# Regioselectivity of the glycosylation of *N*-dimethylmaleoyl-protected hexosamine acceptors. An experimental and DFT approach.

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**Supplementary Information**

NMR Spectra and Cartesian coordinates of most stable conformers

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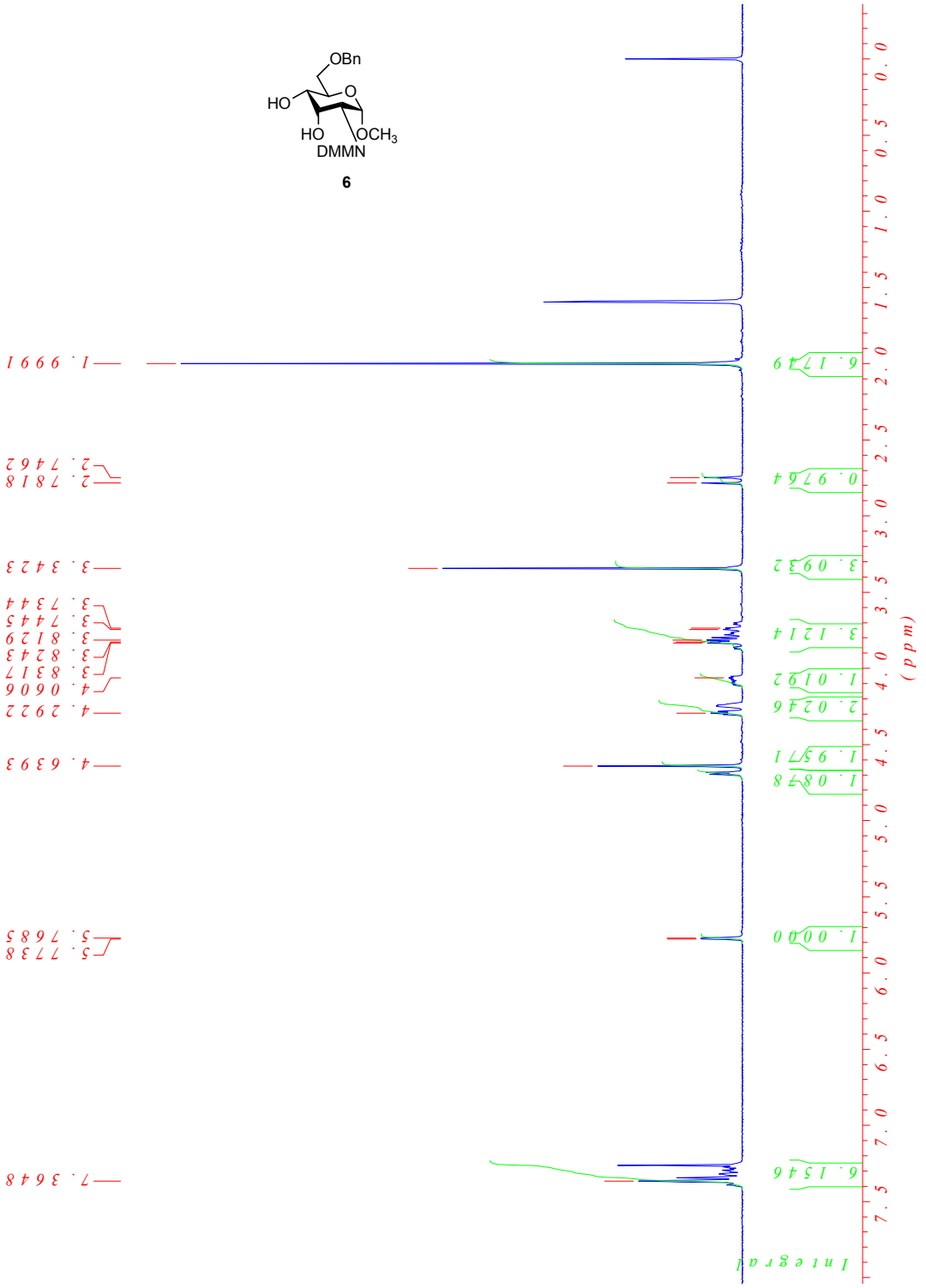
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3.8243
3.8317
4.0606
4.2922
4.6393
5.7738
5.7685
7.3648
6.1749
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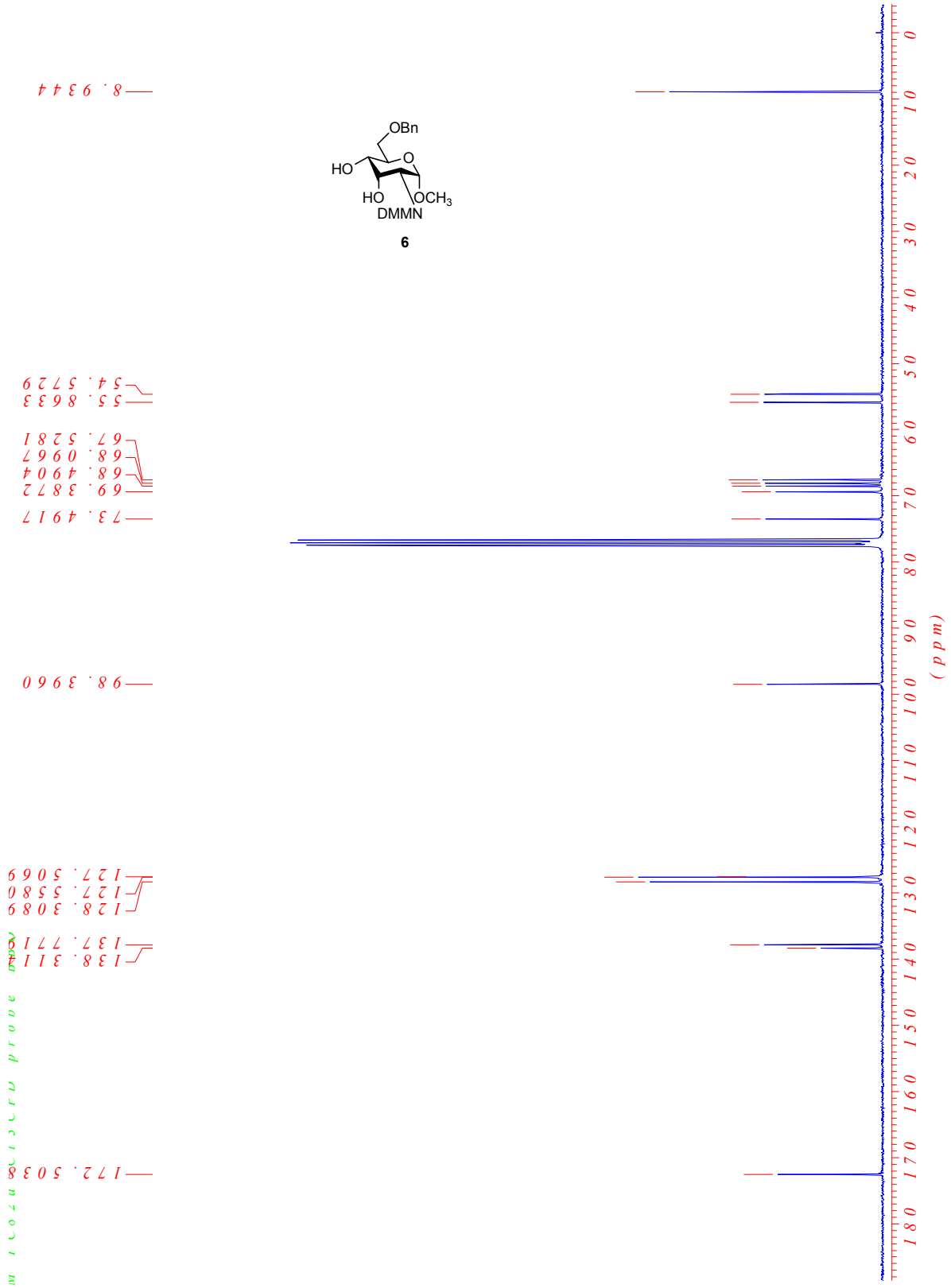
3.0932
3.1214
1.0192
2.0246
1.9371
1.0878
1.0000
6.1546
Integral
(ppm)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HO
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6.8.4904
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7.3.4917
9.8.3960
1.2.7.5069
1.2.7.5580
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1.3.8.3114
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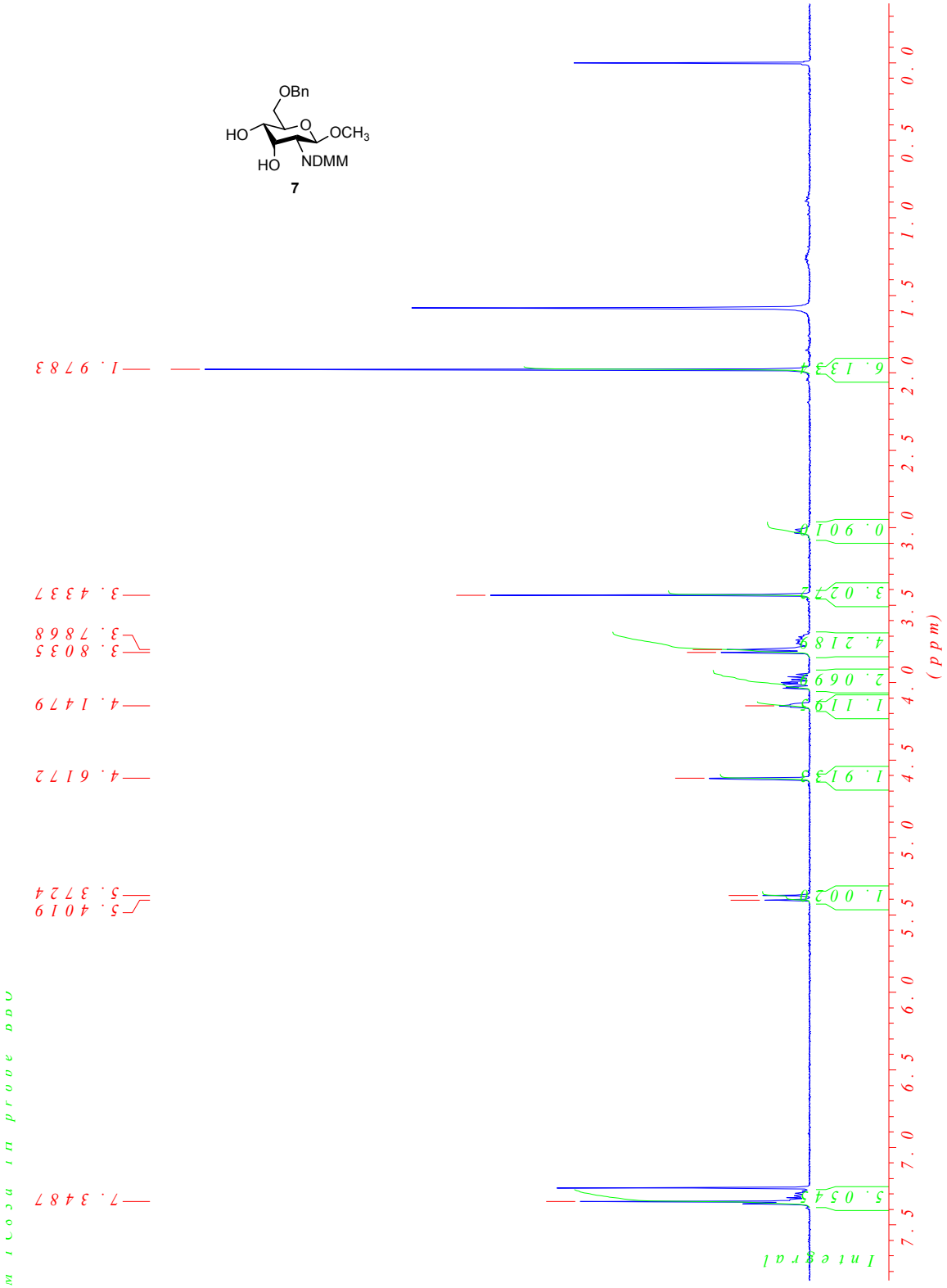
( ppm )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OCH3
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4.1479
4.6172
5.4019
5.3724
7.3487
6.1333
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3.0273
4.2189
2.0699
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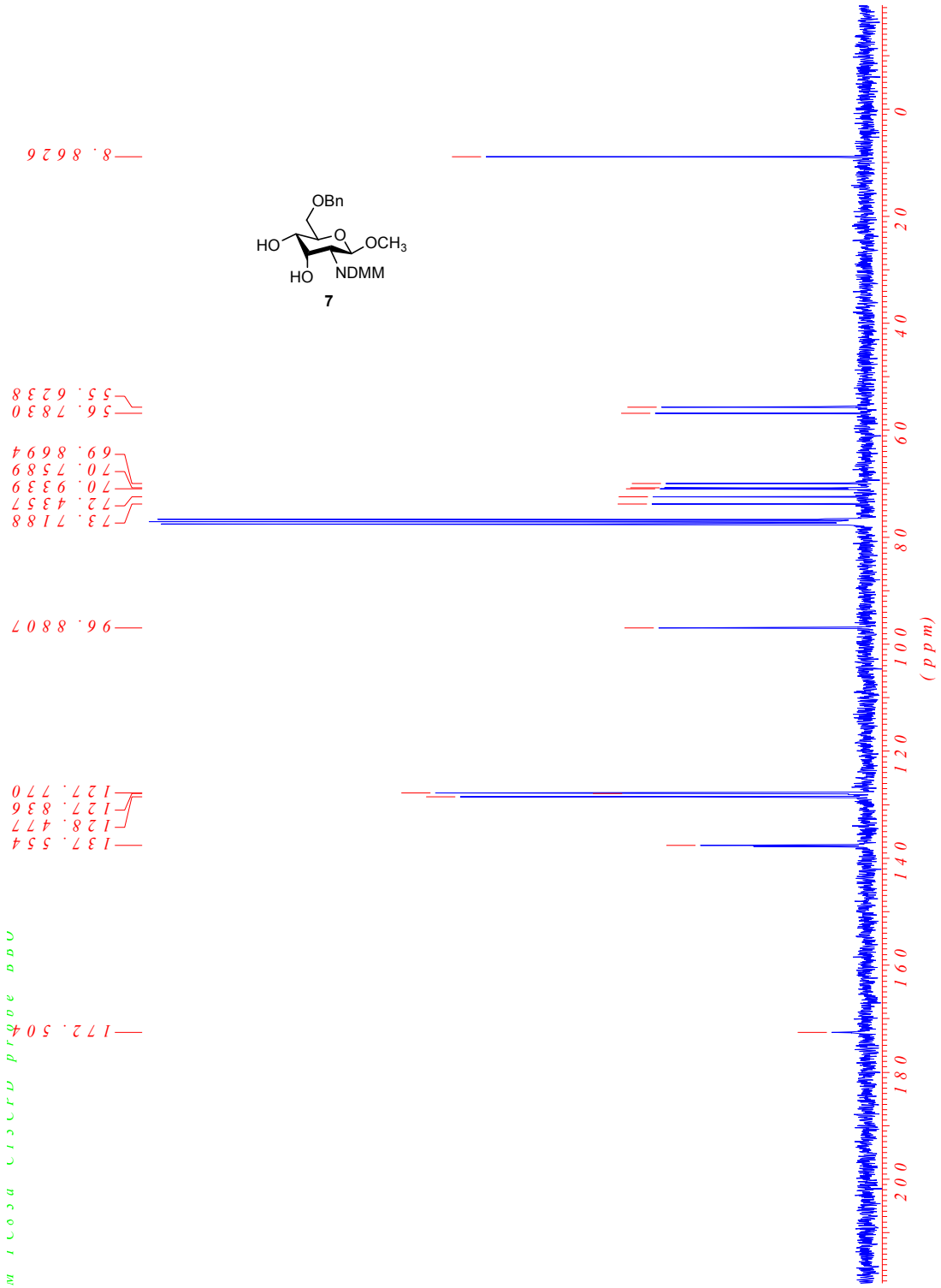
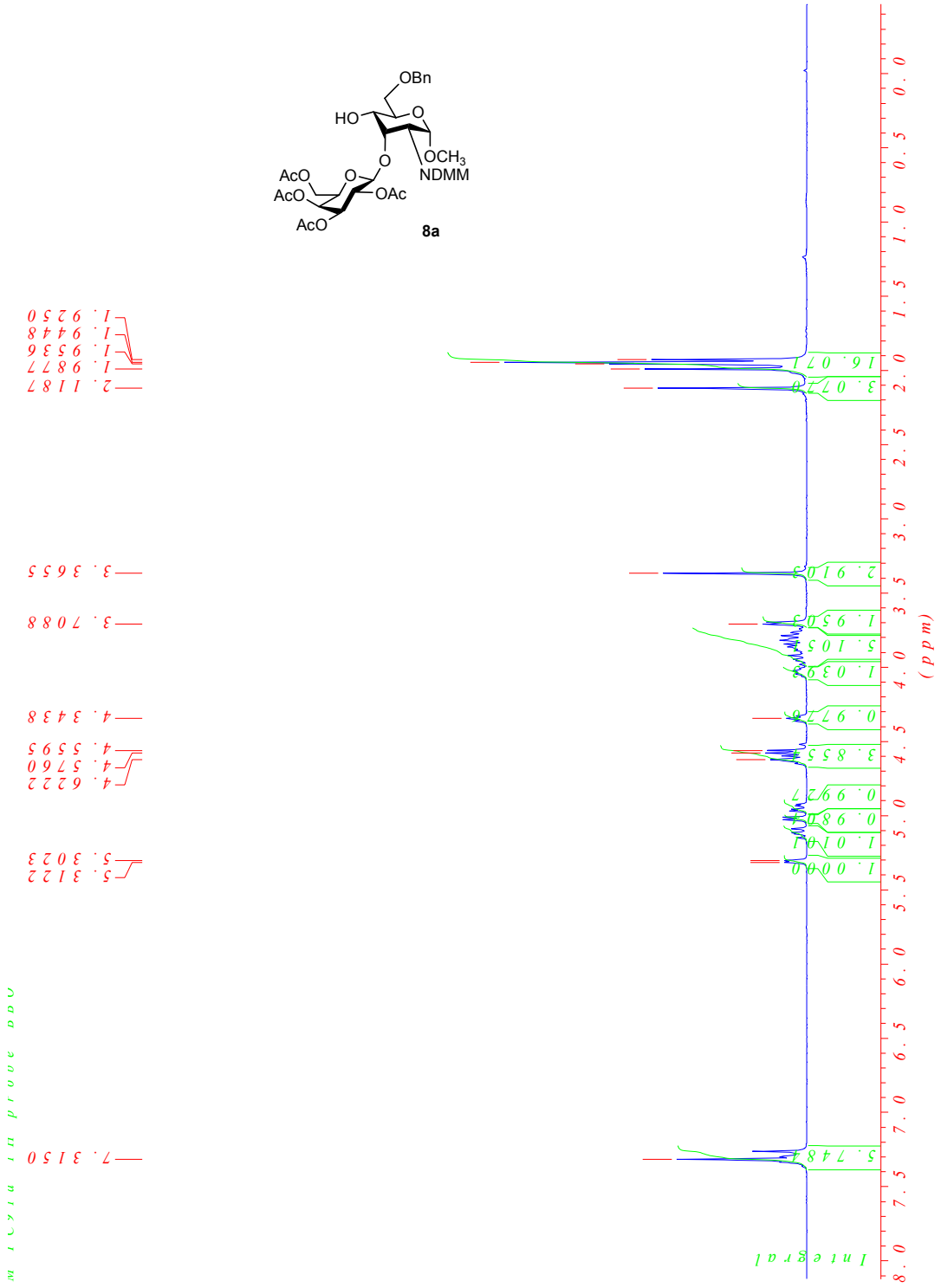
1.9133
1.0023
5.0543
Integral
(ppm)

