Supplementary Materials

Intramolecular interactions in derivatives of uracil tautomers

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Table of Contents

Table S1. Dipole moments μ (in Debye) and the difference in μ between formamide and the gas phase, Δμ = μ(f) – μ(gas).

	5-NH2		5-NO2		5-NO2(90°)		6-NO2		6-NO2(90°)		6-NH2	
	μ	Δμ	μ	Δμ	μ	Δμ	μ	Δμ	μ	Δμ	μ	Δμ
u1	4.5	1.9	4.9	2.5	4.7	2.0	0.5	0.5	1.1	0.8	6.2	3.2
u2	2.3	1.1	7.0	3.2	6.3	2.4	4.5	1.6	4.2	1.5	4.8	2.1
u3	5.9	2.6	2.2	1.1	2.3	1.2	2.8	1.3	2.6	1.3	6.6	3.3
u4	2.6	1.0	3.8	1.5	2.8	0.7	3.3	1.0	2.8	0.8	3.2	1.4
u5	3.3	1.3	4.7	1.7	3.7	1.0	5.8	2.0	5.4	1.7	1.9	0.9
u6	3.8	1.9	1.8	0.6	1.3	0.4	4.7	1.8	4.5	1.6	4.2	1.9

Table S2. Relative energies (in kcal·mol^{-1}) of 5-NH2 uracil tautomers in all studied environments.

E_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	range
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	9.5	10.7	11.3	11.6	11.6	11.9	12.1	12.2	12.2	12.2	2.7
u3	14.6	13.8	13.2	13.0	12.9	12.7	12.5	12.5	12.4	12.4	-2.2
u4	14.4	16.1	17.0	17.3	17.4	17.7	17.9	18.0	18.1	18.1	3.6
u5	15.5	16.9	17.6	17.8	17.9	18.1	18.3	18.3	18.4	18.4	2.9
u6	18.1	19.3	19.8	19.9	20.0	20.1	20.2	20.2	20.3	20.3	2.1

Table S3. Solvation energies (in kcal·mol^{-1}) of 5-NH2 uracil tautomers in all studied environments.

E_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-5.0	-7.7	-8.7	-8.9	-9.8	-10.5	-10.8	-11.0	-11.1	-11.0
u2	0.0	-3.8	-5.8	-6.6	-6.7	-7.4	-7.9	-8.2	-8.3	-8.3	-8.3
u3	0.0	-5.9	-9.1	-10.3	-10.6	-11.7	-12.6	-13.0	-13.2	-13.3	-13.2
u4	0.0	-3.4	-5.1	-5.8	-5.9	-6.6	-7.0	-7.3	-7.4	-7.4	-7.4
u5	0.0	-3.7	-5.7	-6.4	-6.5	-7.3	-7.8	-8.0	-8.2	-8.2	-8.2
u6	0.0	-3.8	-6.0	-6.9	-7.0	-7.9	-8.4	-8.7	-8.9	-9.0	-8.9

Table S4. Relative Gibbs energies (in kcal·mol^{-1}) of 5-NH2 uracil tautomers in all studied environments.

G_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	9.4	10.5	11.1	11.4	11.4	11.7	11.8	11.8	11.9	11.9	2.4
u3	14.1	13.4	13.0	12.8	12.8	12.6	12.4	12.3	12.2	12.2	-1.9
u4	14.3	15.9	16.7	17.0	17.1	17.4	17.6	17.6	17.7	17.7	3.3
u5	15.4	16.6	17.2	17.5	17.5	17.7	17.8	17.9	17.9	17.9	2.6
u6	17.8	18.5	19.4	19.6	19.7	19.8	19.8	19.9	19.9	19.9	2.1

Table S5. Solvation Gibbs energies (in kcal·mol^{-1}) of 5-NH2 uracil tautomers in all studied environments.

