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Supporting Information

Pd-Catalyzed C-H Activation in Water: Synthesis of Bis(Indolyl)methanes from Indoles and Benzyl Alcohols

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General procedure: A mixture of indole **1** (0.5 mmol), palladium(II) acetate (6 mg, 0.025 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 18 mg, 0.05 mmol) and benzyl alcohol **2** (1.5 mmol) in H_2O (2 mL) was heated at 60 ^oC for 16 h in a sealed tube. After cooling, the reaction mixture was poured into water and extracted with EtOAc. The organic layer was washed with brine, dried over $MgSO_4$ and concentrated in vacuo. The residue was purified by flash column chromatography (silica gel, hexanes/EtOAc) to give desired product **3**.

Bis(5-methoxyindol-3-yl)(phenyl)methane 3a[1]

Following the general procedure, **3a** was obtained as a white solid. 77 mg (81%); mp 213-216 °C; IR (KBr) (cm^{-1}) 3392, 3319; ^1H NMR (400 MHz, $CDCl_3$): δ 3.69 (s, 6H), 5.77 (s, 1H), 6.66 (dd, *J*=4.0, 2.0 Hz, 2H), 6.78-6.84 (m, 4H), 7.18-7.30 (m, 5H), 7.33-7.37 (m, 2H), 7.81 (brs, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 40.3, 55.8, 102.0, 111.7, 111.9, 119.3, 124.4, 126.1, 127.5, 128.2, 128.7, 131.9, 143.9, 153.7; MS (EI): *m/z* (%) 382 (M^+, 100).

Bis(5-methoxyindol-3-yl)(4-methylphenyl)methane 3b[2]

Following the general procedure, **3b** was obtained as a pale yellow solid. 59 mg (60%); mp 202-204 °C; IR (KBr) (cm^{-1}) 3348; ^1H NMR (400 MHz, $CDCl_3$): δ 2.32 (s, 3H), 3.69 (s, 6H), 5.73 (s, 1H), 6.66 (s, 2H), 6.80 (m, 4H), 7.08 (d, *J*=8.0 Hz, 2H), 7.20-7.25 (m, 4H), 7.80 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ ; 21.1, 39.9, 55.9, 102.0, 111.6, 111.8, 119.5, 124.4, 127.5, 128.6, 128.9, 131.9, 135.4, 140.9, 153.7; MS (EI): *m/z* (%) 396 (M^+, 100).

Bis(5-methoxyindol-3-yl)(4-ethylphenyl)methane 3c

Following the general procedure, **3c** was obtained as a white solid. 100 mg (97%); mp 180-182 °C; IR (KBr) (cm^{-1}) 3402; ^1H NMR (400 MHz, $CDCl_3$): δ 1.21 (t, *J*=8.0 Hz, 3H), 2.62 (q, *J*=8.0 Hz, 2H), 3.68 (s, 6H), 5.73 (s, 1H), 6.66 (d, *J*=4.0 Hz, 2H), 6.78-6.84 (m, 4H), 7.10 (d, *J*=8.0 Hz, 2H), 7.20-7.28 (m, 4H), 7.79 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 15.6, 28.5, 39.9, 55.8, 102.0, 111.6, 111.8, 119.6, 124.4, 127.6, 127.7, 128.6, 131.9, 141.1, 141.9, 153.7; MS (EI): *m/z* (%) 410 (M^+, 100). Anal. Calcd for $C_{27}H_{26}N_2O_2$: C, 79.00; H, 6.38; N, 6.82. Found: C, 78.83; H, 6.43; N, 6.71.

Bis(5-methoxyindol-3-yl)(4-methoxyphenyl)methane 3d[3]

Following the general procedure, **3d** was obtained as an off-white solid. 67 mg (65%); mp 186-188 °C; IR (KBr) (cm^{-1}) 3332; ^1H NMR (400 MHz, DMSO-d_6): δ 3.59 (s, 6H), 3.71 (s, 3H), 5.68 (s, 1H), 6.65-7.00 (m, 8H), 7.20-7.30 (m, 4H), 10.6 (brs, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 54.9, 55.2, 101.5, 110.4, 111.9, 113.3, 118.0, 124.2, 127.0, 129.2, 131.8, 137.0, 152.6, 157.3; MS (EI): *m/z* (%) 412 (M^+, 100).

Bis(5-methoxyindol-3-yl)(3-methylphenyl)methane 3e

Following the general procedure, **3e** was obtained as a white solid. 93 mg (94%); mp 193-195 °C; IR (KBr) (cm^{-1}) 3394; ^1H NMR (400 MHz, $CDCl_3$): δ 2.29 (s, 3H), 3.69 (s, 6H), 5.72 (s, 1H), 6.66 (dd, *J*=2.0, 0.4 Hz, 2H), 6.80-6.84 (m, 4H), 7.01 (t, *J*=6.8 Hz, 1H), 7.10-7.20 (m, 3H), 7.20-7.26 (m, 2H), 7.80 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 40.2, 55.9, 102.0, 111.6, 111.8, 119.4, 124.4, 125.7, 126.9, 127.6, 128.1, 129.4, 131.9, 137.6, 143.8, 153.7; MS (EI): *m/z* (%) 396 (M^+, 100); HRMS-EI: *m/z* (M^+) calcd for $C_{26}H_{24}N_2O_2$ 396.1838, found 396.1837.

Bis(5-methoxyindol-3-yl)(4-fluorophenyl)methane 3f[4]

Following the general procedure, **3f** was obtained as a pale yellow solid. 73 mg (73%); mp 145-147 °C; IR (KBr) (cm^{-1}) 3461, 3405; ^1H NMR (400 MHz, $CDCl_3$): δ 3.69 (s, 6H), 5.75 (s, 1H), 6.63 (d, *J*=2.0 Hz, 2H), 6.77 (d, *J*=4.0 Hz, 2H), 6.84 (dd, *J*=8.0, 4.0 Hz, 2H), 6.96 (t, *J*=8.0 Hz, 2H), 7.20-7.35 (m, 2H), 7.83 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 39.5, 55.9, 101.9, 111.7, 112.0, 114.8, 115.1, 119.1, 124.4, 127.4, 130.0, 130.1, 131.9, 139.6, 139.6, 153.8, 160.2, 162.6; MS (EI): *m/z* (%) 400 (M^+, 100).

Bis(5-methoxyindol-3-yl)(2-methylphenyl)methane 3g

Following the general procedure, **3g** was obtained as a white solid. 86 mg (87%); mp 177-179 °C; IR (KBr) (cm^{-1}) 3419; ^1H NMR (400 MHz, $CDCl_3$): δ 2.38 (s, 3H), 3.69 (s, 6H), 5.89 (s, 1H), 6.57 (d, *J*=2.0 Hz, 2H), 6.76 (d, *J*=2.4 Hz, 2H), 6.83 (dd, *J*=8.8, 2.4 Hz, 2H), 7.00-7.15 (m, 3H), 7.15-7.25 (m, 3H), 7.79 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 19.6, 36.4, 55.9, 102.0, 111.6, 111.7, 118.7, 124.7, 125.8, 126.1, 127.6, 128.4, 130.2, 131.9, 136.0, 141.9, 153.7; MS (EI): *m/z* (%) 396 (M^+, 100); Anal. Calcd for $C_{26}H_{24}N_2O_2$: C, 78.76; H, 6.10; N, 7.07. Found: C, 78.49; H, 6.11; N, 6.83.

Bis(5-methoxyindol-3-yl)(2-thienyl)methane 3h

Following the general procedure, **3h** was obtained as an off-white solid. 54 mg (56%); mp 190-192 °C; IR (KBr) (cm^{-1}) 3390, 3325; ^1H NMR (400 MHz, $CDCl_3$): δ 3.71 (s, 6H), 6.05 (s, 1H), 6.80-6.86 (m, 4H), 6.88 (d, *J*=2,4 Hz, 2H), 6.90-6.95 (m, 2H), 7.15 (dd, *J*=4.4, 1.6 Hz, 1H), 7.24 (dd, *J*=8.4, 0.4 Hz, 2H), 7.84 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 35.4, 55.9, 101.8, 111.8, 112.0, 119.3, 123.6, 124.0, 125.2, 126.4, 127.2, 131.8, 148.6, 153.8; MS (EI): *m/z* (%) 388 (M^+, 100); Anal. Calcd for $C_{23}H_{20}N_2O_2S$: C, 71.11; H, 5.19; N, 7.21. Found: C, 70.76; H, 5.09; N, 6.98.

Bis(indol-3-yl)(phenyl)methane 3i[5]

Following the general procedure, **3i** was obtained as a brown solid. 47 mg (58%); mp 141-143 °C; IR (KBr) (cm^{-1}) 3398; ^1H NMR (400 MHz, $CDCl_3$): δ 5.87 (s, 1H), 6.59 (s, 2H), 6.99 (dd, *J*=8.0, 8.0 Hz, 2H), 7.15 (dd, *J*=8.0, 8.0 Hz, 2H), 7.18-7.40 (m, 9H), 7.78 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 40.2, 111.0, 119.2, 119.7, 119.9, 121.9, 123.6, 126.1, 127.1, 128.2, 128.7, 136.7, 144.0; MS (EI): *m/z* (%) 322

(M^+, 100).

Bis(5-methylindol-3-yl)(phenyl)methane 3j[6]

Following the general procedure, **3j** was obtained as a brown solid. 65 mg (74%); mp 183-185 °C; IR (KBr) (cm^{-1}) 3422; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.34 (s, 6H), 5.82 (s, 1H), 6.57 (d, *J*=4.0 Hz, 2H), 6.99 (d, *J*=8.0 Hz, 2H). 7.15-7.40 (m, 9H), 7.79 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 21.5, 40.0, 110.7, 119.3, 119.5, 123.5, 123.9, 126.0, 127.3, 128.2, 128.4, 128.7, 135.0, 144.2; MS (EI): *m/z* (%) 350 (M^+, 100).

Bis(5-fluoroindol-3-yl)(phenyl)methane 3k

Following the general procedure, **3k** was obtained as an off-white solid. 50 mg (56%); mp 169-171 °C; IR (KBr) (cm^{-1}) 3465, 3424; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.73 (s, 1H), 6.72 (s, 2H), 6.90 (td, *J*=9.2, 2.4 Hz, 2H), 6.98 (dd, *J*=9.2, 2.4 Hz, 2H), 7.20-7.35 (m, 7H), 7.93 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 40.2, 104.7, 104.9, 110.3, 110.5, 111.6, 111.7, 119.5, 119.5, 125.2, 126.4, 127.3, 127.4, 128.4, 128.6, 133.2, 143.2, 156.4, 158.7; MS (EI): *m/z* (%) 358 (M^+, 100); HRMS-EI: *m/z* (M^+) calcd for $C_{23}H_{16}F_2N_2$ 358.1282, found 358.1283.

