

Supplementary information

Acid-modulated peptide synthesis for application on oxide biosensor interfaces

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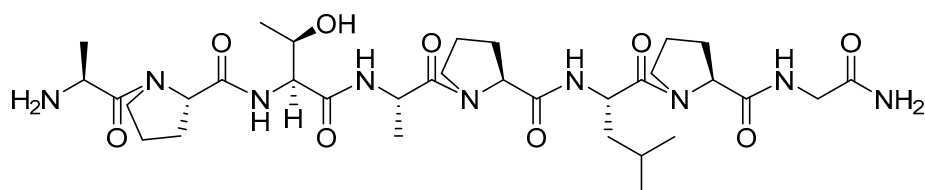
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Figure S1



Chemical Formula: $C_{33}H_{55}N_9O_9$
Exact Mass: 721,41

mV

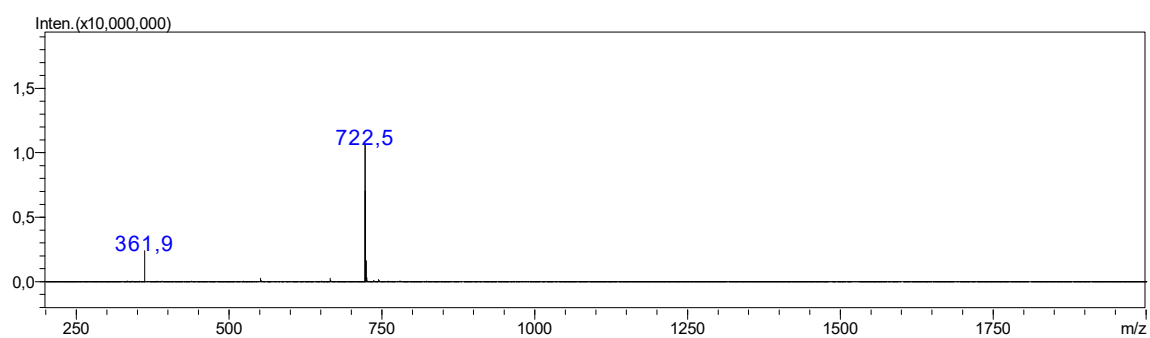
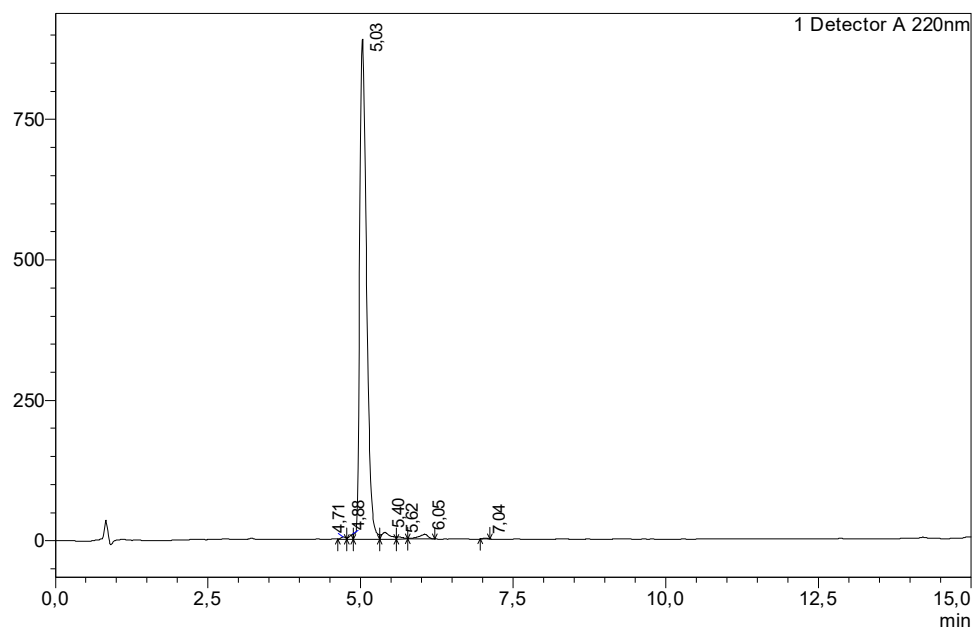
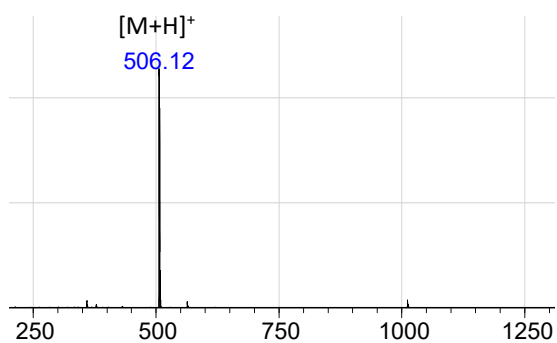
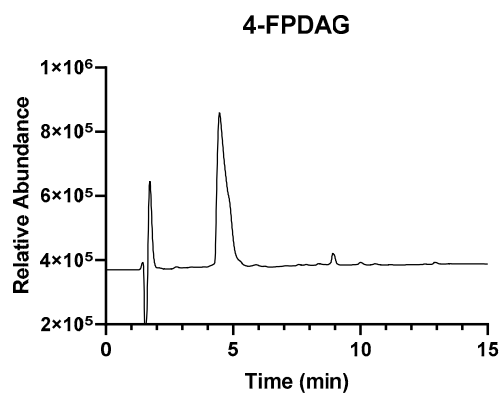
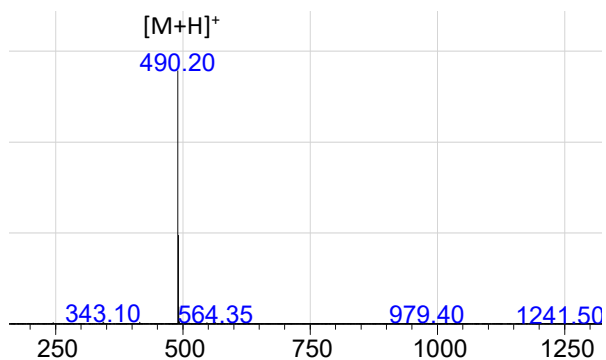
