

How DNA is Damaged by External Electric Fields: Selective Mutation vs. Random Degradation (SUPPORTING INFORMATION)

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Computational Details

ONIOM approach: The geometry of the central guanine:cytosine (GC) base pair was fully optimized at the M06-2X/6-311G(d,p) level¹ and the rest of the system was frozen in space and described with M06-2X/6-31G(d) for border basis pairs and PM6² for the sugar-phosphate backbone. For the records, the phosphate groups are protonated to ensure the electrical neutrality of the system. The M06-2X functional has been shown to provide an accurate description of van der Waals interactions¹ and is particularly efficient for the treatment of the GC hydrogen-bonds.³ This partial optimization procedure retains the characteristic double helix form while allowing to relax the central base pairs for every electric field strengths. Single-point calculations have been performed in the aqueous media characteristic of living cells. The well-known polarisable continuum model (PCM)⁴ is used through single point energy calculations performed on the gas phase geometries. These single-point calculations have been performed with larger basis sets (including diffuse functions) aiming to provide the most accurate results. The used level of theory can be shortened as: PCM-(M06-2X/6-311++G(d,p):M06-2X/6-31+G(d):PM6)//M06-2X/6-311G(d,p):M06-2X/6-31G(d):PM6. We computed the equilibrium constant using the usual expression:

$$K_{\text{eq}} = e^{-\Delta G/RT} \quad (\text{S-1})$$

where R is the ideal gas constant, T is the temperature (298.15 K), and ΔG is the Gibbs free energy obtained from the ONIOM PCM-(M06-2X/6-311++G(d,p):M06-2X/6-31+G(d):PM6) energies and the thermal corrections from the M06-2X/6-311G(d,p):M06-2X/6-31G(d):PM6 optimizations. All these calculations have been performed with the ONIOM scheme⁵ as implemented in Gaussian09.⁶

Molecular Dynamics: The system was formed starting from a DNA dG₃:dC₃ dodecamer structure (built up with the 3DNA software⁷) placed in a cubic box of 66 Å filled with water 9181 molecules and 22 sodium cations to counterbalance the total electric charge. The final

system contained 28319 atoms. To account for the interactions within the system particles, the AMBER parambsc0 force field⁸ was used for the DNA residues and the TIP3P model⁹ for the water molecules. After minimization, MD simulations has been carried out with the GROMACS-4.5.5 program package¹⁰ using a time step of 2 fs, keeping all bonds involving hydrogen atoms frozen. Van der Waals interactions were evaluated using a cut-off radius of 9 Å and the electrostatic part was computed using the Particle Mesh Ewald (PME)¹¹ method with a 9 Å cut-off radius for the real part. The system was equilibrated with the Berendsen thermostat¹² ($\tau_T = 0.1$ ps) for 1 ns. For the production phase, the thermostat was replaced by the Nosé-Hoover algorithm^{13,14} ($\tau_T = 1.0$ ps) and a constant electric field was included when necessary in the selected direction as implemented in GROMACS software.

Additional MD simulations

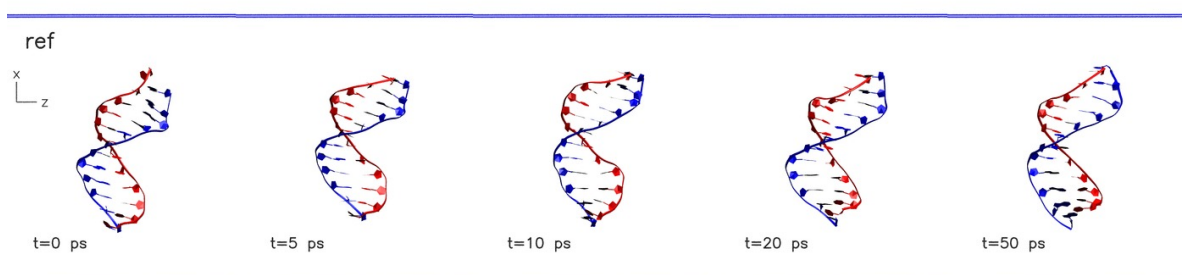


Figure S-1: Time evolution of undamaged model **B**, that is, without any electric field perturbation.

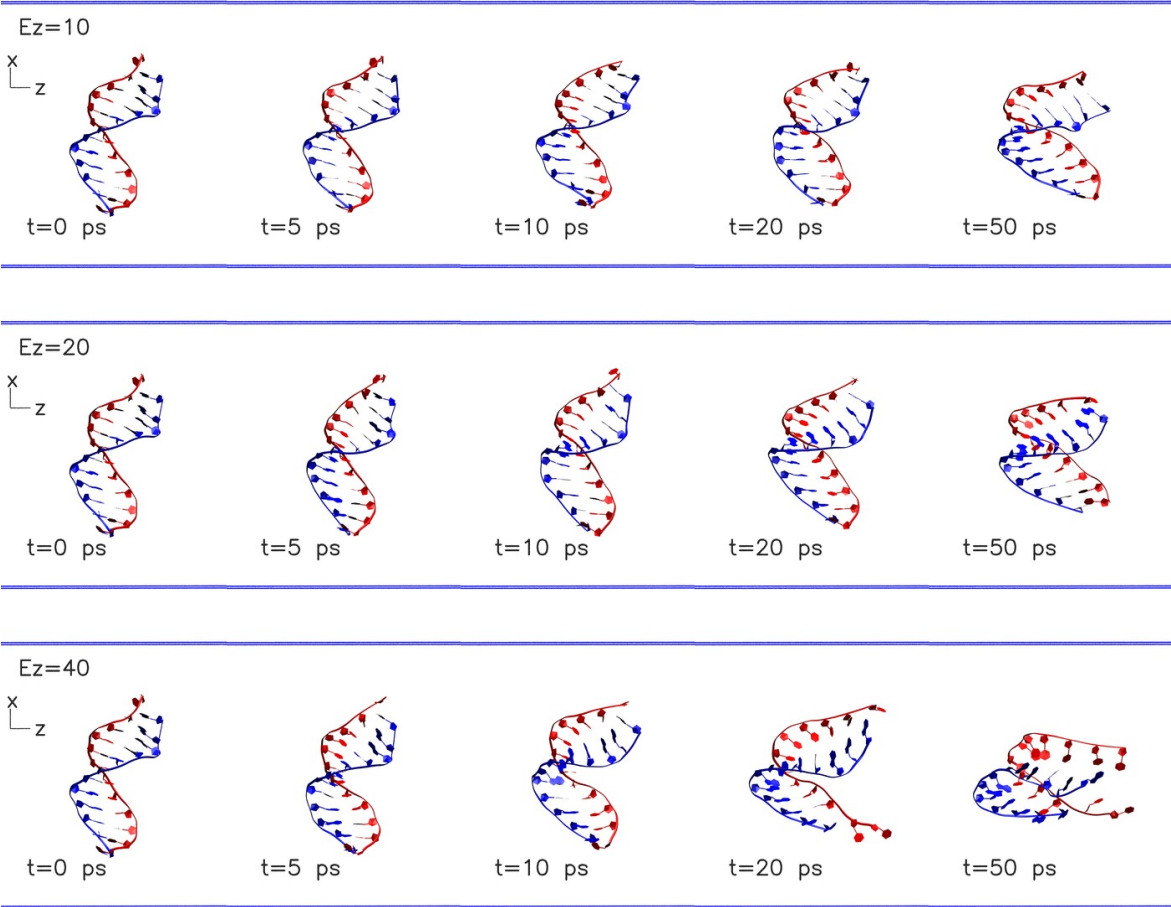


Figure S-2: Time evolution of model **B** under less intense Z-fields (strengths are given in $1/10^{-4}$ au).

