54325300
H	2.82424500	-1.33708700	-2.79826400
H	2.98621300	-3.09950000	-2.85518500
H	1.41009000	-2.34378000	-3.12828800
C	-0.05396700	-3.93906300	-1.13418700
H	-1.03637200	-3.79918300	-0.67554900

H	-0.14340800	-3.67215300	-2.18817900
H	0.20154400	-5.00321600	-1.07676700
C	0.26963100	-3.58392300	2.00137300
H	0.68951100	-4.53360100	2.35232500
H	0.17587800	-2.92365900	2.86818000
H	-0.73383600	-3.78004800	1.61589700
C	2.96303300	-1.97891500	2.55821600
H	2.19257000	-1.91750000	3.33162900
H	3.62454800	-2.81117400	2.82601900
H	3.55246100	-1.05871400	2.59050600
C	4.33636500	-1.40011400	-0.28707700
H	4.77532600	-0.94579200	0.60213900
H	4.97180600	-2.24528400	-0.57855600
H	4.37530800	-0.67312000	-1.10111600
H	-1.49609800	1.28938800	-2.26240300
C	-0.68988100	3.21349900	-1.57460700
H	0.05530800	3.57568300	-0.86666000
H	-0.56424800	3.71284500	-2.53677900
O	-1.99806900	3.60247900	-1.13930700
C	-2.30552800	3.29148100	0.12423600
O	-1.55832400	2.78678900	0.93649100
O	-3.56551300	3.63710500	0.33175300
C	-4.08075900	3.34028000	1.63020400
H	-5.06451200	3.80552700	1.66314000
H	-4.16433900	2.25809800	1.75932800
H	-3.43320200	3.75682600	2.40516300
C	2.62011400	1.58149700	-0.58457900
C	2.61896000	2.89984200	-1.38042800
C	3.56597500	1.71572400	0.61726400
H	2.99974300	0.80982600	-1.26643900
C	4.03726000	3.27936400	-1.81950000
H	2.21504800	3.70354400	-0.74875800
H	1.96689800	2.80855800	-2.25660600
C	4.98573100	2.11379200	0.20816600
H	3.15859900	2.48905000	1.28558600
H	3.56895900	0.78345300	1.19370900
C	4.98111300	3.40055500	-0.62069700
H	4.00965500	4.22047600	-2.37884000
H	4.41801500	2.51349800	-2.51026200
H	5.60953700	2.23648600	1.10035800
H	5.43950000	1.30759400	-0.38419200
H	5.99569600	3.63610600	-0.95850200
H	4.65552900	4.23771600	0.01210400

TS2_c1

C	2.80819200	-1.58628400	-0.83756800
C	1.80468100	-2.61584000	-1.12418900
C	1.04241400	-2.18978800	-2.23167900
C	1.47989500	-0.84886000	-2.57337700
C	2.65160900	-0.54584400	-1.78127400

Rh	0.78610900	-0.72032400	-0.51825300
C	0.66983100	1.35357400	-0.08716900
C	-0.67795400	1.06096500	-0.36393400
C	-1.82844200	1.70934400	-0.47568400
C	-1.26711900	-0.89784000	-0.45372900
C	-2.24033900	-1.09833700	-1.38469200
C	-3.35655500	-1.74520000	-0.74311000
H	-2.20360000	-0.75533800	-2.40932600
C	-3.02250400	-1.92960700	0.61453700
C	-4.60475100	-2.17091400	-1.21053400
C	-3.89271100	-2.53172600	1.52030100
C	-5.47875800	-2.76987900	-0.31730100
H	-4.87844200	-2.03308000	-2.25202800
C	-5.12396200	-2.94746800	1.02868900
H	-3.62212500	-2.66218700	2.55918700
H	-6.45164300	-3.10660200	-0.66063500
H	-5.82934000	-3.41627500	1.70722900
N	-1.72621000	-1.41467300	0.78061400
N	0.41769600	-1.19797800	1.55038200
C	-0.86230100	-1.54047400	1.82990100
C	1.30928400	-1.28075200	2.54663700
N	-1.29792600	-1.97123400	3.01004100
C	0.94610400	-1.72767300	3.80380000
H	2.31650400	-0.95815900	2.31234700
C	-0.39287000	-2.07078300	3.97886800
H	1.66841600	-1.79863800	4.60651800
H	-0.75952900	-2.43404600	4.93534500
C	-0.02559400	-2.97257000	-2.92410500
H	-0.67317000	-2.32886000	-3.52174900
H	0.43800300	-3.69936800	-3.60088700
H	-0.65703300	-3.51750600	-2.21820600
C	1.68573900	-3.92363600	-0.40744000
H	1.84631300	-3.80560500	0.66817900
H	0.69817900	-4.36781400	-0.55241700
H	2.43414000	-4.63320200	-0.77863500
C	3.90997900	-1.71469400	0.16754700
H	4.81408000	-2.10090000	-0.31752400
H	4.15568100	-0.75358800	0.62770400
H	3.64465900	-2.41923900	0.95994100
C	3.55963400	0.62506000	-1.97934800
H	4.28448700	0.70256500	-1.16678700
H	4.11624100	0.49339600	-2.91445500
H	3.02485700	1.57580700	-2.04816100
C	0.98717100	-0.02205900	-3.71967300
H	1.15008500	1.04283100	-3.53391600
H	1.51914600	-0.28842800	-4.64042800
H	-0.08113500	-0.17255400	-3.89299200
H	-2.76111200	1.19108900	-0.67187900
C	1.06898100	1.80410500	1.29547200
H	1.00295500	2.89539900	1.35576500

H	0.43092600	1.36589400	2.06165100
O	2.40199900	1.40357000	1.63756400
C	3.37628600	2.12834700	1.07468400
O	3.22063500	3.08643300	0.35777200
O	4.54178400	1.59562300	1.43443500
C	5.69891600	2.31410400	0.98568000
H	5.71448100	3.31346000	1.42469500
H	6.55122800	1.73195900	1.33148800
H	5.70195600	2.39747400	-0.10346300
H	1.22314100	1.85313900	-0.88213500
C	-1.91381000	3.20178600	-0.28995900
C	-2.58930800	3.85401300	-1.50936200
C	-2.68953900	3.52999900	0.99971200
H	-0.90114700	3.61783300	-0.19645200
C	-2.74668900	5.36523400	-1.31627200
H	-3.58072800	3.39947100	-1.65129200
H	-2.00840000	3.64031500	-2.41459900
C	-2.84919600	5.04173300	1.18525600
H	-3.68197100	3.05977300	0.94730300
H	-2.17586000	3.08728700	1.86211200
C	-3.51732800	5.68533400	-0.03265400
H	-3.25392800	5.79730400	-2.18545200
H	-1.75178300	5.82937900	-1.26836500
H	-3.42909800	5.24318100	2.09234500
H	-1.85882200	5.49402000	1.33655800
H	-3.59065300	6.76919000	0.10526900
H	-4.54504600	5.30715700	-0.12409800

TS2_d1

C	-0.34544000	-2.54517400	1.92170800
C	0.43279300	-1.60183700	2.64155500
C	-0.35151700	-0.39821200	2.72693800
C	-1.65483700	-0.65254500	2.15795500
C	-1.64951100	-1.96876200	1.62908600
Rh	-0.03190500	-0.78334000	0.57962300
C	-0.71840200	0.41943700	-1.05598700
C	0.09316900	1.24632900	-0.25273500
H	-0.27393600	0.04598300	-1.97764400
C	0.11000700	2.51011400	0.16399700
C	1.73612100	0.25138100	0.22354000
C	2.62341700	0.93139500	1.00531300
C	3.93213100	0.82703500	0.41822900
H	2.37162100	1.52834000	1.87063400
C	3.81962100	0.03829000	-0.74234900
C	5.17830200	1.34733900	0.78356100
C	4.91411700	-0.25957000	-1.54928000
C	6.27503200	1.05766800	-0.01246400
H	5.28036200	1.96266100	1.67205700
C	6.14186800	0.26374000	-1.16130700
H	4.80964500	-0.86346900	-2.44007300

H	7.25054100	1.45311600	0.25125000
H	7.01708100	0.05633800	-1.76848300
N	2.46415200	-0.33675000	-0.84847200
N	0.76713700	-1.86974200	-1.05236900
C	1.96145500	-1.42704000	-1.50736800
C	0.18023000	-2.87561900	-1.71203000
N	2.62979800	-1.96769900	-2.52094500
C	0.80585500	-3.49706700	-2.77545300
H	-0.80745600	-3.16026400	-1.36753000
C	2.05947000	-3.00193200	-3.13107000
H	0.34054700	-4.31869500	-3.30405000
H	2.62336500	-3.44131500	-3.94945600
C	-2.20187900	0.58692800	-1.16841200
H	-2.44740400	1.33540000	-1.93219500
H	-2.66734100	0.89038300	-0.23261100
O	-2.72296200	-0.67232600	-1.61261600
C	-4.00516700	-0.91494400	-1.32658100
O	-4.72591800	-0.21382300	-0.65472300
O	-4.33473300	-2.07432600	-1.88236700
C	-5.68450800	-2.49354500	-1.64884300
H	-5.79263900	-3.43181100	-2.19009800
H	-5.85669800	-2.64581400	-0.58052700
H	-6.38690400	-1.74821400	-2.02651600
C	0.01417900	0.83556800	3.49002900
H	-0.30434100	1.74137500	2.96734700
H	-0.48254200	0.82277200	4.46723700
H	1.09021700	0.89201700	3.66643100
C	1.80486000	-1.79514000	3.20438500
H	2.27189100	-2.70194500	2.81309800
H	2.45730800	-0.95220700	2.95491500
H	1.76126900	-1.88403900	4.29550800
C	0.04752800	-3.95001800	1.59431200
H	-0.18000900	-4.60226100	2.44539200
H	-0.50823600	-4.33241100	0.73439900
H	1.11571300	-4.03621200	1.38095600
C	-2.81762600	-2.72875600	1.07942200
H	-2.61444700	-3.16831400	0.09879500
H	-3.08628200	-3.54492500	1.75991900
H	-3.69180000	-2.08195000	0.98059100
C	-2.79852800	0.30514800	2.23779100
H	-3.60027500	0.06478800	1.53626700
H	-3.21776800	0.28803500	3.25081300
H	-2.46493500	1.32945600	2.04248900
H	0.76596600	2.81495600	0.97503800
C	-0.70392500	3.60203800	-0.47569400
C	-1.84801800	4.03887800	0.46082600
C	0.18290000	4.80542700	-0.84060900
H	-1.15276200	3.21876400	-1.40232800
C	-2.66487200	5.18360200	-0.14655900
H	-1.41877900	4.36222400	1.42076800

H	-2.50090700	3.18314400	0.67442100
C	-0.64053400	5.94424000	-1.44948700
H	0.68354300	5.16529600	0.07025800
H	0.97056500	4.48613200	-1.53237300
C	-1.77518400	6.37320400	-0.51574400
H	-3.44623100	5.49209500	0.55616800
H	-3.17624700	4.81828300	-1.04804500
H	0.01336000	6.79369100	-1.67345100
H	-1.06406800	5.61153400	-2.40747700
H	-2.37493000	7.16019200	-0.98490700
H	-1.34770000	6.80469200	0.40004100

TS2_a1'

C	-0.35262300	-0.17421100	2.94495600
C	0.43795700	0.89683100	2.48382100
C	-0.42871500	1.78157900	1.72880000
C	-1.78715000	1.32963000	1.89154400
C	-1.74523000	0.09665800	2.57559000
Rh	-0.51526000	-0.17991300	0.70576900
C	-1.32123300	-0.18665000	-1.29264200
C	-0.05210700	0.41404900	-1.38224400
C	0.49958300	1.28920100	-2.22883900
C	1.24296100	-0.66303200	-0.25874200
C	2.52541000	-0.20720800	-0.17904700
C	3.41267300	-1.26746800	-0.58404000
H	2.82847400	0.79188700	0.09793500
C	2.63002000	-2.39677100	-0.88506500
C	4.80286000	-1.32890500	-0.72345500
C	3.18892000	-3.59568200	-1.31708500
C	5.37145900	-2.51790900	-1.15310600
H	5.41636200	-0.46189900	-0.49913900
C	4.57279500	-3.63362800	-1.44454200
H	2.57443600	-4.45483000	-1.54790500
H	6.44776000	-2.58924600	-1.27142500
H	5.04356500	-4.54995800	-1.78574500
N	1.28649500	-2.03465200	-0.64974100
N	-0.73794300	-2.28363000	0.40015800
C	0.27364300	-2.87339700	-0.27924200
C	-1.78992500	-3.04499300	0.72505000
N	0.32328900	-4.16488400	-0.59442100
C	-1.81996600	-4.39685200	0.44147800
H	-2.61259100	-2.53977000	1.21694800
C	-0.70707600	-4.91436200	-0.22005100
H	-2.66526300	-5.01430900	0.71623200
H	-0.64410900	-5.96976400	-0.47140900
C	-0.05852800	3.11259100	1.15547900
H	-0.32318300	3.19298200	0.09762300
H	-0.57953000	3.91113600	1.69586100
H	1.01186000	3.28882800	1.25450600

C	1.89694000	1.09293000	2.74498200
H	2.44843500	0.15152000	2.68144700
H	2.35015900	1.79337100	2.04040200
H	2.03153400	1.49699000	3.75510500
C	0.10869400	-1.34043500	3.76096400
H	-0.06970900	-1.15689100	4.82676900
H	-0.42249700	-2.25737000	3.48878100
H	1.17744300	-1.52036600	3.62364900
C	-2.92615400	-0.67632700	3.07372800
H	-2.66810000	-1.71293700	3.30533900
H	-3.29366500	-0.22341800	4.00213100
H	-3.75418300	-0.67152400	2.35896100
C	-2.99617300	2.13168200	1.53596200
H	-3.89159900	1.51613500	1.43343000
H	-3.18508900	2.86072900	2.33381900
H	-2.85407300	2.69537700	0.61094400
H	-0.11487100	1.44743800	-3.11277700
C	1.81097700	2.00349800	-2.26931400
H	2.59575300	1.46659800	-1.74097500
H	2.11040700	2.13237000	-3.31113900
O	1.69183500	3.34176700	-1.74892000
C	2.46179500	3.67687400	-0.71832800
O	3.19625500	2.93888700	-0.09280800
O	2.27327000	4.96388500	-0.46678600
C	3.04575900	5.49707500	0.61269000
H	2.80947100	6.55938600	0.63758100
H	2.76533600	5.02238400	1.55686000
H	4.11157900	5.34392300	0.43324900
H	-1.36619100	-1.23034300	-1.60708600
C	-2.62687200	0.53700500	-1.53642700
C	-2.90747700	0.66876200	-3.04790000
C	-3.78956900	-0.21383400	-0.87151100
H	-2.55647600	1.54889200	-1.11985900
C	-4.25137200	1.36111000	-3.30347600
H	-2.91730400	-0.33386100	-3.49864400
H	-2.10882600	1.23102500	-3.54191400
C	-5.13626100	0.46907300	-1.11730600
H	-3.82228600	-1.23421500	-1.28363800
H	-3.59359700	-0.31885300	0.20114400
C	-5.40497800	0.62841900	-2.61569300
H	-4.43005100	1.42860900	-4.38168200
H	-4.19915000	2.39249400	-2.92768300
H	-5.94058700	-0.10363500	-0.64222100
H	-5.13136700	1.46135900	-0.64455300
H	-6.34569400	1.16495100	-2.77694100
H	-5.52585300	-0.36508400	-3.06937900

TS2_b1'

C	1.70171500	-2.75626100	1.23070000
C	1.28096500	-3.28596500	-0.00458500

C	2.10082000	-2.68505900	-1.04189100
C	3.14750900	-1.92114800	-0.39653400
C	2.86474000	-1.89638600	0.98696500
Rh	1.11879000	-1.00849500	-0.05657800
C	1.58482600	0.66613400	-1.27949500
C	0.24979700	0.46528200	-1.66363800
C	-0.59781900	1.06127500	-2.49149400
C	-0.86969600	-0.96064700	-0.58680900
C	-1.64626600	-1.74982300	-1.37885400
C	-2.97294400	-1.79427700	-0.81623300
H	-1.31872100	-2.23081900	-2.29069900
C	-2.97543500	-0.98123500	0.33461200
C	-4.15098600	-2.43534900	-1.21176200
C	-4.11736700	-0.78168500	1.10352900
C	-5.29271500	-2.25195500	-0.44767100
H	-4.16809700	-3.06200400	-2.09841800
C	-5.27236100	-1.43518100	0.69309000
H	-4.10494600	-0.13234600	1.96792000
H	-6.21771300	-2.74062300	-0.73603100
H	-6.18479600	-1.30125200	1.26522000
N	-1.67169400	-0.48194600	0.47595000
N	0.25649900	0.20925900	1.48808100
C	-1.09771900	0.18791200	1.51460500
C	0.88070700	0.88327500	2.45945700
N	-1.84977500	0.75284600	2.45613200
C	0.18088800	1.51592600	3.46942700
H	1.96355000	0.90645800	2.40536900
C	-1.20790300	1.40150700	3.42148400
H	0.68723900	2.05982800	4.25614200
H	-1.83302100	1.85132900	4.18854000
C	2.03935500	-3.01071800	-2.50207900
H	2.37860400	-2.17100200	-3.11441600
H	2.67694900	-3.87255200	-2.73046200
H	1.02080200	-3.25637700	-2.81122400
C	0.17731000	-4.27142500	-0.21534500
H	-0.64548200	-4.11443800	0.48632800
H	-0.23462600	-4.20653900	-1.22385300
H	0.56010000	-5.28844500	-0.07329900
C	1.13101200	-3.05695100	2.58060900
H	1.74255300	-3.80595500	3.09671100
H	1.10200500	-2.16286000	3.21089500
H	0.11328500	-3.44666500	2.50491300
C	3.70605200	-1.25789300	2.04736000
H	3.13235600	-1.06774500	2.95828800
H	4.53503500	-1.92111000	2.32069200
H	4.13884800	-0.31276200	1.70507700
C	4.32677900	-1.28499600	-1.06171500
H	4.58647000	-0.33059900	-0.59511600
H	5.19707400	-1.94633300	-0.98019800
H	4.15174600	-1.10858100	-2.12578800

H	-0.10695400	1.84675500	-3.06486900
C	-2.08095000	0.96224400	-2.72889600
H	-2.35991100	1.67940100	-3.50389700
H	-2.39308900	-0.03561800	-3.03306100
O	-2.83346200	1.22540000	-1.54706300
C	-2.65009900	2.43916300	-1.01892800
O	-2.04120600	3.34837900	-1.53172500
H	2.32042500	0.24016300	-1.96369300
O	-3.23519100	2.45723700	0.17279400
C	-3.09968900	3.68210000	0.89253600
H	-3.62052200	3.51996700	1.83504500
H	-2.04335200	3.90340800	1.07067600
H	-3.55290100	4.50797200	0.34029500
C	2.07551700	1.92787200	-0.56950300
C	3.15333500	2.62016200	-1.42403000
C	0.97775500	2.93862600	-0.21527900
H	2.57545700	1.62128000	0.36337000
C	3.74751500	3.82513700	-0.68840500
H	2.70261300	2.94728000	-2.37175800
H	3.94661500	1.90624200	-1.68037100
C	1.56318000	4.12624500	0.55201400
H	0.50313400	3.30306500	-1.13310700
H	0.17566000	2.46748700	0.36203800
C	2.66258500	4.81714100	-0.25966700
H	4.48778500	4.32147300	-1.32456500
H	4.28545700	3.46791100	0.20178100
H	0.76779500	4.83939400	0.79463700
H	1.97897400	3.77597900	1.50925400
H	3.10658300	5.63536500	0.31707600
H	2.21265900	5.26861200	-1.15407700

TS2_c1'

C	-2.56852700	-0.85423600	1.68172000
C	-1.41536200	-1.54892100	2.25774400
C	-0.50136500	-0.58350800	2.73514400
C	-1.01727500	0.71575500	2.36230700
C	-2.34346100	0.53238700	1.82136300
Rh	-0.72813800	-0.40302500	0.48092900
C	-0.99106900	0.58177000	-1.39246000
C	0.29494300	0.98536700	-0.99843500
H	-1.06643800	-0.19137200	-2.15541300
C	1.12054000	1.97631000	-1.32640700
C	1.29041700	-0.50389900	0.09806900
C	2.40001000	-0.10528500	0.77755700
C	3.50436900	-0.95051900	0.39057200
H	2.44816200	0.72227100	1.46974800
C	3.01927400	-1.88781200	-0.54093800
C	4.85526400	-0.96446000	0.74766700
C	3.83783800	-2.85191300	-1.12111200
C	5.68163100	-1.92031600	0.17535200

H	5.24499700	-0.24200600	1.45852800
C	5.17624100	-2.85058900	-0.74387800
H	3.45019500	-3.56425200	-1.83669300
H	6.73424400	-1.94923300	0.43769100
H	5.84582200	-3.58576900	-1.17846000
N	1.64530100	-1.62193500	-0.70074700
N	-0.58828300	-2.09956900	-0.81640500
C	0.66888800	-2.44388100	-1.18094400
C	-1.60011500	-2.82294800	-1.31238200
N	0.97766900	-3.48804900	-1.94566100
C	-1.37067300	-3.92496500	-2.11368600
H	-2.59844500	-2.48877000	-1.05080600
C	-0.03597600	-4.22328000	-2.38908500
H	-2.18542400	-4.51853100	-2.50738400
H	0.23111800	-5.08022400	-3.00187700
H	0.74653300	2.51259100	-2.20373900
C	-2.08114100	1.60239900	-1.48287300
H	-2.04178000	2.10767300	-2.45616500
H	-1.98725100	2.36784400	-0.70873600
O	-3.32921100	0.91701900	-1.36495100
C	-4.41015800	1.70345900	-1.46495300
O	-4.39530700	2.88922600	-1.67857800
O	-5.48322600	0.94474300	-1.25715400
C	-6.73497900	1.63903800	-1.34409400
H	-7.49716700	0.88124700	-1.17116100
H	-6.78840100	2.42134400	-0.58402000
H	-6.85376800	2.08517900	-2.33333500
C	0.75737400	-0.87060200	3.48880800
H	1.40927200	0.00323000	3.53671500
H	0.51134300	-1.15847300	4.51707400
H	1.32767300	-1.68379600	3.03257000
C	-1.28362100	-3.03157500	2.40387500
H	-1.72414600	-3.56163000	1.55507900
H	-0.23602800	-3.33190000	2.48418500
H	-1.80234200	-3.36732100	3.30916000
C	-3.84128500	-1.49319900	1.21920700
H	-4.59099400	-1.45753700	2.01829500
H	-4.25230200	-0.97802900	0.34638100
H	-3.69352100	-2.54747000	0.97053200
C	-3.34922000	1.62028900	1.63217300
H	-4.23599400	1.25899400	1.11061000
H	-3.66445100	1.97446500	2.62139300
H	-2.95084400	2.48753400	1.10011700
C	-0.44460800	2.04339300	2.74374100
H	-0.61848400	2.78971500	1.96404800
H	-0.91406600	2.40288500	3.66724600
H	0.63126300	1.98277000	2.92017200
C	2.43997200	2.47116100	-0.82260500
C	3.20082800	3.21651600	-1.93132500
C	2.29754700	3.36880900	0.41929800

H	3.04292500	1.60063700	-0.53784400
C	4.57183100	3.68337700	-1.43582900
H	2.61146300	4.08778900	-2.25328700
H	3.31450800	2.56509100	-2.80577800
C	3.66778800	3.83341400	0.92025800
H	1.68011900	4.24190600	0.16421100
H	1.76134300	2.82811600	1.20646100
C	4.44788700	4.55478000	-0.18284000
H	5.08808400	4.23127500	-2.23115200
H	5.18885900	2.80279800	-1.20723400
H	3.54642100	4.48576400	1.79200800
H	4.24185000	2.95674400	1.25556000
H	5.44094700	4.83794200	0.18193400
H	3.92719800	5.48769900	-0.43933700

TS2_d1'

C	-3.00528900	1.47875300	0.41680400
C	-1.91809900	2.25543900	1.01881200
C	-1.20516400	2.90237600	-0.01188800
C	-1.75085900	2.43537600	-1.27153600
C	-2.93465100	1.64851100	-0.98378600
Rh	-1.03197300	0.65614000	-0.25298000
C	-1.11890000	-0.88012100	-1.72264800
C	0.26540400	-0.85885600	-1.51847600
C	1.31274500	-1.64450200	-1.71333900
C	1.01615000	0.77390800	-0.38807700
C	1.91382200	1.50897100	-1.10106500
C	3.10102600	1.67168700	-0.30010600
H	1.77110200	1.86015800	-2.11355800
C	2.89094300	0.99668700	0.92157800
C	4.33272000	2.29046800	-0.54092700
C	3.87184400	0.91580000	1.90793900
C	5.31358800	2.22029900	0.43587500
H	4.51511700	2.80638500	-1.47846900
C	5.08309000	1.54202500	1.64298500
H	3.69668500	0.38141700	2.83168600
H	6.27577200	2.69256500	0.26662000
H	5.87039000	1.50077200	2.38857900
N	1.59737000	0.45694100	0.85970500
N	-0.36773900	-0.58631900	1.40252500
C	0.91935200	-0.33958100	1.74374000
C	-1.06953300	-1.39696600	2.20326900
N	1.53209600	-0.80702300	2.82406500
C	-0.50921100	-1.93715100	3.34937500
H	-2.08390600	-1.62411500	1.89014800
C	0.81102600	-1.59420600	3.62097800
H	-1.07833700	-2.59336400	3.99491100
H	1.31876200	-1.96679200	4.50652900
C	-0.07953300	3.86952700	0.16271700
H	0.57629100	3.88713900	-0.70931000

H	-0.48210000	4.87844300	0.30773300
H	0.53536600	3.62050900	1.03157900
C	-1.68870400	2.38927700	2.49083800
H	-1.94273400	1.46407600	3.01598700
H	-0.64616200	2.63128200	2.71259600
H	-2.31601000	3.18842200	2.90220700
C	-4.09156500	0.80869800	1.19766900
H	-4.67197600	1.55909700	1.74684500
H	-4.77641700	0.27343300	0.53804400
H	-3.69696200	0.09704400	1.92874600
C	-3.91543400	1.17575900	-2.00848200
H	-4.52061000	0.34069100	-1.65450100
H	-4.58548400	2.00386400	-2.26862200
H	-3.42017300	0.85755900	-2.92925700
C	-1.34179600	2.90909300	-2.63099100
H	-1.53394100	2.14932600	-3.39317600
H	-1.90415100	3.80877900	-2.90688100
H	-0.27815500	3.15571800	-2.66172800
C	-1.84951200	-2.14854600	-1.35512000
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O	-3.26220500	-1.94015000	-1.41306000
C	-3.97638900	-2.20058700	-0.32119800
O	-3.54872600	-2.57327200	0.74991200
O	-5.25288500	-1.97224700	-0.60260900
C	-6.17846700	-2.29035500	0.44493100
H	-5.98283700	-1.67911300	1.32919900
H	-7.16148900	-2.06922500	0.03366800
H	-6.10054800	-3.34690100	0.70777900
H	-1.50069300	-0.39122500	-2.62001000
H	1.07033100	-2.45892700	-2.40532400
C	2.71961500	-1.66317700	-1.20956100
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C	3.73093100	-1.41016300	-2.33960400
H	2.86562200	-0.87823500	-0.47410800
C	4.44232800	-2.98666900	0.06280500
H	2.89779800	-3.82831500	-1.20377600
H	2.29010800	-3.15299500	0.31089500
C	5.15658400	-1.40619400	-1.77957900
H	3.63044000	-2.19053500	-3.10779800
H	3.50866200	-0.45086500	-2.82164300
C	5.47096000	-2.70874200	-1.03751000
H	4.65523200	-3.94295100	0.55279200
H	4.51565700	-2.20739900	0.83486800
H	5.87504600	-1.24817900	-2.59114100
H	5.26374700	-0.55733200	-1.08921600
H	6.47719900	-2.66337900	-0.60750700
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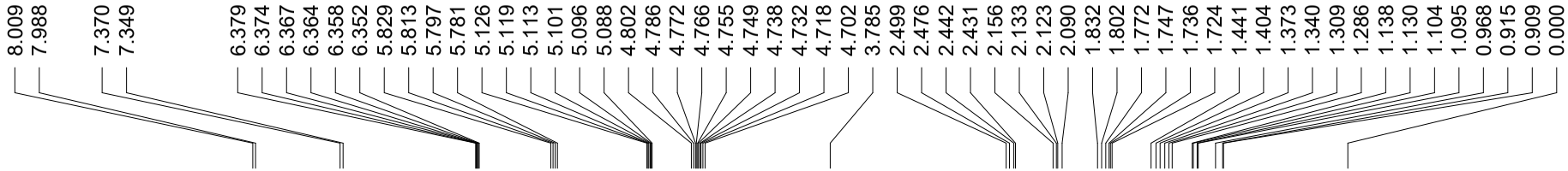

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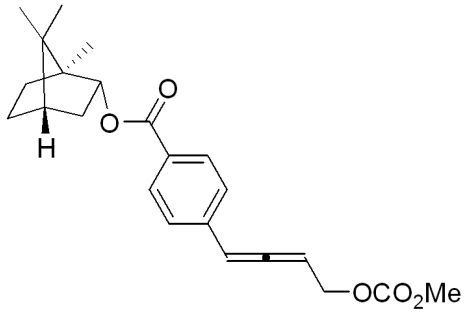

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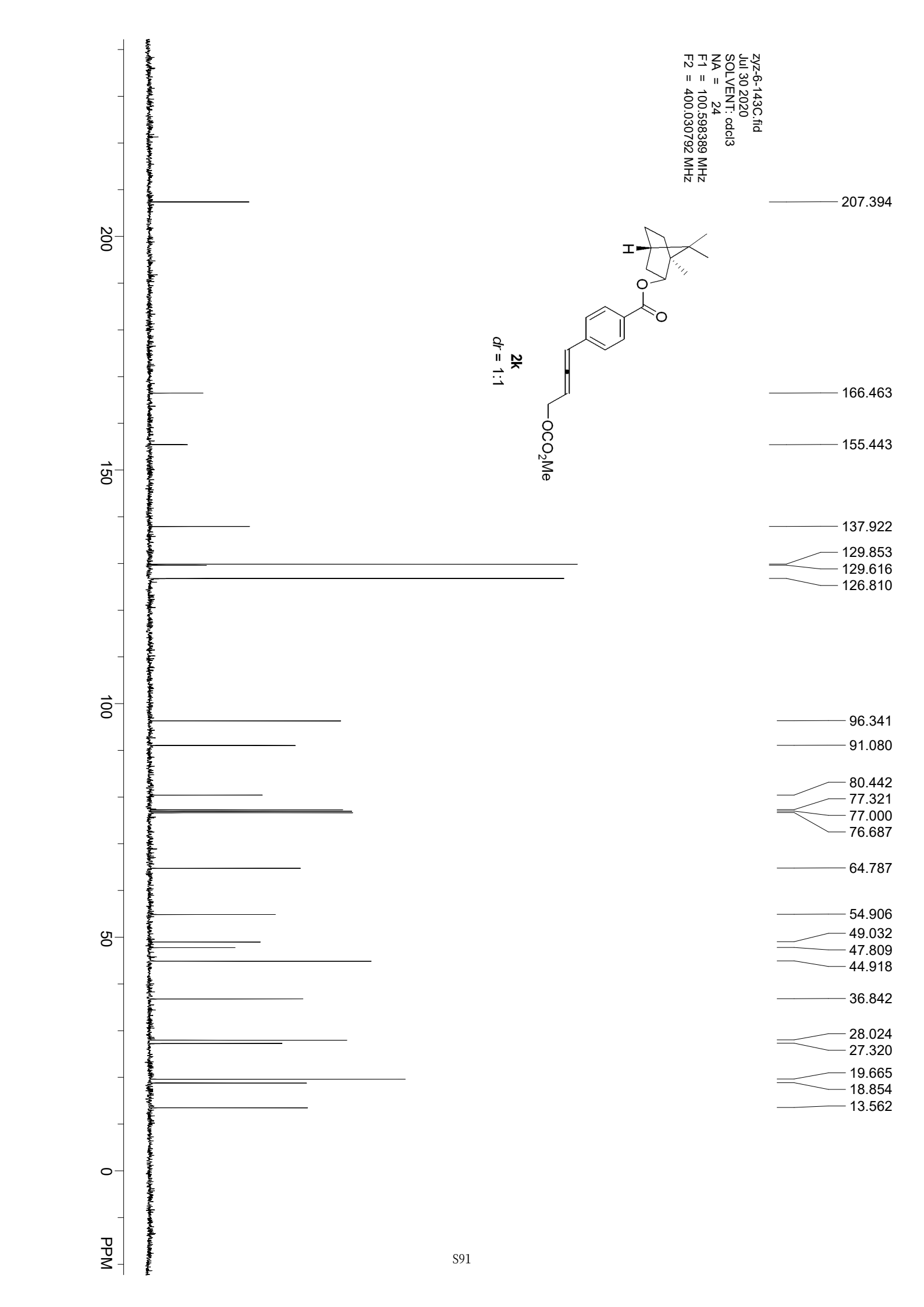
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SAMPLE INFORMATION

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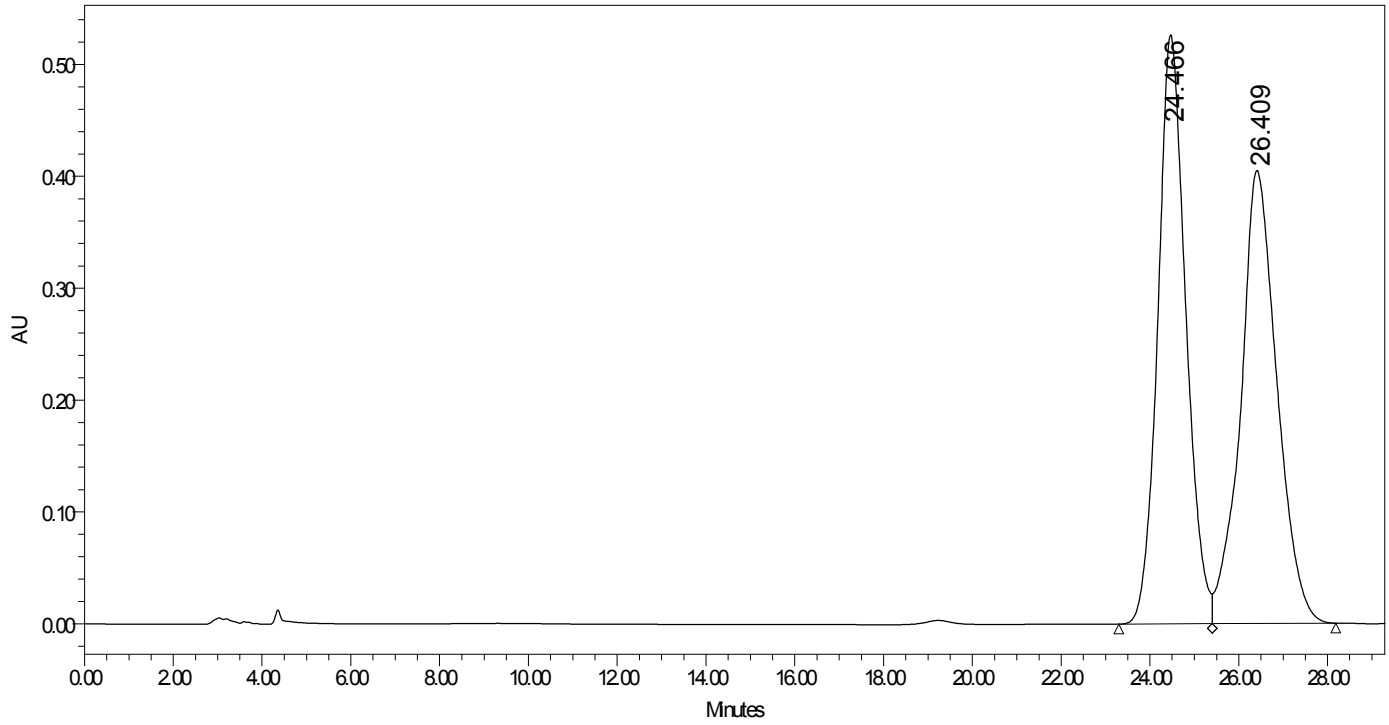
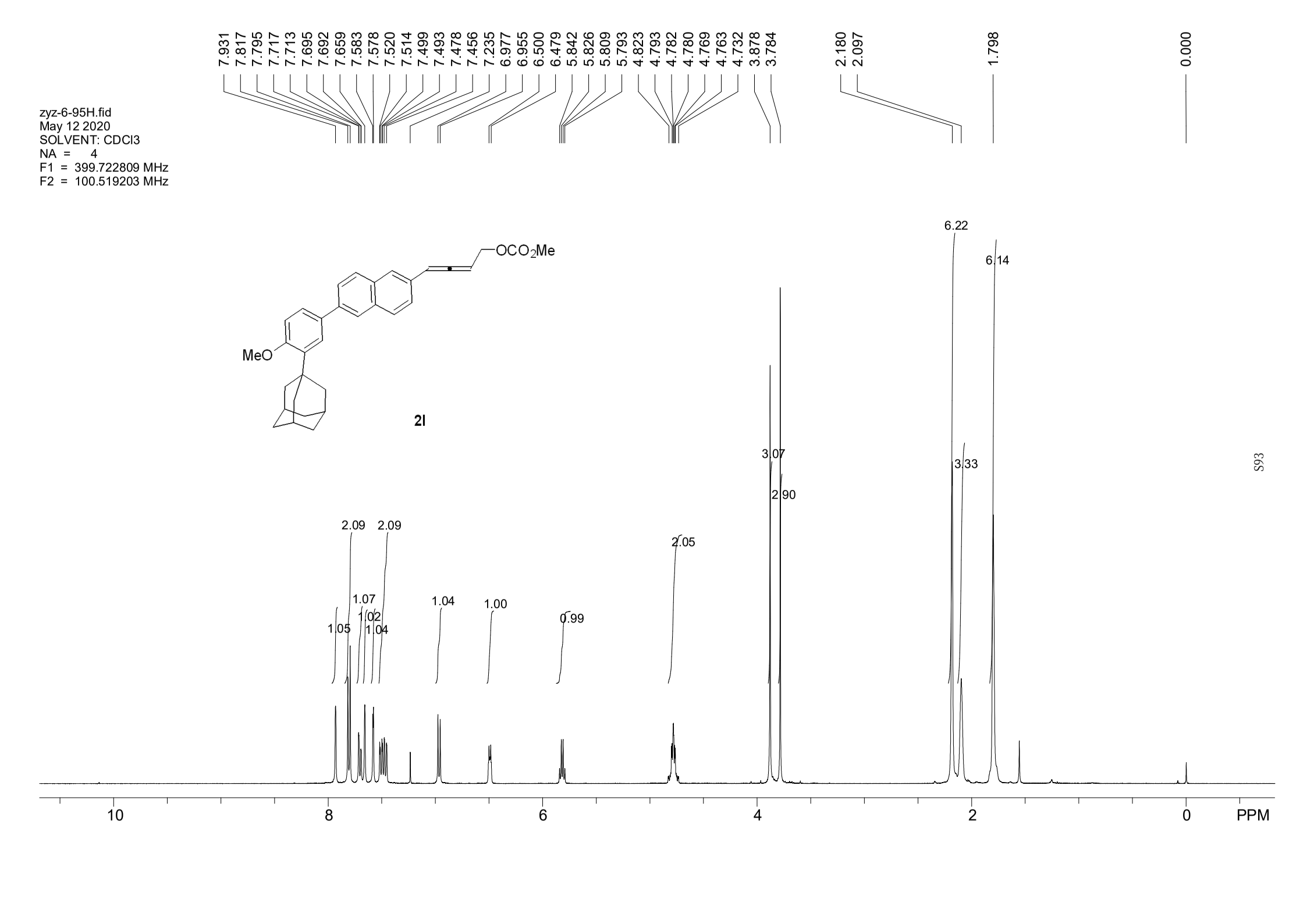
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	100.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 214nm
Date Acquired:	7/30/2020 2:32:15 PM EDT		
Date Processed:	7/30/2020 5:43:06 PM EDT		

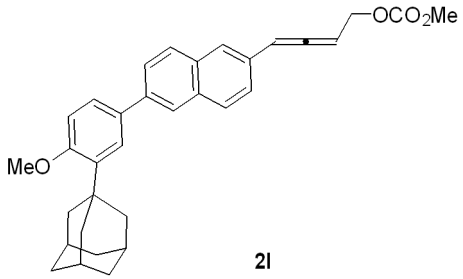


	RT	Area	%Area	Height
1	24.466	23004002	49.96	526399
2	26.409	23039387	50.04	404917

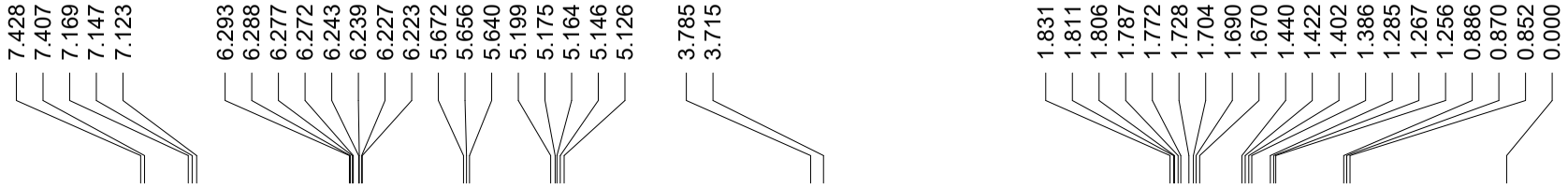

7.931
7.817
7.795
7.717
7.713
7.695
7.692
7.659
7.583
7.578
7.520
7.514
7.499
7.493
7.478
7.456
7.235
6.977
6.955
6.500
6.479
5.842
5.826
5.809
5.793
4.823
4.793
4.782
4.780
4.769
4.763
4.732
3.878
3.784
2.180
2.097
1.798
0.000
zyz-6-95H.fid
May 12 2020
SOLVENT: CDCl3
NA = 4
F1 = 399.722809 MHz
F2 = 100.519203 MHz
OCO2Me
MeO
2l
6.22
6.14
3.33
3.07
2.90
2.09
2.09
2.05
1.07
1.04
1.02
1.05
1.04
1.00
0.99
S93
10
8
6
4
2
0
PPM

zyz-6-95C.fid
May 12 2020
SOLVENT: cdcl3
NA = 60
F1 = 100.598389 MHz
F2 = 400.030792 MHz

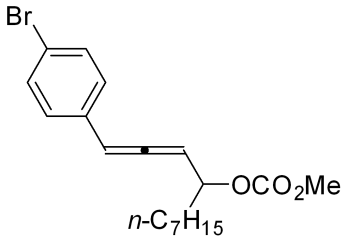
207.126
158.540
155.542
138.969
138.809
133.157
132.951
132.324
130.198
128.461
128.071
126.045
125.777
125.479
124.959
124.814
112.034
97.159
90.904
77.321
77.000
76.686
65.330
55.097
54.875
40.574
37.102
29.087



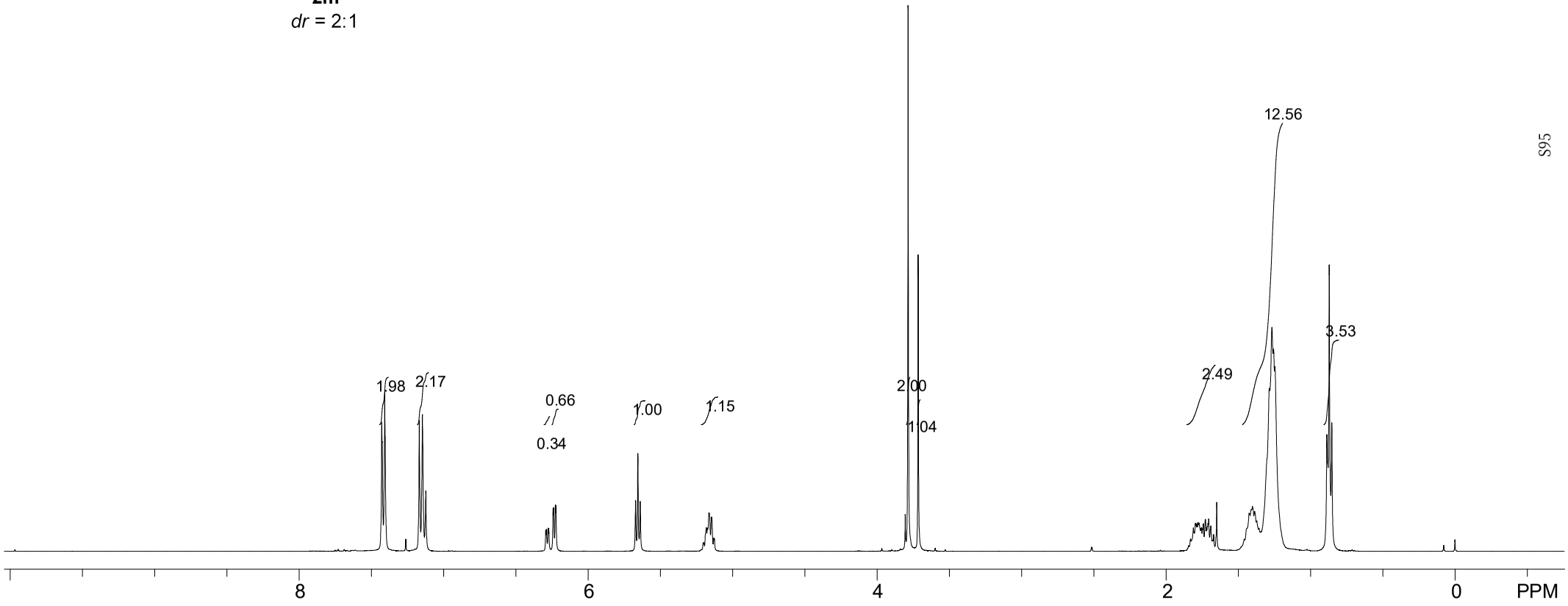
2l

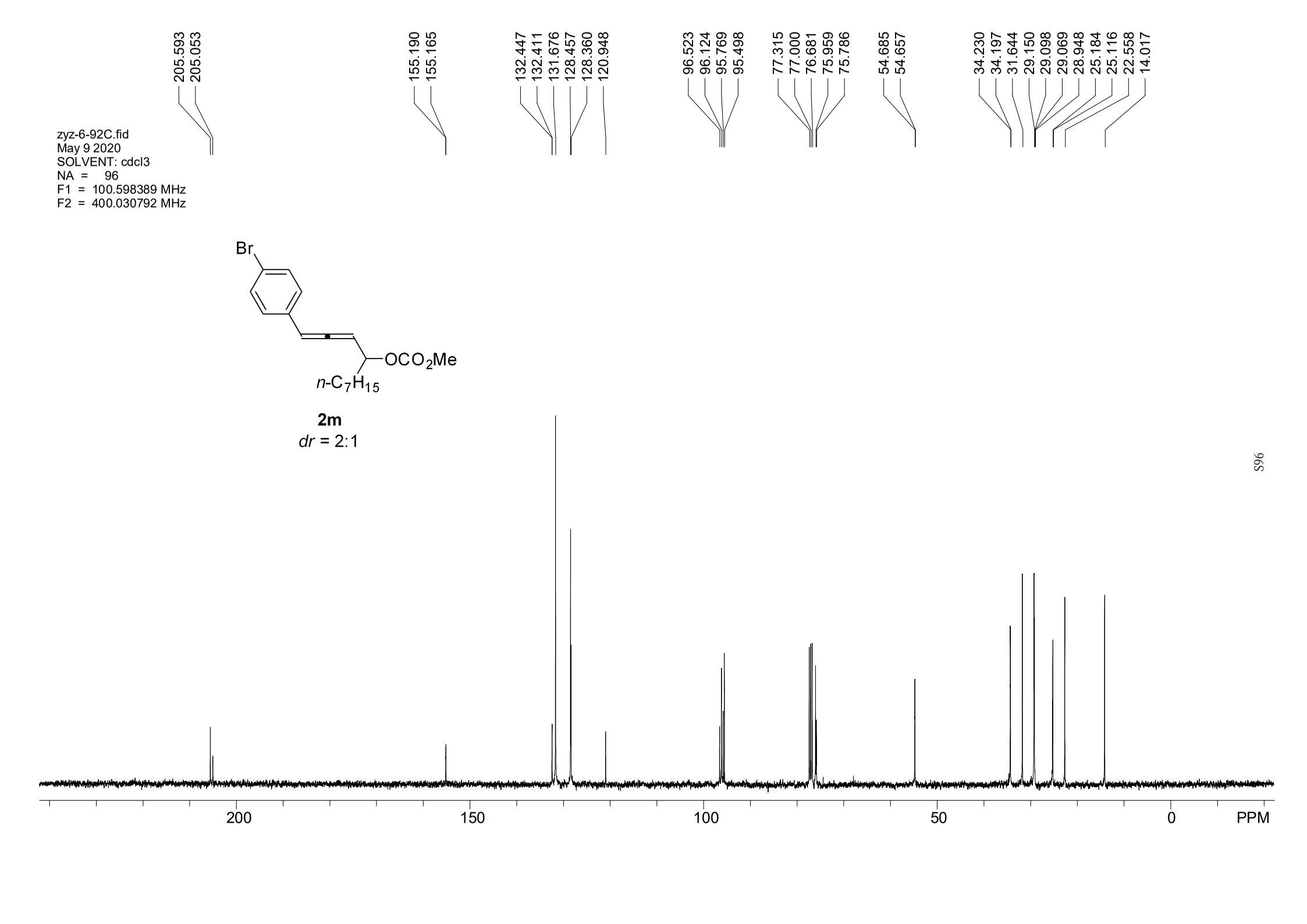


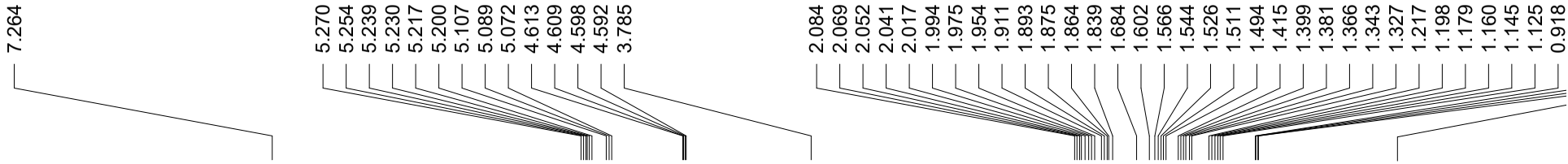
zyz-6-92H.fid
May 9 2020
SOLVENT: CDCl3
NA = 8
F1 = 400.031616 MHz
F2 = 100.596855 MHz



