Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Hydrolysis of the Damaged Deoxythymidine Glycol Nucleoside and Comparison to Canonical DNA

Lex Navarro-Whyte, Jennifer L. Kellie, Stefan A. P. Lenz and Stacey D. Wetmore*,[1]

Department of Chemistry and Biochemistry, University of Lethbridge, 4401 University Drive, Lethbridge, Alberta, T1K 3M4, Canada

Supporting Information (10 Pages)

[1] Corresponding author. E-mail: stacey.wetmore@uleth.ca.

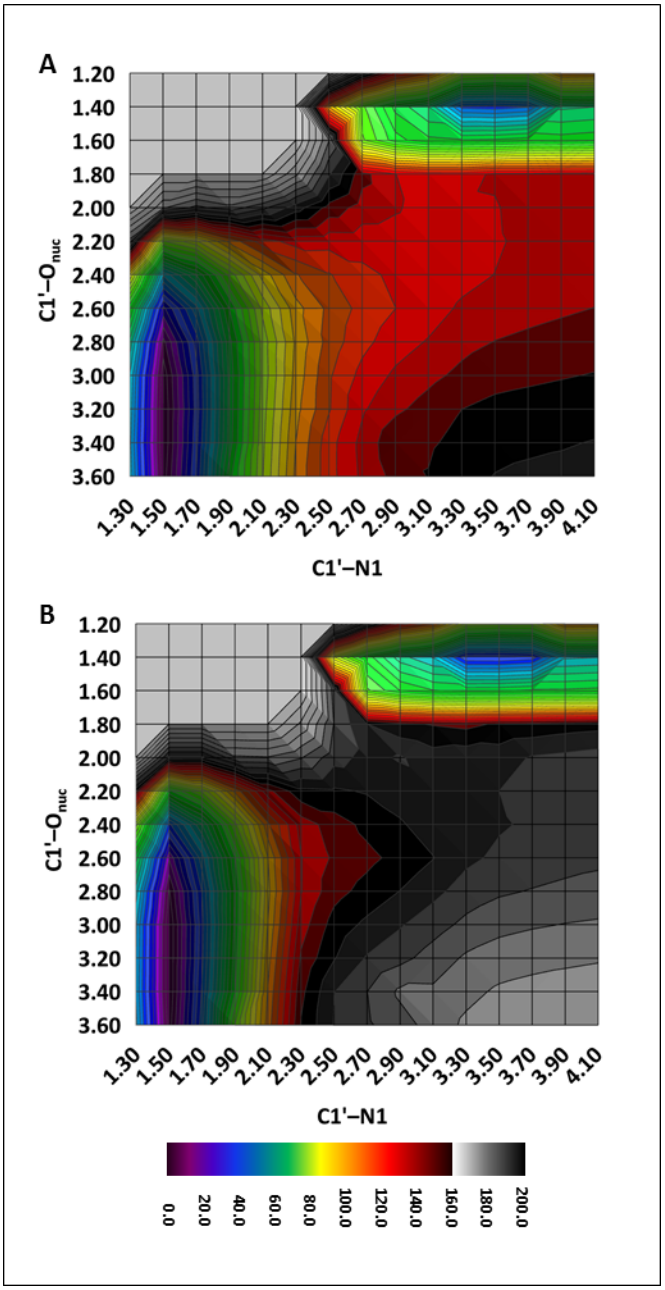

Figure S1. (A) B3LYP-D3 and (B) M06-2X reaction potential energy surface for the hydrolysis of deoxythymidine (dT)

