Supplemental data for

Hydroxyl radical scavenging activity of melatonin and its related indolamines

Aiswarya Purushothaman [a], Achutha. A. S[b], Deepa Janardanan[a]*

[a]Department of Chemistry, School of Physical Sciences, Central University of Kerala, Kasaragod, Kerala-671320, India

[b]PG and Research Department of Chemistry, Sree Narayana College Kollam, Kerala-691001, India

Email: deepa.j@cukerala.ac.in

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Table S1. Relative Energies (ΔE, kcal/mol) and Gibbs free energies (ΔG, kcal/mol) of all the stationary points on the PES of OH radical addition to indolamines computed at the B1 level of theory

Stationary point	ΔE(B1)[a]	ΔG (B1)
RC	0.0	0.0
Melatonin+ •OH		
I-1M	-28.0	-19.3
TS-2M	16.7 (7.2)[b]	20.7 (15.5)
I-2M	-13.7 (-0.8)	-5.8 (10.1)
TS-3M	7.2	15.7
I-3M	-4.6	6.4
PC-M	-123.6	100.1
NAT+ •OH		
I-1T	-20.6	-13.1
TS-2T	22.1 (7.1)	25.9 (16.2)
I-2T	-6.2 (-1.4)	1.6 (10.6)
TS-3T	14.1	22.4
I-3T	3.5	14.0
PC-T	-117.9	-95.4
NAS+ •OH		
I-1S	-22.7	-7.8
TS-2S	22.1 (7.1)	33.3 (18.0)
I-2S	-7.9 (-0.8)	6.6 (14.2)
TS-3S	12.5	25.8
I-3S	0.6	15.7
PC-S	-118.3	-127.1

[a]B1 = UB3LYP/6-31G*; [b] Values in parentheses are energies computed by including an explicit water molecule.

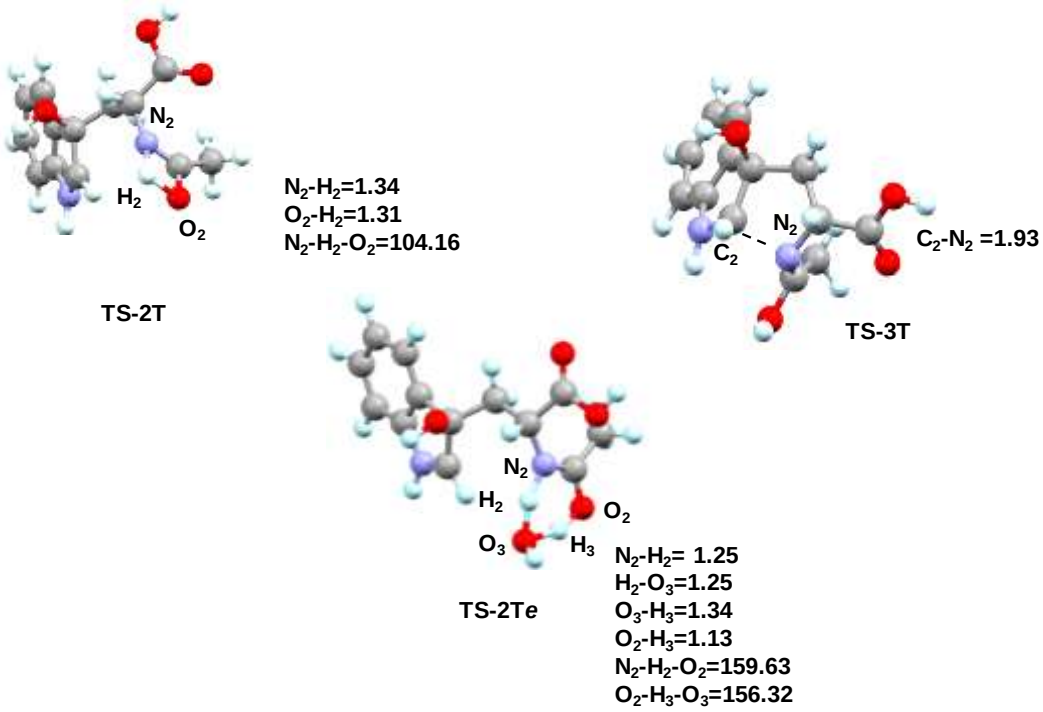

Figure S1. UB3LYP/6-31G* optimized geometries of transition states in the reaction of hydroxyl radical with NAT [Distances in Å, angles in ^{o}].

