Supplementary Material

Synthesis, structural characterization, biological activity and molecular docking study of 4,7-dihydroxycoumarin modified by aminophenols derivatives

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Table S1. The experimental and theoretical bond lengths

Bond distance (Å)	Experimental	Theoretical		
	3b	**3a**	**3b**	**3c**
O1–C2	1.376 (4)	1.396	1.395	1.395
C2–C3	1.436 (4)	1.457	1.458	1.458
C3–C4	1.436 (4)	1.452	1.453	1.452
C4–C10	1.472 (4)	1.467	1.466	1.467
C10–C5	1.386 (5)	1.403	1.402	1.402
C5–C6	1.378 (5)	1.382	1.382	1.382
C6–C7	1.376 (5)	1.398	1.398	1.399
C7–C8	1.361 (6)	1.383	1.383	1.383
C8–C9	1.378 (5)	1.394	1.394	1.394
C9–C10	1.374 (5)	1.394	1.394	1.394
C9–O1	1.375 (4)	1.360	1.360	1.360
C3–C1'	1.424 (4)	1.422	1.422	1.423
O4—C7	1.412 (4)	1.392	1.391	1.392
O4—C3'	1.288 (5)	1.375	1.375	1.375
O5—C3'	1.192 (6)	1.999	1.199	1.199
C3'—C4'	1.488 (6)	1.503	1.503	1.503
C1'– C2'	1.485 (4)	1.496	1.499	1.500
C1'– N1	1.321 (4)	1.333	1.334	1.333
N1–C1"	1.443 (4)	1.419	1.418	1.420
C1"– C2"	1.375 (5)	1.403	1.393	1.394
C2"– C3"	1.388 (4)	1.394	1.393	1.391
C3"– C4"	1.374 (5)	1.392	1.396	1.396
C4"– C5"	1.381 (5)	1.393	1.392	1.396
C5"– C6"	1.380 (5)	1.391	1.390	1.387
C6"– C1"	1.373 (5)	1.394	1.398	1.397
C2–O2	1.209 (4)	1.208	1.208	1.208
C4–O3	1.249 (4)	1.250	1.250	1.250
C2"–O6	/	1.363	/	/
C3"–O6	1.356 (4)	/	1.365	/
C4"–O6	/	/	/	1.365
AAE (Å)	**/**	**/**	**0.02**	**/**
R	**/**	**/**	**0.97**	**/**

Table S2. The experimental and theoretical bond angles

Bond angle (°)	Experimental	Theoretical		
	3b	**3a**	**3b**	**3c**
C9–O1–C2	121.9 (3)	123.0	123.0	123.0
O1–C9–C10	121.7 (3)	122.1	122.1	122.1
O1–C2–C3	119.5 (3)	117.6	117.6	117.6
O1–C2–O2	113.2 (3)	115.0	115.1	115.0
C3–C2–O2	127.3 (3)	127.5	127.3	127.4
C2–C3–C4	120.0 (3)	120.7	120.6	120.7
C2–C3–C1'	119.6 (3)	118.9	118.9	118.9
C4–C3–C1'	120.4 (3)	120.4	120.5	120.4
C3–C4–C10	116.9 (3)	116.9	116.9	116.9
C3–C4–O3	123.9 (3)	123.7	123.6	123.6
C10–C4–O3	119.2 (3)	119.4	119.5	119.5
C4–C10–C5	121.7 (3)	121.5	121.5	121.5
C4–C10–C9	119.9 (3)	119.7	119.7	119.7
C5–C10–C9	118.4 (3)	118.9	118.8	118.8
C10–C5–C6	120.7 (4)	121.0	121.0	121.0
C5–C6–C7	118.6 (4)	118.6	118.6	118.6
C6–C7–C8	122.4 (4)	122.0	122.0	122.0
C7–C8–C9	117.9 (4)	118.4	118.4	118.4
C8–C9–C10	122.0 (3)	121.2	121.2	121.2
C8–C9–O1	116.3 (3)	116.7	116.7	116.7
C8—C7—O4	117.1 (4)	116.6	116.5	116.5
C6—C7—O4	120.2 (4)	121.3	121.4	121.4
O5—C3'—O4	120.3 (5)	123.7	123.7	123.7
O5—C3'—C4'	125.0 (5)	126.6	126.7	126.6
O4—C3'— C4'	114.6 (5)	109.6	109.6	109.6
C3–C1'–N1	118.9 (3)	118.2	118.0	118.2
C3–C1'–C2'	124.0 (3)	123.5	123.2	123.2
N1–C1'–C2'	117.1 (3)	118.2	118.7	118.6
C1'–N1–C1"	125.3 (3)	127.5	128.9	128.4
N1–C1"–C2"	119.1 (3)	120.8	121.1	121.7
C1"–C2"–C3"	119.7 (3)	119.7	119.5	120.3
C2"–C3"–C4"	119.9 (3)	120.3	120.4	120.0
C3"–C4"–C5"	119.5 (3)	120.3	119.4	119.9
C4"–C5"–C6"	121.0 (3)	119.5	120.8	119.8
C5"–C6"– C1"	118.5 (3)	120.8	119.2	120.6
C6"-C1"-N1	119.5 (3)	119.6	118.2	118.8

C1"–C2"–O6	/	117.5	/	/
O6–C2"– C3"	/	122.9	/	/
C2"–C3"–O6	122.8 (3)	/	116.8	/
O6–C3"– C4"	117.6 (3)	/	122.8	/
C3"–C4"–O6	/	/	/	122.8
O6–C4"– C5"	/	/	/	117.3
AAE (º)	**/**	**/**	**0.91**	**/**
R	**/**	**/**	**0.97**	**/**

Table S3. The experimental and theoretical dihedal angles

Dihedral angle (º)	Experimental	Theoretical		
	3b	**3a**	**3b**	**3c**
O3—C4—C10—C9	-178.0 (3)	179.4	179.6	179.6
C3—C4—C10—C9	1.6 (5)	-0.3	0.4	0.3
O3—C4—C10—C5	1.8 (5)	-0.4	0.2	0.2
C3—C4—C10—C5	-178.7 (3)	179.9	-179.0	-179.1
C1'—C3—C4—O3	-2.7 (5)	0.7	0.2	-1.3
C9—O1—C2—O2	179.8 (3)	178.0	176.8	176.4
C9—O1—C2—C3	-0.9 (3)	-1.8	-2.8	-2.9
C4—C3—C2—O2	-178.5 (5)	-178.1	-175.5	-175.5
C1'—C3—C2—O2	-178.0 (3)	0.9	3.9	3.7
C1'—C3—C4—C10	177.8 (3)	-179.6	177.8	178.0
C2—C3—C4—O3	176.9 (3)	179.9	178.0	178.0
C2—C3—C4—C10	-2.7 (5)	-0.6	-2.8	-2.8
O1—C9—C8—C7	179.5 (3)	-179.0	-179.3	-179.3
C2—O1—C9—C10	-0.2 (5)	0.9	0.4	0.4
O1—C9—C8—C7	-179.5 (3)	179.9	179.7	179.7
C10—C9—C8—C7	0.2 (6)	-0.1	-0.1	-0.1
C5—C10—C9—O1	-179.9 (3)	-179.9	-179.7	-179.7
C4—C10—C9—O1	179.2 (3)	0.2	0.8	0.9
C5—C10—C9—C8	-0.6 (5)	0.1	0.1	0.1
C4—C10—C9—C8	179.2 (3)	-179.9	-179.4	-179.4
C9—C8—C7—C6	0.1 (6)	0.2	0.1	0.1
C4—C3—C2—O1	2.4 (5)	1.6	4.0	4.0
C1'—C3—C2—O1	-178.0 (3)	-179.4	-176.6	-176.7
C9—C10—C5—C6	0.8 (5)	0.0	-0.1	-0.1
C4—C10—C5—C6	-179.0 (3)	179.8	179.3	179.3
C10—C5—C6—C7	-0.5 (6)	0.1	0.2	0.2
C8—C7—C6—C5	0.1 (6)	-0.2	-0.2	-0.2

C4—C3— C1'— C2'	-179.6 (3)	-176.9	-173.5	-174.1
C2—C3— C1'— C2'	0.8 (5)	4.0	7.1	6.7
C9—C8—C7—O4	-173.8 (3)	176.5	176.4	176.4
C3'—O4—C7—C8	-96.7 (5)	125.2	126.4	126.2
C7—O4—C3'—O5	-3.5 (8)	-1.4	-1.4	-1.4
C7—O4—C3'—C4'	179.1 (4)	179.1	179.0	179.0
C1'—N1—C1''—C2''	-78.6 (4)	-61.9	-51.7	-55.5
C1'— N1— C1"— C6"	101.9 (4)	122.9	132.1	128.3
N1— C1"— C2"— C3"	179.7 (3)	-176.8	-177.7	-177.7
N1— C1"— C6"— C5"	-179.8 (3)	176.4	177.3	-177.3
N1— C1"— C2"—O6	/	3.1	/	/
O6— C2"— C3"— C4"	/	-178.7	/	/
O6—C3''—C2''—C1''	-179.8 (3)	/	-179.7	/
O6—C3''—C4''—C5''	-178.8 (3)	/	-179.2	/
C2"— C3"— C4"—O6	/	/	/	179.8
O6— C4"— C5"— C6"	/	/	/	179.7
C1"— C6"— C5"— C4"	0.3 (3)	-0.1	0.1	0.1
C2''— C3''— C4''— C5''	1.1 (5)	-0.1	0.1	0.1
C3''— C4''— C5''— C6''	-1.2 (6)	-0.4	-0.7	-0.1
AAE (°)	/	/	**3.13**	/
R	/	/	**0.96**	/

