

SUPPLEMENTARY MATERIAL

Can we predict specific numbers of catalytically important molecules of water in H/D exchange in aromatic systems? A combined NMR and DFT study

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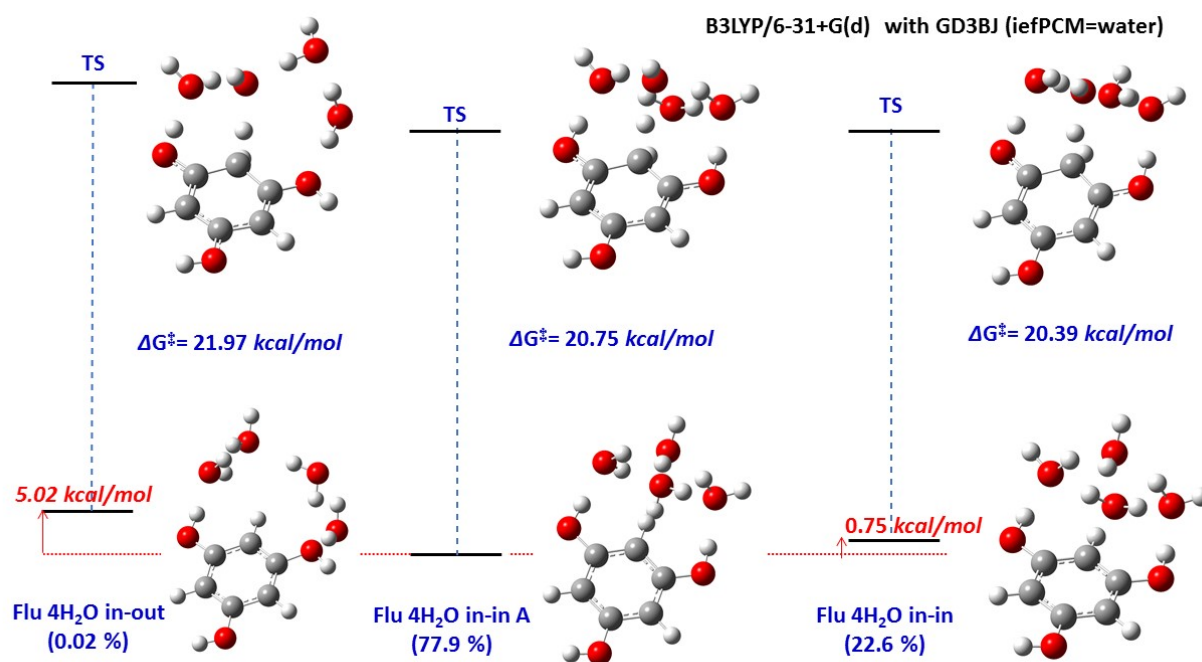


Fig. S1 The mechanistic pathway of the aromatic hydrogen exchange process of the complex of the neutral phloroglucinol with four molecules of H₂O and the two phenol -OH groups in the “in-in” configuration at the B3LYP/6-31+G(d)/GD3BJ level. In parenthesis are the Boltzmann populations (Tables 2 and S2).

CAM-B3LYP/6-31+G(d) with GD3BJ

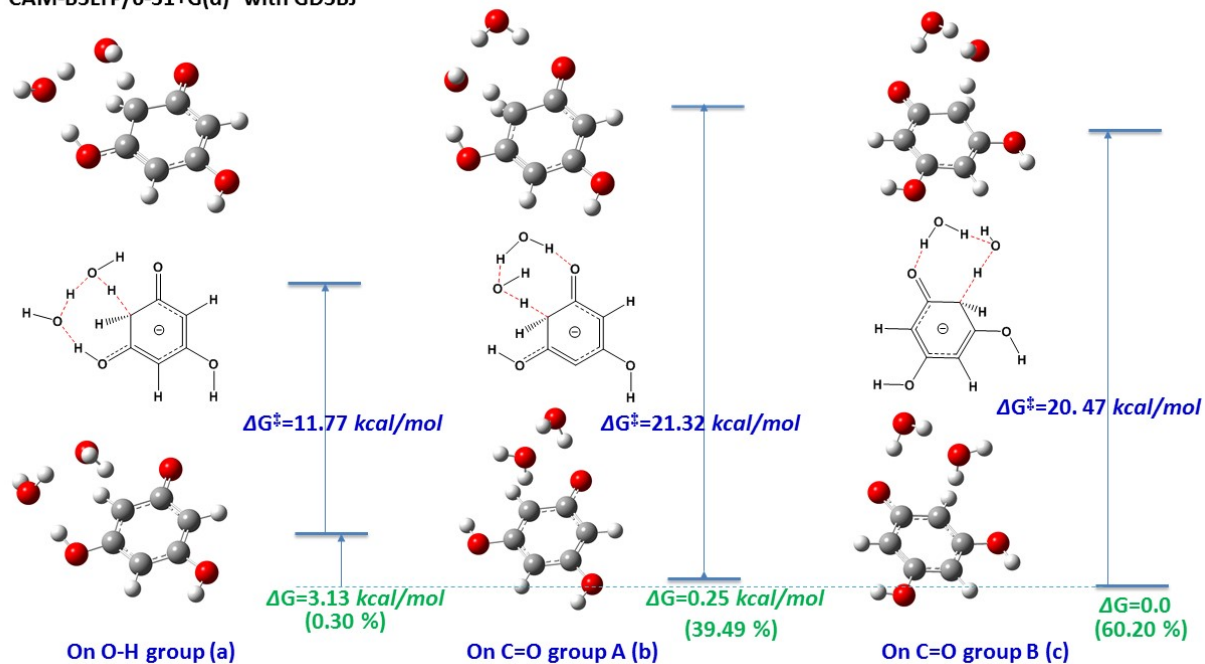


Fig. S2 Three possible mechanistic pathways of the aromatic hydrogen exchange process of the complex of the phloroglucinol anion with two molecules of H_2O : one molecule of H_2O on the phenol -OH group (a), and one molecule of H_2O on the C=O bond (b) and (c), at the CAM-B3LYP/6-31+G(d)/GD3BJ level. In parenthesis are the Boltzmann populations (Tables 2 and S3).

