molecules

MDPI

SUPPLEMENTARY MATERIALS FOR

Identification, Characterization, and Optimization of Integrin $\alpha_v\beta_6$-Targeting Peptides from a One-Bead One-Compound (OBOC) Library: Towards the Development of Positron Emission Tomography (PET) Imaging Agents

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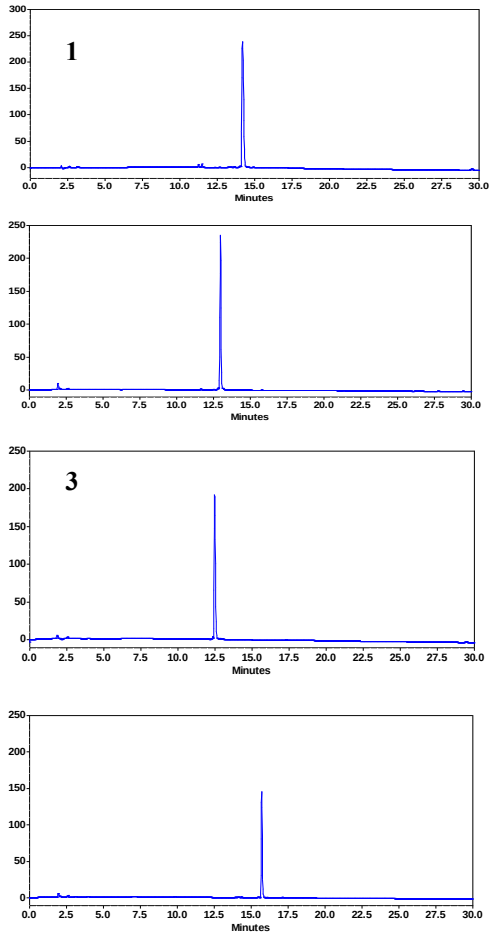
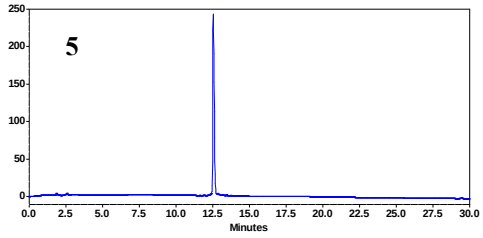
SUPPLEMENTARY TABLE S1. Analytical data of all synthetic peptides showing retention time, purity and mass confirmation.

ID	Sequence	t_R [min]	Purity [%]	Mass (g/mol) Calc.	Mass (g/mol) Obs.
1	VGDLTYLKK(FB)	14.2	>96	1156. 6	1157.6
2	RGDLMKLAK(FB)	13.0	>99	1151. 6	1152.6
3	RGDLADLRK(FB)	12.5	>99	1163.6	1164.5
4	GIDLTSLTK(FB)	15.7	>97	1067.5	1090.7
5	RGDLRELAK(FB)	12.6	>99	1177.6	1178.5
1a	FB-VGDLTYLKK	15.1	>99	1156.6	1157.6
1b	Ac-VGDLTYLKK(FB)	16.5	>99	1198.6	1199.8
1c	Me-VGDLTYLKK(FB)	14	>99	1170.6	1171.7
1d	PEG_{12}-VGDLTYLKK(FB)	15.6	>99	1756.0	1757.1
1e	FB-VGDLTYLKK(FB)	19	>99	1278.6	1279.6
1f	VGDLTYLKK(FB)-PEG_{28}	15.4	>99	2460.4	2461.4
1g	Ac-VGDLTYLKK(FB)-PEG_{28}	17.7	>95	2502.4	2503.8
1h	FB-VGDLTYLKK(FB)-PEG_{28}	19.7	>99	2582.4	2583.6
1i	VGDLTYLKK(FB)KVART	12.8	>99	1711.9	1713.0

