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**SUPPLEMENTARY INFORMATION**

**for**

# Use of π–π forces to steer the assembly of chromone derivatives into hydrogen bonded supramolecular layers: Crystal structures and Hirshfeld Surface Analyses

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**Table S1.** Selected bond lengths (Å), bond angles (°) for the title compounds.

| | Compound **1** | | Compound **2** | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| | XRD | DFT | XRD | DFT | $MOGUL_{(mean)}$[$] | XRD-DFT | XRD-MOGUL | XRD-DFT | XRD-MOGUL |
| O(1)–C(9) | 1.354(2) | 1.358 | 1.366(2) | 1.380 | 1.37(2) | -0.004 | -0.016 | -0.014 | -0.004 |
| O(1)–C(5) | 1.372(2) | 1.382 | 1.376(2) | 1.393 | 1.37(1) | -0.010 | 0.002 | -0.017 | 0.006 |
| O(2)–C(7) | 1.231(2) | 1.241 | 1.240(2) | 1.244 | 1.24(2) | -0.010 | -0.009 | -0.004 | 0.000 |
| O(3)–C(3) | 1.356(2) | 1.363 | -- | -- | 1.37(2) | -0.007 | -0.014 | -- | -- |
| O(3)–C(11) | 1.431(2) | 1.430 | -- | -- | 1.42(2) | 0.001 | 0.011 | -- | -- |
| C(6)–C(1) | 1.427(2) | 1.428 | 1.400(2) | 1.409 | 1.40(1) | -0.001 | 0.027 | -0.009 | 0.000 |
| C(6)–C(7) | 1.470(2) | 1.478 | 1.470(2) | 1.486 | 1.46(2) | -0.008 | 0.010 | -0.016 | 0.010 |
| C(2)–C(1) | 1.374(2) | 1.387 | 1.374(2) | 1.390 | 1.39(1) | -0.013 | -0.016 | -0.016 | -0.016 |
| C(8)–C(9) | 1.328(2) | 1.345 | 1.345(2) | 1.358 | 1.32(1) | -0.017 | 0.008 | -0.013 | 0.025 |
| C(8)–C(7) | 1.451(2) | 1.460 | 1.443(2) | 1.461 | 1.45(2) | -0.009 | 0.001 | -0.018 | -0.007 |
| | | | | | | | | | |
| C(9)–O(1)–C(5) | 118.57(11) | 118.43 | 118.89(10) | 119.05 | 118(1) | 0.14 | 0.57 | -0.16 | 0.89 |
| C(5)–C(6)–C(1) | 117.20(13) | 117.19 | 117.61(11) | 117.61 | 117(1) | 0.01 | 0.20 | 0.00 | 0.61 |
| O(2)–C(7)–C(8) | 121.57(13) | 121.35 | 123.59(11) | 123.23 | 120(1) | 0.22 | 1.57 | 0.36 | 3.59 |
| O(2)–C(7)–C(6) | 123.89(13) | 124.37 | 122.02(12) | 122.91 | 122(1) | -0.48 | 1.89 | -0.89 | 0.02 |
| C(8)–C(7)–C(6) | 114.54(12) | 114.28 | 114.39(11) | 113.86 | 117(1) | 0.26 | 2.46 | 0.53 | -2.61 |
| C(4)–C(5)–C(6) | 123.62(13) | 123.69 | 121.88(11) | 122.08 | 122(1) | -0.07 | 1.62 | -0.20 | -0.12 |