Table S1 Computed activation enthalpy ($\Delta H_{comp}^{\ddagger}$), activation entropy ($-T\Delta S_{comp}^{\ddagger}$) and Gibbs activation energy ($\Delta G_{comp}^{\ddagger}$), for neutral phloroglucinol for various molecular water solvation species and computational methods

Calculation method	$\Delta H_{comp}^{\ddagger}$ kcal mol ⁻¹	$\Delta S_{comp}^{\ddagger}$ cal mol ⁻¹	$-T\Delta S_{comp}^{\ddagger}$ kcal mol ⁻¹	$\Delta G_{comp}^{\ddagger}$ kcal mol ⁻¹	Imaginary frequency cm ⁻¹
Phloroglucinol complex with 2H₂O (IefPCM=H₂O)					
B3LYP/6-31+G(d)	21.53	-7.94	2.10	27.11	-746.98
CAM-B3LYP/6-31+G(d)	21.77	-17.58	5.24	27.01	-891.08
PBE0/6-31+G(d)	19.81	-12.43	3.68	23.45	-802.65
APFD/6-31+G(d)	17.21	-11.32	3.38	20.59	-843.46
ω B97XD/6-31+G(d)	22.65	-11.87	3.54	26.19	-693.18
M06-2X/6-31+G(d)	22.30	-13.57	4.05	26.35	-1141.12
B3LYP/6-31+G(d) with GD3BJ	19.57	-12.02	3.58	23.15	-740.39
CAM-B3LYP/6-31+G(d) with GD3BJ	20.98	-12.39	3.70	24.68	-891.97
PBE0/6-31+G(d) with GD3BJ	19.35	-12.77	3.81	23.16	-802.44
Phloroglucinol complex with 3H₂O (IefPCM=H₂O) (conformation "in-out")					
B3LYP/6-31+G(d) (21.03 %)	26.06	-13.86	4.13	30.19	-259.77
Ketone	16.53	-16.91	5.04	21.57	
CAM-B3LYP/6-31+G(d) (34.95 %)	27.41	-13.91	4.15	31.56	-422.76
ketone	17.96	-17.96	5.48	23.44	
PBE0/6-31+G(d) (10.72 %)	25.66	-11.56	3.45	29.11	-192.9
ketone	17.66	-11.34	3.38	21.04	
APFD/6-31+G(d) ((10.94 %)	23.34	-9.84	2.93	26.28	-182.97
ketone	14.18	-14.38	4.29	18.47	
ω B97XD/6-31+G(d) ((17.12 %)	27.49	-11.32	3.37	30.86	-262.48
ketone	18.78	-14.11	4.21	22.98	
M06-2X/6-31+G(d) (1.34 %)	30.22	-5.42	1.62	31.84	-491.76
ketone	17.13	-15.65	4.67	21.80	
B3LYP/6-31+G(d) with GD3BJ (14.19 %)	24.33	-11.34	3.38	27.52	-207.01
ketone	15.95	-15.10	4.50	20.45	
CAM-B3LYP/6-31+G(d) with GD3BJ (16.10 %)	26.71	-10.74	3.20	29.71	-389.14
ketone	16.99	-15.88	4.73	21.72	
PBE0/6-31+G(d) with GD3BJ (9.65 %)	24.64	-10.46	3.12	27.76	-182.64
ketone	14.92	-16.32	4.87	19.78	
Phloroglucinol complex with 3H₂O (IefPCM=H₂O) (conformation "in-out A")					
B3LYP/6-31+G(d) (0.16%)	23.09	-14.17	4.22	27.31	-259.77
CAM-B3LYP/6-31+G(d) (0.12%)	24.03	-13.94	4.168	28.18	-422.76
PBE0/6-31+G(d) (0.13 %)	22.47	-13.52	4.03	26.50	-192.9
APFD/6-31+G(d) (0.046%)	20.14	-9.70	2.89	23.03	-182.97
ω B97XD/6-31+G(d) ((0.48 %)	24.65	-13.77	4.11	28.75	-262.48
M06-2X/6-31+G(d) (0.13 %)	26.92	-11.72	3.55	30.47	-491.76
B3LYP/6-31+G(d) with GD3BJ (0.82 %)	21.24	-15.39	4.59	25.832	-207.01
CAM-B3LYP/6-31+G(d) with GD3BJ (0.14 %)	23.11	-12.67	3.78	26.89	-389.14
PBE0/6-31+G(d) with GD3BJ (0.13 %)	21.38	-12.84	3.83	25.21	-182.64
Phloroglucinol complex with 3H₂O (IefPCM=H₂O) (conformation "in-in")					

B3LYP/6-31+G(d) (12.71 %)	19.44	-15.63	4.66	24.10	-754.2
ketone	14.12	-17.44	5.20	19.32	
CAM-B3LYP/6-31+G(d) (37.72 %)	20.46	-15.43	4.60	25.06	-911.4
ketone	10.52	-23.06	6.88	17.40	
PBE0/6-31+G(d) (48.63 %)	18.35	-16.12	4.80	23.15	-583.2
ketone	11.91	-17.64	5.26	17.17	
APFD/6-31+G(d) (58.52 %)	15.59	-15.23	4.54	20.13	-537.1
ketone	10.05	-15.13	4.51	14.57	
ω B97XD/6-31+G(d) (52.04 %)	20.68	-14.75	4.40	25.08	-696.4
ketone	14.83	-16.39	4.89	19.72	
M06-2X/6-31+G(d) (50.57%)	22.76	-16.39	4.89	27.23	-748.3
ketone	13.30	-15.00	4.47	18.02	
B3LYP/6-31+G(d) with GD3BJ (46.80 %)	17.15	-15.13	4.51	21.66	-698.9
ketone	12.03	-15.65	4.67	16.70	
CAM-B3LYP/6-31+G(d) with GD3BJ (46.39 %)	19.33	-14.80	4.41	23.99	-880.5
ketone	9.45	-20.13	6.00	15.45	
PBE0/6-31+G(d) with GD3BJ (51.47 %)	17.13	-15.16	4.52	21.65	-548.40
ketone	10.81	-15.64	4.66	15.48	
Phloroglucinol complex with 3H₂O (IefPCM=H₂O) (conformation "in-in A")					
B3LYP/6-31+G(d) (66.09 %)	19.52	-18.66	5.56	25.08	-754.2
CAM-B3LYP/6-31+G(d) (27.22 %)	20.41	-16.23	4.85	25.66	-911.4
PBE0/6-31+G(d) (40.53 %)	18.42	-15.50	4.62	23.05	-583.2
APFD/6-31+G(d) (30.51 %)	15.66	-13.73	4.09	19.75	-537.1
ω B97XD/6-31+G(d) (17.12 %)	20.61	-13.92	4.15	24.76	-696.4
M06-2X/6-31+G(d) (47.96%)	23.14	-13.63	4.06	27.20	-748.3
B3LYP/6-31+G(d) with GD3BJ(38.19 %)	17.16	-14.70	4.38	21.54	-698.9
CAM-B3LYP/6-31+G(d) with GD3BJ (37.37 %)	19.36	-14.28	4.25	23.62	-880.5
PBE0/6-31+G(d) with GD3BJ (38.75 %)	17.14	-14.58	4.34	21.48	-548.40
Phloroglucinol complex with 4H₂O (conformation "in-out")					
B3LYP/6-31+G(d) (0.03%)	18.60	-18.46	5.50	24.10	-318.1
ketone	16.63	-17.77	5.30	21.93	
CAM-B3LYP/6-31+G(d) (0.06%)	19.25	-18.29	5.45	24.71	-479.7
ketone	16.64	-16.07	4.79	21.43	
PBE0/6-31+G(d) (0.11%)	17.75	-19.77	5.89	23.64	-208.4
ketone	14.87	-13.40	3.99	18.87	
APFD/6-31+G(d) (2.30%)	23.73	-0.22	0.07	23.79	-157.61
ketone	18.37	-0.92	0.27	18.64	
ω B97XD/6-31+G(d) (0.92%)	27.52	-1.35	0.40	27.92	-278.2
ketone	22.19	-1.49	0.45	22.64	
M06-2X/6-31+G(d) (2.58%)	30.91	-0.72	0.40	31.12	-433.6
ketone	22.42	-1.01	0.45	22.72	
B3LYP/6-31+G(d) with GD3BJ (0.02%)	17.14	-16.20	4.83	21.97	-235.7
ketone	19.51	-1.56	0.47	19.98	
CAM-B3LYP/6-31+G(d) with GD3BJ (1.75 %)	25.74	-5.61	1.67	27.41	-430.5
ketone	16.43	-11.41	3.40	19.83	
PBE0/6-31+G(d) with GD3BJ (1.75%)	24.18	-4.22	1.26	25.44	-167.2
ketone	14.66	-11.23	3.35	18.01	

