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Research Article

SUPPLEMENTARY INFORMATION

SYNTHESIS, CHARACTERIZATION, ANTICANCER ACTIVITY, AND COMPUTATIONAL STUDY OF UMBELLIFERONE SCHIFF'S BASES

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Acetylation of 4-methylumbelliferone

4-methylumbelliferone (0.038 mol. 8.29 g) dissolved in pyridine (48 mL) solvent and catalytic amount of piperidine (0.1 mL) was added to it then the mixture cooled to 0–5 °C for 30 minutes and acetyl chloride (0.056 mol. 4.39 g) was added slowly dropwise. The mixture was stirred for 48 hours at room temperature. The resultant dark red reaction mixture was poured into ice-cold water (140 mL), and the product was adjusted to pH 1–2 using 2 N hydrochloric acid. The resulting precipitate was filtered under suction, washed with water until neutral, and then dried. The solid product was recrystallized in ethanol/water (1:1), and the yellowish crystals with a recorded melting point of 137 °C.

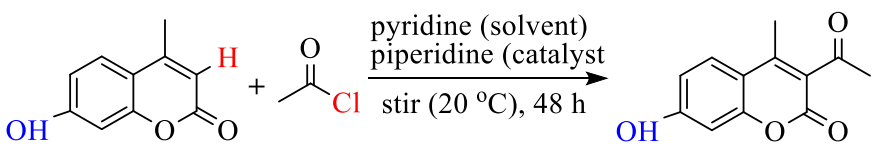

Figure S1: Acetylation of 4-methylumbelliferone

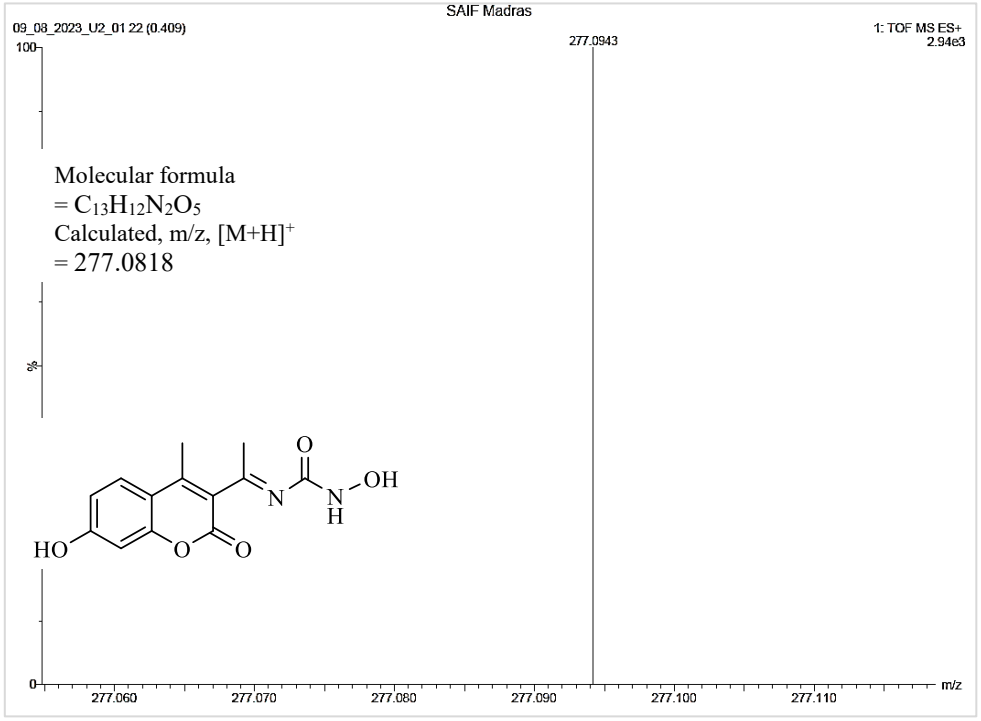

Figure S2: ESI-HRMS of compound 1a

