

Supporting Information

New library of Iodo-quinoline derivatives obtained by an alternative synthetic pathway and their antimicrobial activity.

Cristina M. Al-Matarneh^{1,2*}, Alina Nicolescu³, Ioana C. Marinas², Madalina D. Gaboreanu², Sergiu Shova⁴, Andrei Dascalu¹, Mihaela Sillion⁵, Mariana Pinteala¹

¹Center of Advanced Research in Bionanoconjugates and Biopolymers, "Petru Poni"
Institute of Macromolecular Chemistry of Romanian Academy, 41A Grigore
Ghica Voda Alley, Iasi 700487, Romania;

²Research Institute of the University of Bucharest-ICUB, 91-95 Spl.
Independentei, 050095 Bucharest, Romania;

³NMR Laboratory "Petru Poni" Institute of Macromolecular Chemistry of Romanian
Academy, 41A Grigore Ghica Voda Alley, Iasi 700487, Romania;

⁴Department of Inorganic Polymers "Petru Poni" Institute of Macromolecular
Chemistry of Romanian Academy, 41A Grigore Ghica Voda Alley, Iasi 700487,
Romania;

⁵Physics of Polymers and Polymeric Materials Department, "Petru Poni" Institute
of Macromolecular Chemistry, 41A Grigore Ghica Voda Alley, 700487, Iasi,
Romania;

almarneh.cristina@icmpp.ro;

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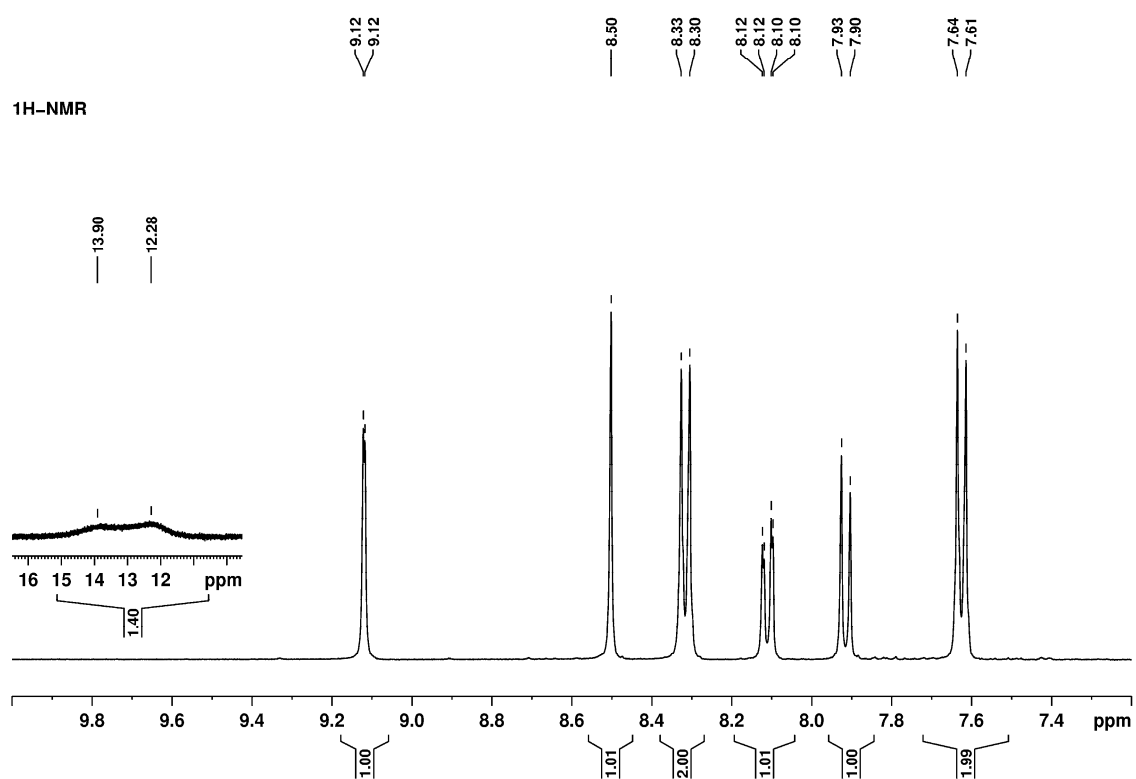


Figure S1.A. The ¹H-NMR spectrum corresponding to compound **4c**, recorded in DMSO-d₆, at 400.1 MHz.

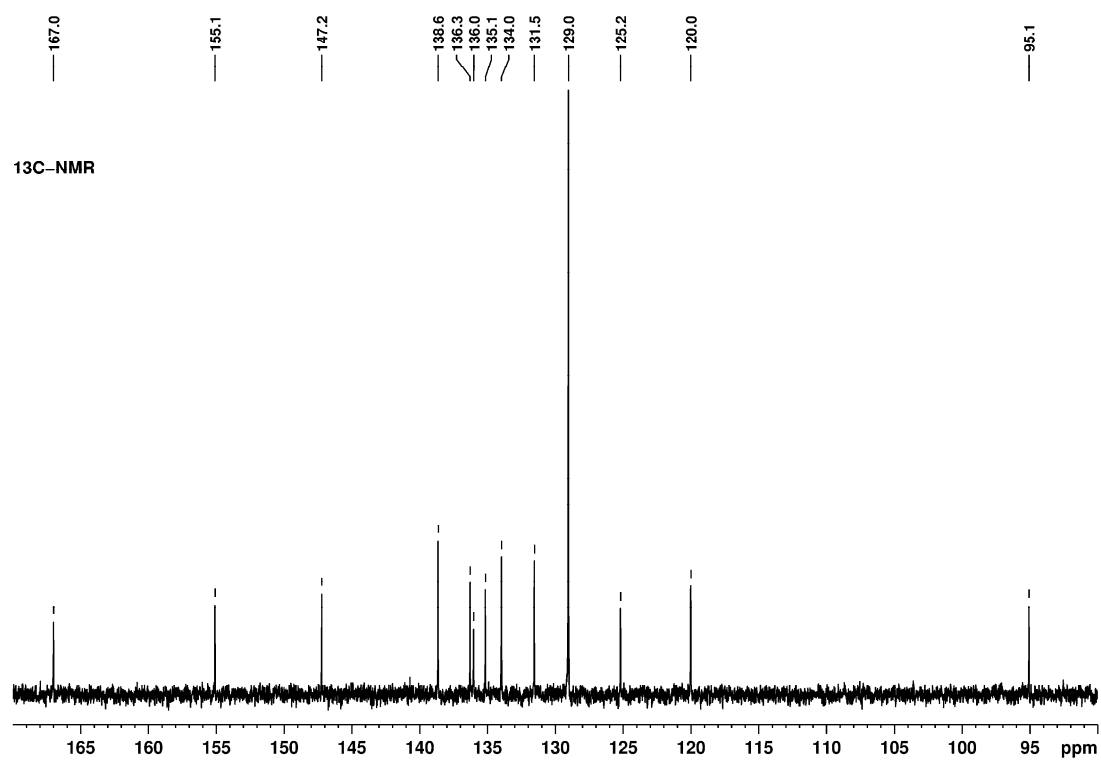


Figure S1.B. The ¹³C-NMR spectrum corresponding to compound **4c**, recorded in DMSO-d₆, at 100.6 MHz.

