

Supplementary Information for:

**Triplet Formation of 6-Azauridine and Singlet Oxygen Sensitization with UV Light
Irradiation**

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6-azauridine (6AUd) Optimized Structure:

	Coordinates (Angstroms)		
	X	Y	Z
N	0	0	0
C	0	0	1.375924
N	1.260268	0	1.953716
N	2.414543	-0.0916	1.268241
C	2.371854	-0.1273	-0.02437
C	1.131472	-0.06762	-0.80649
C	3.075332	-0.59897	4.835942
C	1.805906	-1.2631	5.366362
C	0.889336	-1.23704	4.132183
C	1.315443	0.087132	3.449058
O	2.619508	0.373057	3.857992
O	1.067317	-0.08084	-2.02865
O	-1.03211	-0.00482	2.048254
O	-0.46269	-1.27045	4.532854
O	1.274302	-0.44457	6.396264
O	4.633401	-2.33773	5.240483
C	4.079114	-1.55434	4.193132
H	-0.92496	0.005863	-0.45677
H	3.317961	-0.20144	-0.55712
H	3.575214	-0.04307	5.637595
H	1.999179	-2.28613	5.719663
H	1.131709	-2.07977	3.465203
H	0.630506	0.900105	3.724492
H	-0.98777	-0.91185	3.793666
H	0.311639	-0.60083	6.419079
H	5.294449	-2.94675	4.85197
H	4.841489	-0.95356	3.67651
H	3.583595	-2.17872	3.433778

Uridine Optimized Structure:

	Coordinates (Angstroms)		
	X	Y	Z
H	0	0	0
O	0	0	0.979744
C	1.346428	0	1.428318
H	1.907831	0.863651	1.038149
H	1.88316	-0.91068	1.122078
C	1.306949	0.042826	2.954483
H	0.677986	-0.7771	3.31991
O	2.649076	-0.16554	3.478745
C	3.134464	1.003007	4.092617
H	3.169787	0.888489	5.184876
N	4.540942	1.226315	3.639347
C	5.159027	0.402962	2.724873
H	4.531851	-0.38552	2.330158
C	6.453543	0.558066	2.359392
H	6.911335	-0.10478	1.633254
C	7.254005	1.609099	2.949112
O	8.43381	1.857513	2.707734
N	6.547909	2.385775	3.884119
H	7.061064	3.156596	4.332715
C	5.234748	2.255556	4.256554
O	4.708274	3.007637	5.085715
C	0.840805	1.371473	3.541963
H	0.138628	1.886807	2.871262
C	2.161069	2.143025	3.704458
H	2.474788	2.564688	2.735353
O	2.008997	3.144526	4.682473
H	2.908832	3.338127	5.013719
O	0.261176	1.115463	4.811737
H	0.324982	1.942606	5.325932