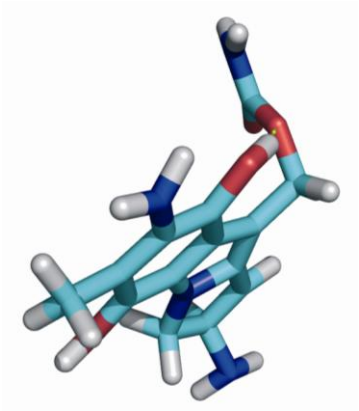
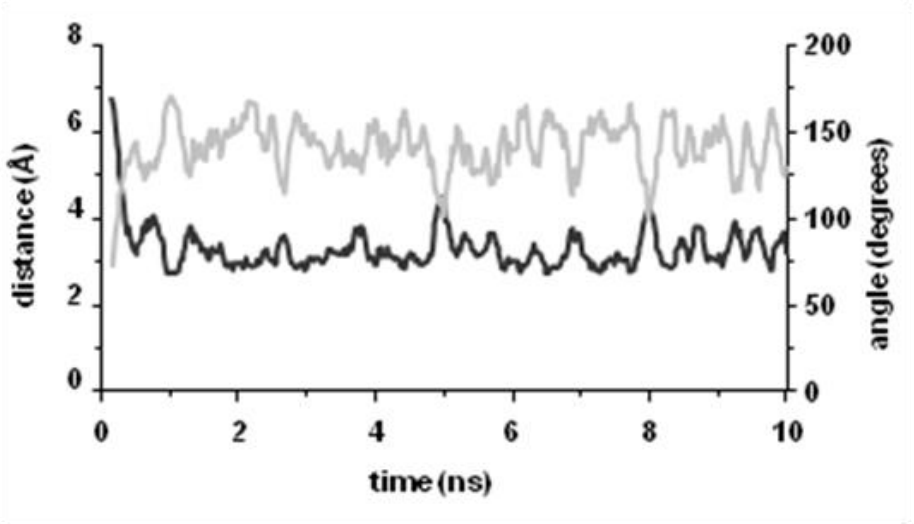
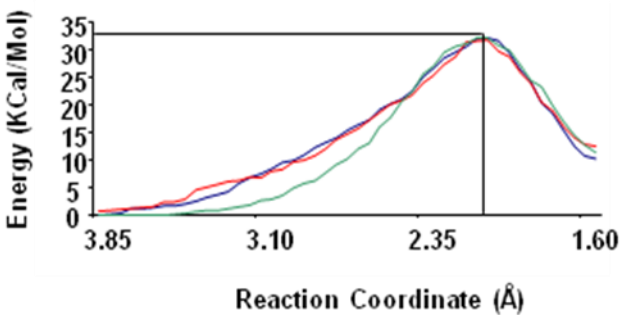
Electronic Supplementary Information



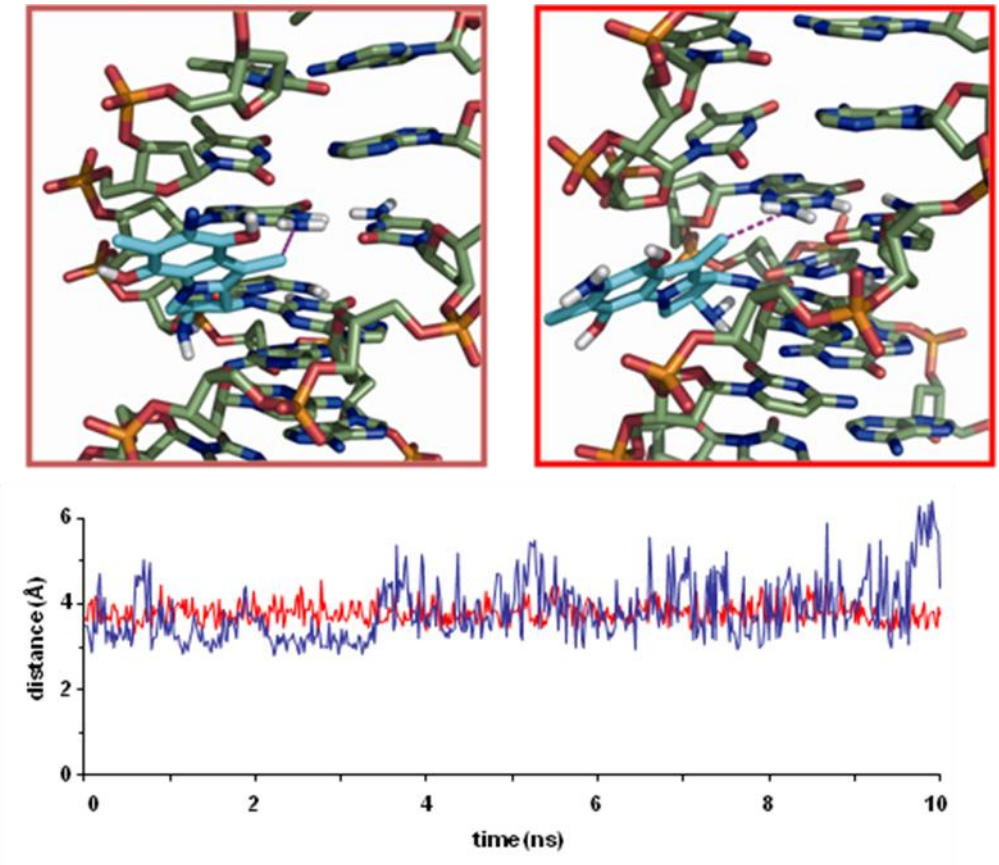
Supplementary Figure S1: representative structure of MMC^+ obtained during the MD simulation in aqueous solution. An internal hydrogen bond between the phenol group at C8 and OM is detected.



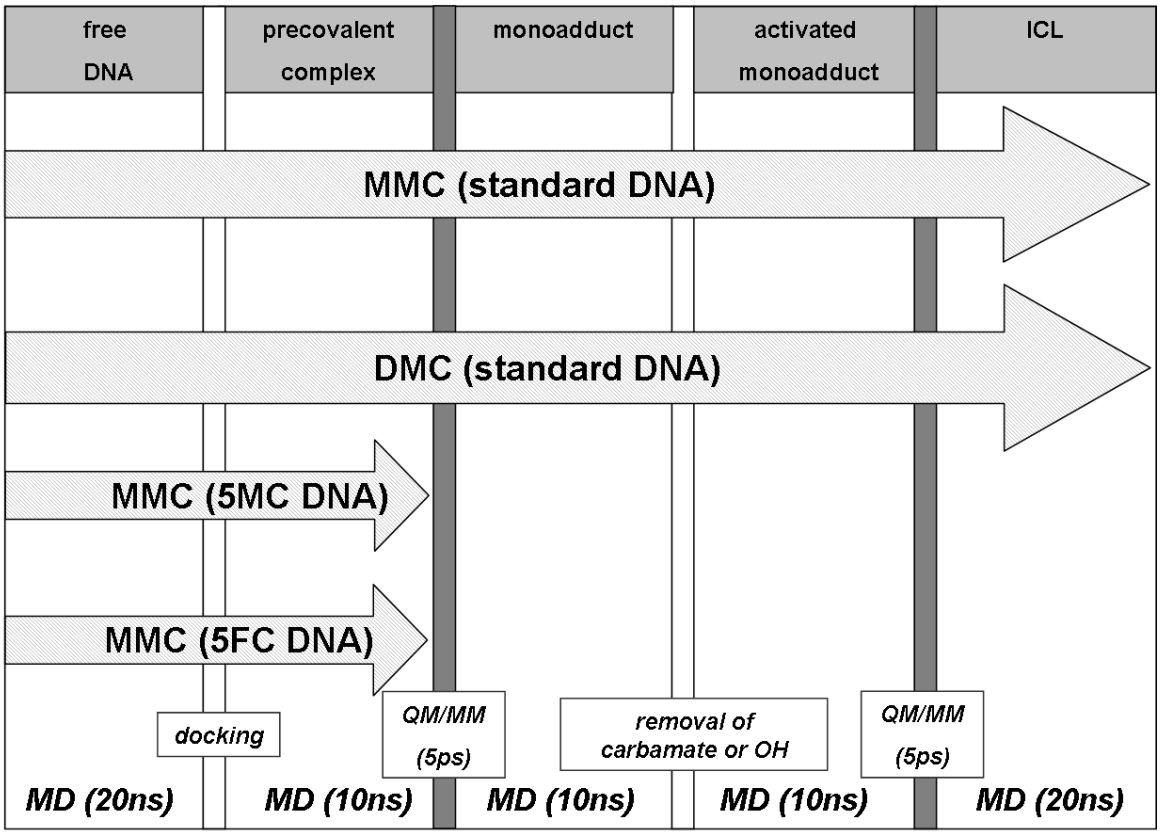
Supplementary Figure S2: O5(MMC^+)–OP^1(T23) distance (black, left axis) and O5-H5-OP^1 angle (grey, right axis) showing the feasibility of a good hydrogen bond.



Supplementary Figure S3: Free energy profiles during the formation of the MMC-monoadducts in standard (blue), 5MC- (red) and 5FC-containing (green) DNA.



Supplementary Figure S4: *Top*: Representative structures of the α- and β-monoadducts containing the unmasked second reactive group that originates upon removal of either the carbamate (MMC, left) or the hydroxyl group (DMC, right) . *Bottom*: Time evolution of the distance between N^2(G22) and C10 of the drug showing the feasibility of the second nucleophilic attack that will lead to the α-(blue) and β-(red) ICLs.