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| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| C(3)–O(3)–C(11) | 117.05(11) | 117.46 | -- | -- | 117(1) | -0.41 | 0.05 | -- | -- |
| O(3)–C(3)–C(4) | 124.60(13) | 124.47 | -- | -- | 120(4) | 0.13 | 4.60 | -- | -- |
| O(3)–C(3)–C(2) | 115.39(12) | 115.57 | -- | -- | 119(4) | -0.18 | -3.61 | -- | -- |
| C(8)–C(9)–O(1) | 123.43(13) | 123.85 | 122.98(11) | 122.44 | 123(1) | -0.42 | 0.43 | 0.54 | -0.02 |
| | | | | | | | | | |
| C(9)–C(8)–C(7)–O(2) | 179.8(2) | -179.83 | -179.77(11) | 179.89 | 179(2) | 0.03 | 0.80 | 0.12 | 0.77 |
| C(11)–O(3)–C(3)–C(4) | 6.5(2) | 1.31 | -- | -- | 5(2) | 5.19 | 1.50 | -- | -- |
| C(11)–O(3)–C(3)–C(2) | -173.9(2) | 178.68 | -- | -- | 176(2) | 4.78 | 2.10 | -- | -- |
| C(7)–C(8)–C(9)–O(1) | 0.1(2) | -0.30 | -1.00(18) | -0.38 | 4(1) | 0.20 | 3.90 | 0.62 | 3.00 |
| C(5)–O(1)–C(9)–C(8) | -0.7(2) | 0.13 | 0.79(16) | 0.59 | 2(1) | 0.57 | 1.30 | 0.20 | 1.21 |

[$]Computer programs used: MOGUL run on the CSD.

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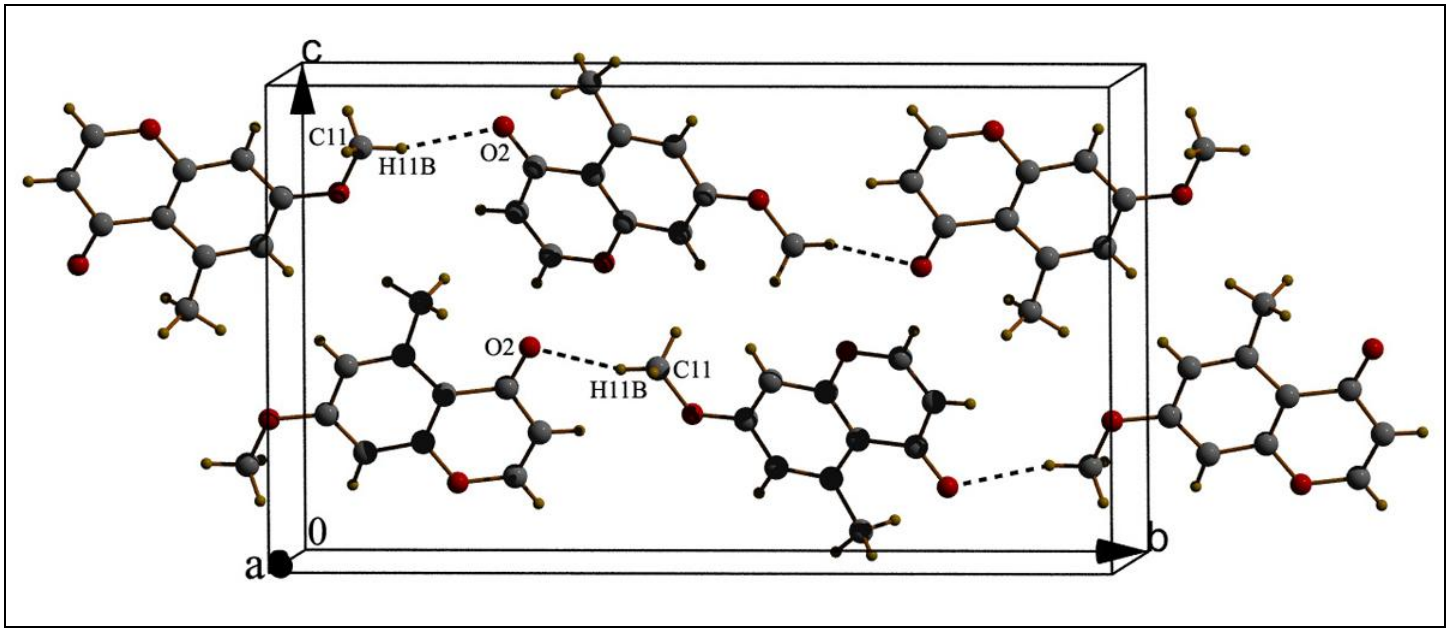


Figure S1: Formation of 1D parallel chains running along [0 1 0] direction in **1**.