Phloroglucinol complex with 4H ₂ O (conformation “in-in”)					
B3LYP/6-31+G(d) (8.64 %)	18.48	-11.69	3.48	21.96	-758.4
ketone	14.07	-11.80	3.52	17.58	
CAM-B3LYP/6-31+G(d) (5.64 %)	19.22	-11.00	3.28	22.50	-940.8
ketone	13.89	-10.39	3.10	16.99	
PBE0/6-31+G(d) (4.51%)	17.22	-11.20	3.34	20.55	-613.0
ketone	12.03	-10.86	3.24	15.26	
APFD/6-31+G(d) (8.02%)	14.56	-11.63	3.47	18.03	-605.3
ketone	10.23	-10.27	3.06	13.29	
ω B97XD/6-31+G(d) (7.40%)	19.44	-11.98	3.57	23.01	-784.1
ketone	14.85	-10.97	3.27	18.12	
M06-2X/6-31+G(d) (16.85%)	21.98	-11.99	3.57	25.56	-817.1
ketone	13.56	-12.03	3.59	17.15	
B3LYP/6-31+G(d) with GD3BJ (22.03%)	16.13	-14.30	4.26	20.39	-757.4
ketone	12.23	-11.24	3.35	15.58	
CAM-B3LYP/6-31+G(d) with GD3BJ (4.04%)	18.12	-10.76	3.21	21.33	-927.8
Ketone	13.09	-10.47	3.12	16.21	
PBE0/6-31+G(d) with GD3BJ	15.97	-11.95	3.56	19.53	-603.7
ketone(4.56%)	11.10	-10.96	3.27	14.37	
Phloroglucinol complex with 4H ₂ O (conformation “in-in A”)					
B3LYP/6-31+G(d) (91.10%)	19.47	-12.49	3.72	23.19	-651.1
ketone	16.75	-10.10	2.91	19.73	
CAM-B3LYP/6-31+G(d) (94.30%)	20.15	-12.36	3.69	23.84	-846.5
ketone	16.95	-9.02	2.69	19.64	
PBE0/6-31+G(d) (95.38%)	18.27	-12.57	3.75	22.02	-507.4
ketone	14.90	-9.33	2.78	17.68	
APFD/6-31+G(d) (89.68%)	15.55	-10.67	3.18	18.73	-520.4
ketone	13.49	-9.17	2.73	16.23	
ω B97XD/6-31+G(d) (91.69%)	20.53	-12.04	3.59	24.12	-670.4
ketone	17.60	-9.012	2.69	20.29	
M06-2X/6-31+G(d) (80.56%)	22.62	-11.29	3.37	25.99	-768.4
ketone	16.34	-10.32	3.08	19.42	
B3LYP/6-31+G(d) with GD3BJ (77.95%)	17.13	-12.13	3.62	20.75	-643.1
ketone	15.23	-8.60	2.56	17.80	
CAM-B3LYP/6-31+G(d) with GD3BJ (91.28%)	19.11	-11.77	3.51	20.62	-835.4
Ketone	16.28	-8.55	2.55	18.82	
PBE0/6-31+G(d) with GD3BJ	17.04	-12.77	3.81	20.85	-500.4
ketone(93.68%)	14.13	-9.06	2.70	16.83	

Table S2: Computed activation enthalpy ($\Delta H_{comp}^{\ddagger}$), entropy difference between *TS* and complexes ($\Delta S_{(TS-R)}$), activation entropy ($-T\Delta S_{comp}^{\ddagger}$) and equilibrium Gibbs energies ($\Delta G_{comp}^{\ddagger}$), for taxifolin for various molecular solvation species with a variety of computational methods in continuum (IEFPCM=water)

Calculation method	Taxifolin (IEFPCM=water)					Imaginary frequency cm ⁻¹
	TS at 6 position	$\Delta H_{comp}^{\ddagger}$ kcal mol ⁻¹	$\Delta S_{(TS-R)}$ cal mol ⁻¹	$-T\Delta S^{\ddagger}$ kcal mol ⁻¹	$-T\Delta S^{\ddagger}$ kcal mol ⁻¹	
B3LYP/6-31+G(d)	6 enone	50.78	-3.13	0.93	51.71	
	TS at 6 position	58.11	-0.90	0.27	58.38	-2086.5

	TS at 8 position	58.82	-0.86	0.26	59.08	-2091.8
	8 enone	51.22	-3.54	1.06	52.28	
Taxifolin (IEFPCM=water)						
M06-2X/6-31+G(d)	TS at 6 position	62.80	-1.92	0.57	63.37	-2099.7
	6 enone	52.04	-2.81	0.84	52.88	
	TS at 8 position	63.70	-1.43	0.43	64.13	-2101.3
	8 enone	52.52	-3.78	1.13	53.65	
Taxifolin + H ₂ O (IEFPCM=water)						
B3LYP/6-31+G(d)	TS at 6 position	32.76	-9.01	2.69	35.44	
	6 enone	23.25	-14.90	4.44	27.70	-1272.9
	TS at 8 position	34.36	-5.912	1.76	36.13	
	8 enone	23.74	-14.46	4.31	28.05	-1296.1
Taxifolin + H ₂ O (IEFPCM=water)						
M06-2X/6-31+G(d)	TS at 6 position	33.65	-7.05	2.10	35.75	-1132.6
	6 enone	20.13	-9.07	2.71	22.84	
	TS at 8 position	29.103	-5.34	1.59	35.94	-1155.7
	8 enone	20.63	-10.40	3.10	23.73	
Taxifolin + 2H ₂ O (IEFPCM=water)						
B3LYP/6-31+G(d)	TS at 6 position	20.16	-17.91	5.34	25.50	-1039.4
	6 enone	13.00	-12.37	3.69	16.69	
	TS at 8 position	20.73	-19.07	5.69	26.41	-1089.0
	8 enone	13.39	-18.61	5.55	18.94	
Taxifolin + 2H ₂ O (IEFPCM=water)						
M06-2X/6-31+G(d)	TS at 6 position	20.73	-11.85	3.53	24.26	-1175.8
	6 enone	9.98	-10.72	3.20	13.17	
	TS at 8 position	21.45	-9.922	2.96	24.41	-1194.3
	8 enone	10.42	-13.17	3.93	14.34	
Taxifolin + 2H ₂ O (IEFPCM=water)						
B3LYP/6-31+G(d) with GD3BJ	TS at 6 position	19.03	-5.96	1.78	20.81	-1155.4
	6 enone	11.28	-11.15	3.33	14.61	
	TS at 8 position	17.81	-13.79	4.123	21.93	-1214.7
	8 enone	11.66	-9.11	2.72	14.37	
Taxifolin + 2H ₂ O (IEFPCM=water)						
APFD/6-31+G(d)	TS at 6 position	15.73	-15.73	5.06	20.79	-1047.9
	6 enone	8.95	-12.65	3.77	12.72	
	TS at 8 position	16.31	-14.96	4.46	20.77	-1089.8
	8 enone	9.03	-12.44	3.71	12.74	
Taxifolin + 2H ₂ O (IEFPCM=water)						
wB97XD/6-31+G(d)	TS at 6 position	20.14	-16.55	4.93	25.08	-1049.0
	6 enone	13.03	-11.60	3.46	16.49	
	TS at 8 position	20.47	-12.48	3.72	24.19	-1117.9
	8 enone	13.43	-11.89	3.54	16.97	
Taxifolin + 2H ₂ O (IEFPCM=water)						
PBE0/6-31+G(d)	TS at 6 position	17.82	-14.46	4.31	22.13	-1041.6
	6 enone	9.91	-11.25	3.35	13.27	
	TS at 8 position	18.56	-14.48	4.32	22.88	-1092.5
	8 enone	10.29	-11.39	3.39	13.68	
Taxifolin + 2H ₂ O (IEFPCM=water)						
PBE0/6-31+G(d) with GD3BJ	TS at 6 position	16.59	-14.13	4.21	20.80	-1137.8
	6 enone	9.08	-11.00	3.28	12.36	
	TS at 8 position	17.34	-13.21	3.94	21.28	-1095.6
	8 enone	9.37	-9.67	2.884	12.24	
Taxifolin + 2H ₂ O (IEFPCM=water)						
CAM-B3LYP/6-31+G(d)	TS at 6 position	20.57	-14.08	4.20	24.78	-1140.9
	6 enone	13.12	-11.95	3.56	16.68	

