Dual Roles of Glycosyl Torsion Angle Conformation and Stereochemical Configuration in Butadiene Oxide-Derived N1 β-Hydroxyalkyl Deoxyinosine Adducts: A Structural Perspective [†]

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Supporting Information

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Running Title: Butadiene Oxide-Derived Inosine N1 Adduct

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Table S1. ^{1}H NMR Assignments for the *ras61 R*-N1-BDO-(61,2) adduct.

	H1'	H2'	H2''	H3'	H4'	H5'	H5''	H8	H6	CH_3	H5	H2
C^{1}	5.45	1.58	2.08	4.42					7.02		5.10	
G^{2}	5.13	2.43	2.54	4.79	4.01	3.79	3.68	7.37				
G^{3}	5.44	2.54	2.43	4.16	3.84	3.92	3.95	7.28				
A^{4}	5.93	2.34	2.58	4.78				7.59				7.38
C^{5}	5.55	1.64	1.76	4.51	3.83	3.73	3.71		6.63		4.71	
X^{6}	5.32	1.95	2.43	4.57				7.20				7.31
A^{7}	5.27	2.60	2.32		4.03	3.68		7.63				6.85
G^{8}	5.00	2.30	2.36					7.20				
A^{9}	5.67	2.40	2.62	4.78	3.84	3.91	3.94	7.57				
A^{10}	5.75	2.30	2.61	4.76	4.17	3.94		7.49				6.83
G^{11}	5.71	2.08	1.97	4.33	4.00	3.85	3.91	7.02				
C^{12}	5.61	2.06	2.35	4.39	3.85	3.59	3.53		7.30		5.38	
T^{13}	5.95	2.02	2.40	4.66	4.02	3.84	3.84		7.14	1.41		
T^{14}	5.91	1.98	2.34		3.89	3.97	3.93		6.94	1.40		
C^{15}	5.75	2.19	1.84	4.59	4.00	3.92	3.88		7.07		5.13	
T^{16}	5.89	2.12	1.90	4.65	3.81	3.87	3.91		6.83	1.46		
T^{17}	5.42	1.56	1.85	4.49	3.72	3.83			6.68	1.34		
G^{18}	5.64	2.49	2.56		4.07	3.71	3.78	7.46				
T^{19}	5.81	1.97	2.27	4.61	3.98	3.87	3.91		6.80	1.15		
C^{20}	5.71	1.87	2.16	4.56					7.03		5.32	
C^{21}	5.31	1.76	2.08	4.56	3.85	3.82	3.78		6.96		5.16	
G^{22}	5.93	2.39	2.10	4.43	3.93	3.8	3.84	7.42				

Table S2. NOE Restraints Used in the rMD Calculations for the *ras61 R*-N1-BDO-(61,2) adduct.

```
#
# 1      CYT    H3'      1        CYT    H6       4.23     5.17
 &rst
  ixpk= 0, nxpk= 0, iat=  24,  13, r1= 3.73, r2= 4.23, r3= 5.17, r4= 5.67, &end
#
# 1      CYT    H3'      1        CYT    H2'      2.12     2.58
 &rst
  ixpk= 0, nxpk= 0, iat=  24,  26, r1= 1.62, r2= 2.12, r3= 2.58, r4= 3.08,  &end
#
# 1      CYT    H2'2     1        CYT    H2'      1.58     2.02
 &rst
  ixpk= 0, nxpk= 0, iat=  27,  26, r1= 1.08, r2= 1.58, r3= 2.02, r4= 2.52,  &end
#
# 2      GUA    H8       1        CYT    H6       4.54     5.56
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  13, r1= 4.04, r2= 4.54, r3= 5.56, r4= 6.06,  &end
#
# 2      GUA    H8       1        CYT    H2'      3.36     4.1
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  26, r1= 2.86, r2= 3.36, r3= 4.10, r4= 4.60,  &end
#
# 1      CYT    H1'      2        GUA    H8       5.81     7.11
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  43, r1= 5.31, r2= 5.81, r3= 7.11, r4= 7.61,  &end
#
```

```
# 1      CYT   H1'     2        GUA   H5'2    4        6
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  35, r1= 3.50, r2= 4.00, r3= 6.00, r4= 6.50,  &end
#
# 2      GUA   H8      2        GUA   H1'     3.77     4.61
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  40, r1= 3.27, r2= 3.77, r3= 4.61, r4= 5.11,  &end
#
# 2      GUA   H3'     2        GUA   H2'     2.29     2.79
 &rst
  ixpk= 0, nxpk= 0, iat=  57,  59, r1= 1.79, r2= 2.29, r3= 2.79, r4= 3.29,  &end
#
# 2      GUA   H2'2    2        GUA   H1'     2.02     2.58
 &rst
  ixpk= 0, nxpk= 0, iat=  60,  40, r1= 1.52, r2= 2.02, r3= 2.58, r4= 3.08,  &end
#
# 2      GUA   H4'     2        GUA   H8      4.97     6.33
 &rst
  ixpk= 0, nxpk= 0, iat=  37,  43, r1= 4.47, r2= 4.97, r3= 6.33, r4= 6.83,  &end
#
# 2      GUA   H8      2        GUA   H5'     4.7      5.9
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  34, r1= 4.20, r2= 4.70, r3= 5.90, r4= 6.40,  &end
#
# 2      GUA   H8      2        GUA   H5'2    6.03     7.37
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  35, r1= 5.53, r2= 6.03, r3= 7.37, r4= 7.87,  &end
```

```
#
# 2      GUA   H4'     2        GUA   H1'     2.92    3.56
 &rst
  ixpk= 0, nxpk= 0, iat=  37,  40, r1= 2.42, r2= 2.92, r3= 3.56, r4= 4.06,  &end
#
# 2      GUA   H1'     2        GUA   H5'2    4.85    6.15
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  35, r1= 4.35, r2= 4.85, r3= 6.15, r4= 6.65,  &end
#
# 3      GUA   H8      2        GUA   H1'     3.82    4.66
 &rst
  ixpk= 0, nxpk= 0, iat=  76,  40, r1= 3.32, r2= 3.82, r3= 4.66, r4= 5.16,  &end
#
# 3      GUA   H8      2        GUA   H3'     4.12    4.88 change
 &rst
  ixpk= 0, nxpk= 0, iat=  76,  57, r1= 3.62, r2= 4.12, r3= 5.00, r4= 5.38,  &end
#
# 3      GUA   H3'     2        GUA   H1'     5.42    6.62
 &rst
  ixpk= 0, nxpk= 0, iat=  90,  40, r1= 4.92, r2= 5.42, r3= 6.62, r4= 7.12,  &end
#
# 3      GUA   H5'     2        GUA   H1'     4.42    5.58 change
 &rst
  ixpk= 0, nxpk= 0, iat=  67,  40, r1= 3.92, r2= 4.22, r3= 5.58, r4= 6.08,  &end
#
# 3      GUA   H4'     2        GUA   H1'     5.11    6.25
 &rst
```

```
  ixpk= 0, nxpk= 0, iat=  70,  40, r1= 4.61, r2= 5.11, r3= 6.25, r4= 6.75,  &end
#
# 3      GUA   H1'     3       GUA   H8      3.31    4.05
 &rst
  ixpk= 0, nxpk= 0, iat=  73,  76, r1= 2.81, r2= 3.31, r3= 4.05, r4= 4.55,  &end
#
# 3      GUA   H3'     3       GUA   H8      4.46    5.44 change
 &rst
  ixpk= 0, nxpk= 0, iat=  90,  76, r1= 3.96, r2= 4.16, r3= 5.44, r4= 5.94,  &end
#
# 3      GUA   H8      3       GUA   H4'     5.2     6.8
 &rst
  ixpk= 0, nxpk= 0, iat=  76,  70, r1= 4.70, r2= 5.20, r3= 6.80, r4= 7.30,  &end
#
# 3      GUA   H8      3       GUA   H5'     4.84    6.16
 &rst
  ixpk= 0, nxpk= 0, iat=  76,  67, r1= 4.34, r2= 4.84, r3= 6.16, r4= 6.66,  &end
#
# 3      GUA   H5'2    3       GUA   H8      4.43    5.41
 &rst
  ixpk= 0, nxpk= 0, iat=  68,  76, r1= 3.93, r2= 4.43, r3= 5.41, r4= 5.91,  &end
#
# 3      GUA   H1'     3       GUA   H3'     3.15    3.85
 &rst
  ixpk= 0, nxpk= 0, iat=  73,  90, r1= 2.65, r2= 3.15, r3= 3.85, r4= 4.35,  &end
#
# 4      ADE   H1'     3       GUA   H3'     3.5     4.1
```

```
# &rst
#  ixpk= 0, nxpk= 0, iat= 106,  90, r1= 3.00, r2= 3.50, r3= 4.10, r4= 4.60,  &end
#
# 4       ADE    H1'      3         GUA    H3'      2.74     3.34
# &rst
#  ixpk= 0, nxpk= 0, iat= 106,  90, r1= 2.24, r2= 2.74, r3= 3.34, r4= 3.84,  &end
#
# 4       ADE    H8       3         GUA    H8       4.69     5.73
 &rst
  ixpk= 0, nxpk= 0, iat= 109,  76, r1= 4.19, r2= 4.69, r3= 5.73, r4= 6.23,  &end
#
# 3       GUA    H1'      4         ADE    H8       3.04     4.04
 &rst
  ixpk= 0, nxpk= 0, iat=  73, 109, r1= 2.54, r2= 3.04, r3= 4.04, r4= 4.54,  &end
#
# 4       ADE    H8       4         ADE    H1'      3.37     4.43
 &rst
  ixpk= 0, nxpk= 0, iat= 109, 106, r1= 2.87, r2= 3.37, r3= 4.43, r4= 4.93,  &end
#
# 4       ADE    H3'      4         ADE    H1'      6.07     7.41
# &rst
#  ixpk= 0, nxpk= 0, iat= 122, 106, r1= 5.57, r2= 6.07, r3= 7.41, r4= 7.91,  &end
#
# 4       ADE    H2'      4         ADE    H1'      2.77     3.23
 &rst
  ixpk= 0, nxpk= 0, iat= 124, 106, r1= 2.27, r2= 2.77, r3= 3.23, r4= 3.73,  &end
#
```

```
# 4      ADE   H2      4        ADE   H1'     4.12    5.04
 &rst
  ixpk= 0, nxpk= 0, iat= 118, 106, r1= 3.62, r2= 4.12, r3= 5.04, r4= 5.54,  &end
#
# 5      CYT   H6      4        ADE   H1'     3.3     4.04
 &rst
  ixpk= 0, nxpk= 0, iat= 141, 106, r1= 2.80, r2= 3.30, r3= 4.04, r4= 4.54,  &end
#
# 5      CYT   H6      4        ADE   H3'     5.27    6.43
 &rst
  ixpk= 0, nxpk= 0, iat= 141, 122, r1= 4.77, r2= 5.27, r3= 6.43, r4= 6.93,  &end
#
# 5      CYT   H1'     4        ADE   H1'     4.86    6.14
 &rst
  ixpk= 0, nxpk= 0, iat= 138, 106, r1= 4.36, r2= 4.86, r3= 6.14, r4= 6.64,  &end
#
# 5      CYT   H5      4        ADE   H1'     5.18    6.34
 &rst
  ixpk= 0, nxpk= 0, iat= 143, 106, r1= 4.68, r2= 5.18, r3= 6.34, r4= 6.84,  &end
#
# 5      CYT   H6      4        ADE   H8      3.83    4.69    change
 &rst
  ixpk= 0, nxpk= 0, iat= 141, 109, r1= 3.33, r2= 3.83, r3= 4.99, r4= 5.19,  &end
#
# 5      CYT   H6      4        ADE   H2'2    3.13    3.83    change
 &rst
  ixpk= 0, nxpk= 0, iat= 141, 125, r1= 2.63, r2= 2.93, r3= 3.83, r4= 4.33,  &end
```

```
#
# 5      CYT    H6      4         ADE    H2'      3.55     4.33
 &rst
  ixpk= 0, nxpk= 0, iat= 141, 124, r1= 3.05, r2= 3.55, r3= 4.33, r4= 4.83,  &end
#
# 5      CYT    H1'     4         ADE    H2       3.79     4.63
 &rst
  ixpk= 0, nxpk= 0, iat= 138, 118, r1= 3.29, r2= 3.79, r3= 4.63, r4= 5.13,  &end
#
# 5      CYT    H5      4         ADE    H2'2     3.22     3.94
 &rst
  ixpk= 0, nxpk= 0, iat= 143, 125, r1= 2.72, r2= 3.22, r3= 3.94, r4= 4.44,  &end
#
# 19     THY    H1'     4         ADE    H2       4.57     5.59
# &rst
#  ixpk= 0, nxpk= 0, iat= 592, 118, r1= 4.07, r2= 4.57, r3= 5.59, r4= 6.09,  &end
#
# 5      CYT    H6      5         CYT    H1'      3.79     4.63
 &rst
