ELECTRONIC SUPPLEMENTARY MATERIAL

Iron(III)-catalyzed tandem annulation of indolyl-substituted *p*-quinone methides with ynamides for the synthesis of cyclopenta[*b*]indoles

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General

All moisture or oxygen-sensitive reactions were carried out under an argon atmosphere in oven flasks. The solvent used was purified by distillation over the drying agent indicated and was transferred under argon: THF (Na). All reactions were monitored by thin-layer chromatography (TLC) on silica gel F_{254} plates using UV light as visualizing agent (if applicable). The products were purified by flash column chromatography on silica gel (200–300 meshes) from the Anhui Liangchen Silicon Material Company in China.

^{1}H NMR and ^{13}C NMR spectra were recorded in $CDCl_3$ or $(CD_3)_2SO$ on Bruker AVANCE^{III} 400 MHz, Bruker AVANCE^{III} HD 400 MHz or Bruker AVANCE NEO 600 MHz instrument. Chemical shifts were denoted in ppm (δ) and calibrated by using residual undeuterated solvent (*7.26 ppm for residual undeuterated $CDCl_3$, 2.50 ppm for residual undeuterated $(CD_3)_2SO$ or tetramethylsilane (0.00 ppm)*) as internal reference for ^{1}H NMR and the deuterated solvent (*$CDCl_3$ (77.00 ppm), $(CD_3)_2SO$ (39.50 ppm) or tetramethylsilane (0.00 ppm)*) as internal standard for ^{13}C NMR. The following abbreviations were used to explain the multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, dd = double doublet, br = broad, m = multiplet. The high-resolution mass spectral analysis (HRMS) data were measured on a Bruker ApexII mass spectrometer by means of the ESI technique. The IR spectra were recorded on a Nicolet Nexus 670 FT-IR spectrometer. The X-ray single-crystal determination was performed on an Agilent SuperNova or a Rigaku XtaLAB Synergy R single crystal diffractometer. The melting points were measured on a Kolfer melting point apparatus without calibration (Beijing Tech Instrument Co., LTD).

1. Preparation of Indolyl-Substituted *p*-Quinone Methides

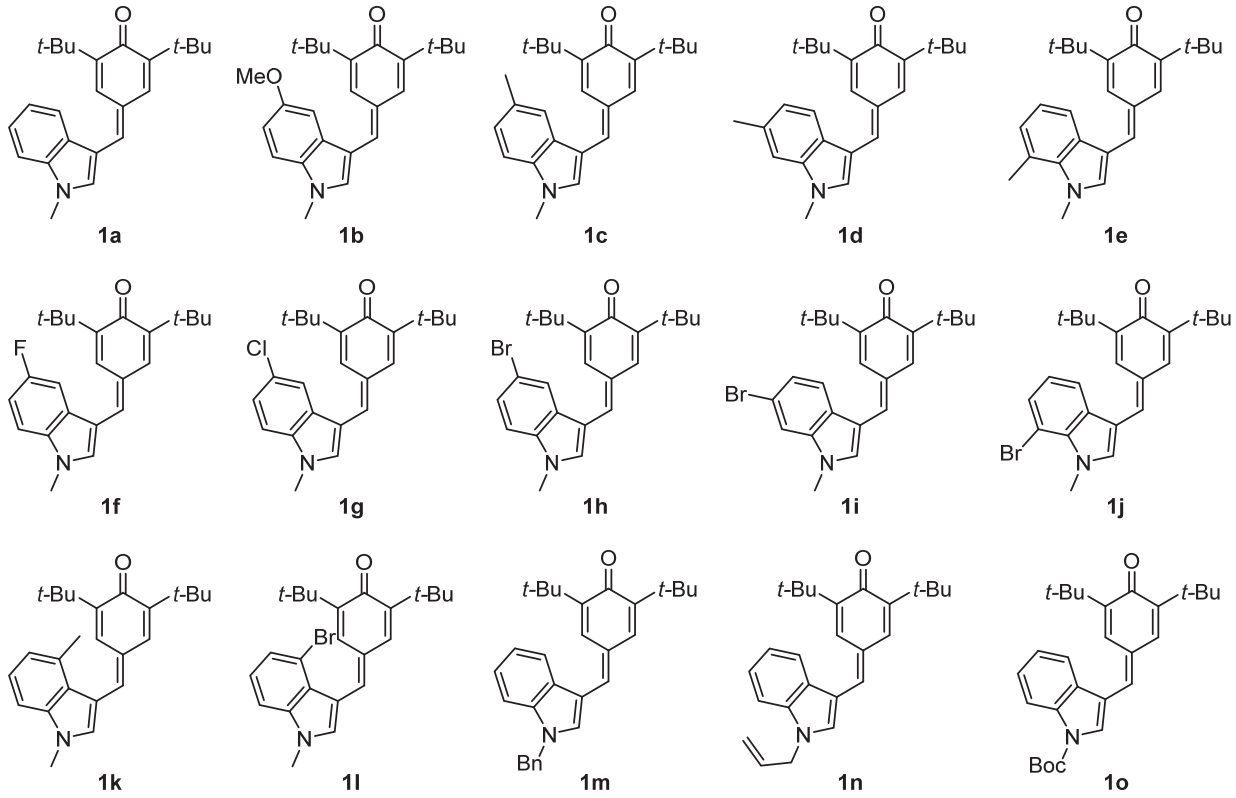
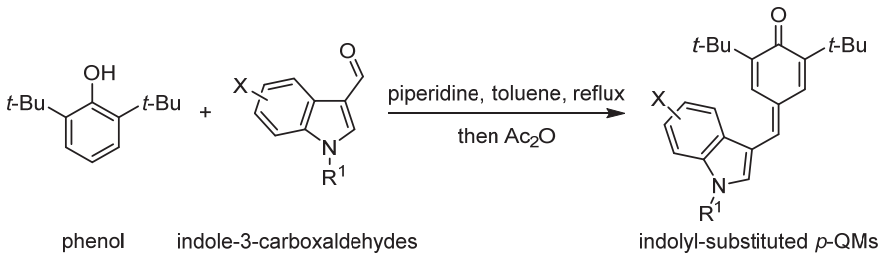


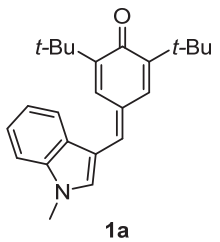
Figure S1. Indolyl-substituted *p*-quinone methides employed in tandem reaction

The indolyl-substituted *p*-quinone methides **1a–1o**[1] were prepared according to the reported methods. The General Procedure was as follows:



In a Dean-Stark apparatus, the solution of 2,6-di-*tert*-butylphenol (20 mmol) and indole-3-carboxaldehydes (20 mmol) in toluene was heated to reflux for 1 h. Piperidine (40 mmol) was added dropwise via the syringe within 2 h and then held to reflux for 12 h. After cooling just below the boiling point of the reaction mixture, acetic anhydride (40 mmol) was added and stirred for 0.5 h. Then the mixture was poured into ice-water and extracted with CH_2Cl_2. The combined organic phases were dried over Na_2SO_4. After filtration, the filtrate was concentrated under reduced pressure. The crude products were purified by flash column chromatography on silica gel with the elution of petroleum ether/ethyl acetate to give the corresponding indolyl-substituted *p*-quinone methides **1a**–**1o**.

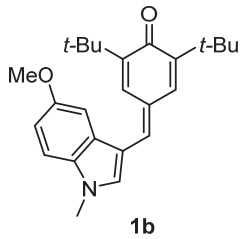
2,6-Di-*tert*-butyl-4-((1-methyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1a

1a:**^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.79 (d, J = 8.4 Hz, 1H), 7.71 (d, J = 2.4 Hz, 1H), 7.46 (s, 1H), 7.41–7.36 (m, 2H), 7.36–7.32 (m, 1H), 7.30–7.25 (m, 1H), 7.11 (d, J = 1.8 Hz, 1H), 3.89 (s, 3H), 1.375 (s, 9H), 1.367 (s, 9H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 186.3, 148.0, 145.9, 137.0, 135.4, 134.8, 131.4, 128.1, 128.0, 127.9, 123.4, 121.3, 119.2, 112.9, 109.9, 35.4, 34.9, 33.6, 29.7, 29.6 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2953, 1620, 1548, 1513, 1485, 1358, 1292, 1246, 1117, 1041, 950 cm^{-1}.

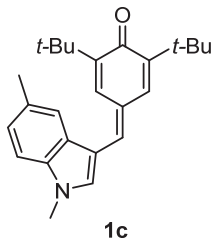
2,6-Di-*tert*-butyl-4-((5-methoxy-1-methyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1b

1b:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.69 (d, J = 2.4 Hz, 1H), 7.43 (s, 1H), 7.33 (s, 1H), 7.24 (d, J = 2.4 Hz, 1H), 7.21 (d, J = 2.0 Hz, 1H), 7.12 (d, J = 2.4 Hz, 1H), 6.98 (dd, J = 8.8, 2.4 Hz, 1H), 3.90 (s, 3H), 3.86 (s, 3H), 1.374 (s, 9H), 1.368 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 155.6, 147.9, 145.7, 135.4, 134.9, 132.2, 131.7, 128.8, 127.9, 127.4, 113.6, 112.5, 110.8, 100.8, 55.8, 35.4, 34.9, 33.7, 29.7, 29.6 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2920, 2093, 1643, 1513, 1358, 1292, 1245, 1117, 1043 cm^{-1}.

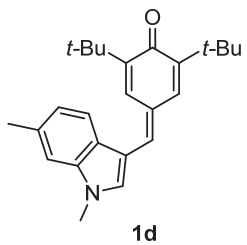
2,6-Di-*tert*-butyl-4-((1,5-dimethyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1c

1c:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.70 (d, J = 2.4 Hz, 1H), 7.58 (s, 1H), 7.39 (s, 1H), 7.33 (s, 1H), 7.22 (d, J = 8.4 Hz, 1H), 7.13 (dd, J = 8.4, 1.2 Hz, 1H), 7.09 (d, J = 2.4 Hz, 1H), 3.80 (s, 3H), 2.48 (s, 3H), 1.38 (s, 9H), 1.37 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.2, 147.6, 145.6, 135.48, 135.46, 135.2, 131.6, 130.8, 128.2, 128.1, 127.4, 124.9, 119.0, 112.5, 109.6, 35.3, 34.8, 33.5, 29.6, 29.5, 21.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2954, 2090, 1627, 1549, 1514, 1485, 1357, 1247, 1119 cm^{-1}.

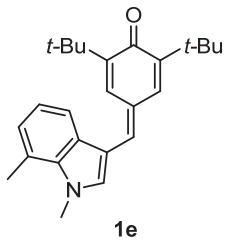
2,6-Di-*tert*-butyl-4-((1,6-dimethyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1d

1d:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.71 (d, J = 2.4 Hz, 1H), 7.68 (d, J = 2.4 Hz, 1H), 7.40 (s, 1H), 7.36 (s, 1H), 7.16 (s, 1H), 7.14–7.07 (m, 2H), 3.85 (s, 3H), 2.52 (s, 3H), 1.37 (s, 9H), 1.36 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 147.8, 145.8, 137.5, 135.5, 135.1, 133.4, 131.1, 128.0, 127.7, 125.9, 123.1, 118.9, 112.9, 109.9, 35.4, 34.9, 33.5, 29.7, 29.6, 21.8 ppm. **IR** (film): $\bar{\upsilon}$ = 3441, 2954, 2079, 1625, 1548, 1515, 1466, 1357, 1305, 1248, 1116 cm^{-1}.

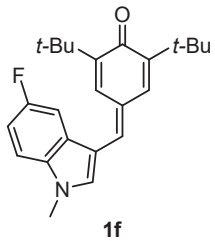
2,6-Di-*tert*-butyl-4-((1,7-dimethyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1e

1e:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.68 (d, J = 2.4 Hz, 1H), 7.62 (d, J = 8.0 Hz, 1H), 7.35 (s, 2H), 7.40–7.32 (m, 2H), 7.02 (d, J = 6.8 Hz, 1H), 4.14 (s, 3H), 2.78 (s, 3H), 1.37 (s, 9H), 1.36 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 147.9, 145.8, 135.7, 135.4, 134.7, 133.0, 129.3, 128.0, 127.9, 126.1, 121.9, 121.5, 117.1, 112.5, 37.7, 35.4, 34.9, 29.7, 29.6, 19.6 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2946, 2064, 1634, 1545, 1453, 1357, 1252, 1077, 953, 744 cm^{-1}.

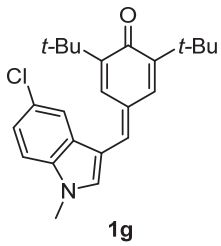
2,6-Di-*tert*-butyl-4-((5-fluoro-1-methyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1f

1f:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.65 (d, J = 2.0 Hz, 1H), 7.48 (s, 1H), 7.42 (dd, J = 9.2, 2.4 Hz, 1H), 7.28 (dd, J = 8.8, 4.0 Hz, 1H), 7.24 (s, 1H), 7.11–7.03 (m, 2H), 3.88 (s, 3H), 1.37 (s, 9H), 1.36 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 158.9 (d, $^{1}J_{C\text{-}F}$ = 236.6 Hz), 148.1, 146.0, 135.3, 134.0, 133.6, 132.6, 128.7 (d, $^{3}J_{C\text{-}F}$ = 9.6 Hz), 128.0, 127.8, 112.7 (d, $^{4}J_{C\text{-}F}$ = 4.6 Hz), 111.7 (d, $^{2}J_{C\text{-}F}$ = 26.2 Hz), 110.8 (d, $^{3}J_{C\text{-}F}$ = 9.7 Hz), 104.5 (d, $^{2}J_{C\text{-}F}$ = 24.1 Hz), 35.4, 34.9, 33.8, 29.6, 29.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2090, 1633, 1553, 1482, 1288, 1111, 1021, 952 cm^{-1}.

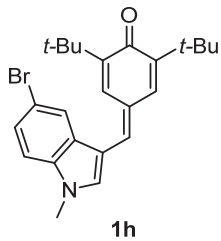
2,6-Di-*tert*-butyl-4-((5-chloro-1-methyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1g

1g:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.76–7.73 (m, 1H), 7.64 (d, J = 2.4 Hz, 1H), 7.44 (s, 1H), 7.29–7.25 (m, 2H), 7.23 (s, 1H), 7.07 (d, J = 2.4 Hz, 1H), 3.87 (s, 3H), 1.37 (s, 9H), 1.36 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 148.2, 146.2, 135.4, 135.3, 133.6, 132.2, 129.0, 128.4, 127.8, 127.3, 123.6, 118.9, 112.4, 111.0, 35.4, 34.9, 33.7, 29.6, 29.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2954, 2082, 1626, 1551, 1515, 1470, 1358, 1285, 1246, 1125, 728 cm^{-1}.

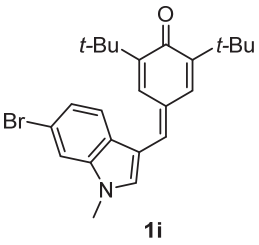
4-((5-Bromo-1-methyl-1*H*-indol-3-yl) methylene)-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one



1h

1h:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.89 (d, J = 1.2 Hz, 1H), 7.63 (d, J = 2.0 Hz, 1H), 7.41 (s, 1H), 7.37 (dd, J = 8.8, 1.6 Hz, 1H), 7.20 (d, J = 9.2 Hz, 2H), 7.07 (d, J = 2.0 Hz, 1H), 3.85 (s, 3H), 1.37 (s, 9H), 1.36 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 148.2, 146.1, 135.7, 135.2, 133.6, 132.1, 129.5, 128.4, 127.8, 126.1, 122.0, 114.7, 112.3, 111.4, 35.4, 34.9, 33.7, 29.6, 29.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3362, 2954, 1602, 1550, 1516, 1469, 1355, 1284, 1253, 1125, 946, 855, 817, 620 cm^{-1}.

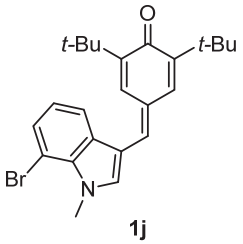
4-((6-Bromo-1-methyl-1*H*-indol-3-yl) methylene)-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one



1i

1i:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.66–7.60 (m, 2H), 7.52 (d, J = 1.6 Hz, 1H), 7.41 (s, 1H), 7.35 (dd, J = 8.4, 1.6 Hz, 1H), 7.27 (s, 1H), 7.08 (d, J = 2.4 Hz, 1H), 3.85 (s, 3H), 1.362 (s, 9H), 1.356 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.4, 148.3, 146.2, 137.8, 135.3, 133.7, 131.6, 128.6, 127.7, 126.8, 124.4, 120.5, 116.9, 113.0, 112.9, 35.4, 34.9, 33.6, 29.6, 29.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3396, 2955, 1611, 1550, 1515, 1468, 1359, 1297, 1243, 1129, 1057, 1030, 844, 801, 739 cm^{-1}.

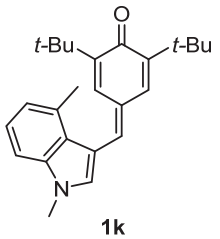
4-((7-Bromo-1-methyl-1*H*-indol-3-yl) methylene)-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one



1j

1j:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.69 (dd, J = 8.0, 0.8 Hz, 1H), 7.63 (d, J = 2.4 Hz, 1H), 7.45 (d, J = 7.2 Hz, 1H), 7.37 (s, 1H), 7.28 (s, 1H), 7.09 (d, J = 2.0 Hz, 1H), 7.06 (t, J = 8.0 Hz, 1H), 4.25 (s, 3H), 1.362 (s, 9H), 1.356 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.4, 148.4, 146.3, 135.2, 133.8, 133.5, 133.3, 131.1, 128.8, 128.3, 127.8, 122.2, 118.4, 112.3, 104.5, 37.8, 35.4, 34.9, 29.6, 29.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3426, 2948, 1550, 1521, 1451, 1301, 1128, 1076, 1019, 946, 799, 776, 733 cm^{-1}.

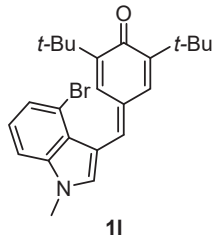
2,6-Di-*tert*-butyl-4-((1,4-dimethyl-1*H*-indol-3-yl) methylene) cyclohexa-2,5-dien-1-one



1k

1k:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.69 (s, 1H), 7.67–7.63 (m, 1H), 7.31 (s, 1H), 7.24–7.18 (m, 2H), 7.12–7.06 (m, 1H), 7.04–6.97 (m, 1H), 3.86 (s, 3H), 2.78 (s, 3H), 1.37 (s, 9H), 1.36 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.6, 148.1, 145.9, 138.1, 137.6, 135.1, 132.2, 131.7, 128.3, 128.1, 126.4, 123.3, 123.1, 114.0, 107.9, 35.3, 34.9, 33.6, 29.7, 29.6, 21.2 ppm. **IR** (film): $\bar{\upsilon}$ = 3440, 2954, 1634, 1545, 1517, 1460, 1355, 1300, 1252, 1072, 909, 744 cm^{-1}.

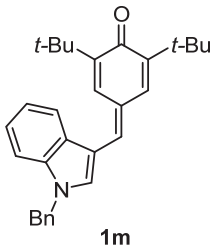
4-((4-Bromo-1-methyl-1*H*-indol-3-yl) methylene)-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one



1l

1l:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 8.14 (s, 1H), 7.60 (d, J = 2.4 Hz, 1H), 7.40 (d, J = 7.6 Hz, 1H), 7.32 (d, J = 8.8 Hz, 2H), 7.18–7.10 (m, 2H), 3.88 (s, 3H), 1.36 (s, 9H), 1.35 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.7, 148.3, 146.1, 138.4, 136.4, 135.3, 132.9, 128.3, 127.9, 125.8, 125.6, 123.9, 114.8, 113.3, 109.3, 35.3, 34.9, 33.7, 29.6, 29.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3404, 2954, 1603, 1546, 1518, 1449, 1358, 1296, 1131, 1019, 946, 735 cm^{-1}.

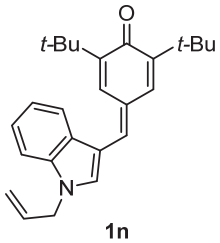
4-((1-Benzyl-1*H*-indol-3-yl) methylene)-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one



1m

1m:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.84–7.78 (m, 1H), 7.61 (d, J = 2.0 Hz, 1H), 7.45 (s, 1H), 7.41–7.38 (m, 2H), 7.38–7.32 (m, 3H), 7.32–7.21 (m, 4H), 7.10 (d, J = 2.4 Hz, 1H), 5.36 (s, 2H), 1.35 (s, 9H), 1.29 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.3, 148.0, 146.0, 136.7, 135.6, 135.2, 134.5, 130.6, 129.1, 128.4 (2C), 128.3, 128.0, 127.5, 123.5, 121.5, 119.3, 113.3, 110.3, 50.7, 35.4, 34.9, 29.57, 29.56 ppm. **IR** (film): $\bar{\upsilon}$ = 3409, 2920, 1632, 1551, 1514, 1468, 1387, 1358, 1088, 1043, 1020 cm^{-1}.

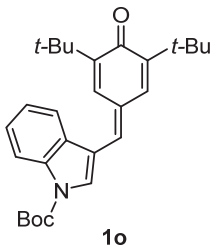
4-((1-Allyl-1*H*-indol-3-yl) methylene)-2,6-di-*tert*-butylcyclohexa-2,5-dien-1-one



1n

1n:**^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.80 (d, J = 7.6 Hz, 1H), 7.70 (d, J = 2.4 Hz, 1H), 7.52 (s, 1H), 7.41–7.36 (m, 2H), 7.35–7.30 (m, 1H), 7.30–7.24 (m, 1H), 7.11 (d, J = 2.4 Hz, 1H), 6.11–5.99 (m, 1H), 5.32 (d, J = 10.4 Hz, 1H), 5.22 (d, J = 17.2 Hz, 1H), 4.80 (d, J = 5.6 Hz, 2H), 1.364 (s, 9H), 1.361 (s, 9H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 186.4, 148.0, 146.0, 136.5, 135.3, 134.6, 132.2, 130.4, 128.3, 128.2, 128.1, 123.4, 121.4, 119.3, 118.7, 113.2, 110.2, 49.3, 35.4, 34.9, 29.60, 29.56 ppm. **IR** (film): $\bar{\upsilon}$ = 3444, 2956, 2079, 1634, 1551, 1516, 1472, 1354, 1246, 1121 cm^{-1}.

***tert*-Butyl 3-((3,5-di-*tert*-butyl-4-oxocyclohexa-2,5-dien-1-ylidene) methyl)-1*H*-indole-1-carboxylate**



1o

1o:**^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.22 (d, J = 7.2 Hz, 1H), 7.93 (s, 1H), 7.73–7.68 (m, 2H), 7.41 (t, J = 7.2 Hz, 1H), 7.34 (t, J = 7.2 Hz, 1H), 7.23 (s, 1H), 7.10 (d, J = 1.8 Hz, 1H), 1.70 (s, 9H), 1.358 (s, 9H), 1.355 (s, 9H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 186.7, 149.0, 148.9, 147.2, 135.3, 134.7, 131.8 (2C), 129.6, 127.7, 127.1, 125.5, 123.5, 119.0, 116.9, 115.4, 84.7, 35.5, 35.0, 29.5 (2C), 28.1 ppm. **IR** (film): $\bar{\upsilon}$ = 3443, 2958, 2074, 1633, 1447, 1376, 1173, 1137, 1095, 1021 cm^{-1}.

2. Preparation of Ynamides

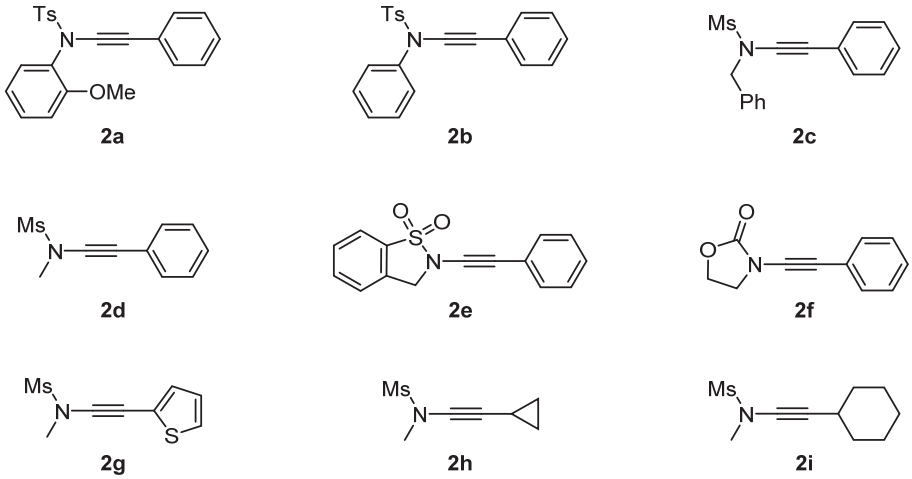
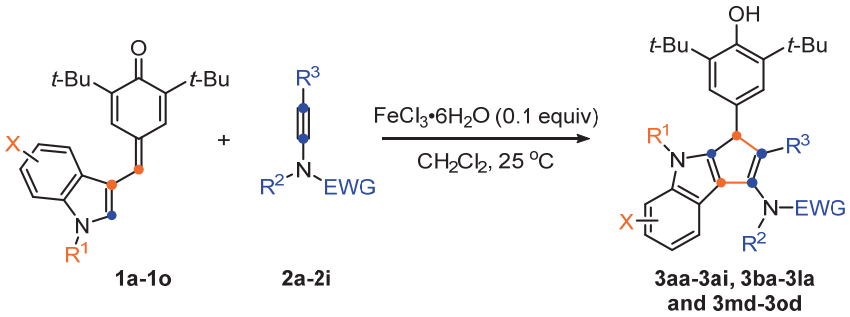


Figure S2. Ynamides employed in tandem reaction

The ynamides **2a**–**2c**[2a], **2d**[2b], **2e**[2c], **2f**[2d], **2g**–**2h**[2e], and **2i**[2f] were prepared according to the reported methods.

3. Tandem (2+2) Annulation/*retro*-4π Electrocyclization/Imino-Nazarov Cyclization Reaction of Indolyl-Substituted *p*-QMs with Ynamides

3.1. General Procedure for Tandem Annulation

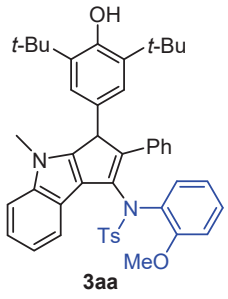


1a-1o **2a-2i** **3aa-3ai, 3ba-3la and 3md-3od**

To a solution of indolyl-substituted *p*-quinone methides **1a**–**1o** (0.1 mmol) and ynamides **2a**–**2i** (0.11 mmol) in CH_2Cl_2 (1.0 mL) was added $FeCl_3 \cdot 6H_2O$ (0.01 mmol). The resulting mixture was stirred at 25 °C for the indicated time. The solvent was concentrated under reduced pressure, and then the resulting residue was purified by flash column chromatography on silica gel with the elution of petroleum ether/dichloromethane to give the corresponding products **3aa–3ai**, **3ba**–**3la** and **3md**–**3od**.

3.2. Spectroscopic Data for Aminocyclopenta[*b*]indoles 3

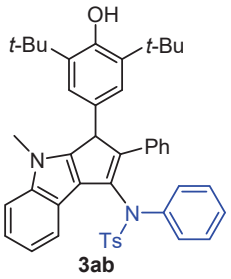
***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**



3aa

3aa: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3 \cdot 6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3aa** (66.0 mg, 91% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.92 (br, 1H), 7.67 (d, J = 7.8 Hz, 2H), 7.29 (d, J = 8.2 Hz, 1H), 7.22–7.12 (m, 4H), 7.10 (t, J = 7.4 Hz, 1H), 7.03 (t, J = 7.3 Hz, 1H), 6.93 (t, J = 7.5 Hz, 2H), 6.85–6.57 (m, 6H), 6.52 (t, J = 7.2 Hz, 1H), 4.97 (s, 1H), 4.60 (s, 1H), 3.53 (s, 3H), 3.39 (s, 3H), 2.42 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.0, 152.6, 149.7, 142.7, 142.0, 140.8, 138.6, 135.8, 135.7, 135.1, 130.2 (2C), 129.5, 128.8, 128.6, 128.1, 127.1, 126.4, 125.8, 124.7, 122.0, 121.7, 120.9, 120.4, 119.8, 119.5, 111.6, 109.1, 54.8, 51.5, 34.1, 30.7, 30.2, 21.5 ppm. **IR** (film): $\tilde{\upsilon}$ = 3361, 2921, 1598, 1462, 1433, 1349, 1265, 1161, 1090, 1029, 738, 588 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{49}N_2O_4S$ [M + H]$^+$: 725.3408; found: 725.3401.

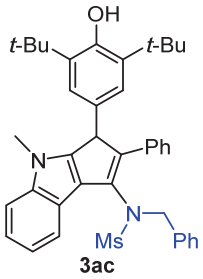
***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-4-methyl-*N*-phenylbenzenesulfonamide**



3ab

3ab: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2b** (38.2 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3ab** (60.4 mg, 87% yield, 2:1 *dr*, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$, mixed isomers of **3ab** (*2:1 dr*)) δ = 7.80–7.45 (m, 4.96H, major + minor), 7.36 (br, 1.65H, major + minor), 7.30–7.17 (m, 5.67H, major + minor), 7.17–7.01 (m, 12.18H, major + minor), 6.96 (br, 3.32H, major + minor), 6.78 (br, 2.61H, major + minor), 6.59 (br, 0.52H, minor), 5.08 (br, 0.44H, minor), 5.00 (s, 1.00H, major), 4.95 (s, 1.08H, major), 4.74 (br, 0.42H, minor), 3.52 (s, 4.45H, major + minor), 2.35 (br, 1.46H, minor), 2.29 (s, 3.03H, major), 1.36 (br, 8.64H, minor), 1.24 (s, 18.00H, major) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.6 (major + minor), 151.0 (major + minor), 143.3 (2major), 143.2 (minor), 142.3 (major + minor), 140.7 (major + 2minor), 137.6 (major + minor), 136.0 (major + minor), 134.5 (major + minor), 134.1 (minor), 133.5 (major), 129.2 (2major + 3minor), 128.4 (2major), 127.7 (2major + 2minor), 126.3 (major + minor), 126.0 (2major), 125.8 (minor), 125.0 (minor), 124.8 (minor), 124.6 (minor), 124.5 (major), 122.0 (major), 120.9 (major + minor), 120.6 (major + minor), 120.1 (major), 119.7 (major + minor), 119.3 (minor), 118.5 (minor), 109.4 (major + minor), 51.0 (minor), 50.4 (major), 34.1 (major + minor), 30.6 (major + minor), 30.2 (major + minor), 21.4 (major + minor) ppm. **IR** (film): $\bar{\upsilon}$ = 3630, 3382, 2956, 1597, 1483, 1433, 1357, 1233, 1163, 1090, 1033, 933, 735, 693, 586, 546 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{45}H_{47}N_2O_3S$ $[M + H]^+$: 695.3302; found: 695.3295.

***N*-Benzyl-*N*-(3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl) methanesulfonamide**

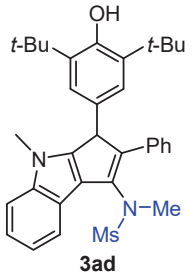


3ac

3ac: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2c** (31.4 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.5 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3ac** (60.0 mg, 95% yield, 2:1 *dr*, light yellow solid, mp = 216–217 °C). **^{1}H NMR** (600 MHz, $CDCl_3$, mixed isomers of **3ac** (*2:1 dr*)) δ = 7.82–7.72 (m, 1.50H, major + minor), 7.40–7.31 (m, 3.07H, major + minor), 7.29–7.20 (m, 6.88H, major + minor), 7.17–6.94(m, 8.07H, major + minor), 6.93–6.59 (m, 5.13H, major + minor), 5.37 (s, 0.40H, minor), 5.35 (s, 0.48H, minor),5.00 (br, 2.13H, major), 4.84 (br, 1.97H, major), 4.70 (br, 0.56H, minor), 4.64 (s, 0.51H, minor), 3.54 (s, 4.54H, major + minor), 2.99 (br, 1.50H, minor), 2.67 (s, 3.00H, major), 1.27 (s, 27.07H, major + minor) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.7 (major + minor), 151.5 (minor), 150.6 (major), 142.5 (major + minor), 140.8 (major + minor), 136.4 and 135.9 (2major + 2minor), 134.9 (minor), 134.6 (major), 133.0 (minor), 132.3 (major), 129.8 (major + minor), 129.2 (minor), 128.9 (major + minor), 128.6 (major), 128.1 (major), 127.7 (minor), 127.4 (major + minor), 126.5 (major + minor), 125.5 (major + minor), 124.7 (major + minor), 120.8 (major + minor), 120.5 (major + minor), 120.1 (major + minor), 119.5 (major + minor), 117.6 (major), 117.2 (minor), 109.9 (major + minor), 53.6 (major + minor), 51.3 (major + minor), 40.4 (major + minor), 34.1 (major + minor), 30.7 (major + minor), 30.2 (major + minor) ppm. **IR**

(film): $\bar{\upsilon}$ = 3361, 2956, 2921, 1601, 1456, 1433, 1338, 1153, 1066, 1021, 732, 697, 578, 556 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{40}H_{45}N_2O_3S$ $[M + H]^+$: 633.3145; found: 633.3139.

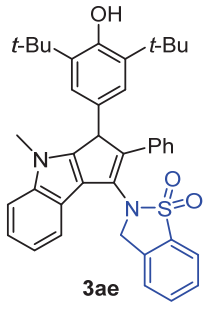
_N_-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-_N_-methylmethanesulfonamide



3ad

3ad: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2d** (23.0 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ad** (48.5 mg, 87% yield, light yellow powder). **^{1}H NMR** (400 MHz, $CDCl_3$) δ = 7.83–7.72 (m, 1H), 7.36 (d, *J* = 7.5 Hz, 2H), 7.33–7.27 (m, 1H), 7.27–7.17 (m, 4H), 7.13 (t, *J* = 7.3 Hz, 1H), 6.88 (br, 2H), 5.03 (s, 1H), 4.85 (s, 1H), 3.54(s, 3H), 3.50 (s, 3H), 2.75 (s, 3H), 1.30 (s, 18H) ppm. **^{13}C NMR** (100 MHz, $CDCl_3$) δ = 152.7, 151.5, 140.8, 140.5, 136.2, 135.0, 134.9, 128.3, 128.1, 126.6, 125.7, 124.7, 120.8, 120.5, 120.2, 119.6, 117.5, 109.9, 50.6, 39.3, 37.1, 34.2, 30.7, 30.2 ppm. **IR** (film): $\bar{\upsilon}$ = 3631, 3382, 2957, 1598, 1482, 1434, 1138, 1234, 1146, 1069, 1019, 963, 734, 695, 576 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{34}H_{41}N_2O_3S$ $[M + H]^+$: 557.2832; found: 557.2825.

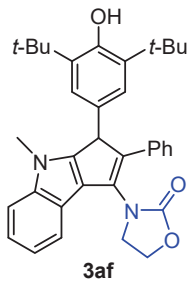
2-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-2,3-dihydrobenzo[*d*]isothiazole 1,1-dioxide



3ae

3ae: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2e** (29.6 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 5.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1.5/1) afforded **3ae** (24.7 mg, 40% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.93 (d, *J* = 7.7 Hz, 1H), 7.64 (t, *J* = 7.4 Hz, 1H), 7.59 (t, *J* = 8.6 Hz, 3H), 7.51 (d, *J* = 8.0 Hz, 1H), 7.36 (d, *J* = 7.6 Hz, 1H), 7.28–7.25 (m, 1H), 7.18 (t, *J* = 7.5 Hz, 2H), 7.14 (t, *J* = 7.7 Hz, 1H), 7.10 (t, *J* = 7.3 Hz, 1H), 7.03 (t, *J* = 7.7 Hz, 1H), 6.98 (s, 2H), 5.02 (s, 1H), 4.91 (s, 1H), 4.80 (d, *J* = 14.4 Hz, 1H), 4.75 (d, *J* = 14.4 Hz, 1H), 3.56 (s, 3H), 1.32 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.7, 151.3, 142.7, 140.7, 136.1, 135.6, 134.4, 133.7, 132.7, 129.9, 129.2, 128.5, 128.0, 126.7, 125.6, 124.8, 124.5, 121.8, 120.9, 120.8, 120.2, 120.0, 118.1, 109.6, 51.4, 50.8, 34.3, 30.7, 30.3 ppm. **IR** (film): $\bar{\upsilon}$ = 3631, 3389, 3054, 2958, 2872, 1598, 1518, 1481, 1433, 1311, 1173, 757, 738, 564 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{39}H_{41}N_2O_3S$ $[M + H]^+$: 617.2832; found: 617.2822.

3-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl) oxazolidin-2-one

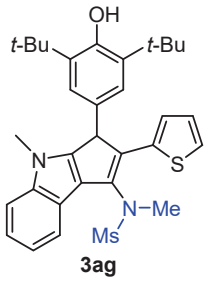


3af

3af: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2f** (20.6 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 2.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3af** (13.5 mg, 25% yield, yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.70–7.63 (m, 1H), 7.28–7.25 (m, 1H), 7.22 (d, *J* = 4.8 Hz, 4H), 7.19–7.11 (m, 3H), 6.90 (s, 2H), 5.04 (s, 1H), 4.77 (s, 1H), 4.47–4.40 (m, 2H), 3.79–3.73 (m, 1H), 3.70–3.64 (m, 1H), 3.54(s, 3H), 1.31 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ

= 156.7, 152.7, 150.9, 140.7, 136.0, 135.3, 134.3, 132.3, 128.3, 128.1, 126.5, 125.7, 124.9, 120.9, 120.8, 120.2, 120.0, 117.6, 109.5, 62.8, 50.8, 45.8, 34.2, 30.7, 30.2 ppm. **IR** (film): $\bar{\upsilon}$ = 3630, 3399, 3054, 2957, 1758, 1596, 1483, 1432, 1398, 1231, 1094, 1039, 737, 701 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{35}H_{39}N_2O_3$ $[M + H]^+$: 535.2955; found: 535.2948.

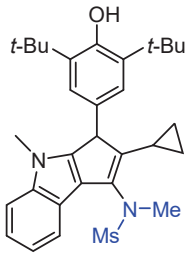
***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-(thiophen-2-yl)-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-methylmethanesulfonamide**



3ag

3ag: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2g** (23.7 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.5 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ag** (36.7 mg, 65% yield, light green powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.77 (br, 1H), 7.31–7.27 (m, 1H), 7.23–7.17 (m, 2H), 7.17–6.90 (m, 3H), 6.85 (br, 2H), 5.11 (s, 1H), 4.77 (br, 1H), 3.52 (s, 3H), 3.47 (s, 3H), 3.10 (s, 3H), 1.35 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 153.0, 151.8, 140.8, 137.0, 136.5, 135.2, 133.8, 126.4 (2C), 124.8, 124.6, 124.3, 120.9, 120.4 (2C), 119.7, 116.7, 109.9, 50.6, 38.9, 36.1, 34.3, 30.6, 30.3 ppm. **IR** (film): $\bar{\upsilon}$ = 3379, 2956, 1598, 1481, 1460, 1433, 1338, 1145, 1120, 1068, 1021, 734, 695 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{32}H_{39}N_2O_3S_2$ $[M + H]^+$: 563.2397; found: 563.2383.

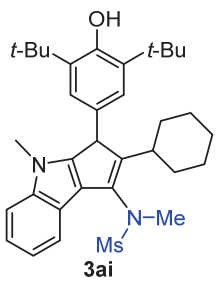
***N*-(2-Cyclopropyl-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-methylmethanesulfonamide**



3ah

3ah: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2h** (19.0 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.5 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3ah** (42.7 mg, 82% yield, brown foam). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.60 (br, 1H), 7.29–7.22 (m, 1H), 7.18–7.08 (m, 2H), 6.92 (br, 2H), 5.12 (s, 1H), 4.22 (br, 1H), 3.46 (br, 3H), 3.42 (s, 3H), 3.04 (s, 3H), 1.89 (br, 1H), 1.37 (s, 18H), 0.83–0.73 (m, 1H), 0.70–0.34 (m, 2H), 0.31–0.21 (m, 1H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.7, 150.4, 144.1, 140.3, 136.3, 134.1, 125.8, 124.5, 120.1, 119.7 (2C), 118.9, 116.1, 109.8, 49.5, 37.8, 36.9, 34.2, 30.5, 30.2, 10.4, 7.3, 5.8 ppm. **IR** (film): $\bar{\upsilon}$ = 3630, 3430, 2957, 1611, 1468, 1433, 1341, 1235, 1147, 1068, 961, 737, 519 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{31}H_{41}N_2O_3S$ $[M + H]^+$: 521.2832; found: 521.2829.

***N*-(2-Cyclohexyl-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-methylmethanesulfonamide**

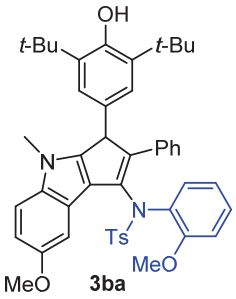


3ai

3ai: According to the above *General Procedure* by using **1a** (34.7 mg, 0.1 mmol), **2i** (23.7 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3ai** (32.1 mg, 57% yield, 1:1 *dr*, yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$, mixed isomers of **3ai** (*1:1 dr*)) δ = 7.69–7.52 (m, 1.88H, major + minor), 7.31–7.24 (m, 1.88H, major + minor), 7.20–7.12 (m, 3.75H, major + minor), 7.09–6.45 (m, 3.62H, major + minor), 5.12 (s, 0.86H, minor), 5.10 (s,

1.00H, major), 4.46 (s, 0.86H, minor), 4.41 (s, 1.02H, major), 3.48 (s, 3.05H, major), 3.43 (s, 5.15H, minor), 3.38 (s, 3.01H, major), 3.05 (s, 3.00H, major), 3.02 (s, 2.57H, minor), 2.90–2.80 (m, 1.88H, major + minor), 1.92–1.83 (m, 0.87H, minor), 1.76–1.70 (m, 2.88H, major + minor), 1.62–1.56 (m, 2.06H, major), 1.55–1.45 (m, 5.15H, major + minor), 1.37 (s, 33.51H, major + minor), 1.29–1.24 (m, 2.08H, major), 1.20–1.12 (m, 1.86H, major + minor), 1.02–0.84 (m, 1.97H, major + minor), 0.58–0.42 (m, 1.87H, major + minor) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.8 (major + minor), 151.5 (major), 151.0 (minor), 149.7 (minor), 149.4 (major), 140.4 (minor), 140.3 (major), 136.2 (major + minor), 131.9 (major + minor), 126.4 (minor), 126.0 (major), 124.8 (major + minor), 120.1 (major + minor), 119.9 (minor), 119.8 (2C, major), 119.6 (minor), 119.0 (minor), 118.8 (major), 116.1 (minor), 115.5 (major), 109.9 (major + minor), 48.8 (minor), 48.6 (major), 38.6 (major), 38.2 (minor), 38.1 (minor), 37.9 (minor), 37.8 (major), 37.4 (major), 34.7 (major), 34.2 (major + minor), 32.8 (minor), 32.3 (minor), 31.2 (major), 30.5 (major + minor), 30.3 (major + minor), 27.1 (minor), 27.0 (major), 26.9 (major + minor), 26.25 (major), 26.15 (minor) ppm. **IR** (film): $\bar{\upsilon}$ = 3417, 2957, 1610, 1482, 1433, 1338, 1225, 1146, 1054, 962, 739, 696 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{34}H_{46}N_2O_3SNa$ $[M + Na]^+$: 585.3121; found: 585.3115.

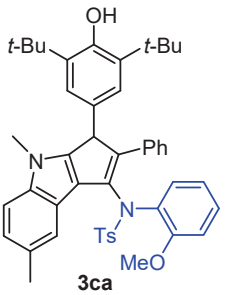
***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-7-methoxy-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**



3ba

3ba: According to the above *General Procedure* by using **1b** (37.7 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ba** (50.0 mg, 66% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.68 (d, J = 7.1 Hz, 2H), 7.62 (br, 1H), 7.22–7.12 (m, 3H), 7.10 (t, J = 7.6 Hz, 1H), 7.02 (t, J = 7.0 Hz, 1H), 6.91 (t, J = 7.4 Hz, 2H), 6.86 (d, J = 8.6 Hz, 1H), 6.81–6.58 (m, 6H), 6.56–6.48 (m, 1H), 4.97 (s, 1H), 4.59 (br, 1H), 3.89 (s, 3H), 3.50 (s, 3H), 3.41 (s, 3H), 2.40 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.0, 154.1, 152.5, 150.2, 142.8, 141.2, 138.4, 136.2, 135.8, 135.7, 135.1, 130.2, 129.8, 129.5, 128.8, 128.5, 128.0, 127.0, 126.3, 126.0, 124.7, 122.0, 120.7, 119.8, 111.6, 110.4, 109.6, 104.2, 56.0, 54.8, 51.5, 34.1, 30.7, 30.2, 21.5 ppm. **IR** (film): $\tilde{\upsilon}$ = 3632, 3377, 2955, 1597, 1497, 1462, 1434, 1347, 1265, 1160, 1091, 1028, 735, 699, 586 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{47}H_{51}N_2O_5S$ $[M + H]^+$: 755.3513; found: 755.3505.

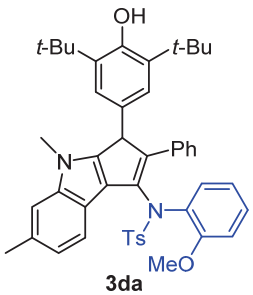
***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4,7-dimethyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**



3ca

3ca: According to the above *General Procedure* by using **1c** (36.1 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ca** (51.8 mg, 70% yield, light yellow solid, mp = 209–210 °C). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.66 (d, J = 7.9 Hz, 2H), 7.43 (br, 1H), 7.15 (d, J = 8.3 Hz, 3H), 7.10 (t, J = 7.0 Hz, 1H), 7.06 (t, J = 7.4 Hz, 1H), 7.02–6.96 (m, 3H), 6.88–6.62 (m, 6H), 6.55 (t, J = 7.2 Hz, 1H), 4.96 (s, 1H), 4.58 (br, 1H), 3.49 (s, 3H), 3.37 (s, 3H), 2.42 (s, 3H), 2.41 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 155.9, 152.5, 150.1, 142.6, 142.1, 139.2, 138.7, 135.8, 135.5, 135.2, 130.3, 130.1, 129.6, 128.8, 128.5, 128.3, 128.1, 127.2, 126.4, 125.9, 124.7, 121.8, 121.7, 121.6, 120.0, 119.9, 111.5, 108.7, 54.6, 51.4, 34.1, 30.6, 30.2, 21.6, 21.5 ppm. **IR** (film): $\tilde{\upsilon}$ = 3362, 2920, 1598, 1462, 1433, 1349, 1161, 1088, 1042, 736, 579, 558 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{47}H_{51}N_2O_4S$ $[M + H]^+$: 739.3564; found: 739.3555.

***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4,6-dimethyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**

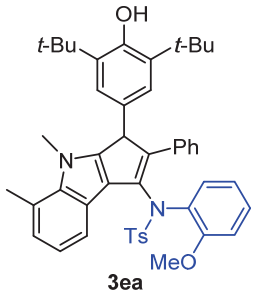


3da

3da: According to the above *General Procedure* by using **1d** (36.1 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3da** (53.9 mg, 73% yield, light yellow solid, mp = 198–199 °C). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.78 (br, 1H), 7.66 (d, J = 7.9 Hz, 2H), 7.15 (d, J = 6.9 Hz, 2H), 7.10 (t, J = 7.5 Hz, 1H), 7.07 (s, 1H), 7.02 (t, J = 7.03 Hz, 1H), 6.97 (d, J = 7.9 Hz, 1H), 6.92 (t, J = 7.6 Hz, 2H), 6.82–6.61 (m, 6H), 6.53 (t, J = 7.4 Hz, 1H), 4.96 (s, 1H), 4.58 (br, 1H), 3.49 (s, 3H), 3.40 (s, 3H),

2.51 (s, 3H), 2.41 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.0, 152.5, 149.3, 142.6, 141.9, 141.2, 138.6, 135.8, 135.7, 135.2, 130.1 (3C), 129.5, 128.8, 128.5, 128.1, 127.1, 126.3, 126.0, 124.7, 121.6, 121.1, 120.7, 119.9, 119.6, 111.5, 109.3, 54.8, 51.5, 34.1, 30.6, 30.2, 21.9, 21.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3360, 2920, 1597, 1433, 1348, 1160, 1088, 1042, 817, 699, 586, 557 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{47}H_{51}N_2O_4S$ $[M + H]^+$: 739.3564; found: 739.3558.

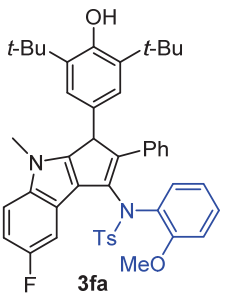
_N_-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4,5-dimethyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-_N_-(2-methoxyphenyl)-4-methylbenzenesulfonamide



3ea

3ea: According to the above *General Procedure* by using **1e** (36.1 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ea** (60.0 mg, 81% yield, light yellow solid, mp = 199–200 °C). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.79 (br, 1H), 7.65 (d, *J* = 6.3 Hz, 2H), 7.21–7.06 (m, 3H), 7.05–6.97 (m, 2H), 6.94–6.89 (m, 3H), 6.85–6.35 (m, 7H), 4.96 (s, 1H), 4.56 (br, 1H), 3.81 (s, 3H), 3.40 (s, 3H), 2.74 (s, 3H), 2.40 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.3–155.3 (1C), 152.5, 150.4, 142.6, 142.3, 139.4, 138.6, 135.8, 135.7–135.2 (1C), 135.1, 130.1, 129.5 (2C), 128.7, 128.4, 128.0, 127.0, 126.3, 126.0, 124.7, 123.6, 122.5, 121.1, 120.9, 120.2, 119.9, 119.6, 111.5, 54.7, 51.7, 34.5, 34.1, 30.2, 21.5, 19.9 ppm. **IR** (film): $\bar{\upsilon}$ = 3634, 3361, 2956, 2921, 1597, 1497, 1433, 1348, 1265, 1161, 1089, 1028, 746, 589, 557 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{47}H_{51}N_2O_4S$ $[M + H]^+$: 739.3564; found: 739.3557.

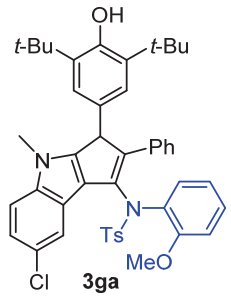
_N_-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-7-fluoro-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-_N_-(2-methoxyphenyl)-4-methylbenzenesulfonamide



3fa

3fa: According to the above *General Procedure* by using **1f** (36.5 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.2 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3fa** (72.9 mg, 98% yield, light yellow solid, mp = 199–200 °C). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.66 (d, *J* = 8.1 Hz, 2H), 7.24 (s, 1H), 7.20 (d, *J* = 7.8 Hz, 2H), 7.15 (dd, *J* = 8.9, 4.5 Hz, 1H), 7.12–7.01 (m, 2H), 6.98 (t, *J* = 7.4 Hz, 2H), 6.92–6.88 (m, 1H), 6.84–6.59 (m, 5H), 6.57–6.45 (m, 2H), 4.98 (s, 1H), 4.56 (s, 1H), 3.50 (s, 3H), 3.40 (s, 3H), 2.44 (s, 3H), 1.25 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 157.9 (d, $^1J_{C\text{-}F}$ = 231.0 Hz), 156.2, 152.6, 151.3, 143.1, 142.3, 138.5, 137.3, 135.9, 135.1 (2C), 130.7, 129.6 (2C), 129.0, 128.8, 128.1, 127.3, 126.6, 125.5, 124.7, 121.7 (d, $^3J_{C\text{-}F}$ = 11.1 Hz), 120.6, 119.7, 111.5, 109.4 (d, $^3J_{C\text{-}F}$ = 9.9 Hz), 108.4 (d, $^2J_{C\text{-}F}$ = 25.1 Hz), 107.0 (d, $^2J_{C\text{-}F}$ = 24.6 Hz), 54.8, 51.7, 34.1, 30.8, 30.2, 21.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3632, 3366, 2956, 1597, 1497, 1463, 1351, 1161, 1090, 1027, 736, 585, 558 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{48}FN_2O_4S$ $[M + H]^+$: 743.3313; found: 743.3307.

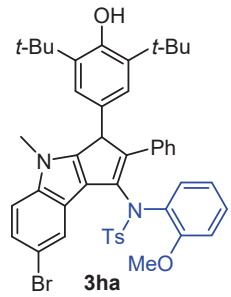
***N*-(7-Chloro-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**



3ga

3ga: According to the above *General Procedure* by using **1g** (38.1 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.2 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ga** (72.2 mg, 95% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.63 (d, J = 8.0 Hz, 2H), 7.25 (br, 1H), 7.22 (d, J = 7.9 Hz, 2H), 7.17–7.03 (m, 6H), 6.88 (br, 2H), 6.79–6.61 (m, 3H), 6.50 (d, J = 4.5 Hz, 2H), 4.99 (s, 1H), 4.57 (s, 1H), 3.50 (s, 3H), 3.39 (s, 3H), 2.46 (s, 3H), 1.26 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.2, 152.7, 151.2, 143.3 (2C), 139.0, 138.5, 136.0, 135.1, 134.8, 131.4, 129.7, 129.3, 129.1, 129.0, 128.0, 127.4, 126.8, 125.3, 125.1, 124.7, 122.2, 121.3, 120.4, 120.0, 119.8, 111.4, 110.0, 54.7, 51.6, 34.2, 30.8, 30.2, 21.7 ppm. **IR** (film): $\bar{\upsilon}$ = 3363, 2921, 1597, 1496, 1433, 1351, 1161, 1088, 1022, 592, 579, 557 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{48}ClN_2O_4S$ $[M + H]^+$: 759.3018; found: 759.3016.