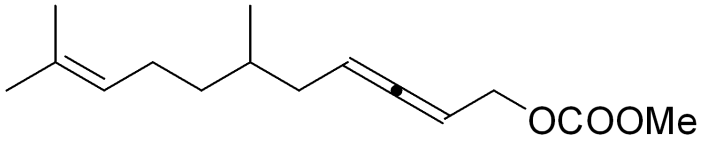
2m
dr = 2:1




205.593
205.053
155.190
155.165
132.447
132.411
131.676
128.457
128.360
120.948
96.523
96.124
95.769
95.498
77.315
77.000
76.681
75.959
75.786
54.685
54.657
34.230
34.197
31.644
29.150
29.098
29.069
28.948
25.184
25.116
22.558
14.017
zyz-6-92C.fid
May 9 2020
SOLVENT: cdcl3
NA = 96
F1 = 100.598389 MHz
F2 = 400.030792 MHz
Br
OCO2Me
n-C7H15
2m
dr = 2:1
S96
200
150
100
50
0
PPM

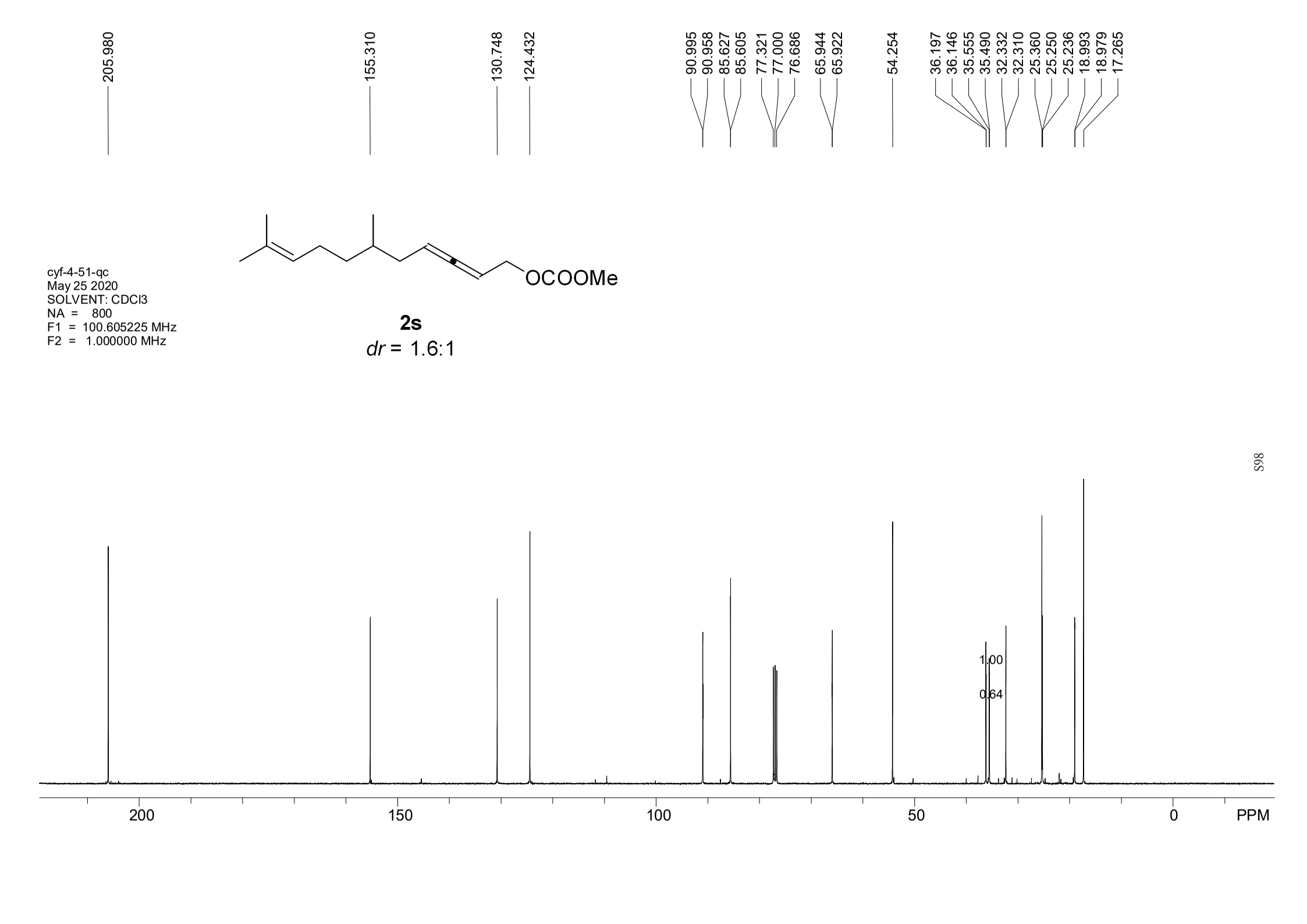


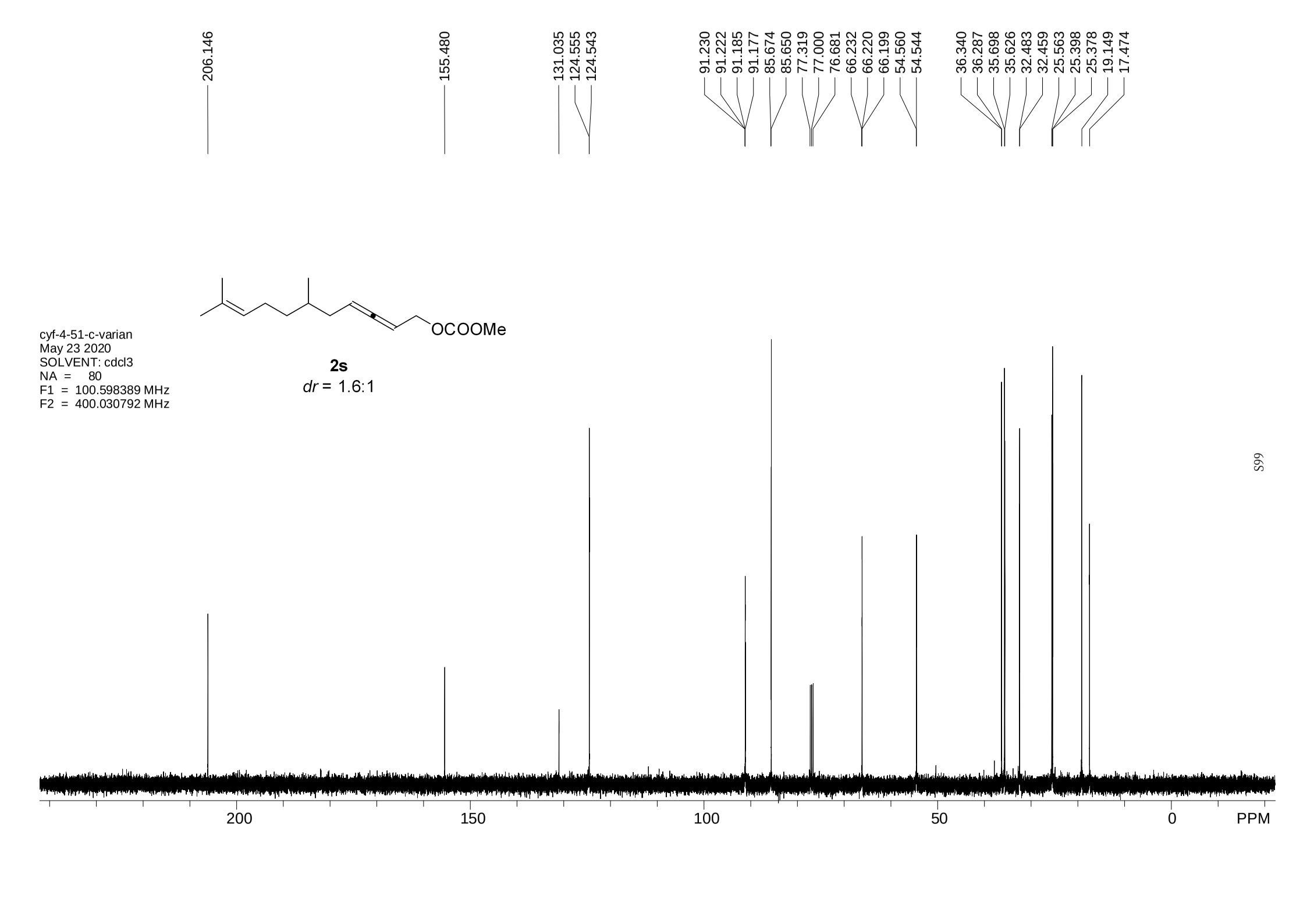
cyf-4-51-h
May 23 2020
SOLVENT: CDCl3
NA = 4
F1 = 399.722809 MHz
F2 = 100.519203 MHz



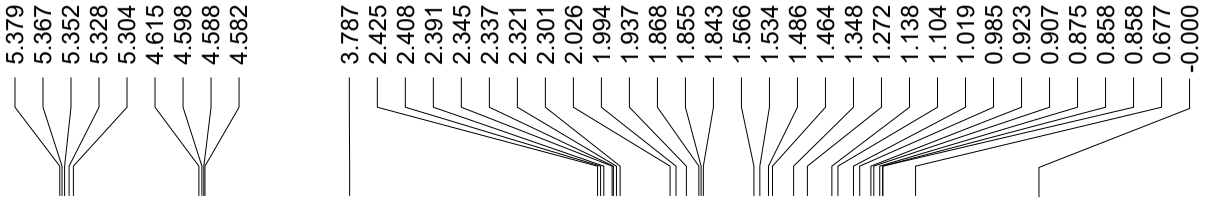
2s

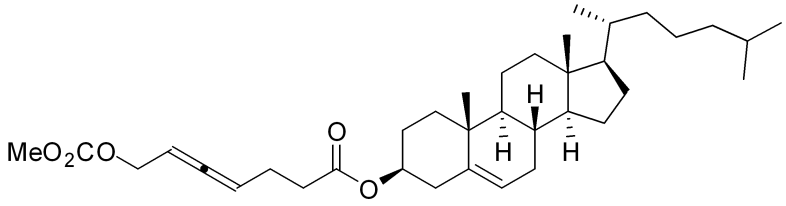
dr = 1.6:1


205.980
155.310
130.748
124.432
90.995
90.958
85.627
85.605
77.321
77.000
76.686
65.944
65.922
54.254
36.197
36.146
35.555
35.490
32.332
32.310
25.360
25.250
25.236
18.993
18.979
17.265
OCOOMe
cyf-4-51-qc
May 25 2020
SOLVENT: CDCl3
NA = 800
F1 = 100.605225 MHz
F2 = 1.000000 MHz
2s
dr = 1.6:1
1.00
0.64
200
150
100
50
0
PPM


206.146
155.480
131.035
124.555
124.543
91.230
91.222
91.185
91.177
85.674
85.650
77.319
77.000
76.681
66.232
66.220
66.199
54.560
54.544
36.340
36.287
35.698
35.626
32.483
32.459
25.563
25.398
25.378
19.149
17.474
OCOOMe
2s
dr = 1.6:1
cyf-4-51-c-varian
May 23 2020
SOLVENT: cdcl3
NA = 80
F1 = 100.598389 MHz
F2 = 400.030792 MHz
200
150
100
50
0
PPM

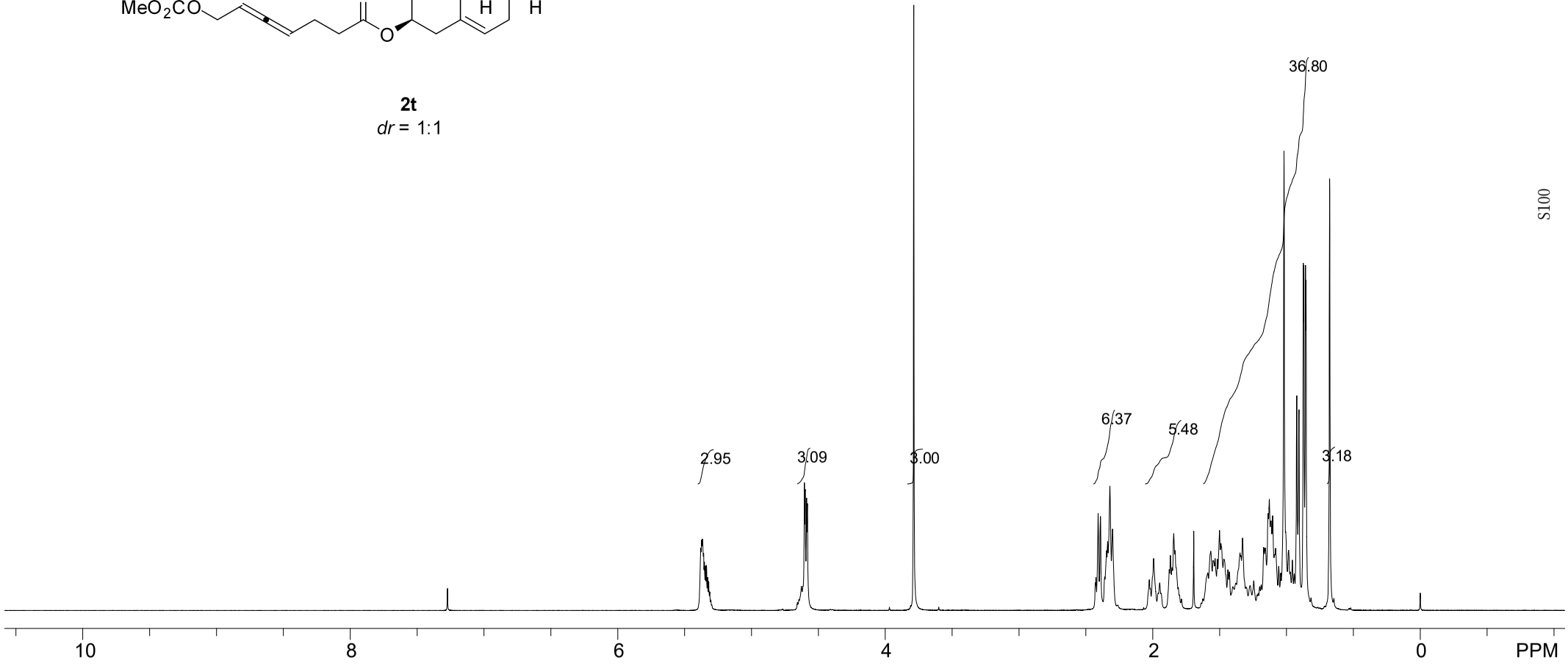
zyz-6-111H.fid
May 30 2020
SOLVENT: CDCl3
NA = 4
F1 = 400.031616 MHz
F2 = 100.596855 MHz





2t

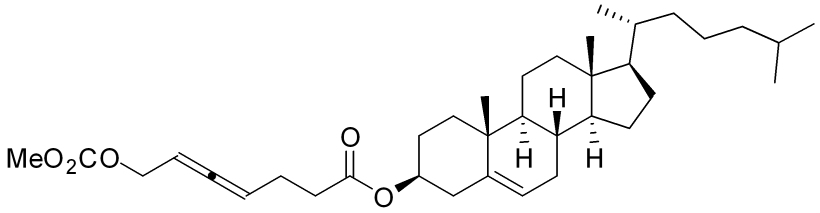
dr = 1:1



zyz-6-111C.fid
May 30 2020
SOLVENT: cdcl3
NA = 84
F1 = 100.598389 MHz
F2 = 400.030792 MHz

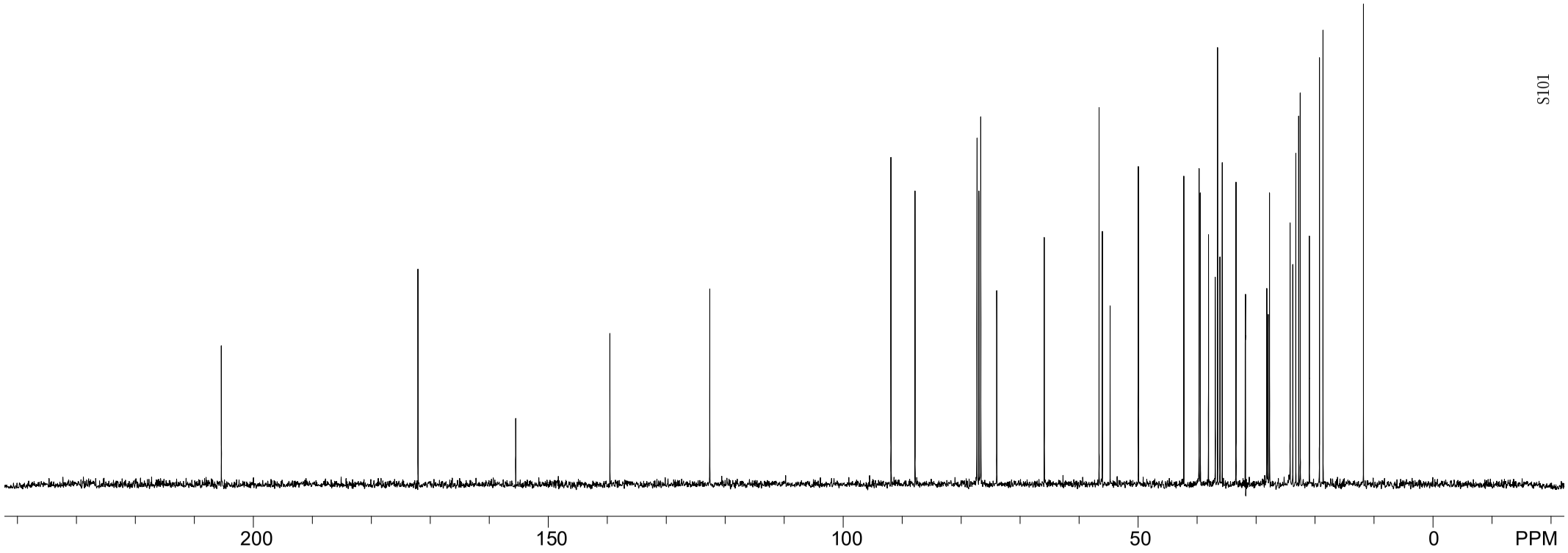
205.434 172.098 155.517 139.564 122.625

77.319 91.919 87.827 77.006 76.685 73.977 65.924 56.632 56.074 54.759 49.964 42.255 39.677 39.471 38.071 36.932 36.534 36.137 35.746 33.414 31.846 31.800 28.191 27.961 27.732 24.237 23.785 23.273 22.784 22.524 20.979 19.258 18.669 11.809



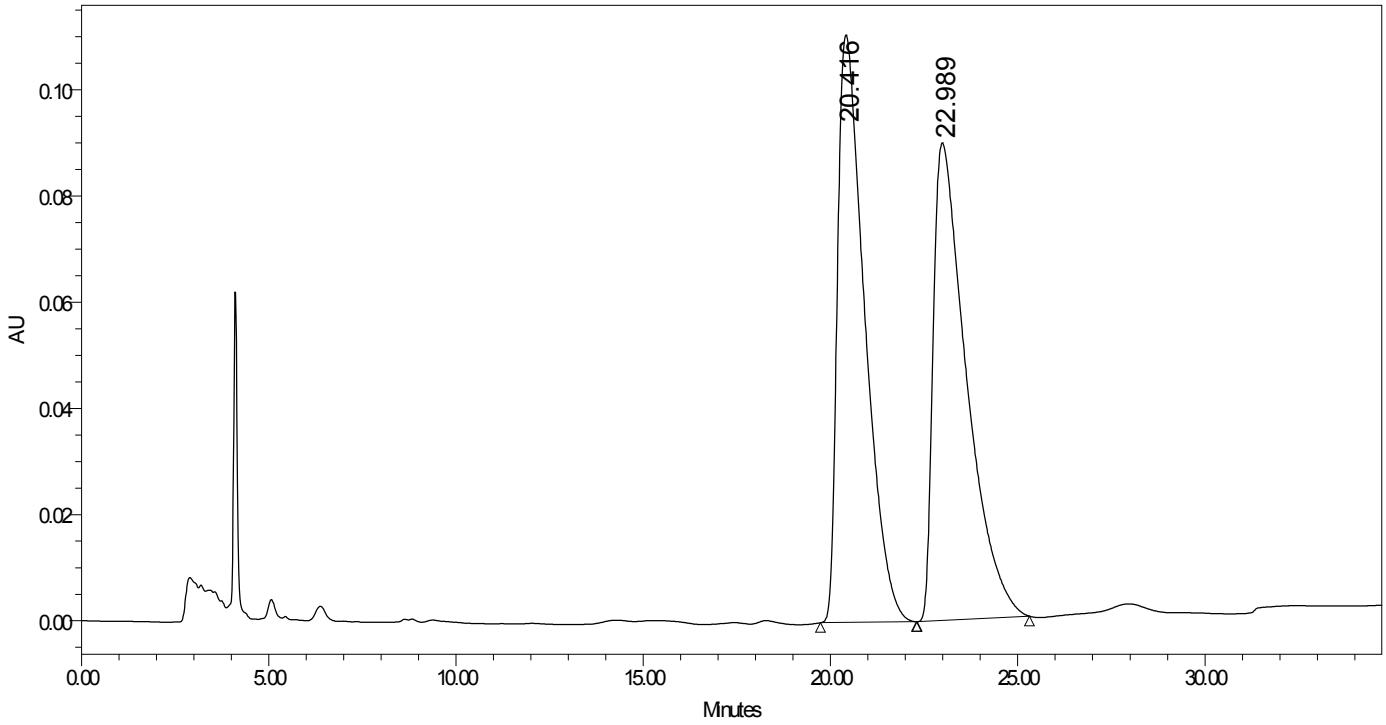
2t

dr = 1:1

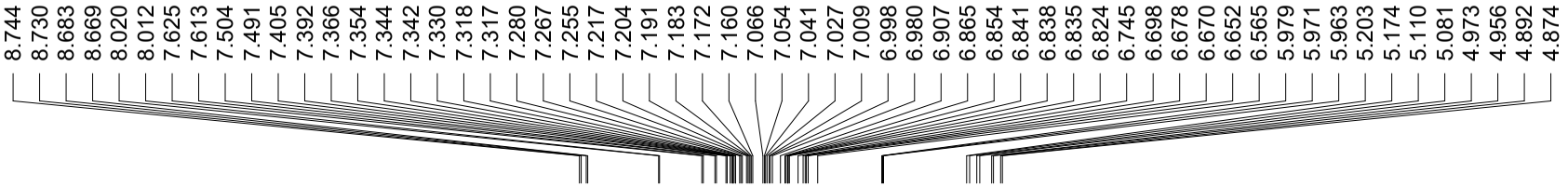


SAMPLE INFORMATION

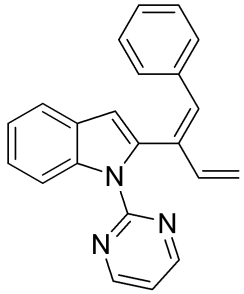
Sample Name:	zyz-6-111-od-h-200-1-1-214	Acquired By:	System
Sample Type:	Unknown	Sample Set Name:	
Vial:	1	Acq. Method Set:	HPLC
Injection #:	48	Processing Method:	Default
Injection Volume:	10.00 ul	Channel Name:	W2489 ChA
Run Time:	100.0 Minutes	Proc. Chnl. Descr.:	W2489 ChA 214nm
Date Acquired:	7/24/2020 2:33:43 PM EDT		
Date Processed:	7/24/2020 5:37:43 PM EDT		



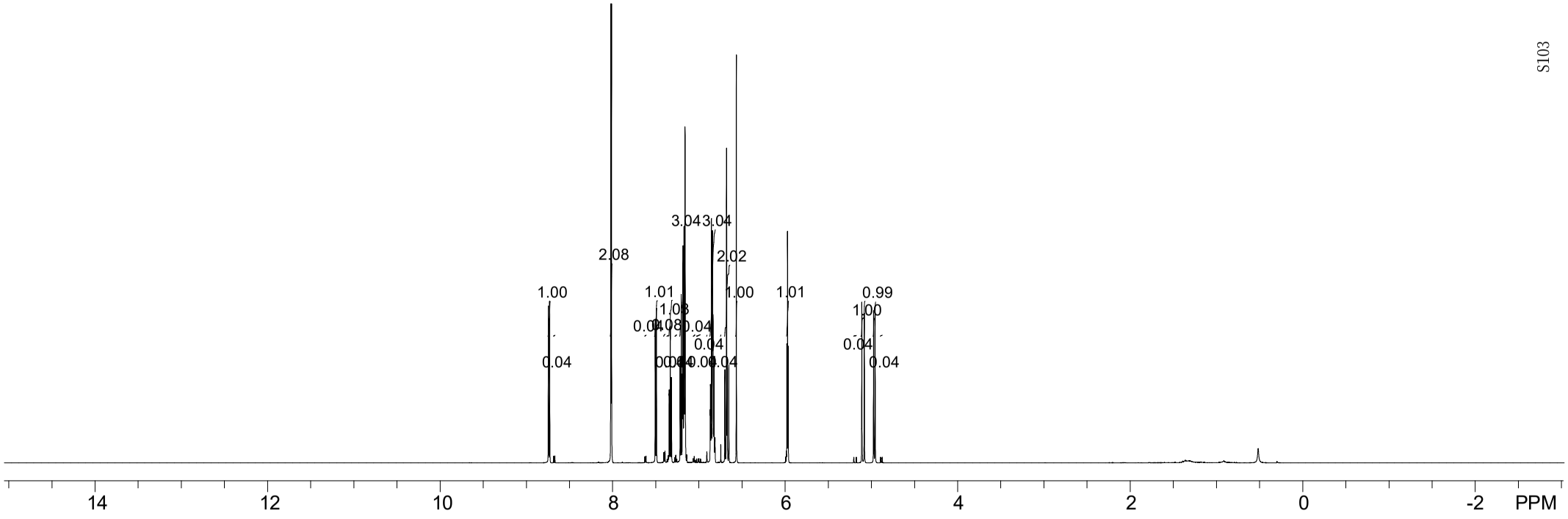
	RT	Area	%Area	Height
1	20.416	5576354	50.14	110641
2	22.989	5545985	49.86	89967

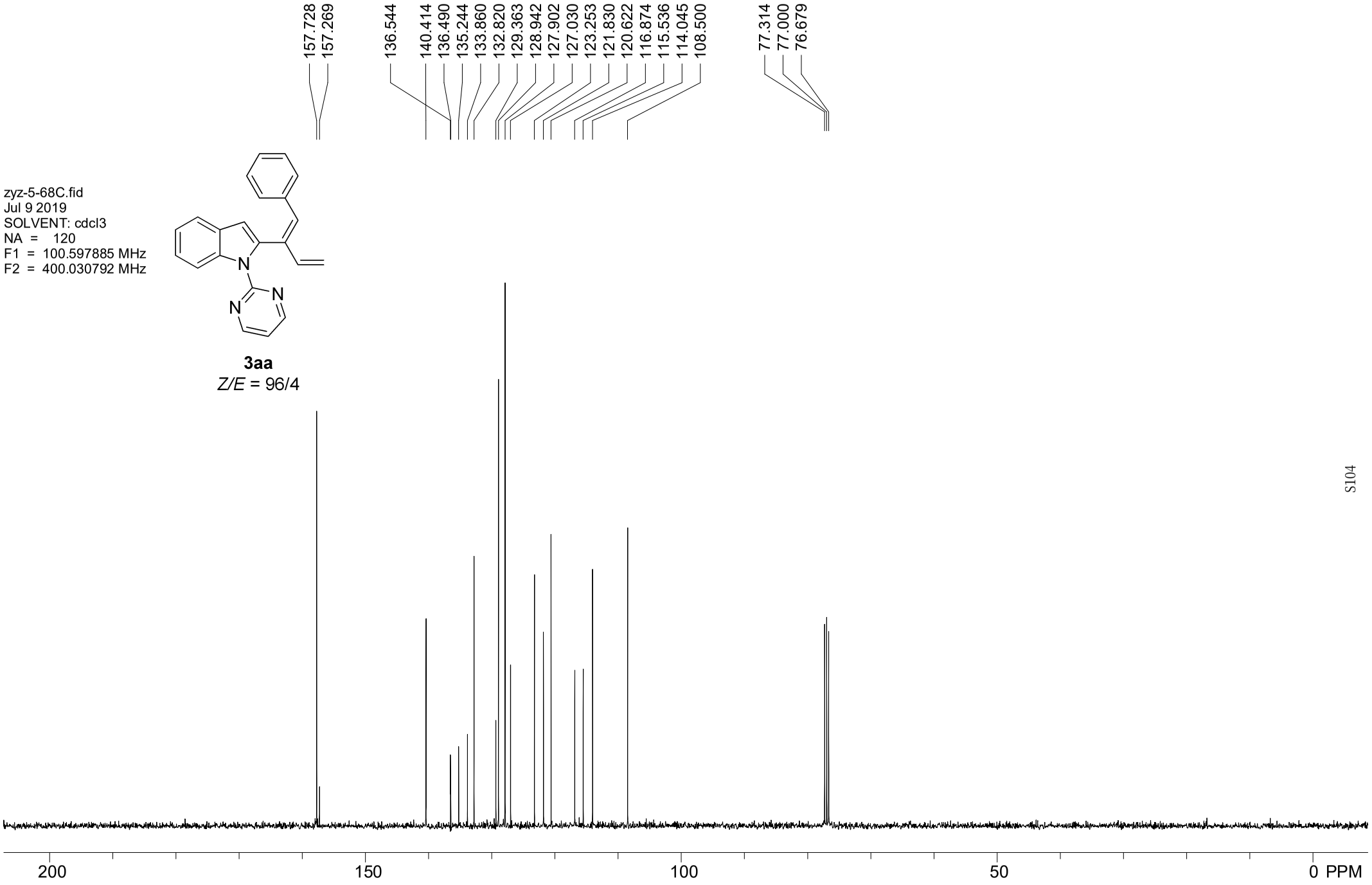


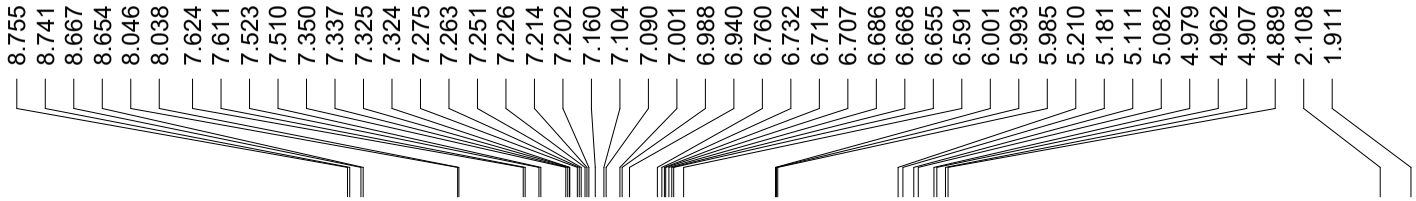
zyz-5-68-H-Q.fid
Sep 14 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz



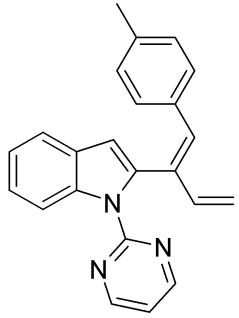
3aa
Z/E = 96/4



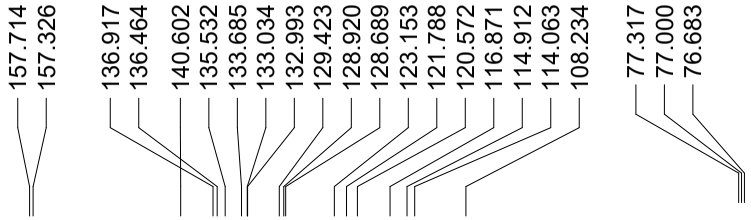

157.728
157.269
136.544
140.414
136.490
135.244
133.860
132.820
129.363
128.942
127.902
127.030
123.253
121.830
120.622
116.874
115.536
114.045
108.500
77.314
77.000
76.679
zyz-5-68C.fid
Jul 9 2019
SOLVENT: cdcl3
NA = 120
F1 = 100.597885 MHz
F2 = 400.030792 MHz
N
N
N
3aa
Z/E = 96/4
200
150
100
50
0 PPM



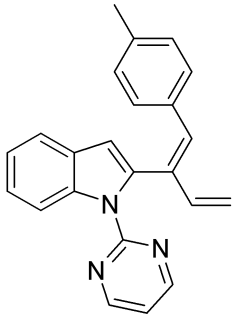
zyz-5-82-h-Q.fid
Sep 15 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz



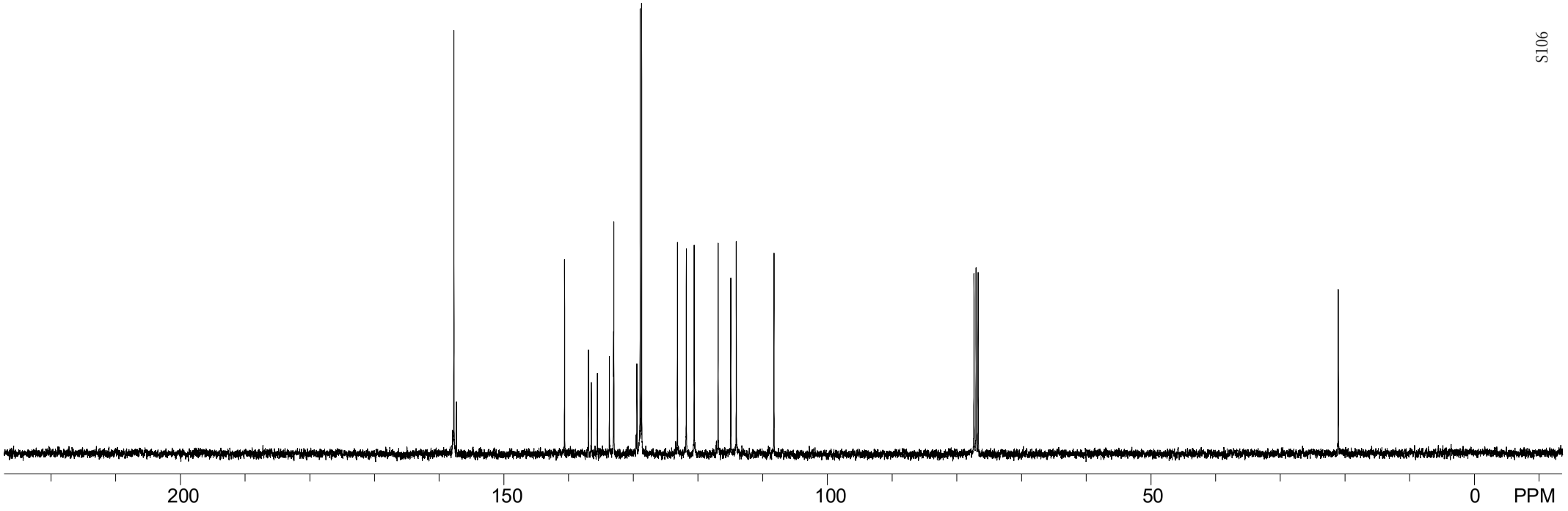
3ab
Z/E = 96/4

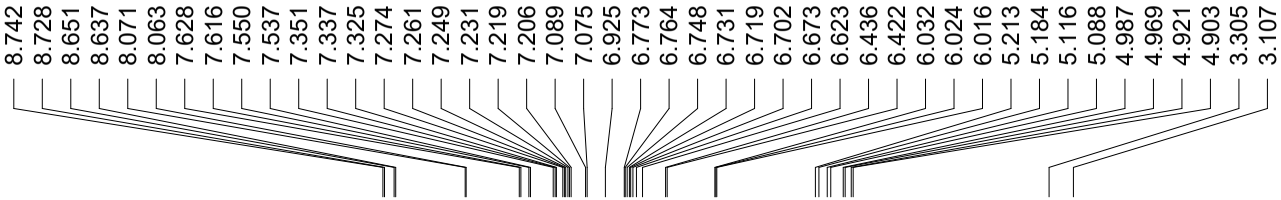


zyz-5-82C.fid
Jul 22 2019
SOLVENT: cdcl3
NA = 80
F1 = 100.599144 MHz
F2 = 400.030792 MHz

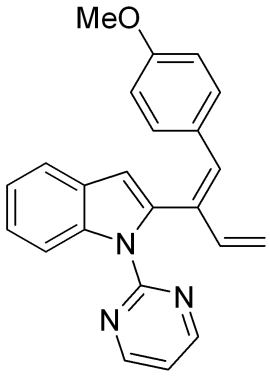


3ab
Z/E = 96/4

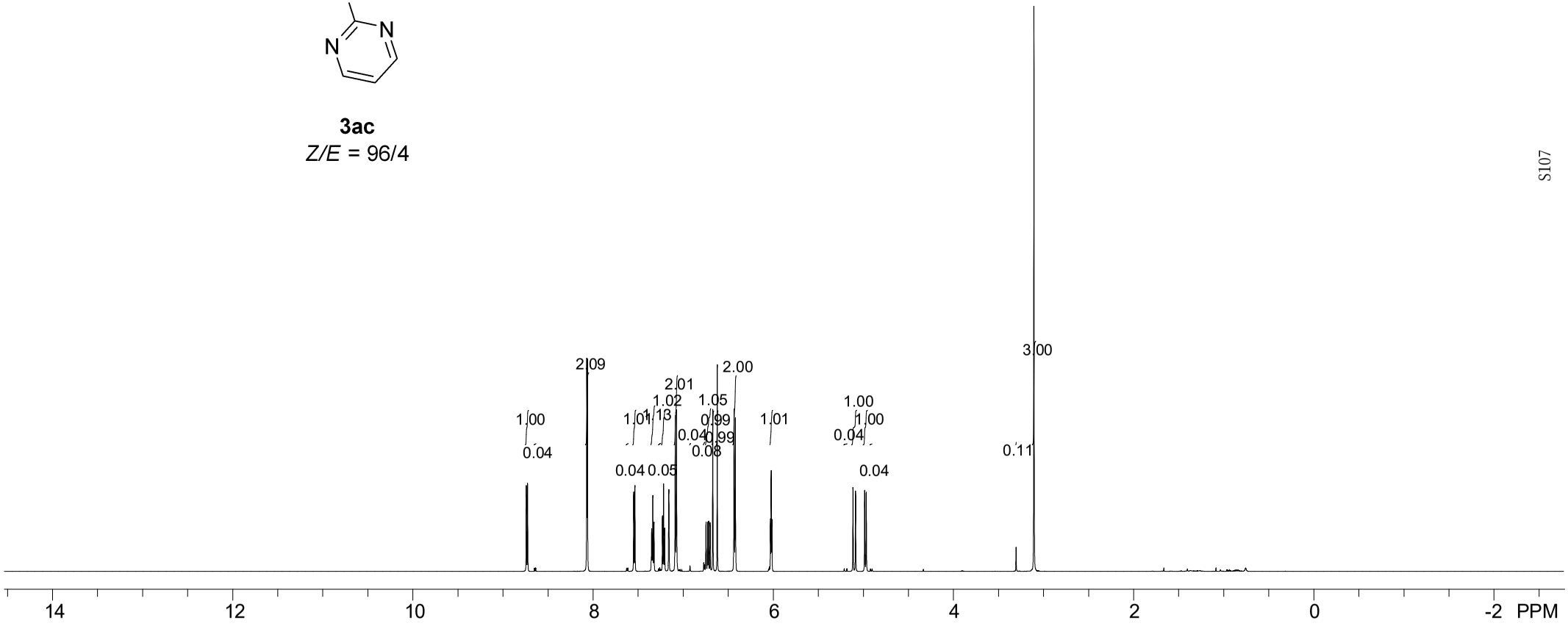




zyz-6-171-H-Q.fid
Oct 13 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz

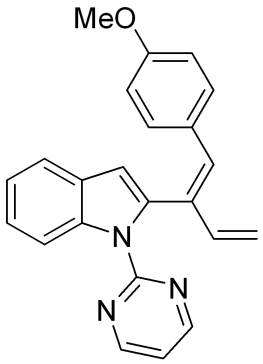


3ac
Z/E = 96/4

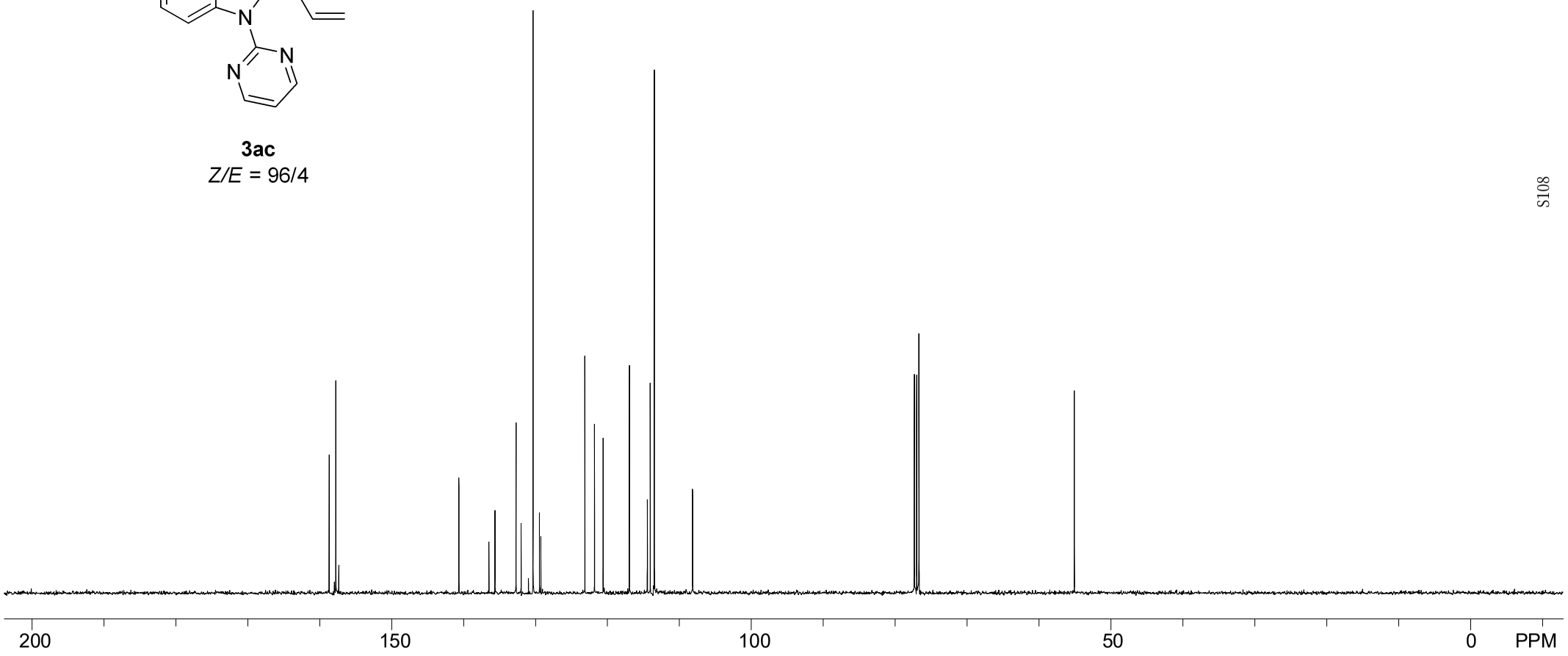


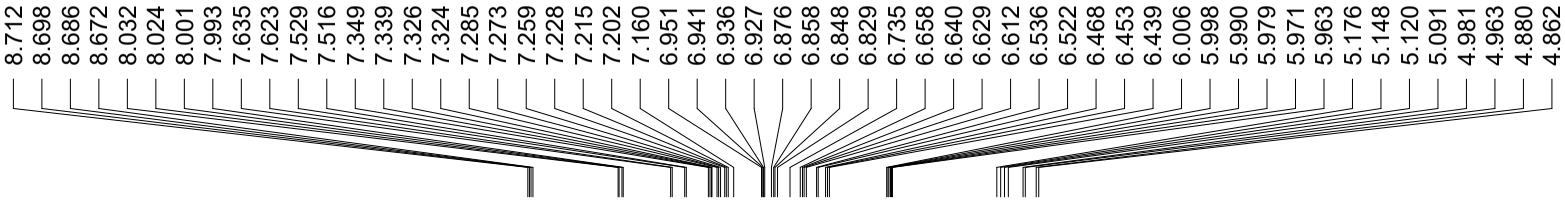
zyz-5-75C.fid
Jul 12 2019
SOLVENT: cdcl3
NA = 264
F1 = 100.599144 MHz
F2 = 400.030792 MHz

158.700
157.973
157.774
157.361
136.483
140.667
135.650
132.713
132.002
130.992
130.350
129.463
129.256
123.138
121.800
120.599
116.951
114.450
114.053
113.487
108.164
77.321
77.000
76.686
55.074

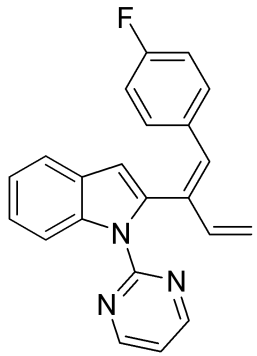


3ac
Z/E = 96/4

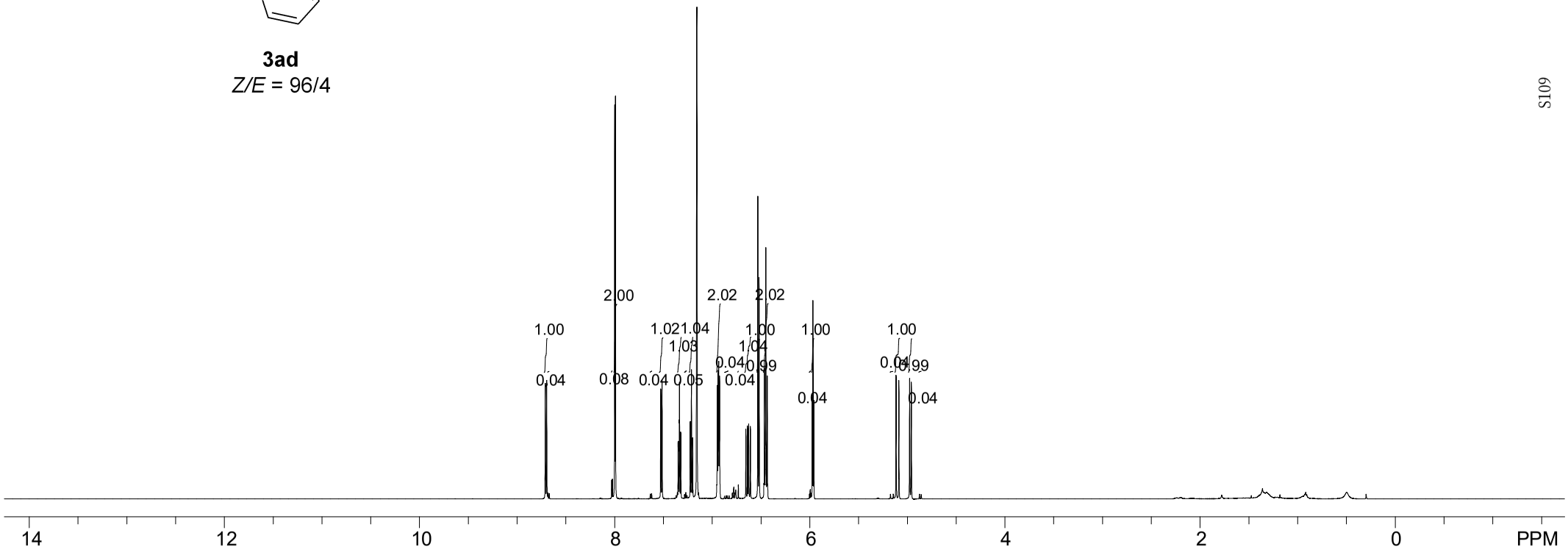


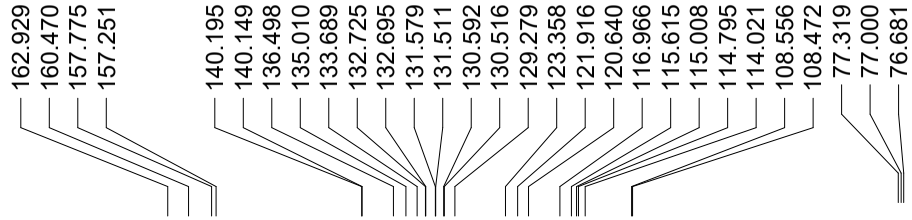


zyz-5-81--H-Q.fid
Sep 18 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz

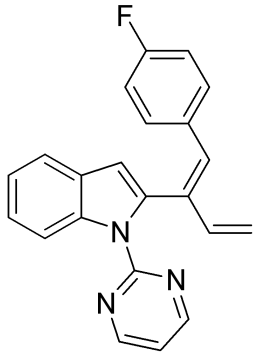


3ad
Z/E = 96/4

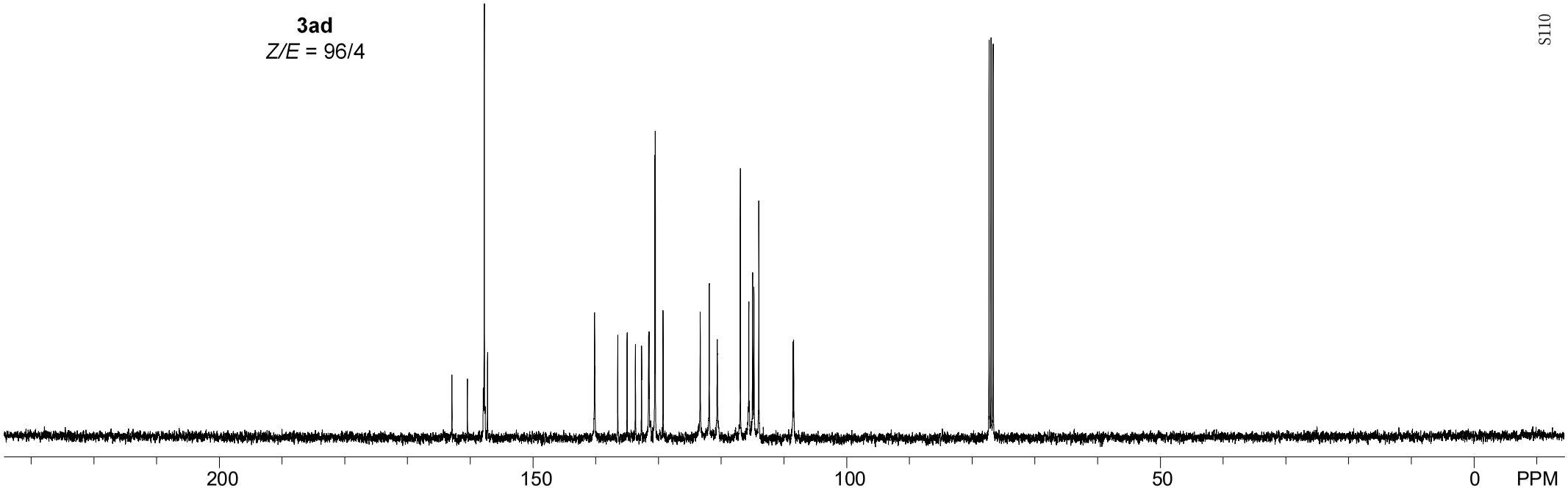




zyz-5-81C.fid
Jul 18 2019
SOLVENT: cdcl3
NA = 324
F1 = 100.520737 MHz
F2 = 399.722015 MHz