SUPPLEMENTARY FIGURE S1





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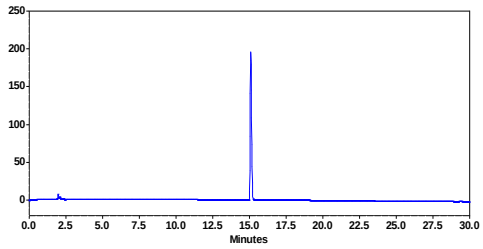

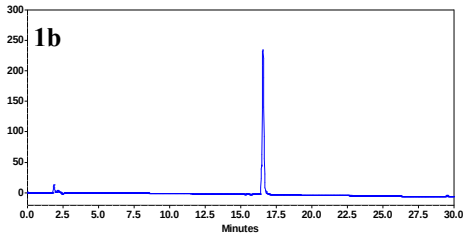

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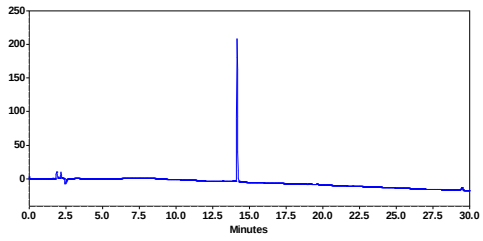

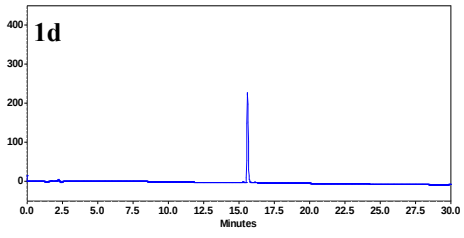

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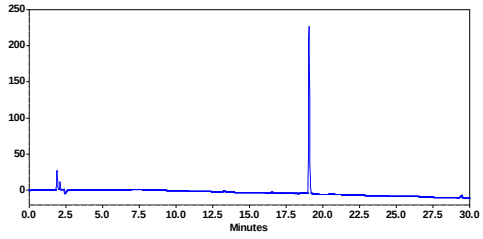

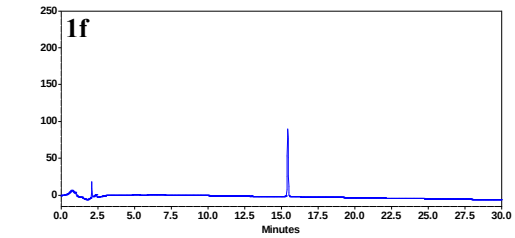

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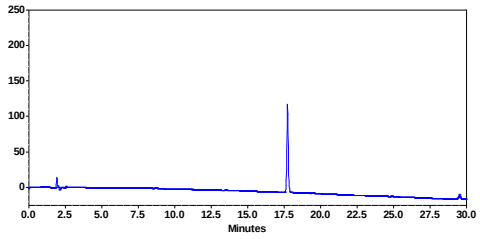

