

Supplemental Material for:  
Rheostats and toggle switches for modulating protein function  
File 5: Physicochemical trends: Positions 46-54

Meinhardt, Manley, Parente and Swint-Kruse

**List of Figures**

S25	Physicochemical trends: Position 46, Accessible surface area . . . . .	3
S26	Physicochemical trends: Position 46, Side chain branching . . . . .	4
S27	Physicochemical trends: Position 46, Charge/polarity/aromaticity . . . . .	5
S28	Physicochemical trends: Position 46, Hydrophobicity . . . . .	6
S29	Physicochemical trends: Position 48, Accessible surface area . . . . .	7
S30	Physicochemical trends: Position 48, Side chain branching . . . . .	8
S31	Physicochemical trends: Position 48, Charge/polarity/aromaticity . . . . .	9
S32	Physicochemical trends: Position 48, Helical propensity (N' scale) . . . . .	10
S33	Physicochemical trends: Position 48, Hydrophobicity . . . . .	11
S34	Physicochemical trends: Position 50, Accessible surface area . . . . .	12
S35	Physicochemical trends: Position 50, Side chain branching . . . . .	13
S36	Physicochemical trends: Position 50, Charge/polarity/aromaticity . . . . .	14
S37	Physicochemical trends: Position 50, Helical propensity (N1 scale) . . . . .	15
S38	Physicochemical trends: Position 50, Hydrophobicity . . . . .	16
S39	Physicochemical trends: Position 51, Accessible surface area . . . . .	17
S40	Physicochemical trends: Position 51, Side chain branching . . . . .	18
S41	Physicochemical trends: Position 51, Charge/polarity/aromaticity . . . . .	19
S42	Physicochemical trends: Position 51, Helical propensity (N2 scale) . . . . .	20
S43	Physicochemical trends: Position 51, Hydrophobicity . . . . .	21
S44	Physicochemical trends: Position 52, Accessible surface area . . . . .	22
S45	Physicochemical trends: Position 52, Side chain branching . . . . .	23
S46	Physicochemical trends: Position 52, Charge/polarity/aromaticity . . . . .	24
S47	Physicochemical trends: Position 52, Helical propensity (N3 scale) . . . . .	25
S48	Physicochemical trends: Position 52, Hydrophobicity . . . . .	26
S49	Physicochemical trends: Position 54, Accessible surface area . . . . .	27
S50	Physicochemical trends: Position 54, Side chain branching . . . . .	28
S51	Physicochemical trends: Position 54, Charge/polarity/aromaticity . . . . .	29
S52	Physicochemical trends: Position 54, Helical propensity (C4 scale) . . . . .	30
S53	Physicochemical trends: Position 54, Helical propensity (Midpoint scale) . . . . .	31
S54	Physicochemical trends: Position 54, Hydrophobicity . . . . .	32

**Figures S25-S54.** Physico-chemical trends: positions 46-54. Repression assay data for each position were color-coded according to various physico-chemical scales. For example, Figures S25-S28 show results for position 46 color-coded by accessible surface area of the free side chain [46], side chain branching, charge/polarity/aromaticity, and hydrophobicity [45]. 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.

