Supplementary Material for:

Pyranose ring puckering thermodynamics for common vertebrate monosaccharides and idose with the CHARMM force field

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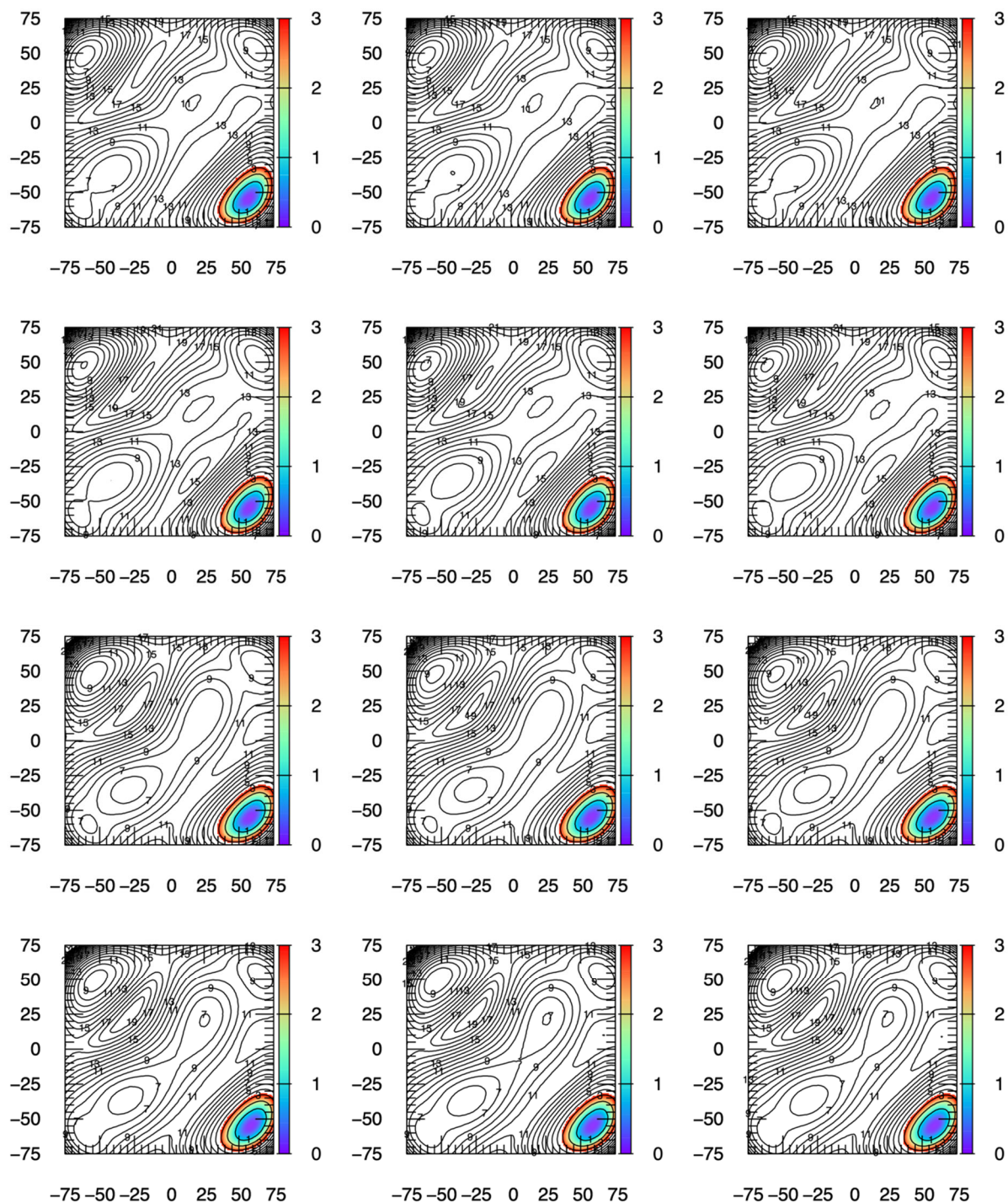* Correspondence: oguvench@une.edu; Tel.: +01-207-221-4171

Figure S1. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of D-glucose (Glc) and the corresponding O-methyl glycosides. First row: αGlc; second row: MeαGlc; third row: βGlc; fourth row: MeβGlc. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