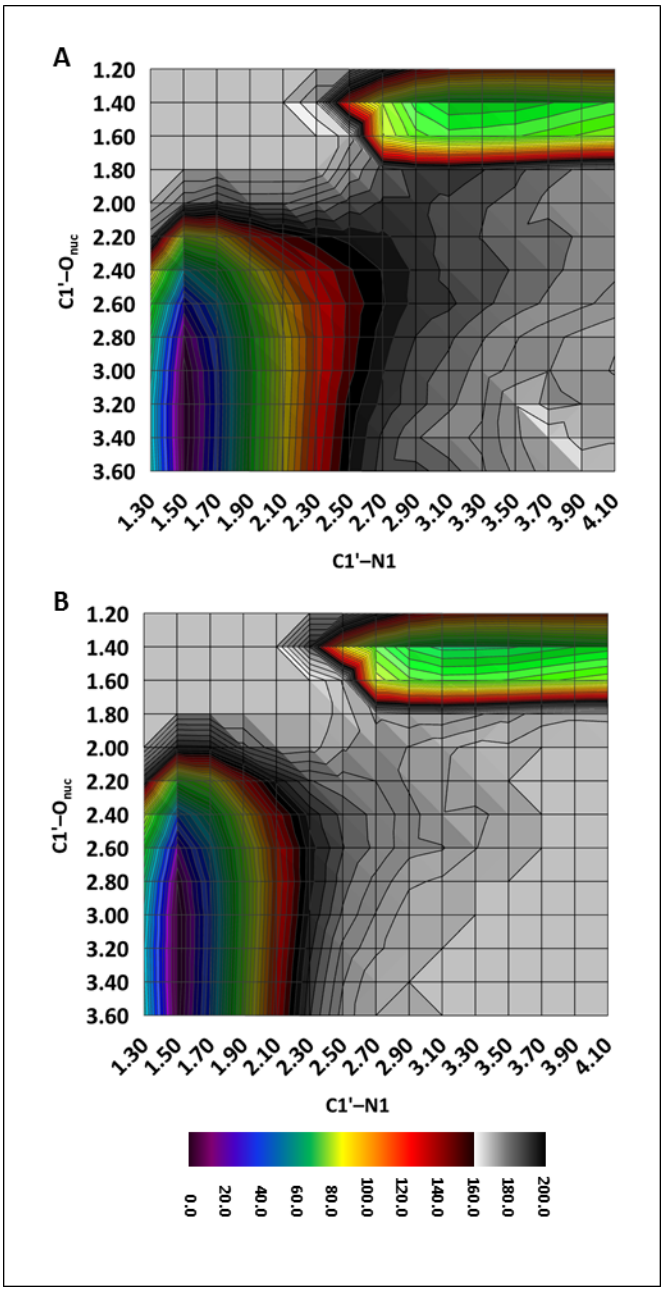

Figure S2. (A) B3LYP-D3 and (B) M06-2X reaction potential energy surface for the hydrolysis of deoxythymidine glycol (dTg)

Table S1. Comparison of the Relative Potential Energy for the Deglycosylation of Deoxythymidine Glycol (dT) Calculated Using a Variety of Methods.[a]

	PCM-B3LYP/ 6-31+G(d)	PCM-B3LYP/ 6-311+G(2df,2p)	PCM-B3LYP-D3/ 6-311+G(2df,2p)	PCM-M06-2X/ 6-311+G(2df,2p)
		Relaxed[b]		
RC	0.0	0.0	0.0	0.0
TSC	163.3	164.3	171.1	196.7
PC	63.8	64.1	74.3	69.2
		Constrained[c]		
RC	0.0	0.0	0.0	0.0
TSC	162.9	164.5	172.5	196.8
PC	66.5	66.0	76.3	69.4

[a]Relative energies were determined using PCM-B3LYP/6-31+G(d) geometries. [b]Geometries were fully optimized. [c]Relative energies on constrained geometries from the potential energy surface.

Table S2. Cartesian coordinates for the optimized constrained stationary points on the thymine potential energy surface.