	TS_at 8_position	21.29	-14.67	4.38	25.67	-1188.7
	8_enone	13.55	-11.91	3.55	17.10	
Taxifolin + 2H ₂ O (IEFPCM=water)						
CAM-B3LYP/6-31+G(d) with GD3BJ	TS_at 6_position	19.44	-10.92	3.26	22.69	-1209.7
	6_enone	12.32	-10.07	3.00	15.33	
	TS_at 8_position	20.14	-11.58	3.45	23.59	-1263.4
	8_enone	12.65	-9.65	2.97	15.61	
Taxifolin + 3H ₂ O (IEFPCM=water)						
B3LYP/6-31+G(d)	TS_at 6_position	25.12	-8.11	2.42	27.54	-1030.7
	TS_at 6_position	24.13	-12.22	3.64	27.77	
	TS_at 8_position	25.83	-7.13	2.13	27.95	-1022.0
	Taxifolin + 3H ₂ O (IEFPCM=water)					
M06-2X/6-31+G(d)	TS_at 6_position	25.34	-9.57	2.85	28.20	-1222.4
	TS_at 6_position	24.16	-9.38	2.80	26.96	
	TS_at 8_position	26.06	-7.38	2.20	28.26	-1241.7
	Taxifolin + 3H ₂ O (IEFPCM=water)					
B3LYP/6-31+G(d) with GD3BJ	TS_at 6_position	22.72	-9.76	2.91	25.63	-1094.4
	TS_at 6_position	21.59	-15.87	4.73	25.32	
	TS_at 8_position	23.53	-6.09	1.82	24.72	-1113.5
	Taxifolin + 3H ₂ O (IEFPCM=water)					
APFD/6-31+G(d)	TS_at 6_position	20.74	-7.51	2.234	22.98	-1043.8
	TS_at 6_position	19.40	-10.66	3.18	22.58	
	TS_at 8_position	21.62	-6.46	1.93	23.55	-1076.6
	Taxifolin + 3H ₂ O (IEFPCM=water)					
wB97XD/6-31+G(d)	TS_at 6_position	25.06	-7.79	2.32	27.38	-1005.9
	TS_at 6_position	23.89	-9.66	2.88	26.77	
	TS_at 8_position	25.77	-5.37	1.60	27.37	-1032.4
	Taxifolin + 3H ₂ O (IEFPCM=water)					
PBE0/6-31+G(d)	TS_at 6_position	23.06	-9.85	2.94	26.00	-1036.7
	TS_at 6_position	21.83	-10.33	3.08	24.91	
	TS_at 8_position	23.80	-8.45	2.52	26.32	-1046.5
	Taxifolin + 3H ₂ O (IEFPCM=water)					
PBE0/6-31+G(d) with GD3BJ	TS_at 6_position	20.45	-15.85	4.73	25.18	-1116.1
	TS_at 6_position	21.69	-7.86	2.34	24.03	
	TS_at 8_position	22.60	-13.45	4.01	24.67	-1146.50
	Taxifolin + 3H ₂ O (IEFPCM=water)					
CAM-B3LYP/6-31+G(d)	TS_at 6_position	25.78	-11.22	3.34	29.12	-1120.3
	TS_at 6_position	24.68	-11.10	3.31	27.99	
	TS_at 8_position	26.52	-7.68	2.291	28.81	-1137.1
	Taxifolin + 3H ₂ O (IEFPCM=water)					
CAM-B3LYP/6-31+G(d) with GD3BJ	TS_at 6_position	24.51	-9.23	2.75	27.26	-1166.8
	TS_at 6_position	23.45	-12.07	3.60	27.05	
	TS_at 8_position	25.42	-7.52	2.24	27.66	-1189.6
Taxifolin + 4H ₂ O (IEFPCM=water)						
B3LYP/6-31+G(d)	TS_at 6_position	24.08	4.21	-1.2550	22.82	-1077.96