Bis(5-cyanoindol-3-yl)(phenyl)methane 3l[7]

Following the general procedure, **3l** was obtained as an off-white solid. 84 mg (90%); mp 246-249 °C; IR (KBr) (cm^{-1}) 3319, 2220; ^{1}H NMR (400 MHz, $CDCl_3$): δ 5.84 (s, 1H), 6.81 (s, 2H), 7.25-7.35 (m, 5H), 7.40-7.45 (m, 4H), 7.67 (s, 2H), 8.34 (brs, 2H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 40.0, 102.7, 112.2, 119.9, 120.7, 125.2, 125.5, 126.6, 127.0, 128.4, 128.7, 138.4, 142.2; MS (EI): *m/z* (%) 372 (M^+, 100).

Bis(5-carbomethoxyindol-3-yl)(phenyl)methane 3m

Following the general procedure, **3l** was obtained as an off-white solid. 92 mg (84%); mp 226-228 °C; IR (KBr) (cm^{-1}) 3325, 1689; ^{1}H NMR (400 MHz, DMSO-d_6): δ 3.76 (s, 6H), 6.02 (s, 1H), 6.88 (s, 2H), 7.21 (dd, *J*=7.2, 7.2 Hz, 1H), 7.30 (dd, *J*=7.6, 7.6 Hz, 2H), 7.35 (d, *J*=7.2 Hz, 2H), 7.45 (d, *J*=8.8 Hz, 2H), 7.70 (dd, *J*=8.4, 1.2 Hz, 2H), 8.02 (s, 2H), 11.3 (brs, 2H); ^{13}C NMR (100 MHz, DMSO-d_6): δ 51.6, 111.5, 119.4, 119.8, 121.7, 122.1, 125.6, 126.1, 126.1, 128.2, 139.3, 144.2, 167.2; MS (EI): *m/z* (%) 438 (M^+, 100); HRMS-EI: *m/z* (M^+) calcd for $C_{27}H_{22}N_2O_4$ 438.1580, found 438.1579.

Bis(2-methylindol-3-yl)(phenyl)methane 3n[5]

Following the general procedure, **3l** was obtained as a brown solid. 86 mg (98%); mp 251-254 °C; IR (KBr) (cm^{-1}) 3395; ^{1}H NMR (400 MHz, $CDCl_3$): δ 2.06 (s, 6H), 6.00 (s, 1H), 6.85 (dd, *J*=8.0, 8.0 Hz, 2H), 6.97 (d, *J*=8.0 Hz, 2H), 7.03 (dd, *J*=8.0, 8.0 Hz, 2H), 7.20-7.30 (m, 7H), 7.73 (brs, 2H); ^{13}C NMR (100

MHz, $CDCl_3$): δ 12.4, 39.3, 109.9, 113.4, 119.1, 119.3, 120.6, 126.0, 128.1, 129.0, 129.1, 131.8, 135.0, 143.7; MS (EI): *m/z* (%) 350 (M^+, 98.8), 130 (100).

Bis(1-methylindol-3-yl)(phenyl)methane 3o[5]

Following the general procedure, **3l** was obtained as an off-white solid. 64 mg (73%); mp 199-201 °C; IR (KBr) (cm^{-1}) 1473; ^1H NMR (400 MHz, $CDCl_3$): δ 3.66 (s, 6H), 5.88 (s, 1H), 6.52 (s, 2H), 6.98 (dd, *J*=8.0, 6.0 Hz, 2H), 7.16-7.30 (m, 7H), 7.32-7.40 (m, 4H); ^{13}C NMR (100 MHz, $CDCl_3$): δ 32.7, 40.1, 190.0, 118.2, 118.6, 120.0, 121.4, 126.0, 127.4, 128.2, 128.2, 128.7, 137.4, 144.4; MS (EI): *m/z* (%) 350 (M^+, 100).

References

(1) S. Whitney, R. Grigg, A. Derrick, A. Keep, *Org. Lett.* 2007, **9**, 3299–3302.

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(3) M. Chakrabarty, A. Mukherji, S. Karmakar, S. Arima, Y. Harigaya, *Heterocycles,* 2006, **68**, 331-338.

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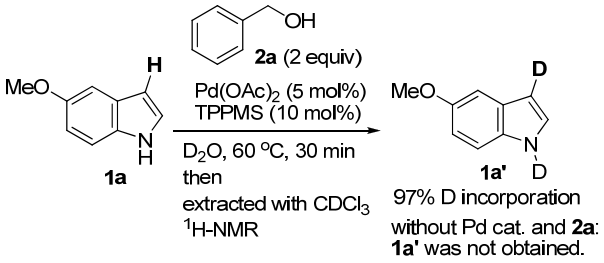
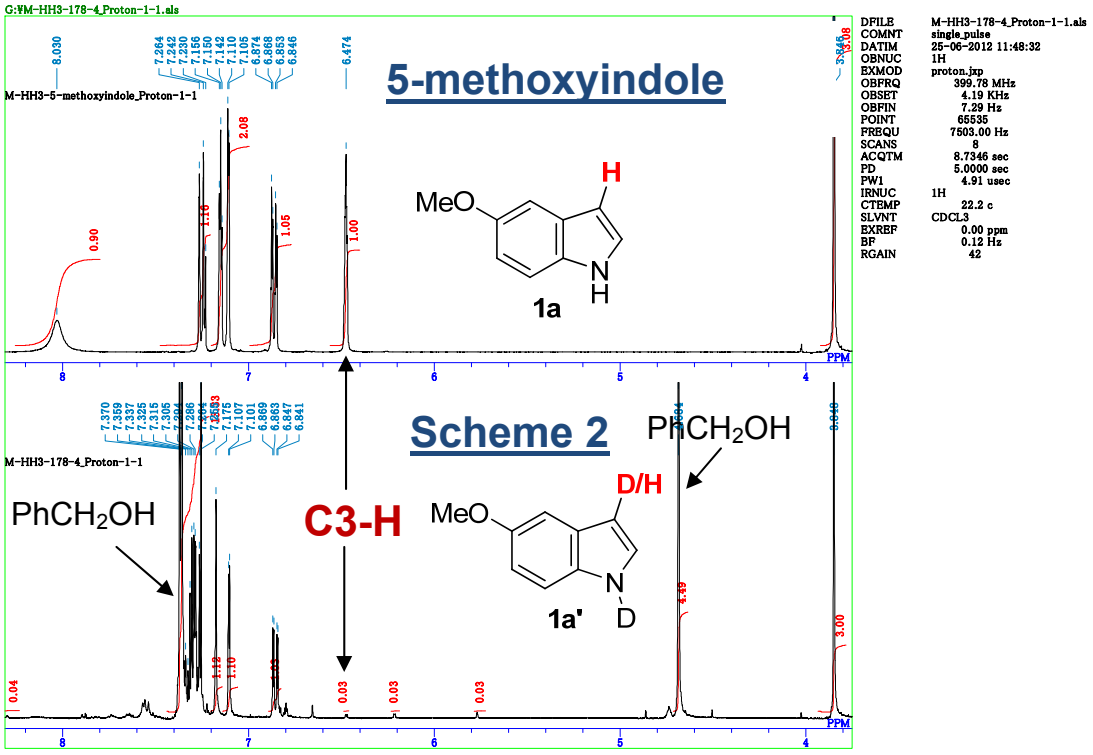
Scheme 2. C-H bond Activation at the C3-position of indole 1a.[a]

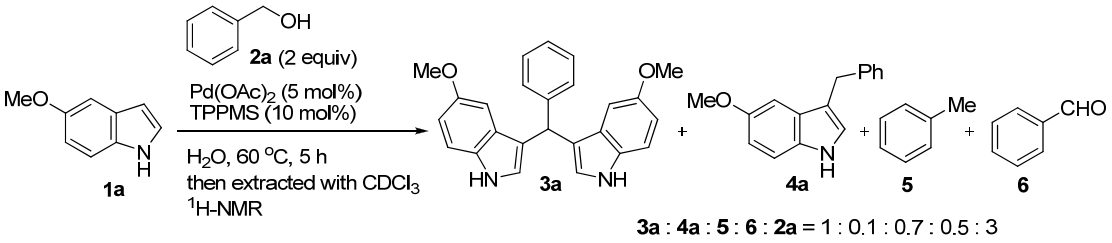


A mixture of **1a** (37 mg, 0.25 mmol), palladium(II) acetate (3 mg, 0.0125 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 9 mg, 0.025 mmol) and benzyl alcohol **2a** (54 mg, 0.5 mmol) in D_2O (0.75 mL) was heated at 60 °C for 30 min in a sealed tube. After cooling, the reaction mixture was extracted with $CDCl_3$ (8 mL), then the organic layer was analyzed by ^{1}H-NMR spectroscopy.

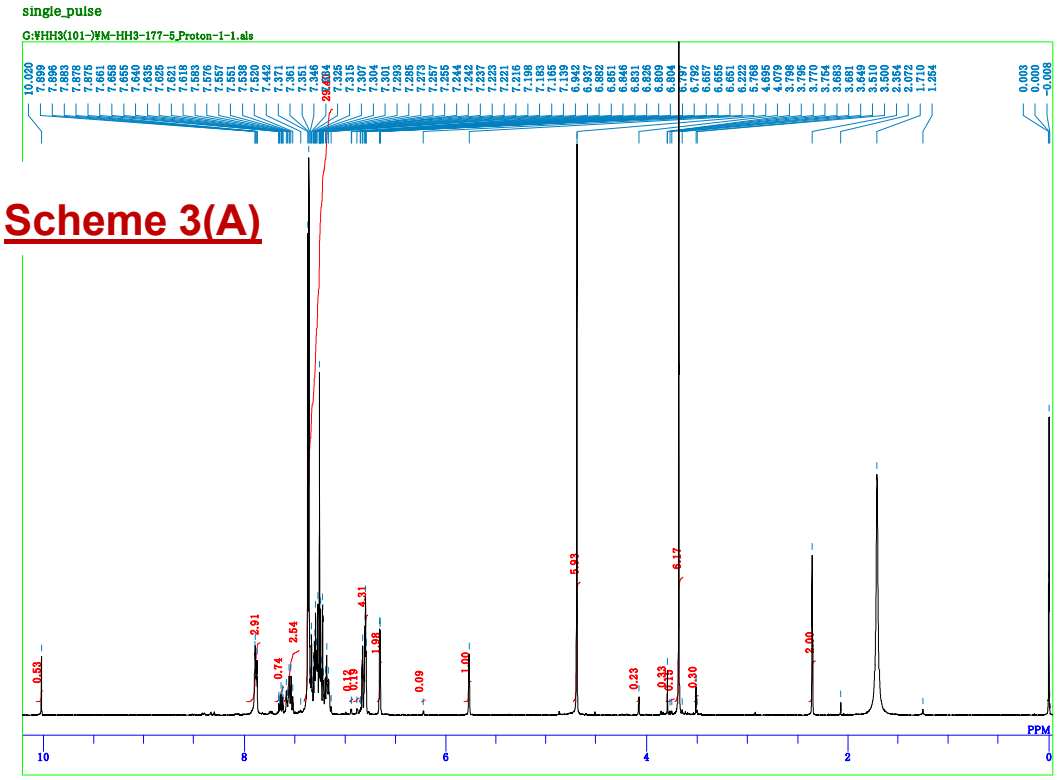


0.03H: 97% D incorporation

Scheme 3 (A). ^{1}H NMR experiments to monitor the reaction.

