Table S1 The geometric (bonds and selected angles) and toplogical parameters in the chromone derivatives (distance in Å, angles in °, ? in e/ Å^3, ∇^2? in e/ Å^5). The first line refers to the *Mul_exp* model, while the second and third ones refer to the *SP_theor* model and *OPT_theo* model.

	compound **I**	compound **II**	?		∇^2?	
			I	**II**	**I**	**II**
O1-C2	1.3821(3)	1.3906(3)	1.80(2)	1.90(2)	-11.9(1)	-13.3(1)
	1.3821	1.3906	1.84	1.81	-10.8	-11.0
	1.3941	1.3964	1.80	1.79	-11.1	-11.1
O1-C9	1.3791(3)	1.3744(3)	2.12(2)	2.02(2)	-14.1(1)	-13.6(1)
	1.3791	1.3744	1.84	1.86	-8.4	-8.0
	1.3655	1.3637	1.89	1.90	-7.2	-7.2
O2-C2	1.2272(3)	1.2165(3)	2.80(2)	2.87(2)	-34.3(1)	-33.0(1)
	1.2272	1.2165	2.72	2.78	-9.9	-7.8
	1.2043	1.2049	2.85	2.84	-5.5	-5.6
O4-C4	1.2562(3)	1.2569(2)	2.42(2)	2.57(2)	-16.2(1)	-15.7(1)
	1.2562	1.2569	2.52	2.51	-8.9	-8.9
	1.2445	1.2488	2.57	2.55	-7.1	-7.5
N1-C31	1.3216(3)	1.3258(2)	2.24(2)	2.27(2)	-18.6(1)	-17.9(1)
	1.3216	1.3258	2.30	2.29	-20.5	-20.7
	1.3334	1.3292	2.26	2.27	-21.4	-20.7
N1-H1	1.0090(3)	1.0088(2)	2.02(2)	2.12(2)	-16.4(1)	-22.1(1)
	1.0090	1.0088	2.27	2.29	-45.8	-46.3
	1.0263	1.0333	2.17	2.15	-41.8	-40.8
N1-H2	1.0102(3)	-	2.15(2)			-20.0(1)
	1.0102	-	2.29			-40.2
	1.0081	-	2.30			-40.5
N1-C33	-	1.4618(3)		1.70(2)		-8.9(1)
	-	1.4618		1.70		-15.1
		1.4574		1.72		-15.6
C2-C3	1.4524(3)	1.4616(2)	1.76(2)	1.79(2)	-11.7(1)	-10.9(1)
	1.4524	1.4616	1.89	1.84	-17.2	-16.6
	1.4651	1.4635	1.84	1.85	-16.4	-16.5
C3-C4	1.4526(3)	1.4469(2)	1.82(2)	1.83(2)	-10.9(1)	-10.5(1)
	1.4526	1.4469	1.90	1.92	-17.2	-17.6
	1.4590	1.4540	1.88	1.89	-16.8	-17.1
C3-C31	1.4327(3)	1.4301(2)	1.87(2)	1.86(2)	-12.7(1)	-12.9(1)
	1.4327	1.4301	1.93	1.93	-17.4	-17.6
	1.4108	1.4211	2.01	1.97	-19.1	-18.3
C31-C311	1.4934(3)	1.4922(2)	1.70(2)	1.68(2)	-10.6(1)	-8.1(1)
	1.4934	1.4922	1.77	1.78	-15.8	-16.1
	1.4903	1.4902	1.78	1.76	-16.1	-15.8
C4-C10	1.4778(2)	1.4713(3)	1.70(2)	1.81(2)	-9.9(1)	-11.8(1)
	1.4778	1.4713	1.83	1.85	-16.5	-17.0
	1.4728	1.4718	1.85	1.85	-16.9	-17.0