Supplementary Figure S5: Schematic representation of the different molecular complexes and techniques employed during the study of the reactions between MMC and DMC with the DNA oligonucleotides.

AMBER PREP FILES FOR MMC^+, DMC^+, 5-methyl-cytosine (5MC), 5-fluorocytosine (5FC), MMC-DNA monoadduct, DMC-DNA monoadduct, activated monoadduct and ICLs.

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0    0    2

MMC+
MNA.data
MNA INT 1
CORRECT OMIT DU BEG
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   1  DUMM  DU    M   0  -1  -2   0.0000   0.0000   0.0000   0.00000
   2  DUMM  DU    M   1   0  -1   1.7142   0.0000   0.0000   0.00000
   3  DUMM  DU    M   2   1   0   1.7139  60.0035 -90.0000   0.00000
   4  C1    CC    M   3   1   2   1.8081 125.2992 138.5085  -0.107758
   5  H1    HA    E   4   3   1   1.0673  75.2649  22.0074   0.196170
   6  C2    CT    M   4   3   1   1.5294 141.3323 258.9744   0.461678
   7  H2    HC    E   6   4   3   1.0832 107.8133  38.2064   0.030597
   8  N3    NT    B   6   4   3   1.4385 110.9918 156.4472  -1.097330
   9  H31   H     E   8   6   4   0.9981 118.1344 214.6330   0.433418
  10  H32   H     E   8   6   4   0.9993 117.9280  67.7379   0.433418
  11  C4    CT    M   6   4   3   1.5835 103.7579 282.3043  -0.088190
  12  H41   HC    E  11   6   4   1.0770 113.1085 125.2981   0.094765
  13  H42   HC    E  11   6   4   1.0778 110.5053 249.4844   0.094765
  14  N5    N2    M  11   6   4   1.4738 101.8811   6.5806   0.034748
  15  C6    CB    M  14  11   6   1.3079 137.7514 178.7114   0.093363
  16  C7    CA    M  15  14  11   1.4053 130.7339 357.9256   0.122615
  17  O8    OH    S  16  15  14   1.3873 116.3064 359.8220  -0.525990
  18  H8    HO    E  17  16  15   0.9681 113.3918 237.8675   0.406319
  19  C9    CA    M  16  15  14   1.3533 118.4193 176.3481   0.090496
  20  C10   CT    3  19  16  15   1.5063 119.9125 184.6373  -0.077929
  21  H101  HC    E  20  19  16   1.0787 110.7062  11.1528   0.066707
  22  H102  HC    E  20  19  16   1.0833 109.6068 130.4821   0.066707
  23  H103  HC    E  20  19  16   1.0861 110.8739 250.1324   0.066707
  24  C11   CA    M  19  16  15   1.4604 121.8982   4.2911   0.059848
  25  N12   N2    B  24  19  16   1.3649 119.6230 177.9162  -0.676411
  26  H121  H     E  25  24  19   0.9981 117.3720 174.9334   0.350286
  27  H122  H     E  25  24  19   0.9932 123.1237 345.1746   0.350286
  28  C13   CA    M  24  19  16   1.3551 120.4758 356.5455   0.142966
  29  O14   OH    S  28  24  19   1.3748 119.5271 180.9536  -0.487506
  30  H14   HO    E  29  28  24   0.9859 111.7590 237.6658   0.373540
  31  C15   CB    M  28  24  19   1.4211 119.2704 359.2240  -0.049679
  32  C16   CC    M  31  28  24   1.3653 132.8160 184.4347   0.017982
  33  C17   CT    3  32  31  28   1.4999 128.1634   1.2898   0.046768
  34  H171  HC    E  33  32  31   1.0773 111.0659 136.2747   0.134279
  35  H172  HC    E  33  32  31   1.0741 109.6581  13.9121   0.134279
  36  O18   OS    S  33  32  31   1.4538 110.3775 252.0078  -0.432400
  37  C19   C     B  36  33  32   1.3560 118.0497  82.5269   0.922287
  38  O20   O     E  37  36  33   1.2213 122.5661 357.3986  -0.594454
  39  N21   N     B  37  36  33   1.3270 111.3914 177.4351  -0.951931
  40  H211  H     E  39  37  36   0.9969 119.5128 180.9609   0.442576
  41  H212  H     E  39  37  36   0.9963 120.6669 357.9132   0.442576
  42  C22   CC    M   4   3   1   1.3267  62.8081 168.6436  -0.020565

IMPROPER
 C7   C15  C6   N5
 C6   C13  C15  C16
 C9   C13  C11  N12
 C7   C10  C9   C11

LOOP
 C6  C15
 C22 N5
 C1  C22

DONE
STOP
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DMC+
DMC.data
DMC INT 1
CORRECT OMIT DU BEG
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   2  DUMM  DU     M   1   0  -1   1.7152   0.0000   0.0000   0.00000
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   5  H1    HA     E   4   2   1   1.0627  17.5794  19.8035   0.190681
   6  C2    CT     M   4   2   1   1.4858 105.3775 213.5106   0.474506
   7  H2    HC     E   6   4   2   1.0895 112.4630 317.0778   0.052349
   8  N3    NT     B   6   4   2   1.4637 112.3300  84.8862  -1.151601
   9  H31   H      E   8   6   4   0.9970 118.8616  57.0949   0.448147
  10  H32   H      E   8   6   4   1.0231 111.6254 290.7907   0.448147
  11  C4    CT     M   6   4   2   1.5213  98.0429 201.6351  -0.086180
  12  H41   HC     E  11   6   4   1.0900 109.4919 115.2468   0.106372
  13  H42   HC     E  11   6   4   1.0895 111.1349 238.8411   0.106372
  14  N5    N2     M  11   6   4   1.4733 106.3634 357.8692   0.122252
  15  C6    CB     M  14  11   6   1.3419 137.1472 177.6360   0.013039
  16  C7    CA     M  15  14  11   1.4127 130.0937   4.4450   0.115683
  17  O8    OH     S  16  15  14   1.3662 119.3267 358.5538  -0.544045
  18  H8    HO     E  17  16  15   0.9632 114.6483 351.6282   0.420926
  19  C9    CA     M  16  15  14   1.4106 120.0487 185.7963   0.107912
  20  C10   CT     3  19  16  15   1.5272 120.7658 177.4117   0.044303
  21  H101  HC     E  20  19  16   1.0913 109.0736 264.6300   0.032262
  22  H102  HC     E  20  19  16   1.0911 110.7812  24.3618   0.032262
  23  H103  HC     E  20  19  16   1.0884 110.4762 143.6953   0.032262
  24  C11   CA     M  19  16  15   1.4116 118.3723   2.6175   0.051405
  25  N12   N2     B  24  19  16   1.3470 120.5414 173.3221  -0.729382
  26  H121  H      E  25  24  19   1.0146 117.3743 185.4478   0.350621
  27  H122  H      E  25  24  19   1.0068 121.7954 355.1018   0.350621
  28  C13   CA     M  24  19  16   1.4146 120.6326 358.3038   0.170825
  29  O14   OH     S  28  24  19   1.3702 118.6877 174.9865  -0.455208
  30  H14   HO     E  29  28  24   0.9641 113.3923 220.2506   0.377895
  31  C15   CB     M  15  14  11   1.3823 107.4654 190.8827  -0.077235
  32  C16   CC     M  31  15  14   1.4424 108.5450 356.0500   0.143998
  33  C17   CT     3  32  31  15   1.5140 125.1109 178.1091   0.072333
  34  H171  HC     E  33  32  31   1.0551 102.9783 175.7546   0.133537
  35  H172  HC     E  33  32  31   1.0925 113.7161  50.6016   0.133537
  36  O18   OH     S  33  32  31   1.4219 109.6285 280.9019  -0.629121
  37  H18   HO     E  36  33  32   0.9598 109.4817 359.8184   0.452791
  38  C22   CC     M   4   2   1   1.3586 130.4235  59.8028  -0.181899

