

Supplemental Material for:
Rheostats and toggle switches for modulating protein function
File 6: Physicochemical trends: Positions 55-59

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Figures S55-S72. Physico-chemical trends: positions 55-59. Repression assay data for each position were color-coded according to various physico-chemical scales. For example, Figures S55-S57 show results for position 55 color-coded by accessible surface area of the free side chain [46], side chain branching, and charge/polarity/aromaticity. The relevant parameter can be determined from the legend in the lower right hand corner of each graph. Positions 50-58 have potential to participate in an alpha helix, and repression assay results were also compared to both average and position-specific helical propensities [47]. For simplicity, only one helix color scale is used as a legend, with magenta corresponding to high propensity and green corresponding to low propensity. Since wild-type LacI and PurR have different length helices [20], we compared multiple helical scales to results for each position. However, no scale showed good correlation with the functional assay among all chimeras.

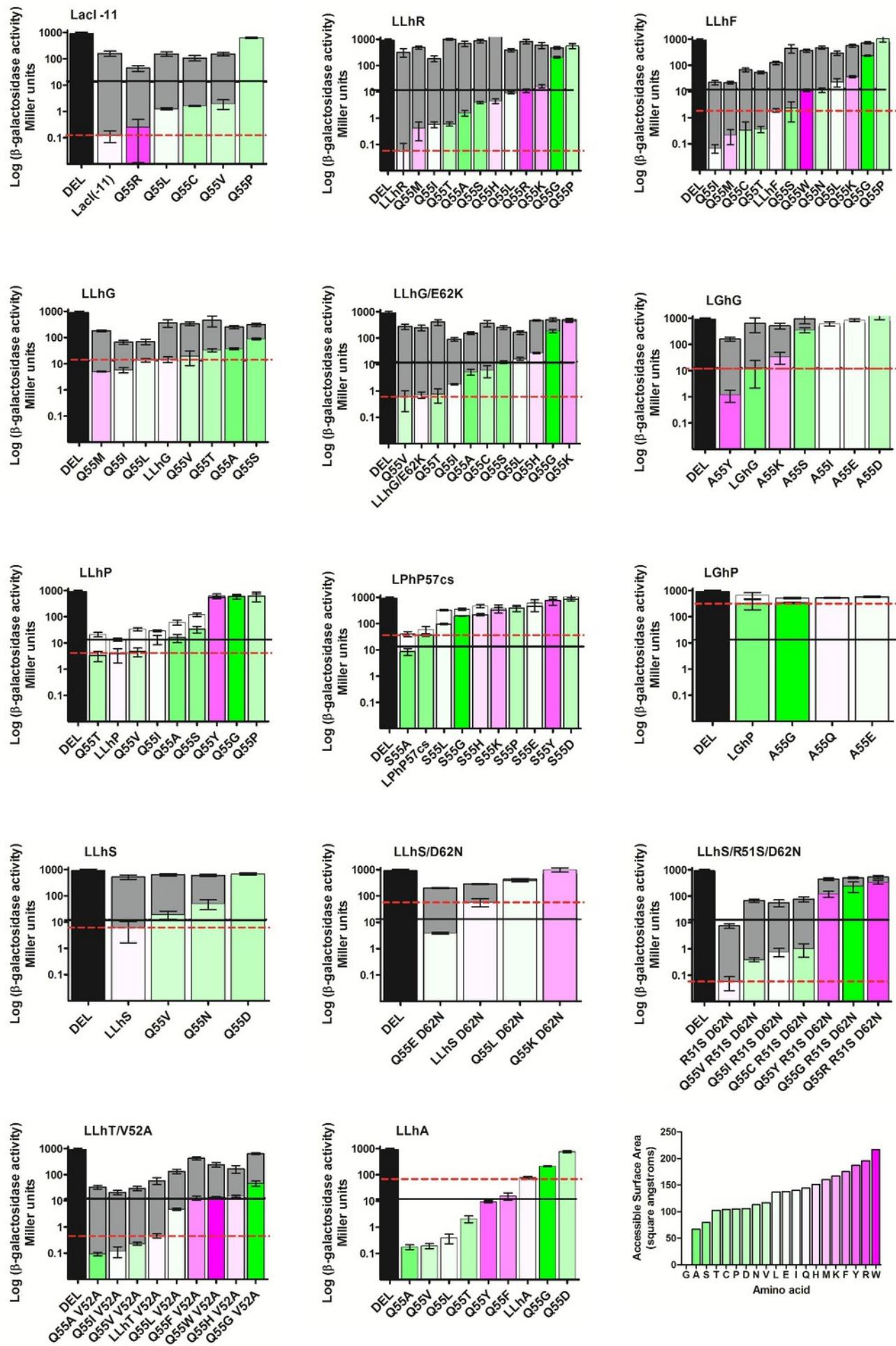


Figure S55: Physicochemical trends: Position 55, Accessible surface area

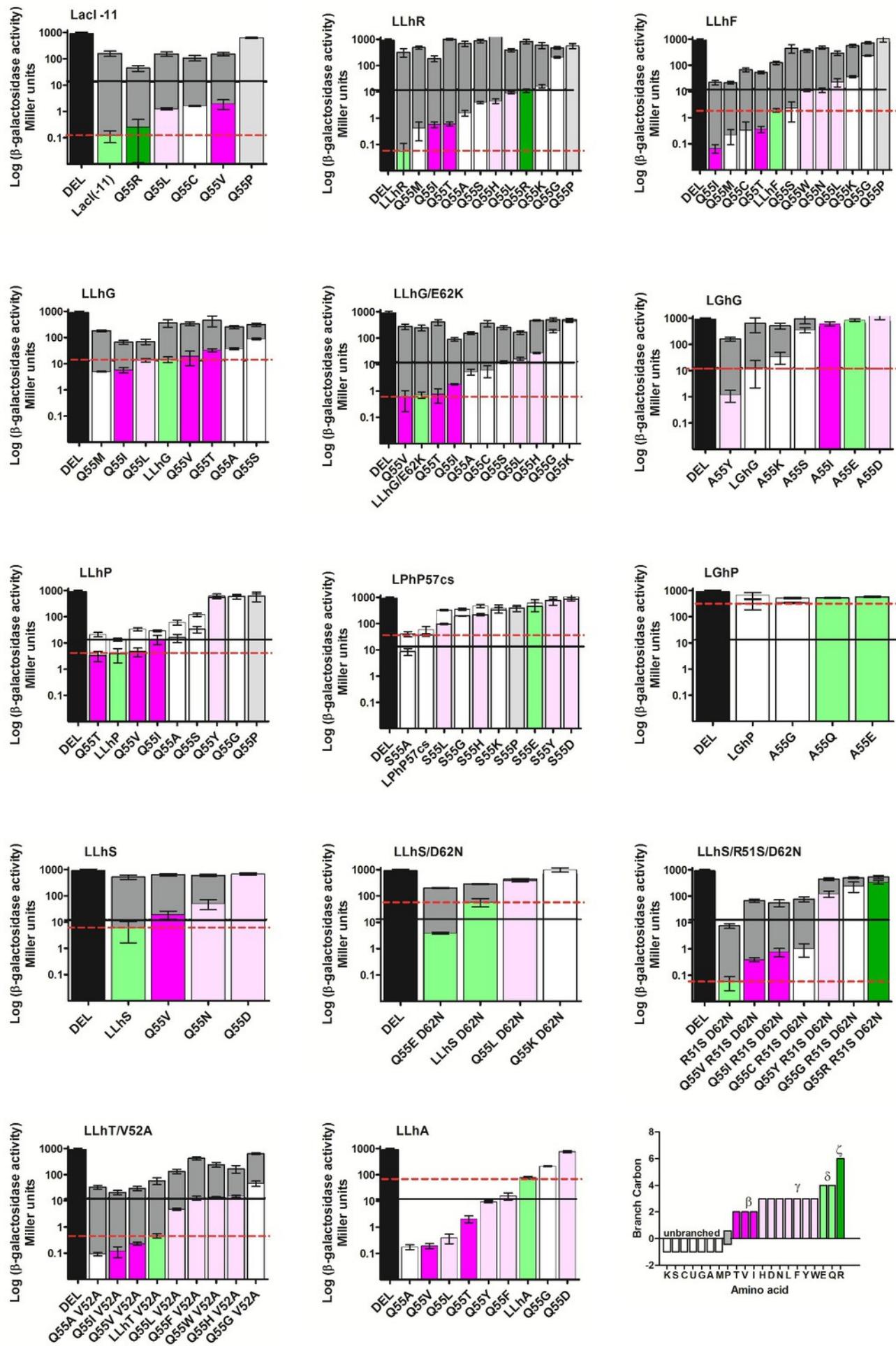


Figure S56: Physicochemical trends: Position 55, Side chain branching

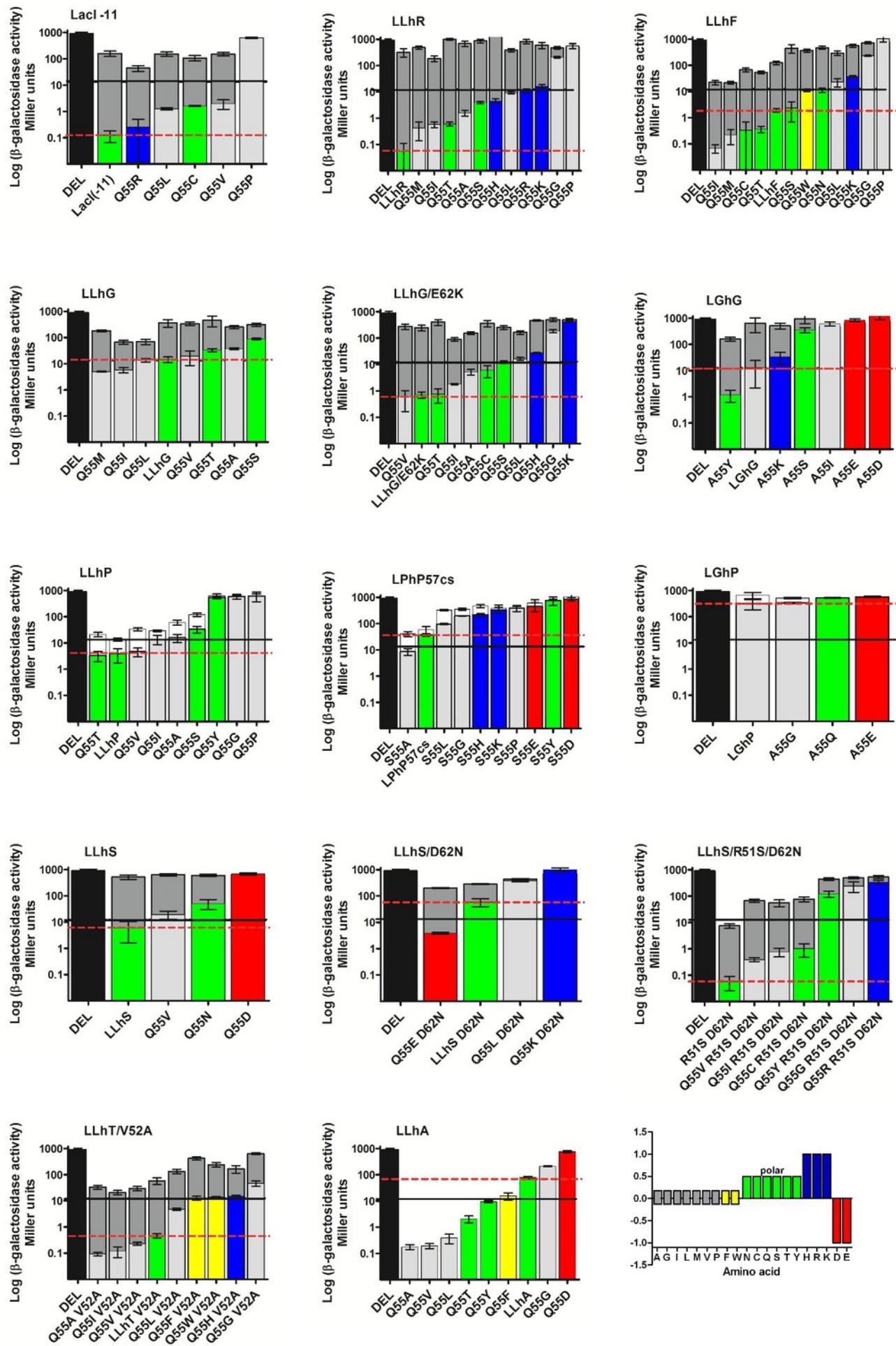


Figure S57: Physicochemical trends: Position 55, Charge/polarity/aromaticity

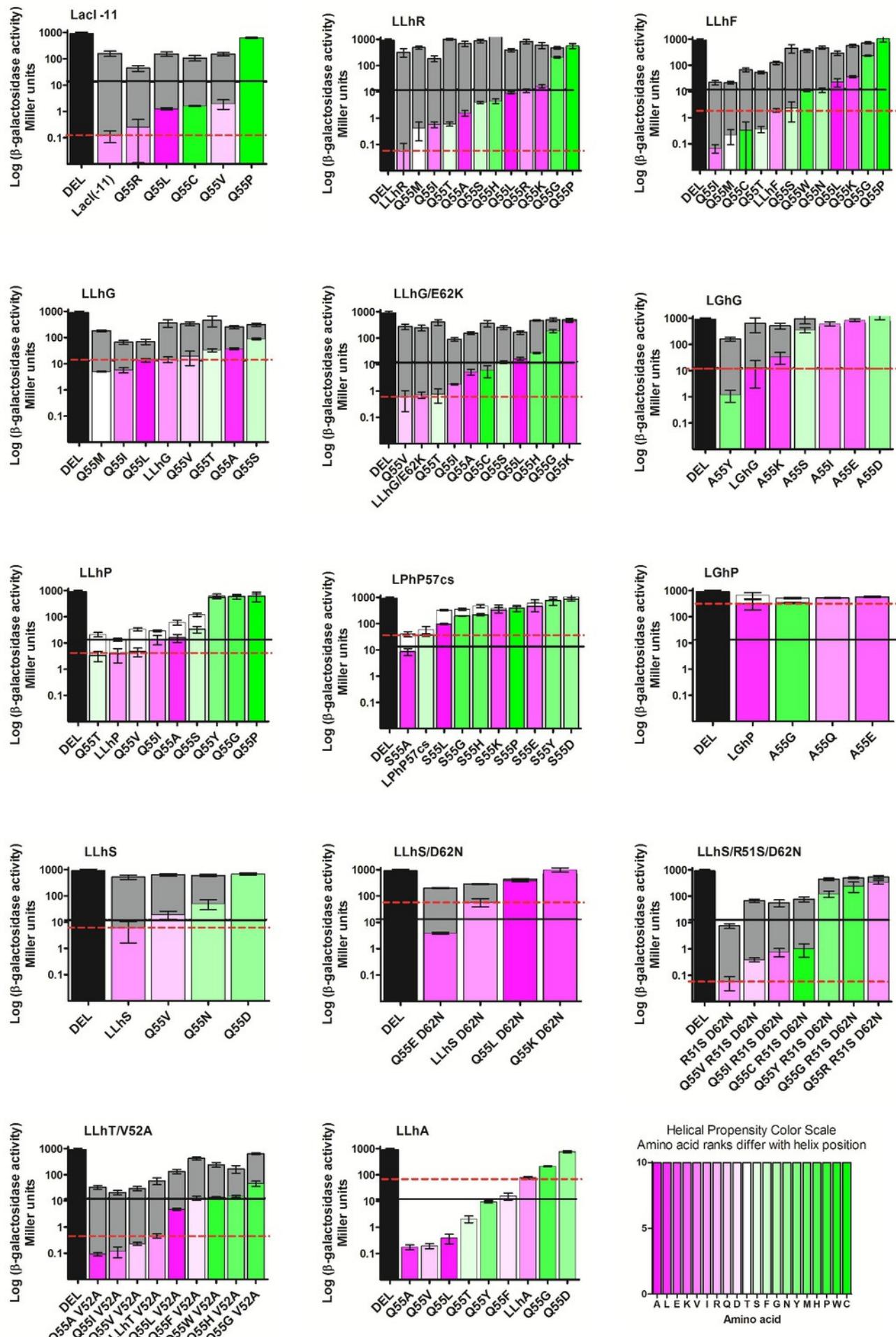


Figure S58: Physicochemical trends: Position 55, Helical propensity (C3 scale)

