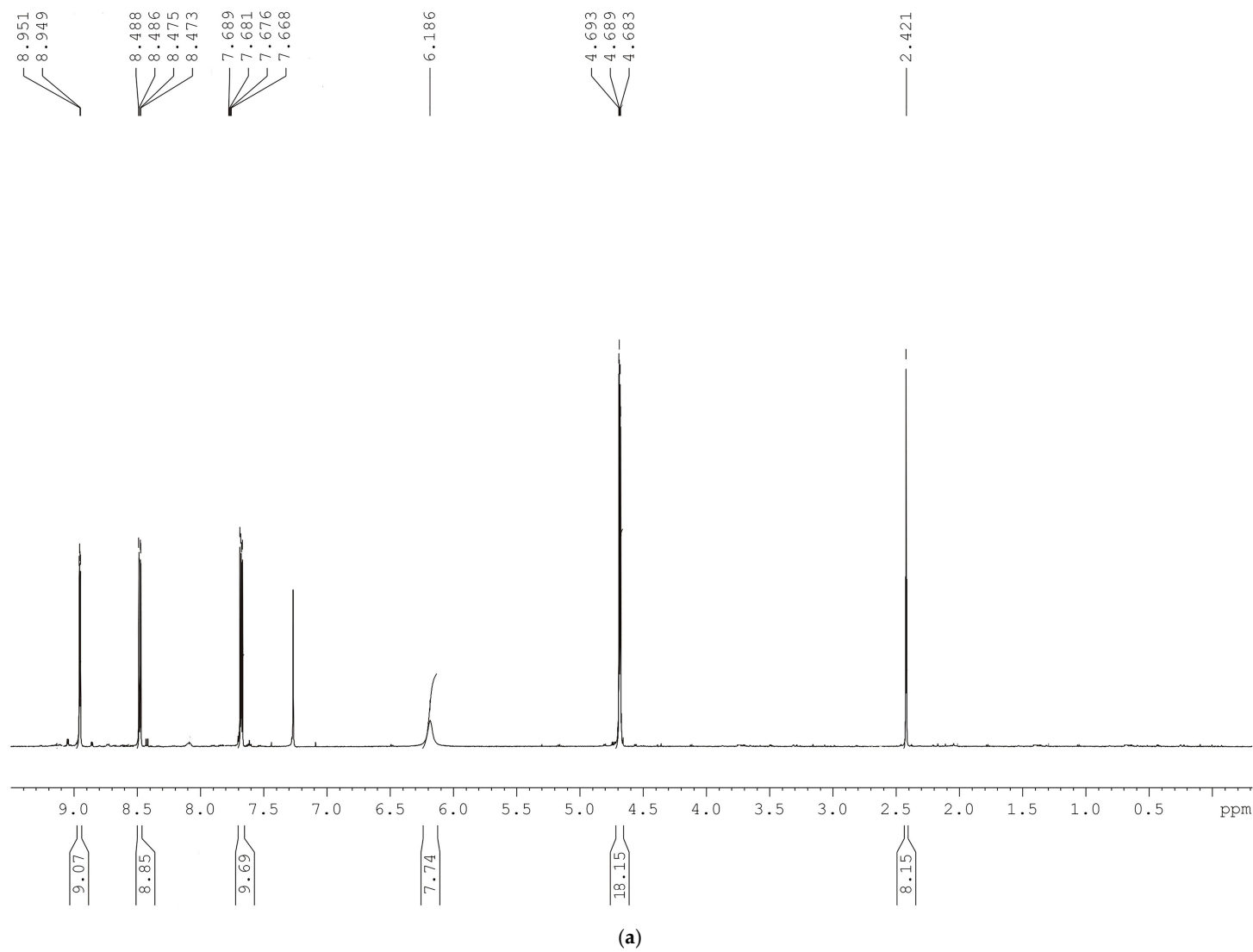


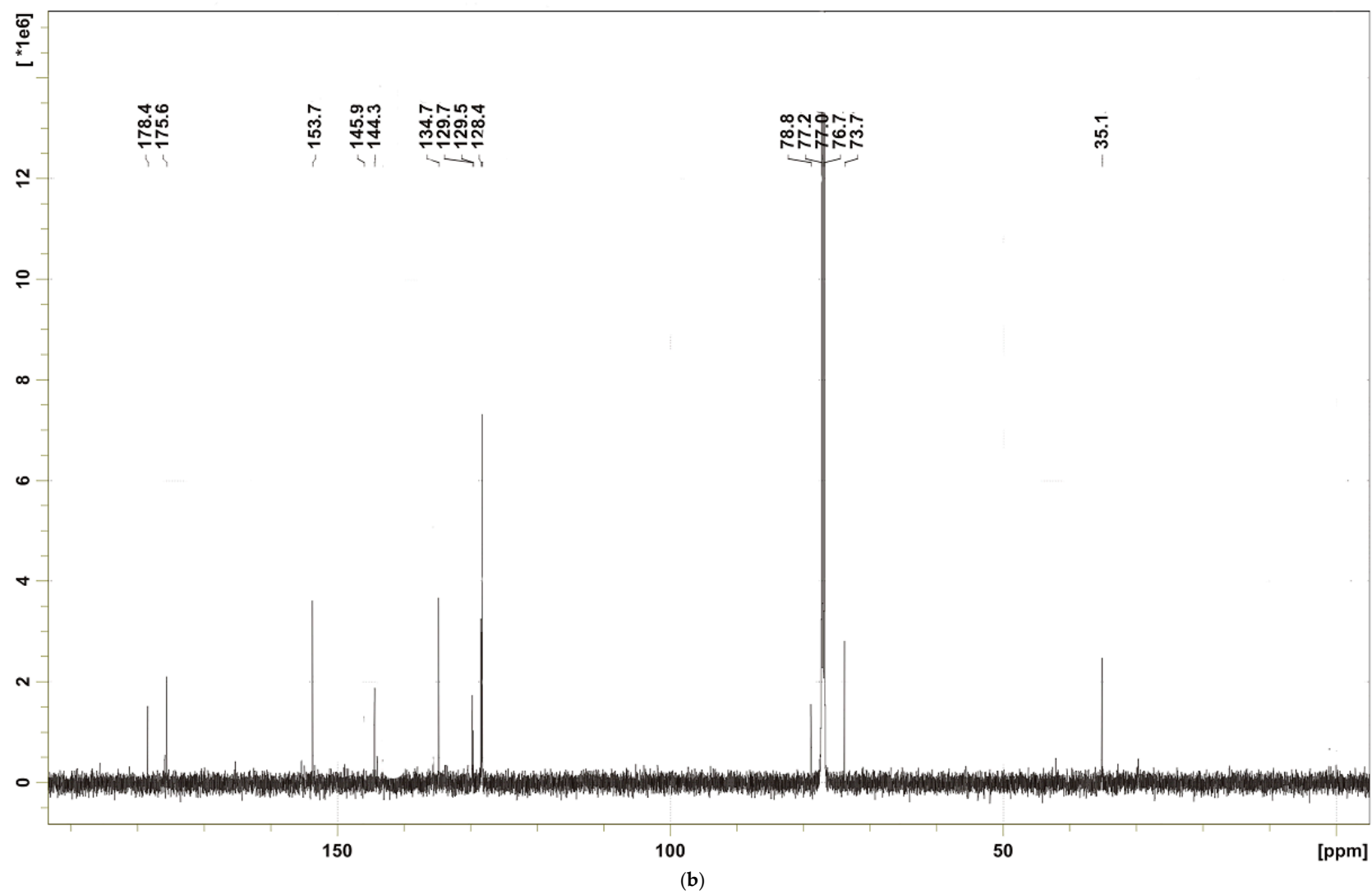
Supplementary Materials: New Acetylenic Amine Derivatives of 5,8-Quinolinediones: Synthesis, Crystal Structure and Antiproliferative Activity

Monika Kadela-Tomanek, Maria Jastrzębska, Ewa Bębenek, Elwira Chrobak, Małgorzata Latocha, Joachim Kusz, Dorota Tarnawska and Stanisław Boryczka

Table S1. Selected geometric parameters given by X-ray diffraction experiment and theoretical calculations for compounds **2a** and **3a**.

Bond Lengths (Å)	Experimental	Calculated	Bond Angles (°)	Experimental	Calculated
<i>6-chloro-7-propargylamine-5,8-quinolinedione 2a</i>					
Cl1–C6	1.7434 (1)	1.7472	C7–N2–C9	130.95	128.89
N2–C7	1.3418 (1)	1.3587	C7–N2–H2N	112.92	110.38
C2–H2	0.9500 (1)	1.0877	C9–N2–H2N	116.12	114.73
C2–C3	1.3885 (1)	1.4023	Cl1–C6–C7	122.57	122.84
O1–C5	1.2271 (1)	1.2275	N2–C9–H9A	107.39	106.18
O2–C8	1.2166 (1)	1.2204	C9–C10–C11	176.37	179.73
N2–H2N	0.8303 (1)	1.0178	C10–C11–H11	180.00	179.92
C9–H9A	0.8306 (2)	1.0899	C2–N1–C8A–C8	176.28	179.08
C9–H9B	0.9362 (1)	1.0948	H2N–N2–C7–C6	−174.12	−178.58
C9–C10	1.4634 (2)	1.4689	O1–C5–C6–Cl1	1.08	2.89
C10–C11	1.1818 (2)	1.2092	C9–C10–C11–H11	146.53	145.45
C11–H11	0.9500 (1)	1.0666	N2–C9–C10–C11	−176.36	−178.47
<i>7-chloro-6-propargylamine-5,8-quinolinedione 3a</i>					
Cl1–C7	1.7370	1.7447	C6–N2–C9	130.01	128.03
N2–C6	1.3360	1.3637	C6–N2–H2N	114.27	114.23
C2–H2	0.9500	1.0879	C9–N2–H2N	115.59	114.23
C2–C3	1.3905	1.4012	Cl1–C7–C6	122.19	122.39
O1–C5	1.2197	1.2199	N2–C9–H9A	109.09	110.18
O2–C8	1.2319	1.2280	C9–C10–C11	178.58	179.61
N2–H2N	0.8447	1.0172	C10–C11–H11	180.00	179.49
C9–H9A	0.9900	1.0901	C2–N1–C8A–C8	178.66	179.15
C9–H9B	0.9900	1.0948	H2N–N2–C6–C7	−175.66	−174.52
C9–C10	1.4753	1.4691	O2–C8–C7–Cl1	1.97	2.08
C10–C11	1.1908	1.2094	C9–C10–C11–H11	146.84	145.08
C11–H11	0.9500	1.0666	N2–C9–C10–C11	−175.23	−176.98





