

Modeling DNA oxidation in water

– Electronic Supporting Information (ESI) –

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Section S1: Adopted constraints in geometry optimizations

C1'-C1' distances and C1'-C3'...C3'-C1' dihedral angles involving consecutive ribose rings have been held fixed for all the steps in all the sequences.

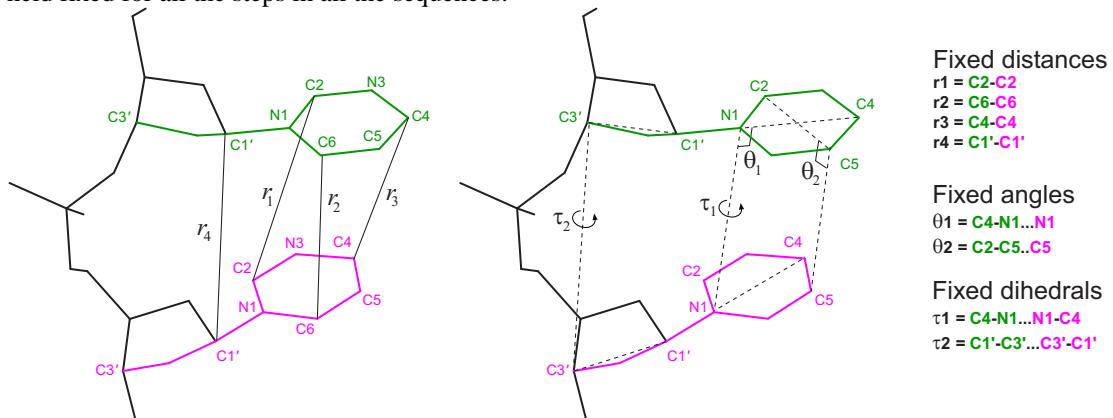


Figure S1: Internal coordinates held fixed in 5'-Pyrimidine-Pyrimidine-3' steps. C6 has to be replaced with N for 6-deaza uracil.

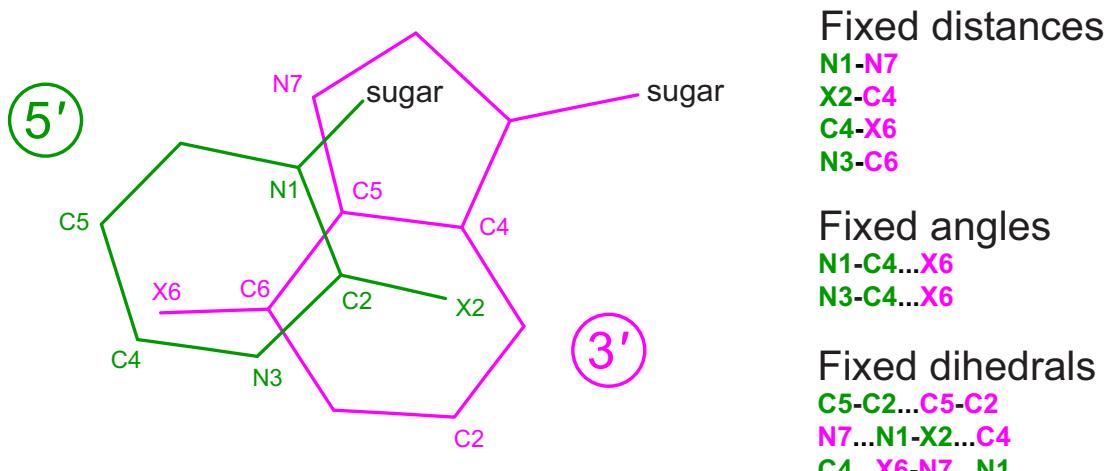
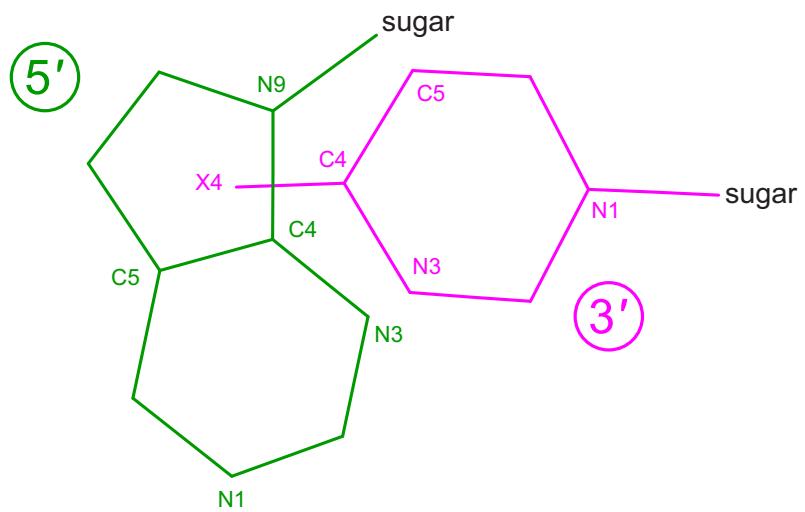


Figure S2: Constrained inter base coordinates for 5'-Pyrimidine-Purine-3' steps. X symbols denote heteroatoms.



Fixed distances

N9-C5

N3-N3

C5-X4

C4-C4

Fixed angles

N9-C5...X4

N1-C5...X4

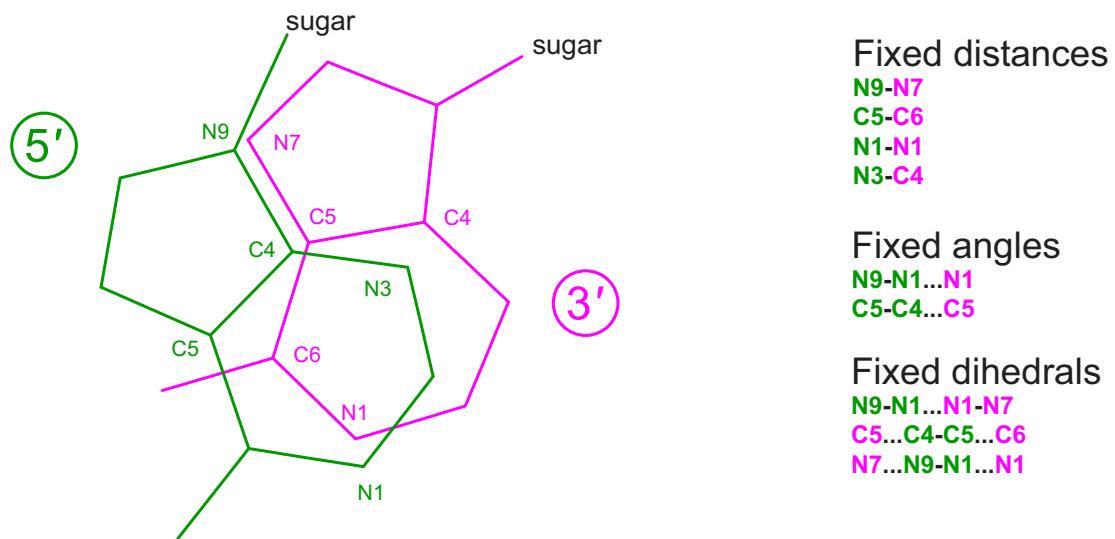
Fixed dihedrals

N1-N3...C4-N1

C5...N9-N3...N3

C5...X4-C5...N9

Figure S3: Constrained inter base coordinates for 5'-Purine-Pyrimidine-3' steps. X symbols denote heteroatoms.



Fixed distances

N9-N7

C5-C6

N1-N1

N3-C4

Fixed angles

N9-N1...N1

C5-C4...C5

Fixed dihedrals

N9-N1...N1-N7

C5...C4-C5...C6

N7...N9-N1...N1

Figure S4: Constrained inter base coordinates for 5'-Purine-Purine-3' steps.

Section S2: Optimized geometries of free and embedded DNA nucleobases

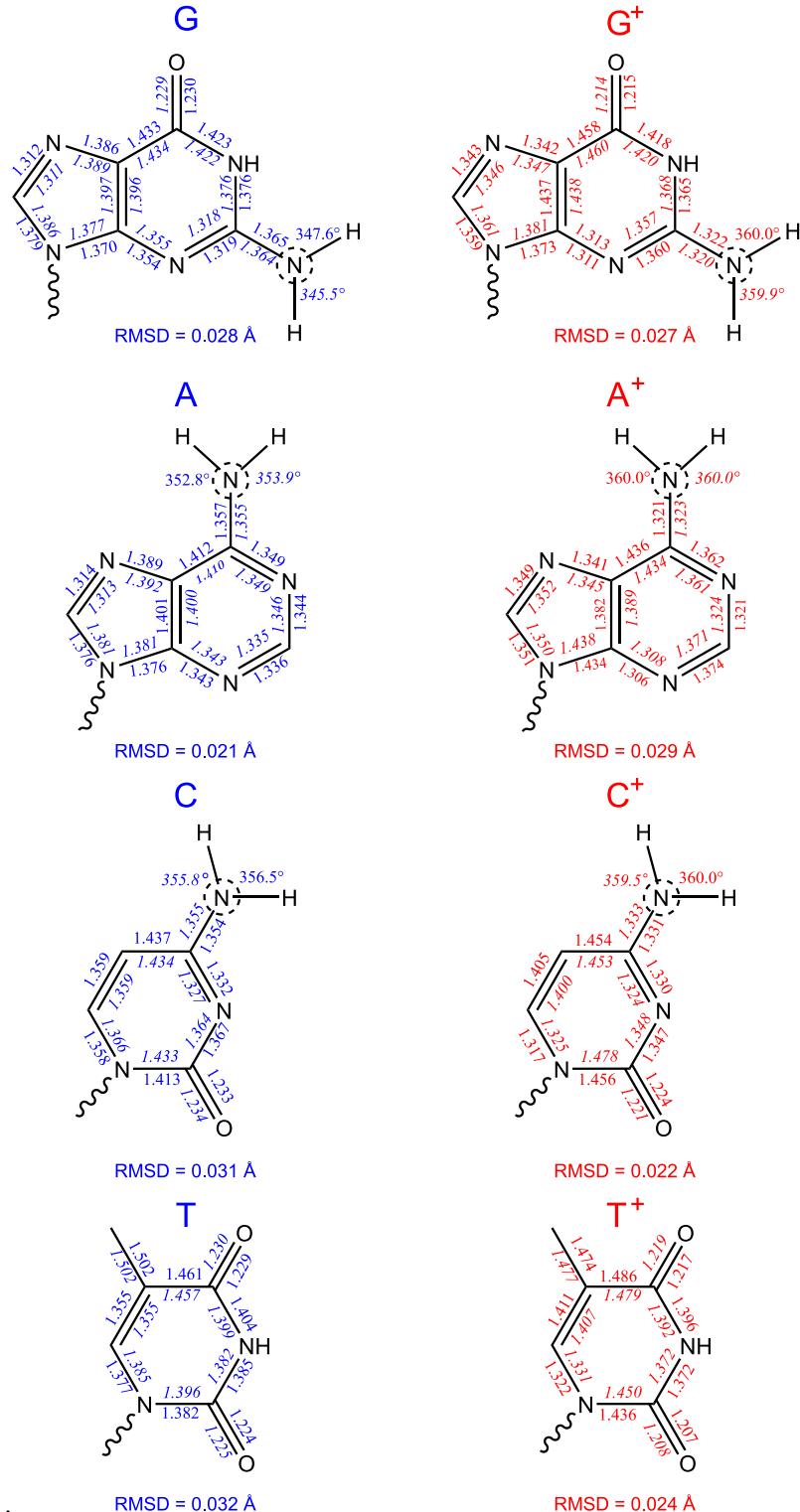


Figure S5: Geometric parameters (bond lengths in Å, angles in degrees) for neutral (blue) and singly ionized (red) free DNA nucleobases (roman font) and DNA nucleobases in XXYX single strands (italicized font) optimized at the PCM/B3LYP-D/TZVP level.

Section S3: local base steps coordinates and puckering conformations of single strands

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XACX cation
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1 X/A       0.13      0.43      3.20      6.64      2.40      33.15
  2 A/C       0.48      0.44      3.38      4.00      0.97      36.76
  3 C/X       0.49      0.58      3.33      4.88      0.89      36.96
  ~~~~~
  ave.       0.37      0.48      3.30      5.17      1.42      35.63
  s.d.       0.20      0.09      0.09      1.35      0.85      2.14
*****
base Puckering
  1 C2'-endo
  2 C1'-exo
  3 O4'-endo
  4 C2'-endo

XACX neutral
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1 X/A       0.12      0.40      3.21      6.33      2.11      33.03
  2 A/C       0.46      0.44      3.38      3.85      2.44      36.95
  3 C/X       0.49      0.56      3.39      3.97      1.10      37.10
  ~~~~~
  ave.       0.36      0.47      3.33      4.72      1.89      35.70
  s.d.       0.21      0.08      0.10      1.40      0.70      2.31
*****
base Puckering
  1 C2'-endo
  2 C1'-exo
  3 O4'-endo
  4 C2'-endo

XAGX cation
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1 X/A       0.15      0.42      3.22      6.48      1.64      32.97
  2 A/G       0.33      0.37      3.30      4.94      1.97      35.47
  3 G/X       0.80      0.66      3.24      5.99     -1.16      39.33
  ~~~~~
  ave.       0.43      0.48      3.25      5.81      0.82      35.92
  s.d.       0.33      0.15      0.04      0.79      1.72      3.20
*****
base Puckering
  1 C2'-endo
  2 C2'-endo
  3 C1'-exo
  4 C2'-endo

XAGX neutral
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1 X/A       0.15      0.41      3.23      6.15      1.76      33.01
  2 A/G       0.34      0.37      3.28      5.32      2.27      35.30
  3 G/X       0.83      0.69      3.11      7.87      0.11      39.12
  ~~~~~
  ave.       0.44      0.49      3.21      6.45      1.38      35.81
  s.d.       0.35      0.17      0.09      1.30      1.12      3.08
*****
base Puckering
  1 C2'-endo
  2 C1'-exo
  3 C1'-exo
  4 C2'-endo

XATX cation
Local base step parameters
  step      Shift      Slide      Rise      Tilt      Roll      Twist
  1 X/A       0.10      0.42      3.19      6.61      2.72      33.17
  2 A/T       0.32      0.31      3.58      1.12     -0.80      36.02
  3 T/X       0.61      0.52      3.33      4.57      1.08      39.03

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~~~~~
ave.      0.34      0.42      3.37      4.10      1.00      36.07
s.d.      0.25      0.10      0.20      2.78      1.76      2.93
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 O4'-endo
4 C2'-endo

XATX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/A      0.09      0.40      3.19      6.68      2.20      33.00
2 A/T      0.36      0.37      3.46      2.92      0.01      36.01
3 T/X      0.62      0.49      3.33      4.52      0.76      39.20
~~~~~
ave.      0.36      0.42      3.33      4.71      0.99      36.07
s.d.      0.26      0.07      0.13      1.88      1.11      3.10
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 O4'-endo
4 C2'-endo

XCAX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.28      0.48      3.27      4.86      2.68      33.39
2 C/A      0.41      0.48      3.27      5.47      2.63      37.05
3 A/X      0.63      0.62      3.30      5.19      -1.16     37.46
~~~~~
ave.      0.44      0.53      3.28      5.17      1.38      35.97
s.d.      0.18      0.08      0.02      0.30      2.21      2.24
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XCAX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.27      0.47      3.30      4.51      2.69      33.32
2 C/A      0.43      0.48      3.30      5.14      2.90      36.85
3 A/X      0.67      0.67      3.15      7.19      0.52      37.15
~~~~~
ave.      0.46      0.54      3.25      5.61      2.04      35.77
s.d.      0.20      0.12      0.09      1.40      1.32      2.13
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 O4'-endo
4 C2'-endo

XAAAX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/A      0.05      0.48      3.42      3.76      -1.64     33.22
2 A/A      0.37      0.45      3.31      4.79      1.99      35.97
3 A/X      0.59      0.66      3.18      8.73      -2.86     37.32
~~~~~
ave.      0.34      0.53      3.30      5.76      -0.83     35.50
s.d.      0.27      0.12      0.12      2.62      2.52      2.09
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C1'-exo

XAAAX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
```

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1 X/A      0.30      1.25      3.28      5.53      5.69      33.01
2 A/A      0.42      0.48      3.29      4.91      2.70      36.14
3 A/X      0.58      0.66      3.22      8.29     -3.04      37.20
~~~~~ ave.    0.44      0.80      3.26      6.24      1.78      35.45
       s.d.   0.14      0.40      0.03      1.47      4.44      2.18
*****base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C1'-exo

XCCX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.45      0.45      3.29      4.77      1.88      35.66
2 C/C      0.43      0.39      3.48      1.33      2.58      36.59
3 C/X      0.38      0.64      3.26      6.05      1.55      35.05
~~~~~ ave.    0.42      0.49      3.34      4.05      2.00      35.76
       s.d.   0.04      0.13      0.12      2.44      0.52      0.78
*****base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C1'-exo

XCCX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.42      0.46      3.28      4.79      2.47      35.32
2 C/C      0.43      0.45      3.41      2.69      2.64      36.25
3 C/X      0.42      0.57      3.31      5.29      1.07      35.77
~~~~~ ave.    0.42      0.49      3.33      4.25      2.06      35.78
       s.d.   0.01      0.07      0.07      1.38      0.86      0.47
*****base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C1'-exo

XCGX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.32      0.50      3.24      5.43      2.67      33.99
2 C/G      0.19      0.45      3.25      5.64      3.07      34.08
3 G/X      0.82      0.64      3.32      4.92     -2.11      40.05
~~~~~ ave.    0.44      0.53      3.27      5.33      1.21      36.04
       s.d.   0.33      0.10      0.05      0.37      2.88      3.47
*****base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XCGX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/C      0.32      0.48      3.27      4.87      2.84      34.13
2 C/G      0.22      0.45      3.27      5.42      2.86      34.04
3 G/X      0.87      0.70      3.14      7.32     -0.46      39.66
~~~~~ ave.    0.47      0.54      3.23      5.87      1.74      35.94
       s.d.   0.35      0.14      0.07      1.28      1.91      3.21
*****base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

```

XCTX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/C	0.40	0.45	3.32	4.37	2.13	35.12
2 C/T	0.27	0.43	3.42	2.47	3.11	34.26
3 T/X	0.60	0.56	3.30	5.54	0.47	38.32
ave.	0.43	0.48	3.35	4.13	1.90	35.90
s.d.	0.17	0.07	0.07	1.55	1.33	2.14

base Puckering

1 C2'-endo	
2 C1'-exo	
3 O4'-endo	
4 C2'-endo	

XCTX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/C	0.36	0.48	3.29	4.52	3.11	34.71
2 C/T	0.28	0.46	3.36	3.75	2.76	34.05
3 T/X	0.63	0.51	3.34	4.73	0.25	38.97
ave.	0.43	0.48	3.33	4.33	2.04	35.91
s.d.	0.18	0.02	0.04	0.51	1.56	2.67

base Puckering

1 C2'-endo	
2 C1'-exo	
3 O4'-endo	
4 C2'-endo	

XGAX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.12	0.34	3.25	5.68	2.62	32.22
2 G/A	0.40	0.55	3.27	5.43	2.12	36.83
3 A/X	0.70	0.61	3.17	7.06	-0.24	38.39
ave.	0.41	0.50	3.23	6.05	1.50	35.81
s.d.	0.29	0.14	0.05	0.88	1.53	3.21

base Puckering

1 C2'-endo	
2 C2'-endo	
3 O4'-endo	
4 C2'-endo	

XGAX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.10	0.33	3.24	5.71	3.23	32.22
2 G/A	0.42	0.55	3.27	5.47	2.44	36.75
3 A/X	0.70	0.61	3.19	6.82	-0.38	38.48
ave.	0.41	0.50	3.23	6.00	1.76	35.81
s.d.	0.30	0.15	0.04	0.72	1.90	3.23

base Puckering

1 C2'-endo	
2 C2'-endo	
3 O4'-endo	
4 C2'-endo	

XGCX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.07	0.30	3.17	6.89	1.87	32.68
2 G/C	0.52	0.48	3.46	2.90	-0.24	38.03
3 C/X	0.49	0.56	3.33	4.81	0.66	37.02
ave.	0.36	0.45	3.32	4.87	0.77	35.91
s.d.	0.25	0.13	0.14	2.00	1.06	2.85

base Puckering

1 C2'-endo	
2 C1'-exo	
3 O4'-endo	

4 C2'-endo

XGCX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.11	0.32	3.21	6.20	2.27	32.49
2 G/C	0.56	0.52	3.34	4.44	2.25	37.87
3 C/X	0.49	0.55	3.36	4.41	0.81	37.10
ave.	0.39	0.46	3.30	5.02	1.78	35.82
s.d.	0.24	0.12	0.08	1.02	0.84	2.91

base Puckering

1 C2'-endo

2 C2'-endo

3 O4'-endo

4 C2'-endo

XGGX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	-0.24	1.07	3.45	2.43	-3.36	32.95
2 G/G	0.35	0.46	3.27	5.38	-0.15	36.08
3 G/X	0.86	0.71	3.13	7.65	-0.59	39.56
ave.	0.32	0.74	3.28	5.15	-1.37	36.20
s.d.	0.55	0.31	0.16	2.62	1.74	3.31

base Puckering

1 C2'-endo

2 C2'-endo

3 C1'-exo

4 C2'-endo

XGGX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.10	0.32	3.27	5.31	2.57	31.95
2 G/G	0.39	0.48	3.25	5.91	1.80	35.97
3 G/X	0.87	0.72	3.09	8.15	-0.00	39.30
ave.	0.45	0.51	3.20	6.46	1.46	35.74
s.d.	0.39	0.20	0.10	1.49	1.32	3.68

base Puckering

1 C2'-endo

2 C1'-exo

3 C1'-exo

4 C2'-endo

XGTX cation

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.05	0.33	3.20	6.25	3.35	32.23
2 G/T	0.40	0.38	3.57	1.25	-1.67	37.07
3 T/X	0.61	0.50	3.29	5.08	0.77	39.12
ave.	0.35	0.40	3.36	4.19	0.82	36.14
s.d.	0.28	0.09	0.19	2.61	2.51	3.54

base Puckering

1 C2'-endo

2 C1'-exo

3 O4'-endo

4 C2'-endo

XGTX neutral

Local base step parameters

step	Shift	Slide	Rise	Tilt	Roll	Twist
1 X/G	0.09	0.33	3.22	5.89	3.04	32.25
2 G/T	0.44	0.43	3.45	2.99	-0.36	37.05
3 T/X	0.62	0.48	3.30	5.04	0.46	39.22
ave.	0.38	0.41	3.32	4.64	1.05	36.17
s.d.	0.27	0.08	0.11	1.49	1.77	3.57

base Puckering

1 C2'-endo

