Supporting Information for

Model Studies of the (6–4) Photoproduct Photoreactivation: Efficient Photosensitized Splitting of Thymine Oxetane Units by Covalently Linked Tryptophan in High Polarity Solvents

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- ^{13}C NMR spectra of compounds **4, 5, 8a, 8b, 1, 2a, 2b** and **3** S11–S18

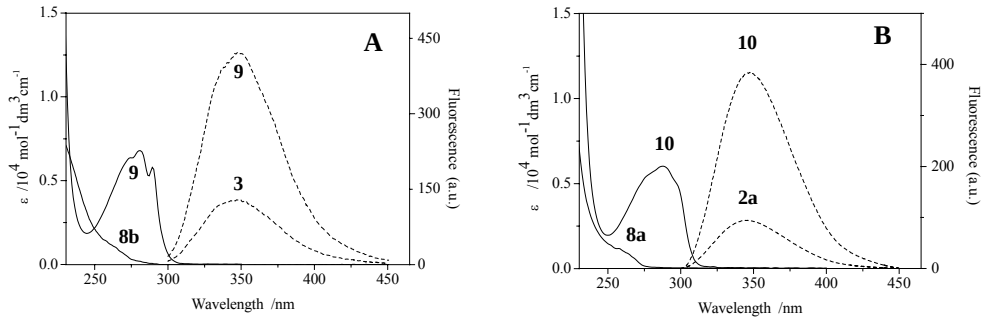


Fig. S1 UV absorption spectra (solid) and/or fluorescence emission spectra (dash) (λ_{ex} = 290 nm) of compounds **9**, **8b** and **3** (A), **10**, **8a** and **2a** (B), in methanol.

The detail for measurement of splitting quantum yields

The absorbances at 270 nm (A_{270}) were measured at certain time intervals. The A_{270} change (ΔA_{270}) of the solution depends on the splitting reaction. The change of mole extinction coefficients ($\Delta\varepsilon_{270}$) were obtained from those measured of model compounds **1–3** and the splitting products **4**, **5** and benzophenone or benzaldehyde at 270 nm, and the value of $\Delta\varepsilon_{270}$ employed was 1.80×10^4 mol^{-1} $cm^{-1}dm^{-3}$ for **1** and **2**, 1.18×10^4 mol^{-1} $cm^{-1}dm^{-3}$ for **3**, respectively. The splitting concentration (c_{spl}) of the model compound was obtained from $\Delta A_{270}/\Delta\varepsilon_{270}$. The plot of c_{spl} against the irradiation time (t, min) is fitted as a well straight line. The rate of splitting reaction was obtained from the slope (B) of the line (Fig. S2). The intensity of the incident light I_0 was measured using ferrioxalate actinometry. The rate of proton absorbed (I_a) by solution was obtained in term of Beer's law, $I_a = I_0\,(1-10^{-A290})$. The absorbance of the model compound at 290 nm, A_{290} was determined before irradiation. Above these values allow the calculation of the quantum yield in terms of Φ_{spl} = (rate of oxetane split)/(rate of photon absorbed) = BV_0/I_a, wherein V_0 was the volume of irradiation solution, 3×10^{-3} L.

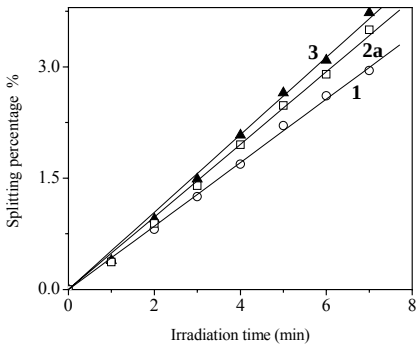


Fig. S2 Splitting rates determined for the model compounds **1**(○), **2a**(□) and **3**(▲) in methanol.

