

Electronic Supplementary Information

Formation of pyrimidine-pyrimidine type DNA intrastrand cross-links:

a theoretical verification

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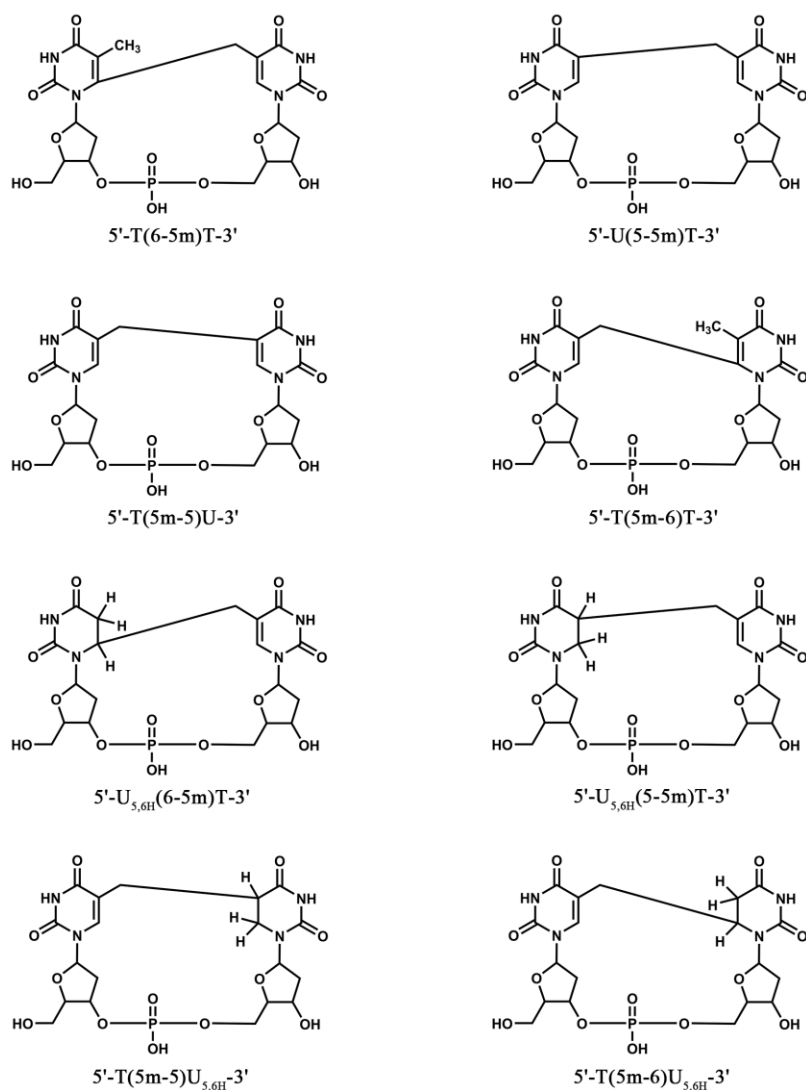


Figure S1 Prototype structures of the eight related closed-shell intrastrand cross-links.

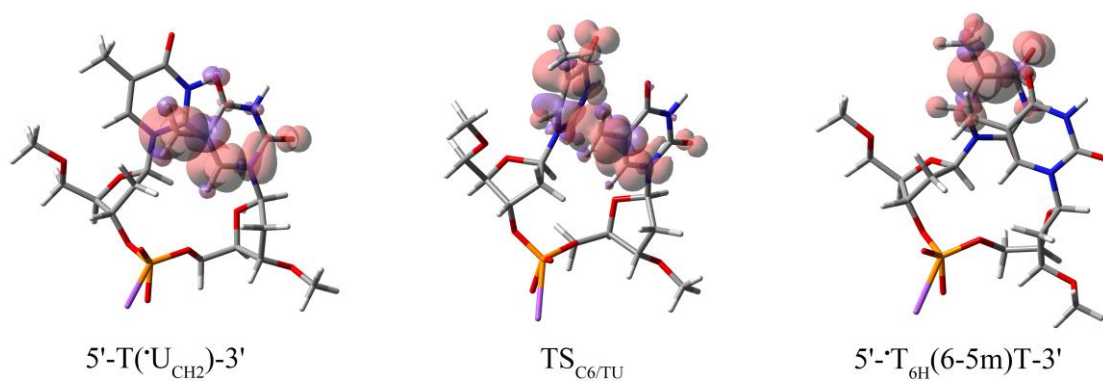


Figure S2 Spin density distributions of related stationary points along the reaction path of $\cdot U_{CH_2}$ radical addition to the C₆ site of its 5' neighboring thymidine.

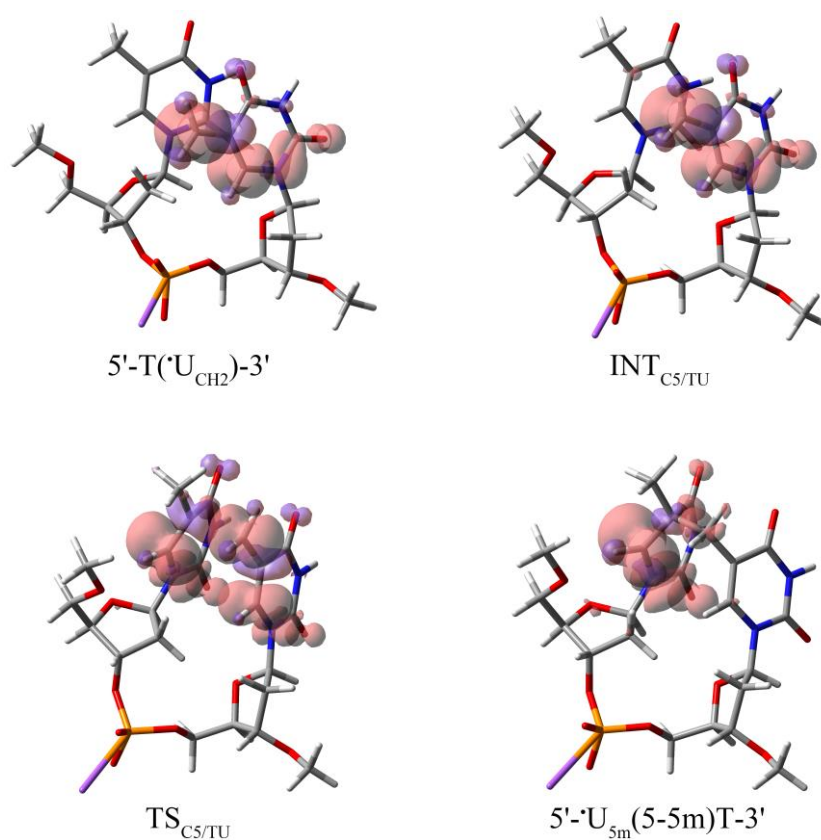


Figure S3 Spin density distributions of related stationary points along the reaction path of $\cdot U_{CH_2}$ radical addition to the C₅ site of its 5' neighboring thymidine.

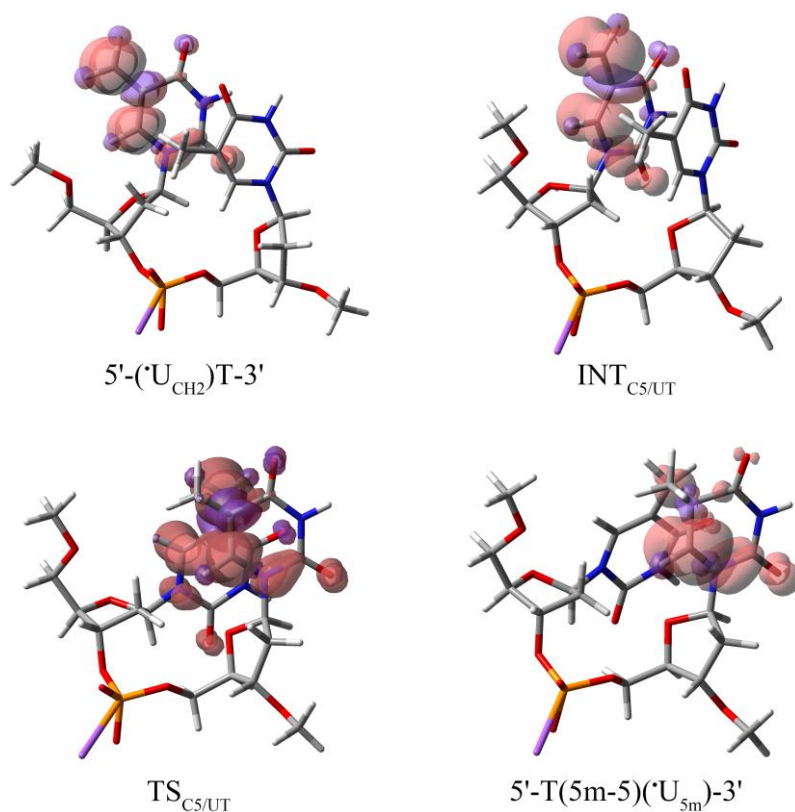


Figure S4 Spin density distributions of related stationary points along the reaction path of U_{CH_2} radical addition to the C_5 site of its 3' neighboring thymidine.

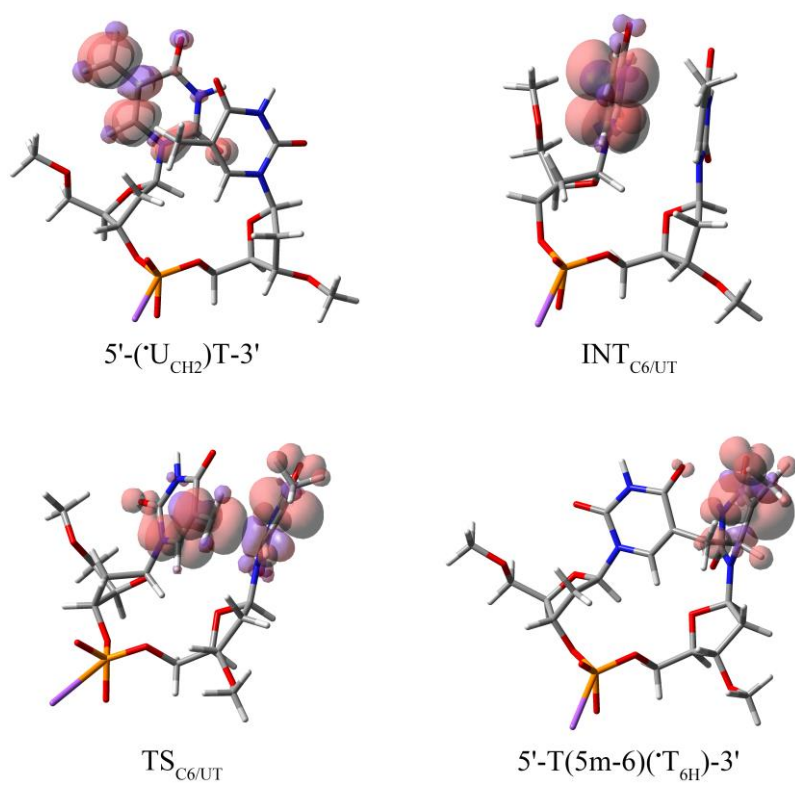


Figure S5 Spin density distributions of related stationary points along the reaction path of U_{CH_2} radical addition to the C_6 site of its 3' neighboring thymidine.

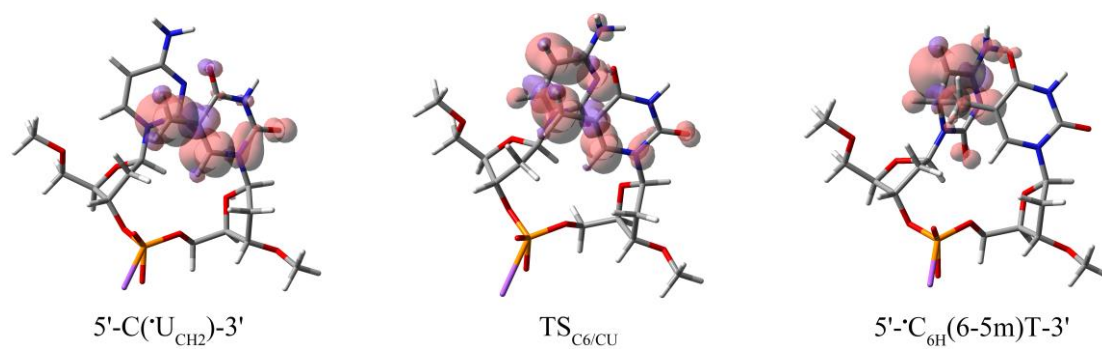


Figure S6 Spin density distributions of related stationary points along the reaction path of U_{CH_2} radical addition to the C_6 site of its 5' neighboring deoxycytidine.

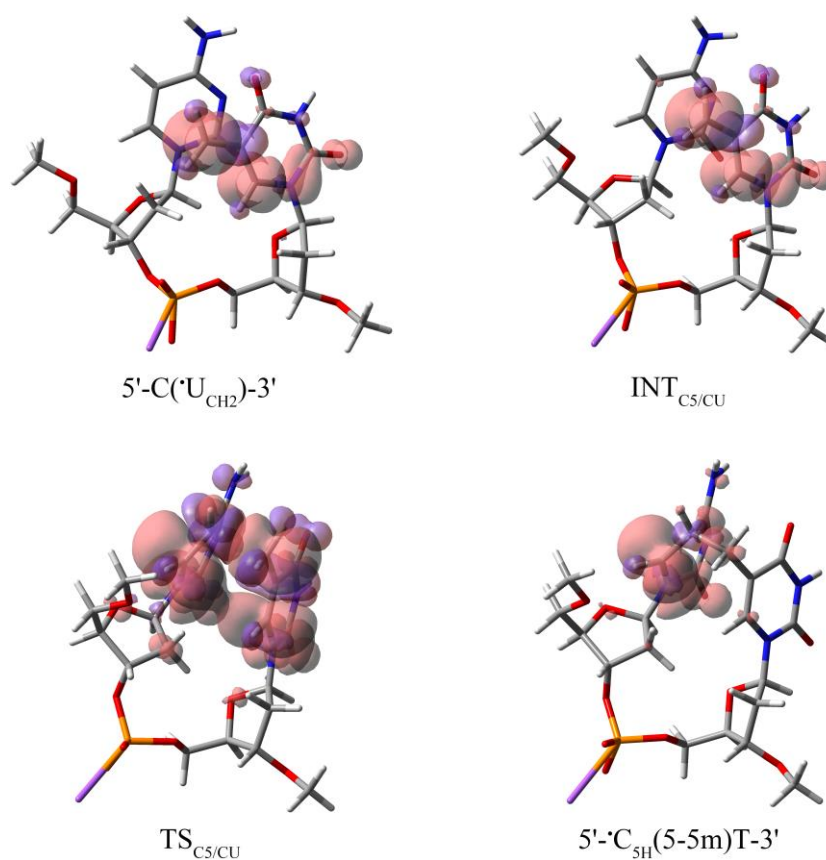


Figure S7 Spin density distributions of related stationary points along the reaction path of U_{CH_2} radical addition to the C_5 site of its 5' neighboring deoxycytidine.

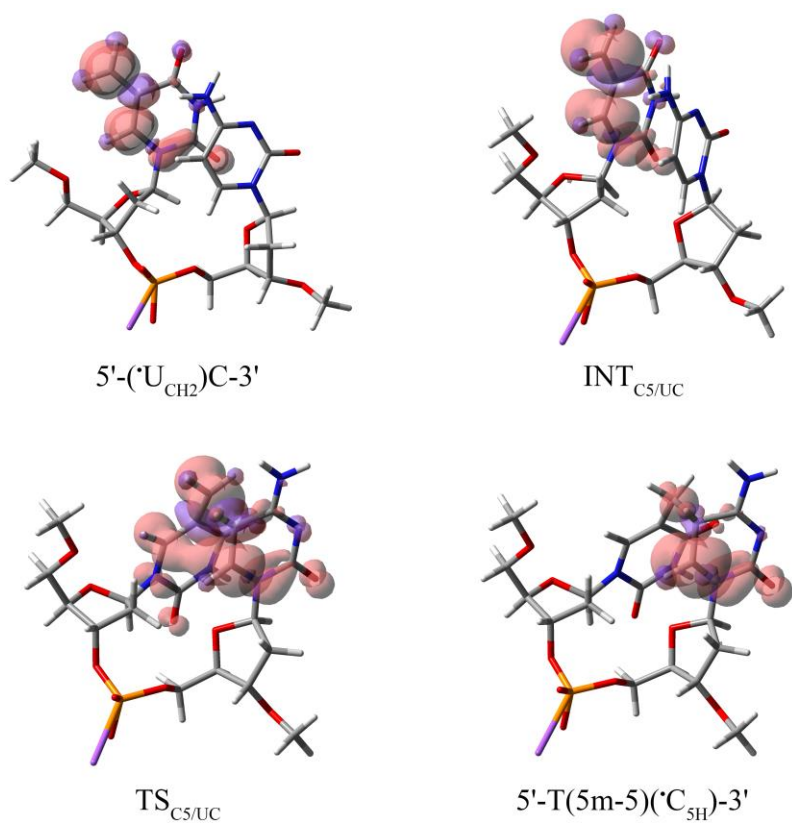


Figure S8 Spin density distributions of related stationary points along the reaction path of $\bullet$ U_{CH2} radical addition to the C₅ site of its 3' neighboring deoxycytidine.

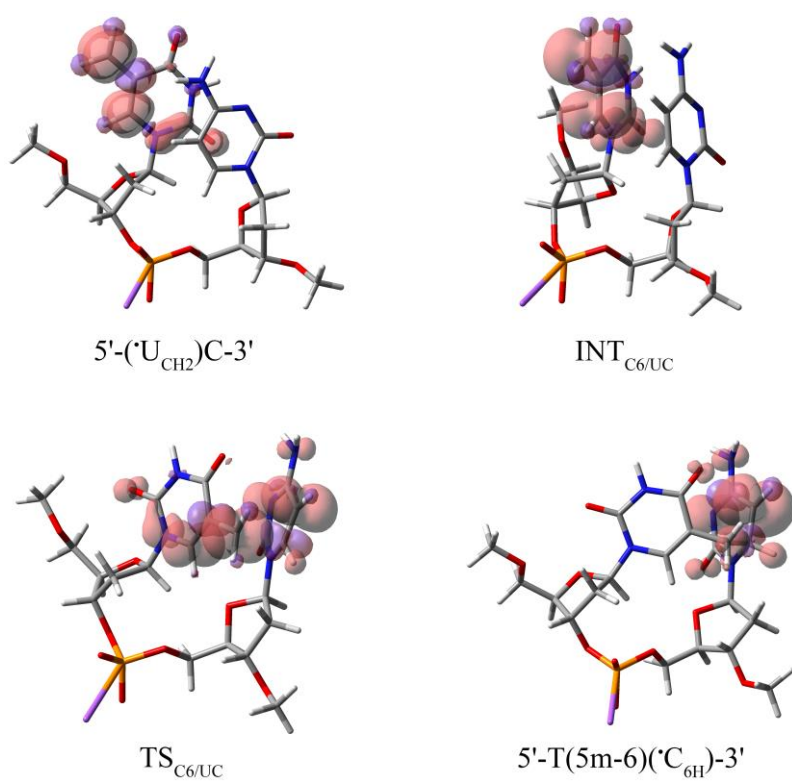


Figure S9 Spin density distributions of related stationary points along the reaction path of $\bullet$ U_{CH2} radical addition to the C₆ site of its 3' neighboring deoxycytidine.

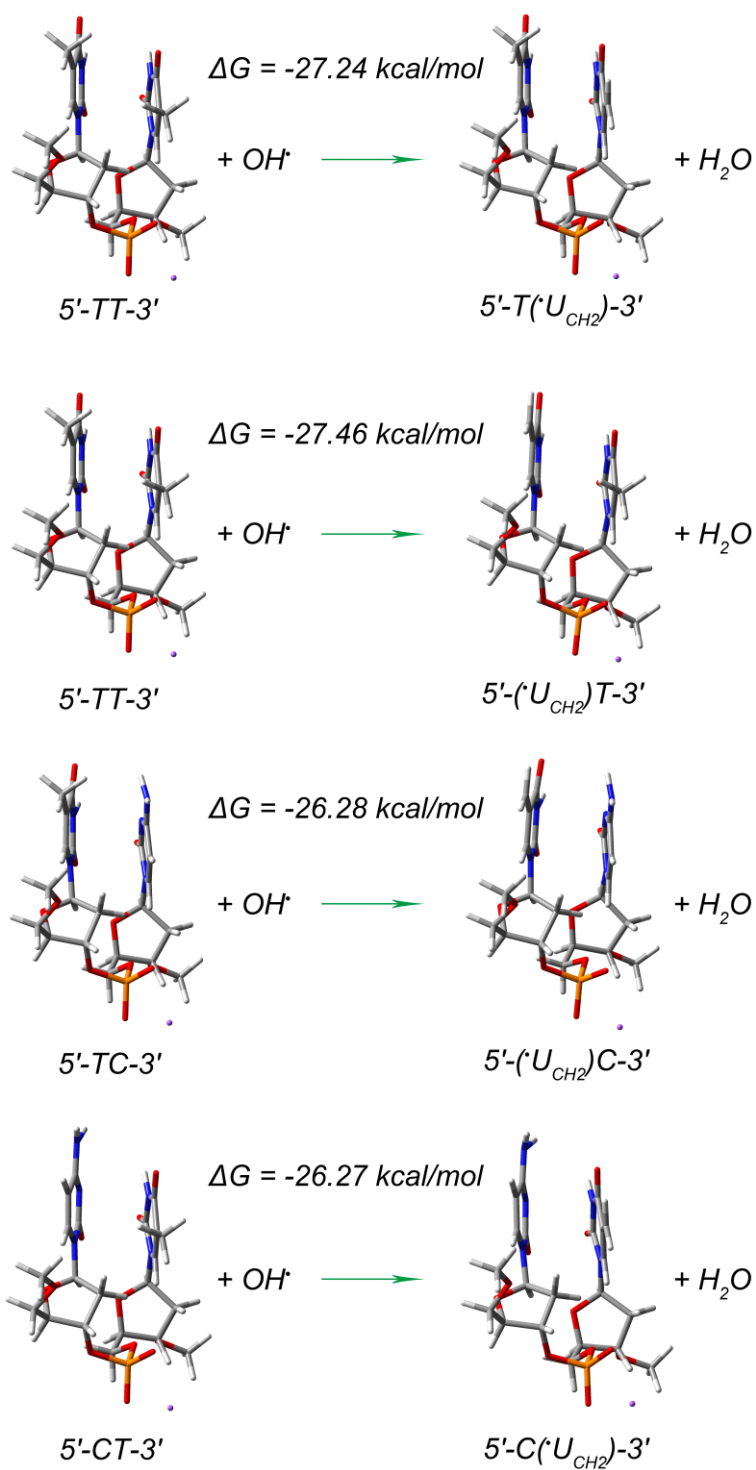


Figure S10 Reaction free energies calculated for $\text{OH}^\bullet$ radical reacting with the canonical 5'-TT-3', 5'-TC-3', and 5'-CT-3' sequences forming the 5'-T(U_{CH_2})-3', 5'-(U_{CH_2})T-3', 5'-(U_{CH_2})C-3', and 5'-C(U_{CH_2})-3' sequences, respectively.