  ixpk= 0, nxpk= 0, iat= 141, 138, r1= 3.29, r2= 3.79, r3= 4.63, r4= 5.13,  &end
#
# 5      CYT    H5      5         CYT    H6       2.2      2.68
 &rst
  ixpk= 0, nxpk= 0, iat= 143, 141, r1= 1.70, r2= 2.20, r3= 2.68, r4= 3.18,  &end
#
# 5      CYT    H3'     5         CYT    H6       2.74     3.36     change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 152, 141, r1= 2.24, r2= 2.74, r3= 3.86, r4= 4.00,  &end
#
# 5      CYT    H5'      5        CYT    H6       4.15     5.07
 &rst
  ixpk= 0, nxpk= 0, iat= 132, 141, r1= 3.65, r2= 4.15, r3= 5.07, r4= 5.57,  &end
#
# 5      CYT    H4'      5        CYT    H6       4.72     5.88
 &rst
  ixpk= 0, nxpk= 0, iat= 135, 141, r1= 4.22, r2= 4.72, r3= 5.88, r4= 6.38,  &end
#
# 5      CYT    H5       5        CYT    H1'      4.86     6.34
 &rst
  ixpk= 0, nxpk= 0, iat= 143, 138, r1= 4.36, r2= 4.86, r3= 6.34, r4= 6.84,  &end
#
# 5      CYT    H3'      5        CYT    H1'      3.37     4.13
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 138, r1= 2.87, r2= 3.37, r3= 4.13, r4= 4.63,  &end
#
# 5      CYT    H3'      5        CYT    H5       5.92     7.24
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 143, r1= 5.42, r2= 5.92, r3= 7.24, r4= 7.74,  &end
#
# 5      CYT    H4'      5        CYT    H1'      4.86     5.94
# &rst
#  ixpk= 0, nxpk= 0, iat= 135, 138, r1= 4.36, r2= 4.86, r3= 5.94, r4= 6.44,  &end
#
# 5      CYT    H5'      5        CYT    H1'      2.32     2.84
```

```
# &rst
#  ixpk= 0, nxpk= 0, iat= 132, 138, r1= 1.82, r2= 2.32, r3= 2.84, r4= 3.34,  &end
#
# 5      CYT    H2'      5        CYT    H5       3.73     4.55
 &rst
  ixpk= 0, nxpk= 0, iat= 154, 143, r1= 3.23, r2= 3.73, r3= 4.55, r4= 5.05,  &end
#
# 5      CYT    H2'2     5        CYT    H5       4.91     5.99
 &rst
  ixpk= 0, nxpk= 0, iat= 155, 143, r1= 4.41, r2= 4.91, r3= 5.99, r4= 6.49,  &end
#
# 6      N1R    H8       5        CYT    H1'      5.49     6.51     change
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 138, r1= 4.99, r2= 5.35, r3= 5.50, r4= 6.00,
&end
#
# 6      N1R    H8       5        CYT    H3'      5.86     7.16     CHANGE
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 152, r1= 5.36, r2= 5.86, r3= 8.56, r4= 8.66,
&end
#
# 6      N1R    H8       5        CYT    H2'2     5.91     7.23
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 155, r1= 5.41, r2= 5.91, r3= 7.23, r4= 7.73,  &end
#
# 6      N1R    H8       5        CYT    H2'      5.85     7.15
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 195, 154, r1= 5.35, r2= 5.85, r3= 7.15, r4= 7.65,  &end
#
# 6      N1R    H5'2    5        CYT    H1'     4.31    5.27
 &rst
  ixpk= 0, nxpk= 0, iat= 162, 138, r1= 3.81, r2= 4.31, r3= 5.27, r4= 5.77,  &end
#
# 6      N1R    H8      6        N1R    HAA   2.23    2.33    change
 &rst
  ixpk= 0, nxpk= 0, iat= 195, 168, r1= 2.33, r2= 2.63, r3= 2.83, r4= 3.95,
&end
#
# 6      N1R    H3'     6        N1R    H8      3.92    5.08    change
 &rst
  ixpk= 0, nxpk= 0, iat= 197, 195, r1= 5.42, r2= 5.89, r3= 5.92, r4= 6.08,  &end
#
# 6      N1R    H3'     6        N1R    HAA   2.7     3.3     change
 &rst
  ixpk= 0, nxpk= 0, iat= 197, 168, r1= 2.20, r2= 2.70, r3= 3.60, r4= 3.80,
&end
#
# 6      N1R    H5'     6        N1R    HAA   4.26    5.2
 &rst
  ixpk= 0, nxpk= 0, iat= 163, 168, r1= 3.76, r2= 4.26, r3= 5.20, r4= 5.70,  &end
#
# 6      N1R    H2      6        N1R    HAA   6.18    7.56
 &rst
  ixpk= 0, nxpk= 0, iat= 179, 168, r1= 5.68, r2= 6.18, r3= 7.56, r4= 8.06,
```

```
&end
#
# 6      N1R    H5'      6        N1R    H8       4.91     6.01
 &rst
  ixpk= 0, nxpk= 0, iat= 163, 195, r1= 4.41, r2= 4.91, r3= 6.01, r4= 6.51,
&end
#
# 6      N1R    H8       6        N1R    H5'2     4.45     6.45
# &rst
#  ixpk= 0, nxpk= 0, iat= 195, 162, r1= 3.95, r2= 4.45, r3= 6.45, r4= 6.95,  &end
#
# 6      N1R    H4'      6        N1R    H8       5.89     7.19
 &rst
  ixpk= 0, nxpk= 0, iat= 165, 195, r1= 5.39, r2= 5.89, r3= 7.19, r4= 7.69,  &end
#
# 6      N1R    H5'      6        N1R    H2'      3.04     3.72
# &rst
#  ixpk= 0, nxpk= 0, iat= 163, 170, r1= 2.54, r2= 3.04, r3= 3.72, r4= 4.22,  &end
#
# 7      ADE    H8       6        N1R    HAA    5.63     6.87
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 168, r1= 5.13, r2= 5.63, r3= 5.80, r4= 6.07,
&end
#
# 7      ADE    H8       6        N1R    H3'      5.2      6.8
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 197, r1= 4.70, r2= 5.20, r3= 6.80, r4= 7.30,
```

```
&end
#
# 7      ADE   H8      6        N1R   H2'     4.45    5.43
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 170, r1= 3.95, r2= 4.45, r3= 5.43, r4= 5.93,  &end
#
# 7      ADE   H2      6        N1R   H2      4.44    5.62    change
 &rst
  ixpk= 0, nxpk= 0, iat= 222, 179, r1= 3.94, r2= 4.44, r3= 5.42, r4= 5.92,  &end
#
# 7      ADE   H4'     6        N1R   H8      4.34    5.34
 &rst
  ixpk= 0, nxpk= 0, iat= 207, 195, r1= 3.84, r2= 4.34, r3= 5.34, r4= 5.84,  &end
# 7      ADE   H8      7        ADE   H1'     4.04    4.94    change
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 210, r1= 3.54, r2= 3.94, r3= 4.94, r4= 5.44,  &end
#
# 7      ADE   H5'     7        ADE   H8      4.87    6.13
 &rst
  ixpk= 0, nxpk= 0, iat= 204, 213, r1= 4.37, r2= 4.87, r3= 6.13, r4= 6.63,  &end
#
# 7      ADE   H4'     7        ADE   H8      4.35    5.65
 &rst
  ixpk= 0, nxpk= 0, iat= 207, 213, r1= 3.85, r2= 4.35, r3= 5.65, r4= 6.15,  &end
#
# 7      ADE   H4'     7        ADE   H1'     2.84    3.56    change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 207, 210, r1= 2.00, r2= 2.34, r3= 3.56, r4= 4.06,  &end
#
# 7      ADE   H2      7        ADE   H1'     4.78    6.22
 &rst
  ixpk= 0, nxpk= 0, iat= 222, 210, r1= 4.28, r2= 4.78, r3= 6.22, r4= 6.72,  &end
#
# 8      GUA   H8      7        ADE   H1'     3.32    4.06    change
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 210, r1= 2.82, r2= 3.12, r3= 4.06, r4= 4.56,  &end
#
# 8      GUA   H8      7        ADE   H8      3.67    4.49    change
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 213, r1= 3.17, r2= 3.67, r3= 4.70, r4= 4.99,  &end
#
# 8      GUA   H1'     7        ADE   H1'     4.96    6.04    change
 &rst
  ixpk= 0, nxpk= 0, iat= 242, 210, r1= 4.06, r2= 4.46, r3= 6.04, r4= 6.54,  &end
#
# 17     THY   H1'     7        ADE   H2      5.19    6.35
# &rst
#  ixpk= 0, nxpk= 0, iat= 527, 222, r1= 4.69, r2= 5.19, r3= 6.35, r4= 6.85,  &end
#
# 7      ADE   H4'     8        GUA   H1'     3       3.66
# &rst
#  ixpk= 0, nxpk= 0, iat= 207, 242, r1= 2.50, r2= 3.00, r3= 3.66, r4= 4.16,  &end
#
# 8      GUA   H8      8        GUA   H1'     3.84    4.7
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 242, r1= 3.34, r2= 3.84, r3= 4.70, r4= 5.20,  &end
#
# 9      ADE   H8      8        GUA   H8      4.83    5.91
 &rst
  ixpk= 0, nxpk= 0, iat= 278, 245, r1= 4.33, r2= 4.83, r3= 5.91, r4= 6.41,  &end
#
# 9      ADE   H4'     9        ADE   H8      4.88    6.12
 &rst
  ixpk= 0, nxpk= 0, iat= 272, 278, r1= 4.38, r2= 4.88, r3= 6.12, r4= 6.62,  &end
#
# 9      ADE   H3'     9        ADE   H1'     3.58    4.38
 &rst
  ixpk= 0, nxpk= 0, iat= 291, 275, r1= 3.08, r2= 3.58, r3= 4.38, r4= 4.88,  &end
#
# 10     ADE   H8      9        ADE   H1'     3.68    4.5
 &rst
  ixpk= 0, nxpk= 0, iat= 310, 275, r1= 3.18, r2= 3.68, r3= 4.50, r4= 5.00,  &end
#
# 10     ADE   H4'     9        ADE   H1'     3       3.6
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 275, r1= 2.50, r2= 3.00, r3= 3.60, r4= 4.10,  &end
#
# 10     ADE   H4'     9        ADE   H1'     2.74    3.34    change
 &rst
  ixpk= 0, nxpk= 0, iat= 304, 275, r1= 2.24, r2= 2.74, r3= 3.64, r4= 3.84,  &end
#
```

```
# 10     ADE    H5'      10       ADE    H8       5.34     6.52
 &rst
  ixpk= 0, nxpk= 0, iat= 301, 310, r1= 4.84, r2= 5.34, r3= 6.52, r4= 7.02,  &end
#
# 10     ADE    H8       10       ADE    H4'      4.87     6.13
 &rst
  ixpk= 0, nxpk= 0, iat= 310, 304, r1= 4.37, r2= 4.87, r3= 6.13, r4= 6.63,  &end
#
# 10     ADE    H1'      10       ADE    H4'      2.64     3.22
 &rst
  ixpk= 0, nxpk= 0, iat= 307, 304, r1= 2.14, r2= 2.64, r3= 3.22, r4= 3.72,  &end
#
# 10     ADE    H3'      10       ADE    H1'      3.86     4.72
 &rst
  ixpk= 0, nxpk= 0, iat= 323, 307, r1= 3.36, r2= 3.86, r3= 4.72, r4= 5.22,  &end
#
# 11     GUA    H8       10       ADE    H3'      4.71     5.75     change
 &rst
  ixpk= 0, nxpk= 0, iat= 342, 323, r1= 4.21, r2= 4.51, r3= 5.75, r4= 6.25,  &end
#
# 11     GUA    H8       10       ADE    H8       5.44     6.64
 &rst
