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Supporting information for article:

Hydrogen-bond-driven supramolecular helical assembly of a coumarin-substituted phthalonitrile derivative: synthesis and *in vitro* anticancer activity against colorectal adenocarcinoma

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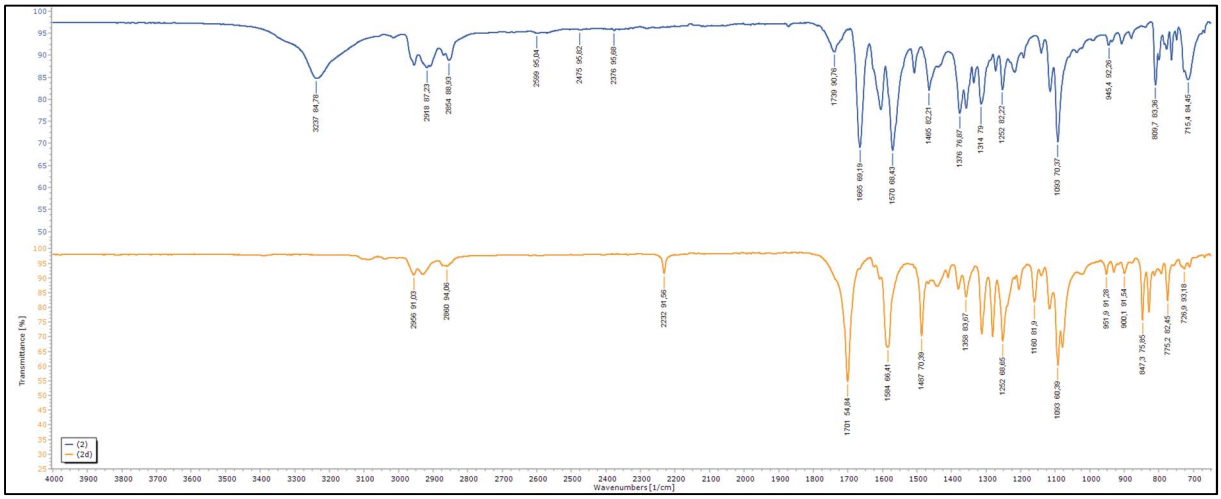


Figure S1 Comparative of the FT-IR spectrum of compounds **2** and **2d**.