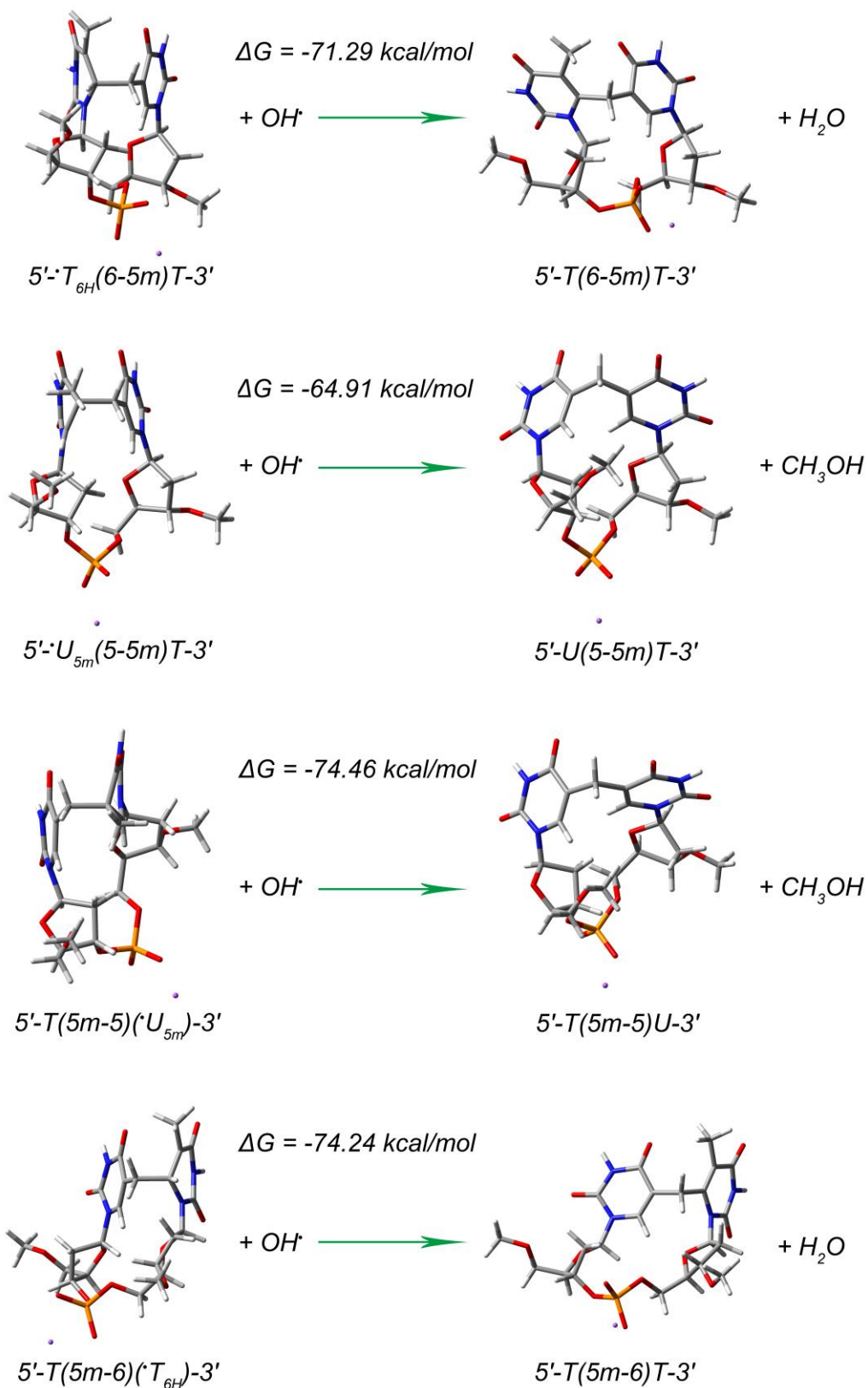


Figure S11 Reaction free energies calculated for formation of the closed-shell 5'-T(6-5m)T-3', 5'-U(5-5m)T-3', 5'-T(5m-5)U-3', and 5'-T(5m-6)T-3 intrastrand cross-links starting from the $\cdot\text{U}_{\text{CH}_2}$ radical adducts, 5'- $\cdot\text{T}_{6\text{H}}(6\text{-}5\text{m})\text{T-}3'$, 5'- $\cdot\text{U}_{5\text{m}}(5\text{-}5\text{m})\text{T-}3'$, 5'-T(5m-5)($\cdot\text{U}_{5\text{m}}\text{)-}3'$, and 5'-T(5m-6)($\cdot\text{T}_{6\text{H}}\text{)-}3'$, respectively.

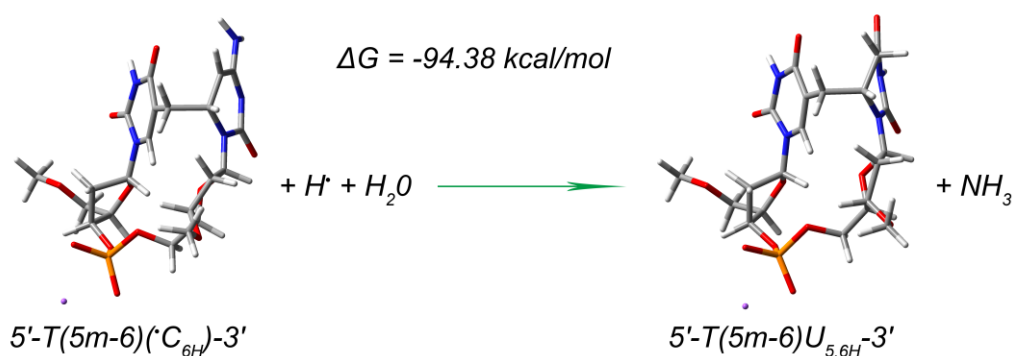
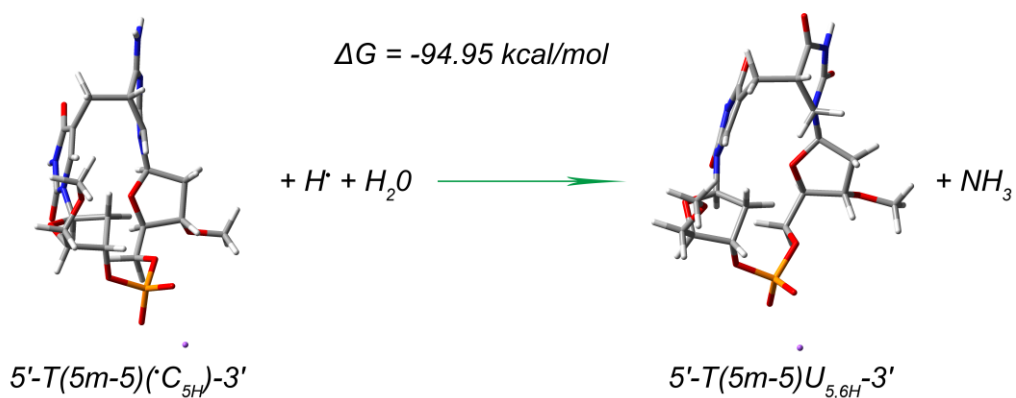
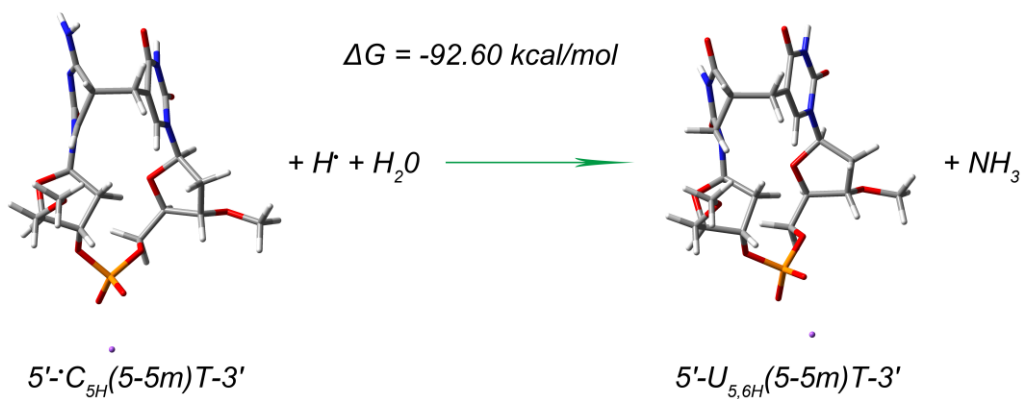
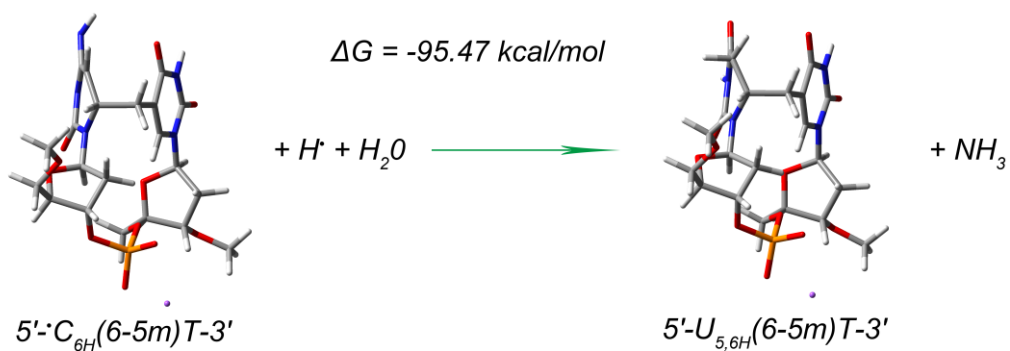


Figure S12 Reaction free energies calculated for formation of the closed-shell 5'-U_{5,6H}(6-5m)T-3', 5'-U_{5,6H}(5-5m)T-3', 5'-T(5m-5)U_{5,6H}-3', and 5'-T(5m-6)U_{5,6H}-3' intrastrand cross-links starting from the •U_{CH2} radical adducts, 5'-•C_{6H}(6-5m)T-3', 5'-•C_{5H}(5-5m)T-3', 5'-T(5m-5)(•C_{5H})-3', and 5'-T(5m-6)(•C_{6H})-3, respectively.

Table S1 Cartesian coordinates of stationary points along the reaction paths of $\cdot\text{U}_{\text{CH}_2}$ radical addition to the C₅ and C₆ sites of its 5' neighboring thymidine starting from the canonical 5'-T($\cdot\text{U}_{\text{CH}_2}$)-3' sequence, respectively.

	5'-T($\cdot\text{U}_{\text{CH}_2}$)-3'		
O	-0.04611600	-0.05144900	0.10808100
C	0.03129800	-0.02822300	1.51688700
C	1.48983100	-0.00921800	1.93155700
O	2.08909600	-1.28759800	1.69070400
C	2.32490000	1.01405800	1.15182600
O	3.28286900	1.55851600	2.06365800
C	2.96267300	0.16432700	0.06105000
C	3.12758300	-1.20052200	0.72937100
N	2.99669500	-2.32691100	-0.19472700
C	4.01611400	-3.25779700	-0.28777900
O	5.04113700	-3.22709400	0.37385800
N	3.78456400	-4.24593100	-1.22306700
C	2.68449900	-4.40011700	-2.06541100
O	2.63876600	-5.32448500	-2.86084700
C	1.63943200	-3.40223400	-1.86928300
C	0.39287200	-3.52241200	-2.69038700
C	1.84272500	-2.44107000	-0.94756300
P	4.42731100	2.58842400	1.51396300
O	4.70399200	3.58855800	2.60142500
O	4.07302300	3.12032300	0.15452500
O	5.70129200	1.57897100	1.33588700
C	6.16200400	0.95338300	2.53621600
C	7.37477600	0.11248000	2.21806100
O	6.98482800	-0.93465900	1.33086700
C	8.51969500	0.87986400	1.53121800
O	9.72717500	0.42215000	2.10784300
C	8.38730700	0.45287300	0.07059900
C	7.87229300	-0.97530600	0.22757400
N	7.15065500	-1.50082700	-0.92129500
C	7.44916000	-2.78548100	-1.34571100
O	8.34129700	-3.46999900	-0.88011700
N	6.66272300	-3.23479100	-2.39207800
C	5.60561900	-2.59317800	-3.01669600
O	5.01378300	-3.12530100	-3.93823300
C	5.28063700	-1.26148900	-2.45560100
C	4.20392300	-0.57369600	-3.01033300
C	6.07026000	-0.80463000	-1.41156300
H	-0.47134800	0.86804300	1.91100000
H	-0.45740500	-0.91445900	1.94729100
H	1.54985000	0.20629000	3.00329800
H	1.71349800	1.82100600	0.74035800
H	3.90702700	0.57999000	-0.28321500
H	2.27376500	0.09872500	-0.78367400
H	4.10989500	-1.31379000	1.19726700
H	-0.32246900	-2.74096000	-2.42753700
H	0.62384500	-3.44040400	-3.75656400
H	-0.07943300	-4.49688600	-2.53705800
H	1.08826800	-1.69161500	-0.72093300
H	6.42134800	1.71636500	3.27852400
H	5.36931600	0.31548100	2.94441200
H	7.75986400	-0.31506500	3.15167500
H	8.42052200	1.96582500	1.66389400
H	9.32800100	0.49581500	-0.48021300

H	7.64963600	1.08432100	-0.42957100
H	8.69218500	-1.67151700	0.41512300
H	3.94210100	0.42342500	-2.68272800
H	3.64232600	-1.03087600	-3.81324600
H	5.88080400	0.14384700	-0.92199200
H	4.52273000	-4.93540800	-1.30952200
H	6.91016500	-4.15144100	-2.74790900
C	10.84033200	1.22880400	1.78105100
H	11.70342100	0.81203300	2.30145600
H	11.04614000	1.23298900	0.70357500
H	10.68397000	2.26437600	2.11089300
Na	4.22280800	5.33493600	1.03686400
C	-1.37900700	-0.12391300	-0.35739500
H	-1.34327100	-0.13170600	-1.44751200
H	-1.87035000	-1.03920700	-0.00287500
H	-1.96050000	0.74358300	-0.02035300

TS_{C6/TU}

O	-0.08876500	-0.21358100	0.25365200
C	0.03743900	-0.09631000	1.65314200
C	1.50376000	0.03952000	2.02160900
O	2.20415200	-1.15680100	1.67376300
C	2.23787800	1.16806200	1.29163700
O	3.29812800	1.59385500	2.15563200
C	2.75545900	0.45663000	0.04979600
C	3.13179300	-0.90784000	0.62235600
N	3.11277200	-2.02643500	-0.30772200
C	3.99913500	-3.06014700	-0.04572200
O	4.78081300	-3.06194900	0.88804200
N	3.93705800	-4.11191400	-0.94081500
C	2.92915500	-4.37116500	-1.87834000
O	2.89633300	-5.44818500	-2.46053000
C	1.99416600	-3.28610200	-2.05671000
C	0.95583100	-3.41574700	-3.12051300
C	2.20450600	-2.09674800	-1.36854600
P	4.44322900	2.61109600	1.58885300
O	4.98518700	3.37750200	2.76249300
O	3.93267300	3.39882100	0.41569400
O	5.57156600	1.56886200	1.02157400
C	6.31464800	0.84029400	2.00104100
C	7.45813600	0.12612200	1.32068900
O	6.93229900	-0.88991400	0.46575000
C	8.34440400	1.03400000	0.44300300
O	9.68744800	0.68974500	0.72055300
C	7.93855500	0.63536200	-0.97615300
C	7.60901000	-0.84051800	-0.77505700
N	6.73070100	-1.42280100	-1.78190000
C	7.16913900	-2.52692900	-2.50158700
O	8.27210700	-3.02442100	-2.37328700
N	6.24054000	-3.01518600	-3.39963600
C	4.94493400	-2.56717900	-3.62822200
O	4.22079600	-3.13691900	-4.42643600
C	4.55605300	-1.39746600	-2.82852600
C	3.20426600	-0.94831500	-2.91454800
C	5.46469200	-0.91215500	-1.92946700
H	-0.51844200	0.78036000	2.02004100
H	-0.36957100	-0.99002800	2.14901300

H	1. 57864600	0. 19219600	3. 10365600
H	1. 59279500	2. 01807100	1. 05436200
H	3. 59222700	0. 98023600	-0. 41101800
H	1. 92772900	0. 39569600	-0. 65403000
H	4. 14776500	-0. 88450100	1. 02674500
H	0. 25021500	-2. 58272200	-3. 08762500
H	1. 43313100	-3. 43406900	-4. 10799600
H	0. 40401300	-4. 35290300	-3. 00981500
H	1. 39243000	-1. 37926400	-1. 30138100
H	6. 70852600	1. 52910900	2. 75527500
H	5. 66269000	0. 10804500	2. 49380700
H	8. 09356200	-0. 33079300	2. 08915800
H	8. 17019900	2. 09850900	0. 64925100
H	8. 72517500	0. 79565300	-1. 71493200
H	7. 04217900	1. 18614700	-1. 27565900
H	8. 51239400	-1. 45439700	-0. 76259000
H	2. 97136400	0. 03740200	-2. 52821100
H	2. 63554400	-1. 26712700	-3. 78118100
H	5. 23746400	-0. 09041300	-1. 25716500
H	4. 57064700	-4. 87670700	-0. 73960400
H	6. 54122600	-3. 82599400	-3. 92901400
C	10. 61717600	1. 62532200	0. 21338100
H	11. 61049200	1. 28056100	0. 50270800
H	10. 57303500	1. 70048200	-0. 88005900
H	10. 44179400	2. 62180700	0. 63953600
Na	4. 49130100	5. 39434100	1. 59867600
C	-1. 42796700	-0. 41268600	-0. 14827100
H	-1. 43150200	-0. 51116500	-1. 23479600
H	-1. 84244600	-1. 32559700	0. 29889900
H	-2. 05821800	0. 43838000	0. 14039500

5'-*T_{6H}(6-5m)T-3'

O	-0. 06999000	0. 09472100	0. 05682400
C	-0. 03058000	0. 01761700	1. 46303500
C	1. 41407000	-0. 01552000	1. 92330700
O	2. 02373500	-1. 22932500	1. 47527700
C	2. 27620200	1. 12311800	1. 35247700
O	3. 26696100	1. 43265800	2. 34495100
C	2. 88969500	0. 46014200	0. 12882800
C	3. 19126300	-0. 91417400	0. 71217600
N	3. 47402100	-1. 98147300	-0. 21158100
C	4. 35740600	-2. 94107300	0. 21640400
O	4. 95165500	-2. 90119100	1. 28177000
N	4. 55532800	-4. 00742800	-0. 65464400
C	3. 70939800	-4. 38985100	-1. 69343900
O	3. 81747100	-5. 49543100	-2. 21155700
C	2. 74376200	-3. 39002200	-2. 08814700
C	1. 84092600	-3. 67713300	-3. 23057800
C	2. 83559900	-2. 00884300	-1. 52698500
P	4. 57014000	2. 33247800	1. 94820000
O	5. 11322000	2. 92192800	3. 21913500
O	4. 24896800	3. 27500300	0. 82207600
O	5. 61599800	1. 21625000	1. 35539100
C	6. 39728200	0. 44825700	2. 27562300
C	7. 71639800	0. 08630100	1. 62732700
O	7. 49994700	-0. 89817400	0. 61260300
C	8. 42283100	1. 27080700	0. 94547200