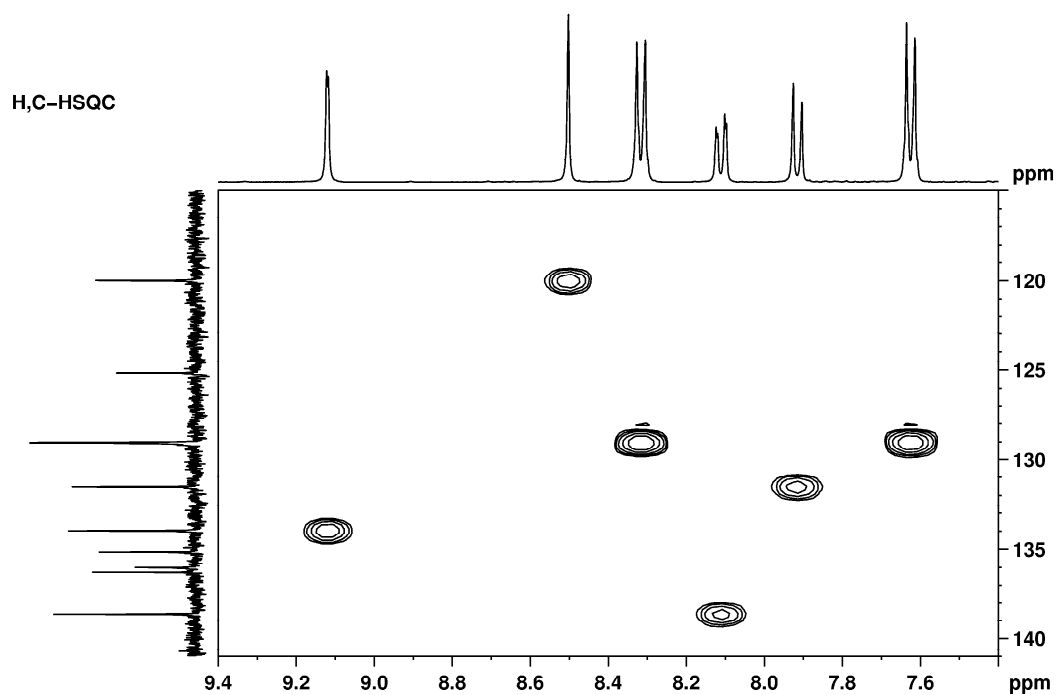


Figure S1.C. Detailed region of the H,C-HSQC spectrum corresponding to compound **4c**, showing the correlation signals for protonated carbons.

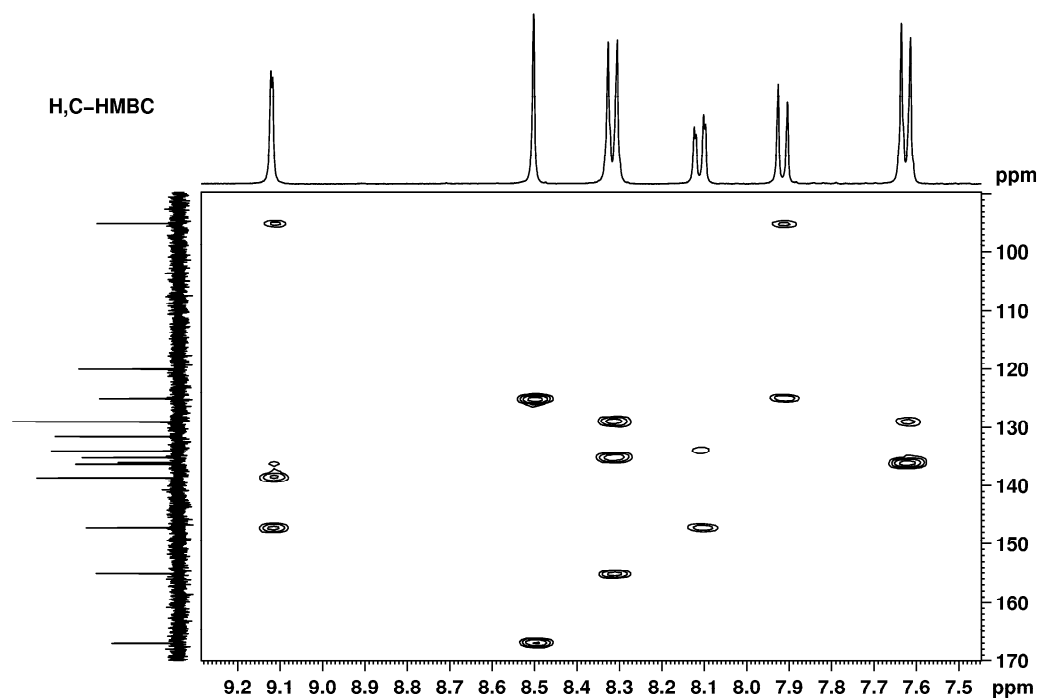


Figure S1.D. The H,C-HMBC spectrum corresponding to compound **4c**, showing 2 or 3 bonds correlation signals between protons and carbons, used mainly to assign quaternary carbons.

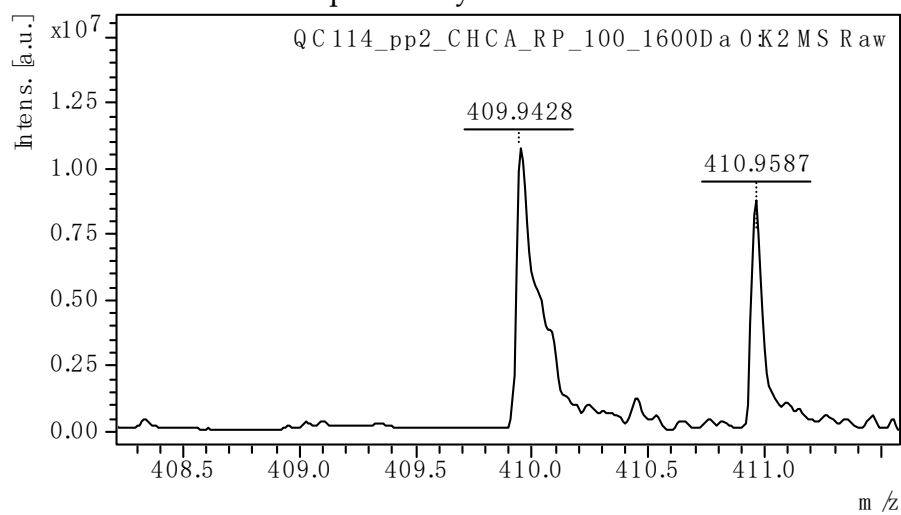


Figure S1. E. MALDI-MS spectra of compound **4c**.

