Supporting Information

Synthesis of Functionalized Pyrroloindolines via Visible-Light-Induced Radical Cascade Reaction: Rapid Synthesis of (±)-Flustraminol B

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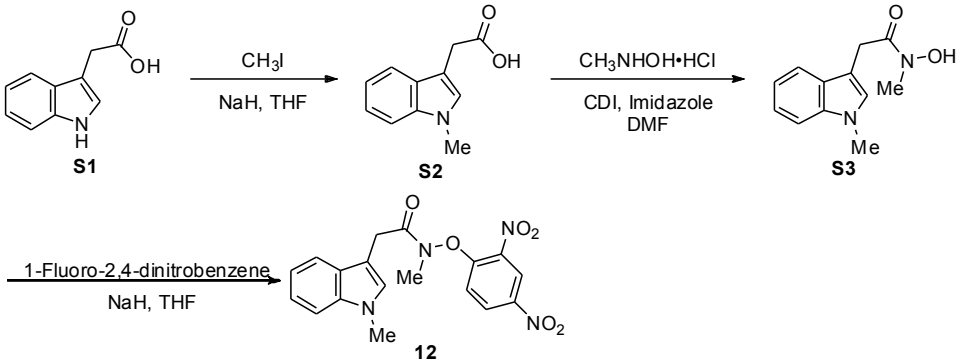
1. General Methods

All commercially available chemicals were used without further purification unless otherwise noted. Reactions were monitored by thin layer chromatography using TLC silica gel 60-F_{254} plates. TLC plates were visualized by UV fluorescence (254 nm) or stained by Cerium Molybdate followed by heating. Purification of the reaction products was carried out by column chromatography using Siliaflash-P60 (40-63 μm) silica gel available from Silicycle. ^{1}H-NMR spectra were recorded on a BRUKER AV-400 (400 MHz) and ^{13}C-NMR spectra were recorded on a BRUKER AV-400 or AV-600 (100 MHz or 150 MHz). Data for ^{1}H-NMR are recorded as follows: chemical shift (δ, ppm), multiplicity (s = singlet, d = doublet, t = triplet, m = multiplet, q = quartet), coupling constant(s) in Hz and integration. Data for ^{13}C-NMR are reported in terms of chemical shift (δ, ppm). IR spectra were recorded on a PerkinElmer Spectrum Two IR spectrometer and only major peaks were reported in cm^{-1}. High-resolution mass spectral analysis (HRMS) data were obtained using Agilent Technologies 6530 Accurate Mass Q-TOF LC/MS. Irradiation of photochemical reactions was carried out using two 6W PAR38 Green LED flood lamps from ABi LED lighting. Yields refer to chromatographically and spectroscopically purified compounds.

2. General procedure for starting materials

For those known starting materials, not described below, please find the syntheses in previous report[1].

2.1 N-(2,4-dinitrophenoxy)-N-methyl-2-(1-methyl-1H-indol-3-yl)acetamide (12)

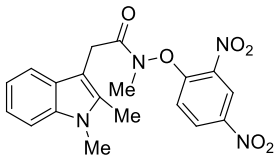


To a solution of indole-3-acetic acid **S1** (15.0 g, 85.7 mmol) in THF (350 mL), NaH (17.1 g, 429 mmol) was added portionwise at 0 °C. The mixture was stirred for 30 minutes and then iodomethane (17.6 mL, 283 mmol) was added dropwise. The reaction was moved to room temperature and the stirring was continued for 16 h. The reaction mixture was then cooled to 0 °C and acidified with 6 N aq. HCl and extracted with EtOAc. The combined organic phase was dried and concentrated. The crude solid was recrystallised from EtOAc/hexane to give the desired product **S2** (15 g, 92%) [2].

The hydroxamic acid **S3** was prepared according to literature's procedure with slight modifications[3]. To a solution of 1-methyl indole-3-acetic acid **S2** (300 mg, 1.6 mmol) in DMF 10 ml, CDI (514 mg, 3.2 mmol) was added in one portion. The mixture was stirred for 30 minutes before hydroxylamine hydrochloric salt (330 mg, 4.7 mmol) and imidazole (108 mg, 1.6 mmol) were added. The reaction was allowed to stir for 12 hours at room temperature and then quenched with water. The mixture was extracted with EtOAc. The extracts were combined, dried and concentrated. The crude oil **S3** was used without further purification.

The obtained hydroxamic acid **S3** was dissolved in THF (15 mL) and cooled to 0 °C. NaH (190 mg, 4.76 mmol) was added portionwise and the mixture was stirred for 1 hour before 1-fluoro-2,4-dinitrobenzene (200 μL, 1.59 mmol) was added. The reaction was moved to room temperature and the stirring was continued for 10 hours. After quenching with water, the mixture was extracted with EtOAc and the combined extracts were dried and concentrated. The residue was purified on silica gel to afford the product **12** (420 mg, 69% over 2 steps); mp 90 ^{o}C.[4] ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.62 (d, *J* = 2.6 Hz, 1H), 7.85 (dd, *J* = 9.3, 2.6 Hz, 1H), 7.42 (d, *J* = 9.3, 1H), 7.14 (dd, *J* = 11.0, 4.1 Hz, 1H), 7.05 – 6.99 (m, 2H), 6.84 (d, *J* = 9.3 Hz, 1H), 6.77 (s, 1H), 3.98 (s, 2H), 3.54 (s, 3H), 3.36 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 155.9, 141.5, 136.3, 135.9, 128.1, 127.5, 127.1, 122.1, 121.3, 119.6, 118.5, 114.3, 109.0, 105.8, 36.2, 32.4, 31.6; ESI HRMS calcd for $C_{18}H_{16}N_4NaO_6$ $[M + Na]^+$ 407.0962, found 407.0962; IR (CH_2Cl_2, cm^{-1}) 1689, 1684, 1533, 1471, 1342, 1254, 1110, 834, 739.

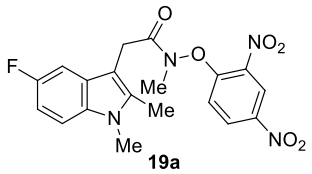
2-(1,2-Dimethyl-1H-indol-3-yl)-N-(2,4-dinitrophenoxy)-N-methylacetamide (18a)



18a

Following the procedure **2.1**, compound **18a** was obtained as yellow solid (61% over 3 steps); mp 130 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.56 (d, *J* = 2.6 Hz, 1H), 7.78 (dd, *J* = 9.3, 2.6 Hz, 1H), 7.31 (d, *J* = 7.8 Hz, 1H), 7.06 (dd, *J* = 7.2, 6.6 Hz, 1H), 7.00 – 6.89 (m, 2H), 6.64 (d, *J* = 9.3 Hz, 1H), 3.94 (s, 2H), 3.41 (s, 3H), 3.33 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.2, 156.0, 141.3, 135.8, 135.4, 134.0, 127.7, 126.8, 121.2, 121.2, 119.7, 117.5, 114.1, 108.3, 102.6, 36.1, 31.6, 29.3, 10.1; HRMS calcd for $C_{19}H_{18}N_4O_6$ $[M + Na]^+$ 421.1119, found 421.1119; IR (CH_2Cl_2, cm^{-1}) 1684, 1604, 1531, 1471, 1341, 1252, 1111, 737.

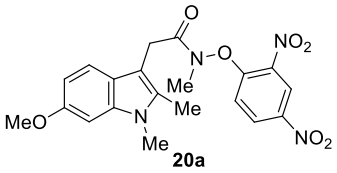
N-(2,4-dinitrophenoxy)-2-(5-fluoro-1,2-dimethyl-1H-indol-3-yl)-N-methylacetamide (19a)



19a

Following the procedure **2.1**, compound **19a** was obtained as yellow solid (57% over 3 steps); mp 145 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, *J* = 2.5 Hz, 1H), 7.93 – 7.88 (m, 1H), 6.99 (dd, *J* = 9.5, 1.9 Hz, 1H), 6.90 (dd, *J* = 8.7, 4.2 Hz, 1H), 6.81 (dd, *J* = 13.8, 5.7 Hz, 2H), 3.88 (s, 2H), 3.42 (s, 3H), 3.34 (s, 3H), 2.21 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.7, 158.9, 156.6, 155.9, 141.6, 136.0, 132.6, 128.1, 127.2, 127.1, 121.4, 114.5, 109.3, 109.1, 109.1, 109.0, 102.9, 102.7, 102.6, 36.2, 31.3, 29.5, 10.3; HRMS calcd for $C_{19}H_{17}FN_4O_6$ $[M + Na]^+$ 439.1024, found 439.1021; IR (CH_2Cl_2, cm^{-1}) 1684, 1605, 1534, 1486, 1343, 1143, 739.

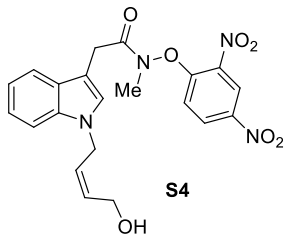
N-(2,4-dinitrophenoxy)-2-(6-methoxy-1,2-dimethyl-1H-indol-3-yl)-N-methylacetamide (20a)



20a

Following the procedure **2.1**, compound **20a** was obtained as yellow solid (67% over 3 steps); mp 90 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.54 (d, *J* = 2.6 Hz, 1H), 7.78 (dd, *J* = 9.3, 2.6 Hz, 1H), 7.14 (d, *J* = 8.6 Hz, 1H), 6.64 (d, *J* = 9.3 Hz, 1H), 6.59 (dd, *J* = 8.6, 2.1 Hz, 1H), 6.34 (d, *J* = 1.6 Hz, 1H), 3.86 (s, 2H), 3.77 (s, 3H), 3.31 (s, 6H), 2.15 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.1, 156.1, 156.0, 141.2, 136.5, 135.3, 132.7, 127.7, 121.2, 121.1, 118.1, 114.2, 109.2, 102.4, 92.1, 77.5, 77.3, 77.1, 76.8, 36.1, 31.6, 29.2, 10.0; HRMS calcd for $C_{20}H_{20}N_4O_7$ $[M + Na]^+$ 451.1224, found 451.1224; IR (CH_2Cl_2, cm^{-1}) 1684, 1605, 1532, 1489,1342, 1254, 1228, 1114, 833, 738.

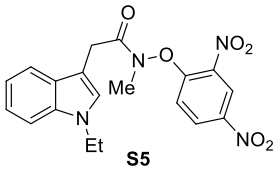
(Z)-N-(2,4-dinitrophenoxy)-2-(1-(4-hydroxybut-2-en-1-yl)-1H-indol-3-yl)-N-methylacetamide (S4)



S4

Following the procedure **2.1**, compound **S4** was obtained as yellow solid (55% over 3 steps); mp 85 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 2.5 Hz, 1H), 7.93 (dd, *J* = 9.3, 2.5 Hz, 1H), 7.44 (t, *J* = 7.2 Hz, 1H), 7.14 – 6.98 (m, 3H), 6.92 – 6.83 (m, 2H), 5.79 – 5.66 (m, 2H), 4.53 – 4.42 (m, 2H), 4.13 (s, 2H), 3.95 (d, *J* = 11.4 Hz, 2H), 3.34 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.5, 155.9, 141.4, 135.9, 135.7, 132.8, 128.5, 127.4, 126.3, 125.4, 122.1, 121.6, 119.7, 118.6, 114.3, 109.3, 106.2, 62.3, 47.5, 36.1, 31.5; HRMS calcd for $C_{21}H_{20}N_4O_7$ $[M + Na]^+$ 463.1224, found 463.1223; IR (CH_2Cl_2, cm^{-1}) 1687, 1605, 1533, 1468, 1343, 1256, 1111, 1065, 740.

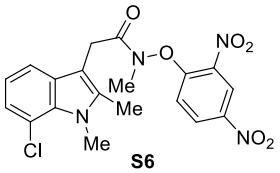
N-(2,4-dinitrophenoxy)-2-(1-ethyl-1H-indol-3-yl)-N-methylacetamide (S5)



S5

Following the procedure **2.1**, compound **S5** was obtained as dark yellow oil (66% over 3 steps). ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.61 (d, *J* = 2.6 Hz, 1H), 7.85 (dd, *J* = 9.3, 2.6 Hz, 1H), 7.43 (d, *J* = 7.9 Hz, 1H), 7.17 – 7.09 (m, 1H), 7.06 (d, *J* = 8.0 Hz, 1H), 7.01 (t, *J* = 7.4 Hz, 1H), 6.85 (s, 1H), 6.82 (d, *J* = 9.3 Hz, 1H), 3.99 (s, 2H), 3.91 (q, *J* = 7.3 Hz, 2H), 3.35 (s, 3H), 1.31 (t, *J* = 7.3 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 176.0, 156.0, 141.4, 135.9, 135.4, 128.2, 127.3, 125.7, 121.9, 121.4, 119.5, 118.6, 114.2, 109.0, 105.8, 40.6, 36.1, 31.7, 15.4; ESI HRMS calcd for $C_{19}H_{18}N_4O_6$ $[M + Na]^+$ 421.1119, found 421.1120; IR (CH_2Cl_2, cm^{-1}) 1688, 1604, 1530, 1467, 1339, 1108, 1063, 735.

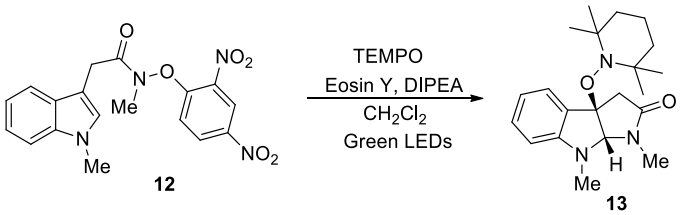
2-(7-Chloro-1,2-dimethyl-1H-indol-3-yl)-N-(2,4-dinitrophenoxy)-N-methylacetamide (S6)



S6

Following the procedure **2.1**, compound **S6** was obtained as yellow solid (64% over 3 steps); mp 95 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.63 (d, *J* = 2.6 Hz, 1H), 8.01 – 7.89 (m, 1H), 7.18 (d, *J* = 7.7 Hz, 1H), 6.97 (d, *J* = 7.1 Hz, 1H), 6.83 (t, *J* = 7.7 Hz, 1H), 6.72 (d, *J* = 9.3 Hz, 1H), 3.91 (s, 2H), 3.80 (s, 3H), 3.33 (s, 3H), 2.23 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.8, 155.8, 141.4, 136.1, 135.29, 131.0, 129.6, 127.8, 122.9, 121.3, 120.3, 116.1, 116.1, 113.8, 103.4, 36.2, 32.1, 31.4, 10.5; HRMS calcd for $C_{19}H_{17}ClN_4O_6$ $[M + Na]^+$ 455.0729, found 455.0725; IR (CH_2Cl_2, cm^{-1}) 1683, 1604, 1530, 1304, 1111, 1066, 734.

3. Radical Process Verified Using TEMPO to Trap C3a Radical



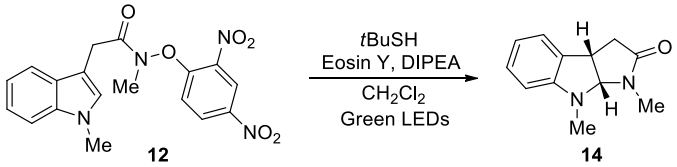
12 **13**

To a solution of indol-3-yl acetamide **12** (38.4 mg, 0.1 mmol) and TEMPO (31 mg, 0.2 mmol) in CH_2Cl_2 (0.1 M) in a vial was added Eosin Y (2 mol %). Nitrogen was bubbled through the solution for 5 minutes. DIPEA (35 μL, 0.2 mmol) was added via syringe and nitrogen was bubbled through the solution for another 10 minutes. The vial was then capped and irradiated under green LEDs for 10 hours. The reaction mixture was concentrated and directly purified on silica gel to give the TEMPO derivative **13** as colorless oil (29 mg, 79%). ^{1}H NMR (400 MHz,

$CDCl_3$) δ7.26 (d, *J* = 8.0 Hz, 1H), 7.19 (td, *J* = 8.0, 1.2 Hz, 1H), 6.79 (td, *J* = 7.5, 0.8 Hz, 1H), 6.46 (d, *J* = 8.0 Hz, 1H), 5.77 (s, 1H), 3.30 – 3.19 (m, 1H), 3.09 (s, 3H), 2.99 (s, 3H), 2.96 – 2.86 (m, 1H), 1.55 – 1.27 (m, 6H), 1.13 (s, 3H), 0.99 (s, 3H), 0.37 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.5, 150.69, 132.8, 129.9, 124.1, 118.9, 108.1, 88.1, 86.8, 60.0, 59.3, 46.6, 40.8, 40.3, 36.7, 33.3, 32.9, 28.3, 20.6, 20.3, 16.9; ESI HRMS calcd for $C_{21}H_{31}N_3NaO_2$ $[M + Na]^+$ 380.2308, found 380.2310; IR (CH_2Cl_2, cm^{-1}) 2927, 1696, 1609, 1492, 1288, 1260, 974, 744.

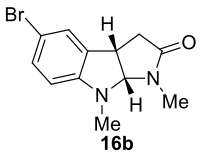
4. General Procedure for Photocatalytic Cyclization

4.1. 1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (14)



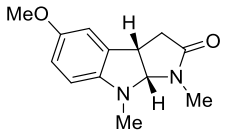
To a solution of indol-3-yl acetamide **12** (38.4 mg, 0.1 mmol) and *t*-BuSH (20 mg, 0.2 mmol) in CH_2Cl_2 (0.1 M) in a vial was added Eosin Y (2 mol %). Nitrogen was bubbled through the solution for 5 minutes. DIPEA (35 μL, 0.2 mmol) was added via syringe and nitrogen was bubbled through the solution for another 10 minutes. The vial was then capped and irradiated under green LED for 10 hours. The reaction mixture was concentrated and directly purified on silica gel to give the title compound **(14)** as colorless solid (16 mg, 78%); mp 130 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (t, *J* = 7.7 Hz, 1H), 7.06 (d, *J* = 7.3 Hz, 1H), 6.74 (t, *J* = 7.4 Hz, 1H), 6.47 (d, *J* = 7.8 Hz, 1H), 5.07 (d, *J* = 8.0 Hz, 1H), 4.07 – 3.97 (m, 1H), 3.07 (s, 3H), 2.94 (s, 3H), 2.92 – 2.85 (m, 1H), 2.59 (dd, *J* = 17.2, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.4, 150.2, 131.0, 128.7, 124.1, 118.7, 107.5, 85.8, 38.5, 36.8, 35.7, 28.4; ESI HRMS calcd for $C_{12}H_{14}N_2O$ $[M + Na]^+$ 225.0998, found 225.1002; IR (CH_2Cl_2, cm^{-1}) 2923, 1679, 1605, 1492, 1398, 1286, 1227, 1006, 745, 694, 662, 593.

5-Bromo-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (16b)



Following the procedure **4.1**, compound **16a** (46.2 mg) gave **16b** as yellowish solid (19.2 mg, 68%) mp 90 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.22 (d, *J* = 8.3 Hz, 1H), 7.14 (s, 1H), 6.31 (d, *J* = 8.3 Hz, 1H), 5.08 (d, *J* = 8.0 Hz, 1H), 4.05 – 3.93 (m, 1H), 3.05 (s, 3H), 2.94 (s, 3H), 2.88 (dd, *J* = 17.3, 10.1 Hz, 1H), 2.55 (dd, *J* = 17.3, 3.2 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.1, 149.3, 133.2, 131.3, 127.1, 110.2, 108.7, 85.7, 38.3, 36.5, 35.5, 28.5; ESI HRMS calcd for $C_{12}H_{13}BrN_2O$ $[M + Na]^+$ 303.0103, found 303.0101; IR (CH_2Cl_2, cm^{-1}) 1674, 1601, 1491,1419, 1398, 1271, 1228, 1086, 1007, 804.

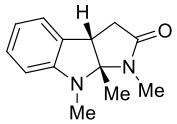
5-Methoxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (17b)



17b

Following the procedure **4.1**, compound **17a** (41.4 mg) gave **17b** as yellowish solid (18.3 mg, 79%); mp 108 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.77 – 6.65 (m, 2H), 6.42 (d, *J* = 8.3 Hz, 1H), 5.00 (d, *J* = 8.0 Hz, 1H), 4.08 – 3.94 (m, 1H), 3.74 (s, 3H), 3.01 (s, 3H), 2.92 (d, *J* = 7.1 Hz, 3H), 2.91 – 2.82 (m, 1H), 2.55 (dd, *J* = 17.2, 3.1 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 173.2, 153.7, 144.7, 132.6, 113.4, 111.3, 108.8, 86.7, 56.0, 38.8, 37.3, 36.7, 28.2; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ $[M + Na]^+$ 255.1104, found 255.1102; IR (CH_2Cl_2, cm^{-1}) 1676, 1493, 1422, 1275, 1226, 1027, 1007, 974, 803, 712.

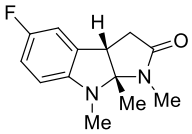
1,8,8a-Trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (18b)



18b

Following the procedure **4.1**, compound **18a** (39.8 mg) gave **18b** as yellowish oil (17.7 mg, 82%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (t, *J* = 7.7 Hz, 1H), 7.04 (d, *J* = 7.2 Hz, 1H), 6.71 (t, *J* = 7.4 Hz, 1H), 6.37 (d, *J* = 7.8 Hz, 1H), 3.61 (d, *J* = 9.0 Hz, 1H), 2.98 (s, 3H), 2.90 (dd, *J* = 17.0, 9.1 Hz, 1H), 2.84 (s, 3H), 2.66 (d, *J* = 17.1 Hz, 1H), 1.63 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 149.6, 129.6, 128.7, 123.9, 118.1, 106.0, 87.3, 46.4, 36.2, 30.0, 26.0, 20.3; ESI HRMS calcd for $C_{13}H_{16}N_2O$ $[M + Na]^+$ 239.1155, found 239.1154; IR (CH_2Cl_2, cm^{-1}) 1672, 1607, 1492, 1417, 1393, 1110, 1090, 796, 691.

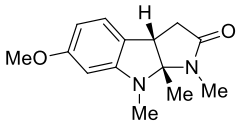
5-Fluoro-1,8,8a-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (19b)



19b

Following the procedure **4.1**, compound **19a** (41.6 mg) gave **19b** as yellowish oil (18.2 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 – 6.71 (m, 2H), 6.22 (dd, *J* = 8.4, 4.0 Hz, 1H), 3.56 (dd, *J* = 15.7, 7.6 Hz, 1H), 2.92 (s, 3H), 2.90 – 2.82 (m, 1H), 2.80 (s, 3H), 2.58 (dd, *J* = 17.0, 2.1 Hz, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 157.7, 155.3, 145.9, 131.0, 130.9, 114.5, 114.3, 111.8, 111.5, 106.1, 106.0, 87.8, 46.3, 46.3, 35.9, 30.4, 26.0, 20.2; ESI HRMS calcd for $C_{13}H_{15}FN_2O$ $[M + Na]^+$ 257.1061, found 257.1060; IR (CH_2Cl_2, cm^{-1}) 1680, 1494, 1393, 1268, 1235, 1113, 1089, 889.

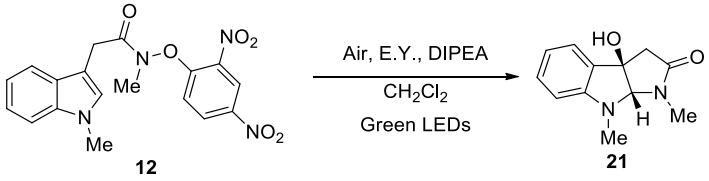
6-Methoxy-1,8,8a-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (20b)



20b

Following the procedure **4.1**, compound **20a** (42.8 mg) gave **20b** as yellowish oil (18.5 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (dd, *J* = 8.0, 1.0 Hz, 1H), 6.21 (dd, *J* = 8.0, 2.2 Hz, 1H), 5.94 (d, *J* = 2.2 Hz, 1H), 3.76 (s, 3H), 3.54 (t, *J* = 13.1 Hz, 1H), 2.95 (s, 3H), 2.87 (dd, *J* = 17.4, 8.5 Hz, 1H), 2.82 (s, 3H), 2.64 – 2.54 (m, 1H), 1.59 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.7, 161.1, 150.9, 124.1, 122.0, 101.8, 93.7, 87.9, 55.4, 45.7, 36.4, 29.9, 25.9, 20.3; ESI HRMS calcd for $C_{14}H_{18}N_2O_2$ $[M + Na]^+$ 269.1260, found 269.1261; IR (CH_2Cl_2, cm^{-1}) 1676, 1619, 1501, 1389, 1229, 1084, 945, 816, 729, 688.

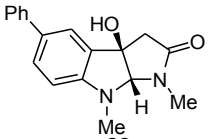
4.2. 3a-hydroxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (21)



12 **21**

To a solution of indol-3-yl acetamide **12** (38.4 mg, 0.1 mmol) in CH_2Cl_2 (0.1 M) in a vial was added Eosin Y (2 mol %). DIPEA (35 μL, 0.2 mmol) was added via syringe and then irradiated under green LED in the open air for 10 hours. The reaction mixture was concentrated and directly purified on silica gel to give the title compound **(21)** as white solid (17 mg, 75%); mp 85 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 – 7.24 (m, 2H), 6.82 (td, *J* = 7.4, 0.7 Hz, 1H), 6.56 (d, *J* = 7.9 Hz, 1H), 4.78 (s, 1H), 3.10 (s, 3H), 2.95 (s, 3H), 2.93 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 150.0, 131.2, 130.9, 123.6, 119.2, 108.6, 92.5, 80.0, 43.5, 36.0, 28.1; ESI HRMS calcd for $C_{12}H_{14}N_2O_2$ $[M + Na]^+$ 241.0947, found 241.0948; IR (CH_2Cl_2, cm^{-1}) 3331, 2723, 1666, 1609, 1492, 1398,1281, 1083, 987, 746.

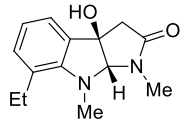
3a-Hydroxy-1,8-dimethyl-5-phenyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (22)



22

Following the procedure **4.2**, 46.0 mg starting material gave **22** as yellowish oil (22.9 mg, 78%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (d, *J* = 7.4 Hz, 1H), 6.75 (d, *J* = 7.4 Hz, 1H), 4.63 (s, 1H), 3.48 (s, 1H), 3.13 (s, 3H), 3.00 (dt, *J* = 15.7, 8.0 Hz, 1H), 2.94 – 2.76 (m, 8H), 2.06 (ddt, *J* = 37.7, 20.8, 8.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 148.7, 146.8, 130.6, 126.9, 121.9, 116.9, 93.9, 80.0, 43.8, 39.0, 32.6, 30.6, 27.3, 25.5; ESI HRMS calcd for $C_{18}H_{18}N_2O_2$ $[M + Na]^+$ 317.1260, found 317.1264; IR (CH_2Cl_2, cm^{-1}) 1667, 1616, 1485, 1398, 1282, 990, 908, 728.

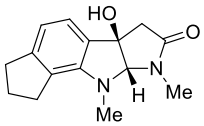
7-Ethyl-3a-hydroxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (23)



23

Following the procedure **4.2**, 41.2 mg starting material gave **23** as yellowish oil (16.7 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.12 (dd, *J* = 11.1, 7.7 Hz, 2H), 6.93 (t, *J* = 7.5 Hz, 1H), 4.63 (s, 1H), 3.10 (s, 3H), 2.89 (t, *J* = 11.0 Hz, 2H), 2.84 (s, 3H), 2.79 – 2.69 (m, 1H), 2.62 (dq, *J* = 14.9, 7.4 Hz, 1H), 1.24 (t, *J* = 7.5 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 149.1, 134.4, 131.3, 130.8, 122.7, 121.5, 94.2, 80.2, 43.3, 41.7, 26.7, 24.7, 13.8; ESI HRMS calcd for $C_{14}H_{18}N_2O_2$ [M + Na]$^+$ 269.1260, found 269.1267; IR (CH_2Cl_2, cm^{-1}) 1667, 1482, 1453, 1417, 1397, 1285, 1087, 1036, 974, 755.

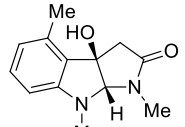
5b-hydroxy-8,9-dimethyl-2,3,5b,6,8a,9-hexahydro-1H-cyclopenta[g]pyrrolo[2,3-b]indol-7(8H)-one (24)



24

Following the procedure **4.2**, 84.8 mg starting material gave **24** as yellowish oil (43.3 mg, 84%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.04 (d, *J* = 7.4 Hz, 1H), 6.75 (d, *J* = 7.4 Hz, 1H), 4.63 (s, 1H), 3.48 (s, 1H), 3.13 (s, 3H), 3.00 (dt, *J* = 15.7, 8.0 Hz, 1H), 2.94 – 2.76 (m, 8H), 2.06 (ddt, *J* = 37.7, 20.8, 8.5 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 148.7, 146.8, 130.6, 126.9, 121.9, 116.9, 93.9, 80.0, 43.8, 39.0, 32.6, 30.6, 27.3, 25.5; ESI HRMS calcd for $C_{15}H_{18}N_2O_2$ [M + Na]$^+$ 281.1260, found 281.1267; IR (CH_2Cl_2, cm^{-1}) 1665, 1595, 1467, 1416, 1397, 1278, 1073, 1006, 729.

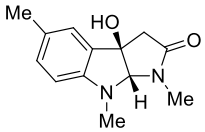
3a-hydroxy-1,4,8-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (25)



25

Following the procedure **4.2**, 75.0 mg starting material gave **25** as yellowish oil (33.3 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (t, *J* = 7.7 Hz, 1H), 6.58 (d, *J* = 7.5 Hz, 1H), 6.38 (d, *J* = 7.9 Hz, 1H), 4.74 (s, 1H), 3.05 (s, 3H), 3.00 – 2.91 (m, 5H), 2.73 (d, *J* = 3.4 Hz, 1H), 2.35 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.3, 150.5, 135.2, 130.5, 128.5, 121.2, 106.2, 93.7, 80.1, 43.0, 36.6, 28.1, 17.4; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ [M + Na]$^+$ 255.1104, found 255.1109; IR (CH_2Cl_2, cm^{-1}) 1665, 1598, 1480, 1284, 982, 749.

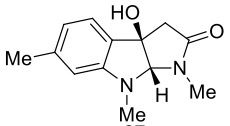
3a-Hydroxy-1,5,8-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (26)



26

Following the procedure **4.2**, 75.0 mg starting material gave **26** as yellowish oil (33.3 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 – 7.00 (m, 2H), 6.47 (d, *J* = 8.0 Hz, 1H), 4.72 (s, 1H), 3.05 (s, 3H), 2.93 (s, 3H), 2.87 (t, *J* = 4.4 Hz, 2H), 2.84 (d, *J* = 6.3 Hz, 1H), 2.28 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 148.0, 131.4, 131.3, 128.9, 124.1, 108.9, 93.1, 80.1, 43.6, 36.8, 28.0, 20.6; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ $[M + Na]^+$ 255.1104, found 255.1104; IR (CH_2Cl_2, cm^{-1}) 1666, 1501, 1398, 1281, 1082, 1048, 995, 806.

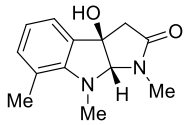
3a-Hydroxy-1,6,8-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (27)



27

Following the procedure **4.2**, 40.0 mg starting material gave **27** as yellowish oil (15.0 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.14 (d, *J* = 7.5 Hz, 1H), 6.62 (d, *J* = 7.5 Hz, 1H), 6.37 (s, 1H), 4.74 (s, 1H), 3.07 (s, 3H), 2.92 (s, 3H), 2.89 (s, 2H), 2.76 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 150.2, 141.0, 128.7, 123.4, 120.0, 109.4, 92.8, 79.7, 43.6, 36.1, 28.0, 21.8; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ $[M + Na]^+$ 255.1104, found 255.1110; IR (CH_2Cl_2, cm^{-1}) 1670, 1515, 1499, 1287, 1084, 10501, 987.

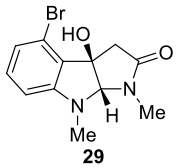
3a-hydroxy-1,7,8-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (28)



28

Following the procedure **4.2**, 40.0 mg starting material gave **28** as yellowish oil (15.3 mg, 66%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.15 (d, *J* = 7.4 Hz, 1H), 7.08 (d, *J* = 7.4 Hz, 1H), 6.90 (t, *J* = 7.4 Hz, 1H), 4.66 (s, 1H), 3.11 (s, 3H), 2.97 – 2.84 (m, 5H), 2.59 (s, 1H), 2.32 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 149.7, 134.0, 133.2, 124.5, 122.4, 121.5, 94.2, 80.3, 43.3, 41.3, 26.8, 18.5; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ $[M + Na]^+$ 255.1104, found 255.1107; IR (CH_2Cl_2, cm^{-1}) 1666, 1469, 1398, 1285, 1265, 1076, 1009, 974, 755.

4-bromo-3a-hydroxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (29)

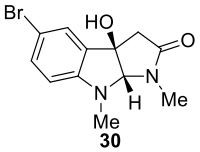


29

Following the procedure **4.2**, 46.3 mg starting material gave **29** as yellowish oil (21.3 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (t, *J* = 8.0 Hz, 1H), 6.87 (d, *J* = 7.9 Hz, 1H), 6.47 (d, *J* = 8.0 Hz, 1H), 4.83 (s, 1H), 3.21 (d, *J* = 18.0 Hz, 1H), 3.18 (s, 1H), 3.08 (s, 3H), 2.97 (s, 3H), 2.93 (d, *J*

= 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 152.0, 131.9, 129.1, 122.3, 118.7, 107.5, 92.4, 80.6, 43.3, 36.2, 28.2; ESI HRMS calcd for $C_{12}H_{13}BrN_2O_2$ $[M + Na]^+$ 319.0053, found 319.0047; IR (CH_2Cl_2, cm^{-1}) 1667, 1598, 1573, 1479, 1426, 1399, 1286, 980, 733.

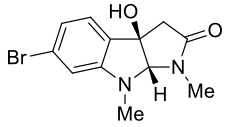
5-bromo-3a-hydroxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (30)



30

Following the procedure **4.2**, 50.0 mg **16a** gave **30** as yellowish oil (23.4 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.36 (d, J = 1.9 Hz, 1H), 7.32 (dd, J = 8.4, 2.0 Hz, 1H), 6.41 (d, J = 8.4 Hz, 1H), 4.78 (s, 1H), 3.06 (s, 4H), 2.93 (d, J = 8.4 Hz, 3H), 2.92 – 2.80 (m, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.6, 149.0, 133.5, 133.3, 126.8, 110.6, 110.0, 92.6, 79.6, 43.5, 35.9, 28.2; ESI HRMS calcd for $C_{12}H_{13}BrN_2O_2$ $[M + Na]^+$ 319.0053, found 319.0050; IR (CH_2Cl_2, cm^{-1}) 1671, 1604, 1491, 1399, 1268, 1099, 992, 810.

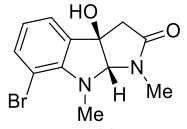
6-bromo-3a-hydroxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (31)



31

Following the procedure **4.2**, 54.0 mg starting material gave **31** as yellowish oil (21.3 mg, 70%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.11 (d, J = 7.9 Hz, 1H), 6.90 (dd, J = 7.9, 1.6 Hz, 1H), 6.66 (s, 1H), 4.79 (d, J = 0.9 Hz, 1H), 3.07 (s, 4H), 2.93 (s, 3H), 2.86 (t, J = 10.2 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 151.1, 130.4, 124.9, 124.5, 121.8, 111.5, 92.4, 79.3, 43.5, 35.5, 28.2; ESI HRMS calcd for $C_{12}H_{13}BrN_2O_2$ $[M + Na]^+$ 319.0053, found 319.0061; IR (CH_2Cl_2, cm^{-1}) 1753, 1672, 1603, 1537, 1491, 1414, 1260, 1137, 983, 831, 737.

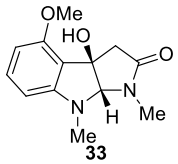
7-bromo-3a-hydroxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (32)



32

Following the procedure **4.2**, 50.0 mg starting material gave **32** yellowish oil (25.3 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.07 (t, J = 8.0 Hz, 1H), 6.87 (d, J = 7.9 Hz, 1H), 6.47 (d, J = 8.0 Hz, 1H), 4.83 (s, 1H), 3.21 (d, J = 18.0 Hz, 1H), 3.18 (s, 1H), 3.08 (s, 3H), 2.97 (s, 3H), 2.93 (d, J = 17.9 Hz, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 152.0, 131.9, 129.1, 122.3, 118.7, 107.5, 92.4, 80.6, 43.3, 36.2, 28.2; ESI HRMS calcd for $C_{12}H_{13}BrN_2O_2$ $[M + Na]^+$ 319.0053, found 319.0060; IR (CH_2Cl_2, cm^{-1}) 1669, 1600, 1467, 1416, 1286, 1252, 1090, 1048, 998, 746.

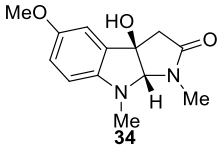
3a-hydroxy-4-methoxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (33)



33

Following the procedure **4.2**, 50.0 mg starting material gave **33** as yellowish oil (22.5 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.20 (t, *J* = 8.0 Hz, 1H), 6.33 (d, *J* = 7.9 Hz, 1H), 6.21 (d, *J* = 7.7 Hz, 1H), 4.78 (d, *J* = 1.6 Hz, 1H), 3.85 (s, 3H), 3.19 (d, *J* = 17.6 Hz, 1H), 3.08 (s, 3H), 2.95 (s, 3H), 2.87 (d, *J* = 14.5 Hz, 1H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 172.3, 156.3, 151.7, 132.2, 116.9, 102.3, 101.7, 92.3, 79.6, 55.3, 43.5, 36.4, 28.0; ESI HRMS calcd for $C_{13}H_{16}N_2O_3$ $[M + Na]^+$ 271.1053, found 271.1057; IR (CH_2Cl_2, cm^{-1}) 1669, 1606, 1484, 1398, 1295, 1258, 1144, 1068, 1048, 988, 754.

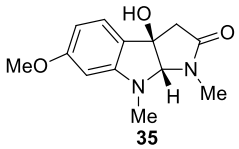
3a-hydroxy-5-methoxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (34)



34

Following the procedure **4.2**, compound **17a** (50.0 mg) gave **34** as yellowish oil (20.3 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.86 (d, *J* = 2.5 Hz, 1H), 6.82 (dd, *J* = 8.5, 2.6 Hz, 1H), 6.51 (d, *J* = 8.5 Hz, 1H), 4.68 (s, 1H), 3.75 (s, 3H), 3.18 (s, 1H), 3.02 (s, 3H), 2.91 (d, *J* = 6.8 Hz, 3H), 2.85 (d, *J* = 4.1 Hz, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 154.0, 144.5, 132.4, 116.7, 110.4, 109.4, 93.8, 80.2, 56.0, 43.7, 37.8, 28.0; ESI HRMS calcd for $C_{13}H_{16}N_2O_3$ $[M + Na]^+$ 271.1053, found 271.1054; IR (CH_2Cl_2, cm^{-1}) 1665, 1494, 1274, 1218, 1026, 994.

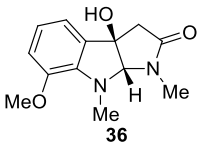
3a-hydroxy-6-methoxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (35)



35

Following the procedure **4.2**, 45.0 mg starting material gave **35** as yellowish oil (21.6 mg, 80%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.13 (d, *J* = 8.2 Hz, 1H), 6.31 (d, *J* = 8.2 Hz, 1H), 6.06 (s, 1H), 4.73 (s, 1H), 3.77 (s, 3H), 3.05 (s, 3H), 2.89 (s, 3H), 2.85 (s, 2H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 162.5, 151.5, 124.3, 124.0, 104.1, 95.0, 92.9, 79.4, 55.4, 43.6, 35.7, 28.0; ESI HRMS calcd for $C_{13}H_{16}N_2O_3$ $[M + Na]^+$ 271.1053, found 271.1054; IR (CH_2Cl_2, cm^{-1})1670, 1619, 1501, 1236, 1084, 987, 829.

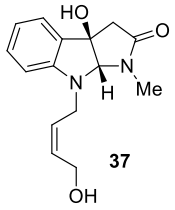
3a-hydroxy-7-methoxy-1,8-dimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (36)



36

Following the procedure **4.2**, 56.0 mg starting material gave **36** as yellowish oil (26.8 mg, 83%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.90 (dd, *J* = 9.8, 4.3 Hz, 2H), 6.81 (d, *J* = 6.8 Hz, 1H), 4.62 (s, 1H), 3.84 (s, 3H), 3.18 (s, 3H), 3.05 (s, 1H), 2.89 (s, 3H), 2.86 (s, 2H); ^{13}C NMR (151 MHz, $CDCl_3$) δ 171.1, 148.1, 139.4, 134.5, 122.7, 116.0, 113.2, 94.2, 80.8, 55.6, 43.5, 40.3, 27.2; ESI HRMS calcd for $C_{13}H_{16}N_2O_3$ $[M + Na]^+$ 271.1053, found 271.1056; IR (CH_2Cl_2, cm^{-1}) 1665, 1593, 1492, 1452, 1418, 1398, 1285, 1232, 999.

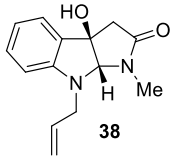
(Z)-3a-hydroxy-8-(4-hydroxybut-2-en-1-yl)-1-methyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (37)



37

Following the procedure **4.2**, compound **S4** (44.0 mg) gave **37** as yellowish oil (17.8 mg, 65%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.21 (dd, *J* = 13.8, 7.3 Hz, 2H), 6.80 (t, *J* = 7.4 Hz, 1H), 6.62 (d, *J* = 8.0 Hz, 1H), 5.79 (dt, *J* = 15.5, 4.7 Hz, 1H), 5.72 – 5.59 (m, 1H), 4.83 (s, 1H), 4.13 (dd, *J* = 16.2, 4.7 Hz, 1H), 4.00 (ddd, *J* = 28.1, 14.3, 4.3 Hz, 2H), 3.93 – 3.75 (m, 2H), 2.86 (d, *J* = 4.8 Hz, 5H), 2.69 (s, 1H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.2, 149.0, 133.0, 132.3, 130.5, 125.2, 124.0, 119.8, 110.3, 90.0, 79.7, 61.8, 51.0, 43.7, 27.7; ESI HRMS calcd for $C_{15}H_{18}N_2O_3$ $[M + Na]^+$ 297.1210, found 297.1208; IR (CH_2Cl_2, cm^{-1}) 1676, 1603, 1489, 1293, 991, 748.

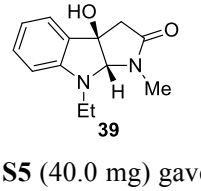
8-Allyl-3a-hydroxy-1-methyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (38)



38

Following the procedure **4.2**, 41.0 mg starting material gave **38** as yellowish oil (17.7 mg, 75%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.28 – 7.16 (m, 2H), 6.81 (t, *J* = 7.0 Hz, 1H), 6.59 (d, *J* = 7.9 Hz, 1H), 5.87 (ddd, *J* = 22.2, 10.4, 5.4 Hz, 1H), 5.24 (dd, *J* = 19.0, 14.3 Hz, 2H), 4.85 (s, 1H), 4.04 (d, *J* = 16.6 Hz, 1H), 3.89 (dd, *J* = 16.6, 5.5 Hz, 1H), 3.25 (s, 1H), 2.87 (d, *J* = 5.3 Hz, 5H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 149.4, 133.6, 131.9, 130.7, 123.7, 119.7, 117.7, 109.8, 91.0, 80.0, 52.7, 43.6, 27.8; ESI HRMS calcd for $C_{14}H_{16}N_2O_2$ $[M + Na]^+$ 267.1104, found 267.1109; IR (CH_2Cl_2, cm^{-1}) 1674, 1605, 1474, 1461, 1279, 1230, 1061, 956, 731.

8-Ethyl-3a-hydroxy-1-methyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (39)

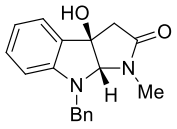


39

Following the procedure **4.2**, compound **S5** (40.0 mg) gave **39** as yellowish solid (17.7 mg, 76%); mp 130 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.24 – 7.16 (m, 2H), 6.77 (td, *J* = 7.4, 0.8 Hz, 1H), 6.58

(d, J = 8.0 Hz, 1H), 4.79 (s, 1H), 3.50 (dq, J = 14.4, 7.2 Hz, 1H), 3.31 (dq, J = 14.3, 7.1 Hz, 1H), 2.86 – 2.80 (m, 5H), 1.17 (t, J = 7.1 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.9, 149.1, 132.3, 130.6, 123.8, 119.4, 109.8, 90.3, 79.9, 43.8, 43.4, 27.5, 13.0; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ [M + Na]$^+$ 255.1104, found 255.1103; IR (CH_2Cl_2, cm^{-1}) 1665, 1607, 1487, 1398, 1268, 1083, 1049, 990, 746.

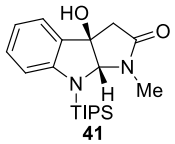
8-benzyl-3a-hydroxy-1-methyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (40)



40

Following the procedure **4.2**, 46.0 mg starting material gave **40** as yellow solid (20.6 mg, 70%); mp 105 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 (dt, J = 20.3, 6.7 Hz, 6H), 7.19 (dd, J = 11.1, 4.2 Hz, 1H), 6.84 (t, J = 7.4 Hz, 1H), 6.55 (d, J = 8.0 Hz, 1H), 4.92 (s, 1H), 4.59 (dd, J = 44.8, 16.2 Hz, 2H), 3.01 – 2.87 (m, 2H), 2.79 (s, 1H), 2.74 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.8, 149.7, 137.8, 131.8, 130.9, 128.8, 127.6, 127.1, 123.8, 119.9, 109.9, 91.4, 80.1, 54.1, 43.5, 27.9; ESI HRMS calcd for $C_{18}H_{18}N_2O_2$ [M + Na]$^+$ 317.1260, found 317.1260; 1665, 1607, 1491, 1395, 1273, 1229, 916, 744, 692.

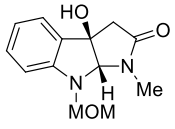
3a-Hydroxy-1-methyl-8-(triisopropylsilyl)-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (41)



41

Following the procedure **4.2**, 55.0 mg starting material gave **41** as yellowish oil (25.2 mg, 67%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (d, J = 7.4 Hz, 1H), 7.24 – 7.14 (m, 1H), 6.90 (dd, J = 12.0, 4.7 Hz, 2H), 5.21 (s, 1H), 2.99 (q, J = 16.4 Hz, 2H), 2.84 (s, 3H), 2.01 (s, 1H), 1.46 (dq, J = 14.7, 7.5 Hz, 3H), 1.22 (d, J = 7.5 Hz, 9H), 1.11 (d, J = 7.5 Hz, 9H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 150.5, 134.1, 130.5, 124.1, 120.8, 114.4, 85.9, 81.0, 41.6, 26.8, 18.9, 18.7, 13.1; ESI HRMS calcd for $C_{20}H_{32}N_2O_2Si$ [M + Na]$^+$ 383.2125, found 383.2121; IR (CH_2Cl_2, cm^{-1}) 1670, 1609, 1489, 1286, 1157, 991, 746.

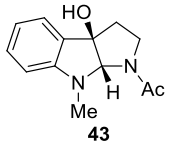
3a-Hydroxy-8-(methoxymethyl)-1-methyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (42)



42

Following the procedure **4.2**, 50.0 mg starting material gave **42** as yellowish oil (24.2 mg, 81%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.31 – 7.18 (m, 2H), 6.90 (t, *J* = 7.3 Hz, 1H), 6.75 (d, *J* = 7.9 Hz, 1H), 4.90 – 4.75 (m, 2H), 4.50 (d, *J* = 10.5 Hz, 1H), 4.06 (s, 1H), 3.24 (s, 3H), 2.84 (s, 2H), 2.81 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.5, 147.7, 133.0, 130.6, 124.3, 121.4, 110.9, 90.0, 82.2, 79.8, 55.3, 43.0, 27.1; ESI HRMS calcd for $C_{13}H_{16}N_2O_3$ $[M + Na]^+$ 271.1053, found 271.1055; IR (CH_2Cl_2, cm^{-1}) 1668, 1608, 1487, 1398, 1157, 1071, 994, 746.

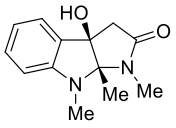
1-(3a-hydroxy-8-methyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-1(2H)-yl)ethanone (43)



43

Following the procedure **4.2**, 40.0 mg starting material gave **43** as yellowish oil (13.4 mg, 53%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.26 – 7.18 (m, 2H), 6.75 (dt, *J* = 7.4, 5.5 Hz, 1H), 6.48 (t, *J* = 6.1 Hz, 1H), 5.45 (s, 1H), 3.75 (ddd, *J* = 10.5, 7.7, 5.1 Hz, 1H), 3.38 (dt, *J* = 10.4, 7.7 Hz, 1H), 2.99 (s, 3H), 2.39 (dt, *J* = 12.9, 7.9 Hz, 1H), 2.30 (ddd, *J* = 11.4, 6.5, 4.6 Hz, 1H), 2.06 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 171.0, 150.9, 130.3, 130.1, 122.7, 118.1, 107.3, 88.3, 86.4, 47.5, 38.4, 34.5, 22.4; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ $[M + Na]^+$ 255.1104, found 255.1105; IR (CH_2Cl_2, cm^{-1}) 1612, 1491, 1417, 1297, 1196, 1129, 1050, 945, 745.

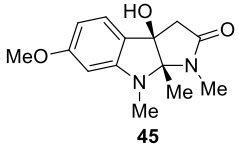
3a-hydroxy-1,8,8a-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (44)



44

Following the procedure **4.2**, compound **18a** (57.0 mg) gave **44** as yellowish oil (17.7 mg, 76%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.30 (dt, *J* = 8.5, 4.2 Hz, 1H), 7.26 – 7.21 (m, 1H), 6.78 (t, *J* = 7.4 Hz, 1H), 6.48 (d, *J* = 7.9 Hz, 1H), 3.03 – 2.96 (m, 4H), 2.86 (d, *J* = 16.9 Hz, 1H), 2.79 (s, 3H), 2.10 (s, 1H), 1.56 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 148.9, 131.0, 130.0, 124.1, 118.5, 107.0, 88.9 81.2, 41.5, 29.9, 25.9, 15.0; ESI HRMS calcd for $C_{13}H_{16}N_2O_2$ $[M + Na]^+$ 255.1104, found 255.1100; 1666, 1609, 1494, 1395, 1101, 1064, 991, 914, 744.

3a-hydroxy-6-methoxy-1,8,8a-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (45)

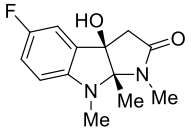


45

Following the procedure **4.2**, compound **20a** (50.0 mg) gave **45** as yellowish oil (21.7 mg, 71%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.16 (t, *J* = 8.6 Hz, 1H), 6.26 (dd, *J* = 8.2, 2.1 Hz, 1H), 5.99 (d, *J* = 2.1 Hz, 1H), 3.77 (s, 3H), 2.96 (s, 3H), 2.83 (dd, *J* = 49.9, 16.9 Hz, 2H), 2.74 (d, *J* = 6.1 Hz, 3H), 2.65 (s, 1H), 1.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.4, 162.6, 150.4, 124.8, 122.9, 103.0, 93.8, 89.5, 80.7, 55.4, 41.6, 29.9, 25.8, 15.0; ESI HRMS calcd for $C_{14}H_{18}N_2O_3$ $[M + Na]^+$

285.1210, found 285.1208; IR (CH_2Cl_2, cm^{-1}) 1667, 1619, 1498, 1419, 1393, 1231, 1091, 1064, 952.

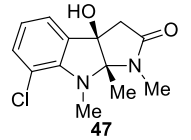
5-fluoro-3a-hydroxy-1,8,8a-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (46)



46

Following the procedure **4.2**, compound **19a** (40.0 mg) gave **46** as yellowish oil (18.5 mg, 77%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 6.99 (d, *J* = 7.6 Hz, 1H), 6.91 (t, *J* = 8.7 Hz, 1H), 6.39 – 6.31 (m, 1H), 2.98 (d, *J* = 10.8 Hz, 1H), 2.94 (s, 3H), 2.91 – 2.77 (m, 2H), 2.74 (s, 3H), 1.51 (s, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 170.2, 157.7, 155.3, 145.1, 131.4, 131.3, 117.1, 116.9, 111.6, 111.3, 107.4, 107.4, 89.6, 81.0, 41.7, 30.4, 26.0, 14.8; ESI HRMS calcd for $C_{13}H_{15}FN_2O_2$ $[M + Na]^+$ 273.1010, found 273.1008; IR (CH_2Cl_2, cm^{-1}) 1667, 1498, 1396, 1267, 1103, 1065, 893, 807.

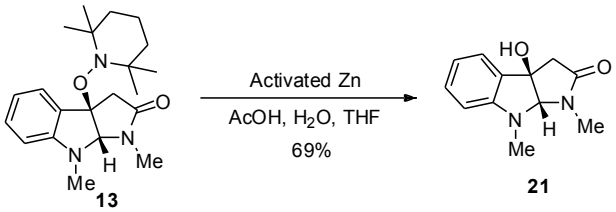
7-chloro-3a-hydroxy-1,8,8a-trimethyl-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (47)



47

Following the procedure **4.2**, compound **S6** (51.0 mg) gave **47** as yellowish oil (21.7 mg, 69%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.18 – 7.14 (m, 2H), 6.75 (td, *J* = 7.7, 1.6 Hz, 1H), 3.25 – 3.22 (m, 3H), 2.78 (td, *J* = 17.0, 10.2 Hz, 2H), 2.71 (d, *J* = 7.1 Hz, 3H), 1.51 (d, *J* = 1.6 Hz, 3H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 169.6, 145.6, 135.0, 132.5, 122.9, 121.1, 117.1, 89.6, 81.1, 41.5, 33.5, 24.9, 14.9; ESI HRMS calcd for $C_{13}H_{15}ClN_2O_2$ $[M + Na]^+$ 289.0714, found 289.0712; IR (CH_2Cl_2, cm^{-1}) 1666, 1475, 1419, 1395, 1272, 1107, 1064, 737.

