

# Coumarin Derivatives: The Influence of Cycloalkyl Groups at the C-3 Position on Intermolecular Interactions; Synthesis, Structure and Spectroscopy

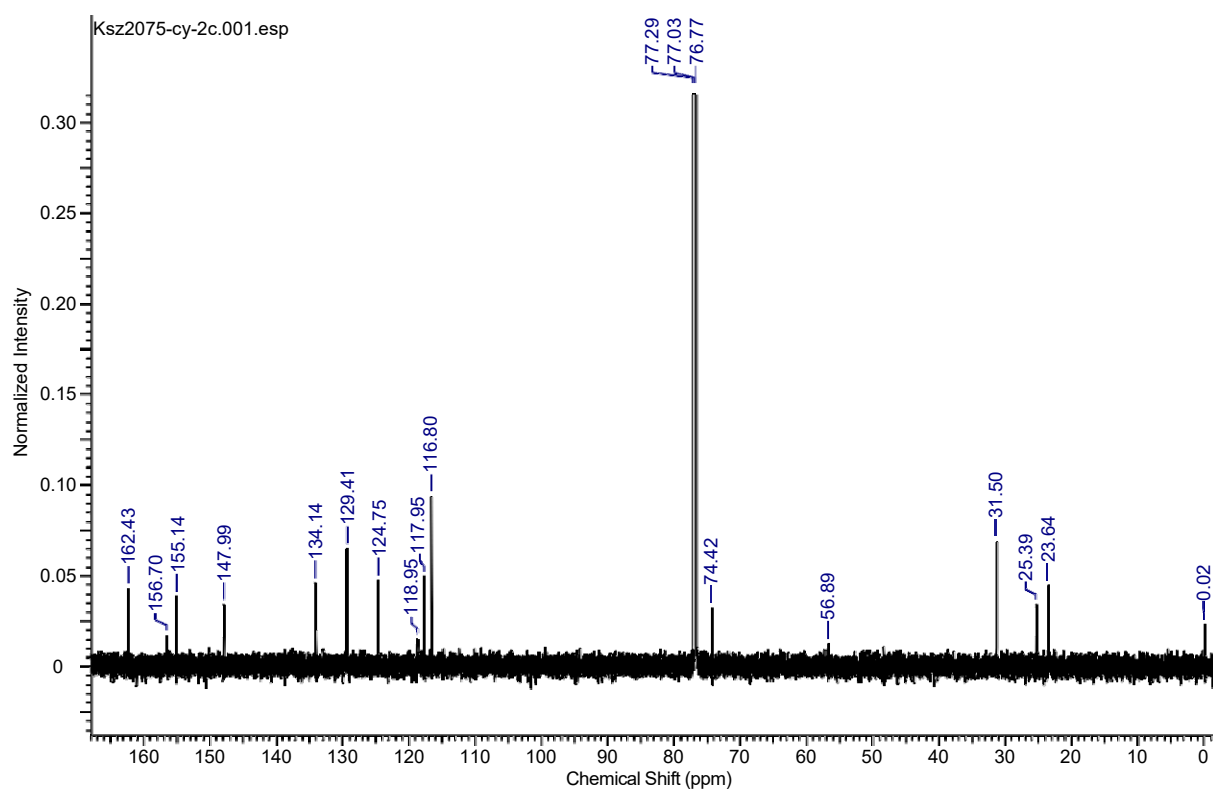
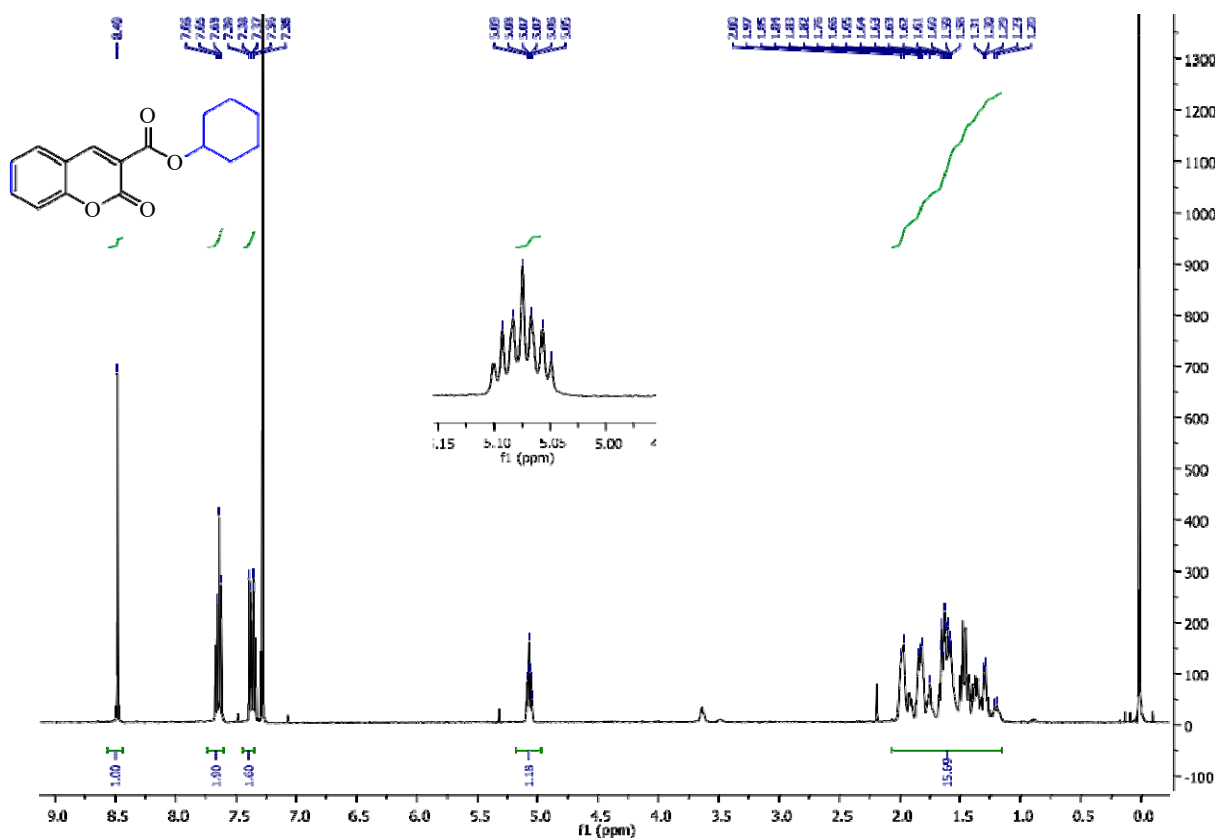
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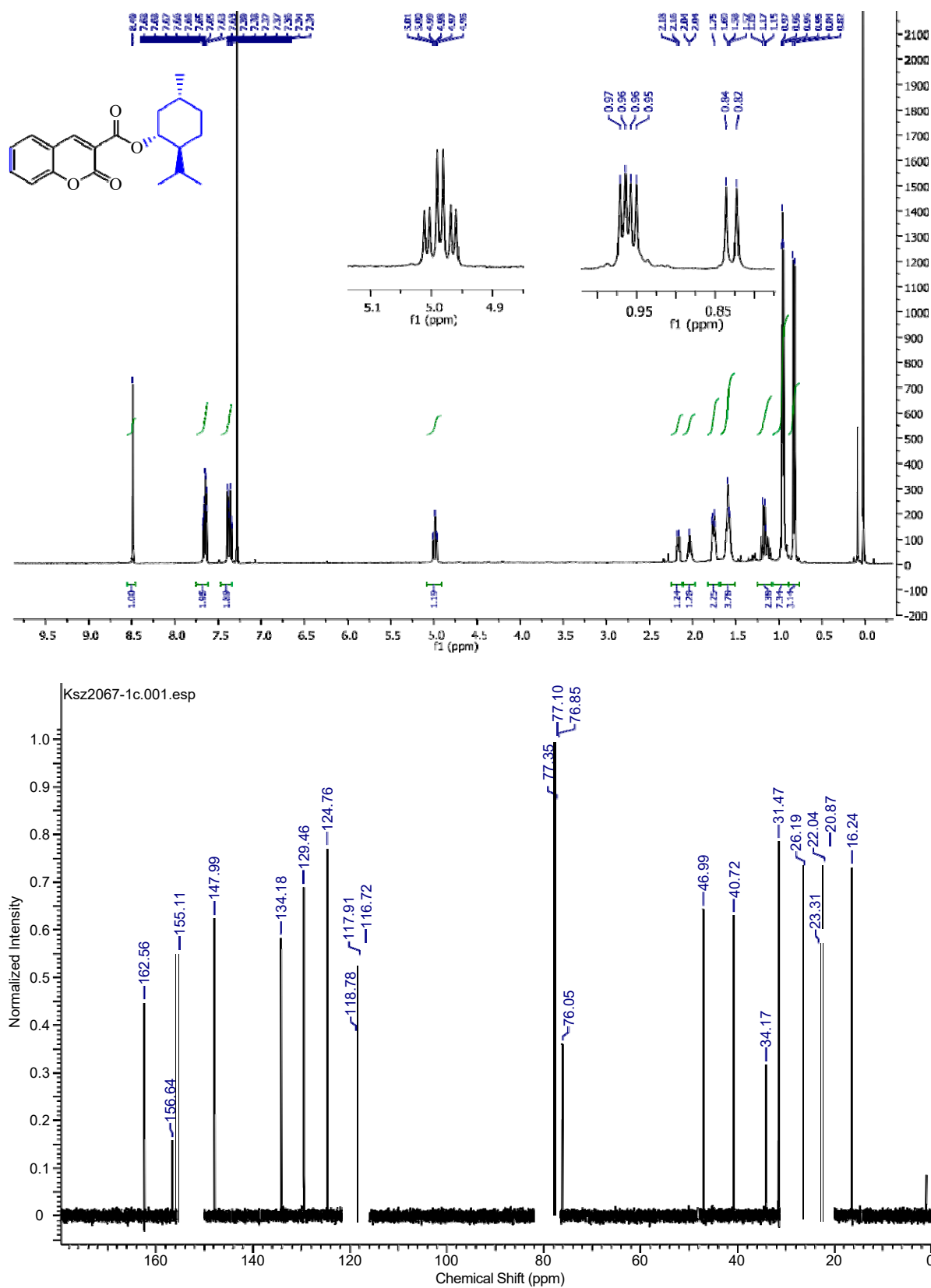