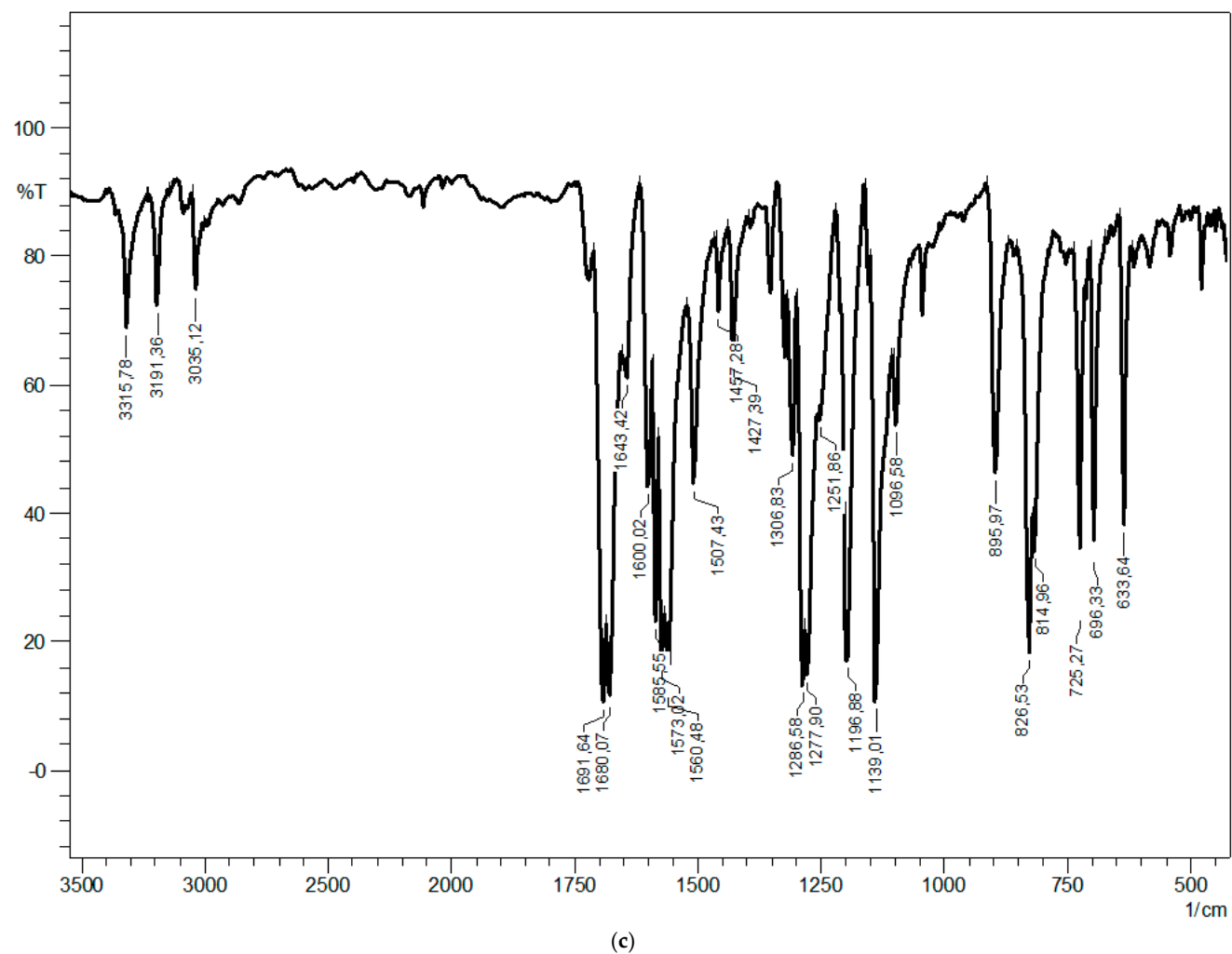
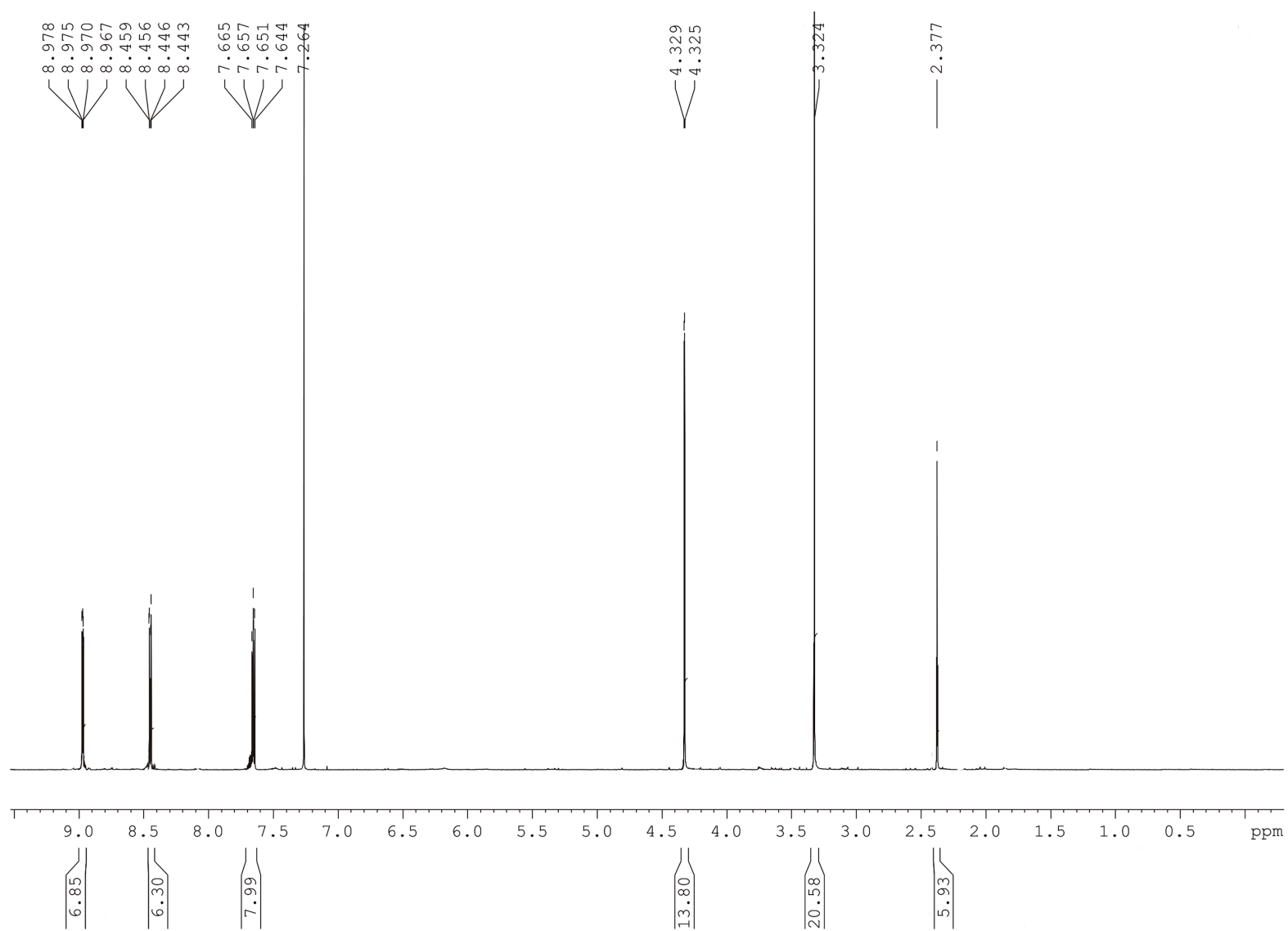
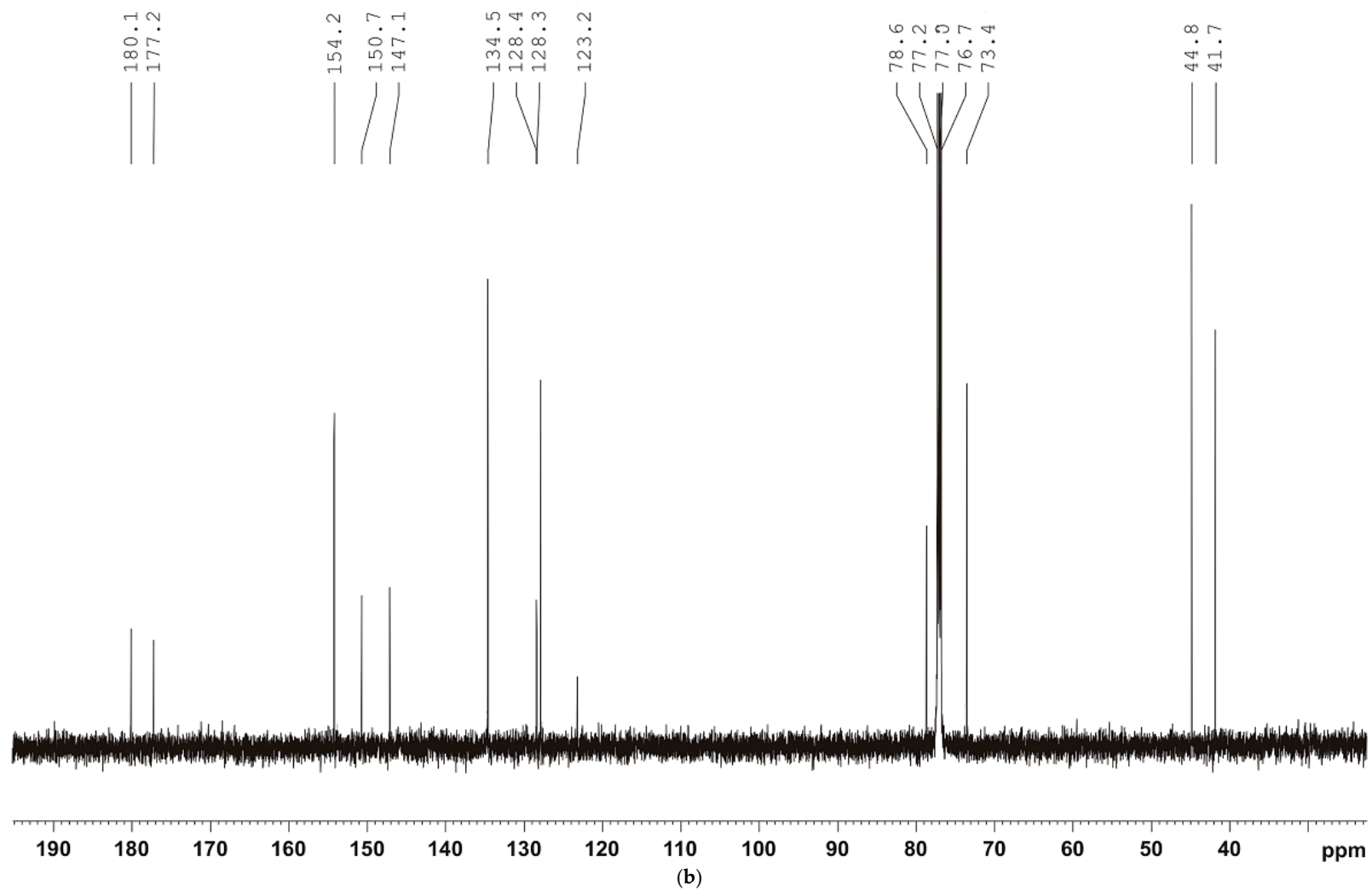
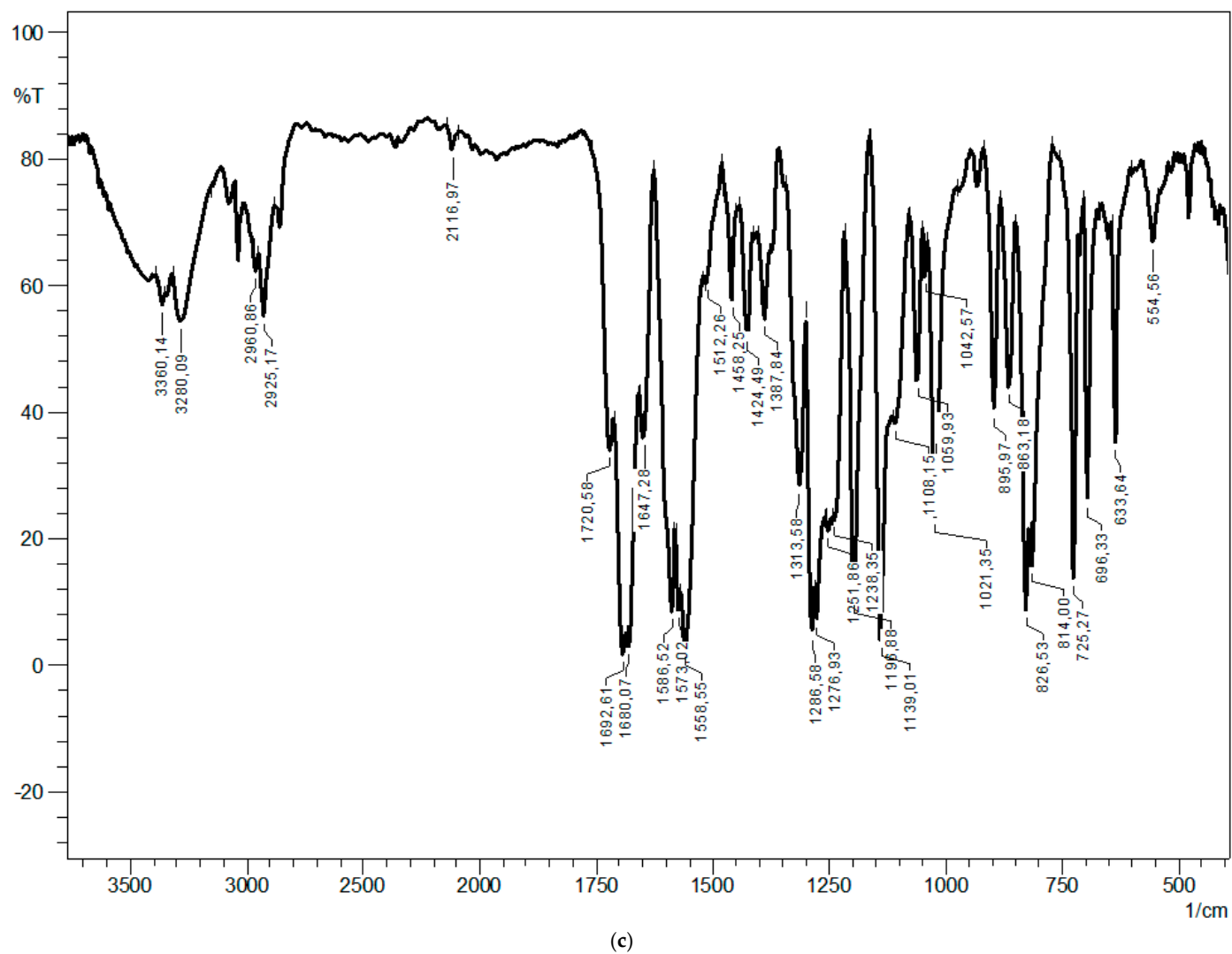


Figure S1. 6-chloro-7-propargylamine-5,8-quinolinedione **2a**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.