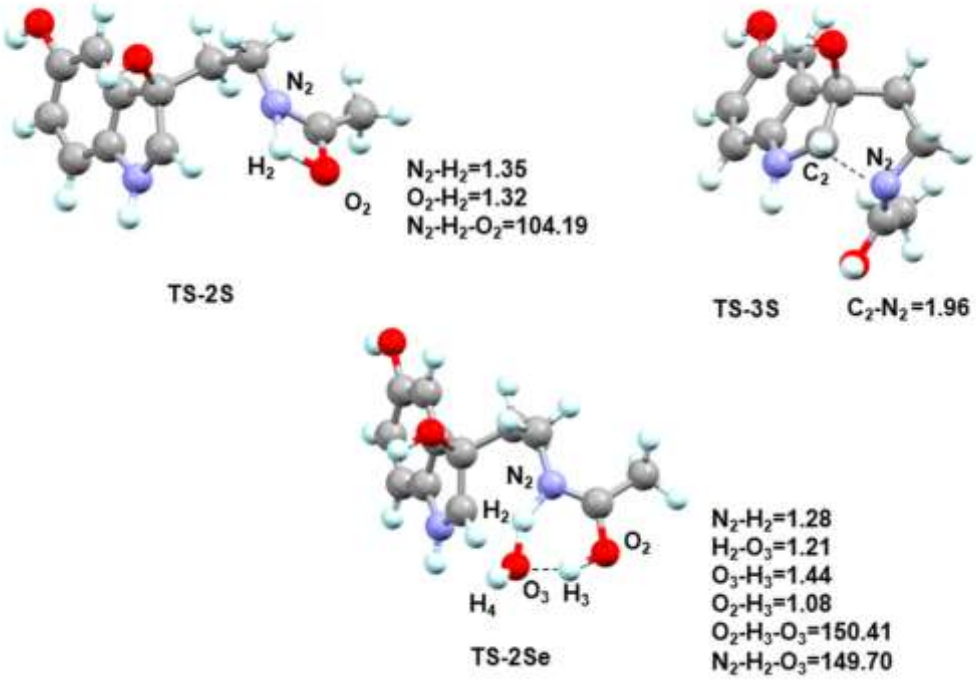

Figure S2. UB3LYP/6-31G* optimized geometries of transition states in the reaction of hydroxyl radical with NAS [Distances in Å, angles in ^{o}].