Induced H₁-mutation at E_{ext}= −80 × 10^{−4} au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.85030100
N	0.19723900	0.00000000	−3.96971900
C	1.49379300	−0.48960200	−4.12344200
N	2.07984600	−0.70995600	−2.99520300
C	1.14108700	−0.37675100	−2.02547900
C	1.16859100	−0.40190300	−0.58718000
O	2.14053000	−0.76478200	0.10648600
C	−1.07987100	0.37140100	−0.70277000
N	−2.17220700	0.74436500	0.00543500
H	−2.23880300	0.55284500	0.99660000
H	−3.01059700	0.92393000	−0.51593400
N	−1.18132400	0.43766000	−2.04213400
C	−0.04216600	0.05104600	−2.60732900
N	−1.09110200	0.22398000	4.98582300
C	0.07909400	−0.08684800	5.61393600
H	0.04965600	−0.07300000	6.70314100
C	1.19964400	−0.42458900	4.93146100
H	2.10846500	−0.67902500	5.45636300
C	1.16576800	−0.40487600	3.49800700
N	2.16002900	−0.74887100	2.72098400
H	3.01957200	−1.04347800	3.15951100
H	2.10217400	−0.75063400	1.62978600
N	0.00896800	−0.01138700	2.91286300
C	−1.17079900	0.27610600	3.58454600
O	−2.19652900	0.52328800	2.99579900

H	1.93382300	-0.61128200	-5.10817300
N	2.10608200	-3.93009000	-3.58428300
C	3.28095100	-4.22282900	-2.92217000
H	4.17435100	-4.45291700	-3.48368200
N	3.17917800	-4.19005300	-1.61664200
C	1.84889900	-3.85431600	-1.39362800
C	1.13780900	-3.66882100	-0.17869500
O	1.54793500	-3.76559200	0.97686800
N	-0.20037500	-3.33363200	-0.41666700
H	-0.78529600	-3.18376300	0.38033100
C	-0.77668100	-3.19354000	-1.66271600
N	-2.07627300	-2.86720600	-1.67598600
H	-2.67556300	-2.72562200	-0.87554900
H	-2.50806700	-2.77125500	-2.58397900
N	-0.10887300	-3.36694400	-2.79999200
C	1.19410400	-3.69222400	-2.58605100
N	-1.34642600	3.91031900	-2.50884100
C	-0.32614200	3.63336300	-3.39565700
H	-0.49688000	3.71778200	-4.45862600
N	0.79649600	3.27774900	-2.82201200
C	0.50528400	3.31946900	-1.46350400
C	1.32332100	3.03661900	-0.33779900
O	2.50102000	2.68281400	-0.31030600
N	0.61957900	3.20732800	0.86025000
H	1.11234100	3.02950600	1.71205200
C	-0.69925600	3.60122200	0.95985100
N	-1.18920700	3.70597800	2.20265900

H	-0.70101000	3.51705200	3.06641100
H	-2.15628000	3.98529000	2.28423000
N	-1.46399700	3.86654500	-0.09570500
C	-0.79433100	3.70639500	-1.26840600
N	2.39698900	2.50971900	5.59830300
C	3.69600600	2.12160800	5.49221300
H	4.27287900	1.91727400	6.38196100
C	4.28894000	1.98431100	4.27599800
H	5.33112600	1.67228400	4.20993900
C	3.48391700	2.26624600	3.12823700
N	3.99566100	2.15326800	1.91683600
H	4.96055900	1.86492200	1.83979800
H	3.42946000	2.35173600	1.10447900
N	2.19440600	2.65159300	3.23131300
C	1.63924900	2.77685400	4.46639900
O	0.46126200	3.12640100	4.63302900
N	-3.80937200	-2.41302600	3.07908400
C	-3.23459900	-2.55321800	4.30354900
H	-3.82268300	-2.40208700	5.19657800
C	-1.92113400	-2.88317500	4.42708800
H	-1.47711400	-2.99131900	5.41666100
C	-1.18501800	-3.07268800	3.21596400
N	0.09435200	-3.39434600	3.26231200
H	0.51965300	-3.49806600	4.17240200
H	0.61671200	-3.52880800	2.40852400
N	-1.75356700	-2.93403300	1.99962400
C	-3.07018000	-2.60312700	1.91986700

O	-3.65479800	-2.45995600	0.83574200
O	4.60637800	-5.76224600	-5.64434200
C	3.48266500	-6.49413200	-6.16895000
H	3.80842700	-7.10641800	-7.00983300
H	3.07612900	-7.13370900	-5.38565700
C	2.40427300	-5.52865000	-6.63297200
H	1.90998900	-6.05515100	-7.44928300
O	1.55319700	-5.18994800	-5.49619600
C	1.83972500	-3.87295900	-5.04916500
H	0.96773900	-3.23812200	-5.20641000
C	2.89966900	-4.17794500	-7.15361800
H	3.80753100	-4.33808800	-7.73520600
C	3.01213700	-3.34298900	-5.87655100
H	4.04268000	-3.01249800	-5.74751600
H	2.35899900	-2.47357800	-5.95158500
O	2.03420900	-3.48400100	-8.03992100
P	2.21801100	-1.90575500	-8.22796100
O	1.91411800	-1.53360600	-9.62769300
O	3.55080500	-1.49883700	-7.72977300
O	1.07926100	-1.33628300	-7.25913100
C	-0.19123400	-2.01154200	-7.20275200
H	-0.40699900	-2.46116200	-8.17186000
H	-0.14898900	-2.78843700	-6.43952100
C	-1.28988200	-1.02326800	-6.84683900
H	-2.17644300	-1.42350500	-7.33847700
O	-1.37244500	-0.91260900	-5.39338400
C	-0.81233300	0.32039400	-4.96666500

H	-1.59190000	0.93918600	-4.52253800
C	-1.07355000	0.41341100	-7.32648500
H	-0.63355700	0.38758800	-8.32328600
C	-0.24126500	1.02565000	-6.19813600
H	0.71406000	1.36847800	-6.59553500
H	-0.77866200	1.86995000	-5.76658700
O	-2.23696800	1.21314200	-7.47815500
P	-2.08971000	2.80635500	-7.47798400
O	-3.07709000	3.39654100	-8.40920200
O	-0.67704400	3.17386900	-7.72169500
O	-2.49073500	3.16165700	-5.97046100
C	-3.56828400	2.43903900	-5.34594300
H	-4.29859500	2.15067900	-6.10198200
H	-3.16792200	1.54716800	-4.86412000
C	-4.24086500	3.31132400	-4.29849300
H	-5.27461900	2.96613000	-4.28959400
O	-3.52058600	3.17315900	-3.03606900
C	-2.74643900	4.33735600	-2.78759200
H	-3.12536700	4.84289900	-1.89948900
C	-4.23180800	4.81527100	-4.57950300
H	-4.40064000	4.97381700	-5.64450900
C	-2.88795000	5.26042100	-3.99916500
H	-2.27886200	5.70089200	-4.78839400
H	-3.05672900	5.99944100	-3.21592700
O	-5.24359000	5.58466300	-3.94646700
O	4.79603100	2.89015400	8.41871000
C	4.09851600	4.11594600	8.70941100

