

Supplementary Information

Conformational Analysis, Experimental and GIAO-DFT ^{13}C NMR Chemical Shift Calculation on 2'-Hydroxy-3,4,5-trimethoxy-chalcone

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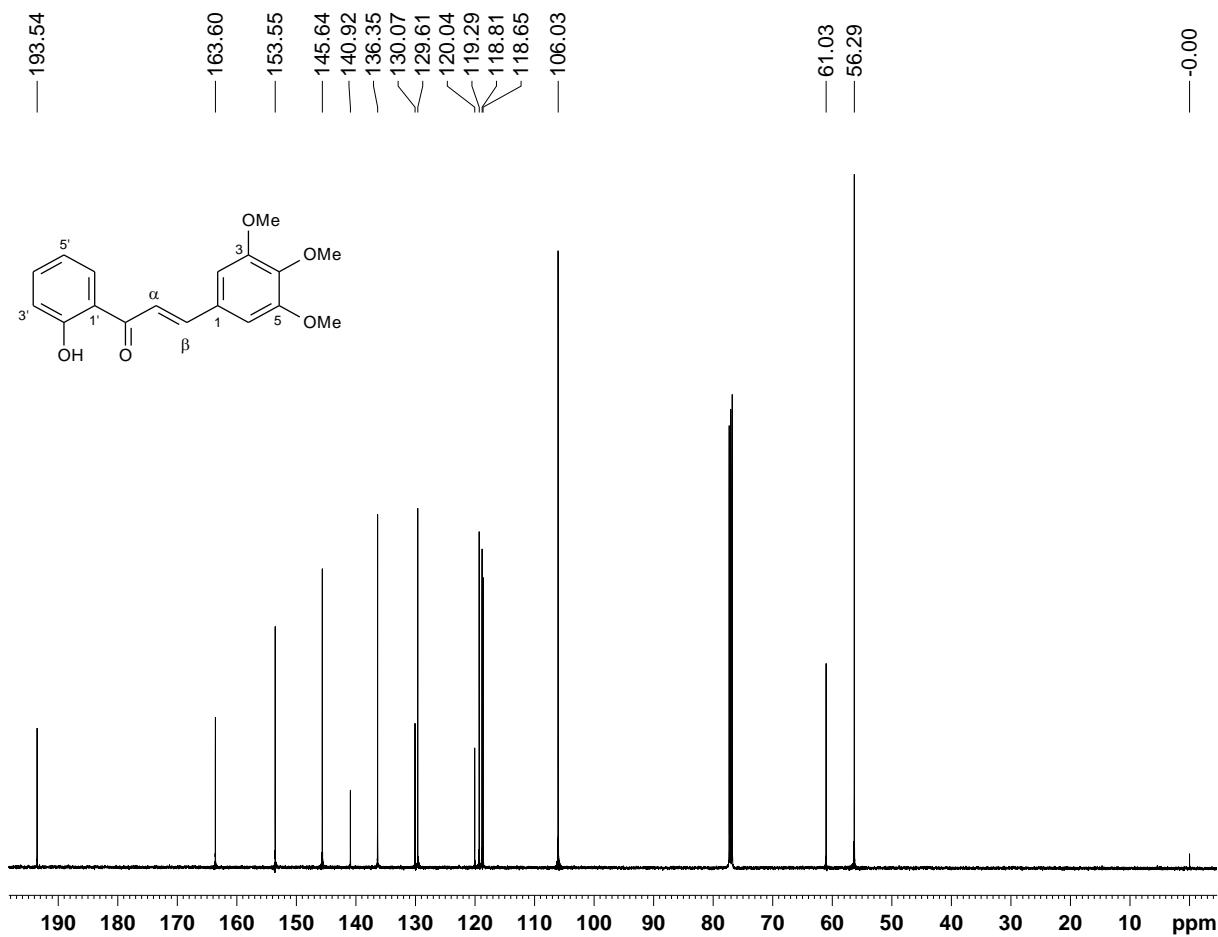


Figure S1. ^{13}C NMR spectrum (125.7 MHz, CDCl_3) of 2'-hydroxy-3,4,5-trimethoxy-chalcone.