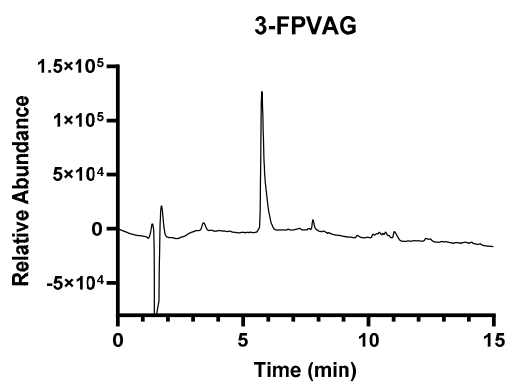
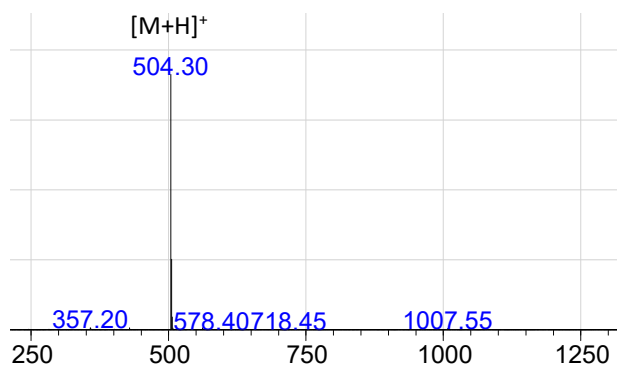
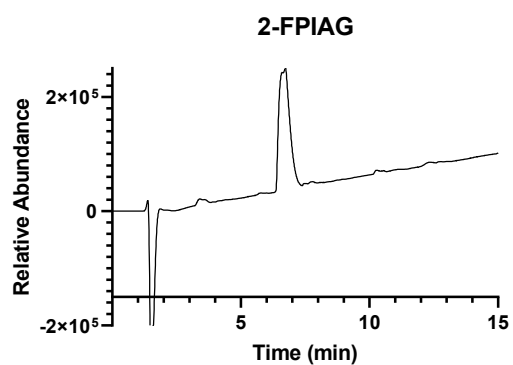
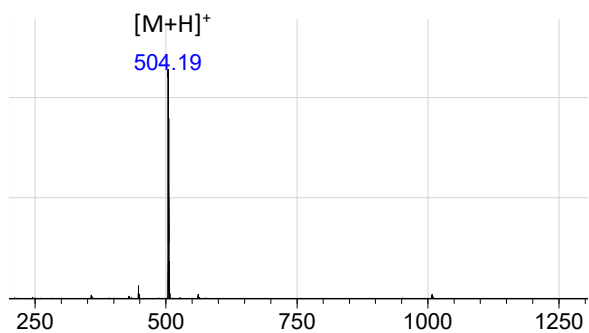
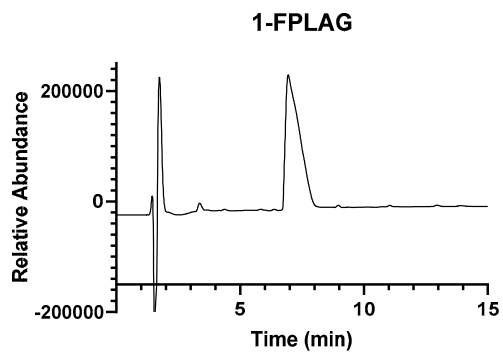
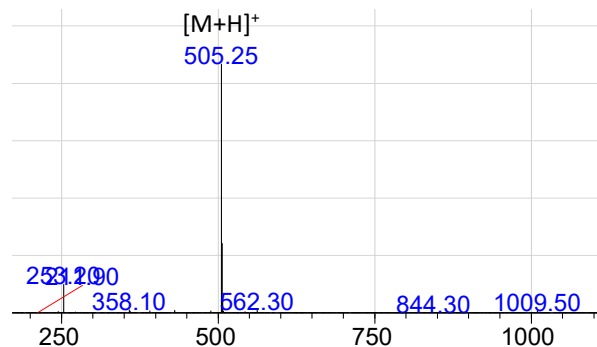
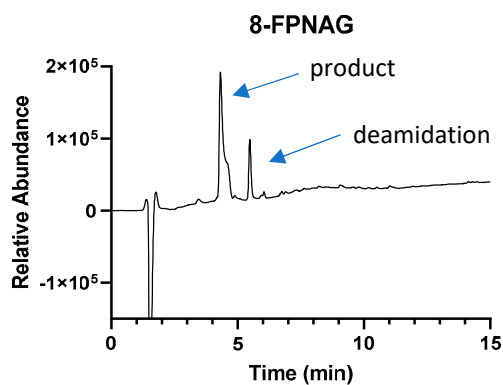
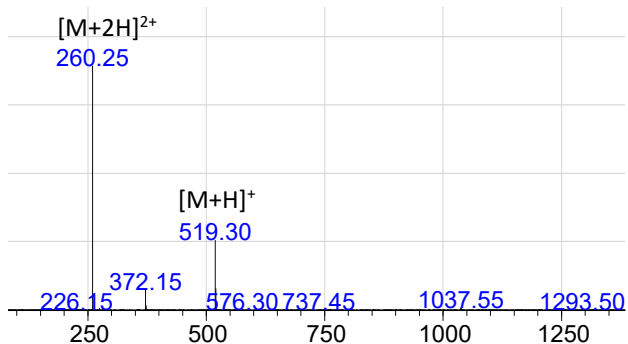
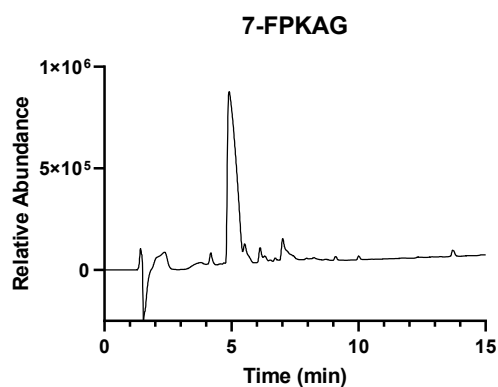
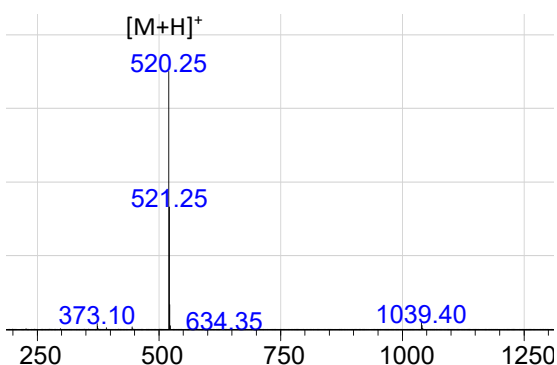
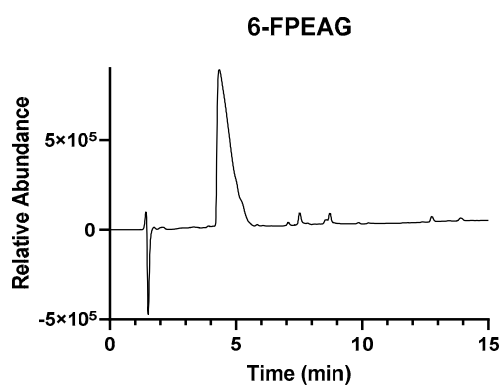
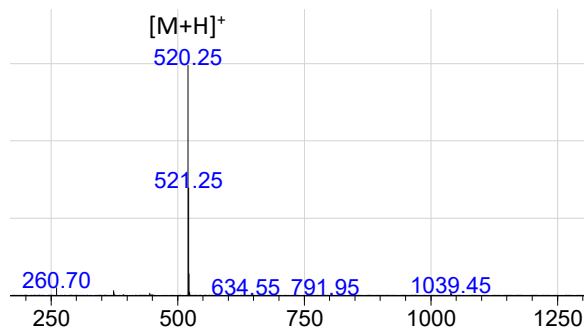
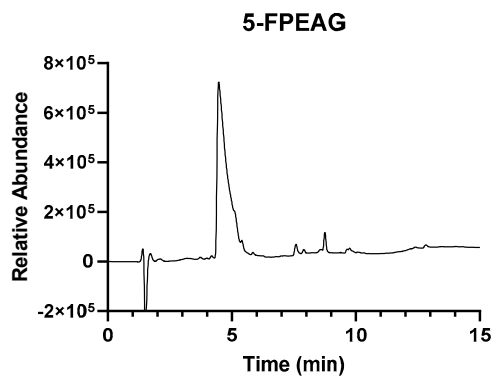