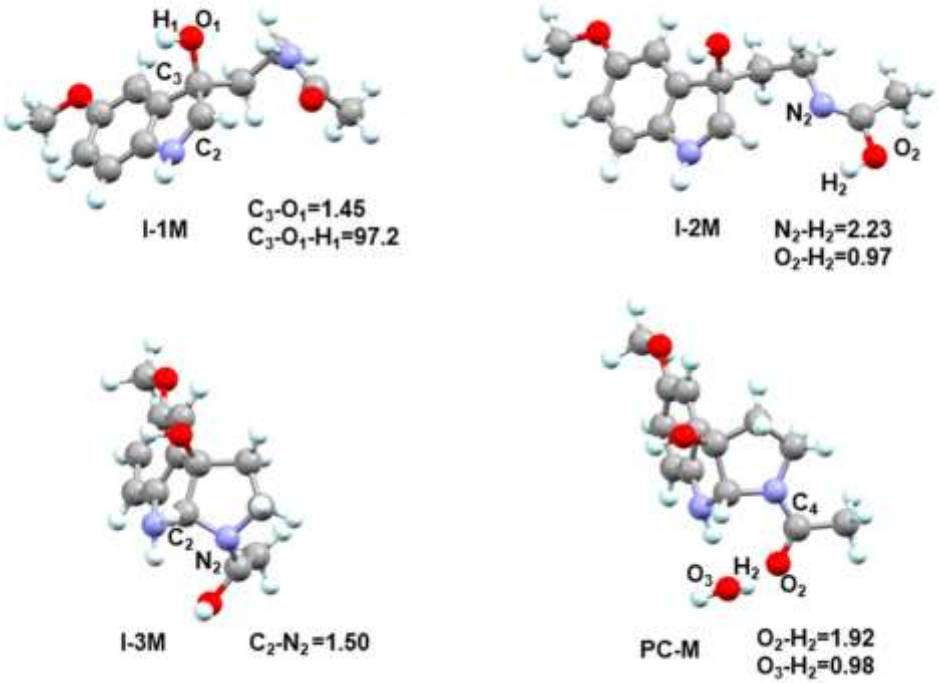

Figure S3. UB3LYP/6-31G* optimized geometries of intermediates and product complex in the reaction of hydroxyl radical with Melatonin [Distances in Å, angles in ^{o}].

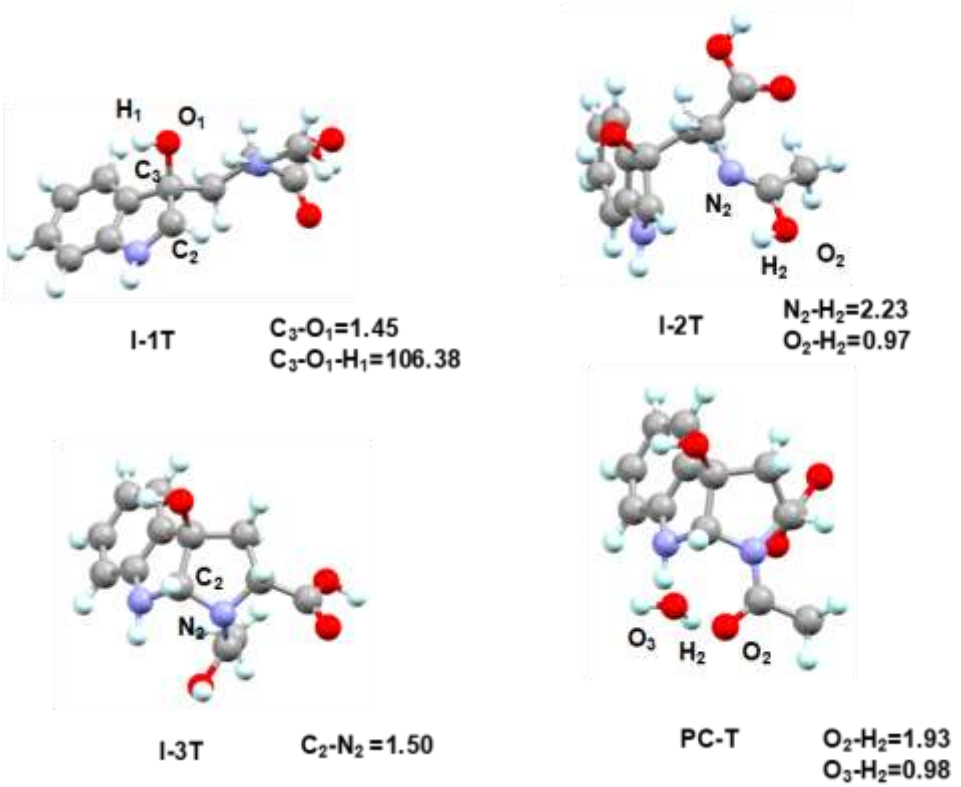

Figure S4. UB3LYP/6-31G* optimized geometries of intermediates and product complex in the reaction of hydroxyl radical with NAT [Distances in Å, angles in ^{o}].

