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DFT and Molecular Docking Studies of Melatonin and Some Analogues Interaction with Xanthine Oxidase as a Possible Antiradical Mechanism

Brenda Manzanilla, Minerva Martinez-Alfaro, Juvencio Robles*

Departamento de Farmacia, DCNE, Universidad de Guanajuato, Noria Alta S/N. Col. Noria Alta, C. P. 36050, Guanajuato, Gto., México.

***Corresponding author:** Juvencio Robles, email: roblesj@ugto.mx

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Supplementary Information

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Table S1. Atoms studied for hydrogen atom transfer (HAT) mechanism for Mel at M06-2X/6-31+G*. Values in kcal/mol.

Atom	Do	ΔG			
		$OH^{\bullet}$	$CH_3O^{\bullet}$	$HOO^{\bullet}$	$NO_2^{\bullet}$
N1	85.73	-29.10[a] -24.34[b]	-14.59[a] -9.29[b]	3.30[a] 8.28[b]	4.47[a] 11.07[b]
N2	102.36	-9.99[a] -6.25[b]	4.83[a] 8.41[b]	22.41[a] 26.38[b]	23.58[a] 19.16[b]
C7	104.78	-4.31[a] -2.57[b]	10.42[a] 11.86[b]	28.09[a] 30.05[b]	29.26[a] 32.83[b]
C8	95.83	-28.31[a] -25.54[b]	-14.12[a] -12.16[b]	4.09[a] 7.08[b]	5.26[a] 9.87[b]
C9	96.38	-23.23[a] -22.03[b]	-9.58[a] -8.15[b]	9.17[a] 10.59[b]	10.34[a] 13.38[b]

[a] water
[b] pentyl ethanoate

Table S2. Atoms studied for hydrogen atom transfer (HAT) mechanism for AMK at M06-2X/6-31+G*. Values in kcal/mol.

Atom	Do	ΔG			
		$OH^{\bullet}$	$CH_3O^{\bullet}$	$HOO^{\bullet}$	$NO_2^{\bullet}$
N1	96.39	-24.50[a] -19.58[b]	-10.09[a] -5.08[b]	7.90[a] 13.04[b]	16.02[a] 15.82[b]
N2	103.89	-9.57[a] -6.52[b]	5.87[a] 7.33[b]	22.83 [a] 26.11[b]	29.91[a] 28.89[b]
C8	98.29	-27.03[a] -23.54[b]	-13.71[a] -10.29[b]	5.37[a] 9.08[b]	14.57[a] 11.86[b]
C9	97.06	-24.57[a] -21.88[b]	-10.57[a] -8.10[b]	7.83[a] 10.74[b]	16.35[a] 13.53[b]

[a] water
[b] pentyl ethanoate

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Table S3. Atoms studied for hydrogen atom transfer (HAT) mechanism for AFMK at M06-2X/6-31+G*. Values in kcal/mol.

Atom	Do	ΔG			
		$OH^{\bullet}$	$CH_3O^{\bullet}$	$HOO^{\bullet}$	$NO_2^{\bullet}$
N1	105.15	-21.68[a] -17.56[b]	-8.54[a] -3.64[b]	10.72[a] 15.07[b]	11.90[a] 17.85[b]
N2	107.67	-11.54[a] -5.84[b]	2.90[a] 8.93[b]	20.86[a] 26.79[b]	22.03[a] 29.57[b]
C8	94.75	-26.83[a] -23.30[b]	-13.27[a] -9.20[b]	5.57[a] 9.33[b]	6.74[a] 12.11[b]
C9	99.00	-24.50[a] -20.95[b]	-11.29[a] -6.69[b]	7.90[a] 11.67[b]	9.07[a] 14.46[b]
C12	86.46	-19.43[a] -21.34[b]	-4.91[a] -8.00[b]	12.97[a] 11.28[b]	14.14[a] 14.07[b]

[a] water
[b] pentyl ethanoate

Table S4. Atoms studied for hydrogen atom transfer (HAT) mechanism for 6OHM at M06-2X/6-31+G*. Values in kcal/mol.

Atom	Do	ΔG			
		$OH^{\bullet}$	$CH_3O^{\bullet}$	$HOO^{\bullet}$	$NO_2^{\bullet}$
N1	102.59	-31.35[a] -26.98[b]	-16.64[a] -12.08[b]	1.05[a] 5.70[b]	8.86[a] 8.43[b]
N2	102.62	-10.83[a] -7.12[b]	3.43[a] 7.08[b]	21.57[a] 25.56[b]	29.82[a] 28.28[b]
C4	104.14	-5.45[a] -2.67[b]	9.01[a] 12.06[b]	26.95[a] 30.01[b]	35.00[a] 32.74[b]
C7	105.56	5.40[a] -0.08[b]	20.06[a] 14.55[b]	37.80[a] 32.60[b]	45.67[a] 35.32[b]
C8	95.28	-23.85[a] -22.25[b]	-10.89[a] -8.41[b]	8.55[a] 10.43[b]	18.10[a] 13.16[b]
C9	95.28	-23.85[a] -22.25[b]	-10.89[a] -8.41[b]	8.55[a] 10.43[b]	18.10[a] 13.16[b]
O13	84.32	-42.46[a] -35.98[b]	-28.10[a] -20.64[b]	-10.06[a] -3.30[b]	-1.90[a] -0.58[b]

[a] water
[b] pentyl ethanoate

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Table S5. Atoms studied for hydrogen atom transfer (HAT) mechanism for Ir at M06-2X/6-31+G*. Values in kcal/mol.