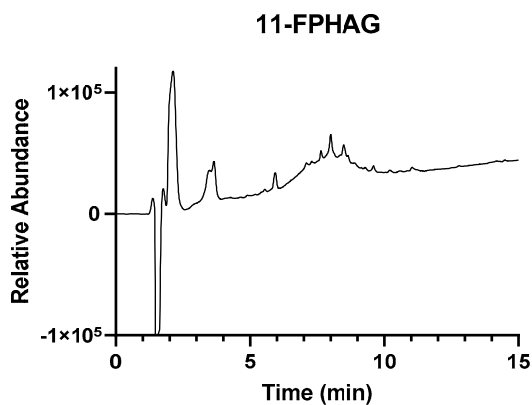
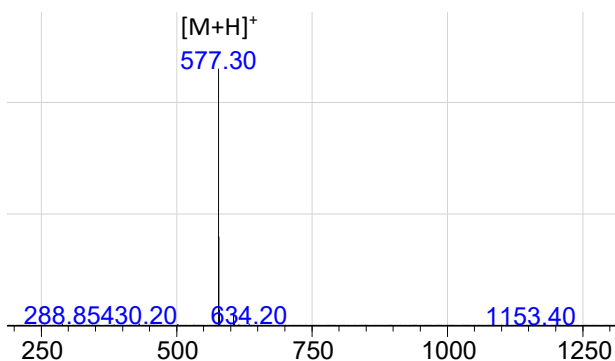
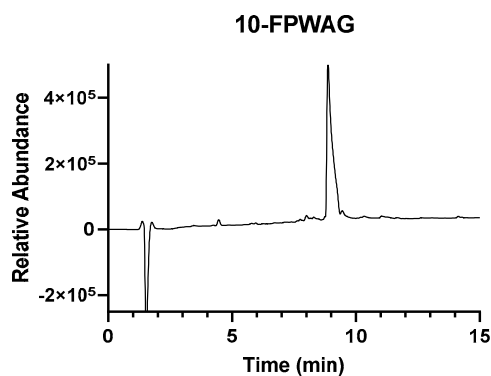
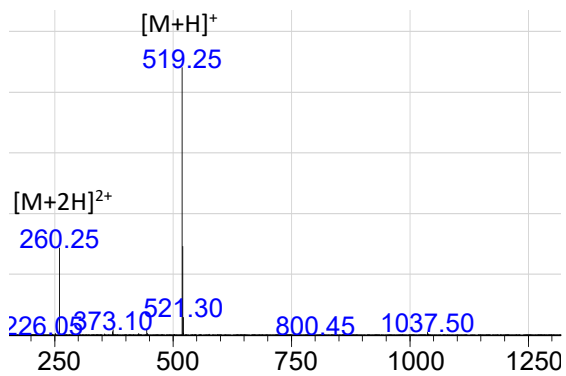
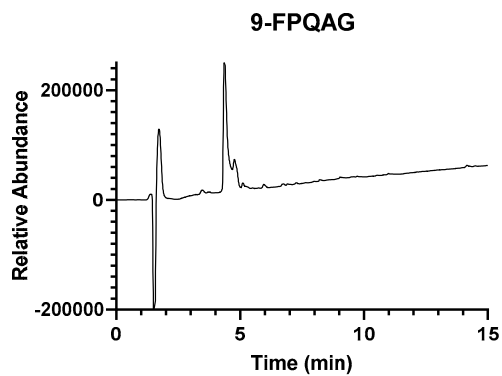
Table S1

Entry	Peptides ¹	Protecting group	Theoretical Mass (Da)	Experimental Mas (Da) ²	HPLC retention time (min)	Gradient ³	Purity ⁴
1	FPLAG	None	503.26	504.19	6.8	5-40% ^a	98%
2	FPIAG	None	503.26	504.30	6.5	5-40% ^a	95%
3	FPVAG	None	489.25	490.20	6.0	5-40% ^a	94%
4	FPDAG	OFm	505.21	506.12	4.2	5-40% ^a	96%
5	FPEAG	OFm	519.22	520.25	4.2	5-40% ^a	95%
6	FPEAG ⁵	OFm	519.22	520.25	4.2	5-40% ^a	95%
7	FPKAG	Fmoc	518.27	519.30	5.0	5-40% ^a	86%
8	FPNAG	None	504.22	505.25	4.5	5-40% ^a	80%
9	FPQAG	None	518.24	519.25	4.5	5-40% ^a	96%
10	FPWAG	None	576.26	577.30	8.9	5-40% ^a	96%
11	FPHAG	None	527.24	n.d.	-	-	-
12	FPHAG	Dnp	527.24	528.10	0.4	5-95% ^b	74%
13	FPHAG	Trt	527.24	528.31	3.0	5-40% ^a	91%
14	FPMAG	None	521.22	522.20	4.2	5-40% ^a	76%
15	FPCAG	None	493.19	n.d.	-	-	-
16	FPCAG	Fm	493.19	493.55	1.2	5-95% ^b	58%
17	FPCAG	Fm/DODT	493.19	493.35	1.2	5-95% ^b	75%
18	FPSAG	None	477.21	478.20	4.0	5-40% ^a	77%
19	FPSAG	tBu	477.21	478.33	4.0	5-40% ^a	82%
20	FPTAG	None	491.23	492.25	4.0	5-40% ^a	81%
21	FPTAG ⁶	tBu	491.23	492.39	4.0	5-40% ^a	81%
22	FPYAG	None	553.24	554.30	6.0	5-40% ^a	56%
23	FPYAG	2-Br-Z	553.24	554.34	6.0	5-40% ^a	95%

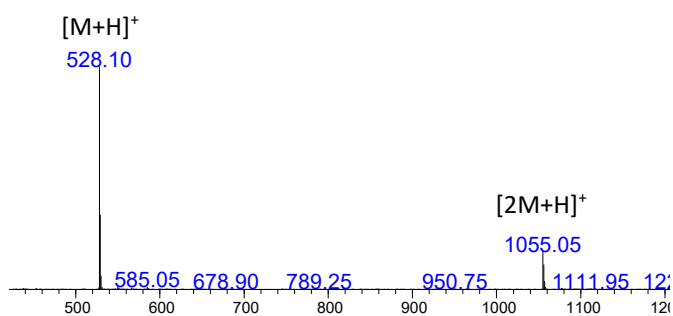
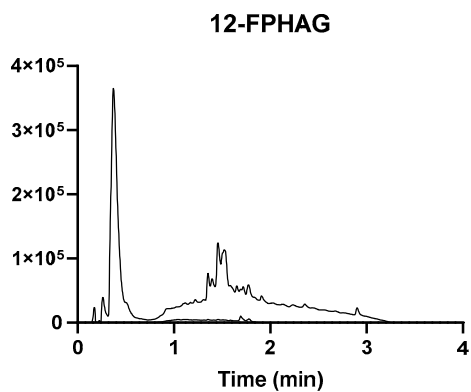
¹ All peptides are C-terminal carboxylic acid; ² Determined by LC-MS; ³ Linear MeCN (+0.036% TFA) into H₂O (+0.045% TFA) over 15 min (a) or 5 min (b); ⁴ Determined by analytical HPLC. n.d : not determined.



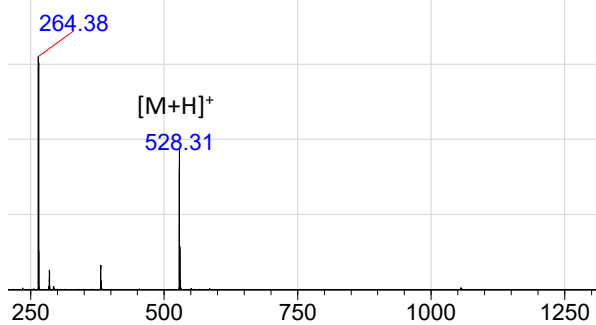
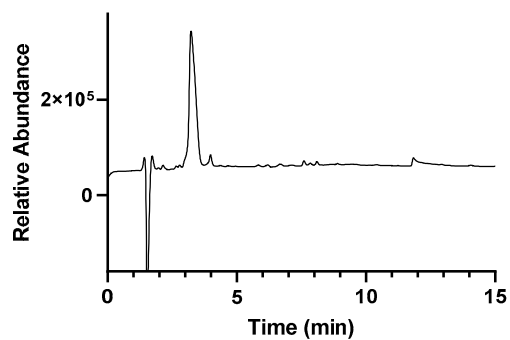