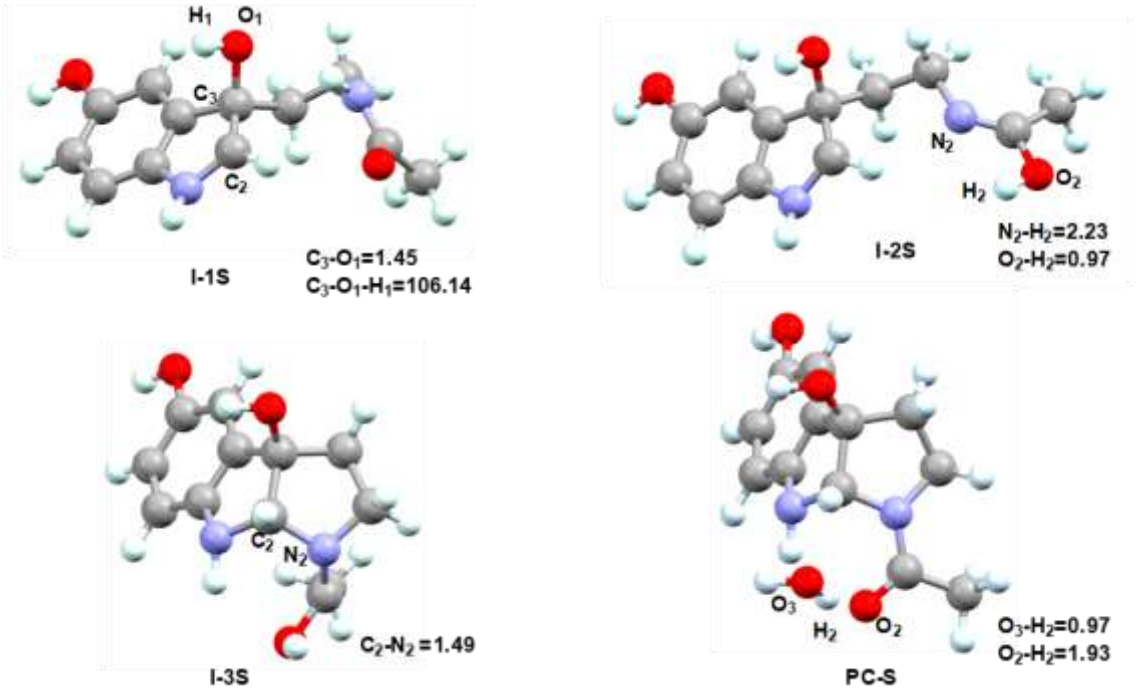

Figure S5. UB3LYP/6-31G* optimized geometries of intermediates and product complex in the reaction of hydroxyl radical with NAS [Distances in Å, angles in ^{o}].

