SUPPLEMENTARY INFORMATION

Quantitative analysis of intermolecular interactions in 2,2'-((4-bromophenyl)methylene)bis(3-hydroxy-5,5-dimethylcyclohex-2-en-1-one): Insights from crystal structure, PIXEL, Hirshfeld surfaces and QTAIM analysis

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Table of Contents

	[1]) for these pairs are given.
4	Figure S3. Structural superimposition of experimental (orange) and optimized monomer in gas (blue) and ethanol solvent (purple) phases.
5	Figure S4. Molecular graphs obtained from QTAIM analysis for six molecular pairs (motif I to VI). Bond critical points (BCP) are denoted by small green spheres.
6.	Figure S5. FT-IR spectrum of the title compound (a) experimental (b) monomer (c) dimer-IV (d) dimer-III (e) dimer-II and (f) dimer-I.
7	Figure S6. FT-Raman of the title compound (a) experimental (b) monomer (c) dimer-IV (d) dimer-III (e) dimer-II and (f) dimer-I.

Table S1. Selected torsion angles in the title compound and its related analogs (°). The CSD refcode is given.

Compound code	τ_1	τ_2	τ_3
X-ray (4-Br)	–55.3(5)	48.8(5)	–7.7(6)
Gas phase (4-Br)	–45.0	53.7	-28.7
Ethanol (4-Br)	-47.7	51.9	-23.9
QIKCOC (4-NMe2)	–55.1(3)	49.1(2)	–3.5(3)
QIKCAO (4-OH)	–51.4(5)	52.5(4)	–0.2(5)
QIKCES (4-Me)	–54.2(2)	50.4(2)	–4.0(2)
QIKCIW (4-OMe)	–55.9(2)	52.2(2)	–1.0(2)
PUFTEP01 (4-Cl)	–43.8(2)	52.6(2)	–30.2(2)
QIKBOB (4-F)	–51.1(4) 47.1(3)	52.9(3) –49.5(3)	–24.8(4) 23.9(3)
QEDVEC (4-OET)	54.6(8)	–46.5(2)	12.5(2)
IRODID (4-NO2)	54.0(7)	–45.9(8)	28.5(7)
TOHDAV (4-H) (unsubstituted)	52.1(2) 44.6(2)	–48.9(2) –53.0(2)	14.8(2) 25.5(2)