Table S4. The experimental and calculated chemical shifts (ppm) in the ^{1}H NMR septrum of investigated compounds

^{1}H NMR Compound	Experimental			Theoretical		
	3a	**3b**	**3c**	**3a**	**3b**	**3c**
C4'(CH_3)-3H	2.32	2.32	2.31	2.36	2.39	2.36
C2'(CH_3)-3H	2.61	2.63	2.56	2.63	2.86	2.62
C6"-H	7.15	6.81	6.88	7.67	7.12	7.49
C8-H	7.15	7.20	7.23	7.14	7.10	7.10
C2"-H	/	7.20	6.88	/	7.11	7.49
C6-H	7.15	7.20	7.23	7.32	7.25	7.18
C4"-H	7.15	6.81	/	7.72	7.02	/
C3"-H	6.94	/	7.12	7.12	/	7.32
C5"-H	7.15	6.81	7.12	7.39	7.63	7.10
C5-H	8.03	8.01	8.00	8.41	8.46	8.47
N1-H	15.17	15.37	15.24	15.39	15.14	15.08
AAE	/	/	/	**0.24**	**0.21**	**0.23**
R	/	/	/	**0.999**	**0.998**	**0.998**

Table S5. The experimental and calculated chemical shifts (ppm) in the ^{13}C NMR spectrum of investigated compounds

^{13}C NMR Compound	Experimental			Theoretical		
	3a	**3b**	**3c**	**3a**	**3b**	**3c**
C2' (CH_3)	20.59	20.63	20.49	17.55	17.89	17.88
C4'(CH_3)	21.08	21.06	21.05	16.87	16.23	16.26
C3	96.69	96.92	96.73	97.00	96.92	97.58
C8	109.88	112.46	109.84	108.57	110.15	110.26
C10	116.64	116.14	116.09	117.42	117.98	118.13
C3"	117.75	154.93	117.71	114.07	158.79	114.56
C6	118.07	119.17	118.04	117.82	118.63	117.85
C5"	119.12	126.72	117.71	120.31	131.52	114.56
C6"	119.49	117.61	126.85	128.32	116.66	128.03
C4''	123.25	115.47	153.82	130.57	113.07	158.75
C1''	127.16	130.53	127.10	123.49	139.41	129.50
C5	129.65	127.15	127.00	126.61	127.88	128.11
C2''	151.54	109.88	126.85	152.99	112.64	128.03
C7	153.86	136.81	154.83	157.78	159.35	159.13
C9	154.87	153.86	157.35	157.72	156.99	156.87
C2	161.42	158.36	161.48	161.91	163.05	162.97
C1'	168.68	168.64	168.64	179.80	177.63	177.74
C3'	176.02	175.75	175.75	172.45	175.02	175.12
C4	179.60	179.70	179.50	181.46	181.47	181.42
AAE	/	/	/	**3.31**	**4.13**	**2.42**
R	/	/	/	**0.996**	**0.993**	**0.998**

Table S6. The experimental, unscaled and scaled theoretical wavelengths and PED analysis parameters for **3a**

Mode	**Assignments of 3a**	**Exp. values**	**B3LYP-D3BJ/6-311++g(d,p)**		
		IR (cm^{-1})	**Calc. (Unscaled) (cm^{-1})**	**Calc. (Scaled) (cm^{-1})**	**PED (%) of 3a**
92	OH stretching (C)	**3220**	3637	3517	ν_{OH}(100)
91	HC stretching (A)		3112	3009	ν_{HC}(98)

90	HC stretching (A)		3109	3006	$\nu_{HC}(98)$
89	HC stretching (A)		3096	2994	$\nu_{HC}(99)$
88	HC stretching (C)		3095	2993	$\nu_{HC}(98)$
87	HC stretching (C)		3081	2979	$\nu_{HC}(97)$
86	HC stretching (C)		3074	2973	$\nu_{HC}(98)$
85	HC stretching ($-CH_3$, A)		3055	2954	$\nu_{HC}(98)$
84	HC stretching (C)		3051	2950	$\nu_{HC}(98)$
83	HC stretching ($-CH_3$, B)		3046	2946	$\nu_{HC}(99)$
82	HC stretching ($-CH_3$, B)		3027	2927	$\nu_{HC}(99)$
81	HC stretching ($-CH_3$, A)		3009	2910	$\nu_{HC}(100)$
80	HC stretching ($-CH_3$, B) NH stretching (NH)		2996	2897	$\nu_{CH}(85) + \nu_{NH}(6)$
79	NH stretching (NH) NHO bending HO Hbond stretching	**3084**	2963	2865	$\nu_{NH}(76) + \delta_{NHO}(6) + \nu_{HO}(4)$
78	HC stretching ($-CH_3$, A)		2951	2854	$\nu_{CH}(99)$
77	C=O stretching (A) CC stretching (A) CCO bending (A)	**1767**	1780	1721	$\nu_{C=O}(87) + \nu_{CC}(4) + \delta_{CCO}(2)$
76	C=O stretching (B) CC stretching (B) CCO bending (B)	**1710**	1732	1675	$\nu_{C=O}(85) + \nu_{CC}(5) + \delta_{CCO}(3)$
75	CNH bending CO stretching (C) CC stretching (C)	**1605**	1625	1571	$\delta_{CNH}(11) + \nu_{CO}(16) + \nu_{CC}(19)$
74	CNH bending HNC bending CC stretching (A, B)		1619	1566	$\delta_{CNH}(10) + \delta_{HNC}(17) + \nu_{CC}(7)$
73	CC stretching (A, B)	**1614**	1611	1558	$\nu_{CC}(39)$
72	CC stretching (A, B)		1600	1547	$\nu_{CC}(42)$
71	CNH bending HNC bending CC stretching (A, B)		1594	1541	$\delta_{CNH}(12) + \delta_{HNC}(7) + \nu_{CC}(15)$
70	OC stretching (A,C) NC stretching (A,C)		1571	1519	$\nu_{OC}(32) + \nu_{NC}(14) + \nu_{CC}(13)$

	CC stretching (A,C)				
69	CCH bending (B)		1515	1465	δ_{CCH} (36)
68	CCH bending (A, C)	**1464**	1499	1450	δ_{CCH} (35)
67	CCH bending (B) CC stretching (B) COH bending (B)	**1442**	1478	1429	δ_{CCH}(17) + ν_{CC}(7) + δ_{COH}(7)
66	CCH bending (-CH_3) CC stretching (C)		1463	1415	δ_{CCH}(46) + ν_{CC}(6)
65	OC stretching (A) CC stretching (A) HCC bending (-CH_3) CCH bending (-CH_3 A)		1448	1400	ν_{OC} (8) + ν_{CC} (7) + δ_{HCC}(6) + δ_{CCH}(5)
64	HCH bending (-CH_3, A) HCCO torsion (w.t) (A)		1446	1398	δ_{CCH} (48) + τ_{HCCO} (17)
63	HCH bending (-CH_3, A) CCH bending (-CH_3, A)		1442	1394	δ_{HCH} (46) + δ_{CCH} (20)
62	HCH bending (-CH_3) CCH bending (-CH_3)		1440	1393	δ_{HCC} (48) + δ_{CCH} (17)
61	HCH bending (-CH_3) CCH bending (-CH_3) NC stretching		1421	1374	δ_{HCH} (29) + δ_{CCH} (13) + ν_{NC} (9)
60	CCH bending (-CH_3) HCH bending (-CH_3)		1383	1337	δ_{CCH} (35) + δ_{HCH} (48)
59	CCH bending (-CH_3, A) HCH bending (-CH_3, A)	**1346**	1373	1328	δ_{CCH} (35) + δ_{HCH} (34)
58	CC stretching (C) OC stretching (C) NC stretching (C)		1346	1302	ν_{CC} (20) + ν_{OC} (11) + ν_{NC} (6)
57	CC stretching (A)		1341	1297	ν_{CC} (60)
56	COH bending (B) CC stretching (B) CCH bending (B)		1330	1286	δ_{CCH} (28) + ν_{CC} (11) + δ_{CCH} (7)
55	CC stretching (A ,B) CCH bending (A, B)		1304	1261	ν_{CC} (21) + δ_{CCH} (8)
54	CCH bending (B) CC stretching (B)		1295	1252	δ_{CCH} (22) + ν_{CC} (18)
53	OC stretching (C) CC stretching (A,C) CCH bending (A,C)		1260	1218	ν_{OC} (30) + ν_{CC} (12) + δ_{CCH} (5)
52	OC stretching (A) CC stretching (A, C)		1251	1210	ν_{OC} (39) + ν_{CC} (11)
51	CN stretching CC stretching (A, B) CCH bending (A, B)		1246	1205	ν_{CN} (11) + ν_{CC} (13) + δ_{CCH} (7)

