Table S4: Electronic energies, Zero-Point Vibrational Energies, Thermal Energies, Entropies and relative free energies for species calculated at B3LYP\LANL2DZ for structures shown in Figure 6. Italicized relative free energy values are in kcal mol^{-1} while values in parentheses are in kJ mol^{-1}.

Structure	Electronic energy (Hartrees)	ZPE (kcal mol^{-1})	$H_{298}^{o} - H_{0}^{o}$ (kcal mol^{-1})	Entropy (cal mol^{-1} K^{-1})	Relative free energy at 298 K
1A	-1639.2886242	312.6	19.6	196.8	*0.0* (0.0)
$TS_{(1A\rightarrow 1D)}$	-1639.2696380	312.8	19.8	200.6	*11.1* (46.4)
1D	-1639.2817215	311.3	20.0	202.8	*3.1* (13.0)
$TS_{(1D\rightarrow OxPtH)}$ + Carnosine	-1639.2181703	311.7	19.9	201.9	*42.0* (175.7)
$TS_{(1D\rightarrow Car)}$ + OxPt	-1639.1995789	310.5	19.8	201.5	*52.5* (219.7)
OxPtH + Car	-1639.2368711	312.7	20.3	207.3	*30.0* (125.5)
Car + OxPtH	-1639.2798599	313.6	19.2	201.1	*5.4* (22.6)