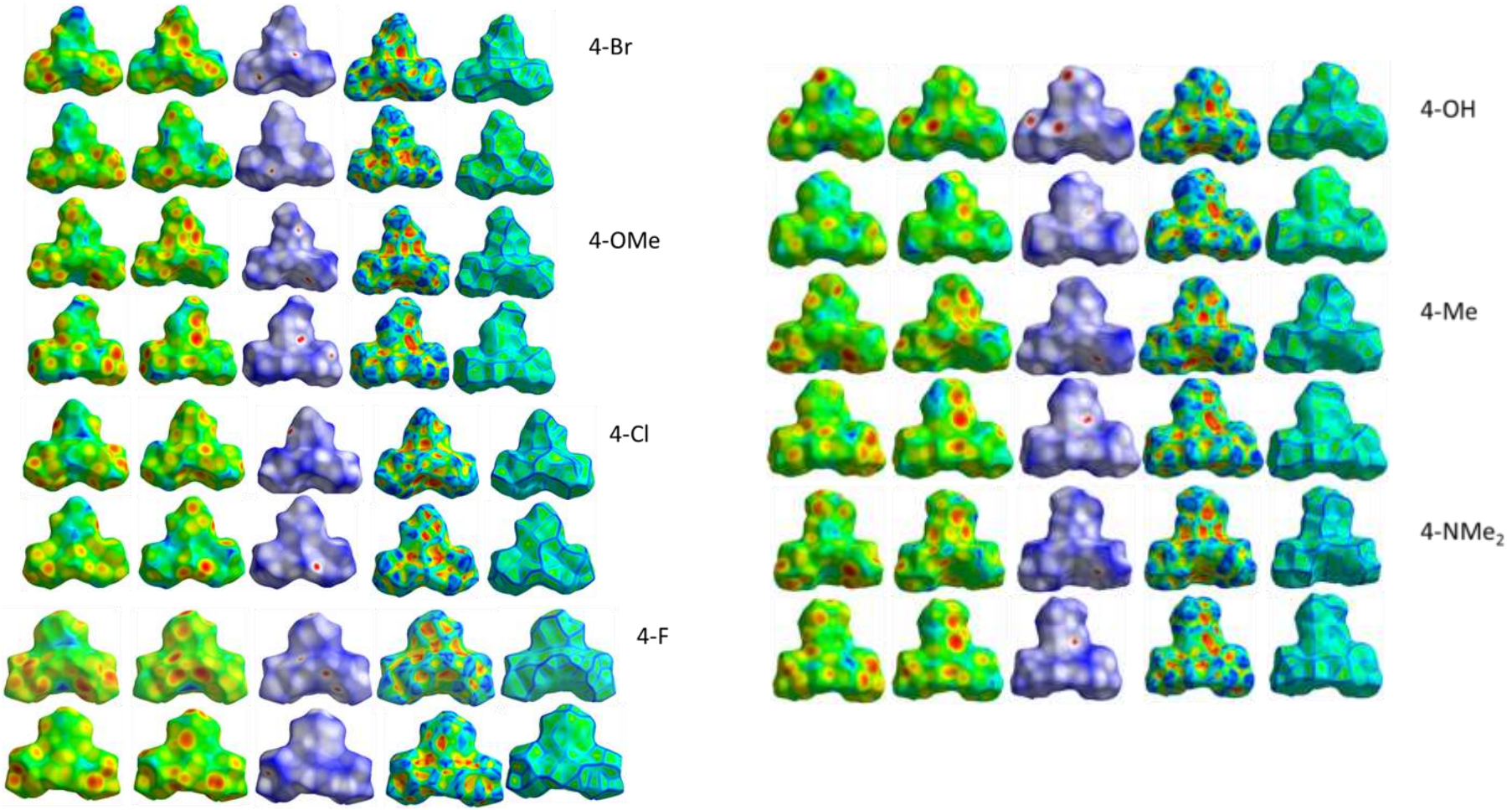
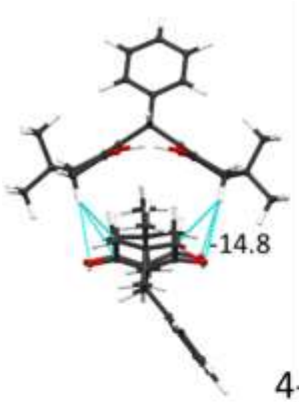
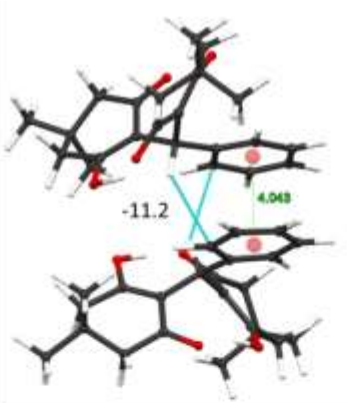
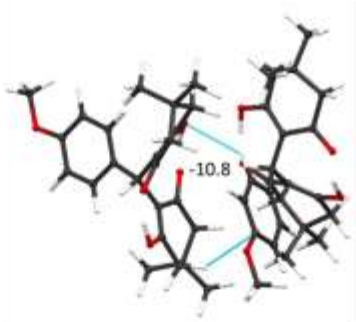


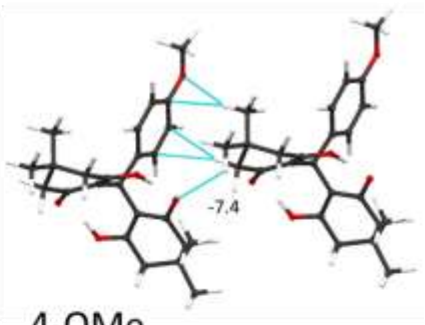
Figure S1. Two different orientations of Hirshfeld surfaces mapped with different properties such as d_i (column-1), d_e (column-2), d_{norm} (column-3) , shape index (column-4)and curvedness (column-5) for the title compound and its related analogs.