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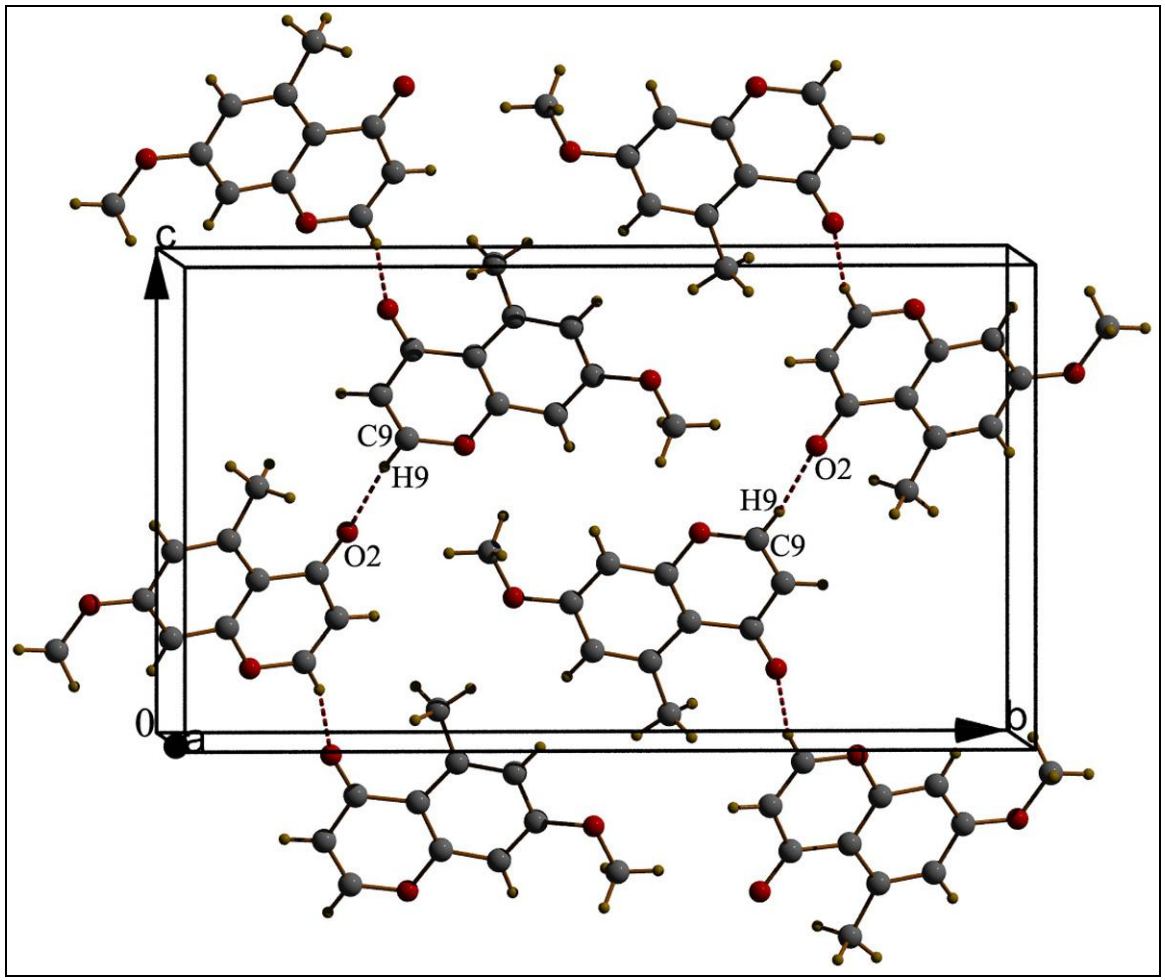


Figure S2: Formation of 1D parallel chains running along [0 0 1] direction in **1**.

