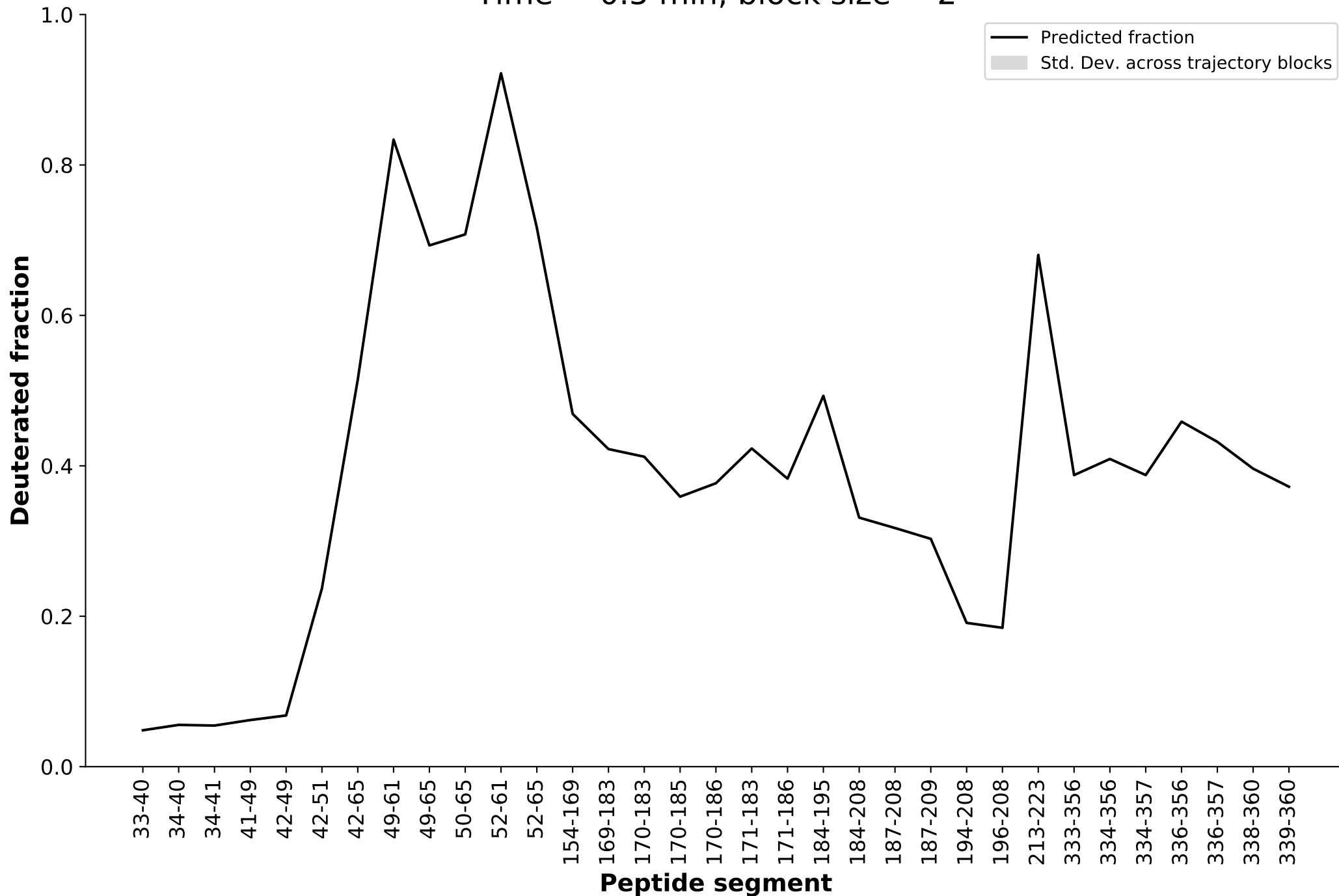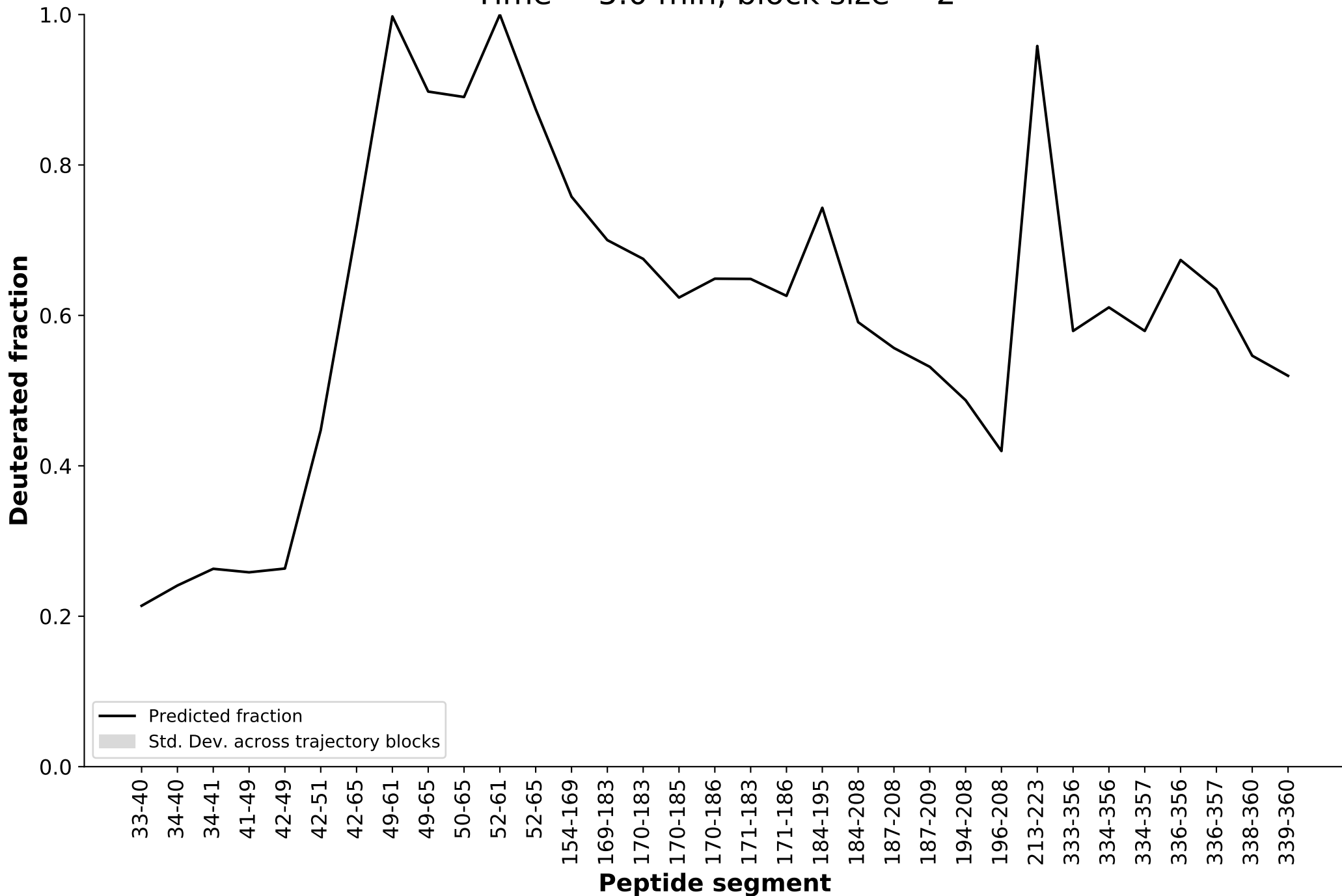**By-segment predicted deuterated fractions**