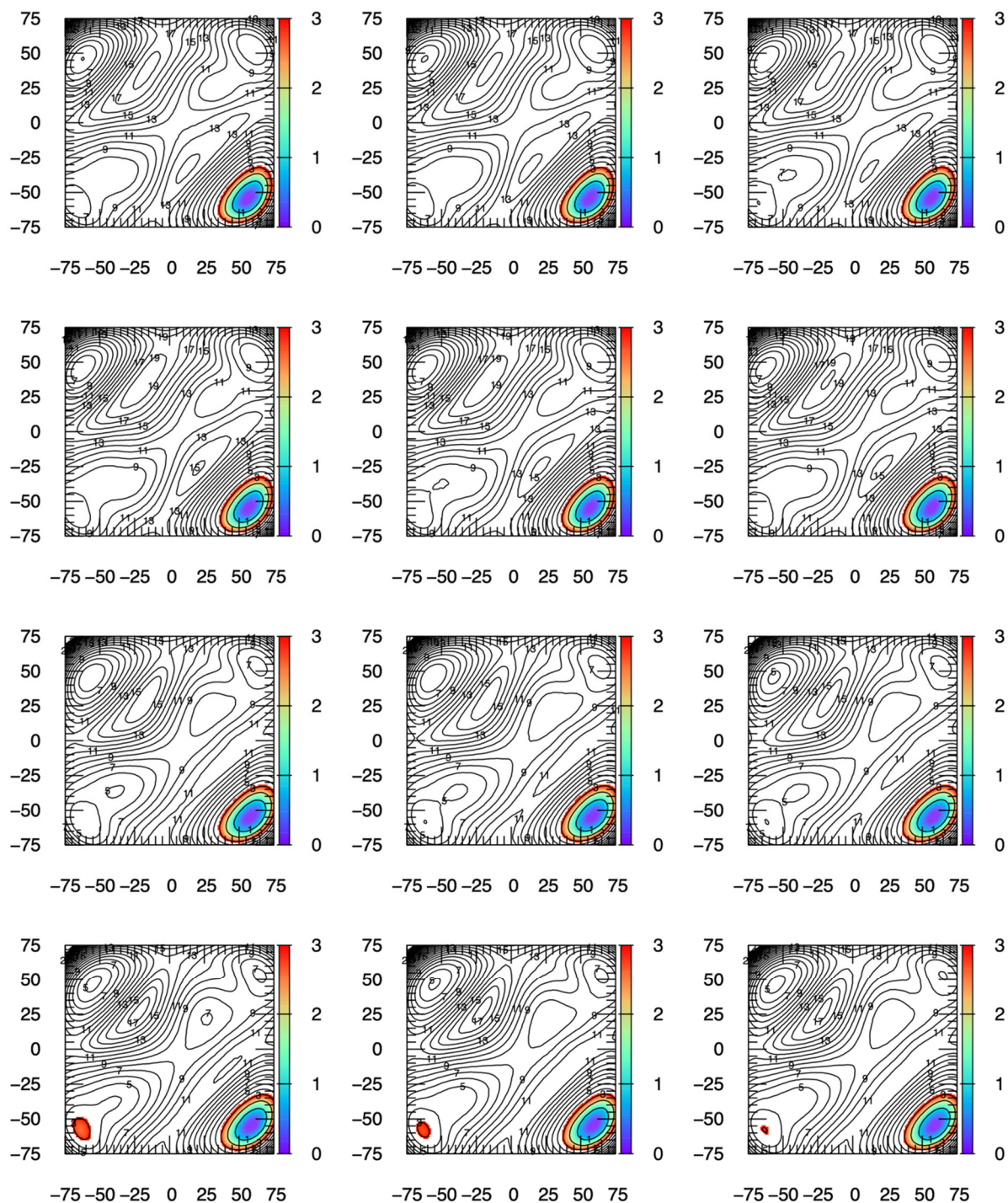
Figure S2. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of N-acetyl-D-glucosamine (GlcNAc) and the corresponding O-methyl glycosides. First row: αGlcNAc; second row: MeαGlcNAc; third row: βGlcNAc; fourth row: MeβGlcNAc. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
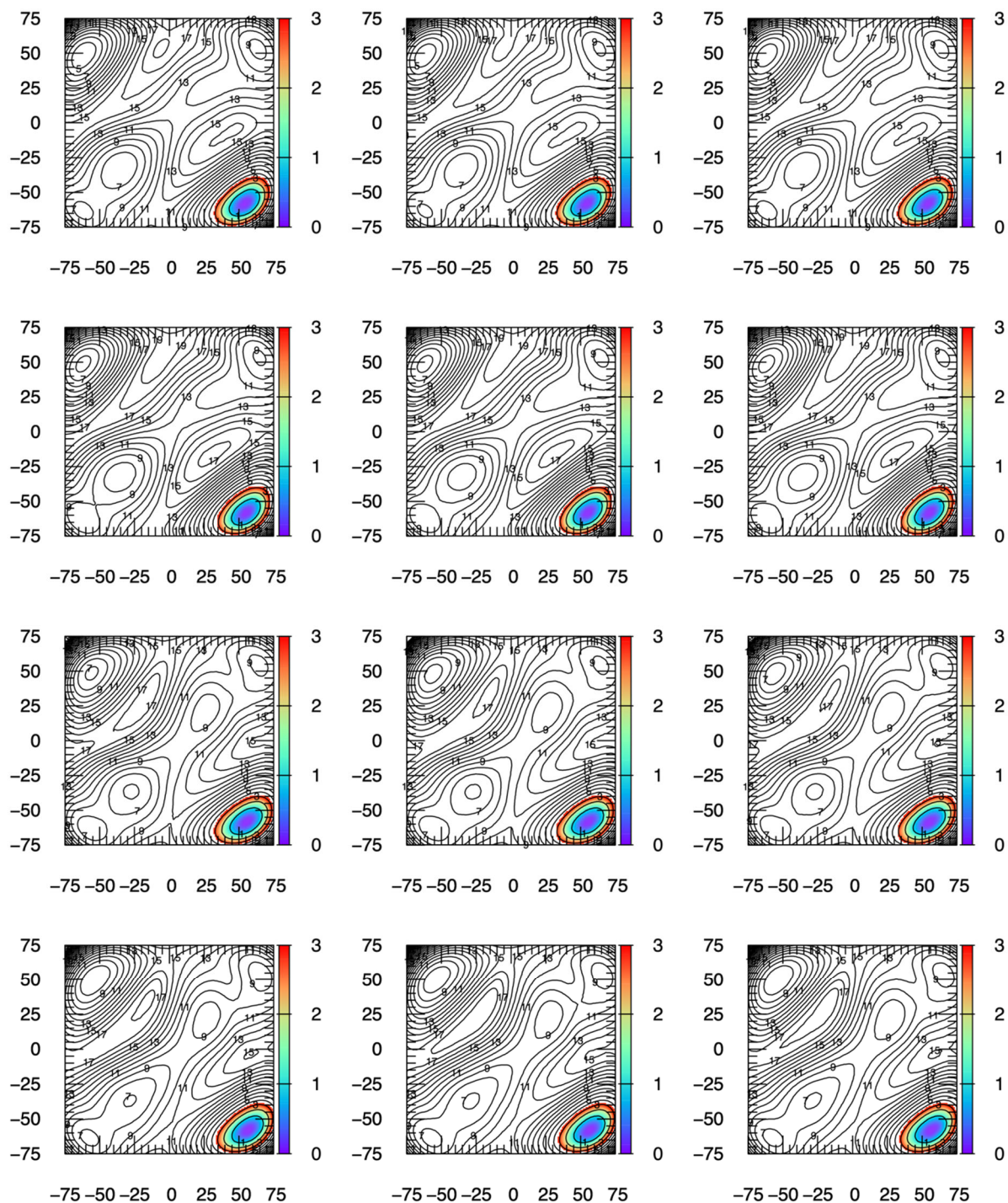
Figure S3. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of D-galactose (Gal) and the corresponding O-methyl glycosides. First row: αGal; second row: MeαGal; third row: βGal; fourth row: MeβGal. