Supporting Information

***Rec. Nat. Prod*. 12:6 (2018) 634-637**

Quinolone Alkaloids Along with Other Constituents from Zanthoxylum rhetsa and their Chemotaxonomic Significance

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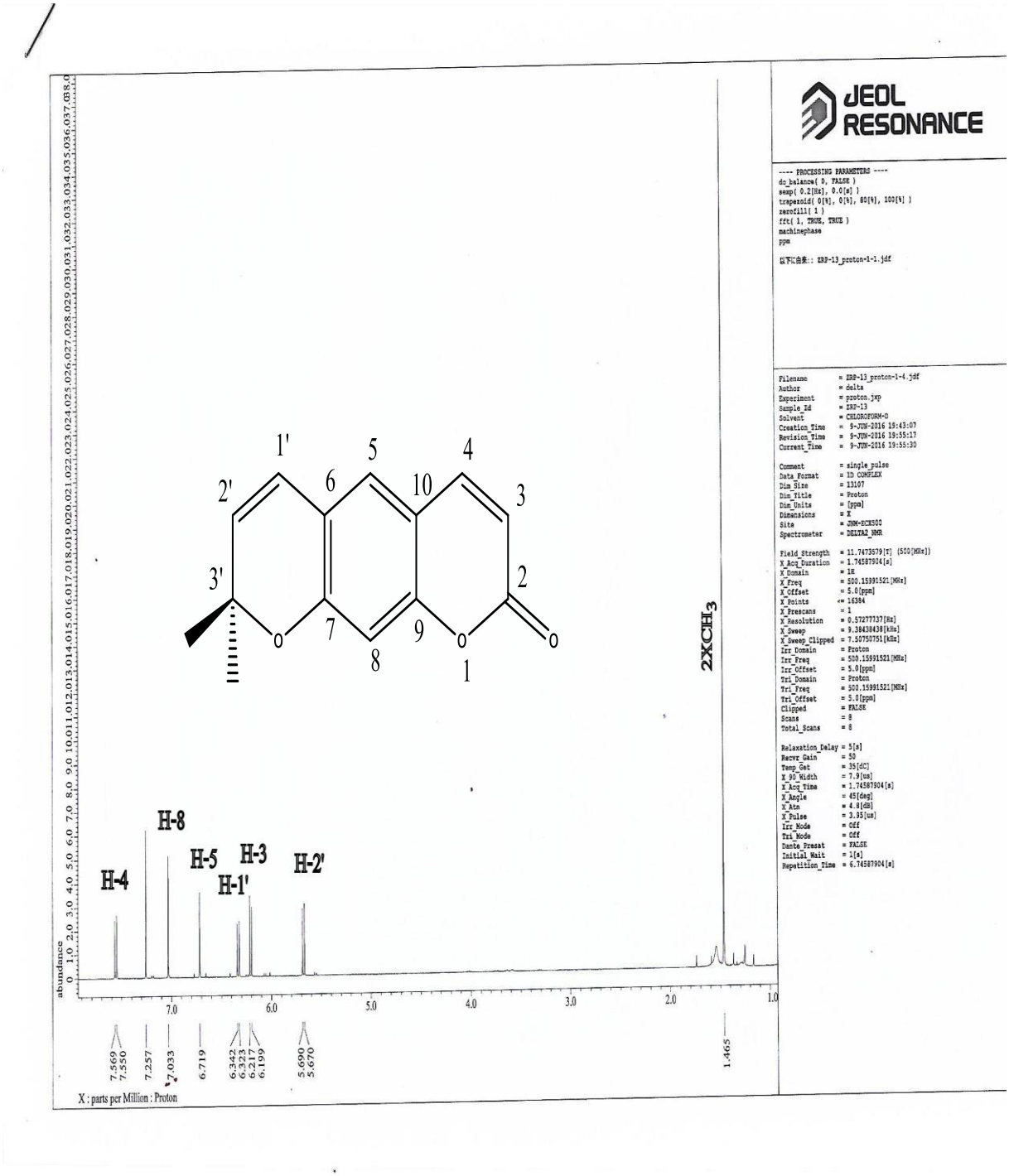
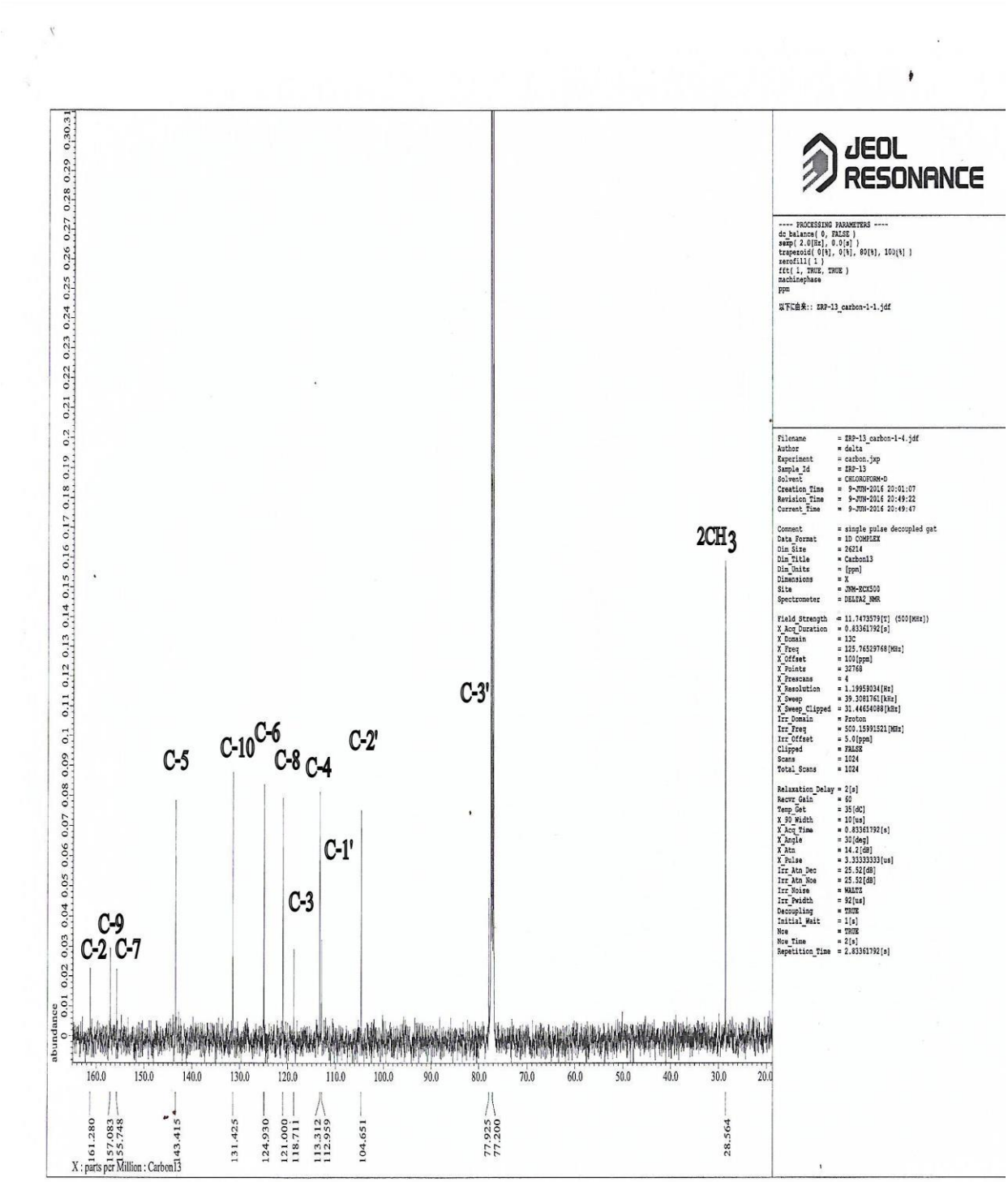


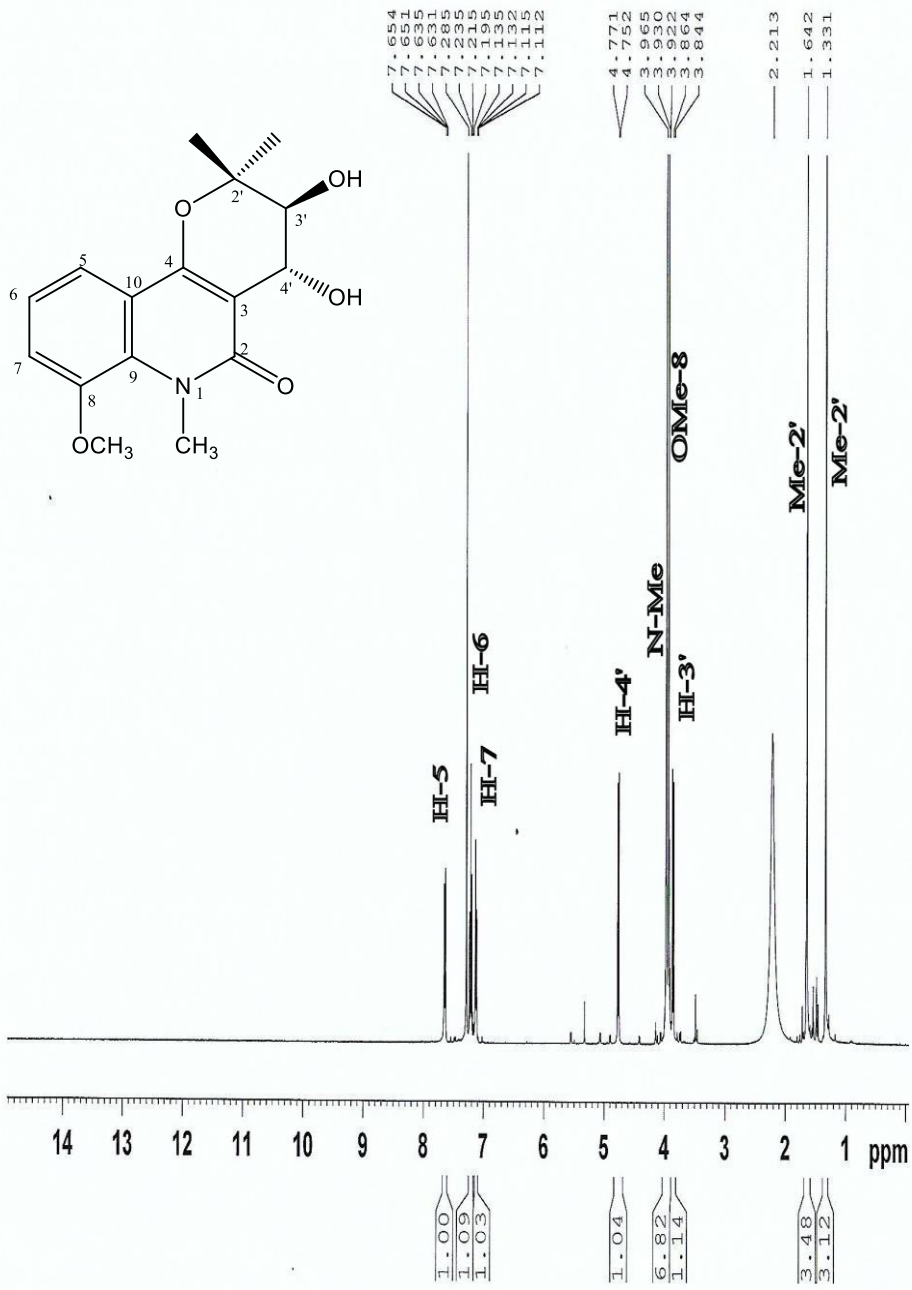
S1: ^{1}H NMR (500 MHz, $CDCl_3$) Spectrum of Compound **1**(Xanthyletin).



S2: ^{13}C NMR spectrum (150 MHz, $CDCl_3$) of Compound 1(Xanthyletin).

*Xanthyletin **(1)***: white crystals; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.56 (1H, d, *J*= 9.5 Hz, H-4), 7.03 (1H, s, H-5), 6.72 (1H, s, H-8), 6.33 (1H, d, *J*= 10.0 Hz, H-4′), 6.21 (1H, d, *J*= 9.5 Hz, H-3), 5.68 (1H, d, *J*= 10 Hz, H-3′), 1.47 (6H, s, 2 x Me, H-5′, 6′).

Wazed Miah Science Research Center (WMSRC)
Jahangirnagar University
Sample: DU_ZRP_12



BRUKER

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PROCNO 1

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P1 14.75 us
PLW1 12.00000000 W

F2 - Processing parameters
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SF 400.2300000 MH
WDW EM
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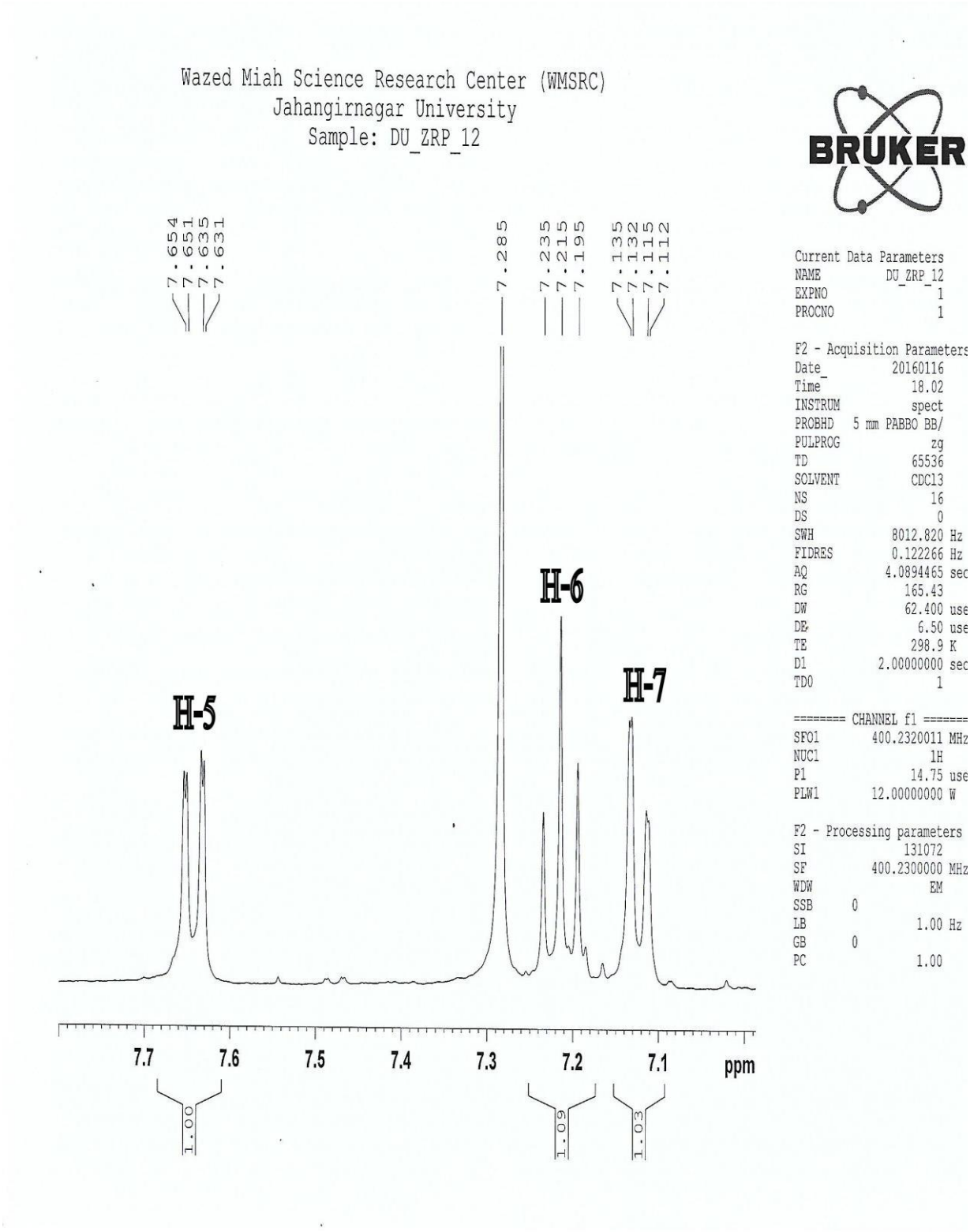
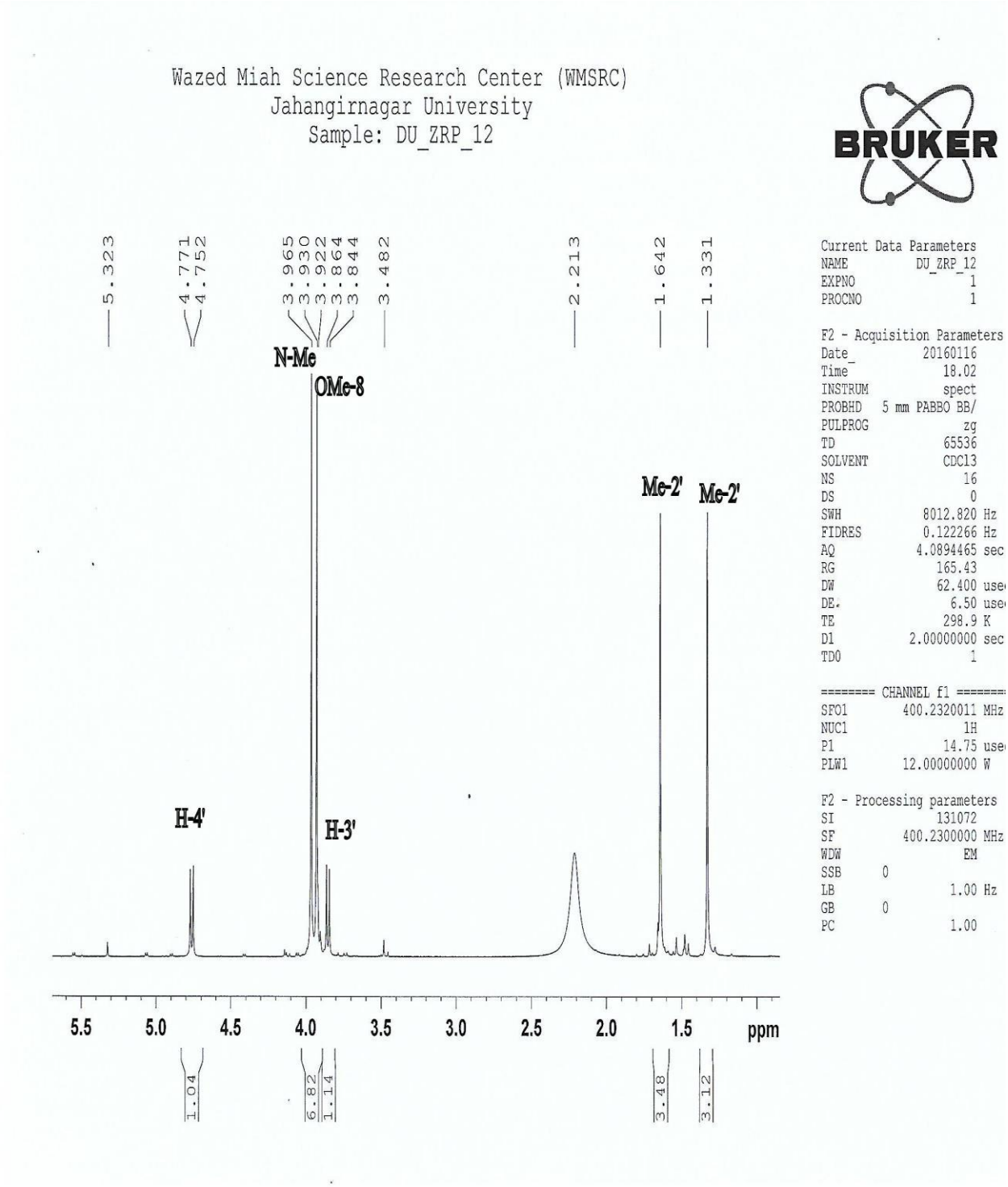
LB 1.00 Hz
GB 0
PC 1.00

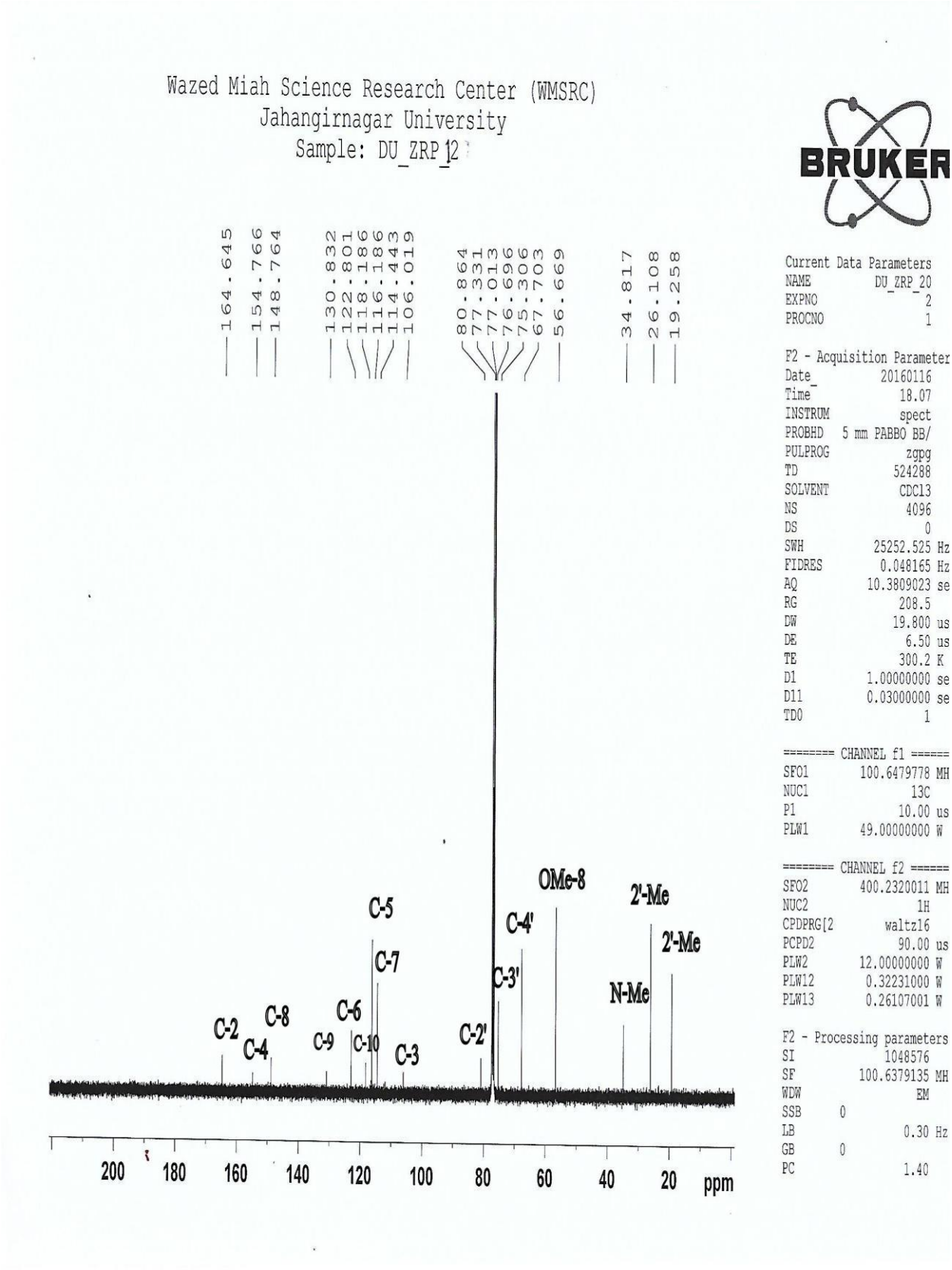
S3: ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound 2 (Zanthodioline)



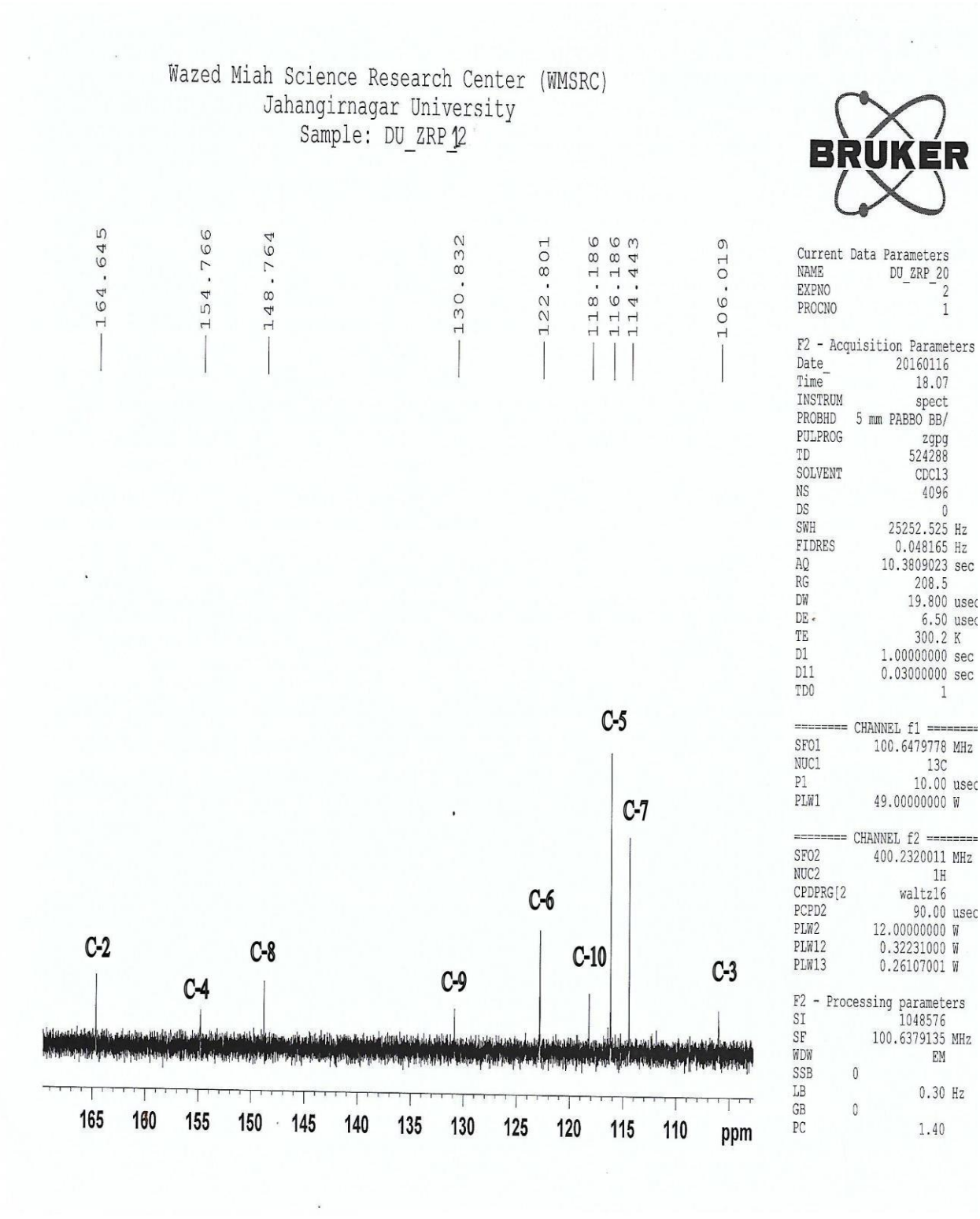
S4 : Partially expanded ^{1}H NMR spectrum (400 MHz, $CDCl_3$) of Compound 2



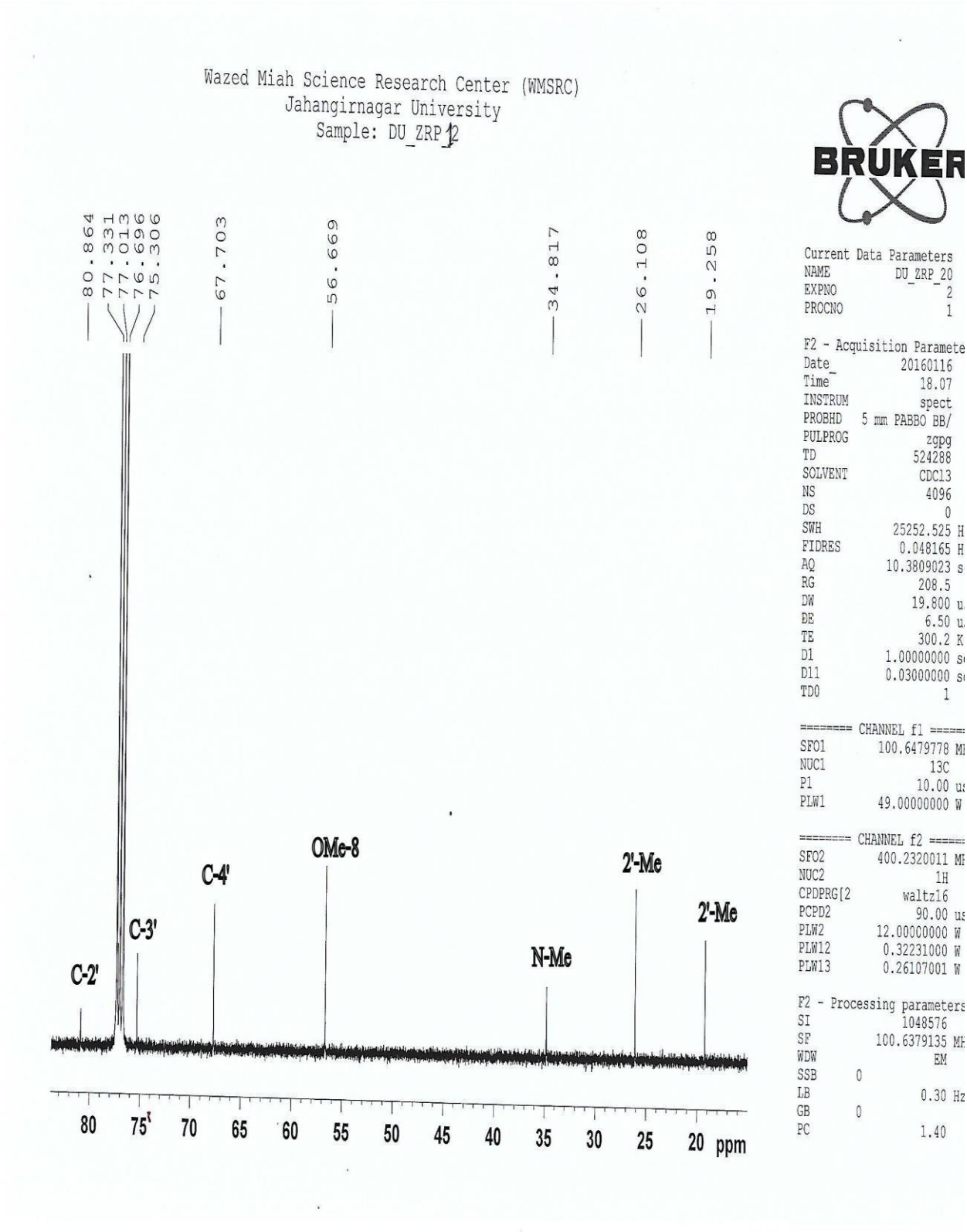
S5 : Partially expanded ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound 2 (Zanthodioline)