H	4.44040100	4.51036800	9.66619400
H	4.30386900	4.83929800	7.92030400
C	2.60158400	3.85984500	8.77271700
H	2.23555000	4.59967700	9.48459300
O	2.04886200	3.95642600	7.42494700
C	1.74516300	2.66084500	6.92961100
H	0.66848200	2.56955400	6.78712400
C	2.18420400	2.46975400	9.25679600
H	2.84728500	2.16712700	10.06725500
C	2.20996100	1.64125700	7.97095200
H	2.92356200	0.82439300	8.07867500
H	1.21731800	1.23316700	7.78120400
O	0.88121600	2.35563500	9.80960900
P	0.37360600	1.14568200	9.86985600
O	-0.44137900	1.07273100	11.10309800
O	1.40218900	0.09358300	9.71015900
O	-0.58820200	1.15372200	8.59123700
C	-1.28524200	2.36647500	8.24966200
H	-1.50044700	2.92989200	9.15759800
H	-0.65868300	2.96390700	7.58739500
C	-2.58707600	2.03514900	7.53843700
H	-3.25163600	2.85695500	7.80468300
O	-2.31910400	1.87976100	6.11168700
C	-2.35535500	0.50535600	5.75658300
H	-3.18662300	0.32819100	5.07418800
C	-3.25199600	0.71912700	7.94656000
H	-3.14445000	0.59138800	9.02359500

C	-2.56633200	-0.30320900	7.03790500
H	-2.05574500	-1.04795400	7.64844100
H	-3.31329500	-0.79504600	6.41496400
O	-4.65008600	0.61824600	7.72011200
P	-5.15490200	-0.59408700	7.69952600
O	-6.50928200	-0.51545600	8.29077900
O	-4.24390800	-1.59494400	8.29849900
O	-5.27146100	-0.84992600	6.12442000
C	-5.62673300	0.24803600	5.26327400
H	-6.27719700	0.93672500	5.80223700
H	-4.71962100	0.76695100	4.95382300
C	-6.34865100	-0.27078300	4.03036500
H	-7.02005000	0.54212200	3.75415800
O	-5.35789900	-0.63818100	3.02302400
C	-5.24826700	-2.05157300	2.94113500
H	-5.58445000	-2.38578000	1.95972400
C	-7.17784400	-1.54100500	4.23004200
H	-7.67467200	-1.48655500	5.19858600
C	-6.14892400	-2.65380900	4.02100200
H	-6.07810900	-3.25837400	4.92508400
H	-6.45834800	-3.28339400	3.18688100
O	-8.23416700	-1.76030000	3.30674100
H	-5.33947000	5.26024700	-3.05882800
H	-3.99977500	3.20143300	-8.47844700
H	2.48940100	-0.96582000	-10.12202800
H	-7.92343100	-1.50082500	2.44743600
H	-6.94285100	-1.24565300	8.70610100

H	-0.82347900	0.27375700	11.43475400
H	4.63055300	2.30793600	9.15125400
H	4.94369500	-5.24179900	-6.36435000

Induced H₁-mutation at E_{ext}= -100 × 10⁻⁴ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.87346900
N	0.19518300	0.00000000	-3.97290400
C	1.49040000	-0.49539100	-4.12807500
N	2.07482000	-0.71579300	-2.99955600
C	1.13775000	-0.37966400	-2.02970200
C	1.16955300	-0.40681800	-0.58833000
O	2.13996500	-0.77433900	0.09589000
C	-1.07883800	0.37168300	-0.70043300
N	-2.17026100	0.74161700	0.00751900
H	-2.23089200	0.56204700	1.00234800
H	-3.00888300	0.93079600	-0.50961400
N	-1.18265900	0.43985300	-2.04407300
C	-0.04511300	0.05143900	-2.60794800
N	-1.08791100	0.22422800	4.99262300
C	0.07616700	-0.08332700	5.63058000
H	0.03892100	-0.06610600	6.72008400
C	1.20141900	-0.42249000	4.95461500
H	2.10705600	-0.67668000	5.48500900
C	1.17208500	-0.40582900	3.52482300
N	2.17575400	-0.75553500	2.75814800
H	3.03509000	-1.04189900	3.20164500

H	2.12117000	-0.76126000	1.68945000
N	0.02002600	-0.01547400	2.93047900
C	-1.16221600	0.27749300	3.59596100
O	-2.18095800	0.52880200	2.99532700
H	1.93093900	-0.61643700	-5.11324900
N	2.10608200	-3.93009000	-3.58428300
C	3.28095100	-4.22282900	-2.92217000
H	4.17435100	-4.45291700	-3.48368200
N	3.17917800	-4.19005300	-1.61664200
C	1.84889900	-3.85431600	-1.39362800
C	1.13780900	-3.66882100	-0.17869500
O	1.54793500	-3.76559200	0.97686800
N	-0.20037500	-3.33363200	-0.41666700
H	-0.78529600	-3.18376300	0.38033100
C	-0.77668100	-3.19354000	-1.66271600
N	-2.07627300	-2.86720600	-1.67598600
H	-2.67556300	-2.72562200	-0.87554900
H	-2.50806700	-2.77125500	-2.58397900
N	-0.10887300	-3.36694400	-2.79999200
C	1.19410400	-3.69222400	-2.58605100
N	-1.34642600	3.91031900	-2.50884100
C	-0.32614200	3.63336300	-3.39565700
H	-0.49688000	3.71778200	-4.45862600
N	0.79649600	3.27774900	-2.82201200
C	0.50528400	3.31946900	-1.46350400
C	1.32332100	3.03661900	-0.33779900
O	2.50102000	2.68281400	-0.31030600

N	0.61957900	3.20732800	0.86025000
H	1.11234100	3.02950600	1.71205200
C	-0.69925600	3.60122200	0.95985100
N	-1.18920700	3.70597800	2.20265900
H	-0.70101000	3.51705200	3.06641100
H	-2.15628000	3.98529000	2.28423000
N	-1.46399700	3.86654500	-0.09570500
C	-0.79433100	3.70639500	-1.26840600
N	2.39698900	2.50971900	5.59830300
C	3.69600600	2.12160800	5.49221300
H	4.27287900	1.91727400	6.38196100
C	4.28894000	1.98431100	4.27599800
H	5.33112600	1.67228400	4.20993900
C	3.48391700	2.26624600	3.12823700
N	3.99566100	2.15326800	1.91683600
H	4.96055900	1.86492200	1.83979800
H	3.42946000	2.35173600	1.10447900
N	2.19440600	2.65159300	3.23131300
C	1.63924900	2.77685400	4.46639900
O	0.46126200	3.12640100	4.63302900
N	-3.80937200	-2.41302600	3.07908400
C	-3.23459900	-2.55321800	4.30354900
H	-3.82268300	-2.40208700	5.19657800
C	-1.92113400	-2.88317500	4.42708800
H	-1.47711400	-2.99131900	5.41666100
C	-1.18501800	-3.07268800	3.21596400
N	0.09435200	-3.39434600	3.26231200