50	CN stretching CC stretching (A, B) CCH bending (A, B)		1237	1196	ν_{CN} (8) + ν_{CC} (8) + δ_{CCH} (18)
49	CN stretching CC stretching (A, B) CCH bending (A, B)		1198	1158	ν_{CN} (6) + ν_{CC} (23) + δ_{CCH} (6)
48	CO stretching (C) CC stretching (A, B) CCH bending (B) CCO bending (B)	**1211**	1190	1151	ν_{CO} (23) + ν_{CC} (15) + δ_{CCH} (14) + δ_{CCO} (9)
47	COH bending (B) CC stretching (B) CCH bending (B)		1164	1126	δ_{COH} (29) + ν_{CC} (9) + δ_{CCH} (15)
46	CC stretching (A,C) CCH bending (A, C) OC stretching (A, C)	**1110**	1154	1116	ν_{CC} (22) + δ_{CCH} (10) + ν_{OC} (5)
45	OC stretching (A, B) CCH bending (A, B) HCC bending (A, B)		1131	1094	ν_{OC} (29) + δ_{CCH} (14) + δ_{HCC} (9)
44	OC stretching (A, B) CCH bending (A, B)		1115	1078	ν_{OC} (6) + δ_{CCH} (38)
43	COH bending (B) CCC bending (B) CC stretching (B)		1100	1064	δ_{COH} (13) + δ_{CCC} (22) + ν_{CC} (9)
42	CCH bending (-CH_3, A) HCCO torsion (w.t) (-CH_3, A)		1048	1013	δ_{CCH} (57) + τ_{HCCO} (29)
41	CC stretching (B) CCH bending (B)		1043	1009	ν_{CC} (42) + δ_{CCH} (6)
40	CCH bending (-CH_3) HCCN torsion (w.t) (B) CC stretching (B)	**1026**	1040	1006	δ_{CCH} (46) + τ_{HCCN} (13) + ν_{CC} (5)
39	OC stretching (C) CC stretching (B) CCH bending (A, B, -CH_3) CCC stretching (B)		1009	976	ν_{OC} (10) + ν_{CC} (7) + δ_{CCH} (7) + δ_{CCC} (5)
38	CCH bending (A, B) CC stretching (B, -CH_3)		1005	972	δ_{CCH} (30) + ν_{CC} (5)
37	OC stretching (C) CC stretching (A, C) CCH bending (A, C)		991	958	ν_{OC} (8) + ν_{CC} (6) + δ_{CCH} (10)
36	HCCC torsion (w.t) (B) CCCH torsion (w.t) (B)		971	939	τ_{HCCC} (64) + τ_{CCCH} (5)
35	HCCH torsion (w.t) (A, C)		970	938	τ_{HCCH} (40) + τ_{CCCH} (28)

	CCCH torsion (w.t) (A, C)				
34	OC stretching (C) OCO bending (A, C) CCO bending (A, C) CC stretching (A, B)		956	924	ν_{OC} (20) + δ_{OCO} (5) + δ_{CCO} (5) + ν_{CC} (5)
33	HCCH torsion (w.t) (B) HCCN torsion (w.t) (B) CCCH torsion (w.t) (B)		936	905	τ_{HCCH} (36) + τ_{CCCN} (11) + τ_{CCCH} (9)
32	OHNC torsion NHOC torsion HNCC torsion		915	885	τ_{OHNC} (40) + τ_{NHOC} (19) + τ_{NHCC} (11)
31	CO stretching (B,C) OCCH torsion (w.t) (A, B) CC stretching COC bending (A, B)		901	871	ν_{CO} (29) + τ_{OCCH} (8) + ν_{CC} (8) + δ_{COC} (5)
30	CC stretching (B,C) CCC bending (A, B) COH bending (A, C)		884	855	ν_{CC} (15) + δ_{CCC} (5) + δ_{COH} (5)
29	HCCO torsion (w.t) (B) OCCH torsion (w.t) (B) CCCH torsion (w.t) (B) HCCC torsion (w.t) (B)		860	832	τ_{HCCO} (19) + τ_{OCCH} (18) + τ_{CCCH} (10) + τ_{HCCC} (10)
28	CC stretching (B) COH bending (C) OC stretching (B) HCCO torsion (w.t) (C, B)		859	831	ν_{CC} (22) + δ_{COH} (4) + ν_{OC} (4) + τ_{HCCO} (4)
27	HCCO torsion (w.t) (B) CCCH torsion (w.t) (B) HCCC torsion (w.t) (B)		839	811	τ_{HCCO} (12) + τ_{CCCH} (8) + τ_{HCCC} (12)
26	OCCH torsion (w.t) (A) HCCC torsion (w.t) (A) CCCH torsion (w.t) (A)		827	800	τ_{OCCH} (15) + τ_{HCCC} (23) + τ_{CCCH} (8)
25	CO stretching (C) OC stretching (C) CC stretching (A)		792	766	ν_{CO} (6) + ν_{OC} (6) + ν_{CC} (8)
24	CO stretching (C) OC stretching (C) CC stretching (B) CCC bending (B)		784	758	ν_{CO} (12) + ν_{OC} (9) + ν_{CC} (6) + δ_{CCC} (4)
23	CCCC torsion (A,B, C) CCCO torsion (C) OCCC torsion (C)	**735**	768	743	τ_{CCCC} (7) + τ_{CCCO} (5) + τ_{OCCC} (12)
22	HCCC torsion (w.t) (B) HCCO torsion (w.t) (B) CCCH torsion (w.t) (B)		748	723	τ_{HCCC} (27) + τ_{HCCO} (11) + τ_{CCCH} (10)

21	HCCC torsion (w.t) (B) OCCN torsion (w.t) (B) CCCC torsion (w.t) (B) CC stretching (B)		740	716	τ_{HCCC} (5) + τ_{OCCN} (5) + τ_{CCCO} (4) + ν_{CC} (4)
20	CCCO torsion (w.t) (B) COCC torsion (w.t) (B)		733	709	τ_{CCCO} (40) + τ_{COCC} (8)
19	CC stretching (A,B) OCO bending (A, B, C) CCC bending (A, B, C)		707	684	ν_{CC} (13) + δ_{OCO} (8) + δ_{CCC} (4)
18	CC stretching (A,B) CCC bending (A, B, C) OC stretching (A,B)		695	672	ν_{CC} (15) + δ_{CCC} (7) + ν_{OC} (3)
17	CCN bending (A, C) CCO bending (A, C) OCO bending (A, C)		688	665	δ_{CCN} (5) + δ_{CCO} (10) + δ_{OCO} (4)
16	CCCC torsion (w.t) (A, C) HCCC torsion (w.t) (A, C)		676	654	τ_{CCCC} (16) + τ_{HCCC} (5)
15	CCC bending (A, B, C) CCO bending (C)		650	629	δ_{CCC} (15) + δ_{CCO} (3)
14	CCCC torsion (w.t) (A, C) CCCH torsion (w.t) (A, C) OCOC torsion (w.t) (A, C) COCC torsion (w.t) (A, C)		612	592	τ_{HCCC} (6) + τ_{CCCC} (6) + τ_{HCCC} (4) + τ_{CCCC} (4)
13	CCC bending (A, B, C) CCO bending (C) CC stretching (A, B, C)		592	572	δ_{CCC} (12) + δ_{CCO} (5) + ν_{CC} (5)
12	OCOC torsion (w.t) (A,C=O) HCCO torsion (w.t) (A, C=O)		580	561	τ_{OCOC} (8) + τ_{HCCO} (22)
11	HCCC torsion (w.t) (A, C) HCCO torsion (w.t) (A, C) OCOC torsion (w.t) (A, C)		576	557	τ_{HCCC} (5) + τ_{HCCO} (8) + τ_{OCOC} (4)
10	CCC bending (B) CC stretching (B)		559	541	δ_{CCC} (19) + ν_{CC} (5)
9	CCCC torsion (B) HCCC torsion (B)		553	535	τ_{CCCC} (16) + τ_{HCCC} (4)
8	CC stretching (A, C) CCO bending (A, C) CCC bending (A, C) COH bending (A, C)		526	509	ν_{CC} (12) + δ_{CCO} (9) + δ_{CCC} (6) + δ_{COH} (4)
7	CCN bending CCO bending (A, B, C)		512	495	δ_{CCN} (8) + δ_{CCO} (15)

6	CCO bending (B) NCC bending CCC bending (B) OCCC torsion (B)		478	462	δ_{CCO} (10) + δ_{NCC} (6) + δ_{CCC} (4) + τ_{OCCC} (3)
5	CCO bending (C) NCC bending CCN bending CCCC torsion (A, C)		465	450	δ_{CCO} (10) + δ_{NCC} (8) + δ_{CCN} (4) + τ_{CCCC} (4)
4	CCCC torsion (A, C) OCCC torsion (A, C) CCCO torsion (A, C)		458	443	τ_{CCCC} (20) + τ_{OCCC} (5) + τ_{CCCO} (4)
3	CCO bending (B) CC stretching (A, C) COC bending (B)	**445**	457	442	δ_{CCO} (23) + ν_{CC} (9) + δ_{COC} (7)
2	COH bending (A) HO H bending CCO bending (A,C) OCO bending (A,C)		438	424	δ_{COH} (11) + ν_{HO} (10) + δ_{CCO} (8) + δ_{OCO} (7)
1	CCO bending (A) CCC bending (A)		409	396	δ_{CCO} (34) + δ_{CCC} (4)
R		**0.991**			

Table S7. The experimental, unscaled and scaled theoretical wavelengths and PED analysis parameters for **3b**

