Structural Analysis and Multipole Modelling of Quercetin Monohydrate – A Quantitative and Comparative Study

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SUPPORTING INFORMATION

Supplementary Tables S1-S7

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Table S1. Atom-types assignment in quercetin monohydrate.

Atom label	Atom-type
O1	Occ
O3, O5, O7, O13, O14	Och
O4	O=c[cc]
C2, C3, C5, C7, C9, C13, C14,	Co[x]cc
C4	C=occ
C6, C8, C12, C15, C16	Ccch
C10	C1.5c1.5c1.5c
C11	C1c1.5c1.5c
H3, H5, H7, H13, H14	Ho[cc]
H6, H8, H12, H15, H16	Hc[cc]
O1W	Ohh
H1W, H2W	Ho[h]

The numbers in atom-type name denote bond orders *i.e.* 1 – single, 1.5 - intermediate, 2 – double bonds. The atomic symbols in between the brackets code the neighbours of the neighbours of the first atom.

Table S2. Comparison of the X-H distances for the IAM_UR and TAAM_UR models.

Bond	$d_{\mathrm{IAM\_UR}}$(Å)	$d_{\mathrm{TAAM\_UR}}$(Å)
O3-H3	0.909(27)	0.967(14)
O5-H5	0.921(25)	1.000(13)
O7-H7	0.822(26)	0.908(13)
O13-H13	0.841(26)	0.972(13)
O14-H14	0.880(25)	0.965(13)
O1W-H1W	0.900(28)	1.007(14)
O1W-H2W	0.923(28)	1.014(14)
Average (rmsd)	0.885(37)	0.976(33)
Average (neutron)	0.967(10)	
$(d_{\mathrm{model}} - d_{\mathrm{neutron}})/\sigma_{\mathrm{neutron}}$	-8.21	0.91
C6-H6	0.904(22)	1.046(10)
C8-H8	0.955(22)	1.040(10)
C12-H12	0.976(22)	1.045(09)
C15-H15	1.010(23)	1.083(10)
C16-H16	0.943(23)	1.059(10)
Average (rmsd)	0.957(35)	1.055(16)
Average (neutron)	1.083(11)	
$(d_{\mathrm{model}} - d_{\mathrm{neutron}})/\sigma_{\mathrm{neutron}}$	-11.42	-2.57

Table S3. Hirshfeld test values with the corresponding distances for the quercetin molecule for the IAM_R, TAAM_R and TAAM_THEO_R models. DMSDA ($Å^2 * 10^4$)

Bond	IAM_R DMSDA	IAM_R *d* (Å)	TAAM_R DMSDA	TAAM_R *d* (Å)	TAAM_THEO_R DMSDA	TAAM_THEO_R *d* (Å)
O1-C2	-8	1.3708(16)	-2	1.3666(9)	-6	1.3654(8)
O1-C9	-5	1.3645(16)	1	1.3582(9)	-4	1.3560(8)
O3-C3	2	1.3576(16)	-3	1.3534(9)	-2	1.3515(8)
O4-C4	-16	1.2752(16)	5	1.2752(9)	0	1.2688(8)
O5-C5	-7	1.3603(16)	-7	1.3524(9)	-5	1.3512(8)
O7-C7	-20	1.3525(16)	-6	1.3466(9)	-3	1.3448(8)
O13-C13	1	1.3707(15)	5	1.3656(9)	5	1.3633(8)
C14-C14	-7	1.3584(16)	-4	1.3529(9)	-2	1.3511(8)
C2-C3	-4	1.3744(18)	3	1.3766(10)	1	1.3760(9)
C2-C11	17	1.4635(18)	3	1.4640(10)	-4	1.4633(9)
C3-C4	-12	1.4330(18)	-15	1.4341(10)	-3	1.4357(9)
C6-C5	-10	1.3718(19)	-6	1.3800(10)	3	1.3800(9)
C6-C7	-3	1.4051(18)	-4	1.4078(10)	2	1.4070(9)
C8-C7	-2	1.3896(19)	-6	1.3922(10)	1	1.3923(9)
C8-C9	-12	1.3836(19)	-8	1.3900(10)	2	1.3894(9)
C10-C4	-20	1.4278(18)	-8	1.4267(10)	-1	1.4284(9)
C10-C5	-14	1.4192(18)	-5	1.4214(10)	-7	1.4204(9)
C10-C9	-2	1.4009(18)	1	1.3999(9)	-2	1.4014(9)
C11-C12	-5	1.4087(18)	4	1.4088(10)	2	1.4083(9)
C11-C16	-4	1.4027(18)	-4	1.4044(10)	-5	1.4045(9)
C12-C13	-5	1.3830(19)	-3	1.3865(10)	1	1.3877(9)
C13-C14	2	1.3987(18)	1	1.4028(10)	2	1.4009(9)
C14-C15	8	1.3881(19)	6	1.3937(10)	0	1.3937(9)
C16-C15	2	1.3914(19)	1	1.3912(10)	0	1.3916(9)
rmsd	7.7(60)		4.7(30)		2.6(19)	

Table S4. Topological properties of the electron density for the covalent bonds of quercetin monohydrate for the TAAM_OPT (first entry) and THEO_OPT (second entry in italics) models.

Bond	d_{AB}	$d_{A...CP}$	$d_{B...CP}$	$\rho(\mathbf{r}_{CP})$	$\nabla^2\rho(\mathbf{r}_{CP})$	λ_1	λ_2	λ_3	ε
O1-	1.3659	0.8295	0.5368	1.99	-15.06	13.98	-13.82	-15.21	0.09
C2		*0.8285*	*0.5380*	*1.85*	*-10.37*	*14.13*	*-11.88*	*-12.62*	*0.06*
O1-	1.3571	0.8309	0.5263	2.02	-16.03	13.50	-14.08	-15.45	0.09
C9		*0.8303*	*0.5274*	*1.89*	*-12.30*	*13.33*	*-12.39*	*-13.24*	*0.06*
O3-	1.3562	0.8202	0.5361	2.01	-15.16	13.98	-13.88	-15.26	0.09
C3		*0.8106*	*0.5457*	*1.97*	*-12.70*	*14.74*	*-13.02*	*-14.43*	*0.10*
O4-	1.2832	0.7886	0.4946	2.59	-27.96	12.17	-18.81	-21.32	0.12
C4		*0.8088*	*0.4744*	*2.36*	*-22.21*	*13.10*	*-17.31*	*-18.00*	*0.04*
O5-	1.3544	0.8220	0.5324	2.01	-15.56	13.65	-13.90	-15.31	0.09
C5		*0.8207*	*0.5339*	*1.98*	*-14.68*	*12.80*	*-13.17*	*-14.31*	*0.08*
O7-	1.3499	0.8223	0.5278	2.02	-15.92	13.47	-14.00	-15.39	0.09
C7		*0.8247*	*0.5253*	*1.98*	*-15.50*	*12.17*	*-13.38*	*-14.29*	*0.06*
O13-C13	1.3659	0.8202	0.5458	1.98	-14.27	14.37	-13.60	-15.04	0.10
		0.8226	*0.5433*	*1.90*	*-12.01*	*13.87*	*-12.33*	*-13.55*	*0.09*
O14-C14	1.3511	0.8219	0.5294	2.02	-15.76	13.58	-13.97	-15.37	0.09
		0.8180	*0.5333*	*1.99*	*-14.39*	*13.28*	*-13.25*	*-14.41*	*0.08*
C2-	1.3830	0.6900	0.6932	2.25	-21.76	10.19	-13.91	-18.05	0.23
C3		*0.7023*	*0.6808*	*2.14*	*-18.85*	*9.91*	*-12.22*	*-16.53*	*0.26*
C2-	1.4602	0.7448	0.7155	1.92	-14.60	11.31	-11.60	-14.30	0.19
C11		*0.7642*	*0.6960*	*1.82*	*-13.06*	*10.49*	*-10.68*	*-12.88*	*0.17*
C3-	1.4347	0.7337	0.7010	2.05	-17.88	10.49	-12.74	-15.63	0.18
C4		*0.7114*	*0.7234*	*1.97*	*-15.83*	*10.58*	*-11.78*	*-14.63*	*0.19*
C6-	1.3829	0.6844	0.6985	2.18	-20.02	10.12	-13.38	-16.76	0.20
C5		*0.6575*	*0.7254*	*2.11*	*-17.88*	*10.23*	*-12.33*	*-15.78*	*0.22*