C5-C6	1.3932(3)	1.3905(2)	2.00(2)	2.01(2)	-15.2(1)	-15.4(1)
	1.3932	1.3905	2.08	2.09	-20.5	-20.8
	1.3851	1.3851	2.12	2.12	-21.3	-21.3
C5-C10	1.4078(3)	1.4090(3)	1.88(2)	1.91(2)	-13.4(1)	-13.4(1)
	1.4078	1.4090	2.02	1.85	-19.5	-18.9
	1.4031	1.4033	2.04	2.04	-19.9	-19.9
C6-C7	1.4084(3)	1.4065(3)	1.96(2)	1.89(2)	-10.9(1)	-11.1(1)
	1.4084	1.4065	2.03	2.04	-19.8	-19.9
	1.4016	1.4018	2.06	2.06	-20.3	-20.3
C7-C8	1.3965(3)	1.3955(3)	1.99(2)	2.00(2)	-15.1(1)	-15.1(1)
	1.3965	1.3955	2.07	2.07	-20.3	-20.3
	1.3878	1.3876	2.10	2.10	-21.0	-21.0
C8-C9	1.4015(2)	1.3995(3)	1.96(2)	2.03(2)	-16.3(1)	-15.5(1)
	1.4015	1.3995	2.07	2.08	-20.6	-20.9
	1.3959	1.3963	2.10	2.10	-21.2	-21.2
C9-C10	1.3978(3)	1.3963(3)	1.99(3)	1.99(2)	-14.4(1)	-13.9(1)
	1.3978	1.3963	2.09	2.09	-20.7	-20.9
	1.3959	1.3954	2.10	2.10	-21.0	-21.1
C3111-C312	1.4033(3)	1.3982(2)	1.89(2)	1.89(2)	-13.0(1)	-12.4(1)
	1.4033	1.3982	2.04	2.06	-19.8	-20.0
	1.3987	1.3969	2.06	2.06	-20.2	-20.2
C311-C316	1.4032(2)	1.4001	1.87(2)	1.90(2)	-13.9(1)	-13.2(1)
	1.4032	1.4001	2.04	2.05	-19.6	-19.8
	1.3985	1.3964	2.06	2.06	-20.0	-20.1
C312-C313	1.3975(3)	1.3968(3)	1.89(2)	1.93(2)	-14.5(1)	-15.1(1)
	1.3975	1.3968	2.06	2.07	-20.2	-20.41
	1.3895	1.3919	2.10	2.09	-21.1	-20.8
C313-C314	1.4026(3)	1.3989(3)	1.90(2)	1.93(2)	-16.8(1)	-15.7(1)
	1.4026	1.3989	2.06	2.08	-20.2	-20.8
	1.3954	1.3940	2.08	2.09	-20.8	-20.8
C314-C315	1.4023(3)	1.4018(2)	1.92(2)	1.93(2)	-15.2(1)	-14.2(1)
	1.4023	1.4018	2.05	2.05	-20.1	-20.2
	1.3922	1.3934	2.09	2.09	-20.9	-20.9
C315-C316	1.4022(3)	1.3993(3)	1.92(2)	1.92(2)	-15.2(1)	-14.9(1)
	1.4022	1.3993	2.05	2.06	-19.9	-20.2
	1.3938	1.3926	2.08	2.09	-20.8	-20.8
C5-H5	1.0847	1.0822	1.91(2)	1.83(2)	-17.1(1)	-16.0(1)
	1.0847	1.0822	1.92	1.93	-23.8	-24.1
	1.0834	1.0829	1.92	1.92	-23.9	-23.9
C6-H6	1.0830	1.0828	1.82(2)	1.80(2)	-15.9(1)	-15.8(1)
	1.0830	1.0828	1.90	1.91	-23.4	-23.5
	1.0842	1.0843	1.90	1.90	-23.4	-23.3
C7-H7	1.0823	1.0826	1.82(2)	1.80(2)	-15.0(1)	-15.9(1)
	1.0823	1.0826	1.91	1.92	-23.7	-23.7
	1.0842	1.0824	1.91	1.91	-23.5	-23.5
C8-H8	1.0835	1.0821	1.91(2)	1.82(2)	-15.4(1)	-15.9(1)
	1.0835	1.0821	1.90	1.91	-23.4	-23.4
	1.0828	1.0828	1.90	1.90	-23.4	-23.4

