Supporting Information

Circular Dichroism Spectra of Uridine Derivatives: *ChiraSac* Study

Tomoo Miyahara[a] , Hiroshi Nakatsuji[a,b*] and Takehiko Wada[b]

[a] *Quantum Chemistry Research Institute (QCRI), JST-CREST, Kyodai Katsura Venture Plaza, North building 107, 1-36 Goryo-Oohara, Nishikyo-ku, Kyoto, 615-8245, Japan,;*
[b] *Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, 2-1-1, Katahira, Aoba-ku, Sendai 980-8577, Japan*

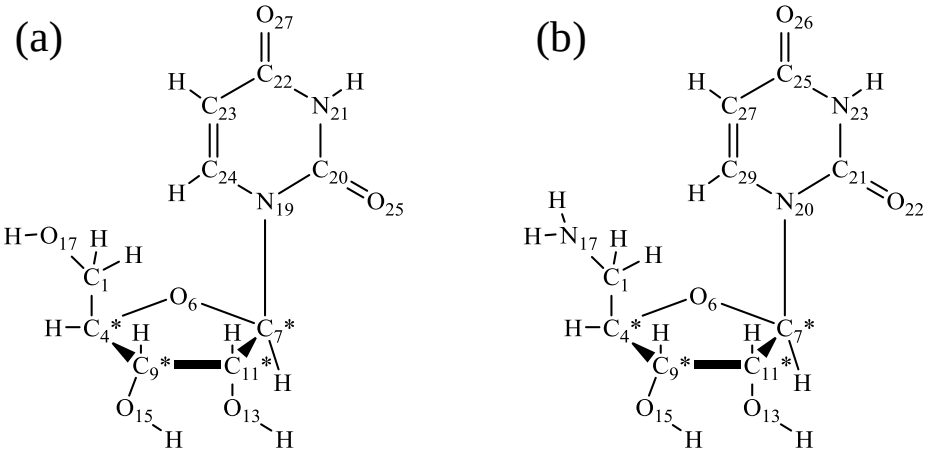

Figure S1. Atom labels of (a) uridine and (b) NH2-uridine. The chiral carbons are marked with *.