Figure S3 The ^{1}H NMR spectrum of compound **4**

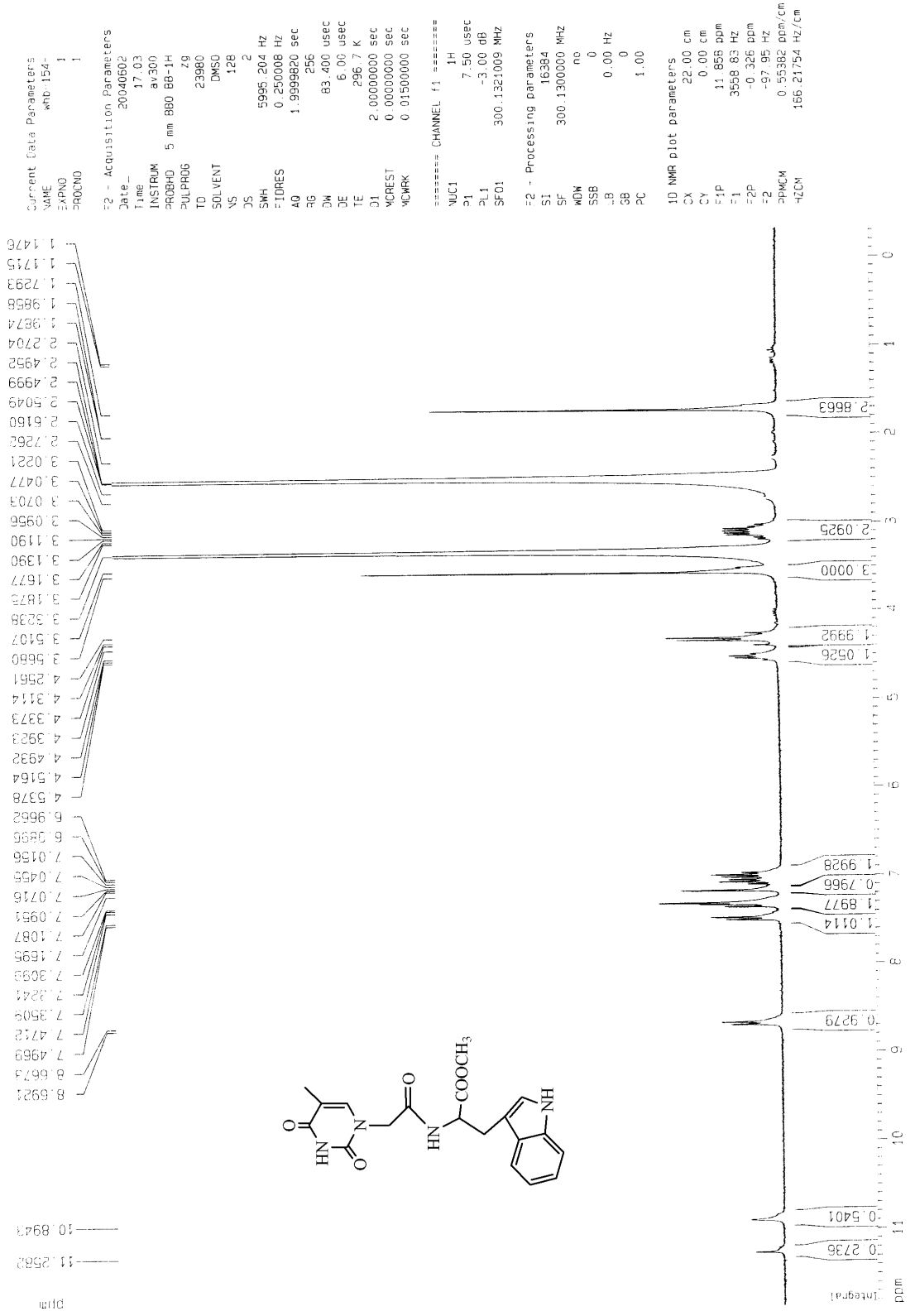


Figure S4 The ^{1}H NMR spectrum of compound **5**

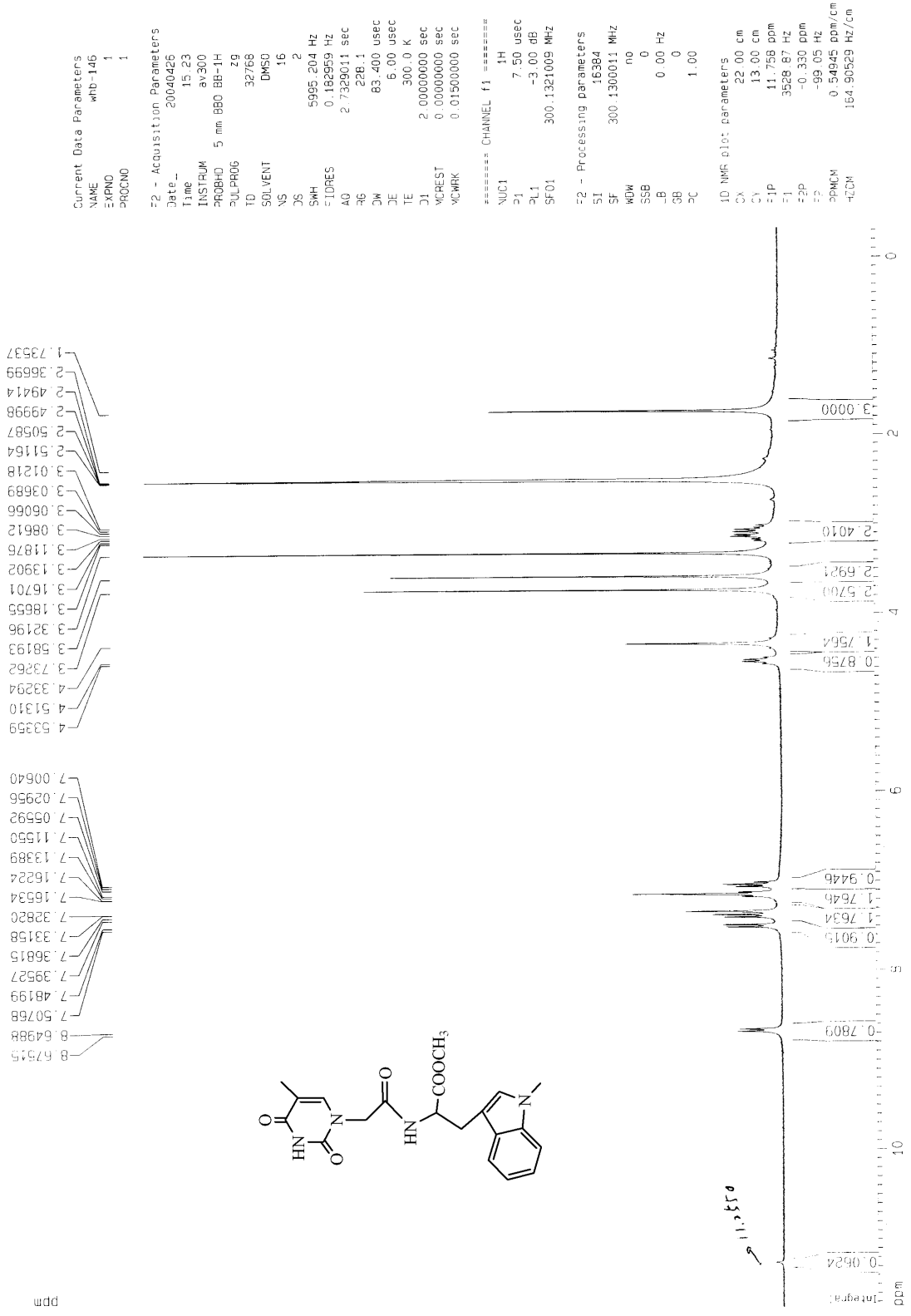