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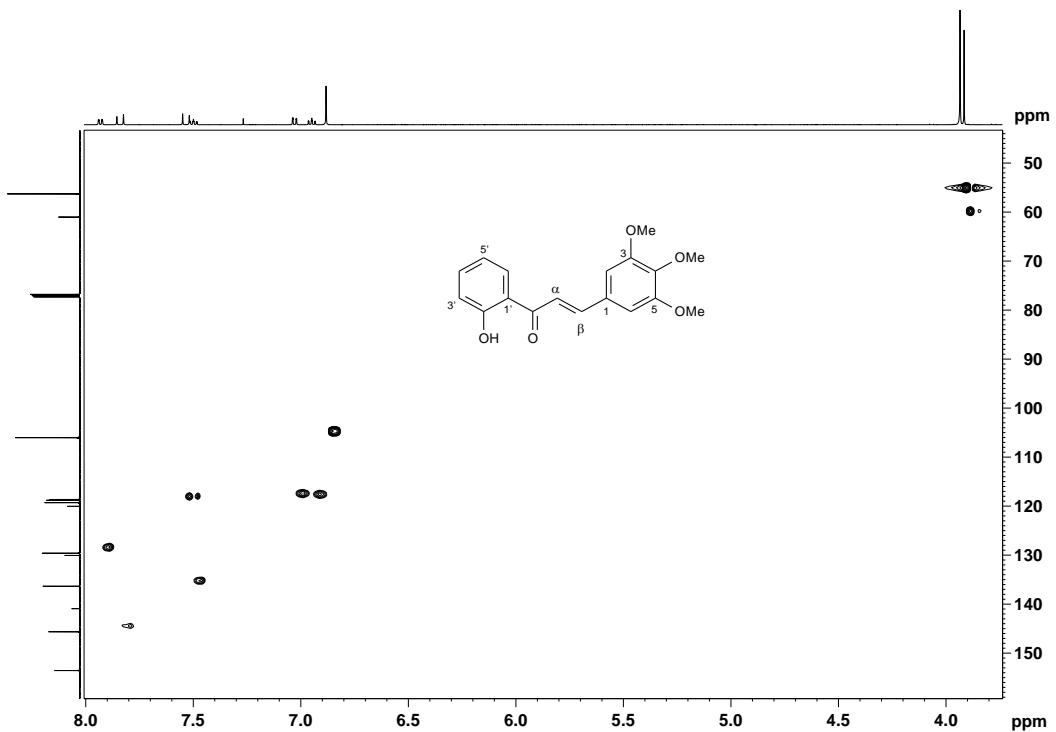


Figure S2. HSQC NMR contour map (500 MHz, CDCl_3) of 2'-hydroxy-3,4,5-trimethoxy-chalcone.