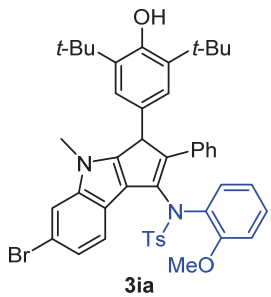
***N*-(7-Bromo-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**



3ha

3ha: According to the above *General Procedure* by using **1h** (42.5 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ha** (77.8 mg, 97% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.63 (d, J = 8.2 Hz, 2H), 7.45 (br, 1H), 7.25–7.19 (m, 3H), 7.16–7.04 (m, 5H), 6.90 (br, 2H), 6.81–6.61 (m, 3H), 6.56–6.44 (m, 2H), 4.99 (s, 1H), 4.56 (s, 1H), 3.49 (s, 3H), 3.39 (s, 3H), 2.47 (s, 3H), 1.26 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.2, 152.7, 151.1, 143.4, 143.2, 139.3, 138.4, 136.0, 135.1, 134.7, 131.5, 129.7 (2C), 129.2, 129.0, 127.9, 127.5, 126.9, 125.3, 124.7, 124.3, 123.0, 122.7, 119.8 (2C), 112.8, 111.4, 110.5, 54.7, 51.6, 34.2, 30.7, 30.2, 21.8 ppm. **IR** (film): $\bar{\upsilon}$ = 3631, 3411, 2956, 1598, 1496, 1464, 1434, 1349, 1264, 1162, 1057, 1026, 788, 730, 663, 591, 555 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{48}BrN_2O_4S$ $[M + H]^+$: 803.2513; found: 803.2507.

***N*-(6-Bromo-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**

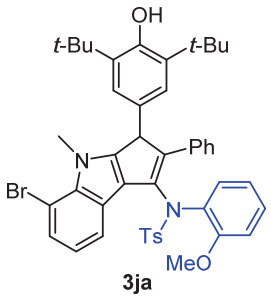


3ia

3ia: According to the above *General Procedure* by using **1i** (42.5 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.5 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ia** (74.6 mg, 93% yield, light yellow solid, mp = 205–206 °C). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.81 (br, 1H), 7.66 (d, J = 8.0 Hz, 2H), 7.43 (d, J = 1.3 Hz, 1H), 7.25–7.22 (m, 1H), 7.19 (d, J = 7.5 Hz, 2H), 7.12–7.08 (m, 1H), 7.05 (t, J = 7.4 Hz, 1H), 6.91 (t, J = 7.6 Hz, 2H), 6.75 (d, J = 8.2 Hz, 1H), 6.66 (br, 2H), 6.58 (br, 2H), 6.52–6.41 (m, 2H), 4.99 (s, 1H), 4.57 (s, 1H), 3.49 (s, 3H), 3.40 (s, 3H), 2.43 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.2, 152.7, 150.1, 142.9, 142.5, 141.5, 138.4, 135.9, 135.1, 134.9, 130.1, 129.9, 129.5, 129.0, 128.8, 128.1,

127.2, 126.6, 125.3, 124.6, 123.3, 122.6, 121.2, 120.6, 119.7, 113.9, 112.3, 111.6, 54.9, 51.7, 34.1, 30.8, 30.2, 21.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3404, 2957, 1597, 1497, 1468, 1434, 1348, 1264, 1162, 1091, 1029, 857, 748, 587, 556 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{48}BrN_2O_4S$ $[M + H]^+$: 803.2513; found: 803.2507.

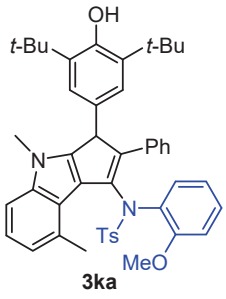
***N*-(5-Bromo-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**



3ja

3ja: According to the above *General Procedure* by using **1j** (42.5 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3ja** (78.6 mg, 98% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.99 (br, 1H), 7.66 (d, J = 7.0 Hz, 2H), 7.31 (d, J = 7.6 Hz, 1H), 7.16 (br, 2H), 7.11–7.08 (m, 1H), 7.03 (t, J = 7.4 Hz, 1H), 7.00–6.94 (m, 1H), 6.89 (t, J = 7.5 Hz, 2H), 6.83–6.40 (m, 7H), 4.99 (s, 1H), 4.56 (s, 1H), 3.92 (s, 3H), 3.39 (s, 3H), 2.41 (s, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 156.0, 152.7, 151.2, 142.9 (2C), 138.4, 136.6, 135.9, 134.8 (2C), 129.9 (2C), 129.5, 128.9, 128.7, 128.0, 127.1, 126.6, 125.8, 125.3, 124.8, 124.6, 121.5, 121.2, 120.5, 119.7, 111.6, 103.6, 54.8, 52.0, 34.7, 34.1, 30.2, 21.5 ppm. **IR** (film): $\bar{\upsilon}$ = 3633, 3378, 2956, 1598, 1497, 1435, 1350, 1265, 1162, 1104, 1028, 733, 662, 589, 549 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{48}BrN_2O_4S$ $[M + H]^+$: 803.2513; found: 803.2503.

***N*-(3-(3,5-Di-*tert*-butyl-4-hydroxyphenyl)-4,8-dimethyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-(2-methoxyphenyl)-4-methylbenzenesulfonamide**

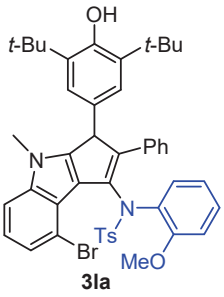


3ka

3ka: According to the above *General Procedure* by using **1k** (36.1 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1.5/1) afforded **3ka** (65.1 mg, 88% yield, 4:1 *dr*, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$, mixed isomers of **3ka** (*4:1 dr*)) δ = 7.71 (d, J = 7.9 Hz, 0.97H, major), 7.76 (d, J = 8.1 Hz, 0.52H, minor), 7.57 (d, J = 8.1 Hz, 1.97H, major), 7.22–7.12 (m, 3.78H, major + minor), 7.08–7.02 (m, 1.53H, major + minor), 6.97–6.92 (m, 1.54H, major + minor), 6.89–6.86 (m, 2.41H, major + minor), 6.85–6.74 (m, 4.57H, major + minor), 6.69 (d, J = 7.3 Hz, 2.01H, major), 6.67–6.59 (m, 2.85H, major + minor), 6.11 (d, J = 7.7 Hz, 0.48H, minor), 5.16 (s, 0.25H, minor), 4.92 (s, 1.00H, major), 4.88 (s, 0.99H, major), 4.41 (s, 0.24H, minor), 3.59–3.50 (m, 6.76H, major + minor), 3.35 (s, 0.73H, minor), 3.07 (s, 0.74H, minor), 3.00 (s, 2.94H, major), 2.30 (s, 0.75H, minor), 2.26 (s, 2.96H, major), 1.34 (s, 4.48H, minor), 1.17 (s, 18.08H, major) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 153.6 (minor), 152.9 (minor), 152.7 (major), 152.4 (major), 150.3 (major), 148.9 (minor), 142.2 (minor), 141.9 (major), 141.8 (major), 141.3 (major), 141.2 (minor), 140.8 (minor), 139.5 (major), 139.1 (minor), 137.2 (major), 137.0 (minor), 136.2 (minor), 135.8 (major), 134.9 (minor), 134.6 (major), 133.8 (major), 132.6 (minor), 131.9 (minor), 131.7 (major), 129.2 (minor), 129.0 (major), 128.6 (minor), 128.3 (minor), 127.9 (major), 127.8 (major), 126.9 (major), 126.7 (minor), 126.4 (major + minor), 126.3 (minor), 126.2 (major), 126.1 (minor), 126.0 (minor), 125.7 (major), 125.3 (major), 124.9 (minor),

124.4 (major), 122.4 (minor), 122.2 (2minor), 122.0 (2major), 121.6 (major), 121.0 (major), 120.9 (minor), 120.7 (major), 120.0 (minor), 112.2 (major), 111.7 (minor), 106.8 (major), 106.6 (minor), 54.4 (major + minor), 51.6 (minor), 49.8 (major), 34.3 (minor), 34.1 (major), 30.8 (minor), 30.7 (major), 30.4 (minor), 30.2 (major), 22.8 (major + minor), 21.4 (minor), 21.3 (major) ppm. **IR** (film): $\bar{\upsilon}$ = 3613, 3364, 2952, 2922, 1598, 1500, 1431, 1348, 1267, 1160, 1088, 1021, 940, 727, 687, 588 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{47}H_{51}N_2O_4S$ [*M* + H]$^+$: 739.3564; found: 739.3553.

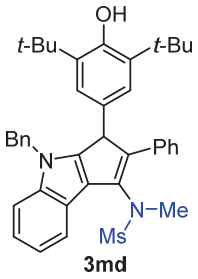
_N_-(8-Bromo-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-4-methyl-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-_N_-(2-methoxyphenyl)-4-methylbenzenesulfonamide



3la

3la: According to the above *General Procedure* by using **1l** (42.5 mg, 0.1 mmol), **2a** (41.5 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 6.0 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 1/1) afforded **3la** (71.5 mg, 89% yield, 4:1 *dr*, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$, mixed isomers of **3la** (*4:1 dr*)) δ = 7.88 (d, *J* = 8.0 Hz, 0.95H, major), 7.67 (d, *J* = 7.7 Hz, 0.20H, minor), 7.63 (d, *J* = 8.1 Hz, 0.47H, minor), 7.57 (d, *J* = 8.1 Hz, 1.95H, major), 7.48 (d, *J* = 8.0 Hz, 0.24H, minor), 7.45 (d, *J* = 7.6 Hz, 0.96H, major), 7.29 (d, *J* = 8.2 Hz, 0.24H, minor), 7.26–7.23 (m, 1.00H, major), 7.15 (t, *J* = 8.1 Hz, 1.00H, major), 7.10–7.01 (m, 1.51H, major + minor), 6.91 (d, *J* = 8.2 Hz, 1.49H, major + minor), 6.88–6.82 (m, 3.81H, major + minor), 6.82–6.73 (m, 3.20H, major + minor), 6.72–6.67 (m, 2.27H, major + minor), 6.67–6.63 (m, 2.49H, major + minor), 6.09 (d, *J* = 7.8 Hz, 0.46H, minor), 5.20 (s, 0.23H, minor), 4.92 (s, 1.01H, major), 4.89 (s, 1.00H, major), 4.41 (s, 0.23H, minor), 3.544 (s, 2.98H, major), 3.536 (s, 0.69H, minor), 3.52 (s, 2.96H, major), 3.23 (s, 0.69H, minor), 2.27 (s, 0.68H, minor), 2.23 (s, 2.94H, major), 1.35 (s, 4.30H, minor), 1.17 (s, 18.15H, major) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 153.6 (minor), 153.1 (minor), 152.6 (major), 152.5 (major), 151.4 (major), 150.1 (minor), 142.9 (major), 141.9 (major), 141.8 (3minor), 141.6 (major), 139.7 (major), 139.5 (minor), 136.4 (major + 2minor), 135.9 (major), 134.4 (minor), 134.2 (major), 133.9 (major), 132.9 (minor), 129.2 (minor), 129.1 (major), 128.6 (minor), 128.0 (minor), 127.8 (2C, major), 127.6 (minor), 126.8 (major), 126.6 (major + minor), 126.3 (minor), 126.2 (major + minor), 125.8 (major), 125.7 (major), 125.4 (2minor), 125.2 (major), 124.9 (minor), 124.4 (major), 122.9 (minor), 122.6 (major), 121.6 (minor), 121.4 (major + minor), 120.9 (major), 120.3 (major), 119.9 (minor), 114.1 (major + minor), 111.9 (major), 111.3 (minor), 108.4 (major), 108.3 (minor), 54.4 (major), 54.1 (minor), 51.5 (minor), 49.7 (major), 34.3 (minor), 34.1 (major), 31.0 (minor), 30.8 (major), 30.3 (minor), 30.1 (major), 21.3 (major + minor) ppm. **IR** (film): $\bar{\upsilon}$ = 3633, 3372, 2956, 1598, 1500, 1433, 1350, 1266, 1159, 1089, 1029, 1003, 726, 679, 662, 588, 543 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{46}H_{48}BrN_2O_4S$ [*M* + H]$^+$: 803.2513; found: 803.2507.

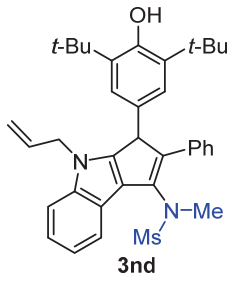
***N*-(4-Benzyl-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-methylmethanesulfonamide**



3md

3md: According to the above *General Procedure* by using **1m** (42.3 mg, 0.1 mmol), **2d** (23.0 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.5 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3md** (52.5 mg, 83% yield, light brown powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.78 (d, J = 7.9 Hz, 1H), 7.39 (d, J = 7.2 Hz, 2H), 7.27–7.21 (m, 2H), 7.20–7.16 (m, 2H), 7.16–7.05 (m, 5H), 6.88 (br, 2H), 6.68 (d, J = 5.9 Hz, 2H), 5.30 (d, J = 16.2 Hz, 1H), 5.05–4.91 (m, 2H), 4.77 (br, 1H), 3.54 (s, 3H), 2.80 (br, 3H), 1.24 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.8, 151.9, 140.4 (2C), 136.4 (2C), 135.1, 134.9, 128.4, 128.1 (2C), 127.3, 126.6, 126.4, 125.9, 124.5, 121.0, 120.7, 120.4, 119.6, 117.5, 110.7, 50.7, 48.3, 39.3, 37.1, 34.1, 30.1 ppm. **IR** (film): $\bar{\upsilon}$ = 3630, 3393, 3058, 2957, 1599, 1481, 1453, 1434, 1343, 1145, 1068, 1021, 962, 772, 737, 695 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{40}H_{45}N_2O_3S$ [M + H]$^+$: 633.3145; found: 633.3136.

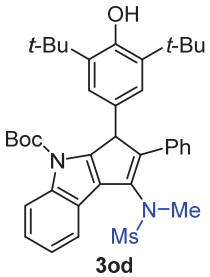
***N*-(4-Allyl-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-2-phenyl-3,4-dihydrocyclopenta[*b*]indol-1-yl)-*N*-methylmethanesulfonamide**



3nd

3nd: According to the above *General Procedure* by using **1n** (37.3 mg, 0.1 mmol), **2d** (23.0 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 1.3 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3nd** (57.8 mg, 99% yield, orange powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.76 (d, J = 7.1 Hz, 1H), 7.39 (d, J = 7.6 Hz, 2H), 7.28–7.23 (m, 3H), 7.22–7.16 (m, 2H), 7.14 (t, J = 7.4 Hz, 1H), 6.88 (br, 2H), 5.51–5.36 (m, 1H), 5.03 (s, 1H), 4.94 (d, J = 10.3 Hz, 1H), 4.90–4.72 (m, 2H), 4.64–4.56 (m, 1H), 4.47 (dd, J = 16.6, 6.2 Hz, 1H), 3.52 (s, 3H), 2.78 (br, 3H), 1.30 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.8, 151.4, 140.7, 140.1, 136.3, 135.0 (2C), 132.0, 128.1 (2C), 126.6, 125.9, 124.6, 120.9, 120.6, 120.3, 119.7, 117.6, 116.9, 110.4, 50.7, 46.9, 39.3, 37.1, 34.2, 30.2 ppm. **IR** (film): $\bar{\upsilon}$ = 3630, 3399, 3054, 2957, 1598, 1516, 1481, 1455, 1434, 1341, 1146, 1020, 962, 770, 736, 694, 518 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{36}H_{43}N_2O_3S$ [M + H]$^+$: 583.2989; found: 583.2985.

***tert*-Butyl 3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)-1-(*N*-methylmethylsulfonamido)-2-phenylcyclopenta[*b*]indole-4(3*H*)-carboxylate**

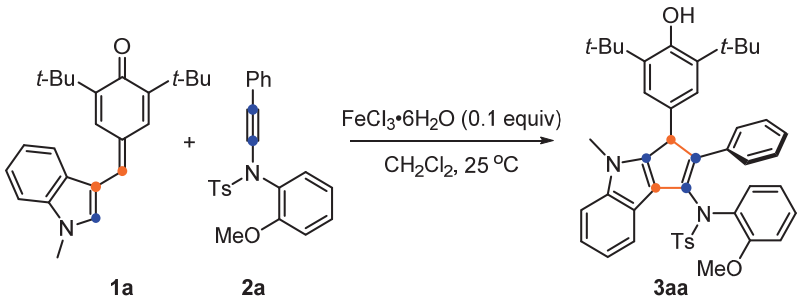


3od

3od: According to the above *General Procedure* by using **1o** (43.3 mg, 0.1 mmol), **2d** (23.0 mg, 0.11 mmol) and $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol) in CH_2Cl_2 (1.0 mL) for 0.5 h at 25 °C, the chromatographic purification ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) afforded **3od** (56.6 mg, 88% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 8.30 (br, 1H), 7.90–7.72 (m, 1H), 7.38–7.28 (m, 4H), 7.28–7.15 (m, 3H), 6.60 (br, 2H), 5.14 (br, 1H), 4.98 (s, 1H), 3.38 (br, 3H), 2.56 (s, 3H), 1.32 (s, 9H), 1.22 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 152.5, 149.2, 146.1, 140.0, 135.6, 134.6, 132.0, 129.3, 128.0, 127.5, 126.3, 126.1, 124.3 (2C), 123.9, 123.3, 122.9, 119.6, 115.9, 83.6, 54.5, 39.6, 37.6, 34.1, 30.1, 27.7 ppm. **IR** (film): $\bar{\upsilon}$ = 3632, 3432, 3055, 2959, 1733, 1594,

1481, 1435, 1339, 1320, 1155, 1119, 963, 738, 701, 518 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{38}H_{47}N_2O_5S$ $[M + H]^+$: 643.3200; found: 643.3199.

3.3. General Procedure for Synthesis of 3aa on Gram Scale

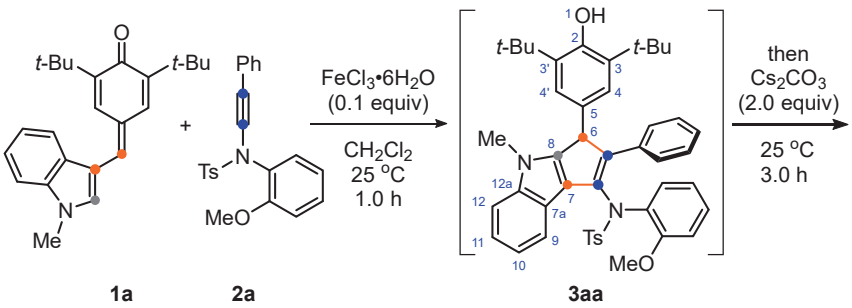


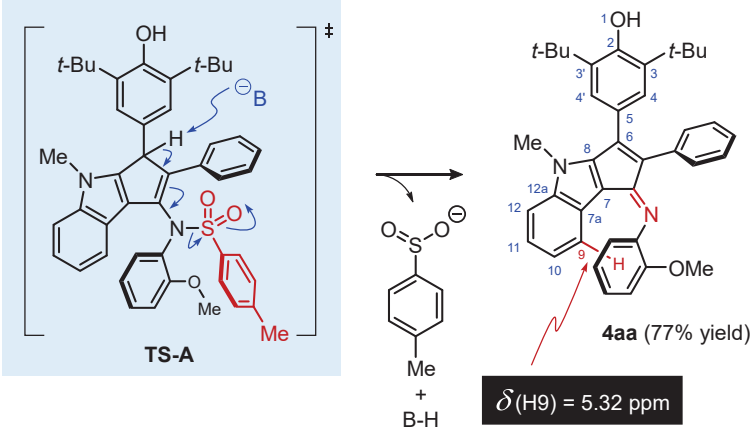
1a **2a** **3aa**

To a solution of indolyl-substituted *p*-quinone methides **1a** (3.0 mmol, 1.041 g) and ynamides **2a** (3.3 mmol, 1.244 g) in CH_2Cl_2 (30 mL) was added $FeCl_3 \cdot 6H_2O$ (0.3 mmol, 81.1 mg). The resulting mixture was stirred at 25 °C for the 1.0 h. The solvent was concentrated under reduced pressure, and then the resulting residue was purified by flash column chromatography on silica gel with the elution of petroleum ether/ dichloromethane ($V_{\text{petroleum ether}}/V_{\text{dichloromethane}}$ = 3:1) to give the corresponding products **3aa** (1.760 g, 81% yield, light yellow powder).

4. Oxidative Desulfonylation of 3aa

We have investigated a one-pot protocol for the removal of the sulfonyl group at the exocyclic nitrogen of the product **3aa** in the presence of Cs_2CO_3. An unusual α,β-unsaturated imine **4aa**, which resulted from an elimination of the sulfonamide moiety in **3aa** via **TS-A**, was isolated in a total yield of 77% yield. This desulfonylation to some extent shows the unique structural influence of aminocyclopenta[*b*]indoles in exocyclic *N*-Ts deprotection.

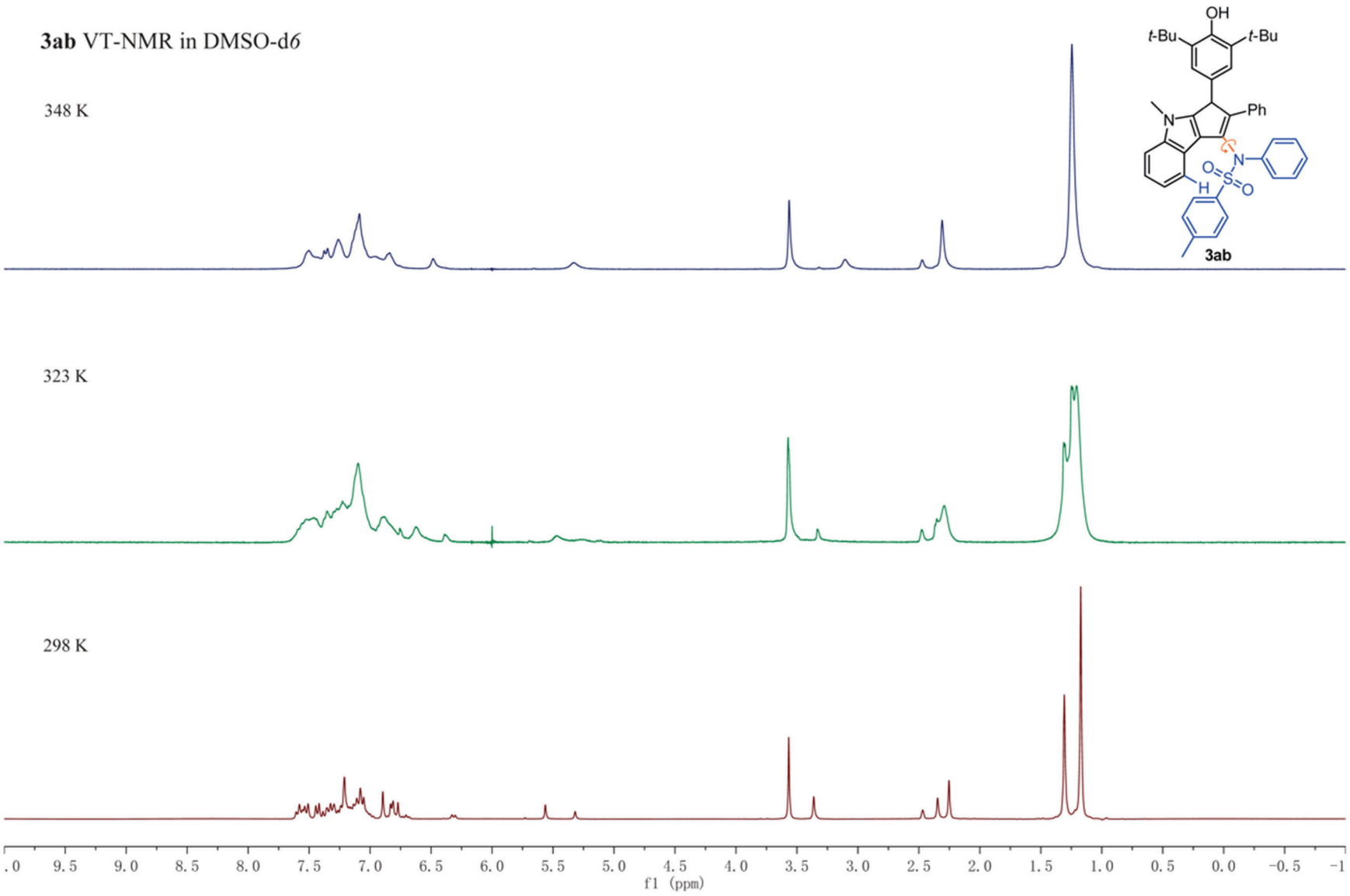




General Procedure: To a solution of indolyl-substituted *p*-quinone methide **1a** (34.7 mg, 0.1 mmol) and ynamide **2a** (41.5 mg, 0.11 mmol) in CH_2Cl_2 (1.0 mL) was added $FeCl_3·6H_2O$ (2.7 mg, 0.01 mmol). The resulting mixture was stirred at 25 °C for 1.0 h. At the end of tandem annulation, Cs_2CO_3 (65.2 mg, 0.2 mmol) was added to the reaction mixture and stirred at 25 °C for 3.0 h. The solvent was concentrated under reduced pressure, and then the resulting residue was purified by flash column chromatography on silica gel with the elution of petroleum ether/dichloromethane ($V_{petroleum\ ether}/V_{dichloromethane}$ = 2/1) to give the corresponding product **4aa** (43.8 mg, 77% yield, light yellow powder). **^{1}H NMR** (600 MHz, $CDCl_3$) δ = 7.37–7.31 (m, 2H), 7.23–7.18 (m, 3H), 7.17–7.13 (m, 3H), 7.10 (d, J = 8.2 Hz, 1H), 7.04–6.98 (m, 2H), 6.97–6.93 (m, 1H), 6.91 (dd, J = 7.5, 1.6 Hz, 1H), 6.74 (t, J = 7.9 Hz, 1H), 5.32 (d, J = 8.2 Hz, 1H), 5.29 (s, 1H), 3.75 (s, 3H), 3.57 (s, 3H), 1.34 (s, 18H) ppm. **^{13}C NMR** (150 MHz, $CDCl_3$) δ = 163.3, 155.0, 153.9, 150.2, 143.7, 141.9, 139.7, 139.0, 135.8, 133.4, 131.4, 127.4, 126.6, 126.4, 124.6, 123.5, 123.2, 121.7, 121.2, 120.8, 120.6, 119.9, 112.1, 109.7, 106.3, 56.0, 34.3, 31.6, 30.2 ppm. **IR** (film): $\bar{\upsilon}$ = 3627, 3404, 3055, 2957, 1633, 1604, 1490, 1456, 1434, 1385, 1247, 1114, 1025, 744, 696 cm^{-1}. **HRMS** (ESI): *m/z* calcd for $C_{39}H_{41}N_2O_2$ $[M + H]^+$: 569.3163; found: 569.3155.

For its 2D NMR spectra (^{1}H-^{1}H COSY, HSQC, and HMBC), please see pages S113-S118.

5. Variable Temperature NMR Experiments of Atropisomer 3ab



6. Determination of the Structure of Products

6.1. X-Ray Crystallographic Data of Compound 3ac

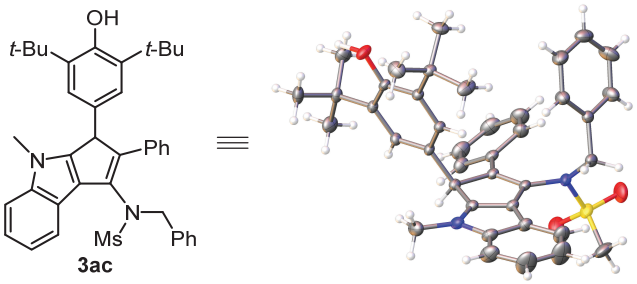


Figure S3. ORTEP drawing of **3ac** (20% ellipsoid probability)

The single crystal of **3ac**, which was used for the determination of its relative configurations via X-ray crystallography (Figure S3), was recrystallized from dichloromethane and methanol. The intensity data were collected on an Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer using graphite-monochromated Mo Kα radiation.

Crystal data and structure refinement for 3ac	
CCDC number	2152044
Empirical formula	$C_{40}H_{44}N_2O_3S$
Formula weight	632.83
Temperature/K	293(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	15.3974(8)
b/Å	11.0390(5)
c/Å	21.2880(11)
α/°	90.00
β/°	99.266(6)
γ/°	90.00
Volume/Å^3	3571.2(3)
Z	4
ρ_{calc}g/cm^3	1.177
μ/mm^{-1}	0.129
F(000)	1352.0
Crystal size/mm^3	0.21 × 0.15 × 0.14
Radiation	Mo Kα (λ = 0.71073)
2Θ range for data collection/°	6.89 to 57.194

Index ranges	$-20 \leq h \leq 18$, $-12 \leq k \leq 14$, $-14 \leq l \leq 28$
Reflections collected	14336
Independent reflections	8101 [R_{int} = 0.0473, R_{sigma} = 0.0886]
Data/restraints/parameters	8101/0/425
Goodness-of-fit on F^2	1.015
Final R indexes [I>=2σ (I)]	R_1 = 0.0684, wR_2 = 0.1322
Final R indexes [all data]	R_1 = 0.1502, wR_2 = 0.1779
Largest diff. peak/hole / e $Å^{-3}$	0.18/–0.29

6.2. X-Ray Crystallographic Data of Compound 3ca

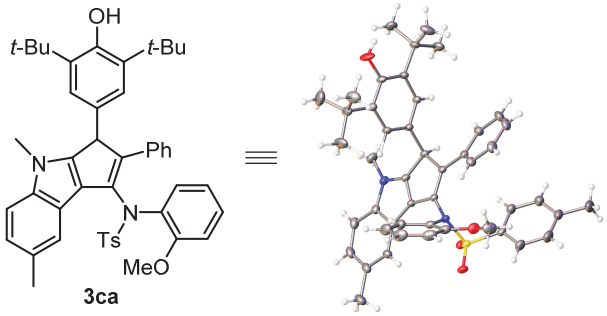


Figure S4. ORTEP drawing of **3ca** (20% ellipsoid probability)

The single crystal of **3ca**, which was used for the determination of its relative configurations via X-ray crystallography (Figure S4), was recrystallized from dichloromethane and methanol. The intensity data were collected on a Rigaku XtaLAB Synergy R (DW system, HyPix) diffractometer using graphite-monochromated Cu Kα radiation.

Crystal data and structure refinement for 3ca	
CCDC number	2152045
Empirical formula	$C_{47}H_{50}N_2O_4S$
Formula weight	738.95
Temperature/K	291.7(2)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.55370(10)
b/Å	12.93580(10)
c/Å	30.0737(3)
α/°	90
β/°	93.7820(10)
γ/°	90
Volume/Å^3	4096.74(6)
Z	4
ρ_{calc}g/cm^3	1.198
μ/mm^{-1}	1.054
F(000)	1576.0
Crystal size/mm^3	0.11 × 0.07 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.89 to 152.874
Index ranges	$-11 \le h \le 13$, $-16 \le k \le 15$, $-37 \le l \le 37$

Reflections collected	32293
Independent reflections	8231 [R_{int} = 0.0277, R_{sigma} = 0.0228]
Data/restraints/parameters	8231/1/499
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0424, wR_2 = 0.1170
Final R indexes [all data]	R_1 = 0.0466, wR_2 = 0.1199
Largest diff. peak/hole / e $Å^{-3}$	0.26/–0.33

6.3. X-Ray Crystallographic Data of Compound 3da

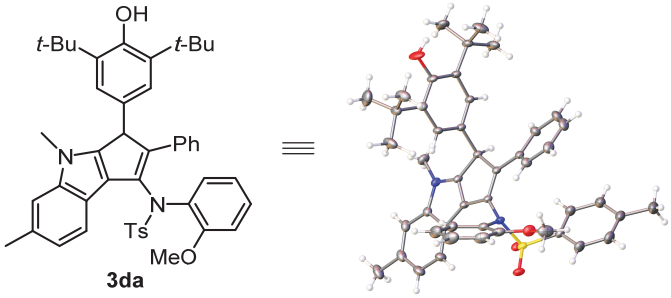


Figure S5. ORTEP drawing of **3da** (20% ellipsoid probability)

The single crystal of **3da**, which was used for the determination of its relative configurations via X-ray crystallography (Figure S5), was recrystallized from dichloromethane and methanol. The intensity data were collected on a Rigaku XtaLAB Synergy R (DW system, HyPix) diffractometer using graphite-monochromated Cu Kα radiation.

Crystal data and structure refinement for 3da	
CCDC number	2152046
Empirical formula	$C_{47}H_{50}N_2O_4S$
Formula weight	738.95
Temperature/K	302.48(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.54220(10)
b/Å	12.89340(10)
c/Å	30.3311(4)
α/°	90
β/°	95.1050(10)
γ/°	90
Volume/Å^3	4106.40(7)
Z	4
ρ_{calc}g/cm^3	1.195
μ/mm^{-1}	1.051
F(000)	1576.0
Crystal size/mm^3	0.15 × 0.12 × 0.11
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.85 to 152.792
Index ranges	$-13 \le h \le 13$, $-12 \le k \le 15$, $-37 \le l \le 37$

Reflections collected	36576
Independent reflections	8265 [R_{int} = 0.0525, R_{sigma} = 0.0443]
Data/restraints/parameters	8265/0/498
Goodness-of-fit on F^2	1.083
Final R indexes [I>=2σ (I)]	R_1 = 0.0483, wR_2 = 0.1294
Final R indexes [all data]	R_1 = 0.0577, wR_2 = 0.1365
Largest diff. peak/hole / e $Å^{-3}$	0.24/–0.42

6.4. X-Ray Crystallographic Data of Compound 3ea

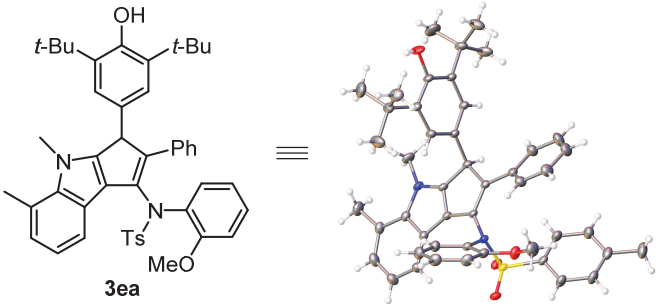


Figure S6. ORTEP drawing of **3ea** (20% ellipsoid probability)

The single crystal of **3ea**, which was used for the determination of its relative configurations via X-ray crystallography (Figure S6), was recrystallized from dichloromethane and methanol. The intensity data were collected on a Rigaku XtaLAB Synergy R (DW system, HyPix) diffractometer using graphite-monochromated Cu Kα radiation.

Crystal data and structure refinement for 3ea	
CCDC number	2152047
Empirical formula	$C_{47}H_{50}N_2O_4S$
Formula weight	738.95
Temperature/K	302.34(10)
Crystal system	triclinic
Space group	P–1
a/Å	12.4470(2)
b/Å	13.1078(3)
c/Å	15.0372(2)
α/°	105.888(2)
β/°	96.944(2)
γ/°	114.393(2)
Volume/Å^3	2070.93(7)
Z	2
ρ_{calc}g/cm^3	1.185
μ/mm^{-1}	1.042
F(000)	788.0
Crystal size/mm^3	0.15 × 0.06 × 0.05
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	6.342 to 152.784
Index ranges	$-15 \le h \le 15$, $-16 \le k \le 16$, $-18 \le l \le 17$

Reflections collected	26451
Independent reflections	8323 [R_{int} = 0.0484, R_{sigma} = 0.0489]
Data/restraints/parameters	8323/0/498
Goodness-of-fit on F^2	1.050
Final R indexes [I>=2σ (I)]	R_1 = 0.0469, wR_2 = 0.1247
Final R indexes [all data]	R_1 = 0.0611, wR_2 = 0.1344
Largest diff. peak/hole / e $Å^{-3}$	0.20/–0.47

6.5. X-Ray Crystallographic Data of Compound 3fa

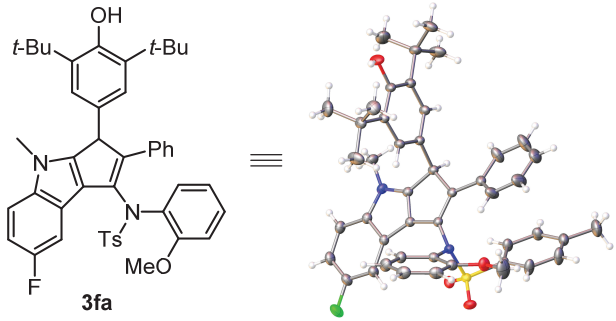


Figure S7. ORTEP drawing of **3fa** (20% ellipsoid probability)

The single crystal of **3fa**, which was used for the determination of its relative configurations via X-ray crystallography (Figure S7), was recrystallized from dichloromethane and methanol. The intensity data were collected on an Agilent SuperNova (Dual, Cu at zero, Eos) diffractometer using graphite-monochromated Cu Kα radiation.

Crystal data and structure refinement for 3fa	
CCDC number	2152048
Empirical formula	$C_{46}H_{47}FN_2O_4S$
Formula weight	742.91
Temperature/K	293(2)
Crystal system	triclinic
Space group	P-1
a/Å	12.2295(10)
b/Å	12.9142(10)
c/Å	14.2096(12)
α/°	95.174(7)
β/°	99.059(7)
γ/°	113.378(8)
Volume/Å^3	2005.2(3)
Z	2
ρ_{calc}g/cm^3	1.230
μ/mm^{-1}	1.117
F(000)	788.0
Crystal size/mm^3	0.15 × 0.12 × 0.09
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	9.048 to 133.182
Index ranges	$-14 \le h \le 14$, $-14 \le k \le 15$, $-13 \le l \le 16$

Reflections collected	12108
Independent reflections	6924 [R_{int} = 0.0213, R_{sigma} = 0.0296]
Data/restraints/parameters	6924/2/500
Goodness-of-fit on F^2	1.027
Final R indexes [I>=2σ (I)]	R_1 = 0.0478, wR_2 = 0.1251
Final R indexes [all data]	R_1 = 0.0570, wR_2 = 0.1348
Largest diff. peak/hole / e $Å^{-3}$	0.21/–0.37

6.6. X-Ray Crystallographic Data of Compound 3ia

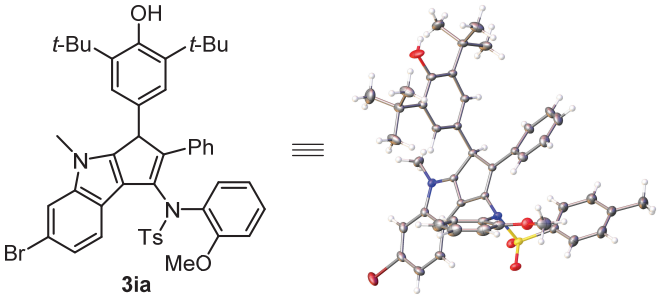


Figure S8. ORTEP drawing of **3ia** (20% ellipsoid probability)

The single crystal of **3ia**, which was used for the determination of its relative configurations via X-ray crystallography (Figure S8), was recrystallized from dichloromethane and methanol. The intensity data were collected on a Rigaku XtaLAB Synergy R (DW system, HyPix) diffractometer using graphite-monochromated Cu Kα radiation.

Crystal data and structure refinement for 3ia	
CCDC number	2152049
Empirical formula	$C_{46}H_{47}BrN_2O_4S$
Formula weight	803.82
Temperature/K	303.78(10)
Crystal system	monoclinic
Space group	$P2_1/c$
a/Å	10.55960(10)
b/Å	12.86910(10)
c/Å	30.3703(3)
α/°	90
β/°	96.1700(10)
γ/°	90
Volume/Å^3	4103.19(7)
Z	4
ρ_{calc}g/cm^3	1.301
μ/mm^{-1}	2.193
F(000)	1680.0
Crystal size/mm^3	0.18 × 0.15 × 0.12
Radiation	Cu Kα (λ = 1.54184)
2Θ range for data collection/°	5.854 to 152.902
Index ranges	$-13 \le h \le 13$, $-16 \le k \le 13$, $-31 \le l \le 38$

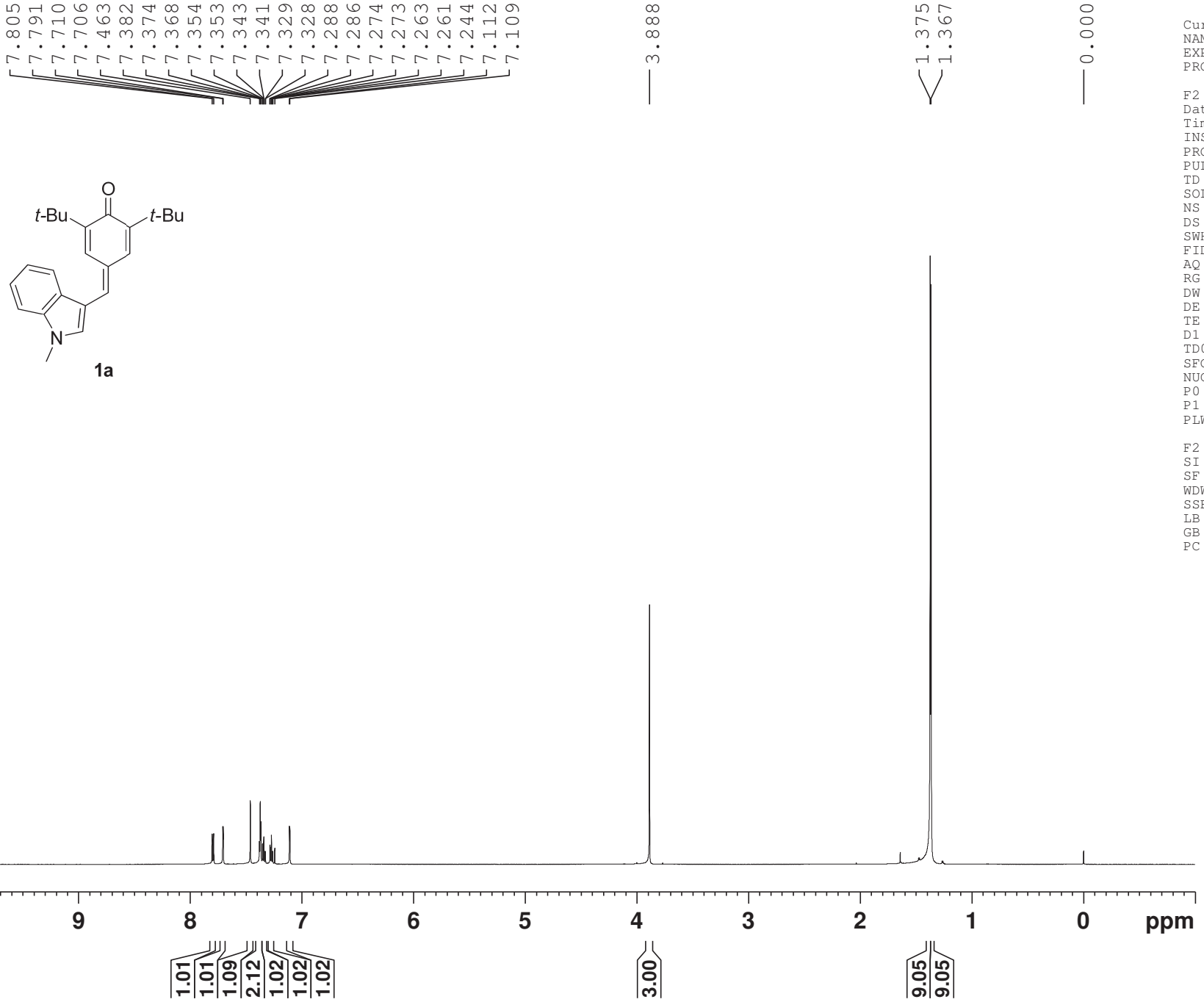
Reflections collected	29600
Independent reflections	8255 [R_{int} = 0.0556, R_{sigma} = 0.0497]
Data/restraints/parameters	8255/2/497
Goodness-of-fit on F^2	1.045
Final R indexes [I>=2σ (I)]	R_1 = 0.0470, wR_2 = 0.1260
Final R indexes [all data]	R_1 = 0.0548, wR_2 = 0.1316
Largest diff. peak/hole / e $Å^{-3}$	0.33/–0.76

7. References

(1) (a) M. Mäurer, W. Hiller, B. Müller and H. B. Stegmann, *Chem. Ber.*, 1992, **125**, 857; (b) D. Richter, N. Hampel, T. Singer, A. R. Ofial and H. Mayr, *Eur. J. Org. Chem.*, 2009, **2009**, 3203; (c) W.-D. Chu, L.-F. Zhang, X. Bao, X.-H. Zhao, C. Zeng, J.-Y. Du, G.-B. Zhang, F.-X. Wang, X.-Y. Ma and C.-A. Fan, *Angew. Chem.*, *Int. Ed.*, 2013, **52**, 9229; (d) Y. F. Wong, Z. Wang, J. Sun, *Org. Biomol. Chem.*, 2016, **14**, 5751; (e) S. Li, Y. Liu, B. Huang, T. Zhou, H. Tao, Y. Xiao, L. Liu, J. Zhang, *ACS Catal.*, 2017, **7**, 2805.

(2) (a) B. Yao, Z. Liang, T. Niu and Y. Zhang, *J. Org. Chem.*, 2009, **74**, 4630; (b) C. Schotes and A. Mezzetti, *Angew. Chem., Int. Ed.*, 2011, **50**, 3072; (c) A. S. Reddy and K. C. K. Swamy, *Angew. Chem., Int. Ed.*, 2017, **56**, 6984; (d) T. Hamada, X. Ye and S. S. Stahl, *J. Am. Chem. Soc.*, 2008, **130**, 833; (e) A. Mukherjee, R. B. Dateer, R. Chaudhuri, S. Bhunia, S. N. Karad and R.-S. Liu, *J. Am. Chem. Soc.*, 2011, **133**, 15372; (f) C. Schotes, R. Bigler and A. Mezzetti, *Synthesis*, 2012, **44**, 513.