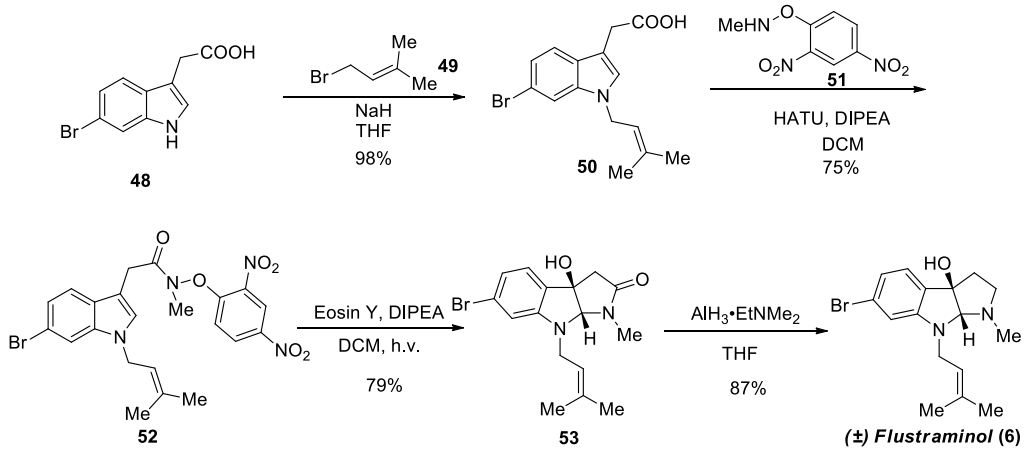
4.3 Reduction of TEMPO derivative (13) to compound (21)



13 **21**

A solution of TEMPO derivative **13** in HOAc/H_2O/THF (0.3 mL: 0.1 mL: 0.1 mL) under argon was added activated zinc powder in one portion. The suspension was heated to 50 ^oC for 24 hours and then cooled to room temperature and filtered. The filtrate was poured into water and the mixture was extracted with EtOAc. The combined organic layer was washed with saturated $NaHCO_3$ aqueous solution, water and brine and dried. Then the solvent was evaporated and the crude product was purified on silica gel to give compound **21** as colorless oil (69%).

5. Total Synthesis of (±)-Flustraminol



To a solution of 6-bromoindole-3-acetic acid **48** (310 mg, 1.22 mmol) in THF (15 mL), NaH (146 mg, 3.66 mmol) was added portionwise. The mixture was stirred for 30 minutes at 0 °C and then dimethylallylbormide **49** (236 mg, 1.59 mmol) was added dropwise. The reaction was moved to room temperature and the stirring was continued for 16 hours. The reaction mixture was then cooled to 0 °C and acidified with 6 N aq. HCl and extracted with EtOAc. The combined organic phase was dried and concentrated. The residue was purified on silica gel to give product **50** as dark yellow oil (385 mg, 98%).[2]

To a solution of the obtained indole-3-acetic acid **50** (100 mg, 0.31 mmol) and O-(2,4-dinitrophenyl)-N-methylhydroxylamine **51** (80 mg, 0.37 mmol) in CH_2Cl_2 (5 mL), HATU (118 mg, 0.31 mmol) was added. DIPEA (154 uL, 0.93 mmol) was added via syringe while the mixture was stirred vigorously. The reaction was allowed to stir for 12 hours and then quenched with water. The mixture was extracted with EtOAc. The combined extracts were dried and concentrated. The residue was purified on silica gel to give the product **52** as orange solid (120 mg, 75%); mp 95 ^{o}C. ^{1}H NMR (400 MHz, $CDCl_3$) δ 8.67 (d, J = 2.3 Hz, 1H), 8.01 (dd, J = 9.3, 2.0 Hz, 1H), 7.30 (d, J = 8.4 Hz, 1H), 7.24 (s, 1H), 7.10 – 7.05 (m, 1H), 6.97 (d, J = 9.3 Hz, 1H), 6.83 (s, 1H), 5.12 (t, J = 6.5 Hz, 1H), 4.39 (d, J = 6.9 Hz, 2H), 3.92 (s, 2H), 3.34 (s, 3H), 1.78 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 175.5, 155.9, 141.6, 137.4, 136.5, 136.1, 128.8, 127.0, 126.3, 122.6, 121.7, 120.0, 118.7, 115.4, 114.5, 112.4, 106.1, 43.9, 36.2, 31.1, 25.6, 18.0; ESI HRMS calcd for $C_{22}H_{21}BrN_4O_6$ $[M + Na]^+$ 539.0537, found 539.0545; IR (CH_2Cl_2, cm^{-1}) 3110, 2933, 1690, 1605, 1533, 1468, 1342, 1255, 1231, 1163, 1100, 834, 770.

6-bromo-3a-hydroxy-1-methyl-8-(3-methylbut-2-en-1-yl)-3,3a,8,8a-tetrahydropyrrolo[2,3-b]indol-2(1H)-one (53)

Following the procedure **4.2**, compound **52** (40.0 mg) gave **53** as yellowish oil (15.1 mg, 79%). ^{1}H NMR (400 MHz, $CDCl_3$) δ 7.06 (d, J = 7.8 Hz, 1H), 6.86 (d, J = 7.8 Hz, 1H), 6.68 (s, 1H), 5.18 (s, 1H), 4.81 (s, 1H), 4.00 – 3.80 (m, 3H), 2.87 – 2.68 (m, 5H), 1.72 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 172.0, 150.8, 136.3, 131.3, 125.0, 124.2, 122.1, 119.7, 112.7, 90.5, 79.2, 47.2, 43.5, 27.8,

25.6, 18.1; ESI HRMS calcd for $C_{16}H_{19}BrN_2O_2$ $[M + Na]^+$ 373.0522, found 373.0527; IR (CH_2Cl_2, cm^{-1}) 1605, 1487, 1456, 1312, 1249, 1158, 1023, 937, 746..

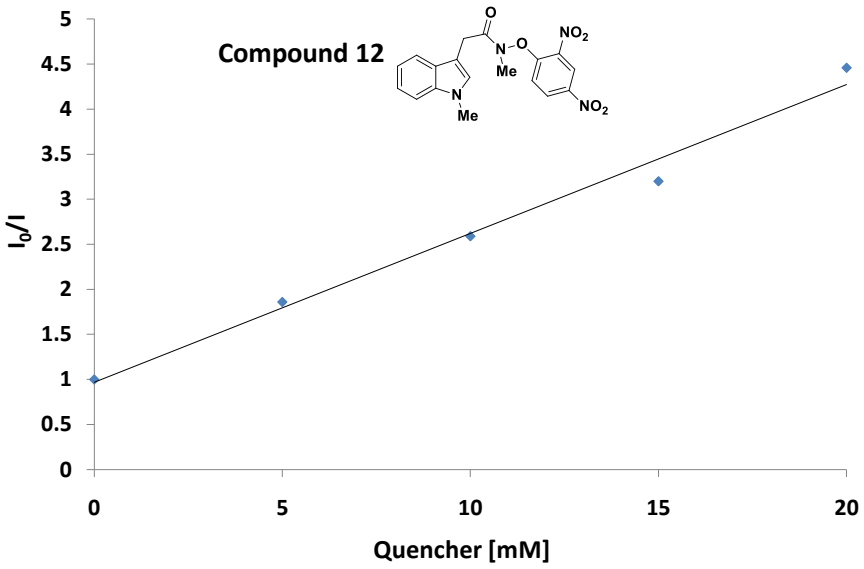
***(±)-Flustraminol* (6)**

Following the reported procedure with slight modification[5], alane-N,N-dimethylethylamine complex (1 M solution in THF, 85 μL, 0.084 mmol) was added to a solution of **53** (15.0 mg, 0.042 mmol) in 2 mL THF under nitrogen at room temperature. The reaction mixture was stirred at the 60 ^oC for 5 min, treated with 5 mL saturated potassium tartrate, and stirred until the solution became clear. The mixture was extracted with AcOEt and the organic layer was washed with brine, dried and concentrated under reduced pressure. The residue was purified on silica gel column to give flustraminol B (12.5 mg, 87%) as a colorless oil. ^1H NMR (400 MHz, $CDCl_3$) δ 7.07 (d, J = 7.8 Hz, 1H), 6.83 (dd, J = 7.8, 1.6 Hz, 1H), 6.62 (s, 1H), 5.19 (d, J = 5.8 Hz, 1H), 4.35 (s, 1H), 3.85 (d, J = 6.5 Hz, 2H), 2.88 – 2.77 (m, 1H), 2.67 (dd, J = 15.8, 7.8 Hz, 1H), 2.54 (s, 3H), 2.29 (dt, J = 14.6, 7.4 Hz, 1H), 2.19 – 2.10 (m, 1H), 1.73 (s, 6H); ^{13}C NMR (100 MHz, $CDCl_3$) δ 152.3, 135.43, 131.4, 124.5, 123.7, 120.7, 119.8, 111.2, 95.6, 87.9, 53.1, 46.3, 40.1, 38.8, 25.6, 18.1; ESI HRMS calcd for $C_{16}H_{21}BrN_2O$ $[M + Na]^+$ 359.0729, found 359.0730; IR (CH_2Cl_2, cm^{-1}) 1673, 1602, 1484, 1444, 1310, 1246, 1158, 1098, 1025, 922, 797.

6. Emission Quenching Experiments – Stern-Volmer Studies

Emission intensities were recorded using a Steady State emission spectra recorded on Horiba Fluorolog®-3 model FL1039A/40A spectrofluorometer, equipped with a 450 watt steady state xenon illuminator and single-grating emission monochromator and a photomultiplier tube (room-temperature R928P).

Experimental procedures: All the Eosin Y solutions were excited at 400 nm and the emission intensity was collected at 555 nm. A screw-top quartz cuvette was charged with a 0.1 mM solution of Eosin Y in MeOH (2.0 mL) and the initial emission was collected. Another two series of samples, 0.1 mM Eosin Y in MeOH with compound **12** or DIPEA as quencher in gradient concentrations (5 mM, 10 mM, 15 mM and 20 mM), were tested and the emissions were collected.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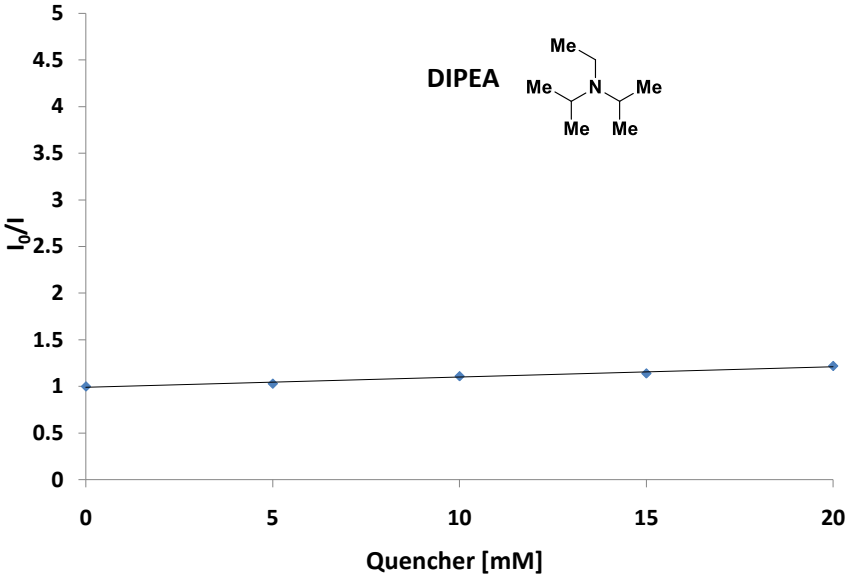
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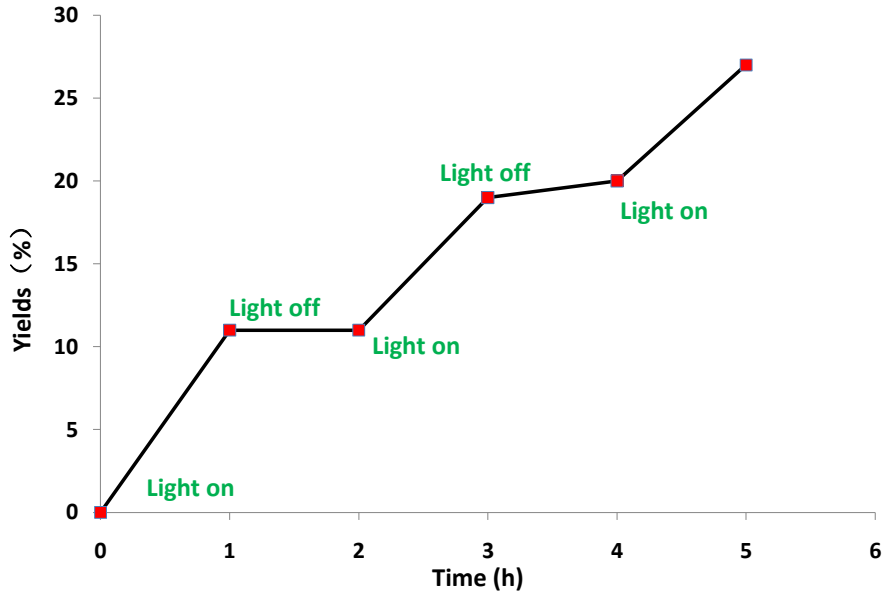
10
15
20

7. Light ON – Light OFF Experiments

A flask with septum stopper was charged with substrate **12** (76 mg, 0.2 mmol) in $CDCl_3$ (5 mL), and Eosin Y (2.5 mg, 0.004 mmol) was added. DIPEA (51 mg, 0.4 mmol) was added via syringe and air was bubbled through the solution for 5 minutes. The flask was irradiated under green LED in the open air for 1 h at which point a reaction aliquot (0.5 mL) was taken via syringe for ^{1}H NMR analysis. Yields of compound **21** were calculated using anisole as an internal standard. The green LED was switched off and the mixture was stirred in the dark for 1h at which point a reaction aliquot (0.5 mL) was taken for ^{1}H NMR analysis. The green LED was then switched ON and OFF and ON and OFF alternatively and ^{1}H NMR yields were calculated using anisole as an internal standard.



8. Crystal Structure Solution and Refinement

Data collection of three structures was performed on a Bruker D8 VENTURE X-ray diffractometer with PHOTON 100 CMOS shutterless detector equipped with a Mo-target X-ray tube (λ = 0.71073 Å) at T = 100(2) K. Data reduction and integration were performed with the Bruker software package SAINT (version 8.38A).[6] Data were corrected for absorption effects, using the empirical methods as implemented in SADABS (version 2016/2).[7] The structures were solved by SHELXT (version 2018/2)[8] and refined by full-matrix least-squares procedures using the Bruker SHELXTL (version 2018/3)[9] software package. All non-hydrogen atoms were refined anisotropically. In the structure of Compound **15**, the coordinates of H-atoms on C7 and C10 were refined independently, while other H-atoms were included at calculated positions and refined as riders, with U_{iso}(H) = 1.2 U_{eq}(C) and U_{iso}(H) = 1.5 U_{eq}(C) for methyl groups. In the structure of Compound **39**, the coordinates of H-atom on O1 were refined independently, while other H-atoms

were included at calculated positions and refined as riders, with $U_{iso}(H) = 1.2\ U_{eq}(C)$ and $U_{iso}(H) = 1.5\ U_{eq}(C)$ for methyl groups. The structure of Compound **15** was refined as an inversion twin with the parameter of BASF refined to 0.43249. Selected crystallographic data for Compound **15 and 39** are shown in Table S1. Crystallographic data have been deposited with Cambridge Crystallographic Data Centre: Deposition number CCDC 1841089 and 1841090 for Compound **15** and Compound **39**, respectively. Copies of the data can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html (or from the Cambridge Crystallographic Data Centre, 12, Union Road, Cambridge, CB2 1EZ, UK; Fax: +44 1223 336033; e-mail: deposit@ccdc.cam.ac.uk).

Table S1. Crystallographic data for Compound **15 and 39**.

	15	**39**
Empirical formula	$C_{12}H_{14}N_2O$	$C_{13}H_{16}N_2O_2$
Formula weight	202.25	232.28
Temperature (K)	100(2)	100(2)
Wavelength (Å)	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic
Space group	$P2_12_12_1$	$C2/c$
a (Å)	5.7386(4)	28.7011(14)
b (Å)	9.5416(7)	9.3880(5)
c (Å)	18.3137(13)	8.9139(4)
α (°)	90.00	90.00
β (°)	90.00	99.230(2)
γ (°)	90.00	90.00
V (Å^3)	1002.77(12)	2370.7(2)
Z	4	8
ρ_{calcd} (g·cm^{-3})	1.340	1.302
μ (mm^{-1})	0.087	0.089
F(000)	432	992
Crystal size (mm)	0.08×0.09×0.28	0.06×0.11×0.31
θ range for data collection (°)	3.083-30.490	2.876-30.582
Reflections collected	12225	56256
Independent reflections	3055 [R_{int} = 0.0380]	3644 [R_{int} = 0.0409]
Transmission factors (min/max)	0.9011/1	0.9641/1
Data/restraints/params.	3055/0/147	3644/0/159
$R1$,[a] $wR2$[b] ($I > 2\sigma(I)$)	0.0449, 0.0903	0.0483, 0.1152
$R1$,[a] $wR2$[b] (all data)	0.0572, 0.0960	0.0619, 0.1233
Quality-of-fit[c]	1.052	1.063

[a] $R1 = \Sigma||F_o|-|F_c||/\Sigma|F_o|$. [b] $wR2 = [\Sigma[w(F_o^2-F_c^2)^2]/\Sigma[w(F_o^2)^2]]$.
[c] Quality-of-fit = $[\Sigma[w(F_o^2-F_c^2)^2]/(N_{obs}-N_{params})]^{½}$, based on all data

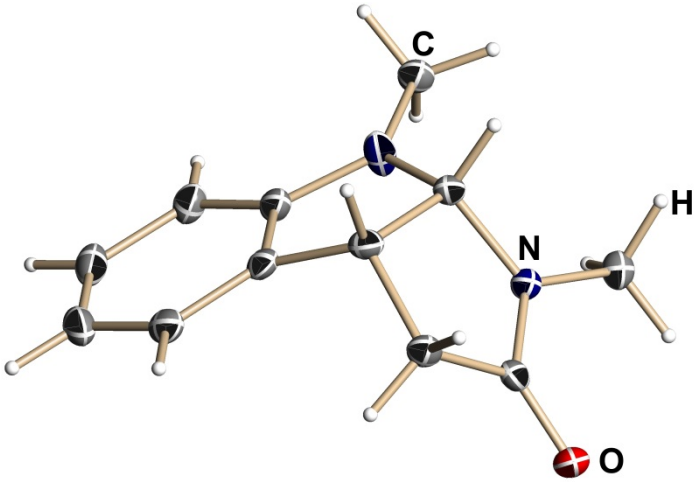


Figure S1. ORTEP drawing of the Compound **15** drawn with thermal ellipsoids at the 50% probability level. Color scheme used: N blue, O red, C grey, H white.

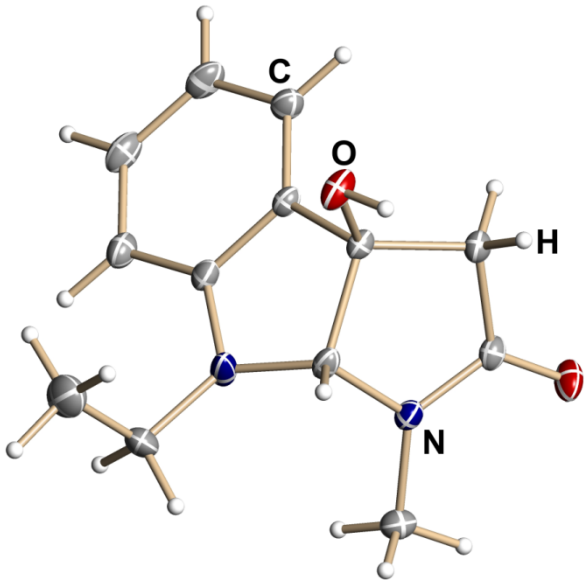


Figure S2. ORTEP drawing of the Compound **39** drawn with thermal ellipsoids at the 50% probability level. Color scheme used: N blue, O red, C grey, H white.

9. References

[1] K. Wu, Y. Du, T. Wang, *Org. Lett.* 2017, **19**, 5669

[2] P. A. Woods, L. C. Morrill, T. Lebl, A. M. Z. Slawin, R. A. Bragg, A. D. Smith, *Org. Lett.* 2010, **12**, 2660.

[3] D. Li, T. Wu, K. Liang, C. Xia, *Org. Lett.* 2016, **18**, 2228.

[4] J. Davies, T. D. Svejstrup, D. F. Reina, N. S. Sheikh, D. Leonori, *J. Am. Chem. Soc.* 2016, **138**, 8092.

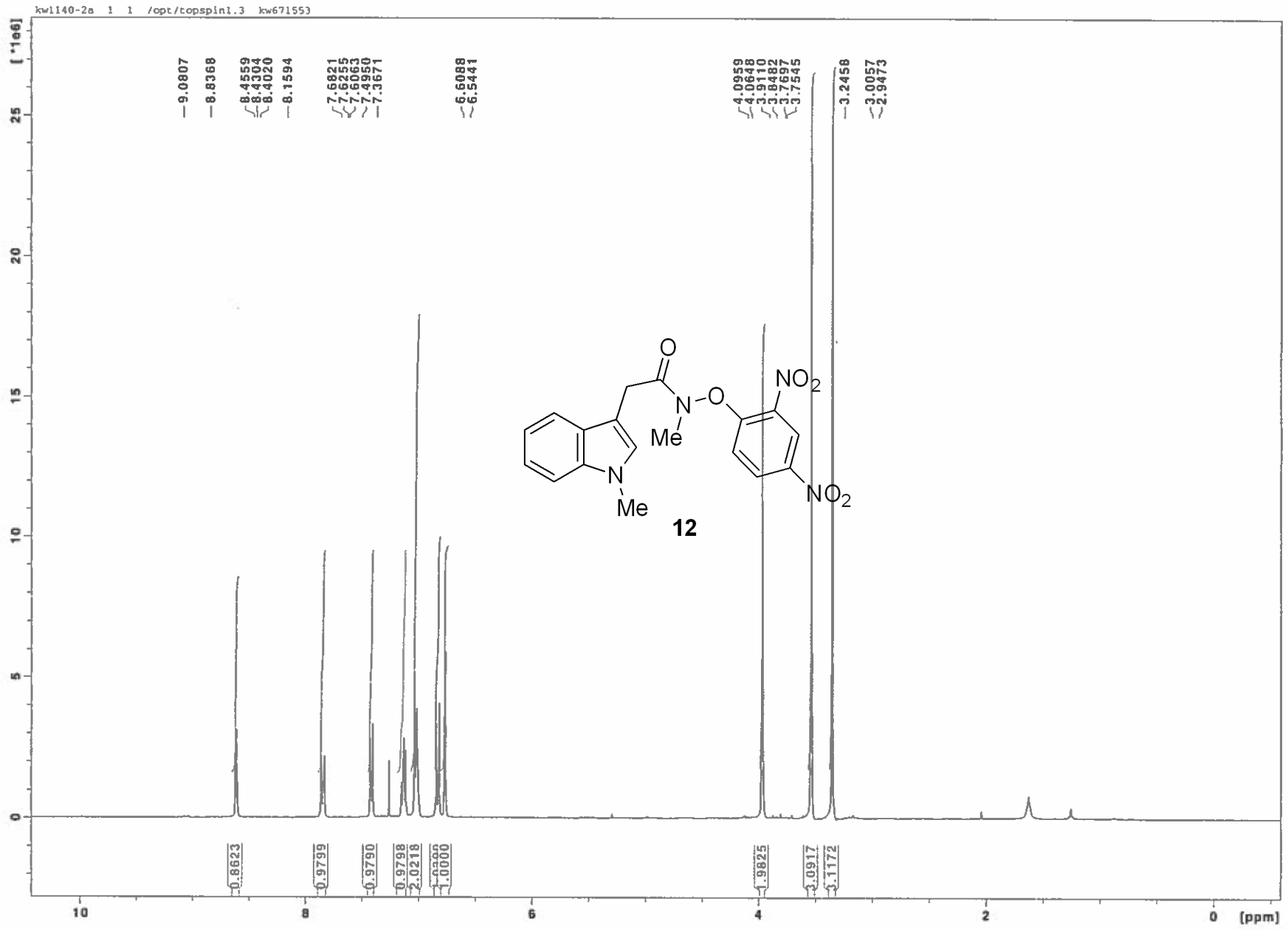
[5] T. Kawasaki, M. Shinada, D. Kamimura, M. Ohzono, A. Ogawa, *Chem. Commun.* 2006, 420.

[6] SAINT; part of Bruker APEX3 software package (version 2016.9-0): Bruker AXS, 2016.

[7] SADABS; part of Bruker APEX3 software package (version 2016.9-0): Bruker AXS, 2016.

[8] G. M. Sheldrick, *Acta Cryst.* 2015, **A71**, 3-8.

[9] G. M. Sheldrick, *Acta Cryst.* 2015, **C71**, 3-8.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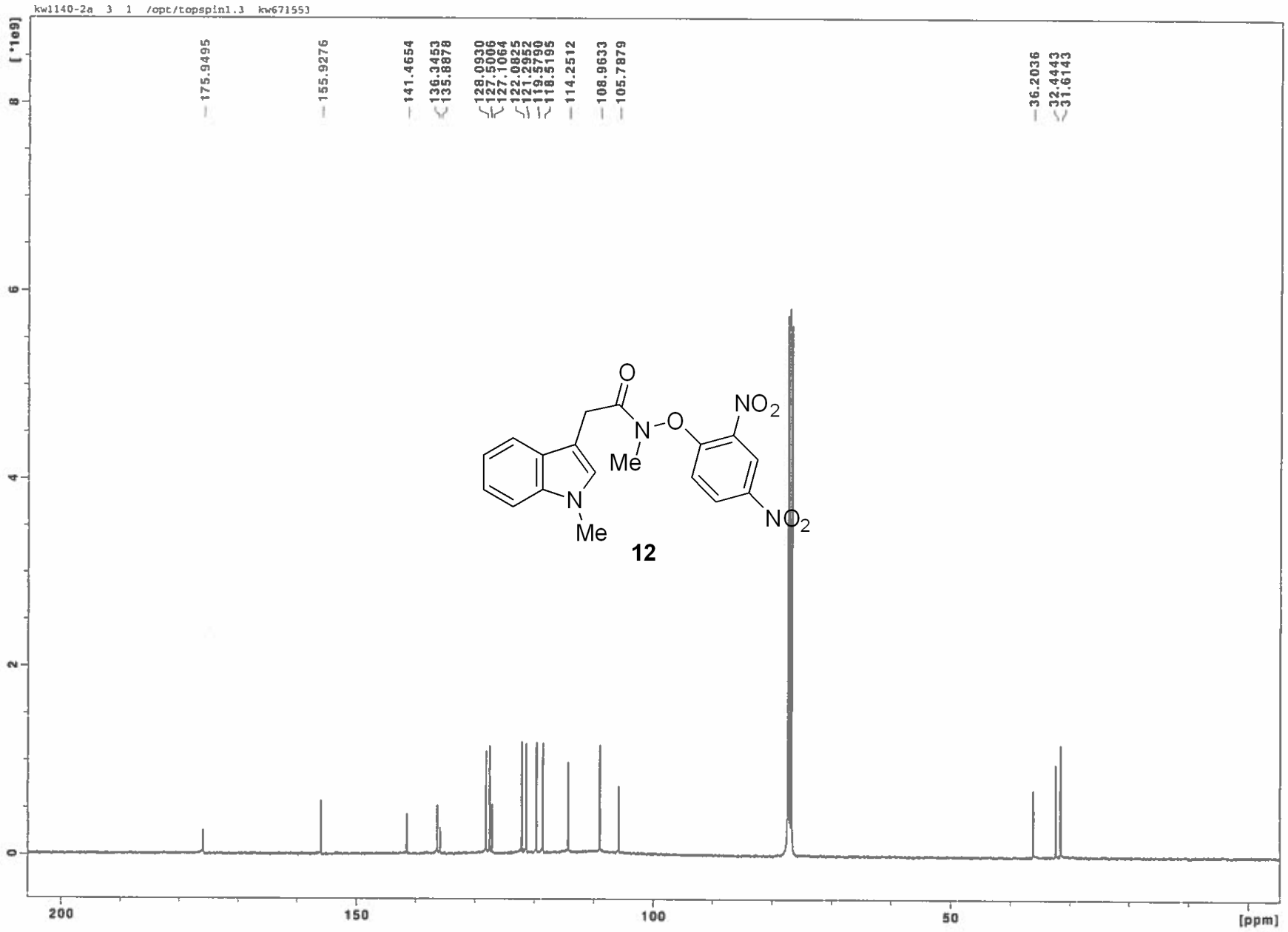
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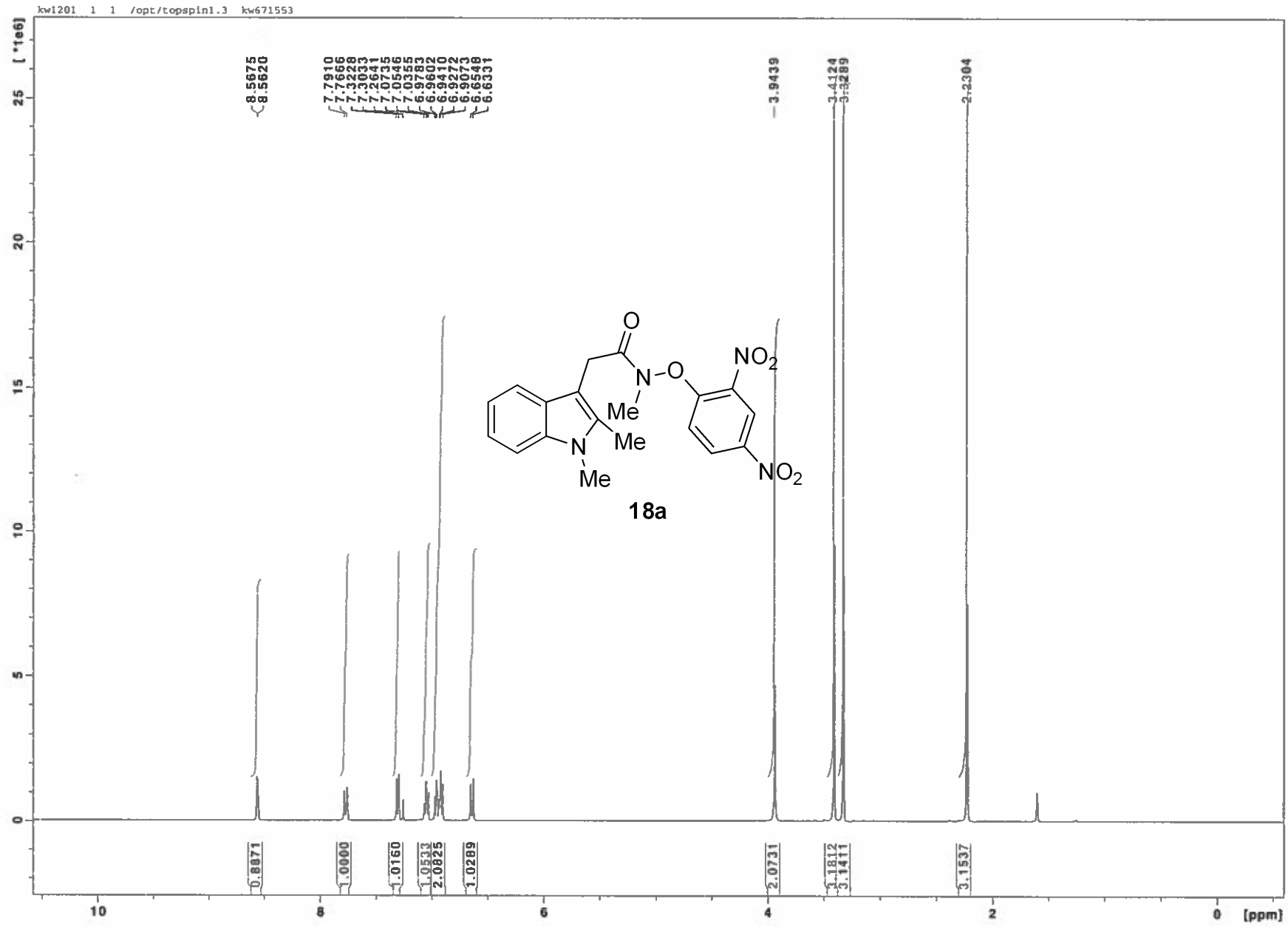
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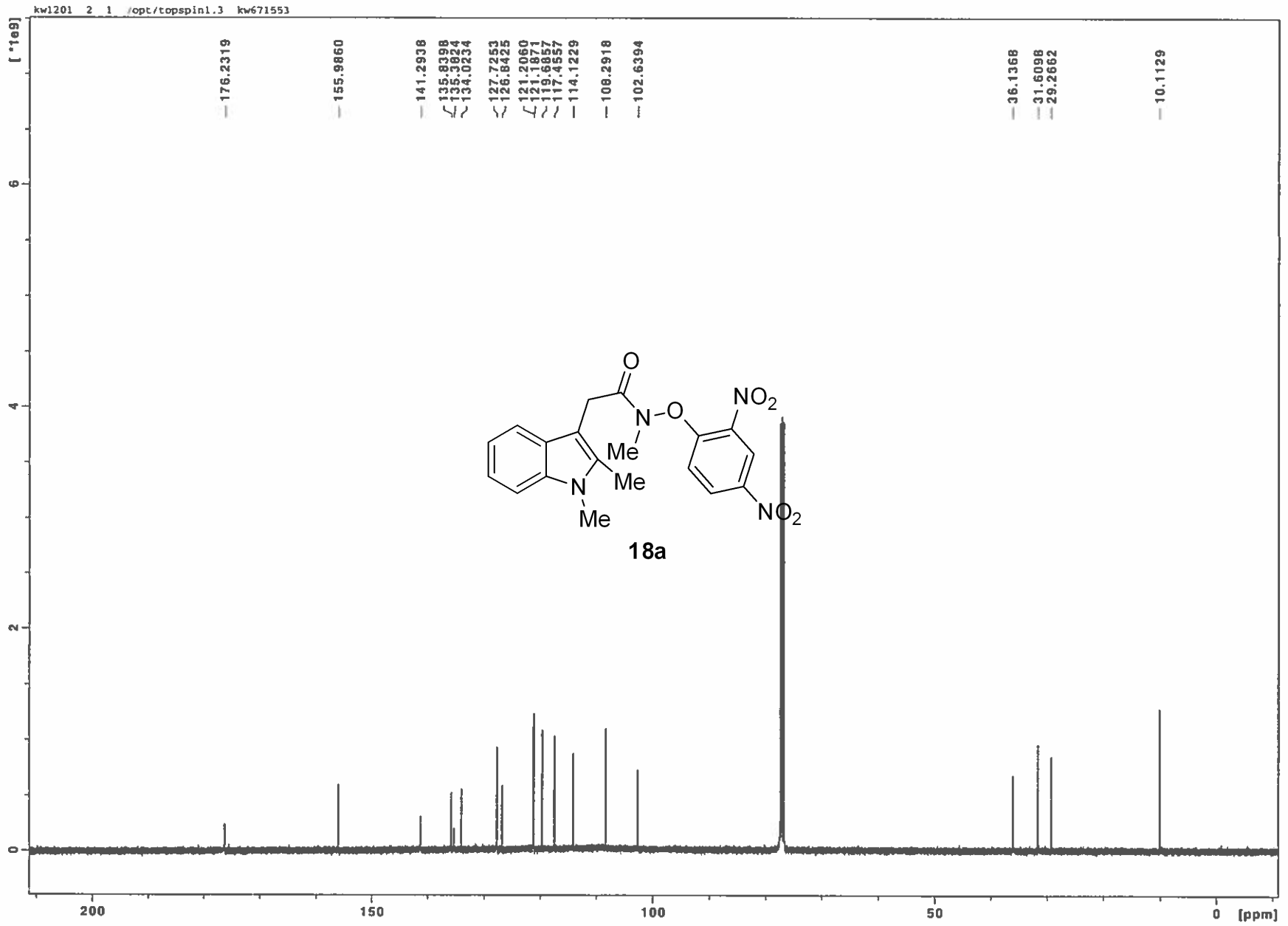
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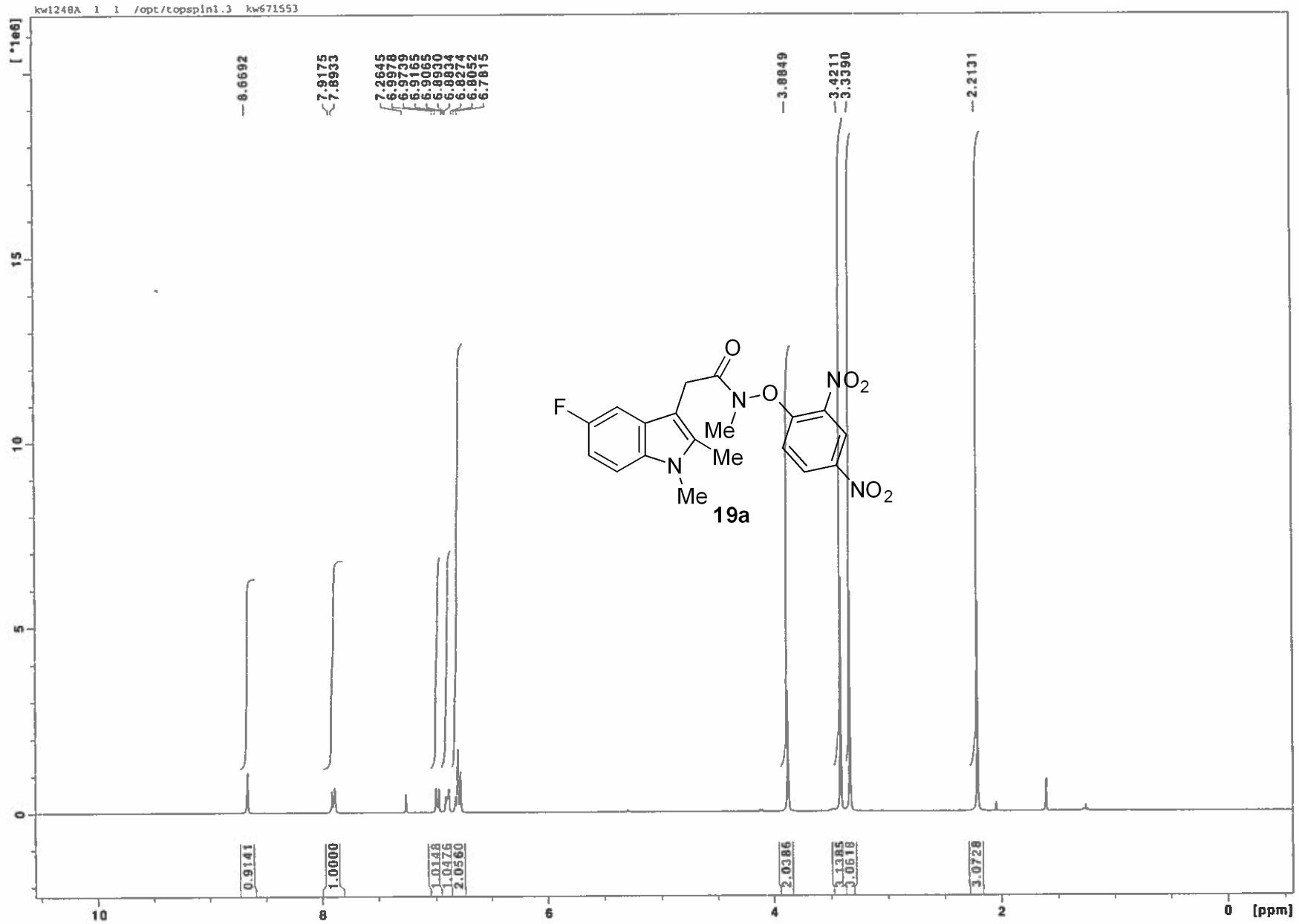
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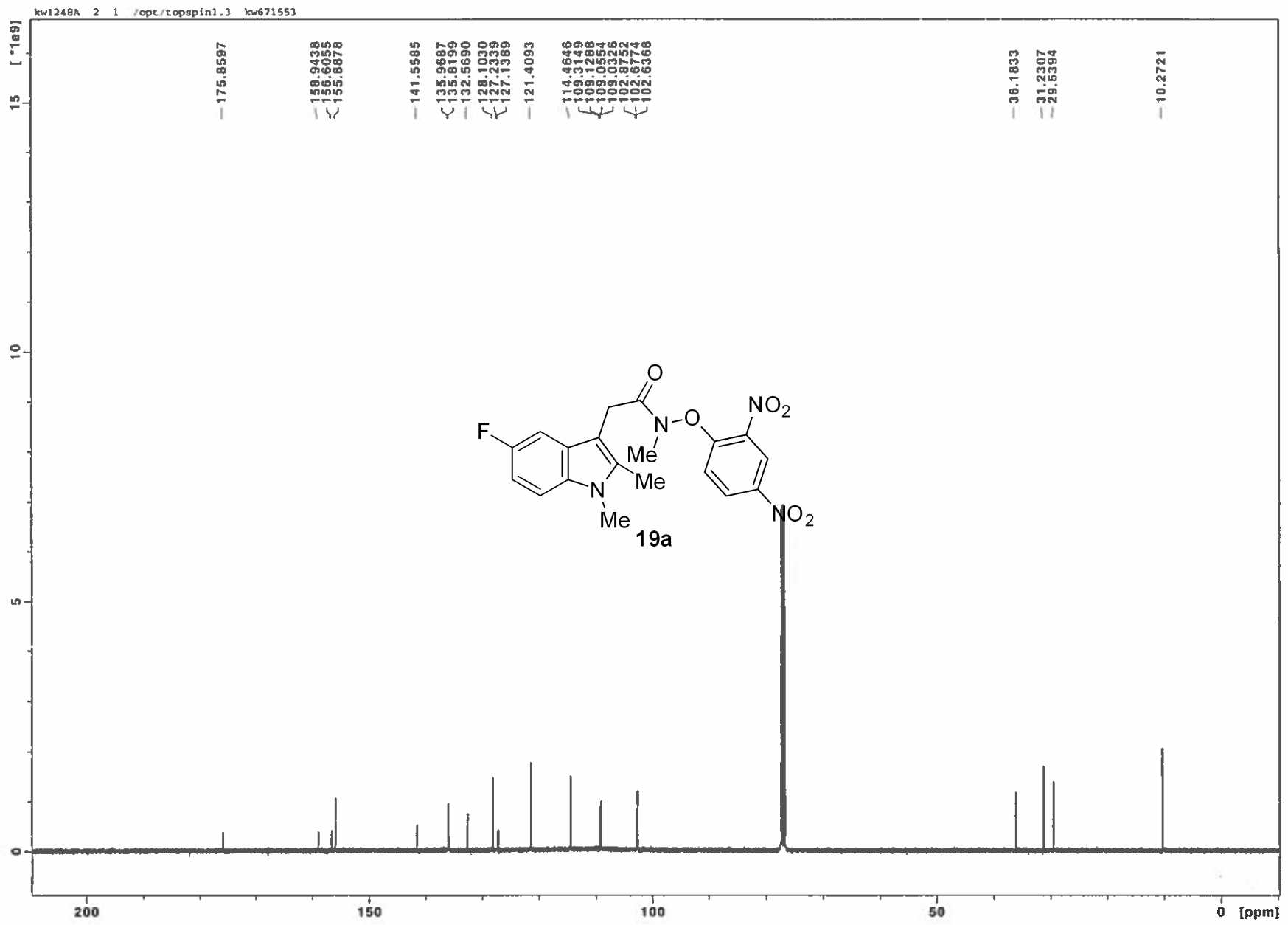
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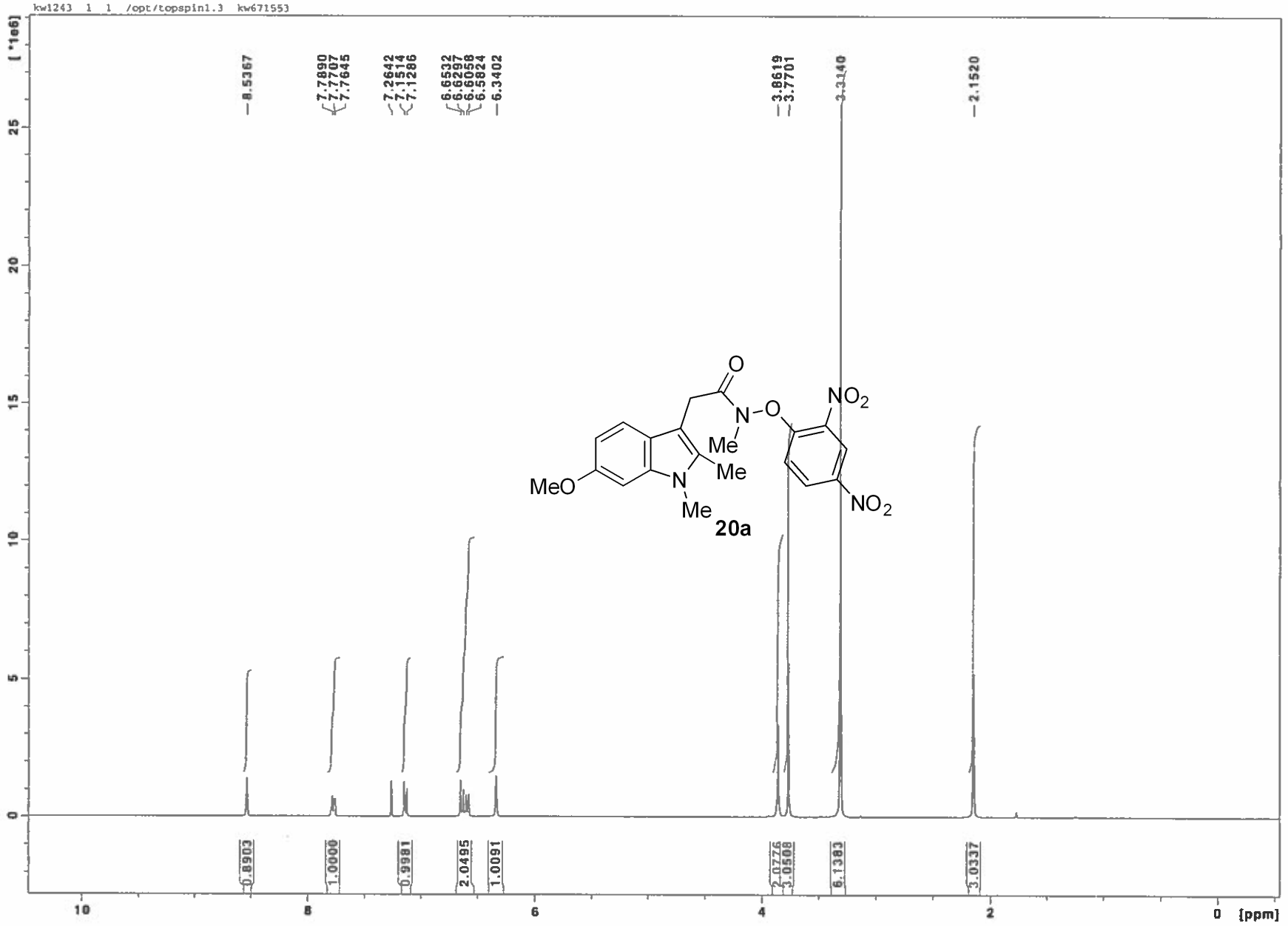
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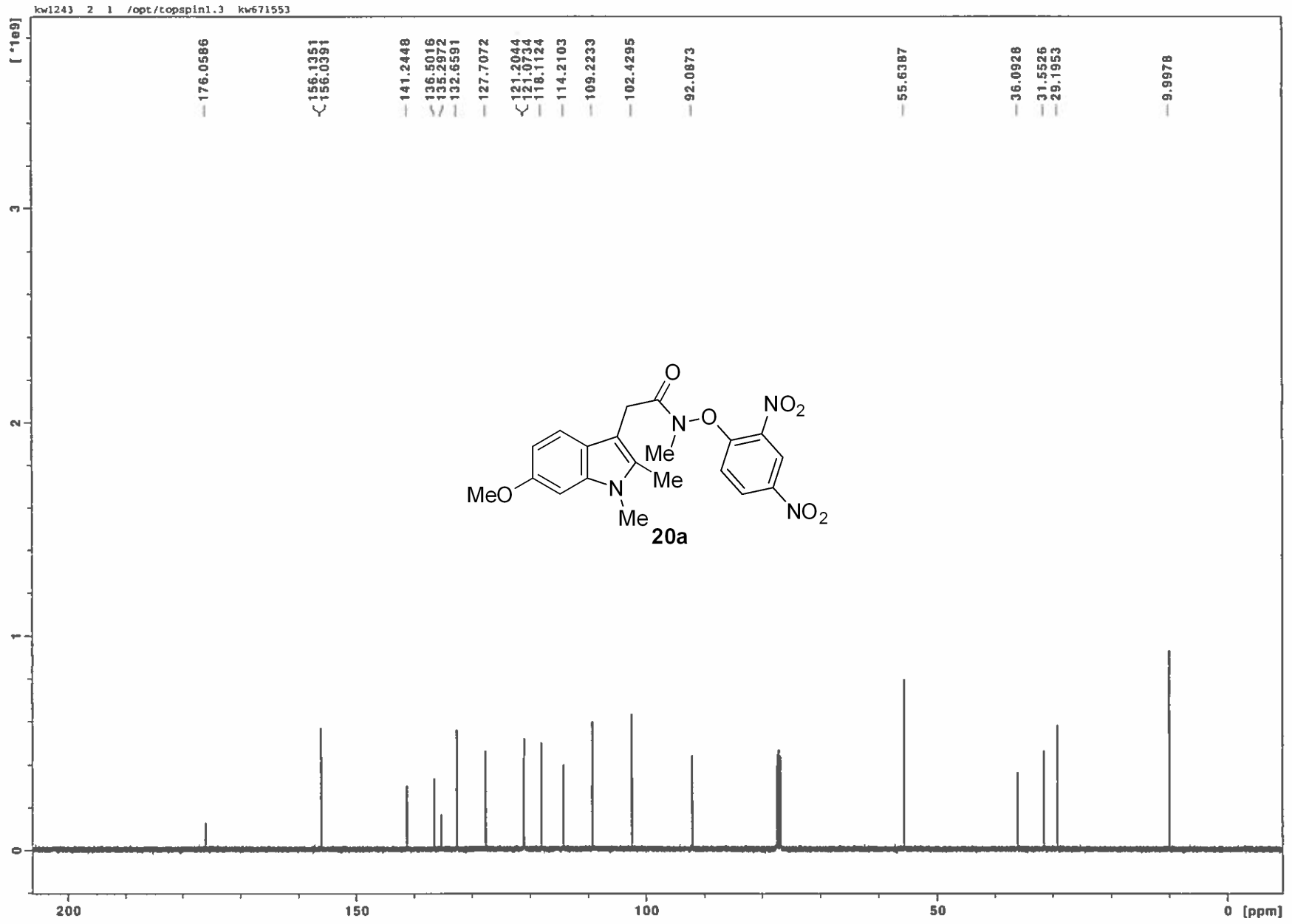
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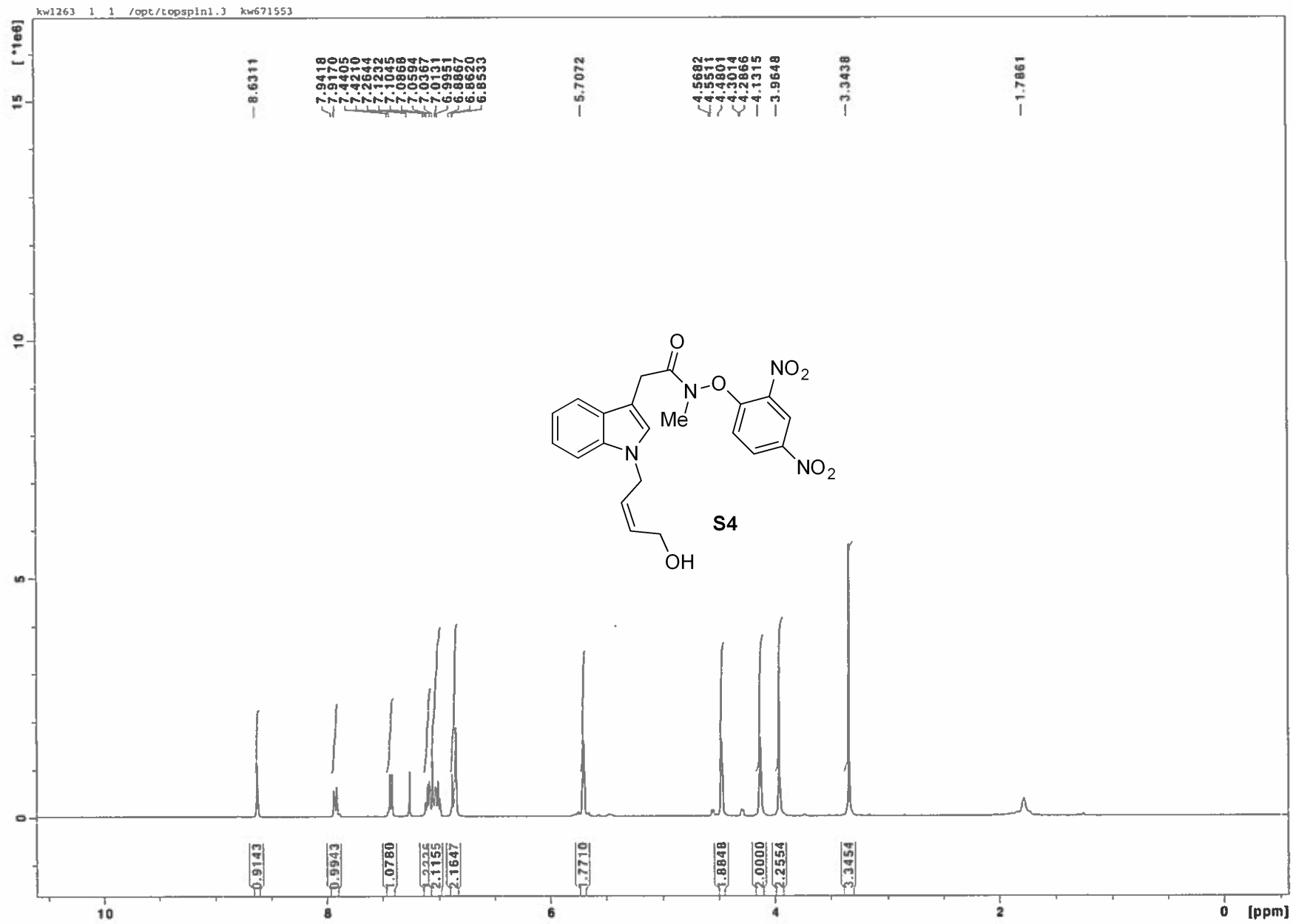
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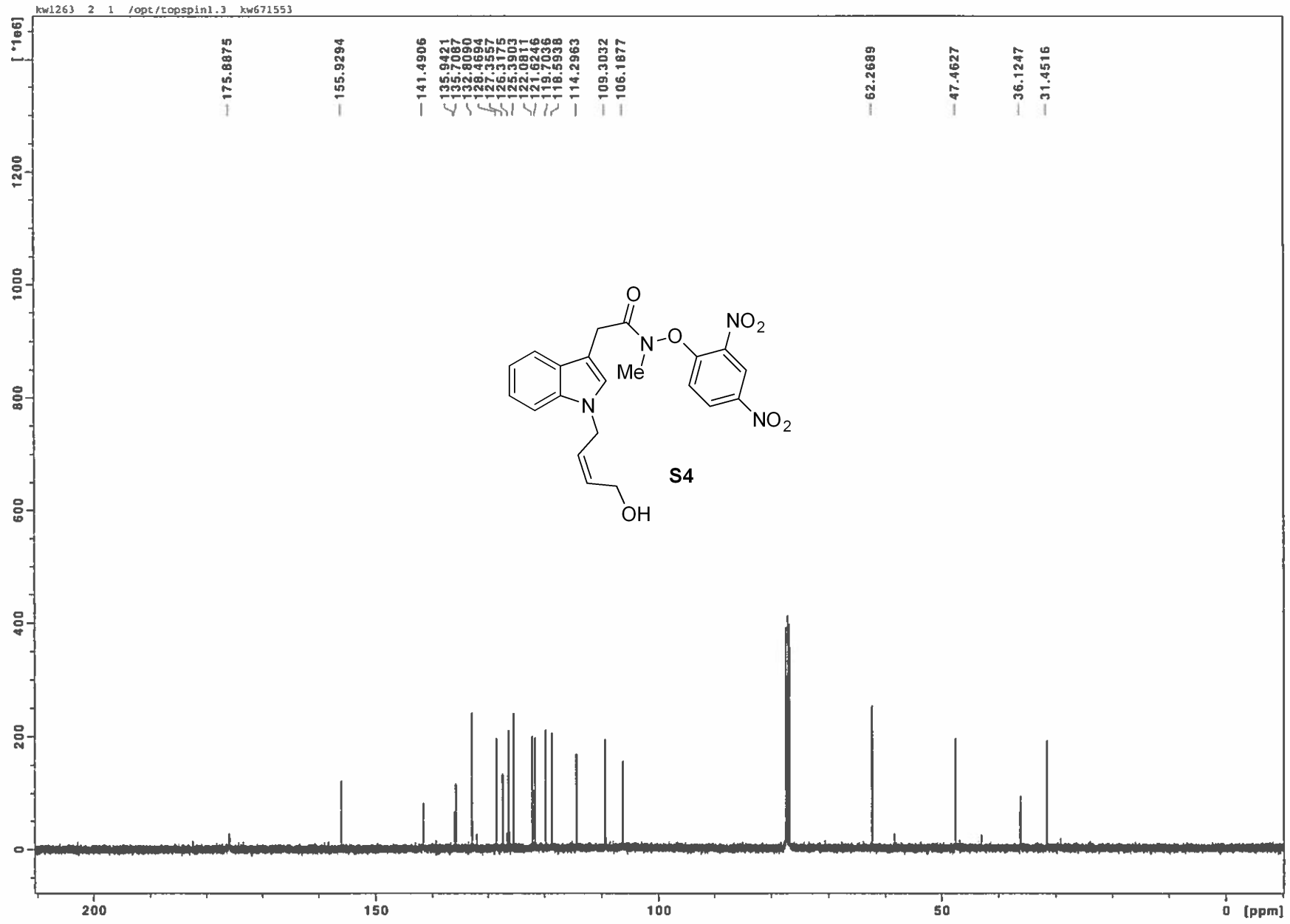
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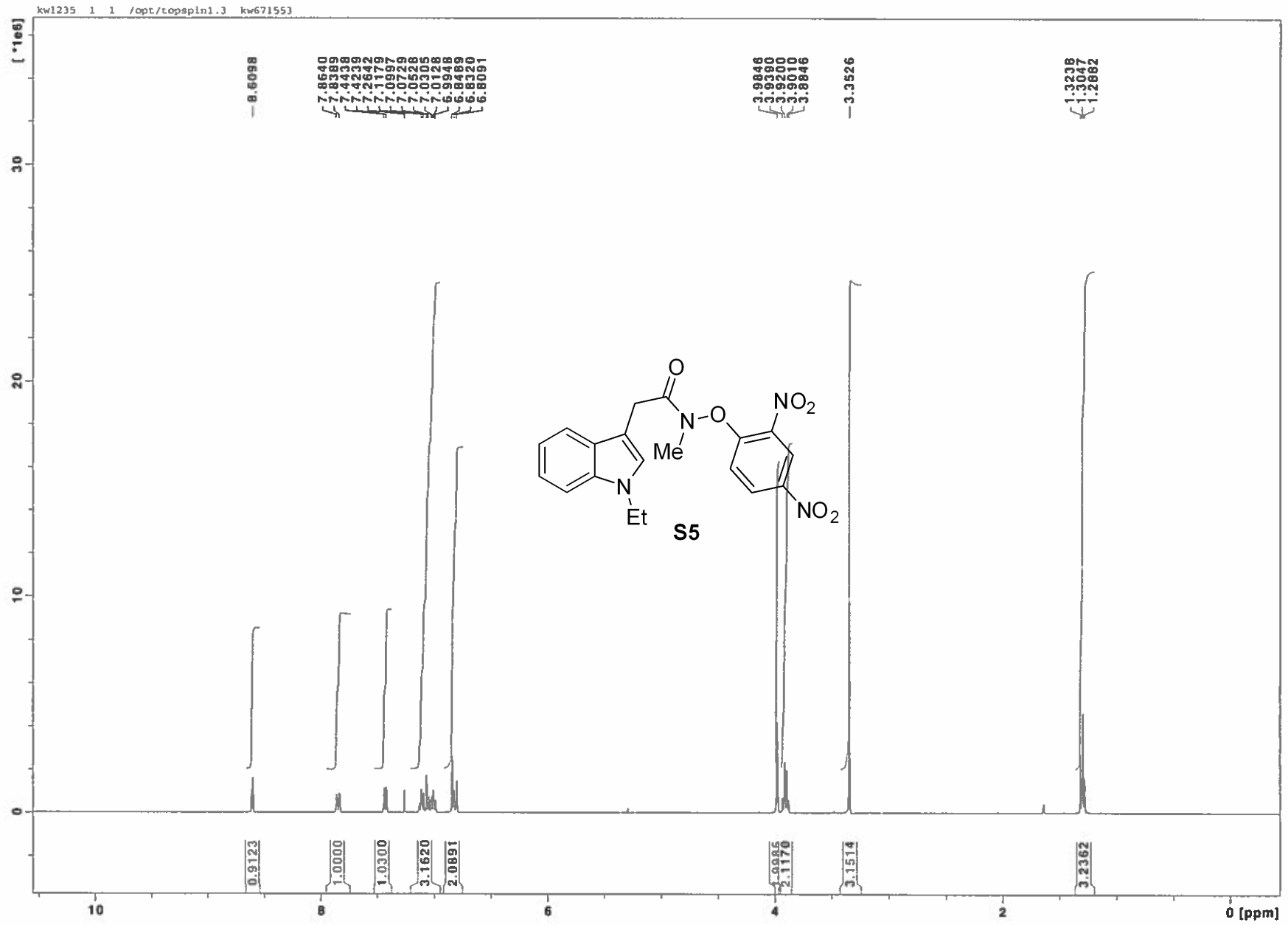
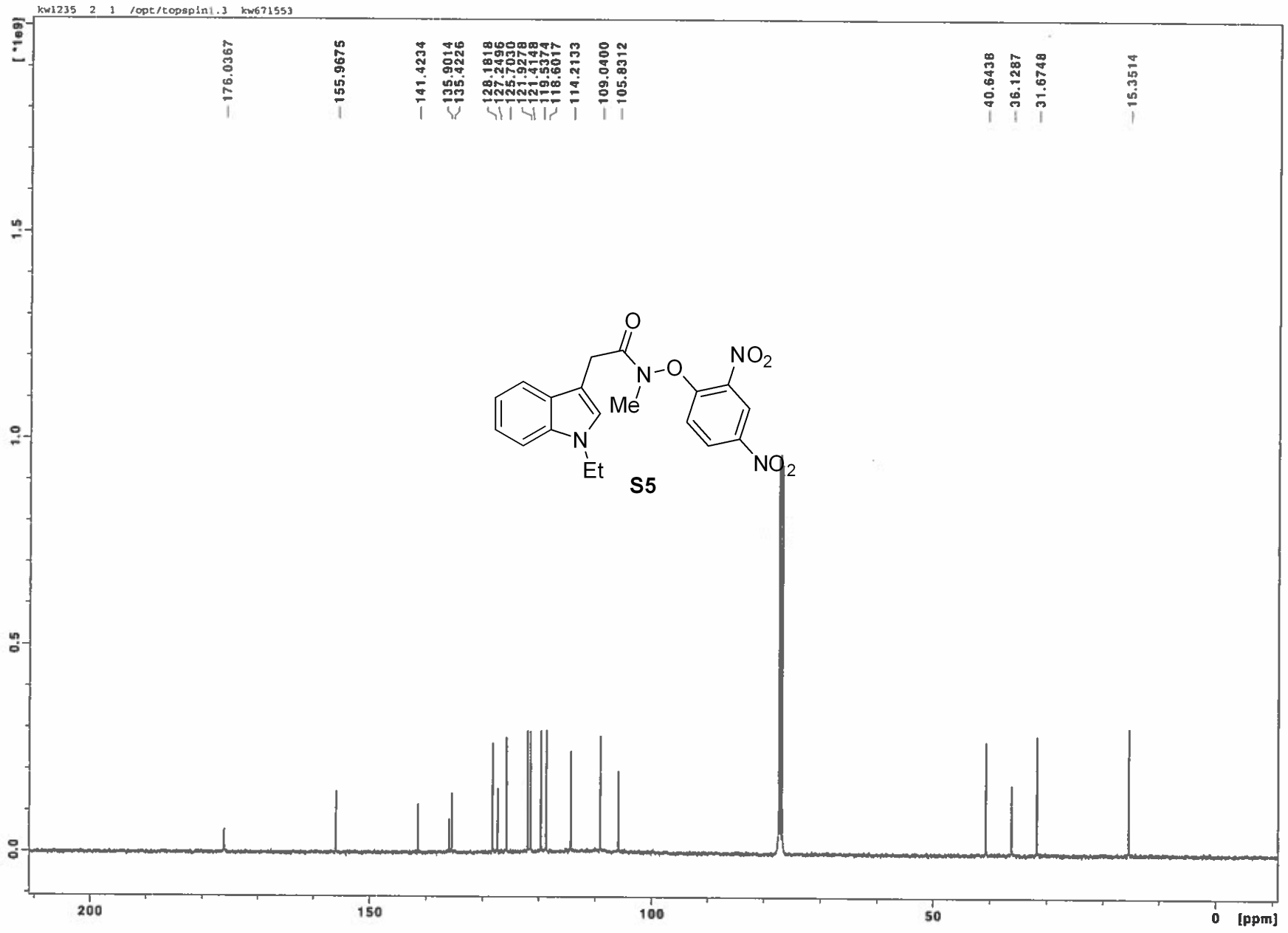
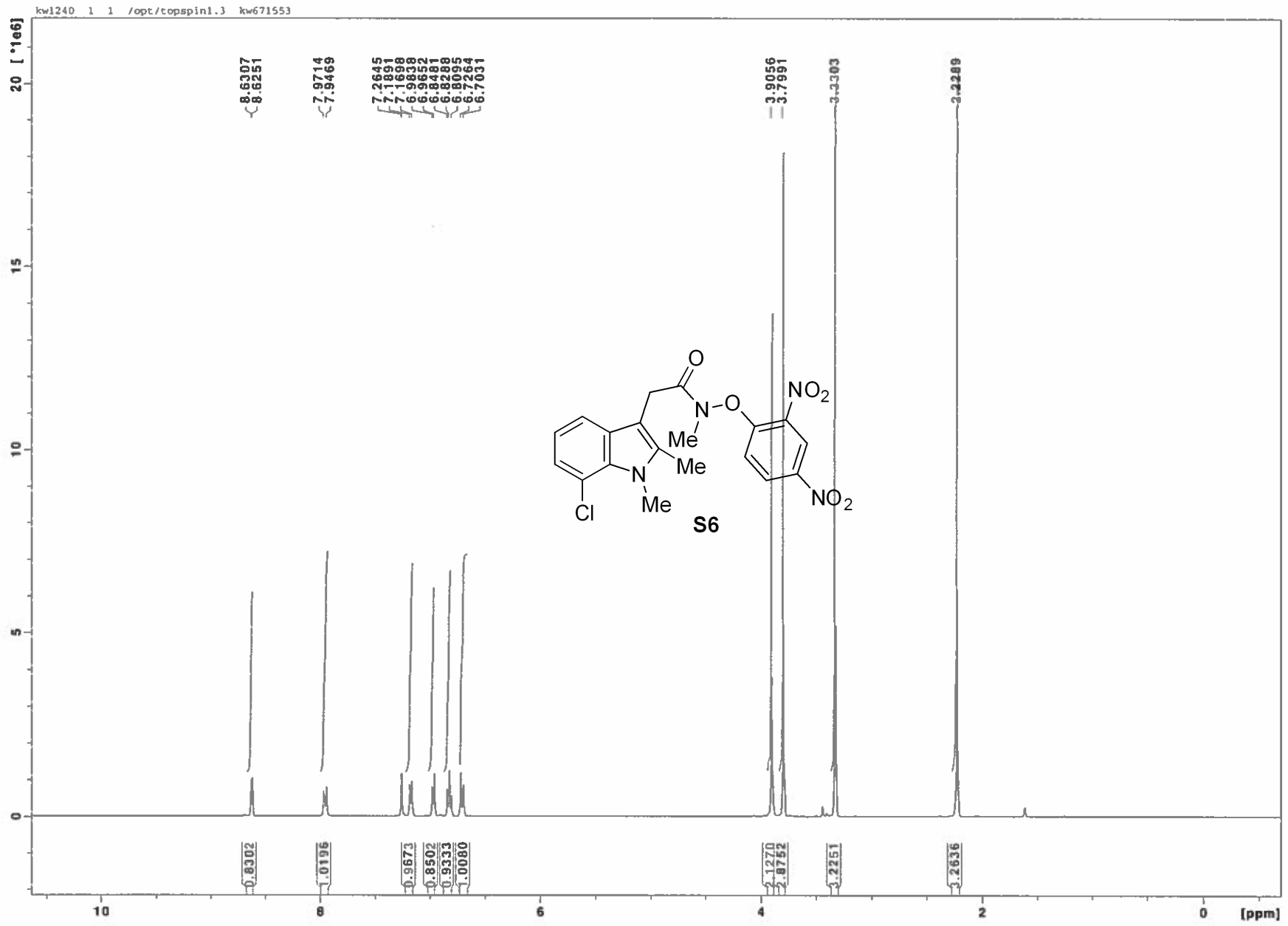
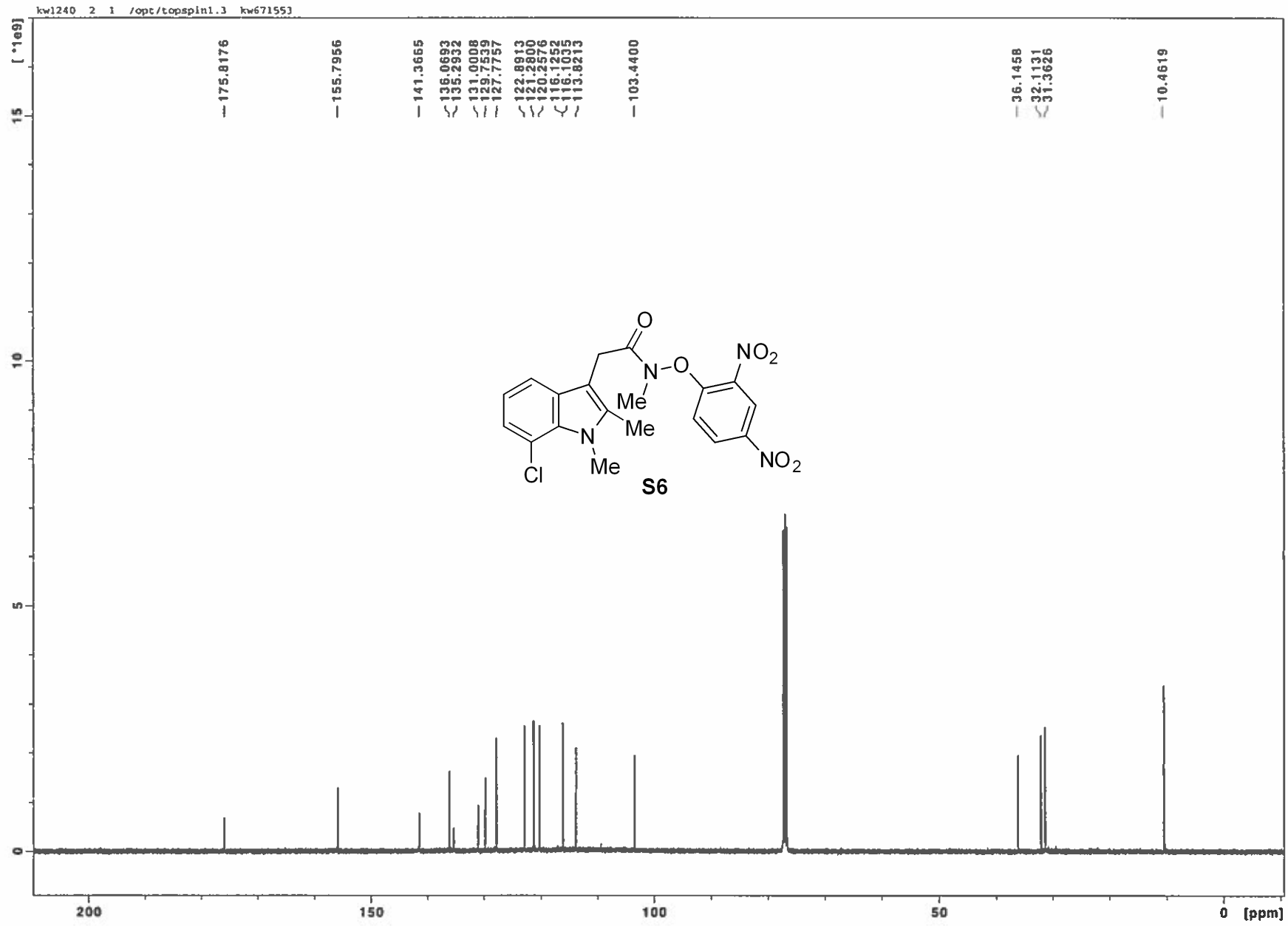
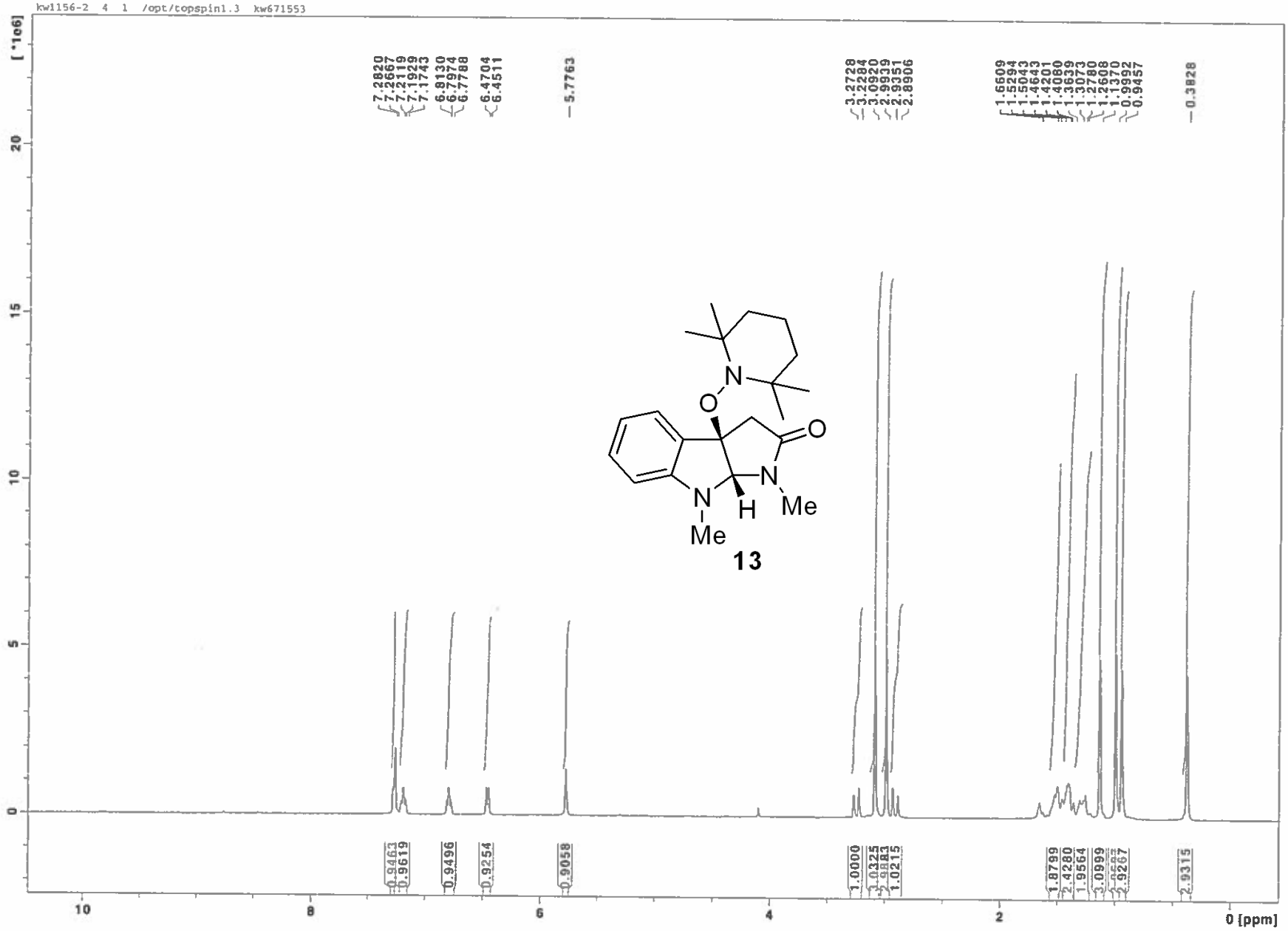
600
400
200
0
200
150
100
50
0 [ppm]
O
N
O
Me
N
NO2
NO2
OH
S4