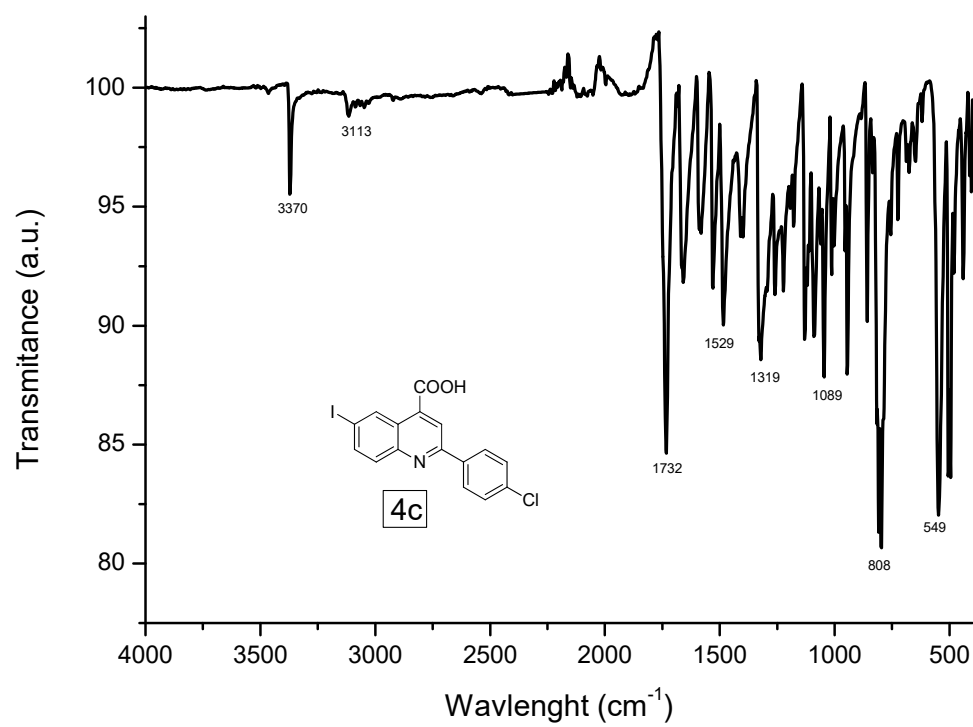


Figure S1.F. FT-IR spectrum of compound **4c**.

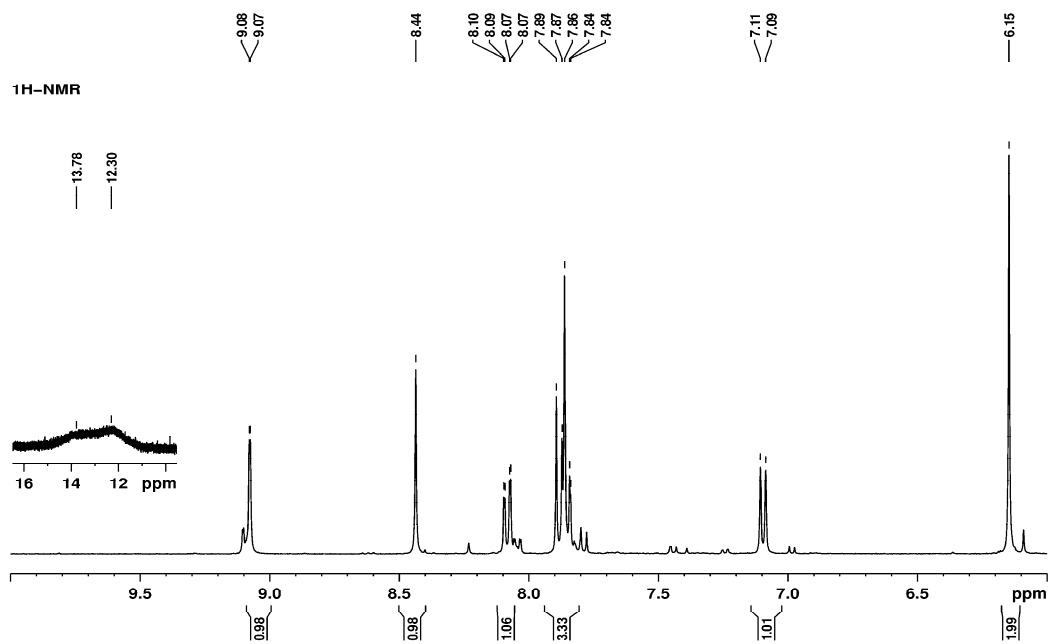


Figure S2.A. The ¹H-NMR spectrum corresponding to compound **4t**, recorded in DMSO-d₆, at 400.1 MHz.

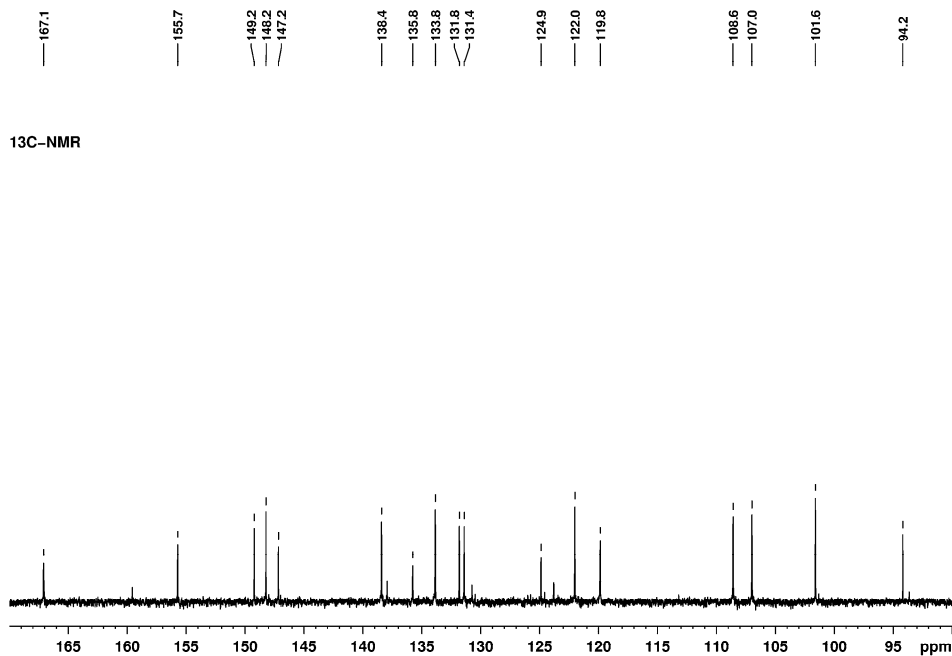


Figure S2.B. The ¹³C-NMR spectrum corresponding to compound **4t**, recorded in DMSO-d₆, at 100.6 MHz.