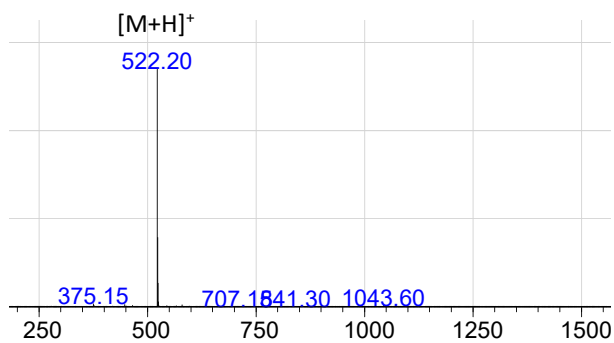
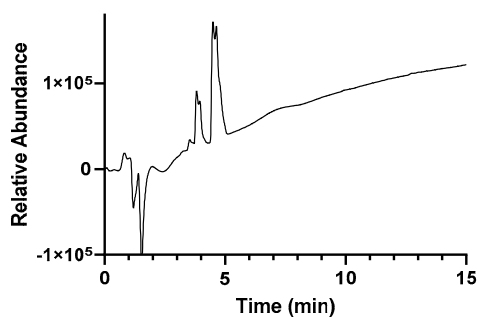
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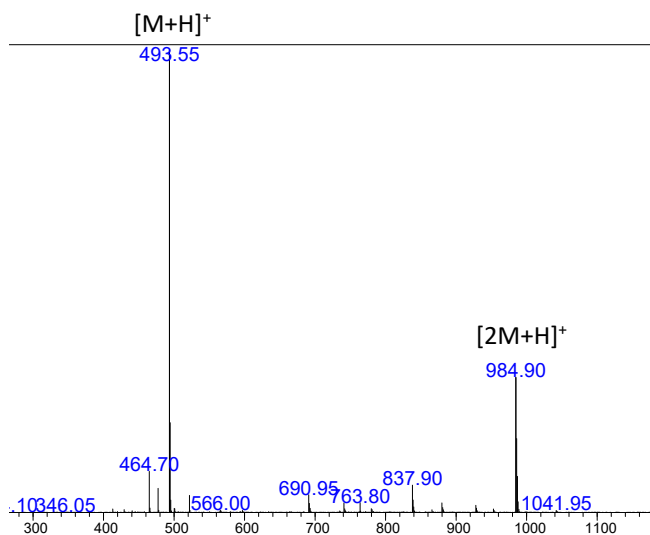
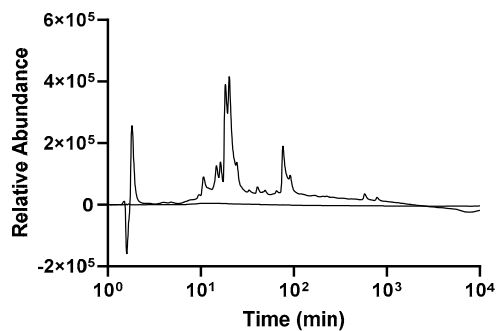
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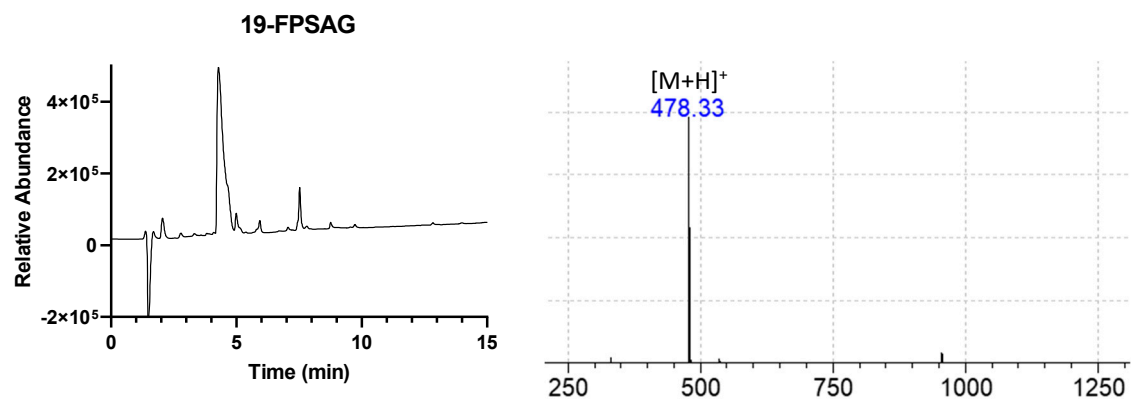
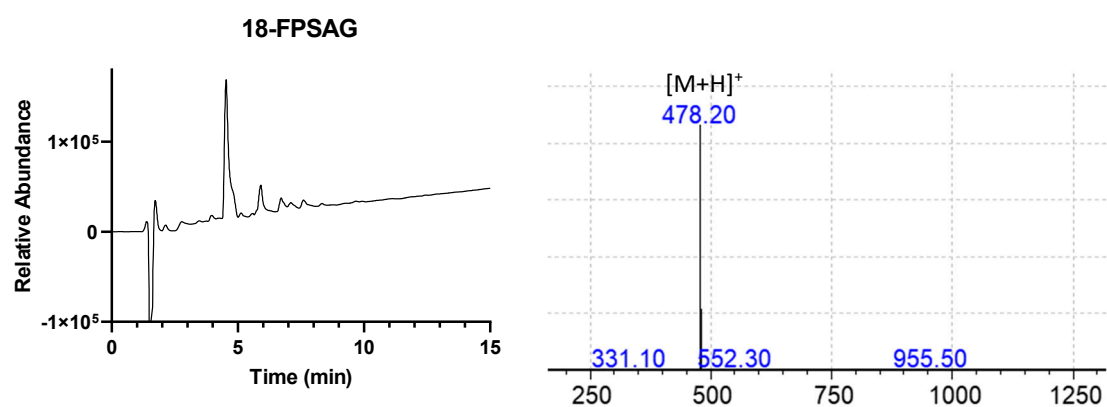
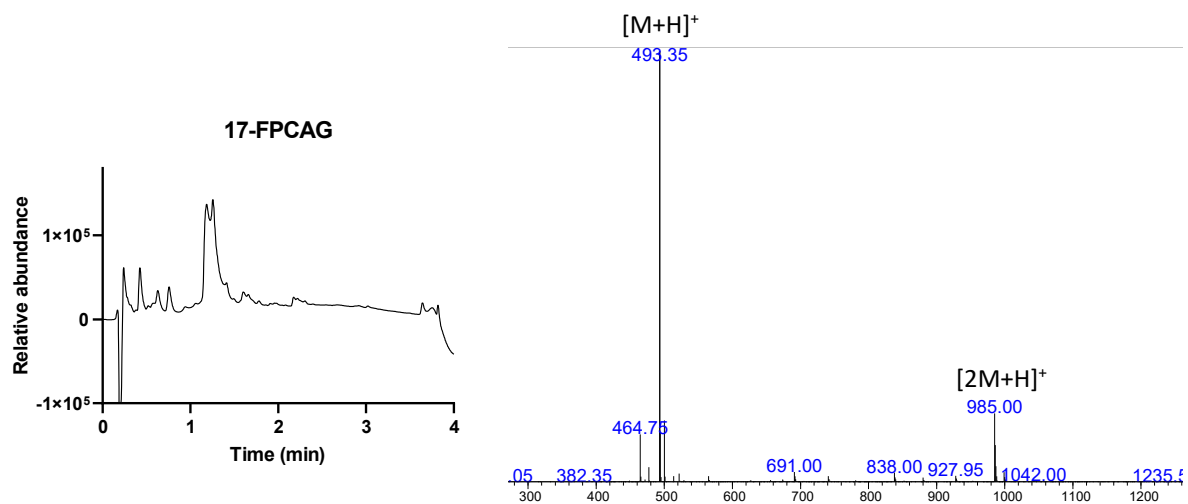


