

Supporting Information

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Anti-urease Secondary Metabolites from *Seriphidium quettense*

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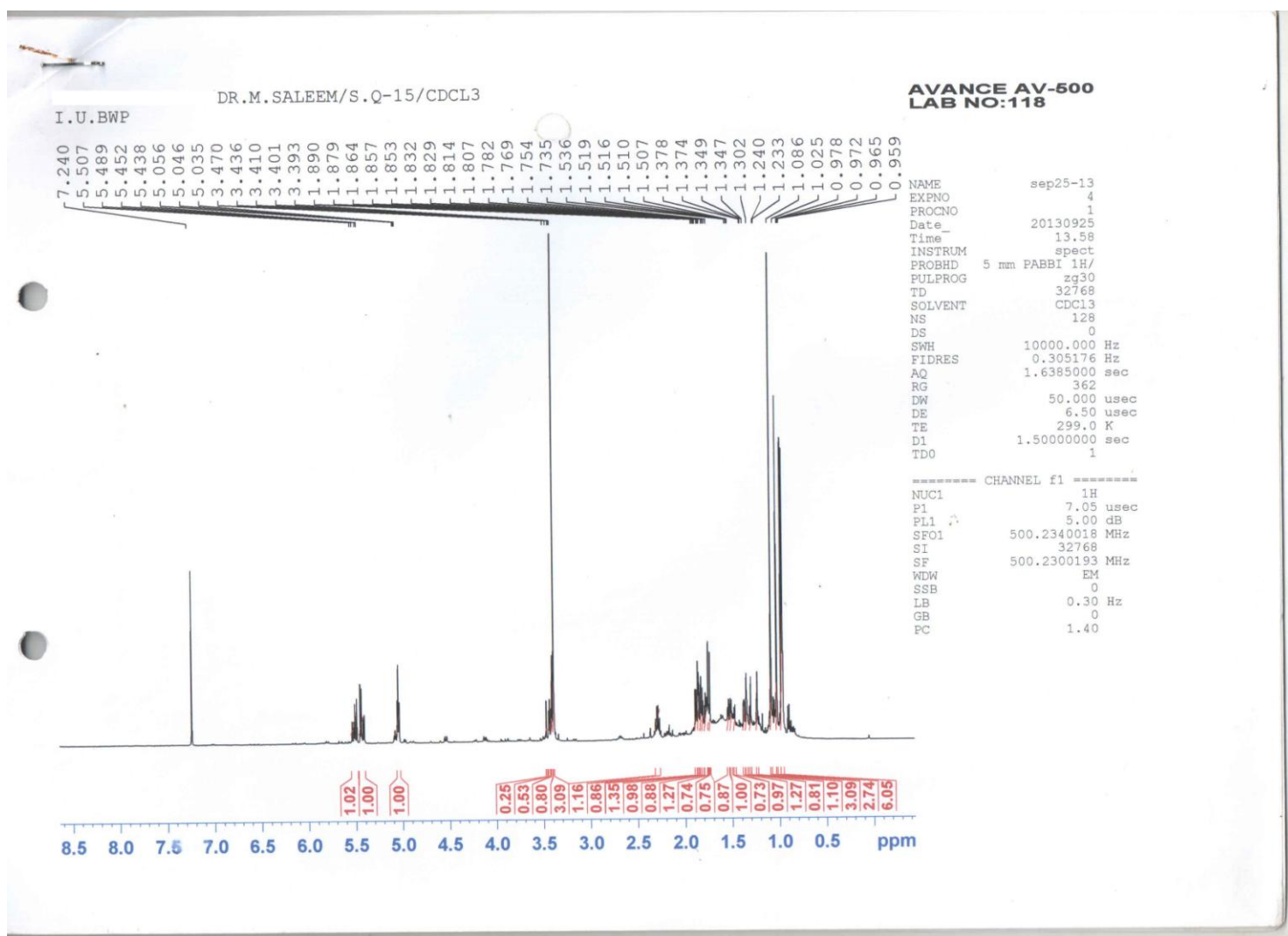
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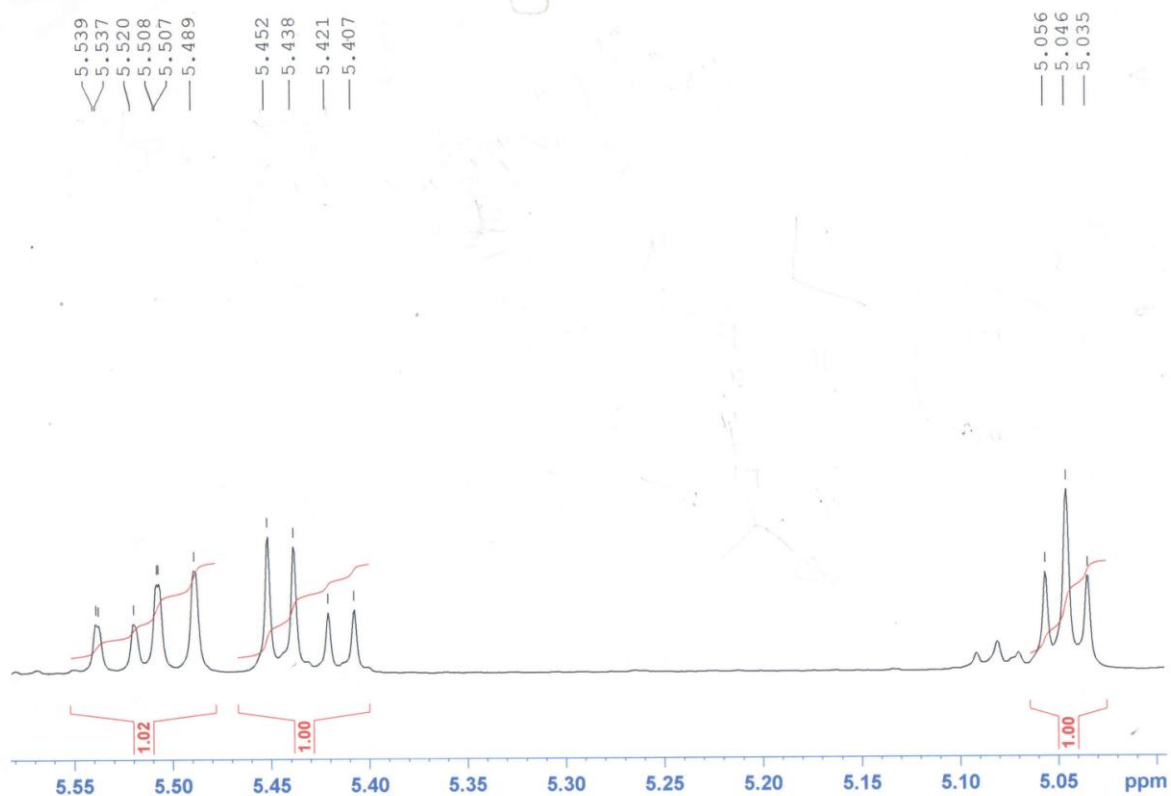


S1: ¹H-NMR (600 MHz, CDCl₃) Spectrum of Compound 1

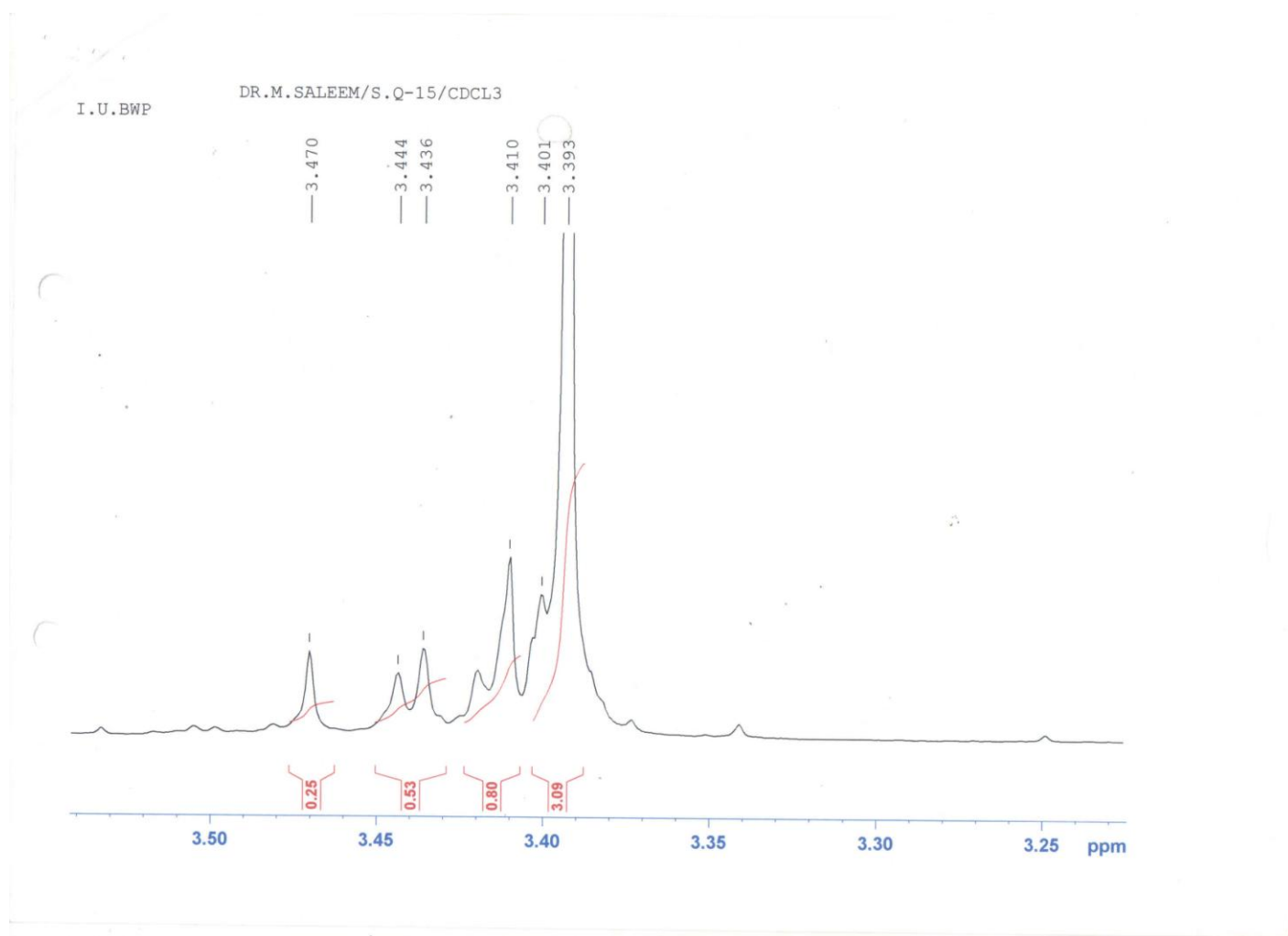
Spectroscopic data of seriphilidine (1): white amorphous powder (20 mg); IR ν_{max} (KBr) cm^{-1} : 3410, 1645; ¹H-NMR (CDCl₃; 600 MHz): δ (ppm) 5.53 (1H, dd, J = 15.5, 9.5 Hz, H-10), 5.45 (1H, dd, J = 15.5, 7.0 Hz, H-11), 5.05 (1H, t, J = 5.0 Hz, H-2), 3.93 (3H, s, 2-OMe), 3.41 (1H, br s, H-9), 2.30 (1H, m, H-12), 1.89 (1H, d, J = 5.5 Hz, H-3), 1.85 (1H, d, J = 4.5 Hz, H-7), 1.78 (2H, m, H-8), 1.75 (1H, d, J = 9.5 Hz, H-5), 1.51 (1H, dd, J = 5.4, 1.8 Hz, H-7), 1.37 (1H, d, J = 5.5 Hz, H-3), 1.08 (3H, s, Me-15), 1.02 (3H, s, Me-16), 0.97 (3H, d, J = 6.5 Hz, Me-13) and 0.96 (3H, d, J = 6.5 Hz, Me-14); ¹³C-NMR (CDCl₃; 150 MHz): δ (ppm) 142.0 (C-11), 122.5 (C-10), 105.5 (C-2), 83.5 (C-9), 72.3 (C-6), 57.2 (C-5), 47.8 (C-3), 46.0 (C-4), 39.5 (C-7), 31.4 (C-12), 31.0 (C-15), 22.7 (C-13, 14), 21.6 (C-8), 15.8 (C-16) and 56.0 (2-OMe); EIMS: m/z 268 [M]⁺; HR-EIMS: m/z 268.2435 [M]⁺ (calcd. 268.2475 for C₁₆H₂₈O₃).