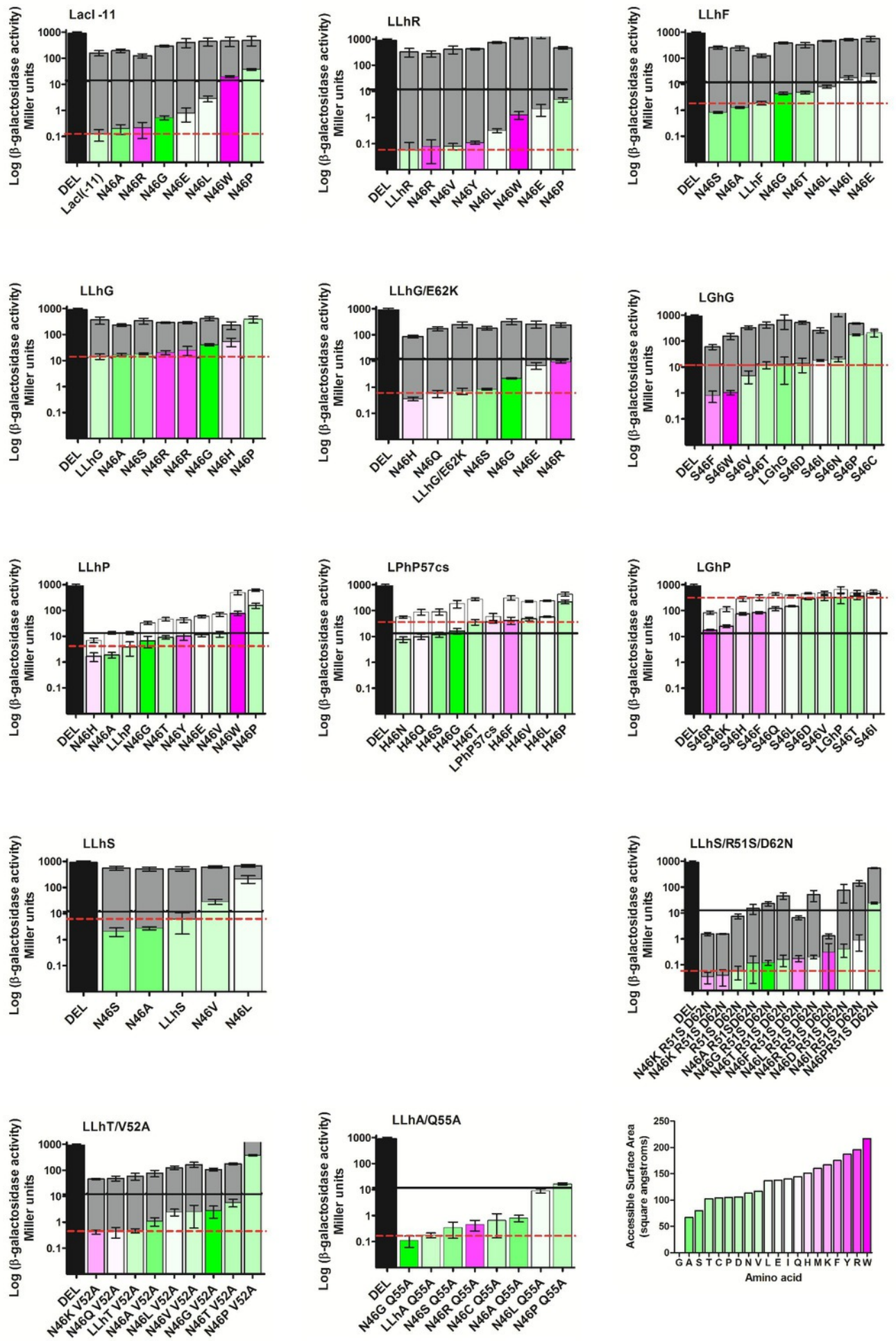


Figure S25: Physicochemical trends: Position 46, Accessible surface area

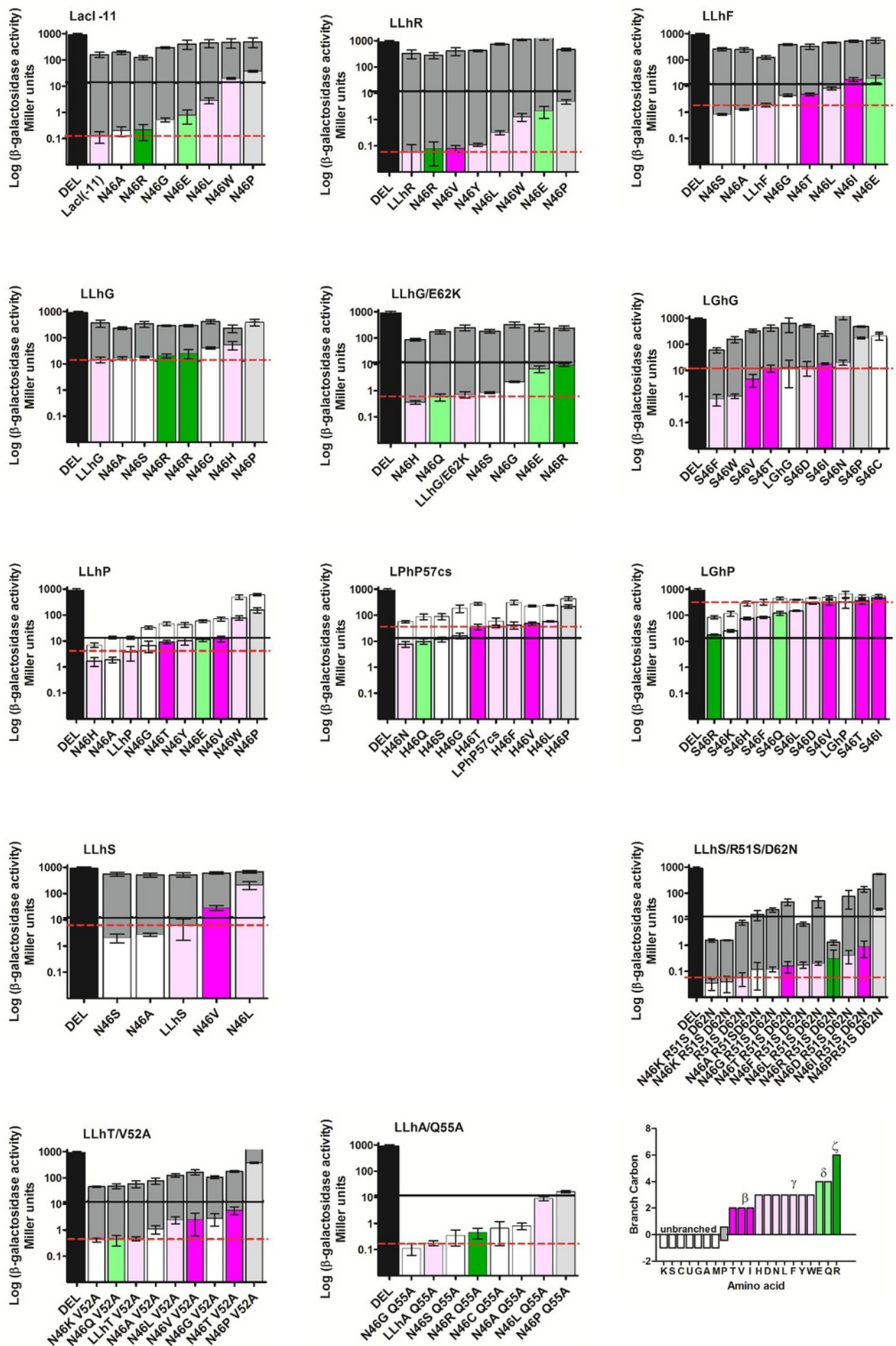


Figure S26: Physicochemical trends: Position 46, Side chain branching



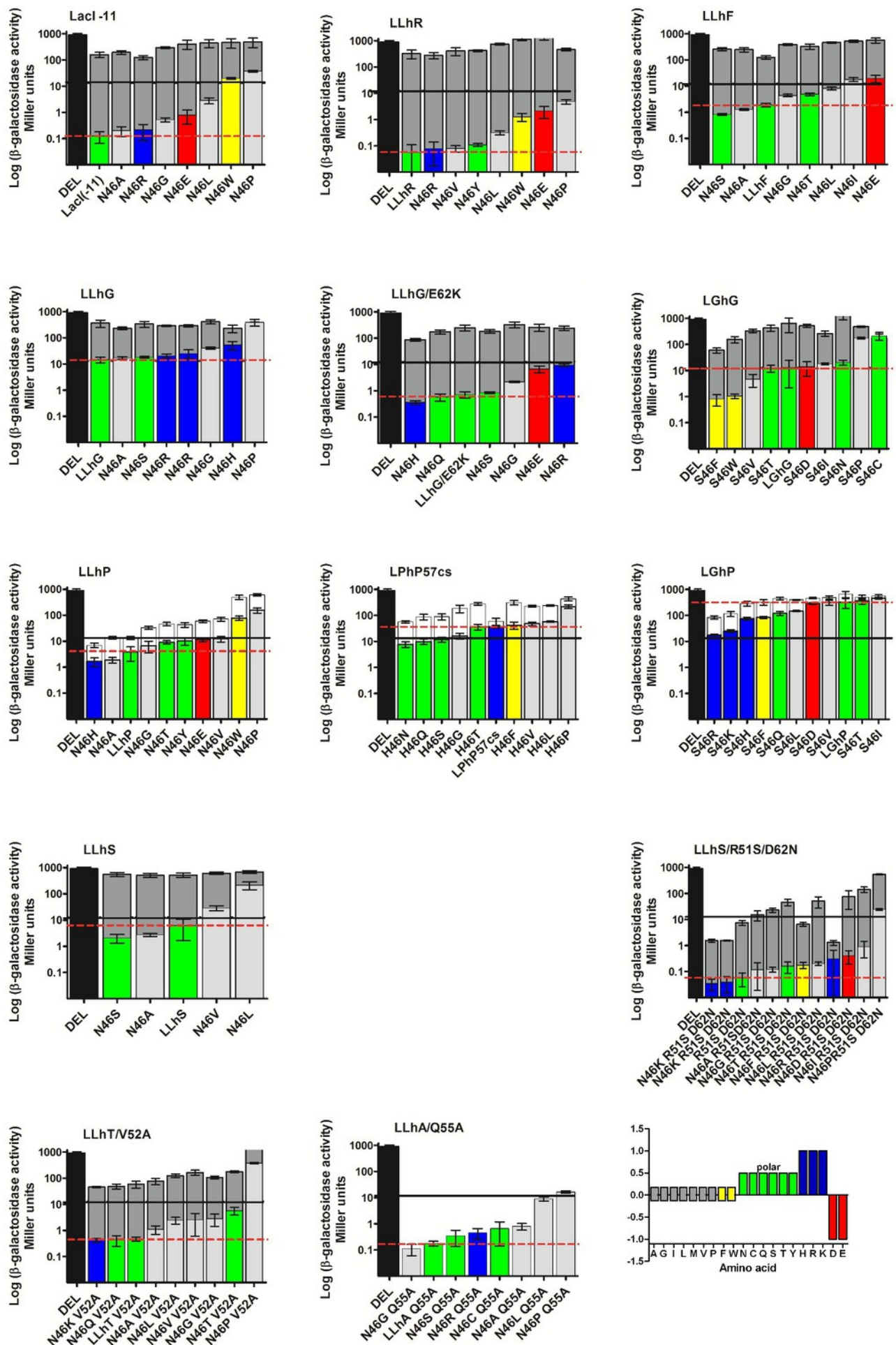


Figure S27: Physicochemical trends: Position 46, Charge/polarity/aromaticity

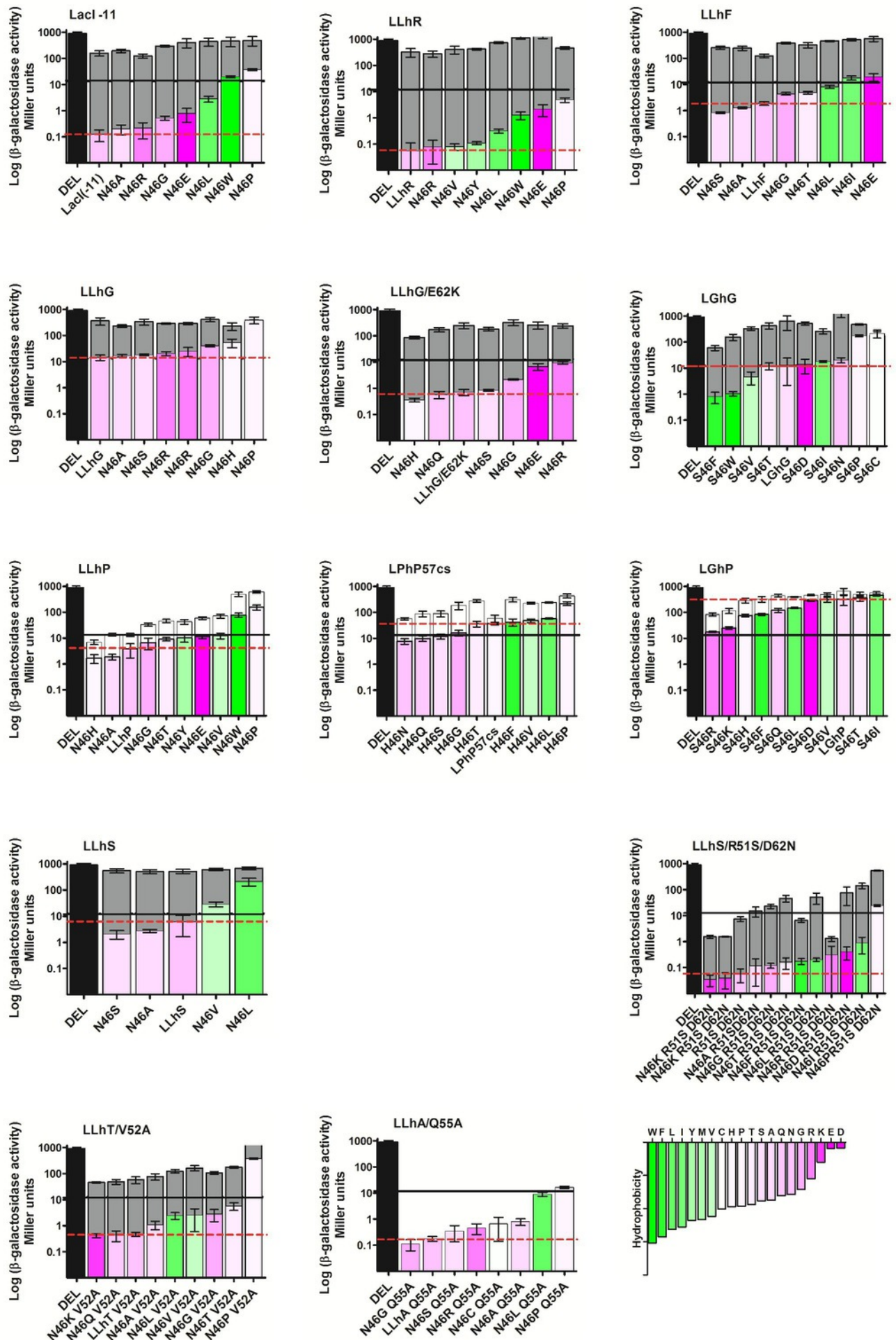


Figure S28: Physicochemical trends: Position 46, Hydrophobicity



