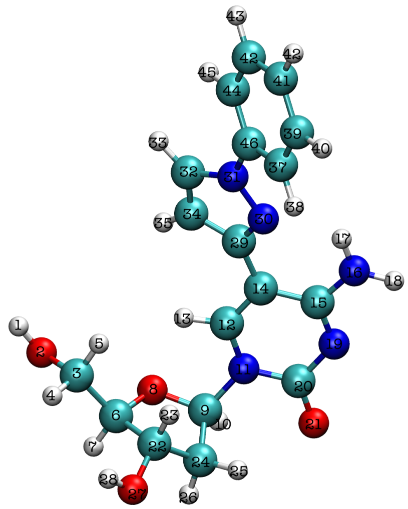
Electronic Supporting Information

Photophysical Investigation of Two Emissive Nucleosides Exhibiting Gigantic Stokes Shifts

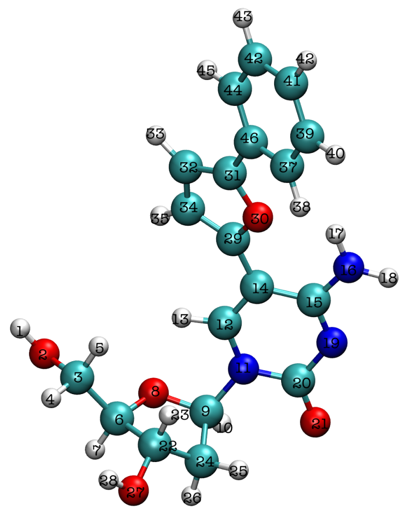
J. Stendevad[a], M. Hornum[a], D. Wüstner[b] and J. Kongsted[a*]

[a]Department of Physics, Chemistry and Pharmacy, University of Southern Denmark, DK-5230 Odense M, Denmark
[b]Department of Biochemistry and Molecular Biology, University of Southern Denmark, DK-5230 Odense M, Denmark
*E-mail: kongsted@sdu.dk



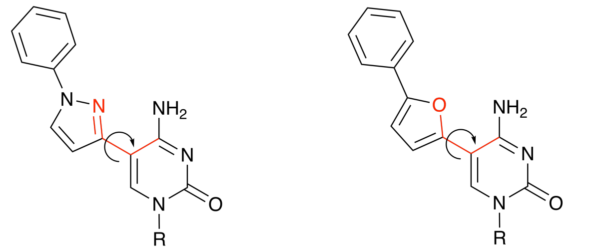
Atom number	Atom name	Atom type	Charge
1	HO5′	HO	0.473993
2	O5′	OH	-0.770348
3	C5′	CI	0.250576
4	H5′	H1	0.024864
5	H5″	H1	0.024864
6	C4′	CT	0.263568
7	H4′	H1	0.043960
8	O4′	OS	-0.633003
9	C1′	CT	0.528779
10	H1′	H2	0.064454
11	N1	N*	-0.535041
12	C6	CM	0.330269
13	H6	H4	0.167746
14	C5	CM	-0.775230
15	C4	CA	1.229087
16	N4	N2	-1.181323
17	H41	H	0.480702
18	H42	H	0.480702
19	N3	NC	-1.087081
20	C2	C	1.220941
21	O2	O	-0.783015
22	C3′	CT	0.550780
23	H3′	H1	-0.029535
24	C2′	CT	-0.382145
25	H2′	HC	0.115065
26	H2″	HC	0.129704
27	O3′	OH	-0.881779
28	HO3′	HO	0.499459
29	C1py	cc	0.611178
30	N1py	nd	-0.490978
31	N2py	na	0.085730
32	C2py	cd	-0.047969
33	H2py	ha	0.171579
34	C3py	cc	-0.524713
35	H3py	ha	0.257062
36	C1ph	ca	0.210468
37	C2ph	ca	-0.236806
38	H2ph	ha	0.159077
39	C3ph	ca	-0.088375
40	H3ph	ha	0.143872
41	C4ph	ca	-0.202818
42	H4ph	ha	0.153912
43	C5ph	ca	-0.088375
44	H5ph	ha	0.143872
45	C6ph	ca	-0.236806
46	H6ph	ha	0.159077