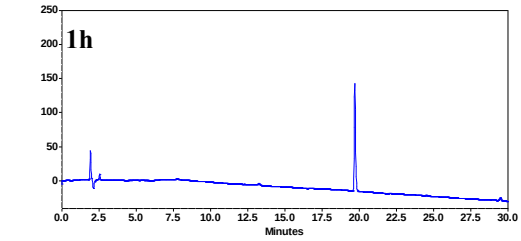

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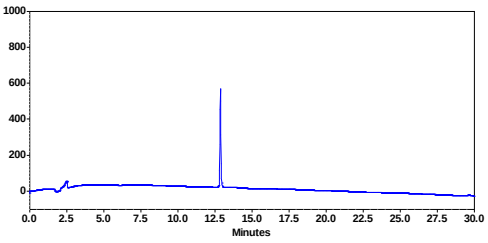
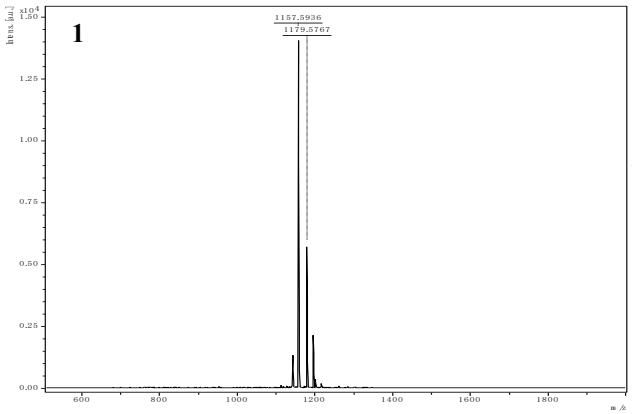
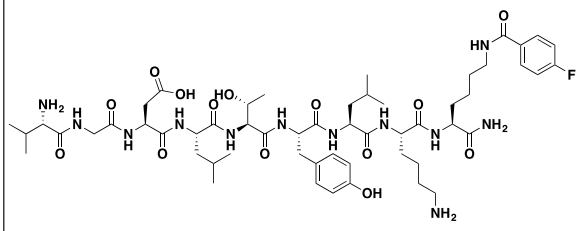


SUPPLEMENTARY FIGURE S2.





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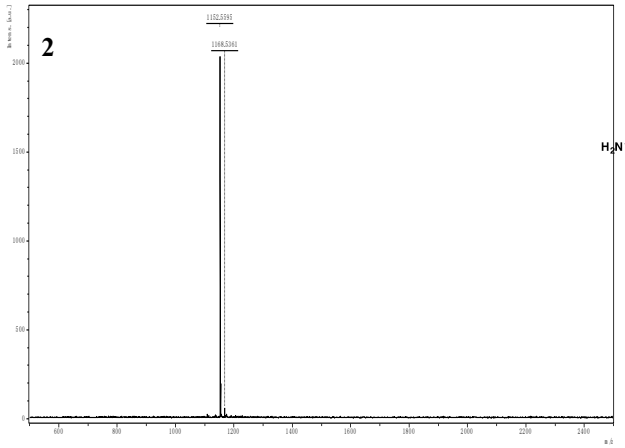

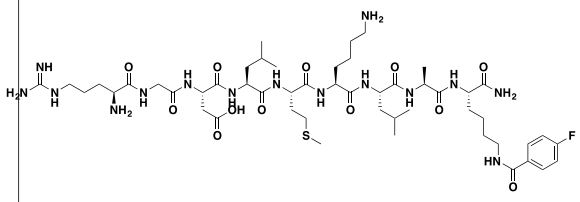

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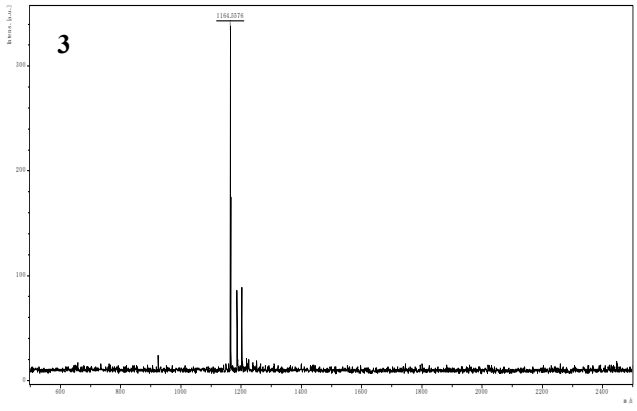

