Supporting Information

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Theoretical study of mechanisms for the hydrolytic deamination of cytosine via steered molecular dynamic simulations

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Table S1

Cartesian coordinates of the reactant (in Å), intermediate, transition states and product geometries obtained by electronic structure calculations at PCM-M06-2X/6-311++G(d,p) level of all the mechanisms studied.

C-W structure. Reactive

N	1.965637	0.425248	-0.013735
C	2.040429	-0.928075	0.011605
H	3.033997	-1.355653	0.031185
C	0.913191	-1.672818	0.011786
H	0.943449	-2.751522	0.031612
C	-0.327708	-0.952376	-0.016152
N	-1.486547	-1.624331	-0.019833
H	-1.501295	-2.630316	0.003851
H	-2.360222	-1.110237	-0.029736
N	-0.385931	0.376944	-0.040642
C	0.754004	1.120248	-0.040834
O	0.768568	2.345680	-0.062800
H	2.806636	0.986233	-0.014472
O	-3.143316	0.853527	-0.157622
H	-3.529652	1.364581	0.558252
H	-2.175022	0.976408	-0.085751

Table S2

Cartesian coordinates (in Å) obtained from SMD simulations for intermediate and transition states of all the mechanisms studied.

A-pathway. TS1a structure

N	22.4160004	18.5189991	21.5569992
C	22.1119995	17.1450005	21.3670006
H	22.9309998	16.5060005	21.4080009
C	20.9489994	16.7770004	20.8689995
H	20.6320000	15.7290001	20.7110004
C	20.0030003	17.8409996	20.5279999
N	18.7560005	17.6529999	20.1720009
H	18.4480000	16.6739998	20.0410004
H	18.3689995	18.8080006	19.8799992
N	20.4239998	19.1900005	20.5760002
C	21.5429993	19.5240002	21.2010002
O	21.8320007	20.6410007	21.6480007
H	23.3519993	18.7240009	21.9820004
O	18.2000008	19.9689999	19.5930004
H	17.3330002	20.3649998	19.9400005
H	19.4680004	19.8610001	20.1529999

A-pathway. I1a structure

N	21.9389992	18.4559994	22.5930004
C	22.3299999	17.7409992	21.5330009
H	23.1350002	17.0030003	21.2830009
C	21.4039993	17.9759998	20.5400009
H	21.3239994	17.3980007	19.6329994
C	20.1259995	18.7290001	20.6770000
N	19.3320007	18.8409996	19.5079994
H	19.6250000	18.2670002	18.7329998
H	17.8239994	20.2689991	20.1550007
N	19.9239998	19.4850006	21.8090000
C	20.7830009	19.3069992	22.8020000
O	20.6520004	19.8969994	23.8999996
H	22.5410004	18.2339993	23.4120007
O	17.3619995	19.7560005	20.9290009
H	16.3950005	19.9599991	21.0860004
H	19.0139999	19.7490005	22.1660004

A-pathway. TS2a structure

N	18.8139992	21.0660000	25.0890007
C	20.0949993	20.7639999	25.4960003
H	20.4939995	21.3920002	26.4279995
C	21.0550003	20.3999996	24.5410004
H	22.0370007	20.3869991	25.1450005
C	20.5799999	20.0300007	23.2159996
N	21.3299999	19.4769993	22.1079998
H	22.3090000	19.7070007	22.3409996
H	20.9200001	18.3929996	22.2229996
N	19.2390003	20.3610001	22.8700008
C	18.2880001	20.6399994	23.8560009
O	17.0979996	20.6140003	23.6739998
H	17.9890003	21.3530006	25.7740002
O	19.9860001	18.0590000	23.3589993
H	20.5370007	17.5289993	23.9939995
H	19.0139999	19.7490005	22.1660004

A-path. I2a structure

N	16.1369991	21.4549999	22.2940006
C	15.5900002	20.8549995	23.3260002
H	14.5620003	21.1140003	23.6270008
C	16.3250008	20.0820007	24.2310009
H	15.9770002	19.6250000	25.1429996
C	17.6620007	19.6730003	23.9440002
N	18.6030006	19.5930004	25.1930008
H	18.0620003	19.6970005	26.0559998
H	19.4519997	20.0939999	25.0939999
N	18.2430000	20.3959999	22.8369999
C	17.4640007	21.1079998	21.9309998
O	17.7880001	21.4729996	20.8899994
H	15.8710003	22.2180004	21.7110004
O	17.7049999	18.2099991	23.6760006
H	18.4850006	17.8059998	24.1989994
H	19.0300007	20.0330009	22.2619991

A-pathway. TS3a structure

N	19.1049995	21.6180000	22.4120007
C	18.2929993	21.3530006	23.4589996
H	17.7999992	22.2140007	23.7999992
C	18.2619991	20.0139999	23.9220009
H	17.5830002	19.7460003	24.6630001
C	19.0179996	18.8430004	23.2970009
N	20.2919998	18.1959991	24.3549995
H	20.2189999	18.3649998	25.4629993
H	21.3910007	18.3759995	24.0650005
N	19.6739998	19.3460007	22.0690002
C	19.7339993	20.6560001	21.7950001
O	20.5349998	21.0569992	20.8640003
H	19.0459995	22.5489998	21.9720001
O	18.3969994	17.5909996	23.1949997
H	19.3859997	17.3020000	24.0590000
H	20.4029999	18.7000008	21.6060009