Table 1 Parameters for **X**



Atom number	Atom name	Atom type	Charge
1	HO5′	HO	0.477441
2	O5′	OH	-0.767316
3	C5′	CI	0.255320
4	H5′	H1	0.022485
5	H5″	H1	0.022485
6	C4′	CT	0.253235
7	H4′	H1	0.046924
8	O4′	OS	-0.621557
9	C1′	CT	0.501430
10	H1′	H2	0.073491
11	N1	N*	-0.552469
12	C6	CM	0.402904
13	H6	H4	0.133124
14	C5	CM	-0.840701
15	C4	CA	1.278848
16	N4	N2	-1.216603
17	H41	H	0.491026
18	H42	H	0.491026
19	N3	NC	-1.101316
20	C2	C	1.239734
21	O2	O	-0.777680
22	C3′	CT	0.558666
23	H3′	H1	-0.028029
24	C2′	CT	-0.374418
25	H2′	HC	0.108342
26	H2″	HC	0.132019
27	O3′	OH	-0.881855
28	HO3′	HO	0.499041
29	C1fu	cc	0.510022
30	O1fu	os	-0.273080
31	C2fu	cc	0.118953
32	C3fu	cd	-0.253135
33	H3fu	ha	0.207901
34	C4fu	cd	-0.401707
35	H4fu	ha	0.239184
36	C1ph	ca	0.080552
37	C2ph	ca	-0.155245
38	H2ph	ha	0.120344
39	C3ph	ca	-0.121897
40	H3ph	ha	0.144495
41	C4ph	ca	-0.181704
42	H4ph	ha	0.152023
43	C5ph	ca	-0.121897
44	H5ph	ha	0.144495
45	C6ph	ca	-0.155245
46	H6ph	ha	0.120344

Table 2 Parameters for **Y**



X **Y**

Figure 1 Illustration of dihedral angle, ζ, in nucleosides **X** (left) and **Y** (right).

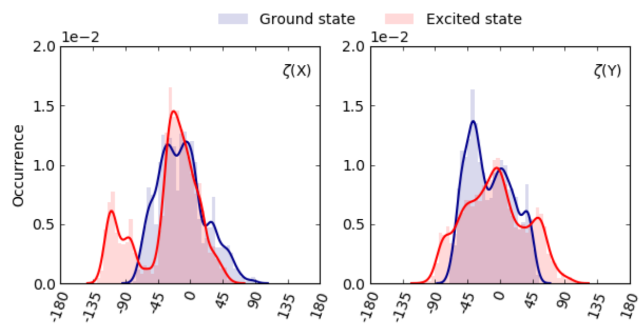


Figure 2 Histogram showing the distribution of dihedral angle, ζ, in nucleosides **X** (left) and **Y** (right) over the ground and excited state trajectories (water).

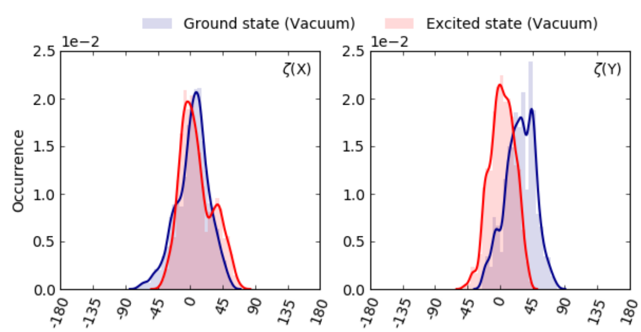
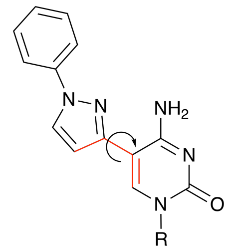


Figure 3 Histogram showing the distribution of dihedral angle, ζ, in nucleosides **X** (left) and **Y** (right) over the ground and excited state trajectories (vacuum).



X **Y**

Figure 4 Illustration of dihedral angle, θ in nucleosides **X** (left) and **Y** (right).

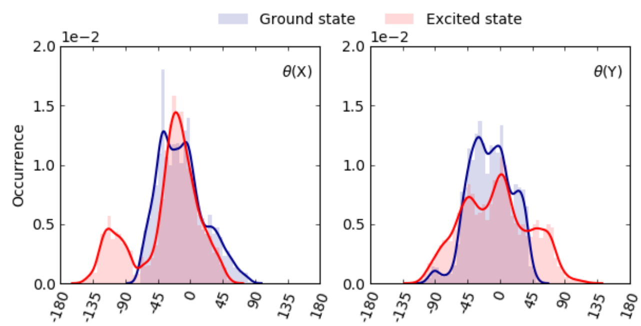


Figure 5 Histogram showing the distribution over the ground and excited state trajectories (water) of dihedral angle θ in nucleosides **X** (left) and **Y** (right).

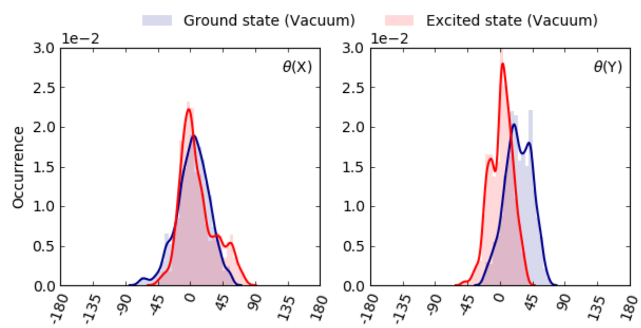


Figure 6 Histogram showing the distribution over the ground and excited state trajectories (vacuum) of dihedral angle θ in nucleosides **X** (left) and **Y** (right).