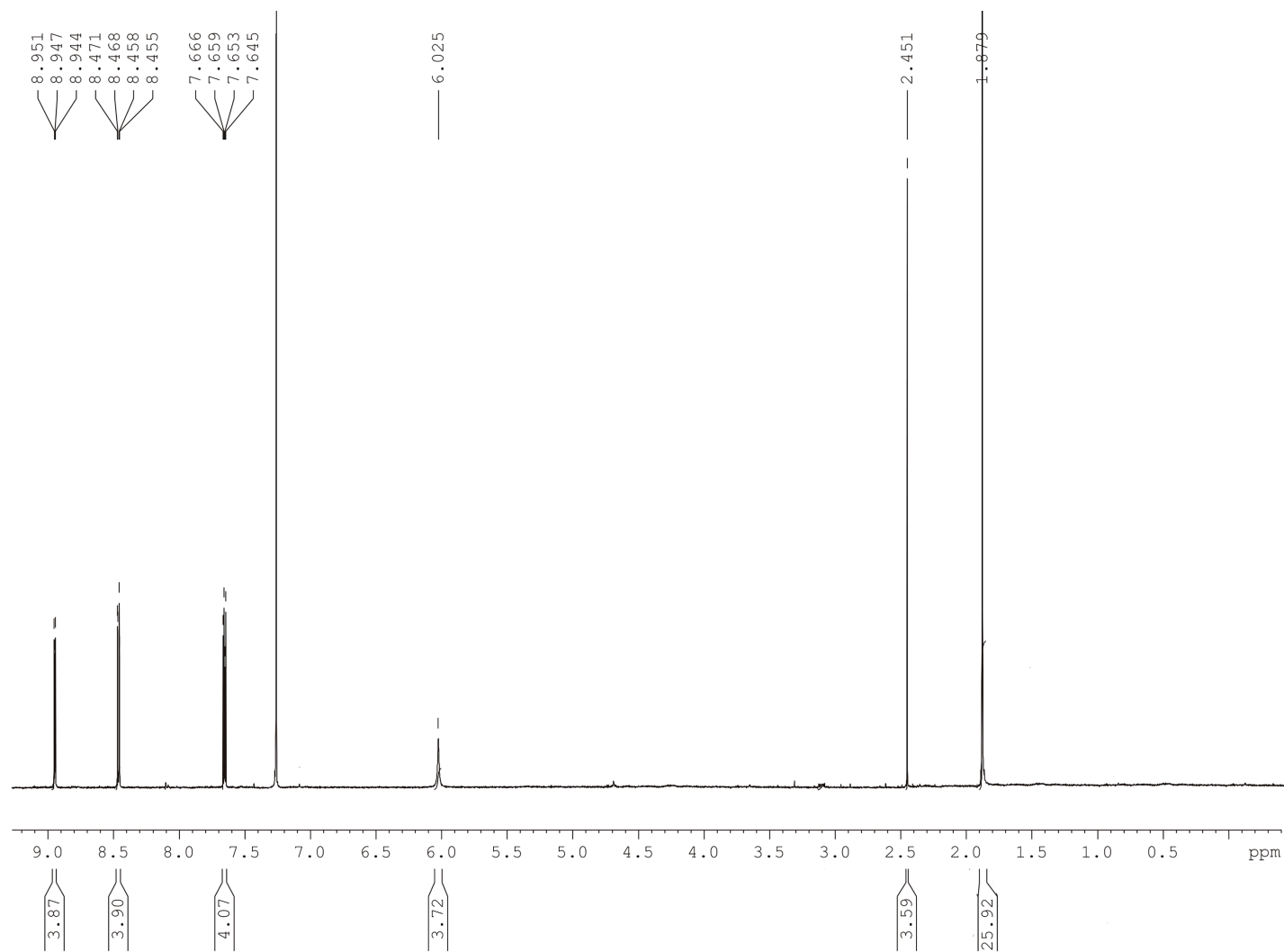


(a)

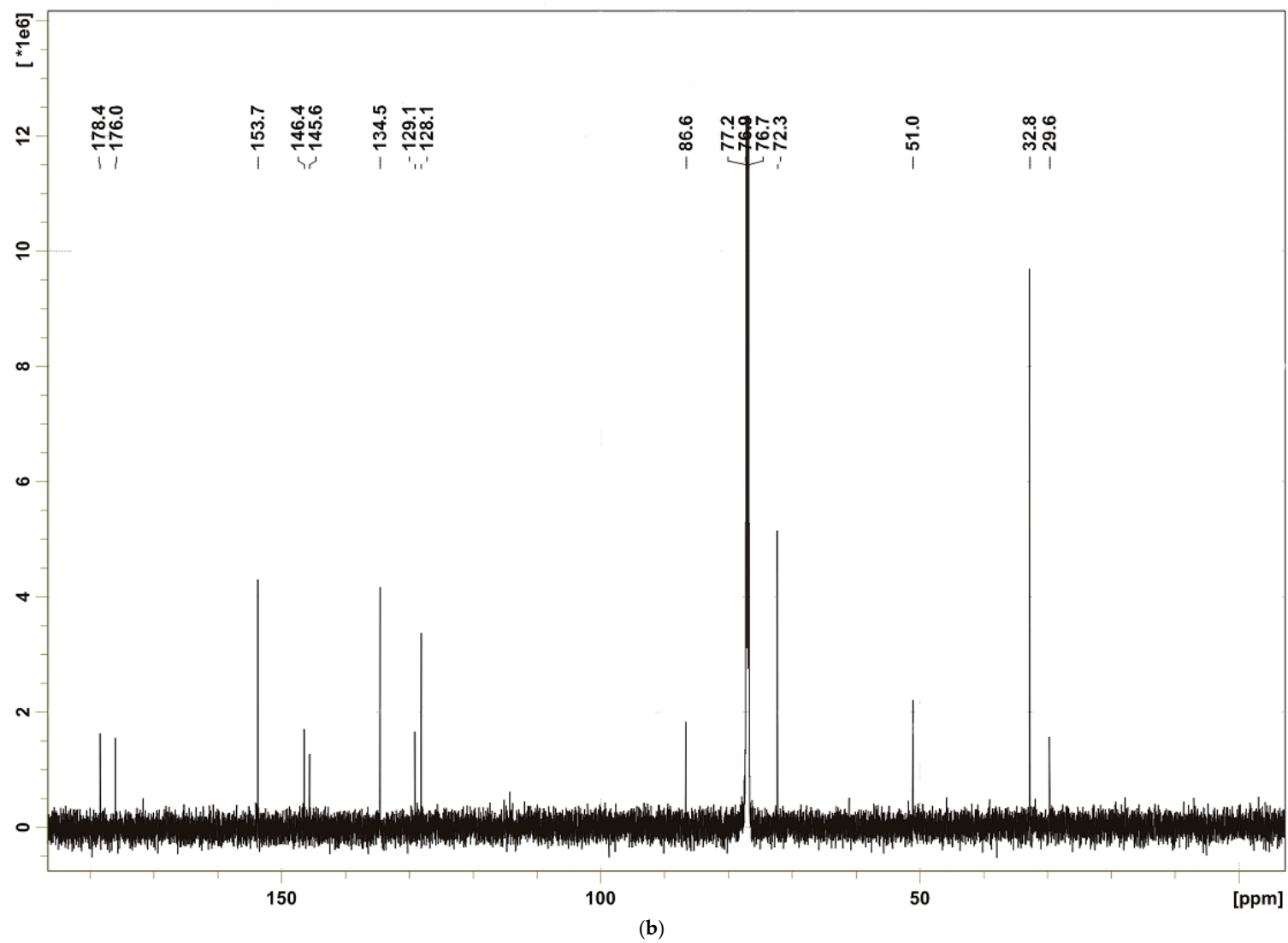




FigureS2. 6-chloro-7-(*N*-methylpropargylamine)-5,8-quinolinedione **2b**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.



(a)



