Supporting Information

Analysis of sequence-defined oligomers through advanced polymer chromatography mass spectrometry hyphenation

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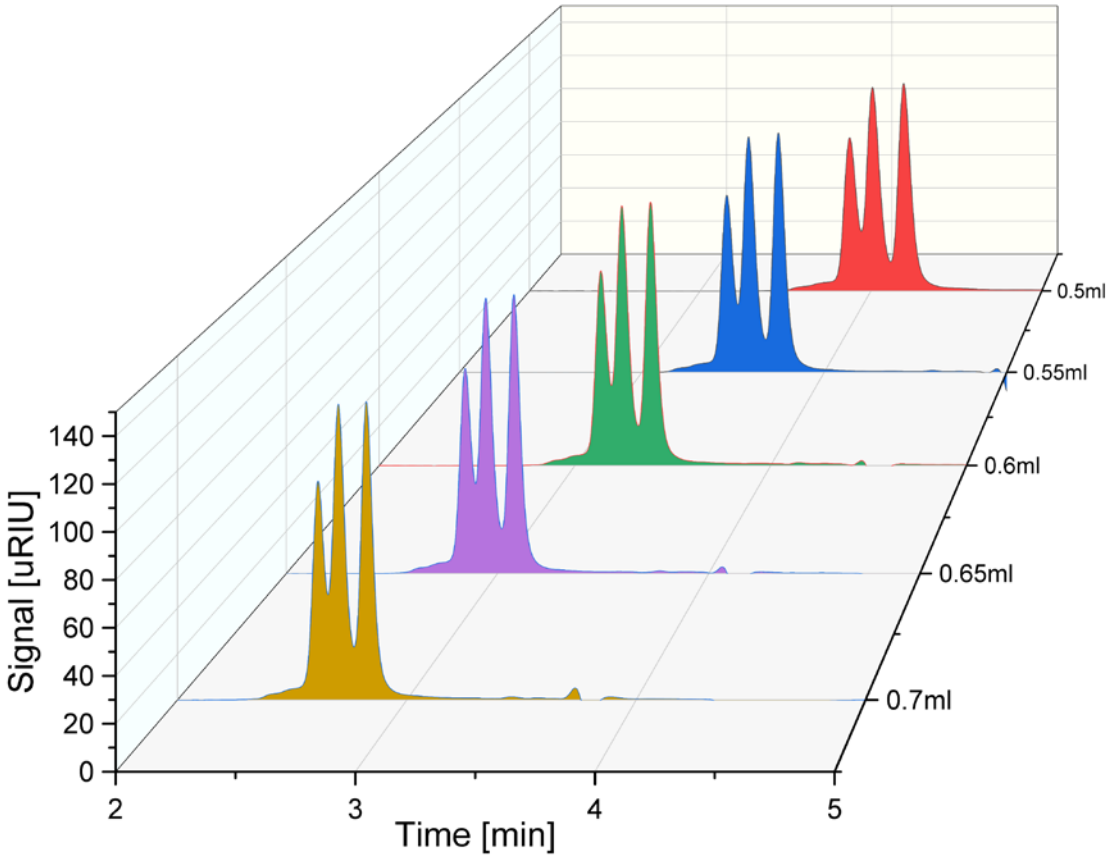

Figure S 1: Elution profiles of the mixture of tetramer, hexamer and octamer with alternating order of monomer units with different flow rate within an APC measurement.

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Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x