kw1235 1 1 /opt/topspin1.3 kw671553
[*1e6]
8.6098
7.8640
7.8389
7.4438
7.4239
7.2642
7.1179
7.0997
7.0729
7.0528
7.0305
7.0128
6.9948
6.8469
6.8320
6.8091
3.9846
3.9360
3.9200
3.9010
3.8846
3.3526
1.3238
1.3047
1.2882
0.9123
1.0000
1.0300
3.1620
2.0891
1.0085
2.1170
3.1514
3.2362
10
8
6
4
2
0 [ppm]
O
N-O
Me
N
Et
NO2
NO2
S5

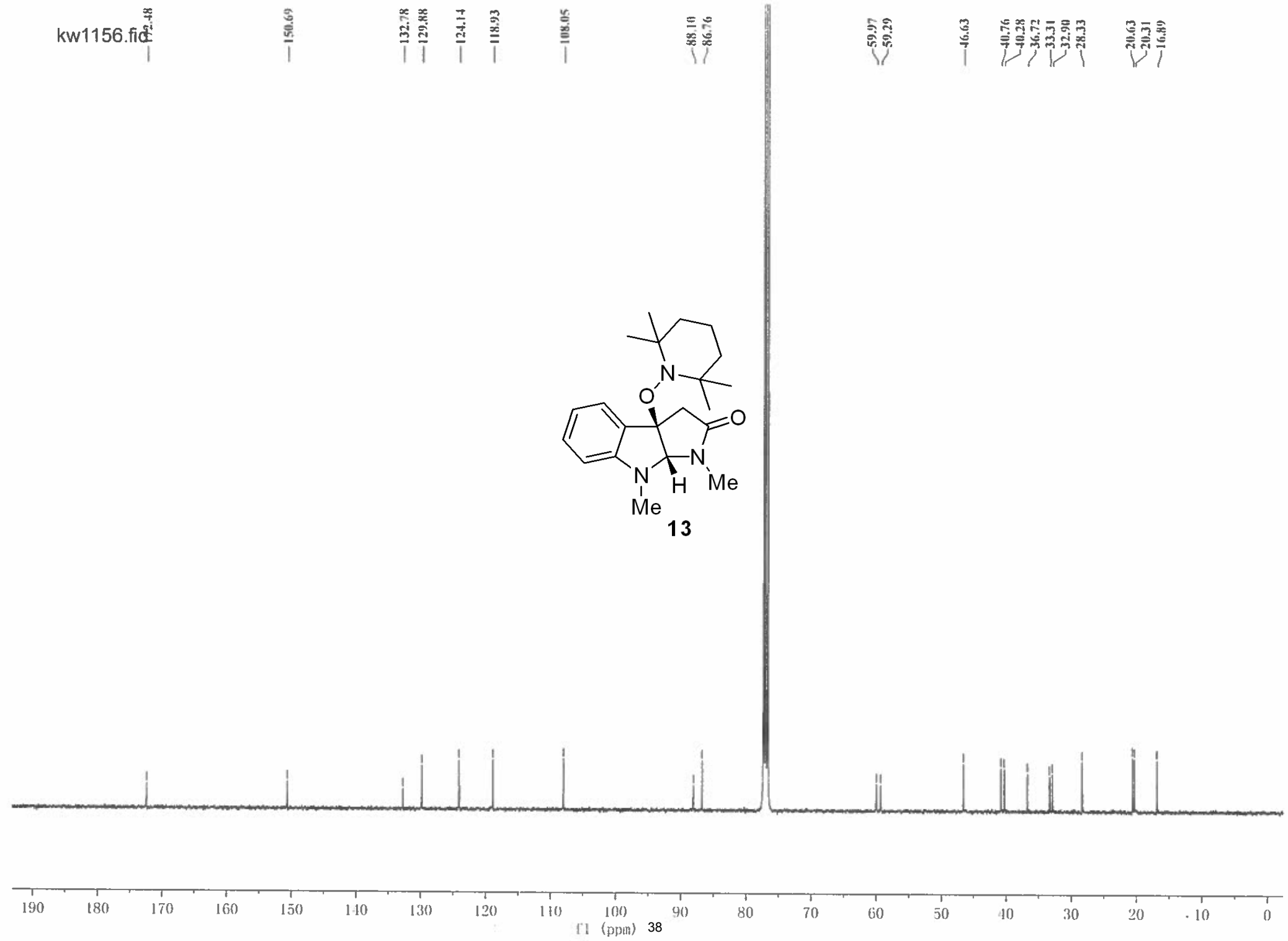

kw1235 2 1 /opt/topspin1.3 kw671553
176.0367
155.9675
141.4234
135.9014
135.4226
128.1818
127.2496
125.7030
121.9278
121.4148
119.5374
118.6017
114.2133
109.0400
105.8312
40.6438
36.1287
31.6748
15.3514
O
N
O
Me
N
Et
NO2
NO2
S5
[*1e9]
1.5
1.0
0.5
0.0
200
150
100
50
0
[ppm]

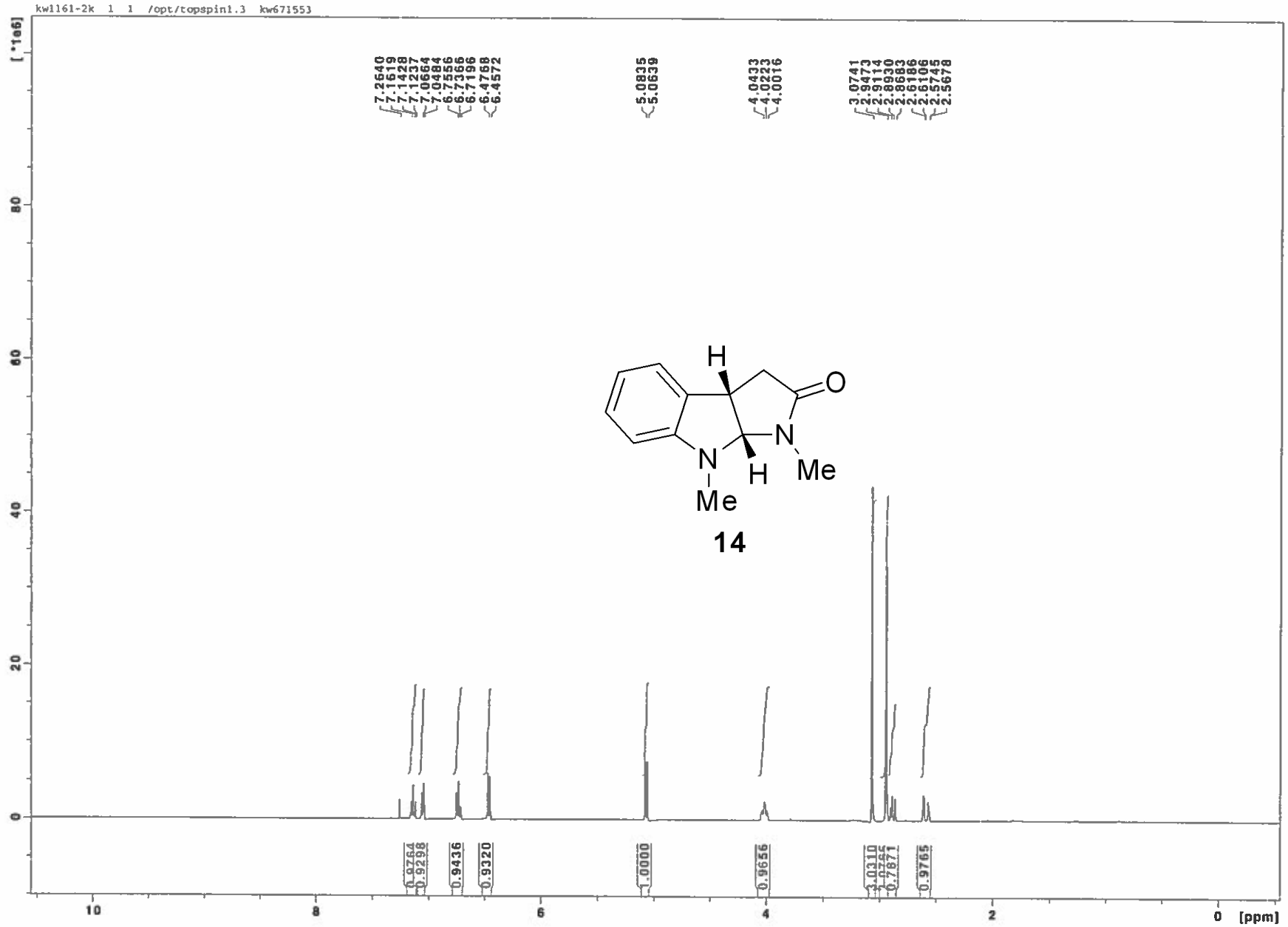

kw1240 1 1 /opt/topspin1.3 kw671553
20 [*1e6]
15
10
5
0
8.6307
8.6251
7.9714
7.9469
7.2645
7.1891
7.1698
6.9838
6.9652
6.8481
6.8288
6.8095
6.7264
6.7031
3.9056
3.7991
3.3303
3.2289
0.8302
1.0196
0.9673
0.8502
0.9333
1.0080
2.1270
2.8752
3.2251
3.2636
10
8
6
4
2
0
[ppm]
O
N
O
Me
Me
N
Me
Cl
NO2
NO2
S6


kw1240 2 1 /opt/topspin1.3 kw67155j
[*1e9]
175.8176
155.7956
141.3665
136.0693
135.2932
131.0008
129.7539
127.7757
122.8913
121.2800
120.2576
116.1252
116.1035
113.8213
103.4400
36.1458
32.1131
31.3626
10.4619
O
N
O
NO2
NO2
Me
Me
N
Me
Cl
S6
200
150
100
50
0
[ppm]

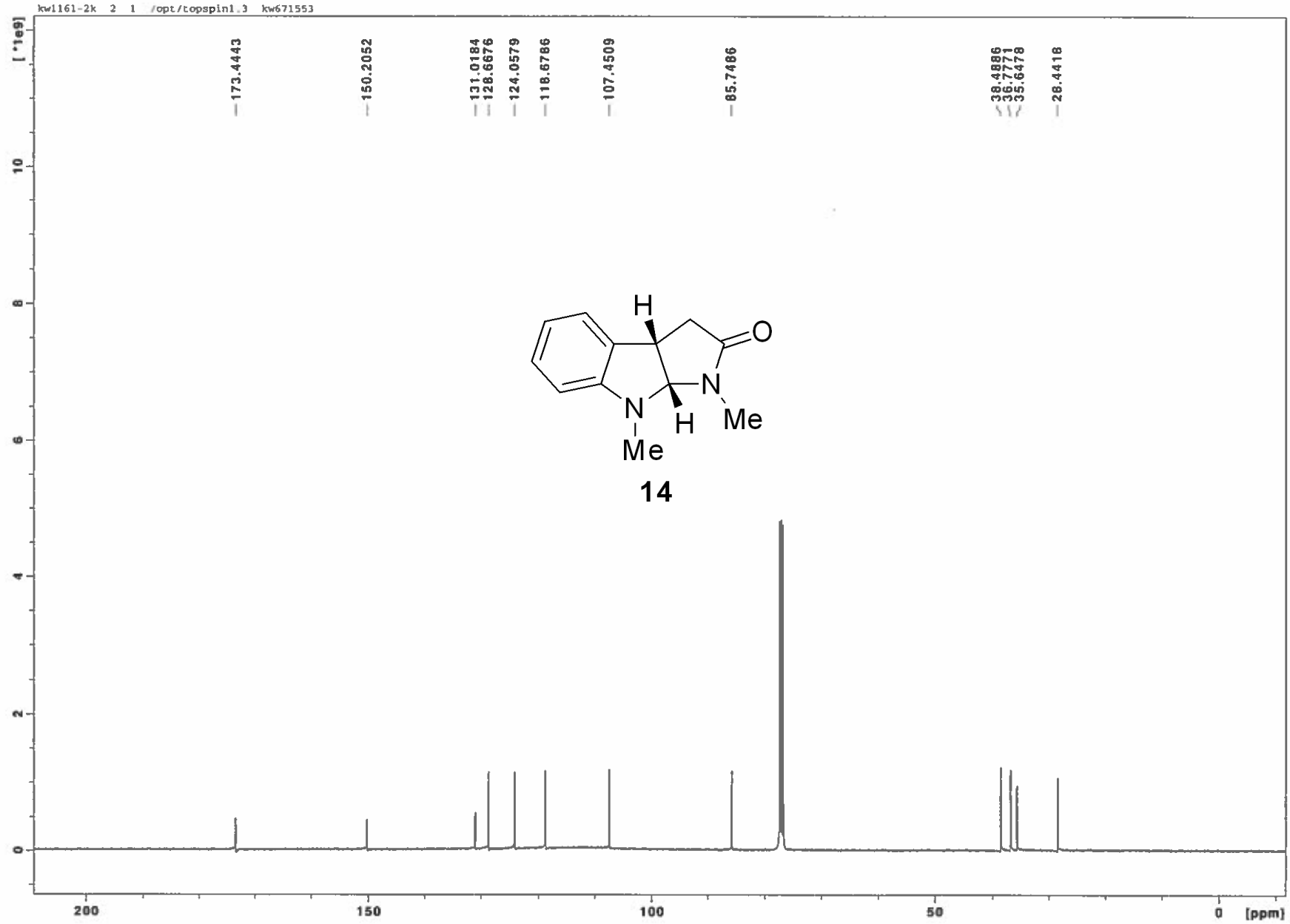

kw1156-2 4 1 /opt/topspin1.3 kw671553
[*1e6]
7.2820
7.2667
7.2119
7.1929
7.1743
6.8130
6.7974
6.7788
6.4704
6.4511
5.7763
3.2728
3.2884
3.0920
2.9939
2.9351
2.8906
1.6609
1.5294
1.5043
1.4643
1.4201
1.4080
1.3639
1.3073
1.2780
1.2608
1.1370
0.9992
0.9457
0.3828
0.9463
0.9619
0.9496
0.9254
0.9058
1.0000
1.0325
2.9881
1.0215
1.8799
2.4280
1.9564
3.0999
2.9267
2.9315
10
8
6
4
2
0 [ppm]
N
O
O
N
N
H
Me
Me

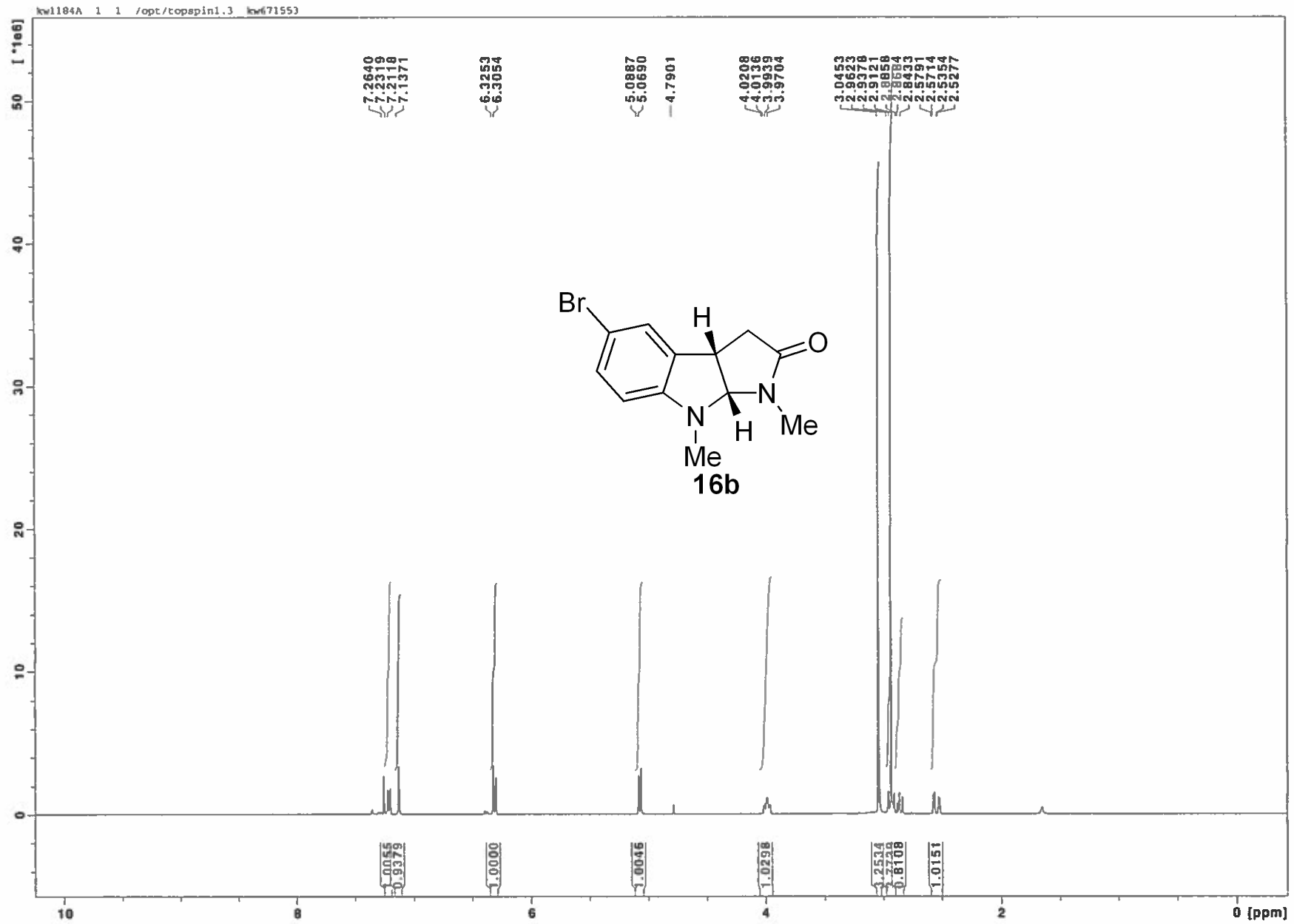
13

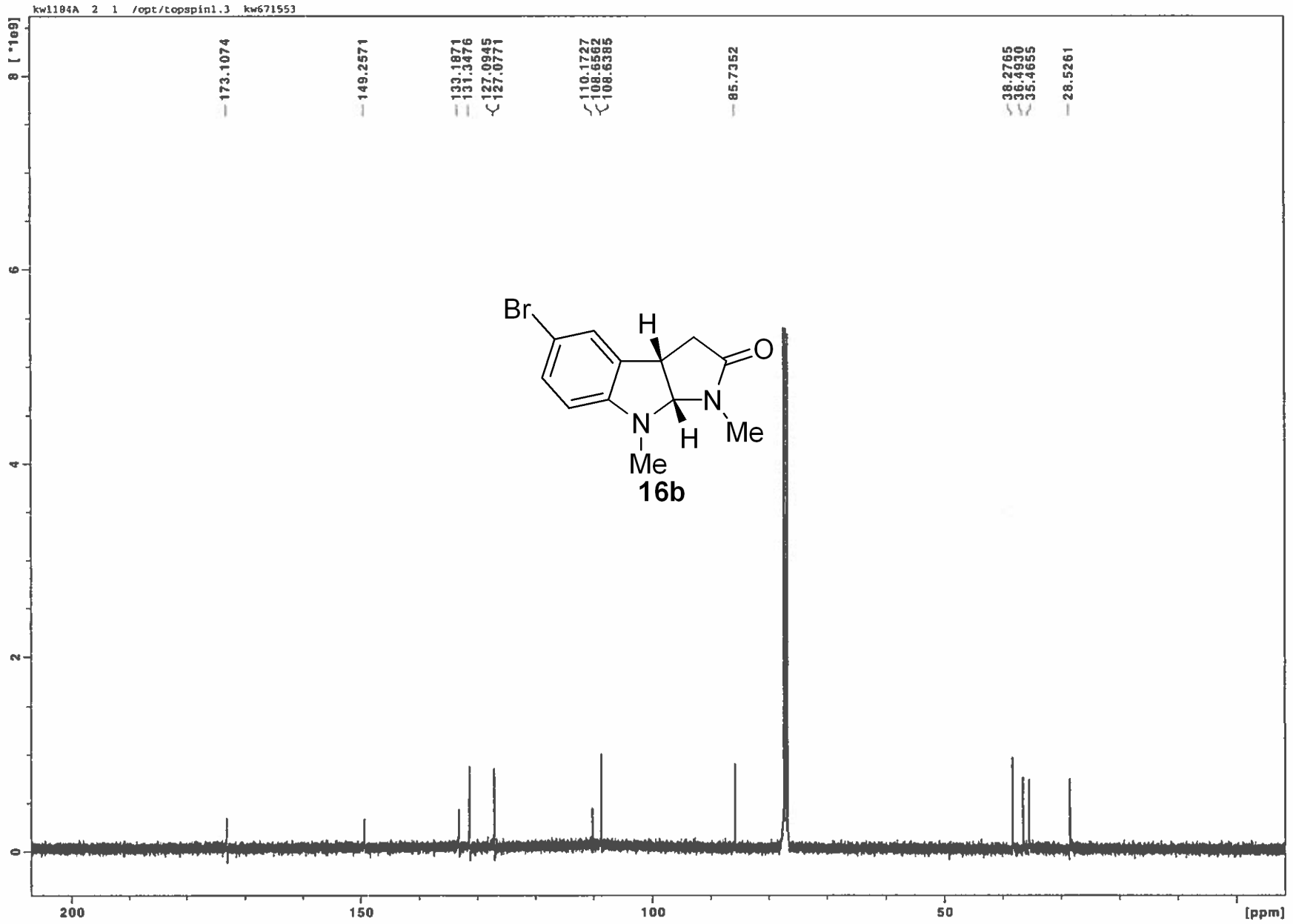

kw1156.fid
172.48
150.69
132.78
129.88
124.14
118.93
108.05
88.10
86.76
59.97
59.29
46.63
40.76
40.28
36.72
33.31
32.90
28.33
20.63
20.31
16.89
O
N
O
N
N
H
Me
Me
13
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

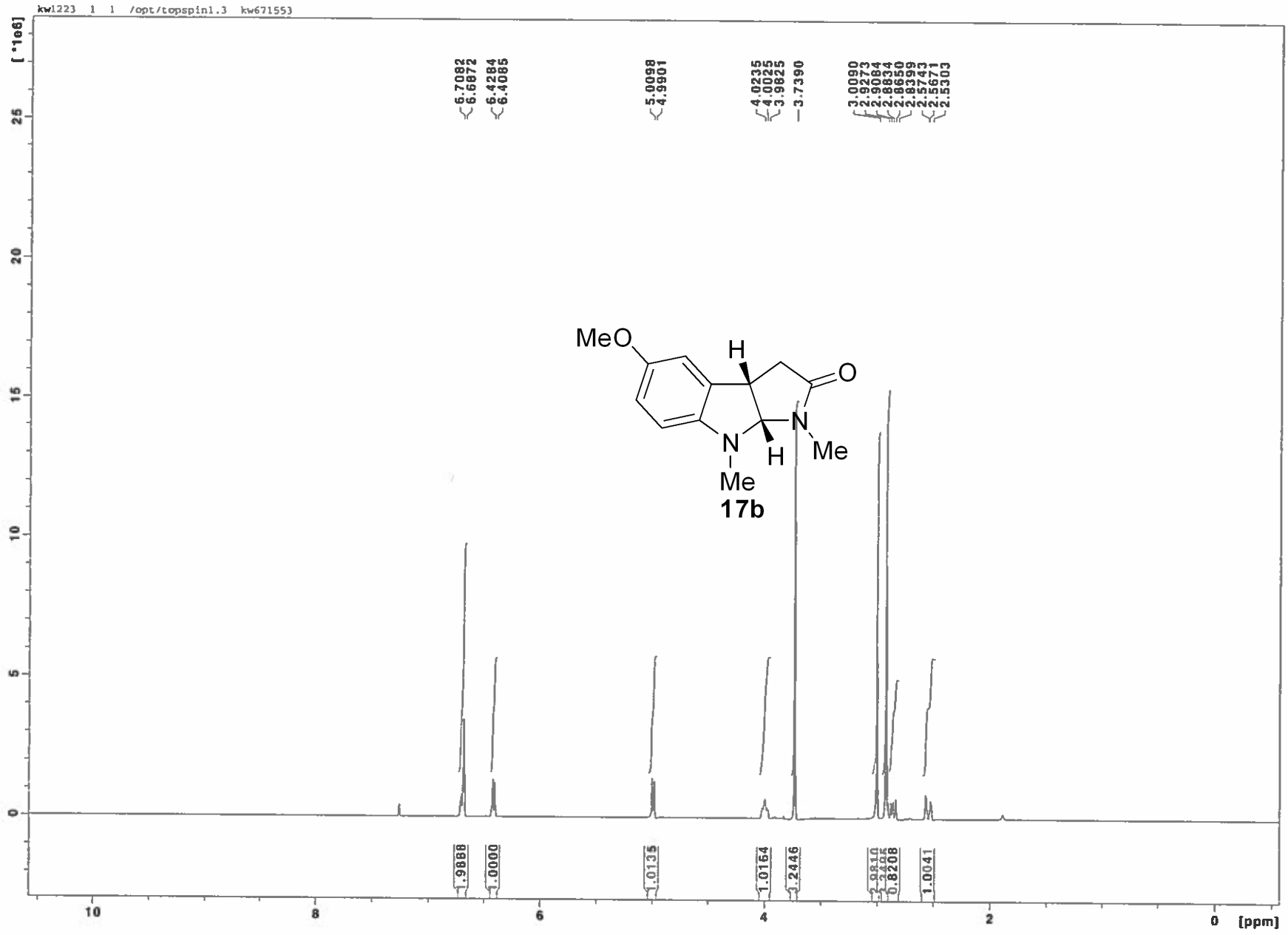

kw1161-2k 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2640
7.1619
7.1428
7.1237
7.0664
7.0484
6.7556
6.7366
6.7196
6.4768
6.4572
5.0835
5.0639
4.0433
4.0223
4.0016
3.0741
2.9473
2.9114
2.8930
2.8683
2.6186
2.6106
2.5745
2.5678
0.9764
0.9298
0.9436
0.9320
1.0000
0.9656
3.0310
3.0365
0.7871
0.9765
[ppm]
H
O
N
N
H
Me
Me

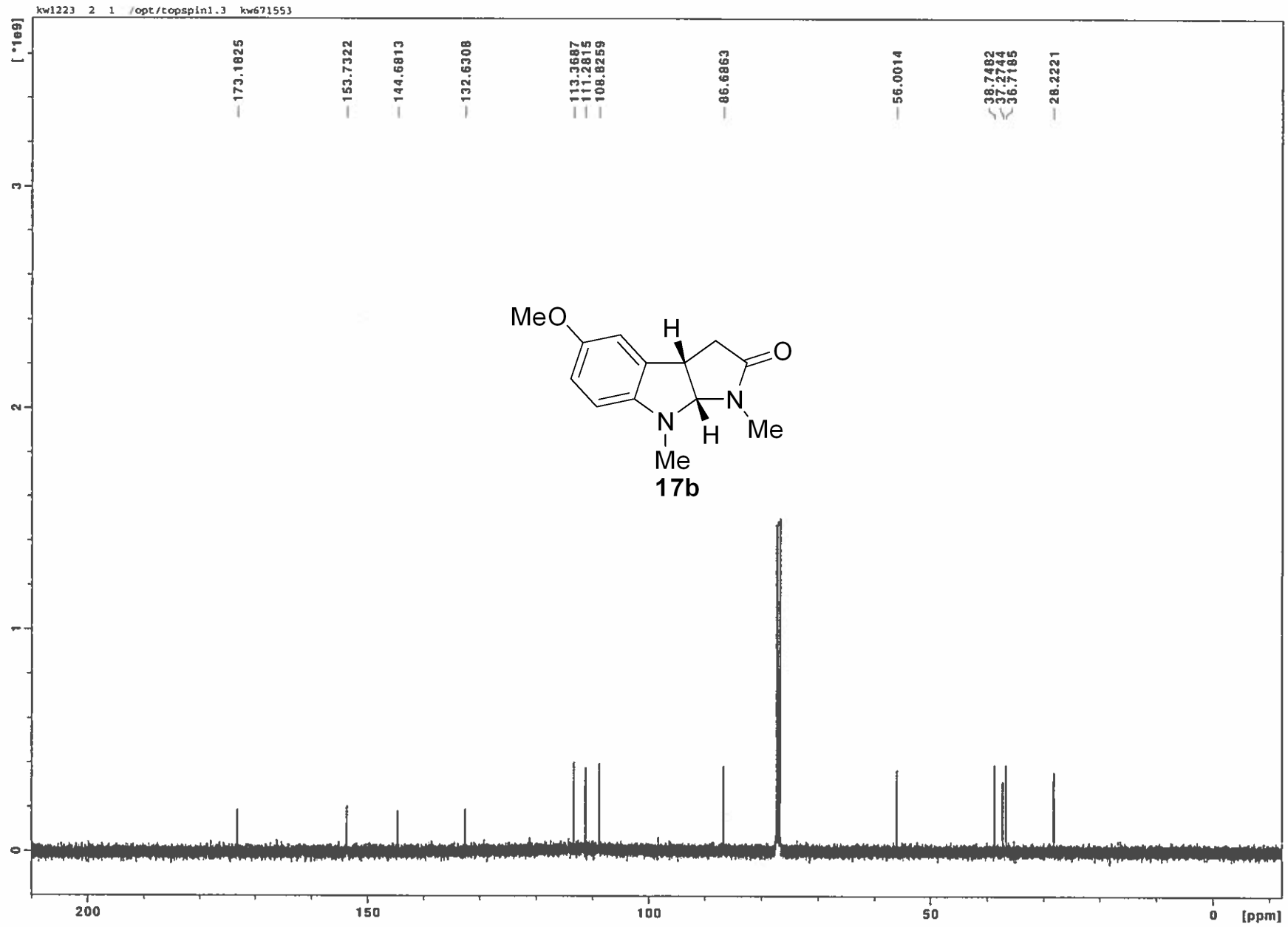
14

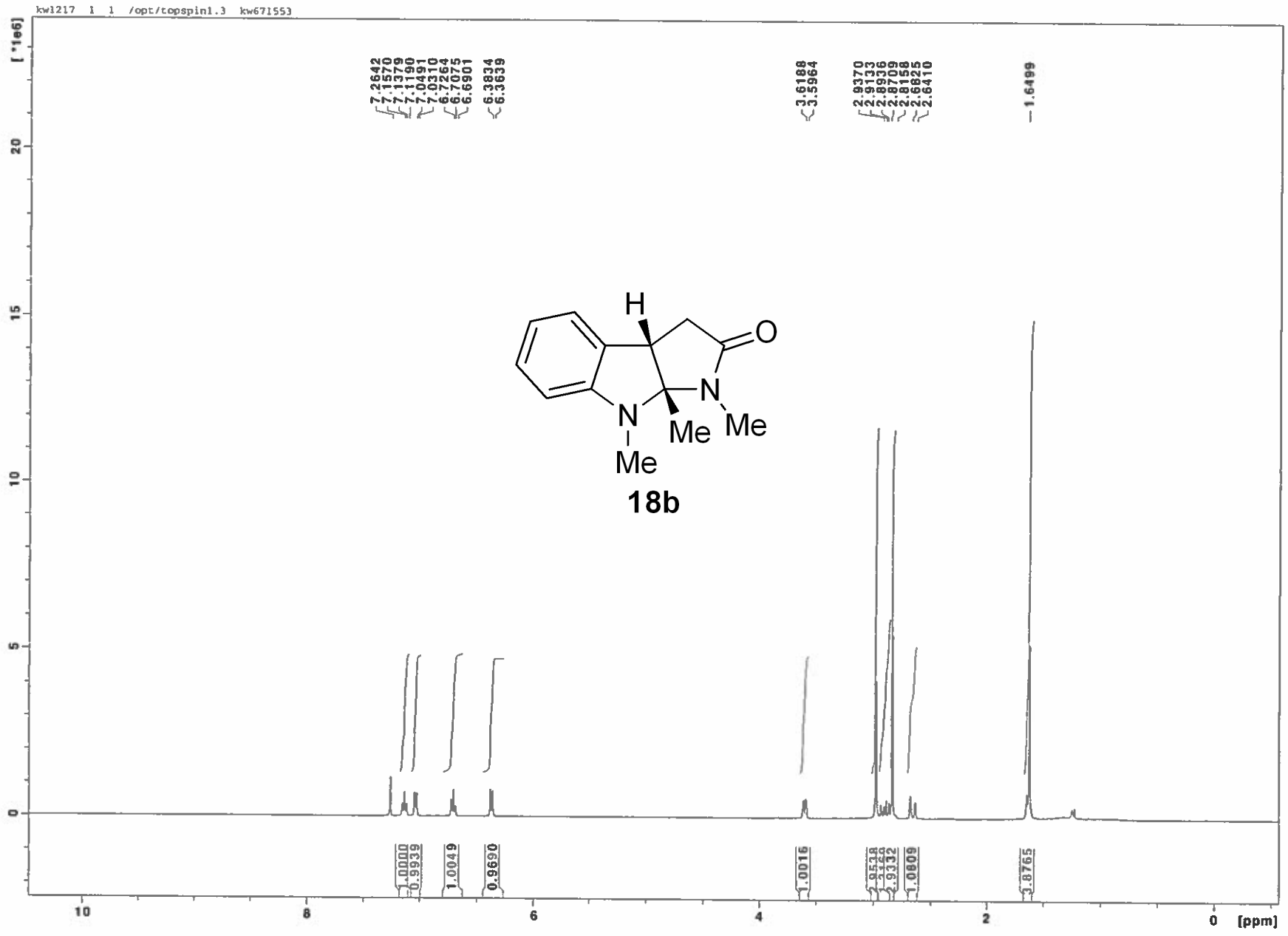

kw1161-2k 2 1 /opt/topspin1.3 kw671553
[*1e9]
173.4443
150.2052
131.0184
128.6676
124.0579
118.6786
107.4509
85.7486
38.4886
36.7771
35.6478
28.4418
H
O
N
N
H
Me
Me
14
200
150
100
50
0
[ppm]


kw1104A 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2640
7.2319
7.2118
7.1371
6.3253
6.3054
5.0887
5.0690
4.7901
4.0208
4.0136
3.9939
3.9704
3.0453
2.9623
2.9378
2.9121
2.8858
2.8433
2.5791
2.5714
2.5354
2.5277
1.0055
0.9379
1.0000
1.0046
1.0298
1.2534
0.8108
1.0151
Br
H
O
N
N
Me
H
Me
16b
10
8
6
4
2
0 [ppm]