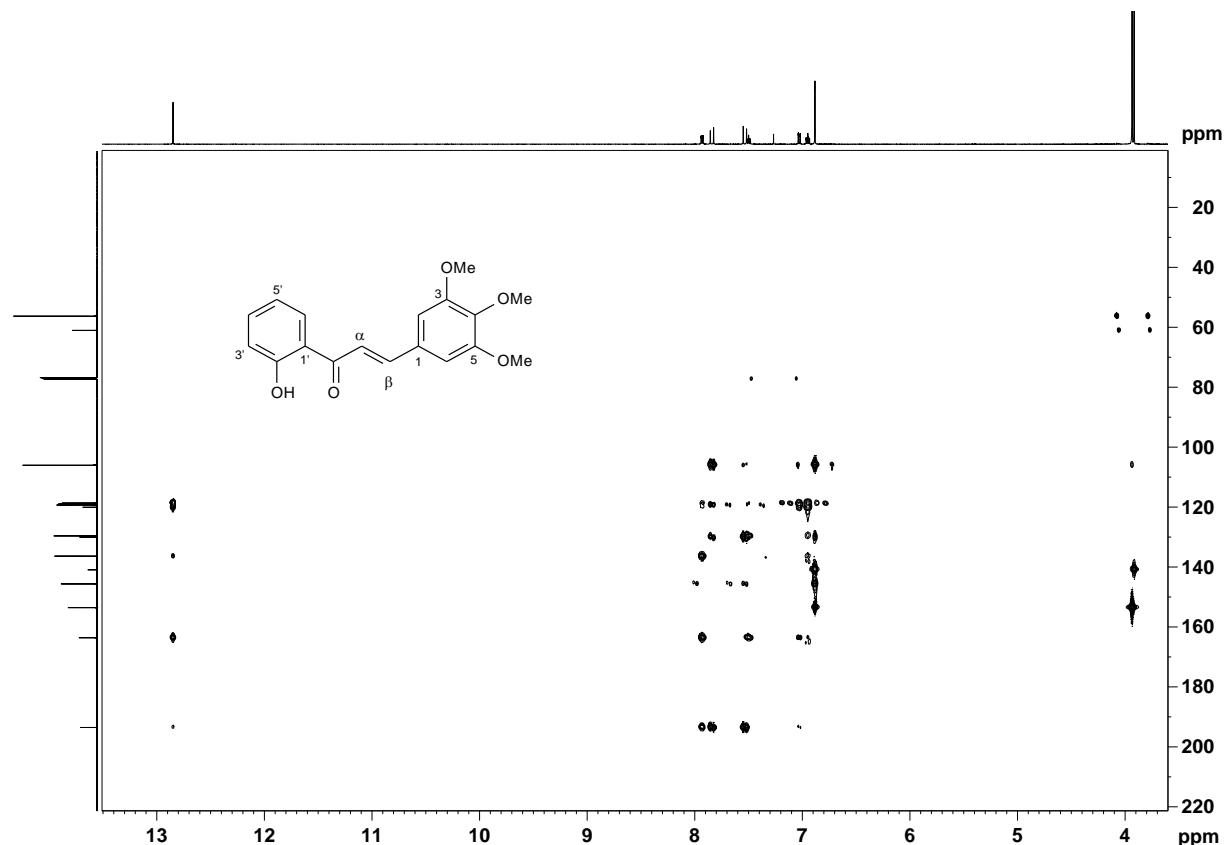


Figure S3. HMBC NMR contour map (500 MHz, CDCl_3) of 2'-hydroxy-3,4,5-trimethoxy-chalcone.

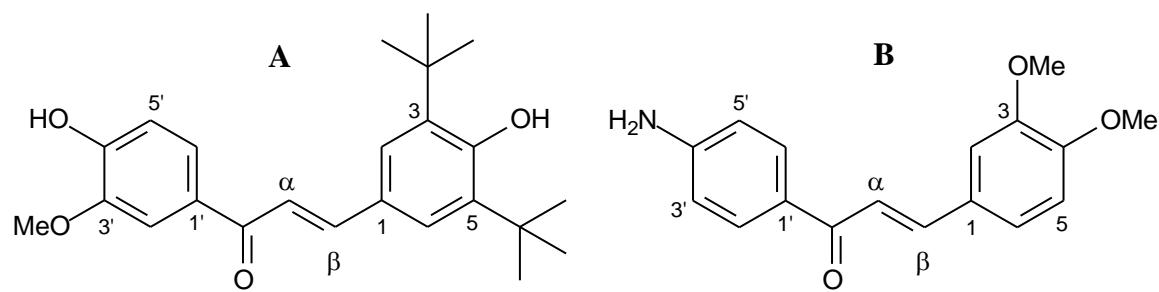


Figure S4. Structure of (*E*)-1-(4-hydroxy-3-methoxyphenyl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)prop-2-en-1-one (A) and (*E*)-1-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one (B).

