Supplementary Information

Gallic acid-cholesterol conjugate synthesis, spectroscopic characterization and quantum chemical calculations: Experimental and theoretical approach

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Table S1— Theoretical (B3LYP/6-31G(d,p)) and experimental ($CDCl_3$) ^1H and ^{13}C NMR chemical shifts (δ, δC, ppm) for compound **3**

^{13}C NMR			^1H NMR		
Atom	Calculated	Experimental	Atom	Calculated	Experimental
C-1	38.03	37.04	37OCH3(s)	4.21	3.91
C-2	35.08	28.25	36OCH3(s)	4.19	3.90
C-3	74.42	74.82	35OCH3(s)	4.19	3.48
C-4	42.06	38.23	34H(s)	7.69	7.41
C-5	141.57	139.63	30H(s)	7.80	7.41
C-6	127.98	122.84	27H(d)	1.55	1.00
C-7	38.84	31.95	26H(d)	1.44	0.92
C-8	40.70	31.88	25H(d)	1.47	0.91
C-9	49.49	50.88	24H(m)	2.19	1.60
C-10	45.66	35.81	23H(q)	1.68	1.25
C-11	31.77	22.58	22H(m)	1.94	1.25
C-12	46.80	39.73	21H(m)	1.72	1.21
C-13	50.64	42.32	20H(m)	1.96	1.68
C-14	53.43	56.25	19H(s)	1.48	1.32
C-15	39.93	29.72	18H(s)	1.45	1.03
C-16	61.68	27.89	17H(m)	2.25	1.45
C-17	31.95	56.69	16H(m)	1.91	1.51
C-18	29.38	19.43	15H(m)	2.22	1.51
C-19	33.39	21.07	14H(m)	2.68	1.45
C-20	47.35	36.66	12H(m)	2.28	1.57
C-21	46.28	36.19	11H(m)	1.82	1.35
C-22	36.97	24.31	9H(m)	1.81	1.57
C-23	47.70	39.52	8H(m)	2.71	1.35
C-24	38.45	28.03	7H(m)	2.53	1.95
C-25	32.49	23.84	6H(m)	5.95	5.41
C-26	38.45	22.85	4H(d)	2.90	2.44
C-27	26.14	19.43	3H(m)	4.29	4.84
C-28	163.13	165.64	2H(m)	2.20	1.71
C-29	105.55	125.88	1H(t)	2.09	1.11
C-30	118.00	106.72			
C-31	144.53	152.87			
C-32	144.66	142.00			
C-33	143.97	152.87			
C-34	116.47	106.72			
C-35	64.20	56.12			
C-36	62.97	60.92			
C-37	64.31	56.12			

Table S2— Topological parameters for intramolecular interaction in compound; electron density (ρ_{BCP}), Laplacian of electron density ($\Delta^2\rho_{BCP}$), electron kinetic energy density (G_{BCP}), electron potential energy density (V_{BCP}), total electron energy density (H_{BCP}), Hydrogen bond energy (E_{HB}) at bond critical point (BCP)

Interactions	$\boldsymbol{\rho}_{\mathbf{BCP}}$	$\Delta^2\rho_{BCP}$	$\boldsymbol{G}_{\mathbf{BCP}}$	$\boldsymbol{V}_{\mathbf{BCP}}$	$\boldsymbol{H}_{\mathbf{BCP}}$	$\boldsymbol{E}_{\mathbf{HB}}$
H7-H17	0.012461	0.046070	0.009456	-0.007394	0.002062	-0.003697
H22-H27	0.010104	0.037715	0.007651	-0.005873	0.001778	-0.002936
H12-H17	0.009256	0.035246	0.007139	-0.005467	0.001672	-0.002733
H1-H11	0.011013	0.037873	0.007842	-0.006216	0.001626	-0.003108
H18-H19	0.011709	0.039262	0.008179	-0.006543	0.001636	-0.003271
H35-O4	0.010930	0.039076	0.008580	-0.007392	0.001188	-0.003696
H37-O4	0.011932	0.047770	0.009360	-0.008025	0.001335	-0.004012