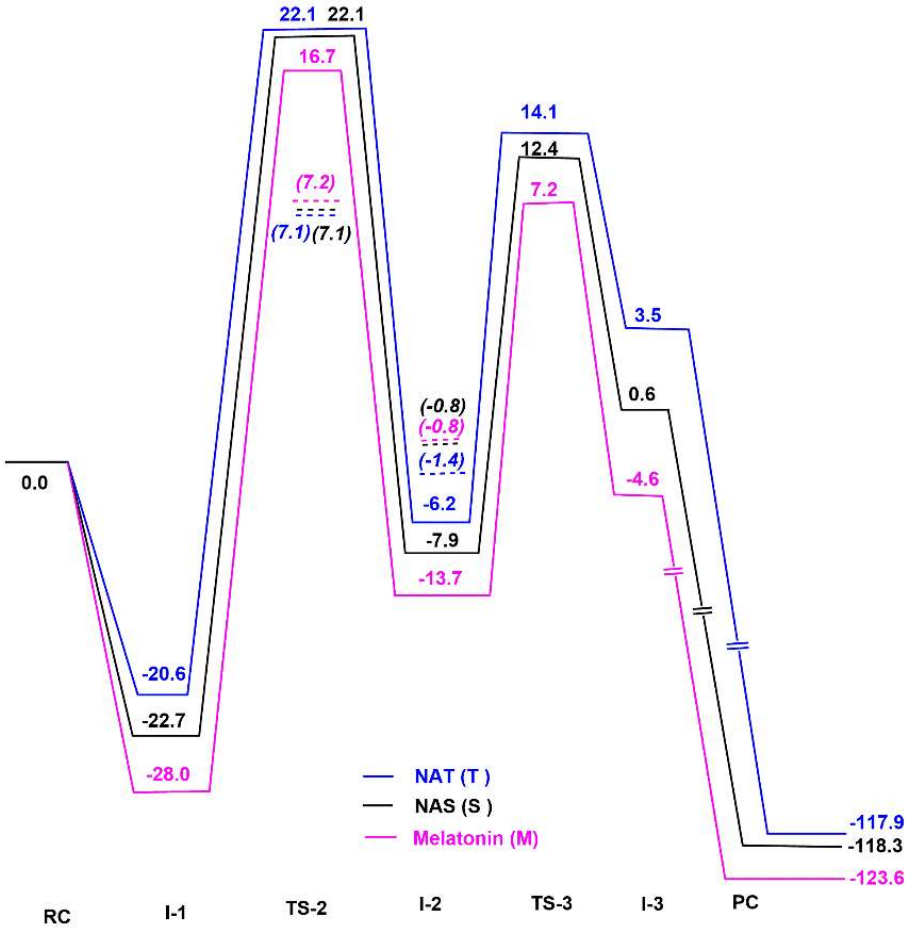

Figure S6. Energy profile (B1 energies in kcal/mol) calculated in the gas phase for the hydroxyl radical scavenging by melatonin, NAS and NAT (relative energy with the inclusion of an explicit solvent molecule is denoted in italics within parentheses).

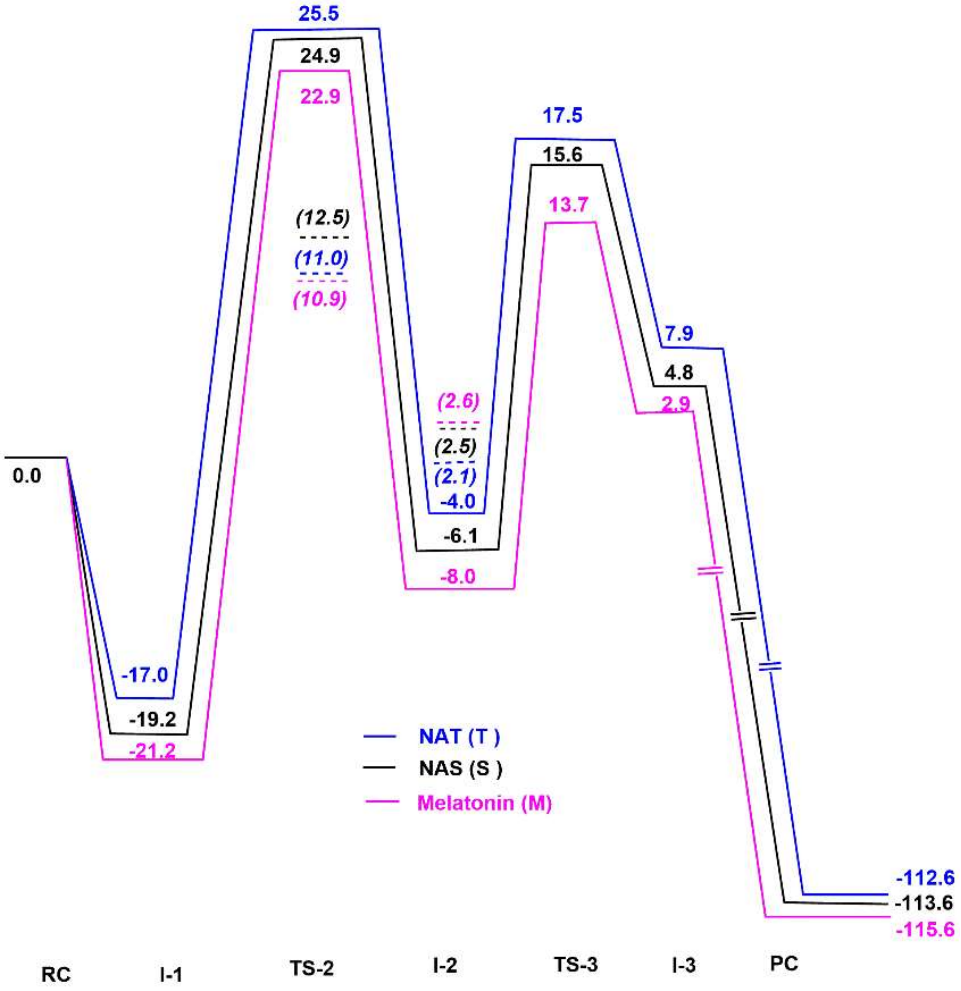

Figure S7. Energy profile (B2 energies in kcal/mol) calculated in the gas phase for the hydroxyl radical scavenging by melatonin, NAS and NAT (relative energy with the inclusion of an explicit solvent molecule is denoted in italics within parentheses).