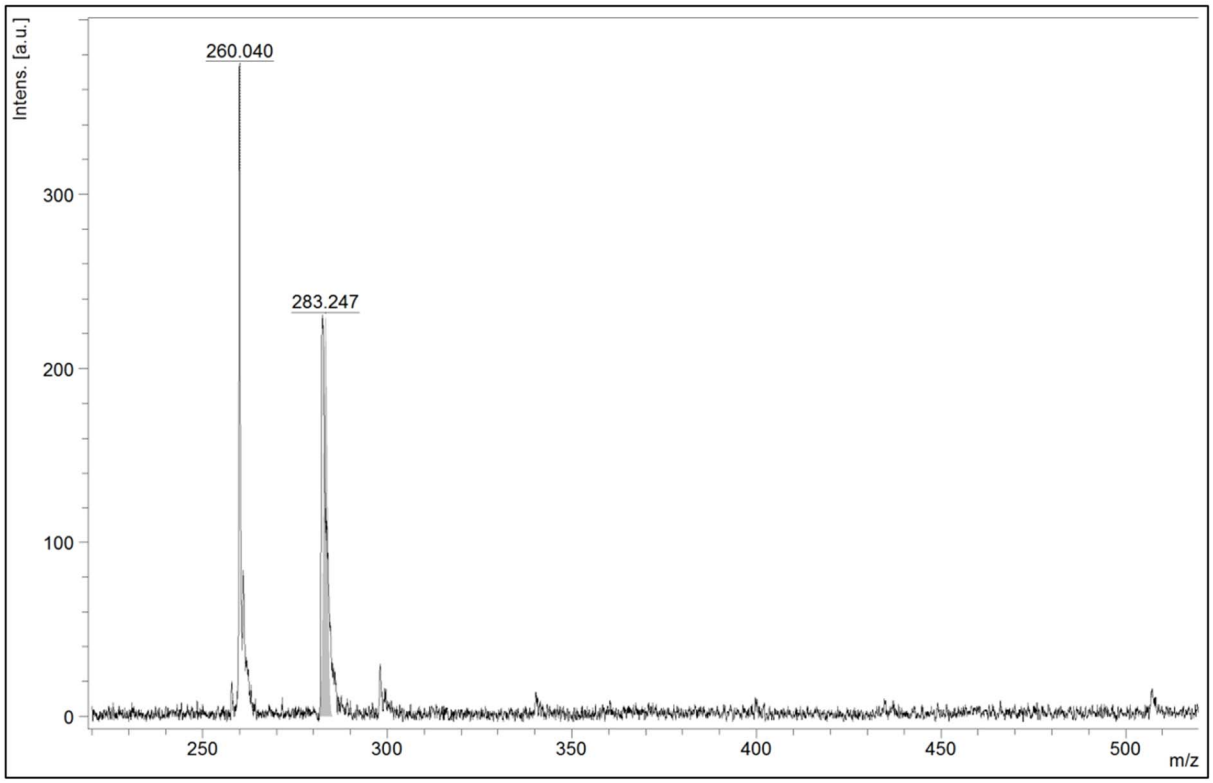


Figure S2 Positive ion in reflection mode MALDI-TOF mass spectrum of compound **2** in DHB matrix.

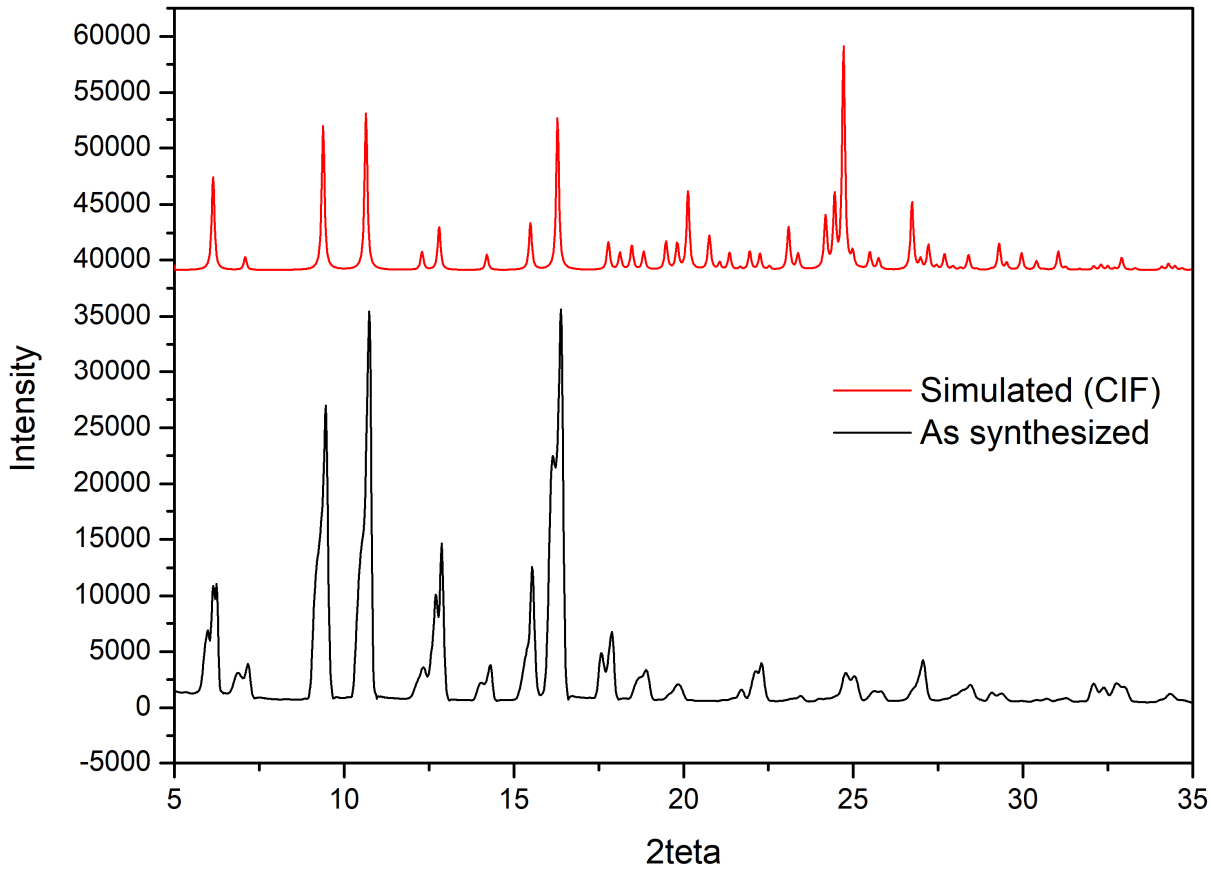


Figure S3 Compared XRD graphs of compound **2d**.