	TS_at 8_position	26.51	-2.740	0.806	27.32	-1051.77
	TS_at 8_position	24.18	0.849	-0.253	23.93	-1051.77
	Taxifolin + 4H ₂ O (IEFPCM=water)					
M06-2X/6-31+G(d)	TS_at 6_position	25.34	-9.57	2.85	28.20	-1222.4
	TS_at 6_position	24.16	-9.38	2.80	26.96	
	TS_at 8_position	26.06	-7.38	2.20	28.26	-1241.7
	Taxifolin + 3H ₂ O (IEFPCM=water)					
B3LYP/6-31+G(d) with GD3BJ	TS_at 6_position	22.87	3.889	-1.160	21.71	-1201.71
	TS_at 8_position	24.22	1.539	-0.459	23.76	-1201.64
A	TS_at 8_position	23.66	2.147	-0.640	23.02	-1201.64
B	Taxifolin + 4H ₂ O (IEFPCM=water)					
APFD/6-31+G(d)	TS_at 6_position	20.95	3.54	-1.055	19.89	-1068.46
A	TS_at 8_position	22.06	-3.173	0.946	23.00	-1068.60
B	TS_at 8_position	21.57	4.483	-1.337	20.23	-1068.60
	Taxifolin + 3H ₂ O (IEFPCM=water)					
wB97XD/6-31+G(d)	TS_at 6_position	25.14	3.532	-1.053	24.08	-1082.11
A	TS_at 6_position	25.96	-7.971	2.377	28.33	-1084.27
B	TS_at 8_position	25.97	1.474	-0.439	25.53	-1084.27
	Taxifolin + 4H ₂ O (IEFPCM=water)					
PBE0/6-31+G(d)	TS_at 6_position	22.41	3.505	-1.045	21.37	-1065.26
A	TS_at 8_position	24.86	-4.418	1.317	26.17	-1062.98
B	TS_at 8_position	22.63	0.909	-0.271	22.36	-1062.98
	Taxifolin + 4H ₂ O (IEFPCM=water)					
PBE0/6-31+G(d) with GD3BJ	TS_at 6_position	21.78	2.76	-0.823	20.96	-1177.43
A	TS_at 6_position	23.19	-5.14	1.532	24.72	-1177.32
B	TS_at 8_position	22.52	2.76	-0.823	22.17	-1177.32
	Taxifolin + 4H ₂ O (IEFPCM=water)					
CAM-B3LYP/6-31+G(d)	TS_at 6_position	25.31	4.49	-1.339	23.97	-1168.34
A	TS_at 8_position	27.33	-3.21	0.957	28.28	-1161.98
B	TS_at 8_position	25.32	1.364	-0.407	24.91	-1161.98
	Taxifolin + 4H ₂ O (IEFPCM=water)					
CAM-B3LYP/6-31+G(d) with GD3BJ	TS_at 6_position	24.78	3.456	-1.030	23.75	-1241.54
A	TS_at 8_position	25.80	-6.702	1.998	27.80	-1242.46
B	TS_at 8_position	23.45	1.135	-0.338	25.11	-1242.46

Table S3 Computed activation enthalpy ($\Delta H_{comp}^{\ddagger}$), activation entropy ($-T\Delta S_{comp}^{\ddagger}$) and Gibbs activation energy (ΔG^{\ddagger}) for phloroglucinol anion for various molecular water solvation species and computational methods.

Calculation method	$\Delta H_{comp}^{\ddagger}$ kcal mol ⁻¹	$\Delta S_{comp}^{\ddagger}$ cal mol ⁻¹	$-T\Delta S_{comp}^{\ddagger}$ kcal mol ⁻¹	$\Delta G_{comp}^{\ddagger}$ kcal mol ⁻¹	<i>imaginary</i>
Phloroglucinol anion complex with 2H₂O (one H₂O on OH)					
B3LYP/6-31+G(d) (0.16 %)	11.04	-8.94	2.67	13.70	-1027.7
CAM-B3LYP/6-31+G(d) (0.32 %)	11.89	-8.39	2.50	14.39	-1144.1
PBE0/6-31+G(d)	10.79	-8.43	2.51	13.30	-817.8

APFD/6-31+G(d)	9.84	-6.70	2.00	11.83	-788.3
ω B97XD/6-31+G(d) (0.37%)	12.90	-7.73	2.31	15.21	-996.4
ω B97XD/aug-cc-pVDZ (0.22 %)	13.74	-8.39	2.50	16.24	-854.5
M06-2X/6-31+G(d) (0.39 %)	14.93	-9.74	2.91	17.83	-975.4
B3LYP/6-31+G(d) with GD3BJ (0.26 %)	10.64	-7.94	2.37	13.01	-979.5
CAM B3LYP/6-31+G(d) with GD3BJ (0.30 %)	11.77	-7.76	2.31	14.08	-1117.6
PBE0/6-31+G(d) with GD3BJ	10.68	-7.97	2.38	13.05	-782.6
Phloroglucinol anion complex with 2H₂O (1 H₂O on C=O (B))					
B3LYP/6-31+G(d) (55.21 %)	17.11	-9.65	2.88	19.99	-366.3
CAM-B3LYP/6-31+G(d) (38.73 %)	17.95	-8.62	2.57	20.58	-536.4
PBE0/6-31+G(d)	a	a	a	a	a
APFD/6-31+G(d)	a	a	a	a	a
ω B97XD/6-31+G(d) (57.92 %)	18.76	-8.76	2.61	21.37	-388.0
ω B97XD/aug-cc-pVDZ (62.72 %)	20.96	-8.926	2.66	23.62	-216.0
M06-2X/6-31+G(d) (72.33 %)	22.68	-8.22	2.45	25.13	-239.4
B3LYP/6-31+G(d) with GD3BJ (65.89 %)	17.28	-8.65	2.58	19.86	-239.2
CAM B3LYP/6-31+G(d) with GD3BJ (60.20 %)	18.02	-8.02	2.39	20.47	-476.5
PBE0/6-31+G(d) with GD3BJ	a	a	a	a	a
Phloroglucinol anion complex with 2H₂O (one H₂O on C=O (A))					
B3LYP/6-31+G(d) (44.62 %)	17.62	-9.73	2.90	20.52	-296.2
CAM B3LYP/6-31+G(d) (60.95 %)	18.42	-10.96	3.27	21.69	-1344.4
PBE0/6-31+G(d)	17.00	-10.46	3.12	20.11	-1177.1
APFD/6-31+G(d)	16.32	-9.48	2.83	19.15	-1159.9
ω B97XD/6-31+G(d) (41.71 %)	19.14	-10.12	3.02	22.16	-1283.2
ω B97XD/aug-cc-pVDZ (37.05 %)	20.19	-9.69	2.89	23.08	-1209.8
M06-2X/6-31+G(d) (27.27 %)	20.22	-13.06	3.89	24.12	-1263.22
B3LYP/6-31+G(d) with GD3BJ (33.85 %)	17.12	-9.37	2.79	19.91	-1206.6
CAM B3LYP/6-31+G(d) with GD3BJ (39.49 %)	18.28	-8.80	2.62	21.32	-1327.5
PBE0/6-31+G(d) with GD3BJ	16.79	-9.79	2.92	19.71	-1156.4
Phloroglucinol anion complex with 3H₂O					
B3LYP/6-31+G(d)	10.10	-9.40	2.80	12.90	-1252.6
CAM-B3LYP/6-31+G(d)	10.97	-8.01	2.39	13.36	-1258.6
PBE0/6-31+G(d)	9.60	-7.40	2.21	11.80	-1007.0
APFD/6-31+G(d)	9.08	-7.29	2.18	11.26	-937.7
ω B97XD/6-31+G(d)	11.70	-7.95	2.37	14.07	-1148.7
M06-2X/6-31+G(d)	14.20	-7.65	2.28	16.47	-1055.1
B3LYP/6-31+G(d) with GD3BJ	9.58	-6.86	2.05	11.63	-1125.5
CAM-B3LYP/6-31+G(d) with GD3BJ	10.81	-7.17	2.14	12.95	-1231.9
PBE0/6-31+G(d) with GD3BJ	9.46	-6.75	2.21	11.48	-970.8
Phloroglucinol anion complex with 4H₂O					
B3LYP/6-31+G(d)	11.82	-14.04	4.19	16.01	-1102.1
CAM-B3LYP/6-31+G(d)	10.81	-7.17	2.14	12.95	-1197.5
PBE0/6-31+G(d)	11.00	-15.72	4.69	15.68	-922.3
APFD/6-31+G(d)	10.20	-14.41	4.30	14.49	-853.7
ω B97XD/6-31+G(d)	12.69	-12.00	3.58	16.27	-1071.0
M06-2X/6-31+G(d)	15.25	-8.26	2.46	17.71	-982.6
B3LYP/6-31+G(d) with GD3BJ	10.79	-14.31	4.27	15.06	-1038.5
CAM-B3LYP/6-31+G(d) with GD3BJ	12.07	-13.04	3.89	15.96	-1167.5
PBE0/6-31+G(d) with GD3BJ	10.57	-13.31	3.97	14.53	-871.6

^a A transition state could not be determined.