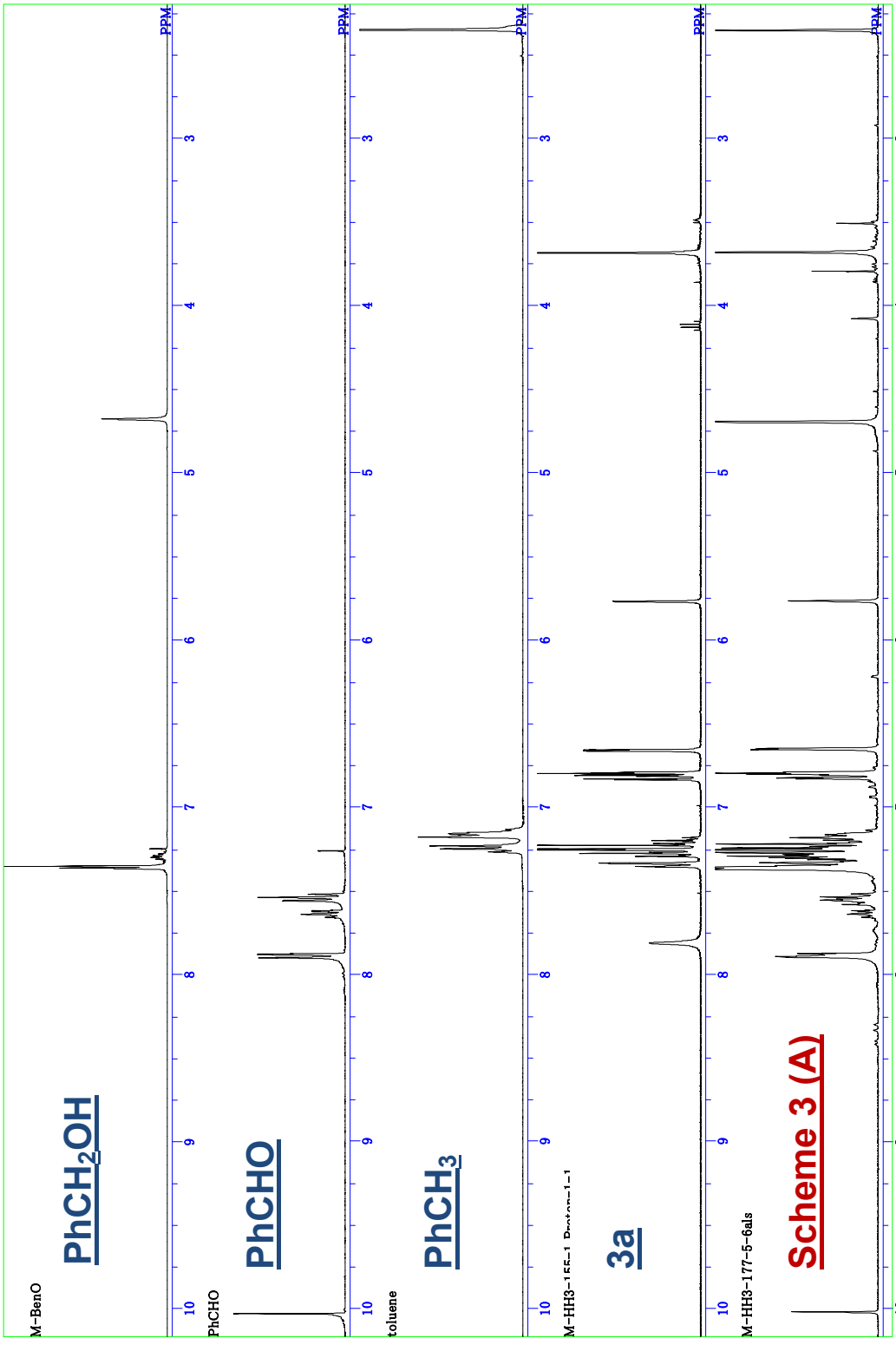


A mixture of **1a** (74 mg, 0.5 mmol), palladium(II) acetate (6 mg, 0.025 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 18 mg, 0.05 mmol) and benzyl alcohol **2a** (108 mg, 1.0 mmol) in H_2O (2 mL) was heated at 60 °C for 5 h in a sealed tube. After cooling, the reaction mixture was extracted with $CDCl_3$ (8 mL), then the organic layer was analyzed by ^{1}H-NMR spectroscopy.



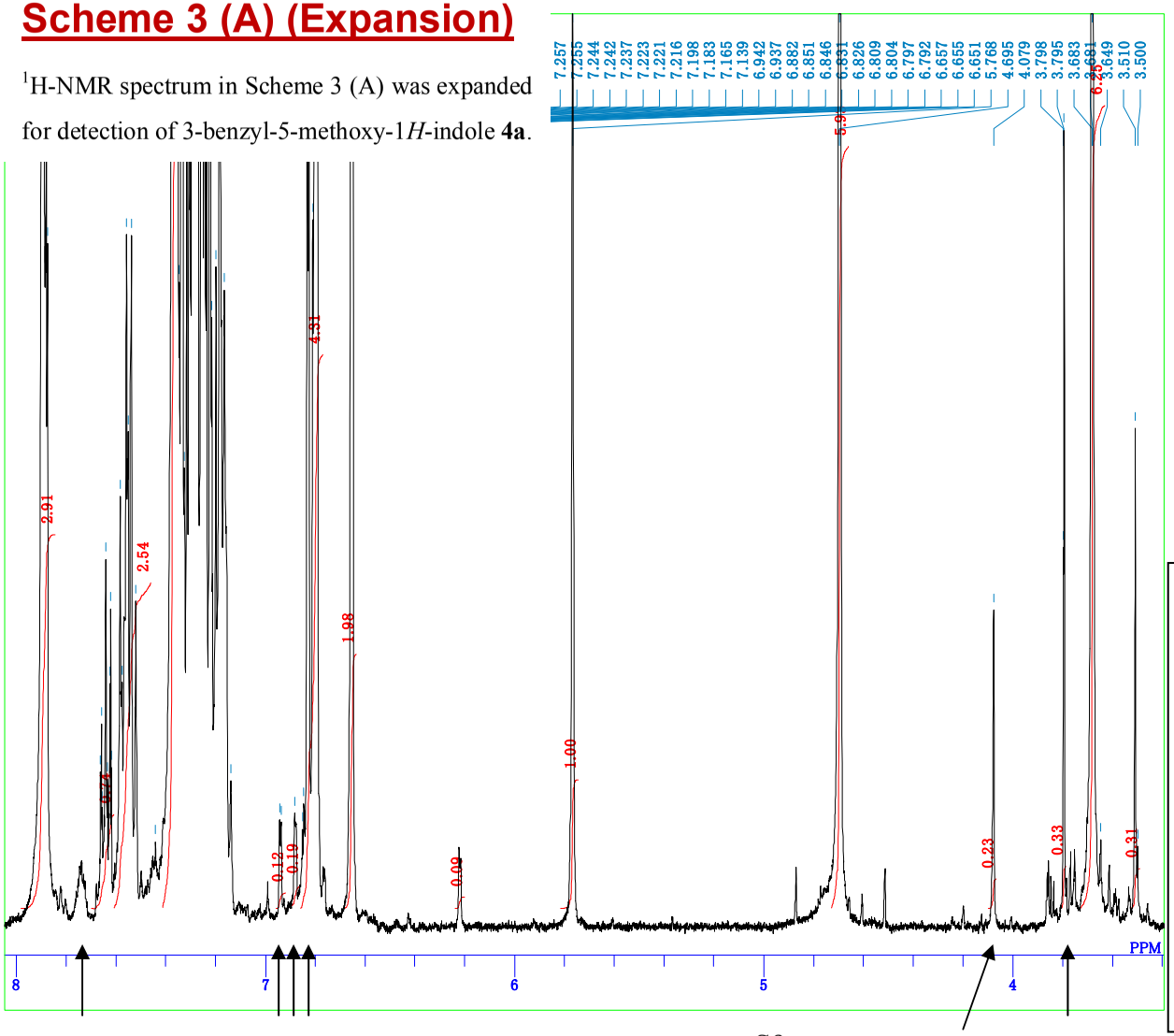
Product ratio was determined by integration.

	desired **3a**	3-benzylated **4a**	toluene **5**	benzaldehyde **6**	$PhCH_2OH$ **2a**
Signal δ	5.76 (methine-**H**)	3.79 (O**CH$_3$**)	2.35 (**CH$_3$**)	10.0 (**CH**O)	4.69 (**CH$_2$**)
Integral value	1.00 (1H)	0.33 (3H)	2.00 (3H)	0.53 (1H)	5.93 (2H)
Calculated ratio	1	0.1	0.7	0.5	3



Scheme 3 (A) (Expansion)

^{1}H-NMR spectrum in Scheme 3 (A) was expanded for detection of 3-benzyl-5-methoxy-1*H*-indole **4a**.



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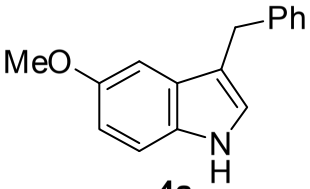


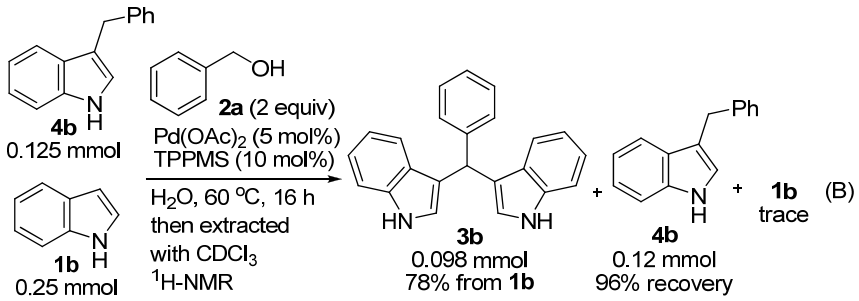
4a

Ref) Whitney, S.; Grigg, R.; Derrick, A.; Keep, A. *Org. Lett.* **2007**, *9*, 3299–3302.