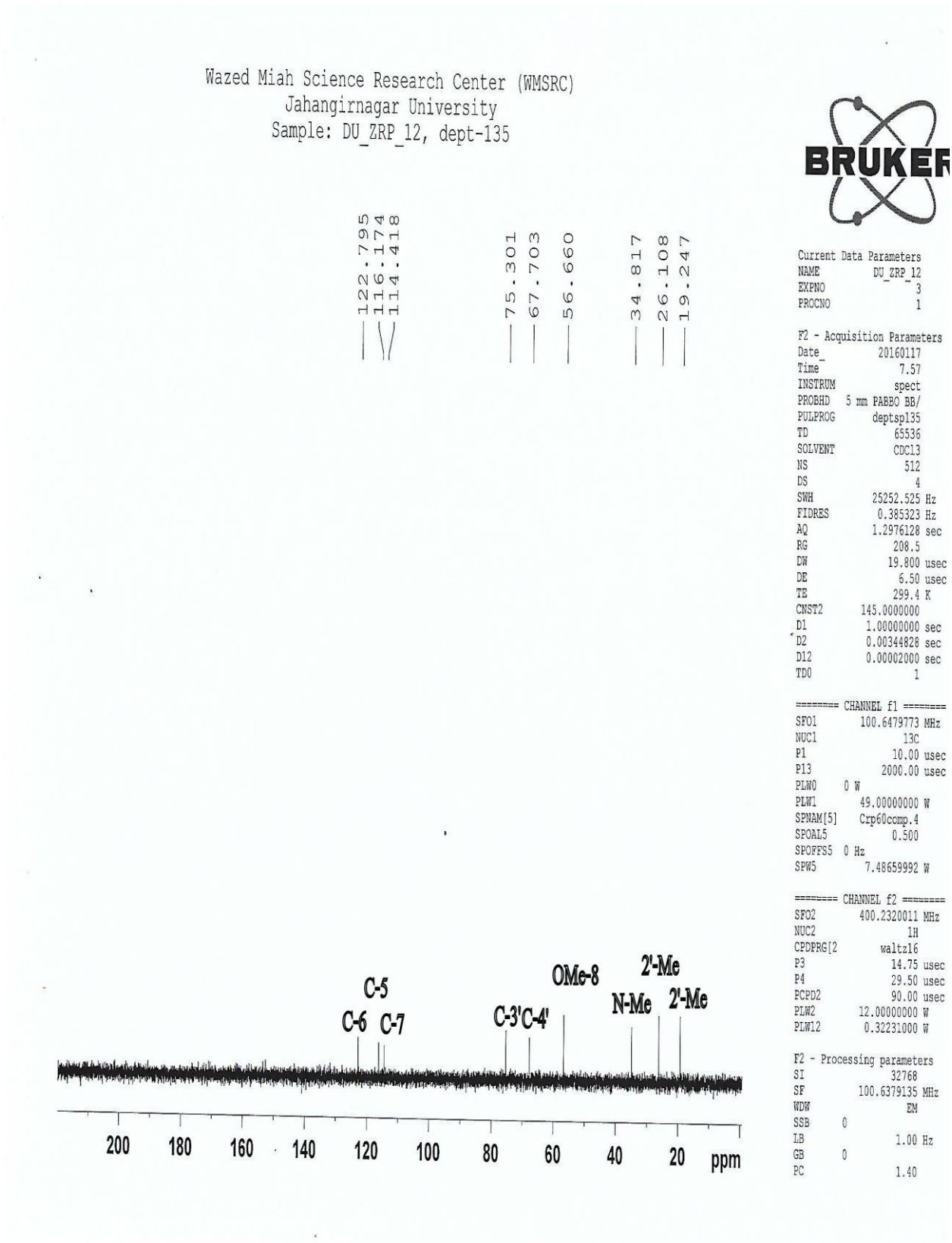
S6: ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



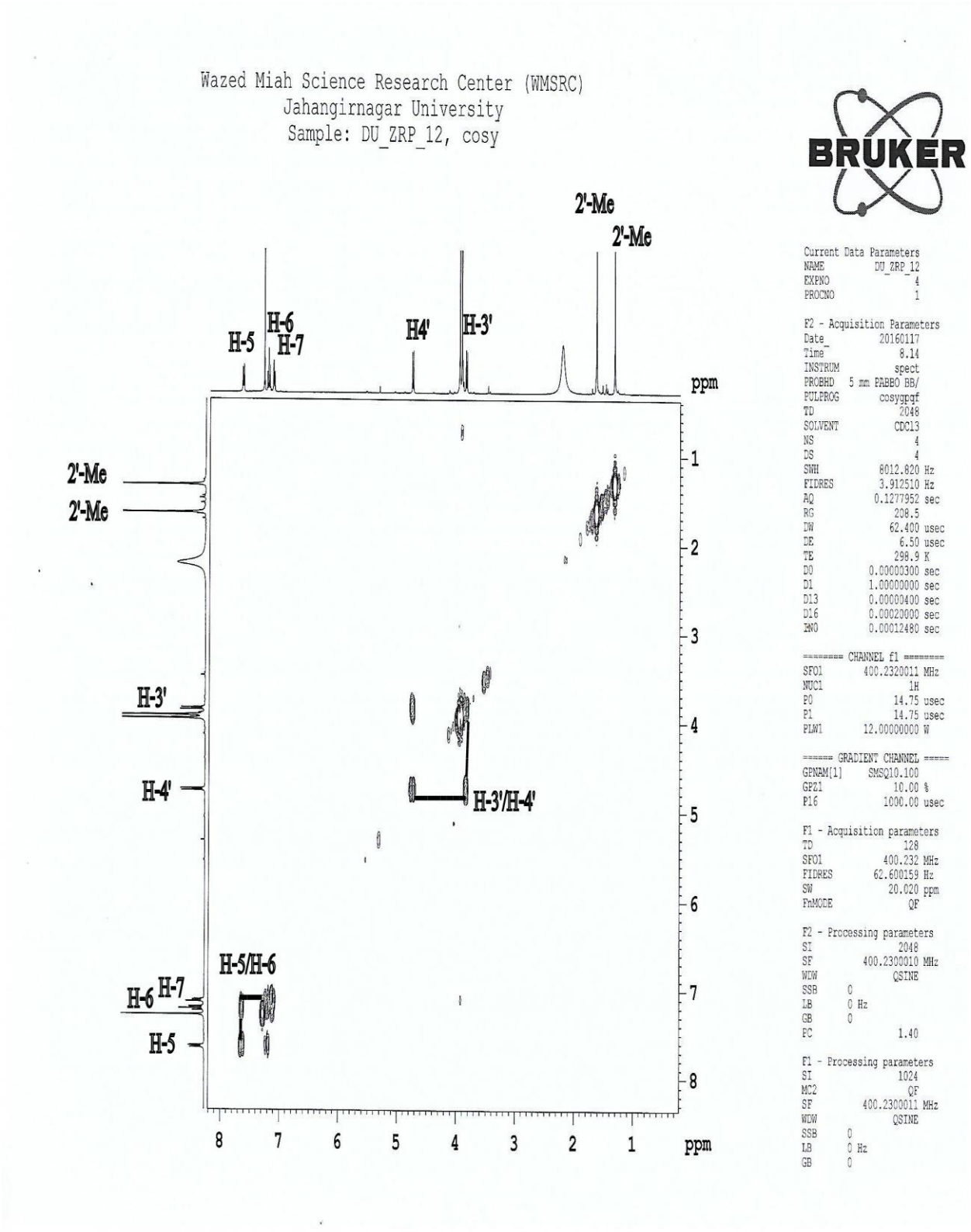
S7 : Partially expanded ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



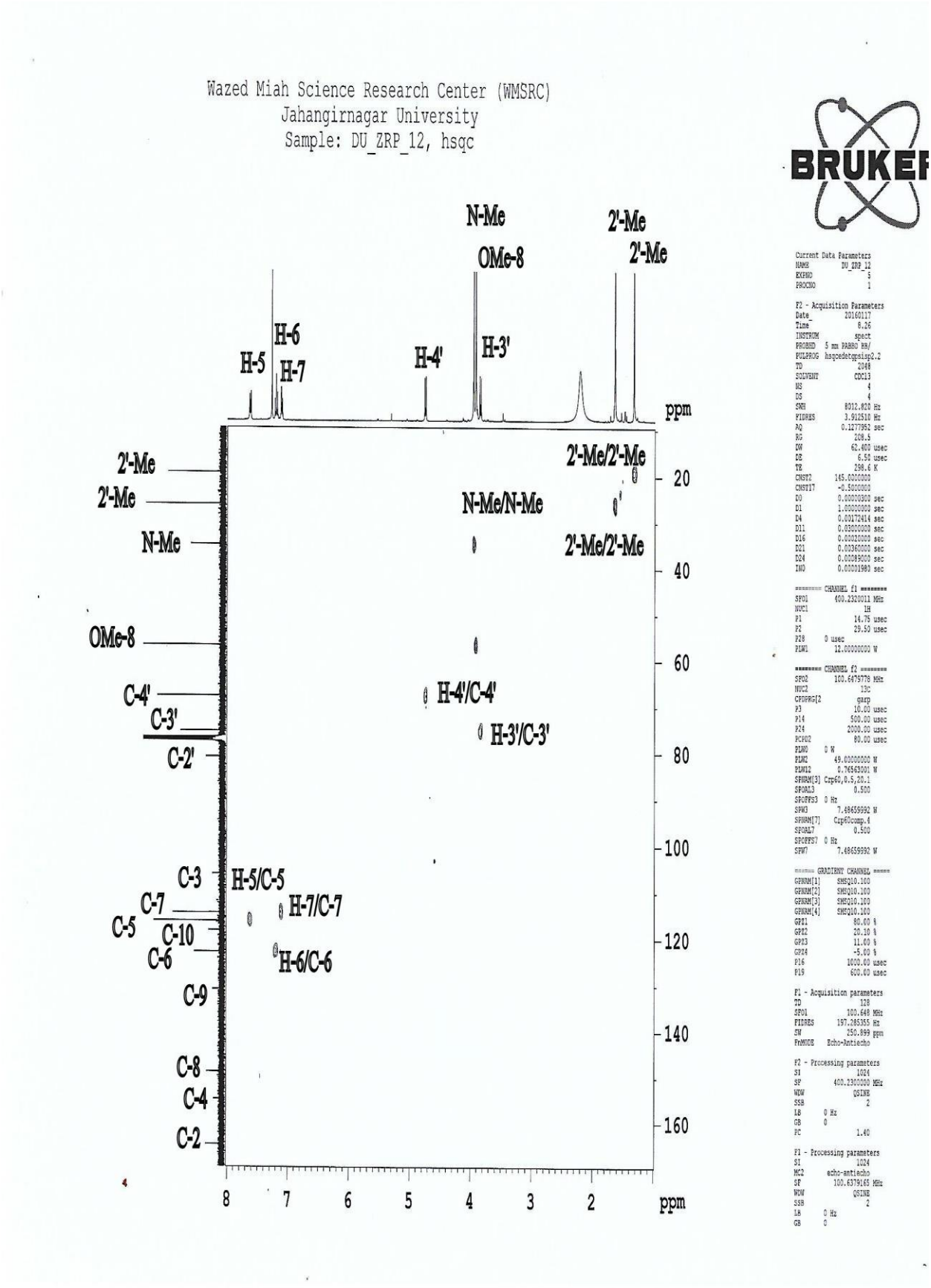
S8 : Partially expanded ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



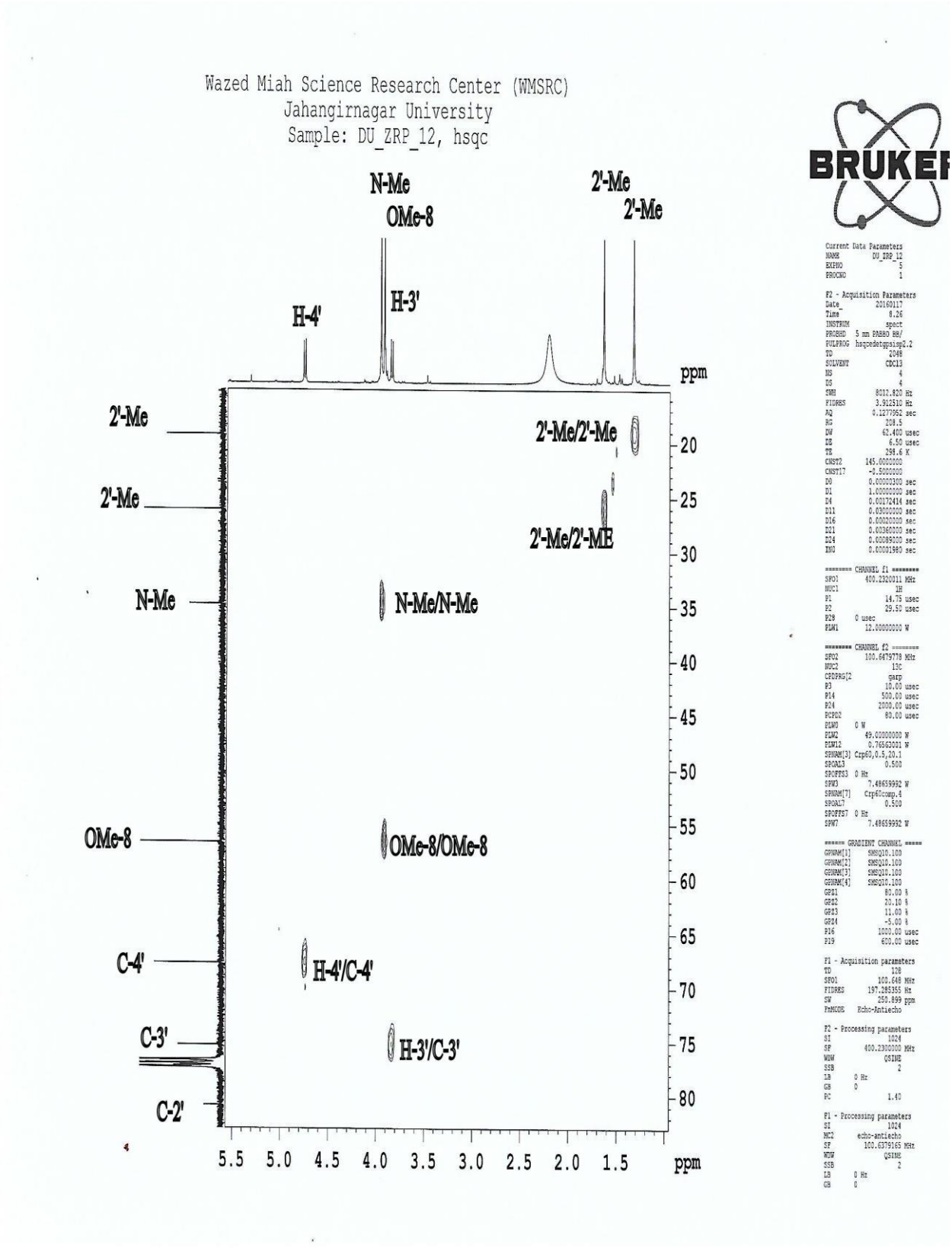
S9: DEPT-135 spectrum of Compound **2** (Zanthodioline)



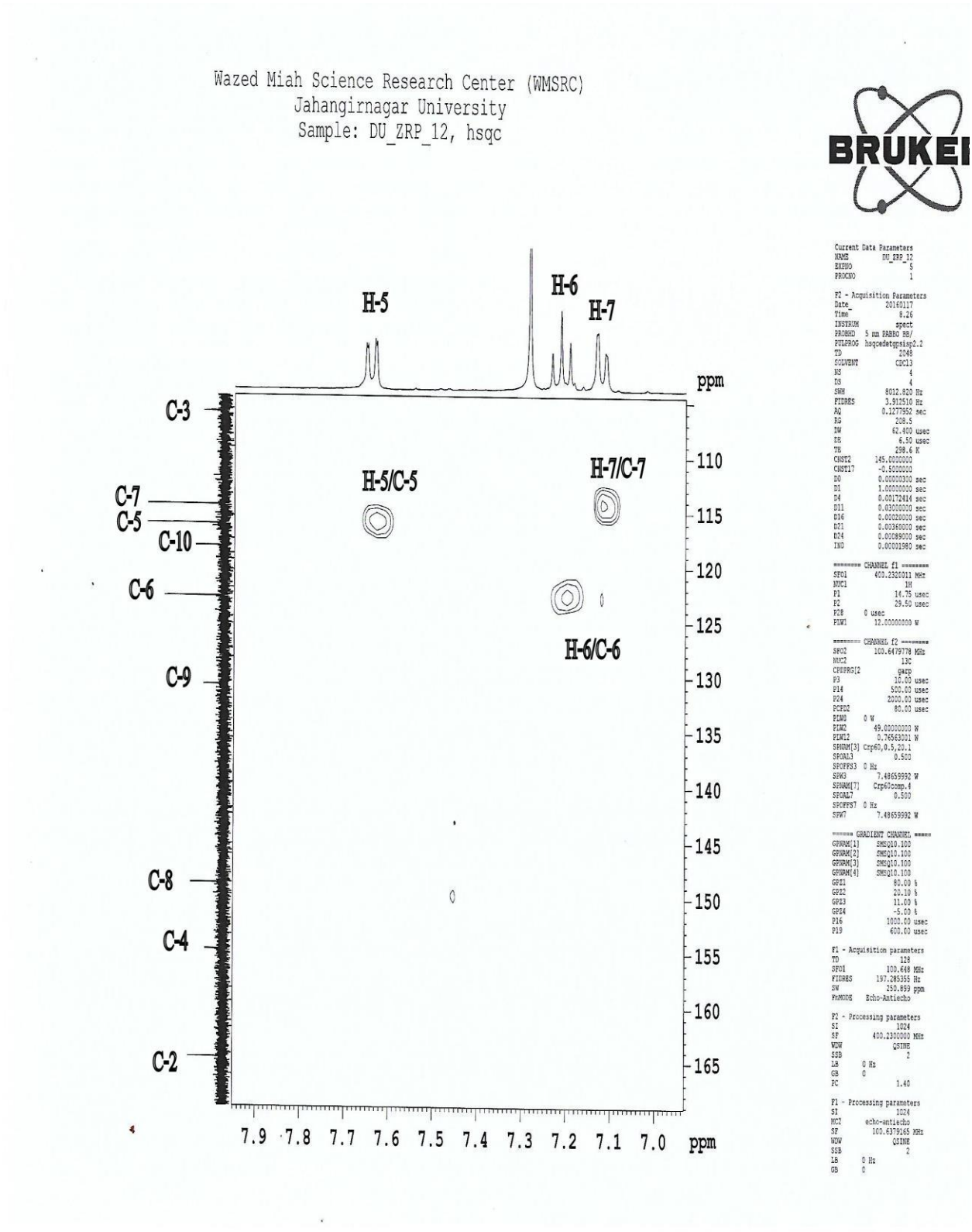
S10: COSY-NMR spectrum (400 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



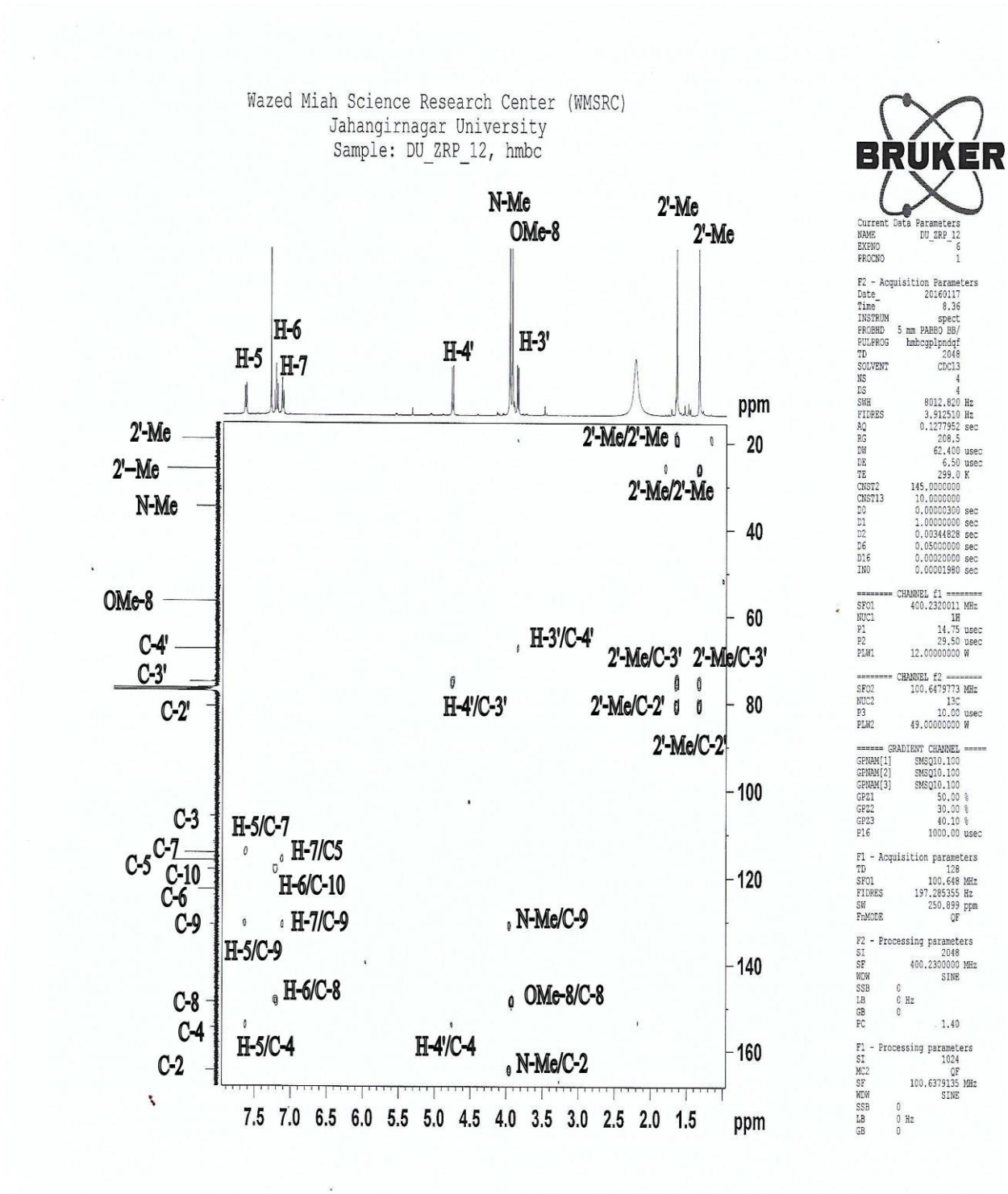
S11 : HSQC- NMR spectrum (400 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



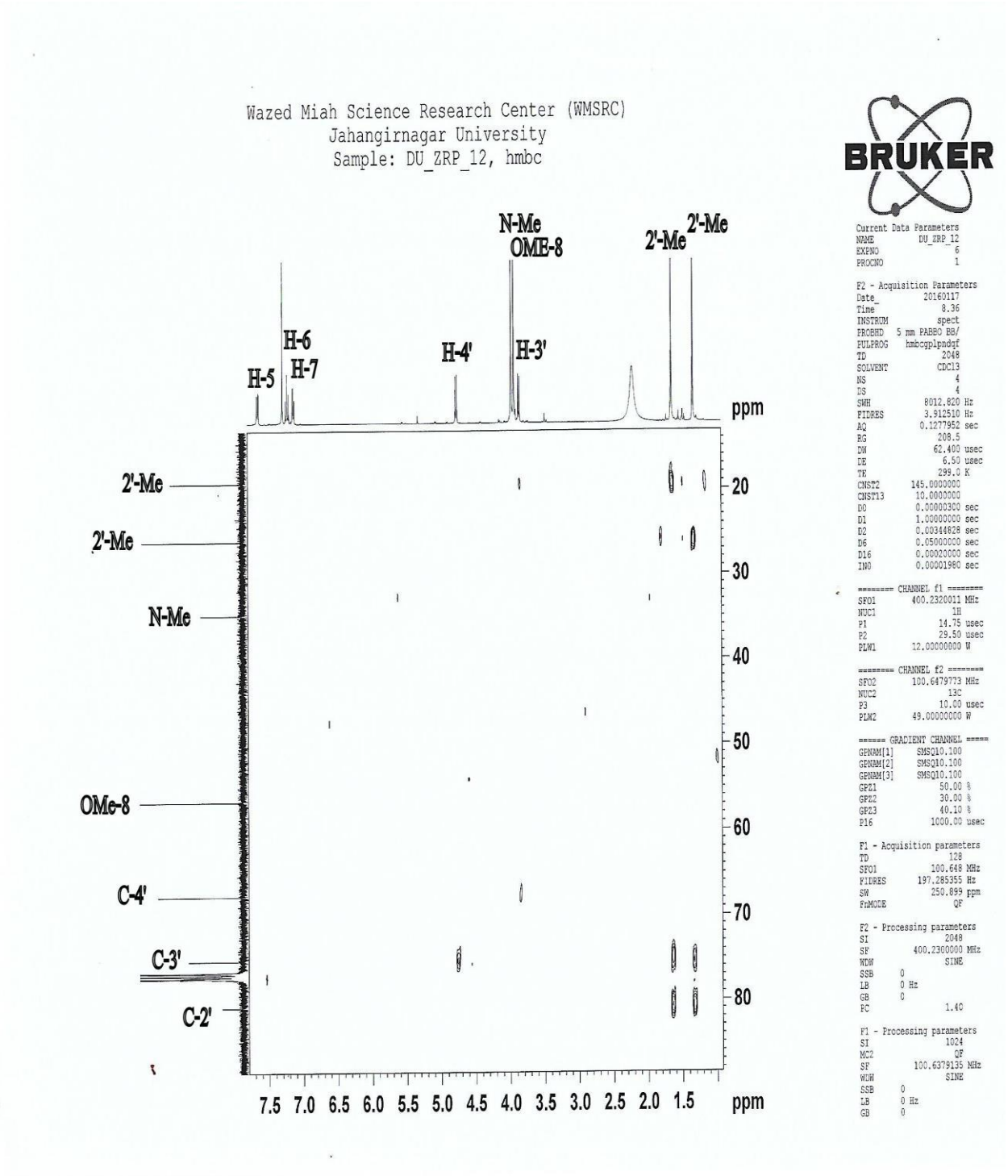
S12: Partially expanded HSQC- NMR spectrum (400 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