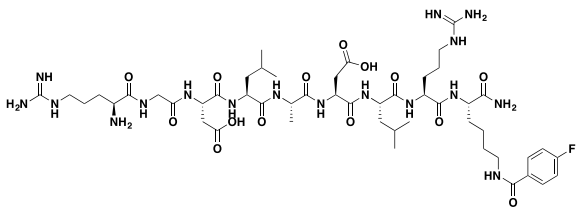

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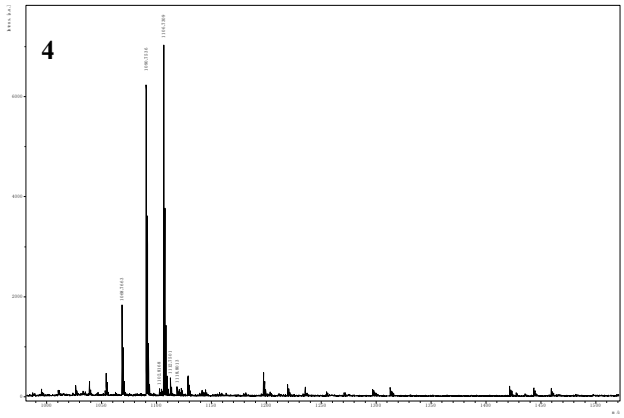

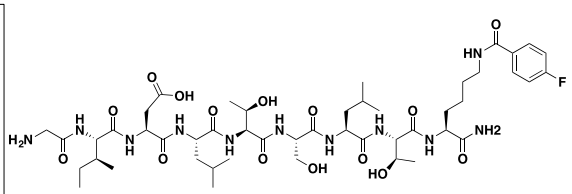

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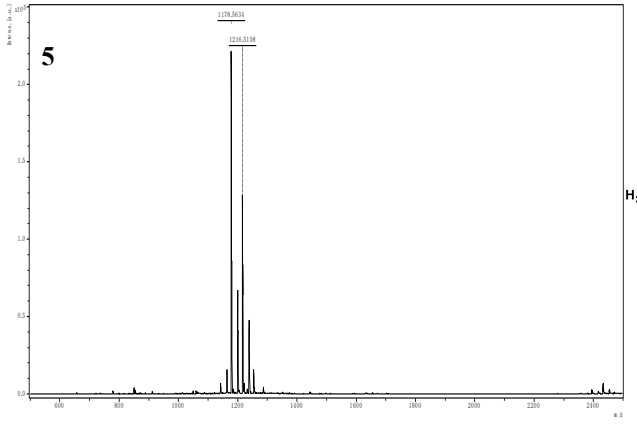
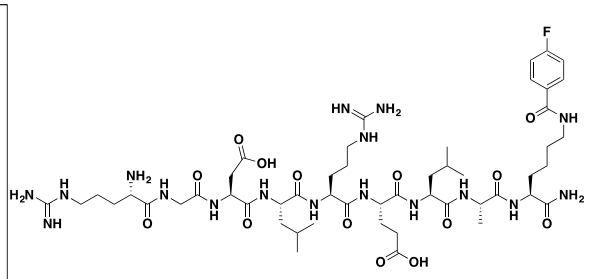
SUPPLEMENTARY FIGURE S2 (CONTINUED)





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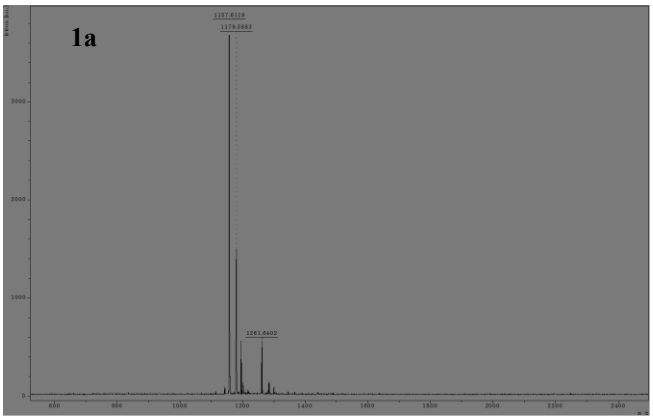