3-Benzyl-5-methoxy-1*H*-indole

^{1}H NMR (500 MHz, $CDCl_3$): δ 3.78 (s, 3H,CH_3), 4.06 (s, 2H, CH_2), 6.81 (d, 1H, *J*=2.1 Hz), 6.83 (dd, 1H, *J*=2.1, 8.8 Hz), 6.94 (d, 1H, *J*= 2.1 Hz), 7.19-7.16 (m, 2H), 7.28-7.24 (m, 4H) , 7.76 (br s, 1H, NH)

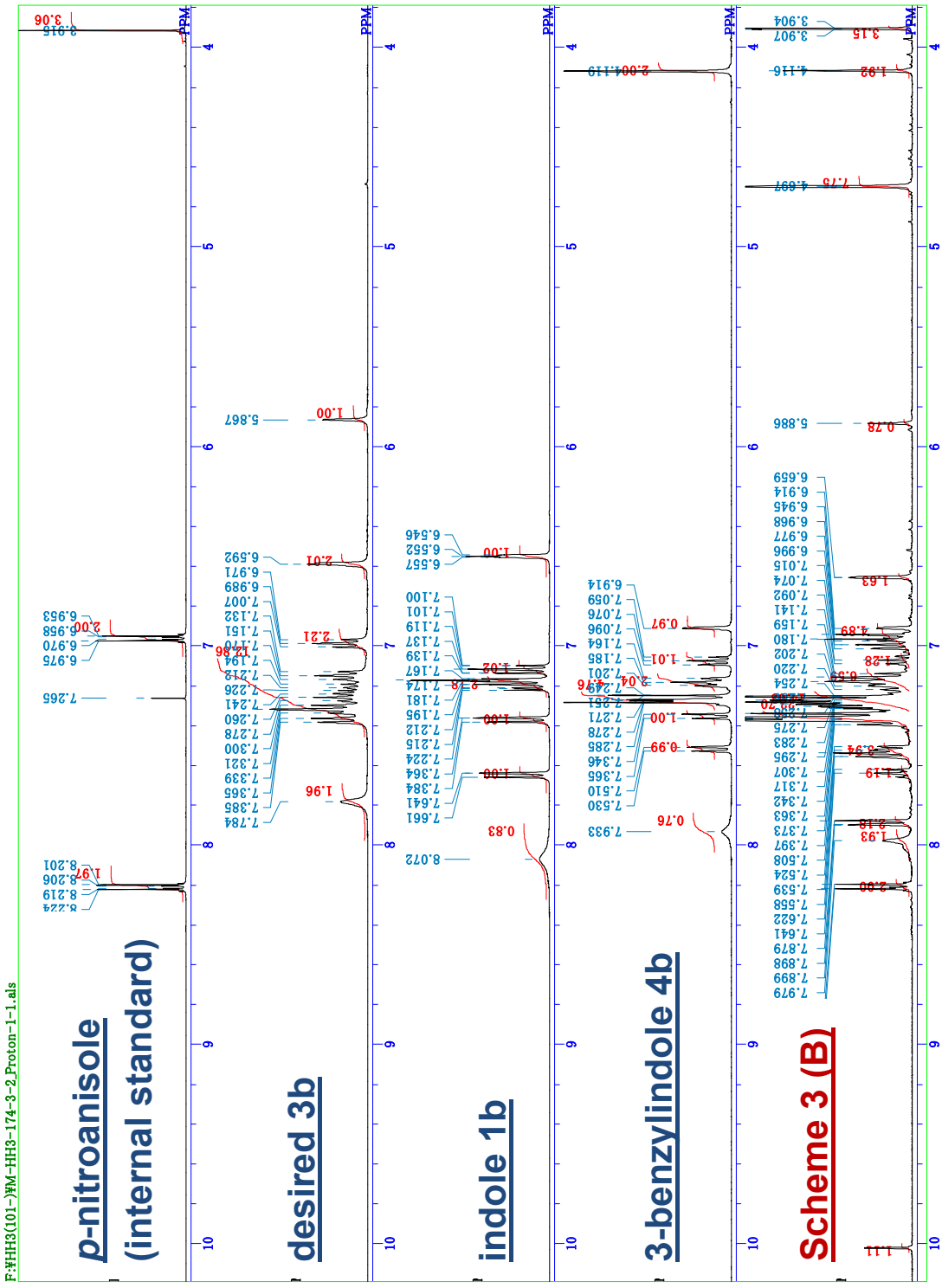
Scheme 3 (B). ^{1}H NMR experiments to monitor the reaction.

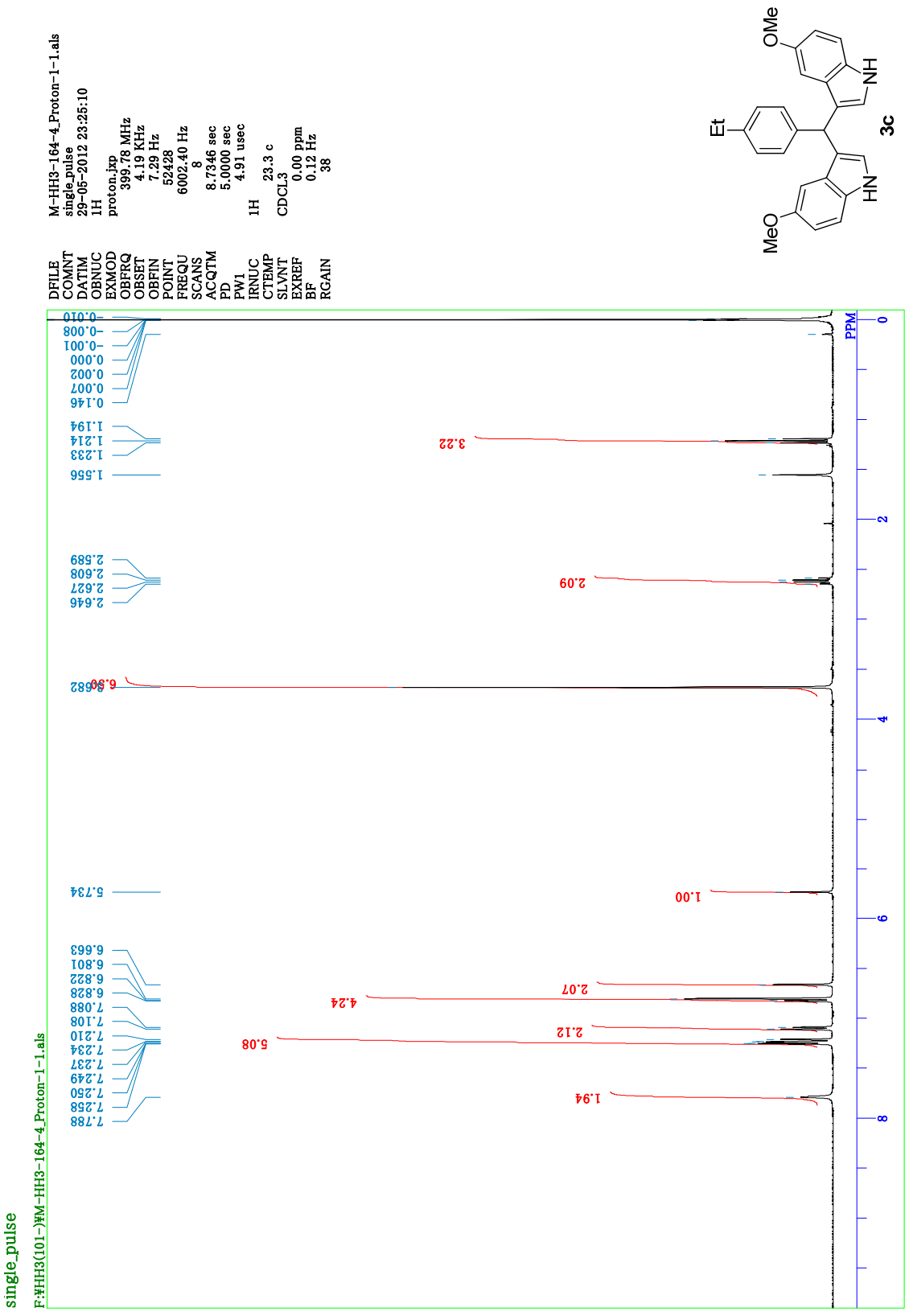


A mixture of 3-benzylindole **4b** (26 mg, 0.125 mmol), **1b** (30 mg, 0.25 mmol), palladium(II) acetate (3 mg, 0.0125 mmol), sodium diphenylphosphinobenzene-3-sulfonate (TPPMS, 9 mg, 0.025 mmol) and benzyl alcohol **2a** (77 μL, 0.7 mmol) in H_2O (2 mL) was heated at 60 °C for 16 h in a sealed tube. After the reaction mixture was cooled, *p*-nitroanisole (19 mg, 0.125 mmol, internal standard) was added to the reaction mixture, which was extracted with $CDCl_3$ (10 mL), then the organic layer was analyzed by ^{1}H-NMR spectroscopy.

Conversion yield and recovery were calculated by integration.

	desired **3b**	3-benzylindole **4b**	*p*-nitroanisole **internal standard**
Signal δ	5.89 (methine-**H**)	4.12 (C**H$_2$**)	8.21 (Ar-**H**x2)
Integral value	0.78 (1H)	1.92 (2H)	2.0 (2H)
			19 mg (0.125 mmol)
Calculated ratio	0.098 mmol 78% from **1b**	0.12 mmol 96% recovery	