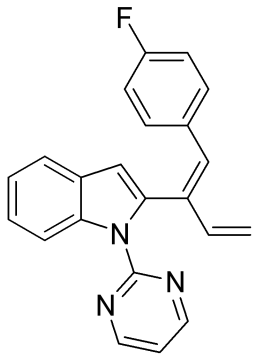
3ad
Z/E = 96/4



-0.000

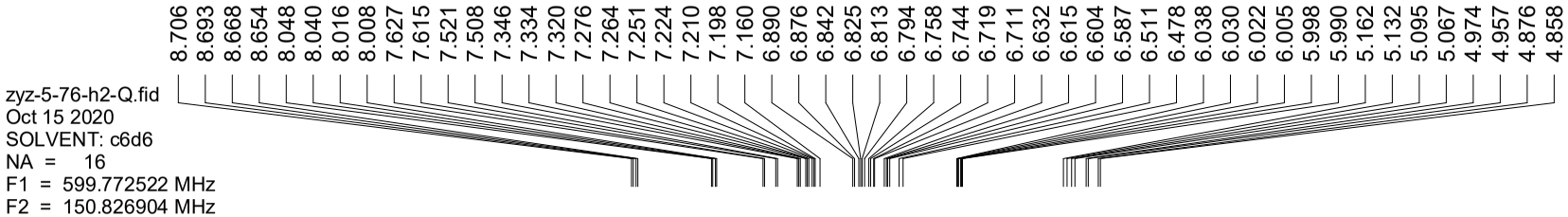
-114.627

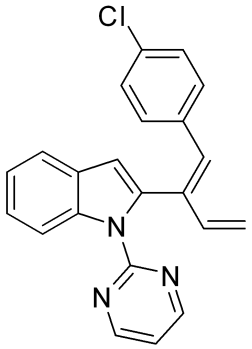
zyz-5-81F.fid
Jul 18 2019
SOLVENT: CDCl3
F1 = 376.065857 MHz
F2 = 100.519203 MHz



3ad
Z/E = 96/4

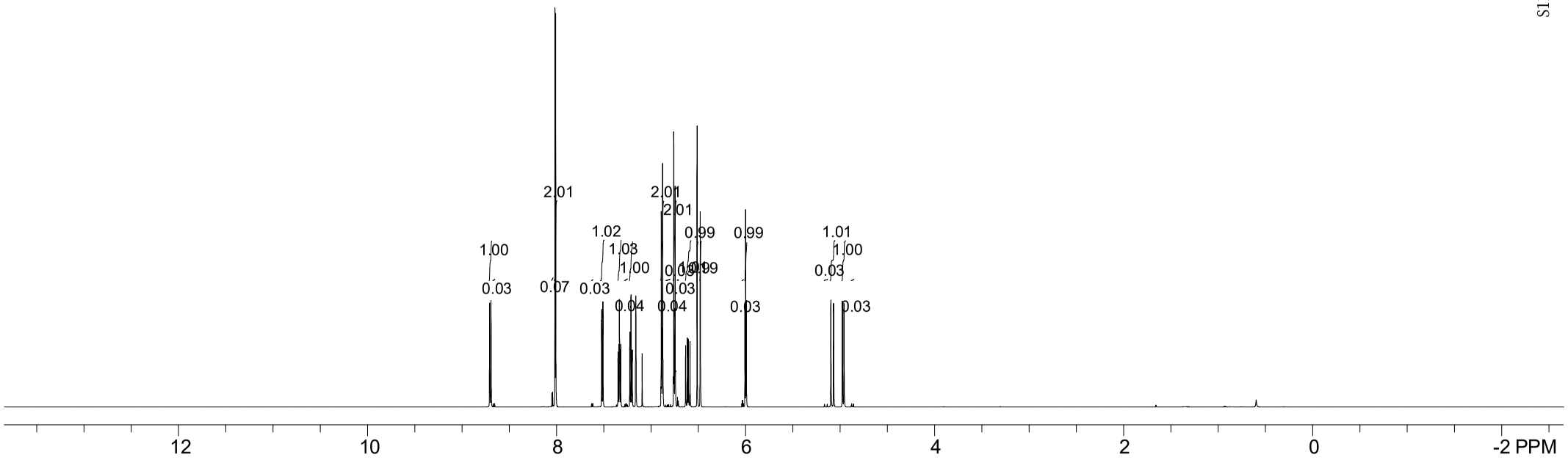
50 0 -50 -100 -150 -200 -250 -300 PPM

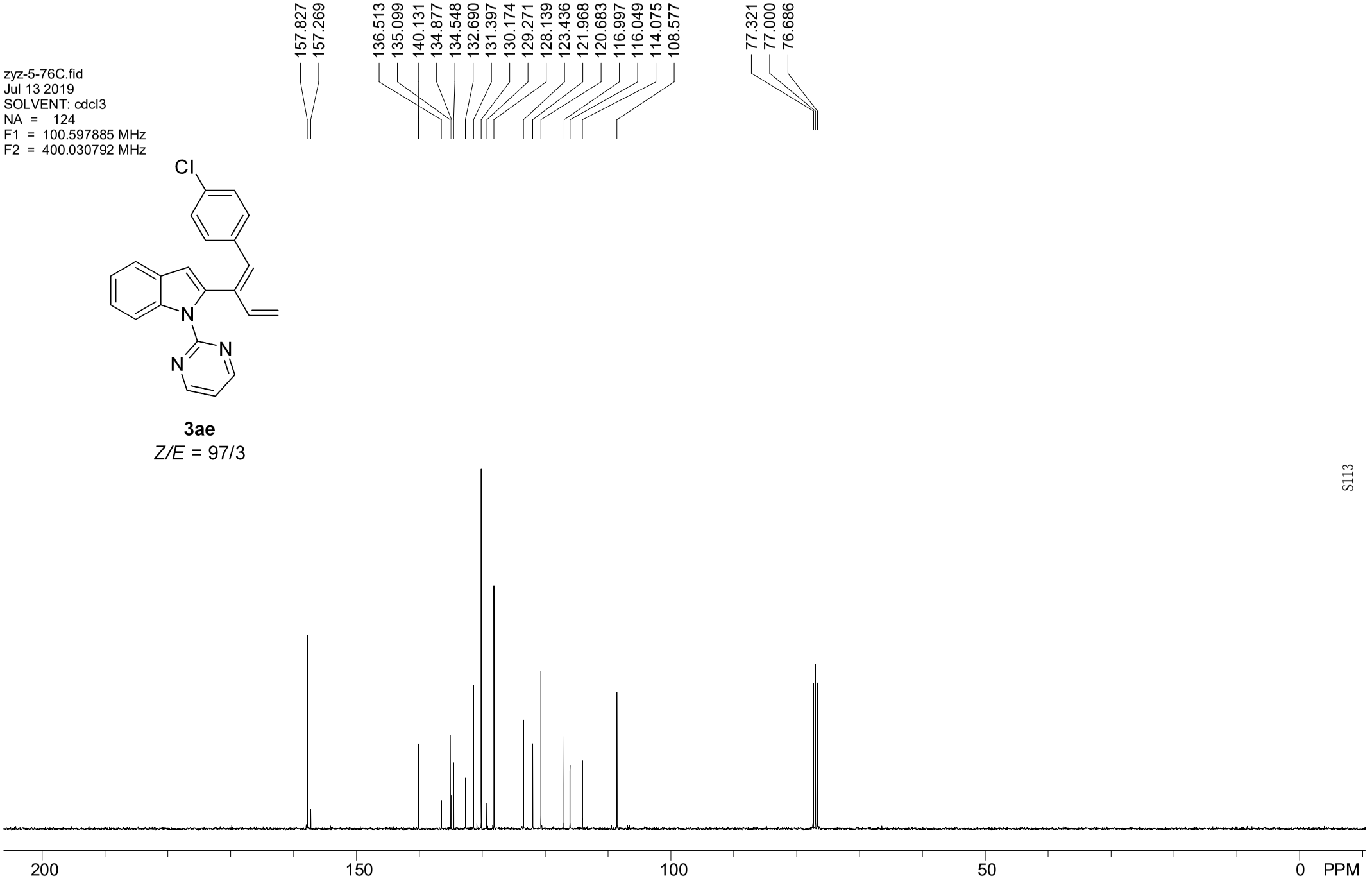

8.706
8.693
8.668
8.654
8.048
8.040
8.016
8.008
7.627
7.615
7.521
7.508
7.346
7.334
7.320
7.276
7.264
7.251
7.224
7.210
7.198
7.160
6.890
6.876
6.842
6.825
6.813
6.794
6.758
6.744
6.719
6.711
6.632
6.615
6.604
6.587
6.511
6.478
6.038
6.030
6.022
6.005
5.998
5.990
5.162
5.132
5.095
5.067
4.974
4.957
4.876
4.858
zyz-5-76-h2-Q.fid
Oct 15 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz

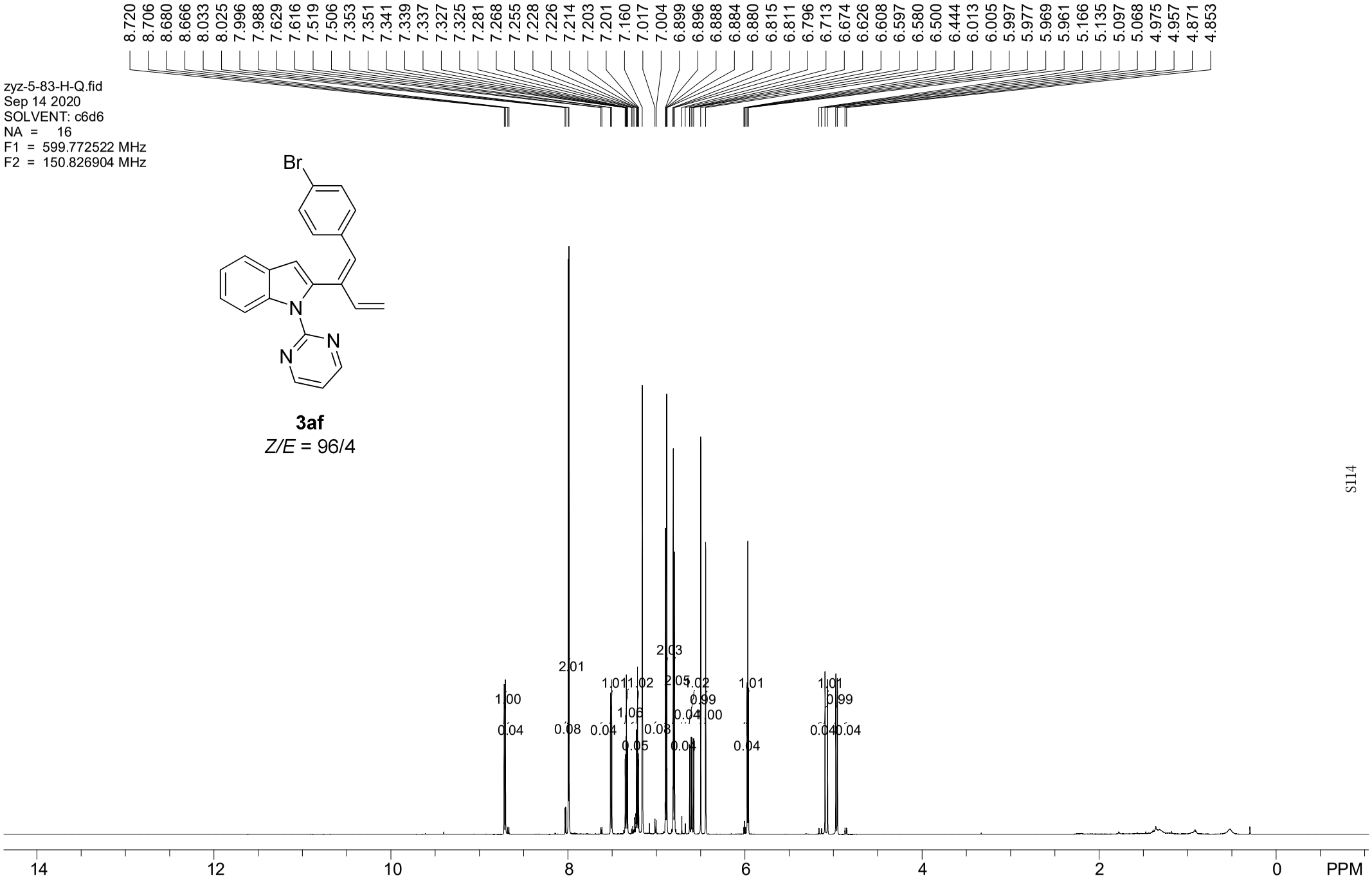

Cl
N
N
N

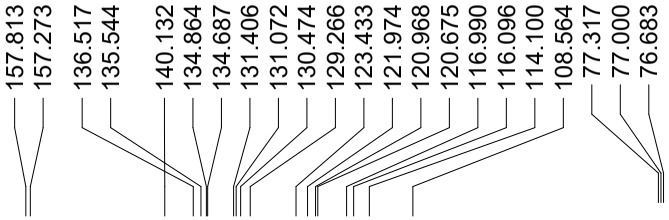
3ae

Z/E = 97/3

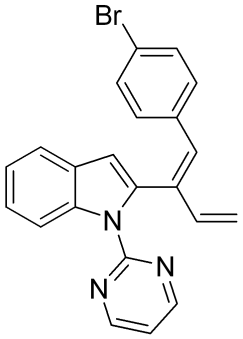

1.00
0.03
2.01
0.07
1.02
1.03
1.00
0.03
0.04
2.01
2.01
0.03
0.04
0.99
0.99
0.03
0.99
0.03
1.01
1.00
0.03
0.03
12
10
8
6
4
2
0
-2 PPM


157.827
157.269
136.513
135.099
140.131
134.877
134.548
132.690
131.397
130.174
129.271
128.139
123.436
121.968
120.683
116.997
116.049
114.075
108.577
77.321
77.000
76.686
zyz-5-76C.fid
Jul 13 2019
SOLVENT: cdcl3
NA = 124
F1 = 100.597885 MHz
F2 = 400.030792 MHz
Cl
N
N
N
3ae
Z/E = 97/3
S113
200
150
100
50
0
PPM

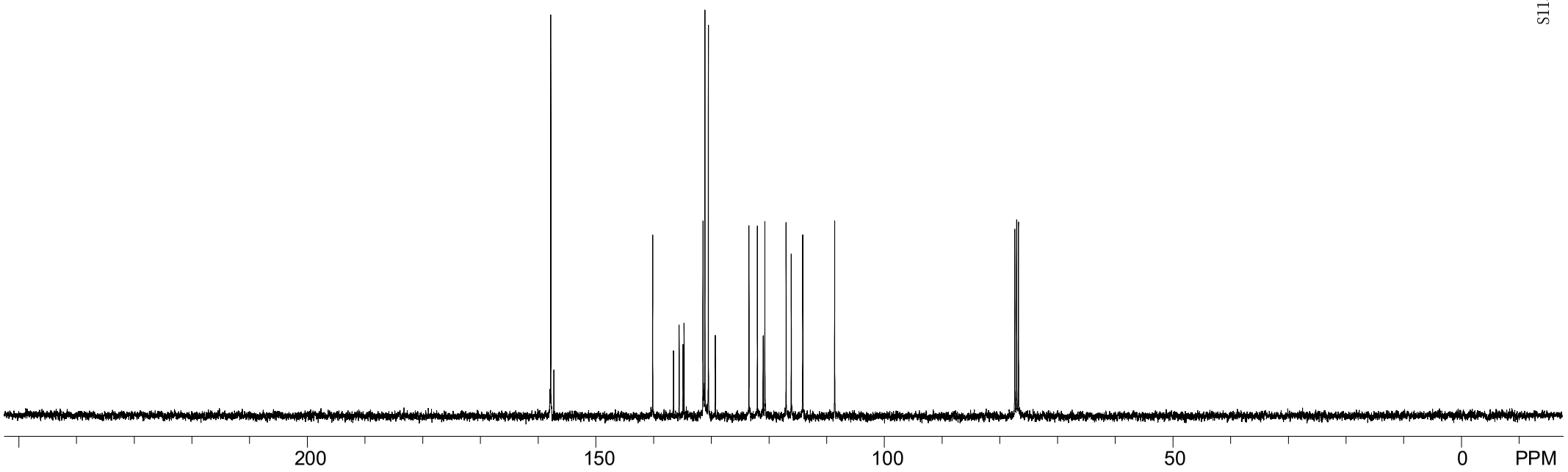

8.720 8.706 8.680 8.666 8.033 8.025 7.996 7.988 7.629 7.616 7.519 7.506 7.353 7.351 7.341 7.339 7.337 7.327 7.325 7.281 7.268 7.255 7.228 7.226 7.214 7.203 7.201 7.160 7.017 7.004 6.899 6.896 6.888 6.884 6.880 6.815 6.811 6.796 6.713 6.674 6.626 6.608 6.597 6.580 6.500 6.444 6.013 6.005 5.997 5.977 5.969 5.961 5.166 5.135 5.097 5.068 4.975 4.957 4.871 4.853
zyz-5-83-H-Q.fid
Sep 14 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz
Br
N
N
N
3af
Z/E = 96/4
1.00
0.04
2.01
0.08
1.01
0.04
1.02
1.06
0.05
2.03
0.08
2.05
0.04
1.02
0.99
1.00
0.04
1.01
0.04
1.01
0.99
0.04
0.04
14
12
10
8
6
4
2
0
PPM

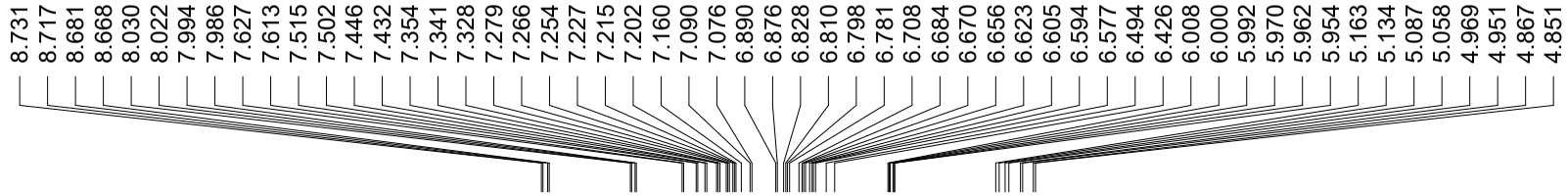


zyz-5-83C.fid
Jul 20 2019
SOLVENT: cdcl3
NA = 160
F1 = 100.599144 MHz
F2 = 400.030792 MHz

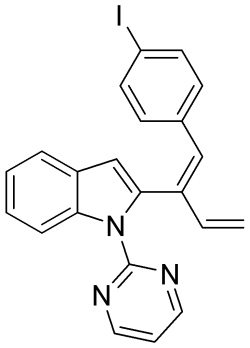


3af
Z/E = 96/4

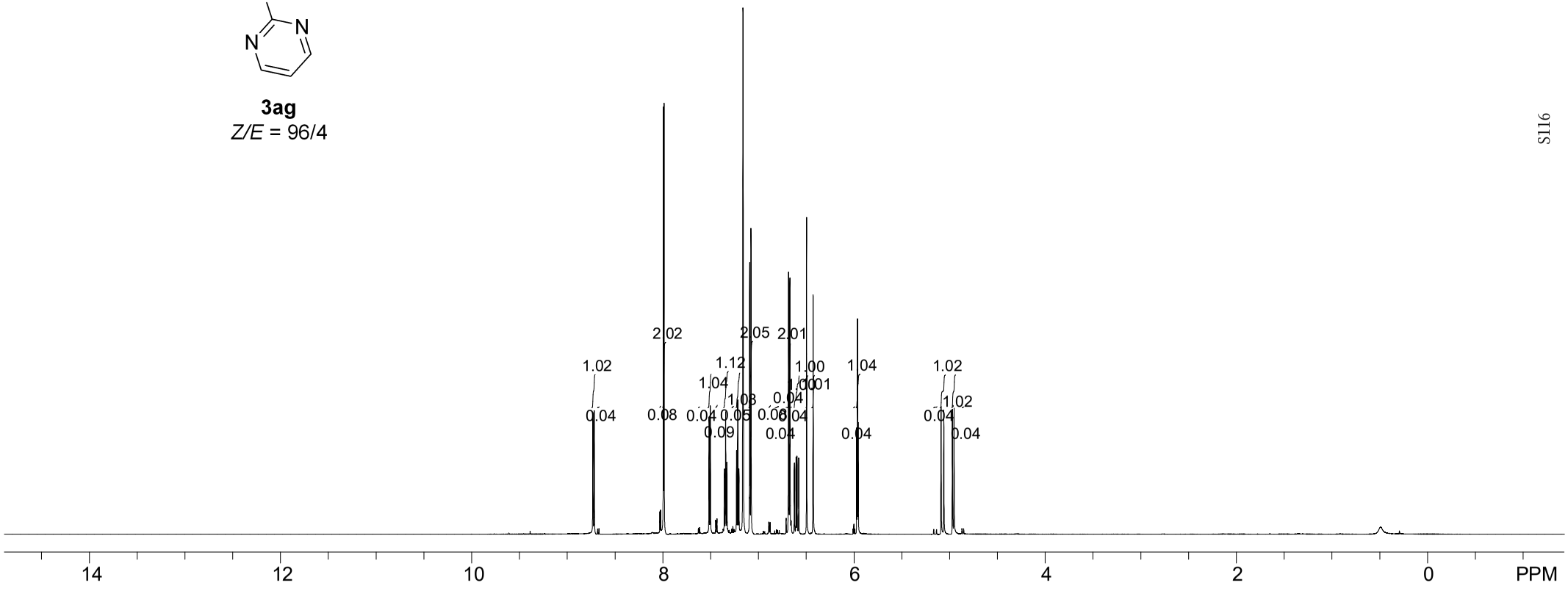


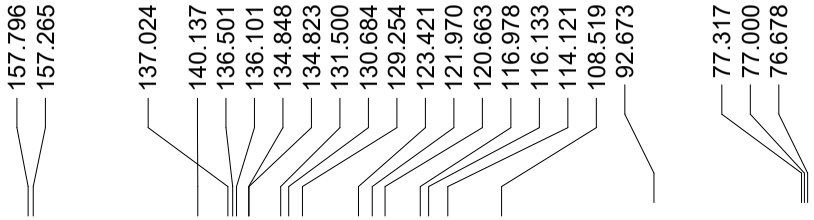


zyz-5-86-D6-H-q.fid
Sep 10 2020
SOLVENT: c6d6
NA = 8
F1 = 599.772522 MHz
F2 = 150.826904 MHz

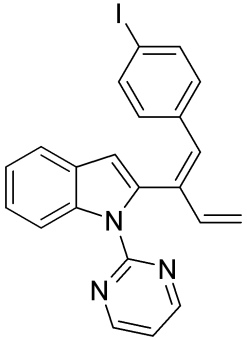


3ag
Z/E = 96/4

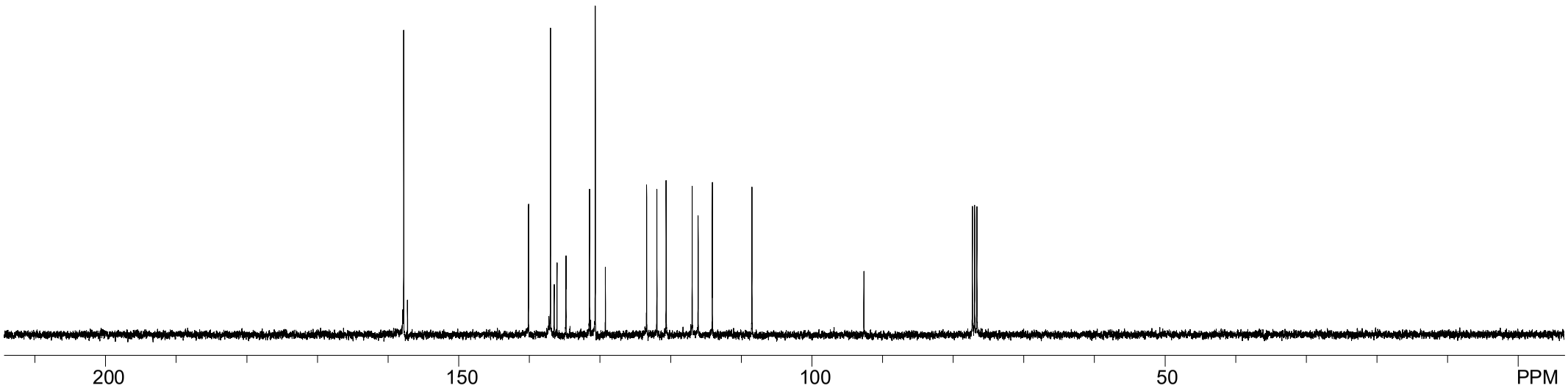


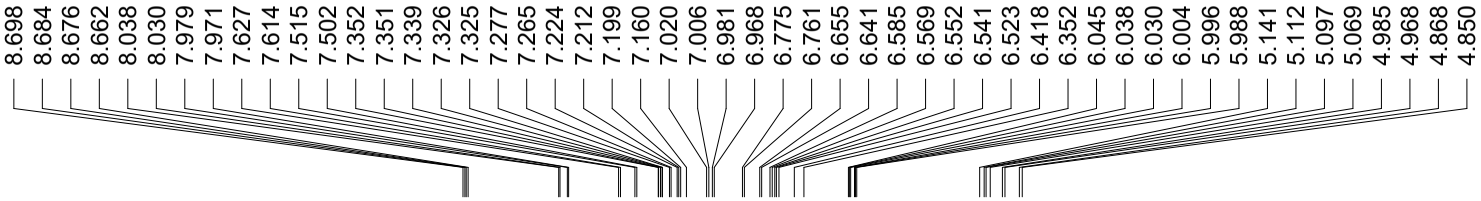


zyz-5-86C.fid
Jul 22 2019
SOLVENT: cdcl3
NA = 8
F1 = 100.599144 MHz
F2 = 400.030792 MHz

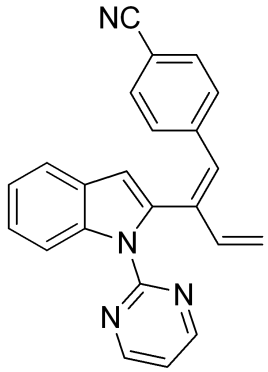


3ag
Z/E = 96/4

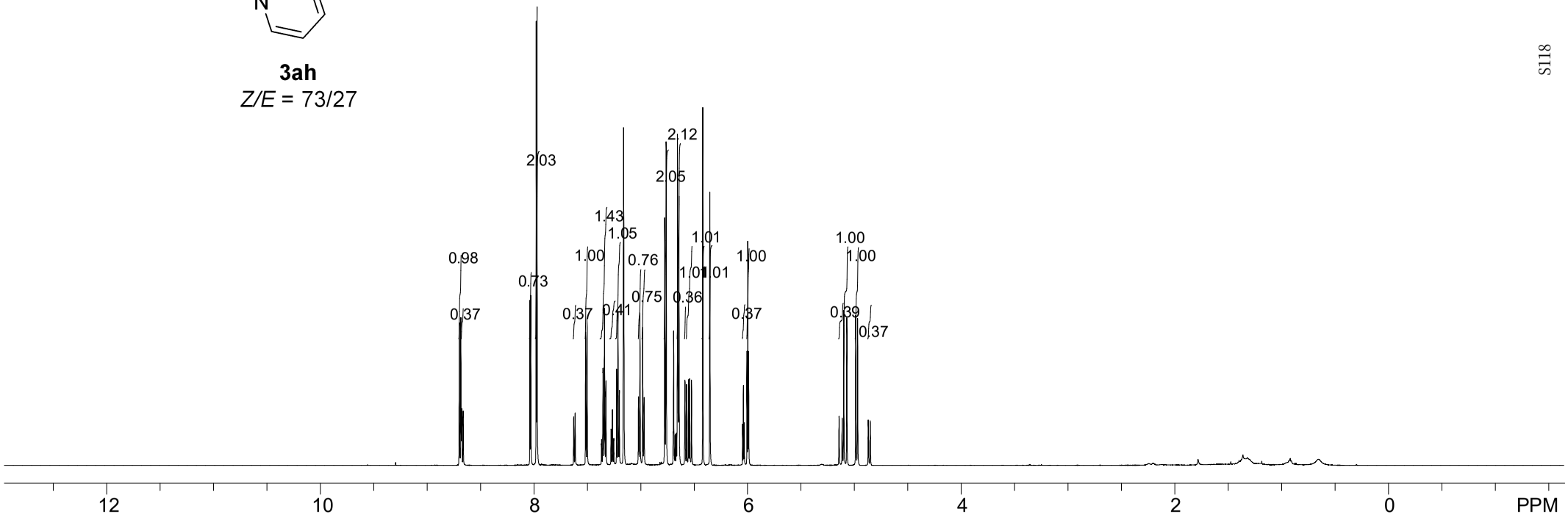


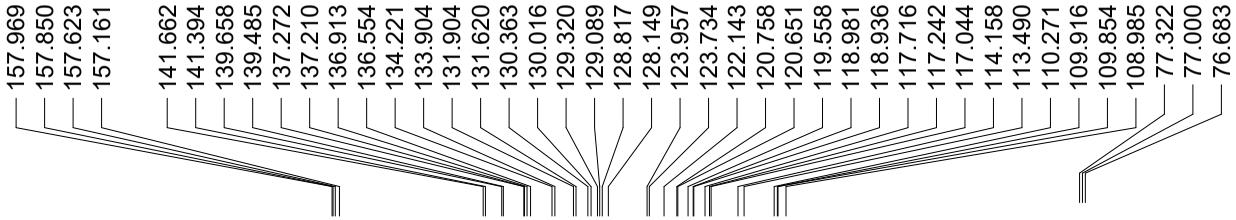


zyz-5-122-h-Q.fid
Sep 15 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz

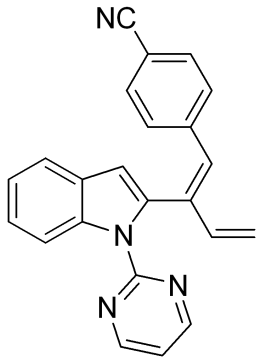


3ah
Z/E = 73/27

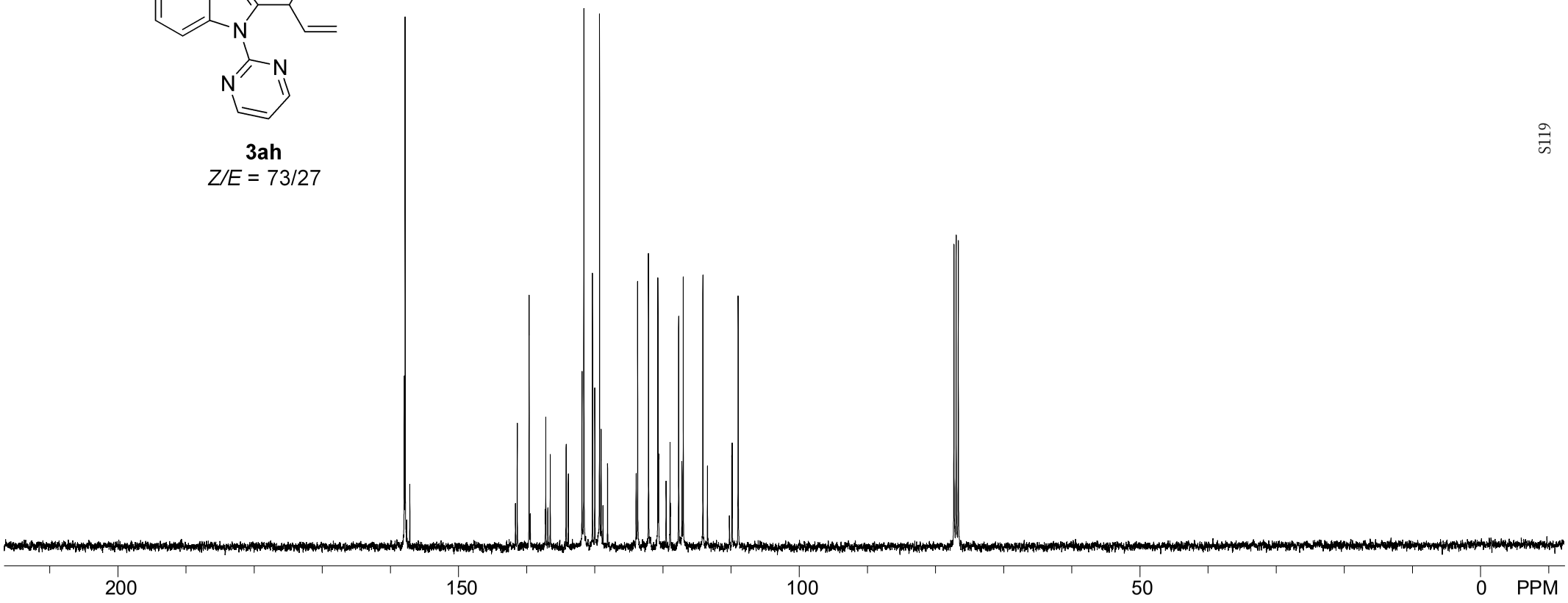


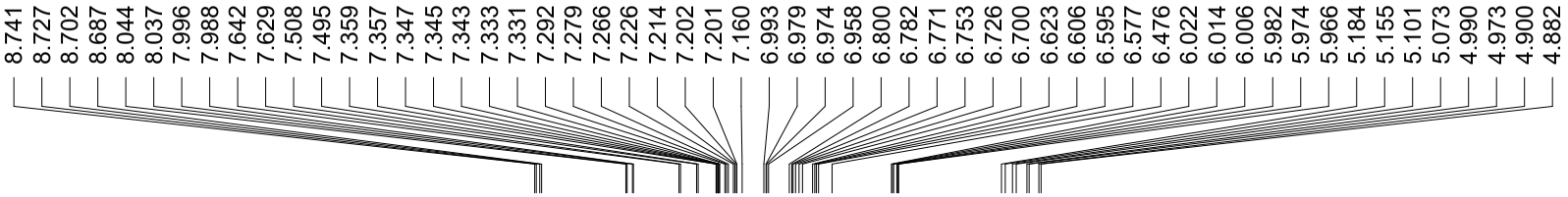


zyz-5-122C.fid
Sep 23 2019
SOLVENT: cdcl3
NA = 440
F1 = 100.599144 MHz
F2 = 400.030792 MHz

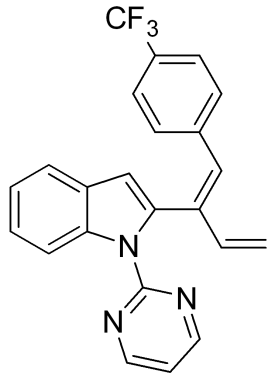


3ah
Z/E = 73/27

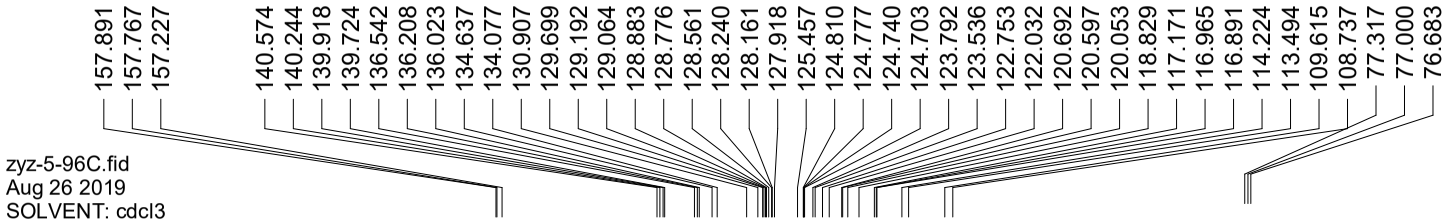




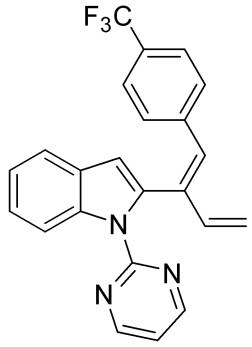
zyz-5-96-H-Q.fid
Sep 14 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz



3ai
Z/E = 96/4

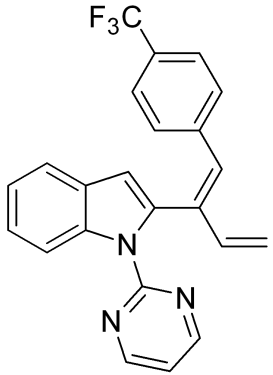


zyz-5-96C.fid
Aug 26 2019
SOLVENT: cdcl3
NA = 160
F1 = 100.599144 MHz
F2 = 400.030792 MHz

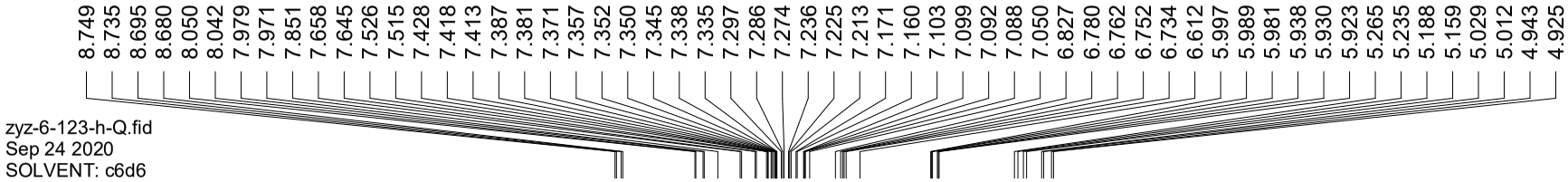


3ai
Z/E = 96/4

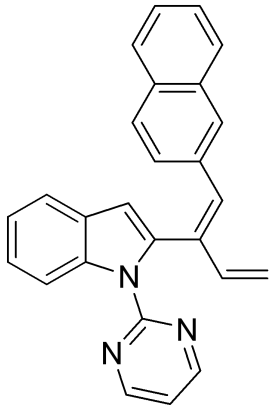
zyz-5-96F.fid
Aug 26 2019
SOLVENT: CDCl3
NA = 8
F1 = 376.365509 MHz
F2 = 100.596855 MHz
SW1 = 156250.00 Hz



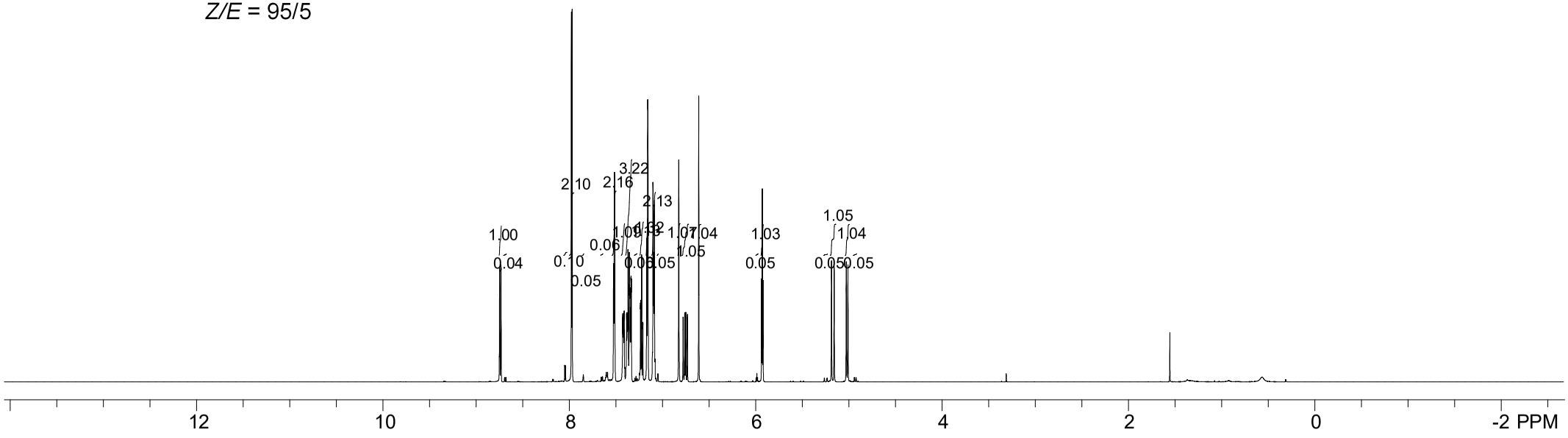
3ai
Z/E = 96/4



zyz-6-123-h-Q.fid
Sep 24 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz

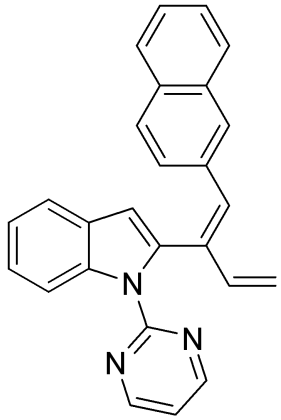


3aj
Z/E = 95/5

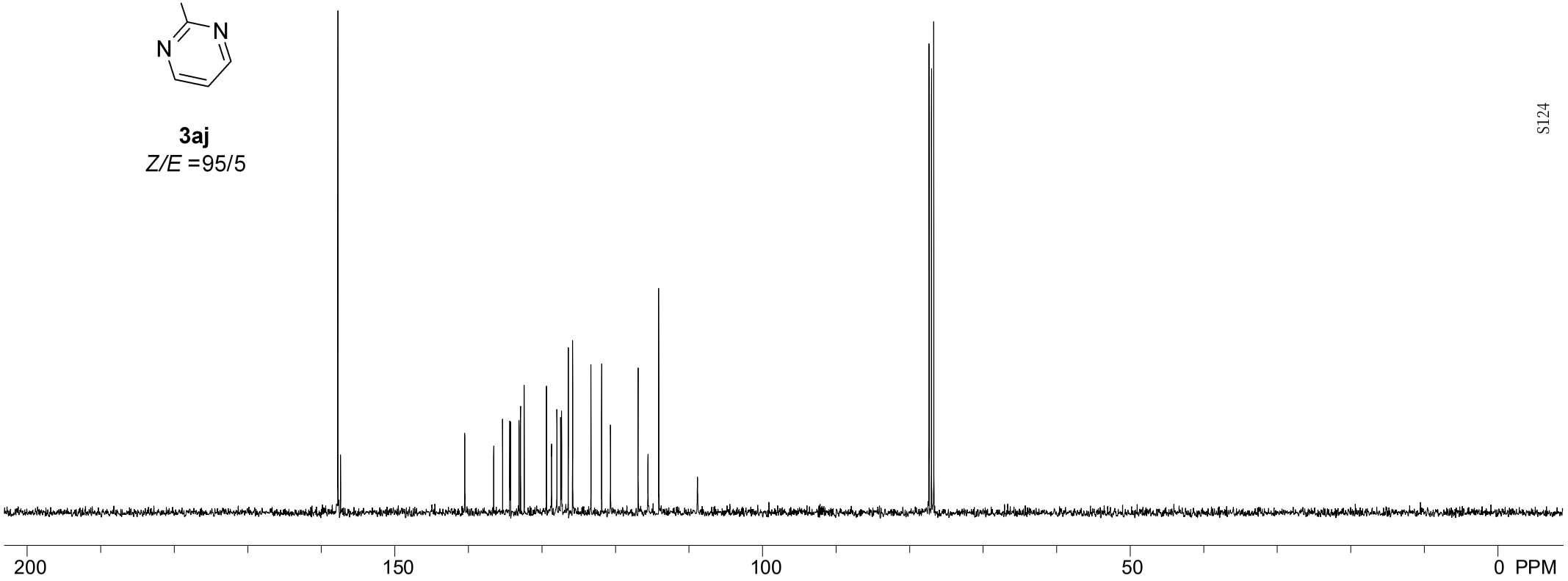


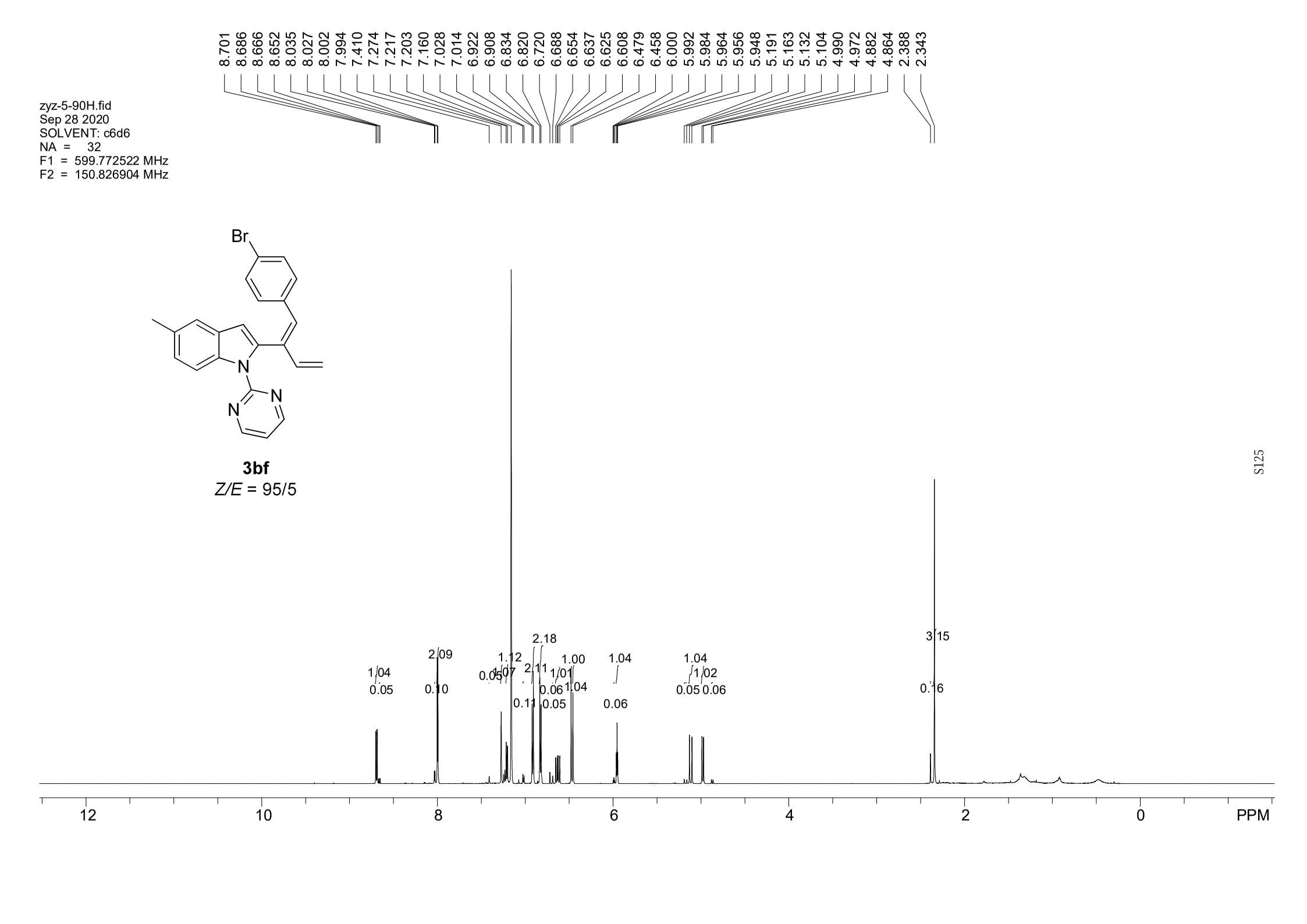
zyz-5-123C.fid
Sep 22 2019
SOLVENT: cdcl3
NA = 160
F1 = 100.520737 MHz
F2 = 399.722015 MHz