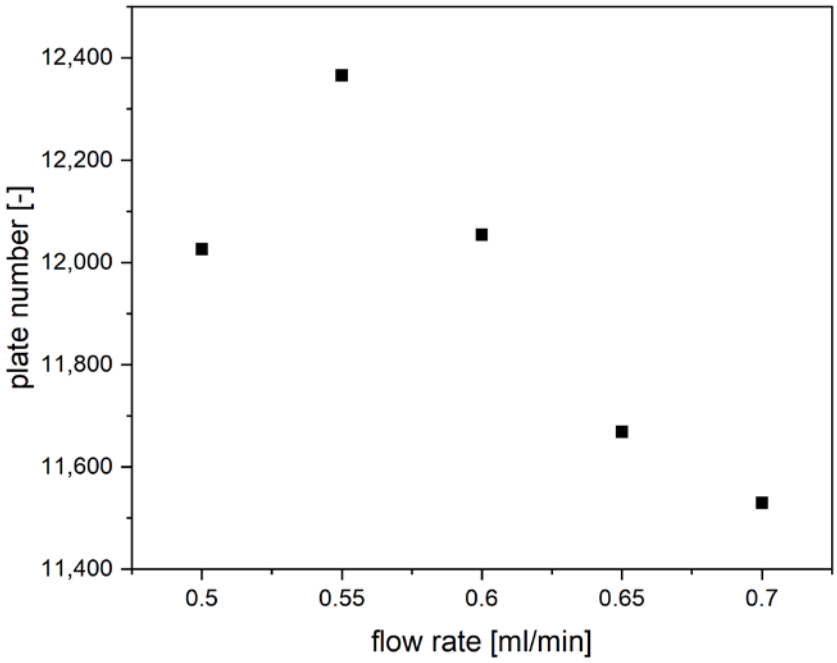
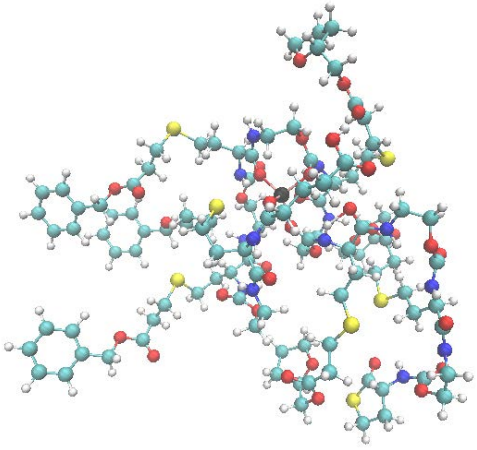
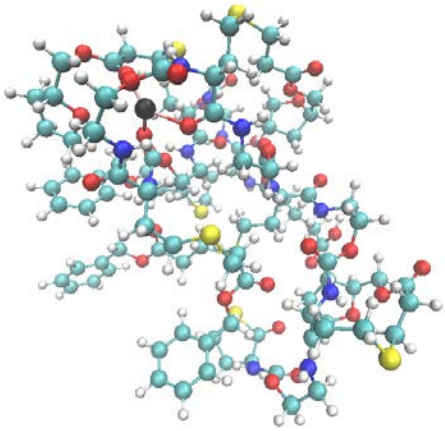


Figure S 2: Influence of the flow rate to the calculated number of plates with constant measurement conditions. Calculated for the hexamer sample with alternating order of monomer units.

Table S 1: Optimized structures of B3T3 and BT3 singly and doubly charged with the added ion coloured in black.