A. Thymine reactant with constrained glycosidic bond (1.5 Å) and nucleophile distance (3.4 Å)

H	-1.14888300	-0.53128500	-0.56291000
H	-1.55628100	0.08888500	1.74286400
H	-0.16481100	1.19433300	1.74935700
H	-2.02812900	2.71499300	-1.31726900
H	-0.97223000	4.58118900	-0.25028900
H	0.15961400	3.87385800	-1.43248300
H	1.18144900	4.28192700	0.63475100
O	0.61480800	3.49716600	0.57050600
C	-0.34560200	3.70626300	-0.47232800
O	-0.49094900	1.35420700	-1.09458800
C	-0.51376000	0.26690700	-0.18075900
H	1.68406600	1.54717900	0.28258700
H	2.47833900	-3.08704100	-0.52868800
C	3.48865300	-1.33413800	-0.10543400
O	4.59690400	-1.87736200	-0.11874800
N	2.33895200	-2.09687300	-0.34764800
C	1.03124400	-1.66725400	-0.37739500
O	0.10053100	-2.44915200	-0.61759600
N	0.86479000	-0.32169200	-0.12462600
C	1.94689700	0.50573400	0.12147900
C	3.23409600	0.07634500	0.14581300
C	-1.24480900	2.48457500	-0.58634000
C	-1.89607700	2.01642300	0.74071400
C	-1.00891400	0.83077900	1.15605800
H	-3.38865500	0.94034700	-0.04461000
O	-3.27197700	1.68602100	0.59331400
H	-1.86767200	2.81125400	1.48891000
O	-3.69357900	-0.42283800	-1.16717000
H	-4.42024700	-0.23576100	-1.78240600
H	-3.95787500	-1.24212700	-0.67323000
O	-1.82999200	-3.75213100	0.92397400
H	-1.13225400	-3.30412000	0.39487600
H	-1.74875000	-4.69695800	0.71763500
O	-4.28067600	-2.70133300	0.24912600
H	-4.74204100	-2.49672000	1.07791400
H	-3.41562600	-3.10561400	0.51563700
C	4.39792200	0.98925300	0.41374800
H	5.10015500	0.98996300	-0.42845600
H	4.05687200	2.01519000	0.57923100
H	4.95832000	0.66451000	1.29860400

B. Thymine dissociative transition state with constrained glycosidic bond (2.9 Å) and nucleophile distance (2.8 Å)

H	0.66126900	0.59095900	-0.74806000
H	1.75277600	0.47346900	1.67312300
H	0.95086000	-1.08377100	1.41785100
H	4.02014900	-1.47045800	-1.04617600
H	3.48917200	-3.74671000	-0.37238700
H	2.52121800	-3.30412300	-1.80025200
H	1.17244700	-4.25530900	-0.14827100
O	1.46884500	-3.34465300	0.00728100
C	2.66595800	-3.11289700	-0.72964100
O	2.07340400	-0.78589300	-1.21022200
C	1.40430000	-0.11455600	-0.36535700
H	-2.01915800	-2.50551200	0.16371900

H	-3.41138300	1.97152000	-0.54029200
C	-4.13691500	0.15270100	0.10982400
O	-5.28324500	0.60141600	0.31996800
N	-3.14273200	1.00562800	-0.37702300
C	-1.83072400	0.65071200	-0.66057200
O	-1.03848500	1.54425100	-1.09584100
N	-1.44903800	-0.62330800	-0.46348900
C	-2.38058200	-1.48740400	0.01558500
C	-3.69522700	-1.20241500	0.31842900
C	3.08489500	-1.67362300	-0.52289800
C	3.09950300	-1.14394400	0.93114300
C	1.73854200	-0.41772100	1.04019000
H	4.05956300	0.55923800	0.71387200
O	4.19839600	-0.29371700	1.18964100
H	3.17038300	-1.97357900	1.63497600
O	3.34660900	1.89945500	-0.25955100
H	3.75797200	2.13241100	-1.10700000
H	2.92197400	2.73162000	0.08491900
O	-0.54989900	4.00333400	-0.06070800
H	-0.78547300	3.12158200	-0.45610600
H	-0.78167300	4.66533800	-0.73117600
O	2.09072000	4.13361800	0.64710600
H	2.12229700	4.22836300	1.61223500
H	1.12677200	4.09342300	0.40779600
C	-4.66263600	-2.22865800	0.84281000
H	-5.52778500	-2.34840500	0.17756100
H	-4.17436300	-3.20429200	0.94096700
H	-5.05807400	-1.94766500	1.82781200