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
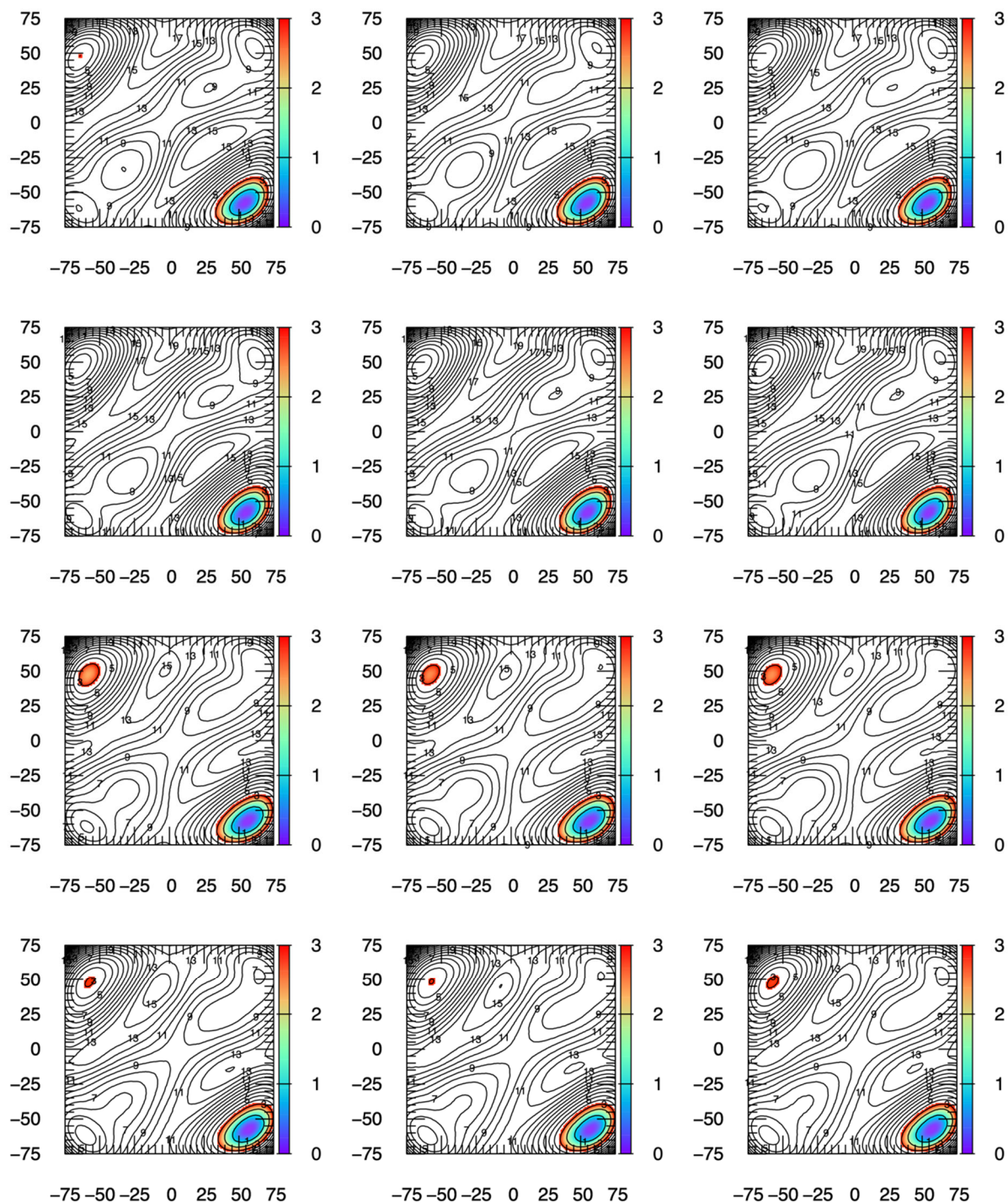
Figure S4. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of *N*-acetyl-D-galactosamine (GalNAc) and the corresponding O-methyl glycosides. First row: αGalNAc; second row: MeαGalNAc; third row: βGalNAc; fourth row: MeβGalNAc. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
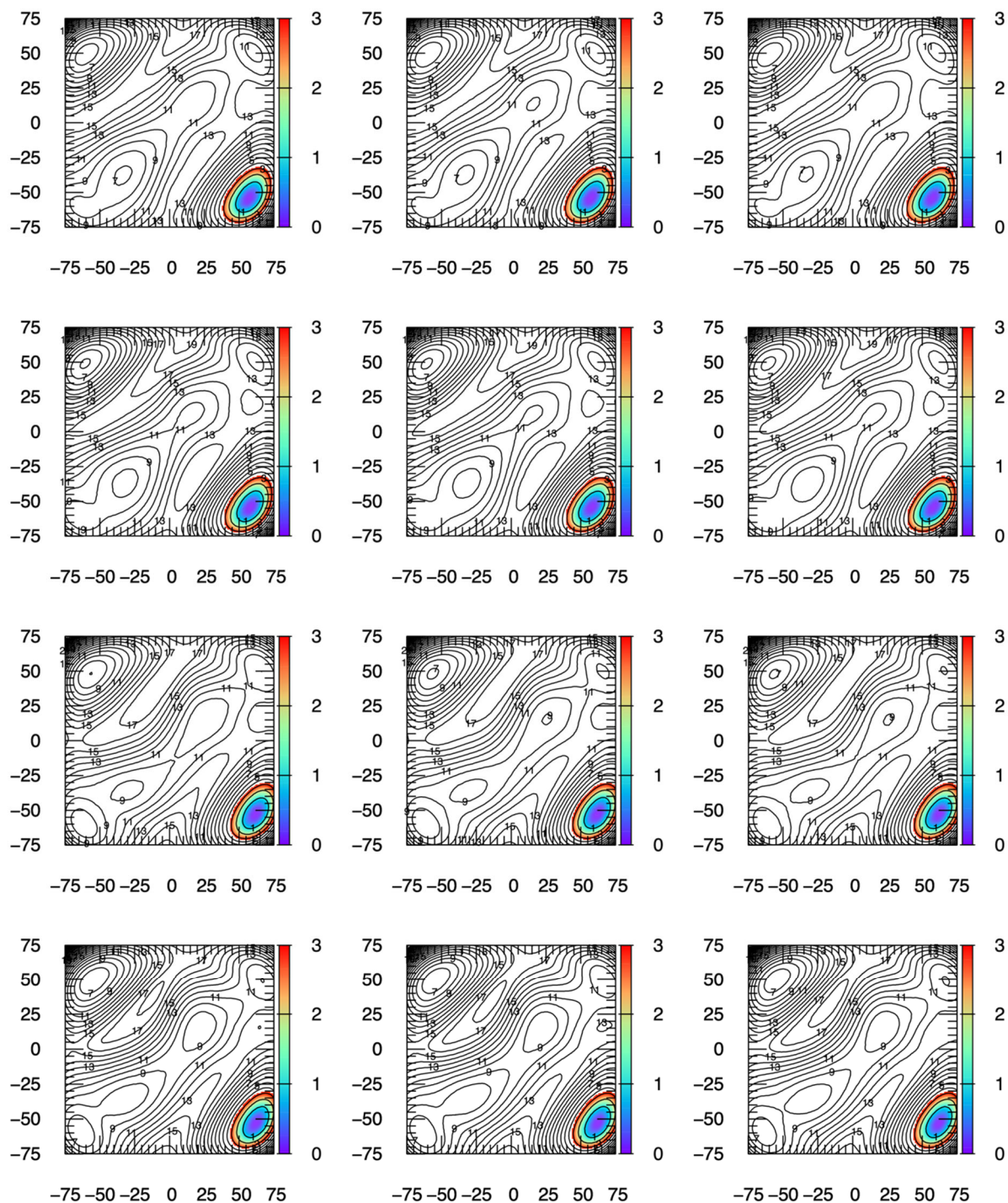