B_3T_3	BT_3
1*Li^+	
	

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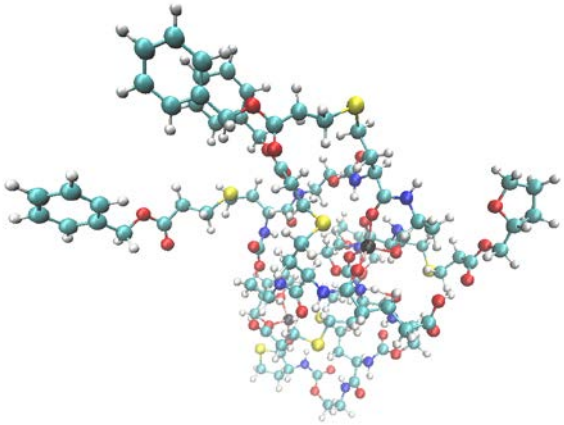	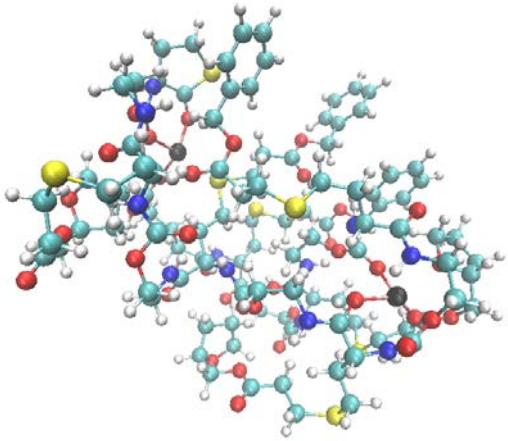
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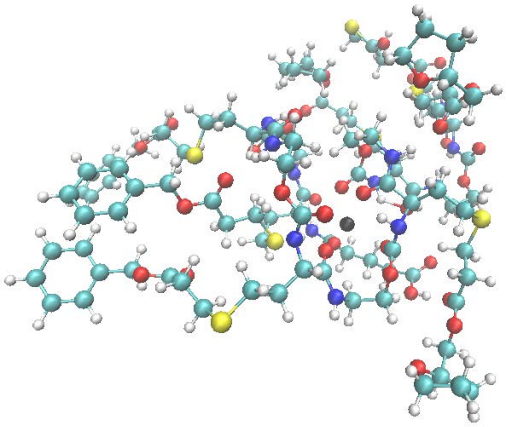	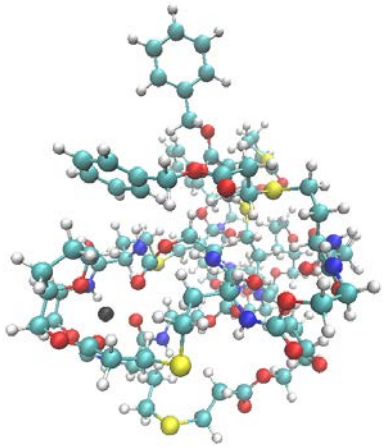
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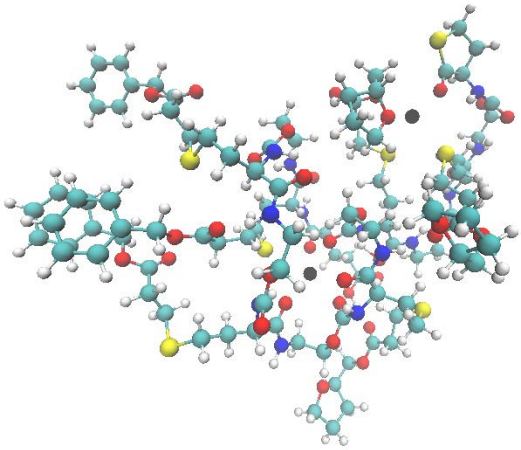	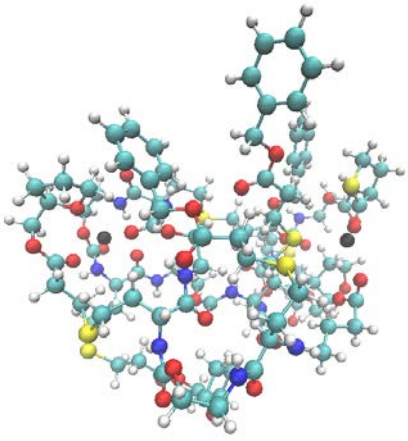