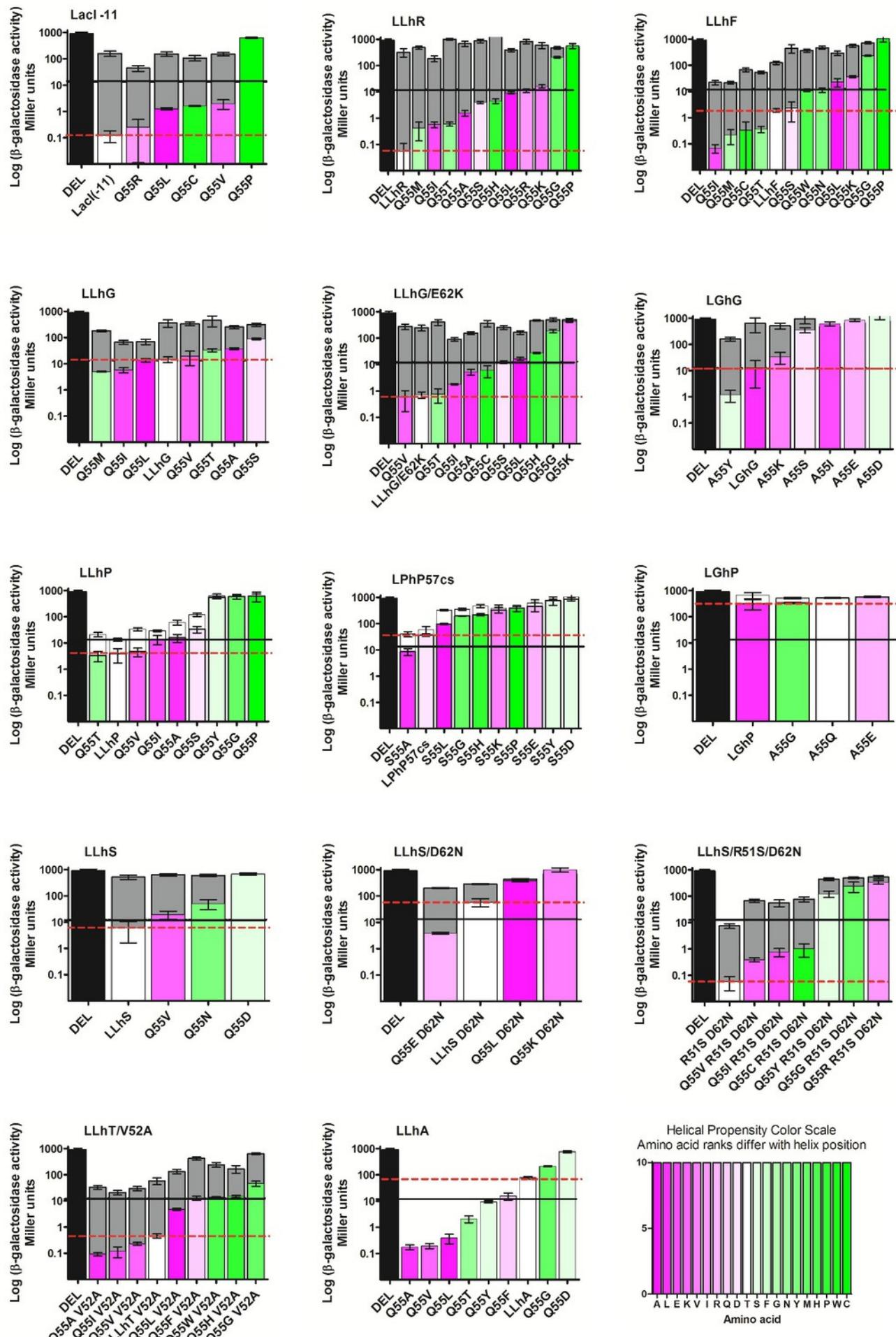


Figure S59: Physicochemical trends: Position 55, Helical propensity (C4 scale)