Figure S5. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of D-mannose (Man) and the corresponding O-methyl glycosides. First row: αMan; second row: MeαMan; third row: βMan; fourth row: MeβMan. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
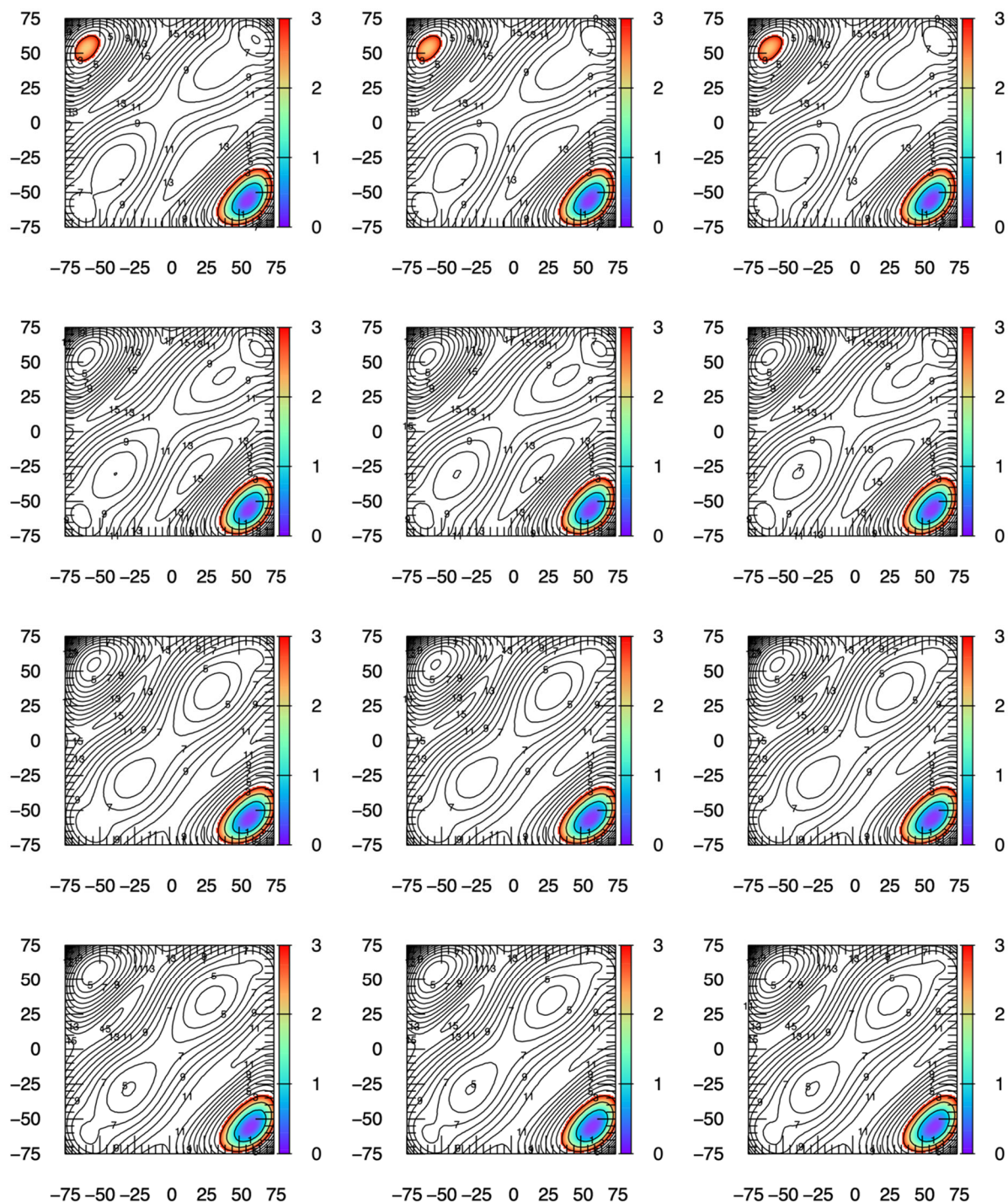
Figure S6. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of D-xylose (Xyl) and the corresponding O-methyl glycosides. First row: αXyl; second row: MeαXyl; third row: βXyl; fourth row: MeβXyl. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.