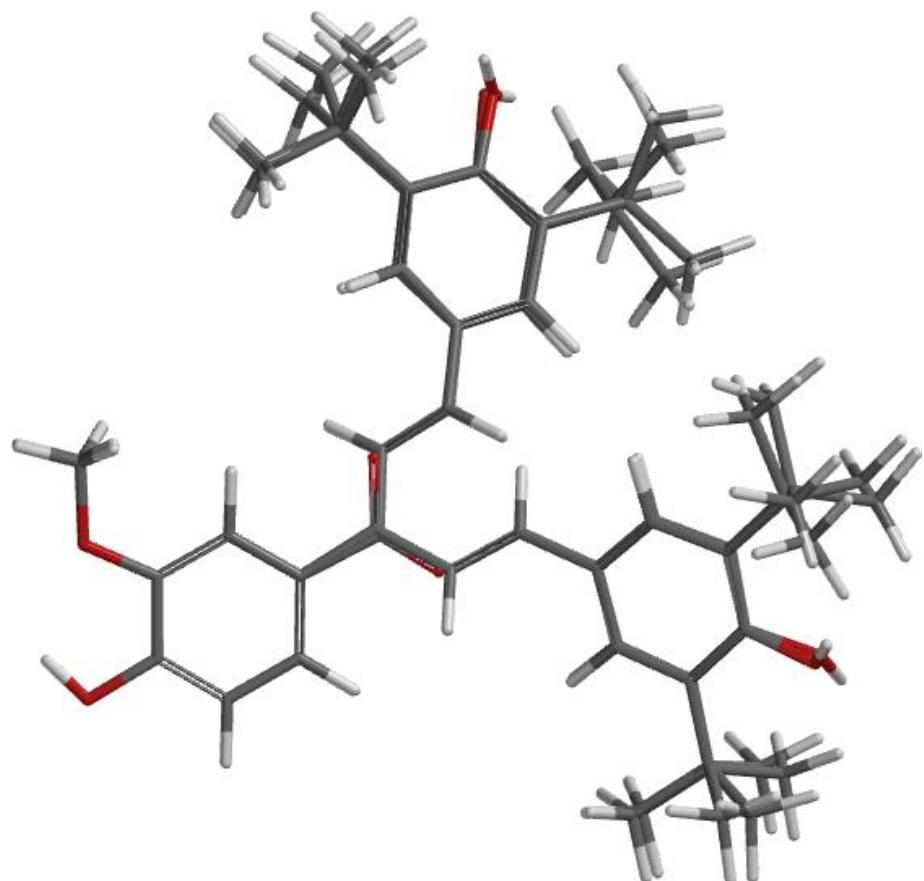


Figure S5. Superposition of the four lowest energy conformations of (*E*)-1-(4-hydroxy-3-methoxyphenyl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)prop-2-en-1-one molecule.

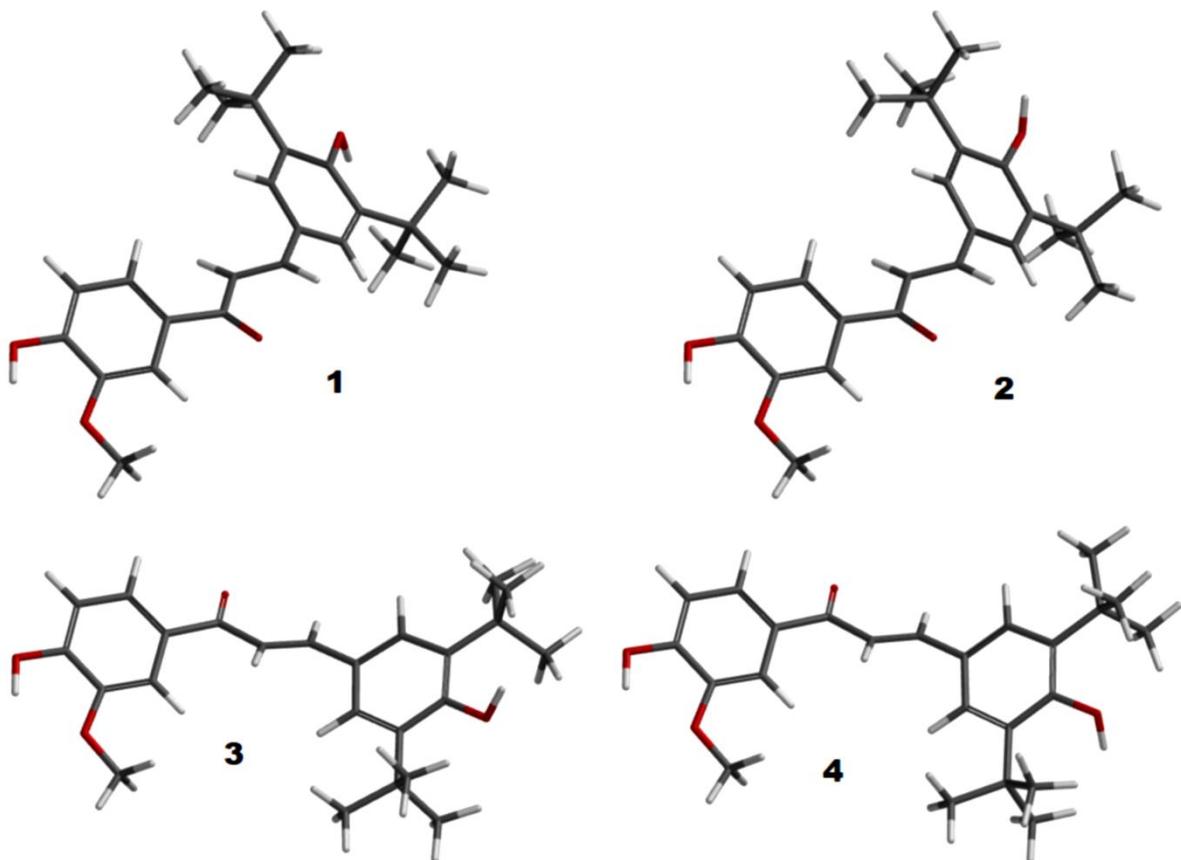


Figure S6. DFT-optimized structures of the four more stable conformers, 1, 2, 3 and 4, respectively, of (E)-1-(4-hydroxy-3-methoxyphenyl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)prop-2-en-1-one. For relative energies and abundances of the conformers, see Table S1.