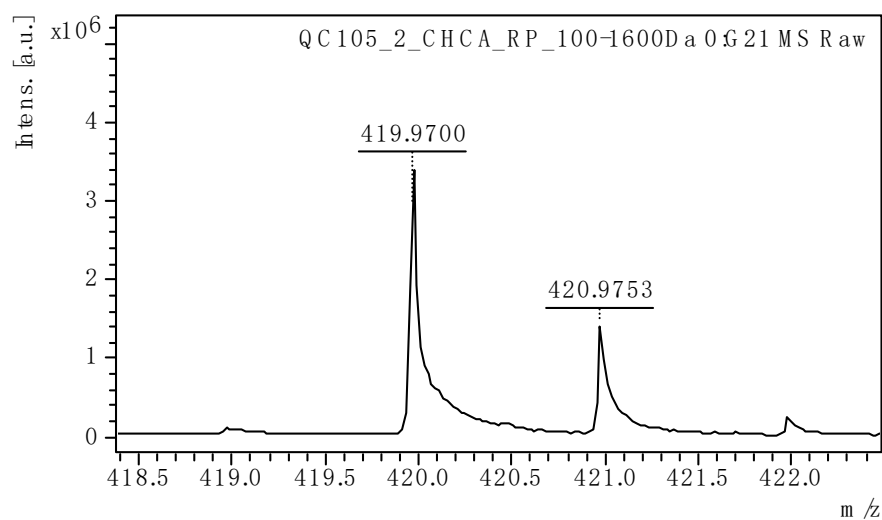


Figure S2.C. MALDI-MS spectrum of the compound **4t**.

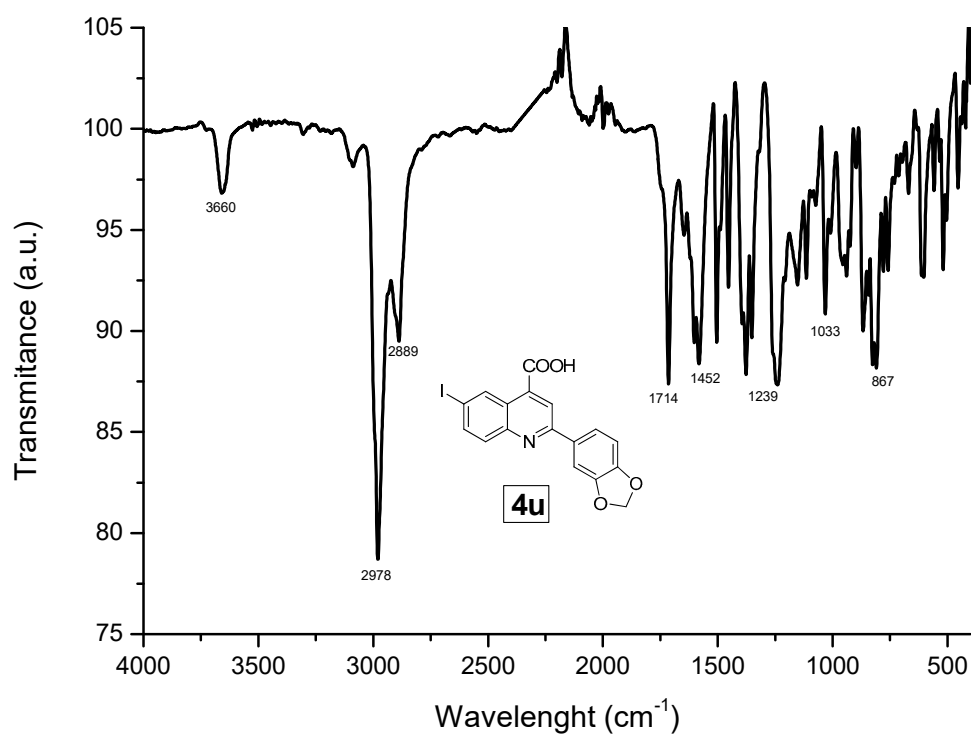


Figure S2.D. FT-IR spectrum of compound **4t**.

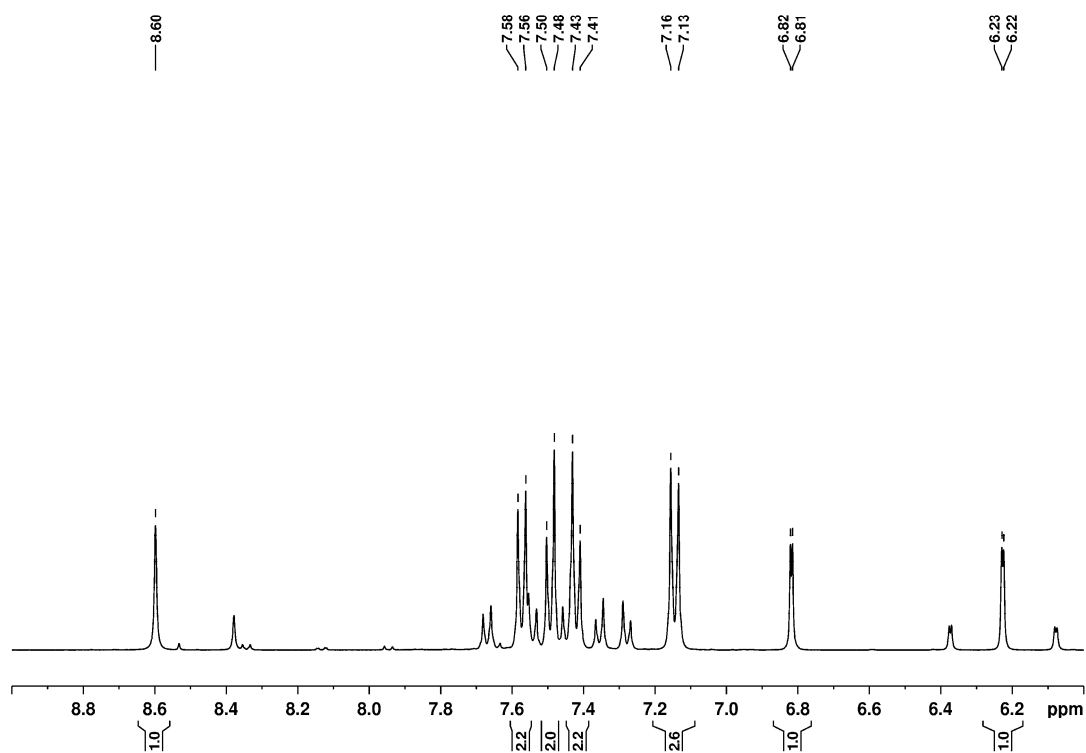


Figure S3.A. The ^1H -NMR spectrum corresponding to compound **8c**, recorded in DMSO-d_6 , at 400.1 MHz.

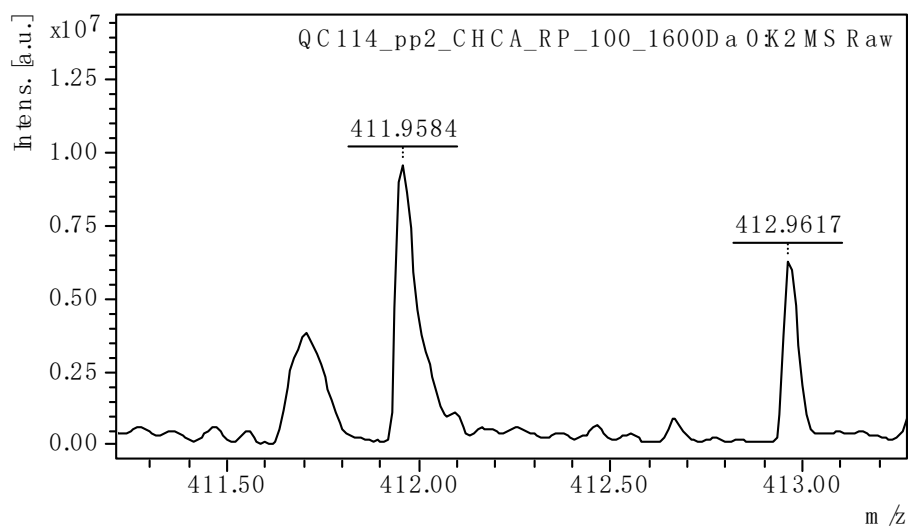


Figure S3.B. MALDI-MS spectra of compound **8c**.