G_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-5.0	-7.7	-8.7	-8.9	-9.8	-10.4	-10.8	-10.9	-11.0	-10.9
u2	0.0	-4.0	-6.0	-6.7	-6.9	-7.6	-8.1	-8.4	-8.5	-8.5	-8.5
u3	0.0	-5.7	-8.8	-10.0	-10.2	-11.4	-12.2	-12.6	-12.8	-12.9	-12.8
u4	0.0	-3.4	-5.3	-6.0	-6.1	-6.8	-7.2	-7.5	-7.6	-7.6	-7.6
u5	0.0	-3.8	-5.8	-6.6	-6.7	-7.4	-8.0	-8.2	-8.4	-8.4	-8.4
u6	0.0	-4.3	-6.1	-6.8	-7.0	-7.8	-8.4	-8.7	-8.8	-8.9	-8.8

Table S6. Relative energies (in kcal·mol^{-1}) of 5-NO2 uracil tautomers in all studied environments.

E_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	10.1	11.0	11.5	11.7	11.8	11.9	12.0	12.1	12.1	12.1	2.1
u3	10.2	10.6	10.9	11.0	11.0	11.1	11.2	11.2	11.2	11.2	1.1
u4	11.8	14.4	15.8	16.3	16.4	17.0	17.4	17.6	17.7	17.7	5.9
u5	12.9	15.1	16.4	16.8	16.9	17.4	17.7	17.8	17.9	17.9	5.0
u6	5.4	8.7	10.5	11.1	11.2	11.9	12.3	12.6	12.7	12.7	7.3

Table S7. Solvation energies (in kcal·mol^{-1}) of 5-NO2 uracil tautomers in all studied environments.

E_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-6.4	-9.9	-11.2	-11.4	-12.7	-13.6	-14.1	-14.3	-14.4	-14.3
u2	0.0	-5.5	-8.5	-9.6	-9.7	-10.9	-11.7	-12.1	-12.3	-12.3	-12.3
u3	0.0	-5.9	-9.2	-10.4	-10.6	-11.8	-12.6	-13.1	-13.3	-13.4	-13.3
u4	0.0	-3.8	-5.9	-6.6	-6.8	-7.5	-8.0	-8.3	-8.4	-8.5	-8.4
u5	0.0	-4.1	-6.4	-7.3	-7.4	-8.3	-8.8	-9.2	-9.3	-9.4	-9.3
u6	0.0	-3.1	-4.8	-5.5	-5.6	-6.2	-6.7	-6.9	-7.0	-7.1	-7.0

Table S8. Relative Gibbs energies (in kcal·mol^{-1}) of 5-NO2 uracil tautomers in all studied environments.

G_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	10.0	10.6	11.2	11.4	11.6	11.7	11.8	11.9	12.0	12.0	2.0
u3	9.9	10.3	10.6	10.7	11.3	10.9	11.0	11.1	11.1	11.1	1.4
u4	11.5	13.6	15.2	15.8	16.5	16.5	17.0	17.2	17.3	17.4	5.8
u5	12.7	14.3	15.7	16.2	16.9	16.9	17.2	17.4	17.5	17.6	4.8
u6	6.4	9.3	11.0	11.6	12.3	12.4	12.9	13.1	13.3	13.3	6.9

Table S9. Solvation Gibbs energies (in kcal·mol^{-1}) of 5-NO2 uracil tautomers in all studied environments.

G_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-6.2	-9.6	-10.9	-11.7	-12.5	-13.4	-13.9	-14.2	-14.3	14.3
u2	0.0	-5.6	-8.4	-9.5	-10.2	-10.8	-11.6	-12.0	-12.2	-12.3	12.3
u3	0.0	-5.8	-9.0	-10.1	-10.4	-11.5	-12.4	-12.8	-13.0	-13.1	13.1
u4	0.0	-4.1	-5.9	-6.6	-6.8	-7.5	-8.0	-8.3	-8.4	-8.4	8.4
u5	0.0	-4.6	-6.6	-7.4	-7.6	-8.4	-8.9	-9.2	-9.4	-9.4	9.4
u6	0.0	-3.2	-5.0	-5.7	-5.8	-6.5	-6.9	-7.2	-7.3	-7.3	7.3

Table S10. Relative energies (in kcal·mol^{-1}) of 5-NO2(90°) uracil tautomers in all studied environments.

