






Supporting Information for:

## **A Study of Antioxidant Properties and a Pharmacokinetic Investigation of Chalcones and Pyrazolines**

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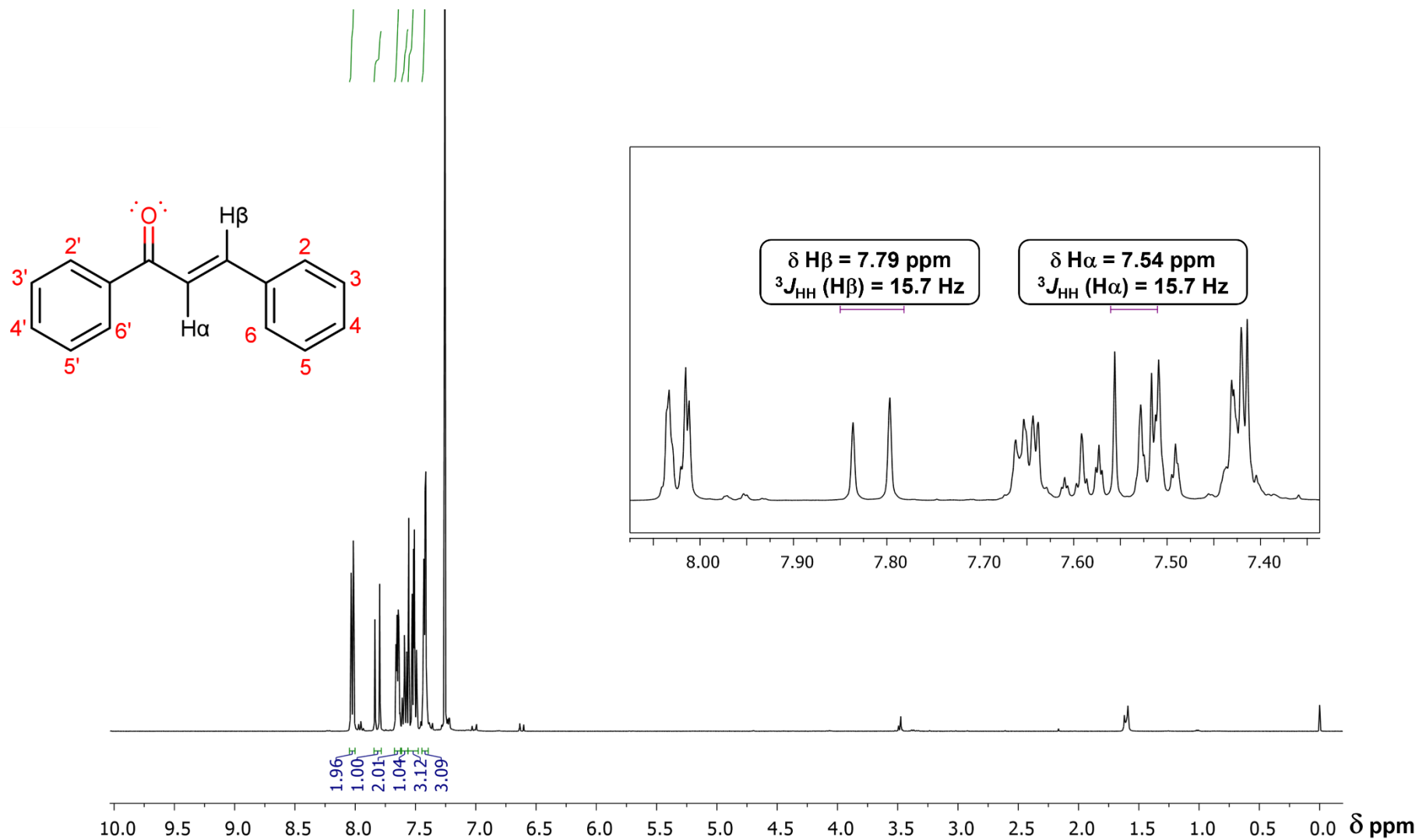
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**Table S1.** Bioavailability results determined by Lipinski, Ghose, Veber, Egan and Muegge.

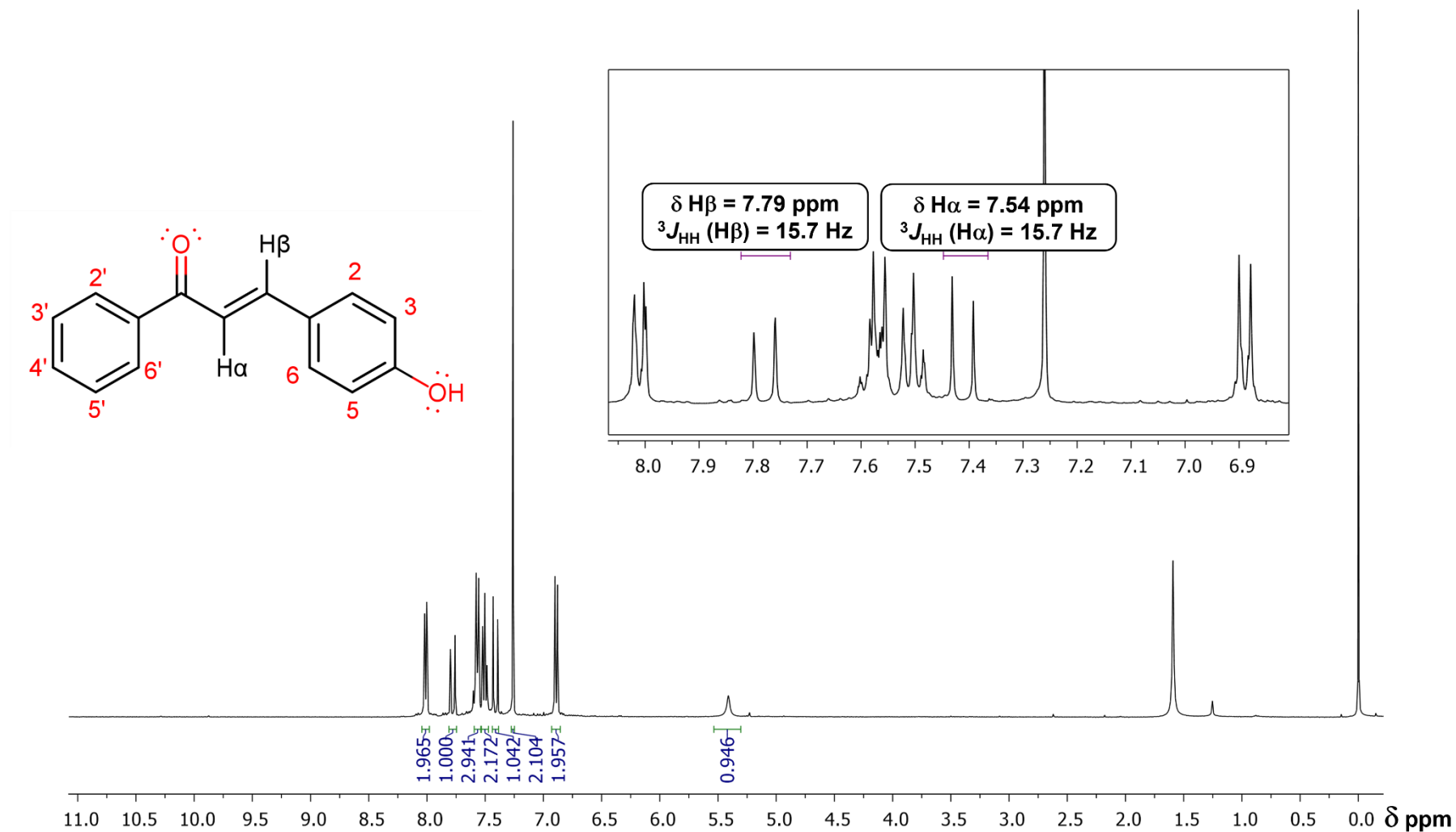
COMPOUND	NRBs	LIPINSKI	GHOSE	VEBER	EGAN	MUEGGE	BIOVABILITY
1a	3	Yes; 0 violations	No	No	No	No	0.55
1b	3	Yes; 0 violations	No	No	No	No	0.55
1c	3	Yes; 0 violations	No	No	No	No	0.55
2a	3	Yes; 0 violations	No	No	No	No	0.55
2b	3	Yes; 0 violations	No	No	No	No	0.55
2c	3	Yes; 0 violations	No	No	No	No	0.55
2d	3	Yes, 1 violation	No	No	No	No, 1 violation	0.55

**Table S2.** Warning indications about false positive reactions (PAINS)

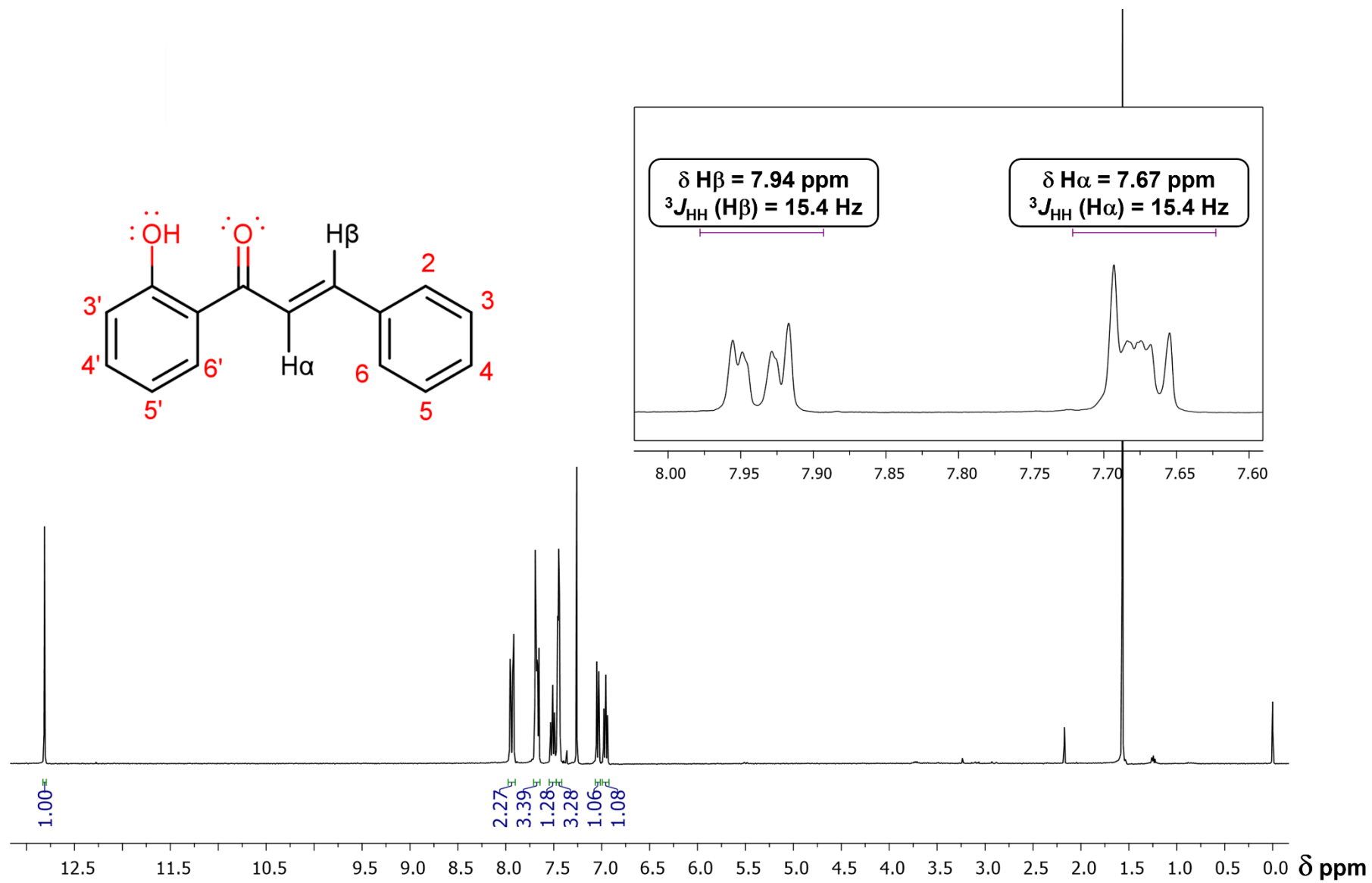
COMPOUND	PAINS
1a	No alert
1b	No alert
1c	No alert
2a	No alert
2b	1 alert: hzone_phenol_A
2c	No alert
2d	No alert