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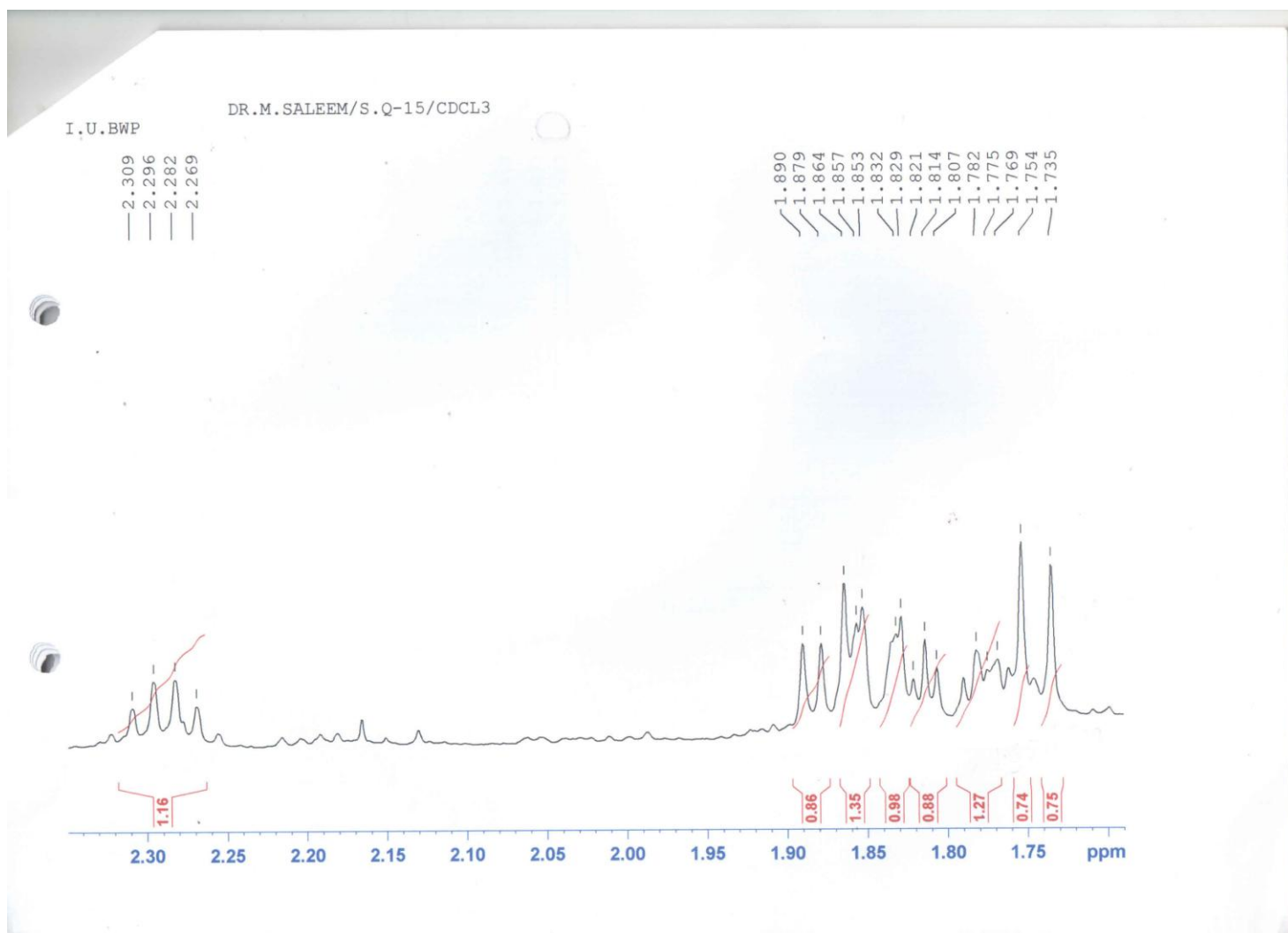
DR.M.SALEEM/S.Q-15/CDCL₃



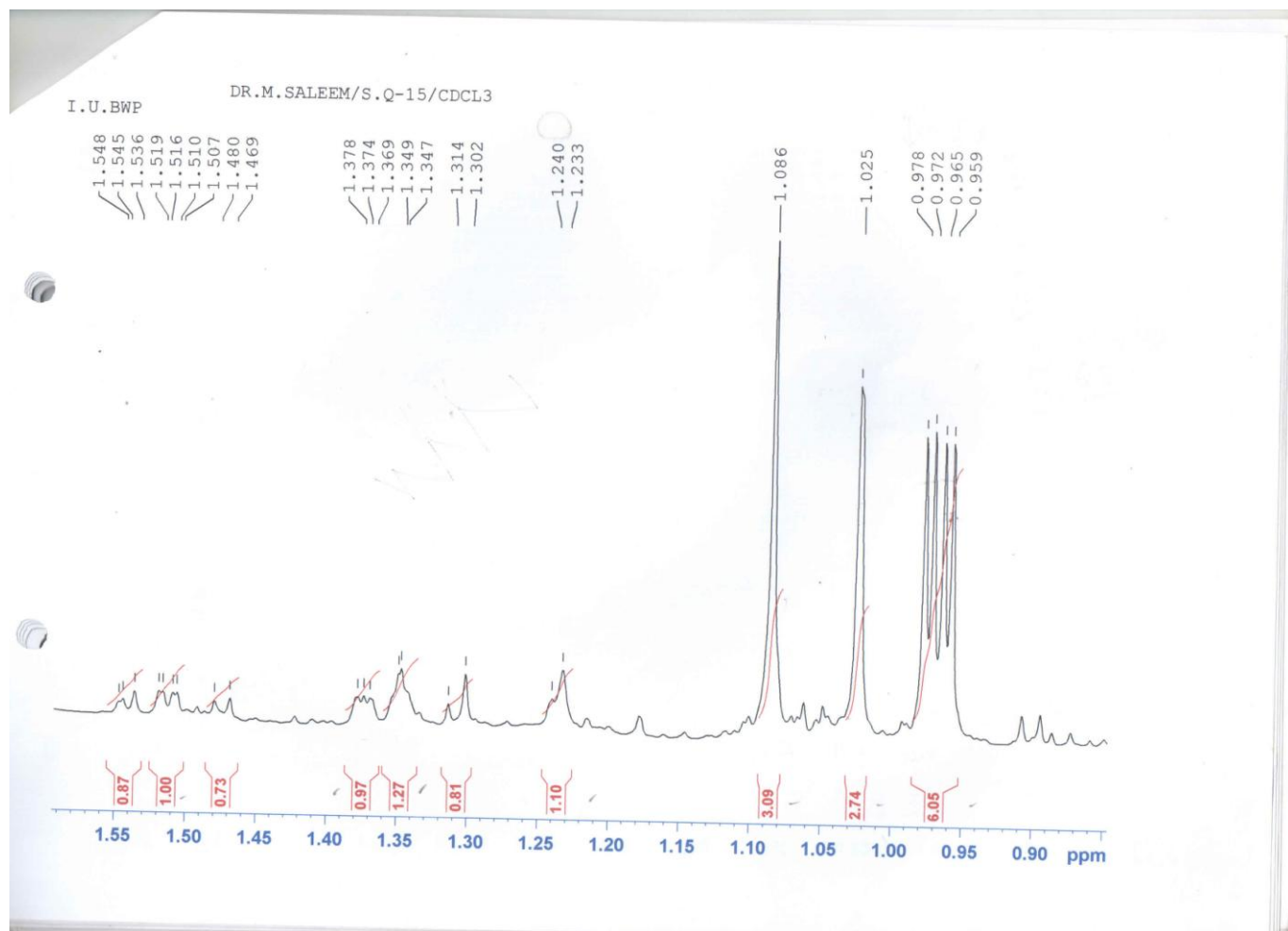
S2: ^1H -NMR Spectrum of Compound **1** (From 5.00 to 5.60 ppm)



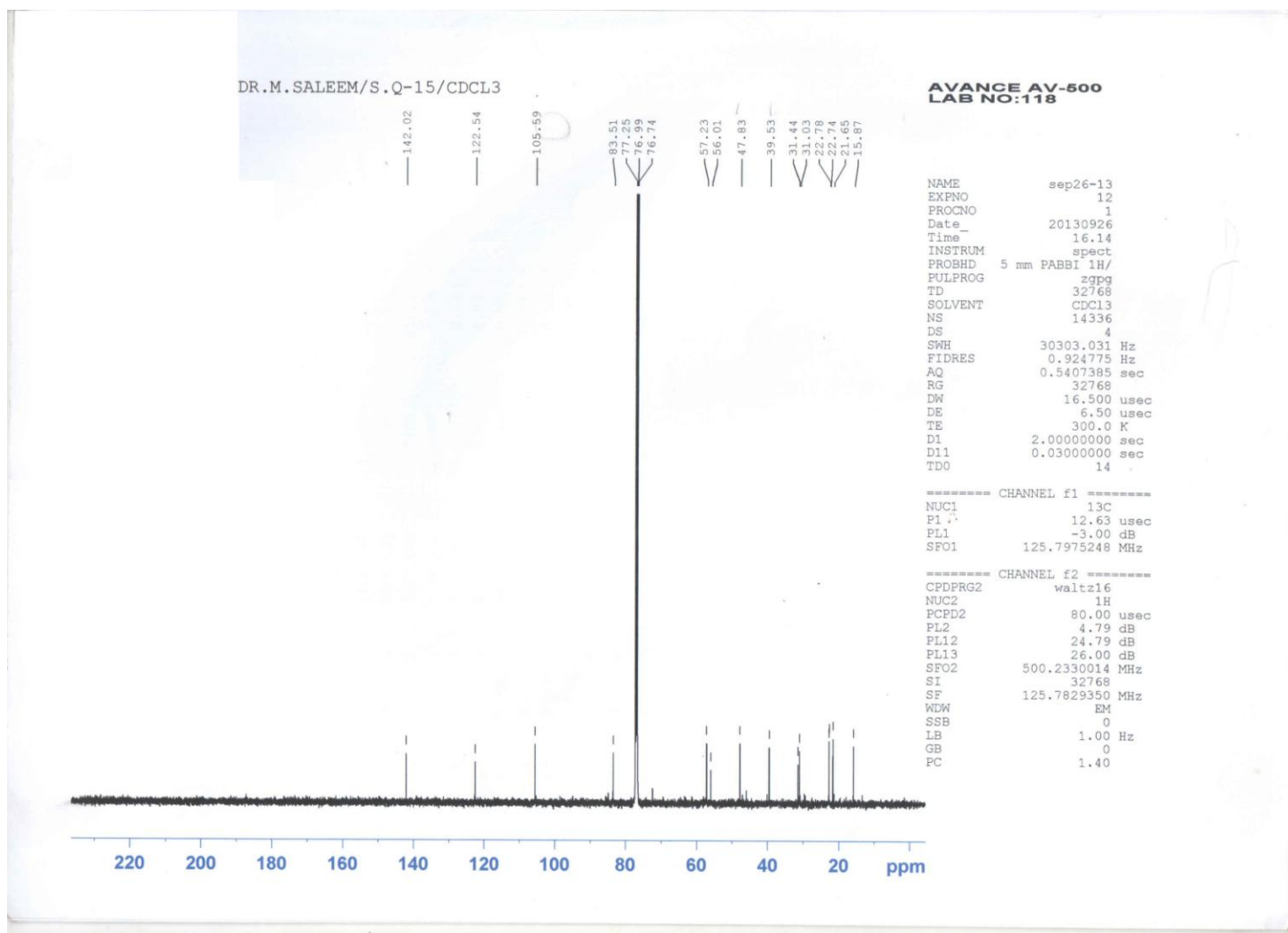
S3: ^1H -NMR Spectrum of Compound **1** (From 3.25 to 3.50 ppm)