```

2 C1'-exo
3 O4'-endo
4 C2'-endo

XXAX cation
Local base step parameters
  step   Shift   Slide   Rise   Tilt   Roll   Twist
  1 X/X    0.45    0.51   3.32   5.04  -0.29  35.47
  2 X/A    0.16    0.48   3.31   4.63   4.64  32.90
  3 A/X    0.74    0.59   3.30   5.29  -1.62  38.81
  ~~~~~
  ave.    0.45    0.53   3.31   4.99   0.91  35.73
  s.d.    0.29    0.05   0.01   0.33   3.30  2.96
*****base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXAX neutral
Local base step parameters
  step   Shift   Slide   Rise   Tilt   Roll   Twist
  1 X/X    0.44    0.50   3.33   4.94  -0.19  35.44
  2 X/A    0.15    0.46   3.29   4.96   4.23  32.69
  3 A/X    0.78    0.64   3.14   7.37   0.15  38.49
  ~~~~~
  ave.    0.46    0.53   3.25   5.76   1.40  35.54
  s.d.    0.31    0.09   0.10   1.40   2.46  2.90
*****base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXCX cation
Local base step parameters
  step   Shift   Slide   Rise   Tilt   Roll   Twist
  1 X/X    0.44    0.44   3.40   3.52   0.20  35.50
  2 X/C    0.42    0.41   3.39   2.96   2.47  35.89
  3 C/X    0.43    0.59   3.39   3.81   1.16  35.76
  ~~~~~
  ave.    0.43    0.48   3.39   3.43   1.28  35.72
  s.d.    0.01    0.09   0.01   0.44   1.14  0.20
*****base Puckering
1 C2'-endo
2 C2'-endo
3 O4'-endo
4 C2'-endo

XXCX neutral
Local base step parameters
  step   Shift   Slide   Rise   Tilt   Roll   Twist
  1 X/X    0.44    0.45   3.39   3.85  -0.00  35.41
  2 X/C    0.34    0.50   3.29   4.22   4.00  35.00
  3 C/X    0.50    0.50   3.45   2.90   0.25  36.73
  ~~~~~
  ave.    0.43    0.48   3.38   3.65   1.41  35.71
  s.d.    0.08    0.03   0.08   0.68   2.24  0.91
*****base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXGX cation
Local base step parameters
  step   Shift   Slide   Rise   Tilt   Roll   Twist
  1 X/X    0.45    0.50   3.31   5.39  -0.31  35.24
  2 X/G    0.14    0.38   3.31   4.36   4.91  32.28
  3 G/X    0.78    0.61   3.34   4.67  -2.05  39.65
  ~~~~~
  ave.    0.46    0.50   3.32   4.81   0.85  35.72
  s.d.    0.32    0.11   0.02   0.53   3.62  3.71

```

```
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXGX neutral
Local base step parameters
step Shift Slide Rise Tilt Roll Twist
1 X/X 0.45 0.49 3.33 5.05 -0.26 35.36
2 X/G 0.16 0.39 3.32 4.46 4.65 32.27
3 G/X 0.84 0.68 3.12 7.57 -0.31 39.18
~~~~~ ave. 0.48 0.52 3.26 5.69 1.36 35.60
s.d. 0.34 0.15 0.12 1.65 2.85 3.46
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XXTX cation
Local base step parameters
step Shift Slide Rise Tilt Roll Twist
1 X/X 0.45 0.47 3.36 4.54 -0.18 35.50
2 X/T 0.28 0.43 3.38 3.23 3.14 33.72
3 T/X 0.56 0.58 3.29 5.50 1.03 37.94
~~~~~ ave. 0.43 0.49 3.34 4.42 1.33 35.72
s.d. 0.14 0.08 0.04 1.14 1.68 2.12
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 O4'-endo
4 C2'-endo

XXTX neutral
Local base step parameters
step Shift Slide Rise Tilt Roll Twist
1 X/X 0.45 0.48 3.34 4.88 -0.28 35.43
2 X/T 0.20 0.50 3.29 4.62 4.09 32.66
3 T/X 0.63 0.49 3.35 4.47 0.23 39.04
~~~~~ ave. 0.43 0.49 3.33 4.66 1.35 35.71
s.d. 0.21 0.01 0.03 0.21 2.39 3.20
*****
base Puckering
1 C2'-endo
2 C2'-endo
3 C1'-exo
4 C2'-endo

XTAX cation
Local base step parameters
step Shift Slide Rise Tilt Roll Twist
1 X/T 0.23 0.47 3.24 5.58 2.43 32.50
2 T/A 0.35 0.45 3.27 5.43 3.44 36.53
3 A/X 0.71 0.57 3.29 5.26 -1.22 38.50
~~~~~ ave. 0.43 0.50 3.27 5.42 1.55 35.85
s.d. 0.25 0.06 0.03 0.16 2.45 3.06
*****
base Puckering
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTAX neutral
Local base step parameters
step Shift Slide Rise Tilt Roll Twist
1 X/T 0.23 0.46 3.25 5.42 2.42 32.40
2 T/A 0.36 0.45 3.27 5.53 3.24 36.33
3 A/X 0.74 0.62 3.15 7.18 0.29 38.22
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    ave.      0.44      0.51      3.22      6.04      1.98      35.65
    s.d.      0.27      0.09      0.06      0.99      1.52      2.97
*****base Puckering*****
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTCX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/T      0.26      0.45      3.29      5.03      2.17      32.82
2 T/C      0.55      0.39      3.41      2.15      3.24      38.74
3 C/X      0.48      0.59      3.31      5.61      -0.28     36.13
~~~~~ave.      0.43      0.48      3.34      4.26      1.71      35.90
s.d.      0.15      0.10      0.06      1.85      1.80      2.97
*****base Puckering*****
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTCX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/T      0.22      0.47      3.25      5.48      2.69      32.30
2 T/C      0.55      0.43      3.37      3.02      3.33      38.49
3 C/X      0.52      0.55      3.34      5.04      -0.59     36.75
~~~~~ave.      0.43      0.48      3.32      4.52      1.81      35.85
s.d.      0.18      0.06      0.06      1.31      2.11      3.19
*****base Puckering*****
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTGX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/T      0.23      0.49      3.23      5.91      2.39      32.25
2 T/G      0.31      0.37      3.25      5.51      3.58      35.60
3 G/X      0.78      0.62      3.32      4.96      -1.91     39.65
~~~~~ave.      0.44      0.49      3.27      5.46      1.35      35.84
s.d.      0.30      0.13      0.05      0.48      2.89      3.71
*****base Puckering*****
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTGX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/T      0.23      0.46      3.26      5.43      2.46      32.39
2 T/G      0.34      0.37      3.28      5.30      3.31      35.57
3 G/X      0.84      0.68      3.12      7.52      -0.17     39.22
~~~~~ave.      0.47      0.51      3.22      6.08      1.87      35.73
s.d.      0.33      0.16      0.08      1.24      1.81      3.42
*****base Puckering*****
1 C2'-endo
2 C1'-exo
3 C1'-exo
4 C2'-endo

XTTX cation
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/T      0.28      0.44      3.30      4.62      2.00      33.61
2 T/T      0.42      0.32      3.44      2.10      2.15      36.45

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3 T/X      0.61      0.61      3.30      7.47     -1.76     37.26
~~~~~
ave.      0.44      0.46      3.35      4.73      0.80     35.77
s.d.      0.16      0.15      0.08      2.69      2.22     1.91
*****
base   Puckering
1    C2'-endo
2    C1'-exo
3    C1'-exo
4    C1'-exo