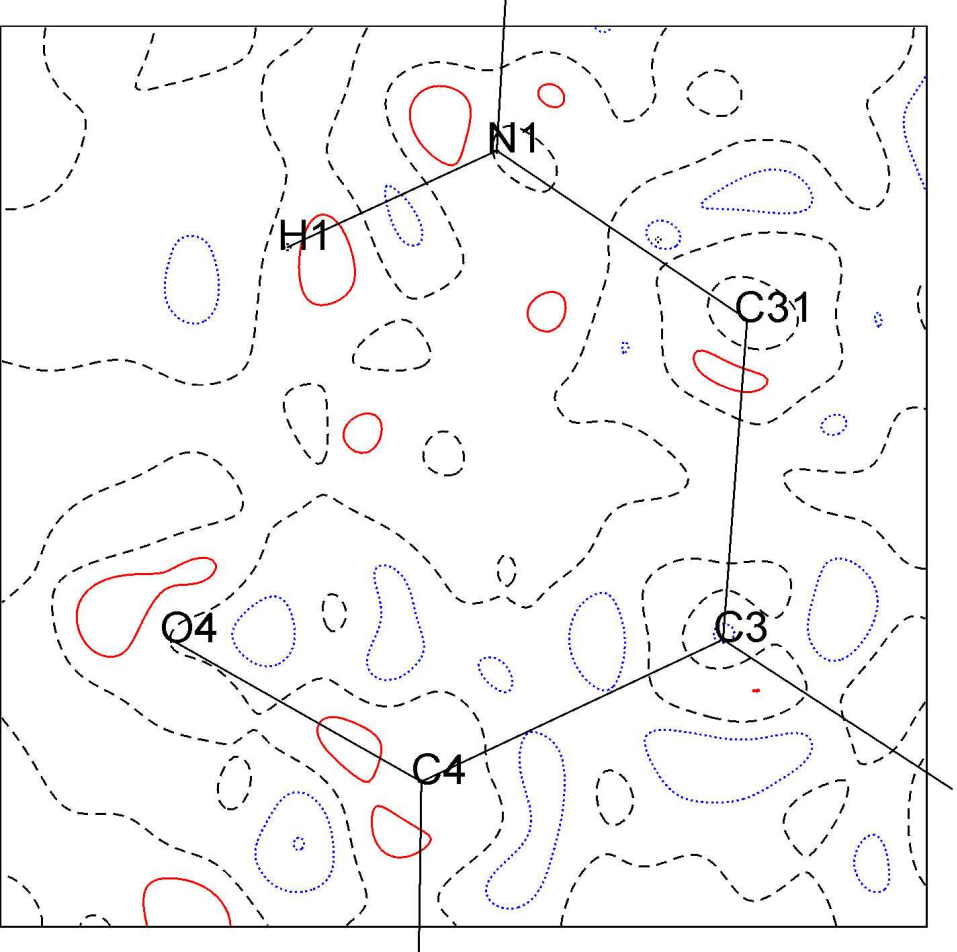
C312-H312	1.0842	1.0829	1.71(2)	1.78(2)	-17.1(1)	-16.3(1)
	1.0842	1.0829	1.91	1.91	-23.6	-23.6
	1.0833	1.0841	1.91	1.90	-23.6	-23.4
C313-H313	1.0833	1.0834	1.82(2)	1.70(2)	-15.8(1)	-13.8(1)
	1.0833	1.0834	1.91	1.91	-23.5	-23.6
	1.0838	1.0840	1.90	1.90	-23.4	-23.4
C314-H314	1.0817	1.0828	1.72(2)	1.78(2)	-16.9(1)	-16.9(1)
	1.0817	1.0828	1.92	1.65	-23.7	-23.5
	1.0840	1.0840	1.90	1.90	-23.5	-23.5
C315-H315	1.0830	1.0828	1.81(2)	1.70(2)	-14.1(1)	-13.9(1)
	1.0830	1.0828	1.91	1.91	-23.5	-23.5
	1.0839	1.0840	1.90	1.90	-23.4	-23.4
C316-H316	1.0838	1.0828	1.81(2)	1.77(2)	-14.9(1)	-16.3(1)
	1.0838	1.0828	1.91	1.91	-23.4	-23.6
	1.0843	1.0844	1.90	1.90	-23.3	-23.3
C33-H33A		1.0584		1.86(2)		-9.3(1)
		1.0584		2.01		-25.9
		1.0886		2.06		-26.0
C33-H33B		1.0660		1.75(2)		-9.9(1)
		1.0660		-		-
		-		-		-
C33-H33C		1.0599		1.78(2)		-9.7(1)
		1.0599		2.01		-25.9
		1.0939		2.09		-26.1
C33-H33D		1.0606		1.62(2)		-9.4(1)
		1.0606		-		-
		-		-		-
C33-H33E		1.0591		1.66(2)		-9.4(1)
		1.0591		2.02		-26.2
		1.0939		2.06		-26.0
C33-H33F		1.0588		1.66(2)		-9.3(1)
		1.0588		-		-
		-		-		-