C. Thymine intermediate complex with constrained glycosidic bond (2.9 Å) and nucleophile distance (2.8 Å)

H	-0.38531600	0.00862000	0.01557100
H	-2.47166100	1.52967300	-0.76783300
H	-2.38864800	0.11921200	-1.83475400
H	-3.69460400	-1.74349500	1.34599600
H	-4.57408400	-2.97681100	-0.56808400
H	-2.96221900	-3.59556700	-0.12995000
H	-3.08653100	-3.19590600	-2.42234200
O	-3.01909200	-2.41272400	-1.85358600
C	-3.50160900	-2.73880600	-0.55263200
O	-1.83554900	-1.31607900	0.52908400
C	-1.46224000	-0.22524700	-0.01479300
H	1.55418100	-1.35683600	1.47996400
H	4.29294200	0.97074300	-1.60344800
C	4.39217600	-0.52953200	-0.19150300
O	5.61151000	-0.72897200	-0.37763100
N	3.73371600	0.45207000	-0.93293000
C	2.38697800	0.79216300	-0.84158900
O	1.96479300	1.71503200	-1.59564400
N	1.61794400	0.12053800	0.03909500
C	2.21970300	-0.84438400	0.78370400
C	3.54393400	-1.22412100	0.74249500
C	-3.31796000	-1.53293700	0.34421100
C	-3.81442700	-0.16995300	-0.19227800
C	-2.52876600	0.44017600	-0.79110200
H	-3.65357700	0.93758000	1.41565500
O	-4.37936900	0.63689300	0.82549200
H	-4.58876300	-0.31258800	-0.94631100
O	-1.84755200	1.18929700	1.88537200
H	-1.44506400	0.79712300	2.67795600

H	-1.43360400	2.09405500	1.77237400
O	-0.29161300	3.12234800	-1.26561100
H	0.52965900	2.55761000	-1.36749600
H	-0.12857000	3.91805100	-1.79627600
O	-0.72668600	3.57579600	1.37541900
H	-1.34516700	4.31582600	1.48388100
H	-0.55203000	3.50189200	0.39710900
C	4.12120500	-2.30789900	1.61225200
H	4.92408800	-1.92738700	2.25743900
H	3.34692000	-2.73868800	2.25650500
H	4.55491700	-3.12085300	1.01514700

D. Thymine associative transition state with constrained glycosidic bond (3.3 Å) and nucleophile distance (2.0 Å)

H	-0.50540900	0.19691900	0.10505100
H	-2.71487300	1.56281500	-0.78800300
H	-2.35126200	0.15477700	-1.80775400
H	-3.73039300	-1.83266400	1.23365400
H	-4.36988800	-3.12360100	-0.71901700
H	-2.73765400	-3.60364300	-0.19154400
H	-2.81208500	-3.20157600	-2.49902800
O	-2.80196500	-2.42511000	-1.91735200
C	-3.32487300	-2.79376900	-0.64267300
O	-1.86098200	-1.24729100	0.54635200
C	-1.56872100	-0.06183300	0.11108100
H	1.48997700	-1.20441800	1.52962200
H	4.43469000	0.92066800	-1.50768000
C	4.37233900	-0.65491500	-0.17789900
O	5.55241500	-0.99671500	-0.40902200
N	3.82900100	0.44138900	-0.84831000
C	2.53750800	0.94153400	-0.70269700
O	2.22183000	1.94891300	-1.39982800
N	1.70769600	0.32840800	0.16402700
C	2.19869000	-0.74273300	0.84043500
C	3.46240600	-1.28596600	0.74174700
C	-3.29288400	-1.58210900	0.26558300
C	-3.88112500	-0.27049900	-0.30556900
C	-2.62426200	0.47611400	-0.79353600
H	-3.98782300	0.80743300	1.33047800
O	-4.61544300	0.46265700	0.66616600
H	-4.57545100	-0.47852400	-1.11960900
O	-1.97823000	1.07730400	1.70314500
H	-1.52031300	0.67775900	2.46536000
H	-1.59669700	2.01833700	1.59342200
O	0.03528200	3.45844000	-1.12231200
H	0.83024800	2.84945200	-1.18759900
H	0.34665700	4.32688900	-1.42266000
O	-0.99253800	3.47169800	1.36344100
H	-1.68216000	4.15395700	1.40334500
H	-0.59969400	3.52344400	0.44412100
C	3.91204500	-2.48188500	1.53682900
H	4.77402600	-2.24649700	2.17506600
H	3.10308600	-2.84142700	2.18221600
H	4.21844800	-3.31149600	0.88602000