E_rel	gas	thf	water	*range*
u1	0.0	0.0	0.0	0.0
u2	9.1	11.0	11.6	2.5
u3	11.8	12.0	12.0	0.2
u4	11.6	16.0	17.1	5.6
u5	12.6	16.5	17.4	4.8
u6	15.8	19.7	20.6	4.8

Table S11. Solvation energies (in kcal·mol^{-1}) of 5-NO2(90°) uracil tautomers in all studied environments.

E_solv	gas	thf	water	*range*
u1	0.0	-10.6	-13.2	13.2
u2	0.0	-8.7	-10.7	10.7
u3	0.0	-10.4	-13.0	13.0
u4	0.0	-6.2	-7.6	7.6
u5	0.0	-6.8	-8.4	8.4
u6	0.0	-6.7	-8.4	8.4

Table S12. Relative energies (in kcal·mol^{-1}) of 6-NH2 uracil tautomers in all studied environments.

E_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	6.6	8.3	9.3	9.6	9.7	10.0	10.3	10.4	10.5	10.5	3.8
u3	10.3	10.2	10.0	9.9	9.9	9.8	9.7	9.7	9.7	9.7	-0.6
u4	8.1	11.1	12.7	13.3	13.4	14.0	14.4	14.6	14.7	14.7	6.5
u5	8.5	11.4	12.9	13.5	13.6	14.2	14.5	14.7	14.8	14.9	6.4
u6	12.4	14.4	15.3	15.6	15.6	15.9	16.1	16.2	16.3	16.3	3.9

Table S13. Solvation energies (in kcal·mol^{-1}) of 6-NH2 uracil tautomers in all studied environments.

E_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-6.5	-9.9	-11.2	-11.4	-12.7	-13.5	-14.0	-14.2	-14.2	-14.2
u2	0.0	-4.8	-7.3	-8.2	-8.4	-9.3	-9.9	-10.2	-10.3	-10.4	-10.3
u3	0.0	-6.7	-10.3	-11.6	-11.9	-13.2	-14.1	-14.6	-14.8	-14.9	-14.8
u4	0.0	-3.5	-5.4	-6.0	-6.2	-6.8	-7.3	-7.5	-7.6	-7.7	-7.6
u5	0.0	-3.6	-5.5	-6.1	-6.3	-7.0	-7.4	-7.7	-7.8	-7.9	-7.8
u6	0.0	-4.6	-7.1	-8.0	-8.2	-9.2	-9.8	-10.1	-10.3	-10.4	-10.3

Table S14. Relative Gibbs energies (in kcal·mol^{-1}) of 6-NH2 uracil tautomers in all studied environments.

G_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	6.6	8.1	9.2	9.5	9.6	9.9	10.1	10.3	10.4	10.4	3.8
u3	10.1	9.9	9.8	9.7	9.7	9.5	9.4	9.4	9.3	9.3	0.8
u4	8.4	11.1	12.8	13.3	13.4	13.9	14.3	14.5	14.6	14.7	6.2
u5	8.7	11.4	13.0	13.5	13.6	14.1	14.5	14.7	14.8	14.8	6.2
u6	12.5	14.4	15.4	15.6	15.7	15.9	16.1	16.2	16.2	16.2	3.7

Table S15. Solvation Gibbs energies (in kcal·mol^{-1}) of 6-NH2 uracil tautomers in all studied environments.