Table S4 Computed activation enthalpy ($\Delta H_{comp}^{\ddagger}$), entropy difference between *TS* and complexes ($\Delta S_{(TS-R)}$), activation entropy ($-T\Delta S_{comp}^{\ddagger}$) and equilibrium Gibbs energies ($\Delta G_{comp}^{\ddagger}$), for the C(6)-H of ionic taxifolin with three water molecules, with a variety of computational methods in continuum (IEFPCM=water)

Calculation method	$\Delta H_{comp}^{\ddagger}$ <i>kcal mol⁻¹</i>	$\Delta S_{comp}^{\ddagger}$ <i>cal mol⁻¹</i>	$-T\Delta S_{comp}^{\ddagger}$ <i>kcal mol⁻¹</i>	$\Delta G_{comp}^{\ddagger}$ <i>kcal mol⁻¹</i>	<i>Imaginary</i> <i>cm⁻¹</i>
Ionic Taxifolin + 3H₂O (IEFPCM=water) C(6)-H					
B3LYP-D/6-31+G(d)	22.27	5.23	1.56	23.83	-1014.38
PBE-D/6-31+G(d)	23.06	5.71	1.70	24.76	-736.08
ωB97X-D/6-31+G(d)	23.56	3.18	0.95	24.51	-940.37
CAM-B3LYP-D/6-31+G(d)	22.17	4.29	1.27	23.44	-907.14

Ionic taxifolin +3H₂O

Cartesian Coordinates

Geometries of minimized structures and transition states

Minimized

Taxifolin_anion_3H2O_at C6 wB97XD_631G+d_water

-1 1

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C      -0.12673500  -0.36853000  -0.72042200
C      -0.76810200   0.83057200  -0.28037400
C      -2.15407800   0.83939700   0.00548800
H       1.65085500  -1.32464300  -1.40344000
C       1.19289100  -0.39302500  -1.08697500
C       0.03408200   2.01187500  -0.19427500
C       1.99731800   0.79914700  -1.02833900
O      -0.83219300  -1.52862800  -0.80111100
O      -0.52532600   3.16207800   0.23101200
H      -1.47233800   2.97649200   0.43420800
O       3.22577200   0.78754400  -1.35900500
O      -2.79535900   1.82116700   0.44714000
O      -4.07370400  -0.50803400   0.53374400
H      -4.26483100   0.41185000   0.78940300
C      -2.00498800  -1.64201900   0.02093800
H      -1.69153200  -1.60585100   1.07420500

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C	-2.91599900	-0.45000200	-0.26182400
H	-3.18333700	-0.46203500	-1.33236900
O	2.83791500	-1.94657200	1.73337300
H	2.49444300	-1.05013700	1.94183700
C	-2.64449100	-2.97668300	-0.29349700
H	-3.52940100	-3.11905300	0.33254300
H	-2.94632100	-3.02022500	-1.34543400
H	-1.94128800	-3.79001500	-0.09276400
C	1.36955000	1.99689300	-0.53405300
H	3.35837600	-2.20518800	2.50445200
H	1.95536800	2.90912500	-0.46914600
O	1.88957300	0.61258300	2.33146500
H	2.56261800	1.13485500	2.78747400
H	1.71643800	1.09322300	1.50104200
O	4.45322000	-1.56700700	-0.58560800
H	4.05089400	-0.74279900	-0.94422500
H	3.92417400	-1.75640200	0.21413100

Transition State

Taxifolin_anion_3H2O_at C6_part_wB97XD_631G+d_water.

Imaginary Frequency: -940.37 cm⁻¹

-1 1

C	-0.35167600	-0.65517200	-0.62235400
C	-0.78179400	0.69583900	-0.30946800
C	-2.14983100	0.96918600	0.01138000
H	1.15286000	-1.96607800	-1.35835600
C	0.89106400	-0.94519100	-1.10630100
C	0.13765300	1.72742500	-0.42404000
C	1.85756000	0.09844600	-1.30604500
O	-1.22635700	-1.66281200	-0.47324700
O	-0.19149100	2.97615600	-0.19391400
H	-1.14715100	2.99534800	0.07482000

O	2.97277600	-0.10445600	-1.81394700
O	-2.57540700	2.09619400	0.31926600
O	-4.23469500	0.01744000	0.74634200
H	-4.32176600	0.97576500	0.85645700
C	-2.37653700	-1.47053700	0.37978100
H	-2.01826400	-1.34256300	1.40903000
C	-3.10876800	-0.20106300	-0.05851300
H	-3.39591800	-0.31738100	-1.11781100
O	3.26419400	-0.96799300	2.06977900
H	3.18474700	0.21775200	1.92796900
C	-3.22138200	-2.71844600	0.26348300
H	-4.09381100	-2.62971200	0.91408600
H	-3.56074800	-2.85664400	-0.76717800
H	-2.64455500	-3.59371800	0.57007800
C	1.54086100	1.47068700	-0.77111700
H	3.72879800	-1.14747300	2.89175500
H	1.95484600	2.26265600	-1.39953200
O	3.04376000	1.41425700	1.74638900
H	3.91205100	1.79950400	1.59500600
H	2.11825000	1.51812200	0.20996500
O	4.28140900	-2.08414900	-0.15003400
H	3.90457900	-1.52427800	-0.84581600
H	3.92966300	-1.69544100	0.69362300

Minimized

Taxifolin_anion_3H2O_at C6 CAM-B3LYP-D_631G+d_water

-1 1

C	-0.18173500	-0.41656500	-0.73770100
C	-0.79099500	0.79803500	-0.30049500
C	-2.16538000	0.83705700	0.01693400
H	1.56185200	-1.41213800	-1.44497600
C	1.12708000	-0.47028000	-1.12937900
C	0.03170700	1.96471700	-0.24808000
C	1.95021600	0.70803400	-1.10569500
O	-0.91495100	-1.56319800	-0.78757700
O	-0.50558800	3.12797700	0.17360900
H	-1.45490400	2.95528000	0.39898900
O	3.17106900	0.67114400	-1.46516500
O	-2.77679100	1.83996600	0.45943400
O	-4.09338700	-0.45338700	0.62865700
H	-4.25228200	0.47781900	0.87716300
C	-2.06980300	-1.64244300	0.06727800
H	-1.72695000	-1.59777100	1.10969700
C	-2.95936700	-0.43671200	-0.20680800
H	-3.26357700	-0.46030700	-1.26604000
O	3.12220300	-1.76201600	1.87637400
H	2.72854300	-0.87271600	2.04018000
C	-2.74369500	-2.96469800	-0.21286800
H	-3.61911700	-3.07786800	0.43113200
H	-3.06624800	-3.01711900	-1.25762500
H	-2.05539800	-3.79062800	-0.01462300
C	1.35684000	1.92248100	-0.61551900
H	3.68936200	-1.94466300	2.63979700
H	1.95829500	2.82543500	-0.58510200
O	1.98473700	0.73104500	2.27553200
H	2.56175700	1.34949800	2.74895300