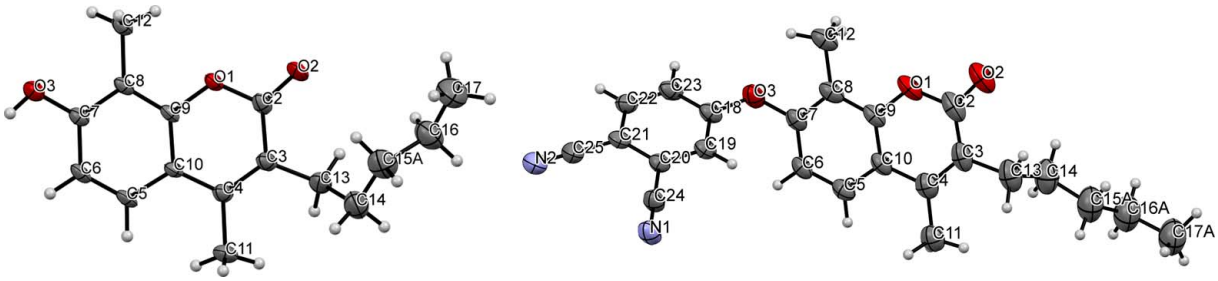


Figure S4 Numbered representations of coumarin crystals in ellipsoid style. The disordered parts in crystal structures are omitted for clarity.

Table S1 Bond Lengths for compound **2** (CCDC2158229).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.375(8)	C6	C7	1.407(8)
O1	C9	1.375(7)	C7	C8	1.386(8)
O2	C2	1.220(7)	C8	C9	1.384(8)
O3	C7	1.347(8)	C8	C12	1.498(9)
C2	C3	1.446(9)	C9	C10	1.400(8)
C3	C4	1.371(9)	C13	C14	1.501(9)
C3	C13	1.497(11)	C14	C15A	1.486(10)
C4	C10	1.416(9)	C14	C15B	1.529(12)
C4	C11	1.515(9)	C15A	C16	1.552(10)
C5	C6	1.359(8)	C15B	C16	1.546(13)
C5	C10	1.410(9)	C16	C17	1.531(11)

Table S2 Bond Angles for compound **2** (CCDC2158229).

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C9	O1	C2	121.9(5)	C9	C8	C7	117.1(5)
O1	C2	C3	119.3(5)	C9	C8	C12	122.2(5)
O2	C2	O1	115.4(6)	O1	C9	C8	115.7(5)
O2	C2	C3	125.3(6)	O1	C9	C10	119.7(5)
C2	C3	C13	116.4(6)	C8	C9	C10	124.6(5)
C4	C3	C2	118.7(6)	C5	C10	C4	125.1(5)
C4	C3	C13	124.8(6)	C9	C10	C4	119.4(5)
C3	C4	C10	121.0(5)	C9	C10	C5	115.5(6)
C3	C4	C11	120.3(6)	C3	C13	C14	116.6(8)
C10	C4	C11	118.7(5)	C13	C14	C15B	134.0(12)
C6	C5	C10	121.9(6)	C15A	C14	C13	115.4(9)
C5	C6	C7	120.3(6)	C14	C15A	C16	110.9(9)
O3	C7	C6	121.1(5)	C14	C15B	C16	108.9(11)
O3	C7	C8	118.4(5)	C17	C16	C15A	106.2(10)
C8	C7	C6	120.5(6)	C17	C16	C15B	127.7(17)
C7	C8	C12	120.7(6)				

Table S3 Torsion Angles for compound **2** (CCDC2158229).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C2	C3	C4	-1.0(9)	C6	C5	C10	C9	1.4(10)
O1	C2	C3	C13	-179.2(6)	C6	C7	C8	C9	-1.1(9)
O1	C9	C10	C4	-0.2(8)	C6	C7	C8	C12	179.8(6)
O1	C9	C10	C5	179.5(6)	C7	C8	C9	O1	-179.6(5)
O2	C2	C3	C4	-179.5(6)	C7	C8	C9	C10	0.9(9)
O2	C2	C3	C13	2.2(10)	C8	C9	C10	C4	179.3(6)
O3	C7	C8	C9	179.5(5)	C8	C9	C10	C5	-1.1(9)
O3	C7	C8	C12	0.4(9)	C9	O1	C2	O2	179.7(5)
C2	O1	C9	C8	-179.9(5)	C9	O1	C2	C3	1.0(8)
C2	O1	C9	C10	-0.4(8)	C10	C5	C6	C7	-1.6(11)
C2	C3	C4	C10	0.4(9)	C11	C4	C10	C5	2.5(9)
C2	C3	C4	C11	178.3(6)	C11	C4	C10	C9	-177.8(6)
C2	C3	C13	C14	100.1(8)	C12	C8	C9	O1	-0.5(8)
C3	C4	C10	C5	-179.4(7)	C12	C8	C9	C10	-180.0(6)
C3	C4	C10	C9	0.2(9)	C13	C3	C4	C10	178.4(6)
C3	C13	C14	C15A	-75.1(10)	C13	C3	C4	C11	-3.6(11)
C3	C13	C14	C15B	-128(2)	C13	C14	C15A	C16	-74.0(13)
C4	C3	C13	C14	-78.0(10)	C13	C14	C15B	C16	32(4)
C5	C6	C7	O3	-179.2(6)	C14	C15A	C16	C17	178.2(11)
C5	C6	C7	C8	1.5(10)	C14	C15B	C16	C17	125.6(19)
C6	C5	C10	C4	-179.0(6)					