8. Copies of NMR Spectra

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DS                     2
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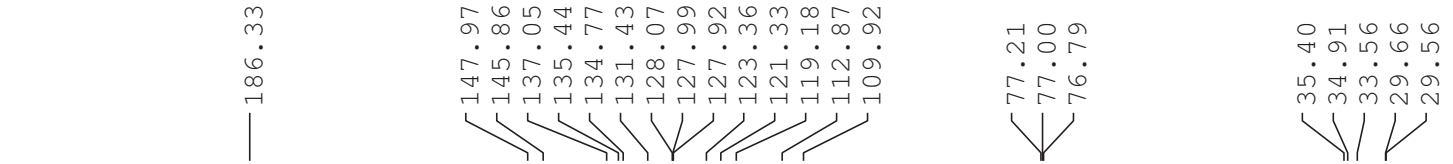

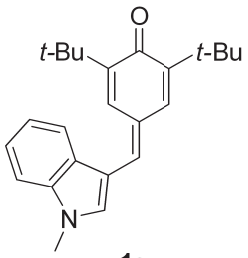

1a

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P0                 4.00 usec
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PLW1         87.25299835 W
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NUC2                  1H
CPDPRG[2          waltz65
PCPD2             70.00 usec
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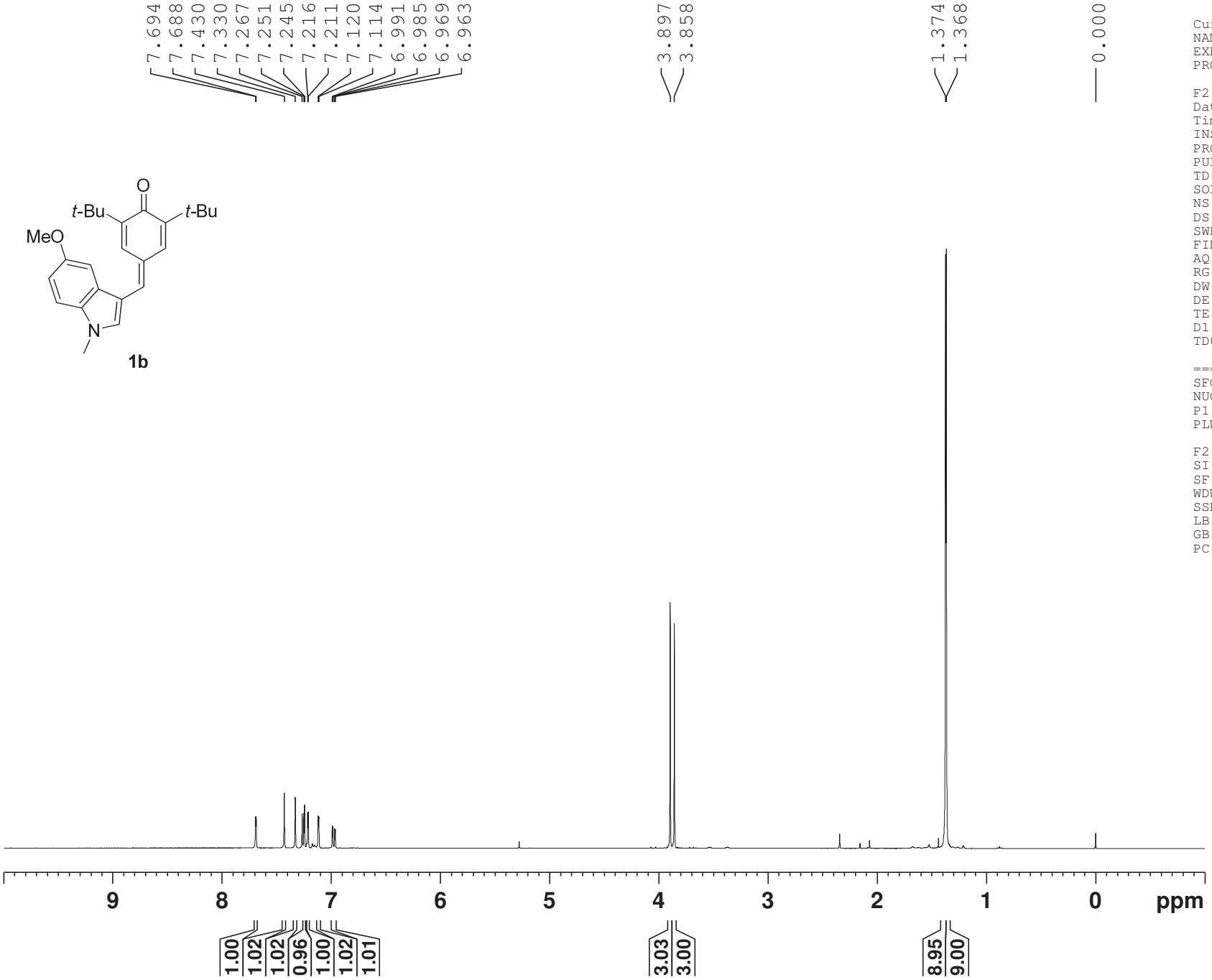
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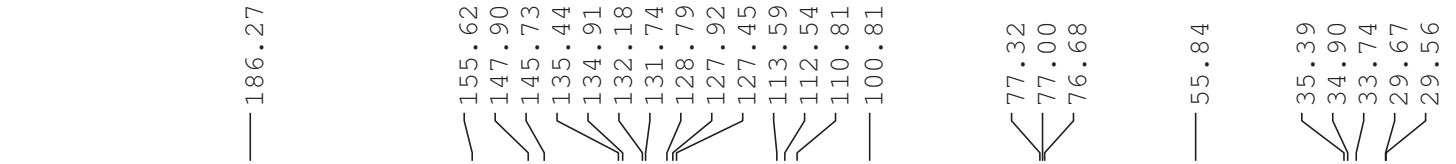

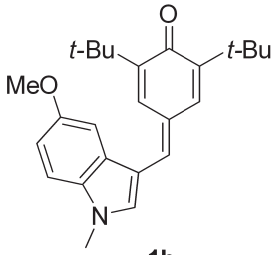

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NS                       32
DS                        2
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DE                    6.50 usec
TE                   296.4 K
D1               2.00000000 sec
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TD0                       1

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P1                   15.50 usec
PLW1           25.00000000 W

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NUC2                    1H
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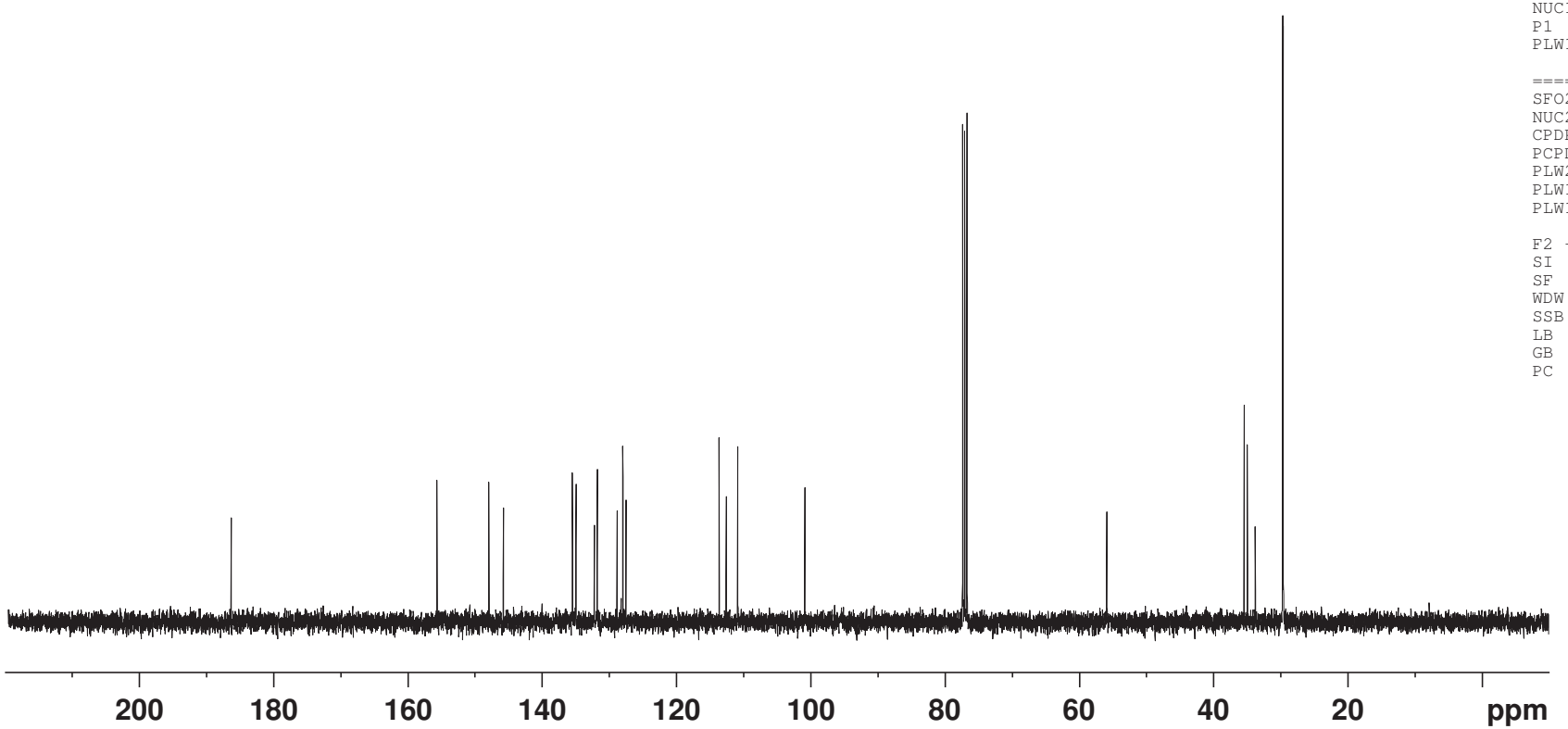

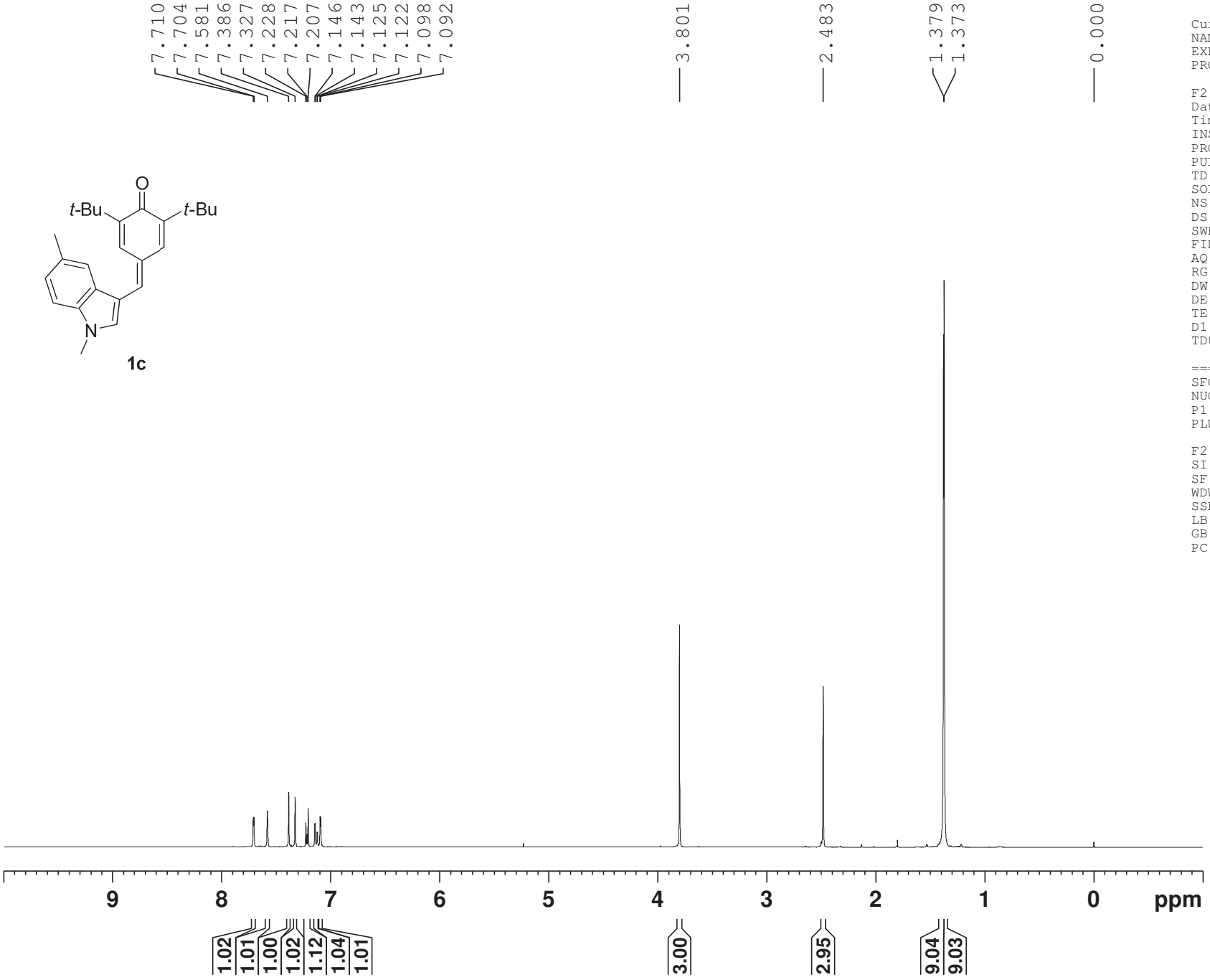


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TE                   296.0 K
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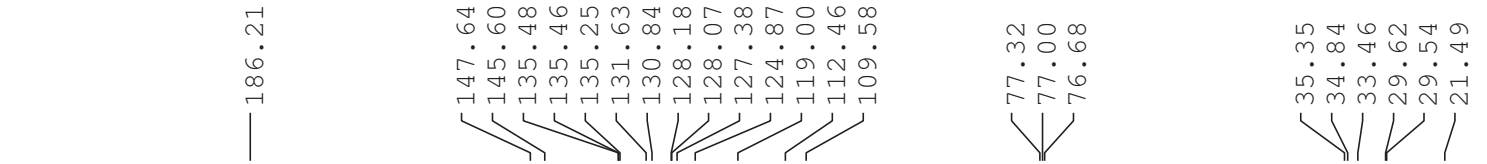

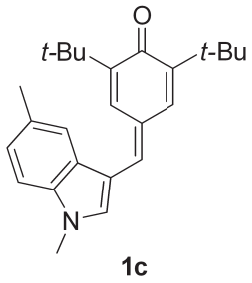

1c

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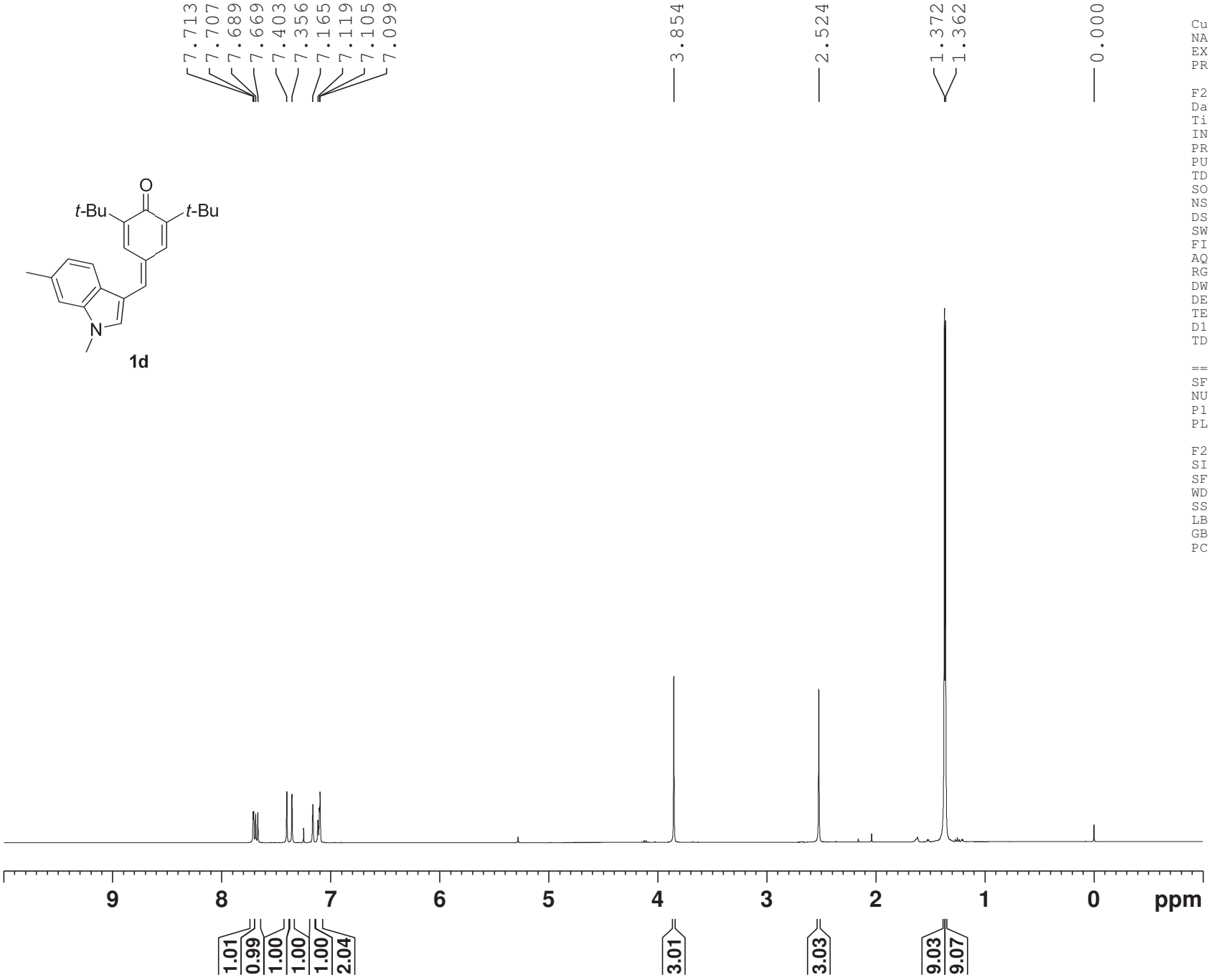


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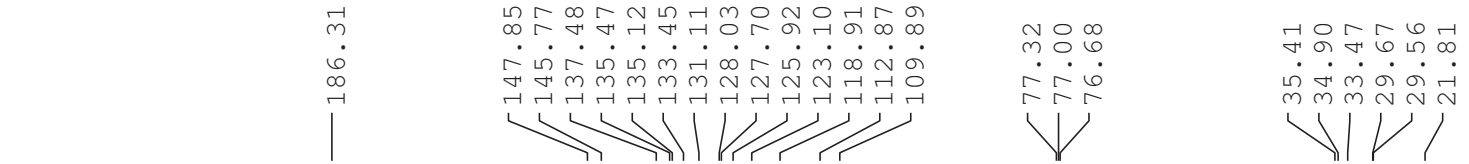
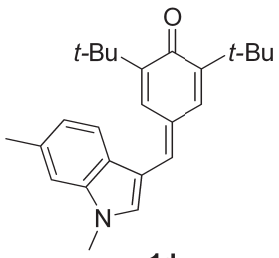
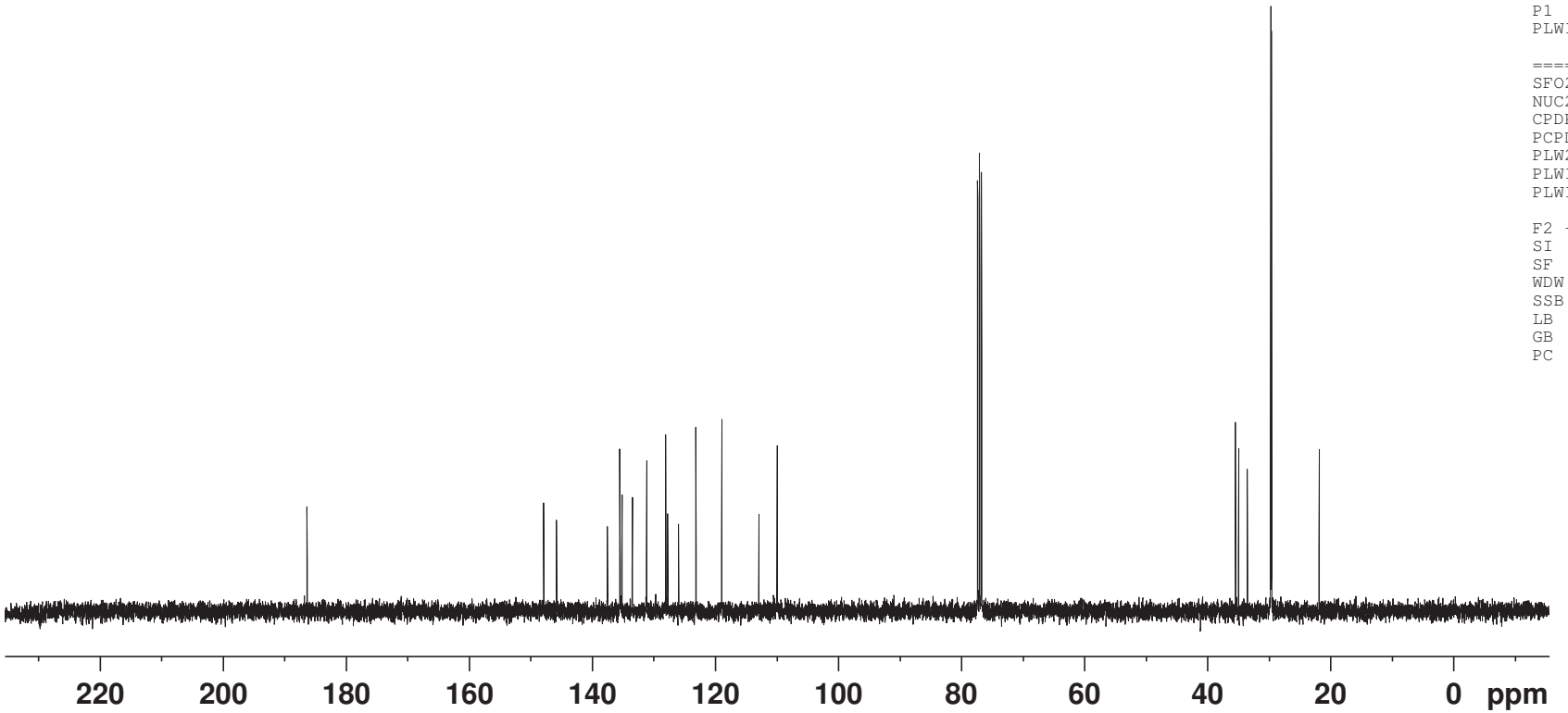
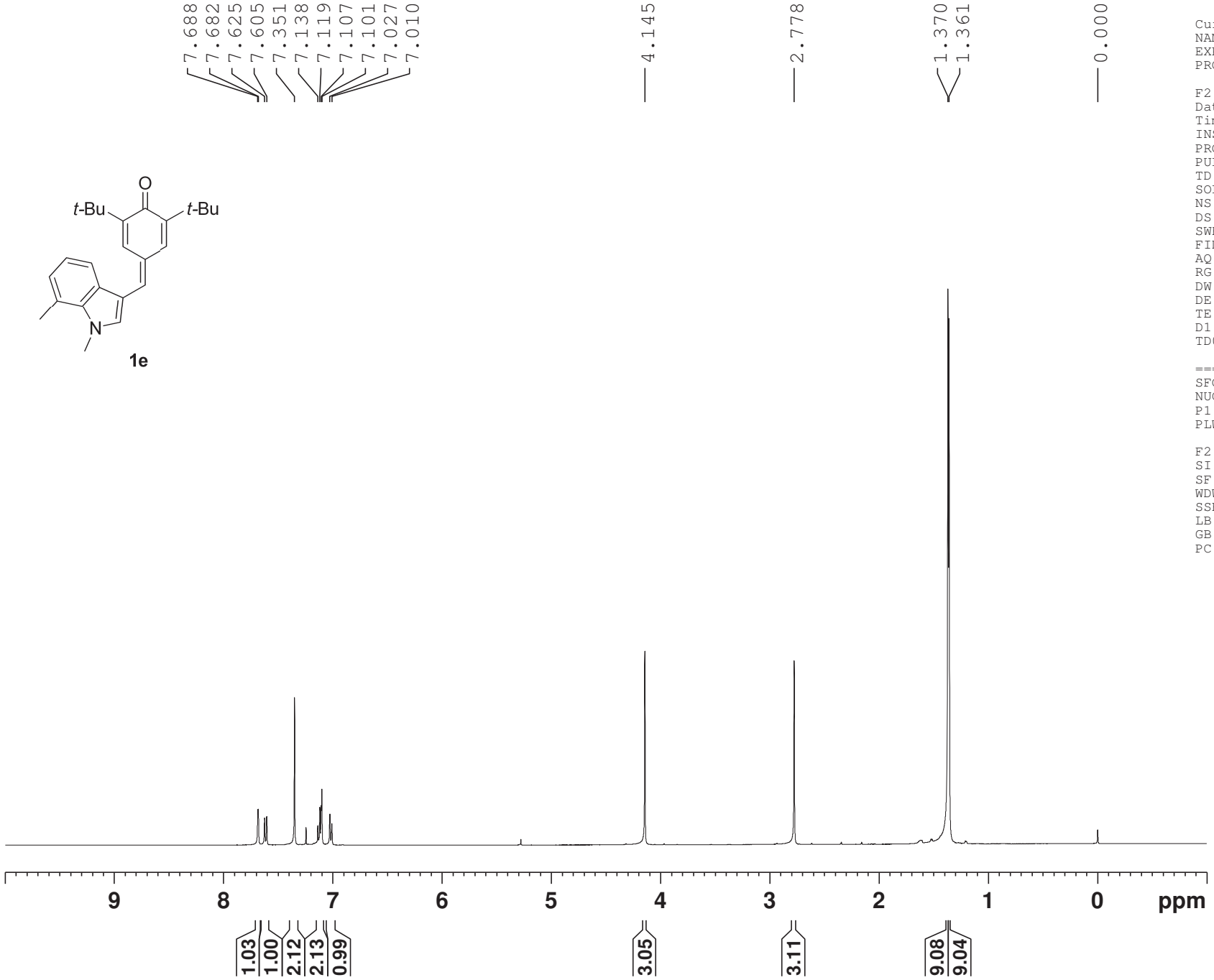




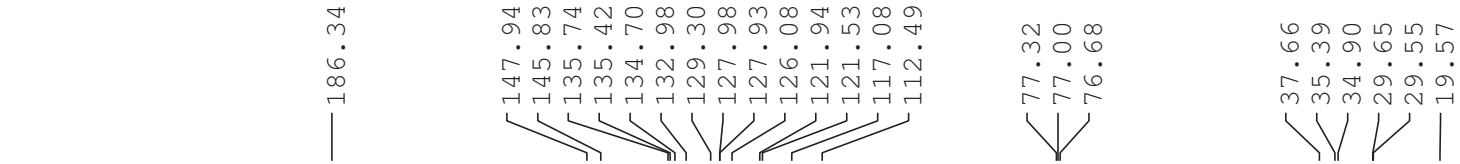
1d

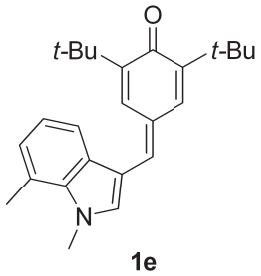
```
Current Data Parameters
NAME                  6-Me
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                  9.21
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       2
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ               1.2976128 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  295.1 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6238364 MHz
NUC1                    13C
P1                   15.50 usec
PLW1           25.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2            waltz16
PCPD2                80.00 usec
PLW2           19.50000000 W
PLW12           0.51492000 W
PLW13           0.32955000 W

F2 - Processing parameters
SI                      32768
SF             100.6127729 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```





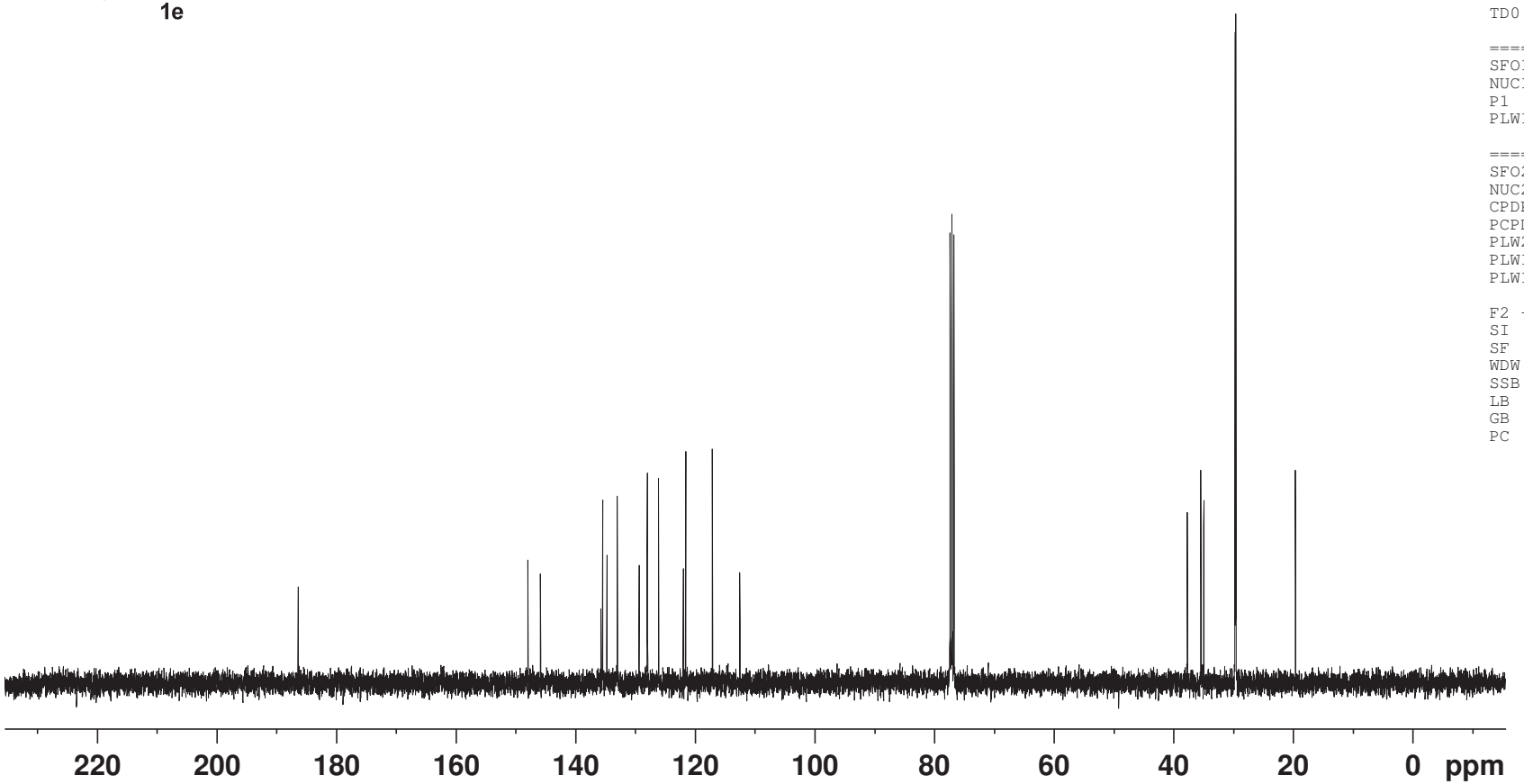

```
Current Data Parameters
NAME                  7-Me
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                   8.28
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                        4
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                      114
DW                   62.400 usec
DE                    6.50 usec
TE                   294.1 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    12.40 usec
PLW1           19.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300152 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

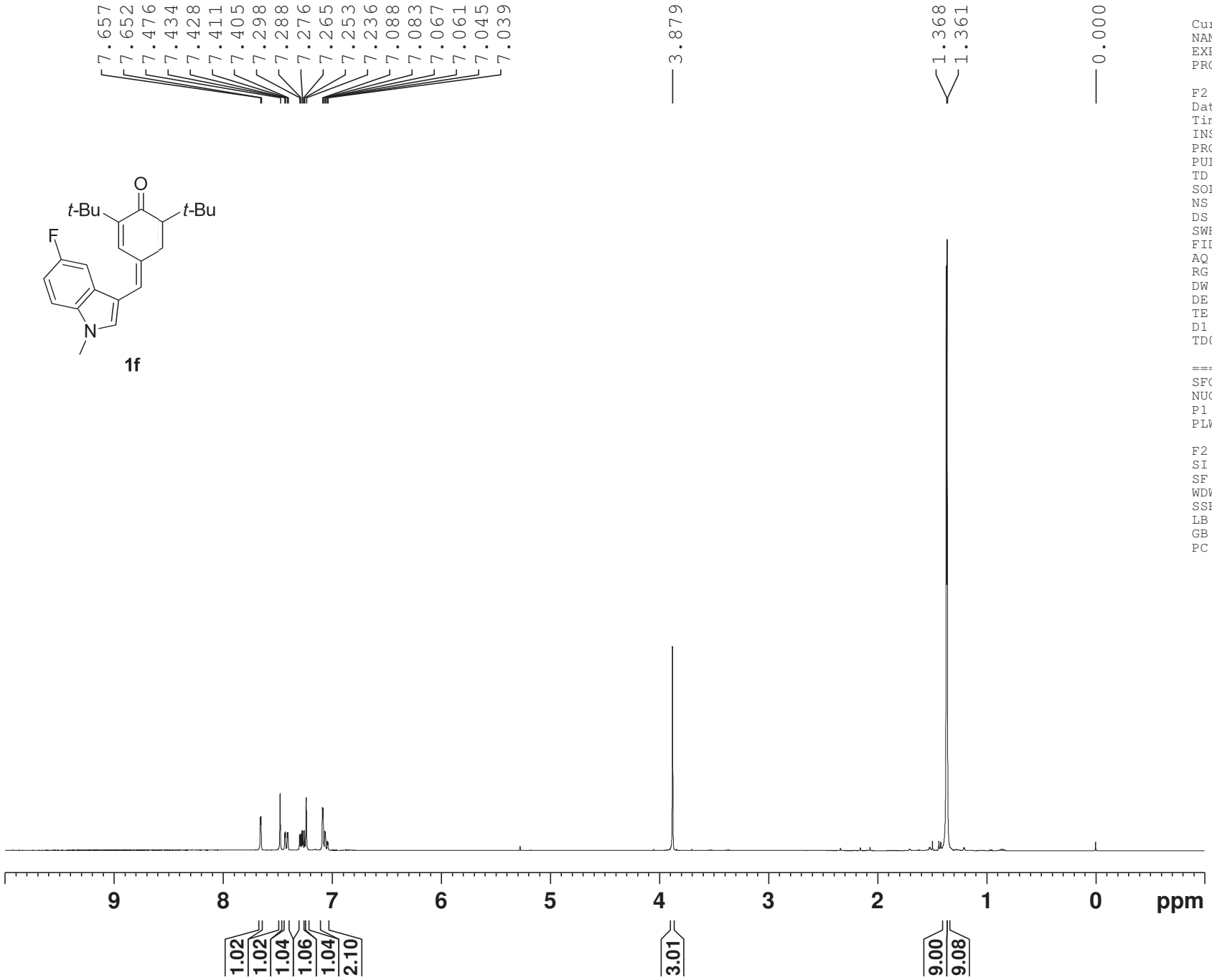




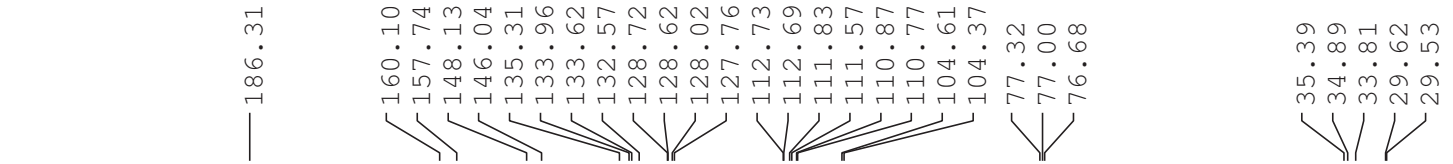
1e

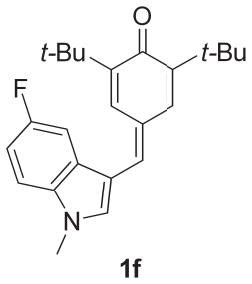
```
Current Data Parameters
NAME                  7-Me
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                  8.32
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      64
DS                       2
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ                1.2976128 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  295.3 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6238364 MHz
NUC1                    13C
P1                   15.50 usec
PLW1           25.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           19.50000000 W
PLW12           0.51492000 W
PLW13           0.32955000 W

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





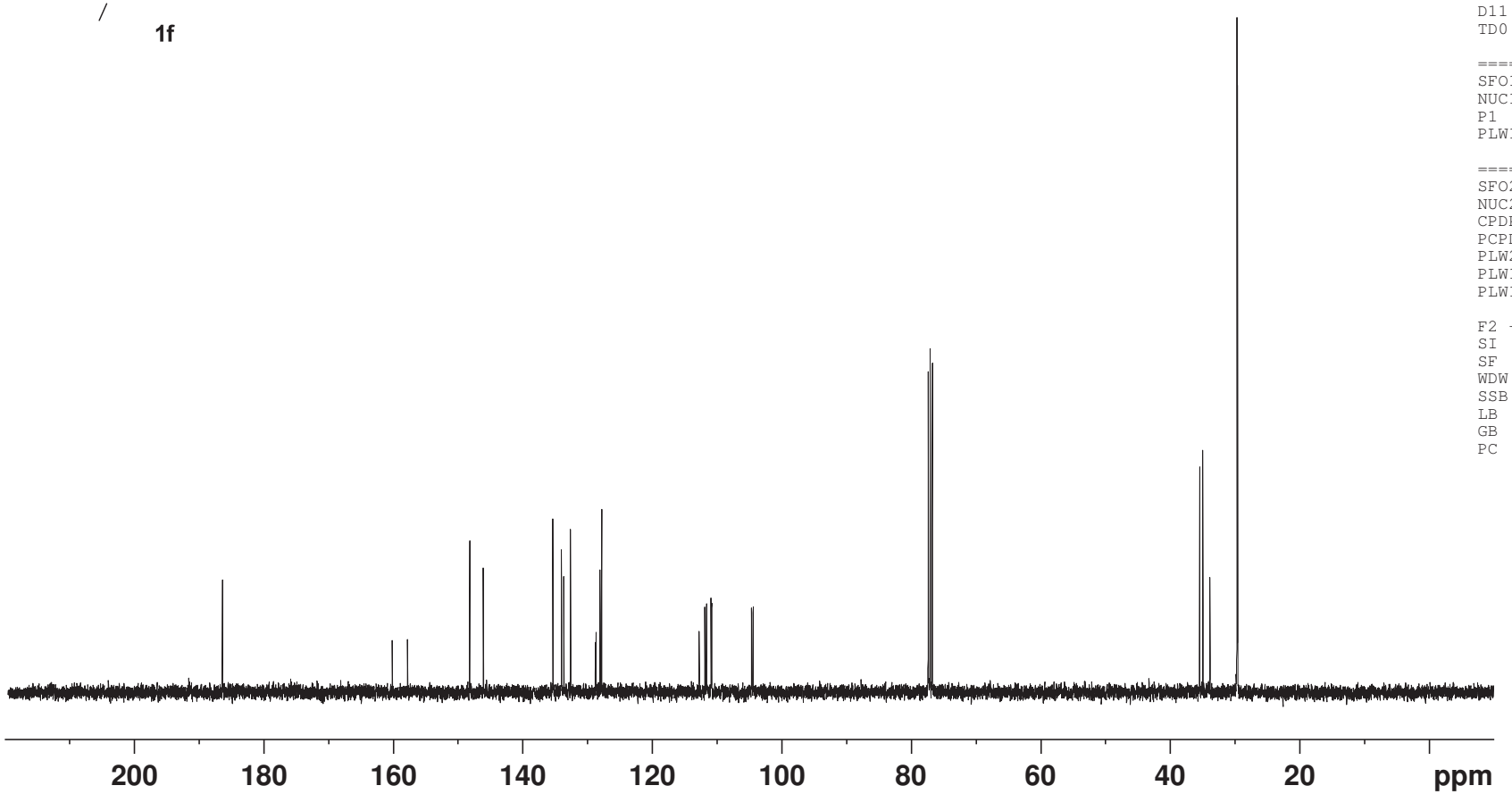

```
Current Data Parameters
NAME                  5-F
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180608
Time                8.25
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                     4
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                   114
DW                62.400 usec
DE                 6.50 usec
TE                295.8 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 12.40 usec
PLW1         19.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300126 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

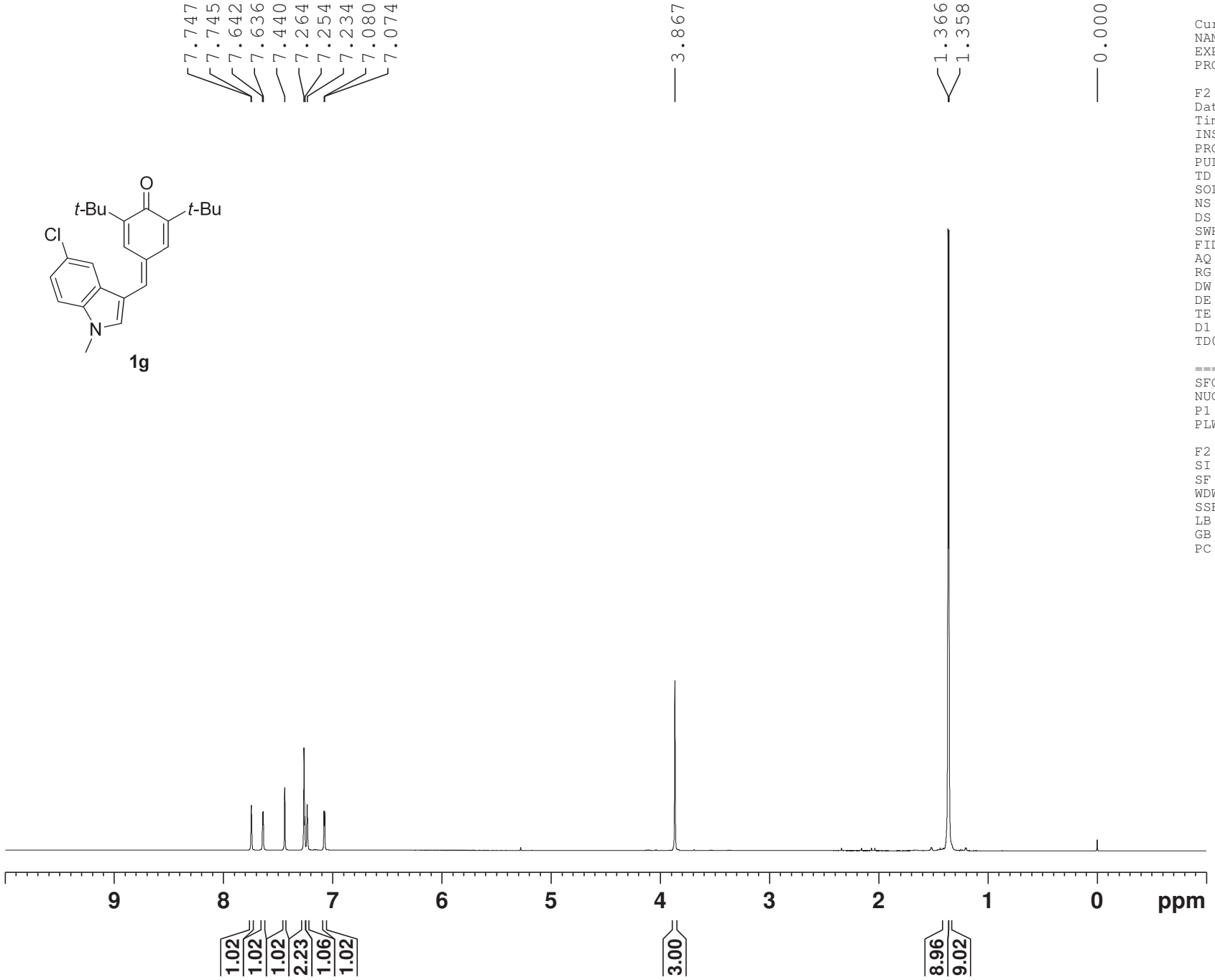




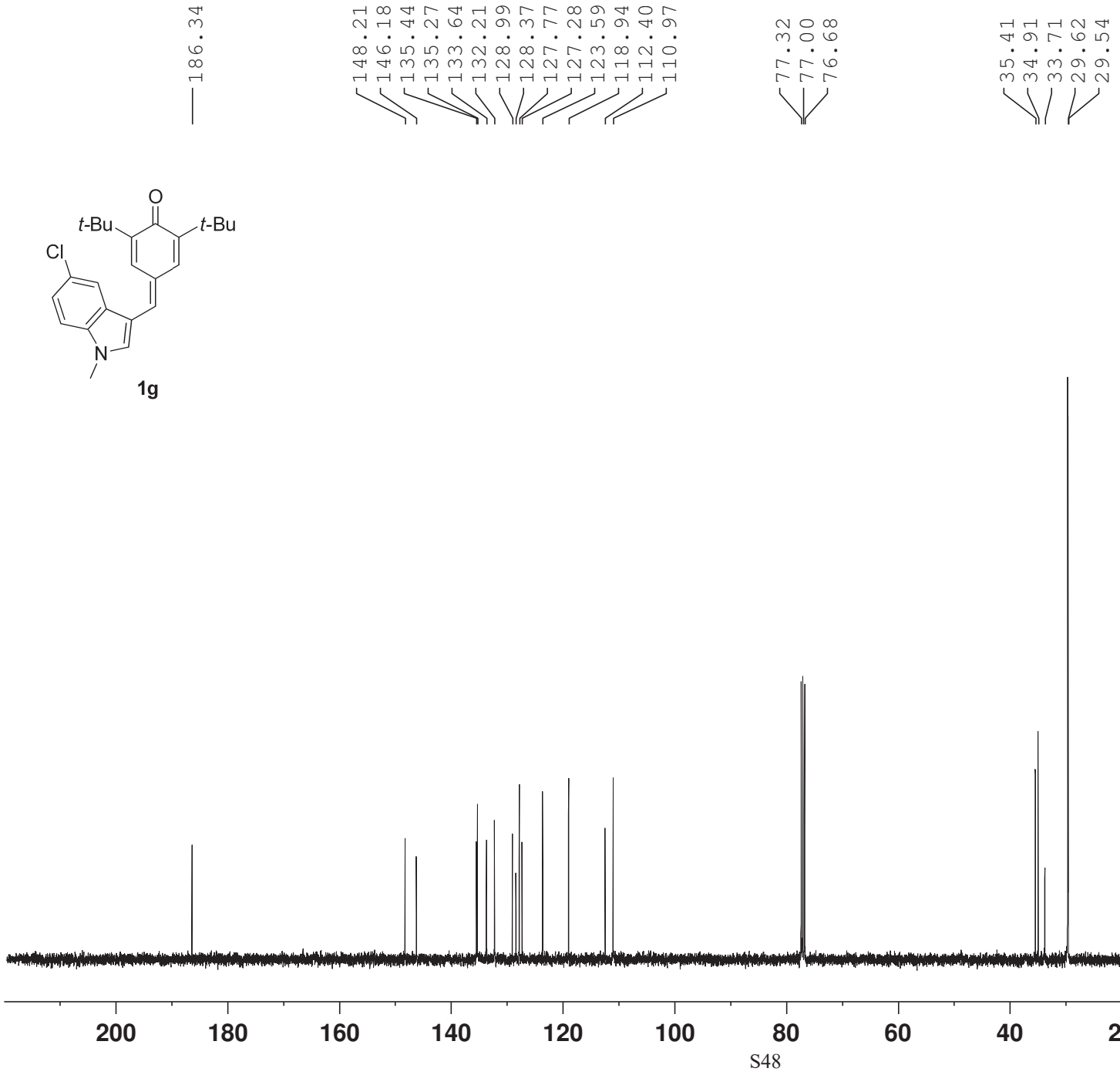
1f

```
Current Data Parameters
NAME                  5-F
EXPNO                  11
PROCNO                  1

F2 - Acquisition Parameters
Date_           20180608
Time                8.27
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                   32
DS                    2
SWH           24038.461 Hz
FIDRES         0.366798 Hz
AQ             1.3631488 sec
RG                 2050
DW               20.800 usec
DE                6.50 usec
TE               296.4 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6228298 MHz
NUC1                13C
P1                15.50 usec
PLW1        25.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        19.50000000 W
PLW12        0.51492000 W
PLW13        0.32955000 W

F2 - Processing parameters
SI                 32768
SF          100.6127750 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

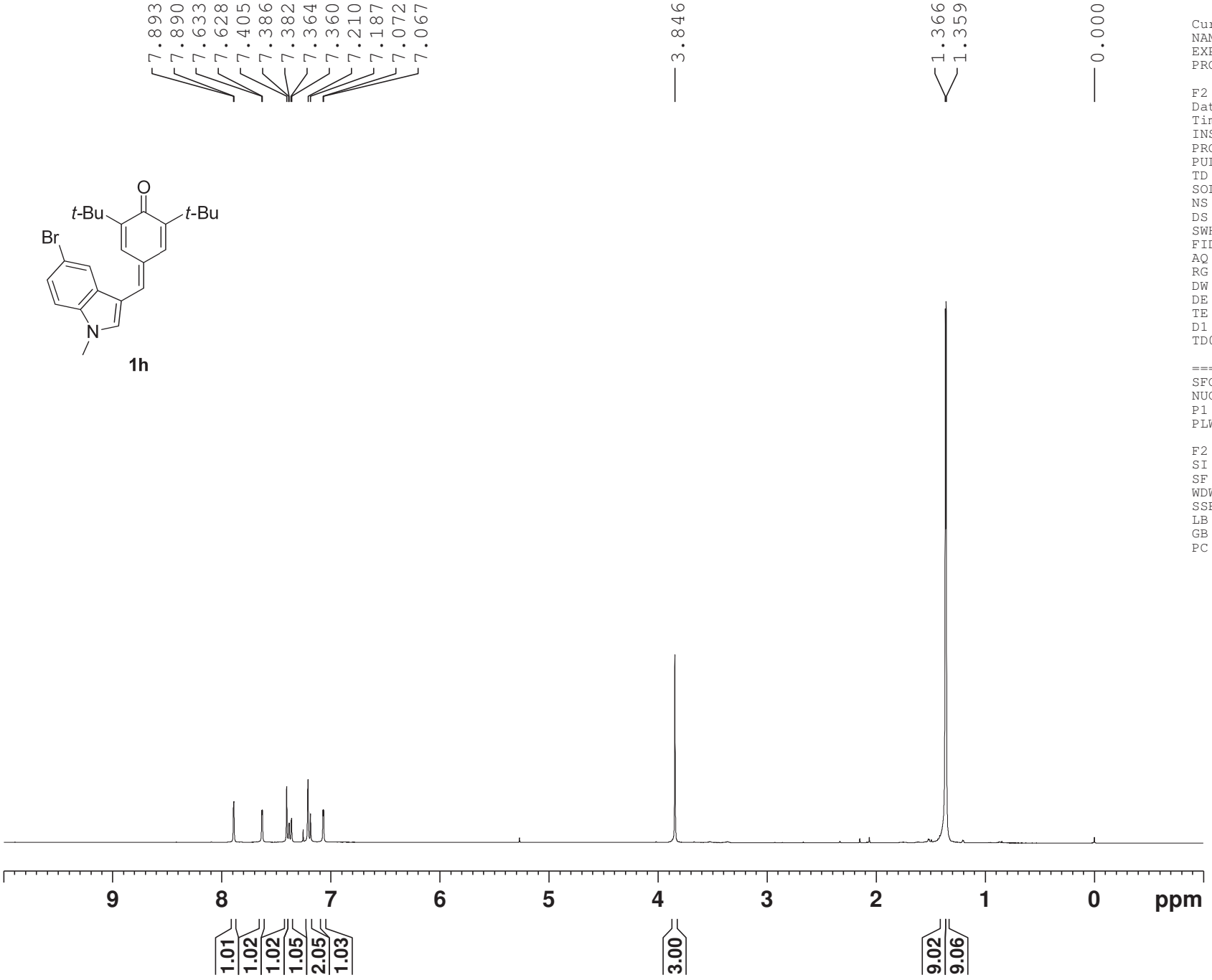




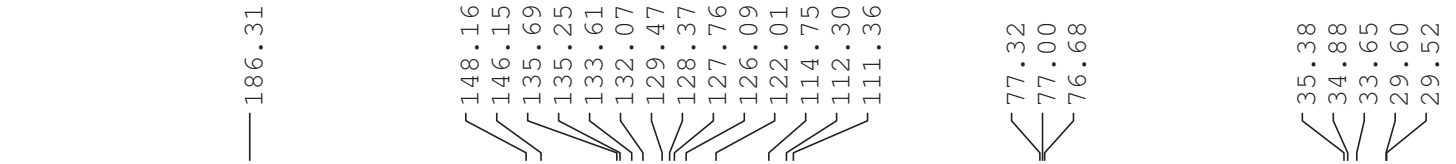

```
Current Data Parameters
NAME                  5-Cl
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180608
Time                   8.11
INSTRUM               spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDCl3
NS                        4
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                      144
DW                   62.400 usec
DE                    6.50 usec
TE                   295.8 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    12.40 usec
PLW1           19.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300118 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

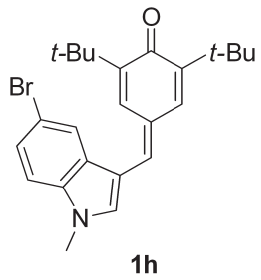



```
Current Data Parameters
NAME                  5-Cl
EXPNO                   12
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180608
Time                   8.15
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        2
SWH               24038.461 Hz
FIDRES             0.366798 Hz
AQ                 1.3631488 sec
RG                     2050
DW                   20.800 usec
DE                    6.50 usec
TE                   296.5 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            100.6228298 MHz
NUC1                    13C
P1                    15.50 usec
PLW1            25.00000000 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2            19.50000000 W
PLW12            0.51492000 W
PLW13            0.32955000 W

F2 - Processing parameters
SI                      32768
SF              100.6127744 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```



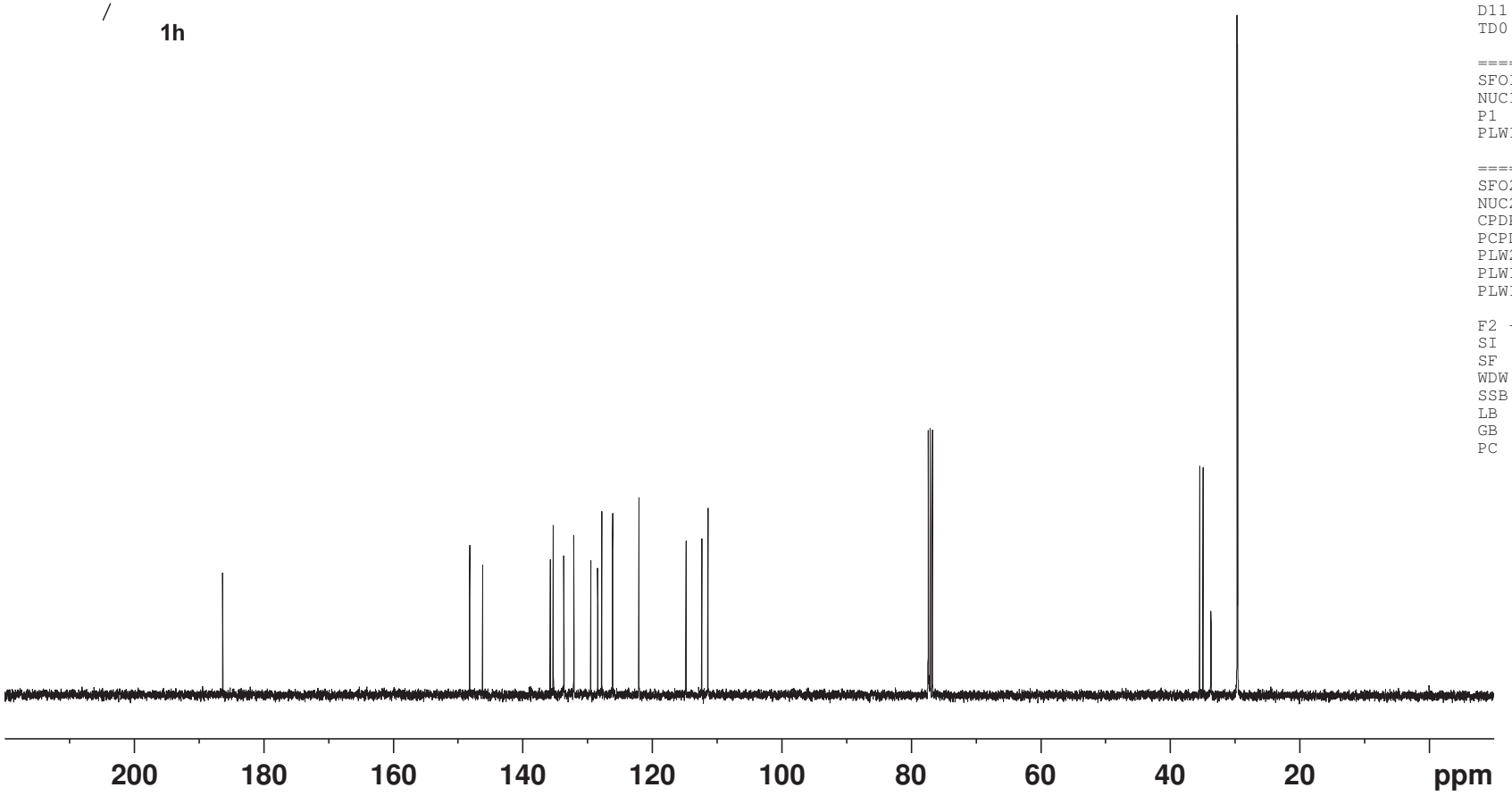

```
Current Data Parameters
NAME                  5-Br
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180714
Time                  1.29
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                        4
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                      101
DW                   62.400 usec
DE                    6.50 usec
TE                   297.1 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    12.40 usec
PLW1           19.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300119 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