XTTX neutral
Local base step parameters
step      Shift      Slide      Rise      Tilt      Roll      Twist
1 X/T      0.25      0.45      3.27      5.03      2.37     33.13
2 T/T      0.43      0.37      3.38      3.42      2.12     36.15
3 T/X      0.64      0.57      3.35      6.58     -1.67     38.01
~~~~~
ave.      0.44      0.46      3.33      5.01      0.94     35.76
s.d.      0.20      0.10      0.05      1.58      2.27     2.46
*****
base   Puckering
1    C2'-endo
2    C1'-exo
3    C1'-exo
4    C1'-exo

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Section S4: results obtained by using the TZVP basis set

Table S1: Predicted (PCM-B3LYP-D/TZVP) adiabatic ionization potentials (eV) of nucleobases (Y) and of XXYX single stranded oligonucleotides

	Y	XXYX
G	5.79	5.82
A	6.20	6.25
C	6.55	6.50
T	6.55	6.52

Table S2: Adiabatic ionization potentials (eV, TZVP basis set) of 5'-XYZX-3' single strands

Y (5' side)	Z (3' side)			
	G	A	C	T
5.73	5.77	5.76	5.78	
5.79	6.01	6.17	6.22	
5.75	6.15	6.38	6.38	
5.80	6.23	6.41	6.40	

Table S3: Predicted electronic couplings (eV, TZVP basis set) for 5'-YZ-3' steps

Y (5' side)	Z (3' side)			
	G	A	C	T
0.09	0.16	0.23	0.16	
0.12	0.24	0.16	0.10	
0.25	0.18	0.12	0.13	
0.13	0.08	0.10	0.12	

Table S4: Hole energies (eV) relative to XXGX of single strands predicted by PCM/B3LYP-D/TZVP computations and by using the TB Hamiltonian. Deviations^a of TB from DFT results are in eV

ss	TB	DFT	ss	TB	DFT
XAGA	-0.08	-0.09	XCAC	0.28	0.29
AAGA	-0.09	-0.09	CCAC	0.28	0.28
TGAC	-0.08	-0.06	XTAT	0.38	0.39
TAGC	-0.11	-0.11	TTAT	0.38	0.39
XCGC	-0.14	-0.14	TCAT	0.31	0.32
CCGC	-0.14	-0.15	CTAC	0.34	0.34
XTGT	-0.06	-0.06	CAAC	0.14	0.14
TTGT	-0.06	-0.06	TAAT	0.18	0.19
AGGA	-0.13	-0.11	CAAT	0.15	0.14
CGGC	-0.16	-0.16	TAAC	0.16	0.17
TGGT	-0.12	-0.11	XTCT	0.52	0.52
TGGA	-0.12	-0.14	TTCT	0.51	0.52
CGGT	-0.14	-0.15	TCCT	0.49	0.49
MUE ^a	MSE	RMSD	L. dev. (seq)	R^2	intercep t
7×10^{-3}	-2×10^{-3}	9×10^{-3}	2×10^{-2} (AGGA)	0.999	-4×10^{-4}

^aMUE/MSE denote mean unsigned/signed errors; RMSD is the root mean square deviation. Signed largest deviation is reported for the corresponding sequence. R^2 is the linear correlation coefficient between DFT and TB calculated hole energies. The linear fitting using DFT values as abscissa and TB ones as ordinate returns 0.99 and -4×10^{-4} eV as the slope and the intercept, respectively.

Section S5: Statistical analysis for the symmetric couplings

Table S5: Hole energies (eV) relative to XXGX of single strands predicted by PCM/B3LYP-D/TZV+P computations and by using the TB Hamiltonian with symmetric 5'-YZ-3' couplings, see Eq. (5) in the main text. Deviations of TB from DFT results are in eV

ss	TB	DFT	ss	TB	DFT
XGAX	-0.05	-0.05	XACX	0.34	0.35
XAGX	-0.05	-0.03	XCA _X	0.34	0.33
AAGA	-0.10	-0.10	CCAC	0.28	0.28
TGAC	-0.07	-0.06	XATX	0.40	0.40
TAGC	-0.11	-0.11	XTAX	0.40	0.41
XGCX	-0.07	-0.08	TTAT	0.38	0.38
XCGX	-0.07	-0.07	TCAT	0.32	0.32
CCGC	-0.14	-0.14	CTAC	0.33	0.34
XGTX	-0.03	-0.04	CAAC	0.14	0.14
XTGX	-0.03	-0.02	TAAT	0.18	0.19
TTGT	-0.05	-0.06	CAAT	0.16	0.14
AGGA	-0.13	-0.11	TAAC	0.16	0.17
CGGC	-0.16	-0.16	XCTX	0.57	0.56
TGGT	-0.11	-0.11	XTCX	0.57	0.58
TGGA	-0.12	-0.14	TTCT	0.50	0.52
CGGT	-0.14	-0.15	TCCT	0.49	0.49
MUE ^a	MSE	RMSD	L. dev. (seq)	R^2	intercept
8×10^{-3}	-8×10^{-4}	1×10^{-2}	-2×10^{-2} (TTCT)	0.999	5×10^{-4}

^aMUE/MSE denote mean unsigned/signed errors; RMSD is the root mean square deviation. Signed largest deviation is reported for the corresponding sequence. R^2 is the linear correlation coefficient between DFT and TB calculated hole energies. The linear fitting using DFT values as abscissa and TB predictions as ordinate returns 0.99 and 5×10^{-4} eV as the slope and the intercept, respectively.

Cartesian coordinates

XAAX				XACX			
O	-9.85446	0.10734	0.23297	H	-10.09257	-1.84058	-0.49185
C	-9.67437	-0.86705	-0.79043	H	-10.16045	-0.55730	-1.72748
C	-8.18980	-1.05570	-1.05577	H	-8.06597	-1.91484	-1.72593
O	-7.64945	0.12011	-1.69258	H	-7.95055	-1.67397	1.04509
C	-7.35306	-1.27422	0.22122	H	-7.56224	0.74291	0.93358
O	-6.29748	-2.20087	-0.11703	H	-5.60822	0.09489	-1.32224
C	-6.78674	0.11769	0.48886	H	-4.63298	4.14784	-2.86651
C	-6.51840	0.56363	-0.94262	H	-5.89238	0.09666	1.10928
N	-6.34247	1.99750	-1.13757	H	-3.98302	-4.74062	-1.51267
C	-5.43338	2.41660	-2.12268	H	-4.87698	-3.20964	-1.70604
O	-4.81975	1.63354	-2.82990	H	-2.38592	-3.27933	-2.37250
N	-5.30544	3.79304	-2.19285	H	-1.91853	-4.20774	0.24972
C	-6.02398	4.72131	-1.44239	H	-2.55074	-2.05663	1.21278
O	-5.85430	5.92542	-1.55581	H	-1.01681	-0.84679	-1.14984
C	-6.97928	4.08623	-0.51564	H	-3.70838	-0.18543	1.45351
N	-7.11482	2.81199	-0.38989	H	-0.19075	3.29547	-2.65446
P	-5.45986	-2.90502	1.10358	H	-3.64562	4.69430	1.05254
O	-6.35889	-3.81257	1.91977	H	-2.79864	5.79131	0.03478
O	-4.71148	-1.86689	1.92851	H	-0.76171	-1.89463	1.08512
O	-4.42844	-3.82285	0.24078	H	2.64698	-3.75777	-3.14114
C	-4.08167	-3.71225	-1.15003	H	1.11743	-2.93161	-2.74944
C	-2.75965	-2.99034	-1.38161	H	3.22293	-1.51472	-3.00794
O	-2.96434	-1.56439	-1.35246	H	4.36025	-3.20824	-0.99149
C	-1.68348	-3.30239	-0.31561	H	3.20356	-2.03986	0.77714
O	-0.41662	-3.46592	-0.98739	H	3.48779	0.46954	-0.95177
C	-1.69088	-2.03390	0.53750	H	1.23545	-1.22092	1.63250
C	-1.92255	-0.99262	-0.55003	H	2.36089	4.74933	-0.46619
N	-2.32699	0.31294	-0.10572	H	-1.05459	2.83753	2.99973
C	-3.21471	0.61139	0.90739	H	-0.93577	4.47043	2.53092
N	-3.39572	1.90019	1.07941	H	4.68438	-1.01599	0.62871
C	-2.58359	2.49730	0.12101	H	7.70023	0.61480	-3.67601
C	-2.29580	3.83627	-0.20907	H	6.07721	0.39976	-2.97462
N	-2.83449	4.88219	0.47800	H	7.46328	2.52010	-2.43998
N	-1.45567	4.08660	-1.23249	H	9.32976	0.65948	-1.26964
C	-0.88174	3.03613	-1.85506	H	7.98753	0.44304	0.70752
N	-1.04678	1.73148	-1.62441	H	7.15587	3.34873	0.22245
C	-1.92589	1.52080	-0.63615	H	3.77527	3.78695	3.13854
P	0.82716	-4.10095	-0.11714	H	8.95426	1.89716	1.16101
O	0.52954	-5.53583	0.27051	H	10.29338	2.68965	-0.77049
O	0.120239	-3.20137	1.05082	H	-10.80687	0.18107	0.39620
O	0.198037	-4.11731	-1.26697	H	-7.60198	4.72739	0.09880
C	2.10574	-3.20356	-2.36804	H	5.00651	-0.25458	3.38585
C	2.89423	-1.94294	-2.05078	Na	-5.82689	-2.58735	3.96096
O	2.05855	-0.98890	-1.37545	Na	0.77665	-4.98707	2.64228
C	4.14876	-2.14840	-1.15739	Na	7.67416	-3.96419	0.44988
O	5.25461	-1.52463	-1.83854				
C	3.79527	-1.39321	0.12343	O	9.82464	0.05178	0.29694
C	2.89473	-0.29989	-0.44294	C	9.61883	1.08220	-0.66494
N	2.06658	0.39704	0.51023	C	8.13210	1.21754	-0.94685
C	1.26010	-0.14686	1.49267	O	7.66472	0.05735	-1.66857
N	0.55896	0.75176	2.14954	C	7.26596	1.31556	0.32896
C	0.91664	1.95250	1.56016	O	6.19431	2.24184	0.05079
C	0.50255	3.27047	1.79003	C	6.73296	-0.10281	0.47567
N	-0.45048	3.59752	2.70947	C	6.52445	-0.46339	-0.99172
N	1.05505	4.24190	1.04195	N	6.39563	-1.89423	-1.25434
C	1.95371	3.91437	0.09999	C	5.48094	-2.32423	-2.22829
N	0.240174	2.70076	-0.24412	O	4.83744	-1.54933	-2.91737
C	1.85144	1.75750	0.53707	N	5.38651	-3.70358	-2.31038
P	6.78142	-1.90508	-1.36345	C	6.05457	-4.62323	-1.50177
O	7.15529	-3.29729	-1.83858	O	5.84241	-5.82431	-1.56452
O	6.97616	-1.66793	0.12236	C	7.01897	-3.97857	-0.59143
O	7.60763	-0.83145	-2.27276	N	7.16310	-2.70408	-0.49432
C	7.14635	0.44146	-2.74797	P	5.31740	2.82514	1.30774
C	7.41949	1.61589	-1.81611	O	6.17549	3.69416	2.20563
O	6.35026	1.76967	-0.86444	O	4.58308	1.71060	2.04016
C	8.73801	1.54002	-0.99977	O	4.27373	3.77528	0.49660
O	9.46365	2.74237	-1.27114	C	3.95498	3.73876	-0.90349
C	8.23896	1.47461	0.44884	C	2.68168	2.96634	-1.21209
C	6.95030	2.28041	0.32798	O	2.94394	1.55009	-1.25615
N	6.00394	2.14813	1.42820	C	1.54133	3.17119	-0.18244
C	5.20461	3.24982	1.77628	O	0.33245	3.36327	-0.93950
O	5.24915	4.32533	1.20579	C	1.51333	1.83999	0.55485
N	4.36847	3.01043	2.86103	C	1.86489	0.88660	-0.58693
C	4.18131	1.78803	3.49512	N	2.30092	-0.42496	-0.17529
O	3.38187	1.63005	4.40430	C	3.20550	-0.71501	0.82722
C	5.06506	0.73918	2.95502	N	3.44969	-1.99889	0.96238
N	5.90400	0.92634	1.99582	C	2.66259	-2.60439	-0.01280

C	2.44549	-3.93952	-0.40829	H	-3.64959	-4.26400	3.16847	
N	3.02496	-4.99010	0.23435	H	-8.85747	-2.64992	1.16832	
N	1.61579	-4.18508	-1.44340	H	-10.01258	-3.32203	-0.86760	
C	0.98579	-3.14554	-2.02249	H	10.77509	0.01656	0.48284	
N	1.08287	-1.85138	-1.72806	H	-4.79894	-0.19490	3.25682	
C	1.94479	-1.63988	-0.72988	Na	5.59297	2.34961	4.15405	
P	-1.01153	3.95663	-0.20813	Na	-1.59147	4.82283	2.48828	
O	-0.79779	5.38659	0.24573	Na	-8.29122	4.49413	-0.57198	
O	-1.53469	3.01898	0.86847					XAGX
O	-1.97517	3.99629	-1.52205	O	9.87517	0.03536	0.27874	
C	-2.10762	2.91238	-2.45614	C	9.69522	1.06306	-0.69124	
C	-2.88599	1.70414	-1.94934	C	8.21217	1.23210	-0.97397	
O	-2.04057	0.80610	-1.23844	O	7.71754	0.07506	-1.68282	
C	-4.07064	2.02326	-1.01149	C	7.35050	1.36468	0.30223	
O	-5.25286	2.01977	-1.82691	O	6.30464	2.31987	0.01981	
C	-3.98355	0.93971	0.09084	C	6.77912	-0.03737	0.46079	
C	-2.91697	-0.01465	-0.44879	C	6.56028	-0.40335	-1.00367	
N	-2.08533	-0.72808	0.50375	N	6.38248	-1.83052	-1.25472	
C	-1.92372	-2.14077	0.34431	C	5.45551	-2.23683	-2.22681	
O	-2.59806	-2.74084	-0.49751	O	4.83829	-1.44468	-2.92055	
N	-1.03189	-2.77271	1.15439	N	5.31751	-3.61298	-2.29996	
C	-0.34598	-2.09904	2.06828	C	5.96925	-4.54968	-1.49672	
N	0.50889	-2.79229	2.86447	O	5.73041	-5.74552	-1.56239	
C	-0.48161	-0.68616	2.25310	C	6.95046	-3.92917	-0.58791	
C	-1.34640	-0.03800	1.42532	N	7.12844	-2.65880	-0.49335	
P	-6.74460	2.13802	-1.15267	P	5.44997	2.93280	1.27872	
O	-7.65012	2.75573	-2.19669	O	6.33417	3.78249	2.16932	
O	-6.69561	2.78597	0.21278	O	4.69083	1.83971	2.01792	
O	-7.12323	0.55134	-0.92553	O	4.42814	3.90954	0.47089	
C	-7.03750	-0.30332	-2.07471	C	4.08144	3.86729	-0.92221	
C	-7.31304	-1.73561	-1.67112	C	2.78544	3.12115	-1.20296	
O	-6.25293	-2.20826	-0.81665	O	3.02084	1.70107	-1.24393	
C	-8.63532	-1.94337	-0.90350	O	1.66789	3.35317	-0.15422	
O	-9.21517	-3.15387	-1.39511	O	0.44818	3.57399	-0.88470	
C	-8.16195	-2.08409	0.54143	C	1.62571	2.02370	0.59073	
C	-6.82904	-2.80266	0.34026	C	1.94018	1.06257	-0.55254	
N	-5.90233	-2.67867	1.45877	N	2.35109	-0.25837	-0.15187	
C	-5.14683	-3.78810	1.85988	C	3.24800	-0.56906	0.85030	
O	-5.26953	-4.90431	1.38713	N	3.45530	-1.85812	0.98901	
N	-4.23325	-3.49151	2.86189	C	2.64341	-2.44193	0.02251	
C	-4.00945	-2.24569	3.44012	C	2.39152	-3.77277	-0.36703	
O	-3.16058	-2.06073	4.29882	N	2.94728	-4.83760	0.26739	
C	-4.88906	-1.20854	2.88172	N	1.54411	-3.99901	-1.39206	
N	-5.75896	-1.42985	1.95708	C	0.94715	-2.94222	-1.98018	
H	9.98452	2.05226	-0.29484	N	1.09111	-1.64504	-1.70781	
H	10.13659	0.85724	-1.60916	C	1.96269	-1.45904	-0.70888	
H	7.97490	2.11052	-1.56356	P	-0.88331	4.13424	-0.10199	
H	7.84227	1.66130	1.19147	O	-0.65677	5.54212	0.41167	
H	7.51387	-0.73507	0.90014	O	-1.39017	3.14882	0.93811	
H	5.61121	-0.00273	-1.37586	O	-1.86876	4.23444	-1.39742	
H	7.63478	-4.61095	0.03898	C	-1.99959	3.20207	-2.38723	
H	4.69819	-4.06505	-2.96443	C	2.79706	1.98092	-1.94940	
H	5.82180	-0.15496	1.06794	O	-1.97227	1.05150	-1.24579	
H	3.79900	4.78180	-1.19773	C	-4.01225	2.27718	-1.03834	
H	4.78759	3.32615	-1.47858	O	-5.17942	2.18214	-1.87056	
H	2.32889	3.29323	-2.19896	C	-3.90110	1.22806	0.08694	
H	1.71737	4.03211	0.46754	C	-2.85903	0.25240	-0.45887	
H	2.31405	1.82132	1.30007	N	-2.06908	-0.46664	0.51368	
H	1.01563	0.73728	-1.26230	C	-1.25988	0.06612	1.50656	
H	3.66435	0.08509	1.39901	N	-0.51248	-0.83581	2.09989	
H	0.31290	-3.40554	-2.83740	C	-0.82692	-2.02217	1.45734	
H	3.81151	-4.78922	0.83783	C	-0.38614	-3.35643	1.71646	
H	3.06162	-5.87041	-0.26381	O	0.41143	-3.77919	2.55069	
H	0.54666	1.64437	1.01072	N	-1.01696	-4.25446	0.81508	
H	-2.65723	3.33916	-3.29961	C	-1.93100	-3.93872	-0.15994	
H	-1.11826	2.59238	-2.79868	N	-2.36373	-4.95680	-0.95936	
H	-3.29379	1.18676	-2.83248	N	-2.35568	-2.71014	-0.37576	
H	-3.96272	3.01109	-0.56485	C	-1.78952	-1.81278	0.46926	
H	-3.64838	1.40550	1.02003	P	-6.67910	2.36992	-1.22526	
H	-3.37773	-0.77911	-1.07812	O	-7.55357	2.97141	-2.30446	
H	-1.48627	1.04014	1.41960	O	-6.62345	3.07000	0.11382	
H	0.10494	-0.14584	2.98605	O	-7.10604	0.80574	-0.94188	
H	0.74978	-3.72885	2.56331	C	-7.06835	-0.09061	-2.06209	
H	1.24296	-2.28350	3.33846	C	-7.34865	-1.50476	-1.59735	
H	-4.92985	0.42249	0.25597	O	-6.26009	-1.96802	-0.77370	
H	-7.77382	0.00557	-2.82775	C	-8.63458	-1.65983	-0.76118	
H	-6.03448	-0.23587	-2.51113	O	-9.23678	-2.89634	-1.14937	
H	-7.33451	-2.34282	-2.58520	C	-8.09639	-1.71231	0.66871	
H	-9.31949	-1.09712	-1.03963	C	-6.79057	-2.47077	0.45068	
H	-7.98143	-1.09669	0.97066	N	-5.79370	-2.29999	1.50358	

C	-4.95461	-3.37963	1.81751	N	2.29051	-0.41850	-0.16253
O	-4.98177	-4.45220	1.23853	C	3.22537	-0.71120	0.81001
N	-4.09602	-3.12475	2.87950	N	3.45576	-1.99652	0.94820
C	-3.89046	-1.89076	3.48400	C	2.62410	-2.60117	0.00980
O	-3.04699	-1.69883	4.34465	C	2.40563	-3.93672	-0.37910
C	-4.82282	-0.86674	2.98688	N	2.98873	-4.98730	0.25840
N	-5.69502	-1.07246	2.06112	N	1.56284	-4.17929	-1.40213
H	10.08459	2.02670	-0.32870	C	0.91530	-3.14202	-1.96907
H	10.20743	0.81790	-1.63348	N	1.00875	-1.84668	-1.67719
H	8.07583	2.12196	-1.60013	C	1.89621	-1.63471	-0.69533
H	7.93824	1.70036	1.16096	P	-0.99828	3.96143	-0.20714
H	7.54332	-0.68693	0.88971	O	-0.78946	5.38875	0.25534
H	5.66305	0.08445	-1.39183	O	-1.51771	3.01524	0.86437
H	7.55024	-4.57653	0.04273	O	-1.96180	4.00015	-1.52113
H	4.62018	-3.95770	-2.95345	C	-2.07490	2.92384	-2.46654
H	5.86758	-0.06012	1.05417	C	-2.86172	1.71151	-1.98373
H	3.94584	4.91125	-1.22316	O	-2.03047	0.80531	-1.26235
H	4.89347	3.42907	-1.50804	C	-4.06468	2.02601	-1.06772
H	2.42146	3.45078	-2.18509	O	-5.23293	1.99748	-1.90077
H	1.87587	4.21084	0.49082	C	-3.98426	0.95455	0.04670
H	2.43705	1.99444	1.32366	C	-2.91822	-0.00594	-0.48143
H	1.07618	0.93453	-1.21380	N	-2.09740	-0.71770	0.48631
H	3.72939	0.22090	1.41693	C	-1.95657	-2.09822	0.33256
H	0.25678	-3.19096	-2.78380	O	-2.55720	-2.76410	-0.50300
H	3.72797	-4.66087	0.88523	N	-1.09495	-2.68232	1.24193