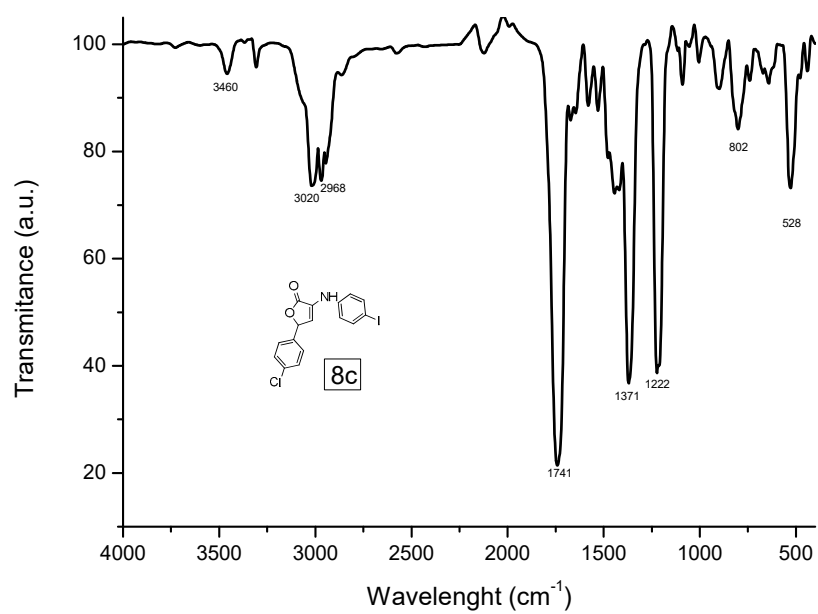


Figure S3.C. FT-IR spectrum of compound **8c**.

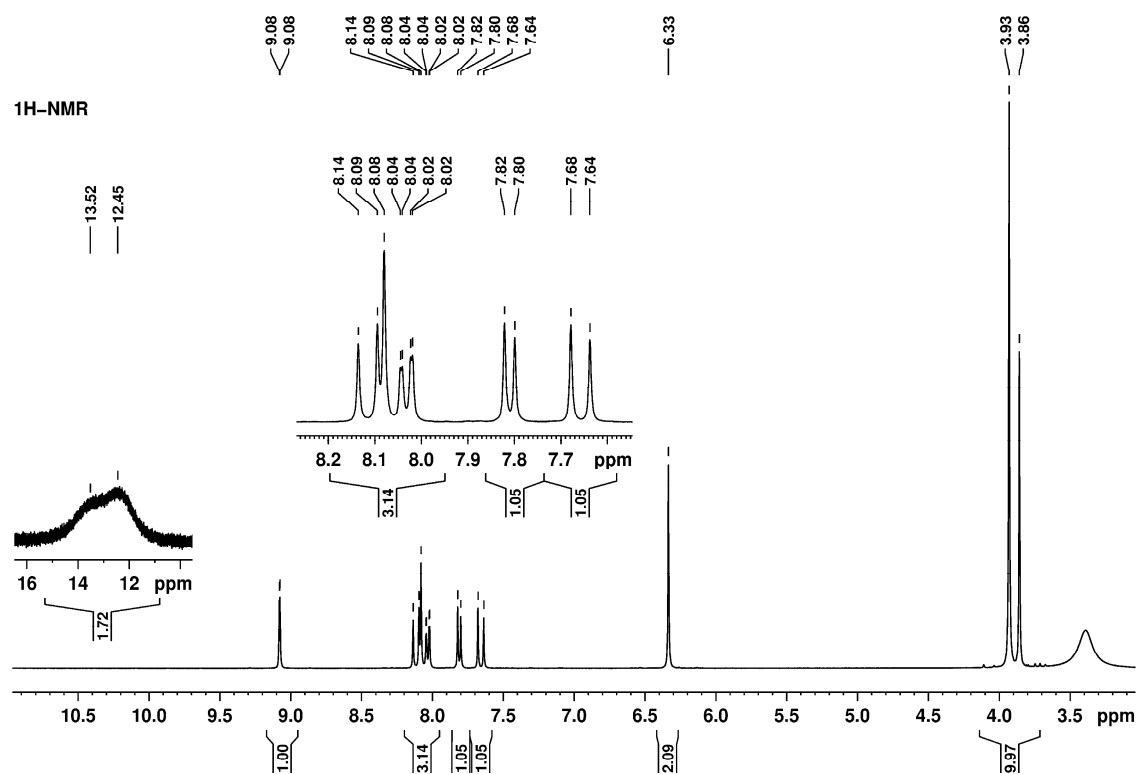


Figure S4.A. The ¹H-NMR spectrum corresponding to compound **5n**, recorded in DMSO-d₆, at 400.1 MHz.

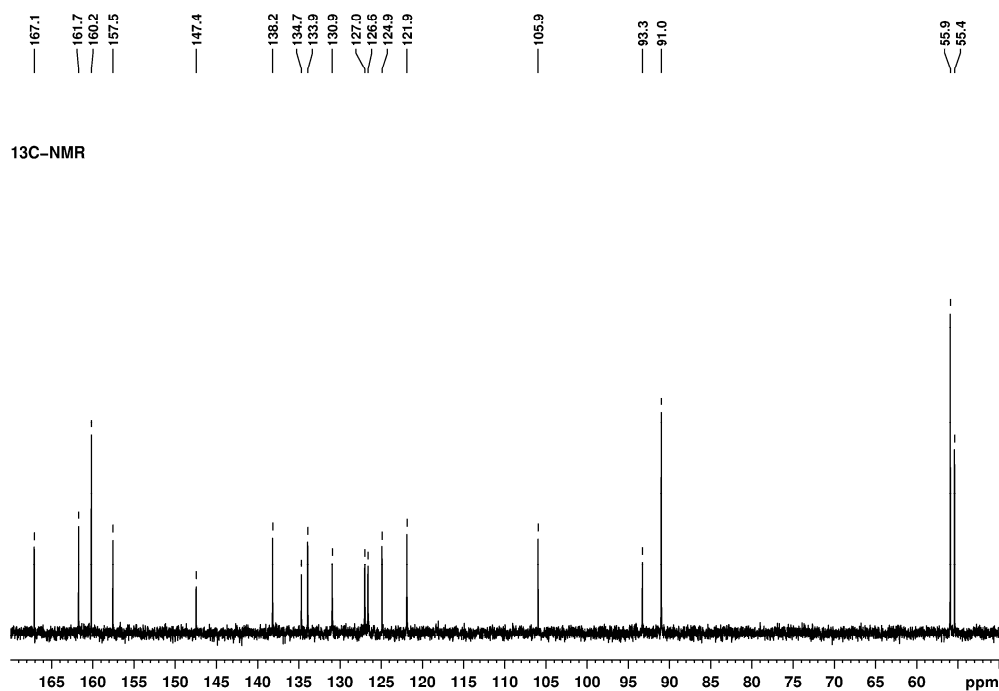


Figure S4.B. The ¹³C-NMR spectrum corresponding to compound **5n**, recorded in DMSO-d₆, at 100.6 MHz.