  ixpk= 0, nxpk= 0, iat= 342, 310, r1= 4.94, r2= 5.44, r3= 6.64, r4= 7.14,  &end
#
# 11     GUA    H1'      11       GUA    H8       3.45     4.07
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 342, r1= 2.95, r2= 3.45, r3= 4.07, r4= 4.57,  &end
```

```
#
# 11    GUA   H3'     11       GUA   H8      3.26    3.98    change
 &rst
  ixpk= 0, nxpk= 0, iat= 356, 342, r1= 2.76, r2= 3.10, r3= 3.98, r4= 4.48,  &end
#
# 11    GUA   H4'     11       GUA   H3'     2.65    3.23
 &rst
  ixpk= 0, nxpk= 0, iat= 336, 356, r1= 2.15, r2= 2.65, r3= 3.23, r4= 3.73,  &end
#
# 11    GUA   H3'     11       GUA   H2'     2.18    2.66
 &rst
  ixpk= 0, nxpk= 0, iat= 356, 358, r1= 1.68, r2= 2.18, r3= 2.66, r4= 3.16,  &end
#
# 11    GUA   H3'     11       GUA   H2'2    2.62    3.2
 &rst
  ixpk= 0, nxpk= 0, iat= 356, 359, r1= 2.12, r2= 2.62, r3= 3.20, r4= 3.70,  &end
#
# 11    GUA   H1'     11       GUA   H3'     4.28    5.24  change
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 356, r1= 3.78, r2= 4.00, r3= 5.24, r4= 5.74,  &end
#
# 12    CYT   H6      12       CYT   H1'     3.59    4.39
 &rst
  ixpk= 0, nxpk= 0, iat= 374, 371, r1= 3.09, r2= 3.59, r3= 4.39, r4= 4.89,  &end
#
# 12    CYT   H5      12       CYT   H6      2.19    2.61
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 376, 374, r1= 1.69, r2= 2.19, r3= 2.61, r4= 3.11,  &end
#
# 12     CYT    H4'      12       CYT    H6       4.41     5.39
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 374, r1= 3.91, r2= 4.41, r3= 5.39, r4= 5.89,  &end
#
# 12     CYT    H3'      12       CYT    H1'      4.01     4.89
 &rst
  ixpk= 0, nxpk= 0, iat= 385, 371, r1= 3.51, r2= 4.01, r3= 4.89, r4= 5.39,  &end
#
# 12     CYT    H2'2     12       CYT    H1'      2.04     2.5
 &rst
  ixpk= 0, nxpk= 0, iat= 388, 371, r1= 1.54, r2= 2.04, r3= 2.50, r4= 3.00,  &end
#
# 13     THY    H6       12       CYT    H1'      4.69     5.73
 &rst
  ixpk= 0, nxpk= 0, iat= 404, 371, r1= 4.19, r2= 4.69, r3= 5.73, r4= 6.23,  &end
#
# 13     THY    H6       12       CYT    H3'      4.01     4.91
 &rst
  ixpk= 0, nxpk= 0, iat= 404, 385, r1= 3.51, r2= 4.01, r3= 4.91, r4= 5.41,  &end
#
# 13     THY    H6       12       CYT    H6       3.5      4.5
 &rst
  ixpk= 0, nxpk= 0, iat= 404, 374, r1= 3.00, r2= 3.50, r3= 4.50, r4= 5.00,  &end
#
# 13     THY    M7       12       CYT    H6       4.53     5.53     change
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 374, r1= 4.03, r2= 4.33, r3= 6.64, r4= 7.14,
 igr1= 407, 408, 409,
 &end
#
# 13     THY    H6       13       THY    H1'      3.35     4.25
 &rst
  ixpk= 0, nxpk= 0, iat= 404, 401, r1= 2.85, r2= 3.35, r3= 4.25, r4= 4.75,  &end
#
# 13     THY    H3'      13       THY    H6       4.09     5.01
 &rst
  ixpk= 0, nxpk= 0, iat= 417, 404, r1= 3.59, r2= 4.09, r3= 5.01, r4= 5.51,  &end
#
# 13     THY    H4'      13       THY    H6       4.23     5.17
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 404, r1= 3.73, r2= 4.23, r3= 5.17, r4= 5.67,  &end
#
# 13     THY    H3'      13       THY    H1'      3.47     4.53
 &rst
  ixpk= 0, nxpk= 0, iat= 417, 401, r1= 2.97, r2= 3.47, r3= 4.53, r4= 5.03,  &end
#
# 13     THY    H3'      13       THY    H2'      4.42     5.4
# &rst
#  ixpk= 0, nxpk= 0, iat= 417, 419, r1= 3.92, r2= 4.42, r3= 5.40, r4= 5.90,  &end
#
# 14     THY    H6       13       THY    H3'      4.08     4.98
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 436, 417, r1= 3.58, r2= 4.08, r3= 4.98, r4= 5.48,  &end
#
# 14     THY    H6       13       THY    H6       4.13     4.87
 &rst
  ixpk= 0, nxpk= 0, iat= 436, 404, r1= 3.63, r2= 4.13, r3= 4.87, r4= 5.37,  &end
#
# 14     THY    M7       13       THY    H1'      3.64     4.46
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 401, r1= 3.14, r2= 3.64, r3= 5.36, r4= 5.86,
 igr1= 439, 440, 441,
 &end
#
# 13     THY    H4'      14       THY    H6       5.47     6.69
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 436, r1= 4.97, r2= 5.47, r3= 6.69, r4= 7.19,  &end
#
# 15     CYT    H6       14       THY    H1'      3.82     4.66
 &rst
  ixpk= 0, nxpk= 0, iat= 468, 433, r1= 3.32, r2= 3.82, r3= 4.66, r4= 5.16,  &end
#
# 15     CYT    H6       15       CYT    H1'      3.64     4.44
 &rst
  ixpk= 0, nxpk= 0, iat= 468, 465, r1= 3.14, r2= 3.64, r3= 4.44, r4= 4.94,  &end
#
# 15     CYT    H3'      15       CYT    H1'      3.56     4.36
 &rst
  ixpk= 0, nxpk= 0, iat= 479, 465, r1= 3.06, r2= 3.56, r3= 4.36, r4= 4.86,  &end
```

```
#
# 15     CYT    H2'2    15       CYT    H1'      2.32     2.84 change
 &rst
  ixpk= 0, nxpk= 0, iat= 482, 465, r1= 1.82, r2= 2.12, r3= 2.84, r4= 3.34,  &end
#
# 15     CYT    H2'     15       CYT    H5       4.64     5.68
 &rst
  ixpk= 0, nxpk= 0, iat= 481, 470, r1= 4.14, r2= 4.64, r3= 5.68, r4= 6.18,  &end
#
# 16     THY    H6      15       CYT    H3'      4.45     5.43
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 479, r1= 3.95, r2= 4.45, r3= 5.43, r4= 5.93,  &end
#
# 16     THY    M7      15       CYT    H2'      4.12     4.88
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 481, r1= 3.62, r2= 4.12, r3= 5.86, r4= 6.36,
 igr1= 501, 502, 503,
 &end
#
# 16     THY    H6      16       THY    H1'      2.75     3.35  change
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 495, r1= 2.25, r2= 2.75, r3= 3.85, r4= 4.00,  &end
#
# 16     THY    H4'     16       THY    H6       4.82     6.18  change
 &rst
  ixpk= 0, nxpk= 0, iat= 492, 498, r1= 4.32, r2= 4.42, r3= 6.18, r4= 6.68,  &end
#
```

```
# 16     THY    M7       16        THY    H1'      4.79     5.85
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 495, r1= 4.29, r2= 4.79, r3= 7.03, r4= 7.53,
 igr1= 501, 502, 503,
 &end
#
# 16     THY    H2'      16        THY    M7       3.88     4.74
 &rst
  ixpk= 0, nxpk= 0, iat= 513,  -1, r1= 3.38, r2= 3.88, r3= 5.69, r4= 6.19,
 igr2= 501, 502, 503,
 &end
#
# 17     THY    H6       16        THY    H1'      4.25     5.19
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 495, r1= 3.75, r2= 4.25, r3= 5.19, r4= 5.69,  &end
#
# 17     THY    H6       16        THY    H3'      3.67     4.49     change
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 511, r1= 3.17, r2= 3.67, r3= 4.99, r4= 5.19,  &end
#
# 17     THY    H4'      16        THY    H6       4.77     5.83
# &rst
#  ixpk= 0, nxpk= 0, iat= 524, 498, r1= 4.27, r2= 4.77, r3= 5.83, r4= 6.33,  &end
#
# 17     THY    H4'      16        THY    H1'      2.98     3.64
 &rst
  ixpk= 0, nxpk= 0, iat= 524, 495, r1= 2.48, r2= 2.98, r3= 3.64, r4= 4.14,  &end
```

```
#
# 17    THY   H6      16      THY   H6      4.38    5.58
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 498, r1= 3.88, r2= 4.38, r3= 5.58, r4= 6.08,  &end
#
# 17    THY   H6      16      THY   H2'     3.51    4.29 change
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 513, r1= 3.01, r2= 3.21, r3= 4.29, r4= 4.79,  &end
#
# 17    THY   H4'     16      THY   H2'     3.11    3.81    change
 &rst
  ixpk= 0, nxpk= 0, iat= 524, 513, r1= 2.61, r2= 3.11, r3= 4.00, r4= 4.31,  &end
#
# 17    THY   M7      16      THY   H1'     4       6
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 495, r1= 3.50, r2= 4.00, r3= 7.21, r4= 7.71,
 igr1= 533, 534, 535,
 &end
#
# 17    THY   M7      16      THY   H2'     4.73    5.79
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 513, r1= 4.23, r2= 4.73, r3= 6.95, r4= 7.45,
 igr1= 533, 534, 535,
 &end
#
# 17    THY   M7      16      THY   H2'2    4.34    5.3
 &rst
```

```
 ixpk= 0, nxpk= 0, iat=  -1, 514, r1= 3.84, r2= 4.34, r3= 6.36, r4= 6.86,
igr1= 533, 534, 535,
 &end
#
# 17    THY   H6      17      THY   H1'     2.7     3.3      change
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 527, r1= 2.20, r2= 2.70, r3= 3.50, r4= 3.80,  &end
#
# 17    THY   H6      17      THY   H4'     3.72    4.54
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 524, r1= 3.22, r2= 3.72, r3= 4.54, r4= 5.04,  &end
#
# 17    THY   H5'     17      THY   H6      4.89    5.97
# &rst
#  ixpk= 0, nxpk= 0, iat= 521, 530, r1= 4.39, r2= 4.89, r3= 5.97, r4= 6.47,  &end
#
# 17    THY   H1'     17      THY   H4'     2.93    3.57
 &rst
  ixpk= 0, nxpk= 0, iat= 527, 524, r1= 2.43, r2= 2.93, r3= 3.57, r4= 4.07,  &end
#
# 17    THY   H3'     17      THY   H1'     3.56    4.36
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 527, r1= 3.06, r2= 3.56, r3= 4.36, r4= 4.86,  &end
#
# 18    GUA   H8      17      THY   H1'     5.11    6.25
 &rst
  ixpk= 0, nxpk= 0, iat= 562, 527, r1= 4.61, r2= 5.11, r3= 6.25, r4= 6.75,  &end
```

```
#
# 18    GUA   H8      17      THY   H3'     4.41    5.39
 &rst