Table S4 Bond Lengths for compound **2d** (CCDC2158230).

Atom	Atom	Length/Å	Atom	Atom	Length/Å
O1	C2	1.363(8)	C8	C12	1.515(8)
O1	C9	1.381(6)	C9	C10	1.376(8)
O2	C2	1.218(7)	C13	C14	1.527(7)
O3	C7	1.409(6)	C14	C15A	1.540(8)
O3	C18	1.362(6)	C14	C15B	1.480(15)
N1	C24	1.154(6)	C15A	C16A	1.520(9)
N2	C25	1.151(7)	C15B	C16B	1.507(17)
C2	C3	1.435(9)	C16A	C17A	1.537(9)
C3	C4	1.365(8)	C16B	C17B	1.501(17)
C3	C13	1.508(8)	C18	C19	1.396(6)
C4	C10	1.457(8)	C18	C23	1.381(7)
C4	C11	1.488(8)	C19	C20	1.383(7)
C5	C6	1.354(7)	C20	C21	1.394(7)
C5	C10	1.403(7)	C20	C24	1.408(7)
C6	C7	1.379(7)	C21	C22	1.391(7)
C7	C8	1.370(7)	C21	C25	1.419(8)
C8	C9	1.387(8)	C22	C23	1.348(7)

Table S5 Bond Angles for compound **2d** (CCDC2158230).

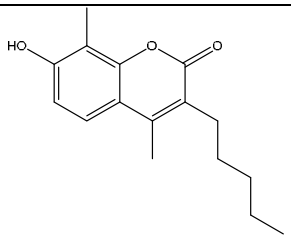
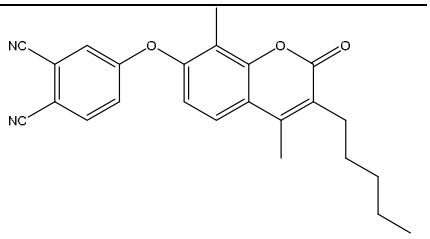
Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
C2	O1	C9	121.2(5)	C9	C10	C4	119.7(5)
C18	O3	C7	120.2(4)	C9	C10	C5	117.2(5)
O1	C2	C3	119.6(6)	C3	C13	C14	112.9(5)
O2	C2	O1	114.2(7)	C13	C14	C15A	106.1(6)
O2	C2	C3	126.2(7)	C15B	C14	C13	125.3(11)
C2	C3	C13	116.8(6)	C16A	C15A	C14	112.0(8)
C4	C3	C2	120.6(6)	C14	C15B	C16B	103.2(13)
C4	C3	C13	122.6(7)	C15A	C16A	C17A	110.6(8)
C3	C4	C10	118.3(6)	C17B	C16B	C15B	119.9(17)
C3	C4	C11	122.9(6)	O3	C18	C19	124.2(5)
C10	C4	C11	118.8(5)	O3	C18	C23	115.4(5)
C6	C5	C10	120.7(5)	C23	C18	C19	120.4(5)
C5	C6	C7	119.4(5)	C20	C19	C18	119.0(5)
C6	C7	O3	120.1(5)	C19	C20	C21	120.4(5)
C8	C7	O3	116.8(5)	C19	C20	C24	119.0(5)
C8	C7	C6	123.0(5)	C21	C20	C24	120.6(5)
C7	C8	C9	115.7(5)	C20	C21	C25	120.4(5)
C7	C8	C12	122.0(6)	C22	C21	C20	118.5(5)
C9	C8	C12	122.3(5)	C22	C21	C25	121.1(5)
O1	C9	C8	115.5(5)	C23	C22	C21	121.6(5)
C10	C9	O1	120.6(5)	C22	C23	C18	120.0(5)
C10	C9	C8	123.9(5)	N1	C24	C20	178.3(6)
C5	C10	C4	123.2(5)	N2	C25	C21	178.8(8)

Table S6 Torsion Angles for compound **2d** (CCDC2158230).