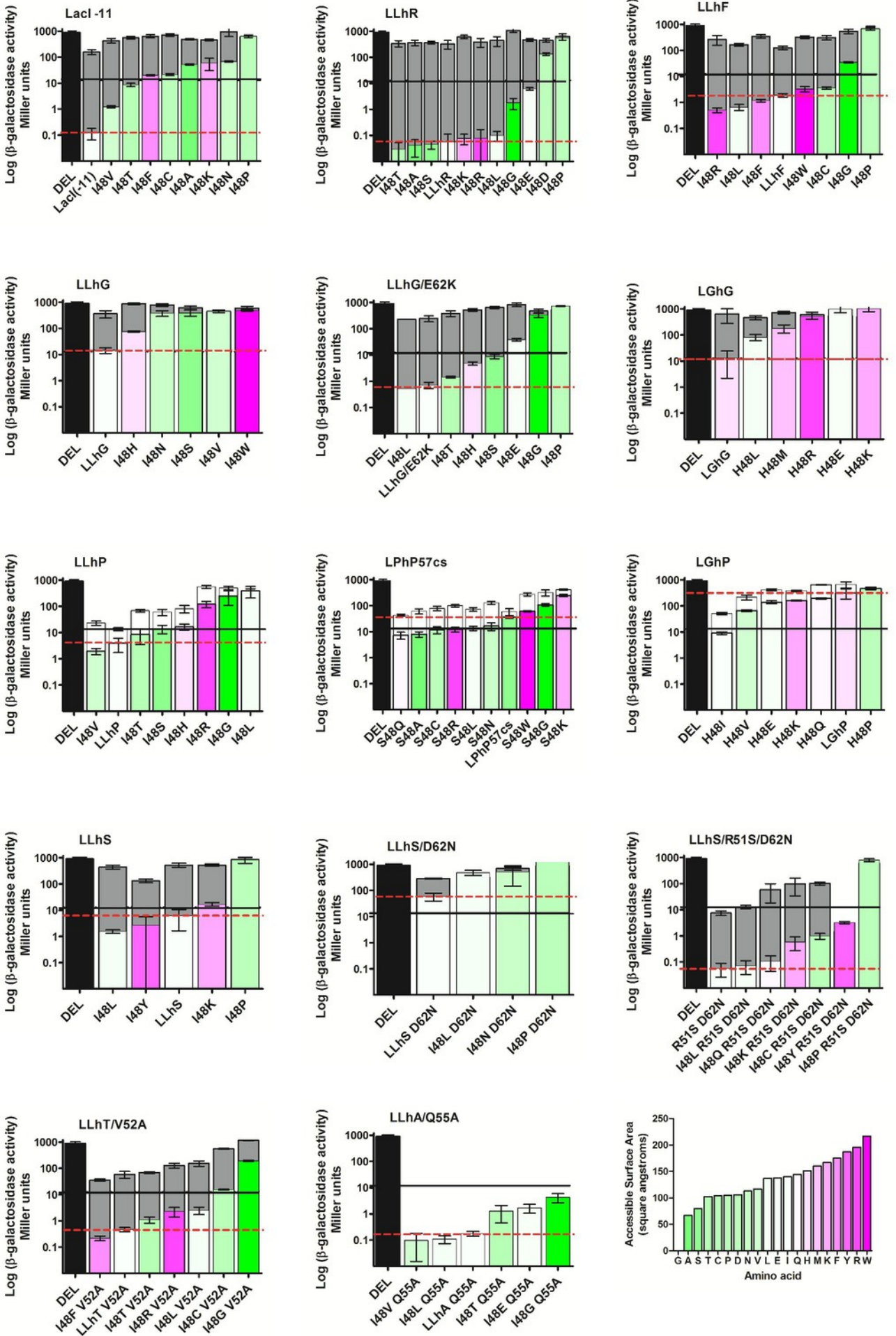


Figure S29: Physicochemical trends: Position 48, Accessible surface area

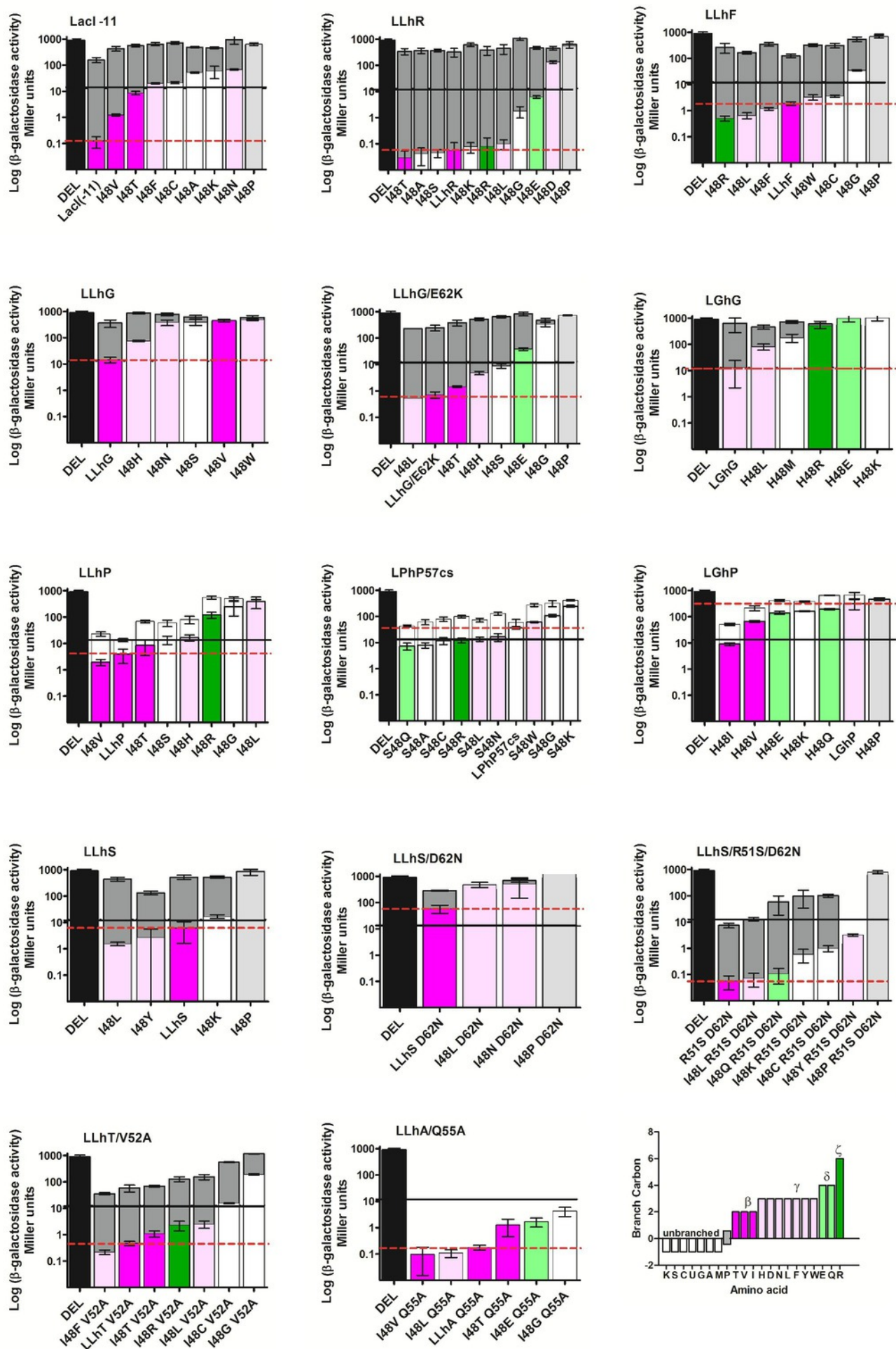


Figure S30: Physicochemical trends: Position 48, Side chain branching



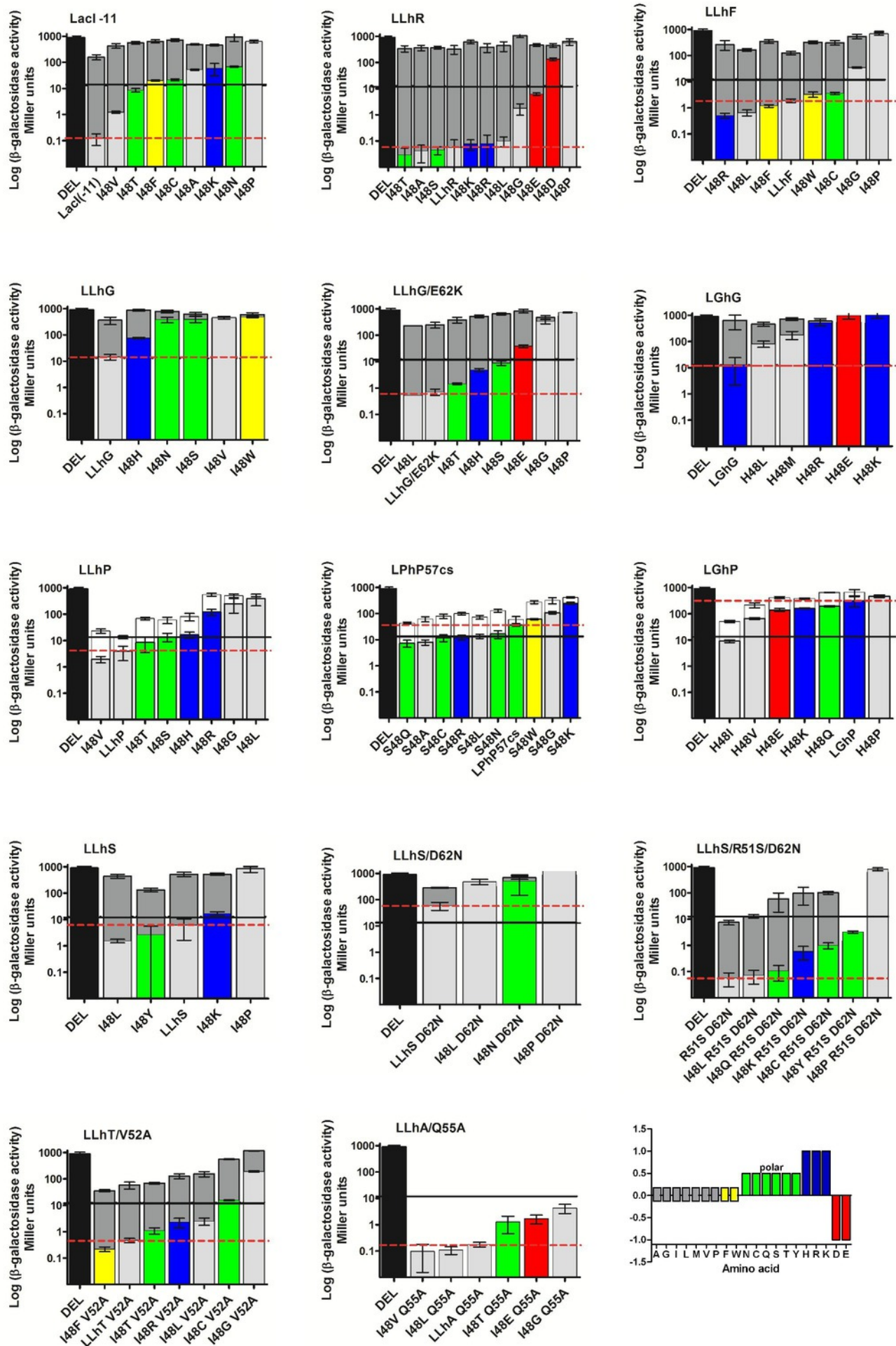


Figure S31: Physicochemical trends: Position 48, Charge/polarity/aromaticity



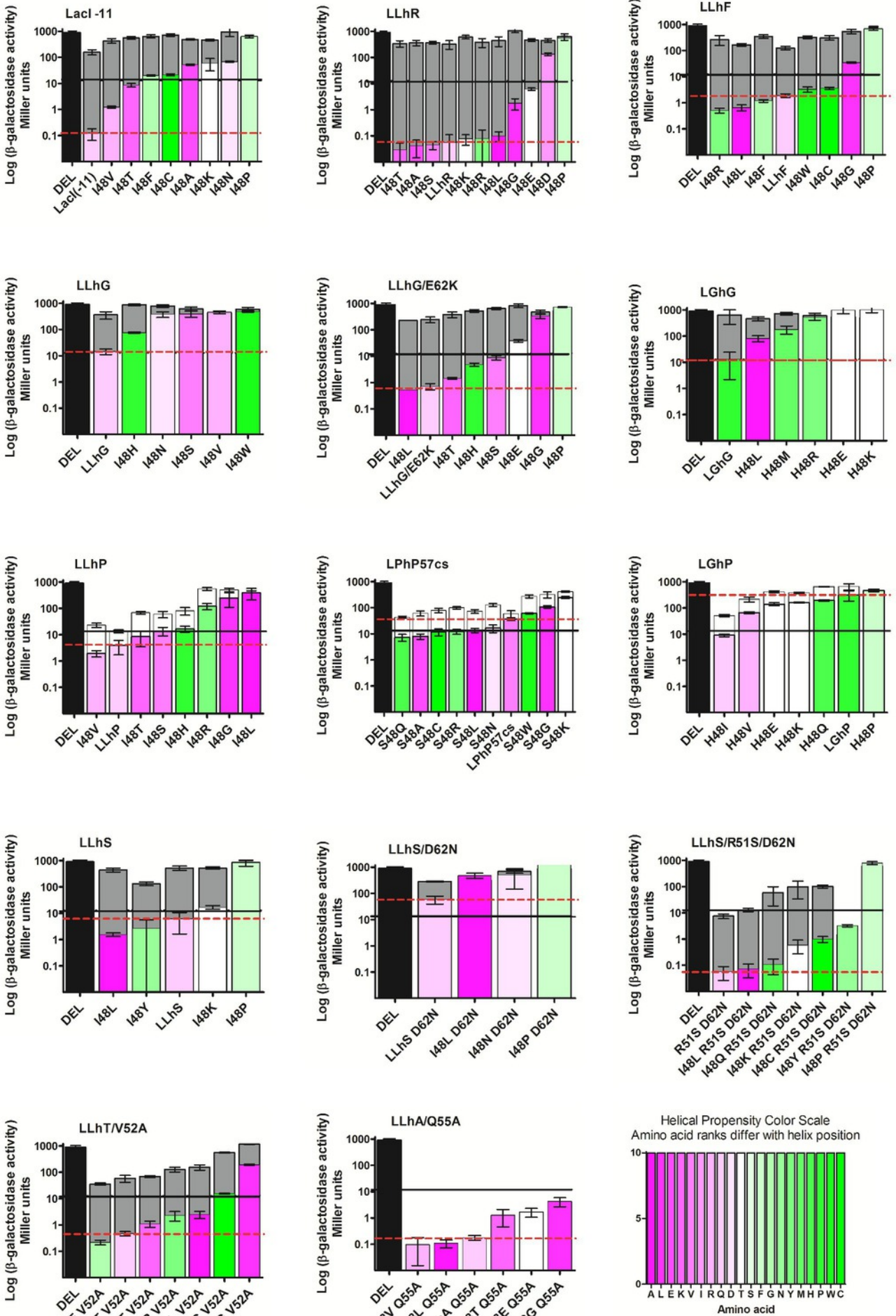


Figure S32: Physicochemical trends: Position 48, Helical propensity (N' scale)

