

Supplementary Material

Synthesis and stability studies of constrained peptide–antimony bicycles

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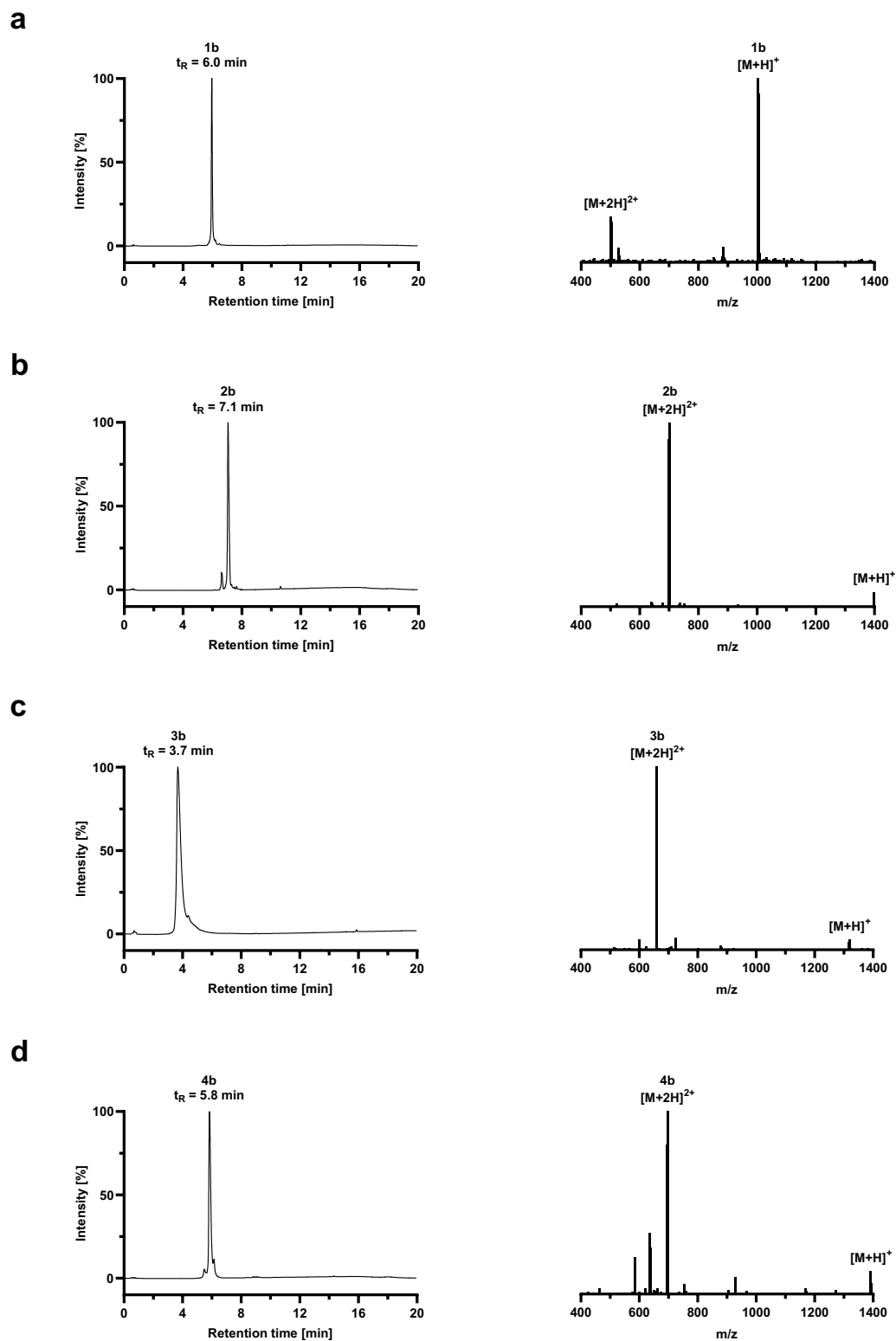
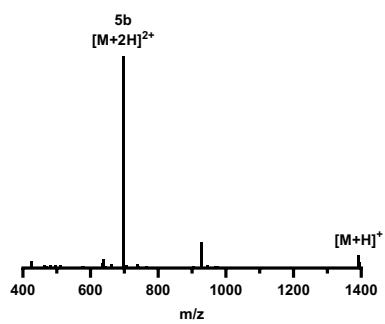
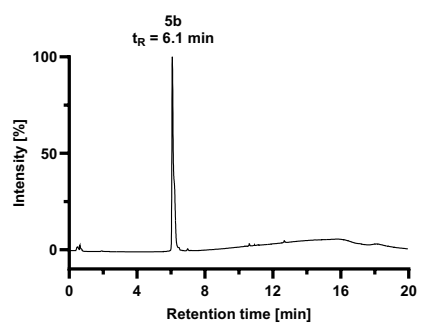
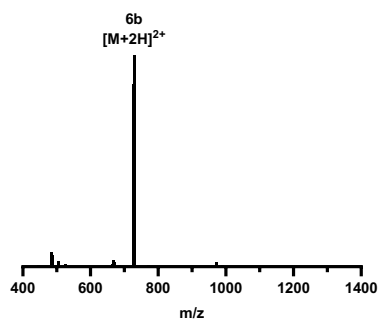
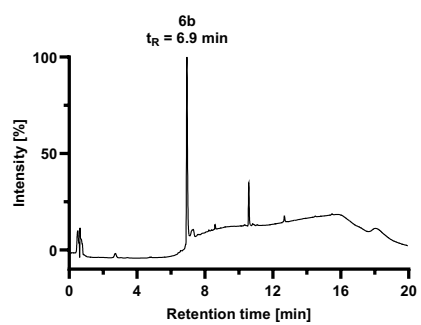