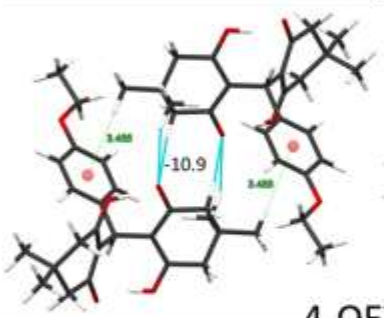
4-H

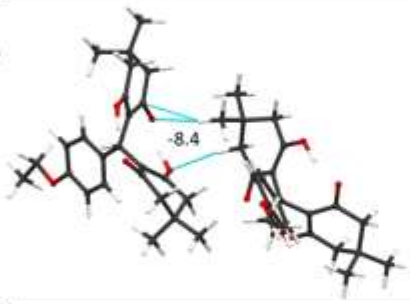




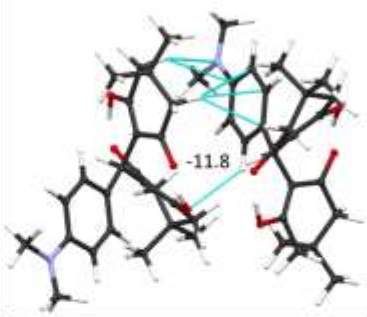


4-OMe

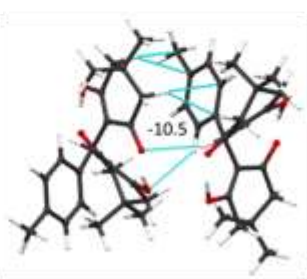


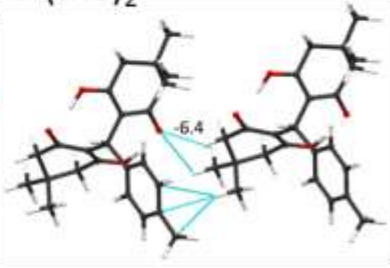


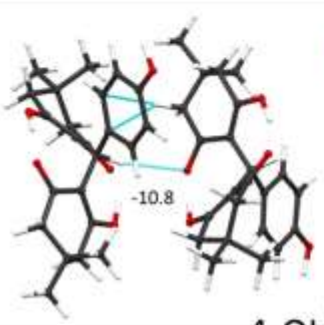
4-OET

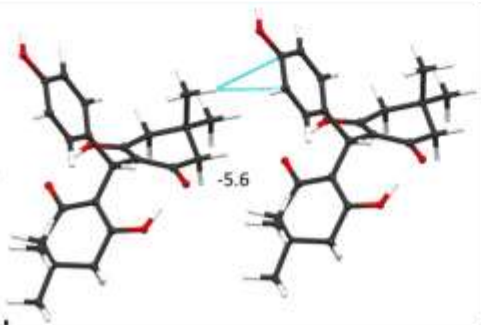


4-N(Me)$_2$

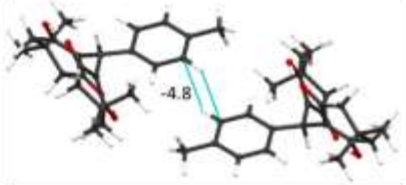