C6-	1.4090	0.6978	0.7113	2.10	-18.09	10.68	-12.76	-16.01	0.20
C7		*0.6744*	*0.7347*	*2.01*	*-16.05*	*10.60*	*-11.89*	*-14.76*	*0.19*
C8-	1.3963	0.6877	0.7086	2.15	-19.29	10.43	-13.23	-16.50	0.20
C7		*0.6695*	*0.7268*	*2.06*	*-17.08*	*10.36*	*-12.19*	*-15.26*	*0.20*
C8-	1.3878	0.6871	0.7007	2.16	-19.64	10.24	-13.27	-16.62	0.20
C9		*0.6589*	*0.7289*	*2.08*	*-17.31*	*10.45*	*-12.17*	*-15.58*	*0.22*
C10-	1.4269	0.7148	0.7121	2.00	-16.71	10.54	-12.46	-14.78	0.16
C4		*0.6957*	*0.7312*	*1.94*	*-14.58*	*11.16*	*-11.71*	*-14.03*	*0.16*
C10-	1.4211	0.6936	0.7276	2.04	-16.80	11.07	-12.35	-15.52	0.20
C5		*0.6924*	*0.7288*	*1.96*	*-15.18*	*10.70*	*-11.67*	*-14.21*	*0.18*
C10-	1.4061	0.6762	0.7299	2.05	-17.42	10.65	-12.53	-15.54	0.19
C9		*0.6774*	*0.7287*	*2.02*	*-15.97*	*10.72*	*-11.97*	*-14.72*	*0.19*
C11-C12	1.4122	0.7087	0.7034	2.05	-16.88	10.82	-12.53	-15.17	0.17
		0.7096	*0.7026*	*1.95*	*-14.38*	*11.05*	*-11.57*	*-13.86*	*0.17*
C11-C16	1.4072	0.7087	0.6985	2.07	-17.46	10.71	-12.80	-15.37	0.17
		0.7042	*0.7031*	*1.99*	*-15.32*	*10.64*	*-11.79*	*-14.17*	*0.17*
C12-C13	1.3874	0.6858	0.7017	2.16	-19.67	10.22	-13.27	-16.62	0.20
		0.6731	*0.7144*	*2.09*	*-17.47*	*10.37*	*-12.31*	*-15.52*	*0.21*
C13-C14	1.4099	0.7051	0.7051	2.17	-19.60	10.79	-13.23	-17.16	0.23
		0.7024	*0.7078*	*2.06*	*-18.21*	*9.72*	*-12.24*	*-15.69*	*0.22*
C14-C15	1.3978	0.7064	0.6915	2.13	-18.86	10.46	-13.01	-16.31	0.20
		0.7227	*0.6751*	*2.06*	*-17.08*	*10.23*	*-12.21*	*-15.10*	*0.19*
C16-C15	1.3895	0.6945	0.6950	2.11	-18.47	10.24	-13.05	-15.65	0.17
		0.6946	*0.6949*	*2.04*	*-15.93*	*11.12*	*-12.22*	*-14.83*	*0.18*
O3-	0.9832	0.7484	0.2348	2.39	-52.38	28.68	-40.15	-40.92	0.02
H3		*0.7396*	*0.2436*	*2.37*	*-43.43*	*32.18*	*-37.59*	*-38.02*	*0.01*
O5-	0.9948	0.7511	0.2437	2.34	-48.23	28.65	-38.05	-38.82	0.02
H5		*0.7484*	*0.2464*	*2.31*	*-41.99*	*31.81*	*-36.70*	*-37.10*	*0.01*

O7-	0.9864	0.7493	0.2371	2.38	-51.36	28.66	-39.59	-40.42	0.02
H7		*0.7463*	*0.2401*	*2.34*	*-45.89*	*31.09*	*-38.25*	*-38.74*	*0.01*
O13-H13	0.9926	0.7506	0.2420	2.35	-49.05	28.66	-38.44	-39.26	0.02
		0.7495	*0.2431*	*2.29*	*-42.94*	*31.13*	*-36.76*	*-37.31*	*0.01*
O14-H14	0.9788	0.7476	0.2312	2.41	-54.19	28.67	-41.01	-41.84	0.02
		0.7368	*0.2420*	*2.40*	*-45.67*	*32.16*	*-38.65*	*-39.18*	*0.01*
O1W-H1W	0.9735	0.7385	0.2350	2.52	-53.53	30.66	-41.79	-42.40	0.01
		0.7314	*0.2421*	*2.45*	*-44.39*	*31.24*	*-37.48*	*-38.15*	*0.02*
O1W-H2W	0.9747	0.7387	0.2360	2.52	-53.04	30.68	-41.63	-42.09	0.01
		0.7352	*0.2394*	*2.42*	*-44.18*	*31.06*	*-37.37*	*-37.88*	*0.01*
C6-	1.0823	0.7033	0.3789	1.85	-19.18	14.86	-16.56	-17.48	0.05
H6		*0.6880*	*0.3942*	*1.81*	*-15.38*	*16.69*	*-15.60*	*-16.46*	*0.05*
C8-	1.0798	0.7018	0.3780	1.86	-19.37	14.87	-16.66	-17.58	0.05
H8		*0.6846*	*0.3952*	*1.81*	*-15.40*	*16.64*	*-15.53*	*-16.50*	*0.06*
C12-H12	1.0794	0.7012	0.3782	1.86	-19.39	14.83	-16.66	-17.56	0.05
		0.6944	*0.3850*	*1.84*	*-16.46*	*16.81*	*-16.29*	*-16.99*	*0.04*
C15-H15	1.0832	0.7040	0.3793	1.85	-19.11	14.85	-16.53	-17.43	0.05
		0.6883	*0.3949*	*1.81*	*-15.62*	*16.27*	*-15.56*	*-16.34*	*0.05*
C16-H16	1.0825	0.7030	0.3795	1.85	-19.17	14.80	-16.53	-17.44	0.05
		0.6893	*0.3932*	*1.83*	*-16.28*	*16.05*	*-15.82*	*-16.50*	*0.04*

The distances are given in Å, electron density $\rho(\mathbf{r}_{CP})$ in eÅ^{-3}. The Laplacian $\nabla^2\rho(\mathbf{r}_{CP})$, Hessian eigenvalues λ_1, λ_2, λ_3 are in eÅ^{-5}. The ellipticity ε is dimensionless. The distances, d_{AB}, are the same for both models because the same optimized geometry was used.

Table S5. Topological properties of the electron density at ring critical points of quercetin monohydrate for the TAAM_OPT (first entry) and THEO_OPT (second entry in italics) models. The values of $\rho(\mathbf{r}_{CP})$ are given in eÅ^{-3} and $\nabla^2\rho(\mathbf{r}_{CP})$ in eÅ^{-5}.

Ring label	$\rho(\mathbf{r}_{CP})$	$\nabla^2\rho(\mathbf{r}_{CP})$
A (C11...C14)	0.1210	3.59
	0.1115	*3.78*
B (O1...C4)	0.1169	3.62
	0.1178	*3.78*
C (C8...C5)	0.1037	3.56
	0.1063	*3.72*
D (O5...C4)	0.1065	2.85
	0.1220	*2.89*
E (C3...C12)	0.0687	1.69
	0.0634	*1.90*

Table S6. Monopole charges obtained for the TAAM_OPT and THEO_OPT models. The charge values are given in |e|.