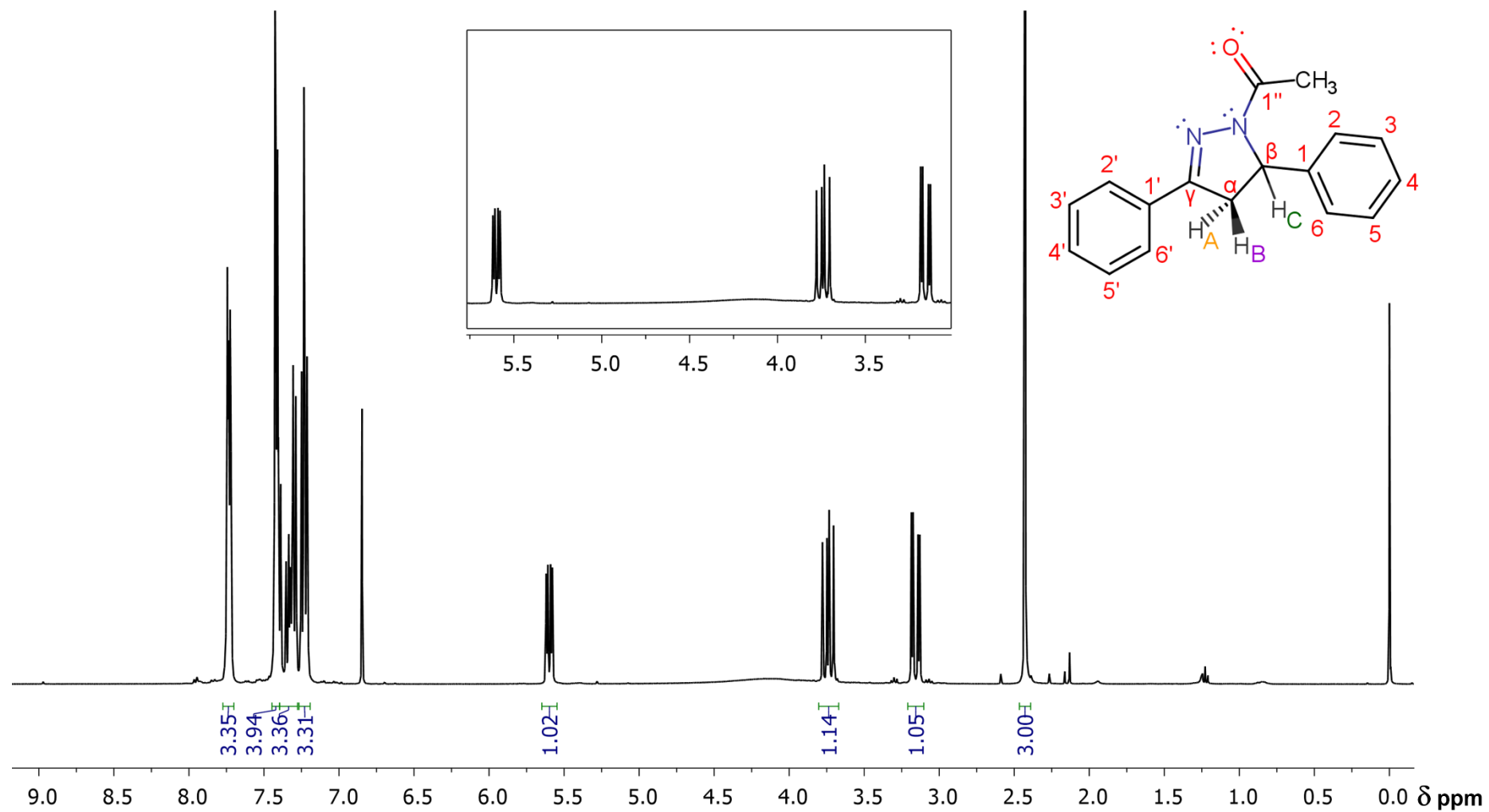
**Figure S1.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **1a**.



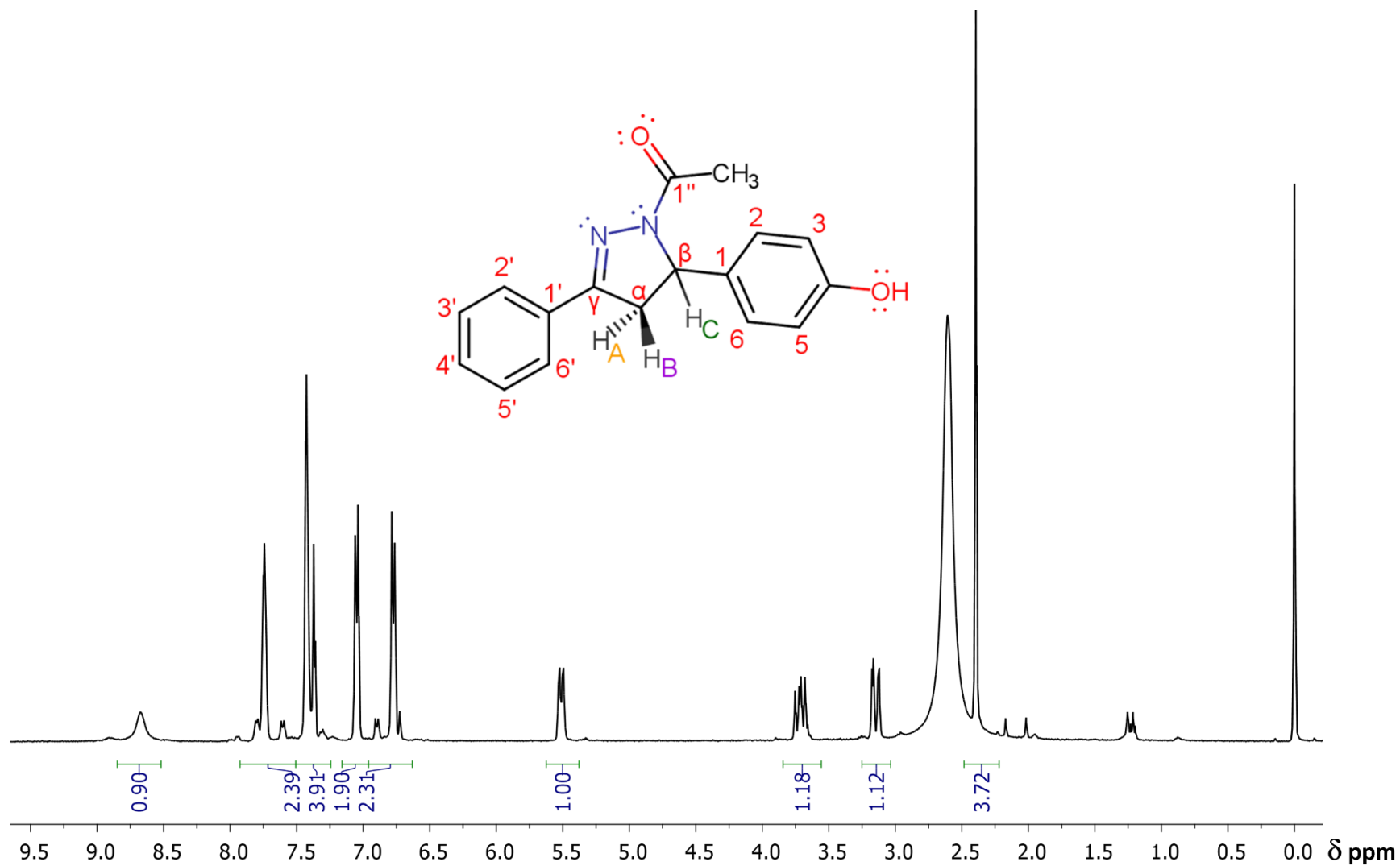
**Figure S2.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **1b**.