H	0.51965300	-3.49806600	4.17240200
H	0.61671200	-3.52880800	2.40852400
N	-1.75356700	-2.93403300	1.99962400
C	-3.07018000	-2.60312700	1.91986700
O	-3.65479800	-2.45995600	0.83574200
O	4.60637800	-5.76224600	-5.64434200
C	3.48266500	-6.49413200	-6.16895000
H	3.80842700	-7.10641800	-7.00983300
H	3.07612900	-7.13370900	-5.38565700
C	2.40427300	-5.52865000	-6.63297200
H	1.90998900	-6.05515100	-7.44928300
O	1.55319700	-5.18994800	-5.49619600
C	1.83972500	-3.87295900	-5.04916500
H	0.96773900	-3.23812200	-5.20641000
C	2.89966900	-4.17794500	-7.15361800
H	3.80753100	-4.33808800	-7.73520600
C	3.01213700	-3.34298900	-5.87655100
H	4.04268000	-3.01249800	-5.74751600
H	2.35899900	-2.47357800	-5.95158500
O	2.03420900	-3.48400100	-8.03992100
P	2.21801100	-1.90575500	-8.22796100
O	1.91411800	-1.53360600	-9.62769300
O	3.55080500	-1.49883700	-7.72977300
O	1.07926100	-1.33628300	-7.25913100
C	-0.19123400	-2.01154200	-7.20275200
H	-0.40699900	-2.46116200	-8.17186000
H	-0.14898900	-2.78843700	-6.43952100

C	-1.28988200	-1.02326800	-6.84683900
H	-2.17644300	-1.42350500	-7.33847700
O	-1.37244500	-0.91260900	-5.39338400
C	-0.81233300	0.32039400	-4.96666500
H	-1.59190000	0.93918600	-4.52253800
C	-1.07355000	0.41341100	-7.32648500
H	-0.63355700	0.38758800	-8.32328600
C	-0.24126500	1.02565000	-6.19813600
H	0.71406000	1.36847800	-6.59553500
H	-0.77866200	1.86995000	-5.76658700
O	-2.23696800	1.21314200	-7.47815500
P	-2.08971000	2.80635500	-7.47798400
O	-3.07709000	3.39654100	-8.40920200
O	-0.67704400	3.17386900	-7.72169500
O	-2.49073500	3.16165700	-5.97046100
C	-3.56828400	2.43903900	-5.34594300
H	-4.29859500	2.15067900	-6.10198200
H	-3.16792200	1.54716800	-4.86412000
C	-4.24086500	3.31132400	-4.29849300
H	-5.27461900	2.96613000	-4.28959400
O	-3.52058600	3.17315900	-3.03606900
C	-2.74643900	4.33735600	-2.78759200
H	-3.12536700	4.84289900	-1.89948900
C	-4.23180800	4.81527100	-4.57950300
H	-4.40064000	4.97381700	-5.64450900
C	-2.88795000	5.26042100	-3.99916500
H	-2.27886200	5.70089200	-4.78839400

H	-3.05672900	5.99944100	-3.21592700
O	-5.24359000	5.58466300	-3.94646700
O	4.79603100	2.89015400	8.41871000
C	4.09851600	4.11594600	8.70941100
H	4.44040100	4.51036800	9.66619400
H	4.30386900	4.83929800	7.92030400
C	2.60158400	3.85984500	8.77271700
H	2.23555000	4.59967700	9.48459300
O	2.04886200	3.95642600	7.42494700
C	1.74516300	2.66084500	6.92961100
H	0.66848200	2.56955400	6.78712400
C	2.18420400	2.46975400	9.25679600
H	2.84728500	2.16712700	10.06725500
C	2.20996100	1.64125700	7.97095200
H	2.92356200	0.82439300	8.07867500
H	1.21731800	1.23316700	7.78120400
O	0.88121600	2.35563500	9.80960900
P	0.37360600	1.14568200	9.86985600
O	-0.44137900	1.07273100	11.10309800
O	1.40218900	0.09358300	9.71015900
O	-0.58820200	1.15372200	8.59123700
C	-1.28524200	2.36647500	8.24966200
H	-1.50044700	2.92989200	9.15759800
H	-0.65868300	2.96390700	7.58739500
C	-2.58707600	2.03514900	7.53843700
H	-3.25163600	2.85695500	7.80468300
O	-2.31910400	1.87976100	6.11168700

C	-2.35535500	0.50535600	5.75658300
H	-3.18662300	0.32819100	5.07418800
C	-3.25199600	0.71912700	7.94656000
H	-3.14445000	0.59138800	9.02359500
C	-2.56633200	-0.30320900	7.03790500
H	-2.05574500	-1.04795400	7.64844100
H	-3.31329500	-0.79504600	6.41496400
O	-4.65008600	0.61824600	7.72011200
P	-5.15490200	-0.59408700	7.69952600
O	-6.50928200	-0.51545600	8.29077900
O	-4.24390800	-1.59494400	8.29849900
O	-5.27146100	-0.84992600	6.12442000
C	-5.62673300	0.24803600	5.26327400
H	-6.27719700	0.93672500	5.80223700
H	-4.71962100	0.76695100	4.95382300
C	-6.34865100	-0.27078300	4.03036500
H	-7.02005000	0.54212200	3.75415800
O	-5.35789900	-0.63818100	3.02302400
C	-5.24826700	-2.05157300	2.94113500
H	-5.58445000	-2.38578000	1.95972400
C	-7.17784400	-1.54100500	4.23004200
H	-7.67467200	-1.48655500	5.19858600
C	-6.14892400	-2.65380900	4.02100200
H	-6.07810900	-3.25837400	4.92508400
H	-6.45834800	-3.28339400	3.18688100
O	-8.23416700	-1.76030000	3.30674100
H	-5.33947000	5.26024700	-3.05882800

H	-3.99977500	3.20143300	-8.47844700
H	2.48940100	-0.96582000	-10.12202800
H	-7.92343100	-1.50082500	2.44743600
H	-6.94285100	-1.24565300	8.70610100
H	-0.82347900	0.27375700	11.43475400
H	4.63055300	2.30793600	9.15125400
H	4.94369500	-5.24179900	-6.36435000

Induced H₂-mutation at E_{ext}= +60 × 10⁻⁴ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.04186400
N	0.18207400	0.00000000	-3.92516200
C	1.48686400	-0.45496000	-4.07886000
N	2.08695700	-0.67555700	-2.95478600
C	1.13905600	-0.36134200	-1.99826300
C	1.16686900	-0.38538100	-0.60845600
O	2.17781300	-0.73645900	0.09797700
C	-1.13134700	0.38566500	-0.67433900
N	-2.19126100	0.70846100	0.08322300
H	-2.17162900	0.70679800	1.10050100
H	-2.97171100	1.11777200	-0.40114500
N	-1.19687900	0.43413600	-1.98669400
C	-0.06162400	0.05432400	-2.58612000
N	-1.11931300	0.22623300	5.00960700
C	0.05899600	-0.10637800	5.62547500
H	0.04627700	-0.13221700	6.71495800
C	1.15097500	-0.40906000	4.90459300