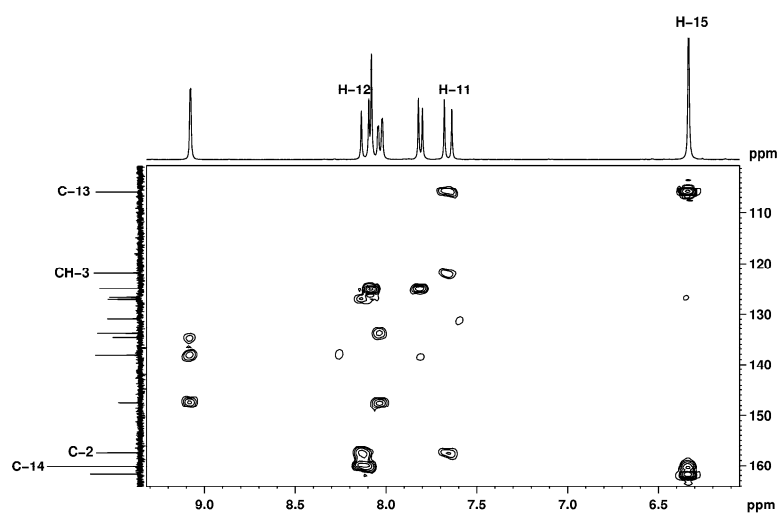


Figure S4.C. The H,C-HMBC spectrum corresponding to compound **5n**, recorded in DMSO-d₆, showing correlation signals between vinylic protons and either quinoline's CH-3 or benzaldehyde's C-14 carbon atoms.

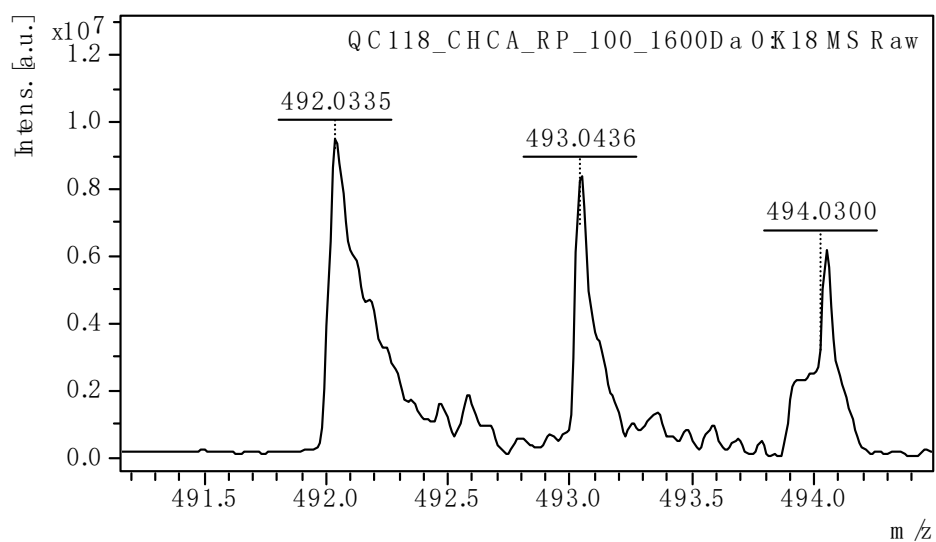


Figure S4.D. Maldi-MS spectrum corresponding to compound **5n**.

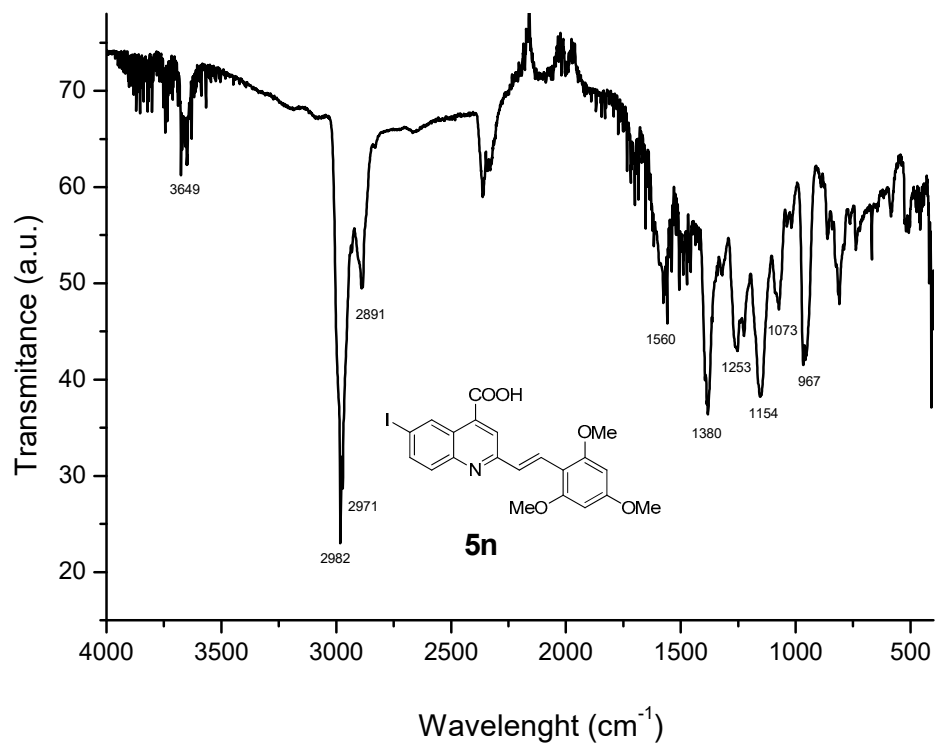


Figure S4.E. FT-IR spectrum of compound **5n**.