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O
OCH3
NDMM
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AcO
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OAc
AcO
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1.9877
2.1187
3.6555
3.7088
4.3438
4.5595
4.5760
4.6222
5.3023
5.3122
7.3150
16.071
3.0720
2.9103
1.9503
5.1053
1.0393
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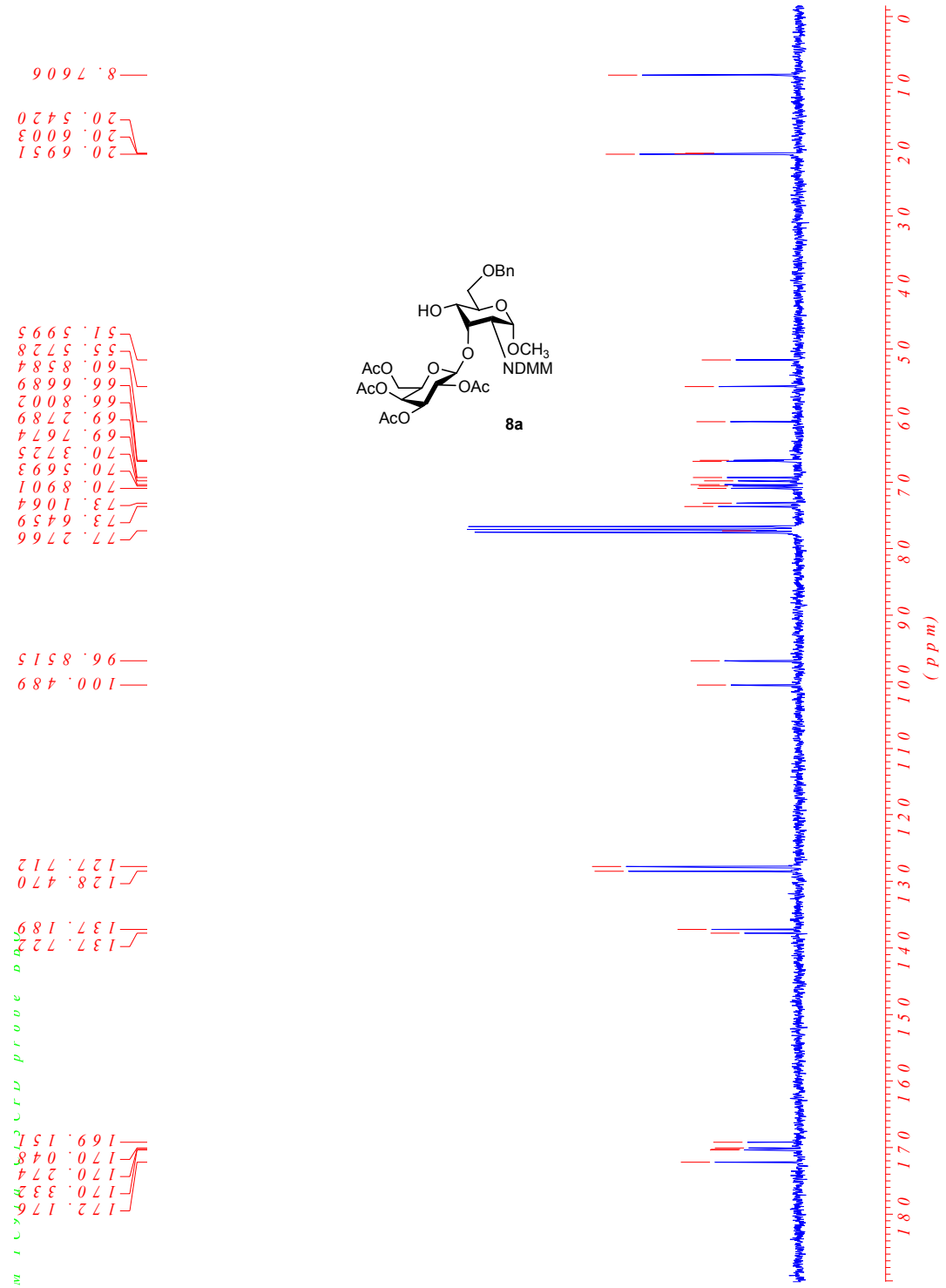
3.8555
0.9927
0.9830
1.0101
1.0000
5.7484
Integral
Normalized Area
(ppm)