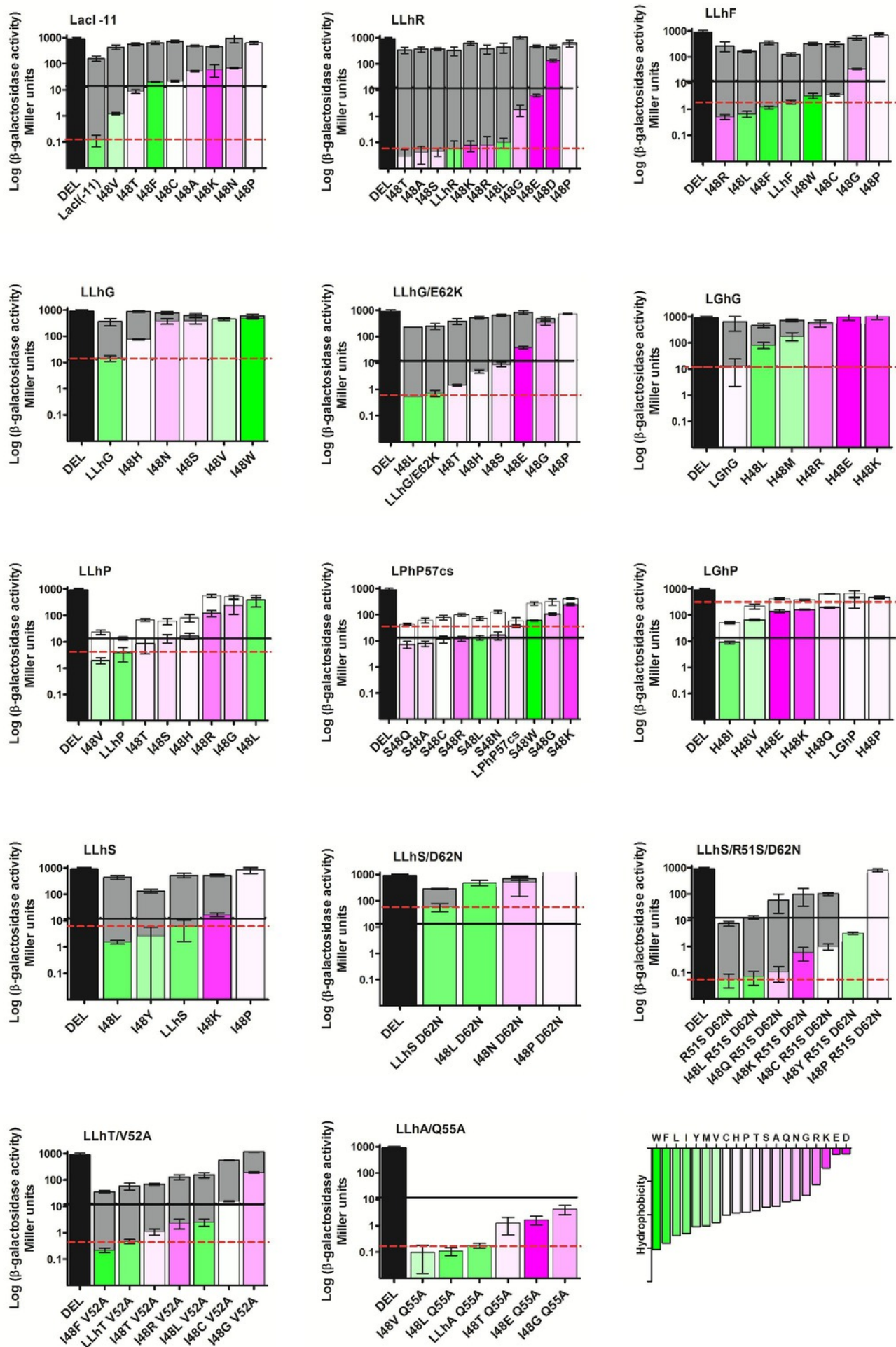


Figure S33: Physicochemical trends: Position 48, Hydrophobicity



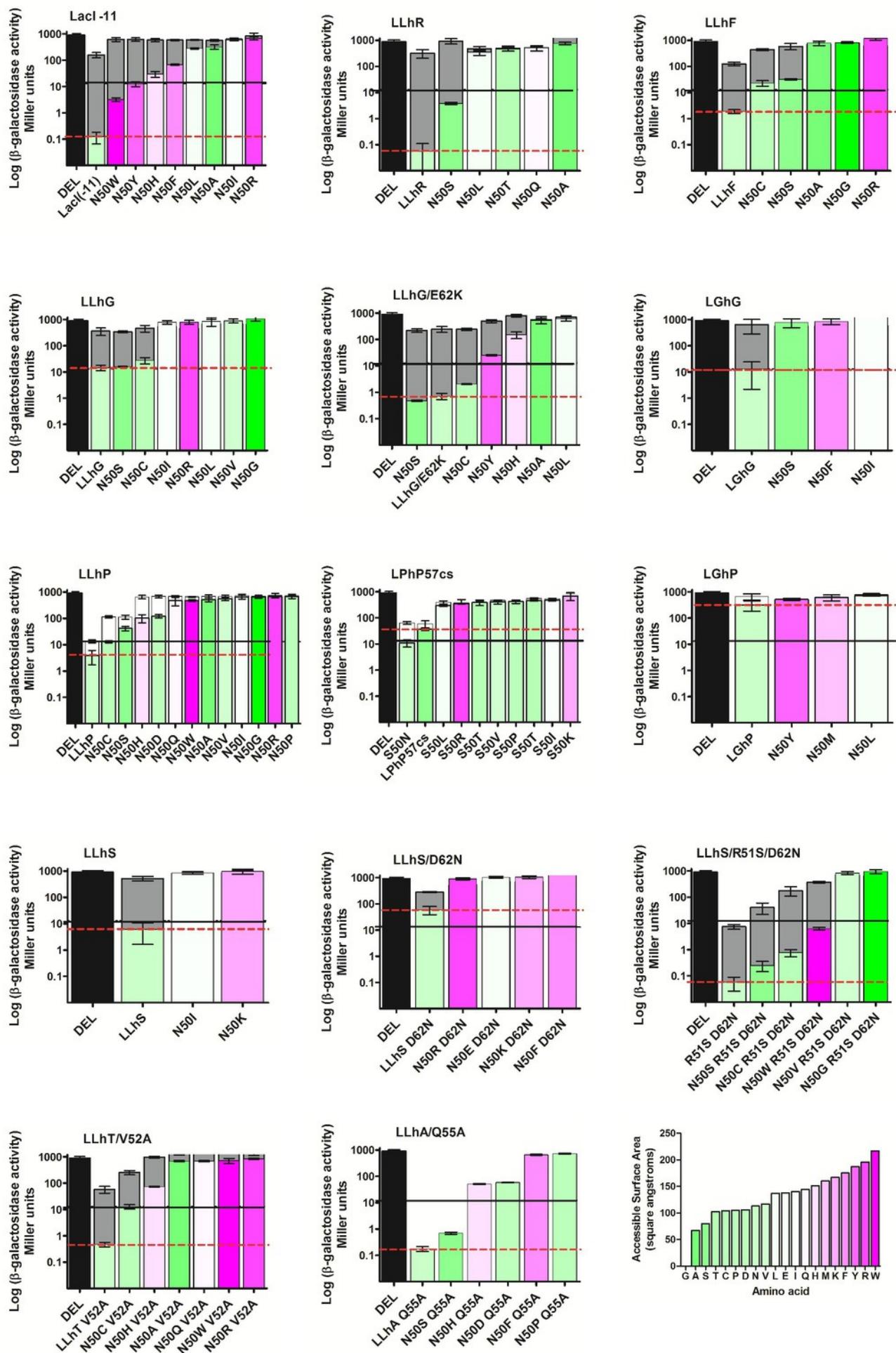


Figure S34: Physicochemical trends: Position 50, Accessible surface area

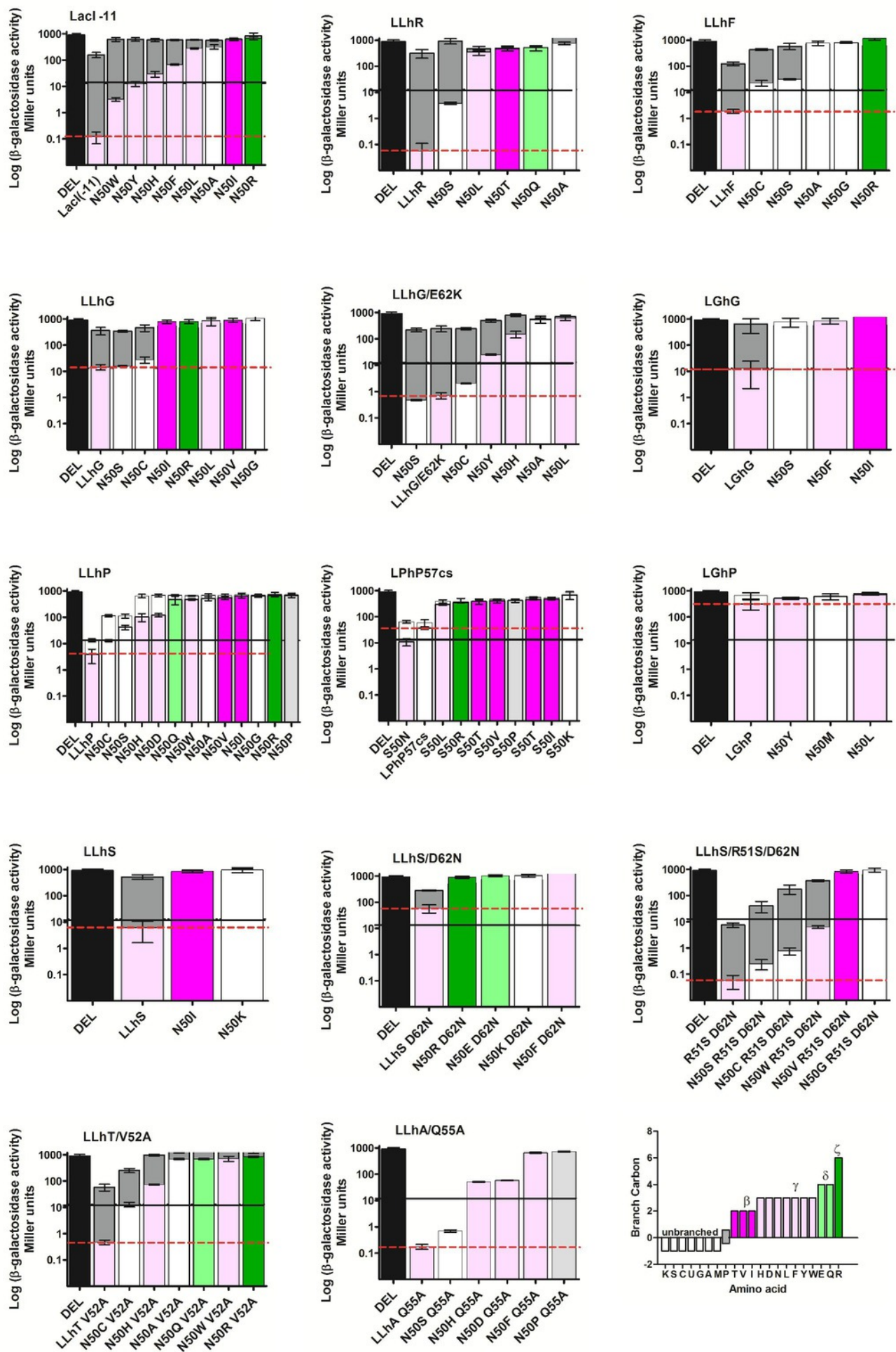


Figure S35: Physicochemical trends: Position 50, Side chain branching



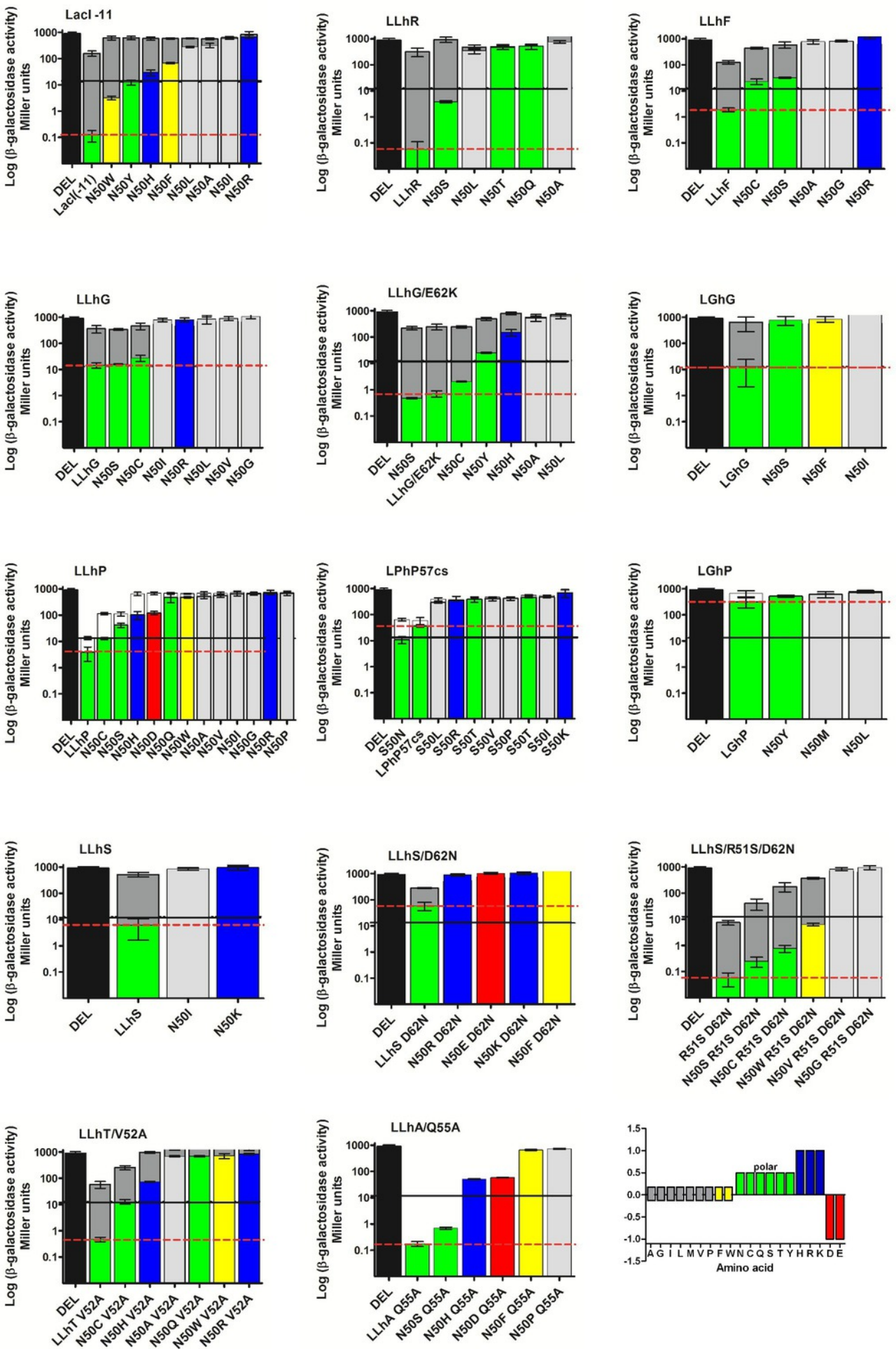


Figure S36: Physicochemical trends: Position 50, Charge/polarity/aromaticity



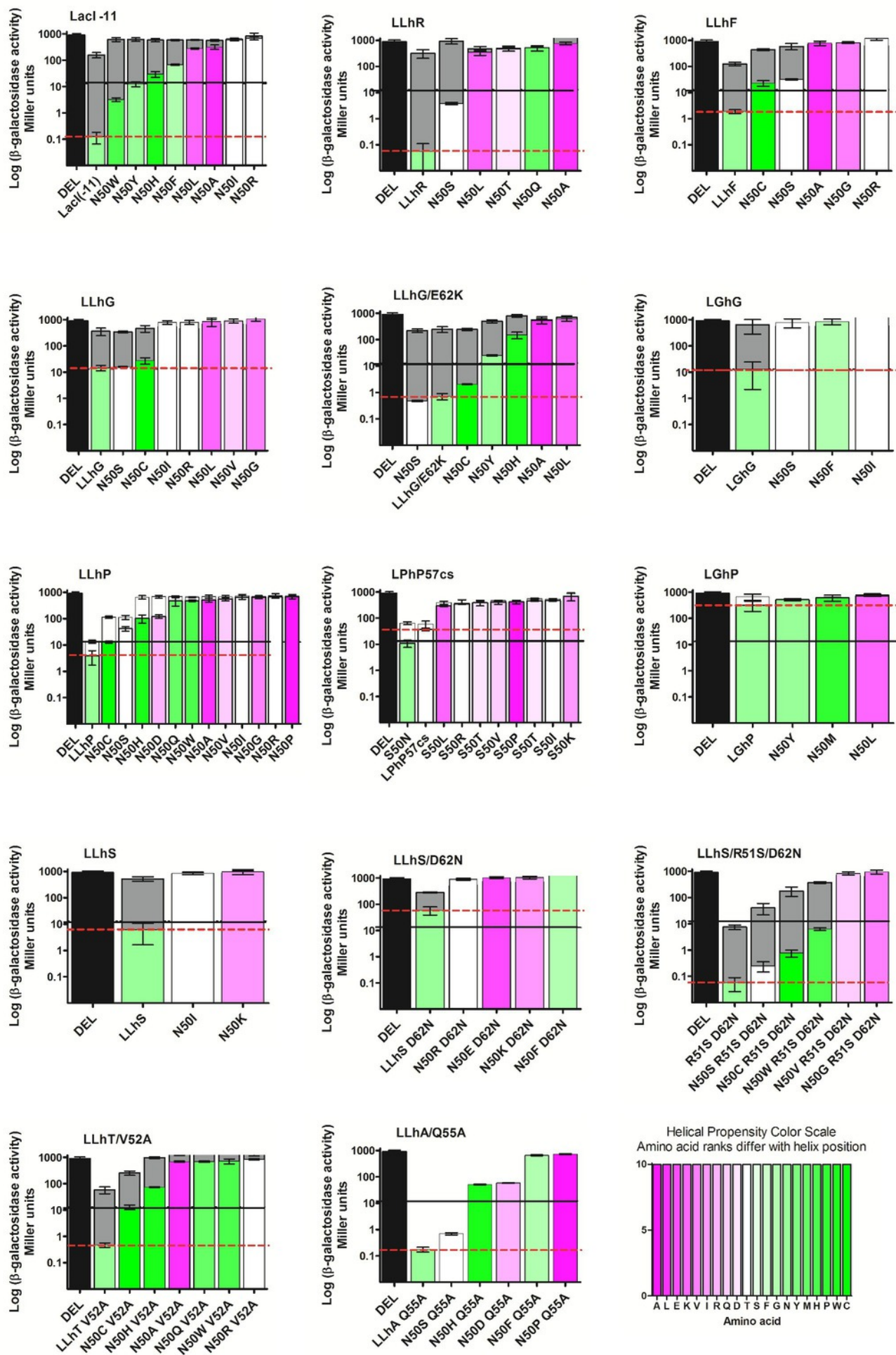


Figure S37: Physicochemical trends: Position 50, Helical propensity (N1 scale)