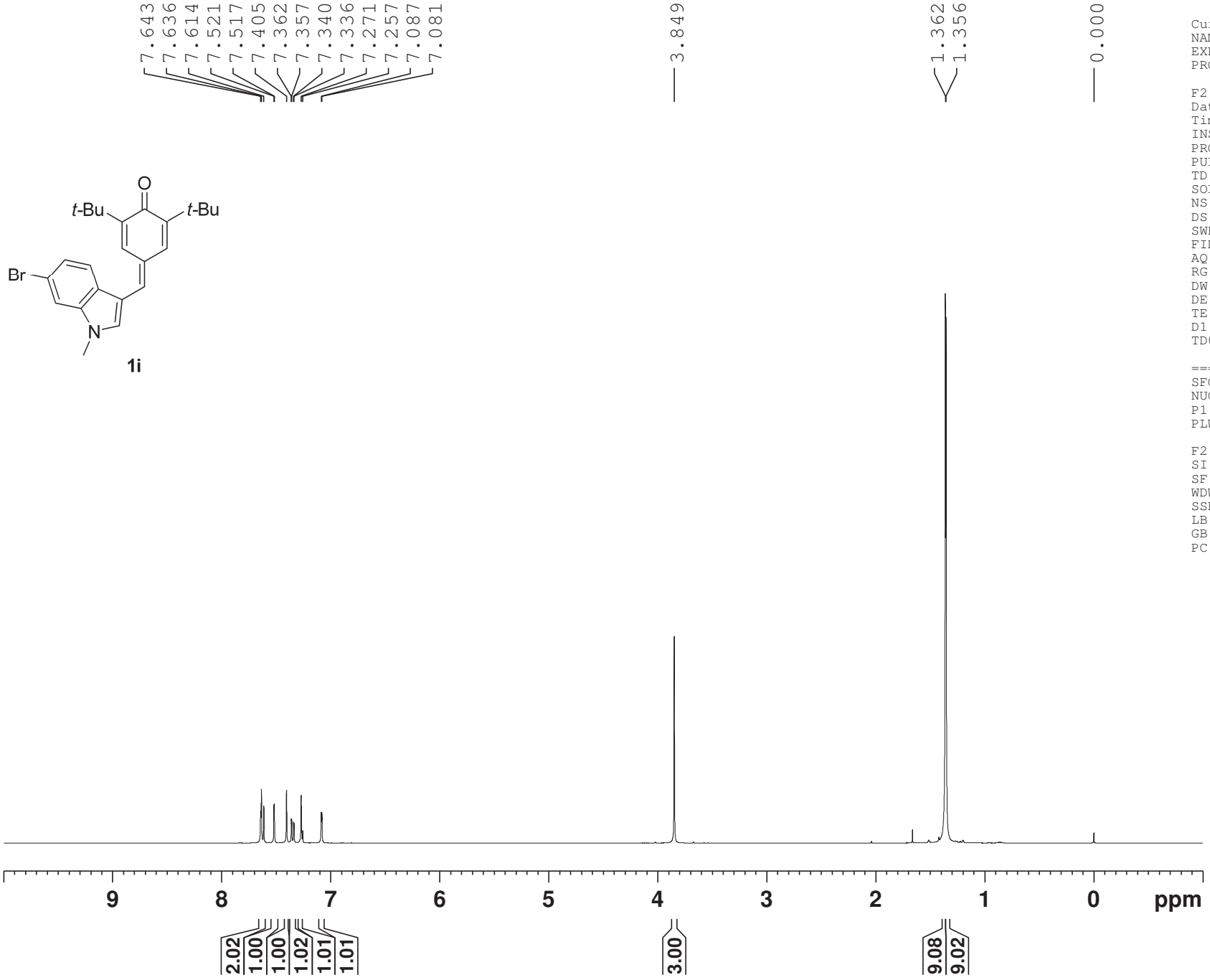


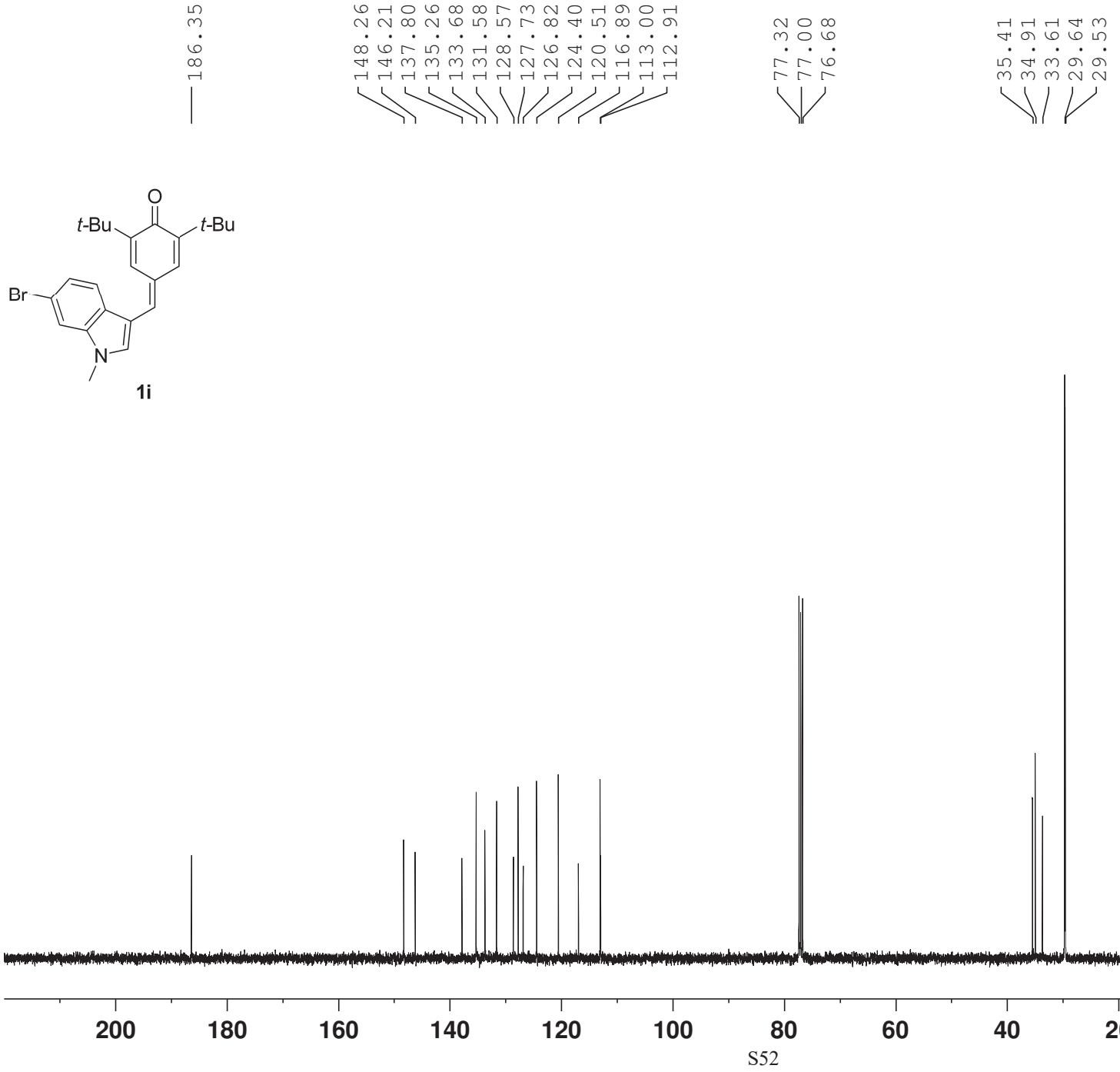


1h

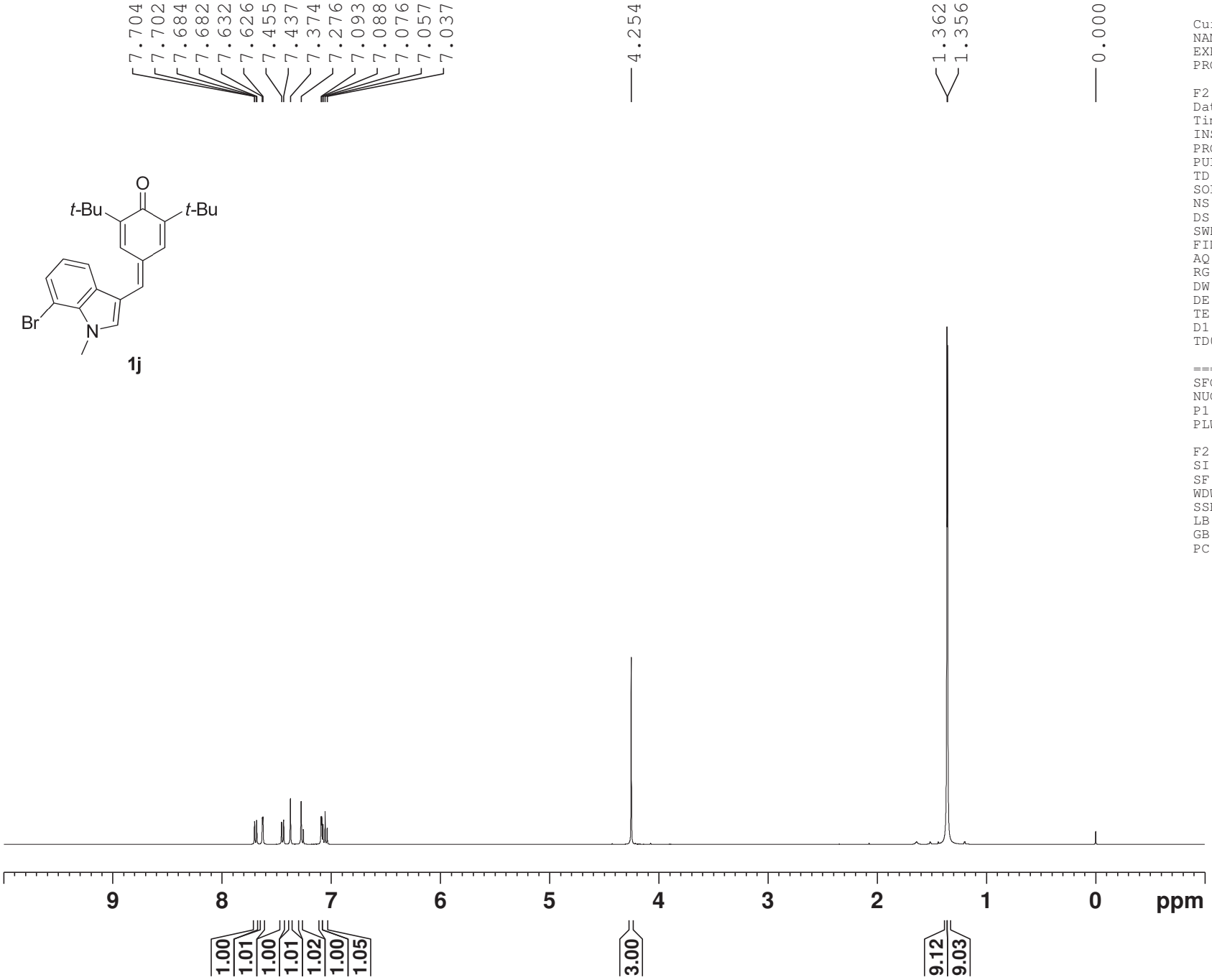
```
Current Data Parameters
NAME                  5-Br
EXPNO                   12
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180714
Time                   1.33
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       64
DS                        2
SWH               25252.525 Hz
FIDRES             0.385323 Hz
AQ                1.2976128 sec
RG                     2050
DW                   19.800 usec
DE                    6.50 usec
TE                   297.8 K
D1                2.00000000 sec
D11               0.03000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1            100.6238364 MHz
NUC1                    13C
P1                    15.50 usec
PLW1            25.00000000 W

======== CHANNEL f2 ========
SFO2            400.1316005 MHz
NUC2                    1H
CPDPRG[2             waltz16
PCPD2                 80.00 usec
PLW2            19.50000000 W
PLW12            0.51492000 W
PLW13            0.32955000 W

F2 - Processing parameters
SI                      32768
SF              100.6127776 MHz
WDW                        EM
SSB          0
LB                     1.00 Hz
GB           0
PC                     1.40
```

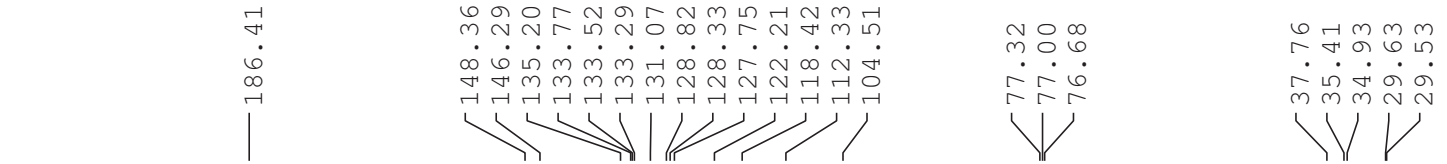


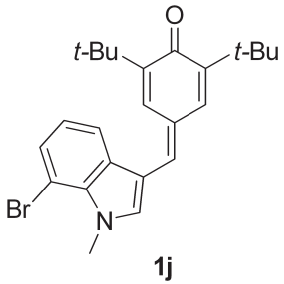

7.643
7.636
7.614
7.521
7.517
7.405
7.362
7.357
7.340
7.336
7.271
7.257
7.087
7.081
3.849
1.362
1.356
0.000
O
t-Bu
t-Bu
Br
N
1i
Current Data Parameters
NAME 6-Br
EXPNO 14
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210811
Time 9.11
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 80.6
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 12.40 usec
PLW1 19.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300120 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
2.02
1.00
1.00
1.02
1.01
1.01
3.00
9.08
9.02




```
Current Data Parameters
NAME                  6-Br
EXPNO                   15
PROCNO                   1

F2 - Acquisition Parameters
Date_              20210811
Time                  9.18
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     128
DS                       2
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ                1.2976128 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  294.2 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6228303 MHz
NUC1                    13C
P1                   15.50 usec
PLW1           25.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           19.50000000 W
PLW12           0.45497999 W
PLW13           0.29119000 W

F2 - Processing parameters
SI                    32768
SF             100.6127750 MHz
WDW                      EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

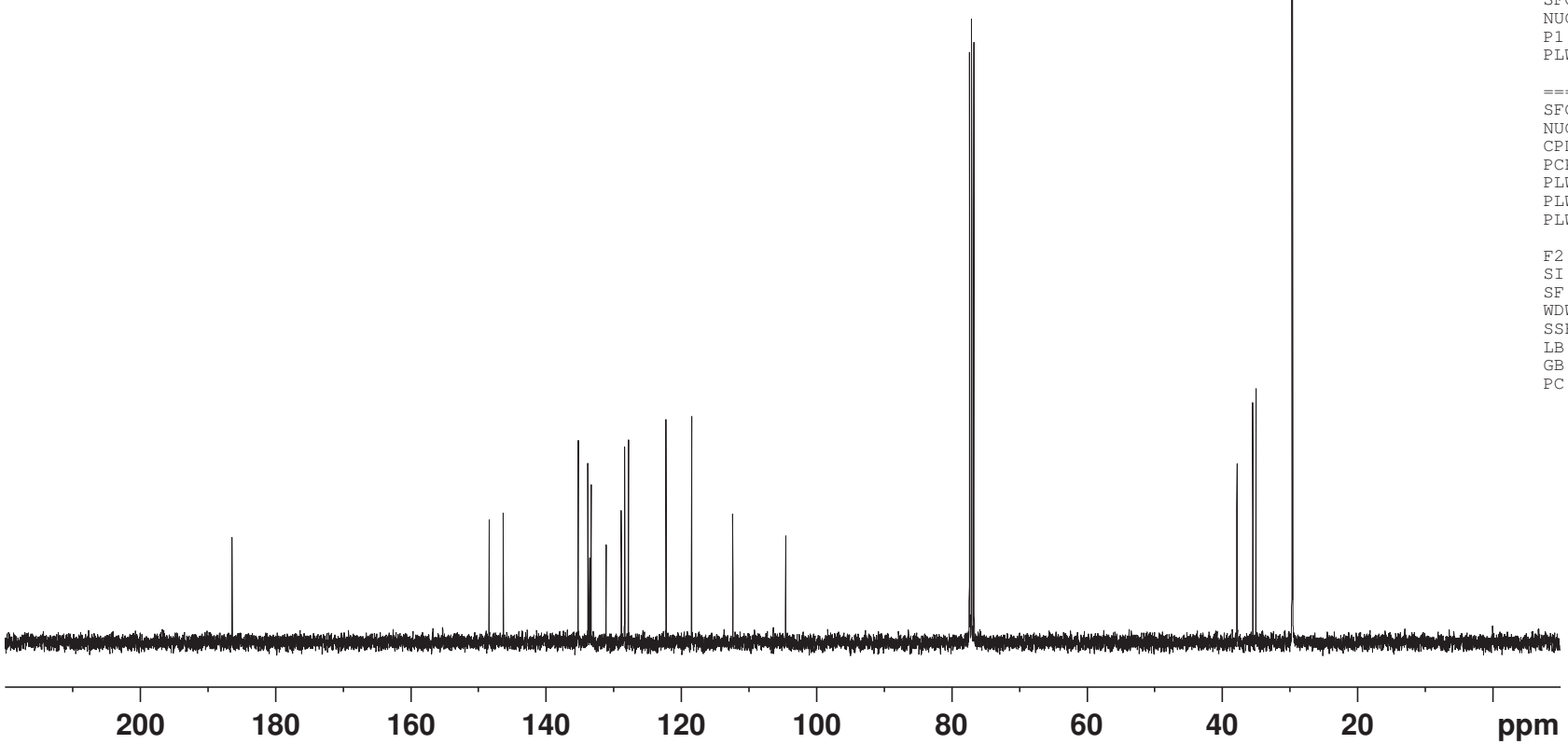

7.704
7.702
7.684
7.682
7.632
7.626
7.455
7.437
7.374
7.276
7.093
7.088
7.076
7.057
7.037
4.254
1.362
1.356
0.000
O
t-Bu
t-Bu
Br
N
1j
Current Data Parameters
NAME 7-Br
EXPNO 18
PROCNO 1
F2 - Acquisition Parameters
Date_ 20210811
Time 9.24
INSTRUM spect
PROBHD 5 mm PABBO BB/
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 8012.820 Hz
FIDRES 0.122266 Hz
AQ 4.0894465 sec
RG 101
DW 62.400 usec
DE 6.50 usec
TE 293.2 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
SFO1 400.1324710 MHz
NUC1 1H
P1 12.40 usec
PLW1 19.00000000 W
F2 - Processing parameters
SI 65536
SF 400.1300126 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.00
1.01
1.00
1.01
1.02
1.00
1.05
3.00
9.12
9.03

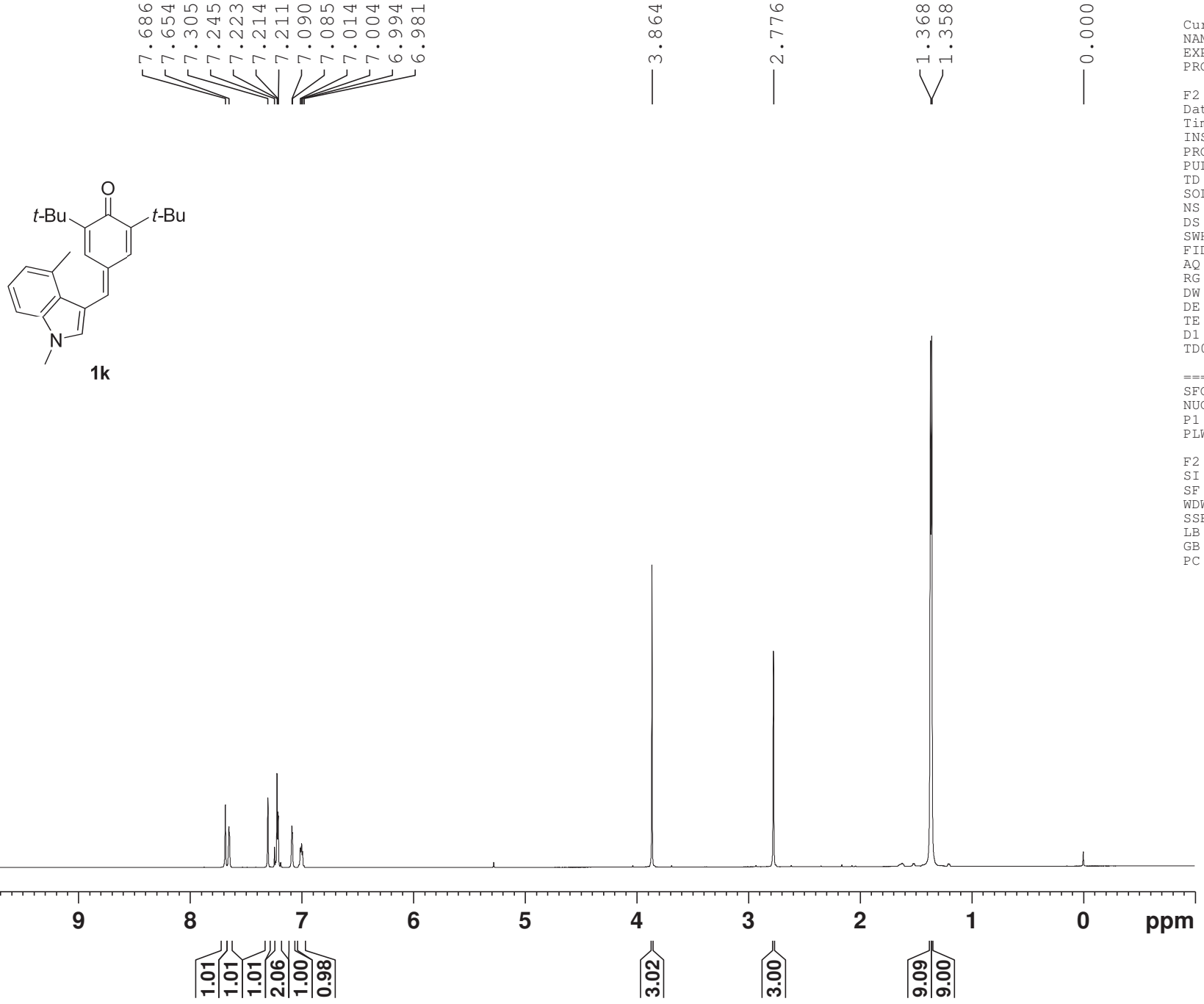




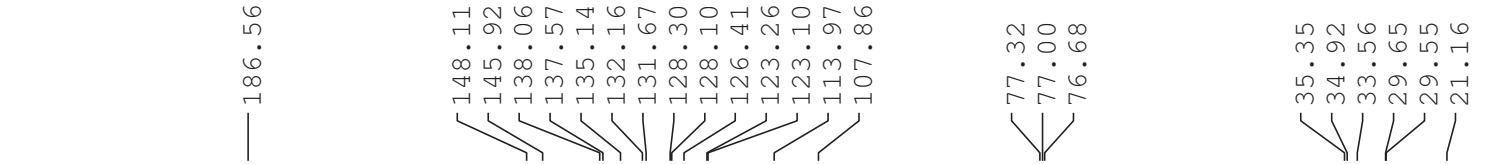
1j

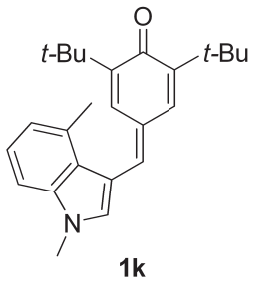
```
Current Data Parameters
NAME                 7-Br
EXPNO                  19
PROCNO                  1

F2 - Acquisition Parameters
Date_             20210811
Time                 9.32
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                    128
DS                      2
SWH             25252.525 Hz
FIDRES          0.385323 Hz
AQ              1.2976128 sec
RG                   2050
DW                 19.800 usec
DE                  6.50 usec
TE                 294.3 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          100.6238364 MHz
NUC1                  13C
P1                 15.50 usec
PLW1          25.00000000 W

======== CHANNEL f2 ========
SFO2          400.1316005 MHz
NUC2                  1H
CPDPRG[2          waltz16
PCPD2              80.00 usec
PLW2          19.50000000 W
PLW12          0.45497999 W
PLW13          0.29119000 W

F2 - Processing parameters
SI                   32768
SF            100.6127737 MHz
WDW                     EM
SSB       0
LB                  1.00 Hz
GB        0
PC                  1.40
```





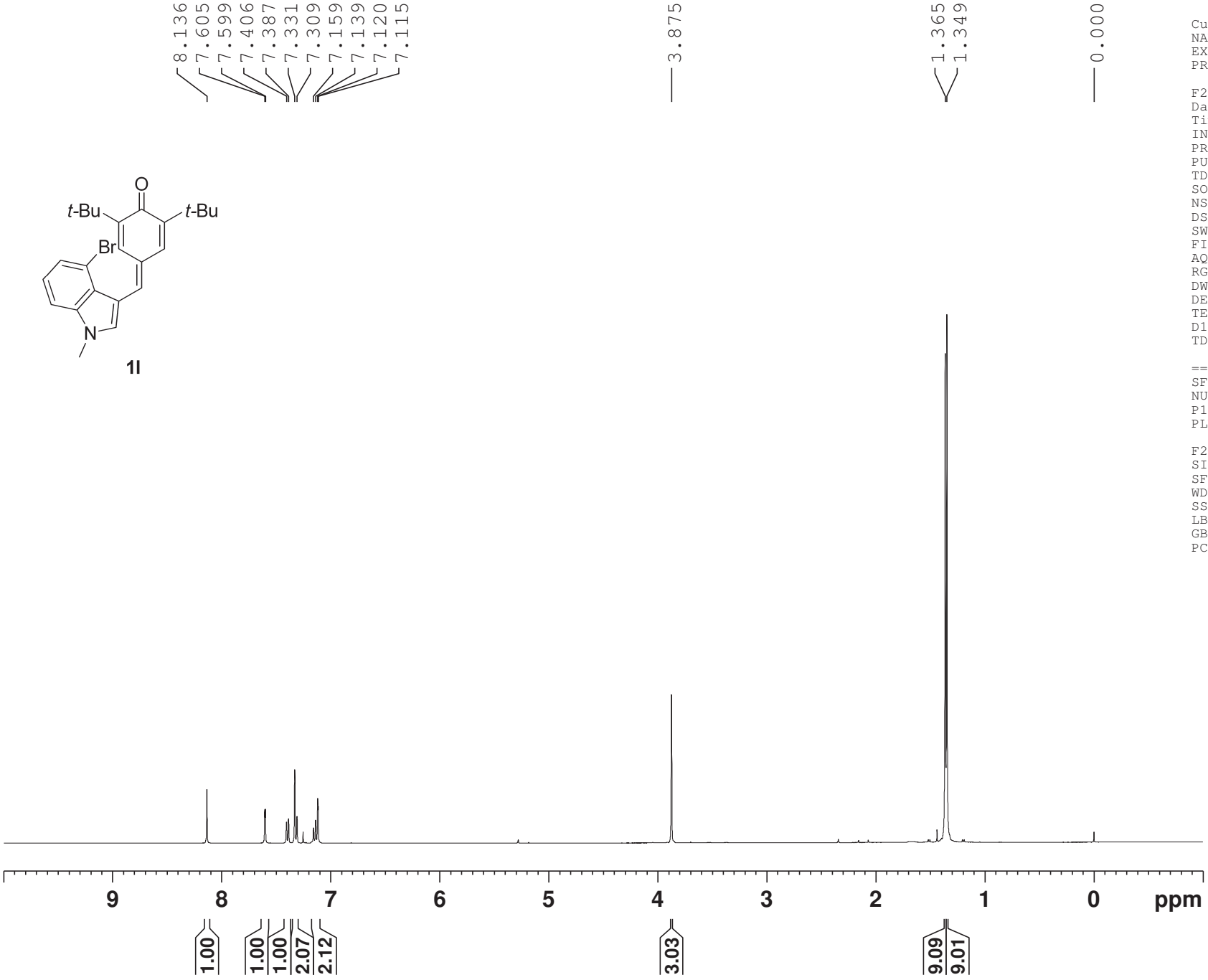

```
Current Data Parameters
NAME                  4-Me
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                  8.59
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG               zg30
TD                   65536
SOLVENT              CDC13
NS                       4
DS                       2
SWH               8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     101
DW                  62.400 usec
DE                   6.50 usec
TE                  293.9 K
D1              1.00000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                   1H
P1                  12.40 usec
PLW1           19.00000000 W

F2 - Processing parameters
SI                   65536
SF             400.1300153 MHz
WDW                    EM
SSB          0
LB                   0.30 Hz
GB           0
PC                   1.00
```



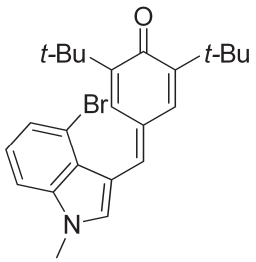


1k

```
Current Data Parameters
NAME                  4-Me
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                  9.02
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      50
DS                       2
SWH              25252.525 Hz
FIDRES           0.385323 Hz
AQ               1.2976128 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  295.1 K
D1              2.00000000 sec
D11             0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6238364 MHz
NUC1                    13C
P1                   15.50 usec
PLW1           25.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           19.50000000 W
PLW12           0.51492000 W
PLW13           0.32955000 W

F2 - Processing parameters
SI                      32768
SF             100.6127734 MHz
WDW                        EM
SSB         0
LB                    1.00 Hz
GB          0
PC                    1.40
```

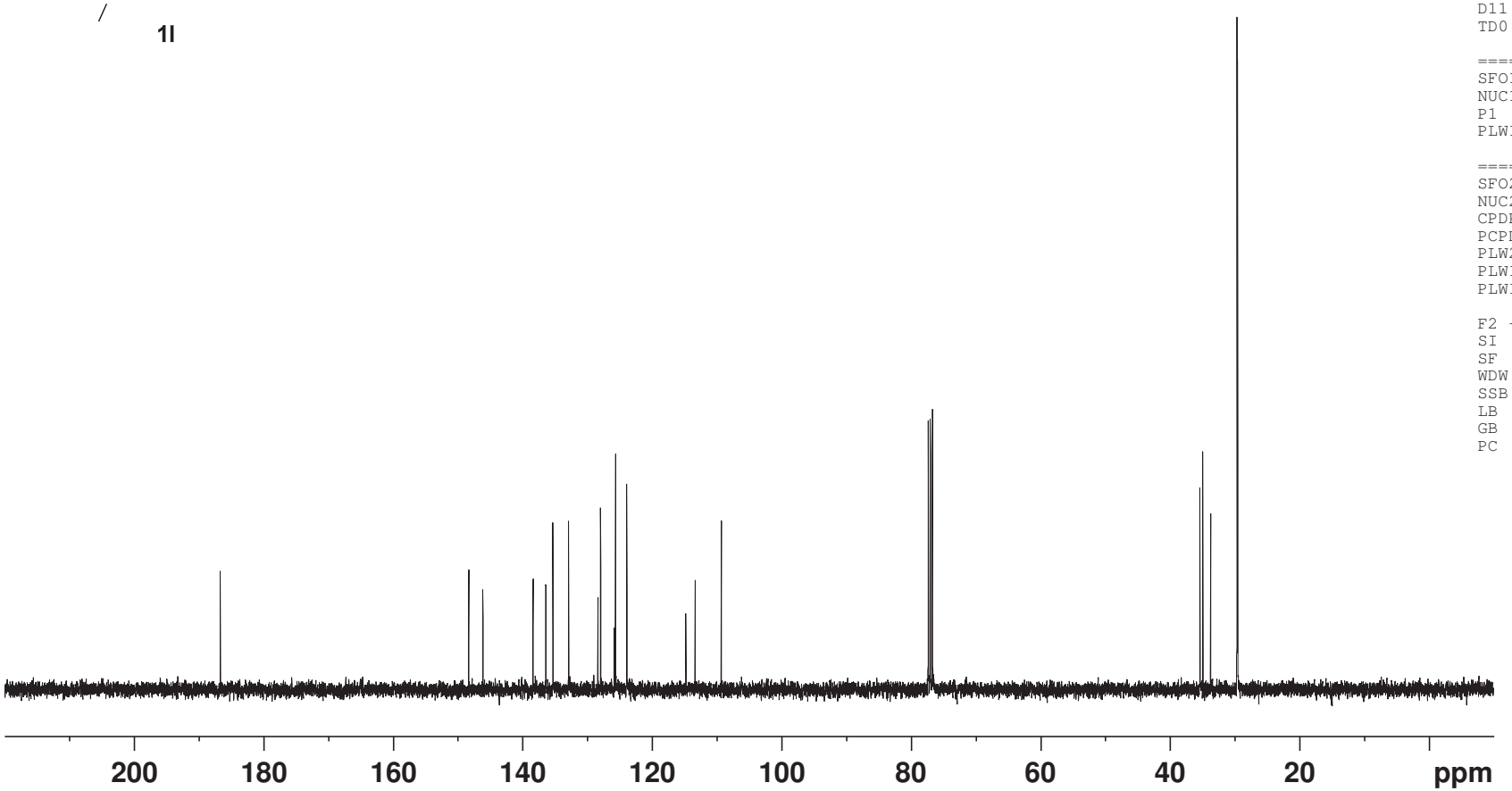



```
Current Data Parameters
NAME                  4-Br
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                  8.50
INSTRUM              spect
PROBHD   5 mm PABBO BB/
PULPROG                zg30
TD                    65536
SOLVENT               CDC13
NS                        4
DS                        2
SWH                8012.820 Hz
FIDRES            0.122266 Hz
AQ                4.0894465 sec
RG                     80.6
DW                   62.400 usec
DE                    6.50 usec
TE                   293.9 K
D1              1.00000000 sec
TD0                       1

======== CHANNEL f1 ========
SFO1           400.1324710 MHz
NUC1                     1H
P1                    12.40 usec
PLW1           19.00000000 W

F2 - Processing parameters
SI                    65536
SF             400.1300120 MHz
WDW                      EM
SSB       0
LB                    0.30 Hz
GB        0
PC                    1.00
```

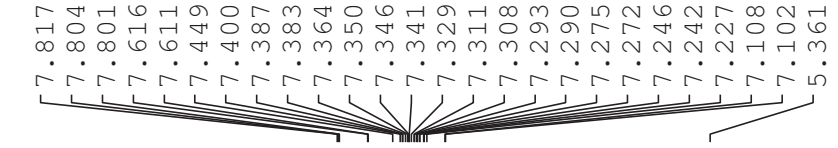


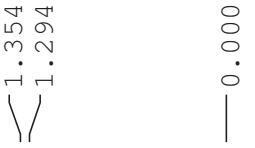
1l

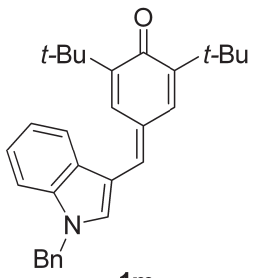
186.68
148.31
146.11
138.37
136.39
135.31
132.89
128.34
127.93
125.81
125.63
123.88
114.77
113.33
109.29
77.32
77.00
76.68
35.35
34.91
33.68
29.63
29.53




```
Current Data Parameters
NAME                  4-Br
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                   8.53
INSTRUM               spect
PROBHD    5 mm PABBO BB/
PULPROG              zgpg30
TD                    65536
SOLVENT               CDCl3
NS                       50
DS                        2
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ               1.2976128 sec
RG                     2050
DW                   19.800 usec
DE                    6.50 usec
TE                   295.1 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6238364 MHz
NUC1                    13C
P1                   15.50 usec
PLW1           25.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           19.50000000 W
PLW12           0.51492000 W
PLW13           0.32955000 W

F2 - Processing parameters
SI                      32768
SF             100.6127745 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

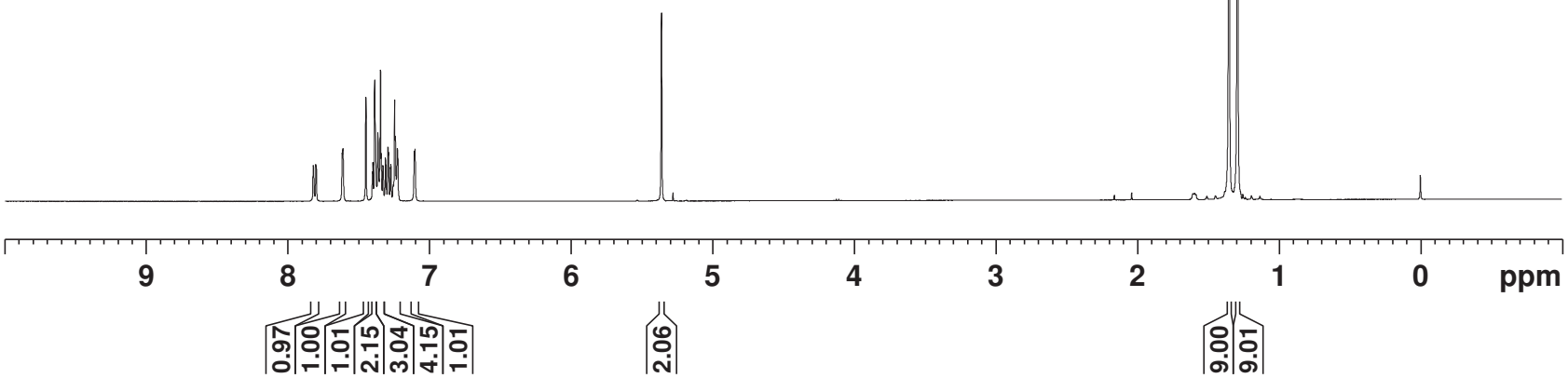


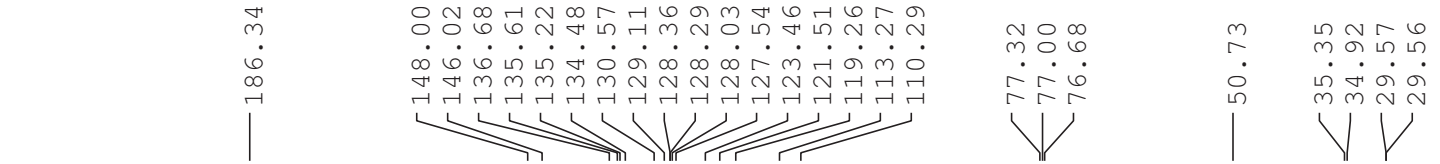


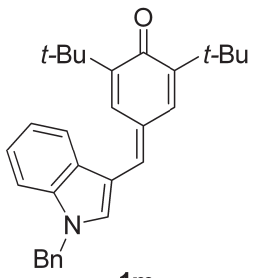


1m

```
Current Data Parameters
NAME                  N-Bn
EXPNO                   10
PROCNO                   1

F2 - Acquisition Parameters
Date_           20180810
Time                 9.28
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDC13
NS                      4
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ             4.0894465 sec
RG                    114
DW                 62.400 usec
DE                  6.50 usec
TE                 293.8 K
D1            1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 12.40 usec
PLW1         19.00000000 W

F2 - Processing parameters
SI                  65536
SF           400.1300152 MHz
WDW                    EM
SSB       0
LB                  0.30 Hz
GB        0
PC                  1.00
```

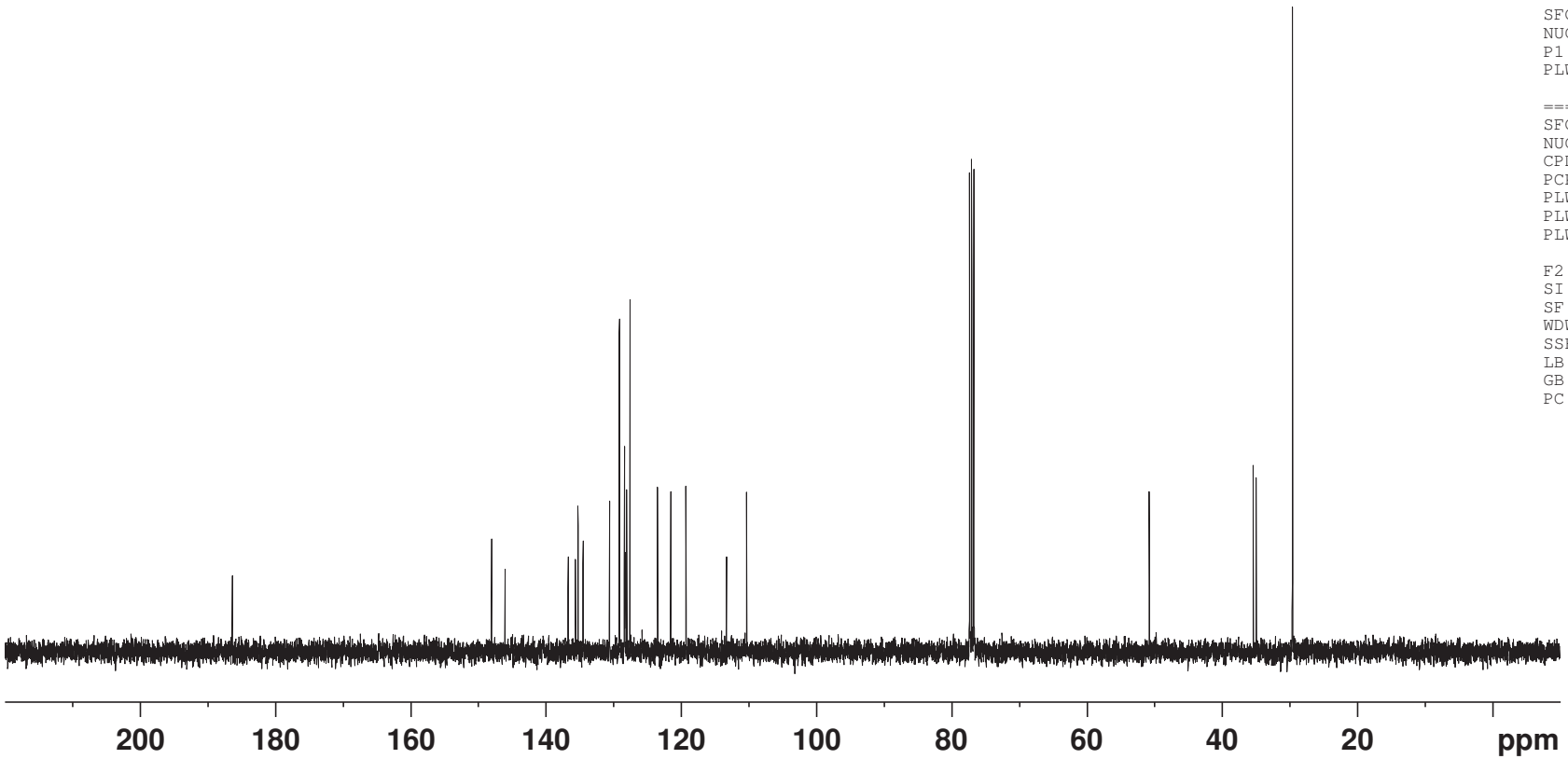


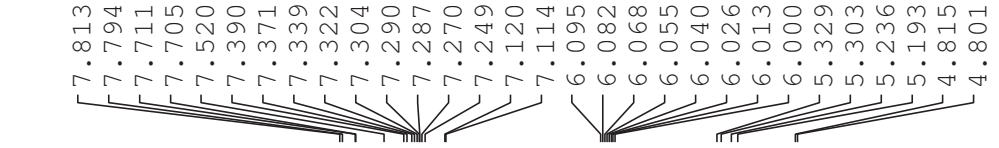


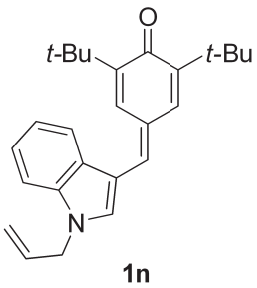


1m

```
Current Data Parameters
NAME                  N-Bn
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_              20180810
Time                  9.31
INSTRUM              spect
PROBHD    5 mm PABBO BB/
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                      50
DS                       2
SWH              25252.525 Hz
FIDRES            0.385323 Hz
AQ                1.2976128 sec
RG                    2050
DW                  19.800 usec
DE                   6.50 usec
TE                  295.0 K
D1               2.00000000 sec
D11              0.03000000 sec
TD0                      1

======== CHANNEL f1 ========
SFO1           100.6238364 MHz
NUC1                    13C
P1                   15.50 usec
PLW1           25.00000000 W

======== CHANNEL f2 ========
SFO2           400.1316005 MHz
NUC2                    1H
CPDPRG[2           waltz16
PCPD2                80.00 usec
PLW2           19.50000000 W
PLW12           0.51492000 W
PLW13           0.32955000 W

F2 - Processing parameters
SI                      32768
SF             100.6127729 MHz
WDW                        EM
SSB          0
LB                    1.00 Hz
GB           0
PC                    1.40
```

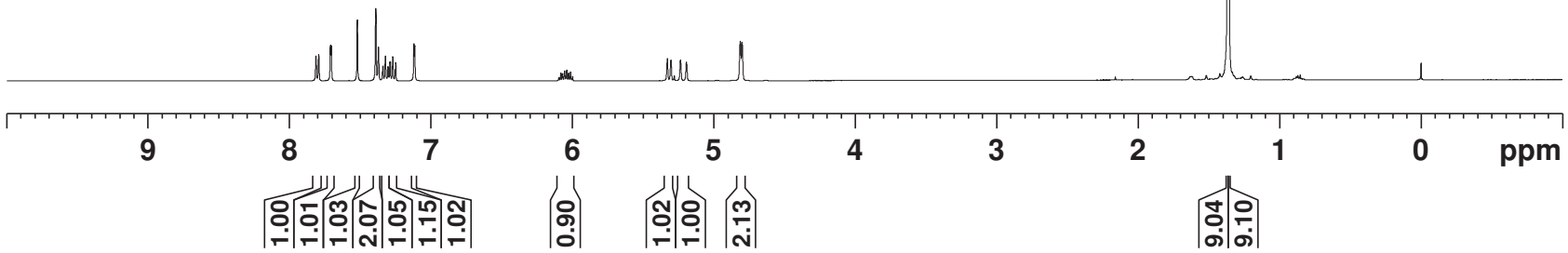


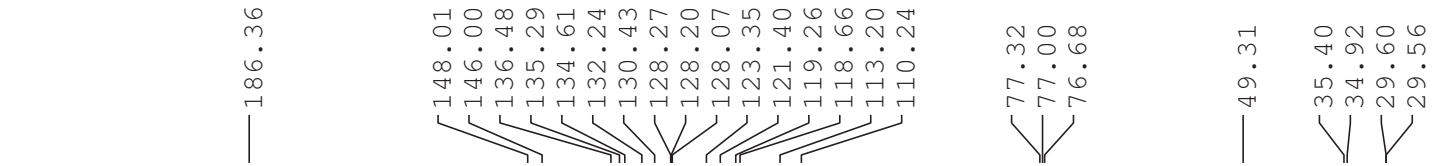


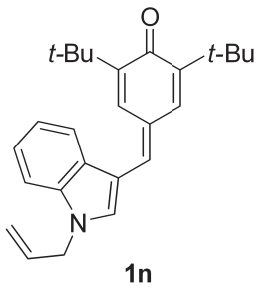


1n

```
Current Data Parameters
NAME              N-allyl
EXPNO                  10
PROCNO                  1

F2 - Acquisition Parameters
Date_            20180810
Time                 9.08
INSTRUM             spect
PROBHD   5 mm PABBO BB/
PULPROG              zg30
TD                  65536
SOLVENT             CDC13
NS                      4
DS                      2
SWH              8012.820 Hz
FIDRES           0.122266 Hz
AQ               4.0894465 sec
RG                    101
DW                 62.400 usec
DE                  6.50 usec
TE                 293.9 K
D1              1.00000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1          400.1324710 MHz
NUC1                  1H
P1                 12.40 usec
PLW1          19.00000000 W

F2 - Processing parameters
SI                  65536
SF            400.1300142 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

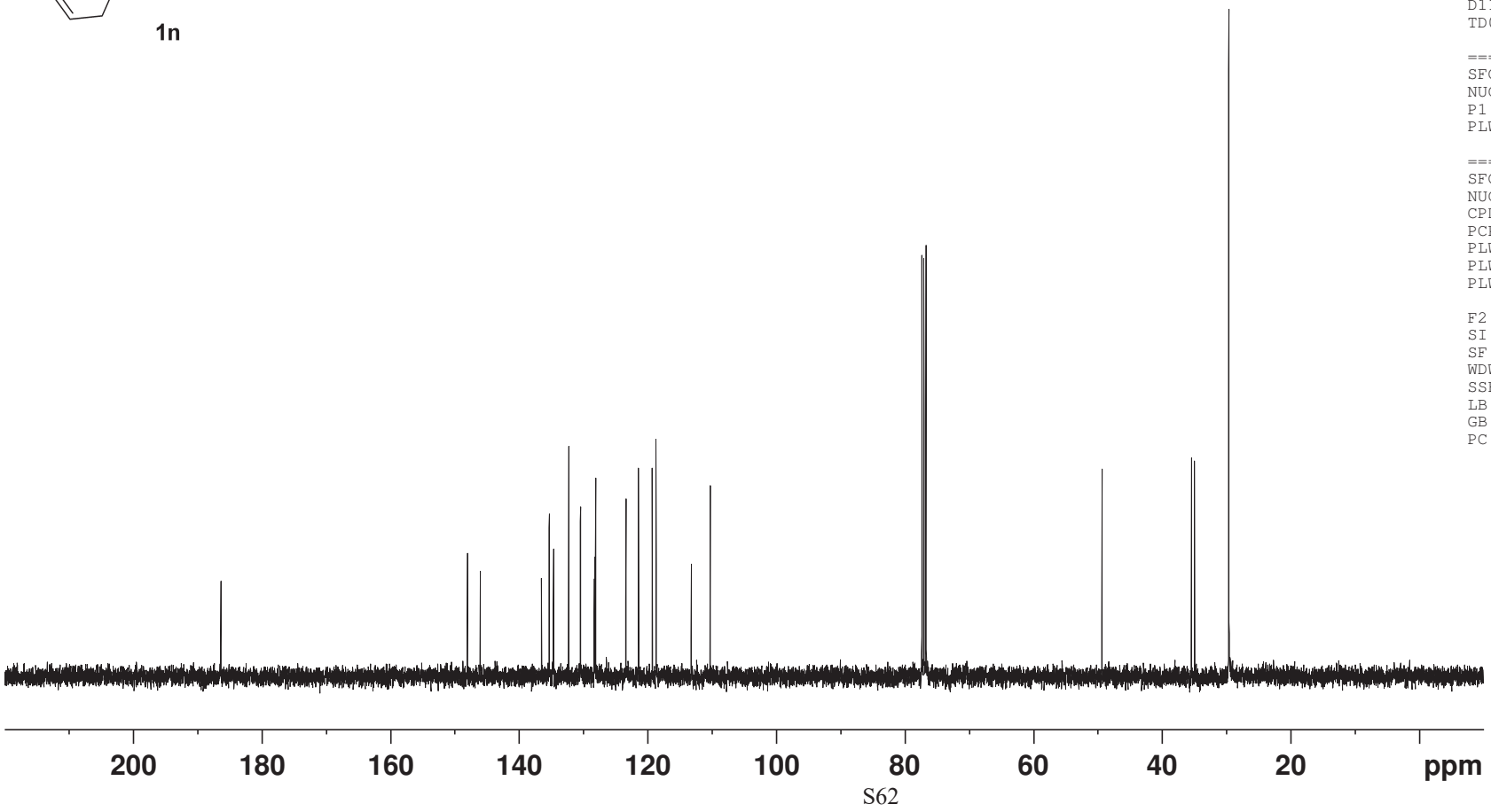


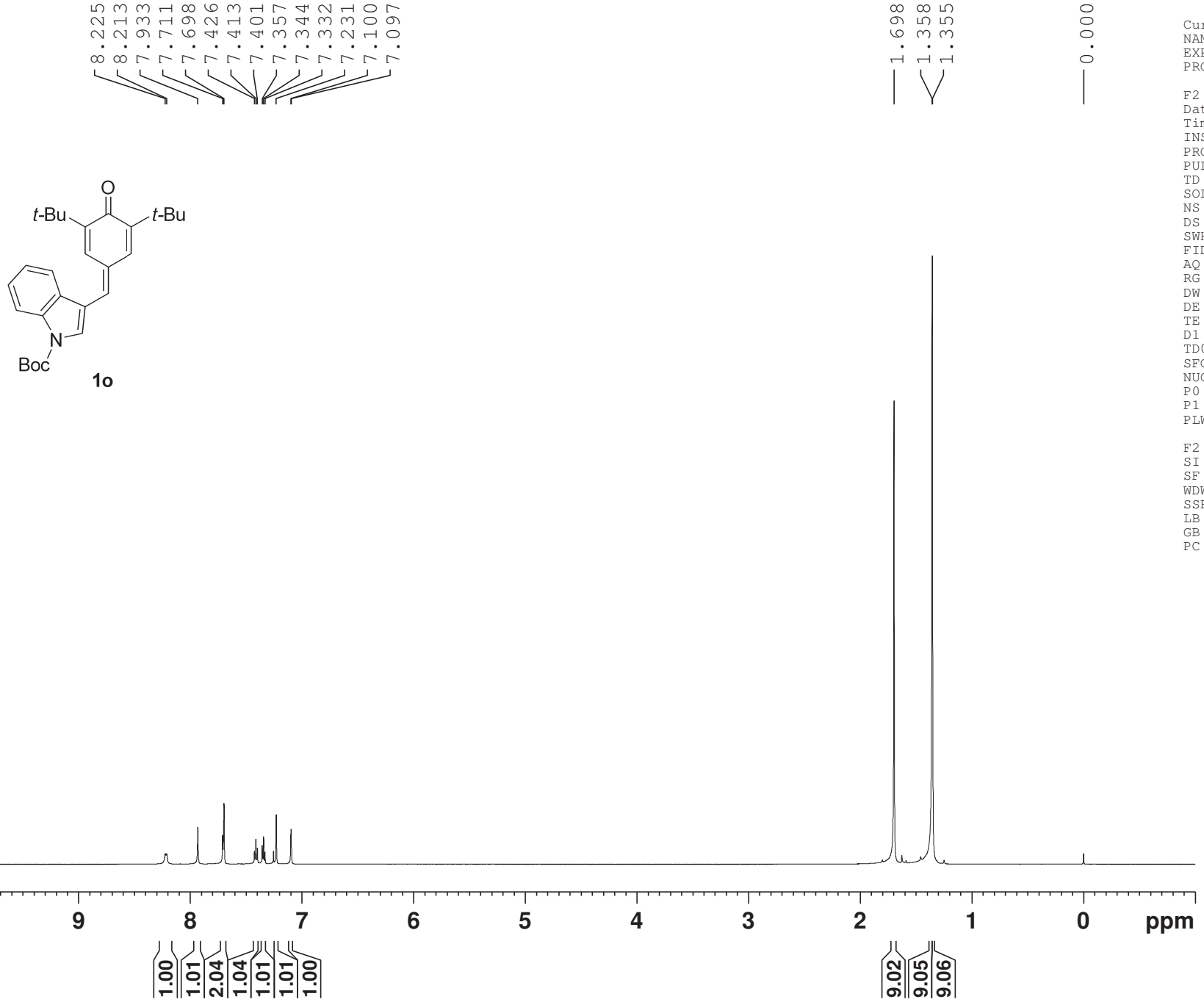




1n

```
Current Data Parameters
NAME            N-allyl
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20180810
Time               9.12
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                65536
SOLVENT           CDCl3
NS                   50
DS                    2
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                 2050
DW               19.800 usec
DE                6.50 usec
TE               295.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        100.6238364 MHz
NUC1                13C
P1                15.50 usec
PLW1        25.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        19.50000000 W
PLW12        0.51492000 W
PLW13        0.32955000 W

F2 - Processing parameters
SI                 32768
SF          100.6127732 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

