Supporting Information for Publication

Excited State Dynamics of 6-Thioguanine

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a)

Ground State		S1		S2	
Tautomer	Rel. kJ/mol	Character	Vert. E, eV	Character	Vert. E, ev
9e 6TG	9	ππ*	4.66 (0.193)	nπ*	5.17 (.004)
7e 6TG	29.8	ππ*	4.44 (0.159)	nπ*	4.95 (0.004)
9e G			5.12 (0.107)		5.475 (0.003)

b)

Ground State		T1		T2		T3	
Tautomer	Rel. kJ/mol	Character	Vert. E, eV	Character	Vert. E, ev	Character	Vert. E, ev
9e 6TG	9	ππ*	3.598	ππ*	4.698	nπ*	4.909
7e 6TG	29.8	ππ*	3.591	ππ*	4.306	nπ*	4.672
9e G			4.006		4.822		5.393

Table S1. a) Singlet and b) triplet excited state analysis at CCSD/6-31+G(2d,p) for ground state and EOM-CCSD/6-31+G(2d,p) for excited states. Values in parenthesis correspond to oscillator strengths of the transition. Ground state energies are relative to 7k tautomer for 6-TG.

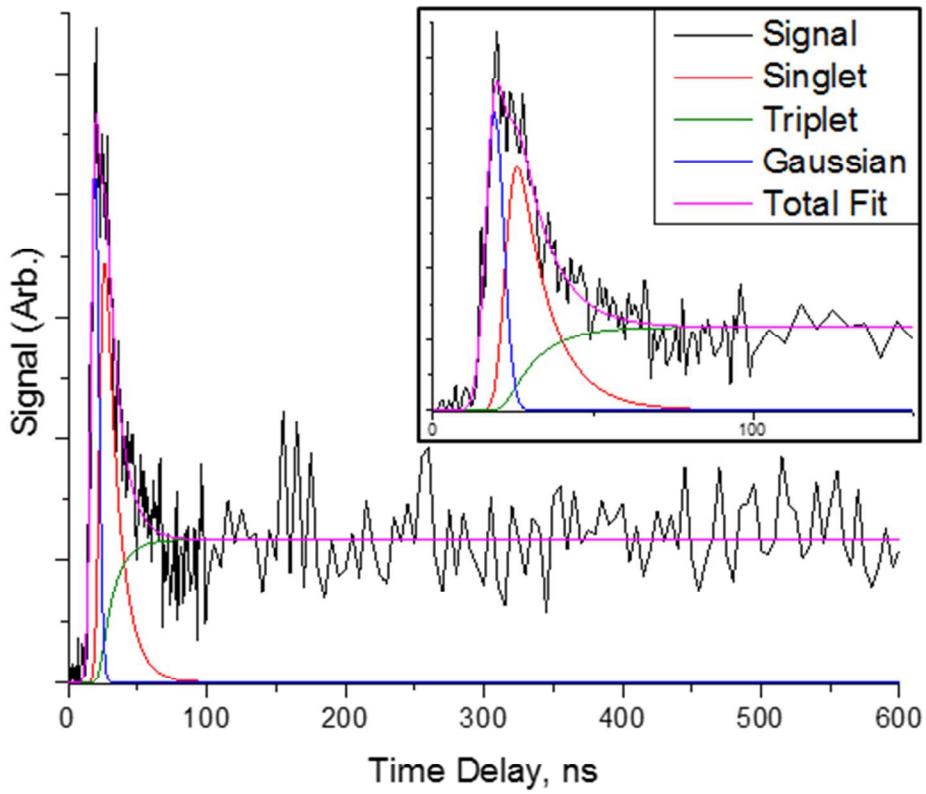

Figure S1. Nanosecond pump probe trace of 9-enol guanine at its origin of 32873 cm^{-1}. The singlet lifetime is fit as a bi-exponential of fluorescence (13 ns) and a second decay (40 ns) which feeds a dark state with a lifetime longer than the experiment allows. The inset shows a magnified portion of the fitting.