Atom	Do	ΔG			
		$OH^{\bullet}$	$CH_3O^{\bullet}$	$HOO^{\bullet}$	$NO_2^{\bullet}$
N1	66.92	-41.49[a] -47.41[b]	-26.58[a] -31.26[b]	-9.09[a] -14.79[b]	-7.92[a] -12.01[b]
O5	67.76	-40.70[a] -47.41[b]	-25.79[a] -33.80[b]	-8.30[a] -16.07[b]	-7.13[a] -13.29[b]
C4	92.63	-14.54[a] -23.06[b]	0.23[a] -8.11[b]	17.86[a] 9.56[b]	19.04[a] 12.35[b]
C6	108.97	-5.04[a] -10.11[b]	11.63[a] 5.86[b]	27.36[a] 22.51[b]	28.53[a] 25.29[b]
C9	103.99	-4.41[a] -12.51[b]	10.33[a] 1.94[b]	27.99[a] 20.11[b]	29.16[a] 22.90[b]
C10	103.48	-5.01[a] -12.97[b]	10.23[a] 1.79[b]	27.39[a] 19.66[b]	28.56[a] 22.44[b]
C11	103.80	9.54[a] -11.39[b]	25.05[a] 3.54[b]	41.94[a] 21.23[b]	43.11[a] 24.02[b]
C13	84.94	-22.46[a] -29.72[b]	-7.99[a] -14.22[b]	9.94[a] 2.90[b]	11.11[a] 5.69[b]
Ca	103.26	7.58[a] -12.82[b]	22.89[a] 1.33[b]	39.98[a] 19.80[b]	41.16[a] 22.59[b]
Cb	102.36	-6.16[a] -13.08[b]	8.48[a] 2.14[b]	26.24[a] 19.55[b]	27.41[a] 22.33[b]
Cc	104.34	-4.53[a] -11.95[b]	10.27[a] 2.92[b]	27.87[a] 20.68[b]	29.04[a] 23.46[b]
Cd	102.53	-6.20[a] -13.54[b]	8.61[a] 1.46[b]	26.20[a] 19.09[b]	27.37[a] 21.87[b]
Ce	103.97	9.07[a] -12.31[b]	22.99[a] 2.35[b]	41.47[a] 20.31[b]	42.64[a] 23.10[b]

[a] water
[b] pentyl ethanoate

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Table S6. Atoms studied for hydrogen atom transfer (HAT) mechanism for It at M06-2X/6-31+G*. Values in kcal/mol.

Atom	Do	ΔG			
		$OH^{\bullet}$	$CH_3O^{\bullet}$	$HOO^{\bullet}$	$NO_2^{\bullet}$
N1	64.11	-45.97[a] -1.71[b]	-31.34[a] 13.81[b]	-13.57[a] 30.91[b]	-12.39[a] 33.70[b]
O5	67.16	-40.86 -40.64[b]	-25.47[a] -25.19[b]	-8.46[a] -8.02[b]	-7.29[a] -5.24[b]
C4	90.24	-18.68[a] -18.04[b]	-4.30[a] -3.47[b]	13.72[a] 14.58[b]	14.89[a] 17.37[b]
C6	109.58	-4.37[a] -1.37[b]	10.82[a] 13.88[b]	28.03[a] 31.26[b]	29.20[a] 34.04[b]
C9	103.58	-4.66[a] -4.04[b]	10.67[a] 11.16[b]	27.74[a] 28.58[b]	28.92[a] 31.36[b]
C10	102.79	-5.70[a] -5.02[b]	9.67[a] 10.19[b]	26.70[a] 27.60[b]	27.87[a] 30.39[b]
C11	103.66	-4.17[a] -3.46[b]	10.78[a] 11.83[b]	28.23[a] 29.16[b]	29.40[a] 31.95[b]
C13	84.90	-22.29[a] -22.20[b]	-6.95[a] -6.80[b]	10.11[a] 10.42[b]	11.28[a] 13.20[b]
Cb	105.07	-3.04[a] -2.19[b]	12.12[a] 13.04[b]	29.36[a] 30.44[b]	30.53[a] 33.22[b]
Cc	102.93	-4.60[a] -4.24[b]	10.92[a] 10.85[b]	27.80[a] 28.39[b]	28.98[a] 31.17[b]
Cd	103.10	-5.08[a] -4.33[b]	10.08[a] 10.87[b]	27.32[a] 28.30[b]	28.49[a] 31.08[b]
Ce	103.47	-4.24[a] -3.77[b]	11.14[a] 11.51[b]	28.16[a] 28.85[b]	29.34[a] 31.63[b]

[a] water
[b] pentyl ethanoate