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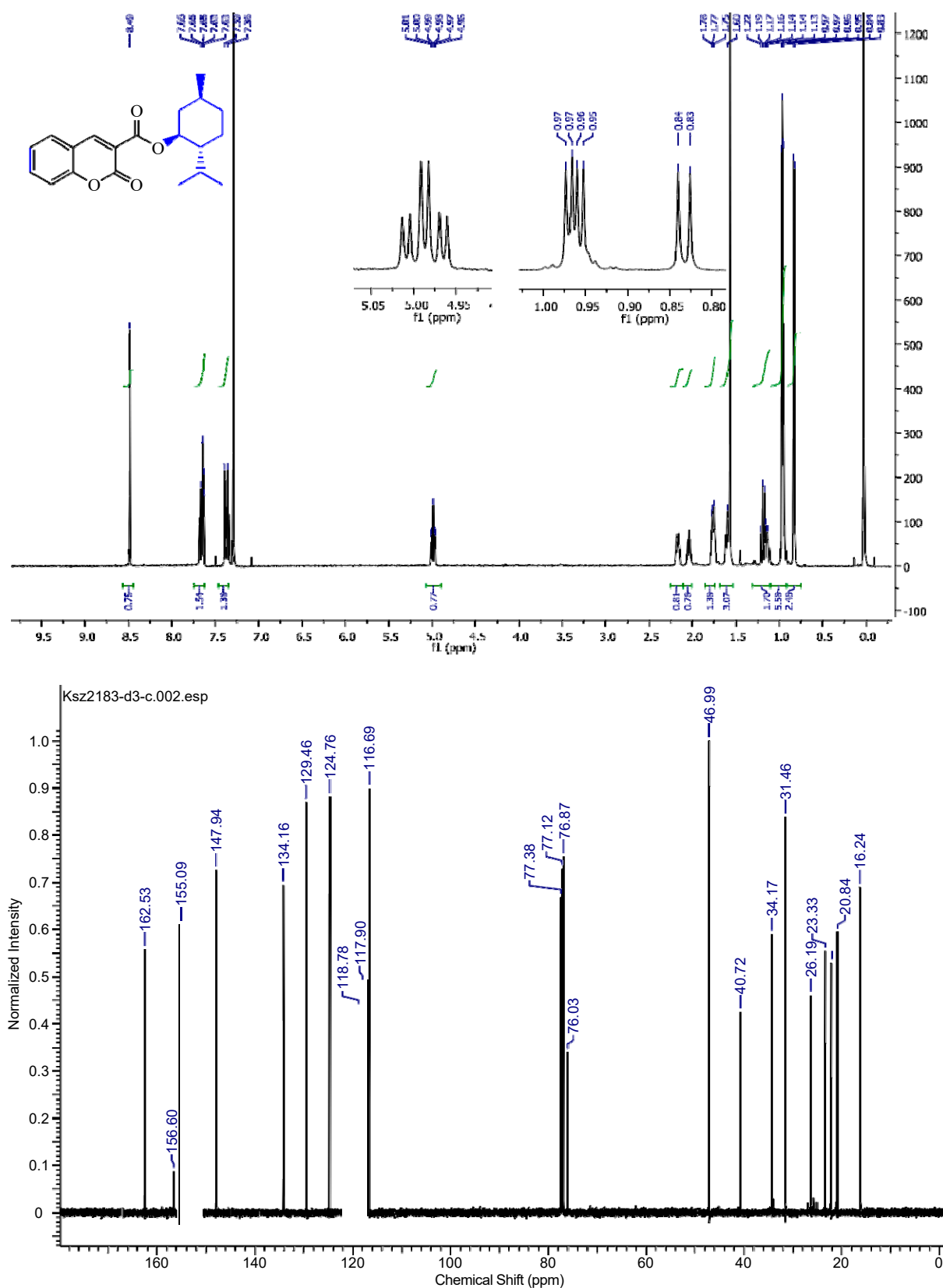
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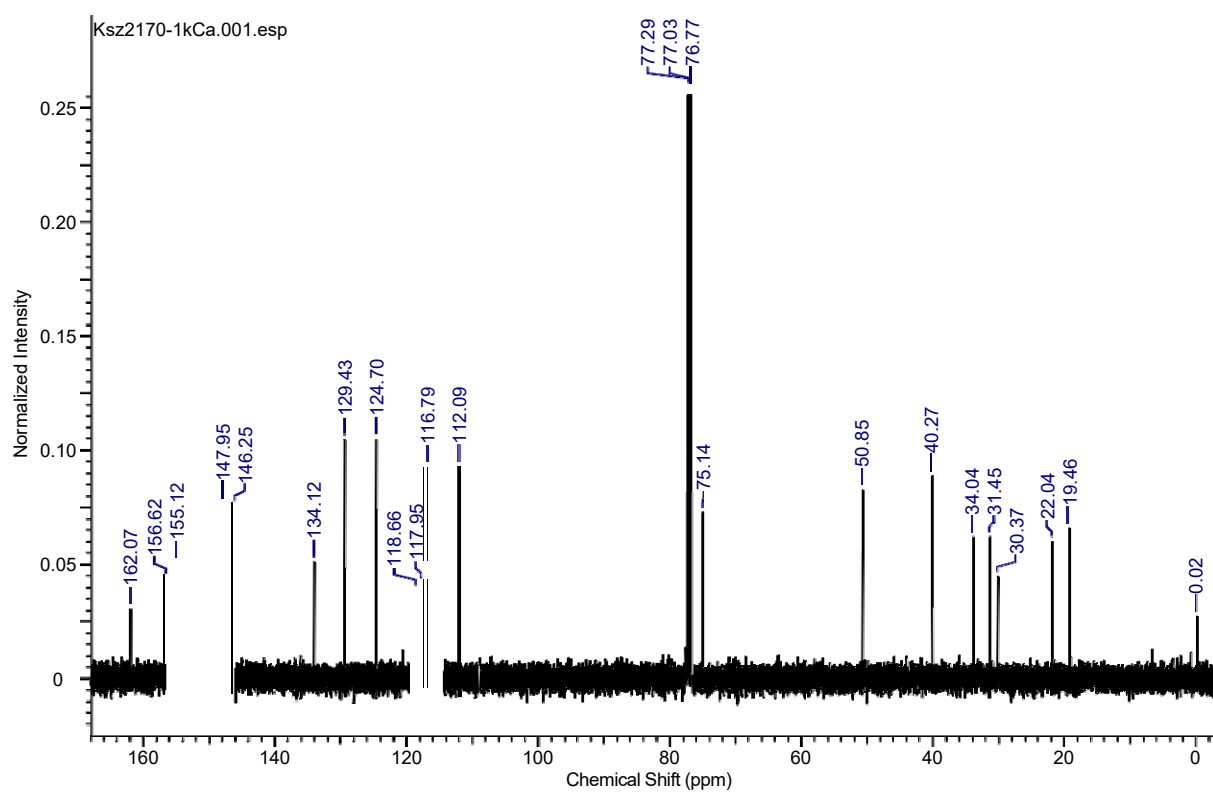
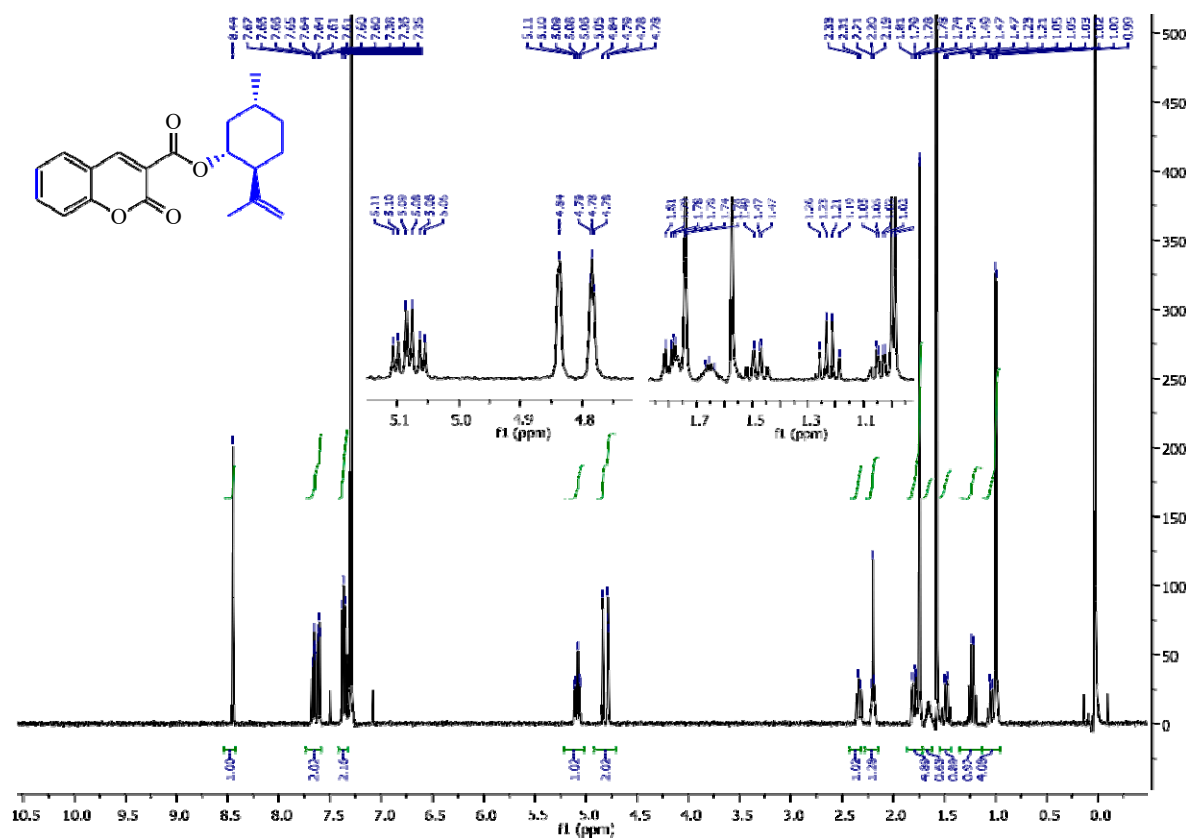
**Figure S-1.** <sup>1</sup>H NMR (500 MHz), and <sup>13</sup>C NMR (126 MHz) of cyclohexyl 2-oxo-2H-chromene-3-carboxylate (CMR-1) in CDCl<sub>3</sub>.