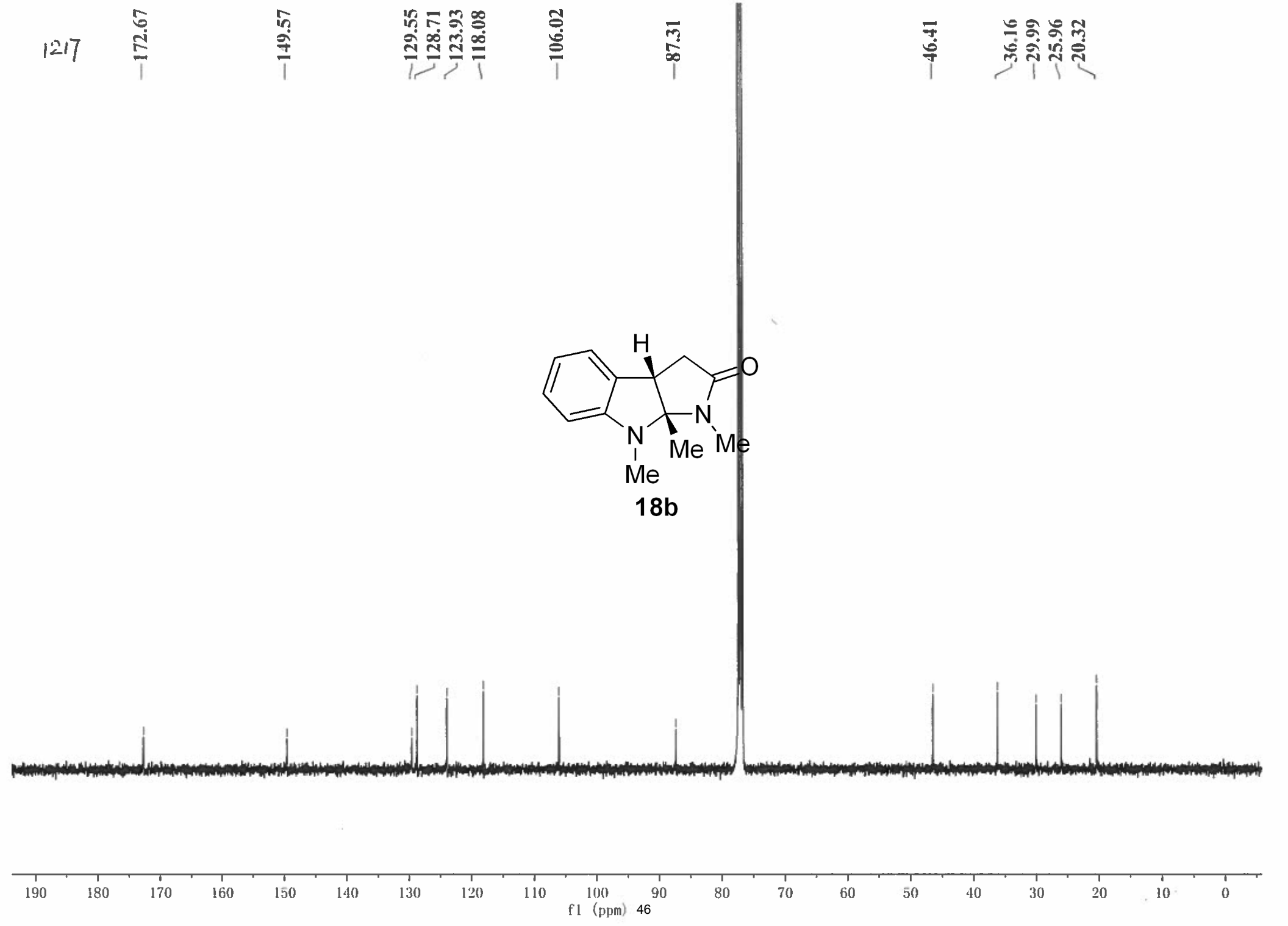

kw1104A 2 1 /opt/topspin1.3 kw671553
8 [*10^9]
6
4
2
0
173.1074
149.2571
133.1871
131.3476
127.0945
127.0771
110.1727
108.6562
108.6385
85.7352
38.2765
36.4930
35.4655
28.5261
Br
H
O
N
Me
N
H
Me
16b
200
150
100
50
[ppm]

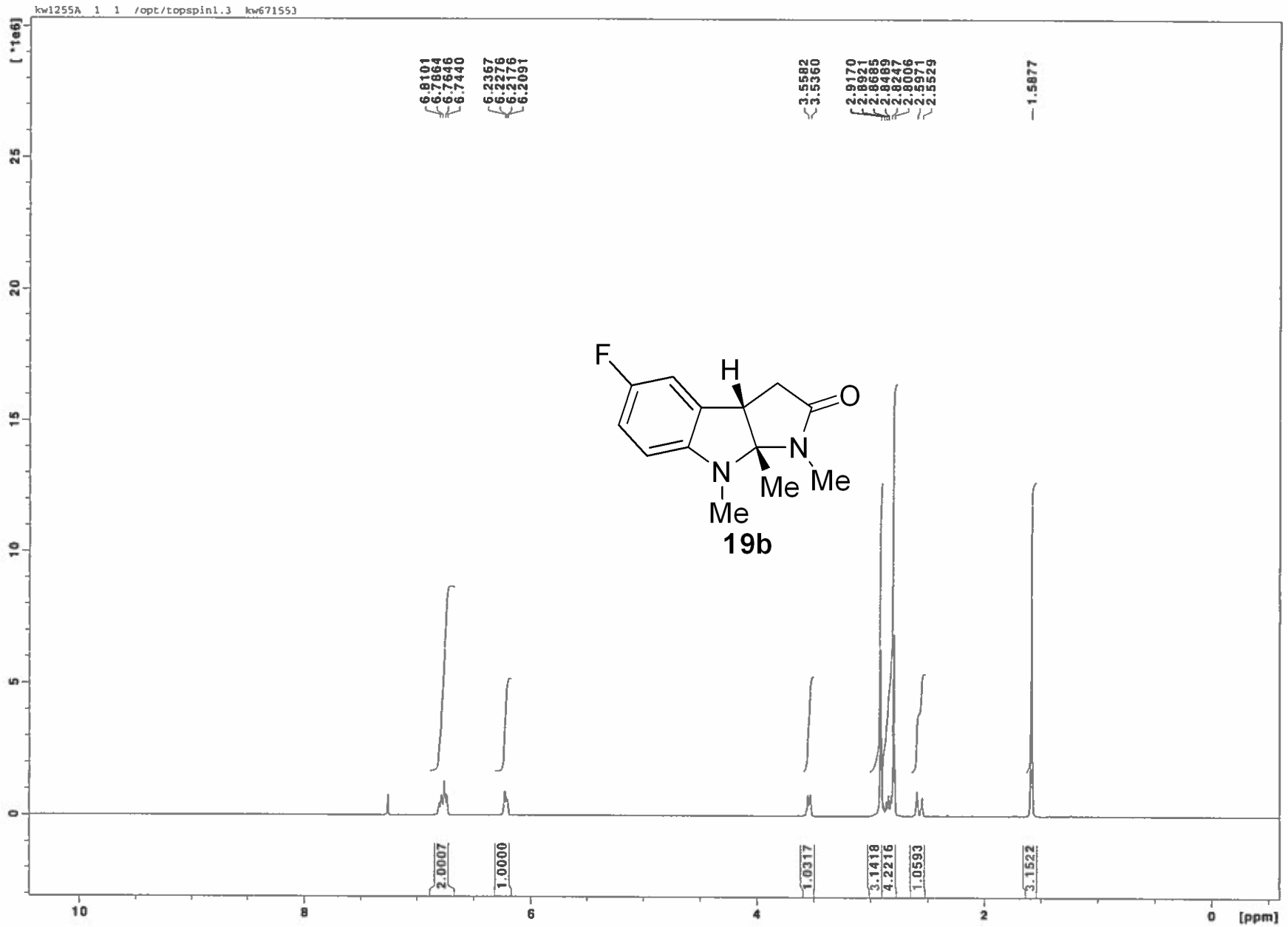

kw1223 1 1 /opt/topspin1.3 kw671553
6.7082
6.6872
6.4284
6.4085
5.0098
4.9901
4.0235
4.0025
3.9825
3.7390
3.0090
2.9273
2.9084
2.8834
2.8650
2.8399
2.5743
2.5671
2.5303
MeO
H
O
N
Me
N
H
Me
17b
1.9888
1.0000
1.0135
1.0164
2.2446
0.8208
1.0041
10
8
6
4
2
0
[ppm]

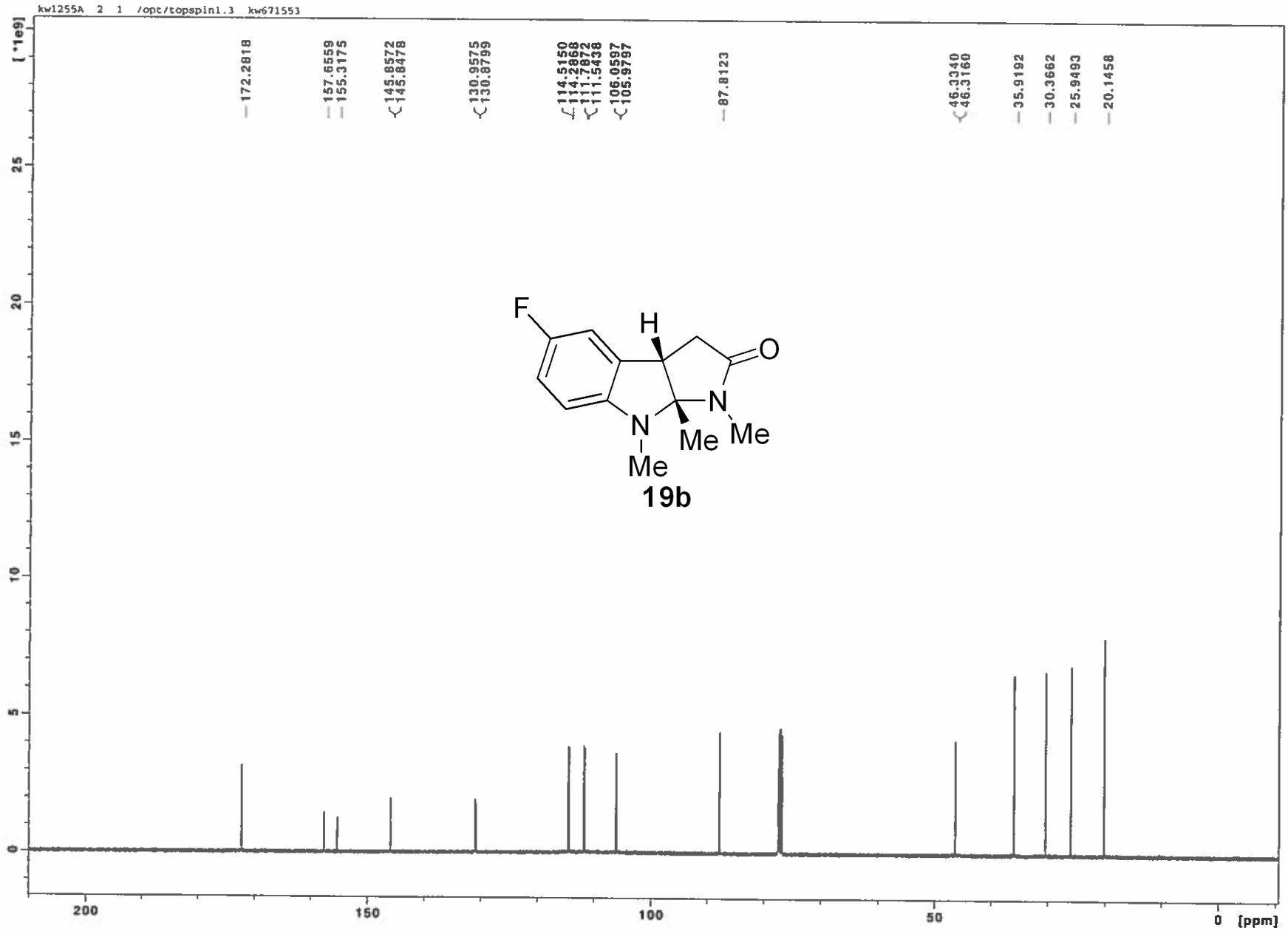

kw1223 2 1 /opt/topspin1.3 kw671553
[*1e9]
173.1825
153.7322
144.6813
132.6308
113.3687
111.2815
108.8259
86.6863
56.0014
38.7482
37.2744
36.7185
28.2221
MeO
H
O
N
Me
N
H
Me
17b
0
1
2
3
200
150
100
50
0
[ppm]

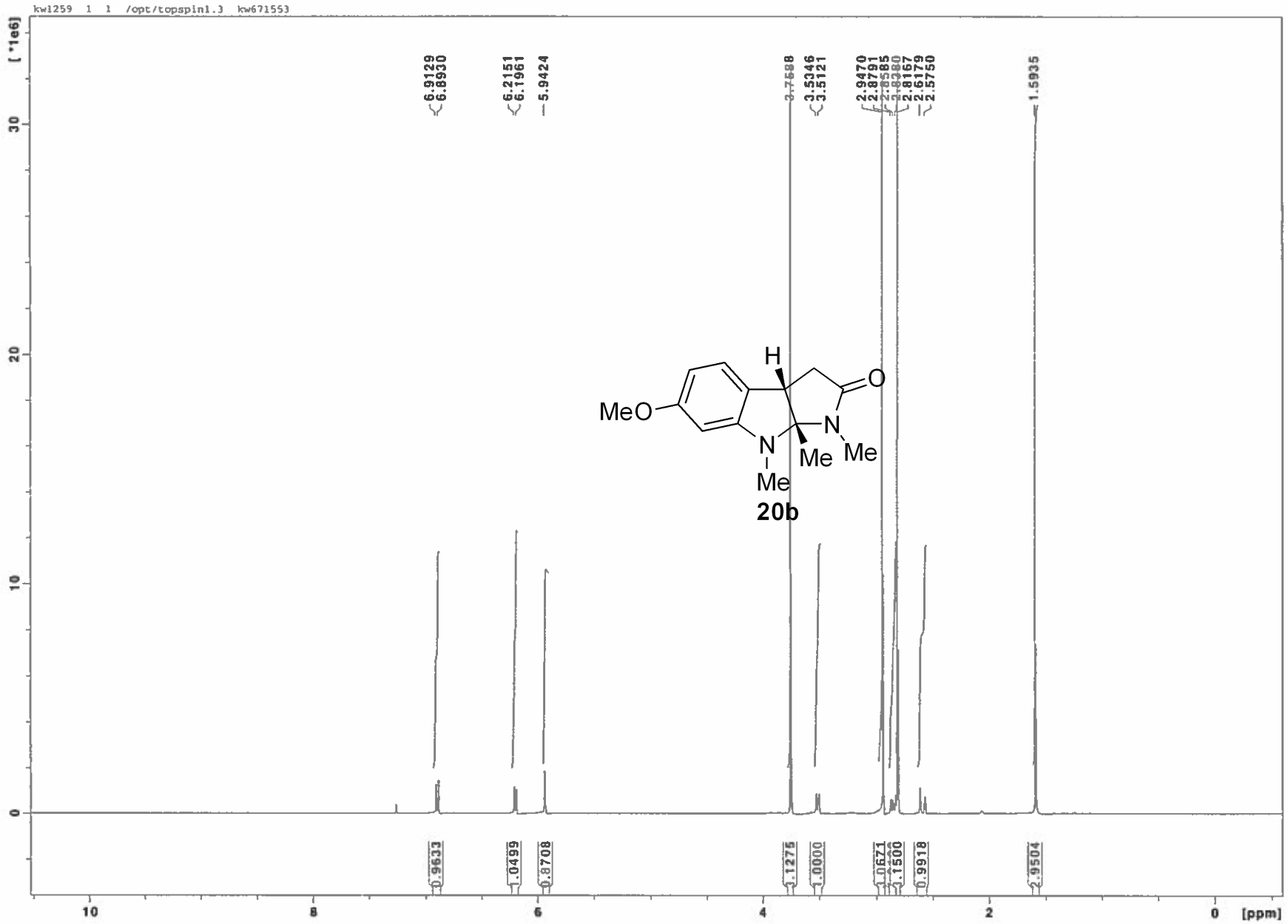

kw1217 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2642
7.1570
7.1379
7.1190
7.0491
7.0310
6.7264
6.7075
6.6901
6.3834
6.3639
3.6188
3.5964
2.9370
2.9133
2.8936
2.8709
2.8558
2.6825
2.6410
1.6499
H
O
N
N
Me
Me
Me
18b
1.0000
0.9939
1.0049
0.9690
1.0016
2.9538
2.9448
2.9332
1.0809
3.8765
10
8
6
4
2
0
[ppm]

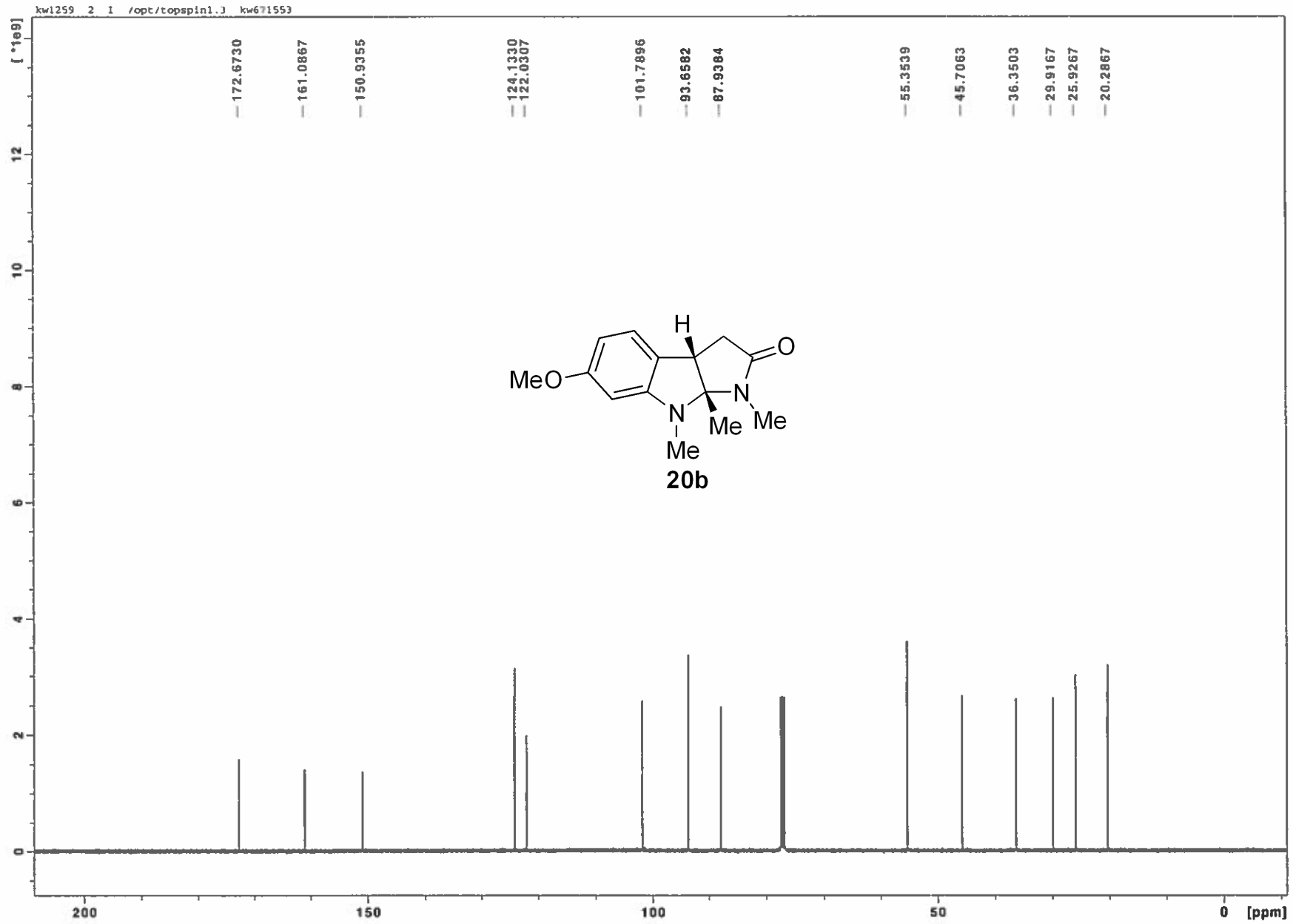
127


172.67
149.57
129.55
128.71
123.93
118.08
106.02
87.31
46.41
36.16
29.99
25.96
20.32
H
O
N
N
Me
Me
Me
18b
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

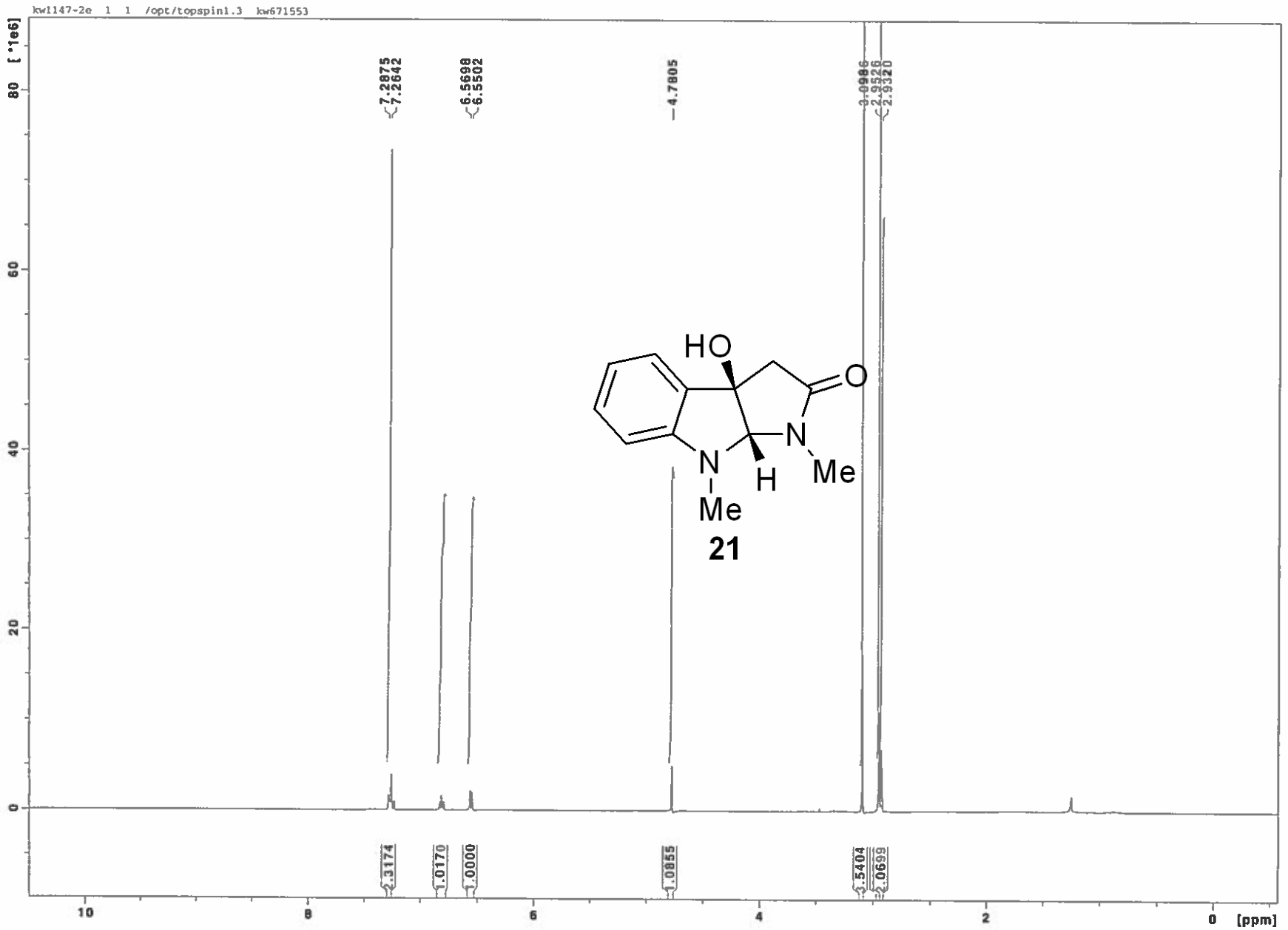

kw1255A 1 1 /opt/topspin1.3 kw671553
[*1e6]
6.8101
6.7864
6.7646
6.7440
6.2367
6.2276
6.2176
6.2091
3.5582
3.5360
2.9170
2.8921
2.8685
2.8489
2.8247
2.8006
2.5971
2.5529
1.5877
F
H
O
N
N
Me
Me
Me
19b
2.0007
1.0000
1.0317
3.1418
4.2216
1.0593
3.1522
10
8
6
4
2
0
[ppm]

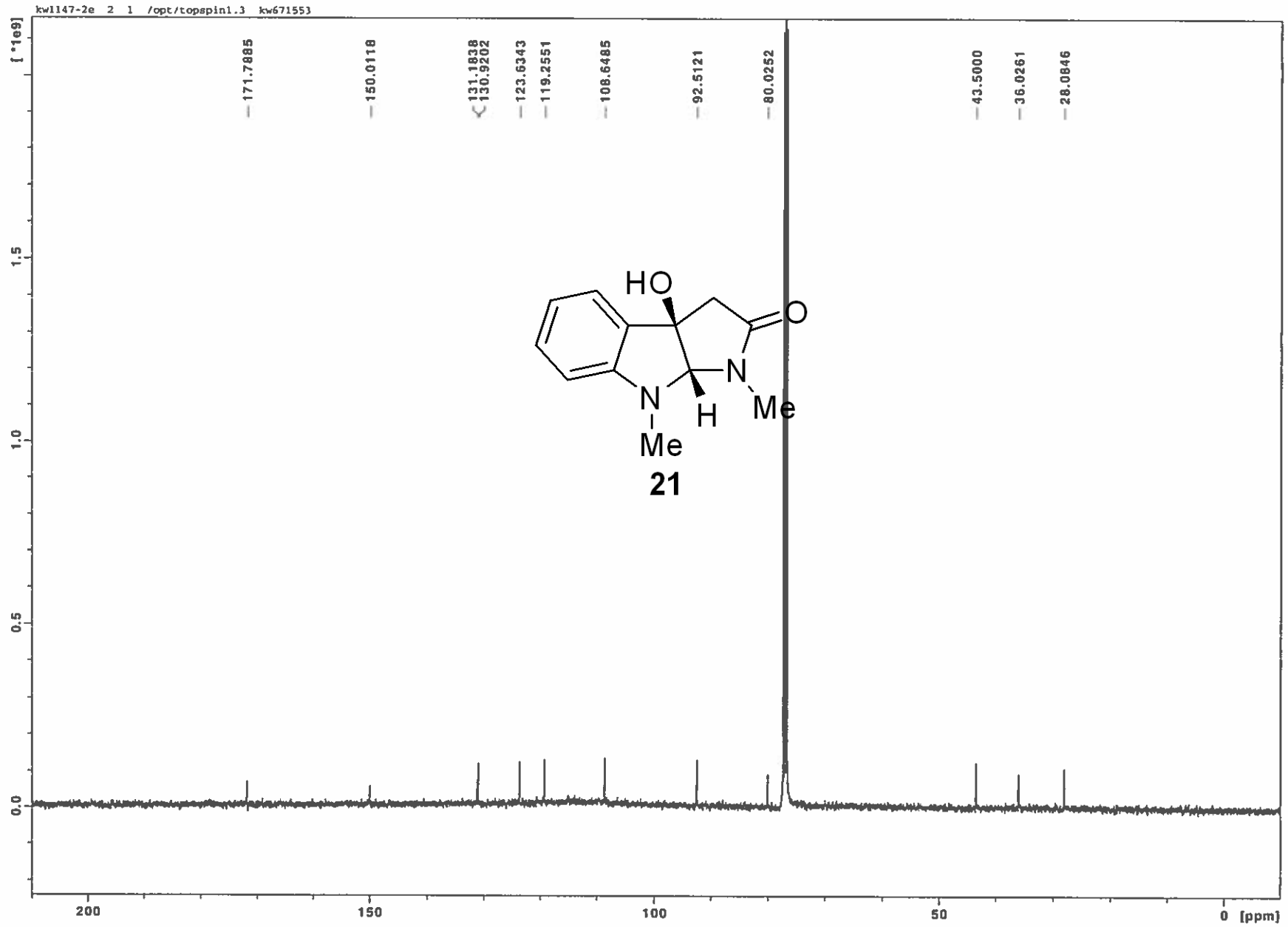

kw1255A 2 1 /opt/topspin1.3 kw671553
[*1e9]
172.2818
157.6559
155.3175
145.8572
145.8478
130.9575
130.8799
114.5150
114.2868
111.7872
111.5438
106.0597
105.9797
87.8123
46.3340
46.3160
35.9192
30.3662
25.9493
20.1458
F
H
O
N
N
Me
Me
Me
19b
0
5
10
15
20
25
200
150
100
50
0
[ppm]

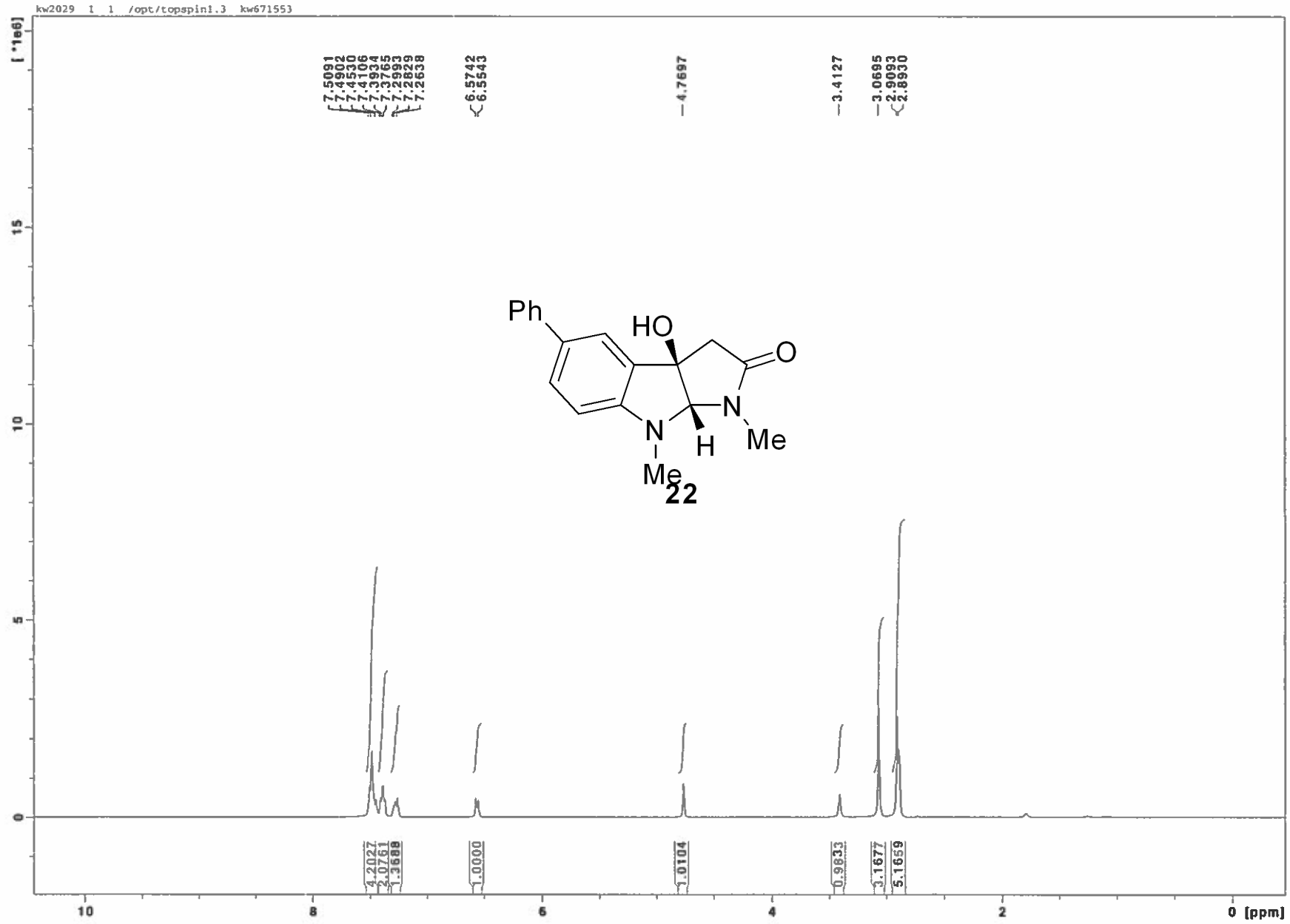

kw1259 1 1 /opt/topspin1.3 kw671553
[*1e6]
6.9129
6.8930
6.2151
6.1961
5.9424
3.7688
3.5346
3.5121
2.9470
2.8791
2.8585
2.8380
2.8167
2.6179
2.5750
1.5935
0.9633
1.0499
0.8708
1.1275
1.0000
1.0621
1.1444
1.1500
0.9918
2.9504
[ppm]
MeO
H
O
N
Me
N
Me
Me
20b

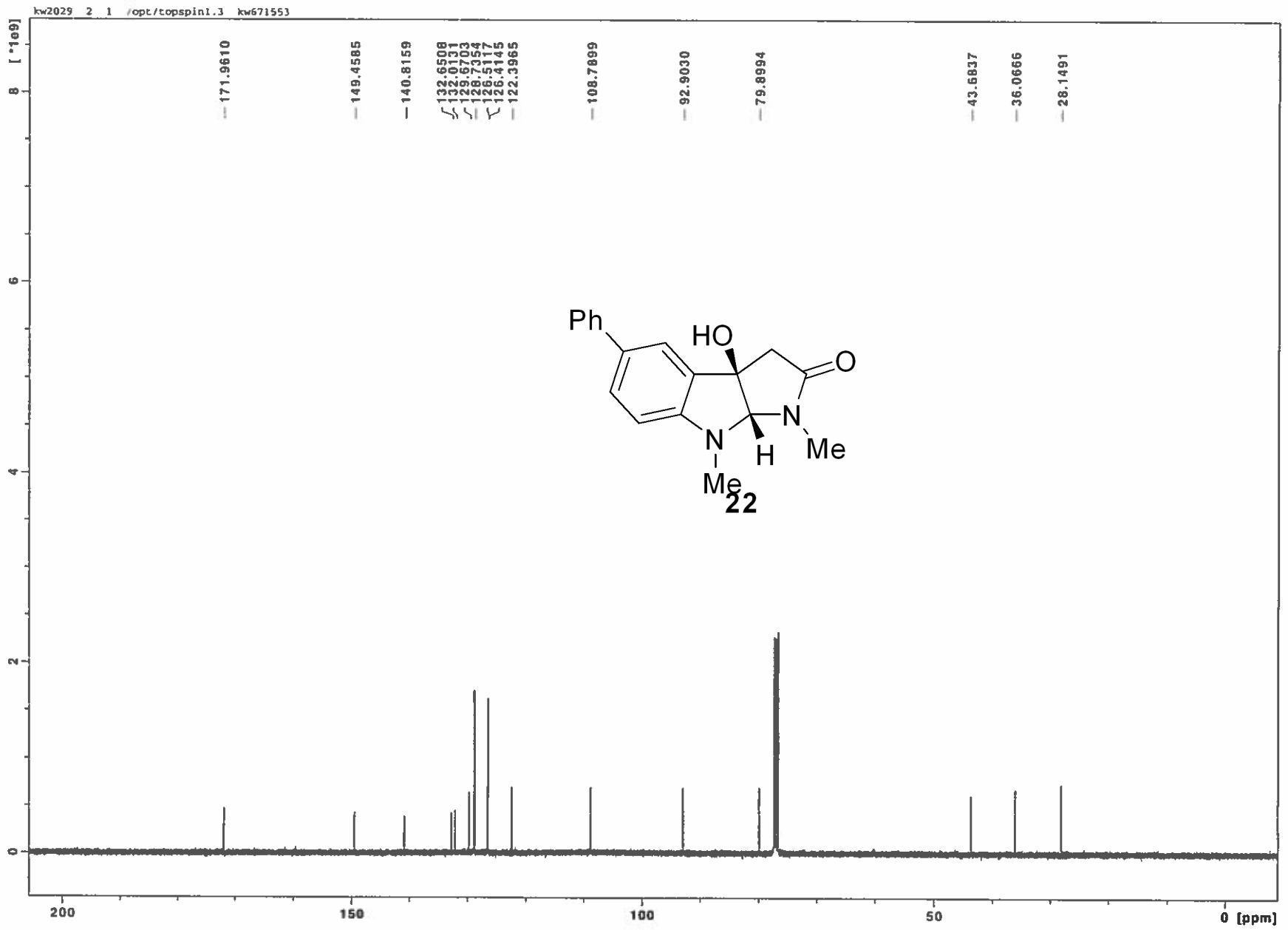

kw1259 2 1 /opt/topspin1.3 kw671553
[*1e9]
172.6730
161.0867
150.9355
124.1330
122.0307
101.7896
93.6582
87.9384
55.3539
45.7063
36.3503
29.9167
25.9267
20.2867
MeO
H
O
N
N
Me
Me
Me
0
2
4
6
8
10
12
200
150
100
50
0
[ppm]

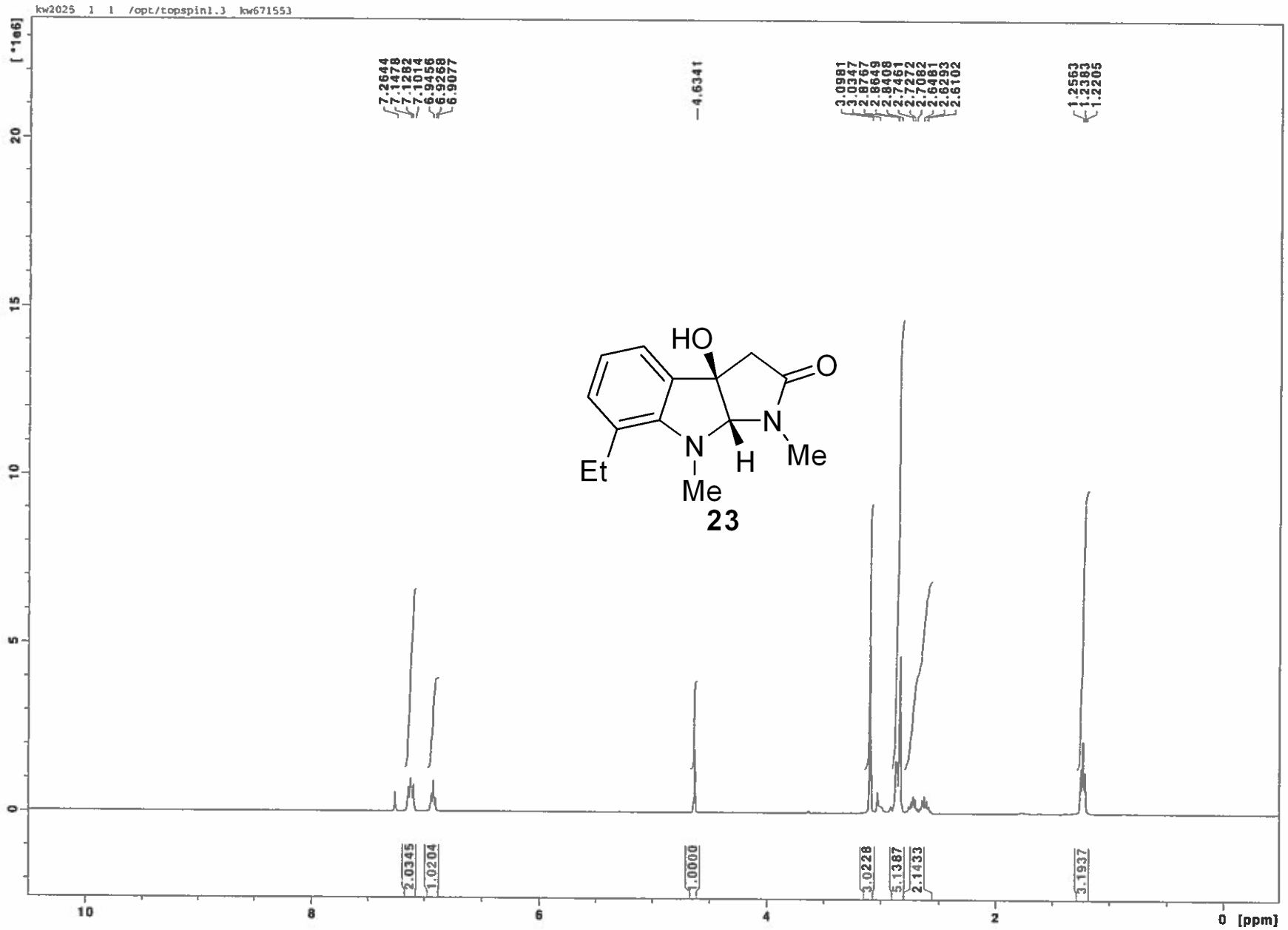
20b

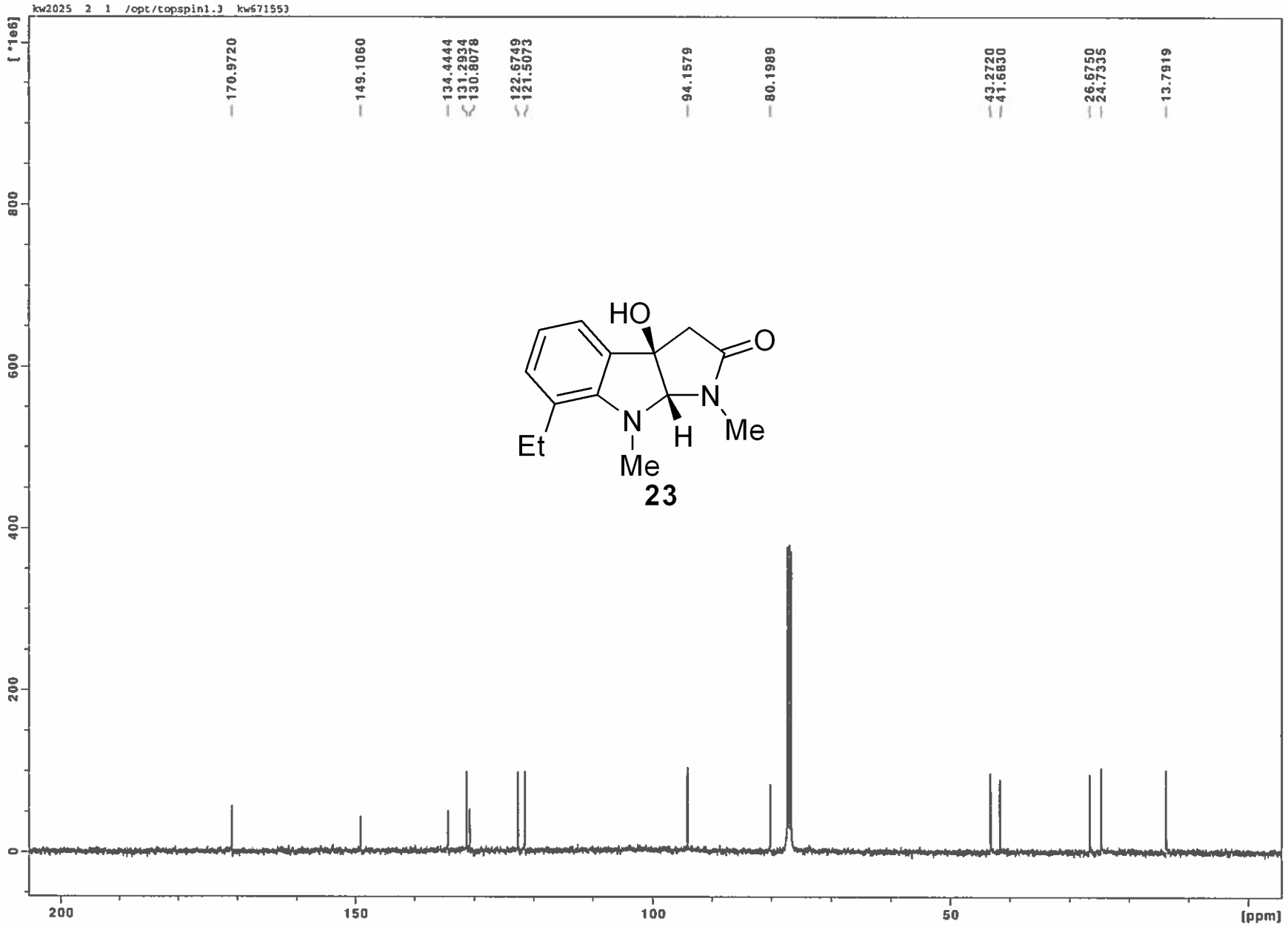

kw1147-2e 1 1 /opt/topspin1.3 kw671553
[*1e6]
80
60
40
20
0
7.2875
7.2642
6.5698
6.5502
4.7805
3.0986
2.9526
2.9320
HO
O
N
Me
N
H
Me
21
2.3174
1.0170
1.0000
1.0855
3.5404
2.0699
10
8
6
4
2
0
[ppm]

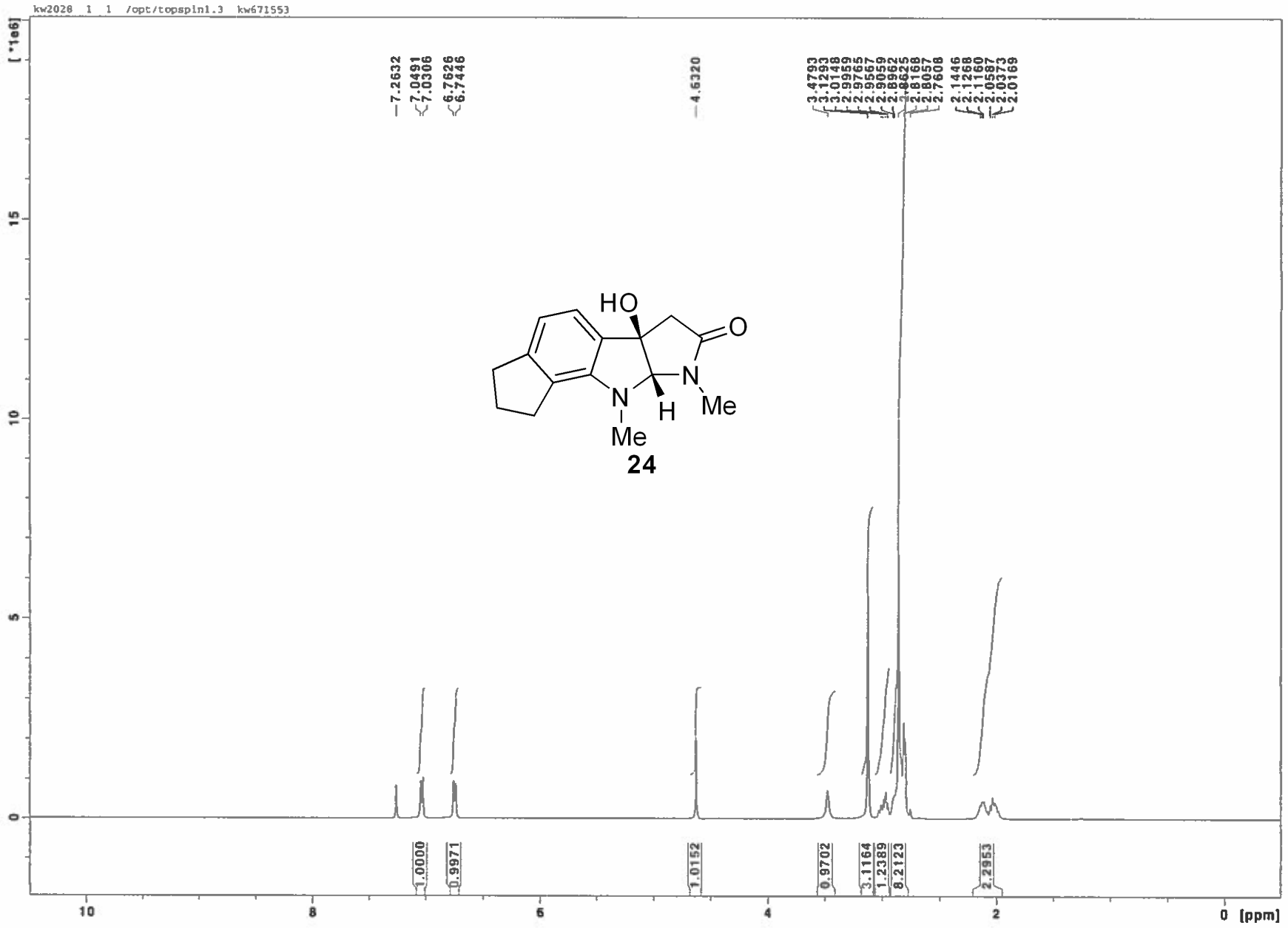

kw1147-2e 2 1 /opt/topspin1.3 kw671553
[*1e9]
1.5
1.0
0.5
0.0
171.7885
150.0118
131.1838
130.9202
123.6343
119.2551
108.6485
92.5121
80.0252
43.5000
36.0261
28.0846
HO
O
N
N
Me
H
Me
21
200
150
100
50
0 [ppm]

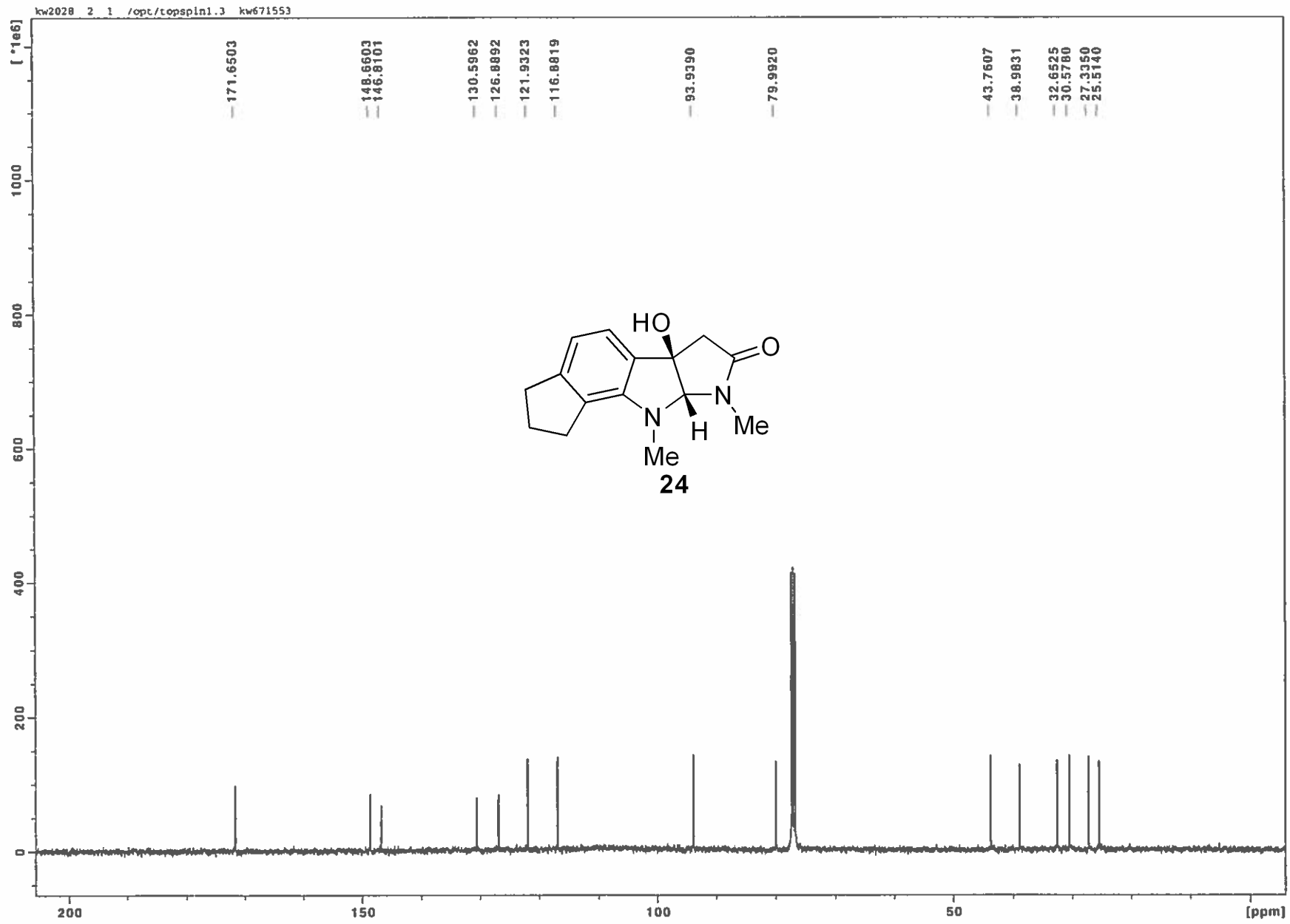

kw2029 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.5091
7.4902
7.4530
7.4106
7.3934
7.3765
7.2993
7.2829
7.2638
6.5742
6.5543
4.7697
3.4127
3.0695
2.9093
2.8930
Ph
HO
O
N
N
Me
H
Me
22
4.2027
2.0761
1.3688
1.0000
1.0104
0.9633
3.1677
5.1659
10
8
6
4
2
0 [ppm]


kw2029 2 1 /opt/topspin1.3 kw671553
171.9610
149.4585
140.8159
132.6508
132.0131
129.6703
128.7364
126.5117
126.4145
122.3965
108.7899
92.9030
79.8994
43.6837
36.0666
28.1491
Ph
HO
O
N
Me
N
H
Me
22
[*1e9]
8
6
4
2
0
200
150
100
50
0 [ppm]

