Dominant Carbons in *Trans* and *Cis*-resveratrol Isomerization

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Supporting Information

Potential energy scan (PES) for tarns and cis resveratrol have been reported for $\delta = \angle C_{(6)}\text{-}C_{(5)}\text{-}C_{(8)}\text{-}C_{(9)}$ along with comparison between calculated NMR using different DFT models i.e. B3PW91, B3LYP and M06-2X, in DMSO and gas phase has been illustrated for C, H and O atoms as well as the comparison of energy terms for the *trans* and *cis* – resveratrol, is provided additionally.

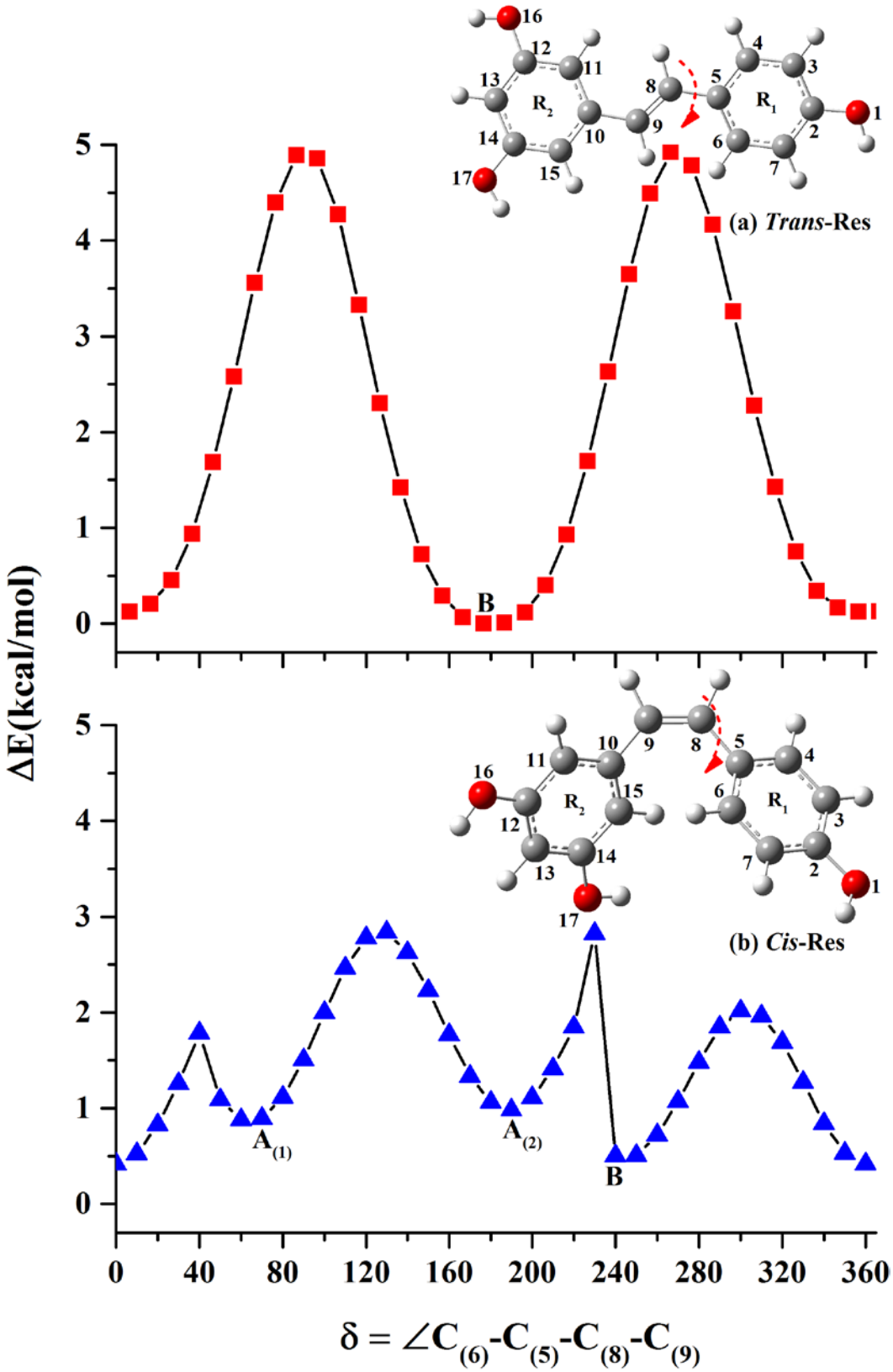

Figure S1: Potential Energy Scan (PES) curve of (a) trans and (b) cis resveratrol through rotation of $\delta = \angle C_{(6)}\text{-}C_{(5)}\text{-}C_{(8)}\text{-}C_{(9)}$ at the B3LYP/6-31+G* level of theory.

Table S1: The calculated NMR (in ppm) isotropic chemical shifts (with respect to TMS for ^{13}C and ^{1}H NMR along with H_2O for ^{17}O NMR, respectively) for *trans* and *cis* resveratrol[1] in DMSO and gas phase.