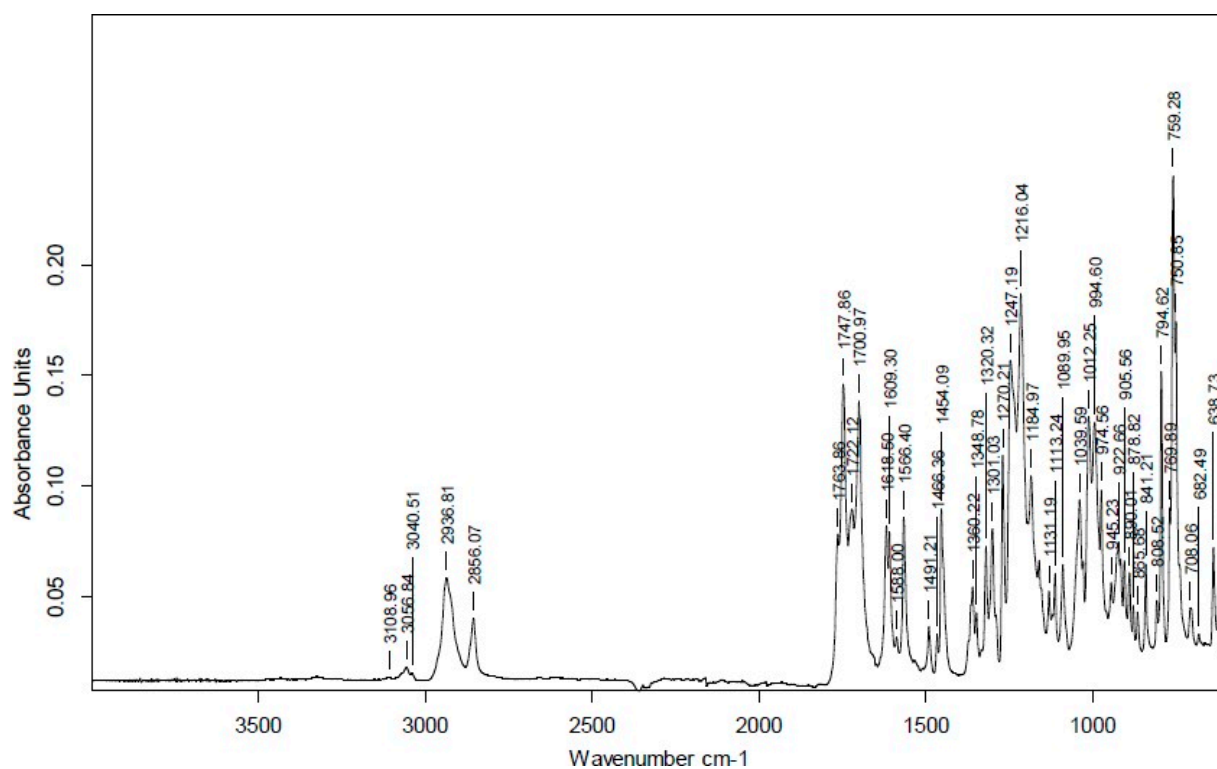
**Figure S-2.** <sup>1</sup>H NMR (500 MHz), and <sup>13</sup>C NMR (126 MHz) of (1*R*,2*S*,5*R*)-2-isopropyl-5-methylcyclohexyl 2-oxo-2*H*-chromene-3-carboxylate (**CMR-2**) in CDCl<sub>3</sub>.