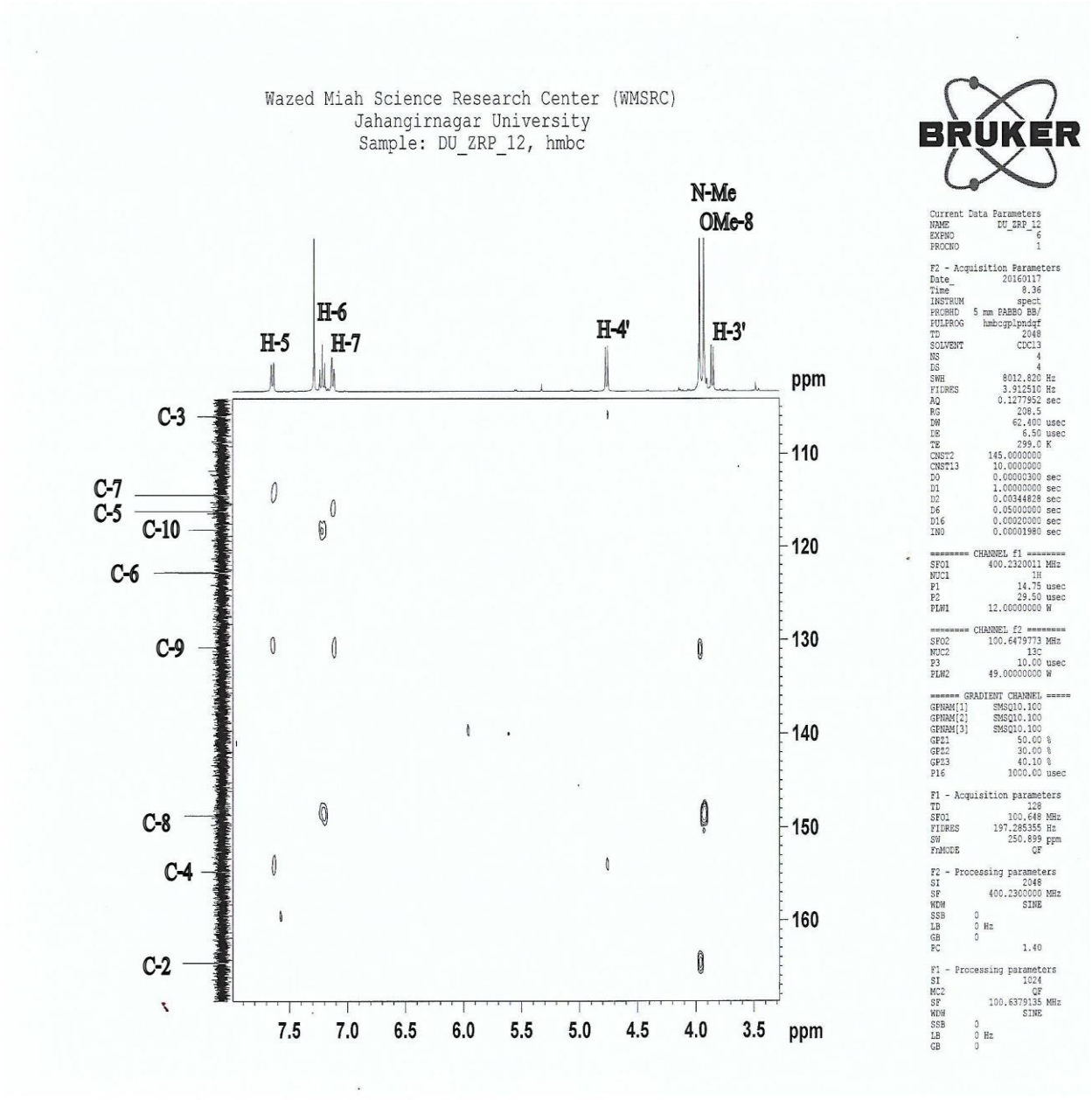
S13: Partially expanded HSQC-NMR spectrum (400 MHz, $CDCl_3$) of Compound **2** (Zanthodioline)



S14: HMBC- NMR spectrum (400 MHz, $CDCl_3$) of Compound 2 (Zanthodioline)

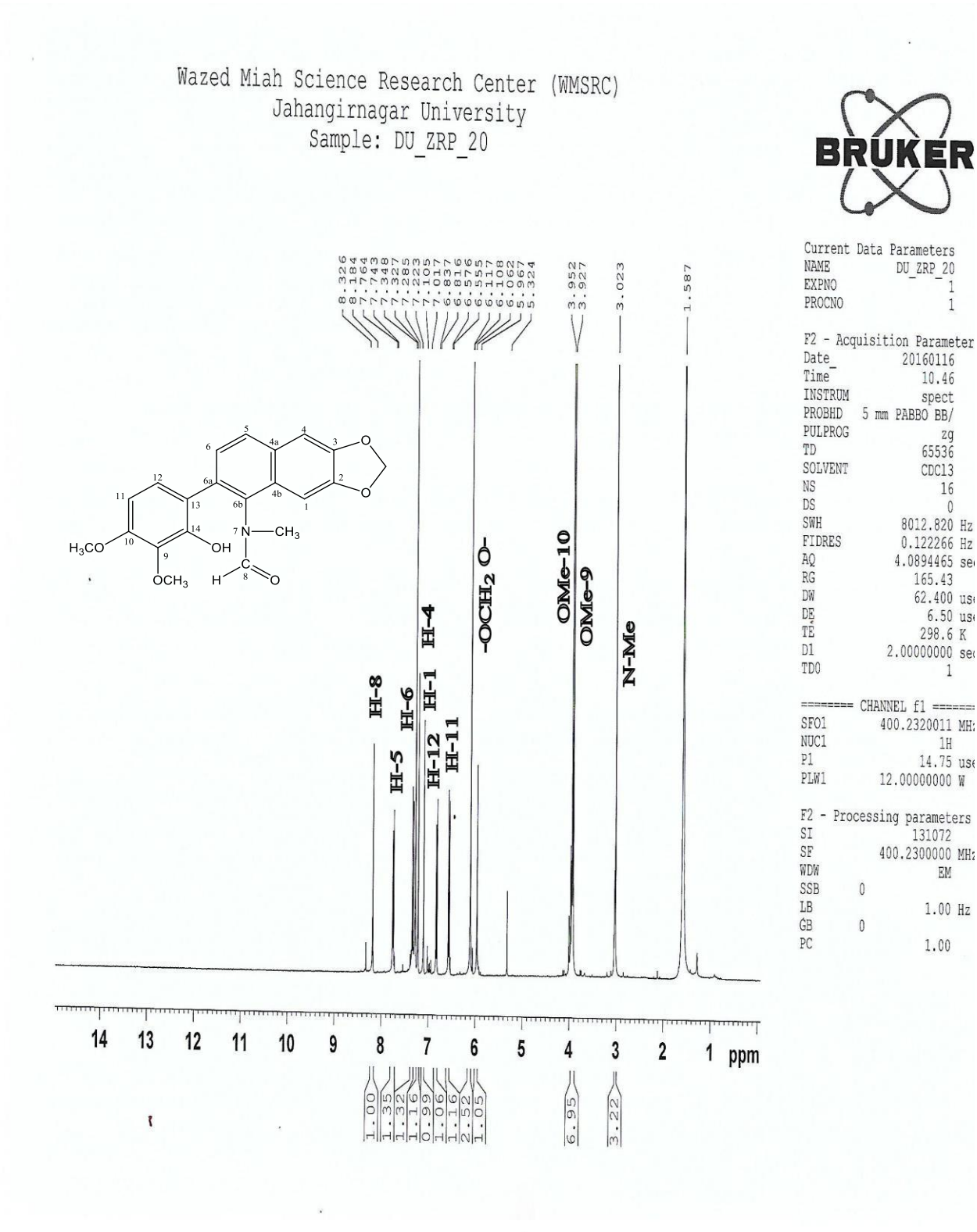


S15 : Partially expanded HMBC- NMR spectrum (400 MHz, $CDCl_3$) of Compound 2 (Zanthodioline)

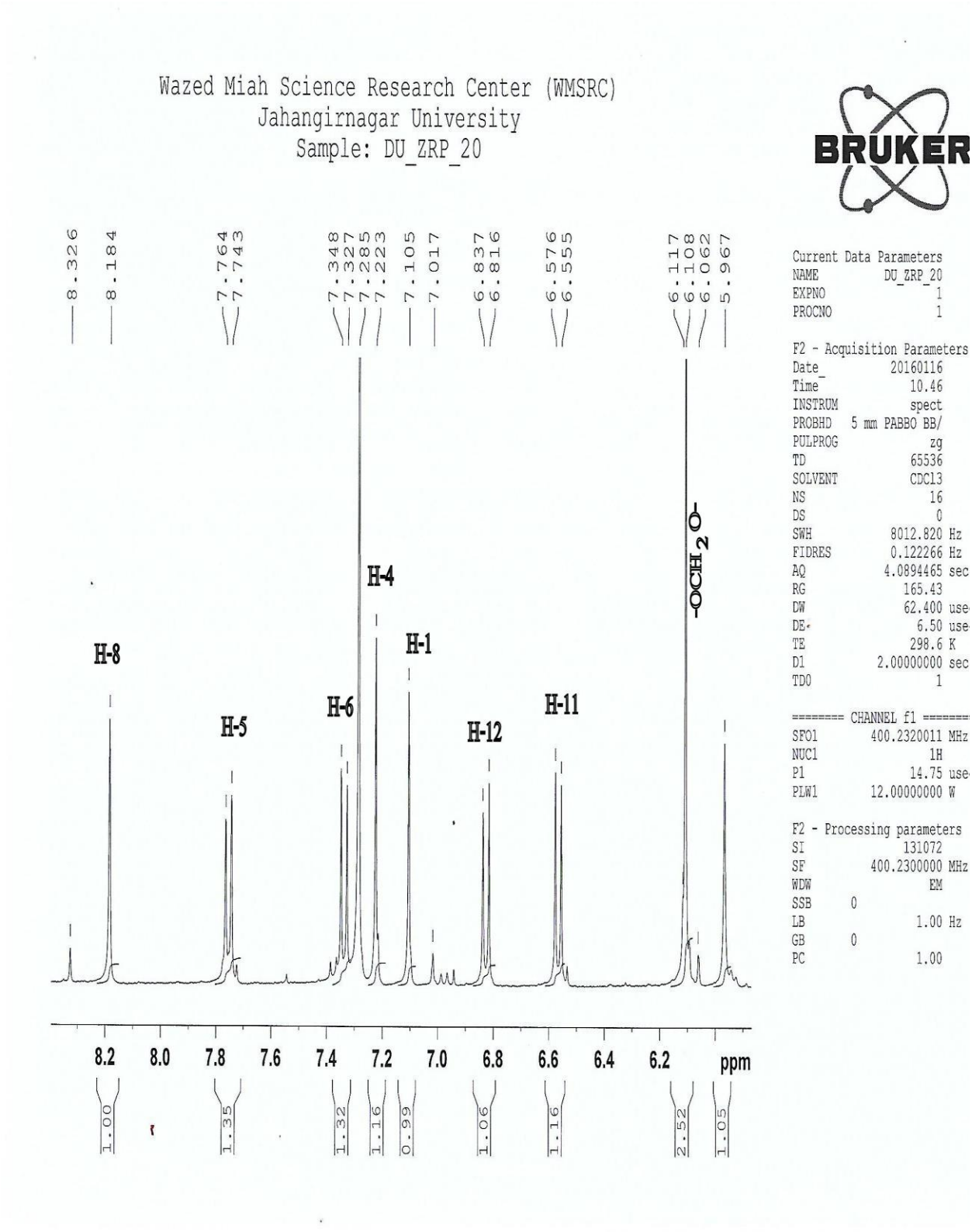


S16: Partially expanded HMBC- NMR spectrum (400 MHz, $CDCl_3$) of Compound 2 (Zanthodioline).

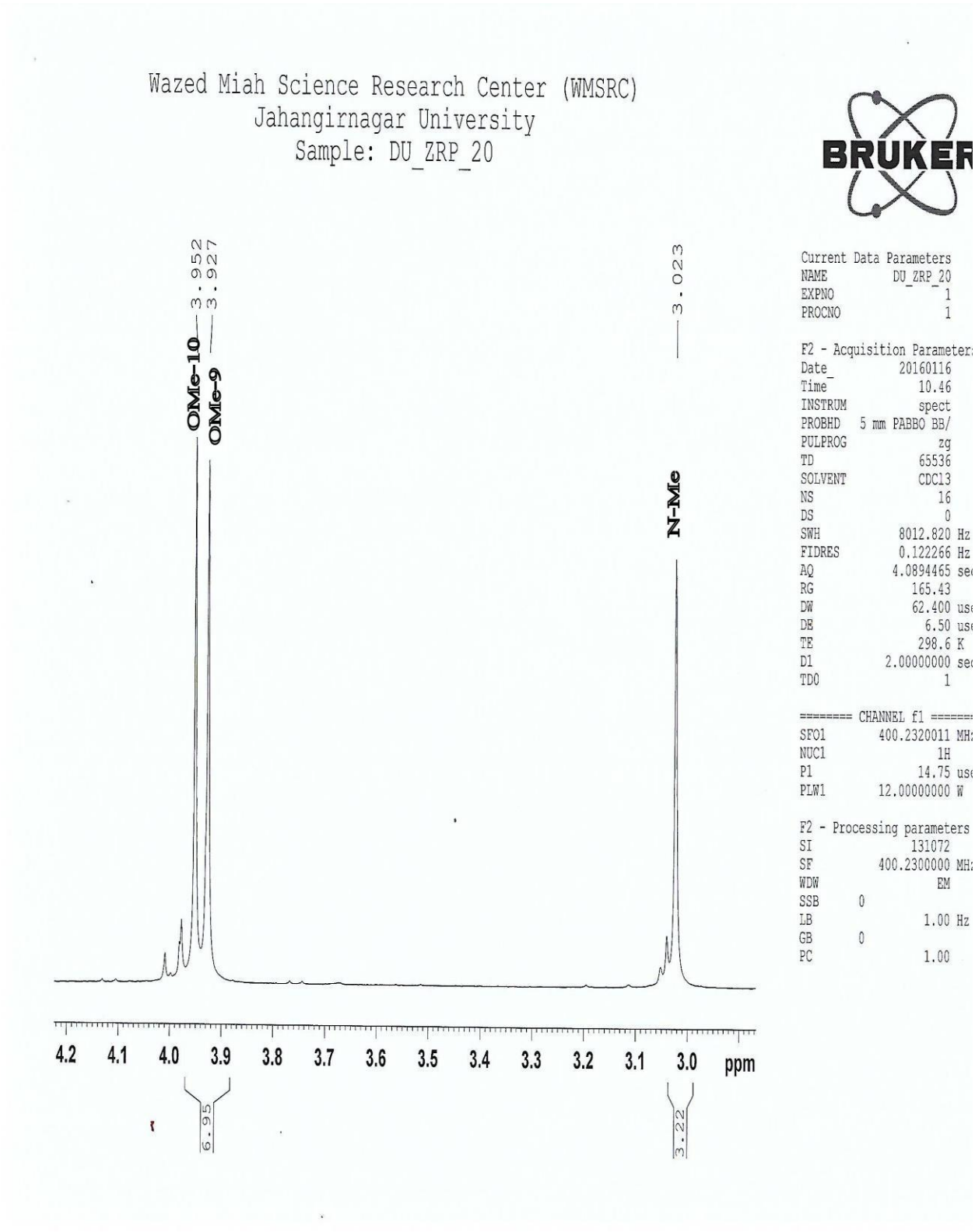
*Zanthodioline (**2**)*: white crystals; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 7.64 (dd, *J*= 8.0, 1.2 Hz, H-5), 7.22 (1H, t, *J* = 8.0 Hz, H-6), 7.12 (1H, dd, *J*= 8.0, 1.2 Hz, H-7), 4.76 (1H, d, *J*= 8 Hz, H-4′), 3.97 (3H, s, N-Me), 3.93 (3H, s, OMe-8), 3.84 (1H, d, *J*= 8 Hz, H-3′), 1.64 (3H s, H-2′ Me), 1.33 (3H, s, H-2′ Me). ^{13}C-NMR (125 MHz, $CDCl_3$): δ 164.6 (C-2), 154.8 (C-4), 148.8 (C-8), 130.8 (C-9), 122.8 (C-6), 118.2 (C-10), 116.2 (C-5), 114.4 (C-7), 106.0 (C-3), 80.9 (C-2′), 75.3 (C-3′), 67.7 (C-4′), 56.7 (OMe-8), 34.8 (N-Me), 26.1 (C-2′ Me), 19.3 (C-2′ Me).



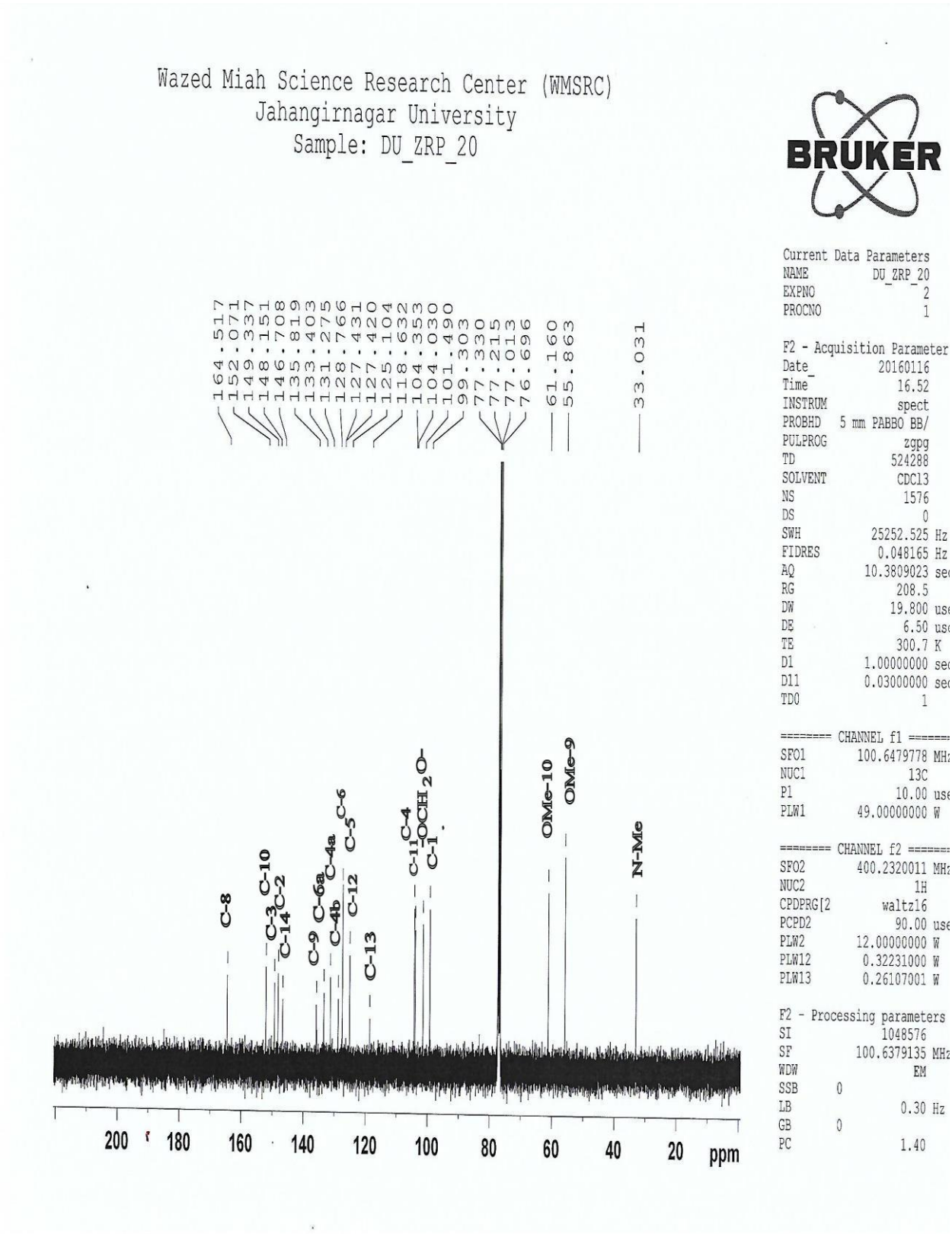
S17 : ^{1}H NMR (400 MHz, $CDCl_3$) Spectrum of Compound **3** (Arnottianamide).



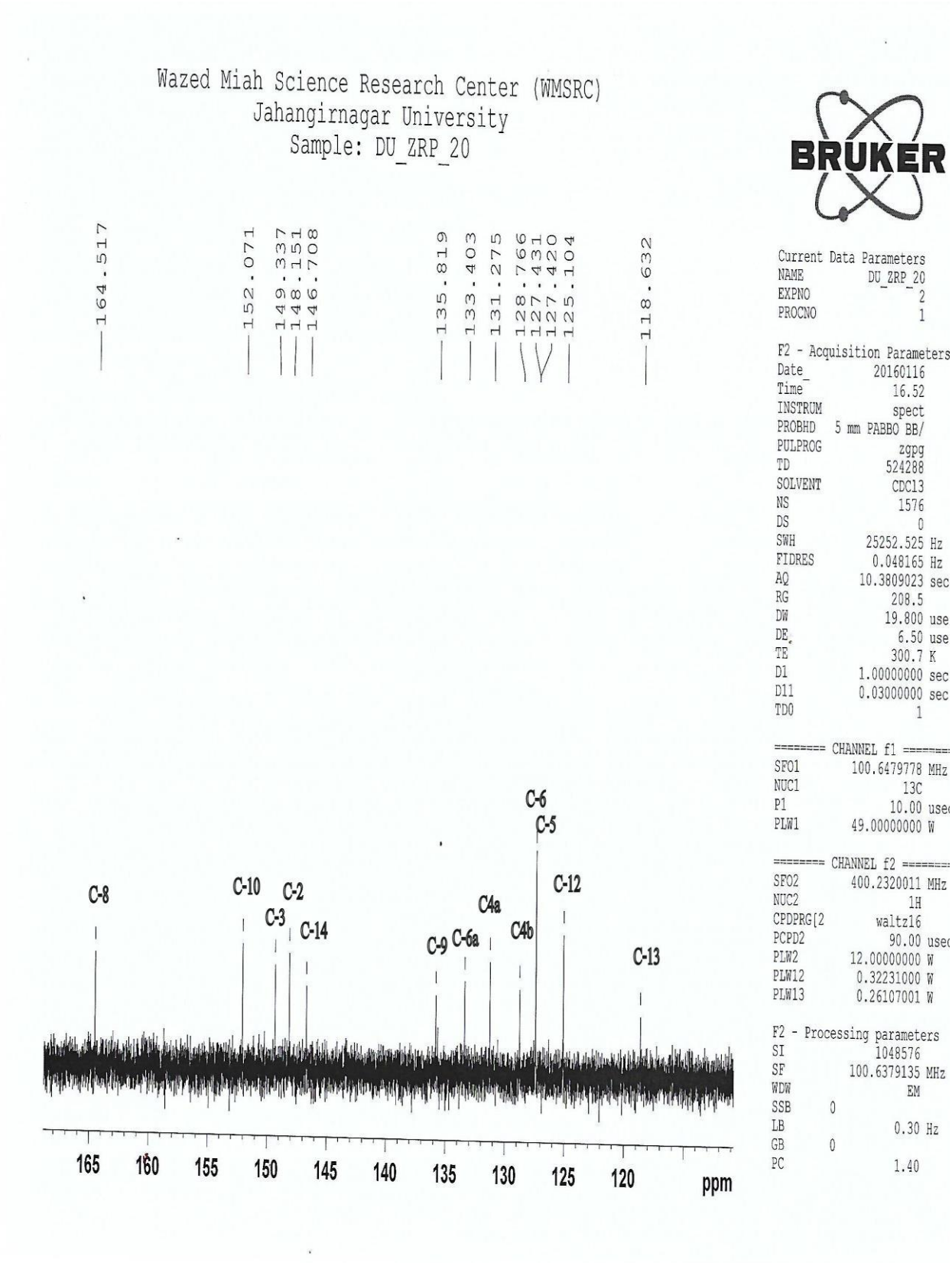
S18 : Partially expanded ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound 3 (Arnottianamide).



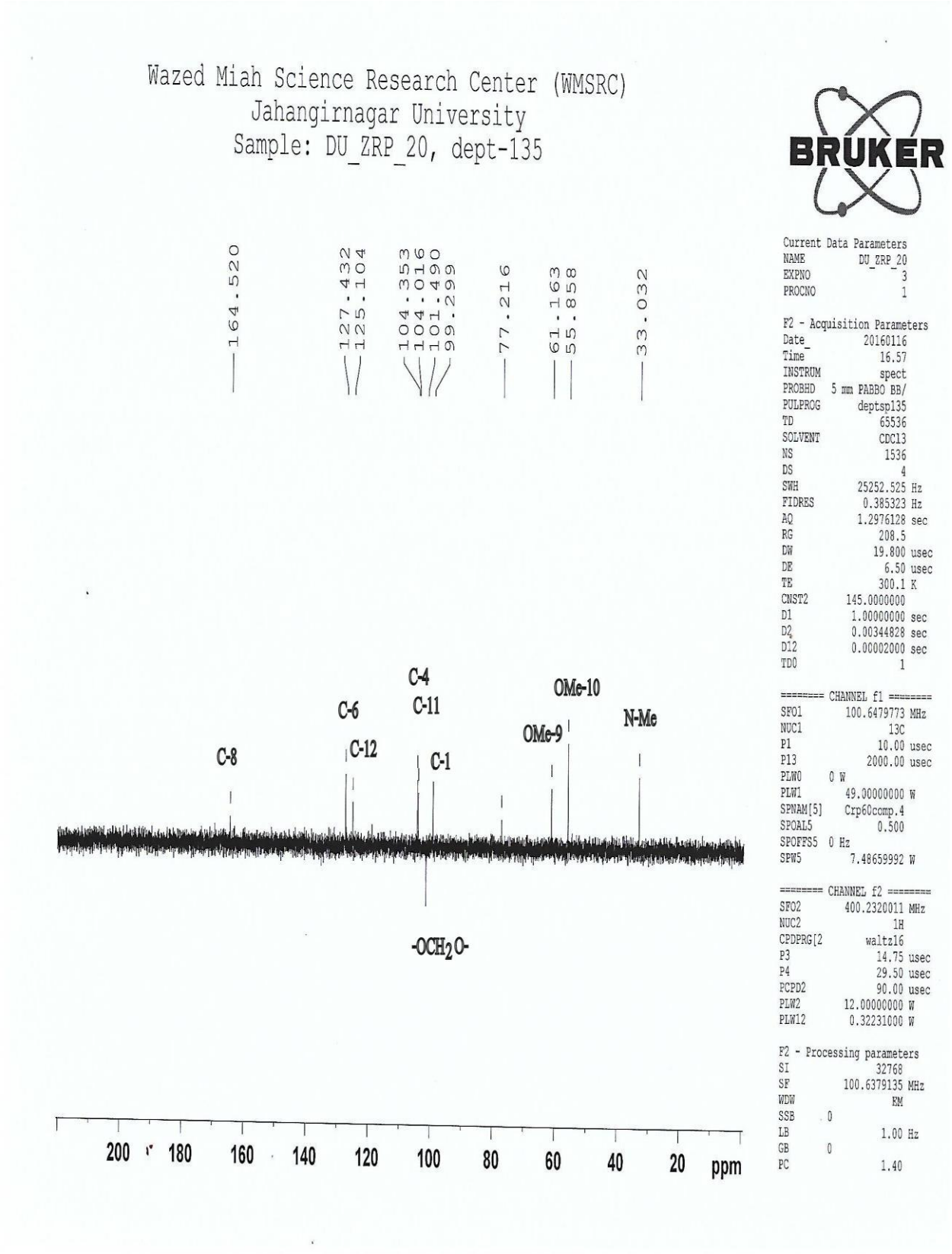
S19 : Partially expanded ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound 3 (Arnottianamide).



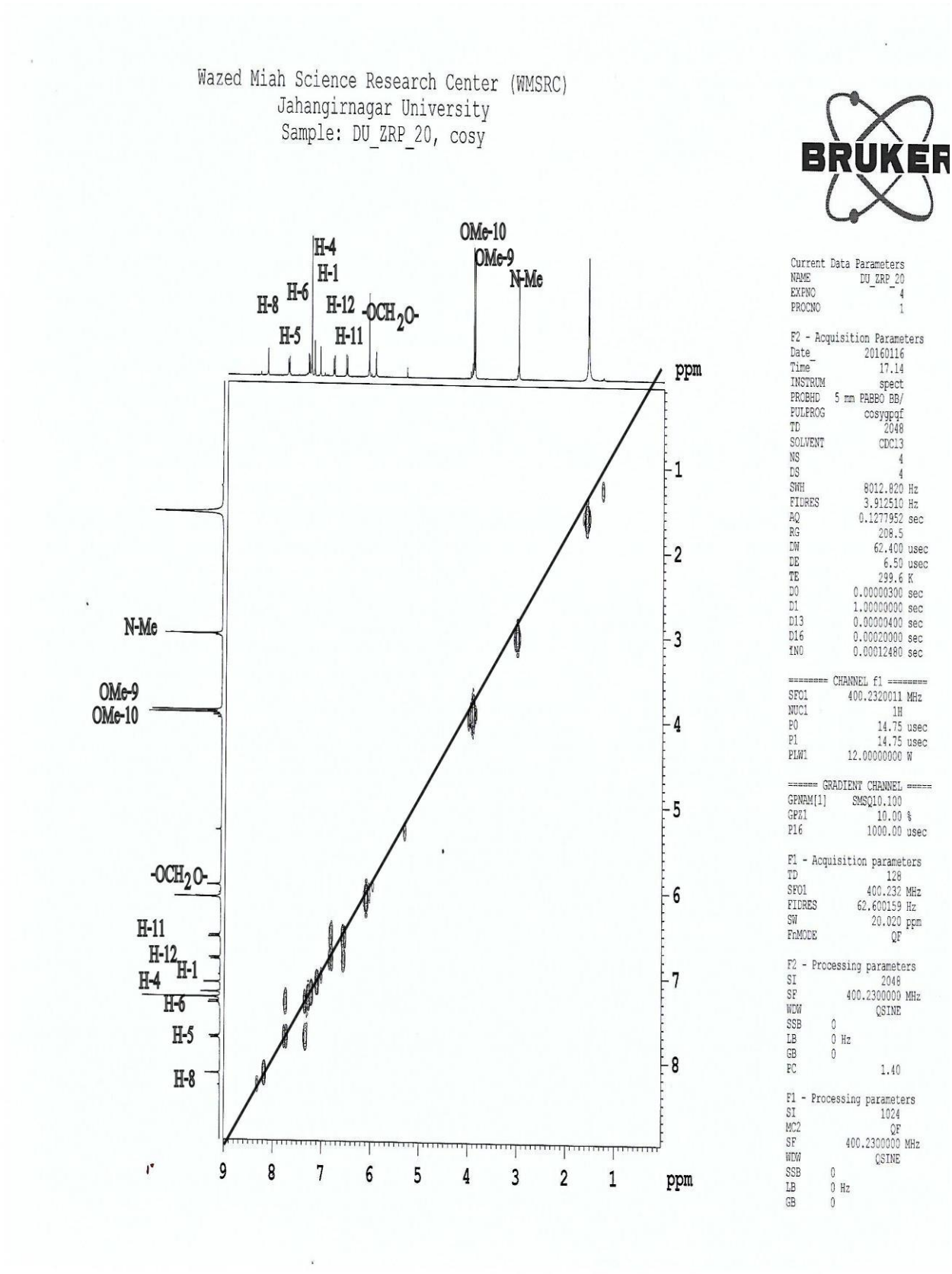
S20 : ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).