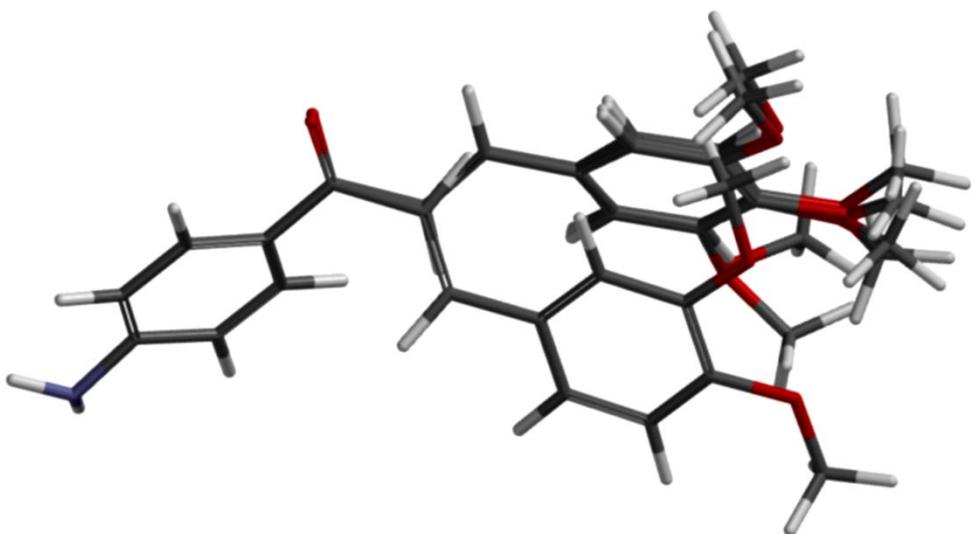


Figure S7. Superposition of the five lowest energy conformations of (E)-1-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one molecule.