Figure S5 The ^{1}H NMR spectrum of compound **8a**

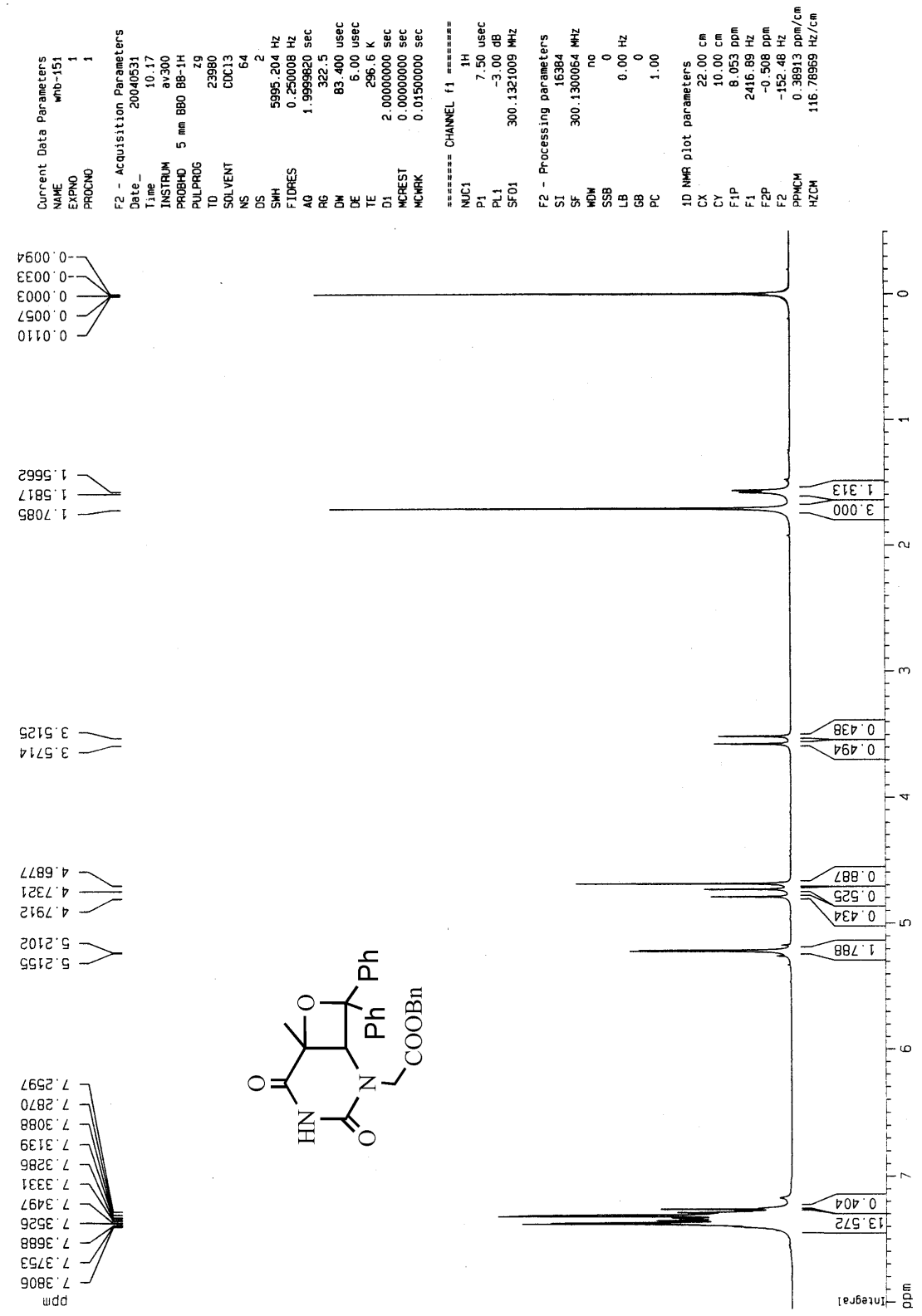


Figure S6 The ^{1}H NMR spectrum of compound **8b**

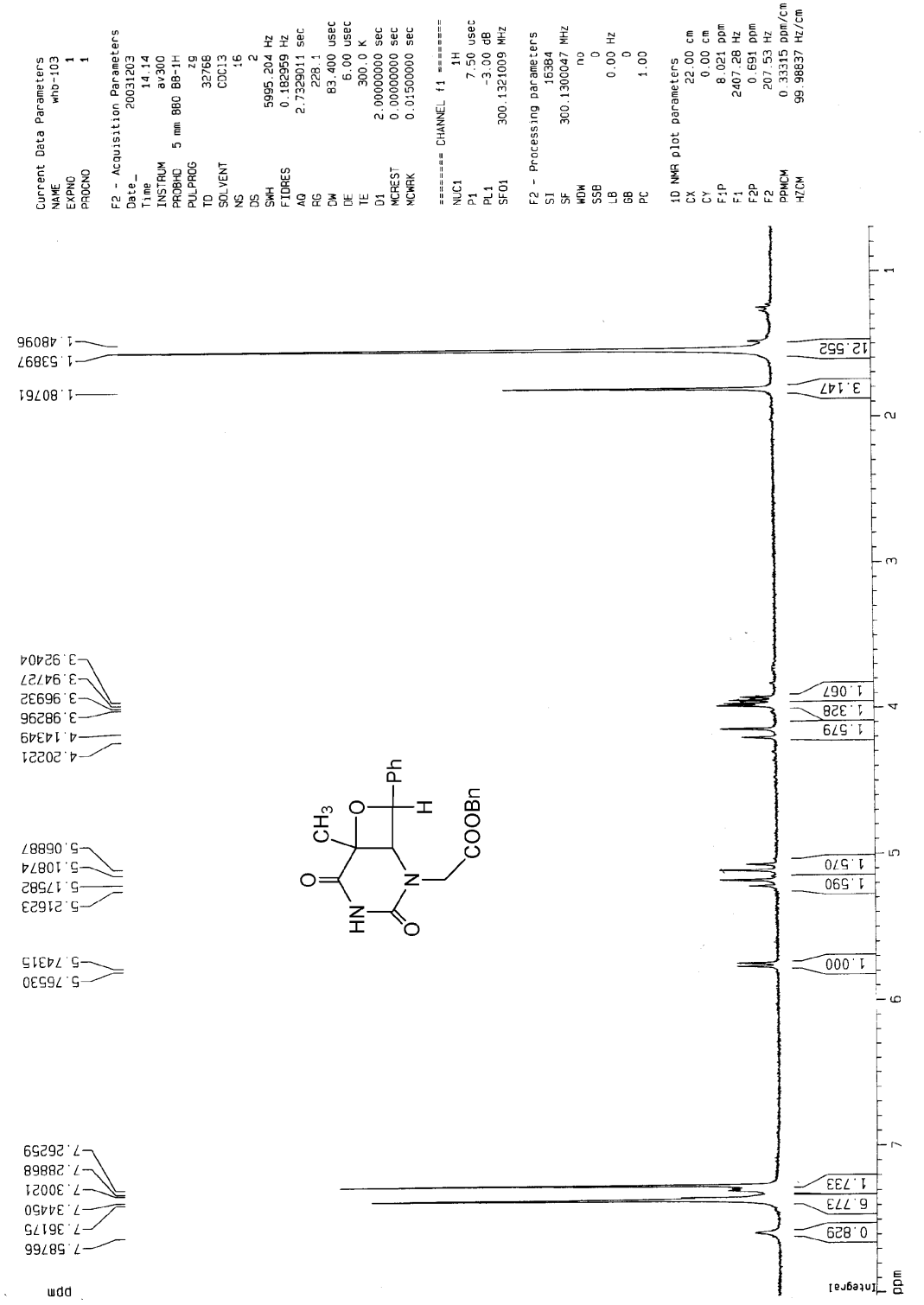


Figure S7 The ^{1}H NMR spectrum of compound **1**