Figure S1. LCMS traces (254 nm) and ESI+ spectra of antimony-peptide bicycles. (a) 1b, (b) 2b, (c) 3b, (d) 4b, (e) 5b, (f) 6b, (g) 7b.

e



f



g

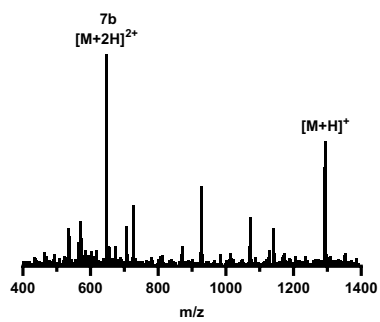
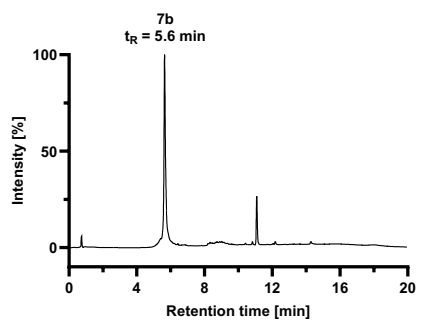


Figure S1. (Cont.)

Table S1. LCMS gradient 1 using MeCN in ultrapure H₂O, whereby both solvents contained 0.1% formic acid as an additive.

Time (min)	H₂O (%)	MeCN (%)
0	95	5
10	10	90
13	10	90
14	95	5
20	95	5

This gradient was used for the analysis of **1b**, **2b**, **4b** and **7b**.

Table S2. LCMS gradient 2 using MeCN in ultrapure H₂O, whereby both solvents contained 0.1% formic acid as an additive.

Time (min)	H₂O (%)	MeCN (%)
0	80	20
2	80	20
20	5	87.5

This gradient was used for the analysis of **3b**, **5b** and **6b**.