G_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-6.5	-10.1	-11.3	-11.6	-12.8	-13.7	-14.2	-14.4	-14.5	14.5
u2	0.0	-5.0	-7.5	-8.5	-8.7	-9.6	-10.2	-10.5	-10.6	-10.7	10.7
u3	0.0	-6.7	-10.4	-11.7	-12.0	-13.4	-14.4	-14.9	-15.2	-15.3	15.3
u4	0.0	-3.8	-5.8	-6.5	-6.6	-7.3	-7.8	-8.1	-8.2	-8.2	8.2
u5	0.0	-3.8	-5.8	-6.5	-6.7	-7.4	-7.9	-8.1	-8.3	-8.3	8.3
u6	0.0	-4.6	-7.2	-8.2	-8.4	-9.4	-10.1	-10.5	-10.7	-10.7	10.7

Table S16. Relative energies (in kcal·mol^{-1}) of 6-NO2 uracil tautomers in all studied environments.

E_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	9.9	9.3	9.1	9.0	9.0	8.9	8.8	8.8	8.8	8.8	1.1
u3	11.4	11.3	11.2	11.2	11.1	11.1	11.0	11.0	11.0	11.0	0.4
u4	11.7	12.4	12.8	13.0	13.0	13.2	13.3	13.3	13.3	13.3	1.6
u5	12.9	13.3	13.4	13.4	13.4	13.4	13.4	13.4	13.4	13.4	0.5
u6	16.2	15.9	15.5	15.4	15.4	15.2	15.1	15.0	15.0	15.0	1.3

Table S17. Solvation energies (in kcal·mol^{-1}) of 6-NO2 uracil tautomers in all studied environments.

E_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-4.3	-6.5	-7.4	-7.5	-8.3	-8.9	-9.2	-9.3	-9.4	9.4
u2	0.0	-4.9	-7.4	-8.3	-8.5	-9.3	-9.9	-10.3	-10.4	-10.5	10.5
u3	0.0	-4.4	-6.8	-7.6	-7.8	-8.7	-9.3	-9.6	-9.7	-9.8	9.8
u4	0.0	-3.6	-5.4	-6.1	-6.2	-6.9	-7.4	-7.6	-7.7	-7.8	7.8
u5	0.0	-4.0	-6.1	-6.9	-7.1	-7.9	-8.4	-8.7	-8.8	-8.9	8.9
u6	0.0	-4.6	-7.2	-8.2	-8.4	-9.4	-10.0	-10.4	-10.6	-10.6	10.6

Table S18. Relative Gibbs energies (in kcal·mol^{-1}) of 6-NO2 uracil tautomers in all studied environments.

G_rel	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
u2	9.2	8.9	8.6	8.6	8.5	8.5	8.4	8.4	8.4	8.4	0.8
u3	11.2	11.1	11.0	10.9	10.9	10.9	10.9	10.8	10.8	10.8	0.3
u4	11.3	12.2	12.6	12.7	12.8	12.9	13.0	13.0	13.1	13.1	1.7
u5	12.3	12.9	13.0	13.1	13.1	13.1	13.1	13.1	13.1	13.1	0.8
u6	15.7	15.3	15.0	14.9	14.8	14.7	14.7	14.7	14.7	14.6	1.0

Table S19. Solvation Gibbs energies (in kcal·mol^{-1}) of 6-NO2 uracil tautomers in all studied environments.

G_solv	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f	*range*
u1	0.0	-4.3	-6.6	-7.4	-7.6	-8.4	-9.0	-9.3	-9.5	-9.6	9.6
u2	0.0	-4.6	-7.2	-8.1	-8.3	-9.2	-9.8	-10.2	-10.3	-10.4	10.4
u3	0.0	-4.4	-6.8	-7.6	-7.8	-8.7	-9.3	-9.7	-9.8	-9.9	9.9
u4	0.0	-3.4	-5.3	-6.0	-6.2	-6.9	-7.4	-7.6	-7.8	-7.8	7.8
u5	0.0	-3.6	-5.8	-6.6	-6.8	-7.6	-8.2	-8.5	-8.7	-8.7	8.7
u6	0.0	-4.7	-7.3	-8.2	-8.4	-9.4	-10.0	-10.4	-10.5	-10.6	10.6

Table S20. Relative energies (in kcal·mol^{-1}) of 6-NO2(90°) uracil tautomers in all studied environments.