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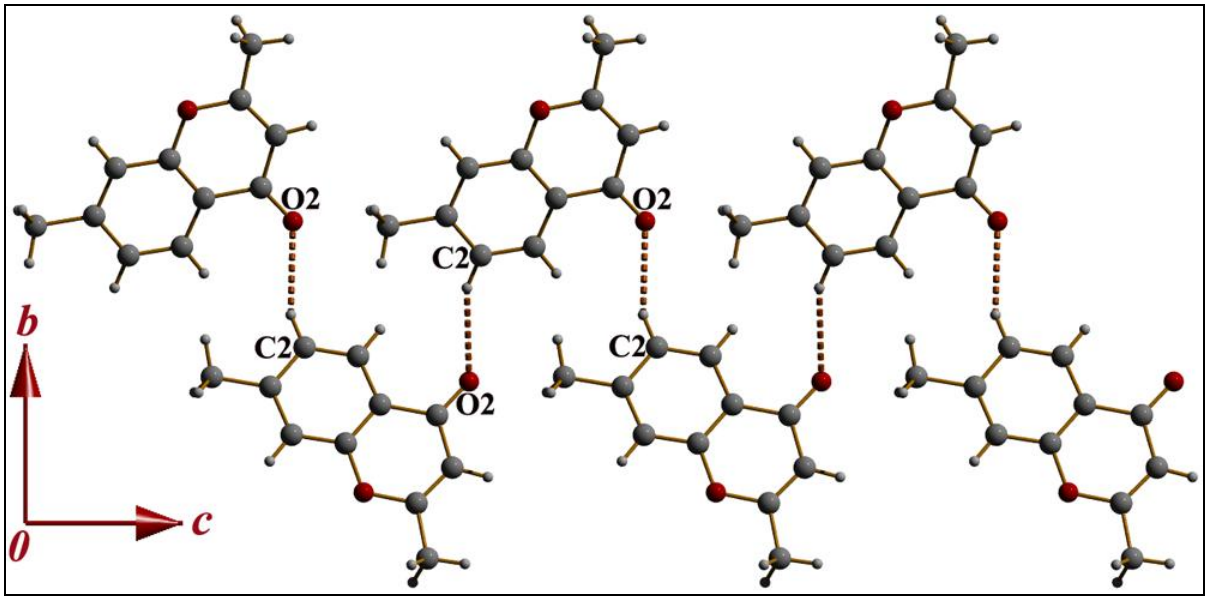


Figure S3: Propagation of 1D zigzag chain along [0 0 1] direction in compound **2**.

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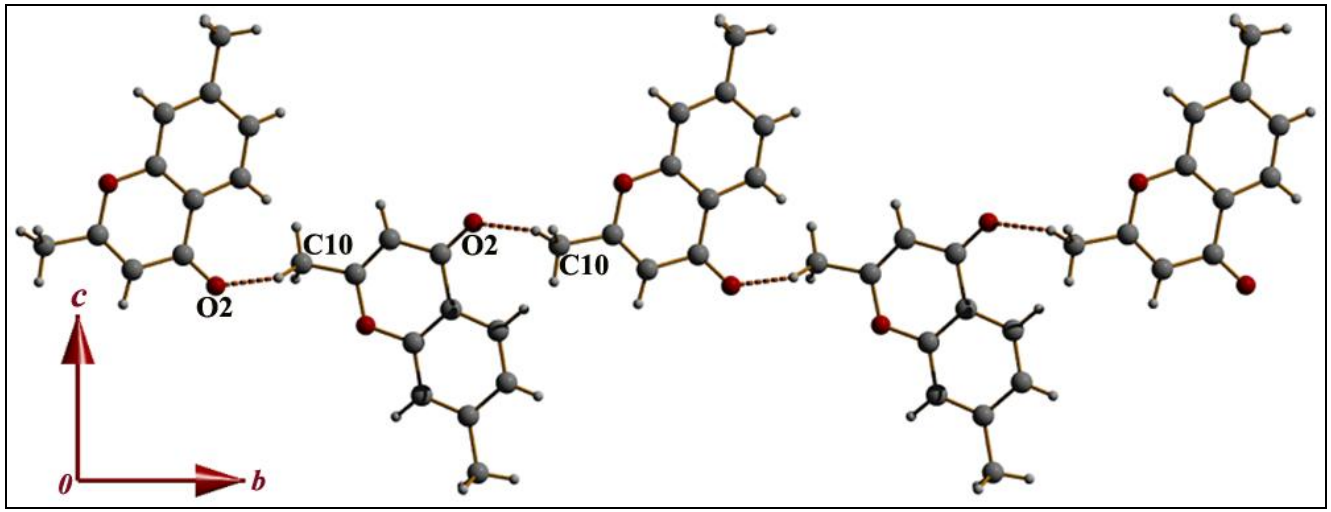


Figure S4: Propagation of 1D zigzag chain along [0 1 0] direction in compound **2**.