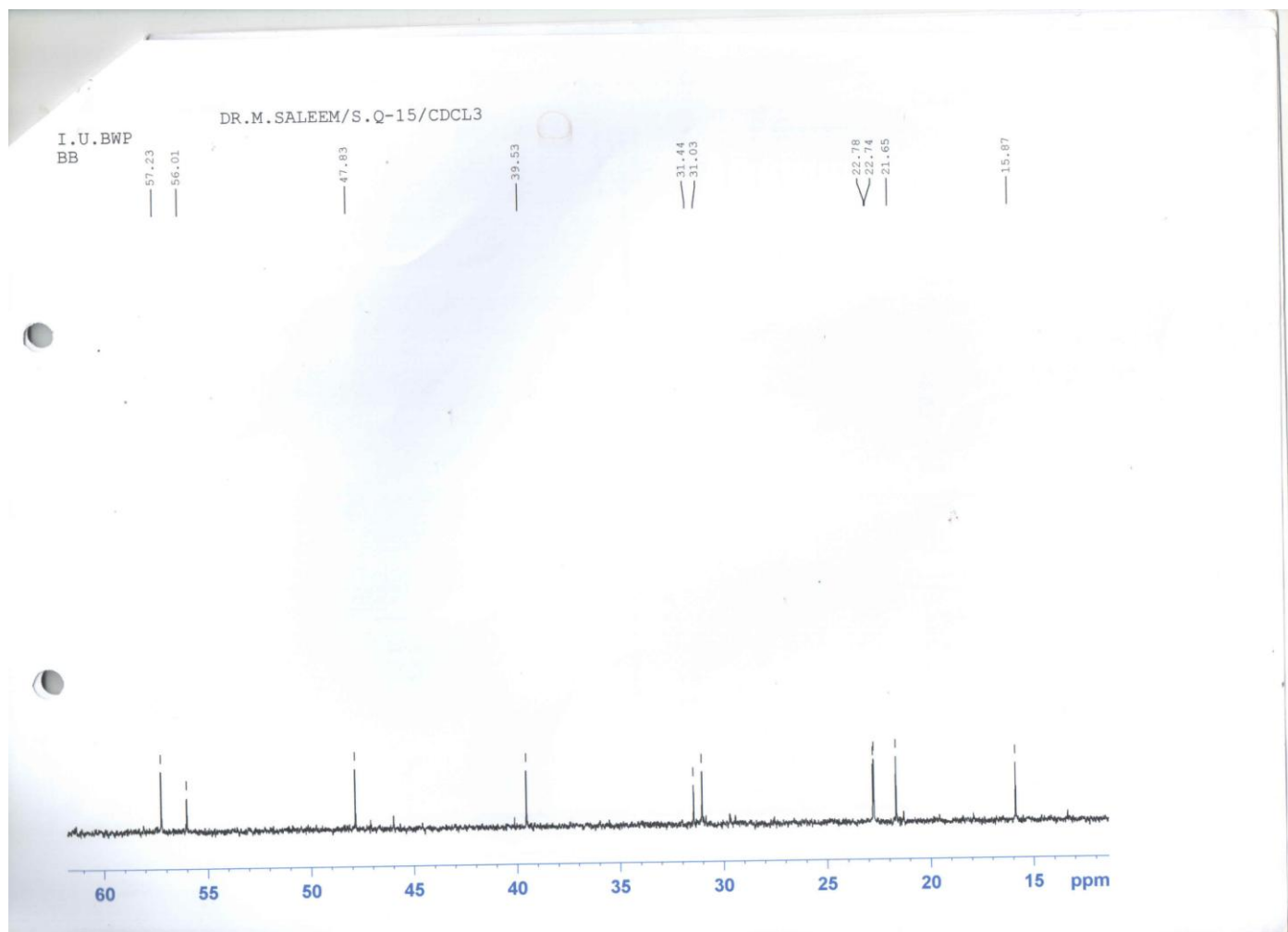
S4: ^1H -NMR Spectrum of Compound **1** (From 1.70 to 2.30 ppm)



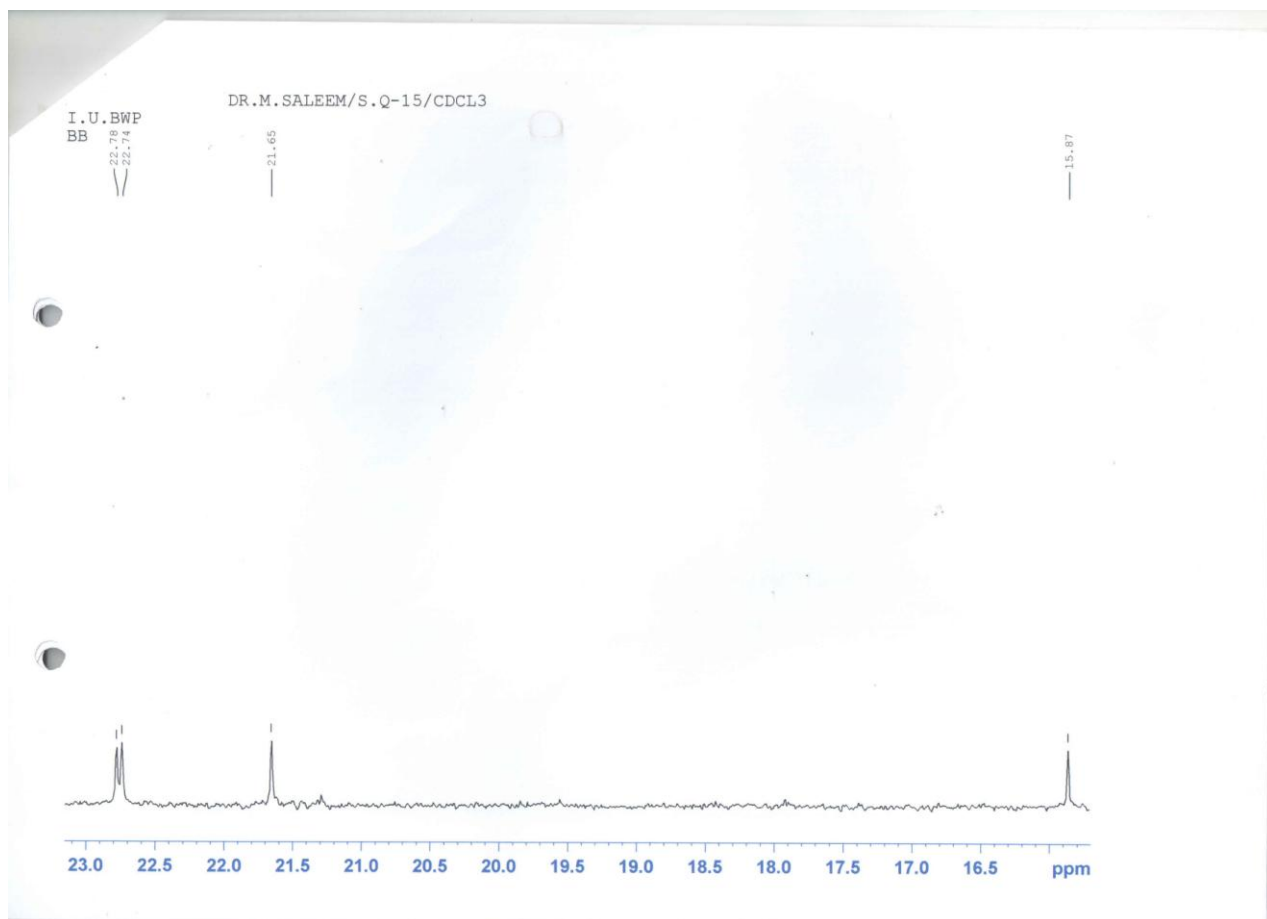
S5: ^1H -NMR Spectrum of Compound **1** (From 0.85 to 1.55 ppm)



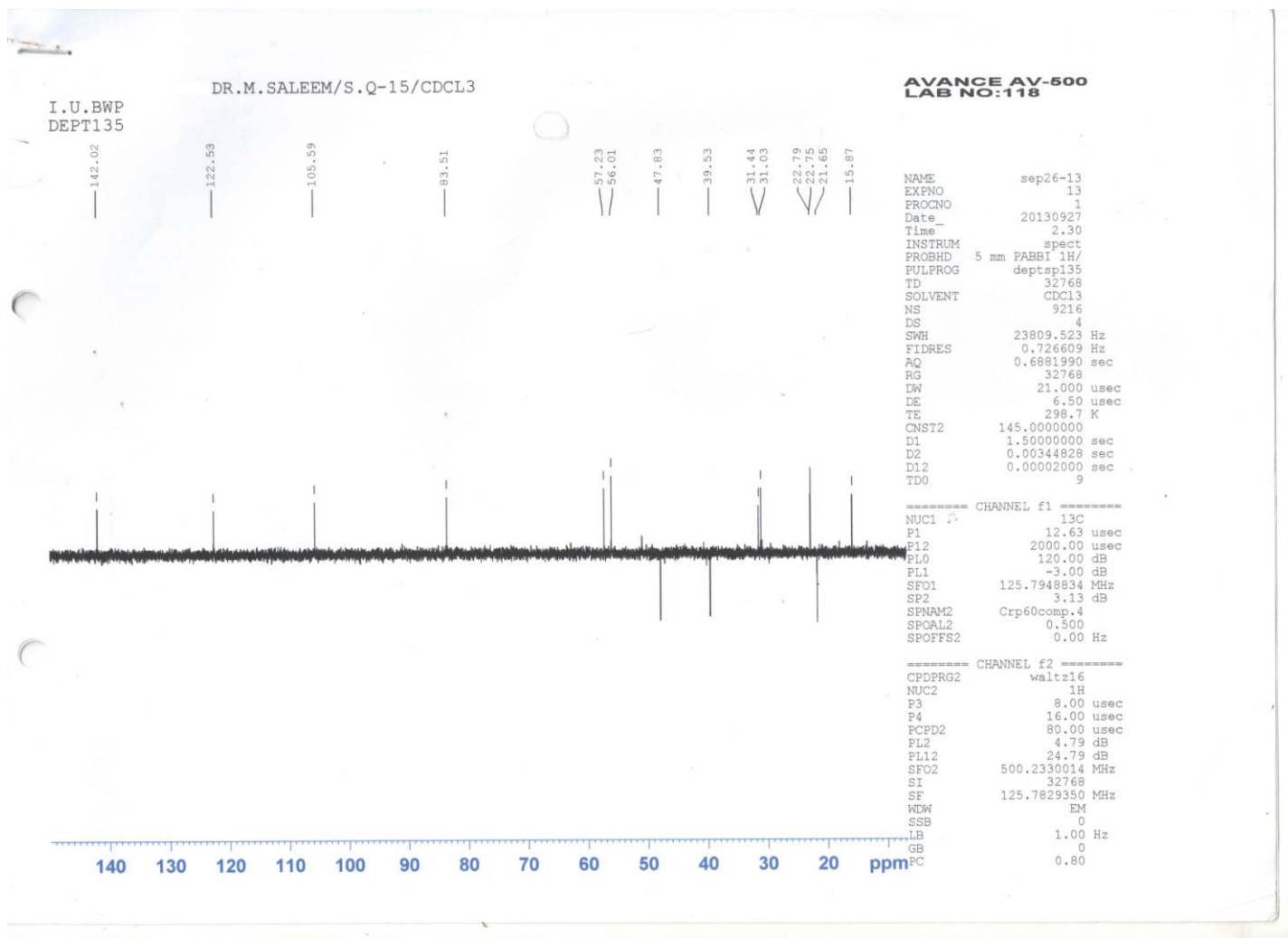
S6: ¹³C-NMR BB Spectrum of Compound **1** (From 00 to 220 ppm)



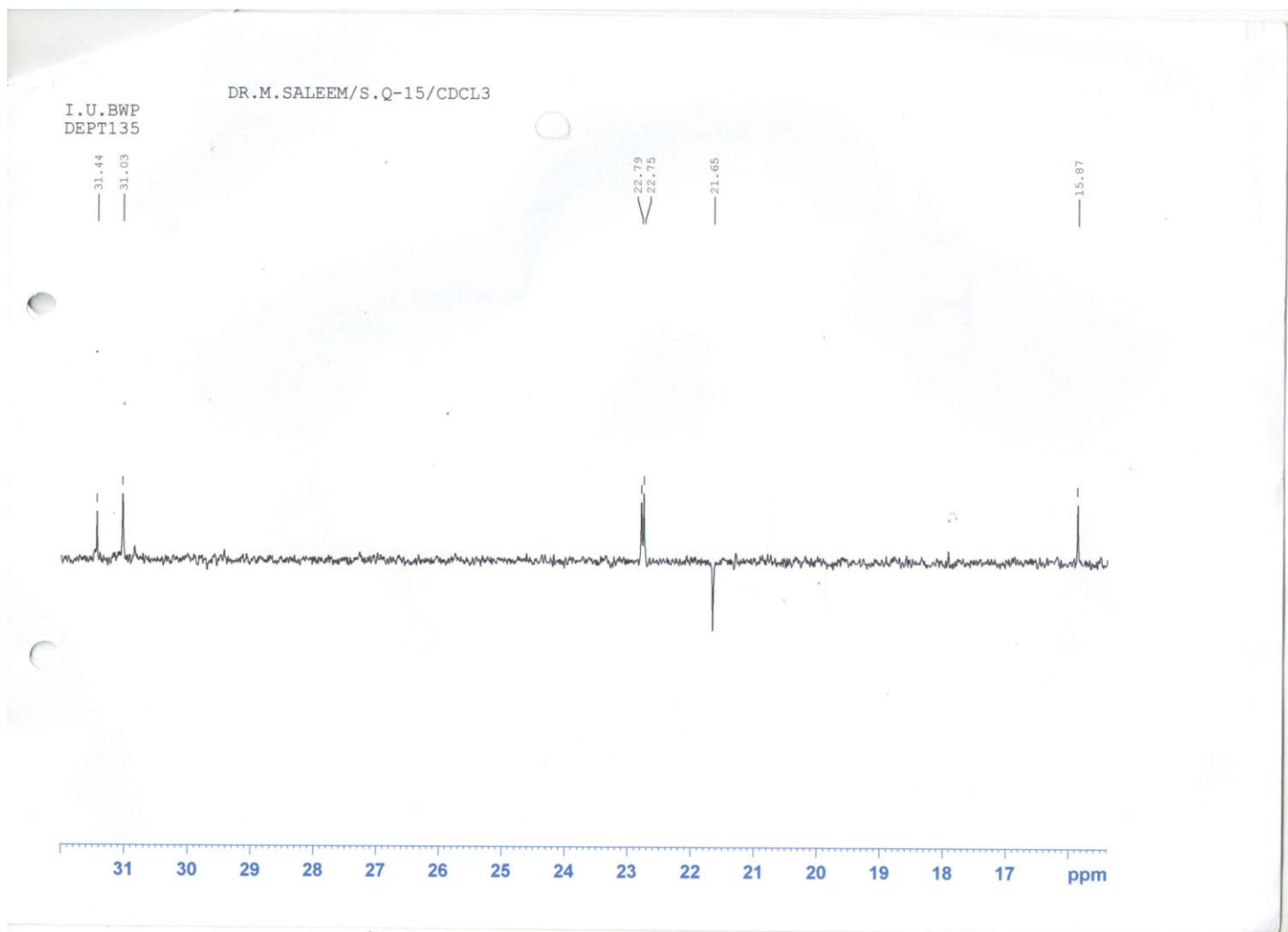
S7: ^{13}C -NMR BB Spectrum of Compound **1** (From 10 to 60 ppm)