Atom Label	TAAM_OPT	THEO_OPT
O13	-0.23	-0.29
H13	0.21	0.23
O4	-0.17	-0.38
O1	-0.22	-0.20
O7	-0.23	-0.23
H7	0.21	0.23
O5	-0.23	-0.24
H5	0.21	0.21
O14	-0.23	-0.23
H14	0.21	0.20
O3	-0.23	-0.26
H3	0.21	0.21
O1W	-0.34	-0.21
H1W	0.17	0.10
H2W	0.17	0.11
C10	0.10	0.22
C2	0.04	0.04
C8	-0.03	0.18
H8	0.08	0.05
C9	0.04	-0.09
C6	-0.03	0.21
H6	0.08	0.03
C11	-0.03	-0.03
C7	0.04	-0.15
C3	0.04	0.12
C4	-0.08	0.01
C12	-0.03	0.08
H12	0.08	0.07
C13	0.04	0.01
C14	0.04	0.01
C5	0.04	-0.14
C16	-0.03	-0.04
H16	0.08	0.06
C15	-0.03	0.02
H15	0.08	0.06

Table S7. Computed Electrostatic Potential surface quantities for the TAAM_OPT and THEO_OPT models.

Surface quantity	TAAM_OPT	THEO_OPT
$V_{S,\max}$	50.8	45.6
$V_{S,\min}$	-48.1	-37.0
$\overline{V}_S^+$	18.2	14.2
$\overline{V}_S^-$	-11.6	-10.2
$\overline{V}_S$	1.2	2.0
Π	14.7	12.4
σ_+^2	177.4	156.7
σ_-^2	86.8	86.8
σ_{tot}^2	264.2	243.5
ν	0.221	0.229

The quantities: $V_{S,\max}$, $V_{S,\min}$, $\overline{V}_S^+$, $\overline{V}_S^-$, $\overline{V}_S$ and Π are given in kcal/mol; σ_+^2, σ_-^2 and σ_{tot}^2 are in (kcal/mol)^2; ν is dimensionless. The following definitions were used to calculate surface quantities:

$$\overline{V}_S^+ = \frac{1}{p}\sum_{i=1}^{p} V_S^+(\mathbf{r}_i), \qquad \overline{V}_S^- = \frac{1}{n}\sum_{i=1}^{n} V_S^-(\mathbf{r}_i), \qquad \overline{V}_S = \frac{1}{p+n}\sum_{i=1}^{p+n} V_S(\mathbf{r}_i),$$

$$\Pi = \frac{1}{p+n}\sum_{i=1}^{p+n}\left|V_S(\mathbf{r}_i) - \overline{V}_S\right|, \qquad \sigma_+^2 = \frac{1}{p}\sum_{i=1}^{p}[V_S^+(\mathbf{r}_i) - \overline{V}_S^+]^2, \qquad \sigma_-^2 = \frac{1}{n}\sum_{i=1}^{n}[V_S^-(\mathbf{r}_i) - \overline{V}_S^-]^2,$$

$$\sigma_{\text{tot}}^2 = \sigma_+^2 + \sigma_-^2, \; \nu = \frac{\sigma_+^2\sigma_-^2}{(\sigma_{\text{tot}}^2)^2}.$$

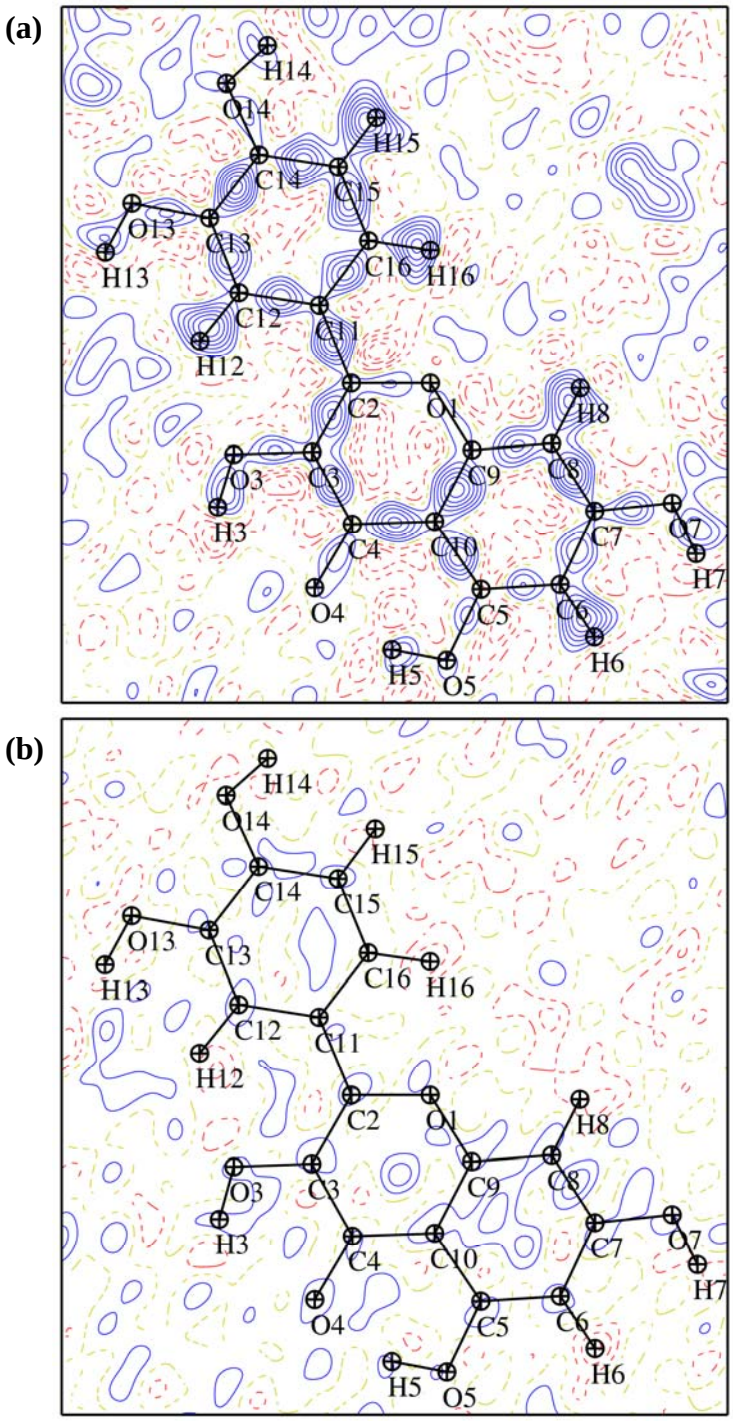


Figure S1. Residual experimental electron density maps in the plane of quercetin molecule for the (a) IAM_R and (b) TAAM_R models. Blue solid lines and red dashed lines denote positive and negative values, respectively. Contour level at ± 0.05 eÅ^{-3}. The zero contours are shown in yellow dashed lines.