4-OH



4-Me

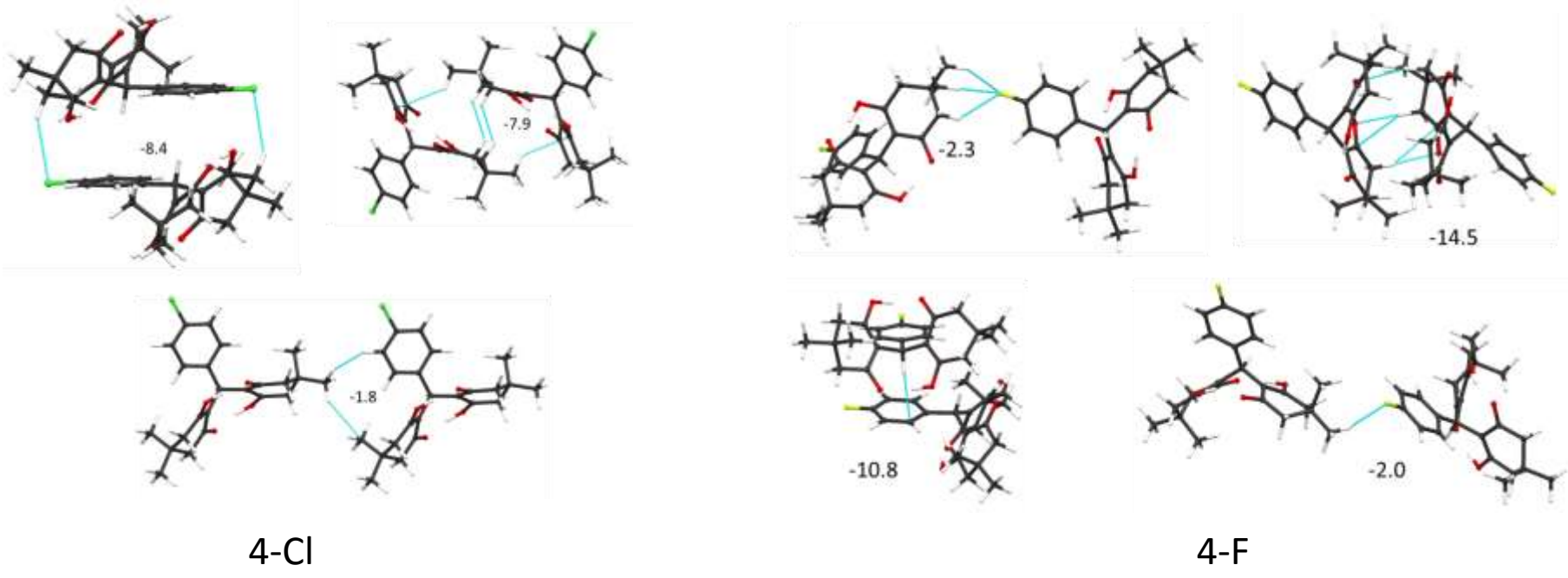
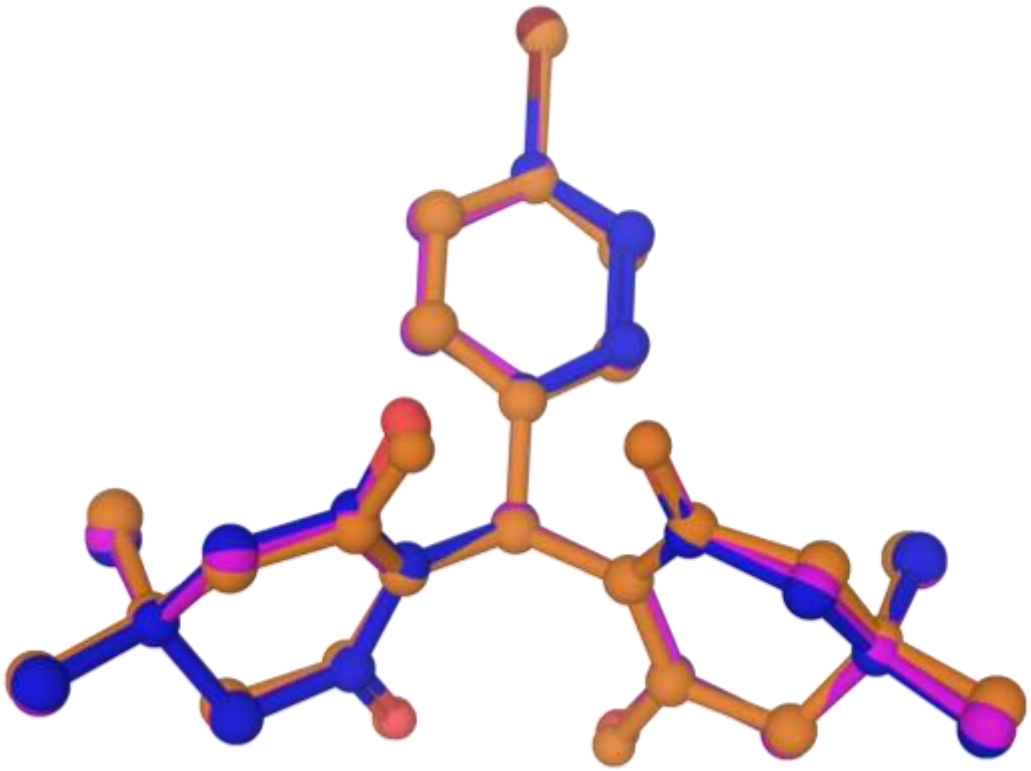


Figure S2. Selected molecular pairs from the crystal structures of closely related analogs of the title compound **I** show the importance of C···H and H···halogen contacts. The intermolecular interaction energies (in kcal mol^{-1}) for these pairs are given.