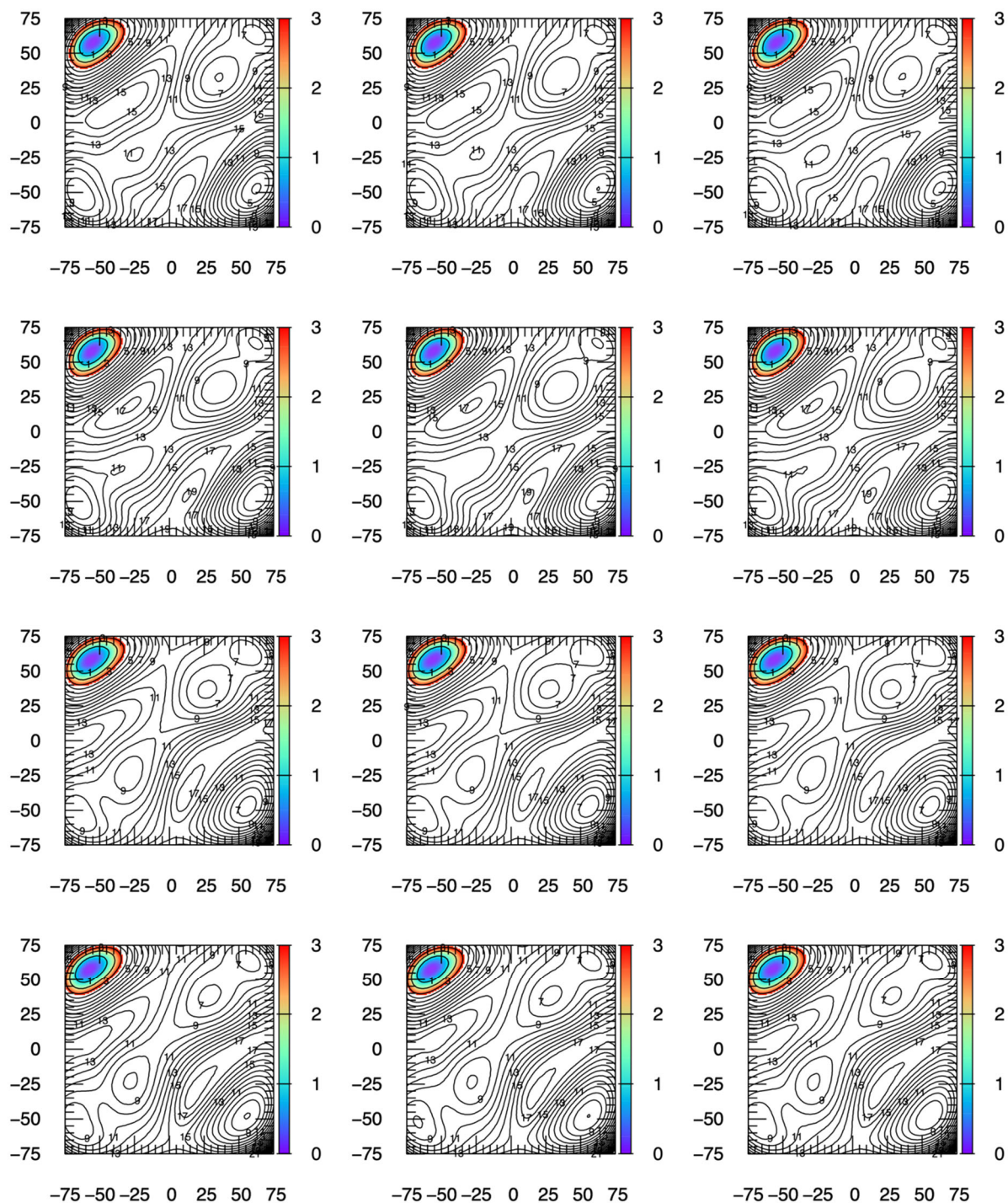**Figure S7.** Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of L-fucose (Fuc) and the corresponding O-methyl glycosides. First row: αFuc; second row: MeαFuc; third row: βFuc; fourth row: MeβFuc. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.