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6
8
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1.00
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0.146
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1.233
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2.627
2.646
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7.108
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7.237
7.249
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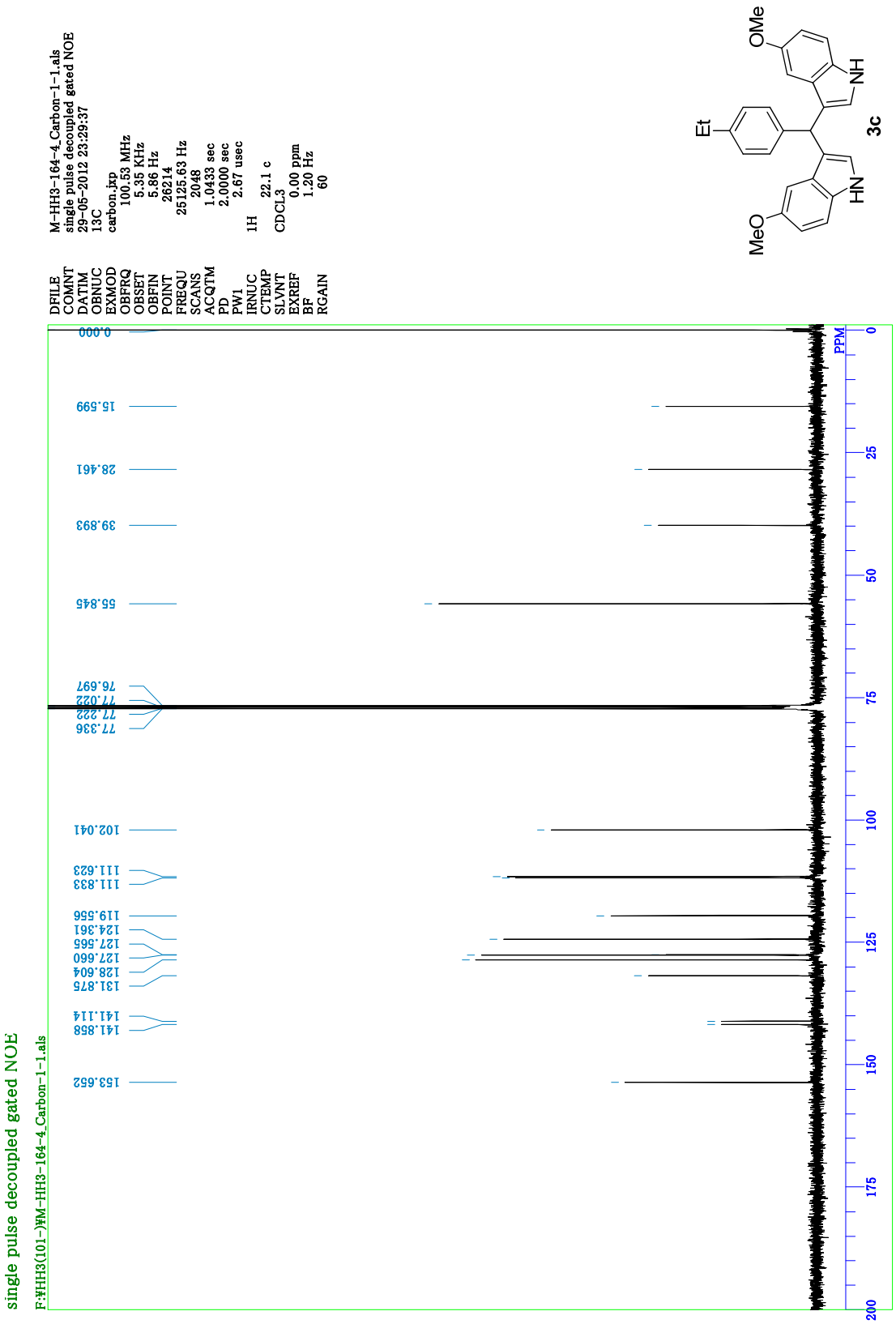
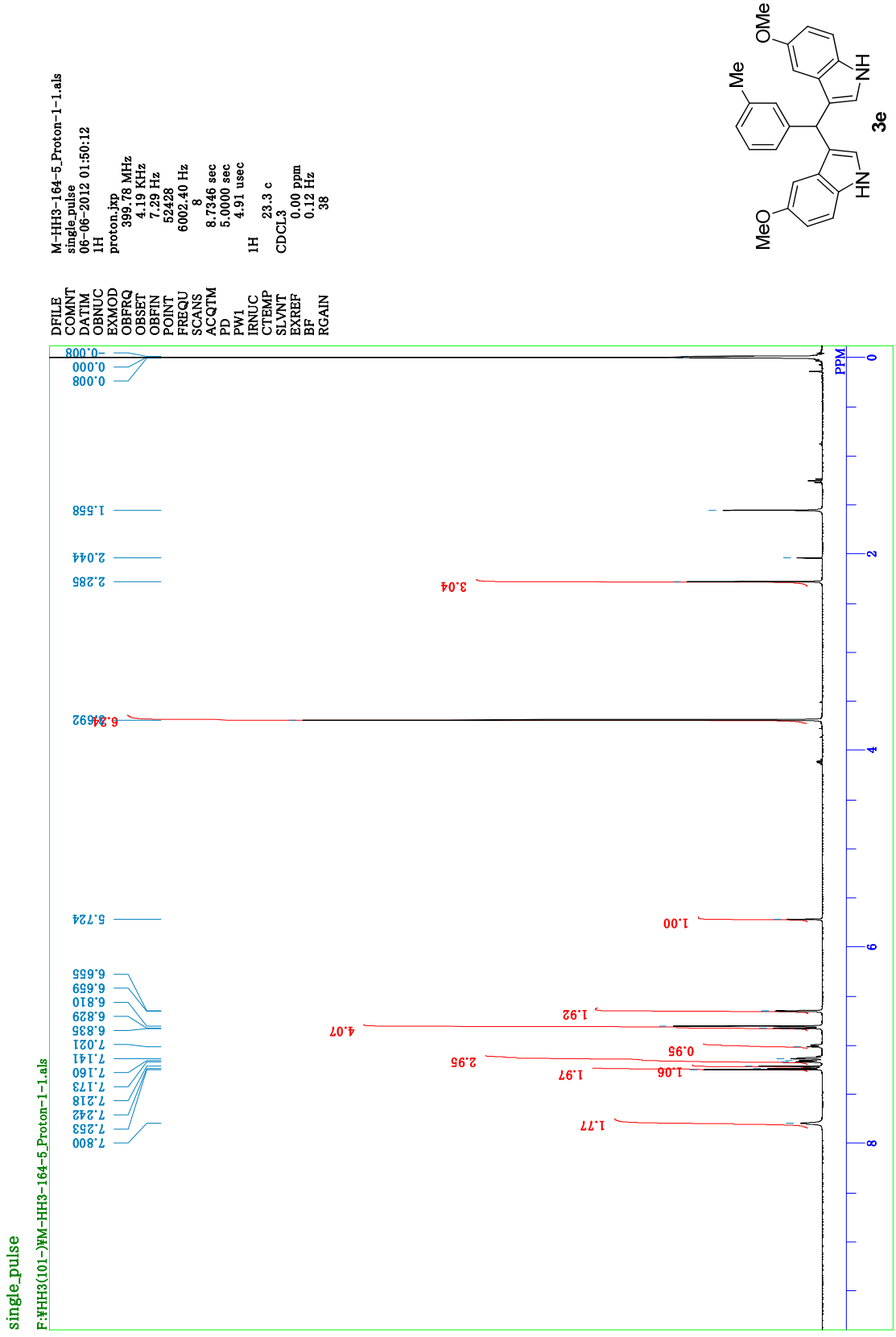
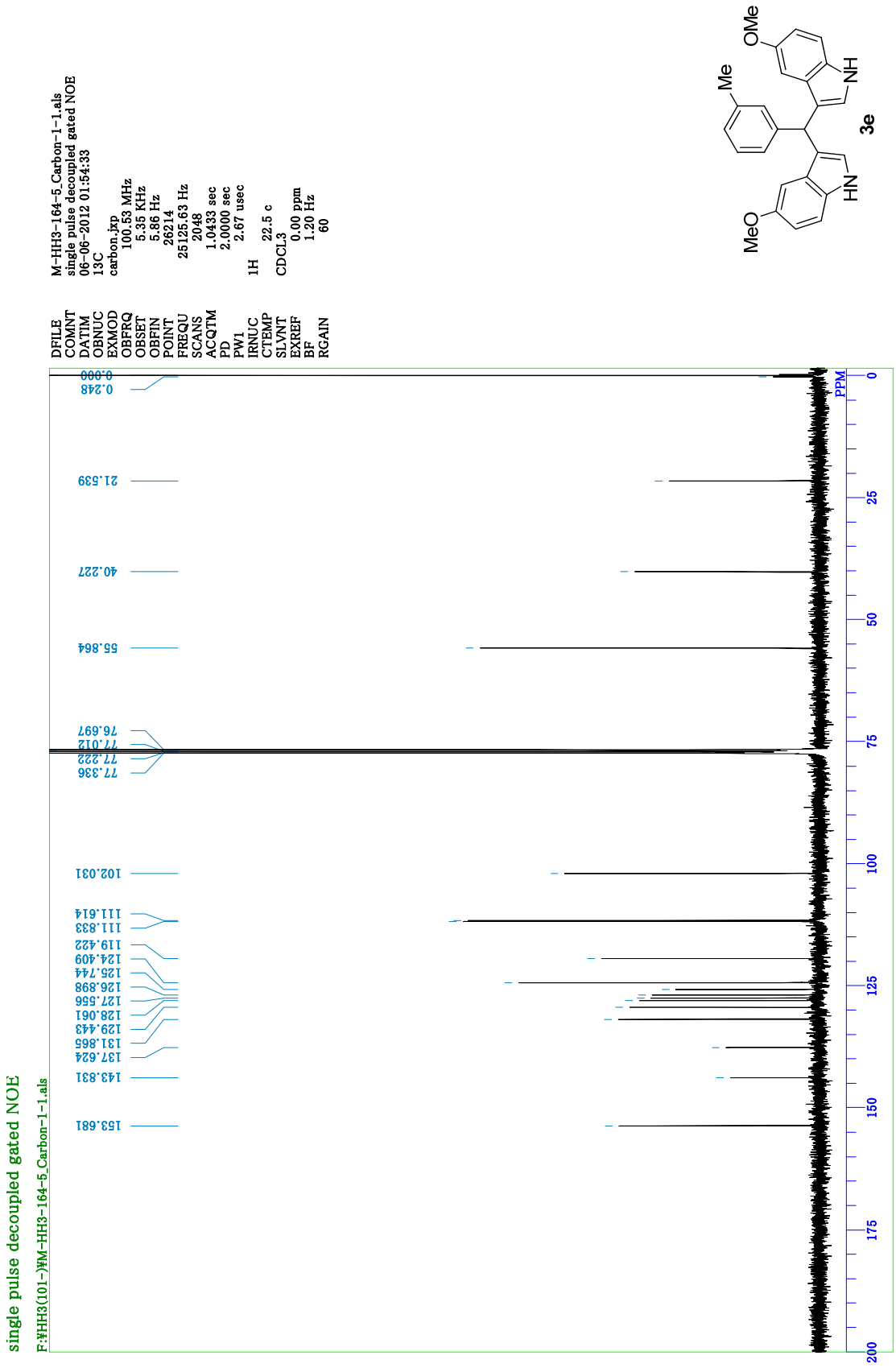
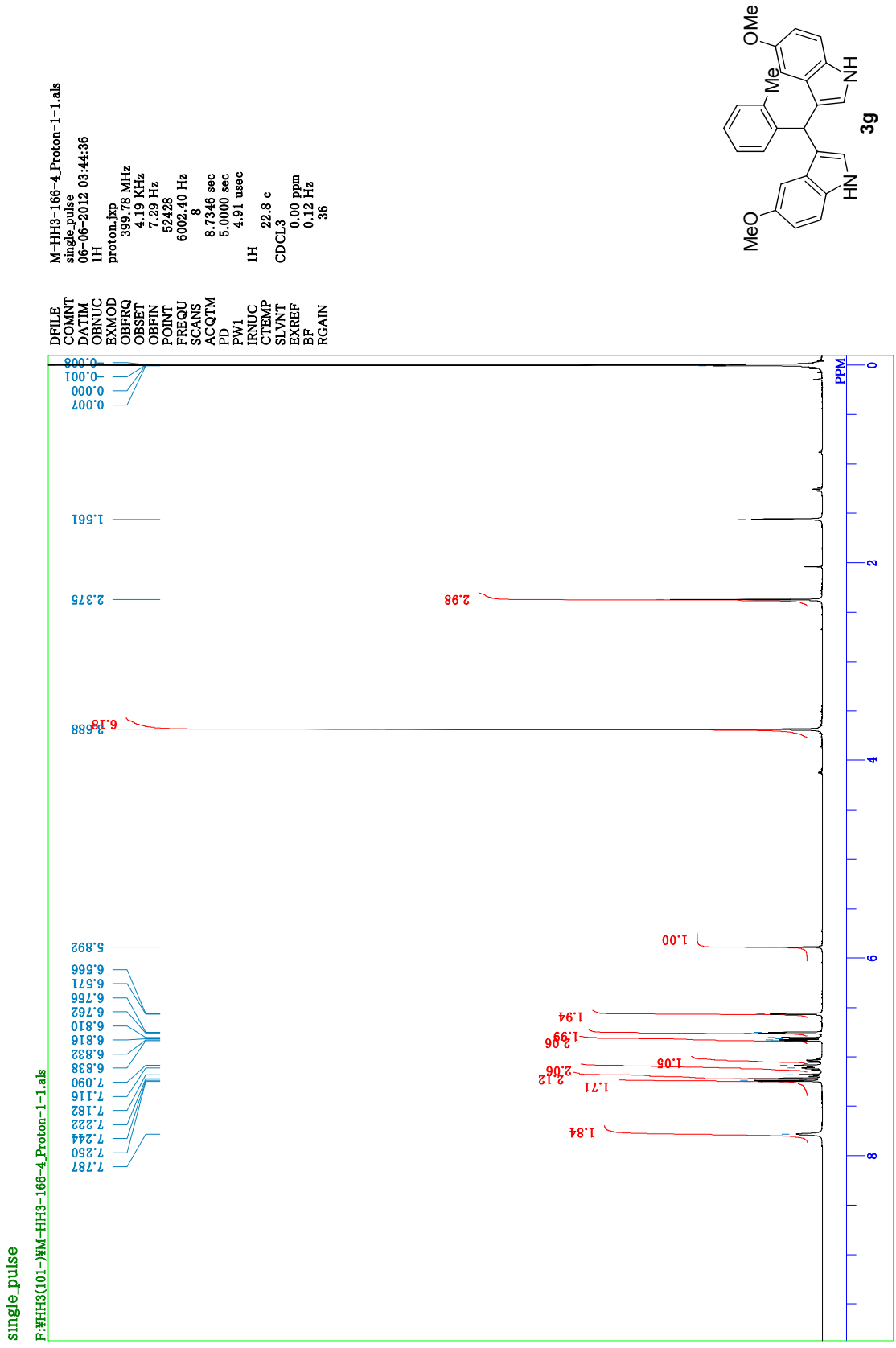
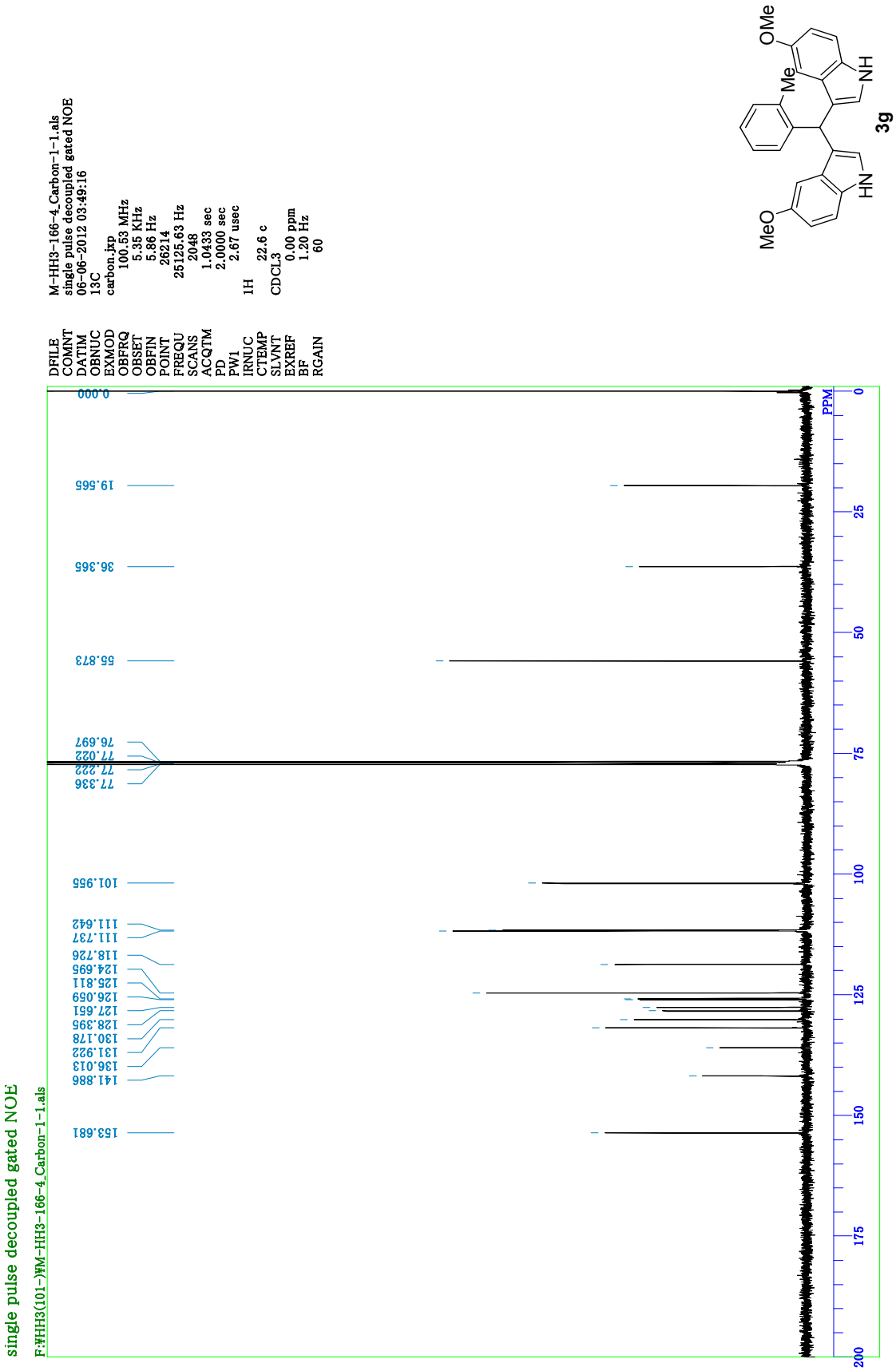
7.258
7.788