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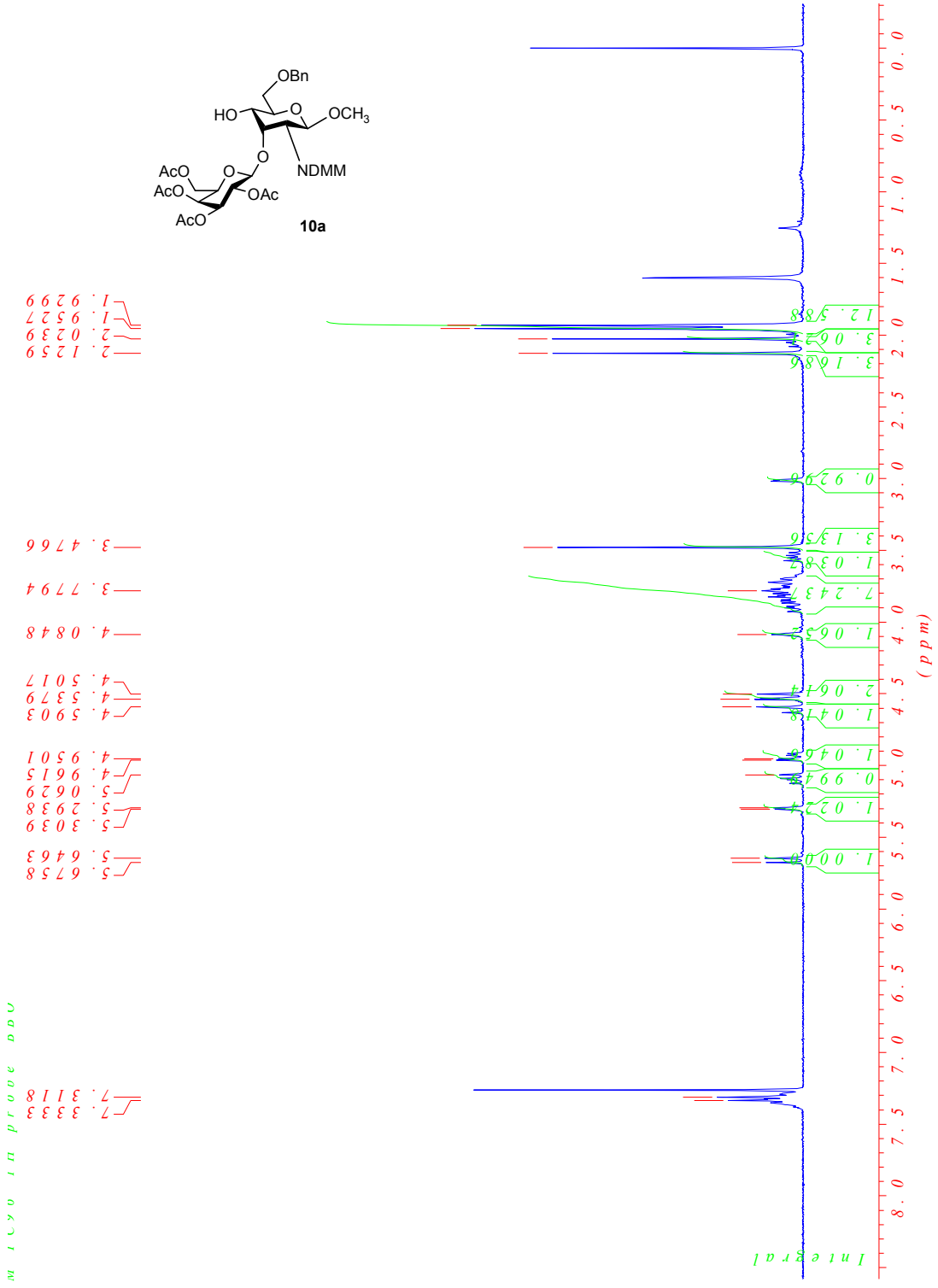
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HO
O
OCH3
O
NDMM
AcO
O
AcO
OAc
AcO
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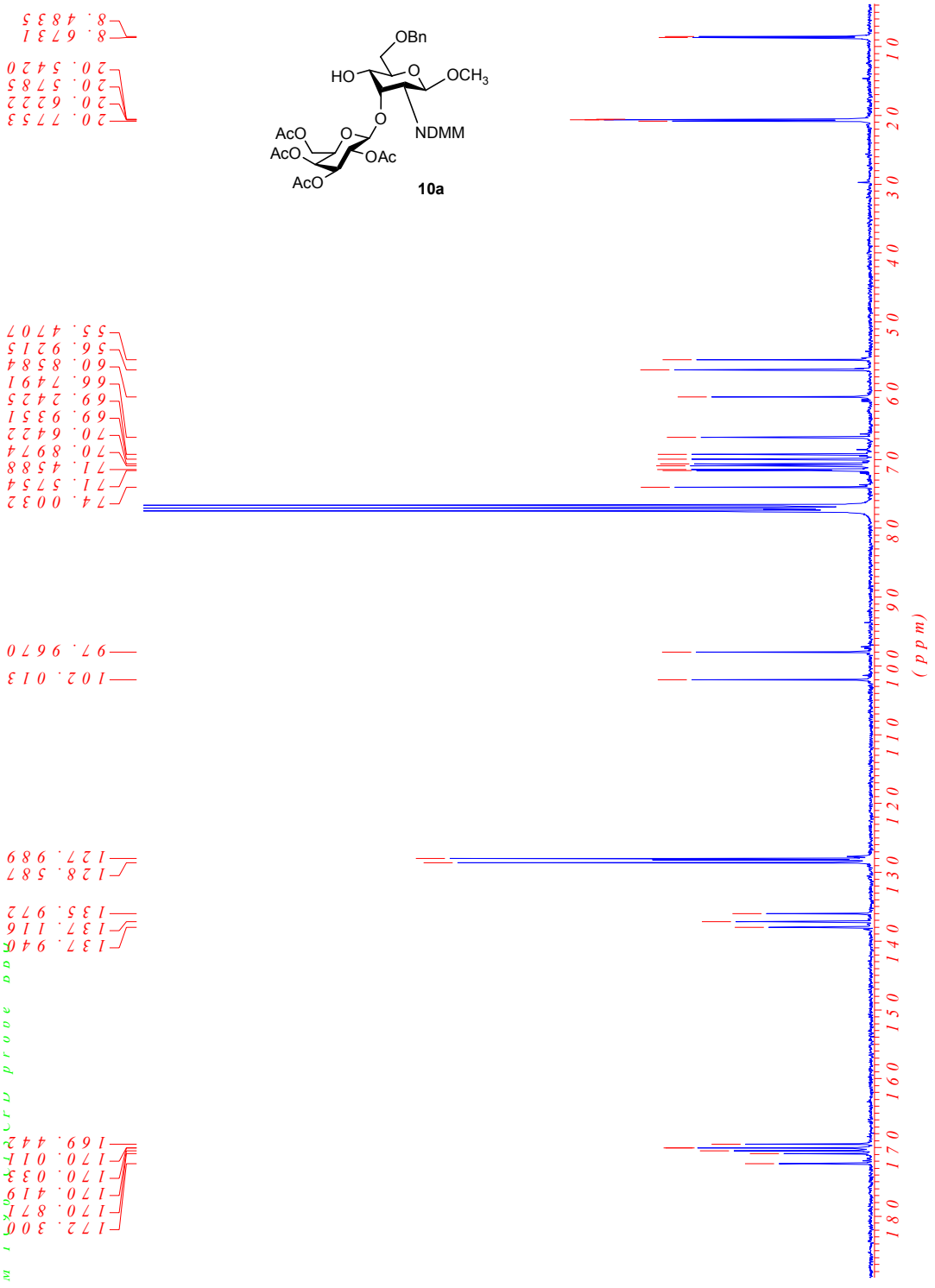
3.0629
2.0239
1.9527
1.9299
0.9296
3.4766
3.7794
4.0848
4.5017
4.5379
4.5903
4.9501
4.9615
5.0629
5.2938
5.3039
5.6463
5.6758
7.3318
7.3333
1.0000
1.0227
0.9947
1.0460
1.0478
2.0647
1.0635
7.2433
1.0382
3.1356
Integral
(ppm)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HO
O
OCH3
O
NDMM
AcO
AcO
O
OAc
AcO
10a
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8.4835
2.0.5420
2.0.5785
2.0.6222
2.0.7753
55.4707
56.9215
60.8584
66.7491
69.2425
69.9351
70.6422
70.8974
71.4588
71.5754
74.0032
97.9670
102.0130
127.9890
128.5870
135.9720
137.1160
137.9400
169.4422
170.0110
170.0330
170.4190
170.8710
172.3000
( ppm )

