Electronic Supplementary Material (ESI) for Chemical Science.

SC-EDG-06-2014-001822

Supporting Information

for

Highly Active Antibacterial Ferrocenoylated or Ruthenocenoylated Arg-Trp Peptides can be Discovered by an L-to-D Substitution Scan

by

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Contents:

Table S1. MALDI-TOF *m*/*z*-values for the FcC(O)- and RcC(O)-WRWRW-NH_2 peptides (FW = formula weight; EM = exact monoisotopic mass).

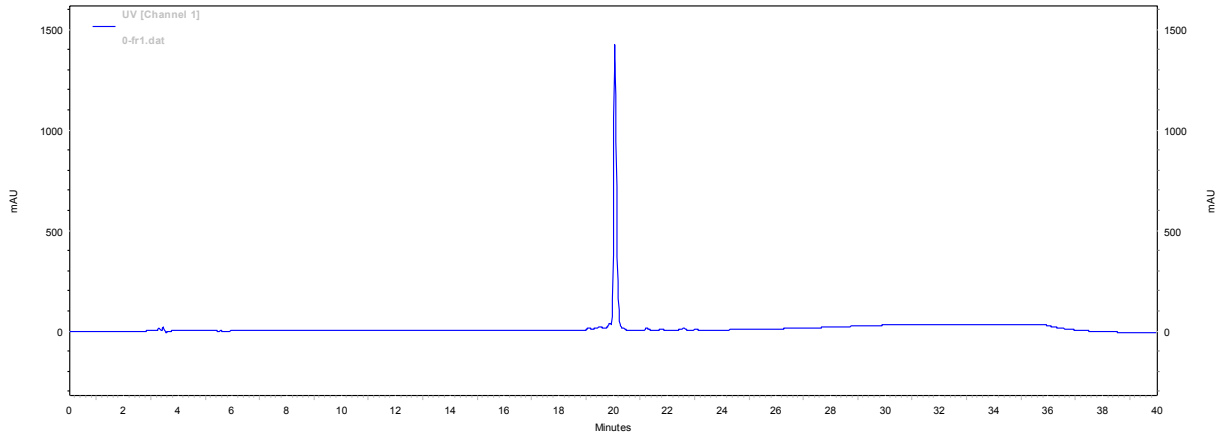
peptide	**FcC(O)-WRWRW-NH_2**			**RcC(O)-WRWRW-NH_2**		
	$[M+H]^+$			$[M+H]^+$		
	found	*calculated (FW)*	*calculated (EM)*	found	*calculated (FW)*	*calculated (EM)*
LLLLL	1100.36[a]	*1101.09*	*1100.47*	1146.27[a]	*1146.31*	*1146.44*
LLLLD	1100.64	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LLLDL	1100.64	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LLDLL	1100.62	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LDLLL	1100.62	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
DLLLL	1100.64	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LLLDD	1100.62	*1101.09*	*1100.47*	1146.39	*1146.31*	*1146.44*
LLDLD	1100.62	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LDLLD	1100.62	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
DLLLD	1100.64	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LLDDL	1100.65	*1101.09*	*1100.47*	1146.39	*1146.31*	*1146.44*
LDLDL	1100.66	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
DLLDL	1100.66	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LDDLL	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DLDLL	1100.66	*1101.09*	*1100.47*	1146.39	*1146.31*	*1146.44*
DDLLL	1100.65	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LLDDD	1100.65	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
LDLDD	1100.65	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
DLLDD	1100.65	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
LDDLD	1100.65	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DLDLD	1100.62	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DDLLD	1100.64	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
LDDDL	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DLDDL	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DDLDL	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DDDLL	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
LDDDD	1100.65	*1101.09*	*1100.47*	1146.38	*1146.31*	*1146.44*
DLDDD	1100.65	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DDLDD	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DDDLD	1100.66	*1101.09*	*1100.47*	1146.39	*1146.31*	*1146.44*
DDDDL	1100.66	*1101.09*	*1100.47*	1146.37	*1146.31*	*1146.44*
DDDDD	1100.64	*1101.09*	*1100.47*	1146.11[a]	*1146.31*	*1146.44*

[a] these *m*/*z*-values were obtained by ESI-MS before, and are taken from: H. B. Albada, A.-I. Chiriac, M. Wenzel, M. Penkova, J. E. Bandow, H.-G. Sahl, N. Metzler-Nolte, *Beilstein J. Org. Chem.* 2012, **8**, 1753.