H	2.95550	-5.72031	-0.22688	C	-0.29743	-2.05829	2.21009
H	0.66073	1.84211	1.05853	O	0.48005	-2.70363	2.90909
H	-2.53653	3.67448	-3.21476	C	-0.48917	-0.61806	2.27824
H	-1.01013	2.88934	-2.73558	C	0.32507	0.15278	3.27773
H	-3.17689	1.49706	-2.86244	C	-1.34865	-0.01880	1.41862
H	-3.96378	3.28293	-0.62169	P	-6.73507	2.12880	-1.24997
H	-3.51200	1.71275	0.98468	O	-7.62219	2.74295	-2.31141
H	-3.33664	-0.51228	-1.08436	O	-6.70063	2.78615	0.11124
H	-1.27301	1.13197	1.69190	O	-7.12290	0.54564	-1.01707
H	-0.70672	-5.21676	0.90014	C	-7.02621	-0.31834	-2.15841
H	-3.21187	-4.74465	-1.47069	C	-7.30675	-1.74656	-1.74436
H	-2.33997	-5.89502	-0.57933	O	-6.25286	-2.21406	-0.87801
H	-4.84919	0.73401	0.30440	C	-8.63520	-1.94390	-0.98402
H	-7.82444	0.20333	-2.80104	O	-9.21330	-3.15846	-1.46750
H	-6.07858	-0.05385	-2.53166	C	-8.17257	-2.07017	0.46498
H	-7.42163	-2.14222	-2.48768	C	-6.83760	-2.79053	0.28304
H	-9.32345	-0.82095	-0.91731	N	-5.92135	-2.64284	1.40870
H	-7.88392	-0.70178	1.02144	C	-5.17946	-3.74585	1.85090
H	-6.96593	-3.54509	0.37062	O	-5.29965	-4.87300	1.40462
H	-4.76349	0.13065	3.40890	N	-4.27881	-3.42764	2.85868
H	-3.47573	-3.88741	3.13551	C	-4.06257	-2.16964	3.41339
H	-8.77060	-2.22296	1.36261	O	-3.22128	-1.96610	4.27574
H	-10.00717	-3.03036	-0.57415	C	-4.92951	-1.14361	2.81740
H	10.82383	-0.01839	0.46925	N	-5.78237	-1.38426	1.88172
Na	5.67522	2.46027	4.13130	H	9.98140	2.00477	-0.49763
Na	-1.34730	4.84653	2.65743	H	10.09768	0.79678	-1.80382
Na	-8.07426	4.84649	-0.78122	H	7.93910	2.05567	-1.71445
XATX							
O	9.83257	0.01039	0.11733	H	7.88071	1.63003	1.04645
C	9.60445	1.03211	-0.84907	H	7.54159	-0.76982	0.78276
C	8.11120	1.16778	-1.09430	H	5.57965	-0.04203	-1.44418
O	7.62428	0.00166	-1.79311	H	7.60946	-4.65362	-0.05721
C	7.28003	1.27782	0.20338	H	4.59068	-4.10803	-2.97881
O	6.20011	2.20128	-0.05032	H	5.85601	-0.18490	0.99471
C	6.75000	-0.13904	0.37615	H	3.80612	4.77693	-1.22851
C	6.49917	-0.50808	-1.08258	H	4.78949	3.32324	-1.53613
N	6.35211	-1.93832	-1.33460	H	2.32798	3.28149	-2.21704
C	5.40392	-2.36742	-2.27660	H	1.74614	4.04845	0.44915
O	4.74163	-1.59029	-2.94531	H	2.33001	1.83708	1.29832
N	5.30337	-3.74635	-2.35141	H	1.00883	0.74779	-1.24859
C	5.98174	-4.66394	-1.54841	H	3.71359	0.08947	1.35706
O	5.75296	-5.86284	-1.59040	H	0.22937	-3.40641	-2.77151
C	6.98032	-4.02077	-0.67383	H	3.77737	-4.78518	0.85910
N	7.13785	-2.74718	-0.59257	H	3.02722	-5.86574	-0.24308
P	5.37007	2.79970	1.23176	H	0.56077	1.67237	1.01374
O	6.27208	3.65537	2.09914	H	-2.61131	3.35582	-3.31587
O	4.64394	1.69698	1.99019	H	-1.07960	2.60835	-2.79521
O	4.31283	3.76002	0.45122	H	-3.25061	1.19981	-2.87796
C	3.96810	3.73239	-0.94294	H	-3.97678	3.01935	-0.62876
C	2.68924	2.96232	-1.23069	H	-3.64888	1.42915	0.97127
O	2.94353	1.54422	-1.26319	H	-3.38057	-0.77023	-1.11135
C	1.55980	3.18322	-0.19228	H	-1.48920	1.05873	1.38380
O	0.34685	3.37629	-0.94203	H	-0.97716	-3.68409	1.13190
C	1.52760	1.85797	0.55525	H	-4.93303	0.44282	0.21393
C	1.86470	0.89477	-0.58105	H	-7.75529	-0.01561	-2.92088
				H	-6.01905	-0.25500	-2.58575
				H	-7.32258	-2.36231	-2.65269

H	-9.31655	-1.09783	-1.13425	C	8.13903	1.86454	0.57936	
H	-7.99498	-1.07810	0.88488	C	6.84577	2.62841	0.31044	
H	-6.98034	-3.86397	0.14633	N	5.83645	2.53052	1.35838	
H	-4.84299	-0.12174	3.17026	C	5.02043	3.64431	1.61444	
H	-3.71070	-4.19704	3.20068	O	5.09973	4.69632	0.00500	
H	-8.87266	-2.62917	1.09288	N	4.12143	3.44784	2.65456	
H	-10.01501	-3.31994	-0.94446	C	3.89748	2.25186	3.32278	
H	10.78743	-0.02538	0.27900	O	3.04139	2.12484	4.18296	
H	0.07476	1.21783	3.24562	C	4.82466	1.18739	2.89620	
H	0.14746	-0.22298	4.29300	N	5.71101	1.33331	1.97294	
H	1.39777	0.03913	3.07332	H	-10.02348	-1.94213	-0.44078	
Na	5.83861	2.24523	4.03571	H	-10.14766	-0.78144	-1.78873	
Na	-1.51614	4.78114	2.51746	H	-7.98611	-2.04120	-1.67298	
Na	-8.27481	4.49836	-0.70648	H	-7.92706	-1.49271	1.07836	
				H	-7.52295	0.87703	0.70200	
			XCA	H	-5.62448	-0.02099	-1.51867	
O	-9.85940	0.07286	0.10011	H	-7.37174	4.74662	-0.26745	
C	-9.64620	-0.98459	-0.83095	H	-4.57360	3.93206	-3.33192	
C	-8.15573	-1.13331	-1.08178	H	-5.85336	0.25645	0.92468	
O	-7.67662	0.01226	-1.82230	H	-3.85740	-4.85656	-0.95847	
C	-7.31847	-1.20098	0.21838	H	-4.82336	-3.41911	-1.38091	
O	-6.26188	-2.16688	0.01403	H	-2.35207	-3.41854	-2.00506	
C	-6.75314	0.20679	0.31698	H	-1.81208	-4.02821	0.71019	
C	-6.51558	0.50259	-1.16144	H	-2.40919	-1.79315	1.43322	
N	-6.29942	1.91069	-1.47284	H	-1.05045	-0.86781	-1.16380	
C	-5.37374	2.26323	-2.46681	H	-3.67783	-0.21462	1.25788	
O	-4.74255	1.45460	-3.12461	H	-4.38226	2.11055	1.83492	
N	-5.24044	3.63633	-2.62532	H	-2.98342	4.99052	0.01614	
C	-5.90705	4.63060	-1.90998	H	-3.98478	4.49019	1.33481	
O	-5.73720	5.82082	-2.12097	H	-0.63962	-1.61737	1.16197	
C	-6.80640	4.06531	-0.89443	H	2.55843	-3.65185	-3.05737	
N	-6.99244	2.80181	-0.72276	H	1.02597	-2.85981	-2.60915	
P	-5.48166	-2.73710	1.34104	H	3.15870	-1.43721	-2.86196	
O	-6.42460	-3.55637	2.20084	H	4.00826	-3.06780	-0.52298	
O	-4.77242	-1.61740	2.09120	H	3.62343	-1.38917	0.98661	
O	-4.40148	-3.73251	0.64022	H	3.31095	0.68318	-1.21666	
C	-4.01974	-3.79543	-0.74261	H	1.31089	-0.85025	1.64593	
C	-2.73264	-3.04376	-1.04502	H	2.22731	4.96792	-0.94313	
O	-2.99211	-1.63570	-1.15566	H	-1.07095	3.33073	2.78773	
C	-1.61750	-3.20117	0.02208	H	-0.92536	4.93698	2.20282	
O	-0.39252	-3.43777	-0.69414	H	4.90401	-0.43976	0.17154	
C	-1.60025	-1.83325	0.69899	H	7.90121	-0.14732	-2.85614	
C	-1.91429	-0.94382	-0.50275	H	6.15341	0.12304	-2.61134	
N	-2.34882	0.41681	-0.23313	H	7.50743	2.20743	-2.59002	
C	-1.81064	1.49175	-1.00881	H	9.37236	0.89441	-0.95485	
O	-0.98590	1.24742	-1.89237	H	7.90786	0.87171	0.96937	
N	-2.23022	2.75713	-0.71885	H	7.03972	3.69366	0.17249	
C	-3.08213	2.96955	0.27758	H	4.74445	0.21491	3.36971	
N	-3.47482	4.24911	0.49723	H	3.50618	4.23002	2.85864	
C	-3.64987	1.91882	1.06058	H	8.81004	2.39399	1.26223	
C	-3.25900	0.65339	0.75500	H	10.09443	3.09848	-0.68861	
P	0.95519	-3.92701	0.10507	H	-10.81152	0.11468	0.27587	
O	0.75660	-5.30241	0.71042	Na	-5.99978	-2.15313	4.12867	
O	1.46175	-2.87086	1.07423	Na	1.46819	-4.47522	2.89396	
O	1.92578	-4.09654	-1.19519	Na	8.06610	-4.75381	-0.76317	
C	2.02535	-3.13253	-2.25590					
C	2.80971	-1.87319	-1.91295					
O	1.98507	-0.92114	-1.24236	XCCX				
C	4.04638	-2.09611	-1.01443	O	-9.87828	0.35066	0.12502	
O	5.19584	-2.06275	-1.87430	C	-9.69104	-0.63156	-0.89000	
C	3.95847	-0.96765	0.03645	C	-8.20415	-0.81277	-1.14360	
C	2.87164	-0.05415	-0.53219	O	-7.67220	0.37181	-1.77338	
N	2.08976	0.70717	0.41374	C	-7.37989	-1.02643	0.14553	
C	1.28409	0.20882	1.42063	O	-6.33687	-1.97952	-0.15984	
N	0.51965	1.11972	1.98299	C	-6.79055	0.36016	0.39417	
C	0.82510	2.28486	1.28953	C	-6.51129	0.77043	-1.04510	
C	0.40371	3.62554	1.42069	N	-6.24619	2.18125	-1.27210	
N	-0.48841	4.03747	2.35743	C	-5.32012	2.53386	-2.26689	
N	0.93252	4.55625	0.60396	O	-4.72204	1.72303	-2.95331	
C	1.84062	4.17419	-0.30697	N	-5.13525	3.90186	-2.39332	
N	2.33382	2.95115	-0.53390	C	-5.76588	4.89552	-1.65282	
C	1.79930	2.05215	0.31242	O	-5.55450	6.08535	-1.82597	
P	6.69984	-2.26780	-1.24323	C	-6.69075	4.33246	-0.65316	
O	7.54882	-2.90569	-2.32167	N	-6.90857	3.07065	-0.49620	
O	6.64678	-2.94184	0.10932	P	-5.51662	-2.66074	1.08755	
O	7.16101	-0.70814	-0.99279	O	-6.42977	-3.55312	1.90539	
C	7.13829	0.16472	-2.13200	O	-4.78073	-1.60838	1.90563	
C	7.41897	1.58535	-1.69014	O	-4.47187	-3.59865	0.26405	
O	6.32059	2.06431	-0.88896	C	-4.07670	-3.49949	-1.11413	
C	8.69608	1.74993	-0.83986	C	-2.75941	-2.76127	-1.31333	
O	9.32564	2.96043	-1.26492	O	-2.98416	-1.34145	-1.28985	
			C	-1.69138	-3.05813	-0.22931		

								XCGX
O	-0.42799	-3.26330	-0.89684	H	7.55172	2.68908	-2.35923	
C	-1.68019	-1.76718	0.58782	H	9.25689	0.65202	-1.19802	
C	-1.91652	-0.75254	-0.52895	H	7.93777	0.56995	0.78910	
N	-2.29754	0.59751	-0.15539	H	7.25583	3.50116	0.24225	
C	-1.74223	1.70925	-0.87710	H	3.83034	4.14894	3.06460	
O	-0.92597	1.50310	-1.77603	H	8.97229	1.98842	1.20612	
N	-2.15979	2.96059	-0.52092	H	10.40493	2.58262	-0.73699	
C	-3.01629	3.13243	0.48239	H	-10.83046	0.41175	0.29469	
N	-3.42653	4.39626	0.74206	H	4.71866	0.02175	3.26865	
C	-3.55459	2.04715	1.24373	H	-7.23113	5.01858	-0.00972	
C	-3.19697	0.79581	0.85384	Na	-5.92107	-2.32320	3.93804	
P	0.81368	-3.90259	-0.03132	Na	0.94217	-4.80086	2.72449	
O	0.51071	-5.33223	0.37198	Na	7.74749	-3.74476	0.38084	
O	1.21189	-2.99923	1.12677					
O	1.95889	-3.93685	-1.18946					
C	2.08090	-3.03314	-2.29912	O	-9.88355	0.16878	0.12592	
C	2.86442	-1.76449	-2.00201	C	-9.70324	-0.86363	-0.83955	
O	2.03780	-0.80576	-1.33174	C	-8.21846	-1.04622	-1.10284	
C	4.13493	-1.94464	-1.12500	O	-7.70888	0.10744	-1.80847	
O	5.22663	-1.35914	-1.86143	C	-7.37729	-1.17954	0.18852	
C	3.81685	-1.13473	0.13285	O	-6.34173	-2.15705	-0.06071	
C	2.90195	-0.06341	-0.45814	C	-6.78324	0.21255	0.33767	
N	2.07612	0.69809	0.46391	C	-6.54064	0.55617	-1.12898	
C	1.97644	2.11925	0.28976	N	-6.30534	1.97025	-1.39414	
O	2.65720	2.66834	-0.58090	C	-5.37425	2.33851	-2.37668	
N	1.15739	2.81618	1.12542	O	-4.75493	1.54006	-3.05826	
C	0.42454	2.17438	2.02410	N	-5.21723	3.71257	-2.49469	
N	-0.39024	2.91571	2.81753	C	-5.87042	4.69483	-1.75302	
C	0.45916	0.75033	2.19096	O	-5.67875	5.88810	-1.92496	
C	1.30087	0.05326	1.38297	C	-6.79016	4.11412	-0.76379	
P	6.76683	-1.72774	-1.42919	N	-6.99378	2.84909	-0.62574	
O	7.13986	-3.12172	-1.89882	P	-5.55543	-2.78699	1.23528	
O	7.00394	-1.46851	0.04632	O	-6.49959	-3.62389	2.07630	
O	7.55465	-0.66560	-2.38548	O	-4.82265	-1.70469	2.01654	
C	7.10871	0.64707	-2.75709	O	-4.50354	-3.77482	0.48332	
C	7.44470	1.76509	-1.77264	C	-4.10514	-3.75945	-0.89662	
O	6.37597	1.95225	-0.82839	C	-2.80349	-3.01190	-1.14477	
C	8.74561	1.58580	-0.94503	O	-3.04205	-1.59680	-1.19767	
O	9.57861	2.71324	-1.22891	C	-1.70817	-3.23446	-0.06863	
C	8.23730	1.58113	0.50522	O	-0.47923	-3.49264	-0.76970	
C	6.99150	2.44709	0.36218	C	-1.65743	-1.88913	0.64997	
N	6.02629	2.39001	1.45031	C	-1.95206	-0.95066	-0.51886	
C	5.31224	3.54773	1.79133	N	-2.35786	0.40527	-0.19386	
O	5.49331	4.63637	1.27529	C	-1.82412	1.50473	-0.93321	
N	4.37587	3.33632	2.79353	O	-1.00426	1.29372	-1.82979	
C	4.08177	2.12600	3.41544	N	-2.24831	2.75933	-0.60027	
O	3.22906	2.02216	4.28405	C	-3.09466	2.94192	0.40747	
C	4.88648	1.02062	2.88061	N	-3.49196	4.21502	0.66568	
N	5.77865	1.16275	1.96216	C	-3.66933	1.86382	1.14499	
H	-10.10582	-1.60454	-0.58539	C	-3.27869	0.61061	0.79397	
H	-10.17461	-0.33100	-1.83132	P	0.82533	-4.05091	0.05753	
H	-8.06562	-1.67114	-1.81215	O	0.55454	-5.43292	0.61829	
H	-7.99385	-1.39878	0.97003	O	1.33238	-3.04036	1.07375	
H	-7.55586	1.00931	0.82257	O	1.83427	-4.21550	-1.21311	
H	-5.63333	0.23990	-1.42211	C	1.96817	-3.24537	-2.26488	
H	-4.45751	4.18937	-3.09294	C	2.77064	-2.00439	-1.90023	
H	-5.90015	0.33103	1.01968	O	1.96183	-1.04302	-1.22102	
H	-3.95147	-4.53097	-1.45930	C	4.00372	-2.26496	-1.00334	
H	-4.86036	-3.01653	-1.70353	O	5.15656	-2.16002	-1.85333	
H	-2.36014	-3.04929	-2.29524	C	3.89009	-1.20014	0.10741	
H	-1.94151	-3.94313	0.36137	C	2.86149	-0.22653	-0.46552	
H	-2.52508	-1.78794	1.28051	N	2.08320	0.54166	0.47820	
H	-1.02130	-0.65586	-1.14618	C	1.26129	0.05710	1.48598	
H	-3.62751	-0.09246	1.30736	N	0.51803	0.98716	2.04100	
H	-4.27801	2.20453	2.03426	C	0.84844	2.14637	1.34778	
H	-2.97289	5.16249	0.26327	C	0.42117	3.50375	1.53553	
H	-3.96233	4.60521	1.57187	O	-0.36491	3.99595	2.34118	
H	-0.74223	-1.62456	1.11853	N	1.07224	4.36037	0.60910	
H	2.62327	-3.59392	-3.06675	C	2.01288	3.99625	-0.32013	
H	1.09103	-2.76967	-2.68255	N	2.50487	4.97776	-1.13156	
H	3.18112	-1.35019	-2.96999	N	2.41322	2.75044	-0.48383	
H	4.34343	-2.99829	-0.91959	C	1.81973	1.88926	0.38051	
H	3.25798	-1.76320	0.83147	P	6.66609	2.35605	-1.23358	
H	3.48311	0.66677	-1.02414	O	7.51721	-2.97569	-2.32118	
H	1.36895	-1.03167	1.39305	O	6.62781	-3.04163	0.11349	
H	-0.16775	0.24710	2.91683	O	7.10959	-0.79261	-0.97614	
H	-0.55788	3.87416	2.53907	C	7.07130	0.08608	-2.11057	
H	-1.14167	2.45582	3.31304	C	7.35639	1.50495	-1.66500	
H	4.72196	-0.73979	0.59302	O	6.26929	1.97969	-0.84563	
H	7.62917	0.86012	-3.69564	C	8.64332	1.66322	-0.83046	
H	6.03036	0.64248	-2.94211	O	9.25276	2.89148	-1.23304	

C	8.10455	1.73565	0.59873	O	0.38694	3.33314	-0.87435
C	6.80617	2.50218	0.36729	C	1.52619	1.70686	0.54737
N	5.80966	2.37073	1.42442	C	1.87283	0.78180	-0.61939
C	4.98529	3.47010	1.70622	N	2.27717	-0.57350	-0.27463
O	5.02508	4.52424	1.09482	C	1.76813	-1.68687	-1.02333
N	4.12722	3.25857	2.77686	O	0.94252	-1.48587	-1.91699
C	3.89959	2.04400	3.41166	N	2.21412	-2.93328	-0.69093
O	3.04715	1.88851	4.27068	C	3.08446	-3.09772	0.30073
C	4.82740	0.99687	2.95647	N	3.54315	-4.35207	0.52753
N	5.70226	1.16393	2.02458	C	3.60028	-2.01079	1.07331
H	4.75976	0.01508	3.41236	C	3.18799	-0.76509	0.72489
H	-10.10600	-1.82229	-0.47871	P	-0.94671	3.88672	-0.09478
H	-10.20231	-0.61572	-1.78803	O	-0.73220	5.29436	0.42339
H	-8.07859	-1.93906	-1.72396	O	-1.45240	2.89744	0.94417
H	-7.98664	-1.49235	1.04063	O	-1.92925	3.98269	-1.39179
H	-7.53884	0.88349	0.74862	C	-2.06248	2.94477	-2.37603
H	-5.65775	0.03201	-1.50459	C	-2.85896	1.72400	-1.93216
H	-4.54065	4.01737	-3.18797	O	-2.03222	0.78121	-1.25519
H	-5.88099	0.22168	0.94369	C	-4.05063	2.01537	-0.99313
H	-3.95541	-4.80865	-1.17148	O	-5.22570	2.01388	-1.81682
H	-4.89683	-3.33584	-1.52003	C	-3.95980	0.91096	0.08945
H	-2.41234	-3.34904	-2.11454	C	-2.92257	-0.04676	-0.49602
H	-1.94081	-4.07342	0.59271	N	-2.10196	-0.82181	0.42242
H	-2.46316	-1.85557	1.38762	C	-1.94335	-2.18553	0.15493
H	-1.08465	-0.86683	-1.17566	O	-2.54951	-2.78707	-0.72416
H	-3.70623	-0.27302	1.25998	N	-1.07456	-2.83447	1.00785
H	-4.40485	2.02626	1.92312	C	-0.28325	-2.27866	2.01543
H	-2.94699	4.96211	0.25506	O	0.46953	-2.98940	2.67719
H	-3.94941	4.42016	1.54314	C	-0.43297	-0.83330	2.15962
H	-0.69105	-1.70987	1.11626	C	0.41603	-0.13566	3.18265
H	2.50600	-3.76780	-3.06137	C	-1.31741	-0.18122	1.36721
H	0.98023	-2.95266	-2.63324	P	-6.72562	2.12613	-1.15901