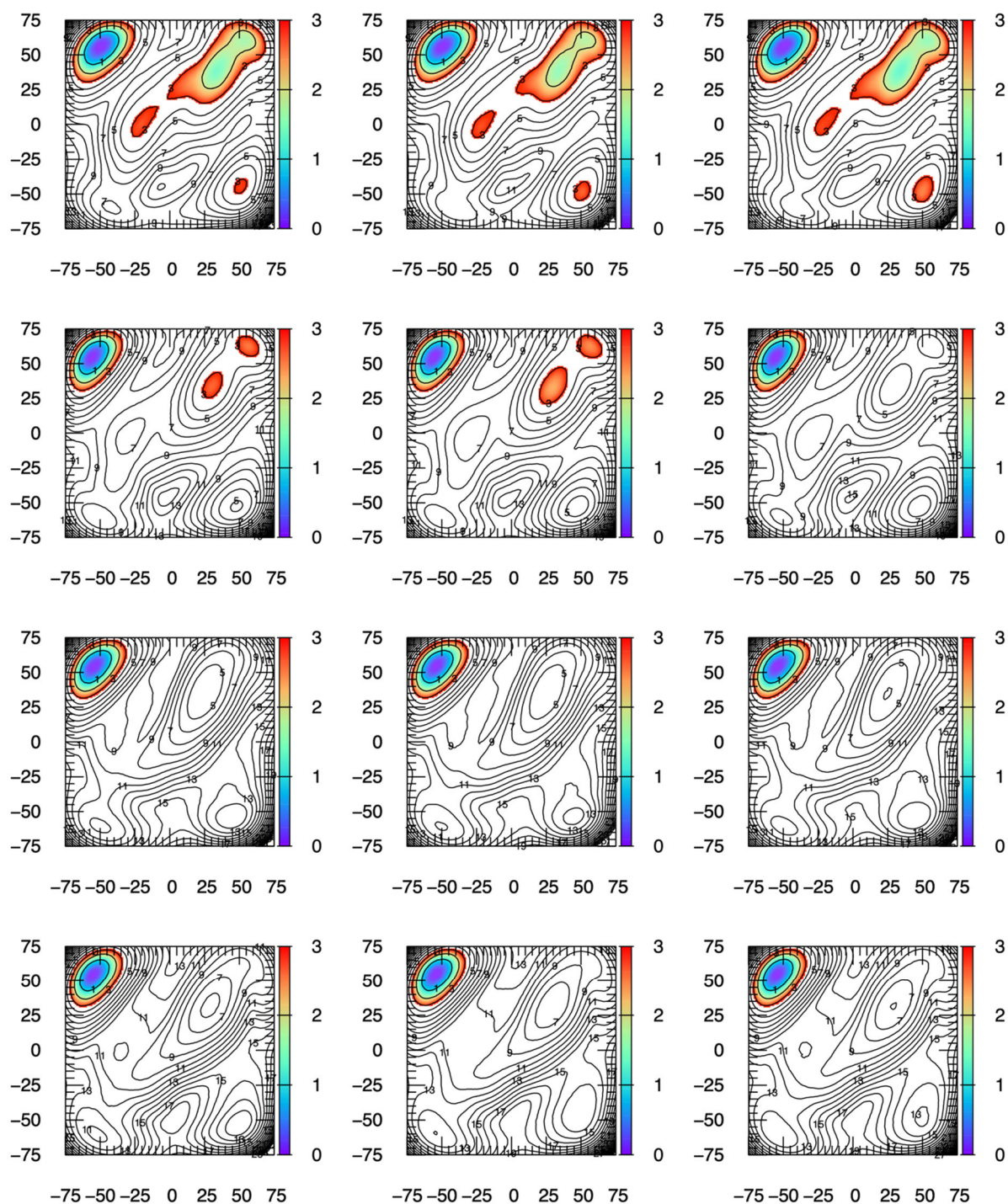**Figure S8.** Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of N-acetyl-D-neuraminate (Neu5Ac) and the corresponding O-methyl glycosides. First row: αNeu5Ac; second row: MeαNeu5Ac; third row: βNeu5Ac; fourth row: MeβNeu5Ac. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
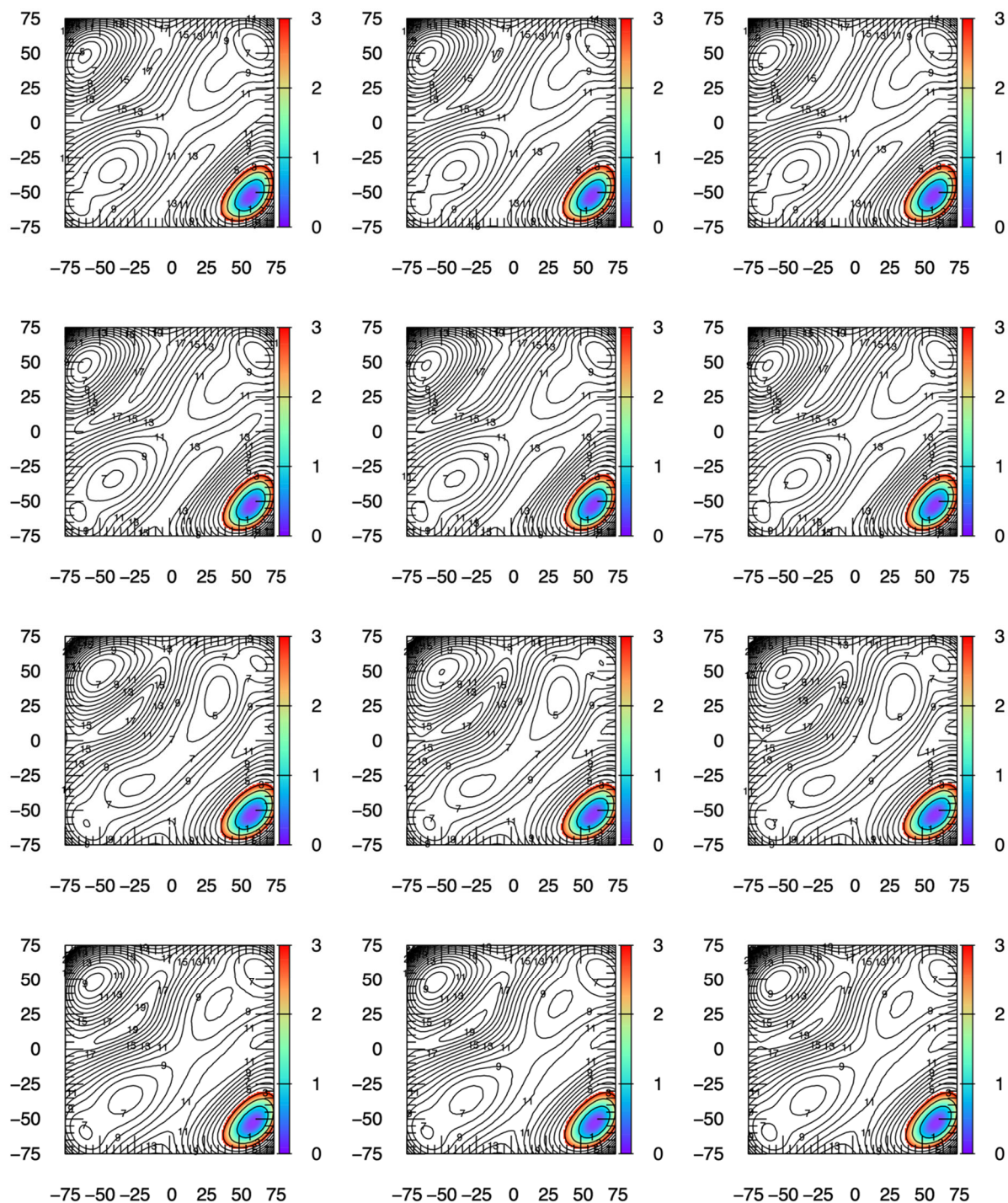
Figure S9. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of D-glucuronate (GlcA) and the corresponding O-methyl glycosides. First row: αGlcA; second row: MeαGlcA; third row: βGlcA; fourth row: MeβGlcA. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
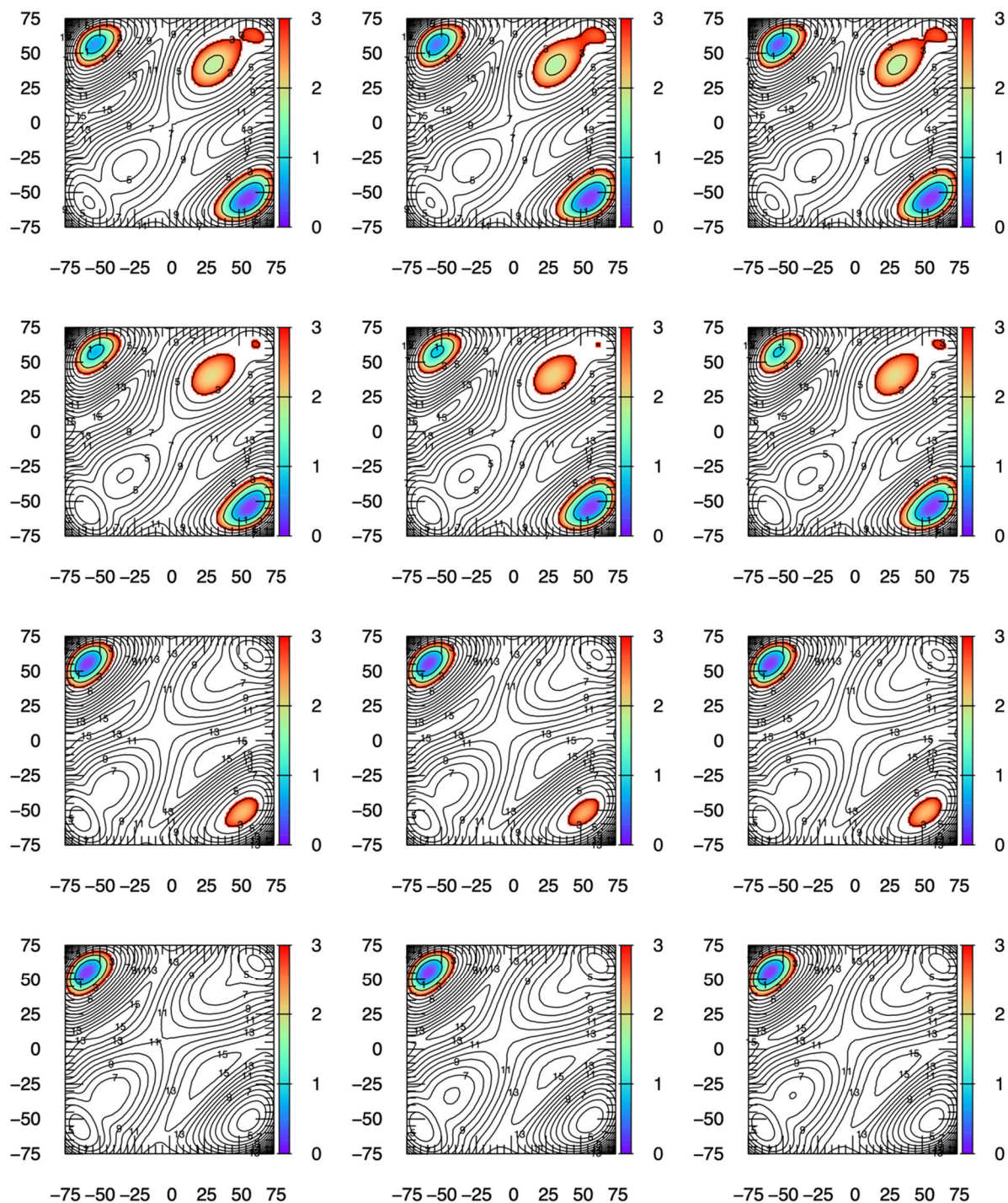
Figure S10. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of L-iduronate (IdoA) and the corresponding O-methyl glycosides. First row: αIdoA; second row: MeαIdoA; third row: βIdoA; fourth row: MeβIdoA. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
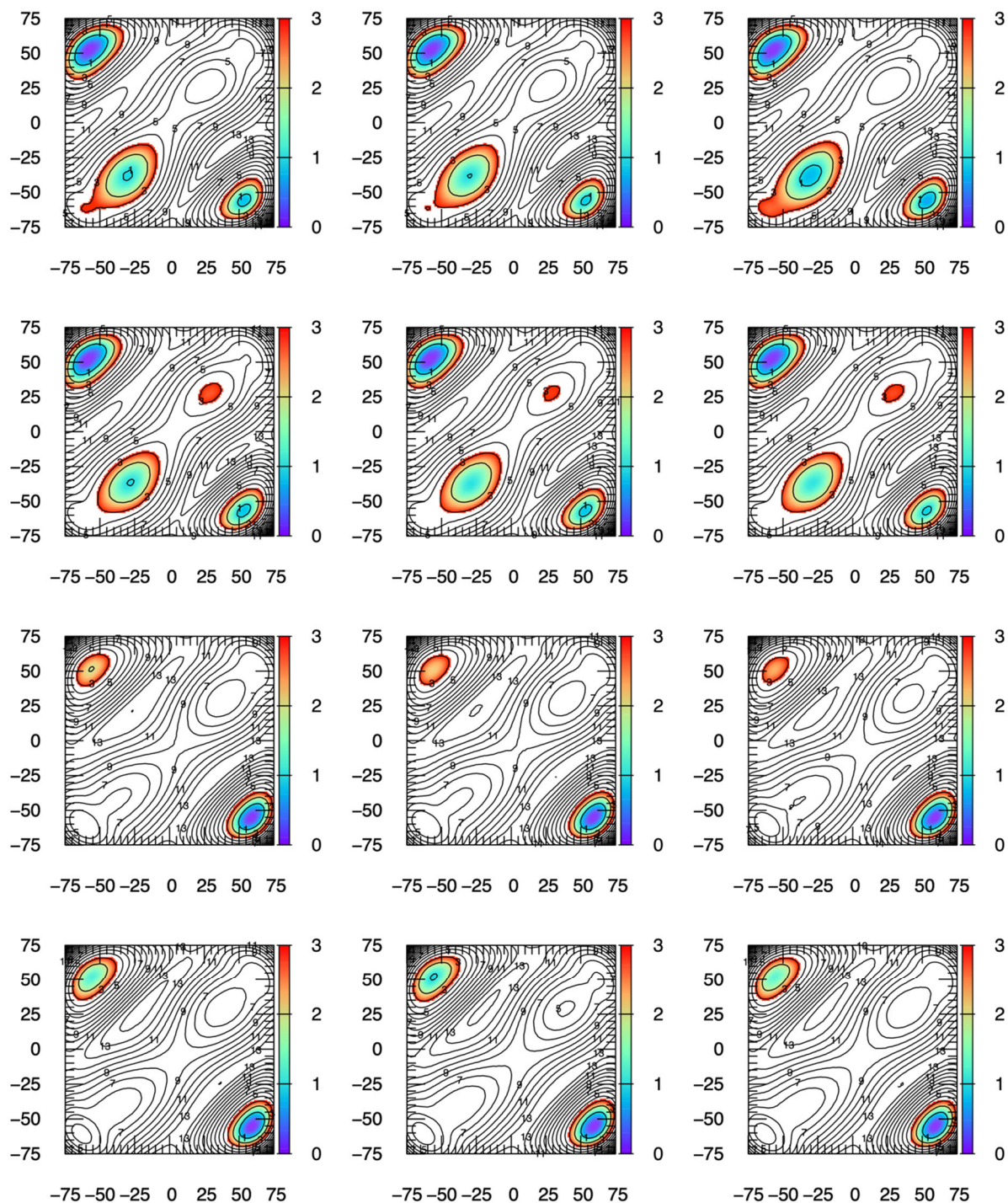