A	B	C	D	Angle/°	A	B	C	D	Angle/°
O1	C2	C3	C4	0.3(8)	C7	C8	C9	C10	-2.9(7)
O1	C2	C3	C13	-178.1(5)	C8	C9	C10	C4	-177.3(5)
O1	C9	C10	C4	0.7(7)	C8	C9	C10	C5	3.3(7)
O1	C9	C10	C5	-178.6(4)	C9	O1	C2	O2	178.7(4)
O2	C2	C3	C4	179.1(6)	C9	O1	C2	C3	-2.3(8)
O2	C2	C3	C13	0.7(9)	C10	C5	C6	C7	-1.7(7)
O3	C7	C8	C9	-176.4(4)	C11	C4	C10	C5	-4.5(7)
O3	C7	C8	C12	3.2(7)	C11	C4	C10	C9	176.2(5)
O3	C18	C19	C20	179.6(5)	C12	C8	C9	O1	-0.6(7)
O3	C18	C23	C22	-178.9(5)	C12	C8	C9	C10	177.5(5)
C2	O1	C9	C8	180.0(5)	C13	C3	C4	C10	-179.5(5)
C2	O1	C9	C10	1.8(7)	C13	C3	C4	C11	1.7(8)
C2	C3	C4	C10	2.1(8)	C13	C14	C15A	C16A	173.0(14)
C2	C3	C4	C11	-176.7(5)	C13	C14	C15B	C16B	70(2)
C2	C3	C13	C14	-93.4(8)	C14	C15A	C16A	C17A	174.6(15)
C3	C4	C10	C5	176.7(4)	C14	C15B	C16B	C17B	157(2)
C3	C4	C10	C9	-2.6(7)	C18	O3	C7	C6	56.2(6)
C3	C13	C14	C15A	-170.4(10)	C18	O3	C7	C8	-127.1(5)
C3	C13	C14	C15B	172.1(12)	C18	C19	C20	C21	-2.5(7)
C4	C3	C13	C14	88.1(7)	C18	C19	C20	C24	177.4(5)
C5	C6	C7	O3	178.6(4)	C19	C18	C23	C22	-0.5(8)
C5	C6	C7	C8	2.1(7)	C19	C20	C21	C22	2.8(7)
C6	C5	C10	C4	179.7(4)	C19	C20	C21	C25	-178.2(5)
C6	C5	C10	C9	-0.9(7)	C20	C21	C22	C23	-2.0(8)
C6	C7	C8	C9	0.1(7)	C21	C22	C23	C18	0.8(8)

C6	C7	C8	C12	179.7(5)	C23	C18	C19	C20	1.3(7)
C7	O3	C18	C19	8.5(7)	C24	C20	C21	C22	-177.1(5)
C7	O3	C18	C23	-173.1(4)	C24	C20	C21	C25	1.9(7)
C7	C8	C9	O1	179.0(4)	C25	C21	C22	C23	179.0(5)

Table S7 Some calculated DFT parameters of compounds **2** and **2d**.

Properties		
Electronic Energy (E)	-23061.20	-34368.22
Dipole Moment (μ)	5.73	8.43
Polarizability (α)	188.90	297.33
LUMO Energy (E_{LUMO})	-1.39	-2.23
HOMO Energy (E_{HOMO})	-5.84	-6.58
Band Gap (E_{GAP})	4.45	4.34
Ionization Potential (IP)	1.39	2.23
Electron Affinity (EA)	5.84	6.58
Electronegativity (χ)	3.62	4.41
Chemical Hardness (η)	2.23	2.18
Global Softness (σ)	0.22	0.23
Electrophilicity index (ω)	2.94	4.46

Equations and notes

$E_{GAP} = E_H – E_L$	$IP = –E_{HOMO}$	$EA = –E_{LUMO}$	$\chi = (IP + EA)/2$
$\eta = (EA – IP)/2$	$\sigma = 1/(2\eta)$	$\omega = \chi^2/(2\eta)$	

Dipole moment unit is Debye (D). Polarizability unit is Hartree (a.u.). HOMO and LUMO energy, Energy gap, Electron affinity, Ionization potential, Chemical hardness, Global softness, Electronegativity and Electrophilicity index unit is Electron Volt (eV).