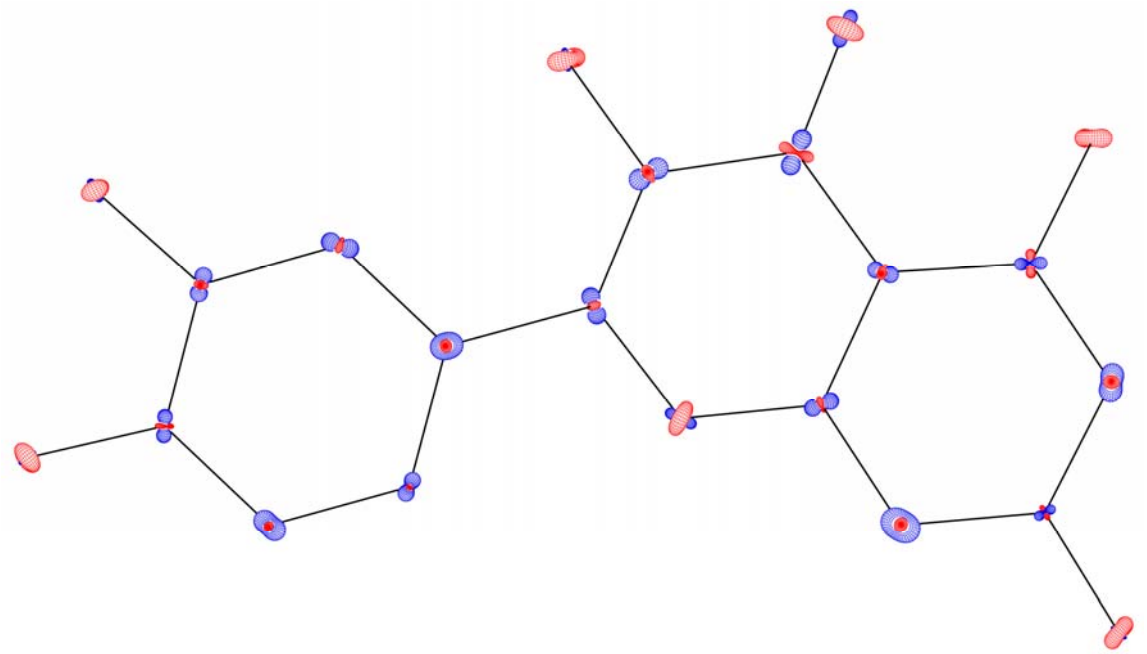
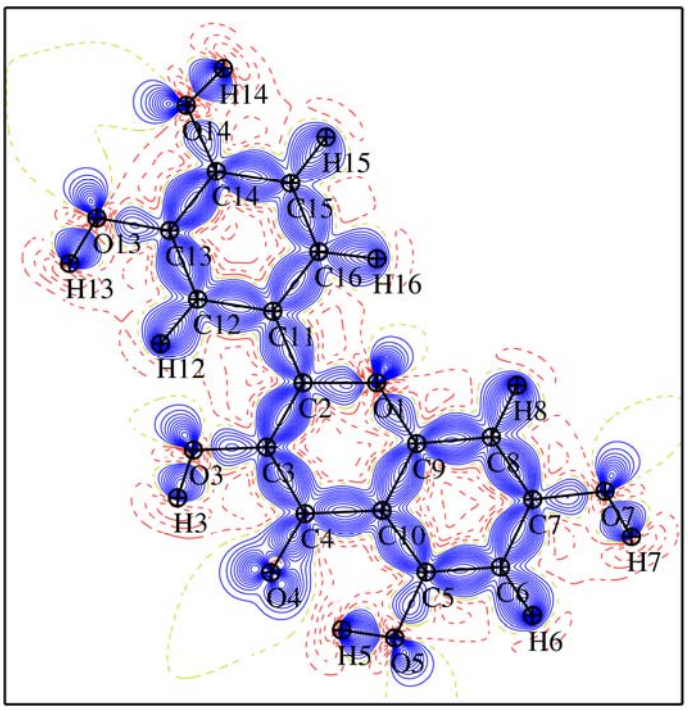


Figure S2. PEANUT[64] representations of the ADP differences between the TAAM_THEO_R and TAAM_R restrained models. The root mean square displacement differences surfaces are shown in scale of 6.15. The positive differences appear in blue, while the negative are in red. Hydrogen atoms were omitted.

(a)



(b)

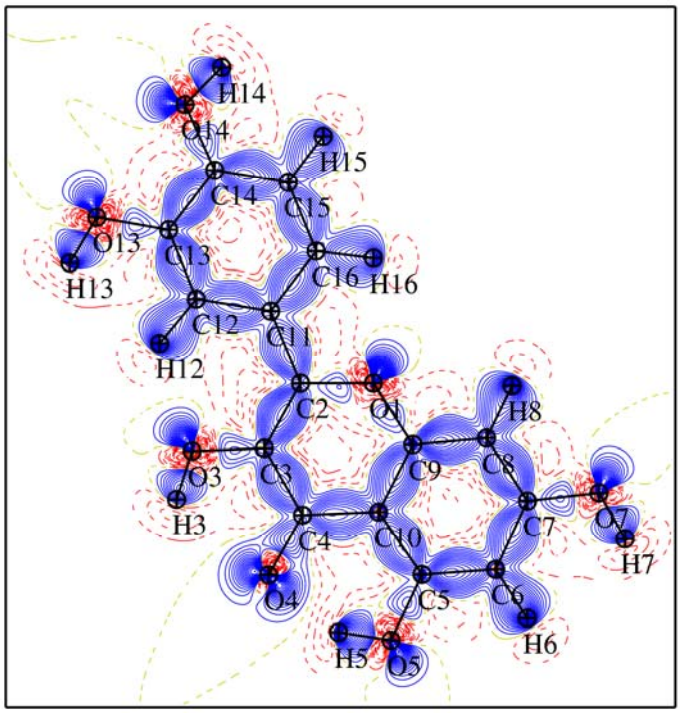


Figure S3. Static deformation density maps in the plane of the quercetin molecule for (a) TAAM_OPT and (b) THEO_OPT models. Blue solid lines and red dashed lines denote positive and negative contours, respectively. Contour level at ± 0.05 eÅ^{-3}. The zero contours are shown in yellow dashed lines.