**Figure S3.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **1c**.

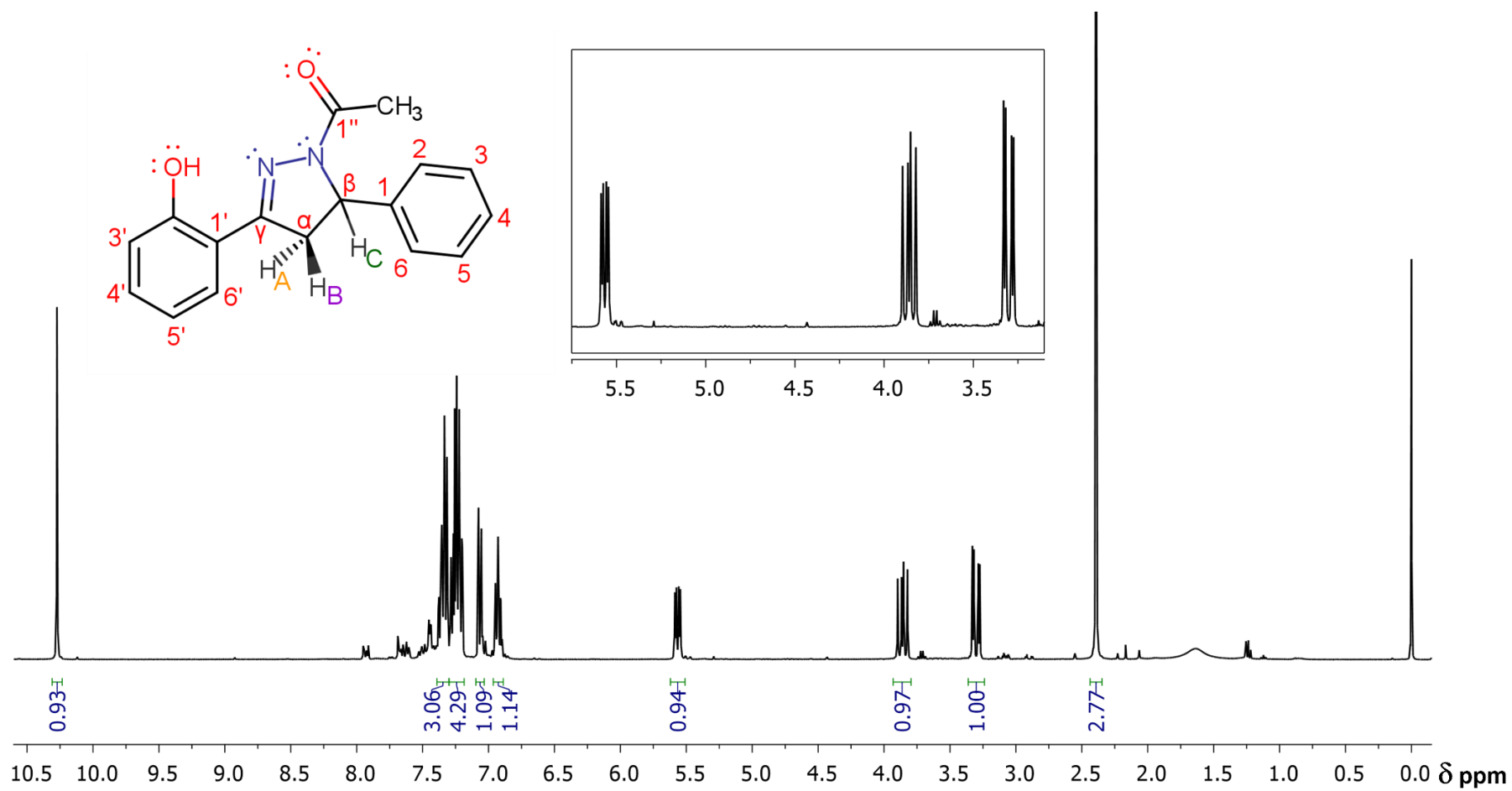


**Figure S4.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **2a**.

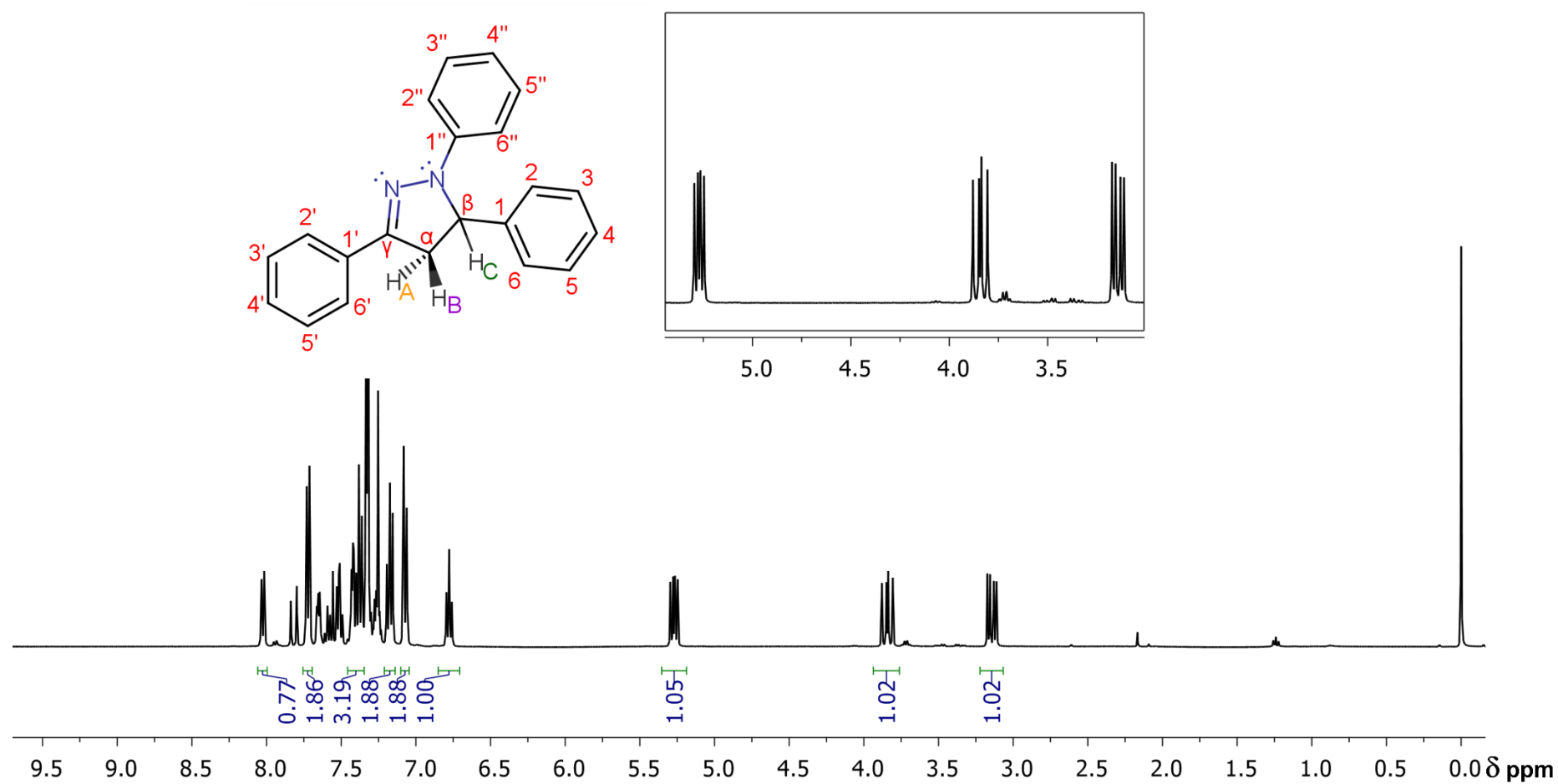


**Figure S5.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ,  $\text{DMSO-d}_6$ ) of compound **2b**.

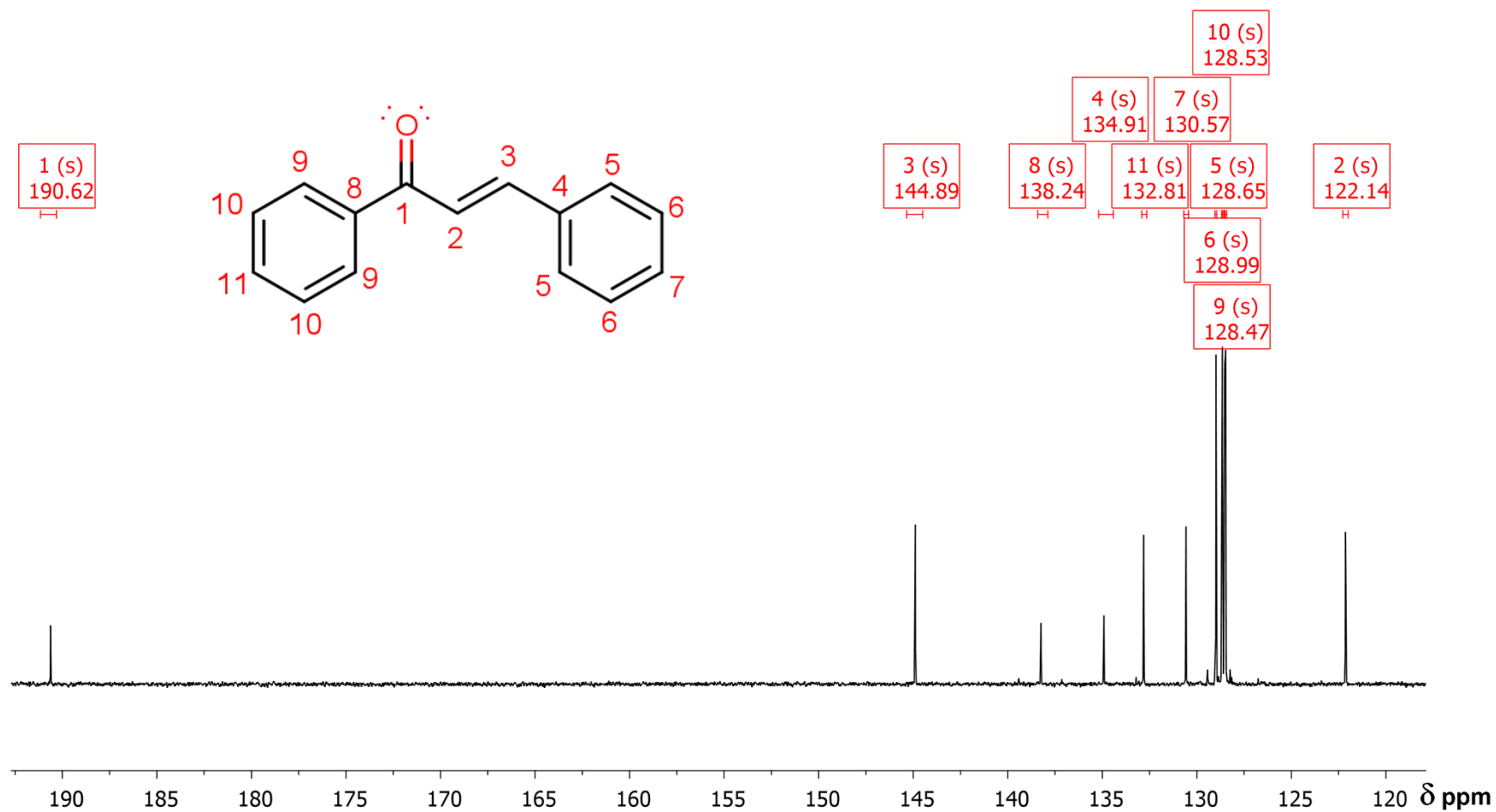




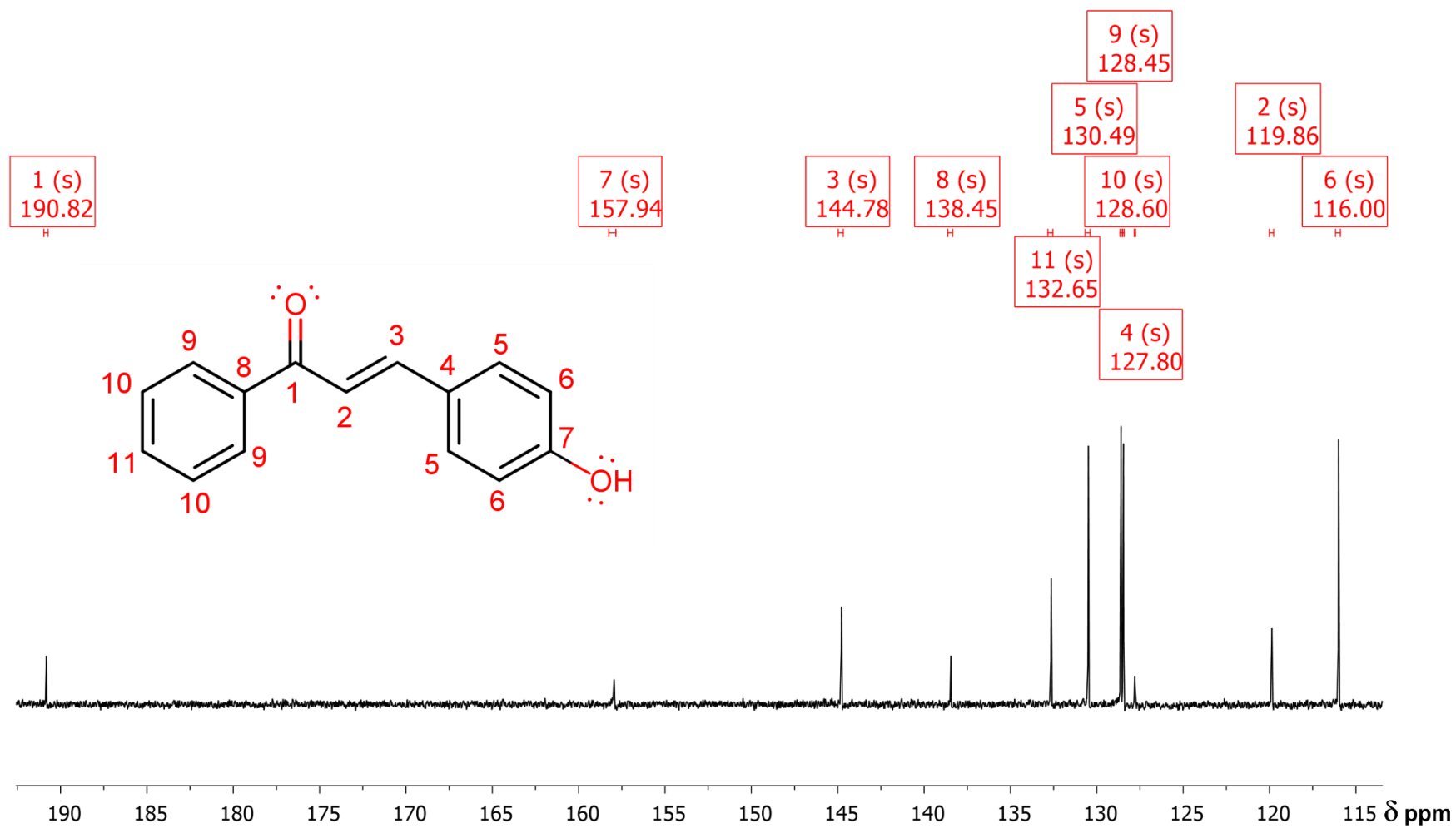
**Figure S6.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **2c**.



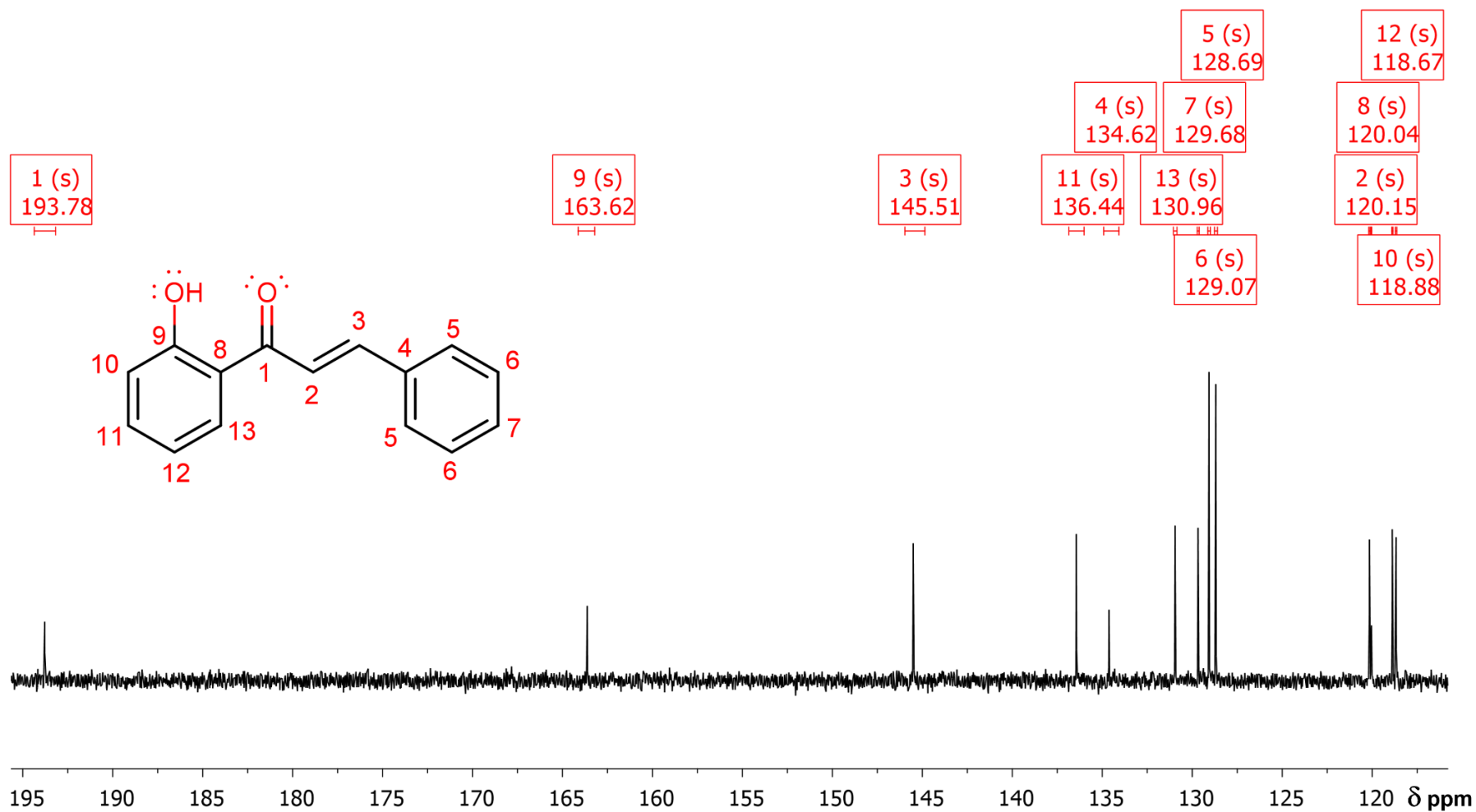
**Figure S7.**  $^1\text{H}$  NMR spectrum (400 MHz,  $\text{CDCl}_3$ ) of compound **3a**.