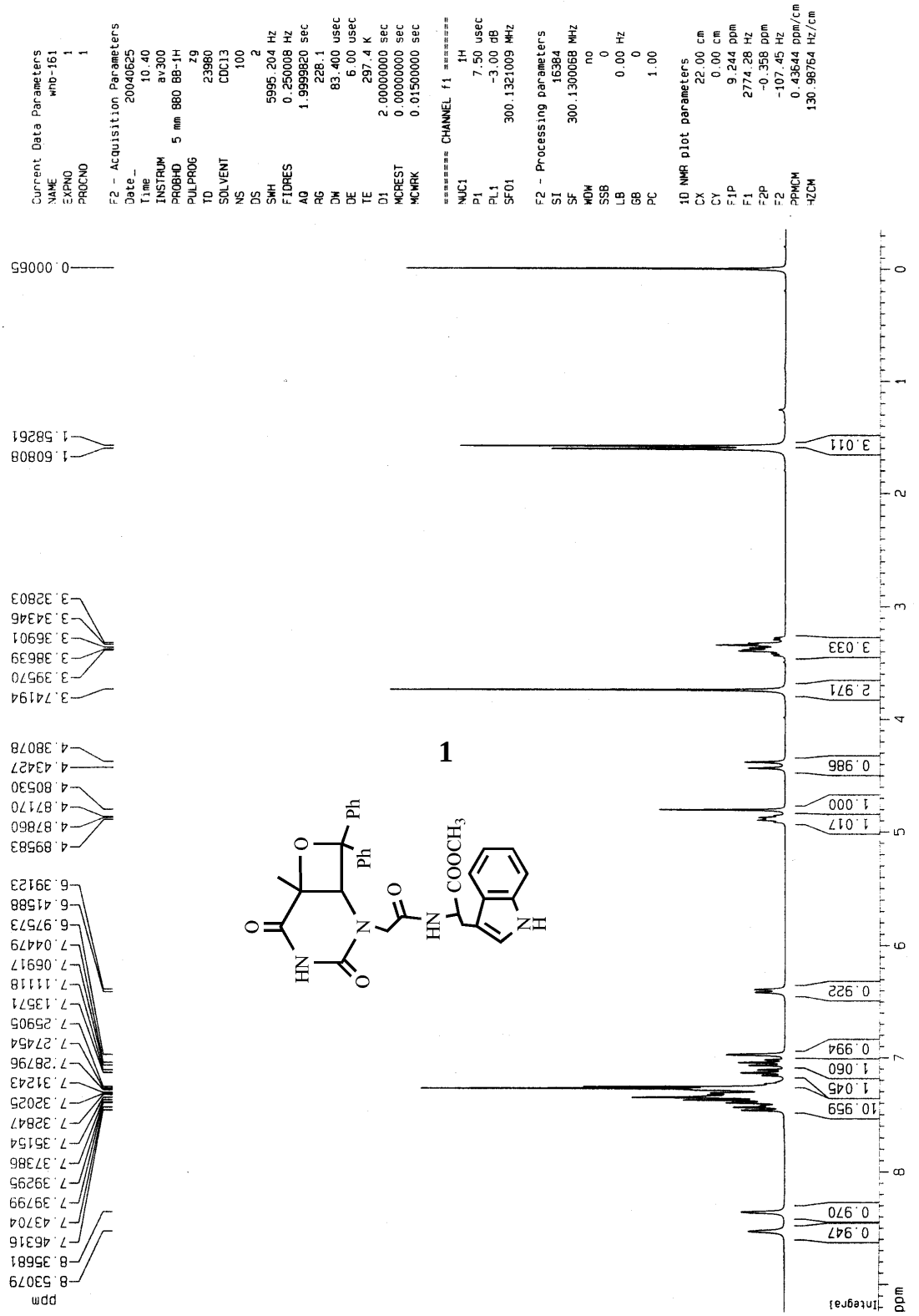


Figure S8 The ^{1}H NMR spectrum of compound **2a**

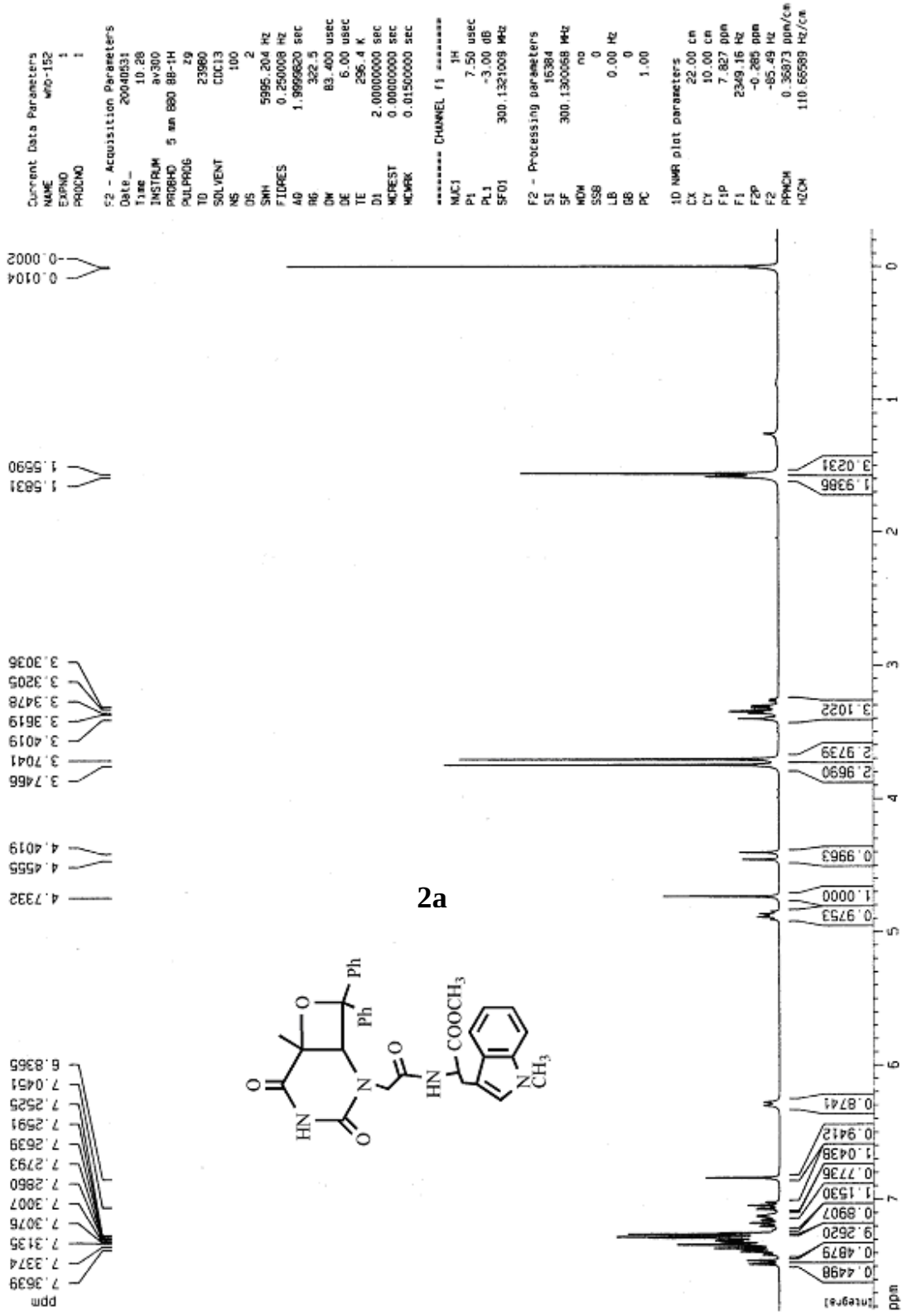
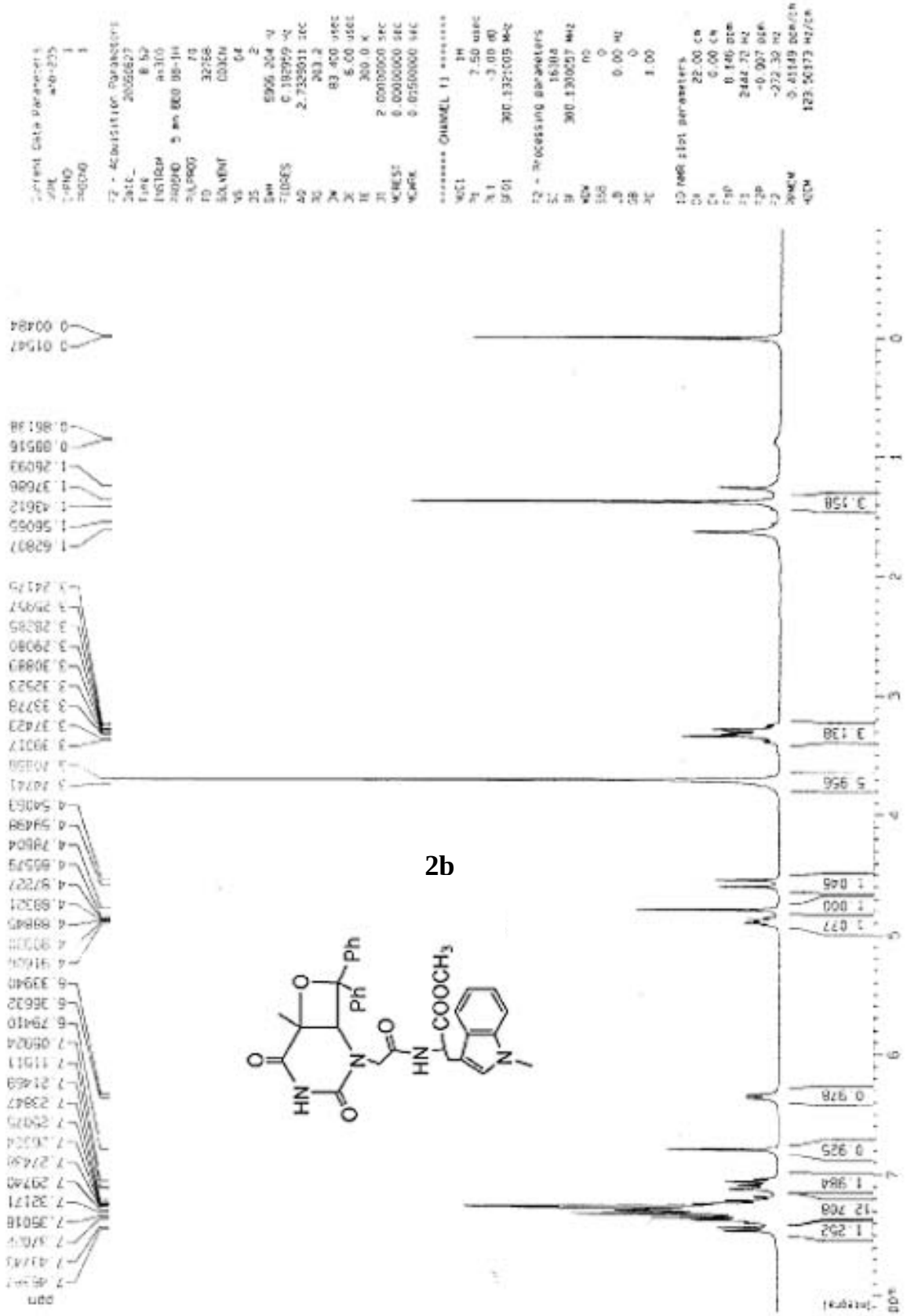


