

Table S1. The energies and 298 K Gibbs energies of the intermediate radicals and transition states in reaction of 2MN-1-OH (R1) and O₂ at BH&HLYP and ROCBS-QB3 levels (all in kJ/mol, relative to R1 + O₂) and T₁-Diagnostics at ROCCSD/6-31+G(d') level

Species (R1 = 2MN-1-OH)	BH&HLYP		ROCBS-QB3		T ₁ -Diag
	ΔE_{0K}	ΔG_{298K}	ΔE_{0K}	ΔG_{298K}	
R1-200-a	-24.9	23.4	-64.6	-16.3	0.0201
R1-200-s	-19.5	28.7	-60.4	-12.1	0.0202
R1-400-a	-5.7	37.7	-37.5	5.9	0.0197
R1-400-s	-9.5	37.0	-45.9	0.6	0.0197
R1-500-a	113.4	157.4			
R1-500-s	111.8	155.3			
R1-700-a	98.0	140.6			
R1-700-s	97.1	139.8			
R1-900-a	116.6	162.6			
R1-900-s	111.2	158.0			
TS(R1 + O₂ → R1-200-a)	46.6	91.7	-14.0	31.1	0.0299
TS(R1 + O₂ → R1-200-s)	42.9	88.6	-13.2	32.5	0.0314
TS(R1 + O₂ → R1-400-a)	48.5	91.4	-5.8	37.1	0.0293
TS(R1 + O₂ → R1-400-s)	41.8	86.6	-12.8	32.1	0.0300
TS(R1 + O ₂ → R1-500-a)	133.0	175.1			
TS(R1 + O ₂ → R1-500-s)	131.6	174.1			
TS(R1 + O ₂ → R1-700-a)	124.1	165.7			
TS(R1 + O ₂ → R1-700-s)	121.7	164.0			
TS(R1 + O ₂ → R1-900-a)	132.4	177.2			
TS(R1 + O ₂ → R1-900-s)	124.1	171.2			
R1-2300-a	34.4	82.9			
R1-2300-s	29.7	77.7			
R1-2400-a	41.5	91.3			
R1-2400-s	33.4	83.9			
R1-2900-a	37.5	89.1	-30.7	20.9	0.0205
R1-2900-s	31.2	83.0	-38.0	13.8	0.0203
R1-2-10-OO-a	99.8	150.8			
R1-2-10-OO-s	96.5	147.5			
R1-3400-a	82.9	128.5			
R1-3400-s	78.4	124.9			
R1-4500-a	96.6	144.9			
R1-4500-s	94.8	143.6			
R1-4900-a	102.1	152.1			
R1-4900-s	94.1	144.3			
R1-4-10-OO-a	130.3	178.5			
R1-4-10-OO-s	96.5	147.5			
TS(R1-200-a → R1-2300-a)	97.1	145.8			
TS(R1-200-s → R1-2300-s)	92.2	141.8			
TS(R1-200-a → R1-2400-a)	138.9	186.7			
TS(R1-200-s → R1-2400-s)	131.1	181.3			
TS(R1-200-a → R1-2900-a)	95.5	147.2	19.3	71.1	0.0299
TS(R1-200-s → R1-2900-s)	80.1	132.4	3.6	55.9	0.0303
TS(R1-200-a → R1-2-10-OO-a)	138.4	189.8			
TS(R1-200-s → R1-2-10-OO-s)	129.1	180.9			
R1C-2OOH	-52.5	-5.7	-100.5	-53.7	0.0205
R1O-2OOH-a	Not Exist				
R1O-2OOH-s	Not Exist				