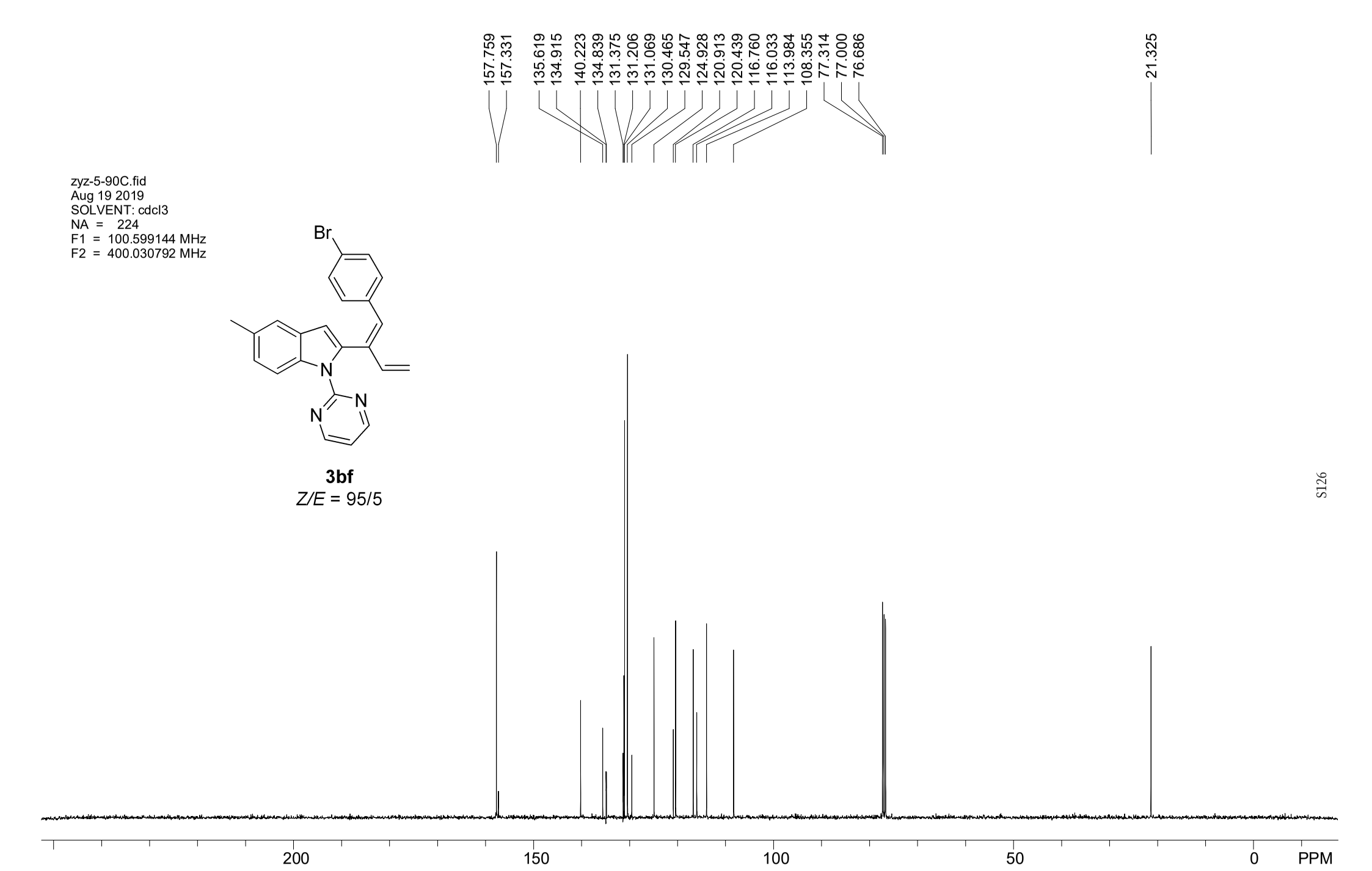
157.760
157.385
136.560
135.351
134.386
134.271
140.501
133.116
132.909
132.412
129.381
128.692
127.965
127.452
127.322
126.411
125.822
123.327
121.880
120.671
116.921
115.574
114.112
108.831
77.321
77.000
76.686

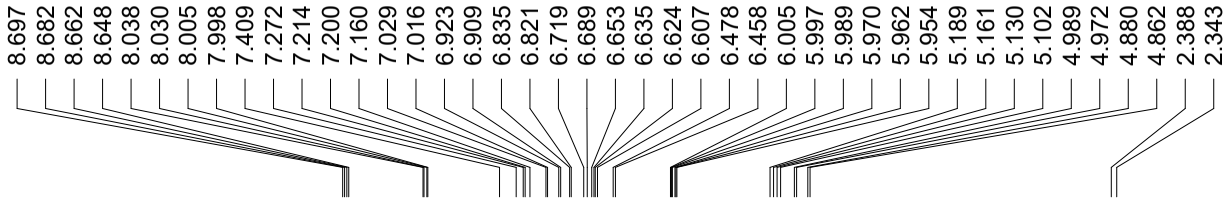


3aj
Z/E =95/5

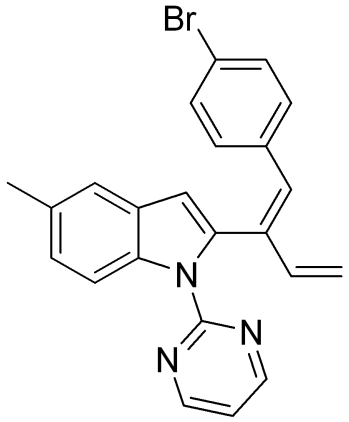



8.701
8.686
8.666
8.652
8.035
8.027
8.002
7.994
7.410
7.274
7.217
7.203
7.160
7.028
7.014
6.922
6.908
6.834
6.820
6.720
6.688
6.654
6.637
6.625
6.608
6.479
6.458
6.000
5.992
5.984
5.964
5.956
5.948
5.191
5.163
5.132
5.104
4.990
4.972
4.882
4.864
2.388
2.343
zyz-5-90H.fid
Sep 28 2020
SOLVENT: c6d6
NA = 32
F1 = 599.772522 MHz
F2 = 150.826904 MHz
Br
N
N
N
3bf
Z/E = 95/5
S125
1.04
0.05
2.09
0.10
0.05
1.12
0.07
2.11
0.11
2.18
0.06
0.05
1.00
1.01
1.04
1.04
0.06
1.04
1.02
0.05
0.06
3.15
0.16
12
10
8
6
4
2
0
PPM

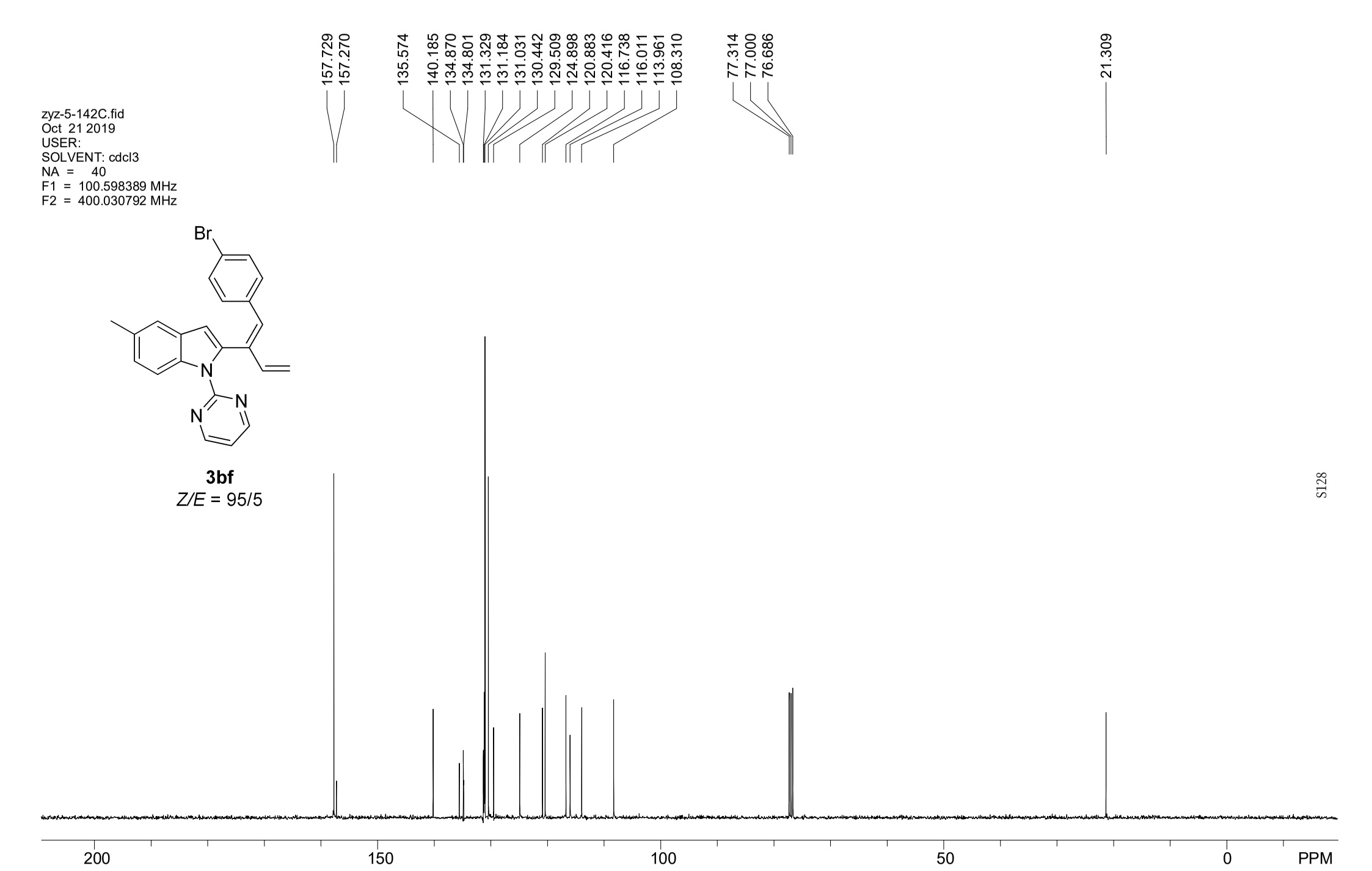

157.759
157.331
135.619
134.915
140.223
134.839
131.375
131.206
131.069
130.465
129.547
124.928
120.913
120.439
116.760
116.033
113.984
108.355
77.314
77.000
76.686
21.325
zyz-5-90C.fid
Aug 19 2019
SOLVENT: cdcl3
NA = 224
F1 = 100.599144 MHz
F2 = 400.030792 MHz
Br
N
N
N
3bf
Z/E = 95/5
S126
200
150
100
50
0
PPM

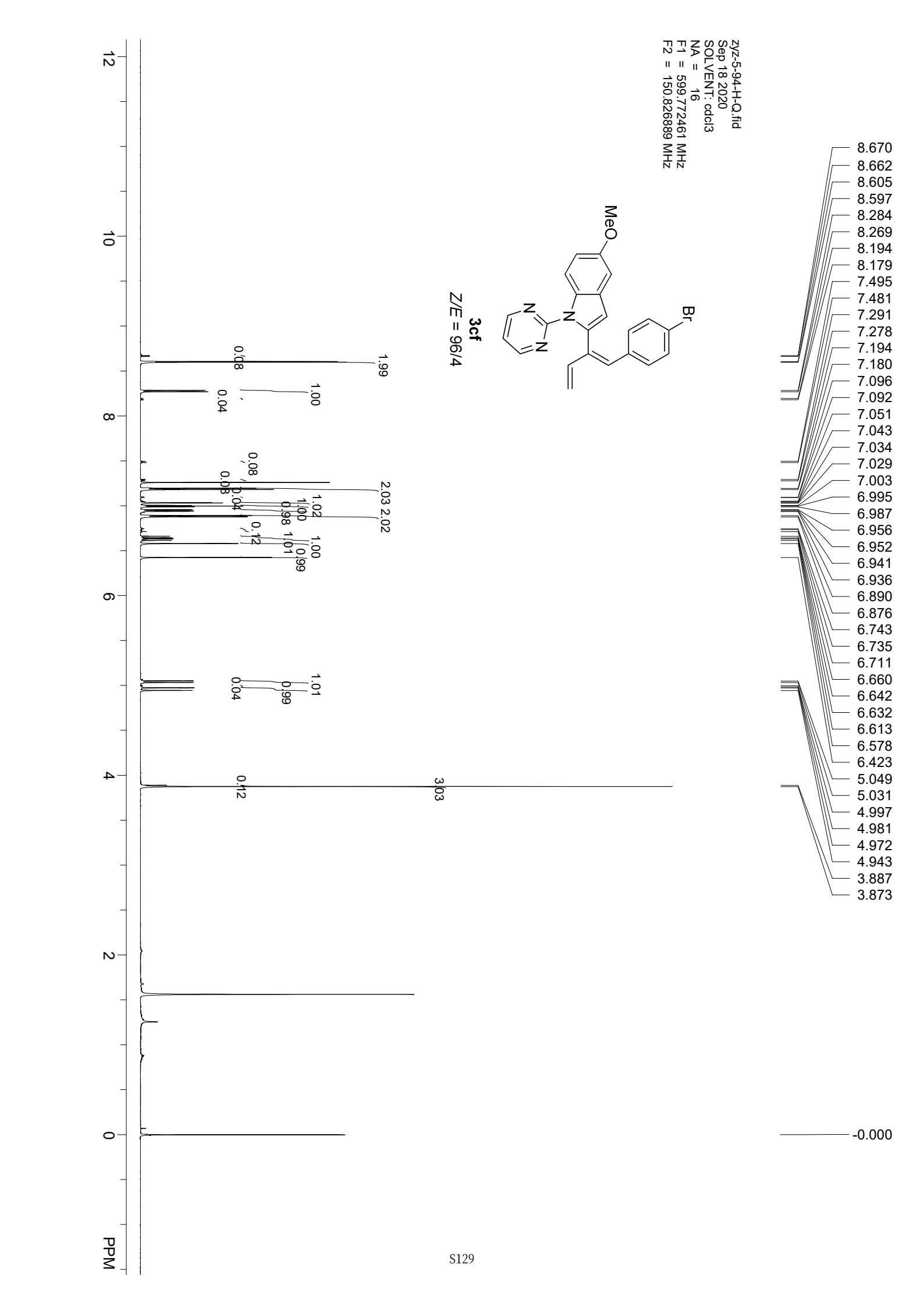


zyz-5-142H
Sep 15 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz



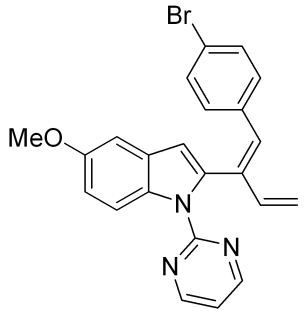
3bf
Z/E = 95/5


157.729
157.270
135.574
140.185
134.870
134.801
131.329
131.184
131.031
130.442
129.509
124.898
120.883
120.416
116.738
116.011
113.961
108.310
77.314
77.000
76.686
21.309
zyz-5-142C.fid
Oct 21 2019
USER:
SOLVENT: cdcl3
NA = 40
F1 = 100.598389 MHz
F2 = 400.030792 MHz
Br
N
N
N
3bf
Z/E = 95/5
S128
200
150
100
50
0
PPM


zyz-5-94-H-Q.fid
Sep 18 2020
SOLVENT: cdcl3
NA = 16
F1 = 599.772461 MHz
F2 = 150.826889 MHz
MeO
Br
N
N
N
3cf
Z/E = 96/4
8.670
8.662
8.605
8.597
8.284
8.269
8.194
8.179
7.495
7.481
7.291
7.278
7.194
7.180
7.096
7.092
7.051
7.043
7.034
7.029
7.003
6.995
6.987
6.956
6.952
6.941
6.936
6.890
6.876
6.743
6.735
6.711
6.660
6.642
6.632
6.613
6.578
6.423
5.049
5.031
4.997
4.981
4.972
4.943
3.887
3.873
-0.000
1.99
1.00
0.04
0.08
0.08
0.08
0.04
1.02
1.00
0.98
2.03
2.02
0.12
1.01
1.00
0.99
1.01
0.99
0.04
3.03
0.12
12
10
8
6
4
2
0
PPM

zyz-5-94C.fid
Aug 23 2019
NA = 320
Solvent = cdcl3
F1 = 100.598389 MHz
F2 = 400.030792 MHz

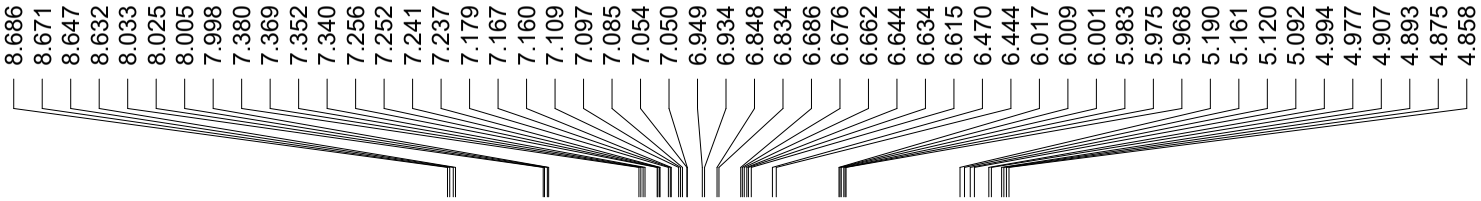
157.783
157.247
155.466
135.612
140.208
135.398
134.939
131.459
131.207
131.092
130.458
130.029
120.951
116.760
116.026
115.277
112.860
108.486
102.574
77.321
77.000
76.686
55.663



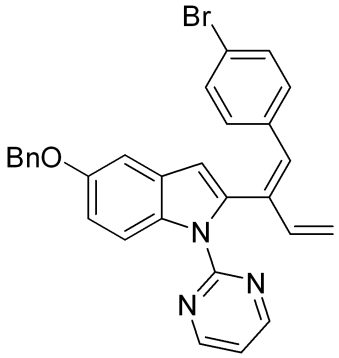
3cf
Z/E = 96/4

S130

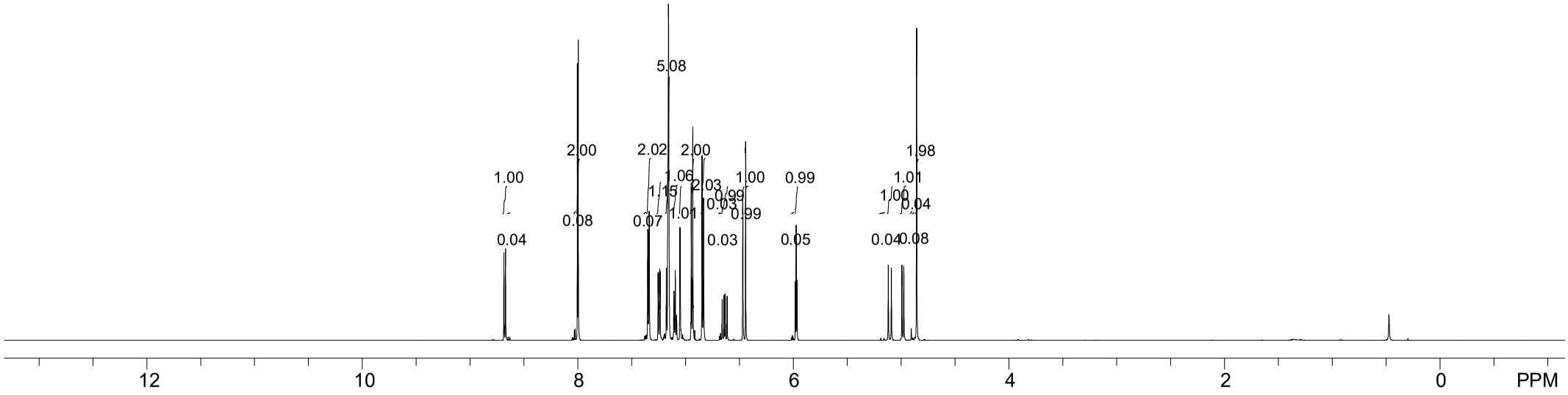
200 150 100 50 0 PPM

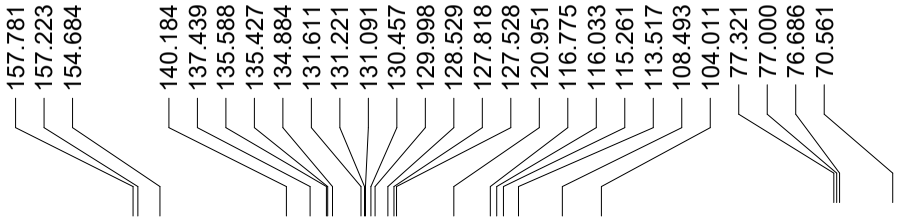


zyz-6-172-h-q.fid
Oct 16 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz

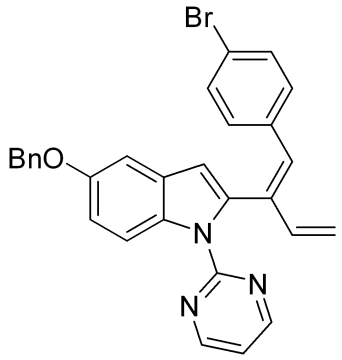


3df
Z/*E* = 96/4

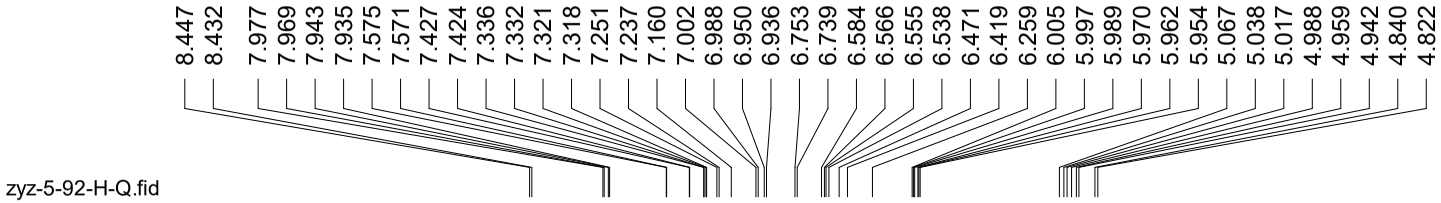




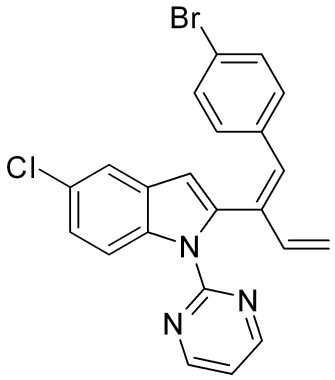
zyz-5-102C.fid
Sep 2 2019
SOLVENT: cdcl3
NA = 176
F1 = 100.597885 MHz
F2 = 400.030792 MHz



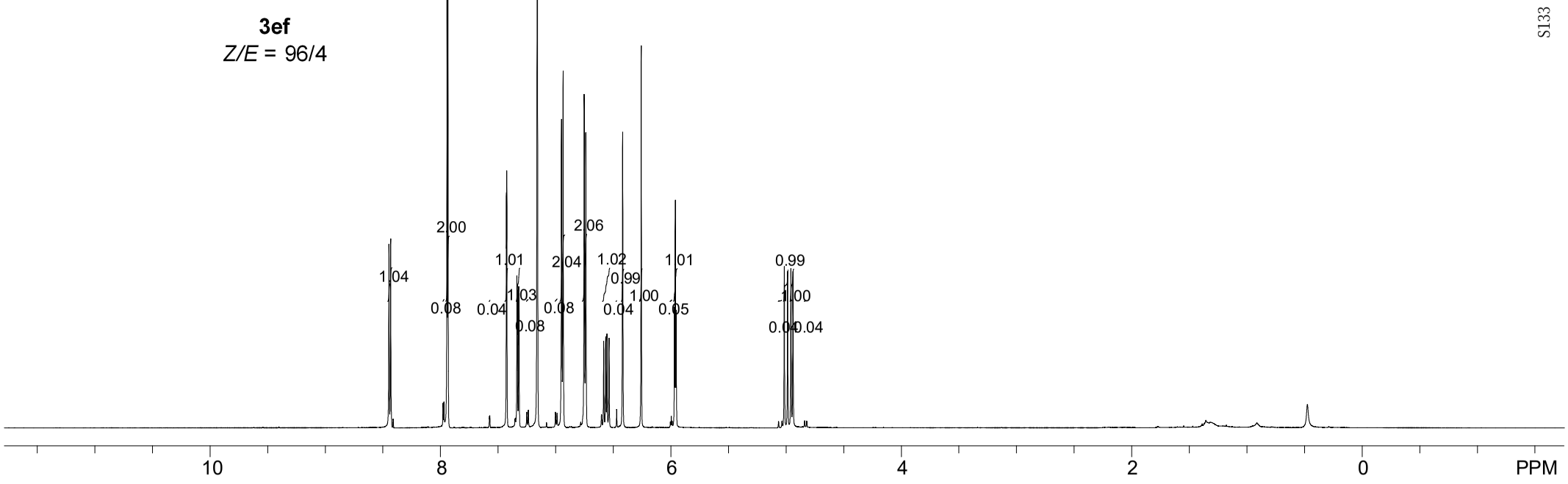
3df
Z/E = 96/4

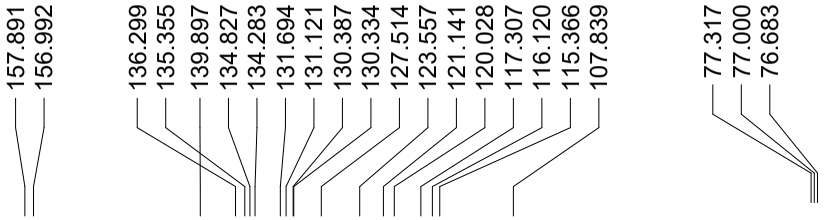


zyz-5-92-H-Q.fid
Sep 14 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz

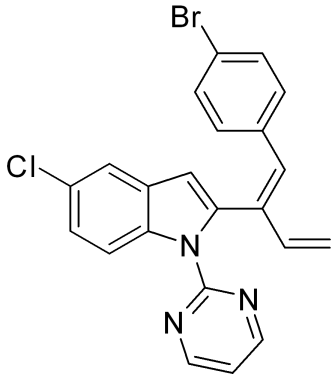


3ef
Z/E = 96/4



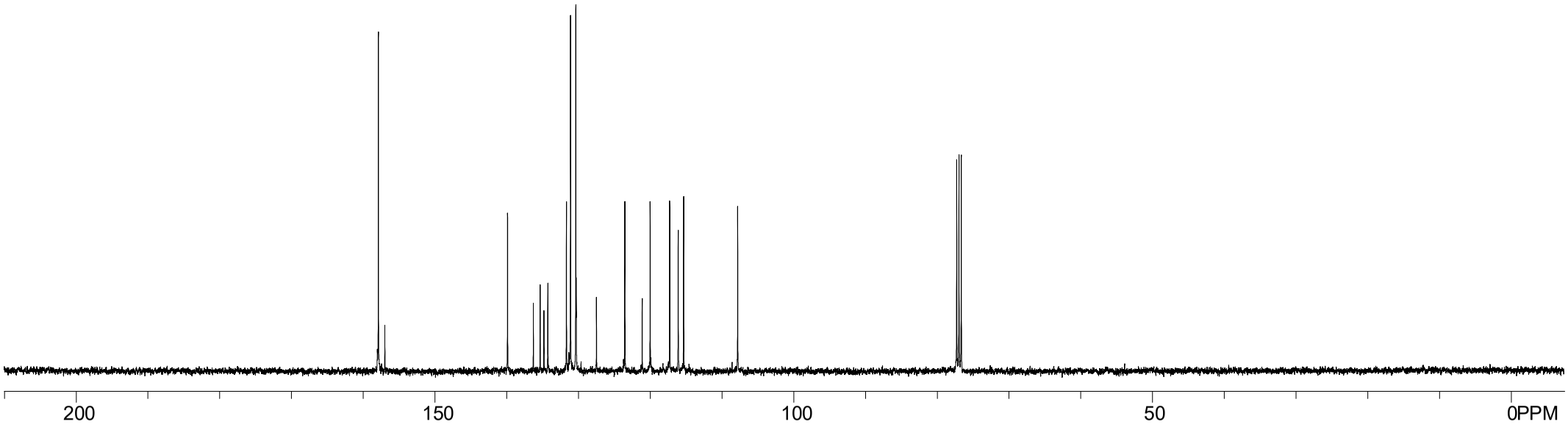


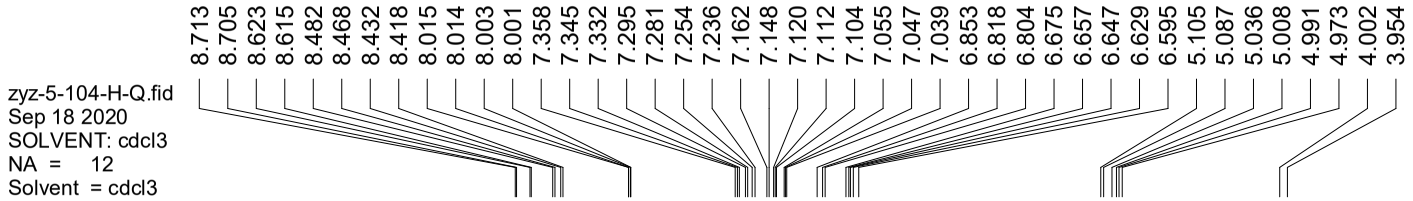
zyz-5-92C.fid
Aug 20 2019
SOLVENT: cdcl3
NA = 268
F1 = 100.599144 MHz
F2 = 400.030792 MHz



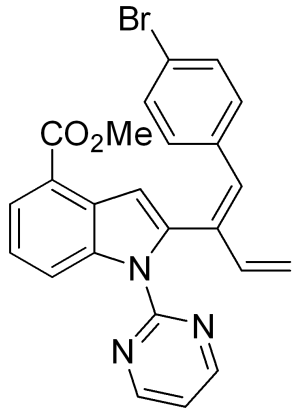
3ef

Z/E = 96/4



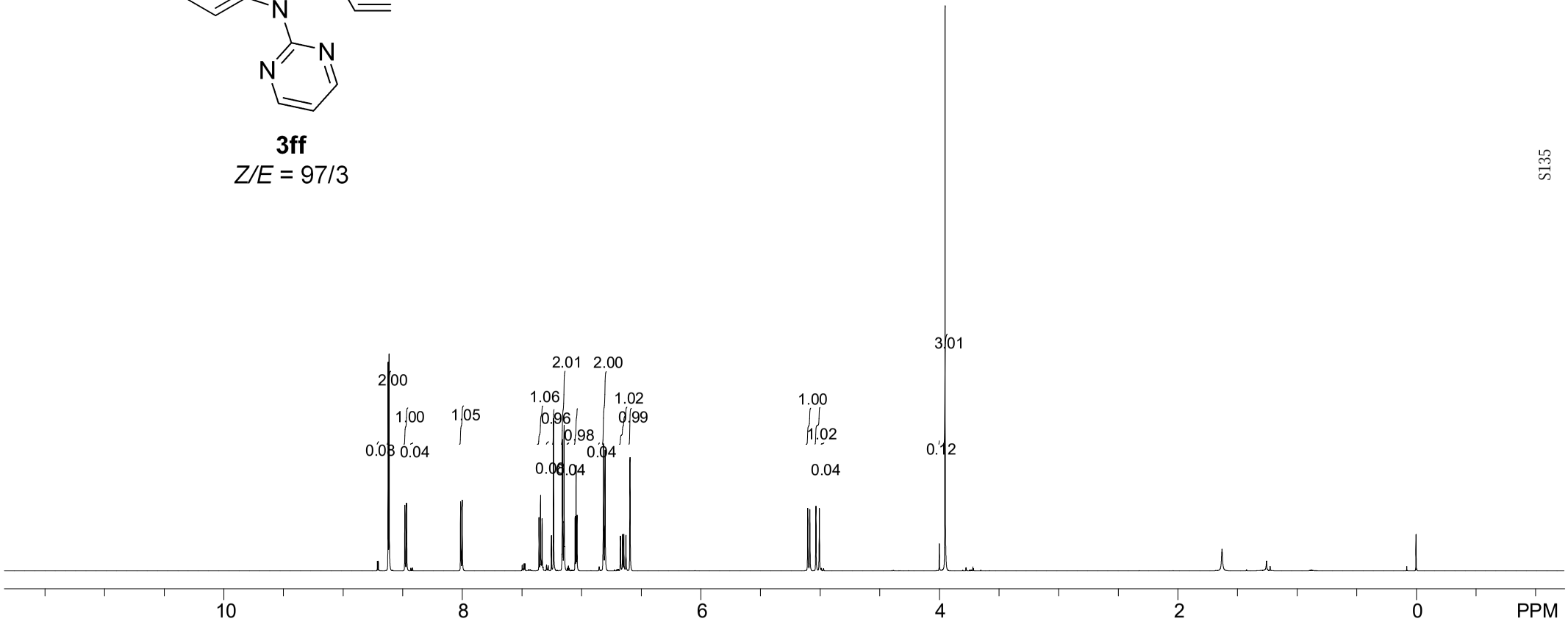


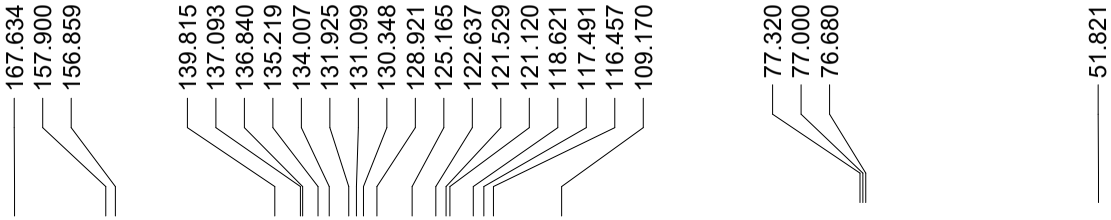
zyz-5-104-H-Q.fid
Sep 18 2020
SOLVENT: cdcl3
NA = 12
Solvent = cdcl3
F1 = 599.772461 MHz
F2 = 150.826889 MHz



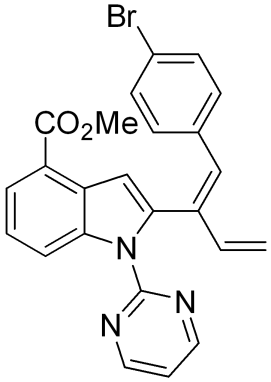
3ff

Z/E = 97/3



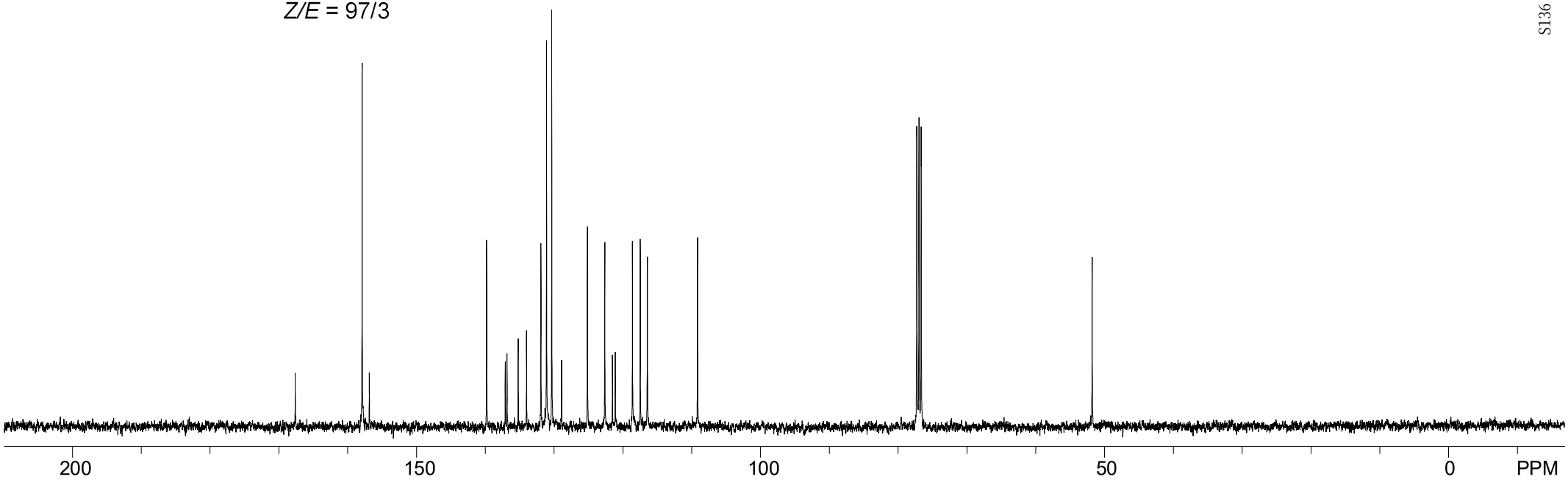


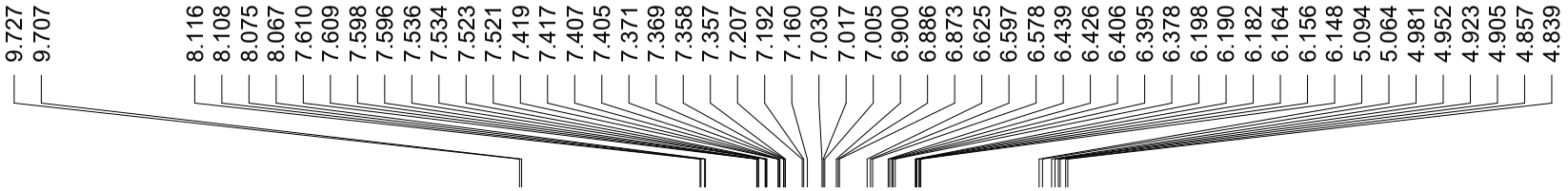
zyz-5-104C.fid
Sep 4 2019
SOLVENT: cdcl3
NA = 200
F1 = 100.597885 MHz
F2 = 400.030792 MHz



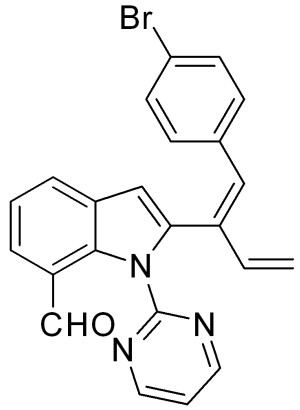
3ff

Z/E = 97/3

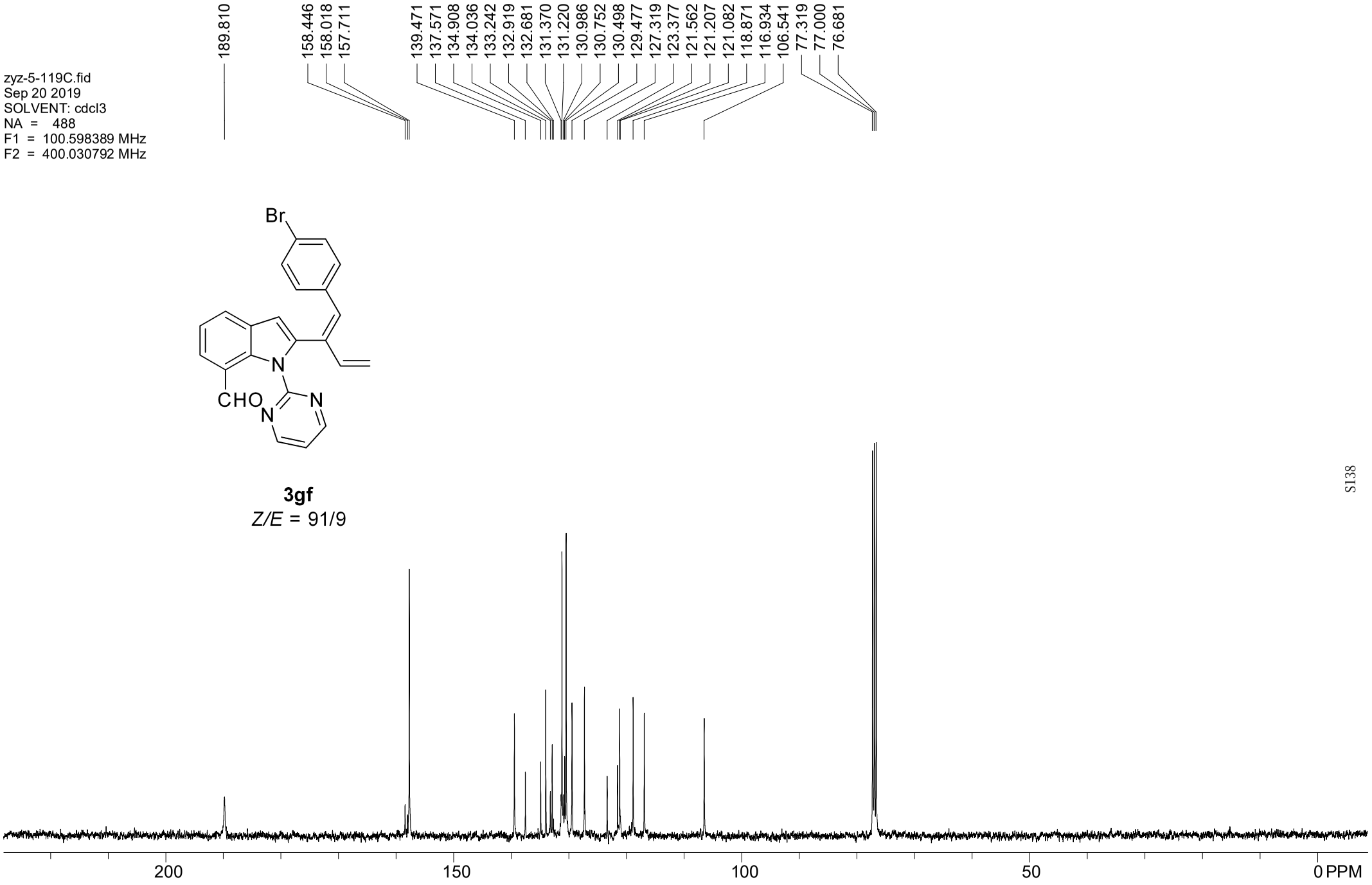


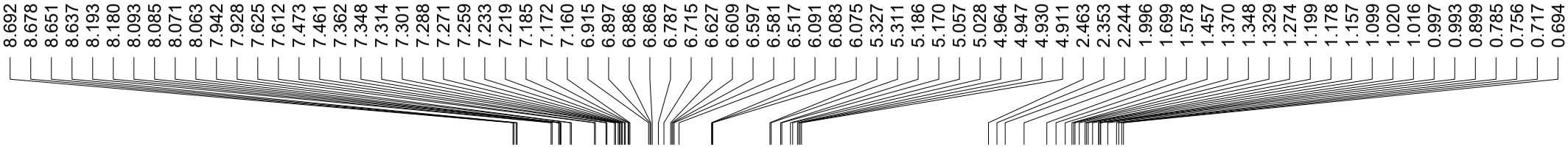


zyz-5-119-h-Q.fid
Sep 15 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz

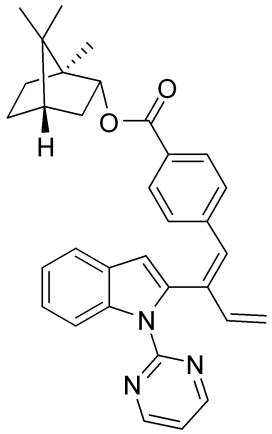


3gf
Z/E = 91/9

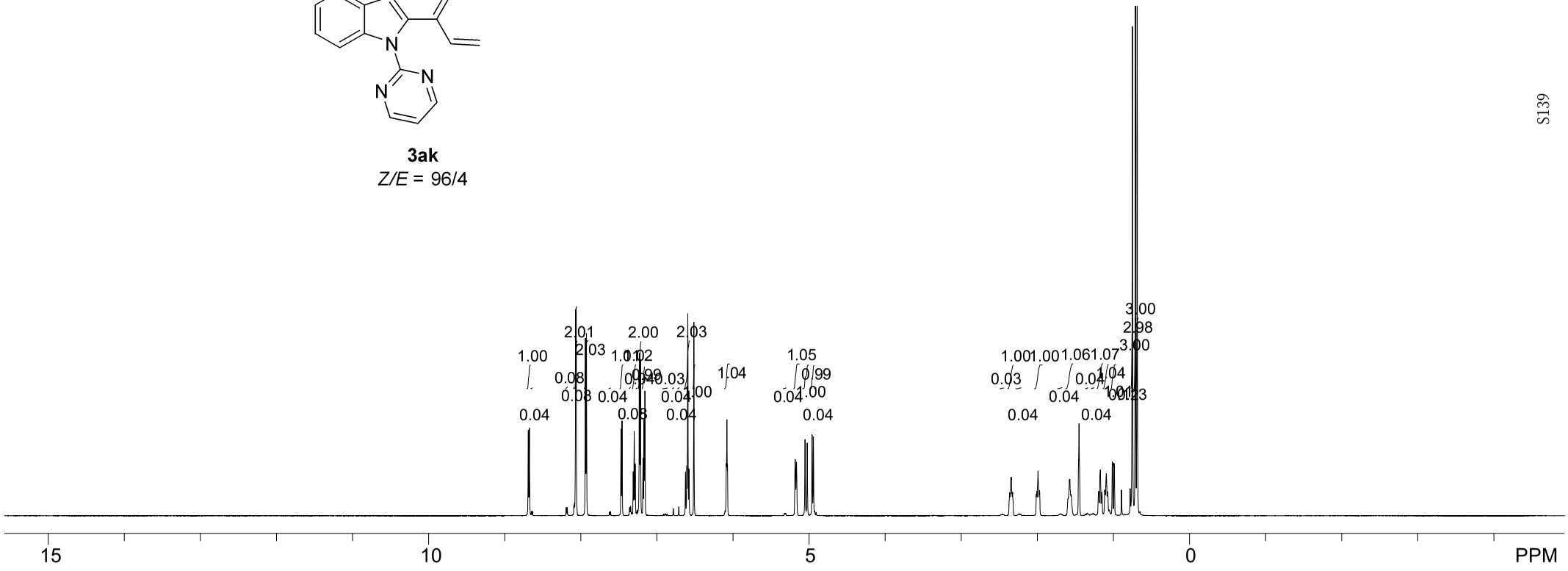

189.810
158.446
158.018
157.711
139.471
137.571
134.908
134.036
133.242
132.919
132.681
131.370
131.220
130.986
130.752
130.498
129.477
127.319
123.377
121.562
121.207
121.082
118.871
116.934
106.541
77.319
77.000
76.681
zyz-5-119C.fid
Sep 20 2019
SOLVENT: cdcl3
NA = 488
F1 = 100.598389 MHz
F2 = 400.030792 MHz
Br
N
CHO
N
N
3gf
Z/E = 91/9
S138
200
150
100
50
0 PPM