Nucleus	B3PW91			B3LYP			M06-2X		
	Trans	***Cis***	$\Delta\delta_{(Cis-Trans)}$	***Trans***	***Cis***	$\Delta\delta_{(Cis-Trans)}$	***Trans***	***Cis***	$\Delta\delta_{(Cis-Trans)}$
^{13}C NMR - DMSO									
$C_{(2)}$	159.0	158.5	0.5	163.6	163.1	0.5	173.0	172.2	0.8
$C_{(3)}$	115.8	115.5	0.3	119.2	118.8	0.4	129.5	130.2	-0.7
$C_{(4)}$	134.1	134.2	-0.1	137.8	137.9	-0.1	149.8	149.3	0.5
$C_{(5)}$	129.8	130.2	-0.4	134.4	134.8	-0.4	143.8	145.2	-1.4
$C_{(6)}$	**125.9**	**130.8**	**-4.9**	**129.3**	**134.7**	**-5.4**	**140.8**	**146.9**	**-6.1**
$C_{(7)}$	115.4	113.8	1.6	118.9	117.2	1.7	128.6	127.4	1.2
$C_{(8)}$	132.6	133.4	-0.8	136.4	137.1	-0.7	147.6	149.0	-1.4
$C_{(9)}$	**127.7**	**130.2**	**-2.5**	**131.3**	**133.8**	**-2.5**	**141.3**	**143.2**	**-1.9**
$C_{(10)}$	141.3	142.4	-1.1	146.1	147.1	-1.0	156.6	159.5	-2.9
$C_{(11)}$	**100.0**	**108.8**	**-8.8**	**103.3**	**112.4**	**-9.1**	**113.2**	**122.3**	**-9.1**
$C_{(12)}$	160.4	160.6	-0.2	165.2	165.4	-0.2	174.3	175.1	-0.8
$C_{(13)}$	99.6	99.1	0.5	102.8	102.2	0.6	112.4	112.0	0.4
$C_{(14)}$	159.8	158.7	1.1	164.6	163.4	1.2	174.2	173.5	0.7
$C_{(15)}$	**107.9**	**104.8**	**3.1**	**111.3**	**108.6**	**2.7**	**120.8**	**118.3**	**2.5**
^{1}H and ^{17}O NMR - DMSO									
$H_{(18)}$	4.93	4.79	0.14	4.77	4.64	0.13	5.20	5.10	0.10
$H_{(19)}$	7.22	7.24	-0.02	7.06	7.08	-0.02	7.68	7.63	0.05
$H_{(20)}$	7.53	7.53	0.00	7.34	7.35	-0.01	7.90	7.95	-0.05
$H_{(21)}$	8.12	7.72	0.40	7.96	7.58	0.38	8.56	8.28	0.28
$H_{(22)}$	7.06	6.75	0.31	6.92	6.60	0.32	7.31	7.13	0.18
$H_{(23)}$	7.54	6.87	0.67	6.19	6.70	-0.51	7.96	7.42	0.54
$H_{(24)}$	6.38	6.70	-0.32	7.12	6.52	0.60	7.58	6.78	0.80
$H_{(25)}$	7.08	6.67	0.41	6.94	6.52	0.42	7.50	7.06	0.44
$H_{(26)}$	6.38	6.35	0.03	6.25	6.21	0.04	6.81	6.99	-0.18
$H_{(27)}$	6.34	6.57	-0.23	6.19	6.47	-0.28	6.72	6.94	-0.22