Figure S11. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for the α- and β-anomers of D-idose (Ido) and the corresponding O-methyl glycosides. First row: αIdo; second row: MeαIdo; third row: βIdo; fourth row: MeβIdo. $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.
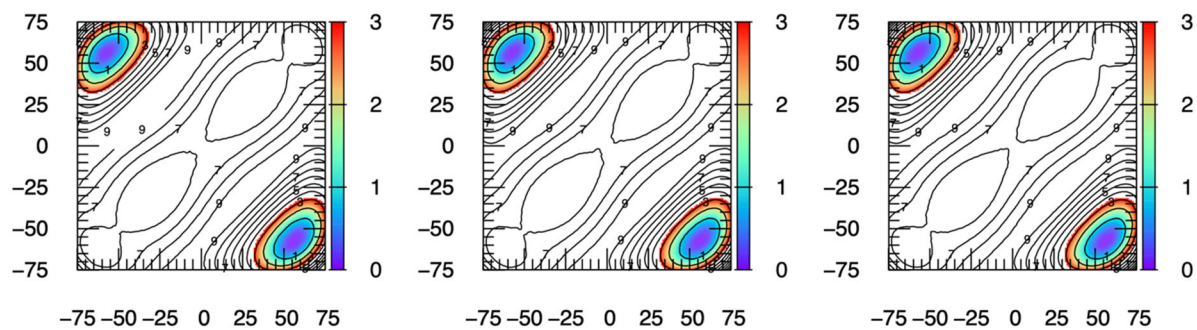
Figure S12. Triplicate eABF $\Delta G(\alpha_1, \alpha_2)$ data for tetrahydropyran (THP). $\Delta G(\alpha_1, \alpha_2)$ is in kcal/mol, with contours drawn every 1 kcal/mol, colored from 0-3 kcal/mol, and labeled every 2 kcal/mol.