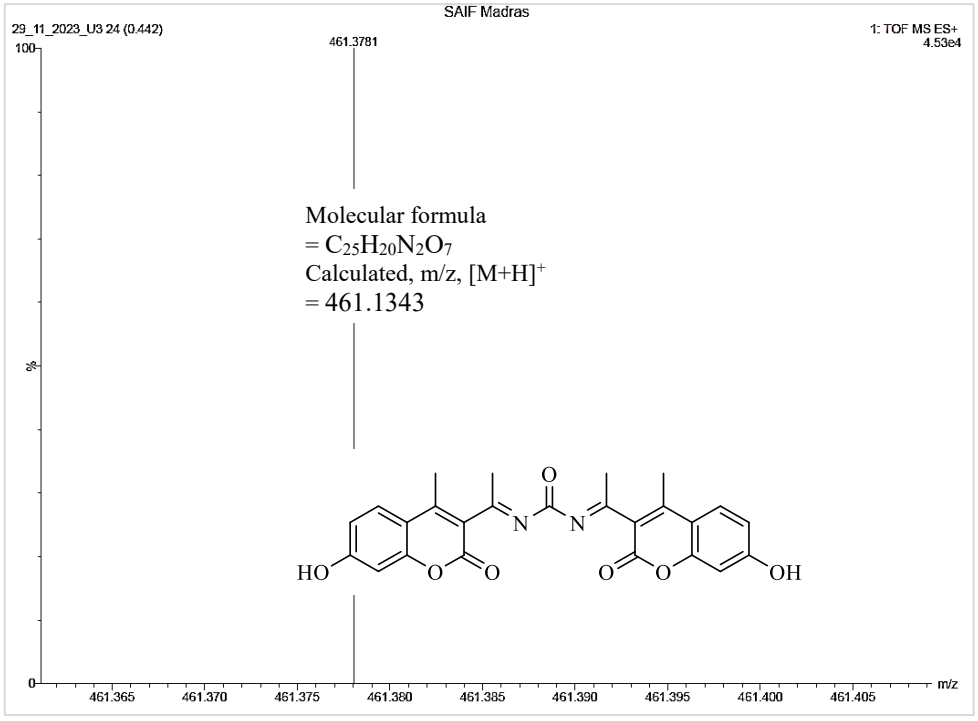

Figure S3: ESI-HRMS of compound 1b

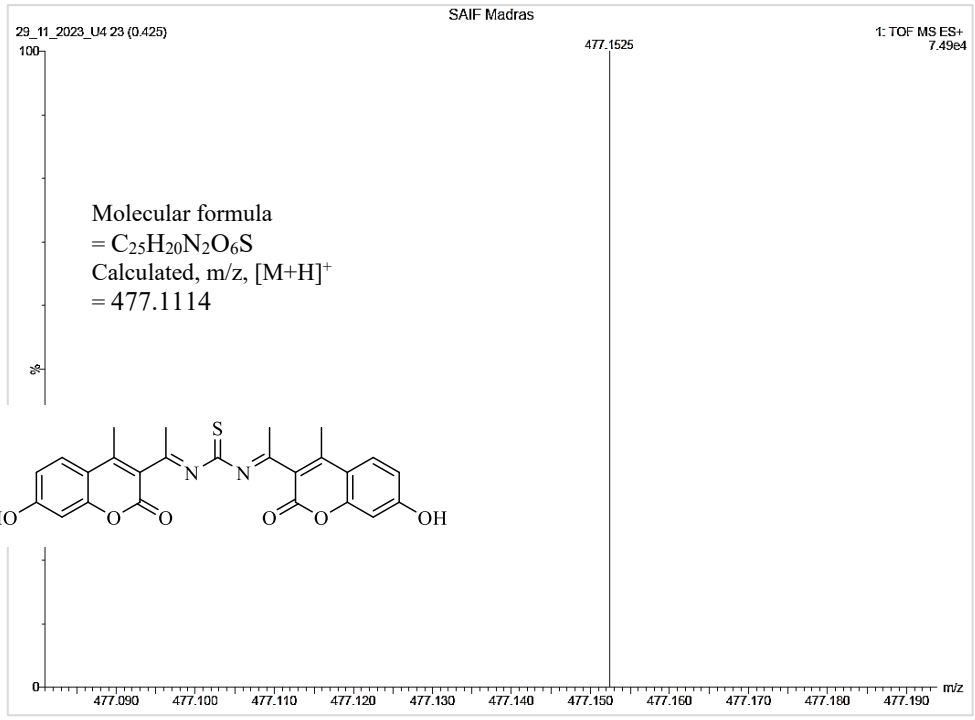

Figure S4: ESI-HRMS of compound 1c

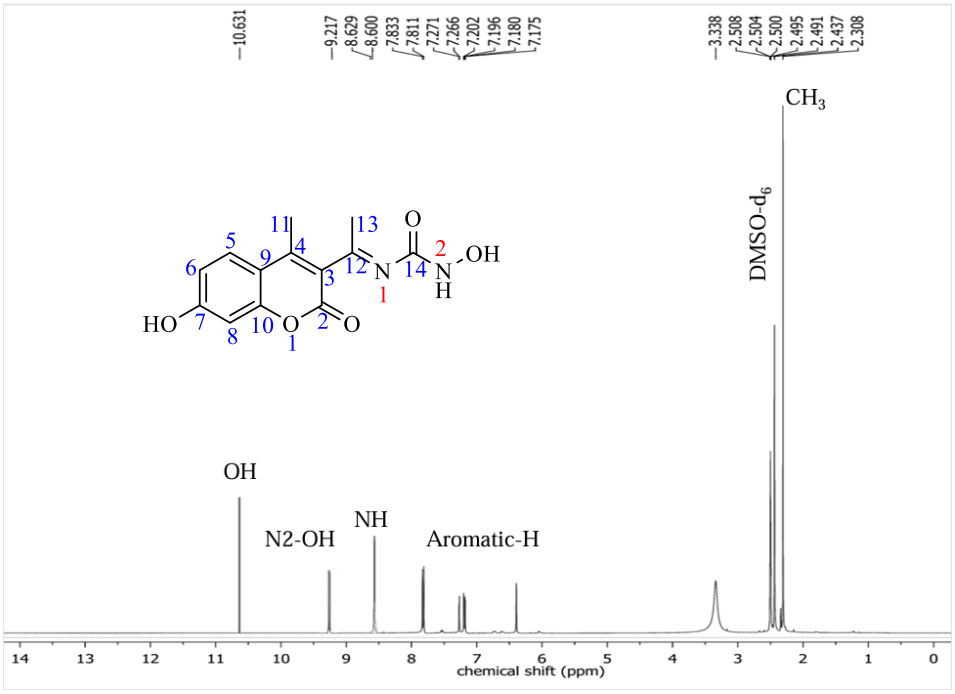

Figure S5: ^{1}H NMR spectra of compound 1a

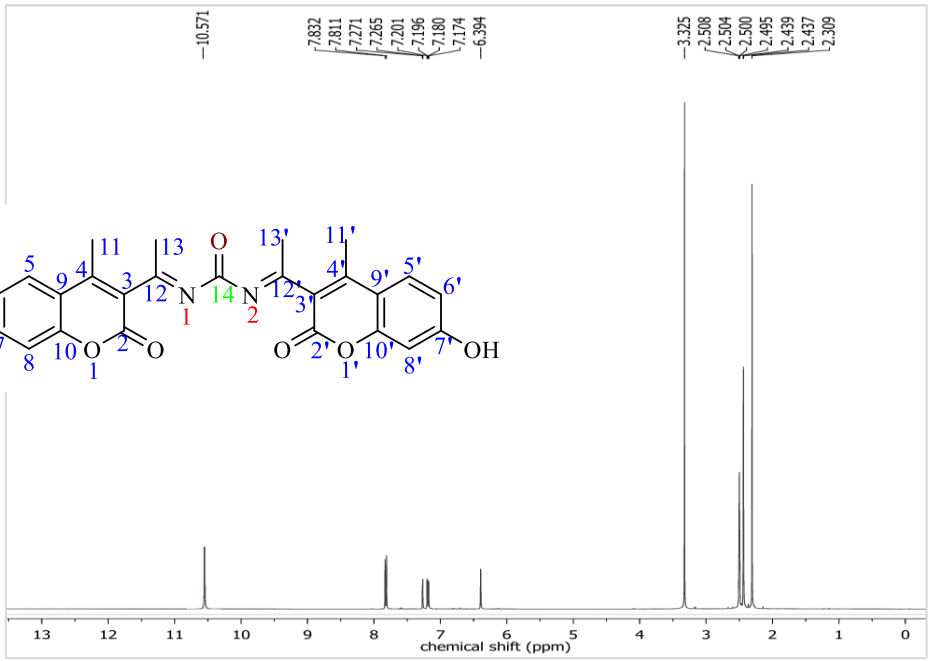