H	1.78861700	1.16050300	1.41855500
O	4.48050800	-1.57972900	-0.60294500
H	4.02953900	-0.79230700	-0.99488900
H	4.04888400	-1.69518900	0.26942800

Transition State

Taxifolin_anion_3H2O_at C6_part_ CAM-B3LYP-D_631G+d_water

Imaginary Frequency: -907.14 cm⁻¹

-1 1

C	-0.36882800	-0.67087000	-0.61816800
C	-0.79478200	0.68352500	-0.32023700
C	-2.15939600	0.96228000	-0.00069800
H	1.13011500	-1.99517800	-1.33524500
C	0.87170600	-0.97055800	-1.09471700
C	0.12837700	1.70788100	-0.44077200
C	1.84228800	0.06496600	-1.29998800
O	-1.25039000	-1.67325600	-0.45888300
O	-0.19467300	2.96185000	-0.22160100
H	-1.15606300	2.99281000	0.04715400
O	2.95939100	-0.14813300	-1.80075400
O	-2.58312100	2.09275000	0.29960700
O	-4.24360900	0.03866500	0.75591300
H	-4.31366200	1.00548400	0.86240300
C	-2.39849500	-1.46750400	0.39684500
H	-2.03413200	-1.32887000	1.42161600
C	-3.12186000	-0.20209600	-0.05441700
H	-3.42116900	-0.33054300	-1.10784500
O	3.33198400	-0.94278100	2.06535700
H	3.21356400	0.23893100	1.92986500
C	-3.24769600	-2.71121100	0.29701400
H	-4.12100300	-2.61190500	0.94572300
H	-3.58737900	-2.86234800	-0.73218800

H	-2.67488000	-3.58635000	0.61374700
C	1.53098000	1.44362500	-0.78281300
H	3.81884800	-1.10197700	2.88624900
H	1.94182000	2.22385100	-1.42892000
O	3.02604100	1.44351200	1.74644200
H	3.88866500	1.85346800	1.58713700
H	2.11078000	1.51399000	0.19175500
O	4.39340000	-2.01423100	-0.16246000
H	3.96525900	-1.47617300	-0.85483600
H	4.03327500	-1.64243700	0.69212500

Minimized

Taxifolin_anion_3H2O_at C6 B3LYP-D_631G+d_water

-1 1

C	-0.16423800	-0.40484500	-0.74055900
C	-0.78238900	0.80989800	-0.30033900
C	-2.16110200	0.84353300	0.01178700
H	1.59326300	-1.39265100	-1.43929500
C	1.15290800	-0.45237900	-1.12481700
C	0.04101200	1.98272300	-0.23508200
C	1.97680000	0.73027500	-1.08949000
O	-0.89464100	-1.56025900	-0.80263500
O	-0.50366900	3.14886200	0.19110400
H	-1.45579800	2.96580400	0.40900700
O	3.20594900	0.69888000	-1.44052200
O	-2.78112300	1.84918900	0.45904500
O	-4.10072500	-0.46022800	0.60934700
H	-4.25179900	0.47187900	0.86725400
C	-2.06194500	-1.64681700	0.05085000
H	-1.72205200	-1.60634000	1.09525800
C	-2.95408400	-0.43583700	-0.22269800
H	-3.25514800	-0.45699000	-1.28427400

O	3.01055100	-1.83064600	1.85362800
H	2.64349100	-0.92830200	2.01872800
C	-2.73061100	-2.97454000	-0.24127500
H	-3.60732100	-3.09564500	0.40147400
H	-3.05230000	-3.02160900	-1.28775300
H	-2.03833800	-3.79975400	-0.04677200
C	1.37340300	1.94454200	-0.59550300
H	3.57310900	-2.02310800	2.62014700
H	1.97355800	2.84867500	-0.55337300
O	1.96293500	0.71479400	2.29265500
H	2.60923800	1.29573600	2.72544400
H	1.77059200	1.14462900	1.43246200
O	4.47949200	-1.59322300	-0.57960000
H	4.04492200	-0.79358000	-0.96993400
H	4.00590500	-1.72701700	0.27020900

Transition State

Taxifolin_anion_3H2O_at C6_part_ B3LYP-D_631G+d_water

Imaginary Frequency: -1014.38 cm⁻¹

-1 1

C	-0.36533600	-0.66469900	-0.62007000
C	-0.78685600	0.68987300	-0.31211200
C	-2.15325800	0.97254700	0.00712700
H	1.13321300	-1.98851700	-1.35669100
C	0.88072000	-0.96413300	-1.10563500
C	0.14748200	1.71661200	-0.42949900
C	1.85597100	0.06851800	-1.30775600
O	-1.24785100	-1.67491100	-0.46702000
O	-0.17647500	2.97709000	-0.20717400
H	-1.14099800	3.00213900	0.06183400
O	2.97668700	-0.14406800	-1.81860200
O	-2.57683600	2.10908400	0.31605300
O	-4.25867400	0.04866000	0.74618000

H	-4.31113000	1.01664500	0.86884600
C	-2.40881500	-1.46947100	0.38818700
H	-2.04683300	-1.34046800	1.41569600
C	-3.12409900	-0.19134500	-0.05964600
H	-3.41829400	-0.31266900	-1.11674700
O	3.26283100	-0.97153600	2.08958600
H	3.19626300	0.24192200	1.92441300
C	-3.26307100	-2.71388100	0.27198500
H	-4.13787000	-2.61821300	0.92112500
H	-3.60239200	-2.85308500	-0.76017500
H	-2.69287400	-3.59490700	0.58134300
C	1.54993900	1.44542400	-0.76708300
H	3.78763900	-1.12685500	2.89016500
H	1.98060700	2.23779200	-1.38659700
O	3.06960600	1.43218700	1.72632300
H	3.94379400	1.76822700	1.47168000
H	2.12866800	1.49047200	0.21932900
O	4.35782700	-2.03926100	-0.13623800
H	3.94770600	-1.49104200	-0.83427000
H	3.97951900	-1.66605800	0.71419800