  ixpk= 0, nxpk= 0, iat= 562, 543, r1= 3.91, r2= 4.41, r3= 5.39, r4= 5.89,  &end
#
# 18    GUA   H8      17      THY   H6      5.13    6.27
 &rst
  ixpk= 0, nxpk= 0, iat= 562, 530, r1= 4.63, r2= 5.13, r3= 6.27, r4= 6.77,  &end
#
# 18    GUA   H8      17      THY   H2'     4.31    5.27 change
 &rst
  ixpk= 0, nxpk= 0, iat= 562, 545, r1= 3.81, r2= 4.21, r3= 5.27, r4= 5.77,  &end
#
# 18    GUA   H4'     18      GUA   H8      4.83    6.17
 &rst
  ixpk= 0, nxpk= 0, iat= 556, 562, r1= 4.33, r2= 4.83, r3= 6.17, r4= 6.67,  &end
#
# 18    GUA   H8      18      GUA   H5'2    5.19    6.35
 &rst
  ixpk= 0, nxpk= 0, iat= 562, 554, r1= 4.69, r2= 5.19, r3= 6.35, r4= 6.85,  &end
#
# 18    GUA   H5'     18      GUA   H8      4.39    5.37
 &rst
  ixpk= 0, nxpk= 0, iat= 553, 562, r1= 3.89, r2= 4.39, r3= 5.37, r4= 5.87,  &end
#
# 18    GUA   H4'     18      GUA   H1'     3.05    3.73    change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 556, 559, r1= 2.55, r2= 2.80, r3= 3.73, r4= 4.23,  &end
#
# 19     THY    H6       18       GUA    H8       3.97     5.03     change
 &rst
  ixpk= 0, nxpk= 0, iat= 595, 562, r1= 3.47, r2= 3.97, r3= 5.23, r4= 5.53,  &end
#
# 19     THY    M7       18       GUA    H8       3.43     4.19
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 562, r1= 2.93, r2= 3.43, r3= 5.03, r4= 5.53,
 igr1= 598, 599, 600,
 &end
#
# 19     THY    M7       18       GUA    H1'      3.65     4.47
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 559, r1= 3.15, r2= 3.65, r3= 5.37, r4= 5.87,
 igr1= 598, 599, 600,
 &end
#
# 19     THY    H6       19       THY    H1'      3.03     3.71
 &rst
  ixpk= 0, nxpk= 0, iat= 595, 592, r1= 2.53, r2= 3.03, r3= 3.71, r4= 4.21,  &end
#
# 19     THY    H4'      19       THY    H6       4.69     5.73     change
 &rst
  ixpk= 0, nxpk= 0, iat= 589, 595, r1= 4.19, r2= 4.39, r3= 5.13, r4= 6.23,  &end
#
# 19     THY    H4'      19       THY    H1'      2.72     3.28
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 589, 592, r1= 2.22, r2= 2.72, r3= 3.28, r4= 3.78,  &end
#
# 19     THY    H3'      19       THY    H1'      3.38     4.14
 &rst
  ixpk= 0, nxpk= 0, iat= 608, 592, r1= 2.88, r2= 3.38, r3= 4.14, r4= 4.64,  &end
#
# 19     THY    M7       19       THY    H1'      5.79     7.07
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 592, r1= 5.29, r2= 5.79, r3= 8.49, r4= 8.99,
 igr1= 598, 599, 600,
 &end
#
# 19     THY    H2'      19       THY    M7       3.75     4.59
 &rst
  ixpk= 0, nxpk= 0, iat= 610,  -1, r1= 3.25, r2= 3.75, r3= 5.51, r4= 6.01,
 igr2= 598, 599, 600,
 &end
#
# 19     THY    H2'2     19       THY    M7       5.11     6.25
 &rst
  ixpk= 0, nxpk= 0, iat= 611,  -1, r1= 4.61, r2= 5.11, r3= 7.51, r4= 8.01,
 igr2= 598, 599, 600,
 &end
#
# 20     CYT    H6       19       THY    H1'      3.68     4.32 change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 627, 592, r1= 3.18, r2= 3.48, r3= 4.32, r4= 4.82,  &end
#
# 20     CYT    H6       19       THY    H3'      4        4.88
 &rst
  ixpk= 0, nxpk= 0, iat= 627, 608, r1= 3.50, r2= 4.00, r3= 4.88, r4= 5.38,  &end
#
# 20     CYT    H6       19       THY    M7       5.67     6.93
 &rst
  ixpk= 0, nxpk= 0, iat= 627,  -1, r1= 5.17, r2= 5.67, r3= 8.32, r4= 8.82,
 igr2= 598, 599, 600,
 &end
#
# 20     CYT    H5       20       CYT    H6       2.1      2.56
 &rst
  ixpk= 0, nxpk= 0, iat= 629, 627, r1= 1.60, r2= 2.10, r3= 2.56, r4= 3.06,  &end
#
# 20     CYT    H3'      20       CYT    H1'      3.57     4.53
 &rst
  ixpk= 0, nxpk= 0, iat= 638, 624, r1= 3.07, r2= 3.57, r3= 4.53, r4= 5.03,  &end
#
# 21     CYT    H6       20       CYT    H1'      4.13     5.05
 &rst
  ixpk= 0, nxpk= 0, iat= 657, 624, r1= 3.63, r2= 4.13, r3= 5.05, r4= 5.55,  &end
#
# 21     CYT    H5       20       CYT    H5       5.14     6.28
 &rst
  ixpk= 0, nxpk= 0, iat= 659, 629, r1= 4.64, r2= 5.14, r3= 6.28, r4= 6.78,  &end
```

```
#
# 21     CYT    H1'      20       CYT    H1'      5.23     6.39
 &rst
  ixpk= 0, nxpk= 0, iat= 654, 624, r1= 4.73, r2= 5.23, r3= 6.39, r4= 6.89,  &end
#
# 21     CYT    H6       21       CYT    H1'      3.72     4.54
 &rst
  ixpk= 0, nxpk= 0, iat= 657, 654, r1= 3.22, r2= 3.72, r3= 4.54, r4= 5.04,  &end
#
# 21     CYT    H3'      21       CYT    H6       2.66     3.26     change
# &rst
#  ixpk= 0, nxpk= 0, iat= 668, 657, r1= 2.16, r2= 2.66, r3= 3.56, r4= 3.76,  &end
#
# 21     CYT    H5       21       CYT    H1'      4.31     5.69
 &rst
  ixpk= 0, nxpk= 0, iat= 659, 654, r1= 3.81, r2= 4.31, r3= 5.69, r4= 6.19,  &end
#
# 21     CYT    H2'      21       CYT    H1'      2.51     3.07
 &rst
  ixpk= 0, nxpk= 0, iat= 670, 654, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
# 21     CYT    H2'      21       CYT    H5       3.34     4.08
# &rst
#  ixpk= 0, nxpk= 0, iat= 670, 659, r1= 2.84, r2= 3.34, r3= 4.08, r4= 4.58,  &end
#
# 21     CYT    H3'      21       CYT    H5       4.54     5.46     change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 668, 659, r1= 4.04, r2= 4.74, r3= 5.86, r4= 5.96,  &end
#
# 22     GUA   H8       21       CYT    H1'      3.61     4.39 change
 &rst
  ixpk= 0, nxpk= 0, iat= 687, 654, r1= 3.11, r2= 4.31, r3= 4.59, r4= 4.89,  &end
#
# 22     GUA   H8       21       CYT    H6       4.05     5.15
 &rst
  ixpk= 0, nxpk= 0, iat= 687, 657, r1= 3.55, r2= 3.85, r3= 5.15, r4= 5.65,  &end
#
# 22     GUA   H3'      21       CYT    H5       4.65     5.35     change
 &rst
  ixpk= 0, nxpk= 0, iat= 701, 659, r1= 4.15, r2= 4.95, r3= 5.80, r4= 6.00,  &end
#
# 22     GUA   H8       21       CYT    H2'      3.52     4.3      change
 &rst
  ixpk= 0, nxpk= 0, iat= 687, 670, r1= 3.02, r2= 3.32, r3= 4.30, r4= 4.80,  &end
#
# 22     GUA   H8       22       GUA    H1'      3.1      3.78
 &rst
  ixpk= 0, nxpk= 0, iat= 687, 684, r1= 2.60, r2= 3.10, r3= 3.78, r4= 4.28,  &end
#
# 22     GUA   H3'      22       GUA    H8       2.11     2.89
 &rst
  ixpk= 0, nxpk= 0, iat= 701, 687, r1= 1.61, r2= 2.11, r3= 2.89, r4= 3.39,  &end
#
# 22     GUA   H4'      22       GUA    H8       4.35     5.65
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 681, 687, r1= 3.85, r2= 4.35, r3= 5.65, r4= 6.15,  &end
#
# 22     GUA   H3'      22       GUA   H1'      3.42     4.18
 &rst
  ixpk= 0, nxpk= 0, iat= 701, 684, r1= 2.92, r2= 3.42, r3= 4.18, r4= 4.68,  &end
#
# 22     GUA   H4'      22       GUA   H3'      2.4      2.94     change
 &rst
  ixpk= 0, nxpk= 0, iat= 681, 701, r1= 1.90, r2= 2.70, r3= 3.14, r4= 3.44,  &end
#
# 1      CYT   H2'      1        CYT   H6       2.19     2.67
 &rst
  ixpk= 0, nxpk= 0, iat=  26,  13, r1= 1.69, r2= 2.19, r3= 2.67, r4= 3.17,
&end
#
# 3      GUA   H1'      3        GUA   H2"      2.14     2.62
 &rst
  ixpk= 0, nxpk= 0, iat=  73,  93, r1= 1.64, r2= 2.14, r3= 2.62, r4= 3.12,  &end
#
# 5      CYT   H2"      5        CYT   H6       2.42     2.96     change
 &rst
  ixpk= 0, nxpk= 0, iat= 155, 141, r1= 1.92, r2= 2.72, r3= 3.20, r4= 3.46,  &end
#
# 5      CYT   H2'      5        CYT   H1'      2.51     3.07
 &rst
  ixpk= 0, nxpk= 0, iat= 154, 138, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
```

```
#
# 6      N1R    H2'      6        N1R    H8      2.1      2.56
 &rst
  ixpk= 0, nxpk= 0, iat= 170, 195, r1= 1.60, r2= 2.10, r3= 2.56, r4= 3.06,  &end
#
# 7      ADE    H1'      6        N1R    H2"     4.09     4.99
 &rst
  ixpk= 0, nxpk= 0, iat= 210, 171, r1= 3.59, r2= 4.09, r3= 4.99, r4= 5.49,  &end
#
# 8      GUA    H8       7        ADE    H2      5.73     7.01
 &rst
  ixpk= 0, nxpk= 0, iat= 245, 222, r1= 5.23, r2= 5.73, r3= 7.01, r4= 7.51,  &end
#
# 9      ADE    H8       9        ADE    H1'     3.26     3.94
 &rst
  ixpk= 0, nxpk= 0, iat= 278, 275, r1= 2.76, r2= 3.26, r3= 3.94, r4= 4.44,  &end
#
# 10     ADE    H8       10       ADE    H1'     3.49     4.27
 &rst
  ixpk= 0, nxpk= 0, iat= 310, 307, r1= 2.99, r2= 3.49, r3= 4.27, r4= 4.77,  &end
#
# 10     ADE    H2"      10       ADE    H1'     2.08     2.54
 &rst
  ixpk= 0, nxpk= 0, iat= 326, 307, r1= 1.58, r2= 2.08, r3= 2.54, r4= 3.04,  &end
#
# 11     GUA    H5"      11       GUA    H3'     2.51     3.07
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 334, 356, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
# 11     GUA   H5'      11       GUA   H3'      3.21     3.79
 &rst
  ixpk= 0, nxpk= 0, iat= 333, 356, r1= 2.71, r2= 3.21, r3= 3.79, r4= 4.29,  &end
#
# 12     CYT   H4'      12       CYT   H1'      2.93     3.47
 &rst
  ixpk= 0, nxpk= 0, iat= 368, 371, r1= 2.43, r2= 2.93, r3= 3.47, r4= 3.97,  &end
#
# 12     CYT   H2'      12       CYT   H1'      2.21     2.71
# &rst
#  ixpk= 0, nxpk= 0, iat= 387, 371, r1= 1.71, r2= 2.21, r3= 2.71, r4= 3.21,  &end
#
# 15     CYT   H5       14       THY   H2'      3.56     4.36
 &rst