O4-C4-C3	123.8(1)	123.4(1)
	123.8	123.4
	123.5	123.4
C4-C3-C31	120.0(1)	120.3(1)
	120.0	120.3
	119.9	120.2
C3-C31-N1	120.3(1)	120.5(1)
	120.3	120.5
	120.4	119.8
C31-N1-H1	120.2(1)	109.9(1)
	120.2	109.9
	117.0	113.1

Table S2 Summary of experimental atomic volumes V_{tot}, V_{001} in Å^3, number of electrons *N*, N_{001} in *e* and net atomic charges *Q* in *e*.

	compound I					*compound II*				
atom	V_{tot}	V_{001}	*N*	N_{001}	*Q*	V_{tot}	V_{001}	*N*	N_{001}	*Q*
O1	17.46	16.03	8.94	8.94	-0.84	17.17	14.55	8.81	8.8	-0.81
O2	19.71	15.78	8.88	8.88	-0.73	19.44	17.16	8.75	8.74	-0.75
O4	16.69	15.71	8.82	8.81	-0.62	15.39	14.07	8.68	8.68	-0.68
N1	15.93	13.69	8.1	8.1	-0.81	12.23	11.96	7.86	7.86	-0.86
C2	10.72	8.49	4.87	4.87	1.03	9.21	7.62	4.98	4.98	1.02
C3	10.95	10.51	6.14	6.14	-0.07	10.97	10.54	6.07	6.07	-0.07
C4	8.25	7.35	5.34	5.34	0.51	7.27	7.26	5.47	5.47	0.53
C5	11.43	10.16	6.11	6.11	0.01	11.04	10.92	6	6	0
C6	12.05	11.83	6.13	6.12	-0.03	11.68	11.48	6.03	6.03	-0.03
C7	12.01	12.59	6.12	6.12	0.02	11.12	11.12	5.97	5.97	0.03
C8	12.53	12.29	6.08	6.08	0.08	12.05	11.63	5.78	5.78	0.22
C9	11.64	9.43	5.65	5.65	0.25	10.29	9.75	5.76	5.76	0.24
C10	11.79	10.09	6.23	6.23	-0.03	10.04	9.92	6.06	6.06	-0.06
C31	9.65	8.7	5.75	5.75	0.25	8.6	8.5	5.71	5.71	0.29
C33						5.92	5.91	5.73	5.73	0.27
C311	9.91	9.4	6.05	6.05	-0.11	8.52	8.51	6.12	6.12	-0.12
C312	11.78	11.73	6.15	6.15	-0.02	11.52	11.35	5.99	5.99	0.01
C313	11.63	11.15	6.11	6.11	-0.01	11.74	11.69	5.89	5.89	0.11
C314	11.98	11.37	6.06	6.06	0.23	10.45	10.36	5.98	5.98	0.12
C315	11.82	11.36	6.07	6.07	-0.06	10.79	10.71	5.61	5.61	0.09
C316	12.67	12.25	6.17	6.16	0.15	12.53	11.8	5.94	5.94	0.26
H1	3.6	3.08	0.47	0.47	0.31	3.11	3.12	0.71	0.71	0.29
H2	2.7	2.67	0.52	0.52	0.38					
H5	6.92	5.44	0.79	0.79	0.05	6.92	5.73	0.95	0.94	0.05
H6	7.14	6.98	0.79	0.78	0.01	7.42	6.94	1.05	1.04	-0.05
H7	6.18	5.85	0.78	0.78	0.02	6.68	6.52	1.1	1.1	-0.01
H8	8.03	7.84	0.83	0.82	0.02	8.07	5.85	1.02	1.02	-0.02