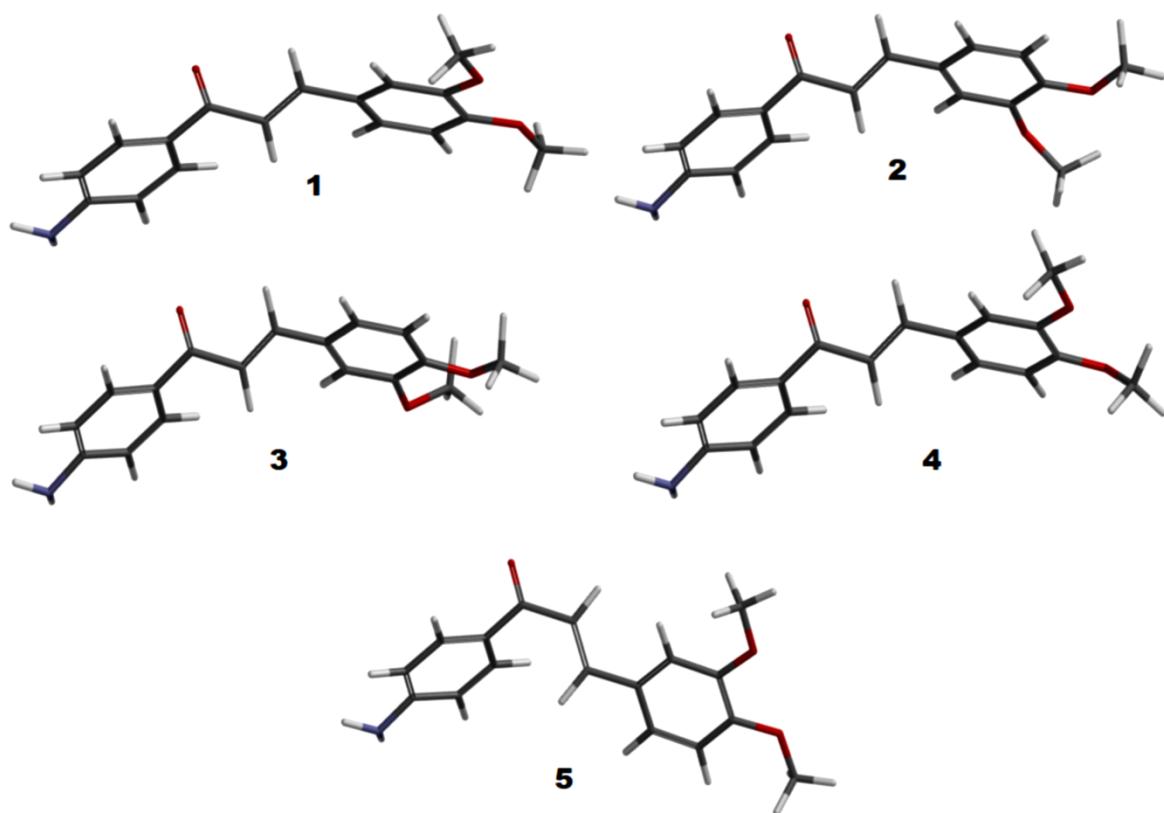


Figure S8. DFT-optimized structures of the five more stable conformers, 1, 2, 3, 4 and 5, respectively, of (E)-1-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one. For relative energies and abundances of the conformers, see Table S3.

Table S1. DFT, thermo chemical parameter and DFT population for the 17 more significant conformations of (*E*)-1-(4-hydroxy-3-methoxyphenyl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)prop-2-en-1-one

Conformer	ΔE^a / (kcal mol ⁻¹)	Bolt. dist. ^b / %	ΔE^c / (kcal mol ⁻¹)	Bolt. dist. ^d / %	ΔE^e / (kcal mol ⁻¹)	Bolt. dist. ^f / %	ΔG^g / (kcal mol ⁻¹)	Bolt. dist. ^h / %
001	0.00	49	0.00	71.4	0.00	53.4	0.00	65.4
002	0.11	41	0.68	20.4	0.16	39.9	0.44	29.0
003	1.28	5.6	1.29	6.6	1.42	3.9	1.56	3.7
004	1.53	3.7	2.54	0.7	1.79	2.0	1.91	2.0
005	3.07	0.3	2.81	0.4	2.60	0.4	—	—
006	3.15	0.2	2.94	0.3	2.63	0.4	—	—
007	3.79	0.1	3.78	0.1	—	—	—	—
008	4.13	0.0	3.79	0.1	—	—	—	—
009	6.24	0.0	4.06	0.0	—	—	—	—
010	6.30	0.0	—	—	—	—	—	—
011	7.80	0.0	—	—	—	—	—	—
012	8.01	0.0	—	—	—	—	—	—
013	8.79	0.0	—	—	—	—	—	—
014	8.91	0.0	—	—	—	—	—	—
015	8.97	0.0	—	—	—	—	—	—
016	9.08	0.0	—	—	—	—	—	—
017	9.39	0.0	—	—	—	—	—	—

^aRelative MMFF energy of conformers obtained from Monte Carlo analysis; ^bMMFF Boltzmann population of the conformers; ^crelative B3LYP/6-31G(d) single point energy of conformers obtained from Monte Carlo analysis; ^dB3LYP/6-31(g) single point energy Boltzmann population of the conformers; ^erelative mPW1PW91/6-31G(d) energy minimization of the conformers; ^fmPW1PW91/6-31G(d) energy minimization Boltzmann population of the conformers; ^grelative mPW1PW91/6-31G(d) sum of electronic and free energy of the conformers; ^hmPW1PW91/6-31G(d) Boltzmann population calculated from ΔG values of the conformers.

Table S2. Calculated (scaled) and differences between experimental ^{13}C NMR chemical shifts (in ppm) in the (*E*)-1-(4-hydroxy-3-methoxyphenyl)-3-(3,5-di-*tert*-butyl-4-hydroxyphenyl)prop-2-en-1-one relative to TMS, for approaches (I) and (II)