  ixpk= 0, nxpk= 0, iat= 470, 451, r1= 3.06, r2= 3.56, r3= 4.36, r4= 4.86,  &end
#
# 15     CYT   H3'      15       CYT   H6       2.93     3.59
 &rst
  ixpk= 0, nxpk= 0, iat= 479, 468, r1= 2.43, r2= 2.93, r3= 3.59, r4= 4.09,  &end
#
# 16     THY   H6       15       CYT   H2'      3        3.8
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 481, r1= 2.50, r2= 3.00, r3= 3.80, r4= 4.30,  &end
#
# 16     THY   M7       15       CYT   H6       4.39     5.21
```

```
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 468, r1= 3.89, r2= 4.39, r3= 6.26, r4= 6.76,
 igr1= 501, 502, 503,
 &end
#
# 16     THY    M7       15        CYT    H2"      4.32     5.28
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 482, r1= 3.82, r2= 4.32, r3= 6.34, r4= 6.84,
 igr1= 501, 502, 503,
 &end
#
# 16     THY    H4'      16        THY    H1'      3.27     4.13
 &rst
  ixpk= 0, nxpk= 0, iat= 492, 495, r1= 2.77, r2= 3.27, r3= 4.13, r4= 4.63,  &end
#
# 16     THY    M7       16        THY    H6       2.25     2.75
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 498, r1= 1.75, r2= 2.25, r3= 3.30, r4= 3.80,
 igr1= 501, 502, 503,
 &end
#
# 16     THY    H2"      16        THY    M7       2.9      5.3
 &rst
  ixpk= 0, nxpk= 0, iat= 514,  -1, r1= 2.40, r2= 2.90, r3= 6.36, r4= 6.86,
 igr2= 501, 502, 503,
 &end
#
```

```
# 17     THY    H4'      16       THY    H1'      2.98     3.64
 &rst
  ixpk= 0, nxpk= 0, iat= 524, 495, r1= 2.48, r2= 2.98, r3= 3.64, r4= 4.14,  &end
#
# 17     THY    M7       16       THY    H6       4.12     5.04
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 498, r1= 3.62, r2= 4.12, r3= 6.05, r4= 6.55,
 igr1= 533, 534, 535,
 &end
#
# 17     THY    H3'      17       THY    H6       2.84     3.48     change
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 530, r1= 2.34, r2= 2.94, r3= 3.78, r4= 3.98,  &end
#
# 17     THY    M7       17       THY    H6       3        3.66
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 530, r1= 2.50, r2= 3.00, r3= 4.40, r4= 4.90,
 igr1= 533, 534, 535,
 &end
#
# 17     THY    H2''     17       THY    H2'      2.15     2.63
# &rst
#  ixpk= 0, nxpk= 0, iat= 546, 545, r1= 1.65, r2= 2.15, r3= 2.63, r4= 3.13,  &end
#
# 17     THY    H2''     17       THY    M7       5.22     6.38
 &rst
  ixpk= 0, nxpk= 0, iat= 546,  -1, r1= 4.72, r2= 5.22, r3= 7.66, r4= 8.16,
```

```
 igr2= 533, 534, 535,
 &end
#
# 17    THY   H2'     17      THY   M7     2.02    4.42
 &rst
  ixpk= 0, nxpk= 0, iat= 545,  -1, r1= 1.52, r2= 2.02, r3= 5.31, r4= 5.81,
 igr2= 533, 534, 535,
 &end
#
# 18    GUA   H8      18      GUA   H1'    3.67    4.49
 &rst
  ixpk= 0, nxpk= 0, iat= 562, 559, r1= 3.17, r2= 3.67, r3= 4.49, r4= 4.99,  &end
#
# 19    THY   H6      18      GUA   H1'    3.25    3.95
 &rst
  ixpk= 0, nxpk= 0, iat= 595, 559, r1= 2.75, r2= 3.25, r3= 3.95, r4= 4.45,  &end
#
# 19    THY   H3'     19      THY   H6     2.93    3.57    change
 &rst
  ixpk= 0, nxpk= 0, iat= 608, 595, r1= 2.43, r2= 3.13, r3= 3.97, r4= 4.17,  &end
#
# 19    THY   H5''    19      THY   H6     4.78    5.84
 &rst
  ixpk= 0, nxpk= 0, iat= 587, 595, r1= 4.28, r2= 4.78, r3= 5.84, r4= 6.34,  &end
#
# 19    THY   H6      19      THY   H5'    3.58    4.62
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 595, 586, r1= 3.08, r2= 3.58, r3= 4.62, r4= 5.12,  &end
#
# 19     THY    H1'      19       THY    H5'      3.72     4.28     change
 &rst
  ixpk= 0, nxpk= 0, iat= 592, 586, r1= 3.22, r2= 3.72, r3= 4.48, r4= 4.78,  &end
#
# 19     THY    H2'      19       THY    H6       3.19     3.89
# &rst
#  ixpk= 0, nxpk= 0, iat= 610, 595, r1= 2.69, r2= 3.19, r3= 3.89, r4= 4.39,  &end
#
# 19     THY    H2''     19       THY    H1'      2.14     2.62
 &rst
  ixpk= 0, nxpk= 0, iat= 611, 592, r1= 1.64, r2= 2.14, r3= 2.62, r4= 3.12,  &end
#
# 19     THY    M7       19       THY    H6       2.66     3.26
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 595, r1= 2.16, r2= 2.66, r3= 3.92, r4= 4.42,
 igr1= 598, 599, 600,
 &end
#
# 19     THY    H4'      19       THY    H2'      3.72     4.68
 &rst
  ixpk= 0, nxpk= 0, iat= 589, 610, r1= 3.22, r2= 3.72, r3= 4.68, r4= 5.18,  &end
#
# 20     CYT    H6       19       THY    H6       3.57     4.43 change
 &rst
  ixpk= 0, nxpk= 0, iat= 627, 595, r1= 3.07, r2= 3.77, r3= 4.63, r4= 4.93,  &end
```

```
#
# 20     CYT    H6       20       CYT    H1'      3.22     3.78
 &rst
  ixpk= 0, nxpk= 0, iat= 627, 624, r1= 2.72, r2= 3.22, r3= 3.78, r4= 4.28,  &end
#
# 21     CYT    H5       20       CYT    H1'      4.6      5.4       change
 &rst
  ixpk= 0, nxpk= 0, iat= 659, 624, r1= 4.10, r2= 4.80, r3= 5.60, r4= 5.90,  &end
#
# 21     CYT    H5       20       CYT    H2'      3.1      3.9
 &rst
  ixpk= 0, nxpk= 0, iat= 659, 640, r1= 2.60, r2= 3.10, r3= 3.90, r4= 4.40,  &end
#
# 21     CYT    H5       20       CYT    H2"      2.99     3.65
 &rst
  ixpk= 0, nxpk= 0, iat= 659, 641, r1= 2.49, r2= 2.99, r3= 3.65, r4= 4.15,  &end
#
# 21     CYT    H5       21       CYT    H6       2.22     2.72
 &rst
  ixpk= 0, nxpk= 0, iat= 659, 657, r1= 1.72, r2= 2.22, r3= 2.72, r4= 3.22,  &end
#
# 21     CYT    H6       21       CYT    H5"      5        6.12      change
 &rst
  ixpk= 0, nxpk= 0, iat= 657, 649, r1= 4.50, r2= 4.80, r3= 5.72, r4= 6.62,  &end
#
# 21     CYT    H2"      21       CYT    H1'      2.24     2.76
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 671, 654, r1= 1.74, r2= 2.24, r3= 2.76, r4= 3.26,  &end
#
# 21     CYT    H3'      21       CYT    H2''     2.63     3.21
 &rst
  ixpk= 0, nxpk= 0, iat= 668, 671, r1= 2.13, r2= 2.63, r3= 3.21, r4= 3.71,  &end
#
# 22     GUA    H8       21       CYT    H3'      5.3      6.48
 &rst
  ixpk= 0, nxpk= 0, iat= 687, 668, r1= 4.80, r2= 5.30, r3= 6.48, r4= 6.98,  &end
#
# 22     GUA    H5'      22       GUA    H8       4.16     5.08     change
 &rst
  ixpk= 0, nxpk= 0, iat= 678, 687, r1= 3.66, r2= 4.56, r3= 5.28, r4= 5.58,  &end
#
# 1      CYT    H1'      1        CYT    H2'      2.86     3.5
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  26, r1= 2.36, r2= 2.86, r3= 3.50, r4= 4.00,
&end
#
# 2      GUA    H2'      2        GUA    H8       2.31     2.83
 &rst
  ixpk= 0, nxpk= 0, iat=  59,  43, r1= 1.81, r2= 2.31, r3= 2.83, r4= 3.33,  &end
#
# 2      GUA    H1'      2        GUA    H5'      4.41     5.59
 &rst
  ixpk= 0, nxpk= 0, iat=  40,  34, r1= 3.91, r2= 4.41, r3= 5.59, r4= 6.09,  &end
#
```

```
# 4      ADE   H8      3        GUA   H3'     4.44    5.56
 &rst
  ixpk= 0, nxpk= 0, iat= 109,  90, r1= 3.94, r2= 4.44, r3= 5.56, r4= 6.06,  &end
#
# 4      ADE   H3'     4        ADE   H8      3.9     4.5
 &rst
  ixpk= 0, nxpk= 0, iat= 122, 109, r1= 3.40, r2= 3.90, r3= 4.50, r4= 5.00,  &end
#
# 5      CYT   H5      4        ADE   H8      3.11    3.81
 &rst
  ixpk= 0, nxpk= 0, iat= 143, 109, r1= 2.61, r2= 3.11, r3= 3.81, r4= 4.31,  &end
#
# 5      CYT   H2'     5        CYT   H6      1.93    2.47
 &rst
  ixpk= 0, nxpk= 0, iat= 154, 141, r1= 1.43, r2= 1.93, r3= 2.47, r4= 2.97,  &end
#
# 5      CYT   H3'     5        CYT   H2'     2.14    2.66
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 154, r1= 1.64, r2= 2.14, r3= 2.66, r4= 3.16,  &end
#
# 5      CYT   H2''    5        CYT   H2'     1.76    2.24
 &rst
  ixpk= 0, nxpk= 0, iat= 155, 154, r1= 1.26, r2= 1.76, r3= 2.24, r4= 2.74,  &end
#
# 6      N1R   H2'     6        N1R   HAA     2.11    2.57
# &rst
#  ixpk= 0, nxpk= 0, iat= 170, 168, r1= 1.61, r2= 2.11, r3= 2.57, r4= 3.07,  &end
```

```
#
# 9      ADE   H3'     9        ADE   H8      3.52    4.3
 &rst
  ixpk= 0, nxpk= 0, iat= 291, 278, r1= 3.02, r2= 3.52, r3= 4.30, r4= 4.80,  &end
#
# 9      ADE   H5'     9        ADE   H8      4.01    4.91
 &rst
  ixpk= 0, nxpk= 0, iat= 269, 278, r1= 3.51, r2= 4.01, r3= 4.91, r4= 5.41,  &end
#
# 9      ADE   H2"     9        ADE   H1'     2.1     2.56
 &rst
  ixpk= 0, nxpk= 0, iat= 294, 275, r1= 1.60, r2= 2.10, r3= 2.56, r4= 3.06,  &end
#
# 9      ADE   H2"     9        ADE   H1'     2.1     2.56
 &rst
  ixpk= 0, nxpk= 0, iat= 294, 275, r1= 1.60, r2= 2.10, r3= 2.56, r4= 3.06,  &end
#
# 10     ADE   H8      9        ADE   H3'     4.23    5.17
 &rst
  ixpk= 0, nxpk= 0, iat= 310, 291, r1= 3.73, r2= 4.23, r3= 5.17, r4= 5.67,  &end
#
# 10     ADE   H8      9        ADE   H2"     2.06    2.54
 &rst
  ixpk= 0, nxpk= 0, iat= 310, 294, r1= 1.56, r2= 2.06, r3= 2.54, r4= 3.04,  &end
#
# 10     ADE   H3'     10       ADE   H8      3.65    4.47
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 323, 310, r1= 3.15, r2= 3.65, r3= 4.47, r4= 4.97,  &end