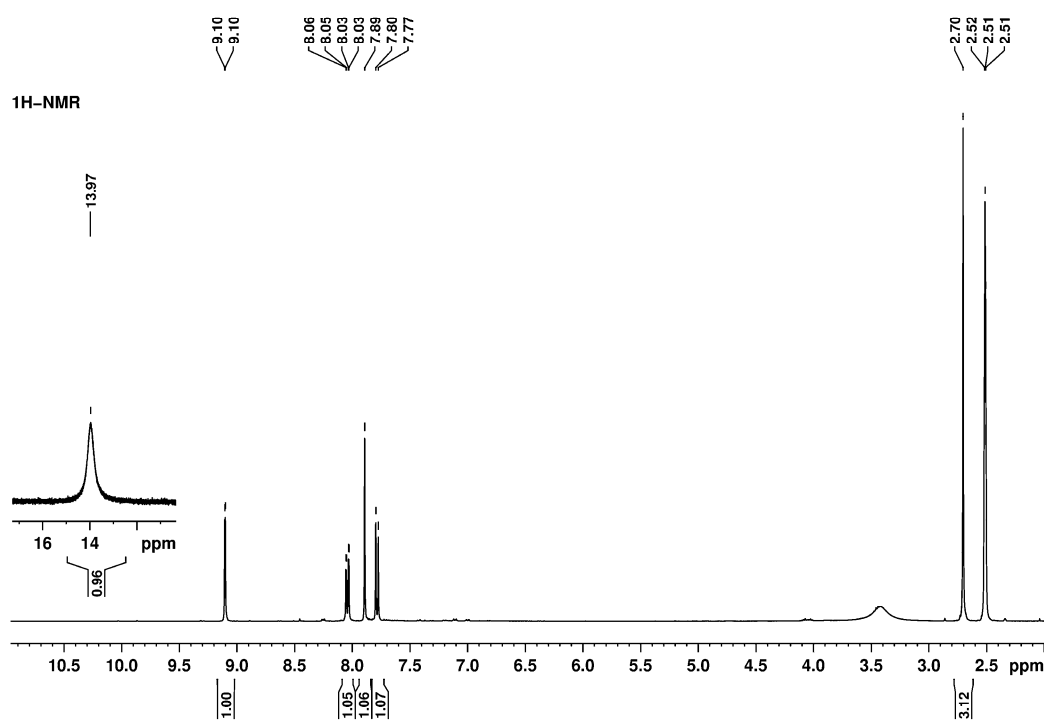


Figure S5.A. The ^1H -NMR spectrum corresponding to compound **7**, recorded in DMSO-d_6 , at 600.1 MHz.

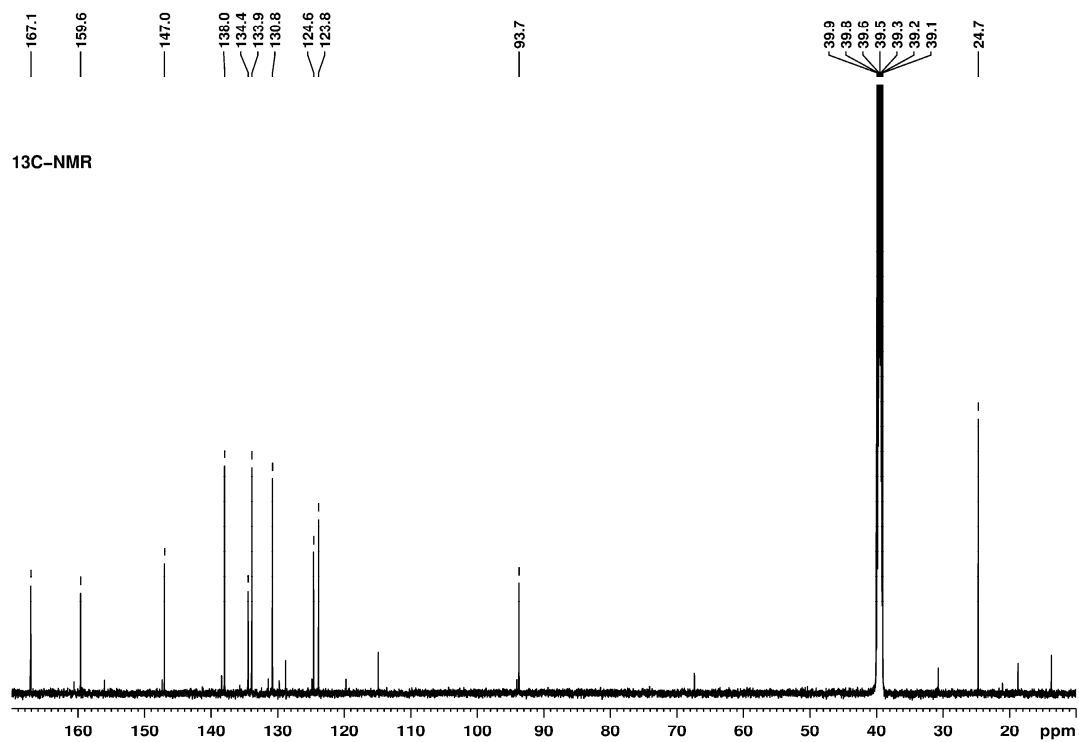


Figure S5.B. The ¹³C-NMR spectrum corresponding to compound **7**, recorded in DMSO-d₆, at 150.9 MHz.

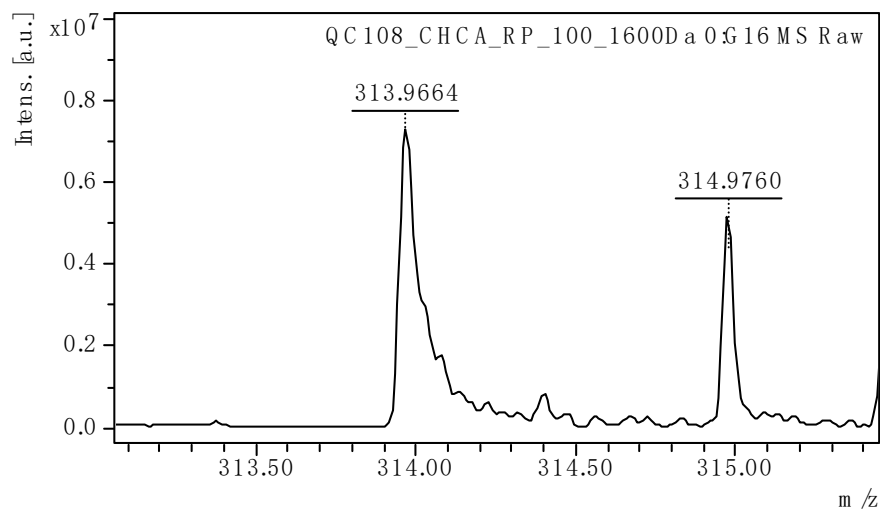


Figure S5.C. Maldi-MS spectrum corresponding to compound **7**.