Cartesian coordinates for the different compounds, as minimized at B3LYP/6-31+G** level

## Compound 6m

Methyl 6-*O*-methyl-2-deoxy-2-dimethylmaleimido-α-D-allopyranoside

Methylated on O3

Energy = -1167.180693 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55201 | 0.00000 | 0.00000 |
| C | 2.16108 | 1.41390 | 0.00000 |
| C | 1.50551 | 2.22259 | -1.13498 |
| C | -0.02788 | 2.20290 | -0.99400 |
| C | -0.74822 | 2.87597 | -2.16373 |
| O | -0.48428 | 0.83731 | -1.02133 |
| O | -0.43024 | 0.35238 | 1.28380 |
| N | 2.08509 | -0.90758 | 1.03100 |
| O | 1.94336 | 2.05317 | 1.29295 |
| O | 2.04854 | 3.52395 | -1.11070 |
| O | -0.31516 | 4.22881 | -2.22963 |
| C | 2.14486 | -0.75637 | 2.37441 |
| C | 2.48327 | -2.03861 | 3.03920 |
| C | 2.62132 | -2.96992 | 2.06704 |
| C | 2.34975 | -2.30134 | 0.74963 |
| O | 1.98512 | 0.33354 | 2.99482 |
| O | 2.33108 | -2.76530 | -0.36015 |
| C | -1.83978 | 0.17819 | 1.50793 |
| C | 2.63813 | -2.12774 | 4.52077 |
| C | 2.97519 | -4.41336 | 2.12885 |
| C | -0.95001 | 4.98488 | -3.26463 |
| C | 2.89246 | 3.10301 | 1.66631 |
| H | -0.36915 | -0.99835 | -0.27228 |
| H | 1.85415 | -0.46184 | -0.94455 |
| H | 3.24370 | 1.35578 | -0.16676 |
| H | 1.76241 | 1.70940 | -2.07768 |
| H | -0.31478 | 2.68461 | -0.05213 |
| H | -1.83344 | 2.82213 | -2.00082 |
| H | -0.51448 | 2.34621 | -3.09982 |
| H | 1.45029 | 4.10185 | -1.62407 |
| H | -2.01744 | 0.43768 | 2.55152 |
| H | -2.13085 | -0.86460 | 1.33045 |
| H | -2.42357 | 0.83561 | 0.85779 |
| H | 2.88811 | -3.14343 | 4.82965 |
| H | 1.71446 | -1.82670 | 5.02679 |
| H | 3.42780 | -1.45376 | 4.87085 |
| H | 3.11799 | -4.75079 | 3.15615 |
| H | 3.89414 | -4.60601 | 1.56327 |
| H | 2.19062 | -5.01917 | 1.66175 |
| H | -2.03531 | 5.01413 | -3.10730 |
| H | -0.54782 | 5.99697 | -3.20794 |
| H | -0.73400 | 4.55670 | -4.25181 |
| H | 2.60014 | 3.41483 | 2.66935 |
| H | 2.80679 | 3.92231 | 0.95810 |
| H | 3.90886 | 2.69607 | 1.67261 |
| H | 1.86586 | 1.16646 | 2.27446 |

Methylated on O4

Energy = -1167.166925 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54610 | 0.00000 | 0.00000 |
| C | 2.16770 | 1.42523 | 0.00000 |
| C | 1.51826 | 2.16530 | -1.17660 |
| C | -0.01443 | 2.16854 | -1.04313 |
| C | -0.70844 | 2.88851 | -2.20215 |
| O | -0.46114 | 0.82203 | -1.09083 |
| O | -0.47798 | 0.40899 | 1.23253 |
| N | 2.10639 | -0.90682 | 0.99599 |
| O | 1.94975 | 2.22577 | 1.12764 |
| O | 1.91095 | 3.59835 | -1.16612 |
| O | -0.12119 | 4.20898 | -2.29226 |
| C | 2.32461 | -0.73058 | 2.36549 |
| C | 2.71170 | -2.06110 | 2.94051 |
| C | 2.72292 | -2.97066 | 1.94321 |
| C | 2.32251 | -2.27379 | 0.67943 |
| O | 2.25657 | 0.32680 | 2.97724 |
| O | 2.18563 | -2.73927 | -0.43292 |
| C | -1.86449 | 0.11924 | 1.47018 |
| C | 3.02574 | -2.19076 | 4.39271 |
| C | 3.04986 | -4.42537 | 1.93984 |
| C | -0.61944 | 5.04363 | -3.35950 |
| C | 3.31804 | 3.97308 | -1.31163 |
| H | -0.37108 | -0.99689 | -0.26917 |
| H | 1.82505 | -0.45819 | -0.95655 |
| H | 3.24571 | 1.29353 | -0.19536 |
| H | 1.83204 | 1.74867 | -2.14094 |
| H | -0.27262 | 2.63913 | -0.08723 |
| H | -1.78157 | 2.98070 | -2.01048 |
| H | -0.55170 | 2.34801 | -3.14402 |
| H | 2.01740 | 1.67433 | 1.94205 |
| H | 1.17283 | 4.09565 | -1.75178 |
| H | -2.07072 | 0.43811 | 2.49176 |
| H | -2.05434 | -0.95688 | 1.37371 |
| H | -2.50778 | 0.66765 | 0.77451 |
| H | 3.29008 | -3.21633 | 4.65535 |
| H | 2.16890 | -1.88160 | 5.00133 |
| H | 3.85734 | -1.53252 | 4.66760 |
| H | 3.30228 | -4.78325 | 2.93931 |
| H | 3.89366 | -4.62875 | 1.27101 |
| H | 2.20380 | -5.00872 | 1.56011 |
| H | -1.69418 | 5.19232 | -3.22572 |
| H | -0.10362 | 6.00018 | -3.27752 |
| H | -0.41665 | 4.58177 | -4.33100 |
| H | 3.32961 | 5.05764 | -1.40799 |
| H | 3.74050 | 3.49069 | -2.19577 |
| H | 3.82219 | 3.67038 | -0.39574 |

## Compound 7m

Methyl 6-*O*-methyl-2-deoxy-2-dimethylmaleimido-β-D-allopyranoside

Methylated on O3

Energy = -1167.178051 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55109 | 0.00000 | 0.00000 |
| C | 2.08915 | 1.43814 | 0.00000 |
| C | 1.47824 | 2.19269 | -1.19558 |
| C | -0.06172 | 2.07147 | -1.19849 |
| C | -0.70045 | 2.62488 | -2.47356 |
| O | -0.42629 | 0.68516 | -1.16516 |
| O | -0.41193 | -1.31599 | -0.04305 |
| N | 2.10934 | -0.86226 | 1.05333 |
| O | 1.71815 | 2.05801 | 1.27110 |
| O | 1.92388 | 3.52986 | -1.14173 |
| O | -0.31217 | 3.98557 | -2.60842 |
| C | 1.98901 | -0.74511 | 2.38826 |
| C | 2.35703 | -1.99884 | 3.08064 |
| C | 2.69838 | -2.89332 | 2.12269 |

| | | | |
|---|---|---|---|
| C | 2.54510 | -2.22156 | 0.78568 |
| O | 1.63225 | 0.32146 | 2.98666 |
| O | 2.74949 | -2.64461 | -0.31832 |
| C | -1.83616 | -1.50855 | 0.02801 |
| C | 2.33655 | -2.10511 | 4.56978 |
| C | 3.17764 | -4.29735 | 2.21689 |
| C | -0.87684 | 4.63139 | -3.75295 |
| C | 2.53610 | 3.18852 | 1.71123 |
| H | -0.41504 | 0.51553 | 0.88594 |
| H | 1.85561 | -0.48104 | -0.93416 |
| H | 3.18281 | 1.44773 | -0.07484 |
| H | 1.85460 | 1.68932 | -2.10243 |
| H | -0.46780 | 2.59819 | -0.32305 |
| H | -1.79314 | 2.53670 | -2.40025 |
| H | -0.36392 | 2.03556 | -3.34009 |
| H | 1.37161 | 4.04400 | -1.76238 |
| H | 1.59732 | 1.14669 | 2.27812 |
| H | -1.99106 | -2.58597 | 0.07906 |
| H | -2.32513 | -1.10418 | -0.86121 |
| H | -2.24368 | -1.03215 | 0.92901 |
| H | 2.64801 | -3.09781 | 4.89692 |
| H | 1.33176 | -1.91061 | 4.96060 |
| H | 3.00494 | -1.36498 | 5.02332 |
| H | 3.24217 | -4.63401 | 3.25213 |
| H | 4.16432 | -4.39619 | 1.74988 |
| H | 2.50569 | -4.96587 | 1.66662 |
| H | -1.97233 | 4.62610 | -3.69477 |
| H | -0.51791 | 5.66110 | -3.74339 |
| H | -0.55633 | 4.13752 | -4.67919 |
| H | 2.12718 | 3.48689 | 2.67693 |
| H | 2.45060 | 3.99046 | 0.98325 |
| H | 3.57695 | 2.86734 | 1.81899 |