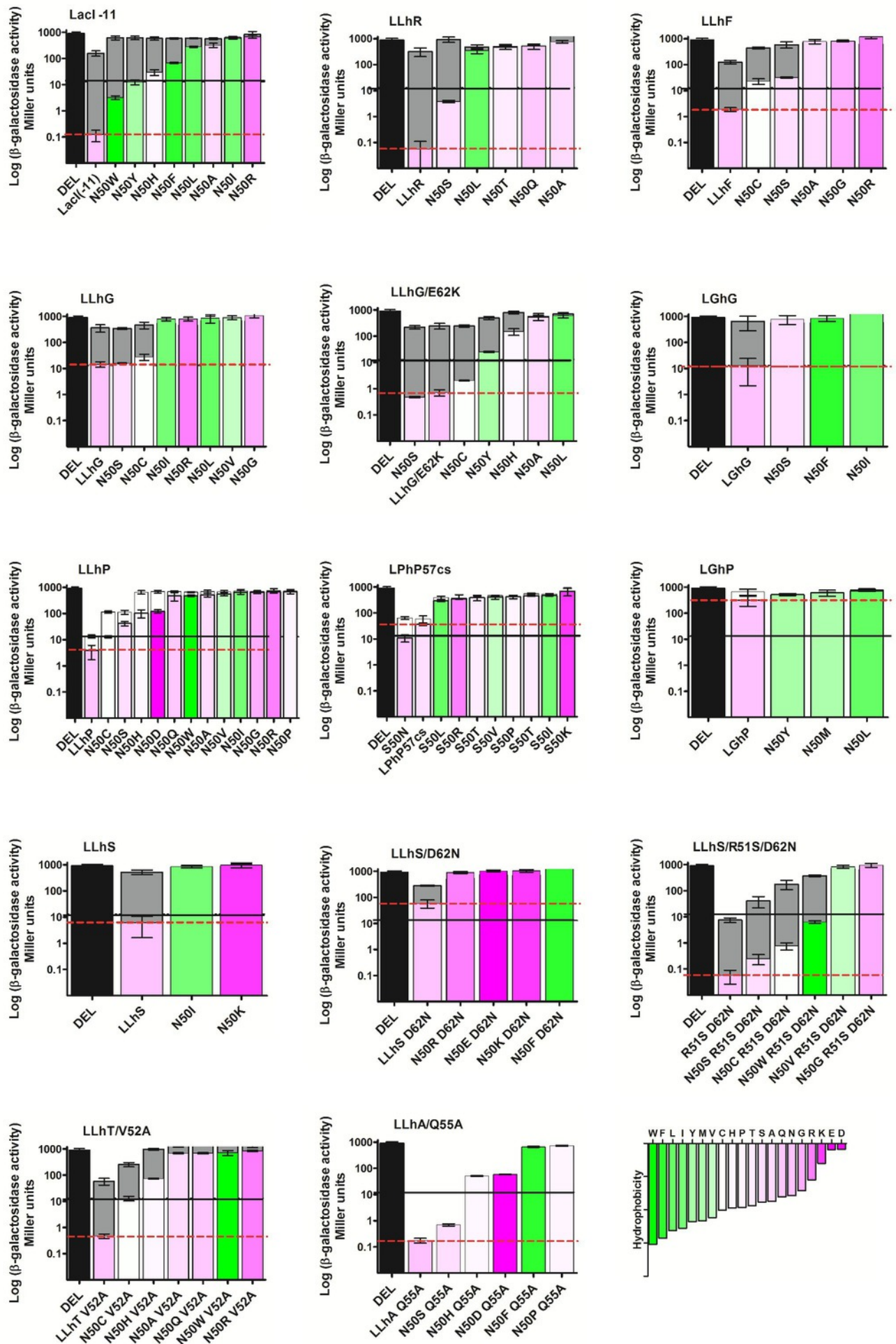


Figure S38: Physicochemical trends: Position 50, Hydrophobicity



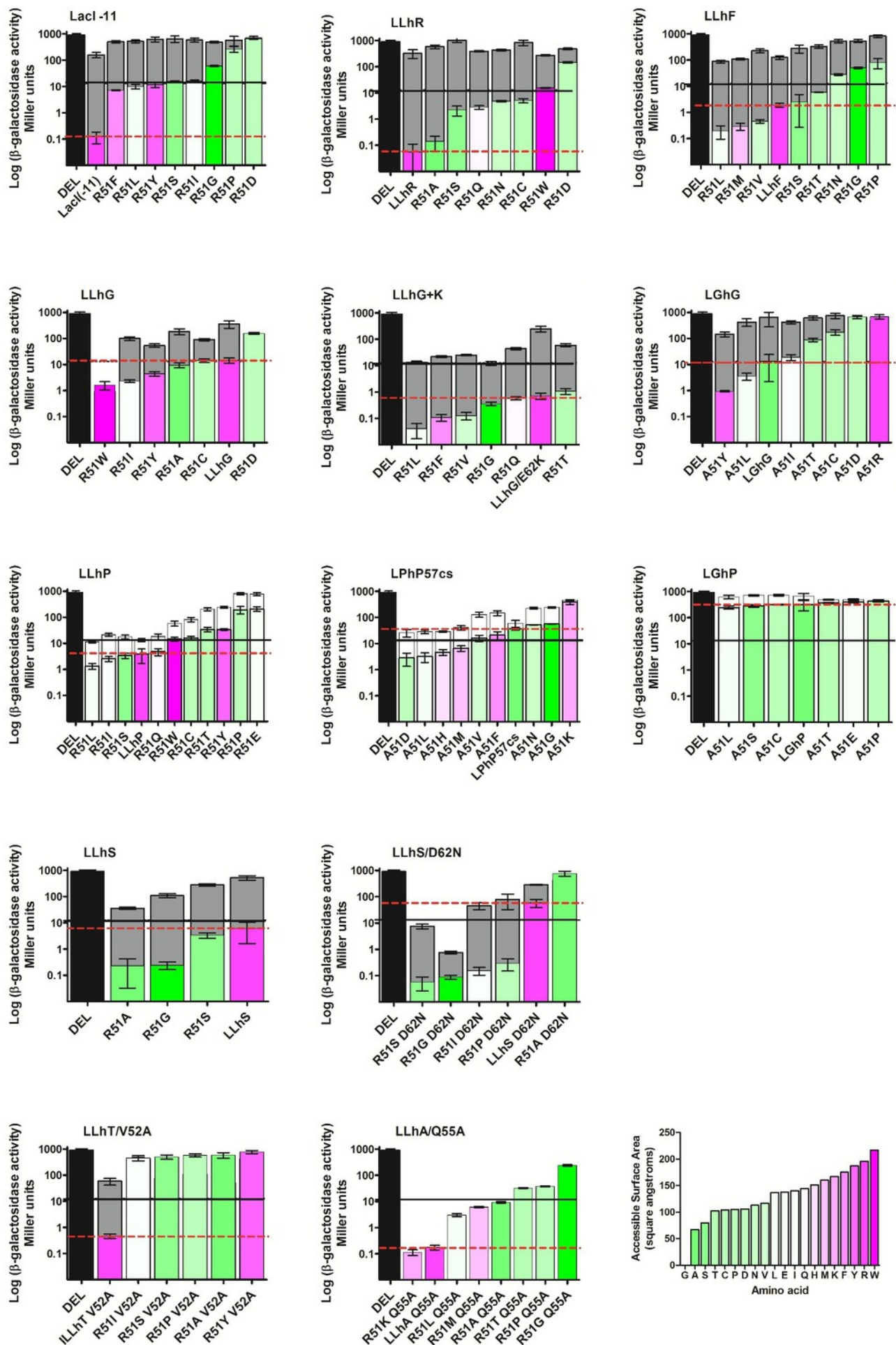


Figure S39: Physicochemical trends: Position 51, Accessible surface area



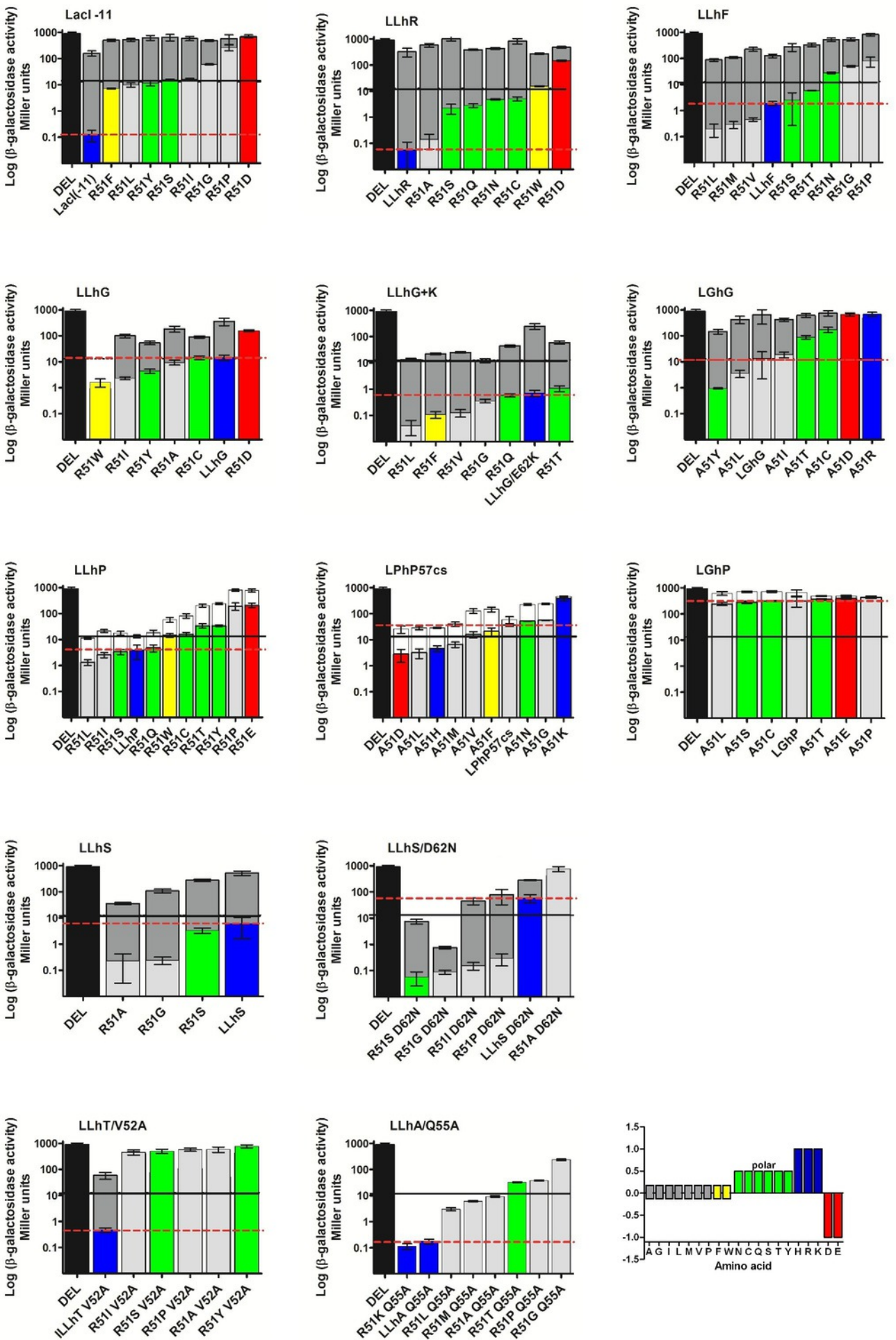


Figure S41: Physicochemical trends: Position 51, Charge/polarity/aromaticity



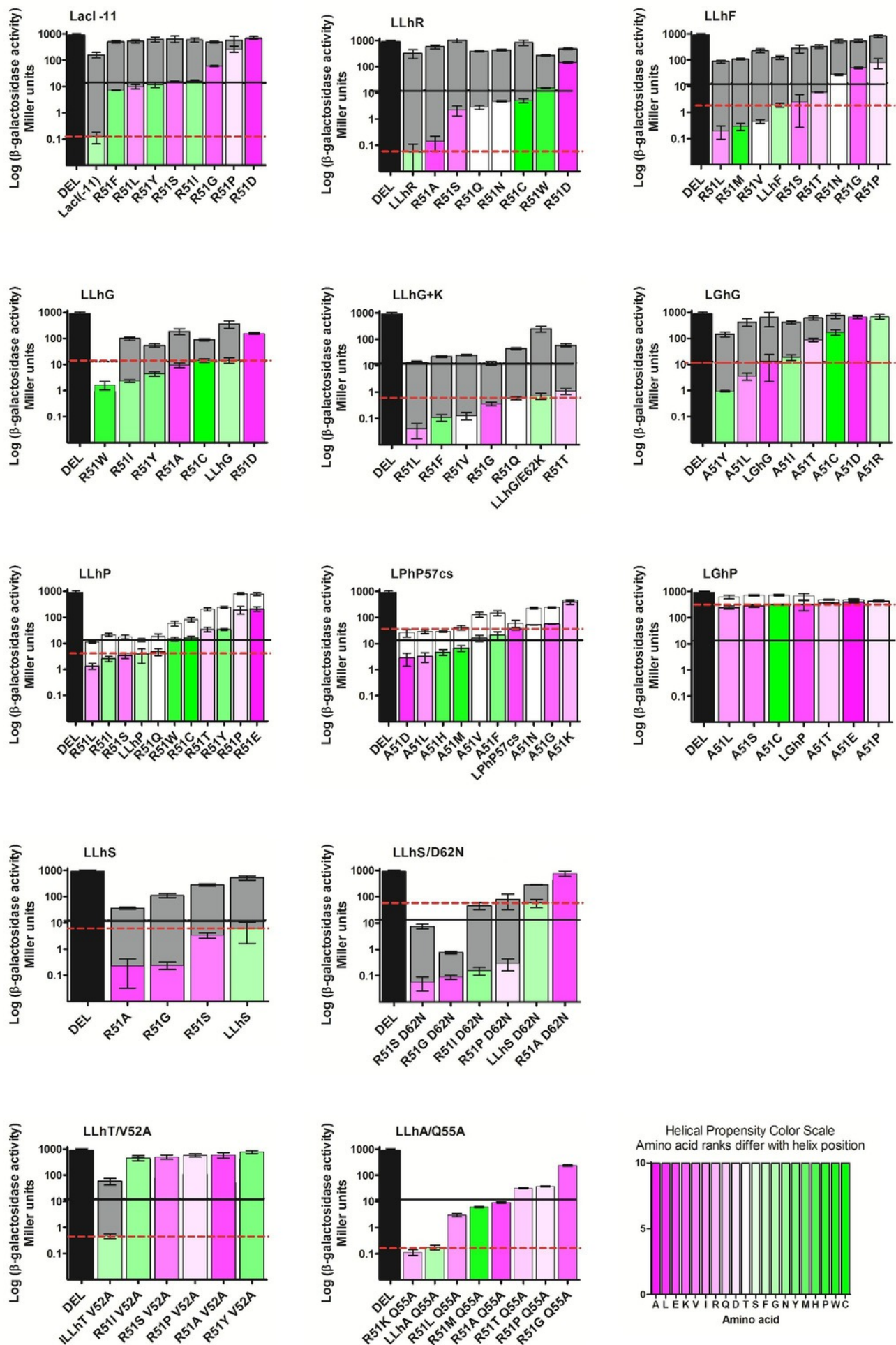


Figure S42: Physicochemical trends: Position 51, Helical propensity (N2 scale)