14-FPMAG

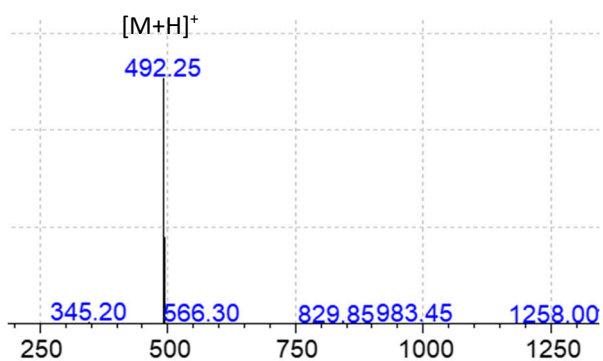
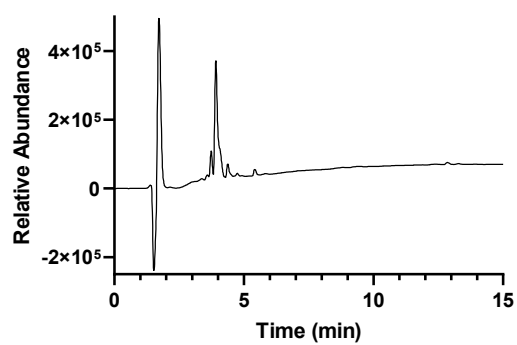


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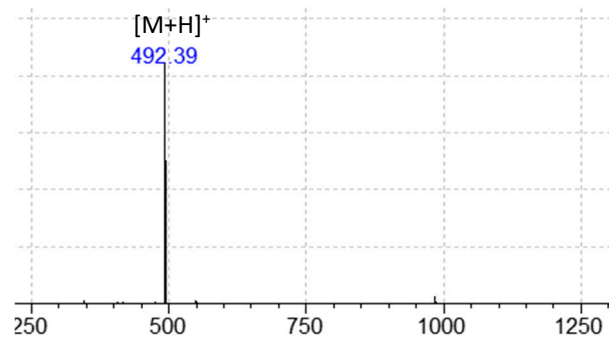
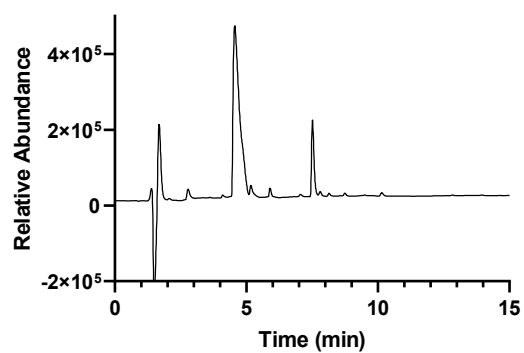




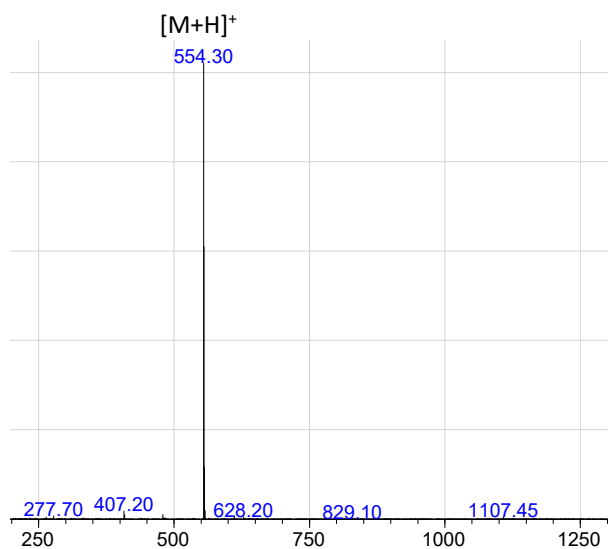
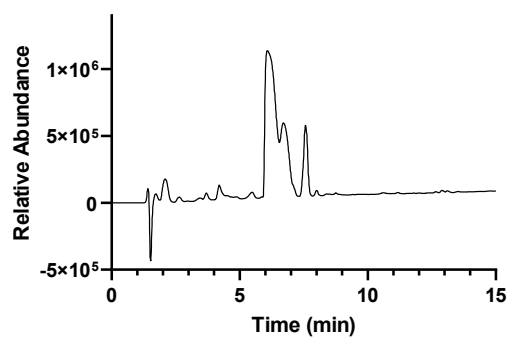
20-FPTAG