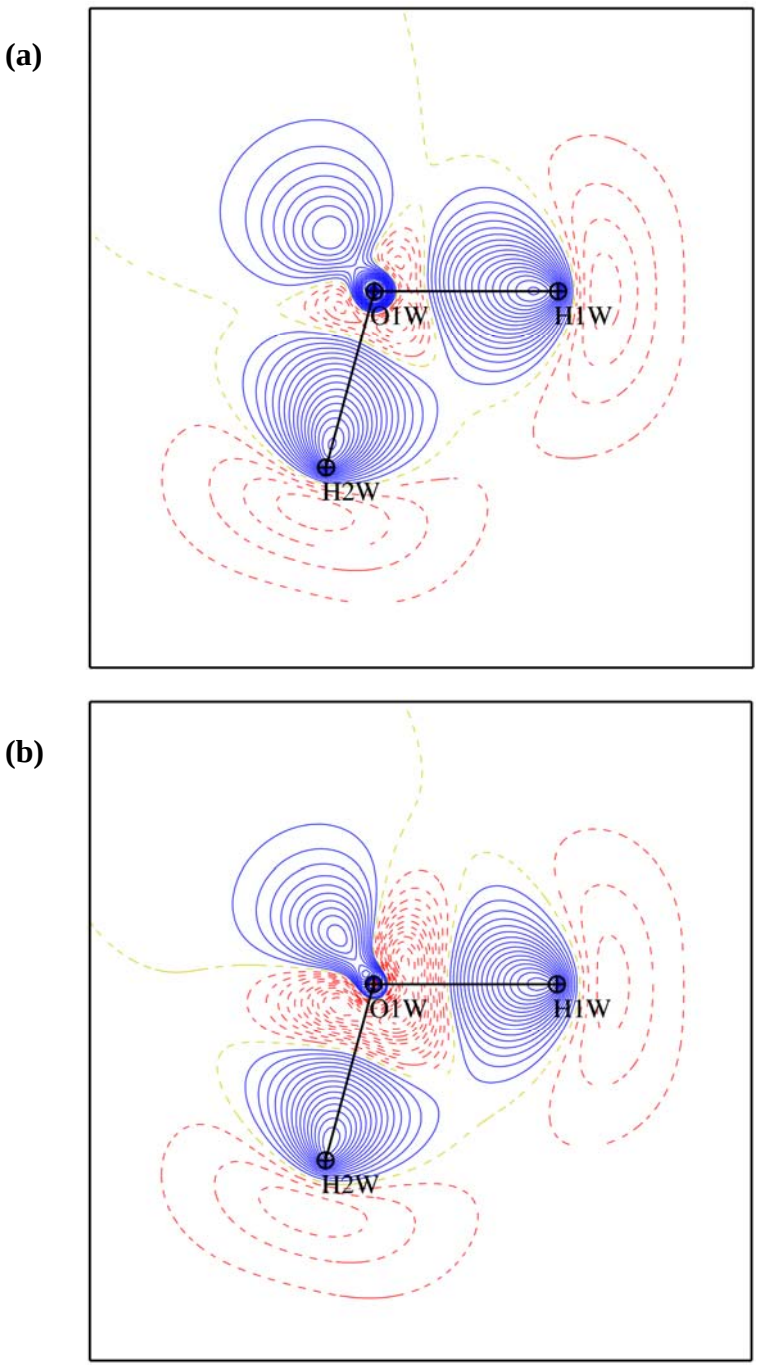
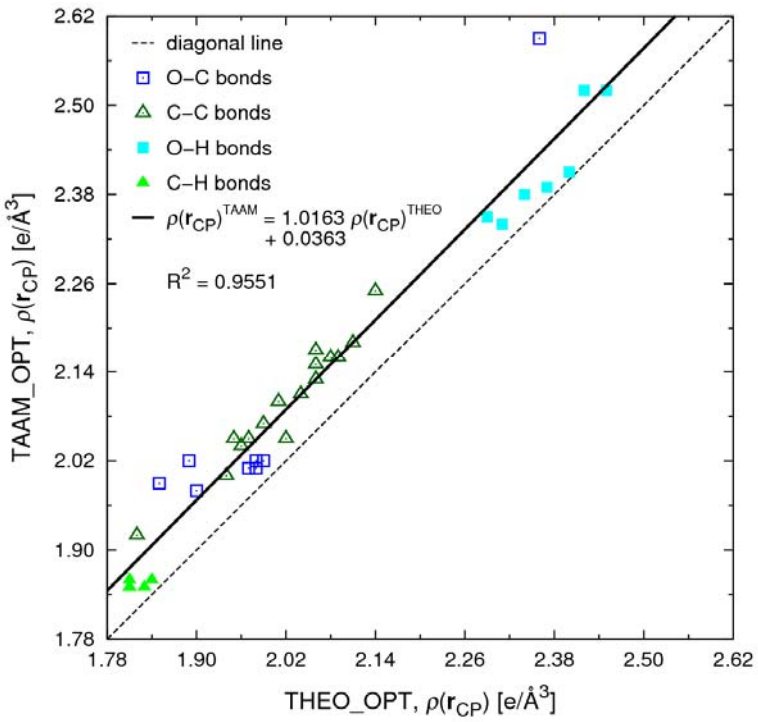
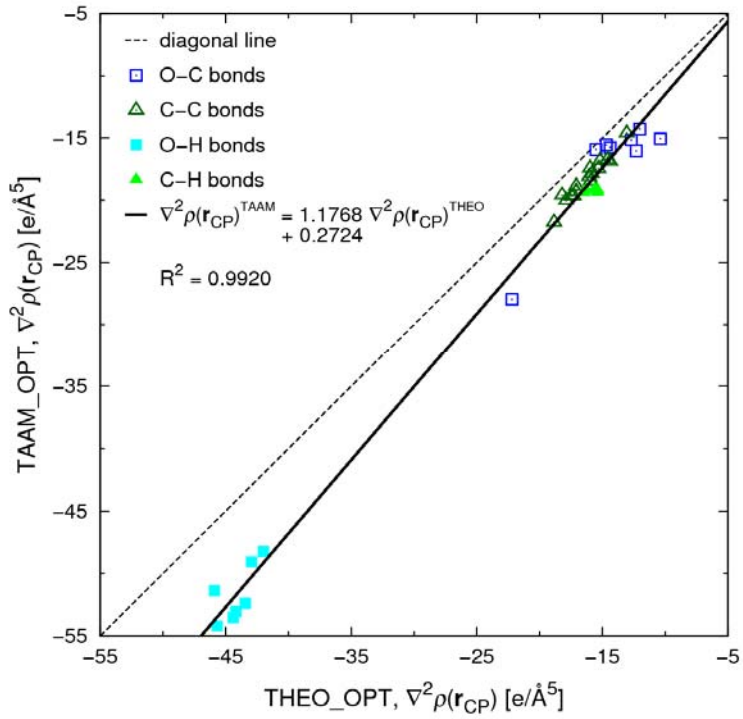


Figure S4. Static deformation density maps for the water molecule in quercetin monohydrate presented in the plane defined by H1W, O1W and H2W atoms for (a) TAAM_OPT and (b) THEO_OPT models, respectively. Blue solid lines and red dashed lines denote positive and negative values, respectively. Contour level at ±0.05 eÅ^{-3}. The zero contours are shown in yellow dashed lines.

(a)


diagonal line
O–C bonds
C–C bonds
O–H bonds
C–H bonds
$\rho(\mathbf{r}_{CP})^{TAAM} = 1.0163\ \rho(\mathbf{r}_{CP})^{THEO} + 0.0363$
$R^2 = 0.9551$
TAAM_OPT, $\rho(\mathbf{r}_{CP})$ [e/Å^3]
THEO_OPT, $\rho(\mathbf{r}_{CP})$ [e/Å^3]
1.78
1.90
2.02
2.14
2.26
2.38
2.50
2.62

(b)


diagonal line
O–C bonds
C–C bonds
O–H bonds
C–H bonds
$\nabla^2\rho(\mathbf{r}_{CP})^{TAAM} = 1.1768\ \nabla^2\rho(\mathbf{r}_{CP})^{THEO} + 0.2724$
$R^2 = 0.9920$
TAAM_OPT, $\nabla^2\rho(\mathbf{r}_{CP})$ [e/Å^5]
THEO_OPT, $\nabla^2\rho(\mathbf{r}_{CP})$ [e/Å^5]
−5
−15
−25
−35
−45
−55