Minimized

Taxifolin_anion_3H2O_at C6 PBE-D_631G+d_water

-1 1

C	-0.17778400	-0.42026900	-0.73088800
C	-0.78683100	0.79537700	-0.29558300
C	-2.16289900	0.83557200	0.01430600
H	1.57164200	-1.41315900	-1.43796000
C	1.13422900	-0.47042200	-1.12377200
C	0.03270800	1.96582200	-0.24004000
C	1.95736900	0.70952600	-1.10160000
O	-0.90637200	-1.56676400	-0.77803600
O	-0.51000800	3.12284700	0.18040600
H	-1.45910100	2.93415300	0.40117500
O	3.17631400	0.67615500	-1.46228200
O	-2.77707300	1.83796800	0.45950200
O	-4.09838000	-0.44855600	0.59519000
H	-4.23648200	0.48405900	0.85062900
C	-2.06191900	-1.63684800	0.07172300
H	-1.72349600	-1.57953100	1.11723500
C	-2.95360000	-0.43646800	-0.21790700
H	-3.23675200	-0.46614600	-1.28554800
O	3.09193900	-1.76410900	1.87454100
H	2.70526800	-0.86963100	2.02230200
C	-2.73331500	-2.96116300	-0.19462000
H	-3.61180300	-3.06542100	0.44831800
H	-3.05344200	-3.02685300	-1.24030300
H	-2.04661200	-3.78633500	0.01712500
C	1.36099600	1.92344200	-0.60739000
H	3.69126900	-1.90750400	2.61926400
H	1.96264900	2.82785800	-0.57540200
O	1.98396900	0.74168700	2.26308900
H	2.61218600	1.34750400	2.68057100

H	1.77942700	1.14912200	1.39739700
O	4.45925800	-1.59336600	-0.59944400
H	4.01772500	-0.80232200	-0.99161700
H	4.01662100	-1.70009700	0.26771600

Transition State

Taxifolin_anion_3H2O_at C6_part_6_PBE-D_631G+d_water

Imaginary Frequency: -736.08 cm⁻¹

-1 1

C	-0.36271500	-0.66428100	-0.61599900
C	-0.78859700	0.68151900	-0.30326700
C	-2.15333200	0.95757800	0.00668300
H	1.14224500	-1.97331900	-1.36215100
C	0.88243800	-0.95196100	-1.10374600
C	0.13623600	1.71483700	-0.41735200
C	1.84693600	0.08894500	-1.30157700
O	-1.23571700	-1.67314500	-0.46502700
O	-0.20050800	2.96277800	-0.19330100
H	-1.16542000	2.96969000	0.07281700
O	2.96239500	-0.10974800	-1.81578000
O	-2.58266000	2.08603700	0.31764500
O	-4.24533100	0.02709900	0.71914500
H	-4.29210500	0.99228900	0.84774400
C	-2.38436700	-1.46957600	0.38467200
H	-2.02374100	-1.32809600	1.41252400
C	-3.11140300	-0.20665800	-0.06833700
H	-3.38852500	-0.33391000	-1.13067700
O	3.31426000	-0.97468100	2.06771800
H	3.17212900	0.25909500	1.91221200
C	-3.23037600	-2.71319000	0.28473000
H	-4.10639900	-2.61202400	0.93109900
H	-3.56806200	-2.86751500	-0.74558100
H	-2.65875900	-3.58840100	0.60664100

C	1.53213500	1.45001900	-0.74914500
H	3.86910100	-1.10793600	2.84740500
H	1.98001800	2.25623900	-1.33732700
O	2.97905800	1.40536500	1.73167500
H	3.83681700	1.79839800	1.52006000
H	2.09845900	1.47034000	0.25678700
O	4.37638900	-1.99604900	-0.16005000
H	3.95426000	-1.44706700	-0.84553200
H	4.00514900	-1.63241700	0.69780500

Minimized

Minimized

Taxifolin_anion_3H2O_at C8 CAM-B3LYP-D_631G+d_water

-1 1

C	-0.43640500	-0.71426400	-0.72310300
C	-0.58371700	0.66528800	-0.40143600
C	-1.85141300	1.18865600	-0.06479600
H	0.84958800	-2.29372500	-1.36361900
C	0.76919900	-1.24084900	-1.11320000
C	0.58052100	1.49239300	-0.49504500
C	1.93356600	-0.40140300	-1.24098800
O	-1.50484100	-1.55160900	-0.64660800
O	0.47640600	2.80320500	-0.18895400
H	-0.46258400	2.97784500	0.07246000
O	3.04991300	-0.88619000	-1.61133200
O	-2.07460200	2.37324500	0.28131800
O	-4.06264100	0.67315600	0.71149500
H	-3.89751200	1.62386400	0.86285500
C	-2.57918900	-1.16661800	0.23231900
H	-2.18818300	-1.14915600	1.25844800
C	-3.03178400	0.23780600	-0.14368600

H	-3.38064900	0.22466900	-1.18927200
O	3.13955000	0.46815800	2.09839400
H	2.56292400	-0.32958700	2.13906300
C	-3.66383700	-2.20816900	0.09530400
H	-4.49438200	-1.96667100	0.76293700
H	-4.03694400	-2.24054200	-0.93322500
H	-3.27745700	-3.19549200	0.36183100
C	1.79097800	0.98503900	-0.89661300
H	2.67389600	1.06061700	1.48540900
H	2.65113000	1.64097800	-0.98820600
O	1.47845600	-1.74584100	1.95383300
H	0.68080100	-1.68827500	2.50231100
H	1.16281300	-1.68562200	1.03005300
O	5.07853400	-0.31560000	0.16707900
H	4.42065300	-0.50413000	-0.54402800
H	4.52218900	-0.05023600	0.92865000

Transition State

Taxifolin_anion_3H2O_at C8_part_ CAM-B3LYP-D_631G+d_water

Imaginary Frequency: -878.06 cm⁻¹

-1 1

C	0.45945400	-0.47154200	0.62732200
C	0.73920400	0.78105800	0.12938000
C	2.08585400	1.10160000	-0.25032200
H	-0.84531700	-1.47048800	1.98241200
C	-0.88627600	-0.84320500	1.08762800
C	-0.32847800	1.77482400	0.10919400
C	-1.87557600	0.27960200	1.23744200
O	1.34306700	-1.45215300	0.67398500
O	-0.05550600	2.97030600	-0.42105300
H	0.88631300	2.98610100	-0.72119100
O	-2.95408400	0.05167500	1.81396300

O	2.43367100	2.16301200	-0.78493300
O	4.28028900	0.23034300	-0.70851500
H	4.27280700	1.15236700	-1.02698700
C	2.56891500	-1.32783600	-0.10229000
H	2.28117900	-1.45394600	-1.15266400
C	3.14027100	0.06864100	0.09406500
H	3.38953600	0.20884000	1.15899200
O	-2.07000800	-2.41790800	-1.11170800
H	-2.87782600	-1.60596700	-1.58244800
C	3.49098100	-2.43414700	0.34448200
H	4.40824700	-2.40225200	-0.24793000
H	3.74891400	-2.31827800	1.40133800
H	3.01493000	-3.40668700	0.19769800
C	-1.56614000	1.53842800	0.63219700
H	-2.57750700	-3.14650200	-0.72549400
H	-2.31113000	2.32590600	0.63610700
O	-3.60812400	-0.76794400	-2.00873200
H	-4.09071500	-1.14510300	-2.75775700
H	-1.31694800	-1.50254100	0.27265100
O	-5.10517600	0.31603800	-0.05034400
H	-4.47293000	0.31790100	0.69340300
H	-4.59183100	-0.09084500	-0.80400700