$H_{(28)}$	4.60	4.78	-0.18	4.44	4.61	-0.17	4.76	4.56	0.20
$H_{(29)}$	4.61	4.30	0.31	4.46	4.16	0.30	4.67	4.34	0.33
$O_{(1)}$	112.02	110.82	-1.2	112.90	111.79	-1.11	116.68	115.93	-0.75
$O_{(16)}$	109.48	109.29	-0.19	110.73	110.51	-0.22	114.13	112.69	-1.44
$O_{(17)}$	109.29	109.16	-0.13	110.75	110.39	-0.36	113.76	113.11	-0.65
^{1}H and ^{17}O NMR - Gas									
$H_{(18)}$	3.90	3.84	-0.06	3.76	3.70	-0.06	3.96	4.21	0.25
$H_{(19)}$	7.08	7.16	0.08	6.93	7.01	0.08	7.48	7.50	0.02
$H_{(20)}$	7.36	7.34	-0.02	7.18	7.17	-0.01	7.68	7.74	0.06
$H_{(21)}$	7.88	7.58	-0.30	7.74	7.44	-0.30	8.33	8.13	-0.20
$H_{(22)}$	6.63	6.32	-0.31	6.49	6.19	-0.30	7.06	6.69	-0.37
$H_{(23)}$	7.33	6.71	-0.62	7.20	6.55	-0.65	7.70	7.25	-0.45
$H_{(24)}$	6.96	6.61	-0.35	5.98	6.44	0.46	7.31	6.68	-0.63
$H_{(25)}$	7.05	6.61	-0.44	6.92	6.48	-0.44	7.42	7.00	-0.42
$H_{(26)}$	6.10	6.04	-0.06	5.98	5.91	-0.07	6.51	6.62	0.11
$H_{(27)}$	5.94	6.26	0.32	5.81	6.15	0.34	6.38	6.64	0.26
$H_{(28)}$	3.76	3.89	0.13	3.62	3.76	0.14	3.91	3.76	-0.15
$H_{(29)}$	3.70	3.48	-0.22	3.57	3.34	-0.23	3.79	3.52	-0.27
$O_{(1)}$	114.55	113.51	-1.04	116.06	114.94	-1.12	119.73	120.44	0.71
$O_{(16)}$	113.52	113.11	-0.41	115.27	114.74	-0.53	118.23	116.96	-1.27
$O_{(17)}$	111.84	112.24	0.40	113.80	113.92	0.12	116.96	116.34	-0.62

[1]using the basis set 6-311++G**

Table S2: Comparison of energy terms for the *trans* and *cis* - resveratrol (kcal. mol^{-1})[*].

Energy Fragment	*Trans*-R	*Cis*-R	$\Delta(\Delta E_i)$[a]
ΔE_{Estat}	-3715.50	-3707.72	-7.78
ΔE_{Pauli}	7918.79	7846.29	72.50
ΔE_{Orb}	-20431.77	-20362.60	-69.17
ΔE_{Int}	-16228.48	-16224.03	-4.45
ΔE_{Ster}	4203.28	4138.57	64.71
ΔE_{XC}	-15952.13	-15947.18	-4.95

[*]using the DFT based B3LYP model and 6-311++G^{**} basis sets

[a](ΔE(*trans*-R) – ΔE(*cis*-R))