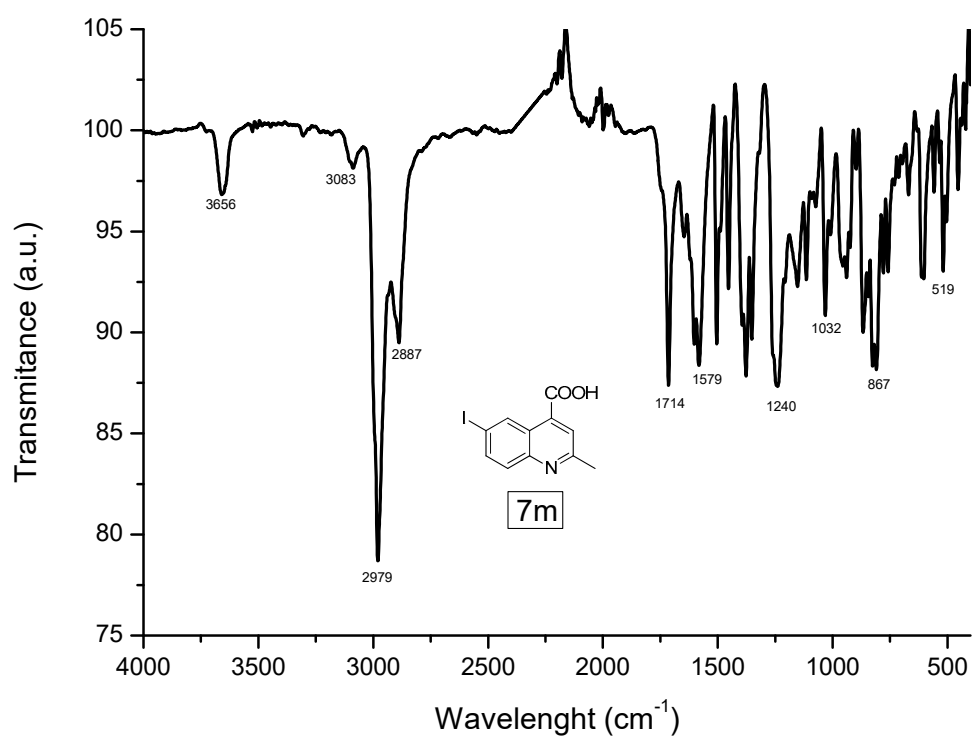


Figure S5.D. FT-IR spectrum of compound 7.

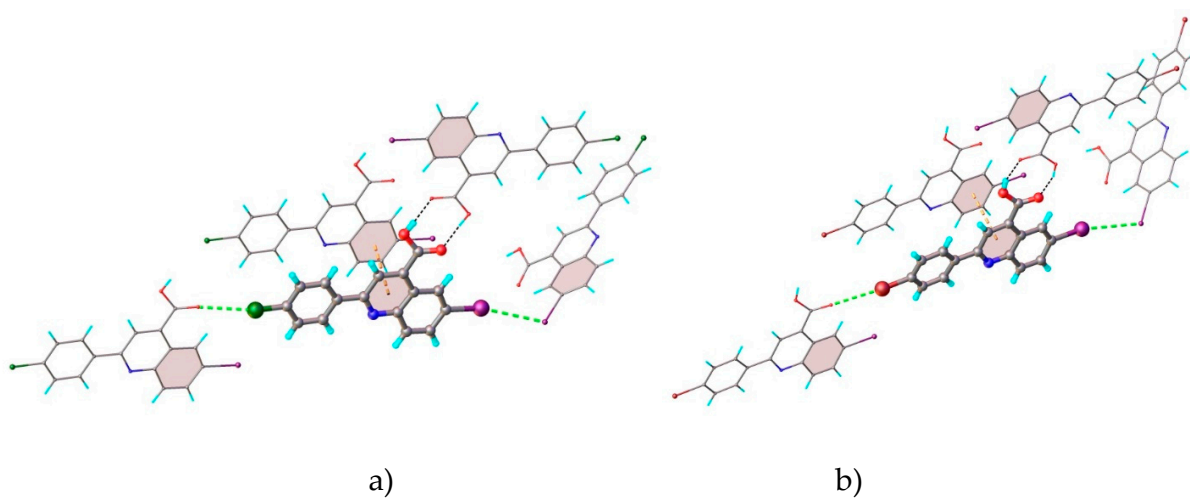


Figure S6. View of the asymmetric unit (large atoms and bonds radii) showing its interaction with adjacent molecules for **4c** (a) and **4d** (b). Hydrogen and halogen bonds are shown as dotted lines with black and green color, respectively.

H-bonds parameters:

For **4c**: O2-H...O1 [O2-H 0.84 Å, H...O1($-x, -y, 1 - z$) 1.84 Å, O2...O1 2.683(3) Å, \angle O2HO1 177.2°.

For **4d**: O2-H...O1 [O2-H 0.86 Å, H...O1($-x, -y, 1 - z$) 1.85 Å, O2...O1 2.674(6) Å, \angle O2HO1 160.6°.

For **4c**: [C14-Cl1...O1] C14-Cl1 1.744(1) Å, Cl1...O1($1 - x, y - 1, z$) 3.211(1) Å, \angle C14Cl1O1 169.3(1)°.

Halogen bond parameters:

For **4d**: [C14-Br1...O1] C14-Br1 1.891(7) Å, Br1...O1($1 - x, y - 1, z$) 3.314(5) Å, \angle C14Br1O1 162.2(4)°.

I...I contacts: 3.8052(1) (for **4c**) Å; 3.9115(8) Å (for **4d**);

Centroid-to-centroid distances (orange dotted lines): 3.5512 Å (for **4c**);
3.5878(1) Å (for **4d**);

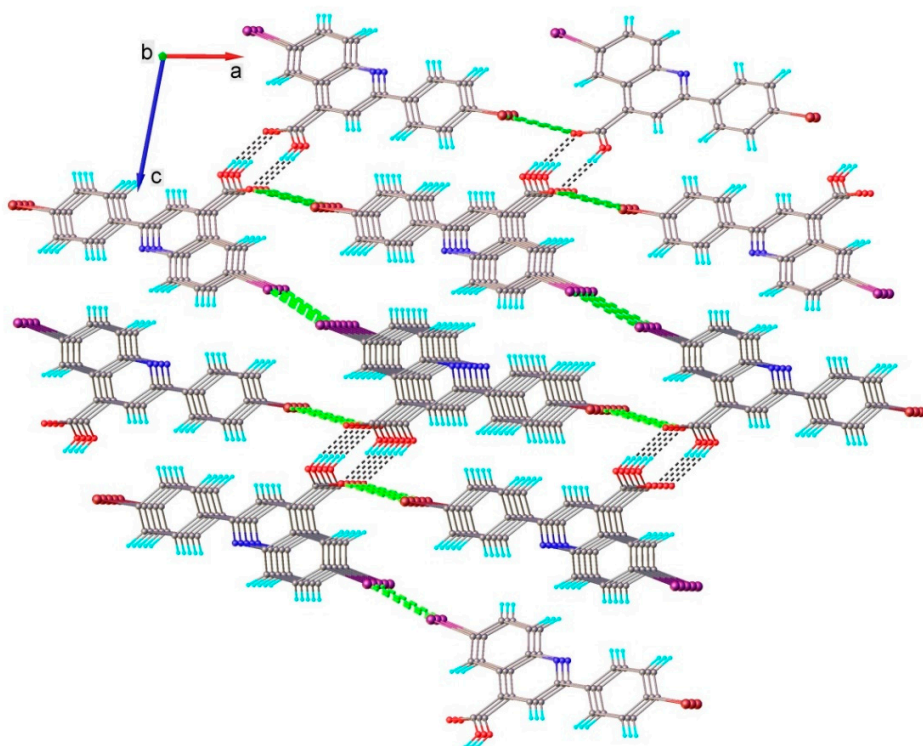


Figure S7. Crystal packing viewed along *b* axis for **4d**.