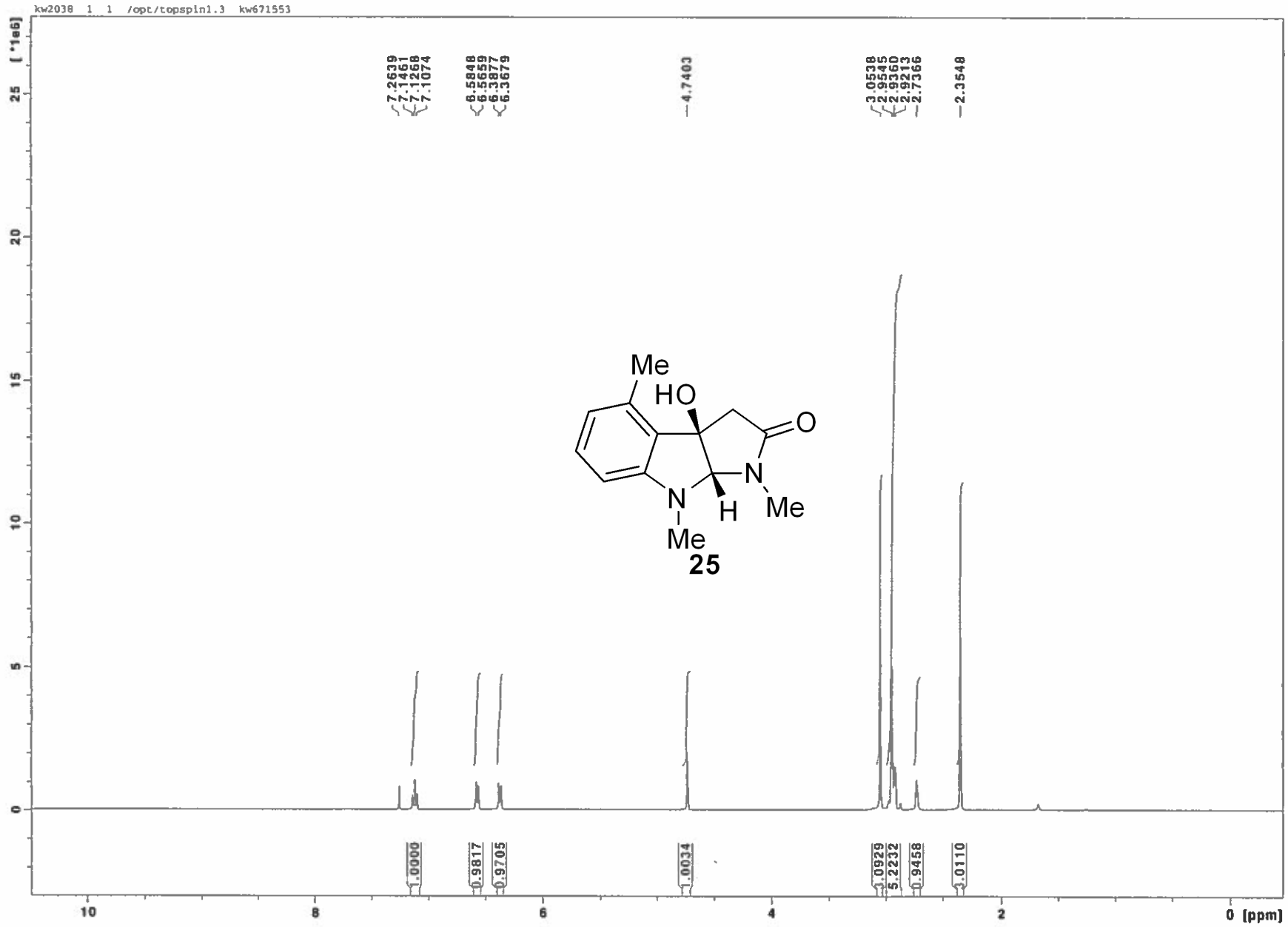

kw2025 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2644
7.1478
7.1282
7.1014
6.9456
6.9268
6.9077
4.6341
3.0981
3.0347
2.8767
2.8649
2.8408
2.7461
2.7272
2.7082
2.6481
2.6293
2.6102
1.2563
1.2383
1.2205
HO
O
N
N
H
Me
Et
Me
23
2.0345
1.0204
1.0000
3.0228
5.1387
2.1433
3.1937
10
8
6
4
2
0 [ppm]


kw2025 2 1 /opt/topspin1.3 kw671553
[*1e6]
800
600
400
200
0
170.9720
149.1060
134.4444
131.2934
130.8078
122.6749
121.5073
94.1579
80.1989
43.2720
41.6830
26.6750
24.7335
13.7919
HO
O
N
Me
N
H
Et
Me
23
200
150
100
50
[ppm]

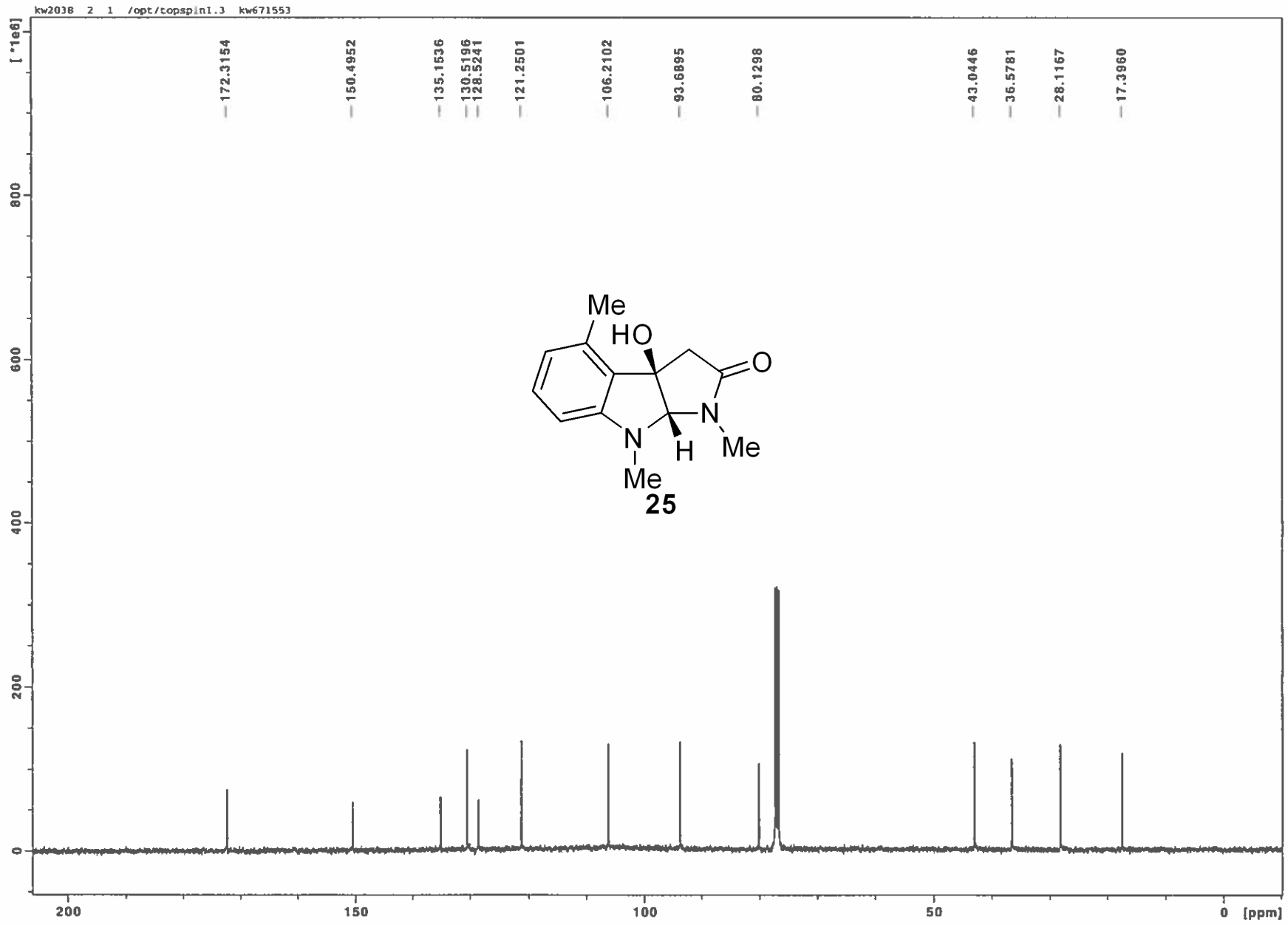

kw2020 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2632
7.0491
7.0306
6.7626
6.7446
4.6320
3.4793
3.1293
3.0148
2.9959
2.9765
2.9567
2.9059
2.8962
2.8625
2.8168
2.8057
2.7608
2.1446
2.1268
2.1160
2.0587
2.0373
2.0169
HO
O
N
N
H
Me
Me
24
1.0000
0.9971
1.0152
0.9702
3.1164
1.2389
8.2123
2.2953
10
8
6
4
2
0 [ppm]

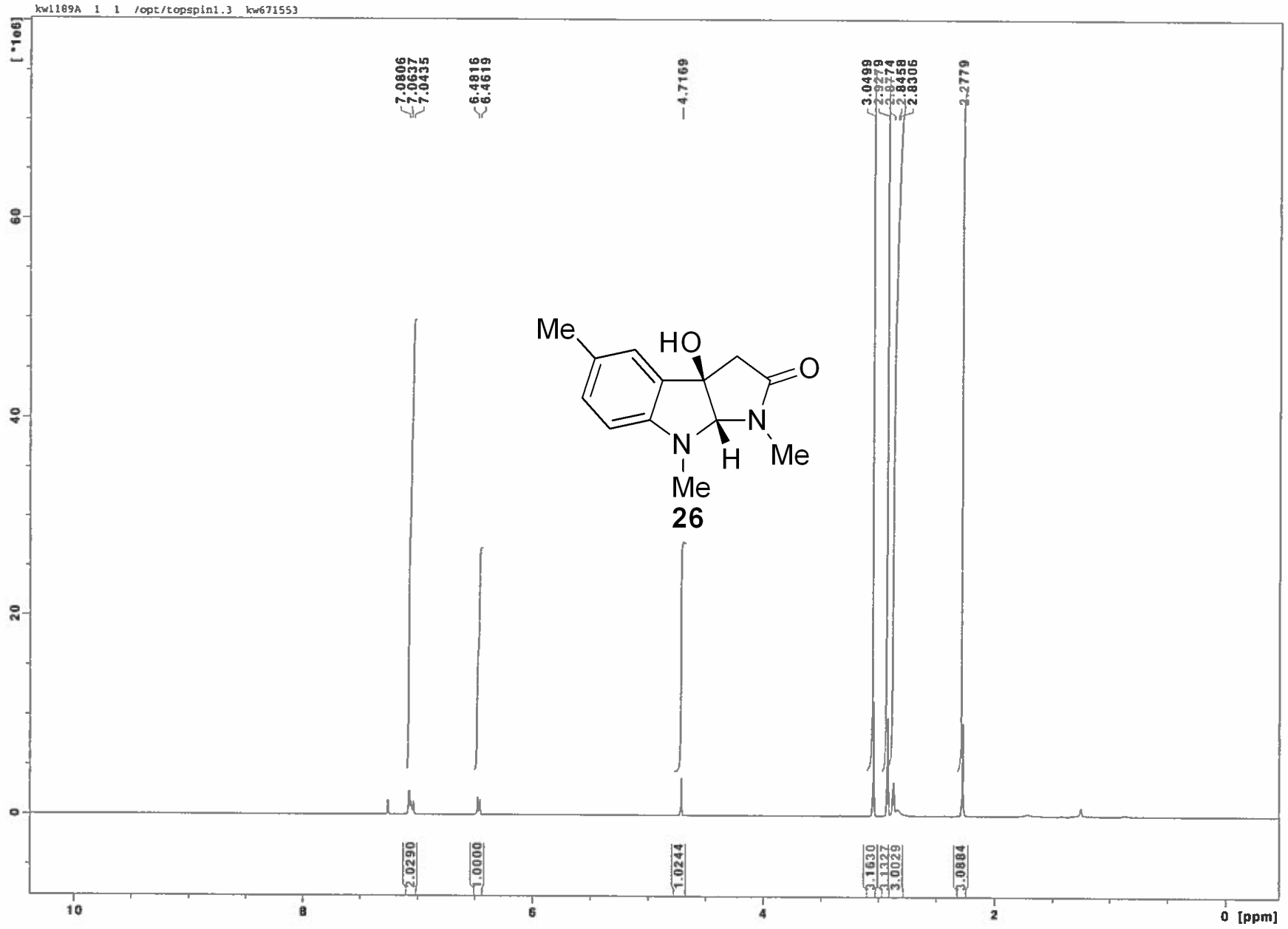

kw2028 2 1 /opt/topspin1.3 kw671553
[*1e6]
171.6503
148.6603
146.8101
130.5962
126.8892
121.9323
116.8819
93.9390
79.9920
43.7607
38.9831
32.6525
30.5780
27.3350
25.5140
1000
800
600
400
200
0
200
150
100
50
[ppm]
HO
O
N
N
Me
H
Me

24

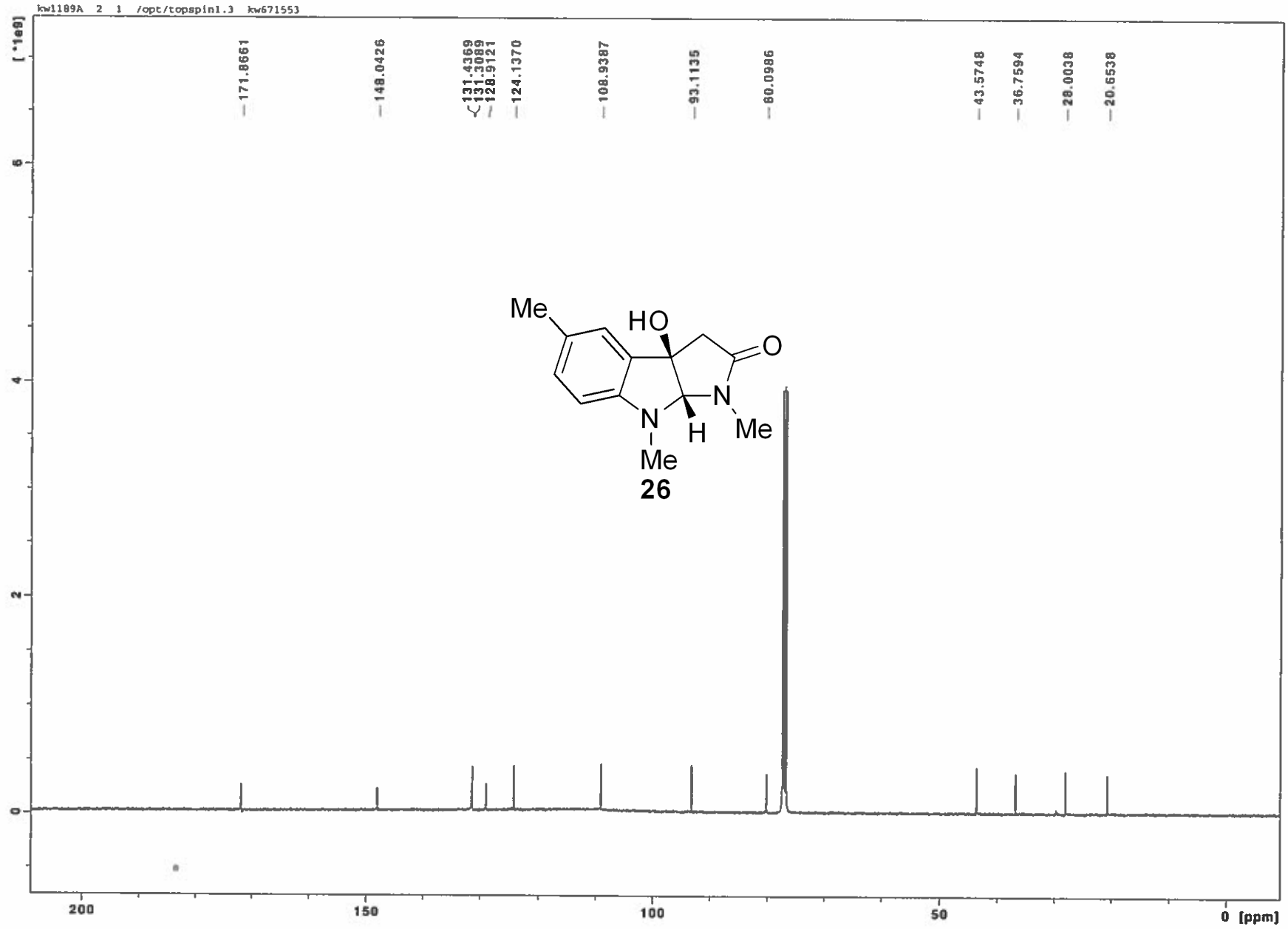

kw2038 1 1 /opt/topspin1.3 kw671553
[*1e6]
25
20
15
10
5
0
7.2639
7.1461
7.1268
7.1074
6.5848
6.5659
6.3877
6.3679
4.7403
3.0538
2.9545
2.9360
2.9213
2.7366
2.3548
1.0000
0.9817
0.9705
1.0034
3.0929
5.2232
0.9458
3.0110
10
8
6
4
2
0 [ppm]
Me
HO
O
N
N
H
Me
Me

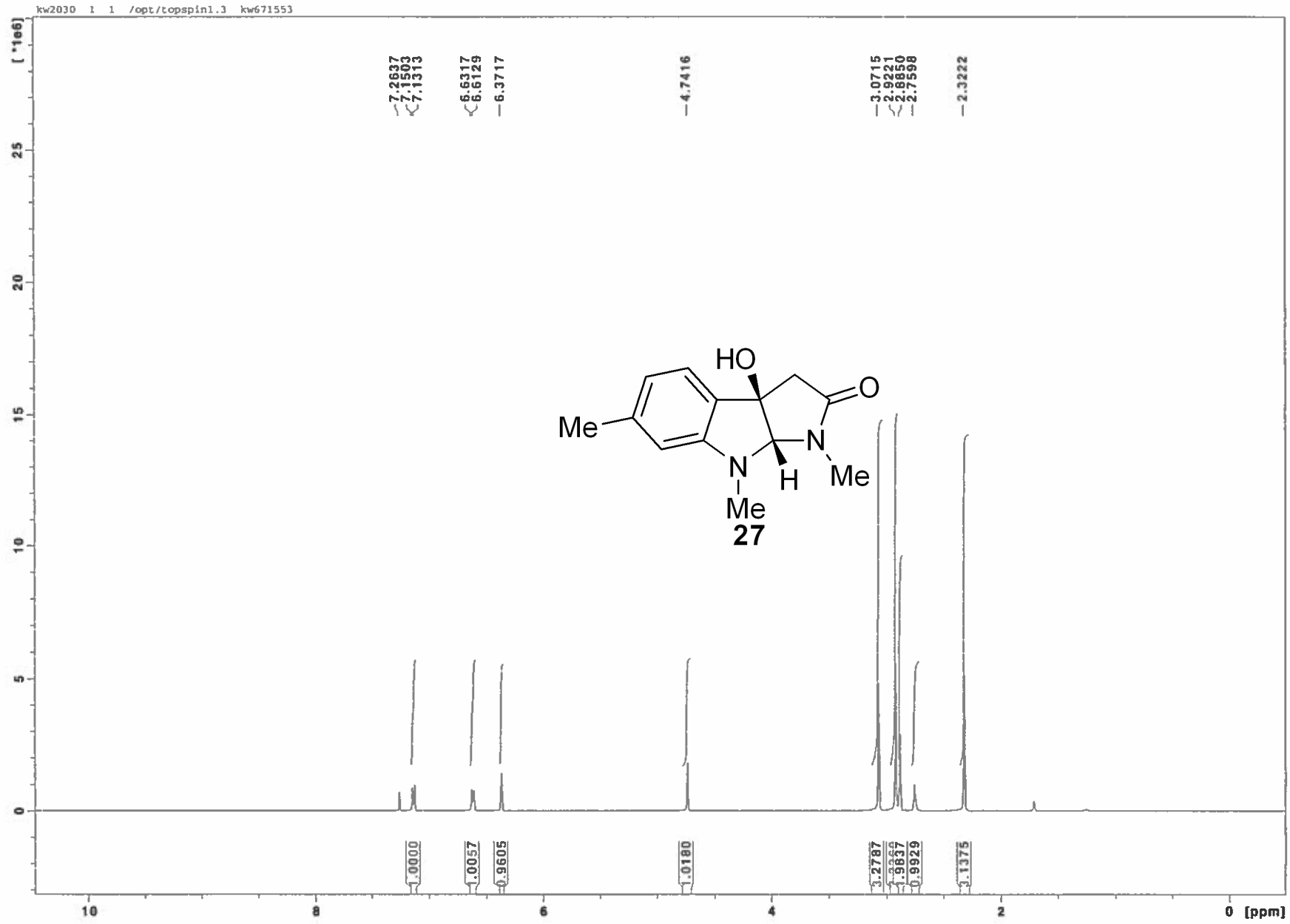
25

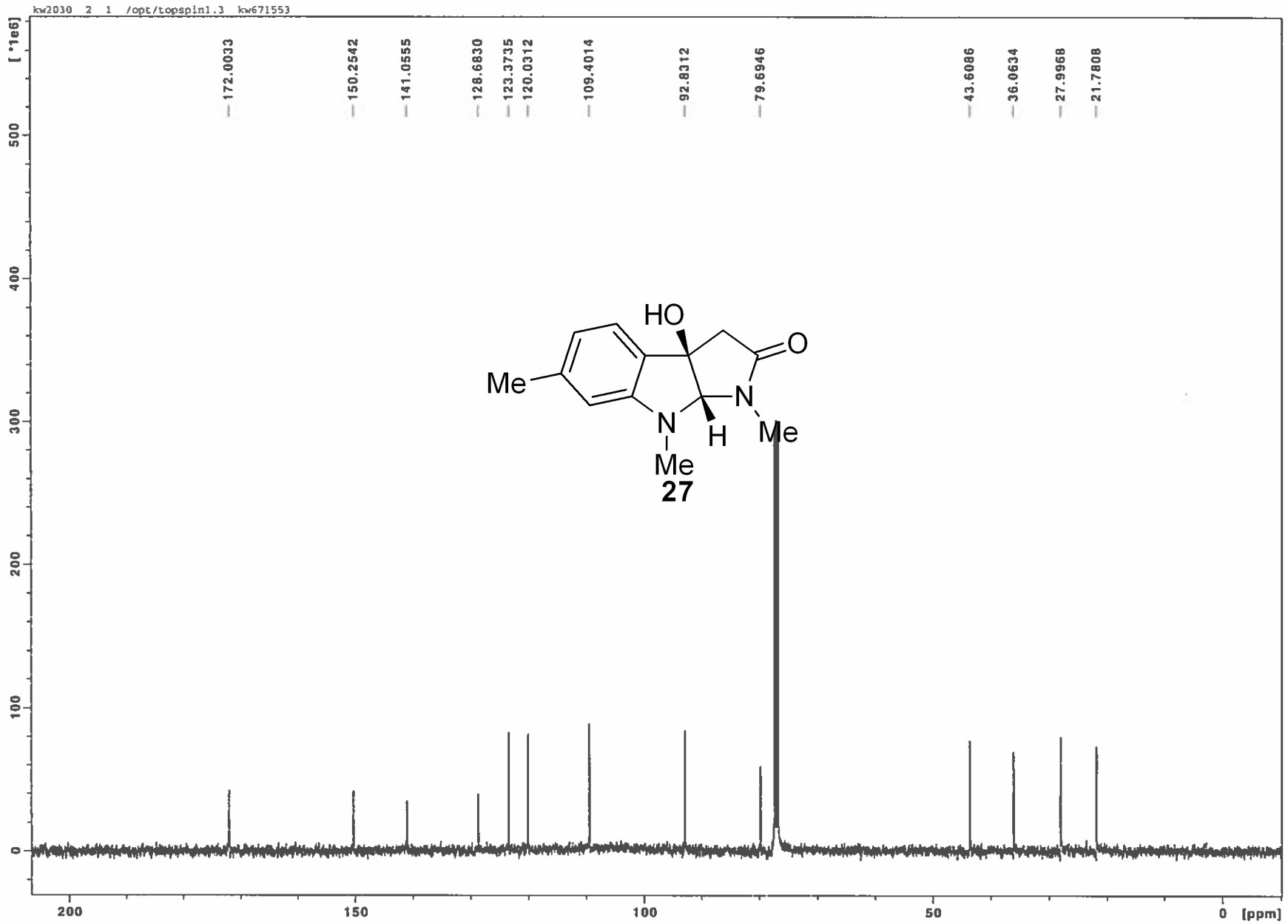

kw2038 2 1 /opt/topspin1.3 kw671553
[*1e6]
800
600
400
200
0
172.3154
150.4952
135.1536
130.5196
128.5241
121.2501
106.2102
93.6895
80.1298
43.0446
36.5781
28.1167
17.3960
Me
HO
O
N
Me
N
H
Me
25
200
150
100
50
0 [ppm]

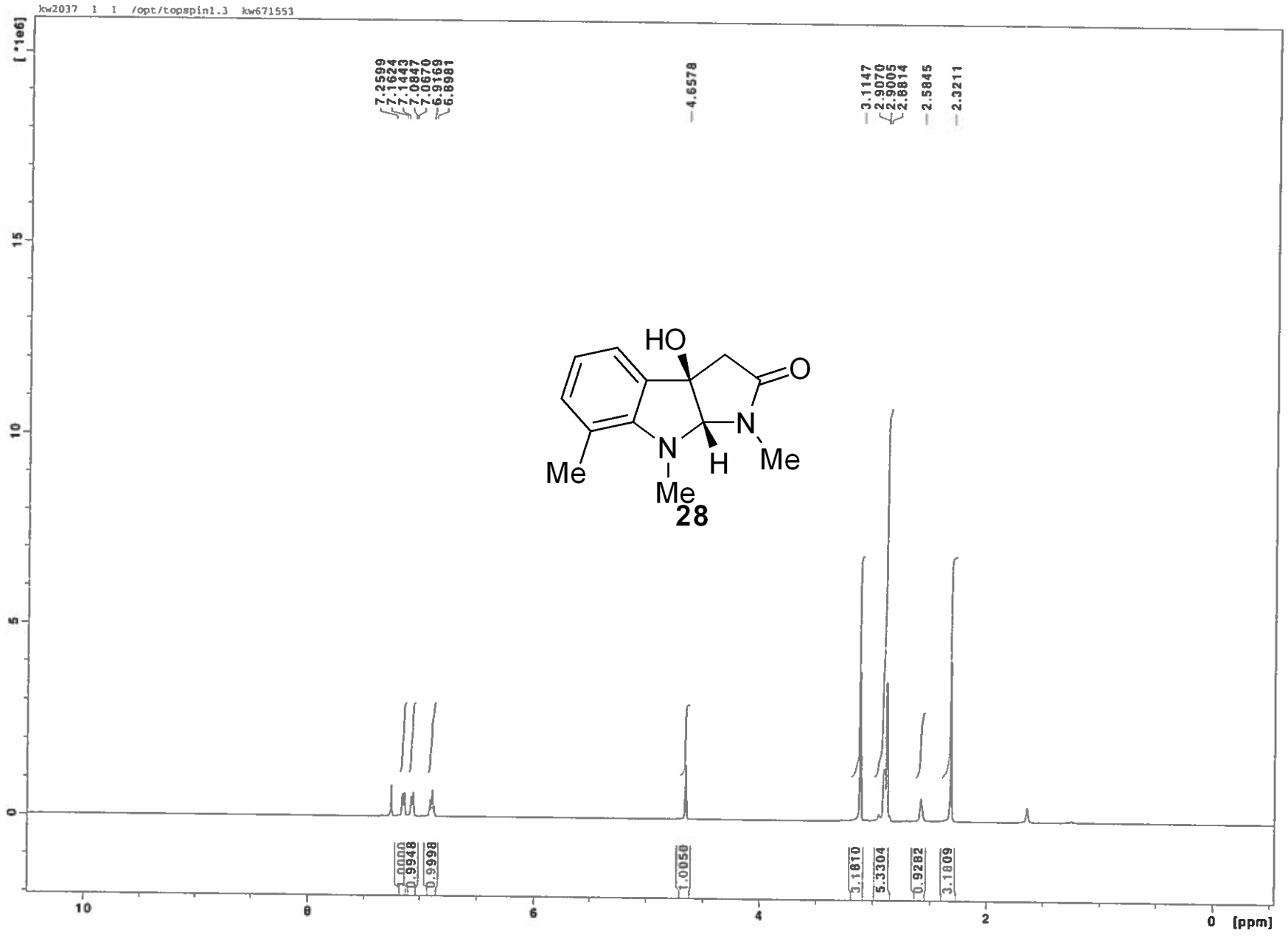

kw1109A 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.0806
7.0637
7.0435
6.4816
6.4619
4.7169
3.0499
2.9279
2.8774
2.8458
2.8306
2.2779
Me
HO
O
N
Me
N
H
Me
2.0290
1.0000
1.0244
3.1630
1.1327
3.0029
3.0884
10
8
6
4
2
0 [ppm]

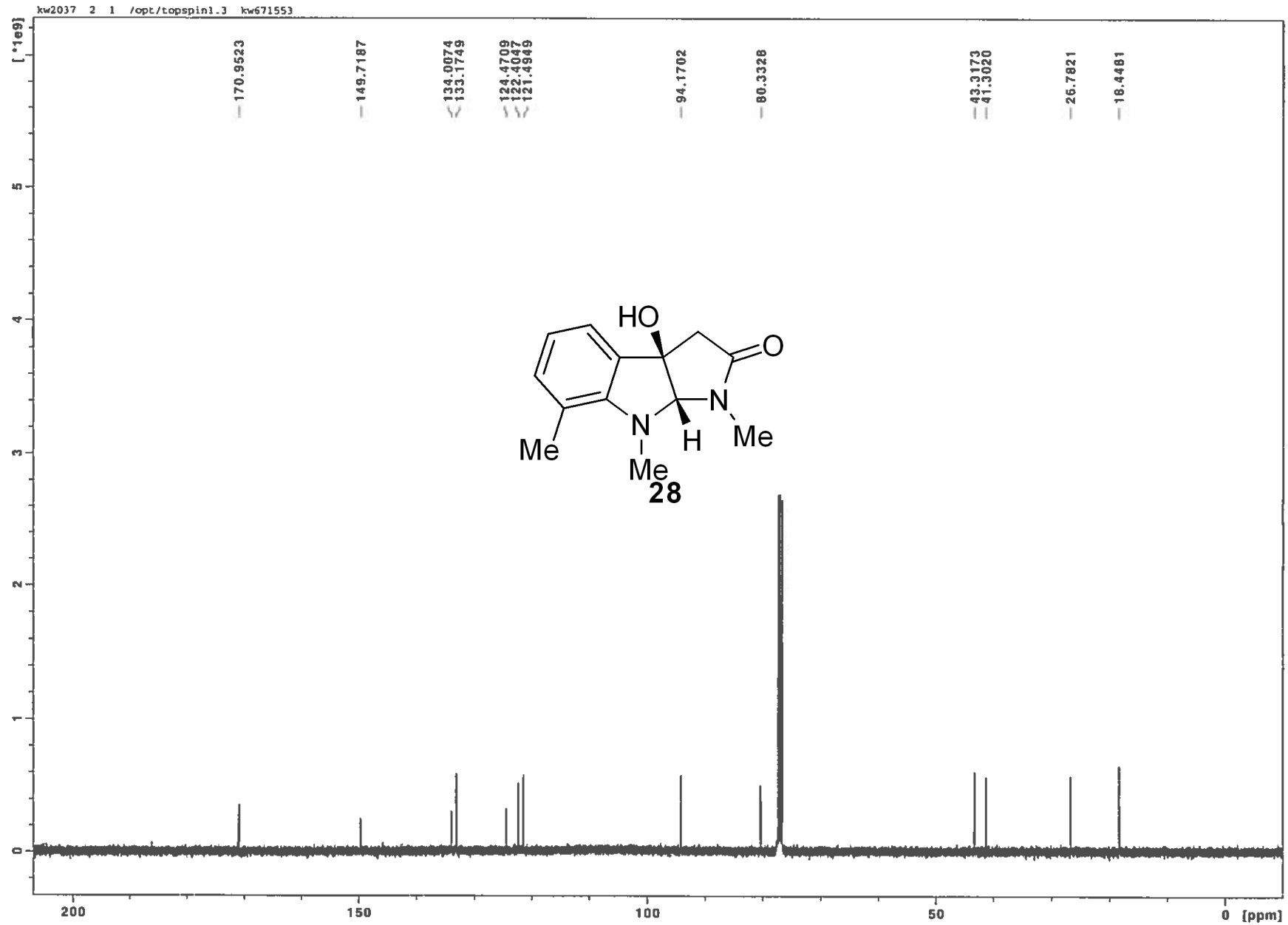
26

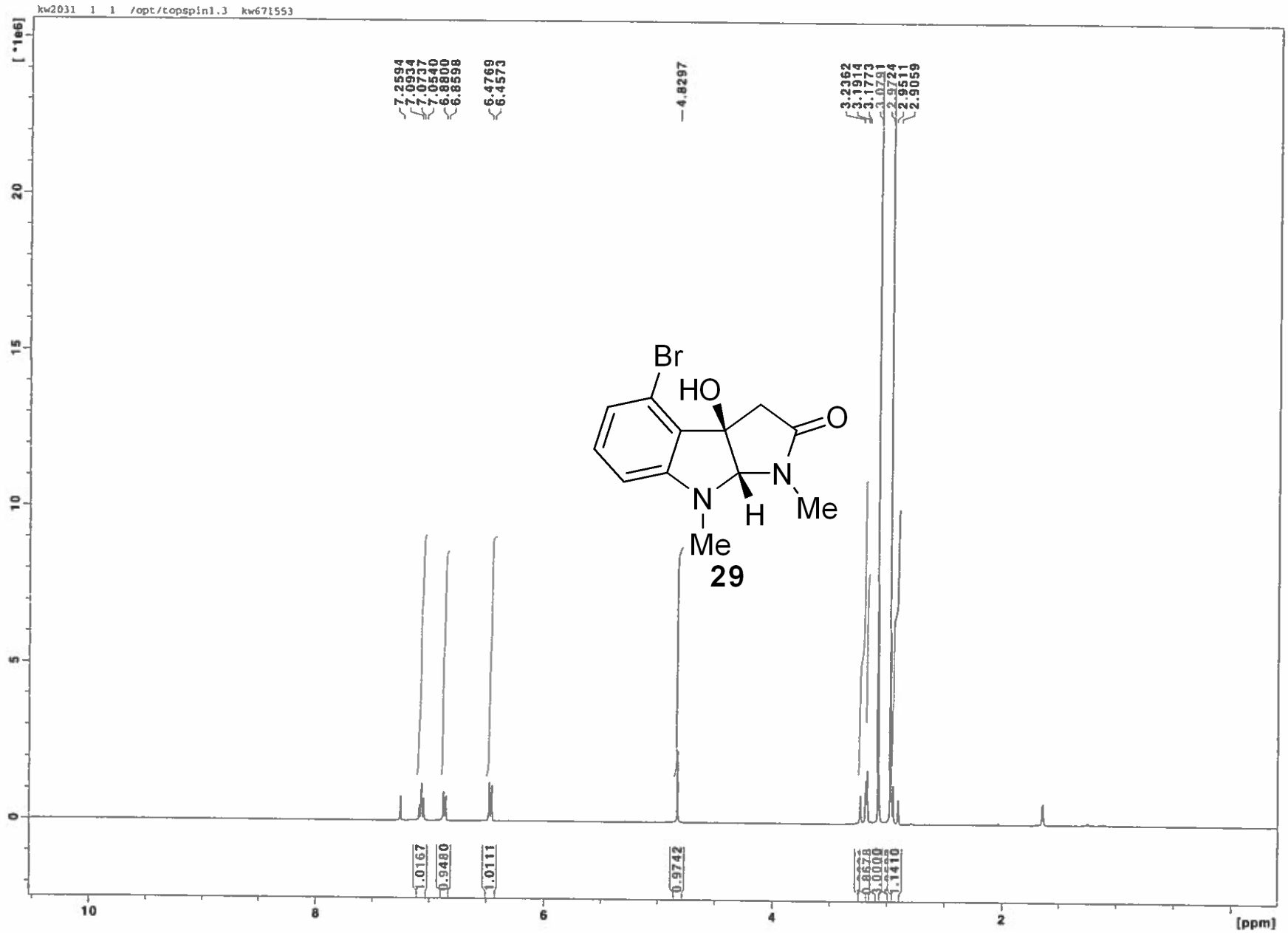

kw1189A 2 1 /opt/topspin1.3 kw671553
[*1e8]
171.8661
148.0426
131.4369
131.3089
128.9121
124.1370
108.9387
93.1135
80.0986
43.5748
36.7594
28.0038
20.6538
Me
HO
O
N
N
H
Me
Me
26
200
150
100
50
0 [ppm]

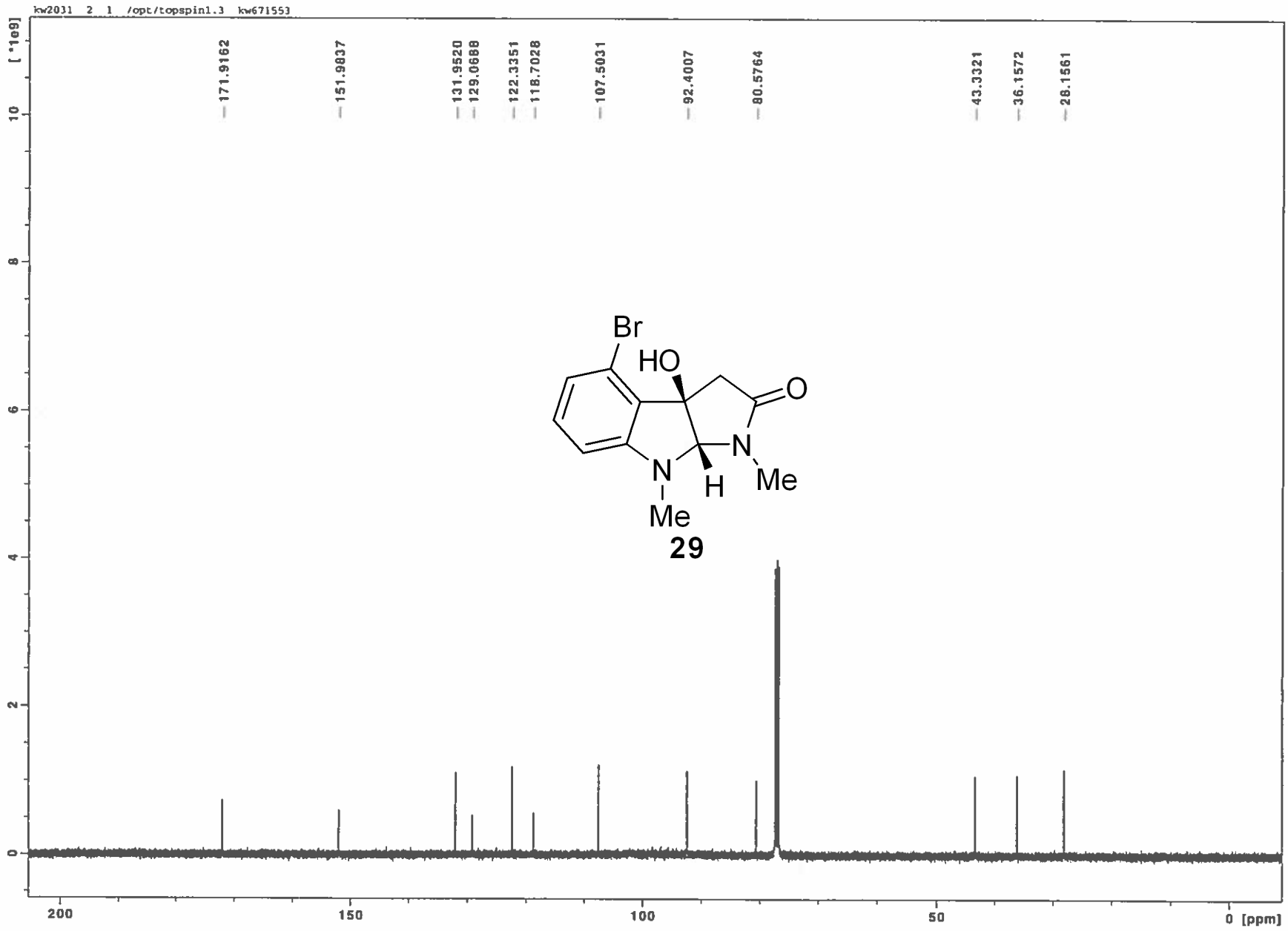

kw2030 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2637
7.1503
7.1313
6.6317
6.6129
6.3717
4.7416
3.0715
2.9221
2.8850
2.7598
2.3222
HO
O
Me
N
N
H
Me
Me
27
1.0000
1.0057
0.9605
1.0180
3.2787
1.9637
0.9929
3.1375
10
8
6
4
2
0 [ppm]

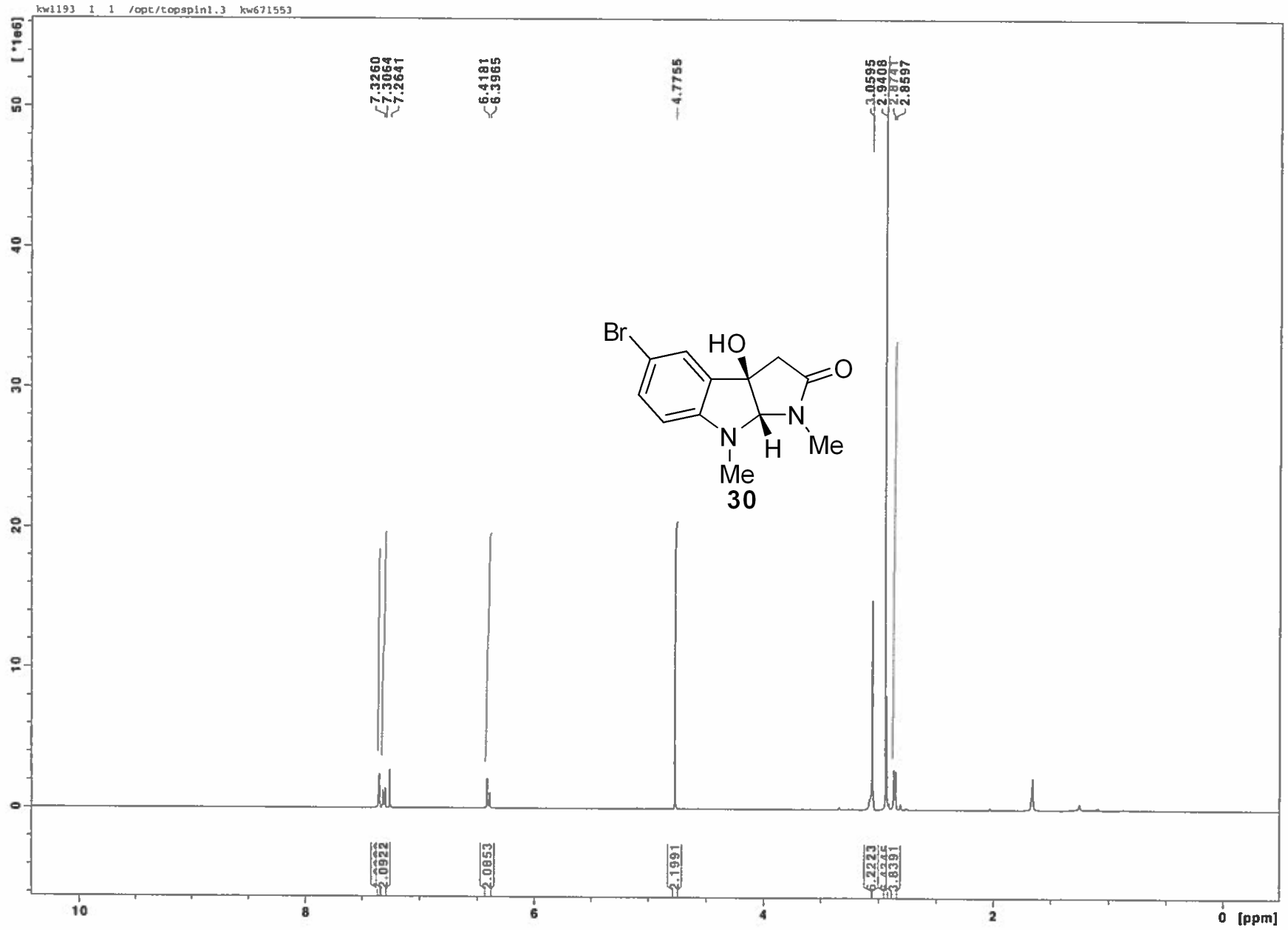

kw2030 2 1 /opt/topspin1.3 kw671553
[*1e6]
172.0033
150.2542
141.0555
128.6830
123.3735
120.0312
109.4014
92.8312
79.6946
43.6086
36.0634
27.9968
21.7808
HO
O
Me
N
N
H
Me
Me
27
200
150
100
50
0
[ppm]

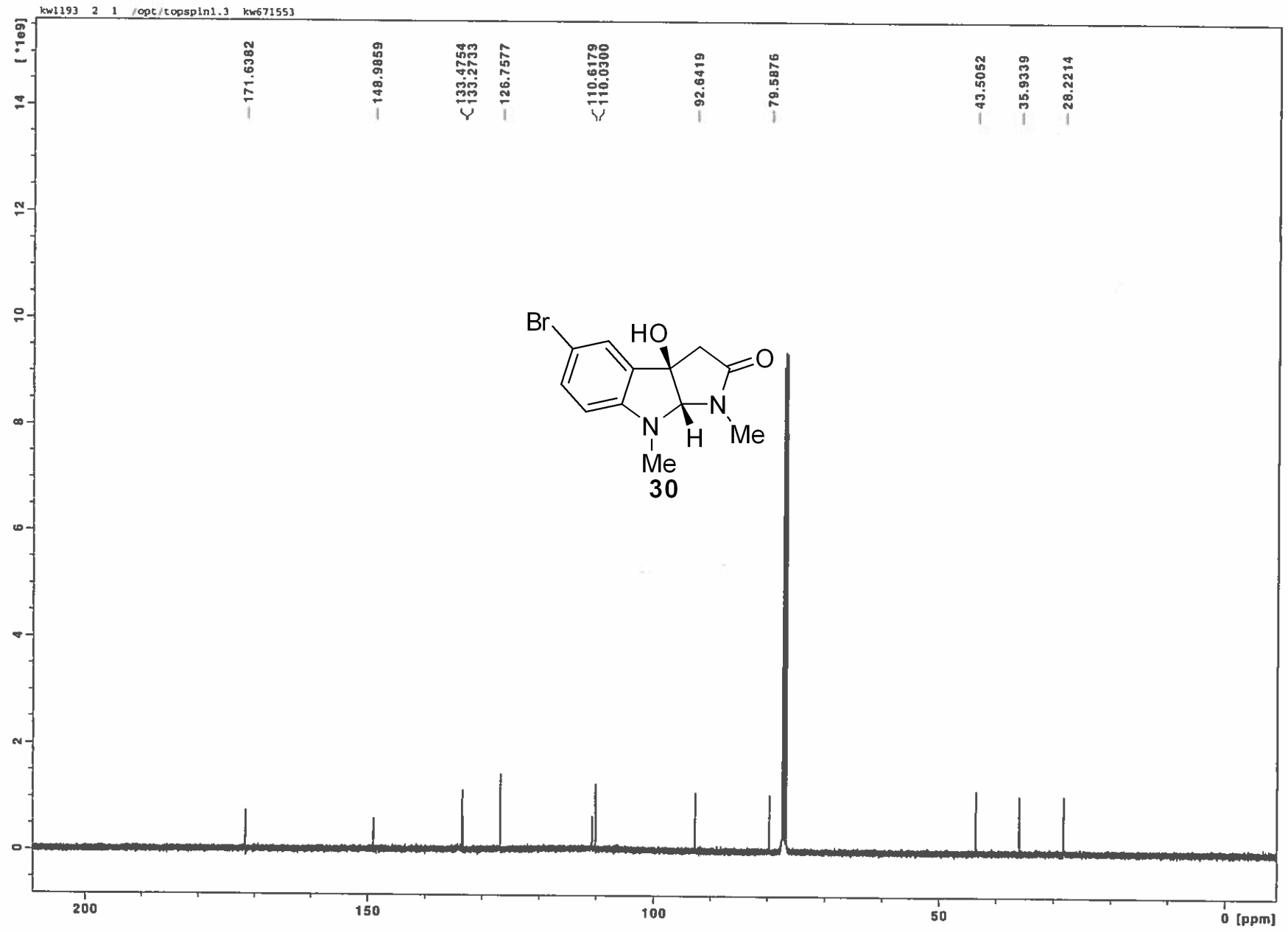

kw2037 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2599
7.1624
7.1443
7.0847
7.0670
6.9169
6.8981
4.6578
3.1147
2.9070
2.9005
2.8814
2.5845
2.3211
HO
O
N
N
Me
Me
H
Me
28
1.0000
0.9948
0.9998
1.0050
3.1810
5.3304
0.9282
3.1809
10
8
6
4
2
0
[ppm]

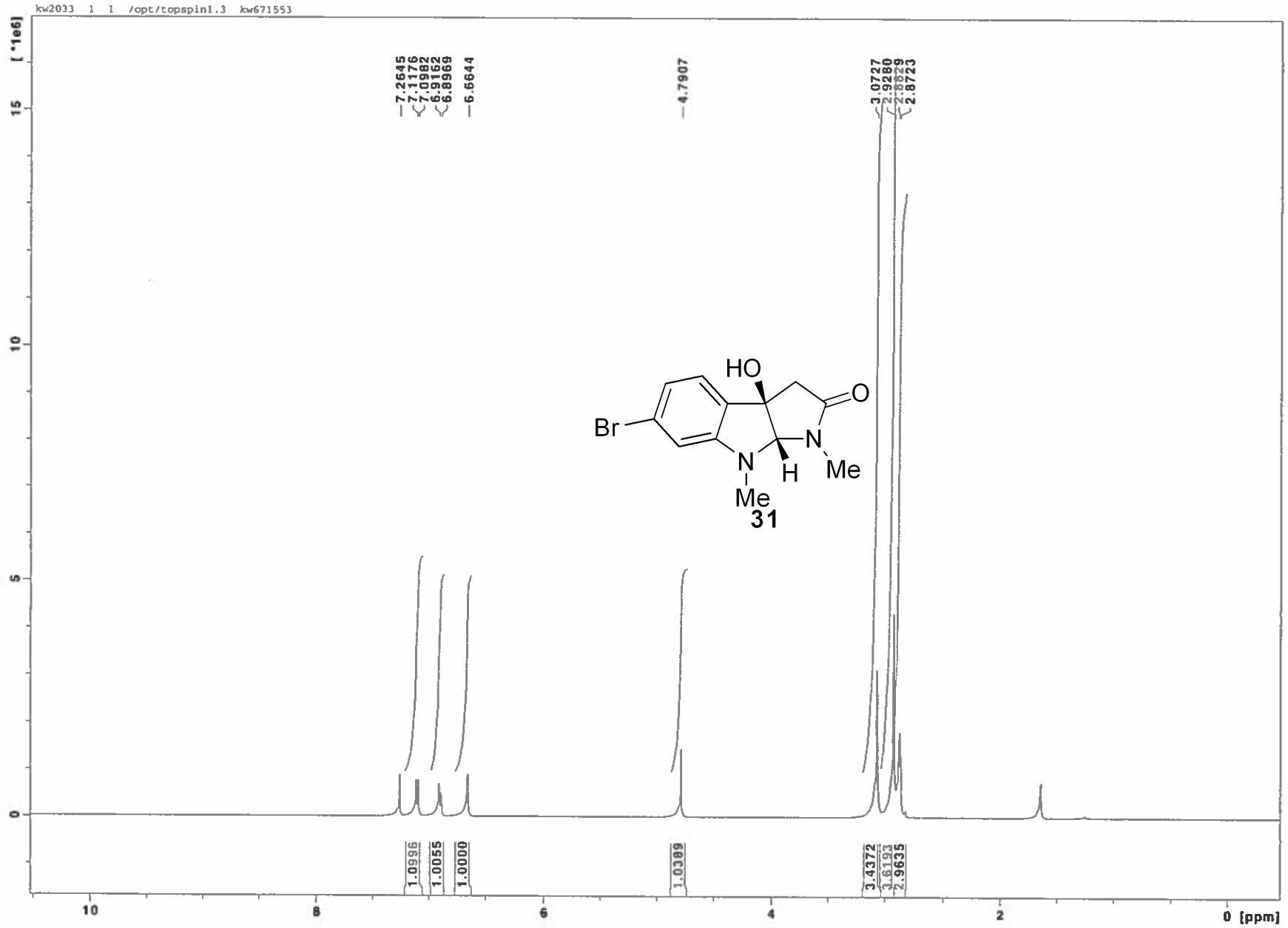

kw2037 2 1 /opt/topspin1.3 kw671553
[*1e9]
170.9523
149.7187
134.0074
133.1749
124.4709
122.4047
121.4949
94.1702
80.3328
43.3173
41.3020
26.7821
18.4481
HO
O
N
N
H
Me
Me
Me
28
200
150
100
50
0 [ppm]