H	2.08095400	-0.67924100	5.39032900
C	1.07363100	-0.33175400	3.44071000
N	2.06558600	-0.63585100	2.66148000
H	2.88284500	-0.96264000	3.16469400
H	2.06534000	-0.69541800	1.14501300
N	-0.09134100	0.08018800	2.87331300
C	-1.20053500	0.32753600	3.56943500
O	-2.29269000	0.60995800	3.08689300
H	1.91677900	-0.57521900	-5.06644500
N	2.10608200	-3.93009000	-3.58428300
C	3.28095100	-4.22282900	-2.92217000
H	4.17435100	-4.45291700	-3.48368200
N	3.17917800	-4.19005300	-1.61664200
C	1.84889900	-3.85431600	-1.39362800
C	1.13780900	-3.66882100	-0.17869500
O	1.54793500	-3.76559200	0.97686800
N	-0.20037500	-3.33363200	-0.41666700
H	-0.78529600	-3.18376300	0.38033100
C	-0.77668100	-3.19354000	-1.66271600
N	-2.07627300	-2.86720600	-1.67598600
H	-2.67556300	-2.72562200	-0.87554900
H	-2.50806700	-2.77125500	-2.58397900
N	-0.10887300	-3.36694400	-2.79999200
C	1.19410400	-3.69222400	-2.58605100
N	-1.34642600	3.91031900	-2.50884100
C	-0.32614200	3.63336300	-3.39565700
H	-0.49688000	3.71778200	-4.45862600

N	0.79649600	3.27774900	-2.82201200
C	0.50528400	3.31946900	-1.46350400
C	1.32332100	3.03661900	-0.33779900
O	2.50102000	2.68281400	-0.31030600
N	0.61957900	3.20732800	0.86025000
H	1.11234100	3.02950600	1.71205200
C	-0.69925600	3.60122200	0.95985100
N	-1.18920700	3.70597800	2.20265900
H	-0.70101000	3.51705200	3.06641100
H	-2.15628000	3.98529000	2.28423000
N	-1.46399700	3.86654500	-0.09570500
C	-0.79433100	3.70639500	-1.26840600
N	2.39698900	2.50971900	5.59830300
C	3.69600600	2.12160800	5.49221300
H	4.27287900	1.91727400	6.38196100
C	4.28894000	1.98431100	4.27599800
H	5.33112600	1.67228400	4.20993900
C	3.48391700	2.26624600	3.12823700
N	3.99566100	2.15326800	1.91683600
H	4.96055900	1.86492200	1.83979800
H	3.42946000	2.35173600	1.10447900
N	2.19440600	2.65159300	3.23131300
C	1.63924900	2.77685400	4.46639900
O	0.46126200	3.12640100	4.63302900
N	-3.80937200	-2.41302600	3.07908400
C	-3.23459900	-2.55321800	4.30354900
H	-3.82268300	-2.40208700	5.19657800

C	-1.92113400	-2.88317500	4.42708800
H	-1.47711400	-2.99131900	5.41666100
C	-1.18501800	-3.07268800	3.21596400
N	0.09435200	-3.39434600	3.26231200
H	0.51965300	-3.49806600	4.17240200
H	0.61671200	-3.52880800	2.40852400
N	-1.75356700	-2.93403300	1.99962400
C	-3.07018000	-2.60312700	1.91986700
O	-3.65479800	-2.45995600	0.83574200
O	4.60637800	-5.76224600	-5.64434200
C	3.48266500	-6.49413200	-6.16895000
H	3.80842700	-7.10641800	-7.00983300
H	3.07612900	-7.13370900	-5.38565700
C	2.40427300	-5.52865000	-6.63297200
H	1.90998900	-6.05515100	-7.44928300
O	1.55319700	-5.18994800	-5.49619600
C	1.83972500	-3.87295900	-5.04916500
H	0.96773900	-3.23812200	-5.20641000
C	2.89966900	-4.17794500	-7.15361800
H	3.80753100	-4.33808800	-7.73520600
C	3.01213700	-3.34298900	-5.87655100
H	4.04268000	-3.01249800	-5.74751600
H	2.35899900	-2.47357800	-5.95158500
O	2.03420900	-3.48400100	-8.03992100
P	2.21801100	-1.90575500	-8.22796100
O	1.91411800	-1.53360600	-9.62769300
O	3.55080500	-1.49883700	-7.72977300

O	1.07926100	-1.33628300	-7.25913100
C	-0.19123400	-2.01154200	-7.20275200
H	-0.40699900	-2.46116200	-8.17186000
H	-0.14898900	-2.78843700	-6.43952100
C	-1.28988200	-1.02326800	-6.84683900
H	-2.17644300	-1.42350500	-7.33847700
O	-1.37244500	-0.91260900	-5.39338400
C	-0.81233300	0.32039400	-4.96666500
H	-1.59190000	0.93918600	-4.52253800
C	-1.07355000	0.41341100	-7.32648500
H	-0.63355700	0.38758800	-8.32328600
C	-0.24126500	1.02565000	-6.19813600
H	0.71406000	1.36847800	-6.59553500
H	-0.77866200	1.86995000	-5.76658700
O	-2.23696800	1.21314200	-7.47815500
P	-2.08971000	2.80635500	-7.47798400
O	-3.07709000	3.39654100	-8.40920200
O	-0.67704400	3.17386900	-7.72169500
O	-2.49073500	3.16165700	-5.97046100
C	-3.56828400	2.43903900	-5.34594300
H	-4.29859500	2.15067900	-6.10198200
H	-3.16792200	1.54716800	-4.86412000
C	-4.24086500	3.31132400	-4.29849300
H	-5.27461900	2.96613000	-4.28959400
O	-3.52058600	3.17315900	-3.03606900
C	-2.74643900	4.33735600	-2.78759200
H	-3.12536700	4.84289900	-1.89948900

C	-4.23180800	4.81527100	-4.57950300
H	-4.40064000	4.97381700	-5.64450900
C	-2.88795000	5.26042100	-3.99916500
H	-2.27886200	5.70089200	-4.78839400
H	-3.05672900	5.99944100	-3.21592700
O	-5.24359000	5.58466300	-3.94646700
O	4.79603100	2.89015400	8.41871000
C	4.09851600	4.11594600	8.70941100
H	4.44040100	4.51036800	9.66619400
H	4.30386900	4.83929800	7.92030400
C	2.60158400	3.85984500	8.77271700
H	2.23555000	4.59967700	9.48459300
O	2.04886200	3.95642600	7.42494700
C	1.74516300	2.66084500	6.92961100
H	0.66848200	2.56955400	6.78712400
C	2.18420400	2.46975400	9.25679600
H	2.84728500	2.16712700	10.06725500
C	2.20996100	1.64125700	7.97095200
H	2.92356200	0.82439300	8.07867500
H	1.21731800	1.23316700	7.78120400
O	0.88121600	2.35563500	9.80960900
P	0.37360600	1.14568200	9.86985600
O	-0.44137900	1.07273100	11.10309800
O	1.40218900	0.09358300	9.71015900
O	-0.58820200	1.15372200	8.59123700
C	-1.28524200	2.36647500	8.24966200
H	-1.50044700	2.92989200	9.15759800