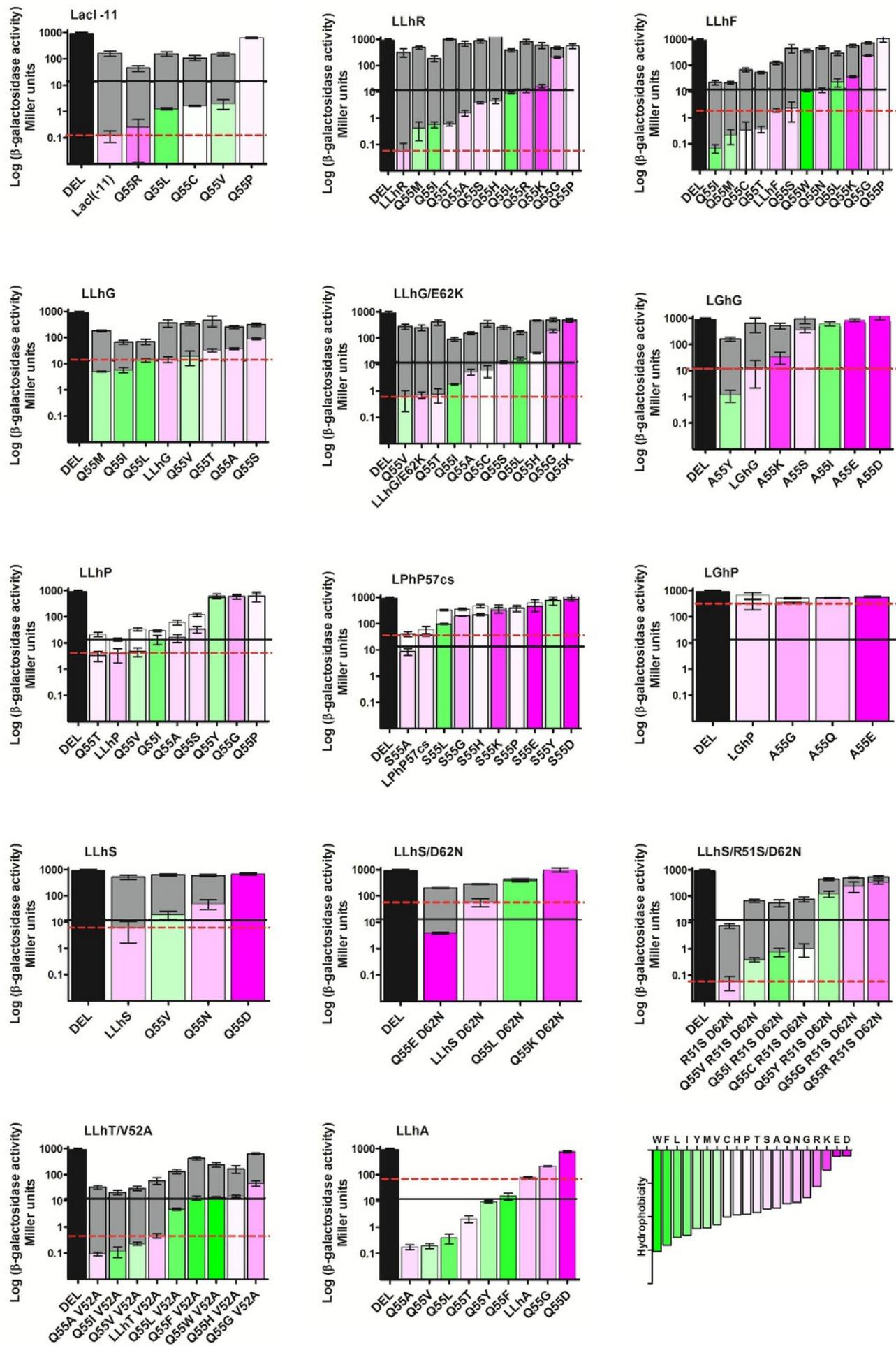


Figure S60: Physicochemical trends: Position 55, Hydrophobicity

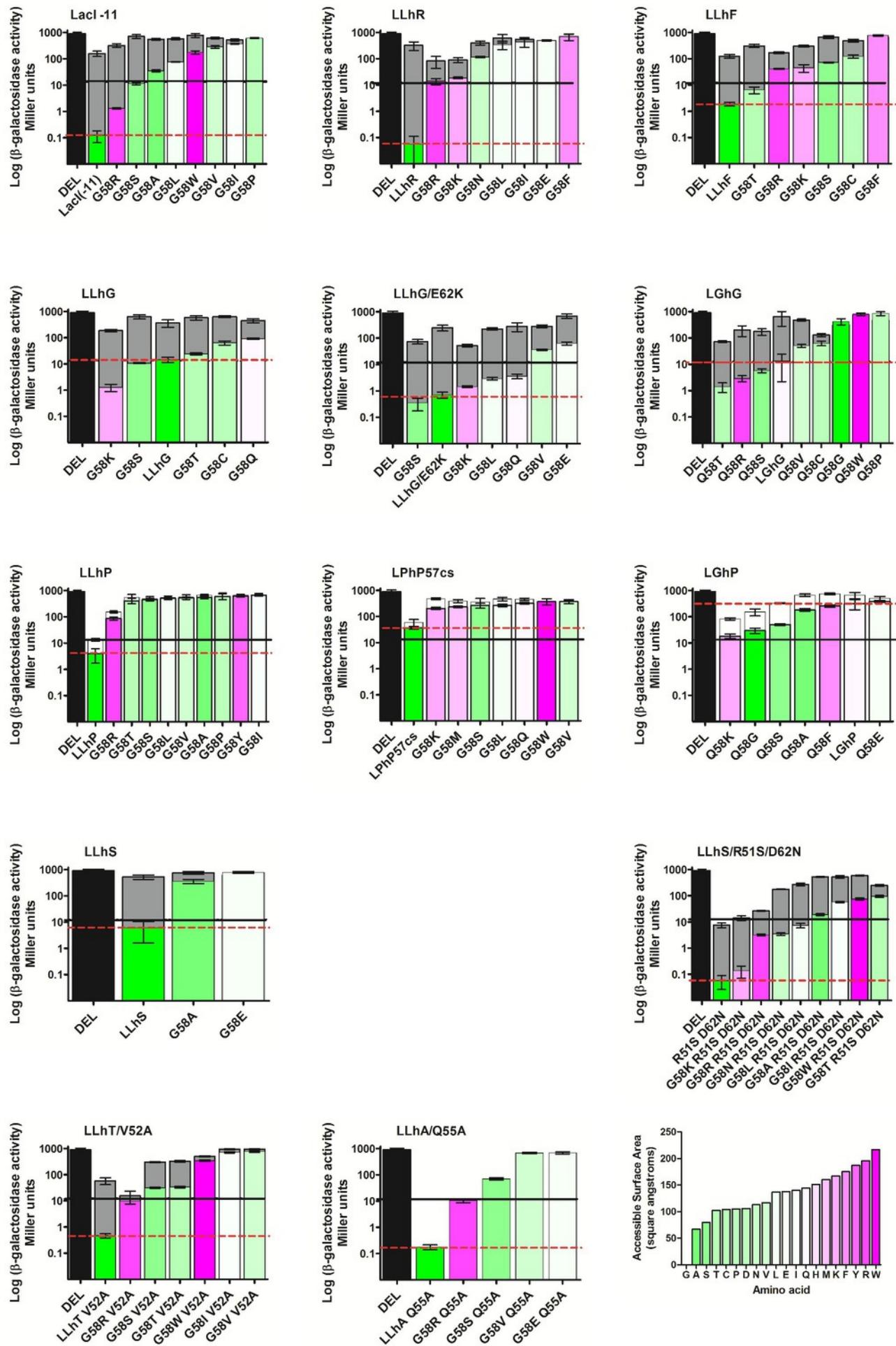


Figure S61: Physicochemical trends: Position 58, Accessible surface area

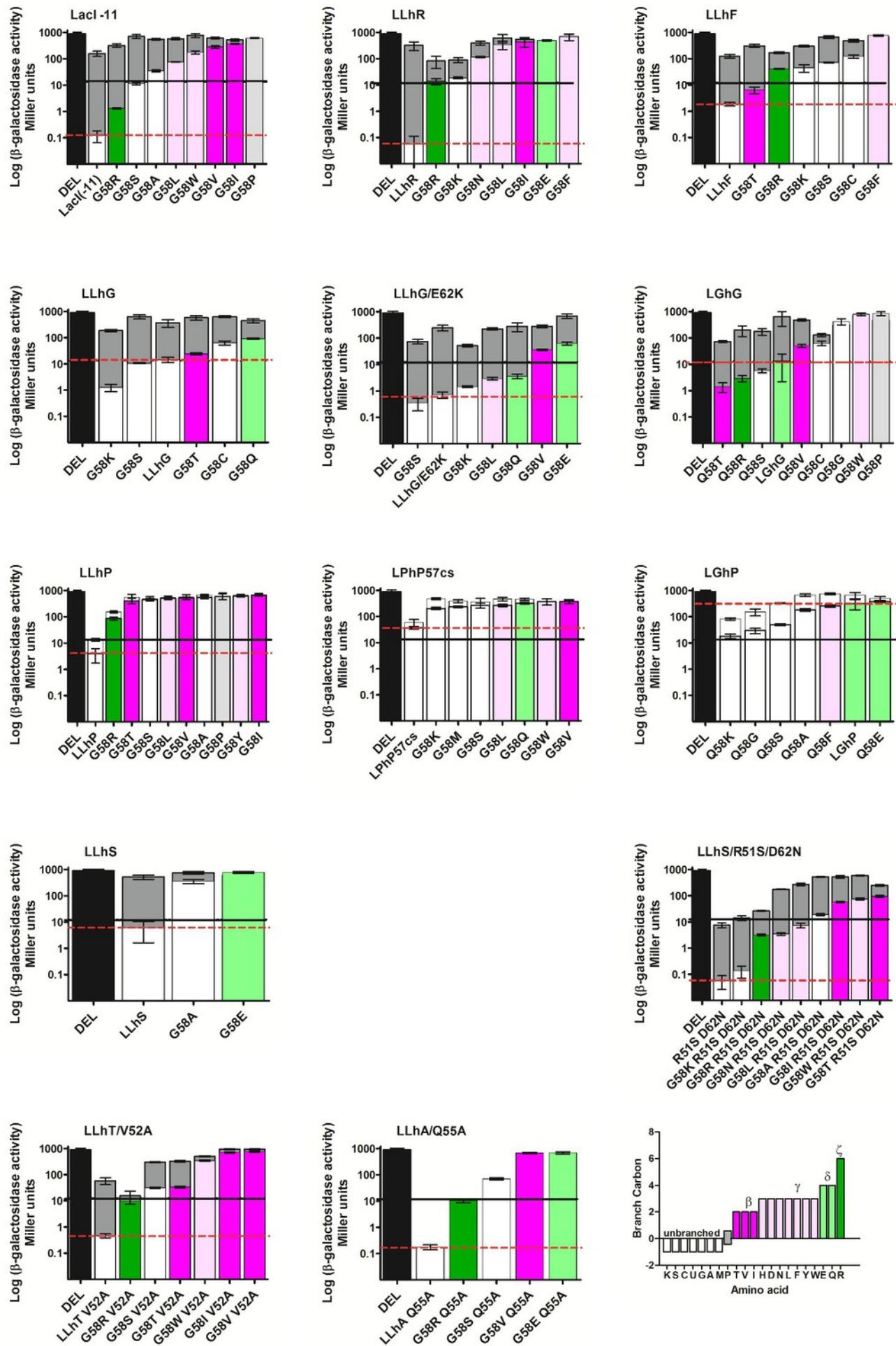


Figure S62: Physicochemical trends: Position 58, Side chain branching