IMPROPER
 C7   C15  C6   N5
 C6   C13  C15  C16
 C9   C13  C11  N12
 C7   C10  C9   C11

LOOP
 C6  C15
 C22 N5
 C1  C22

DONE
STOP
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5MC.data
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CORRECT OMIT DU BEG
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   6   O2P   O2    E   4   1   2   1.4907 148.5323 122.8410  -0.7545
   7   O5'   OS    M   4   1   2   1.5823  42.2503 132.7391  -0.4128
   8   C5'   CI    M   7   4   1   1.4096 119.0125 109.6841  -0.0111
   9   H5'1  H1    E   8   7   4   1.0902 109.5307 122.6459   0.0662
  10   H5'2  H1    E   8   7   4   1.0901 109.5057   2.6113   0.0662
  11   C4'   CT    M   8   7   4   1.5027 109.5079 242.6301   0.0721
  12   H4'   H1    E  11   8   7   1.0903 108.7974  17.8616   0.0887
  13   O4'   OS    S  11   8   7   1.4429 108.7818 137.8474  -0.3124
  14   C1'   CT    B  13  11   8   1.4162 110.8906 115.2571   0.1421
  15   H1'   H2    E  14  13  11   1.0899 106.5238 107.4191   0.0851
  16   N1    N*    S  14  13  11   1.4678 107.2760 226.7210  -0.054283
  17   C6    CM    B  16  14  13   1.3631 120.7320  60.0161  -0.168892
  18   H6    H4    E  17  16  14   1.0898 119.9275 359.7695   0.196567
  19   C5    CM    B  17  16  14   1.3283 120.2181 179.7685  -0.039121
  20   C51   CT    3  19  17  16   1.4939 119.6981 178.5209  -0.283416
  21   H511  HC    E  20  19  17   1.0906 109.5042 325.5594   0.086524
  22   H512  HC    E  20  19  17   1.0901 109.4897  85.5859   0.086524
  23   H513  HC    E  20  19  17   1.0901 109.4801 160.6337   0.086524
  24   C4    CA    B  19  17  16   1.4328 119.0361 358.8897   0.608709
  25   N4    N2    B  24  19  17   1.3188 121.6766 183.0450  -0.866133
  26   H41   H     E  25  24  19   1.0302 119.9979 358.1684   0.401555
  27   H42   H     E  25  24  19   1.0303 119.9906 178.1519   0.401555
  28   N3    NC    S  24  19  17   1.3248 120.1954   1.1970  -0.715006
  29   C2    C     S  28  24  19   1.3503 120.4517 359.7750   0.730138
  30   O2    O     E  29  28  24   1.2318 121.5643 178.9773  -0.590049
  31   C3'   CT    M  11   8   7   1.5224 111.7199 255.6649   0.1645
  32   H3'   H1    E  31  11   8   1.0904 111.0672  21.9562   0.0623
  33   C2'   CT    B  31  11   8   1.5187 103.3798 262.1936  -0.0561
  34   H2'1  HC    E  33  31  11   1.0899 104.2081 212.1208   0.0486
  35   H2'2  HC    E  33  31  11   1.0898 104.2226  92.0959   0.0486
  36   O3'   OS    M  31  11   8   1.4254 111.0644 141.9800  -0.4998

IMPROPER
 C6   C2   N1   C1'
 N1   N3   C2   O2
 C4   H41  N4   H42
 N1   C5   C6   H6
 C6   C4   C5   C5
 N3   C5   C4   N4

LOOP
 C1'  C2'
 C2   N1

DONE
STOP
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5FC.data
5FC INT 1
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   3   DUMM DU    M   2   1   0   1.7141  59.9872 -90.0000   0.00000
   4   P    P     M   2   1   3   2.3519 102.8903  82.6663   0.985430
   5   O1P  O2    E   4   2   1   1.4774  64.9890 197.2207  -0.718327
   6   O2P  O2    E   4   2   1   1.4809  59.0901 348.1034  -0.718327
   7   O5'  OS    M   4   2   1   1.5941 103.5344  96.2536  -0.241912
   8   C5'  CI    M   7   4   2   1.4486 118.7635 129.0080  -0.080361
   9   H5'1 H1    E   8   7   4   1.0871 113.2007  89.9906   0.067076
  10   H5'2 H1    E   8   7   4   1.0912 108.7754 330.6867   0.067076
  11   C4'  CT    M   8   7   4   1.5121 109.7885 213.9196   0.253120
  12   H4'  H1    E  11   8   7   1.0895 108.6202 160.4756   0.083045
  13   O4'  OS    S  11   8   7   1.4620 108.7076 279.2058  -0.369232
  14   C1'  CT    B  13  11   8   1.4147 109.8083 106.3629   0.039775
  15   H1'  H2    E  14  13  11   1.0828 109.9510 114.1402   0.166181
  16   N1   N*    S  14  13  11   1.4885 107.8118 232.5314  -0.049889
  17   C6   CM    B  16  14  13   1.3565 121.2723  81.8255  -0.044172
  18   H6   H4    E  17  16  14   1.0647 120.8250   1.4511   0.172042
  19   C5   CM    B  17  16  14   1.3621 121.3395 179.7777  -0.005665
  20   F5   F     E  19  17  16   1.0899 120.2368 180.9219  -0.215007
  21   C4   CA    B  19  17  16   1.4304 116.6922   0.6635   0.695439
  22   N4   N2    B  21  19  17   1.3238 120.1478 179.6551  -0.926795
  23   H41  H     E  22  21  19   1.0148 118.7408 175.3518   0.410614
  24   H42  H     E  22  21  19   0.9994 119.6149 354.5054   0.410614
  25   N3   NC    S  21  19  17   1.3382 121.4500 359.2389  -0.766650
  26   C2   C     S  25  21  19   1.3554 120.8857   0.6418   0.780061
  27   O2   O     E  26  25  21   1.2299 117.3287 180.3243  -0.662521
  28   C3'  CT    M  11   8   7   1.5277 116.2964  36.4618   0.181949
  29   H3'  H1    E  28  11   8   1.0921 111.6861  32.1967   0.078359
  30   C2'  CT    B  28  11   8   1.5204 102.8626 273.5618  -0.057999
  31   H2'1 HC    E  30  28  11   1.0775 107.8695  87.3817   0.053334
  32   H2'2 HC    E  30  28  11   1.0755 122.9561 204.4826   0.053334
  33   O3'  OS    M  28  11   8   1.4243 112.1882 156.3259  -0.641033

IMPROPER
 C6   C2   N1   C1'
 N1   N3   C2   O2
 C4   H41  N4   H42
 N1   C5   C6   H6
 C6   C4   C5   C5
 N3   C5   C4   N4

LOOP
 C1'  C2'
 C2   N1

DONE
STOP
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0    0    2

Modified first guanine covalently bonded to MMC
GMA.data
GMA INT 1
CORRECT OMIT DU BEG
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   2  DUMM  DU    M   1   0  -1   1.5507   0.0000   0.0000   0.00000
   3  DUMM  DU    M   2   1   0   1.4598 109.5046 -90.0000   0.00000
   4  P     P     M   3   2   1   1.6098 109.4815 171.8037   1.07350
   5  O1P   O2    E   4   3   2   1.4757 107.8660 128.9552  -0.75450
   6  O2P   O2    E   4   3   2   1.4826 107.0798   3.4750  -0.75450
   7  O5'   OS    M   4   3   2   1.5946 105.9670 246.7517  -0.41280
   8  C5'   CI    M   7   4   3   1.4491 118.8038 313.0108  -0.01110
   9  H5'1  H1    E   8   7   4   1.0895 109.7875  93.9948   0.06620
  10  H5'2  H1    E   8   7   4   1.0896 109.7503 333.8969   0.06620
  11  C4'   CT    M   8   7   4   1.5112 109.7559 213.9956   0.07210
  12  H4'   H1    E  11   8   7   1.0906 107.7490 156.3048   0.08870
  13  O4'   OS    S  11   8   7   1.4633 108.6274 279.0603  -0.31240
  14  C1'   CT    B  13  11   8   1.3949 111.5744 107.8753  -0.090196
  15  H1'   H2    E  14  13  11   1.0093 119.8636 113.4915   0.073923
  16  N9    N*    S  14  13  11   1.4628 109.0420 232.3016  -0.001596
  17  C8    CK    B  16  14  13   1.3930 126.5881  79.3409   0.150746
  18  H8    H5    E  17  16  14   1.0629 121.6263   0.4003   0.169314
  19  N7    NB    S  17  16  14   1.2926 111.8010 180.7062  -0.557905
  20  C5    CB    S  19  17  16   1.3844 105.7664   0.1348   0.238612
  21  C6    C     B  20  19  17   1.4266 130.1384 179.8183   0.529446
  22  O6    O     E  21  20  19   1.2056 131.9219 359.6613  -0.523593
  23  N1    NA    B  21  20  19   1.4378 109.7013 179.9680  -0.479606
  24  H1    H     E  23  21  20   1.0007 113.1710 180.1423   0.341750
  25  C2    CA    B  23  21  20   1.3541 125.6099   0.0676   0.336728
  26  N2    N2    B  25  23  21   1.3690 116.8536 180.7562  -0.379035
  27  H22   H     E  26  25  23   0.9967 119.2255 354.2878   0.319880
  28  C1    CT    B  26  25  23   1.4424 120.4474 173.5182   0.050474
  29  H11   HC    E  28  26  25   1.0835 103.2665 333.4524  -0.002830
  30  C21   CT    3  28  26  25   1.5580 112.0006 214.8592   0.210357
  31  H2    HC    E  30  28  26   1.0782 113.8990  18.3638   0.061006
  32  N31   N3    3  30  28  26   1.5360 109.9070 145.7215  -0.565438
  33  H31   H     E  32  30  28   1.0178 110.8497 223.2633   0.381371
  34  H32   H     E  32  30  28   1.0190 110.2273 101.4153   0.381371
  35  H33   H     E  32  30  28   1.0182 110.5451 340.2503   0.381371
  36  C41   CT    3  30  28  26   1.5512 103.9528 261.8929  -0.061161
  37  H41   HC    E  36  30  28   1.0773 116.2187 203.3156   0.097063
  38  H42   HC    E  36  30  28   1.0817 109.6605  72.9852   0.097063
  39  N5    N2    S  36  30  28   1.4538  98.3564 319.4666   0.076165
  40  C61   CB    S  39  36  30   1.3735 138.3439 210.9405  -0.097532
  41  C7    CA    B  40  39  36   1.3820 130.2455   0.5304   0.204247
  42  O8    OH    S  41  40  39   1.3909 115.6979   1.3519  -0.602760
  43  H88   HO    E  42  41  40   0.9658 113.4836 220.2069   0.448677
  43  C9    CA    B  41  40  39   1.3716 119.0190 180.8515  -0.027554
  44  C10   CT    3  44  41  40   1.5128 121.2229 176.9890  -0.196565
  45  H101  HC    E  45  44  41   1.0858 110.6428 130.6879   0.085476
  46  H102  HC    E  45  44  41   1.0857 110.2625 248.3155   0.085476
  47  H103  HC    E  45  44  41   1.0796 112.3737  10.0772   0.085476
  48  C11   CA    B  44  41  40   1.4191 119.7581 359.6987   0.037467
  49  N12   N2    B  49  44  41   1.3711 120.9228 179.7409  -0.695826
  50  H121  H     E  50  49  44   0.9955 118.3684 179.6910   0.344397
  51  H122  H     E  50  49  44   0.9918 122.7541 359.7868   0.344397
  52  C13   CA    B  49  44  41   1.3834 120.4037   0.1286   0.321327
  53  O14   OH    S  53  49  44   1.3966 118.2325 180.9384  -0.497586
  55  H14   HO    E  54  53  49   0.9701 112.1294  91.6167   0.381704
  54  C15   CB    S  53  49  44   1.3884 119.9383   0.1877  -0.278328
  55  C16   CC    B  56  53  49   1.4583 133.9797 179.8322   0.022496
  56  C17   CT    3  57  56  53   1.4955 128.5548 358.7011   0.034859
  57  H171  HC    E  58  57  56   1.0739 110.7849 191.8127   0.117799
  58  H172  HC    E  58  57  56   1.0781 113.0571  62.8287   0.117799
  59  O18   OS    S  58  57  56   1.4643 107.7873 307.3385  -0.353773
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  60   C19    C      B   61   58   57    1.3621 117.0801 134.8037   0.894227
  61   O20    O      E   62   61   58    1.2158 121.9035  26.6266  -0.613284
  62   N21    N      B   62   61   58    1.3344 111.2884 204.8474  -1.031107
  63   H211   H      E   64   62   61    0.9956 119.5194 184.2416   0.548170
  64   H212   H      E   64   62   61    0.9936 120.0944   1.1124   0.548170
  65   C22    CC     E   57   56   53    1.3512 105.8634 179.2058  -0.090689
  66   N3     NC     S   25   23   21    1.2931 123.4868   0.0000  -0.231293
  67   C4     CB     E   16   14   13    1.3521 127.3597 260.3045  -0.031994
  68   C3'    CT     M   11    8    7    1.5272 116.4108  36.3269   0.16450
  69   H3'    H1     E   70   11    8    1.0901 111.0785  33.6484   0.06230
  70   C2'    CT     B   70   11    8    1.5198 102.8652 273.6188  -0.05610
  71   H2'1   HC     E   72   70   11    1.0898 111.3656 205.0787   0.04860
  72   H2'2   HC     E   72   70   11    1.0898 111.3543  85.0500   0.04860
  73   O3'    OS     M   70   11    8    1.4254 112.1999 156.3781  -0.49980