H	-0.65868300	2.96390700	7.58739500
C	-2.58707600	2.03514900	7.53843700
H	-3.25163600	2.85695500	7.80468300
O	-2.31910400	1.87976100	6.11168700
C	-2.35535500	0.50535600	5.75658300
H	-3.18662300	0.32819100	5.07418800
C	-3.25199600	0.71912700	7.94656000
H	-3.14445000	0.59138800	9.02359500
C	-2.56633200	-0.30320900	7.03790500
H	-2.05574500	-1.04795400	7.64844100
H	-3.31329500	-0.79504600	6.41496400
O	-4.65008600	0.61824600	7.72011200
P	-5.15490200	-0.59408700	7.69952600
O	-6.50928200	-0.51545600	8.29077900
O	-4.24390800	-1.59494400	8.29849900
O	-5.27146100	-0.84992600	6.12442000
C	-5.62673300	0.24803600	5.26327400
H	-6.27719700	0.93672500	5.80223700
H	-4.71962100	0.76695100	4.95382300
C	-6.34865100	-0.27078300	4.03036500
H	-7.02005000	0.54212200	3.75415800
O	-5.35789900	-0.63818100	3.02302400
C	-5.24826700	-2.05157300	2.94113500
H	-5.58445000	-2.38578000	1.95972400
C	-7.17784400	-1.54100500	4.23004200
H	-7.67467200	-1.48655500	5.19858600
C	-6.14892400	-2.65380900	4.02100200

H	-6.07810900	-3.25837400	4.92508400
H	-6.45834800	-3.28339400	3.18688100
O	-8.23416700	-1.76030000	3.30674100
H	-5.33947000	5.26024700	-3.05882800
H	-3.99977500	3.20143300	-8.47844700
H	2.48940100	-0.96582000	-10.12202800
H	-7.92343100	-1.50082500	2.44743600
H	-6.94285100	-1.24565300	8.70610100
H	-0.82347900	0.27375700	11.43475400
H	4.63055300	2.30793600	9.15125400
H	4.94369500	-5.24179900	-6.36435000

Induced H₂-mutation at E_{ext}= +80 × 10⁻⁴ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.03889100
N	0.18409600	0.00000000	-3.92450900
C	1.48969000	-0.45310500	-4.07838400
N	2.09031300	-0.67368800	-2.95362100
C	1.14176800	-0.36048200	-1.99837200
C	1.16561600	-0.38346200	-0.61263200
O	2.18476500	-0.73444700	0.09201100
C	-1.13042900	0.38565700	-0.67713200
N	-2.19712400	0.70286200	0.07781300
H	-2.16439100	0.73504700	1.09290400
H	-2.95690900	1.14863700	-0.40848800
N	-1.19403700	0.43437100	-1.98734100
C	-0.05995300	0.05464700	-2.58896100

N	-1.11706000	0.22476500	5.02095200
C	0.05668500	-0.11135400	5.64518000
H	0.03729700	-0.14056400	6.73494800
C	1.15177900	-0.41327200	4.93059200
H	2.07928000	-0.68636000	5.42034500
C	1.08460600	-0.33158100	3.46371700
N	2.08023000	-0.63179900	2.69242700
H	2.89140500	-0.96350300	3.20301800
H	2.07067000	-0.69924700	1.11685800
N	-0.07817900	0.08426700	2.88992800
C	-1.19019900	0.33054900	3.57585300
O	-2.28187400	0.61690200	3.09643500
H	1.91882900	-0.57345100	-5.06645700
N	2.10608200	-3.93009000	-3.58428300
C	3.28095100	-4.22282900	-2.92217000
H	4.17435100	-4.45291700	-3.48368200
N	3.17917800	-4.19005300	-1.61664200
C	1.84889900	-3.85431600	-1.39362800
C	1.13780900	-3.66882100	-0.17869500
O	1.54793500	-3.76559200	0.97686800
N	-0.20037500	-3.33363200	-0.41666700
H	-0.78529600	-3.18376300	0.38033100
C	-0.77668100	-3.19354000	-1.66271600
N	-2.07627300	-2.86720600	-1.67598600
H	-2.67556300	-2.72562200	-0.87554900
H	-2.50806700	-2.77125500	-2.58397900
N	-0.10887300	-3.36694400	-2.79999200

C	1.19410400	-3.69222400	-2.58605100
N	-1.34642600	3.91031900	-2.50884100
C	-0.32614200	3.63336300	-3.39565700
H	-0.49688000	3.71778200	-4.45862600
N	0.79649600	3.27774900	-2.82201200
C	0.50528400	3.31946900	-1.46350400
C	1.32332100	3.03661900	-0.33779900
O	2.50102000	2.68281400	-0.31030600
N	0.61957900	3.20732800	0.86025000
H	1.11234100	3.02950600	1.71205200
C	-0.69925600	3.60122200	0.95985100
N	-1.18920700	3.70597800	2.20265900
H	-0.70101000	3.51705200	3.06641100
H	-2.15628000	3.98529000	2.28423000
N	-1.46399700	3.86654500	-0.09570500
C	-0.79433100	3.70639500	-1.26840600
N	2.39698900	2.50971900	5.59830300
C	3.69600600	2.12160800	5.49221300
H	4.27287900	1.91727400	6.38196100
C	4.28894000	1.98431100	4.27599800
H	5.33112600	1.67228400	4.20993900
C	3.48391700	2.26624600	3.12823700
N	3.99566100	2.15326800	1.91683600
H	4.96055900	1.86492200	1.83979800
H	3.42946000	2.35173600	1.10447900
N	2.19440600	2.65159300	3.23131300
C	1.63924900	2.77685400	4.46639900

O	0.46126200	3.12640100	4.63302900
N	-3.80937200	-2.41302600	3.07908400
C	-3.23459900	-2.55321800	4.30354900
H	-3.82268300	-2.40208700	5.19657800
C	-1.92113400	-2.88317500	4.42708800
H	-1.47711400	-2.99131900	5.41666100
C	-1.18501800	-3.07268800	3.21596400
N	0.09435200	-3.39434600	3.26231200
H	0.51965300	-3.49806600	4.17240200
H	0.61671200	-3.52880800	2.40852400
N	-1.75356700	-2.93403300	1.99962400
C	-3.07018000	-2.60312700	1.91986700
O	-3.65479800	-2.45995600	0.83574200
O	4.60637800	-5.76224600	-5.64434200
C	3.48266500	-6.49413200	-6.16895000
H	3.80842700	-7.10641800	-7.00983300
H	3.07612900	-7.13370900	-5.38565700
C	2.40427300	-5.52865000	-6.63297200
H	1.90998900	-6.05515100	-7.44928300
O	1.55319700	-5.18994800	-5.49619600
C	1.83972500	-3.87295900	-5.04916500
H	0.96773900	-3.23812200	-5.20641000
C	2.89966900	-4.17794500	-7.15361800
H	3.80753100	-4.33808800	-7.73520600
C	3.01213700	-3.34298900	-5.87655100
H	4.04268000	-3.01249800	-5.74751600
H	2.35899900	-2.47357800	-5.95158500