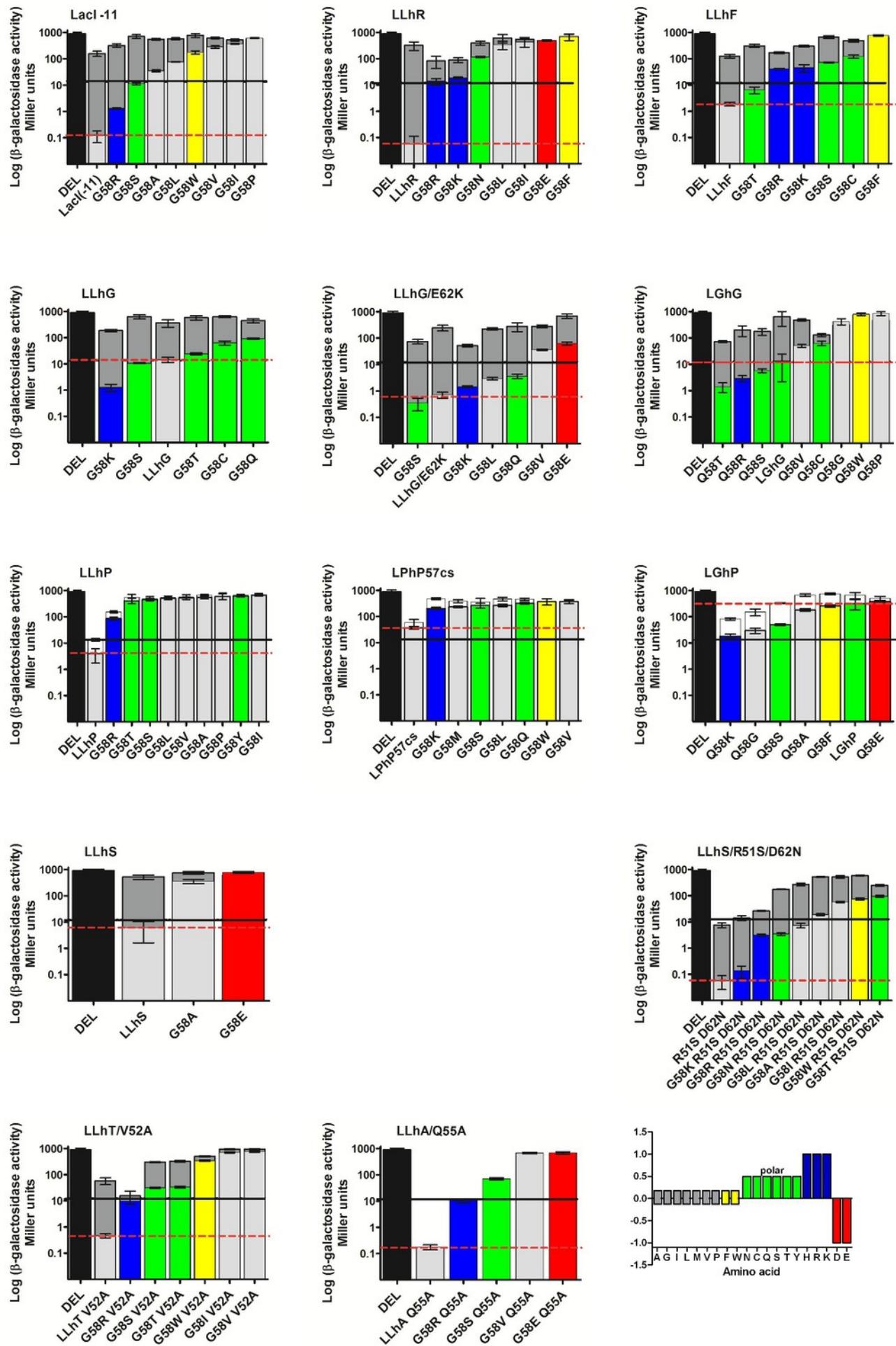


Figure S63: Physicochemical trends: Position 58, Charge/polarity/aromaticity

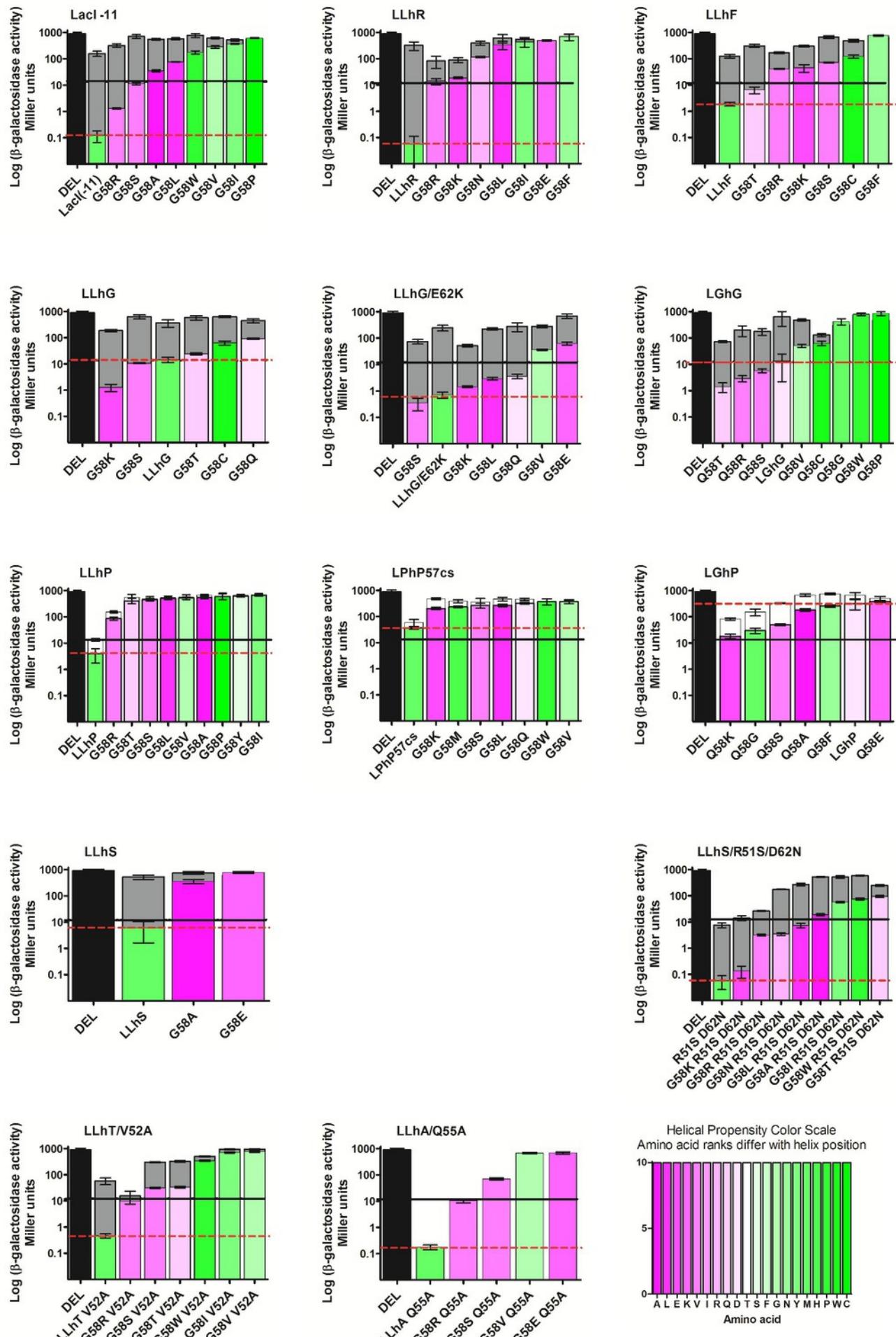


Figure S64: Physicochemical trends: Position 58, Helical propensity (C1 scale)

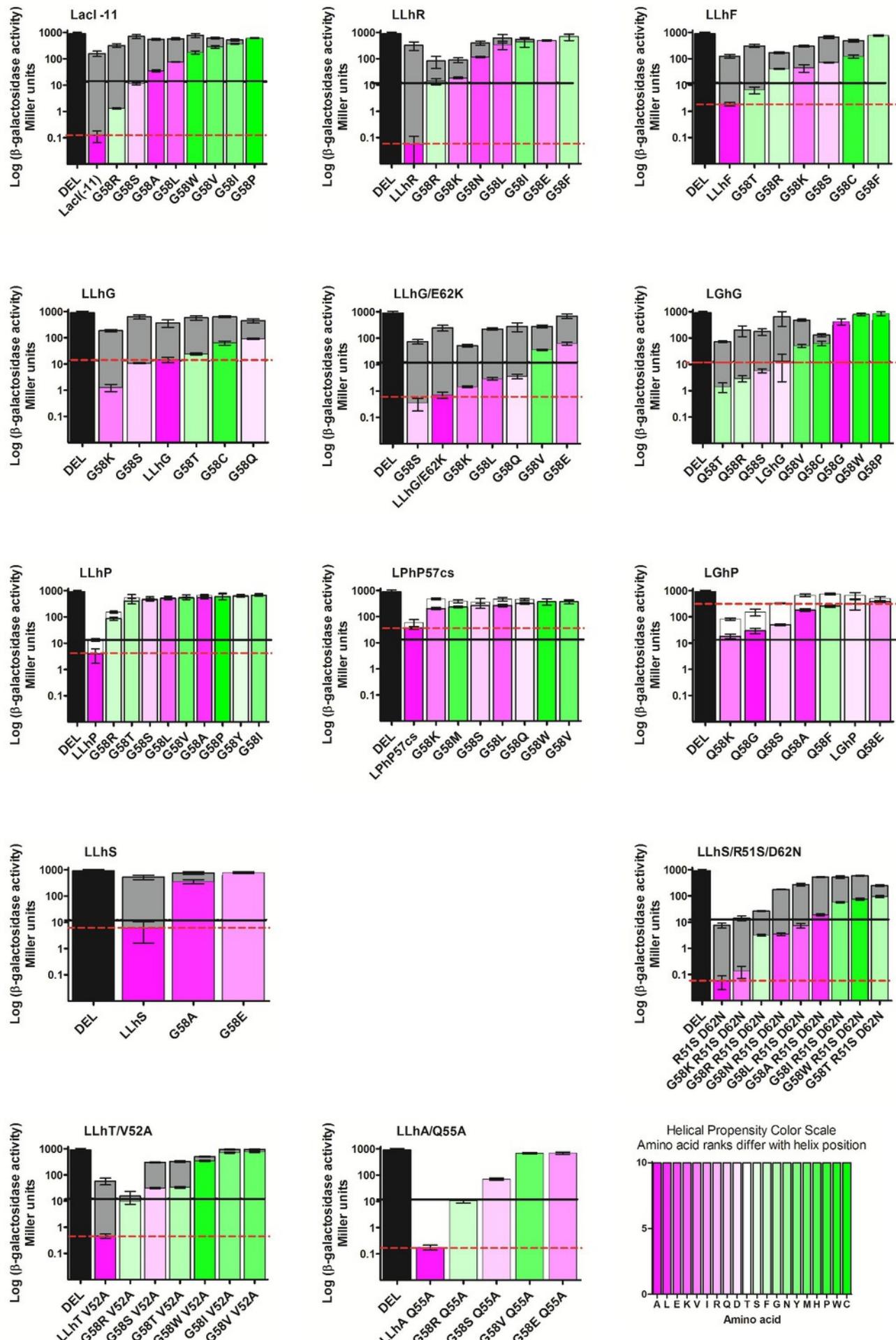


Figure S65: Physicochemical trends: Position 58, Helical propensity C_{cap} scale)