Nuclei	δ_{exp}	Approach (I)		Approach (II)	
		$\delta_{\text{calc}}^{\text{a}} (\delta_{\text{scal}})^{\text{b}}$	$\neq \delta_{\text{calc}} (\delta_{\text{scal}})$	$\delta_{\text{calc}}^{\text{a}} (\delta_{\text{scal}})^{\text{b}}$	$\neq \delta_{\text{calc}} (\delta_{\text{scal}})$
C1	126.4	121.6 (126.5)	-4.79 (0.07)	120.8 (125.6)	-5.57 (-0.75)
*C2	125.8	120.5 (125.3)	3.52 (-0.45)	120.3 (125.1)	-5.50 (-0.71)
*C3	136.5	131.5 (136.9)	-4.97 (0.38)	130.9 (136.2)	-5.62 (-0.29)
C4	156.4	151.1 (157.5)	-5.28 (1.06)	150.7 (157.0)	-5.74 (0.57)
*C5	136.5	131.5 (136.9)	-11.25 (0.38)	130.9 (136.2)	-5.62 (-0.29)
*C6	125.8	120.5 (125.3)	-5.26 (-0.45)	120.3 (125.1)	-5.50 (-0.71)
**C7	34.4	36.2 (36.8)	1.85 (2.44)	34.5 (35.0)	0.09 (0.59)
**C8	30.2	31.3 (31.7)	1.14 (1.49)	29.5 (29.8)	-0.68 (-0.43)
α	118.8	110.7 (115.1)	-8.06 (-3.74)	109.9 (117.1)	-8.93 (-1.67)
β	145.6	142.2 (148.1)	-3.38 (2.51)	141.5 (147.4)	-4.06 (1.79)
β'	189	175.8 (183.4)	-13.18 (-5.61)	175.6 (183.2)	-13.38 (-5.82)
C1'	131.5	125.7 (130.8)	-5.80 (-0.73)	124.9 (130.0)	-6.56 (-1.53)
C2'	123.5	119.0 (123.8)	-4.48 (0.25)	118.0 (122.7)	-5.47 (-0.79)
C3'	113.7	109.0 (113.2)	-4.68 (-0.45)	108.0 (112.2)	-5.72 (-1.54)
C4'	150.1	144.1 (150.1)	-6.00 (-0.01)	143.6 (149.5)	-6.54 (-0.58)
C5'	146.9	138.9 (144.6)	-8.02 (-2.29)	138.3 (144.0)	-8.56 (-2.86)
C6'	110.6	108.1 (112.3)	-2.47 (1.72)	107.3 (111.5)	-3.29 (0.86)
OMe-5'	56.1	54.7 (56.2)	-1.45 (0.06)	53.1 (54.5)	-3.00 (-1.56)

^aCalculated chemical shifts ($\delta_{\text{calc}} = \sigma_{\text{TMS}} - \sigma_{\text{aver}}$ or σ_{lowe}) obtained by TMS subtraction; ^bscaled chemical shifts ($\delta_{\text{scal}} = 1.05\delta_{\text{calc}} - 1.22$) obtained by the generated universal scaling factor.¹ *The δ_{calc} and δ_{scal} for C2 and C6, C3 and C5 were arithmetically averaged; **the δ_{calc} and δ_{scal} for C7 and C8, were arithmetically averaged from the two *t*-butyl carbons and of the methyl carbons of the two *t*-butyl ligands, respectively.

Table S3. DFT, thermo chemical parameter and DFT population for the 15 more significant conformations of (*E*)-1-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one

Conformer	$\Delta E^a /$ (kcal mol ⁻¹)	Bolt. dist. ^b / %	$\Delta E^c /$ (kcal mol ⁻¹)	Bolt. dist. ^d / %	$\Delta E^e /$ (kcal mol ⁻¹)	Bolt. dist. ^f / %	$\Delta G^g /$ (kcal mol ⁻¹)	Bolt. dist. ^h / %
001	0.00	20.5	0.00	71.4	0.00	53.4	0.00	69.3
002	0.08	17.8	0.68	20.4	0.16	39.9	0.99	11.2
003	0.15	15.9	1.29	6.6	1.42	3.9	1.00	11.0
004	0.17	15.4	2.54	0.7	1.79	2.0	1.44	4.8
005	0.27	12.9	2.81	0.4	2.60	0.4	1.95	1.9
006	0.41	10.3	2.94	0.3	2.63	0.4	—	—
007	0.89	4.6	3.78	0.1	—	—	—	—
008	1.37	2.0	3.79	0.1	—	—	—	—
009	3.16	0.1	4.06	0.0	—	—	—	—
010	3.18	0.1	—	—	—	—	—	—
011	3.26	0.1	—	—	—	—	—	—
012	3.29	0.1	—	—	—	—	—	—
013	3.37	0.1	—	—	—	—	—	—
014	3.69	0.0	—	—	—	—	—	—
015	4.36	0.0	—	—	—	—	—	—