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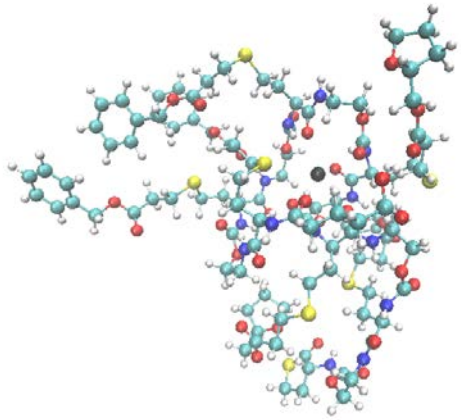	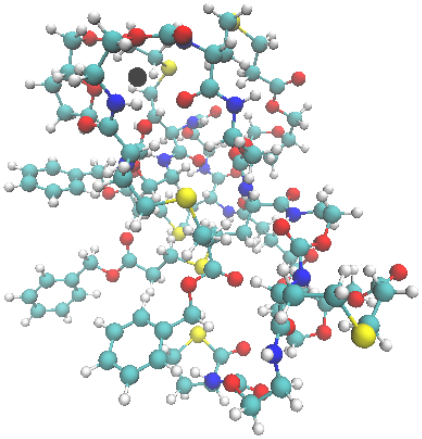
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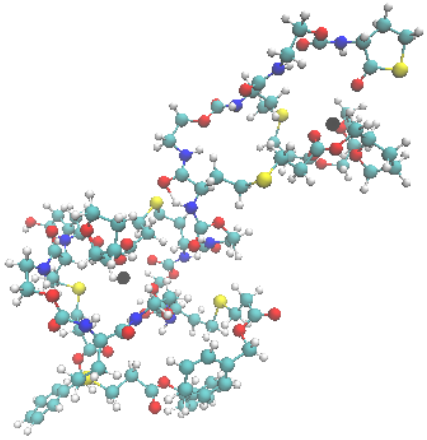	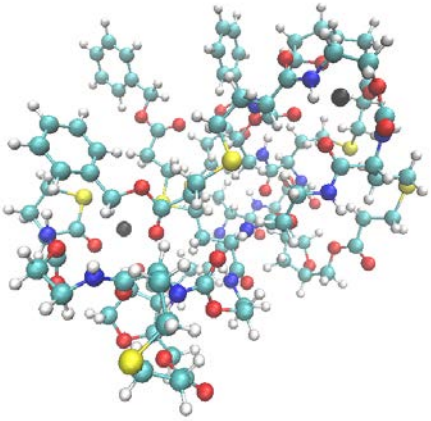
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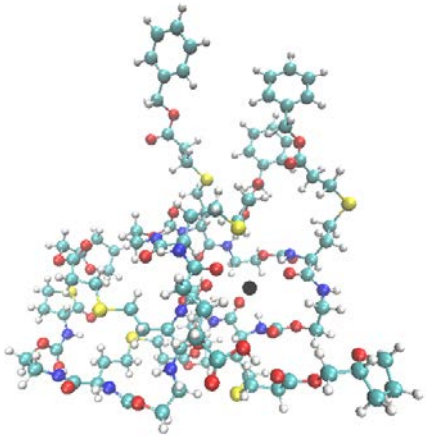	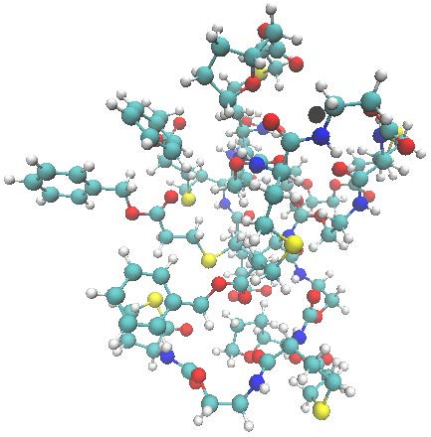