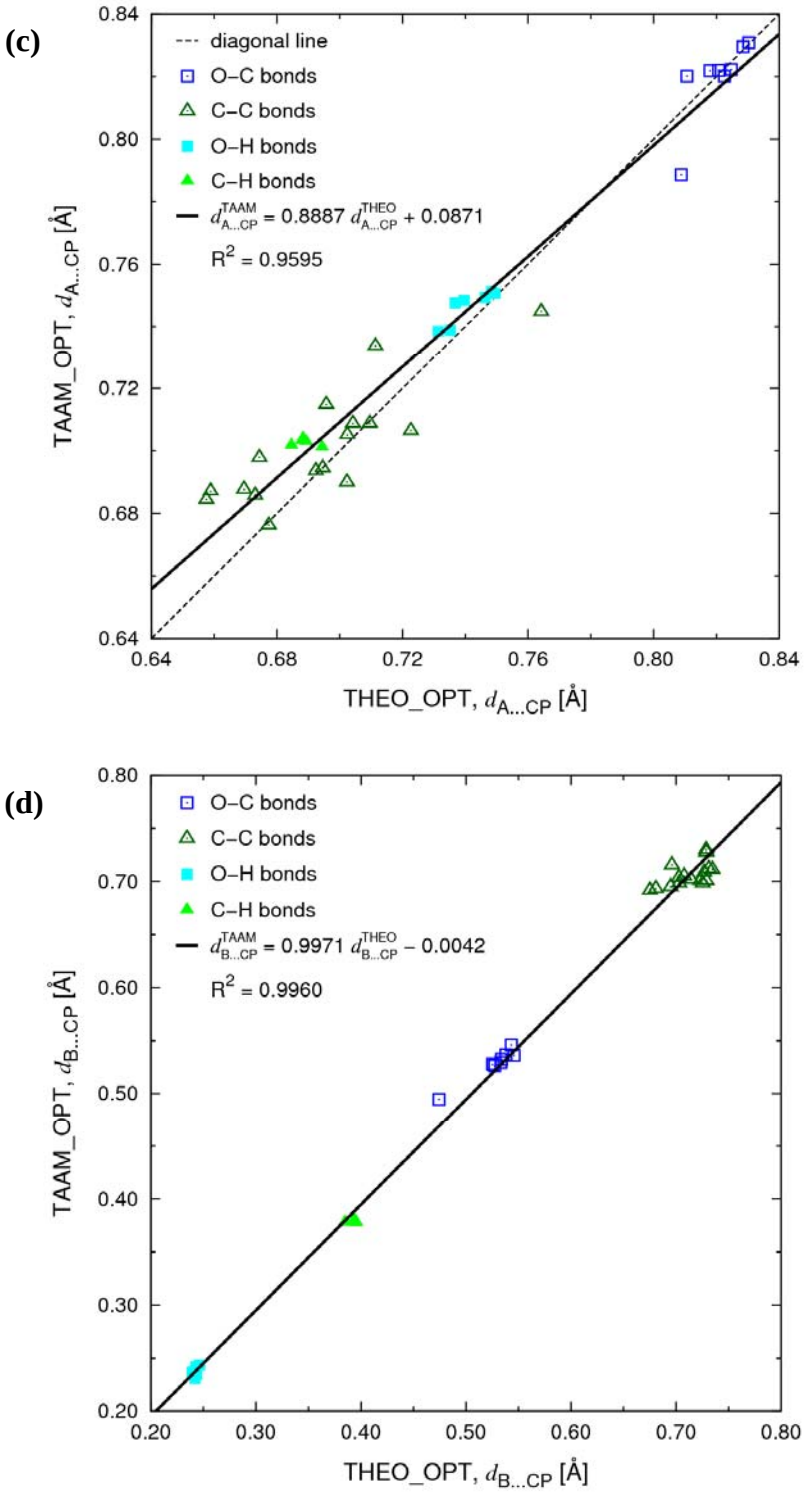
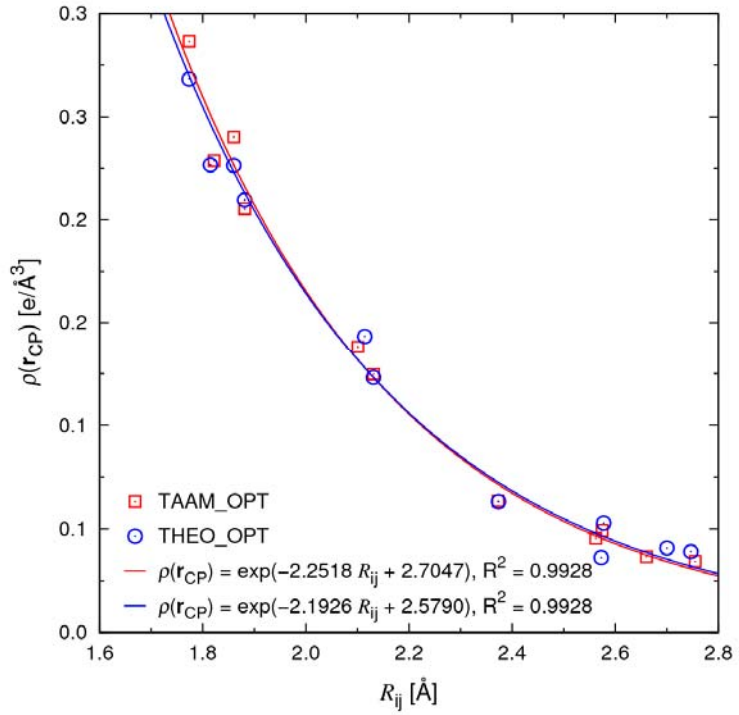
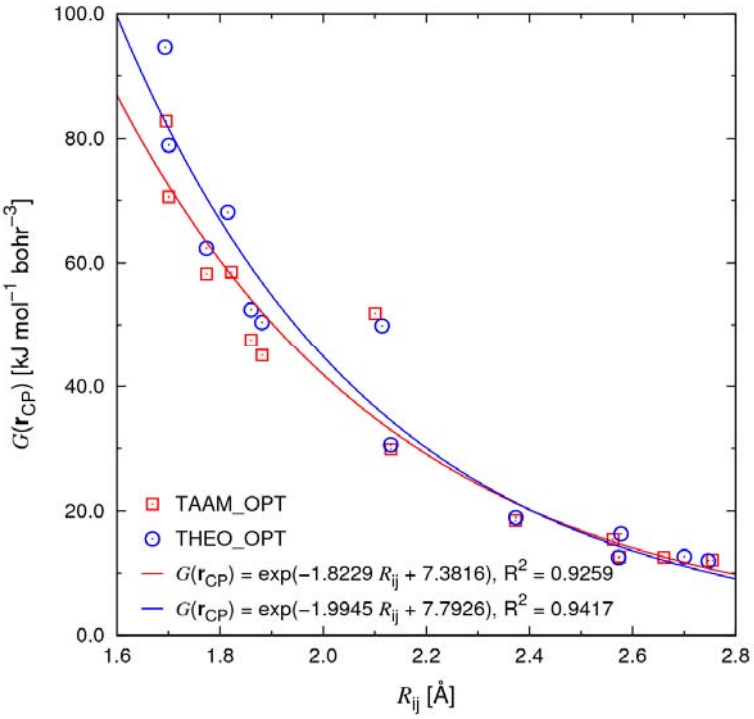


Figure S5. Correlation between topological properties of the total electron density of the covalent bonds for the TAAM_OPT and THEO_OPT models. Plots show the relative correlation of (a) $\rho(\mathbf{r}_{CP})$, (b) $\nabla^2 \rho(\mathbf{r}_{CP})$ (c) $d_{A...CP}$ and (d) $d_{B...CP}$ values between TAAM_OPT and THEO_OPT.

(a)


0.3
0.3
0.2
0.2
0.1
0.1
0.0
1.6
1.8
2.0
2.2
2.4
2.6
2.8
$\rho(\mathbf{r}_{CP})$ [e/Å^3]
R_{ij} [Å]
TAAM_OPT
THEO_OPT
$\rho(\mathbf{r}_{CP})$ = exp(−2.2518 R_{ij} + 2.7047), R^2 = 0.9928
$\rho(\mathbf{r}_{CP})$ = exp(−2.1926 R_{ij} + 2.5790), R^2 = 0.9928

(b)


100.0
80.0
60.0
40.0
20.0
0.0
1.6
1.8
2.0
2.2
2.4
2.6
2.8
$G(\mathbf{r}_{CP})$ [kJ mol^{-1} bohr^{-3}]
R_{ij} [Å]
TAAM_OPT
THEO_OPT
$G(\mathbf{r}_{CP})$ = exp(−1.8229 R_{ij} + 7.3816), R^2 = 0.9259
$G(\mathbf{r}_{CP})$ = exp(−1.9945 R_{ij} + 7.7926), R^2 = 0.9417