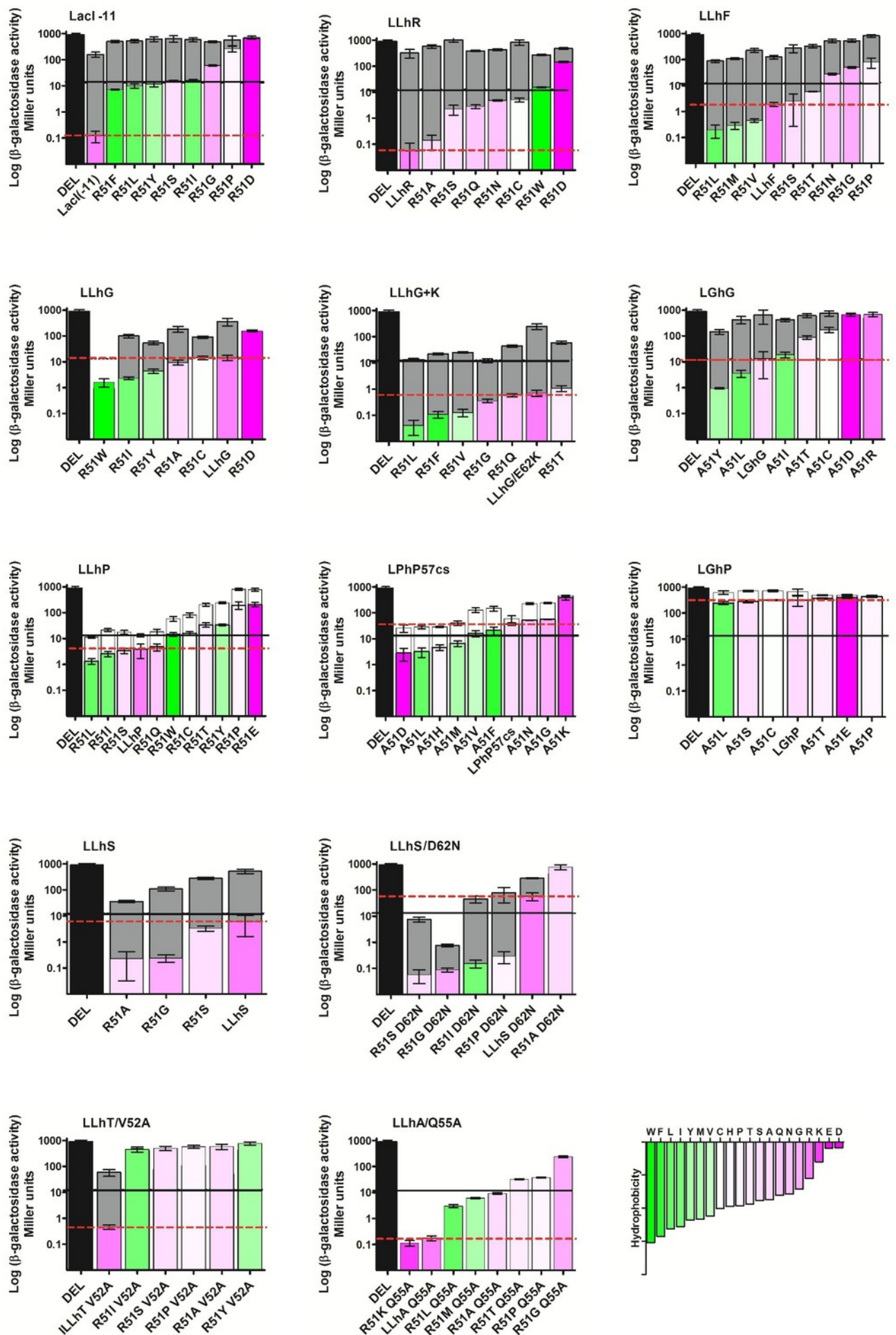


Figure S43: Physicochemical trends: Position 51, Hydrophobicity

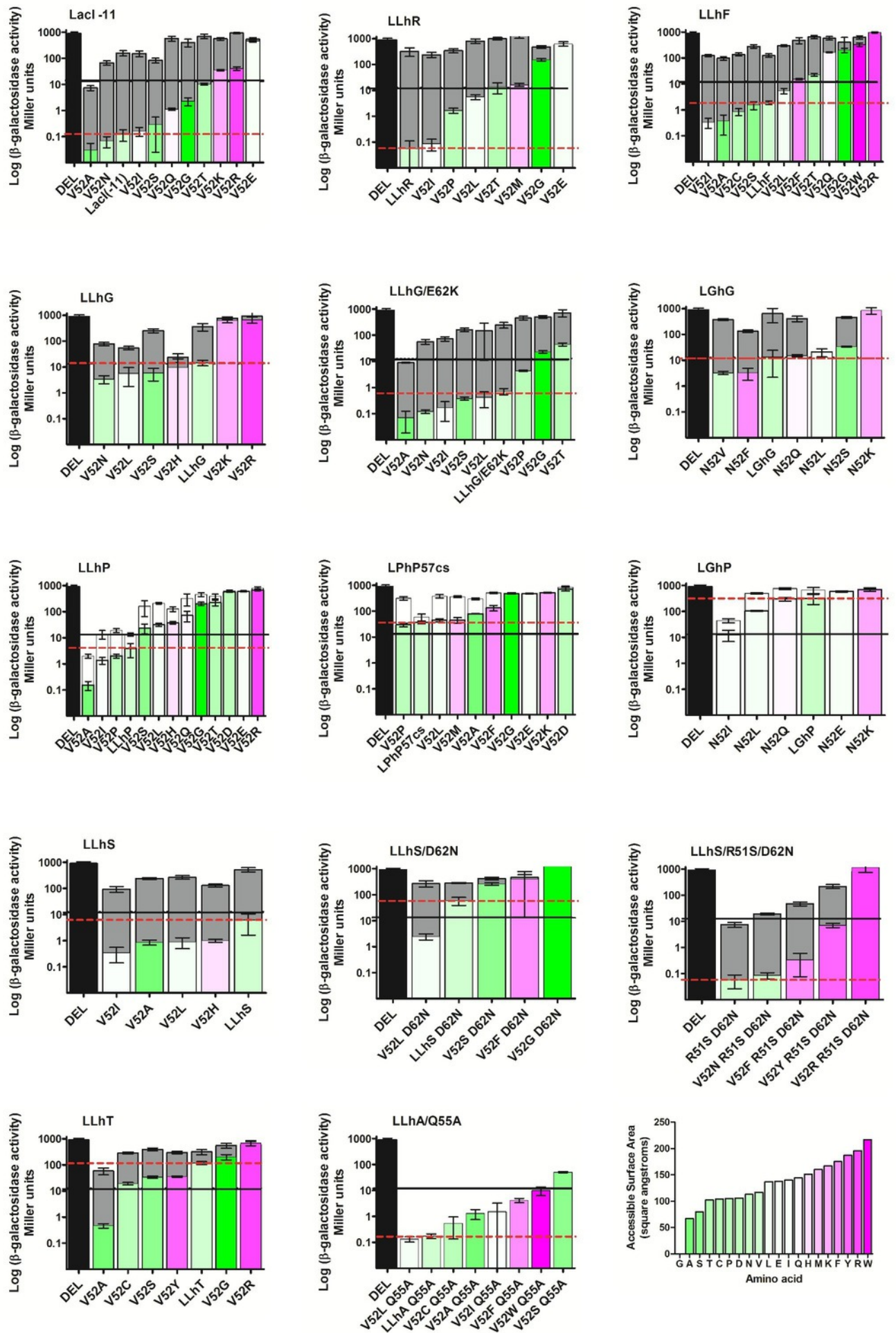


Figure S44: Physicochemical trends: Position 52, Accessible surface area



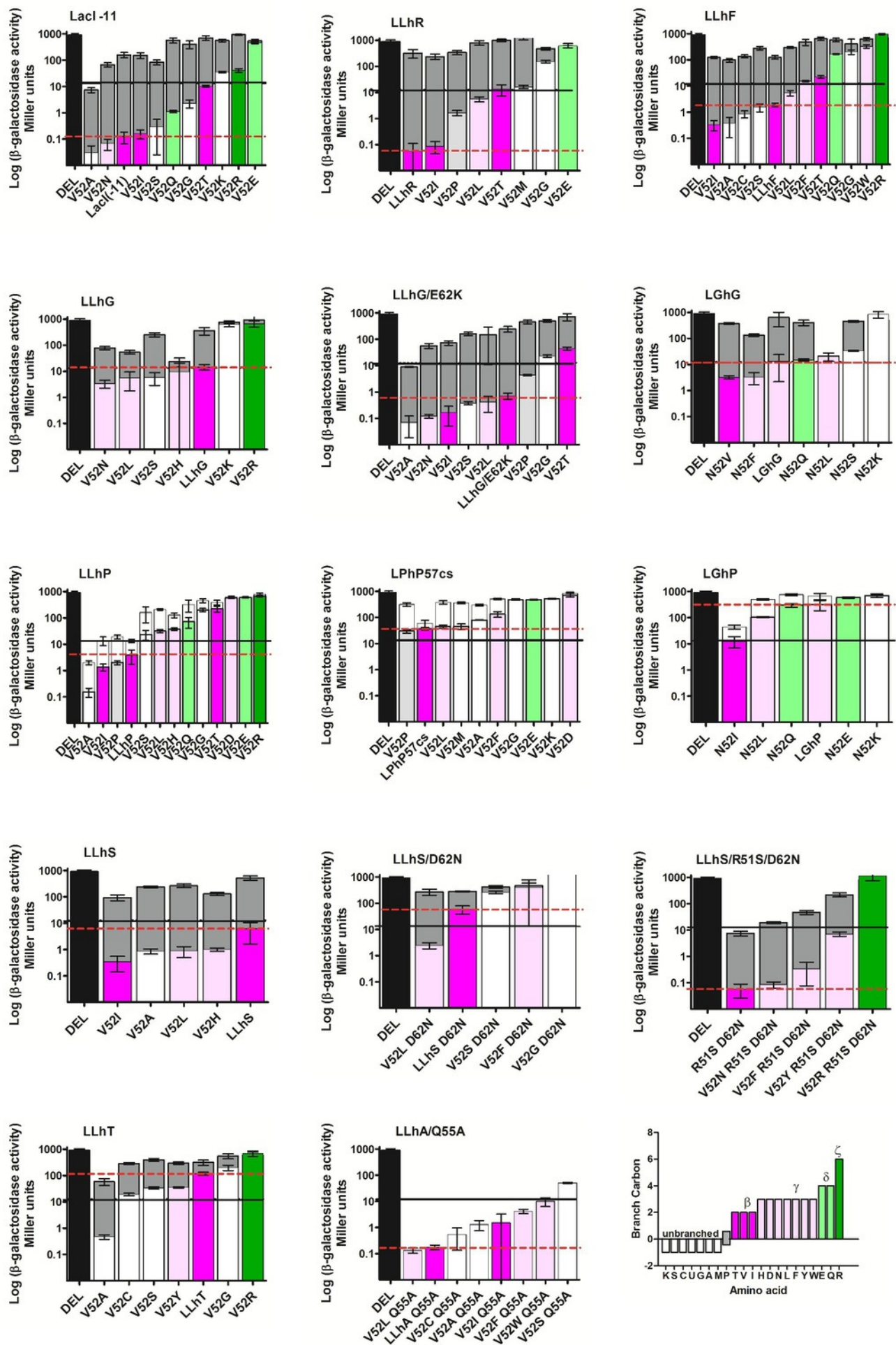


Figure S45: Physicochemical trends: Position 52, Side chain branching

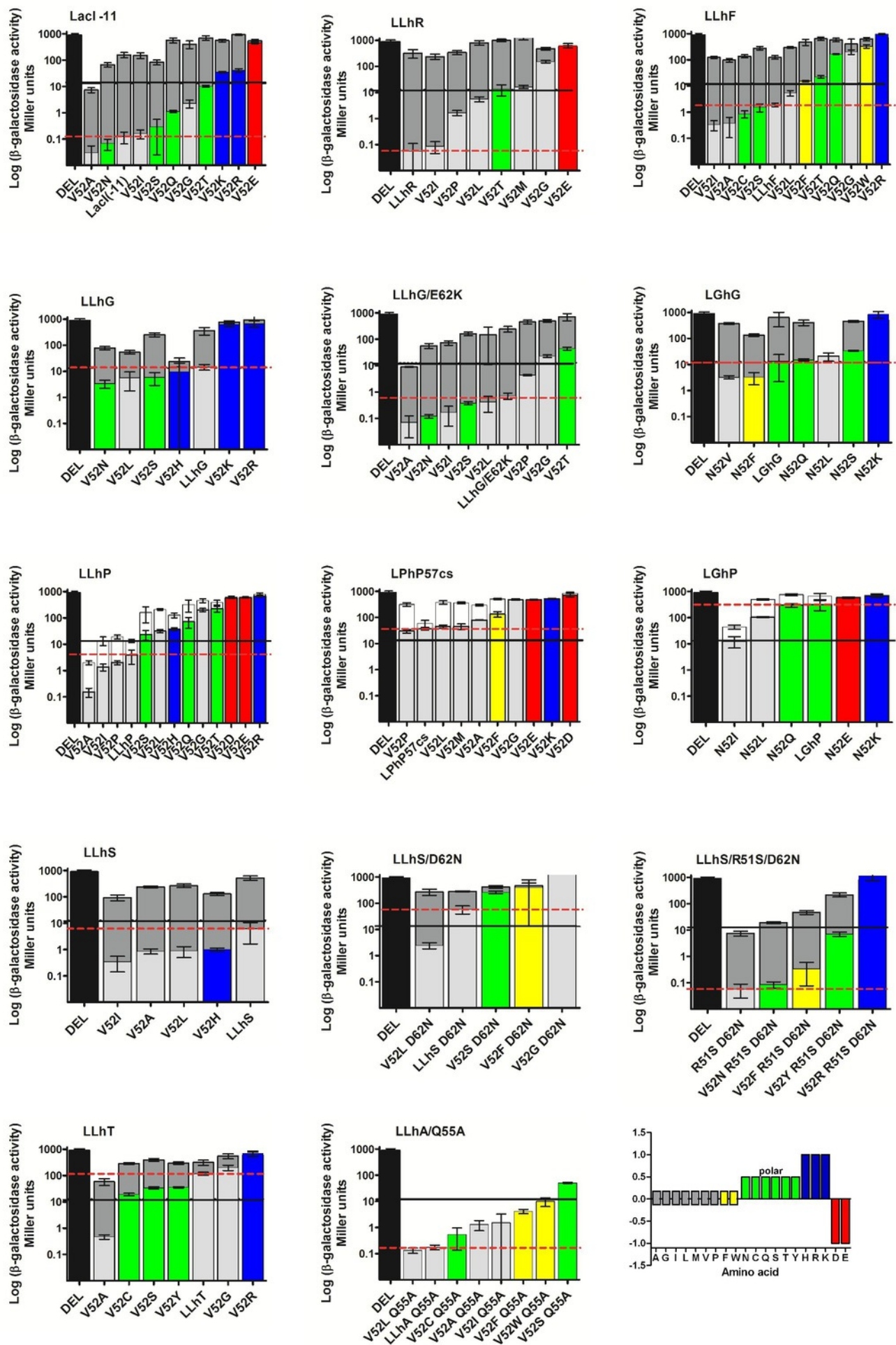


Figure S46: Physicochemical trends: Position 52, Charge/polarity/aromaticity



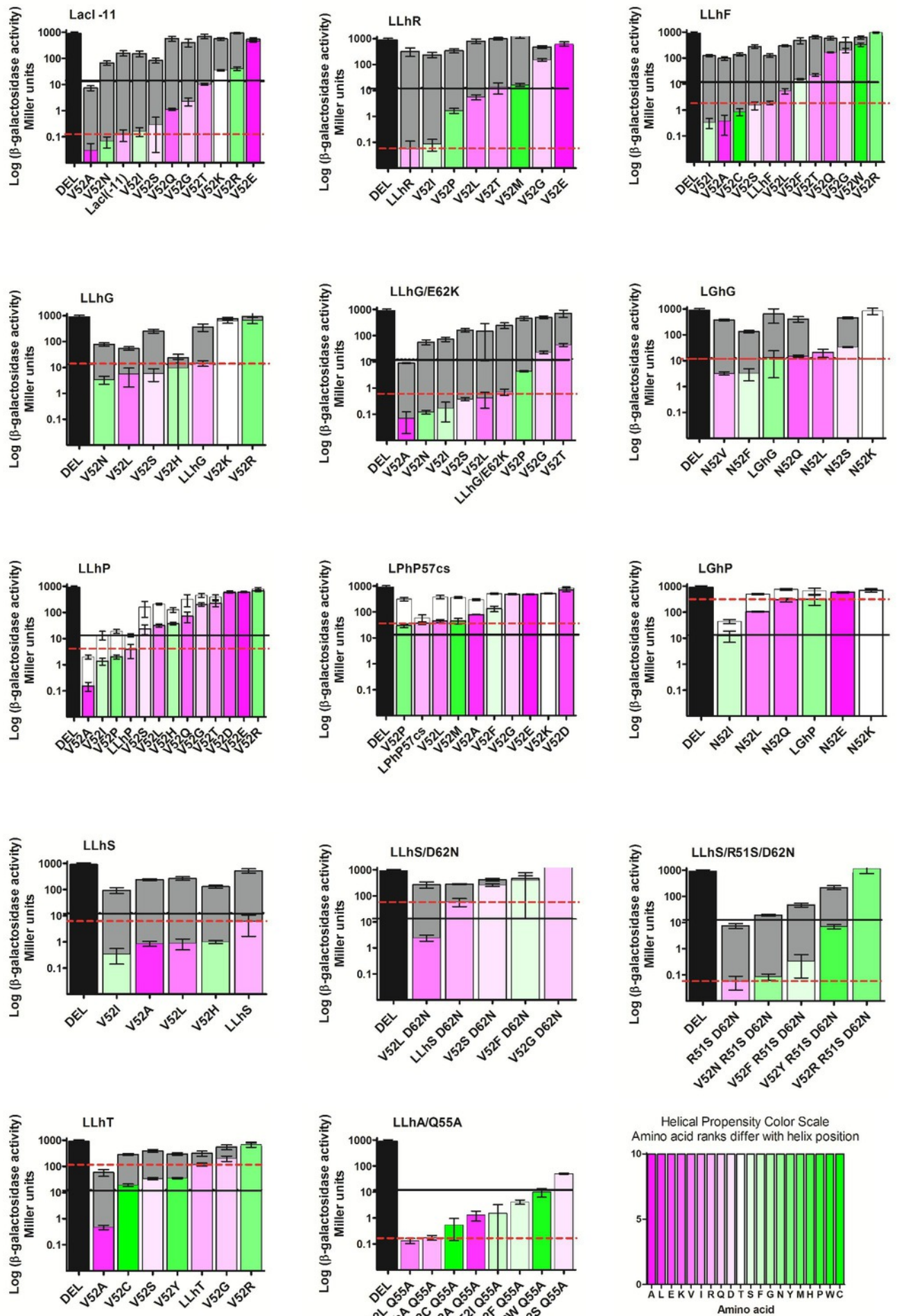


Figure S47: Physicochemical trends: Position 52, Helical propensity (N3 scale)