Figure S9 The ^{1}H NMR spectrum of compound **2b**



2b

Figure S10 The ^{1}H NMR spectrum of compound **3**

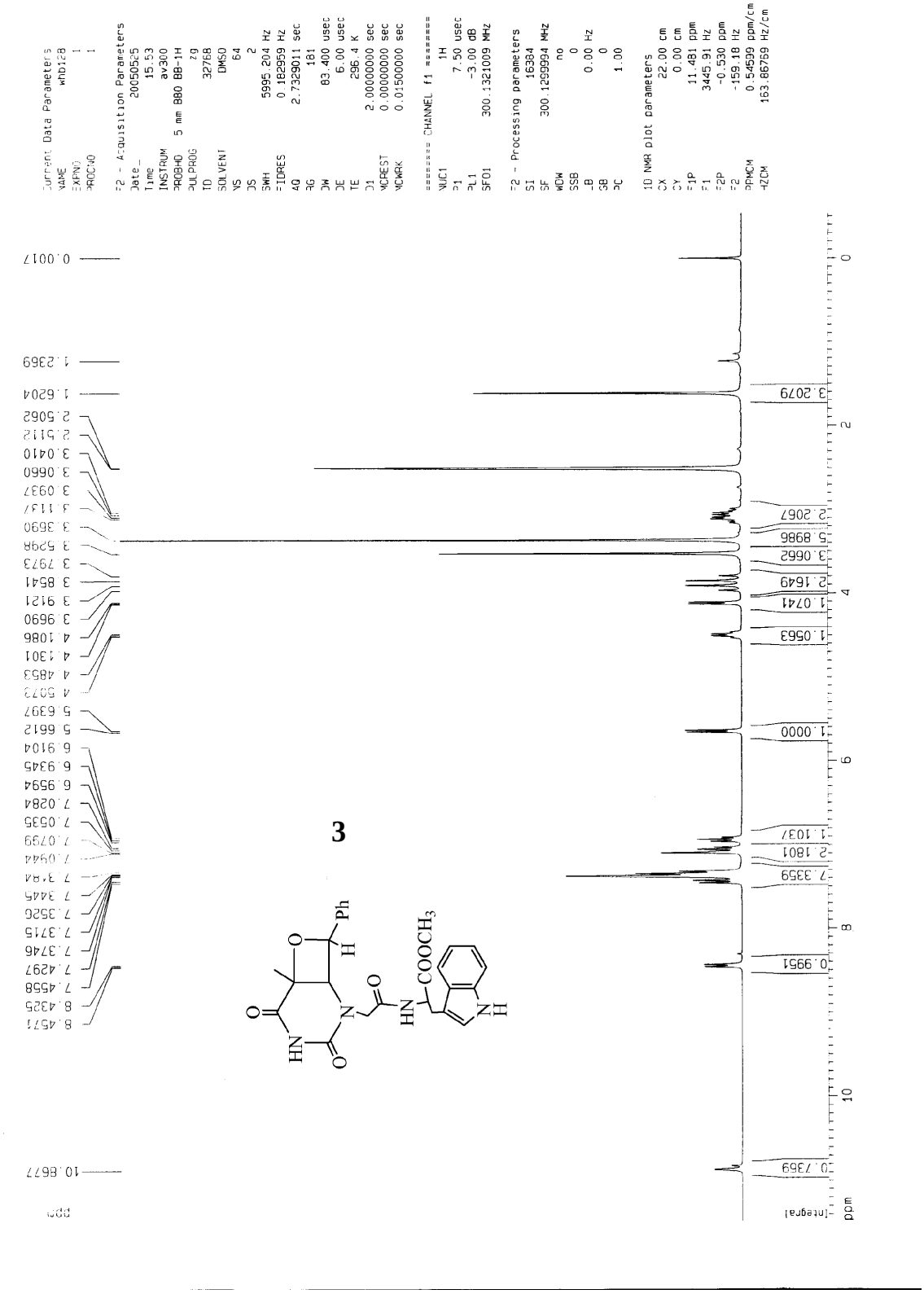


Figure S11 The ^{13}C NMR spectrum of compound **4**