21-FPTAG



22-FPYAG



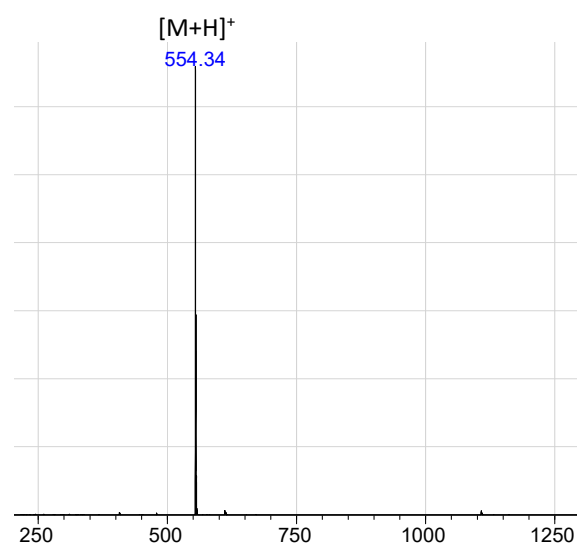
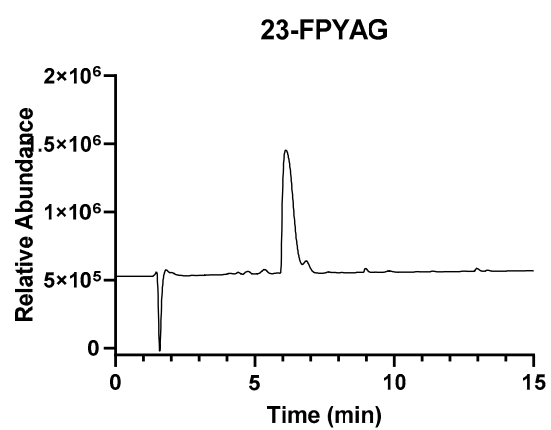
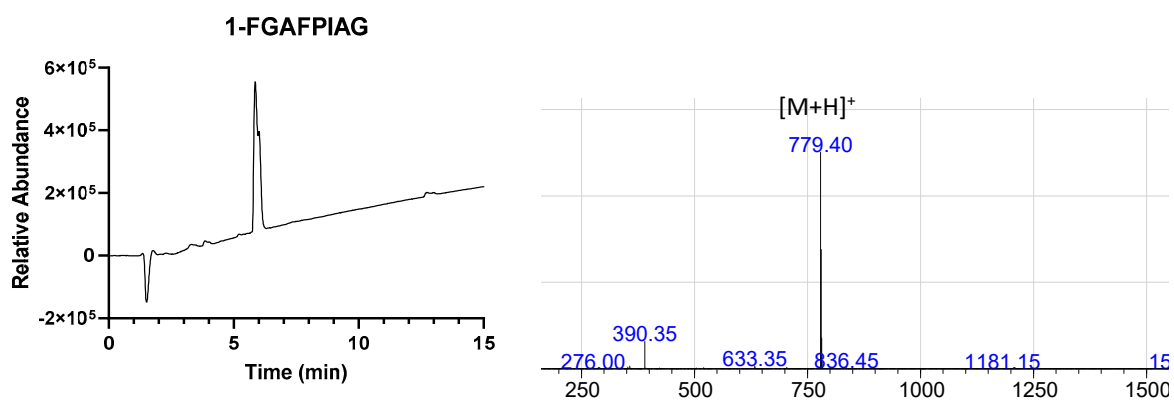
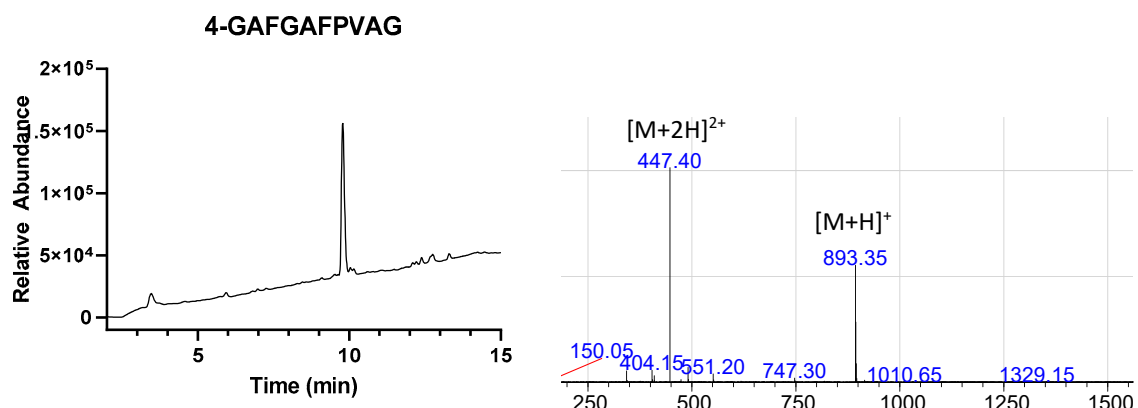
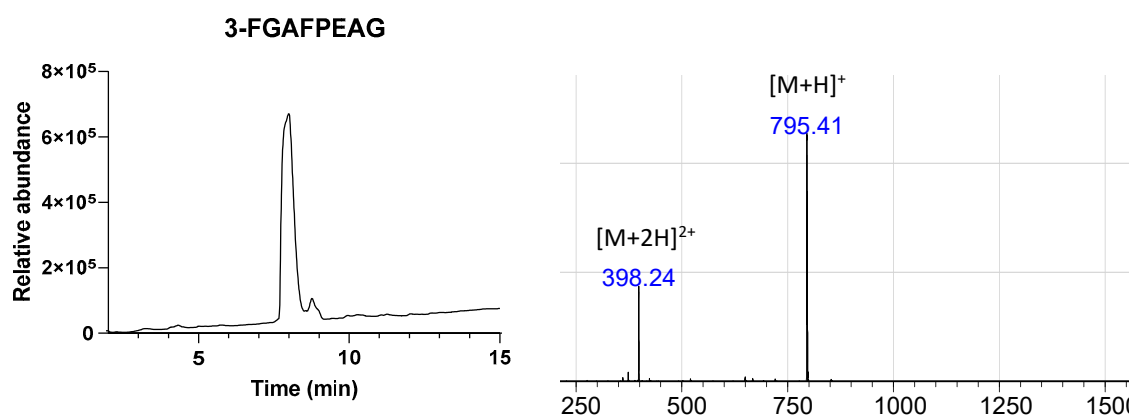
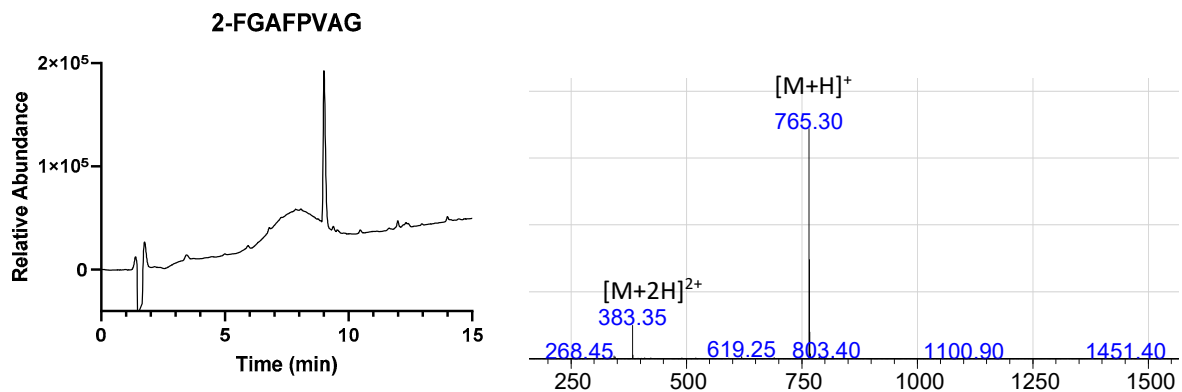


Table S2

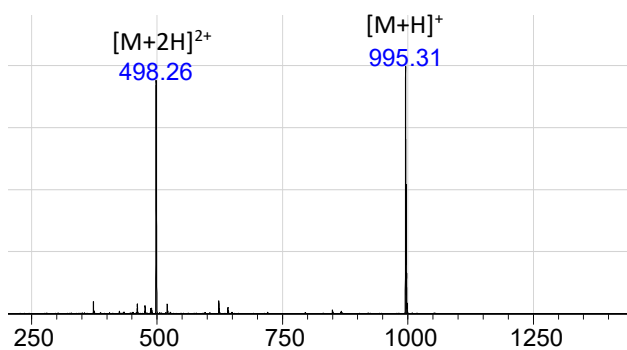
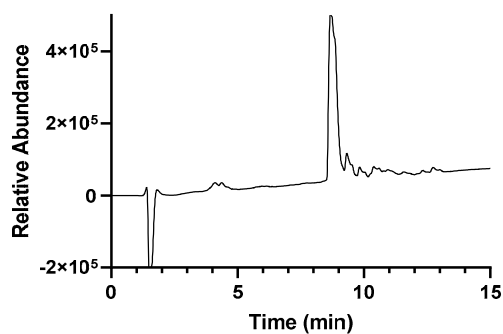
Entry	Peptides ¹	Theoretical Mass (Da)	Experimental Mas (Da) ²	HPLC retention time (min) ³	Gradient	Purity ⁴
1	FGAFPIAG	778.39	779.40	6.0	5-40%	94%
2	FGAFPVAG	764.38	765.30	9.1	5-40%	91%
3	FGAFPEAG	794.35	795.41	7.9	5-40%	97%
4	GAFGAFPVAG	892.43	893.35	10	5-40%	90%
5	EAFGAFPEAG	994.43	995.31	8.5	5-40%	89%
6	GDEAFGAFPEAG	1166.48	1167.47	9	5-40%	80%
7	FGAFGAFGAFPIAG	1328.64	1330.60	13.5	5-40%	76%
8	DYKG	481.21	482.25	1.6	5-40%	60%
9	DYKG ⁵	481.21	482.26	1.6	5-40%	77%
10	DYKGG	538.23	539.25	2.8	0-30%	62%
11	DYKGG ⁵	538.23	539.36	1.6	5-40%	72%
12	DYKD	539.21	540.25	3.8	0-40%	63%
13	DYKDD	654.24	655.20	4.9	0-20%	63%
14	DYKK	552.28	553.20	2.1	0-40%	57%

¹ All peptides are C-terminal carboxylic acid; ² Determined by LC-MS; ³ Linear MeCN (+0.036% TFA) into H₂O (+0.045% TFA) over 15 min; ⁴ Determined by analytical HPLC; ⁵ Asp (D) protected as OFm ester; Tyr (Y) protected with 2-Br-Z.