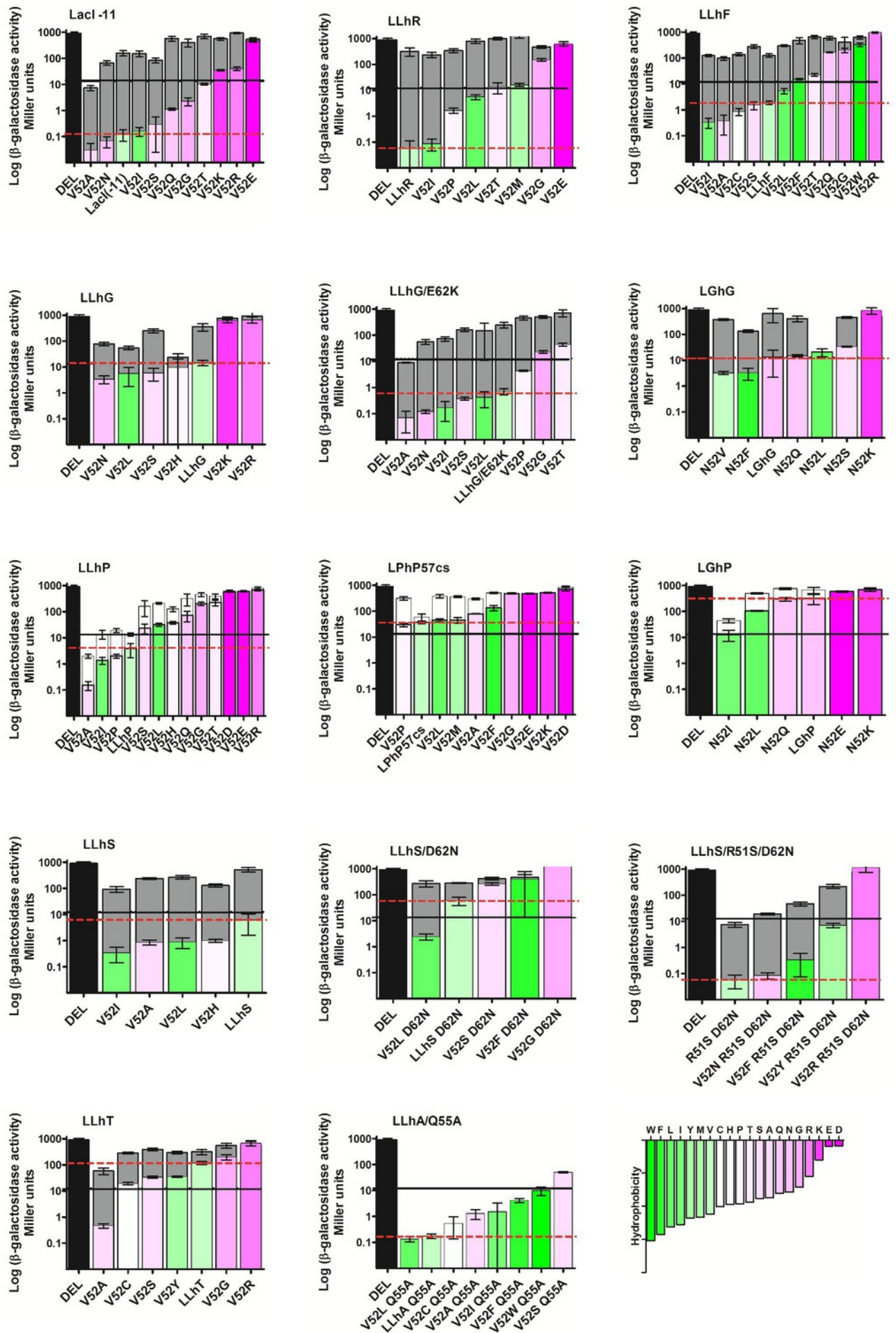


Figure S48: Physicochemical trends: Position 52, Hydrophobicity



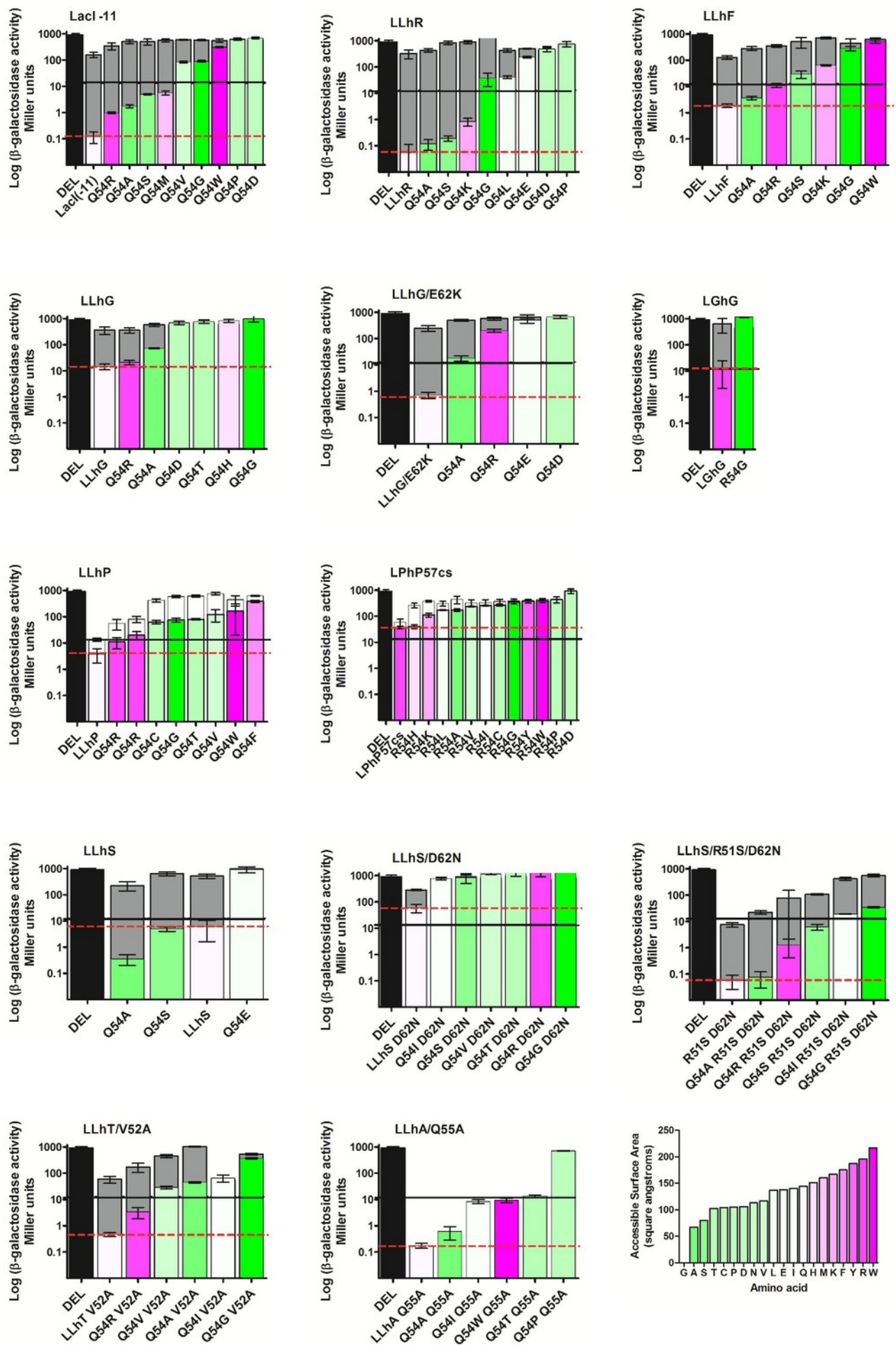


Figure S49: Physicochemical trends: Position 54, Accessible surface area



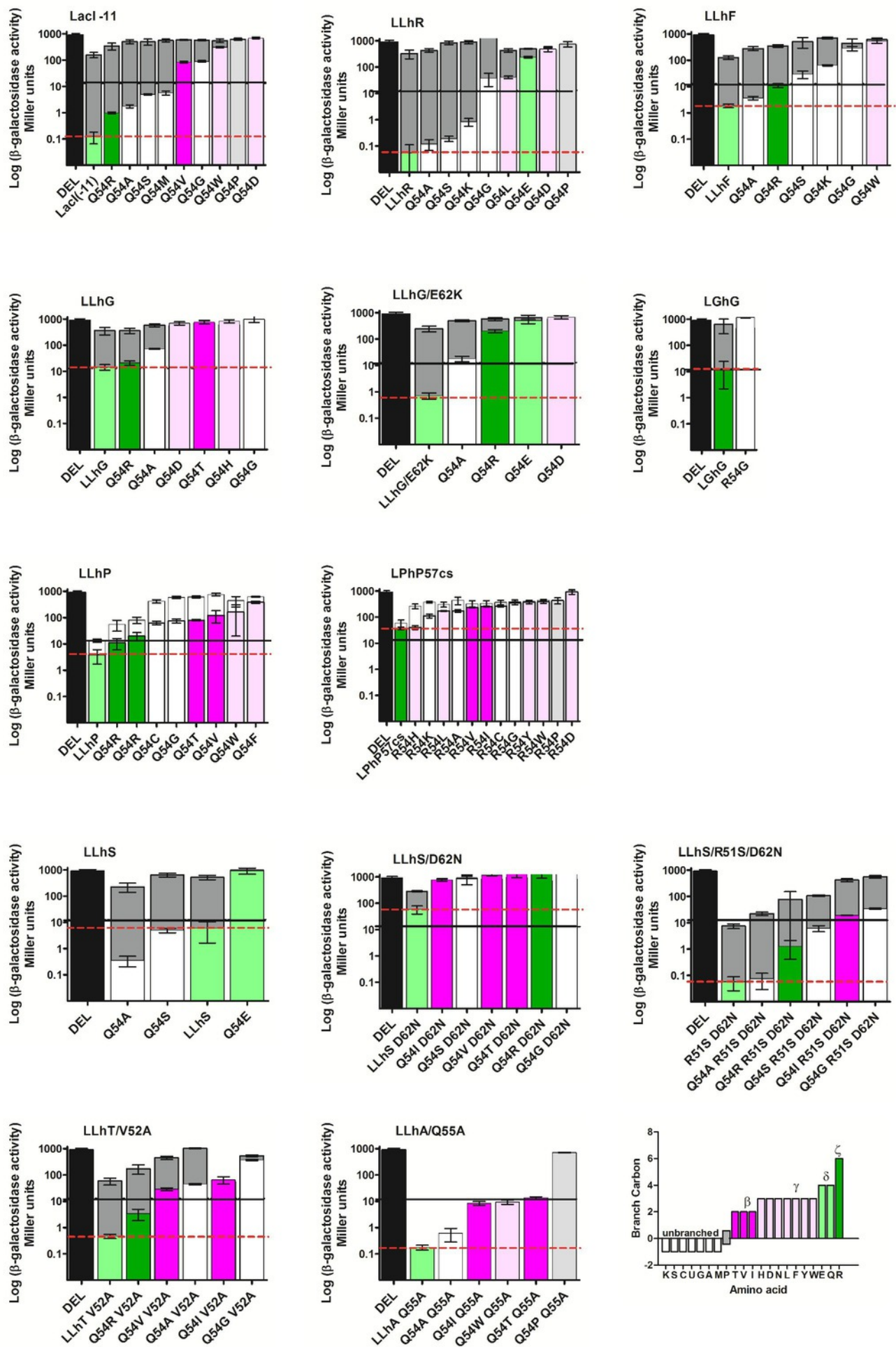


Figure S50: Physicochemical trends: Position 54, Side chain branching