E_rel	gas	thf	water	*range*
u1	0.0	0.0	0.0	0.0
u2	5.4	5.8	6.0	0.6
u3	11.1	11.0	10.9	0.2
u4	7.2	9.9	10.6	3.4
u5	8.1	10.1	10.6	2.5
u6	11.7	12.2	12.2	0.5

Table S21. Solvation energies (in kcal·mol^{-1}) of 6-NO2(90°) uracil tautomers in all studied environments.

E_solv	gas	thf	water	*range*
u1	0.0	-8.5	-10.5	10.5
u2	0.0	-8.0	-9.9	9.9
u3	0.0	-8.6	-10.7	10.7
u4	0.0	-5.8	-7.1	7.1
u5	0.0	-6.4	-8.0	8.0
u6	0.0	-8.0	-10.0	10.0

Table S22. Values of a and determination coefficients of $G = a \cdot 1/\varepsilon + b$ correlations, where G is the total Gibbs energy of a molecule (in hartree) and ε is the dielectric constant of the environment.

	5-NH2		**5-NO2**		**6-NO2**		**6-NH2**	
	a	R^2	a	R^2	a	R^2	a	R^2
u1	0.0178	0.980	0.0232	0.971	0.0155	0.975	0.0235	0.977
u2	0.0138	0.981	0.0199	0.976	0.0169	0.975	0.0174	0.981
u3	0.0209	0.973	0.0212	0.973	0.0160	0.973	0.0247	0.972
u4	0.0124	0.976	0.0136	0.984	0.0127	0.971	0.0134	0.979
u5	0.0136	0.977	0.0152	0.985	0.0142	0.963	0.0135	0.978
u6	0.0142	0.978	0.0119	0.973	0.0172	0.974	0.0174	0.968

Table S23. Values of a and determination coefficients of G_solv(kcal·mol^{-1}) = $a \cdot 1/\varepsilon + b$ correlations.

	5-NH2		**5-NO2**		**6-NO2**		**6-NH2**	
	a	R^2	a	R^2	a	R^2	a	R^2
u1	11.1942	0.9796	14.5484	0.9713	9.7176	0.9753	14.7345	0.9771
u2	8.6785	0.9807	12.4949	0.9763	10.5896	0.9746	10.8955	0.9809
u3	13.1180	0.9735	13.3143	0.9732	10.0560	0.9728	15.5109	0.9718
u4	7.7720	0.9765	8.5240	0.9839	7.9690	0.9708	8.3812	0.9793
u5	8.5509	0.9768	9.5250	0.9847	8.9034	0.9628	8.4624	0.9779
u6	8.9180	0.9783	7.4651	0.9727	10.7867	0.9745	10.9279	0.9677

Table S24. cSAR(X) values for the amino group in 5-NH2 uracil tautomers in all studied environments.

tautomer	**gas**	**to**	**chl**	**o-cr**	**thf**	**pyr**	**et**	**dmso**	**water**	**f**
u1	0.067	0.073	0.076	0.076	0.076	0.077	0.078	0.078	0.078	0.078
u2	0.078	0.081	0.082	0.082	0.082	0.082	0.082	0.082	0.081	0.081
u3	0.057	0.072	0.080	0.083	0.083	0.086	0.088	0.089	0.089	0.089
u4	0.068	0.080	0.086	0.088	0.089	0.091	0.092	0.093	0.093	0.093
u5	0.068	0.079	0.085	0.088	0.088	0.090	0.092	0.092	0.093	0.093
u6	0.042	0.067	0.080	0.085	0.086	0.091	0.094	0.096	0.097	0.097

Table S25. cSAR(X) values for the nitro group in 5-NO2 uracil tautomers in all studied environments.