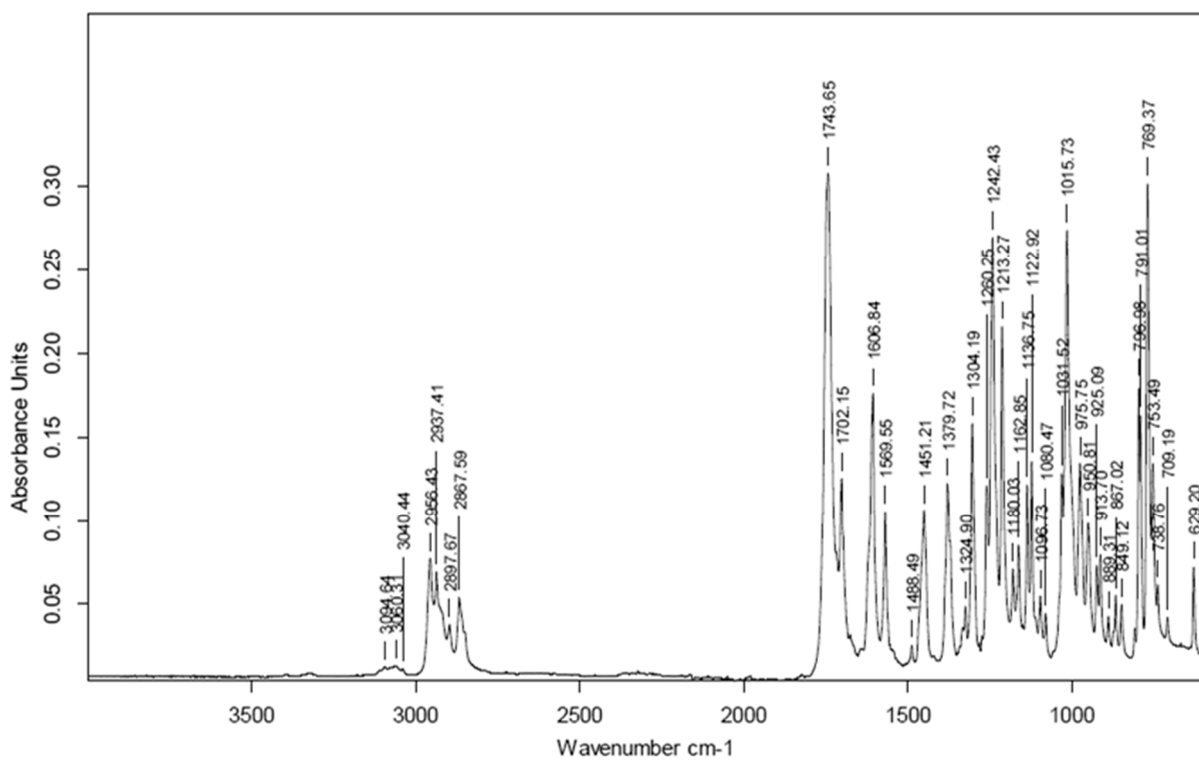
**Figure S-3.** <sup>1</sup>H NMR (500 MHz), and <sup>13</sup>C NMR (126 MHz) of (1*S*,2*R*,5*S*)-2-isopropyl-5-methylcyclohexyl 2-oxo-2*H*-chromene-3-carboxylate (**CMR-3**) in CDCl<sub>3</sub>.



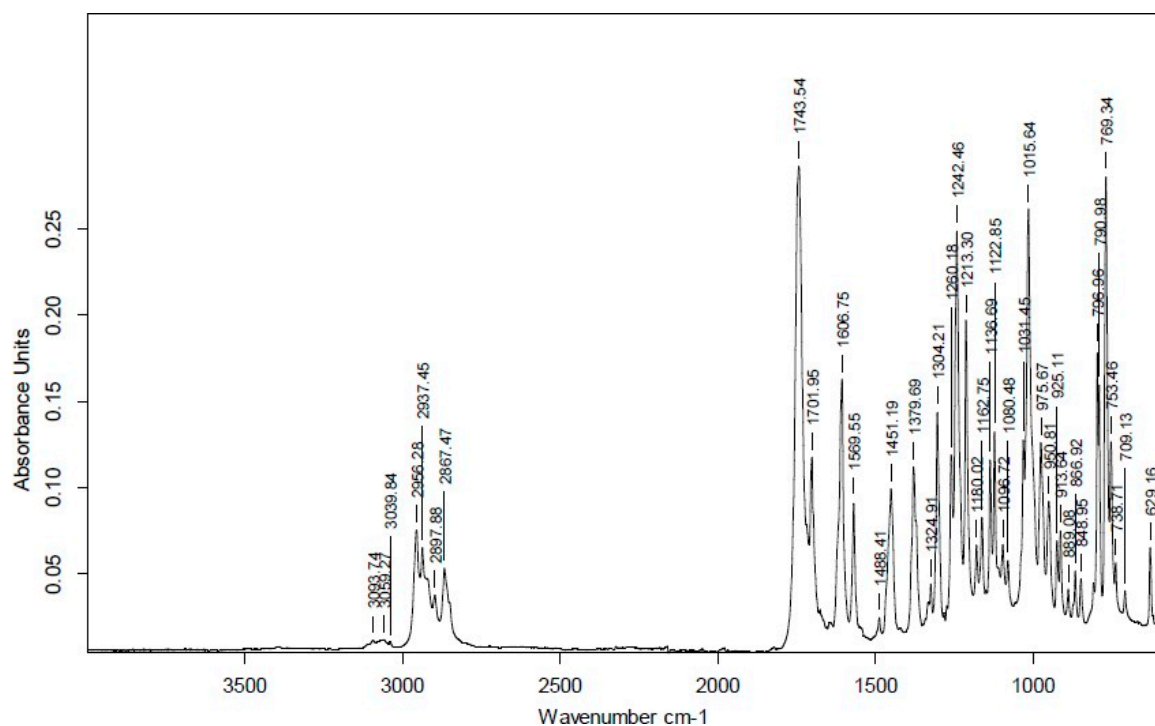
**Figure S-4.** <sup>1</sup>H NMR (500 MHz), and <sup>13</sup>C NMR (126 MHz) of (1*S*,2*R*,5)-2-isopropyl-5-methylcyclohexyl 2-oxo-2*H*-chromene-3-carboxylate (**CMR-3**) in CDCl<sub>3</sub>.



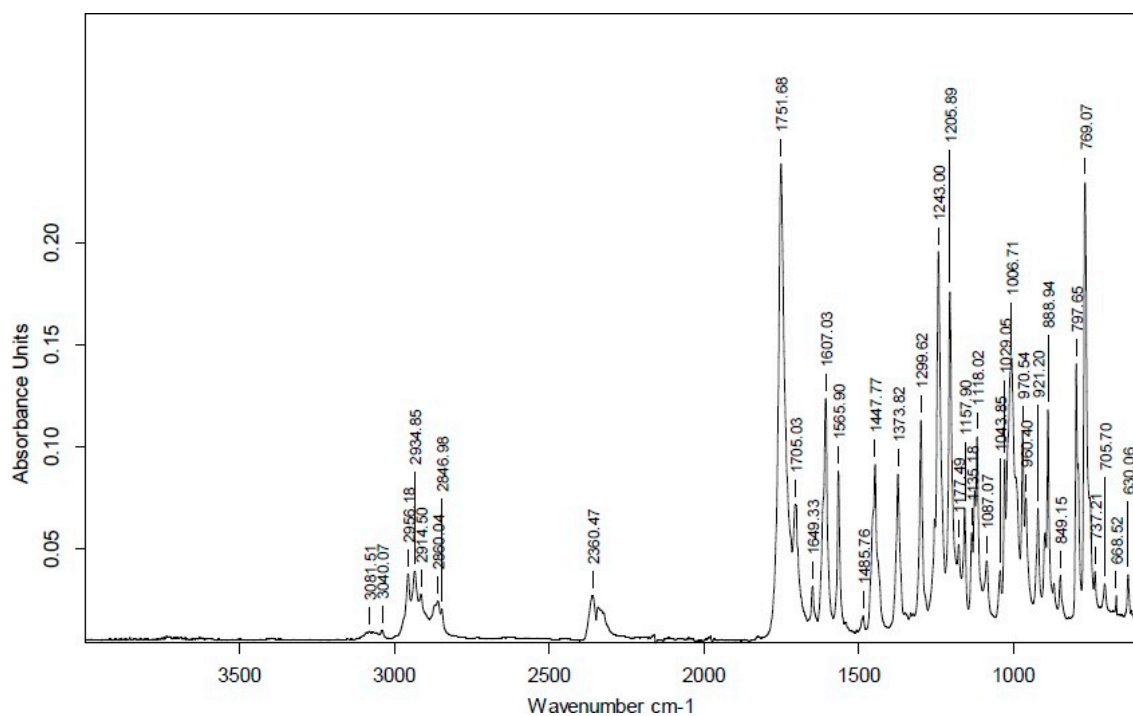
**Figure S-5.** FTIR spectrum of cyclohexyl 2-oxo-2H-chromene-3-carboxylate (CMR-1).