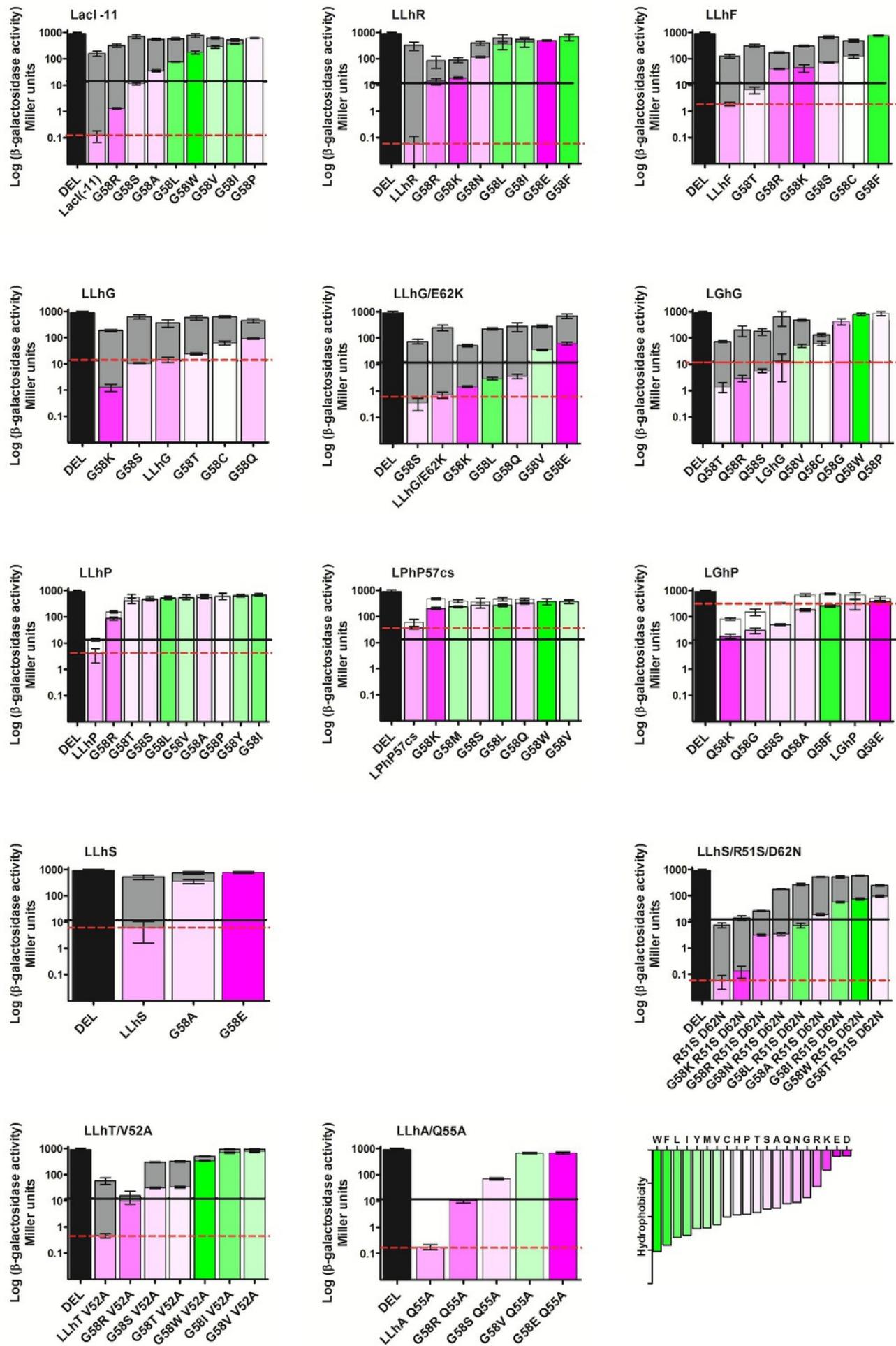


Figure S66: Physicochemical trends: Position 58, Hydrophobicity

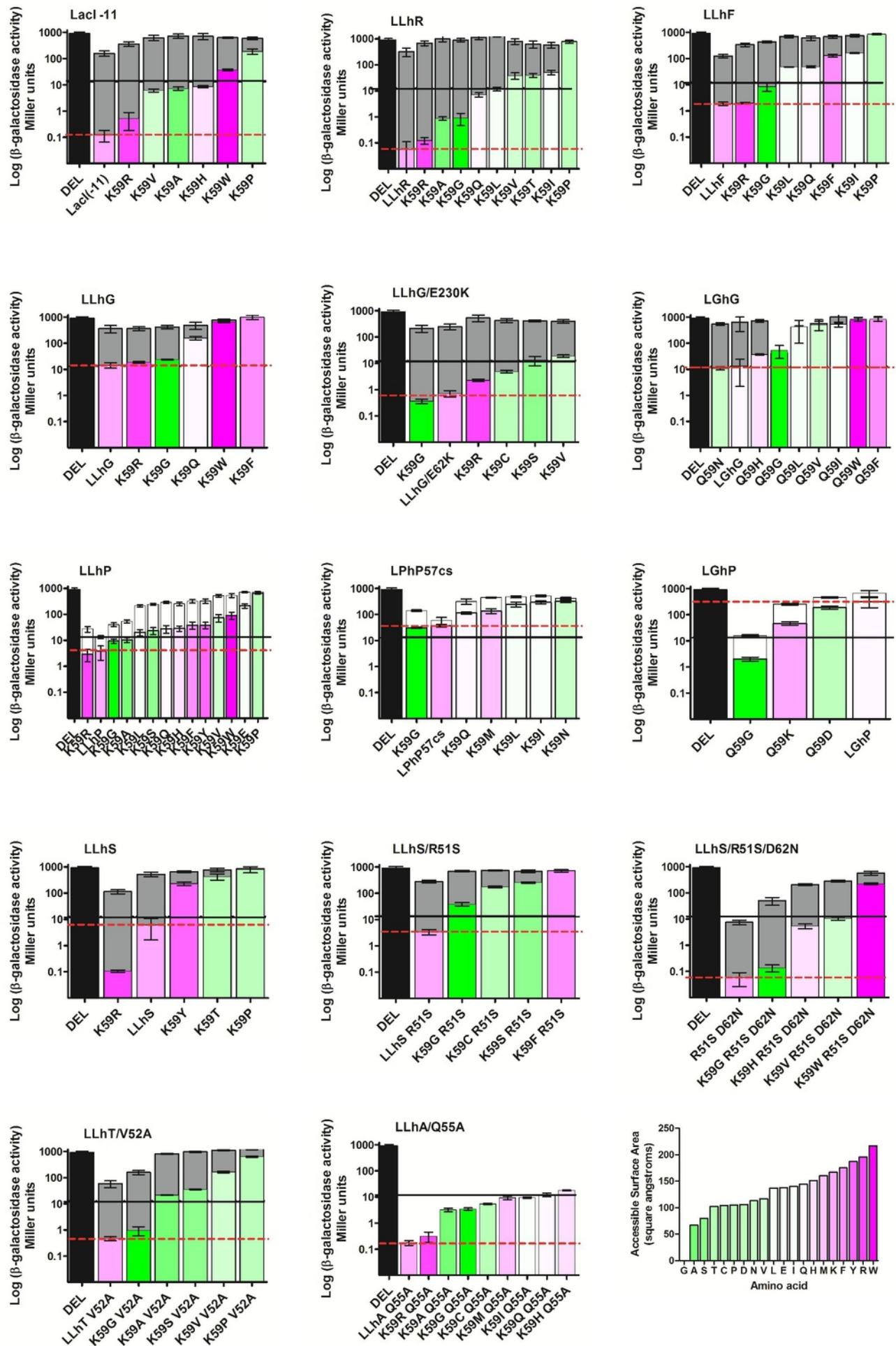


Figure S67: Physicochemical trends: Position 59, Accessible surface area

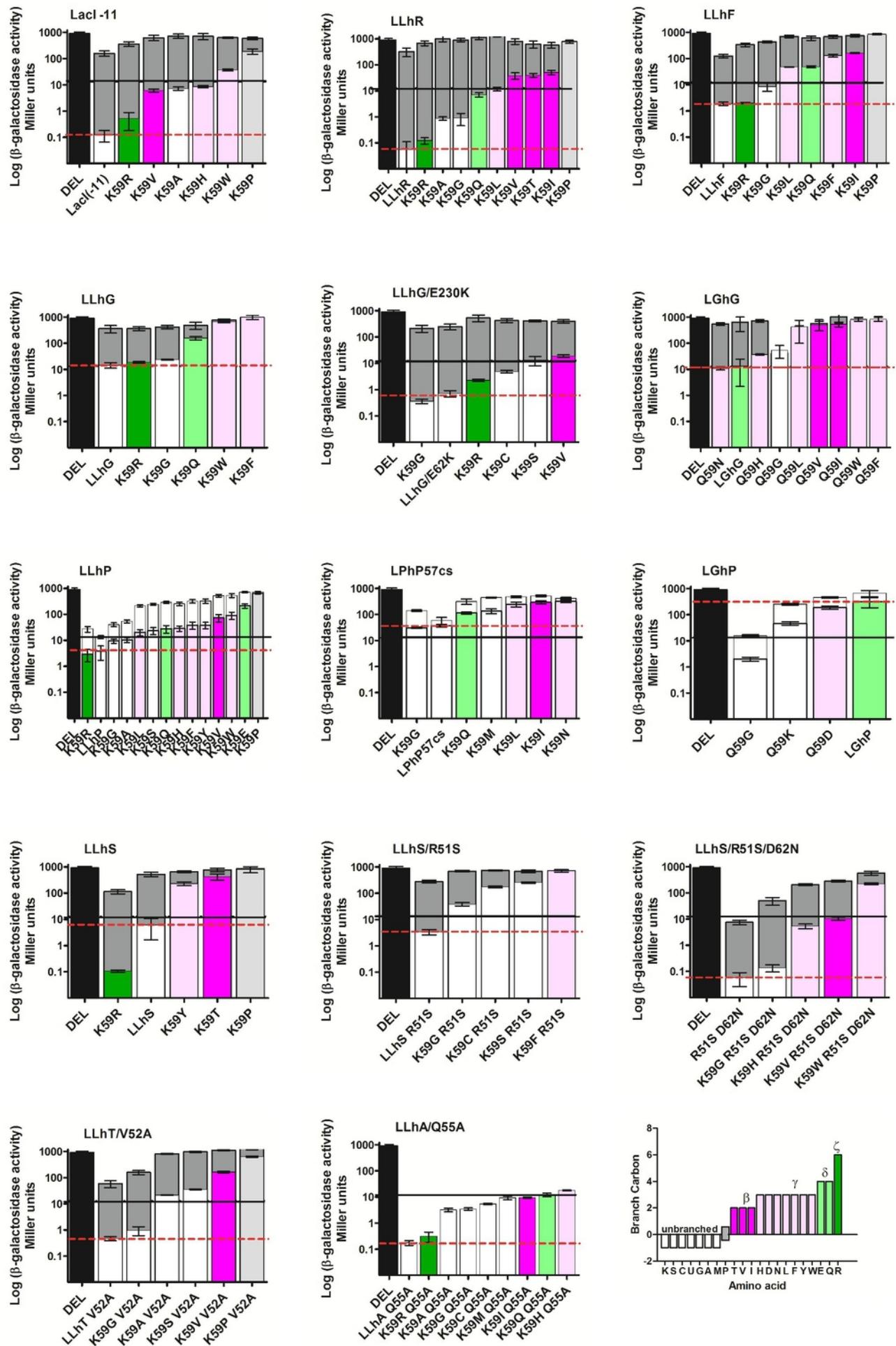