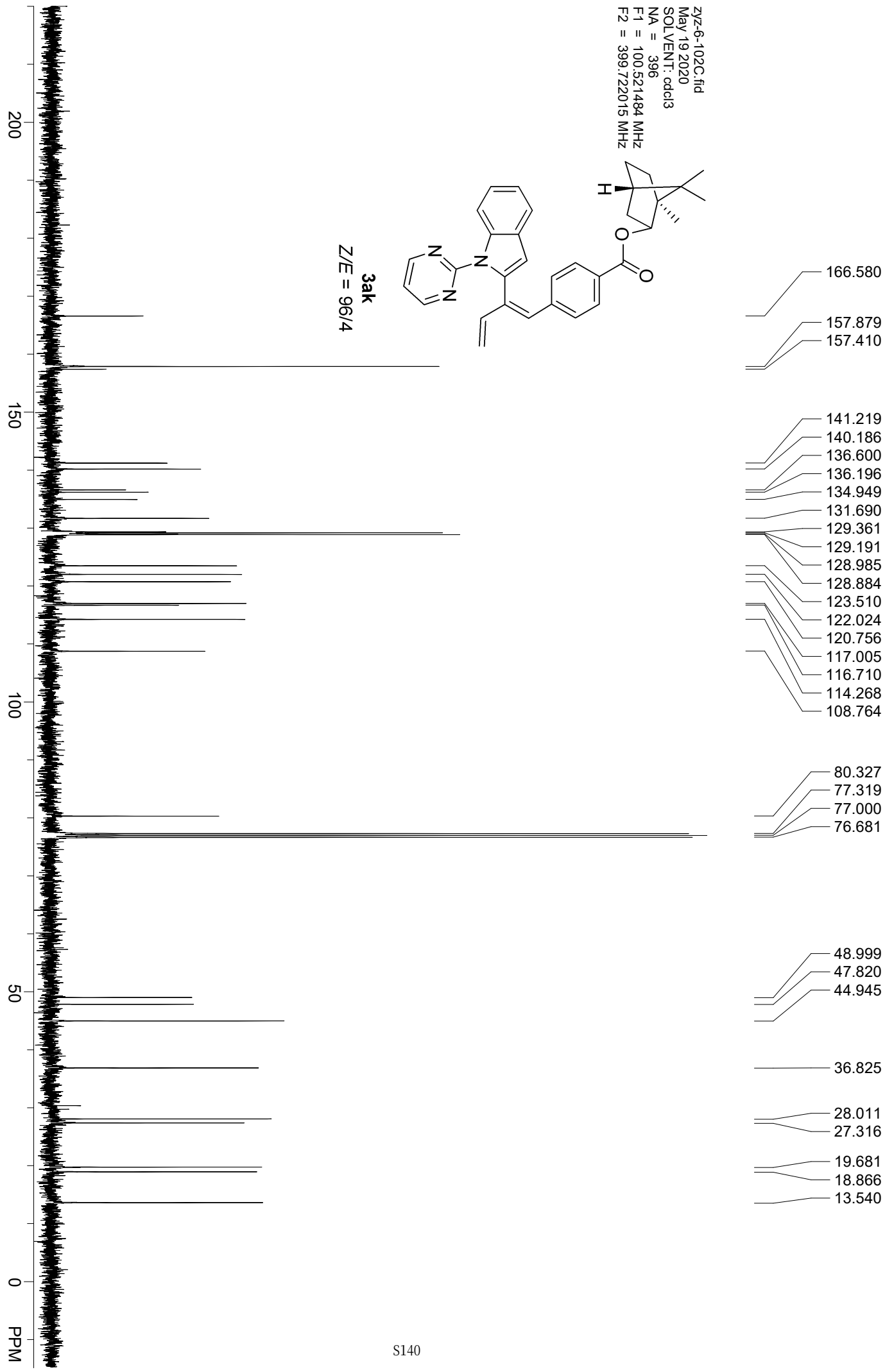


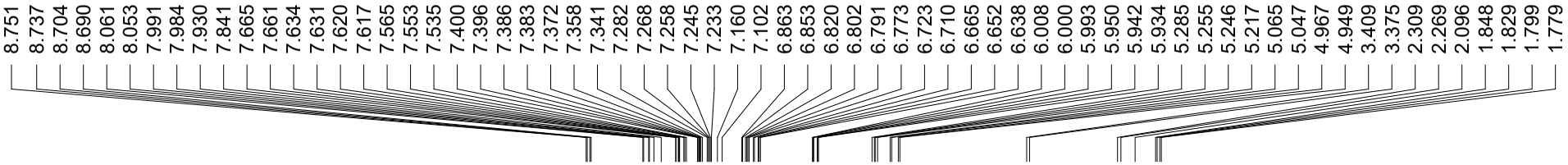
zyz-6-174-h-q.fid
Oct 16 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz



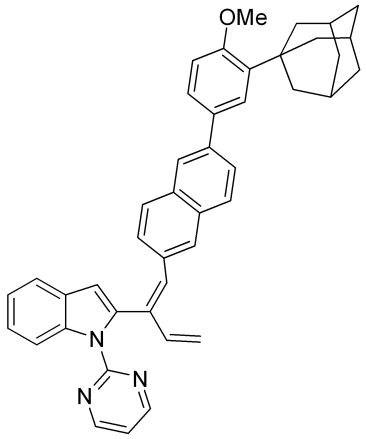
3ak
Z/E = 96/4



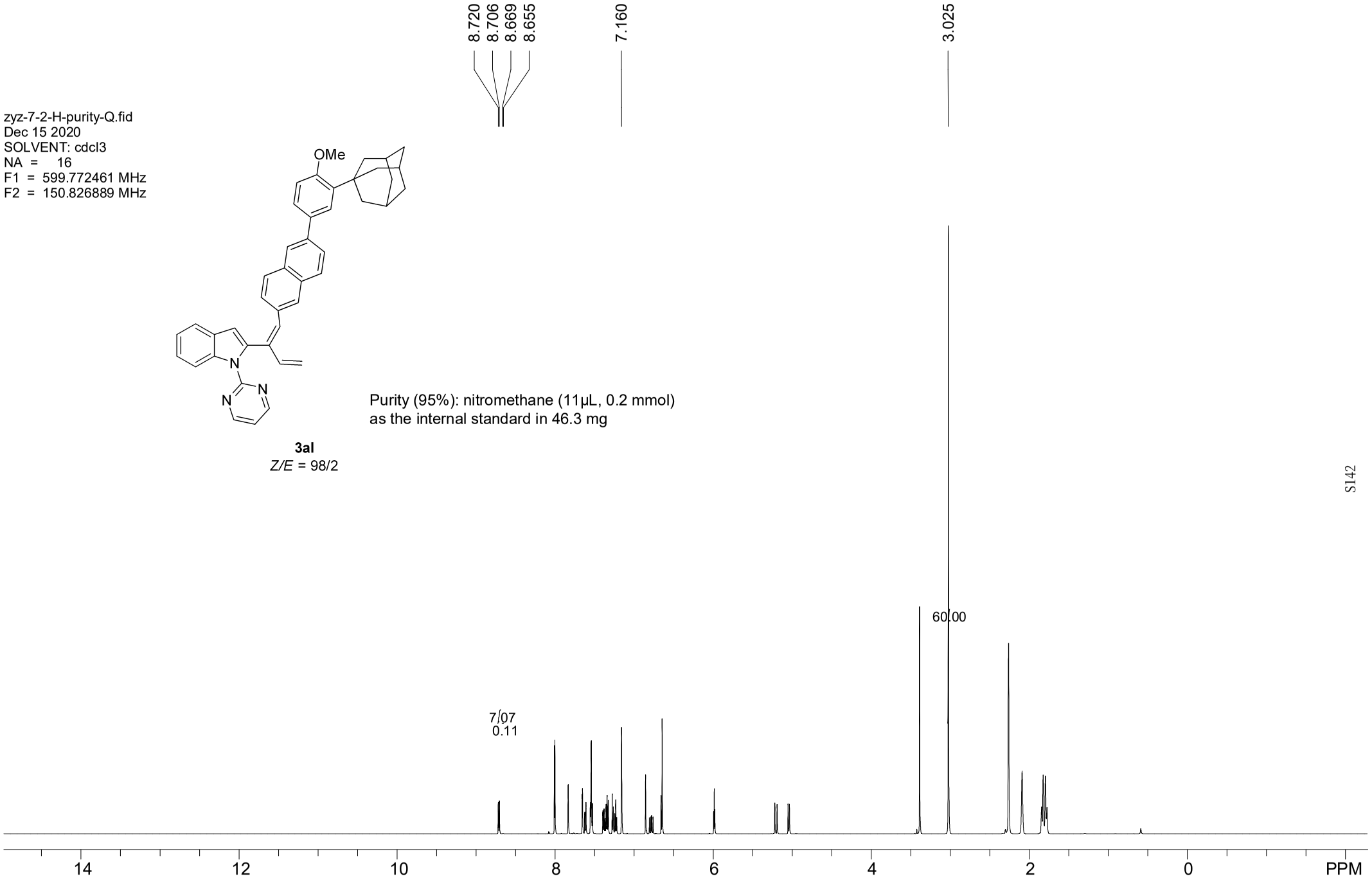

zyz-6-102C.fid
May 19 2020
SOLVENT: cdcl3
NA = 396
F1 = 100.521484 MHz
F2 = 399.722015 MHz
3ak
Z/E = 96/4
166.580
157.879
157.410
141.219
140.186
136.600
136.196
134.949
131.690
129.361
129.191
128.985
128.884
123.510
122.024
120.756
117.005
116.710
114.268
108.764
80.327
77.319
77.000
76.681
48.999
47.820
44.945
36.825
28.011
27.316
19.681
18.866
13.540
200
150
100
50
0
PPM

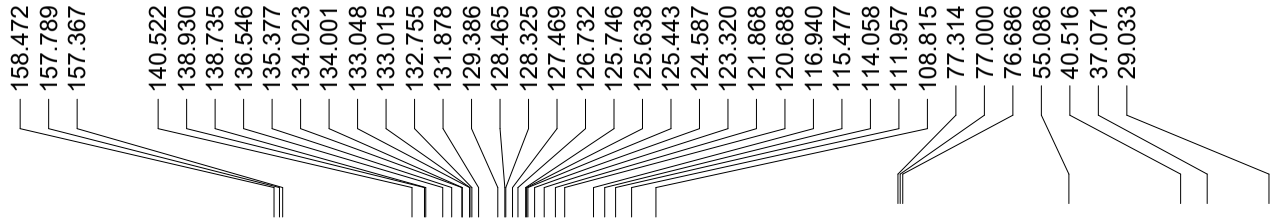


zyz-7-2-H-Q.fid
Dec 15 2020
SOLVENT: cdcl3
NA = 16
F1 = 599.772461 MHz
F2 = 150.826889 MHz

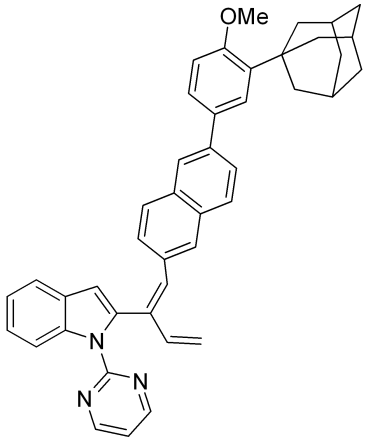


3al
Z/*E* = 98/2

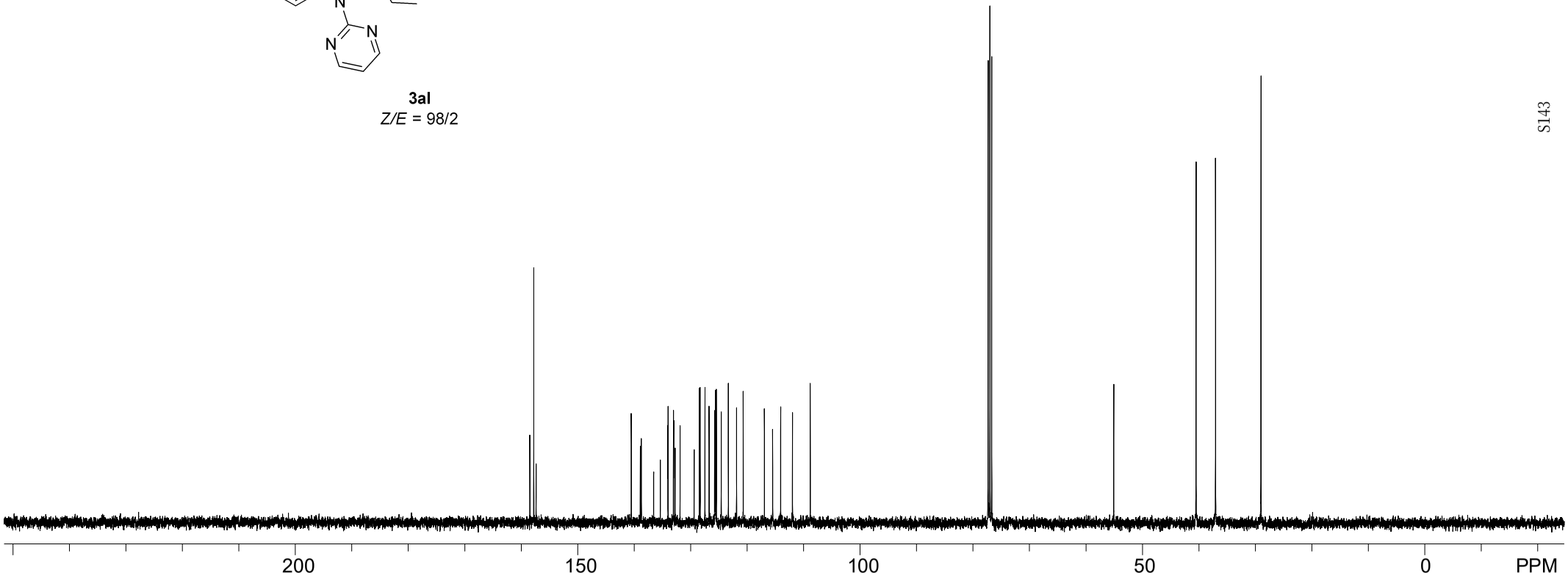

8.720
8.706
8.669
8.655
7.160
3.025
zyz-7-2-H-purity-Q.fid
Dec 15 2020
SOLVENT: cdcl3
NA = 16
F1 = 599.772461 MHz
F2 = 150.826889 MHz
OMe
N
N
N
Purity (95%): nitromethane (11μL, 0.2 mmol)
as the internal standard in 46.3 mg
3al
Z/E = 98/2
S142
60.00
7.07
0.11
14
12
10
8
6
4
2
0
PPM



zyz-7-2C
NA = 151
Solvent = CDCl3
F1 = 100.630371 MHz
F2 = 1.000000 MHz

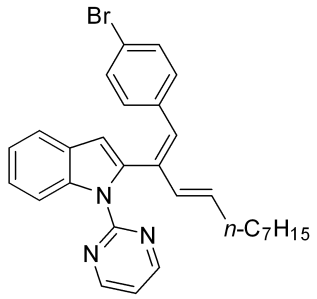


3al
Z/*E* = 98/2

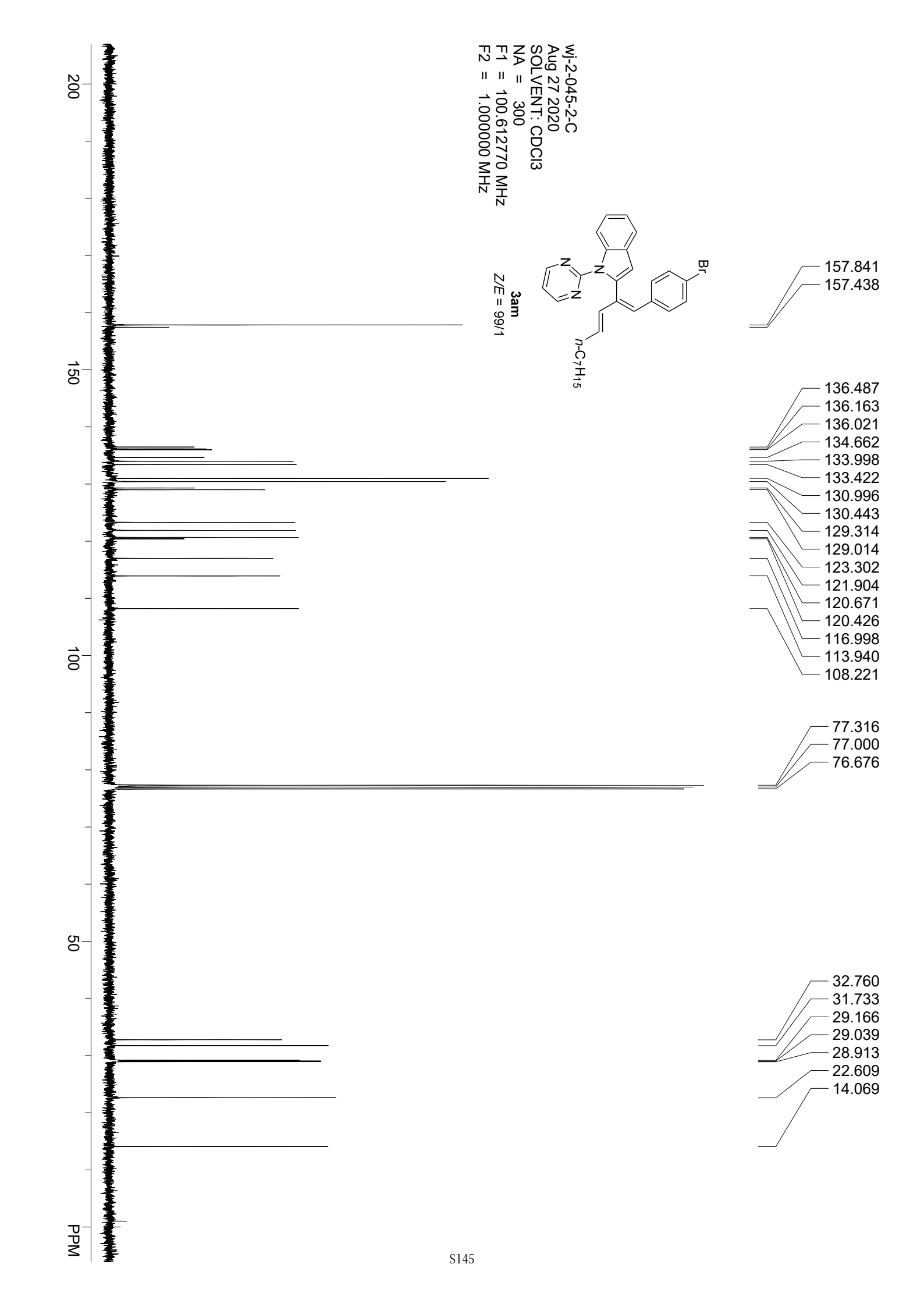


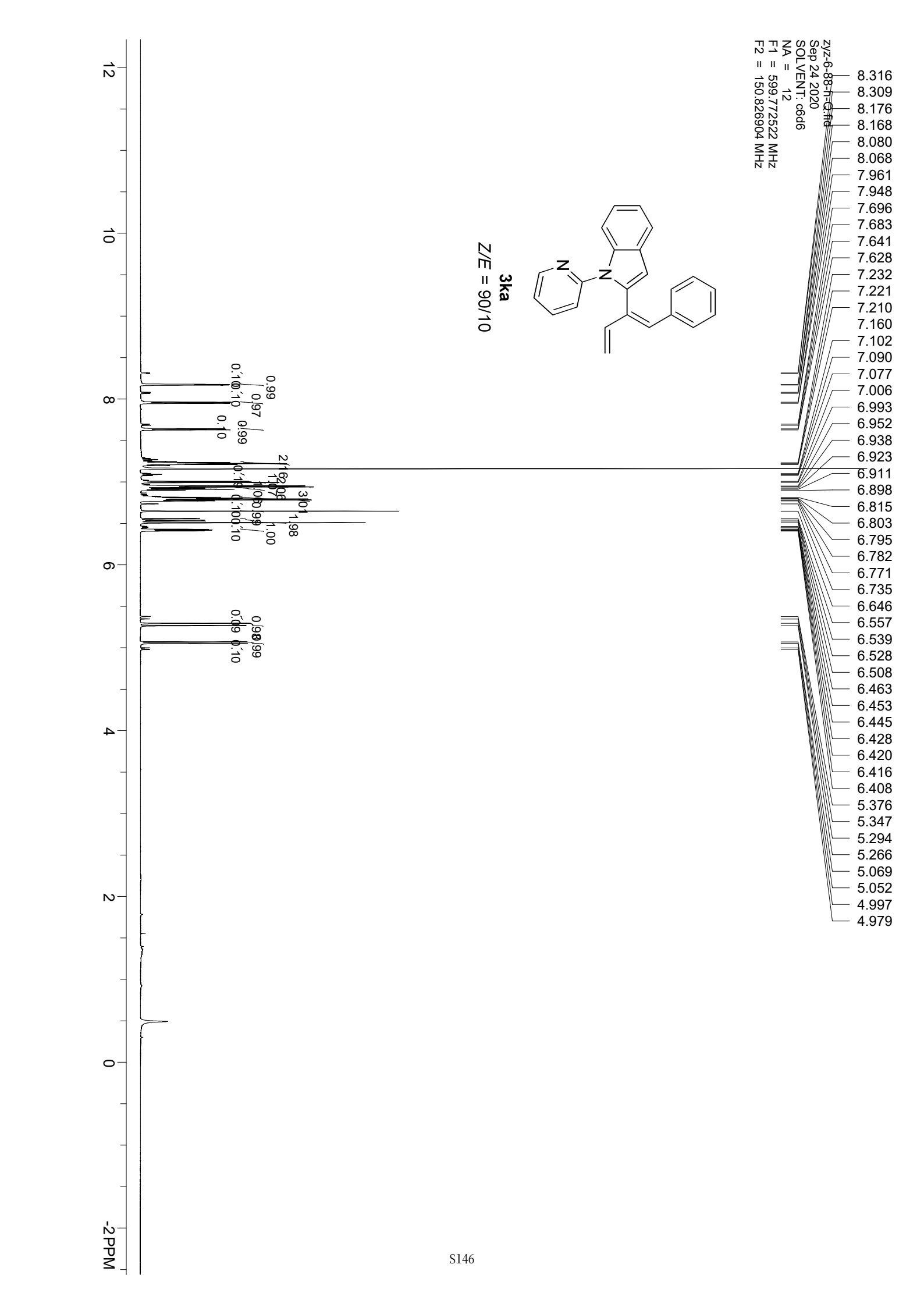
wj-2-45-H-Q.fid
Sep 21 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz

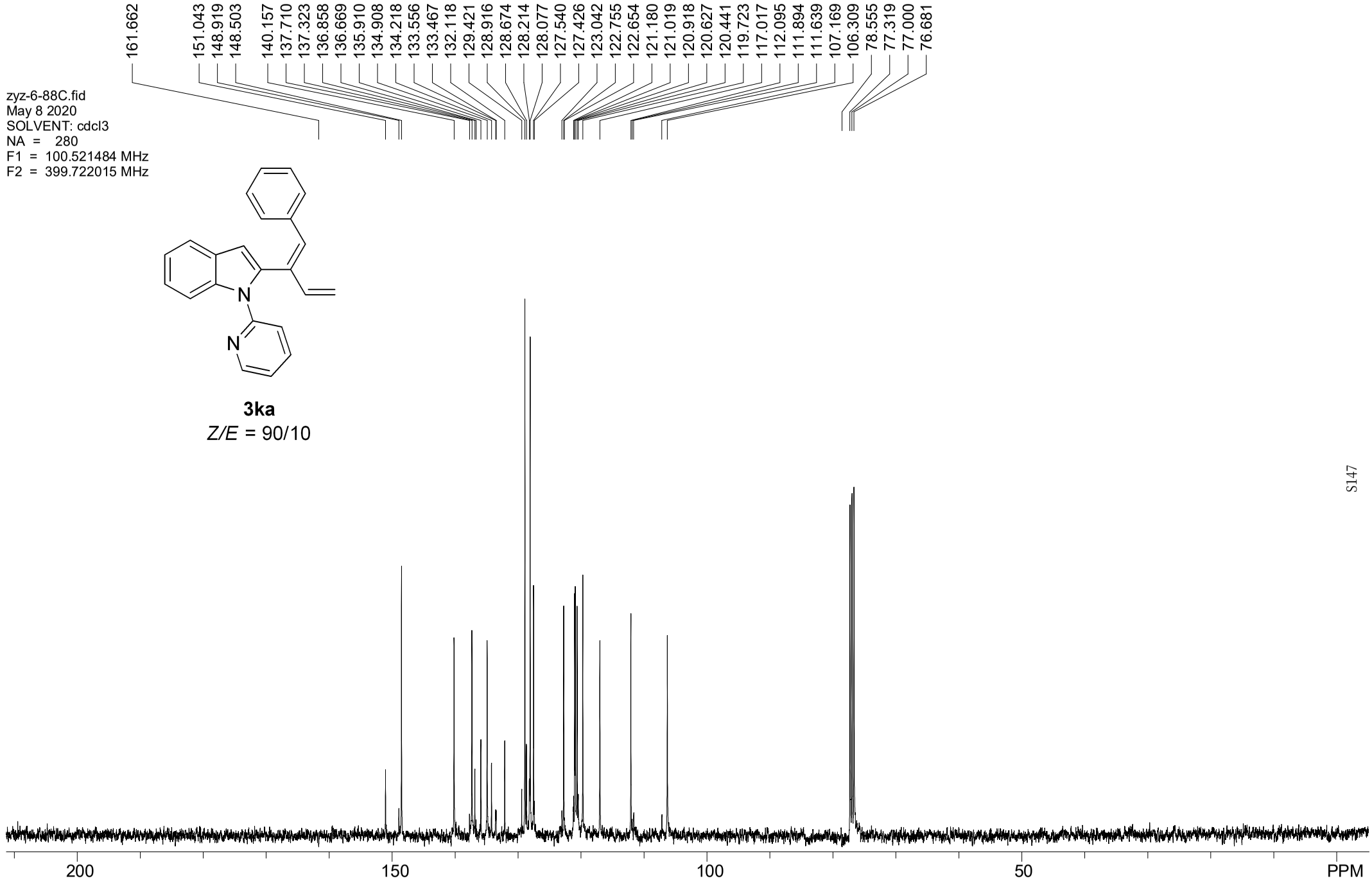
8.707 8.693 8.659 8.645 8.084 8.076 8.051 8.043 7.524 7.511 7.348 7.346 7.335 7.323 7.321 7.223 7.221 7.209 7.197 7.196 7.160 6.943 6.928 6.894 6.880 6.684 6.615 6.587 6.547 6.515 6.472 6.390 6.364 6.064 6.056 6.048 6.030 6.022 6.014 5.601 5.589 5.577 5.564 5.552 1.903 1.893 1.261 1.250 1.238 1.226 1.163 1.158 1.152 1.143 1.139 1.133 1.048 0.896 0.884 0.872



3am
Z/E = 99/1

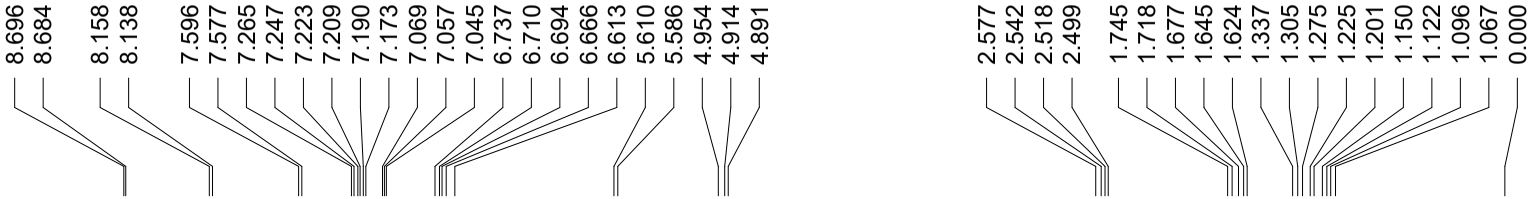

wj-2-045-2-C
Aug 27 2020
SOLVENT: CDCl3
NA = 300
F1 = 100.612770 MHz
F2 = 1.000000 MHz
3am
Z/E = 99/1
Br
n-C7H15
157.841
157.438
136.487
136.163
136.021
134.662
133.998
133.422
130.996
130.443
129.314
129.014
123.302
121.904
120.671
120.426
116.998
113.940
108.221
77.316
77.000
76.676
32.760
31.733
29.166
29.039
28.913
22.609
14.069
200
150
100
50
PPM


zyz-6-88-h-C.fid
Sep 24 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz
8.316
8.309
8.176
8.168
8.080
8.068
7.961
7.948
7.696
7.683
7.641
7.628
7.232
7.221
7.210
7.160
7.102
7.090
7.077
7.006
6.993
6.952
6.938
6.923
6.911
6.898
6.815
6.803
6.795
6.782
6.771
6.735
6.646
6.557
6.539
6.528
6.508
6.463
6.453
6.445
6.428
6.420
6.416
6.408
5.376
5.347
5.294
5.266
5.069
5.052
4.997
4.979
3ka
Z/E = 90/10
12
10
8
6
4
2
0
-2 PPM

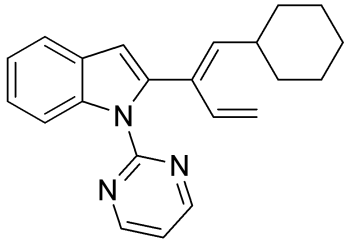

161.662
151.043
148.919
148.503
140.157
137.710
137.323
136.858
136.669
135.910
134.908
134.218
133.556
133.467
132.118
129.421
128.916
128.674
128.214
128.077
127.540
127.426
123.042
122.755
122.654
121.180
121.019
120.918
120.627
120.441
119.723
117.017
112.095
111.894
111.639
107.169
106.309
78.555
77.319
77.000
76.681
zyz-6-88C.fid
May 8 2020
SOLVENT: cdcl3
NA = 280
F1 = 100.521484 MHz
F2 = 399.722015 MHz
N
N
200
150
100
50
PPM

3ka

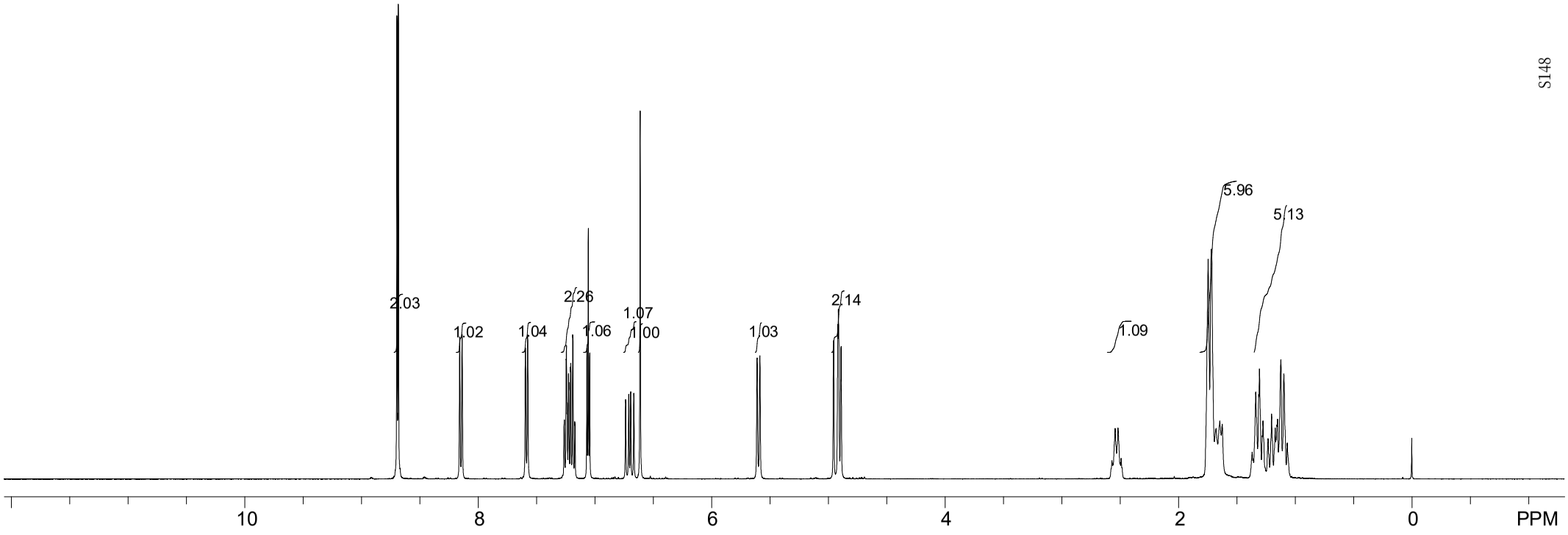
Z/E = 90/10

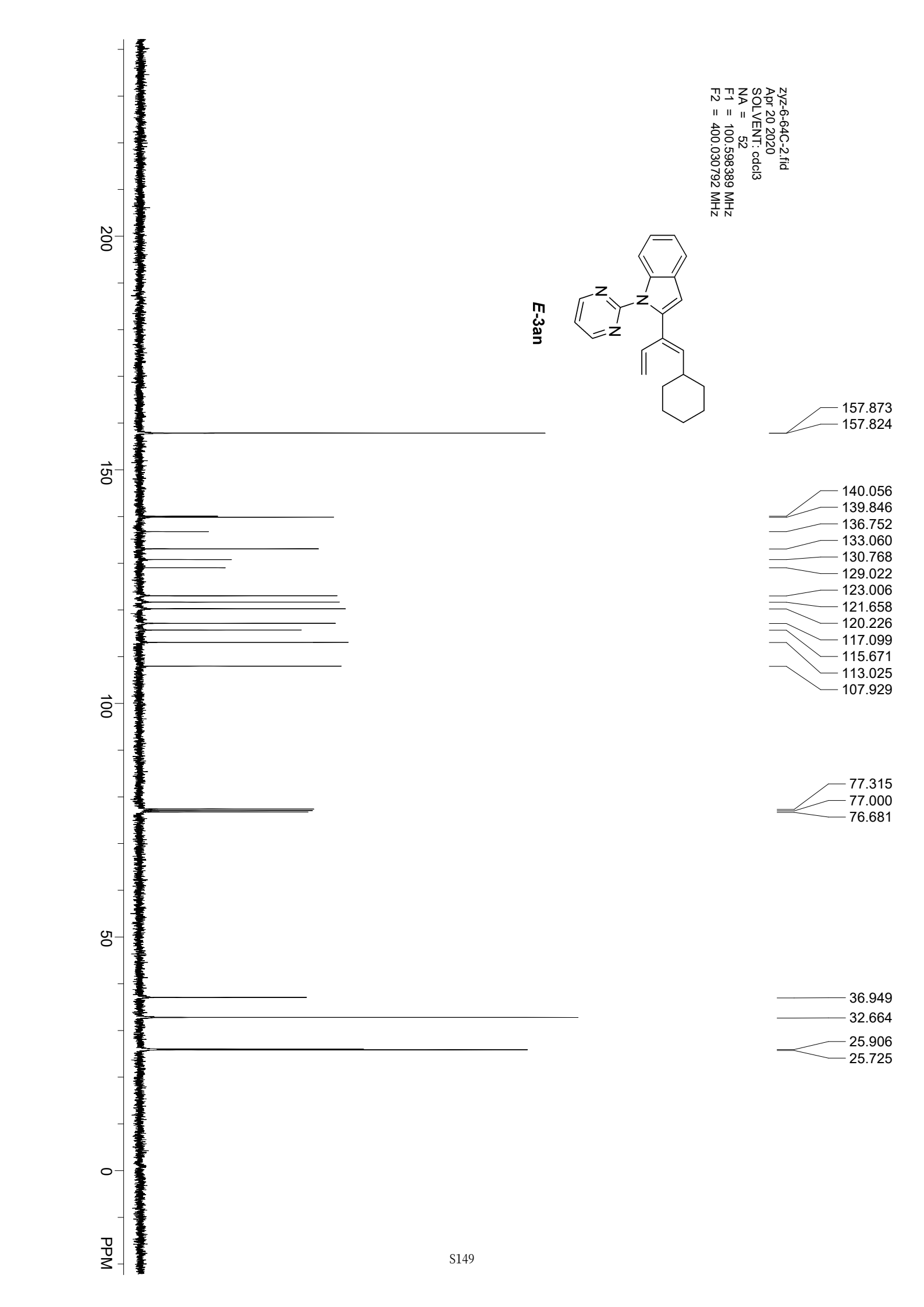


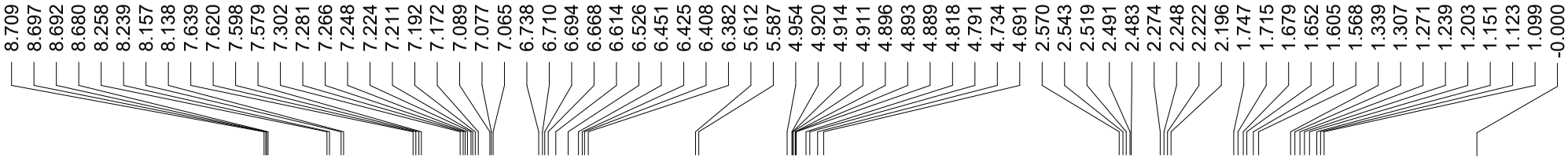
zyz-6-64H-2.fid
Apr 20 2020
SOLVENT: CDCl3
NA = 8
F1 = 399.722809 MHz
F2 = 100.519203 MHz



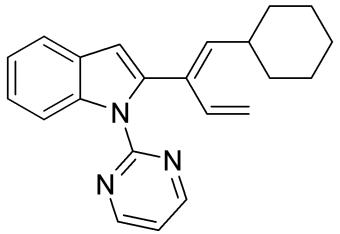
***E*-3an**



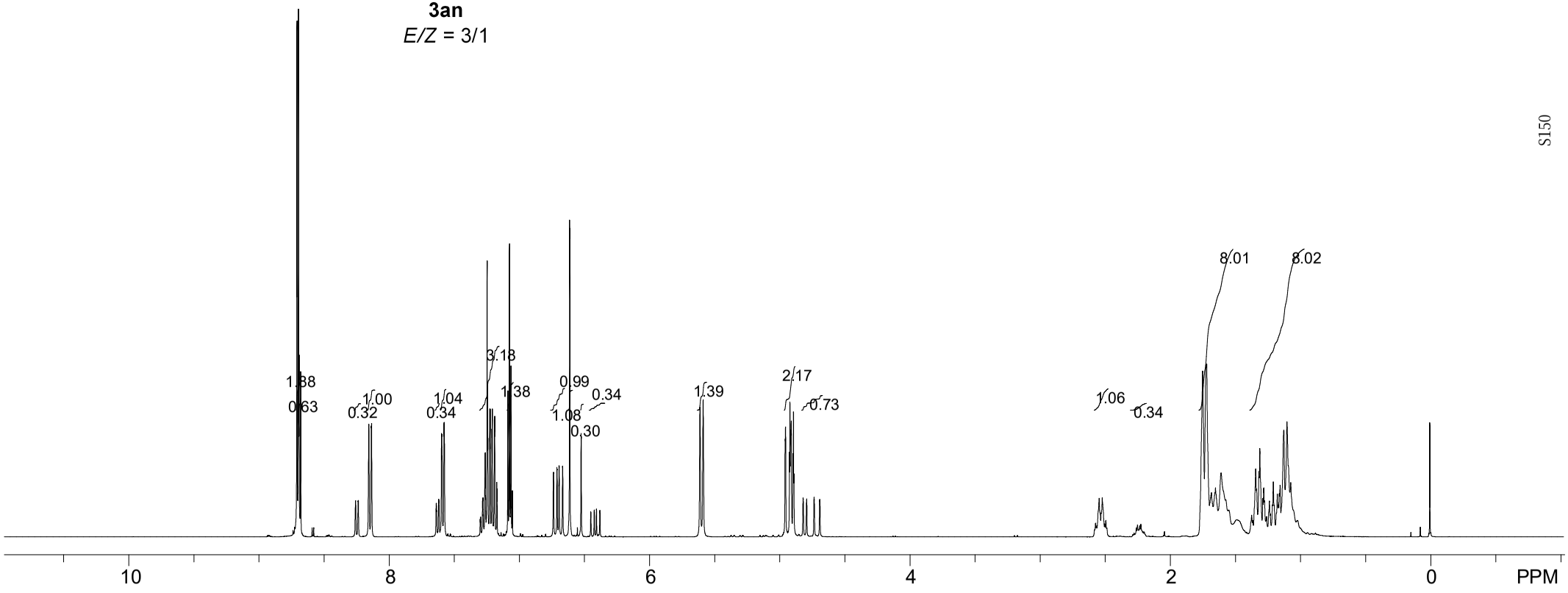

zyz-6-64C-2.fid
Apr 20 2020
SOLVENT: cdcl3
NA = 52
F1 = 100.598389 MHz
F2 = 400.030792 MHz
E-3an
N
N
N
157.873
157.824
140.056
139.846
136.752
133.060
130.768
129.022
123.006
121.658
120.226
117.099
115.671
113.025
107.929
77.315
77.000
76.681
36.949
32.664
25.906
25.725
200
150
100
50
0
PPM



zyz-6-64H-1
USER: nmr
SOLVENT: CDCl3
NA = 16
F1 = 400.100006 MHz
F2 = 1.000000 MHz

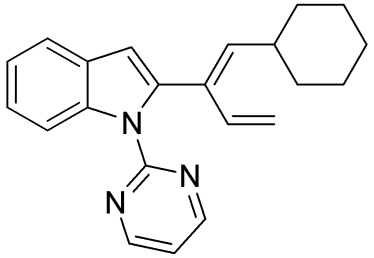


3an
E/Z = 3/1



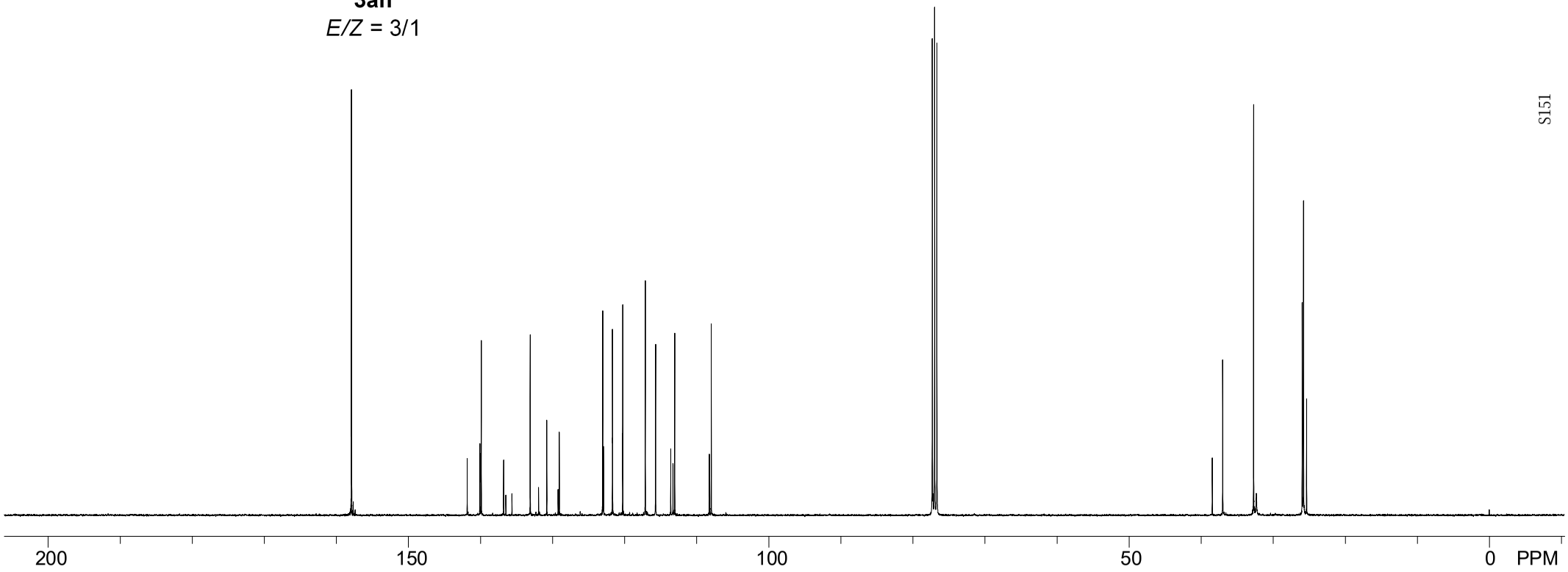
zyz-6-64C-1
USER: nmr
SOLVENT: CDCl3
NA = 14990
F1 = 100.605225 MHz
F2 = 1.000000 MHz

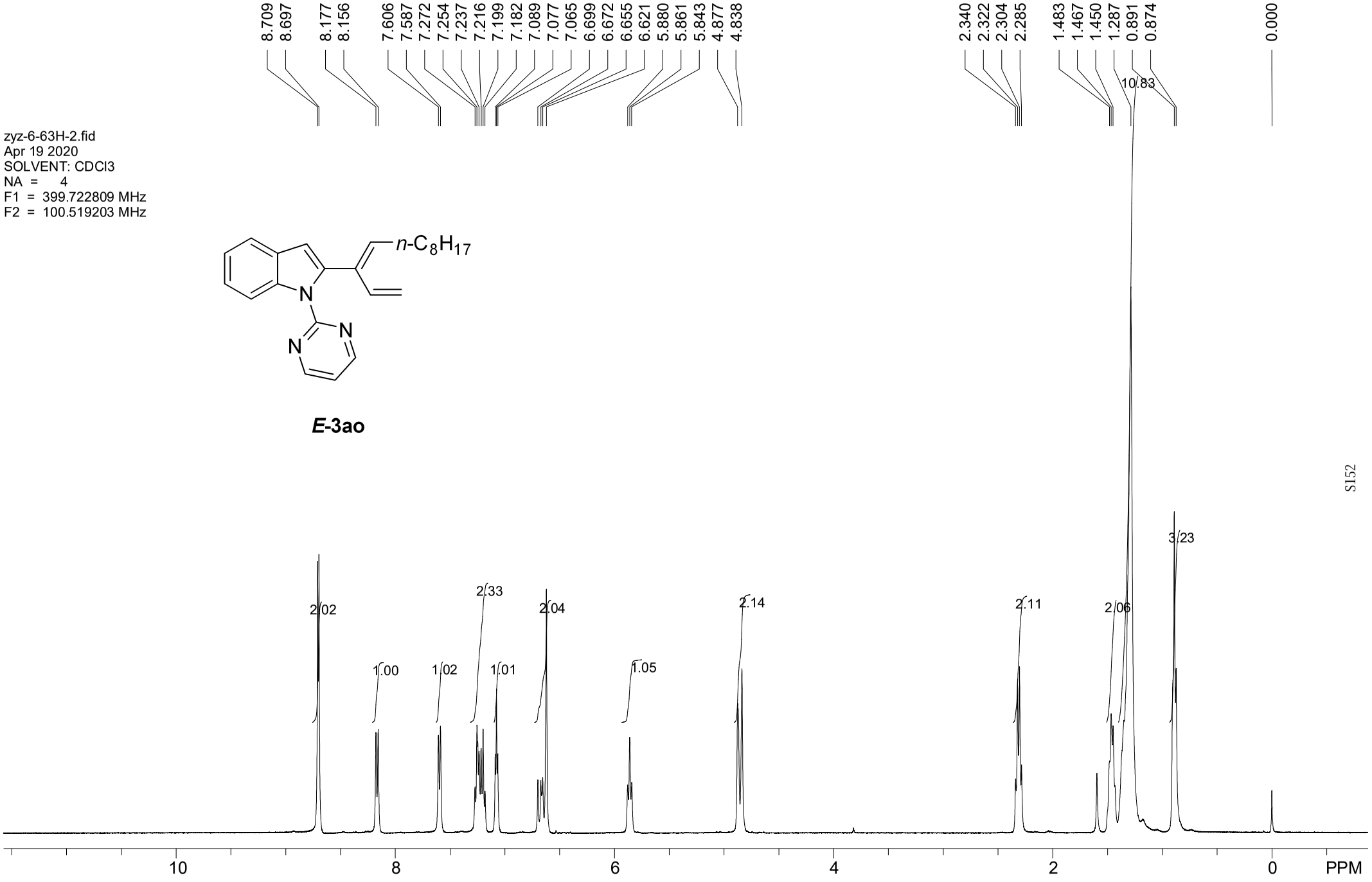
157.925
157.887
157.672
157.412
141.852
140.105
140.074
139.898
136.795
136.489
135.646
133.110
131.946
130.812
129.242
129.073
123.051
122.936
121.695
121.672
120.293
120.270
117.137
115.712
113.613
113.299
113.053
108.250
107.989
77.314
77.000
76.678
38.434
36.986
32.695
25.946
25.754
25.333



3an

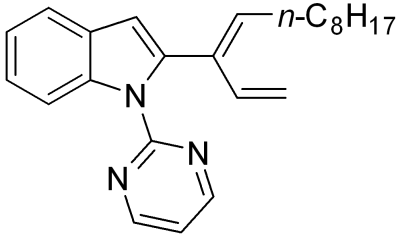
E/Z = 3/1



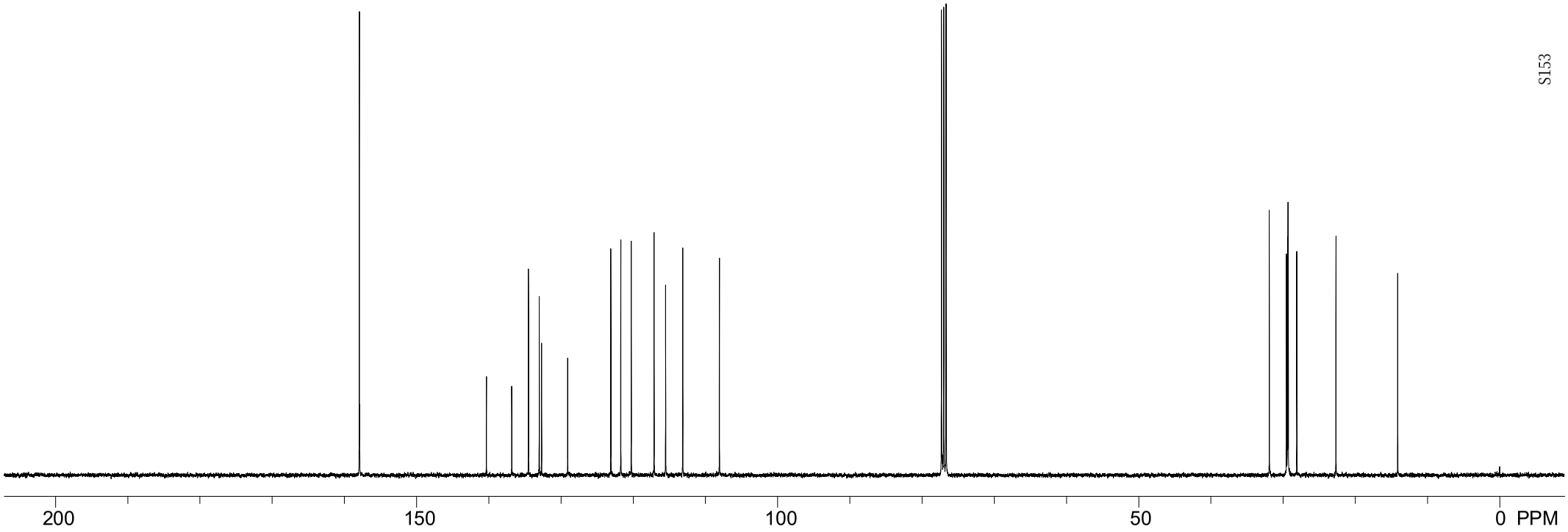

8.709
8.697
8.177
8.156
7.606
7.587
7.272
7.254
7.237
7.216
7.199
7.182
7.089
7.077
7.065
6.699
6.672
6.655
6.621
5.880
5.861
5.843
4.877
4.838
2.340
2.322
2.304
2.285
1.483
1.467
1.450
1.287
0.891
0.874
0.000
10.83
zyz-6-63H-2.fid
Apr 19 2020
SOLVENT: CDCl3
NA = 4
F1 = 399.722809 MHz
F2 = 100.519203 MHz
n-C8H17
N
N
N
E-3ao
S152
2.02
1.00
1.02
2.33
1.01
2.04
1.05
2.14
2.11
2.06
3.23
10
8
6
4
2
0
PPM