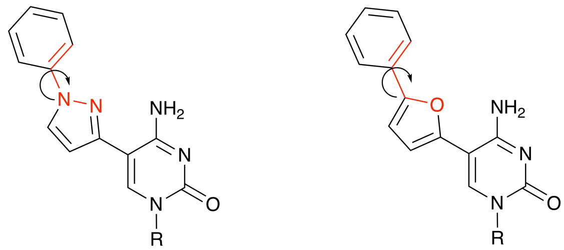


Figure 7 Illustration of dihedral angle, γ in nucleosides **X** (left) and **Y** (right).

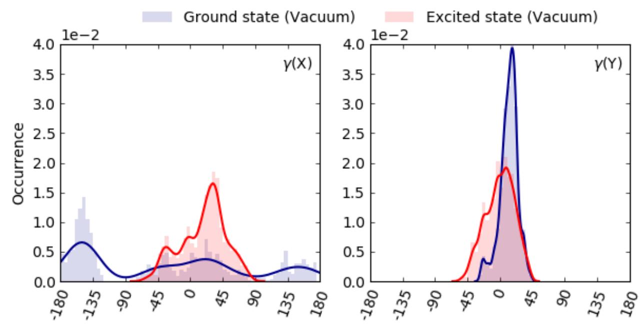


Figure 8 Histogram showing the distribution over the ground and excited state trajectories (vacuum) of dihedral angle γ in nucleosides **X** (left) and **Y** (right).

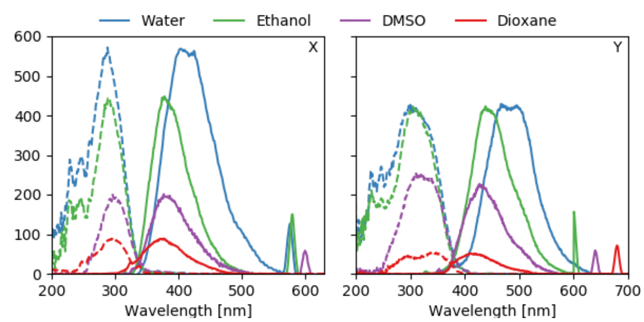


Figure 9 Measured excitation and emission spectra (Raw data) of nucleoside **X** (left) and **Y** (right) in different solvents. Excitation spectra are shown with dashed lines, whereas the solid lines mark the emission spectra.

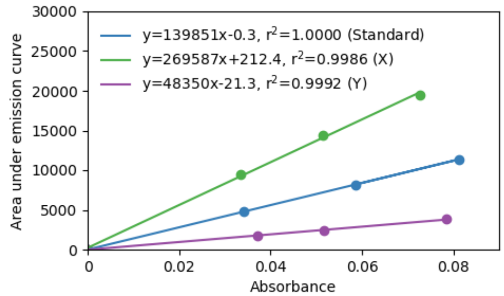


Figure 10 Linear regressions of absorbance as a function of integrated emission of the respective concentrations of **X** and **Y** as well as the standard sample.

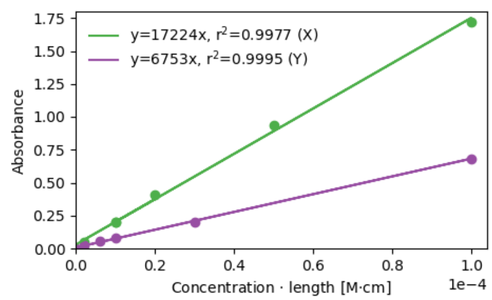


Figure 11 Linear regressions of absorbance as a function of concentration · length for **X** and **Y**

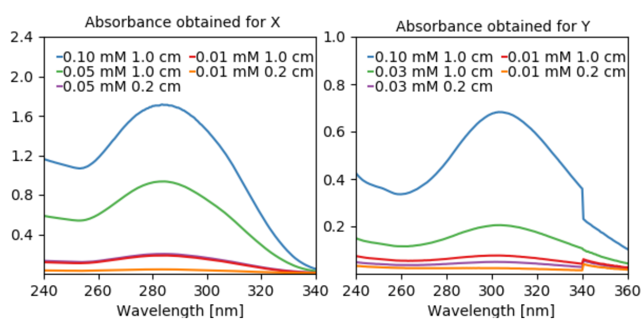


Figure 12 Absorbance spectra for **X** and **Y** obtained for different concentrations and lengths of cuvettes.