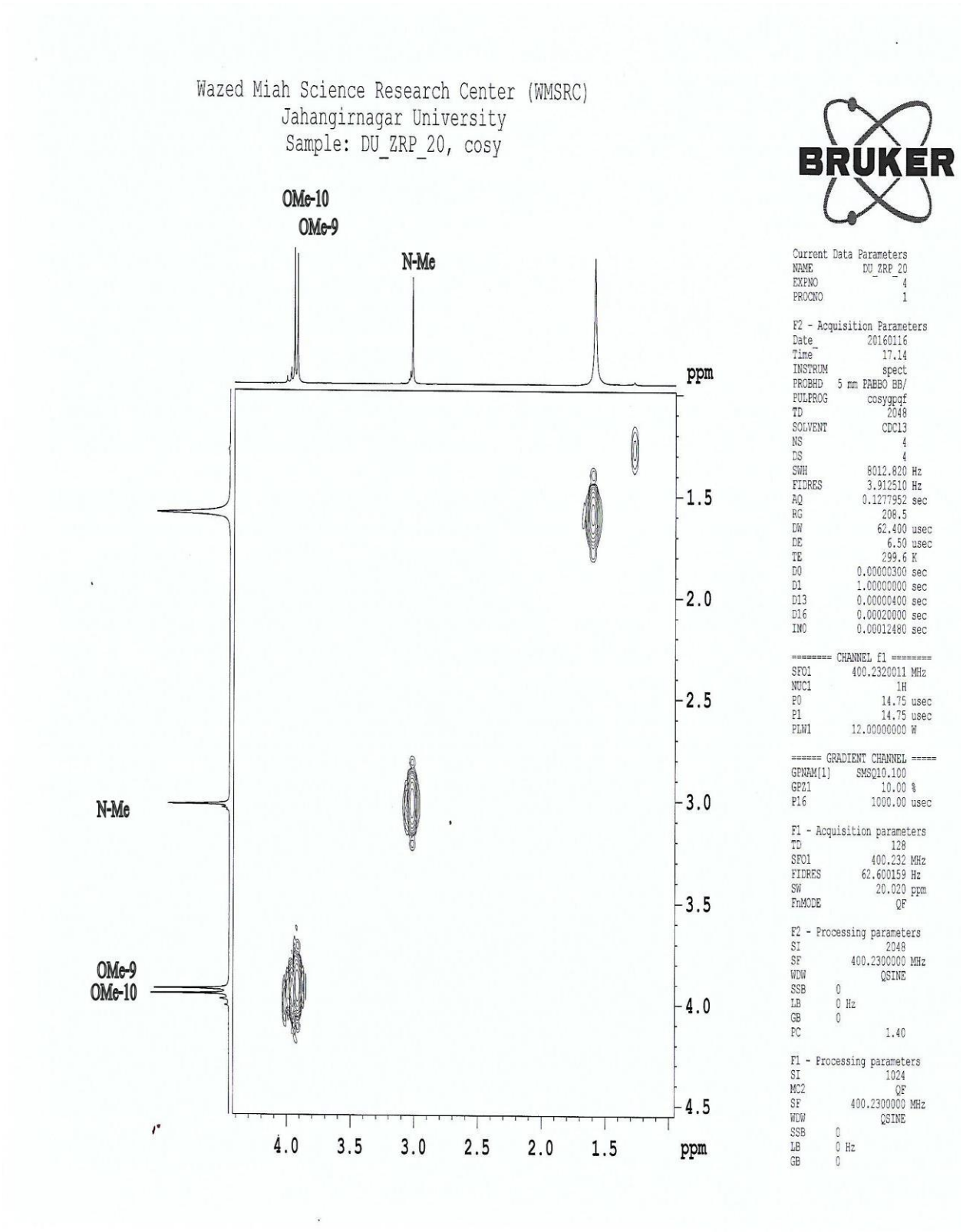
S21: Partially expanded ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).



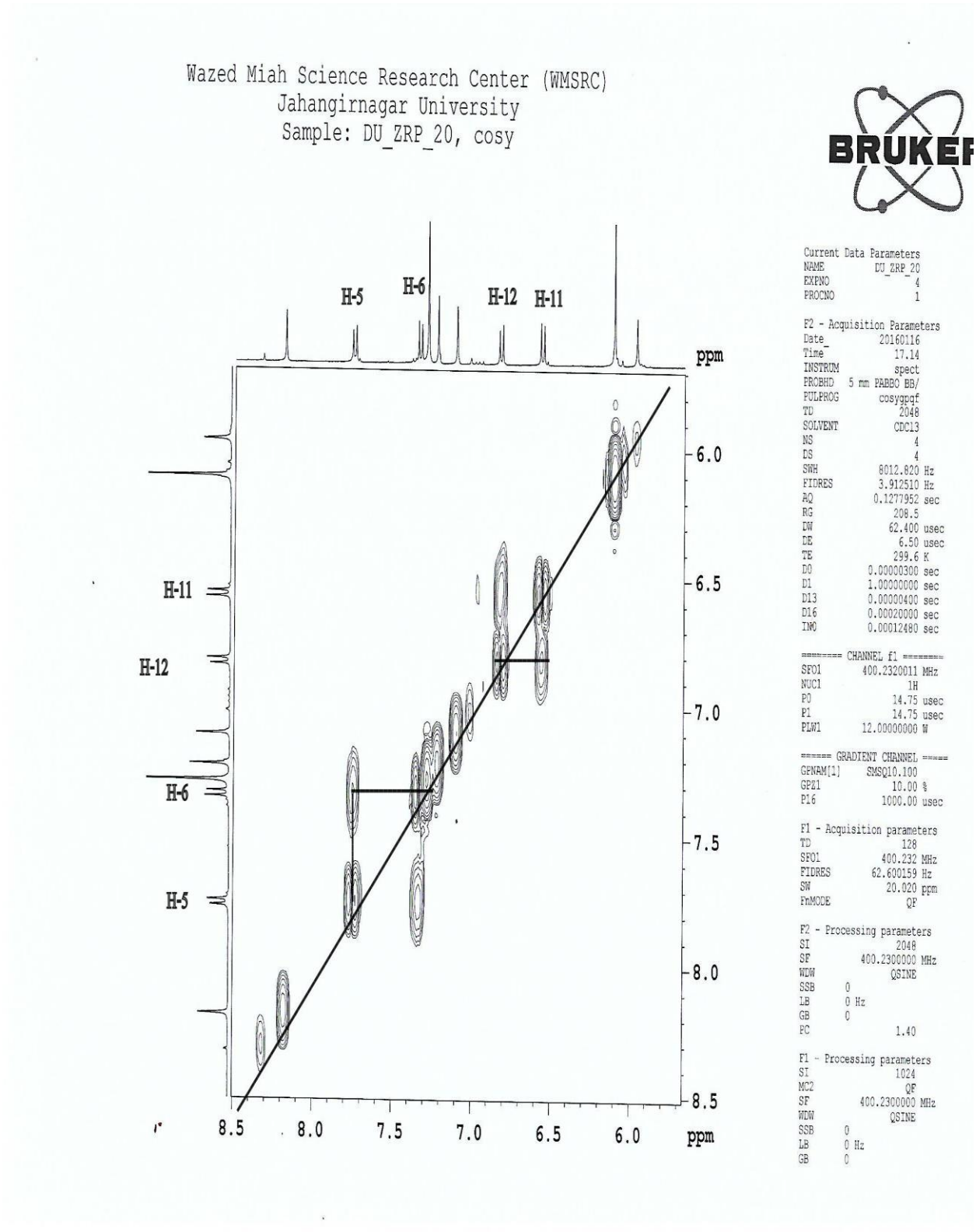
S22 : DEPT-135 NMR spectrum (100 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).



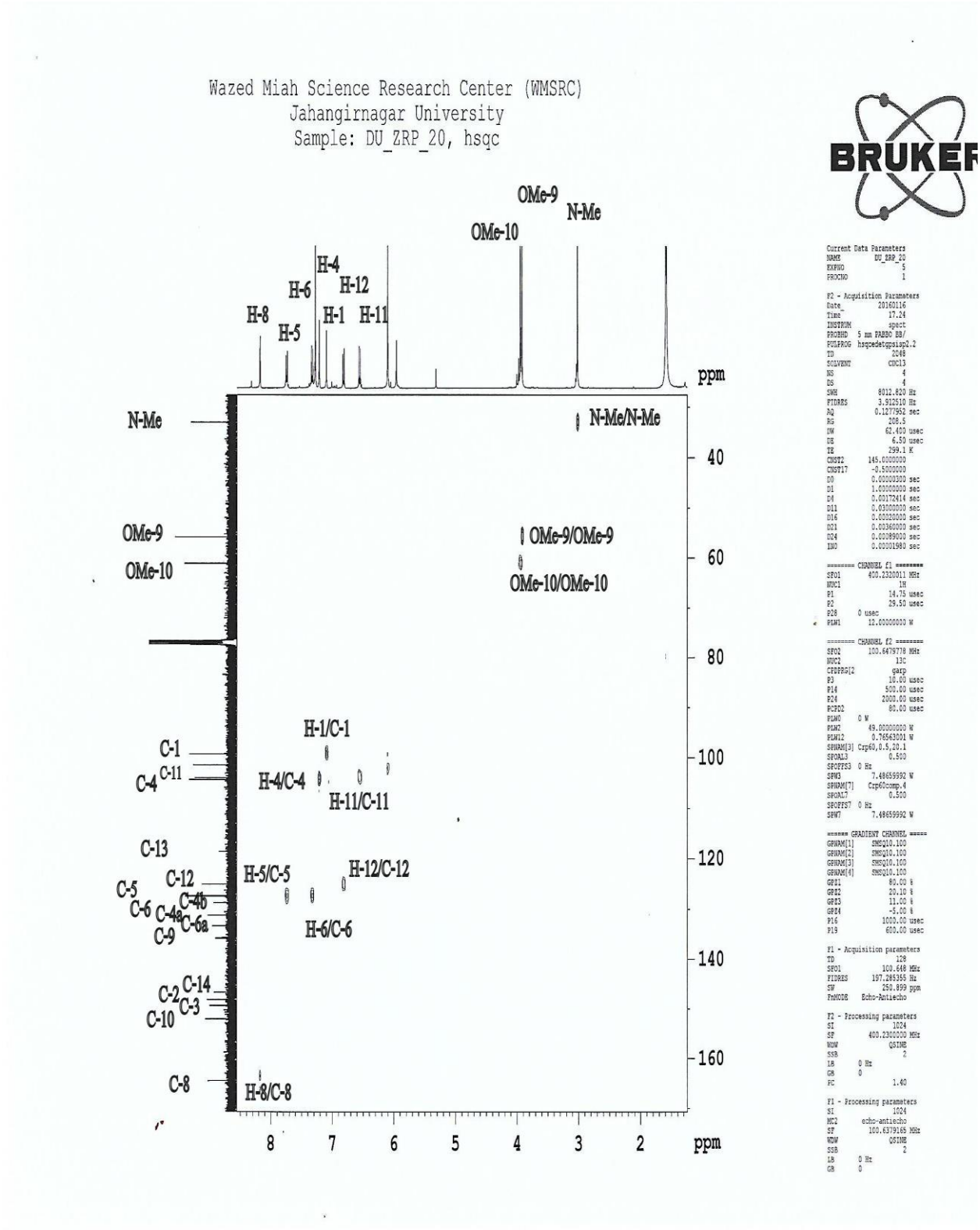
S23: COSY-NMR spectrum (400 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).



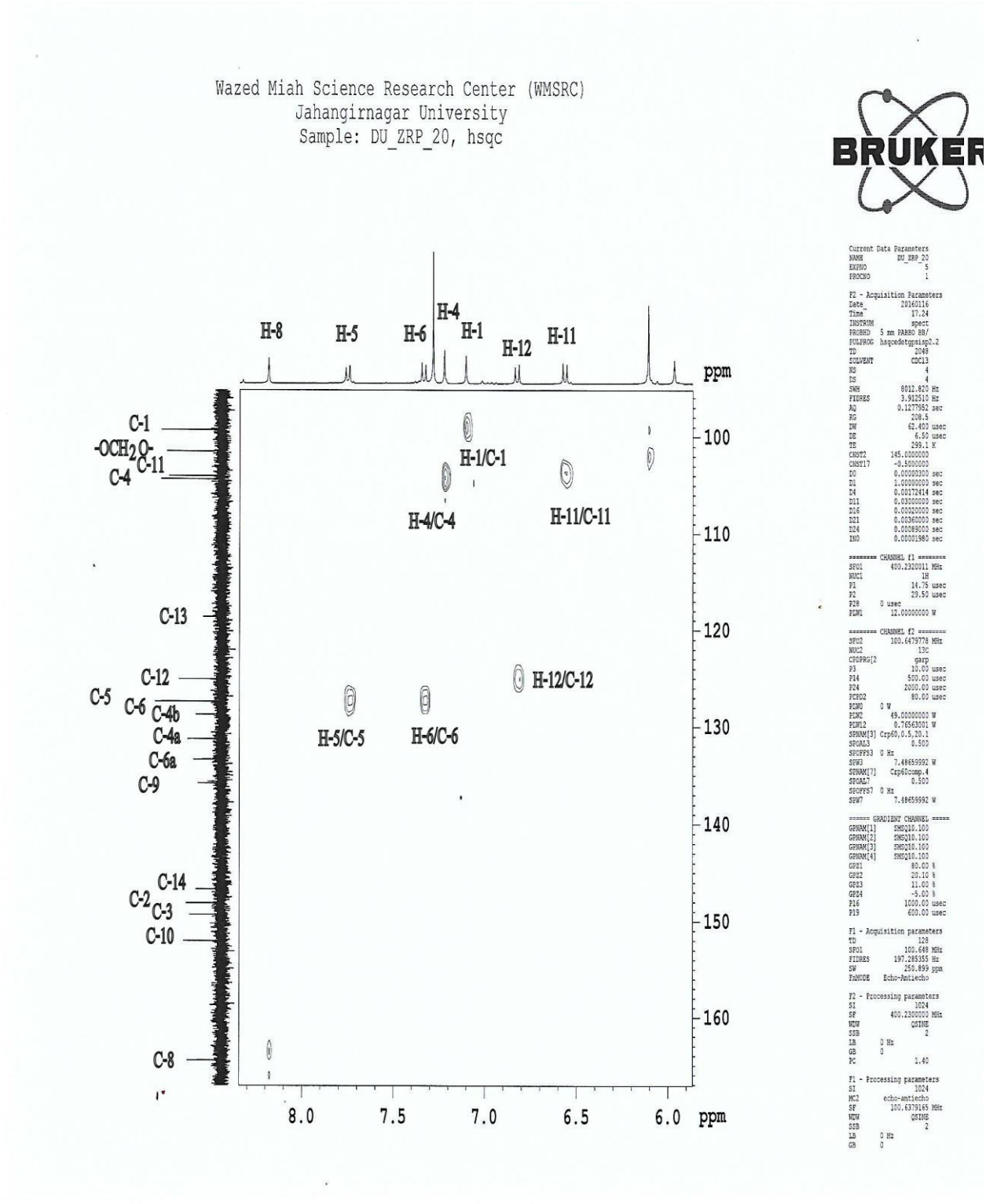
S24 : Partially expanded COSY- NMR spectrum (400 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).



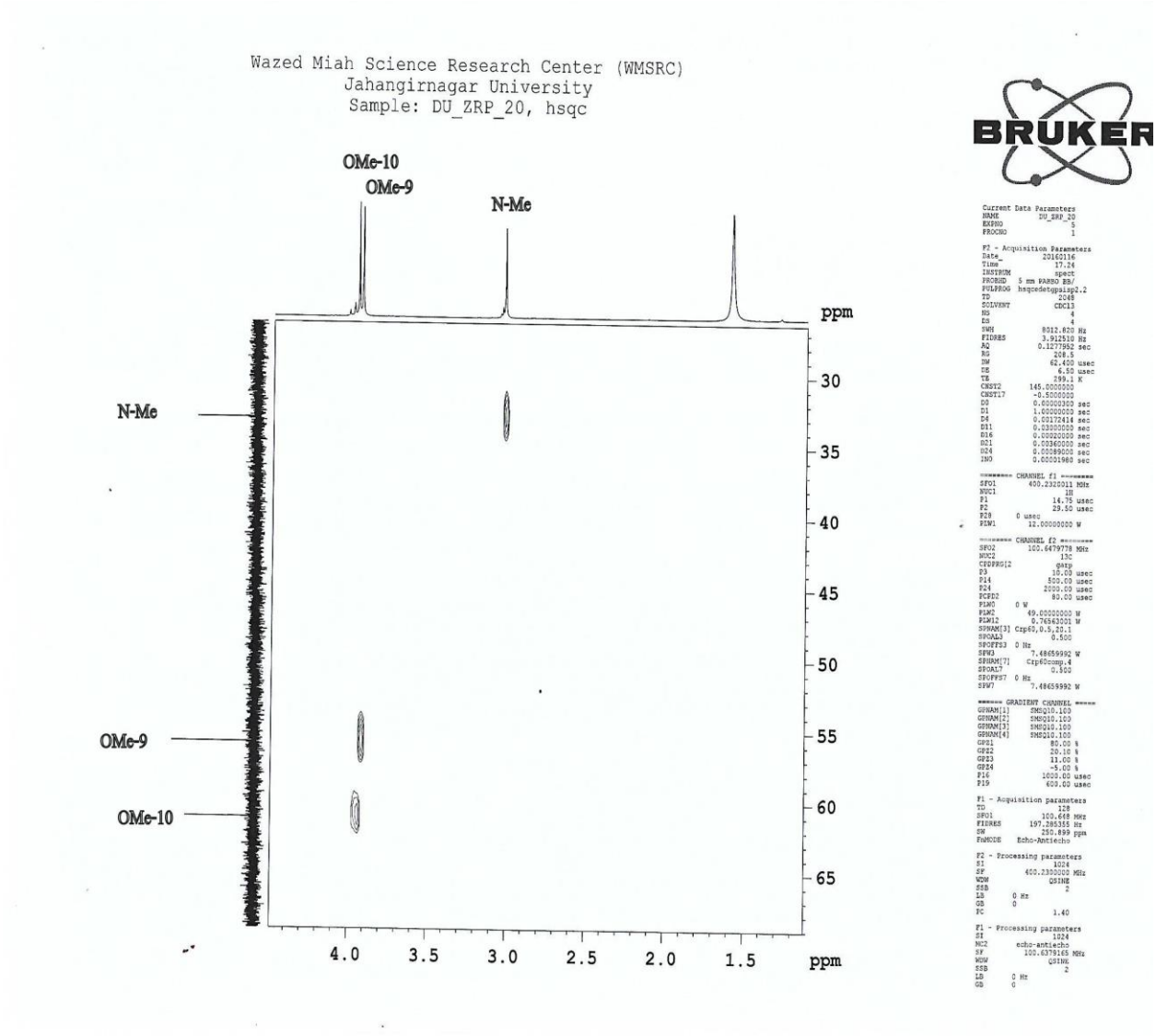
S25 : Partially expanded COSY- NMR spectrum (400 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).



S26 : HSQC- NMR spectrum (400 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).

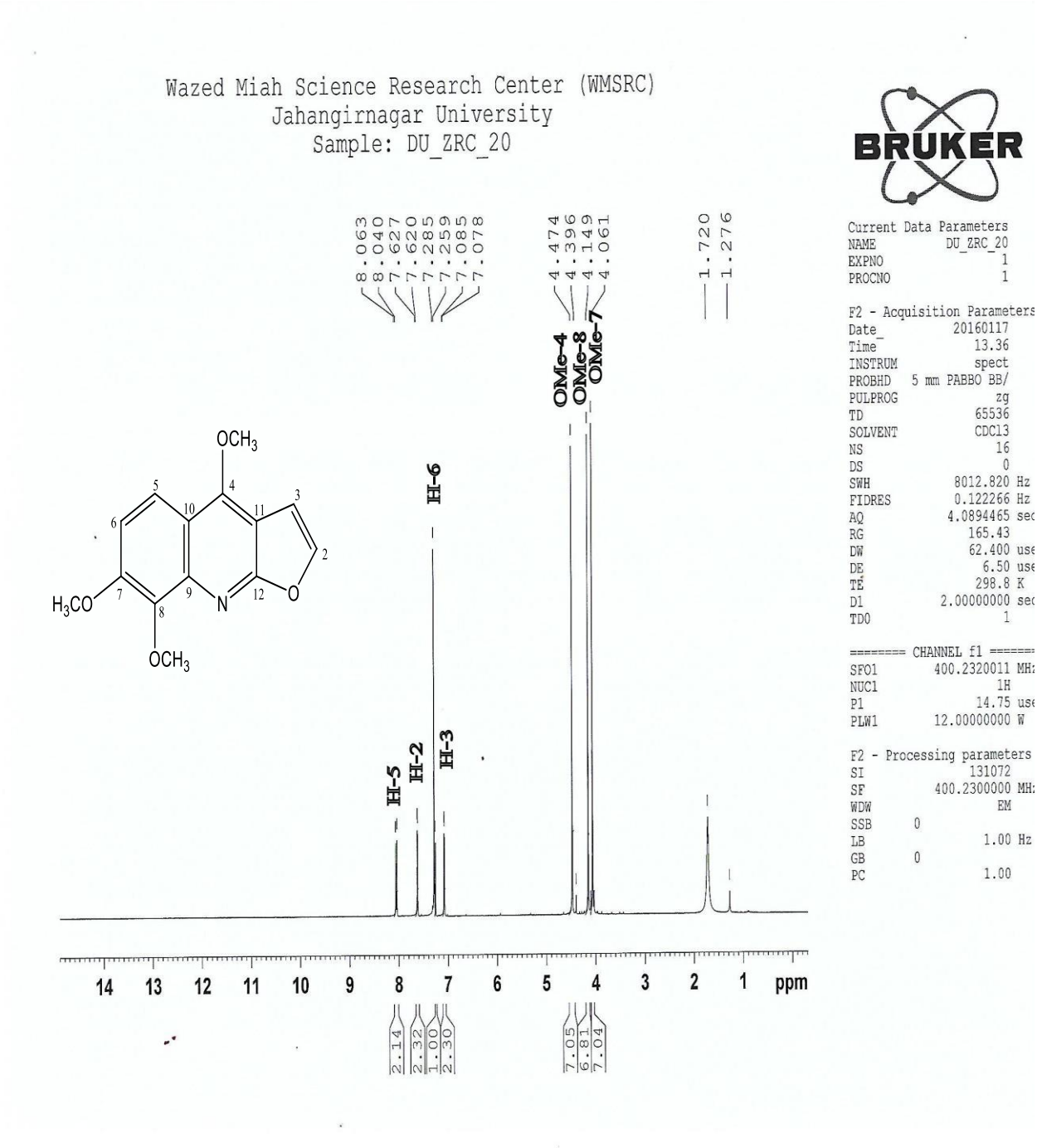


S27 : Partially expanded HSQC- NMR spectrum (400 MHz, $CDCl_3$) of Compound **3** (Arnottianamide).

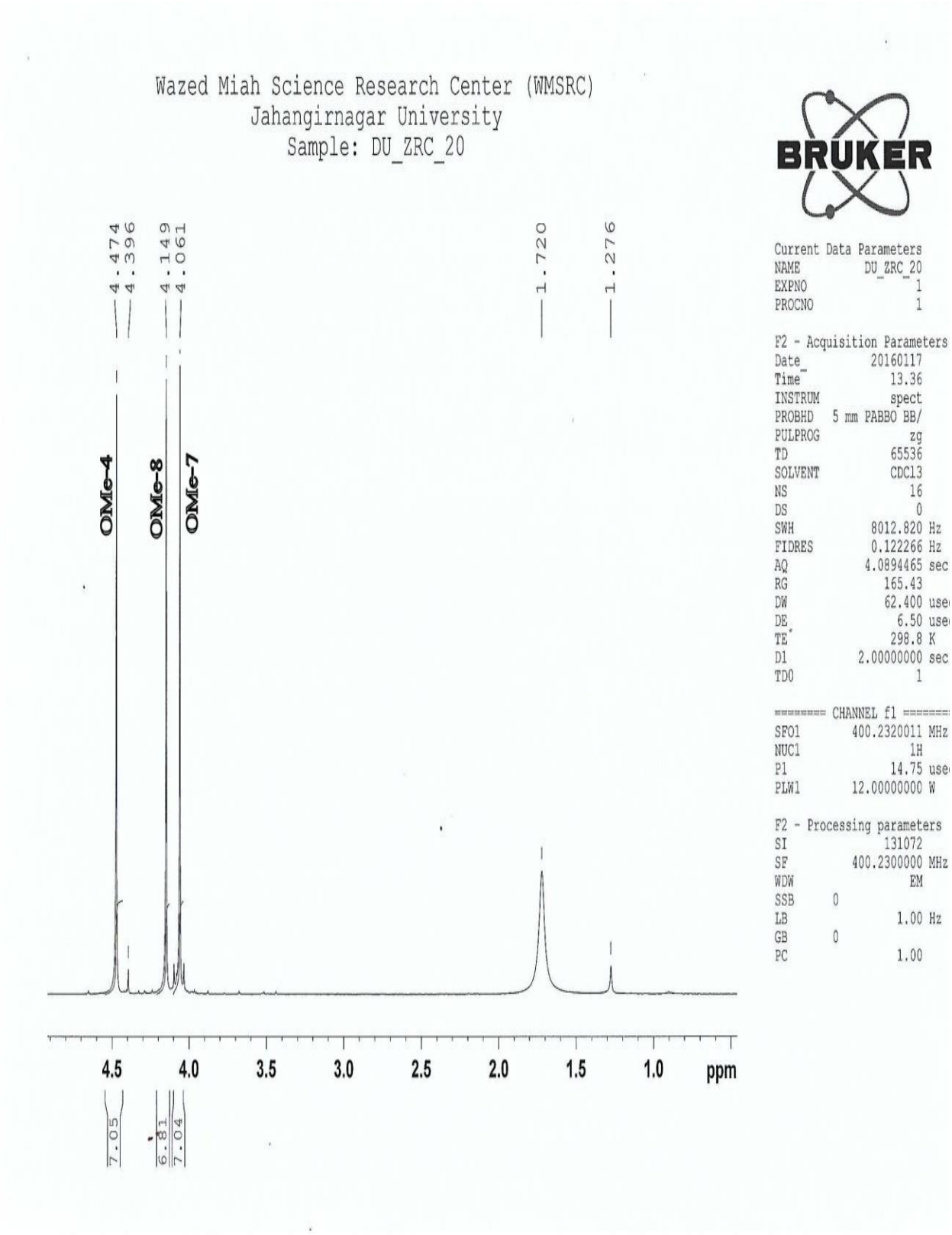


S28: Partially expanded HSQC- NMR spectrum (400 MHz, $CDCl_3$) of Compound 3 (Arnottianamide).