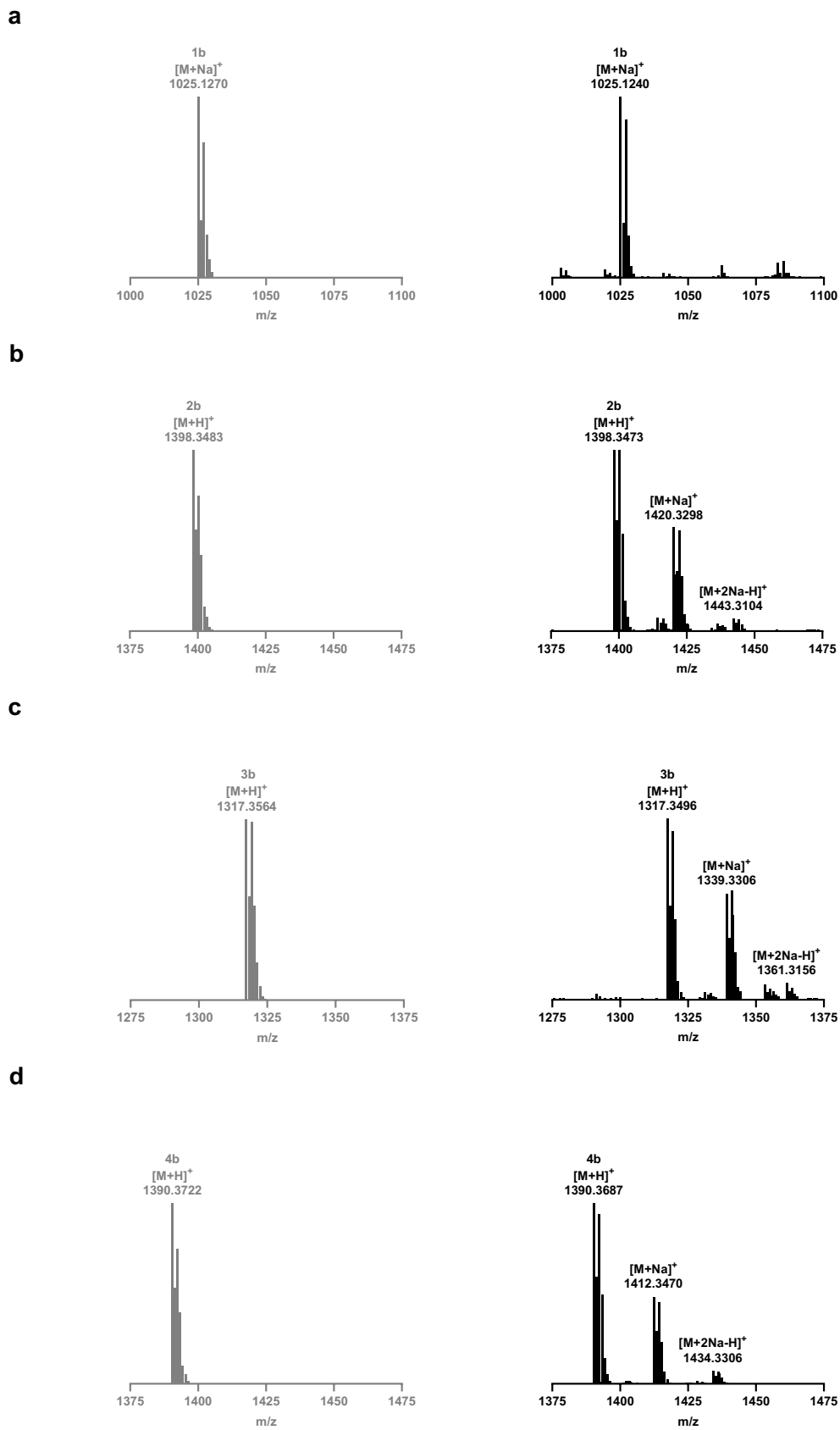
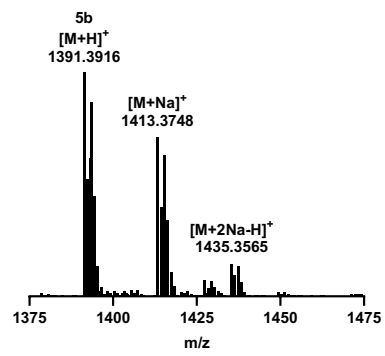
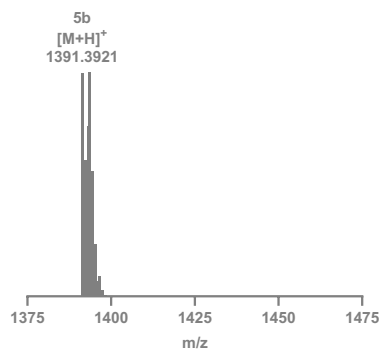
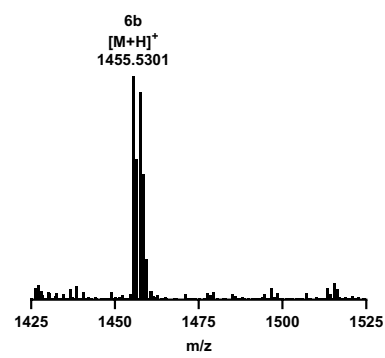
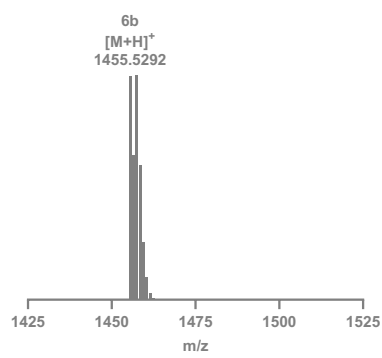