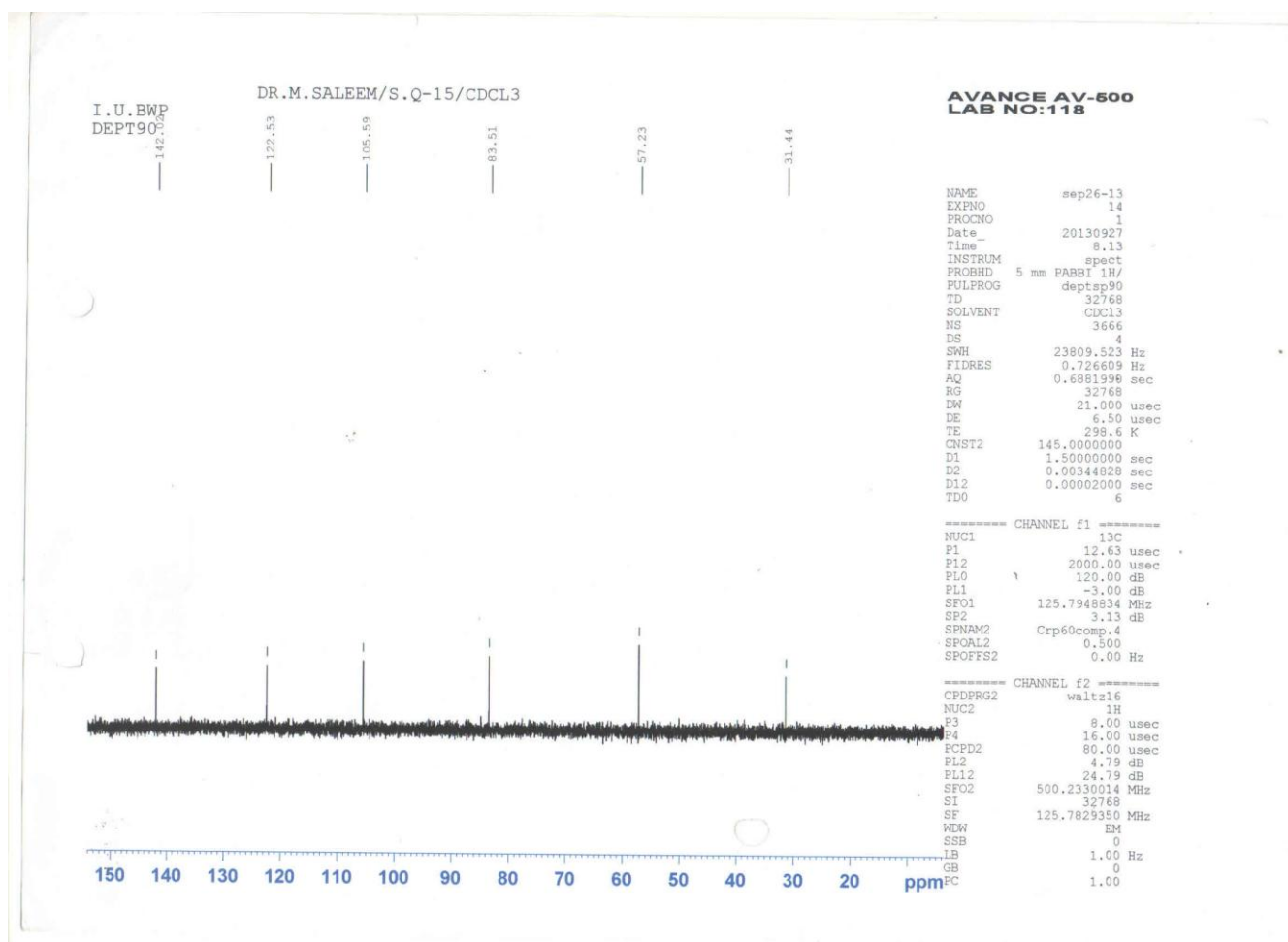
S8: ^{13}C -NMR BB Spectrum of Compound **1** (From 15 to 23 ppm)



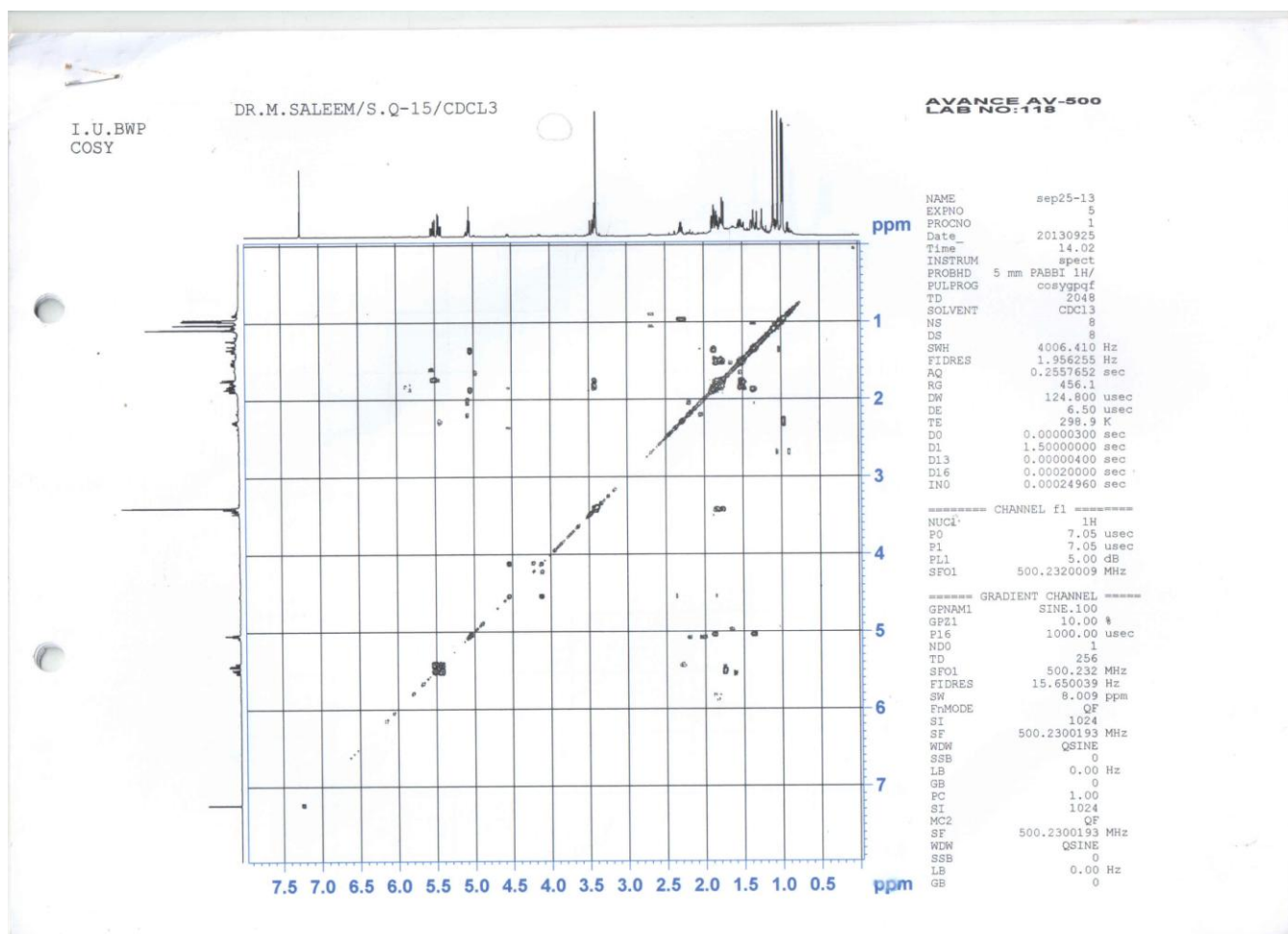
S9: ^{13}C -NMR 135-DEPT Spectrum of Compound **1** (From 10 to 150 ppm)



S10: ^{13}C -NMR 135-DEPT Spectrum of Compound **1** (From 16 to 32 ppm)



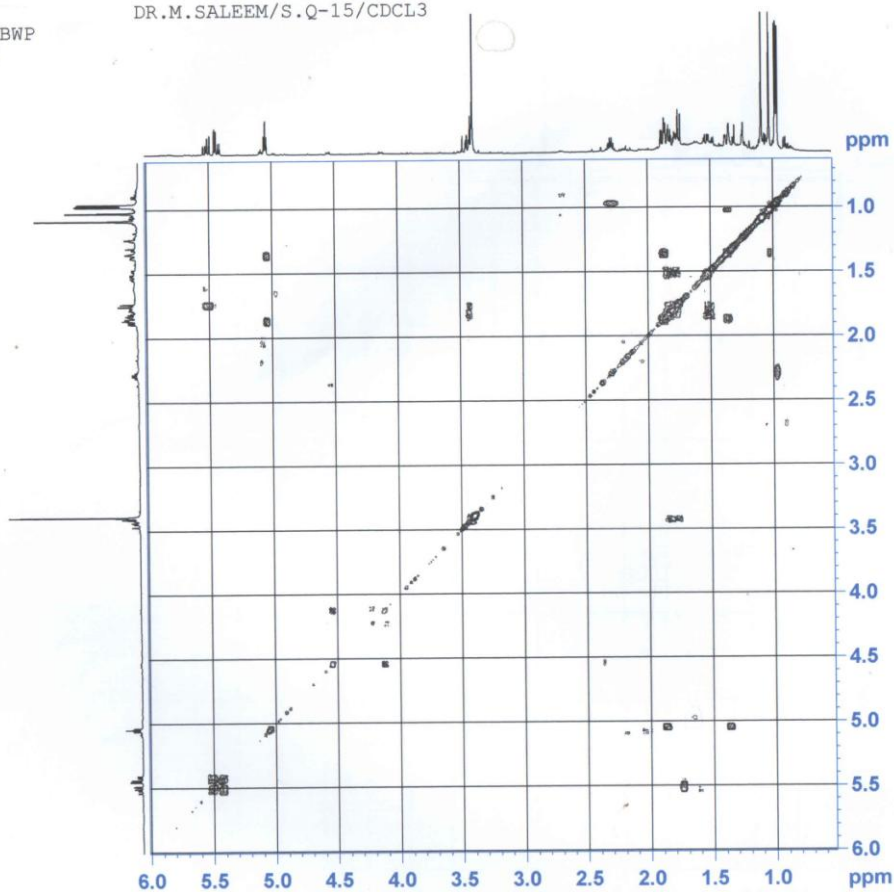
S11: ^{13}C -NMR 90-DEPT Spectrum of Compound **1** (From 10 to 150 ppm)