Mode	**Assignments of 3b**	**Exp. values**	**B3LYP-D3BJ/6-311++g(d,p)**		
		IR (cm^{-1})	**Calc. (Unscaled) (cm^{-1})**	**Calc. (Scaled) (cm^{-1})**	**PED (%) of 3b**
93	OH stretching (C)	**3342**	3642	3522	ν_{OH} (100)
92	CH stretching (A)		3093	2991	ν_{CH}(83)
91	CH stretching (A)		3089	2987	ν_{CH}(99)
90	CH stretching (C)		3083	2981	ν_{CH}(99)
89	CH stretching (A)		3076	2975	ν_{CH}(99)
88	CH stretching (C)		3074	2973	ν_{CH}(99)
87	CH stretching (C)		3057	2956	ν_{CH}(90)
86	CH stretching (C)		3036	2936	ν_{CH}(98)

85	CH stretching (-CH_3, A)		3035	2935	$\nu_{CH}(99)$
84	CH stretching (-CH_3, B)		3035	2935	$\nu_{CH}(98)$
83	CH stretching (-CH_3, B)		3001	2902	$\nu_{CH}(99)$
82	CH stretching (-CH_3, A)		2990	2891	$\nu_{CH}(100)$
81	CH stretching (-CH_3, B) NH stretching (NH)		2942	2845	$\nu_{CH}(97) + \nu_{NH}(1)$
80	NH stretching (NH) NHO bending HO Hbond stretching	**2838**	2933	2836	$\nu_{NH}(81) + \delta_{NHO}(11) + \nu_{HO}(4)$
79	CH stretching (-CH_3, A)		2931	2834	$\nu_{CH}(99)$
78	C=O stretching (A) CC stretching (A) CCO bending (A)	**1764**	1768	1710	$\nu_{C=O}(87) + \nu_{CC}(4) + \delta_{CCO}(3)$
77	C=O stretching (B) CC stretching (B) CCO bending (B)	**1677**	1720	1663	$\nu_{C=O}(80) + \nu_{CC}(4) + \delta_{CCO}(4)$
76	CNH bending (C) CO stretching (C) NHO bending		1629	1575	$\delta_{CNH}(43) + \nu_{CO}(9) + \delta_{NHO}(15)$
75	CC stretching (A, B)	**1620**	1613	1560	$\nu_{CC}(50)$
74	CC stretching (A, B)		1608	1555	$\nu_{CC}(36)$
73	CC stretching (A, B)		1592	1539	$\nu_{CC}(36)$
72	CC stretching (A, B)		1581	1529	$\nu_{CC}(47)$
71	OC stretching (A,C) NC stretching (A,C) CC stretching (A,C)		1561	1510	$\nu_{OC}(32) + \nu_{NC}(13) + \nu_{CC}(12)$
70	CCH bending (A, B)		1497	1448	$\delta_{CCH}(19)$
69	CCH bending (A, C)		1492	1443	$\delta_{CCH}(24)$
68	CCH bending (B) CC stretching (B) COH bending (B)	**1467**	1480	1431	$\delta_{CCH}(17) + \nu_{CC}(7) + \delta_{COH}(7)$
67	HCH bending (-CH_3) CCH bending (-CH_3) NC stretching (C) CC stretching (C)		1471	1422	$\delta_{HCH}(15) + \delta_{CCH}(8) + \nu_{NC}(8) + \nu_{CC}(5)$
66	HCH bending (-CH_3) OC stretching (A) CC stretching (A)		1445	1397	$\delta_{HCH}(21) + \nu_{OC}(5) + \nu_{CC}(5)$

65	HCH bending (-CH_3, A) HCCH torsion (w.t) (A)		1444	1396	δ_{CCH} (35) + τ_{HCCH} (12)
64	HCH bending (-CH_3) CCH bending (-CH_3) HCCH torsion (w.t)		1440	1393	δ_{HCC} (48) + δ_{CCH} (11) + τ_{HCCH} (8)
63	HCH bending (-CH_3, A) CCH bending (-CH_3 A)		1439	1392	δ_{HCC} (45) + δ_{CCH} (21)
62	HCH bending (-CH_3, A) NC stretching (b-II) CCH bending (-CH_3 A)		1419	1372	δ_{HCH} (22) + ν_{NC} (12) + δ_{CCH} (11)
61	CCH bending (-CH_3) HCH bending (-CH_3)		1383	1337	δ_{CCH} (49) + δ_{HCH} (35)
60	CCH bending (-CH_3, A) HCH bending (-CH_3, A)	**1338**	1369	1324	δ_{CCH} (35) + δ_{HCH} (33)
59	CC stretching (C) OC stretching (C) NC stretching (C)		1341	1297	ν_{CC} (21) + ν_{OC} (12) + ν_{NC} (6)
58	CC stretching (A)		1333	1289	ν_{CC} (60)
57	CC stretching (B) CCH bending (B)		1315	1272	ν_{CC} (22) + δ_{CCH} (17)
56	COH bending (B) CC stretching (B) CCH bending (B)		1312	1269	δ_{COH} (17) + ν_{CC} (10) + δ_{CCH} (6)
55	CC stretching (C) OC stretching (C) NC stretching (C)		1297	1254	ν_{CC} (22) + ν_{OC} (5) + ν_{NC} (6)
54	OC stretching (C) CC stretching (A,C) NC stretching (C) CCH bending (A,C)		1265	1223	ν_{OC} (15) + ν_{CC} (7) + ν_{NC} (6) + δ_{CCH} (4)
53	CC stretching (A, C) OC stretching (A) CCH bending (A, C)		1245	1204	ν_{CC} (21) + ν_{OC} (12) + δ_{CCH} (6)
52	CCH bending (A) CC stretching (A, C)		1235	1194	δ_{HCC} (30) + ν_{CC} (11)
51	CC stretching (A, B) OC stretching (A, B) CCH bending (A, B)	**1207**	1211	1171	ν_{CC} (17) + ν_{OC} (7) + δ_{CCH} (4)
50	CO stretching (A, B) CC stretching (A, B) CCH bending (B) CCO bending (A, B)		1186	1147	ν_{CO} (21) + ν_{CC} (16) + δ_{CCH} (15) + δ_{CCO} (10)
49	COH bending (A, B) CC stretching (B) CCH bending (B)		1180	1141	δ_{COH} (27) + ν_{CC} (9) + δ_{CCH} (16)

48	COH bending (B) CCH bending (B)		1160	1122	δ_{COH} (17) + δ_{CCH} (32)
47	CCH bending (A, B) OC stretching (A, B) CN stretching (A, C)		1152	1114	δ_{CCH} (17) + ν_{OC} (8) + ν_{CN} (7)
46	CC stretching (A,B) CCH bending (A, B) OC stretching (A, B)		1148	1110	ν_{CC} (12) + δ_{CCH} (9) + ν_{OC} (9)
45	OC stretching (A, B) CCH bending (A, B)		1124	1087	ν_{OC} (25) + δ_{CCH} (18)
44	CCH bending (A, B) OC stretching (A, B)		1111	1074	δ_{CCH} (37) + ν_{OC} (7)
43	CC stretching (B) CCH bending (B)	**1045**	1087	1051	ν_{CC} (33) + δ_{CCH} (28)
42	CCH bending (-CH_3, A) HCCO torsion (w.t) (-CH_3, A)		1046	1011	δ_{CCH} (57) + τ_{HCCO} (29)
41	CCH bending (-CH_3) HCCN torsion (w.t) (B) HCCO torsion (w.t) (A)		1037	1003	δ_{CCH} (57) + τ_{HCCN} (15) + τ_{HCCO} (6)
40	CCH bending (A, B) CC stretching (B) OC stretching (C)	**999**	1007	974	δ_{CCH} (28) + ν_{CC} (5) + ν_{OC} (5)
39	CCH bending (A, B) CC stretching (B) OC stretching (C)		1005	972	δ_{CCH} (11) + ν_{CC} (5) + ν_{OC} (11)
38	CC stretching (B) CCC bending (A, B) CCH bending (A, B)		999	966	ν_{CC} (10) + δ_{CCC} (5) + δ_{CCH} (4)
37	OC stretching (C) CC stretching (B) CCH bending (A, B)		994	961	ν_{OC} (9) + ν_{CC} (14) + δ_{CCH} (5)
36	CCC bending (A, B) OCO bending (A, B) CN stretching CC stretching (B)		974	942	δ_{CCC} (4) + δ_{OCO} (4) + ν_{CN} (3) + ν_{CC} (3)
35	HCCC torsion (w.t) (A) CCCH torsion (w.t) (A)		968	936	τ_{HCCC} (67) + τ_{CCCH} (10)
34	HCCH torsion (w.t) (B) CCCH torsion (w.t) (B) HCCC torsion (w.t) (B)	**904**	960	928	τ_{HCCH} (60) + τ_{CCCH} (10) + τ_{HCCC} (9)
33	OHNC torsion NHOC torsion OC stretching (B,C) HNCC torsion		938	907	τ_{OHNC} (20) + τ_{NHOC} (12) + ν_{OC} (9) + τ_{NHCC} (7)
32	OHNC torsion		936	905	τ_{OHNC} (11) + τ_{NHOC}