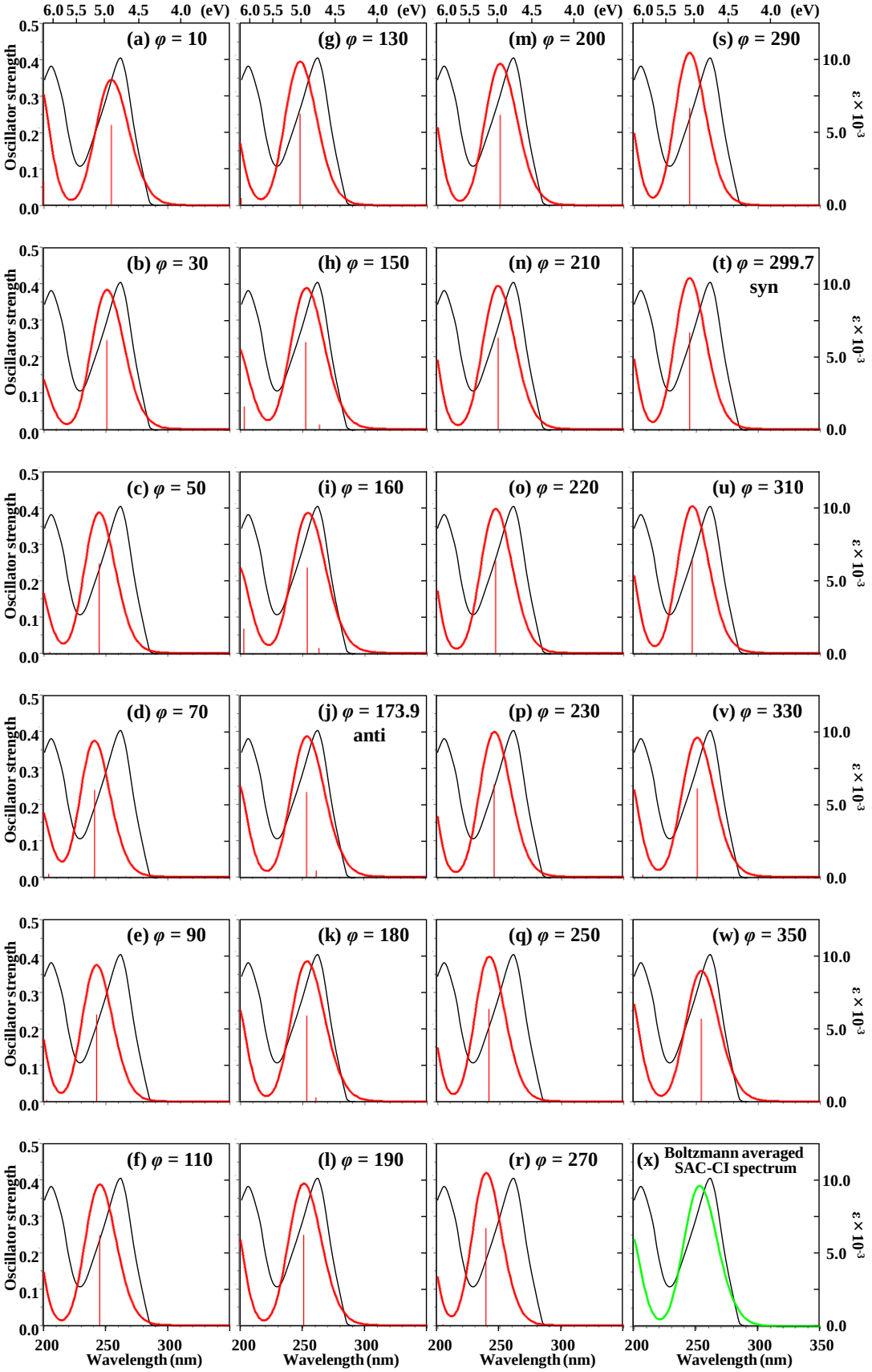

Figure S2. Experimental UV spectrum (black lines)[1] of uridine compared with the SAC-CI UV spectra (red lines) at several conformation angles φ (a-w) and the SAC-CI UV Boltzmann average spectrum (green line) (x).

Table S1. Coordinates (in Å) of the anti conformer of uridine.

Atom (See Figure S1)	X	Y	Z
C_1	-2.337529	2.234397	0.297068
H	-2.041296	3.047515	-0.361300
H	-3.322449	2.463103	0.699213
C_4*	-2.434804	0.957508	-0.515853
H	-3.185656	1.097894	-1.281477
O_6	-1.198962	0.689697	-1.170205
C_7*	-0.576087	-0.448931	-0.687308
H	-0.565255	-1.220438	-1.445276
C_9*	-2.760144	-0.303328	0.280955
H	-3.276309	-0.080746	1.208380
C_{11}*	-1.383444	-0.919090	0.540419
H	-0.953960	-0.488712	1.436199
O_{13}	-1.515851	-2.300052	0.646823
H	-0.649922	-2.694414	0.615072
O_{15}	-3.539709	-1.131802	-0.531780
H	-3.383712	-2.033225	-0.276413
O_{17}	-1.398373	2.058412	1.328489
H	-1.324697	2.849495	1.843185
N_{19}	0.837889	-0.113910	-0.383511
C_{20}	1.651144	-1.149170	-0.015106
N_{21}	2.964797	-0.840133	0.180040
C_{22}	3.570317	0.408999	0.053622
C_{23}	2.635767	1.457328	-0.340911
C_{24}	1.349196	1.156763	-0.537828
O_{25}	1.236776	-2.275103	0.136930
H	3.550525	-1.603347	0.454118
O_{27}	4.741713	0.537350	0.262695
H	3.008743	2.453695	-0.467634
H	0.633946	1.892614	-0.833735

Table S2. Coordinates (in Å) of the syn conformer of uridine.

Atom (See Figure S1)	X	Y	Z
C_1	-2.729213	1.868687	-0.648292
H	-2.356063	2.465823	-1.476840
H	-3.804370	1.999589	-0.599573
C_4*	-2.431943	0.405332	-0.934928
H	-2.996693	0.088084	-1.802659
O_6	-1.040395	0.250963	-1.226877
C_7*	-0.467702	-0.706892	-0.405516
H	-0.510524	-1.683739	-0.869557
C_9*	-2.723831	-0.546108	0.230585
H	-3.428398	-0.121773	0.935889
C_{11}*	-1.339273	-0.756168	0.848064
H	-1.103282	0.058253	1.512872
O_{13}	-1.206772	-2.001011	1.485107
H	-1.128691	-1.885931	2.420282
O_{15}	-3.210713	-1.750217	-0.299582
H	-3.092324	-2.435689	0.345757
O_{17}	-2.210600	2.308592	0.572352
H	-1.260133	2.296766	0.544236
N_{19}	0.952522	-0.430538	-0.214466
C_{20}	1.371126	0.749780	0.358091
N_{21}	2.725897	0.930608	0.407624
C_{22}	3.725391	0.083707	-0.061303
C_{23}	3.199398	-1.134035	-0.674849
C_{24}	1.881561	-1.318719	-0.725615
O_{25}	0.620664	1.575828	0.807687
H	3.022645	1.788136	0.829131
O_{27}	4.878210	0.378775	0.054026
H	3.889395	-1.848613	-1.076088
H	1.463274	-2.198348	-1.174674