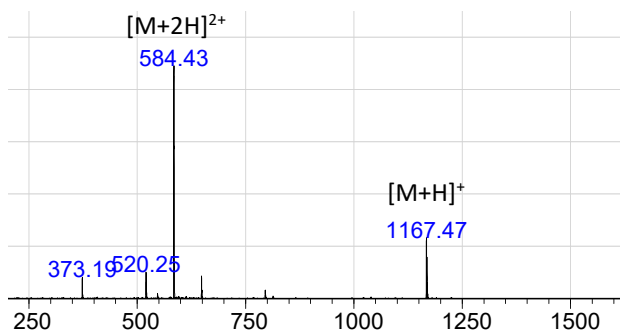
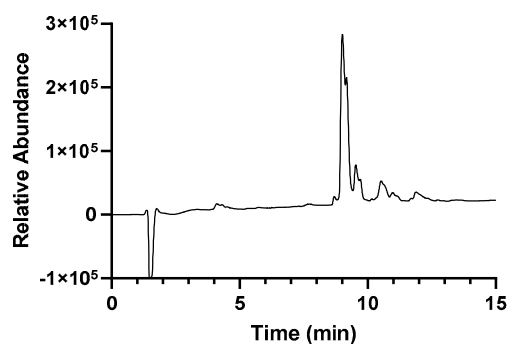




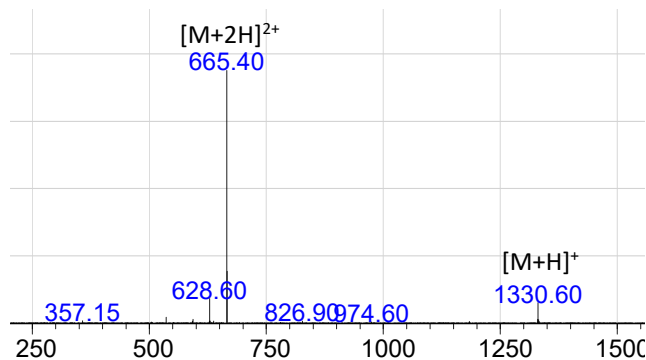
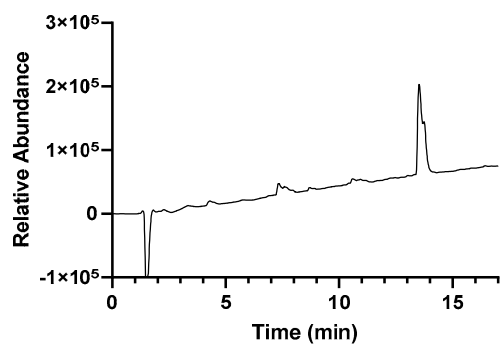
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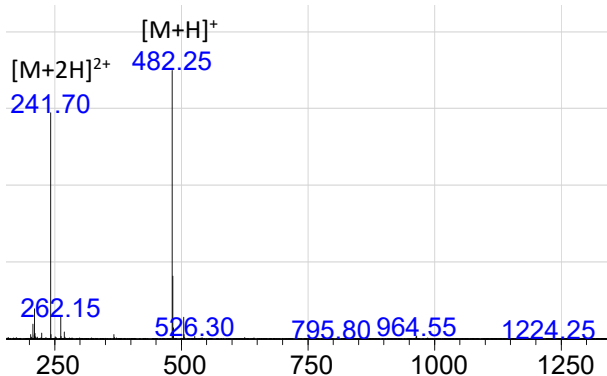
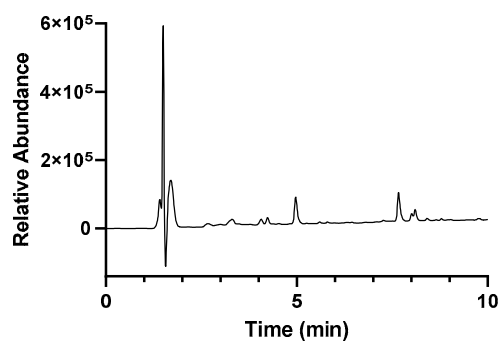
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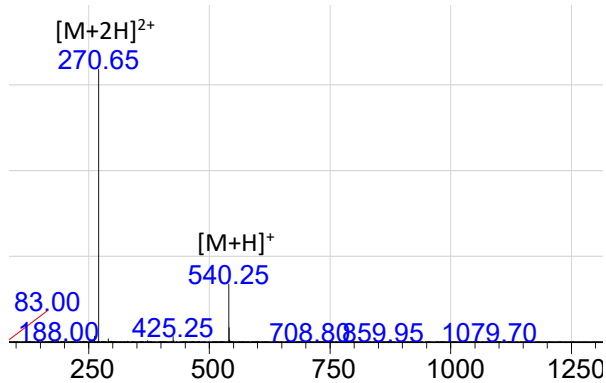
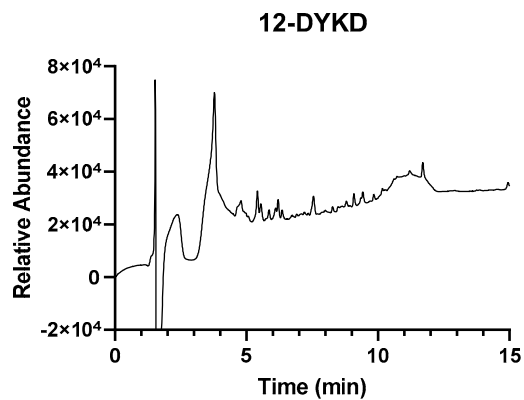
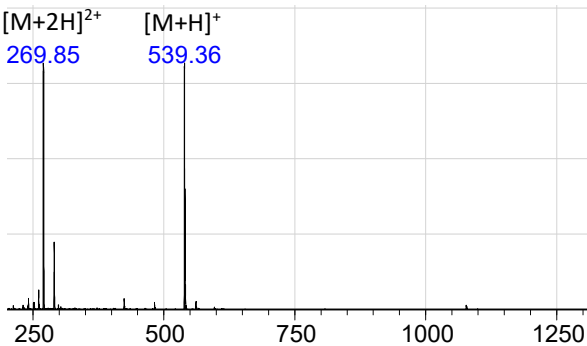
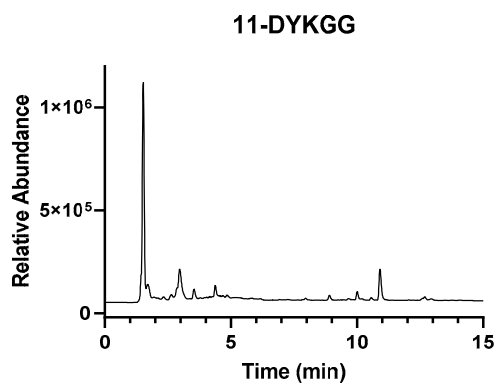
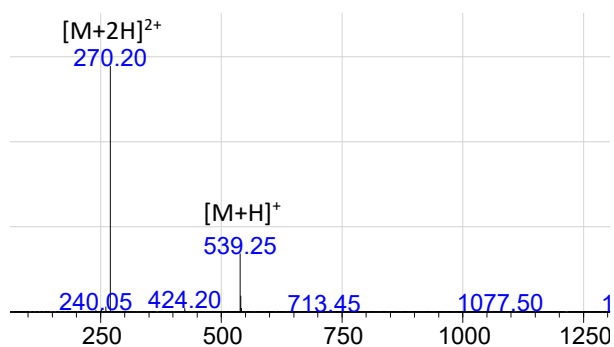
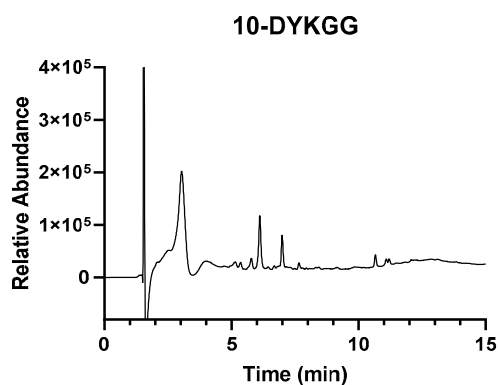
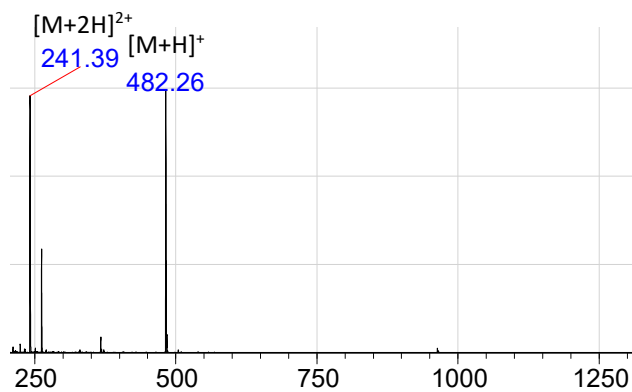
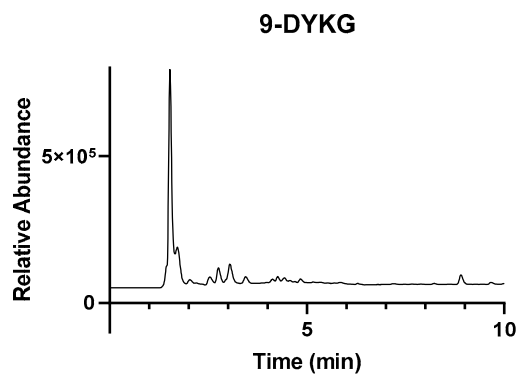