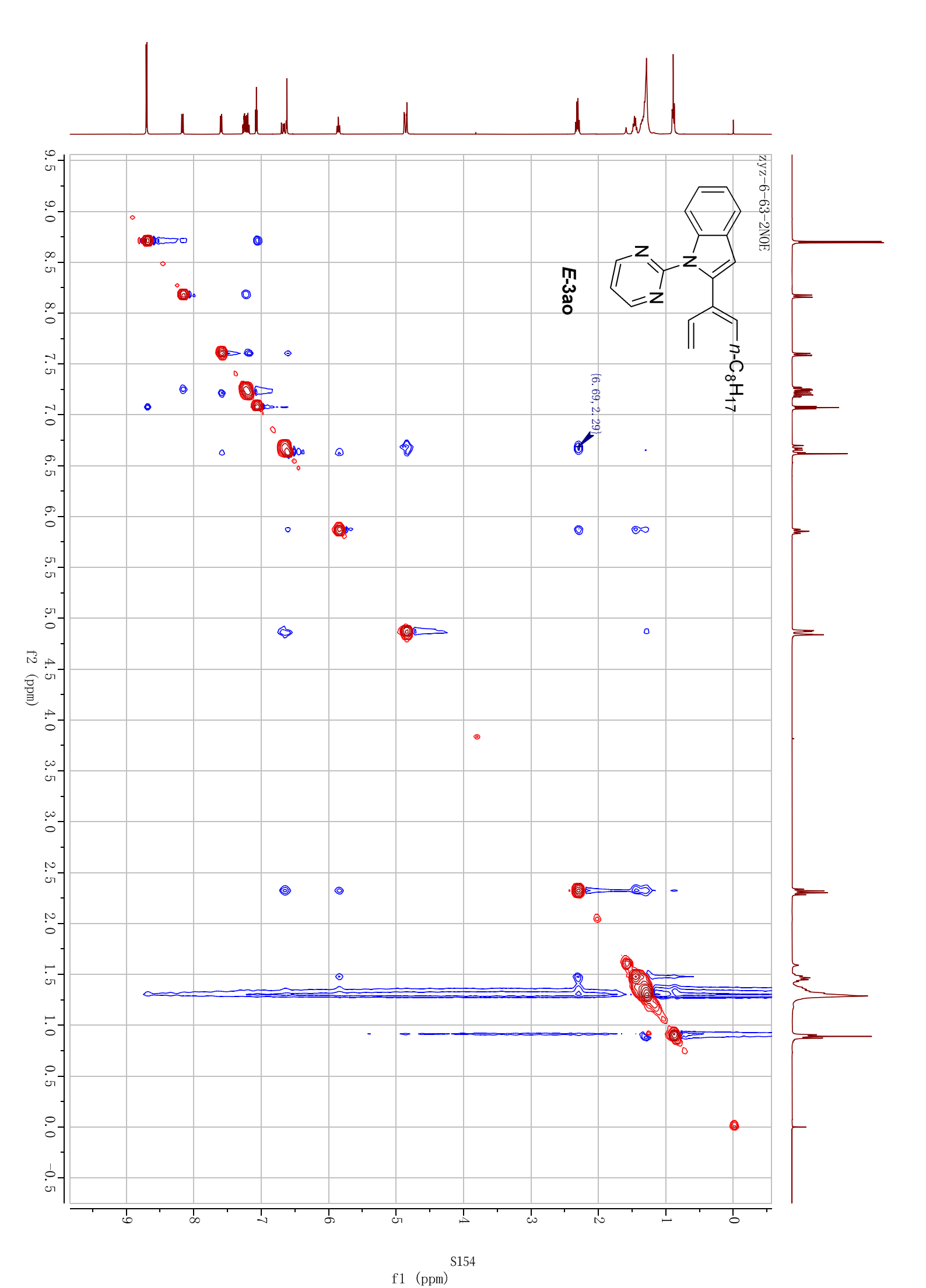
zyz-6-63C-2
USER: nmr
SOLVENT: CDCl3
NA = 1024
F1 = 100.605225 MHz
F2 = 1.000000 MHz

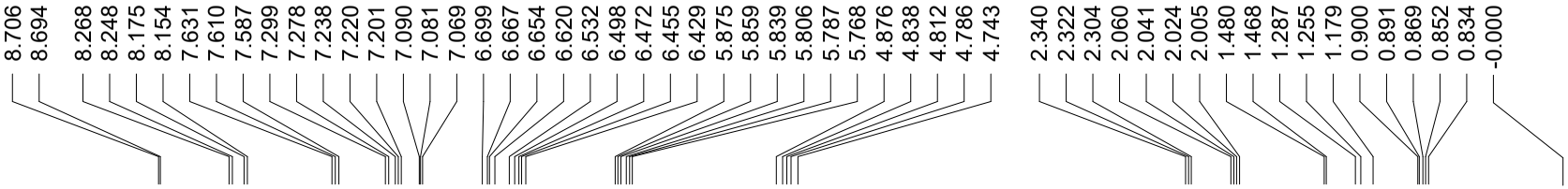
157.933
157.887
140.335
136.826
134.512
133.019
132.697
129.081
123.105
121.726
120.278
117.114
115.520
113.145
108.074
77.322
77.000
76.686
31.883
29.508
29.370
29.302
29.248
28.076
22.652
14.094



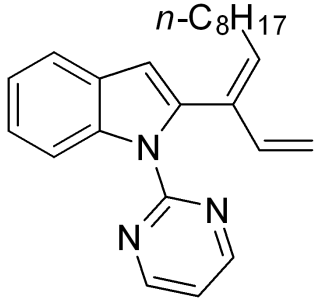
***E*-3ao**




zyz-6-63-2NOE
E-3ao
n-C8H17
6.69, 2.29
f2 (ppm)
f1 (ppm)

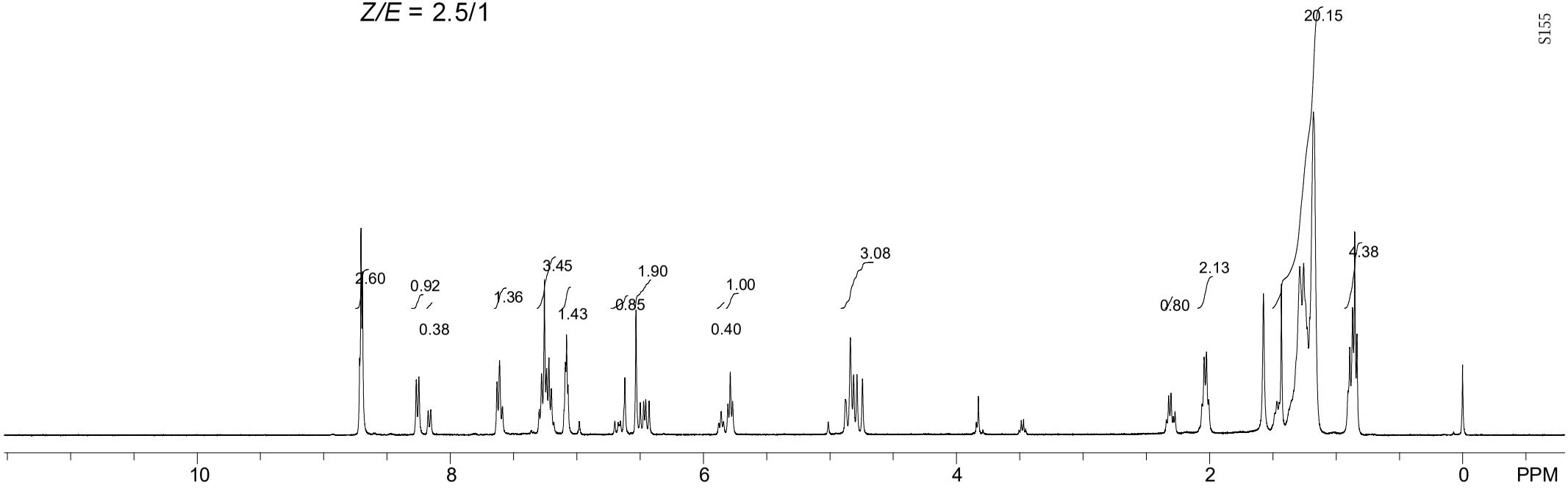


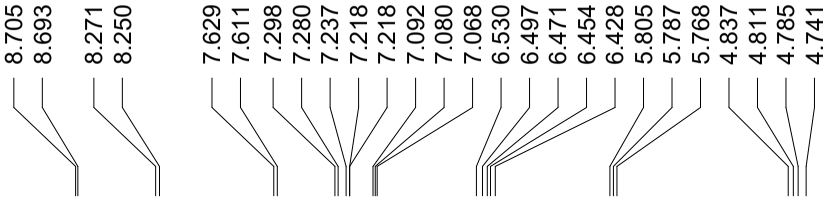
zyz-6-63H-mixture.fid
Apr 19 2020
SOLVENT: CDCl3
NA = 12
F1 = 399.722809 MHz
F2 = 100.519203 MHz



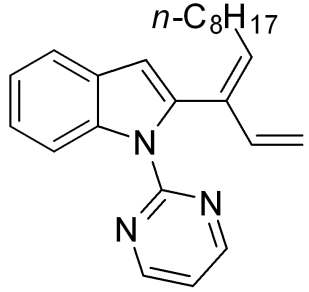
3ao

Z/*E* = 2.5/1

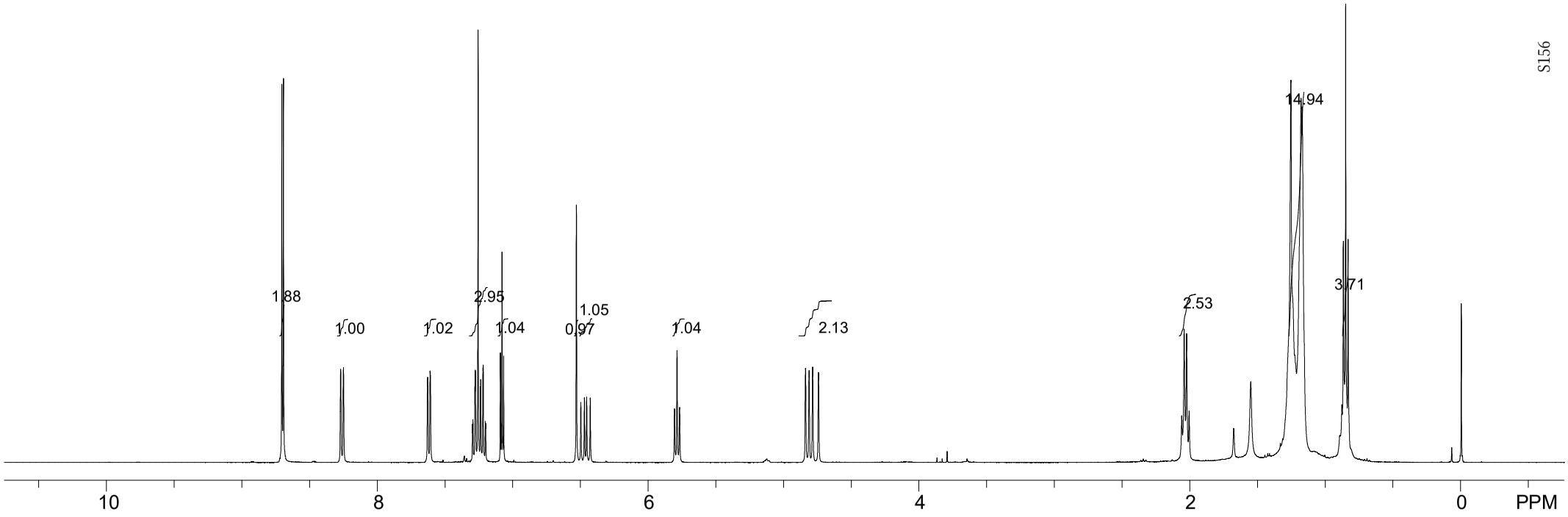


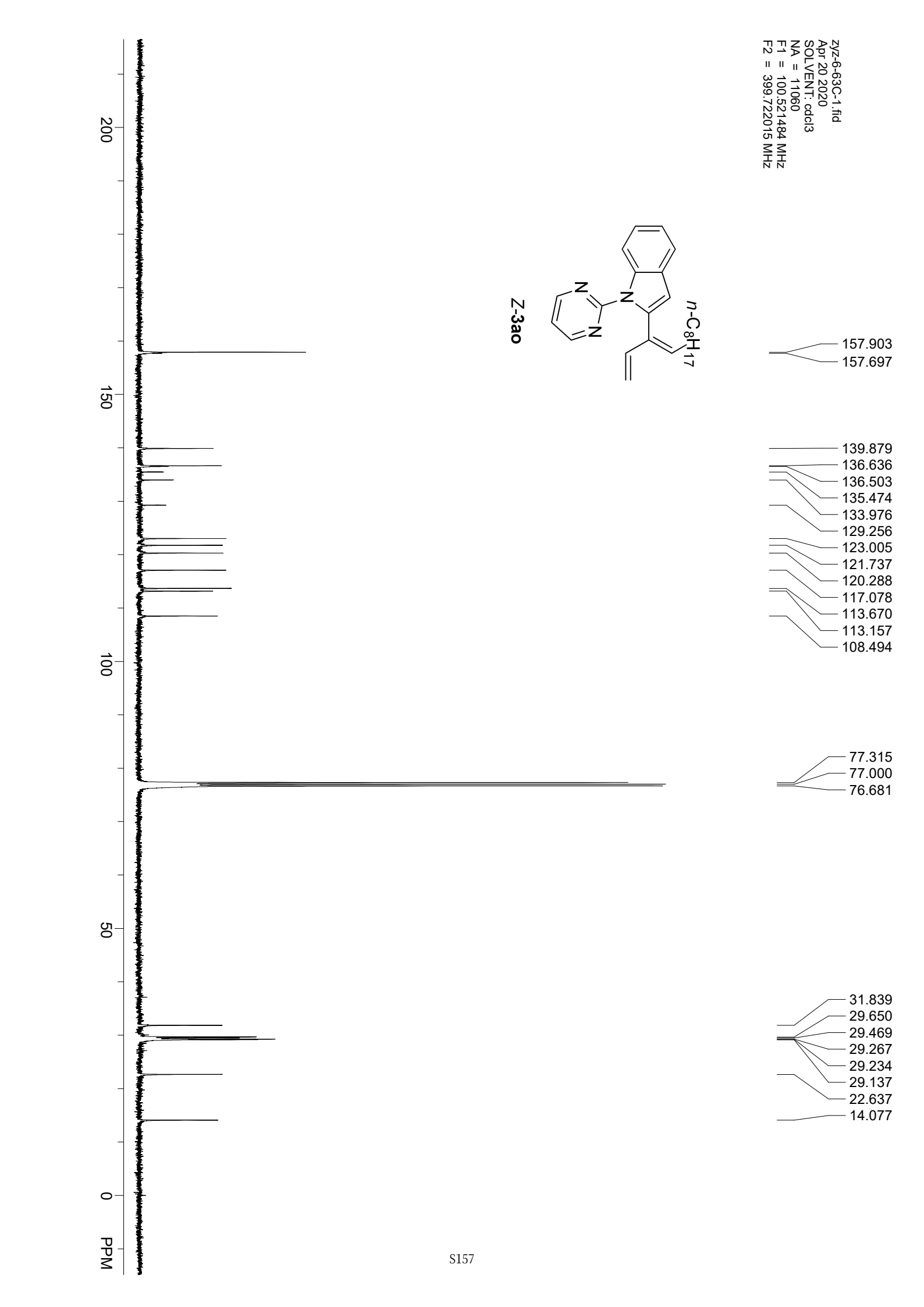


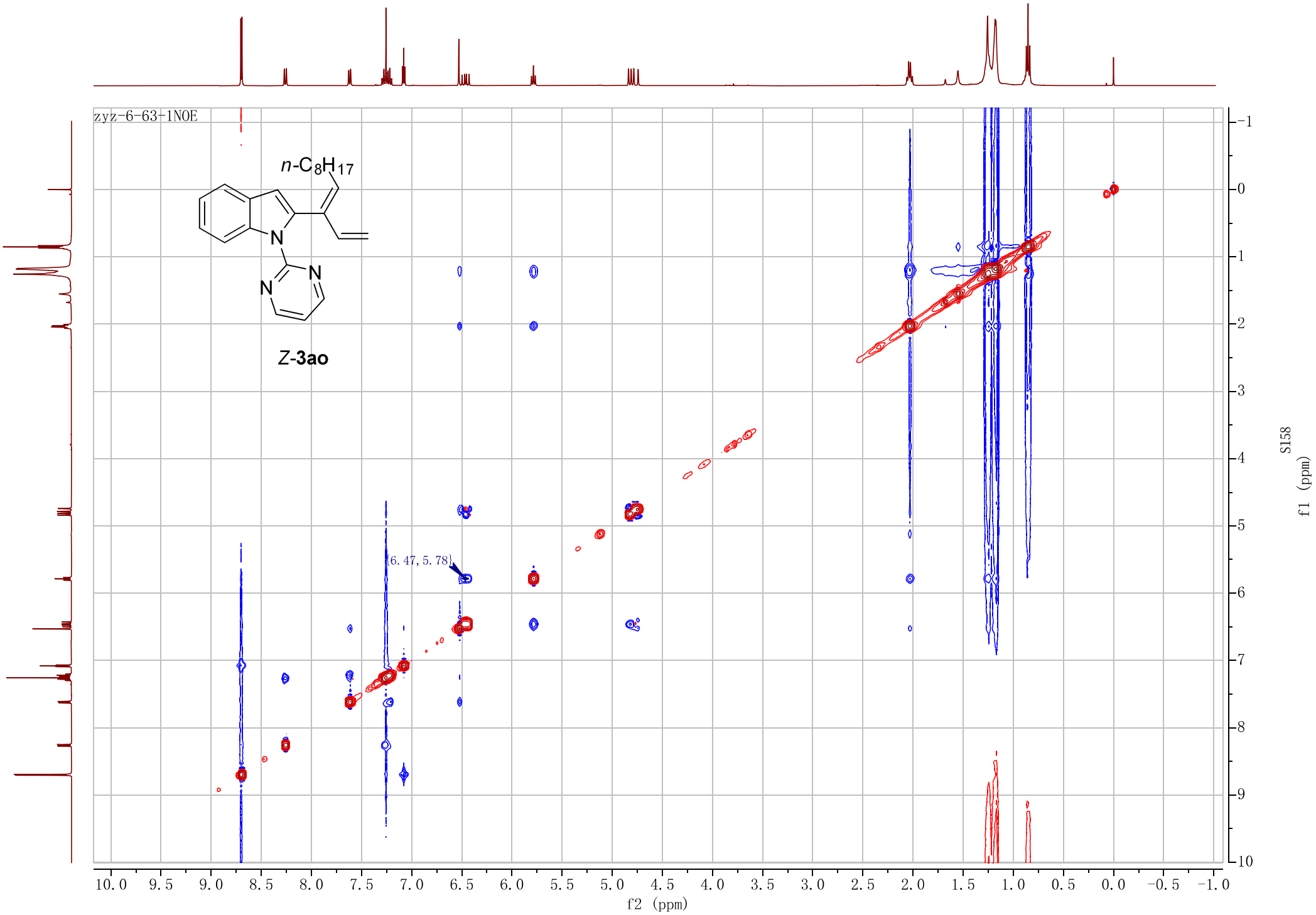
zyz-6-63H-1
SOLVENT: CDCl3
NA = 16
F1 = 400.100006 MHz
F2 = 1.000000 MHz

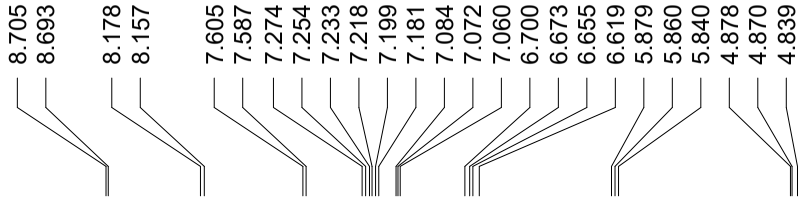


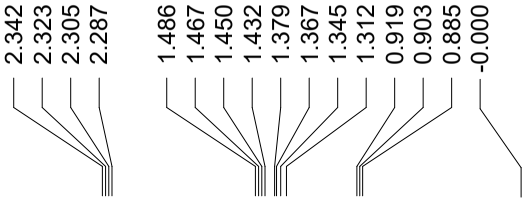
***Z*-3ao**



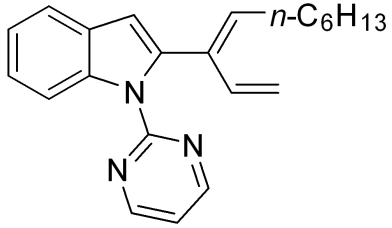

zyz-6-63C-1.fid
Apr 20 2020
SOLVENT: cdcl3
NA = 11060
F1 = 100.521484 MHz
F2 = 399.722015 MHz
Z-3ao
n-C8H17
N
N
N
157.903
157.697
139.879
136.636
136.503
135.474
133.976
129.256
123.005
121.737
120.288
117.078
113.670
113.157
108.494
77.315
77.000
76.681
31.839
29.650
29.469
29.267
29.234
29.137
22.637
14.077
200
150
100
50
0
PPM


zyz-6-63-1NOE
n-C8H17
N
N
N
Z-3ao
(6.47, 5.78)
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 -0.5 -1.0
f2 (ppm)
-1 0 1 2 3 4 5 6 7 8 9 10
S158
f1 (ppm)

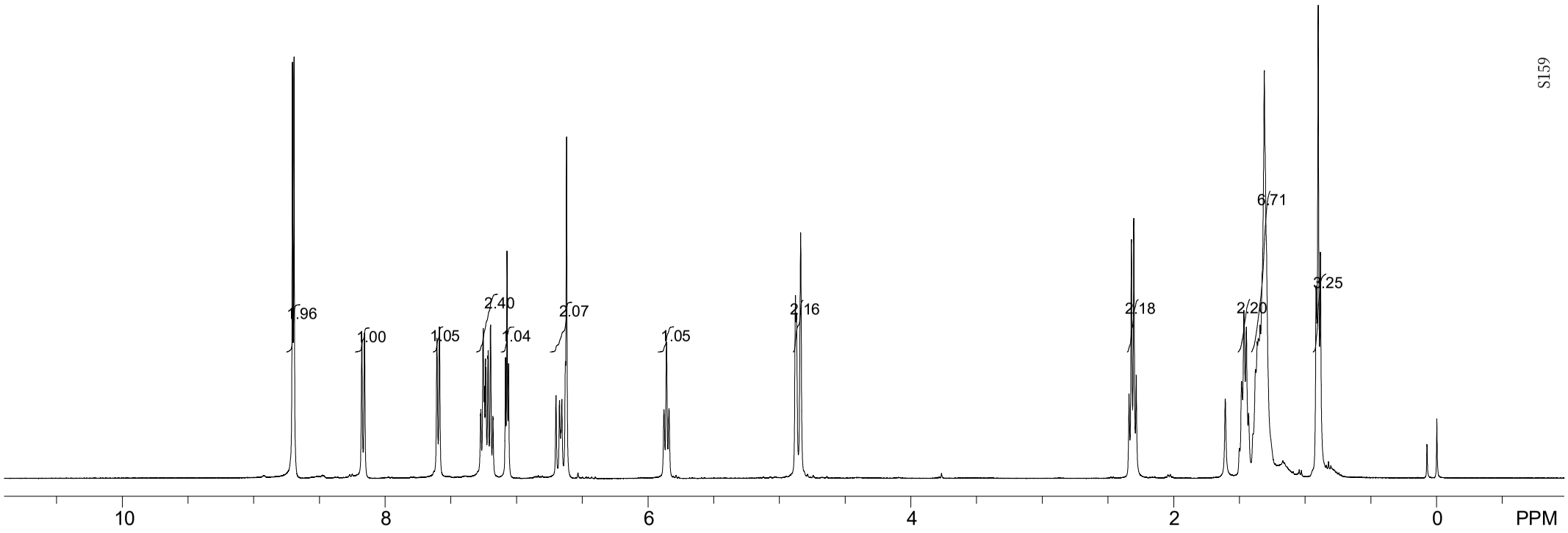


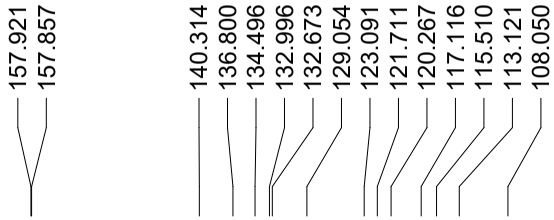


zyz-6-79H-2.fid
Apr 27 2020
SOLVENT: CDCl3
NA = 8
F1 = 400.031616 MHz
F2 = 100.596855 MHz

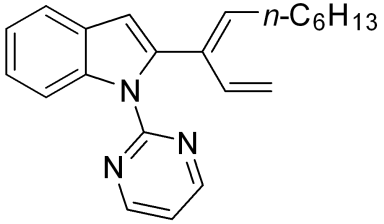


***E*-3ap**

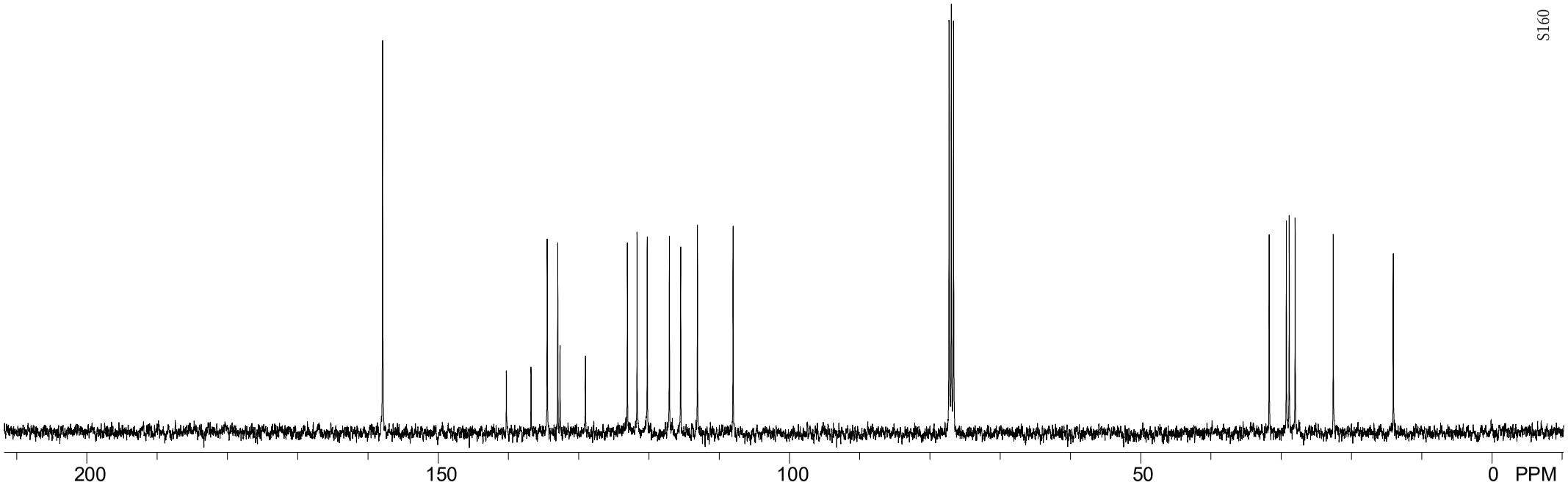


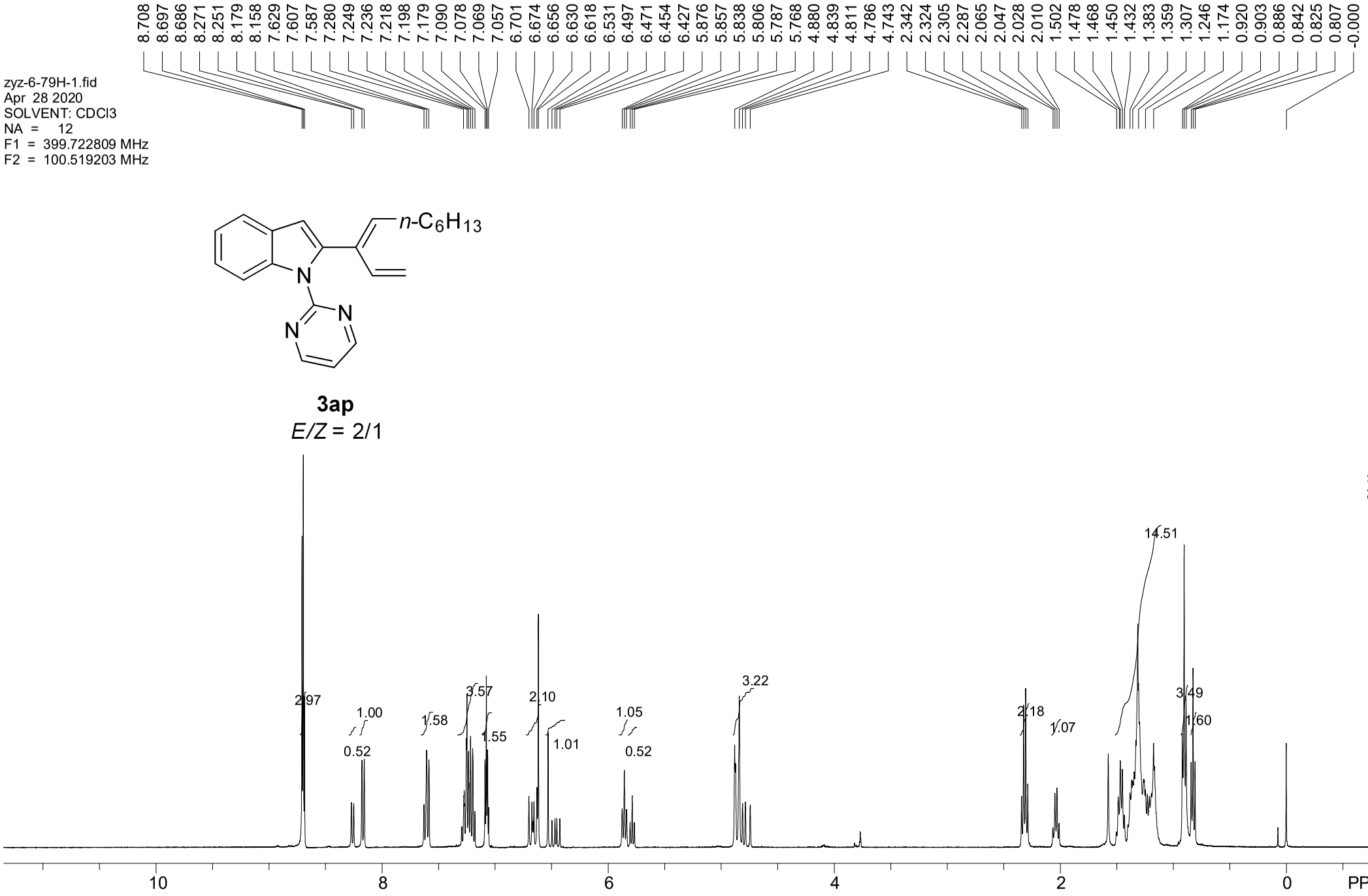


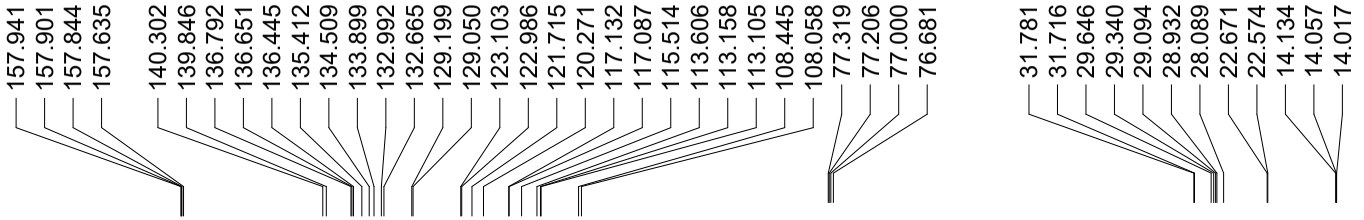
zyz-6-79-2C.fid
Apr 27 2020
SOLVENT: cdcl3
NA = 116
F1 = 100.598389 MHz
F2 = 400.030792 MHz



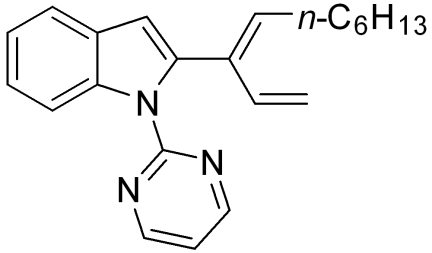
***E*-3ap**




8.708 8.697 8.686 8.271 8.251 8.179 8.158 7.629 7.607 7.587 7.280 7.249 7.236 7.218 7.198 7.179 7.090 7.078 7.069 7.057 6.701 6.674 6.656 6.630 6.618 6.531 6.497 6.471 6.454 6.427 5.876 5.857 5.838 5.806 5.787 5.768 4.880 4.839 4.811 4.786 4.743 2.342 2.324 2.305 2.287 2.065 2.047 2.028 2.010 1.502 1.478 1.468 1.450 1.432 1.383 1.359 1.307 1.246 1.174 0.920 0.903 0.886 0.842 0.825 0.807 -0.000
zyz-6-79H-1.fid
Apr 28 2020
SOLVENT: CDCl3
NA = 12
F1 = 399.722809 MHz
F2 = 100.519203 MHz
n-C6H13
N
N
N
3ap
E/Z = 2/1
S161
2.97
1.00
0.52
1.58
3.57
1.55
2.10
1.01
1.05
0.52
3.22
2.18
1.07
14.51
3.49
1.60
10
8
6
4
2
0
PPM

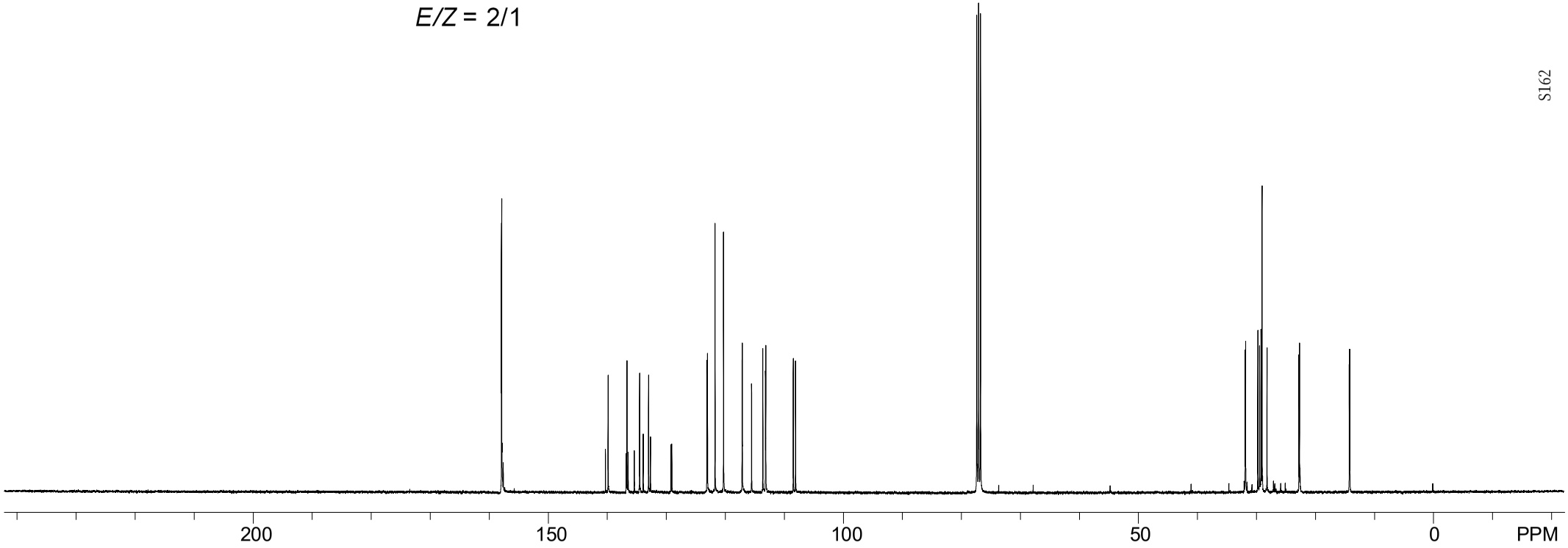


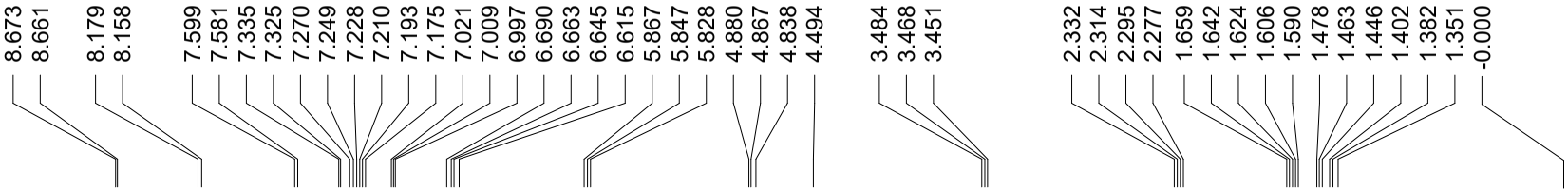
zyz-6-79C-1.fid
Apr 27 2020
SOLVENT: cdcl3
NA = 13152
F1 = 100.598389 MHz
F2 = 400.030792 MHz



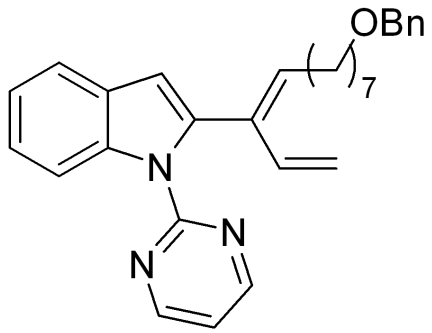
3ap

E/*Z* = 2/1

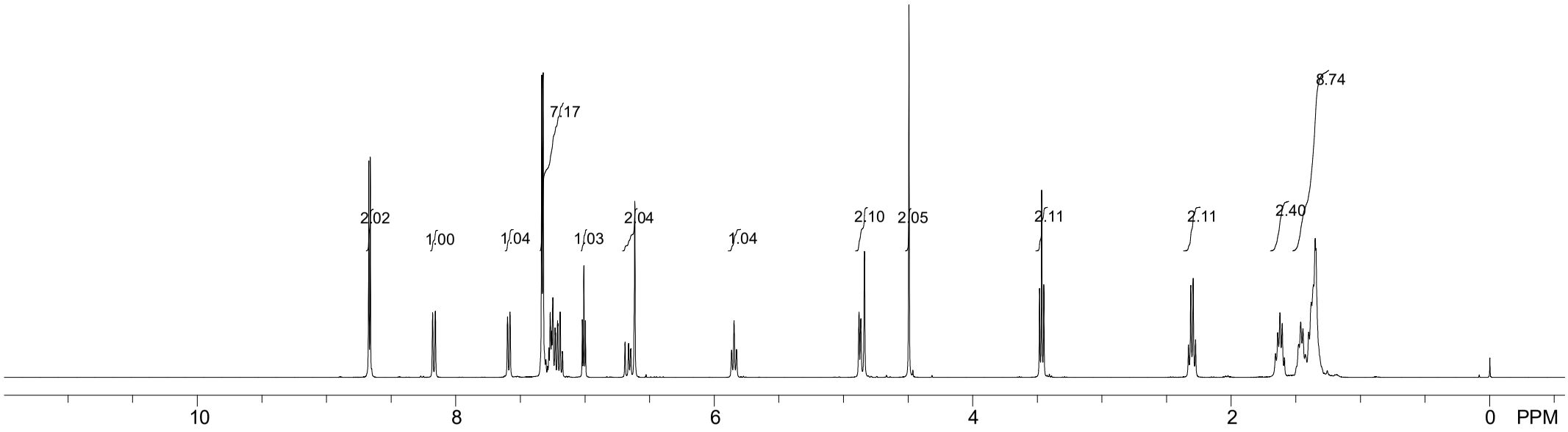


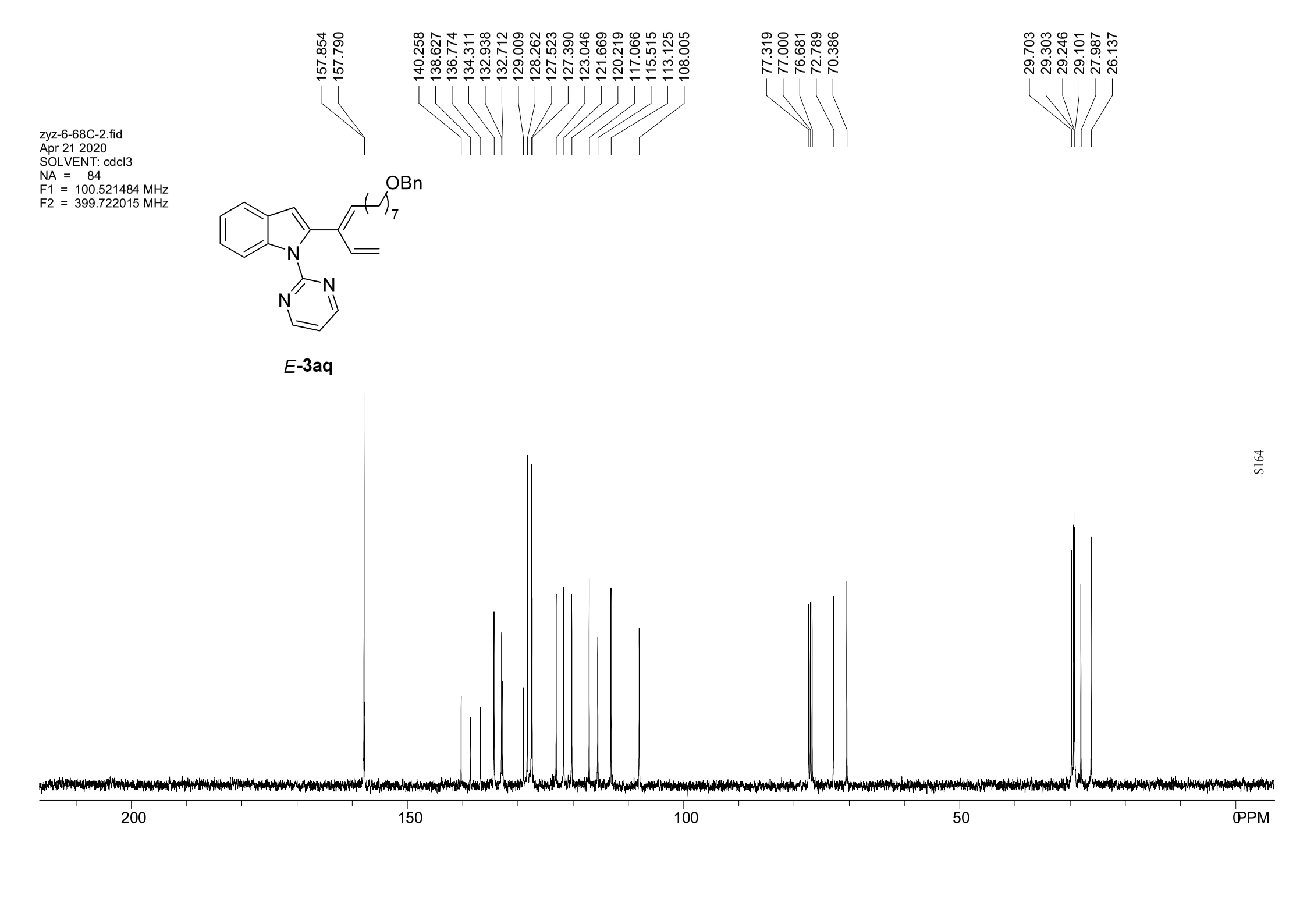


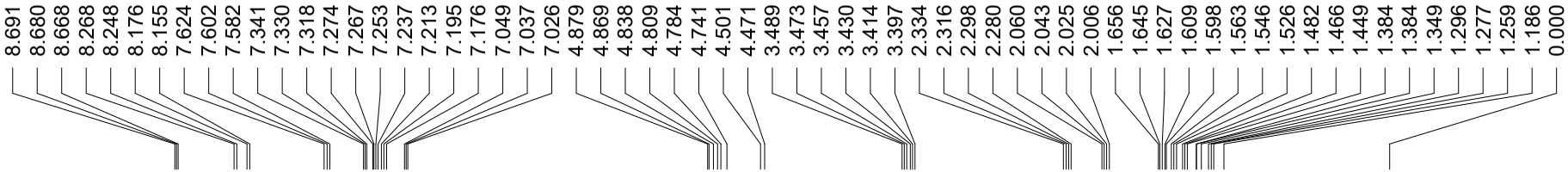
zyz-6-68H-2.fid
Apr 23 2020
SOLVENT: CDCl3
NA = 8
F1 = 399.722809 MHz
F2 = 100.519203 MHz



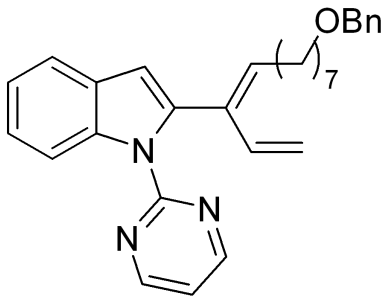
***E*-3aq**




157.854
157.790
140.258
138.627
136.774
134.311
132.938
132.712
129.009
128.262
127.523
127.390
123.046
121.669
120.219
117.066
115.515
113.125
108.005
77.319
77.000
76.681
72.789
70.386
29.703
29.303
29.246
29.101
27.987
26.137
zyz-6-68C-2.fid
Apr 21 2020
SOLVENT: cdcl3
NA = 84
F1 = 100.521484 MHz
F2 = 399.722015 MHz
OBn
7
N
N
N
E-3aq
S164
200
150
100
50
0
PPM