Table S3. Coordinates (in Å) of the anti conformer of NH2-uridine.

Atom (See Figure S1)	X	Y	Z
C_1	2.629732	-2.154800	0.308809
H	2.437911	-3.017849	-0.328577
H	3.665977	-2.215818	0.625342
C_4*	2.483689	-0.895907	-0.531316
H	3.141507	-0.965137	-1.387182
O_6	1.143047	-0.798423	-1.022847
C_7*	0.533256	0.397899	-0.676996
H	0.533936	1.089524	-1.511077
C_9*	2.755884	0.419790	0.192659
H	3.319636	0.273293	1.106218
C_{11}*	1.359761	0.972742	0.491736
H	0.997117	0.555511	1.423343
O_{13}	1.434207	2.359581	0.538036
H	0.551562	2.711333	0.587521
O_{15}	3.449875	1.256539	-0.689839
H	3.281925	2.157207	-0.440226
N_{17}	1.782897	-2.118757	1.495485
H	0.833587	-2.334246	1.257478
H	2.079945	-2.805864	2.161952
N_{20}	-0.883420	0.077912	-0.352306
C_{21}	-1.690714	1.090974	0.091020
O_{22}	-1.282998	2.206881	0.308195
N_{23}	-3.002803	0.771354	0.289178
H	-3.575994	1.516301	0.631903
C_{25}	-3.630210	-0.446884	0.042811
O_{26}	-4.797724	-0.585548	0.262509
C_{27}	-2.719593	-1.453381	-0.494372
H	-3.112435	-2.417445	-0.748038
C_{29}	-1.432144	-1.149925	-0.673238
H	-0.740620	-1.855673	-1.080257

Table S4. Coordinates (in Å) of the syn conformer of NH2-uridine.

Atom (See Figure S1)	X	Y	Z
C_1	-2.874577	1.765176	-0.781543
H	-2.545324	2.325562	-1.656954
H	-3.960865	1.779319	-0.777833
C_4*	-2.435740	0.321560	-0.963884
H	-2.925505	-0.092210	-1.836515
O_6	-1.022802	0.279591	-1.184321
C_7*	-0.443487	-0.685521	-0.373750
H	-0.490788	-1.659803	-0.844114
C_9*	-2.705537	-0.599946	0.234109
H	-3.428405	-0.175071	0.918406
C_{11}*	-1.322830	-0.742385	0.873396
H	-1.130227	0.098556	1.517569
O_{13}	-1.170078	-1.966344	1.546353
H	-0.929224	-1.817310	2.447976
O_{15}	-3.149050	-1.838115	-0.258601
H	-3.038484	-2.489534	0.422444
N_{17}	-2.399669	2.317132	0.478455
H	-1.399146	2.390207	0.479171
H	-2.771587	3.237373	0.618257
N_{20}	0.977284	-0.414230	-0.192686
C_{21}	1.407506	0.730587	0.446143
O_{22}	0.669218	1.517664	0.972000
N_{23}	2.765536	0.914359	0.464544
H	3.072001	1.741131	0.936903
C_{25}	3.752217	0.113680	-0.098993
O_{26}	4.907622	0.407963	-0.000781
C_{27}	3.212517	-1.058632	-0.784280
H	3.891855	-1.735090	-1.262441
C_{29}	1.894468	-1.250059	-0.802651
H	1.467146	-2.096790	-1.303536