#
# 10     ADE    H2'      10       ADE    H8       2.26     2.76
 &rst
  ixpk= 0, nxpk= 0, iat= 325, 310, r1= 1.76, r2= 2.26, r3= 2.76, r4= 3.26,  &end
#
# 11     GUA    H1'      11       GUA    H2'      2.58     3.16
 &rst
  ixpk= 0, nxpk= 0, iat= 339, 358, r1= 2.08, r2= 2.58, r3= 3.16, r4= 3.66,  &end
#
# 12     CYT    H5"      12       CYT    H6       3.76     4.6
 &rst
  ixpk= 0, nxpk= 0, iat= 366, 374, r1= 3.26, r2= 3.76, r3= 4.60, r4= 5.10,  &end
#
# 12     CYT    H5'      12       CYT    H6       4.21     5.15
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 374, r1= 3.71, r2= 4.21, r3= 5.15, r4= 5.65,  &end
#
# 12     CYT    H5'      12       CYT    H3'      2.9      3.5      change
 &rst
  ixpk= 0, nxpk= 0, iat= 365, 385, r1= 2.40, r2= 3.20, r3= 3.80, r4= 4.00,  &end
#
# 12     CYT    H5"      12       CYT    H3'      2.65     3.25
 &rst
  ixpk= 0, nxpk= 0, iat= 366, 385, r1= 2.15, r2= 2.65, r3= 3.25, r4= 3.75,  &end
#
# 12     CYT    H2"      12       CYT    H6       3.15     3.85
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 388, 374, r1= 2.65, r2= 3.15, r3= 3.85, r4= 4.35,  &end
#
# 12     CYT    H2"      12       CYT    H6       3.44     4.2
 &rst
  ixpk= 0, nxpk= 0, iat= 388, 374, r1= 2.94, r2= 3.44, r3= 4.20, r4= 4.70,  &end
#
# 12     CYT    H3'      12       CYT    H2"      3.01     3.67
 &rst
  ixpk= 0, nxpk= 0, iat= 385, 388, r1= 2.51, r2= 3.01, r3= 3.67, r4= 4.17,  &end
#
# 13     THY    H6       12       CYT    H2'      2.91     3.55
 &rst
  ixpk= 0, nxpk= 0, iat= 404, 387, r1= 2.41, r2= 2.91, r3= 3.55, r4= 4.05,  &end
#
# 13     THY    M7       13       THY    H6       0.86     3.26
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 404, r1= 0.36, r2= 0.86, r3= 3.92, r4= 4.42,
 igr1= 407, 408, 409,
 &end
#
# 14     THY    H6       13       THY    H1'      3.44     4.2
 &rst
  ixpk= 0, nxpk= 0, iat= 436, 401, r1= 2.94, r2= 3.44, r3= 4.20, r4= 4.70,  &end
#
# 14     THY    H6       13       THY    H2'      3.15     3.85
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 436, 419, r1= 2.65, r2= 3.15, r3= 3.85, r4= 4.35,  &end
#
# 14     THY    H6       14       THY    H1'      3.55     4.35
 &rst
  ixpk= 0, nxpk= 0, iat= 436, 433, r1= 3.05, r2= 3.55, r3= 4.35, r4= 4.85,  &end
#
# 14     THY    H6       14       THY    H4'      4.5      5.5
 &rst
  ixpk= 0, nxpk= 0, iat= 436, 430, r1= 4.00, r2= 4.50, r3= 5.50, r4= 6.00,  &end
#
# 14     THY    H5"      14       THY    H6       4.9      6.1       change
 &rst
  ixpk= 0, nxpk= 0, iat= 428, 436, r1= 4.40, r2= 4.90, r3= 5.50, r4= 6.60,  &end
#
# 14     THY    H5'      14       THY    H6       3.96     5.04
 &rst
  ixpk= 0, nxpk= 0, iat= 427, 436, r1= 3.46, r2= 3.96, r3= 5.04, r4= 5.54,  &end
#
# 14     THY    H2'      14       THY    H6       2.42     2.96
 &rst
  ixpk= 0, nxpk= 0, iat= 451, 436, r1= 1.92, r2= 2.42, r3= 2.96, r4= 3.46,  &end
#
# 14     THY    M7       14       THY    H6       2.17     2.65
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 436, r1= 1.67, r2= 2.17, r3= 3.18, r4= 3.68,
 igr1= 439, 440, 441,
 &end
```

```
#
# 15    CYT   H5      14      THY   H1'     4.82    5.88
 &rst
  ixpk= 0, nxpk= 0, iat= 470, 433, r1= 4.32, r2= 4.82, r3= 5.88, r4= 6.38,  &end
#
# 15    CYT   H6      14      THY   H2"     3       3.66    change
 &rst
  ixpk= 0, nxpk= 0, iat= 468, 452, r1= 2.50, r2= 2.80, r3= 3.46, r4= 4.16,  &end
#
# 15    CYT   H4'     15      CYT   H6      4.77    5.83
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 468, r1= 4.27, r2= 4.77, r3= 5.83, r4= 6.33,  &end
#
# 15    CYT   H5'     15      CYT   H6      4.11    5.03
 &rst
  ixpk= 0, nxpk= 0, iat= 459, 468, r1= 3.61, r2= 4.11, r3= 5.03, r4= 5.53,  &end
#
# 15    CYT   H5"     15      CYT   H6      4.51    5.51
 &rst
  ixpk= 0, nxpk= 0, iat= 460, 468, r1= 4.01, r2= 4.51, r3= 5.51, r4= 6.01,  &end
#
# 15    CYT   H2'     15      CYT   H1'     2.33    2.85
 &rst
  ixpk= 0, nxpk= 0, iat= 481, 465, r1= 1.83, r2= 2.33, r3= 2.85, r4= 3.35,  &end
#
# 16    THY   H5'     15      CYT   H1'     2.5     3.1     change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 489, 465, r1= 2.00, r2= 2.70, r3= 3.30, r4= 3.60,  &end
#
# 16     THY    H6       15       CYT    H6       4.41     5.19     change
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 468, r1= 3.91, r2= 4.61, r3= 5.39, r4= 5.69,  &end
#
# 16     THY    H3'      16       THY    H6       2.76     3.38     change
 &rst
  ixpk= 0, nxpk= 0, iat= 511, 498, r1= 2.26, r2= 2.46, r3= 3.18, r4= 3.88,  &end
#
# 16     THY    H6       16       THY    H5'      4.27     5.21
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 489, r1= 3.77, r2= 4.27, r3= 5.21, r4= 5.71,  &end
#
# 16     THY    H3'      16       THY    H1'      3.8      4.64
 &rst
  ixpk= 0, nxpk= 0, iat= 511, 495, r1= 3.30, r2= 3.80, r3= 4.64, r4= 5.14,  &end
#
# 16     THY    H2''     16       THY    H6       3.12     3.88
 &rst
  ixpk= 0, nxpk= 0, iat= 514, 498, r1= 2.62, r2= 3.12, r3= 3.88, r4= 4.38,  &end
#
# 16     THY    H3'      16       THY    H2''     2.4      3
 &rst
  ixpk= 0, nxpk= 0, iat= 511, 514, r1= 1.90, r2= 2.40, r3= 3.00, r4= 3.50,  &end
#
# 16     THY    H2''     16       THY    H1'      2.46     3
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 514, 495, r1= 1.96, r2= 2.16, r3= 2.80, r4= 3.50,  &end
#
# 17     THY    H2"      17       THY    H6       2.94     3.6
# &rst
#  ixpk= 0, nxpk= 0, iat= 546, 530, r1= 2.44, r2= 2.94, r3= 3.60, r4= 4.10,  &end
#
# 17     THY    H2'      17       THY    H6       2.66     3.26     change
 &rst
  ixpk= 0, nxpk= 0, iat= 545, 530, r1= 2.16, r2= 2.56, r3= 3.26, r4= 3.76,  &end
#
# 17     THY    H3'      17       THY    H2"      2.9      3.54     change
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 546, r1= 2.40, r2= 2.70, r3= 3.24, r4= 4.04,  &end
#
# 17     THY    H2"      17       THY    H1'      2.46     3
 &rst
  ixpk= 0, nxpk= 0, iat= 546, 527, r1= 1.96, r2= 2.46, r3= 3.00, r4= 3.50,  &end
#
# 19     THY    H6       18       GUA    H2'      3.13     3.87
# &rst
#  ixpk= 0, nxpk= 0, iat= 595, 578, r1= 2.63, r2= 3.13, r3= 3.87, r4= 4.37,  &end
#
# 19     THY    H6       18       GUA    H2'      3.15     3.85     change
# &rst
#  ixpk= 0, nxpk= 0, iat= 595, 578, r1= 2.65, r2= 3.15, r3= 4.15, r4= 4.35,  &end
#
```

```
# 19    THY   M7     18      GUA   H2'     3.15    3.85
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 578, r1= 2.65, r2= 3.15, r3= 4.62, r4= 5.12,
 igr1= 598, 599, 600,
 &end
#
# 19    THY   M7     18      GUA   H2''    3.09    3.77    change
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 579, r1= 2.59, r2= 2.79, r3= 3.53, r4= 5.03,
 igr1= 598, 599, 600,
 &end
#
# 19    THY   H2'    19      THY   H1'     2.53    3.09
 &rst
  ixpk= 0, nxpk= 0, iat= 610, 592, r1= 2.03, r2= 2.53, r3= 3.09, r4= 3.59,  &end
#
# 19    THY   H3'    19      THY   H2'     2.03    2.57
 &rst
  ixpk= 0, nxpk= 0, iat= 608, 610, r1= 1.53, r2= 2.03, r3= 2.57, r4= 3.07,  &end
#
# 20    CYT   H3'    20      CYT   H6      3.27    3.93
 &rst
  ixpk= 0, nxpk= 0, iat= 638, 627, r1= 2.77, r2= 3.27, r3= 3.93, r4= 4.43,  &end
#
# 21    CYT   H2'    21      CYT   H6      2.22    2.78    change
 &rst
  ixpk= 0, nxpk= 0, iat= 670, 657, r1= 1.72, r2= 2.02, r3= 2.78, r4= 3.28,  &end
```

```
#
# 21    CYT   H3'     21      CYT   H2'     2.22    2.78    change
 &rst
  ixpk= 0, nxpk= 0, iat= 668, 670, r1= 1.72, r2= 2.02, r3= 2.78, r4= 3.28,  &end
#
# 21    CYT   H4'     21      CYT   H2'     4.01    4.99    change
 &rst
  ixpk= 0, nxpk= 0, iat= 651, 670, r1= 3.51, r2= 3.81, r3= 4.69, r4= 5.49,  &end
#
# 22    GUA   H5"     22      GUA   H8      5.4     6.6
 &rst
  ixpk= 0, nxpk= 0, iat= 679, 687, r1= 4.90, r2= 5.40, r3= 6.60, r4= 7.10,  &end
#
# 22    GUA   H5'     22      GUA   H1'     3.92    4.48
 &rst
  ixpk= 0, nxpk= 0, iat= 678, 684, r1= 3.42, r2= 3.92, r3= 4.48, r4= 4.98,  &end
#
# 22    GUA   H3'     22      GUA   H2'     2.35    2.87
 &rst
  ixpk= 0, nxpk= 0, iat= 701, 703, r1= 1.85, r2= 2.35, r3= 2.87, r4= 3.37,  &end
#
# 22    GUA   H2"     22      GUA   H8      3.04    3.72
 &rst
  ixpk= 0, nxpk= 0, iat= 704, 687, r1= 2.54, r2= 3.04, r3= 3.72, r4= 4.22,  &end
#
# 1     CYT   H5      1       CYT   H6      2.14    2.62
 &rst
```

```
  ixpk= 0, nxpk= 0, iat=  15,  13, r1= 1.64, r2= 2.14, r3= 2.62, r4= 3.12,
&end
#
# 1      CYT    H2'      1         CYT    H6       2.29     2.79
 &rst
  ixpk= 0, nxpk= 0, iat=  26,  13, r1= 1.79, r2= 2.29, r3= 2.79, r4= 3.29,  &end