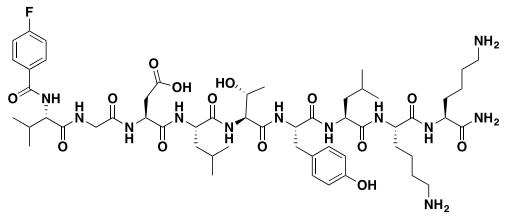

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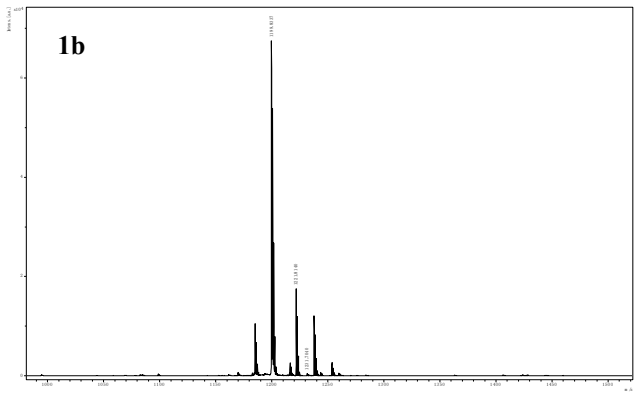

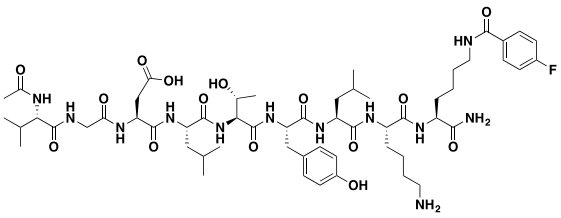

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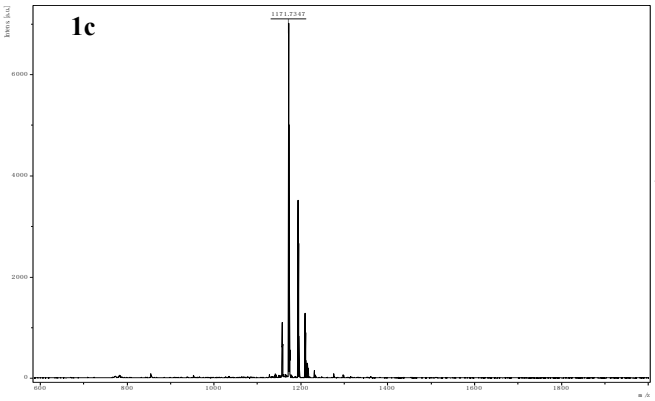

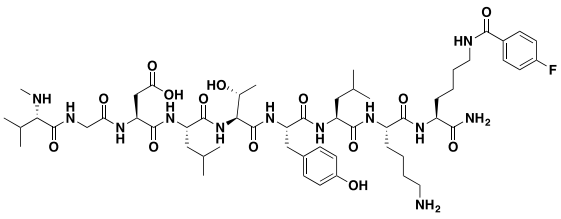

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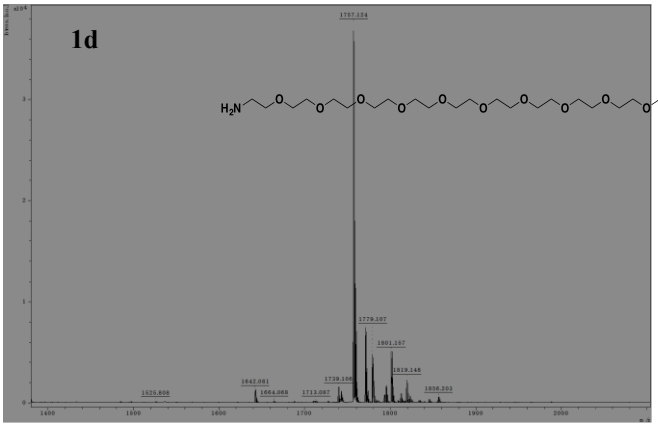
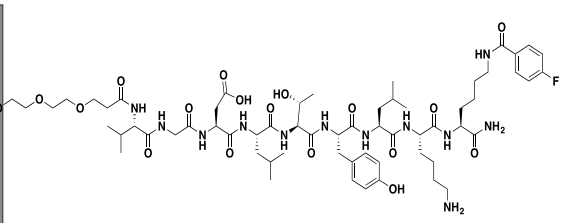
SUPPLEMENTARY FIGURE S2 (CONTINUED)