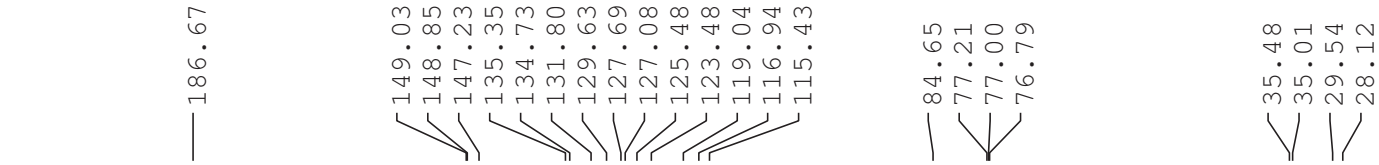


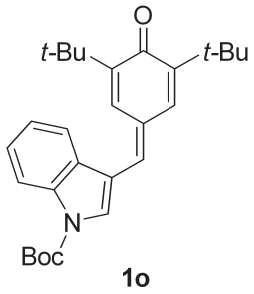


Current Data Parameters
NAME N-Boc
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20210810
Time 10.08 h
INSTRUM Avance
PROBHD Z114607_0847 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 4
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 47.619
DW 42.000 usec
DE 8.79 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.33 usec
P1 10.00 usec
PLW1 25.31200027 W

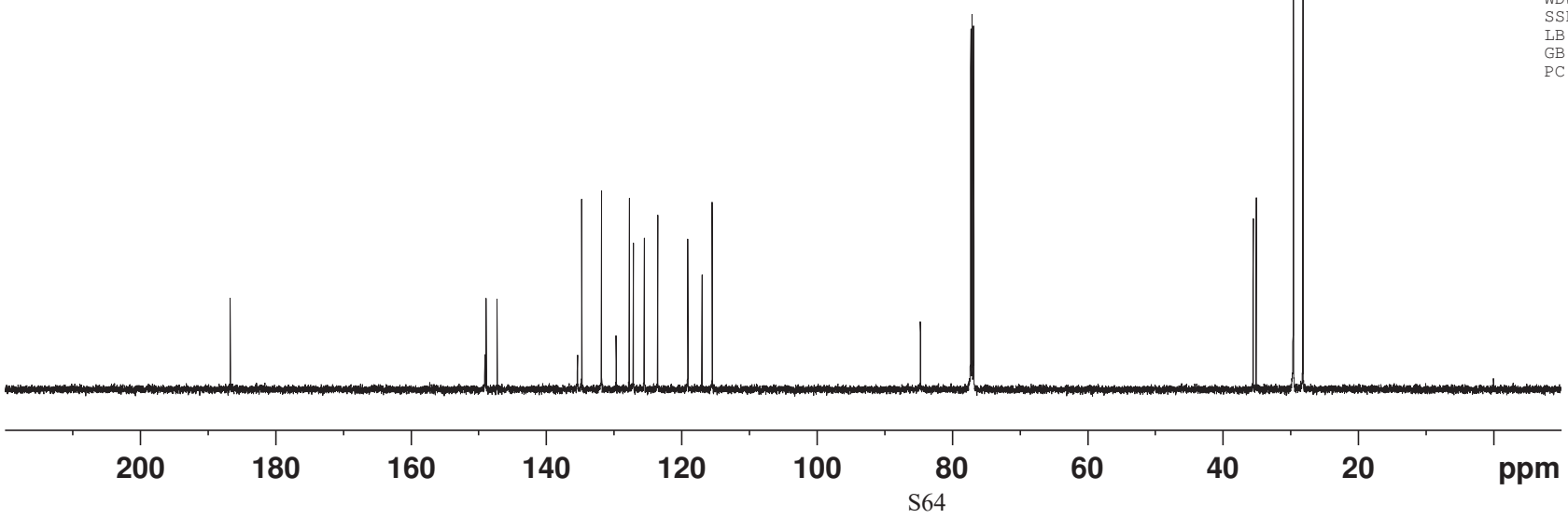
F2 - Processing parameters
SI 65536
SF 600.1300179 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

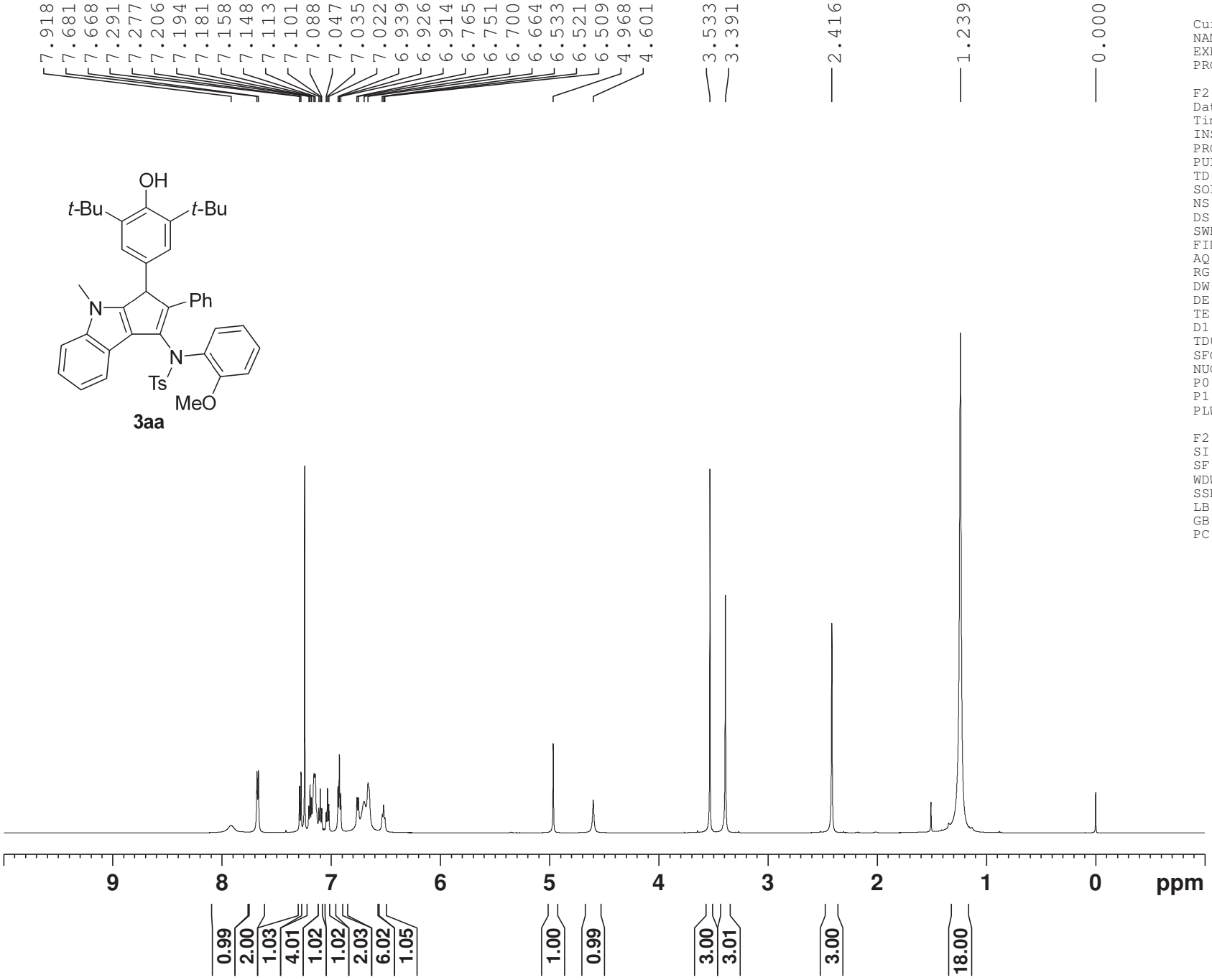




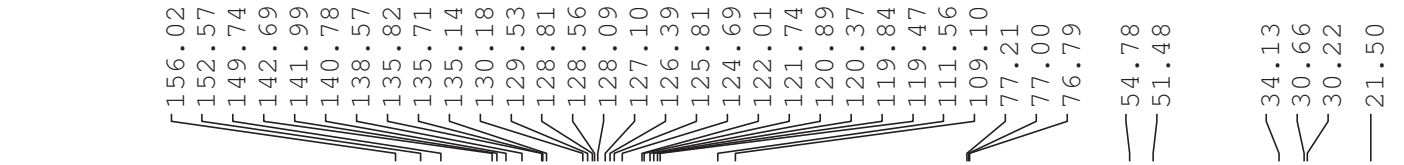
1o

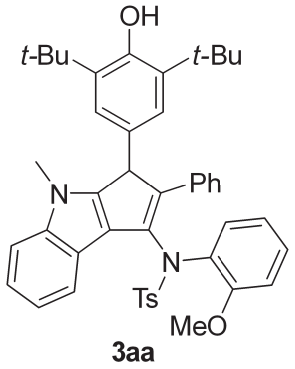
```
Current Data Parameters
NAME                 N-Boc
EXPNO                   11
PROCNO                   1

F2 - Acquisition Parameters
Date_             20210810
Time                10.14 h
INSTRUM             Avance
PROBHD    Z114607_0847 (
PULPROG             zgpg30
TD                   65536
SOLVENT              CDCl3
NS                     128
DS                       4
SWH             37037.035 Hz
FIDRES           1.130281 Hz
AQ              0.8847360 sec
RG                     101
DW                  13.500 usec
DE                   6.50 usec
TE                  298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                      1
SFO1          150.9194079 MHz
NUC1                  13C
P0                   4.00 usec
P1                  12.00 usec
PLW1          87.25299835 W
SFO2          600.1324005 MHz
NUC2                  1H
CPDPRG[2           waltz65
PCPD2                70.00 usec
PLW2          25.31200027 W
PLW12          0.51656997 W
PLW13          0.25983000 W

F2 - Processing parameters
SI                   32768
SF            150.9028146 MHz
WDW                     EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```





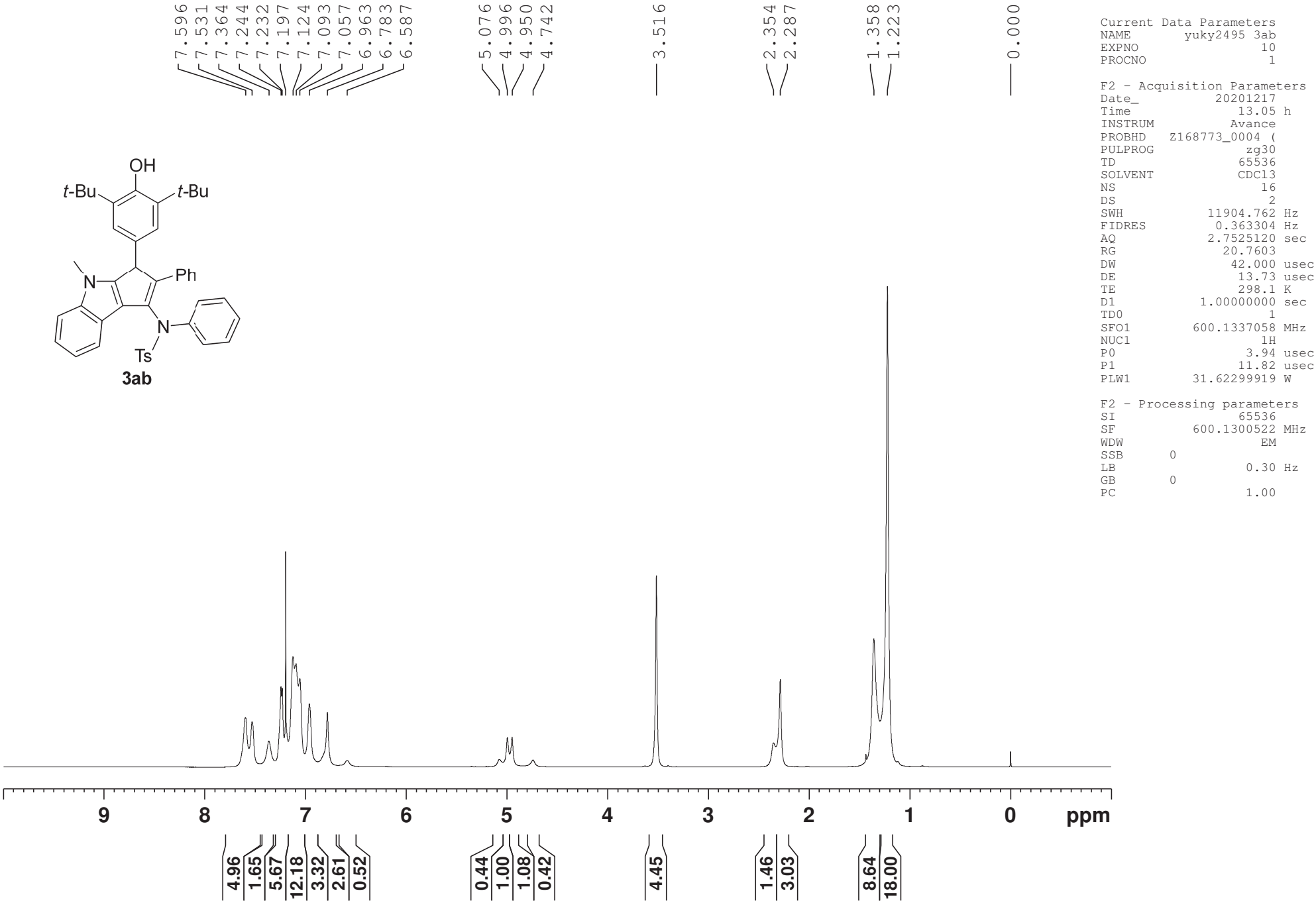

```
Current Data Parameters
NAME       yuky2462 3aa
EXPNO                20
PROCNO                1

F2 - Acquisition Parameters
Date_          20201116
Time              22.59 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               47.619
DW               42.000 usec
DE               13.73 usec
TE               298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                3.94 usec
P1               11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300240 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



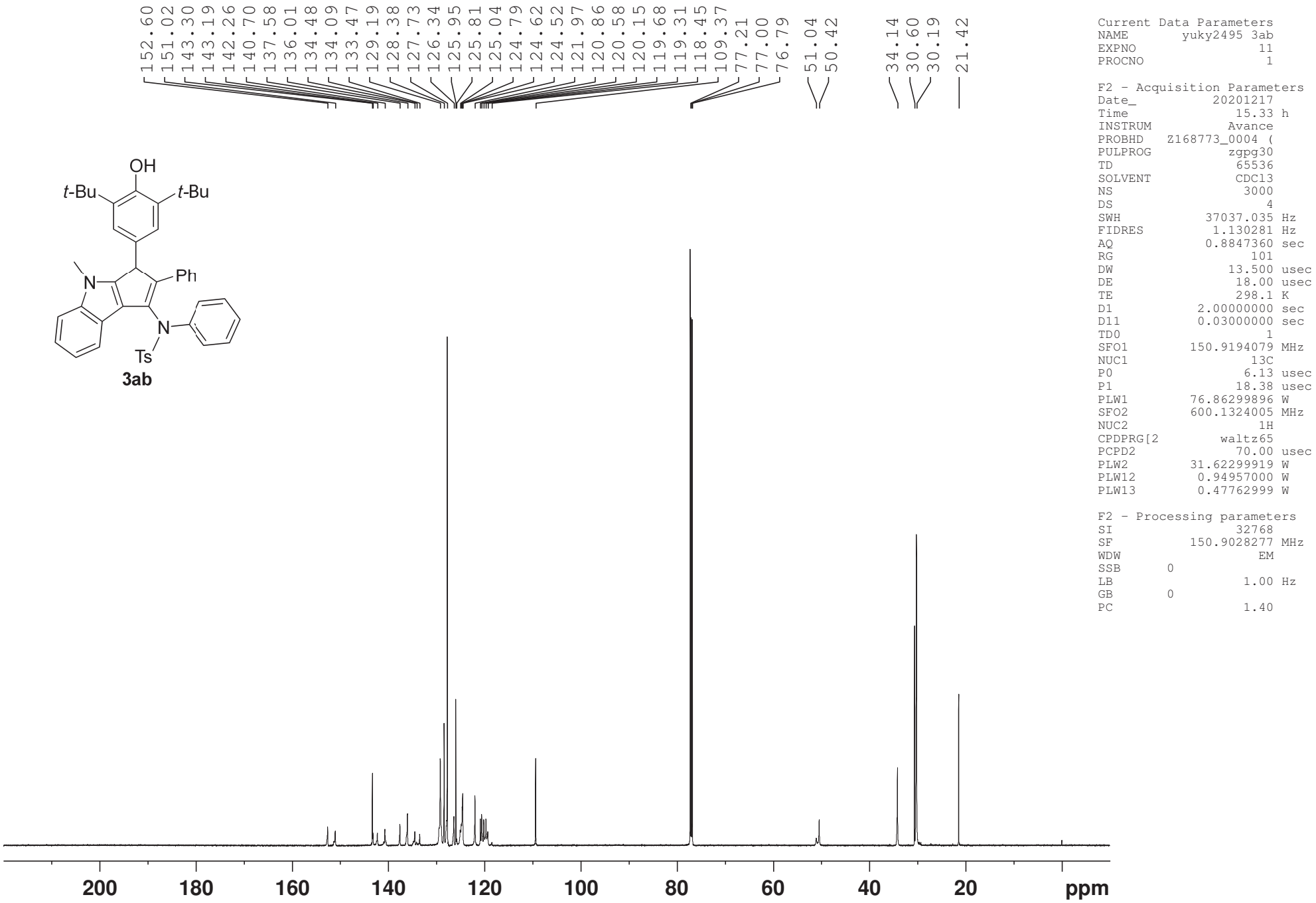


3aa

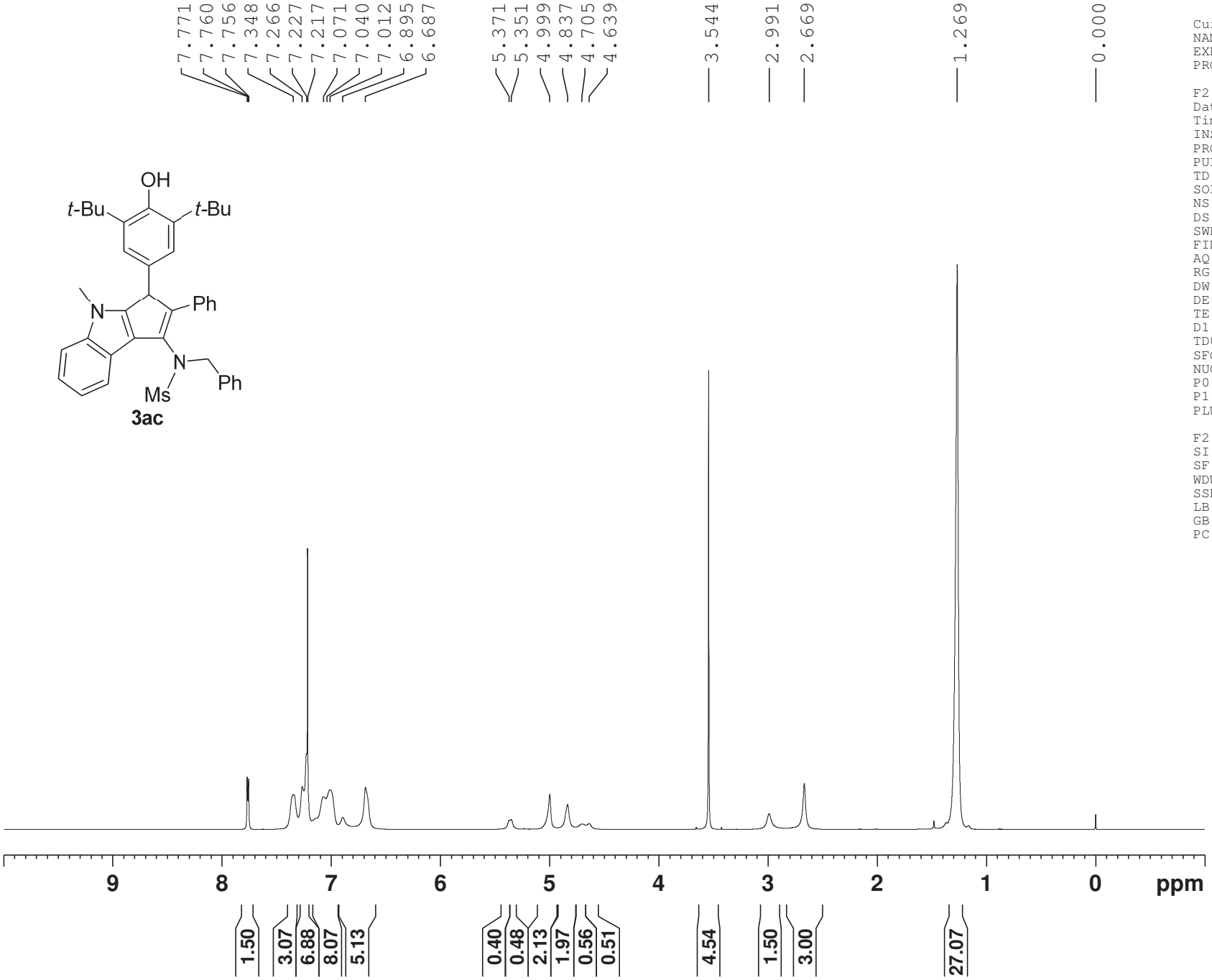
```
Current Data Parameters
NAME        yuky2462 3aa
EXPNO                 21
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201117
Time                1.56 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW                13.500 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                 6.13 usec
P1                18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028160 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



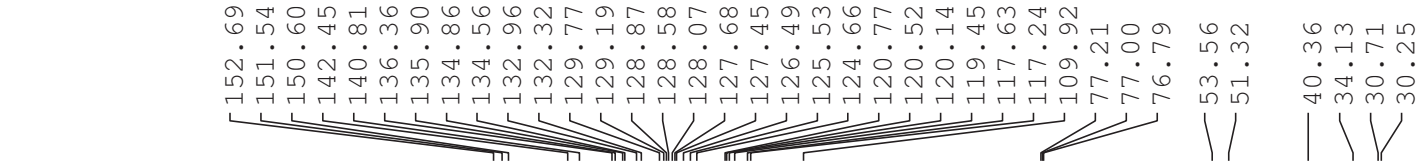

```
Current Data Parameters
NAME       yuky2495 3ab
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201217
Time              13.05 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG              20.7603
DW                42.000 usec
DE                13.73 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                 3.94 usec
P1                11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300522 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

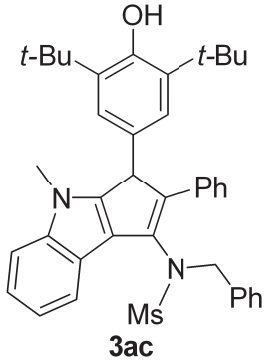



```
Current Data Parameters
NAME        yuky2495 3ab
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201217
Time              15.33 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028277 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



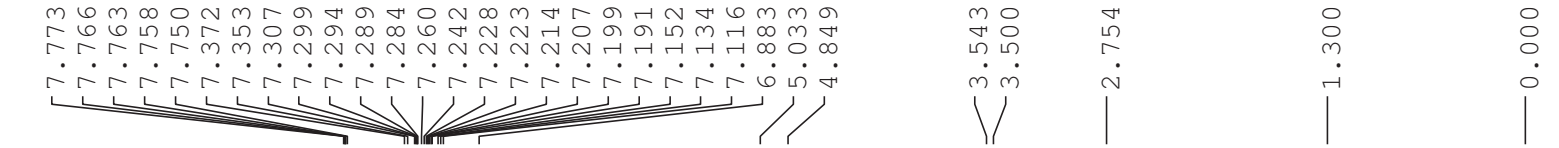

```
Current Data Parameters
NAME       yuky2464 3ac
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201128
Time              14.32 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                     8
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               12.9352
DW                42.000 usec
DE                18.78 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1        600.1337058 MHz
NUC1                1H
P0                 4.33 usec
P1                13.00 usec
PLW1        21.26799965 W

F2 - Processing parameters
SI                 65536
SF          600.1300401 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

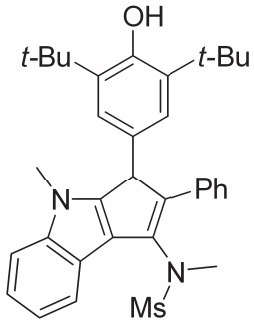




3ac

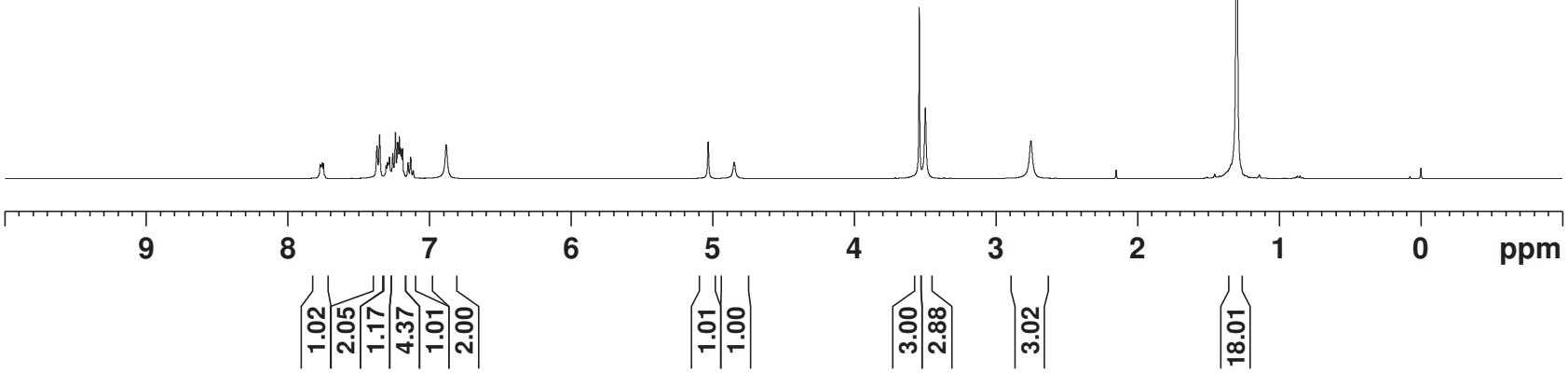
```
Current Data Parameters
NAME       yuky2464 3ac
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201128
Time              16.10 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2000
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1        66.87999725 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2        21.26799965 W
PLW12        0.56160998 W
PLW13        0.28204000 W

F2 - Processing parameters
SI                32768
SF          150.9028236 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

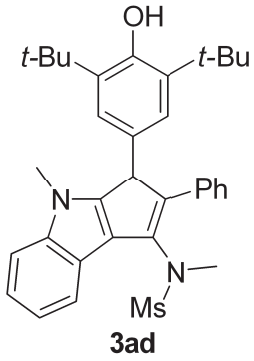




3ad

```
Current Data Parameters
NAME        yuky1914 3ad
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190326
Time                8.37
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                     4
DS                     2
SWH             8012.820 Hz
FIDRES          0.122266 Hz
AQ             4.0894465 sec
RG                  71.8
DW                62.400 usec
DE                 6.50 usec
TE                292.4 K
D1            1.00000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1         400.1324710 MHz
NUC1                   1H
P1                 12.40 usec
PLW1         19.00000000 W

F2 - Processing parameters
SI                 65536
SF           400.1300226 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```





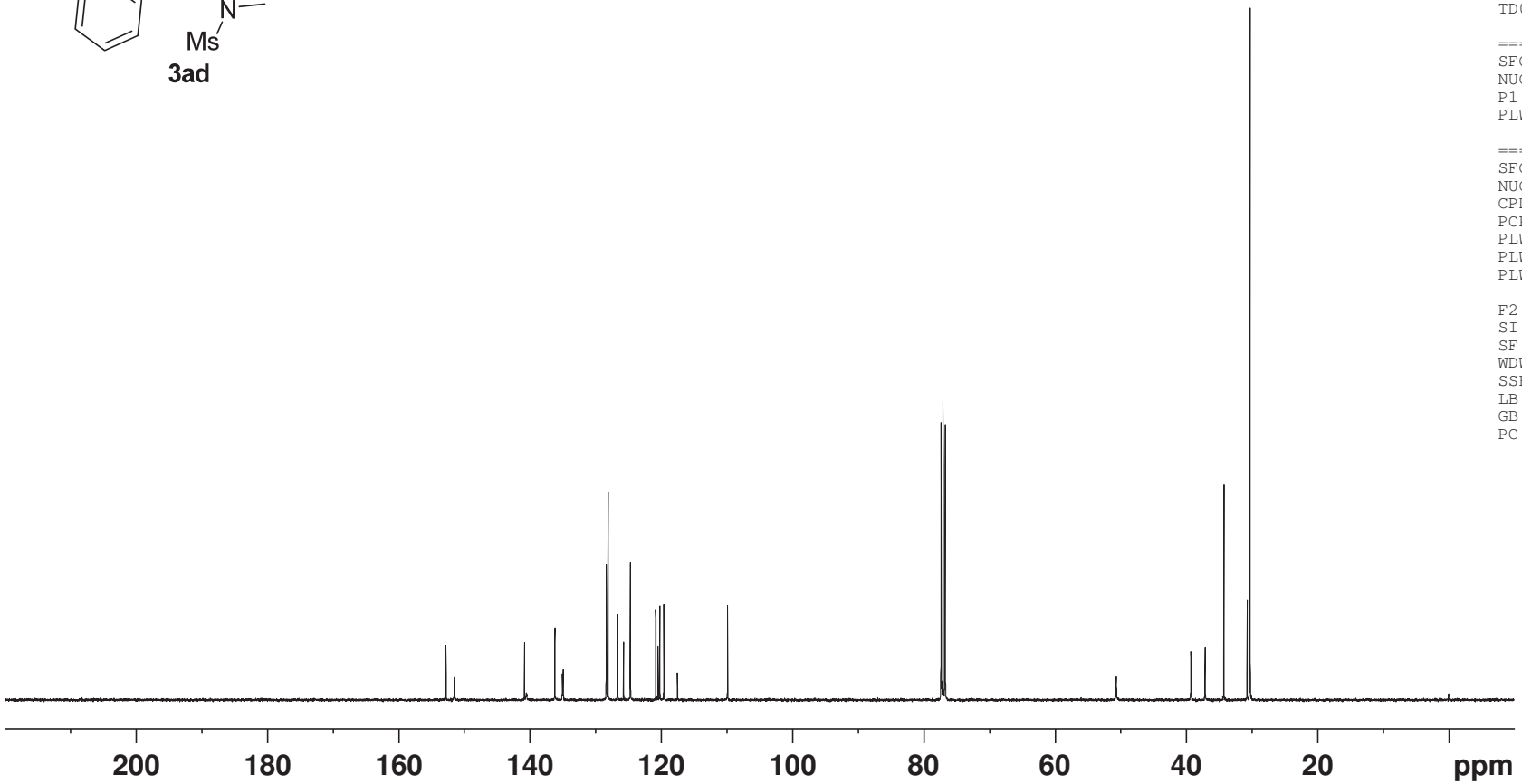
3ad

152.74
151.47
140.79
140.50
136.17
135.02
134.89
128.33
128.07
126.60
125.69
124.67
120.79
120.45
120.18
119.57
117.49
109.86

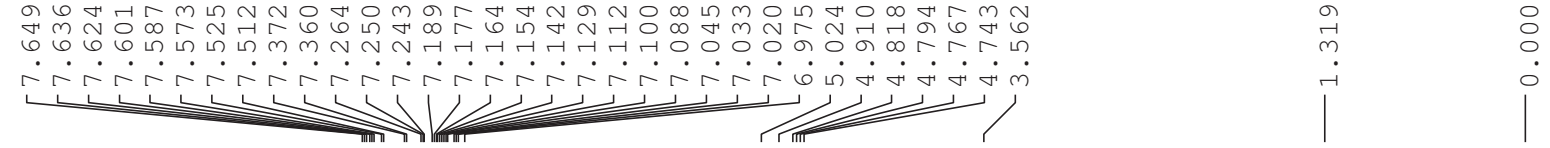
77.32
77.00
76.68

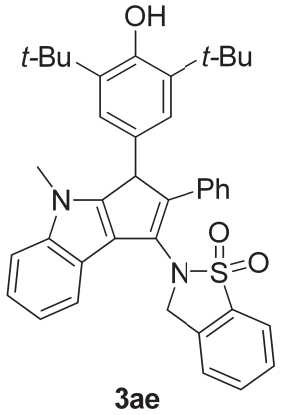
50.61

39.25
37.08
34.22
30.69
30.23



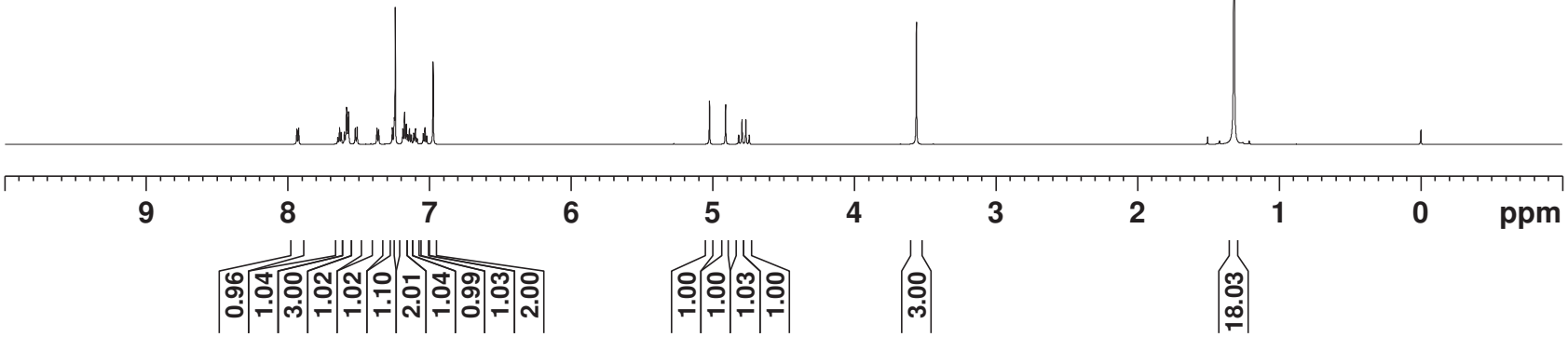

```
Current Data Parameters
NAME        yuky1914 3ad
EXPNO                 15
PROCNO                 1

F2 - Acquisition Parameters
Date_           20190326
Time                9.34
INSTRUM            spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1024
DS                     2
SWH           25252.525 Hz
FIDRES         0.385323 Hz
AQ            1.2976128 sec
RG                  2050
DW                19.800 usec
DE                 6.50 usec
TE                293.5 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
SFO1        100.6238364 MHz
NUC1                13C
P1                15.50 usec
PLW1        25.00000000 W

======== CHANNEL f2 ========
SFO2        400.1316005 MHz
NUC2                1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        19.50000000 W
PLW12        0.51492000 W
PLW13        0.32955000 W

F2 - Processing parameters
SI                 32768
SF          100.6127766 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

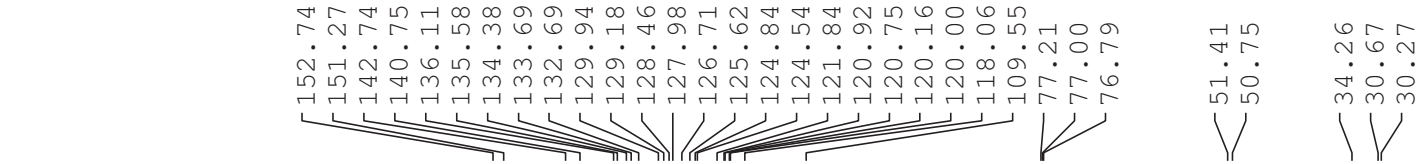


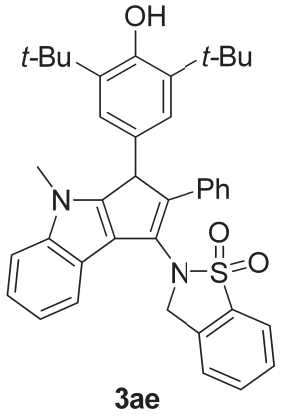


3ae

```
Current Data Parameters
NAME        yuky2466 3ae
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201128
Time                8.34 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG                    32
DW                42.000 usec
DE                18.78 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1        600.1337058 MHz
NUC1                1H
P0                 4.33 usec
P1                13.00 usec
PLW1        21.26799965 W

F2 - Processing parameters
SI                 65536
SF          600.1300246 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

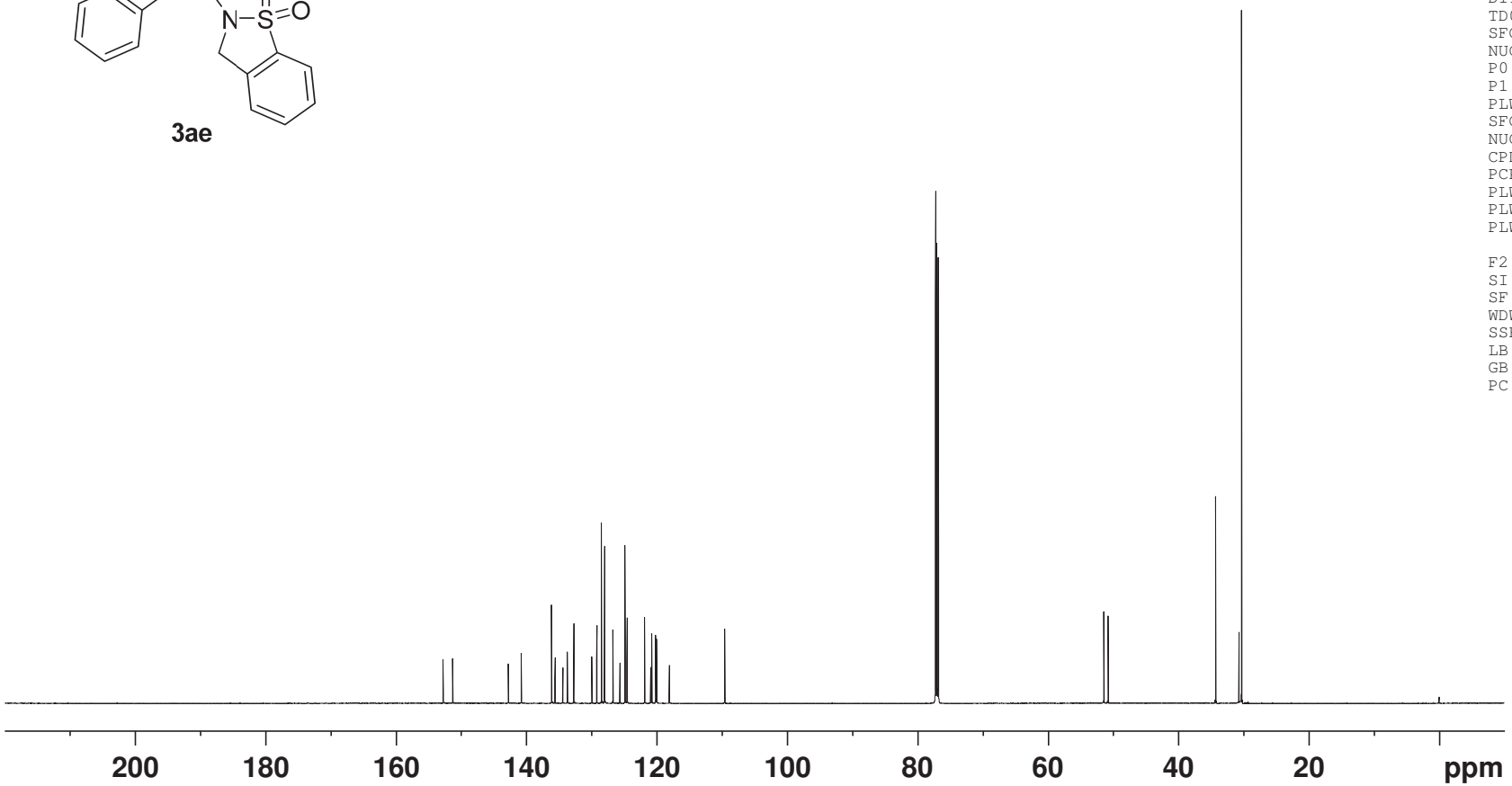


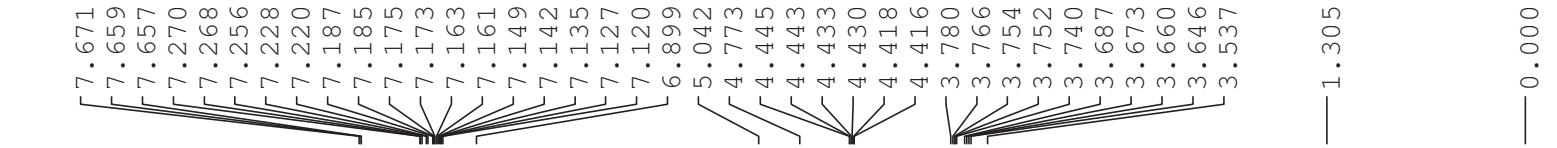


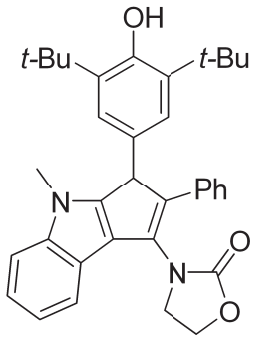


3ae

```
Current Data Parameters
NAME       yuky2466 3ae
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201128
Time              11.01 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0               3.33 usec
P1              10.00 usec
PLW1        66.87999725 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2        21.26799965 W
PLW12        0.56160998 W
PLW13        0.28204000 W

F2 - Processing parameters
SI                 32768
SF          150.9028157 MHz
WDW                   EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

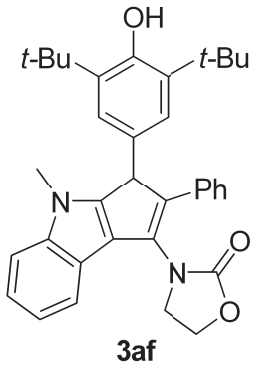






3af

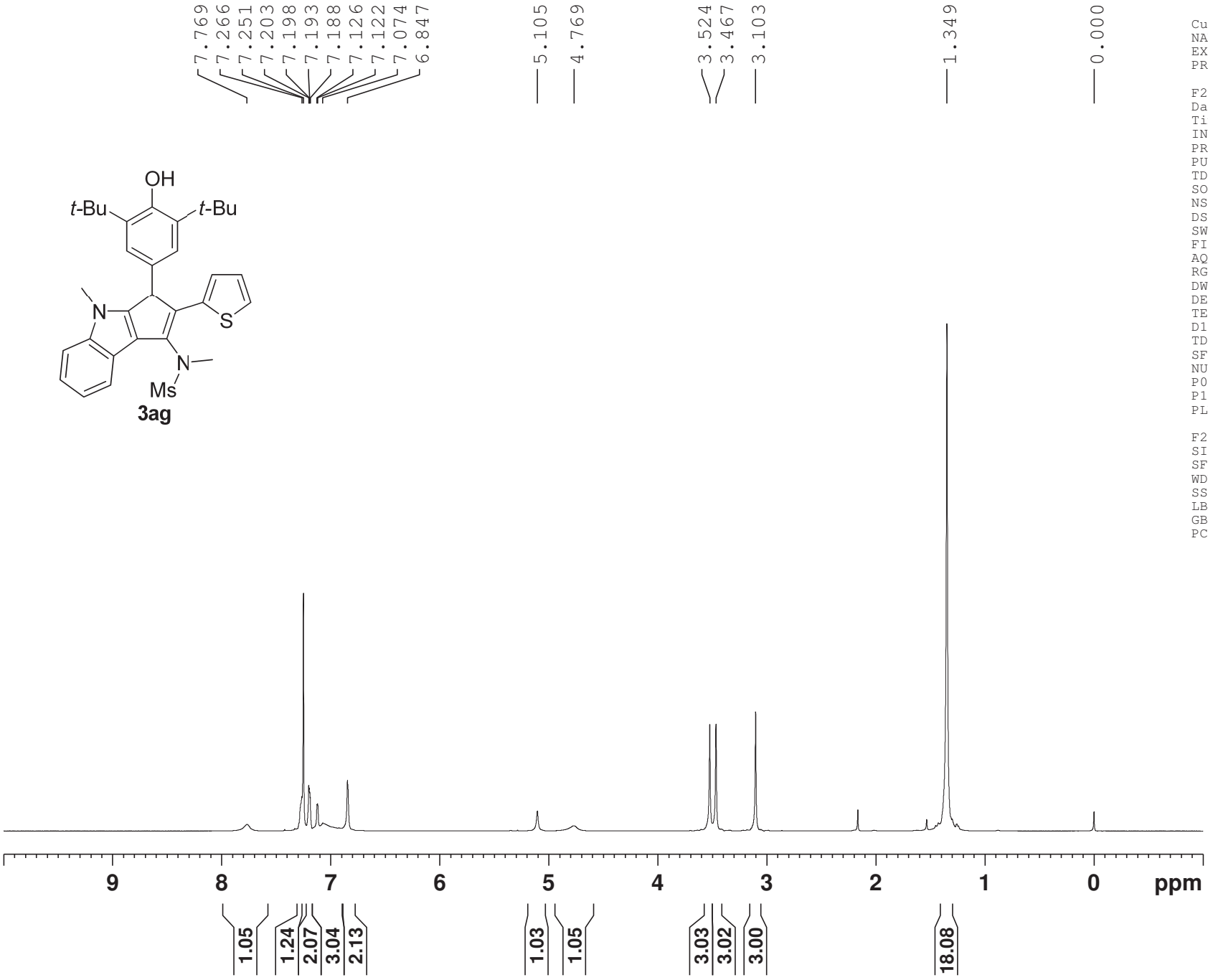
```
Current Data Parameters
NAME        yuky2500 3af
EXPNO                13
PROCNO                1

F2 - Acquisition Parameters
Date_          20201221
Time              18.33 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG              36.0421
DW                42.000 usec
DE                13.73 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                 3.94 usec
P1                11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300332 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



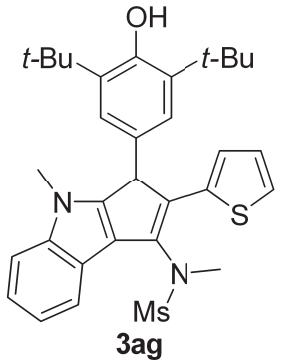
3af

156.70
152.72
150.93
140.73
136.04
135.26
134.30
132.25
128.29
128.13
126.46
125.71
124.88
120.87
120.77
120.20
120.04
117.59
109.55
77.21
77.00
76.79
62.84
50.83
45.85
34.21
30.68
30.23

```
Current Data Parameters
NAME        yuky2500 3af
EXPNO                 14
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201221
Time              19.47 h
INSTRUM            Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                  1500
DS                     4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                   101
DW                13.500 usec
DE                18.00 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        150.9194079 MHz
NUC1                13C
P0                 6.13 usec
P1                18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                 32768
SF          150.9028250 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```




```
Current Data Parameters
NAME      yuky2470-2 3ag
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201203
Time              22.23 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG                    32
DW               42.000 usec
DE               18.78 usec
TE               298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0               4.33 usec
P1              13.00 usec
PLW1         21.26799965 W

F2 - Processing parameters
SI                 65536
SF           600.1300200 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

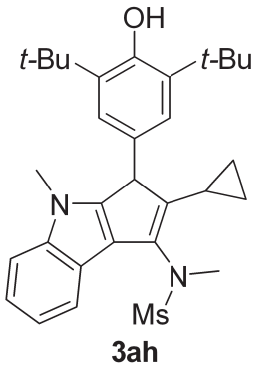


3ag

152.98
151.78
140.84
137.01
136.51
135.15
133.77
126.38
124.82
124.60
124.29
120.91
120.35
119.75
116.68
109.94
77.21
77.00
76.79
50.61
38.92
36.12
34.32
30.60
30.29

```
Current Data Parameters
NAME      yuky2470-2 3ag
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201204
Time               2.29 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 5000
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0               3.33 usec
P1              10.00 usec
PLW1        66.87999725 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2        21.26799965 W
PLW12        0.56160998 W
PLW13        0.28204000 W

F2 - Processing parameters
SI                32768
SF          150.9028139 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

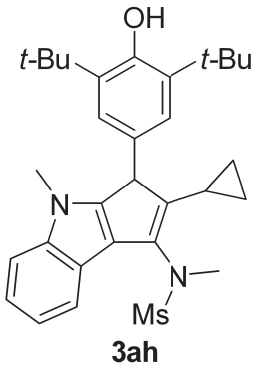
200 180 160 140 120 100 80 60 40 20 ppm



3ah

7.595 7.254 7.249 7.244 7.238 7.198 7.158 7.152 7.147 7.142 7.137 7.131 6.918 5.118 4.218 3.455 3.425 3.038 1.888 1.373 0.791 0.786 0.779 0.609 0.512 0.268 0.262 0.253 0.246 0.000

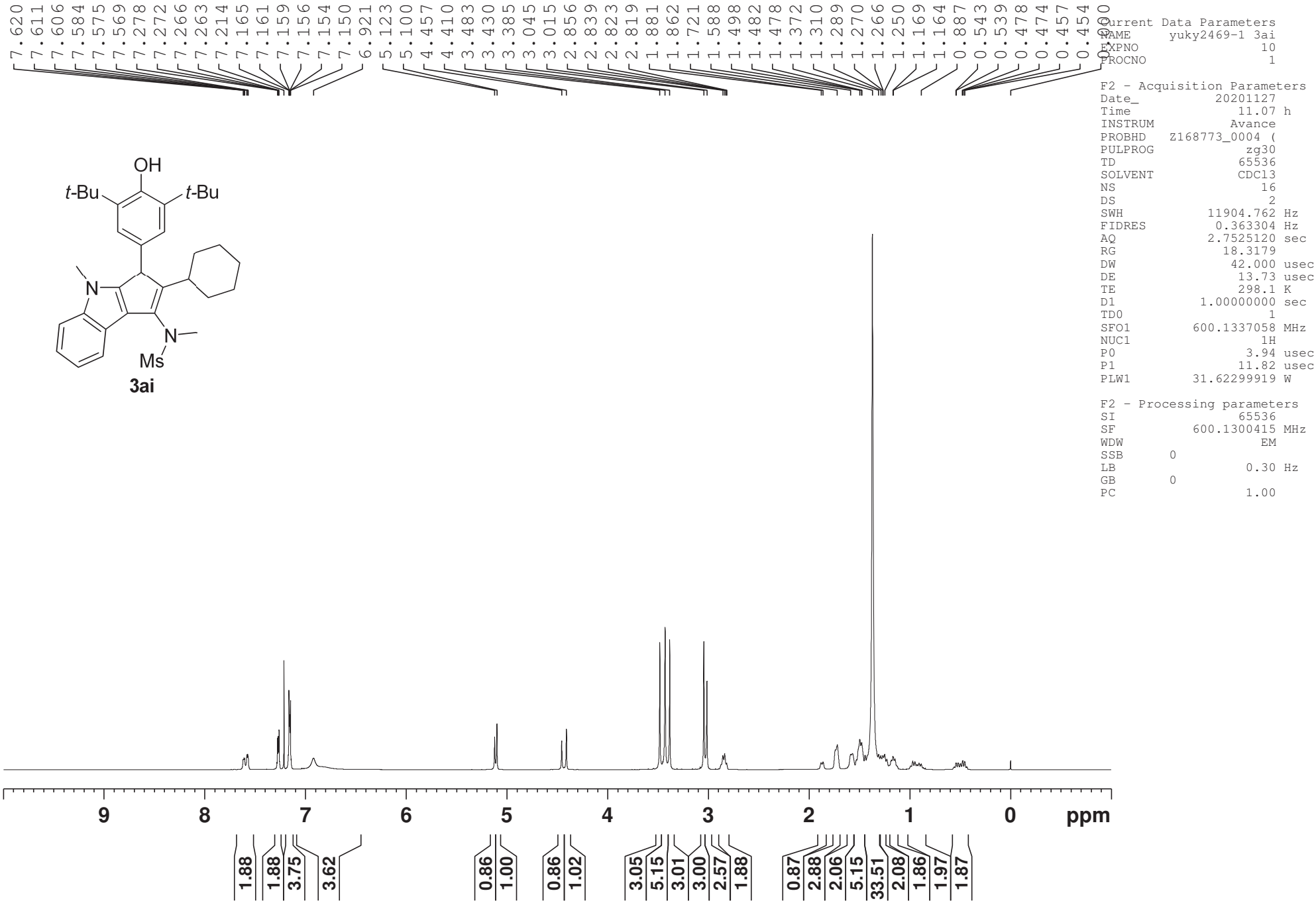
```
Current Data Parameters
NAME        yuky2497 3ah
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201217
Time              12.06 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                     4
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               16.3897
DW                42.000 usec
DE                13.73 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                 3.94 usec
P1                11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300511 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



3ah

152.73
150.38
144.09
140.32
136.26
134.10
125.82
124.48
120.12
119.72
118.91
116.07
109.83
77.21
77.00
76.79
49.49
37.84
36.85
34.20
30.46
30.23
10.36
7.28
5.82

