Table S1 Selected bond lengths (Å) of all the stationary points in various environments at B3LYP/6-311+G(d,p) level.

reactant and transition state	bond	gas	water	benzene	product	bond	gas	water	benzene
Uridine	N1-C2	1.387	1.396	1.400		C4-C5	1.456	1.451	1.454
	C2-N3	1.373	1.381	1.382		C5=C6	1.343	1.344	1.344
	N3-C4	1.415	1.401	1.406		C6-N1	1.365	1.361	1.363
	C4-C5	1.450	1.446	1.450		C2=O8	1.225	1.226	1.226
	C5=C6	1.350	1.349	1.348		C4=O10	1.214	1.223	1.218
	C6-N1	1.377	1.379	1.381		C6···H12	1.274	1.269	1.272
	C2=O7	1.228	1.220	1.217		H12···O13	1.211	1.218	1.214
	C4=O9	1.216	1.227	1.221		N1-C1’	1.507	1.510	1.509
	N1-C1’	1.495	1.466	1.466	*cis*-U5OH	N1-C2	1.374	1.372	1.371
•OH	O-H	0.976	0.977	0.976		C2-N3	1.397	1.389	1.392
cis-U5OH-TS	N1-C2	1.401	1.397	1.399		N3-C4	1.383	1.379	1.380
	C2-N3	1.376	1.376	1.376		C4-C5	1.526	1.524	1.524
	N3-C4	1.406	1.396	1.402		C5-C6	1.474	1.476	1.476
	C4-C5	1.466	1.465	1.465		C6-N1	1.380	1.377	1.378
	C5=C6	1.379	1.383	1.381		C2=O8	1.225	1.234	1.231
	C6-N1	1.353	1.353	1.353		C4=O10	1.212	1.218	1.216
	C2=O7	1.220	1.222	1.221		C5-O13	1.462	1.458	1.455
	C4=O9	1.211	1.219	1.214		N1-C1’	1.506	1.499	1.504
	C5···O12	2.097	2.059	2.081	*trans*-U5OH	N1-C2	1.372	1.370	1.371
	N1-C1’	1.513	1.511	1.512		C2-N3	1.392	1.390	1.391
trans-U5OH-TS	N1-C2	1.397	1.394	1.396		N3-C4	1.383	1.379	1.381
	C2-N3	1.372	1.375	1.373		C4-C5	1.524	1.523	1.524
	N3-C4	1.406	1.397	1.403		C5-C6	1.478	1.476	1.477
	C4-C5	1.463	1.462	1.462		C6-N1	1.380	1.378	1.379
	C5=C6	1.376	1.381	1.377		C2=O7	1.230	1.234	1.232
	C6-N1	1.360	1.357	1.358		C4=O9	1.213	1.218	1.215
	C2=O7	1.224	1.225	1.225		C5-O12	1.452	1.458	1.454
	C4=O9	1.212	1.219	1.215		N1-C1’	1.501	1.501	1.501
	C5···O12	2.083	2.067	2.090	*cis*-U6OH	N1-C2	1.369	1.366	1.368
	N1-C1’	1.501	1.504	1.503		C2-N3	1.391	1.386	1.390
cis-U6OH-TS	N1-C2	1.396	1.392	1.394		N3-C4	1.397	1.393	1.398
	C2-N3	1.374	1.373	1.374		C4-C5	1.443	1.441	1.442
	N3-C4	1.409	1.402	1.406		C5-C6	1.489	1.490	1.491
	C4-C5	1.450	1.445	1.448		C6-N1	1.452	1.459	1.457
	C5=C6	1.384	1.387	1.384		C2=O7	1.226	1.232	1.229
	C6-N1	1.365	1.363	1.364		C4=O9	1.222	1.229	1.226
	C2=O7	1.222	1.226	1.223		C6-O12	1.447	1.434	1.435
	C4=O9	1.216	1.224	1.219		N1-C1’	1.493	1.476	1.477
	C6···O12	2.109	2.106	2.112	*trans*-U6OH	N1-C2	1.366	1.361	1.364
	N1-C1’	1.482	1.488	1.483		C2-N3	1.395	1.391	1.393
trans-U6OH-TS	N1-C2	1.389	1.390	1.389		N3-C4	1.399	1.390	1.395
	C2-N3	1.377	1.375	1.377		C4-C5	1.442	1.441	1.442

	N3-C4	1.410	1.402	1.407		C5-C6	1.490	1.489	1.489
	C4-C5	1.448	1.445	1.446		C6-N1	1.458	1.459	1.458
	C5=C6	1.385	1.388	1.386		C2=O7	1.228	1.233	1.230
	C6-N1	1.368	1.363	1.366		C4=O9	1.223	1.230	1.226
	C2=O7	1.224	1.225	1.225		C6-O12	1.436	1.436	1.436
	C4=O9	1.217	1.224	1.220		N1-C1’	1.495	1.495	1.496
	C6···O12	2.090	2.108	2.110	UN3H8	N1-C2	1.509	1.501	1.517
	N1-C1’	1.502	1.504	1.504		C2-N3	1.318	1.320	1.315
UN3H8-TS	N1-C2	1.408	1.400	1.404		N3-C4	1.358	1.361	1.360
	C2-N3	1.362	1.361	1.362		C4-C5	1.466	1.470	1.470
	N3-C4	1.352	1.350	1.351		C5=C6	1.382	1.393	1.389
	C4-C5	1.432	1.427	1.430		C6-N1	1.332	1.322	1.325
	C5=C6	1.358	1.360	1.359		C2=O7	1.228	1.232	1.229
	C6-N1	1.362	1.361	1.362		C4=O9	1.246	1.241	1.240
	C2=O7	1.228	1.234	1.230		N1-C1’	1.474	1.487	1.479
	C4=O9	1.270	1.278	1.273	UC5H10	N1-C2	1.386	1.384	1.385
	C3···H9	1.283	1.281	1.283		C2-N3	1.379	1.379	1.379
	H9···O12	1.201	1.202	1.202		N3-C4	1.425	1.413	1.420
	N1-C1’	1.493	1.497	1.495		C4-C5	1.439	1.432	1.436
UC5H10-TS	N1-C2	1.386	1.385	1.386		C5=C6	1.333	1.334	1.333
	C2-N3	1.379	1.378	1.379		C6-N1	1.387	1.382	1.385
	N3-C4	1.412	1.404	1.408		C2=O7	1.227	1.230	1.229
	C4-C5	1.443	1.439	1.441		C4=O9	1.211	1.221	1.215
	C5=C6	1.340	1.343	1.341		N1-C1’	1.495	1.500	1.497
	C6-N1	1.381	1.375	1.378	UC6H11	N1-C2	1.398	1.396	1.397
	C2=O7	1.226	1.228	1.227		C2-N3	1.374	1.373	1.374
	C4=O9	1.217	1.223	1.220		N3-C4	1.418	1.409	1.414
	C5···H10	1.315	1.293	1.304		C4-C5	1.463	1.457	1.460
	H10···O12	1.161	1.186	1.173		C5=C6	1.334	1.336	1.335
	N1-C1’	1.498	1.500	1.500		C6-N1	1.347	1.344	1.346
UC6H11-TS	N1-C2	1.397	1.396	1.396		C2=O7	1.224	1.226	1.225
	C2-N3	1.373	1.373	1.373		C4=O9	1.213	1.223	1.217
	N3-C4	1.412	1.402	1.408		N1-C1’	1.493	1.494	1.493

Fig. S1 Optimized geometries of the uridine +H_2O complexes and of transition states along with imaginary frequencies.