TS(R1-200-<i>a</i> → R1C-200H)	88.9	139.2	22.4	72.6	0.0260
TS(R1-200-<i>a</i> → R1O-200H-<i>a</i>)	99.2	150.3	36.4	87.6	0.0353
TS(R1-200-<i>s</i> → R1O-200H-<i>s</i>)	89.4	140.2	20.4	71.1	0.0345
TS(R1C-200H → 2-MN-1-ol + HO₂)	-2.8	42.1	-58.3	-13.5	0.0251
TS(R1C-200H → 2-OOH-naphth-1-ol + CH ₃)	66.3	110.5			
TS(R1C-200H → 2-MN-23-O-1-OH + OH)	21.7	66.7			
R1-20-890-<i>s</i>	-27.0	22.1	-63.7	-14.6	0.0165
R1-90-230-<i>s</i>	-9.6	40.1	-51.0	-1.3	0.0183
TS(R1-2900-<i>s</i> → R1-20-890-<i>s</i>)	95.5	151.0	37.7	90.6	0.0227
TS(R1-2900- <i>s</i> → R1-90-230- <i>s</i>)	Not Found				
TS(R1-400- <i>a</i> → R1-2400- <i>a</i>)	137.6	187.2			
TS(R1-400- <i>s</i> → R1-2400- <i>s</i>)	131.0	181.2			
TS(R1-400- <i>a</i> → R1-3400- <i>a</i>)	128.0	175.2			
TS(R1-400- <i>s</i> → R1-3400- <i>s</i>)	123.3	170.9			
TS(R1-400- <i>a</i> → R1-4500- <i>a</i>)	149.5	198.3			
TS(R1-400- <i>s</i> → R1-4500- <i>s</i>)	147.7	197.1			
TS(R1-400- <i>a</i> → R1-4900- <i>a</i>)	159.2	209.5			
TS(R1-400- <i>s</i> → R1-4900- <i>s</i>)	150.9	202.0			
TS(R1-400- <i>a</i> → R1-4-10-OO- <i>a</i>)	155.2	203.0			
TS(R1-400- <i>s</i> → R1-4-10-OO- <i>s</i>)	148.3	197.2			
R1C-400H	-57.2	-12.9	-96.5	-52.1	0.0179
TS(R1-400-<i>a</i> → R1C-400H)	116.0	166.6	41.9	92.4	0.0223
TS(R1C-400H → 2-MN-1-ol + HO₂)	-1.0	42.5	-43.1	0.4	0.0289

Table S2. The energies and 298 K Gibbs energies of the intermediate radicals and transition states in reaction of 2MN-3-OH (R3) and O₂ at BH&HLYP and ROCBS-QB3 levels (all in kJ/mol, relative to R3 + O₂)

Species (R2 = 2MN-2-OH)	M06-2X		ROCBS-QB3		<i>T</i> ₁ - <i>Diag</i>
	ΔE_{0K}	ΔG_{298K}	ΔE_{0K}	ΔG_{298K}	
R3-200- <i>a</i>	59.0	105.8			
R3-200- <i>s</i>	75.4	120.3			
R3-400-<i>a</i>	-43.7	1.4	-75.0	-29.8	0.0202
R3-400-<i>s</i>	-40.0	5.7	-74.4	-28.7	0.0202
TS(R3 + O ₂ → R3-200- <i>a</i>)	99.9	144.4			
TS(R3 + O ₂ → R3-200- <i>s</i>)	96.9	142.1			
TS(R3 + O₂ → R3-400-<i>a</i>)	36.2	77.8	-15.5	26.2	0.0309
TS(R3 + O₂ → R3-400-<i>s</i>)	37.6	79.2	-13.9	27.6	0.0323
R3-2400-<i>a</i>	-47.3	2.7	-107.8	-57.8	0.0210
R3-2400-<i>s</i>	-56.9	-6.8	-117.0	-66.9	0.0209
TS(R3-400-<i>a</i> → R3-2400-<i>a</i>)	44.1	94.1	-19.7	31.1	0.0263
TS(R3-400-<i>s</i> → R3-2400-<i>s</i>)	30.5	80.7	-32.4	18.2	0.0269
TS(R3-400- <i>a</i> → R3C-400H)	69.8	66.2			
TS(R3-400- <i>a</i> → R3O-200H- <i>a</i>)	68.8	53.3			
TS(R3-400- <i>s</i> → R3O-200H- <i>s</i>)	79.6	67.6			
R3-40-120- <i>s</i>	-163.5	-155.2			
TS(R3-2400- <i>s</i> → R3-40-120- <i>s</i>)	14.2	64.4			