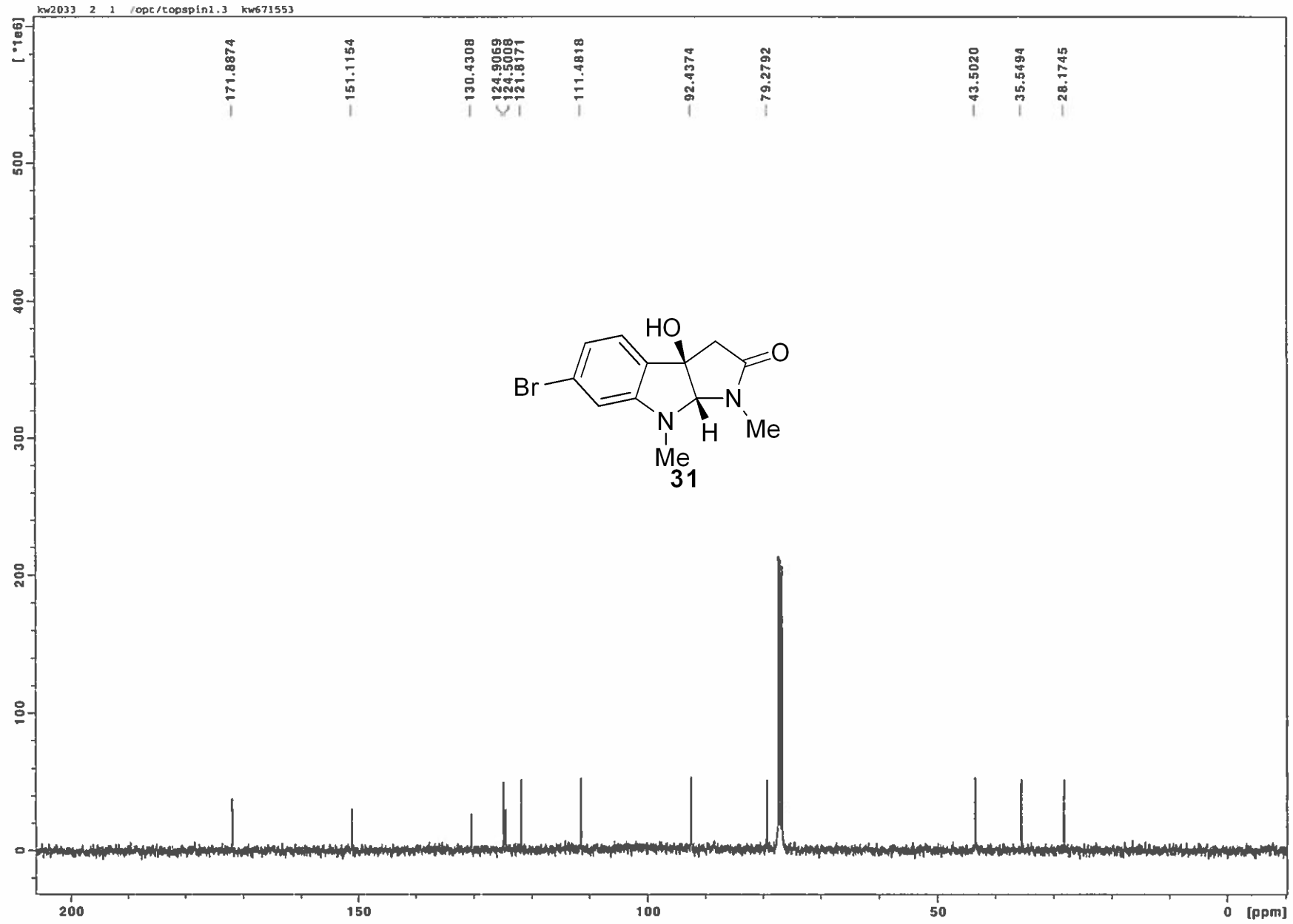

kw2031 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2594
7.0934
7.0737
7.0540
6.8800
6.8598
6.4769
6.4573
4.8297
3.2362
3.1914
3.1773
3.0791
2.9724
2.9511
2.9059
Br
HO
O
N
N
Me
H
Me
29
1.0167
0.9480
1.0111
0.9742
0.8678
3.0000
2.1410
10
8
6
4
2
[ppm]

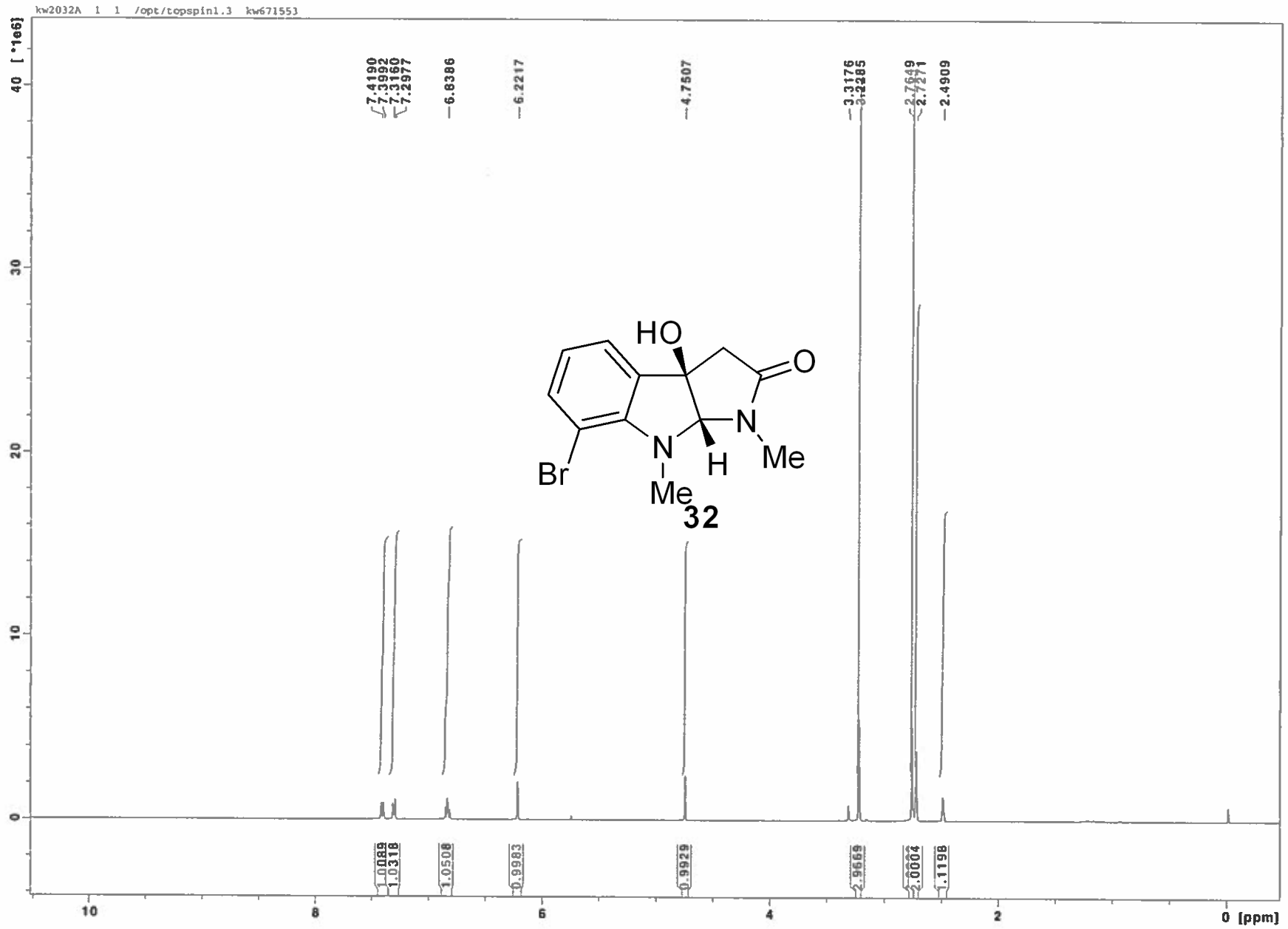

kw2031 2 1 /opt/topspin1.3 kw671553
[*10⁸]
171.9162
151.9837
131.9520
129.0688
122.3351
118.7028
107.5031
92.4007
80.5764
43.3321
36.1572
28.1561
Br
HO
O
N
N
H
Me
Me
29
200
150
100
50
0 [ppm]

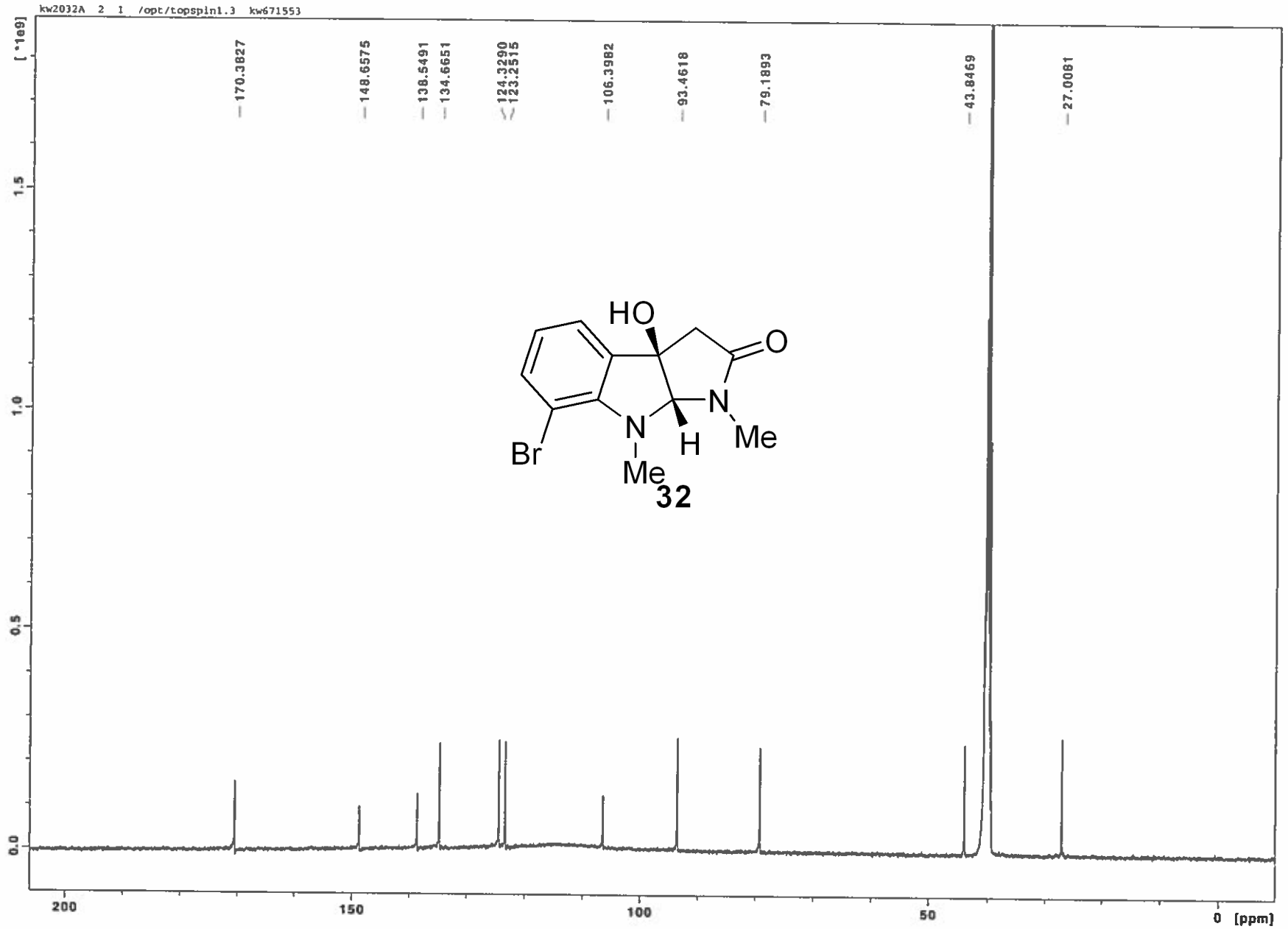

kw1193 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.3260
7.3064
7.2641
6.4181
6.3965
4.7755
3.0595
2.9408
2.8741
2.8597
Br
HO
O
N
Me
N
H
Me
30
2.0922
2.0853
2.1991
6.2223
3.8391
10
8
6
4
2
0 [ppm]

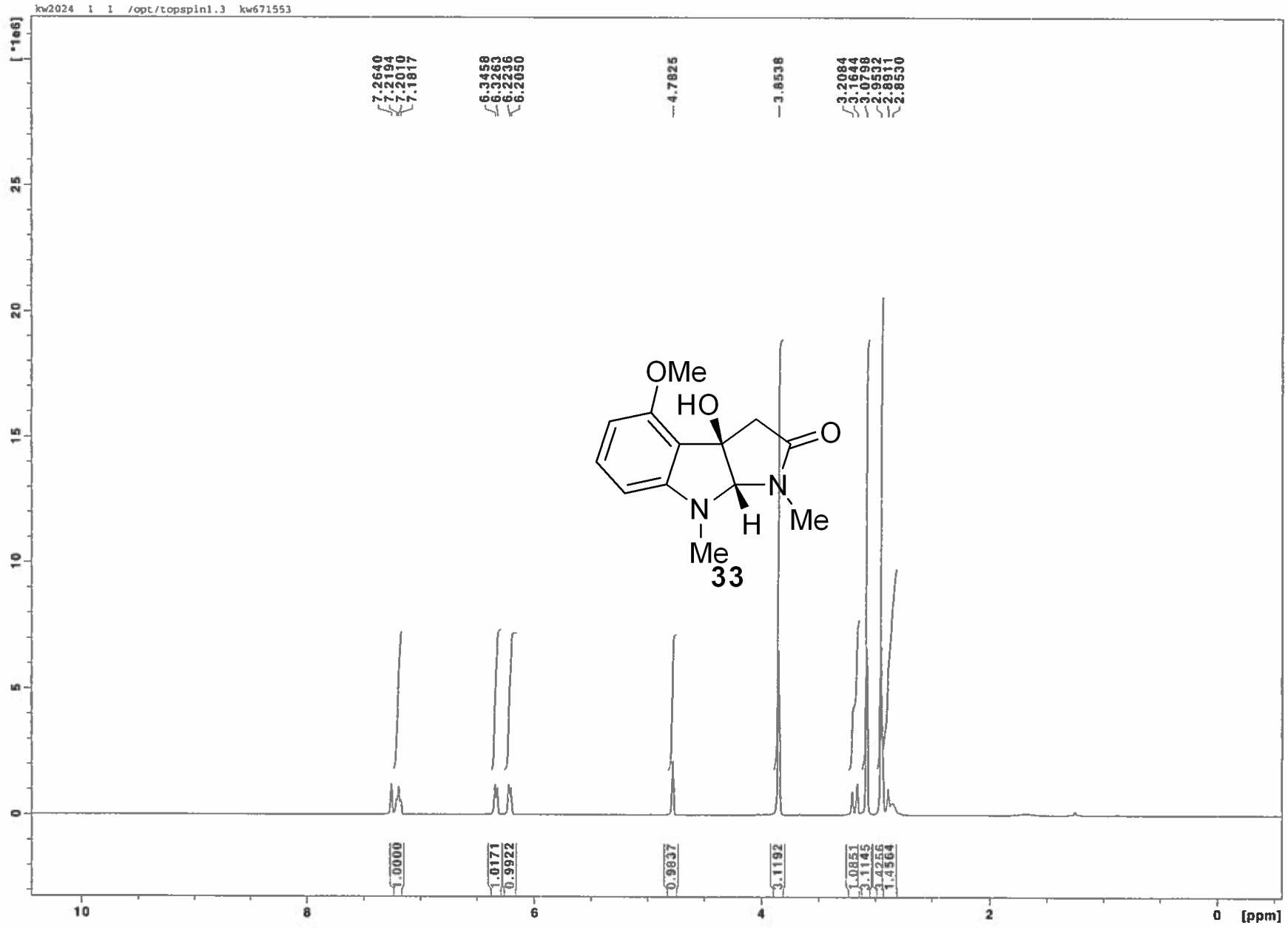

kw1193 2 1 /opt/topspin1.3 kw671553
171.6382
148.9859
133.4754
133.2733
126.7577
110.6179
110.0300
92.6419
79.5876
43.5052
35.9339
28.2214
[*1e9]
14
12
10
8
6
4
2
0
200
150
100
50
0 [ppm]
Br
HO
O
N
Me
N
H
Me
30

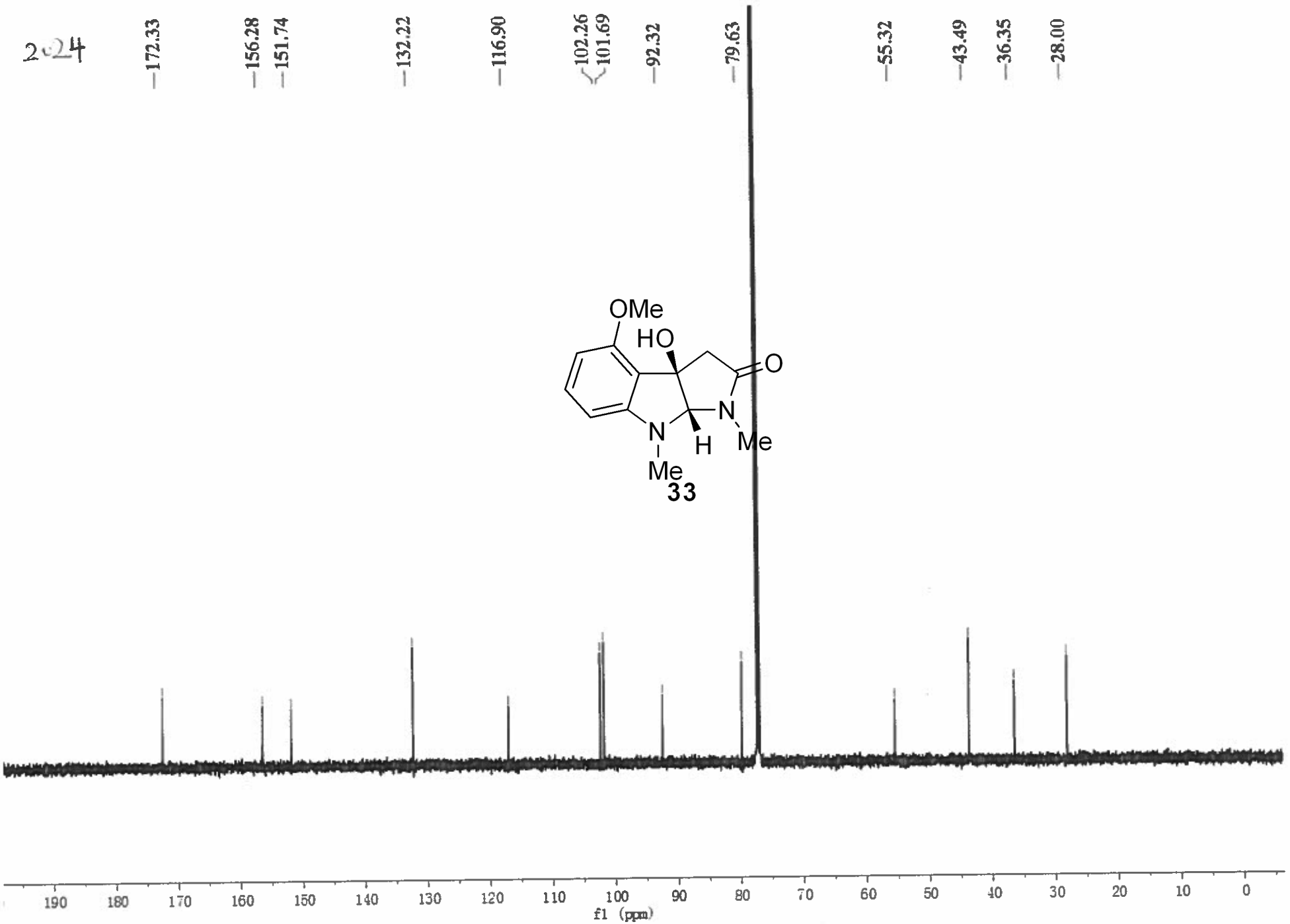

kw2033 1 1 /opt/topspin1.3 kw671553
7.2645
7.1176
7.0982
6.9162
6.8969
6.6644
4.7907
3.0727
2.9280
2.8829
2.8723
HO
O
Br
N
N
H
Me
Me
31
1.0996
1.0055
1.0000
1.0389
3.4372
3.6193
2.9635
10
8
6
4
2
0 [ppm]

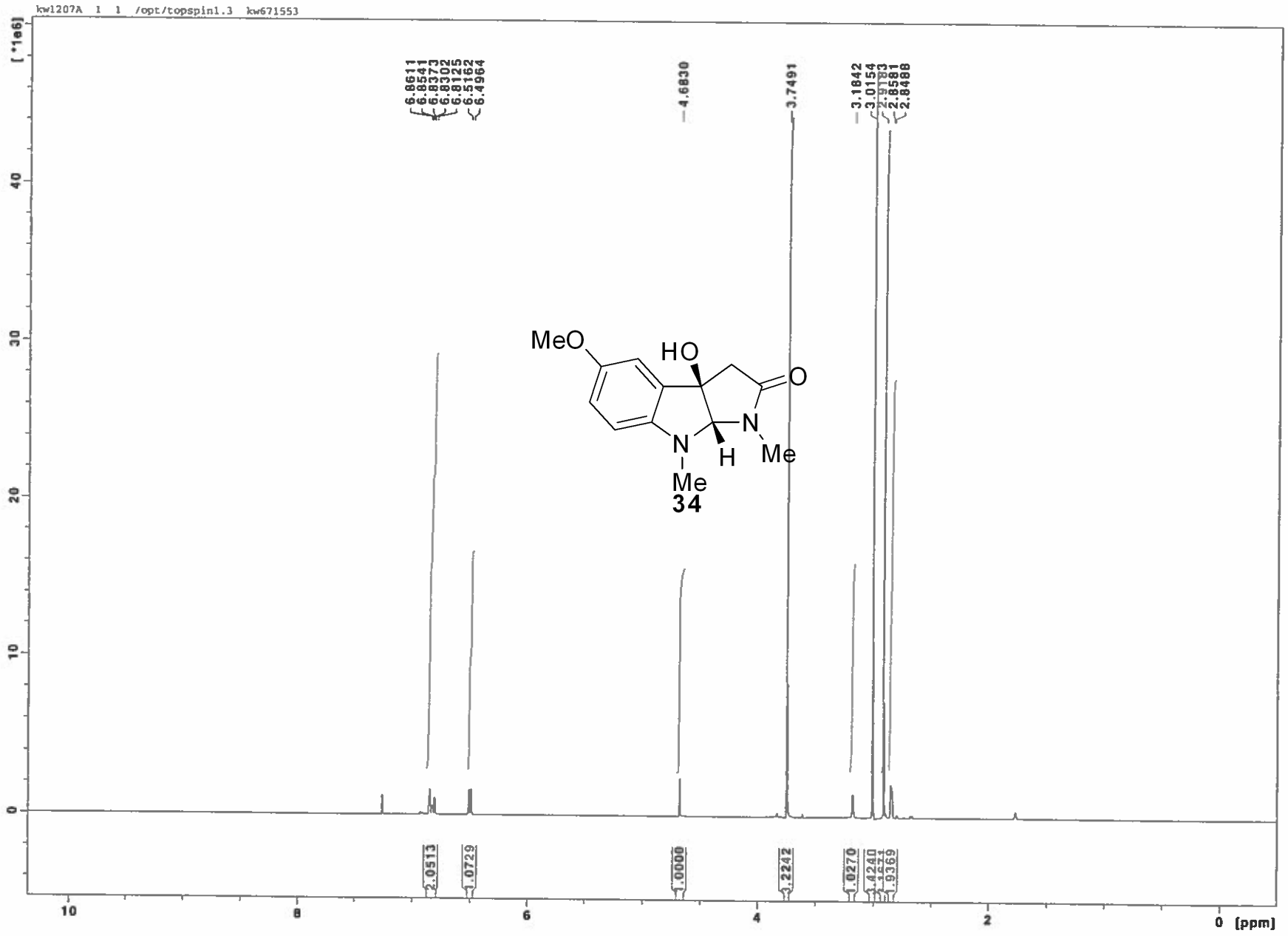

kw2033 2 1 /opt/topspin1.3 kw671553
[*1e6]
171.8874
151.1154
130.4308
124.9069
124.5008
121.8171
111.4818
92.4374
79.2792
43.5020
35.5494
28.1745
HO
O
Br
N
Me
N
H
Me
31
500
400
300
200
100
0
200
150
100
50
0
[ppm]

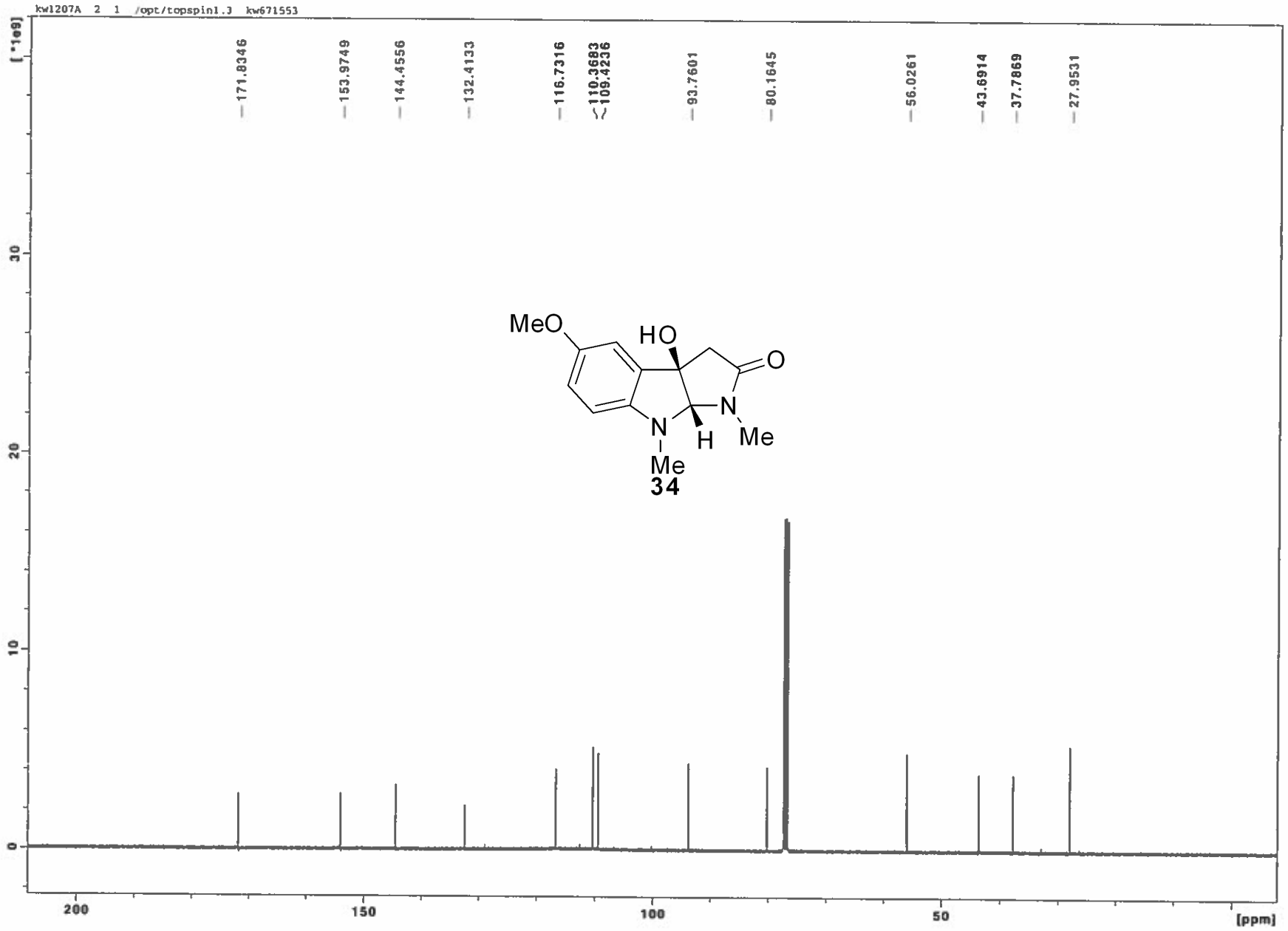

kw2032A 1 1 /opt/topspin1.3 kw671553
7.4190
7.3992
7.3160
7.2977
6.8386
6.2217
4.7507
3.3176
3.2285
2.7649
2.7271
2.4909
HO
O
N
Me
N
H
Me
Br
32
1.0089
1.0318
1.0508
0.9983
0.9929
2.9669
2.0004
1.1198
10
8
6
4
2
0 [ppm]

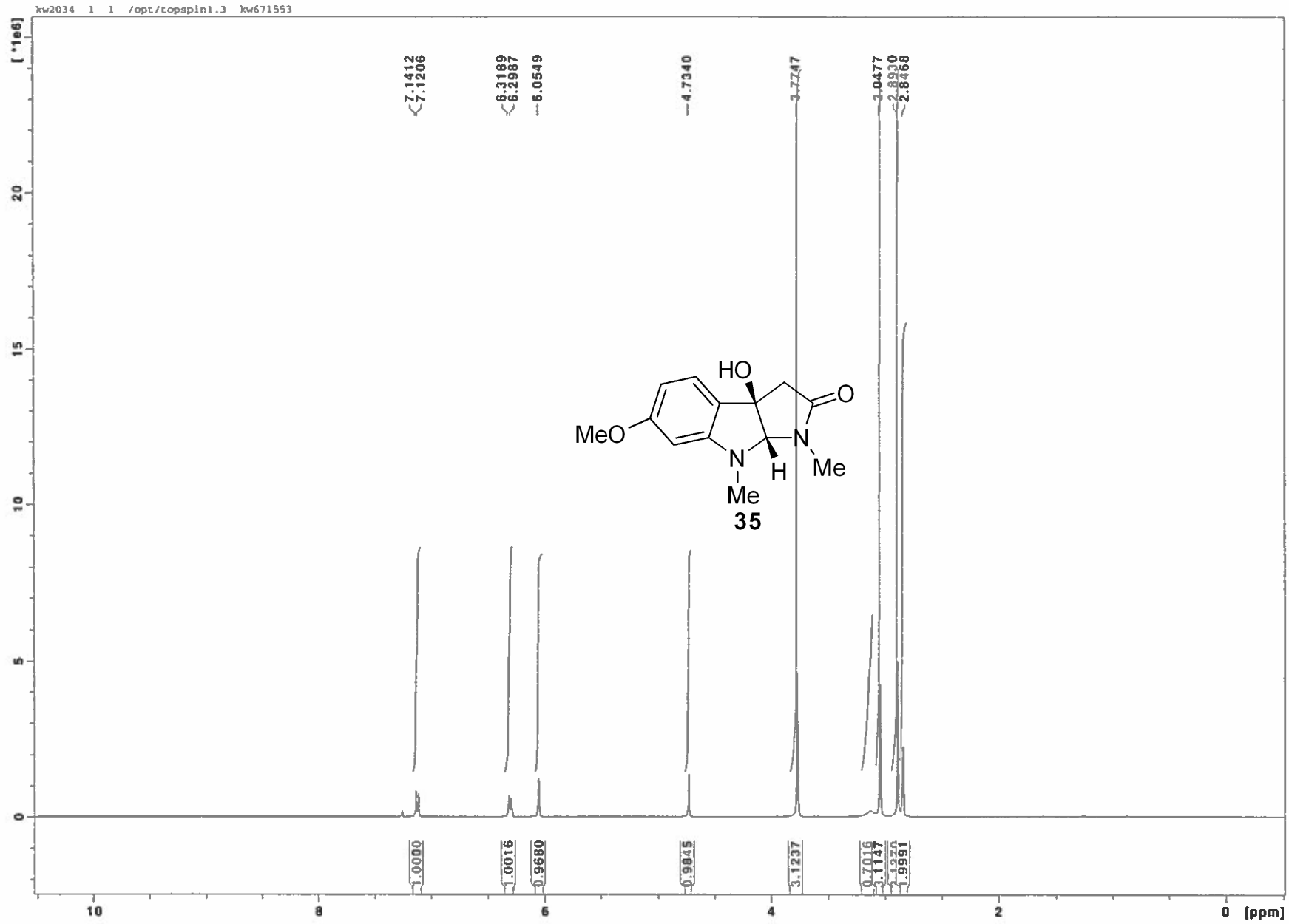

kw2032A 2 1 /opt/topspin1.3 kw671553
[*1e9]
1.5
1.0
0.5
0.0
170.3827
148.6575
138.5491
134.6651
124.3290
123.2515
106.3982
93.4618
79.1893
43.8469
27.0081
200
150
100
50
0 [ppm]
HO
O
N
N
H
Me
Br
Me
32

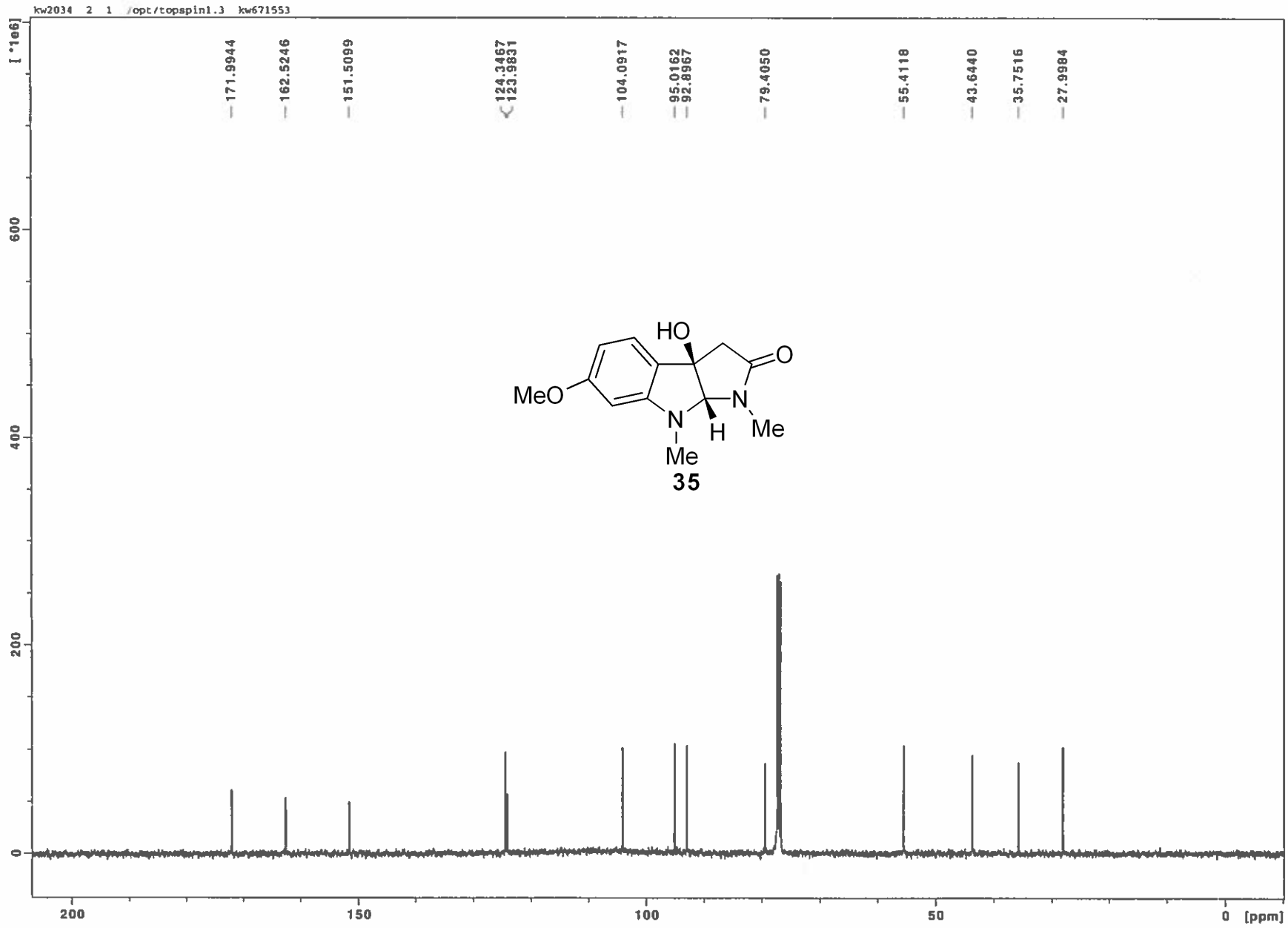

kw2024 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2640
7.2194
7.2010
7.1817
6.3458
6.3263
6.2236
6.2050
4.7825
3.8538
3.2084
3.1644
3.0798
2.9532
2.8911
2.8530
OMe
HO
O
N
N
H
Me
Me
33
1.0000
1.0171
0.9922
0.9837
3.1192
1.0851
3.1145
1.4256
1.4564
10
8
6
4
2
0
[ppm]

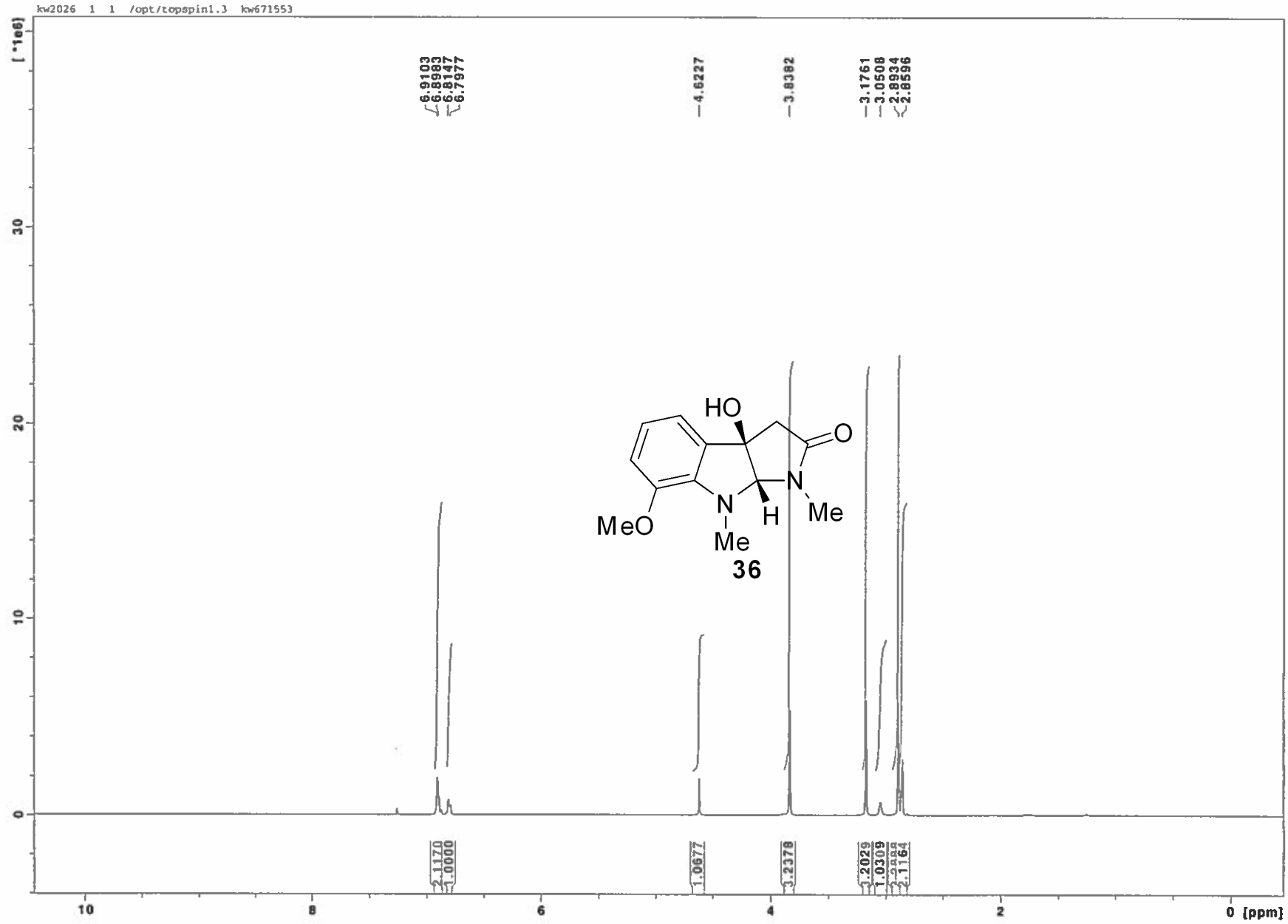

2024
172.33
156.28
151.74
132.22
116.90
102.26
101.69
92.32
79.63
55.32
43.49
36.35
28.00
OMe
HO
O
N
N
H
Me
Me
33
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
10
0
f1 (ppm)

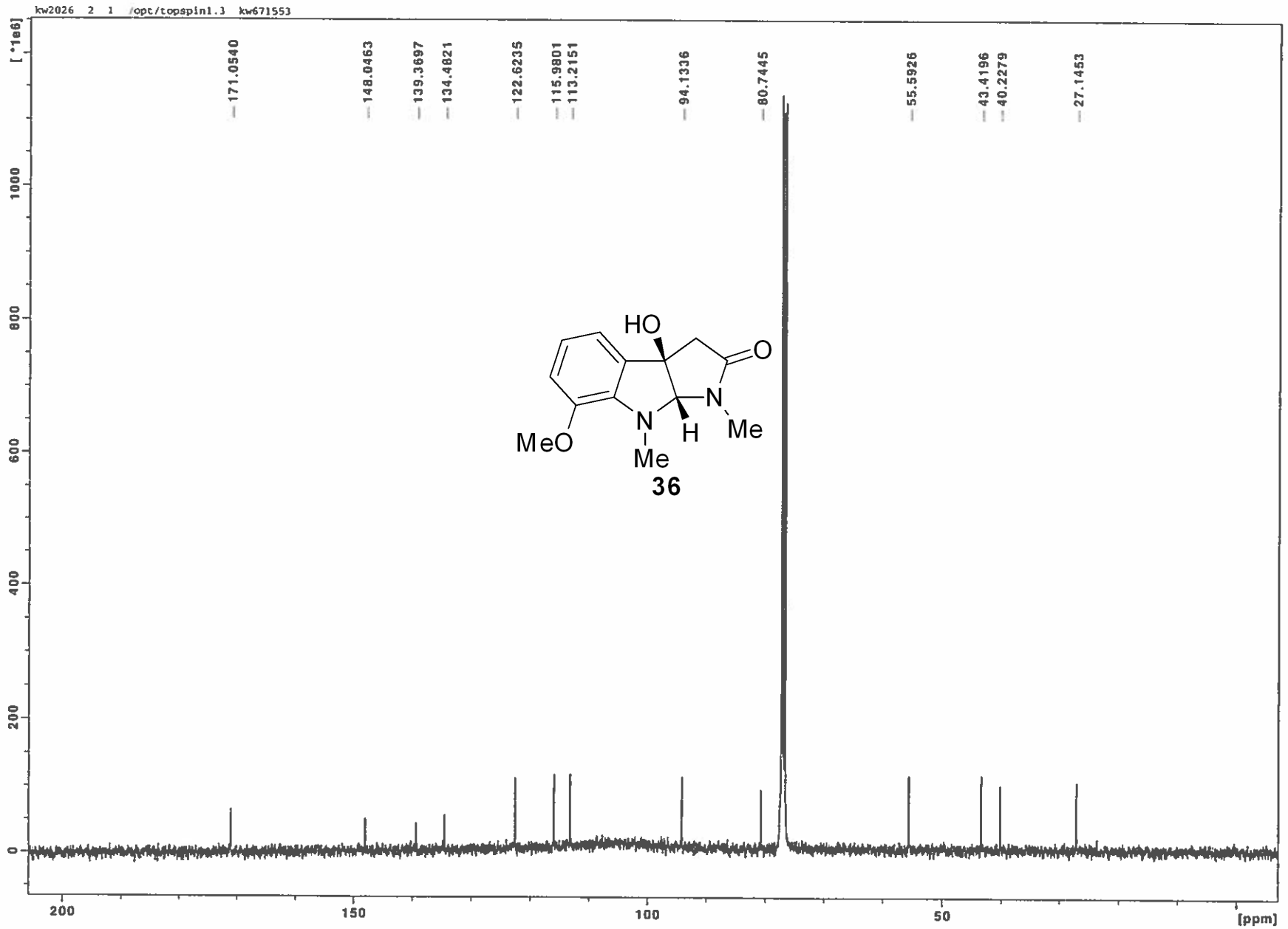

kw1207A 1 1 /opt/topspin1.3 kw671553
[*1e6]
6.8611
6.8541
6.8373
6.8302
6.8125
6.5162
6.4964
4.6830
3.7491
3.1842
3.0154
2.9183
2.8581
2.8488
MeO
HO
O
N
Me
N
H
Me
34
2.0513
1.0729
1.0000
3.2242
1.0270
3.4240
1.9369
10
8
6
4
2
0 (ppm)

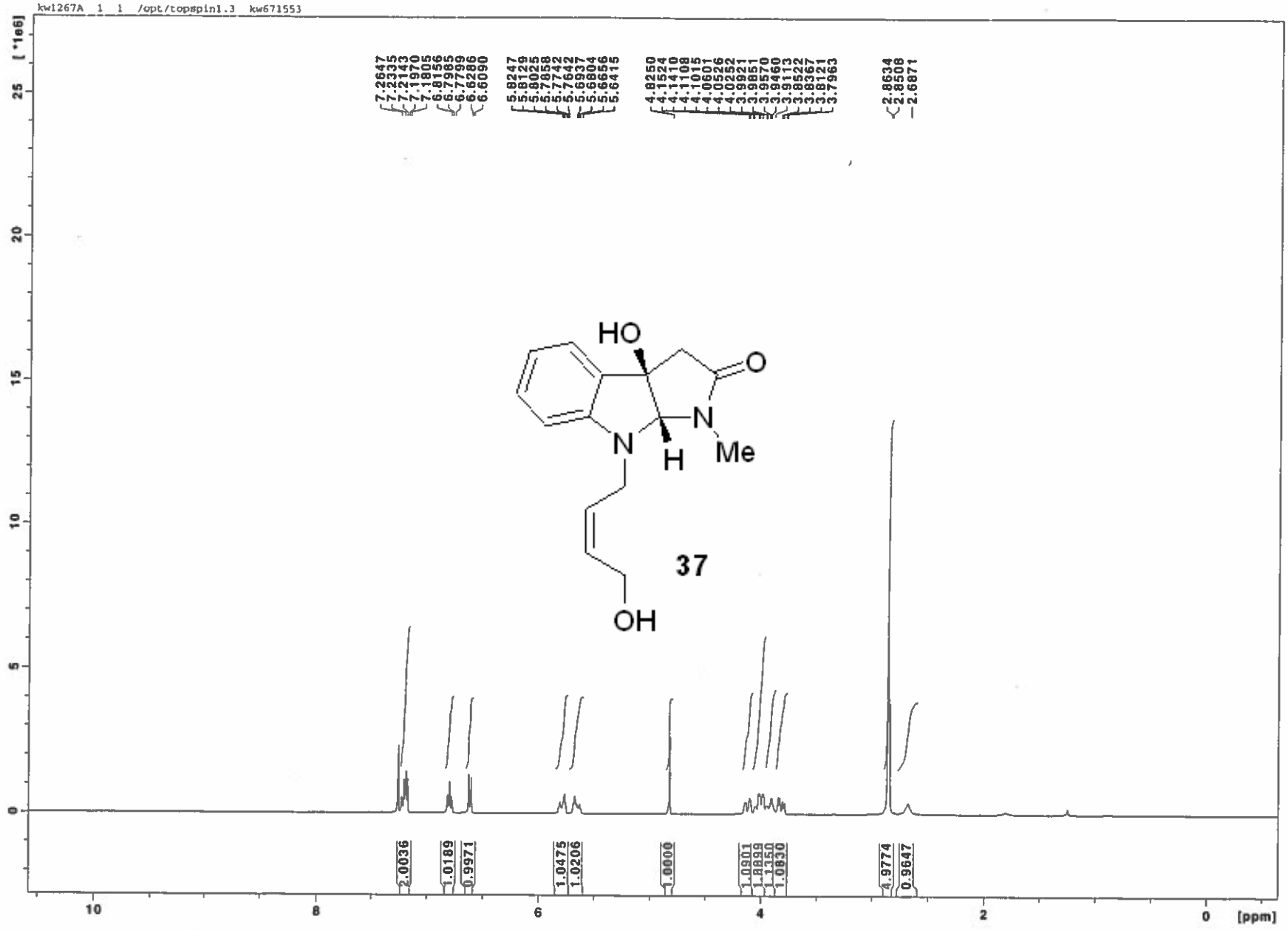

kw1207A 2 1 /opt/topspin1.3 kw671553
[*1e9]
171.8346
153.9749
144.4556
132.4133
116.7316
110.3683
109.4236
93.7601
80.1645
56.0261
43.6914
37.7869
27.9531
MeO
HO
O
N
Me
N
H
Me
34
30
20
10
0
200
150
100
50
[ppm]

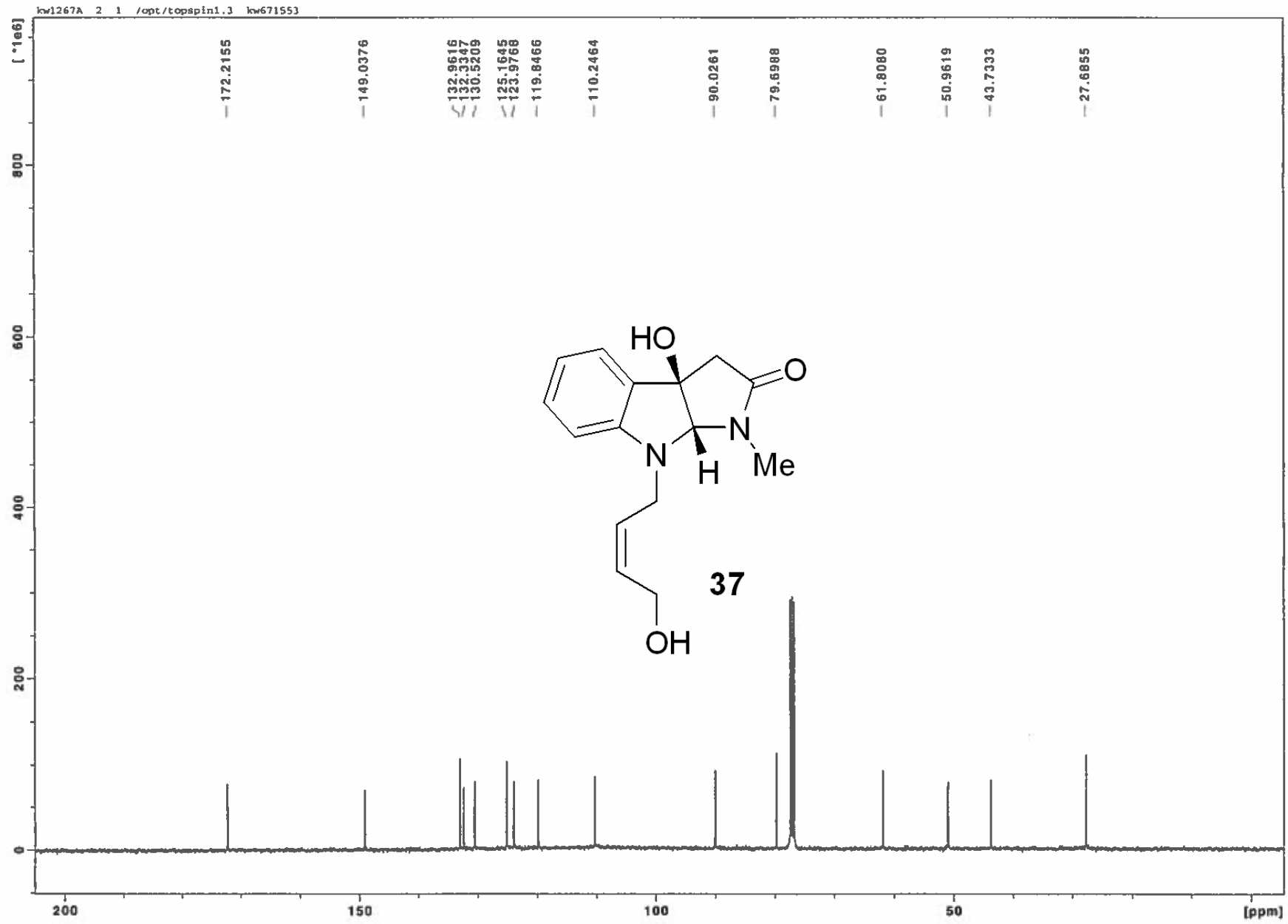

kw2034 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.1412
7.1206
6.3189
6.2987
6.0549
4.7340
3.7747
3.0477
2.8930
2.8468
HO
O
MeO
N
N
H
Me
Me
35
1.0000
1.0016
0.9680
0.9845
3.1237
0.7016
3.1147
1.9991
10
8
6
4
2
0
[ppm]