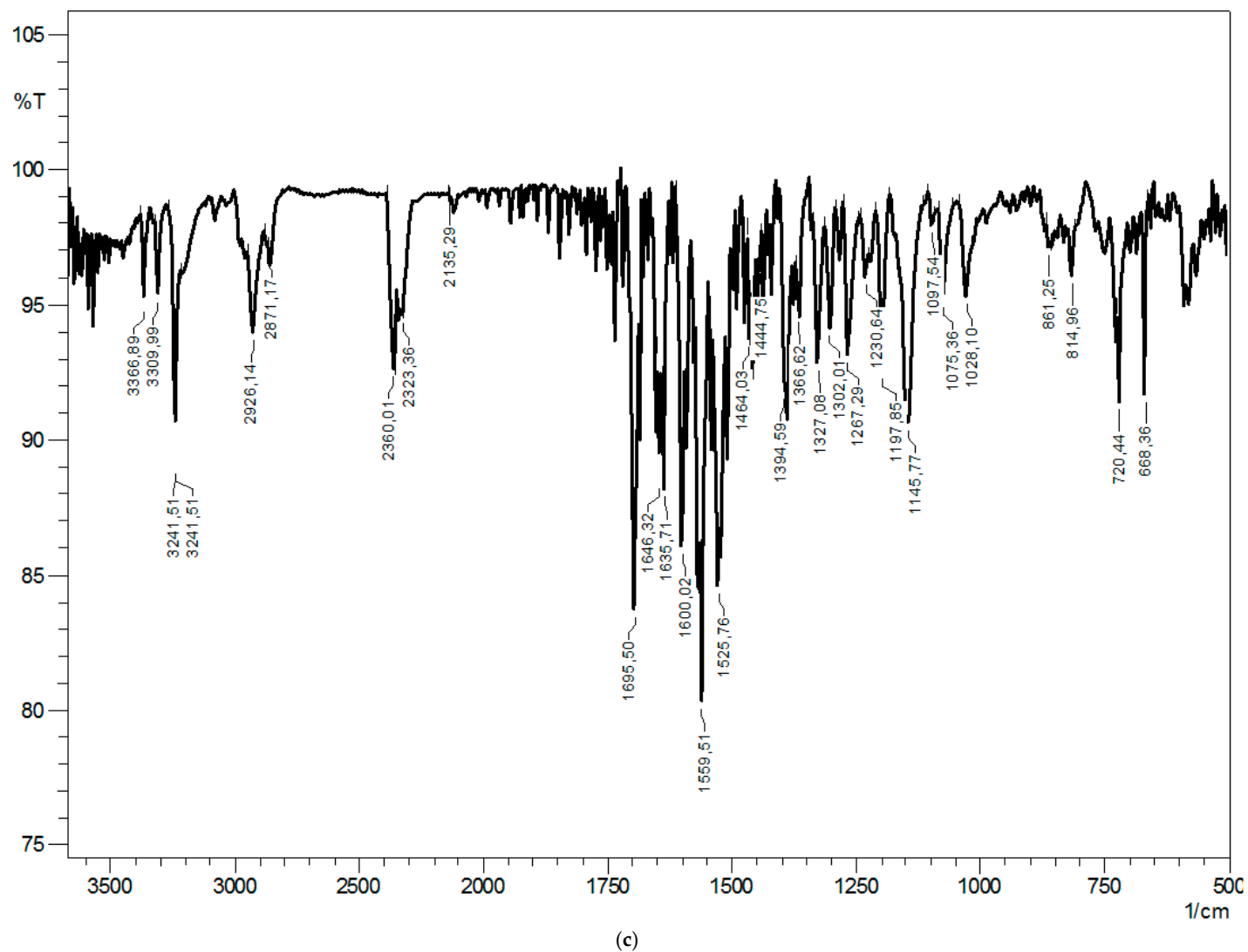
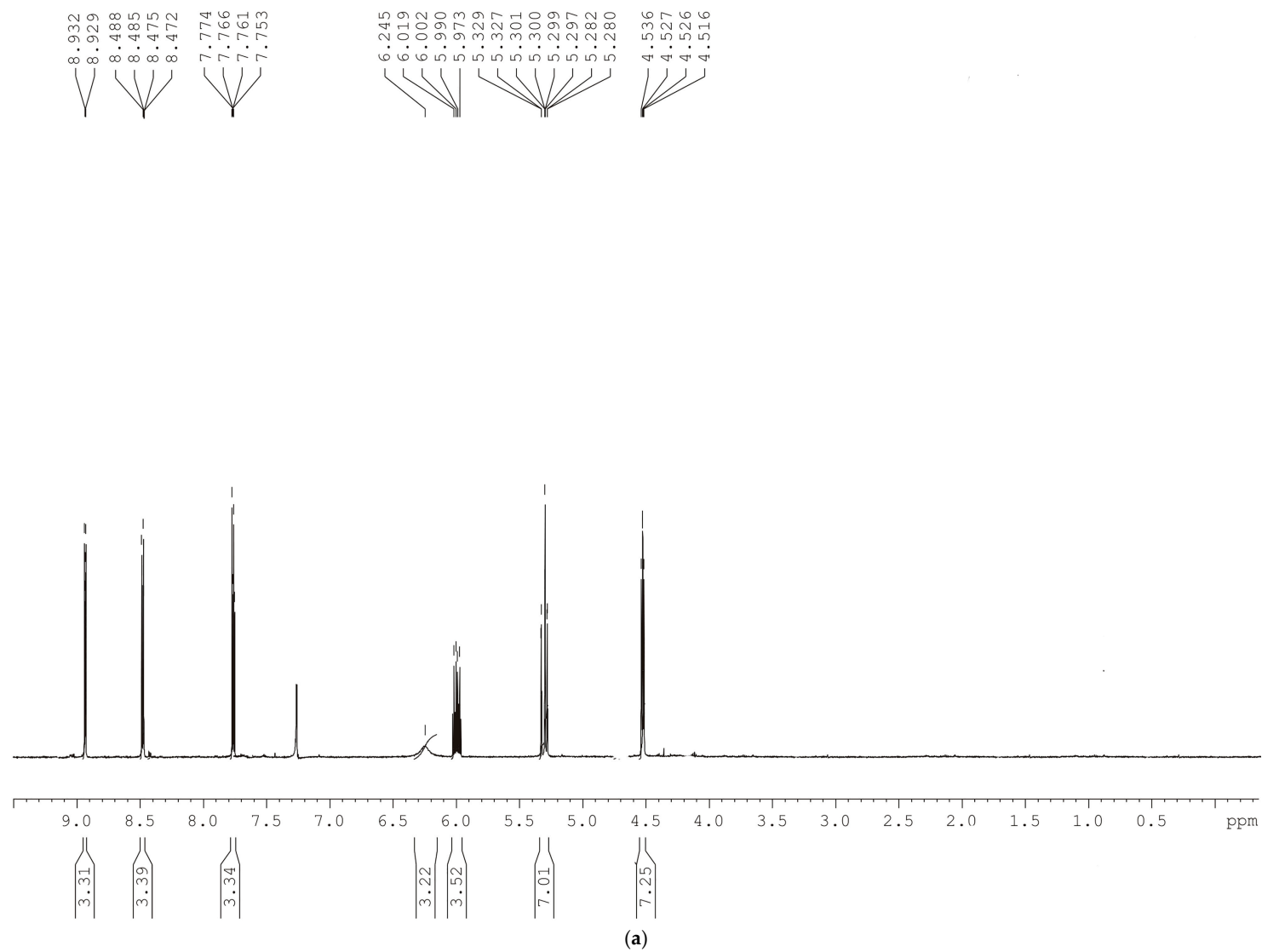
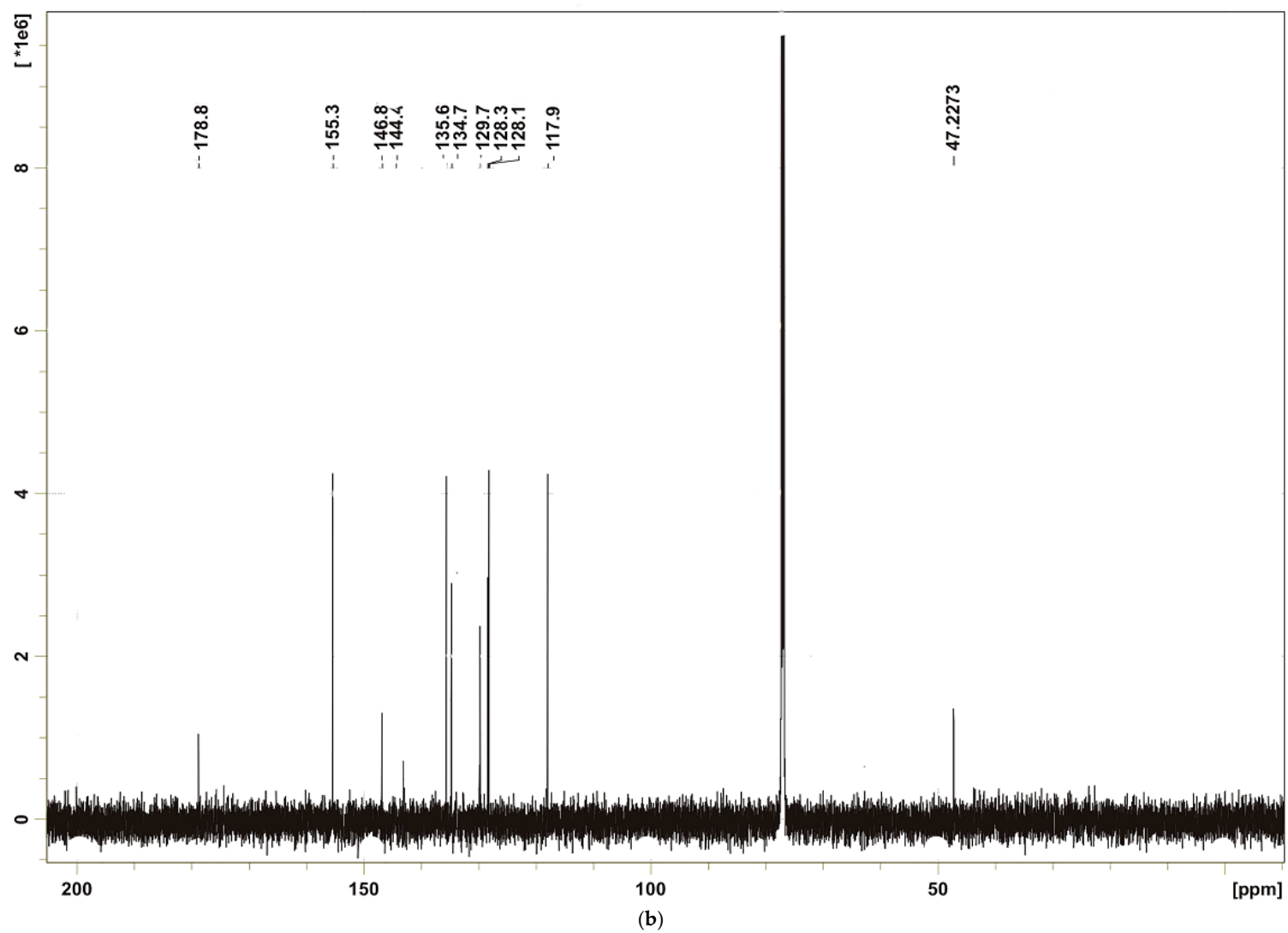


Figure S3. 6-chloro-7-(1,1-dimethylpropargylamine)-5,8-quinolinedione 2c, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.