Table S5. 1st excited states of uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	4.62	0.0001	-0.31	0.003	0.65	97.4
20	4.61	0.0003	6.47	0.008	0.65	18.1
30	4.73	0.0003	5.65	0.009	0.65	43.2
40	4.81	0.0001	1.58	0.006	0.67	73.1
50	4.72	0.0005	-9.03	0.011	0.69	150.6
60	4.69	0.0006	-8.83	0.011	0.69	148.2
70	4.66	0.0005	-8.66	0.011	0.69	146.9
80	4.67	0.0004	-8.68	0.011	0.68	145.7
90	4.67	0.0002	-4.36	0.007	0.68	135.9
100	4.67	0.0001	0.39	0.003	0.67	82.7
110	4.67	0.0002	8.22	0.009	0.66	13.7
120	4.70	0.0010	15.83	0.019	0.66	23.3
130	4.71	0.0018	16.75	0.022	0.66	30.8
140	4.71	0.0058	30.98	0.040	0.66	29.7
150	4.70	0.0120	44.32	0.057	0.67	31.7
160	4.71	0.0136	46.19	0.061	0.69	35.9
170	4.75	0.0146	47.62	0.063	0.71	37.4
173.9	4.74	0.0162	50.76	0.067	0.71	37.8
180	4.75	0.0115	42.91	0.056	0.71	36.4
190	4.77	0.0017	17.11	0.022	0.68	30.0
200	4.75	0.0002	3.65	0.005	0.67	36.1
210	4.76	0.0002	2.83	0.004	0.67	40.3
220	4.75	0.0004	5.25	0.007	0.68	38.2
230	4.73	0.0006	8.19	0.011	0.68	33.1
240	4.73	0.0009	10.36	0.013	0.68	29.9
250	4.74	0.0010	12.94	0.015	0.68	21.6
260	4.72	0.0004	5.54	0.007	0.68	32.6
270	4.72	0.0002	3.73	0.006	0.68	48.6
280	4.72	0.0002	-3.51	0.004	0.68	151.7
290	4.73	0.0003	-5.92	0.007	0.68	156.7
299.7	4.74	0.0006	-8.42	0.011	0.68	150.1
300	4.74	0.0006	-8.43	0.011	0.68	149.5
310	4.72	0.0012	-11.93	0.016	0.67	144.8
320	4.70	0.0018	-14.31	0.019	0.66	145.2
330	4.68	0.0017	-13.84	0.019	0.66	145.3
340	4.69	0.0025	-18.26	0.025	0.66	146.0
350	4.66	0.0020	-15.91	0.021	0.65	149.0
360	4.63	0.0007	-8.85	0.013	0.65	141.7

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S6. 2nd excited states of uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	4.87	0.22	35.30	0.25	1.09	84.3
20	4.87	0.22	27.12	0.24	1.07	85.5
30	4.94	0.24	-47.93	0.25	1.16	97.2
40	5.00	0.26	-54.59	0.26	1.21	97.7
50	5.07	0.25	-56.71	0.26	1.18	98.4
60	5.11	0.25	-48.71	0.26	1.15	97.6
70	5.14	0.24	-44.34	0.25	1.09	97.4
80	5.14	0.24	-39.16	0.26	1.02	96.9
90	5.11	0.24	-35.00	0.26	0.95	96.5
100	5.09	0.25	-34.80	0.26	0.89	96.9
110	5.05	0.25	-34.84	0.26	0.84	97.2
120	5.03	0.25	-40.93	0.26	0.81	98.8
130	5.00	0.25	-42.94	0.26	0.80	99.2
140	4.96	0.25	-49.76	0.26	0.80	100.8
150	4.90	0.24	-49.72	0.25	0.81	100.6
160	4.88	0.24	-38.42	0.25	0.84	97.9
170	4.91	0.24	-34.39	0.25	0.92	96.6
173.9	4.89	0.23	-35.89	0.25	0.94	96.7
180	4.89	0.24	-22.24	0.25	0.99	93.9
190	4.93	0.25	14.35	0.26	1.09	87.7
200	4.95	0.25	24.33	0.26	1.13	86.3
210	4.98	0.25	17.52	0.26	1.15	87.4
220	5.02	0.25	12.08	0.26	1.17	88.2
230	5.04	0.25	12.96	0.26	1.19	88.1
240	5.07	0.25	16.59	0.26	1.24	87.7
250	5.13	0.25	21.52	0.26	1.29	87.1
260	5.17	0.26	25.97	0.27	1.33	86.6
270	5.18	0.27	16.41	0.27	1.40	88.0
280	5.09	0.27	3.20	0.27	1.41	89.6
290	5.06	0.27	9.95	0.27	1.38	88.8
299.7	5.06	0.26	15.70	0.27	1.37	88.1
300	5.06	0.26	16.00	0.27	1.37	88.1
310	5.02	0.26	22.87	0.27	1.33	87.2
320	4.97	0.25	31.02	0.27	1.29	86.0
330	4.94	0.24	35.65	0.26	1.26	85.3
340	4.89	0.23	43.91	0.26	1.20	83.9
350	4.88	0.23	43.81	0.25	1.15	83.4
360	4.86	0.22	41.38	0.25	1.10	83.4