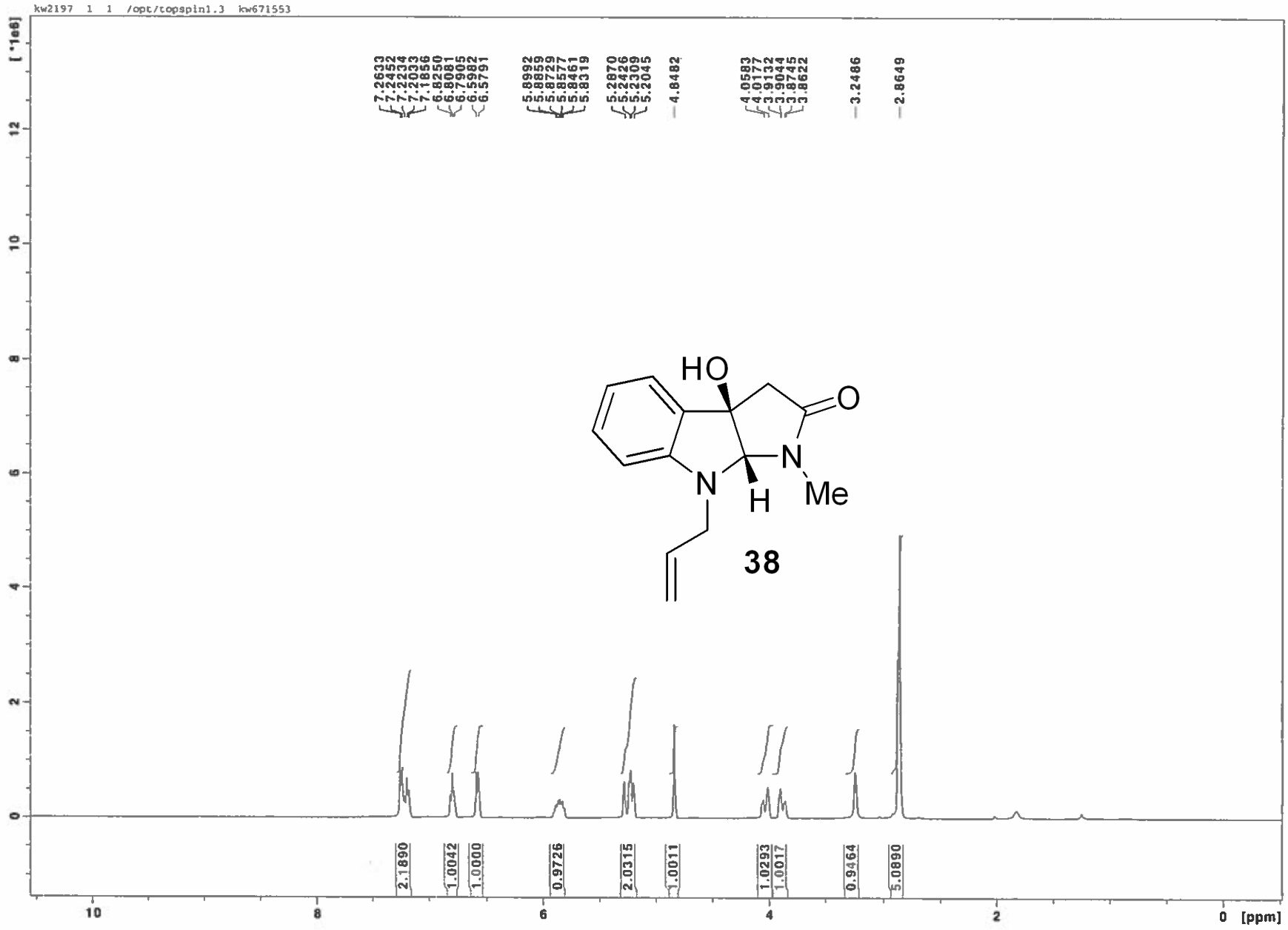

kw2034 2 1 /opt/topspin1.3 kw671553
[*1e6]
171.9944
162.5246
151.5099
124.3467
123.9831
104.0917
95.0162
92.8967
79.4050
55.4118
43.6440
35.7516
27.9984
600
400
200
0
200
150
100
50
0 [ppm]
HO
O
MeO
N
N
Me
H
Me
35

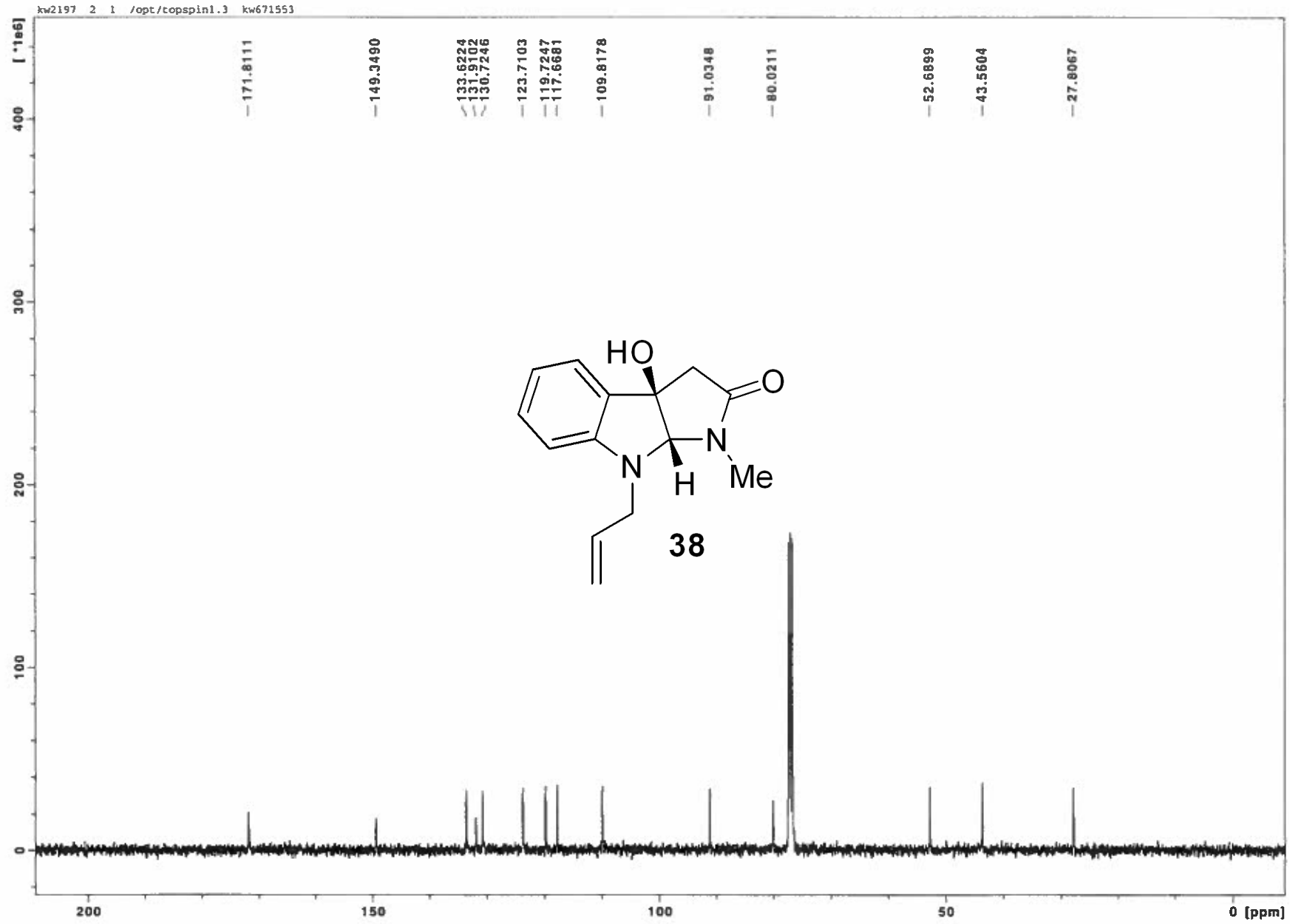

kw2026 1 1 /opt/topspin1.3 kw671553
[*1e6]
6.9103
6.8983
6.8147
6.7977
4.6227
3.8382
3.1761
3.0508
2.8934
2.8596
HO
O
N
N
H
Me
MeO
Me
36
2.1170
1.0000
1.0677
3.2378
3.2029
1.0309
2.1164
10
8
6
4
2
0 [ppm]

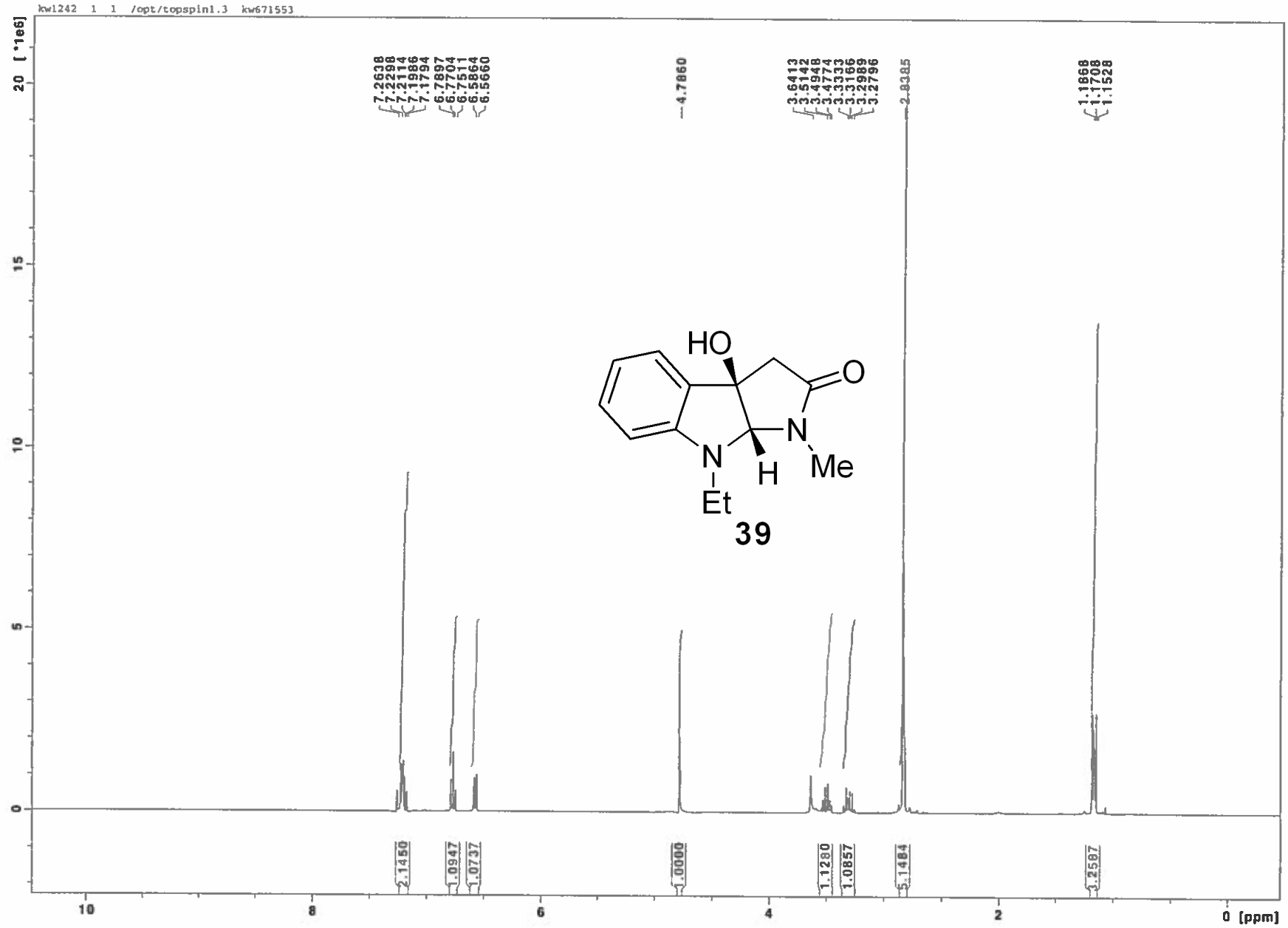

kw2026 2 1 /opt/topspin1.3 kw671553
[*1e6]
171.0540
148.0463
139.3697
134.4821
122.6235
115.9801
113.2151
94.1336
80.7445
55.5926
43.4196
40.2279
27.1453
1000
800
600
400
200
0
200
150
100
50
[ppm]
HO
O
N
Me
N
H
MeO
Me
36

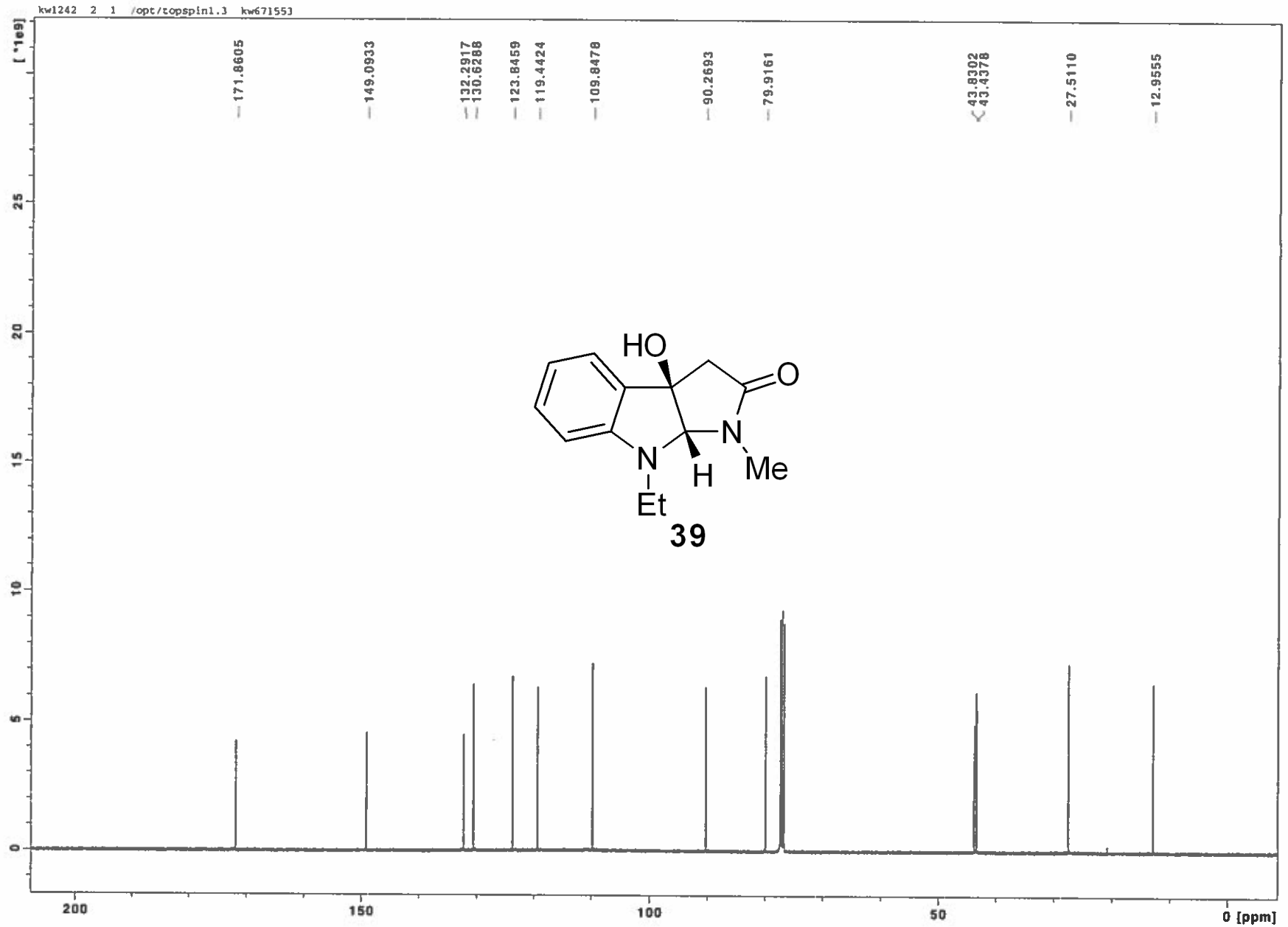

kw1267A 1 1 /opt/topspin1.3 kw671553
7.2647
7.2335
7.2143
7.1970
7.1805
6.8156
6.7985
6.7799
6.6286
6.6090
5.8247
5.8129
5.8025
5.7858
5.7742
5.7642
5.6937
5.6804
5.6656
5.6415
4.8250
4.1524
4.1410
4.1108
4.1015
4.0601
4.0526
4.0252
3.9921
3.9851
3.9570
3.9460
3.9113
3.8522
3.8367
3.8121
3.7963
2.8634
2.8508
2.6871
HO
O
N
N
H
Me
OH
37
2.0036
1.0189
0.9971
1.0475
1.0206
1.0000
1.0901
1.0899
1.1150
1.0830
4.9774
0.9647
[*1e6]
[ppm]

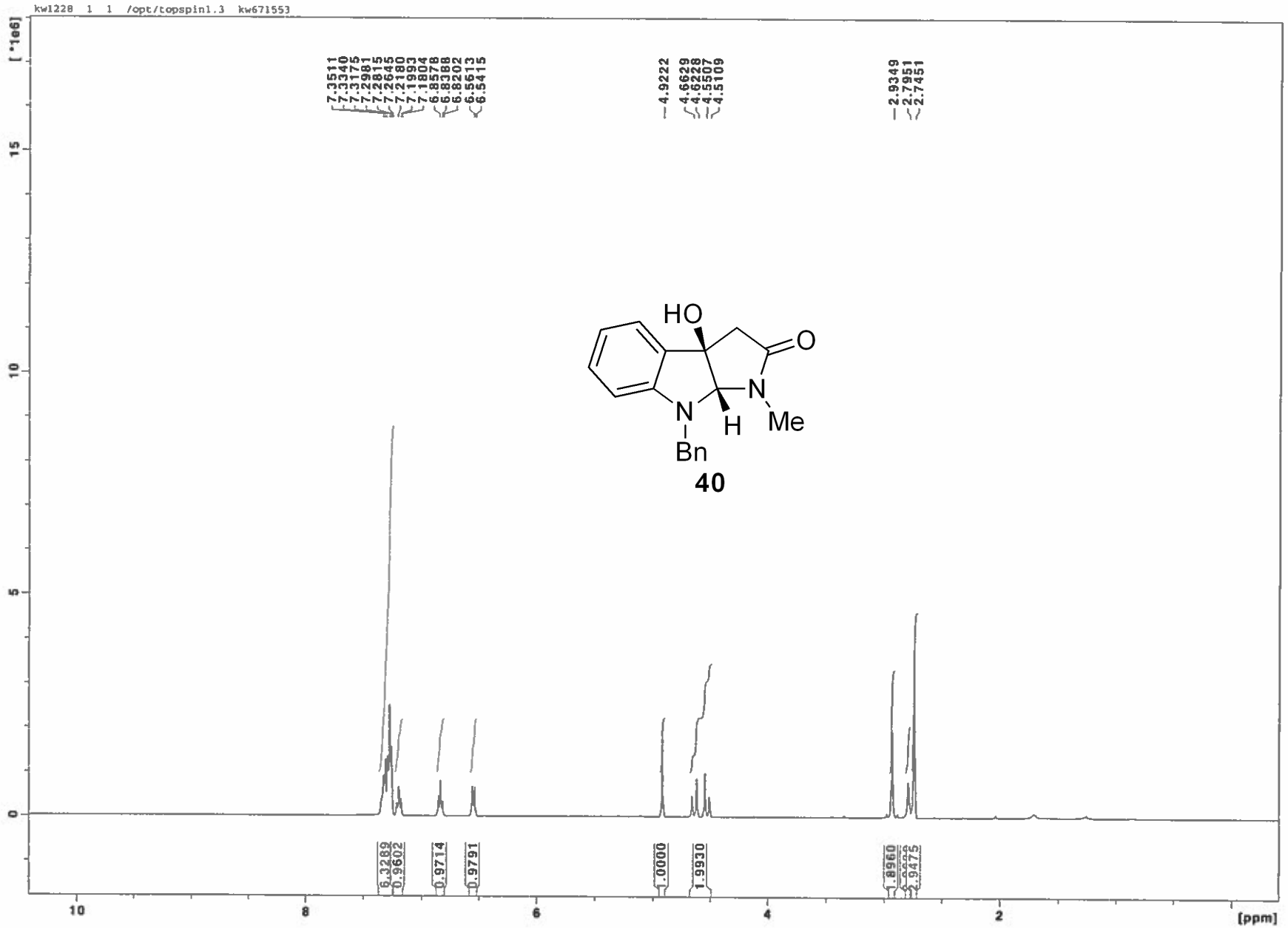

kw1267A 2 1 /opt/topspin1.3 kw671553
[*1e6]
172.2155
149.0376
132.9616
132.3387
130.5209
125.1645
123.9768
119.8466
110.2464
90.0261
79.6988
61.8080
50.9619
43.7333
27.6855
HO
O
N
N
H
Me
37
OH
800
600
400
200
0
200
150
100
50
[ppm]


kw2197 1 1 /opt/topspin1.3 kw671553
7.2633
7.2452
7.2234
7.2033
7.1856
6.8250
6.8081
6.7905
6.5982
6.5791
5.8992
5.8859
5.8729
5.8577
5.8461
5.8319
5.2870
5.2426
5.2309
5.2045
4.8482
4.0583
4.0177
3.9132
3.9044
3.8745
3.8622
3.2486
2.8649
HO
O
N
N
H
Me
38
2.1890
1.0042
1.0000
0.9726
2.0315
1.0011
1.0293
1.0017
0.9464
5.0890
[ppm]

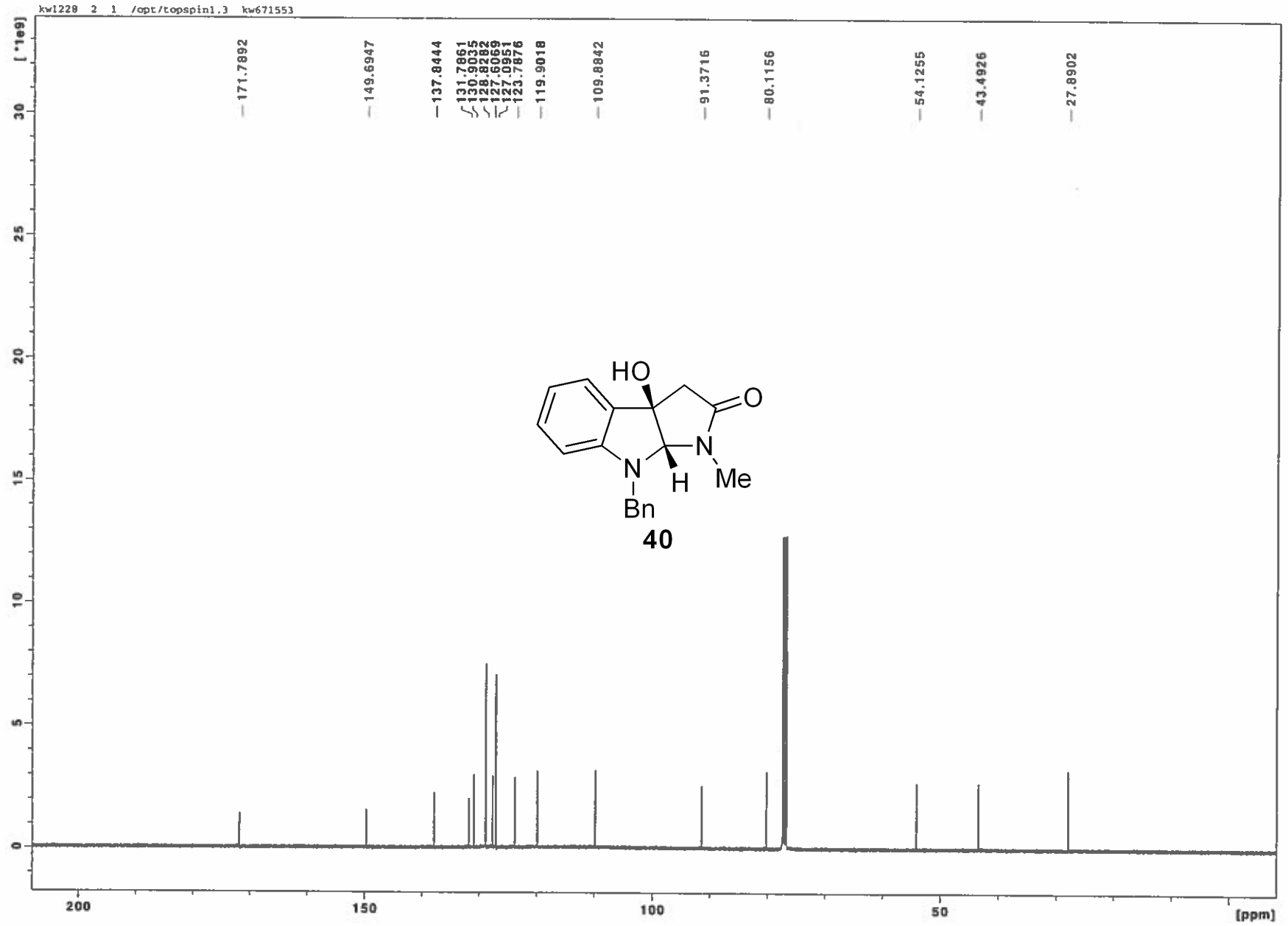

kw2197 2 1 /opt/topspin1.3 kw671553
[*1e6]
171.8111
149.3490
133.6224
131.9102
130.7246
123.7103
119.7247
117.6681
109.8178
91.0348
80.0211
52.6899
43.5604
27.8067
HO
O
N
N
H
Me
38
400
300
200
100
0
200
150
100
50
0 [ppm]

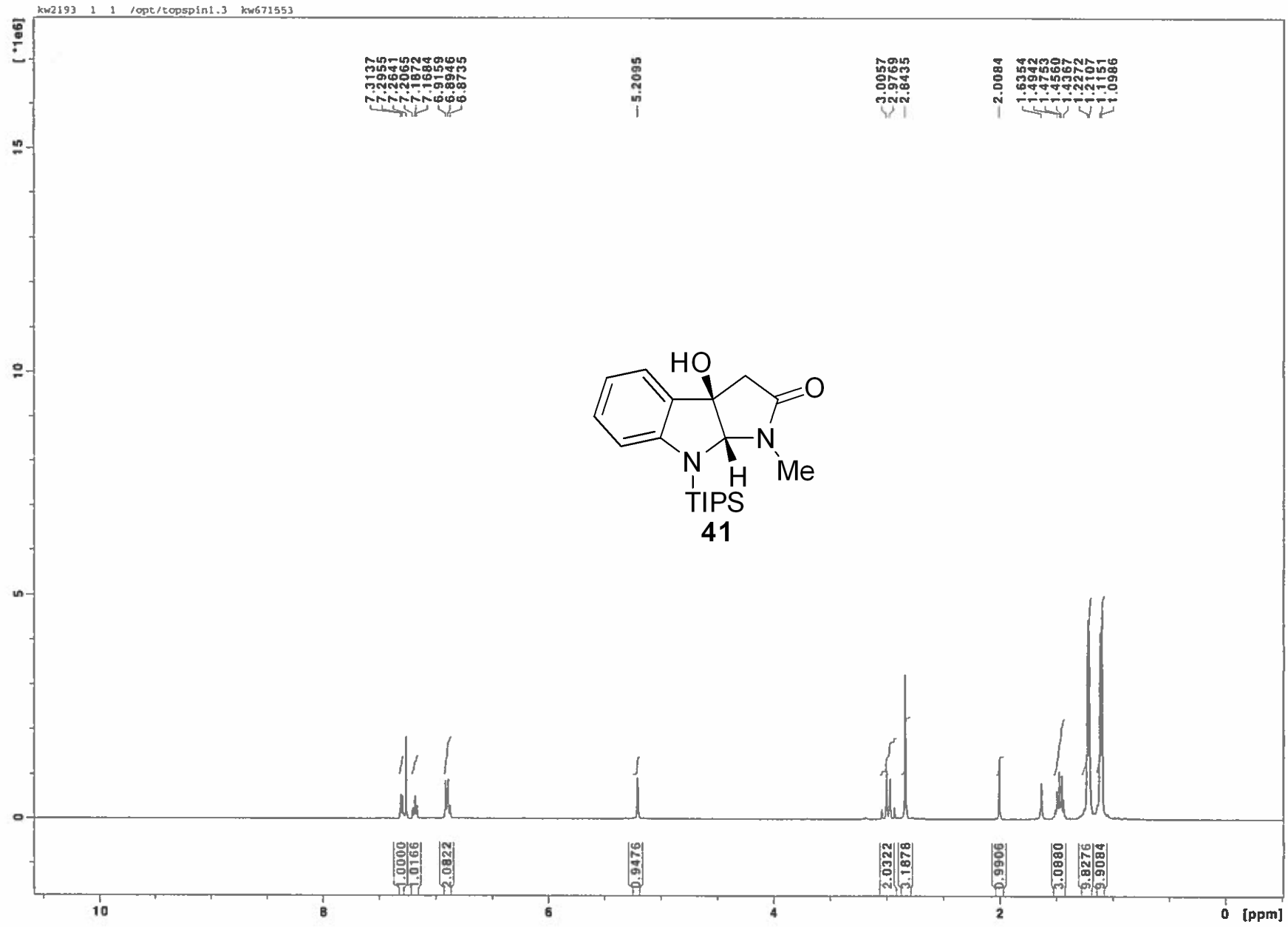

kw1242 1 1 /opt/topspin1.3 kw671553
7.2638
7.2298
7.2114
7.1986
7.1794
6.7897
6.7704
6.7511
6.5864
6.5660
4.7860
3.6413
3.5142
3.4948
3.4774
3.3333
3.3166
3.2989
3.2796
2.8385
1.1668
1.1708
1.1528
HO
O
N
N
H
Me
Et
39
2.1450
1.0947
1.0737
1.0000
1.1280
1.0857
5.1484
3.2587
20 [*1e6]
15
10
5
0
10
8
6
4
2
0 [ppm]

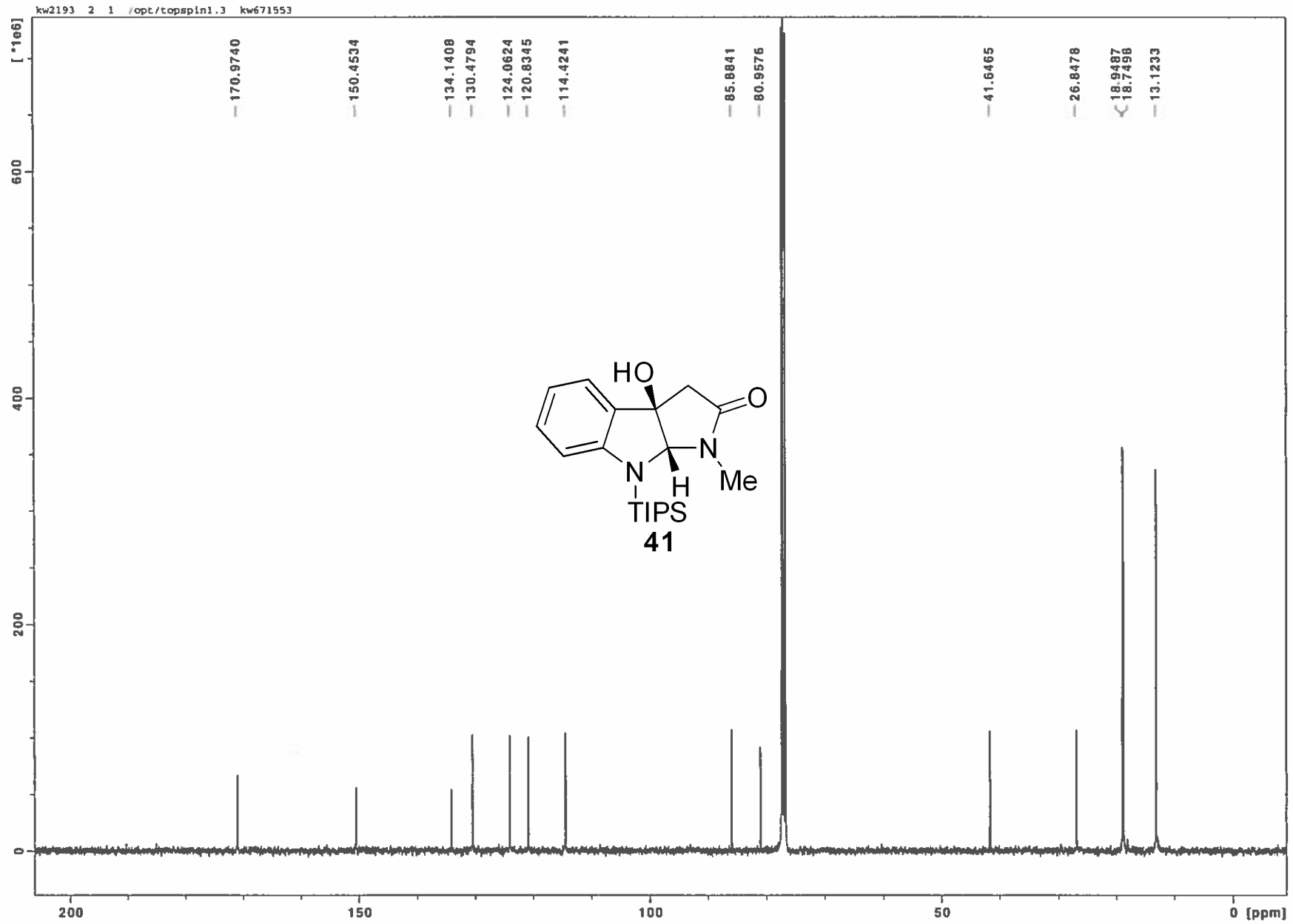

kw1242 2 1 /opt/topspin1.3 kw67155J
171.8605
149.0933
132.2917
130.6288
123.8459
119.4424
109.8478
90.2693
79.9161
43.8302
43.4378
27.5110
12.9555
HO
O
N
N
H
Me
Et
39
200
150
100
50
0 [ppm]

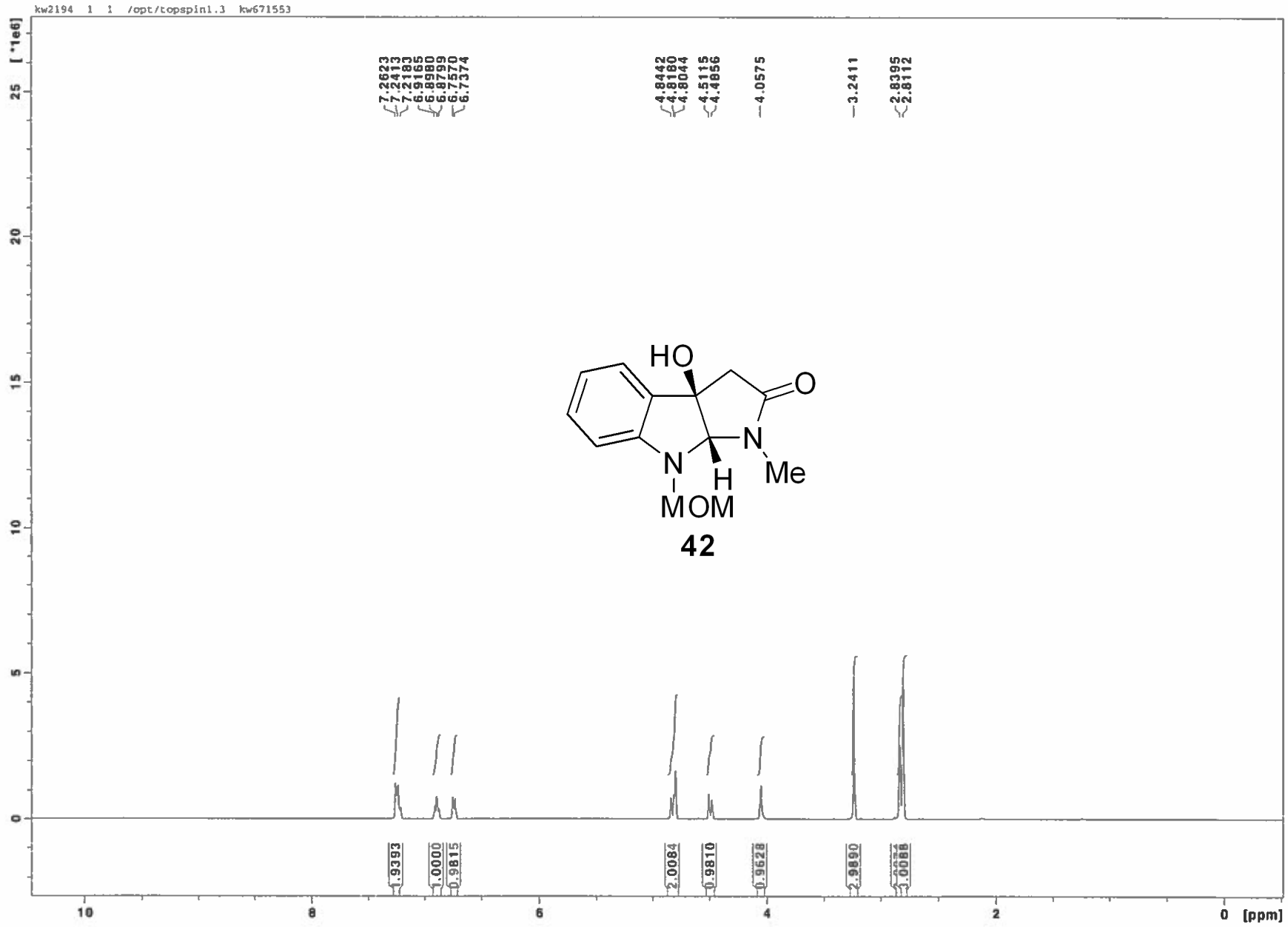

kw1228 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.3511
7.3340
7.3175
7.2981
7.2815
7.2645
7.2180
7.1993
7.1804
6.8578
6.8388
6.8202
6.5613
6.5415
4.9222
4.6629
4.6229
4.5507
4.5109
2.9349
2.7951
2.7451
HO
O
N
N
H
Me
Bn
6.3289
0.9602
0.9714
0.9791
1.0000
1.9930
1.8960
2.9475
10
8
6
4
2
[ppm]

40

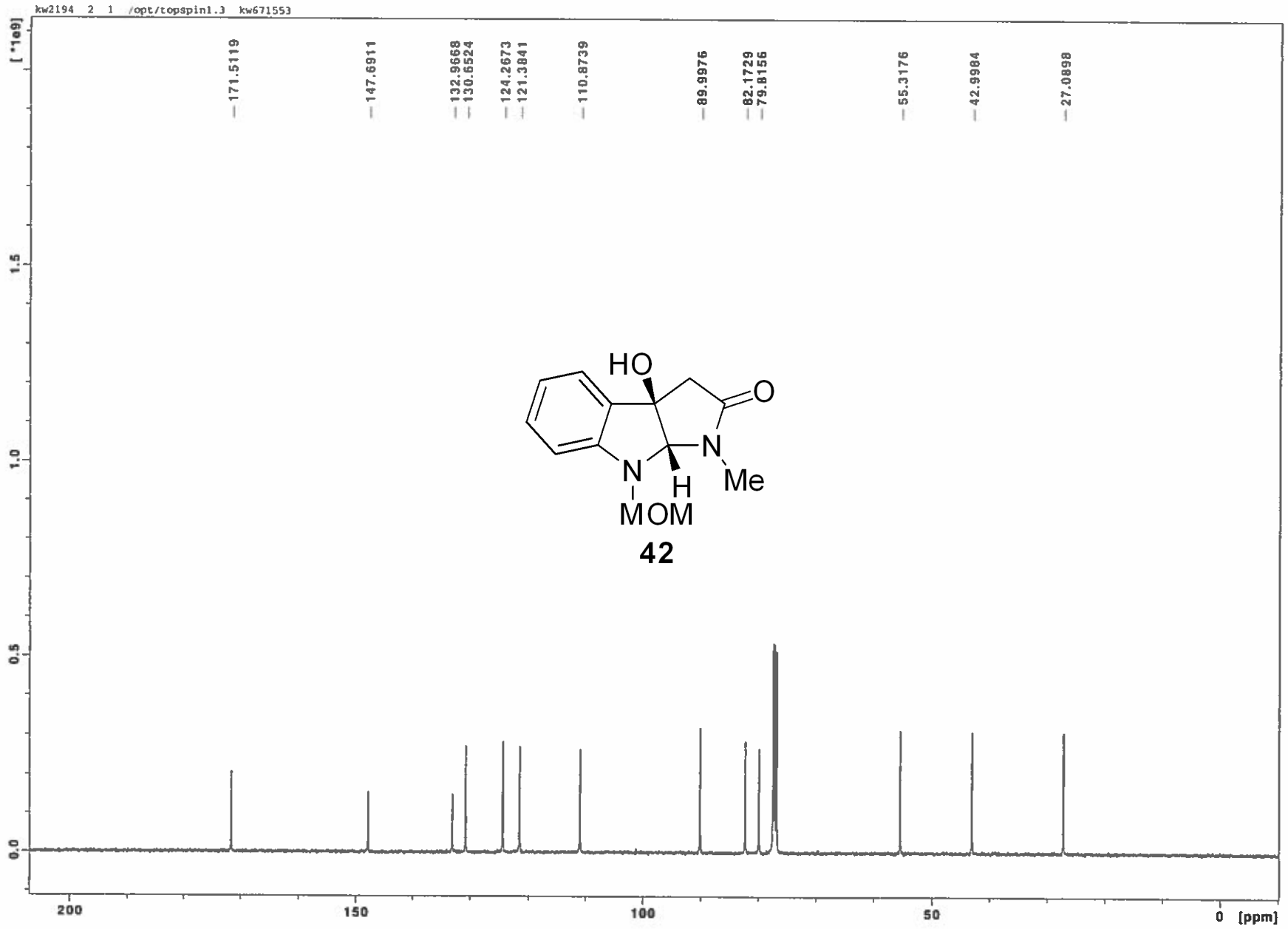

kw1228 2 1 /opt/topspin1.3 kw671553
[*1e9]
171.7892
149.6947
137.8444
131.7661
130.9035
128.8282
127.6069
127.0951
123.7876
119.9018
109.8842
91.3716
80.1156
54.1255
43.4926
27.8902
HO
O
N
N
H
Me
Bn
40
200
150
100
50
[ppm]


kw2193 1 1 /opt/topspin1.3 kw671553
7.3137
7.2955
7.2641
7.2065
7.1872
7.1684
6.9159
6.8946
6.8735
5.2095
3.0057
2.9769
2.8435
2.0084
1.6354
1.4942
1.4753
1.4560
1.4367
1.2272
1.2107
1.1151
1.0986
HO
O
N
N
H
Me
TIPS
41
1.0000
1.0166
2.0822
0.9476
2.0322
3.1878
0.9906
3.0880
9.8276
9.9084
[*1e6]
[ppm]

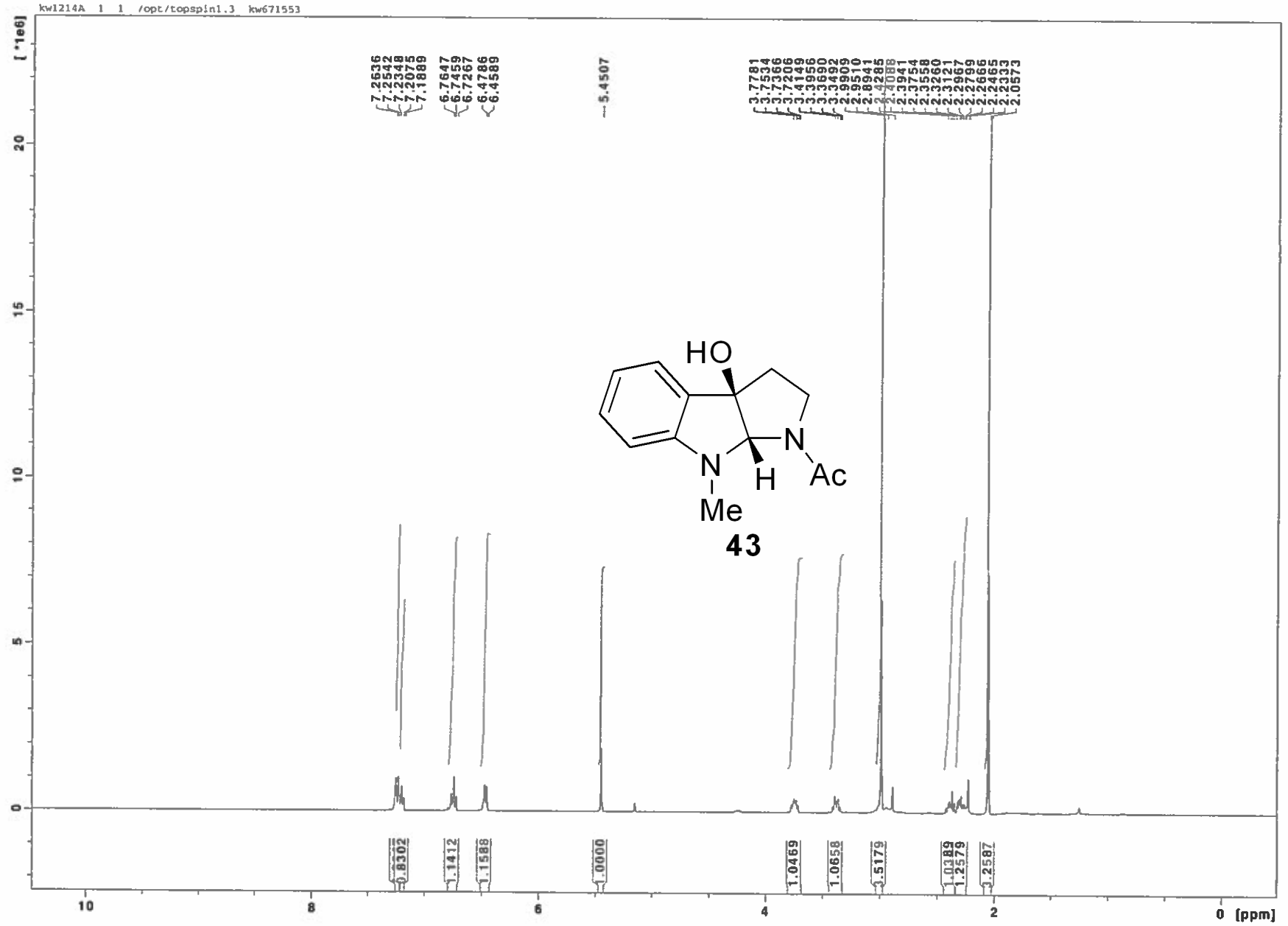

kw2193 2 1 /opt/topspin1.3 kw671553
[*1e6]
600
400
200
0
170.9740
150.4534
134.1408
130.4794
124.0624
120.8345
114.4241
85.8841
80.9576
41.6465
26.8478
18.9487
18.7498
13.1233
HO
O
N
Me
N
H
TIPS
41
200
150
100
50
0 [ppm]

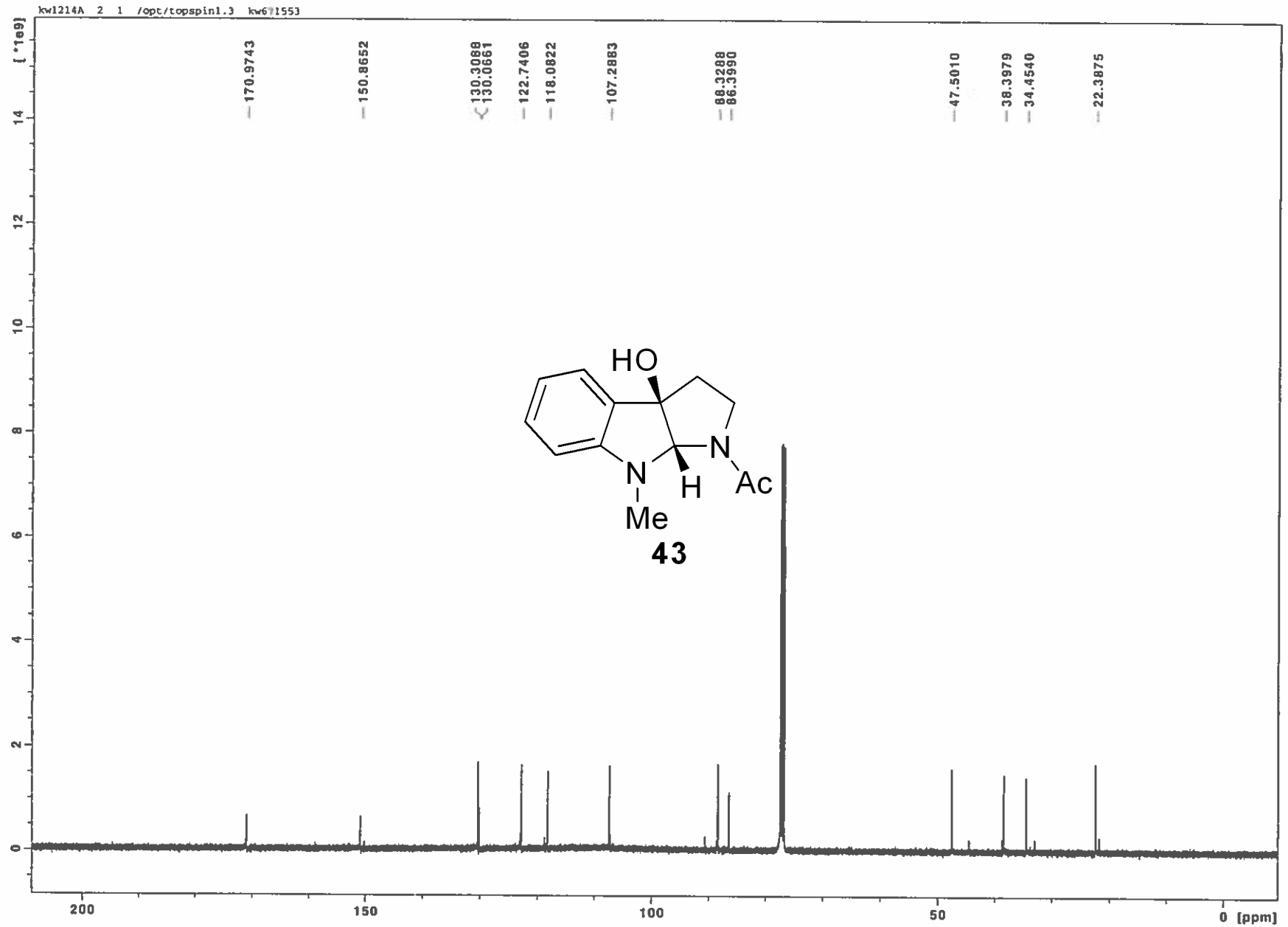

kw2194 1 1 /opt/topspin1.3 kw671553
[*1e6]
25
20
15
10
5
0
7.2623
7.2413
7.2183
6.9165
6.8980
6.8799
6.7570
6.7374
4.8442
4.8180
4.8044
4.5115
4.4856
4.0575
3.2411
2.8395
2.8112
HO
O
N
N
H
Me
MOM
1.9393
1.0000
0.9815
2.0084
0.9810
0.9628
2.9890
3.0088
10
8
6
4
2
0
[ppm]

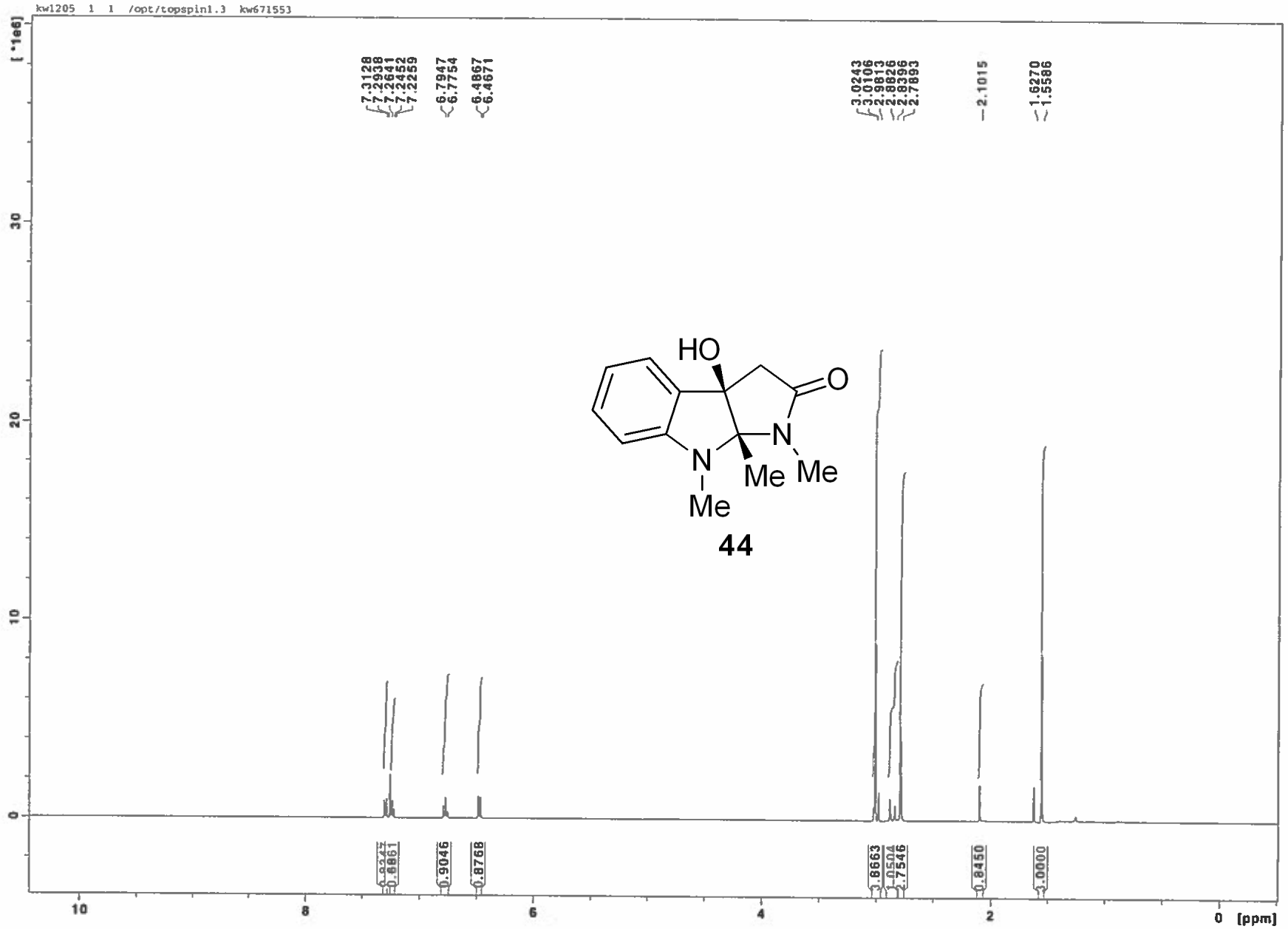
42

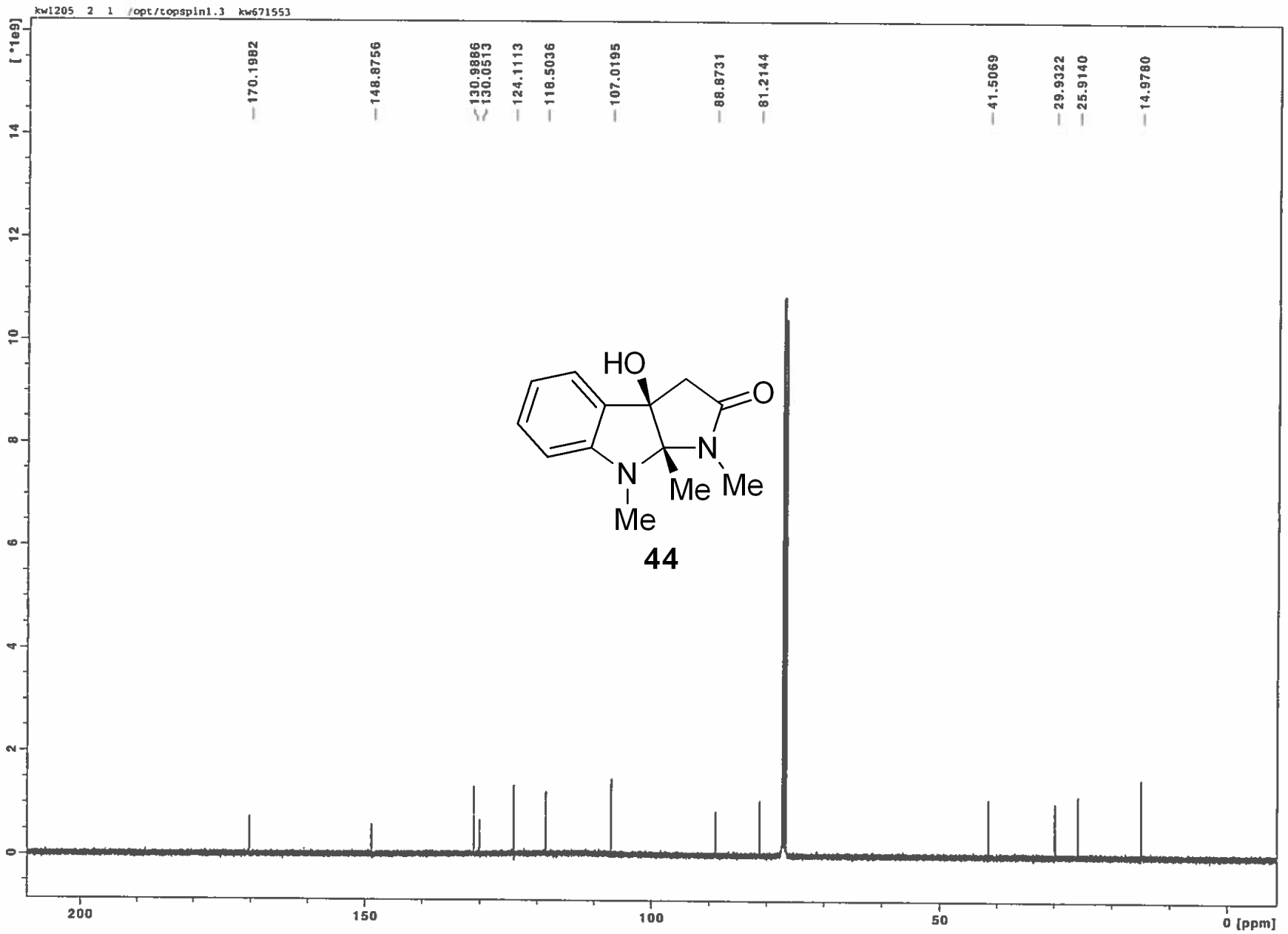

kw2194 2 1 /opt/topspin1.3 kw671553
[*1e9]
171.5119
147.6911
132.9668
130.6524
124.2673
121.3841
110.8739
89.9976
82.1729
79.8156
55.3176
42.9984
27.0898
1.5
1.0
0.5
0.0
200
150
100
50
0 [ppm]
HO
O
N
N
Me
H
MOM