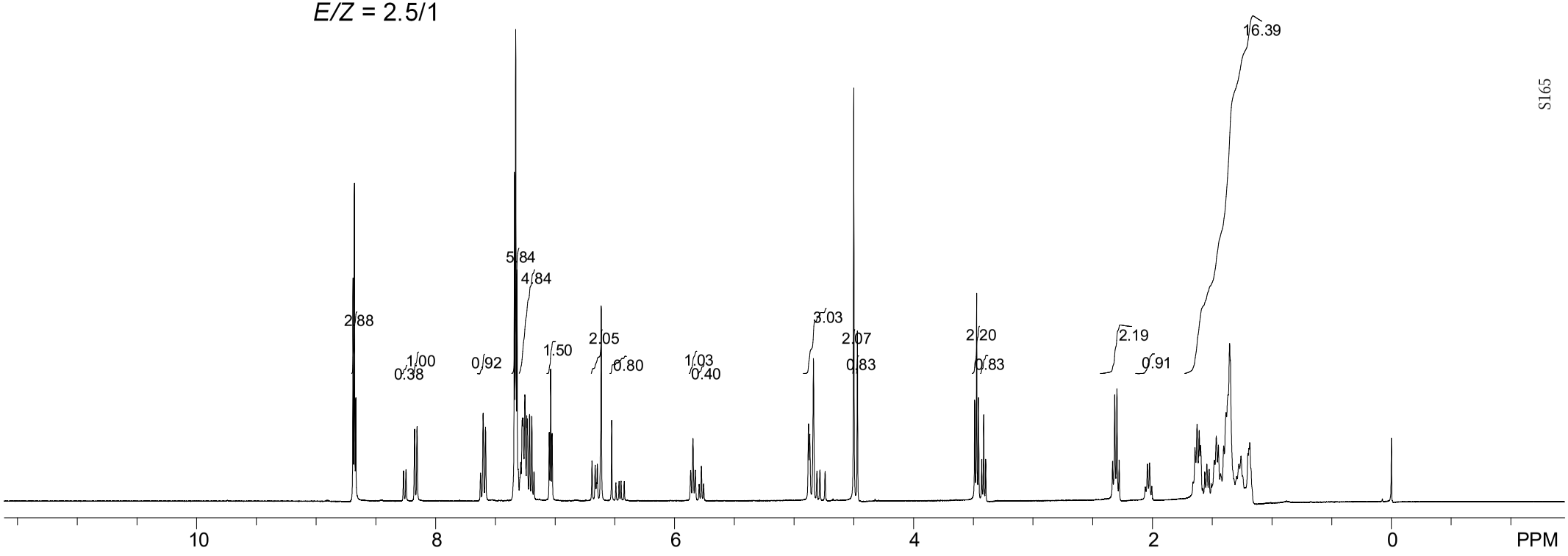


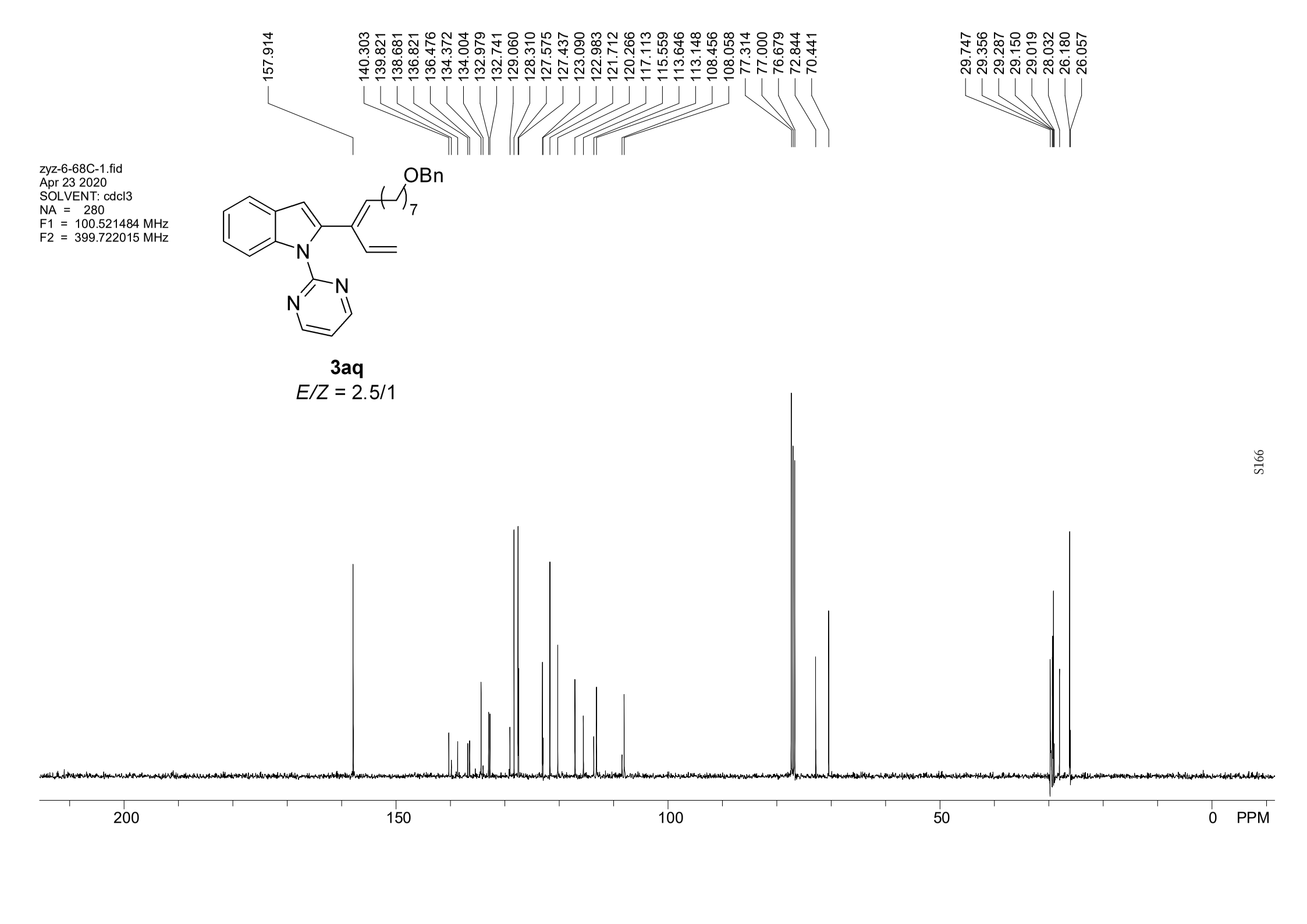
zyz-6-68H-1.fid
Apr 23 2020
SOLVENT: CDCl3
NA = 8
F1 = 399.722809 MHz
F2 = 100.519203 MHz

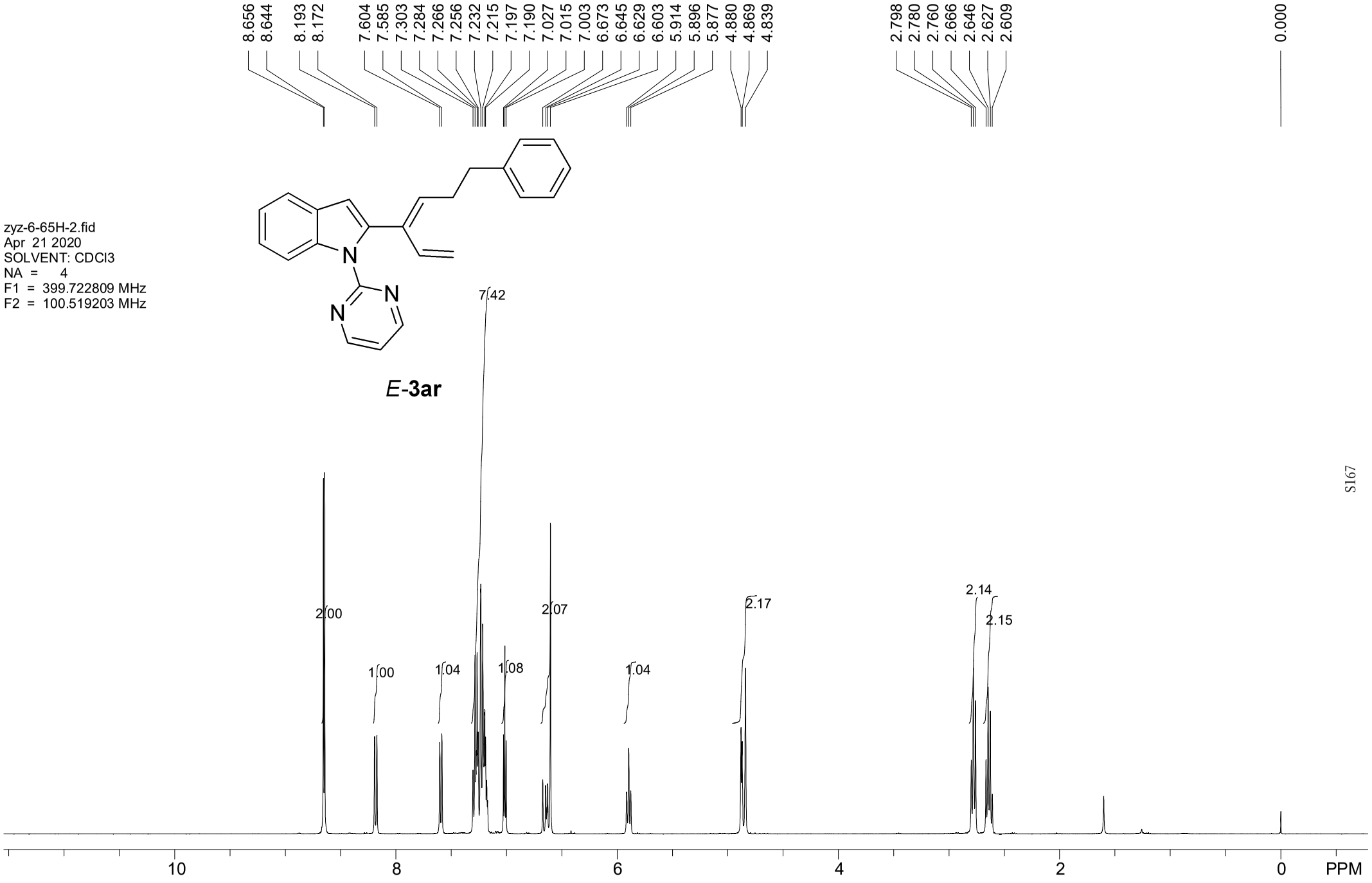


3aq

E/Z = 2.5/1

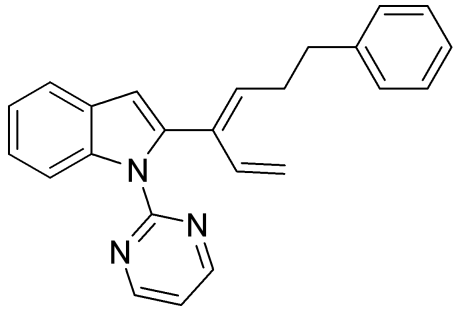



157.914
140.303
139.821
138.681
136.821
136.476
134.372
134.004
132.979
132.741
129.060
128.310
127.575
127.437
123.090
122.983
121.712
120.266
117.113
115.559
113.646
113.148
108.456
108.058
77.314
77.000
76.679
72.844
70.441
29.747
29.356
29.287
29.150
29.019
28.032
26.180
26.057
zyz-6-68C-1.fid
Apr 23 2020
SOLVENT: cdcl3
NA = 280
F1 = 100.521484 MHz
F2 = 399.722015 MHz
OBn
7
N
N
N
3aq
E/Z = 2.5/1
S166
200
150
100
50
0
PPM

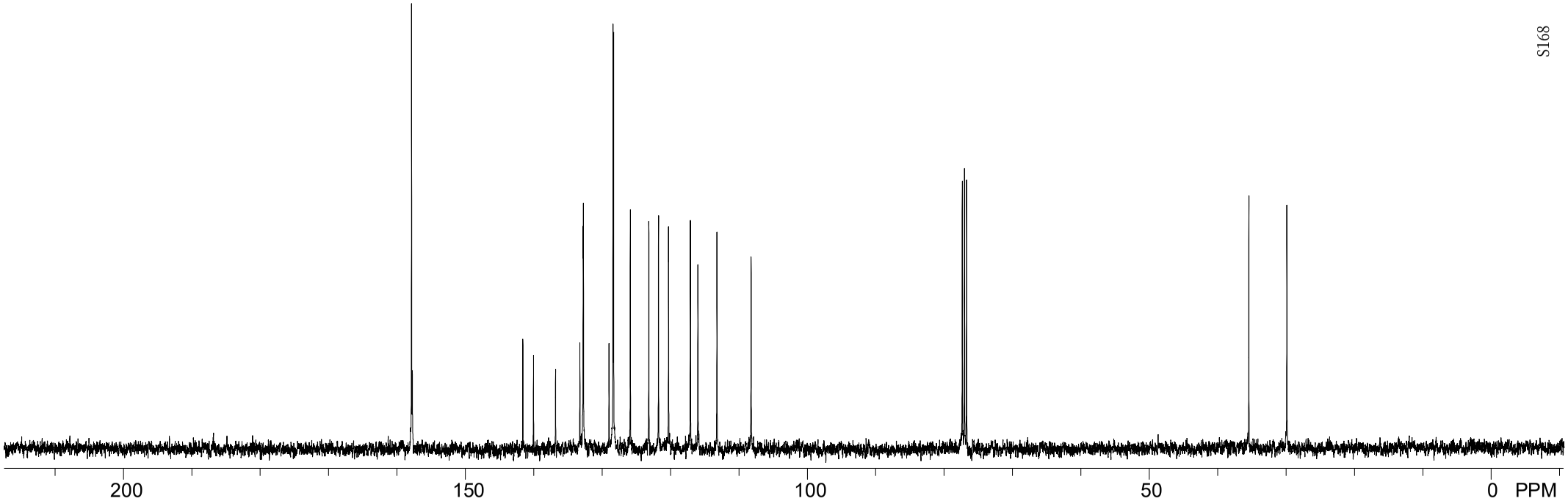

8.656
8.644
8.193
8.172
7.604
7.585
7.303
7.284
7.266
7.256
7.232
7.215
7.197
7.190
7.027
7.015
7.003
6.673
6.645
6.629
6.603
5.914
5.896
5.877
4.880
4.869
4.839
2.798
2.780
2.760
2.666
2.646
2.627
2.609
0.000
zyz-6-65H-2.fid
Apr 21 2020
SOLVENT: CDCl3
NA = 4
F1 = 399.722809 MHz
F2 = 100.519203 MHz
N
N
N
E-3ar
7.42
2.00
1.00
1.04
1.08
2.07
1.04
2.17
2.14
2.15
10
8
6
4
2
0
PPM

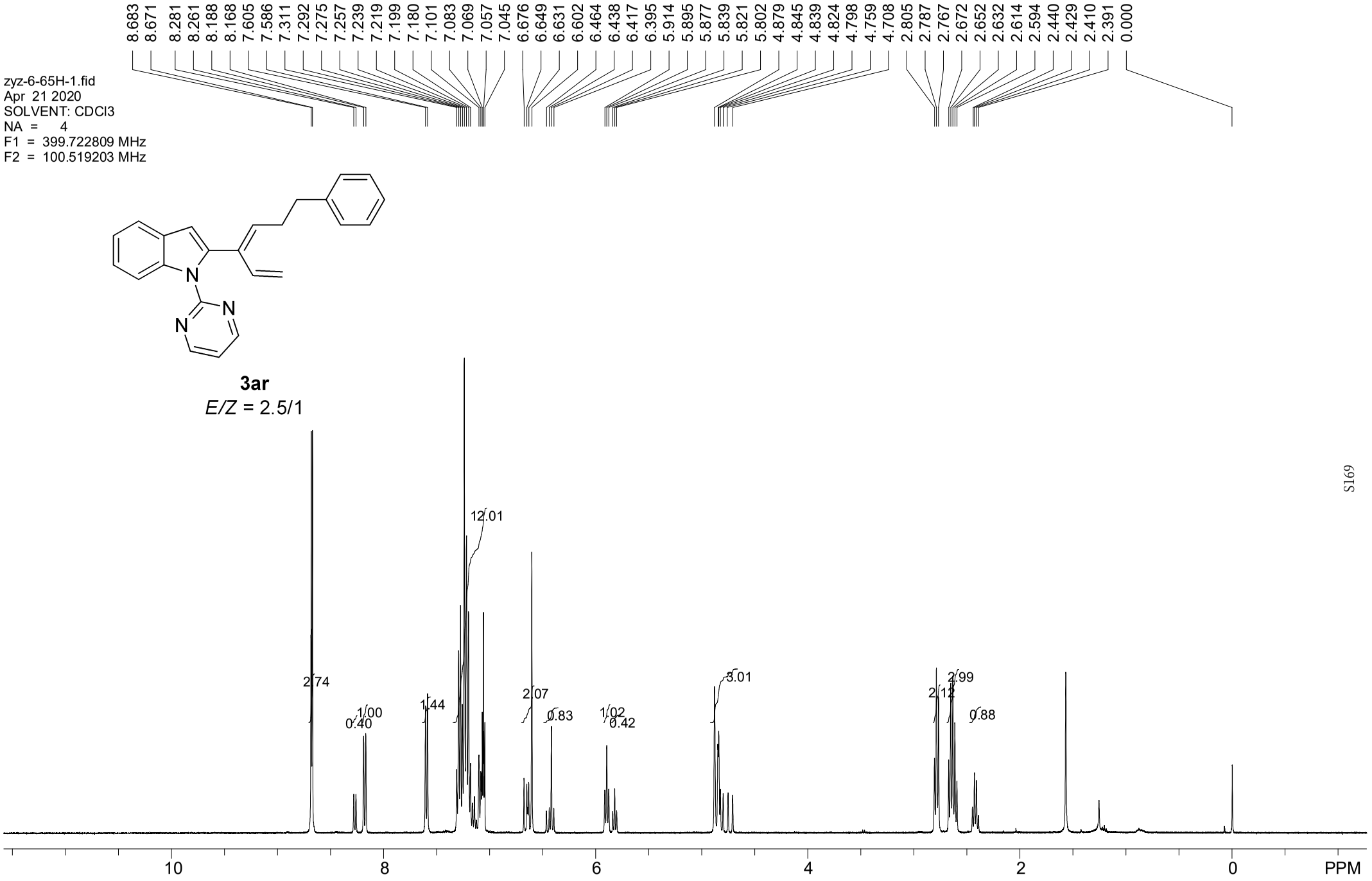
157.866
157.749
141.591
140.032
136.802
133.245
132.764
132.728
128.985
128.408
128.315
125.868
123.163
121.745
120.284
117.086
115.988
113.202
108.203
77.319
77.000
76.685
35.493
29.949

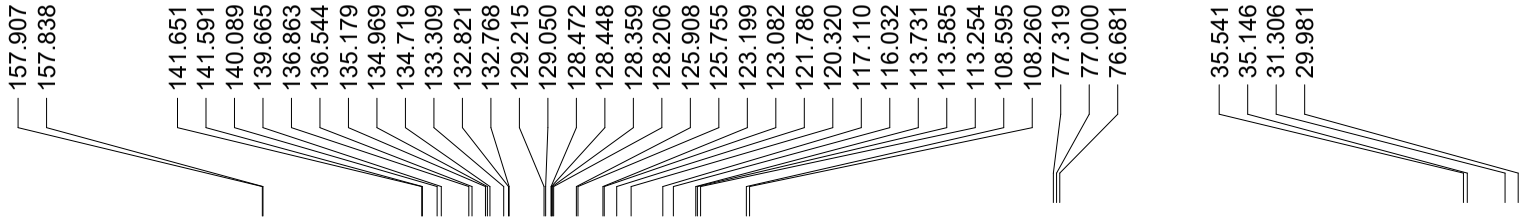
zyz-6-65C-2.fid
Apr 21 2020
SOLVENT: cdcl3
NA = 64
F1 = 100.521484 MHz
F2 = 399.722015 MHz



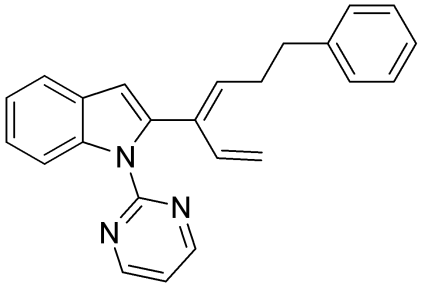
***E*-3ar**




8.683
8.671
8.281
8.261
8.188
8.168
7.605
7.586
7.311
7.292
7.275
7.257
7.239
7.219
7.199
7.180
7.101
7.083
7.069
7.057
7.045
6.676
6.649
6.631
6.602
6.464
6.438
6.417
6.395
5.914
5.895
5.877
5.839
5.821
5.802
4.879
4.845
4.839
4.824
4.798
4.759
4.708
2.805
2.787
2.767
2.672
2.652
2.632
2.614
2.594
2.440
2.429
2.410
2.391
0.000
zyz-6-65H-1.fid
Apr 21 2020
SOLVENT: CDCl3
NA = 4
F1 = 399.722809 MHz
F2 = 100.519203 MHz
N
N
N
3ar
E/Z = 2.5/1
2.74
1.00
0.40
1.44
12.01
2.07
0.83
1.02
0.42
3.01
2.12
2.99
0.88
10
8
6
4
2
0
PPM

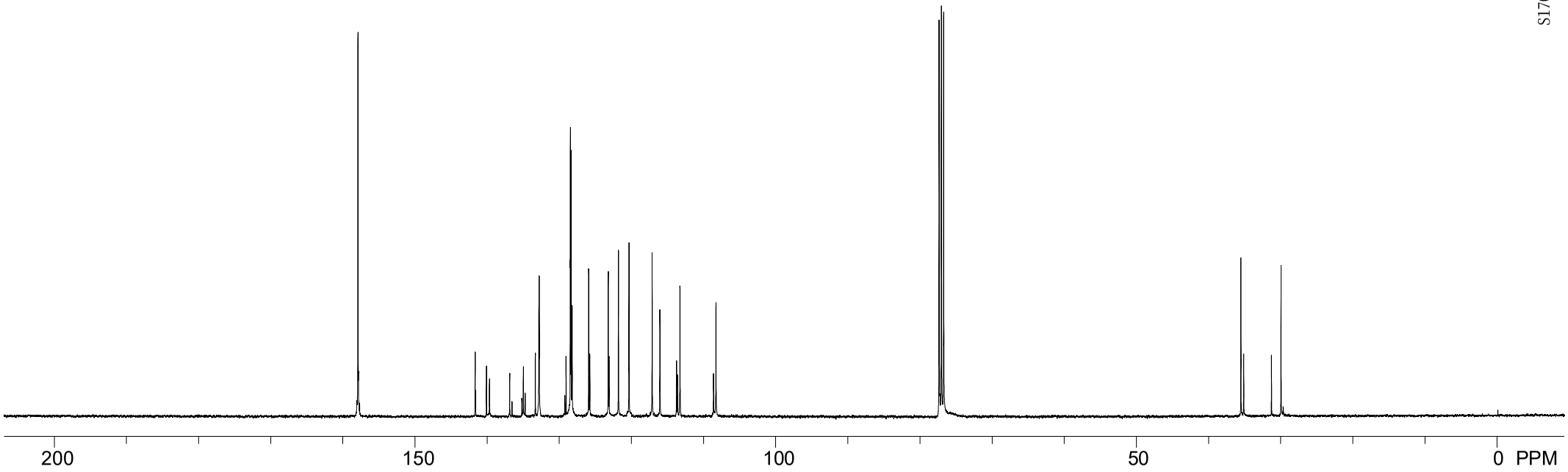


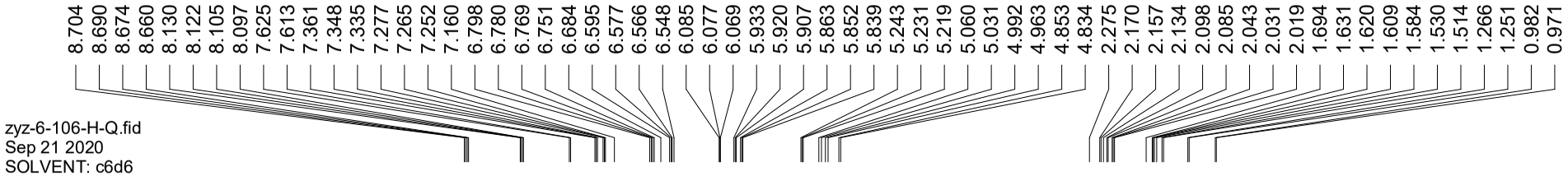
zyz-6-65C-1.fid
Apr 21 2020
SOLVENT: cdcl3
NA = 14388
F1 = 100.521484 MHz
F2 = 399.722015 MHz



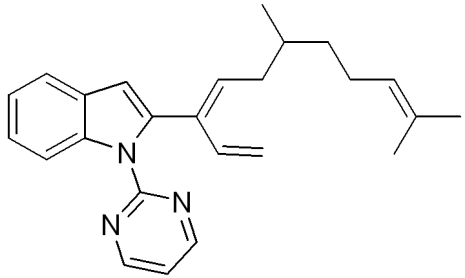
3ar

E/Z = 2.5/1



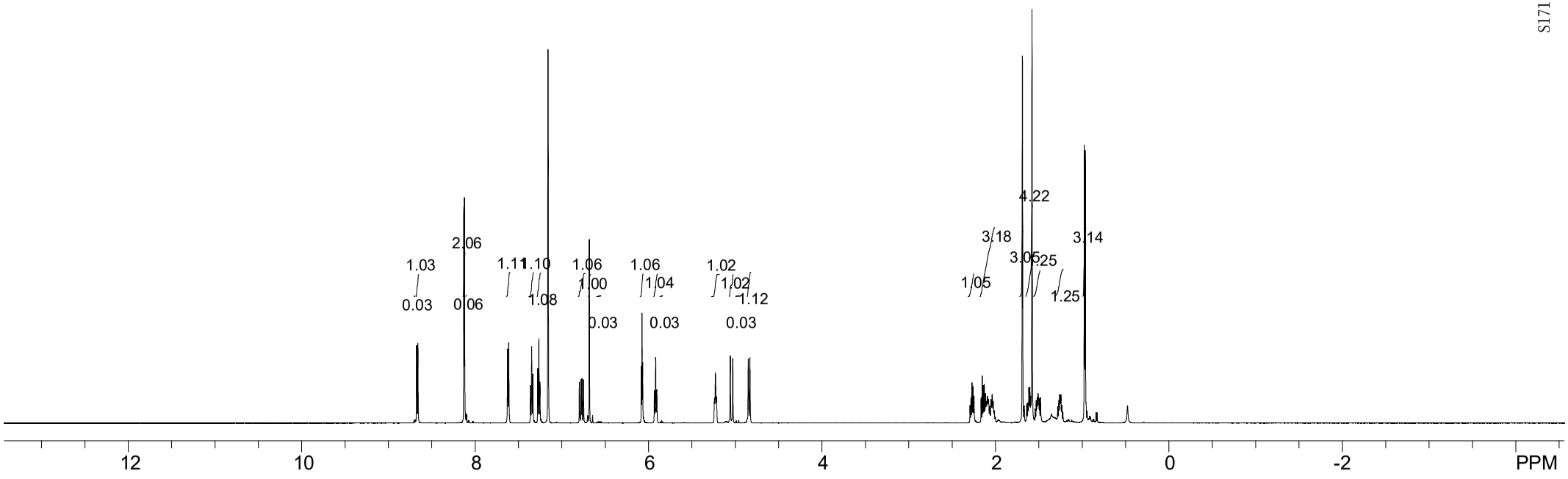


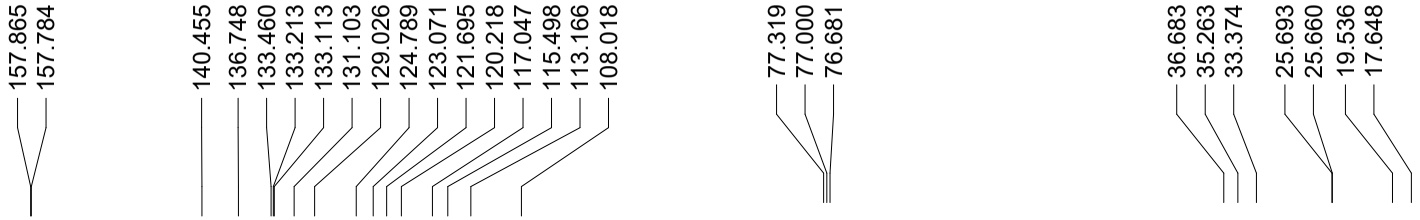
zyz-6-106-H-Q.fid
Sep 21 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz



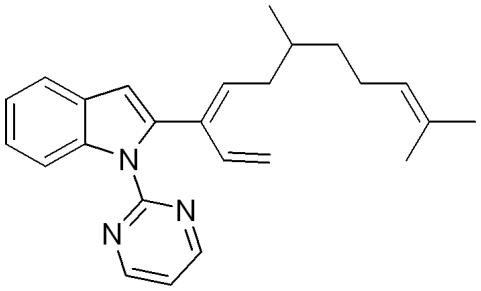
3as

E/Z = 97/3



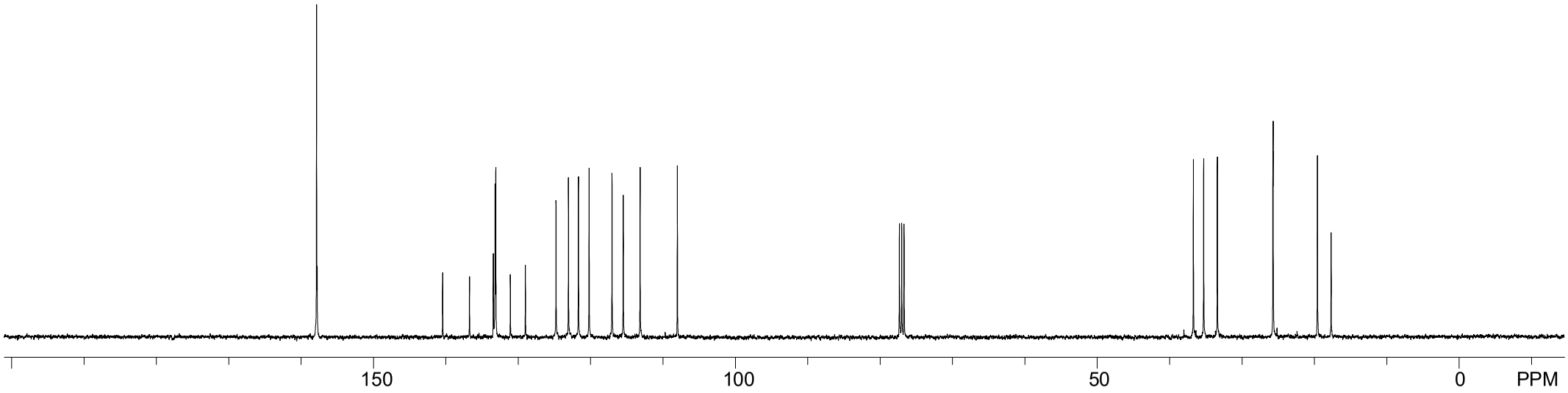


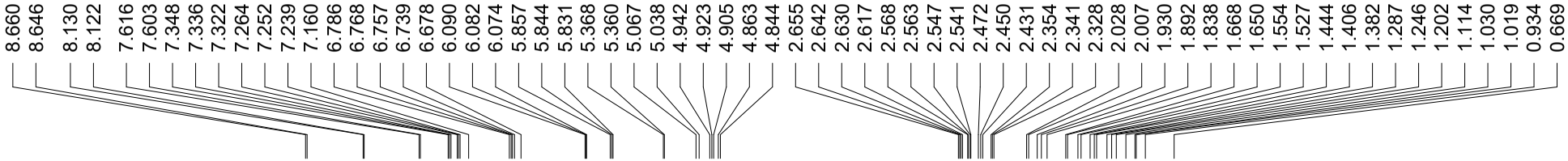
zyz-6-106C.fid
May 24 2020
SOLVENT: cdcl3
NA = 152
F1 = 100.598389 MHz
F2 = 400.030792 MHz



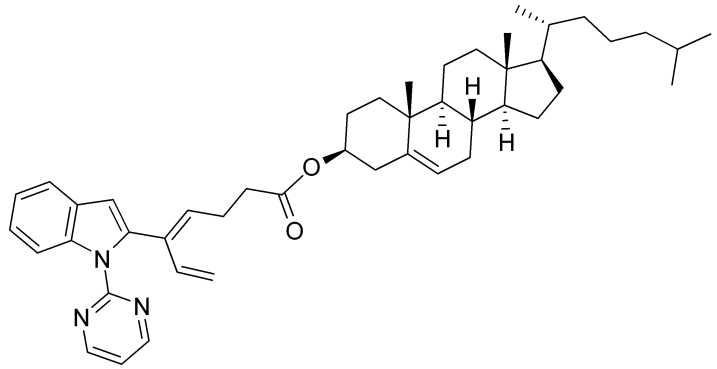
3as

E/Z = 97/3

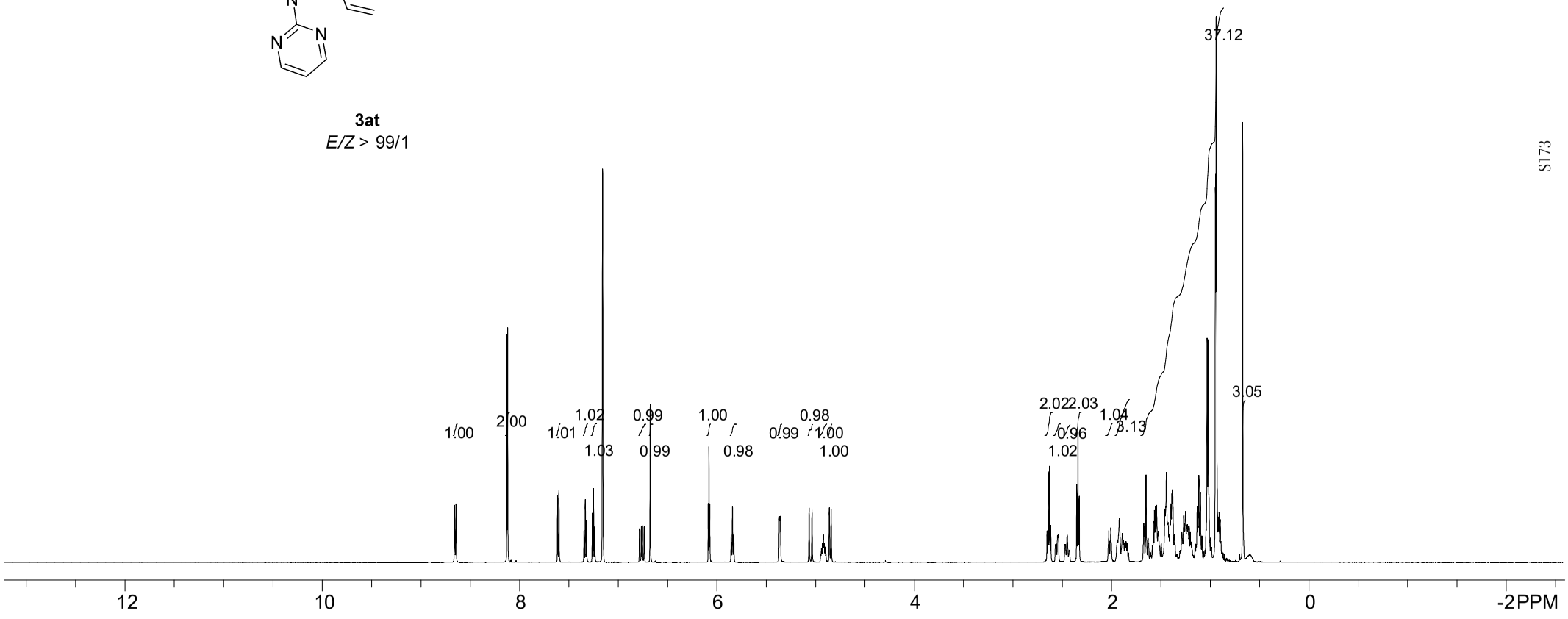


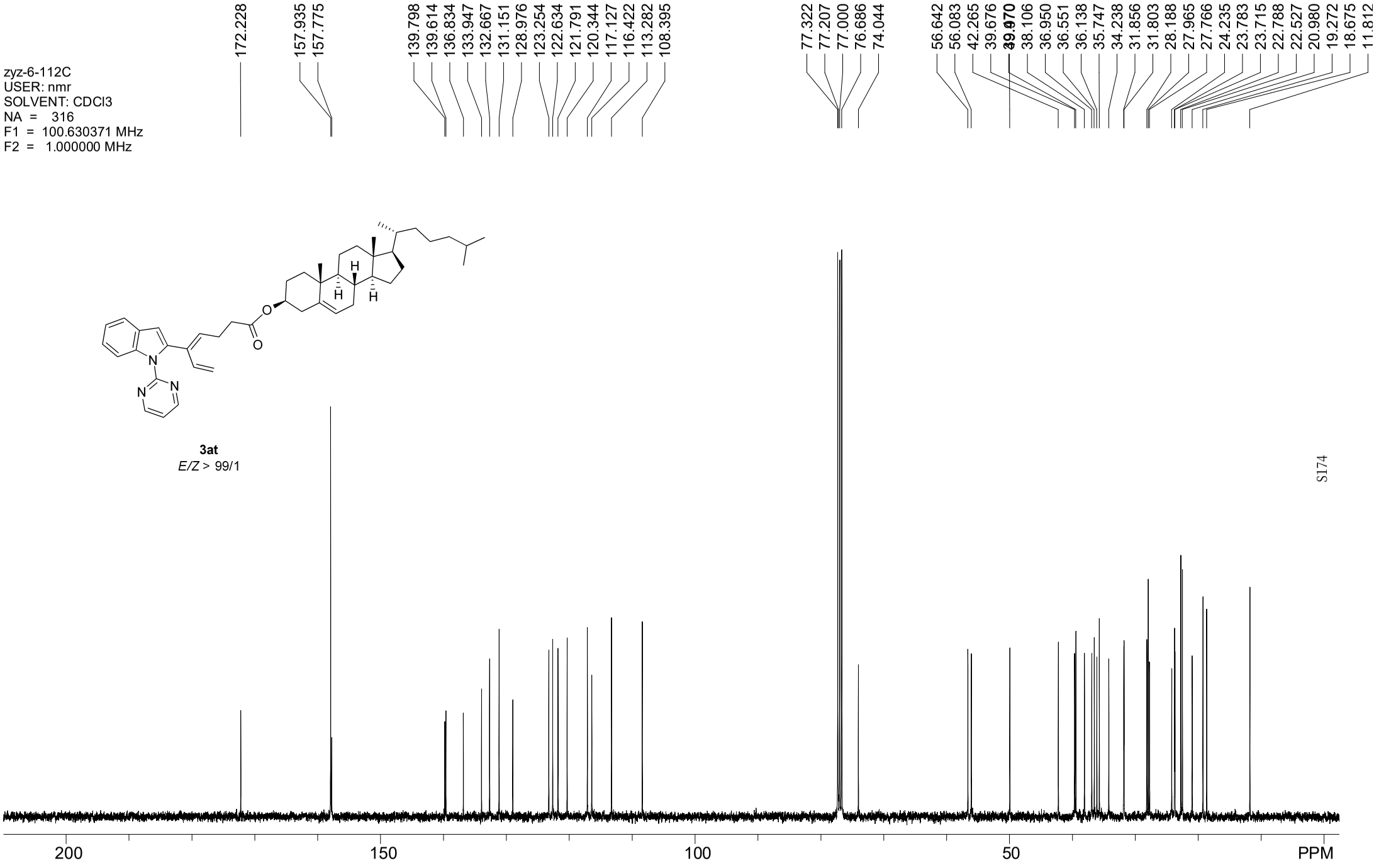


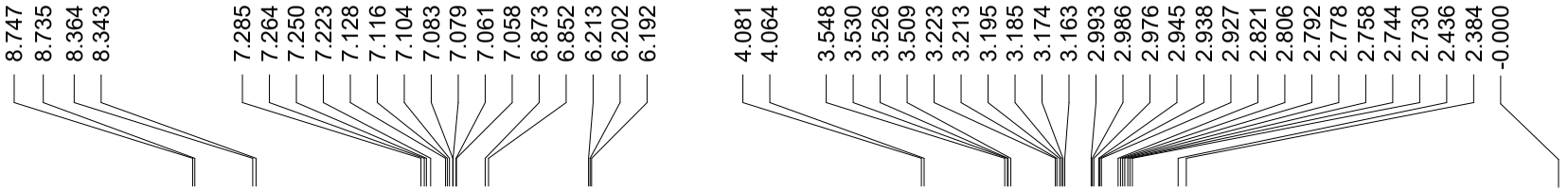
zyz-6-112-h1-Q.fid
Sep 24 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz



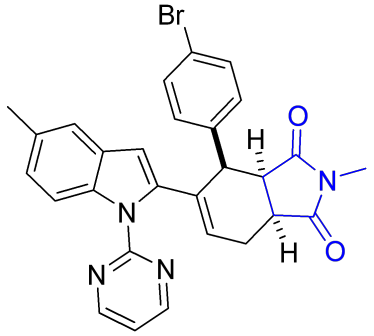
3at
E/Z > 99/1




172.228
157.935
157.775
139.798
139.614
136.834
133.947
132.667
131.151
128.976
123.254
122.634
121.791
120.344
117.127
116.422
113.282
108.395
77.322
77.207
77.000
76.686
74.044
56.642
56.083
42.265
39.676
38.106
36.950
36.551
36.138
35.747
34.238
31.856
31.803
28.188
27.965
27.766
24.235
23.783
23.715
22.788
22.527
20.980
19.272
18.675
11.812
zyz-6-112C
USER: nmr
SOLVENT: CDCl3
NA = 316
F1 = 100.630371 MHz
F2 = 1.000000 MHz
O
O
N
N
N
H
H
H
3at
E/Z > 99/1
S174
200
150
100
50
PPM

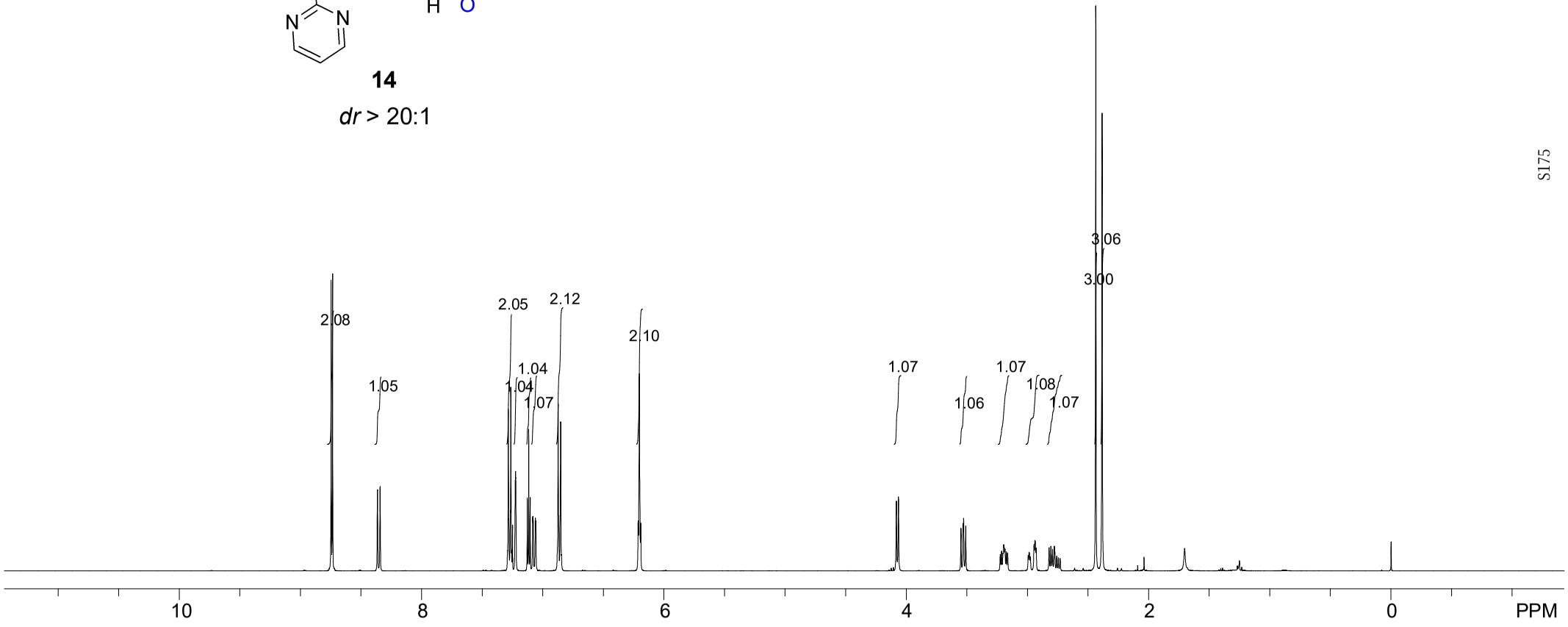


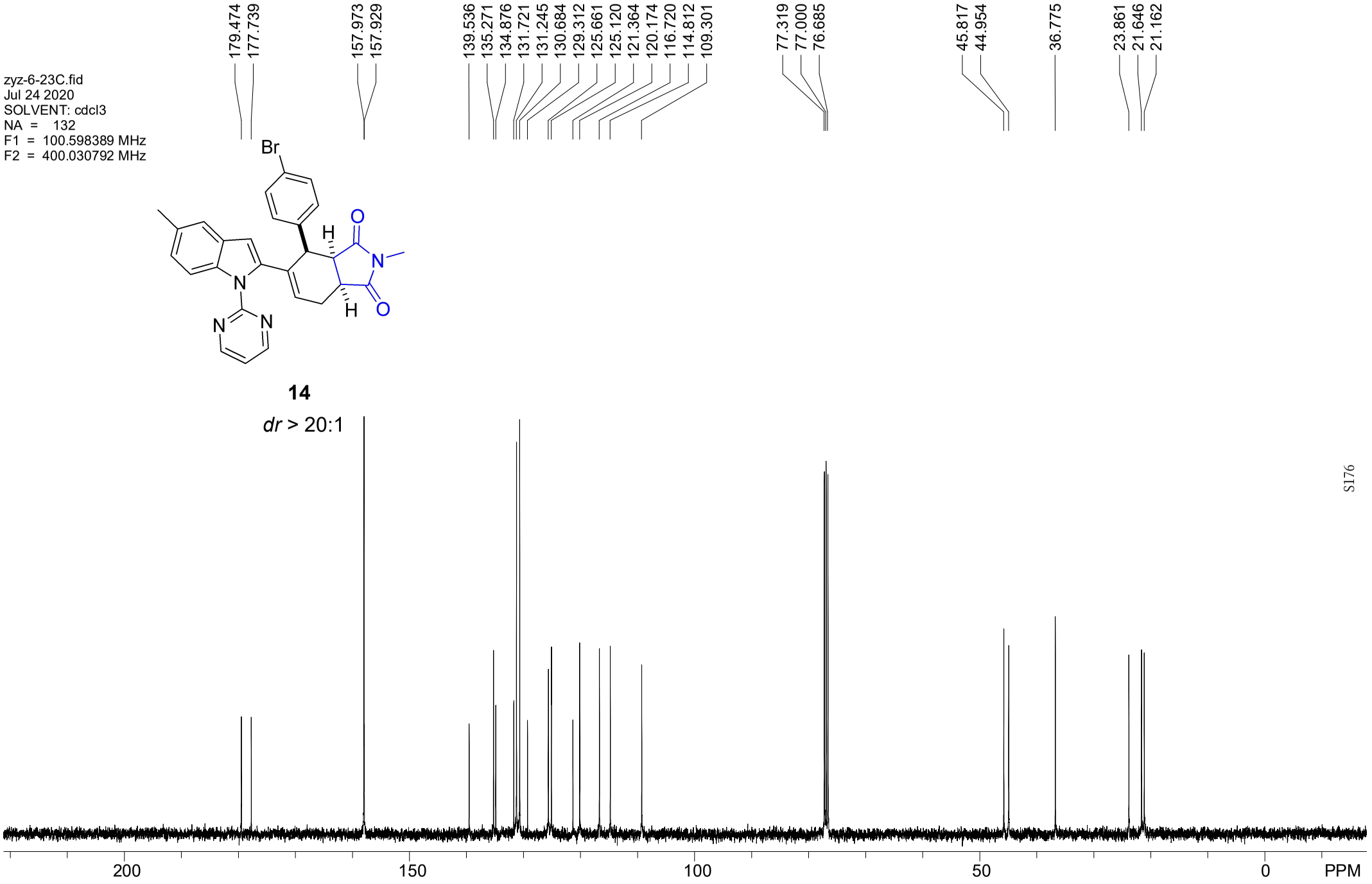
zyz-6-23H.fid
Jul 24 2020
SOLVENT: CDCl3
NA = 12
F1 = 399.722809 MHz
F2 = 100.519203 MHz