HPLC-traces of the L-to-D substituted RcC(O)-WRWRW-NH_2 peptides

Conditions: Analytical HPLC was performed on an automated HPLC system using a C_{18}-AQ RP column (250 × 4.6 mm) at a flow-rate of 1 mL/min. A linear gradient of 5% buffer B per min was started after 5 min of buffer A (**A**: H_2O/MeCN/TFA, 95:5:0.1, v/v/v; **B**: MeCN/H_2O/TFA, 95:5:0.1, v/v/v).

RcC(O)-LLLLL-NH_2 (20.1 min)



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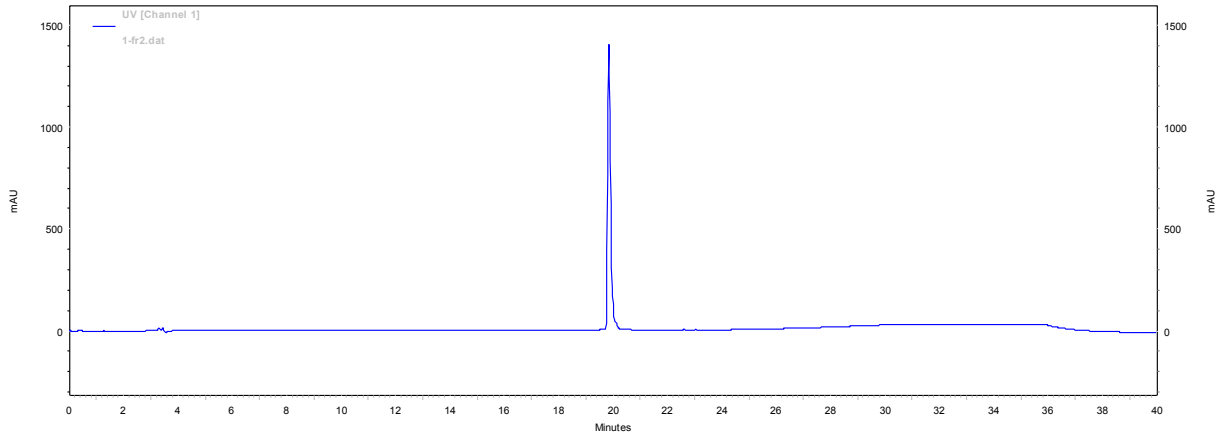

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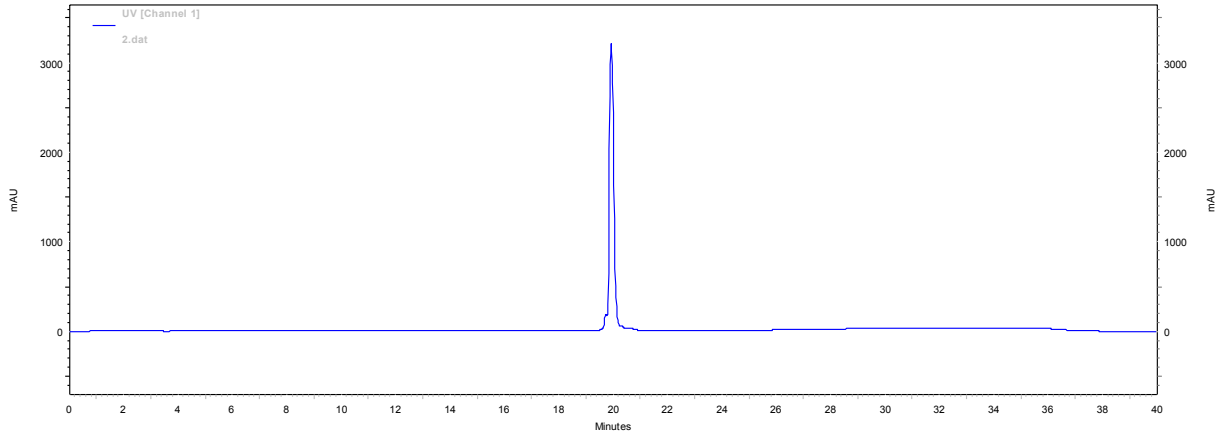