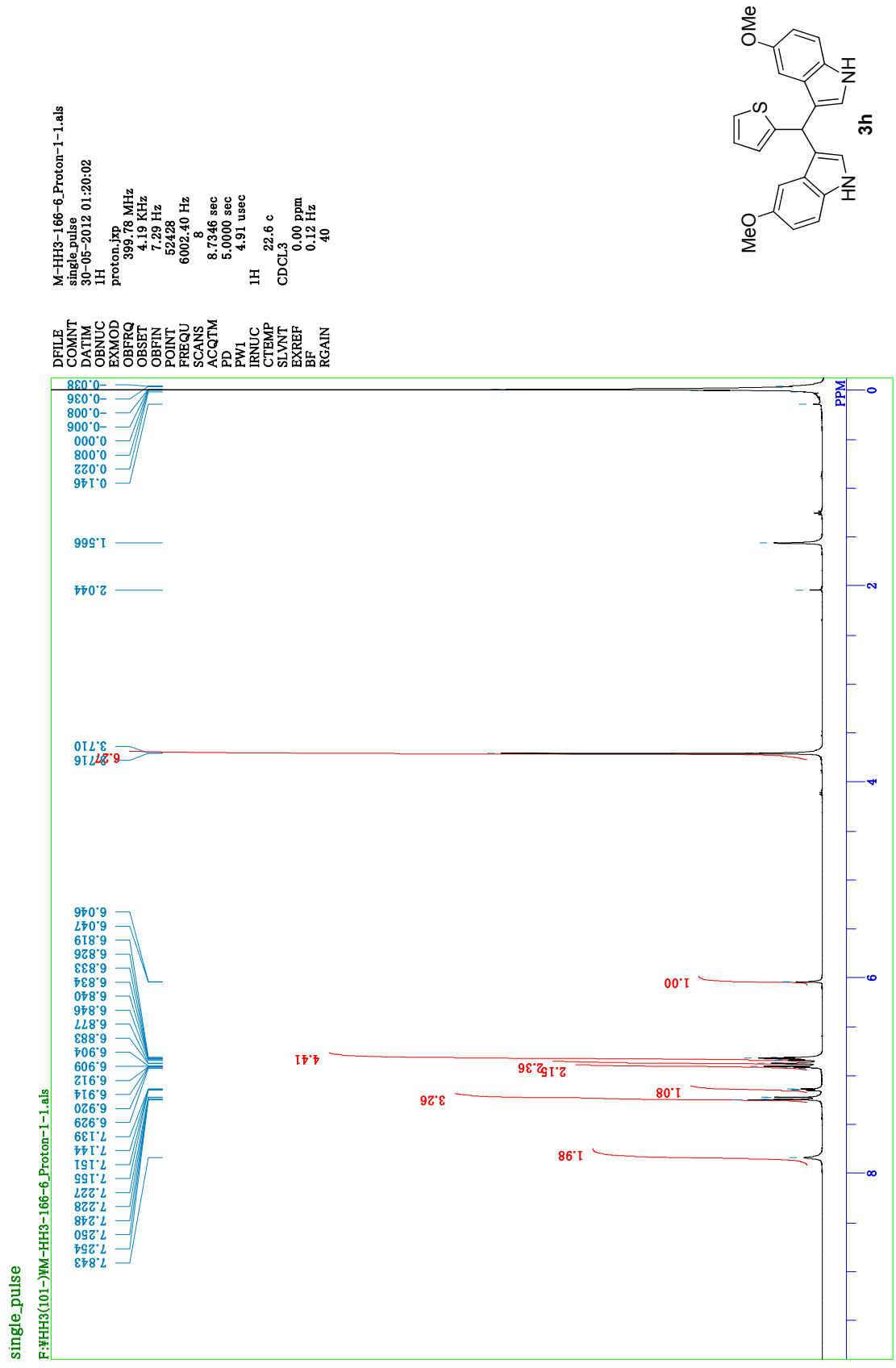

M-HH3-164-4_Carbon-1-1.als
single pulse decoupled gated NOE
29-05-2012 23:29:37
13C
carbon.jxp
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.63 Hz
2048
1.0433 sec
2.0000 sec
2.67 usec
1H
22.1 c
CDCL3
0.00 ppm
1.20 Hz
60
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OMe
NH
Et
3c
HN
MeO
single pulse decoupled gated NOE
F:¥HH3(101-)¥M-HH3-164-4_Carbon-1-1.als
PPM