tautomer	**gas**	**to**	**chl**	**o-cr**	**thf**	**pyr**	**et**	**dmso**	**water**	**f**
u1	-0.163	-0.193	-0.210	-0.217	-0.218	-0.225	-0.229	-0.232	-0.233	-0.234
u2	-0.166	-0.202	-0.222	-0.230	-0.234	-0.239	-0.244	-0.247	-0.249	-0.249
u3	-0.180	-0.202	-0.213	-0.217	-0.218	-0.222	-0.225	-0.226	-0.227	-0.227
u4	-0.173	-0.197	-0.210	-0.215	-0.216	-0.221	-0.225	-0.226	-0.227	-0.228
u5	-0.172	-0.198	-0.211	-0.216	-0.217	-0.222	-0.225	-0.227	-0.228	-0.228
u6	-0.136	-0.144	-0.149	-0.150	-0.150	-0.152	-0.153	-0.153	-0.153	-0.153

Table S26. cSAR(X) values for the nitro group in 5-NO2(90°) uracil tautomers in all studied environments.

tautomer	gas	thf	water	range
u1	-0.121	-0.157	-0.166	-0.045
u2	-0.127	-0.170	-0.180	-0.053
u3	-0.136	-0.158	-0.162	-0.026
u4	-0.138	-0.169	-0.175	-0.037
u5	-0.139	-0.169	-0.175	-0.037
u6	-0.157	-0.167	-0.167	-0.009

Table S27. cSAR(X) values for the amino group in 6-NH2 uracil tautomers in all studied environments.

	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f
u1	0.215	0.258	0.283	0.293	0.295	0.305	0.312	0.316	0.317	0.318
u2	0.201	0.224	0.237	0.242	0.243	0.248	0.251	0.253	0.254	0.254
u3	0.234	0.277	0.302	0.312	0.314	0.324	0.331	0.335	0.337	0.338
u4	0.206	0.227	0.239	0.243	0.244	0.249	0.252	0.253	0.254	0.254
u5	0.214	0.232	0.241	0.245	0.245	0.248	0.250	0.252	0.252	0.252
u6	0.208	0.229	0.240	0.244	0.245	0.249	0.252	0.253	0.254	0.254

Table S28. cSAR(X) values for the nitro group in 6-NO2 uracil tautomers in all studied environments.

	gas	to	chl	o-cr	thf	pyr	et	dmso	water	f
u1	-0.001	0.000	0.000	0.001	0.001	0.001	0.001	0.002	0.002	0.002
u2	-0.052	-0.069	-0.078	-0.081	-0.081	-0.084	-0.086	-0.087	-0.087	-0.088
u3	0.004	0.004	0.005	0.005	0.005	0.006	0.006	0.006	0.006	0.006
u4	-0.042	-0.060	-0.068	-0.071	-0.072	-0.074	-0.076	-0.077	-0.078	-0.078
u5	-0.035	-0.056	-0.066	-0.070	-0.071	-0.075	-0.077	-0.079	-0.079	-0.080
u6	-0.036	-0.055	-0.065	-0.068	-0.069	-0.072	-0.074	-0.076	-0.076	-0.076

Table S29. cSAR(X) values for the nitro group in 6-NO2(90°) uracil tautomers in all studied environments.

	gas	thf	water
u1	0.001	0.002	0.004
u2	-0.030	-0.059	-0.065
u3	0.013	0.015	0.017
u4	-0.021	-0.049	-0.055
u5	-0.015	-0.049	-0.057
u6	-0.018	-0.049	-0.055

Table S30. Geometry data in the gas phase (_g) and formamide (_f), obtained at B97D3/aug-cc-pVDZ level (all distances in Å). In ortho1 and ortho2 columns the lengths of the closest *ortho* contacts of H or O atoms of NH_2 or NO_2 substituents are given. Ortho1 contact is in the direction of lower atom indexing in the uracil (for example 4 for the 5 substitution), while ortho2 higher (6 for the 5 substitution). dNH1 and dNO1 is the appropriate NH or NO bond length.