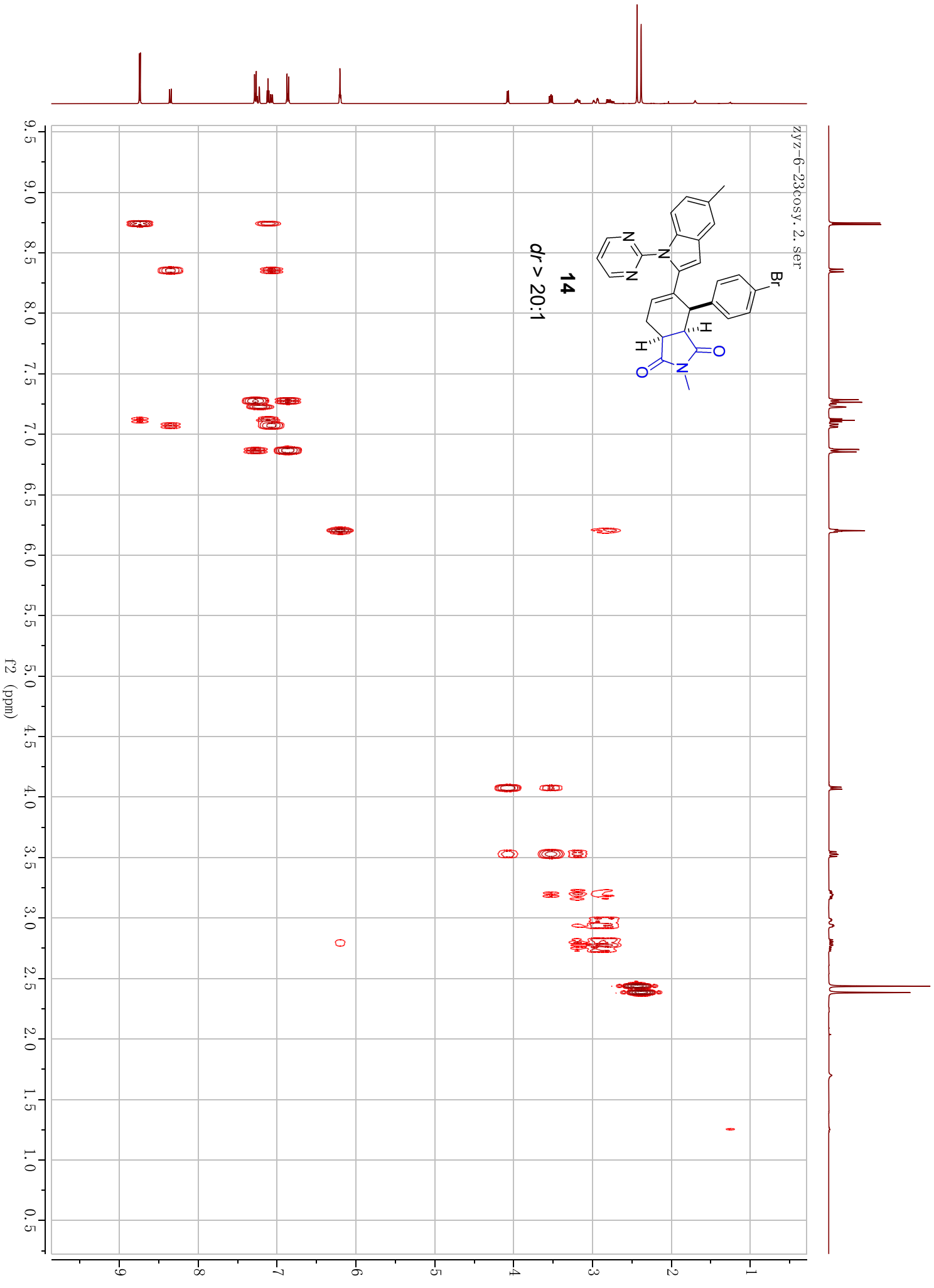


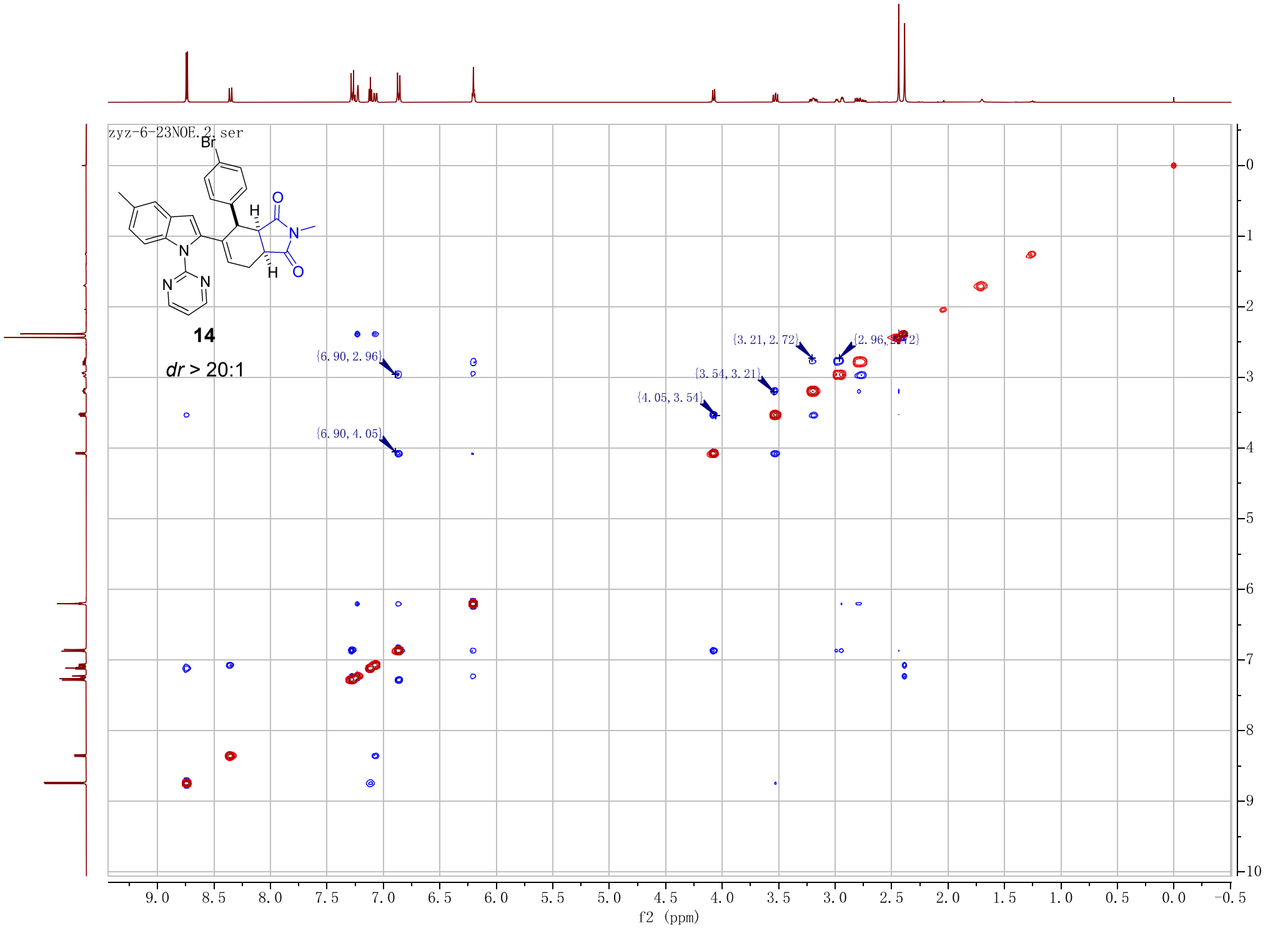
14

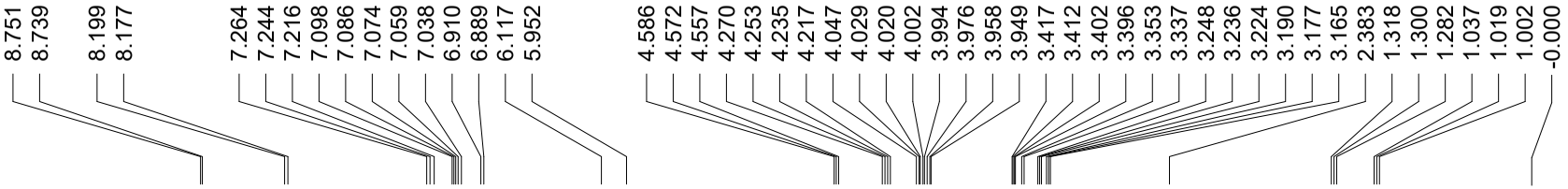
dr > 20:1



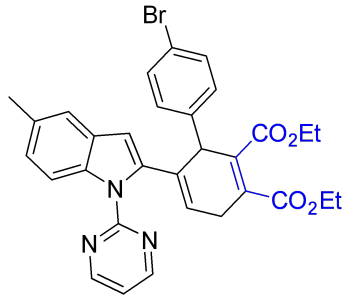

179.474
177.739
157.973
157.929
139.536
135.271
134.876
131.721
131.245
130.684
129.312
125.661
125.120
121.364
120.174
116.720
114.812
109.301
77.319
77.000
76.685
45.817
44.954
36.775
23.861
21.646
21.162
zyz-6-23C.fid
Jul 24 2020
SOLVENT: cdcl3
NA = 132
F1 = 100.598389 MHz
F2 = 400.030792 MHz
Br
O
H
N
N
N
N
H
O
14
dr > 20:1
S176
200
150
100
50
0
PPM


zyz-6-23cosy.2.ser
14
dr > 20:1
Br
N
N
N
H
H
O
O
N
f2 (ppm)
f1 (ppm)

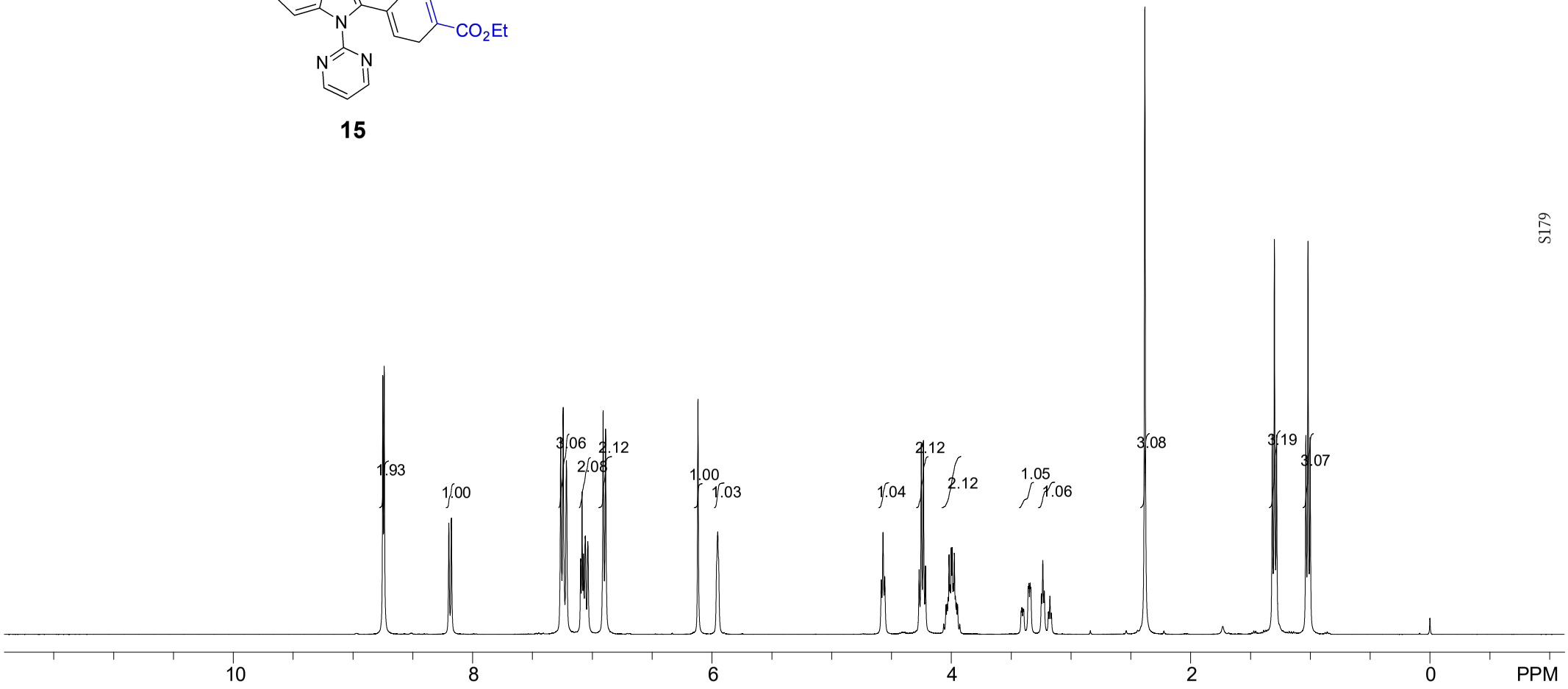

zyz-6-23NOE.2.ser
Br
O
H
N
O
N
N
H
O
14
dr > 20:1
{6.90, 2.96}
{6.90, 4.05}
{4.05, 3.54}
{3.54, 3.21}
{3.21, 2.72}
{2.96, 2.72}
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
-0.5
f2 (ppm)
0
1
2
3
4
5
6
7
8
9
10
f1 (ppm)
S178

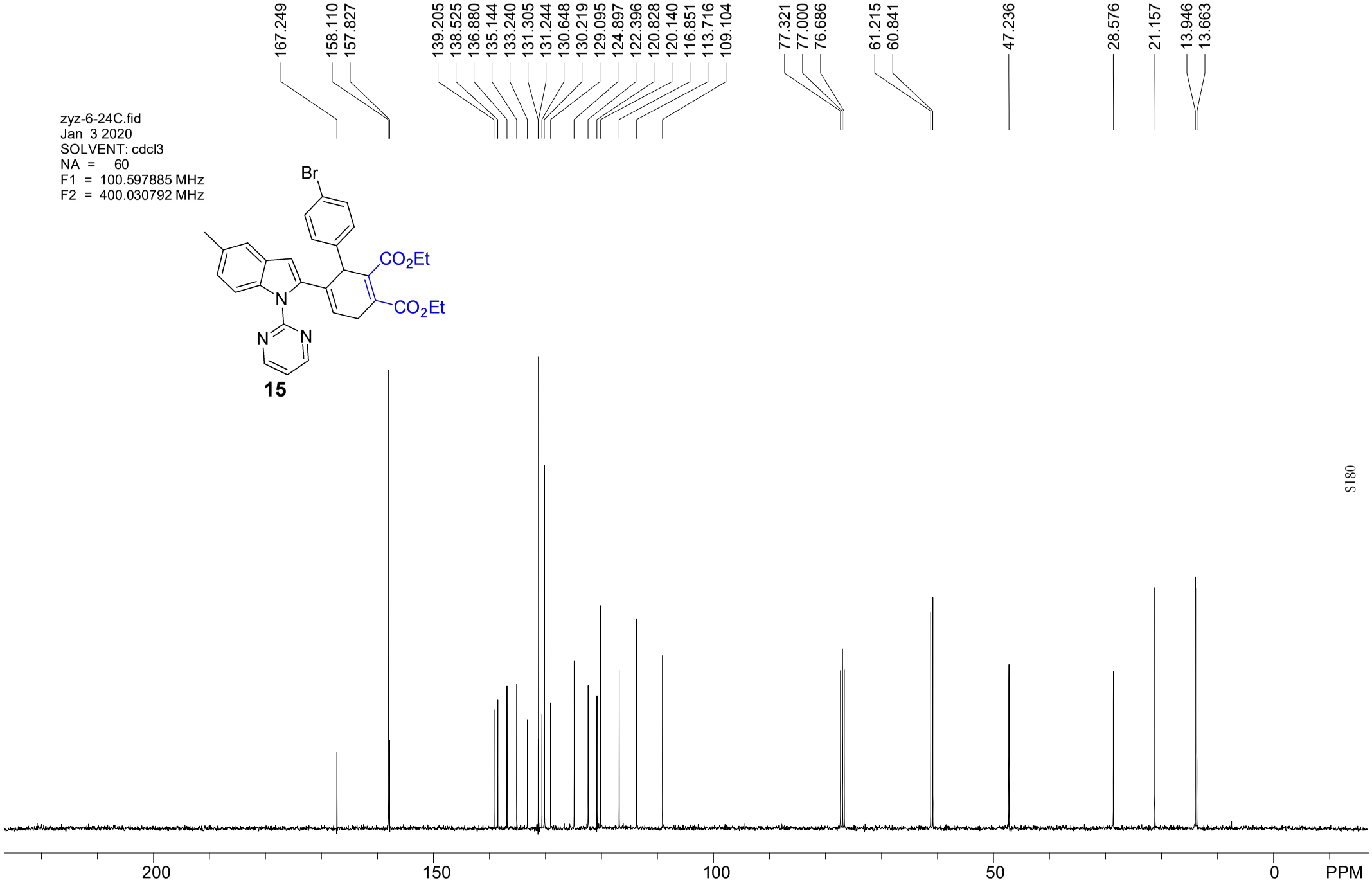


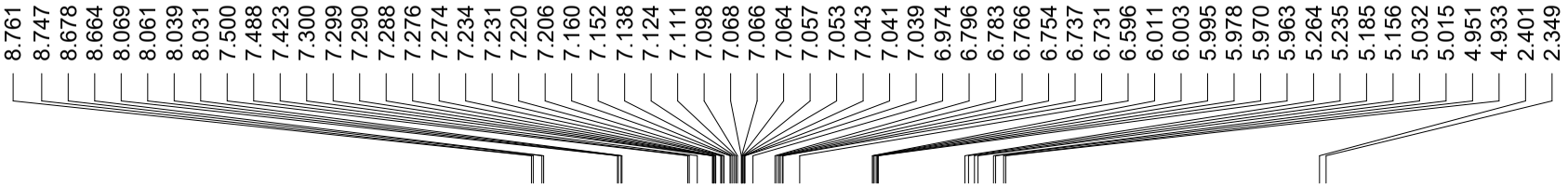
zyz-6-24H
Jan 1 2020
SOLVENT: CDCl3
NA = 8
F1 = 400.031219 MHz
F2 = 100.596855 MHz



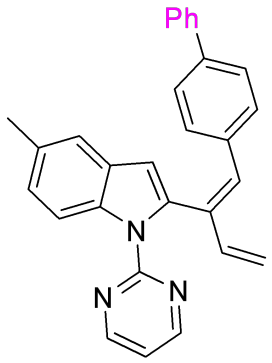
15




167.249
158.110
157.827
139.205
138.525
136.880
135.144
133.240
131.305
131.244
130.648
130.219
129.095
124.897
122.396
120.828
120.140
116.851
113.716
109.104
77.321
77.000
76.686
61.215
60.841
47.236
28.576
21.157
13.946
13.663
zyz-6-24C.fid
Jan 3 2020
SOLVENT: cdcl3
NA = 60
F1 = 100.597885 MHz
F2 = 400.030792 MHz
Br
CO2Et
CO2Et
N
N
N
15
S180
200
150
100
50
0
PPM

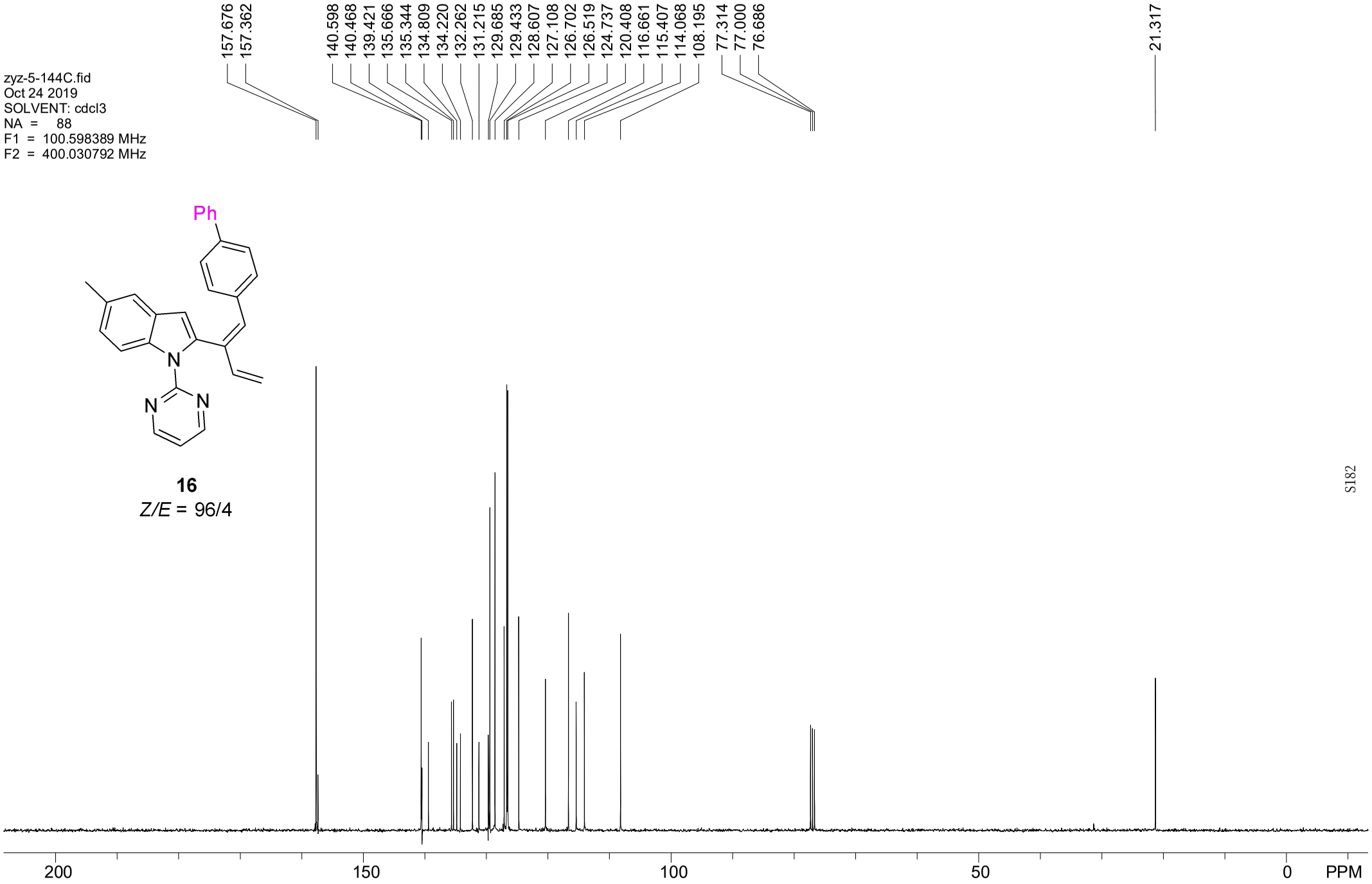


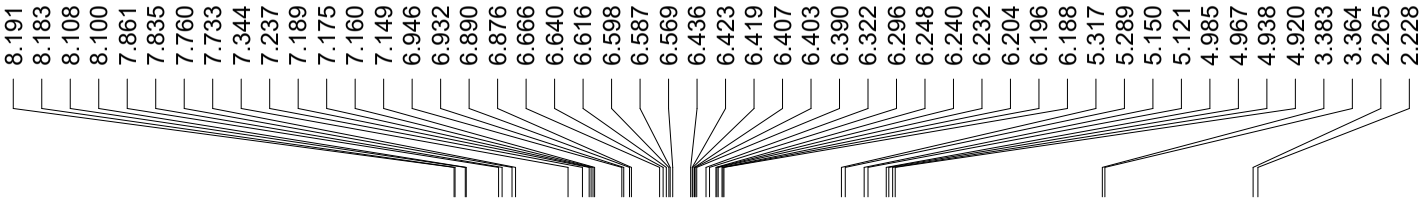
zyz-5-144-h-Q.fid
Sep 15 2020
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz



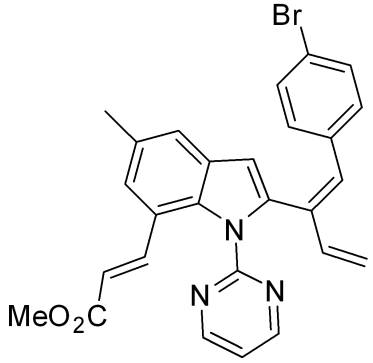
16
Z/E = 96/4

S181


157.676
157.362
140.598
140.468
139.421
135.666
135.344
134.809
134.220
132.262
131.215
129.685
129.433
128.607
127.108
126.702
126.519
124.737
120.408
116.661
115.407
114.068
108.195
77.314
77.000
76.686
21.317
zyz-5-144C.fid
Oct 24 2019
SOLVENT: cdcl3
NA = 88
F1 = 100.598389 MHz
F2 = 400.030792 MHz
Ph
N
N
N
16
Z/E = 96/4
S182
200
150
100
50
0
PPM

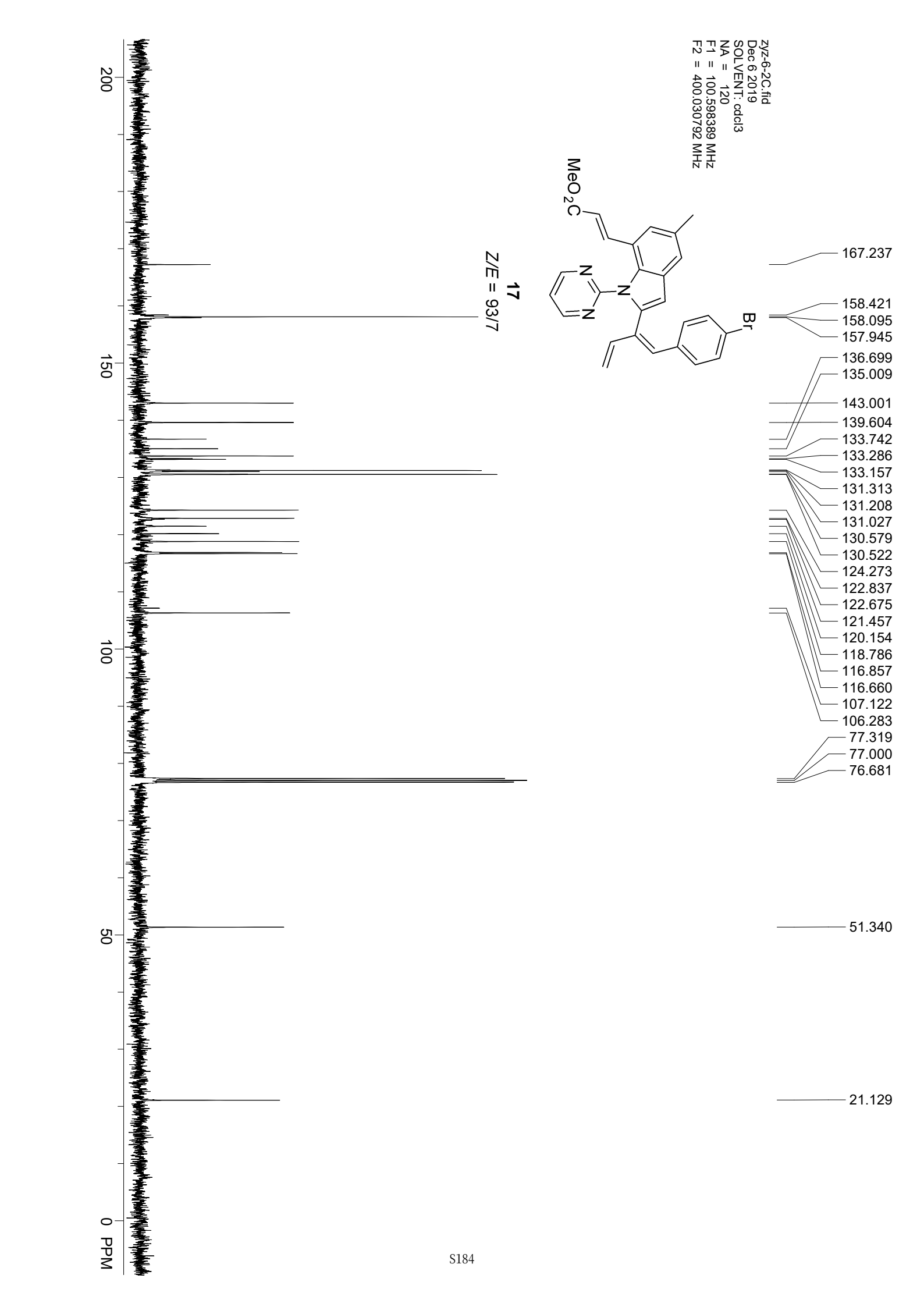


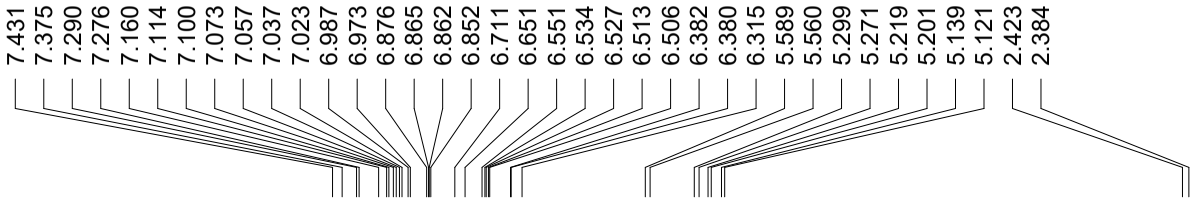
zyz-6-2-h1-Q.fid
Sep 24 2020
SOLVENT: c6d6
NA = 12
F1 = 599.772522 MHz
F2 = 150.826904 MHz



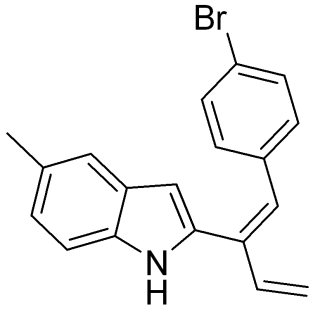
17
Z/E = 93/7

S183

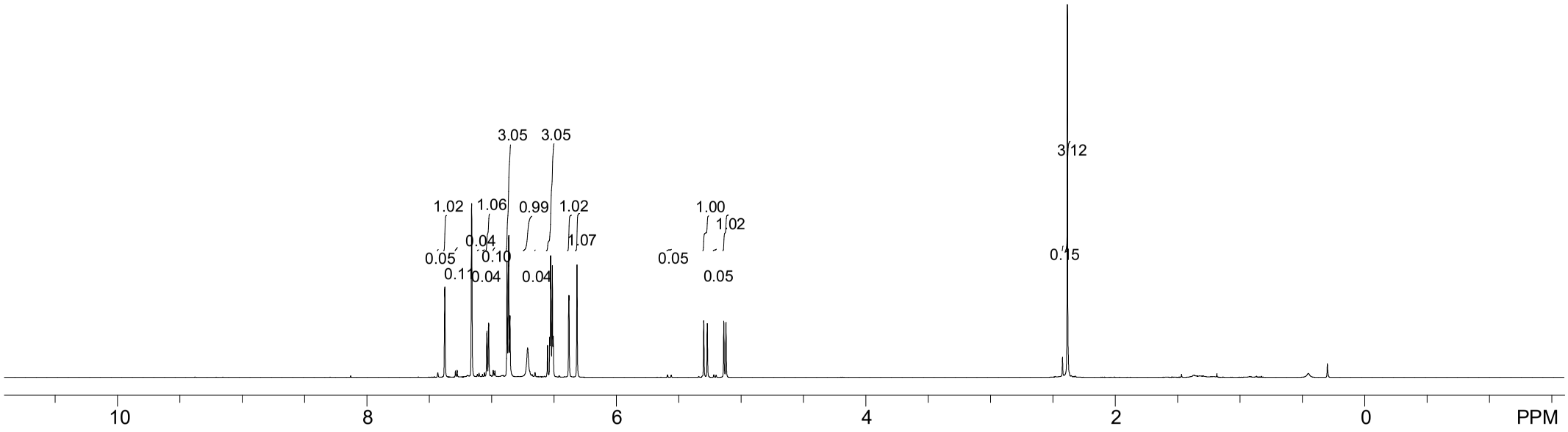

zyz-6-2C.fid
Dec 6 2019
SOLVENT: cdcl3
NA = 120
F1 = 100.598389 MHz
F2 = 400.030792 MHz
MeO2C
N
N
N
Br
17
Z/E = 93/7
167.237
158.421
158.095
157.945
136.699
135.009
143.001
139.604
133.742
133.286
133.157
131.313
131.208
131.027
130.579
130.522
124.273
122.837
122.675
121.457
120.154
118.786
116.857
116.660
107.122
106.283
77.319
77.000
76.681
51.340
21.129
200
150
100
50
0 PPM

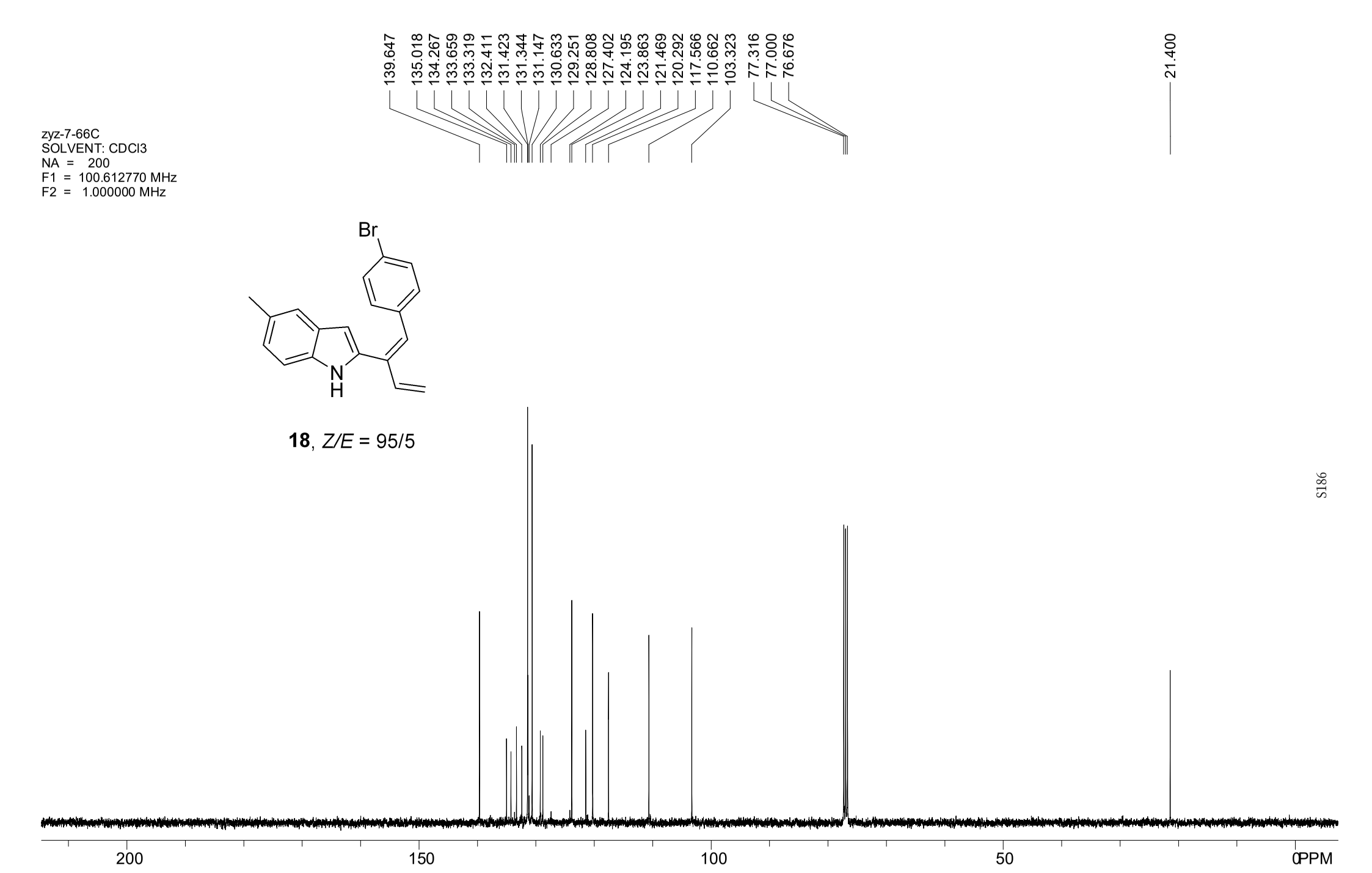


zyz-7-66-Q.fid
Jun 23 2021
SOLVENT: c6d6
NA = 16
F1 = 599.772522 MHz
F2 = 150.826904 MHz

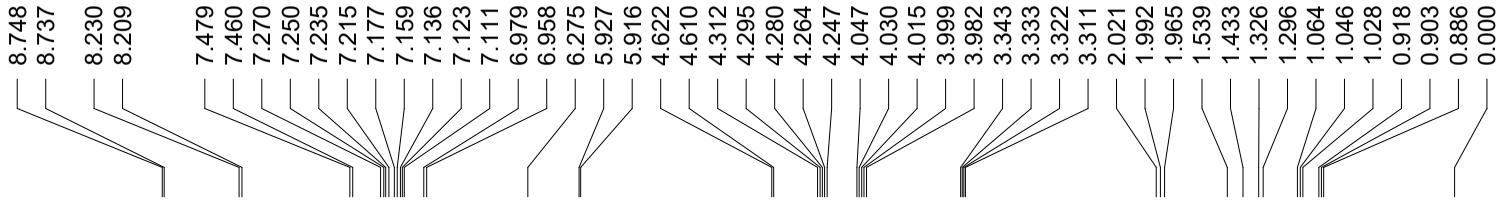


18, *Z/E* = 95/5

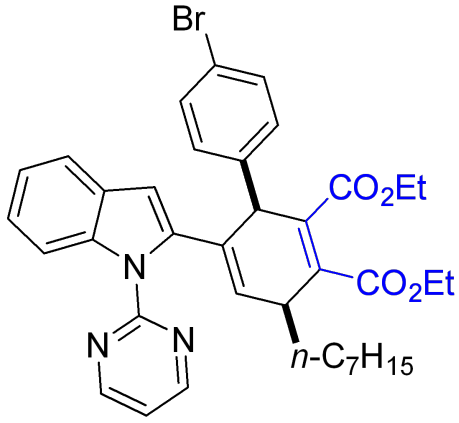



139.647
135.018
134.267
133.659
133.319
132.411
131.423
131.344
131.147
130.633
129.251
128.808
127.402
124.195
123.863
121.469
120.292
117.566
110.662
103.323
77.316
77.000
76.676
21.400
zyz-7-66C
SOLVENT: CDCl3
NA = 200
F1 = 100.612770 MHz
F2 = 1.000000 MHz
Br
N
H
200
150
100
50
0
PPM

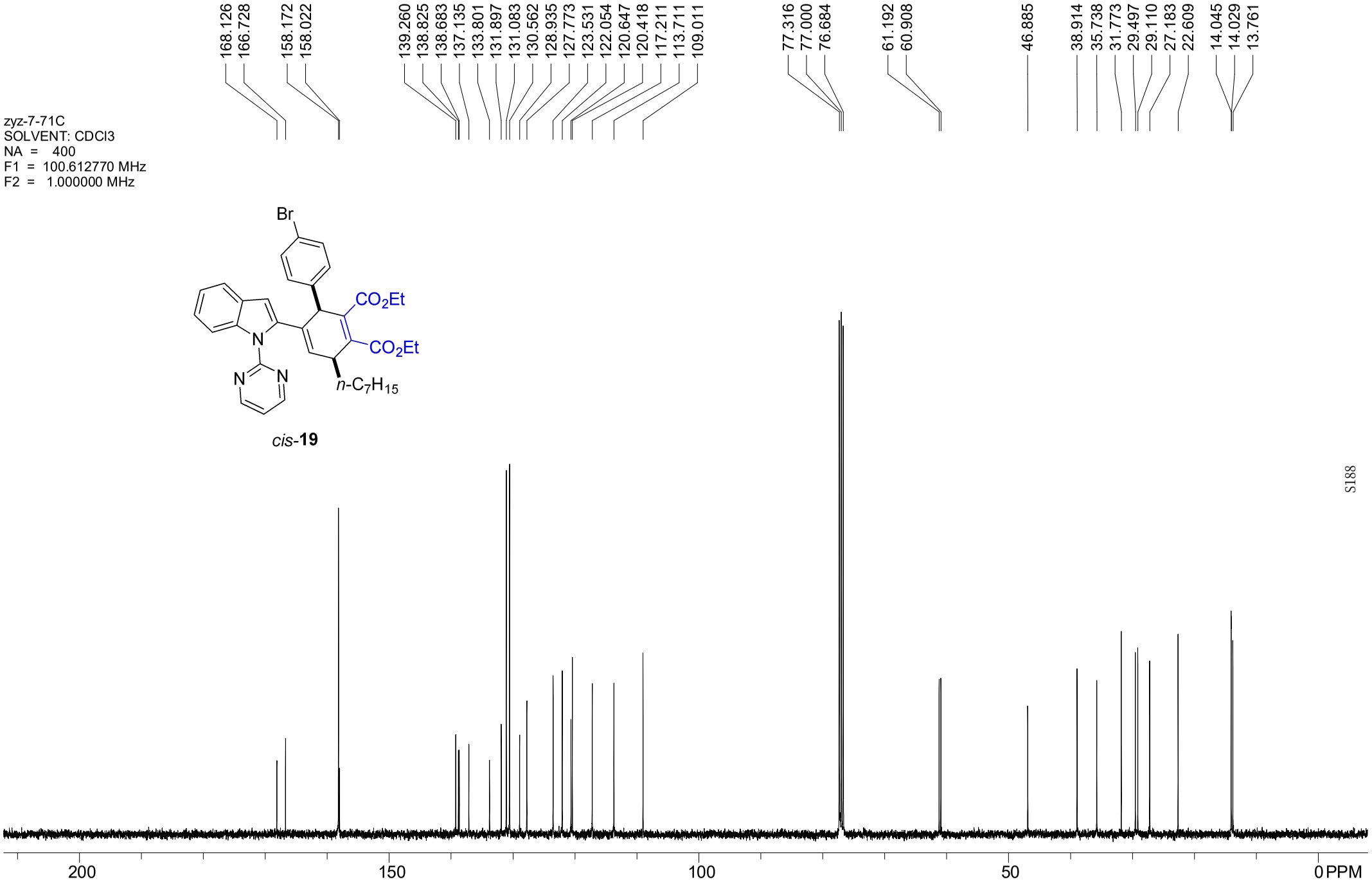
18, *Z/E* = 95/5

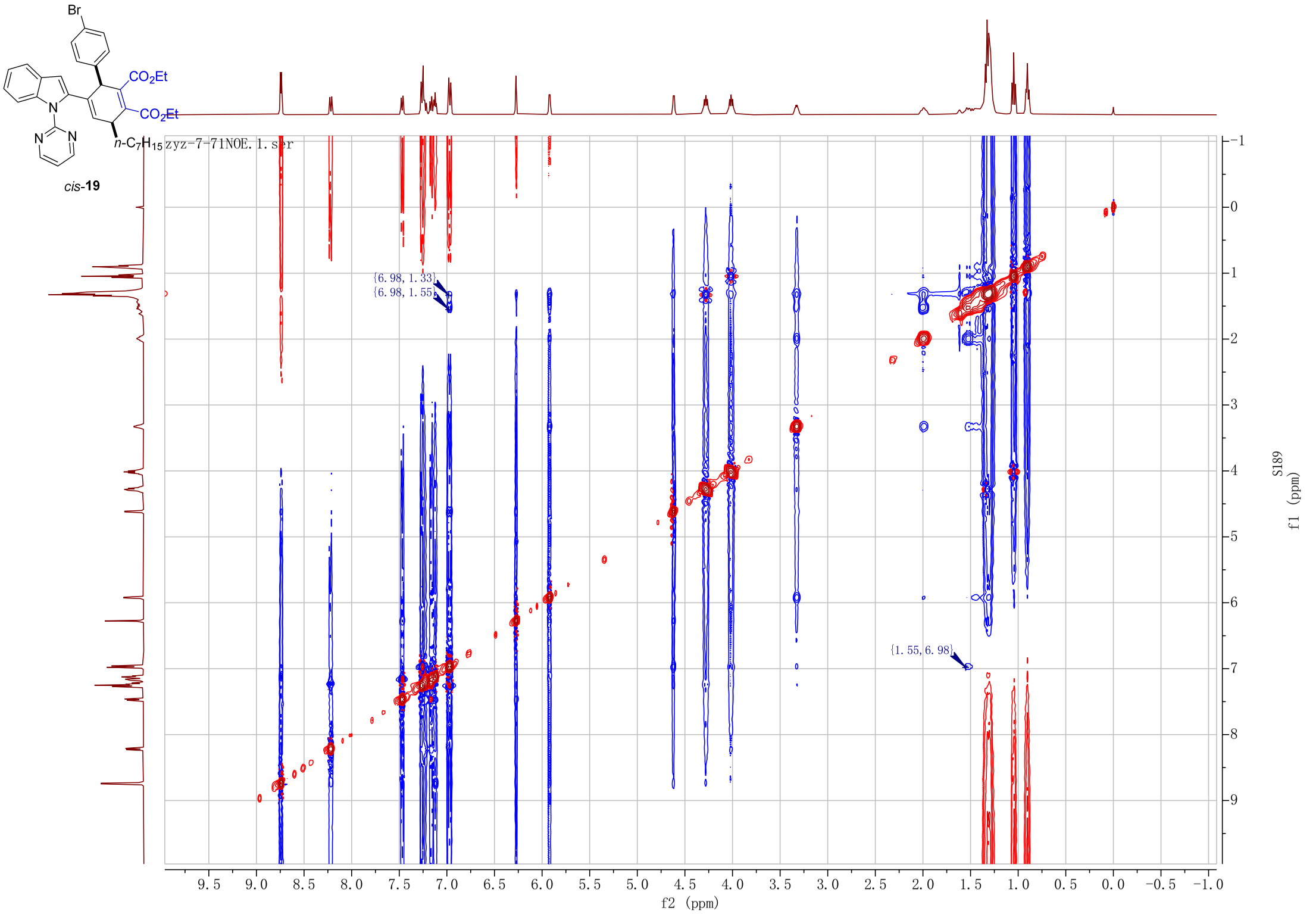


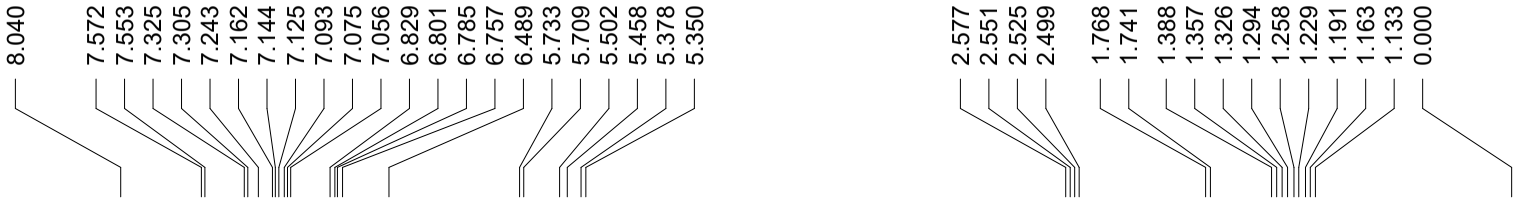
zyz-7-71H
SOLVENT: CDCl3
NA = 16
F1 = 400.130005 MHz
F2 = 1.000000 MHz



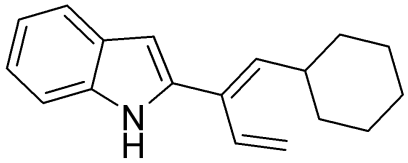
cis-**19**


168.126
166.728
158.172
158.022
139.260
138.825
138.683
137.135
133.801
131.897
131.083
130.562
128.935
127.773
123.531
122.054
120.647
120.418
117.211
113.711
109.011
77.316
77.000
76.684
61.192
60.908
46.885
38.914
35.738
31.773
29.497
29.110
27.183
22.609
14.045
14.029
13.761
zyz-7-71C
SOLVENT: CDCl3
NA = 400
F1 = 100.612770 MHz
F2 = 1.000000 MHz
Br
CO2Et
CO2Et
N
N
N
n-C7H15
cis-19
S188
200
150
100
50
0 PPM

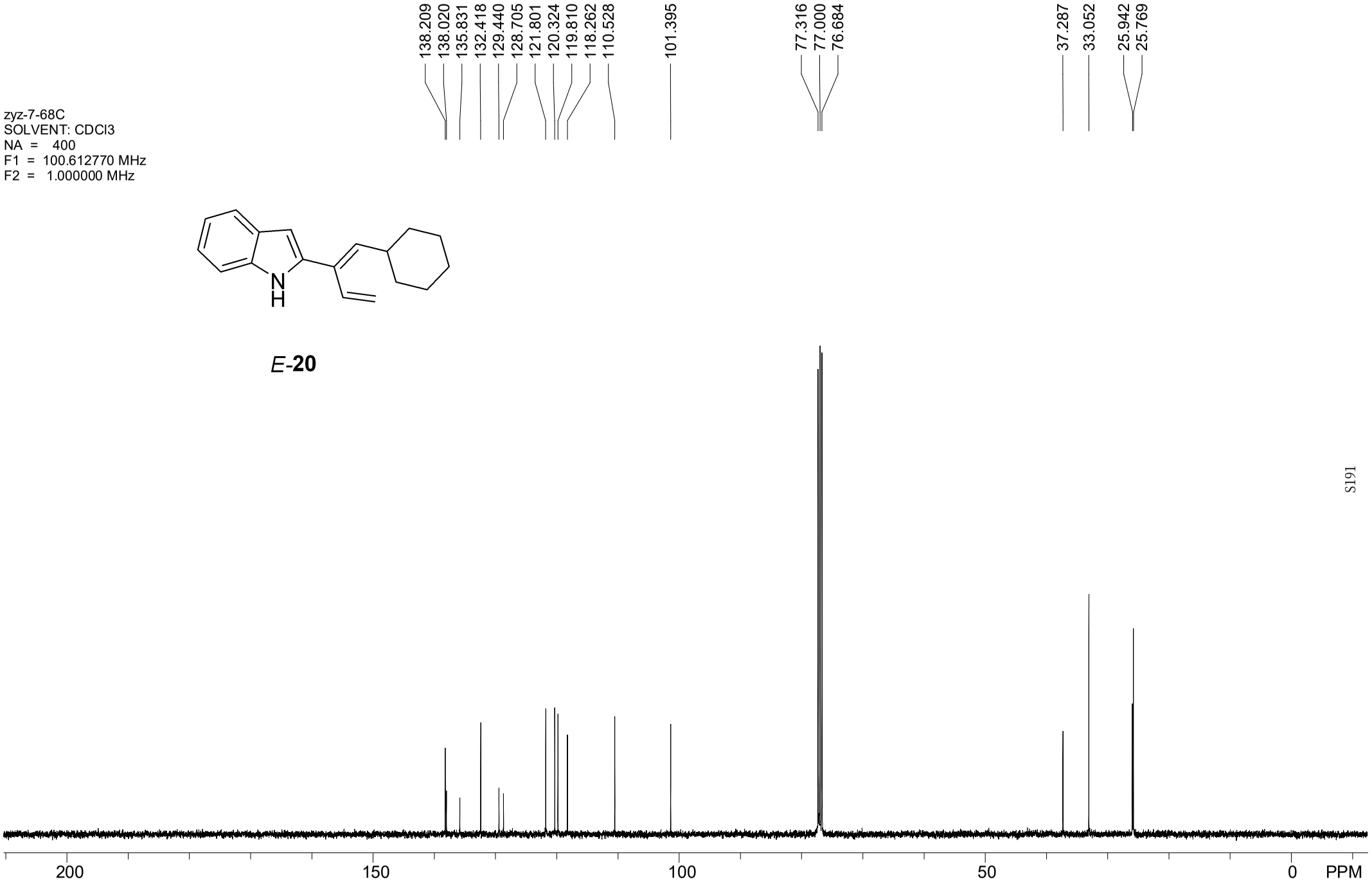

Br
CO2Et
CO2Et
n-C7H15
N
N
N
cis-19
zyz-7-71NOE.1.ser
{6.98, 1.33}
{6.98, 1.55}
{1.55, 6.98}
f2 (ppm)
f1 (ppm)
S189



zyz-7-68H
SOLVENT: CDCl3
NA = 8
F1 = 400.130005 MHz
F2 = 1.000000 MHz



E-**20**


138.209
138.020
135.831
132.418
129.440
128.705
121.801
120.324
119.810
118.262
110.528
101.395
77.316
77.000
76.684
37.287
33.052
25.942
25.769
zyz-7-68C
SOLVENT: CDCl3
NA = 400
F1 = 100.612770 MHz
F2 = 1.000000 MHz
N
H
E-20
200
150
100
50
0
PPM