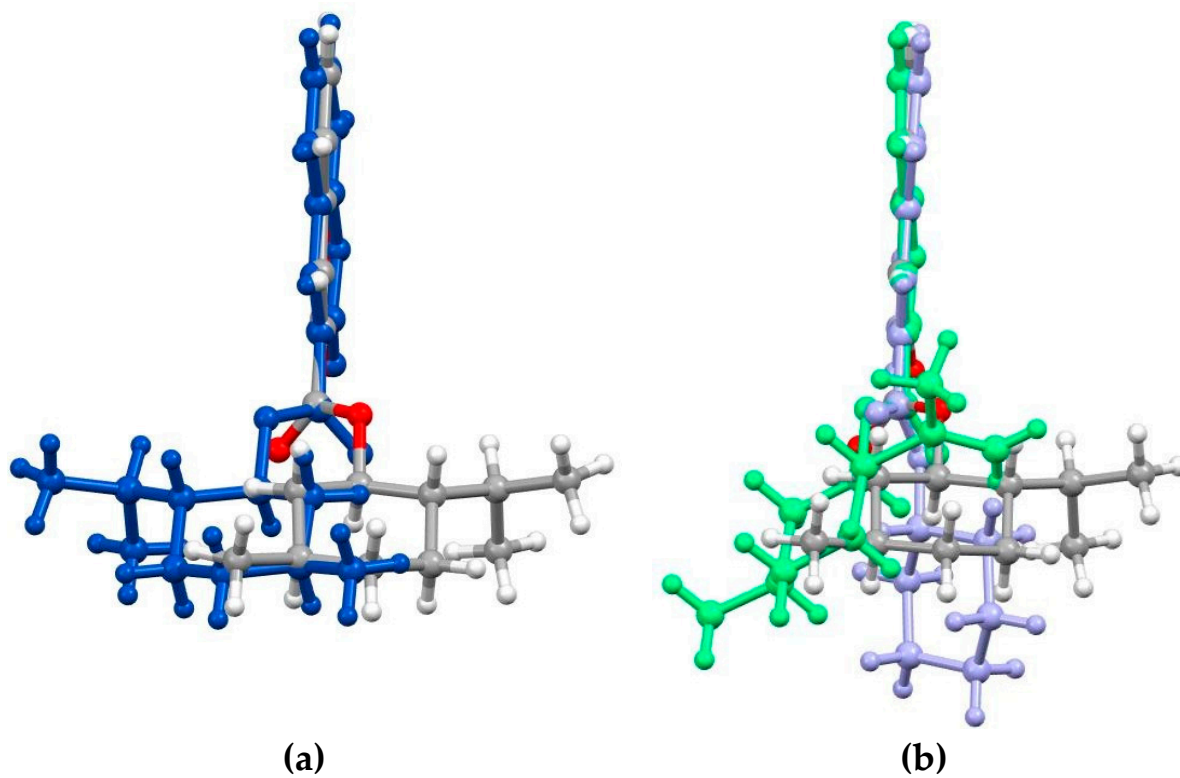
**Figure S-6.** FTIR spectrum of (1R,2S,5R)-2-isopropyl-5-methylcyclohexyl 2-oxo-2H-chromene-3-carboxylate (CMR-2)



**Figure S-7.** FTIR spectrum of (1S,2R,5S)-2-isopropyl-5-methylcyclohexyl 2-oxo-2H-chromene-3-carboxylate (CMR-3).



**Figure S-8.** FTIR of spectrum (1R,2S,5R)-5-methyl-2-(prop-1-en-2-yl)cyclohexyl 2-oxo-2H-chromene-3-carboxylate (CMR-4).

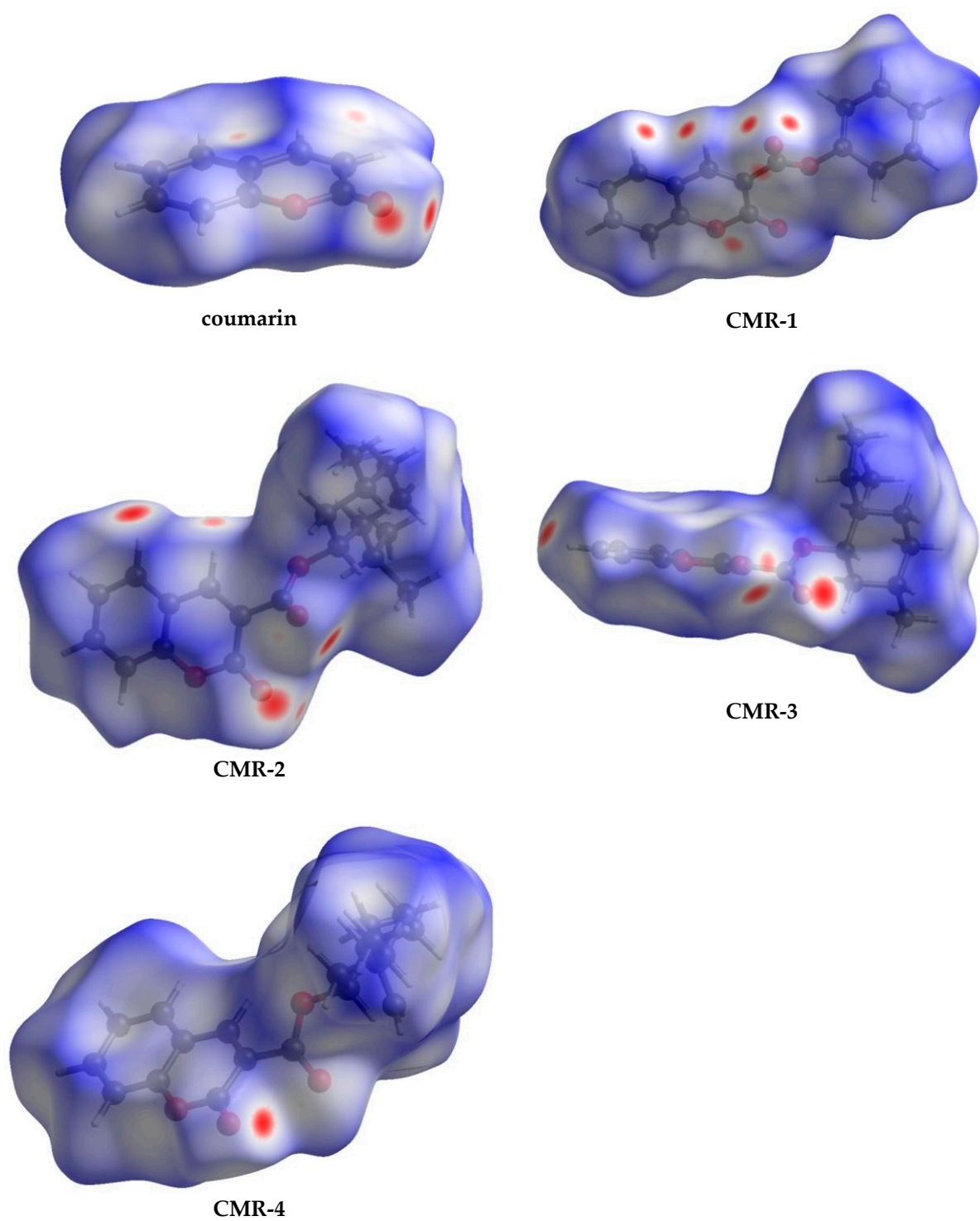


**Figure S-9.** Molecular fitting of conformers:

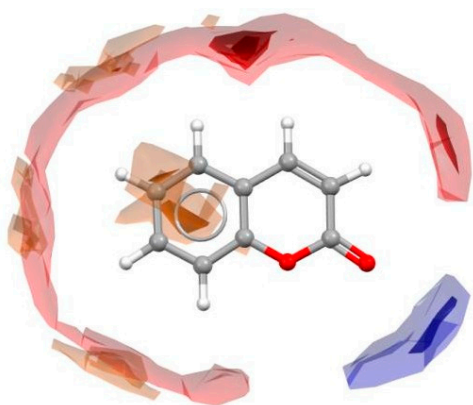
(a) CMR 2 and CMR 3 (navy blue), and

(b) CMR 1 (light blue), CMR 2 and CMR 4 (green) fitted through the coumarin rings.