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S7. 3rd excited states of uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	5.81	0.0001	5.64	0.008	0.72	32.3
20	5.77	0.0002	4.88	0.018	0.72	70.0
30	5.90	0.0005	6.39	0.018	0.78	65.8
40	6.02	0.0003	6.03	0.017	0.81	65.5
50	6.05	0.0030	6.80	0.027	0.78	72.1
60	6.04	0.0061	3.40	0.040	0.77	84.1
70	6.07	0.0083	1.88	0.049	0.74	87.2
80	6.08	0.0075	2.12	0.049	0.71	86.7
90	6.12	0.0040	5.50	0.035	0.70	77.5
100	6.18	0.0012	9.01	0.017	0.71	44.8
110	6.19	0.0011	7.14	0.018	0.73	58.6
120	6.20	0.0061	6.53	0.043	0.75	78.8
130	6.17	0.0190	4.69	0.078	0.75	85.6
140	6.10	0.0401	-4.93	0.110	0.73	93.3
150	6.10	0.0611	-9.58	0.133	0.71	95.5
160	6.11	0.0667	-8.62	0.140	0.70	94.8
170	6.18	0.0643	-6.78	0.137	0.67	94.1
173.9	6.20	0.0578	-6.34	0.130	0.65	94.1
180	6.24	0.0495	-6.74	0.121	0.63	94.9
190	6.29	0.0001	3.69	0.007	0.82	46.7
200	6.26	0.0048	0.50	0.038	0.86	89.1
210	6.25	0.0029	-0.01	0.028	0.83	90.0
220	6.26	0.0017	-0.82	0.020	0.80	92.8
230	6.25	0.0004	-1.57	0.009	0.77	103.2
240	6.23	0.0002	-3.88	0.012	0.75	116.0
250	6.18	0.0010	-6.38	0.022	0.75	112.5
260	6.11	0.0010	-9.79	0.021	0.76	125.5
270	6.06	0.0028	7.82	0.030	0.75	71.2
280	6.04	0.0018	3.27	0.019	0.74	77.5
290	6.04	0.0007	0.79	0.012	0.72	84.9
299.7	6.05	0.0002	-3.62	0.006	0.73	148.7
300	6.05	0.0002	-3.75	0.006	0.73	148.4
310	6.02	0.0011	-6.83	0.019	0.73	117.0
320	6.01	0.0037	-8.62	0.032	0.74	110.0
330	5.99	0.0056	-6.95	0.038	0.76	103.2
340	5.96	0.0052	-2.64	0.034	0.76	95.4
350	5.91	0.0033	-0.06	0.025	0.75	90.2
360	5.86	0.0011	4.53	0.011	0.74	60.3

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S8. 4th excited states of uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	6.20	0.07	-13.31	0.15	0.29	107.34
20	6.20	0.08	-10.84	0.15	0.33	101.89
30	6.26	0.07	22.36	0.15	0.49	73.10
40	6.34	0.08	15.44	0.16	0.46	78.01
50	6.30	0.08	5.95	0.16	0.39	84.47
60	6.31	0.08	-3.74	0.16	0.33	94.05
70	6.30	0.10	-9.52	0.17	0.36	98.73
80	6.35	0.10	-7.49	0.18	0.48	94.99
90	6.39	0.09	-4.42	0.17	0.61	92.39
100	6.41	0.08	-1.10	0.16	0.66	90.58
110	6.37	0.06	6.81	0.14	0.69	85.98
120	6.39	0.05	7.50	0.13	0.68	85.16
130	6.40	0.05	-12.27	0.14	0.55	99.17
140	6.38	0.07	-16.22	0.16	0.41	103.84
150	6.35	0.07	-4.78	0.16	0.55	93.04
160	6.33	0.08	0.79	0.17	0.68	89.61
170	6.33	0.09	2.55	0.18	0.76	88.91
173.9	6.31	0.10	0.85	0.18	0.76	89.65
180	6.31	0.11	1.73	0.19	0.78	89.33
190	6.34	0.16	-8.29	0.22	0.60	93.55
200	6.38	0.14	-7.59	0.21	0.48	94.26
210	6.43	0.11	-5.59	0.19	0.37	94.65
220	6.43	0.06	-8.37	0.15	0.25	103.08
230	6.41	0.05	-10.61	0.14	0.27	106.63
240	6.40	0.05	-12.39	0.14	0.30	107.26
250	6.40	0.06	-11.04	0.14	0.32	104.27
260	6.43	0.06	-7.70	0.15	0.27	101.15
270	6.47	0.06	1.19	0.14	0.15	86.68
280	6.41	0.08	-6.11	0.17	0.38	95.42
290	6.40	0.11	-7.09	0.20	0.66	93.13
299.7	6.41	0.13	-10.41	0.21	0.76	93.76
300	6.41	0.13	-10.29	0.21	0.76	93.69
310	6.37	0.10	-10.60	0.19	0.48	96.57
320	6.31	0.07	-10.35	0.17	0.18	110.09
330	6.27	0.06	-9.20	0.15	0.11	123.48
340	6.24	0.06	-9.27	0.15	0.12	121.91
350	6.22	0.06	-9.88	0.14	0.15	117.29
360	6.20	0.06	-11.43	0.14	0.21	111.26