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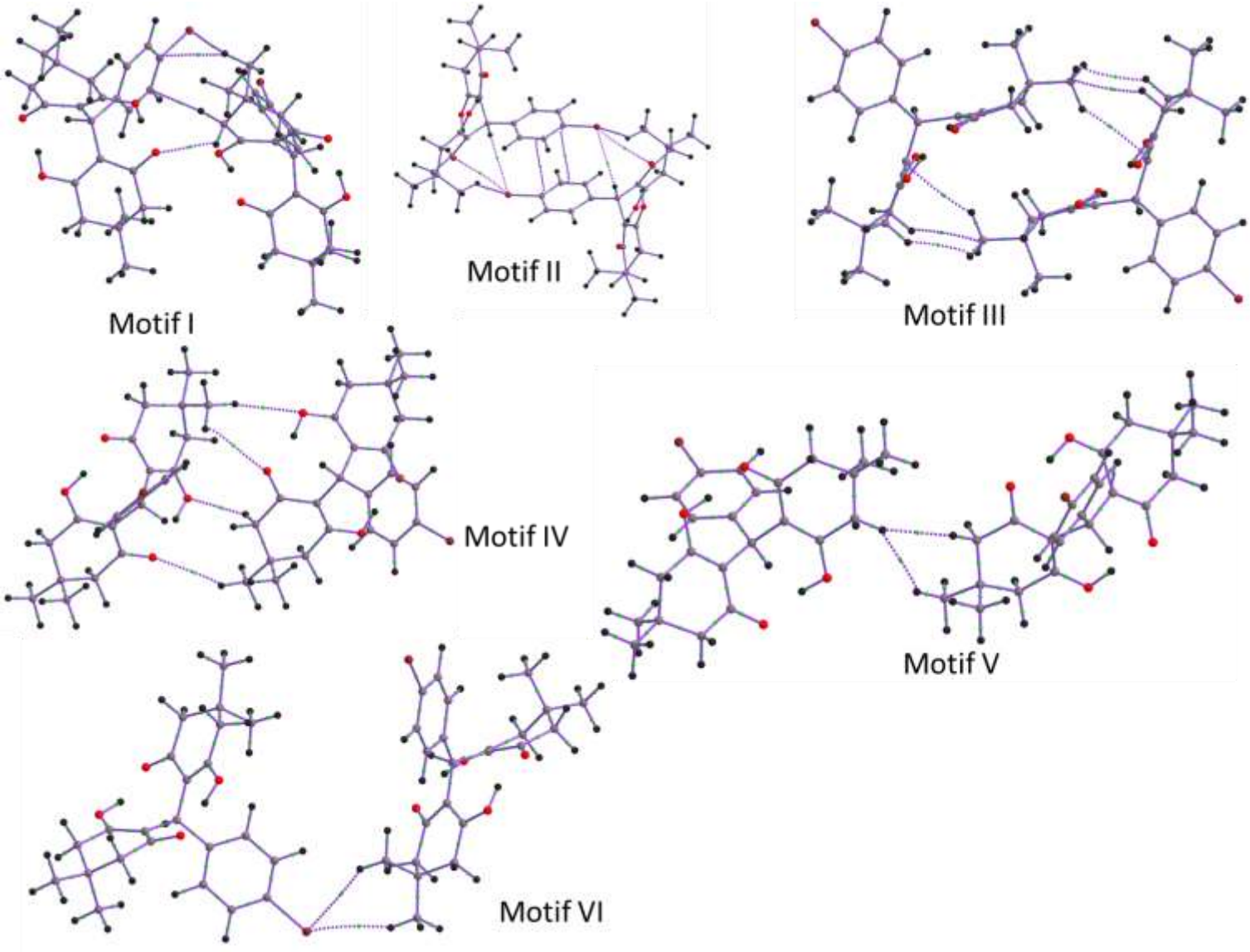