	NHOC torsion OC stretching (B,C) CN stretching				(6) + ν_{OC} (9) + ν_{CN} (5)
31	CO stretching (B,C) OCCH torsion (w.t) (A, B) CC stretching COC bending (A, B)		898	868	ν_{CO} (28) + τ_{OCCH} (9) + ν_{CC} (7) + δ_{COC} (5)
30	HCCN torsion (w.t) (B) OCCH torsion (w.t) (B) CCCH torsion (w.t) (B) HCCC torsion (w.t) (B)		878	849	τ_{HCCN} (21) + τ_{OCCH} (19) + τ_{CCCH} (11) + τ_{HCCC} (9)
29	CC stretching (B) OCCH torsion (w.t) (B) HCCH torsion (w.t) (C, B) HCCO torsion (w.t) (C, B)		865	836	ν_{CC} (12) + τ_{OCCH} (7) + τ_{HCCH} (7) + τ_{HCCO} (7)
28	CC stretching (A, C) HCCH torsion (w.t) (A, C) HCCO torsion (w.t) (A, C) CCCH torsion (w.t) (A, C)		862	834	ν_{CC} (15) + τ_{HCCH} (7) + τ_{HCCO} (5) + τ_{CCCO} (5)
27	HCCO torsion (w.t) (A) OCCH torsion (w.t) (A) CCCH torsion (w.t) (A) HCCC torsion (w.t) (A)		858	830	τ_{HCCO} (19) + τ_{OCCH} (17) + τ_{CCCH} (10) + τ_{HCCC} (9)
26	OCCH torsion (w.t) (A) HCCC torsion (w.t) (A) CCCH torsion (w.t) (A)		823	796	τ_{OCCH} (16) + τ_{HCCC} (23) + τ_{CCCH} (8)
25	CO stretching (C) OC stretching (C) CC stretching (A) COC bending (C)		789	763	ν_{CO} (9) + ν_{OC} (8) + ν_{CC} (5) + δ_{COC} (5)
24	HCCO torsion (w.t) (B) HCCC torsion (w.t) (B) CCCH torsion (w.t) (B) HCCC torsion (w.t) (B)		783	757	τ_{HCCO} (10) + τ_{HCCC} (7) + τ_{CCCH} (7) + τ_{HCCC} (5)
23	CCCC torsion (A,B, C) CCCO torsion (C) OCCC torsion (C)		765	740	τ_{CCCC} (7) + τ_{CCCO} (11) + τ_{OCCC} (5)
22	OC stretching (B) CC stretching (B) CCCH torsion (w.t) (B) HCCO torsion (w.t) (B)		752	727	ν_{OC} (7) + ν_{CC} (6) + τ_{CCCH} (6) + τ_{HCCO} (5)
21	CCCO torsion (w.t) (B) COCC torsion (w.t) (B)		731	707	τ_{CCCO} (41) + τ_{COCC} (8)

20	COC bending (C) CNC bending CC stretching (A,B)		721	697	δ_{COC} (5) + δ_{CNC} (5) + ν_{CC} (8)
19	CC stretching (A,B) OC stretching (A,B) OCO bending (A, B, C) CCC bending (A, B, C)		703	680	ν_{CC} (8) + ν_{OC} (8) + δ_{OCO} (6) + δ_{CCC} (5)
18	CCC bending (A, C) CC stretching (A, C) CCH bending (A, C)		692	669	δ_{CCC} (12) + ν_{CC} (6) + δ_{CCH} (4)
17	HCCC torsion (w.t) (B) CCCC torsion (w.t) (B)		681	659	τ_{HCCC} (16) + τ_{CCCC} (14)
16	CCCC torsion (w.t) (A, C) HCCC torsion (w.t) (A, C)		677	655	τ_{CCCC} (11) + τ_{HCCC} (10)
15	CCC bending (A, B, C) CC stretching (A, B, C) CCO bending (C)		653	631	δ_{CCC} (9) + ν_{CC} (4) + δ_{CCO} (4)
14	CCCC torsion (w.t) (A, C) CCCH torsion (w.t) (A, C) OCOC torsion (w.t) (A, C) COCC torsion (w.t) (A, C)		612	592	τ_{HCCC} (6) + τ_{CCCC} (6) + τ_{HCCC} (4) + τ_{CCCC} (4)
13	HCCC torsion (w.t) (A, C) CCCC torsion (w.t) (A, C) OCCC torsion (w.t) (A, C)		595	575	τ_{HCCC} (6) + τ_{CCCC} (8) + τ_{OCCC} (4)
12	OCOC torsion (w.t) (A,C=O) HCCO torsion (w.t) (A, C=O)	**569**	581	562	τ_{OCOC} (12) + τ_{HCCO} (27)
11	CCO bending (C) OCO bending (C) CC stretching (A, B, C) CCC bending (A, B, C)		576	557	δ_{CCC} (10) + δ_{CCC} (8) + ν_{CC} (5) + δ_{CCC} (4)
10	HCCC torsion (w.t) (A, C) NCCC torsion (w.t) (A, C) CCCC torsion (w.t) (A, C) HCCN torsion (w.t) (A, C)		570	551	τ_{HCCC} (9) + τ_{NCCC} (6) + τ_{CCCC} (5) + τ_{HCCN} (5)
9	CCC bending (B) OC stretching (B)		534	516	δ_{CCC} (38) + ν_{OC} (12)
8	CC stretching (A, C) CCO bending (A, C) CCC bending (A, C)		526	509	ν_{CC} (13) + δ_{CCO} (8) + δ_{CCC} (10)
7	NCC bending CCC bending (A, B, C) CCO bending (C)		515	498	δ_{NCC} (8) + δ_{CCC} (13) + δ_{CCO} (5)

6	CCO bending (B) NCC bending		470	454	δ_{CCO} (30) + δ_{NCC} (24)
5	CCO bending (C) CC stretching (A, C) COC bending (C)	**441**	459	444	δ_{CCO} (19) + ν_{CC} (6) + δ_{COC} (5)
4	CCCC torsion (A, C) OCCC torsion (A, C) CCCO torsion (A, C)		458	443	τ_{CCCC} (17) + τ_{OCCC} (4) + τ_{CCCO} (4)
3	CCCC torsion (A, C) CCCO torsion (A, C) CCCN torsion (A, C)		456	441	τ_{CCCC} (16) + τ_{CCCO} (4) + τ_{CCCN} (3)
2	COH bending (A) HO H bending CCO bending (A,C) CCC bending (A,C)		441	426	δ_{COH} (12) + ν_{HO} (10) + δ_{CCO} (8) + δ_{CCC} (7)
1	CCO bending (A) CCC bending (A)		410	396	δ_{CCO} (33) + δ_{CCC} (4)
R		**0.998**			

Table S8. The experimental, unscaled and scaled theoretical wavelengths and PED analysis parameters for **3c**

Mode	**Assignments of 3c**	**Exp. values**	**B3LYP-D3BJ/6-311++g(d,p)**		
		IR (cm^{-1})	**Calc. (Unscaled) (cm^{-1})**	**Calc. (Scaled) (cm^{-1})**	**PED (%) of 3c**
92	OH stretching (C)	**3212**	3640	3520	ν_{OH} (100)
91	HC stretching (A)		3093	2991	ν_{HC}(98)
90	CH stretching (A)		3089	2987	ν_{CH}(99)
89	HC stretching (C)		3077	2976	ν_{HC}(97)
88	HC stretching (A)		3076	2975	ν_{HC}(98)
87	HC stretching (C)		3070	2969	ν_{HC}(97)
86	HC stretching (C)		3059	2958	ν_{HC}(99)
85	HC stretching (C)		3036	2936	ν_{HC}(98)
84	CH stretching (-CH_3, A)		3035	2935	ν_{CH}(98)
83	CH stretching (-CH_3, B)		3032	2932	ν_{CH}(98)

82	CH stretching (-CH_3, B)		3000	2901	$\nu_{CH}(100)$
81	CH stretching (-CH_3, A)		2990	2891	$\nu_{CH}(99)$
80	NH stretching (NH) NHO bending HO Hbond stretching	**2850**	2950	2853	$\nu_{NH}(81) + \delta_{NHO}(11) + \nu_{HO}(4)$
79	HC stretching (-CH_3) NH stretching (NH)		2941	2844	$\nu_{HC}(98) + \nu_{HN}(1)$
78	CH stretching (-CH_3, A)		2931	2834	$\nu_{CH}(99)$
77	C=O stretching (A) CC stretching (A) OCC bending (A) OCO bending (A)	**1768**	1768	1710	$\nu_{C=O}(84) + \nu_{CC}(2) + \delta_{OCC}(2) + \delta_{OCO}(1)$
76	C=O stretching (B) CC stretching (B) OCC bending (B) OCO bending (B)	**1716**	1718	1661	$\nu_{C=O}(79) + \nu_{CC}(5) + \delta_{OCC}(3) + \delta_{OCO}(1)$
75	CNH bending (C) CO stretching (C) NHO bending	**1618**	1624	1570	$\delta_{CNH}(43) + \nu_{CO}(13) + \delta_{NHO}(6)$
74	CC stretching (A, B)		1613	1560	$\nu_{CC}(31)$
73	CC stretching (A, B)	**1550**	1610	1557	$\nu_{CC}(33)$
72	CC stretching (A, B)		1593	1540	$\nu_{CC}(36)$
71	CC stretching (A, B)		1584	1532	$\nu_{CC}(51)$
70	OC stretching (A,C) NC stretching (A,C) CC stretching (A,C)		1562	1510	$\nu_{OC}(32) + \nu_{NC}(13) + \nu_{CC}(8)$
69	CCH bending (B)		1516	1466	$\delta_{CCH}(32)$
68	CCH bending (A)	**1442**	1495	1446	$\delta_{CCH}(37)$
67	HCH bending (-CH_3) NC stretching (C) CC stretching (C) CCN bending (-CH_3)		1474	1425	$\delta_{HCH}(13) + \nu_{NC}(11) + \nu_{CC}(9) + \delta_{CCN}(8)$
66	HCH bending (-CH_3) OC stretching (A) CC stretching (A,B) HCC bending (-CH_3)		1445	1397	$\delta_{HCH}(7) + \nu_{OC}(5) + \nu_{CC}(5) + \delta_{HCC}(4)$
65	HCH bending (-CH_3, A) HCCO torsion (w.t) (A)		1443	1395	$\delta_{HCH}(49) + \tau_{HCCO}(18)$
64	CCH bending (A, C) CC stretching (A, C)		1442	1394	$\delta_{CCH}(12) + \nu_{CC}(10)$