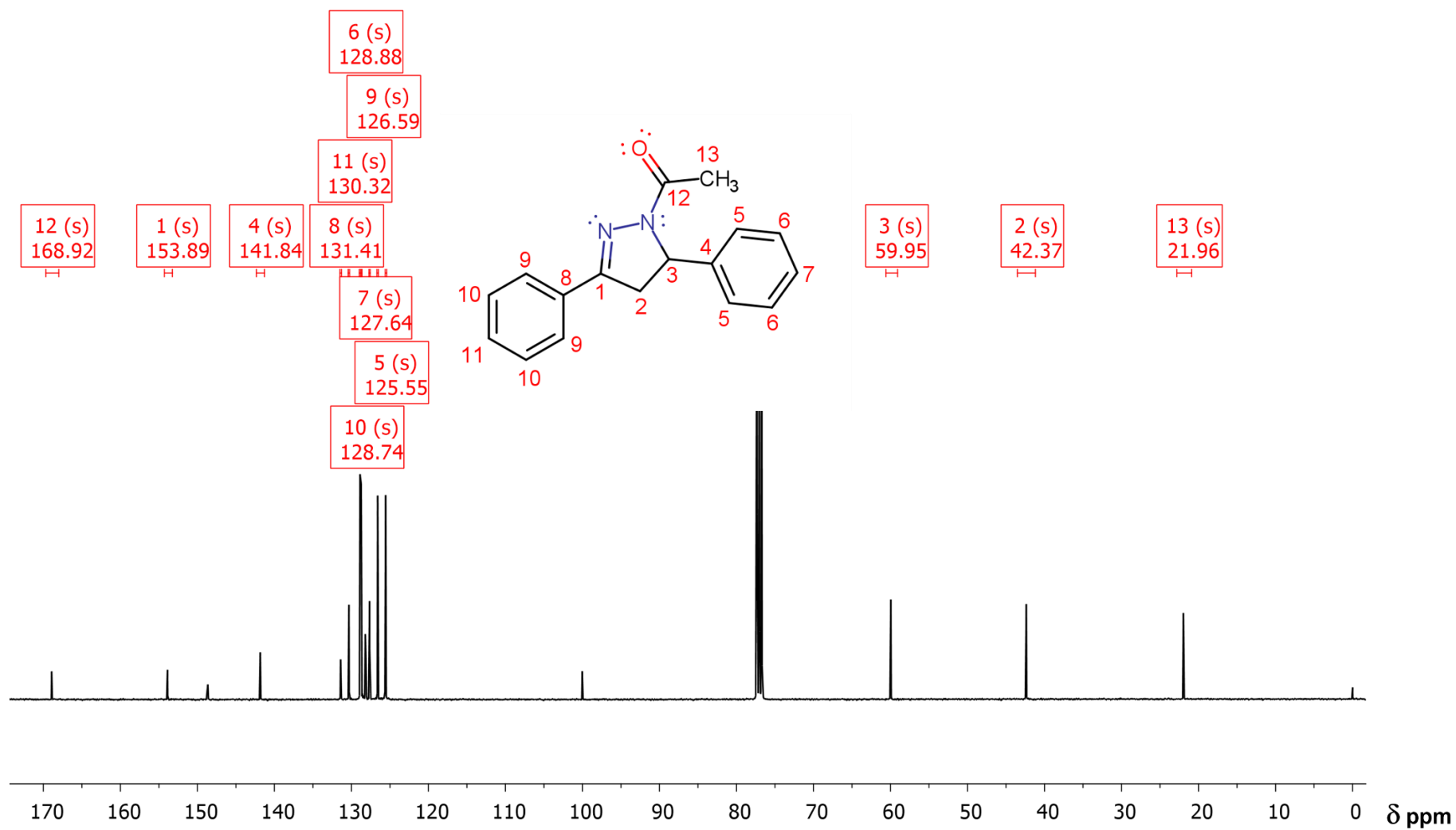
**Figure S8.** <sup>13</sup>C NMR spectrum (100 MHz, CDCl<sub>3</sub>) of compound **1a**.



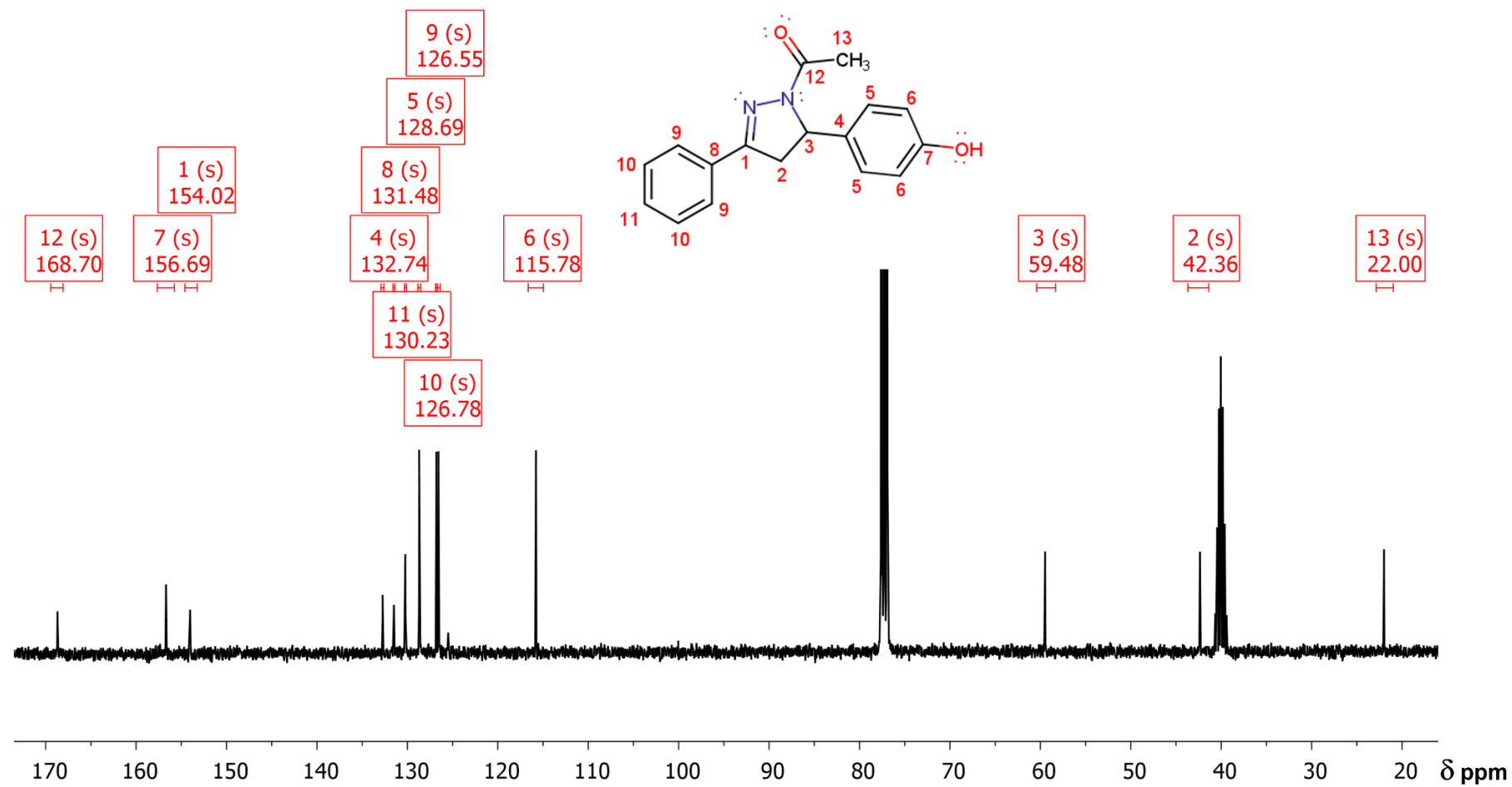
**Figure S9.** <sup>13</sup>C NMR spectrum (100 MHz, CDCl<sub>3</sub>) of compound **1b**.



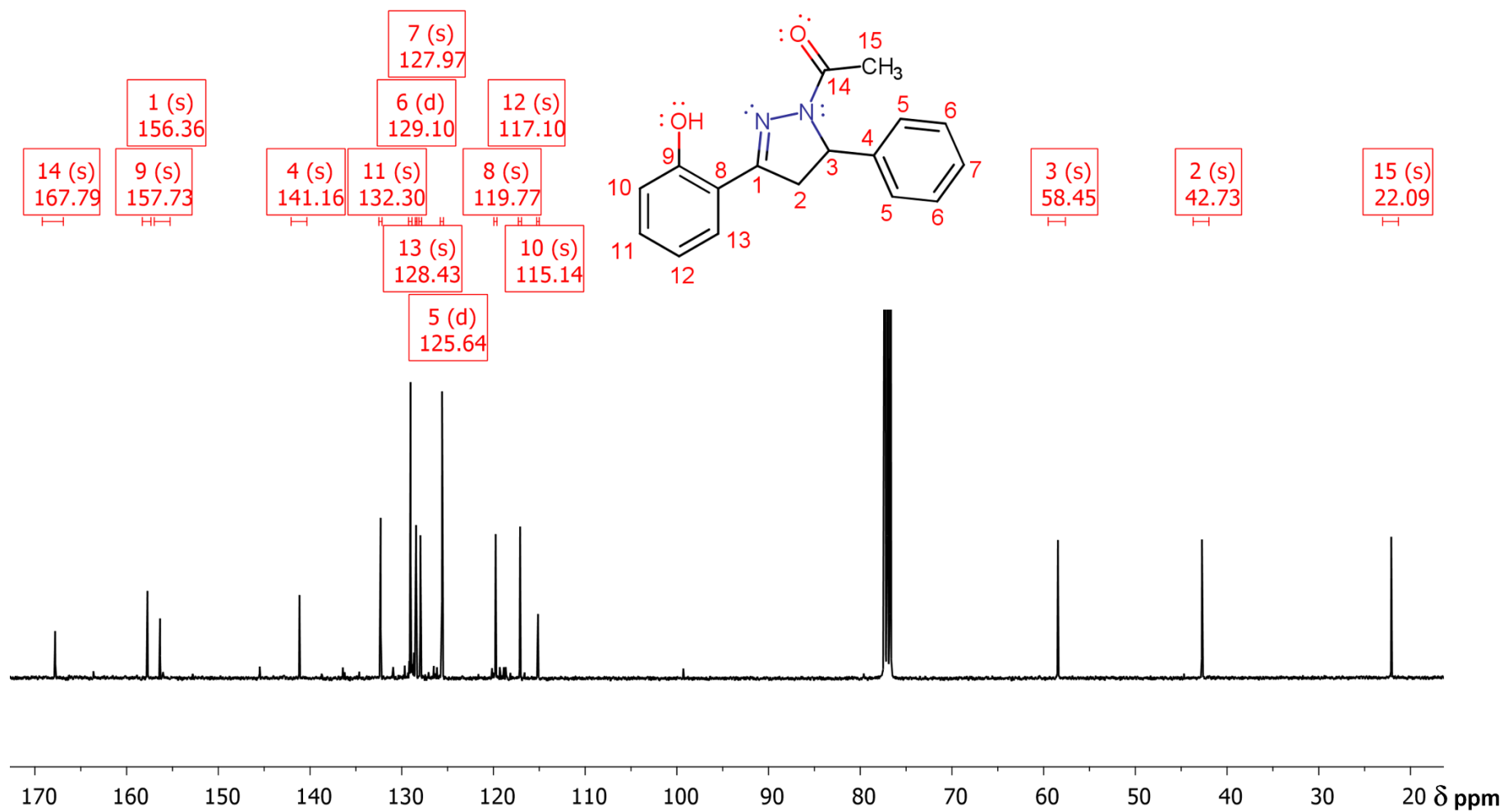
**Figure S10.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ) of compound **1c**.