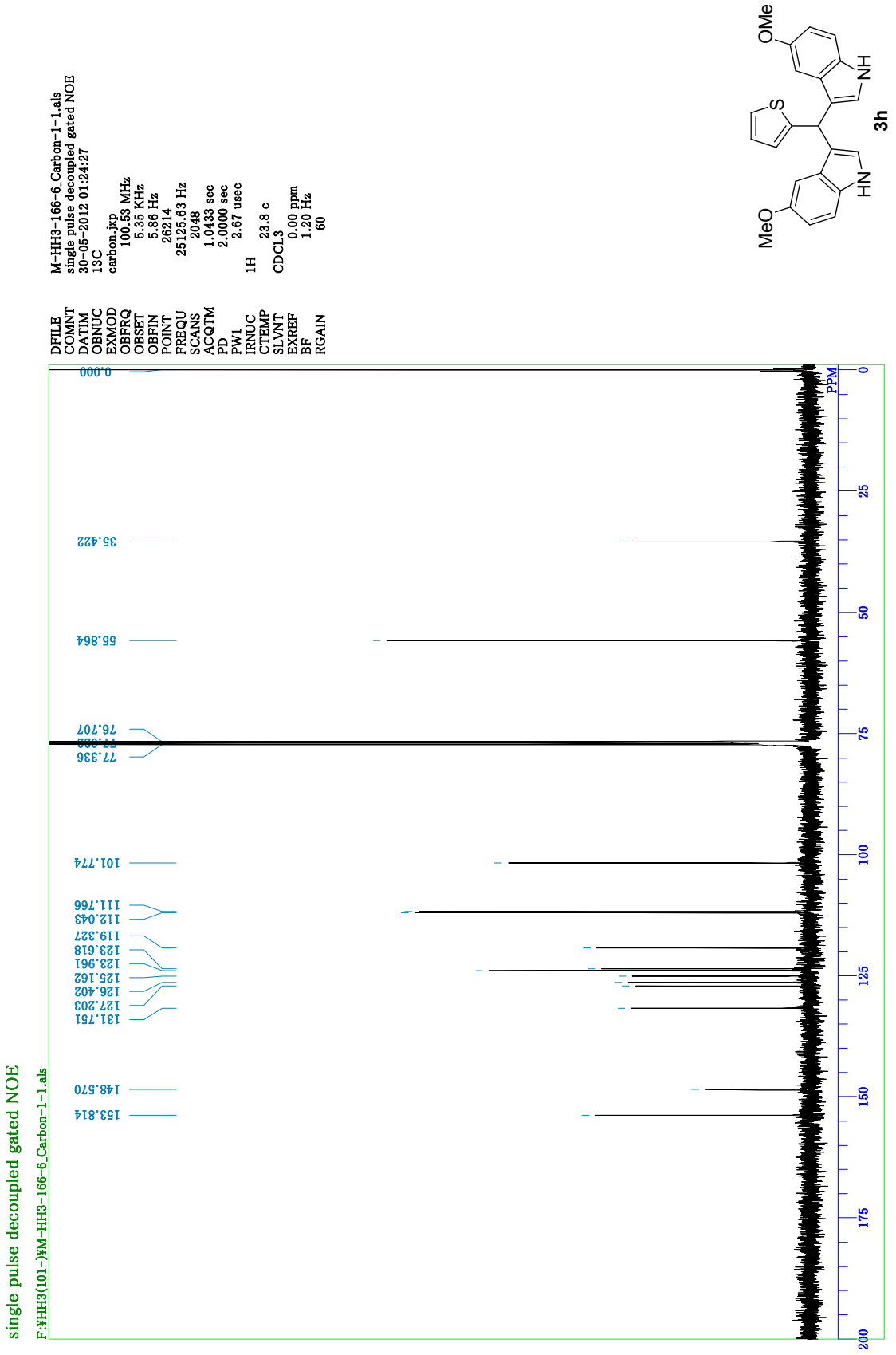

single_pulse
F:¥HH3(101-)¥M-HH3-164-5_Proton-1-1.als
M-HH3-164-5_Proton-1-1.als
single_pulse
06-06-2012 01:50:12
1H
proton.jxp
399.78 MHz
4.19 KHz
7.29 Hz
52428
6002.40 Hz
8
8.7346 sec
5.0000 sec
4.91 usec
1H
23.3 c
CDCl3
0.00 ppm
0.12 Hz
38
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OMe
NH
Me
HN
MeO
3e
PPM

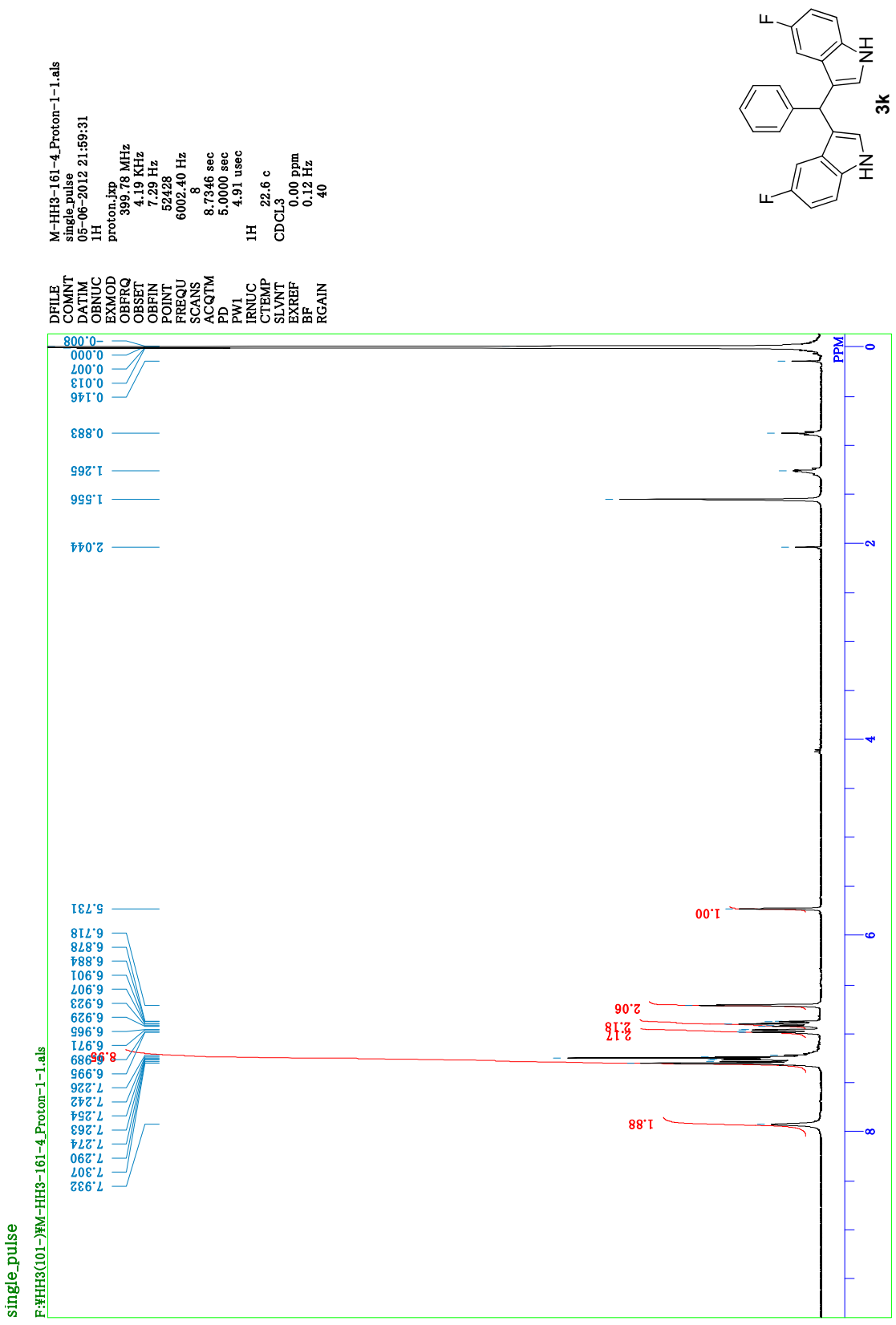

single pulse decoupled gated NOE
F:¥HH3(101-)¥M-HH3-164-5_Carbon-1-1.als
M-HH3-164-5_Carbon-1-1.als
single pulse decoupled gated NOE
06-06-2012 01:54:33
13C
carbon.jxp
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.63 Hz
2048
1.0433 sec
2.0000 sec
2.67 usec
1H
22.5 c
CDCl3
0.00 ppm
1.20 Hz
60
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
0.000
0.248
21.539
40.227
55.864
76.697
77.012
77.222
77.336
102.031
111.614
111.833
119.422
124.409
125.744
126.898
127.556
128.061
129.443
131.865
137.624
143.831
153.681
PPM
0
25
50
75
100
125
150
175
200
Me
OMe
NH
HN
MeO
3e