Figure S68: Physicochemical trends: Position 59, Side chain branching

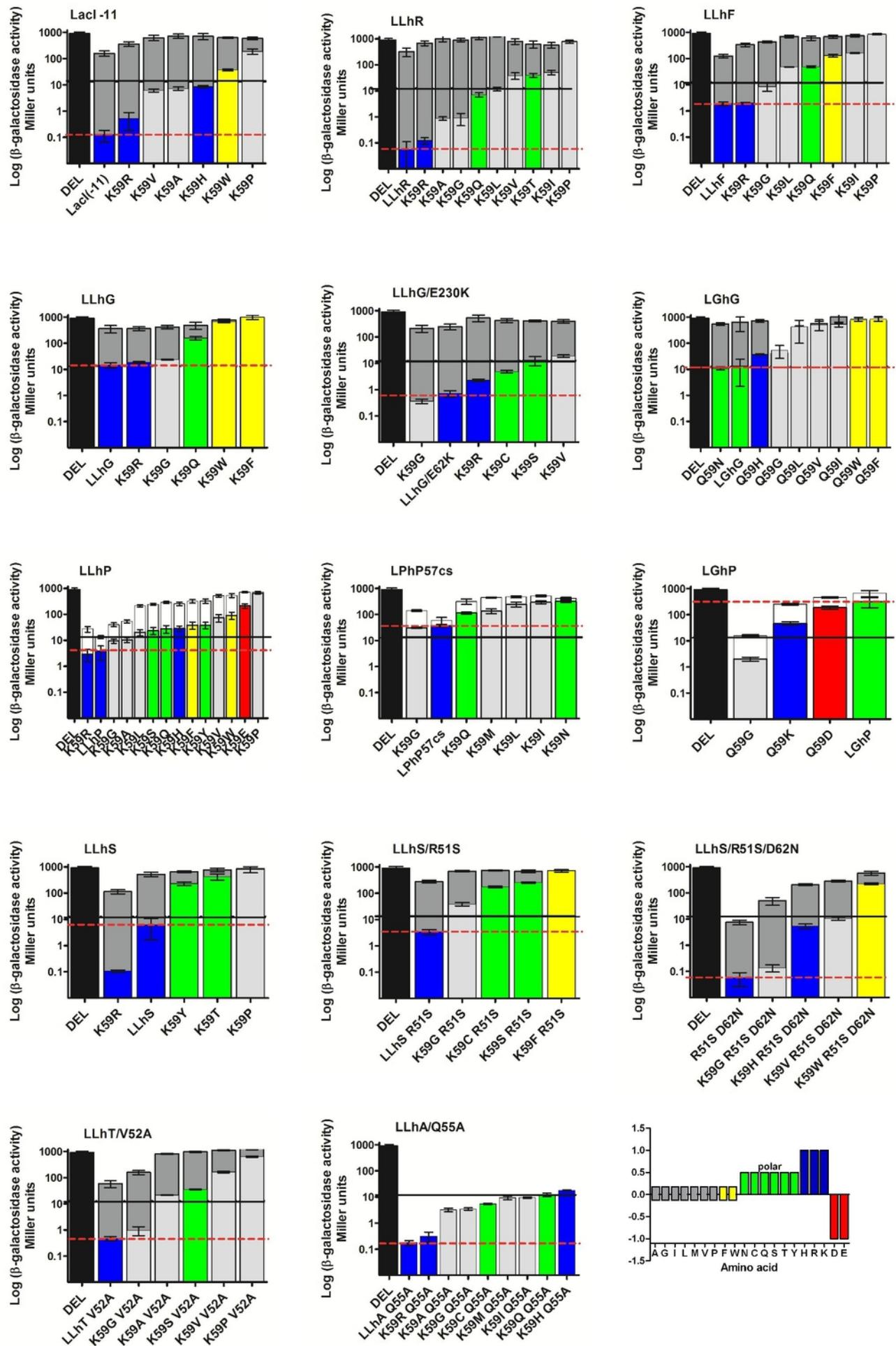


Figure S69: Physicochemical trends: Position 59, Charge/polarity/aromaticity

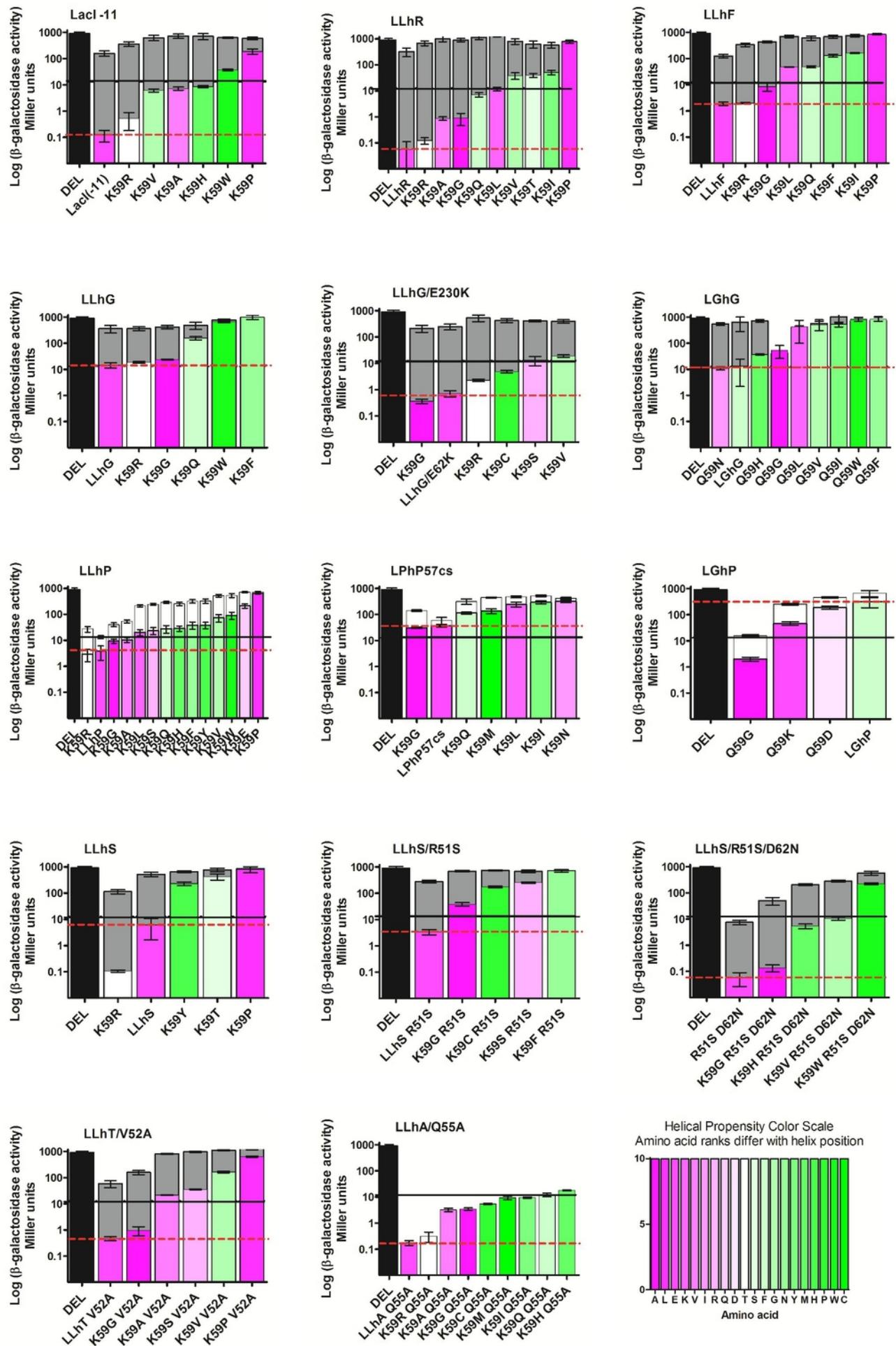


Figure S70: Physicochemical trends: Position 59, Helical propensity (C' scale)