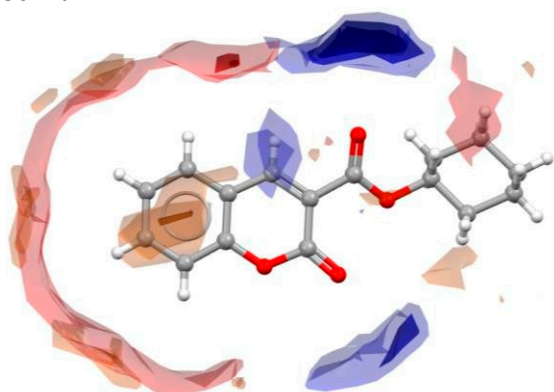
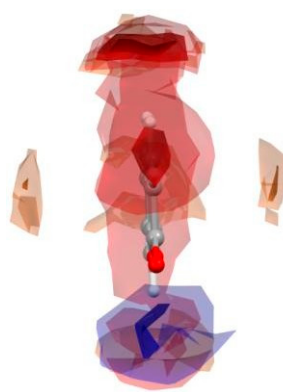




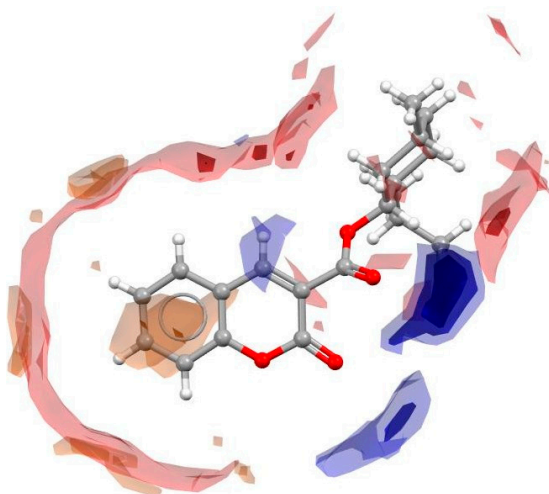
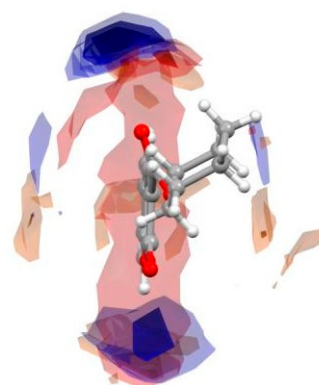
**Figure S-10.** Hirshfeld surfaces for molecules of coumarin and esters **CMR 1-4**.



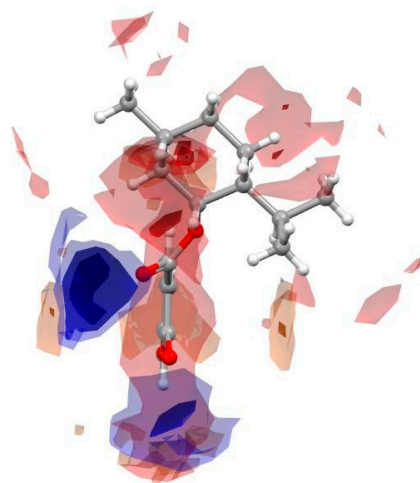
coumarin

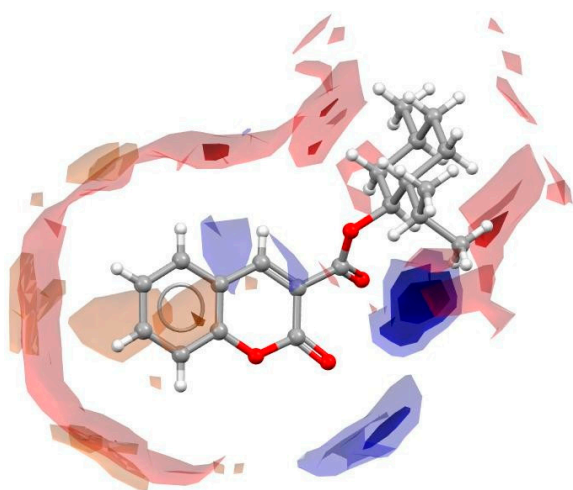


CMR-1

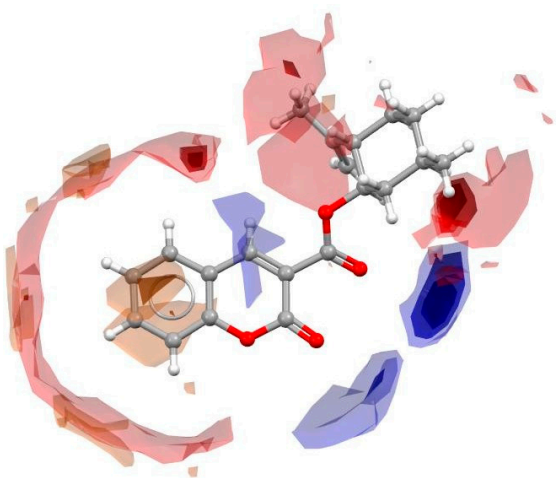
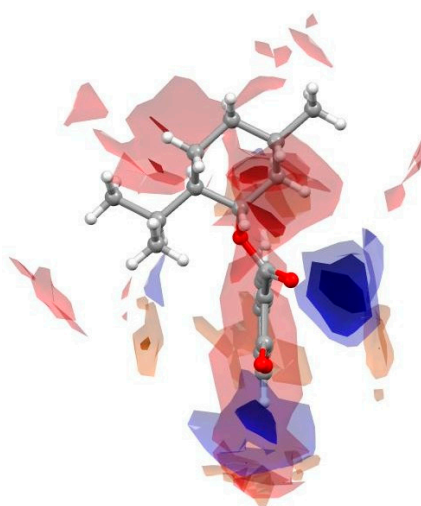


CMR-2

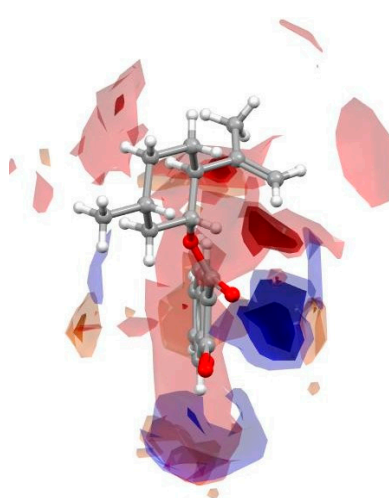




CMR-3

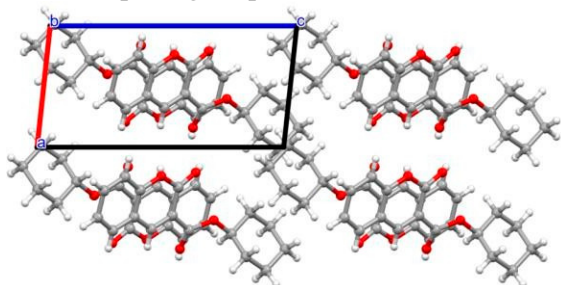


CMR-4

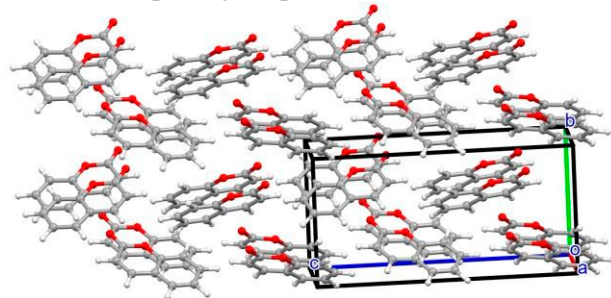


**Figure S-11.** Full Interaction Maps for the molecules of coumarin and esters **CMR 1-4**. Left column –perpendicular view to the coumarin ring; right column - view along the ring.