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S9. 1st excited states of NH2-uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	4.65	0.0003	-7.75	0.010	0.64	151.8
20	4.70	0.0001	-1.75	0.003	0.64	139.0
30	4.72	0.0002	3.33	0.006	0.65	51.6
40	4.76	0.0001	-2.70	0.005	0.67	129.0
50	4.78	0.0001	-2.62	0.003	0.68	147.0
60	4.68	0.0004	-7.04	0.008	0.69	154.3
70	4.68	0.0005	-8.81	0.010	0.69	154.1
80	4.67	0.0004	-8.17	0.011	0.68	146.8
90	4.68	0.0003	-4.78	0.007	0.68	140.4
100	4.67	0.0001	0.30	0.003	0.67	82.8
110	4.68	0.0002	6.04	0.008	0.66	26.8
120	4.69	0.0005	10.84	0.014	0.66	29.4
130	4.71	0.0012	13.62	0.017	0.66	29.5
140	4.72	0.0038	25.14	0.032	0.66	29.2
150	4.71	0.0119	44.63	0.057	0.67	31.3
160	4.72	0.0115	42.06	0.055	0.69	34.3
170	4.75	0.0127	42.98	0.057	0.71	37.6
176.7	4.72	0.0013	13.19	0.016	0.67	22.8
180	4.72	0.0027	19.64	0.024	0.67	26.3
190	4.75	0.0006	8.29	0.010	0.67	20.5
200	4.78	0.0003	5.33	0.007	0.67	26.9
210	4.77	0.0002	3.57	0.006	0.67	45.2
220	4.72	0.0003	5.44	0.008	0.68	38.2
230	4.71	0.0005	7.58	0.010	0.68	31.4
240	4.70	0.0005	6.91	0.009	0.68	32.6
250	4.71	0.0007	8.76	0.010	0.68	24.6
260	4.73	0.0007	8.93	0.010	0.69	21.3
270	4.75	0.0004	5.23	0.007	0.68	35.0
280	4.75	0.0001	-0.26	0.005	0.67	93.4
290	4.73	0.0004	-7.45	0.009	0.68	162.1
296.4	4.73	0.0007	-8.37	0.010	0.67	155.7
300	4.74	0.0010	-11.26	0.014	0.67	156.1
310	4.73	0.0020	-16.39	0.021	0.67	150.0
320	4.70	0.0028	-20.13	0.026	0.66	148.5
330	4.65	0.0033	-22.13	0.029	0.66	148.3
340	4.65	0.0046	-25.54	0.034	0.65	148.4
350	4.65	0.0038	-23.62	0.031	0.64	148.7
360	4.64	0.0017	-16.85	0.022	0.64	148.7