A-pathway. U-A structure. Product

N	20.1520004	18.3959999	21.1700001
C	19.8050003	17.0400009	21.1520004
H	20.3260002	16.3859997	21.8209991
C	18.8670006	16.6070004	20.2590008
H	18.7049999	15.5489998	20.1879997
C	18.3250008	17.4979992	19.2409992
N	17.4279995	13.6190004	18.8479996
H	17.5610008	14.6709995	18.7409992
H	16.8379993	13.4709997	19.6809998
N	18.6030006	18.8439999	19.4099998
C	19.5070000	19.3369999	20.3390007
O	19.7859993	20.5680008	20.3920002
H	20.8980007	18.6849995	21.7759991
O	17.5580006	17.1580009	18.3400002
H	16.8220005	13.2849998	18.1359997
H	18.1959991	19.5960007	18.8129997

B-pathway. TS1b structure

N	22.4529991	17.2010002	21.8579998
C	21.7730007	16.1140003	22.3099995
H	21.9899998	15.5139999	23.2819996
C	20.5440006	15.7950001	21.6910000
H	20.0000000	14.8669996	21.9680004
C	20.0709991	16.7350006	20.6770000
N	18.2290001	17.4960003	21.3770008
H	17.8740005	17.5809994	22.3740005
H	18.2870007	18.4759998	21.0890007
N	20.7700005	17.7520008	20.2460003
C	21.9860001	17.9990005	20.8020000
O	22.7019997	19.0279999	20.6089993
H	23.3379993	17.5529995	22.2819996
O	18.9930000	16.1159992	19.5949993
H	19.0809994	16.5830002	18.7859993
H	18.3379993	16.7570000	20.2789993

B-pathway. I1b structure

N	23.1320000	17.4349995	21.3619995
C	22.5879993	16.2570000	21.6140003
H	23.0760002	15.7320004	22.4740009
C	21.4340000	15.8760004	20.9309998
H	21.1459999	14.8439999	20.8840008
C	20.9610004	16.7590008	19.8999996
N	19.0650005	17.3040009	21.5139999
H	18.5079994	16.6149998	22.1870003
H	18.4899998	18.1520004	21.8110008
N	21.4650002	17.9580002	19.6980000
C	22.6240005	18.2549992	20.4379997
O	23.2380009	19.3519993	20.2350006
H	24.0039997	17.7250004	21.7229996
O	19.9230003	16.3570004	19.0130005
H	20.0499992	16.8379993	18.1410007
H	18.7910004	17.0540009	20.5599995

B-pathway. TS2b structure

N	19.9029999	17.5660000	21.5699997
C	19.5620003	16.2649994	21.4500008
H	20.1900005	15.5270004	21.9860001
C	18.6709995	15.7980003	20.5410004
H	18.4410000	14.7159996	20.4500008
C	18.1930008	16.8320007	19.6389999
N	16.8959999	14.0360003	18.5359993
H	17.8230000	14.0310001	18.0669994
H	16.3199997	13.2720003	18.0990009
N	18.5419998	18.1030006	19.7679996
C	19.3799992	18.5860004	20.7530003
O	19.4769993	19.8020000	20.9860001
H	20.5300007	17.9139996	22.3010006
O	17.2749996	16.7880001	18.6840000
H	16.8040009	14.0000000	19.5900002
H	17.6879997	17.9860001	18.7549992

B-pathway. U-A structure. Product

N	20.152000	18.396000	21.170000
C	19.805000	17.040000	21.152000
H	20.326000	16.386000	21.821000
C	18.867000	16.607000	20.259000
H	18.705000	15.549000	20.188000
C	18.325000	17.498000	19.241000
N	18.603000	18.844000	19.410000
C	19.507000	19.337000	20.339000
O	19.786000	20.568000	20.392000
H	20.898000	18.685000	21.776000
O	17.558000	17.158000	18.340000
H	18.196000	19.596000	18.813000
N	15.187950	17.802420	21.877150
H	15.724090	17.001130	22.331380
H	15.776640	18.645530	21.957820
H	15.179290	17.682000	20.891680

Table S3

Enthalpies and free energies (in kcal·mol^{-1}) in solution phase obtained from electronic structure calculations at PCM-M06-2X/6-311++G(d,p) level for all the mechanisms studied.

	Structure	ΔH	ΔG
A-pathway	**TS1a**	14.99	15.42
	I1a	5.64	4.17
	TS2a	49.42	50.39
	I2a	13.10	14.84
	TS3a	44.87	46.75
	U-A	-3.18	-3.58
B-pathway	**TS1b**	56.99	55.88
	I1b	6.96	6.58
	TS2b	32.49	31.50
	U-A	-3.18	-3.58