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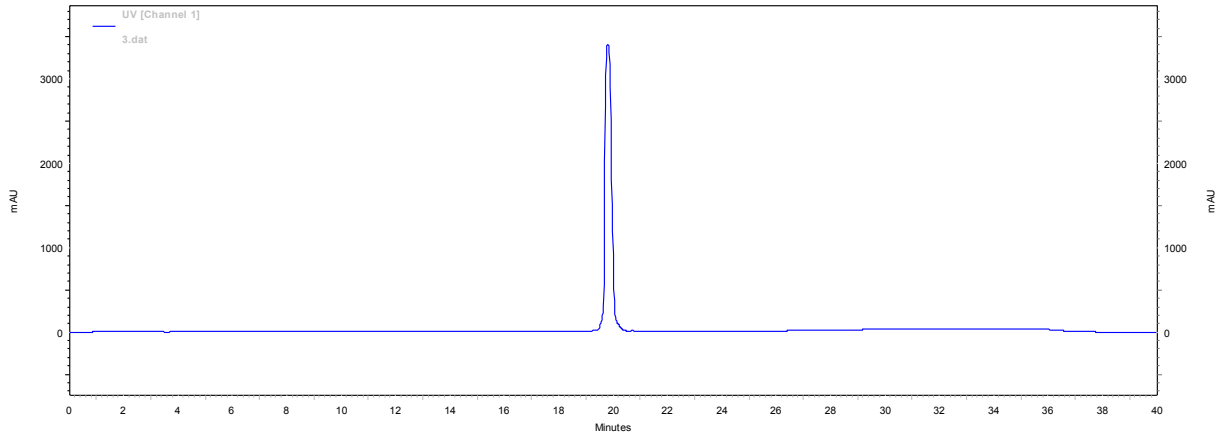

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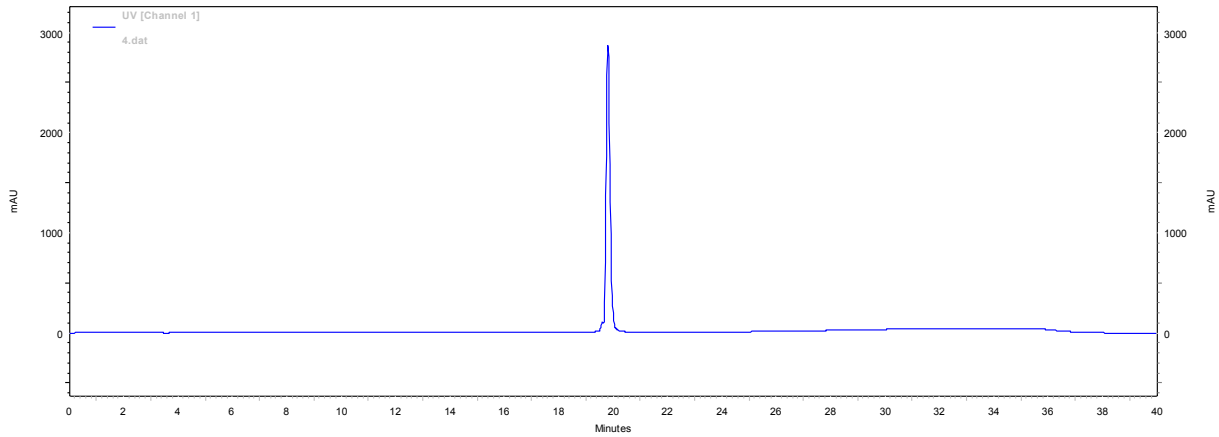