Figure S12 The ^{13}C NMR spectrum of compound **5**

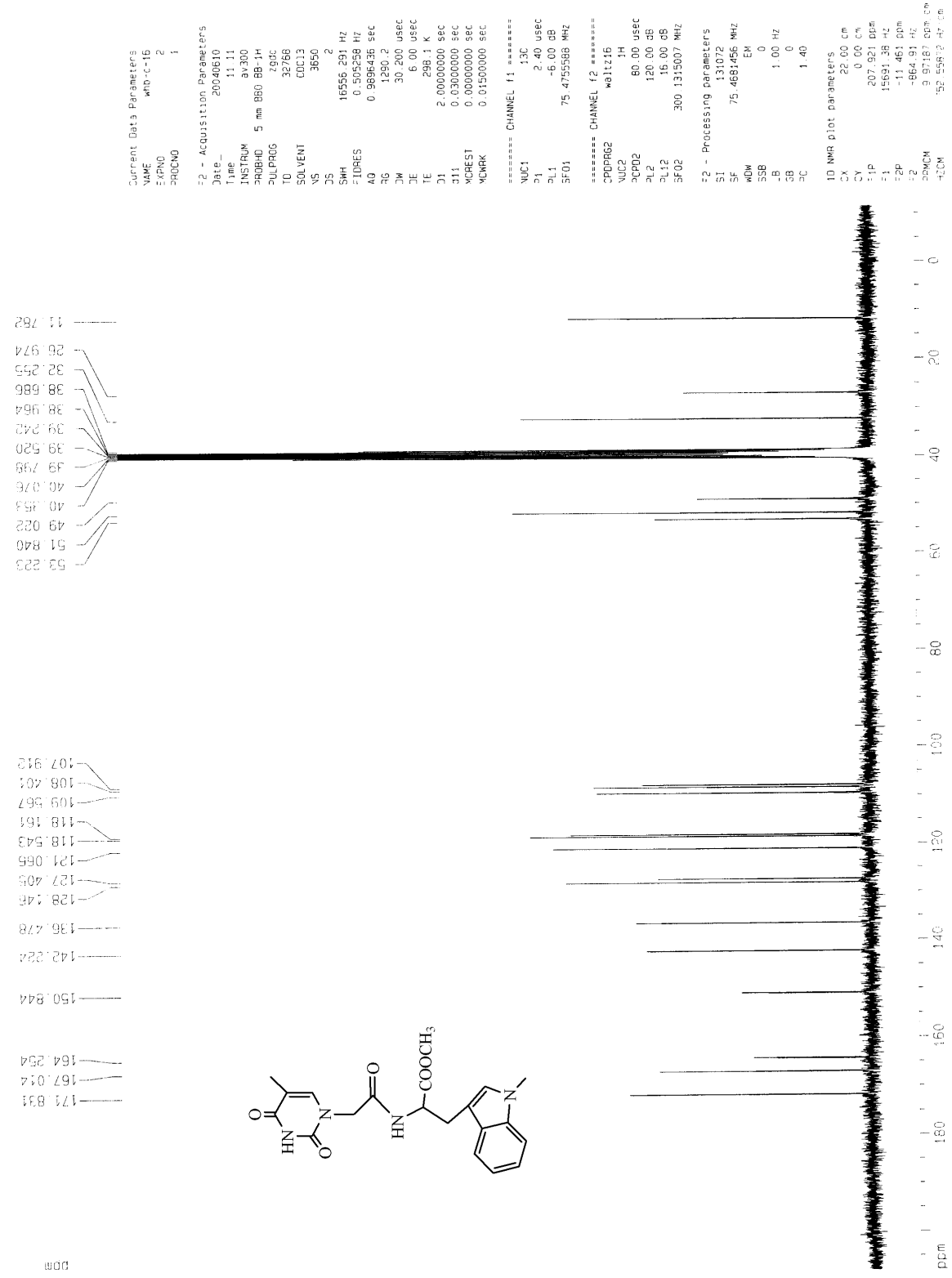


Figure S13 The ^{13}C NMR spectrum of compound **8a**

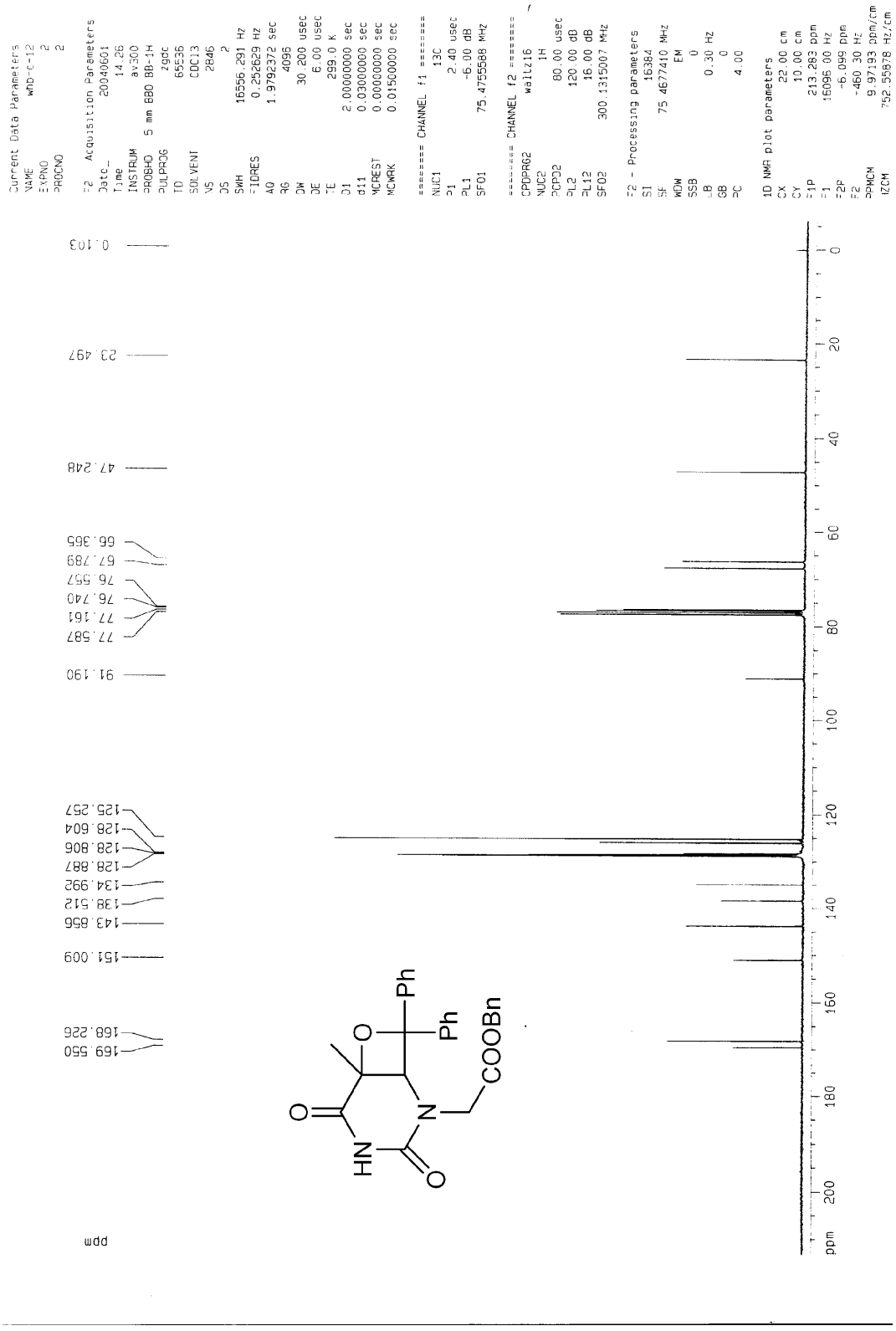


Figure S14 The ^{13}C NMR spectrum of compound **8b**