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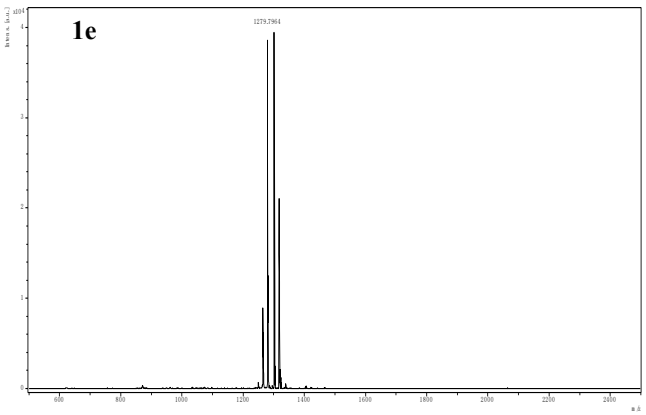

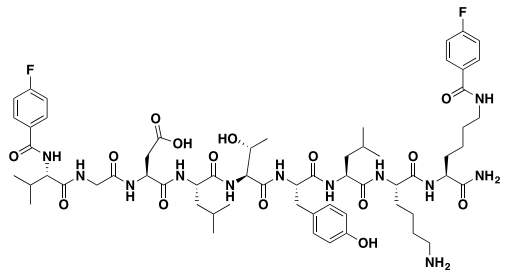

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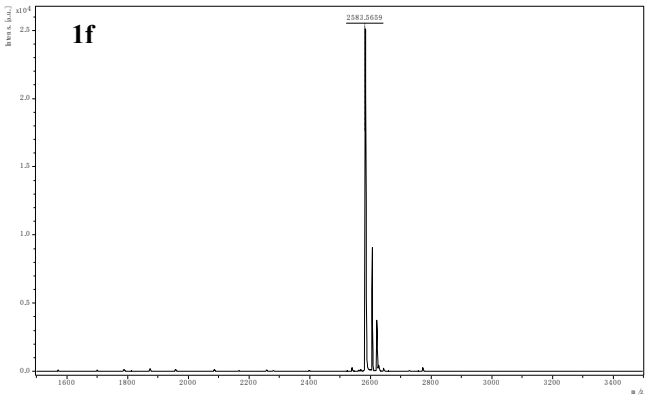

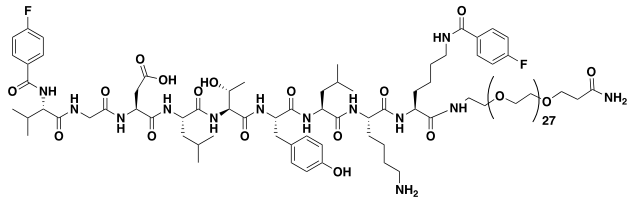

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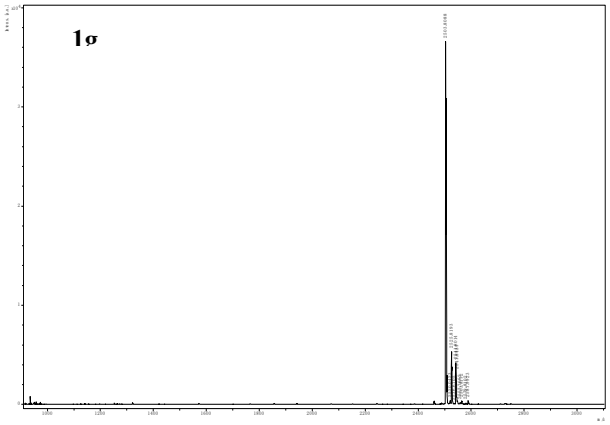
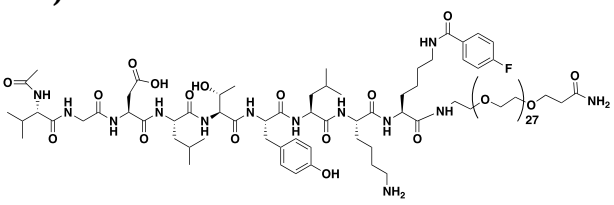
SUPPLEMENTARY FIGURE S2 (CONTINUED)