O	9.80631300	1.13264000	1.20146100
C	8.09374100	1.05157100	-0.53200700
C	8.07908200	-0.47274400	-0.60571200
N	7.27346800	-1.03571000	-1.68473400
C	7.85951700	-1.92139600	-2.57849700
O	9.04730900	-2.18644200	-2.58979400
N	6.96987400	-2.47909000	-3.47415100
C	5.59092000	-2.29955100	-3.54375300
O	4.92542200	-2.92045900	-4.35967200
C	5.06229100	-1.34431700	-2.57699000
C	3.58802200	-1.08367100	-2.54284600
C	5.91974300	-0.79274700	-1.69182500
H	-0.53888800	0.88440700	1.91389700
H	-0.53877200	-0.89365900	1.81303300
H	1.43710500	0.02716200	3.01849100
H	1.69944500	2.02102800	1.11737500
H	3.76384400	0.99029300	-0.24713000
H	2.11599500	0.40561500	-0.63860600
H	4.05446600	-0.84820400	1.37702400
H	0.93798100	-3.06342200	-3.19066800
H	2.36310100	-3.46205900	-4.17274400
H	1.57139700	-4.73482100	-3.24210500
H	1.81829500	-1.61712700	-1.39940500
H	6.58387500	1.03495300	3.17989100
H	5.86076000	-0.47084200	2.53857400
H	8.38290500	-0.32780000	2.39260300
H	8.05474700	2.23473700	1.32307000
H	8.82308800	1.49459900	-1.21151300
H	7.10182100	1.45682500	-0.75066200
H	9.08407700	-0.88061300	-0.73288200
H	3.40332700	-0.04172600	-2.28176200
H	3.16394900	-1.25103700	-3.53659900
H	5.58668000	-0.12707300	-0.89848100
H	5.18895800	-4.71715900	-0.30765700
H	7.37591200	-3.13737300	-4.12957200
C	10.55149400	2.28745800	0.87312400
H	11.58913700	2.08807400	1.14310500
H	10.50415800	2.52007500	-0.19783100
H	10.19217800	3.15895800	1.43631400
Na	5.05260000	5.07333500	2.17888900
C	-1.39156900	0.10499300	-0.43855800
H	-1.33314600	0.16128700	-1.52616600
H	-1.92891800	-0.80872300	-0.15185300
H	-1.95016000	0.97194600	-0.06105900

INT_{CS/TU}

O	-0.12487700	-0.19465500	0.22063500
C	0.03257500	-0.15174000	1.62271400
C	1.50649400	-0.00404500	1.94432200
O	2.19197900	-1.23360400	1.69025100
C	2.19680600	1.07009200	1.09459900
O	3.11436900	1.76574500	1.94320800
C	2.90759300	0.26098600	0.01252600
C	3.17785600	-1.08678200	0.68465300
N	3.06531500	-2.23234400	-0.22261300
C	4.17124600	-3.02624700	-0.46243700
O	5.28420600	-2.81281800	-0.00839700

N	3. 91399800	-4. 10440600	-1. 28575200
C	2. 71437900	-4. 45489300	-1. 90591900
O	2. 64767600	-5. 45484600	-2. 60226500
C	1. 61080600	-3. 54551000	-1. 62266900
C	0. 28718600	-3. 82877500	-2. 26274400
C	1. 83826700	-2. 50612200	-0. 79520100
P	3. 86157100	3. 09578700	1. 35742500
O	4. 22048000	3. 96289500	2. 53150300
O	3. 06250700	3. 71866600	0. 24789100
O	5. 20847100	2. 45952700	0. 68883400
C	6. 10740300	1. 81400300	1. 58885800
C	7. 17021900	1. 10588300	0. 78848600
O	6. 56425300	0. 03903300	0. 06142500
C	7. 90560700	1. 99540900	-0. 24331300
O	9. 28904400	1. 87753600	0. 02174800
C	7. 51902400	1. 36274100	-1. 58330500
C	7. 28331400	-0. 08191100	-1. 15374700
N	6. 51757600	-0. 90551700	-2. 06919600
C	7. 01733400	-2. 15688800	-2. 39747900
O	8. 10326600	-2. 57302600	-2. 04009000
N	6. 18568500	-2. 90240400	-3. 21493700
C	4. 91596400	-2. 58748100	-3. 67779600
O	4. 30678700	-3. 35917100	-4. 39434400
C	4. 40447400	-1. 27904400	-3. 21307000
C	3. 11363400	-0. 90891300	-3. 58186400
C	5. 25167700	-0. 51001200	-2. 43276300
H	-0. 52016600	0. 70249300	2. 04206200
H	-0. 35246800	-1. 07244500	2. 08464100
H	1. 61528800	0. 24189300	3. 00572400
H	1. 48471000	1. 78296400	0. 67425700
H	3. 83653200	0. 73728500	-0. 30128800
H	2. 24309500	0. 12992800	-0. 84606600
H	4. 18463300	-1. 13987200	1. 10595000
H	-0. 46538000	-3. 10982800	-1. 93339200
H	0. 36832900	-3. 77472600	-3. 35281200
H	-0. 05618600	-4. 83682200	-2. 01402200
H	1. 05308700	-1. 80844400	-0. 51436300
H	6. 57171500	2. 55436800	2. 24922700
H	5. 56429000	1. 08346300	2. 20049700
H	7. 92627700	0. 70673500	1. 47773600
H	7. 59312100	3. 04540300	-0. 17220200
H	8. 29475700	1. 45973900	-2. 34429800
H	6. 59238400	1. 80842400	-1. 95452600
H	8. 23403000	-0. 59792700	-0. 99577600
H	4. 95140400	0. 46514400	-2. 07359200
H	4. 71049500	-4. 70527400	-1. 46608200
H	6. 56547000	-3. 79619000	-3. 50701600
C	10. 06418400	2. 85699100	-0. 63884900
H	11. 10425100	2. 68877100	-0. 35709300
H	9. 97722500	2. 78395400	-1. 73008500
H	9. 76405200	3. 86747300	-0. 33177300
C	-1. 47165500	-0. 38601100	-0. 16410900
H	-1. 49974400	-0. 40617900	-1. 25432400
H	-1. 86258700	-1. 33413100	0. 22736400
H	-2. 10395600	0. 43386100	0. 19975700
H	2. 70088300	0. 04767400	-3. 28763200
H	2. 52035100	-1. 57538000	-4. 19252700
Na	3. 11989400	5. 77653900	1. 44470600

TS _{C5/TU}			
O	-0.00905900	-0.02586400	0.03618700
C	0.01131000	-0.02046500	1.44717100
C	1.45360600	-0.00848500	1.91642800
O	2.05131500	-1.28816400	1.69414600
C	2.31628900	1.01494600	1.16655900
O	3.22456900	1.59870400	2.10549400
C	3.04345700	0.16758800	0.12714600
C	3.14684400	-1.20183100	0.80023100
N	3.04593000	-2.32607400	-0.13005200
C	4.04863900	-3.27368300	-0.17052100
O	5.11806000	-3.16742000	0.40908000
N	3.73824200	-4.39176000	-0.92959200
C	2.63439600	-4.58147700	-1.75496100
O	2.42603200	-5.65398900	-2.28939400
C	1.78907900	-3.37814100	-1.91018000
C	0.44931400	-3.59285200	-2.56890600
C	1.90164100	-2.43910700	-0.89574800
P	3.83782100	3.06814000	1.74704700
O	4.49194400	3.59144700	2.99367500
O	2.79963400	3.93196000	1.08616000
O	4.95323800	2.70651600	0.61206500
C	6.21447300	2.22124400	1.06973800
C	6.97013400	1.63037900	-0.09687600
O	6.46496100	0.32258600	-0.38098500
C	6.86375700	2.43872300	-1.41768400
O	8.18121500	2.70104800	-1.85549100
C	6.13117200	1.46416800	-2.35356700
C	6.65331700	0.15623000	-1.77881500
N	6.06746400	-1.09207900	-2.22201000
C	6.91806300	-2.19312900	-2.18064800
O	8.04097800	-2.15456800	-1.71460500
N	6.39960800	-3.33665400	-2.74966500
C	5.14990300	-3.51450800	-3.32398100
O	4.85598700	-4.57164900	-3.85313100
C	4.24921500	-2.35586700	-3.19568400
C	2.87731500	-2.55734600	-3.55574600
C	4.76465900	-1.20113400	-2.67216600
H	-0.50594600	0.87158200	1.83206600
H	-0.49521200	-0.91145600	1.84611300
H	1.47761600	0.20854700	2.98943300
H	1.70849800	1.80212800	0.71404300
H	4.02665000	0.56958400	-0.12563600
H	2.42516100	0.10026900	-0.77180300
H	4.09246400	-1.33064900	1.33122800
H	-0.05417200	-2.63627800	-2.72557100
H	0.56965100	-4.09056900	-3.53222300
H	-0.18825700	-4.22423200	-1.94368900
H	1.14410900	-1.68602100	-0.70710500
H	6.78567400	3.04776800	1.50354600
H	6.07847300	1.44788100	1.83502100
H	8.03436900	1.55976800	0.16433400
H	6.31390400	3.37686500	-1.27978200
H	6.37502600	1.61230000	-3.40663600
H	5.05191900	1.56061400	-2.20429300
H	7.72414100	0.07577500	-1.99190600

H	4.16464300	-0.30315400	-2.59278300
H	4.41669300	-5.14414400	-0.88898100
H	7.03019400	-4.13017900	-2.77327100
C	8.23989000	3.68532700	-2.86816200
H	9.29253700	3.83590200	-3.11021300
H	7.70849600	3.37458500	-3.77617100
H	7.80959600	4.63290600	-2.51874700
C	-1.32069000	-0.10111400	-0.48474600
H	-1.23987100	-0.09353600	-1.57244000
H	-1.81955800	-1.02476400	-0.16371100
H	-1.92232800	0.75739700	-0.16015700
H	2.24692400	-1.67913500	-3.66059300
H	2.68396300	-3.37105600	-4.24819600
Na	3.10197000	5.54517000	2.80627200

5'-*U_{5m}(5-5m)T-3'

O	0.02681900	0.02615700	-0.03335300
C	0.00684200	0.01225700	1.37690400
C	1.43431300	-0.01031500	1.88837300
O	2.01863300	-1.29149600	1.64538000
C	2.33595100	1.02116200	1.19625500
O	3.23271100	1.54973200	2.17933700
C	3.07365700	0.19234900	0.15118400
C	3.15098400	-1.19107200	0.79590000
N	3.08661100	-2.28584900	-0.16664500
C	4.02324600	-3.29145300	-0.11547100
O	5.02948900	-3.27091500	0.57587000
N	3.72876900	-4.39018500	-0.92497200
C	2.73301700	-4.50287300	-1.88434800
O	2.45610100	-5.57367000	-2.38016200
C	2.07922600	-3.17536300	-2.25166400
C	0.68668100	-3.42456300	-2.82735800
C	1.98481900	-2.36696100	-1.00541100
P	3.94417500	2.98337800	1.85930100
O	4.56193300	3.46727800	3.14019200
O	2.99049900	3.90493300	1.15147700
O	5.09652800	2.56490800	0.78140300
C	6.27886700	1.96027700	1.30204100
C	7.09758100	1.39538100	0.16558500
O	6.55073700	0.14285800	-0.25615800
C	7.17411800	2.29024600	-1.10116300
O	8.54185500	2.55165000	-1.34002000
C	6.56288000	1.39522900	-2.19090700
C	6.93206300	0.03325200	-1.62040900
N	6.34497200	-1.15084800	-2.21071800
C	7.19417000	-2.24180900	-2.40031900
O	8.36954100	-2.24492100	-2.08866300
N	6.59210700	-3.32455500	-2.99853700
C	5.26468200	-3.46170800	-3.38602600
O	4.88516500	-4.47806600	-3.94342500
C	4.41463200	-2.31858700	-3.05239400
C	2.94843800	-2.44834200	-3.34808400
C	4.99677300	-1.23379400	-2.49858500
H	-0.50580900	0.90761000	1.76089000
H	-0.52682400	-0.87502500	1.74805300
H	1.42778400	0.17670500	2.96763000
H	1.75864400	1.83837000	0.75688400

H	4.06344500	0.59272300	-0.07641800
H	2.46695700	0.14530600	-0.75744400
H	4.07227300	-1.33453000	1.36522600
H	0.23497300	-2.47407500	-3.12472500
H	0.74925600	-4.07618200	-3.70018100
H	0.04254700	-3.89867500	-2.08309300
H	1.17005100	-1.68470300	-0.80061800
H	6.86458100	2.71235800	1.83940600
H	6.02512500	1.14964200	1.99624200
H	8.12653200	1.23745900	0.51591900
H	6.62215400	3.22839500	-0.97167200
H	6.98346300	1.58029700	-3.18046700
H	5.47762600	1.52909500	-2.22180900
H	8.01435000	-0.10769600	-1.69281700
H	4.41865600	-0.35343600	-2.23886000
H	4.30893400	-5.20572300	-0.76459500
H	7.20278700	-4.11388200	-3.17755000
C	8.75061300	3.59962100	-2.26511800
H	9.82860800	3.72966400	-2.36691300
H	8.32725900	3.36861100	-3.25068800
H	8.30499500	4.53577800	-1.90441300
C	-1.26954500	-0.02743100	-0.59201900
H	-1.15704000	-0.01886100	-1.67694900
H	-1.79182300	-0.94431500	-0.28895000
H	-1.86834900	0.83876900	-0.28251800
H	2.50137600	-1.45971900	-3.48871600
H	2.83927400	-3.01130800	-4.28083500
Na	3.26913400	5.47162300	2.92018300

Table S2 Cartesian coordinates of stationary points along the reaction paths of $^{\bullet}\text{U}_{\text{CH}_2}$ radical addition to the C₅ and C₆ sites of its 3' neighboring thymidine starting from the canonical 5'-($^{\bullet}\text{U}_{\text{CH}_2}$)T-3' sequence, respectively.

5'-($^{\bullet}\text{U}_{\text{CH}_2}$)T-3'			
O	0.99732200	-0.51564200	-0.33740400
C	0.43127100	-0.31243100	0.93879700
C	1.51609300	0.13575200	1.89819900
O	2.39853400	-0.95324700	2.19177000
C	2.39379500	1.26355500	1.34028300
O	2.71925400	2.11957200	2.43858900
C	3.60050600	0.51062400	0.79878900
C	3.71603600	-0.68362400	1.74445400
N	4.24355200	-1.89285800	1.10766600
C	5.33470300	-2.52545600	1.67582100
O	5.90898800	-2.13996300	2.67992700
N	5.75305900	-3.65617100	0.99561900
C	5.23708600	-4.21202400	-0.16563600
O	5.74745500	-5.19864600	-0.66083400
C	4.03295300	-3.52350500	-0.68386100
C	3.40635500	-4.05162500	-1.80744800
C	3.59246200	-2.40448200	0.00499900
P	3.78522600	3.34273000	2.24153000
O	3.33790500	4.48027800	3.11664200
O	4.02262100	3.63585100	0.78757400
O	5.15144600	2.67271100	2.83940200

C	5. 10376900	2. 29732300	4. 21798300
C	6. 45258800	1. 75409900	4. 62613300
O	6. 71614400	0. 57786000	3. 86414100
C	7. 63081600	2. 71583700	4. 39089200
O	8. 48640600	2. 59979800	5. 51124700
C	8. 27614900	2. 16086800	3. 12214300
C	8. 00195700	0. 66666700	3. 27628000
N	7. 98991100	-0. 08967900	2. 03520400
C	8. 65660800	-1. 30577900	1. 99812000
O	9. 34994800	-1. 73132100	2. 90367200
N	8. 49409900	-1. 99641800	0. 81408200
C	7. 71540700	-1. 64628300	-0. 28512300
O	7. 65296200	-2. 37829600	-1. 26146800
C	7. 00444800	-0. 37913300	-0. 14232700
C	6. 16089300	0. 06532800	-1. 29775800
C	7. 15879000	0. 30703600	1. 00896100
H	-0. 35215900	0. 45893400	0. 89004300
H	-0. 02345800	-1. 24116200	1. 31304600
H	1. 04754300	0. 46423400	2. 83162500
H	1. 88446300	1. 84116300	0. 56462800
H	4. 49713600	1. 12627400	0. 78975800
H	3. 38138700	0. 18032300	-0. 21871100
H	4. 38509600	-0. 47518600	2. 58473700
H	4. 84713600	3. 16624800	4. 83371300
H	4. 34062300	1. 52313000	4. 35959600
H	6. 42099900	1. 50643200	5. 69401700
H	7. 29377000	3. 75485700	4. 27314700
H	9. 34245600	2. 37894500	3. 04737200
H	7. 76732500	2. 56912900	2. 24625200
H	8. 75230300	0. 19261000	3. 91246700
H	5. 75627800	1. 06543700	-1. 13344700
H	6. 75881000	0. 07760900	-2. 21310100
H	5. 33141900	-0. 63106200	-1. 46564300
H	6. 62711700	1. 23504300	1. 19950000
H	6. 56179600	-4. 11762000	1. 39655700
H	9. 00762100	-2. 86823100	0. 75027400
C	0. 04565600	-0. 96066100	-1. 28309800
H	0. 56796100	-1. 10109700	-2. 23026100
H	-0. 40371700	-1. 91228500	-0. 97131300
H	-0. 75218100	-0. 21887400	-1. 41502400
H	2. 68769100	-1. 87480600	-0. 27668100
C	9. 46900700	3. 61357200	5. 56733000
H	10. 04857300	3. 44918700	6. 47648700
H	10. 14714000	3. 58176300	4. 70571200
H	9. 00416200	4. 60747500	5. 60964200
H	3. 81093500	-4. 93680400	-2. 27792500
H	2. 51584600	-3. 59249200	-2. 21730800
Na	3. 39869400	5. 91223000	1. 21507300

INT_{CS/UT}

O	0. 00072600	0. 01431300	0. 11849400
C	0. 06361700	-0. 10252200	1. 52316500
C	1. 51874600	-0. 14160700	1. 94974200
O	2. 10961100	-1. 38252300	1. 54890900
C	2. 36586600	0. 96302800	1. 30636100
O	3. 37912300	1. 33669300	2. 25001100
C	2. 97457000	0. 26002800	0. 10175200

C	3. 16104600	-1. 16402600	0. 62250900
N	3. 07851400	-2. 18629900	-0. 42006200
C	4. 10874500	-3. 10003900	-0. 55423700
O	5. 10656100	-3. 12982400	0. 14288000
N	3. 92508300	-4. 00557000	-1. 58920100
C	2. 87184200	-4. 09544400	-2. 48694100
O	2. 90728100	-4. 89681300	-3. 40422300
C	1. 76524200	-3. 15166100	-2. 22334800
C	0. 63795900	-3. 20507500	-3. 04058800
C	1. 93571400	-2. 24931800	-1. 18840100
P	4. 30075700	2. 64631900	1. 92415100
O	4. 94191100	3. 06895400	3. 21568500
O	3. 51863800	3. 67586100	1. 15894300
O	5. 42699600	2. 05079200	0. 90001200
C	6. 36040800	1. 11849000	1. 43709700
C	7. 03148900	0. 37202300	0. 31055300
O	6. 07126100	-0. 38423000	-0. 41133700
C	7. 71701400	1. 22599900	-0. 75780900
O	9. 00012900	1. 56364700	-0. 29800100
C	7. 69272000	0. 30172700	-1. 99286900
C	6. 71488700	-0. 82630300	-1. 59287200
N	5. 68128400	-1. 10503100	-2. 58274600
C	5. 71596500	-2. 30411100	-3. 27287700
O	6. 55615000	-3. 16989100	-3. 09103400
N	4. 70350300	-2. 44243100	-4. 19903000
C	3. 62193000	-1. 58918000	-4. 42644600
O	2. 76520900	-1. 88227900	-5. 24301600
C	3. 64007400	-0. 36862600	-3. 62417500
C	4. 67268600	-0. 18032500	-2. 77999400
H	-0. 43603300	0. 75367700	2. 00120900
H	-0. 43694500	-1. 02309700	1. 85738200
H	1. 57213000	-0. 06249800	3. 04065600
H	1. 77466900	1. 84201000	1. 03941500
H	3. 92213300	0. 70050900	-0. 19874700
H	2. 26492000	0. 27930000	-0. 72868700
H	4. 13508000	-1. 30031800	1. 09549500
H	1. 15945100	-1. 54253000	-0. 91025900
H	7. 12531600	1. 64442200	2. 01803700
H	5. 84947300	0. 40265900	2. 09248800
H	7. 79208000	-0. 29466600	0. 74729900
H	7. 12489600	2. 13453400	-0. 94007400
H	8. 69133300	-0. 10340000	-2. 17337100
H	7. 35565900	0. 80961300	-2. 89866600
H	7. 22689300	-1. 77483300	-1. 41753900
H	4. 76429200	0. 71245300	-2. 17075100
H	4. 71857700	-4. 61566100	-1. 75827000
H	4. 68226000	-3. 33355900	-4. 68443800
C	9. 64306600	2. 51086800	-1. 12734200
H	10. 61598700	2. 72331400	-0. 68294400
H	9. 79173600	2. 12068500	-2. 14244100
H	9. 06156800	3. 44000200	-1. 18956900
C	-1. 32602100	-0. 00929200	-0. 36775500
H	-1. 27615800	0. 08788100	-1. 45323100
H	-1. 82370200	-0. 95311200	-0. 10969000
H	-1. 91077100	0. 82300900	0. 04456400
H	-0. 19078600	-2. 52577900	-2. 88620700
H	0. 59124400	-3. 92742800	-3. 84313700
C	2. 49016400	0. 57807100	-3. 76947800

H	2. 63973600	1. 47283900	-3. 16215800
H	2. 35747400	0. 87573600	-4. 81294000
H	1. 56212100	0. 08820700	-3. 45100900
Na	4. 13728800	5. 28451500	2. 81381300