63	HCH bending (-CH_3, A) CCH bending (-CH_3 A)		1439	1392	δ_{HCC} (45) + δ_{CCH} (20)
62	HCH bending (-CH_3) NC stretching CCH bending (-CH_3)		1416	1369	δ_{HCH} (19) + ν_{NC} (12) + δ_{CCH} (9)
61	CCH bending (-CH_3) HCH bending (-CH_3)	**1346**	1382	1336	δ_{CCH} (34) + δ_{HCH} (49)
60	CCH bending (-CH_3, A) HCH bending (-CH_3, A)		1370	1325	δ_{CCH} (35) + δ_{HCH} (34)
59	CC stretching (A, C) OC stretching (C)		1343	1299	ν_{CC} (25) + ν_{OC} (11)
58	CC stretching (A, C)		1332	1288	ν_{CC} (53)
57	COH bending (B) CCH bending (B)		1331	1287	δ_{COH} (18) + δ_{CCH} (32)
56	CC stretching (B) CCH bending (B)	**1263**	1301	1258	ν_{CC} (6) + δ_{CCH} (32)
55	CC stretching (C) CN stretching (A, C)		1292	1249	ν_{CC} (23) + ν_{CN} (7)
54	OC stretching (C) CC stretching (C)		1253	1212	ν_{OC} (47) + ν_{CC} (20)
53	CC stretching (A, C) OC stretching (A)		1247	1206	ν_{CC} (27) + ν_{OC} (20)
52	CCH bending (A) CC stretching (A, C)		1239	1198	δ_{CCH} (28) + ν_{CC} (8)
51	CN stretching NHO bending CC stretching (A, B) CCH bending (A, C)		1227	1187	ν_{CN} (13) + δ_{NHO} (6) + ν_{CC} (5) + δ_{CCH} (5)
50	CC stretching (A, B) CN stretching (A, B) CCH bending (B)		1191	1152	ν_{CC} (20) + ν_{CN} (8) + δ_{CCH} (5)
49	CO stretching (C) CC stretching (B) CCH bending (B) CCO bending (C)	**1205**	1184	1145	ν_{CO} (20) + ν_{CC} (13) + δ_{CCH} (12) + δ_{CCO} (8)
48	COH bending (B) CCH bending (B) CC stretching (B)		1166	1128	δ_{COH} (11) + δ_{CCH} (25) + ν_{CC} (9)
47	COH bending (B) CCH bending (B) CC stretching (B)		1162	1124	δ_{COH} (39) + δ_{CCH} (16) + ν_{CC} (16)
46	CC stretching (A,B) CCH bending (A, B) OC stretching (A, B)		1149	1111	ν_{CC} (21) + δ_{CCH} (10) + ν_{OC} (5)
45	OC stretching (A, B)		1126	1089	ν_{OC} (27) + δ_{CCH} (21)

	CCH bending (A, B)				
44	CCH bending (A, B) OC stretching (A, B)		1112	1075	δ_{CCH} (36) + ν_{OC} (7)
43	CCH bending (B)	**1027**	1105	1069	δ_{CCH} (54)
42	CCH bending (-CH_3, A) HCCO torsion (w.t) (-CH_3, A)		1046	1011	δ_{CCH} (57) + τ_{HCCO} (29)
41	CCH bending (-CH_3) HCCN torsion (w.t) (B) HCCO torsion (w.t) (A)		1038	1004	δ_{CCH} (59) + τ_{HCCN} (15) + τ_{HCCO} (6)
40	CCH bending (A, B) CCC bending (A, B)		1015	982	δ_{CCH} (12) + δ_{CCC} (33)
39	CCH bending (A, B) CC stretching (B) OC stretching (C)		1006	973	δ_{CCH} (12) + ν_{CC} (7) + ν_{OC} (11)
38	CC stretching (B) CCH bending (A, B)		1003	970	ν_{CC} (5) + δ_{CCH} (31)
37	OC stretching (C) CC stretching (B) CCH bending (A, B)		989	956	ν_{OC} (8) + ν_{CC} (6) + δ_{CCH} (10)
36	HCCH torsion (w.t) (B) CCCH torsion (w.t) (B) HCCC torsion (w.t) (B)		968	936	τ_{HCCH} (40) + τ_{CCCH} (27) + τ_{HCCC} (10)
35	HCCH torsion (w.t) (B) HCCN torsion (w.t) (B) HCCC torsion (w.t) (B) OCCH torsion (w.t) (B)	**921**	957	925	τ_{HCCH} (34) + τ_{CCCN} (10) + τ_{HCCC} (8) + τ_{OCCH} (6)
34	CO stretching (C) OCO bending (C) CCO bending (A, B) CC stretching (A, C)		955	923	ν_{CO} (18) + δ_{OCO} (5) + δ_{CCO} (5) + ν_{CC} (4)
33	HCCH torsion (w.t) (B) OHNC torsion HCCN torsion (w.t) (B) NHOC torsion		938	907	τ_{HCCH} (21) + τ_{OHNC} (10) + τ_{HCCN} (10) + τ_{NHOC} (6)
32	OHNC torsion HCCH torsion (w.t) (B) NHOC torsion NHCC torsion		927	896	τ_{OHNC} (21) + τ_{HCCH} (13) + τ_{NHOC} (12) + τ_{NHCC} (7)
31	CO stretching (B,C) OCCH torsion (w.t) (A, B) CC stretching COC bending (A, B)		897	867	ν_{CO} (28) + τ_{OCCH} (9) + ν_{CC} (7) + δ_{COC} (5)
30	CC stretching (A, B)		876	847	ν_{CC} (23) + δ_{COC} (12)

	COC bending (A, B)				
29	HCCO torsion (w.t) (C, B) OCCH torsion (w.t) (B) CCCH torsion (w.t) (C, B) HCCC torsion (w.t) (C, B)		858	830	τ_{HCCO} (19) + τ_{OCCH} (17) + τ_{CCCH} (10) + τ_{HCCC} (9)
28	CC stretching (B) OCCH torsion (w.t) (B) HCCC torsion (w.t) (B) HCCN torsion (w.t) (B)		850	822	ν_{CC} (13) + τ_{OCCH} (9) + τ_{HCCC} (8) + τ_{HCCN} (5)
27	OC stretching (B) CC stretching (B) OCCH torsion (w.t) (B)		831	804	ν_{OC} (8) + ν_{CC} (16) + τ_{OCCH} (7)
26	OCCH torsion (w.t) (A) HCCC torsion (w.t) (A) CCCH torsion (w.t) (A)		826	799	τ_{OCCH} (15) + τ_{HCCC} (23) + τ_{CCCH} (8)
25	OCCH torsion (w.t) (B) HCCC torsion (w.t) (B) CCCH torsion (w.t) (B)	**779**	802	776	τ_{OCCH} (17) + τ_{HCCC} (15) + τ_{CCCH} (21)
24	CC stretching (A,B) CO stretching (B) OC stretching (A,B)		789	763	ν_{CC} (7) + ν_{CO} (10) + ν_{OC} (4)
23	OC stretching (B) CCC bending (A, B) CN stretching CNC bending		785	759	ν_{OC} (9) + δ_{CCC} (7) + ν_{CN} (4) + δ_{CNC} (3)
22	CCCC torsion (A,B, C) CCCO torsion (C) OCCC torsion (C)		765	740	τ_{CCCC} (13) + τ_{CCCO} (7) + τ_{OCCC} (6)
21	CCCO torsion (w.t) (B) COCC torsion (w.t) (B)		732	708	τ_{CCCO} (33) + τ_{COCC} (6)
20	CCCO torsion (w.t) (A, B) CCCC torsion (A, B) COC bending (C)		724	700	τ_{CCCO} (5) + τ_{CCCC} (5) + δ_{COC} (2)
19	CC stretching (B) OCO bending (C) COC bending (B)		705	682	ν_{CC} (12) + δ_{OCO} (8) + δ_{COC} (3)
18	CCC bending (A) CC stretching (A,B) OC stretching (C)		694	671	δ_{CCC} (15) + ν_{CC} (8) + ν_{OC} (3)
17	CCN bending CCO bending (A, B, C) OCO bending (A, B, C)		691	668	δ_{CCN} (5) + δ_{CCO} (10) + δ_{OCO} (3)
16	HCCC torsion (w.t) (B) CCCC torsion (w.t) (B)		673	651	τ_{HCCC} (16) + τ_{CCCC} (5)
15	CCC bending (B)		650	629	δ_{CCC} (40)