**Figure S11.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ) of compound **2a**.

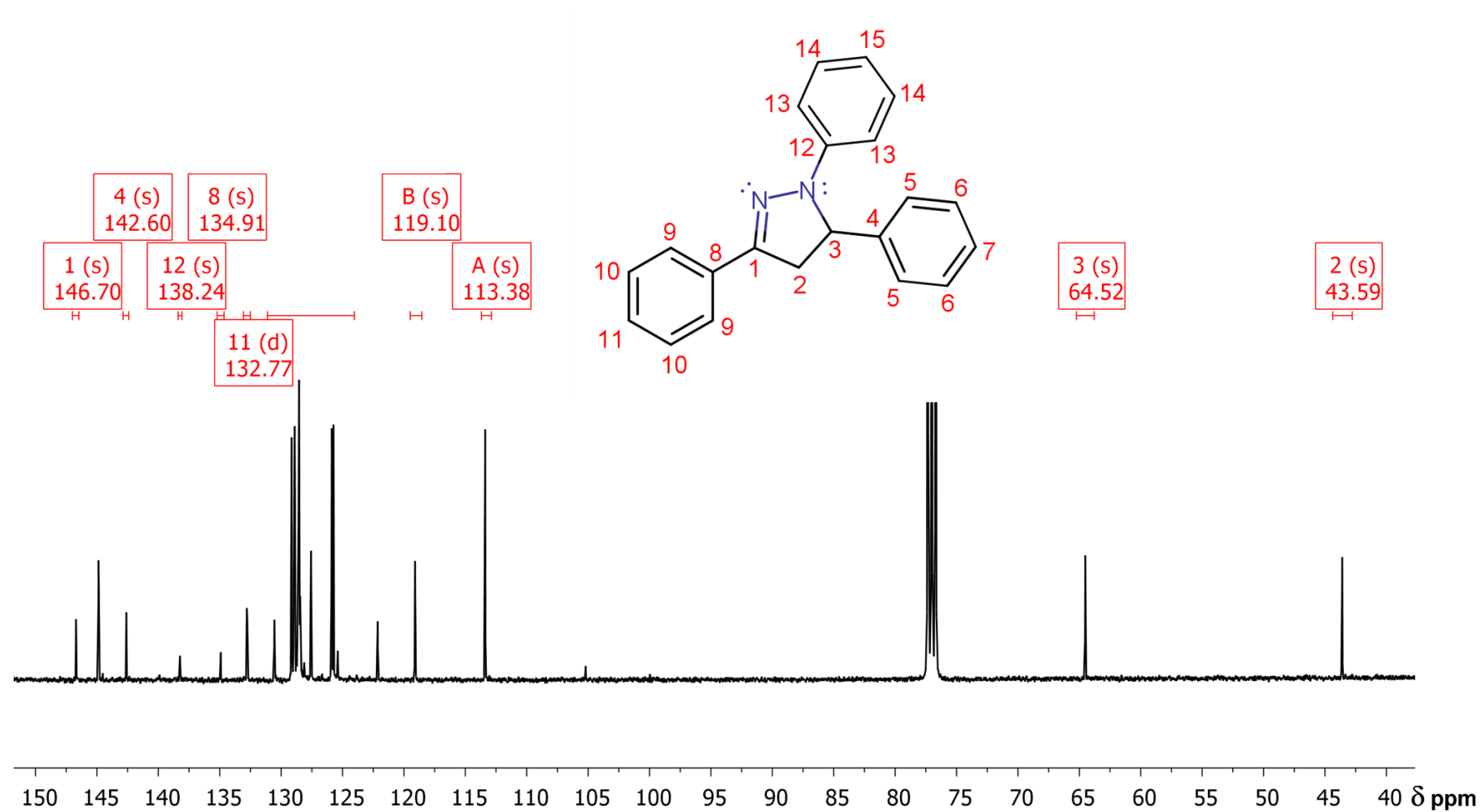


**Figure S12.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3/\text{DMSO-d}_6$ ) of compound **2b**.



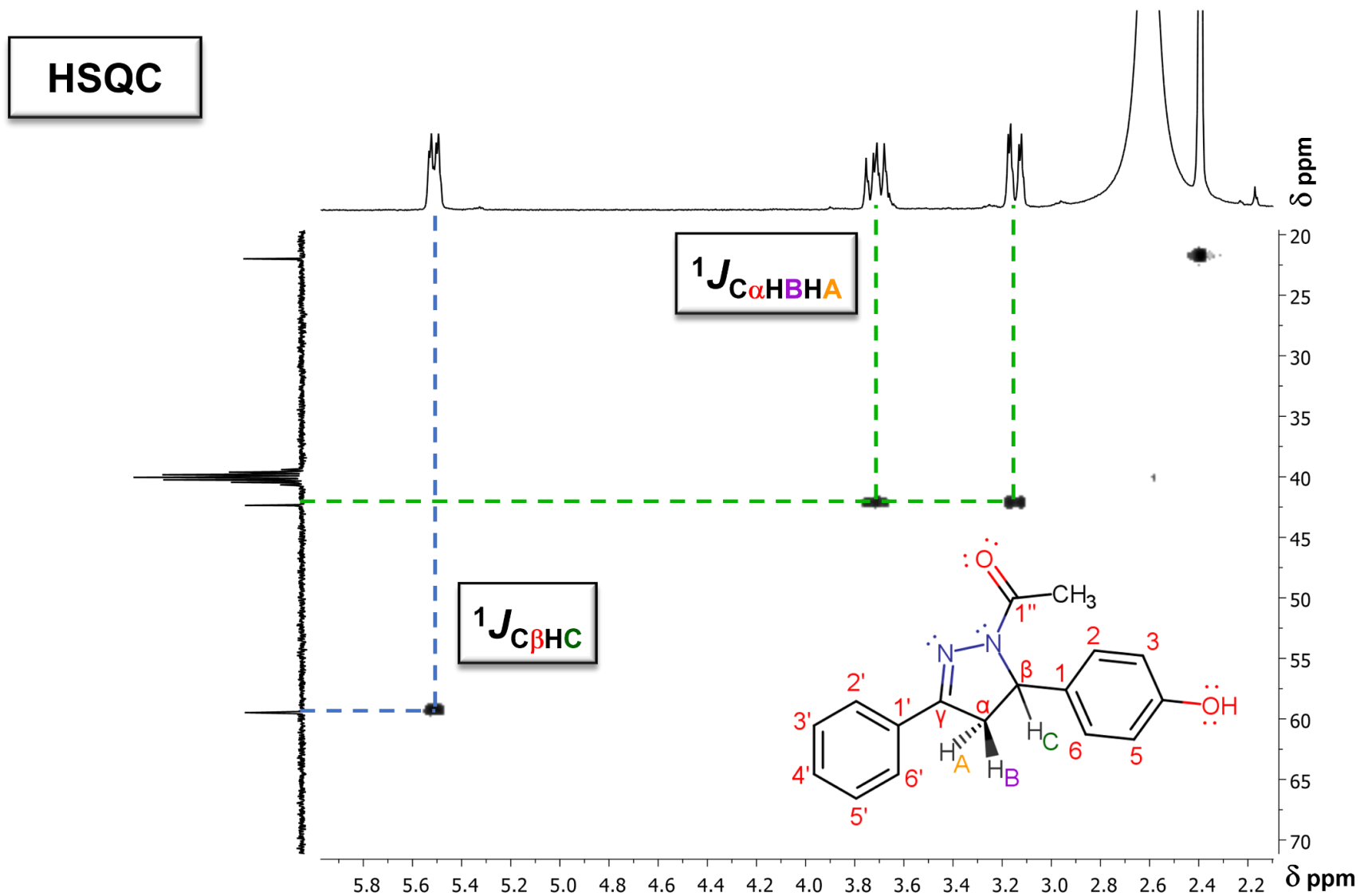
**Figure S13.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ) of compound **2c**.





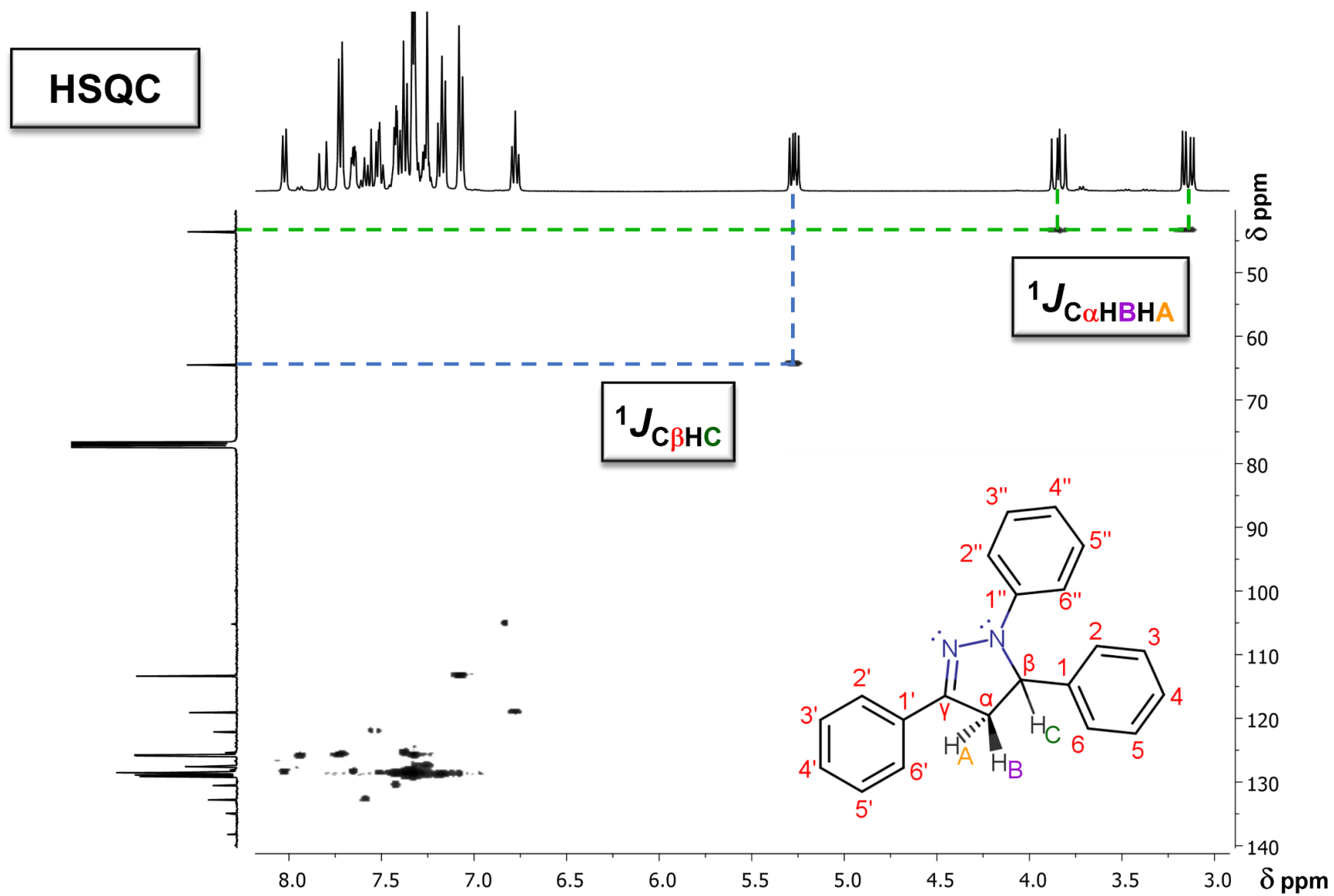
**Figure S14.**  $^{13}\text{C}$  NMR spectrum (100 MHz,  $\text{CDCl}_3$ ) of compound **3a**.



