

Supplementary Table S2. Values of total and relative energies in gas phase and in toluene solvent of (*E*)-*N*-((2-((-methylbut-2-en-1-yl)thio)-1*H*-indol-3-yl)methylene)methanamine oxide **1**, TSs and CAs.

System	Gas phase		Toluene	
	<u>E (in a.u)</u>	<u>ΔE(kcal/mol)</u>	<u>E (in a.u)</u>	<u>ΔE (kcal/mol)</u>
1	-1165.2998		-1165.3134	
TS2n	-1165.2700	18.7	-1165.2787	21.8
TS2x	-1165.2442	34.9	-1165.2545	37.0
TS3n	-1165.2513	30.5	-1165.2628	31.8
CA2n	-1165.3277	-17.5	-1165.3378	-15.3
CA2x	-1165.3210	-13.3	-1165.3327	-12.1
CA3n	-1165.3144	-9.1	-1165.3258	-7.7