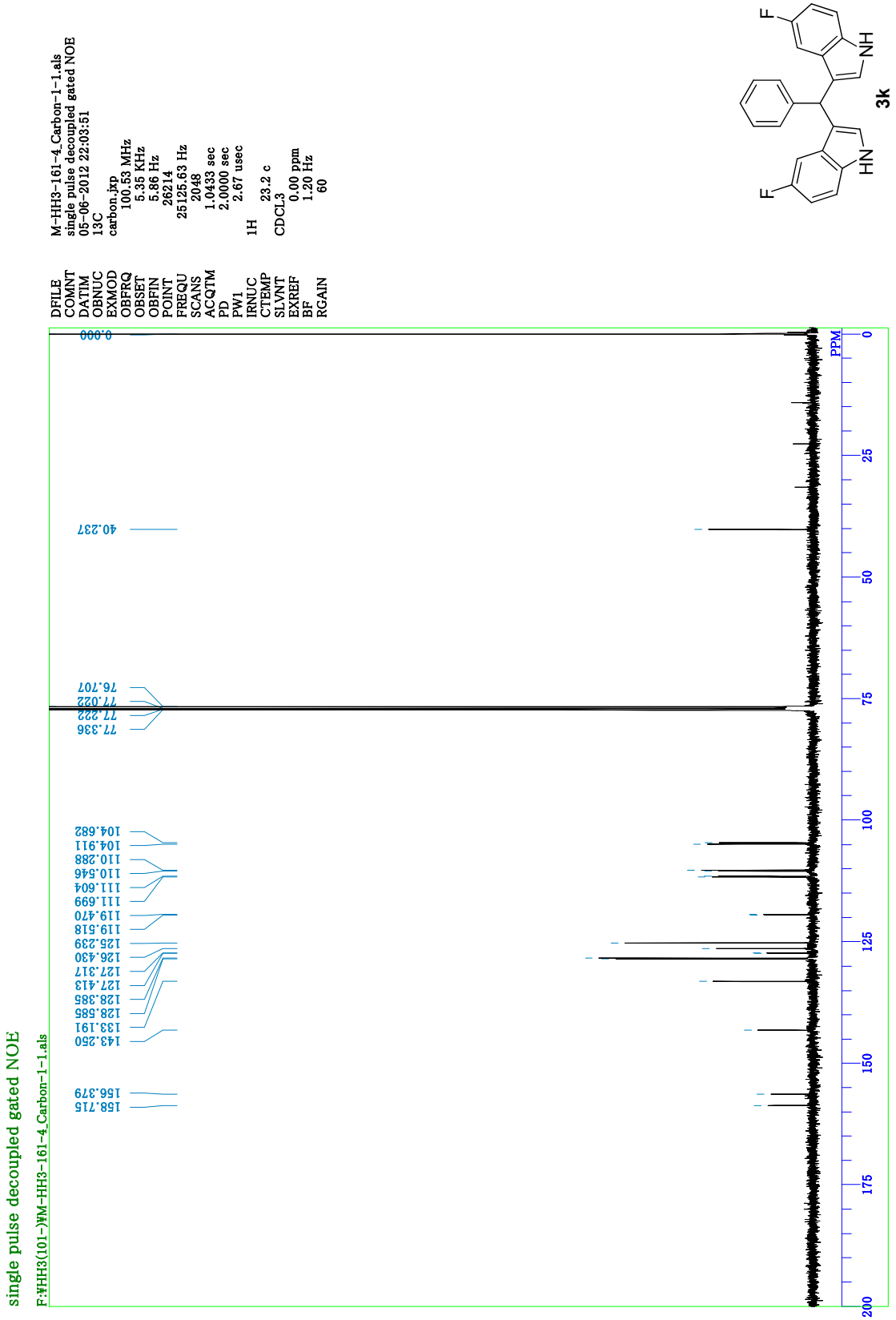


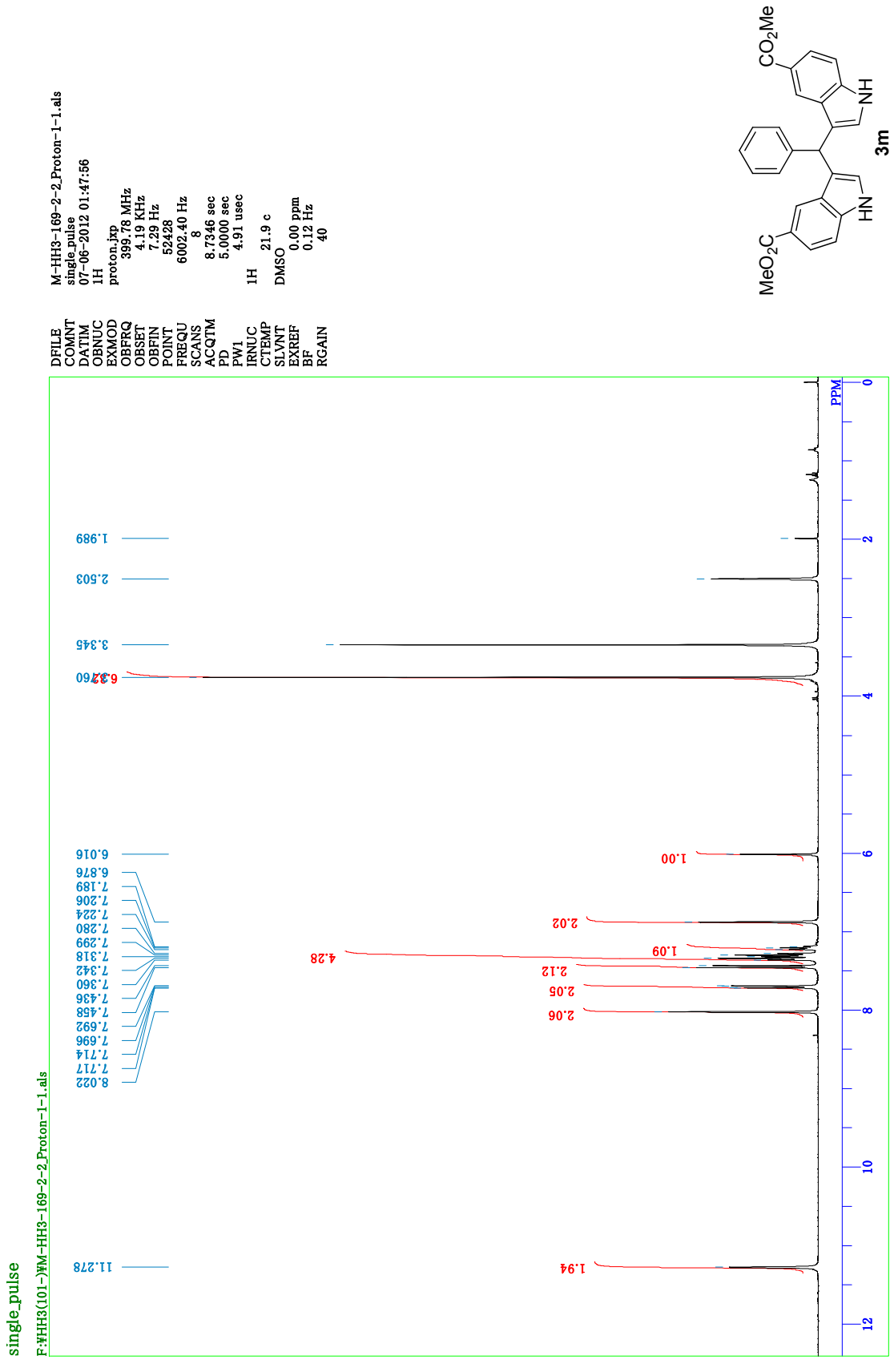

M-HH3-166-4_Carbon-1-1.als
single pulse decoupled gated NOE
06-06-2012 03:49:16
13C
carbon.jxp
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.63 Hz
2048
1.0433 sec
2.0000 sec
2.67 usec
1H
22.6 c
CDCL3
0.00 ppm
1.20 Hz
60
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OMe
Me
NH
HN
MeO
3g
single pulse decoupled gated NOE
F:¥HH3(101-)¥M-HH3-166-4_Carbon-1-1.als
PPM
0.000
19.565
36.365
55.873
76.697
77.022
77.222
77.336
101.955
111.642
111.737
118.726
124.696
125.811
126.059
127.651
128.396
130.178
131.922
136.013
141.886
153.681

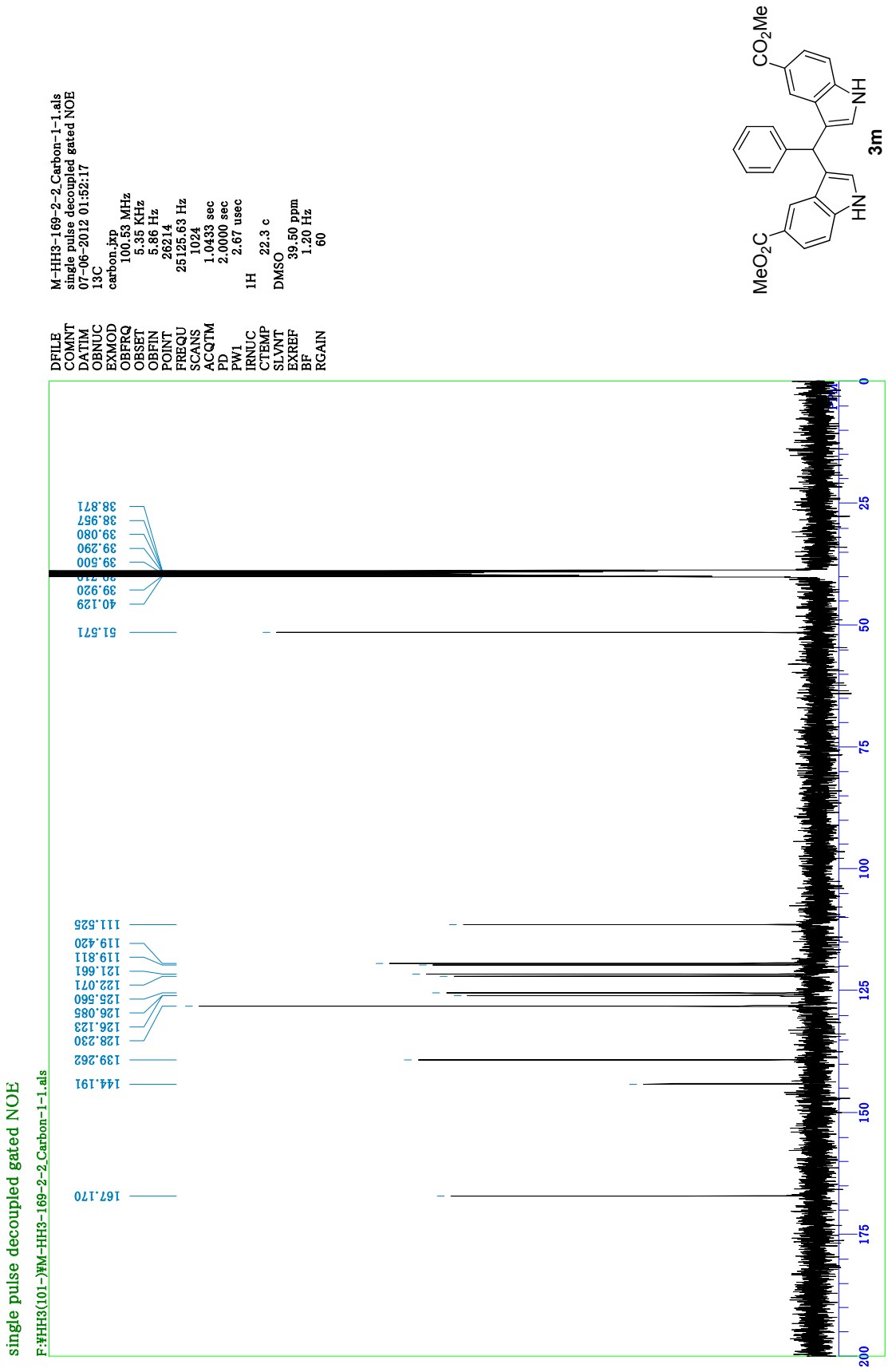



M-HH3-166-6_Carbon-1-1.als
single pulse decoupled gated NOE
30-05-2012 01:24:27
13C
carbon.jxp
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.63 Hz
2048
1.0433 sec
2.0000 sec
2.67 usec
1H
23.8 c
CDCL3
0.00 ppm
1.20 Hz
60
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
OMe
NH
S
HN
MeO
3h
single pulse decoupled gated NOE
F:¥HH3(101-)¥M-HH3-166-6_Carbon-1-1.als
0.000
35.422
55.864
76.707
77.029
77.336
101.774
111.766
112.043
119.327
123.618
123.961
125.162
126.402
127.203
131.751
148.570
153.814
PPM
0
25
50
75
100
125
150
175
200








single pulse decoupled gated NOE
F:¥HH3(101-)¥M-HH3-169-2-2_Carbon-1-1.als
M-HH3-169-2-2_Carbon-1-1.als
single pulse decoupled gated NOE
07-06-2012 01:52:17
13C
carbon.jxp
100.53 MHz
5.35 KHz
5.86 Hz
26214
25125.63 Hz
1024
1.0433 sec
2.0000 sec
2.67 usec
1H
22.3 c
DMSO
39.50 ppm
1.20 Hz
60
DFILE
COMNT
DATIM
OBNUC
EXMOD
OBFRQ
OBSET
OBFIN
POINT
FREQU
SCANS
ACQTM
PD
PW1
IRNUC
CTEMP
SLVNT
EXREF
BF
RGAIN
38.871
38.957
39.080
39.290
39.500
39.710
39.920
40.129
51.571
111.525
119.420
119.811
121.661
122.071
125.560
126.085
126.123
128.230
139.262
144.191
167.170
0
25
50
75
100
125
150
175
200
ppm
CO_2Me
NH
HN
MeO_2C
3m