	5-NH2					**5-NO2**				
	dCN	dNH1	dNH2	ortho1	ortho2	dCN	dNO1	dNO2	ortho1	ortho2
u1_g	1.3969	1.0188	1.0149	2.3202	2.6802	1.4671	1.2280	1.2418	2.8197	2.3662
u2_g	1.3920	1.0149	1.0141	2.3792	2.6025	1.4674	1.2305	1.2395	2.8636	2.4459
u3_g	1.4079	1.0165	1.0166	2.3723	2.6111	1.4639	1.2307	1.2416	2.6874	2.3402
u4_g	1.4028	1.0160	1.0161	2.4429	2.5406	1.4666	1.2325	1.2389	2.6986	2.3849
u5_g	1.4030	1.0160	1.0161	2.4525	2.5294	1.4661	1.2330	1.2384	2.7022	2.3965
u6_g	1.4405	1.0202	1.0202	2.1013	2.9164	1.4406	1.2633	1.2293	1.6700	2.4633
u1_f	1.3989	1.0181	1.0163	2.4131	2.5979	1.4512	1.2364	1.2440	2.7988	2.3795
u2_f	1.3953	1.0175	1.0159	2.4440	2.5453	1.4509	1.2383	1.2442	2.8147	2.3957
u3_f	1.4041	1.0174	1.0173	2.4444	2.5518	1.4510	1.2370	1.2435	2.6767	2.3698
u4_f	1.4000	1.0167	1.0169	2.4701	2.5079	1.4535	1.2379	1.2425	2.6787	2.3750
u5_f	1.4002	1.0167	1.0169	2.4751	2.5021	1.4531	1.2380	1.2425	2.6807	2.3735
u6_f	1.4217	1.0223	1.0189	2.2289	2.5045	1.4342	1.2632	1.2328	1.6839	2.4658
	5-NO2 (90°)					**6-NH2**				
	dCN	dNO1	dNO2	ortho1	ortho2	dCN	dNH1	dNH2	ortho1	ortho2
u1_g	1.4783	1.2297	1.2297	2.8990	3.2812	1.3857	1.0143	1.0161	2.4712	2.3787
u2_g	1.4782	1.2303	1.2302	2.9204	3.2542	1.3748	1.0113	1.0125	2.5173	2.4269
u3_g	1.4794	1.2308	1.2309	2.8152	3.3150	1.3789	1.0134	1.0142	2.5118	2.3733
u4_g	1.4767	1.2315	1.2315	2.8422	3.2865	1.3742	1.0114	1.0129	2.5434	2.4508
u5_g	1.4765	1.2316	1.2316	2.8417	3.2838	1.3723	1.0110	1.0128	2.5459	2.4405
u6_g	1.4749	1.2350	1.2345	2.8676	3.3045	1.3739	1.0112	1.0132	2.5326	2.4377
u1_f	1.4754					1.3610	1.0123	1.0127	2.4898	2.3174
u2_f	1.4747					1.3633	1.0115	1.0123	2.5064	2.4492
u3_f	1.4771					1.3546	1.0116	1.0120	2.5306	2.3481
u4_f	1.4737					1.3635	1.0116	1.0125	2.5269	2.4769
u5_f	1.4735					1.3637	1.0115	1.0125	2.5223	2.4734
u6_f	1.4755					1.3632	1.0114	1.0125	2.5118	2.4730

	6-NO2					**6-NO2 (90°)**		
	dCN	dNO1	dNO2	ortho1	ortho2	dCN	dNO1	dNO2
u1_g	1.4941	1.2257	1.2358	2.5196	2.2005	1.4907	1.2289	1.2289
u2_g	1.5201	1.2321	1.2253	2.4413	2.6386	1.4987	1.2283	1.2282
u3_g	1.4934	1.2271	1.2341	2.5406	2.2470	1.4902	1.2287	1.2286
u4_g	1.5209	1.2331	1.2237	2.4681	2.6616	1.4986	1.2282	1.2281
u5_g	1.5247	1.2338	1.2223	2.4577	2.6627	1.5000	1.2280	1.2279
u6_g	1.5249	1.2348	1.2215	2.4279	2.6676	1.5006	1.2281	1.2279
u1_f	1.4897	1.2278	1.2349	2.5116	2.2153	1.4917		
u2_f	1.5149	1.2332	1.2285	2.4480	2.6407	1.5011		
u3_f	1.4879	1.2284	1.2341	2.5406	2.2483	1.4909		
u4_f	1.5144	1.2332	1.2277	2.4805	2.6580	1.5007		
u5_f	1.5163	1.2333	1.2275	2.4758	2.6576	1.5016		
u6_f	1.5170	1.2333	1.2272	2.4571	2.6589	1.5018		

Table S31. Differences between CN bond lengths in formamide and the gas phase, $\Delta d_{CN} = d_{CN}(f) - d_{CN}(gas)$.