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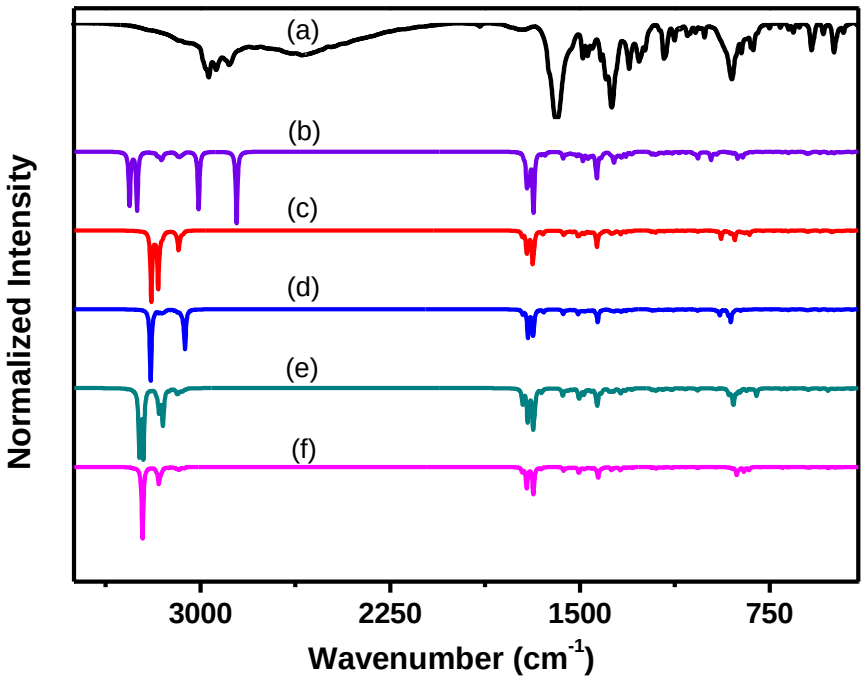

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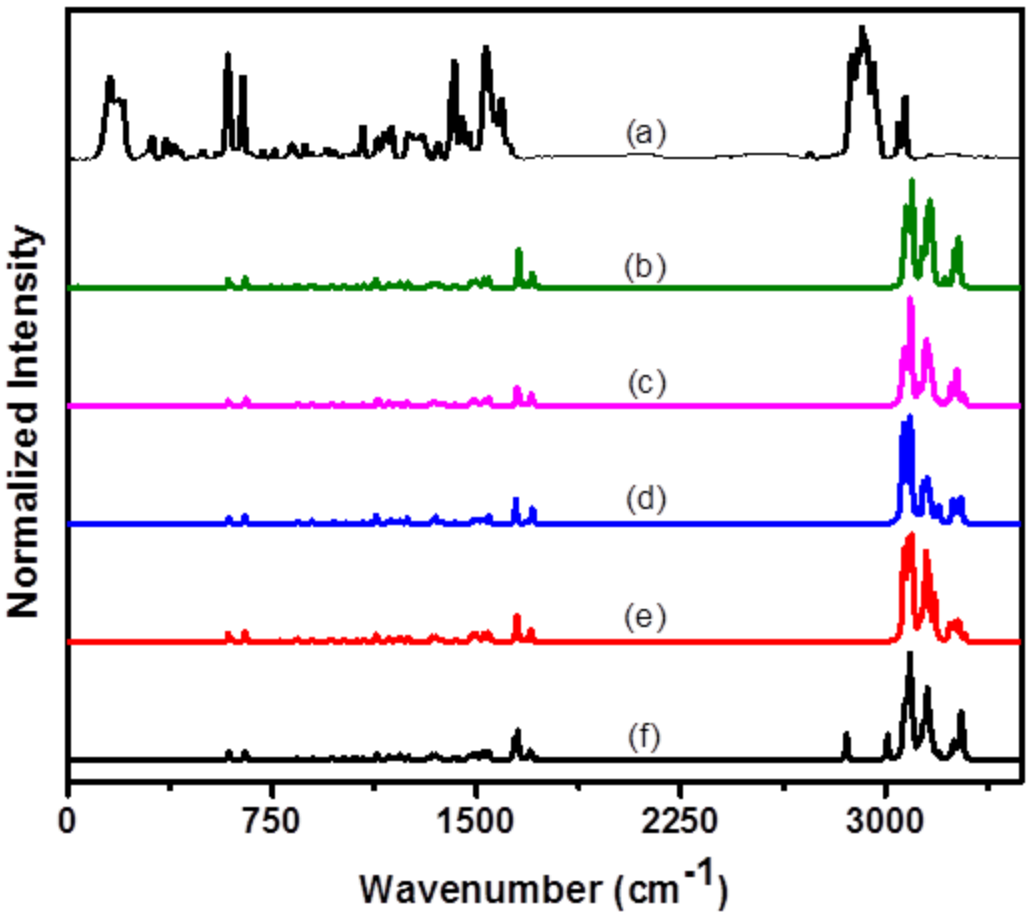

Figure S6. FT-Raman of the title compound (a) experimental (b) monomer (c) dimer-IV (d) dimer-III (e) dimer-II and (f) dimer-I.