H312	6.22	5.79	0.75	0.75	-0.03	7.43	6.98	1.03	1.03	-0.03
H313	6.9	6.33	0.87	0.86	0.04	6.19	5.92	0.98	0.98	0.02
H314	6.68	5.95	0.86	0.85	0.02	6.84	5.92	1.01	1.01	-0.01
H315	6.45	6	0.84	0.83	-0.03	6.67	6.5	0.95	0.95	-0.05
H316	6.13	5.9	0.81	0.81	0.02	6.08	5.81	0.73	0.72	0.07
H33A						5.81	5.81	1.1	1.1	-0.1
H33B						5.25	5.25	1.09	1.09	0.03
H33C						7.56	6.19	1.09	1.08	-0.03
H33D						4.06	4.06	0.99	0.99	0.01
H33E						5.94	5.29	0.99	0.98	0.01
H33F						5.55	5.53	0.99	0.99	0.02
sum	31.5	291.7	138.1	138.0	0.01	337.5	318.2	149.0	149.0	0.01


N1
H1
C31
O4
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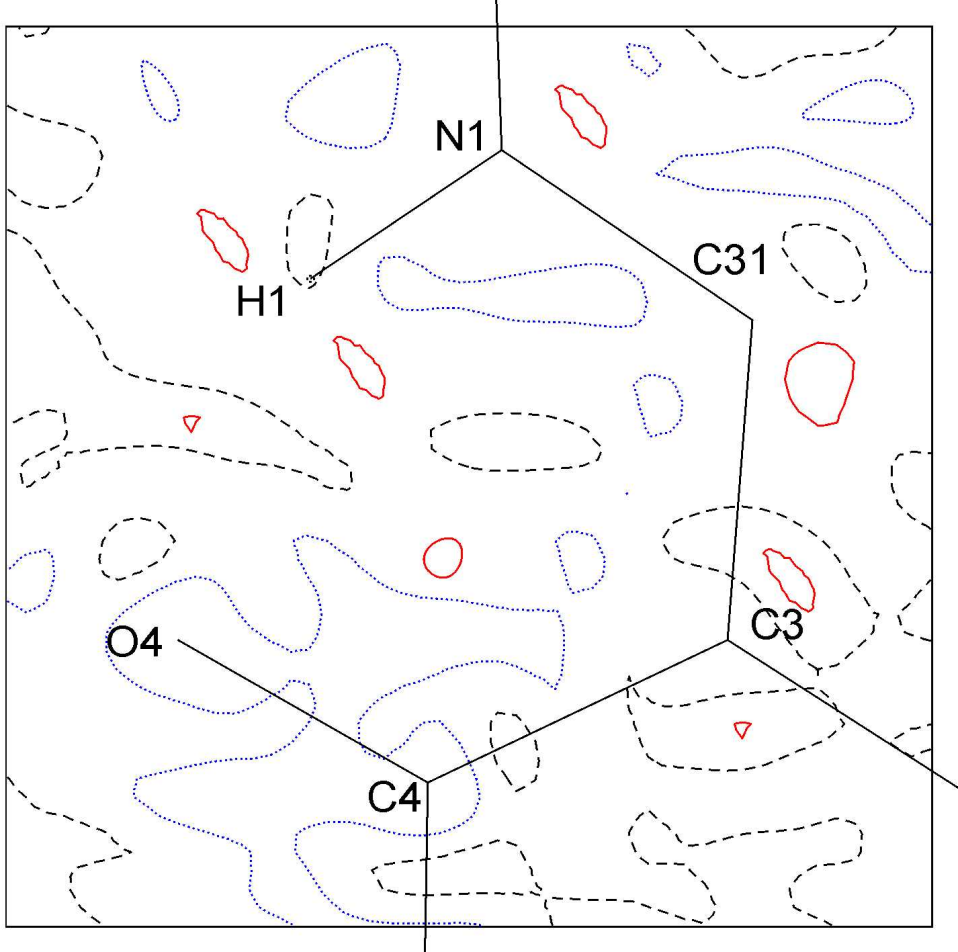
C4


N1
H1
C31
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