H	3.13053	-1.56339	-2.84244	O	-7.61275	2.78005	-2.19661
H	3.98067	-3.26532	-0.57124	O	-6.68810	2.73420	0.22461
H	3.48413	-1.67012	1.00596	O	-7.11677	0.53627	-0.98545
H	3.34920	0.50669	-1.12024	C	-7.02735	-0.28210	-2.16105
H	1.26086	-1.00170	1.70992	C	-7.31621	-1.72485	-1.80635
H	0.80330	5.33569	0.68528	O	-6.26134	-2.23792	-0.96786
H	3.37429	4.73075	-1.58885	C	-8.63880	-1.94205	-1.04357
H	2.48526	5.92778	-0.78146	O	-9.22321	-3.14116	-1.55649
H	4.84093	-0.71354	0.32978	C	-8.16419	-2.11121	0.39903
H	7.82485	-0.22154	-2.84637	C	-6.84616	-2.84889	0.17731
H	6.08026	0.04570	-2.57708	N	-5.90836	-2.77367	1.29057
H	7.43134	2.13229	-2.56229	C	-5.15066	-3.90307	1.62811
H	9.32741	0.81868	-0.97649	O	-5.27035	-4.99060	1.09258
H	7.88335	0.73124	0.96339	N	-4.23961	-3.66307	2.64788
H	6.99634	3.57189	0.26220	C	-4.02021	-2.45184	3.29671
H	3.51509	4.03526	3.00930	O	-3.17512	-2.31593	4.16855
H	8.78175	2.24964	1.28726	C	-4.88457	-1.38037	2.78183
H	10.02523	3.02656	-0.66090	N	-5.74922	-1.54911	1.84135
H	-10.83345	0.23100	0.30746	H	10.02402	1.79828	-0.42922
H	-7.35149	4.78643	-0.12363	H	10.16023	0.60954	-1.75128
Na	-6.06635	-2.25235	4.03380	H	8.01524	1.89818	-1.70842
Na	1.08571	-4.63113	2.87997	H	7.88703	1.41974	1.05099
Na	8.05464	-4.83528	-0.78109	H	7.47141	-0.95827	0.72525
XCTX							
O	9.82177	-0.20335	0.14732	H	5.62258	-0.09736	-1.55032
C	9.64191	0.83821	-0.80831	H	7.33634	-4.84660	-0.18374
C	8.15904	1.00146	-1.09375	H	4.56994	-4.08498	-3.28941
O	7.67904	-0.15328	-1.81815	H	5.80200	-0.31819	0.89798
C	7.29532	1.10984	0.18537	H	3.82838	4.67593	-1.21311
O	6.25242	2.07747	-0.06807	H	4.80786	3.22547	-1.54747
C	6.71539	-0.29117	0.30892	H	2.33483	3.18319	-2.17559
C	6.50262	-0.61981	-1.16554	H	1.81385	3.88955	0.53756
N	6.28419	-2.03131	-1.45440	H	2.29964	1.66260	1.31744
C	5.35029	-2.40128	-2.43551	H	1.03327	0.69105	-1.31033
O	4.70413	-1.60529	-3.09417	H	3.59421	0.12451	1.19924
N	5.23391	-3.77737	-2.58520	H	4.33217	-2.16109	1.85722
C	5.90731	-4.76047	-1.85955	H	3.08664	-5.12226	0.05725
O	5.75658	-5.95355	-2.06800	H	4.06209	-4.55947	1.36880
C	6.78202	-4.17677	-0.83257	H	0.54516	1.52326	0.97331
N	6.96091	-2.91018	-0.67590	H	-2.60065	3.41444	-3.20402
P	5.42007	2.67023	1.21715	H	-1.07370	2.63027	-2.72479
O	6.32735	3.50537	2.09927	H	-3.26244	1.25189	-2.84158
O	4.67840	1.56576	1.95806	H	-3.95659	2.99571	-0.52687
O	4.38101	3.66004	0.44976	H	-3.59230	1.35580	1.01666
C	3.99886	3.63103	-0.93436	H	-3.41233	-0.77023	-1.15278
C	2.71723	2.85651	-1.19887	H	-1.45216	0.89672	1.40001
O	2.98197	1.44498	-1.24606	H	-0.96322	-3.82785	0.83560
C	1.59682	3.06194	-0.14289	H	-4.91187	0.40882	0.26774
				H	-7.75533	0.05670	-2.90918
				H	-6.02044	-0.20841	-2.58716

H	-7.34387	-2.30090	-2.74004		C	-7.32208	-1.60390	-1.57902
H	-9.31973	-1.09074	-1.16322		O	-6.24181	-2.04567	-0.73286
H	-7.96622	-1.13321	0.84203		C	-8.62356	-1.78574	-0.77161
H	-7.01640	-3.91155	-0.00454		O	-9.20304	-3.02358	-1.18925
H	-4.78321	-0.38543	3.20138		C	-8.11529	-1.85148	0.66833
H	-3.66610	-4.45527	2.92235		C	-6.79082	-2.58251	0.46831
H	-8.86659	-2.67591	1.01918		N	-5.82522	-2.41152	1.54842
H	-10.02036	-3.31699	-1.03105		C	-4.98658	-3.48335	1.88607
H	10.76933	-0.25345	0.34423		O	-5.02024	-4.57175	1.33903
H	0.19427	0.93581	3.20646		N	-4.12139	-3.19557	2.93162
H	0.24349	-0.55651	4.18107		C	-3.94164	-1.95528	3.53350
H	1.48159	-0.26821	2.95483		O	-3.11036	-1.76227	4.40482
Na	5.86349	2.10835	4.02463		C	-4.86887	-0.93995	3.01021
Na	-1.43197	4.60074	2.66270		N	-5.72993	-1.17058	2.07940
Na	-8.24853	4.49065	-0.54542		H	10.02046	2.08939	-0.30708
					H	10.15701	0.86894	-1.59964
					H	8.01528	2.15663	-1.58323
				XGAX				
O	9.82725	0.10236	0.31938		H	7.86983	1.76160	1.17743
C	9.64031	1.11891	-0.66116		H	7.50994	-0.63504	0.93266
C	8.15652	1.27254	-0.95001		H	5.61907	0.07751	-1.35939
O	7.67317	0.10693	-1.65188		H	7.53268	-4.53368	0.18289
C	7.28934	1.40656	0.32145		H	4.66368	-3.99560	-2.88367
O	6.22904	2.34083	0.02450		H	5.82502	-0.03017	1.08586
C	6.73790	-0.00119	0.49479		H	3.86782	4.90948	-1.23519
C	6.52618	-0.38706	-0.96555		H	4.82877	3.43309	-1.50687
N	6.37860	-1.82076	-1.20079		H	2.35986	3.43622	-2.21012
C	5.46532	-2.25344	-2.16969		H	1.78829	4.21182	0.44950
O	4.85326	-1.48380	-2.89332		H	2.40063	2.01393	1.30867
N	5.33661	-3.63312	-2.21485		H	1.02490	0.90699	-1.20118
C	5.98661	-4.55340	-1.38845		H	3.67833	0.23581	1.45175
O	5.78400	-5.75453	-1.46039		H	1.30167	-4.89914	-1.62547
C	6.93953	-3.90606	-0.47357		H	-0.68608	-2.49987	-3.19897
N	7.11168	-2.63217	-0.40619		H	-0.44813	-4.16138	-2.93855
P	5.38040	2.96748	1.28094		H	0.62399	1.83780	1.06787
O	6.26958	3.84529	2.14004		H	-2.62610	3.57725	-3.23882
O	4.64933	1.87896	2.05397		H	-1.08987	2.81087	-2.75999
O	4.33167	3.90879	0.46680		H	-3.24953	1.40299	-2.83589
C	4.00672	3.86654	-0.93202		H	-4.00998	3.22108	-0.60575
C	2.71850	3.11148	-1.22459		H	-3.58869	1.66131	1.01180
O	2.96119	1.69195	-1.25909		H	-3.36299	-0.58393	-1.02656
C	1.59700	3.34014	-0.18161		H	-1.30033	1.14251	1.69731
O	0.37276	3.52442	-0.91403		H	-2.18886	-4.80246	-0.56046
C	1.58068	2.02196	0.58473		H	1.18840	-2.85780	2.92370
C	1.89363	1.04970	-0.54961		H	1.12388	-4.47646	2.40329
N	2.32383	-0.26196	-0.13998		H	-4.90156	0.66154	0.31709
C	3.21461	-0.56009	0.87972		H	-7.80922	0.09361	-2.79076
N	3.43181	-1.84537	1.01610		H	-6.06384	-0.12763	-2.48997
C	2.65075	-2.44210	0.02692		H	-7.36373	-2.24213	-2.47095
C	2.41747	-3.82105	-0.27363		H	-9.31904	-0.95302	-0.93125
O	2.87246	-4.83461	0.25694		H	-7.92667	-0.84329	1.04144
N	1.53372	-3.94381	-1.37528		H	-6.94388	-3.65828	0.36541
C	0.84664	-2.90508	-1.97228		H	-4.81747	0.06596	3.41237
N	-0.03487	-3.23745	-2.95952		H	-3.49373	-3.94703	3.20241
N	1.04100	-1.63746	-1.66892		H	-8.79533	-2.38426	1.33953
C	1.96596	-1.46375	-0.69697		H	-9.98716	-3.17130	-0.63637
P	-0.96029	4.09445	-0.14141		H	10.77671	0.05429	0.50740
O	-0.73429	5.50836	0.35492		Na	5.83235	2.46970	4.09848
O	-1.46928	3.12155	0.90980		Na	-1.42523	4.84317	2.60890
O	-1.94296	4.17701	-1.43993		Na	-8.17743	4.73449	-0.73065
C	-2.07775	3.12459	-2.40787					
C	-2.86299	1.90790	-1.93718					
O	-2.02503	0.99807	-1.22368		XGCX			
C	-4.07018	2.21494	-1.01975		O	9.81689	0.04859	0.34101
O	-5.24122	2.13006	-1.84691		C	9.62501	1.04426	-0.65982
C	-3.95859	1.16960	0.10989		C	8.14063	1.18347	-0.95310
C	-2.89851	0.20353	-0.41929		O	7.66500	0.00181	-1.63343
N	-2.09743	-0.48425	0.56658		C	7.27168	1.33624	0.31506
C	-1.27995	0.07189	1.53762		O	6.20630	2.25849	0.00133
N	-0.51480	-0.80680	2.15192		C	6.72723	-0.07141	0.51333
C	-0.85094	-2.01193	1.54911		C	6.51818	-0.48286	-0.94024
C	-0.37761	-3.31411	1.73650		N	6.37151	-1.91841	-1.15101
N	0.60679	-3.63190	2.62414		C	5.45541	-2.37816	-2.10352
N	-0.90497	-4.28839	0.96324		O	4.82050	-1.63784	-2.83671
C	-1.81722	-3.97065	0.03431		N	5.34685	-3.76036	2.13362
N	-2.31448	-2.76572	-0.26618		C	6.00380	-4.66318	-1.29747
C	-1.80860	-1.82879	0.54660		O	5.80377	-5.86615	-1.34225
P	-6.74103	2.28448	-1.19393		C	6.96895	-3.99397	-0.41242
O	-7.62978	2.87652	-2.26653		N	7.12835	-2.71675	-0.36229
O	-6.69371	2.97659	0.14957		P	5.34430	2.89620	1.24350
O	-7.13625	0.71026	-0.91880		O	6.22092	3.79557	2.09317
C	-7.06069	-0.18467	-2.03802		O	4.61767	1.81414	2.02942
					O	4.29244	3.81477	0.40745

C	3.97366	3.73737	-0.99130	H	-3.38638	-0.73792	-0.98530
C	2.69384	2.96529	-1.27382	H	-1.48435	1.16435	1.44359
O	2.94577	1.54642	-1.27441	H	0.11597	0.03512	3.03928
C	1.55974	3.21024	-0.24675	H	0.76256	-3.55482	2.74967
O	0.34481	3.37227	-1.00202	H	1.25733	-2.07868	3.45939
C	1.53610	1.90773	0.54034	H	-4.92128	0.52083	0.32217
C	1.86926	0.91331	-0.57144	H	-7.75143	-0.03930	-2.78998
N	2.29781	-0.38789	-0.12146	H	-6.01360	-0.26317	-2.45203
C	3.19870	-0.65584	0.89916	H	-7.31155	-2.37723	-2.47681
N	3.42617	-1.93739	1.06786	H	-9.30510	-1.09443	-0.97823
C	2.63982	-2.55747	0.10303	H	-7.96723	-1.01370	1.03268
C	2.43086	-3.94530	-0.18739	H	-6.96130	-3.81790	0.35420
O	2.89336	-4.94820	0.35426	H	-4.80105	-0.03583	3.30919
N	1.54283	-4.09498	-1.28875	H	-3.62578	-4.09822	3.33964
C	0.86173	-3.08358	-1.92144	H	-8.84315	-2.55911	1.28737
N	0.00756	-3.43729	-2.92654	H	-9.98578	-3.31608	-0.72530
N	1.04708	-1.81262	-1.63661	H	10.76659	0.00895	0.52983
C	1.93369	-1.61180	-0.63979	Na	5.79669	2.44152	4.06935
P	-0.98668	4.00850	-0.28380	Na	-1.46228	4.97875	2.39868
O	-0.74821	5.45085	0.11557	Na	-8.31608	4.50012	-0.63309
O	-1.51280	3.11812	0.83053				
O	-1.96197	4.01292	-1.58965				
C	-2.10666	2.90439	-2.49261	XGGX			
C	-2.88811	1.71448	-1.94854	O	9.87254	0.07228	0.35013
O	-2.04380	0.83515	-1.21340	C	9.70736	1.06769	-0.65560
C	-4.07154	2.06482	-1.01917	C	8.22787	1.23582	-0.95775
O	-5.25561	2.02066	-1.83092	O	7.73273	0.05922	-1.63323
C	-3.97513	1.02659	0.12455	C	7.35606	1.41504	0.30552
C	-2.91764	0.04747	-0.38839	O	6.31738	2.36562	-0.01549
N	-2.08097	-0.63365	0.58439	C	6.77646	0.02210	0.50580
C	-1.90258	-2.04790	0.45933	C	6.56917	-0.39363	-0.94681
O	-2.54083	-2.67181	-0.39387	N	6.38952	-1.82726	-1.14719
N	-1.03599	-2.65561	1.31467	C	5.47696	-2.27346	-2.11135
C	-0.33817	-1.94873	2.19421	O	4.86517	-1.51891	-2.85013
N	0.51891	-2.60844	3.01587	N	5.34439	-3.65297	-2.13600
C	-0.47378	-0.53135	2.32915	C	5.99878	-4.56482	-1.30597
C	-1.34369	0.08708	1.48419	O	5.80038	-5.76724	-1.36834
P	-6.74940	2.14586	-1.16257	C	6.95122	-3.90622	-0.39789
O	-7.65669	2.73347	-2.22238	N	7.12398	-2.63179	-0.34581
O	-6.70734	2.82536	0.18770	P	5.45228	3.01345	1.21943
O	-7.11947	0.56303	-0.89871	O	6.32821	3.89700	2.08532
C	-7.02004	-0.32312	-2.02235	O	4.69786	1.93966	1.99028
C	-7.29367	-1.74471	-1.58002	O	4.43057	3.95824	0.37447
O	-6.23574	-2.19273	-0.70946	C	4.08082	3.85624	-1.01506
C	-8.61690	-1.93144	-0.80953	C	2.78240	3.10177	-1.26274
O	-9.18885	-3.16228	-1.25784	O	3.01650	1.68113	-1.26353
C	-8.14655	-2.01688	0.64104	C	1.67421	3.36512	-0.21240
C	-6.81385	-2.74253	0.46913	O	0.44812	3.56303	-0.93857
N	-5.88705	-2.57748	1.58255	C	1.63869	2.05890	0.57382
C	-5.12090	-3.66873	2.01315	C	1.94193	1.06354	-0.54295
O	-5.23030	-4.79733	1.56708	N	2.35968	-0.24566	-0.10938
N	-4.21460	-3.33883	3.01104	C	3.24811	-0.53432	0.91441
C	-4.00499	-2.07701	3.55891	N	3.44802	-1.81976	1.07775
O	-3.16524	-1.86362	4.41991	C	2.64933	-2.42278	0.11164
C	-4.88525	-1.06071	2.96449	C	2.42504	-3.80508	-0.19097
N	-5.75010	-1.31353	2.04323	O	2.87507	-4.82014	0.33632
H	9.99900	2.02387	-0.32477	N	1.52337	-3.92631	-1.28373
H	10.14418	0.77874	-1.59262	C	0.83823	-2.89359	-1.88969
H	7.99465	2.05457	-1.60306	N	-0.09728	-3.25024	-2.82503
H	7.84951	1.70975	1.16497	N	1.07300	-1.62546	-1.62941
H	7.50194	-0.69466	0.96183	C	1.98578	-1.45382	-0.64523
H	5.61023	-0.02642	-1.34275	P	-0.86796	4.16740	-0.16400
H	7.58108	-4.60576	0.24167	O	-0.61525	5.58664	0.30421
H	4.66643	-4.13481	-2.78811	O	-1.38084	3.22275	0.91058
H	5.81380	-0.09465	1.10397	O	-1.86329	4.24226	-1.45378
H	3.82644	4.77182	-1.31869	C	-2.00394	3.19015	-2.42097
H	4.80227	3.29905	-1.55283	C	-2.80172	1.98178	-1.95134
H	2.34081	3.26431	-2.26940	O	-1.97683	1.06977	-1.22383
H	1.73957	4.09570	0.36826	C	-4.01679	2.30340	-1.04790
H	2.34595	1.91264	1.27593	O	-5.18483	2.17720	-1.87473
H	1.01174	0.75131	-1.23310	C	-3.90035	1.29092	0.10908
H	3.66113	0.15732	1.44762	C	-2.86362	0.29720	-0.41278
H	1.34917	-5.05854	-1.54119	N	-2.07601	-0.39679	0.58099
H	-0.65097	-2.70993	-3.17797	C	-1.25982	0.16382	1.55231
H	-0.40087	-4.36331	-2.89347	N	-0.50528	-0.71887	2.16482
H	0.57428	1.73285	1.01493	C	-0.82833	-1.92541	1.55830
H	-2.65975	3.31077	-3.34389	C	-0.37323	-3.24674	1.84818
H	-1.12139	2.56964	-2.83274	O	0.42822	-3.64867	2.68647
H	-3.29889	1.17289	-2.81555	N	-1.00659	-4.17356	0.96525
H	-3.96846	3.07078	-0.61332	C	-1.88818	-3.87571	-0.04368
H	-3.62746	1.52948	1.02935	N	-2.23088	-4.89396	-0.89578
				N	-2.33852	-2.66080	-0.27243

C	-1.79385	-1.74256	0.56760	C	6.92211	-4.03113	-0.47850
P	-6.68439	2.37346	-1.23048	N	7.09447	-2.75646	-0.44117
O	-7.56347	2.94816	-2.32049	P	5.39834	2.86989	1.16492
O	-6.62787	3.10255	0.09289	O	6.30236	3.75408	2.00125
O	-7.10387	0.81396	-0.91232	O	4.67217	1.79503	1.96134
C	-7.06675	-0.10605	-2.01332	O	4.34247	3.80503	0.35222
C	-7.34487	-1.51104	-1.51940	C	3.98843	3.72228	-1.03746
O	-6.25679	-1.95591	-0.68505	C	2.70283	2.94981	-1.28805
C	-8.63077	-1.65195	-0.68157	O	2.94929	1.53027	-1.27571
O	-9.22339	-2.90300	-1.03646	C	1.58290	3.21069	-0.24877
C	-8.09431	-1.66140	0.74999	O	0.36335	3.37664	-0.99520
C	-6.78515	-2.42010	0.55566	C	1.55442	1.91328	0.54608
N	-5.78768	-2.21019	1.60183	C	1.87403	0.91040	-0.56031
C	-4.93589	-3.27304	1.94062	N	2.29601	-0.39171	-0.10398
O	-4.94810	-4.35696	1.38267	C	3.22507	-0.66688	0.88704
N	-4.07995	-2.98638	2.99705	N	3.43675	-1.95000	1.05508
C	-3.89944	-1.74053	3.58489	C	2.60858	-2.56932	0.12424
O	-3.05804	-1.51890	4.44054	C	2.40313	-3.95446	-0.17255
C	-4.83847	-0.73670	3.05749	O	2.86929	-4.95952	0.36098
N	-5.70336	-0.96998	2.13167	N	1.49943	-4.09021	-1.26330
H	10.09941	2.04075	-0.32221	C	0.79029	-3.07441	-1.86570
H	10.22645	0.78782	-1.58430	N	-0.09503	-3.42720	-2.84407
H	8.10316	2.10539	-1.61423	N	0.97331	-1.80640	-1.57336
H	7.93888	1.77566	1.15755	C	1.89400	-1.61523	-0.60132
H	7.53329	-0.61589	0.96386	P	-0.97079	4.00177	-0.27439
H	5.67559	0.08137	-1.35970	O	-0.74140	5.44201	0.13593
H	4.67245	-4.02194	-2.80223	O	-1.49484	3.10096	0.83312
H	5.85874	0.02311	1.08986	O	-1.94314	4.00596	-1.58258
H	3.94748	4.88679	-1.35998	C	-2.06270	2.90814	-2.50202
H	4.89085	3.39120	-1.58271	C	-2.85275	1.71061	-1.98895
H	2.41058	3.40211	-2.25128	O	-0.20483	0.82356	-1.24022
H	1.88688	4.24203	0.40451	C	-4.05922	2.05167	-1.08637
H	2.45669	2.05221	1.29975	O	-5.22615	1.98175	-1.91857
H	1.07181	0.91783	-1.19220	C	-3.97459	1.02316	0.06673
H	3.72251	0.26815	1.46728	C	-2.91408	0.04148	-0.43177
H	1.30306	-4.88146	-1.54628	N	-0.209506	-0.64018	0.55932
H	-0.70233	-2.47893	-3.08361	C	-1.94566	-2.02249	0.44349
H	-0.62062	-4.09932	-2.62492	O	-2.51735	-2.71218	-0.39411
H	0.67802	1.89339	1.05641	N	-1.11333	-2.58002	1.39614
H	-2.54610	3.64607	-3.25438	C	-0.29390	-1.92438	2.32637
H	-1.01805	2.86722	-2.76988	O	0.48482	-2.54442	3.04620