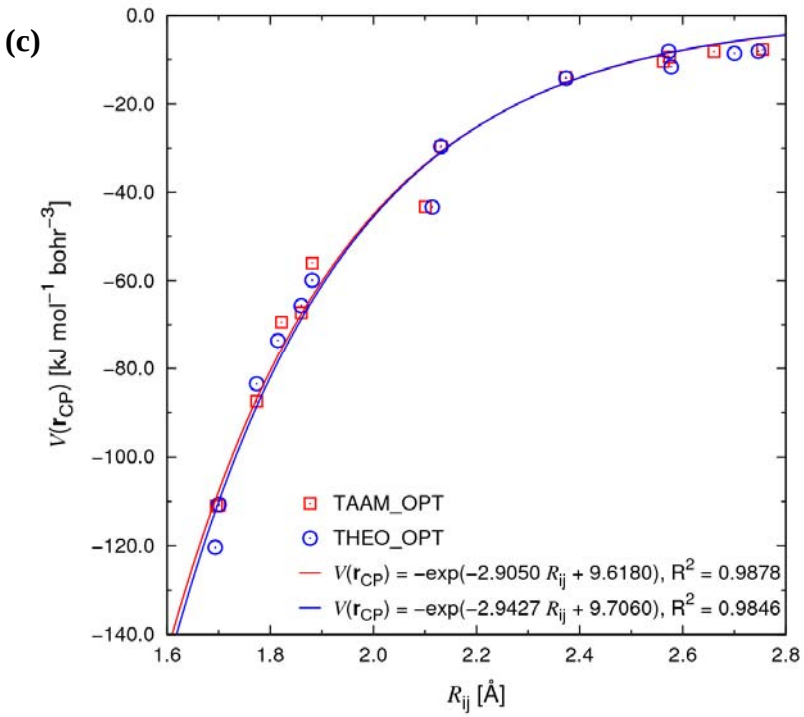
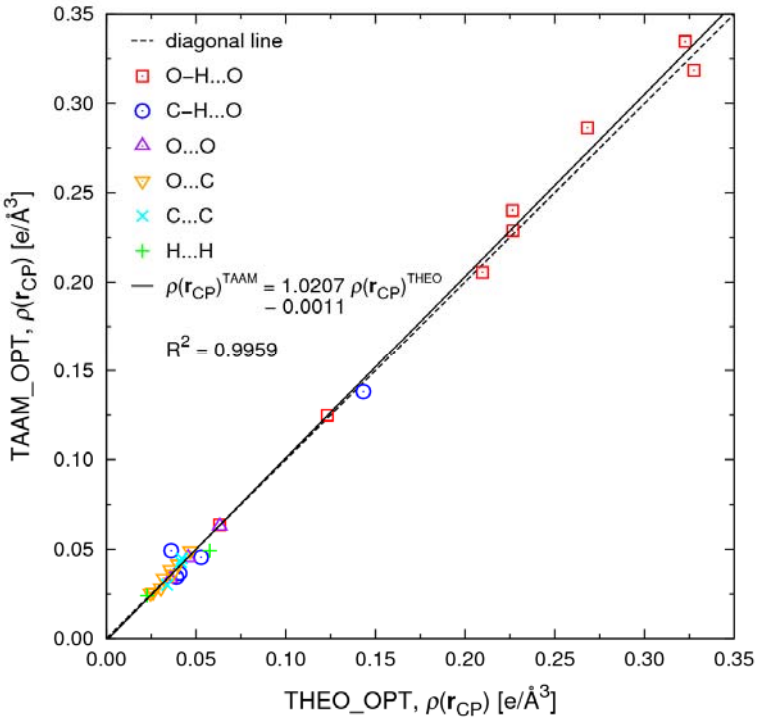
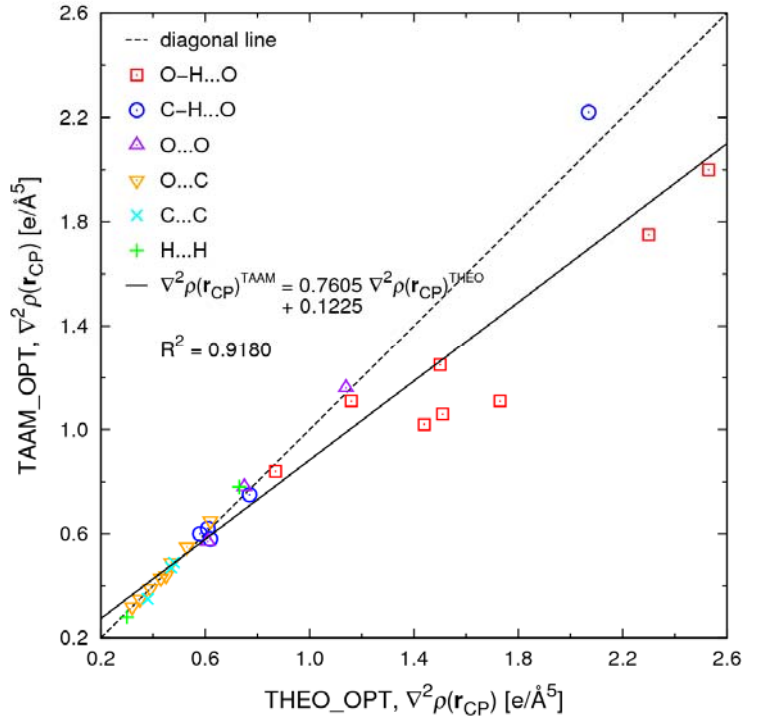


Figure S6. Plots of dependencies between (a) $\rho(\mathbf{r}_{CP})$ and R_{ij}; (b) $G(\mathbf{r}_{CP})$ and R_{ij}; (c) $V(\mathbf{r}_{CP})$ and R_{ij} for X-H...O contacts. Dependencies shown for both TAAM_OPT (blue data points) and THEO_OPT (red data points) models.

(a)


diagonal line
O–H...O
C–H...O
O...O
O...C
C...C
H...H
$\rho(\mathbf{r}_{CP})^{TAAM} = 1.0207\ \rho(\mathbf{r}_{CP})^{THEO} - 0.0011$
$R^2 = 0.9959$
TAAM_OPT, $\rho(\mathbf{r}_{CP})$ [e/Å^3]
THEO_OPT, $\rho(\mathbf{r}_{CP})$ [e/Å^3]
0.00
0.05
0.10
0.15
0.20
0.25
0.30
0.35

(b)


diagonal line
O–H...O
C–H...O
O...O
O...C
C...C
H...H
$\nabla^2\rho(\mathbf{r}_{CP})^{TAAM} = 0.7605\ \nabla^2\rho(\mathbf{r}_{CP})^{THEO} + 0.1225$
$R^2 = 0.9180$
TAAM_OPT, $\nabla^2\rho(\mathbf{r}_{CP})$ [e/Å^5]
THEO_OPT, $\nabla^2\rho(\mathbf{r}_{CP})$ [e/Å^5]
0.2
0.6
1.0
1.4
1.8
2.2
2.6