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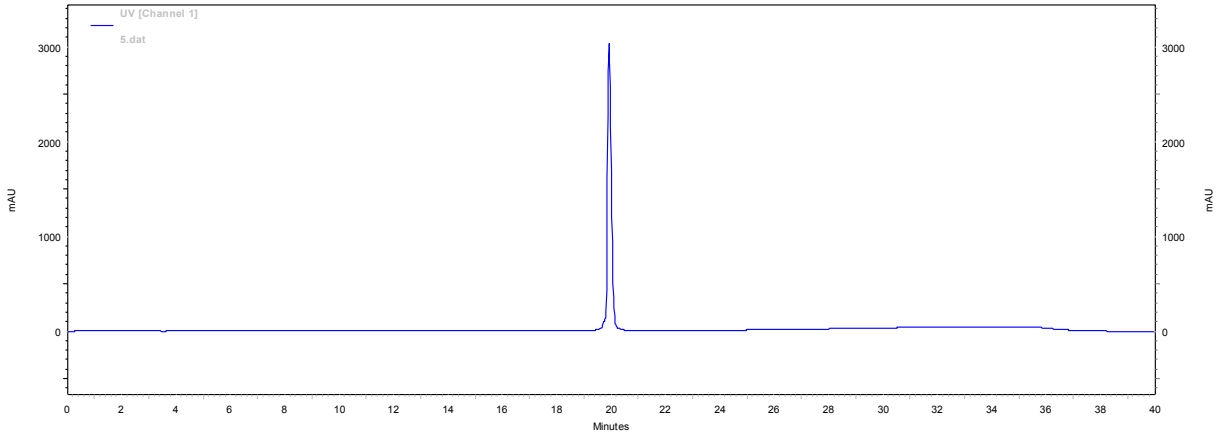

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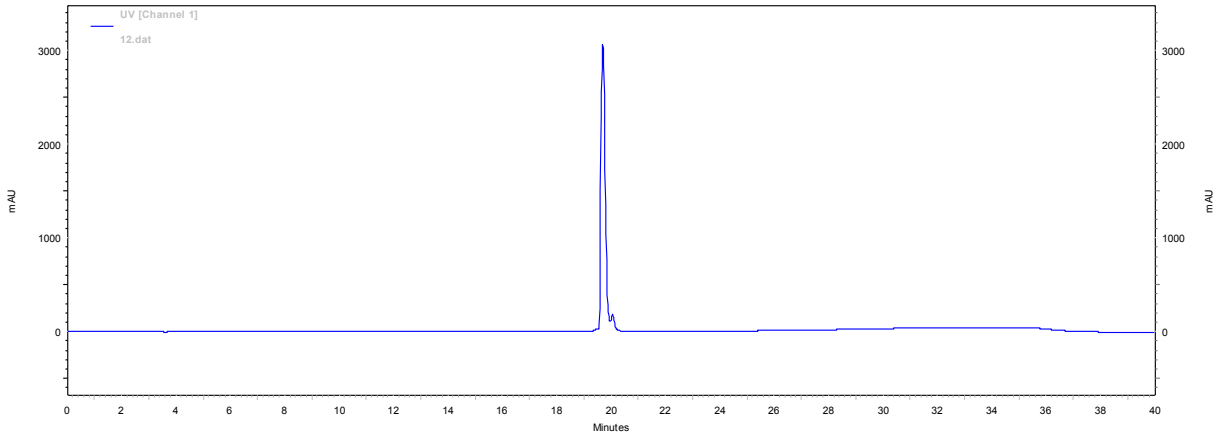