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   C1   N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2
 C41  C61  N5   C22
 C1   C16  C22  N5
 C7   C15  C61  N5
 C9   C13  C11  N12
 C21  C22  C1   N2
 C13  C16  C15  C61

LOOP
 C1'  C2'
 C4   C5
 N5   C22
 C61  C15
 C22  C1
 C4   N9

DONE
STOP
```

```
0    0    2

Modified First Guanine covalently bonded to DMC
GDC.data
GDC INT 1
CORRECT OMIT DU BEG
0.00000
   1  DUMM  DU     M   0  -1  -2   0.0000   0.0000   0.0000   0.00000
   2  DUMM  DU     M   1   0  -1   1.7146   0.0000   0.0000   0.00000
   3  DUMM  DU     M   2   1   0   1.7139  59.9969 -90.0000   0.00000
   4  P     P      M   1   2   3   5.7201 111.9836 291.0711   1.07350
   5  O1P   O2     E   4   1   2   1.4749 119.7162  50.0352  -0.75450
   6  O2P   O2     E   4   1   2   1.4785 118.8360 219.2088  -0.75450
   7  O5'   OS     M   4   1   2   1.6021  37.5749 132.0207  -0.41280
   8  C5'   CI     M   7   4   1   1.4248 118.9456 299.7463  -0.01110
   9  H5'1  H1     E   8   7   4   1.0907 110.0932  71.9653   0.06620
  10  H5'2  H1     E   8   7   4   1.0909 108.7006 313.8732   0.06620
  11  C4'   CT     M   8   7   4   1.5248 113.2894 194.0929   0.07210
  12  H4'   H1     E  11   8   7   1.0925 108.4905 170.2909   0.08870
  13  O4'   OS     S  11   8   7   1.4215 111.8989 290.5628  -0.31240
  14  C1'   CT     B  13  11   8   1.4141 109.3653 117.5153  -0.090196
  15  H1'   H2     E  14  13  11   1.0897 109.4893  98.5528   0.073923
  16  N9    N*     S  14  13  11   1.4774 107.4530 219.3298  -0.001596
  17  C8    CK     B  16  14  13   1.3738 126.7138  69.2664   0.150746
  18  H8    H5     E  17  16  14   1.0839 122.5168   5.4627   0.169314
  19  N7    NB     S  17  16  14   1.3029 114.3423 187.1852  -0.557905
  20  C5    CB     S  19  17  16   1.3993 103.4494   0.4421   0.238612
  21  C6    C      B  20  19  17   1.4350 130.3430 177.5570   0.529446
  22  O6    O      E  21  20  19   1.2286 129.3617 359.9178  -0.523593
  23  N1    NA     B  21  20  19   1.3837 113.3227 179.4668  -0.479606
  24  H1    H      E  23  21  20   1.0153 114.3394 177.9732   0.341750
  25  C2    CA     B  23  21  20   1.3769 125.0621   0.1635   0.336728
  26  N2    N2     B  25  23  21   1.3390 110.7241 179.5442  -0.379035
  27  H22   H      E  26  25  23   1.0183 111.5860 354.6159   0.319880
  28  C1    CT     B  26  25  23   1.4770 140.6415 181.0435  -0.082618
  29  H11   HC     E  28  26  25   1.0883  97.2937 131.6880   0.208403
  30  C21   CT     3  28  26  25   1.5385 112.0054 240.5704  -0.157904
  31  H2    HC     E  30  28  26   1.0925 111.5894 301.0929   0.198411
  32  N31   N3     3  30  28  26   1.4711 111.2296  70.2531  -0.151075
  33  H31   H      E  32  30  28   1.0157 109.9915 293.5859   0.287377
  34  H32   H      E  32  30  28   1.0186 112.5078 173.6498   0.287377
  35  H33   H      E  32  30  28   1.0102 109.3482  49.4897   0.287377
  36  C41   CT     3  30  28  26   1.5196  98.2353 185.3961  -0.186922
  37  H41   HC     E  36  30  28   1.0870 111.0060  85.9143   0.255941
  38  H42   HC     E  36  30  28   1.0896 113.2337 209.1665   0.255941
  39  N5    N2     S  36  30  28   1.4590 105.9094 329.6579   0.181172
  40  C61   CB     S  39  36  30   1.3246 136.6508 191.2051  -0.359320
  41  C7    CA     B  40  39  36   1.4287 126.5875 358.5318   0.374278
  42  O8    OH     S  41  40  39   1.2327 124.2490   4.8172  -0.648299
  43  H88   HO     E  42  41  40   0.9603 109.5058  56.4033   0.441862
  44  C9    CA     B  41  40  39   1.4570 114.0605 185.6119  -0.018231
  45  C10   CT     3  44  41  40   1.5321 117.6909 174.2241  -0.032504
  46  H101  HC     E  45  44  41   1.0875 113.3109 176.1748   0.039666
  47  H102  HC     E  45  44  41   1.0923 108.7377 297.6023   0.039666
  48  H103  HC     E  45  44  41   1.0894 109.0203  54.9970   0.039666
  49  C11   CA     B  44  41  40   1.3623 121.0613 354.6366   0.015773
  50  N12   N2     B  49  44  41   1.3524 123.6832 177.1728  -0.908107
  51  H121  H      E  50  49  44   1.0199 114.8446 187.8083   0.421200
  52  H122  H      E  50  49  44   1.0074 118.5094 350.2279   0.421200
  53  C13   CA     B  49  44  41   1.4811 123.2355 359.4428   0.457905
  54  O14   OH     S  53  49  44   1.2292 120.2422 185.2234  -0.618378
  55  H14   HO     E  54  53  49   0.9597 109.5223 132.2934   0.440889
  56  C15   CB     S  40  39  36   1.3753 107.1986 178.4885  -0.288534
  57  C16   CC     B  56  40  39   1.4513 109.4729   0.4971  -0.172464
  58  C17   CT     3  57  56  40   1.5180 121.8560 185.6183   0.846720
  59  H171  HC     E  58  57  56   1.0822 110.3874 152.5726  -0.150574
  60  H172  HC     E  58  57  56   1.0849 105.8355  37.9614  -0.150574
  61  O18   OH     S  58  57  56   1.4208 114.1077 278.0869  -0.785208
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  62  H18   HO     E  61  58  57   0.9606 109.2408 125.1983   0.433409
  63  C22   CC     E  57  56  40   1.3743 102.8672   4.0532   0.020879
  64  N3    NC     S  25  23  21   1.3465 122.4953 359.2169  -0.231293
  65  C4    CB     E  64  25  23   1.3777 113.8776   1.6441  -0.031994
  66  C3'   CT     M  11   8   7   1.5247 109.3298  50.8067   0.16450
  67  H3'   H1     E  66  11   8   1.0914 112.4336  20.1678   0.06230
  68  C2'   CT     B  66  11   8   1.5213 101.1117 261.3994  -0.05610
  69  H2'1  HC     E  68  66  11   1.0878 109.5841  85.4433   0.04860
  70  H2'2  HC     E  68  66  11   1.0780 111.1855 206.0222   0.04860
  71  O3'   OS     M  66  11   8   1.4046 106.6317 141.4279  -0.49980