H	-3.18217	1.47423	-2.85100	C	-0.48212	-0.48427	2.34493
H	-3.97135	3.32230	-0.66395	C	0.33610	0.31968	3.31489
H	-3.50293	1.80358	0.98735	C	-1.34506	0.08719	1.46953
H	-3.34578	-0.48356	-1.01459	P	-6.72908	2.14021	-1.27354
H	-1.27284	1.23479	1.70691	O	-7.61054	2.73063	-2.35289
H	-0.69435	-5.13297	1.07638	O	-6.68837	2.83619	0.06814
H	-3.07112	-4.70602	-1.43131	O	-7.12545	0.56672	-0.99651
H	-2.19047	-5.83964	-0.53300	C	-7.01927	-0.33486	-2.10769
H	-4.84757	0.80607	0.34948	C	-7.29587	-1.75020	-1.64823
H	-7.82371	0.17142	-2.75774	O	-6.24241	-2.18786	-0.76563
H	-6.07739	-0.07811	-2.48448	C	-8.62472	-1.92658	-0.88402
H	-7.41512	-2.16661	-2.39667	O	-9.19702	-3.15961	-1.32589
H	-9.32525	-0.82253	-0.86155	C	-8.16390	-2.00102	0.56934
H	-7.88731	-0.64022	1.07356	C	-6.82872	-2.72636	0.41358
H	-6.95493	-3.49731	0.51060	N	-5.91280	-2.54254	1.53407
H	-3.45159	-3.73649	3.26974	C	-5.16698	-3.62966	2.00784
H	-8.76712	-2.15496	1.45741	O	-5.28161	-4.76929	1.59272
H	-9.99187	-3.02844	-0.45679	N	-4.26933	-3.27968	3.00773
H	10.81947	0.01777	0.54887	C	-4.06005	-2.00604	3.52888
H	7.54581	-4.52601	0.26473	O	-3.22369	-1.77590	4.38921
H	-4.79059	0.27022	3.45789	C	-4.92735	-1.00013	2.90059
Na	5.72749	2.59658	4.07397	N	-5.77717	-1.27018	1.97025
Na	-1.28799	4.97255	2.57818	H	10.00750	1.96993	-0.51779
Na	-8.07978	4.85984	-0.84511	H	10.11904	0.71176	-1.77627
				H	7.97269	1.99560	-1.74987
				H	7.89830	1.67477	1.02555
XGTX				H	7.53149	-0.72816	0.85109
O	9.83258	0.00197	0.17153	H	5.59065	-0.06063	-1.41250
C	9.62219	0.98872	-0.83467	H	7.53542	-4.64536	0.17215
C	8.13186	1.13063	-1.09475	H	4.58201	-4.17176	-2.82311
O	7.63754	-0.05697	-1.75079	H	5.85107	-0.11708	1.03081
C	7.29613	1.29909	0.19371	H	3.83216	4.75552	-1.36445
O	6.22787	2.22582	-0.09632	H	4.80344	3.28336	-1.61812
C	6.74925	-0.10427	0.41691	H	2.33537	3.23823	-2.28160
C	6.50191	-0.52552	-1.02788	H	1.77497	4.09897	0.35853
N	6.33396	-1.96010	-1.22634	H	2.36534	1.91480	1.28007
C	5.38703	-2.41667	-2.15395	H	1.01026	0.74930	-1.21389
O	4.73121	-1.66946	-2.86143	H	3.71628	0.14376	1.41419
N	5.27651	-3.79724	-2.18352	H	1.30308	-5.05067	-1.52546
C	5.94598	-4.69945	-1.35677	H	-0.76691	-2.70205	-3.06531

H	-0.49982	-4.35442	-2.79876	N	0.17896	-4.07083	2.44938
H	0.59172	1.74813	1.02111	N	-1.23572	-4.54726	0.68266
H	-2.60008	3.32161	-3.35997	C	-2.12901	-4.14080	-0.20542
H	-1.06956	2.58126	-2.82588	N	-2.59475	-2.86984	-0.42222
H	-3.23896	1.17533	-2.87036	C	-2.01823	-2.01059	0.37779
H	-3.97921	3.06162	-0.68513	P	-6.72151	2.41866	-1.23256
H	-3.63175	1.53167	0.97025	O	-7.55761	3.07126	-2.31061
H	-3.38028	-0.74186	-1.03488	O	-6.65795	3.08317	0.12333
H	-1.48349	1.16339	1.40031	O	-7.19490	0.86149	-0.99349
H	-0.99412	-3.58465	1.31643	C	-7.19546	0.00418	-2.14529
H	-4.92377	0.52121	0.25919	C	-7.52913	-1.41234	-1.72880
H	-7.74598	-0.06124	-2.88335	O	-6.45728	-1.94128	-0.92112
H	-6.01034	-0.28120	-2.53206	C	-8.82449	-1.55185	-0.90083
H	-7.30846	-2.39429	-2.53676	O	-9.48237	-2.73470	-1.35916
H	-9.30925	-1.08910	-1.06445	C	-8.29532	-1.70893	0.52269
H	-7.98776	-0.99459	0.95427	C	-7.00963	-2.49323	0.26802
H	-6.97137	-3.80360	0.31124	N	-6.02155	-2.39235	1.34205
H	-4.84422	0.03188	3.22351	C	-5.26810	-3.52521	1.68558
H	-3.69955	-4.03719	3.37268	O	-5.34303	-4.59392	1.10519
H	-8.86425	-2.53843	1.21561	N	-4.41656	-3.32367	2.76866
H	-9.99861	-3.30620	-0.79838	C	-4.14770	-2.10224	3.37324
H	10.78580	-0.03733	0.34177	O	-3.29309	-1.95640	4.23356
H	0.07680	1.38145	3.25660	C	-5.01982	-1.02727	2.86610
H	0.17104	-0.03049	4.34127	N	-5.87521	-1.17947	1.91549
H	1.40750	0.20905	3.10254	H	10.44487	0.59866	-0.06866
Na	5.89201	2.37751	3.97523	H	10.27874	-0.67471	-1.30537
Na	-1.43197	4.93499	2.42411	H	8.77450	1.32043	-1.55146
Na	-8.16005	4.59658	-0.82653	H	8.10726	1.03537	1.14978
				H	6.95063	-1.01963	0.90410
				H	5.68533	-0.14292	-1.71680
				H	4.42028	-4.16759	-3.17743
				H	5.57677	0.11112	0.66907
				H	4.19815	4.34023	-0.81087
				H	4.88113	2.89259	-1.60125
				H	2.46400	3.24810	-2.07177
				H	2.03318	3.81061	0.63191
				H	2.52839	1.52125	1.30965
				H	0.89823	0.62846	-1.12071
				H	1.78969	-3.76988	-0.96866
				H	0.73932	1.48978	1.17797
				H	-2.46813	3.78186	-2.94892
				H	-0.98848	2.87189	-2.55332
				H	-3.18832	1.59332	-2.85787
				H	-4.01876	3.22048	-0.52636
				H	-3.59960	1.55570	0.99494
				H	-3.49404	-0.58136	-1.17550
				H	-1.33828	0.91121	1.57713
				H	-2.55568	-4.90707	-0.84475
				H	0.60704	-3.42642	3.10750
				H	0.40326	-5.06051	2.51217
				H	-4.97353	0.66529	0.26442
				H	-7.94151	0.35330	-2.86988
				H	-6.20624	0.01919	-2.61736
				H	-7.62282	-2.01675	-2.63986
				H	-9.47172	-0.67362	-1.01120
				H	-8.05161	-0.72860	0.93612
				H	-7.20925	-3.55825	0.13750
				H	-3.87884	-4.13397	3.06316
				H	-8.98883	-2.23713	1.18350
				H	-10.26287	-2.86248	-0.79639
				H	10.32517	-1.53946	0.85368
				H	7.26892	-4.92030	-0.14316
				H	4.13162	-1.96184	2.07090
				H	-4.91929	-0.03803	3.29958
				Na	7.11723	4.69384	3.06463
				Na	-1.07998	4.28629	3.03048
				Na	-8.07018	4.91418	-0.73566
							XXAX
				O	9.51237	-1.10940	0.56378
				C	9.78979	-0.14521	-0.44609
				C	8.49232	0.49316	-0.91751
				O	7.73704	-0.42577	-1.73018
				C	7.56689	0.92439	0.23272
				O	6.97441	2.18234	-0.13982
				C	6.55142	-0.21882	0.30616
				C	6.46243	-0.67403	-1.14982
				N	6.14374	-2.09554	-1.33772
				C	5.25307	-2.46798	-2.35365
				O	4.63570	-1.67556	-3.04595
				N	5.09494	-3.84276	-2.47113

C	5.75810	-4.82338	-1.73689	H	-3.22213	1.53702	-2.86601
O	5.57183	-6.01697	-1.91025	H	-3.99084	3.19557	-0.53293
C	6.68652	-4.23931	-0.75583	H	-3.58179	1.52360	0.98737
N	6.87568	-2.97305	-0.60647	H	-3.50034	-0.60508	-1.18979
P	6.11326	3.03536	0.97716	H	-1.37445	0.86519	1.60889
O	6.44761	4.49985	0.78652	H	-2.54849	-4.93217	-0.91240
O	6.27686	2.44548	2.35960	H	0.72397	-3.40342	2.91952
O	4.56835	2.74165	0.49815	H	0.56251	-5.01696	2.32673
C	4.18267	3.26081	-0.78270	H	-4.96328	0.64355	0.26420
C	2.79832	2.75997	-1.13951	H	-7.96447	0.34546	-2.81823
O	2.85099	1.33578	-1.36194	H	-6.22927	0.00407	-2.57547
C	1.72332	2.99676	-0.05242	H	-7.66368	-2.02173	-2.57407
O	0.50055	3.31107	-0.74578	H	-9.48123	-0.65707	-0.92854
C	1.62971	1.63886	0.62293	H	-8.03640	-0.71533	1.00116
C	1.83349	0.72060	-0.57903	H	-7.23315	-3.55507	0.19873
N	2.23617	-0.63750	-0.22566	H	-3.74403	-4.12531	2.95012
C	1.67837	-1.71671	-0.92618	H	-8.98456	-2.21350	1.26719
O	0.87021	-1.57657	-1.82857	H	-10.28508	-2.83999	-0.69200
N	2.14514	-2.94594	-0.48851	H	10.35932	-1.49466	0.83478
C	3.01939	-3.16333	0.57492	H	7.27469	-4.91134	-0.13979
O	3.38474	-4.28283	0.90170	H	4.13171	-1.97022	2.05829
C	3.45102	-1.91201	1.21627	H	-4.88560	-0.07095	3.35537
N	3.07530	-0.74494	0.82288	Na	7.08667	4.63496	3.15950
P	-0.79875	3.87083	0.09075	Na	-1.07294	4.39084	2.92636
O	-0.50544	5.23144	0.68902	Na	-8.06213	4.91291	-0.71137
O	-1.32631	2.84128	1.07671	XXCX cation			
O	-1.80464	4.08594	-1.17393	O	-9.49412	-1.15031	-0.61528
C	-1.97766	3.14185	-2.24352	C	-9.78054	-0.19599	0.40161
C	-2.84037	1.93096	-1.91186	C	-8.48462	0.42413	0.90016
O	-2.07127	0.91242	-1.26894	O	-7.74806	-0.51862	1.70285
C	-4.06000	2.21369	-1.00120	C	-7.54392	0.86921	-0.23318
O	-5.22051	2.18995	-1.84774	O	-6.95686	2.12467	0.15593
C	-3.99398	1.10378	0.06690	C	-6.52648	-0.27257	-0.30630
C	-2.99592	0.11088	-0.52882	C	-6.46039	-0.74613	1.14474
N	-2.23856	-0.67916	0.41465	N	-6.13117	-2.16547	1.32187
C	-1.40651	-0.19846	1.40585	C	-5.21995	-2.54643	2.31706
N	-0.68085	-1.13156	1.97760	O	-4.57088	-1.76074	2.98747
C	-1.03673	-2.30013	1.31046	N	-5.09109	-3.92379	2.44648
C	-0.68514	-3.65708	1.46417	C	-5.78644	-4.89941	1.73302
N	0.17367	-4.08818	2.41992	O	-5.63935	-6.09395	1.93323
N	-1.24850	-4.56684	0.64327	C	-6.68465	-4.30513	0.73038
C	-2.13669	-4.14995	-0.27799	N	-6.85427	-3.03654	0.57616
N	-2.57904	-2.91198	-0.50967	P	-6.08601	2.98531	-0.94757
C	-2.00519	-2.03786	0.33389	O	-6.39050	4.45048	-0.72032
P	-6.71724	2.41807	-1.20575	O	-6.26706	2.42957	-2.34169
O	-7.56417	3.06853	-2.27827	O	-4.54195	2.65154	-0.48474
O	-6.64394	3.09092	0.14621	C	-4.14684	3.14099	0.80432
O	-7.20177	0.86551	-0.95219	C	-2.77073	2.61408	1.14966
C	-7.21507	-0.00164	-2.09588	O	-2.84710	1.18364	1.34294
C	-7.55348	-1.41395	-1.66685	C	-1.68883	2.85631	0.06745
O	-6.47687	-1.94684	-0.87001	O	-0.46688	3.15275	0.77367
C	-8.83944	-1.53988	-0.82251	C	-1.59626	1.50305	-0.61046
O	-9.51299	-2.71923	-1.26776	C	-1.80933	0.57929	0.58905
C	-8.29395	-1.69518	0.59540	N	-2.18040	-0.78253	0.20742
C	-7.01915	-2.49270	0.32851	C	-1.62713	-1.87881	0.89326
N	-6.01461	-2.40431	1.38514	O	-0.79604	-1.77370	1.77727
C	-5.23178	-3.53196	1.67728	N	-2.10120	-3.10311	0.44600
O	-5.33299	-4.59673	1.09374	C	-3.01693	-3.31551	-0.58175
N	-4.33659	-3.33239	2.72158	O	-3.41974	-4.42630	-0.88673
C	-4.08688	-2.12588	3.36286	C	-3.43858	-2.05583	-1.21505
O	-3.23155	-1.99358	4.22316	N	-3.04936	-0.89058	-0.82358
C	-4.98499	-1.05228	2.90416	P	0.85811	3.70689	-0.01733
N	-5.86419	-1.19752	1.97466	O	0.62014	5.07949	-0.60346
H	10.43832	0.65722	-0.06053	O	1.39593	2.68063	-1.00895
H	10.28937	-0.60309	-1.31267	O	1.83998	3.87017	1.27125
H	8.74753	1.36364	-1.53259	C	1.99126	2.88595	2.30506
H	8.10713	1.04359	1.17338	C	2.85603	1.68698	1.93865
H	6.97217	-1.02076	0.91634	O	2.08001	0.68793	1.26066
H	5.68514	-0.12918	-1.68937	C	4.06877	1.98077	1.03163
H	4.44080	-4.14890	-3.18547	O	5.22009	2.02588	1.87452
H	5.58381	0.09587	0.70050	C	4.05391	0.84093	-0.02307
H	4.18151	4.35699	-0.75512	C	3.00823	-0.11872	0.55229
H	4.89014	2.92463	-1.55058	N	2.18905	-0.86815	-0.42692
H	2.48731	3.25766	-2.06603	C	2.07708	-2.34582	-0.28888
H	1.98822	3.81311	0.62596	O	2.78371	-2.86522	0.55954
H	2.46042	1.52345	1.32042	N	1.23858	-3.01619	-1.10455
H	0.91182	0.62438	-1.15618	C	0.51601	-2.36546	-2.00331
H	1.77124	-3.76122	-0.96572	N	-0.34096	-3.03828	-2.77188
H	0.67448	1.48281	1.12036	C	0.59663	-0.92298	-2.15640
H	-2.48251	3.70449	-3.03403	C	1.44907	-0.20786	-1.30616

P	6.70894	2.28467	1.20933	O	6.39585	4.42548	0.68859
O	7.54608	2.97153	2.26390	O	6.25819	2.41683	2.32296
O	6.59007	2.93405	-0.14975	O	4.54351	2.62979	0.45509
O	7.21741	0.73986	0.96877	C	4.15686	3.10381	-0.84306
C	7.23293	-0.12768	2.11300	C	2.77521	2.58798	-1.18515
C	7.58373	-1.53469	1.68017	O	2.83401	1.15769	-1.36782
O	6.51742	-2.06774	0.86684	C	1.69688	2.85269	-0.10597
C	8.88355	-1.64957	0.85290	O	0.47973	3.16562	-0.81388
O	9.57342	-2.80722	1.32815	C	1.58402	1.50780	0.58741
C	8.36095	-1.84098	-0.56809	C	1.79481	0.56653	-0.59775
C	7.08429	-2.63859	-0.30557	N	2.16662	-0.79166	-0.21136
N	6.10645	-2.56757	-1.38977	C	1.61264	-1.88347	-0.89734
C	5.42826	-3.72608	-1.79339	O	0.80176	-1.77793	-1.80033
O	5.62739	-4.83159	-1.32486	N	2.08263	-3.10983	-0.44865
N	4.48974	-3.48660	-2.79002	C	2.97691	-3.32595	0.59483
C	4.18414	-2.25710	-3.36396	O	3.37329	-4.43943	0.90413
O	3.28858	-2.11865	-4.18574	C	3.39593	-2.06879	1.23144
C	5.00062	-1.16728	-2.81633	N	3.02536	-0.90187	0.82801
N	5.87362	-1.33278	-1.88217	P	-0.80298	3.80198	-0.00977
H	-10.41565	0.61677	0.01559	O	-0.49182	5.20204	0.47955
H	-10.29803	-0.66025	1.25417	O	-1.32615	2.85878	1.06232
H	-8.73932	1.28554	1.52823	O	-1.82805	3.93660	-1.26857
H	-8.07297	0.99705	-1.17896	C	-2.01811	2.94790	-2.29318
H	-6.93772	-1.06744	-0.93210	C	-2.88223	1.75564	-1.90113
H	-5.69866	-0.19990	1.70511	O	-2.10814	0.76181	-1.23641
H	-7.27021	-4.96990	0.10409	C	-4.08482	2.06903	-0.97898
H	-4.43780	-4.23648	3.15881	O	-5.25151	2.07918	-1.81679
H	-5.55234	0.04632	-0.68122	C	-4.03427	0.95939	0.09597
H	-4.12835	4.23718	0.79780	C	-3.03381	-0.04106	-0.48465
H	-4.85712	2.80154	1.56809	N	-2.23834	-0.82072	0.45115
H	-2.45054	3.08551	2.08625	C	-2.11426	-2.23475	0.25313
H	-1.94299	3.67921	-0.60593	O	-2.79579	-2.78560	-0.61514
H	-2.42189	1.38659	-1.31394	N	-1.26721	-2.92565	1.06859
H	-0.89897	0.48660	1.18625	C	-0.54518	-2.28230	1.97714
H	-4.13732	-2.10109	-2.04307	N	0.34058	-3.00764	2.70266
H	-1.73554	-3.91886	0.92939	C	-0.60396	-0.86172	2.16403
H	-0.63899	1.36463	-1.10840	C	-1.45913	-0.17060	1.36596
H	2.48604	3.41271	3.12533	P	-6.74919	2.26210	-1.16591
H	1.00953	2.54013	2.64347	O	-7.61126	2.91453	-2.22516
H	3.23191	1.25364	2.87620	O	-6.68841	2.91191	0.19796
H	3.96128	2.93954	0.52381	O	-7.19828	0.69400	-0.94056
H	3.71904	1.24431	-0.98120	C	-7.16177	-0.15851	-2.09471
H	3.46900	-0.86721	1.19864	C	-7.50812	-1.57880	-1.70085
H	1.50428	0.88957	-1.29882	O	-6.45932	-2.12363	-0.87538
H	0.00777	-0.39837	-2.89970	C	-8.82365	-1.72264	-0.90727
H	-0.39058	-4.04838	-2.69661	O	-9.47714	-2.89587	-1.39660
H	-0.85915	-2.58842	-3.51563	C	-8.32822	-1.90207	0.52592
H	5.02364	0.35551	-0.13978	C	-7.04220	-2.69272	0.29091
H	7.97791	0.22330	2.83786	N	-6.08462	-2.62430	1.38963
H	6.24571	-0.12926	2.58903	C	-5.38631	-3.77499	1.77640
H	7.68516	-2.14827	2.58427	O	-5.55878	-4.87567	1.28306
H	9.50588	-0.75235	0.95229	N	-4.47105	-3.54094	2.79335
H	8.10199	-0.87302	-1.00209	C	-4.19272	-2.31771	3.39574
H	7.29698	-3.69838	-0.15470	O	-3.35548	-2.19252	4.27642
H	4.84311	-0.16046	-3.18787	C	-4.99420	-1.22474	2.82756
H	3.95626	-4.29523	-3.09649	N	-5.86521	-1.38848	1.89236
H	9.06487	-2.37021	-1.21692	H	10.41493	0.55900	-0.02947
H	10.36100	-2.91764	0.77162	H	10.27632	-0.72499	-1.25862
H	-10.34036	-1.51694	-0.91300	H	8.73716	1.23544	-1.53411
Na	-7.04873	4.64422	-3.09380	H	8.07914	0.97710	1.17467
Na	1.39191	4.33621	-2.80369	H	6.94261	-1.09166	0.95127
Na	7.97119	4.81750	0.66490	H	5.67693	-0.23534	-1.67677
XXCX							
O	9.48131	-1.19485	0.61969	H	7.23287	-5.00617	-0.06440
C	9.76924	-0.25009	-0.40565	H	4.41955	-4.26847	-3.13541
C	8.47644	0.37973	-0.90075	H	5.55539	0.02125	0.70874
O	7.72577	-0.55793	-1.69578	H	4.15156	4.20019	-0.85218
C	7.54448	0.83935	0.23332	H	4.86674	2.74484	-1.59826
O	6.95897	2.09128	-0.16843	H	2.46257	3.05792	-2.12547
C	6.52533	-0.30030	0.32516	H	1.96622	3.67794	0.55953
C	6.44309	-0.78113	-1.12221	H	2.40511	1.39212	1.29686
N	6.11072	-2.20001	-1.29269	H	0.88114	0.47133	-1.18875
C	5.20932	-2.58061	-2.29703	H	4.08556	-2.11678	2.06702
O	4.57602	-1.79418	-2.98146	H	1.71261	-3.92389	0.93034