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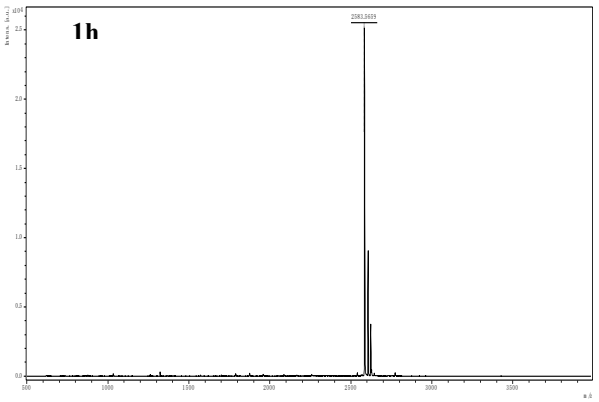

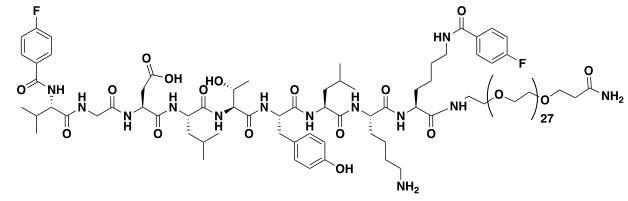

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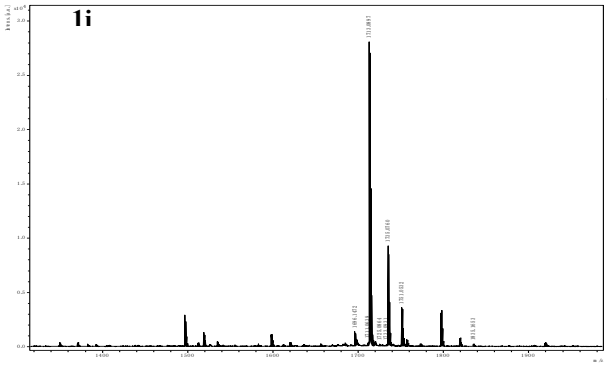

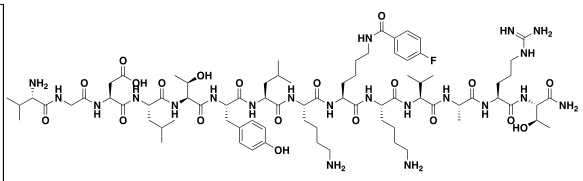

1i

SUPPLEMENTARY TABLE S2. Analytical Radio-HPLC chromatogram confirming the purity of [^{18}F]peptides

ID	Sequence FB =[^{18}F]FB	t_R [min]	RCP [%]	RCY [%]	Molar activity [Ci/μmol]
1	VGDLTYLKK(FB)	14.2	>99	5.4 ± 1.2	>1
2	RGDLMKLAK(FB)	13.6	78	4	NA
3	RGDLADLRK(FB)	12.5	>99	13.4	>1
5	RGDLRELAK(FB)	12.7	>99	13.2 ± 10.1	>1
1a	FB-VGDLTYLKK	15.7	>99	6.5	>1
1f	VGDLTYLKK(FB)-PEG_{28}	16.7	>99	12.8	>1
1h	[^{19}F]FB-VGDLTYLKK(FB)-PEG_{28}	19.8	>99	10.9	>1

1i	VGDLTYLKK(FB)KVART	12.7	>99	2.8	>1

SUPPLEMENTARY FIGURE S3