Figure S6: ^{1}H NMR spectra of compound 1b

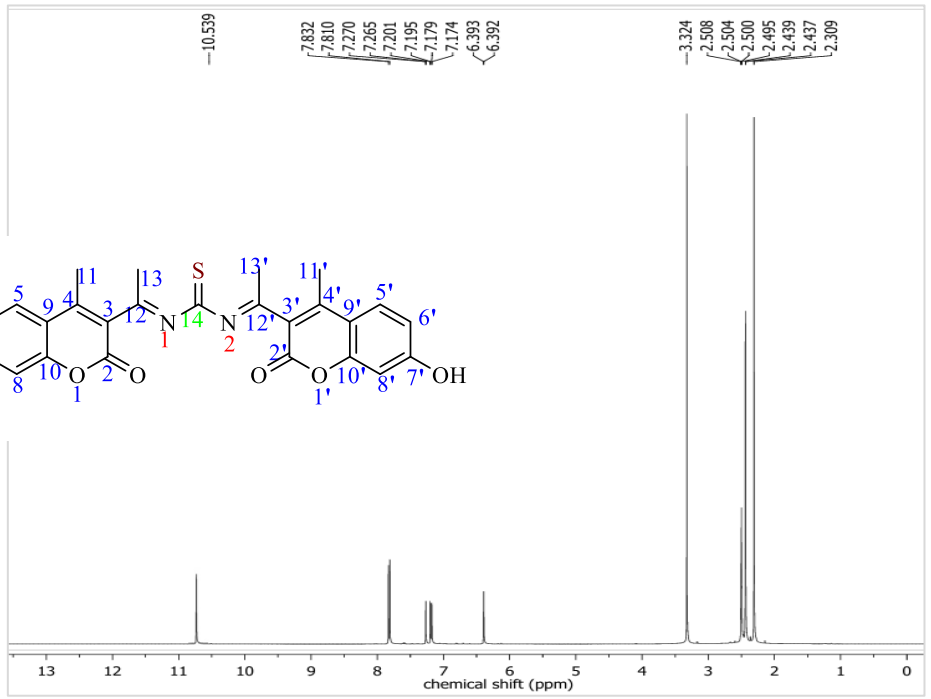

Figure S7: ^{1}H NMR spectra of compound 1c

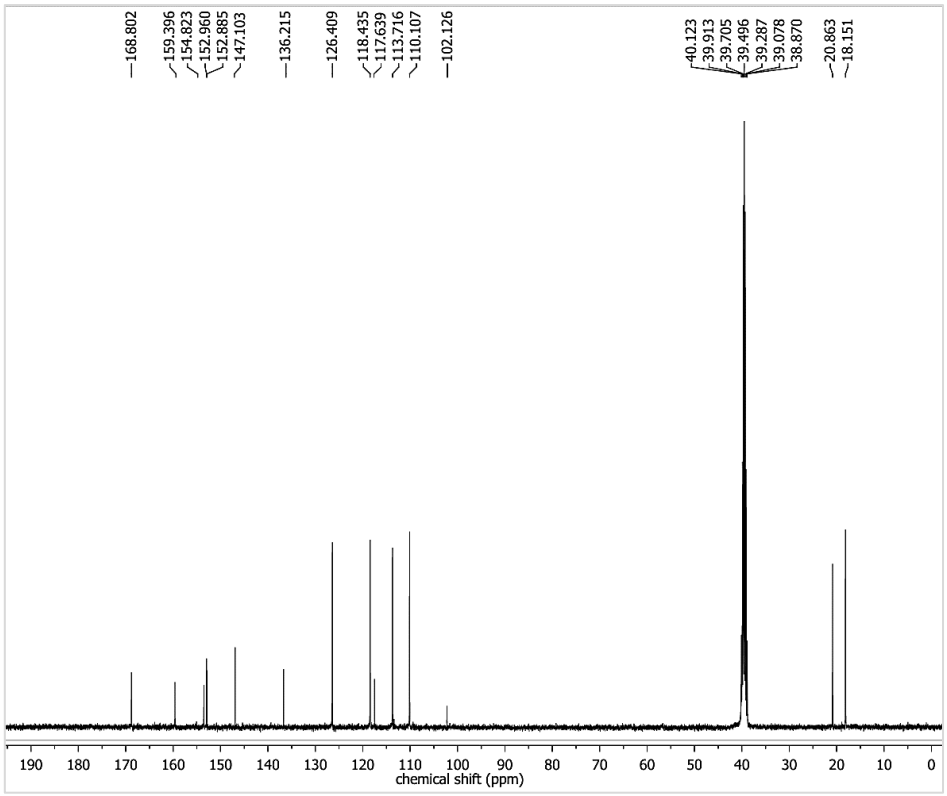

Figure S8: ^{13}C NMR spectra of compound 1a

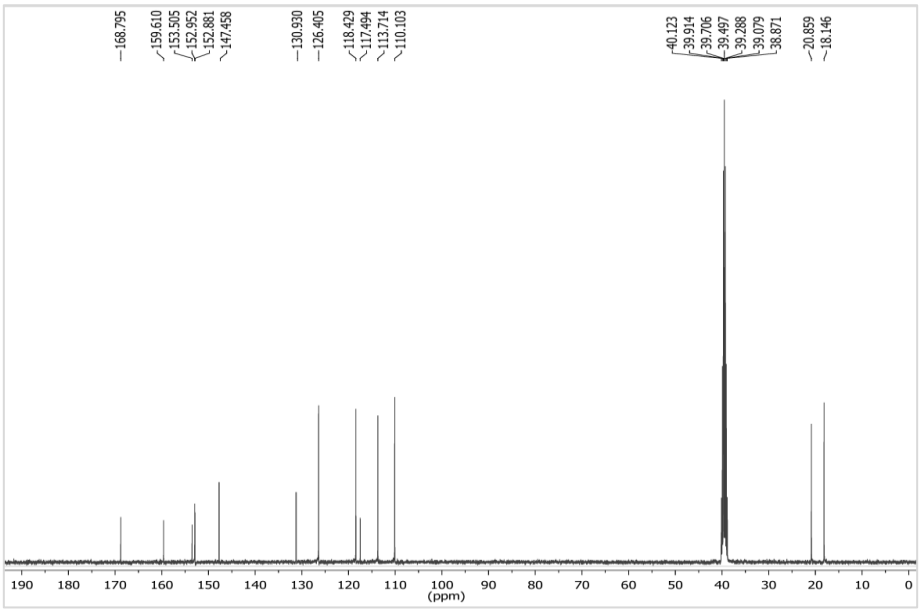

Figure S9: ^{13}C NMR spectra of compound 1b