N	5.07016	-3.95729	-2.42000	H	0.62294	1.37503	1.07740
C	5.75247	-4.93352	-1.69626	H	-2.52623	3.47982	-3.10257
O	5.59613	-6.12830	-1.88868	H	-1.04805	2.59173	-2.65404
C	6.65276	-4.34021	-0.69450	H	-3.28444	1.33050	-2.83403
N	6.82733	-3.07199	-0.54218	H	-3.98546	3.04963	-0.51275
P	6.08447	2.96276	0.92379	H	-3.64712	1.38664	1.02426
				H	-3.53384	-0.75816	-1.13891
				H	-1.53828	0.91401	1.37439

H	0.02800	-0.35650	2.88395	C	-7.13061	0.13920	-2.13094	
H	0.29045	-4.01647	2.64950	C	-7.48785	-1.26906	-1.70691	
H	0.77392	-2.60576	3.52179	O	-6.43006	-1.80705	-0.88581	
H	-5.00624	0.49911	0.27905	C	-8.79198	-1.38115	-0.88861	
H	-7.88540	0.19299	-2.84110	O	-9.46195	-2.56061	-1.33823	
H	-6.15877	-0.13924	-2.53632	C	-8.27661	-1.52826	0.54047	
H	-7.58225	-2.17138	-2.62173	C	-6.99960	-2.33300	0.30651	
H	-9.46374	-0.83965	-1.02174	N	-6.02322	-2.23103	1.39039	
H	-8.08436	-0.92948	0.95805	C	-5.29730	-3.36973	1.76548	
H	-7.25106	-3.75272	0.13532	O	-5.38490	-4.44909	1.20590	
H	-4.84333	-0.21950	3.20568	N	-4.45506	-3.15962	2.85279	
H	-3.93474	-4.34791	3.09765	C	-4.15334	-1.92867	3.42480	
H	-9.04092	-2.43312	1.16379	O	-3.29222	-1.77855	4.27780	
H	-10.26965	-3.02814	-0.85191	C	-5.00076	-0.85066	2.88956	
H	10.32581	-1.57121	0.91011	N	-5.85347	-1.00793	1.93679	
Na	7.04494	4.62923	3.06458	H	10.49894	0.51148	-0.09291	
Na	-1.15821	4.60766	2.74652	H	10.30620	-0.78125	-1.30554	
Na	-8.12337	4.73254	-0.63376	H	8.83603	1.23427	-1.58434	
XXGX cation								
O	9.51192	-1.20131	0.58484	H	6.97423	1.01095	1.12483	
C	9.82288	-0.27941	-0.45423	H	5.72096	-1.02166	0.92405	
C	8.54906	0.38954	-0.94783	H	7.23062	-4.94562	-0.04231	
O	7.76505	-0.52244	-1.74075	H	4.37871	-4.21125	-3.07790	
C	7.63425	0.88196	0.18581	H	5.62295	0.13056	0.66623	
O	7.08425	2.14773	-0.22441	H	4.31381	4.33306	-0.88309	
C	6.58227	-0.22586	0.28735	H	4.96597	2.85583	-1.64428	
C	6.48490	-0.72243	-1.15476	H	2.55170	3.24784	-2.10507	
N	6.13369	-2.14201	-1.29811	H	2.15033	3.86602	0.59171	
C	5.23077	-2.52495	-2.29850	H	2.60792	1.57874	1.30540	
O	4.62428	-1.73989	-3.00892	H	0.94472	0.67912	-1.09963	
N	5.04424	-3.89873	-2.37701	H	4.13829	-1.91742	2.13071	
C	5.69603	-4.87136	-1.62286	H	1.77424	-3.73035	-0.88344	
O	5.48389	-6.06535	-1.76043	H	0.81732	1.57775	1.18528	
C	6.64766	-4.27912	-0.66919	H	-2.35836	3.83911	-2.97361	
N	6.85780	-3.01285	-0.55179	H	-0.89499	2.91193	-2.55839	
P	6.24273	3.05559	0.86296	H	-3.12044	1.66949	-2.84940	
O	6.58512	4.50689	0.60266	H	-3.92306	3.34664	-0.54755	
O	6.41688	2.52538	2.26808	H	-3.50180	1.70911	1.00286	
O	4.68877	2.75261	0.41661	H	-3.47343	-0.47054	-1.12768	
C	4.28615	3.23710	-0.87244	H	-1.26397	1.01021	1.59966	
C	2.88096	2.76184	-1.17885	H	-1.09716	-5.39684	0.83992	
O	2.89467	1.33176	-1.37443	H	-3.56853	-4.64651	-1.58413	
C	1.84818	3.04292	-0.06201	H	-2.64595	-5.93558	-0.86410	
O	0.60847	3.36777	-0.71852	H	-4.90623	0.83147	0.31473	
C	1.75195	1.70015	0.64131	H	-7.86466	0.49304	-2.86551	
C	1.88647	0.75711	-0.55209	H	-6.13668	0.13742	-2.59317	
N	2.26282	-0.60582	-0.18511	H	-7.58242	-1.87979	-2.61356	
C	1.68017	-1.68284	-0.86138	H	-9.42592	-0.49558	-1.01548	
O	0.85659	-1.53441	-1.75048	H	-8.02301	-0.54658	0.94456	
N	2.13282	-2.91043	-0.40208	H	-7.21307	-3.39691	0.18988	
C	3.00859	-3.12256	0.66991	H	-4.88144	0.14733	3.29751	
O	3.36502	-4.24081	1.00404	H	-3.92794	-3.97123	3.16282	
C	3.45773	-1.86674	1.28812	H	-8.98229	-2.03954	1.20173	
N	3.10667	-0.70495	0.86306	H	-10.24840	-2.67134	-0.78012	
P	-0.67068	3.92101	0.14803	H	10.34485	-1.60708	0.86895	
O	-0.36302	5.26050	0.78034	Na	7.24321	4.73080	2.97741	
O	-1.19943	2.86906	1.11397	Na	-0.94432	4.40261	3.00030	
O	-1.69037	4.16988	-1.09833	Na	-7.97166	5.06099	-0.74779	
C	-1.86709	3.25419	-2.19088	XXGX				
C	-2.75535	2.05666	-1.88783	O	9.52402	-1.16242	0.62998	
O	-2.01349	1.01614	-1.23290	C	9.82895	-0.22479	-0.39683	
C	-3.98587	2.35627	-0.99867	C	8.54802	0.42776	-0.89354	
O	-5.13278	2.30985	-1.85550	O	7.78254	-0.49413	-1.69288	
C	-3.93187	1.27133	0.09887	C	7.62123	0.90103	0.23897	
C	-2.95540	0.25696	-0.49130	O	7.05569	2.16178	-0.16459	
N	-2.18868	-0.53618	0.47023	C	6.58405	-0.22192	0.32834	
C	-1.34993	-0.06201	1.43104	C	6.49833	-0.70511	-1.11858	
N	-0.64184	-1.02666	2.04766	N	6.15288	-2.12280	-1.28209	
C	-1.01893	-2.16852	1.44058	C	5.25617	-2.49675	-2.29211	
C	-0.64031	-3.56305	1.64978	O	4.65143	-1.70547	-2.99686	
O	0.11311	-4.03246	2.47812	N	5.07815	-3.87061	-2.38993	
N	-1.32001	-4.41023	0.73558	C	5.72681	4.85025	-1.64143	
C	-2.26254	-4.03379	-0.18149	O	5.52562	-6.04346	-1.80023	
N	-2.84700	-4.94505	-0.93725	C	6.65914	-4.26542	-0.66458	
N	-2.63848	-2.74208	-0.36017	N	6.86627	-3.00001	-0.53283	
C	-2.01420	-1.90590	0.43610	P	6.20160	3.05288	0.92791	
P	-6.63825	2.55450	-1.23184	O	6.55060	4.50812	0.69828	
O	-7.46594	3.21049	-2.31453	O	6.35797	2.49852	2.32584	
O	-6.56938	3.22647	0.12006	O	4.65400	2.76137	0.45523	
O	-7.12981	1.00428	-0.98515	C	4.27541	3.25515	-0.83781	

C	2.88413	2.76606	-1.18282	H	-3.64869	-4.76634	-1.51117	
O	2.91811	1.33688	-1.37526	H	-2.80236	-5.97190	-0.66837	
C	1.81346	3.04088	-0.09991	H	-4.89289	0.80648	0.31561	
O	0.59636	3.36725	-0.79798	H	-7.91431	0.47495	-2.78165	
C	1.69457	1.69638	0.59787	H	-6.18454	0.10612	-2.54050	
C	1.88480	0.75492	-0.58808	H	-7.65408	-1.89504	-2.51754	
N	2.25496	-0.60435	-0.21043	H	-9.44582	-0.48826	-0.88621	
C	1.68352	-1.68583	-0.89219	H	-7.99142	-0.52582	1.03706	
O	0.88211	-1.56020	-1.80235	H	-7.23154	-3.39415	0.29750	
N	2.12997	-2.91615	-0.43422	H	-4.83070	0.12209	3.37710	
C	3.00001	-3.13624	0.63105	H	-3.76299	-3.95678	3.06162	
O	3.36994	-4.25466	0.95469	H	-8.95893	-2.00474	1.33834	
C	3.43875	-1.88413	1.26104	H	-10.27254	-2.65823	-0.60295	
N	3.08744	-0.71588	0.84646	H	10.36130	-1.55500	0.91979	
P	-0.69242	3.95937	0.03344	Na	7.18774	4.69106	3.07598	
O	-0.38000	5.32892	0.60112	Na	-0.92604	4.52897	2.86187	
O	-1.22592	2.95660	1.04320	Na	-7.97146	5.04943	-0.71676	
O	-1.70261	4.15985	-1.23010					
C	-1.89289	3.19628	-2.27901					
C	-2.77501	2.00663	-1.92125	O	9.47068	-1.17302	0.57966	
O	-2.01985	0.98392	-1.26847	C	9.76596	-0.23708	-0.45167	
C	-3.98305	2.32565	-1.00650	C	8.47662	0.38860	-0.96095	
O	-5.15115	2.29432	-1.84261	O	7.73360	-0.55369	-1.75808	
C	-3.91884	1.24090	0.08665	C	7.53547	0.85221	0.16395	
C	-2.95239	0.21453	-0.50381	O	6.95453	2.10446	-0.24398	
N	-2.19922	-0.57442	0.44457	C	6.51359	-0.28524	0.24949	
C	-1.35970	-0.09122	1.43594	C	6.44607	-0.77453	-1.19621	
N	-0.65377	-1.03145	2.01585	N	6.11683	-2.19579	-1.35858	
C	-1.02478	-2.20069	1.36003	C	5.20509	-2.58471	-2.34994	
C	-0.65837	-3.56530	1.59803	O	4.55994	-1.80425	-3.03038	
O	0.10200	-4.05548	2.43047	N	5.06796	-3.96266	-2.46151	
N	-1.33953	-4.42073	0.68841	C	5.75876	-4.93244	-1.73641	
C	-2.26634	-4.04478	-0.25600	O	5.60089	-6.12876	-1.91708	
N	-2.79200	-5.02985	-1.03949	C	6.66939	-4.33039	-0.74951	
N	-2.61663	-2.79010	-0.45697	N	6.84505	-3.06090	-0.61047	
C	-1.98786	-1.93399	0.38492	P	6.08076	2.98119	0.84405	
P	-6.64141	2.54342	-1.19413	O	6.38708	4.44282	0.59832	
O	-7.48973	3.18990	-2.26811	O	6.25528	2.44380	2.24612	
O	-6.55457	3.22975	0.15015	O	4.53854	2.64179	0.37938	
O	-7.13751	0.99758	-0.92206	C	4.14555	3.11763	-0.91555	
C	-7.16901	0.12124	-2.05826	C	2.76212	2.59897	-1.24412	
C	-7.53029	-1.28142	-1.61616	O	2.82796	1.16580	-1.42425	
O	-6.46017	-1.82698	-0.81861	C	1.70022	2.85889	-0.14706	
C	-8.81392	-1.37624	-0.76536	O	0.46533	3.16378	-0.82570	
O	-9.50231	-2.55643	-1.18485	C	1.60443	1.51270	0.54183	
C	-8.26426	-1.51012	0.65300	C	1.80091	0.57413	-0.64718	
C	-7.00260	-2.33165	0.39770	N	2.17698	-0.78277	-0.24827	
N	-5.99096	-2.23037	1.44740	C	1.62052	-1.88736	-0.91963	
C	-5.21275	-3.35675	1.74998	O	0.78999	-1.78941	-1.80501	
O	-5.29988	-4.42117	1.16173	N	2.09000	-3.10885	-0.46086	
N	-4.33985	-3.15839	2.81294	C	3.00286	-3.31385	0.57067	
C	-4.05887	-1.94069	3.42130	O	3.41521	-4.41928	0.87842	
O	-3.19726	-1.79954	4.27365	C	3.40693	-2.04795	1.20773	
C	-4.94260	-0.86615	2.94429	N	3.01714	-0.88491	0.80776	
N	-5.82746	-1.01668	2.02015	P	-0.82811	3.72493	0.01260	
H	10.48900	0.57320	-0.02180	O	-0.55407	5.08914	0.60096	
H	10.32754	-0.71005	-1.24898	O	-1.33619	2.69699	1.02044	
H	8.82497	1.27991	-1.52473	O	-1.85488	3.89796	-1.23765	
H	8.15607	1.03045	1.18134	C	-2.01512	2.94065	-2.29603	
H	6.98565	-1.01844	0.95811	C	-2.87015	1.73137	-1.94609	
H	5.73671	-0.15544	-1.67535	O	-2.09347	0.73518	-1.26257	
H	7.23356	-4.93682	-0.03504	C	-4.09534	2.01339	-1.05146	
H	4.42055	-4.17736	-3.10080	O	-5.23817	2.03251	-1.90498	
H	5.61876	0.11727	0.70816	C	-4.06942	0.88337	0.01526	
H	4.29029	4.35152	-0.83650	C	-3.02323	-0.07208	-0.55968	
H	4.97788	2.89030	-1.59715	N	-2.19653	-0.83059	0.41639	
H	2.57876	3.24840	-2.11933	C	-2.10819	-2.26659	0.23916	
H	2.09414	3.86316	0.56491	O	-2.76851	-2.83819	-0.59529	
H	2.52218	1.57754	1.29857	N	-1.24910	-2.89473	1.10620	
H	0.96350	0.66844	-1.16809	C	-0.44547	-2.30666	2.07927	
H	4.11308	-1.93860	2.10850	O	0.33417	-2.95695	2.75320	
H	1.75557	-3.72991	-0.91320	C	-0.58242	-0.83725	2.18108	
H	0.73609	1.56365	1.09573	C	0.24128	-0.11418	3.17151	
H	-2.38956	3.75057	-3.08054	C	-1.45798	-0.16932	1.30492	
H	-0.92354	2.83886	-2.64035	P	-6.73799	2.28095	-1.25959	
H	-3.17128	1.60494	-2.86618	O	-7.56775	2.95792	-2.32613	
H	-3.89953	3.31778	-0.56277	O	-6.64163	2.93421	0.09918	
H	-3.47797	1.67580	0.98651	O	-7.23377	0.73160	-1.02432	
H	-3.48125	-0.49968	-1.14702	C	-7.22137	-0.13597	-2.16868	
H	-1.31135	0.97349	1.62539	C	-7.55220	-1.54763	-1.73777	
H	-1.11969	-5.40522	0.79825	O	-6.48956	-2.05410	-0.90242	

C	-8.86607	-1.68621	-0.93490	C	1.70492	2.86267	-0.17999
O	-9.53285	-2.84734	-1.43418	O	0.48216	3.18716	-0.87157
C	-8.36774	-1.88422	0.49335	C	1.58473	1.52454	0.52392
C	-7.07063	-2.65408	0.24761	C	1.78680	0.56942	-0.64992
N	-6.12104	-2.58220	1.35568	N	2.16069	-0.78326	-0.24413
C	-5.42202	-3.73118	1.74930	C	1.60656	-1.88429	-0.91464
O	-5.59917	-4.83623	1.27153	O	0.79382	-1.79109	-1.81763
N	-4.48345	-3.48032	2.74412	N	2.07149	-3.10556	-0.44639
C	-4.19845	-2.24839	3.32359	C	2.96719	-3.30853	0.59959
O	-3.27858	-2.09117	4.11550	O	3.37135	-4.41630	0.91634
C	-5.06375	-1.17783	2.81522	C	3.37188	-2.04317	1.23070
N	-5.93123	-1.35207	1.87751	N	3.00291	-0.88132	0.81077
H	10.40873	0.57529	-0.07764	P	-0.78289	3.82405	-0.03812
H	10.27918	-0.71905	-1.29692	O	-0.45609	5.22053	0.44973
H	8.74123	1.24160	-1.59628	O	-1.28406	2.87752	1.04171
H	8.06238	0.99076	1.10942	O	-1.83366	3.96110	-1.27522
H	6.92194	-1.07425	0.88455	C	-2.02784	2.98008	-2.30645
H	5.68441	-0.23422	-1.76219	C	-2.88957	1.78639	-1.91685
H	7.25814	-4.99062	-0.12140	O	-2.11762	0.79110	-1.24764
H	4.41116	-4.28080	-3.16816	C	-4.09653	2.10063	-1.00048
H	5.54064	0.04153	0.62087	O	-5.25934	2.08981	-1.84128
H	4.13859	4.21386	-0.92418	C	-4.03743	1.00470	0.08950
H	4.84958	2.75927	-1.67637	C	-3.04514	-0.00104	-0.49353
H	2.43300	3.06330	-2.18105	N	-2.25191	-0.78692	0.44205
H	1.97595	3.68209	0.51732	C	-2.13881	-2.16084	0.21923
H	2.43130	1.40051	1.24396	O	-2.76354	-2.77161	-0.63954
H	0.88223	0.47277	-1.23017	N	-1.28135	-2.80452	1.09129
H	4.08229	-2.08715	2.05506	C	-0.47319	-2.23715	2.08190
H	1.73129	-3.92726	-0.94530	O	0.29299	-2.94367	2.73532
H	0.64830	1.38794	1.04116	C	-0.60219	-0.79087	2.19963
H	-2.52625	3.48452	-3.09491	C	0.25522	-0.08439	3.21013
H	-1.03719	2.60948	-2.65804	C	-1.45985	-0.14023	1.37686
H	-3.23117	1.29983	-2.88996	P	-6.76424	2.25632	-1.20100
H	-4.00786	2.97859	-0.55168	O	-7.62283	2.91085	-2.26143
H	-3.73019	1.29838	0.96727	O	-6.71856	2.89427	0.16877
H	-3.48377	-0.81811	-1.20997	O	-7.19895	0.68194	-0.99455
H	-1.17797	-3.90385	0.99530	C	-7.13737	-0.15977	-2.15556
H	-5.03658	0.39468	0.14199	C	-7.46811	-1.58698	-1.77608
H	-7.96419	0.20166	-2.90198	O	-6.42718	-2.11618	-0.92987
H	-6.22913	-0.12079	-2.63366	C	-8.79896	-1.75700	-1.01263
H	-7.62470	-2.16683	-2.64090	O	-9.42553	-2.93315	-1.52944
H	-9.49747	-0.79580	-1.03784	C	-8.33305	-1.94558	0.42856
H	-8.13538	-0.91670	0.94303	C	-7.02758	-2.71011	0.21433
H	-7.26065	-3.71509	0.07553	N	-6.09999	-2.63670	1.33799
H	-3.92948	-4.27960	3.03892	C	-5.38409	-3.77704	1.72359
H	-9.07396	-2.43377	1.12235	O	-5.53531	-4.87871	1.22624
H	-10.33218	-2.96968	-0.89721	N	-4.47135	-3.52856	2.74031
H	-0.02219	0.94454	3.21928	C	-4.21843	-2.30245	3.34897
H	0.13381	-0.58701	4.15661	O	-3.36837	-2.16055	4.21492
H	1.30642	-0.21210	2.90526	C	-5.05809	-1.22728	2.80241
H	-1.52889	0.92831	1.28580	N	-5.92147	-1.40327	1.86210
H	-4.94078	-0.17539	3.21053	H	10.40501	0.52062	-0.11605
H	10.31314	-1.54576	0.88047	H	10.25306	-0.77899	-1.32706
Na	7.04034	4.66228	2.97555	H	8.72616	1.19053	-1.61835
Na	-1.10128	4.28926	2.85968	H	8.07159	0.96108	1.09346
Na	-8.03234	4.80161	-0.73549	H	6.92423	-1.10267	0.89480
XXTX							
O	9.46417	-1.21844	0.56122	H	5.65500	-0.27694	-1.74100
C	9.75274	-0.28953	-0.47835	H	7.21849	-5.02710	-0.07365
C	8.46191	0.34210	-0.97675	H	4.38084	-4.32728	-3.13103
O	7.70400	-0.59743	-1.76262	H	5.54222	0.01375	0.64081
C	7.53453	0.81704	0.15445	H	4.16104	4.18564	-0.95979
O	6.95488	2.06799	-0.25841	H	4.86155	2.71607	-1.69250
C	6.51006	-0.31690	0.25963	H	2.45241	3.04245	-2.20986
C	6.42349	-0.81472	-1.18197	H	1.99221	3.68758	0.47852
N	6.09220	-2.23655	-1.33342	H	2.40301	1.41135	1.23604
C	5.18764	-2.62937	-2.32955	H	0.86894	0.46571	-1.23312
O	4.55769	-1.85132	-3.02680	H	4.04788	-2.08013	2.07775
N	5.03767	-4.00698	-2.42543	H	1.71380	-3.92527	-0.92831
C	5.71457	-4.97375	-1.68435	H	0.62273	1.40294	1.01279
O	5.54276	-6.17081	-1.84758	H	-2.54286	3.51595	-3.10888
C	6.63303	-4.36863	-0.70668	H	-1.06015	2.62766	-2.67656
N	6.81714	-3.09914	-0.57926	H	-3.28643	1.35906	-2.85053
P	6.08729	2.95480	0.82678	H	4.00706	3.08762	-0.54569
O	6.40641	4.41354	0.57784	H	-3.63852	1.44300	1.00745
O	6.25942	2.42064	2.23064	H	-3.55761	-0.71324	-1.14489
O	4.54418	2.62596	0.36305	H	-1.19658	-3.80586	0.95173
C	4.15748	3.08943	-0.93890	H	-5.00791	0.54788	0.28842
C	2.77017	2.58017	-1.26748	H	-7.85705	0.18747	-2.90771
O	2.82020	1.14747	-1.43637	H	-6.12983	-0.12310	-2.58524
				H	-7.51205	-2.17688	-2.70056
				H	-9.44819	-0.88133	-1.13184

H	-8.11609	-0.97433	0.87759	O	-9.33372	-2.99511	-1.32587