TS_{C5/UT}

O	-0. 04151800	0. 02549100	0. 08610500
C	0. 00873500	-0. 04808700	1. 49239600
C	1. 45908900	-0. 05340700	1. 93254600
O	2. 07454800	-1. 26646200	1. 47005000
C	2. 28556700	1. 10387500	1. 33411200
O	3. 30565400	1. 45079500	2. 28434200
C	2. 91829400	0. 43309800	0. 13025200
C	3. 25099300	-0. 91333600	0. 76222900
N	3. 62053200	-1. 95112400	-0. 18288800
C	4. 89880700	-2. 48575700	-0. 08166900
O	5. 61974100	-2. 34925700	0. 89048800
N	5. 29117400	-3. 21249700	-1. 18775400
C	4. 64189100	-3. 33360300	-2. 41267400
O	5. 18068200	-3. 91114500	-3. 34313300
C	3. 31021100	-2. 72069300	-2. 45100800
C	2. 65307500	-2. 55289500	-3. 71506600
C	2. 87674300	-2. 07757100	-1. 33242500
P	4. 28517000	2. 72466700	1. 98360400
O	5. 10807200	2. 93528300	3. 22269000
O	3. 49857900	3. 88946100	1. 45337100
O	5. 23241700	2. 21038800	0. 75166100
C	6. 16658300	1. 16348400	0. 99516600
C	6. 73952500	0. 65833300	-0. 30892600
O	5. 76417600	0. 00145500	-1. 12612300
C	7. 37977000	1. 74493300	-1. 20460200
O	8. 77545500	1. 64571500	-1. 03236300
C	6. 90252300	1. 36591600	-2. 61728800
C	6. 38438400	-0. 05449800	-2. 39911300
N	5. 44672300	-0. 53709300	-3. 40634700
C	6. 01345600	-1. 24995000	-4. 45894700
O	7. 18128300	-1. 59567100	-4. 47840100
N	5. 15807100	-1. 49580500	-5. 51182800
C	3. 81342200	-1. 16098800	-5. 61384100
O	3. 20085300	-1. 36905300	-6. 64614300
C	3. 22972400	-0. 60852000	-4. 37857300
C	4. 13786800	-0. 09748400	-3. 44644300
H	-0. 50809700	0. 81179800	1. 94607200
H	-0. 48084300	-0. 96673700	1. 84898900
H	1. 50783700	-0. 01206600	3. 02654400
H	1. 67835500	1. 98208200	1. 10083700
H	3. 78572500	0. 95110400	-0. 26617400
H	2. 15655700	0. 31459000	-0. 64146600
H	4. 08935700	-0. 83480000	1. 45423400
H	1. 89861400	-1. 60821000	-1. 28613800
H	6. 99916900	1. 54334700	1. 59846500
H	5. 70034600	0. 33473900	1. 53817500
H	7. 53319600	-0. 06243700	-0. 06161200
H	7. 03445000	2. 74689800	-0. 91810300
H	7. 70351700	1. 40851300	-3. 35808900
H	6. 07539300	2. 00324100	-2. 94288700
H	7. 20941000	-0. 77362700	-2. 38248100

H	3.83923500	0.54116200	-2.62422700
H	6.22178600	-3.61045500	-1.12945500
H	5.57726600	-1.96406600	-6.30647800
C	9.47082100	2.76405500	-1.54444900
H	10.53222500	2.59870500	-1.35664200
H	9.31437400	2.88079300	-2.62442600
H	9.15313000	3.68802700	-1.04360000
C	-1.36643500	0.02893900	-0.40133200
H	-1.31377400	0.08307900	-1.48945300
H	-1.89814600	-0.88633900	-0.10956900
H	-1.92579200	0.89475800	-0.02270900
H	1.59025200	-2.33117700	-3.69865700
H	2.97801200	-3.20464000	-4.52053400
C	1.88465300	0.06338900	-4.52000400
H	1.41236000	0.18711500	-3.54146900
H	1.98810600	1.05038900	-4.97934800
H	1.23160900	-0.53813500	-5.15339700
Na	4.41028900	5.20673700	3.24214700

5'-T(5m-5)(^{*}U_{5m})-3'

O	-0.00182600	-0.00147100	-0.01381200
C	-0.00706400	-0.00576700	1.39519200
C	1.42443800	-0.00472500	1.89219000
O	2.04178600	-1.24579200	1.50965100
C	2.28807800	1.11777300	1.27462000
O	3.26575500	1.50870400	2.25159700
C	2.97235800	0.37836100	0.14167200
C	3.26521900	-0.92754300	0.87022000
N	3.71718100	-2.00748000	0.01159300
C	5.00705400	-2.48580600	0.21731700
O	5.64588500	-2.29784000	1.23708900
N	5.51028500	-3.21883400	-0.83728700
C	4.98430300	-3.33243000	-2.12001600
O	5.61922400	-3.88358200	-3.00642500
C	3.65339200	-2.75220400	-2.27351300
C	3.08282700	-2.59927500	-3.64486200
C	3.08867300	-2.16199100	-1.20534000
P	4.26961900	2.76022000	1.93464700
O	5.06574500	2.99561100	3.18659200
O	3.50902700	3.91854400	1.35491100
O	5.23897000	2.19925500	0.74075300
C	6.16758200	1.16151800	1.04228300
C	6.80487500	0.63691700	-0.22436300
O	5.88684900	-0.07775700	-1.06174500
C	7.45058300	1.71961800	-1.12303000
O	8.84469600	1.63596300	-0.92383500
C	7.00896700	1.31162000	-2.53735200
C	6.55867400	-0.12952100	-2.31183200
N	5.69578900	-0.68518300	-3.34462700
C	6.34740800	-1.34057900	-4.37163300
O	7.54263500	-1.57919900	-4.37484300
N	5.54693500	-1.66834800	-5.45950100
C	4.17976500	-1.52160200	-5.58747500
O	3.62201300	-1.73917300	-6.64330600
C	3.45697600	-1.17788100	-4.29674700
C	4.35592100	-0.32668600	-3.45337600
H	-0.53040500	0.88090000	1.78545500

H	-0.52180400	-0.90034900	1.77676300
H	1.43165200	0.08741700	2.98422900
H	1.69777800	1.98489700	0.96807400
H	3.85838700	0.86728200	-0.25076100
H	2.24299700	0.21543800	-0.65302700
H	4.04763900	-0.80042600	1.61856900
H	2.09497300	-1.72584600	-1.25284000
H	6.96894700	1.55836900	1.67602700
H	5.68337600	0.33867200	1.57861100
H	7.61018500	-0.04964000	0.07654300
H	7.09131400	2.72226100	-0.85768400
H	7.81415000	1.38894900	-3.27071200
H	6.15257600	1.90270700	-2.87454800
H	7.42228000	-0.79964400	-2.24322200
H	3.96657700	0.27120300	-2.63976600
H	6.44809700	-3.57852700	-0.69949600
H	6.04877000	-2.03880800	-6.25821400
C	9.53897800	2.75382000	-1.43802300
H	10.59814400	2.60155100	-1.22760900
H	9.40271100	2.85458300	-2.52232600
H	9.20282200	3.68155800	-0.95647200
C	-1.30690000	-0.00786200	-0.55152400
H	-1.21217900	-0.00932800	-1.63812500
H	-1.86106900	-0.90159400	-0.23563400
H	-1.86967800	0.88158800	-0.23868900
H	1.99267300	-2.66549700	-3.61369000
H	3.44595300	-3.40791100	-4.28438100
C	2.16974900	-0.41387900	-4.60836500
H	1.62548800	-0.21751900	-3.67945900
H	2.39006900	0.54072900	-5.09177800
H	1.53547700	-1.00632400	-5.26962900
Na	4.37018900	5.27006400	3.14437200

INT_{C6/UT}

O	0.73891100	-1.15324600	-0.00968000
C	0.63666200	-0.47066000	1.21929400
C	2.02153900	-0.08436600	1.70427300
O	2.78578100	-1.22826600	2.08933300
C	2.91536300	0.61251600	0.67517000
O	3.79314600	1.49500100	1.38782300
C	3.57954400	-0.57184100	-0.03008000
C	3.52373800	-1.70733700	1.01690800
N	2.95615700	-2.95389700	0.39358500
C	1.90467700	-3.67514500	0.91937000
O	1.34051300	-3.47360100	1.98051700
N	1.49685700	-4.73714200	0.11141400
C	2.03031700	-5.19294600	-1.07974000
O	1.57190200	-6.17466400	-1.63903800
C	3.17971400	-4.40100400	-1.56204000
C	3.80253400	-4.77951300	-2.74706100
C	3.57547900	-3.33602200	-0.77083300
P	5.41305600	1.39302900	1.49392500
O	5.84155500	2.52734500	2.38289900
O	6.07654800	1.30248600	0.14639400
O	5.64367900	-0.04364100	2.23817600
C	5.32867100	-0.09680800	3.63103100
C	5.69561200	-1.45179100	4.18965300

O	4. 77222800	-2. 42996400	3. 72035700
C	7. 10678600	-1. 96644500	3. 81447300
O	7. 78405200	-2. 24862000	5. 02107400
C	6. 80569100	-3. 23754300	3. 00489200
C	5. 48149700	-3. 64759600	3. 63655200
N	4. 66619600	-4. 61918600	2. 91737500
C	3. 55228700	-5. 08602800	3. 61070500
O	3. 23316000	-4. 67475500	4. 70904000
N	2. 84766700	-6. 07118200	2. 95249700
C	3. 17207900	-6. 70800100	1. 75839100
O	2. 46194200	-7. 59833900	1. 31782800
C	4. 38694700	-6. 20616500	1. 12248900
C	4. 84692700	-6. 88453800	-0. 13251500
C	5. 05245000	-5. 19740300	1. 72181000
H	0. 01693900	0. 43328000	1. 11092500
H	0. 18072400	-1. 12120000	1. 97821700
H	1. 91641200	0. 54045400	2. 59625000
H	2. 34477800	1. 23107400	-0. 02200000
H	4. 59473600	-0. 34871400	-0. 35742800
H	2. 96842300	-0. 83340700	-0. 89406800
H	4. 50693700	-1. 98832600	1. 39748000
H	4. 43186200	-2. 73513300	-1. 05465700
H	5. 89305700	0. 67694800	4. 16107000
H	4. 25527300	0. 07222000	3. 77545500
H	5. 64987300	-1. 39486400	5. 28615200
H	7. 66792900	-1. 23055500	3. 22487100
H	7. 59191100	-3. 99061300	3. 08100600
H	6. 65741400	-2. 96120800	1. 95648200
H	5. 64712100	-4. 04922400	4. 64505400
H	5. 65850900	-6. 32727400	-0. 60457300
H	5. 19953900	-7. 89668600	0. 09032000
H	4. 02416900	-6. 97581900	-0. 84630900
H	0. 74289400	-5. 28924100	0. 50562900
H	2. 01458700	-6. 39513100	3. 43052100
C	-0. 46071500	-1. 80927800	-0. 36036400
H	-0. 29148200	-2. 30772900	-1. 31652700
H	-0. 72667200	-2. 55818100	0. 39829300
H	-1. 28922200	-1. 09615200	-0. 46486000
C	9. 17474600	-2. 42968900	4. 84694700
H	9. 60347000	-2. 60102400	5. 83491800
H	9. 40169200	-3. 29253200	4. 20840300
H	9. 63360500	-1. 53643400	4. 40314500
Na	7. 32560100	3. 25963700	0. 69529400
H	4. 65607500	-4. 23404200	-3. 12862000
H	3. 43005100	-5. 63396600	-3. 29500200
H	5. 95820000	-4. 79622400	1. 28369800

TS_{C6/UT}

O	0. 28229400	-0. 01601600	-0. 17247600
C	0. 07685400	-0. 08139300	1. 21837300
C	1. 39537400	0. 04049500	1. 96575300
O	2. 05160600	-1. 23431800	2. 05874500
C	2. 42162900	0. 97324000	1. 30331500
O	3. 24539200	1. 47665600	2. 36738000
C	3. 16256300	-0. 00118400	0. 40022700
C	3. 24652200	-1. 20247800	1. 32528700
N	3. 50268500	-2. 46860200	0. 62335600

C	2. 50939500	-3. 18668800	-0. 02868000
O	1. 34512400	-2. 84902300	-0. 09753100
N	2. 97398100	-4. 36601800	-0. 59970100
C	4. 28252700	-4. 83103200	-0. 69945400
O	4. 52744300	-5. 91668700	-1. 20015800
C	5. 28114900	-3. 90013200	-0. 16816900
C	6. 66556000	-4. 23166500	-0. 19257700
C	4. 82392300	-2. 79493000	0. 48866000
P	4. 78136200	1. 98973500	2. 16717900
O	5. 05704800	2. 97608400	3. 26775800
O	5. 04950400	2. 43328600	0. 75772900
O	5. 64029600	0. 61326100	2. 43089000
C	5. 65429400	0. 16525900	3. 78712800
C	6. 39725800	-1. 13805300	3. 94278200
O	5. 74085800	-2. 20031600	3. 26873800
C	7. 84858500	-1. 20900900	3. 44408400
O	8. 68846600	-0. 82833000	4. 50411500
C	7. 99577300	-2. 69224200	3. 00774700
C	6. 64369000	-3. 29032100	3. 41449800
N	6. 17195200	-4. 44170200	2. 65460200
C	4. 94033200	-4. 94456300	3. 06408800
O	4. 26328500	-4. 42204000	3. 92927700
N	4. 53614700	-6. 09063000	2. 41043400
C	5. 34486600	-6. 97108500	1. 67874200
O	4. 91249500	-8. 06698500	1. 34414800
C	6. 66489800	-6. 46503000	1. 40096300
C	7. 56717700	-7. 29099300	0. 54486100
C	6. 97938200	-5. 16118200	1. 76150500
H	-0. 59991800	0. 72727400	1. 53652900
H	-0. 37803600	-1. 04140200	1. 50012700
H	1. 19060100	0. 37829200	2. 98649200
H	1. 95884600	1. 80686200	0. 76996100
H	4. 13823200	0. 35638500	0. 07233500
H	2. 52836900	-0. 24250100	-0. 45459300
H	4. 09103900	-1. 11030500	2. 01183600
H	5. 51002900	-2. 10259200	0. 96427300
H	6. 14110700	0. 91581100	4. 41808900
H	4. 62437800	0. 02624400	4. 14172900
H	6. 42561900	-1. 35120000	5. 02453200
H	7. 99393700	-0. 53965700	2. 58500600
H	8. 83828600	-3. 17810400	3. 50426600
H	8. 13701100	-2. 75047400	1. 92708700
H	6. 65073100	-3. 57657300	4. 47530100
H	8. 54767600	-6. 82322900	0. 43515500
H	7. 69875900	-8. 28895300	0. 97183800
H	7. 12646700	-7. 42147600	-0. 45089400
H	2. 25572800	-4. 94326200	-1. 02236700
H	3. 63712400	-6. 45109500	2. 70887800
C	-0. 82152500	-0. 51059100	-0. 89551300
H	-0. 59956000	-0. 38904900	-1. 95700500
H	-0. 98110700	-1. 57404800	-0. 67841200
H	-1. 73805700	0. 04633000	-0. 65619400
C	10. 01626700	-0. 57657600	4. 09002800
H	10. 57797000	-0. 26930000	4. 97268300
H	10. 48432700	-1. 47357300	3. 66450300
H	10. 04953500	0. 22497000	3. 34066500
Na	5. 68464400	4. 58357800	1. 64594000
H	7. 37837900	-3. 42408300	-0. 05585700

H	6.98073900	-5.03765400	-0.84552500
H	8.01638600	-4.84801200	1.73903900

5'-T(5m-6)(^{*}T_{6H})-3'

O	-0.03544200	0.08285200	-0.01149500
C	-0.03836700	0.04740900	1.39516200
C	1.38566600	-0.03489000	1.90574500
O	1.90006400	-1.36759400	1.72195100
C	2.35748300	0.90842800	1.16723100
O	3.30896900	1.36083600	2.14320800
C	2.98351900	-0.03844400	0.15515600
C	3.11971100	-1.26466100	1.03663600
N	3.48727500	-2.48682900	0.31296700
C	2.59169200	-3.28864500	-0.38141600
O	1.38974900	-3.12505700	-0.41279700
N	3.20894200	-4.34053400	-1.04596900
C	4.56956000	-4.59859700	-1.21034000
O	4.94593700	-5.57533100	-1.84408500
C	5.42730900	-3.60828200	-0.58090200
C	6.91924000	-3.67299200	-0.67232500
C	4.84106200	-2.63234000	0.13836900
P	4.75237300	1.99777900	1.72187500
O	5.14293700	2.96873500	2.80120600
O	4.74015900	2.50365500	0.30735100
O	5.73798000	0.68341600	1.77604000
C	6.16196100	0.29165300	3.08357400
C	7.11264300	-0.87800800	3.03705000
O	6.48527100	-2.04675500	2.54361300
C	8.36386400	-0.75357500	2.16673900
O	9.32592400	-0.00534900	2.86178300
C	8.74988200	-2.23480000	1.91173700
C	7.54444200	-3.01057500	2.48169200
N	7.10006700	-4.19808600	1.78103400
C	6.13899900	-4.91296600	2.45654400
O	5.70994000	-4.59196500	3.55216600
N	5.66184300	-6.05541100	1.82448700
C	6.28507600	-6.74149600	0.78651000
O	5.93994000	-7.87903900	0.48948300
C	7.33243100	-6.00324700	0.12303700
C	8.01362600	-6.62123100	-1.04240800
C	7.56194500	-4.56018400	0.43655100
H	-0.51115000	0.95594900	1.80061600
H	-0.60213700	-0.82254000	1.76431100
H	1.39448600	0.19898100	2.97573900
H	1.85130900	1.76596300	0.71860200
H	3.92678500	0.31727500	-0.25841200
H	2.26255100	-0.24694600	-0.63884700
H	3.93803100	-1.12340100	1.75499800
H	5.44079300	-1.88513900	0.64774700
H	6.67071200	1.12934100	3.56933100
H	5.29004900	0.01408400	3.68962100
H	7.45183100	-1.04366900	4.07457400
H	8.10373600	-0.25670800	1.22024000
H	9.66162400	-2.48706000	2.45821200
H	8.92681200	-2.42036000	0.85296200
H	7.75621600	-3.31207200	3.51418600
H	8.99177200	-6.16906800	-1.22192300

H	8.12533400	-7.69601700	-0.88768900
H	7.39644200	-6.48168800	-1.93999200
H	2.57139400	-4.97036900	-1.51971800
H	4.97772700	-6.57354000	2.36224800
C	-1.34132900	0.10134900	-0.54366100
H	-1.25233100	0.14053300	-1.62997200
H	-1.89829400	-0.80134400	-0.25906600
H	-1.90073600	0.98055400	-0.19590100
C	10.43571600	0.34008400	2.05727100
H	11.10459700	0.94560900	2.66961700
H	10.97565500	-0.55133500	1.71274300
H	10.12140600	0.92071900	1.18010300
Na	5.42315000	4.64179200	1.13307400
H	7.32209700	-2.65994900	-0.58136900
H	7.23257400	-4.06158400	-1.64578300
H	8.64449800	-4.39408200	0.40039500

Table S3 Cartesian coordinates of stationary points along the reaction paths of $\cdot\text{U}_{\text{CH}_2}$ radical addition to the C₅ and C₆ sites of its 5' neighboring deoxycytidine starting from the canonical 5'-C($\cdot\text{U}_{\text{CH}_2}$)-3' sequence, respectively.