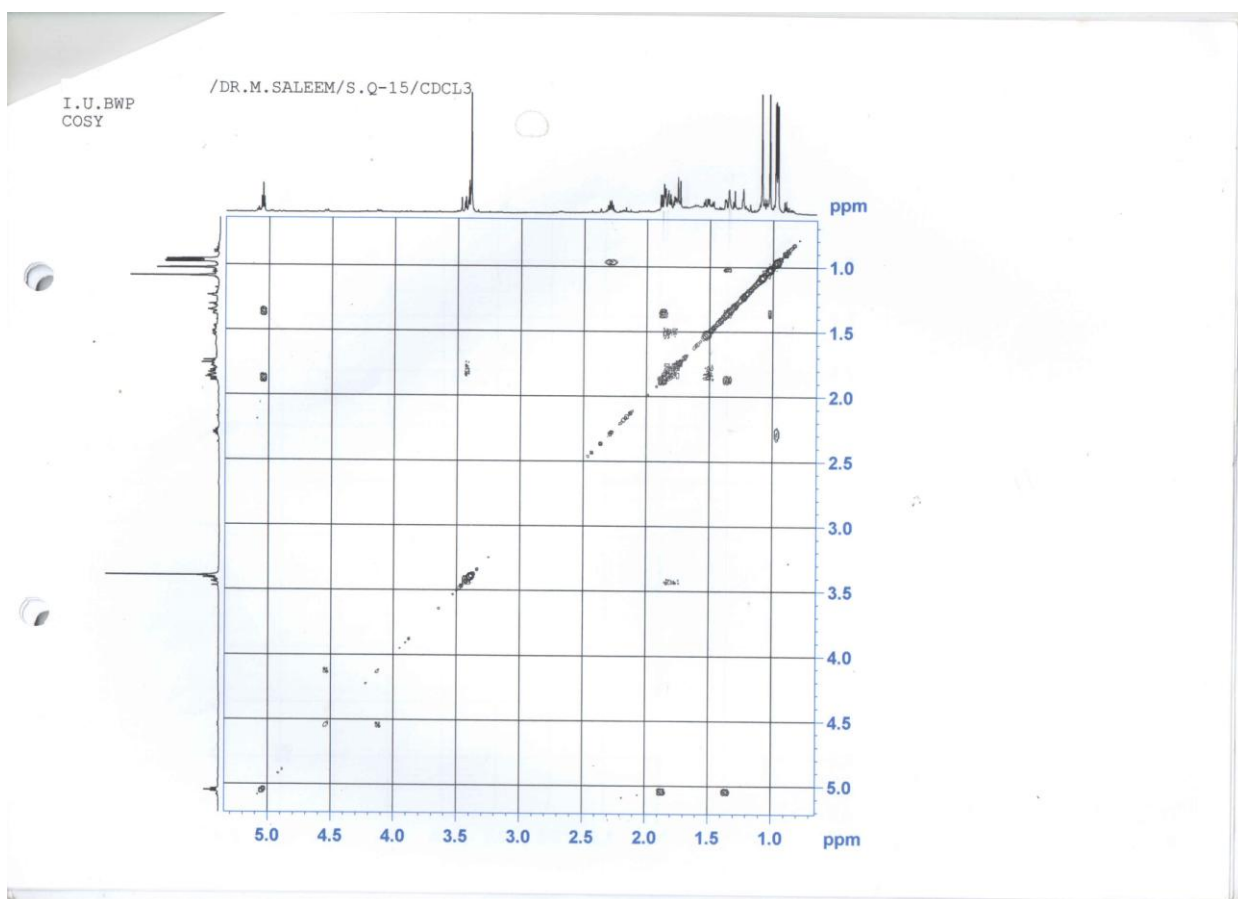
S12: Full COSY (600 MHz) Spectrum of Compound **1**

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COSY

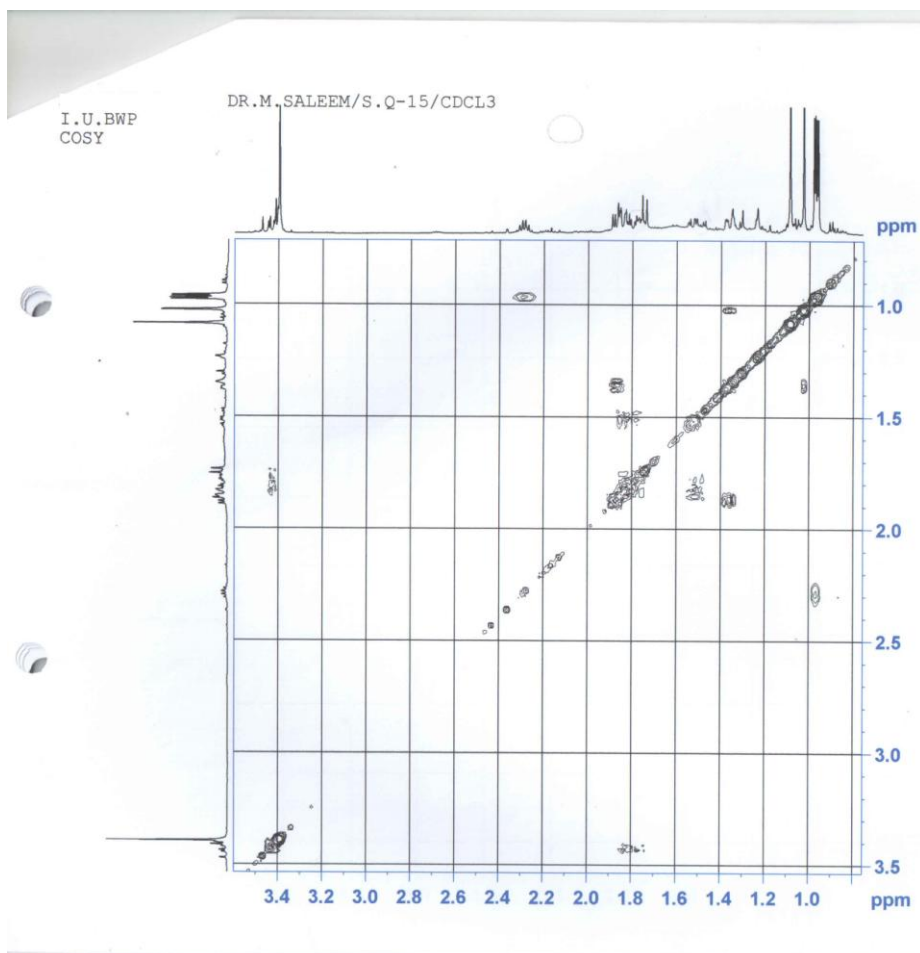
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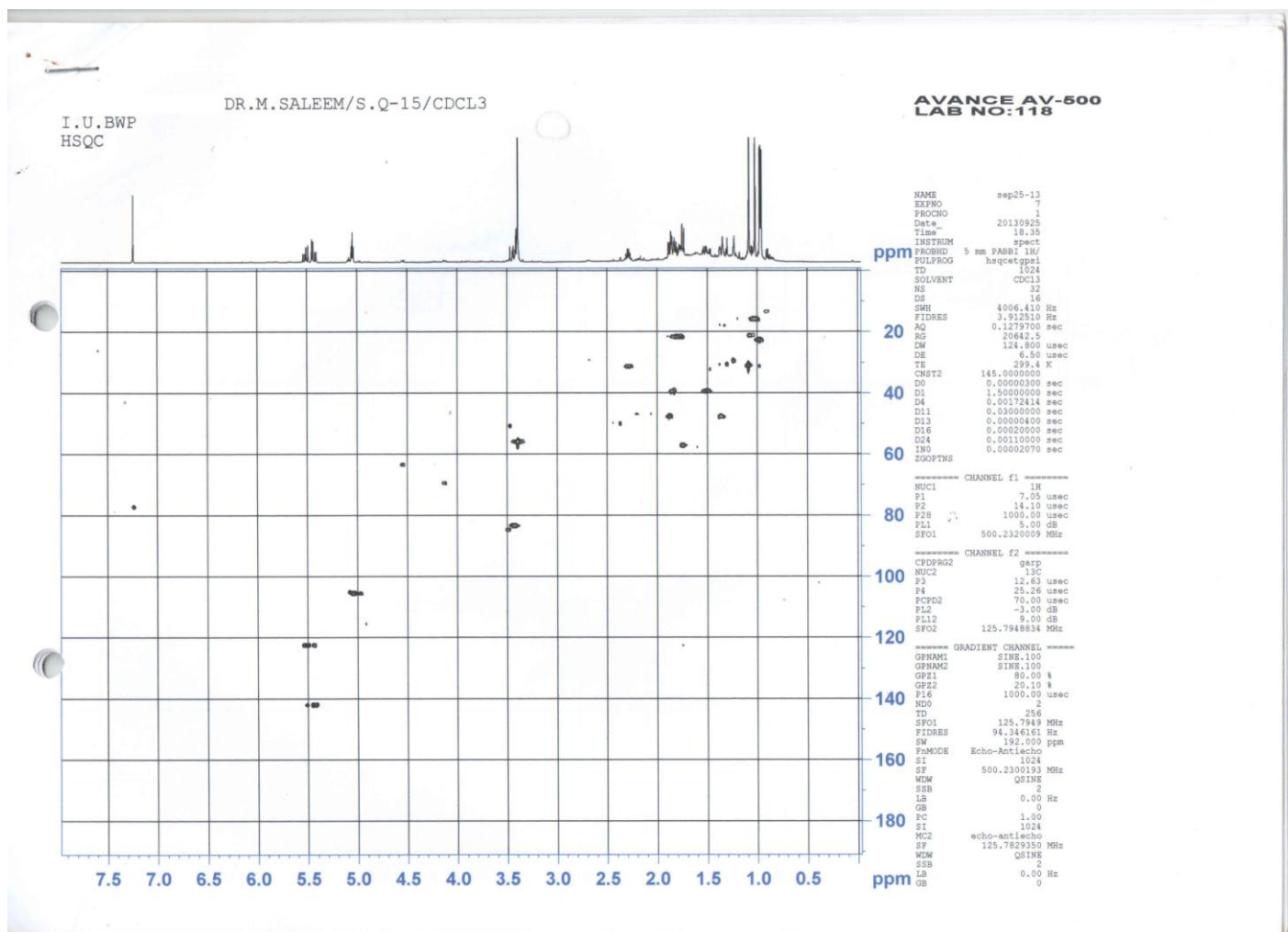
S13: COSY Spectrum of Compound **1** (From 0.5 to 6.0 ppm)



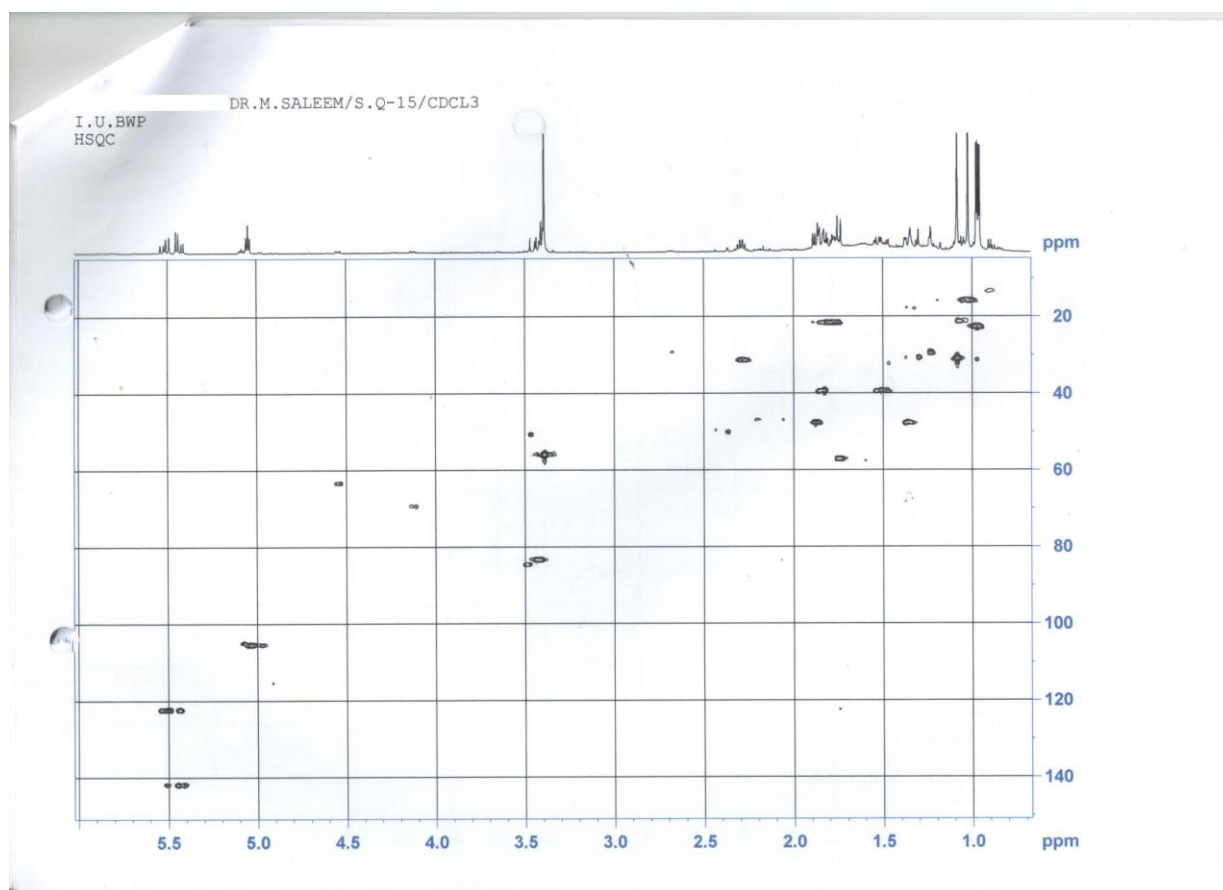
S14: COSY Spectrum of Compound **1** (From 0.5 to 5.5 ppm)