H	-7.21299	-3.77183	0.04143	C	-8.17529	-1.91142	0.54366
H	-3.92259	-4.32725	3.04490	C	-6.87232	-2.65650	0.27066
H	-9.05029	-2.49669	1.04386	N	-5.87202	-2.57235	1.32723
H	-10.22920	-3.08132	-1.00548	C	-5.04899	-3.68443	1.56509
H	0.04523	0.98983	3.21035	O	-5.12047	-4.72700	0.93858
H	0.07409	-0.48265	4.21619	N	-4.15065	-3.49807	2.60709
H	1.31913	-0.23303	2.98651	C	-3.93470	-2.31191	3.29558
H	-1.54550	0.94359	1.37190	O	-3.07587	-2.19108	4.15391
H	-4.93983	-0.22437	3.19788	C	-4.87221	-1.24952	2.89042
H	10.30779	-1.59611	0.85245	N	-5.75639	-1.38520	1.96315
Na	7.05464	4.63375	2.95489	H	9.96470	1.99943	-0.55561
Na	-0.95701	4.57613	2.75693	H	10.07392	0.84413	-1.90951
Na	-8.17074	4.70629	-0.65447	H	7.91721	2.11069	-1.77239
XTAX							
O	9.79605	-0.01733	-0.02230	H	7.45625	-0.81522	0.60734
C	9.58065	1.04512	-0.94705	H	5.55032	0.08637	-1.60470
C	8.08883	1.20045	-1.18546	H	7.32776	-4.67985	-0.37984
O	7.59979	0.05877	-1.92602	H	4.48163	-3.86604	-3.40137
C	7.26367	1.26544	0.12219	H	5.79382	-0.17709	0.82820
O	6.20656	2.23406	-0.06660	H	3.75761	4.88092	-1.02028
C	6.69263	-0.13913	0.22104	H	4.72529	3.44615	-1.44683
C	6.44632	-0.43374	-1.25496	H	2.24079	3.43255	-2.02767
N	6.23021	-1.84381	-1.56269	H	1.75698	4.03488	0.70509
C	5.29246	-2.19735	-2.54456	H	2.34879	1.79968	1.40886
O	4.64781	-1.38957	-3.19074	H	0.96508	0.88643	-1.17877
N	5.15138	-3.57024	-2.69727	H	3.61255	0.25343	1.22025
C	5.83332	-4.56438	-1.99612	H	1.85047	-3.46409	-1.21277
O	5.66186	-5.75404	-2.20529	H	0.57761	1.62413	1.14999
C	6.75116	-3.99869	-0.99644	H	-2.67742	3.77411	-2.97107
N	6.93853	-2.73500	-0.82595	H	-1.13295	2.97675	-2.57723
P	5.42697	2.78478	1.26923	H	-3.24820	1.54478	-2.83685
O	6.36418	3.60793	2.13093	H	-4.12138	3.13609	-0.48728
O	4.73146	1.65297	2.01508	H	-3.66972	1.46086	1.01429
O	4.33536	3.77521	0.57844	H	-3.40860	-0.59843	-1.21029
C	3.93015	3.82278	-0.79819	H	-1.36639	0.86356	1.66948
C	2.64194	3.06314	-1.07433	H	-2.33270	-4.86328	-1.08066
O	2.90649	1.65463	-1.18974	H	0.96960	-3.33235	2.70809
C	1.54597	3.21515	0.01333	H	0.87729	-4.91574	2.06309
O	0.30910	3.46090	-0.67611	H	-4.97060	0.50858	0.23231
C	1.53466	1.84287	0.68117	H	-7.94156	0.15471	-2.85921
C	1.83932	0.96147	-0.52914	H	-6.19205	-0.09150	-2.60244
N	2.28291	-0.39862	-0.26144	H	-7.51515	-2.19643	-2.62566
C	1.75342	-1.44208	-1.03056	H	-9.41111	-0.93503	-0.98498
O	0.92649	-1.28296	-1.91943	H	-7.95728	-0.92195	0.94966
N	2.23649	-2.68843	-0.68496	H	-7.05581	-3.72025	0.10892
C	3.13048	-3.01210	0.34181	H	-3.52973	-4.27915	2.79794
O	3.44318	-4.18701	0.53707	H	-8.84462	-2.45862	1.21405
C	3.63779	-1.86577	1.08091	H	-10.10621	-3.15101	-0.75906
C	4.64391	-2.10839	2.16926	H	10.74914	-0.06374	0.14691
C	3.20802	-0.63048	0.73528	H	4.90402	-1.16801	2.66516
P	-1.01165	3.95791	0.16482	H	4.24599	-2.80846	2.91437
O	-0.76872	5.31598	0.79175	H	5.55980	-2.55410	1.76008
O	-1.50992	2.89116	1.12644	H	-4.80010	-0.28504	3.38125
O	-2.01108	4.16403	-1.10749	Na	5.95364	2.19684	4.05623
C	-2.12639	3.23299	-2.19652	Na	-1.34075	4.42233	3.00448
C	-2.90096	1.96174	-1.87896	Na	-8.20664	4.72981	-0.70407
O	-2.07200	0.99716	-1.22922	XTCX			
C	-4.14013	2.16276	-0.97714	O	9.78304	-0.08264	-0.00766
O	-5.28861	2.10488	-1.83654	C	9.56128	0.97076	-0.94131
C	-4.02893	1.03690	0.07401	C	8.06845	1.11536	-1.18040
C	-2.95636	0.12549	-0.52036	O	7.58612	-0.03564	-1.90934
N	-2.16672	-0.65549	0.40298	C	7.24384	1.18765	0.12678
C	-1.34960	-0.18886	1.41445	O	6.18397	2.15027	-0.06719
N	-0.58613	-1.12032	1.94201	C	6.67737	-0.21984	0.23865
C	-0.89838	-2.26704	1.22557	C	6.43248	-0.52540	-1.23472
C	-0.48564	-3.61076	1.31994	N	6.22031	-1.93433	-1.54322
N	0.40575	-4.04057	2.25529	C	5.26832	-2.29446	-2.51090
N	-1.02577	-4.50876	0.47267	O	4.60025	-1.49222	-3.13960
C	-1.94155	-4.09007	-0.42266	N	5.15455	-3.66902	-2.67873
N	-2.43086	-2.86193	-0.60435	C	5.85325	-4.66042	-1.98703
C	-1.88319	-1.99737	0.26577	O	5.71489	-5.84951	-2.22068
P	-6.79865	2.27185	-1.20841	C	6.73495	-4.08776	-0.95913
O	-7.65657	2.90630	-2.28173	N	6.90946	-2.82257	-0.78547
O	-6.76306	2.92972	0.15252	P	5.38493	2.69204	1.26113
O	-7.22722	0.69948	-0.98095	O	6.31027	3.50878	2.14151
C	-7.18027	-0.15604	-2.13284	O	4.67457	1.55844	1.98969
C	-7.44273	-1.58732	-1.71551	O	4.31131	3.69225	0.55549
O	-6.34372	-2.06288	-0.91306	C	3.90559	3.70833	-0.82169
C	-8.72384	-1.78282	-0.87805	C	2.62827	2.92953	-1.08898

O	2.90296	1.51924	-1.17117	H	-7.88592	0.03712	-2.87764
C	1.51667	3.09971	-0.01716	H	-6.14396	-0.20922	-2.57706
O	0.29556	3.34813	-0.73686	H	-7.45647	-2.31326	-2.67624
C	1.48432	1.73463	0.65813	H	-9.40514	-1.08601	-1.06747
C	1.81202	0.84010	-0.53859	H	-8.01750	-1.13261	0.91234
N	2.22545	-0.52529	-0.23945	H	-7.07574	-3.90236	0.02622
C	1.71532	-1.57305	-1.01318	H	-4.80700	-0.41612	3.24946
O	0.90036	-1.42627	-1.91459	H	-3.68142	-4.47719	2.89738
N	2.20823	-2.81719	-0.66086	H	-8.90924	-2.67861	1.10217
C	3.12937	-3.13873	0.34658	H	-10.11024	-3.30730	-0.92741
O	3.48614	-4.30515	0.50808	H	10.73644	-0.12212	0.16151
C	3.60058	-1.99113	1.10101	H	4.85896	-1.27034	2.68194
C	4.61402	-2.21528	2.18690	H	4.23228	-2.92229	2.93414
C	3.14999	-0.75904	0.76094	H	5.53623	-2.64417	1.77421
P	-1.04358	3.88309	0.04618	Na	5.88274	2.08362	4.04927
O	-0.83459	5.28148	0.59095	Na	-1.54616	4.55092	2.81258
O	-1.54699	2.87328	1.06593	Na	-8.21190	4.56983	-0.59222
O	-2.02322	3.99952	-1.25072				
C	-2.13375	2.99885	-2.27640				
C	-2.91558	1.75028	-1.88757	O	9.82626	-0.08112	0.00945
O	-2.08481	0.80552	-1.22173	C	9.63405	0.96109	-0.94310
C	-4.12995	1.99177	-0.96458	C	8.14625	1.13644	-1.19306
O	-5.29257	1.97970	-1.80644	O	7.64078	-0.01475	-1.90678
C	-4.03560	0.86365	0.09166	C	7.31662	1.24895	0.10828
C	-2.97120	-0.06344	-0.49525	O	6.27760	2.23058	-0.10975
N	-2.14540	-0.83794	0.41679	C	6.72109	-0.14297	0.24063
C	-1.96640	-2.23766	0.15629	C	6.47648	-0.47134	-1.22829
O	-2.61987	-2.77460	-0.74209	N	6.23984	-1.88469	-1.50241
N	-1.10976	-2.93372	0.95418	C	5.29567	-2.24808	-2.47446
C	-0.39394	-2.29600	1.87274	O	4.65960	-1.44679	-3.13713
N	0.46835	-3.02981	2.61451	N	5.13901	-3.62214	-2.59865
C	-0.48833	-0.88314	2.10523	C	5.80878	-4.60922	-1.87620
C	-1.37255	-0.19228	1.34033	O	5.62482	-5.80097	-2.06164
P	-6.79540	2.13161	-1.16237	C	6.73067	-4.03290	-0.88628
O	-7.66022	2.79391	-2.21357	N	6.93321	-2.76819	-0.74282
O	-6.75244	2.75597	0.21418	P	5.50109	2.82492	1.20944
O	-7.22387	0.55374	-0.97192	O	6.44773	3.65211	2.05680
C	-7.14399	-0.28328	-2.13523	O	4.78485	1.72122	1.97706
C	-7.41523	-1.72219	-1.75230	O	4.43079	3.81828	0.49048
O	-6.34053	-2.21271	-0.92572	C	4.01960	3.82696	-0.88533
C	-8.72333	-1.93847	-0.96247	C	2.72153	3.07494	-1.13540
O	-9.32044	-3.13571	-1.46522	O	2.96824	1.66061	-1.21269
C	-8.22061	-2.11009	0.47019	C	1.63037	3.27186	-0.04960
C	-6.90409	-2.84196	0.22038	O	0.39676	3.52701	-0.74188
N	-5.95016	-2.77986	1.31924	C	1.59470	1.91555	0.64902
C	-5.19033	-3.91330	1.63870	C	1.88794	1.00100	-0.53879
O	-5.32019	-4.99597	1.09513	N	2.30338	-0.35867	-0.23514
N	-4.26578	-3.68491	2.64782	C	1.76620	-1.41435	-0.97942
C	-4.03318	-2.48021	3.30326	O	0.94855	-1.27759	-1.88013
O	-3.17828	-2.35412	4.16660	N	2.23256	-2.65886	-0.60416
C	-4.90951	-1.40502	2.81606	C	3.12363	-2.97488	0.42590
N	-5.78951	-1.56378	1.88819	O	3.44838	-4.14525	0.62295
H	9.94023	1.93044	-0.55817	C	3.63904	-1.81904	1.14245
H	10.05528	0.76427	-1.90225	C	4.64812	-2.04765	2.23095
H	7.89124	2.01961	-1.77509	C	3.22685	-0.58566	0.76802
H	7.86036	1.48239	0.98019	P	-0.91410	4.05690	0.09511
H	7.44342	-0.88980	0.63064	O	-0.65595	5.42885	0.68481
H	5.53720	-0.00586	-1.58731	O	-1.41358	3.01981	1.08778
H	7.29958	-4.76392	-0.32615	O	-1.92081	4.23800	-1.17500
H	4.48936	-3.96924	-3.38531	C	-2.04979	3.28123	-2.23985
H	5.77673	-0.25713	0.84482	C	-2.84230	2.02924	-1.89081
H	3.71794	4.75990	-1.06172	O	-2.02479	1.06332	-1.22827
H	4.70713	3.33333	-1.46327	C	-4.07335	2.26841	-0.98595
H	2.23282	3.27286	-2.05425	O	-5.22851	2.18047	-1.83433
H	1.72175	3.92502	0.66953	C	-3.95621	1.18084	0.10293
H	2.28449	1.69040	1.40129	C	-2.91795	0.22764	-0.48598
H	0.95548	0.76761	-1.21163	N	-2.13128	-0.54925	0.44405
H	3.54539	0.12691	1.24958	C	-1.30763	-0.07682	1.45534
H	1.84653	-3.59140	-1.20738	N	-0.56239	-1.01490	1.99210
H	0.51873	1.52914	1.11129	C	-0.88715	-2.16486	1.28875
H	-2.67205	3.49346	-3.08976	C	-0.45766	-3.51926	1.47156
H	-1.13752	2.71327	-2.62852	O	0.33440	-4.00270	2.27881
H	-3.29154	1.30065	-2.82024	N	-1.11321	-4.36529	0.53472
H	-4.06804	2.96300	-0.47416	C	-2.06334	-3.98864	-0.38867
H	-3.69046	1.29073	1.03616	N	-2.55809	-4.96495	-1.20390
H	-3.42877	-0.78414	-1.17624	N	-2.46437	-2.74337	-0.54085
H	-1.50390	0.88625	1.38959	C	-1.86564	-1.89324	0.32919
H	0.13421	-0.38431	2.83778	P	-6.73504	2.37091	-1.20483
H	0.64937	-3.98562	2.33836	O	-7.59150	2.99836	-2.28365
H	1.15395	-2.57401	3.19921	O	-6.68954	3.04683	0.14687
H	-4.98329	0.34380	0.24171	O	-7.17682	0.80561	-0.95613

C	-7.14561	-0.06422	-2.09759	O	-4.75250	-1.62163	1.81389
C	-7.42490	-1.48691	-1.66111	O	-4.40428	-3.63594	0.21108
O	-6.32927	-1.96715	-0.85647	C	-3.99836	-3.56980	-1.16596
C	-8.70364	-1.65361	-0.81541	C	-2.68045	-2.83433	-1.36618
O	-9.31904	-2.87595	-1.22686	O	-2.90458	-1.41211	-1.35877
C	-8.15062	-1.74439	0.60751	C	-1.62324	-3.11903	-0.26937
C	-6.85579	-2.50923	0.35240	O	-0.35038	-3.32274	-0.91710
N	-5.84853	-2.39680	1.40106	C	-1.62422	-1.82167	0.53861
C	-5.02355	-3.50216	1.65617	C	-1.84718	-0.82191	-0.59154
O	-5.07271	-4.54651	1.02880	N	-2.22651	0.53458	-0.23466
N	-4.15208	-3.30914	2.71936	C	-1.67790	1.59363	-0.96492
C	-3.91620	-2.10569	3.37202	O	-0.86289	1.46026	-1.86804
O	-3.05589	-1.96683	4.22596	N	-2.12864	2.83672	-0.55146
C	-4.84570	-1.04884	2.94249	C	-3.03734	3.14374	0.47613
N	-5.73115	-1.19927	2.01774	O	-3.36153	4.31164	0.68231
H	10.03313	1.91812	-0.57405	C	-3.54269	1.98136	1.18412
H	10.12828	0.72692	-1.89756	C	-4.54997	2.19051	2.27767
H	7.99355	2.03450	-1.80352	C	-3.15295	0.75198	0.77177
H	7.93523	1.54604	0.95926	P	0.88361	-3.94010	-0.02283
H	7.47161	-0.82125	0.64807	O	0.58122	-5.36333	0.40058
H	5.59080	0.05430	-1.59556	O	1.26003	-3.01380	1.12484
H	7.29622	-4.70736	-0.25233	O	2.04529	-3.98307	-1.16378
H	4.46533	-3.92466	-3.29608	C	2.16667	-3.10385	-2.29270
H	5.81849	-0.15070	0.84355	C	2.94192	-1.82566	-2.01893
H	3.85835	4.87981	-1.13874	O	2.10946	-0.85661	-1.36606
H	4.80815	3.42197	-1.52486	C	4.21333	-1.98072	-1.13846
H	2.32178	3.42265	-2.09753	O	5.29439	-1.38147	-1.87664
H	1.85878	4.10264	0.62326	C	3.88009	-1.16644	0.11410
H	2.40655	1.87572	1.37939	C	2.96704	-0.10655	-0.49789
H	1.01404	0.92542	-1.18945	N	2.13178	0.66670	0.40924
H	3.64550	0.30299	1.23140	C	2.04364	2.04648	0.20213
H	1.84870	-3.43796	-1.12808	O	2.68503	2.65375	-0.64751
H	0.63304	1.72124	1.11914	N	1.19053	2.69843	1.06981
H	-2.59321	3.81065	-3.02779	C	0.38543	2.14143	2.06754
H	-1.06038	3.00121	-2.61419	O	-0.34933	2.85843	2.74396
H	-3.20251	1.59941	-2.83807	C	0.49354	0.69186	2.17574
H	-4.04973	3.25918	-0.53255	C	-0.36614	-0.00492	3.19110
H	-3.56012	1.63364	1.01450	C	1.34620	0.03183	1.35397
H	-3.39916	-0.49892	-1.15271	P	6.84285	-1.72197	-1.44674
H	-1.30887	0.97841	1.69533	O	7.22131	-3.12792	-1.87351
H	-0.85247	-5.34375	0.60018	O	7.09457	-1.40866	0.01537
H	-3.42948	-4.71638	-1.65662	O	7.60705	-0.68581	-2.44931
H	-2.53425	-5.91799	-0.86241	C	7.14642	0.61592	-2.83993
H	-4.90405	0.68090	0.30823	C	7.46652	1.75106	-1.87183
H	-7.90542	0.24778	-2.82501	O	6.40625	1.92352	-0.91555
H	-6.15828	-0.01844	-2.57137	C	8.78376	1.61422	-1.06086
H	-7.50823	-2.10680	-2.56285	O	9.60087	2.73668	-1.40353
H	-9.38796	-0.80646	-0.94406	C	8.30215	1.65753	0.39723
H	-7.92400	-0.74503	0.98279	C	7.02548	2.47709	0.24620
H	-7.04909	-3.57671	0.23140	N	6.08623	2.42136	1.35753
H	-4.77036	-0.07441	3.41273	C	5.34734	3.56569	1.68848
H	-3.54036	-4.09131	2.93386	O	5.47000	4.64131	1.13003
H	-8.82155	-2.26621	1.29627	N	4.45645	3.35670	2.73273
H	-10.08770	-3.01532	-0.65066	C	4.23762	2.16154	3.41396
H	10.77725	-0.13790	0.18701	O	3.42359	2.06022	4.31919
H	4.92110	-1.09972	2.70513	C	5.06027	1.06658	2.88499
H	4.24731	-2.72695	2.99345	N	5.90634	1.20650	1.92341
H	5.55689	-2.51198	1.82650	H	-10.02023	-1.66239	-0.78902
Na	6.02823	2.25769	3.99978	H	-10.06690	-0.40115	-2.04853
Na	-1.20643	4.58116	2.92662	H	-7.95582	-1.73852	-1.97529
Na	-8.11785	4.84891	-0.73016	H	-7.94228	-1.43391	0.80501
XTTX							
O	-9.80790	0.30002	-0.09376	H	-7.49699	0.96864	0.64788
C	-9.60088	-0.69195	-1.09541	H	-5.53437	0.19428	-1.56104
C	-8.10920	-0.87363	-1.31862	H	-4.36617	4.15664	-3.21936
O	-7.56733	0.30558	-1.95083	H	-5.84680	0.29017	0.87216
C	-7.31093	-1.07149	-0.01074	H	-3.86678	-4.60848	-1.48612
O	-6.26051	-2.02699	-0.28093	H	-4.77680	-3.10249	-1.77424
C	-6.72673	0.31651	0.23386	H	-2.27380	-3.13080	-2.34209
C	-6.42469	0.71772	-1.20334	H	-1.87758	-3.99939	0.32624
N	-6.16814	2.13195	-1.42904	H	-2.47496	-1.83577	1.22367
C	-5.22559	2.49258	-2.40501	H	-0.94121	-0.73684	-1.19637
O	-4.60704	1.68701	-3.07968	H	-3.58214	-0.14407	1.21069
N	-5.04317	3.86228	-2.52158	H	-1.75360	3.62367	-1.07035
C	-5.69468	4.85178	-1.79120	H	-0.69097	-1.67392	1.07400
O	-5.49353	6.04255	-1.96443	H	2.71666	-3.67693	-3.04562
C	-6.62666	4.28006	-0.80314	H	1.17755	-2.85440	-2.68700
N	-6.84176	3.01665	-0.65594	H	3.25504	-1.42631	-2.99383
P	-5.46943	-2.68815	0.99602	H	4.43854	-3.02925	-0.92495
O	-6.40235	-3.56453	1.80801	H	3.31659	-1.79305	0.81058
				H	3.55666	0.61493	-1.06788
				H	1.42941	-1.05191	1.36469

H	1.12811	3.70254	0.93941
H	4.77819	-0.76149	0.58063
H	7.66643	0.82240	-3.78013
H	6.06860	0.59533	-3.02718
H	7.54391	2.67093	-2.46988
H	9.29853	0.67571	-1.28822
H	8.04055	0.65113	0.73040
H	7.25082	3.53526	0.08753
H	3.90458	4.16376	3.00817
H	9.03663	2.11738	1.06533
H	10.43905	2.63009	-0.92620
H	-10.76319	0.36288	0.05665
H	-7.17643	4.96013	-0.16143
H	4.94706	0.07768	3.31600
H	-0.16642	-1.08089	3.19541
H	-0.18097	0.39531	4.19566
H	-1.42993	0.15441	2.97097
H	-4.83757	1.23243	2.72212
H	-4.13904	2.83784	3.06236
H	-5.45071	2.68136	1.88717
Na	-6.02320	-2.21863	3.80177
Na	0.95946	-4.78321	2.75398
Na	7.87249	-3.66621	0.41668