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S10. 2nd excited states of NH2-uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	4.88	0.22	22.01	0.25	1.09	86.4
20	4.93	0.23	-7.60	0.25	1.08	91.2
30	4.97	0.25	-44.63	0.26	1.16	96.7
40	5.02	0.25	-45.13	0.26	1.18	96.6
50	5.06	0.26	-45.83	0.27	1.20	96.5
60	5.07	0.25	-50.54	0.26	1.14	97.9
70	5.10	0.24	-41.63	0.26	1.08	96.8
80	5.13	0.24	-40.11	0.26	1.03	97.0
90	5.11	0.24	-35.20	0.26	0.93	96.7
100	5.08	0.25	-33.72	0.26	0.87	96.8
110	5.05	0.25	-32.45	0.26	0.84	96.7
120	5.01	0.25	-33.31	0.26	0.80	97.2
130	4.99	0.25	-36.35	0.26	0.80	97.8
140	4.93	0.24	-42.16	0.26	0.80	99.1
150	4.89	0.23	-51.01	0.25	0.80	101.0
160	4.89	0.24	-36.60	0.25	0.84	97.5
170	4.90	0.24	-31.11	0.25	0.90	96.1
176.7	4.95	0.25	-4.09	0.26	1.01	90.7
180	4.94	0.25	-11.72	0.26	0.97	92.1
190	4.99	0.25	3.96	0.26	1.04	89.3
200	5.02	0.25	8.83	0.26	1.07	88.6
210	5.02	0.25	7.64	0.26	1.11	88.8
220	5.04	0.25	8.80	0.26	1.13	88.7
230	5.05	0.25	8.10	0.26	1.18	88.8
240	5.10	0.25	16.15	0.26	1.22	87.7
250	5.14	0.25	21.06	0.26	1.27	87.1
260	5.18	0.26	25.23	0.26	1.34	86.7
270	5.18	0.26	22.17	0.27	1.38	87.2
280	5.09	0.27	16.75	0.27	1.40	88.0
290	5.06	0.27	23.90	0.27	1.38	87.1
296.4	5.05	0.27	26.45	0.27	1.36	86.8
300	5.04	0.27	28.97	0.27	1.35	86.5
310	5.02	0.26	34.84	0.27	1.33	85.6
320	5.00	0.25	39.05	0.27	1.29	84.9
330	4.95	0.24	38.67	0.26	1.24	84.7
340	4.91	0.24	46.33	0.26	1.17	83.3
350	4.89	0.23	44.87	0.26	1.13	83.2
360	4.88	0.23	35.96	0.25	1.10	84.3

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S11. 3rd excited states of NH2-uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	5.82	0.0001	-4.39	0.007	0.70	146.6
20	5.89	0.0009	6.67	0.021	0.75	67.4
30	5.91	0.0011	8.81	0.024	0.78	63.9
40	6.00	0.0004	6.95	0.017	0.78	59.4
50	6.08	0.0001	5.74	0.007	0.77	10.1
60	5.99	0.0056	3.61	0.041	0.77	83.8
70	6.02	0.0063	5.05	0.043	0.76	81.7
80	6.04	0.0036	8.43	0.031	0.71	68.6
90	6.13	0.0041	7.84	0.036	0.68	72.2
100	6.15	0.0011	7.47	0.018	0.70	55.5
110	6.17	0.0007	5.07	0.013	0.72	58.0
120	6.16	0.0052	3.43	0.038	0.75	83.4
130	6.15	0.0195	0.43	0.077	0.75	89.6
140	6.08	0.0394	-3.91	0.109	0.70	92.8
150	6.06	0.0633	-8.90	0.138	0.69	95.0
160	6.09	0.0626	-8.61	0.136	0.71	94.8
170	6.16	0.0604	-7.87	0.136	0.69	94.6
176.7	6.19	0.0001	-7.08	0.009	0.81	155.8
180	6.18	0.0019	-7.49	0.019	0.80	119.0
190	6.21	0.0009	-5.28	0.022	0.83	106.6
200	6.24	0.0029	-3.66	0.031	0.83	97.9
210	6.25	0.0038	-1.17	0.033	0.83	92.4
220	6.24	0.0022	-1.36	0.024	0.81	93.9
230	6.21	0.0005	-2.01	0.010	0.78	104.9
240	6.17	0.0000	-3.68	0.007	0.76	135.4
250	6.12	0.0006	-5.58	0.016	0.75	115.7
260	6.07	0.0018	-6.74	0.026	0.75	108.8
270	6.03	0.0036	3.32	0.033	0.77	82.8
280	5.98	0.0020	8.26	0.026	0.74	66.5
290	5.97	0.0003	0.88	0.008	0.72	81.8
296.4	5.95	0.0001	-0.42	0.001	0.71	119.9
300	5.94	0.0003	-2.27	0.006	0.70	121.6
310	5.93	0.0015	-6.85	0.020	0.71	116.2
320	5.92	0.0033	-8.10	0.030	0.73	110.2
330	5.88	0.0041	-6.69	0.035	0.75	103.6
340	5.85	0.0046	-5.85	0.037	0.77	100.9
350	5.85	0.0033	-7.03	0.029	0.75	107.2
360	5.84	0.0015	-9.59	0.020	0.72	127.0

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S12. 4th excited states of NH2-uridine at several angles.