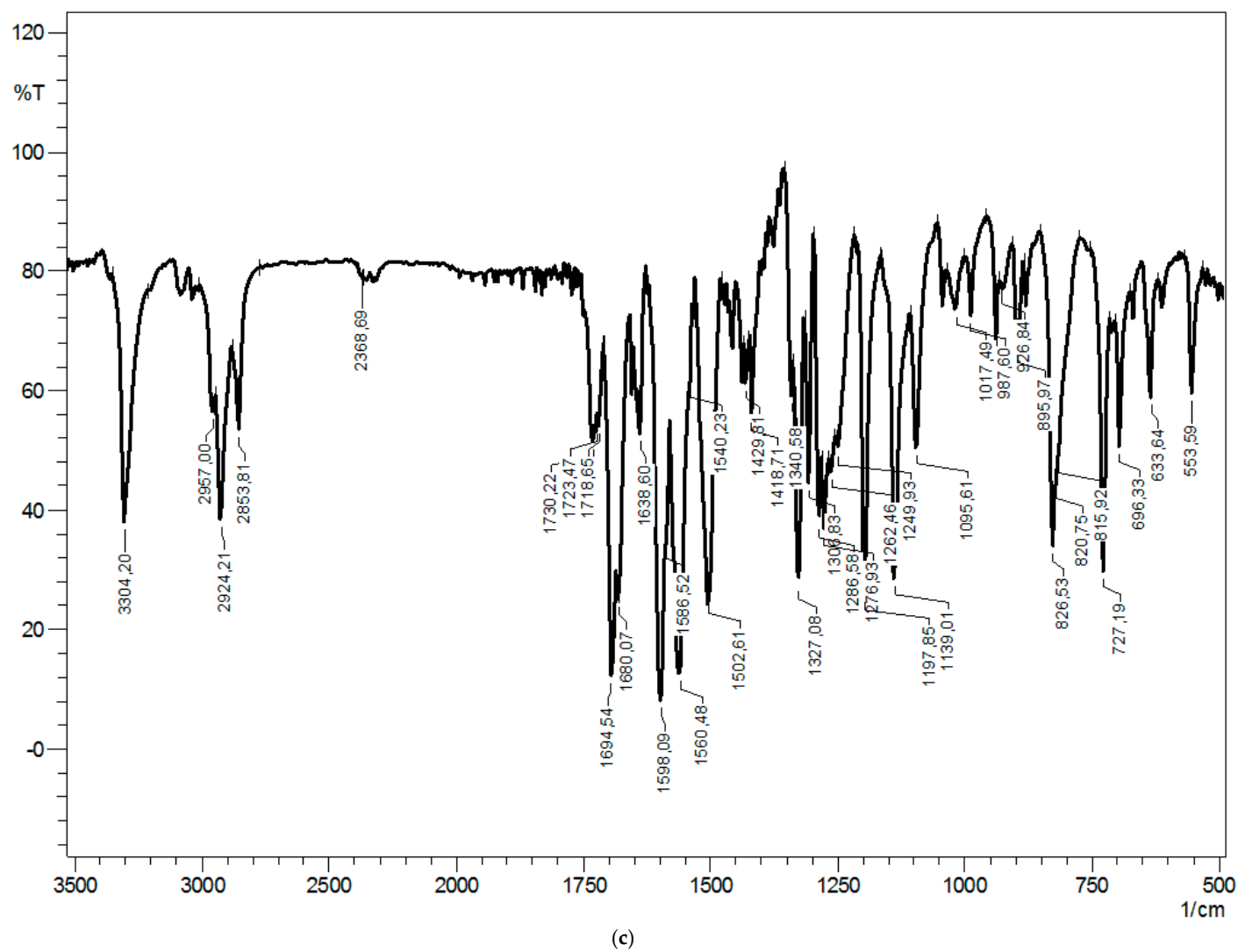
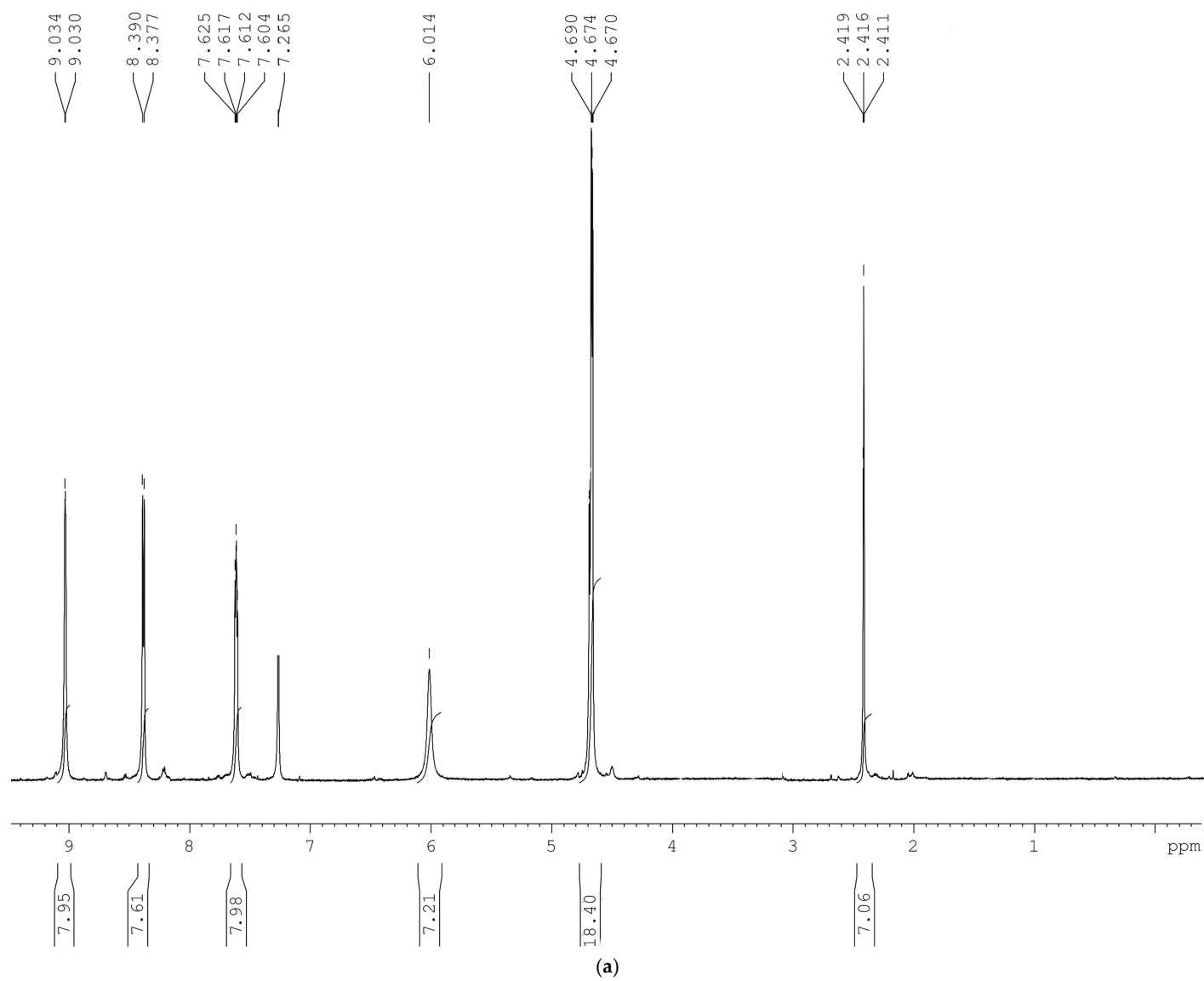
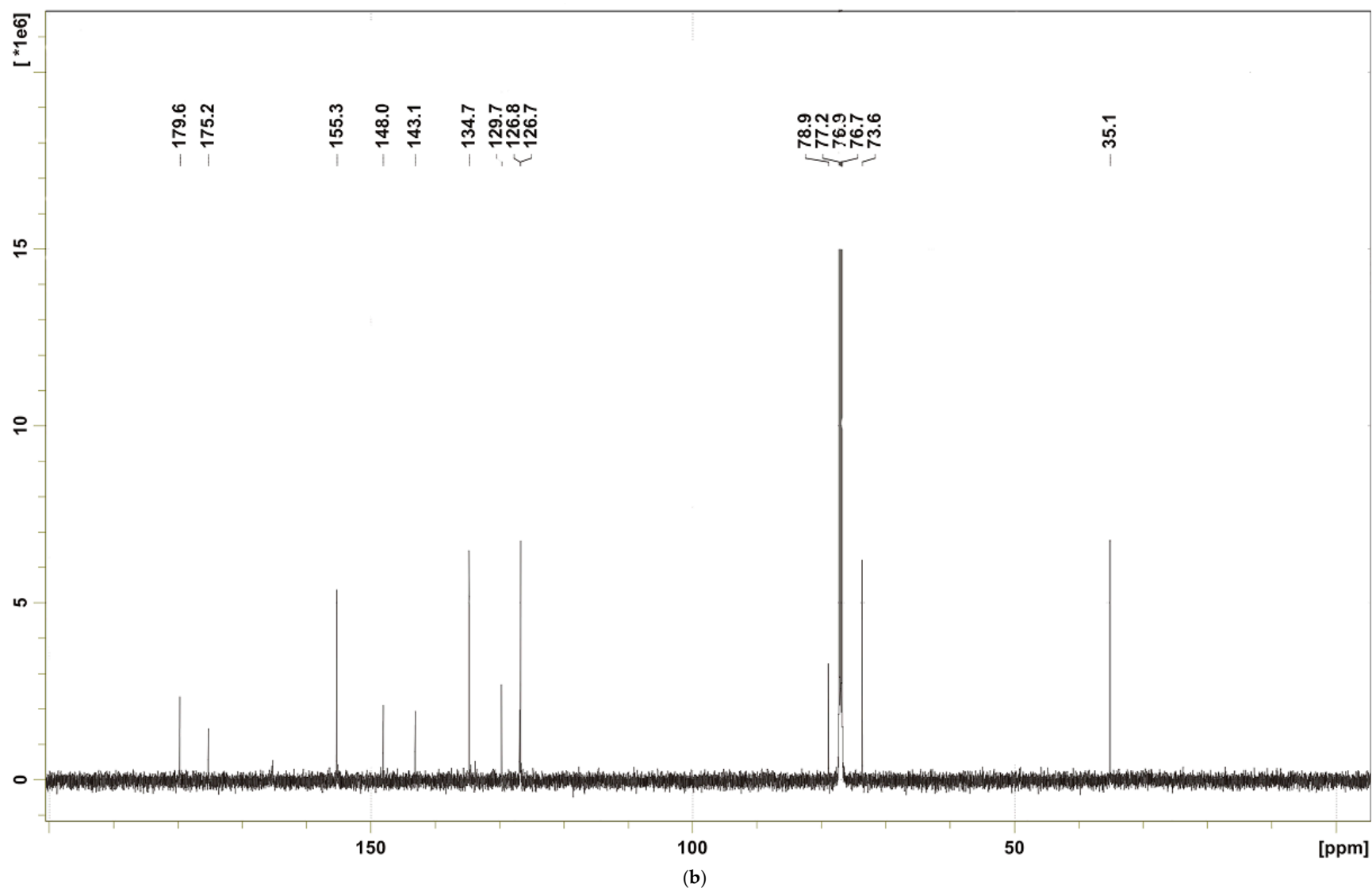


Figure S4. 6-chloro-7-allylamine-5,8-quinolinedione **2d**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.