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   C1   N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2
 C41  C61  N5   C22
 C1   C16  C22  N5
 C7   C15  C61  N5
 C9   C13  C11  N12
 C21  C22  C1   N2
 C13  C16  C15  C61

LOOP
 C1'  C2'
 C4   C5
 N5   C22
 C61  C15
 C22  C1
 C4   N9

DONE
STOP
```

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0    0    2

Activated Monoadduct
GMB.data
GMB INT 1
CORRECT OMIT DU BEG
0.00000
   1   DU   DU     M   0  -1  -2   0.0000   0.0000   0.0000   0.00000
   2   DU   DU     M   1   0  -1   2.0000   0.0000   0.0000   0.00000
   3   DU   DU     M   2   1   0   1.0000   0.0000 -90.0000   0.00000
   4   P    P      M   2   1   3   2.0000 180.0000   0.0000   1.07350
   5   O1P  O2     E   4   2   1   1.5172  64.2983   0.0000  -0.75450
   6   O2P  O2     E   4   2   1   1.4599  56.7706   0.0000  -0.75450
   7   O5'  OS     M   4   2   1   1.6211 141.0667   0.0000  -0.41280
   8   C5'  CI     M   7   4   2   1.4277 117.9994  87.8020  -0.01110
   9   H5'1 H1     E   8   7   4   1.0905 117.3148  38.4066   0.06620
  10   H5'2 H1     E   8   7   4   1.0902 104.0114 281.7556   0.06620
  11   C4'  CT     M   8   7   4   1.5289 112.5281 162.2313   0.07210
  12   H4'  H1     E  11   8   7   1.0900 111.5559 178.3906   0.08870
  13   O4'  OS     S  11   8   7   1.4786 106.8498 295.1284  -0.31240
  14   C1'  CT     B  13  11   8   1.4475 109.3292 116.2392   0.15570
  15   H1'  H2     E  14  13  11   1.0906 111.0174 102.2480   0.08860
  16   N9   N*     S  14  13  11   1.4947 115.8354 227.8053  -0.03790
  17   C8   CK     B  16  14  13   1.3486 126.3958  66.8633   0.13530
  18   H8   H5     E  17  16  14   1.0799 118.2109  11.9717   0.15080
  19   N7   NB     S  17  16  14   1.3339 116.8009 189.4697  -0.51390
  20   C5   CB     S  19  17  16   1.4226 100.5797   0.3012   0.05850
  21   C6   C      B  20  19  17   1.4882 130.3444 180.3825   0.50710
  22   O6   O      E  21  20  19   1.2600 127.3849 348.5150  -0.53010
  23   N1   NA     B  21  20  19   1.3635 112.6229 177.3431  -0.54050
  24   H1   H      E  23  21  20   1.0093 107.8548 183.0836   0.37500
  25   C2   CA     B  23  21  20   1.3437 123.0149 359.0884   0.68340
  26   N2   N2     B  25  23  21   1.3371 113.7386 178.3364  -0.490295
  27   H22  H      E  26  25  23   1.0104 118.9170 350.7094   0.324924
  28   C1   CT     B  26  25  23   1.4941 123.7662 157.9892   0.038317
  29   H11  HC     E  28  26  25   1.0894 104.5648 327.9915   0.126164
  30   C21  CT     3  28  26  25   1.4978 109.6269 206.8399   0.306071
  31   H2   HC     E  30  28  26   1.0903 104.9903 303.1545   0.052448
  32   N31  NT     B  30  28  26   1.4726 114.1531  72.8611  -0.991732
  33   H31  H      E  32  30  28   1.0103 109.5211 100.4852   0.389895
  34   H32  H      E  32  30  28   1.0099 109.5264 340.3997   0.389895
  35   C41  CT     3  30  28  26   1.5346  99.8383 195.2789   0.066318
  36   H41  HC     E  35  30  28   1.0900 111.3261 152.2275   0.062603
  37   H42  HC     E  35  30  28   1.0899 109.3475 275.1616   0.062603
  38   N5   N2     S  35  30  28   1.4703 106.4019  28.3593   0.030090
  39   C61  CB     S  38  35  30   1.3481 137.7121 159.3059  -0.132023
  40   C7   CA     B  39  38  35   1.4130 132.0898   8.3843   0.186079
  41   O8   OH     S  40  39  38   1.3766 123.2105 344.4828  -0.519782
  42   H88  HO     E  41  40  39   0.9596 108.9218  35.6161   0.418230
  43   C9   CA     B  40  39  38   1.4361 115.8401 177.1587   0.109653
  44   C10  CT     3  43  40  39   1.5222 120.6029 169.7373  -0.235035
  45   H101 HC     E  44  43  40   1.0908 110.6403 315.3434   0.097113
  46   H102 HC     E  44  43  40   1.0896 104.5428  76.7885   0.097113
  47   H103 HC     E  44  43  40   1.0894 110.7521 198.3206   0.097113
  48   C11  CA     B  43  40  39   1.3702 120.6771 357.0419   0.068702
  49   N12  N2     B  48  43  40   1.3626 116.8595 174.3588  -0.710275
  50   H121 H      E  49  48  43   1.0102 125.0917 197.3846   0.363299
  51   H122 H      E  49  48  43   1.0101 119.4106  21.6517   0.363299
  52   C13  CA     B  48  43  40   1.3849 123.4720   0.1537   0.201287
  53   O14  OH     S  52  48  43   1.3872 118.2145 176.3497  -0.450982
  54   H14  HO     E  53  52  48   0.9598 110.0702 137.6605   0.374216
  55   C15  CB     S  39  38  35   1.3991 105.5175 186.7479  -0.152831
  56   C16  CC     B  55  39  38   1.4817 107.3280   5.4654   0.122655
  57   C17  CT     B  56  55  39   1.5151 129.0685 178.5067  -0.037432
  58   H171 HC     E  57  56  55   1.0894 109.5184 199.4987   0.151105
  59   H172 HC     E  57  56  55   1.0905 107.4538  80.3294   0.151105
  60   C18  CC     E  38  35  30   1.3314 109.2262 348.3882   0.007632
  61   N3   NC     S  25  23  21   1.3377 126.8670   2.4559  -0.65020
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  62   C4   CB     E  16  14  13   1.3534 128.0421 253.9133   0.29090
  63   C3'  CT     M  11   8   7   1.5329 117.1726  57.1110   0.16450
  64   H3'  H1     E  63  11   8   1.0896 118.4319  17.0873   0.06230
  65   C2'  CT     B  63  11   8   1.4801  97.0368 266.8781  -0.05610
  66   H2'1 HC     E  65  63  11   1.0894 106.9236  81.7710   0.04860
  67   H2'2 HC     E  65  63  11   1.0894 111.0148 204.1459   0.04860
  68   O3'  OS     M  63  11   8   1.4123 111.8090 146.8356  -0.49980

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   C1   N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2
 C41  C61  N5   C18
 C1   C16  C18  N5
 C7   C15  C61  N5
 C9   C13  C11  N12
 C21  C18  C1   N2
 C13  C16  C15  C61

LOOP
 C1'  C2'
 C4   C5
 N5   C18
 C61  C15
 C18  C1
 C4   N9

DONE
STOP
```

```
0    0    2

First modified guanine in the ICL
GMO.data
GMO INT 1
CORRECT OMIT DU BEG
0.00000
   1  DUMM  DU    M   0  -1  -2   0.0000   0.0000   0.0000   0.00000
   2  DUMM  DU    M   1   0  -1   1.5502   0.0000   0.0000   0.00000
   3  DUMM  DU    M   2   1   0   1.4595 109.5041 -90.0000   0.00000
   4  P     P     M   3   2   1   1.6098 109.5229 171.7957   1.07350
   5  O1P   O2    E   4   3   2   1.4760 107.8942 128.9165  -0.75450
   6  O2P   O2    E   4   3   2   1.4829 107.0576   3.4646  -0.75450
   7  O5'   OS    M   4   3   2   1.5945 105.9806 246.7548  -0.41280
   8  C5'   CI    M   7   4   3   1.4498 118.7822 312.9643  -0.01110
   9  H5'1  H1    E   8   7   4   1.0900 109.7613  93.9934   0.06620
  10  H5'2  H1    E   8   7   4   1.0895 109.7582 333.9654   0.06620
  11  C4'   CT    M   8   7   4   1.5109 109.7677 213.9796   0.07210
  12  H4'   H1    E  11   8   7   1.0901 107.7608 156.3397   0.08870
  13  O4'   OS    S  11   8   7   1.4632 108.6489 279.1130  -0.31240
  14  C1'   CT    B  13  11   8   1.4145 109.7846 106.4011   0.15570
  15  H1'   H2    E  14  13  11   1.0901 107.9285 115.7842   0.08860