E. Thymine product with constrained glycosidic bond (3.5 Å) and nucleophile distance (1.4 Å)

H	-1.47897000	0.88009800	-1.66759400
H	-3.44000400	1.94642600	-0.02684200

H	-3.88833700	0.72233700	-1.24344400
H	-2.25122600	-1.75923200	1.18338500
H	-4.16363400	-2.94459400	0.40235000
H	-2.82588900	-3.20764300	-0.74515400
H	-4.82855800	-2.66878500	-1.82574900
O	-4.33945100	-1.93673500	-1.41887800
C	-3.53407200	-2.46216700	-0.35889900
O	-1.75192700	-0.82806800	-0.61032200
C	-1.81969900	0.59412200	-0.66748500
H	0.54440300	-1.47209300	0.07080300
H	4.85519400	0.51200200	-0.10048900
C	3.95278600	-1.34128900	0.14053400
O	5.03010600	-1.94242500	0.24590400
N	3.95127600	0.04971400	-0.04726500
C	2.82788300	0.80812400	-0.17038600
O	3.07324100	2.09321500	-0.33869800
N	1.62327800	0.28560600	-0.11910400
C	1.55779000	-1.07893200	0.05113100
C	2.62726900	-1.92278300	0.18331500
C	-2.75704900	-1.33762800	0.30609100
C	-3.59940300	-0.11111400	0.73818000
C	-3.27922000	0.91691500	-0.35652100
H	-2.32146900	0.68488800	1.99057600
O	-3.23700600	0.35345100	2.04619700
H	-4.66221800	-0.34989100	0.79727800
O	-1.00969800	1.17719400	0.31431200
H	-0.05363800	0.95687600	0.13404700
H	-1.04901300	2.95076100	0.66782800
O	1.22965600	3.82559400	-0.99628100
H	2.25612000	2.65960100	-0.54016900
H	1.70373700	4.66981300	-1.07019100
O	-0.80866600	3.89952200	0.79663500
H	-1.58198400	4.41471300	0.51597100
H	0.49423100	3.97342300	-0.34266100
C	2.49051800	-3.40802000	0.36805200
H	2.94723700	-3.73448300	1.31050600
H	1.43671100	-3.70249000	0.37648900
H	2.99456100	-3.95631000	-0.43736800

F. Thymine concerted transition state with constrained glycosidic bond (2.7 Å) and nucleophile distance (2.2 Å)

H	-1.05589400	0.70333800	1.10534200
H	-2.24431400	0.65124600	-1.31619900
H	-0.73891200	-0.28204900	-1.41440800
H	-2.82282700	-2.78022000	0.75413700
H	-1.40973400	-4.23805800	-0.52136300
H	-0.51062400	-3.70835200	0.92094100
H	0.79371100	-3.47428100	-0.99542600
O	0.08649300	-2.82089700	-0.87700100
C	-0.92332400	-3.37782600	-0.04066900
O	-1.45475700	-1.27656600	1.12132900
C	-1.43896800	-0.13069400	0.54257700
H	1.64969600	-0.99768000	1.77041600
H	3.24779200	1.97765100	-1.55118000
C	3.88608100	0.42092200	-0.35681300
O	5.04888100	0.44526900	-0.81374500
N	2.93709800	1.32293400	-0.83967100
C	1.61037000	1.42266100	-0.42923900
O	0.89179700	2.30995100	-0.97326300
N	1.16928300	0.56658200	0.51367100
C	2.05994300	-0.32910000	1.01245100
C	3.38448300	-0.46946000	0.65804300

C	-1.99367500	-2.33566600	0.20093900
C	-2.49138000	-1.54139800	-1.03044000
C	-1.71295200	-0.21333500	-0.91627600
H	-4.11424700	-0.73035900	-0.30115400
O	-3.89880100	-1.35853800	-1.02157500
H	-2.25427600	-2.07247400	-1.95221300
O	-3.48088500	0.53580600	1.01835900
H	-3.64867500	0.42318000	1.96988500
H	-3.55760500	1.52066500	0.82744700
O	-0.95293700	3.91220000	0.14979600
H	-0.29024900	3.25938400	-0.21324900
H	-0.57790100	4.23660400	0.98350700
O	-3.53348900	3.13772000	0.45697500
H	-4.00682800	3.34334000	-0.36489900
H	-2.59018600	3.42518800	0.31385800
C	4.30208600	-1.49183100	1.27204500
H	5.16454400	-1.02162300	1.76270600
H	3.77006800	-2.08633800	2.02284000
H	4.70539100	-2.18097900	0.51830100

Table S3. Cartesian coordinates for the optimized constrained stationary points on the thymine glycol potential energy surface.