#
# 2      GUA    H3'      2         GUA    H2'      2.29     2.79
 &rst
  ixpk= 0, nxpk= 0, iat=  57,  59, r1= 1.79, r2= 2.29, r3= 2.79, r4= 3.29,  &end
#
# 5      CYT    H2"      5         CYT    H1'      2.26     2.76
 &rst
  ixpk= 0, nxpk= 0, iat= 155, 138, r1= 1.76, r2= 2.26, r3= 2.76, r4= 3.26,  &end
#
# 5      CYT    H3'      5         CYT    H2"      2.38     2.92
 &rst
  ixpk= 0, nxpk= 0, iat= 152, 155, r1= 1.88, r2= 2.38, r3= 2.92, r4= 3.42,  &end
#
# 6      N1R    H2"      6         N1R    H8       2.92     3.56
 &rst
  ixpk= 0, nxpk= 0, iat= 171, 195, r1= 2.42, r2= 2.92, r3= 3.56, r4= 4.06,  &end
#
# 8      GUA    H2'      8         GUA    H1'      2.66     3.26
 &rst
  ixpk= 0, nxpk= 0, iat= 261, 242, r1= 2.16, r2= 2.66, r3= 3.26, r4= 3.76,  &end
#
```

```
# 8      GUA   H2''     8        GUA   H1'     2.19    2.67
 &rst
  ixpk= 0, nxpk= 0, iat= 262, 242, r1= 1.69, r2= 2.19, r3= 2.67, r4= 3.17,  &end
#
# 9      ADE   H8       8        GUA   H1'     3.46    4.22
 &rst
  ixpk= 0, nxpk= 0, iat= 278, 242, r1= 2.96, r2= 3.46, r3= 4.22, r4= 4.72,  &end
#
# 9      ADE   H4'      9        ADE   H3'     2.21    2.69
 &rst
  ixpk= 0, nxpk= 0, iat= 272, 291, r1= 1.71, r2= 2.21, r3= 2.69, r4= 3.19,  &end
#
# 9      ADE   H2'      9        ADE   H1'     3.1     3.8
 &rst
  ixpk= 0, nxpk= 0, iat= 293, 275, r1= 2.60, r2= 3.10, r3= 3.80, r4= 4.30,  &end
#
# 10     ADE   H2''     10       ADE   H8      3.64    4.36    change
 &rst
  ixpk= 0, nxpk= 0, iat= 326, 310, r1= 3.14, r2= 3.44, r3= 4.16, r4= 4.86,  &end
#
# 12     CYT   H3'      12       CYT   H6      2.51    3.07
# &rst
#  ixpk= 0, nxpk= 0, iat= 385, 374, r1= 2.01, r2= 2.51, r3= 3.07, r4= 3.57,  &end
#
# 12     CYT   H3'      12       CYT   H2'     2.21    2.79
 &rst
  ixpk= 0, nxpk= 0, iat= 385, 387, r1= 1.71, r2= 2.21, r3= 2.79, r4= 3.29,  &end
```

```
#
# 13    THY   H6      12      CYT   H2'     2.81    3.43
 &rst
  ixpk= 0, nxpk= 0, iat= 404, 387, r1= 2.31, r2= 2.81, r3= 3.43, r4= 3.93,  &end
#
# 13    THY   H5''    13      THY   H6      4.99    6.11    change
 &rst
  ixpk= 0, nxpk= 0, iat= 396, 404, r1= 4.49, r2= 4.79, r3= 5.51, r4= 6.61,  &end
#
# 13    THY   H5'     13      THY   H6      4.21    5.15
 &rst
  ixpk= 0, nxpk= 0, iat= 395, 404, r1= 3.71, r2= 4.21, r3= 5.15, r4= 5.65,  &end
#
# 13    THY   H4'     13      THY   H1'     2.68    3.28
 &rst
  ixpk= 0, nxpk= 0, iat= 398, 401, r1= 2.18, r2= 2.68, r3= 3.28, r4= 3.78,  &end
#
# 13    THY   H2''    13      THY   H6      2.72    3.28    change
 &rst
  ixpk= 0, nxpk= 0, iat= 420, 404, r1= 2.22, r2= 2.92, r3= 3.58, r4= 3.78,  &end
#
# 13    THY   H2'     13      THY   H1'     4.22    5.18
# &rst
#  ixpk= 0, nxpk= 0, iat= 419, 401, r1= 3.72, r2= 4.22, r3= 5.18, r4= 5.68,  &end
#
# 15    CYT   H6      14      THY   H2'     2.68    3.28    change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 468, 451, r1= 2.18, r2= 2.78, r3= 3.38, r4= 3.78,  &end
#
# 15     CYT    H5       15       CYT    H6       2.32     2.84
 &rst
  ixpk= 0, nxpk= 0, iat= 470, 468, r1= 1.82, r2= 2.32, r3= 2.84, r4= 3.34,  &end
#
# 15     CYT    H4'      15       CYT    H1'      2.85     3.49     change
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 465, r1= 2.35, r2= 2.65, r3= 3.29, r4= 3.99,  &end
#
# 15     CYT    H4'      15       CYT    H3'      2.74     3.34
 &rst
  ixpk= 0, nxpk= 0, iat= 462, 479, r1= 2.24, r2= 2.74, r3= 3.34, r4= 3.84,  &end
#
# 15     CYT    H2'      15       CYT    H6       2.22     2.78
# &rst
#  ixpk= 0, nxpk= 0, iat= 481, 468, r1= 1.72, r2= 2.22, r3= 2.78, r4= 3.28,  &end
#
# 15     CYT    H3'      15       CYT    H2''     2.47     3.03
 &rst
  ixpk= 0, nxpk= 0, iat= 479, 482, r1= 1.97, r2= 2.47, r3= 3.03, r4= 3.53,  &end
#
# 15     CYT    H3'      15       CYT    H2'      2.11     2.69
 &rst
  ixpk= 0, nxpk= 0, iat= 479, 481, r1= 1.61, r2= 2.11, r3= 2.69, r4= 3.19,  &end
#
# 16     THY    H6       15       CYT    H1'      4.33     5.07     change
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 465, r1= 3.83, r2= 4.53, r3= 5.27, r4= 5.57,  &end
#
# 16     THY    H6       15       CYT    H2'      3.38     4.14
 &rst
  ixpk= 0, nxpk= 0, iat= 498, 481, r1= 2.88, r2= 3.38, r3= 4.14, r4= 4.64,  &end
#
# 16     THY    H2'      16       THY    H1'      2.28     2.78
 &rst
  ixpk= 0, nxpk= 0, iat= 513, 495, r1= 1.78, r2= 2.28, r3= 2.78, r4= 3.28,  &end
#
# 17     THY    H6       16       THY    H2"      2.9      4.9
 &rst
  ixpk= 0, nxpk= 0, iat= 530, 514, r1= 2.40, r2= 2.90, r3= 4.90, r4= 5.40,  &end
#
# 17     THY    H3'      17       THY    H2"      2.79     3.41
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 546, r1= 2.29, r2= 2.79, r3= 3.41, r4= 3.91,  &end
#
# 17     THY    H2'      17       THY    H1'      2.86     3.5
 &rst
  ixpk= 0, nxpk= 0, iat= 545, 527, r1= 2.36, r2= 2.86, r3= 3.50, r4= 4.00,  &end
#
# 19     THY    H2'      19       THY    H6       1.73     2.27     change
 &rst
  ixpk= 0, nxpk= 0, iat= 610, 595, r1= 1.23, r2= 1.93, r3= 2.67, r4= 2.77,  &end
#
```

```
# 19     THY    H3'      19       THY    H2"      2.41     2.95
 &rst
  ixpk= 0, nxpk= 0, iat= 608, 611, r1= 1.91, r2= 2.41, r3= 2.95, r4= 3.45,  &end
#
# 20     CYT    H3'      20       CYT    H2"      2.94     3.6
 &rst
  ixpk= 0, nxpk= 0, iat= 638, 641, r1= 2.44, r2= 2.94, r3= 3.60, r4= 4.10,  &end
#
# 21     CYT    H6       20       CYT    H2'      3.1      3.8
 &rst
  ixpk= 0, nxpk= 0, iat= 657, 640, r1= 2.60, r2= 3.10, r3= 3.80, r4= 4.30,  &end
#
# 21     CYT    H6       20       CYT    H2"      2.79     3.41     change
 &rst
  ixpk= 0, nxpk= 0, iat= 657, 641, r1= 2.29, r2= 2.59, r3= 3.21, r4= 3.91,  &end
#
# 21     CYT    H4'      21       CYT    H1'      2.52     3.08     change
 &rst
  ixpk= 0, nxpk= 0, iat= 651, 654, r1= 2.02, r2= 2.62, r3= 3.28, r4= 3.58,  &end
#
# 22     GUA    H8       21       CYT    H2"      3.56     4.24
 &rst
  ixpk= 0, nxpk= 0, iat= 687, 671, r1= 3.06, r2= 3.56, r3= 4.24, r4= 4.74,  &end
#
# 22     GUA    H3'      22       GUA    H2"      2.54     3.06
 &rst
  ixpk= 0, nxpk= 0, iat= 701, 704, r1= 2.04, r2= 2.54, r3= 3.06, r4= 3.56,  &end
```

```
#
# 1      CYT    H1'      1        CYT    H6      3.3      3.9
 &rst
  ixpk= 0, nxpk= 0, iat=  10,  13, r1= 2.80, r2= 3.30, r3= 3.90, r4= 4.40,
&end
#
# 1      CYT    H3'      1        CYT    H2''     2.27     2.73
 &rst
  ixpk= 0, nxpk= 0, iat=  24,  27, r1= 1.77, r2= 2.27, r3= 2.73, r4= 3.23,  &end
#
# 2      GUA    H8       1        CYT    H3'      4.12     4.88     change
 &rst
  ixpk= 0, nxpk= 0, iat=  43,  24, r1= 3.62, r2= 4.12, r3= 5.28, r4= 5.38,  &end
#
# 4      ADE    H8       3        GUA    H2''     2.45     2.99
 &rst
  ixpk= 0, nxpk= 0, iat= 109,  93, r1= 1.95, r2= 2.45, r3= 2.99, r4= 3.49,  &end
#
# 4      ADE    H8       3        GUA    H2'      3.16     3.86
 &rst
  ixpk= 0, nxpk= 0, iat= 109,  92, r1= 2.66, r2= 3.16, r3= 3.86, r4= 4.36,  &end
#
# 4      ADE    H2''     4        ADE    H8       3.34     4.08
 &rst
  ixpk= 0, nxpk= 0, iat= 125, 109, r1= 2.84, r2= 3.34, r3= 4.08, r4= 4.58,  &end
#
# 4      ADE    H2''     4        ADE    H8       3.2      3.9
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 125, 109, r1= 2.70, r2= 3.20, r3= 3.90, r4= 4.40,  &end
#
# 7      ADE   H8      6       N1R   H2"     0.95    3.55
 &rst
  ixpk= 0, nxpk= 0, iat= 213, 171, r1= 0.45, r2= 0.95, r3= 3.55, r4= 4.05,  &end
#
# 9      ADE   H5"     9       ADE   H3'     1.85    2.25    change
 &rst
  ixpk= 0, nxpk= 0, iat= 270, 291, r1= 1.35, r2= 1.85, r3= 2.55, r4= 2.75,  &end
#
# 9      ADE   H2"     9       ADE   H8      4.02    4.98
 &rst
  ixpk= 0, nxpk= 0, iat= 294, 278, r1= 3.52, r2= 3.72, r3= 4.48, r4= 5.48,  &end
#
# 9      ADE   H2'     9       ADE   H8      2.09    2.51
 &rst
  ixpk= 0, nxpk= 0, iat= 293, 278, r1= 1.59, r2= 2.09, r3= 2.51, r4= 3.01,  &end
#
# 10     ADE   H2"     10      ADE   H2'     1.76    2.24
 &rst
  ixpk= 0, nxpk= 0, iat= 326, 325, r1= 1.26, r2= 1.76, r3= 2.24, r4= 2.74,  &end
#
# 11     GUA   H2"     11      GUA   H2'     1.78    2.22
# &rst
#  ixpk= 0, nxpk= 0, iat= 359, 358, r1= 1.28, r2= 1.78, r3= 2.22, r4= 2.72,  &end
#
```

```
# 12     CYT    H2''      12       CYT    H2'      1.77     2.23
 &rst
  ixpk= 0, nxpk= 0, iat= 388, 387, r1= 1.27, r2= 1.77, r3= 2.23, r4= 2.73,  &end
#
# 13     THY    H3'       13       THY    H2''     2.56     3.14
 &rst
  ixpk= 0, nxpk= 0, iat= 417, 420, r1= 2.06, r2= 2.56, r3= 3.14, r4= 3.64,  &end
#
# 14     THY    H4'       13       THY    H1'      3.62     4.38
 &rst
  ixpk= 0, nxpk= 0, iat= 430, 401, r1= 3.12, r2= 3.62, r3= 4.38, r4= 4.88,  &end