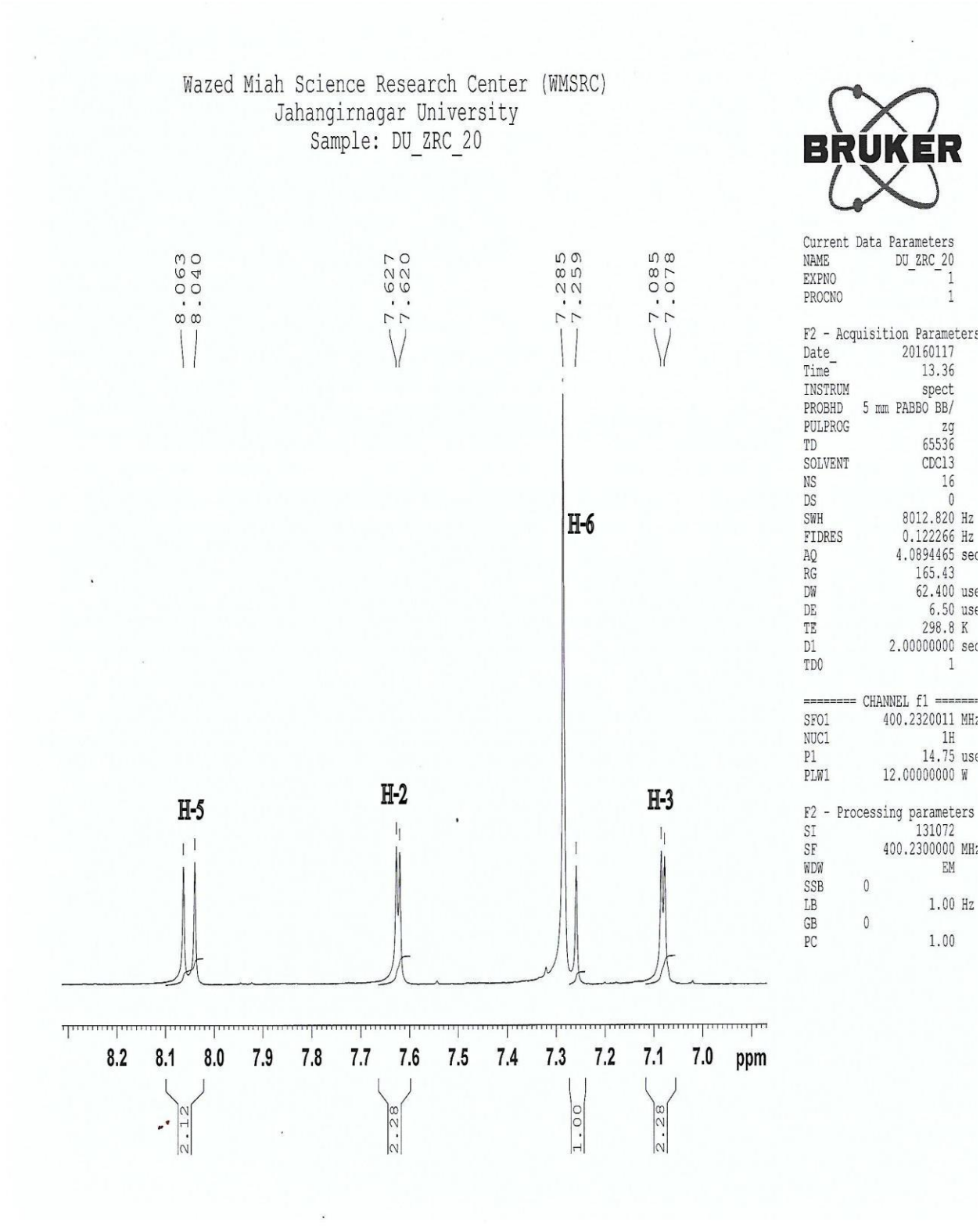
*Arnottianamide (**3**)*: white amorphous; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.18 (1H, s, H-8), 7.75 (1H, d, *J*= 8.4 Hz, H-5), 7.33 (1H, d, *J*= 8.4 Hz, H-6), 7.22 (1H, s, H-4), 7.11 (1H, s, H-1), 6.83 (1H, d, *J*= 8.4 Hz, H-12), 6.57 (1H, d, *J*= 8.4 Hz, H-11), 6.11 (2H, s, OCH_2O), 3.95 (3H, s, OMe-10), 3.93 (3H, s, OMe-9), 3.02 (3H, s, N-Me). ^{13}C-NMR (125 MHz, $CDCl_3$): δ 164.5 (C-8), 152.1 (C-10), 149.3 (C-3), 148.2 (C-2), 146.7 (C-14), 135.8 (C-6b, 9), 133.4 (C-6a), 131.3 (C-4a), 128.8 (C-4b), 127.4 (C-5, 6), 125.1 (C-12), 118.6 (C-13), 104.4 (C-4), 104.0 (C-11), 101.5 (OCH_2O), 99.3 (C-1), 61.2 (OMe-10), 55.9 (OMe-9), 33.0 (N-Me).



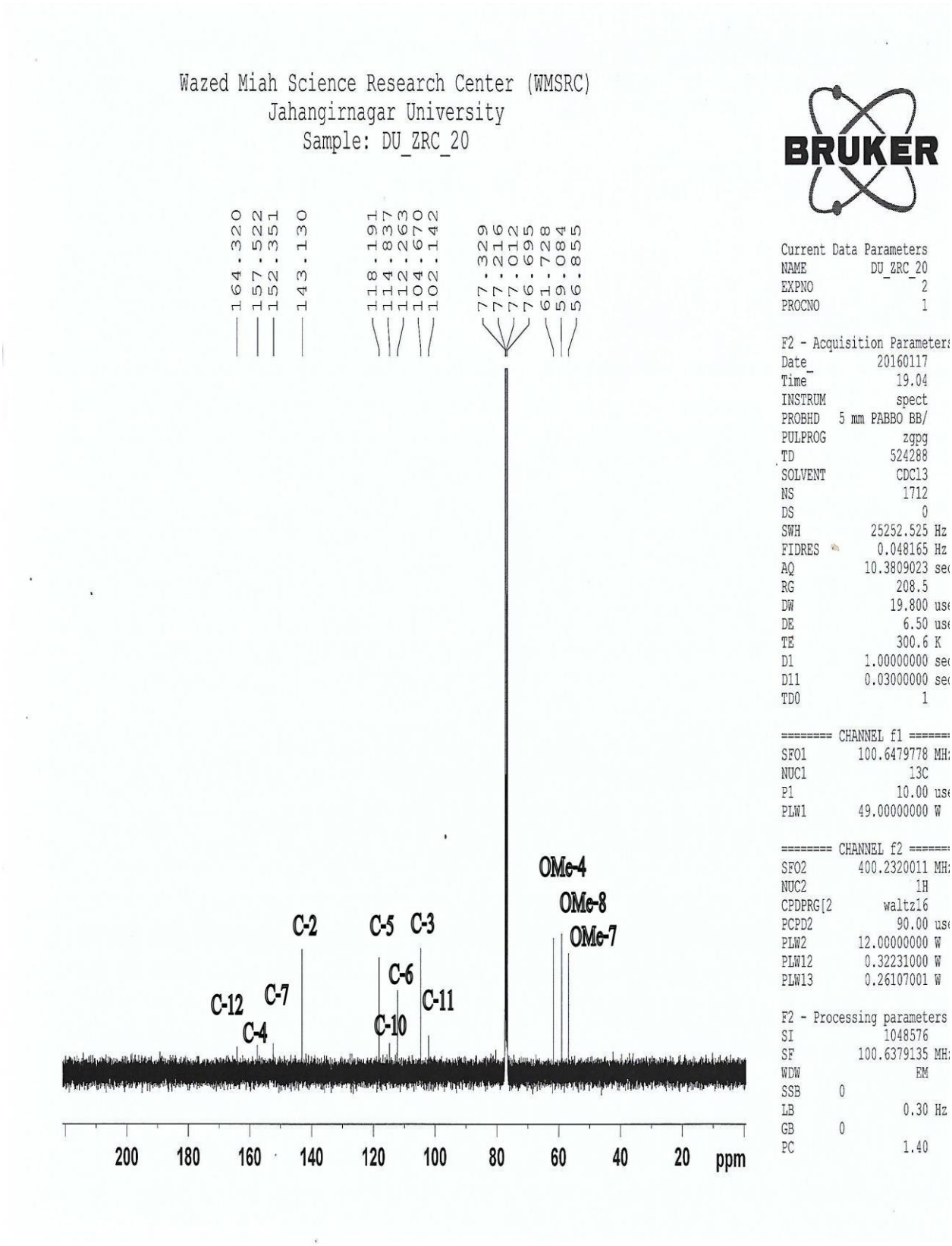
S29: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



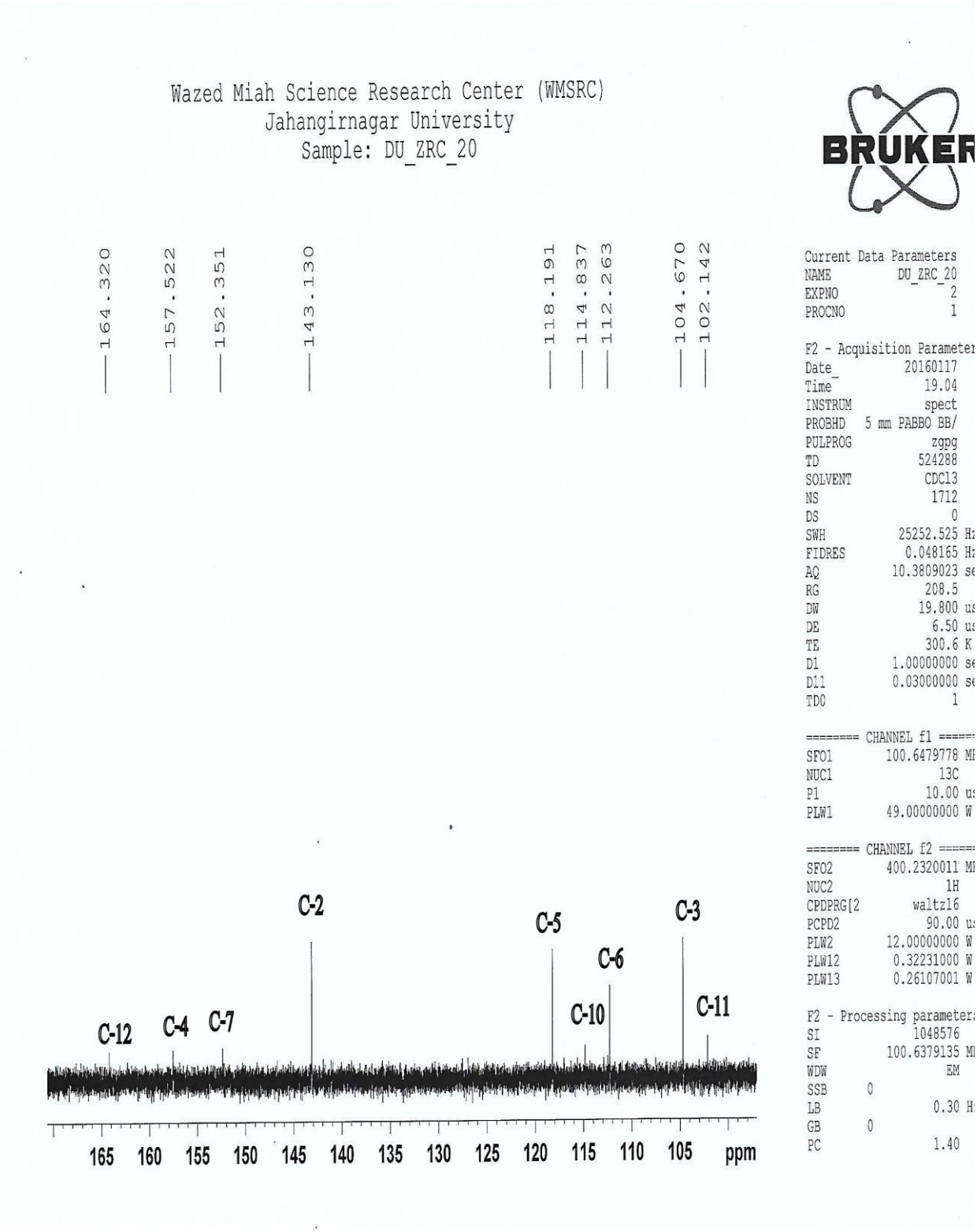
S30: Partially expanded ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



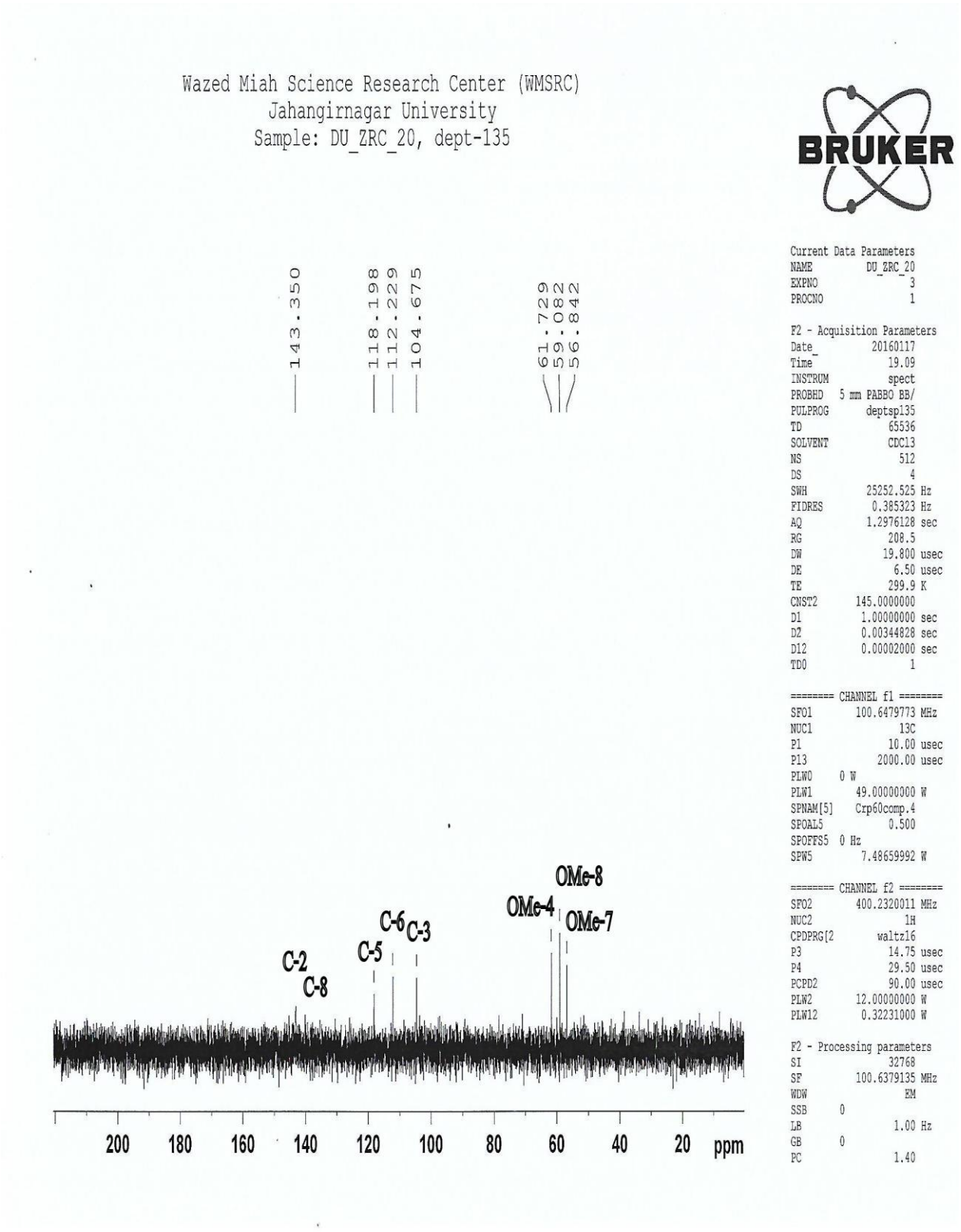
S31: Partially expanded ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine)



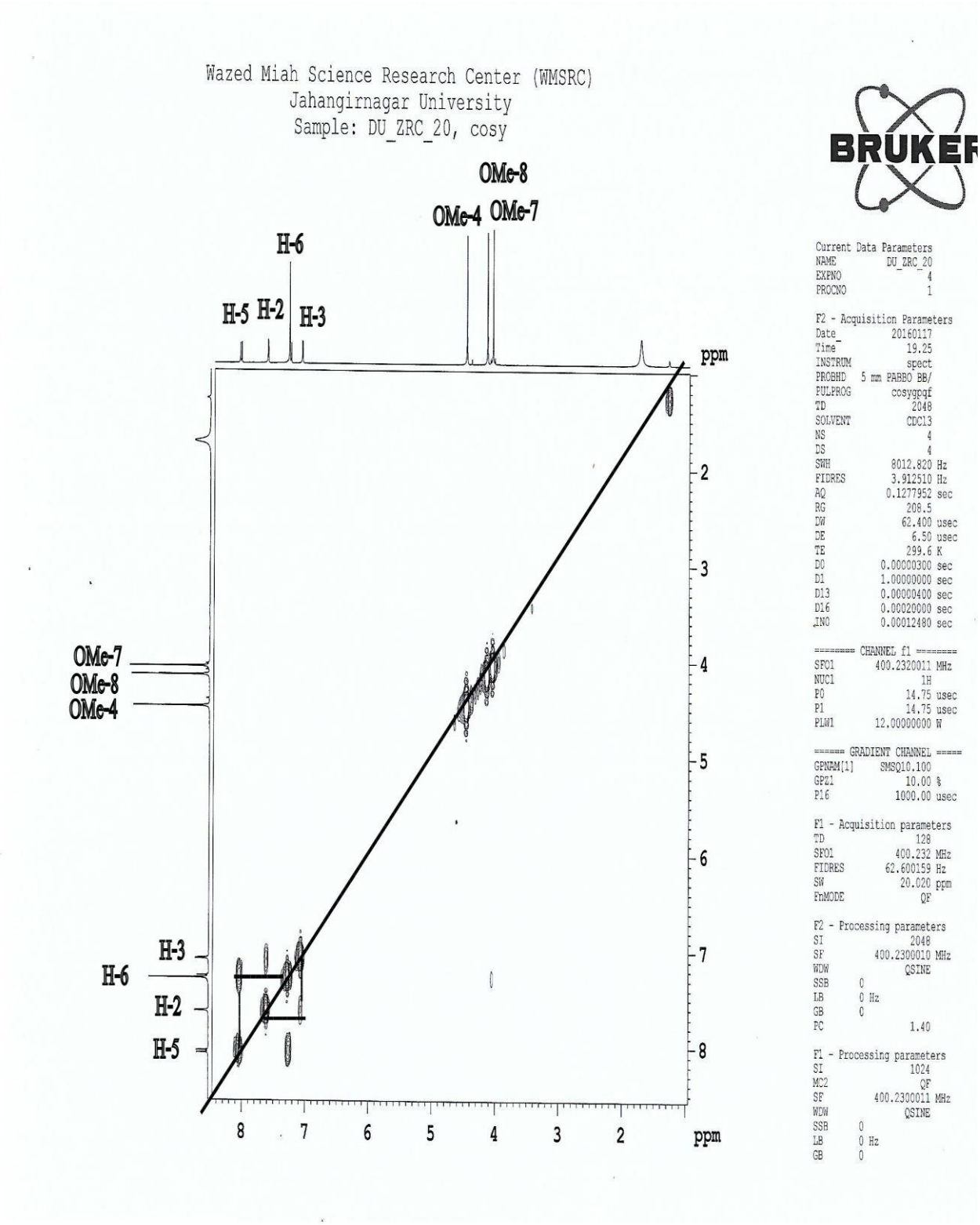
S32: ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine)



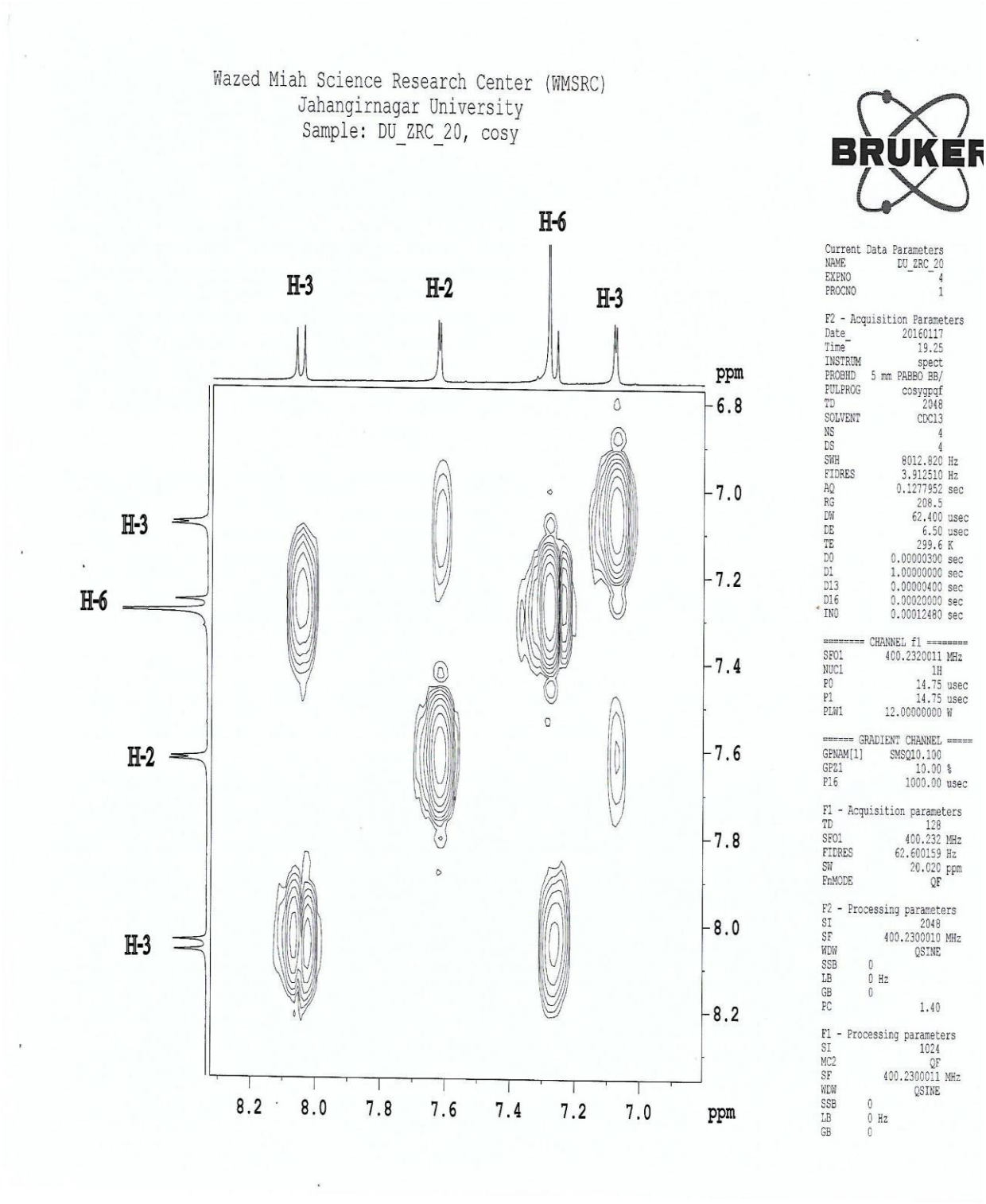
S33: Partially expanded ^{13}C NMR (100 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



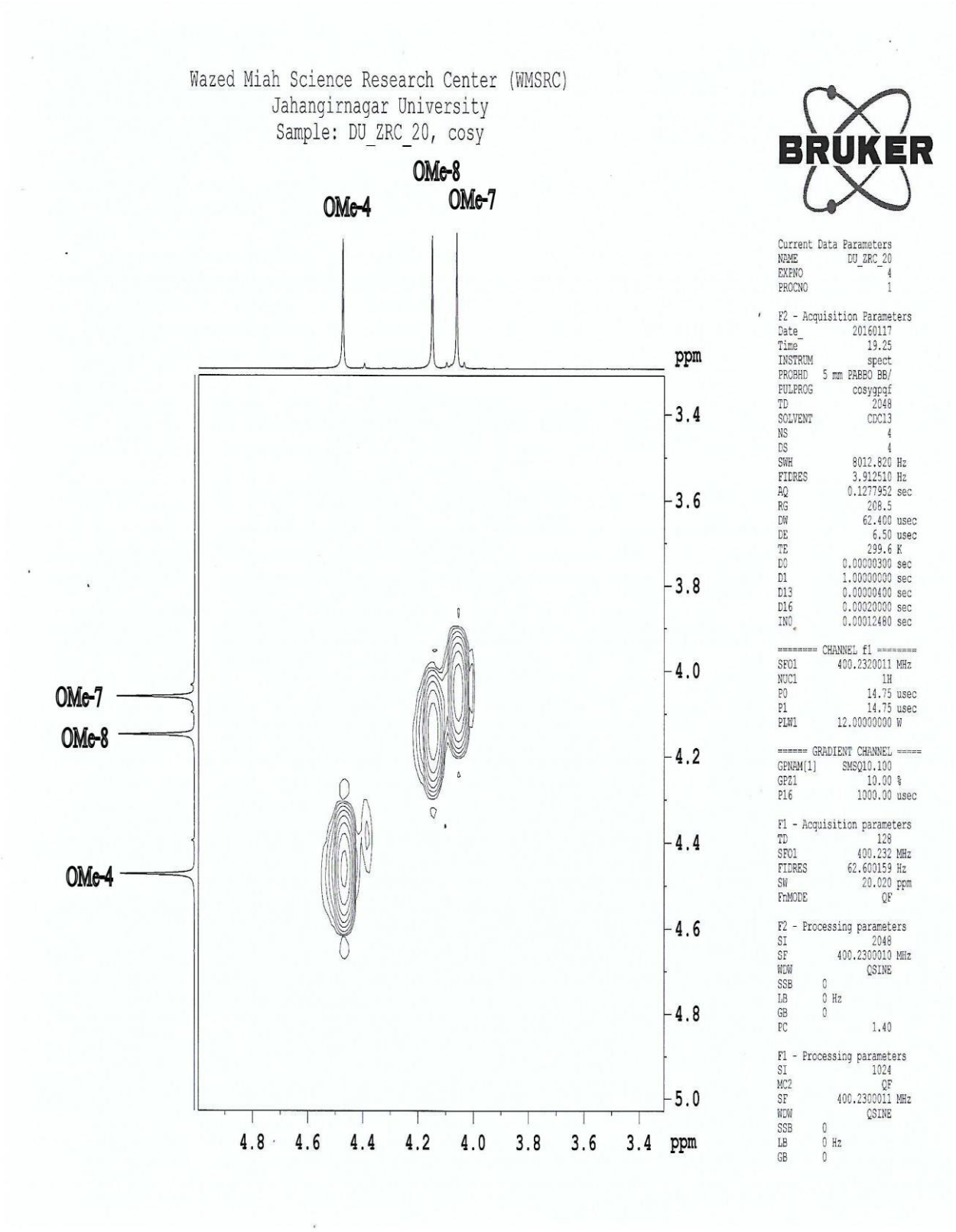
S34 : DEPT-135 NMR (100 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



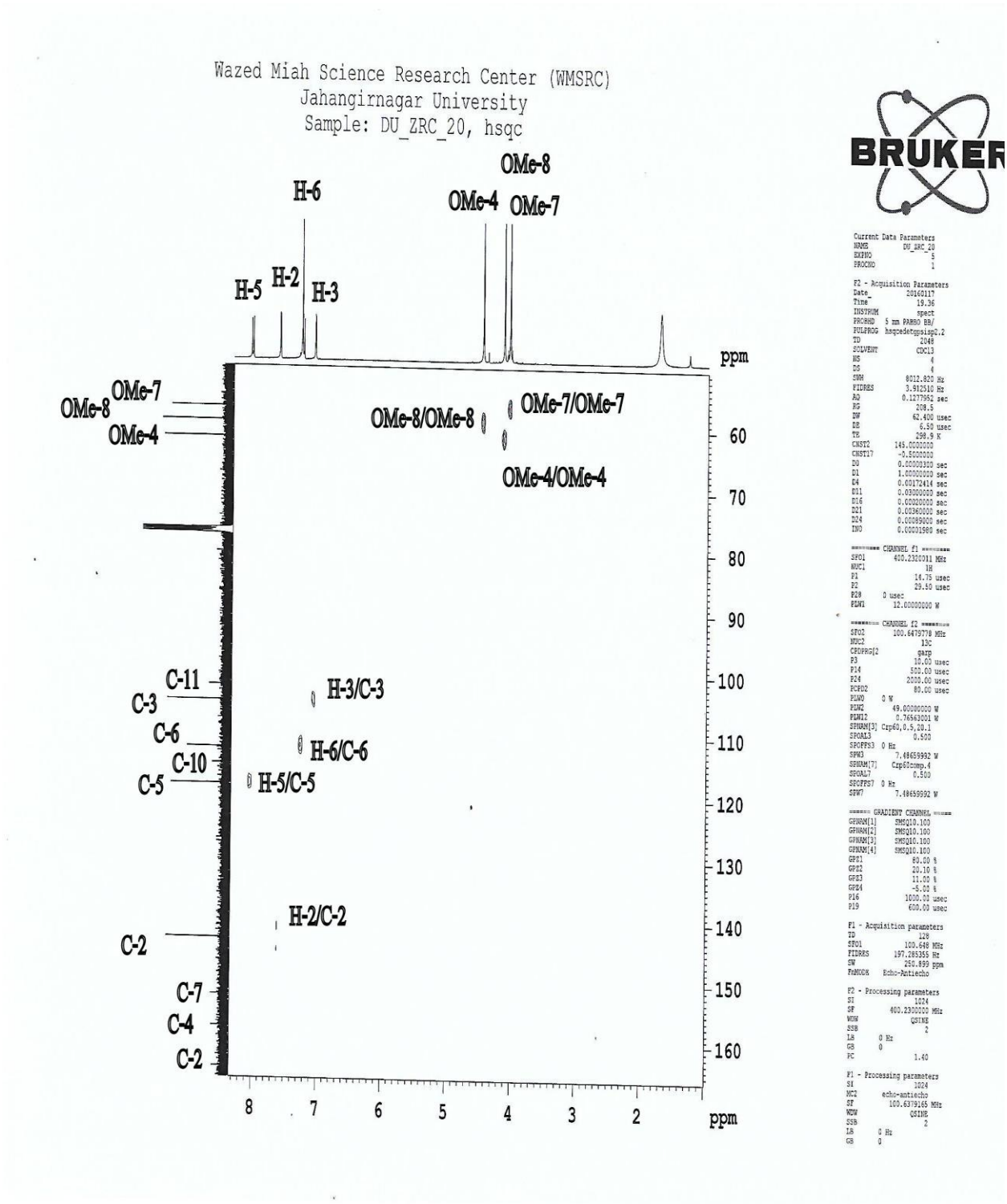
S35 : COSY-NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