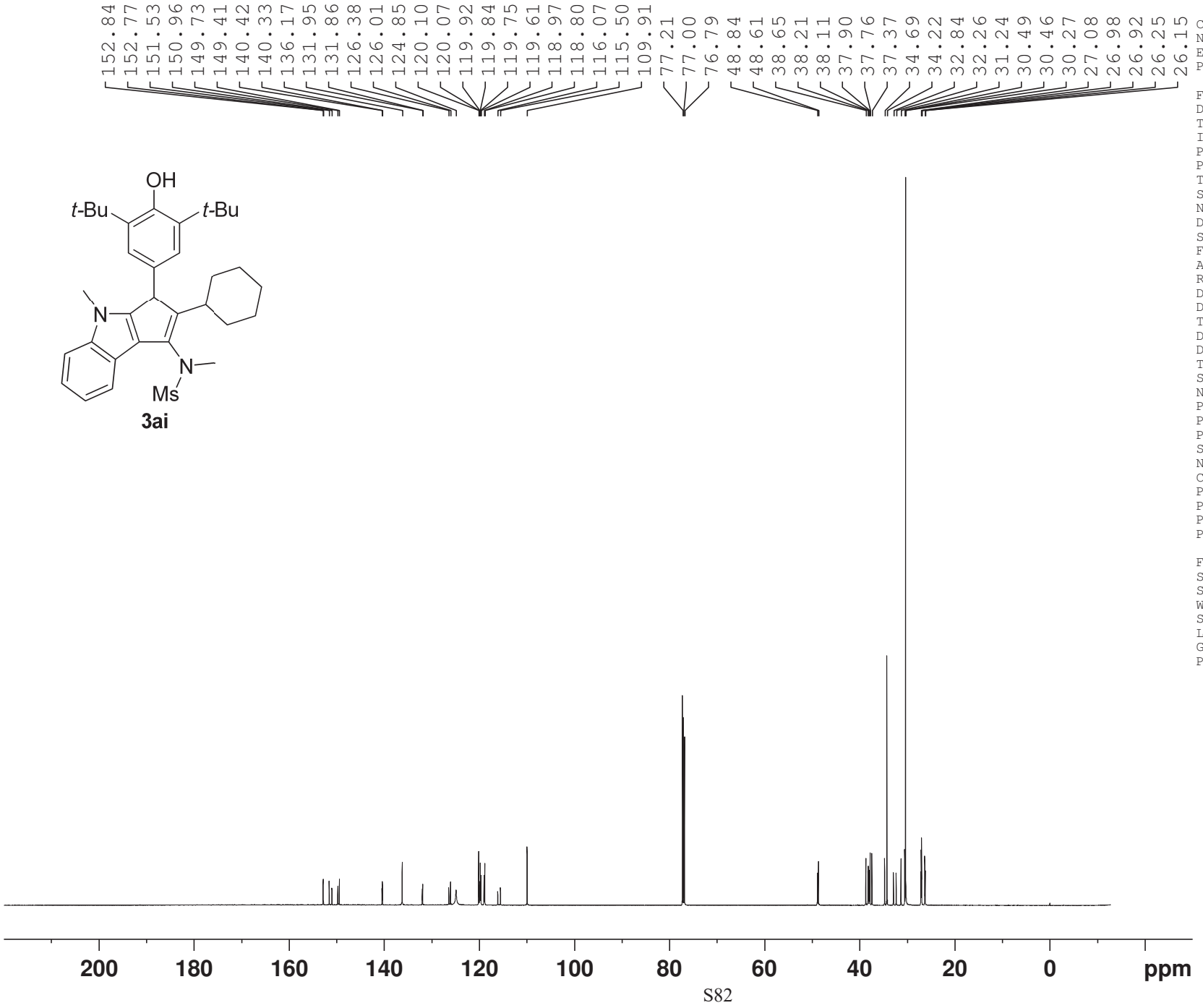
```
Current Data Parameters
NAME        yuky2497 3ah
EXPNO                 13
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201217
Time              12.28 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                  129
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028374 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



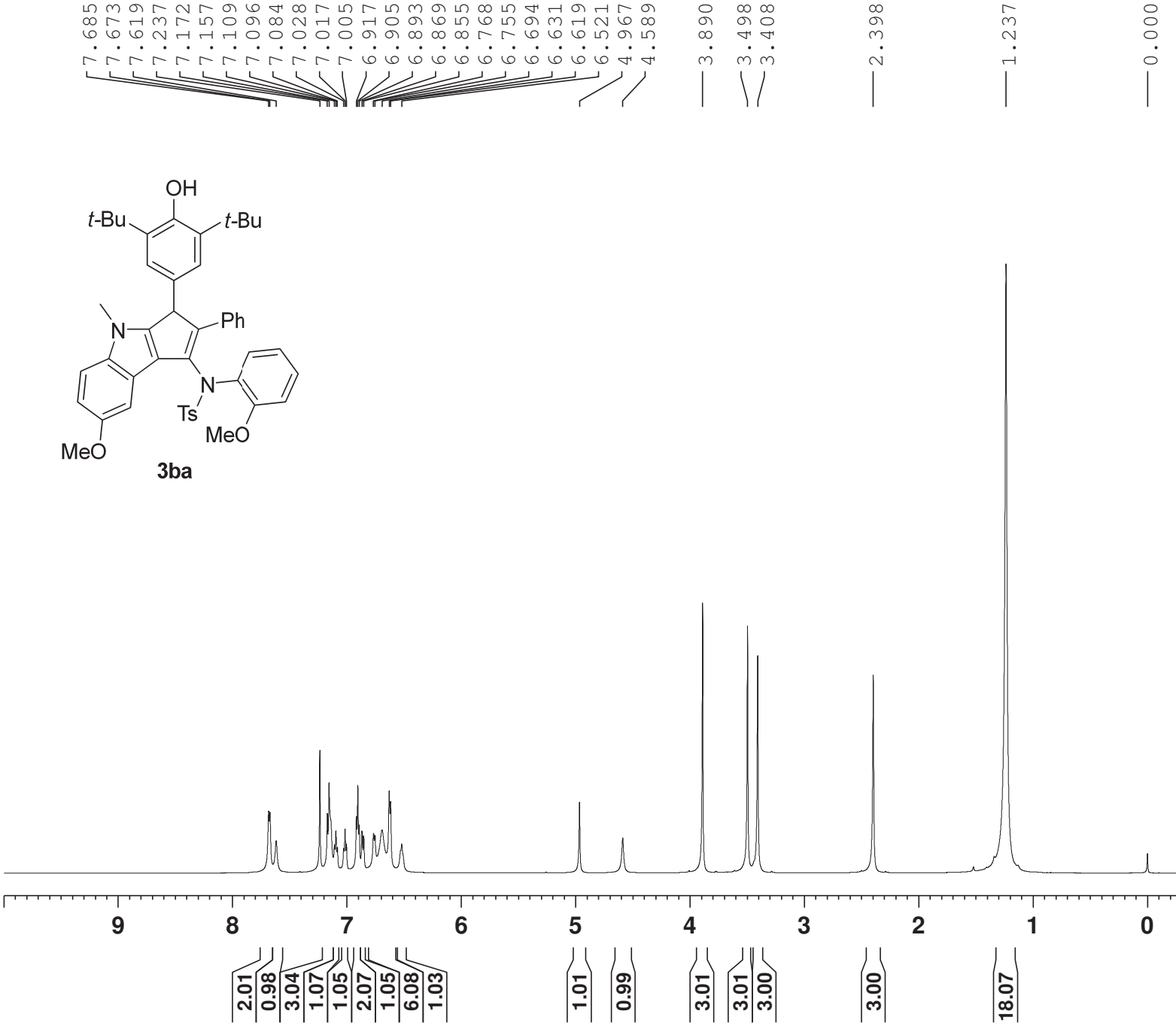
Current Data Parameters
NAME yuky2469-1 3ai
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201127
Time 11.07 h
INSTRUM Avance
PROBHD Z168773_0004 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 18.3179
DW 42.000 usec
DE 13.73 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.94 usec
P1 11.82 usec
PLW1 31.62299919 W

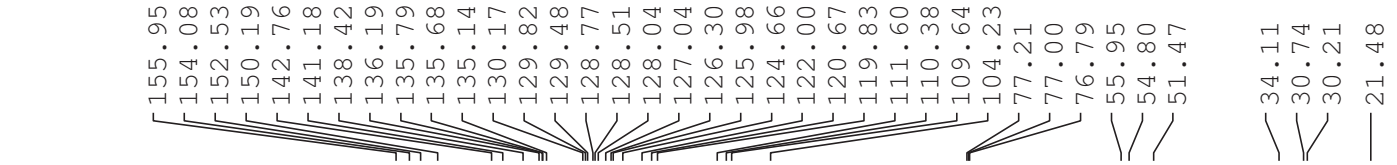
F2 - Processing parameters
SI 65536
SF 600.1300415 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

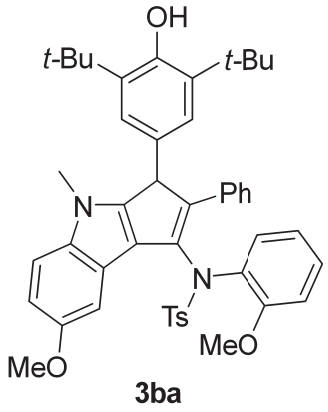



```
Current Data Parameters
NAME      yuky2469-1 3ai
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201127
Time              14.04 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                 32768
SF          150.9028302 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



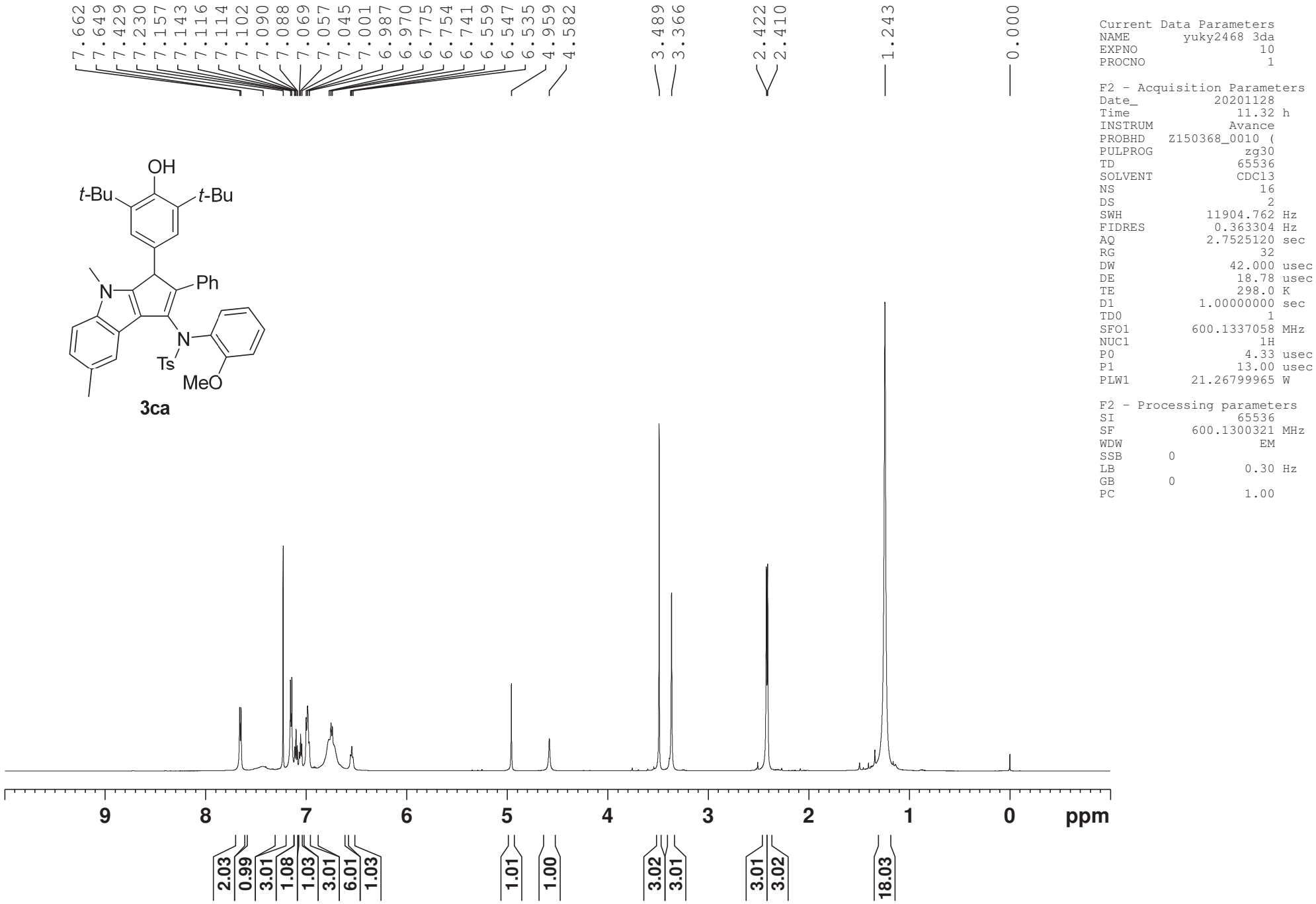

```
Current Data Parameters
NAME        yuky1888 3ca
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201116
Time               15.57 h
INSTRUM            Avance
PROBHD    Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ             2.7525120 sec
RG                47.619
DW                42.000 usec
DE                13.73 usec
TE                298.1 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                 3.94 usec
P1                11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300282 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```



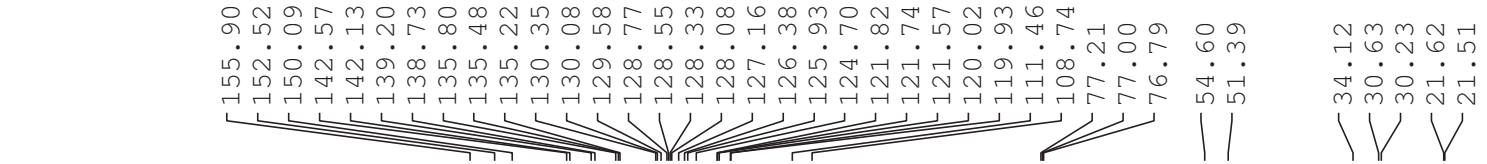


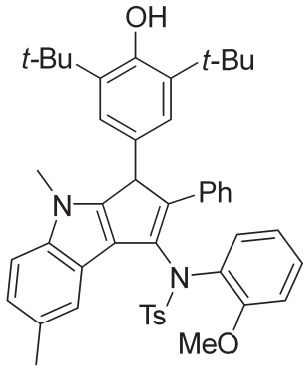
3ba

```
Current Data Parameters
NAME        yuky1888 3ca
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201116
Time              18.54 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028192 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



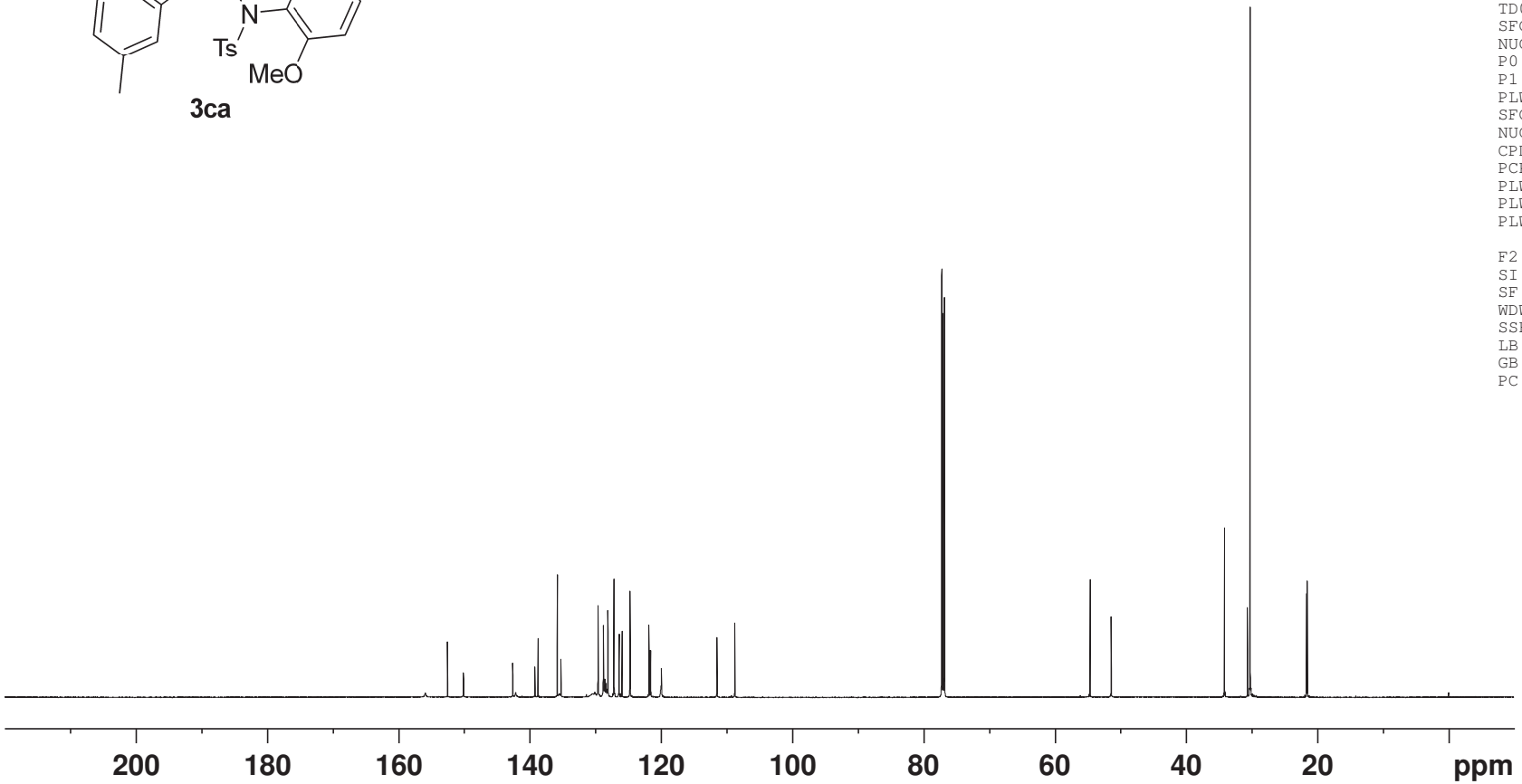

```
Current Data Parameters
NAME        yuky2468 3da
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201128
Time              11.32 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG            zg30
TD                65536
SOLVENT           CDC13
NS                   16
DS                    2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG                   32
DW               42.000 usec
DE               18.78 usec
TE               298.0 K
D1            1.00000000 sec
TD0                   1
SFO1         600.1337058 MHz
NUC1                 1H
P0               4.33 usec
P1              13.00 usec
PLW1         21.26799965 W

F2 - Processing parameters
SI                65536
SF           600.1300321 MHz
WDW                  EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

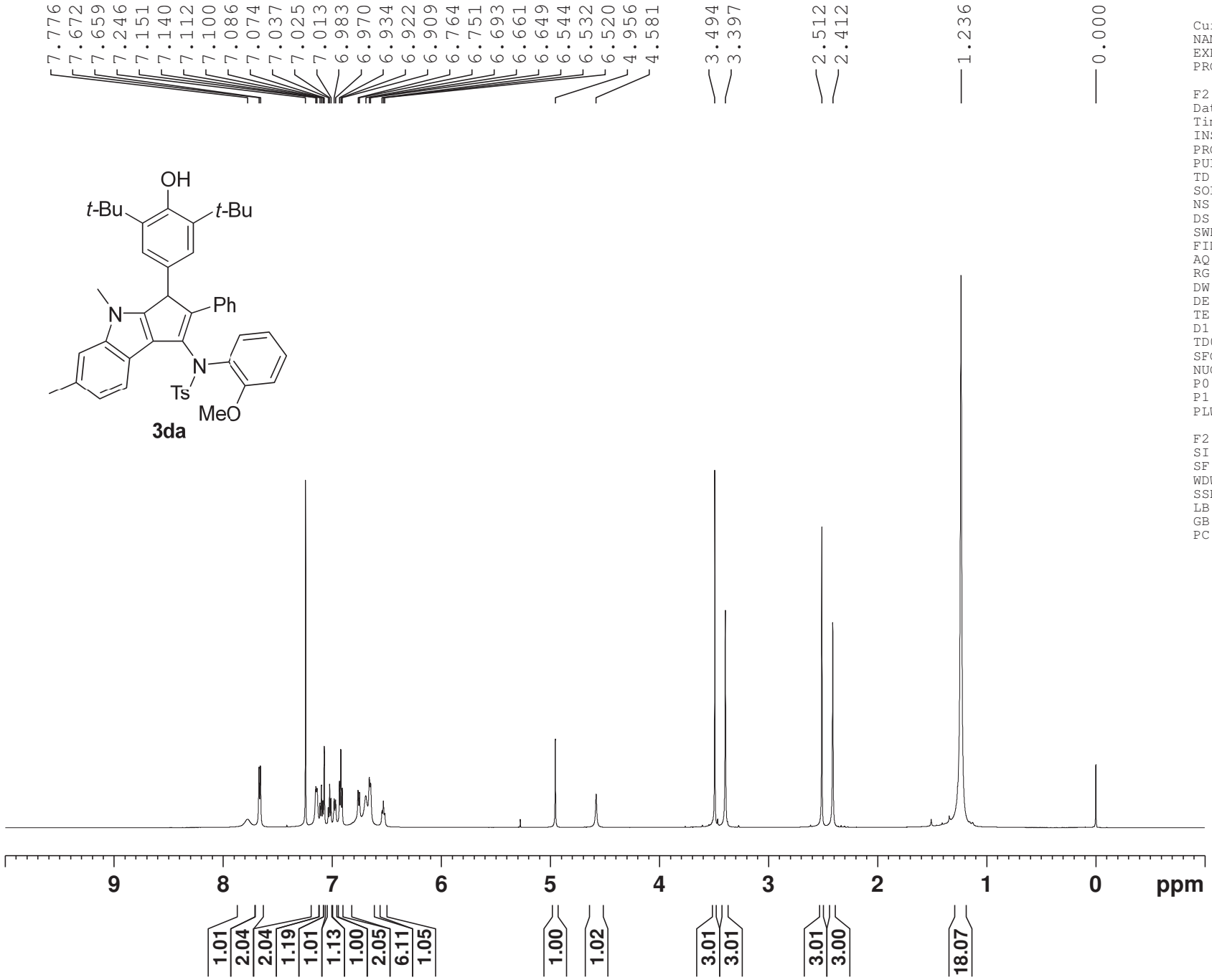




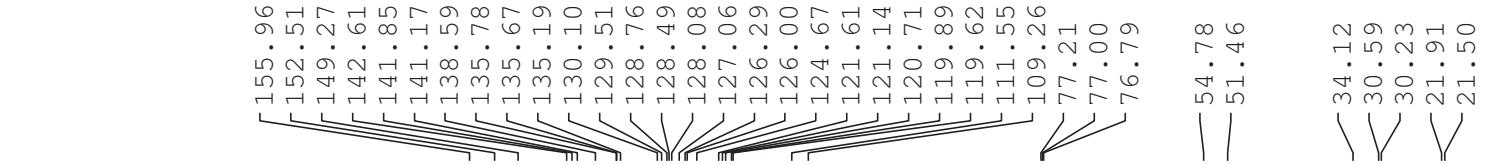
3ca

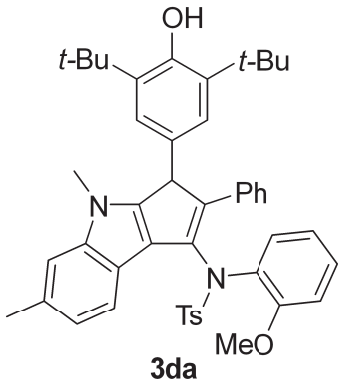
```
Current Data Parameters
NAME        yuky2468 3da
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201128
Time              14.00 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0               3.33 usec
P1              10.00 usec
PLW1        66.87999725 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2        21.26799965 W
PLW12        0.56160998 W
PLW13        0.28204000 W

F2 - Processing parameters
SI                32768
SF          150.9028194 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





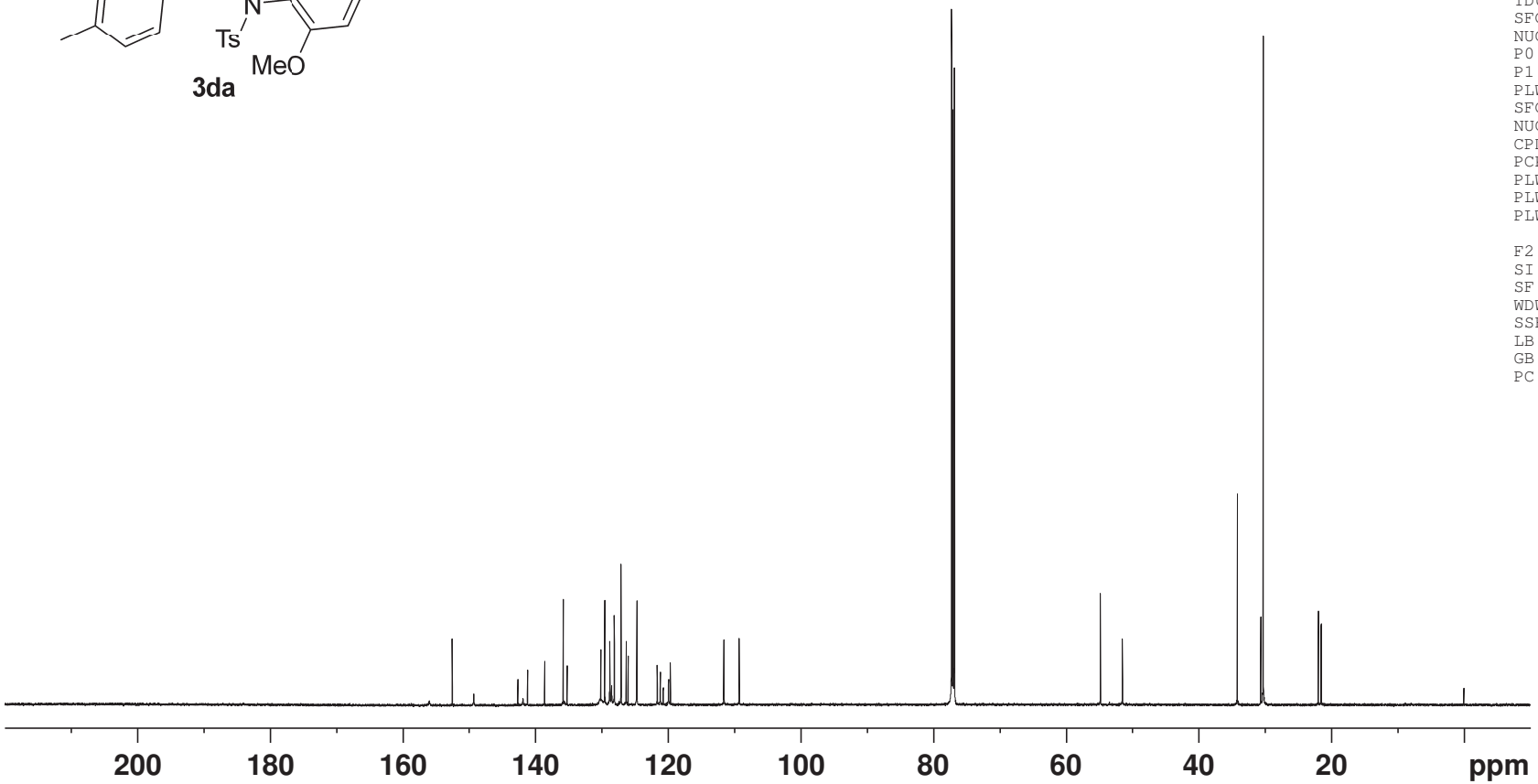

```
Current Data Parameters
NAME        yuky1889 3ea
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201109
Time               15.38 h
INSTRUM            Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               47.619
DW               42.000 usec
DE               13.73 usec
TE               298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                3.94 usec
P1               11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300233 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

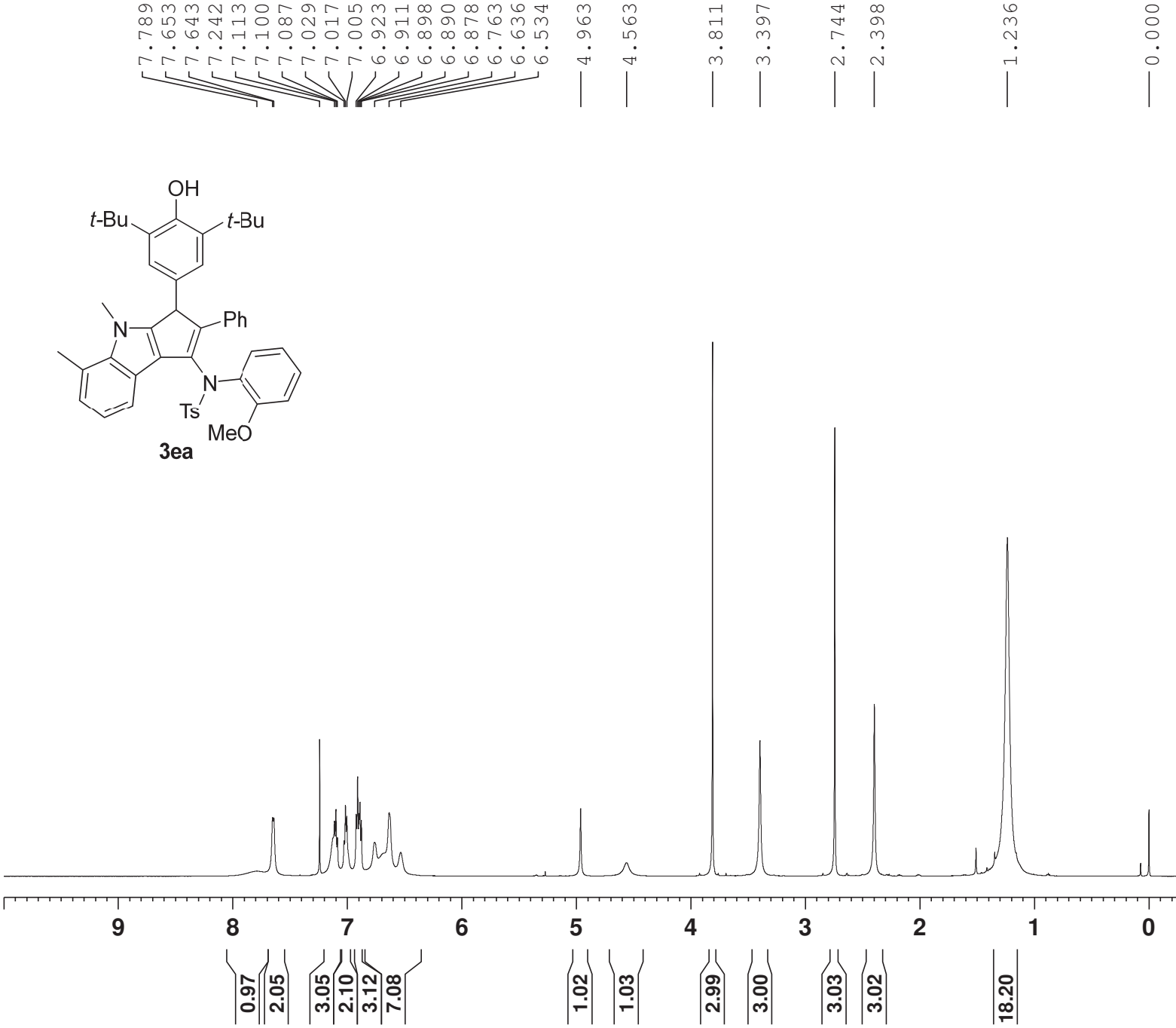




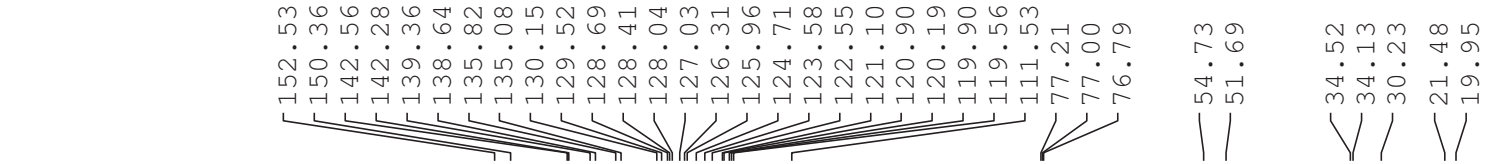
3da

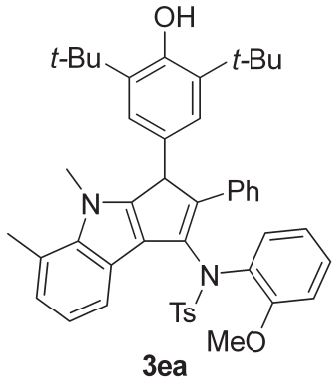
```
Current Data Parameters
NAME        yuky1889 3ea
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201109
Time              17.41 h
INSTRUM            Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2500
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW                13.500 usec
DE                18.00 usec
TE                298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                 6.13 usec
P1                18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                 32768
SF          150.9028151 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```





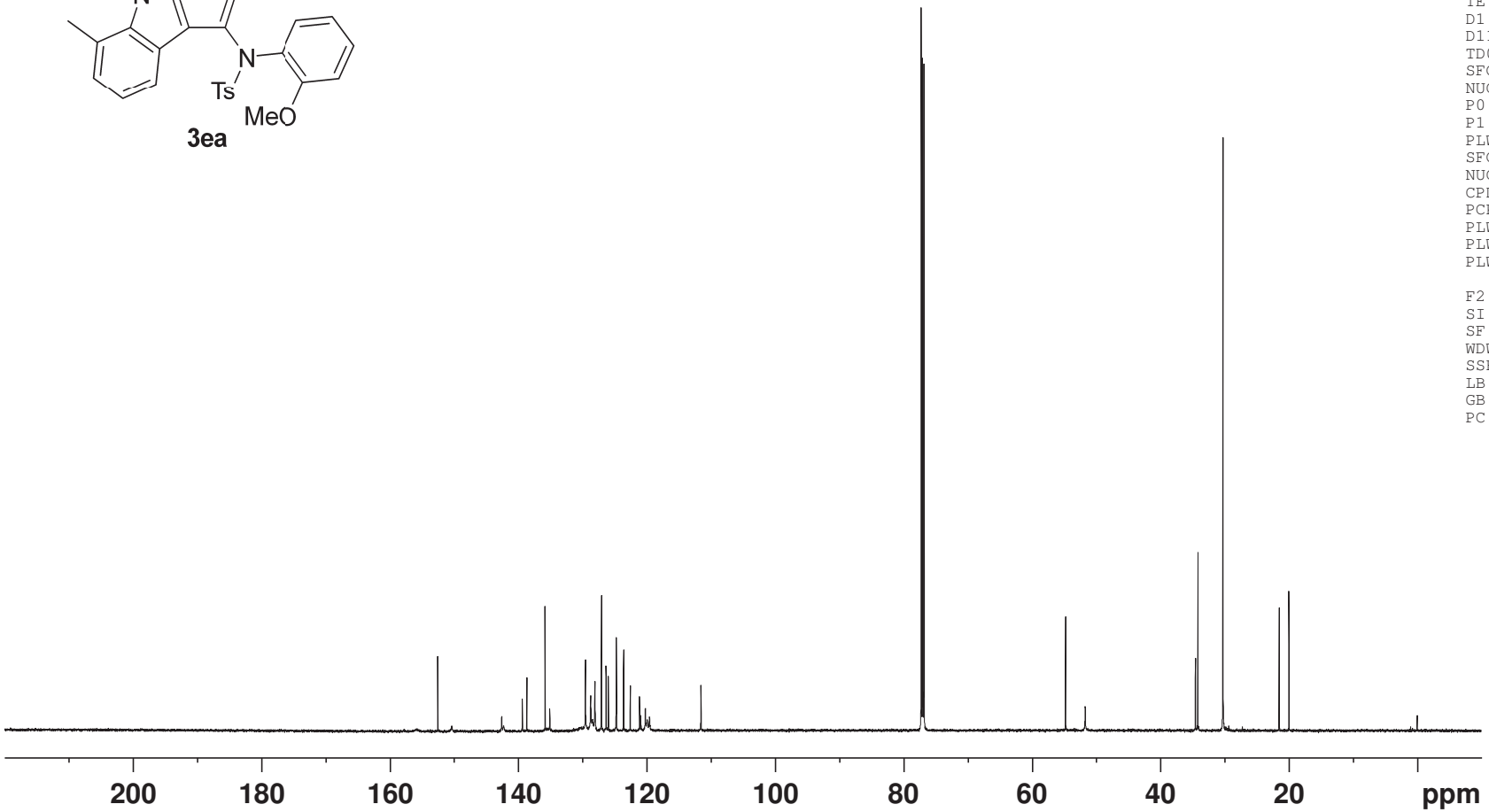

```
Current Data Parameters
NAME       yuky1890 3fa
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201022
Time              11.41 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               47.619
DW               42.000 usec
DE               13.73 usec
TE               298.1 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                3.94 usec
P1               11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300248 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

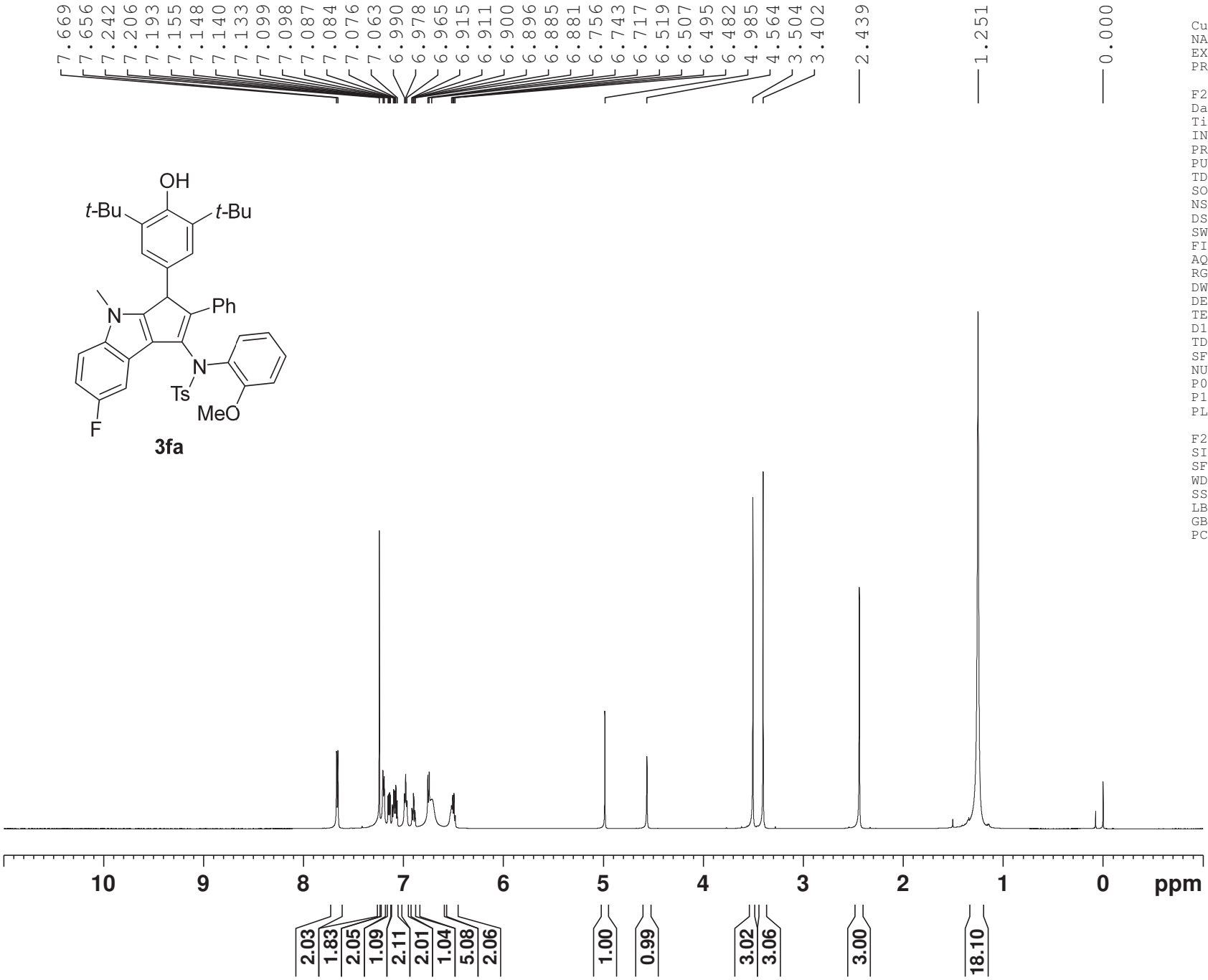




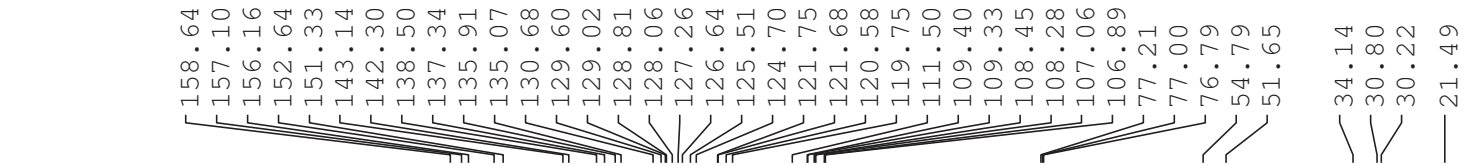
3ea

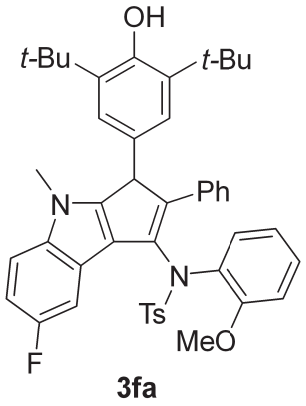
```
Current Data Parameters
NAME        yuky1890 3fa
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201022
Time              13.21 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2048
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                 32768
SF          150.9028164 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





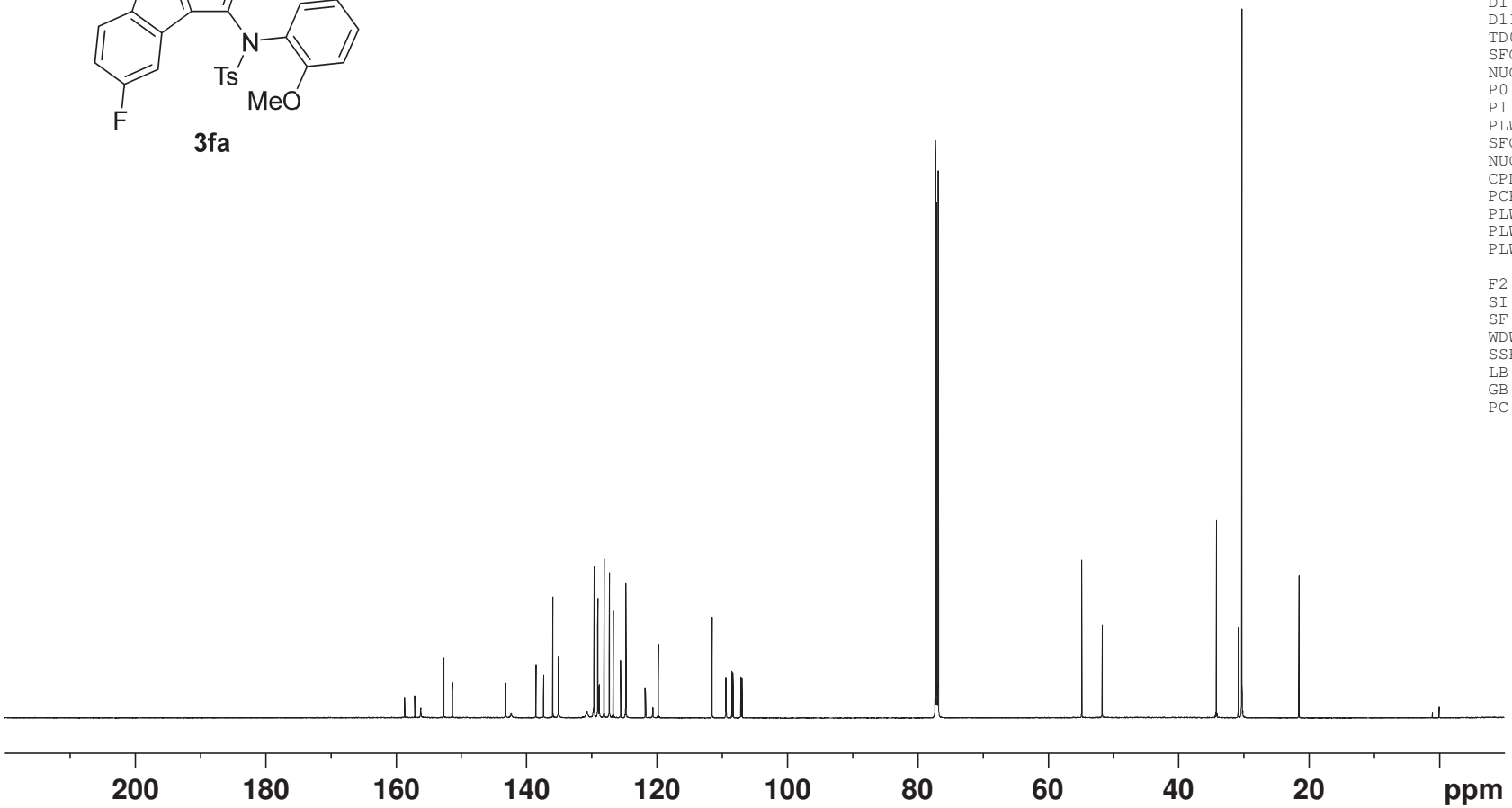

```
Current Data Parameters
NAME        yuky1893 3ha
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201112
Time               11.16 h
INSTRUM            Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG                    32
DW                42.000 usec
DE                18.78 usec
TE                298.0 K
D1           1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                 4.33 usec
P1                13.00 usec
PLW1         21.26799965 W

F2 - Processing parameters
SI                 65536
SF           600.1300249 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

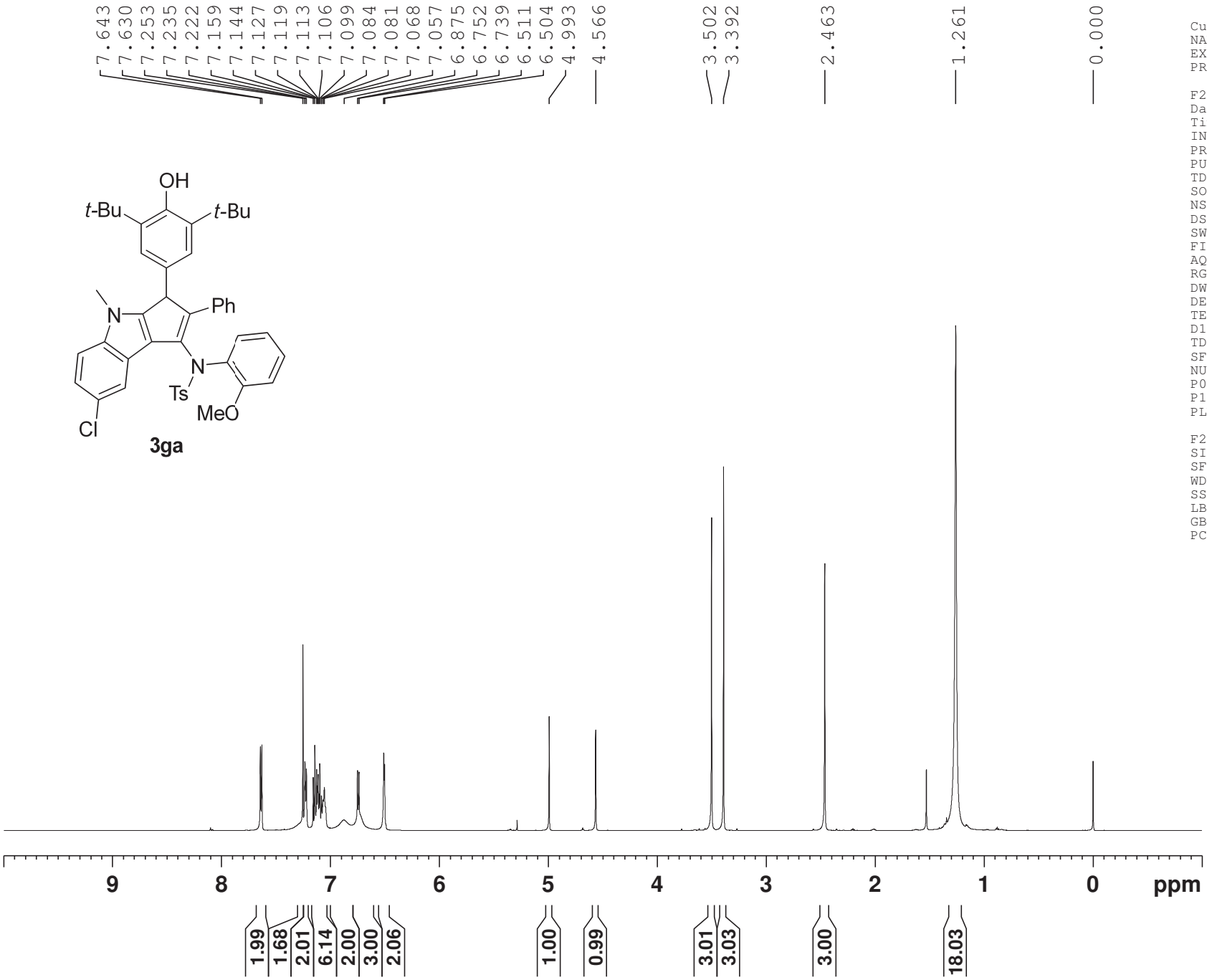




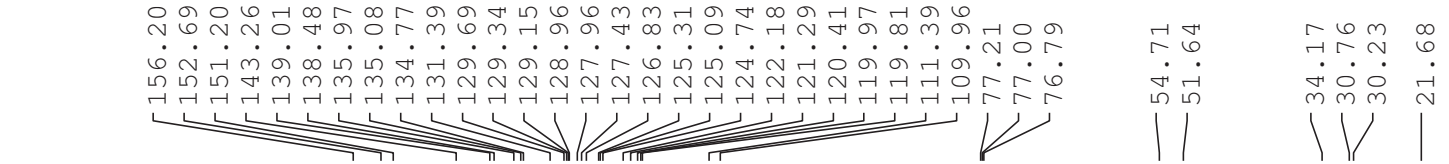
3fa

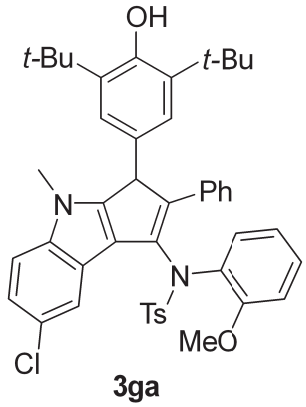
```
Current Data Parameters
NAME        yuky1893 3ha
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201112
Time              14.12 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                3.33 usec
P1               10.00 usec
PLW1         66.87999725 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2         21.26799965 W
PLW12         0.56160998 W
PLW13         0.28204000 W

F2 - Processing parameters
SI                 32768
SF          150.9028161 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





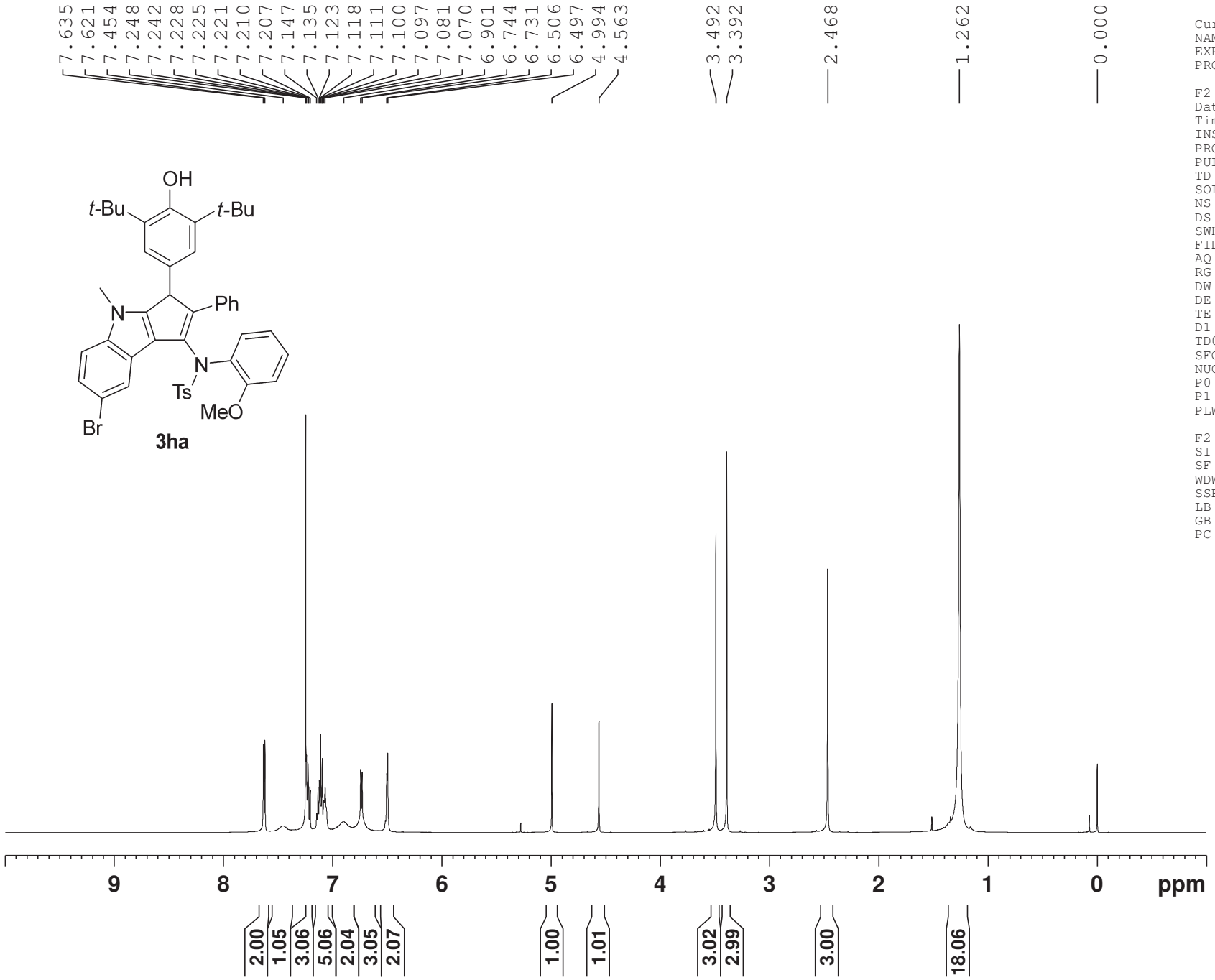

```
Current Data Parameters
NAME        yuky1894 3ia
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201022
Time              12.20 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG                    32
DW               42.000 usec
DE               18.78 usec
TE                298.1 K
D1           1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                4.33 usec
P1               13.00 usec
PLW1         21.26799965 W

F2 - Processing parameters
SI                 65536
SF           600.1300187 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```



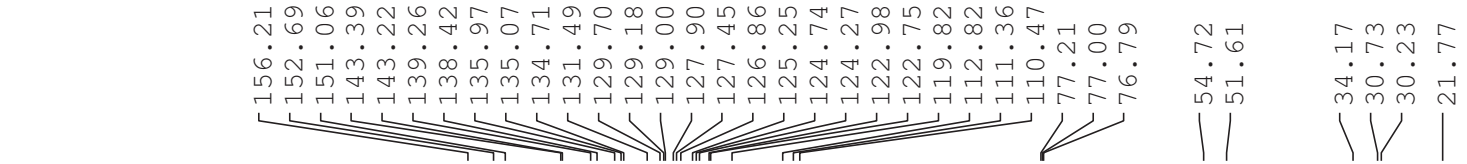


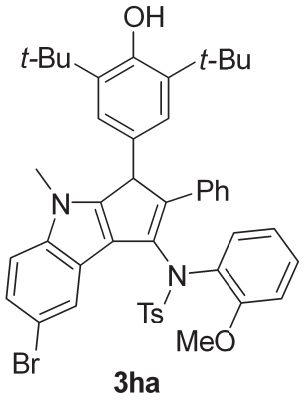
3ga