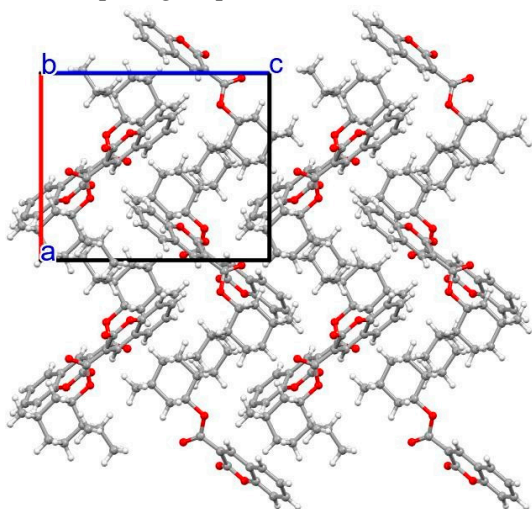
**CMR-1** (space group  $P-1$ )



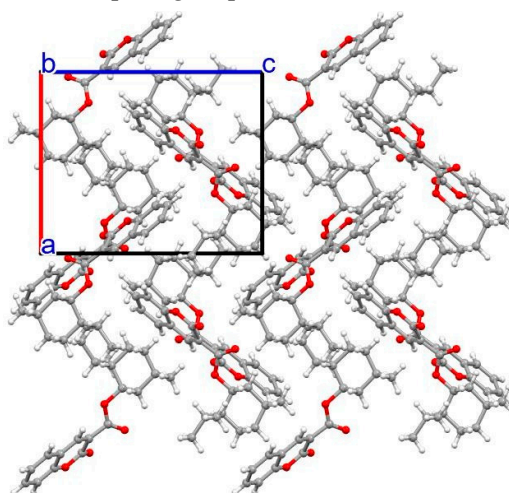
**Coumarin** (space group  $Pc2_1b$ )



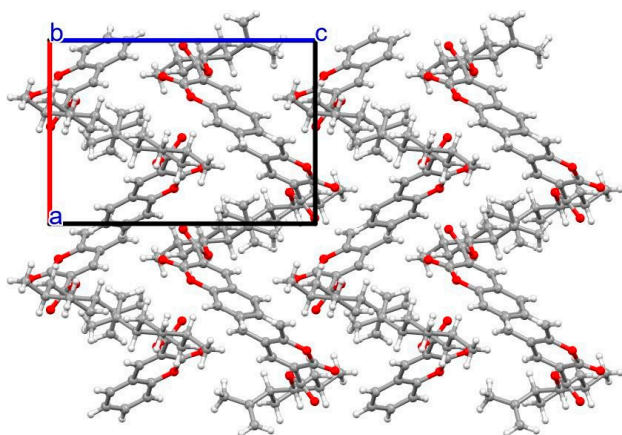
**CMR-2** (space group  $P2_12_12_1$ )



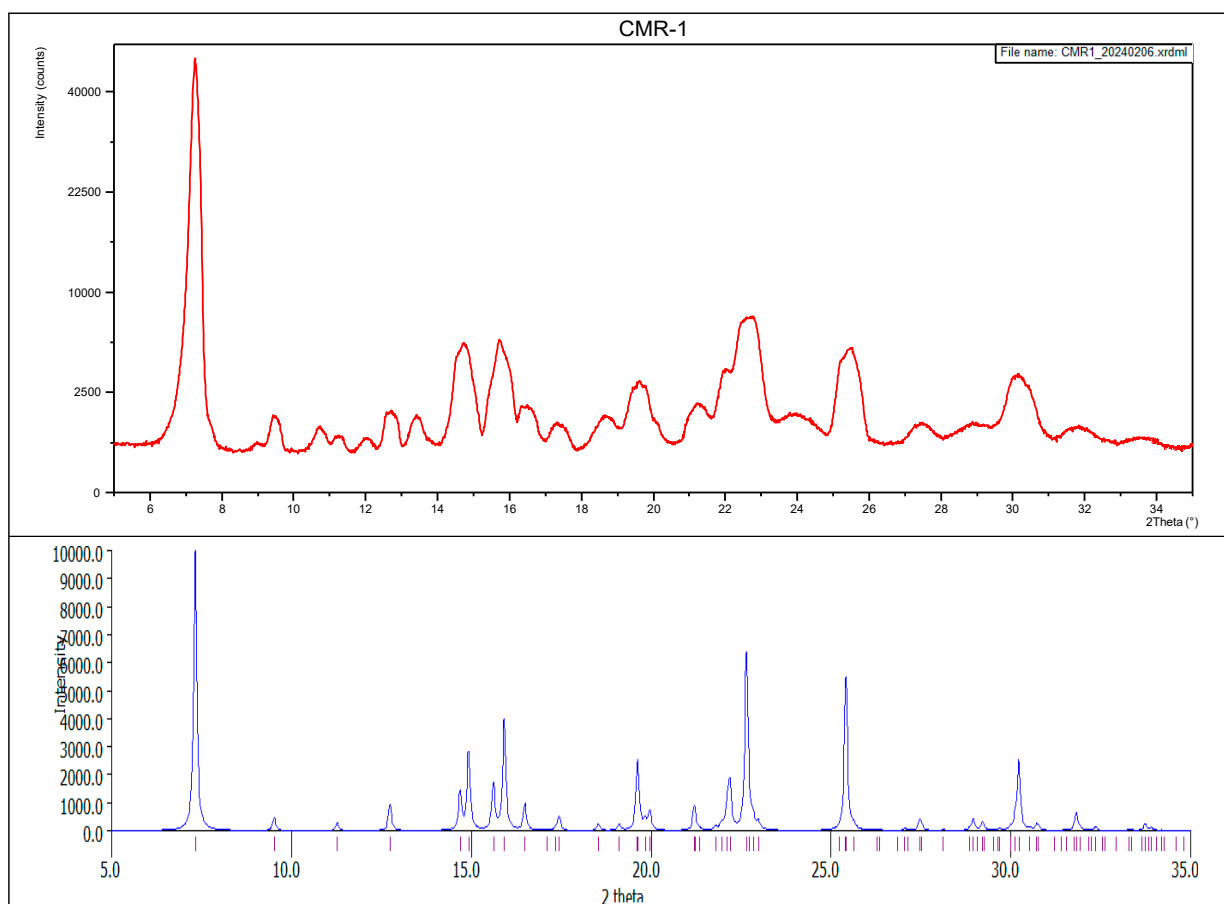
**CMR-3** (space group  $P2_12_12_1$ )