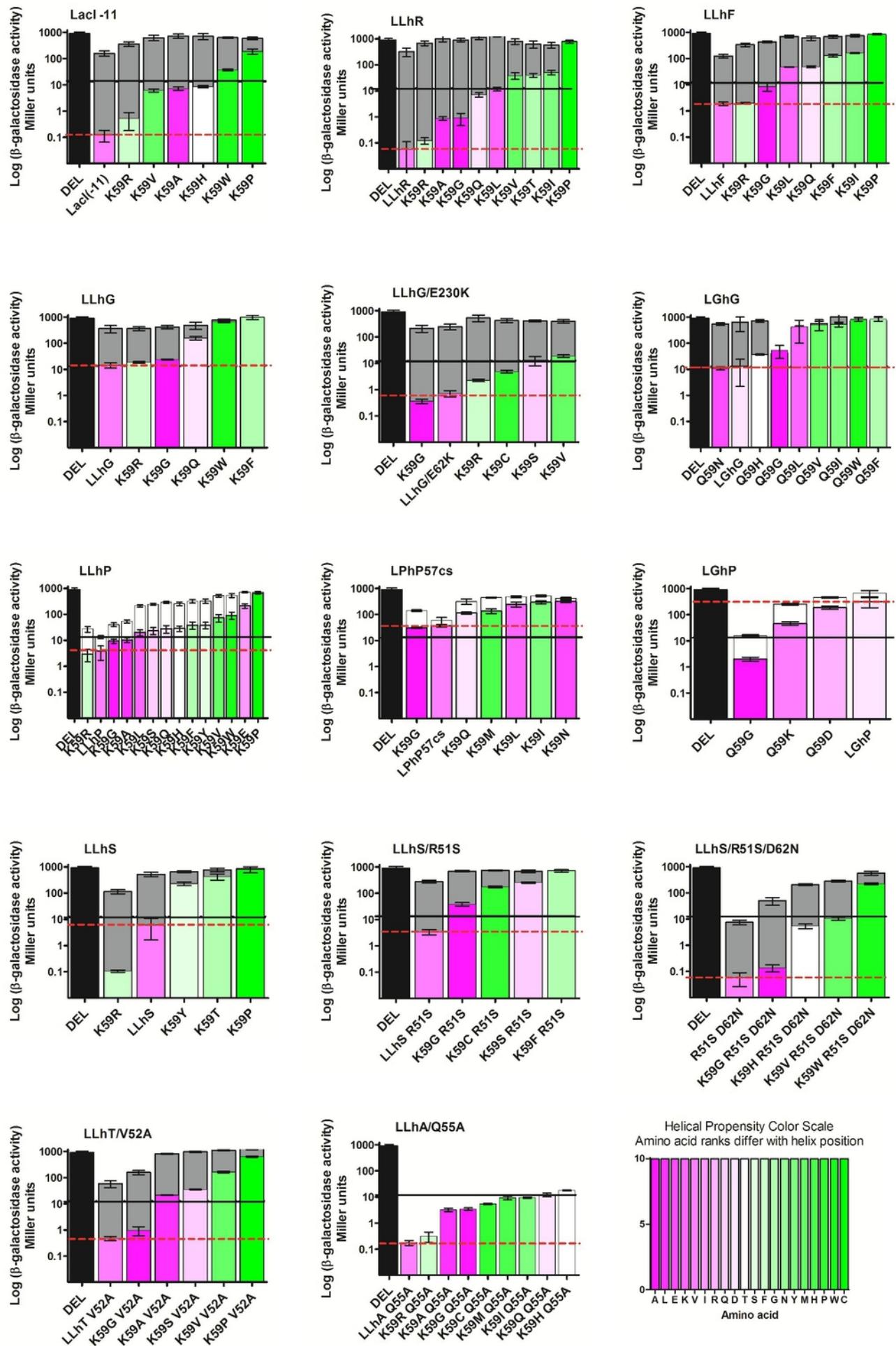


Figure S71: Physicochemical trends: Position 59, Helical propensity (C_{cap} scale)

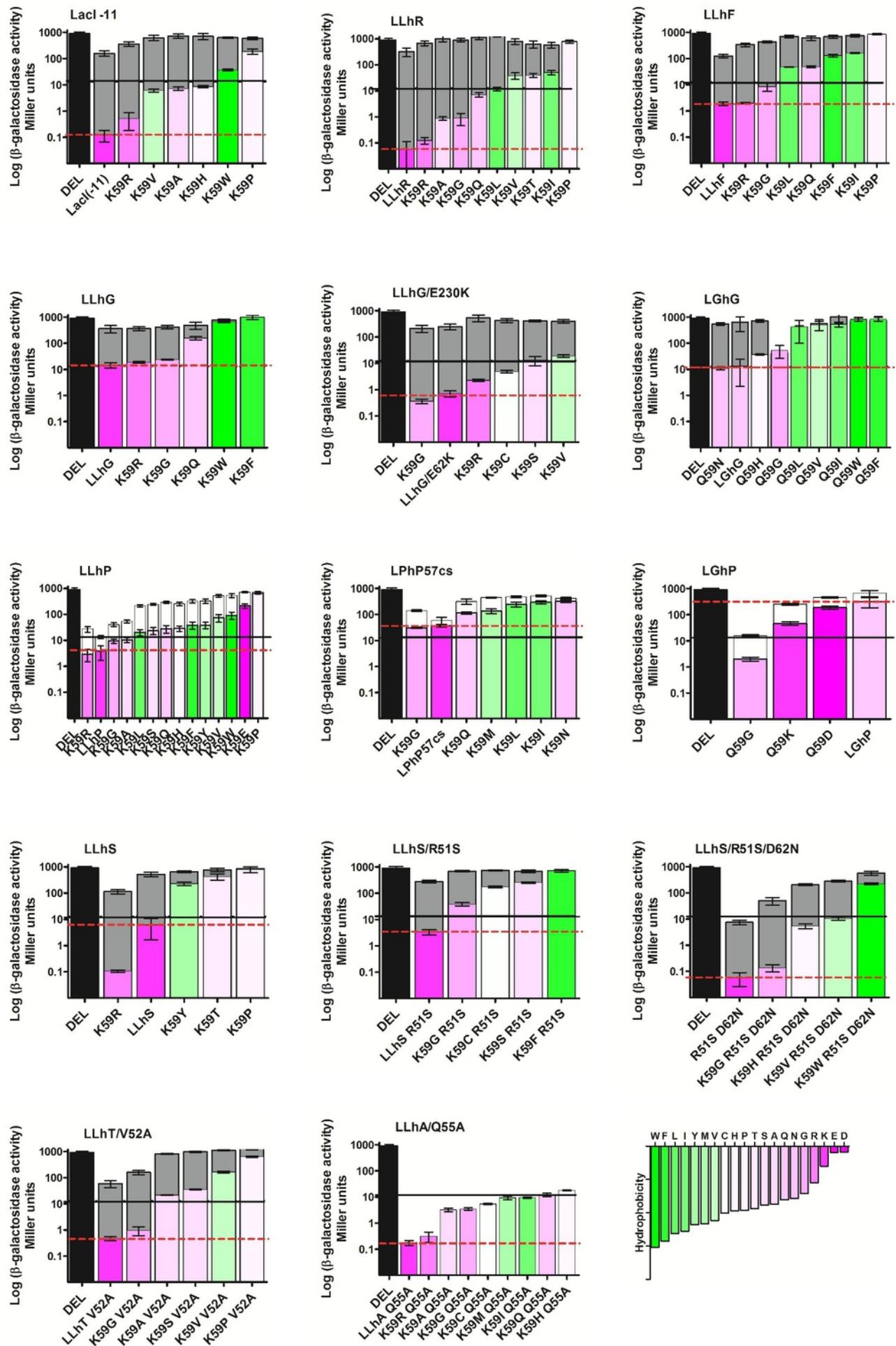


Figure S72: Physicochemical trends: Position 59, Hydrophobicity