

Supplementary Table 1

Calculated energies (B3LYP/6-31G**), relative populations (T=298K) and calculated coupling constants (FC-contribution only, see methods) of GlcNAc, together with the weighted average coupling constant.

| Dihedral Angle [°] | Energy [Hartrees] | GlcNAc α | | GlcNAc α [PCM] | | | GlcNAc β | | |
|--------------------|-------------------|-----------------|---------------|-----------------------|------|---------------|-------------------|------|---------------|
| | | %Pop | J (FC-only) | Energy [Hartrees] | %Pop | J (FC-only) | Energy [Hartrees] | %Pop | J (FC-only) |
| 0 | -819.9921 | 16% | 8.17 | -820.0285 | 0% | 8.17 | -819.9867 | 0% | 7.72 |
| 30 | -819.9927 | 33% | 7.08 | -820.0350 | 92% | 7.08 | -819.9841 | 0% | 6.57 |
| 60 | -819.9930 | 43% | 2.37 | -820.0325 | 6% | 2.37 | -819.9797 | 0% | 3.09 |
| 90 | -819.9902 | 2% | 0.26 | -820.0269 | 0% | 0.26 | -819.9863 | 0% | 0.35 |
| 120 | -819.9903 | 3% | 3.22 | -820.0291 | 0% | 3.22 | -819.9764 | 0% | 4.45 |
| 150 | -819.9896 | 1% | 8.71 | -820.0302 | 1% | 8.71 | -819.9819 | 0% | 9.89 |
| 180 | -819.9898 | 2% | 11.90 | -820.0310 | 1% | 11.90 | -819.9850 | 0% | 12.47 |
| 210 | -819.9880 | 0% | 9.81 | -819.9880 | 0% | 9.81 | -819.9919 | 0% | 8.92 |
| 240 | -819.9822 | 0% | 4.75 | -820.0246 | 0% | 4.75 | -819.9941 | 4% | 3.57 |
| 270 | -819.9731 | 0% | 0.59 | -820.0162 | 0% | 0.59 | -819.9967 | 58% | 0.43 |
| 300 | -819.9768 | 0% | 2.51 | -820.0272 | 0% | 2.51 | -819.9963 | 38% | 1.62 |
| 330 | -819.9791 | 0% | 6.45 | -820.0296 | 0% | 6.45 | -819.9915 | 0% | 5.20 |
| Average J | | | 5.09 | | | 7.29 | | | 1.04 |