**CMR-4** (space group  $P2_12_12_1$ )

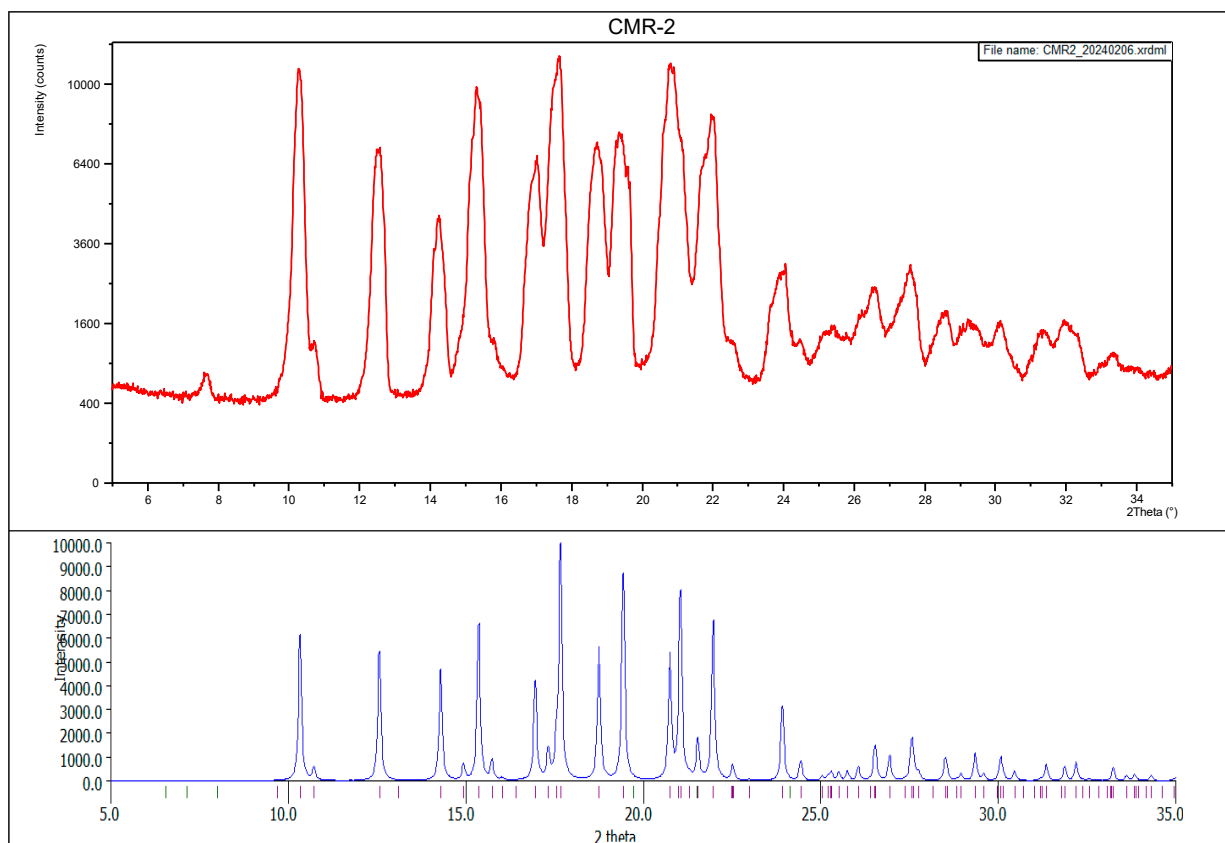


**Figure S-12.** Crystal packing of coumarin esters and coumarin.

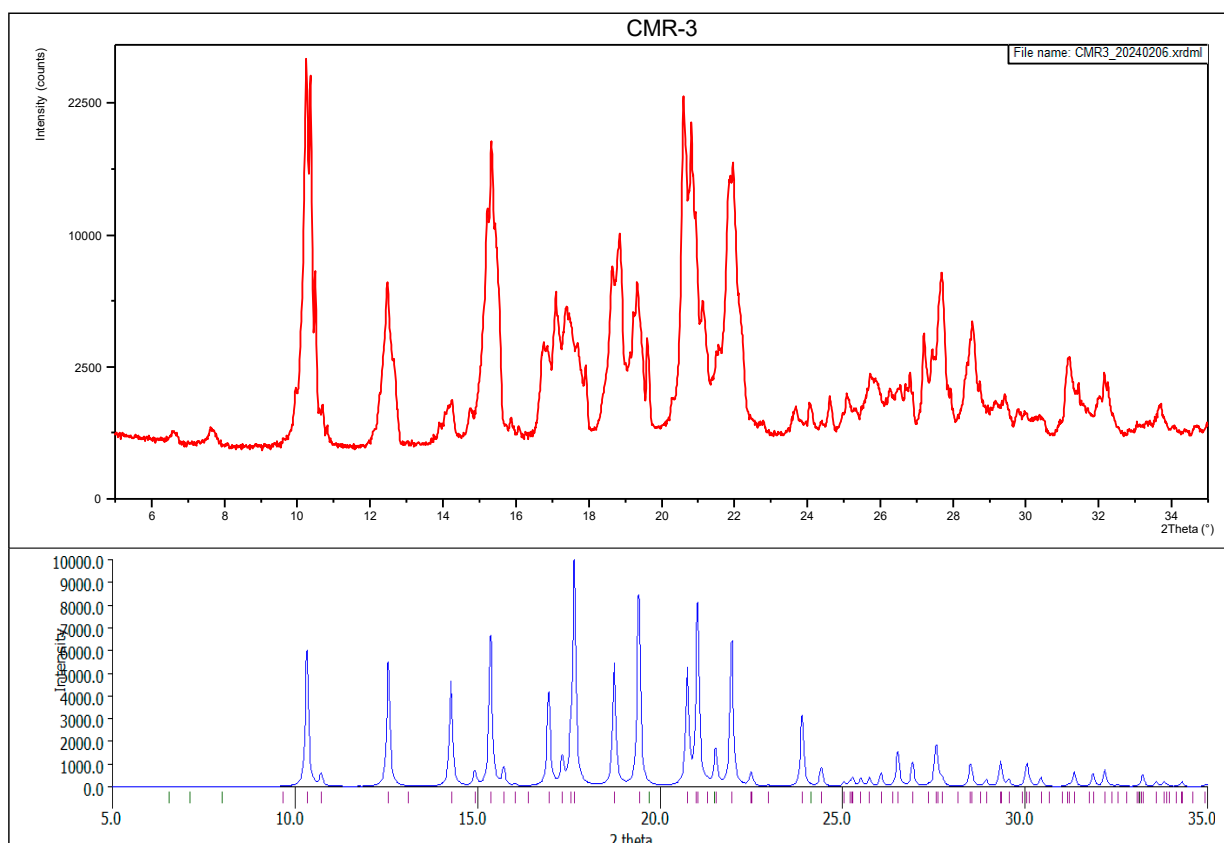


**Figure S-13.** X-Ray powder diffraction patterns for **CMR-1**. Top – red line: the experimental diffractogram; down – blue line: the diffractogram calculated from the single-crystal structural data ( $F^2$  without corrections).

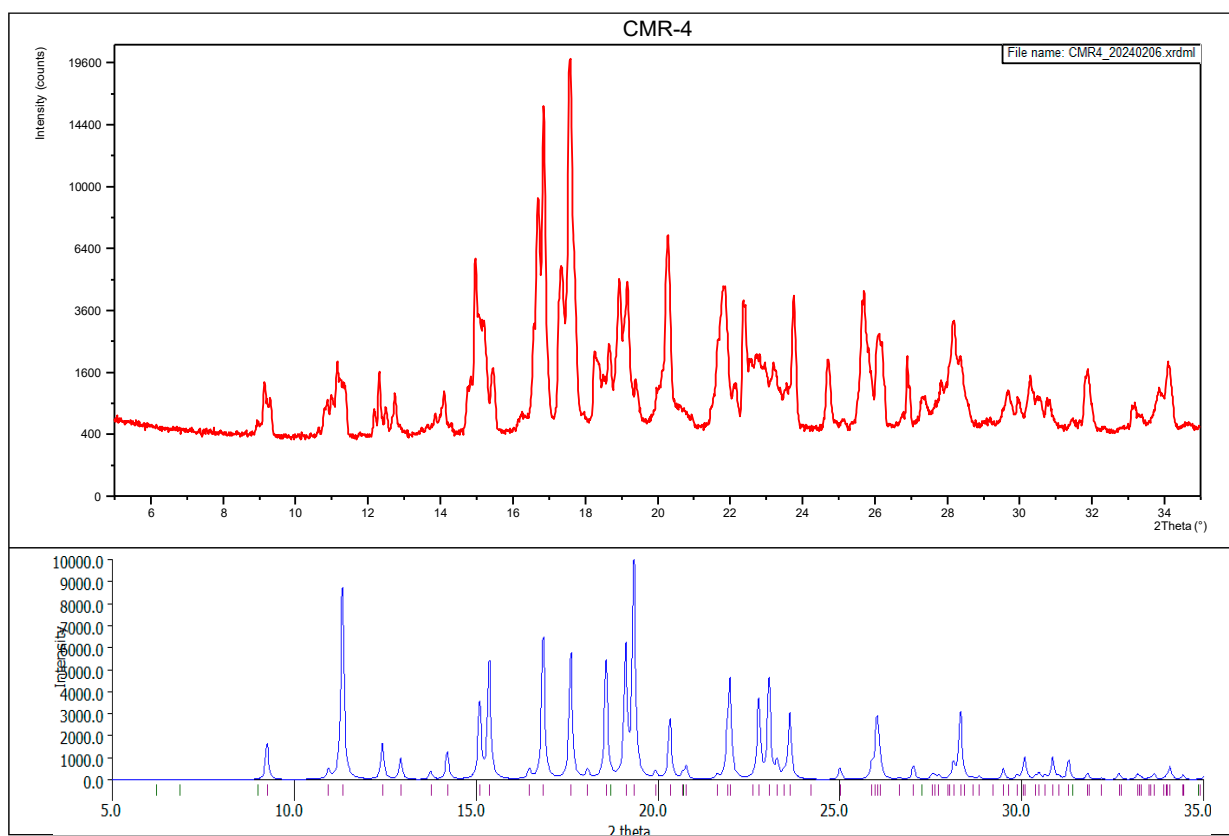




**Figure S-14.** X-Ray powder diffraction patterns for **CMR-2**. Top – red line: the experimental diffractogram; down – blue line: the diffractogram calculated from the single-crystal structural data ( $F^2$  without corrections).



**Figure S-15.** X-Ray powder diffraction patterns for **CMR-3**. Top – red line: the experimental diffractogram; down – blue line: the diffractogram calculated from the single-crystal structural data ( $F^2$  without corrections).



**Figure S-16.** X-Ray powder diffraction patterns for **CMR-4**. Top – red line: the experimental diffractogram; down – blue line: the diffractogram calculated from the single-crystal structural data ( $F^2$  without corrections).