14	CC stretching (A,B) CCC bending (B) OCO bending (B)		629	608	ν_{CC} (8) + δ_{CCC} (4) + δ_{OCO} (4)
13	OCOC torsion (w.t) (A, C) CCCC torsion (w.t) (A, C) OCO bending (A, C) CCCH torsion (w.t) (A,B,C)		608	588	τ_{OCOC} (6) + τ_{CCCC} (5) + δ_{OCO} (5) + τ_{CCCH} (5)
12	OCOC torsion (w.t) (A,C=O) HCCO torsion (w.t) (A, C=O)		579	560	τ_{OCOC} (13) + τ_{HCCO} (34)
11	HCCC torsion (w.t) (A, C) NCCC torsion (w.t) (A, C) CCCC torsion (w.t) (A, C) HCCN torsion (w.t) (A, C)		568	549	τ_{HCCC} (9) + τ_{NCCC} (6) + τ_{CCCC} (5) + τ_{HCCN} (5)
10	CCO bending (C) OCO bending (C) CCC bending (A, B, C)		559	541	δ_{CCO} (11) + δ_{OCO} (6) + δ_{CCC} (9)
9	CC stretching (A, C) CCO bending (A, C) CCC bending (A, C) COH bending (A, C)		526	509	ν_{CC} (12) + δ_{CCO} (8) + δ_{CCC} (6) + δ_{COH} (4)
8	CCCH torsion (w.t) (A, C) HCCC torsion (w.t) (A, C)		517	500	τ_{CCCH} (18) + τ_{HCCC} (16)
7	CCC bending (B) CCN bending (B)		490	474	δ_{CCC} (21) + δ_{CCN} (4)
6	CCCC torsion (A, C) OCCC torsion (A, C) CCCO torsion (A, C)	**451**	461	446	τ_{CCCC} (14) + τ_{OCCC} (3) + τ_{CCCO} (4)
5	CCO bending (C) CC stretching (A, C) COC bending (C)		458	443	δ_{CCO} (24) + ν_{CC} (7) + δ_{COC} (6)
4	CCO bending (B) NCC bending		453	438	δ_{CCO} (17) + δ_{NCC} (17)
3	COH bending (A) HO H bending CCO bending (A,C) OCO bending (A,C)		440	425	δ_{COH} (10) + ν_{HO} (9) + δ_{CCO} (7) + δ_{OCO} (7)
2	CCCC torsion (B) OCCC torsion (B) CCCN torsion (B)		422	408	τ_{CCCC} (34) + τ_{OCCC} (6) + τ_{CCCN} (6)
1	CCO bending (A,C)		409	396	δ_{CCO} (29) + δ_{OCO} (4)

	OCO bending (A,C)				
R		**0.996**			

Table S9. Experimental and calculated electronic transitions for investigation compound

Compounds:	Experimental λ (nm)	TD-B3LYP-D3BJ/6-311++G(d,p)		
		λ(nm)	*f*	Leading configurations
3a	249	239	0.291	HOMO-2→LUMO+1 (58%)
	332	337	0.354	HOMO→LUMO (68%)
3b	248	241	0.198	HOMO-2→LUMO+1 (52%)
	330	334	0.444	HOMO→LUMO (68%)
3c	232	236	0.142	HOMO-2→LUMO+1 (55%)
	249	269	0.143	HOMO→LUMO+1 (56%)
	332	349	0.499	HOMO→LUMO (69%)

l – wave number in nm
f – oscillator strength

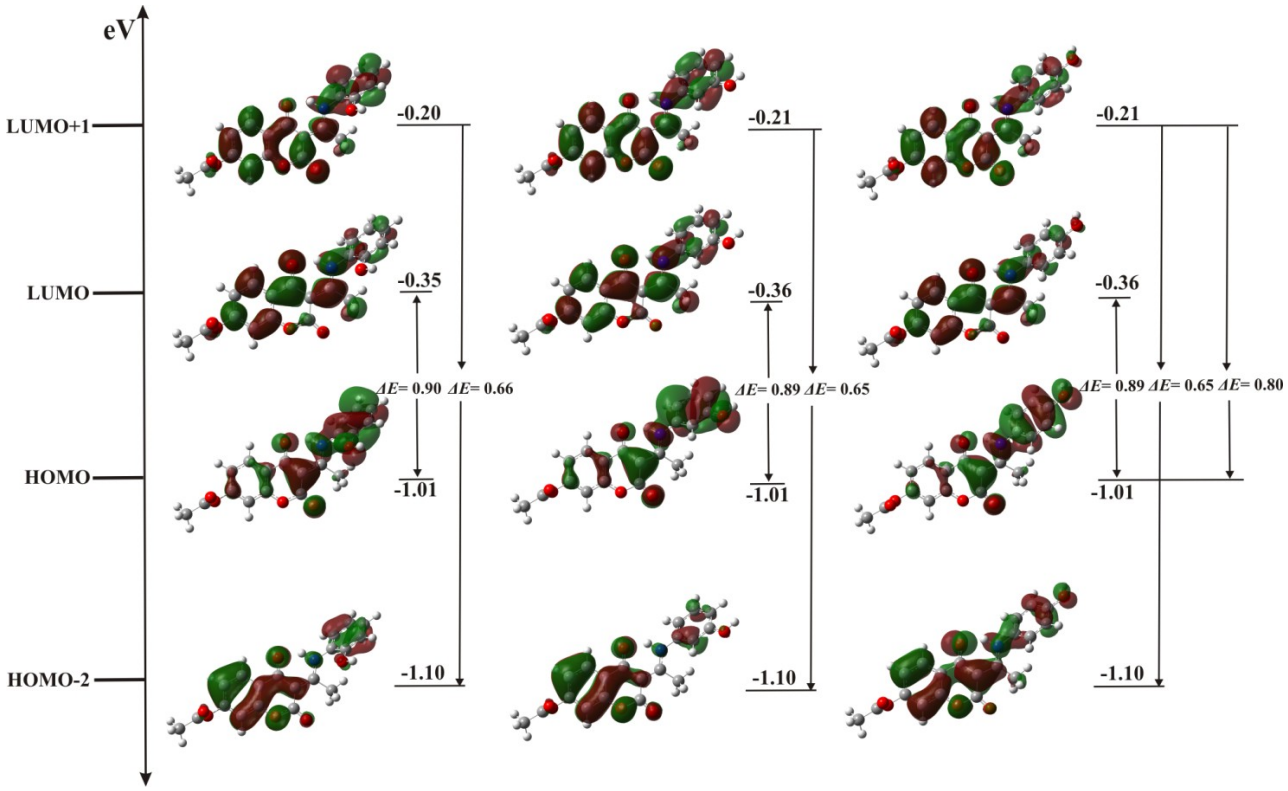

Fig. S1. The plots of the frontier molecular orbitals involved in some computed transitions and the different energy gap of the **3a** (left), **3b** (middle), **3c** (right)

HCT-116

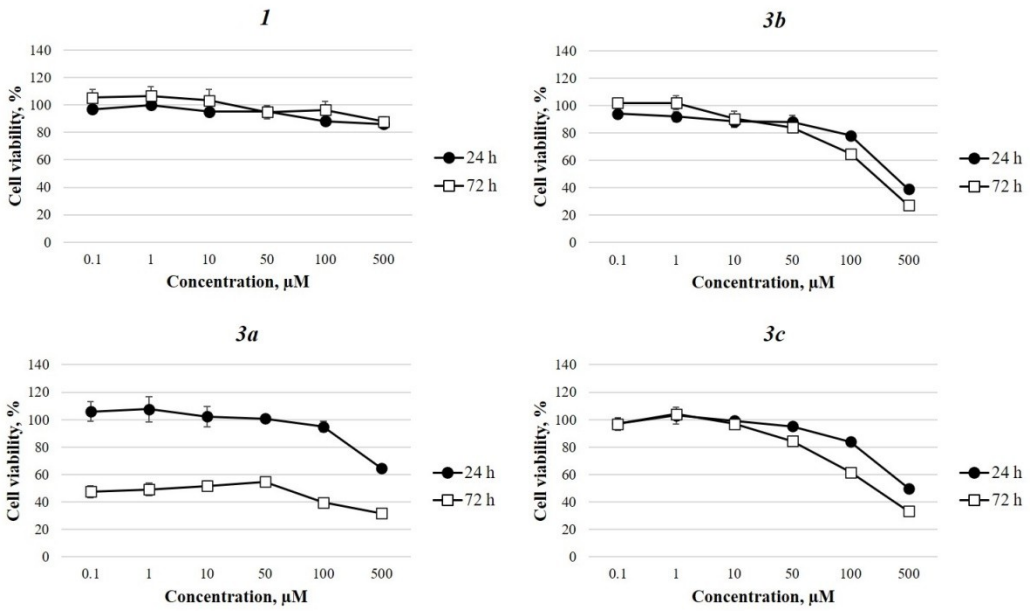

Fig. S2. The viability of HCT-116 cells dependence on various concentrations of 4,7-dihydroxycoumarin derivatives.