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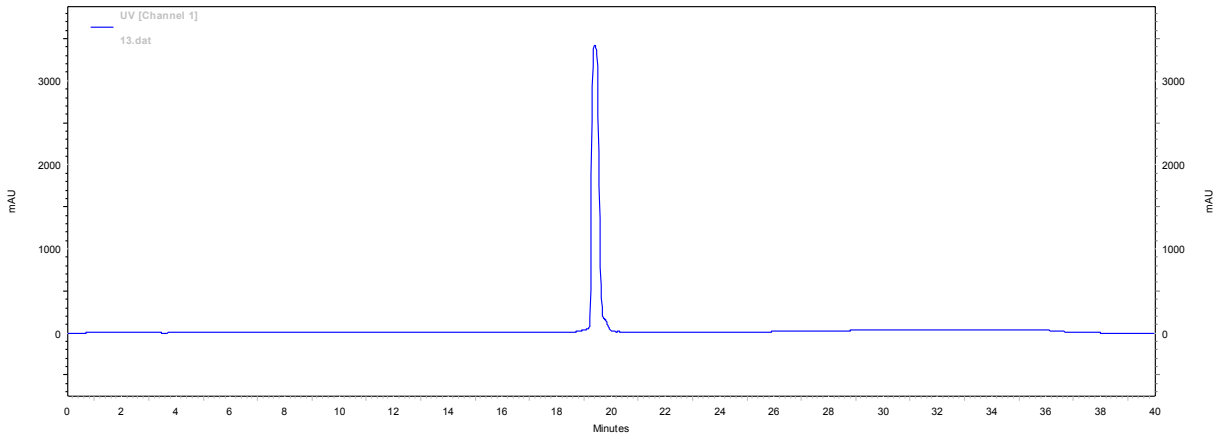

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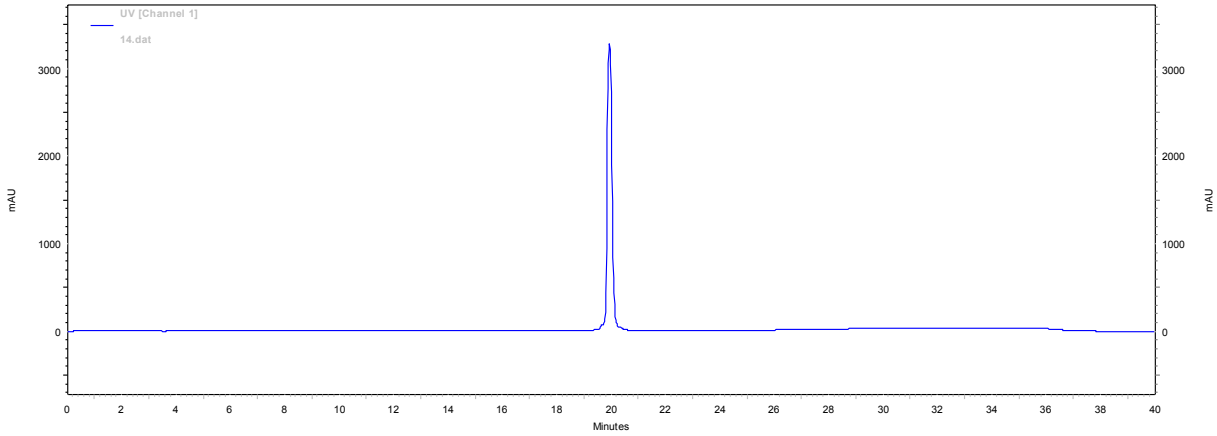

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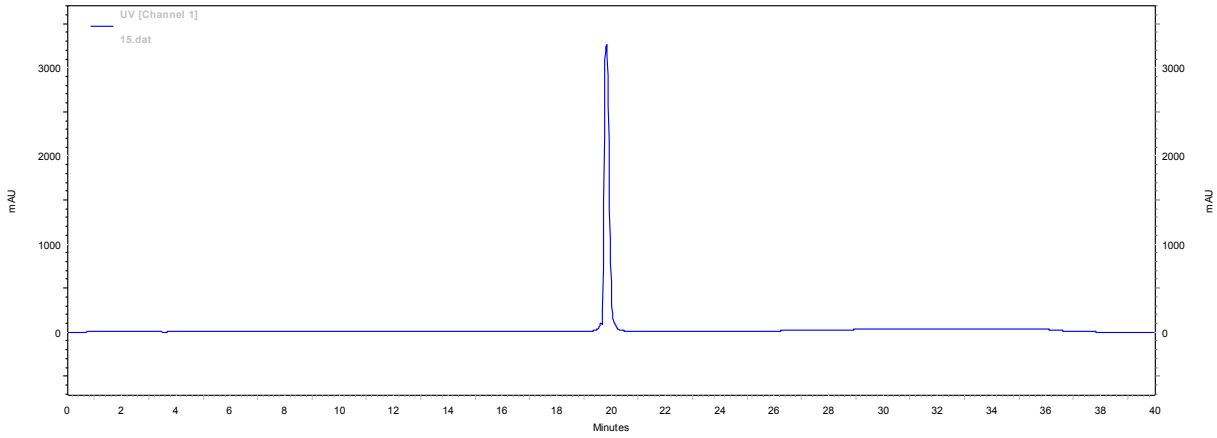