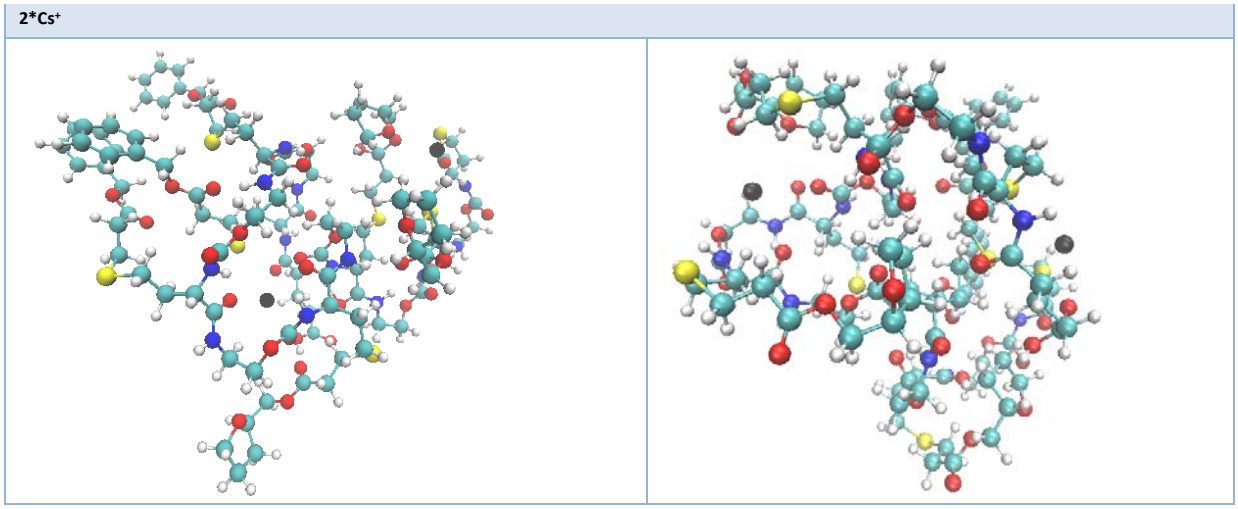

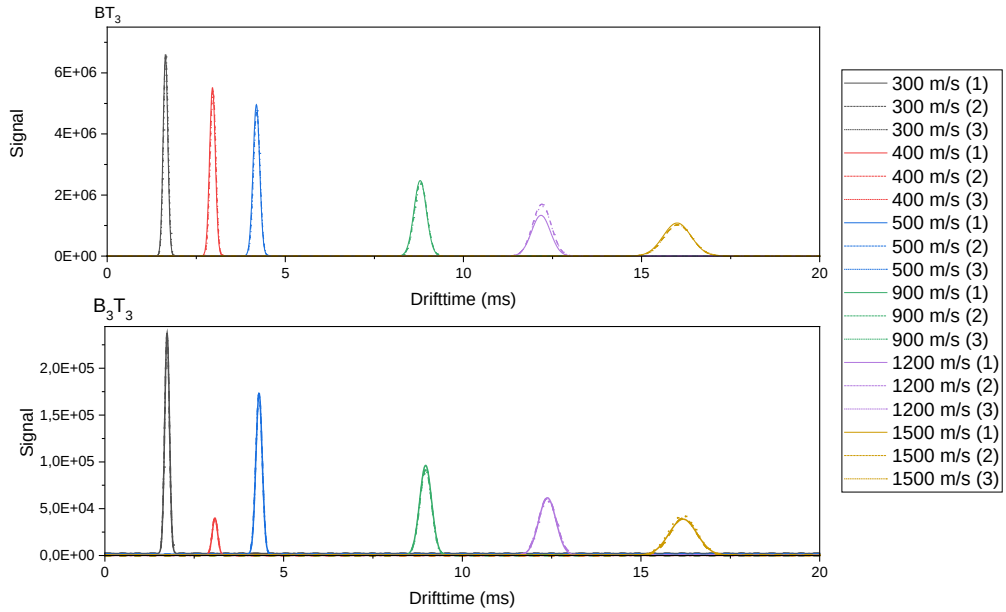

Figure S 3: Drifttime distribution of both hexamers with lithium iodide as ionization agents. Triple measurements of each wave velocity indicated with different types of lines.

Table S 2: absolute drifttimes of both hexamer structures with lithium iodide as ionization agent for all wave velocities and all three measurements.

		First measurement	Second measurement	Third measurement
BT_3	300 m/s	1.64	1.64	1.65
	400 m/s	2.96	2.98	2.97
	500 m/s	4.19	4.20	4.20
	900 m/s	8.79	8.81	8.80
	1200 m/s	12.18	12.21	12.20
	1500 m/s	16.00	16.02	16.01
B_3T_3	300 m/s	1.74	1.74	1.74
	400 m/s	3.08	3.08	3.08
	500 m/s	4.31	4.31	4.31
	900 m/s	8.97	8.98	8.98
	1200 m/s	12.38	12.38	12.39
	1500 m/s	16.18	16.19	16.17