Methylated on O4
Energy = -1167.167000 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54504 | 0.00000 | 0.00000 |
| C | 2.09020 | 1.45271 | 0.00000 |
| C | 1.49191 | 2.14262 | -1.22945 |
| C | -0.04784 | 2.07128 | -1.21414 |
| C | -0.67276 | 2.68588 | -2.46951 |
| O | -0.42214 | 0.70970 | -1.19570 |
| O | -0.43535 | -1.29668 | -0.08069 |
| N | 2.13323 | -0.83481 | 1.03499 |
| O | 1.72562 | 2.23392 | 1.11305 |
| O | 1.80728 | 3.59708 | -1.22778 |
| O | -0.12474 | 4.01905 | -2.60172 |
| C | 1.99744 | -0.71585 | 2.41528 |
| C | 2.51040 | -1.97586 | 3.04074 |
| C | 2.92732 | -2.79763 | 2.05269 |
| C | 2.69135 | -2.10851 | 0.74084 |
| O | 1.55991 | 0.27464 | 2.99350 |
| O | 2.93114 | -2.50371 | -0.37832 |
| C | -1.84885 | -1.48471 | 0.09945 |
| C | 2.51794 | -2.13897 | 4.52355 |
| C | 3.53853 | -4.15645 | 2.09650 |
| C | -0.56066 | 4.76186 | -3.76019 |
| C | 3.20252 | 4.04160 | -1.27128 |
| H | -0.42368 | 0.52437 | 0.87094 |
| H | 1.84503 | -0.48405 | -0.93730 |
| H | 3.18534 | 1.39054 | -0.10032 |
| H | 1.89820 | 1.72339 | -2.15723 |
| H | -0.40286 | 2.60064 | -0.31905 |
| H | -1.76043 | 2.74737 | -2.36848 |
| H | -0.42096 | 2.09024 | -3.35576 |
| H | 1.67504 | 1.67382 | 1.92112 |
| H | 1.11383 | 4.01973 | -1.91314 |
| H | -2.00850 | -2.56257 | 0.11703 |
| H | -2.40817 | -1.04222 | -0.72952 |
| H | -2.17654 | -1.04695 | 1.05069 |
| H | 2.92115 | -3.10936 | 4.81753 |
| H | 1.50400 | -2.04435 | 4.92742 |
| H | 3.11745 | -1.35283 | 4.99581 |
| H | 3.65985 | -4.51169 | 3.12109 |
| H | 4.51852 | -4.15327 | 1.60643 |
| H | 2.91798 | -4.87287 | 1.54651 |
| H | -1.64753 | 4.87491 | -3.72614 |
| H | -0.08764 | 5.74201 | -3.70192 |
| H | -0.25970 | 4.24637 | -4.67776 |
| H | 3.16704 | 5.12188 | -1.40328 |
| H | 3.72081 | 3.55515 | -2.10025 |
| H | 3.64311 | 3.79335 | -0.30767 |

## Compound 11f

Methyl 6-*O*-formyl-2-deoxy-2-dimethylmaleimido-α-D-glucopyranoside

Methylated on O3
Energy = -1241.207106 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.56010 | 0.00000 | 0.00000 |
| C | 2.06273 | 1.46273 | 0.00000 |
| C | 1.44433 | 2.22639 | -1.18107 |
| C | -0.09160 | 2.10523 | -1.12187 |
| C | -0.83739 | 2.79087 | -2.25930 |
| O | -0.47547 | 0.72877 | -1.10820 |
| O | -0.40001 | 0.51690 | 1.23725 |
| N | 2.06284 | -0.83892 | 1.12950 |
| O | 3.52165 | 1.39894 | -0.07964 |
| O | 1.82806 | 3.58037 | -1.07170 |
| O | -0.46819 | 2.32012 | -3.58075 |
| C | 3.04744 | -0.63637 | 2.03250 |
| C | 3.11125 | -1.73308 | 3.03038 |
| C | 2.20711 | -2.66271 | 2.65535 |
| C | 1.53506 | -2.16632 | 1.41012 |
| O | 3.87554 | 0.32416 | 2.03400 |
| O | 0.73941 | -2.73687 | 0.71171 |
| C | -1.80072 | 0.35481 | 1.52323 |
| C | 4.08715 | -1.69763 | 4.15840 |
| C | 1.85216 | -3.98706 | 3.23260 |
| C | 0.48500 | 2.98455 | -4.24156 |
| O | 1.17783 | 3.87510 | -3.78732 |
| C | 4.31644 | 2.62187 | -0.25496 |
| H | -0.38499 | -1.00843 | -0.15758 |
| H | 1.88731 | -0.47943 | -0.92798 |
| H | 1.79494 | 1.97796 | 0.93034 |
| H | 1.81470 | 1.77478 | -2.11255 |
| H | -0.42915 | 2.60026 | -0.20032 |
| H | -0.69486 | 3.87190 | -2.20600 |
| H | -1.89848 | 2.55404 | -2.17360 |
| H | 1.69595 | 3.99217 | -1.94839 |
| H | -1.95422 | 0.74905 | 2.52781 |
| H | -2.07725 | -0.70573 | 1.49316 |
| H | -2.41514 | 0.91141 | 0.80924 |
| H | 4.02398 | -2.60567 | 4.75929 |
| H | 3.89878 | -0.83667 | 4.80943 |
| H | 5.11149 | -1.59684 | 3.78386 |
| H | 2.48179 | -4.23499 | 4.08804 |
| H | 1.95314 | -4.77294 | 2.47620 |
| H | 0.80415 | -3.99589 | 3.55401 |
| H | 0.56370 | 2.60675 | -5.26782 |
| H | 5.33622 | 2.32021 | -0.01335 |

| | | | |
|---|---|---|---|
| H | 3.96157 | 3.40535 | 0.41512 |
| H | 4.24827 | 2.95004 | -1.28826 |
| H | 3.81353 | 0.87943 | 1.07339 |

Methylated on O4
Energy = -1241.199782 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54627 | 0.00000 | 0.00000 |
| C | 2.10413 | 1.45038 | 0.00000 |
| C | 1.47053 | 2.17097 | -1.18754 |
| C | -0.06653 | 2.12092 | -1.09425 |
| C | -0.86222 | 2.88348 | -2.14825 |
| O | -0.45901 | 0.76099 | -1.13280 |
| O | -0.44521 | 0.52471 | 1.20773 |
| N | 2.07514 | -0.81636 | 1.09232 |
| O | 3.50399 | 1.46794 | -0.18072 |
| O | 1.81854 | 3.62814 | -1.24347 |
| O | -0.54314 | 2.55559 | -3.53667 |
| C | 2.84074 | -0.46102 | 2.20493 |
| C | 3.03203 | -1.69296 | 3.04063 |
| C | 2.44986 | -2.73119 | 2.40562 |
| C | 1.82661 | -2.20853 | 1.14579 |
| O | 3.31437 | 0.64691 | 2.42787 |
| O | 1.20702 | -2.81986 | 0.29839 |
| C | -1.81702 | 0.23309 | 1.52617 |
| C | 3.79291 | -1.62288 | 4.32150 |
| C | 2.36004 | -4.17698 | 2.75761 |
| C | 0.41268 | 3.21649 | -4.14619 |
| O | 1.21229 | 3.99030 | -3.61093 |
| C | 3.17588 | 4.15816 | -0.93846 |
| H | -0.38793 | -1.00474 | -0.18521 |
| H | 1.85794 | -0.47612 | -0.93709 |
| H | 1.81916 | 1.95501 | 0.93022 |
| H | 1.84335 | 1.73299 | -2.11899 |
| H | -0.35897 | 2.57467 | -0.13498 |
| H | -0.76221 | 3.96338 | -2.01590 |
| H | -1.90979 | 2.60061 | -2.05076 |
| H | 3.88824 | 1.29290 | 0.69943 |
| H | 1.54297 | 3.91087 | -2.22348 |
| H | -1.99890 | 0.65979 | 2.51264 |
| H | -1.97931 | -0.85031 | 1.55684 |
| H | -2.49727 | 0.68434 | 0.79630 |
| H | 3.87065 | -2.60329 | 4.79379 |
| H | 3.30738 | -0.93428 | 5.02208 |
| H | 4.80285 | -1.23462 | 4.15040 |
| H | 2.85393 | -4.39079 | 3.70692 |
| H | 2.81973 | -4.79203 | 1.97604 |
| H | 1.31316 | -4.49256 | 2.82716 |
| H | 0.43874 | 3.00852 | -5.21931 |
| H | 3.11865 | 5.20717 | -1.22691 |
| H | 3.91965 | 3.60541 | -1.50757 |
| H | 3.33324 | 4.04943 | 0.12970 |