#
# 14     THY    H2'       14       THY    H6       2.2      2.68
 &rst
  ixpk= 0, nxpk= 0, iat= 451, 436, r1= 1.70, r2= 2.20, r3= 2.68, r4= 3.18,  &end
#
# 14     THY    H2''      14       THY    H2'      1.77     2.23
 &rst
  ixpk= 0, nxpk= 0, iat= 452, 451, r1= 1.27, r2= 1.77, r3= 2.23, r4= 2.73,  &end
#
# 15     CYT    H6        14       THY    H6       4.15     4.85     change
 &rst
  ixpk= 0, nxpk= 0, iat= 468, 436, r1= 3.65, r2= 4.15, r3= 5.05, r4= 5.35,  &end
#
# 16     THY    H2''      16       THY    H6       2.49     3.05
# &rst
#  ixpk= 0, nxpk= 0, iat= 514, 498, r1= 1.99, r2= 2.49, r3= 3.05, r4= 3.55,  &end
```

```
#
# 16    THY   H5''    16      THY   H6      4.99    6.09
 &rst
  ixpk= 0, nxpk= 0, iat= 490, 498, r1= 4.49, r2= 4.99, r3= 6.09, r4= 6.59,  &end
#
# 17    THY   H3'     17      THY   H4'     2.08    2.54    change
 &rst
  ixpk= 0, nxpk= 0, iat= 543, 524, r1= 1.58, r2= 2.38, r3= 3.04, r4= 3.14,  &end
#
# 18    GUA   H2'     18      GUA   H8      1.9     3.7
 &rst
  ixpk= 0, nxpk= 0, iat= 578, 562, r1= 1.40, r2= 1.90, r3= 3.70, r4= 4.20,  &end
#
# 18    GUA   H2''    18      GUA   H8      2.99    3.61
 &rst
  ixpk= 0, nxpk= 0, iat= 579, 562, r1= 2.49, r2= 2.99, r3= 3.61, r4= 4.11,  &end
#
# 20    CYT   H6      19      THY   H2'     2.99    3.61    change
 &rst
  ixpk= 0, nxpk= 0, iat= 627, 610, r1= 2.49, r2= 2.79, r3= 3.61, r4= 4.11,  &end
#
# 20    CYT   H2'     20      CYT   H6      2.01    2.59
 &rst
  ixpk= 0, nxpk= 0, iat= 640, 627, r1= 1.51, r2= 2.01, r3= 2.59, r4= 3.09,  &end
#
# 20    CYT   H2''    20      CYT   H6      3.18    3.82    change
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 641, 627, r1= 2.68, r2= 3.38, r3= 4.12, r4= 4.32,  &end
#
# 20     CYT    H3'      20       CYT    H2'      2.06     2.52
 &rst
  ixpk= 0, nxpk= 0, iat= 638, 640, r1= 1.56, r2= 2.06, r3= 2.52, r4= 3.02,  &end
#
# 21     CYT    H4'      21       CYT    H6       4.31     5.27
 &rst
  ixpk= 0, nxpk= 0, iat= 651, 657, r1= 3.81, r2= 4.31, r3= 5.27, r4= 5.77,  &end
#
# 21     CYT    H5''     21       CYT    H6       4.4      5.6
 &rst
  ixpk= 0, nxpk= 0, iat= 649, 657, r1= 3.90, r2= 4.40, r3= 5.60, r4= 6.10,  &end
#
# 21     CYT    H2'      21       CYT    H6       2.23     2.77     change
 &rst
  ixpk= 0, nxpk= 0, iat= 670, 657, r1= 1.73, r2= 2.03, r3= 2.77, r4= 3.27,  &end
#
# 22     GUA    H2''     21       CYT    H6       2.74     3.26
# &rst
#  ixpk= 0, nxpk= 0, iat= 704, 657, r1= 2.24, r2= 2.74, r3= 3.26, r4= 3.76,  &end
#
# 22     GUA    H2''     22       GUA    H2'      1.76     2.24
 &rst
  ixpk= 0, nxpk= 0, iat= 704, 703, r1= 1.26, r2= 1.76, r3= 2.24, r4= 2.74,  &end
#
#
```

```
# 16    THY   H1'     6        N1R    HAN   5.34    6.52    CHANGE
# &rst
#  ixpk= 0, nxpk= 0, iat= 495, 181, r1= 4.84, r2= 5.34, r3= 5.52, r4= 6.02,
#         rk2=0.5, rk3=0.5, ir6=1, ialtd=0,       &end
#
# 17    THY   M7      6        N1R    HAM2 4.4      5.6
 &rst
  ixpk= 0, nxpk= 0, iat=  -1, 186, r1= 2.59, r2= 2.60, r3= 6.73, r4= 7.23,
 igr1= 533, 534, 535,
 &end
#
# 18    GUA   H1'     6        N1R    HAM2 5.74    7.02
# &rst
#  ixpk= 0, nxpk= 0, iat= 559, 186, r1= 5.24, r2= 5.74, r3= 7.02, r4= 7.52,  &end
#
# 19    THY   H6      6        N1R    HAM2 3.65    4.47
# &rst
#  ixpk= 0, nxpk= 0, iat= 595, 186, r1= 3.15, r2= 3.65, r3= 4.47, r4= 4.97, &end
#
# 19    THY   H2'     6        N1R    HAM1 3.84    4.7
# &rst
#  ixpk= 0, nxpk= 0, iat= 610, 185, r1= 3.34, r2= 3.84, r3= 4.70, r4= 5.20, &end
#
# 19    THY   M7      6        N1R    HAM1 4.17    5.09
# &rst
#  ixpk= 0, nxpk= 0, iat=  -1, 185, r1= 3.67, r2= 4.17, r3= 6.11, r4= 6.61,
# igr1= 598, 599, 600,
```

```
# &end
#
# 19    THY   H1'     6        N1R   HAM1 3.91    4.79
# &rst
#  ixpk= 0, nxpk= 0, iat= 592, 185, r1= 3.41, r2= 3.91, r3= 4.79, r4= 5.29, &end
#
# 20    CYT   H1'     6        N1R   HAM1 3.5     4.28
# &rst
#  ixpk= 0, nxpk= 0, iat= 624, 185, r1= 3.00, r2= 3.50, r3= 4.28, r4= 4.78, &end
#
# 7     ADE   H2      6        N1R   HAM2 4.04    4.94
# &rst
#  ixpk= 0, nxpk= 0, iat= 222, 186, r1= 3.54, r2= 4.04, r3= 4.94, r4= 5.44,  &end
#
# 7     ADE   H2      6        N1R   HAN  4.9     6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 222, 181, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# 6     ADE   HAO2 6        N1R   H2     4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# 6     ADE   HAO1 6        N1R   H2     4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 188, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# 6     ADE   HAO2 16       THY   CH3    4.9     6.3
```

```
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 495, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# 6      ADE   HAL   X       H2      XXX   4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 183, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE   HAN   X       N1R    H2      4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 181, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE   HAL   7       N1R    H2      4.9      6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 183, 222, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE   HAL   16      N1R    H1'     4.9      6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 183, 495, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE   HAL   X       N1R    HAO2 4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 183, 189, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE   HAL   X       N1R    HAO1 4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 183, 188, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
```

```
# X      ADE    HAN   X        N1R    HAO2 4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 181, 189, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAO1 X        N1R    HAN   4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 188, 181, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM1 16       N1R    H1'     4.9      6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 185, 495, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM2 16       N1R    H1'     4.9      6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 186, 495, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM1 17       N1R    H1'     4.9      6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 185, 527, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM2 17       N1R    H1'     4.9      6.3
# &rst
#  ixpk= 0, nxpk= 0, iat= 186, 527, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM1 X        N1R    HAN   4.9      6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 181, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
```

```
#
# X     ADE   HAM2 X       N1R   HAN   4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 186, 181, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X     ADE   HAM1 X       N1R   HAL   4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 183, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X     ADE   HAM2 X       N1R   HAL   4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 186, 183, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X     ADE   HAN   5       CYT   H6    4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 181, 141, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X     ADE   HAO1  16      THY   H6    4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 188, 498, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X     ADE   HAO2  16      THY   H6    4.9     6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 498, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X     ADE   HAO1  6       ADE   H2    4.9     6.3
 &rst
```

```
  ixpk= 0, nxpk= 0, iat= 188, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAO2 6          ADE    H2       4.9       6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 189, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM1 6          ADE    H2       4.9       6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM2 6          ADE    H2       4.9       6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 186, 179, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM1 17         THY    H6       4.9       6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 185, 530, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
# X      ADE    HAM2 17         THY    H6       4.9       6.3
 &rst
  ixpk= 0, nxpk= 0, iat= 186, 530, r1= 2.50, r2= 2.80, r3= 6.10, r4= 6.40,  &end
#
```

Figure S1. Atomic Charges on the *R*-N1-BDO-(61,2) Adduct Calculated Using Gaussian 03 and the Hartree-Fock, 3-21G* basis set.