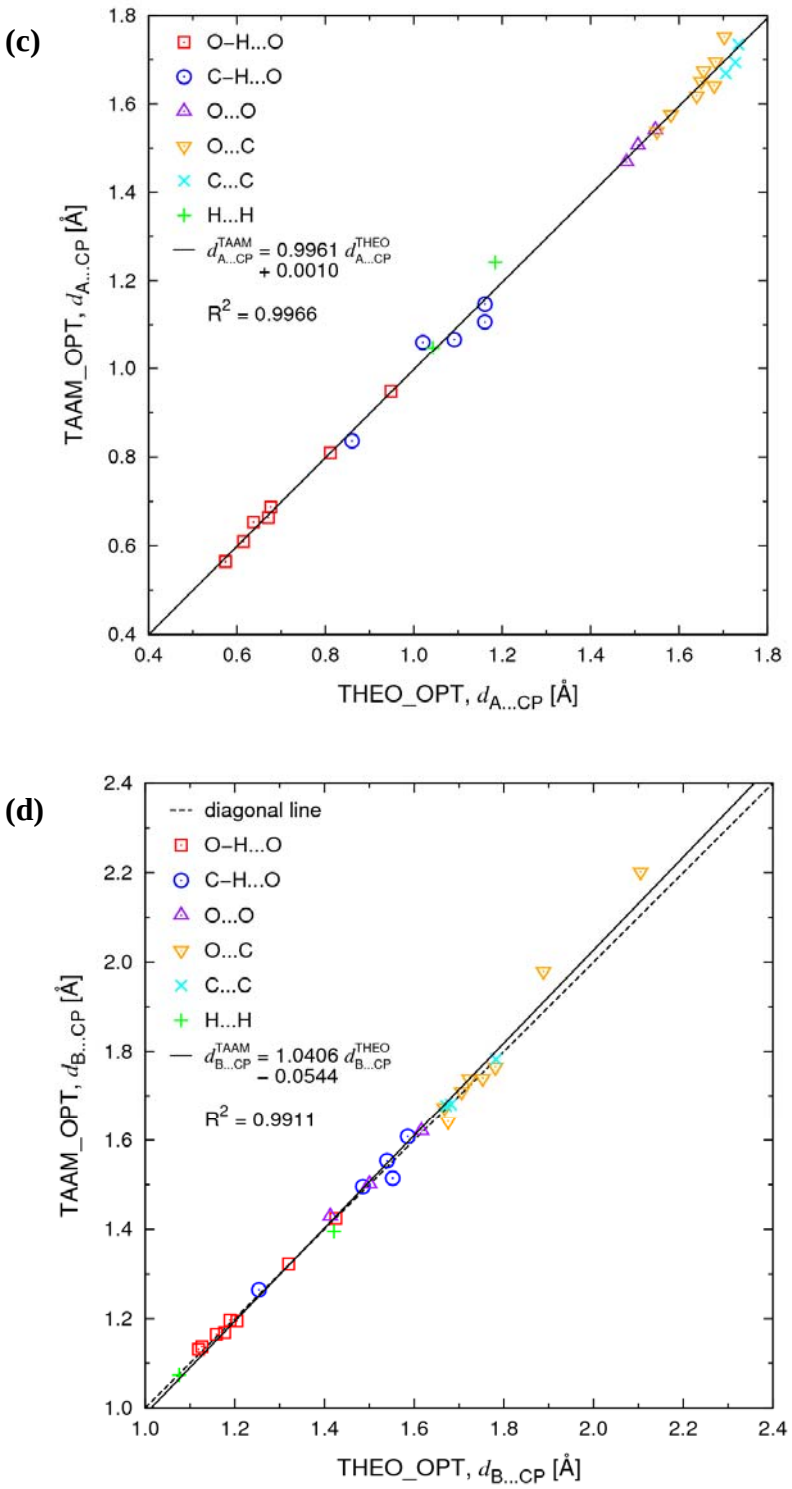


Figure S7. Correlation between topological properties of the total electron density for the weak interactions for the TAAM_OPT and THEO_OPT models. Plots show the relative correlation of (a) $\rho(\mathbf{r}_{CP})$, (b) $\nabla^2 \rho(\mathbf{r}_{CP})$ (c) $d_{A...CP}$ and (d) $d_{B...CP}$ values between TAAM_OPT and THEO_OPT.

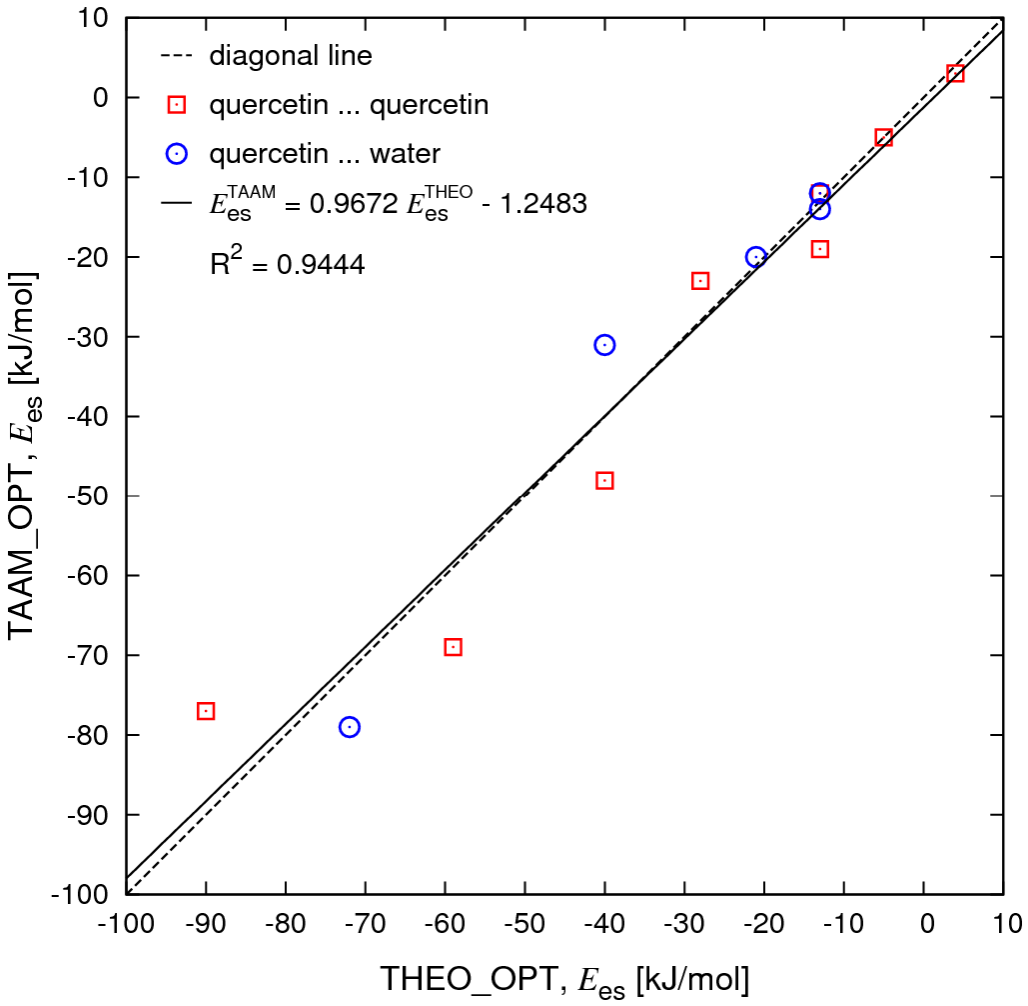


Figure S8. Correlation between electrostatic interaction energies obtained for different pairs of molecules for the TAAM_OPT and THEO_OPT models. Interactions between quercetin molecules are displayed as red squares, whereas quercetin...water short contacts are presented as blue circles.

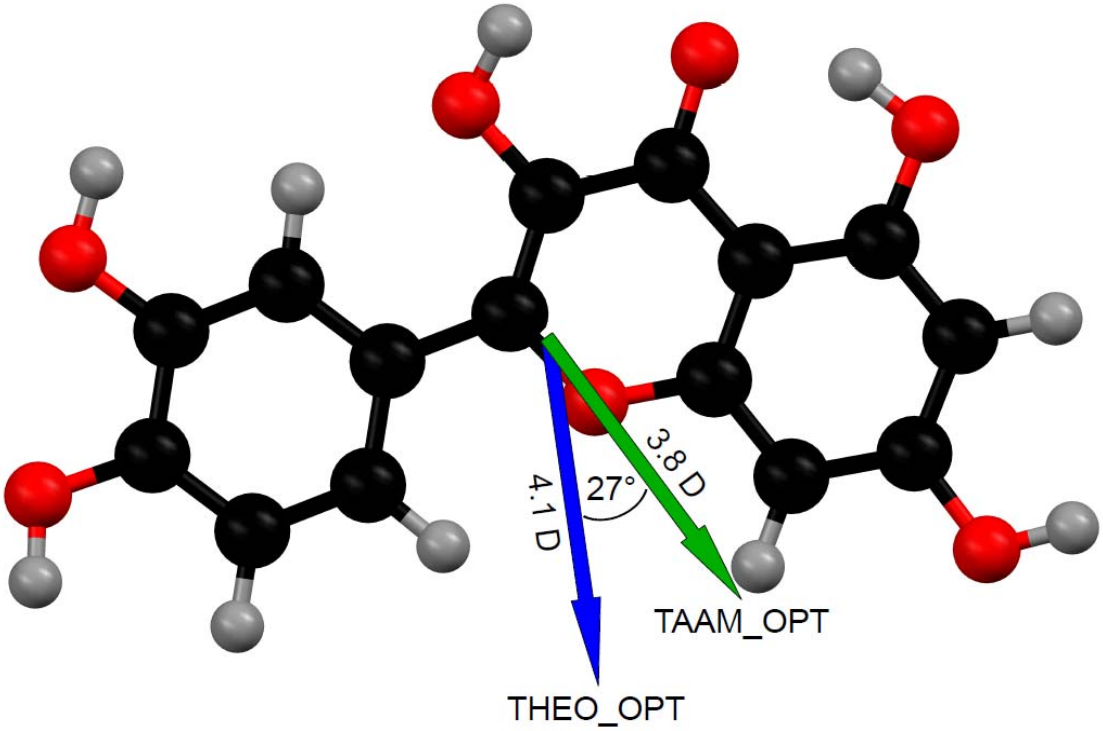


Figure S9. Representation of quercetin molecule with the dipole moment vectors marked for the TAAM_OPT (green arrow) and THEO_OPT (blue arrow) models.