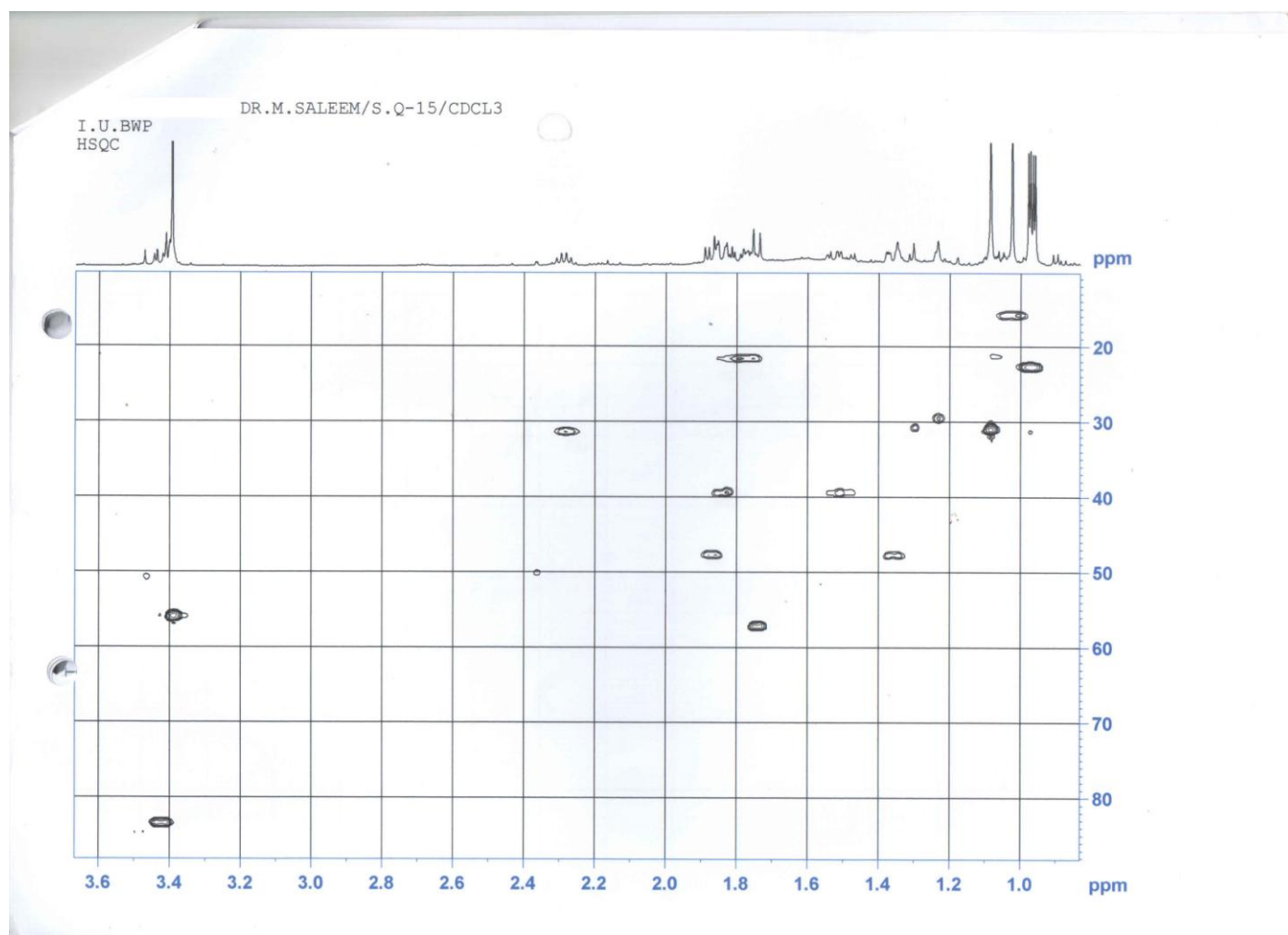
S15: COSY Spectrum of Compound **1** (From 0.5 to 3.4 ppm)



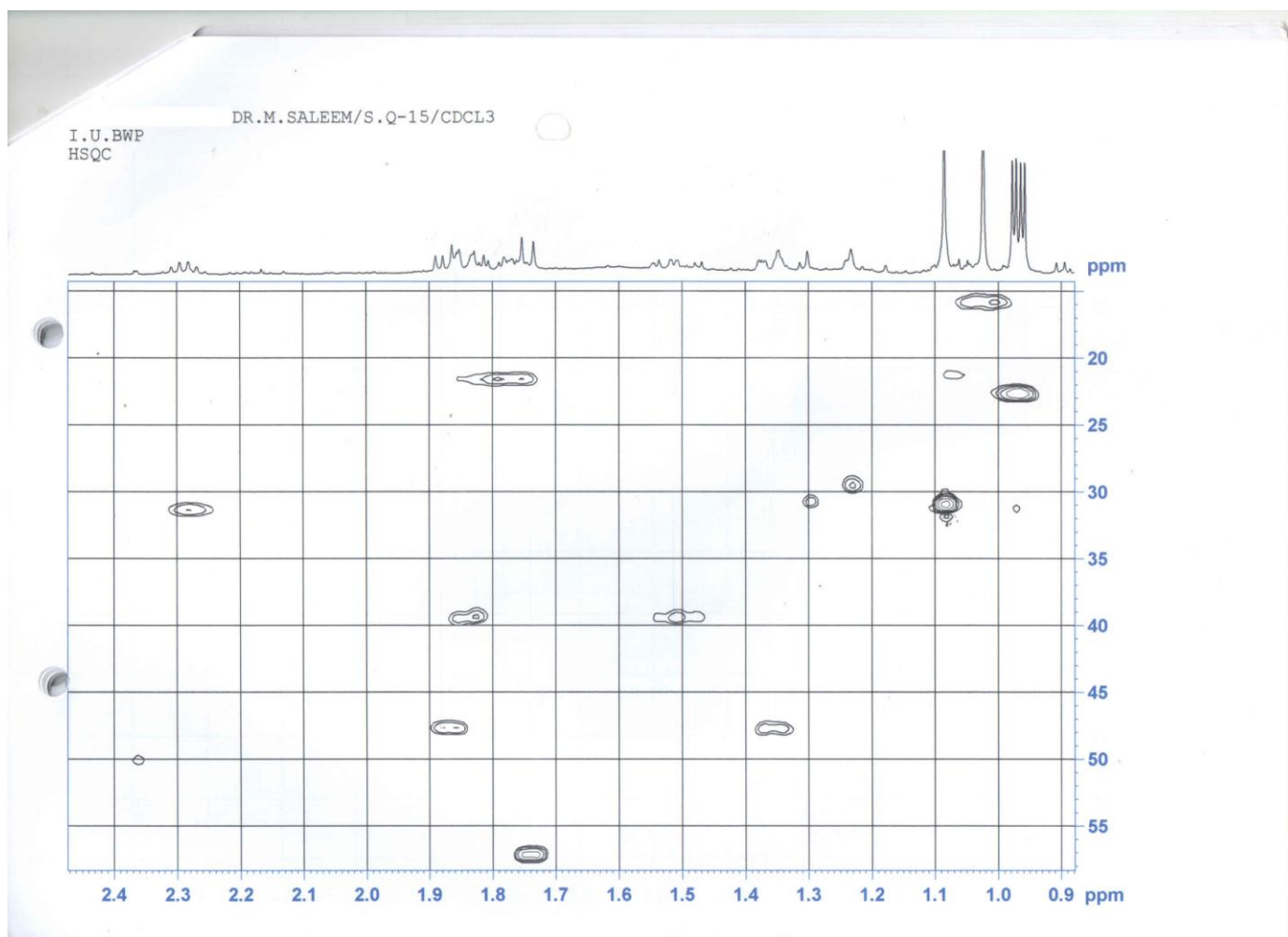
S16: HSQC (600 MHz) Spectrum of Compound **1**



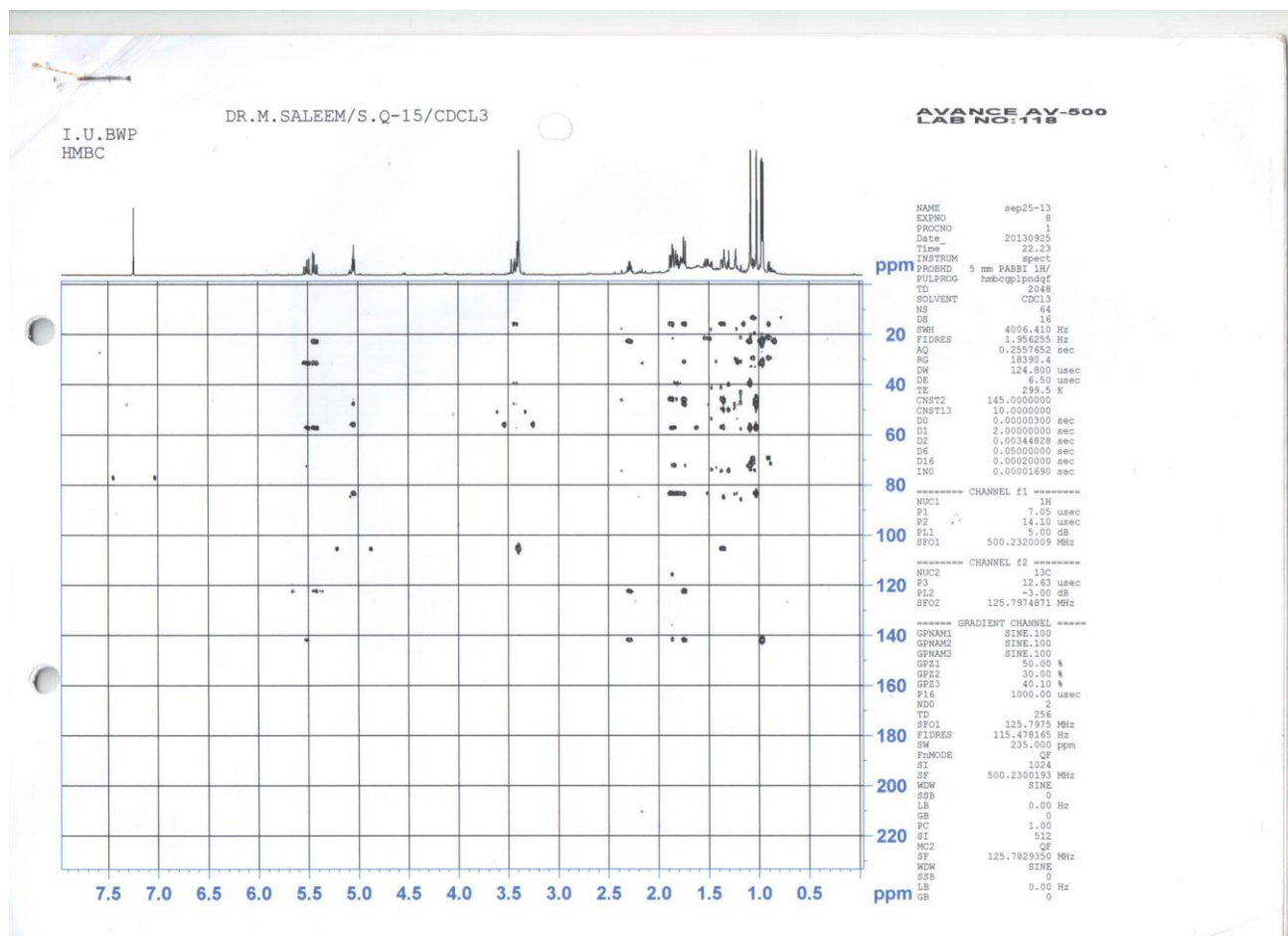
S17: HSQC Spectrum of Compound **1** (From 00 to 150 ppm)



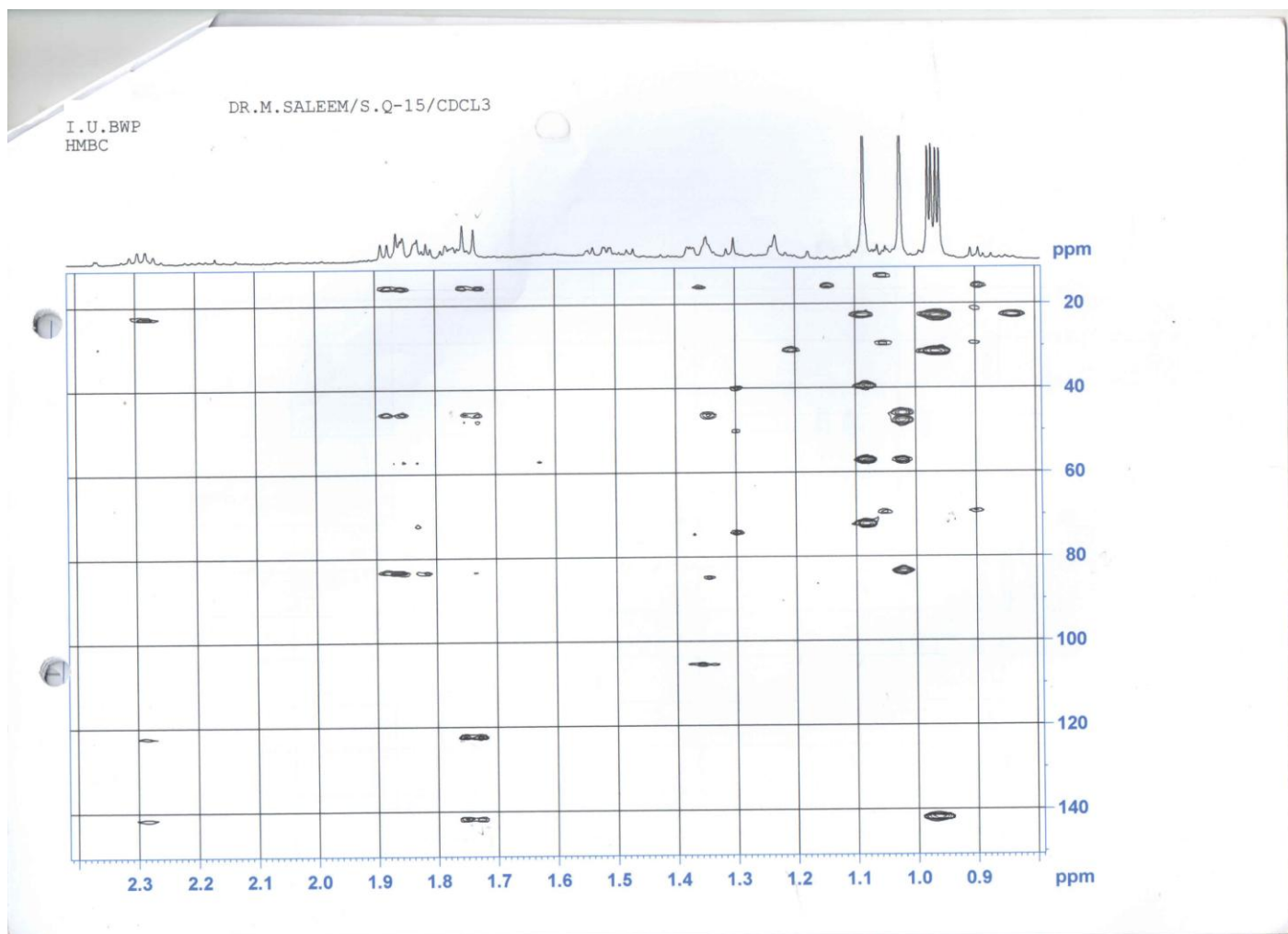
S18: HSQC Spectrum of Compound **1** (From 00 to 90 ppm)