```
Current Data Parameters
NAME        yuky1894 3ia
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201022
Time              14.47 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3000
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0               3.33 usec
P1              10.00 usec
PLW1        66.87999725 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2        21.26799965 W
PLW12        0.56160998 W
PLW13        0.28204000 W

F2 - Processing parameters
SI                32768
SF          150.9028126 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```



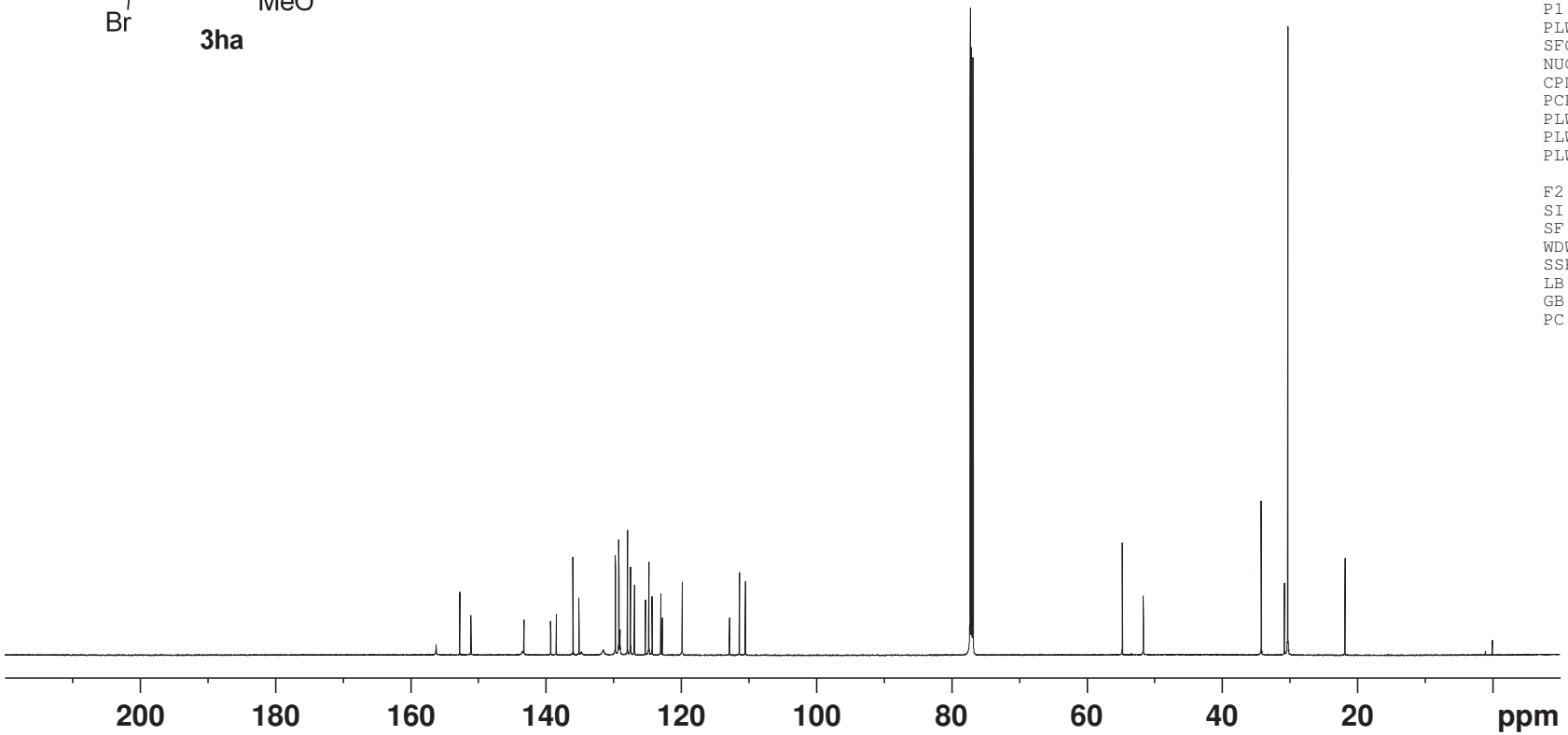

```
Current Data Parameters
NAME        yuky1886 3ja
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201110
Time               20.06 h
INSTRUM            Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH            11904.762 Hz
FIDRES          0.363304 Hz
AQ             2.7525120 sec
RG                    32
DW                42.000 usec
DE                18.78 usec
TE                298.1 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                 4.33 usec
P1                13.00 usec
PLW1         21.26799965 W

F2 - Processing parameters
SI                 65536
SF           600.1300219 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

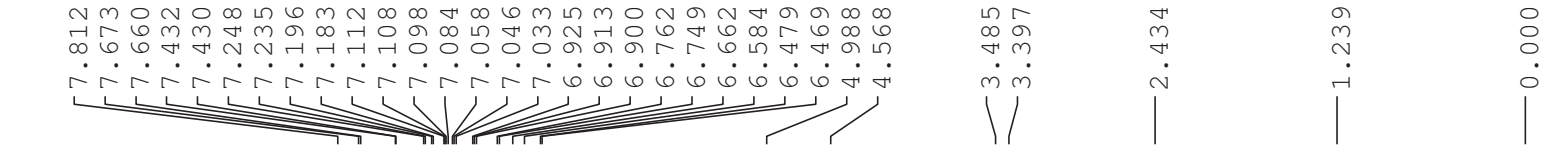


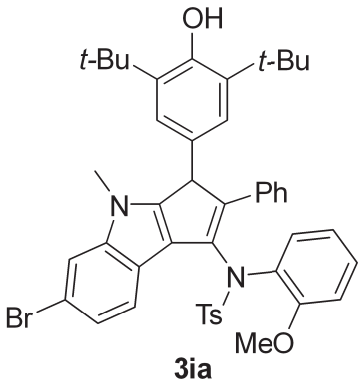


3ha

```
Current Data Parameters
NAME        yuky1886 3ja
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201110
Time              23.03 h
INSTRUM            Avance
PROBHD   Z150368_0010 (
PULPROG            zgpg30
TD                  65536
SOLVENT             CDCl3
NS                   3600
DS                      2
SWH            37037.035 Hz
FIDRES          1.130281 Hz
AQ             0.8847360 sec
RG                    101
DW                13.500 usec
DE                18.00 usec
TE                298.0 K
D1             2.00000000 sec
D11            0.03000000 sec
TD0                     1
SFO1         150.9194079 MHz
NUC1                 13C
P0                3.33 usec
P1               10.00 usec
PLW1         66.87999725 W
SFO2         600.1324005 MHz
NUC2                 1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2         21.26799965 W
PLW12         0.56160998 W
PLW13         0.28204000 W

F2 - Processing parameters
SI                  32768
SF           150.9028147 MHz
WDW                    EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

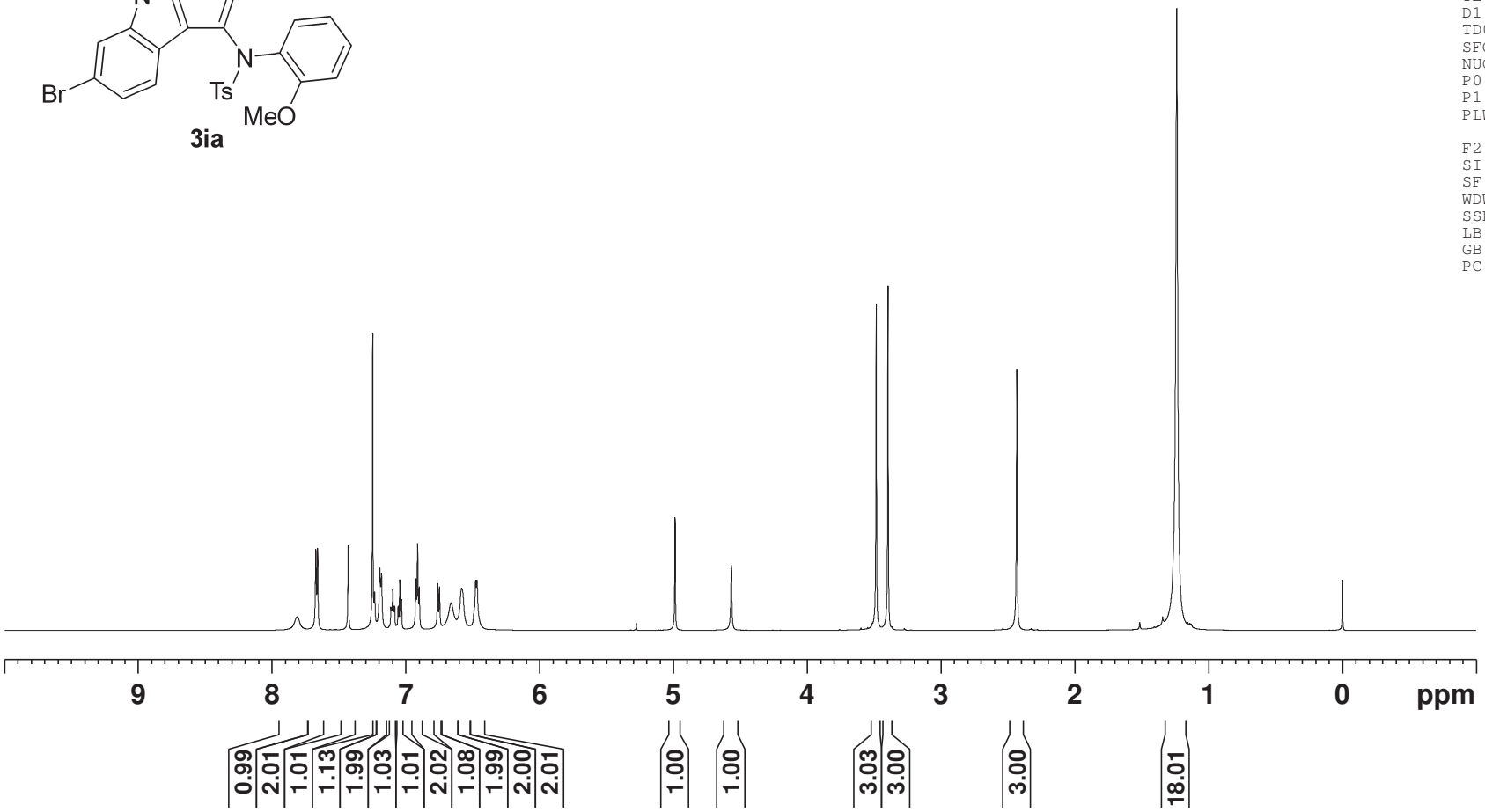


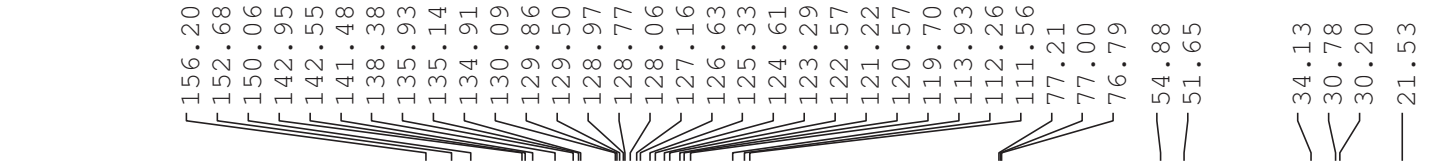


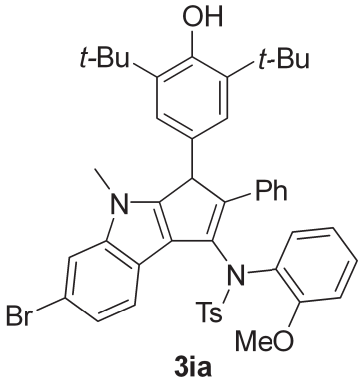


3ia

```
Current Data Parameters
NAME        yuky1891 3ka
EXPNO                 12
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201109
Time               22.37 h
INSTRUM            Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               47.619
DW               42.000 usec
DE               13.73 usec
TE               298.1 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                3.94 usec
P1               11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300220 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

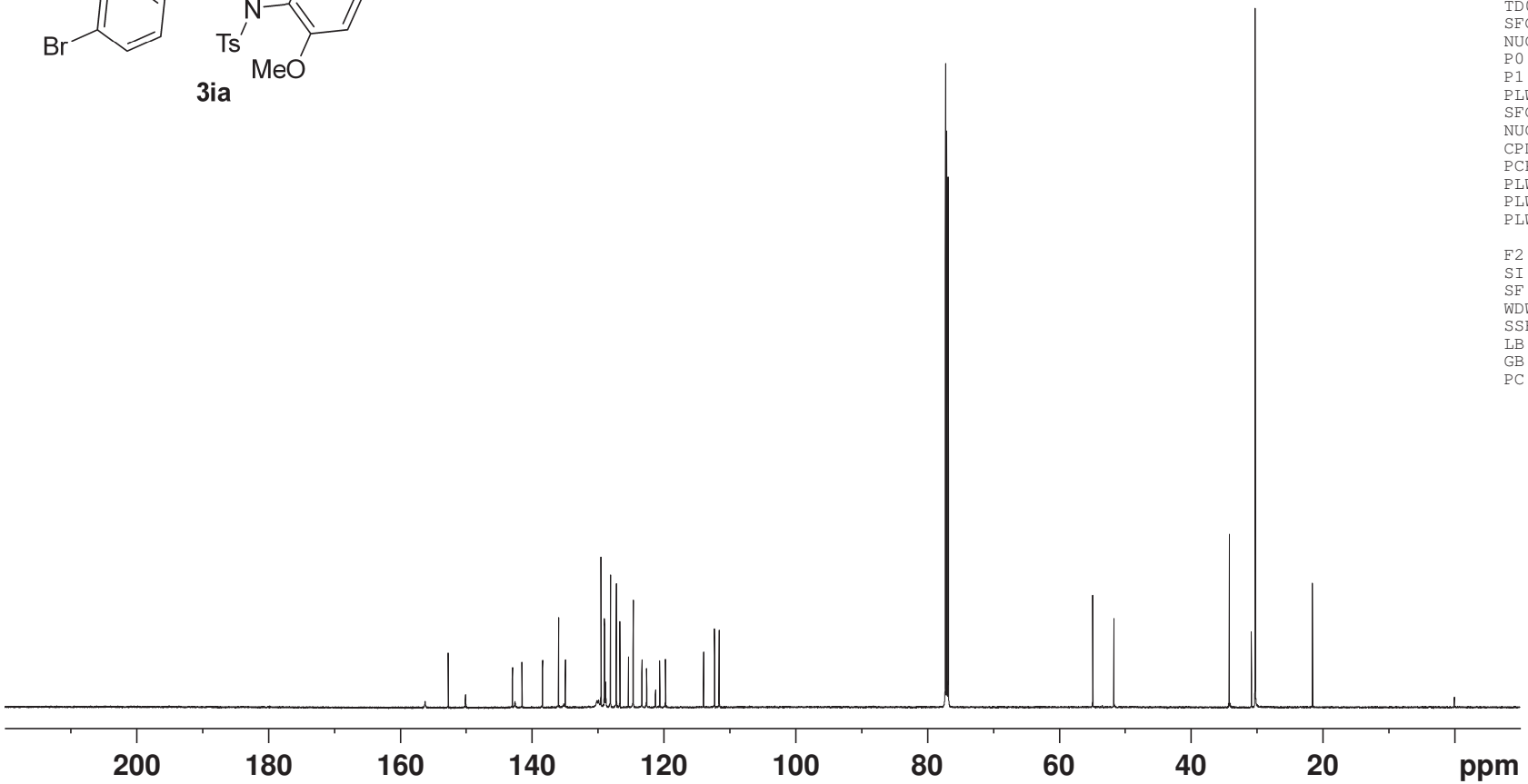


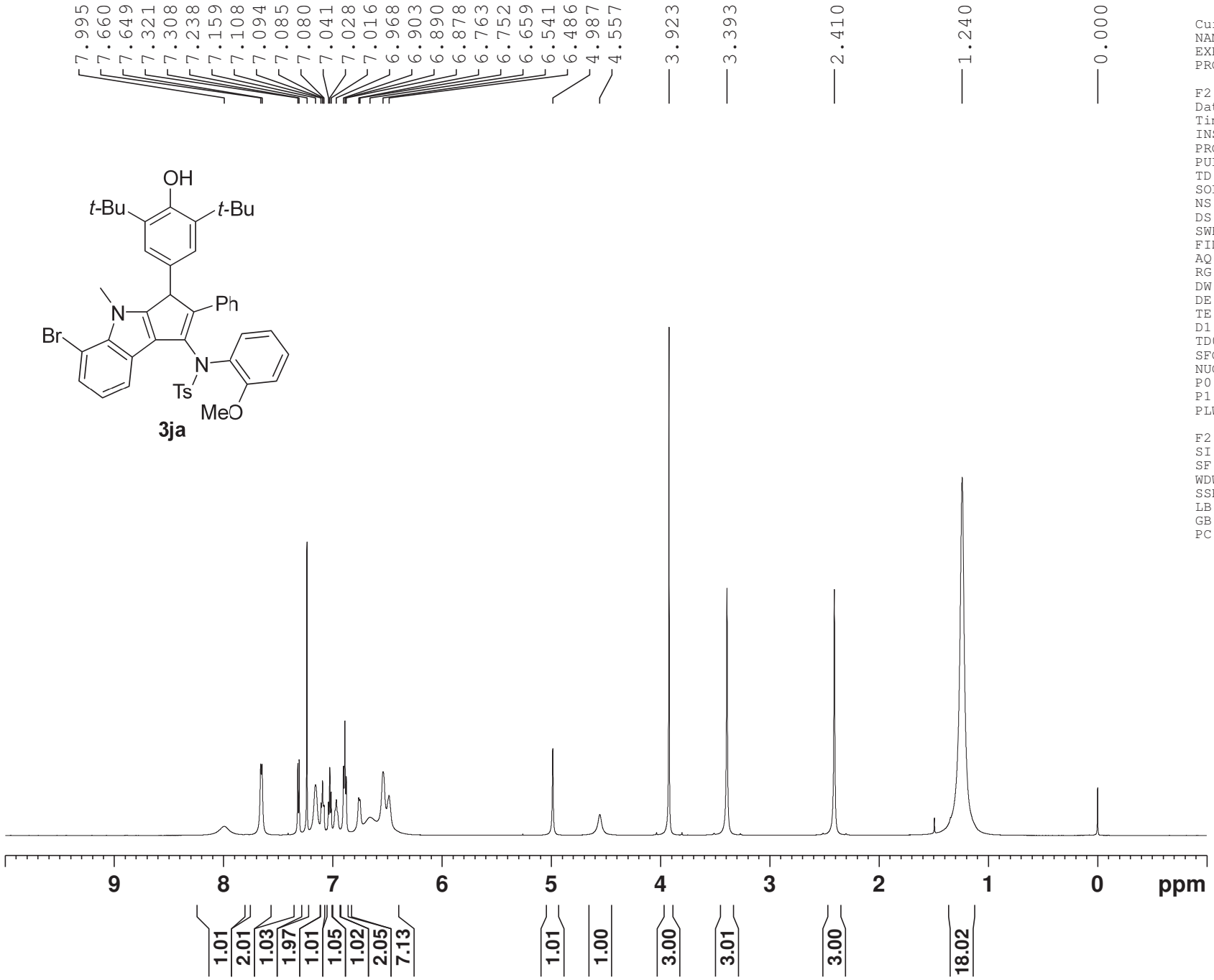




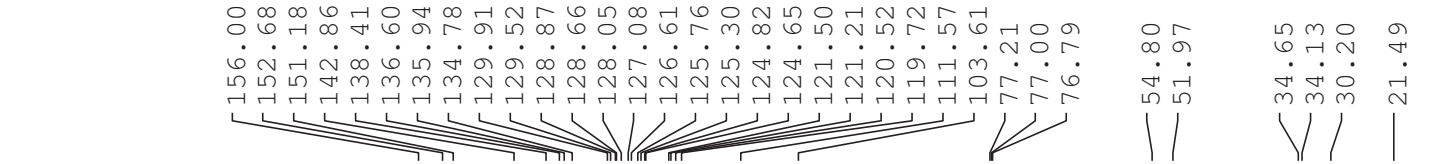
3ia

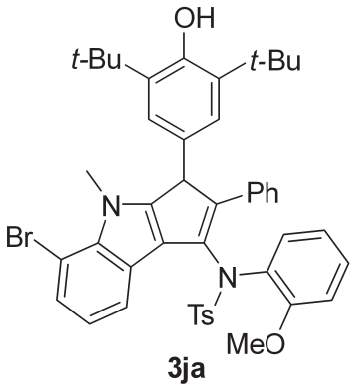
```
Current Data Parameters
NAME        yuky1891 3ka
EXPNO                 13
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201110
Time                1.34 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                 32768
SF           150.9028156 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```





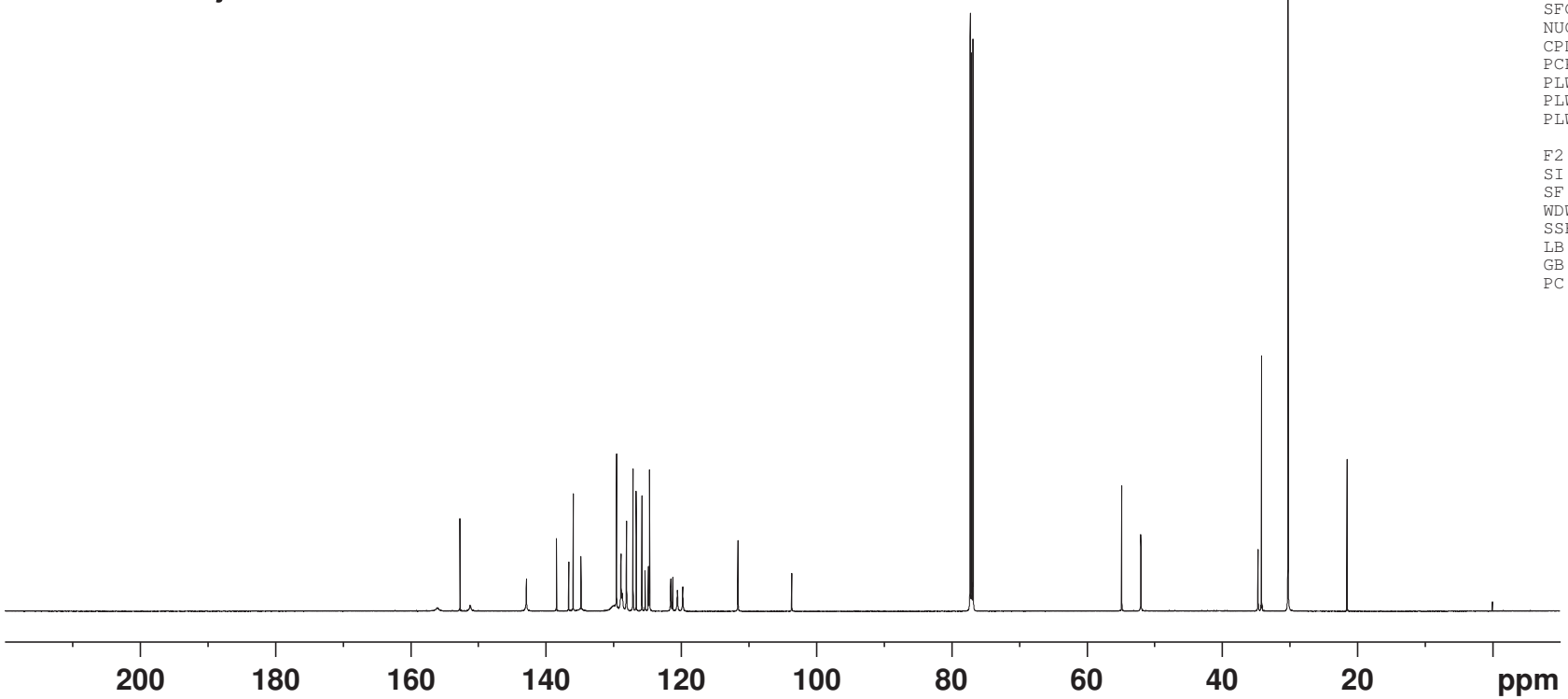

```
Current Data Parameters
NAME       yuky1892 3la
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_          20201112
Time              22.45 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG             zg30
TD                 65536
SOLVENT            CDCl3
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ             2.7525120 sec
RG                    32
DW                42.000 usec
DE                18.78 usec
TE                298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                  1H
P0                 4.33 usec
P1                13.00 usec
PLW1         21.26799965 W

F2 - Processing parameters
SI                 65536
SF           600.1300278 MHz
WDW                   EM
SSB       0
LB                 0.30 Hz
GB        0
PC                 1.00
```

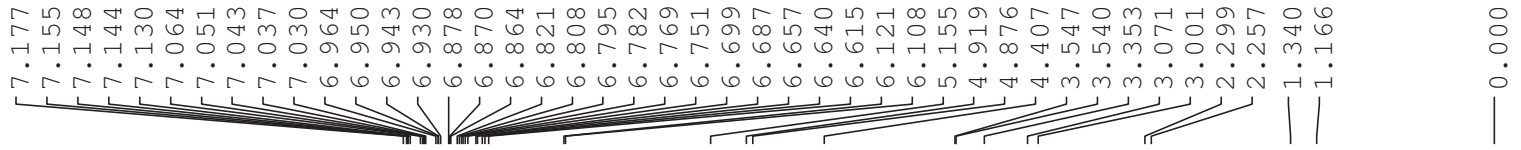


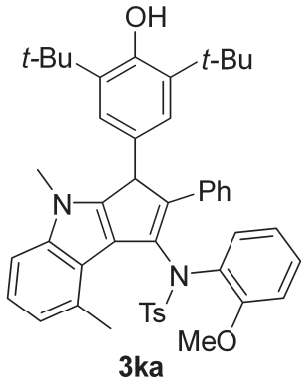


3ja

```
Current Data Parameters
NAME        yuky1892 3la
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201113
Time                1.42 h
INSTRUM           Avance
PROBHD   Z150368_0010 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    2
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0               3.33 usec
P1              10.00 usec
PLW1         66.87999725 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            80.00 usec
PLW2         21.26799965 W
PLW12         0.56160998 W
PLW13         0.28204000 W

F2 - Processing parameters
SI                 32768
SF          150.9028182 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

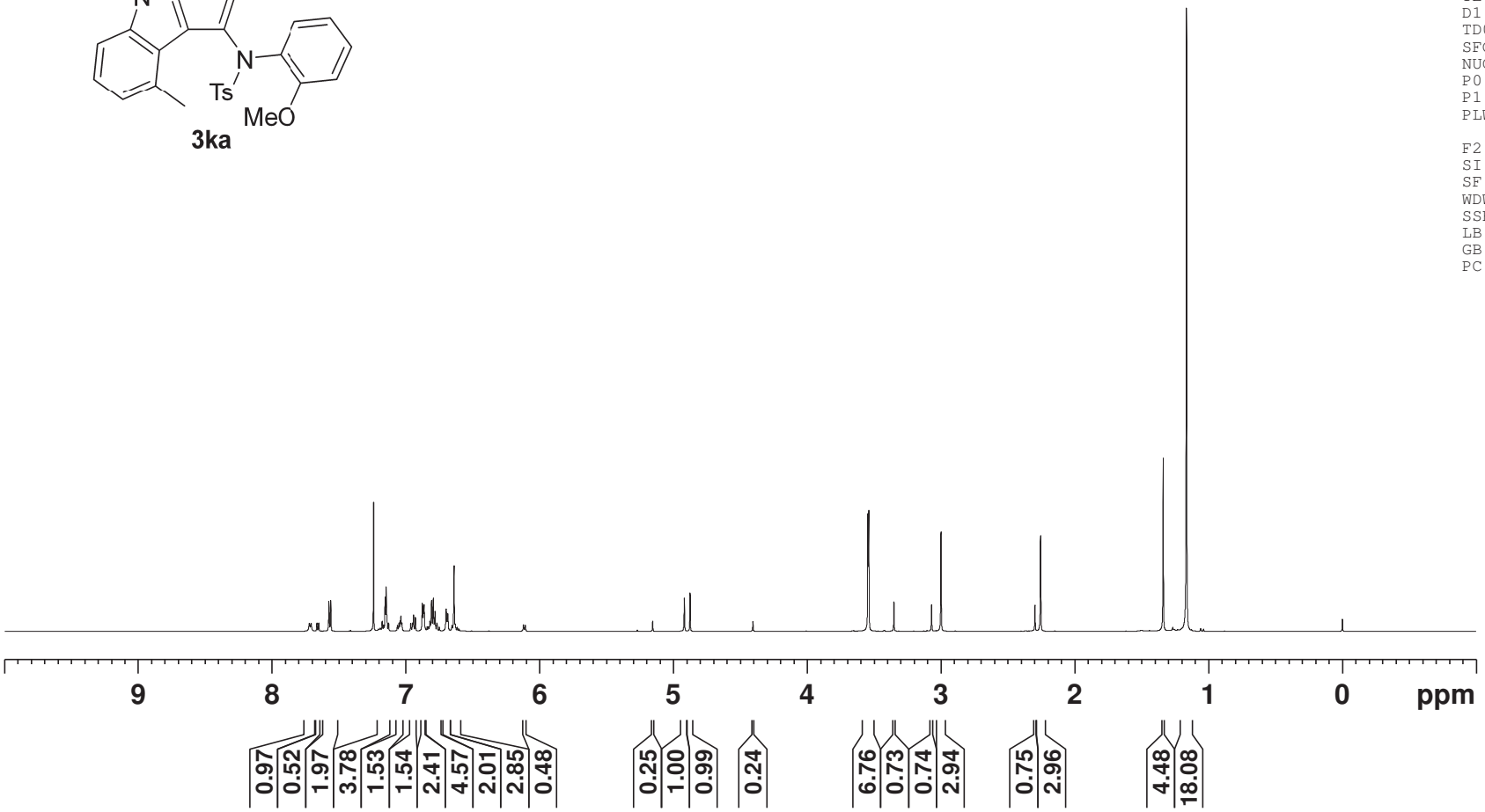


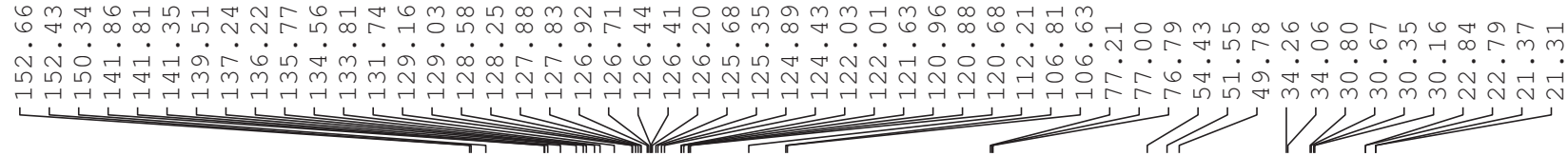


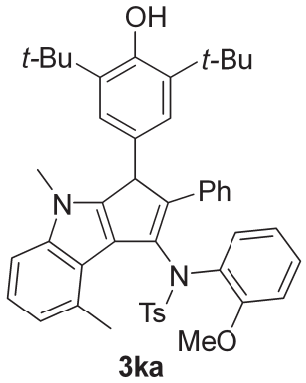


3ka

```
Current Data Parameters
NAME        yuky2463 3ba
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201128
Time                5.14 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               47.619
DW               42.000 usec
DE               13.73 usec
TE               298.0 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                3.94 usec
P1               11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300253 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```

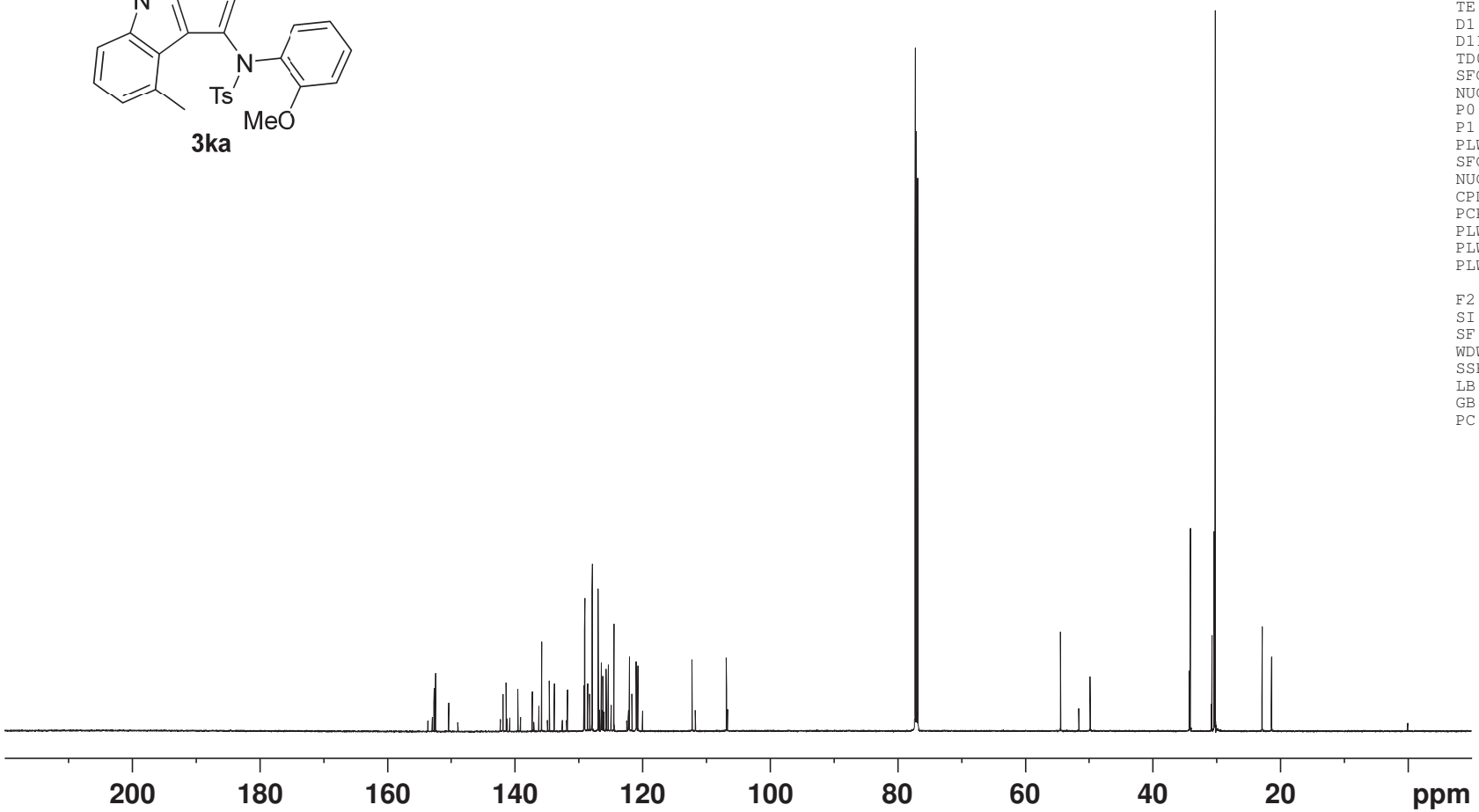


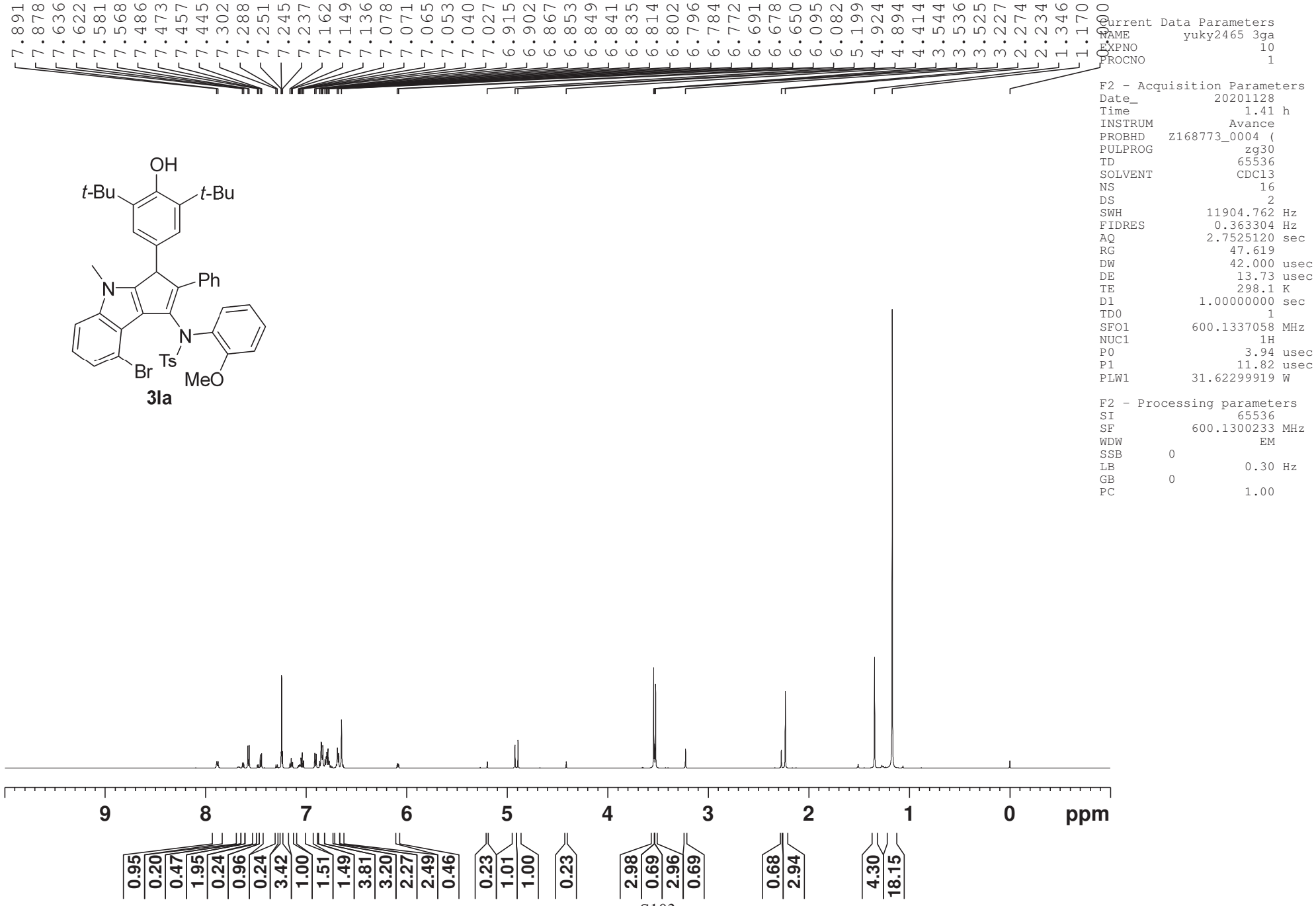


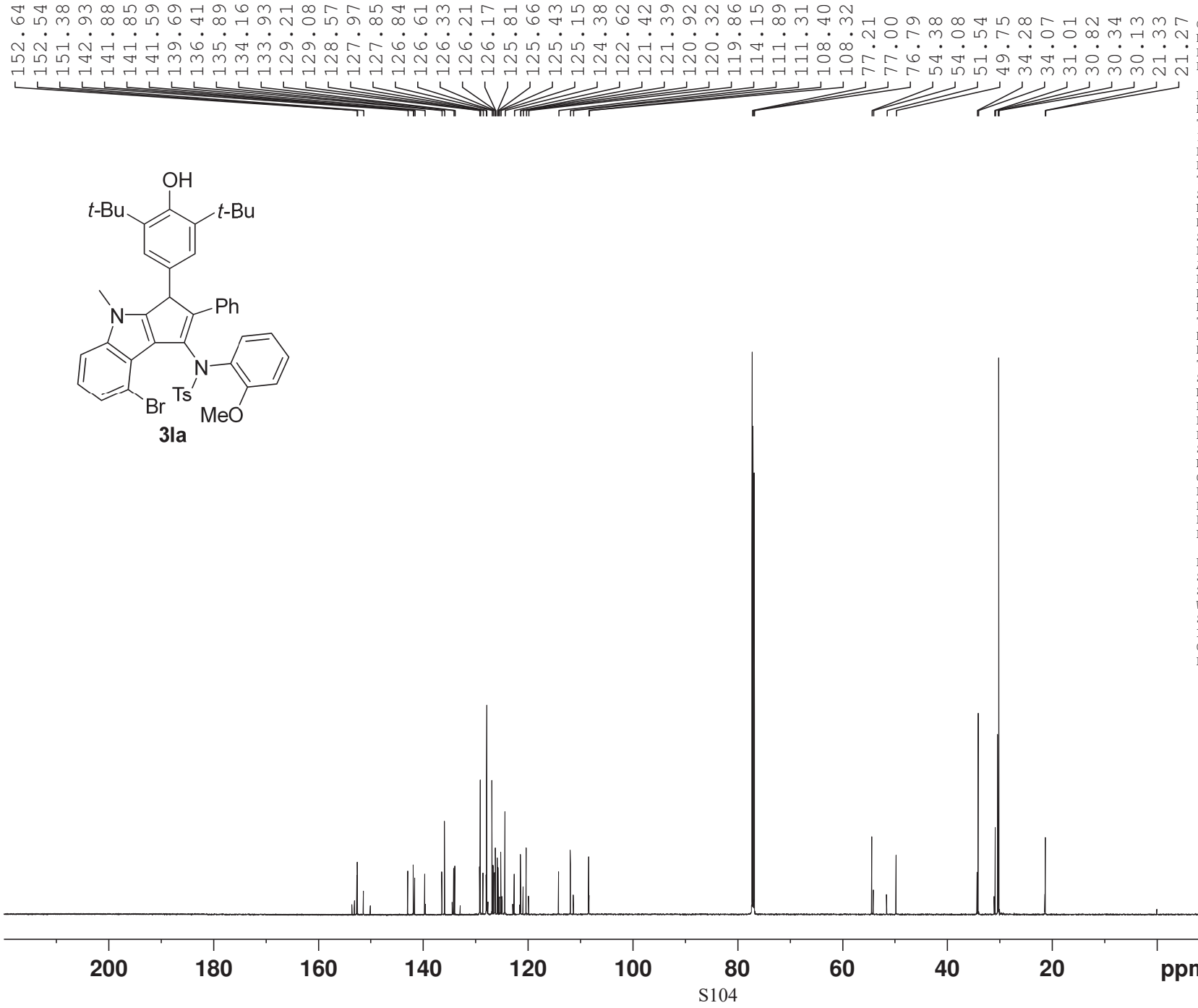


3ka

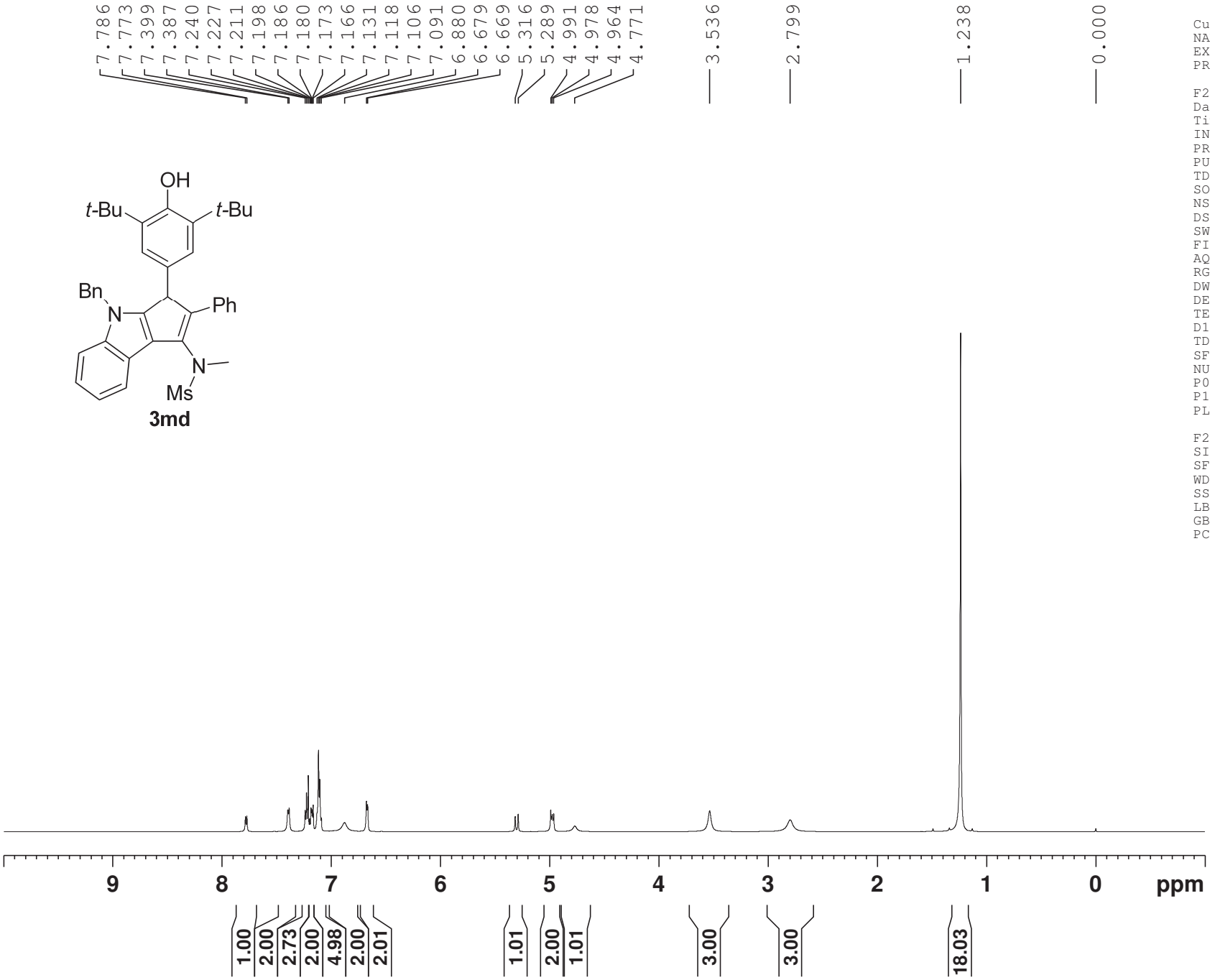
```
Current Data Parameters
NAME        yuky2463 3ba
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201128
Time                8.11 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.1 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1         150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                 32768
SF           150.9028167 MHz
WDW                   EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```




7.891
7.878
7.636
7.622
7.581
7.568
7.486
7.473
7.457
7.445
7.302
7.288
7.251
7.245
7.237
7.162
7.149
7.136
7.078
7.071
7.065
7.053
7.040
7.027
6.915
6.902
6.867
6.853
6.849
6.841
6.835
6.814
6.802
6.796
6.784
6.772
6.691
6.678
6.650
6.095
6.082
5.199
4.924
4.894
4.414
3.544
3.536
3.525
3.227
2.274
2.234
1.346
1.170
0.000
Current Data Parameters
NAME yuky2465 3ga
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201128
Time 1.41 h
INSTRUM Avance
PROBHD Z168773_0004 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 47.619
DW 42.000 usec
DE 13.73 usec
TE 298.1 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.94 usec
P1 11.82 usec
PLW1 31.62299919 W
F2 - Processing parameters
SI 65536
SF 600.1300233 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
OH
t-Bu
t-Bu
Ph
N
N
Ts
Br
MeO
3Ia
9
8
7
6
5
4
3
2
1
0
ppm
0.95
0.20
0.47
1.95
0.24
0.96
0.24
3.42
1.00
1.51
1.49
3.81
3.20
2.27
2.49
0.46
0.23
1.01
1.00
0.23
2.98
0.69
2.96
0.69
0.68
2.94
4.30
18.15




```
Current Data Parameters
NAME       yuky2465 3ga
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201128
Time               4.38 h
INSTRUM          Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3600
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1               13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2         600.1324005 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2            70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028178 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC                1.40
```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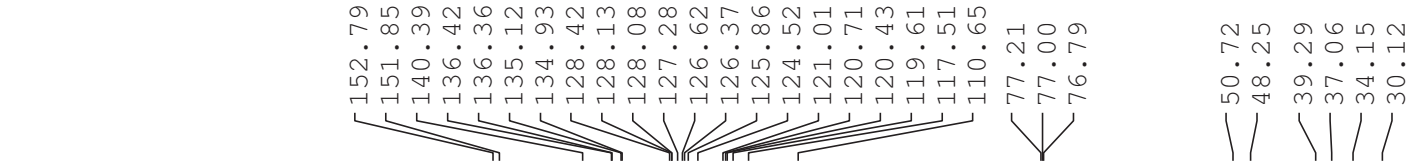
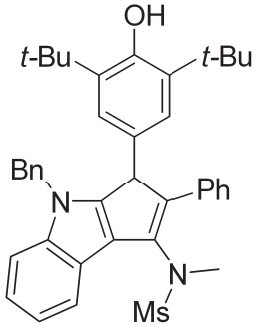
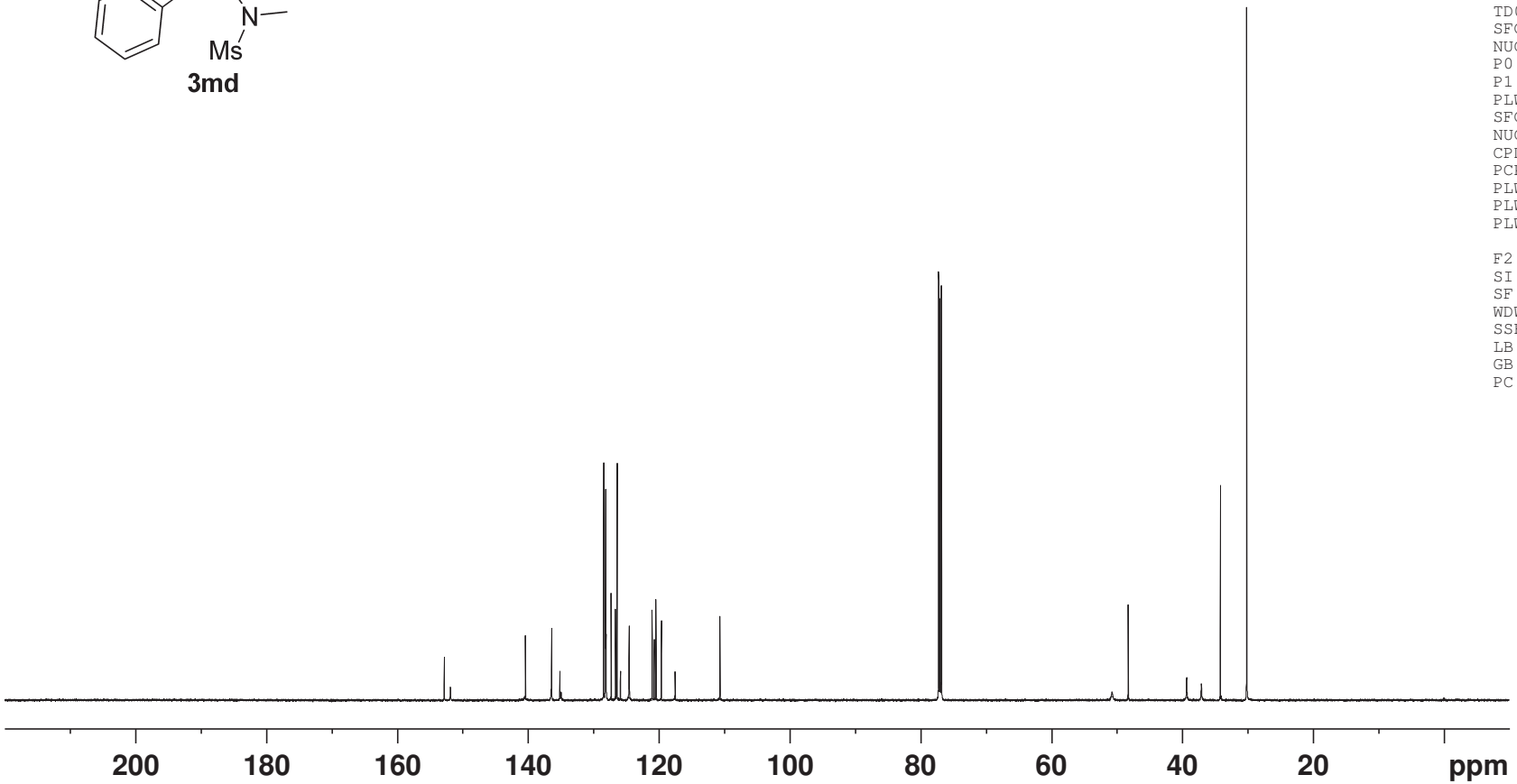
7.773
7.399
7.387
7.240
7.227
7.211
7.198
7.186
7.180
7.173
7.166
7.131
7.118
7.106
7.091
6.880
6.679
6.669
5.316
5.289
4.991
4.978
4.964
4.771
3.536
2.799
1.238
0.000
OH
t-Bu
t-Bu
Bn
N
Ph
N
Ms
3md
Current Data Parameters
NAME yuky2472-3 3nd
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20201123
Time 22.49 h
INSTRUM Avance
PROBHD Z168773_0004 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 29.5786
DW 42.000 usec
DE 13.73 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.94 usec
P1 11.82 usec
PLW1 31.62299919 W
F2 - Processing parameters
SI 65536
SF 600.1300440 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
9
8
7
6
5
4
3
2
1
0
ppm
1.00
2.00
2.73
2.00
4.98
2.00
2.01
1.01
2.00
1.01
3.00
3.00
18.03

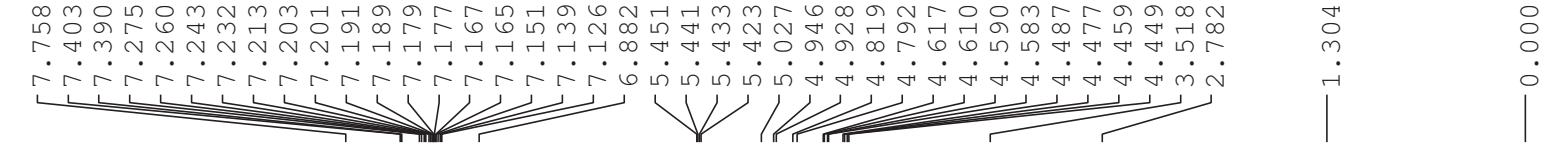


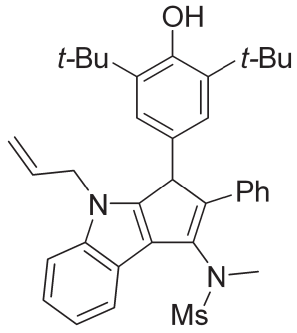


3md