^aRelative MMFF energy of conformers obtained from Monte Carlo analysis; ^bMMFF Boltzmann population of the conformers; ^crelative B3LYP/6-31G(d) single point energy of conformers obtained from Monte Carlo analysis; ^dB3LYP/6-31(g) single point energy Boltzmann population of the conformers; ^erelative mPW1PW91/6-31G(d) energy minimization of the conformers; ^fmPW1PW91/6-31G(d) energy minimization Boltzmann population of the conformers; ^grelative mPW1PW91/6-31G(d) sum of electronic and free energy of the conformers; ^hmPW1PW91/6-31G(d) Boltzmann population calculated from ΔG values of the conformers.

Table S4. Calculated (scaled) and differences between experimental ^{13}C NMR chemical shifts (in ppm) in the (E)-1-(4-aminophenyl)-3-(3,4-dimethoxyphenyl)prop-2-en-1-one relative to TMS, for approaches (I) and (II)

Nuclei	δ_{exp}	Approach (I)		Approach (II)	
		$\delta_{\text{calc}}^{\text{a}} (\delta_{\text{scal}})^{\text{b}}$	$\neq \delta_{\text{calc}} (\delta_{\text{scal}})$	$\delta_{\text{calc}}^{\text{a}} (\delta_{\text{scal}})^{\text{b}}$	$\neq \delta_{\text{calc}} (\delta_{\text{scal}})$
C1	128.01	123.62 (128.58)	-4.39 (0.57)	122.06 (126.95)	-5.95 (-1.06)
C2	121.32	117.73 (122.40)	-3.59 (1.08)	113.09 (117.53)	-8.23 (-3.79)
C3	113.10	107.42 (111.57)	-5.68 (-1.53)	105.67 (109.73)	-7.43 (-3.37)
C4	151.34	144.76 (150.78)	-6.58 (-0.56)	143.88 (149.85)	-7.46 (-1.49)
C5	149.29	143.10 (149.03)	-6.19 (-0.26)	141.94 (147.81)	-7.35 (-1.48)
C6	114.53	114.49 (118.99)	-0.04 (4.46)	111.51 (115.86)	-3.02 (1.33)
C α	122.85	113.11 (117.55)	-9.74 (-5.30)	111.36 (115.70)	-11.49 (-7.15)
C β	145.30	141.01 (146.84)	-4.29 (1.54)	140.28 (146.071)	-5.02 (0.77)
C9	188.97	175.87 (183.44)	-13.10 (-5.53)	175.41 (182.96)	-13.56 (-6.01)
C1'	131.75	124.75 (129.77)	-13.1 (-5.53)	123.56 (128.52)	-8.19 (-3.23)
*C2'	131.58	126.58 (131.69)	-7 (-1.98)	126.58 (131.69)	-5 (0.11)
*C3'	114.36	108.86 (113.09)	-5 (0.11)	107.30 (111.44)	-7.06 (-2.92)
*C4'	155.19	142.64 (148.55)	-12.55 (-6.64)	141.68 (147.55)	-13.51 (-7.64)
*C5'	114.36	108.86 (113.09)	-5.50 (-1.27)	107.30 (111.44)	-7.06 (-2.92)
*C6'	131.58	126.58 (131.69)	-5 (0.11)	126.58 (131.69)	-5 (0.11)
OMe-3	56.01	55.86 (57.43)	-0.15 (1.42)	52.75 (54.17)	-3.26 (-1.84)
OMe-4	56.01	55.86 (57.43)	-0.15 (1.42)	52.75 (54.17)	-3.26 (-1.84)

^aCalculated chemical shifts ($\delta_{\text{calc}} = \sigma_{\text{TMS}} - \sigma_{\text{aver}}$ or σ_{lowe}) obtained by TMS subtraction; ^bscaled chemical shifts ($\delta_{\text{scal}} = 1.05\delta_{\text{calc}} - 1.22$) obtained by the generated universal scaling factor.¹ *The δ_{calc} and δ_{scal} for C2 and C6, C3 and C5 were arithmetically averaged.

Reference

- Costa, F. L. P.; de Albuquerque, A. C. F.; Borges, R. M.; dos Santos Jr., F. M.; de Amorim, M. B.; *J. Comput. Theor. Nanosci.* **2014**, *11*, 219.