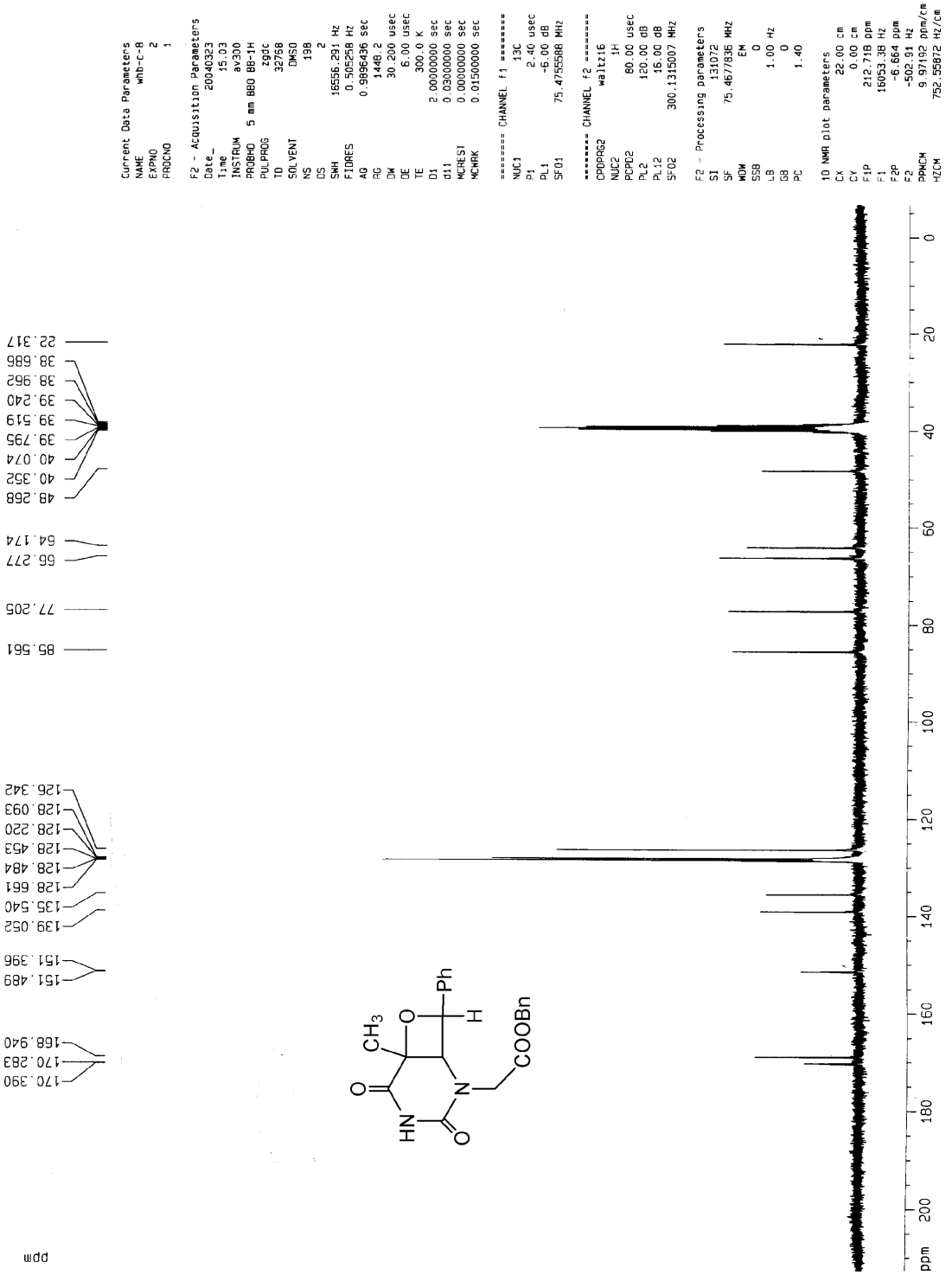


Figure S15 The ^{13}C NMR spectrum of compound **1**

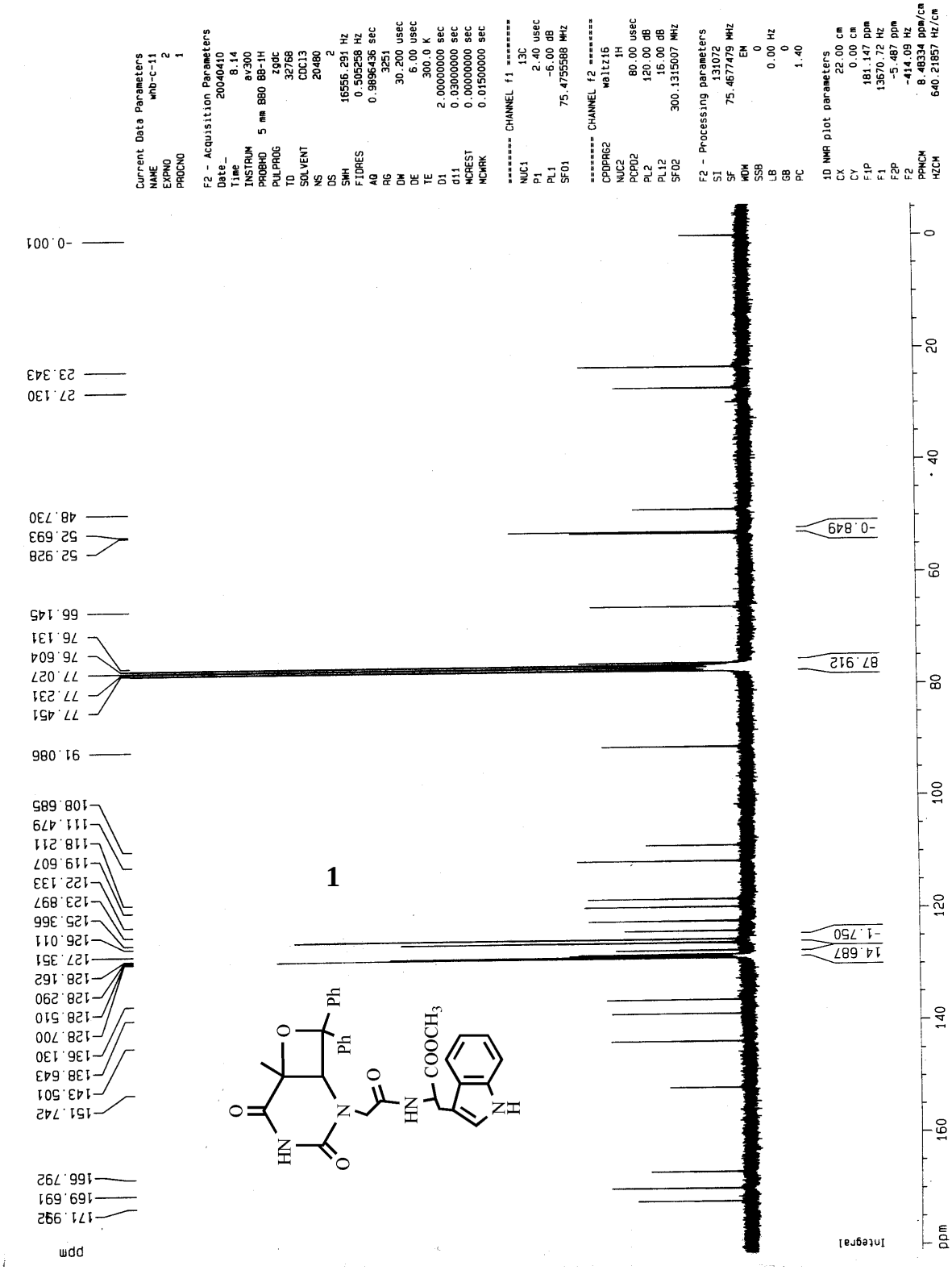


Figure S16 The ^{13}C NMR spectrum of compound **2a**

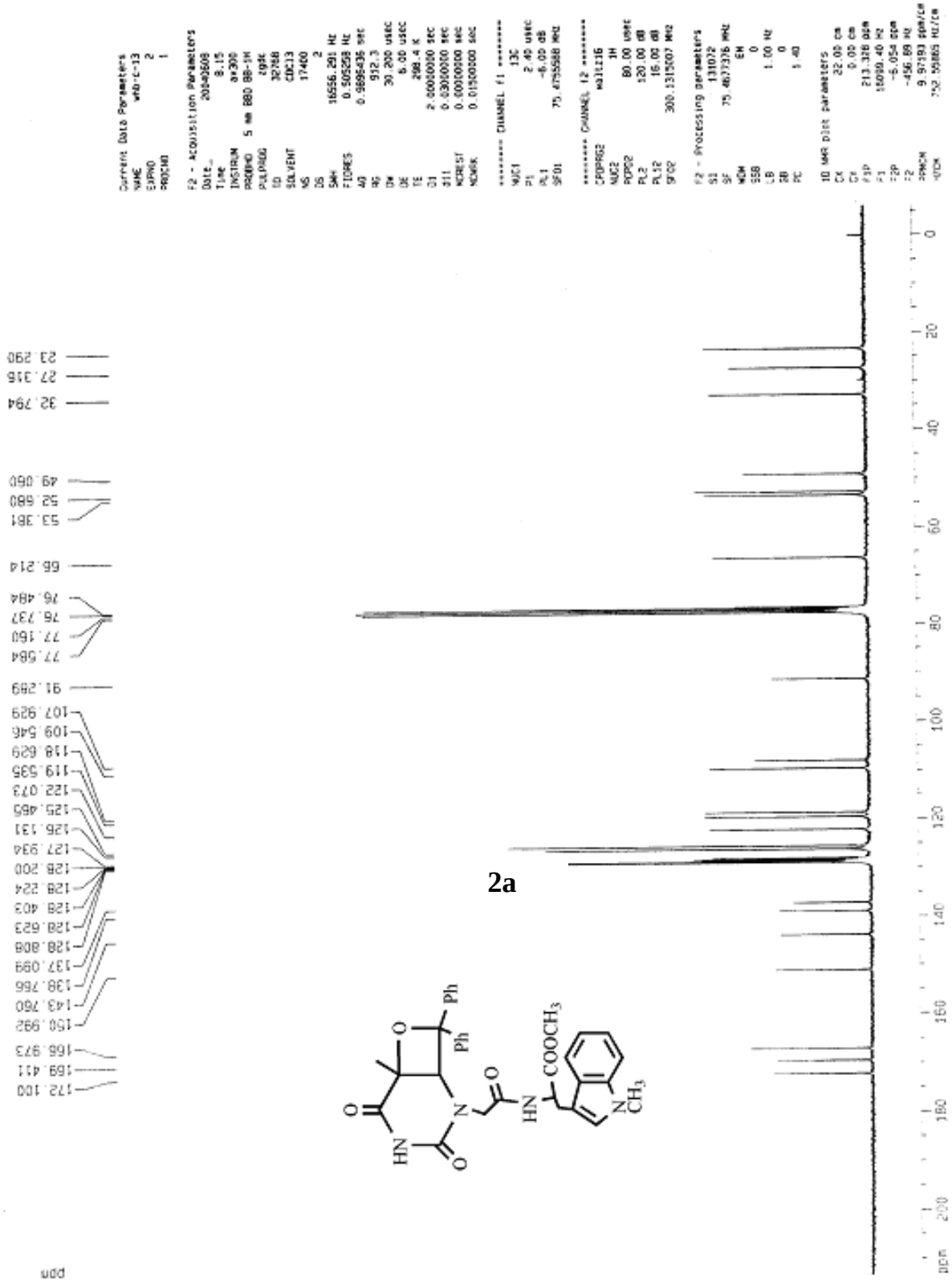