A. Thymine glycol reactant with constrained glycosidic bond (1.5 Å) and nucleophile distance (3.4 Å)

H	1.29497400	-0.53128100	0.82036800
H	2.02641000	-0.23221300	-1.45580100
H	0.64048500	0.81126900	-1.82529900
H	2.08811700	2.86618700	1.16826200
H	1.13341700	4.48728600	-0.28255100
H	-0.13430600	3.92216500	0.83644200
H	-0.74847100	4.05635000	-1.48383400
O	-0.31492400	3.25989100	-1.13714200
C	0.50196900	3.63346100	-0.00898000
O	0.64341700	1.40988300	1.01322100
C	0.72244800	0.21097800	0.26027600
H	-1.58832200	1.32689100	0.90364800
H	-2.12200000	-3.02764700	-0.94601200
C	-3.25895300	-1.48660800	-0.19371600
O	-4.33706200	-1.97515300	-0.49570100
N	-2.07032700	-2.11160900	-0.50888700
C	-0.77407800	-1.62247700	-0.31391900
O	0.18632100	-2.36559500	-0.55024400
N	-0.66461300	-0.34569400	0.13308600
C	-1.81756900	0.55044700	0.17464200
C	-3.09268400	-0.19360300	0.62858600
C	1.40718500	2.48070500	0.40155300
C	2.22142300	1.83114400	-0.74196600
C	1.39844200	0.57514800	-1.07368800
H	3.60006900	0.91510100	0.37991800
O	3.56730300	1.55891600	-0.36905300
H	2.28816300	2.50028400	-1.60249800
O	3.75922400	-0.28006200	1.70833300
H	4.37132600	0.02093900	2.39850600
H	4.14546700	-1.12087100	1.34935300
O	2.75209300	-3.25907100	-1.23053700
H	1.87087900	-2.91490000	-0.96991100
H	2.63111300	-4.21358500	-1.35743500
O	4.69066200	-2.62123600	0.61221900
H	5.51375300	-2.48170100	0.11742300
H	4.01304400	-2.87967300	-0.06348200
C	-3.03736000	-0.57184600	2.11507500
H	-2.92465900	0.33809900	2.71254100
H	-3.97075800	-1.06644400	2.39956700
H	-2.20300900	-1.24347600	2.33427500
O	-4.20436000	0.66051100	0.44899700
H	-4.07051500	1.12172600	-0.40124000
O	-2.09380500	1.13283600	-1.08913700
H	-1.52649700	1.93514700	-1.17644500

B. Thymine Glycol concerted transition state with constrained glycosidic bond (3.1 Å) and nucleophile distance (2.0 Å)

H	-1.06147000	0.76323100	0.43660100
H	-3.00838400	0.75807400	-1.51131000
H	-1.77902000	-0.49873500	-1.75151700
H	-3.61428300	-2.18035700	1.24957600
H	-2.78694300	-3.99161200	-0.20197700
H	-1.59382400	-3.57181600	1.05277600
H	-0.81374900	-3.73017600	-1.27293600
O	-1.12863400	-2.90468200	-0.87049200