Figure S2. Simulated isotope patterns (grey) and high-resolution mass spectra (black) of antimony–peptide bicycles. (a) **1b**, (b) **2b**, (c) **3b**, (d) **4b**, (e) **5b**, (f) **6b**, (g) **7b**.

e



f



g

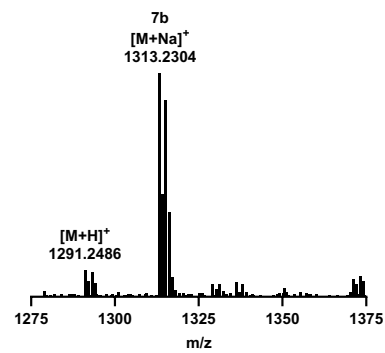
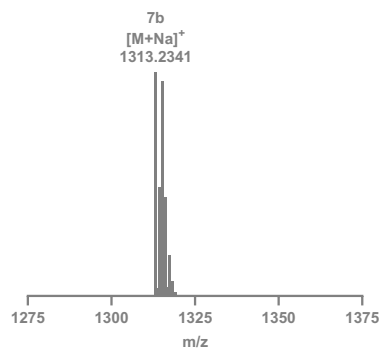


Figure S2. (Cont.)

Table S3. Stability of peptide–Sb^{III} bicycles in EDTA.

Eq. EDTA	1b (%)	2b (%)
0	100	100
0.5	96	88
5	89	93
10	47	68
25	22	49

Table S4. Stability of peptide–Sb^{III} bicycles in GSH.

Eq. GSH	1b (%)	2b (%)
0	100	100
0.5	97	97
5	85	94
10	65	89
25	40	79

Table S5. Gastrodenol competition assay – Sb^{III} and Bi^{III} competition.

Eq. Gastrodenol	1a (%)	1b (%)	1c (%)	2a (%)	2b (%)	2c (%)
0	0	100	0	0	100	0
1	17	1	82	10	3	86
2	14	1	85	9	1	90
5	11	0	88	6	0	94
10	10	0	90	3	0	97

a, linear peptide; **b**, Sb-bicycle; **c**, Bi-bicycle.