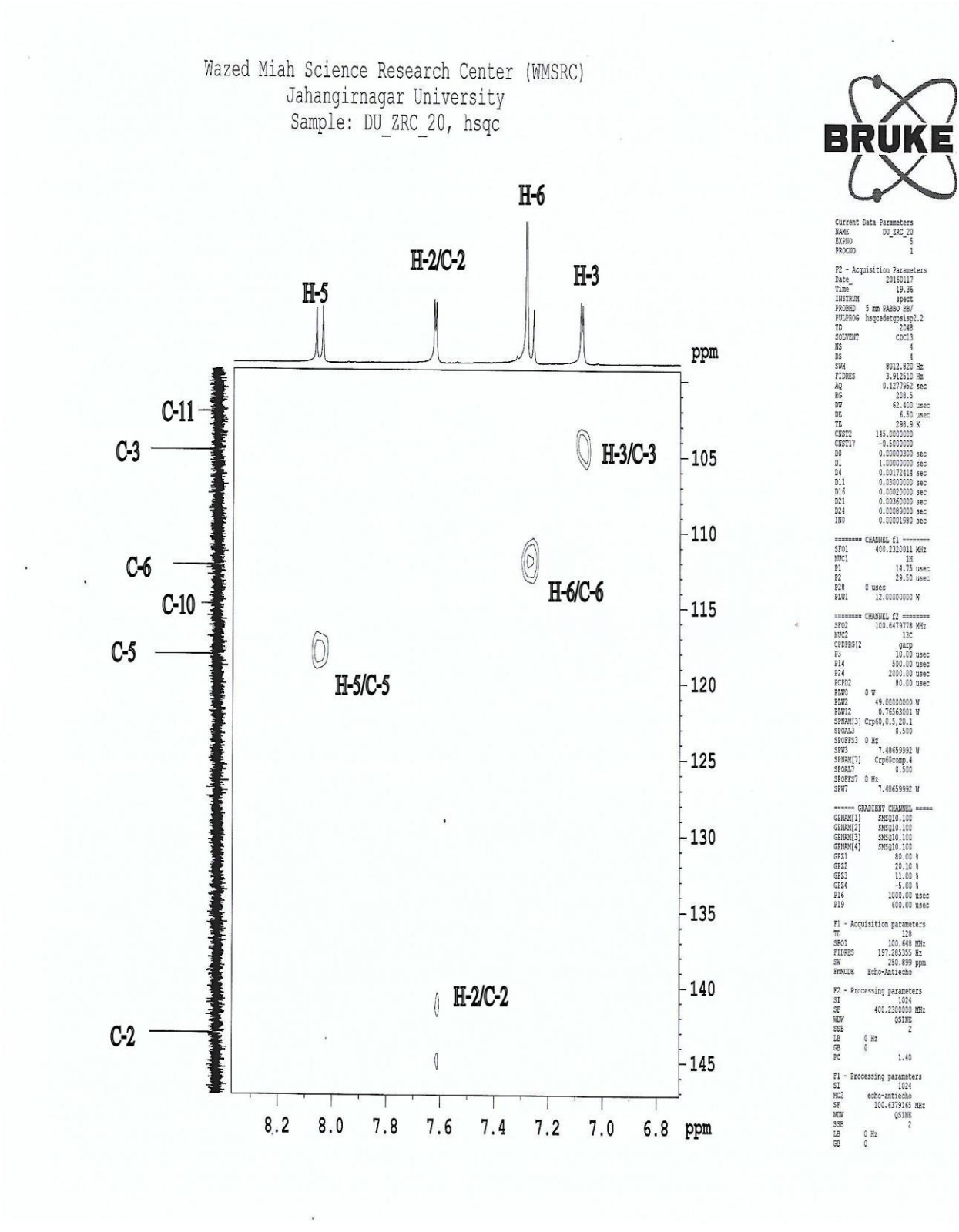
S36 : Partially expanded COSY-NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



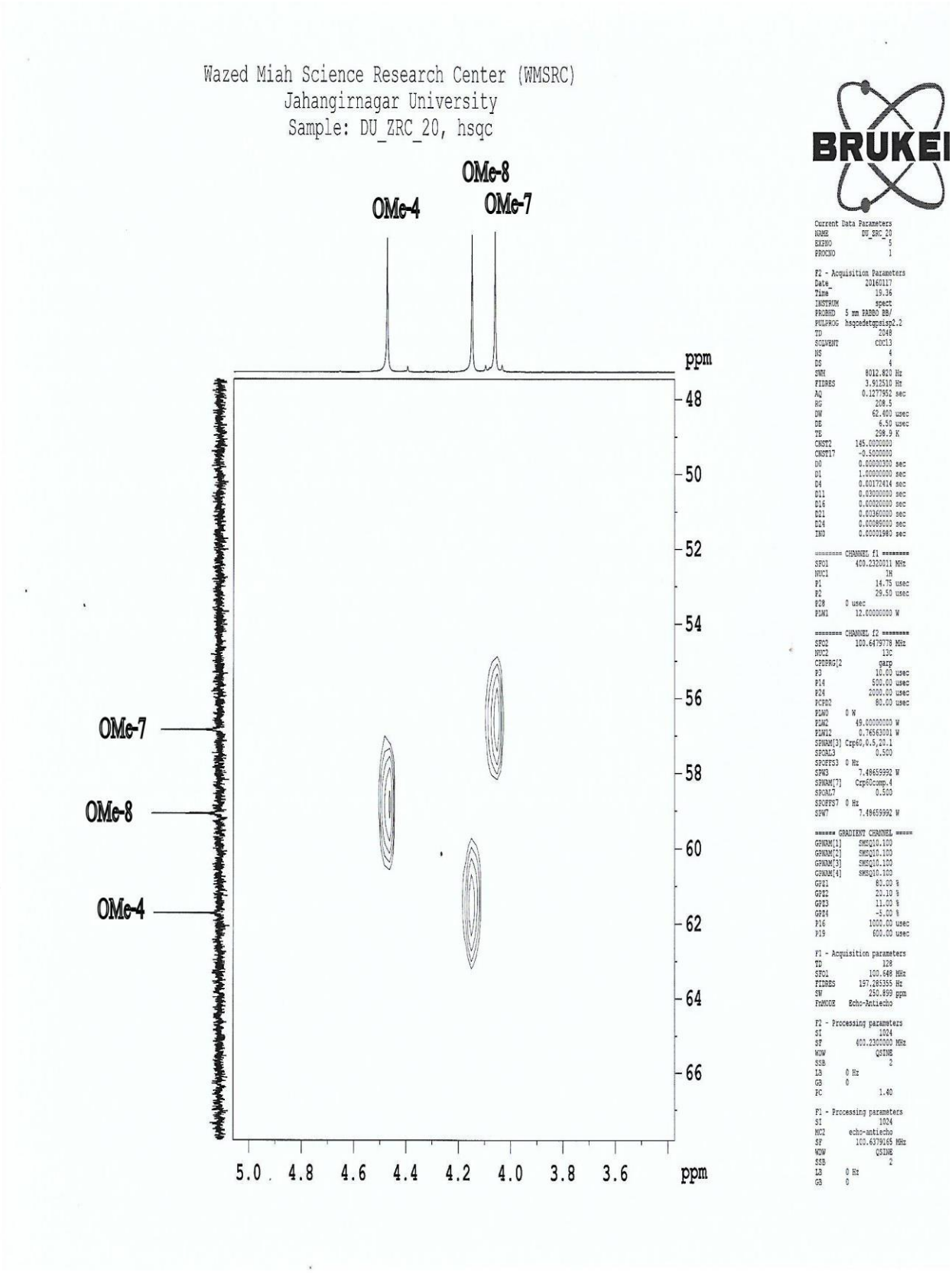
S37 : Partially expanded COSY-NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine)



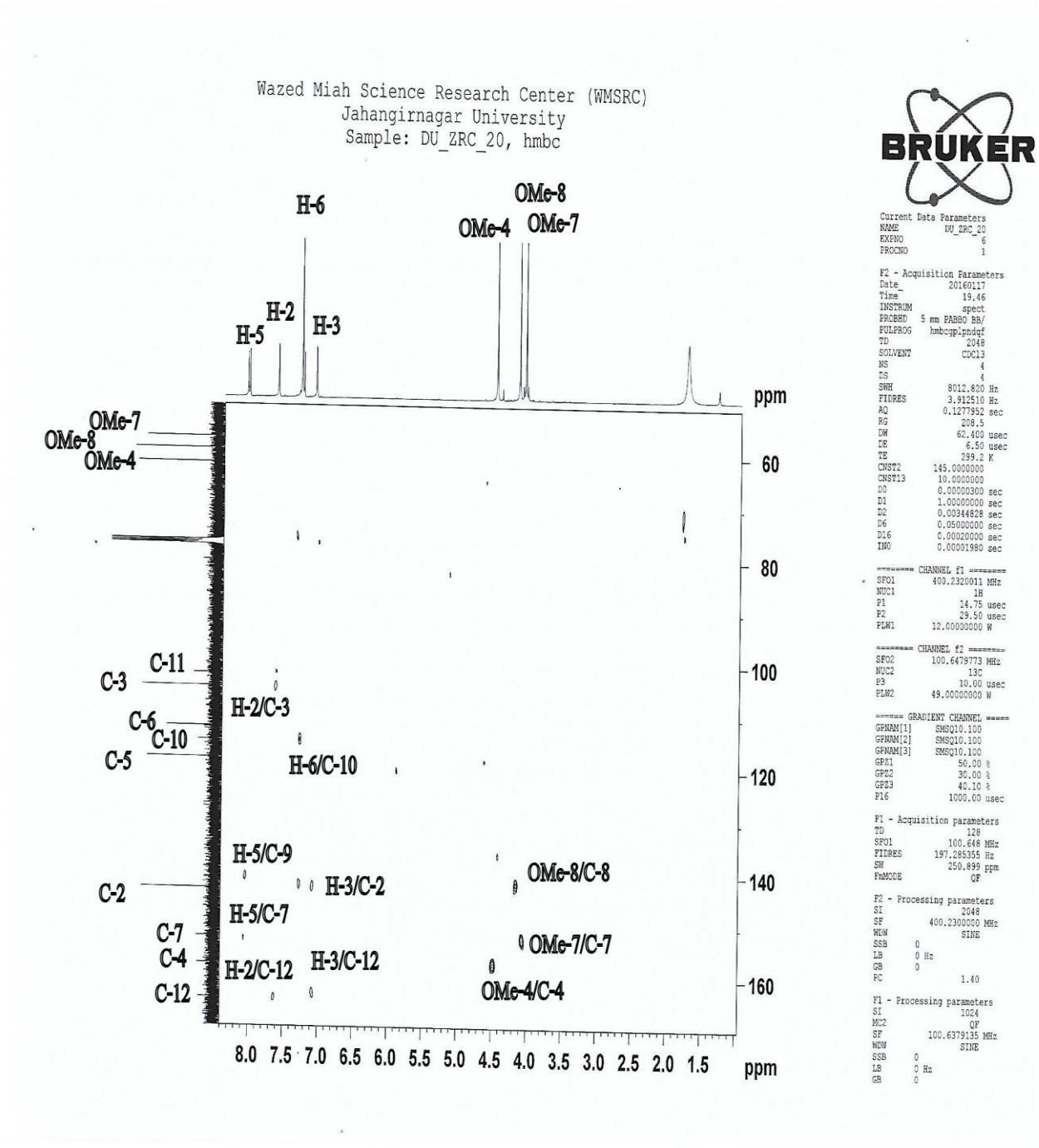
S38: HSQC-NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).



S39: Partially expanded HSQC-NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine).

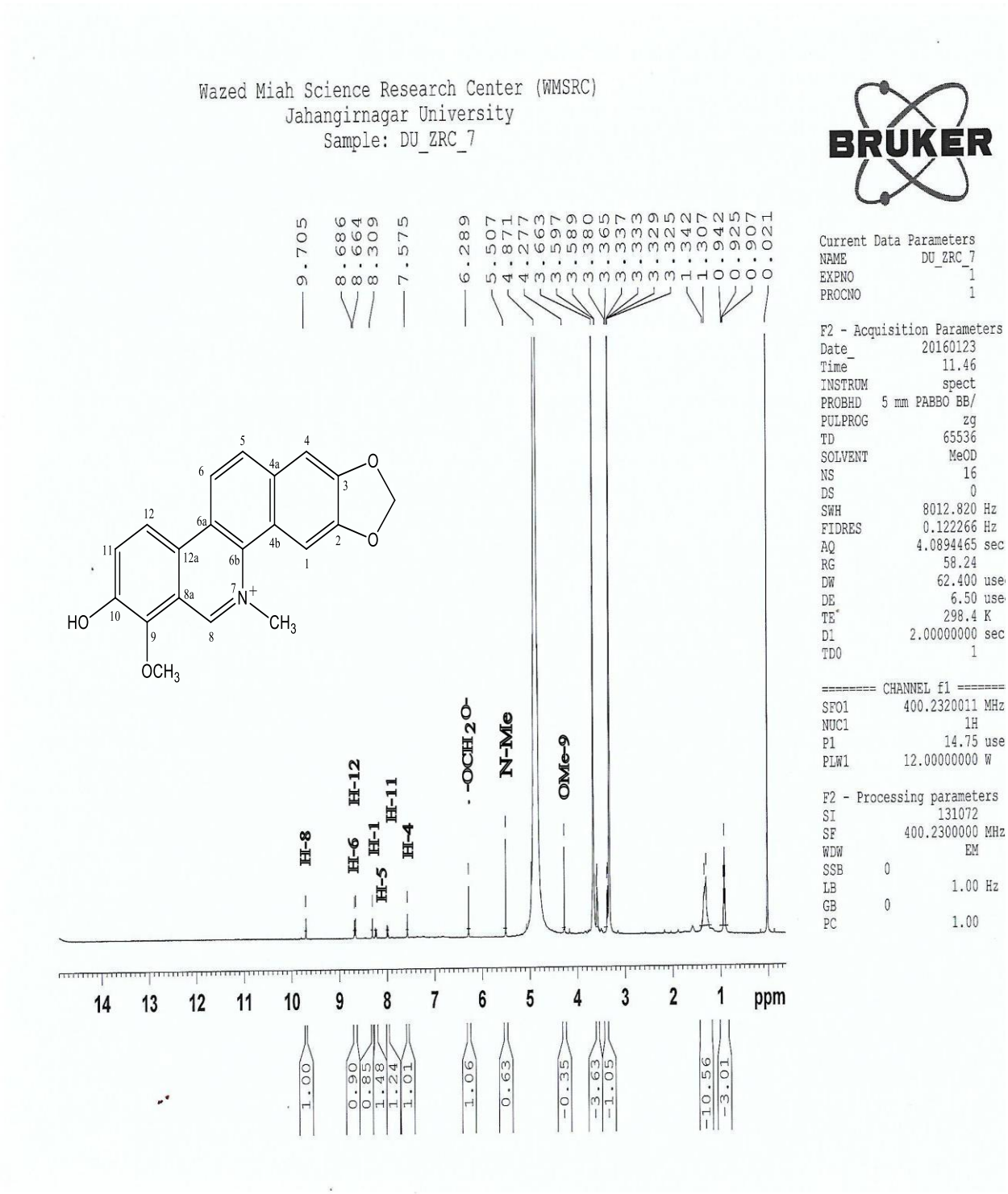


S40: Partially expanded HSQC-NMR (400 MHz, $CDCl_3$) spectrum of Compound **4** (Skimmianine)

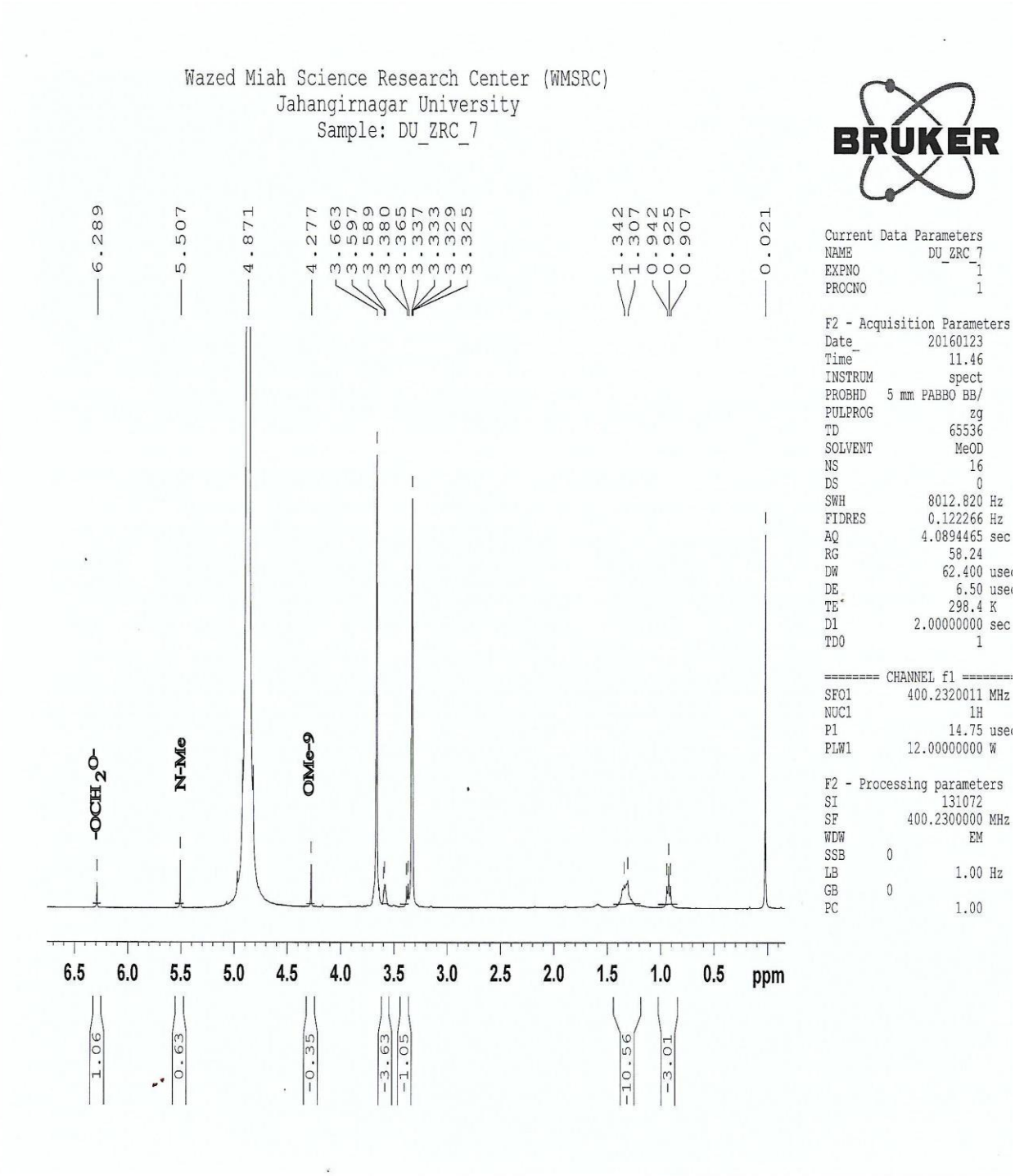


S41: HMBC-NMR (400 MHz, $CDCl_3$) spectrum of Compound 4 (Skimmianine)

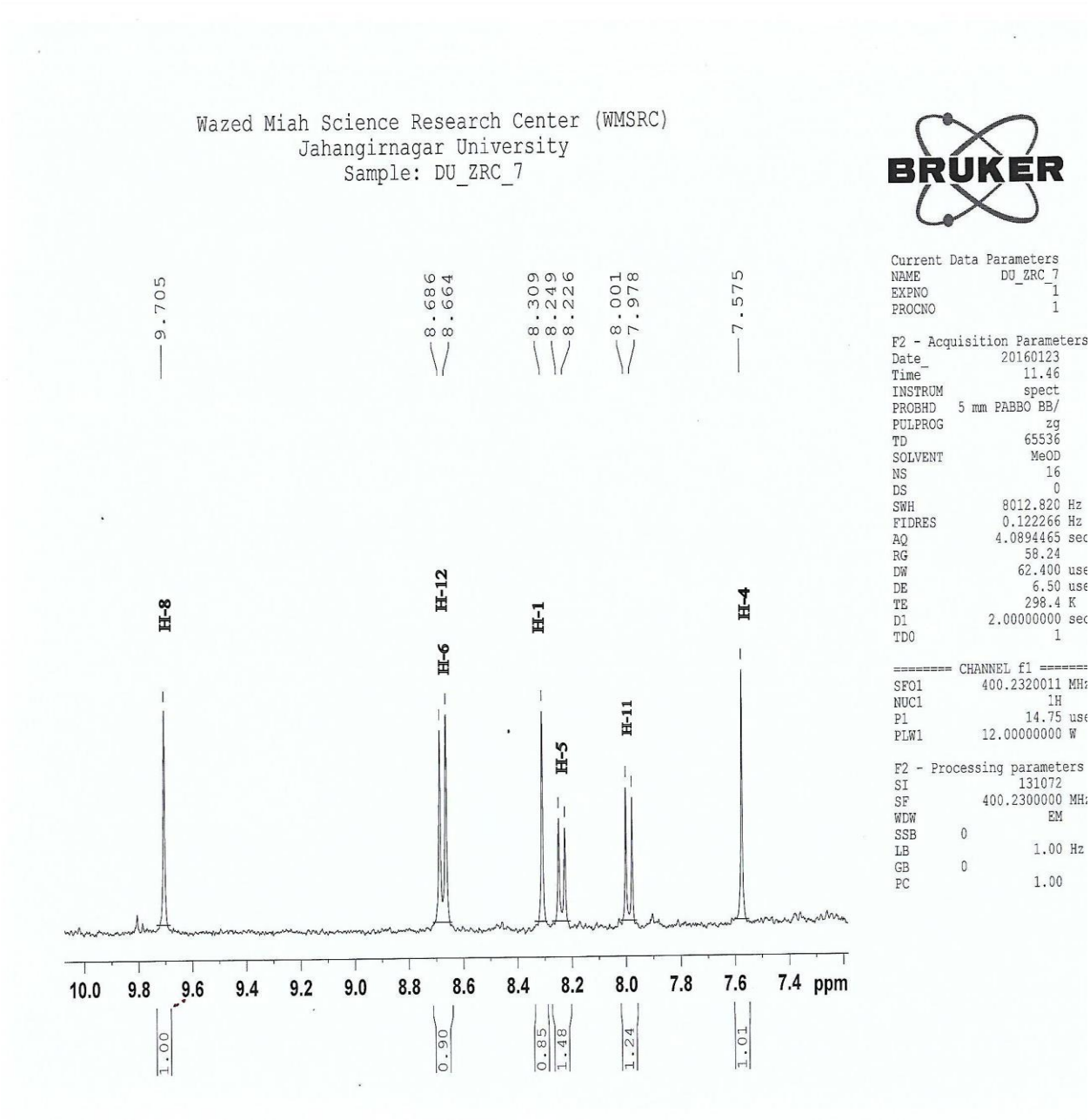
Skimmianine (**4**): colourless crystals; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.05 (1H, d, *J*= 9.2 Hz, H-5), 7.62 (1H, d, *J*= 2.8 Hz, H-2), 7.27 (1H, d, *J*= 9.2 Hz, H-6), 7.08 (1H, d, *J*= 2.8 Hz, H-3), 4.47 (3H, s, OMe-4), 4.15 (3H, s, OMe-8), 4.06 (3H, s, OMe-7). ^{13}C-NMR (125 MHz, $CDCl_3$): δ 164.3 (C-12), 157.5 (C-4), 152.4 (C-7), 143.1 (C-2), 142.0 (C-8), 141.5 (C-9), 118.2 (C-5), 114.8 (C-10), 112.3 (C-6), 104.7 (C-3), 102.1 (C-11), 61.7 (OMe-8), 59.1 (OMe-4), 56.9 (OMe-7).



S42 : ^{1}H-NMR spectrum (400 MHz, $CDCl_3$+CD_3OD) of Compound **5** (Fagaridine).

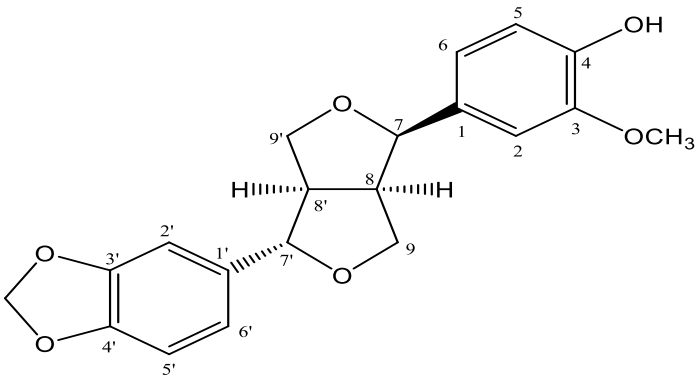


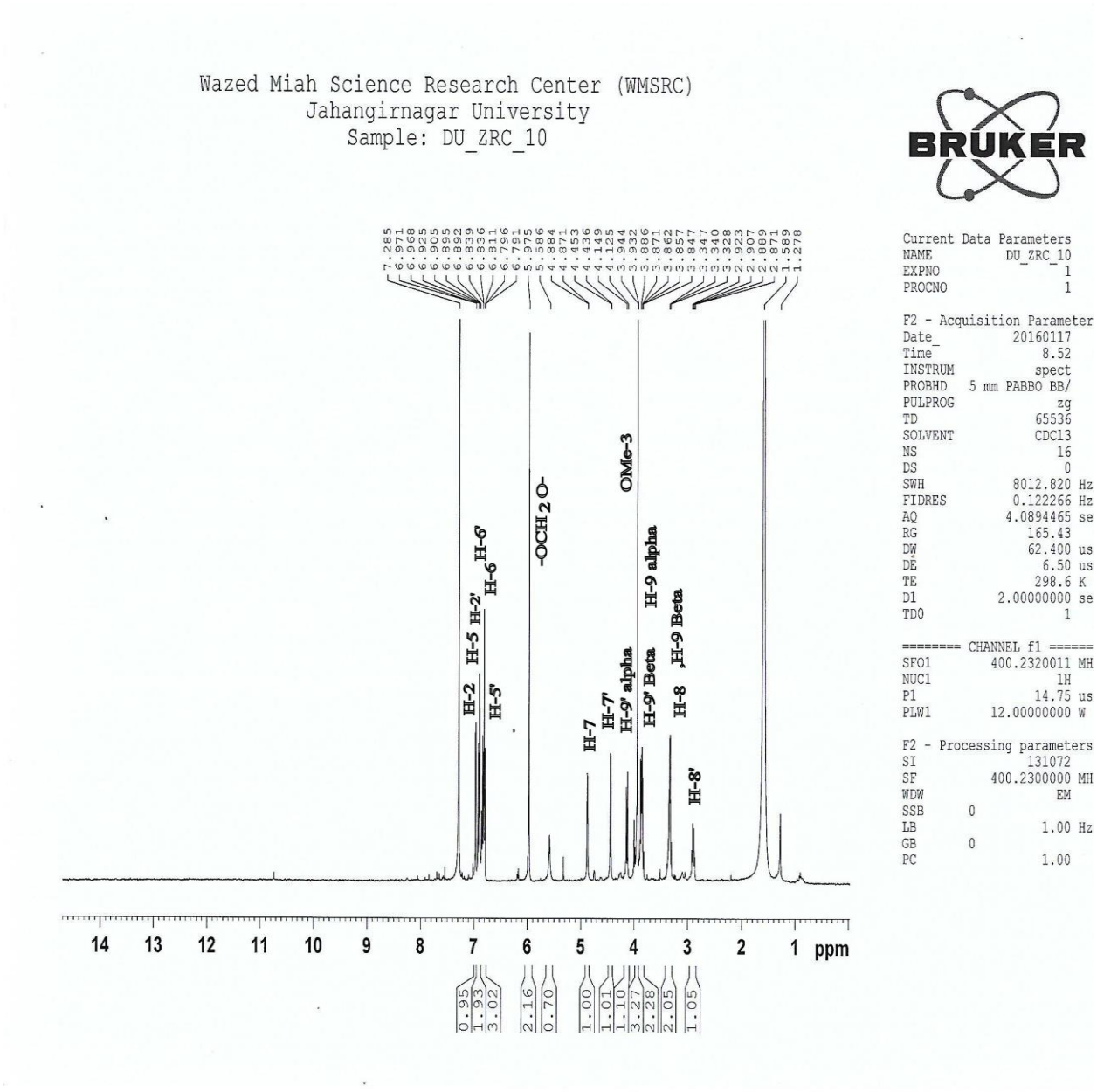
S43 : Expansion of ^{1}H-NMR spectrum (400 MHz, $CDCl_3$+CD_3OD) of Compound **5** (Fagaridine).