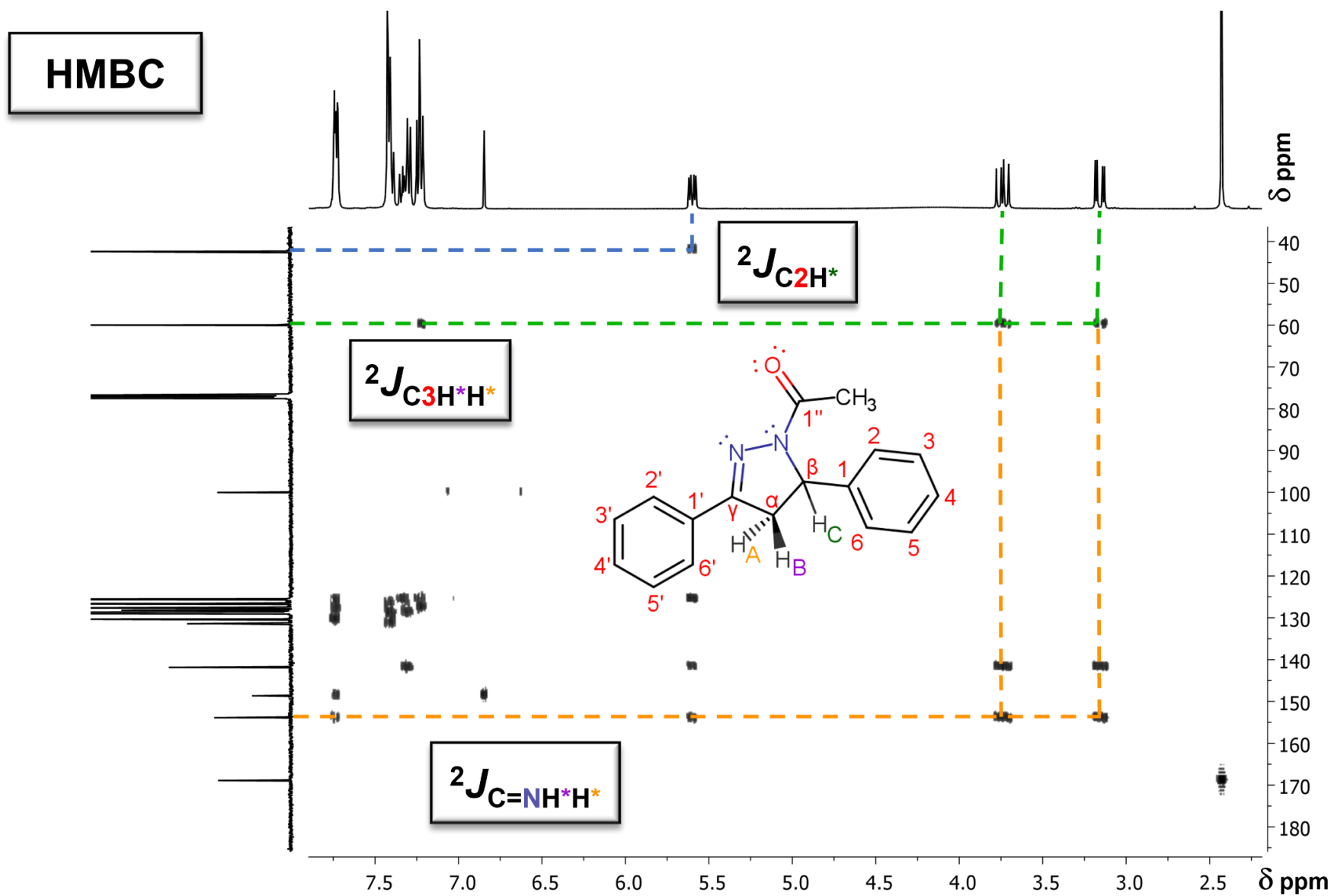


**Figure S16.** HSQC of compound **2b**.





**Figure S18.** HSQC of compound **3a**.



**Figure S19.** HMBC of compound **2a**.

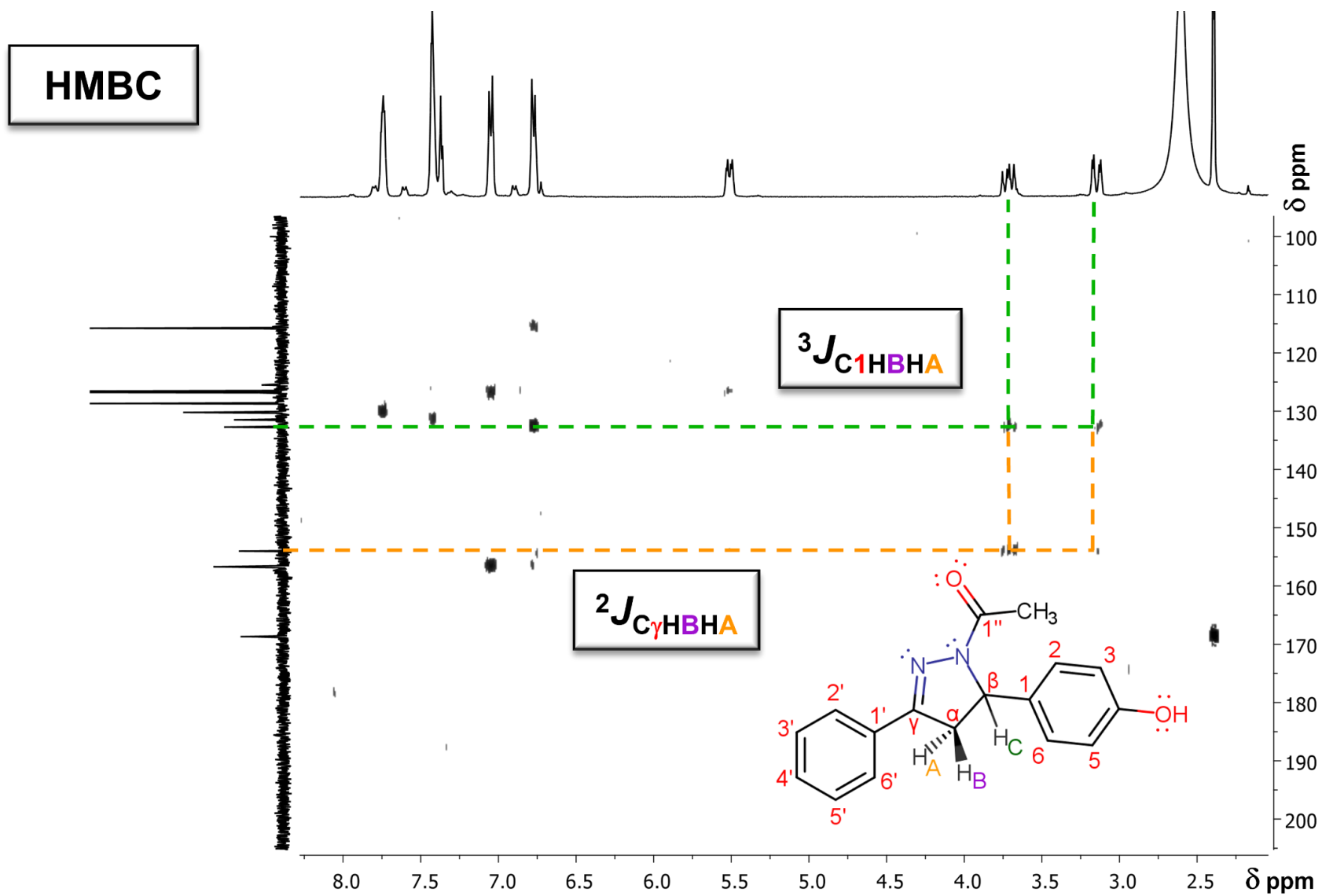
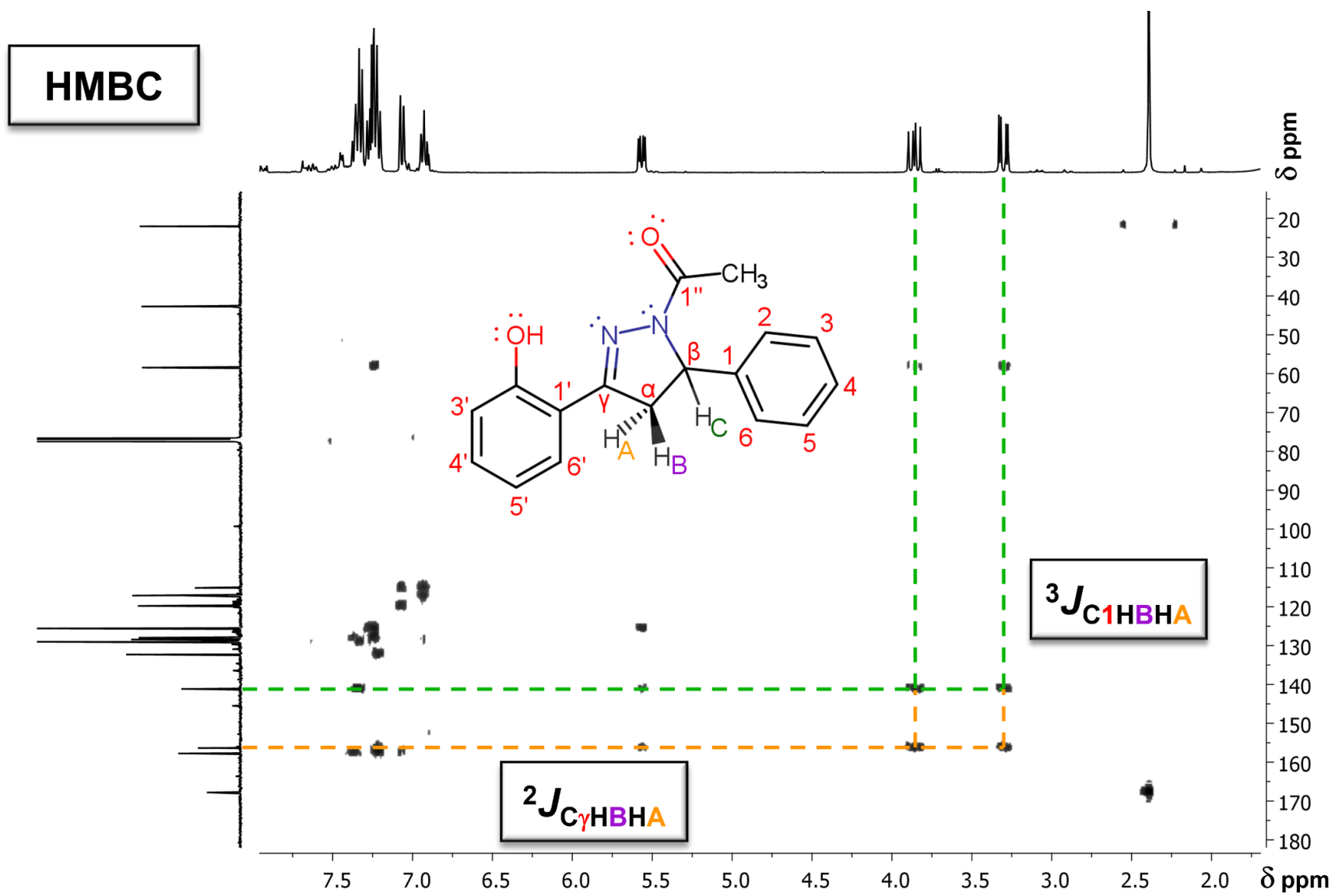
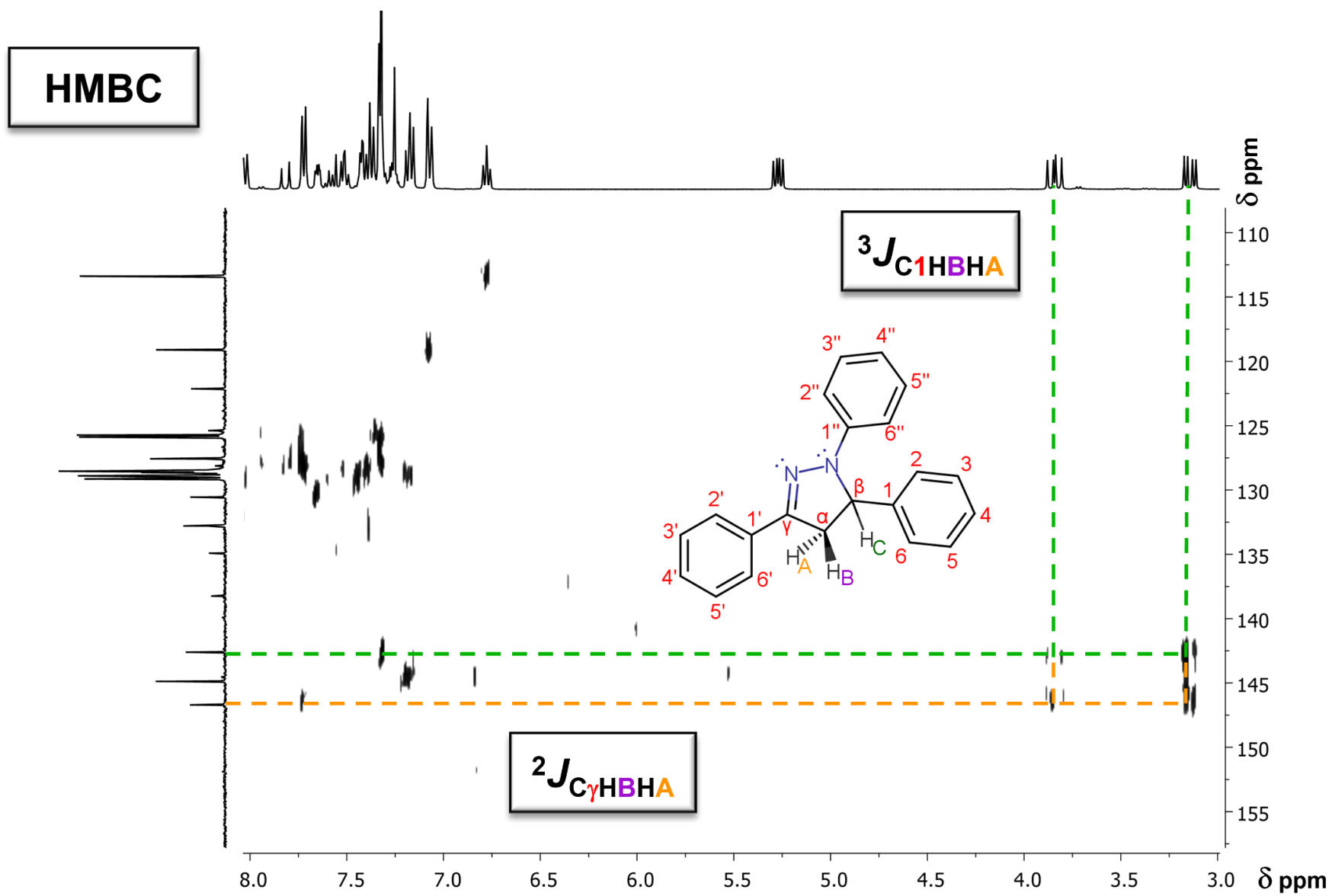


Figure S20. HMBC of compound **2b**.