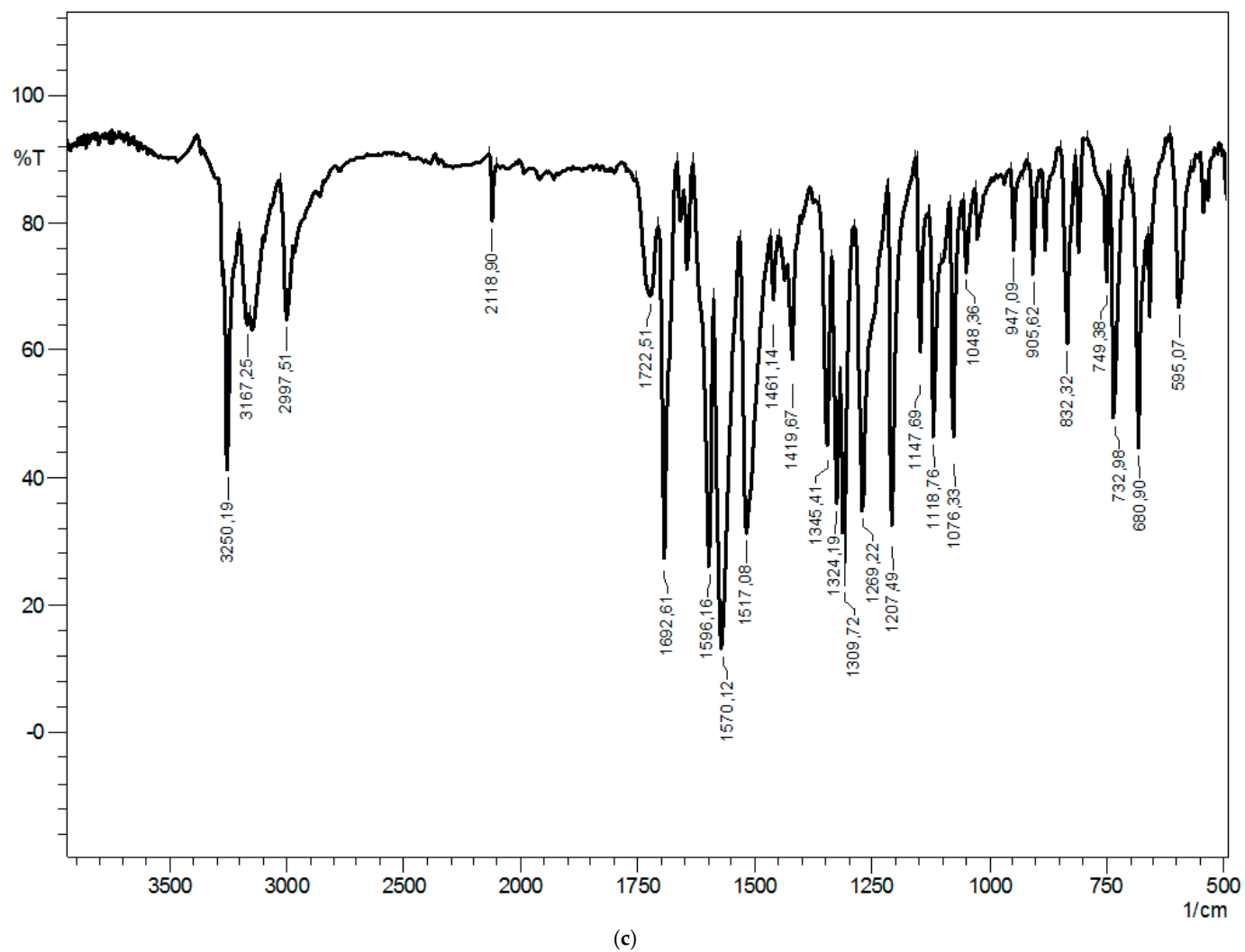
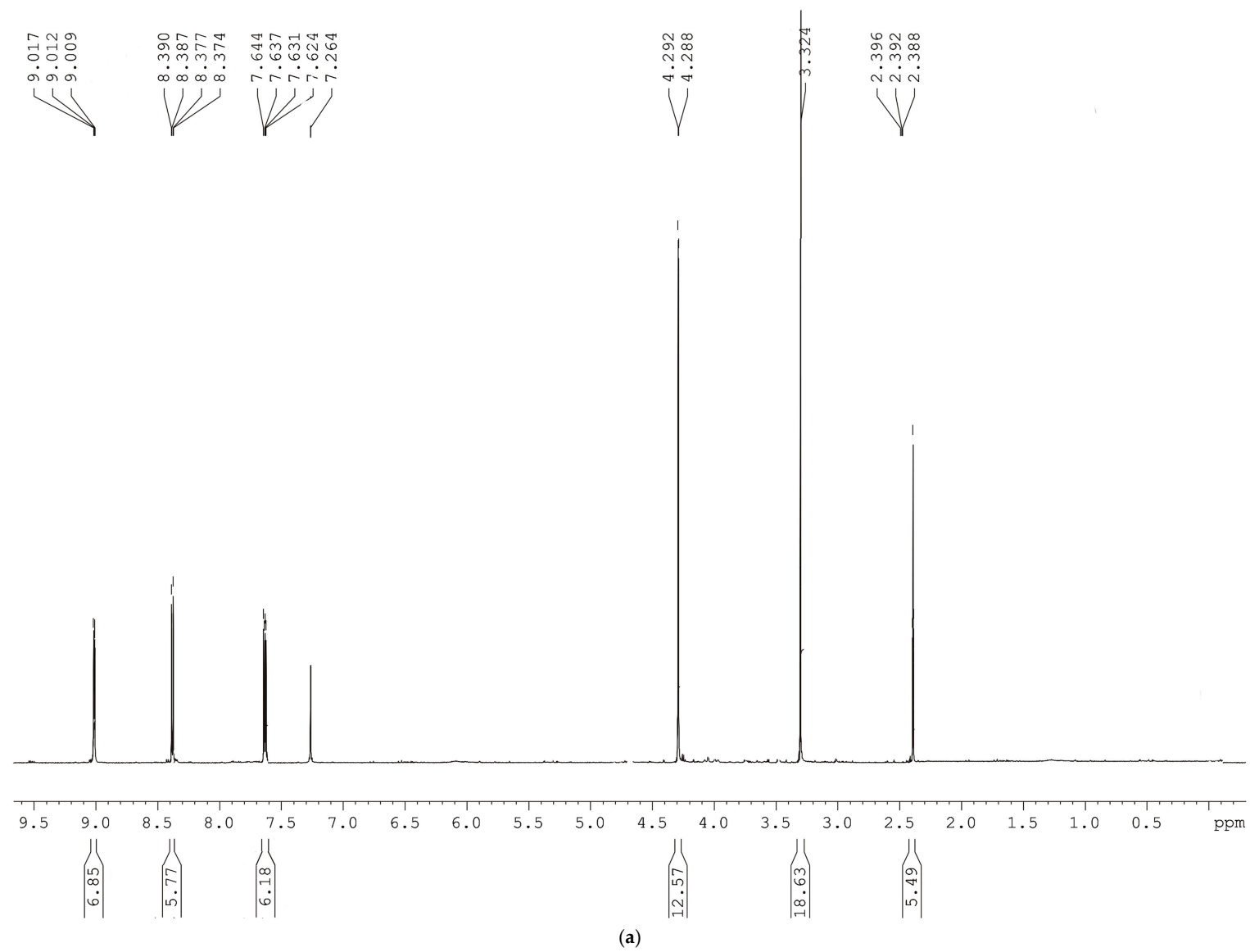
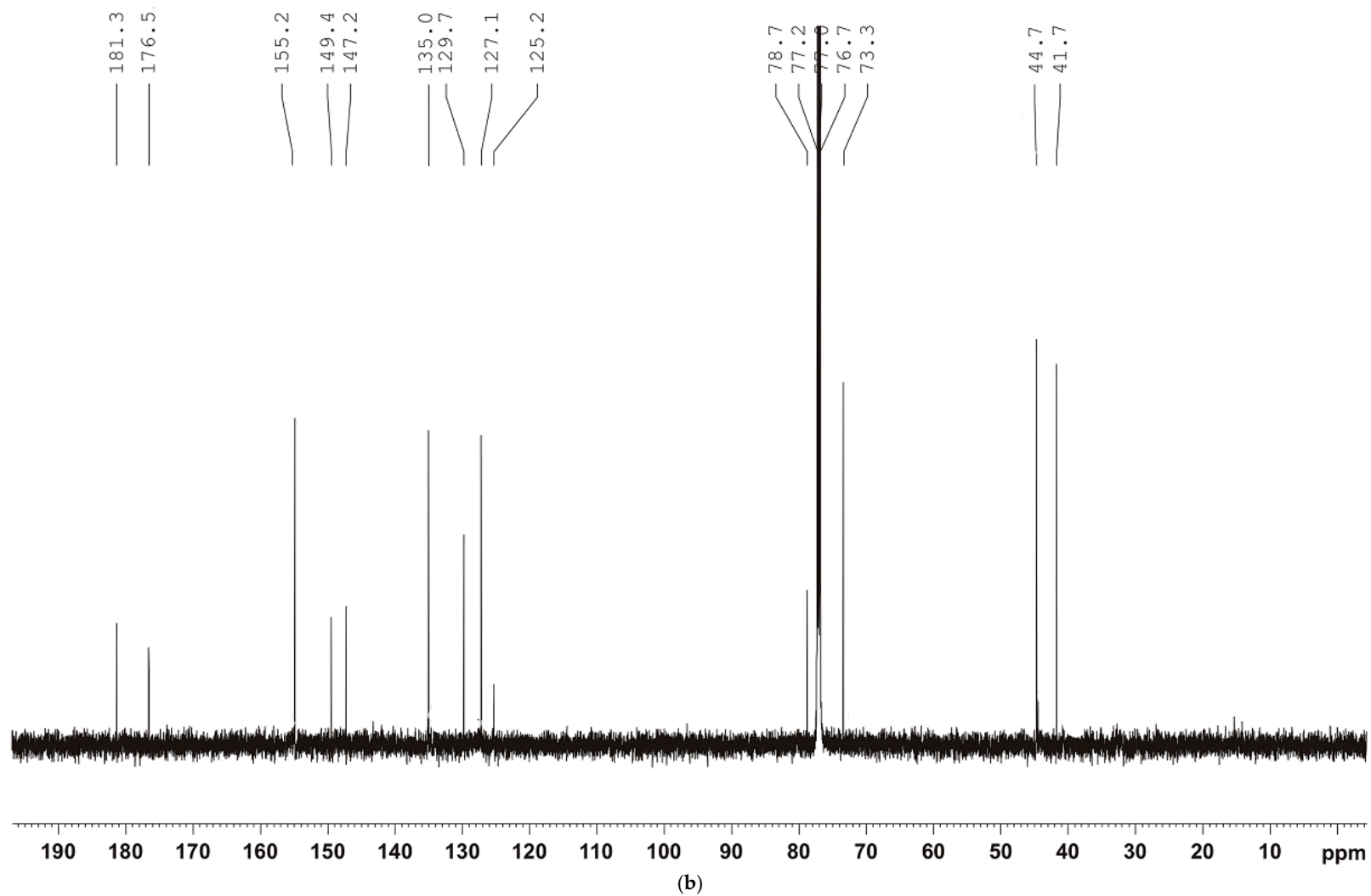


Figure S5. 7-chloro-6-propargylamine-5,8-quinolinedione **3a**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.