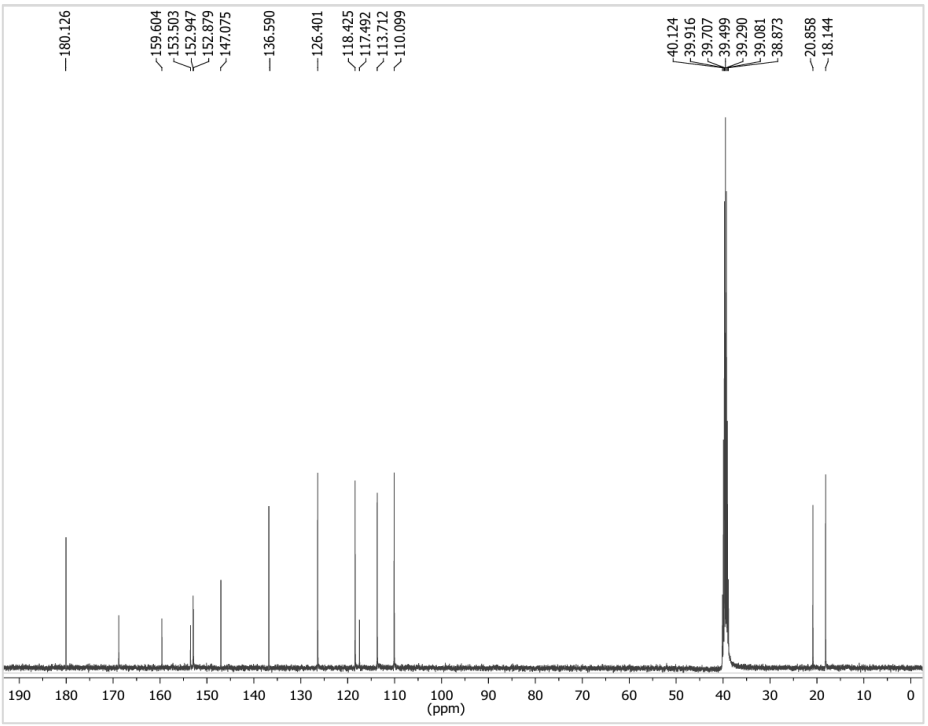

Figure S10: ^{13}C NMR spectra of compound 1c

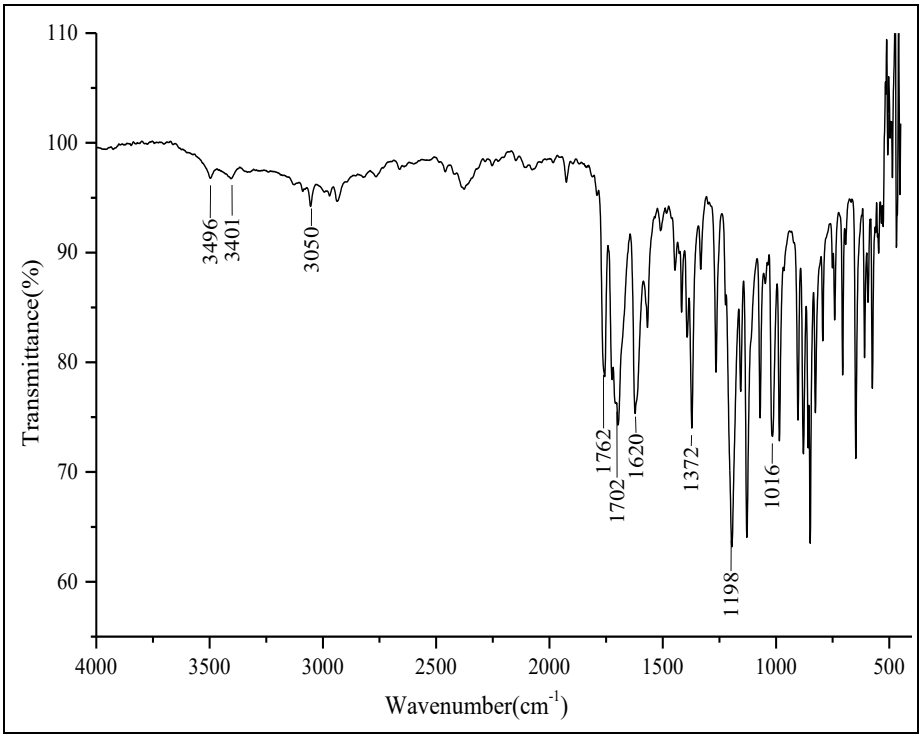

Figure S11: FT-IR spectra of compound 1a

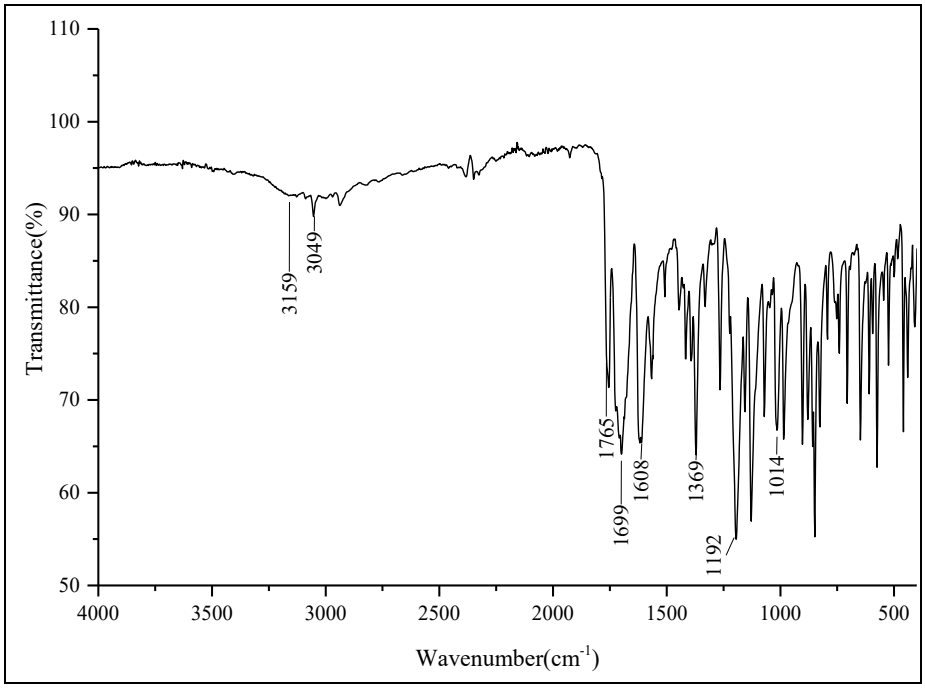

Figure S12: FT-IR spectra of compound 1b

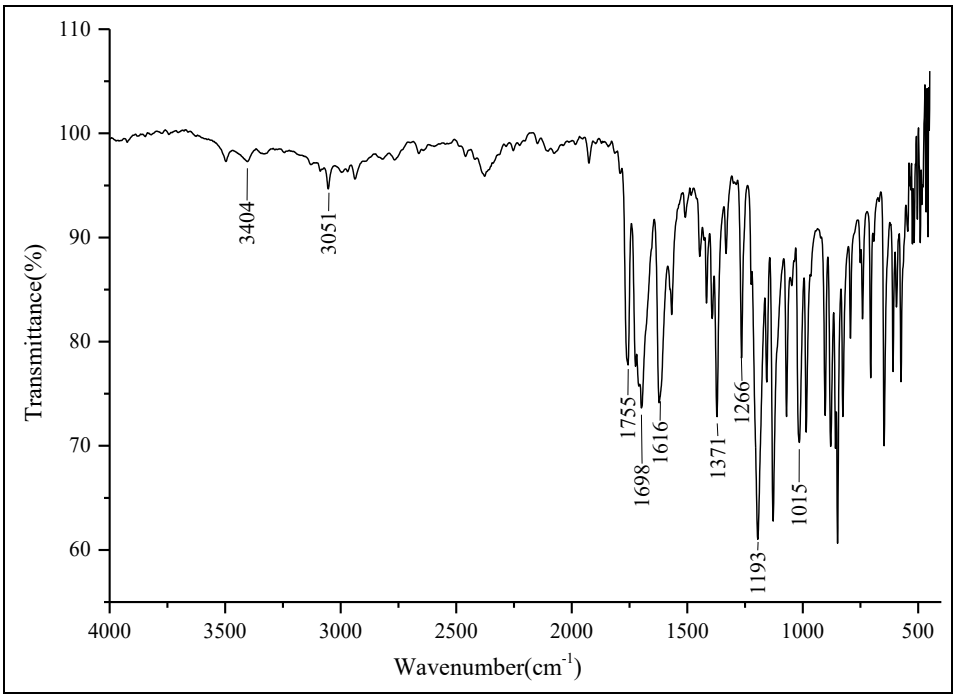