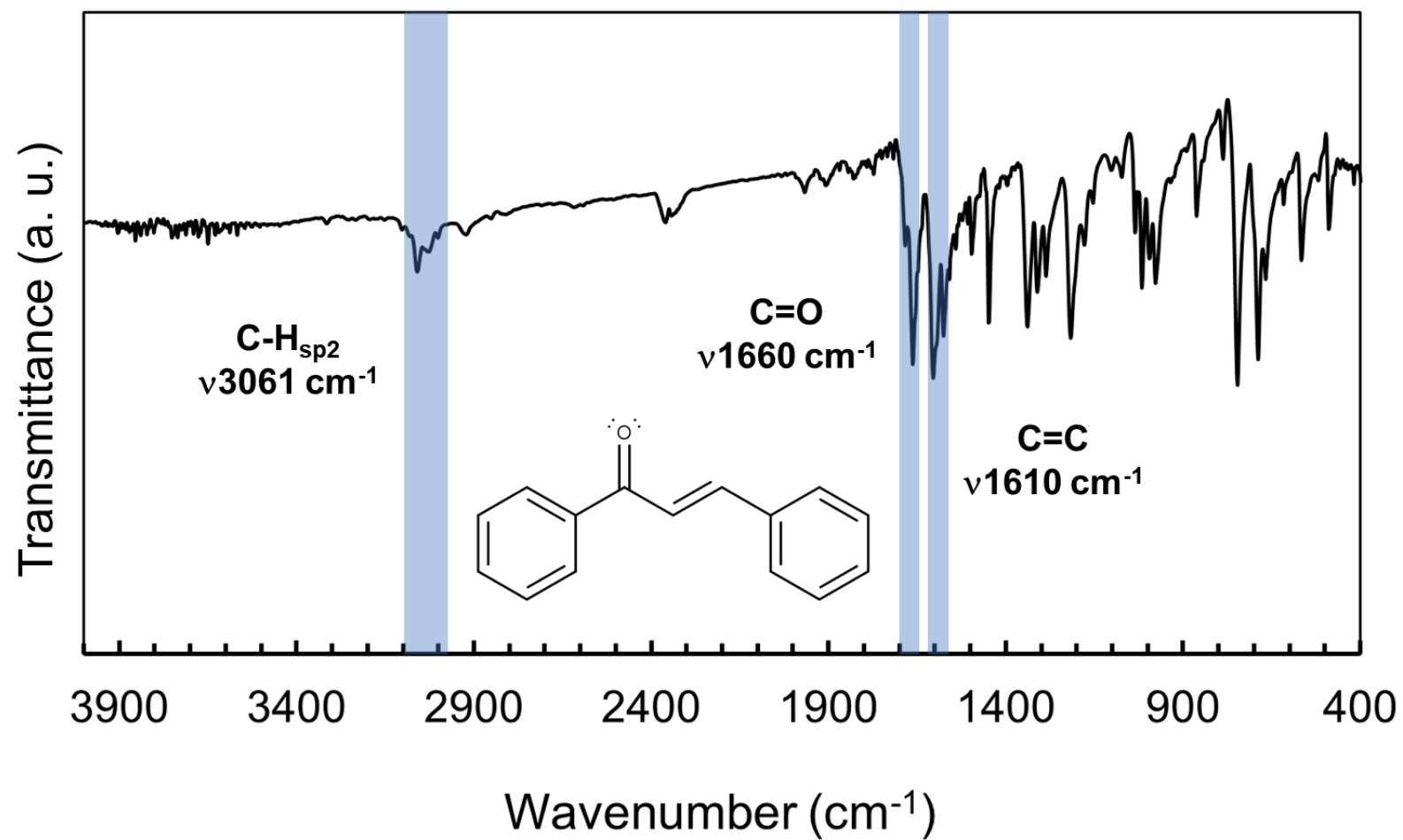


**Figure S21.** HMBC of compound **2c**.

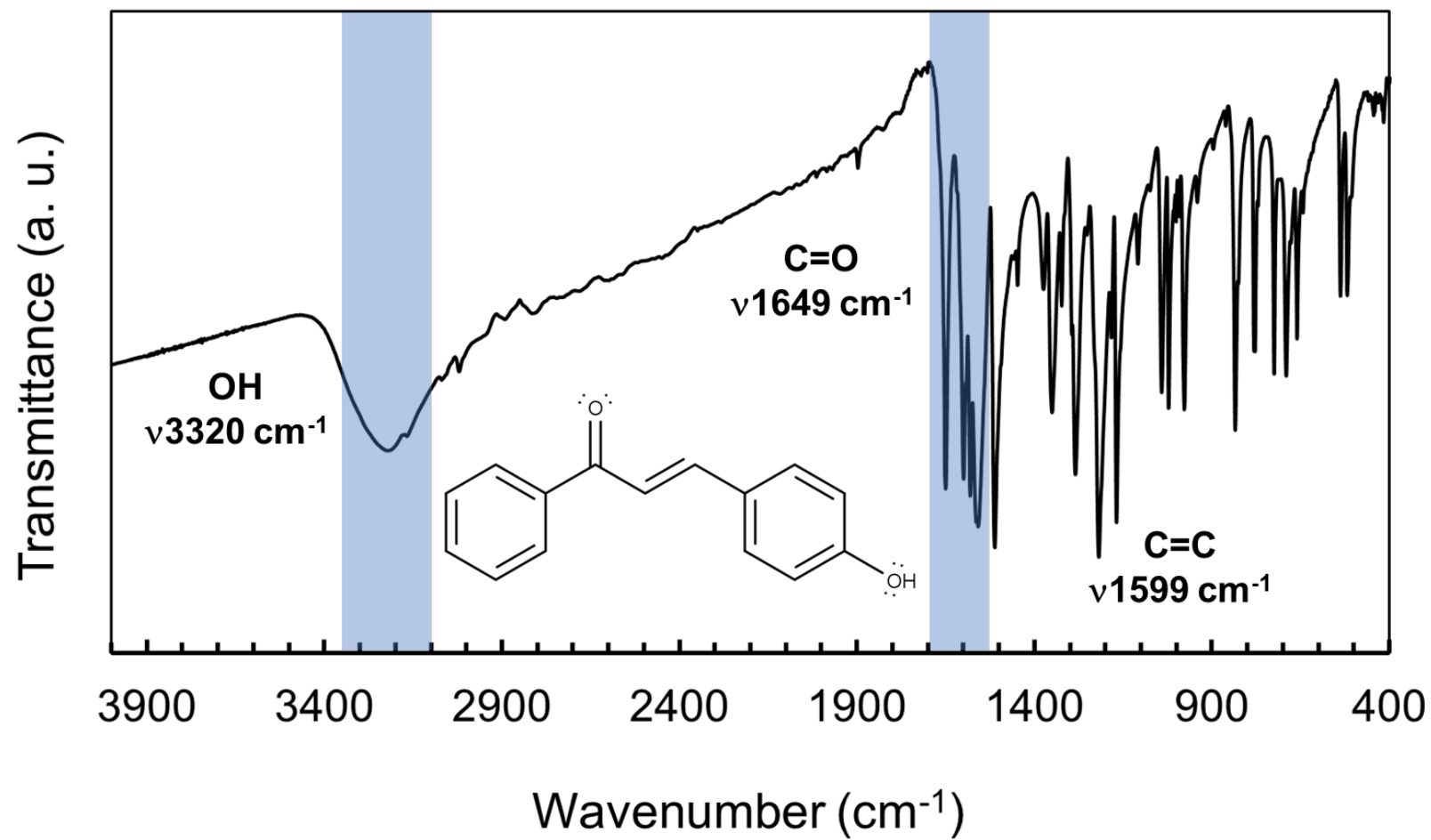




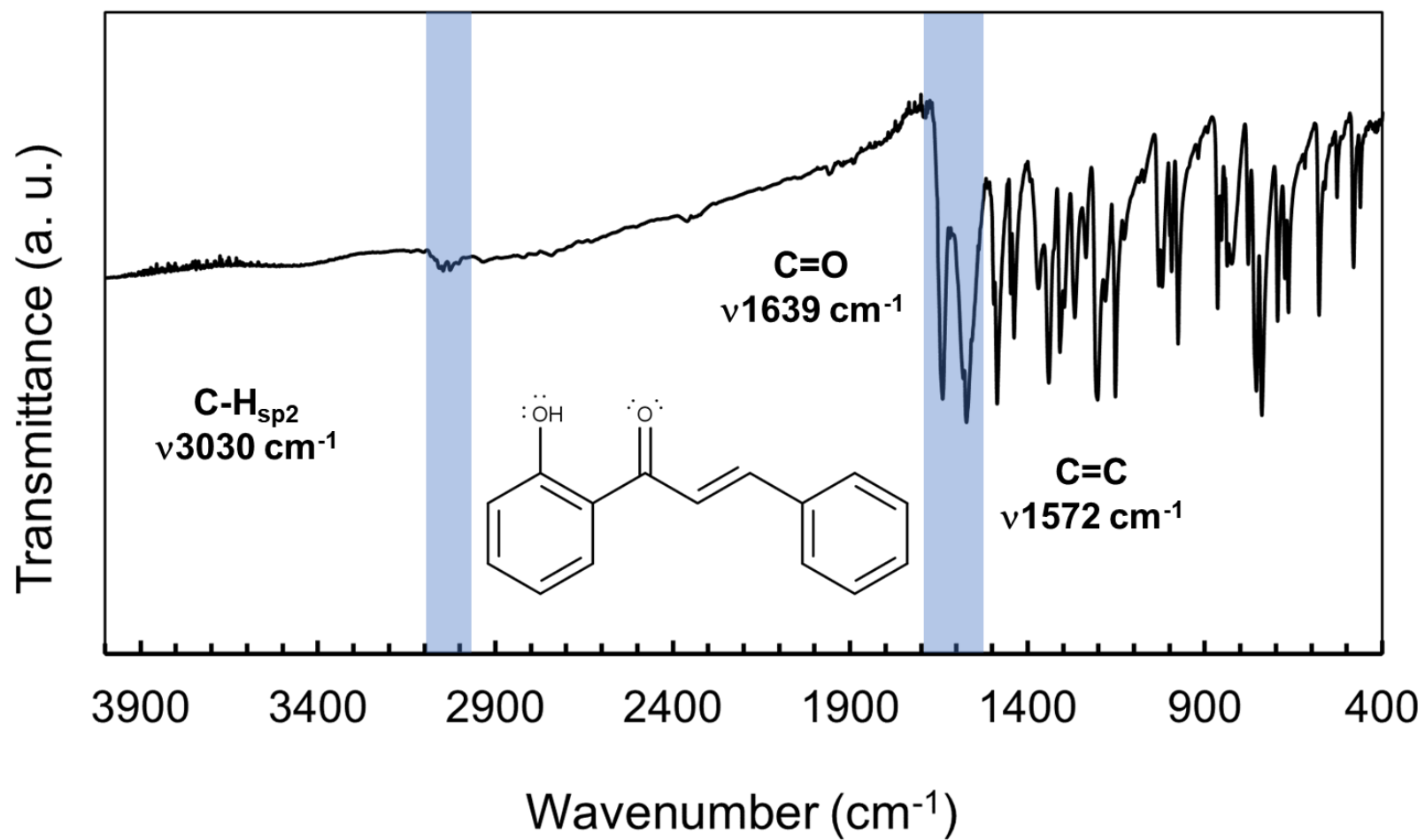
**Figure S22.** HMBC of compound **3a**.



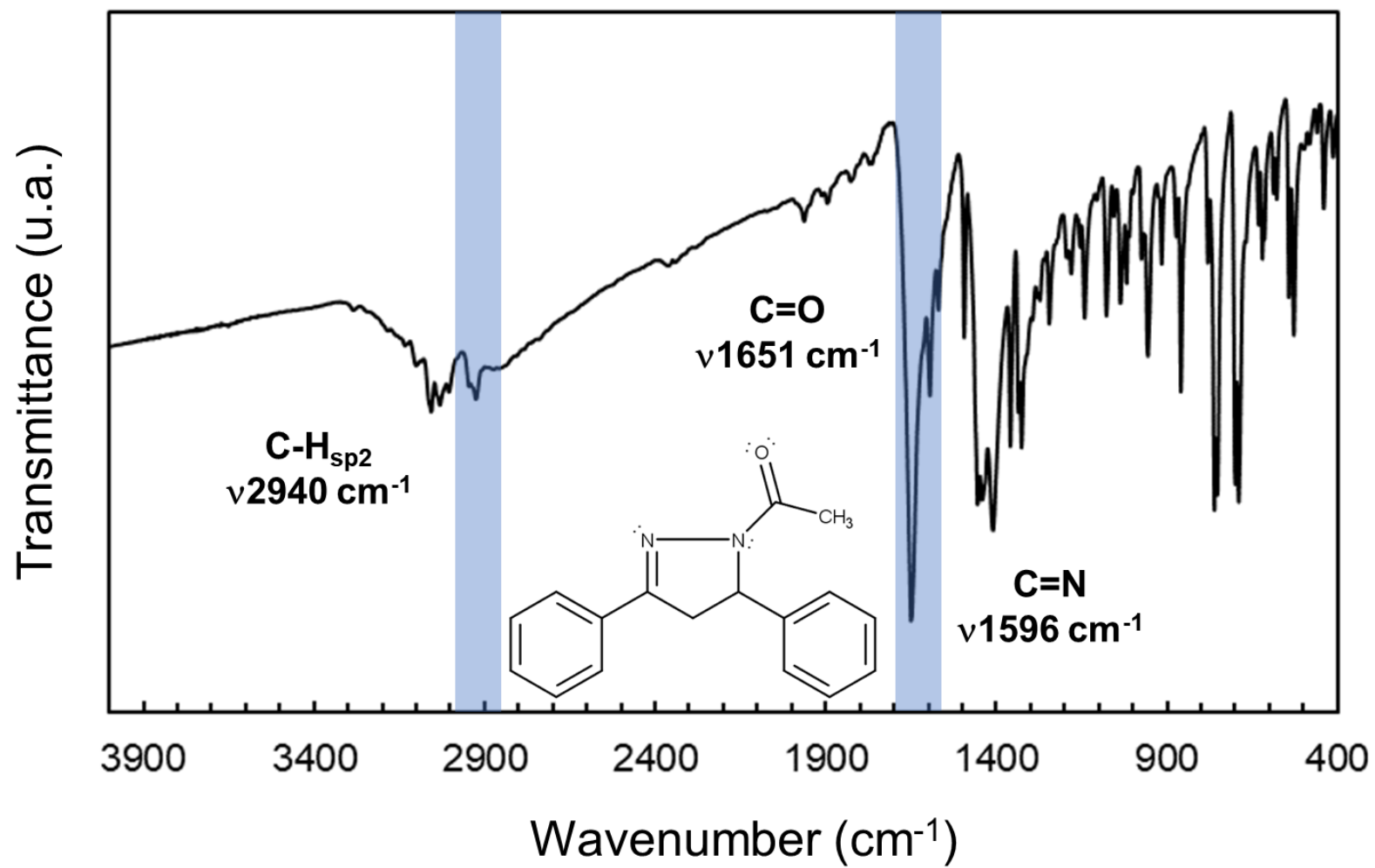
**Figure S23.** FT-IR of compound **1a**.