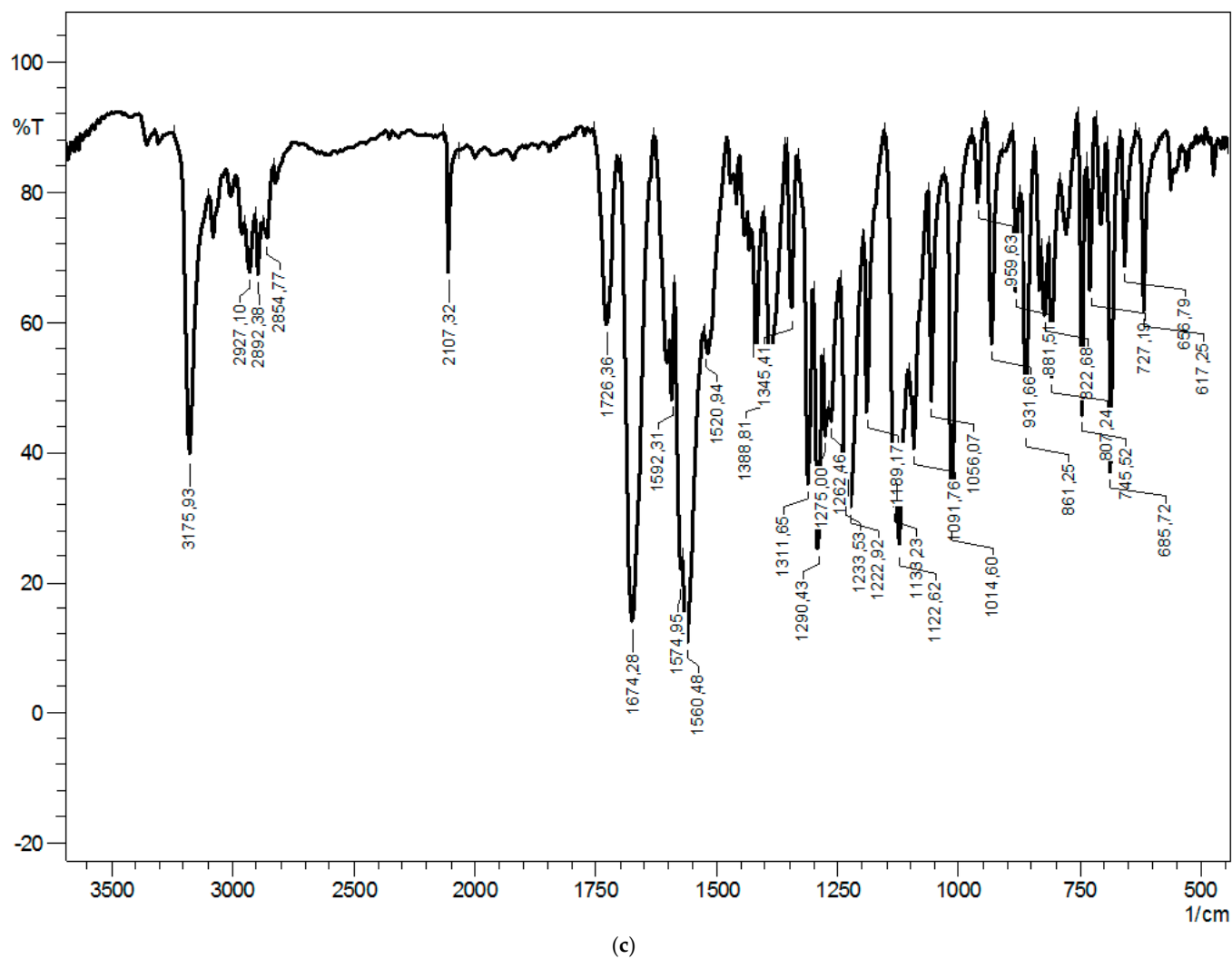
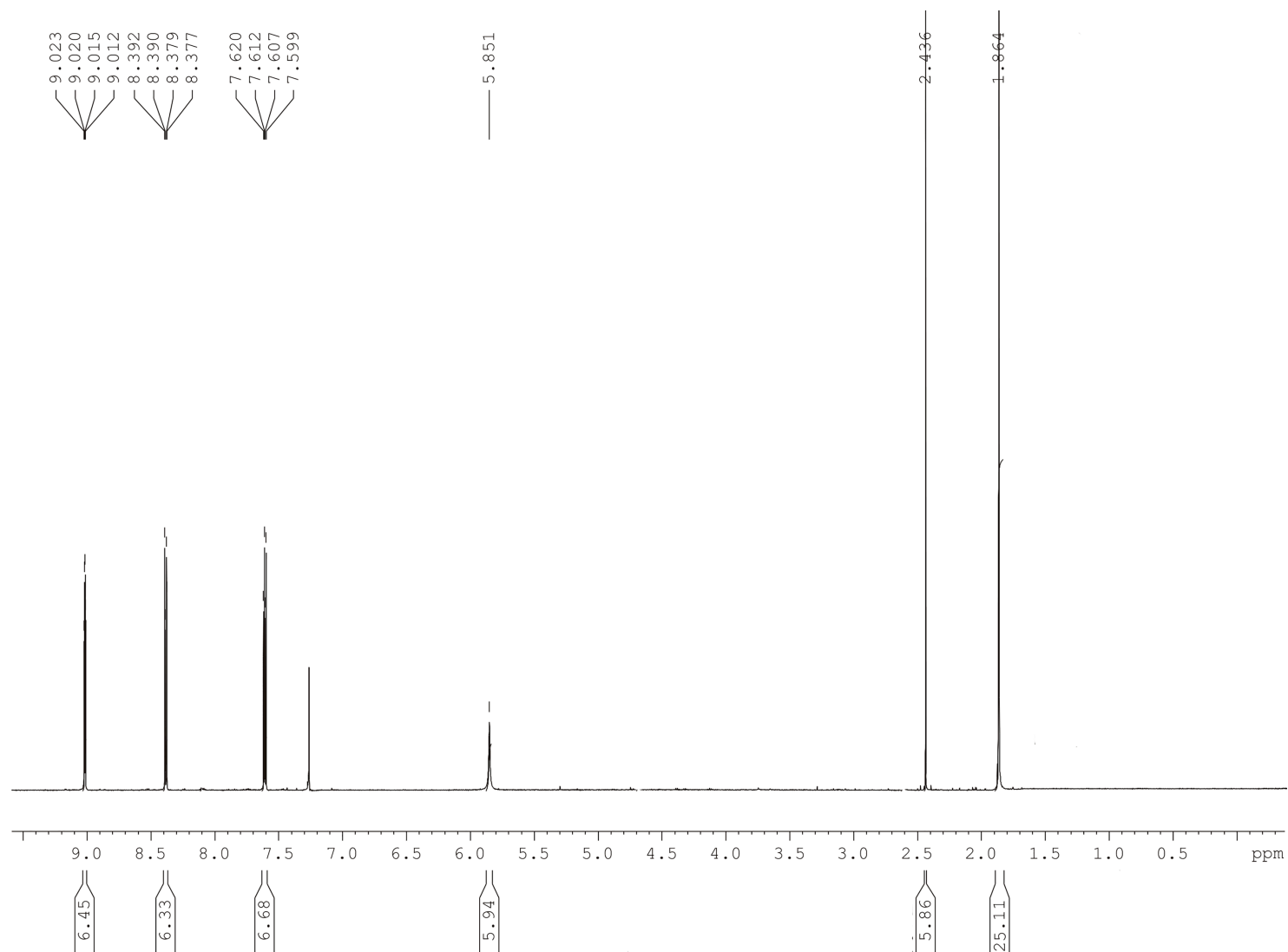
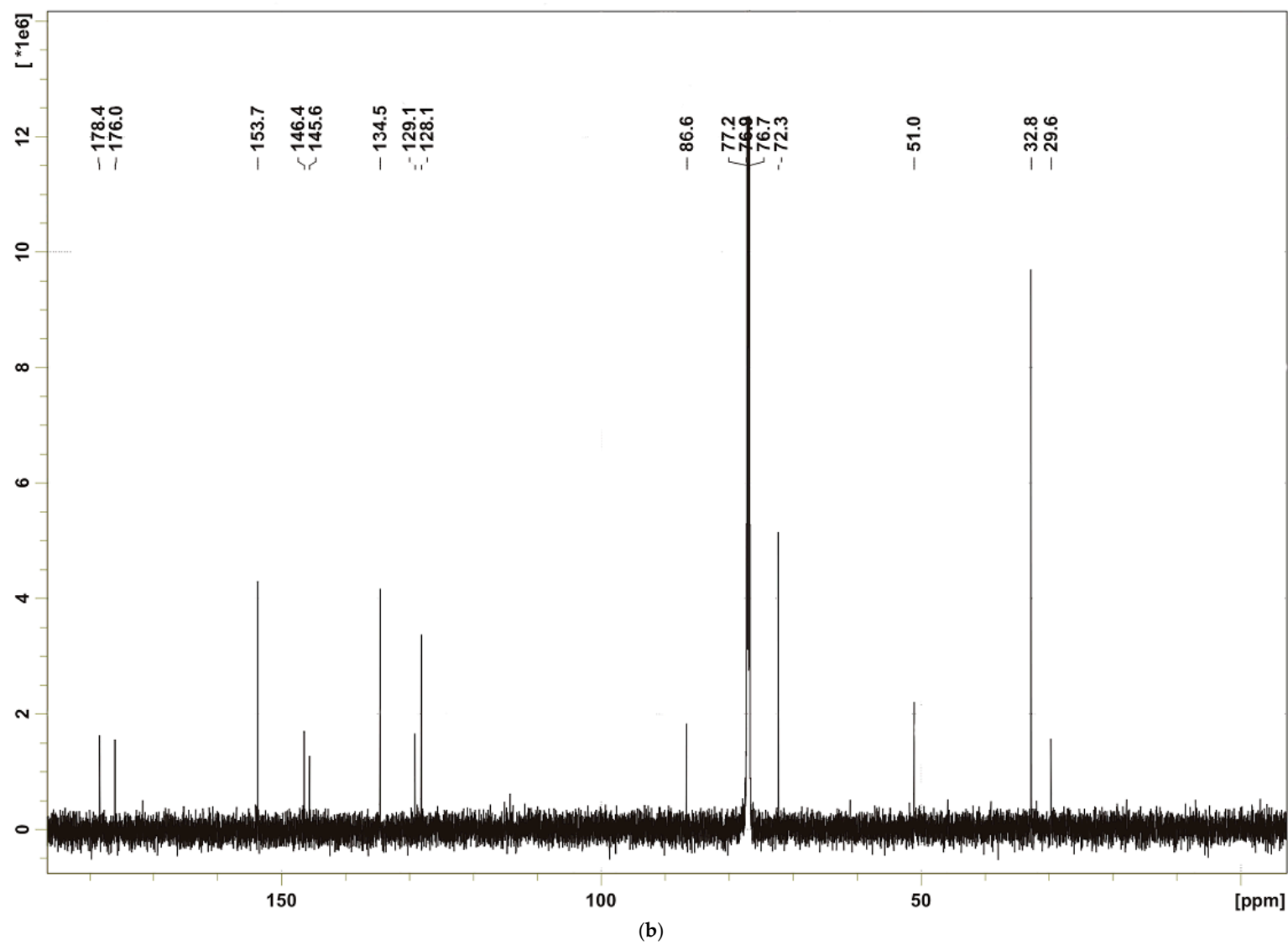


Figure S6. 7-chloro-6-(*N*-methylpropargylamine)-5,8-quinolinedione **3b**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.



(a)