Figure S17 The ^{13}C NMR spectrum of compound **2b**

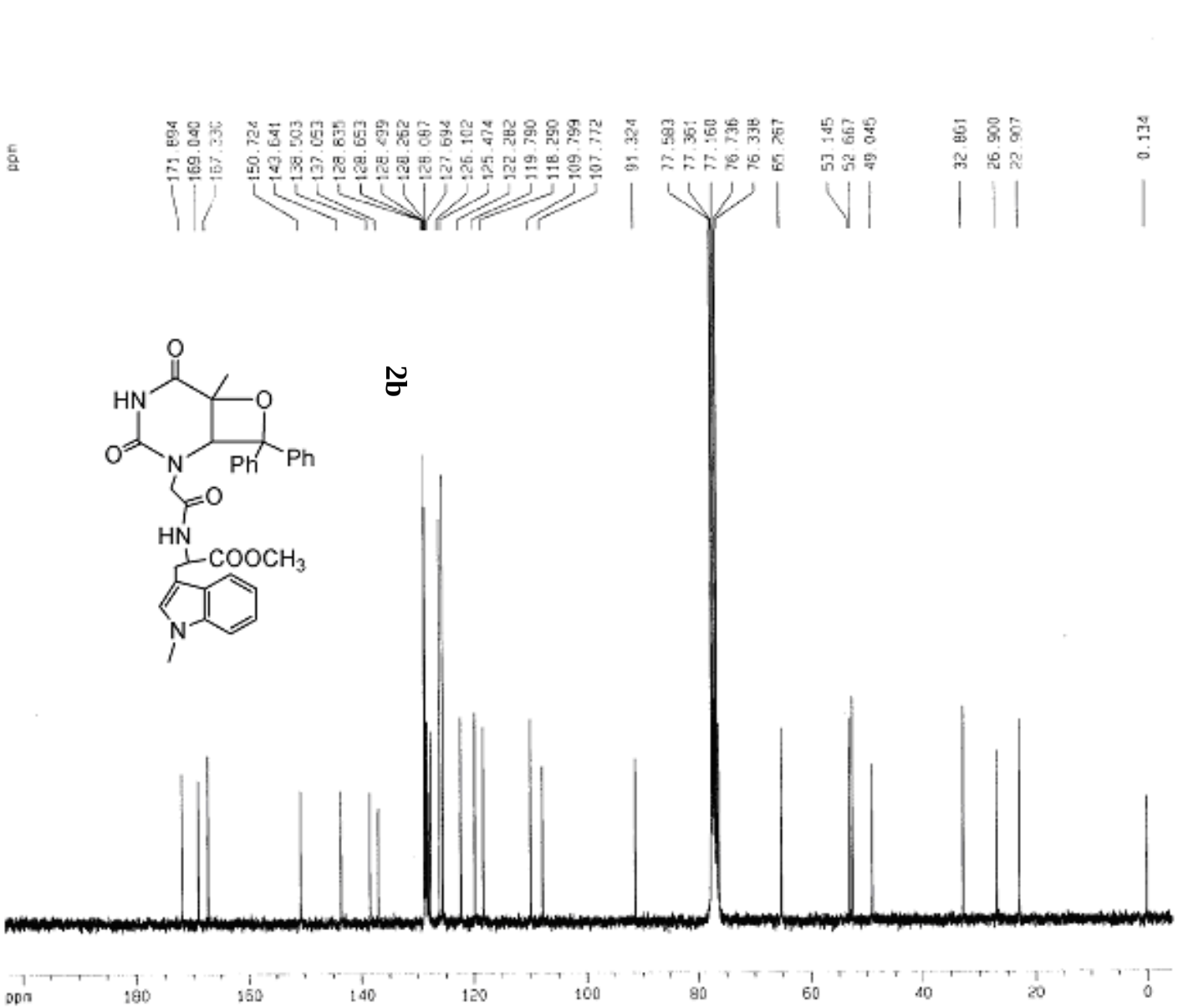



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Figure S18 The ^{13}C NMR spectrum of compound **3**