Time = 0.5 min, block size = 2

**By-segment predicted deuterated fractions**

Time = 5.0 min, block size = 2

Deuterated fraction (y-axis): 0.0, 0.2, 0.4, 0.6, 0.8, 1.0

Peptide segment (x-axis): 33-40, 34-40, 34-41, 41-49, 42-49, 42-51, 42-65, 49-61, 49-65, 50-65, 52-61, 52-65, 154-169, 169-183, 170-183, 170-185, 170-186, 171-183, 171-186, 184-195, 184-208, 187-208, 187-209, 194-208, 196-208, 213-223, 333-356, 334-356, 334-357, 336-356, 336-357, 338-360, 339-360

Legend:
— Predicted fraction
▨ Std. Dev. across trajectory blocks

**By-segment predicted deuterated fractions**

All timepoints (times in min)

Legend:
- Predicted @ time 0.5
- Predicted @ time 5.0

Y-axis: Deuterated fraction

X-axis: Peptide segment

X-axis labels: 33-40, 34-40, 34-41, 41-49, 42-49, 42-51, 42-65, 49-61, 49-65, 50-65, 52-61, 52-65, 154-169, 169-183, 170-183, 170-185, 170-186, 171-183, 171-186, 184-195, 184-208, 187-208, 187-209, 194-208, 196-208, 213-223, 333-356, 334-356, 334-357, 336-356, 336-357, 338-360, 339-360