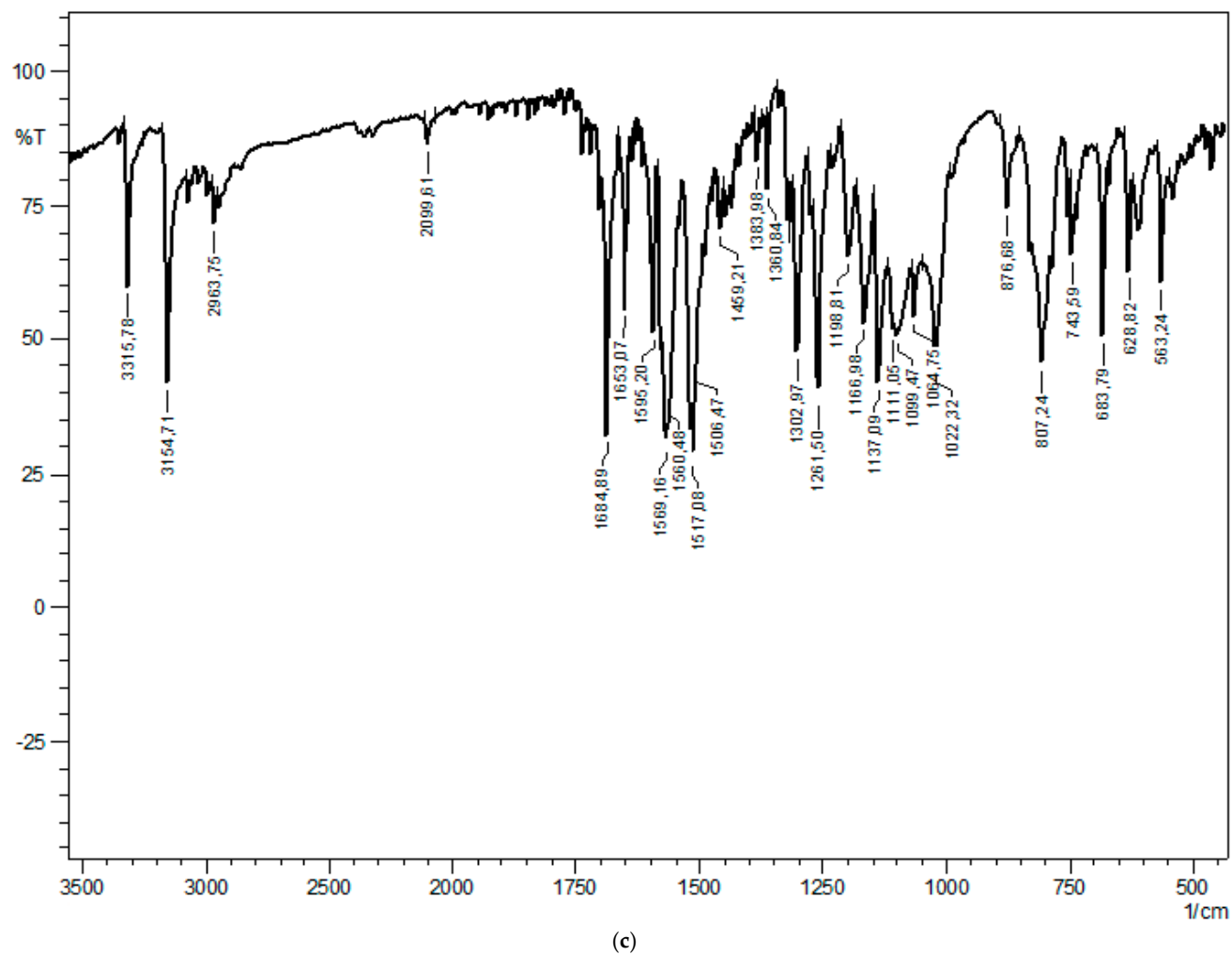
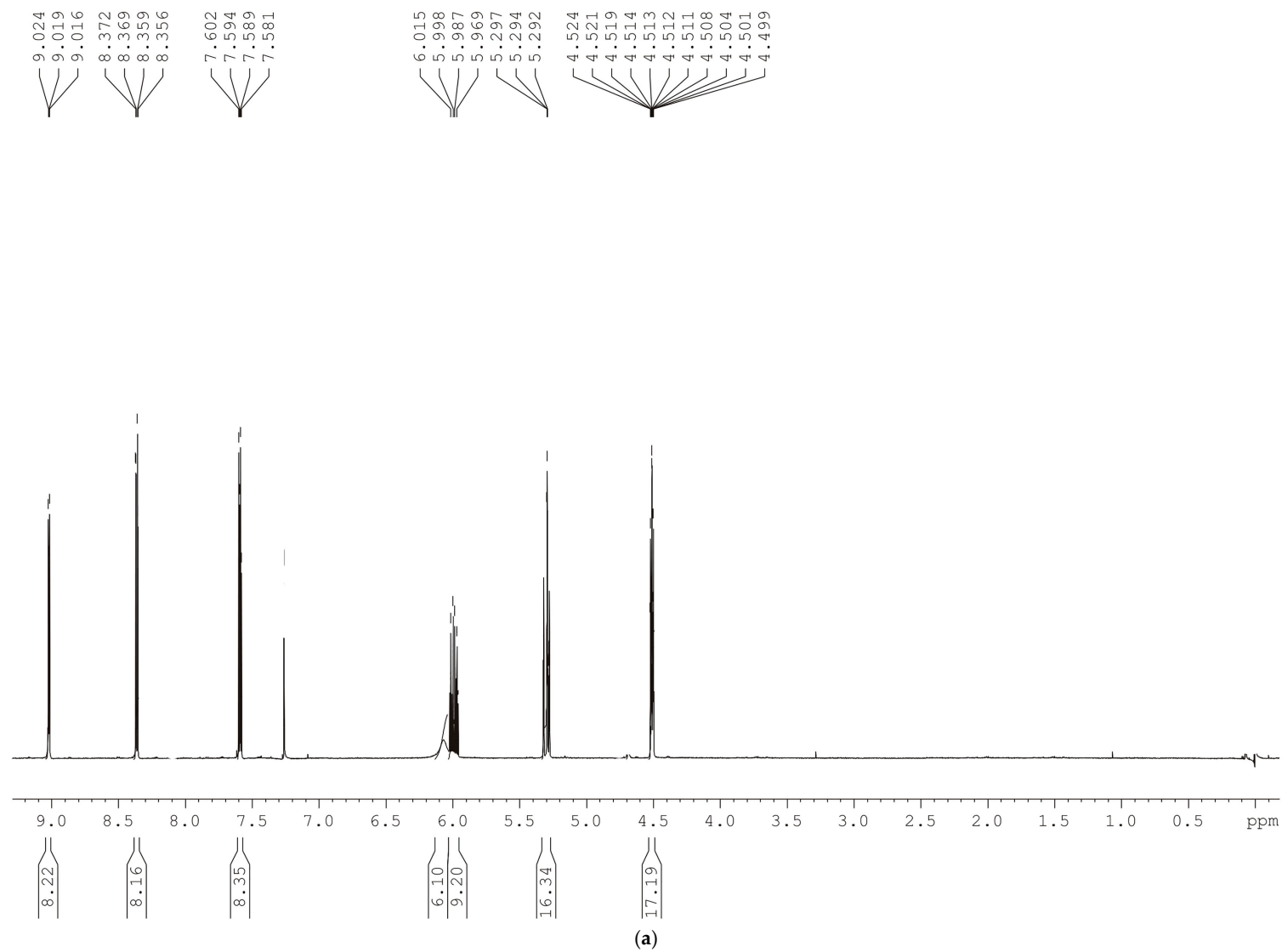
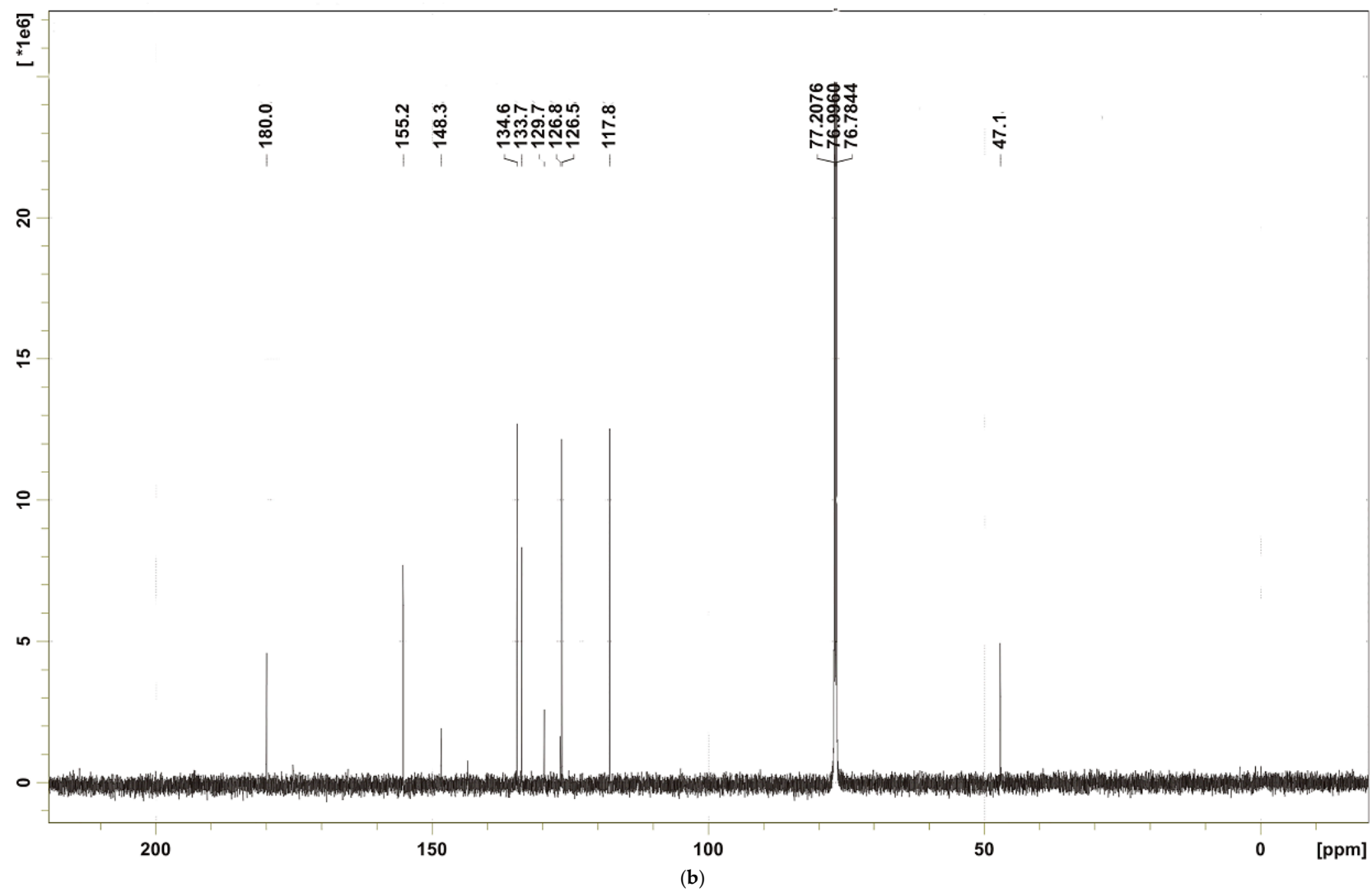


Figure S7. 7-chloro-6-(1,1-dimethylpropargylamine)-5,8-quinolinedione **3c**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum.





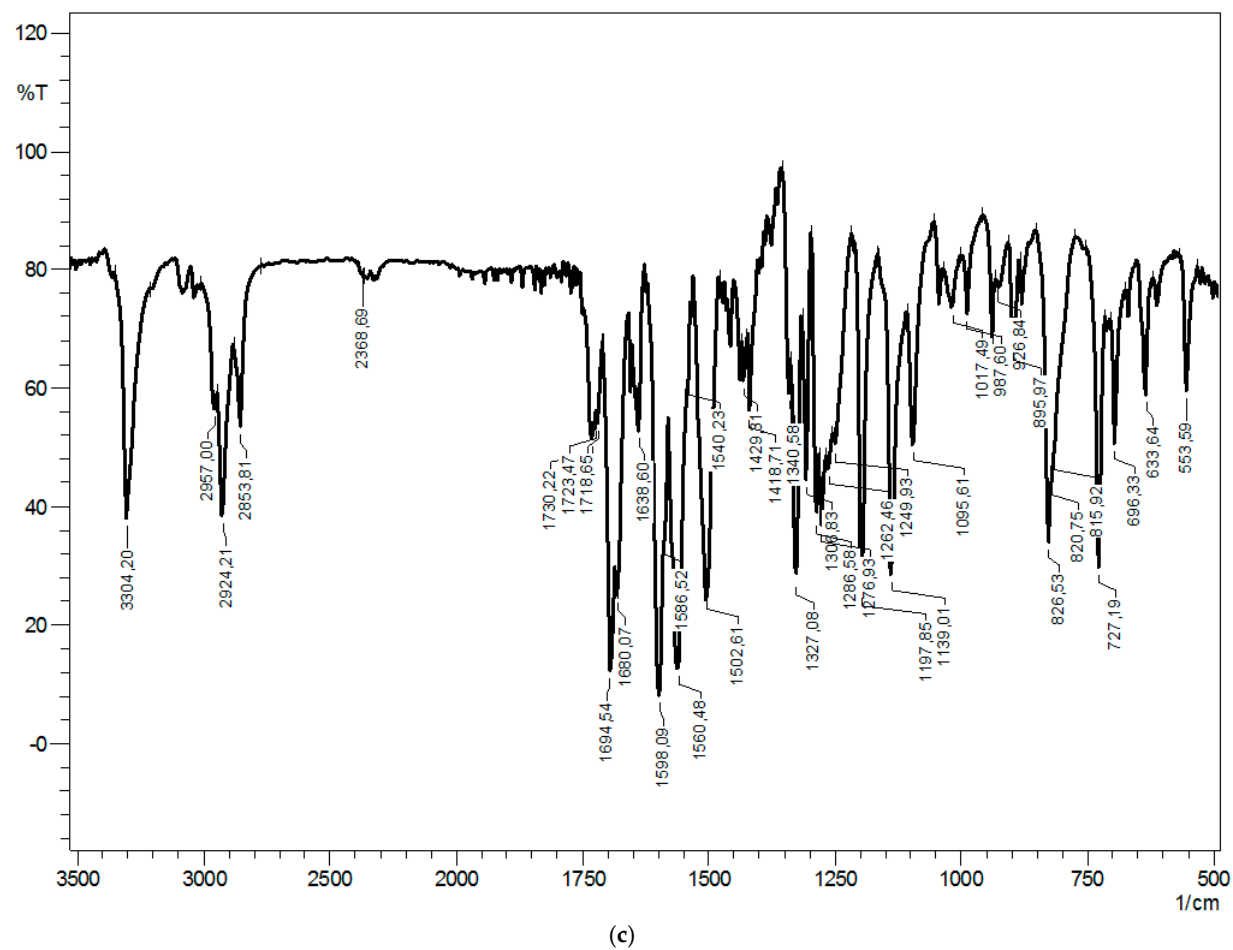


Figure S8. 7-chloro-6-allylamine-5,8-quinolinedione **3d**, (a) ^1H NMR spectrum, (b) ^{13}C NMR spectrum, (c) IR spectrum. Personal communication, 2012.

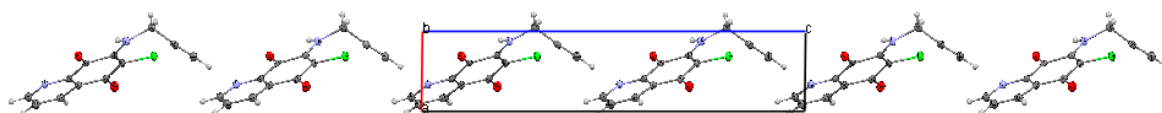


Figure S9. The crystal packing of 6-chloro-7-propargylamine-5,8-quinolinedione **2a**. View along axis “b”.

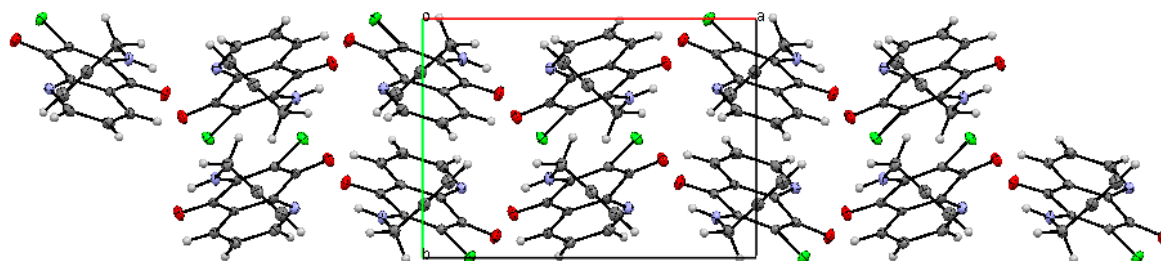


Figure S10. The crystal packing of 7-chloro-6-propargylamine-5,8-quinolinedione **3a**. View along axis “b”.



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