## Compound 11m

Methyl 6-*O*-methyl-2-deoxy-2-dimethylmaleimido-α-D-glucopyranoside

Methylated on O3
Energy = -1167.173536 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55936 | 0.00000 | 0.00000 |
| C | 2.05056 | 1.46424 | 0.00000 |
| C | 1.43743 | 2.23471 | -1.17887 |
| C | -0.09757 | 2.08426 | -1.17549 |
| C | -0.74607 | 2.63129 | -2.44836 |
| O | -0.46854 | 0.70538 | -1.12600 |
| O | -0.40151 | 0.54054 | 1.22546 |
| N | 2.06386 | -0.83084 | 1.13366 |
| O | 3.51380 | 1.41297 | -0.07520 |
| O | 1.80180 | 3.59369 | -1.02835 |
| O | -0.39483 | 4.00358 | -2.56628 |
| C | 3.04556 | -0.61452 | 2.03889 |
| C | 3.11282 | -1.70605 | 3.04245 |
| C | 2.21637 | -2.64384 | 2.66975 |
| C | 1.54384 | -2.15843 | 1.41984 |
| O | 3.86520 | 0.35101 | 2.03750 |
| O | 0.75114 | -2.73745 | 0.72378 |
| C | -1.80346 | 0.39083 | 1.51031 |
| C | 4.08421 | -1.65592 | 4.17358 |
| C | 1.86979 | -3.96706 | 3.25484 |
| C | -0.96349 | 4.64749 | -3.70970 |
| C | 4.29240 | 2.64440 | -0.26656 |
| H | -0.38630 | -1.01085 | -0.13906 |
| H | 1.88712 | -0.48217 | -0.92627 |
| H | 1.77638 | 1.97675 | 0.92904 |
| H | 1.83706 | 1.81384 | -2.11673 |
| H | -0.49183 | 2.62096 | -0.30343 |
| H | -1.83584 | 2.51138 | -2.37773 |
| H | -0.39288 | 2.06239 | -3.32189 |
| H | 1.21598 | 4.11557 | -1.61122 |
| H | -1.95693 | 0.80123 | 2.50841 |
| H | -2.08595 | -0.66859 | 1.49647 |
| H | -2.41277 | 0.94032 | 0.78663 |
| H | 4.02742 | -2.56142 | 4.77853 |
| H | 3.88533 | -0.79355 | 4.81960 |
| H | 5.10880 | -1.54682 | 3.80221 |
| H | 2.49930 | -4.20402 | 4.11354 |
| H | 1.97906 | -4.75744 | 2.50438 |
| H | 0.82124 | -3.98191 | 3.57408 |
| H | -2.05897 | 4.61176 | -3.66517 |
| H | -0.63296 | 5.68638 | -3.68395 |
| H | -0.61875 | 4.17349 | -4.63763 |
| H | 5.32439 | 2.34537 | -0.08106 |
| H | 3.96419 | 3.41151 | 0.43576 |
| H | 4.16562 | 2.99248 | -1.28771 |
| H | 3.80276 | 0.90747 | 1.06220 |

Methylated on O4
Energy = -1167.170588 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54946 | 0.00000 | 0.00000 |
| C | 2.08786 | 1.45609 | 0.00000 |
| C | 1.46718 | 2.15580 | -1.20335 |
| C | -0.07095 | 2.09686 | -1.14897 |
| C | -0.73533 | 2.75837 | -2.35642 |
| O | -0.46425 | 0.73919 | -1.14780 |
| O | -0.44327 | 0.54493 | 1.19782 |
| N | 2.07438 | -0.81422 | 1.09593 |
| O | 3.49309 | 1.51747 | -0.13564 |
| O | 1.81978 | 3.61519 | -1.20276 |
| O | -0.25610 | 4.12242 | -2.37541 |
| C | 2.83562 | -0.45891 | 2.21202 |
| C | 3.03551 | -1.69535 | 3.04066 |
| C | 2.46071 | -2.73370 | 2.39943 |
| C | 1.83751 | -2.20801 | 1.14145 |
| O | 3.29822 | 0.65094 | 2.44545 |
| O | 1.22633 | -2.82028 | 0.28860 |
| C | -1.81879 | 0.27334 | 1.51610 |
| C | 3.79575 | -1.62872 | 4.32207 |
| C | 2.37675 | -4.18201 | 2.74279 |
| C | -0.73349 | 4.93827 | -3.46709 |
| C | 3.14555 | 4.02001 | -1.72799 |

| | | | |
|---|---|---|---|
| H | -0.38859 | -1.00748 | -0.16864 |
| H | 1.86220 | -0.48088 | -0.93435 |
| H | 1.76393 | 1.96793 | 0.91248 |
| H | 1.85218 | 1.74383 | -2.14302 |
| H | -0.40608 | 2.60211 | -0.23256 |
| H | -1.82380 | 2.75079 | -2.24563 |
| H | -0.46019 | 2.24930 | -3.28869 |
| H | 3.85107 | 1.36308 | 0.76004 |
| H | 1.03133 | 4.06373 | -1.74441 |
| H | -1.99736 | 0.71358 | 2.49722 |
| H | -1.99455 | -0.80765 | 1.55889 |
| H | -2.49163 | 0.72480 | 0.77967 |
| H | 3.86931 | -2.60957 | 4.79462 |
| H | 3.31338 | -0.93753 | 5.02207 |
| H | 4.80759 | -1.24513 | 4.15105 |
| H | 2.87914 | -4.40148 | 3.68631 |
| H | 2.83012 | -4.79115 | 1.95304 |
| H | 1.33096 | -4.49971 | 2.81964 |
| H | -1.82444 | 4.99234 | -3.42440 |
| H | -0.31025 | 5.93238 | -3.32419 |
| H | -0.41071 | 4.51939 | -4.42551 |
| H | 3.19336 | 5.09817 | -1.58184 |
| H | 3.20592 | 3.74992 | -2.78428 |
| H | 3.88685 | 3.49204 | -1.13625 |

## Compound 12f

Methyl 6-*O*-formyl-2-deoxy-2-dimethylmaleimido-β-D-glucopyranoside

Methylated on O3
Energy = -1241.195251 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55820 | 0.00000 | 0.00000 |
| C | 1.98100 | 1.48719 | 0.00000 |
| C | 1.46994 | 2.13506 | -1.29775 |
| C | -0.06584 | 1.92418 | -1.38300 |
| C | -0.71356 | 2.45588 | -2.65600 |
| O | -0.40809 | 0.54738 | -1.24382 |
| O | -0.47103 | -1.28186 | 0.13380 |
| N | 2.11188 | -0.82796 | 1.09176 |
| O | 3.41413 | 1.52822 | 0.20060 |
| O | 1.75623 | 3.51526 | -1.25298 |
| O | -0.16779 | 1.89615 | -3.87633 |
| C | 2.78256 | -0.52185 | 2.21231 |
| C | 2.95559 | -1.70148 | 3.09099 |
| C | 2.52124 | -2.77701 | 2.39470 |
| C | 2.06189 | -2.29664 | 1.04753 |
| O | 3.30824 | 0.61603 | 2.47124 |
| O | 1.81600 | -2.92356 | 0.05872 |
| C | -1.90318 | -1.39212 | 0.22493 |
| C | 3.58826 | -1.58537 | 4.43826 |
| C | 2.51337 | -4.22683 | 2.72537 |
| C | 0.81503 | 2.56689 | -4.48836 |
| O | 1.39513 | 3.53897 | -4.04481 |
| C | 4.14883 | 2.78326 | 0.02816 |
| H | -0.38125 | 0.64649 | 0.81705 |
| H | 1.87752 | -0.48083 | -0.92910 |
| H | 1.51760 | 2.02487 | 0.84114 |
| H | 1.96391 | 1.64550 | -2.14804 |
| H | -0.51424 | 2.50545 | -0.55907 |
| H | -0.63619 | 3.54431 | -2.68951 |
| H | -1.76324 | 2.16004 | -2.66291 |
| H | 1.70841 | 3.85309 | -2.16861 |
| H | 3.43426 | 1.13842 | 1.54778 |
| H | -2.10920 | -2.44383 | 0.42145 |
| H | -2.37316 | -1.09047 | -0.71390 |
| H | -2.28387 | -0.77781 | 1.05117 |
| H | 3.71411 | -2.56663 | 4.89750 |
| H | 2.97527 | -0.96867 | 5.10525 |
| H | 4.56914 | -1.10360 | 4.36806 |
| H | 3.00352 | -4.42804 | 3.67879 |
| H | 3.01309 | -4.79926 | 1.93650 |
| H | 1.48318 | -4.59949 | 2.77579 |
| H | 1.03430 | 2.10808 | -5.45983 |
| H | 5.13053 | 2.58658 | 0.46020 |
| H | 3.64257 | 3.59884 | 0.54668 |
| H | 4.23712 | 3.01211 | -1.03099 |

Methylated on O4
Energy = -1241.195200 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54140 | 0.00000 | 0.00000 |
| C | 2.12812 | 1.43839 | 0.00000 |
| C | 1.46813 | 2.23259 | -1.11932 |
| C | -0.06697 | 2.17195 | -0.97415 |
| C | -0.89870 | 3.02182 | -1.93138 |
| O | -0.44322 | 0.82103 | -1.11304 |
| O | -0.42387 | -1.28689 | -0.19547 |
| N | 2.11153 | -0.77019 | 1.09009 |
| O | 3.52272 | 1.41507 | -0.25385 |
| O | 1.83241 | 3.68652 | -1.10193 |
| O | -0.64246 | 2.79316 | -3.35096 |
| C | 1.81374 | -0.60399 | 2.45463 |
| C | 2.36148 | -1.79795 | 3.17851 |
| C | 2.89906 | -2.63953 | 2.26751 |
| C | 2.73621 | -2.03098 | 0.90586 |
| O | 1.22031 | 0.35579 | 2.91744 |
| O | 3.07702 | -2.47480 | -0.16862 |
| C | -1.83272 | -1.50963 | -0.01544 |
| C | 2.25066 | -1.90233 | 4.66243 |
| C | 3.57097 | -3.96105 | 2.42668 |
| C | 0.29275 | 3.48811 | -3.95521 |
| O | 1.12152 | 4.21795 | -3.40322 |
| C | 3.22495 | 4.15055 | -0.85576 |
| H | -0.41486 | 0.43769 | 0.92244 |
| H | 1.85995 | -0.50647 | -0.91829 |
| H | 1.91244 | 1.91503 | 0.96730 |
| H | 1.79979 | 1.84181 | -2.08620 |
| H | -0.32803 | 2.55179 | 0.02968 |
| H | -0.77962 | 4.08784 | -1.72244 |
| H | -1.94451 | 2.74179 | -1.80898 |
| H | 3.93495 | 0.73474 | 0.29935 |
| H | 1.50833 | 4.03836 | -2.04750 |
| H | -1.97805 | -2.58661 | -0.09486 |
| H | -2.40818 | -1.00166 | -0.79437 |
| H | -2.15255 | -1.16536 | 0.97592 |
| H | 2.69685 | -2.82605 | 5.03451 |
| H | 1.20026 | -1.87127 | 4.97260 |
| H | 2.74464 | -1.05371 | 5.14847 |
| H | 3.62474 | -4.26390 | 3.47363 |
| H | 4.58666 | -3.92846 | 2.01698 |
| H | 3.03435 | -4.73302 | 1.86389 |
| H | 0.26996 | 3.35401 | -5.04009 |
| H | 3.18470 | 5.22355 | -1.03724 |
| H | 3.90347 | 3.63695 | -1.53395 |
| H | 3.46061 | 3.92956 | 0.18010 |