```
Current Data Parameters
NAME      yuky2472-3 3nd
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201124
Time               0.27 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2000
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1               13C
P0                6.13 usec
P1               18.38 usec
PLW1         76.86299896 W
SFO2        600.1324005 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2            70.00 usec
PLW2         31.62299919 W
PLW12         0.94957000 W
PLW13         0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028262 MHz
WDW                EM
SSB       0
LB               1.00 Hz
GB        0
PC               1.40
```

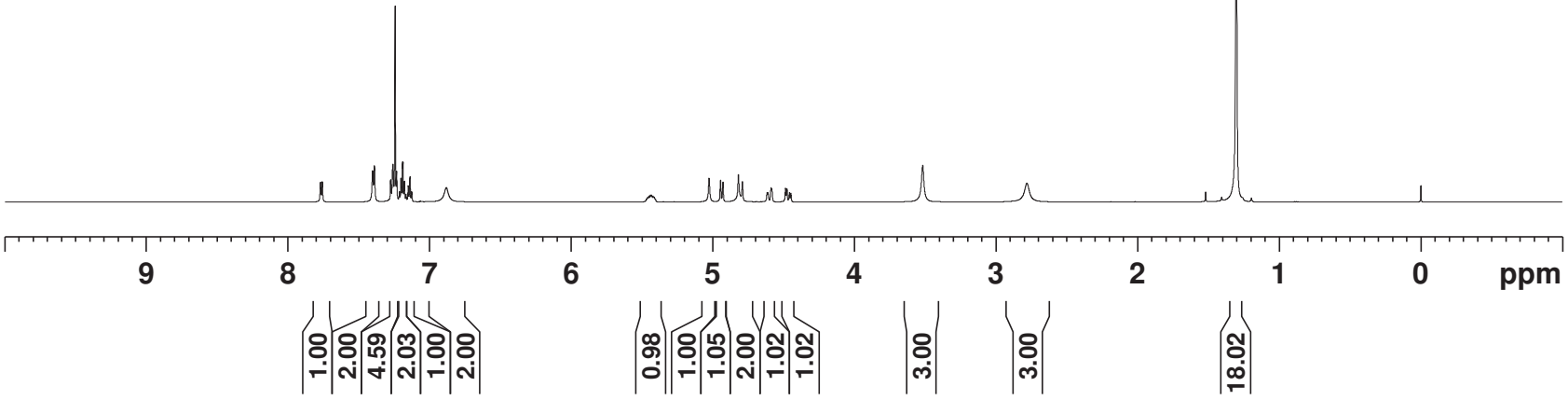


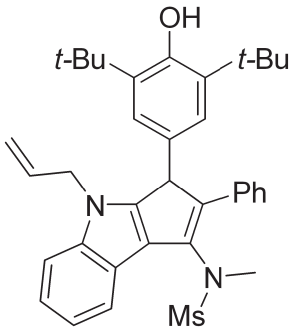




3nd

```
Current Data Parameters
NAME      yuky2472-4 3od
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201120
Time              11.35 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG             zg30
TD                 65536
SOLVENT            CDC13
NS                    16
DS                     2
SWH           11904.762 Hz
FIDRES         0.363304 Hz
AQ            2.7525120 sec
RG               47.619
DW               42.000 usec
DE               13.73 usec
TE               298.1 K
D1            1.00000000 sec
TD0                    1
SFO1         600.1337058 MHz
NUC1                1H
P0                3.94 usec
P1               11.82 usec
PLW1         31.62299919 W

F2 - Processing parameters
SI                 65536
SF           600.1300253 MHz
WDW                   EM
SSB       0
LB                0.30 Hz
GB        0
PC                1.00
```





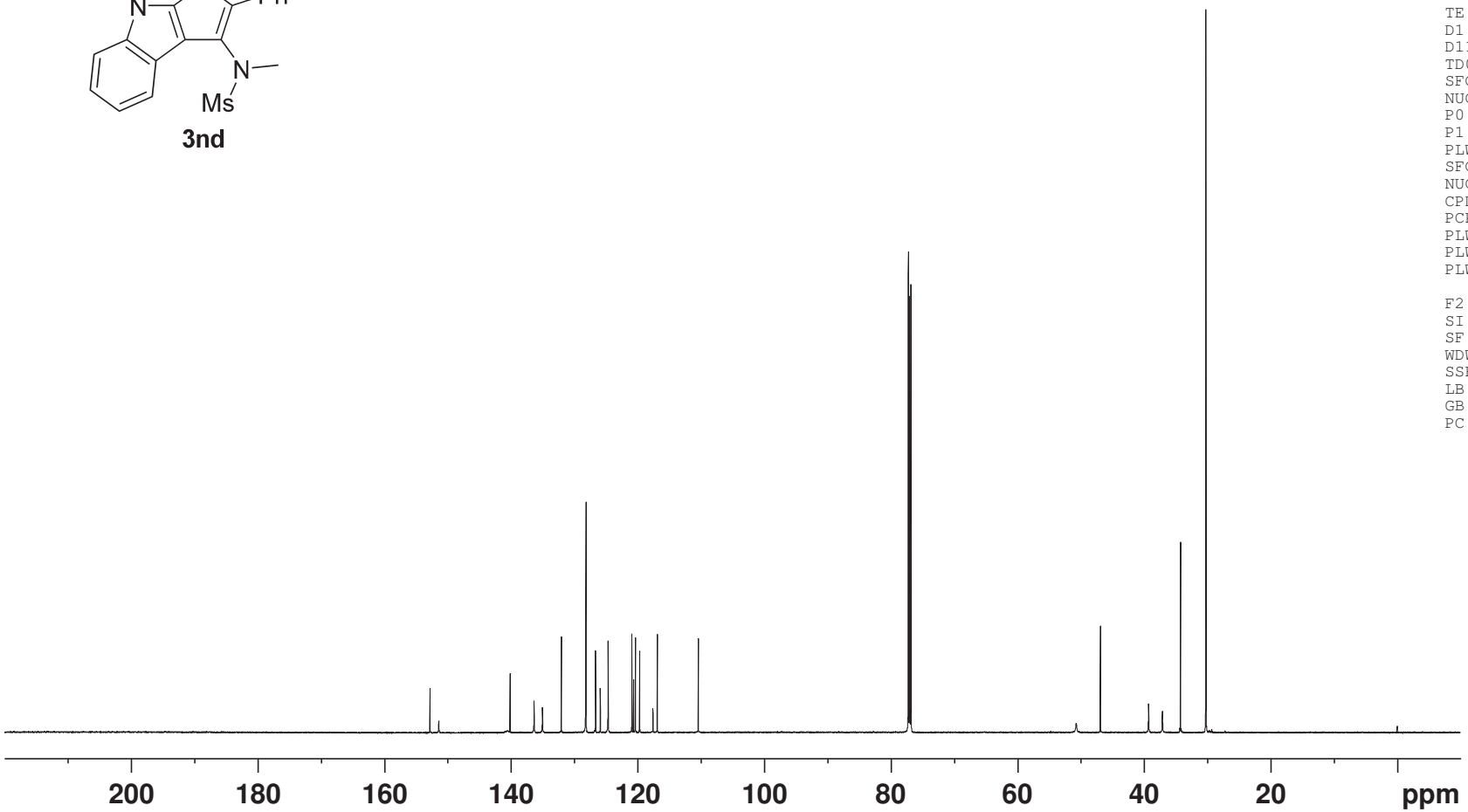
3nd

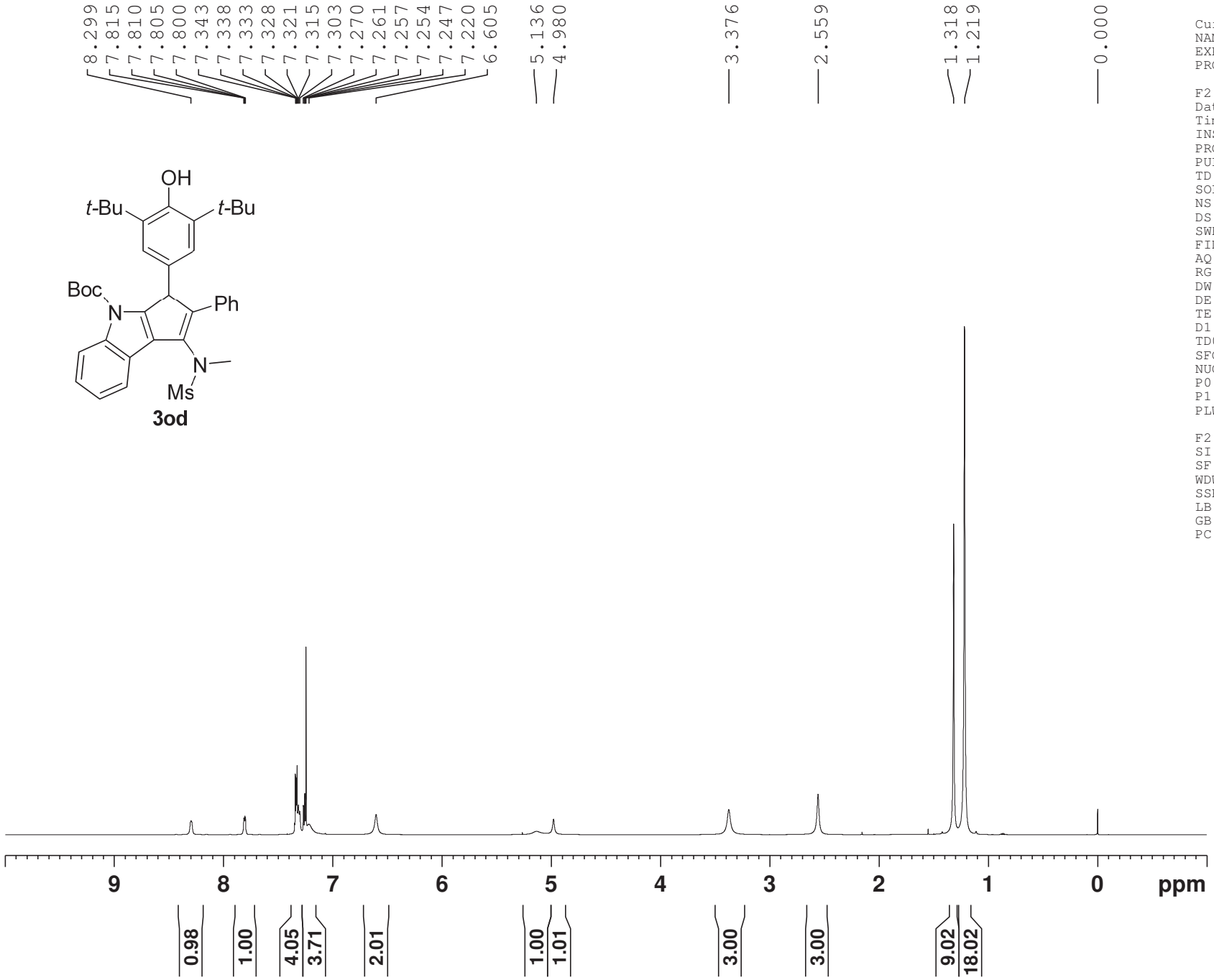
152.78
151.39
140.67
140.10
136.34
135.03
132.01
128.14
126.63
125.87
124.65
120.89
120.60
120.32
119.65
117.55
116.87
110.38

77.21
77.00
76.79

50.68
46.88
39.27
37.07
34.22
30.21

```
Current Data Parameters
NAME      yuky2472-4 3od
EXPNO                12
PROCNO                1

F2 - Acquisition Parameters
Date_          20201120
Time              14.27 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 3500
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1                13C
P0                6.13 usec
P1               18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2            70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028170 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

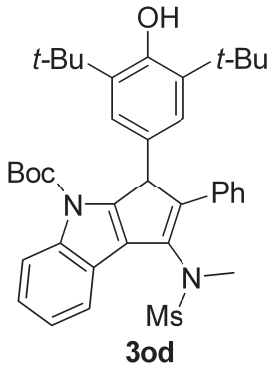




Current Data Parameters
NAME yuky2472-5 3md
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201124
Time 0.58 h
INSTRUM Avance
PROBHD Z168773_0004 (
PULPROG zg30
TD 65536
SOLVENT CDCl3
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 28.8337
DW 42.000 usec
DE 13.73 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.94 usec
P1 11.82 usec
PLW1 31.62299919 W

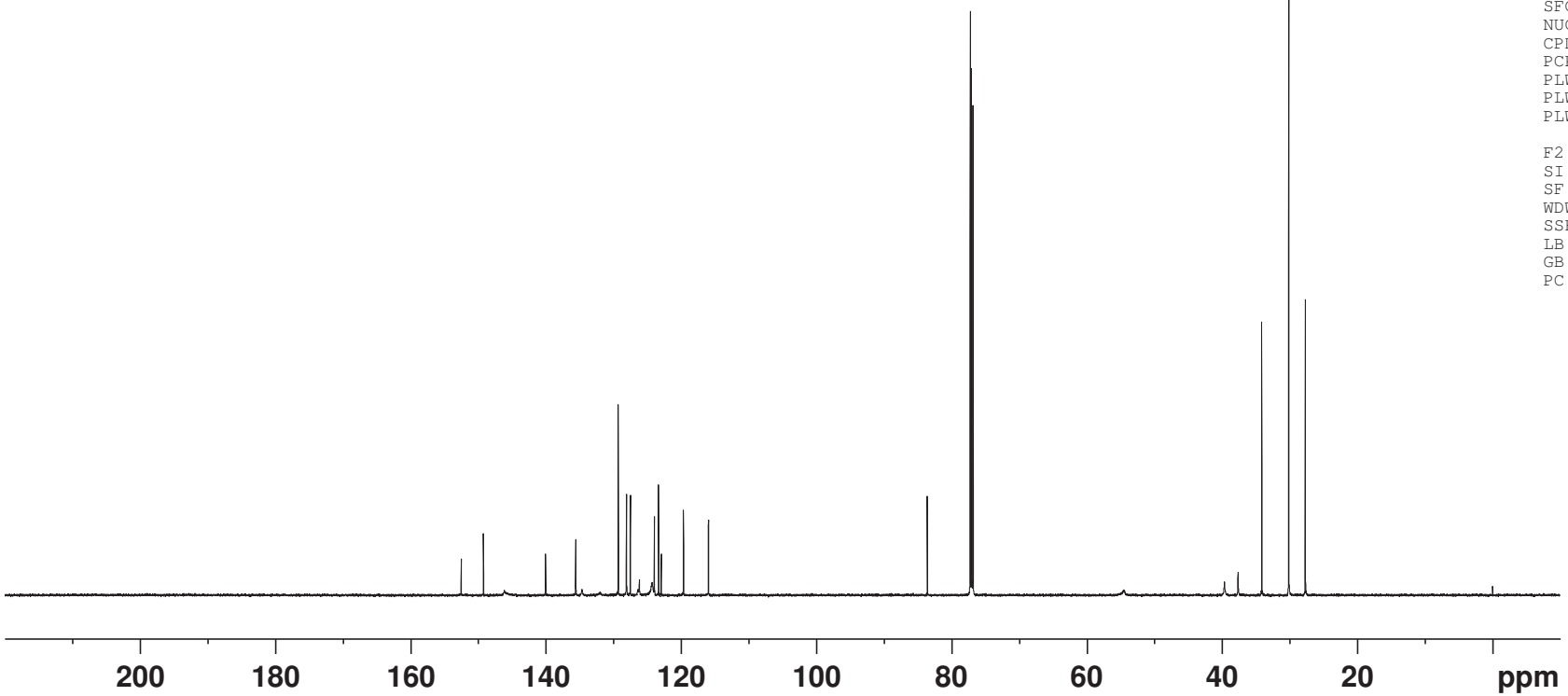
F2 - Processing parameters
SI 65536
SF 600.1300232 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

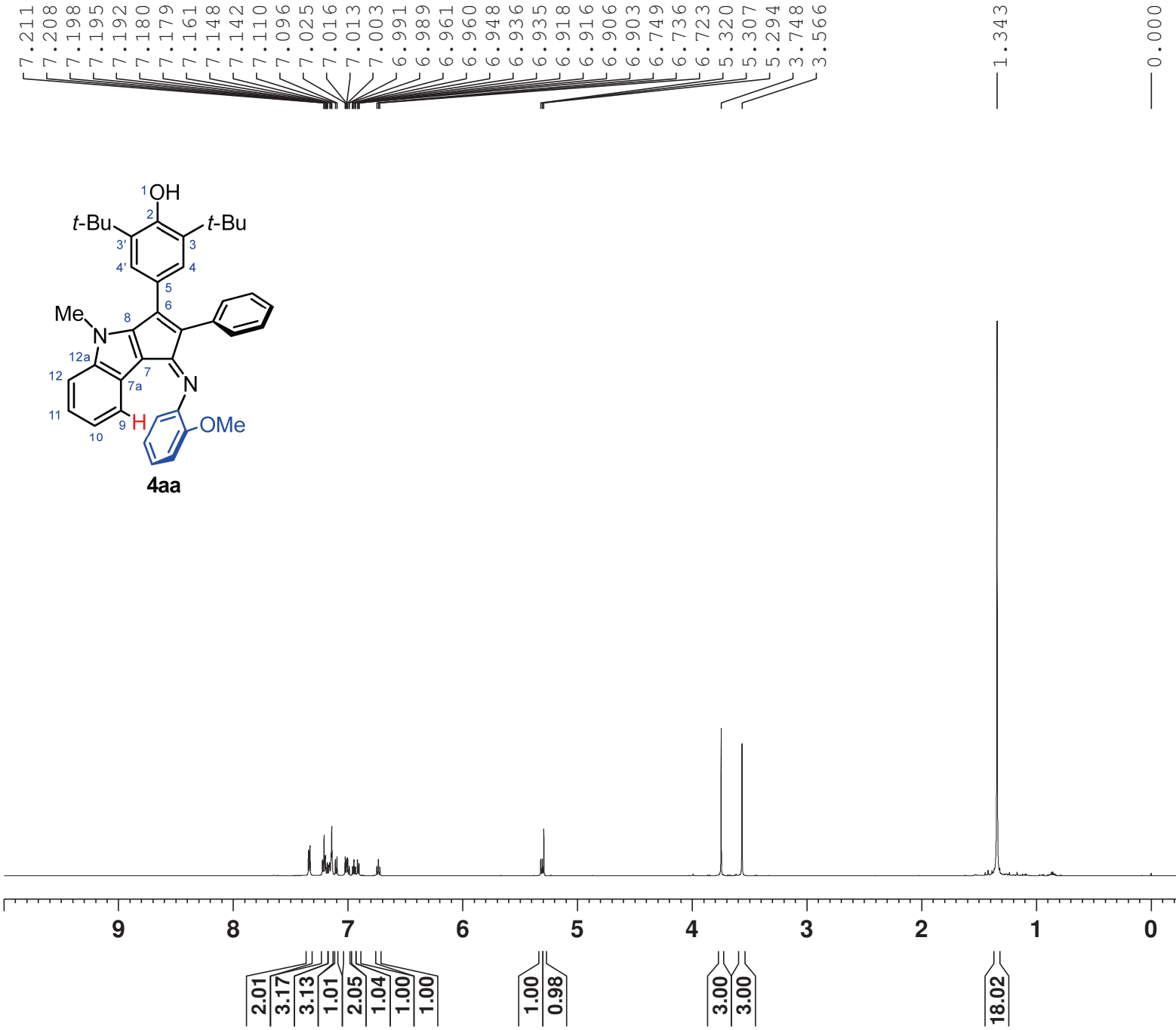


3od

152.50
149.21
146.14
140.03
135.55
134.65
131.96
129.26
128.05
127.49
126.34
126.14
124.29
123.92
123.31
122.91
119.61
115.93
83.56
77.21
77.00
76.79
54.47
39.61
37.60
34.08
30.11
27.65

```
Current Data Parameters
NAME      yuky2472-5 3md
EXPNO                11
PROCNO                1

F2 - Acquisition Parameters
Date_          20201124
Time               2.37 h
INSTRUM          Avance
PROBHD   Z168773_0004 (
PULPROG          zgpg30
TD                65536
SOLVENT           CDCl3
NS                 2000
DS                    4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                  101
DW               13.500 usec
DE               18.00 usec
TE               298.0 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1
SFO1        150.9194079 MHz
NUC1               13C
P0                6.13 usec
P1               18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2               1H
CPDPRG[2        waltz65
PCPD2            70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                32768
SF          150.9028199 MHz
WDW                  EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

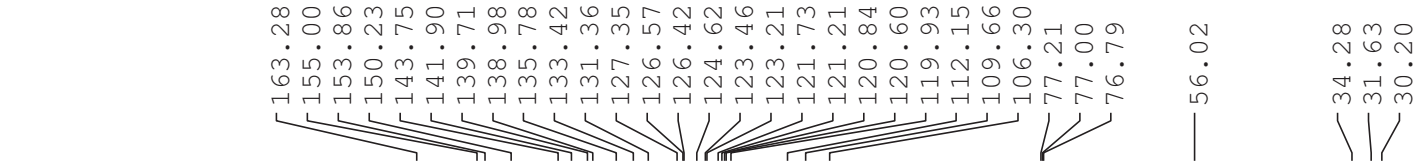


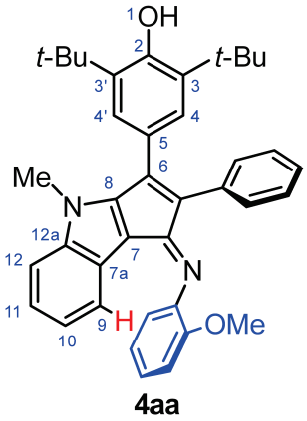


Current Data Parameters
NAME yuky2503
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
Date_ 20201220
Time 5.24 h
INSTRUM Avance
PROBHD Z168773_0004 (
PULPROG zg30
TD 65536
SOLVENT CDC13
NS 16
DS 2
SWH 11904.762 Hz
FIDRES 0.363304 Hz
AQ 2.7525120 sec
RG 24.681
DW 42.000 usec
DE 13.73 usec
TE 298.0 K
D1 1.00000000 sec
TD0 1
SFO1 600.1337058 MHz
NUC1 1H
P0 3.94 usec
P1 11.82 usec
PLW1 31.62299919 W

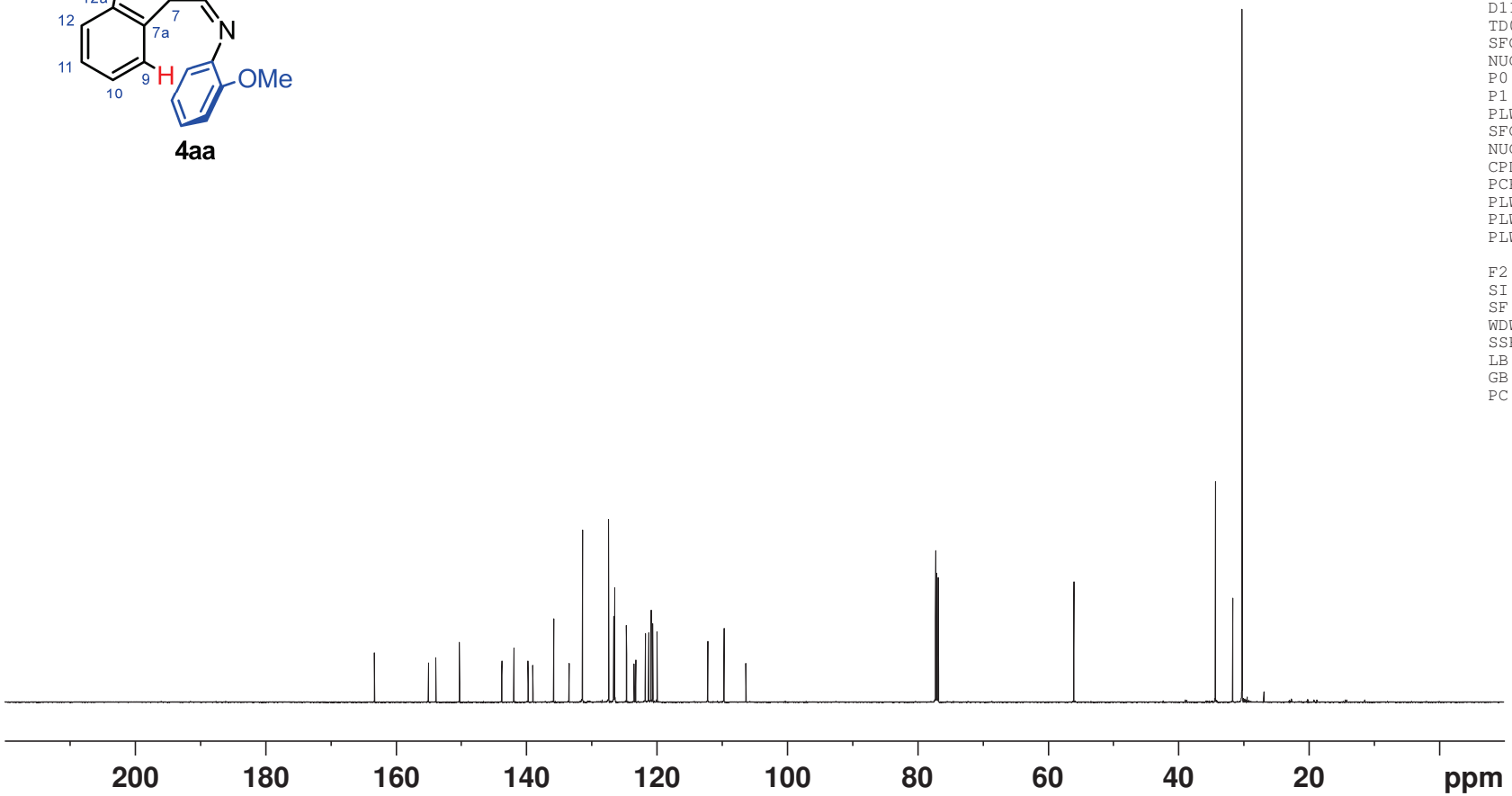
F2 - Processing parameters
SI 65536
SF 600.1300458 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00

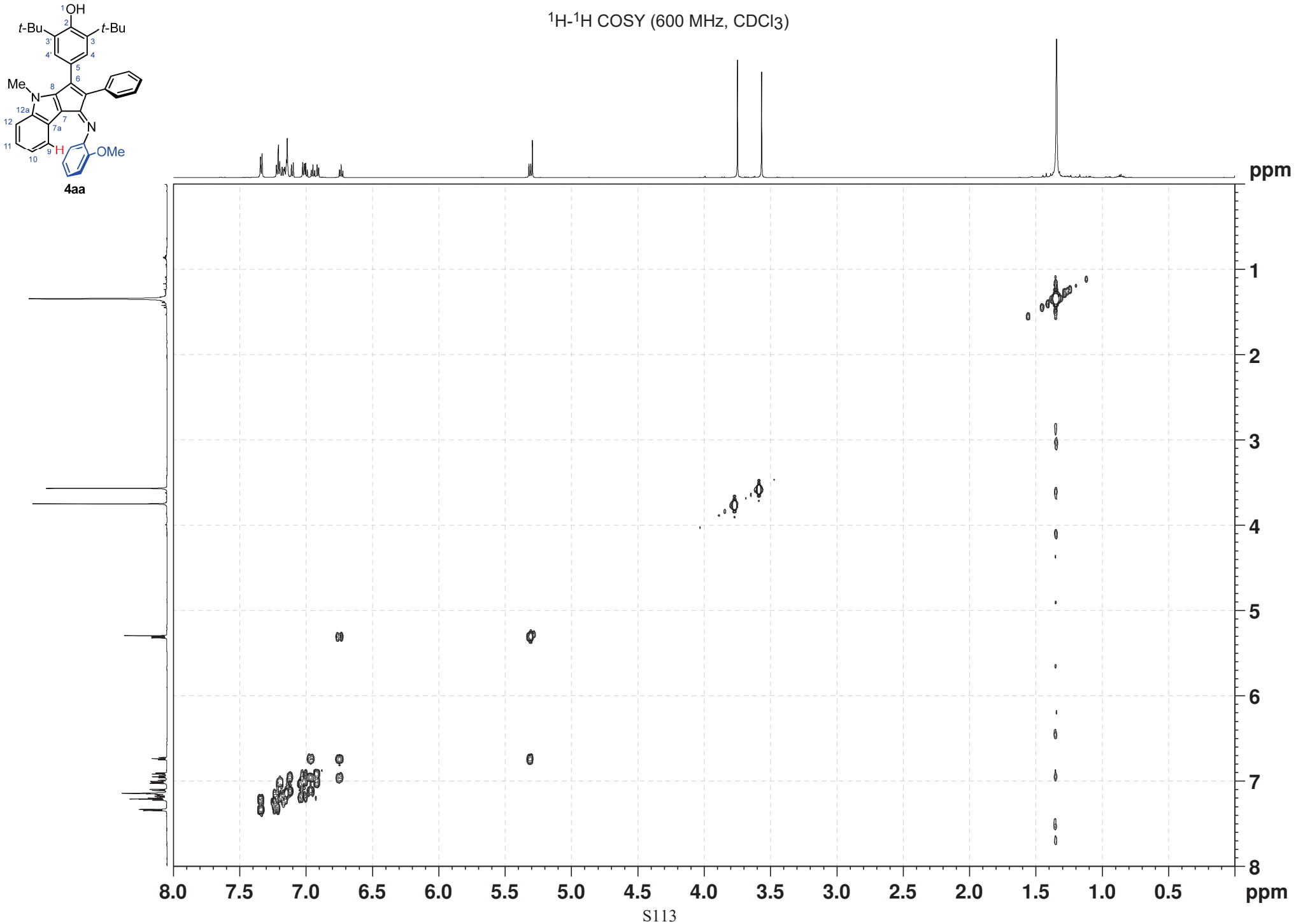


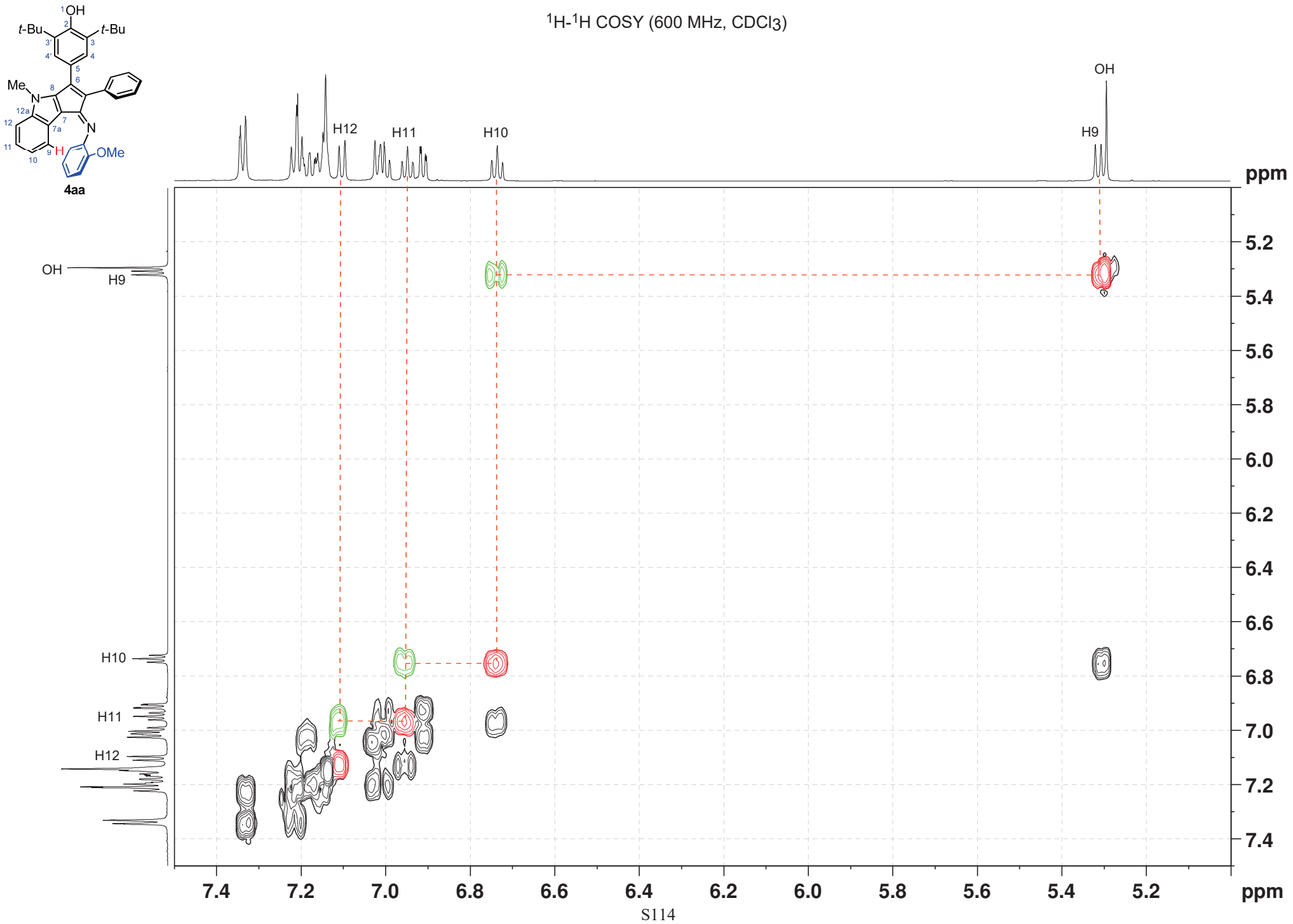


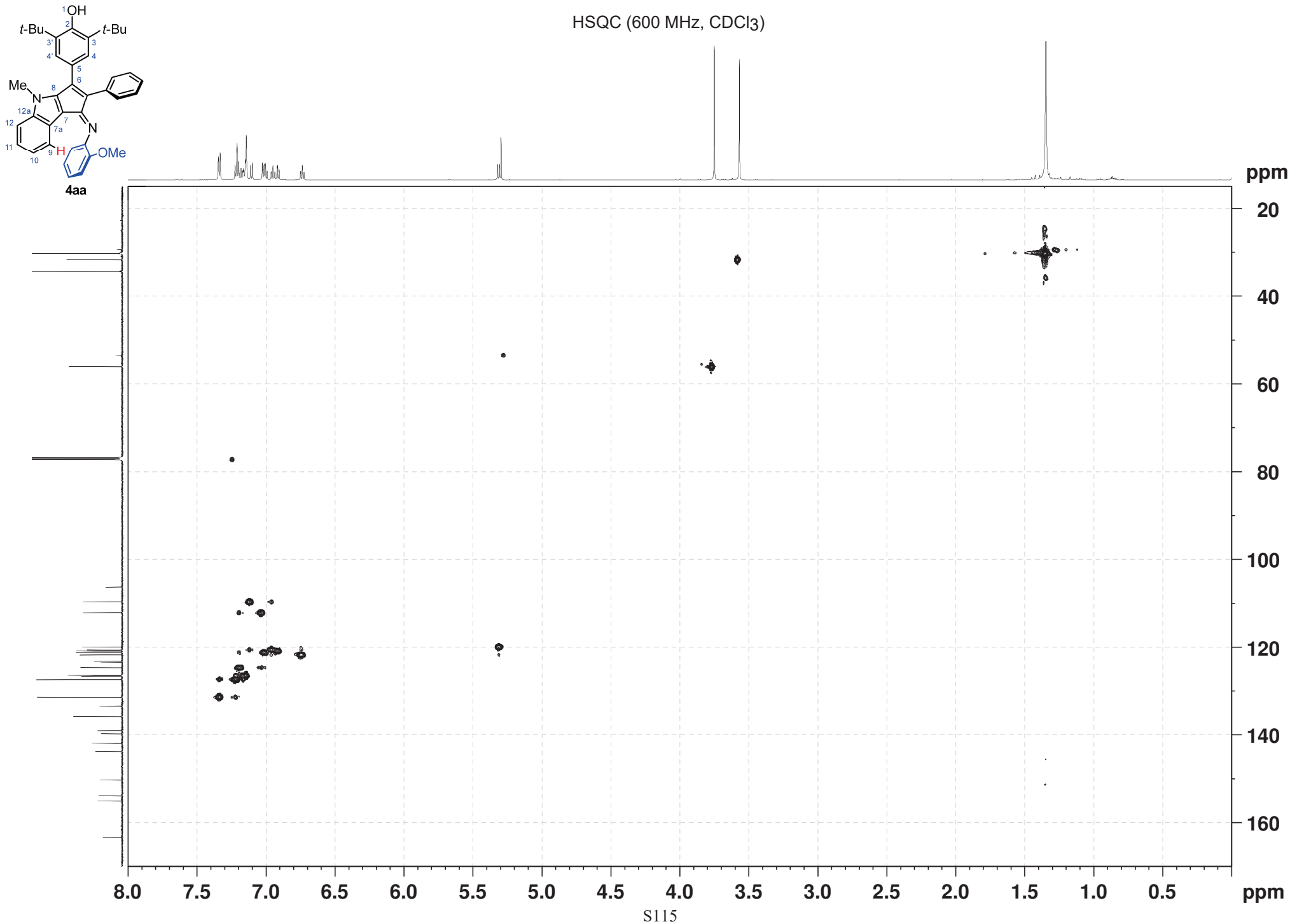
4aa

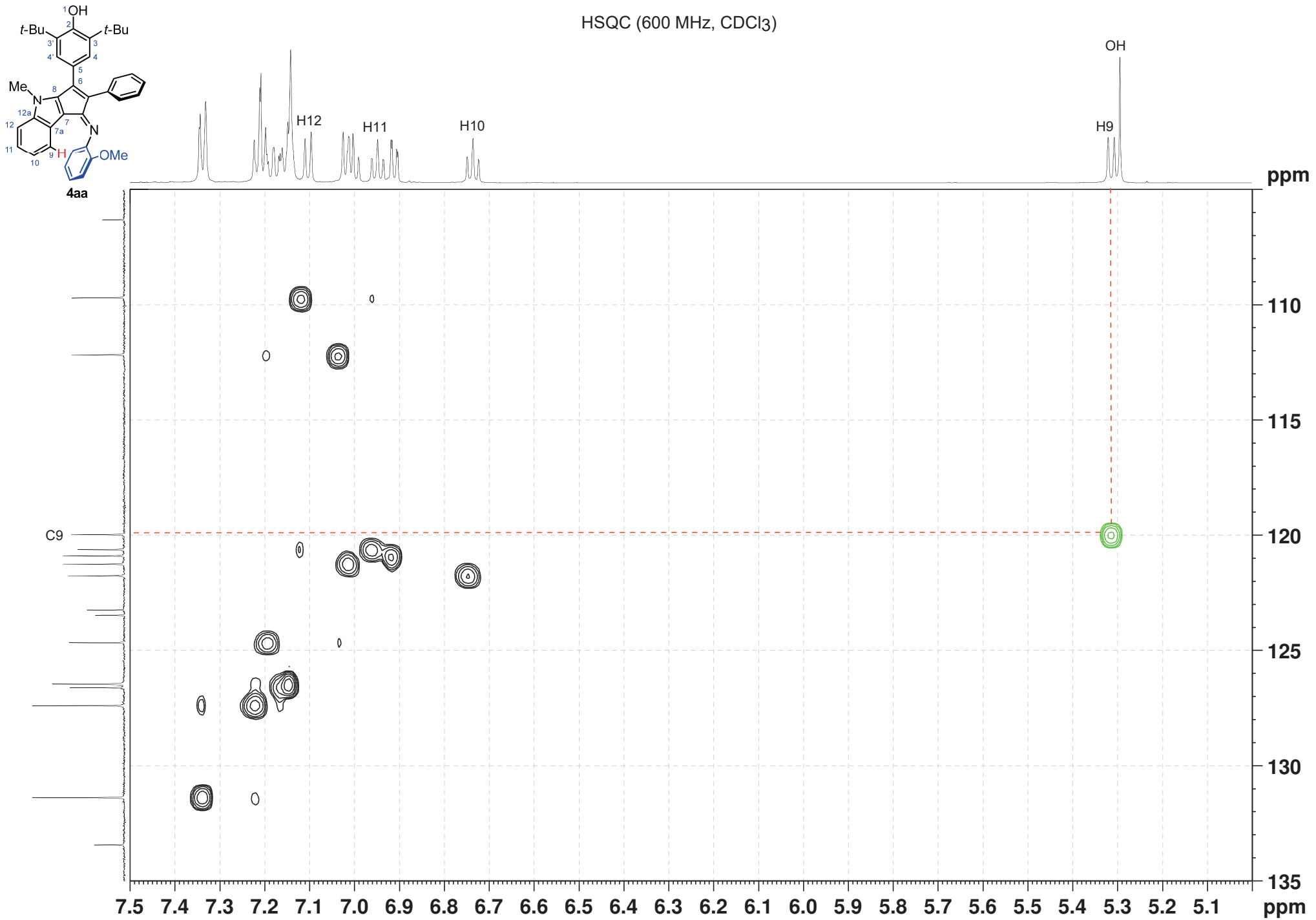
```
Current Data Parameters
NAME            yuky2503
EXPNO                 11
PROCNO                 1

F2 - Acquisition Parameters
Date_           20201220
Time                5.54 h
INSTRUM           Avance
PROBHD   Z168773_0004 (
PULPROG           zgpg30
TD                 65536
SOLVENT            CDCl3
NS                   600
DS                     4
SWH           37037.035 Hz
FIDRES         1.130281 Hz
AQ            0.8847360 sec
RG                   101
DW                13.500 usec
DE                18.00 usec
TE                298.1 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                    1
SFO1        150.9194079 MHz
NUC1                13C
P0                 6.13 usec
P1                18.38 usec
PLW1        76.86299896 W
SFO2        600.1324005 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             70.00 usec
PLW2        31.62299919 W
PLW12        0.94957000 W
PLW13        0.47762999 W

F2 - Processing parameters
SI                 32768
SF          150.9028255 MHz
WDW                   EM
SSB       0
LB                 1.00 Hz
GB        0
PC                 1.40
```

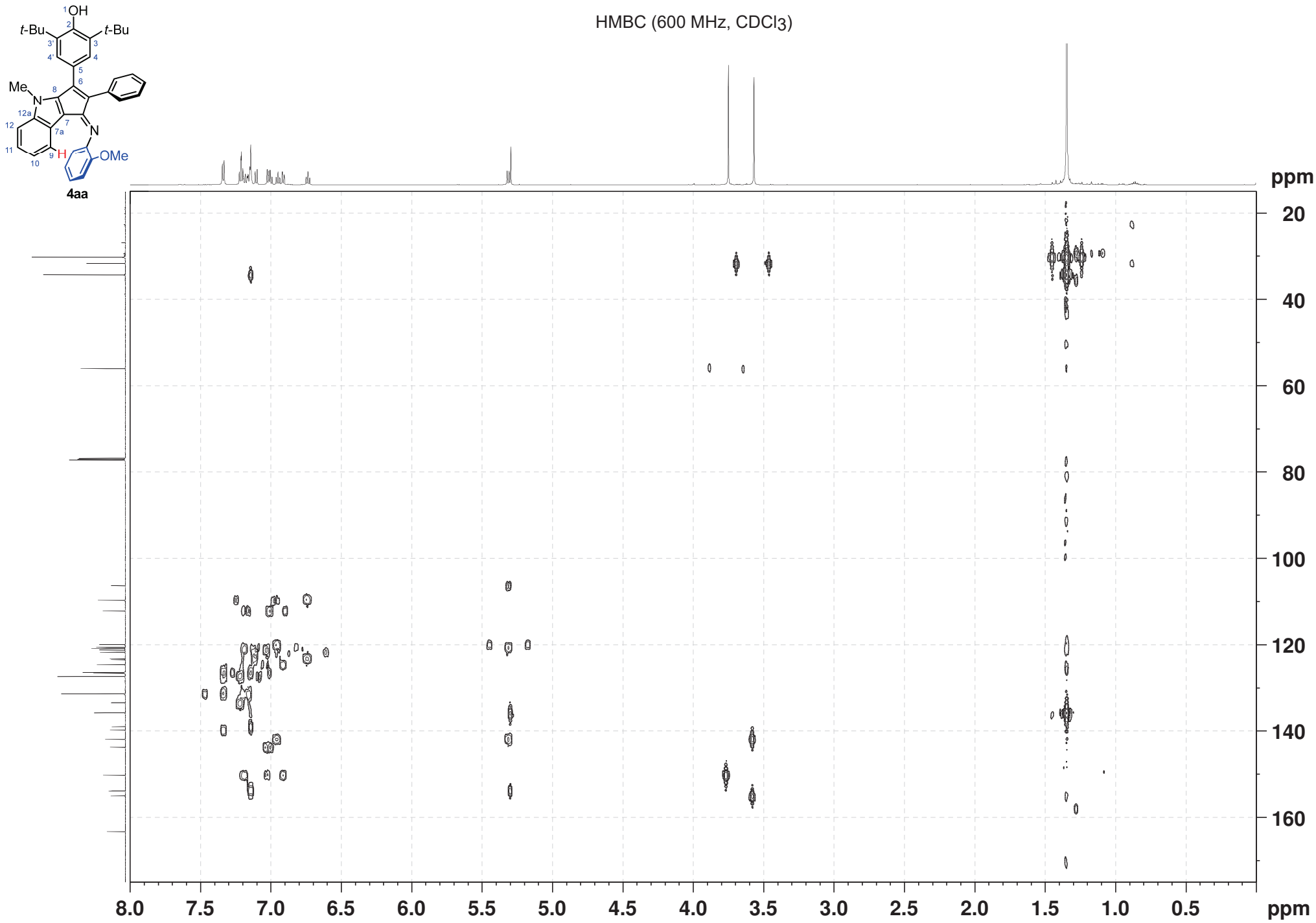


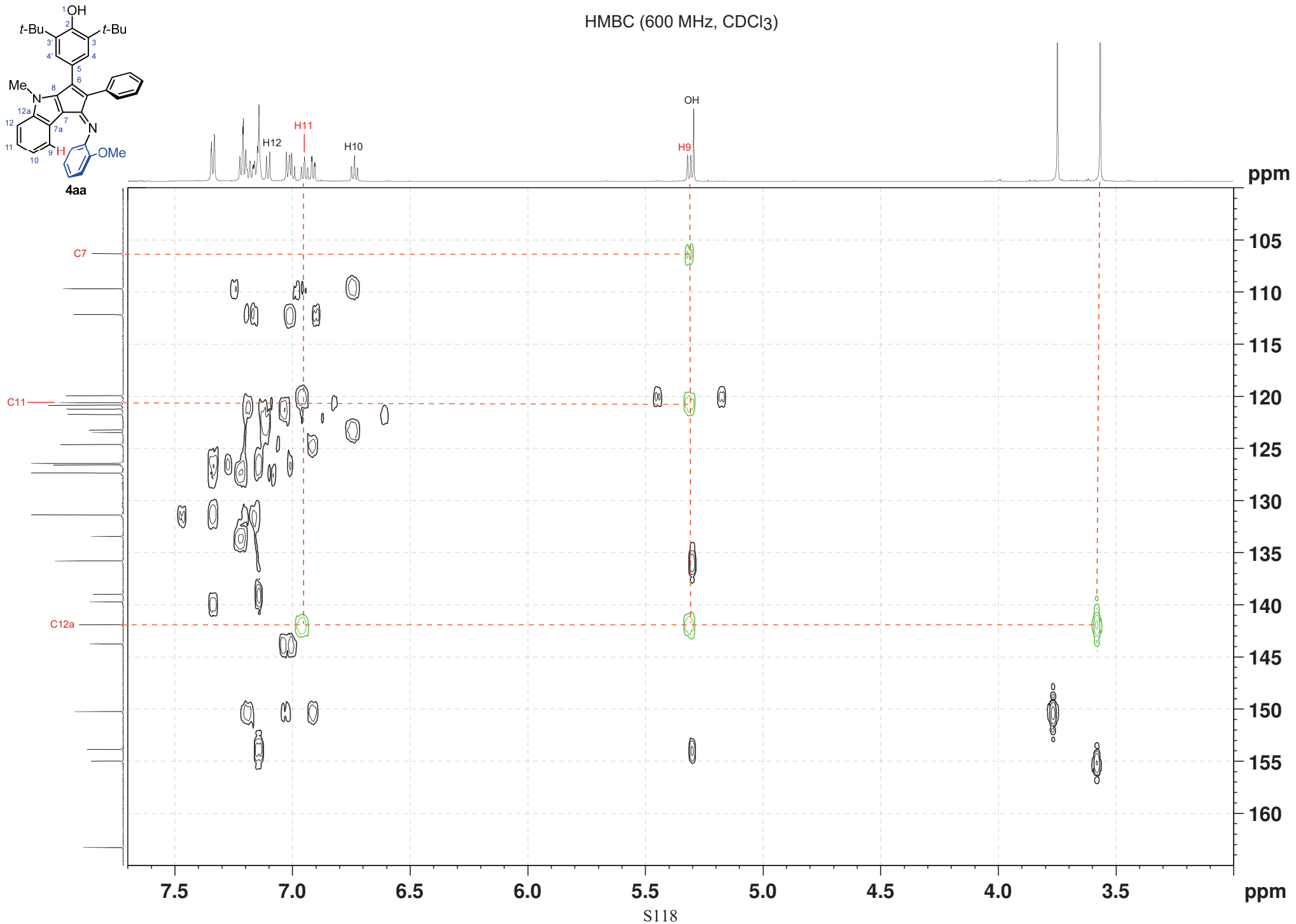

1OH
t-Bu
t-Bu
Me
N
OMe
H
4aa
1H-1H COSY (600 MHz, CDCl3)
ppm
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


^{1}H-^{1}H COSY (600 MHz, CDCl$_3$)
4aa
OH
H12
H11
H10
H9
ppm
7.4
7.2
7.0
6.8
6.6
6.4
6.2
6.0
5.8
5.6
5.4
5.2


HSQC (600 MHz, CDCl3)
4aa
ppm
20
40
60
80
100
120
140
160
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


HSQC (600 MHz, CDCl3)
4aa
H12
H11
H10
H9
OH
C9
ppm
110
115
120
125
130
135
7.5 7.4 7.3 7.2 7.1 7.0 6.9 6.8 6.7 6.6 6.5 6.4 6.3 6.2 6.1 6.0 5.9 5.8 5.7 5.6 5.5 5.4 5.3 5.2 5.1
ppm


HMBC (600 MHz, CDCl3)
4aa
ppm
20
40
60
80
100
120
140
160
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
ppm


HMBC (600 MHz, CDCl3)
4aa
H12
H11
H10
OH
H9
ppm
C7
C11
C12a
105
110
115
120
125
130
135
140
145
150
155
160
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
ppm