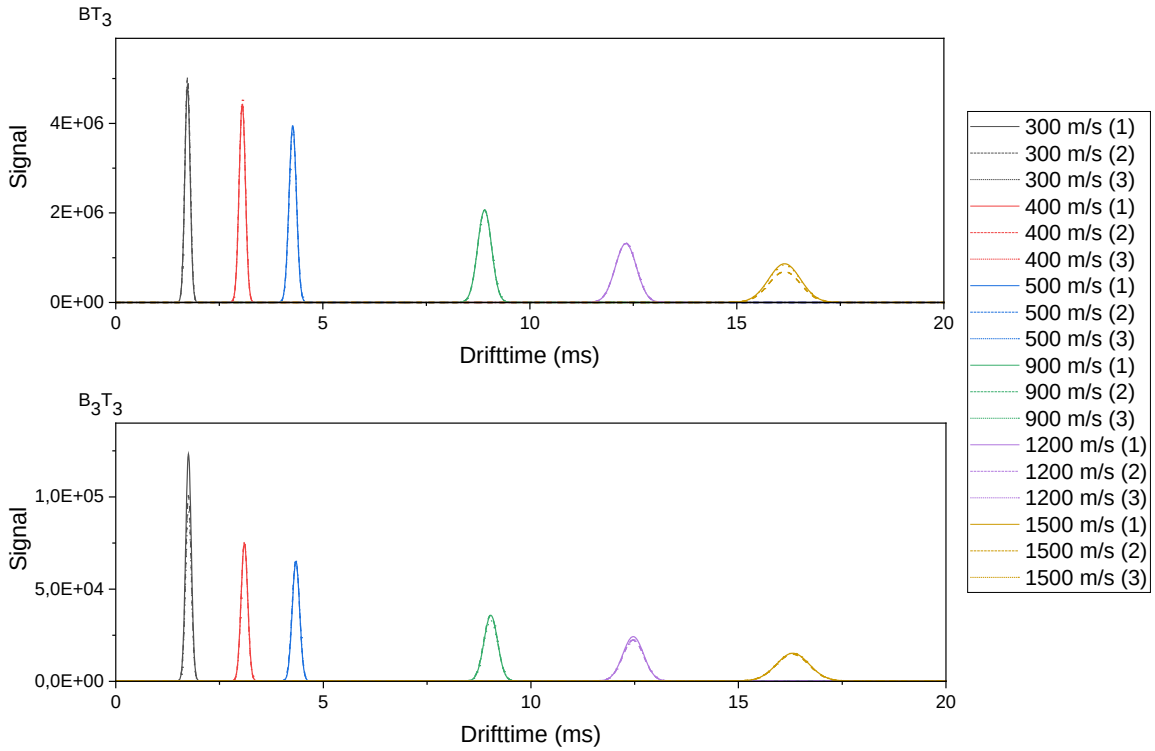

Figure S 4: Drifttime distribution of both hexamers with sodium iodide as ionization agents. Triple measurements of each wave velocity indicated with different types of lines.

Table S 3: Absolute drifttimes of both hexamer structures with sodium iodide as ionization agent for all wave velocities and all three measurements.

		First measurement	Second measurement	Third measurement
BT_3	300 m/s	1.73	1.73	1.73
	400 m/s	3.06	3.06	3.06
	500 m/s	4.27	4.28	4.28
	900 m/s	8.91	8.91	8.91
	1200 m/s	12.32	12.32	12.32
	1500 m/s	16.15	16.15	16.15
B_3T_3	300 m/s	1.75	1.75	1.75
	400 m/s	3.10	3.10	3.10
	500 m/s	4.34	4.34	4.34
	900 m/s	9.03	9.03	9.04
	1200 m/s	12.47	12.47	12.47
	1500 m/s	16.31	16.31	16.31