5'-C($\cdot\text{U}_{\text{CH}_2}$)-3'			
O	-4.77663400	0.48789900	0.35272900
C	-4.59585000	0.42798400	1.75107000
C	-3.11269300	0.40214500	2.06246200
O	-2.55236900	-0.85885400	1.68562200
C	-2.31462200	1.47625300	1.31152600
O	-1.29799000	1.94111400	2.20455700
C	-1.75714700	0.70590600	0.12270500
C	-1.56266300	-0.70575800	0.67796100
N	-1.74538800	-1.75335100	-0.32279600
C	-0.70530700	-2.67675200	-0.58626200
O	0.30775700	-2.67038700	0.10796200
N	-0.87059600	-3.52708700	-1.63921900
C	-1.98577500	-3.51200200	-2.34826200
C	-3.10930400	-2.68393200	-2.01772900
C	-2.92564400	-1.81079600	-1.00162700
P	-0.17072800	2.99698300	1.67352100
O	0.19714600	3.88884600	2.82671300
O	-0.59806400	3.65940500	0.39466900
O	1.06837400	1.98969300	1.32200100
C	1.60503800	1.26706700	2.43235800
C	2.79076700	0.45825500	1.96566900
O	2.33709000	-0.52303600	1.03615200
C	3.88260700	1.28215400	1.25631100
O	5.13001600	0.81295200	1.73055200
C	3.66680400	0.93669300	-0.21597300
C	3.16745600	-0.50217800	-0.11071500
N	2.39808700	-0.96853200	-1.25128300
C	2.69337100	-2.21748000	-1.77323900
O	3.59330300	-2.93178000	-1.36762700
N	1.91136600	-2.58066500	-2.85167600
C	0.81477500	-1.92478800	-3.38300300
O	0.21950800	-2.38491800	-4.34083300
C	0.46886500	-0.65763500	-2.69562200

C	-0.65471300	0.03518800	-3.13749500
C	1.28409800	-0.26381000	-1.64583500
H	-5.05315400	1.30601500	2.23226100
H	-5.06878500	-0.47517300	2.16389900
H	-2.97931600	0.53675000	3.14119000
H	-2.93947500	2.31793800	1.00248400
H	-0.83531300	1.13994600	-0.26077000
H	-2.50702900	0.70355200	-0.67192500
H	-0.55922500	-0.85496800	1.08500500
H	-3.69376300	-1.11976500	-0.66250900
H	1.91757100	1.96567000	3.21639300
H	0.83858200	0.59651100	2.83841100
H	3.24452800	-0.03304900	2.83535800
H	3.77780400	2.35696200	1.45756700
H	4.57412300	1.01775600	-0.81655100
H	2.89766600	1.58713400	-0.63869300
H	4.00013600	-1.19994900	0.00021000
H	-0.94451600	0.97840100	-2.69304300
H	-1.22925500	-0.35785900	-3.96484500
H	1.08351900	0.63158800	-1.06843100
H	2.12700000	-3.48790600	-3.24773000
C	6.20713500	1.66087500	1.38867300
H	7.10901100	1.22708300	1.82211800
H	6.34132300	1.74245100	0.30291900
H	6.05776900	2.66851000	1.79846600
Na	-0.24667500	5.77548000	1.45479700
C	-6.14309900	0.48475500	-0.00839500
H	-6.19424200	0.53268300	-1.09661500
H	-6.63974600	-0.43019000	0.33922200
H	-6.66278300	1.35230800	0.41811500
H	-4.04084100	-2.73306100	-2.56447300
N	-2.06106600	-4.34688400	-3.40560800
H	-1.18510800	-4.71743800	-3.74543000
H	-2.79627700	-4.21990800	-4.08340300

TS_{C6/CU}

O	-0.04944100	0.09862300	0.00073600
C	-0.04598700	0.07718200	1.41052700
C	1.38448600	0.03221700	1.91648900
O	1.99723000	-1.19827000	1.53039900
C	2.28530500	1.13458300	1.35114800
O	3.28841600	1.39243900	2.34198700
C	2.86023400	0.46492900	0.11123400
C	3.07113200	-0.95876800	0.61995500
N	3.09520900	-2.01112800	-0.37614600
C	3.87519300	-3.15286700	-0.08454400
O	4.46646100	-3.22285000	0.98631400
N	3.95475000	-4.14637500	-1.02679200
C	3.11020200	-4.15009400	-2.04801500
C	2.17418600	-3.10833900	-2.28391500
C	2.31435100	-1.94921600	-1.52056300
P	4.56666800	2.33852100	1.97085100
O	5.05943100	2.94790900	3.25334200
O	4.23732800	3.26967200	0.83885600
O	5.64998300	1.24666700	1.40859500
C	6.25281200	0.38573900	2.37738600
C	7.41407600	-0.33892800	1.73866600

O	6.91731400	-1.25149400	0.75811800
C	8.41790900	0.58525500	1.02031300
O	9.71353100	0.13636500	1.36609600
C	8.10580600	0.33979100	-0.45612100
C	7.69232600	-1.12792200	-0.41794300
N	6.87007200	-1.57064100	-1.53720600
C	7.30872100	-2.63364700	-2.31761000
O	8.37146300	-3.20185600	-2.15012100
N	6.43523900	-2.98597200	-3.32642300
C	5.18393600	-2.45019200	-3.60834000
O	4.50142000	-2.90507200	-4.51081000
C	4.79073800	-1.33719500	-2.73540000
C	3.47190300	-0.80022100	-2.87110200
C	5.64544000	-0.98352900	-1.72988200
H	-0.54987000	0.97042300	1.81166500
H	-0.58113300	-0.81005500	1.78061100
H	1.36823900	0.09760300	3.01015600
H	1.74509800	2.05786200	1.12581600
H	3.77588600	0.94460500	-0.23319200
H	2.09916500	0.51689300	-0.66628100
H	4.02544400	-1.03648400	1.14710400
H	1.51379500	-1.21499000	-1.49051600
H	6.61192100	0.97752200	3.22552200
H	5.51604000	-0.34303500	2.73800300
H	7.95315200	-0.89282000	2.51670300
H	8.28596000	1.63611600	1.31087700
H	8.95300300	0.52347700	-1.11842300
H	7.26198700	0.96353100	-0.76500900
H	8.56230000	-1.78819800	-0.39592000
H	3.28194100	0.17317500	-2.43231400
H	2.96301900	-0.99984000	-3.80742100
H	5.40000400	-0.21625200	-1.00129300
H	6.73574800	-3.76528100	-3.90104700
C	10.73241000	1.04531100	1.00233000
H	11.67611200	0.62824900	1.35551500
H	10.79305500	1.18611400	-0.08377600
H	10.57108200	2.02401300	1.47292800
Na	4.76557200	5.10419400	2.29492900
C	-1.35825100	0.10133600	-0.52934700
H	-1.27038900	0.10933200	-1.61641200
H	-1.91261800	-0.79342000	-0.21738600
H	-1.91497000	0.99004000	-0.20431000
H	1.49068600	-3.13746800	-3.12199800
N	3.13471600	-5.22781300	-2.87654000
H	3.92884100	-5.84221600	-2.76635700
H	2.81209300	-5.09644300	-3.82363900

5'-*C_{6H}(6-5m)T-3'

O	-0.01971100	0.04359400	-0.05309800
C	-0.03966900	0.05739700	1.35589200
C	1.38345200	0.04884200	1.87951300
O	2.00099400	-1.19632800	1.55041200
C	2.27451500	1.14026200	1.26291500
O	3.20427100	1.54354700	2.28007400
C	2.95832200	0.38166200	0.13573900
C	3.21794900	-0.94688200	0.83537000
N	3.54691000	-2.07822200	0.01468700

C	4. 31290500	-3. 07930300	0. 60226500
O	4. 69312700	-2. 97181500	1. 76274500
N	4. 66852400	-4. 19835300	-0. 14252900
C	4. 01163000	-4. 46551000	-1. 24753300
C	3. 01575100	-3. 59248300	-1. 79091600
C	3. 00940000	-2. 18316800	-1. 33477600
P	4. 49414800	2. 46245300	1. 88547600
O	4. 92376400	3. 19009200	3. 12850100
O	4. 21324700	3. 28437400	0. 65857200
O	5. 61918900	1. 34491100	1. 46950900
C	6. 30990700	0. 65992000	2. 51781600
C	7. 64945400	0. 17830500	2. 00394500
O	7. 45064100	-0. 89834800	1. 08420600
C	8. 46188600	1. 25065800	1. 25527800
O	9. 81181700	1. 09146900	1. 64555400
C	8. 24741800	0. 87272500	-0. 21059900
C	8. 16641800	-0. 64725000	-0. 11015400
N	7. 44112900	-1. 30218800	-1. 19302100
C	8. 06963600	-2. 29613100	-1. 92929500
O	9. 24158000	-2. 59757900	-1. 79957700
N	7. 24299100	-2. 91832200	-2. 84355100
C	5. 88716600	-2. 69608600	-3. 07037600
O	5. 27521200	-3. 37602900	-3. 88206800
C	5. 31185500	-1. 62913000	-2. 25964100
C	3. 84781700	-1. 33839200	-2. 36228300
C	6. 10537500	-1. 01932800	-1. 35382300
H	-0. 56057000	0. 95437300	1. 72649600
H	-0. 56977800	-0. 82649700	1. 74195500
H	1. 35826700	0. 17631500	2. 96845300
H	1. 70915700	2. 01017000	0. 91965500
H	3. 85538700	0. 88294000	-0. 22580500
H	2. 23284700	0. 27027900	-0. 67163900
H	4. 03896300	-0. 83301200	1. 54714400
H	1. 98352700	-1. 79420300	-1. 33048900
H	6. 46552200	1. 33973000	3. 36097600
H	5. 71818100	-0. 20150200	2. 85118800
H	8. 24269100	-0. 17811200	2. 85416000
H	8. 11078800	2. 26542300	1. 48738000
H	9. 05058100	1. 20614000	-0. 86908800
H	7. 29745100	1. 28293200	-0. 56420000
H	9. 15812200	-1. 10465200	-0. 08510000
H	3. 66484200	-0. 27873500	-2. 18517200
H	3. 49418200	-1. 57364900	-3. 36957000
H	5. 72715800	-0. 26991900	-0. 66281400
H	7. 67898700	-3. 65668200	-3. 38455000
C	10. 64020700	2. 16274300	1. 24158300
H	11. 63635100	1. 96634500	1. 63968900
H	10. 70676600	2. 24698600	0. 15000800
H	10. 27182100	3. 11557000	1. 64389000
Na	4. 69669500	5. 24412100	1. 93207600
C	-1. 32003200	0. 04304100	-0. 60096000
H	-1. 21852800	0. 03005000	-1. 68677800
H	-1. 88478600	-0. 84254600	-0. 28038100
H	-1. 87812300	0. 94003100	-0. 30080800
H	2. 44074600	-3. 87367200	-2. 66388000
N	4. 26238600	-5. 63400100	-1. 89065300
H	5. 06334200	-6. 15484200	-1. 56179800
H	4. 08755900	-5. 67164500	-2. 88416800

INT _{C5/CU}			
O	-0.18851900	-0.23359200	0.40411800
C	0.07330500	-0.25352100	1.79054900
C	1.56342700	-0.07772800	2.00494300
O	2.26001500	-1.26000700	1.60470900
C	2.14524700	1.08174900	1.18515700
O	3.08535500	1.77106500	2.01419200
C	2.81474200	0.38213500	0.00520500
C	3.17656700	-0.99948200	0.55536200
N	3.04738500	-2.07438900	-0.43200800
C	4.19811100	-2.73806500	-0.91269100
O	5.30961400	-2.39338700	-0.51668400
N	4.01615600	-3.73402900	-1.82655700
C	2.80388200	-4.04022400	-2.25620800
C	1.61715100	-3.41052900	-1.75890000
C	1.80075400	-2.42330500	-0.85215500
P	3.61260600	3.23997600	1.53248200
O	4.07856600	3.96938000	2.76201000
O	2.59475000	3.92179700	0.66255500
O	4.88445000	2.85412000	0.58576000
C	6.00539900	2.27603200	1.25209000
C	6.96922300	1.74846800	0.22096100
O	6.38413900	0.63130500	-0.44157200
C	7.37158700	2.76343300	-0.87907700
O	8.77552800	2.91031000	-0.81035100
C	6.91929800	2.07188000	-2.17092600
C	6.96160000	0.60963900	-1.73645200
N	6.24605400	-0.33269100	-2.56956900
C	6.90320300	-1.49583100	-2.94404000
O	8.05586800	-1.75346200	-2.64627700
N	6.15912800	-2.33357300	-3.75098700
C	4.83099800	-2.21973000	-4.12239000
O	4.31601400	-3.04558400	-4.85490700
C	4.14324500	-1.02908600	-3.56943100
C	2.78315700	-0.88393800	-3.81997000
C	4.90601600	-0.14579800	-2.82273900
H	-0.46426700	0.56502800	2.29296200
H	-0.25591900	-1.20469200	2.23378300
H	1.75128100	0.09761600	3.06955000
H	1.37171100	1.78217900	0.86262000
H	3.70061400	0.91989800	-0.33834600
H	2.09404200	0.27676100	-0.81117000
H	4.20726600	-1.04517500	0.91203200
H	0.98573900	-1.85547400	-0.41190600
H	6.50343800	3.03245900	1.86789400
H	5.67676800	1.45241300	1.89747700
H	7.89344900	1.43801900	0.72832200
H	6.88208600	3.73508800	-0.73500100
H	7.57116100	2.28379500	-3.02000000
H	5.89679500	2.36811300	-2.41994500
H	7.99493600	0.25466700	-1.69063400
H	4.47330400	0.75181600	-2.40124700
H	6.63971200	-3.17385100	-4.05009800
C	9.25054700	4.01917800	-1.54548300
H	10.33259900	4.05439700	-1.41380400
H	9.02678100	3.92930300	-2.61592200

H	8.81018700	4.95417500	-1.17468400
C	-1.56347900	-0.38728900	0.11446800
H	-1.67380900	-0.35993500	-0.97003200
H	-1.94267300	-1.34449900	0.49443900
H	-2.14999100	0.42620500	0.56020100
H	2.22959900	-0.03406300	-3.44072400
H	2.26996600	-1.62835400	-4.41288500
Na	2.61774900	5.75363600	2.21522700
H	0.63069900	-3.68898400	-2.10340000
N	2.70345000	-5.01390200	-3.18898000
H	3.54864300	-5.20609600	-3.70898900
H	1.83736300	-5.10771600	-3.69706800

TS_{CS/CU}

O	0.05539500	0.11688700	-0.12942100
C	-0.02425400	0.14290800	1.27898900
C	1.37569400	0.04389800	1.85231100
O	1.89159200	-1.27176600	1.64443900
C	2.36694500	1.01246000	1.19194000
O	3.26191000	1.48789000	2.20388600
C	3.09191300	0.13118200	0.18300900
C	3.06894900	-1.24401000	0.85071900
N	2.99962200	-2.35638000	-0.08868800
C	4.02630000	-3.31905800	-0.12502700
O	5.07546500	-3.11959200	0.48147200
N	3.78762700	-4.47407400	-0.82675400
C	2.75551300	-4.54931600	-1.63468300
C	1.89263600	-3.40422000	-1.91516600
C	1.91542300	-2.43906500	-0.91870400
P	3.94433500	2.95202300	1.97194500
O	4.66218900	3.31352400	3.24108900
O	2.93164100	3.93009600	1.44379500
O	5.00612300	2.65209200	0.76865100
C	6.30492700	2.19103100	1.13984800
C	7.00126800	1.62175300	-0.07388800
O	6.51492400	0.30236900	-0.32904200
C	6.79888500	2.42548200	-1.38604300
O	8.08236300	2.73990000	-1.88605500
C	6.05885000	1.42454700	-2.28742400
C	6.64029300	0.13234900	-1.73327100
N	6.06228700	-1.13026900	-2.14615900
C	6.91800300	-2.22367000	-2.06153300
O	8.02662500	-2.16417800	-1.56204600
N	6.43227000	-3.37818300	-2.63521600
C	5.20545000	-3.57708900	-3.25067200
O	4.94650100	-4.63812900	-3.79140200
C	4.29536600	-2.42164700	-3.17643900
C	2.93629700	-2.63061800	-3.58136500
C	4.77874700	-1.25665000	-2.64723000
H	-0.49424600	1.07879600	1.61818900
H	-0.62907700	-0.69864500	1.64761600
H	1.33285200	0.24325200	2.92866900
H	1.85598600	1.86056800	0.72853600
H	4.10944100	0.47254500	-0.01802900
H	2.51252100	0.10350200	-0.74438500
H	3.95463000	-1.41825700	1.46457700
H	1.15334700	-1.67845300	-0.79082200

H	6.88508000	3.02805000	1.54029300
H	6.23723400	1.41311400	1.90889400
H	8.08104600	1.57936100	0.12299400
H	6.22013100	3.34145100	-1.22008100
H	6.25283000	1.57751200	-3.35025400
H	4.98470400	1.48921100	-2.09185200
H	7.70331000	0.07730600	-1.99265800
H	4.16827400	-0.36347600	-2.60660300
H	7.06551300	-4.16914800	-2.61380200
C	8.05442200	3.72908000	-2.89494200
H	9.08755800	3.92024900	-3.18735900
H	7.49113200	3.40171600	-3.77764600
H	7.60643100	4.65865300	-2.52015800
C	-1.21914800	0.13850500	-0.73894300
H	-1.06485100	0.11753000	-1.81836900
H	-1.81355000	-0.73455300	-0.44039400
H	-1.76948700	1.04882200	-0.46864500
H	2.31304300	-1.75265600	-3.72113400
H	2.76608500	-3.44656200	-4.27745300
Na	3.37023500	5.30241000	3.35642600
H	0.96105900	-3.57458600	-2.44337000
N	2.48987600	-5.71984000	-2.23767200
H	3.20209800	-6.43400100	-2.19830000
H	1.83554400	-5.75830000	-3.00336300

5'-*C₅H(5-5m)T-3'

O	0.00670300	0.02890100	-0.04049800
C	-0.02074600	0.03996900	1.36949500
C	1.40404900	0.01375800	1.88729100
O	1.98188500	-1.26739500	1.64315800
C	2.30704000	1.04791600	1.19851900
O	3.17900400	1.60470800	2.18991700
C	3.07185400	0.21698300	0.17631100
C	3.14170300	-1.16595500	0.82456000
N	3.11663900	-2.26290000	-0.12834400
C	4.12351900	-3.23359200	-0.11419800
O	5.16276900	-3.05429700	0.51600700
N	3.87996900	-4.41212200	-0.79738100
C	2.95086600	-4.45256500	-1.71065700
C	2.23974500	-3.20827400	-2.19764600
C	2.04971300	-2.35860200	-0.99784100
P	3.84543100	3.05986200	1.87484100
O	4.45422600	3.55690800	3.15530000
O	2.86150400	3.95722500	1.17612500
O	5.00630700	2.68466900	0.78981600
C	6.23431600	2.17301100	1.30436900
C	7.06098800	1.61770300	0.16857200
O	6.57799500	0.32083200	-0.18951500
C	7.04728400	2.46637700	-1.13101700
O	8.39132700	2.76903200	-1.44431700
C	6.42120500	1.50845500	-2.15723800
C	6.89263600	0.18654300	-1.56811800
N	6.34617400	-1.04593400	-2.09411700
C	7.21808900	-2.13313000	-2.14582700
O	8.36029800	-2.09763300	-1.72915100
N	6.69052000	-3.25230100	-2.74740700
C	5.40516900	-3.42966900	-3.24503900

O	5.09976200	-4.45990800	-3.82245000
C	4.50640400	-2.29989400	-3.00435800
C	3.05772500	-2.49824700	-3.33759100
C	5.02092000	-1.17751800	-2.46047800
H	-0.52691300	0.94681300	1.73542800
H	-0.56576800	-0.83534100	1.75284100
H	1.39297200	0.20356300	2.96660200
H	1.72588000	1.85193200	0.74021900
H	4.06424200	0.62246300	-0.03219300
H	2.48505300	0.15966300	-0.74517100
H	4.04611600	-1.29596300	1.42309400
H	1.19503000	-1.72106500	-0.81786300
H	6.78233400	2.97856200	1.80241300
H	6.04693600	1.37375500	2.03170100
H	8.10593000	1.53628600	0.49712500
H	6.46605400	3.38802200	-1.01106700
H	6.77129000	1.68319900	-3.17568400
H	5.33105900	1.59095100	-2.12233000
H	7.97670300	0.10463200	-1.69075100
H	4.40150100	-0.30670700	-2.27402000
H	7.32885500	-4.03407900	-2.84128200
C	8.51622000	3.78519400	-2.41867200
H	9.58245900	3.95853600	-2.56847900
H	8.06711900	3.49434200	-3.37656000
H	8.04202600	4.71514600	-2.07871200
C	-1.28916400	0.01712000	-0.60161600
H	-1.17527000	0.00351300	-1.68620400
H	-1.84869800	-0.87276300	-0.28509700
H	-1.85464600	0.91091300	-0.30753600
H	2.57173600	-1.53763000	-3.52742200
H	2.98951500	-3.10562000	-4.24503900
Na	3.12683300	5.53930400	2.93058600
H	1.26634900	-3.47633400	-2.61693200
N	2.60349800	-5.62267500	-2.25701900
H	3.14265900	-6.44353500	-2.02222000
H	2.02101400	-5.65676000	-3.07851000

Table S4 Cartesian coordinates of stationary points along the reaction paths of $\cdot\text{U}_{\text{CH}_2}$ radical addition to the C₅ and C₆ sites of its 3' neighboring deoxycytidine starting from the canonical 5'-($\cdot\text{U}_{\text{CH}_2}$)C-3' sequence, respectively.