C	-2.09327000	-3.21643300	0.14359000
O	-1.95394200	-0.95440500	1.00792600
C	-1.90145200	0.09605800	0.24649400
H	1.24494600	-1.09562000	1.38053600
H	3.56985300	1.65966300	-1.70183000
C	3.88921100	0.00992100	-0.53668800
O	4.99604800	-0.27187300	-0.99774800
N	3.15066200	1.05850500	-0.99864300
C	1.84048500	1.43217100	-0.54386200
O	1.46449200	2.57013800	-0.96180900
N	1.15353400	0.62218300	0.23062800
C	1.70229900	-0.68693600	0.47121600
C	3.23902300	-0.73157800	0.65062200
C	-2.89782500	-1.97004200	0.45339100
C	-3.56876300	-1.25022000	-0.74075300
C	-2.55993100	-0.13397800	-1.07180000
H	-4.74346300	0.00515300	0.20450000
O	-4.85584900	-0.74544500	-0.41006200
H	-3.71441900	-1.93492600	-1.57656400
O	-3.31560700	1.26336800	1.04496300
H	-3.17487500	1.26179700	2.00963900
H	-3.18736100	2.22787400	0.73376100
O	-0.32253900	4.25885000	0.06188100
H	0.30776200	3.55586000	-0.27747600
H	0.03217800	4.54542200	0.91803800
O	-2.94753500	3.71817600	0.24886000
H	-3.35596600	3.90669700	-0.61143500
H	-1.97053900	3.90727200	0.14636000
C	3.68451900	-0.05842300	1.95381900
H	3.21116700	-0.56380500	2.80248800
H	4.77116800	-0.13974900	2.06002500
H	3.40673000	0.99891000	1.97601100
O	3.67728300	-2.08337300	0.70264100
H	3.12735400	-2.56067900	0.05160000
O	1.44503600	-1.61082200	-0.61764200
H	0.52796500	-1.94998600	-0.56508700

C. Thymine Glycol product with constrained glycosidic bond (3.5 Å) and nucleophile distance (1.4 Å)

H	-1.19062400	0.87052500	0.34939900
H	-3.14465800	0.79638200	-1.62196700
H	-1.81329700	-0.38557300	-1.65383700
H	-3.75221600	-2.01938800	1.25498700
H	-2.91688600	-3.87567700	-0.05769500
H	-1.72689100	-3.42091100	1.18997600
H	-0.84760600	-3.73567400	-1.01950700
O	-1.22452500	-2.87905500	-0.76182100
C	-2.21223400	-3.09761500	0.26059500
O	-2.06318700	-0.81590700	1.04279400
C	-2.17564300	0.39783800	0.31563000
H	1.04376500	-1.00883500	1.30482800
H	3.88328100	1.57143600	-1.51695100
C	3.85598300	-0.25666900	-0.56131900
O	4.86650800	-0.69673200	-1.09327400
N	3.35570200	0.98673500	-0.87483400
C	2.15703600	1.48096200	-0.35303900
O	2.02049600	2.77397300	-0.63815400
N	1.30170400	0.79537200	0.31105500
C	1.56520000	-0.63303800	0.41942000
C	3.07046600	-0.98231300	0.55377700
C	-2.97785900	-1.80957300	0.50772900
C	-3.62620900	-1.16301900	-0.74342500

C	-2.66065900	-0.01440000	-1.07133200
H	-4.89222600	0.03744700	0.15413400
O	-4.95731400	-0.70141800	-0.47818400
H	-3.72505200	-1.87783100	-1.56185900
O	-3.14873600	1.22820400	0.88447300
H	-2.95655800	1.33730700	1.83316000
H	-2.96502500	2.95732100	0.23198900
O	0.00256800	4.21620800	0.30212400
H	1.17406600	3.15990600	-0.25698000
H	0.10265200	4.39949800	1.24991600
O	-2.70775700	3.87102800	-0.02596300
H	-3.00923500	3.98358800	-0.94181500
H	-0.96621500	4.05907500	0.15900300
C	3.64342700	-0.55220800	1.91016000
H	3.09061200	-1.05720200	2.70904000
H	4.69692200	-0.84156300	1.97528400
H	3.56611300	0.52830100	2.05995700
O	3.24084900	-2.38435500	0.44651800
H	2.63457400	-2.67301700	-0.26304600
O	1.10241100	-1.33109000	-0.73879400
H	0.22512700	-1.74653100	-0.57847400

Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics

Full citations for References 84 and 86

Frisch, M. J. T., G. W.; Schlegel, H. B. Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J.; Revisions A.02, C.01 and D.01; Gaussian, Inc.: Wallingford CT, 2009.

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, J., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; Pople, J. A.; Revision D.02 ed.; Gaussian, Inc.: Wallingford CT, 2004.