O	2.03420900	-3.48400100	-8.03992100
P	2.21801100	-1.90575500	-8.22796100
O	1.91411800	-1.53360600	-9.62769300
O	3.55080500	-1.49883700	-7.72977300
O	1.07926100	-1.33628300	-7.25913100
C	-0.19123400	-2.01154200	-7.20275200
H	-0.40699900	-2.46116200	-8.17186000
H	-0.14898900	-2.78843700	-6.43952100
C	-1.28988200	-1.02326800	-6.84683900
H	-2.17644300	-1.42350500	-7.33847700
O	-1.37244500	-0.91260900	-5.39338400
C	-0.81233300	0.32039400	-4.96666500
H	-1.59190000	0.93918600	-4.52253800
C	-1.07355000	0.41341100	-7.32648500
H	-0.63355700	0.38758800	-8.32328600
C	-0.24126500	1.02565000	-6.19813600
H	0.71406000	1.36847800	-6.59553500
H	-0.77866200	1.86995000	-5.76658700
O	-2.23696800	1.21314200	-7.47815500
P	-2.08971000	2.80635500	-7.47798400
O	-3.07709000	3.39654100	-8.40920200
O	-0.67704400	3.17386900	-7.72169500
O	-2.49073500	3.16165700	-5.97046100
C	-3.56828400	2.43903900	-5.34594300
H	-4.29859500	2.15067900	-6.10198200
H	-3.16792200	1.54716800	-4.86412000
C	-4.24086500	3.31132400	-4.29849300

H	-5.27461900	2.96613000	-4.28959400
O	-3.52058600	3.17315900	-3.03606900
C	-2.74643900	4.33735600	-2.78759200
H	-3.12536700	4.84289900	-1.89948900
C	-4.23180800	4.81527100	-4.57950300
H	-4.40064000	4.97381700	-5.64450900
C	-2.88795000	5.26042100	-3.99916500
H	-2.27886200	5.70089200	-4.78839400
H	-3.05672900	5.99944100	-3.21592700
O	-5.24359000	5.58466300	-3.94646700
O	4.79603100	2.89015400	8.41871000
C	4.09851600	4.11594600	8.70941100
H	4.44040100	4.51036800	9.66619400
H	4.30386900	4.83929800	7.92030400
C	2.60158400	3.85984500	8.77271700
H	2.23555000	4.59967700	9.48459300
O	2.04886200	3.95642600	7.42494700
C	1.74516300	2.66084500	6.92961100
H	0.66848200	2.56955400	6.78712400
C	2.18420400	2.46975400	9.25679600
H	2.84728500	2.16712700	10.06725500
C	2.20996100	1.64125700	7.97095200
H	2.92356200	0.82439300	8.07867500
H	1.21731800	1.23316700	7.78120400
O	0.88121600	2.35563500	9.80960900
P	0.37360600	1.14568200	9.86985600
O	-0.44137900	1.07273100	11.10309800

O	1.40218900	0.09358300	9.71015900
O	-0.58820200	1.15372200	8.59123700
C	-1.28524200	2.36647500	8.24966200
H	-1.50044700	2.92989200	9.15759800
H	-0.65868300	2.96390700	7.58739500
C	-2.58707600	2.03514900	7.53843700
H	-3.25163600	2.85695500	7.80468300
O	-2.31910400	1.87976100	6.11168700
C	-2.35535500	0.50535600	5.75658300
H	-3.18662300	0.32819100	5.07418800
C	-3.25199600	0.71912700	7.94656000
H	-3.14445000	0.59138800	9.02359500
C	-2.56633200	-0.30320900	7.03790500
H	-2.05574500	-1.04795400	7.64844100
H	-3.31329500	-0.79504600	6.41496400
O	-4.65008600	0.61824600	7.72011200
P	-5.15490200	-0.59408700	7.69952600
O	-6.50928200	-0.51545600	8.29077900
O	-4.24390800	-1.59494400	8.29849900
O	-5.27146100	-0.84992600	6.12442000
C	-5.62673300	0.24803600	5.26327400
H	-6.27719700	0.93672500	5.80223700
H	-4.71962100	0.76695100	4.95382300
C	-6.34865100	-0.27078300	4.03036500
H	-7.02005000	0.54212200	3.75415800
O	-5.35789900	-0.63818100	3.02302400
C	-5.24826700	-2.05157300	2.94113500

H	-5.58445000	-2.38578000	1.95972400
C	-7.17784400	-1.54100500	4.23004200
H	-7.67467200	-1.48655500	5.19858600
C	-6.14892400	-2.65380900	4.02100200
H	-6.07810900	-3.25837400	4.92508400
H	-6.45834800	-3.28339400	3.18688100
O	-8.23416700	-1.76030000	3.30674100
H	-5.33947000	5.26024700	-3.05882800
H	-3.99977500	3.20143300	-8.47844700
H	2.48940100	-0.96582000	-10.12202800
H	-7.92343100	-1.50082500	2.44743600
H	-6.94285100	-1.24565300	8.70610100
H	-0.82347900	0.27375700	11.43475400
H	4.63055300	2.30793600	9.15125400
H	4.94369500	-5.24179900	-6.36435000

Induced H₂-mutation at E_{ext}= +100 × 10⁻⁴ au

N	0.00000000	0.00000000	0.00000000
H	0.00000000	0.00000000	1.03570800
N	0.18634500	0.00000000	-3.92378600
C	1.49329100	-0.44993600	-4.07792700
N	2.09464600	-0.66993200	-2.95235200
C	1.14538200	-0.35912700	-1.99810100
C	1.16604300	-0.38003500	-0.61562300
O	2.19199100	-0.72732100	0.08947500
C	-1.12969200	0.38403400	-0.68004900
N	-2.20471000	0.69333300	0.07251400

H	-2.15271100	0.77169200	1.08313100
H	-2.94199000	1.17386000	-0.41689000
N	-1.19148000	0.43267500	-1.98792100
C	-0.05787400	0.05405000	-2.59153000
N	-1.11424400	0.22354400	5.03273000
C	0.05403900	-0.11844300	5.66537200
H	0.02731600	-0.15348700	6.75536100
C	1.15266000	-0.41914500	4.95723100
H	2.07691800	-0.69727400	5.45122500
C	1.09670500	-0.32963600	3.48779700
N	2.09736100	-0.62481400	2.72489500
H	2.90180700	-0.96377600	3.24189100
H	2.07512100	-0.69760900	1.09921700
N	-0.06237800	0.09191100	2.90749200
C	-1.17794100	0.33707400	3.58274100
O	-2.26799300	0.62971200	3.10619800
H	1.92186100	-0.56977400	-5.06653300
N	2.10608200	-3.93009000	-3.58428300
C	3.28095100	-4.22282900	-2.92217000
H	4.17435100	-4.45291700	-3.48368200
N	3.17917800	-4.19005300	-1.61664200
C	1.84889900	-3.85431600	-1.39362800
C	1.13780900	-3.66882100	-0.17869500
O	1.54793500	-3.76559200	0.97686800
N	-0.20037500	-3.33363200	-0.41666700
H	-0.78529600	-3.18376300	0.38033100
C	-0.77668100	-3.19354000	-1.66271600

N	-2.07627300	-2.86720600	-1.67598600
H	-2.67556300	-2.72562200	-0.87554900
H	-2.50806700	-2.77125500	-2.58397900
N	-0.10887300	-3.36694400	-2.79999200
C	1.19410400	-3.69222400	-2.58605100
N	-1.34642600	3.91031900	-2.50884100
C	-0.32614200	3.63336300	-3.39565700
H	-0.49688000	3.71778200	-4.45862600
N	0.79649600	3.27774900	-2.82201200
C	0.50528400	3.31946900	-1.46350400
C	1.32332100	3.03661900	-0.33779900
O	2.50102000	2.68281400	-0.31030600
N	0.61957900	3.20732800	0.86025000
H	1.11234100	3.02950600	1.71205200
C	-0.69925600	3.60122200	0.95985100
N	-1.18920700	3.70597800	2.20265900
H	-0.70101000	3.51705200	3.06641100
H	-2.15628000	3.98529000	2.28423000
N	-1.46399700	3.86654500	-0.09570500
C	-0.79433100	3.70639500	-1.26840600
N	2.39698900	2.50971900	5.59830300
C	3.69600600	2.12160800	5.49221300
H	4.27287900	1.91727400	6.38196100
C	4.28894000	1.98431100	4.27599800
H	5.33112600	1.67228400	4.20993900
C	3.48391700	2.26624600	3.12823700
N	3.99566100	2.15326800	1.91683600