Hela

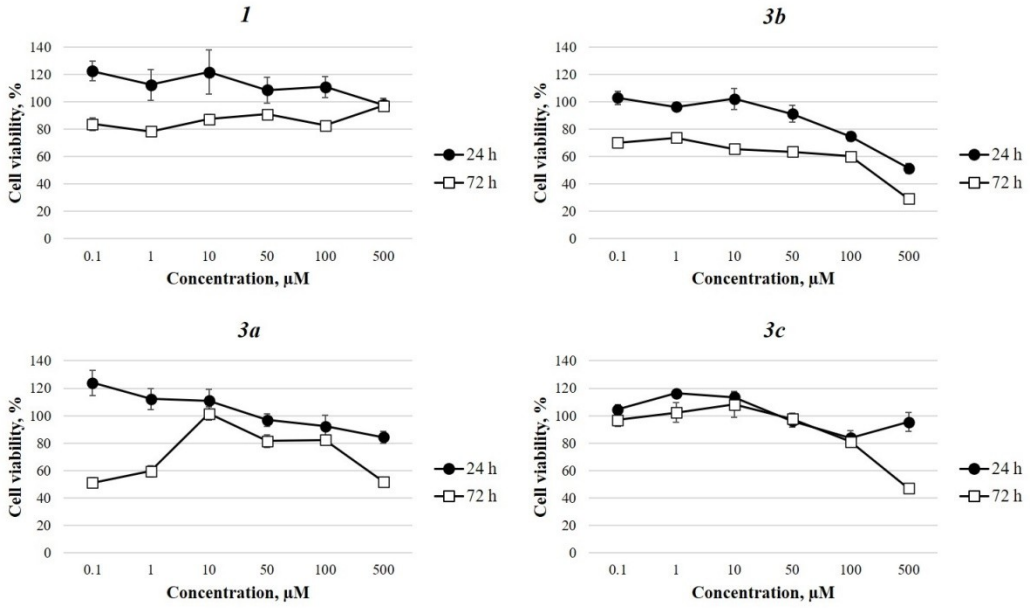

Fig. S3. The viability of HeLA cells dependence on various concentrations of 4,7-dihydroxycoumarin derivatives.

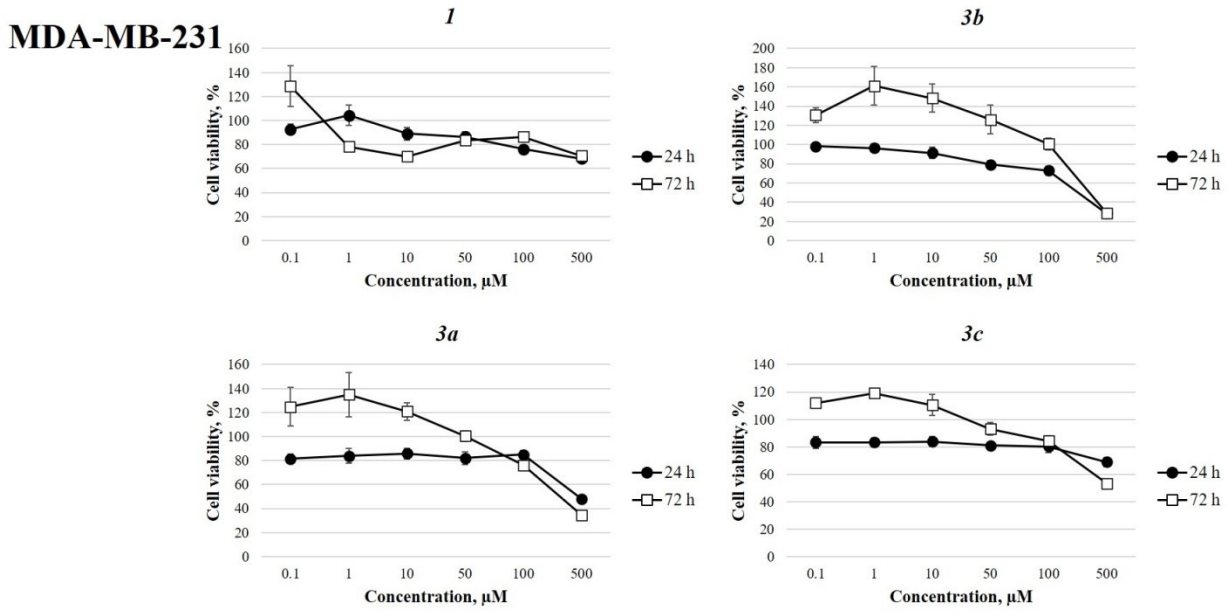

Fig. S4. The viability of MDA-MB-231 cells dependence on various concentrations of 4,7-dihydroxycoumarin derivatives.

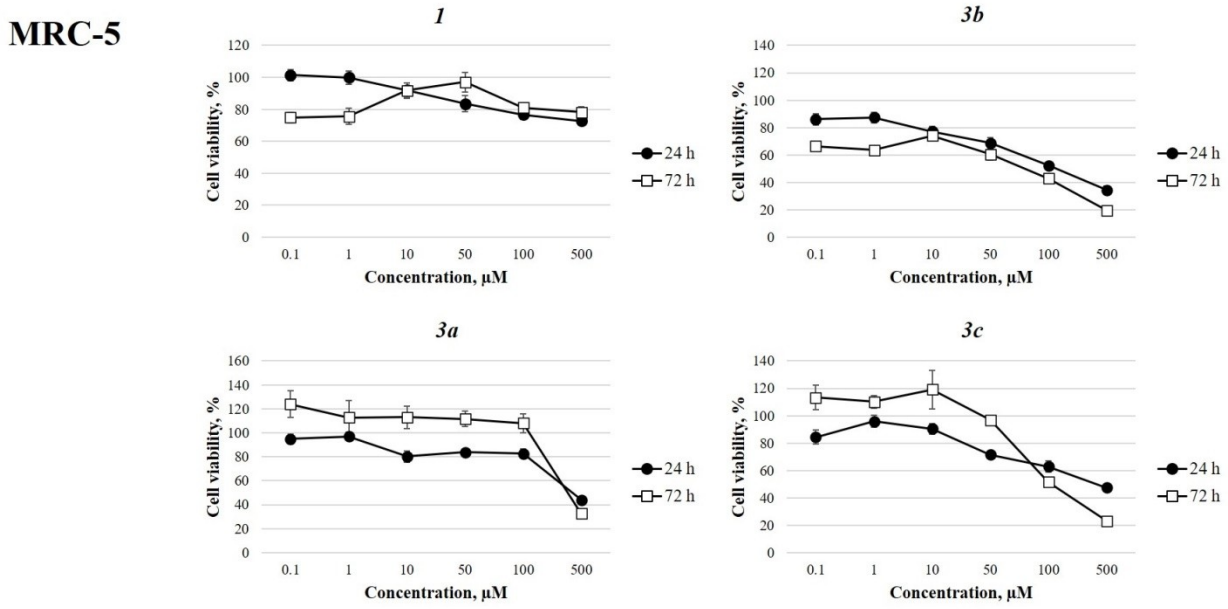

Fig. S5. The viability of MRC-5 cells dependence on various concentrations of 4,7-dihydroxycoumarin derivatives.

Table S10. The type of interactions and corresponding interatomic distance after molecular docking simulations

Conformation	Interaction	Type of interaction	Distance (Å)
EGFR-3a	A:ASP 855:**NH** – 3a:**O6**	Conventional Hydrogen Bond	1.91
	A:LYS 745:**NH** – 3a:**O2**	Conventional Hydrogen Bond	3.01
	A:MET 793:**NH** – 3a:**O7**	Conventional Hydrogen Bond	2.50
	A:ASP 855:**OH** – 3a:**N**	Conventional Hydrogen Bond	2.13
	A:THR790:**C** – 3a	π -Sigma	3.91
	A:ALA 743:**C** – 3a	π -Alkyl	3.98
	A:ALA 743:**C** – 3a	π -Alkyl	4.21
	A:LEU 844:**C** – 3a	π -Alkyl	4.64
	A:VAL 726:**C** – 3a	π -Alkyl	4.29
	A:ALA 726:**C** – 3a	π -Alkyl	4.50
EGFR-3b	A:ARG 836:**NH** – 3b:**O7**	Conventional Hydrogen Bond	1.82
	A:PHE 856:**NH** – 3b:**O6**	Conventional Hydrogen Bond	1.85
	A:LEU 862:**C** – 3b:**O1**	Carbon Hydrogen Bond	3.57
	A:ARG 855:**O** – 3b	π-anion	4.11
	A:MET 766:**C** – 3b	π-sigma	3.89
	A:ALA 859:**C** – 3b	π-sigma	3.49
	A:PHE 723 – 3b	π-π Stacked	4.74
	A:PHE 723 – 3b	π-π Stacked	4.85
	A:ALA 859:**C** – 3b	π -Alkyl	4.46
EGFR-3c	A:ARG 836:**NH** – 3c:**O7**	Conventional Hydrogen Bond	2.10
	A:GLY 857:**O** – 3c:**NH**	Conventional Hydrogen Bond	2.04
	A:ARG 857:**O** – 3c:**NH**	Conventional Hydrogen Bond	2.95
	A:ASP 837:**O** – 3c	π-anion	4.13
	A:ASP 855:**O** – 3c	π-anion	3.76
	A:PHE 723 – 3c	π-π Stacked	4.99
	A:ALA 859:**C** – 3c	π-sigma	3.17
	A:ALA 859:**C** – 3c	π -Alkyl	4.16