Figure S13: FT-IR spectra of compound 1c

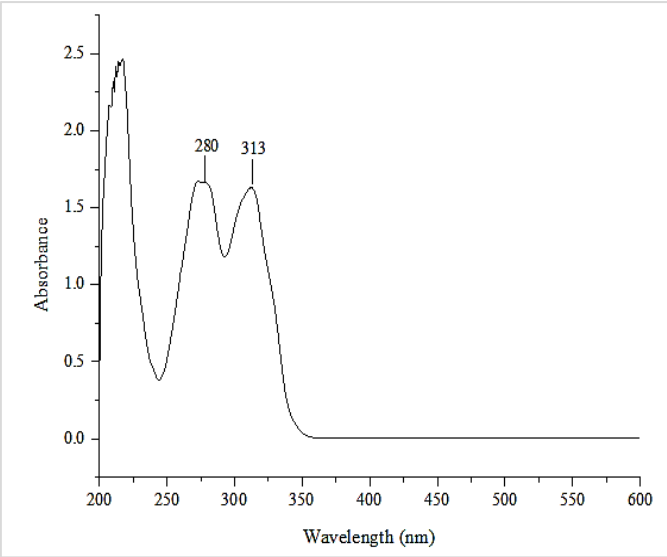

Figure S14: UV-Vis spectra of compound 1a

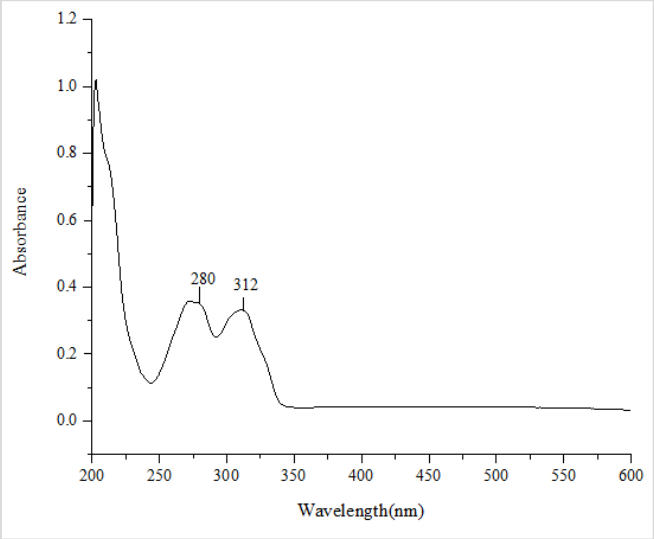

Figure S15: UV-Vis spectra of compound 1b

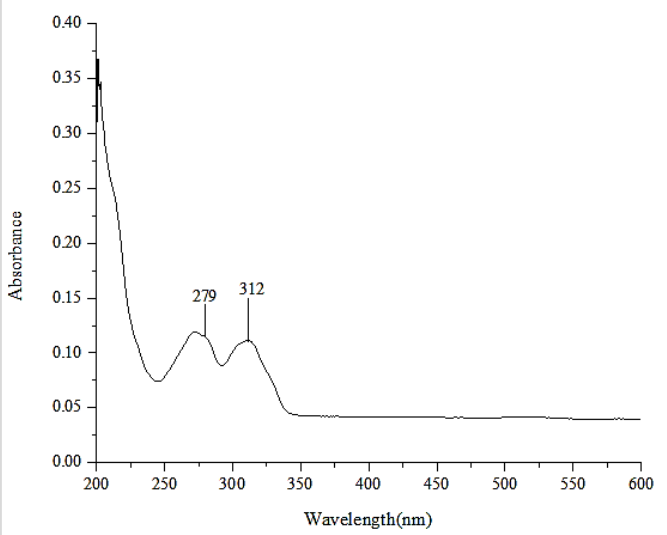

Figure S16: UV-Vis spectra of compound 1c