Δd_{CN}	5-NH2	5-NO2	5-NO2 (90°)	6-NH2	6-NO2	6-NO2 (90°)
u1	0.0020	-0.0158	-0.0030	-0.0247	-0.0044	0.0011
u2	0.0033	-0.0165	-0.0035	-0.0115	-0.0051	0.0024
u3	-0.0037	-0.0128	-0.0024	-0.0244	-0.0055	0.0007
u4	-0.0028	-0.0131	-0.0030	-0.0107	-0.0065	0.0020
u5	-0.0028	-0.0130	-0.0030	-0.0087	-0.0084	0.0016
u6	-0.0188	-0.0064	0.0006	-0.0107	-0.0079	0.0012

Table S32. CO bond lengths of C=O/C-OH groups in 2 and 4 position of the uracil molecule (in the gas phase).

	5-NH2		5-NO2		5-NO2 (90°)		6-NH2		6-NO2		6-NO2 (90°)	
	4-CO	**2-CO**	**4-CO**	**2-CO**	**4-CO**	**2-CO**	**4-CO**	**2-CO**	**4-CO**	**2-CO**	**4-CO**	**2-CO**
u1	1.234	1.229	1.218	1.221	1.222	1.222	1.232	1.227	1.226	1.220	1.225	1.221
u2	1.236	1.358	1.219	1.342	1.223	1.346	1.233	1.353	1.225	1.345	1.225	1.344
u3	1.360	1.229	1.338	1.221	1.345	1.222	1.357	1.228	1.349	1.220	1.349	1.221
u4	1.361	1.360	1.337	1.344	1.344	1.347	1.357	1.356	1.347	1.346	1.347	1.346
u5	1.362	1.361	1.338	1.345	1.345	1.348	1.358	1.356	1.348	1.347	1.348	1.346
u6	1.346	1.354	1.324	1.342	1.350	1.347	1.363	1.355	1.353	1.346	1.354	1.345

Table S33. cSAR(X) values of C=O/C-OH groups in 2 and 4 position of the uracil molecule in the gas phase (=O groups in red, -OH in blue).

	position 4						position 2					
	5-NH2	5-NO2	5-NO2 (90°)	6-NH2	6-NO2	6-NO2 (90°)	5-NH2	6-NH2	5-NO2	6-NO2	5-NO2 (90°)	6-NO2 (90°)
u1	-0.145	-0.170	-0.097	-0.112	-0.112	-0.116	-0.141	-0.126	-0.086	-0.089	-0.095	-0.087
u2	-0.171	-0.193	-0.110	-0.126	-0.128	-0.132	0.169	0.195	0.243	0.240	0.230	0.243
u3	0.144	0.131	0.199	0.182	0.187	0.181	-0.165	-0.153	-0.103	-0.107	-0.116	-0.106
u4	0.123	0.121	0.198	0.177	0.180	0.175	0.140	0.157	0.215	0.210	0.199	0.210
u5	0.117	0.116	0.192	0.172	0.175	0.170	0.141	0.156	0.217	0.209	0.200	0.210
u6	0.100	0.125	0.128	0.178	0.174	0.176	0.169	0.161	0.230	0.214	0.206	0.214

Table S34. Ranges and average values of cSAR(X) of C=O/C-OH groups in 2 and 4 position of the uracil molecule, in the gas phase.

	range	average
C4-OH	0.099	0.159
C2-OH	0.103	0.199
C4=O	0.096	-0.134
C2=O	0.078	-0.115