5'-($\cdot\text{U}_{\text{CH}_2}$)C-3'			
O	0.34425800	-0.33966300	-0.14952100
C	0.11795800	-0.12339000	1.22579300
C	1.45079800	-0.02095800	1.94100600
O	2.08660600	-1.30396700	1.98469500
C	2.44713900	0.92312100	1.25665900
O	3.21283300	1.53544600	2.29930100
C	3.27783300	-0.03009800	0.41015000
C	3.31017000	-1.29502800	1.26937400
N	3.39922300	-2.53260900	0.49285500
C	4.45484200	-3.39720800	0.72411600
O	5.29472700	-3.23970700	1.59206600
N	4.49574800	-4.48439700	-0.13338100
C	3.65905400	-4.77606300	-1.19772700

O	3. 89899200	-5. 71409900	-1. 93739800
C	2. 49304000	-3. 87295500	-1. 31973100
C	1. 53755400	-4. 15453800	-2. 29165000
C	2. 43488200	-2. 79193600	-0. 45555700
P	4. 46780500	2. 51796600	1. 93723500
O	4. 49181900	3. 62298800	2. 95661800
O	4. 45493200	2. 91059100	0. 48725100
O	5. 73873500	1. 51397300	2. 16597000
C	5. 91696300	1. 02956200	3. 49994300
C	7. 16784100	0. 18284400	3. 56135800
O	7. 00232500	-0. 94641100	2. 70789200
C	8. 45502700	0. 89590700	3. 11617600
O	9. 48287000	0. 46914100	3. 98982600
C	8. 65927500	0. 37379400	1. 69642200
C	8. 08875100	-1. 04062800	1. 79852800
N	7. 58876000	-1. 58329400	0. 54573100
C	7. 94021300	-2. 90272600	0. 16300000
O	8. 76360300	-3. 52328100	0. 82652500
N	7. 34983200	-3. 41783700	-0. 95521300
C	6. 46495600	-2. 70569100	-1. 63401000
N	5. 92115100	-3. 26305700	-2. 73115400
C	6. 04677900	-1. 39057000	-1. 23780900
C	6. 62566900	-0. 89478200	-0. 11986200
H	-0. 45022700	0. 80685000	1. 37848400
H	-0. 45948500	-0. 95373500	1. 65794500
H	1. 27324300	0. 31454100	2. 96800800
H	1. 95346800	1. 69412300	0. 65980400
H	4. 26558100	0. 37159200	0. 19710100
H	2. 75457900	-0. 21822300	-0. 52990100
H	4. 16714800	-1. 30637600	1. 94925100
H	1. 61009300	-2. 08605800	-0. 47120000
H	6. 00135700	1. 87241900	4. 19456800
H	5. 05080400	0. 42066500	3. 78418300
H	7. 30407900	-0. 15300500	4. 59670500
H	8. 35267700	1. 98934300	3. 15463900
H	9. 70358000	0. 37465200	1. 38041900
H	8. 07833500	0. 98031300	0. 99747800
H	8. 83315600	-1. 75146200	2. 15940900
H	5. 17228700	-2. 81075400	-3. 23074500
H	5. 28832300	-0. 84183300	-1. 78063700
H	6. 35212600	0. 06204900	0. 31652200
H	5. 33783000	-5. 04556900	-0. 05085700
H	6. 11687200	-4. 23235100	-2. 93245800
C	-0. 85732500	-0. 51984300	-0. 87171600
H	-0. 58814700	-0. 69315800	-1. 91444700
H	-1. 41799200	-1. 38434200	-0. 49312500
H	-1. 49418200	0. 37134500	-0. 80443500
H	1. 65966400	-5. 01947000	-2. 92857700
H	0. 66887000	-3. 52068100	-2. 41693900
C	10. 66554500	1. 23243200	3. 87073700
H	11. 37141100	0. 84955600	4. 60857900
H	11. 11615600	1. 14584700	2. 87445800
H	10. 46950300	2. 29336300	4. 07450000
Na	4. 46956800	5. 19795900	1. 17324100

INT_{C5/UC}

O	0. 08027300	-0. 03503700	-0. 08469100
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C	0.12052500	-0.17163600	1.31908400
C	1.56815000	-0.20533200	1.77071400
O	2.17222700	-1.44351100	1.38643900
C	2.41816100	0.90403300	1.14002900
O	3.38779100	1.31612400	2.11202000
C	3.07767600	0.20159100	-0.03871000
C	3.23593700	-1.22959400	0.47045300
N	3.14955700	-2.25135600	-0.57426300
C	4.13815700	-3.22097900	-0.64548200
O	5.14175200	-3.22628600	0.04566900
N	3.89902200	-4.21062300	-1.58216000
C	2.85726800	-4.30245400	-2.49092900
O	2.83722400	-5.18608500	-3.32833900
C	1.79914600	-3.28405000	-2.30976600
C	0.67529700	-3.34521100	-3.12784300
C	2.00694600	-2.31546000	-1.34262600
P	4.26494700	2.66170500	1.81061600
O	4.77464800	3.16087100	3.13344000
O	3.49324800	3.62248300	0.94988700
O	5.49827500	2.09372700	0.90315600
C	6.44078500	1.24856400	1.55854400
C	7.19118400	0.44180300	0.52769400
O	6.27980200	-0.40109500	-0.15896100
C	7.88434800	1.22668500	-0.58202700
O	9.10118700	1.72593200	-0.09350300
C	8.01644500	0.15857400	-1.68078900
C	6.88477200	-0.84528500	-1.36593400
N	5.83790300	-0.90301400	-2.37977500
C	5.58543500	-2.11789400	-3.06377500
O	6.33809100	-3.07268900	-2.89259200
N	4.48649400	-2.16949400	-3.86808300
C	3.74204200	-1.09224700	-4.06324900
C	4.04541600	0.18341600	-3.47855600
C	5.09495300	0.20960900	-2.62698000
H	-0.39370500	0.67465600	1.79955900
H	-0.37947600	-1.09996000	1.63215000
H	1.60115500	-0.12191600	2.86225200
H	1.81934900	1.76669500	0.83970800
H	4.04404600	0.63655800	-0.28653400
H	2.41645400	0.23921500	-0.90651800
H	4.20422200	-1.37873700	0.95065600
H	1.25952700	-1.56133400	-1.11656900
H	7.15089400	1.85311900	2.13224700
H	5.92574400	0.56275800	2.24186200
H	7.95699200	-0.15330800	1.05038800
H	7.23652500	2.05557700	-0.90776100
H	8.99006600	-0.32748900	-1.57176300
H	7.93577500	0.55025100	-2.69622900
H	7.24439600	-1.86864100	-1.26014300
H	5.38605400	1.10209900	-2.08076000
H	4.69240600	-4.82012200	-1.74634500
C	9.75616200	2.56957200	-1.01999000
H	10.65890400	2.94369800	-0.53586100
H	10.03883400	2.02467400	-1.92958700
H	9.11835500	3.41770900	-1.30149300
C	-1.23847900	-0.06417400	-0.59146800
H	-1.17428600	0.05278600	-1.67412100
H	-1.72977000	-1.01775300	-0.35780100

H	-1.83866800	0.75411500	-0.17318500
H	-0.11808200	-2.61384800	-3.03697400
H	0.58215600	-4.14115700	-3.85398700
Na	3.76171100	5.27279300	2.64607500
H	3.44893300	1.06363100	-3.67491300
N	2.66791700	-1.21360600	-4.86467900
H	2.37295700	-2.14749400	-5.11192900
H	1.97830300	-0.47991700	-4.90404800

TS_{C5/UC}

O	-0.04459300	0.00819800	0.04085700
C	-0.01012400	0.00599500	1.44925400
C	1.43442900	0.00326800	1.90615300
O	2.03780800	-1.23942000	1.51278800
C	2.28577300	1.11921900	1.26364500
O	3.28462700	1.50788300	2.22022300
C	2.94130900	0.37789800	0.11416100
C	3.24199000	-0.93497300	0.82809000
N	3.63549600	-2.02608100	-0.04241600
C	4.91319900	-2.54362000	0.11912200
O	5.61277600	-2.34316800	1.09725300
N	5.33451100	-3.33291100	-0.93200200
C	4.71572600	-3.52981800	-2.16394400
O	5.28129300	-4.15912200	-3.04300000
C	3.38122600	-2.93100800	-2.27006100
C	2.76482400	-2.83532400	-3.56367700
C	2.92118400	-2.22165600	-1.20413300
P	4.28714400	2.75535700	1.88626100
O	5.07548300	3.01453400	3.13872500
O	3.52909500	3.90277800	1.28184100
O	5.26397300	2.17117500	0.71044500
C	6.16781600	1.12060800	1.04078700
C	6.77408600	0.53176700	-0.21146200
O	5.80821300	-0.11457900	-1.04454700
C	7.50608000	1.54143500	-1.12319800
O	8.88177400	1.43405700	-0.83412800
C	7.12511400	1.07786600	-2.54063400
C	6.49894800	-0.29112400	-2.27128100
N	5.59666200	-0.77630100	-3.30475000
C	6.20388100	-1.50096900	-4.36408400
O	7.39642200	-1.77554200	-4.27990200
N	5.44833700	-1.80662600	-5.45947100
C	4.16125700	-1.53665300	-5.46150900
C	3.45340200	-0.98960400	-4.30860800
C	4.28817900	-0.38723000	-3.36386900
H	-0.51963000	0.89490400	1.85269300
H	-0.51683400	-0.88631600	1.84674800
H	1.47070400	0.09972900	2.99731800
H	1.69270300	1.98861100	0.96924800
H	3.82460300	0.86495000	-0.28777900
H	2.19890500	0.22269200	-0.67040300
H	4.05495100	-0.82254700	1.54521300
H	1.94545800	-1.74591200	-1.21400500
H	6.98739600	1.51554900	1.65231600
H	5.66465800	0.33206200	1.60993900
H	7.51870700	-0.21319100	0.10867900
H	7.16092300	2.56596800	-0.93025400

H	7.98532700	1.01401200	-3.20982900
H	6.36969800	1.73271100	-2.98385500
H	7.27206400	-1.05755300	-2.15706500
H	3.94064300	0.27178900	-2.57935000
H	6.26616500	-3.71897700	-0.82981500
C	9.63583200	2.50278200	-1.36788500
H	10.67719900	2.33546800	-1.09027800
H	9.56171400	2.54536200	-2.46210500
H	9.30044300	3.46454900	-0.95789000
C	-1.36506700	0.00075700	-0.45821200
H	-1.30335800	-0.00212900	-1.54700500
H	-1.90924200	-0.89272000	-0.12455200
H	-1.91851400	0.89047300	-0.12967700
H	1.70387000	-2.60593100	-3.59308600
H	3.10856400	-3.53584200	-4.31847300
Na	4.37170400	5.28250300	3.06071600
H	2.47802000	-0.54499800	-4.47018600
N	3.45451900	-1.82257000	-6.56256900
H	3.92587400	-2.22836000	-7.35644500
H	2.47054100	-1.61947700	-6.62851600

5'-T(5m-5)(¹C_{5H})-3'

O	0.03018800	-0.00361600	-0.02961500
C	0.00946500	0.01372500	1.37914800
C	1.43429900	0.00492100	1.89371700
O	2.03890300	-1.25221800	1.55091900
C	2.32203900	1.10010700	1.26275300
O	3.27642300	1.51136800	2.25338700
C	3.02178900	0.32499200	0.16190700
C	3.27749400	-0.97123600	0.91978700
N	3.71258900	-2.08408600	0.09794400
C	4.94664900	-2.65576800	0.38757100
O	5.55314000	-2.47066500	1.42718100
N	5.42811700	-3.48398200	-0.60531700
C	4.92883800	-3.65277100	-1.89407700
O	5.52271900	-4.34283200	-2.70769300
C	3.67514200	-2.95121600	-2.14434000
C	3.18714400	-2.80701000	-3.54814600
C	3.12741200	-2.24686300	-1.13853400
P	4.27983000	2.76082200	1.93122500
O	5.04141600	3.03445600	3.19695000
O	3.53038500	3.90033100	1.30157500
O	5.28038400	2.16693100	0.78169700
C	6.19568300	1.13875500	1.15024900
C	6.87137800	0.55903100	-0.07060800
O	6.00196500	-0.23006100	-0.88709400
C	7.51175300	1.59882900	-1.01995600
O	8.88431800	1.65731500	-0.69958300
C	7.22050600	1.02072600	-2.41531500
C	6.76959700	-0.40098300	-2.07702800
N	6.01950800	-1.08755500	-3.10864700
C	6.76605800	-1.92393000	-3.95986900
O	7.92963700	-2.19439100	-3.68660400
N	6.18174100	-2.36915500	-5.12732800
C	4.90372600	-2.21305600	-5.31530700
C	3.95151300	-1.62358100	-4.30212000
C	4.73118300	-0.69245100	-3.43731800

H	-0.50709800	0.91296800	1.74934100
H	-0.52139500	-0.86804600	1.76854600
H	1.42796700	0.12516100	2.98314500
H	1.74635200	1.96303200	0.91839000
H	3.92621700	0.78773600	-0.22122800
H	2.30748200	0.16364900	-0.64602800
H	4.05394600	-0.84295400	1.67485700
H	2.18264100	-1.72691700	-1.25963800
H	6.97673200	1.55909500	1.79385500
H	5.68863100	0.34042100	1.70341700
H	7.68982300	-0.08267800	0.29126100
H	7.05347600	2.58717500	-0.88670900
H	8.09854300	1.03151700	-3.06482500
H	6.40039600	1.55084500	-2.90750600
H	7.63509200	-1.03315700	-1.86149900
H	4.25313900	-0.00755100	-2.74899600
H	6.31987900	-3.92178000	-0.40349500
C	9.53095500	2.77548400	-1.27107800
H	10.57686400	2.73780300	-0.96428300
H	9.48102600	2.75724300	-2.36739900
H	9.08303800	3.71356600	-0.91723000
C	-1.27013100	-0.00500900	-0.57865700
H	-1.16711100	-0.02075800	-1.66422500
H	-1.83507300	-0.88975500	-0.25644500
H	-1.82775000	0.89300900	-0.28127200
H	2.12176900	-2.56876000	-3.54277300
H	3.32214900	-3.73694600	-4.10661800
Na	4.34051100	5.29965500	3.08115900
H	3.19077000	-1.05078700	-4.84049000
N	4.35955900	-2.63648600	-6.46097100
H	4.94590700	-3.08382400	-7.14997500
H	3.37758700	-2.52626100	-6.65618900

INT_{C6/UC}

O	0.61900500	-1.05992700	-0.07773600
C	0.45702800	-0.25040400	1.06611500
C	1.81247700	0.03009600	1.68833800
O	2.38178000	-1.13383900	2.29357200
C	2.89089000	0.49422400	0.70509000
O	3.76759600	1.38793200	1.40225100
C	3.49720100	-0.83273000	0.23838200
C	3.16927400	-1.82210700	1.38012600
N	2.50348900	-3.05518700	0.82198300
C	1.26641400	-3.52223700	1.22810600
O	0.61348300	-3.12643000	2.17494000
N	0.76952700	-4.55668200	0.43506200
C	1.34968200	-5.20007600	-0.63969200
O	0.78065900	-6.11878300	-1.20628300
C	2.69081100	-4.69039400	-0.98582500
C	3.40460300	-5.32402100	-1.99839700
C	3.17585600	-3.64262400	-0.22022300
P	5.35210800	1.17687700	1.69825300
O	5.79107200	2.38667600	2.47662900
O	6.14024700	0.84833300	0.45972000
O	5.36818600	-0.15639600	2.63999700
C	4.84916300	-0.01375400	3.96448600
C	5.16827900	-1.26307700	4.75156100

O	4.43141600	-2.35861200	4.21004600
C	6.65556800	-1.67098500	4.71702500
O	7.04084800	-1.98188000	6.04053400
C	6.64029500	-2.90493700	3.81094400
C	5.28235100	-3.49051300	4.17270800
N	4.72567700	-4.46142700	3.24009900
C	3.49644500	-5.06900600	3.62204600
O	2.99895100	-4.76089500	4.69687700
N	2.93357500	-5.96808200	2.76333700
C	3.58041300	-6.34308400	1.67364000
C	4.87222400	-5.82995400	1.31409700
C	5.38852800	-4.87889900	2.12443900
H	-0.02482100	0.70291600	0.79781800
H	-0.16560900	-0.76524300	1.81014100
H	1.68312900	0.76895200	2.48451400
H	2.46953600	1.05697900	-0.13173100
H	4.56675600	-0.75939300	0.04262100
H	2.98331000	-1.13089000	-0.67562500
H	4.05424600	-2.17335200	1.91447200
H	4.16342400	-3.23895400	-0.41541700
H	5.31171000	0.85176300	4.45034700
H	3.76394200	0.12521700	3.92029600
H	4.88344900	-1.10052900	5.79925000
H	7.29101400	-0.87158000	4.31322100
H	7.47943100	-3.58190400	3.98034100
H	6.63690600	-2.56192900	2.77176400
H	5.30770300	-3.96538100	5.16095700
H	-0.13233600	-4.90649900	0.73794600
C	-0.61260100	-1.55490000	-0.55812100
H	-0.39662300	-2.17520200	-1.42976300
H	-1.10949700	-2.16507300	0.20860800
H	-1.28314300	-0.73620100	-0.85133600
C	8.43957000	-2.11127100	6.19486600
H	8.63087200	-2.30145700	7.25150500
H	8.84486400	-2.94423600	5.60732400
H	8.95395300	-1.18896400	5.89417800
Na	7.51106200	2.75927000	0.92374100
H	4.40126700	-4.99970500	-2.26913900
H	2.94384300	-6.13551800	-2.54529500
H	6.34816800	-4.42052400	1.92457000
H	5.39264200	-6.16072800	0.42544100
N	3.00024700	-7.26952600	0.88571700
H	3.34385600	-7.42436800	-0.05027900
H	2.04524600	-7.52967500	1.08491800

TS_{C6/UC}

O	0.02742300	-0.07058100	-0.06150100
C	-0.01872300	0.03310800	1.34152900
C	1.38313700	0.02608500	1.92862400
O	1.87480400	-1.31848200	2.05464400
C	2.43442300	0.76392800	1.08422800
O	3.43664000	1.22834600	2.00359600
C	2.93844100	-0.36201300	0.19569200
C	2.96805800	-1.50201500	1.19913100
N	2.97591500	-2.82790000	0.55610400
C	1.83091800	-3.47203900	0.10337800
O	0.70131700	-3.04328400	0.22052500

N	2.09687200	-4.69406800	-0.50360600
C	3.32723400	-5.26986500	-0.81048700
O	3.39287700	-6.37443300	-1.32575200
C	4.47219900	-4.42238700	-0.47353800
C	5.80949400	-4.86315400	-0.70793400
C	4.22259000	-3.27203600	0.21439900
P	4.97306900	1.54606000	1.55194800
O	5.52736200	2.53579600	2.53825700
O	5.06854200	1.89430100	0.09393300
O	5.70249300	0.08854800	1.76257600
C	5.90193200	-0.29691400	3.12340300
C	6.53568000	-1.66133800	3.23077600
O	5.69037900	-2.67477100	2.71487500
C	7.88254900	-1.88623000	2.52528800
O	8.90364100	-1.56756400	3.43734200
C	7.82080700	-3.38464800	2.12547100
C	6.50480000	-3.84489200	2.76534400
N	5.82162300	-4.96970400	2.15146600
C	4.63041000	-5.38695300	2.80296000
O	4.25162600	-4.76829900	3.78939400
N	3.94700700	-6.45787900	2.29675700
C	4.54348000	-7.26074400	1.42649100
C	5.84016900	-7.01064200	0.91017600
C	6.38264900	-5.74726900	1.14545800
H	-0.53352000	0.96174200	1.63441100
H	-0.56587200	-0.81552300	1.77629700
H	1.34325300	0.45713800	2.93398800
H	2.01958600	1.61070600	0.53215000
H	3.90904900	-0.16750900	-0.25930500
H	2.18874000	-0.56991300	-0.56923100
H	3.89235500	-1.49188100	1.78264800
H	5.03401600	-2.63341900	0.54582100
H	6.55726700	0.42623200	3.61960500
H	4.93762300	-0.31174400	3.64846600
H	6.71193800	-1.83886900	4.30522400
H	7.96102900	-1.25191300	1.63156000
H	8.68657000	-3.93896000	2.49433200
H	7.77733400	-3.47747900	1.03851600
H	6.65518500	-4.09240100	3.82502400
H	1.27303500	-5.21421500	-0.78351300
C	-1.21615700	-0.44563000	-0.60799300
H	-1.10446000	-0.46464200	-1.69320400
H	-1.50882400	-1.44319400	-0.25728700
H	-2.00338100	0.27325200	-0.34153400
C	10.17244400	-1.45795500	2.82493500
H	10.88761000	-1.19523500	3.60525700
H	10.48215900	-2.40372800	2.36207900
H	10.17157900	-0.67535000	2.05492900
Na	6.21463900	3.91083600	0.73212600
H	6.58331500	-4.10018700	-0.72443100
H	5.95085800	-5.68454400	-1.40095400
H	7.42975400	-5.56251400	0.93649600
H	6.31803500	-7.69035500	0.21735000
N	3.88300500	-8.39285600	1.06564300
H	4.10580600	-8.79556300	0.16756900
H	2.90704000	-8.42286500	1.32479200

O	-0.03770600	0.05989500	0.00320900
C	-0.02596100	0.03705200	1.40967600
C	1.40468300	-0.01549800	1.90538100
O	1.94556100	-1.33688700	1.71408500
C	2.34839100	0.94991000	1.15770700
O	3.29903300	1.42383200	2.12468000
C	2.98622900	0.01723600	0.14019600
C	3.16000100	-1.20268500	1.02342000
N	3.56184800	-2.41510900	0.30319300
C	2.69093200	-3.23076800	-0.40547500
O	1.48620500	-3.09086200	-0.44809900
N	3.33591800	-4.26684500	-1.06893100
C	4.70324800	-4.49403100	-1.22100700
O	5.10902200	-5.46481800	-1.84734900
C	5.53274700	-3.48522400	-0.58362000
C	7.02569700	-3.52358300	-0.65578700
C	4.92029300	-2.53032500	0.14150800
P	4.72940800	2.08290400	1.69306700
O	5.11006200	3.06462000	2.76639000
O	4.69934700	2.58512500	0.27717700
O	5.73863300	0.78678600	1.74440500
C	6.21254900	0.42714500	3.04469000
C	7.18891200	-0.72153700	2.98912200
O	6.57403000	-1.91594400	2.54849200
C	8.40151600	-0.59049900	2.06718500
O	9.36143400	0.22561900	2.68536000
C	8.83260500	-2.06627200	1.86773700
C	7.65400800	-2.86266500	2.47080100
N	7.21525300	-4.06256400	1.80000600
C	6.32351300	-4.84430200	2.53460300
O	6.02243900	-4.51455400	3.67545100
N	5.75898600	-5.98133300	1.97257700
C	6.25904900	-6.46262200	0.85831400
C	7.32756900	-5.83115100	0.15214400
C	7.65809200	-4.41960500	0.45617600
H	-0.50984300	0.94114000	1.81237400
H	-0.57153300	-0.83872200	1.79241400
H	1.41965300	0.21800600	2.97546100
H	1.81860100	1.79601400	0.71462300
H	3.91718500	0.39388800	-0.28246100
H	2.26309300	-0.20966400	-0.64670500
H	3.97557800	-1.03500600	1.73888000
H	5.50038600	-1.77793800	0.66584800
H	6.71521000	1.28556000	3.49939600
H	5.36662500	0.14003700	3.68225400
H	7.57183200	-0.85115200	4.01688500
H	8.08483100	-0.14843900	1.11017000
H	9.74915700	-2.26387400	2.42900300
H	9.02697000	-2.28909700	0.81943300
H	7.89378300	-3.14310800	3.50193300
H	2.71598600	-4.90981400	-1.54842300
C	-1.34911300	0.07115500	-0.51512500
H	-1.27177600	0.09593100	-1.60273100
H	-1.90291700	-0.82787500	-0.21283800
H	-1.90517200	0.95473600	-0.17300000
C	10.43069900	0.55825300	1.82302500
H	11.09874500	1.22085700	2.37438900

H	10.98941900	-0.33397800	1.51214900
H	10.06695300	1.07503000	0.92501200
Na	5.36488700	4.72970400	1.08869000
H	7.41405400	-2.50647800	-0.55001400
H	7.35700800	-3.90453500	-1.62612300
H	8.74589300	-4.29484800	0.39340800
H	7.76921600	-6.29229200	-0.72170600
N	5.77243100	-7.63366700	0.37442200
H	5.84778500	-7.79663300	-0.61915200
H	4.92962600	-7.97497600	0.81493400

Table S5 Cartesian coordinates of OH^{*}, H₂O, CH₃OH, NH₃, 5'-TT-3', 5'-TC-3', 5'-CT-3', and the eight closed-shell intrastrand cross-links shown in Figure S1, respectively.