  16  N9    N*    S  14  13  11   1.4877 107.7679 232.4945  -0.038777
  17  C8    CK    B  16  14  13   1.3792 129.2830  82.1486   0.123243
  18  H8    H5    E  17  16  14   1.0899 122.9320 359.9051   0.154475
  19  N7    NB    S  17  16  14   1.3081 114.1026 179.8800  -0.559339
  20  C5    CB    S  19  17  16   1.3965 103.9975   0.1633   0.294664
  21  C6    C     B  20  19  17   1.4133 130.2191 179.8644   0.388537
  22  O6    O     E  21  20  19   1.2309 129.0731   0.0000  -0.530049
  23  N1    NA    B  21  20  19   1.4059 111.4324 179.8800  -0.216712
  24  H1    H     E  23  21  20   1.0303 117.4688 179.6679   0.276784
  25  C2    CA    B  23  21  20   1.3798 125.0383 359.6854   0.105208
  26  N2    N2    S  25  23  21   1.3366 116.1488 180.2365  -0.309644
  27  H22   H     E  26  25  23   1.0305 120.0123   0.0000   0.274286
  28  N3    NC    S  25  23  21   1.3304 123.5537   0.7501  -0.211589
  29  C4    CB    E  28  25  23   1.3591 112.3692 359.4493   0.024855
  30  C3'   CT    M  11   8   7   1.5272 116.3826  36.3615   0.16450
  31  H3'   H1    E  30  11   8   1.0901 111.1425  33.6094   0.06230
  32  C2'   CT    B  30  11   8   1.5202 102.8645 273.6140  -0.05610
  33  H2'1  HC    E  32  30  11   1.0903 111.3657 205.0801   0.04860
  34  H2'2  HC    E  32  30  11   1.0894 111.3650  85.0665   0.04860
  35  O3'   OS    M  30  11   8   1.4255 112.2122 156.4009  -0.49980

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 N7   N9   C8   H8
 N1   N3   C2   N2

LOOP
 C1'  C2'
 C4   C5
 C4   N9

DONE
STOP
```

```
0    0    2

Second modified guanine in the ICL
GMM.data
GMM INT 1
CORRECT OMIT DU BEG
0.00000
   1  DUMM  DU    M   0  -1  -2   0.0000   0.0000   0.0000   0.00000
   2  DUMM  DU    M   1   0  -1   1.5502   0.0000   0.0000   0.00000
   3  DUMM  DU    M   2   1   0   1.4595 109.5041 -90.0000   0.00000
   4  P     P     M   3   2   1   1.6098 109.5229 171.7957   1.07350
   5  O1P   O2    E   4   3   2   1.4760 107.8942 128.9165  -0.75450
   6  O2P   O2    E   4   3   2   1.4829 107.0576   3.4646  -0.75450
   7  O5'   OS    M   4   3   2   1.5945 105.9806 246.7548  -0.41280
   8  C5'   CI    M   7   4   3   1.4498 118.7822 312.9643  -0.01110
   9  H5'1  H1    E   8   7   4   1.0900 109.7613  93.9934   0.06620
  10  H5'2  H1    E   8   7   4   1.0895 109.7582 333.9654   0.06620
  11  C4'   CT    M   8   7   4   1.5109 109.7677 213.9796   0.07210
  12  H4'   H1    E  11   8   7   1.0901 107.7608 156.3397   0.08870
  13  O4'   OS    S  11   8   7   1.4632 108.6489 279.1130  -0.31240
  14  C1'   CT    B  13  11   8   1.4145 109.7846 106.4011   0.15570
  15  H1'   H2    E  14  13  11   1.0901 107.9285 115.7842   0.08860
  16  N9    N*    S  14  13  11   1.4877 107.7679 232.4945  -0.038777
  17  C8    CK    B  16  14  13   1.3792 129.2830  82.1486   0.123243
  18  H8    H5    E  17  16  14   1.0899 122.9320 359.9051   0.154475
  19  N7    NB    S  17  16  14   1.3081 114.1026 179.8800  -0.559339
  20  C5    CB    S  19  17  16   1.3965 103.9975   0.1633   0.294664
  21  C6    C     B  20  19  17   1.4133 130.2191 179.8644   0.388537
  22  O6    O     E  21  20  19   1.2309 129.0731   0.0000  -0.530049
  23  N1    NA    B  21  20  19   1.4059 111.4324 179.8800  -0.216712
  24  H1    H     E  23  21  20   1.0303 117.4688 179.6679   0.276784
  25  C2    CA    B  23  21  20   1.3798 125.0383 359.6854   0.105208
  26  N2    N2    B  25  23  21   1.3366 116.1488 180.2365  -0.309644
  27  H22   H     E  26  25  23   1.0305 120.0123   0.0000   0.274286
  28  C1    CT    B  26  25  23   1.5127 117.6538 173.7370   0.050471
  29  H11   HC    E  28  26  25   1.0809 104.2807 342.1348   0.038004
  30  C21   CT    3  28  26  25   1.5724 112.3552 223.5178   0.203713
  31  H2    HC    E  30  28  26   1.0762 115.3011  18.2558   0.087449
  32  N31   N3    3  30  28  26   1.5410 107.4922 145.5955  -0.463291
  33  H31   H     E  32  30  28   1.0190 111.3881 177.5966   0.351639
  34  H32   H     E  32  30  28   1.0219 107.6278  58.7999   0.351639
  35  H33   H     E  32  30  28   1.0178 112.0462 299.1398   0.351639
  36  C41   CT    3  30  28  26   1.5552 105.7249 256.8189   0.002681
  37  H41   HC    E  36  30  28   1.0775 115.2474 210.6396   0.082141
  38  H42   HC    E  36  30  28   1.0818 109.9666  87.2135   0.082141
  39  N5    N2    S  36  30  28   1.4549 100.0325 330.6351  -0.001023
  40  C61   CB    S  39  36  30   1.3479 134.6292 187.9487  -0.119607
  41  C7    C     B  40  39  36   1.4678 126.0789  16.9804   0.401268
  42  O8    O     E  41  40  39   1.2278 119.0215 359.8077  -0.474053
  43  C9    CM    B  41  40  39   1.4451 114.6522 180.0688  -0.063269
  44  C10   CT    3  43  41  40   1.5103 117.5083 179.3860  -0.156271
  45  H101  HC    E  44  43  41   1.0870 111.3755 119.0958   0.068978
  46  H102  HC    E  44  43  41   1.0853 111.4504 240.3782   0.068978
  47  H103  HC    E  44  43  41   1.0803 109.5025 359.8728   0.068978
  48  C11   CM    B  43  41  40   1.3533 121.5368 359.2821   0.014983
  49  N12   N2    B  48  43  41   1.3384 124.9855 180.3719  -0.673605
  50  H121  H     E  49  48  43   0.9994 118.7702 180.1443   0.372075
  51  H122  H     E  49  48  43   0.9966 122.2374 359.5462   0.372075
  52  C13   C     B  48  43  41   1.5272 123.0227 359.7784   0.625178
  53  O14   O     E  52  48  43   1.2130 119.7557 181.9962  -0.450562
  54  C15   CB    S  40  39  36   1.3576 107.7085 196.8374  -0.150074
  55  C16   CC    B  54  40  39   1.4293 108.6265   2.0357  -0.036816
  56  C17   CT    B  55  54  40   1.4987 127.5583 175.6767   0.029926
  57  H171  HC    E  57  55  54   1.0774 108.9511  23.8400   0.086068
  58  H172  HC    E  57  55  54   1.0821 109.0602 143.5287   0.086068
  59  C18   CC    E  55  54  40   1.3565 105.4075 357.8175  -0.110424
  60  N3    NC    S  25  23  21   1.3304 123.5537   0.7501  -0.211589
  61  C4    CB    E  60  25  23   1.3591 112.3692 359.4493   0.024855
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  62  C3'   CT    M  11   8   7   1.5272 116.3826  36.3615   0.16450
  63  H3'   H1    E  62  11   8   1.0901 111.1425  33.6094   0.06230
  64  C2'   CT    B  62  11   8   1.5202 102.8645 273.6140  -0.05610
  65  H2'1  HC    E  64  62  11   1.0903 111.3657 205.0801   0.08860
  66  H2'2  HC    E  64  62  11   1.0894 111.3650  85.0665   0.08860
  67  O3'   OS    M  62  11   8   1.4255 112.2122 156.4009  -0.49980

IMPROPER
 C8   C4   N9   C1'
 C5   N1   C6   O6
 C6   C2   N1   H1
 C2   C1   N2   H22
 N7   N9   C8   H8
 N1   N3   C2   N2
 C41  C61  N5   C18
 C1   C16  C18  N5
 C7   C15  C61  N5
 C9   C13  C11  N12
 C21  C18  C1   N2
 C13  C16  C15  C61

LOOP
 C1'  C2'
 C4   C5
 N5   C18
 C61  C15
 C18  C1
 C4   N9

DONE
STOP
```

Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry

Additions to the *parmbsc0* AMBER force field for non-standard residues MMC^+, DMC^+, 5MC, 5FC, GDC, GMA, GMB, GMO and GMM.

```
#  MMC+

BOND
CC-CC   480.0     1.360         (MMC+)
CB-CC   480.0     1.430         (MMC+)
CM-N2   445.0     1.340         (MMC+)
N2-CC   340.0     1.380         (MMC+)
N2-CB   340.0     1.350         (MMC+)
C -N2   425.0     1.340         (MMC+)
CC-HC   340.0     1.080         (MMC+)
N3-CB   436.0     1.410         (MMC+)
N3-CC   436.0     1.370         (MMC+)
CC-HA   340.0     1.070         (MMC+)

ANGLE
N2-CT-CC     70.0       114.35      (MMC+)
CC-CC-CT     70.0       135.00      (MMC+)
CC-CT-NT     70.0       111.00      (MMC+)
CB-CC-CC     70.0       105.40      (MMC+)
C -CB-CC     65.0       131.80      (MMC+)
N2-CM-C      70.0       112.00      (MMC+)
CM-N2-H      30.0       112.30      (MMC+)
CM-C -CB     70.0       114.96      (MMC+)
CM-CM-N2     70.0       124.97      (MMC+)
CB-N2-CC     70.0       109.30      (MMC+)
CB-C -CM     70.0       114.65      (MMC+)
CB-CB-CC     65.0       108.65      (MMC+)
N2-CB-C      70.0       126.06      (MMC+)
N2-CB-CB     70.0       107.70      (MMC+)
N2-CC-CC     70.0       108.90      (MMC+)
CT-N2-CB     60.0       134.65      (MMC+)
CT-N2-CC     60.0       114.00      (MMC+)
HC-CT-N3     50.0       113.25      (MMC+)
CT-CC-N2     70.0       109.47      (MMC+)
CB-CC-CT     70.0       127,56      (MMC+)
OS-C -N      80.0       110.93      (MMC+)
CC-CT-OS     50.0       106.94      (MMC+)
O -C -N2     80.0       126.20      (MMC+)
C -N2-H      33.0       120.40      (MMC+)
OS-C-N2      80.0       110.40      (MMC+)
HC-CC-CT     50.0       108.00      (MMC+)
HC-CT-NT     50.0       110.10      (MMC+)
CT-CC-CT     40.0       114.0       (MMC+)
CB-CC-HC     50.0       112.0       (MMC+)
N2-CT-OS     50.0       113.0       (MMC+)
CT-N2-CT     50.0        59.80      (MMC+)
CB-N3-CC     70.0       110.70      (MMC+)
N3-CB-C      70.0       127.50      (MMC+)
N3-CB-CB     70.0       107.70      (MMC+)
N3-CC-CC     70.0       108.50      (MMC+)
CT-N3-CB     60.0       134.30      (MMC+)
CT-N3-CC     60.0       115.03      (MMC+)
OH-CA-CB     70.0       121.80      (MMC+)
CA-CB-CC     63.0       134.00      (MMC+)
N2-CA-CA     70.0       118.70      (MMC+)
N2-CB-CA     70.0       130.25      (MMC+)
HA-CC-CT     35.0       126.10      (MMC+)
HA-CC-CC     35.0       123.75      (MMC+)
CC-CT-N3     60.0       109.35      (MMC+)
CC-CC-CC     60.0       144.03      (MMC+)
CT-CM-CA     60.0       121.26      (MMC+)
OS-CT-HC     50.0       111.00      (MMC+)
N2-CT-HC     50.0       107.50      (MMC+)
```

```
DIHE
X -CM-N2-X    4    9.60        180.0            2.          (MMC+)
X -CB-N2-X    4    9.60        180.0            2.          (MMC+)
X -CB-CC-X    4   14.50        180.0            2.          (MMC+)
X -N2-CC-X    4    9.60        180.0            2.          (MMC+)
X -CC-CC-X    4   14.50        180.0            2.          (MMC+)
X -C -N2-X    4    5.80        180.0            2.          (MMC+)


#  DMC+

BOND
CC-CC  480.0    1.360        (DMC+)
CB-CC  480.0    1.430        (DMC+)
CM-N2  445.0    1.340        (DMC+)
N2-CC  340.0    1.380        (DMC+)
N2-CB  340.0    1.350        (DMC+)
C -N2  425.0    1.340        (DMC+)
CC-HC  340.0    1.080        (DMC+)
N3-CB  436.0    1.410        (DMC+)
N3-CC  436.0    1.370        (DMC+)
CC-HA  340.0    1.070        (DMC+)

ANGLE
N2-CT-CC    70.0      114.35     (DMC+)
CC-CC-CT    70.0      135.00     (DMC+)
CC-CT-NT    70.0      111.00     (DMC+)
CB-CC-CC    70.0      105.40     (DMC+)
C -CB-CC    65.0      131.80     (DMC+)
N2-CM-C     70.0      112.00     (DMC+)
CM-N2-H     30.0      112.30     (DMC+)
CM-C -CB    70.0      114.96     (DMC+)
CM-CM-N2    70.0      124.97     (DMC+)
CB-N2-CC    70.0      109.30     (DMC+)
CB-C -CM    70.0      114.65     (DMC+)
CB-CB-CC    65.0      108.65     (DMC+)
N2-CB-C     70.0      126.06     (DMC+)
N2-CB-CB    70.0      107.70     (DMC+)
N2-CC-CC    70.0      108.90     (DMC+)
CT-N2-CB    60.0      134.65     (DMC+)
CT-N2-CC    60.0      114.00     (DMC+)
HC-CT-N3    50.0      113.25     (DMC+)
CT-CC-N2    70.0      109.47     (DMC+)
CB-CC-CT    70.0      127,56     (DMC+)
OS-C -N     80.0      110.93     (DMC+)
CC-CT-OS    50.0      106.94     (DMC+)
CC-CT-OH    50.0      106.94     (DMC+)
O -C -N2    80.0      126.20     (DMC+)
C -N2-H     33.0      120.40     (DMC+)
OS-C-N2     80.0      110.40     (DMC+)
HC-CC-CT    50.0      108.00     (DMC+)
HC-CT-NT    50.0      110.10     (DMC+)
CT-CC-CT    40.0      114.0      (DMC+)
CB-CC-HC    50.0      112.0      (DMC+)
N2-CT-OS    50.0      113.0      (DMC+)
CT-N2-CT    50.0       59.80     (DMC+)
CB-N3-CC    70.0      110.70     (DMC+)
N3-CB-C     70.0      127.50     (DMC+)
N3-CB-CB    70.0      107.70     (DMC+)
N3-CC-CC    70.0      108.50     (DMC+)
CT-N3-CB    60.0      134.30     (DMC+)
CT-N3-CC    60.0      115.03     (DMC+)
OH-CA-CB    70.0      121.80     (DMC+)
CA-CB-CC    63.0      134.00     (DMC+)
N2-CA-CA    70.0      118.70     (DMC+)
N2-CB-CA    70.0      130.25     (DMC+)
HA-CC-CT    35.0      126.10     (DMC+)
```

```
HA-CC-CC    35.0      123.75     (DMC+)
CC-CT-N3    60.0      109.35     (DMC+)
CC-CC-CC    60.0      144.03     (DMC+)
CT-CM-CA    60.0      121.26     (DMC+)
OS-CT-HC    50.0      111.00     (DMC+)
OH-CT-HC    50.0      111.00     (DMC+)
N2-CT-HC    50.0      107.50     (DMC+)

DIHE
X -CM-N2-X    4    9.60        180.0            2.          (DMC+)
X -CB-N2-X    4    9.60        180.0            2.          (DMC+)
X -CB-CC-X    4   14.50        180.0            2.          (DMC+)
X -N2-CC-X    4    9.60        180.0            2.          (DMC+)
X -CC-CC-X    4   14.50        180.0            2.          (DMC+)
X -C -N2-X    4    5.80        180.0            2.          (DMC+)



#  5MC
ANGLE
CT-CM-CA    60.0      121.26    5MC


#  5FC

BOND
CM-F  367.0    1.090   5FC

ANGLE
F -CM-CA    70.0      123.07     5FC
CM-CM-F     70.0      120.24     5FC


#  MMC monoadduct

BOND
CC-CC  480.0    1.360       MMC_adduct
CB-CC  480.0    1.430       MMC_adduct
CM-N2  445.0    1.340       MMC_adduct
N2-CC  340.0    1.380       MMC_adduct
N2-CB  340.0    1.350       MMC_adduct
C -N2  425.0    1.340       MMC_adduct
CC-HC  340.0    1.080       MMC_adduct
N3-CB  436.0    1.410       MMC_adduct
N3-CC  436.0    1.370       MMC_adduct
CC-HA  340.0    1.070       MMC_adduct

ANGLE
N2-CT-CC    70.0      114.35    MMC_adduct
CC-CC-CT    70.0      135.00    MMC_adduct
CB-CC-CC    70.0      105.40    MMC_adduct
C -CB-CC    65.0      131.80    MMC_adduct
N2-CM-C     70.0      112.00    MMC_adduct
CM-N2-H     30.0      112.30    MMC_adduct
CM-C -CB    70.0      114.96    MMC_adduct
CM-CM-N2    70.0      124.97    MMC_adduct
CB-N2-CC    70.0      109.30    MMC_adduct
CB-C -CM    70.0      114.65    MMC_adduct
CB-CB-CC    65.0      108.65    MMC_adduct
N2-CB-C     70.0      126.06    MMC_adduct
N2-CB-CB    70.0      107.70    MMC_adduct
N2-CC-CC    70.0      108.90    MMC_adduct
CT-N2-CB    60.0      134.65    MMC_adduct
CT-N2-CC    60.0      114.00    MMC_adduct
HC-CT-N3    50.0      113.25    MMC_adduct
CT-CC-N2    70.0      109.47    MMC_adduct
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CB-CC-CT    70.0      127,56    MMC_adduct
OS-C -N     80.0      110.93    MMC_adduct