7-FGAFGAFGAFPIAG

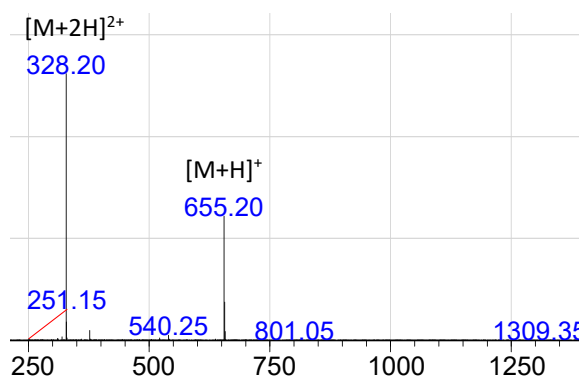
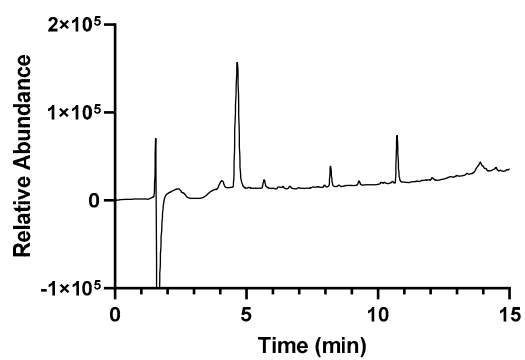


8-DYKG





13-DYKDD



14-DYKK

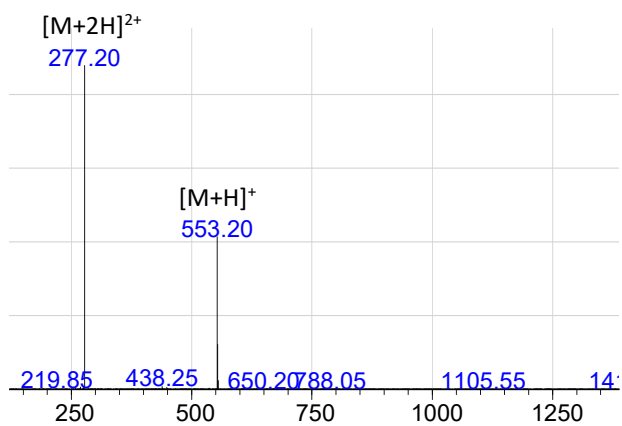
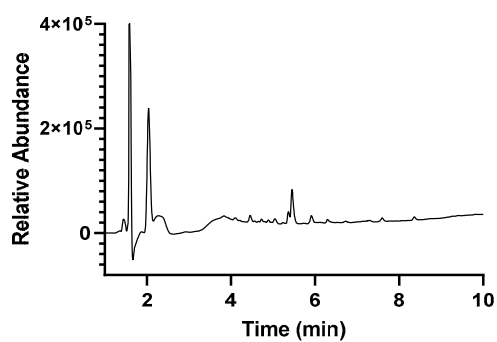


Figure S2

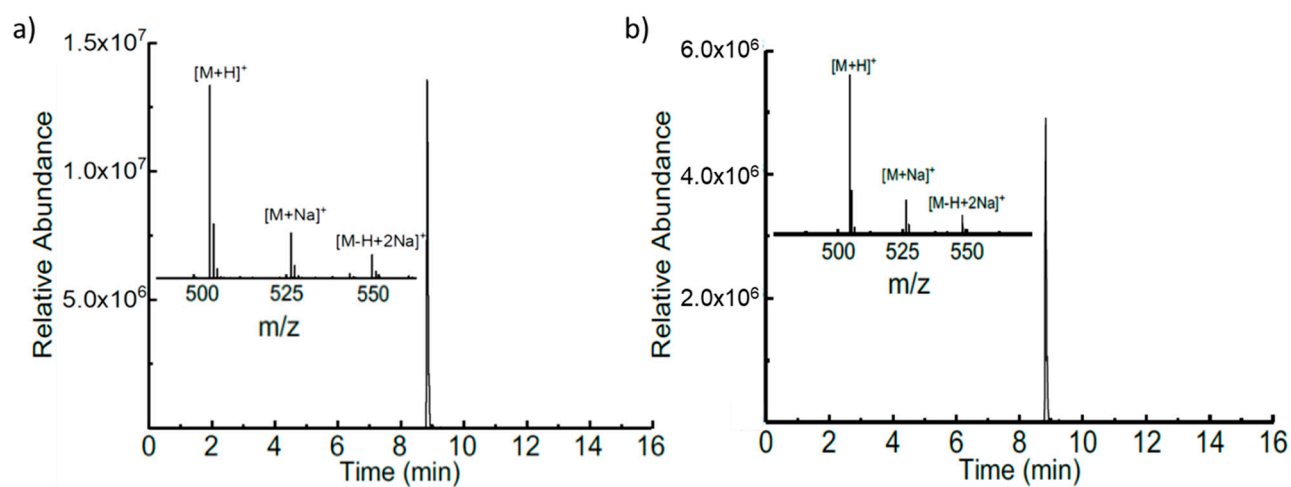


Figure S2: LC-MS of crude FPIAG synthesized on a SPR chip using a) standard cycles and b) fast timing cycles.

Table S3

Amino acid	d_n/d_c (mL/g)	Mass	Volume	d_n/d_c (mol/mL)	$n_A - n_c$	d_A	moles/cm ²	molecules/cm ²
Gly	0.175	75	91	13.125	0.02864	4.497941	9.81494^{-11}	6.12452^{+13}
Ala	0.167	89	108	14.863	0.02863	4.762203	9.17324^{-11}	5.7241^{+13}
Ile	0.179	131	159	23.449	0.11149	5.417502	2.57579^{-10}	1.60729^{+14}
Pro	0.165	115	139	18.975	0.06024	5.180101	1.64453^{-10}	1.02619^{+14}
Phe	0.244	165	200	40.26	0.24304	5.848035	3.53032^{-10}	2.20292^{+14}

Variations in surface density calculated by the De Feijter equation:

$$\tau = \frac{d_A(n_A - n_c)}{d_n/d_c}$$

where d_A is the thickness of the adsorbed layer, d_n/d_c is the refractive index increment of the amino acids as found in literature, n_A and n_c are refractive indexes of adsorbed amino acid layer and the background solution (PBS 0.1X) calculated from experimental data.