OH [*]			
O	0.94556200	-0.03206500	0.00031800
H	0.61962800	0.88834300	0.00031800
H ₂ O			
O	1.06883700	0.15997900	-0.04022800
H	2.03081000	0.20910300	-0.04022800
H	0.79398000	1.08322900	-0.04022800
CH ₃ OH			
C	-0.99109100	0.85666600	0.02405000
H	-0.62183000	-0.17069300	0.03831200
H	-0.63369000	1.33629100	-0.89517700
H	-2.08694000	0.82639400	-0.00303000
O	-0.49993300	1.49455000	1.18828200
H	-0.83119300	2.39919500	1.18728200
NH ₃			
N	0.32878300	0.43793200	0.00576000
H	0.73472200	-0.49427200	0.00571400
H	0.73472900	0.90400900	0.81305700
H	0.73461300	0.90399300	-0.80160000
5'-TT-3'			
O	-0.07860300	-0.12060300	0.15511600
C	0.05907400	-0.06102400	1.55839000
C	1.53234500	-0.00309200	1.91017400
O	2.14732100	-1.27383400	1.66612300
C	2.31525800	1.02530000	1.08249300
O	3.28420200	1.61443300	1.95368200
C	2.93311100	0.16863200	-0.01385000
C	3.14929700	-1.18092500	0.66810400
N	3.01212900	-2.32080700	-0.23960300
C	4.04504100	-3.23752500	-0.34293500
O	5.08267000	-3.17899700	0.29534800
N	3.80861100	-4.24218900	-1.25842900

C	2. 67822100	-4. 44318300	-2. 04822000
O	2. 62710700	-5. 37934600	-2. 82939300
C	1. 60818100	-3. 47799500	-1. 81767100
C	0. 32664200	-3. 66085300	-2. 57060700
C	1. 82375900	-2. 49001600	-0. 92713600
P	4. 45110700	2. 58940000	1. 35680300
O	4. 73406100	3. 64633000	2. 38740400
O	4. 13145300	3. 04744800	-0. 03815300
O	5. 70642400	1. 54628300	1. 25484500
C	6. 11727200	0. 95076400	2. 48811700
C	7. 33853300	0. 09869700	2. 23700500
O	6. 98360800	-0. 95207600	1. 34017400
C	8. 52038400	0. 85063200	1. 60055900
O	9. 69798800	0. 35889700	2. 21021400
C	8. 42932000	0. 44519500	0. 13124800
C	7. 88507100	-0. 97689800	0. 24658000
N	7. 17371400	-1. 45854100	-0. 92598400
C	7. 44801700	-2. 73953300	-1. 38188000
O	8. 32275300	-3. 45370700	-0. 92639900
N	6. 65820100	-3. 13716300	-2. 44111200
C	5. 60698800	-2. 44626500	-3. 03616300
O	4. 98317900	-2. 94288300	-3. 96188600
C	5. 33908200	-1. 13569300	-2. 45114900
C	4. 22119600	-0. 33687500	-3. 04800700
C	6. 11333300	-0. 72972300	-1. 42315200
H	-0. 44583600	0. 83369900	1. 95302500
H	-0. 39113600	-0. 94672700	2. 02988400
H	1. 63153200	0. 23163400	2. 97495100
H	1. 66919000	1. 80819200	0. 67709100
H	3. 85406000	0. 59574300	-0. 40299300
H	2. 21155100	0. 07701700	-0. 82905000
H	4. 14977100	-1. 26847500	1. 10274400
H	-0. 40111700	-2. 89723800	-2. 29006400
H	0. 50088400	-3. 59920100	-3. 64869100
H	-0. 10324400	-4. 64627100	-2. 36952500
H	1. 05888000	-1. 75772500	-0. 67876100
H	6. 34883000	1. 73075300	3. 22202600
H	5. 30635700	0. 32497800	2. 87865900
H	7. 67308800	-0. 32498300	3. 19147200
H	8. 43942200	1. 93667700	1. 74551200
H	9. 38890200	0. 47804100	-0. 38702500
H	7. 72252400	1. 09841700	-0. 38500200
H	8. 68878200	-1. 69348100	0. 42684200
H	4. 18629800	0. 67086200	-2. 63040200
H	4. 35261000	-0. 26244300	-4. 13088500
H	5. 94493100	0. 21674300	-0. 91552600
H	4. 55962000	-4. 91537000	-1. 35998300
H	6. 87527500	-4. 05209100	-2. 81986200
C	10. 83737600	1. 14774500	1. 93448900
H	11. 67544100	0. 70102500	2. 47062200
H	11. 07539100	1. 17056000	0. 86392300
H	10. 69327800	2. 17912400	2. 28245400
Na	4. 42047000	5. 30094900	0. 69130000
C	-1. 42844800	-0. 24383500	-0. 24683600
H	-1. 44236400	-0. 27858100	-1. 33691900
H	-1. 87508900	-1. 16373100	0. 15204400
H	-2. 02007100	0. 61455800	0. 09576300
H	3. 25573400	-0. 82599100	-2. 87423000

5'-TC-3'

O	0.34663400	-0.35201400	-0.13953600
C	0.11853600	-0.13780800	1.23599800
C	1.45053200	-0.03651700	1.95284500
O	2.08609200	-1.31946500	1.99266200
C	2.44589400	0.91055600	1.27069900
O	3.20901400	1.52482600	2.31408200
C	3.27993200	-0.04030900	0.42496800
C	3.31325600	-1.30649600	1.28227700
N	3.41070000	-2.54211400	0.50783900
C	4.47138000	-3.40421500	0.73301000
O	5.31062300	-3.24660000	1.60219800
N	4.50900000	-4.48010100	-0.13177800
C	3.65449800	-4.75817900	-1.19385000
O	3.88275400	-5.69603400	-1.94413100
C	2.51330000	-3.85526100	-1.29863400
C	1.49163300	-4.13542100	-2.35736400
C	2.45485500	-2.80624400	-0.45423400
P	4.45959800	2.51257900	1.95090400
O	4.48254900	3.61554700	2.97250800
O	4.44143400	2.90829000	0.50177700
O	5.73484000	1.51281400	2.17377000
C	5.91927700	1.02716600	3.50641100
C	7.17407400	0.18594700	3.56236700
O	7.01006500	-0.94306800	2.70841500
C	8.45629000	0.90555500	3.11298100
O	9.48870100	0.48608300	3.98477300
C	8.65997700	0.38268900	1.69341300
C	8.09592500	-1.03415600	1.79814600
N	7.59733500	-1.58076900	0.54656500
C	7.95464400	-2.89883500	0.16496000
O	8.78169800	-3.51478600	0.82827800
N	7.36615800	-3.41781000	-0.95254500
C	6.47718000	-2.71101900	-1.63116900
N	5.93877600	-3.27054400	-2.73092200
C	6.05298500	-1.39759500	-1.23597000
C	6.63003300	-0.89801700	-0.11868900
H	-0.44941800	0.79253400	1.38888400
H	-0.46010800	-0.96842800	1.66598400
H	1.27207400	0.29670500	2.98048900
H	1.95092500	1.68048600	0.67355800
H	4.26753800	0.36284300	0.21399700
H	2.75871800	-0.22623700	-0.51677400
H	4.16782100	-1.31407700	1.96564100
H	1.63332400	-2.09344100	-0.47022400
H	6.00217100	1.86933600	4.20205900
H	5.05664900	0.41410200	3.79244900
H	7.31598600	-0.15013500	4.59690900
H	8.34782200	1.99845600	3.15008700
H	9.70362100	0.38800800	1.37527000
H	8.07481500	0.98568100	0.99492200
H	8.84393500	-1.74111100	2.15928700
H	5.17003900	-2.83114100	-3.21191100
H	5.29196600	-0.85258900	-1.77898300
H	6.35202900	0.05778000	0.31709000
H	5.34748900	-5.04751800	-0.05850000

H	6.11964400	-4.24636800	-2.91462500
C	-0.85534300	-0.51838800	-0.86444000
H	-0.58659700	-0.68158800	-1.90891000
H	-1.42094500	-1.38385600	-0.49554900
H	-1.48748300	0.37547000	-0.78811900
H	1.05500500	-5.12914800	-2.22301200
H	0.69048900	-3.39457900	-2.32955900
C	10.66644100	1.25635100	3.86191000
H	11.37636800	0.87853100	4.59848100
H	11.11514600	1.17134300	2.86463200
H	10.46454500	2.31632600	4.06497300
Na	4.45457000	5.19346700	1.19043300
H	1.95197000	-4.11681500	-3.34968200

5'-CT-3'

O	-4.77049800	0.42582800	0.35420500
C	-4.54924200	0.37030900	1.74692400
C	-3.05773400	0.37805500	2.01713200
O	-2.48101500	-0.87283900	1.63128800
C	-2.30370500	1.46549200	1.23964600
O	-1.27916500	1.96292300	2.10537300
C	-1.75792200	0.70053900	0.04216500
C	-1.52583700	-0.70600900	0.59242700
N	-1.72275500	-1.76102300	-0.39899900
C	-0.68946200	-2.69636300	-0.65637600
O	0.35176600	-2.64322100	-0.00753600
N	-0.89830000	-3.61560400	-1.64077400
C	-2.04846400	-3.65191900	-2.29249900
C	-3.15300400	-2.78928700	-1.97858700
C	-2.93286700	-1.86247600	-1.01917800
P	-0.16020900	3.01065900	1.54212300
O	0.18065200	3.95884200	2.65848100
O	-0.57500600	3.61028500	0.22852900
O	1.09616200	2.00398500	1.25593300
C	1.59707600	1.31019700	2.40141900
C	2.78707400	0.47519100	1.99359400
O	2.35499400	-0.50907400	1.05727300
C	3.92596300	1.26331900	1.32216200
O	5.14014100	0.72759200	1.81253100
C	3.72659300	0.95065900	-0.15903000
C	3.18506400	-0.47564600	-0.09136800
N	2.40642000	-0.89015300	-1.24390300
C	2.64033200	-2.14849200	-1.77958900
O	3.51234200	-2.90406900	-1.38676700
N	1.83076500	-2.45977800	-2.84958600
C	0.75917500	-1.73201800	-3.35302800
O	0.11453200	-2.14748800	-4.30429900
C	0.50487400	-0.47303300	-2.65720800
C	-0.65086800	0.34972700	-3.13705400
C	1.32149700	-0.13495300	-1.63877900
H	-5.01341200	1.23750200	2.24095700
H	-4.98915200	-0.54357100	2.17234600
H	-2.89771500	0.52070800	3.09115200
H	-2.95681300	2.28914300	0.94013400
H	-0.85203400	1.14939900	-0.35969000
H	-2.52227200	0.68683100	-0.73856300
H	-0.50811600	-0.83927500	0.96912500

H	-3.69256200	-1.16132900	-0.68124700
H	1.89185200	2.02918400	3.17406900
H	0.81369500	0.65728600	2.80370100
H	3.19112600	-0.01452200	2.88818200
H	3.86587000	2.33811700	1.54156700
H	4.64620700	1.01509800	-0.74260200
H	2.98685500	1.63426000	-0.58124600
H	3.99722500	-1.19959200	0.00037000
H	-0.68600400	1.31806500	-2.63500900
H	-0.56969300	0.51786400	-4.21443700
H	1.17352300	0.77149900	-1.05789400
H	1.98094200	-3.37775600	-3.25048300
C	6.26473100	1.52570500	1.50527500
H	7.13437700	1.04174400	1.95131000
H	6.42621700	1.61509100	0.42389200
H	6.15656700	2.53374100	1.92660700
Na	-0.27013500	5.77788900	1.20908300
C	-6.14600400	0.38344900	0.03151100
H	-6.22919400	0.43368800	-1.05460800
H	-6.60521700	-0.54696700	0.38921800
H	-6.67870700	1.23364400	0.47636900
H	-4.10858000	-2.87518100	-2.47728500
N	-2.18427500	-4.56957700	-3.26553600
H	-1.36734900	-5.08815100	-3.54903200
H	-2.98961700	-4.57149000	-3.86976200
H	-1.59830100	-0.17406500	-2.96435900

5'-T(6-5m)T-3'

O	0.52047300	-1.00081400	1.02602200
C	1.11135200	-0.78766200	2.29045100
C	2.44745100	-0.09211600	2.10884500
O	3.43689200	-0.95683200	1.54412400
C	2.38927700	1.10117800	1.15259800
O	3.30714200	2.11213300	1.59690000
C	2.70328400	0.45350200	-0.19723100
C	3.49073600	-0.82936700	0.15881400
N	2.95118100	-2.02164300	-0.59055100
C	2.23179700	-3.02032700	0.05531100
O	2.29144100	-3.30550200	1.23714200
N	1.39704400	-3.74300100	-0.77969900
C	1.26744300	-3.65526500	-2.15318400
O	0.45119700	-4.35349200	-2.73980600
C	2.20312700	-2.72684000	-2.78362600
C	2.21796200	-2.71087500	-4.28914400
C	3.00631200	-1.96848300	-1.99311800
P	4.69622800	2.56026100	0.88048100
O	5.34085200	3.56333600	1.79690300
O	4.51224700	2.97019200	-0.55695200
O	5.54542300	1.17090100	0.84383500
C	6.15805900	0.68607400	2.04256400
C	7.61828700	0.40692700	1.75146000
O	7.71083600	-0.68564100	0.83500100
C	8.35069100	1.58642200	1.09487100
O	9.67311300	1.58237400	1.59477100
C	8.30709400	1.23898300	-0.39695700
C	8.34676300	-0.28884100	-0.36783800
N	7.64585700	-0.95820800	-1.46398600

C	8.21367100	-2.11334800	-1.99385300
O	9.36354800	-2.45431000	-1.79185600
N	7.35675400	-2.84614600	-2.78893400
C	6.00356900	-2.62271700	-3.03623300
O	5.36933600	-3.38687000	-3.74503000
C	5.47338500	-1.42432500	-2.39558100
C	4.03299600	-1.04420800	-2.63365900
C	6.31604700	-0.66547200	-1.66643700
H	0.45811100	-0.15945700	2.91574100
H	1.27797400	-1.74576300	2.79816700
H	2.82278600	0.21788800	3.08821100
H	1.40193000	1.56842000	1.15039900
H	3.25932600	1.13801100	-0.83605200
H	1.76593600	0.18362000	-0.68564600
H	4.54271900	-0.77025000	-0.10304100
H	1.92237600	-1.73629400	-4.68905900
H	3.21092100	-2.95822500	-4.67069700
H	1.50500800	-3.45175400	-4.65102400
H	6.07534700	1.43128000	2.83986300
H	5.64465200	-0.23353400	2.33773000
H	8.13040600	0.13842500	2.68202600
H	7.85201000	2.54086500	1.31779400
H	9.15233900	1.65067900	-0.95072400
H	7.38248300	1.61707100	-0.83749100
H	9.37098200	-0.66370200	-0.39806200
H	3.88667100	-0.01109500	-2.31610700
H	3.84897200	-1.05804300	-3.70789100
H	5.97372200	0.23790400	-1.16924200
H	0.84693100	-4.45444100	-0.31277400
H	7.76090000	-3.67841200	-3.20378600
C	10.37985600	2.77149300	1.30764700
H	11.36588700	2.67814800	1.76405300
H	10.50436700	2.92912200	0.22901000
H	9.86617400	3.64458300	1.73168900
Na	5.43325700	5.11026000	-0.00889300
C	-0.60304600	-1.85191700	1.11224700
H	-1.01735300	-1.95346400	0.10788100
H	-0.30453800	-2.84048700	1.48679200
H	-1.36701800	-1.43195000	1.77978600

5'-U(5-5m)T-3'

O	0.92529700	0.00200100	-0.92261300
C	0.19253100	0.51240300	0.17083800
C	1.05082800	0.36581100	1.41300000
O	1.19158700	-1.03195200	1.70003000
C	2.46762200	0.93036000	1.19775800
O	2.94817400	1.58161500	2.37682800
C	3.28713000	-0.31434100	0.92470300
C	2.55334200	-1.39675500	1.71554200
N	2.72814200	-2.71500600	1.10019200
C	3.46419300	-3.67598000	1.77882300
O	3.66864600	-3.65232200	2.97840200
N	3.95918200	-4.67705600	0.96513800
C	3.95553600	-4.73131000	-0.42923500
O	4.56884000	-5.60621200	-1.01680600
C	3.14713000	-3.68934300	-1.05945600
C	2.54764000	-2.78327100	-0.26753600

P	4. 02907900	2. 78391600	2. 11395800
O	4. 80006100	3. 00064200	3. 38416900
O	3. 33750000	3. 97425000	1. 50922700
O	4. 97935400	2. 14089600	0. 94679300
C	6. 19133200	1. 48483500	1. 30576800
C	6. 92001500	1. 07324400	0. 04619900
O	6. 24795600	-0. 00747100	-0. 62654600
C	7. 06056800	2. 21490900	-0. 98854800
O	8. 44253800	2. 37700900	-1. 24009500
C	6. 31446000	1. 66613100	-2. 20702300
C	6. 53999200	0. 17400800	-1. 99425200
N	5. 70622000	-0. 71924200	-2. 81512800
C	5. 97184000	-0. 66136600	-4. 17328900
O	6. 80496600	0. 08814600	-4. 65427800
N	5. 21611300	-1. 51984100	-4. 93884800
C	4. 29013000	-2. 46080900	-4. 49969500
O	3. 69436700	-3. 16576000	-5. 29918600
C	4. 12776900	-2. 51745100	-3. 05050600
C	3. 14217200	-3. 55577600	-2. 55091800
C	4. 84177400	-1. 65685100	-2. 28800800
H	-0. 05171800	1. 57324700	0. 01058400
H	-0. 74691300	-0. 04363500	0. 30150300
H	0. 56945500	0. 86354400	2. 26129400
H	2. 47411200	1. 62753300	0. 35464200
H	4. 32887700	-0. 22449300	1. 21826300
H	3. 24556900	-0. 52195000	-0. 14445500
H	2. 91920100	-1. 49113600	2. 74029400
H	1. 91414600	-1. 99339500	-0. 66797500
H	6. 83287900	2. 17140400	1. 86765300
H	5. 99884100	0. 61176800	1. 94035100
H	7. 93008000	0. 74416500	0. 32150600
H	6. 62893600	3. 15278100	-0. 61795500
H	6. 70425000	2. 03439600	-3. 15406700
H	5. 24242100	1. 87246200	-2. 13267800
H	7. 58877900	-0. 07935400	-2. 20388500
H	4. 79270300	-1. 64925600	-1. 20614800
H	4. 50299200	-5. 38713500	1. 44240900
H	5. 38582200	-1. 47400200	-5. 93726900
C	8. 74167500	3. 57617800	-1. 92494500
H	9. 82429300	3. 61398800	-2. 05111000
H	8. 26832400	3. 61407800	-2. 91398700
H	8. 41393400	4. 45045300	-1. 34721200
C	0. 21542400	0. 08100000	-2. 14178100
H	0. 85579400	-0. 34412500	-2. 91623300
H	-0. 72111800	-0. 48879700	-2. 09090900
H	-0. 01762800	1. 12312800	-2. 39435700
H	2. 14249100	-3. 28856700	-2. 91153600
H	3. 39061000	-4. 51762700	-3. 00849600
Na	4. 15987600	5. 30494800	3. 30393000

5'-T(5m-5)U-3'

O	1. 02618400	0. 25719600	-0. 82896500
C	0. 45559000	0. 58845800	0. 41856900
C	1. 45249300	0. 22175900	1. 50093200
O	1. 58273800	-1. 20594900	1. 52598900
C	2. 85277500	0. 79801100	1. 21935100
O	3. 49122500	1. 19197900	2. 43707700