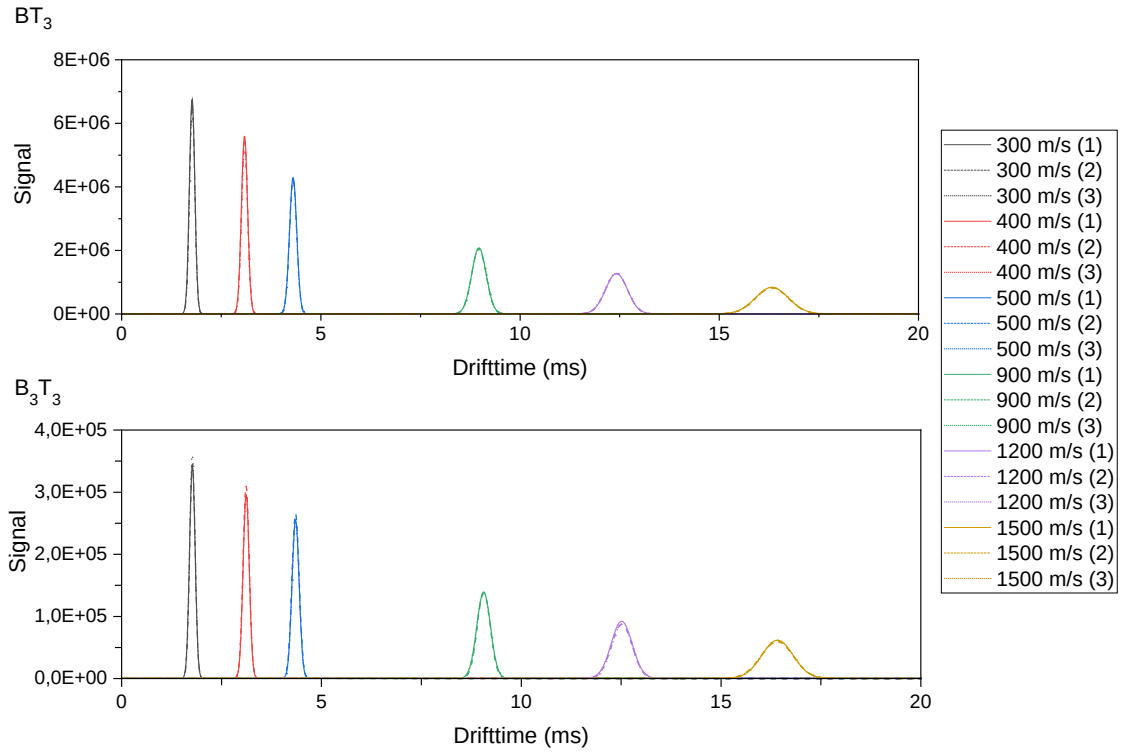

Figure S 5: Drifttime distribution of both hexamers with potassium iodide as ionization agents. Triple measurements of each wave velocity indicated with different types of lines.

Table S 4: Absolute drifttimes of both hexamer structures with potassium iodide as ionization agent for all wave velocities and all three measurements.

		First measurement	Second measurement	Third measurement
BT_3	300 m/s	1.77	1.77	1.77
	400 m/s	3.08	3.09	3.09
	500 m/s	4.30	4.30	4.30
	900 m/s	8.97	8.97	8.97
	1200 m/s	12.42	12.42	12.41
	1500 m/s	16.32	16.32	16.32
B_3T_3	300 m/s	1.77	1.77	1.77
	400 m/s	3.12	3.12	3.12
	500 m/s	4.35	4.35	4.35
	900 m/s	9.06	9.06	9.06
	1200 m/s	12.51	12.52	12.52
	1500 m/s	16.41	16.40	16.41

