

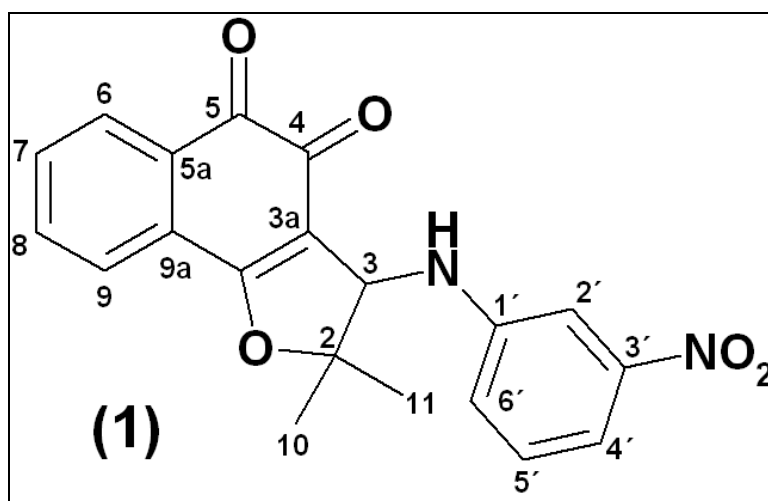
## Supporting information for Manuscript

### “Inner Reorganization During the Radical-Biradical Transition in a Nor- $\beta$ -Lapachone Derivative Possessing Two Redox centres”

By

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**Scheme 1.** Structure of the studied molecule, indicating numbering for each position

**Table 1.** Geometric parameters for the neutral (N), radical anion (RA) and biradical dianion (BD) structures calculated for compound **1** at the BLYP/TZVP level of theory (Distances appear in Angstroms and angles in degrees).

Geometric parameter	N	RA	BD
C-1 --- O-1	1.351	1.390	1.390
C-2 --- O-1	1.536	1.506	1.506
C-2 --- C-3	1.588	1.594	1.594
C-3 --- C-3a	1.521	1.523	1.523
C-3a --- C-4	1.438	1.448	1.448
C-4 --- C-5	1.571	1.511	1.511
C-4 --- O-4	1.241	1.271	1.271
C-5 --- O-5	1.229	1.274	1.274
C-5 --- C-5a	1.497	1.473	1.473
C-5a --- C-6	1.397	1.414	1.414
C-6 --- C-7	1.395	1.388	1.389
C-7 --- C-8	1.396	1.414	1.414
C-8 --- C-9	1.395	1.389	1.389
C-9 --- C-9a	1.400	1.413	1.413
C-9a --- C-5a	1.418	1.443	1.443
C-2 --- C-11	1.524	1.529	1.529
C-2 --- C-10	1.530	1.537	1.537
C-3 --- N-3	1.481	1.478	1.478
N-3 --- C-1'	1.408	1.427	1.427
C-1' --- C-2'	1.410	1.403	1.403
C-2' --- C-3'	1.389	1.419	1.419
C-3' --- C-4'	1.397	1.421	1.422
C-4' --- C-5'	1.392	1.385	1.385
C-5' --- C-6'	1.398	1.409	1.409
C-6' --- C-1'	1.408	1.414	1.414
C-3' --- N-3'	1.492	1.409	1.409
N-3' --- O-3'	1.255	1.318	1.318
N-3' --- H-3'	1.021	1.020	1.020
C-1 --- O-1 --- C-2	107.6	106.7	106.7

C-1 --- C-3a --- C-4	122.5	123.2	123.2
C-3a --- C-4 --- C-5	115.4	115.9	115.9
O-5 --- C-5 --- C-4	120.4	121.4	121.4
C-5 --- C-4 --- O-4	120.1	122.1	122.1
C-4 --- C-5 --- C-5a	118.2	118.2	118.2
C-5 --- C-5a --- C-9a	121.1	122.5	122.5
C-9a --- C-1 --- C-3a	124.9	123.9	123.9
C-5a --- C-6 --- C-7	120.1	121.4	121.4
C-6 --- C-7 --- C-8	120.3	120.4	120.4
C-7 --- C-8 --- C-9	120.5	119.9	119.9
C-8 --- C-9 --- C-9a	120.5	120.5	120.5
C-9 --- C-9a --- C-5a	120.2	120.0	120.0
C-9a --- C-5a --- C-6	119.4	117.8	117.8
C-5a --- C-9a --- C-1	117.5	116.4	116.4
C-3a --- C-1 --- O-1	114.8	114.4	114.4
C-1 --- C-3a --- C-3	109.9	109.8	109.8
C-3a --- C-3 --- C-2	101.3	101.2	101.2
O-1 --- C-2 --- C-3	104.3	105.6	105.6
O-1 --- C-2 --- C-10	105.6	105.7	105.7
O-1 --- C-2 --- C-11	105.3	106.1	106.1
C-10 --- C-2 --- C-11	112.9	112.3	112.3
C-2 --- C-3 --- N-3	114.9	114.2	114.2
C-3a --- C-3 --- N-3	110.3	112.7	112.7
C-3 --- N-3 --- C-1'	122.6	120.7	120.7
N-3 --- C-1' --- C-6'	123.1	122.3	122.3
N-3 --- C-1' --- C-2'	118.3	118.2	118.2
C-1' --- C-2' --- C-3'	119.3	120.8	120.8
C-2' --- C-3' --- C-4'	123.0	119.4	119.4
C-3' --- C-4' --- C-5'	117.0	118.8	118.8
C-4' --- C-5' --- C-6'	121.8	122.5	122.5
C-5' --- C-6' --- C-1'	120.2	118.9	118.9
C-6' --- C-1' --- C-2'	118.6	119.5	119.5
C-2' --- C-3' --- N-3'	118.3	120.6	120.6

C-3' --- N-3' --- O-3'	117.9	119.2	119.2
O-5 --- C-5 --- C-4 --- O-4	-5.0	-0.8	-0.8
C-3a --- C-1 --- O-1 --- C-2	5.5	9.4	9.4
C-1 --- O-1 --- C-2 --- C-3	-12.0	-14.7	-14.7
C-1 --- C-3a --- C-3 --- C-2	-10.9	-9.4	-9.4
O-1 --- C-2 --- C-3 --- N-3	-105.6	-107.0	-107.0
C-2 --- C-3 --- N-3 --- C-1'	-96.1	-93.5	-93.5
C-3 --- N-3 --- C-1' --- C-6'	16.5	16.7	16.7
Improper torsion between line C-1' --- C-6' and C-3a --- C-4	139.6	139.6	132.6