H	4.96055900	1.86492200	1.83979800
H	3.42946000	2.35173600	1.10447900
N	2.19440600	2.65159300	3.23131300
C	1.63924900	2.77685400	4.46639900
O	0.46126200	3.12640100	4.63302900
N	-3.80937200	-2.41302600	3.07908400
C	-3.23459900	-2.55321800	4.30354900
H	-3.82268300	-2.40208700	5.19657800
C	-1.92113400	-2.88317500	4.42708800
H	-1.47711400	-2.99131900	5.41666100
C	-1.18501800	-3.07268800	3.21596400
N	0.09435200	-3.39434600	3.26231200
H	0.51965300	-3.49806600	4.17240200
H	0.61671200	-3.52880800	2.40852400
N	-1.75356700	-2.93403300	1.99962400
C	-3.07018000	-2.60312700	1.91986700
O	-3.65479800	-2.45995600	0.83574200
O	4.60637800	-5.76224600	-5.64434200
C	3.48266500	-6.49413200	-6.16895000
H	3.80842700	-7.10641800	-7.00983300
H	3.07612900	-7.13370900	-5.38565700
C	2.40427300	-5.52865000	-6.63297200
H	1.90998900	-6.05515100	-7.44928300
O	1.55319700	-5.18994800	-5.49619600
C	1.83972500	-3.87295900	-5.04916500
H	0.96773900	-3.23812200	-5.20641000
C	2.89966900	-4.17794500	-7.15361800

H	3.80753100	-4.33808800	-7.73520600
C	3.01213700	-3.34298900	-5.87655100
H	4.04268000	-3.01249800	-5.74751600
H	2.35899900	-2.47357800	-5.95158500
O	2.03420900	-3.48400100	-8.03992100
P	2.21801100	-1.90575500	-8.22796100
O	1.91411800	-1.53360600	-9.62769300
O	3.55080500	-1.49883700	-7.72977300
O	1.07926100	-1.33628300	-7.25913100
C	-0.19123400	-2.01154200	-7.20275200
H	-0.40699900	-2.46116200	-8.17186000
H	-0.14898900	-2.78843700	-6.43952100
C	-1.28988200	-1.02326800	-6.84683900
H	-2.17644300	-1.42350500	-7.33847700
O	-1.37244500	-0.91260900	-5.39338400
C	-0.81233300	0.32039400	-4.96666500
H	-1.59190000	0.93918600	-4.52253800
C	-1.07355000	0.41341100	-7.32648500
H	-0.63355700	0.38758800	-8.32328600
C	-0.24126500	1.02565000	-6.19813600
H	0.71406000	1.36847800	-6.59553500
H	-0.77866200	1.86995000	-5.76658700
O	-2.23696800	1.21314200	-7.47815500
P	-2.08971000	2.80635500	-7.47798400
O	-3.07709000	3.39654100	-8.40920200
O	-0.67704400	3.17386900	-7.72169500
O	-2.49073500	3.16165700	-5.97046100

C	-3.56828400	2.43903900	-5.34594300
H	-4.29859500	2.15067900	-6.10198200
H	-3.16792200	1.54716800	-4.86412000
C	-4.24086500	3.31132400	-4.29849300
H	-5.27461900	2.96613000	-4.28959400
O	-3.52058600	3.17315900	-3.03606900
C	-2.74643900	4.33735600	-2.78759200
H	-3.12536700	4.84289900	-1.89948900
C	-4.23180800	4.81527100	-4.57950300
H	-4.40064000	4.97381700	-5.64450900
C	-2.88795000	5.26042100	-3.99916500
H	-2.27886200	5.70089200	-4.78839400
H	-3.05672900	5.99944100	-3.21592700
O	-5.24359000	5.58466300	-3.94646700
O	4.79603100	2.89015400	8.41871000
C	4.09851600	4.11594600	8.70941100
H	4.44040100	4.51036800	9.66619400
H	4.30386900	4.83929800	7.92030400
C	2.60158400	3.85984500	8.77271700
H	2.23555000	4.59967700	9.48459300
O	2.04886200	3.95642600	7.42494700
C	1.74516300	2.66084500	6.92961100
H	0.66848200	2.56955400	6.78712400
C	2.18420400	2.46975400	9.25679600
H	2.84728500	2.16712700	10.06725500
C	2.20996100	1.64125700	7.97095200
H	2.92356200	0.82439300	8.07867500

H	1.21731800	1.23316700	7.78120400
O	0.88121600	2.35563500	9.80960900
P	0.37360600	1.14568200	9.86985600
O	-0.44137900	1.07273100	11.10309800
O	1.40218900	0.09358300	9.71015900
O	-0.58820200	1.15372200	8.59123700
C	-1.28524200	2.36647500	8.24966200
H	-1.50044700	2.92989200	9.15759800
H	-0.65868300	2.96390700	7.58739500
C	-2.58707600	2.03514900	7.53843700
H	-3.25163600	2.85695500	7.80468300
O	-2.31910400	1.87976100	6.11168700
C	-2.35535500	0.50535600	5.75658300
H	-3.18662300	0.32819100	5.07418800
C	-3.25199600	0.71912700	7.94656000
H	-3.14445000	0.59138800	9.02359500
C	-2.56633200	-0.30320900	7.03790500
H	-2.05574500	-1.04795400	7.64844100
H	-3.31329500	-0.79504600	6.41496400
O	-4.65008600	0.61824600	7.72011200
P	-5.15490200	-0.59408700	7.69952600
O	-6.50928200	-0.51545600	8.29077900
O	-4.24390800	-1.59494400	8.29849900
O	-5.27146100	-0.84992600	6.12442000
C	-5.62673300	0.24803600	5.26327400
H	-6.27719700	0.93672500	5.80223700
H	-4.71962100	0.76695100	4.95382300

C	-6.34865100	-0.27078300	4.03036500
H	-7.02005000	0.54212200	3.75415800
O	-5.35789900	-0.63818100	3.02302400
C	-5.24826700	-2.05157300	2.94113500
H	-5.58445000	-2.38578000	1.95972400
C	-7.17784400	-1.54100500	4.23004200
H	-7.67467200	-1.48655500	5.19858600
C	-6.14892400	-2.65380900	4.02100200
H	-6.07810900	-3.25837400	4.92508400
H	-6.45834800	-3.28339400	3.18688100
O	-8.23416700	-1.76030000	3.30674100
H	-5.33947000	5.26024700	-3.05882800
H	-3.99977500	3.20143300	-8.47844700
H	2.48940100	-0.96582000	-10.12202800
H	-7.92343100	-1.50082500	2.44743600
H	-6.94285100	-1.24565300	8.70610100
H	-0.82347900	0.27375700	11.43475400
H	4.63055300	2.30793600	9.15125400
H	4.94369500	-5.24179900	-6.36435000

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