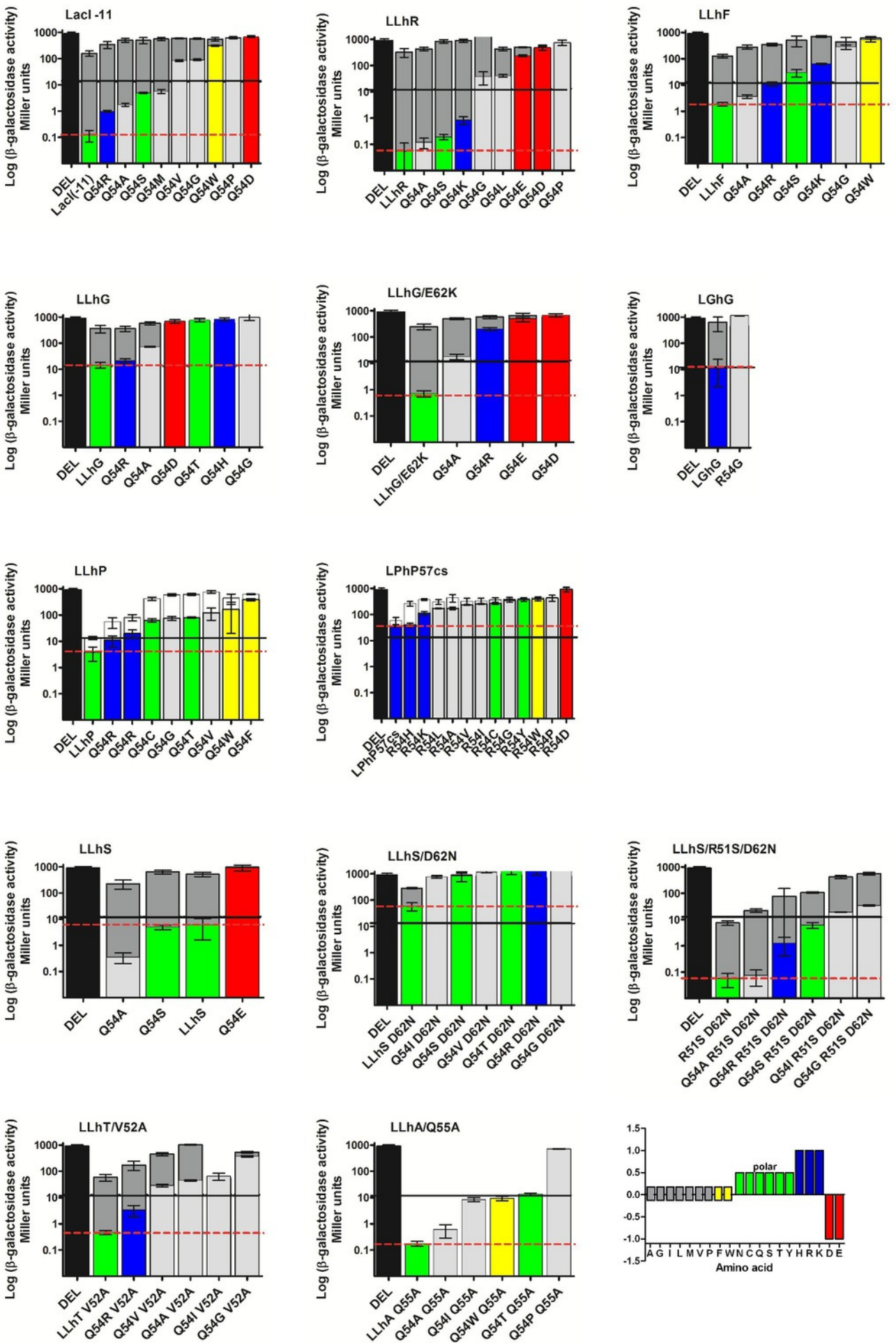


Figure S51: Physicochemical trends: Position 54, Charge/polarity/aromaticity

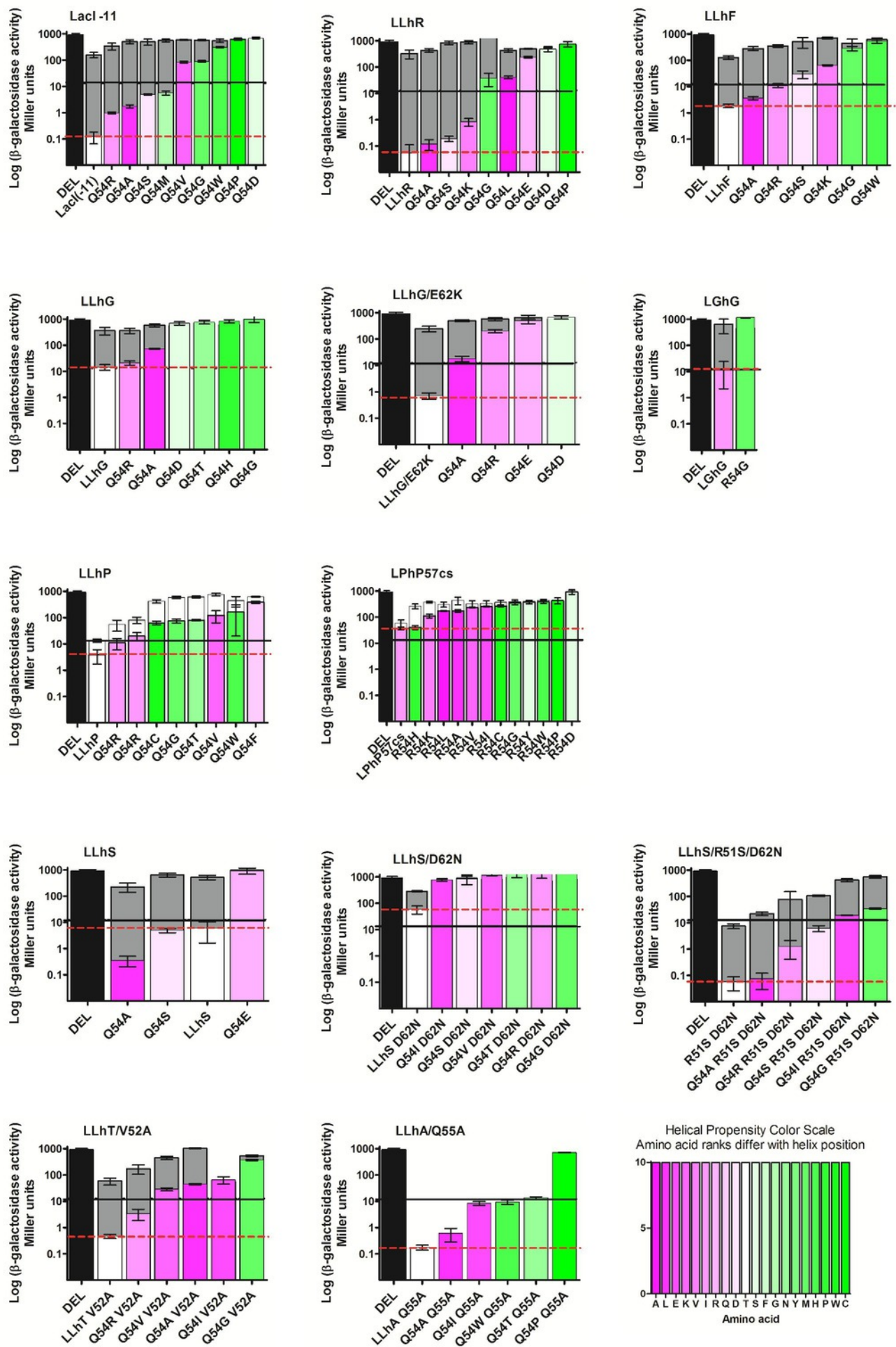


Figure S52: Physicochemical trends: Position 54, Helical propensity (C4 scale)





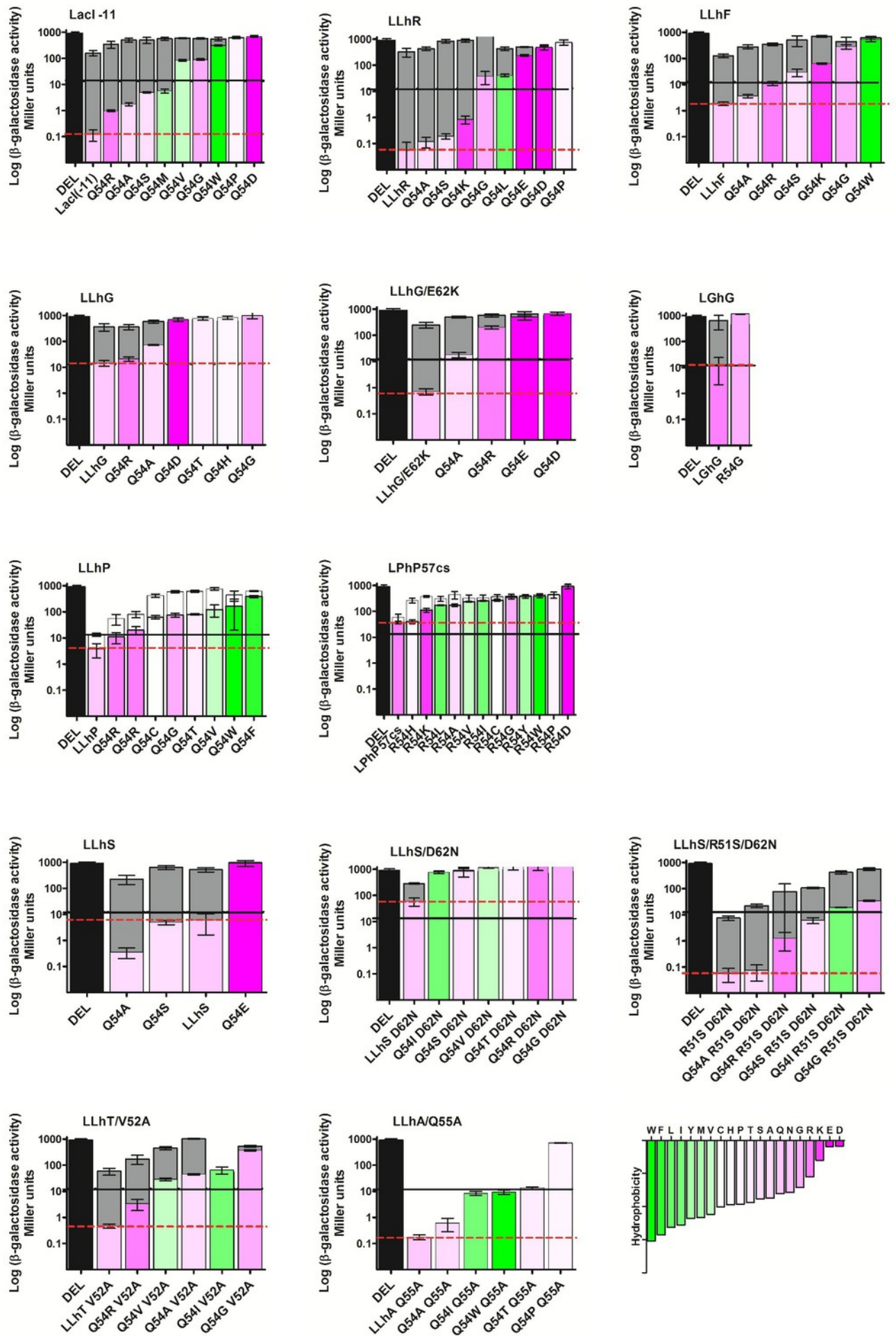


Figure S54: Physicochemical trends: Position 54, Hydrophobicity