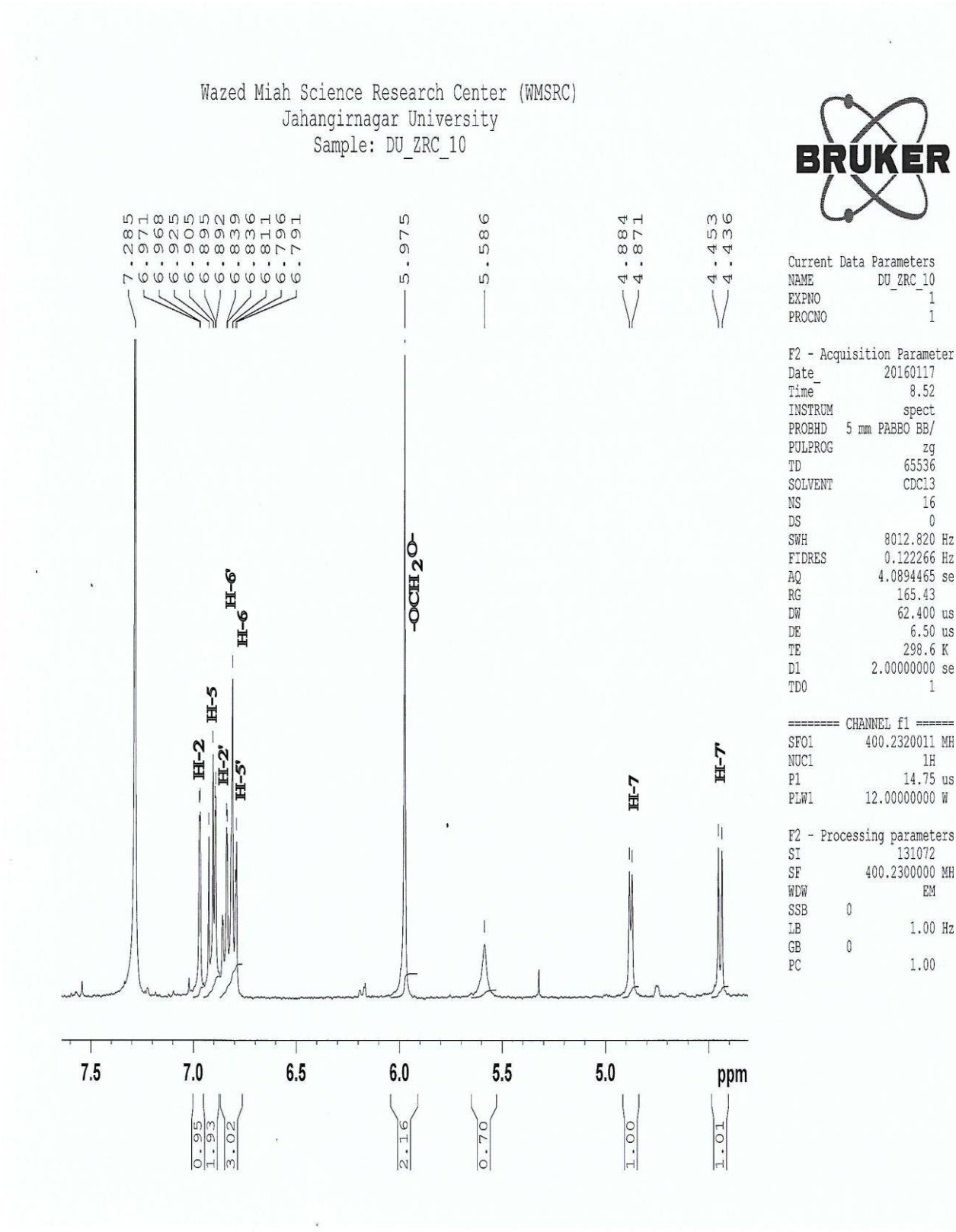
S44 : Expansion of ^{1}H-NMR spectrum (400 MHz, $CDCl_3$+CD_3OD) of Compound **5** (Fagaridine).

*Fagaridine (**5**)*: light yellow powder; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 9.71 (1H, s, H-8), 8.67 (1H, d, *J*= 8.8 Hz, H-12), 8.31 (1H, s, H-1), 8.24 (1H, d, *J*= 9.2 Hz, H-5), 7.99 (1H, d, *J*= 9.2 Hz, H-11), 7.57 (1H, s, H-4), 7.54 (1H, d, *J*= 8.8 Hz, H-6), 6.23 (2H, s, OCH_2O), 5.50 (3H, s, N-Me), 4.28 (3H, s, OMe-9).

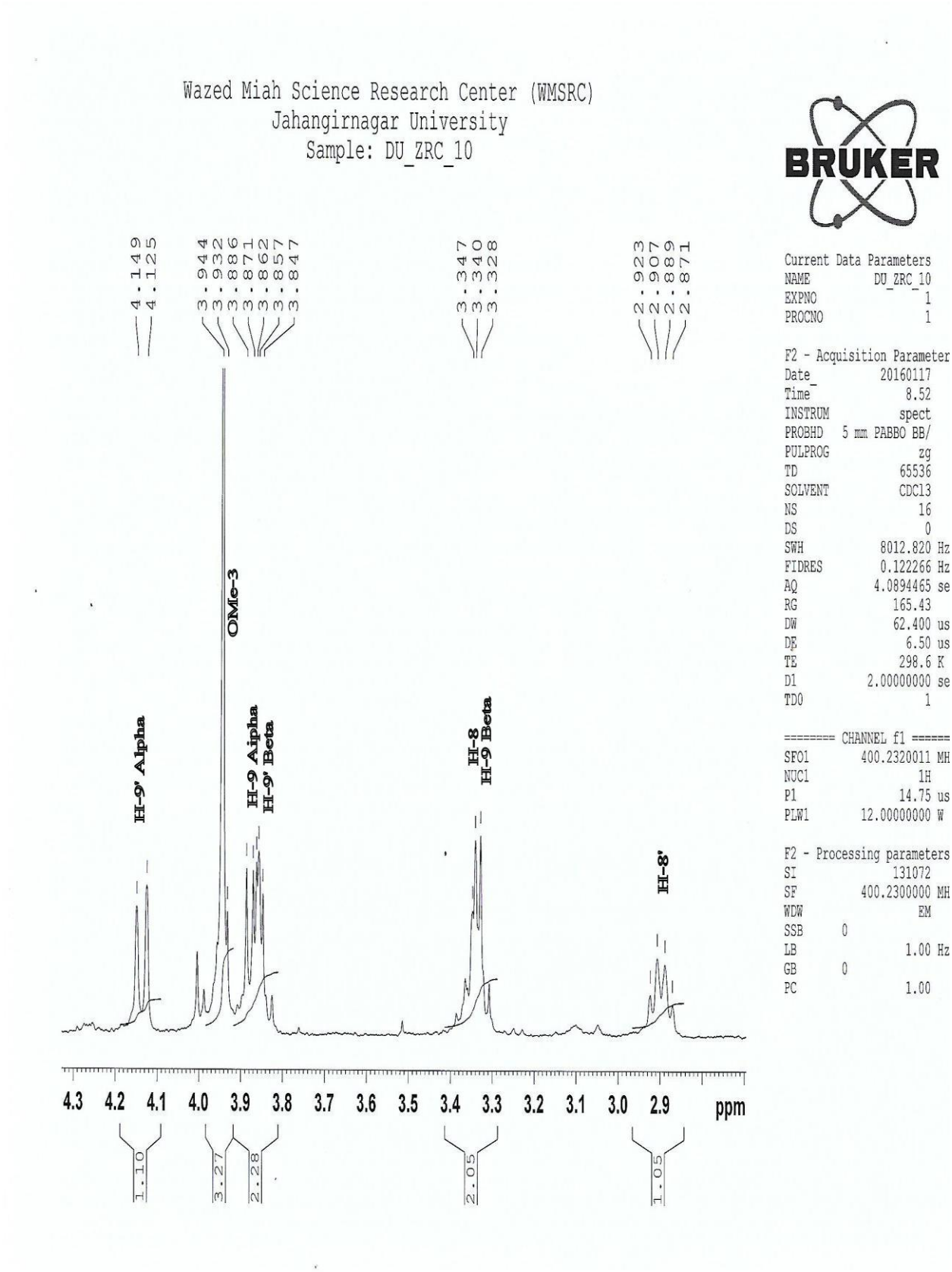




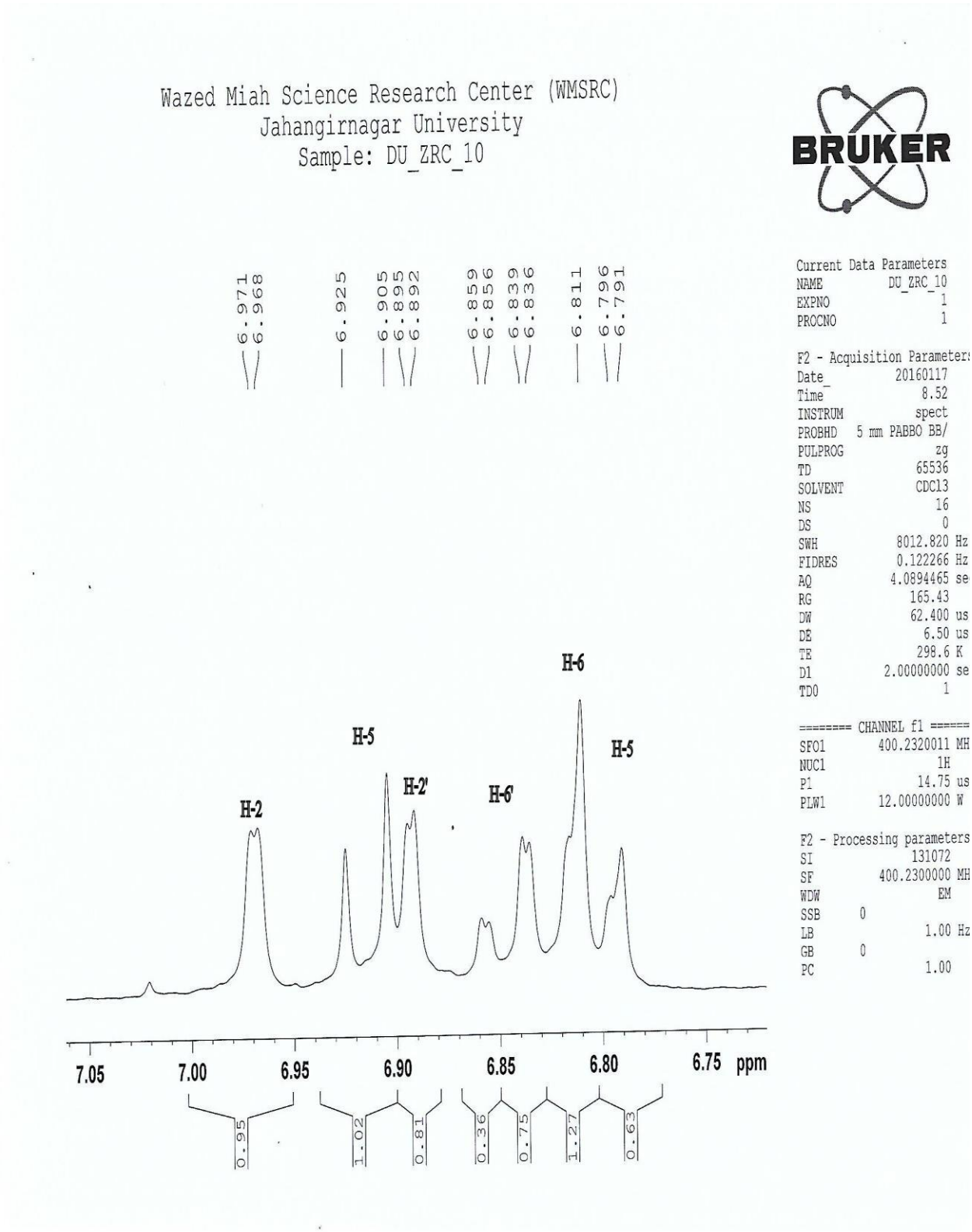
S45: ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of Compound 6 (Pluviatilol).



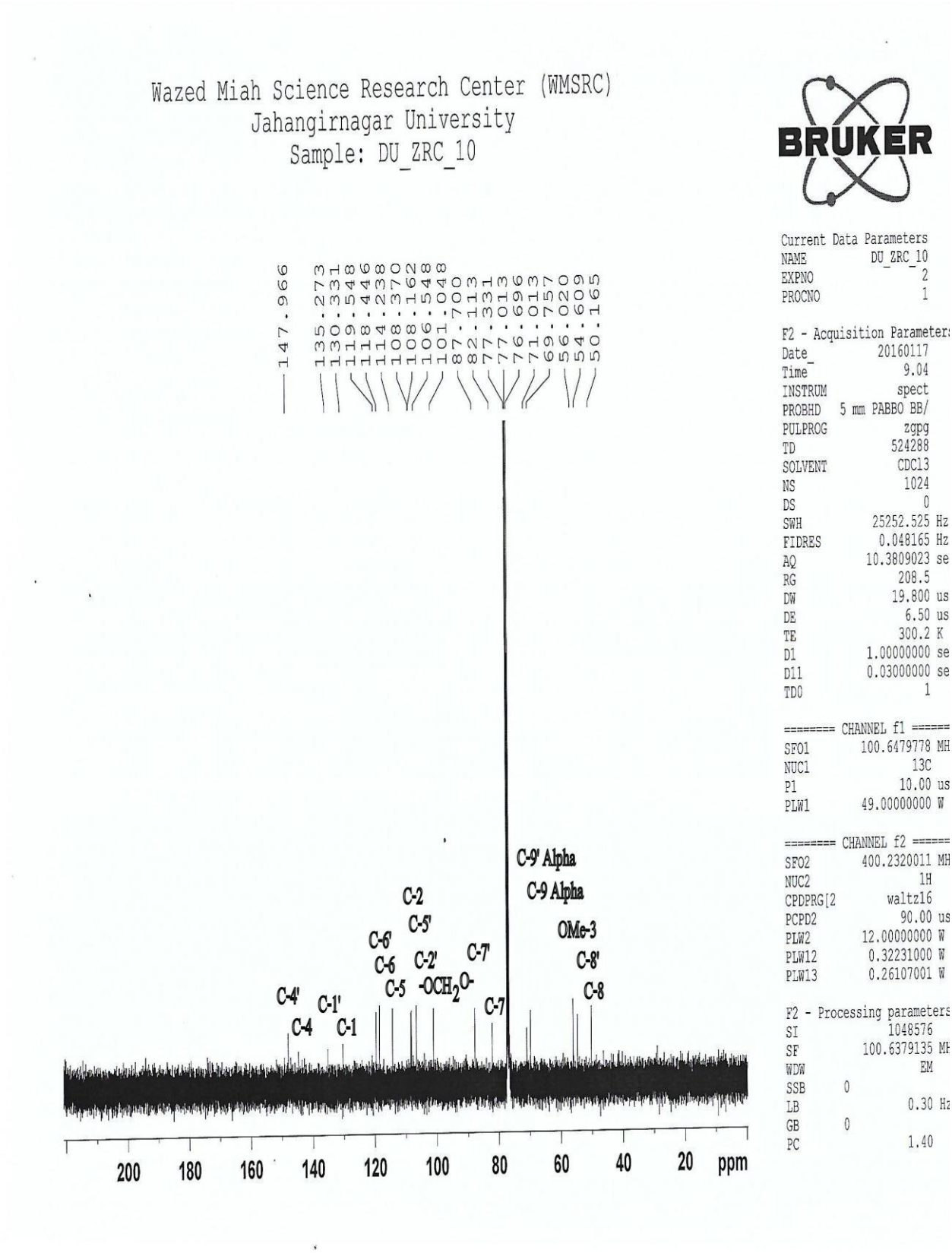
S46 : Partially expanded ^{1}H-NMR spectrum(400 MHz, $CDCl_3$) of Compound 6 (Pluviatilol)



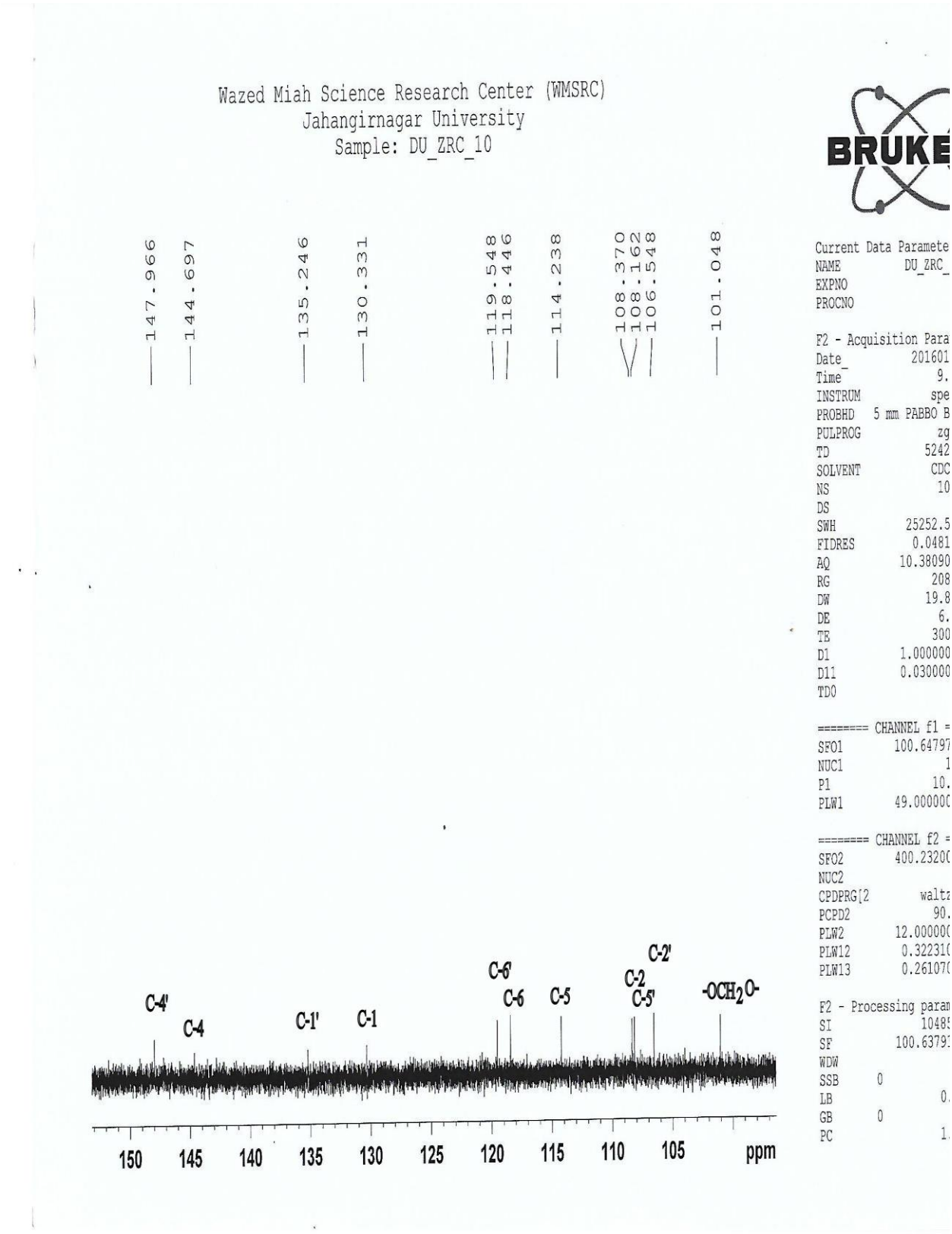
S47: Partially expanded ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of Compound 6 (Pluviatilol).



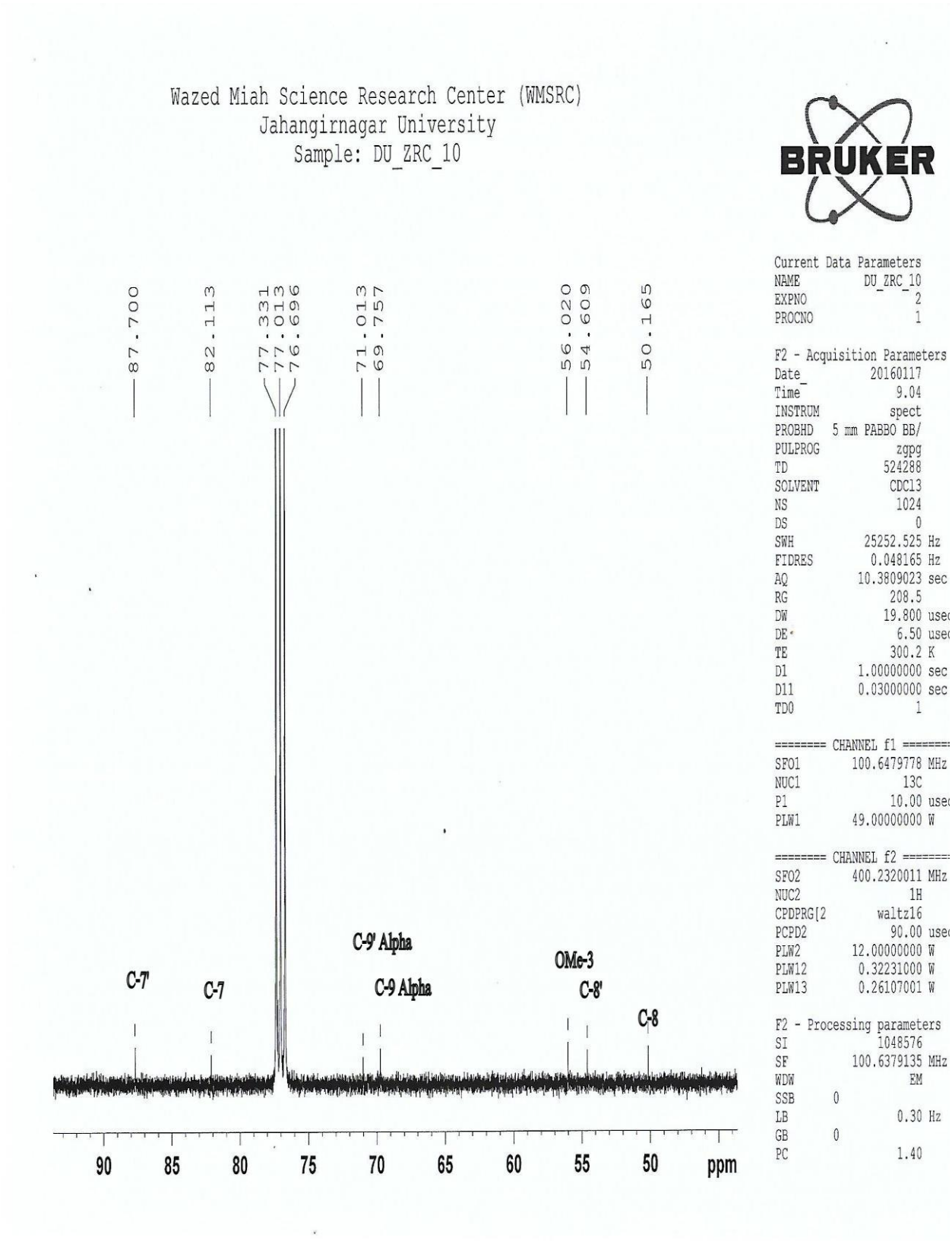
S48: Partially expanded ^{1}H-NMR spectrum (400 MHz, $CDCl_3$) of Compound 6 (Pluviatilol).



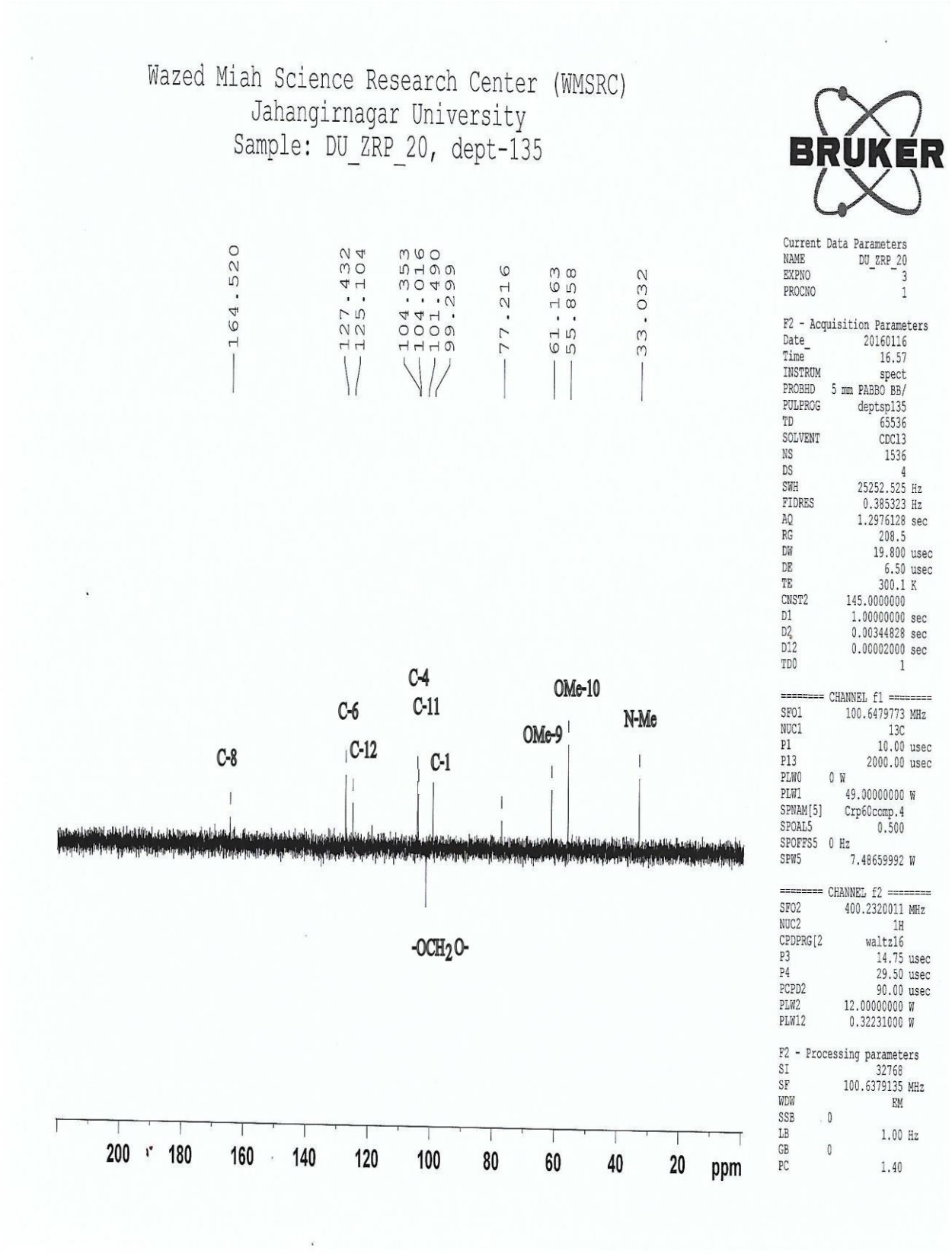
S49 : ^{13}C NMR spectrum (100 MHz, $CDCl_3$) of Compound 6 (Pluviatilol).