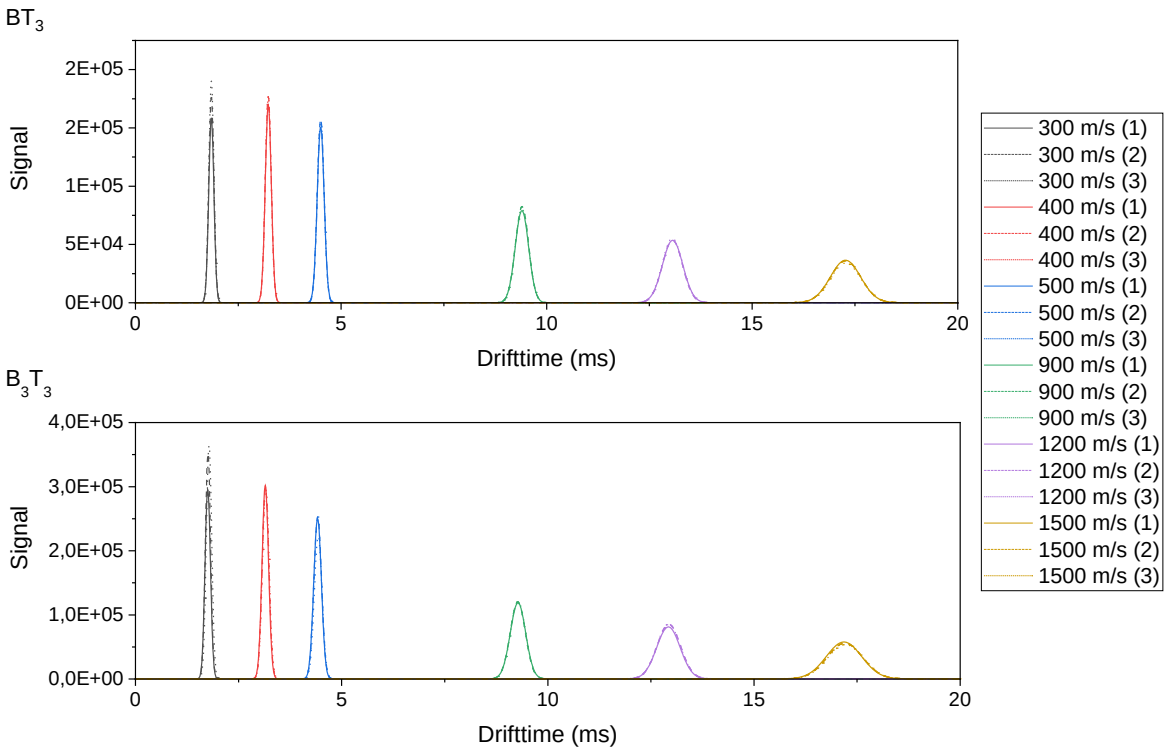

Figure S 6: Drifttime distribution of both hexamers with caesium iodide as ionization agents. Triple measurements of each wave velocity indicated with different types of lines.

Table S 5: Absolute drifttimes of both hexamer structures with caesium iodide as ionization agent for all wave velocities and all three measurements.

		First measurement	Second measurement	Third measurement
BT_3	300 m/s	1.85	1.85	1.85
	400 m/s	3.23	3.23	3.23
	500 m/s	4.50	4.51	4.50
	900 m/s	9.40	9.40	9.40
	1200 m/s	13.06	13.06	13.06
	1500 m/s	17.27	17.27	17.27
B_3T_3	300 m/s	1.75	1.76	1.79
	400 m/s	3.15	3.15	3.16
	500 m/s	4.42	4.42	4.43
	900 m/s	9.28	9.27	9.28
	1200 m/s	12.92	12.93	12.93
	1500 m/s	17.18	17.20	17.22

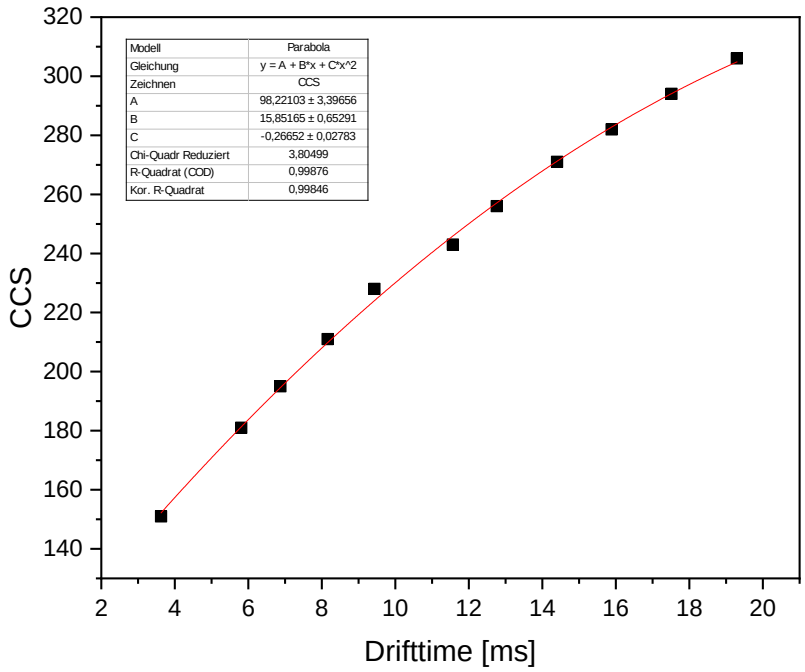

Figure S 7: polyalanine calibration of the CCS versus the drifttime with a wave velocity of 500 m/s.