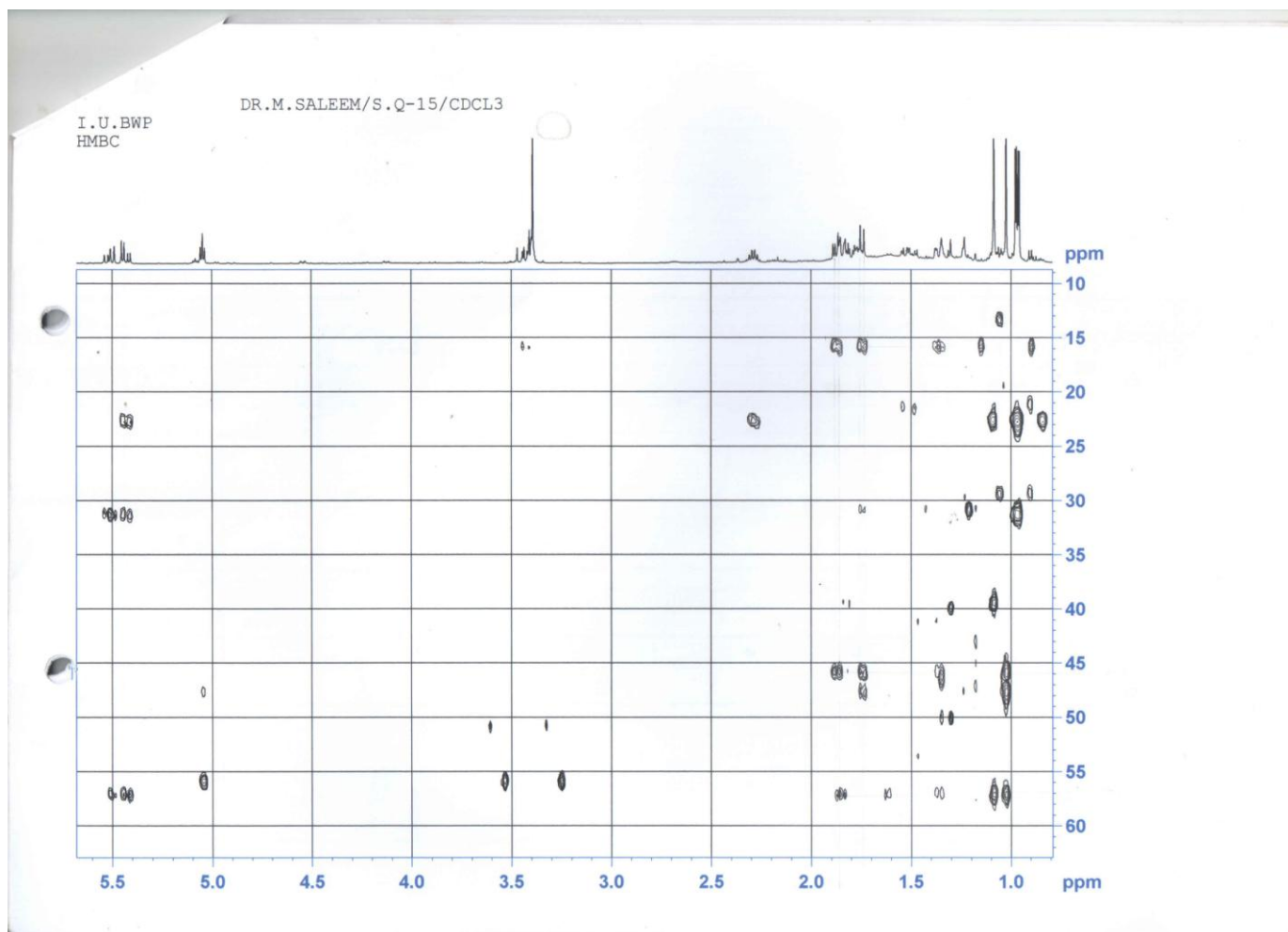
S19: HSQC Spectrum of Compound **1** (From 00 to 60 ppm)



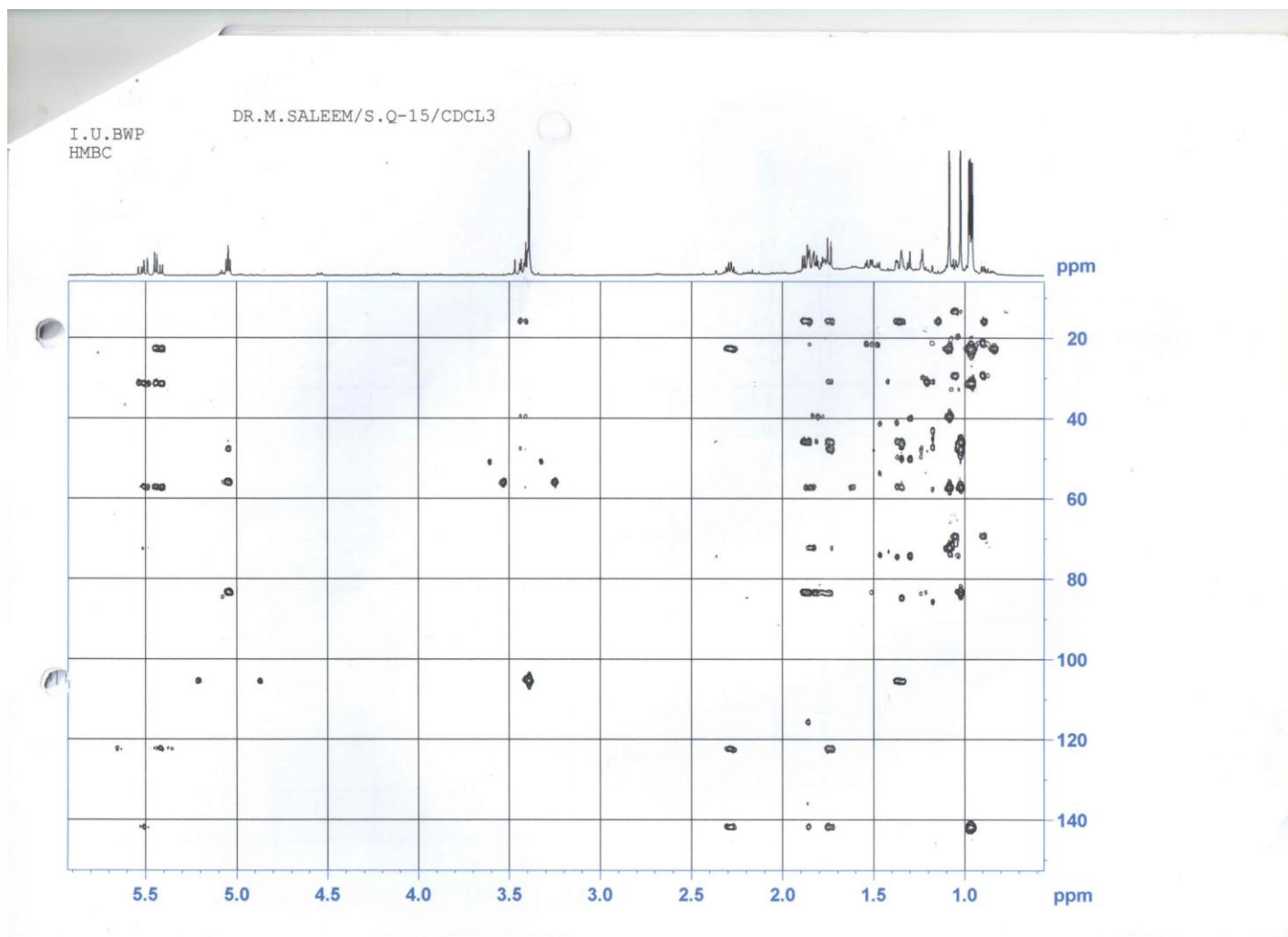
S20: HMBC Spectrum of Compound 1



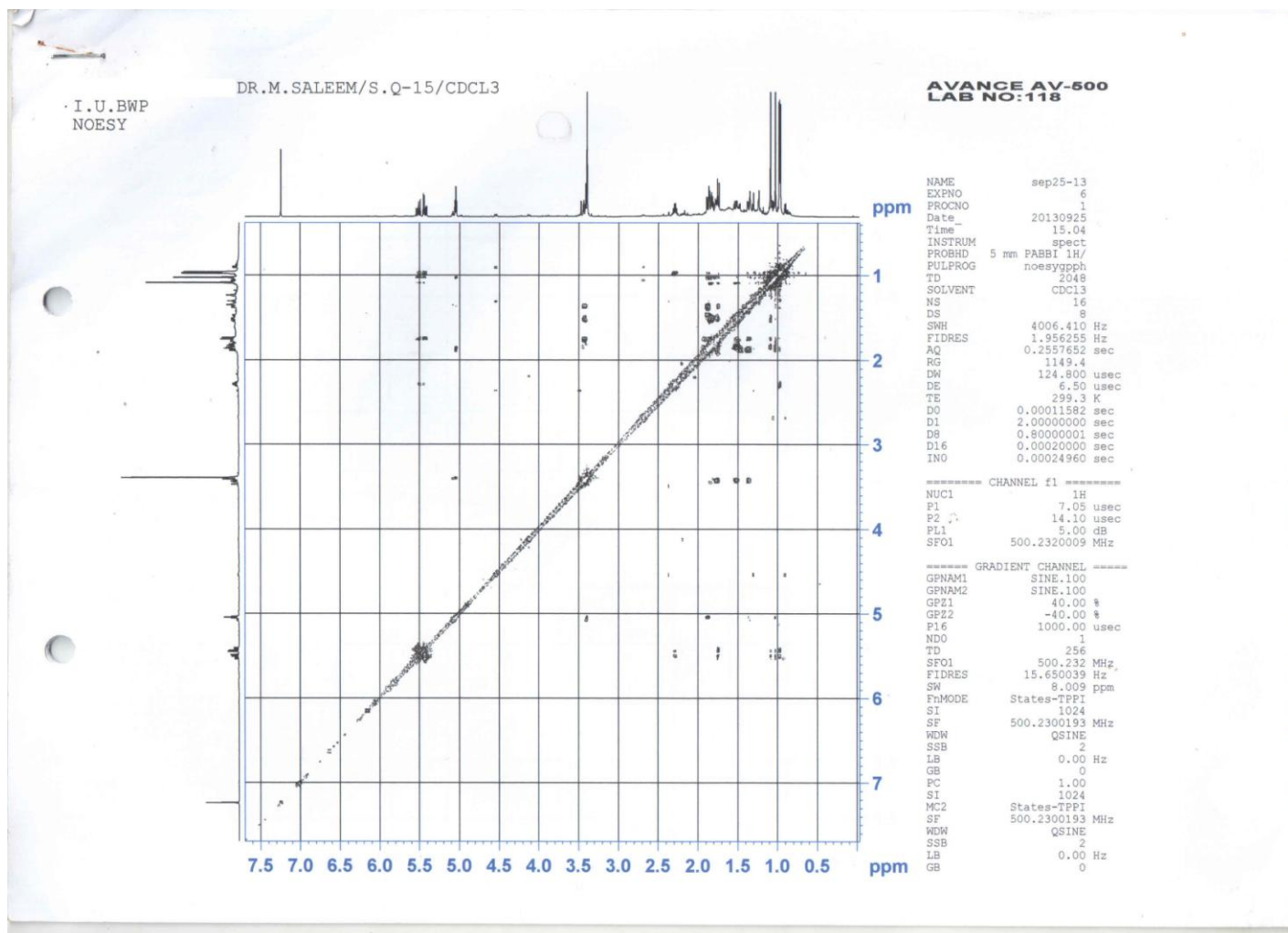
S21: HMBC Spectrum of Compound **1** (From 00 to 150 ppm)