## Compound 12m

Methyl 6-*O*-methyl-2-deoxy-2-dimethylmaleimido-β-D-glucopyranoside

Methylated on O3
Energy = -1167.162157 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55811 | 0.00000 | 0.00000 |
| C | 1.97016 | 1.48779 | 0.00000 |
| C | 1.46308 | 2.14224 | -1.29537 |
| C | -0.06421 | 1.89462 | -1.43619 |
| C | -0.59133 | 2.27241 | -2.82197 |
| O | -0.39892 | 0.51985 | -1.25809 |
| O | -0.47399 | -1.27855 | 0.15886 |
| N | 2.11681 | -0.82257 | 1.09266 |
| O | 3.40351 | 1.54255 | 0.20800 |
| O | 1.72059 | 3.52899 | -1.20423 |
| O | -0.25168 | 3.63024 | -3.06711 |
| C | 2.78146 | -0.51005 | 2.21530 |
| C | 2.95955 | -1.68827 | 3.09549 |
| C | 2.53054 | -2.76655 | 2.40042 |
| C | 2.06830 | -2.29006 | 1.05298 |
| O | 3.29780 | 0.63141 | 2.47535 |
| O | 1.81934 | -2.92090 | 0.06709 |
| C | -1.90521 | -1.38253 | 0.26540 |
| C | 3.59199 | -1.56822 | 4.44249 |
| C | 2.52983 | -4.21603 | 2.73265 |
| C | -0.71600 | 4.12203 | -4.32739 |
| C | 4.12174 | 2.80482 | 0.02187 |
| H | -0.38367 | 0.66364 | 0.80108 |
| H | 1.87776 | -0.48165 | -0.92843 |
| H | 1.49785 | 2.02180 | 0.83794 |
| H | 1.98798 | 1.68934 | -2.15211 |
| H | -0.56794 | 2.51062 | -0.67477 |
| H | -1.68063 | 2.13147 | -2.84447 |
| H | -0.14164 | 1.61423 | -3.58077 |
| H | 1.20615 | 3.96273 | -1.91231 |
| H | 3.42323 | 1.15595 | 1.54992 |
| H | -2.11325 | -2.43126 | 0.47570 |
| H | -2.38404 | -1.08944 | -0.67179 |
| H | -2.27566 | -0.75771 | 1.08839 |
| H | 3.72227 | -2.54860 | 4.90248 |
| H | 2.97680 | -0.95344 | 5.10919 |
| H | 4.57080 | -1.08232 | 4.37132 |
| H | 3.02359 | -4.41326 | 3.68488 |
| H | 3.03002 | -4.78718 | 1.94319 |
| H | 1.50156 | -4.59339 | 2.78666 |
| H | -1.80985 | 4.06143 | -4.38405 |
| H | -0.40653 | 5.16572 | -4.39218 |
| H | -0.27365 | 3.55409 | -5.15582 |
| H | 5.12251 | 2.61032 | 0.40835 |
| H | 3.63120 | 3.60838 | 0.57397 |
| H | 4.15811 | 3.05095 | -1.03656 |

Methylated on O4
Energy = -1167.165589 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54342 | 0.00000 | 0.00000 |
| C | 2.10953 | 1.44466 | 0.00000 |
| C | 1.46287 | 2.22197 | -1.13426 |
| C | -0.07548 | 2.14516 | -1.04205 |
| C | -0.77600 | 2.89232 | -2.17852 |
| O | -0.44387 | 0.79031 | -1.13786 |
| O | -0.42865 | -1.28966 | -0.16160 |
| N | 2.11174 | -0.76243 | 1.09675 |
| O | 3.51191 | 1.45809 | -0.21767 |
| O | 1.81330 | 3.67920 | -1.05116 |
| O | -0.28465 | 4.25133 | -2.13306 |
| C | 1.81352 | -0.59196 | 2.45959 |
| C | 2.38923 | -1.76813 | 3.19160 |
| C | 2.94237 | -2.60494 | 2.28603 |
| C | 2.76105 | -2.01088 | 0.91977 |
| O | 1.19999 | 0.35707 | 2.91830 |
| O | 3.10461 | -2.45870 | -0.15229 |
| C | -1.83511 | -1.50513 | 0.04276 |
| C | 2.28452 | -1.86208 | 4.67656 |
| C | 3.64089 | -3.91175 | 2.45347 |
| C | -0.80042 | 5.13879 | -3.14957 |
| C | 3.14292 | 4.11474 | -1.53726 |
| H | -0.41285 | 0.46437 | 0.90967 |
| H | 1.86686 | -0.51094 | -0.91397 |
| H | 1.86048 | 1.93016 | 0.95368 |
| H | 1.81917 | 1.86662 | -2.10725 |
| H | -0.39276 | 2.58024 | -0.08002 |
| H | -1.85963 | 2.88705 | -2.02784 |
| H | -0.53939 | 2.43743 | -3.14841 |
| H | 3.93667 | 0.84922 | 0.40437 |
| H | 1.01514 | 4.15893 | -1.55779 |
| H | -1.98447 | -2.58302 | -0.01402 |
| H | -2.42094 | -1.01027 | -0.73698 |
| H | -2.13968 | -1.14113 | 1.03180 |
| H | 2.76392 | -2.76580 | 5.05596 |
| H | 1.23415 | -1.86604 | 4.98864 |
| H | 2.74809 | -0.99147 | 5.15339 |
| H | 3.73626 | -4.18754 | 3.50506 |
| H | 4.64025 | -3.87437 | 2.00607 |
| H | 3.09642 | -4.70614 | 1.93029 |
| H | -1.88764 | 5.20029 | -3.05353 |
| H | -0.35899 | 6.11784 | -2.96426 |
| H | -0.52562 | 4.77724 | -4.14553 |
| H | 3.17175 | 5.18999 | -1.36707 |
| H | 3.23395 | 3.86771 | -2.59682 |
| H | 3.88229 | 3.58824 | -0.94111 |

## Compound 14α E

Methyl 4,6-*O*-ethylidene-α-D-allopyranoside

Methylated on O2
Energy = -843.590921 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55916 | 0.00000 | 0.00000 |
| C | 2.23243 | 1.38198 | 0.00000 |
| C | 1.48256 | 2.27037 | -0.99952 |
| C | -0.01378 | 2.28320 | -0.68348 |
| C | -0.70043 | 3.25852 | -1.63499 |
| O | -0.52841 | 0.94873 | -0.86719 |
| O | -0.35190 | 0.18628 | 1.36511 |
| O | 1.86776 | -0.75485 | 1.25260 |
| O | 2.16744 | 1.90465 | 1.31513 |
| O | 2.01275 | 3.57672 | -0.89077 |
| O | -0.05962 | 4.52317 | -1.46676 |
| C | -1.72438 | -0.13085 | 1.70039 |
| C | 1.31844 | 4.50280 | -1.76135 |
| C | 1.89421 | 5.87942 | -1.54436 |
| C | 3.24318 | -0.83627 | 1.80531 |
| H | -0.37942 | -0.96595 | -0.35405 |
| H | 1.93087 | -0.61869 | -0.81803 |
| H | 3.28006 | 1.28343 | -0.32036 |
| H | 1.62673 | 1.87514 | -2.01976 |
| H | -0.17805 | 2.60596 | 0.34878 |
| H | -1.75431 | 3.39978 | -1.38990 |
| H | -0.61921 | 2.90808 | -2.67503 |
| H | 1.13665 | -0.43814 | 1.87427 |
| H | 2.34151 | 2.85923 | 1.26400 |

| | | | |
|---|---|---|---|
| H | -1.83194 | 0.07895 | 2.76383 |
| H | -1.92878 | -1.18778 | 1.49898 |
| H | -2.40106 | 0.50299 | 1.12379 |
| H | 1.46531 | 4.14319 | -2.79399 |
| H | 1.40565 | 6.58917 | -2.21558 |
| H | 2.96674 | 5.87387 | -1.75164 |
| H | 1.72581 | 6.19657 | -0.51203 |
| H | 3.85764 | -1.26790 | 1.01715 |
| H | 3.16551 | -1.51813 | 2.65047 |
| H | 3.56326 | 0.16134 | 2.09879 |

Methylated on O3
Energy = -843.597910 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.55570 | 0.00000 | 0.00000 |
| C | 2.04230 | 1.45145 | 0.00000 |
| C | 1.43013 | 2.18599 | -1.17869 |
| C | -0.10232 | 2.08787 | -1.15131 |
| C | -0.63143 | 2.77626 | -2.40741 |
| O | -0.51672 | 0.71107 | -1.09399 |
| O | -0.37854 | 0.57698 | 1.25950 |
| O | 2.11709 | -0.62927 | 1.13253 |
| O | 1.55567 | 2.08761 | 1.27561 |
| O | 1.82762 | 3.53469 | -1.21541 |
| O | -0.13027 | 4.11232 | -2.38554 |
| C | -1.79110 | 0.54322 | 1.58628 |
| C | 1.27930 | 4.19532 | -2.38119 |
| C | 1.69005 | 5.64543 | -2.34145 |
| C | 2.52539 | 2.25660 | 2.37672 |
| H | -0.41261 | -1.01122 | -0.07338 |
| H | 1.88471 | -0.46709 | -0.93641 |
| H | 3.12947 | 1.53210 | 0.03307 |
| H | 1.79042 | 1.65491 | -2.07833 |
| H | -0.48656 | 2.63345 | -0.28209 |
| H | -1.72054 | 2.84285 | -2.41099 |
| H | -0.30298 | 2.24096 | -3.31094 |
| H | 2.03695 | -1.59143 | 1.07511 |
| H | 0.68551 | 1.57203 | 1.53269 |
| H | -1.88737 | 0.99483 | 2.57291 |
| H | -2.12300 | -0.49785 | 1.62042 |
| H | -2.36857 | 1.10342 | 0.84827 |
| H | 1.67500 | 3.66974 | -3.26745 |
| H | 1.30550 | 6.15838 | -3.22574 |
| H | 2.77947 | 5.72546 | -2.32925 |
| H | 1.28175 | 6.12418 | -1.44789 |
| H | 2.92427 | 1.28157 | 2.65323 |
| H | 1.96640 | 2.71854 | 3.18900 |
| H | 3.29189 | 2.93523 | 2.00708 |