**Figure S24.** FT-IR of compound **1b**.



**Figure S25.** FT-IR of compound **1c**.



**Figure S26.** FT-IR of compound **2a**.

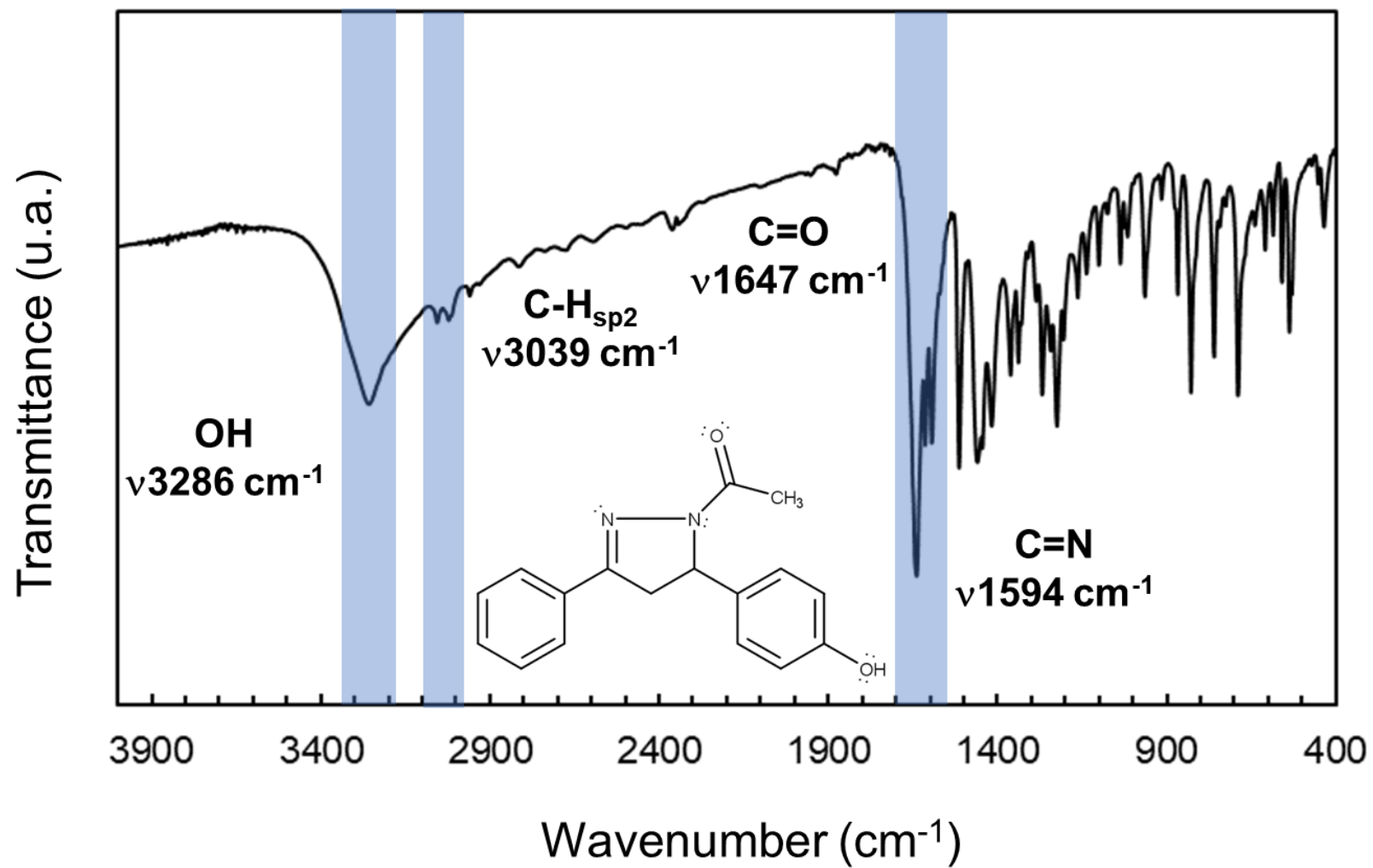
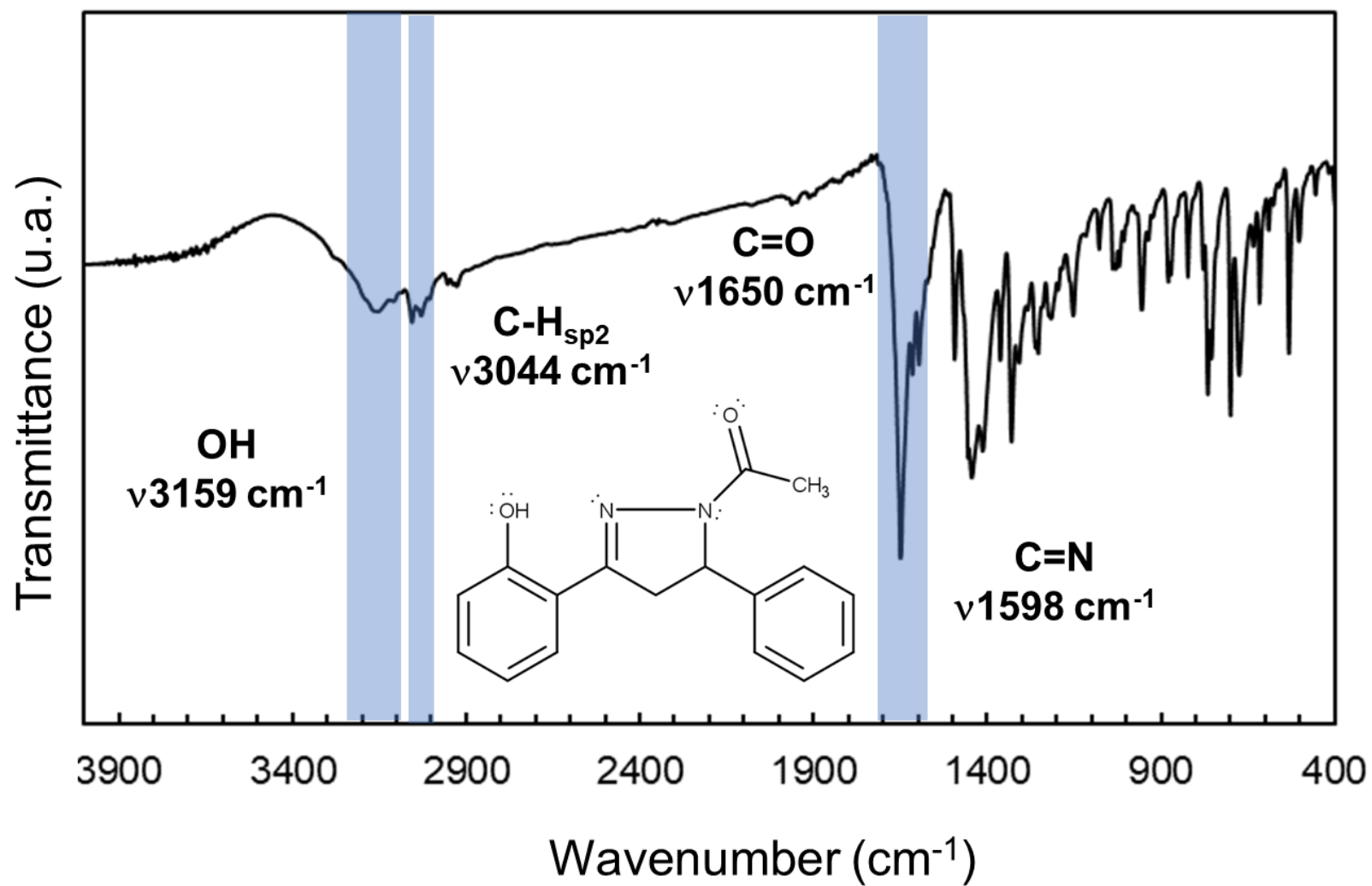
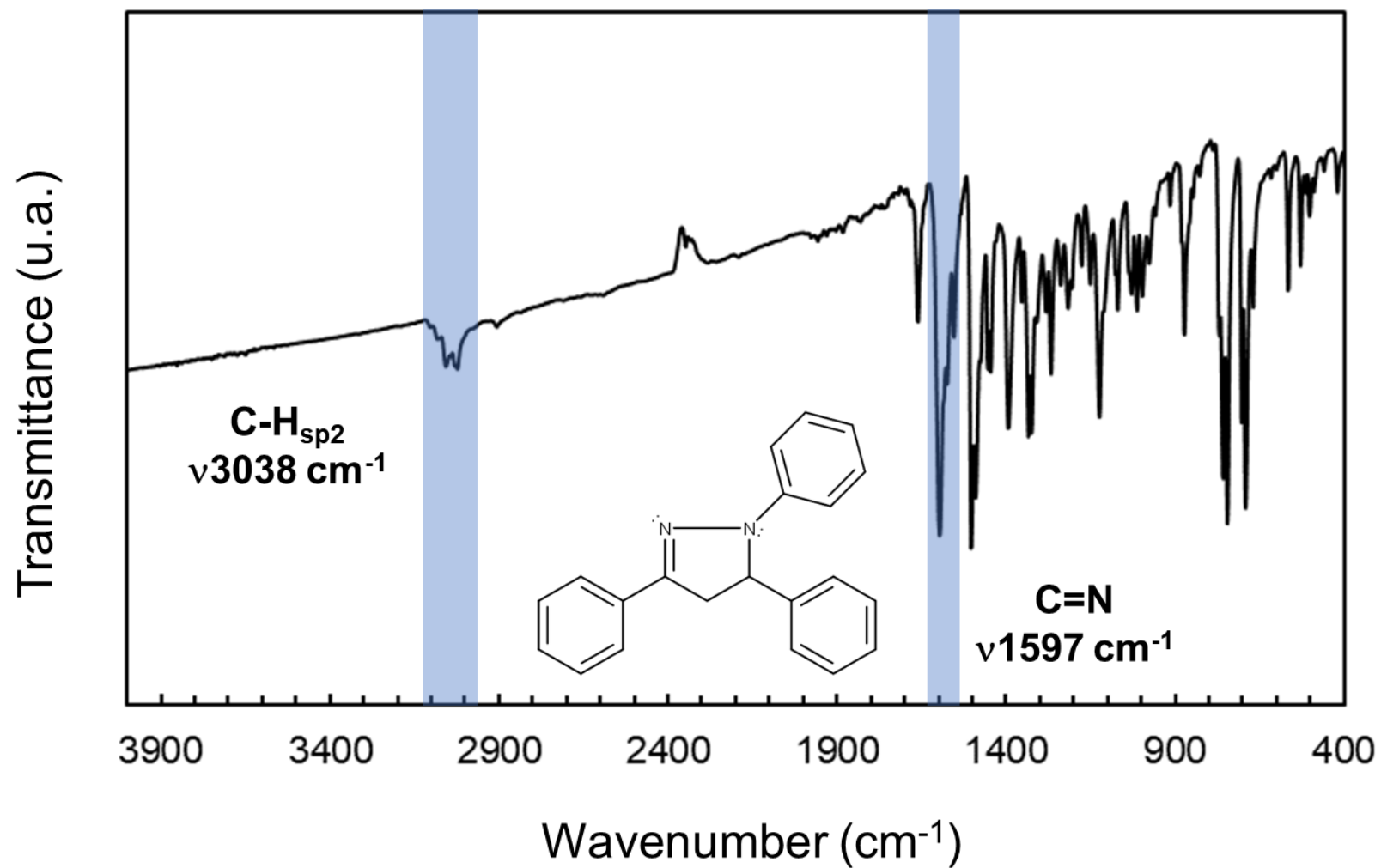


Figure S27. FT-IR of compound **2b**.



**Figure S28.** FT-IR of compound **2c**.



**Figure S29.** FT-IR of compound **3a**.