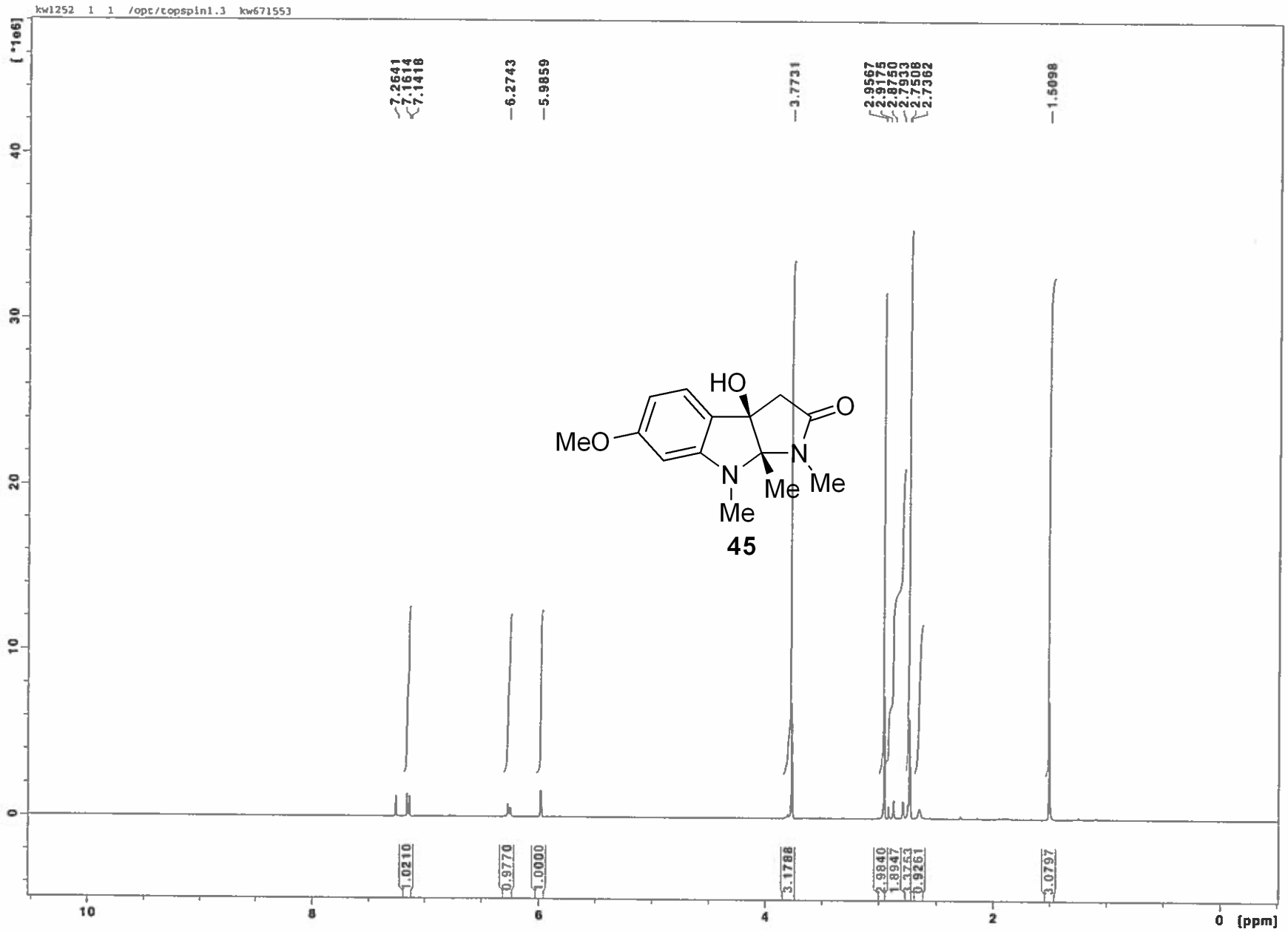
42

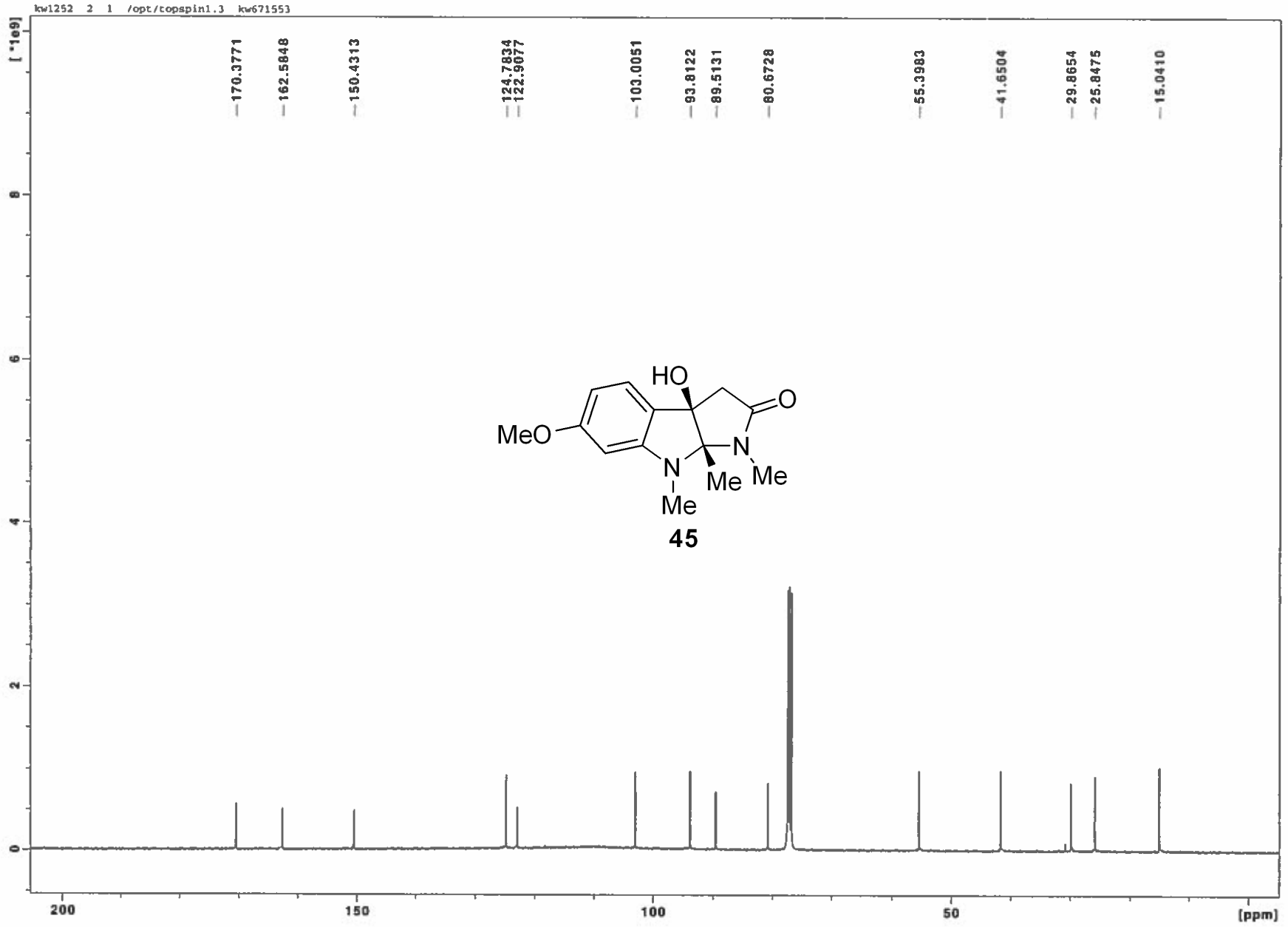

kw1214A 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2636
7.2542
7.2348
7.2075
7.1889
6.7647
6.7459
6.7267
6.4786
6.4589
5.4507
3.7781
3.7534
3.7366
3.7206
3.4149
3.3956
3.3690
3.3492
2.9909
2.9510
2.8941
2.4285
2.3941
2.3754
2.3558
2.3260
2.3121
2.2967
2.2799
2.2666
2.2465
2.2333
2.0573
0.8302
1.1412
1.1588
1.0000
1.0469
1.0658
3.5179
1.0389
1.2579
3.2587
10
8
6
4
2
0 (ppm)
HO
N
N
H
Ac
Me
43


kw1214A 2 1 /opt/topspin1.3 kw6?1553
[*1e9]
170.9743
150.8652
130.3088
130.0661
122.7406
118.0822
107.2883
88.3288
86.3990
47.5010
38.3979
34.4540
22.3875
HO
N
N
H
Ac
Me
43
200
150
100
50
0 [ppm]

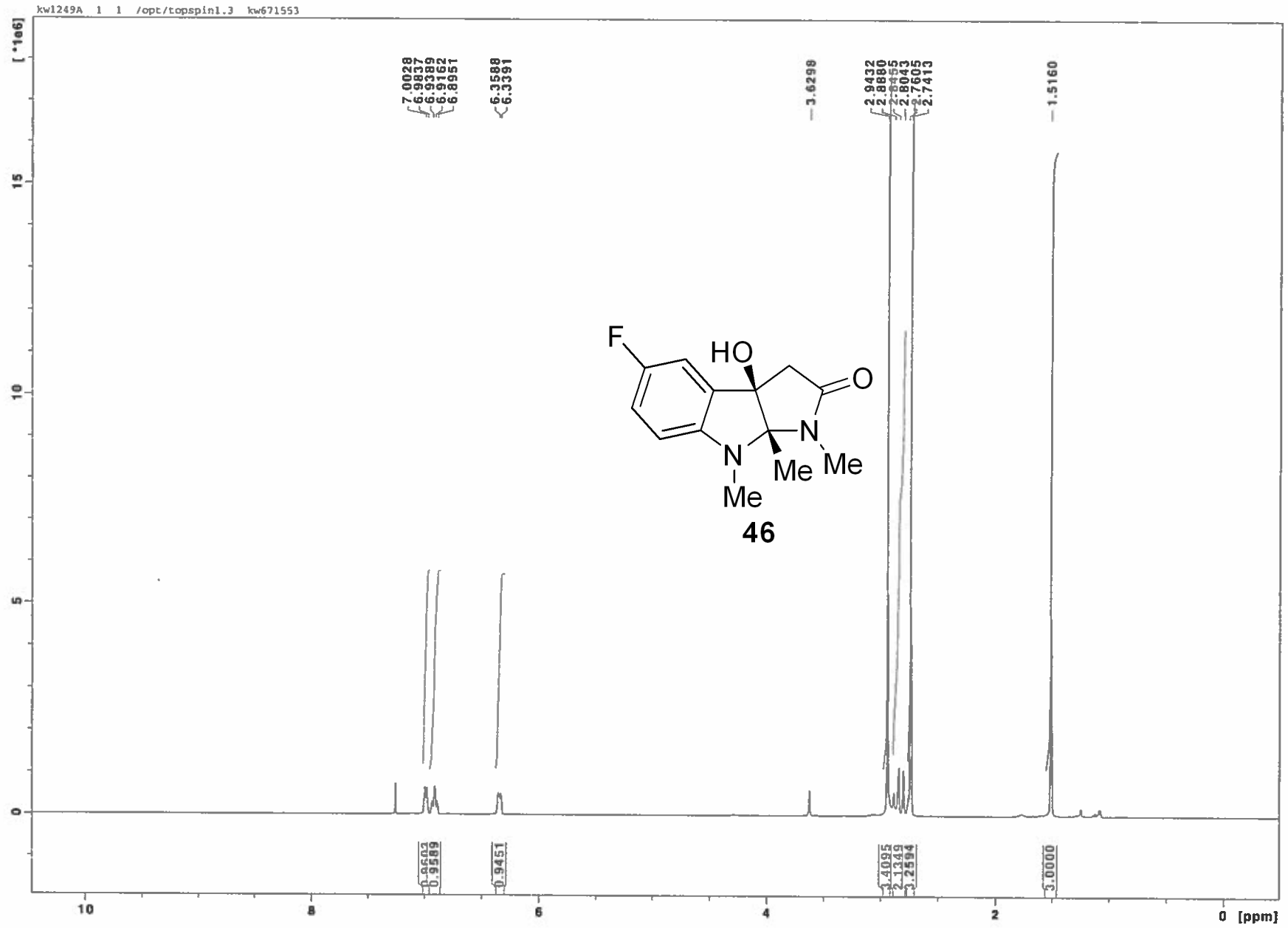

kw1205 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.3128
7.2938
7.2641
7.2452
7.2259
6.7947
6.7754
6.4867
6.4671
3.0243
3.0106
2.9813
2.8826
2.8366
2.7893
2.1015
1.6270
1.5586
HO
O
N
N
Me
Me
Me
44
0.8247
0.6861
0.9046
0.8768
3.8663
1.0504
2.7546
0.8450
3.0000
10
8
6
4
2
0
[ppm]

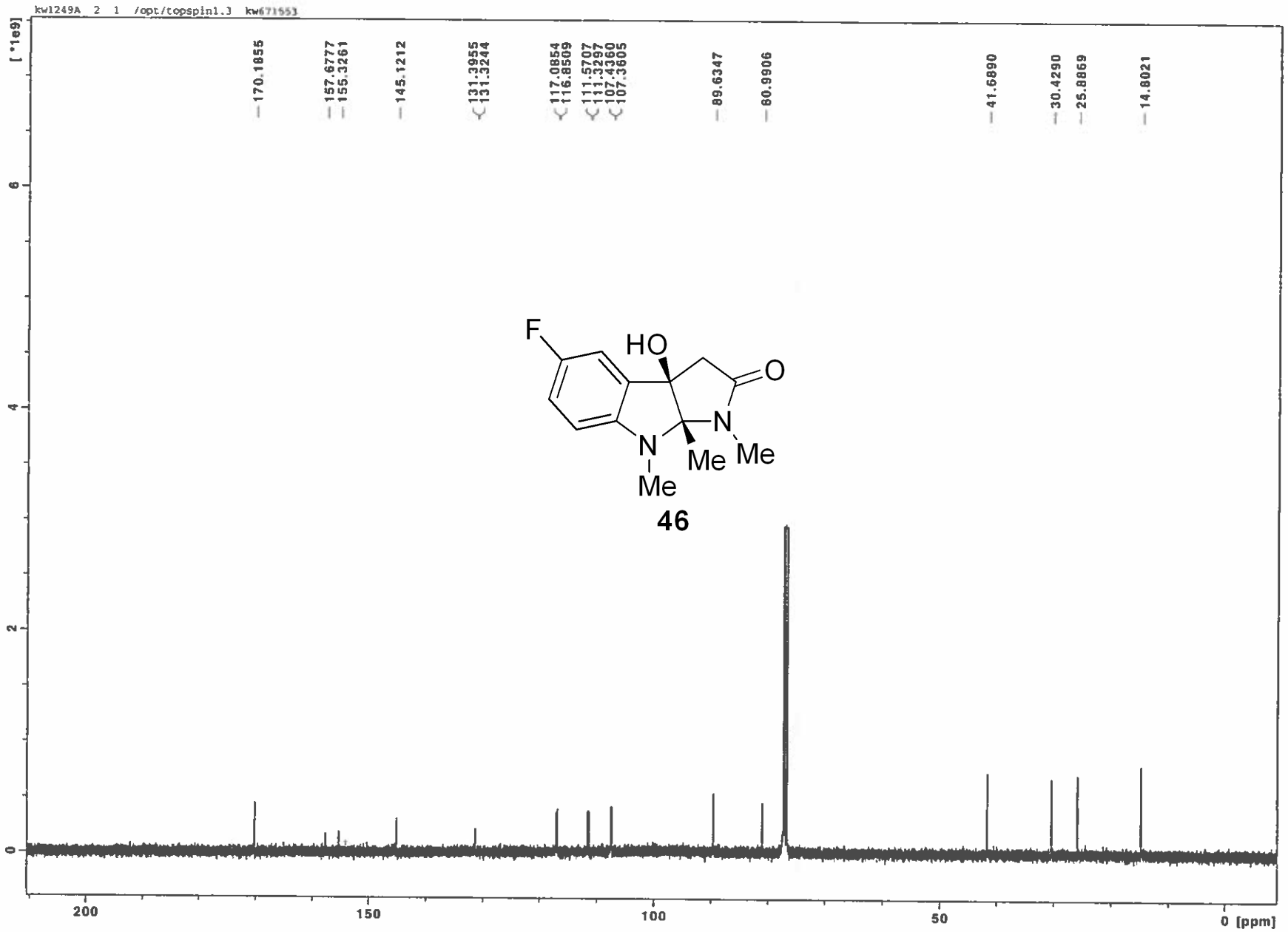

kw1205 2 1 /opt/topspin1.3 kw671553
[*1e9]
170.1982
148.8756
130.9886
130.0513
124.1113
118.5036
107.0195
88.8731
81.2144
41.5069
29.9322
25.9140
14.9780
HO
O
N
N
Me
Me
Me
44
200
150
100
50
0 [ppm]

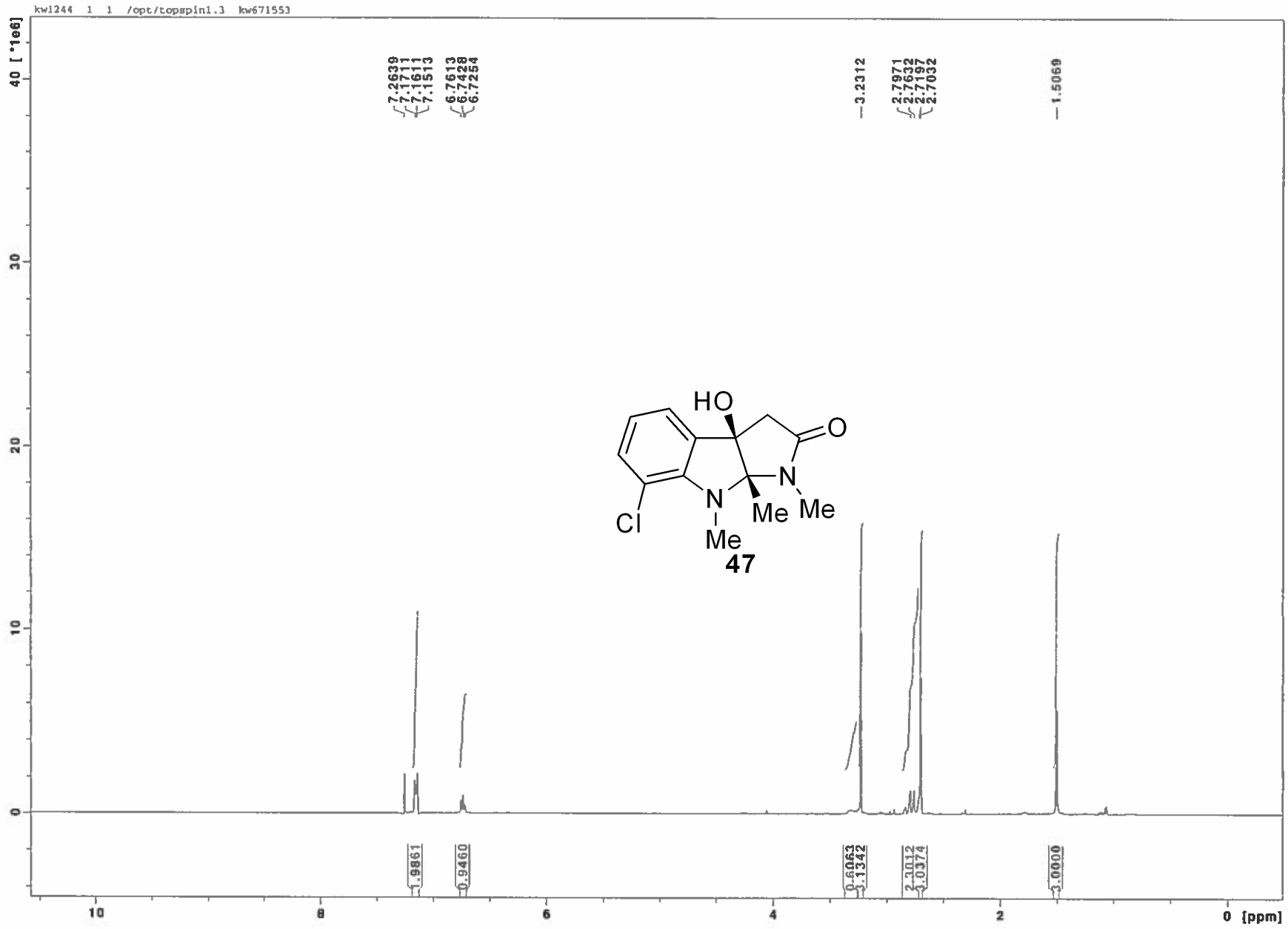

kw1252 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.2641
7.1614
7.1418
6.2743
5.9859
3.7731
2.9567
2.9175
2.8750
2.7933
2.7508
2.7362
1.5098
HO
O
MeO
N
N
Me
Me
Me
45
1.0210
0.9770
1.0000
3.1788
2.9840
1.8947
3.1753
0.9261
3.0797
10
8
6
4
2
0
(ppm)

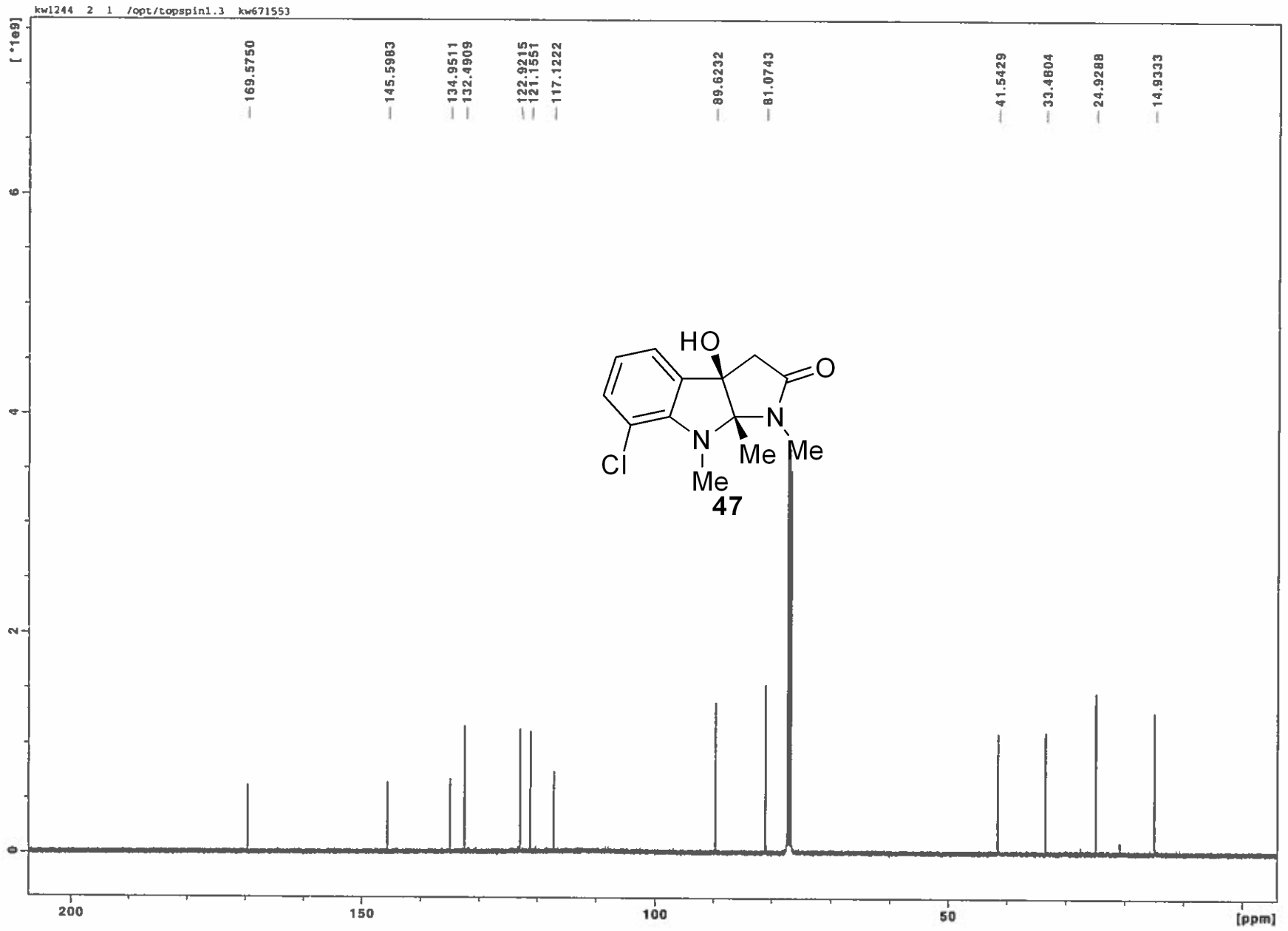

kw1252 2 1 /opt/topspin1.3 kw671553
[*1e9]
170.3771
162.5848
150.4313
124.7834
122.9077
103.0051
93.8122
89.5131
80.6728
55.3983
41.6504
29.8654
25.8475
15.0410
HO
O
MeO
N
N
Me
Me
Me
0
2
4
6
8
200
150
100
50
[ppm]

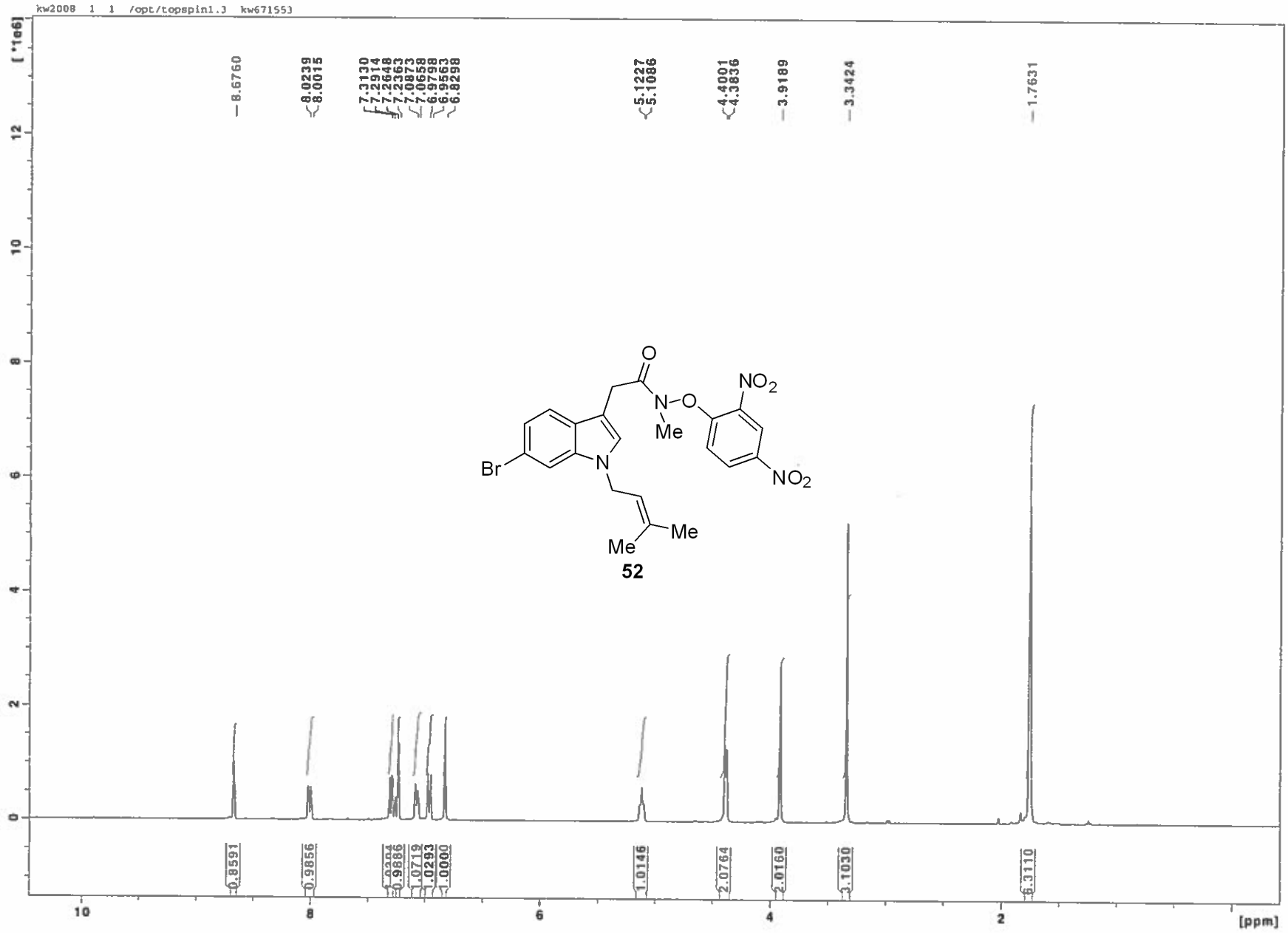
45


kw1249A 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.0028
6.9837
6.9389
6.9162
6.8951
6.3588
6.3391
3.6298
2.9432
2.8886
2.8455
2.8043
2.7605
2.7413
1.5160
F
HO
O
N
Me
N
Me
Me
46
0.9589
0.9451
3.4095
2.1349
3.2594
3.0000
10
8
6
4
2
0 [ppm]


kw1249A 2 1 /opt/topspin1.3 kw671553
[*1e9]
170.1855
157.6777
155.3261
145.1212
131.3955
131.3244
117.0854
116.8509
111.5707
111.3297
107.4360
107.3805
89.6347
80.9906
41.6890
30.4290
25.8869
14.8021
F
HO
O
N
N
Me
Me
Me
46
0
2
4
6
200
150
100
50
0 [ppm]

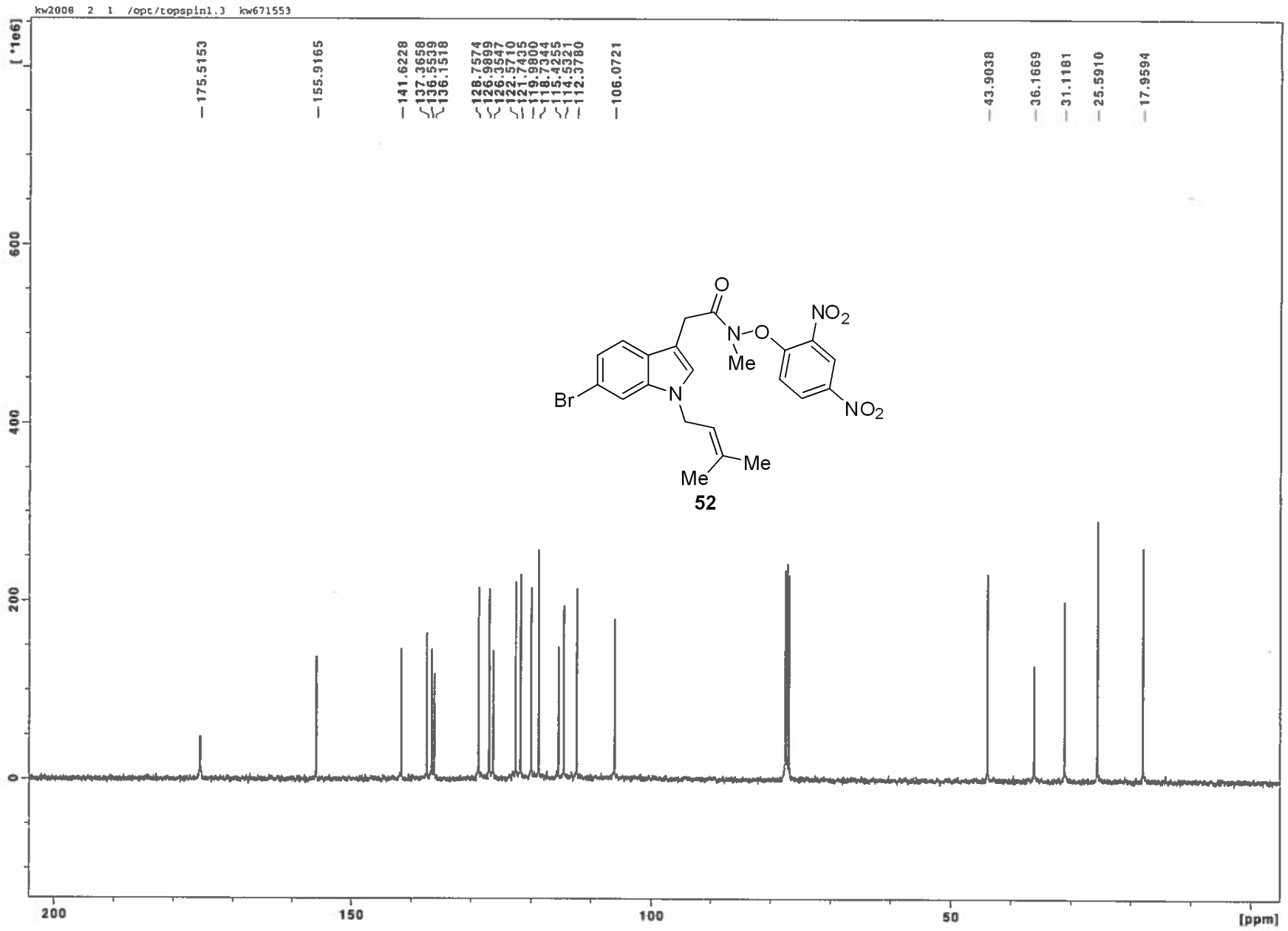

kw1244 1 1 /opt/topspin1.3 kw671553
7.2639
7.1711
7.1611
7.1513
6.7613
6.7428
6.7254
3.2312
2.7971
2.7632
2.7197
2.7032
1.5069
HO
O
N
N
Me
Me
Me
Cl
47
1.9861
0.9460
0.6063
3.1342
2.3012
3.0374
3.0000
40 [*1e6]
30
20
10
0
10
8
6
4
2
0 [ppm]

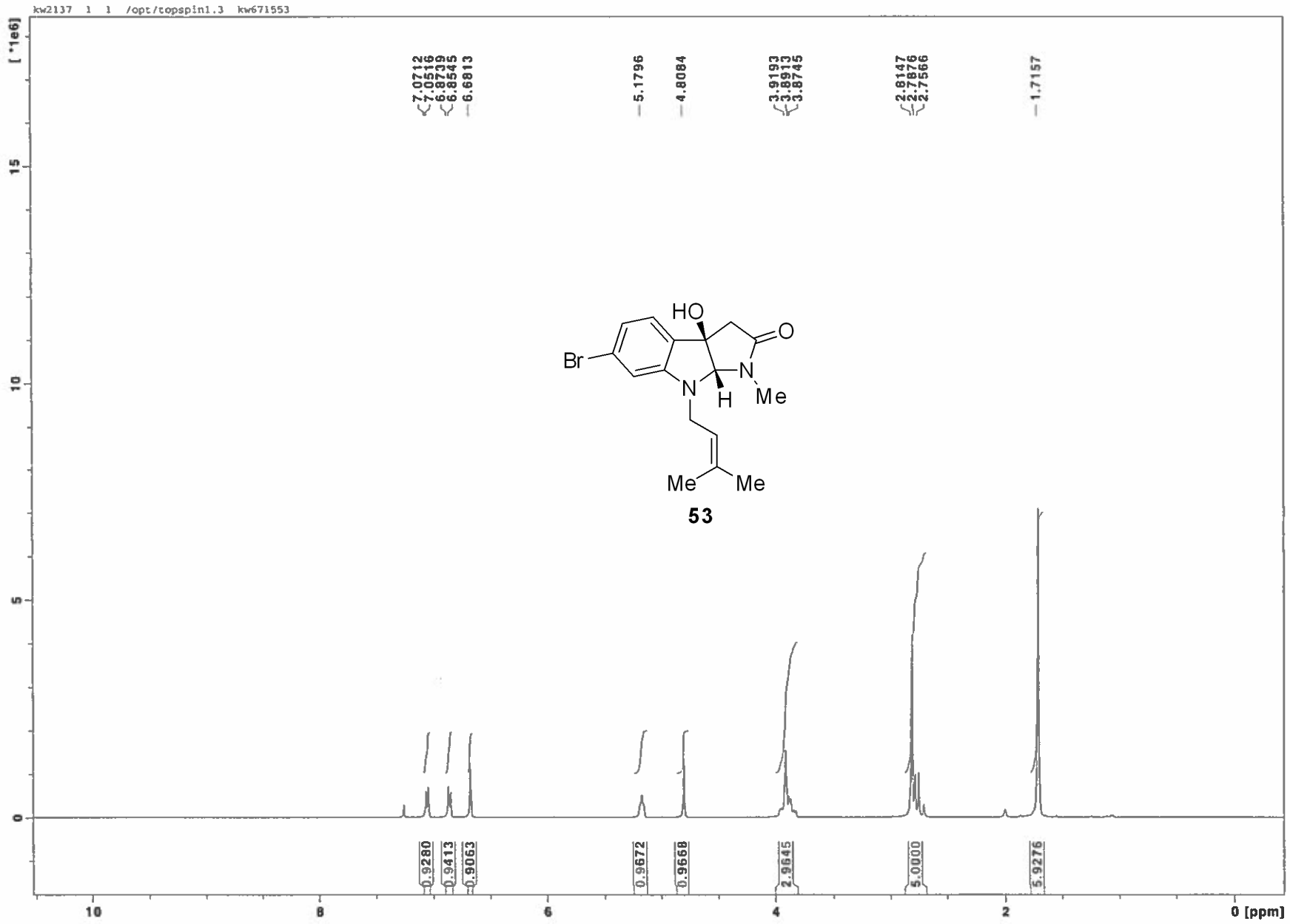

kw1244 2 1 /opt/topspin1.3 kw671553
[*1e8]
169.5750
145.5983
134.9511
132.4909
122.9215
121.1551
117.1222
89.6232
81.0743
41.5429
33.4804
24.9288
14.9333
HO
O
N
N
Me
Me
Me
Cl
47
0
2
4
6
200
150
100
50
[ppm]


kw2008 1 1 /opt/topspin1.3 kw67155j
[*1e6]
8.6760
8.0239
8.0015
7.3130
7.2914
7.2648
7.2363
7.0873
7.0658
6.9798
6.9563
6.8298
5.1227
5.1086
4.4001
4.3836
3.9189
3.3424
1.7631
0.8591
0.9856
1.0719
1.0293
1.0000
1.0146
2.0764
2.0160
3.1030
6.3110
[ppm]

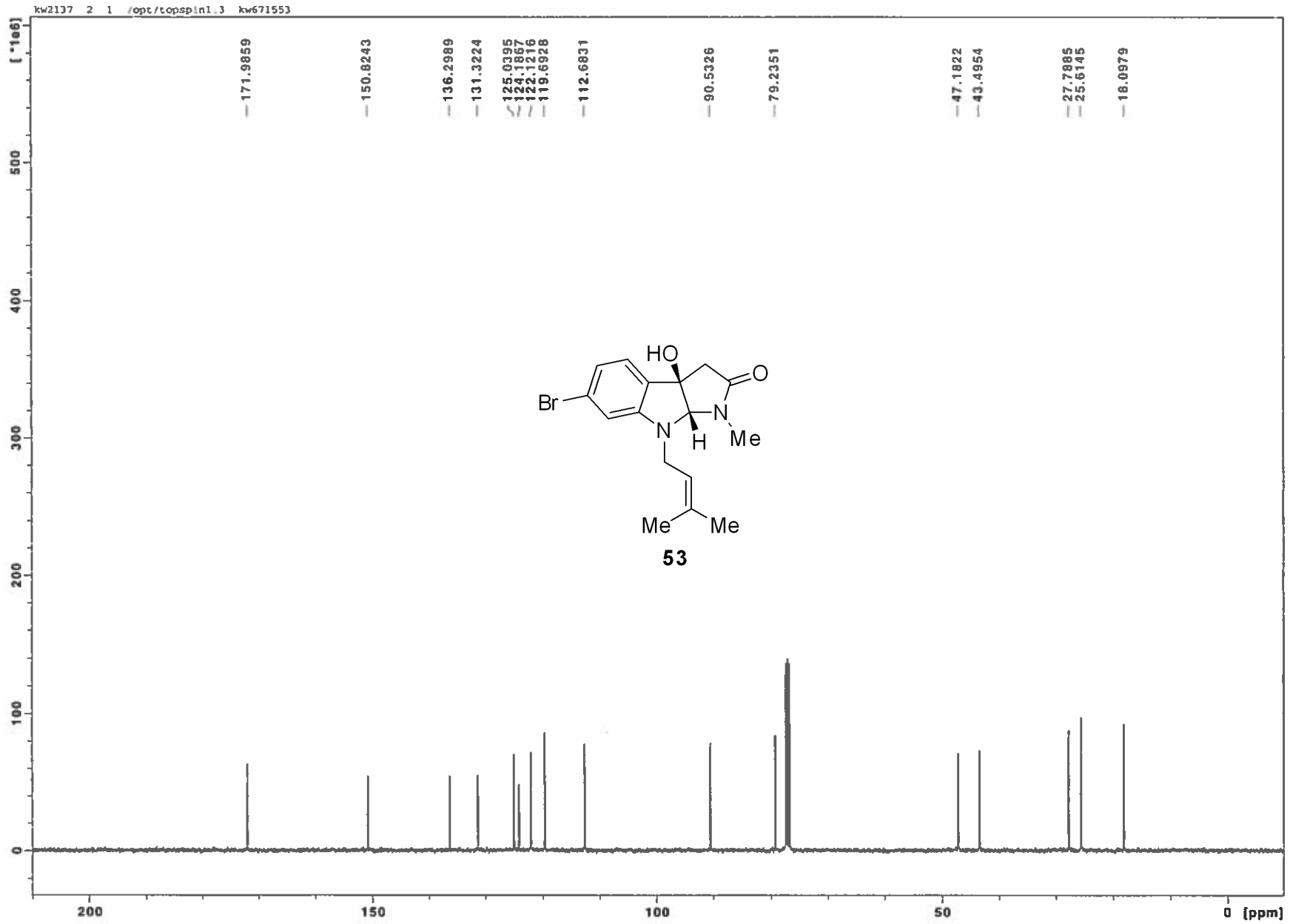
O
N
O
Me
NO2
NO2
Br
N
Me
Me

52

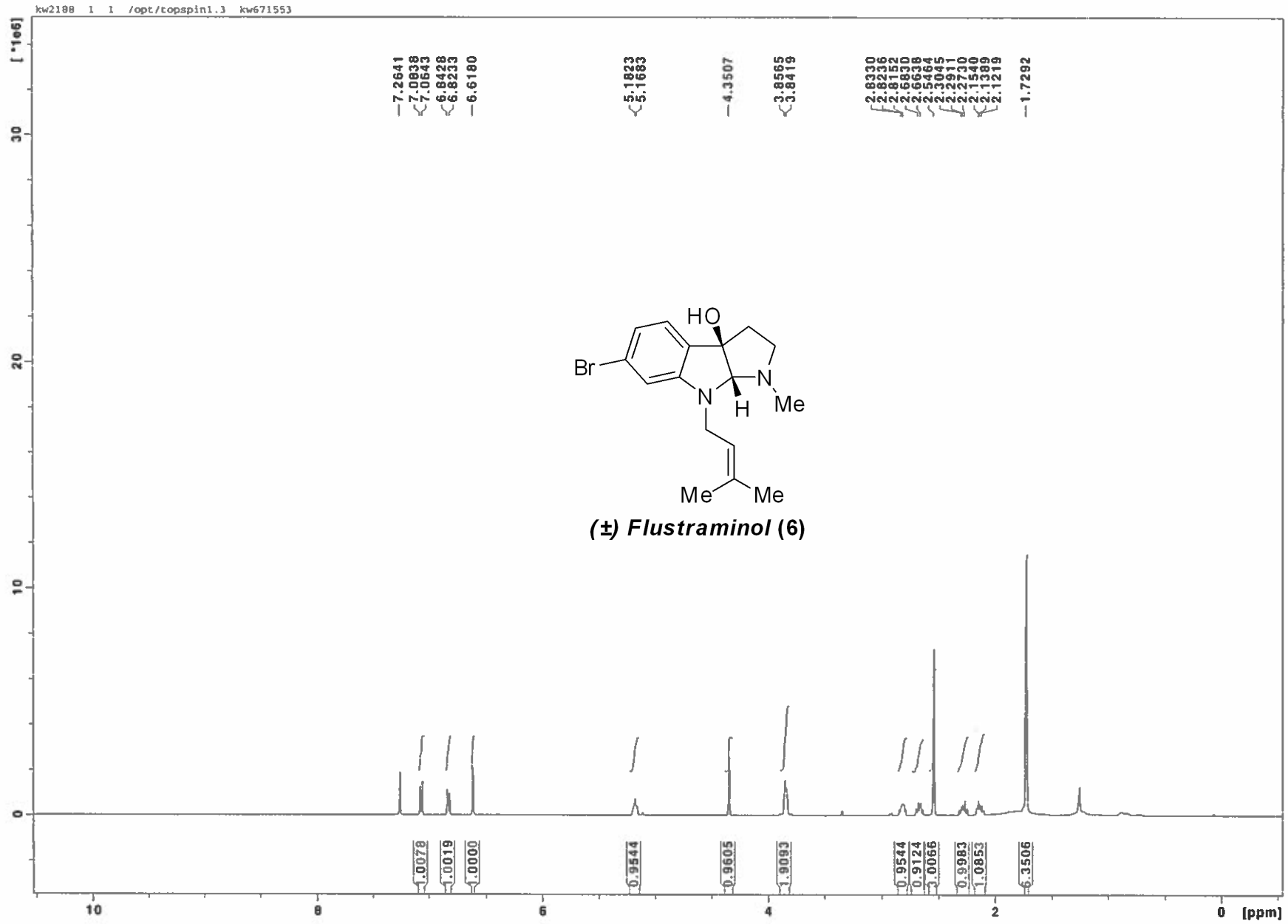

kw2008 2 1 /opt/topspin1.3 kw671553
[*1e6]
600
400
200
0
175.5153
155.9165
141.6228
137.3658
136.5539
136.1518
128.7574
126.9899
126.3547
122.5710
121.7435
119.9800
118.7344
115.4255
114.5321
112.3780
106.0721
43.9038
36.1669
31.1181
25.5910
17.9594
O
N
O
Me
NO2
NO2
Br
N
Me
Me
52
200
150
100
50
[ppm]


kw2137 1 1 /opt/topspin1.3 kw671553
[*1e6]
7.0712
7.0516
6.8739
6.8545
6.6813
5.1796
4.8084
3.9193
3.8913
3.8745
2.8147
2.7876
2.7566
1.7157
HO
O
Br
N
N
H
Me
Me
Me
0.9280
0.9413
0.9063
0.9672
0.9668
2.9645
5.0000
5.9276
10
8
6
4
2
0 [ppm]

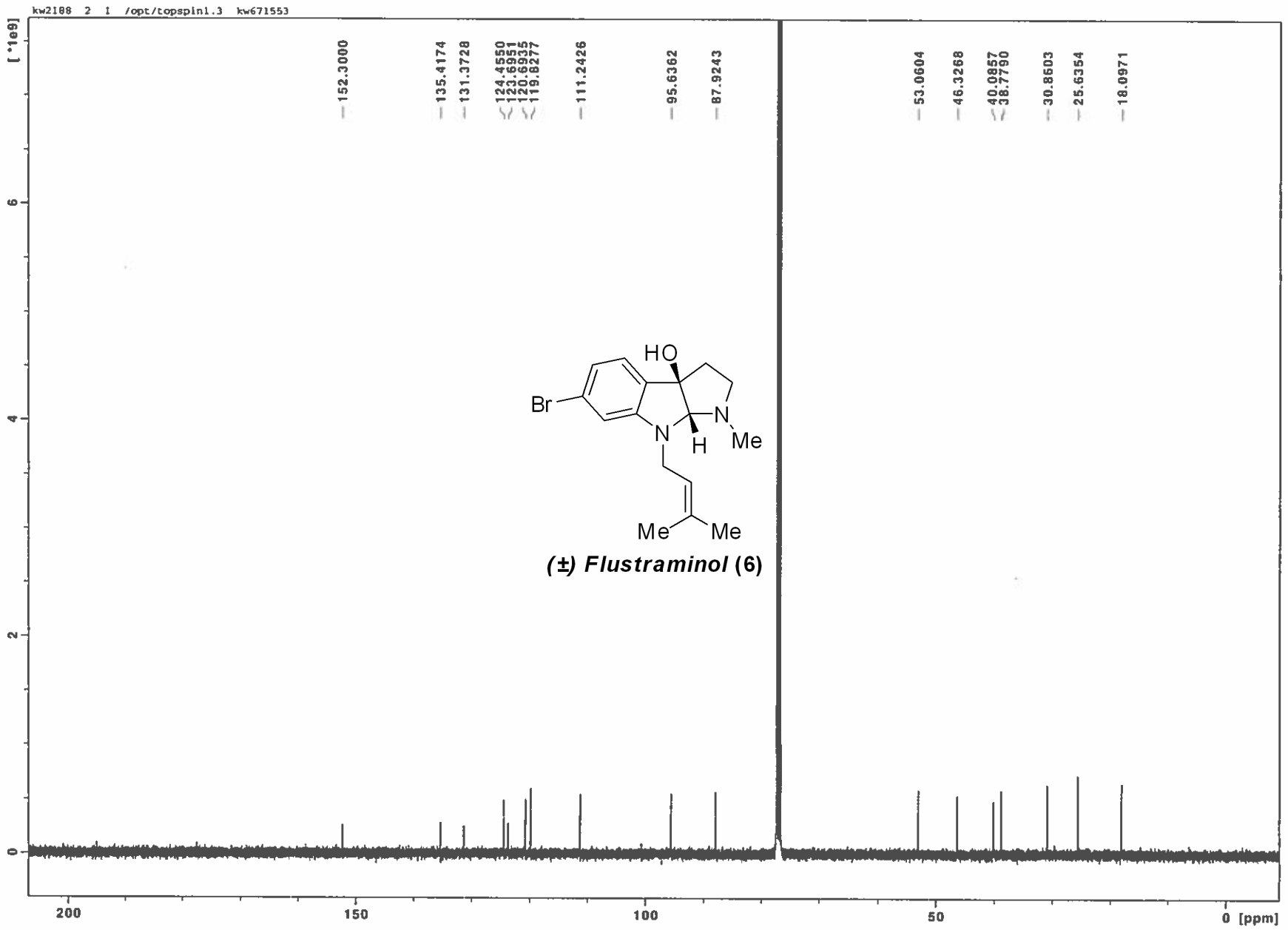
53


kw2137 2 1 /opt/topspin1.3 kw671553
[*1e6]
171.9859
150.8243
136.2989
131.3224
125.0395
124.1867
122.1216
119.6928
112.6831
90.5326
79.2351
47.1822
43.4954
27.7885
25.6145
18.0979
HO
O
Br
N
N
H
Me
Me
Me
200
150
100
50
0 [ppm]

53



***(±) Flustraminol* (6)**



***(±) Flustraminol* (6)**