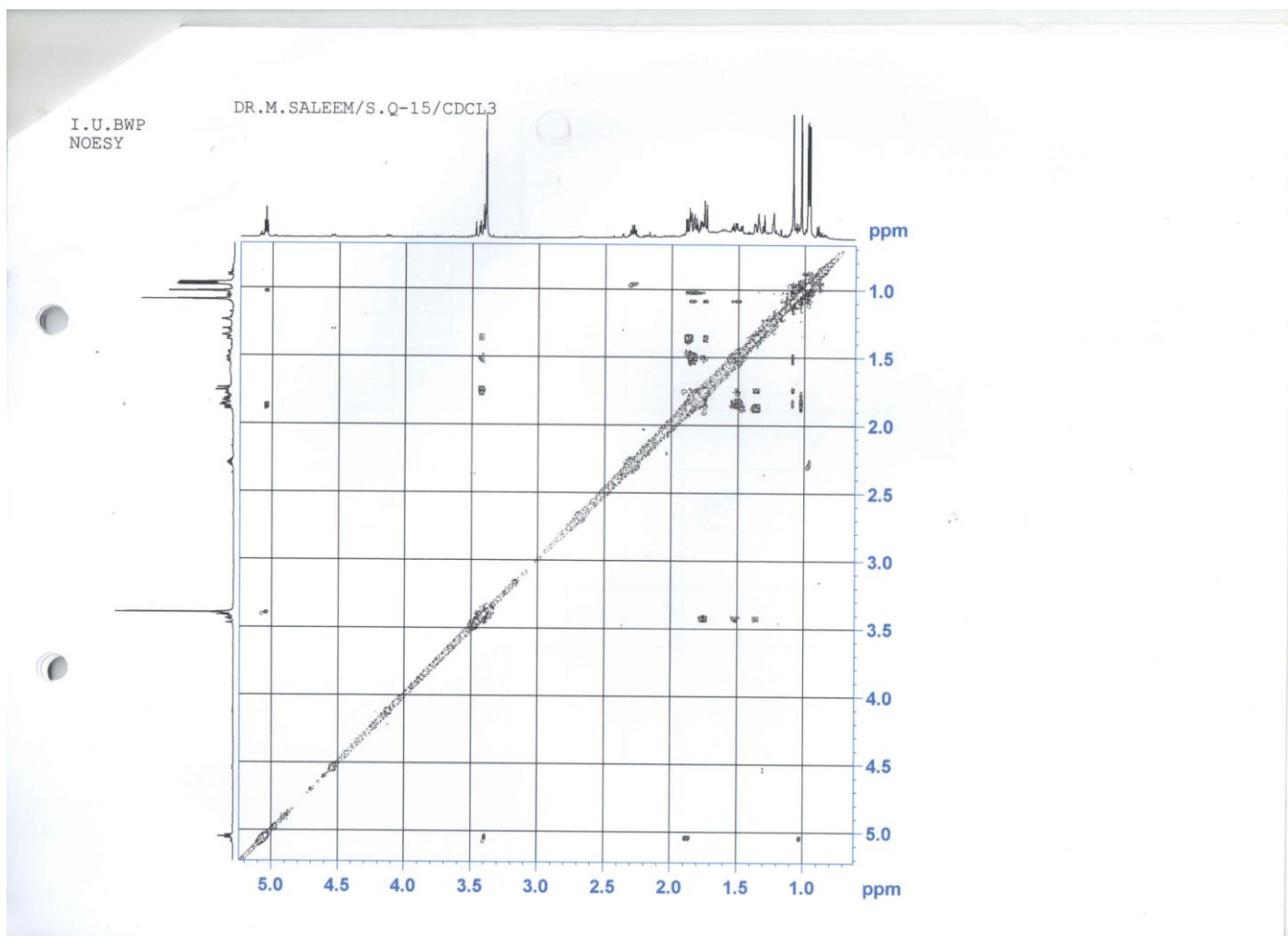
S22: HMBC Spectrum of Compound **1** (From 00 to 60 ppm)



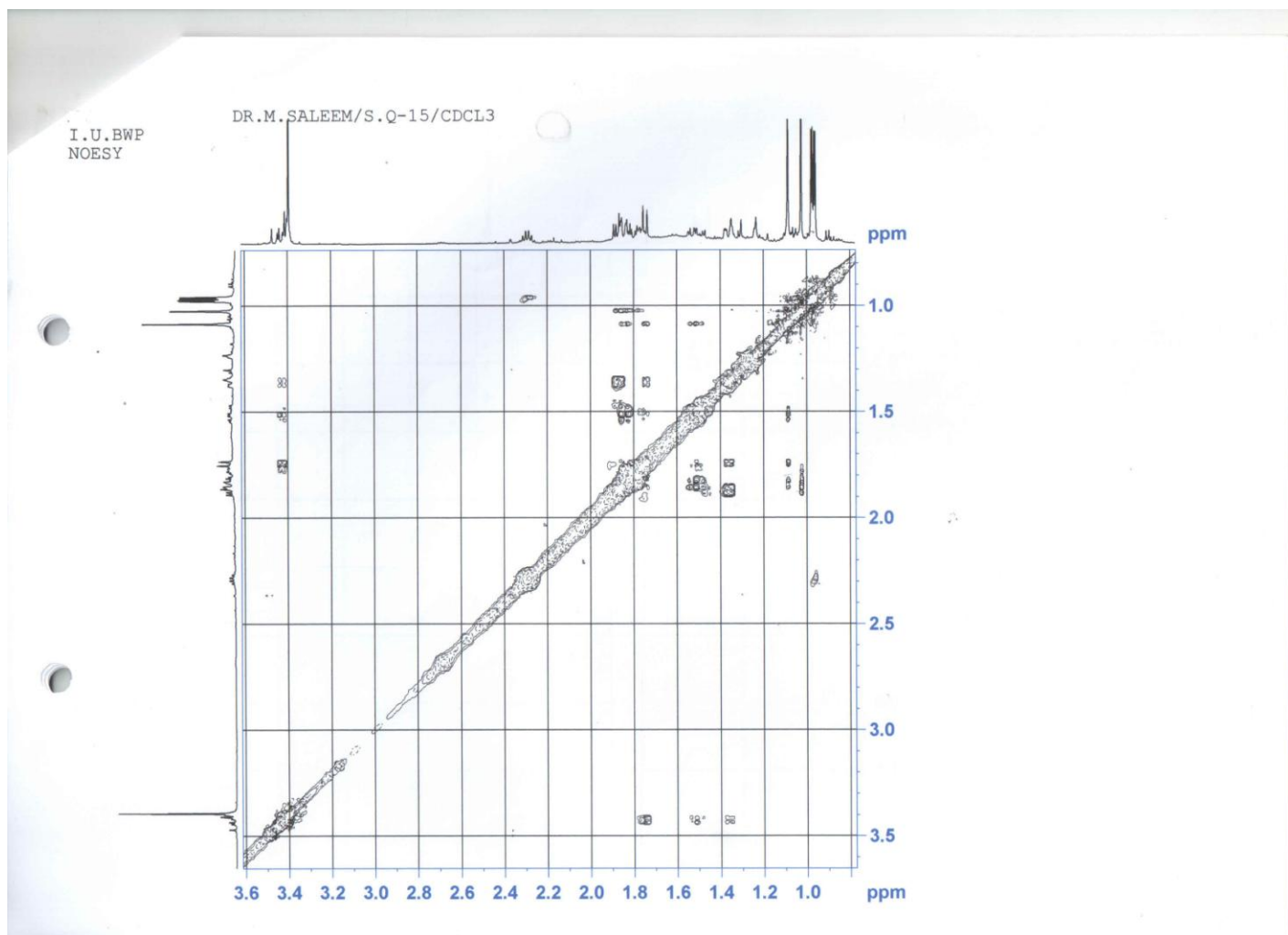
S23: HMBC Spectrum of Compound **1** (From 00 to 150 ppm)



S24: NOESY Spectrum of Compound **1** (From 00 to 8.0 ppm)



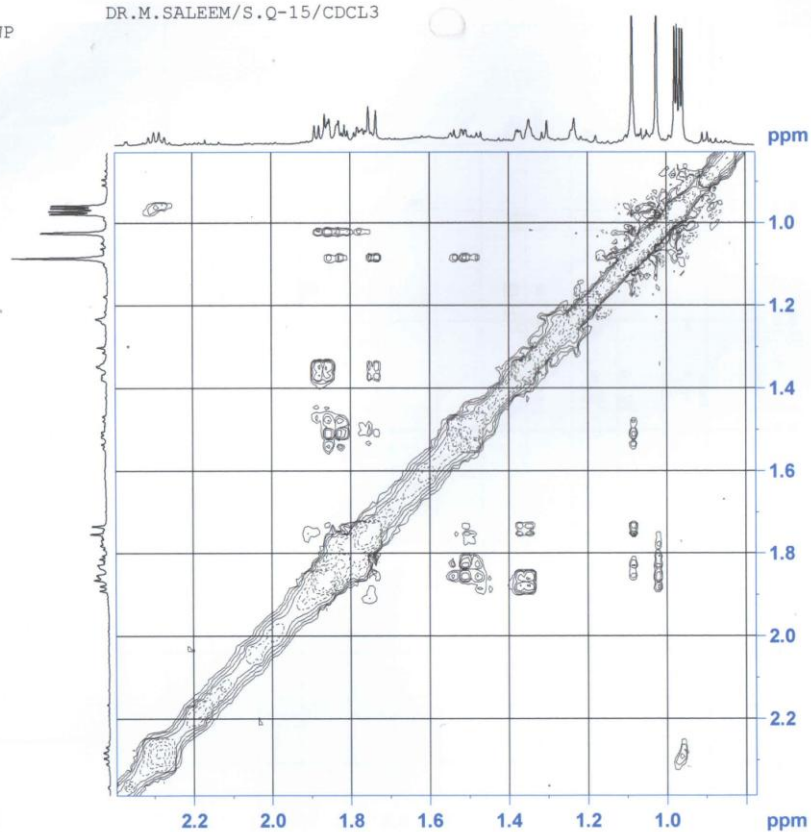
S25: NOESY Spectrum of Compound **1** (From 00 to 5.5 ppm)



S26: NOESY Spectrum of Compound **1** (From 00 to 3.6 ppm)

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NOESY

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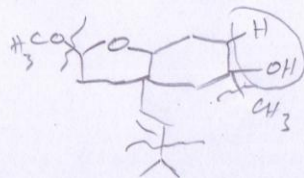
S27: NOESY Spectrum of Compound **1** (From 0.0 to 2.2 ppm)

File Name: S.Q-15
 Sample: M. Imran Touseef/Dr. M. Saleem, Chem Deptt. The Islamia University of Bahawalpur
 Instrument: JEOL JMS600
 Inlet: My Inlet

Date Run: 21-09-2016
 Ionization mode: HRMS⁺

Time Run: 11:35:34
 Run By: Lab 102
 Printed by: Lab 102

Mass	Relative Intensity	Theoretical Delta Mass	Delta [ppm]	Delta [mmu]	RDB	Composition
→ 268.203654	5.6704	268.203845	2.9	0.9	4.9	C ₁₆ H ₂₈ O ₃ → (M) ⁺
253.180167	6.7613	253.180370	1.9	0.8	2.7	C ₁₅ H ₂₅ O ₃ → (M-Me) ⁺
250.193118	16.9562	250.193280	6.3	0.7	8.4	C ₁₆ H ₂₆ O ₂ → (M-18) ⁺
237.185301	27.4628	237.185455	7.9	1.3	14.0	C ₁₅ H ₂₅ O ₂ → (M-OMe) ⁺
225.148997	11.5544	225.149070	2.3	0.9	3.9	C ₁₅ H ₂₁ O ₃ → (M-C ₃ H ₇) ⁺
→ 219.174650	85.67541	219.174890	29.1	8.1	16.3	C ₁₅ H ₂₁ O → (M-OMe-H ₂ O) ⁺
204.151226	22.1345	204.151415	7.0	3.2	4.3	C ₁₄ H ₂₀ O
199.133231	9.5789	199.133420	4.1	1.1	4.3	C ₁₁ H ₁₉ O ₃
192.115454	34.2357	192.115660	19.5	6.7	0.9	C ₁₂ H ₁₆ O ₂
184.109765	22.8764	184.109945	11.2	5.1	3.2	C ₁₀ H ₁₆ O ₃
181.122671	19.4453	181.122855	14.7.5	3.7	6.1	C ₁₁ H ₁₇ O ₂
168.114901	13.3471	168.115030	12.4	6.4	5.5	C ₁₀ H ₁₆ O ₂
150.104299	23.6512	150.104465	11.2	6.3	7.4	C ₁₀ H ₁₄ O



S28: HRMS data of compound **1** (m/z 150-268)