C	3. 58322500	-0. 38393700	0. 61609300
C	2. 92579500	-1. 57737900	1. 30781600
N	2. 99202900	-2. 78204100	0. 47813800
C	3. 75212500	-3. 85514600	0. 92311300
O	4. 05861400	-4. 03207400	2. 08753300
N	4. 14375300	-4. 71805900	-0. 08258600
C	4. 01709600	-4. 54290800	-1. 46091500
O	4. 55003500	-5. 31807700	-2. 23657400
C	3. 18642400	-3. 40082500	-1. 83834600
C	3. 06006100	-3. 02459100	-3. 28186000
C	2. 68509000	-2. 62741100	-0. 85995200
P	4. 60567000	2. 38312500	2. 29459600
O	5. 49389800	2. 32757100	3. 50407300
O	3. 92983200	3. 69086700	1. 98826800
O	5. 41804000	1. 93778800	0. 94538500
C	6. 62496200	1. 19069100	1. 06682800
C	7. 23014200	1. 00162400	-0. 30675000
O	6. 47964100	0. 05358300	-1. 08941500
C	7. 29746300	2. 30342000	-1. 13992300
O	8. 64993900	2. 49031100	-1. 50848400
C	6. 41367100	1. 98007400	-2. 34724400
C	6. 63610200	0. 47497100	-2. 42591700
N	5. 71358800	-0. 26068800	-3. 30503400
C	5. 87138200	0. 01374400	-4. 65342900
O	6. 68669900	0. 81685300	-5. 07499000
N	5. 03039600	-0. 69449800	-5. 48132000
C	4. 10144800	-1. 66593900	-5. 12150200
O	3. 41766000	-2. 21624900	-5. 97044100
C	4. 04655400	-1. 94847400	-3. 69091000
C	4. 85173300	-1. 24298700	-2. 86271800
H	0. 23012700	1. 66444000	0. 46753800
H	-0. 47923600	0. 03151600	0. 57673300
H	1. 09045700	0. 57047700	2. 47376700
H	2. 78777700	1. 64907700	0. 53463500
H	4. 65780000	-0. 35854600	0. 76962700
H	3. 38457400	-0. 39643300	-0. 45583000
H	3. 41440000	-1. 83409300	2. 25045100
H	2. 03764300	-1. 77754400	-1. 06862400
H	7. 33884300	1. 74103100	1. 68796400
H	6. 44552700	0. 21836900	1. 54126600
H	8. 25360800	0. 62492900	-0. 18601600
H	6. 93511200	3. 16818200	-0. 57086400
H	6. 70384000	2. 51142100	-3. 25192700
H	5. 36002800	2. 16576500	-2. 11781900
H	7. 65434400	0. 26579900	-2. 78229300
H	4. 88467900	-1. 40755000	-1. 79256600
H	4. 70408400	-5. 50586300	0. 22286600
H	5. 12155300	-0. 48991400	-6. 47010400
C	8. 91116800	3. 78564700	-2. 00869400
H	9. 97542200	3. 83230700	-2. 24226600
H	8. 33897300	3. 99864200	-2. 92022900
H	8. 67120600	4. 55131600	-1. 25908900
C	0. 15736600	0. 52047600	-1. 91171100
H	0. 67730600	0. 22376800	-2. 82384600
H	-0. 77269000	-0. 05502300	-1. 82023300
H	-0. 09175900	1. 58785800	-1. 96629500
H	2. 04631700	-2. 67146900	-3. 50196100
H	3. 22756000	-3. 90436000	-3. 90967000

Na	4. 95963200	4. 61424500	3. 93601300
5'-T(5m-6)T-3			
O	-0. 11795800	0. 47940100	-0. 27344400
C	-0. 19994400	0. 47535600	1. 13143400
C	1. 17874000	0. 26234800	1. 72044000
O	1. 57124200	-1. 11480200	1. 55071500
C	2. 27786800	1. 11319900	1. 04384300
O	3. 21087600	1. 47640600	2. 07677400
C	2. 87517100	0. 10743800	0. 07384500
C	2. 85715200	-1. 10323800	0. 98640500
N	3. 24468800	-2. 35562500	0. 33934700
C	2. 43715200	-3. 03327100	-0. 56427000
O	1. 27374400	-2. 76514000	-0. 78415700
N	3. 09266500	-4. 07783600	-1. 19672500
C	4. 45300000	-4. 40076500	-1. 18124800
O	4. 87814800	-5. 30366300	-1. 88297900
C	5. 24268800	-3. 54989100	-0. 30258600
C	6. 74787600	-3. 65730200	-0. 22789400
C	4. 59815600	-2. 58971800	0. 38317900
P	4. 76004200	1. 89022900	1. 77184500
O	5. 21743700	2. 75899100	2. 90965700
O	4. 92579300	2. 42637400	0. 37869300
O	5. 54398900	0. 44156100	1. 83990900
C	5. 94630900	-0. 00859100	3. 13552200
C	6. 96885000	-1. 11974000	3. 06634000
O	6. 40482400	-2. 37364800	2. 69493900
C	8. 13384000	-0. 96627300	2. 08614200
O	9. 03270800	-0. 01474800	2. 58651700
C	8. 68432200	-2. 41046000	2. 01597100
C	7. 53705600	-3. 24036400	2. 64472300
N	7. 21921200	-4. 53542800	2. 05437900
C	7. 21128800	-5. 58132800	2. 98140400
O	7. 10095000	-5. 41616300	4. 18342700
N	7. 37113400	-6. 83401500	2. 44352800
C	7. 61361000	-7. 14943100	1. 11577700
O	7. 86733600	-8. 29775400	0. 79131400
C	7. 45708100	-6. 03262400	0. 17873200
C	7. 55873400	-6. 43984000	-1. 26278100
C	7. 20261400	-4. 79315100	0. 66406200
H	-0. 60214100	1. 43351100	1. 49642300
H	-0. 86568700	-0. 32743400	1. 48287700
H	1. 15073700	0. 49284000	2. 79109300
H	1. 88190400	2. 01563100	0. 57342200
H	3. 86616300	0. 37503700	-0. 29097700
H	2. 18155300	-0. 06003700	-0. 75367200
H	3. 59891000	-0. 97530200	1. 78172300
H	5. 14979600	-1. 91230200	1. 02212200
H	6. 39433600	0. 82614300	3. 68024700
H	5. 07368400	-0. 36310200	3. 69959600
H	7. 39673600	-1. 20398400	4. 07974000
H	7. 73967900	-0. 64281900	1. 10985000
H	9. 57229200	-2. 48402100	2. 64903800
H	8. 96279800	-2. 73190500	1. 01187400
H	7. 80603600	-3. 47557300	3. 67503900
H	7. 51264800	-5. 59869500	-1. 94839100
H	8. 50322500	-6. 97228000	-1. 40471400

H	6.75007700	-7.12588100	-1.52458100
H	2.51859100	-4.60751200	-1.84291300
H	7.40107500	-7.59373100	3.11374500
C	-1.38784800	0.59502700	-0.87626600
H	-1.23864900	0.60402200	-1.95657200
H	-2.03185100	-0.25282300	-0.60740700
H	-1.88947800	1.52423200	-0.57345200
C	10.05385500	0.30886500	1.66269000
H	10.68020300	1.07172400	2.12597700
H	10.67198200	-0.56629100	1.42535400
H	9.63009000	0.70386500	0.73019800
Na	5.93586800	4.38713600	1.34495400
H	7.12319700	-2.69985800	0.13076200
H	7.15232200	-3.80365100	-1.22953200

5'-U_{5,6H}(6-5m)T-3'

O	0.00004300	0.08806600	-0.10742100
C	-0.05125100	0.10179300	1.30082000
C	1.35911900	0.07410600	1.85606100
O	1.96507500	-1.18320100	1.54275500
C	2.28182600	1.14996400	1.25772800
O	3.19856000	1.53626200	2.29271900
C	2.97505500	0.37766700	0.14571600
C	3.19765600	-0.95025300	0.85867200
N	3.52443600	-2.08909600	0.04079400
C	4.42030000	-2.98676100	0.55919900
O	4.95646300	-2.88054400	1.64948000
N	4.71972600	-4.08416100	-0.25557500
C	3.98684900	-4.54690700	-1.33059900
C	2.80105100	-3.68515100	-1.67710800
C	2.98706700	-2.21157300	-1.31685700
P	4.52349100	2.41411900	1.91804900
O	4.96429300	3.11760100	3.17069600
O	4.28074900	3.25335100	0.69472900
O	5.61265700	1.26300600	1.50105400
C	6.31761100	0.57244900	2.53666800
C	7.67234900	0.14301300	2.01578800
O	7.50880600	-0.92713000	1.08173400
C	8.44260300	1.25306500	1.27864200
O	9.80289800	1.12102300	1.64159400
C	8.21099100	0.90084800	-0.19151900
C	8.18570900	-0.62294300	-0.12244500
N	7.46267800	-1.28393100	-1.20327900
C	8.11500400	-2.23918400	-1.96873300
O	9.29986200	-2.49849200	-1.86502900
N	7.29775500	-2.87566300	-2.88134400
C	5.92999900	-2.70339100	-3.07801100
O	5.32915000	-3.38219500	-3.89651100
C	5.32553600	-1.68058700	-2.23113600
C	3.85076300	-1.43005300	-2.34130100
C	6.11277700	-1.04742200	-1.33660200
H	-0.56784600	1.00554400	1.66045000
H	-0.60119100	-0.77506600	1.67473600
H	1.31308700	0.20165200	2.94394800
H	1.73870700	2.02915200	0.90242600
H	3.88751800	0.85957300	-0.20248200
H	2.26329700	0.27169600	-0.67400200

H	4.00812400	-0.84743000	1.58408000
H	1.99219000	-1.75596000	-1.29547200
H	6.44906600	1.23507600	3.39726900
H	5.75118700	-0.31563700	2.84083900
H	8.27948700	-0.20507700	2.85957700
H	8.06843100	2.25246000	1.54047900
H	8.98876400	1.27547000	-0.85833600
H	7.24058100	1.28710900	-0.51562200
H	9.19404900	-1.04292300	-0.12956400
H	3.66250100	-0.36299900	-2.21424400
H	3.51785200	-1.69968300	-3.34731900
H	5.72262400	-0.31640400	-0.63236300
H	7.75339800	-3.58241500	-3.44760500
C	10.59688100	2.22041700	1.24456600
H	11.60397600	2.04257000	1.62342800
H	10.64362900	2.32597800	0.15385400
H	10.21105500	3.15616900	1.67016500
Na	4.80545200	5.19007200	1.99489000
C	-1.28811400	0.09835100	-0.68375800
H	-1.16267000	0.08713200	-1.76704100
H	-1.86598500	-0.78373900	-0.37764700
H	-1.84572000	0.99884500	-0.39365700
H	2.59201800	-3.80516100	-2.74059600
H	1.95241700	-4.09366000	-1.11602100
O	4.26501200	-5.59075500	-1.88238300
H	5.43380600	-4.69991300	0.11596000

5'-U_{5,6H}(5-5m)T-3'

O	-0.15241300	-0.17863500	0.09996200
C	-0.09609700	-0.07355900	1.50491300
C	1.34701200	0.12427800	1.92720900
O	2.07773200	-1.09109300	1.76286500
C	2.06934500	1.18576800	1.08802100
O	2.97502800	1.88203800	1.95319200
C	2.81604500	0.35370200	0.05145300
C	3.12118300	-0.94211000	0.80488000
N	3.15680700	-2.12058200	-0.03371000
C	4.17296600	-3.02197400	0.12053100
O	5.14855900	-2.87318200	0.83698600
N	4.04075700	-4.19073900	-0.64433200
C	3.12794400	-4.45364900	-1.65362400
C	2.24518000	-3.26992400	-1.98580700
C	1.91963100	-2.55573700	-0.67958800
P	3.66742500	3.25099200	1.39517800
O	4.20181500	3.99803300	2.58445200
O	2.74181700	3.98405900	0.46583200
O	4.89908800	2.67473900	0.48802800
C	5.98058800	2.07296300	1.19524600
C	6.93533800	1.44241200	0.21258600
O	6.38165600	0.23293000	-0.31466700
C	7.30126400	2.32960100	-1.00671600
O	8.69897000	2.53177000	-0.96170200
C	6.87933600	1.46128700	-2.19943400
C	7.00777800	0.07757400	-1.57563600
N	6.39493300	-1.02847900	-2.29136900
C	7.24102300	-1.95785300	-2.88427100
O	8.45579400	-1.88457100	-2.84955600

N	6.58094000	-2.97439500	-3.53621900
C	5.20744700	-3.16655400	-3.66271900
O	4.77418600	-4.10719000	-4.30770900
C	4.39040000	-2.16571200	-2.97935900
C	2.89467000	-2.33292100	-3.04757800
C	5.02373900	-1.14969200	-2.35743400
H	-0.69940700	0.78078600	1.84893600
H	-0.49063000	-0.98500400	1.97820800
H	1.37106400	0.41237100	2.98382000
H	1.37650100	1.90132700	0.63993400
H	3.72944600	0.84774500	-0.28352300
H	2.15667400	0.16805700	-0.79989300
H	4.09130200	-0.89021900	1.30607200
H	1.29074600	-1.68233800	-0.85556200
H	6.51145600	2.83657800	1.77309400
H	5.60577300	1.30672200	1.88516800
H	7.87214100	1.20774600	0.73615500
H	6.77639400	3.29219300	-0.98289000
H	7.51168500	1.60083000	-3.07776900
H	5.83376100	1.64740600	-2.46533200
H	8.06248400	-0.18771500	-1.45414700
H	4.48218200	-0.36524600	-1.84123200
H	7.17848400	-3.65155400	-3.99671700
C	9.13456700	3.56732400	-1.81887100
H	10.21388400	3.65868300	-1.69197200
H	8.91872200	3.34712300	-2.87176900
H	8.65690200	4.52049100	-1.55665800
C	-1.45818800	-0.44709900	-0.36484100
H	-1.41083800	-0.51580400	-1.45241300
H	-1.83504500	-1.39484700	0.04157000
H	-2.15095100	0.35651500	-0.08232000
H	2.40812000	-1.35557700	-2.96800100
H	2.66154400	-2.73613700	-4.03601600
Na	3.04364000	5.93896400	1.81596300
H	1.32131500	-3.67468100	-2.40458500
H	1.35915900	-3.21955500	-0.00881200
O	3.08193700	-5.53814800	-2.19409800
H	4.73416100	-4.90351400	-0.44917300

5'-T(5m-5)U_{5,6H}-3'

O	-0.01239800	0.04644700	0.05809600
C	-0.00776200	0.01175400	1.46648500
C	1.42638700	-0.01897900	1.95349500
O	2.01859700	-1.26847900	1.56186600
C	2.30682000	1.09177900	1.33780000
O	3.27847700	1.47555000	2.32245400
C	2.98478200	0.34377400	0.20506000
C	3.25155200	-0.96963800	0.92842600
N	3.68739200	-2.05752800	0.07427800
C	4.91566100	-2.64728000	0.35381800
O	5.51457600	-2.50078800	1.40333900
N	5.40077800	-3.44649000	-0.66239500
C	4.91313500	-3.56393400	-1.95830600
O	5.50284100	-4.23256200	-2.79477600
C	3.67382700	-2.83545400	-2.19849000
C	3.16159000	-2.68582000	-3.59417100
C	3.11709500	-2.16803400	-1.17364700

P	4.29011100	2.71986800	2.00550000
O	5.07799700	2.96171500	3.26146400
O	3.54164000	3.87840900	1.41051100
O	5.26130500	2.13631100	0.82548400
C	6.17148400	1.09064100	1.15496000
C	6.83805300	0.54167500	-0.08510800
O	5.98130700	-0.25399300	-0.91313000
C	7.45745700	1.61116400	-1.01852400
O	8.84208000	1.63644000	-0.74772700
C	7.11552500	1.08400800	-2.42203300
C	6.75479200	-0.36758400	-2.10912700
N	6.08068500	-1.12090100	-3.14354600
C	6.91561600	-1.88199400	-3.92744200
O	8.09034700	-2.10347600	-3.68636500
N	6.33890300	-2.40920700	-5.08271700
C	4.99200600	-2.57900600	-5.31509300
C	4.06195100	-1.74668700	-4.45711300
C	4.81787100	-0.63488800	-3.71277800
H	-0.51403000	0.89832400	1.87914900
H	-0.53438300	-0.88216700	1.83320500
H	1.44208500	0.06881100	3.04591800
H	1.72721900	1.96411800	1.02564800
H	3.88105600	0.81340200	-0.18888400
H	2.25173600	0.20303600	-0.58944300
H	4.03155800	-0.85711000	1.68215100
H	2.17344300	-1.64511000	-1.28600200
H	6.96097900	1.48825100	1.80272800
H	5.66620000	0.28052300	1.69190000
H	7.67013300	-0.09211900	0.25844600
H	7.02019400	2.60056100	-0.83463700
H	7.95298500	1.16635700	-3.11850500
H	6.24715100	1.60437600	-2.83572200
H	7.66680700	-0.92858300	-1.88350900
H	4.21511400	-0.24980500	-2.88541800
H	6.28745500	-3.89741400	-0.46688800
C	9.48609900	2.76964800	-1.29225600
H	10.54161200	2.70175800	-1.02615400
H	9.39660400	2.80282700	-2.38561900
H	9.06719600	3.69701200	-0.87987800
C	-1.32197300	0.06800200	-0.46805400
H	-1.23757400	0.09331700	-1.55505800
H	-1.88358300	-0.82708300	-0.16963000
H	-1.87206000	0.95545000	-0.12767600
H	2.15924200	-2.25377400	-3.55050700
H	3.08424700	-3.64825800	-4.10707100
Na	4.38780000	5.23753100	3.20030600
H	3.40110400	-1.26025000	-5.18061200
H	5.01214300	0.19124300	-4.40730200
O	4.59169800	-3.33769500	-6.17467900
H	6.96072200	-3.01403700	-5.60730200

5'-T(5m-6)U_{5,6H}-3'

O	0.05005600	0.02020200	0.00215900
C	0.04733000	0.05527900	1.40859700
C	1.46949300	0.08734400	1.93423000
O	2.06327800	-1.22086100	1.86492000
C	2.40428600	1.01739700	1.14111700

O	3. 36094900	1. 52652000	2. 08344500
C	3. 03146200	0. 04145900	0. 15789600
C	3. 22282300	-1. 14919600	1. 07937500
N	3. 51747300	-2. 40394900	0. 37336800
C	2. 55861700	-3. 22806000	-0. 19878100
O	1. 35905200	-3. 05270700	-0. 13695700
N	3. 10735800	-4. 32058200	-0. 86006000
C	4. 44714900	-4. 60650200	-1. 12068700
O	4. 76593600	-5. 61700500	-1. 73088600
C	5. 36456600	-3. 60036800	-0. 61452100
C	6. 84372800	-3. 70573500	-0. 82374900
C	4. 85156700	-2. 57840300	0. 09527700
P	4. 78851200	2. 16775900	1. 61886600
O	5. 18547400	3. 17103300	2. 66614200
O	4. 74692500	2. 63647300	0. 19214500
O	5. 78903000	0. 86699800	1. 68860500
C	6. 19117400	0. 47464500	3. 00247500
C	7. 14783600	-0. 69046400	2. 96358200
O	6. 53115000	-1. 85333600	2. 44240000
C	8. 42966900	-0. 53042700	2. 13426400
O	9. 41672500	0. 02986200	2. 96347400
C	8. 72782000	-1. 97794200	1. 66222100
C	7. 60845900	-2. 78940200	2. 32955700
N	7. 16740700	-3. 99489800	1. 65878100
C	6. 20174400	-4. 69526900	2. 33699000
O	5. 76500600	-4. 36944200	3. 42656700
N	5. 70864200	-5. 84194300	1. 70325300
C	6. 34036200	-6. 57190700	0. 71662300
C	7. 60764600	-5. 93163500	0. 21772300
C	7. 61941000	-4. 40504100	0. 32085800
H	-0. 48592100	0. 95067700	1. 76599900
H	-0. 45991300	-0. 82971200	1. 82144200
H	1. 44809000	0. 39734100	2. 98418800
H	1. 87412000	1. 84583200	0. 66601300
H	3. 95824200	0. 40038000	-0. 28934300
H	2. 30056000	-0. 21099500	-0. 61315700
H	4. 09806900	-0. 99550000	1. 72383700
H	5. 49749800	-1. 81544700	0. 51767000
H	6. 68846400	1. 31290100	3. 50000400
H	5. 30914000	0. 19214300	3. 59154000
H	7. 46472600	-0. 87240300	4. 00475000
H	8. 24440200	0. 12439300	1. 27132400
H	9. 71931000	-2. 30745600	1. 98049400
H	8. 67155700	-2. 03564000	0. 57463500
H	7. 90005200	-3. 06725100	3. 35105300
H	2. 42561200	-4. 96359700	-1. 24616700
C	-1. 25232800	-0. 09611300	-0. 52487000
H	-1. 16707300	-0. 10432500	-1. 61219500
H	-1. 73108800	-1. 02731500	-0. 19316200
H	-1. 88321200	0. 74959400	-0. 21891600
C	10. 54190900	0. 48849800	2. 24207300
H	11. 23727300	0. 91874100	2. 96349900
H	11. 04271100	-0. 33041200	1. 70980400
H	10. 25479900	1. 25646800	1. 51184600
Na	5. 40911500	4. 80257500	0. 95543500
H	7. 24435100	-2. 69407400	-0. 93764600
H	7. 05351300	-4. 23844700	-1. 75566400
H	8. 66528300	-4. 10383400	0. 23373000

H	7.77190700	-6.24919600	-0.81244500
H	8.41843400	-6.34455000	0.82938000
H	4.94743300	-6.29469700	2.19622900
O	5.92667600	-7.65523200	0.36204500