## Compound 14β E

Methyl 4,6-*O*-ethylidene-β-D-allopyranoside

Methylated on O2
Energy = -843.588394 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54280 | 0.00000 | 0.00000 |
| C | 2.16307 | 1.40534 | 0.00000 |
| C | 1.45153 | 2.29464 | -1.01424 |
| C | -0.06859 | 2.19268 | -0.86406 |
| C | -0.70406 | 3.12751 | -1.88894 |
| O | -0.43271 | 0.82279 | -1.07244 |
| O | -0.40228 | -1.30467 | -0.20098 |
| O | 2.11177 | -0.58181 | 1.26901 |
| O | 1.97683 | 1.85286 | 1.35183 |
| O | 1.88477 | 3.62571 | -0.82665 |
| O | -0.17242 | 4.43021 | -1.63648 |
| C | -1.83141 | -1.51422 | -0.17762 |
| C | 1.22879 | 4.51495 | -1.76538 |
| C | 1.67012 | 5.92592 | -1.46880 |
| C | 1.70484 | -1.89546 | 1.83041 |
| H | -0.39740 | 0.40944 | 0.94791 |
| H | 1.91457 | -0.63546 | -0.80436 |
| H | 3.23534 | 1.34991 | -0.22468 |
| H | 1.71897 | 1.93636 | -2.02355 |
| H | -0.37024 | 2.51712 | 0.14045 |
| H | -1.78637 | 3.19751 | -1.77070 |
| H | -0.47531 | 2.79655 | -2.91298 |
| H | 2.14929 | 0.18460 | 1.90762 |
| H | 2.29192 | 2.76601 | 1.44505 |
| H | -1.97525 | -2.59138 | -0.25383 |
| H | -2.30411 | -1.01228 | -1.02398 |
| H | -2.25705 | -1.14659 | 0.76428 |
| H | 1.52281 | 4.18499 | -2.77622 |
| H | 1.21118 | 6.61036 | -2.18562 |
| H | 2.75685 | 6.00327 | -1.54885 |
| H | 1.35910 | 6.21039 | -0.46036 |
| H | 0.68763 | -1.83038 | 2.20936 |
| H | 2.43520 | -2.10044 | 2.61141 |
| H | 1.77947 | -2.60685 | 1.01230 |

Methylated on O3
Energy = -843.591977 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.54428 | 0.00000 | 0.00000 |
| C | 2.13913 | 1.41446 | 0.00000 |
| C | 1.38971 | 2.34586 | -0.93041 |
| C | -0.13399 | 2.20942 | -0.77787 |
| C | -0.78738 | 3.15784 | -1.78084 |
| O | -0.48858 | 0.85262 | -1.03041 |
| O | -0.36978 | -1.30855 | -0.21770 |
| O | 2.06242 | -0.59286 | 1.19563 |
| O | 1.98854 | 1.84395 | 1.44766 |
| O | 1.80754 | 3.68288 | -0.75399 |
| O | -0.26655 | 4.46533 | -1.53137 |
| C | -1.77862 | -1.58669 | -0.08145 |
| C | 1.12568 | 4.56110 | -1.69247 |
| C | 1.56560 | 5.97706 | -1.41854 |
| C | 2.92972 | 2.86686 | 1.98387 |
| H | -0.38811 | 0.36742 | 0.97023 |
| H | 1.88723 | -0.53527 | -0.89193 |
| H | 3.21728 | 1.40796 | -0.18121 |
| H | 1.64689 | 1.99150 | -1.94560 |
| H | -0.43853 | 2.50722 | 0.23587 |
| H | -1.86805 | 3.21325 | -1.64450 |
| H | -0.57225 | 2.83603 | -2.81043 |
| H | 1.64980 | -1.45917 | 1.34183 |
| H | 2.05423 | 0.96664 | 1.93162 |
| H | -1.88148 | -2.66517 | -0.19382 |
| H | -2.34615 | -1.07390 | -0.86108 |
| H | -2.13427 | -1.28031 | 0.90976 |
| H | 1.40596 | 4.22078 | -2.70364 |
| H | 1.09195 | 6.65017 | -2.13646 |
| H | 2.65035 | 6.06106 | -1.51783 |
| H | 1.26574 | 6.27418 | -0.41018 |
| H | 3.94622 | 2.47868 | 1.90863 |
| H | 2.62376 | 3.02130 | 3.01712 |
| H | 2.77472 | 3.75164 | 1.37306 |

## Compound 1e

Methyl 4,6-*O*-ethylidene-2-deoxy-2-dimethylmaleimido-α-D-glucopyranoside

Methylated on O3

Energy = -1205.282240 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.56590 | 0.00000 | 0.00000 |
| C | 2.08820 | 1.46078 | 0.00000 |
| C | 1.46045 | 2.18257 | -1.19454 |
| C | -0.06834 | 2.10943 | -1.08094 |
| C | -0.67896 | 2.86006 | -2.26090 |
| O | -0.48839 | 0.74823 | -1.09100 |
| O | -0.39189 | 0.48877 | 1.25094 |
| N | 2.05919 | -0.84530 | 1.12840 |
| O | 3.54430 | 1.38943 | -0.06020 |
| O | 1.84645 | 3.54757 | -1.21749 |
| O | -0.16922 | 4.19272 | -2.23911 |
| C | 3.01864 | -0.64183 | 2.05421 |
| C | 3.06277 | -1.73739 | 3.05323 |
| C | 2.17207 | -2.67105 | 2.65591 |
| C | 1.52863 | -2.17720 | 1.39423 |
| O | 3.84722 | 0.32143 | 2.07719 |
| O | 0.75460 | -2.74878 | 0.67327 |
| C | -1.79595 | 0.34355 | 1.53180 |
| C | 4.01093 | -1.69808 | 4.20448 |
| C | 1.81133 | -3.99759 | 3.22441 |
| C | 1.67222 | 5.69352 | -2.26660 |
| C | 1.23455 | 4.25000 | -2.32270 |
| C | 4.31887 | 2.62611 | -0.20477 |
| H | -0.38034 | -1.00792 | -0.17383 |
| H | 1.89337 | -0.48158 | -0.92663 |
| H | 1.80999 | 1.98486 | 0.92257 |
| H | 1.77900 | 1.68066 | -2.12415 |
| H | -0.37842 | 2.60138 | -0.15146 |
| H | -1.76429 | 2.93108 | -2.17291 |
| H | -0.43073 | 2.35776 | -3.20818 |
| H | 3.81386 | 0.86473 | 1.12765 |
| H | -1.94189 | 0.70854 | 2.54851 |
| H | -2.09161 | -0.71050 | 1.46870 |
| H | -2.39889 | 0.93400 | 0.83597 |
| H | 3.93294 | -2.60457 | 4.80561 |
| H | 3.80611 | -0.83578 | 4.84870 |
| H | 5.04429 | -1.59817 | 3.85536 |
| H | 2.41352 | -4.23604 | 4.10203 |
| H | 1.94799 | -4.78449 | 2.47452 |
| H | 0.75281 | -4.01737 | 3.50857 |
| H | 1.22642 | 6.24133 | -3.10000 |
| H | 2.76033 | 5.76359 | -2.33904 |
| H | 1.34161 | 6.14635 | -1.32846 |
| H | 1.56331 | 3.74845 | -3.25010 |
| H | 5.34184 | 2.34495 | 0.04676 |
| H | 3.94126 | 3.39101 | 0.47622 |
| H | 4.25564 | 2.97251 | -1.23265 |

## Compound 2e

Methyl 4,6-*O*-ethylidene-2-deoxy-2-dimethylmaleimido-β-D-glucopyranoside

Methylated on O3

Energy = -1205.270697 Hartrees

| | | | |
|---|---|---|---|
| C | 0.00000 | 0.00000 | 0.00000 |
| C | 1.56329 | 0.00000 | 0.00000 |
| C | 2.00939 | 1.48489 | 0.00000 |
| C | 1.48712 | 2.09602 | -1.30432 |
| C | -0.04890 | 1.93527 | -1.33115 |
| C | -0.57312 | 2.55469 | -2.62334 |
| O | -0.42016 | 0.56704 | -1.23280 |
| O | -0.46376 | -1.28611 | 0.11911 |
| N | 2.10712 | -0.83177 | 1.09257 |
| O | 3.43994 | 1.51066 | 0.20929 |
| O | 1.78671 | 3.47873 | -1.38389 |
| O | -0.14366 | 3.91526 | -2.65376 |
| C | 2.75601 | -0.52962 | 2.22483 |
| C | 2.90343 | -1.70823 | 3.10895 |
| C | 2.47545 | -2.78261 | 2.40615 |
| C | 2.04916 | -2.30226 | 1.04773 |
| O | 3.28444 | 0.60695 | 2.49492 |
| O | 1.82435 | -2.92727 | 0.05291 |
| C | -1.89504 | -1.40266 | 0.22746 |
| C | 3.50891 | -1.59376 | 4.46890 |
| C | 2.44931 | -4.23100 | 2.74187 |
| C | 1.59464 | 5.53344 | -2.59854 |
| C | 1.25562 | 4.06269 | -2.59531 |
| C | 4.16041 | 2.77010 | 0.03354 |
| H | -0.37736 | 0.63301 | 0.82876 |
| H | 1.88291 | -0.48430 | -0.92699 |
| H | 1.54614 | 2.03246 | 0.83471 |
| H | 1.92793 | 1.55887 | -2.16050 |
| H | -0.46633 | 2.50376 | -0.48579 |
| H | -1.66397 | 2.56328 | -2.64875 |
| H | -0.19949 | 2.00069 | -3.49751 |
| H | 3.43460 | 1.12429 | 1.58272 |
| H | -2.09539 | -2.45928 | 0.40245 |
| H | -2.37863 | -1.08003 | -0.69730 |
| H | -2.26521 | -0.80836 | 1.07282 |
| H | 3.60446 | -2.57398 | 4.93720 |
| H | 2.89408 | -0.95976 | 5.11792 |
| H | 4.50100 | -1.13267 | 4.41682 |
| H | 2.91973 | -4.43231 | 3.70521 |
| H | 2.95897 | -4.81101 | 1.96499 |
| H | 1.41515 | -4.59481 | 2.77473 |
| H | 1.20844 | 5.99421 | -3.51054 |
| H | 2.67785 | 5.67271 | -2.56249 |
| H | 1.13740 | 6.02214 | -1.73440 |
| H | 1.71317 | 3.52469 | -3.44404 |
| H | 5.14861 | 2.58925 | 0.45731 |
| H | 3.64958 | 3.57992 | 0.55914 |
| H | 4.23494 | 3.00238 | -1.02626 |