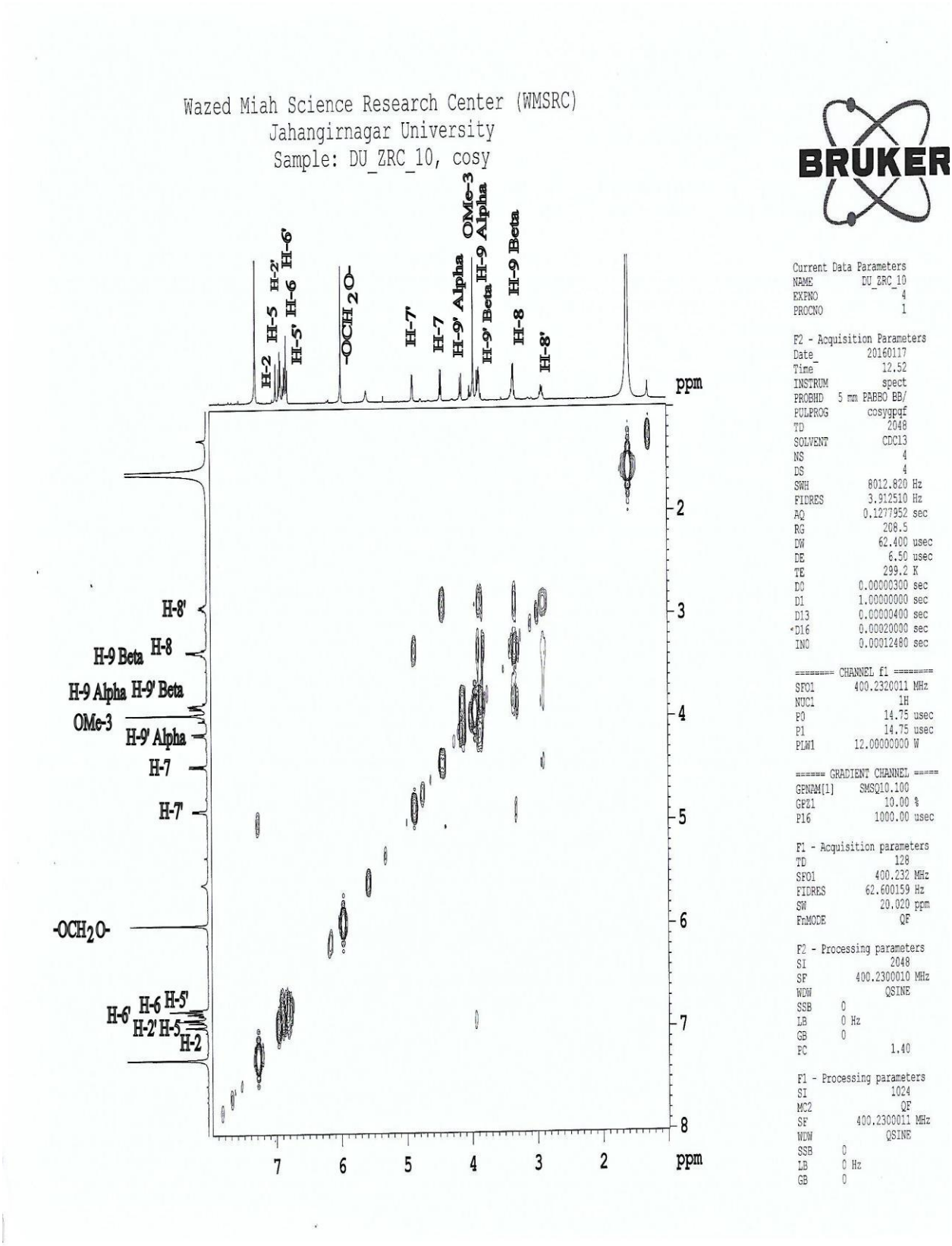
S50: Partially expanded ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of Compound 6 (Pluviatilol)



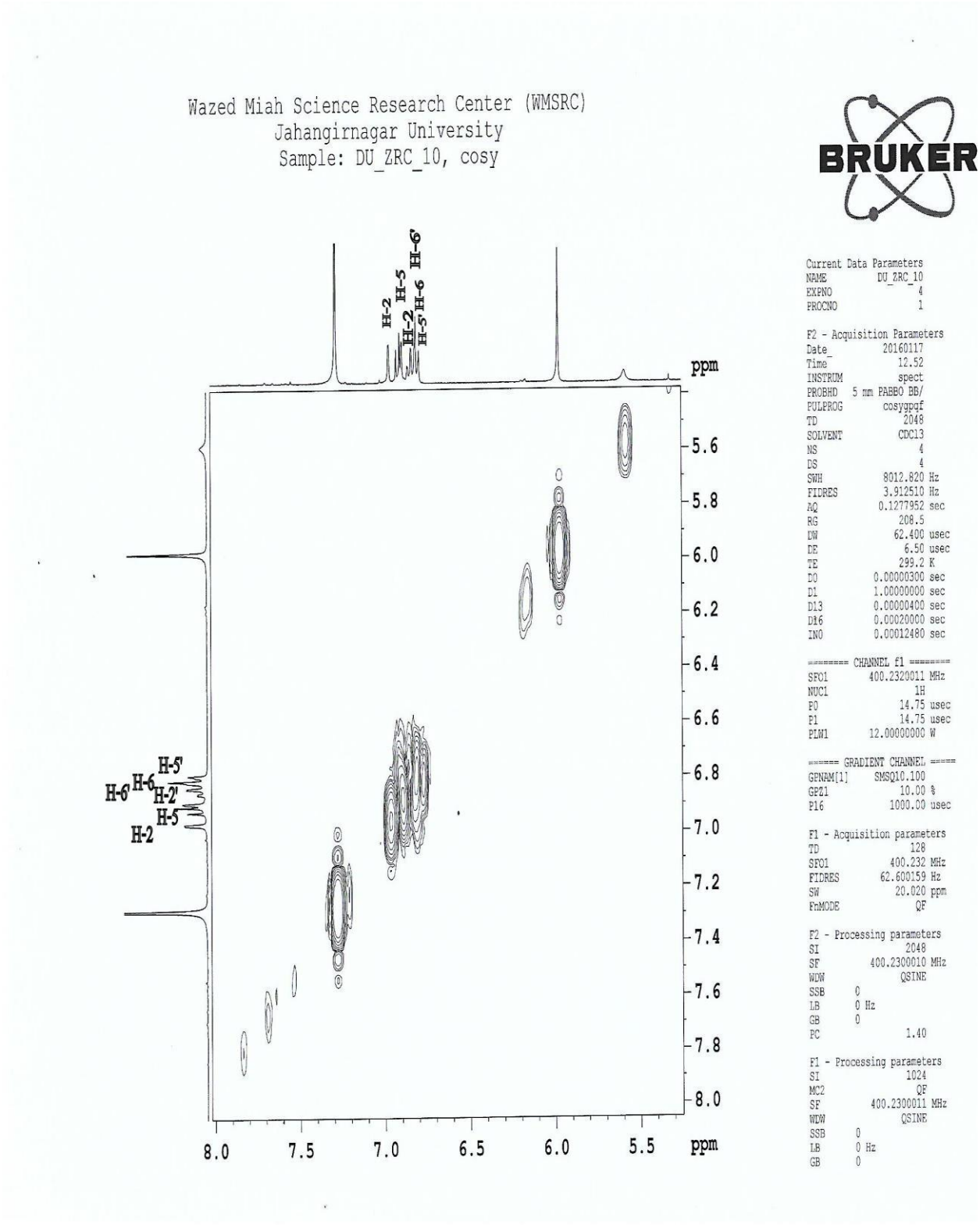
S51: Partially expanded ^{13}C-NMR spectrum (100 MHz, $CDCl_3$) of Compound 6 (Pluviatilol)



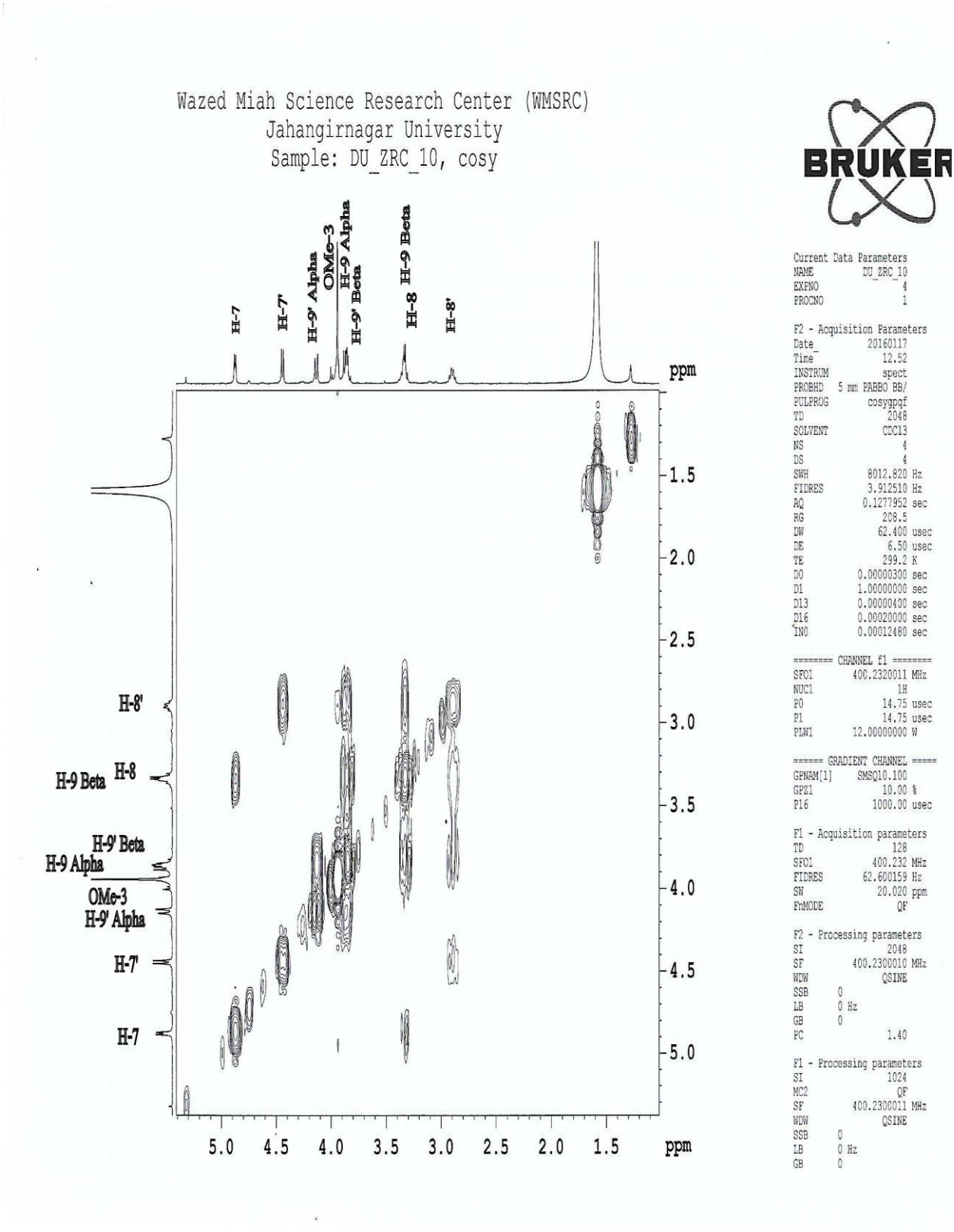
S52: DEPT-135 NMR spectrum (100 MHz, $CDCl_3$) of Compound **6** (Pluviatilol).



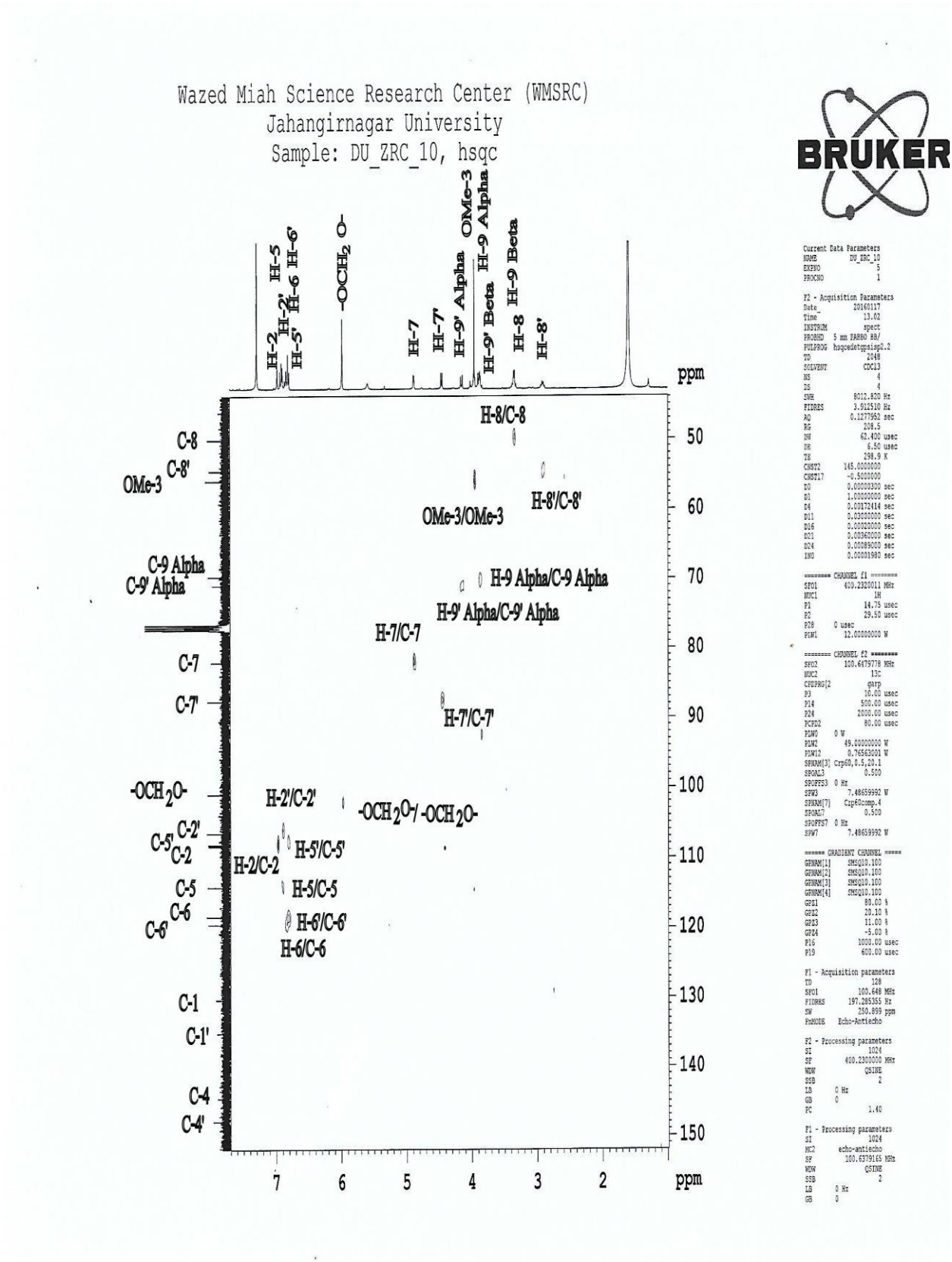
S53: COSY-NMR spectrum (400 MHz, $CDCl_3$) of Compound **6** (Pluviatilol).



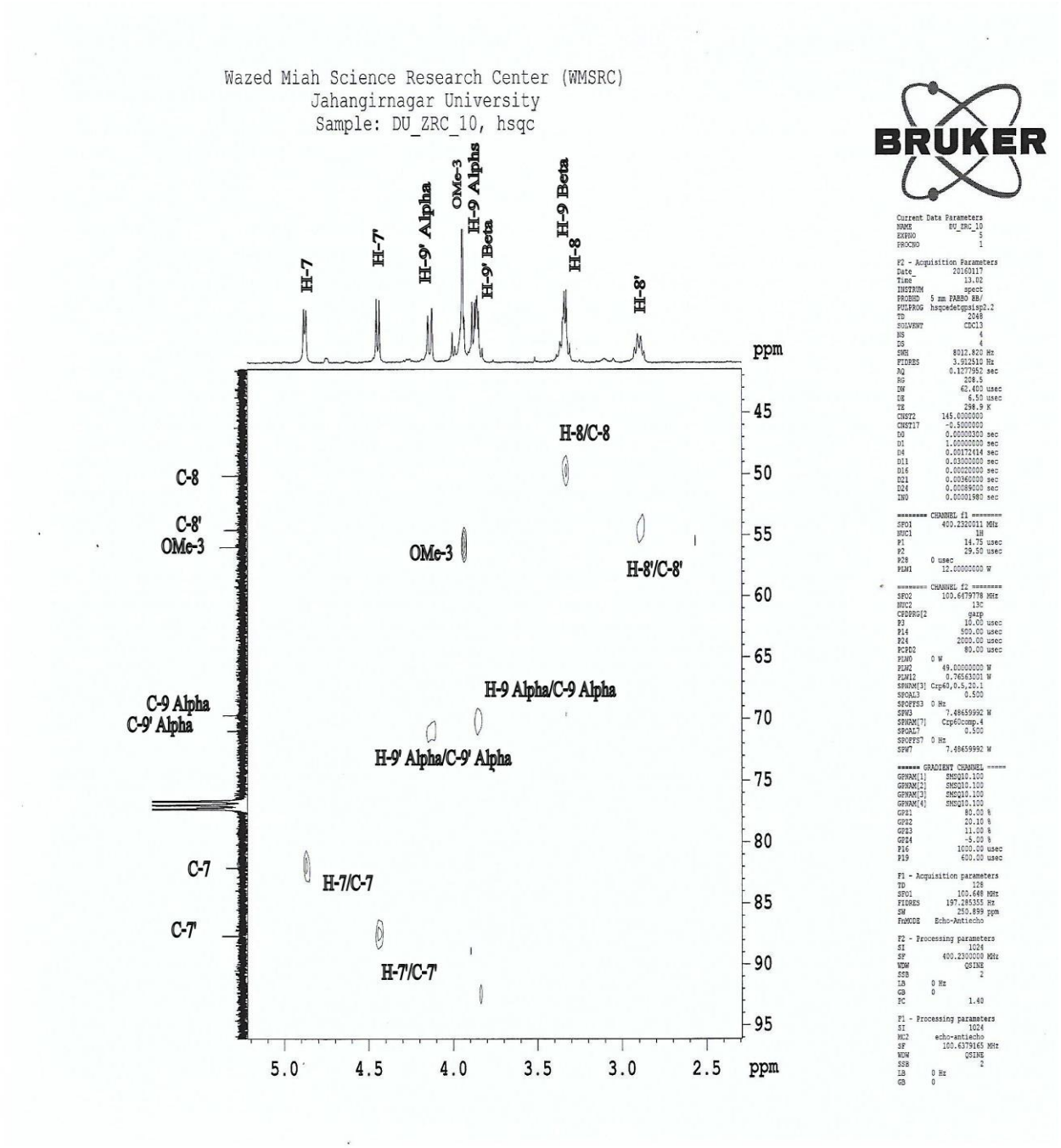
S54 : Partially expanded COSY-NMR spectrum (400 MHz, $CDCl_3$) of Compound **6** (Pluviatilol)



S55 : Partially expanded COSY-NMR spectrum (400 MHz, $CDCl_3$) of Compound **6** (Pluviatilol)

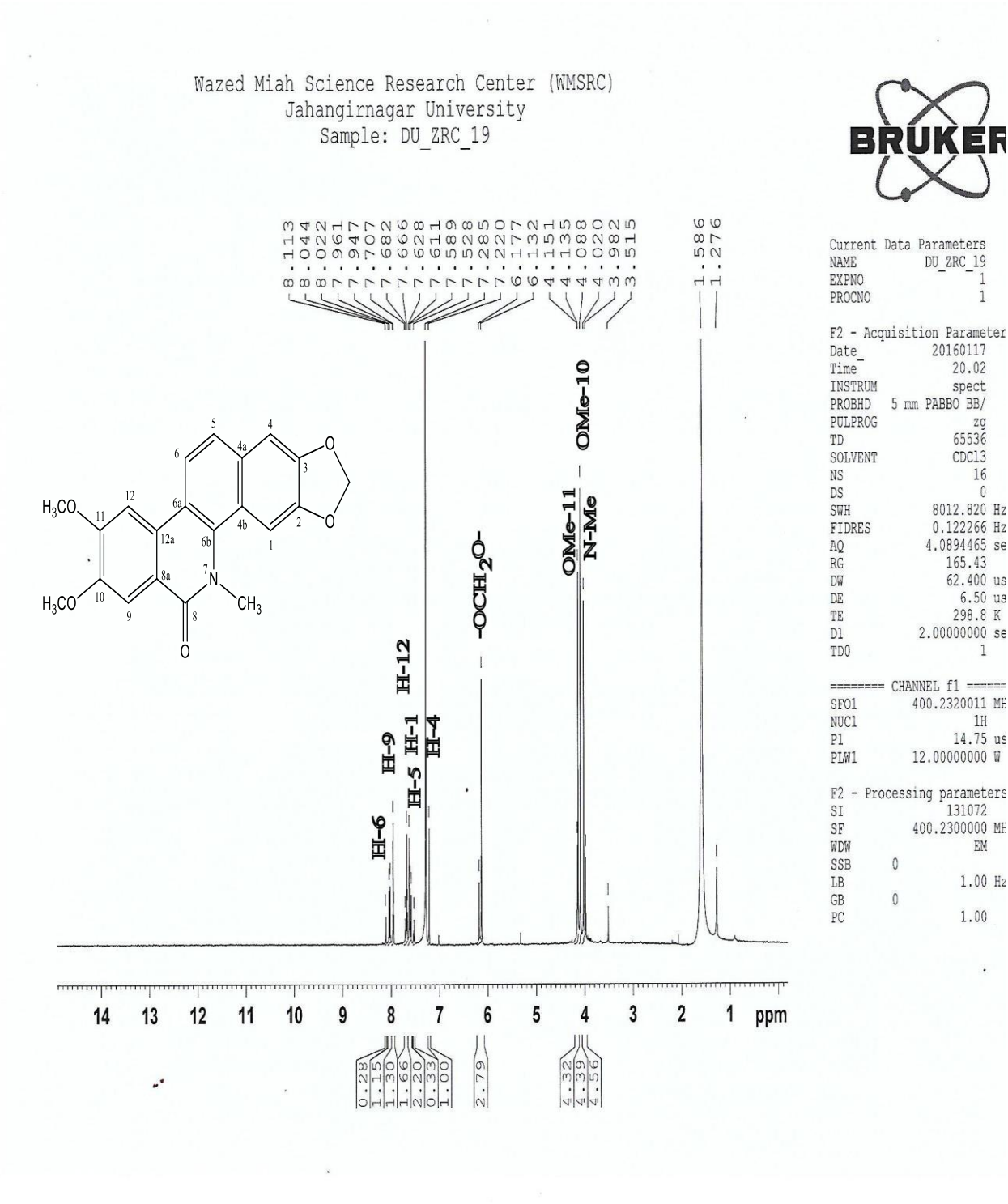


S56: HSQC-NMR spectrum (400 MHz, $CDCl_3$) of Compound **6** (Pluviatilol).

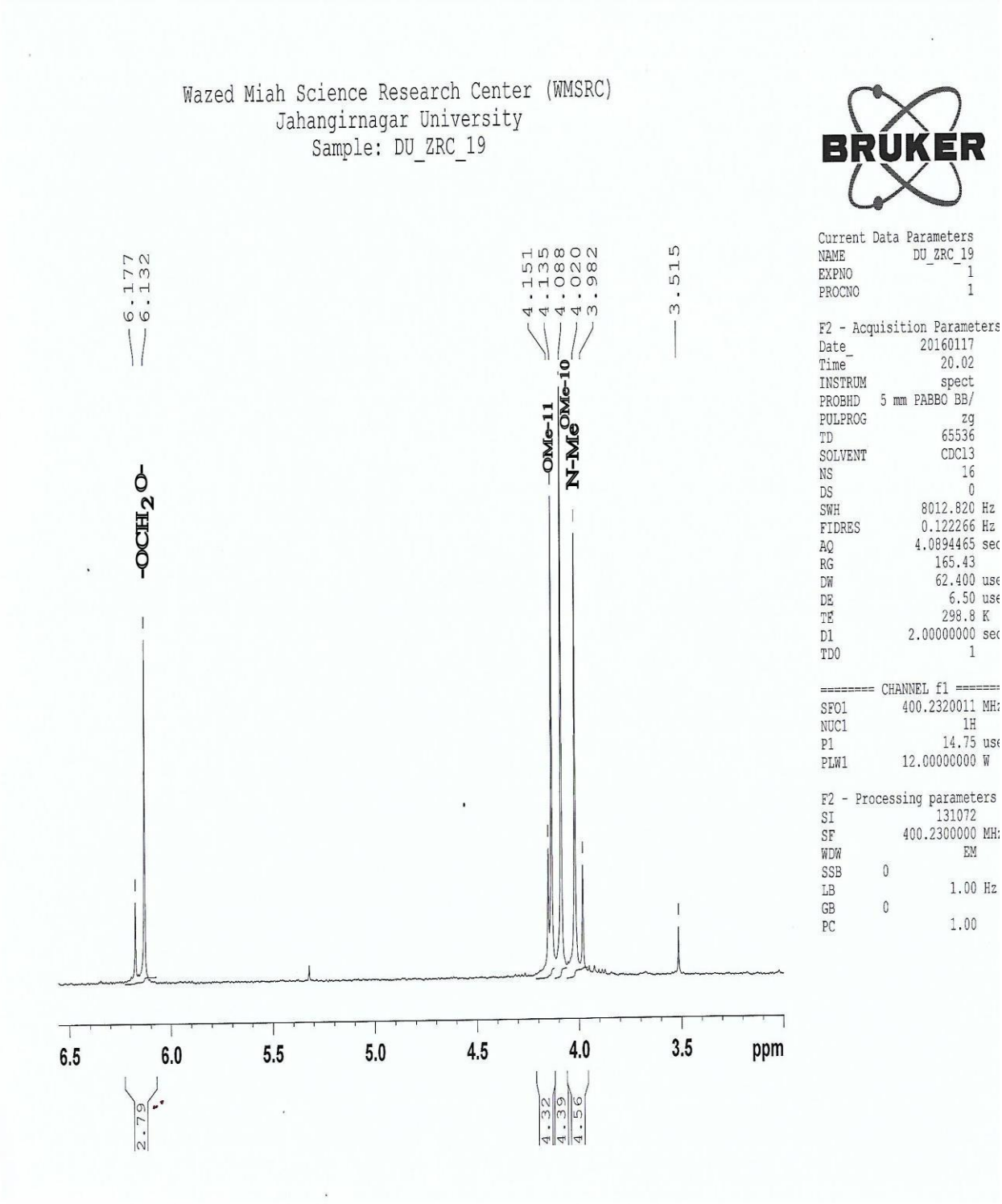


S57: Partially expanded HSQC-NMR spectrum (400 MHz, $CDCl_3$) of Compound **6** (Pluviatilol)

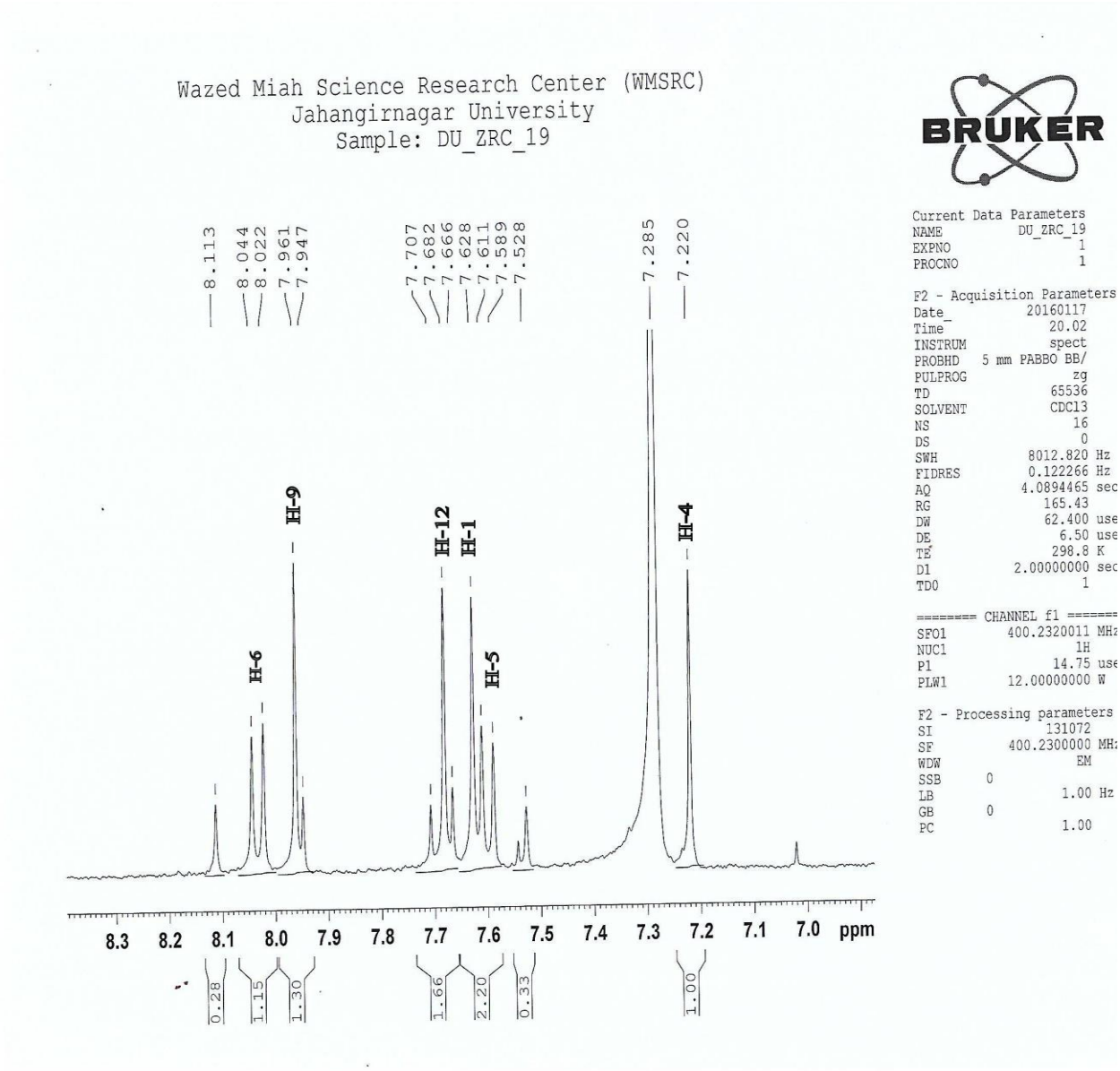
*Pluviatilol (**6**):* white crystals; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 6.97 (1H,d, *J*= 1.2 Hz, H-2), 6.92 (1H, d, *J*= 8.0 Hz, H-5), 6.89 (1H, d, *J*= 1.2 Hz, H-2′), 6.85 (1H, dd, *J*= 8.0, 1.2 Hz, H-6′), 6.81 (1H, dd, *J*=8.0, 2.0 Hz, H-6), 6.80 (1H, d, *J*= 8.0 Hz, H-5′), 5.98 (2H, s, OCH_2O), 4.87 (1H, d, *J*= 5.2 Hz, H-7), 4.44 (1H, d, *J*= 6.8 Hz, H-7′), 4.13 (1H, d, *J*= 9.6 Hz, H-9′α), 3.93 (3H, s, OMe-3), 3.87 (1H, dd, *J*= 9.6, 6.0 Hz, H-9α), 3.86 (1H, m, H-9′β), 3.34 (1H, m, H-8), 3.34 (1H, m, H-9β), 2.89 (1H, dd, *J*= 7.2, 6.4 Hz, H-8′). ^{13}C-NMR (125 MHz, $CDCl_3$): δ 148.0* (C-4′), 147.2* (C-3′), 145.9* (C-3), 144.7* (C-4), 130.3 (C-1), 119.5 (C-6′), 118.4 (C-6), 114.2 (C-5), 108.4 (C-2), 108.2 (C-5′), 106.5 (C-2′), 101.0 (OCH_2O), 87.7 (C-7′), 82.1 (C-7), 71.0 (C-9′), 69.8 (C-9), 56.0 (OMe-3), 54.6 (C-8′), 50.2 (C-8).



S58: ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound **7** (Oxynitidine).



S59: Expansion of ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound **7** (Oxynitidine).



S60: Expansion of ^{1}H NMR (400 MHz, $CDCl_3$) spectrum of Compound **7** (Oxynitidine).

Oxynitidine (**7**): white amorphous; ^{1}H-NMR (500 MHz, $CDCl_3$): δ 8.02 (1H, d, *J*= 8.8 Hz, H-6), 7.96 (1H, s, H-9), 7.68 (1H, s, H-12), 7.63 (1H, s, H-1), 7.60 (1H, d, *J*= 8.8 Hz, H-5), 7.22 (1H, s, H-4), 6.13 (2H, s, OCH_2O), 4.14 (3H, s, OMe-11), 4.08 (3H, s, OMe-11), 4.02 (3H, s, N-Me).