CC-CT-OS    50.0      106.94    MMC_adduct
CC-CT-OH    50.0      106.94    MMC_adduct
O -C -N2    80.0      126.20    MMC_adduct
C -N2-H     33.0      120.40    MMC_adduct
OS-C-N2     80.0      110.40    MMC_adduct
HC-CC-CT    50.0      108.00    MMC_adduct
CT-CC-CT    40.0      114.0     MMC_adduct
CB-CC-HC    50.0      112.0     MMC_adduct
N2-CT-OS    50.0      113.0     MMC_adduct
CT-N2-CT    50.0       59.80    MMC_adduct
CB-N3-CC    70.0      110.70    MMC_adduct
N3-CB-C     70.0      127.50    MMC_adduct
N3-CB-CB    70.0      107.70    MMC_adduct
N3-CC-CC    70.0      108.50    MMC_adduct
CT-N3-CB    60.0      134.30    MMC_adduct
CT-N3-CC    60.0      115.03    MMC_adduct
OH-CA-CB    70.0      121.80    MMC_adduct
CA-CB-CC    63.0      134.00    MMC_adduct
N2-CA-CA    70.0      118.70    MMC_adduct
N2-CB-CA    70.0      130.25    MMC_adduct
HA-CC-CT    35.0      126.10    MMC_adduct
HA-CC-CC    35.0      123.75    MMC_adduct
CC-CT-N3    60.0      109.35    MMC_adduct
CC-CC-CC    60.0      144.03    MMC_adduct
CT-CM-CA    60.0      121.26    MMC_adduct
OS-CT-HC    50.0      111.00    MMC_adduct
OH-CT-HC    50.0      111.00    MMC_adduct
N2-CT-HC    50.0      107.50    MMC_adduct

DIHE
X -CM-N2-X    4    9.60        180.0             2.          MMC_adduct
X -CB-N2-X    4    9.60        180.0             2.          MMC_adduct
X -CB-CC-X    4   14.50        180.0             2.          MMC_adduct
X -N2-CC-X    4    9.60        180.0             2.          MMC_adduct
X -CC-CC-X    4   14.50        180.0             2.          MMC_adduct
X -C -N2-X    4    5.80        180.0             2.          MMC_adduct


#  activated monoadducts

BOND
CC-CC  480.0    1.360       activated monoadduct
CB-CC  480.0    1.430       activated monoadduct
CM-N2  445.0    1.340       activated monoadduct
N2-CC  340.0    1.380       activated monoadduct
N2-CB  340.0    1.350       activated monoadduct
C -N2  425.0    1.340       activated monoadduct
CC-HC  340.0    1.080       activated monoadduct
N3-CB  436.0    1.410       activated monoadduct
N3-CC  436.0    1.370       activated monoadduct
CC-HA  340.0    1.070       activated monoadduct

ANGLE
N2-CT-CC    70.0      114.35    activated monoadduct
CC-CC-CT    70.0      135.00    activated monoadduct
CB-CC-CC    70.0      105.40    activated monoadduct
C -CB-CC    65.0      131.80    activated monoadduct
N2-CM-C     70.0      112.00    activated monoadduct
CM-N2-H     30.0      112.30    activated monoadduct
CM-C -CB    70.0      114.96    activated monoadduct
CM-CM-N2    70.0      124.97    activated monoadduct
CB-N2-CC    70.0      109.30    activated monoadduct
CB-C -CM    70.0      114.65    activated monoadduct
CB-CB-CC    65.0      108.65    activated monoadduct
N2-CB-C     70.0      126.06    activated monoadduct
N2-CB-CB    70.0      107.70    activated monoadduct
```

```
N2-CC-CC    70.0      108.90    activated monoadduct
CT-N2-CB    60.0      134.65    activated monoadduct
CT-N2-CC    60.0      114.00    activated monoadduct
HC-CT-NT    50.0      113.25    activated monoadduct
CT-CC-N2    70.0      109.47    activated monoadduct
CB-CC-CT    70.0      127,56    activated monoadduct
OS-C -N     80.0      110.93    activated monoadduct
CC-CT-OS    50.0      106.94    activated monoadduct
O -C -N2    80.0      126.20    activated monoadduct
C -N2-H     33.0      120.40    activated monoadduct
OS-C-N2     80.0      110.40    activated monoadduct
HC-CC-CT    50.0      108.00    activated monoadduct
CT-CC-CT    40.0      114.0     activated monoadduct
CB-CC-HC    50.0      112.0     activated monoadduct
N2-CT-OS    50.0      113.0     activated monoadduct
CT-N2-CT    50.0       59.80    activated monoadduct
CB-N3-CC    70.0      110.70    activated monoadduct
N3-CB-C     70.0      127.50    activated monoadduct
N3-CB-CB    70.0      107.70    activated monoadduct
N3-CC-CC    70.0      108.50    activated monoadduct
CT-N3-CB    60.0      134.30    activated monoadduct
CT-N3-CC    60.0      115.03    activated monoadduct
OH-CA-CB    70.0      121.80    activated monoadduct
CA-CB-CC    63.0      134.00    activated monoadduct
N2-CA-CA    70.0      118.70    activated monoadduct
N2-CB-CA    70.0      130.25    activated monoadduct
HA-CC-CT    35.0      126.10    activated monoadduct
HA-CC-CC    35.0      123.75    activated monoadduct
CC-CT-N3    60.0      109.35    activated monoadduct
CC-CC-CC    60.0      144.03    activated monoadduct
OS-CT-HC    50.0      111.00    activated monoadduct
N2-CT-HC    50.0      107.50    activated monoadduct

DIHE
X -CM-N2-X    4    9.60        180.0            2.         activated monoadduct
X -CB-N2-X    4    9.60        180.0            2.         activated monoadduct
X -CB-CC-X    4   14.50        180.0            2.         activated monoadduct
X -N2-CC-X    4    9.60        180.0            2.         activated monoadduct
X -CC-CC-X    4   14.50        180.0            2.         activated monoadduct
X -C -N2-X    4    5.80        180.0            2.         activated monoadduct



#  ICLs

BOND
CC-CC  480.0    1.360       ICL
CB-CC  480.0    1.430       ICL
CM-N2  445.0    1.340       ICL
N2-CC  340.0    1.380       ICL
N2-CB  340.0    1.350       ICL
C -N2  425.0    1.340       ICL
CC-HC  340.0    1.080       ICL
N3-CB  436.0    1.410       ICL
N3-CC  436.0    1.370       ICL
CC-HA  340.0    1.070       ICL

ANGLE
N2-CT-CC    70.0      114.35    ICL
CC-CC-CT    70.0      135.00    ICL
CB-CC-CC    70.0      105.40    ICL
C -CB-CC    65.0      131.80    ICL
N2-CM-C     70.0      112.00    ICL
CM-N2-H     30.0      112.30    ICL
CM-C -CB    70.0      114.96    ICL
CM-CM-N2    70.0      124.97    ICL
CB-N2-CC    70.0      109.30    ICL
```

```
CB-C -CM    70.0      114.65    ICL
CB-CB-CC    65.0      108.65    ICL
N2-CB-C     70.0      126.06    ICL
N2-CB-CB    70.0      107.70    ICL
N2-CC-CC    70.0      108.90    ICL
CT-N2-CB    60.0      134.65    ICL
CT-N2-CC    60.0      114.00    ICL
HC-CT-N3    50.0      113.25    ICL
CT-CC-N2    70.0      109.47    ICL
CB-CC-CT    70.0      127,56    ICL
OS-C -N     80.0      110.93    ICL
CC-CT-OS    50.0      106.94    ICL
O -C -N2    80.0      126.20    ICL
C -N2-H     33.0      120.40    ICL
OS-C-N2     80.0      110.40    ICL
HC-CC-CT    50.0      108.00    ICL
CT-CC-CT    40.0      114.0     ICL
CB-CC-HC    50.0      112.0     ICL
N2-CT-OS    50.0      113.0     ICL
CT-N2-CT    50.0       59.80    ICL
CB-N3-CC    70.0      110.70    ICL
N3-CB-C     70.0      127.50    ICL
N3-CB-CB    70.0      107.70    ICL
N3-CC-CC    70.0      108.50    ICL
CT-N3-CB    60.0      134.30    ICL
CT-N3-CC    60.0      115.03    ICL
OH-CA-CB    70.0      121.80    ICL
CA-CB-CC    63.0      134.00    ICL
N2-CA-CA    70.0      118.70    ICL
N2-CB-CA    70.0      130.25    ICL
HA-CC-CT    35.0      126.10    ICL
HA-CC-CC    35.0      123.75    ICL
CC-CT-N3    60.0      109.35    ICL
CC-CC-CC    60.0      144.03    ICL
OS-CT-HC    50.0      111.00    ICL)
N2-CT-HC    50.0      107.50    ICL

DIHE
X -CM-N2-X    4    9.60        180.0            2. ICL
X -CB-N2-X    4    9.60        180.0            2. ICL
X -CB-CC-X    4   14.50        180.0            2. ICL
X -N2-CC-X    4    9.60        180.0            2. ICL
X -CC-CC-X    4   14.50        180.0            2. ICL
X -C -N2-X    4    5.80        180.0            2. ICL
```