φ [a]	EE [b]	Osc [c]	Rot [d]	$\|\mu\|$ [e]	$\|m\|$ [f]	θ [g]
10	6.21	0.06	-12.93	0.14	0.38	103.9
20	6.27	0.06	15.04	0.14	0.39	74.9
30	6.27	0.06	21.00	0.14	0.51	73.4
40	6.30	0.07	23.52	0.15	0.53	73.1
50	6.36	0.08	14.08	0.16	0.46	78.8
60	6.25	0.07	1.87	0.14	0.32	87.7
70	6.24	0.07	-8.18	0.15	0.23	103.0
80	6.26	0.09	-17.46	0.16	0.24	115.2
90	6.40	0.09	-3.98	0.17	0.61	92.2
100	6.41	0.08	2.32	0.16	0.72	88.8
110	6.38	0.06	7.92	0.14	0.71	85.5
120	6.36	0.04	8.94	0.13	0.70	84.3
130	6.36	0.04	-11.67	0.14	0.56	98.7
140	6.30	0.04	-17.96	0.13	0.46	107.1
150	6.30	0.06	-3.19	0.14	0.54	92.3
160	6.32	0.08	1.60	0.16	0.64	89.1
170	6.31	0.10	7.80	0.18	0.75	86.7
176.7	6.38	0.16	-7.34	0.22	0.62	93.1
180	6.37	0.16	-5.06	0.22	0.69	91.9
190	6.42	0.14	-7.31	0.21	0.51	93.9
200	6.46	0.12	-6.29	0.20	0.37	94.9
210	6.46	0.08	-4.16	0.17	0.20	97.2
220	6.44	0.06	-5.58	0.14	0.21	100.5
230	6.40	0.05	-8.00	0.13	0.26	103.6
240	6.40	0.05	-8.13	0.13	0.30	102.6
250	6.39	0.05	-7.05	0.13	0.30	100.1
260	6.42	0.06	-6.66	0.15	0.29	99.0
270	6.45	0.07	-3.53	0.15	0.19	97.2
280	6.41	0.06	-0.46	0.14	0.03	97.0
290	6.43	0.06	-6.63	0.15	0.16	105.8
296.4	6.41	0.05	-9.77	0.14	0.10	133.1
300	6.39	0.05	-10.95	0.13	0.12	135.0
310	6.36	0.05	-11.72	0.13	0.13	130.4
320	6.31	0.05	-11.31	0.13	0.16	121.0
330	6.27	0.04	-9.72	0.13	0.22	109.9
340	6.25	0.04	-8.69	0.12	0.28	104.7
350	6.22	0.04	-12.65	0.12	0.36	107.3
360	6.19	0.04	-16.78	0.12	0.40	109.2

[a] Dihedral angle (in º). [b] Excitation energy (in eV). [c] Oscillator strength. [d] Rotatory strength (10^{-40} cgs). [e] Electronic transition dipole moment (in a.u.). [f] magnetic transition dipole moment (in a.u.). [g] angle in Eq. (2) (in º).

Table S13. Coefficients of HOMO-LUMO configuration of 1st excited states of uridine and NH2-uridine at several angles.

φ [a]	uridine	NH2-uridine	φ [a]	uridine	NH2-uridine
10	0.025	0.032	190	0.065	0.047
20	< 0.01	< 0.01	200	0.017	0.028
30	0.030	0.022	210	0.019	0.021
40	0.017	< 0.01	220	0.031	0.028
50	0.049	0.022	230	0.044	0.037
60	0.050	0.046	240	0.053	0.041
70	0.048	0.052	250	0.060	0.050
80	0.042	0.044	260	0.042	0.053
90	0.023	0.030	270	0.024	0.040
100	< 0.01	< 0.01	280	< 0.01	< 0.01
110	0.026	0.021	290	0.024	0.032
120	0.060	0.046	*syn* [c]	0.044	0.047
130	0.078	0.067	300	0.045	0.062
140	0.143	0.118	310	0.071	0.091
150	0.203	0.201	320	0.091	0.113
160	0.214	0.196	330	0.093	0.126
170	0.218	0.206	340	0.115	0.146
Anti [b]	0.230	0.074	350	0.104	0.132
180	0.193	0.102	360	0.067	0.085

[a] Dihedral angle (in º). [b] 173.9º for uridne and 176.7º for NH2-uridine. [c] 299.7º for uridne and 296.4º for NH2-uridine.

Reference

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