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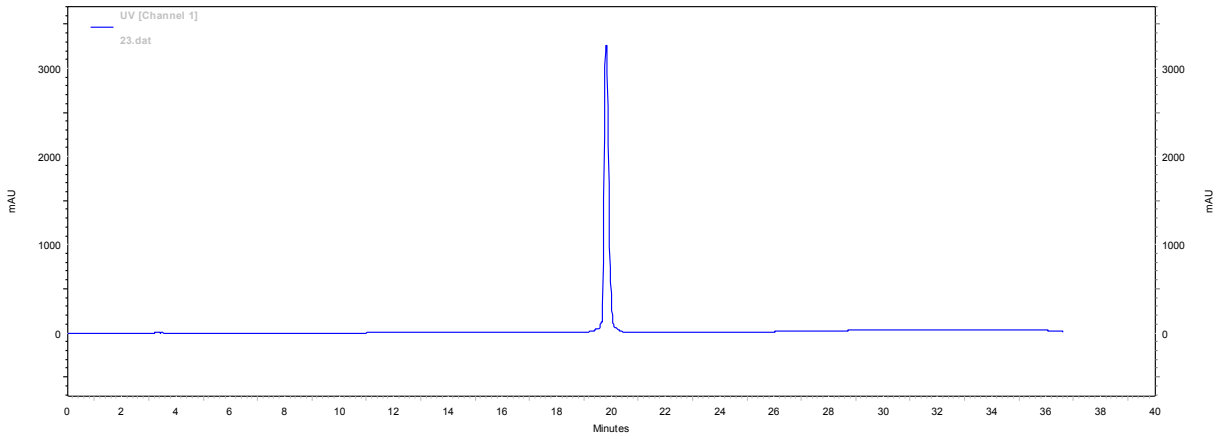

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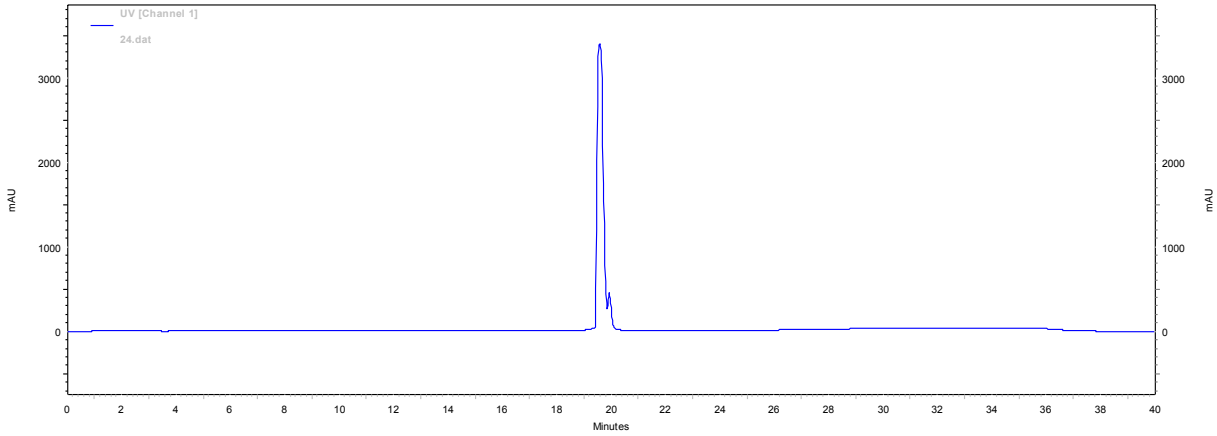

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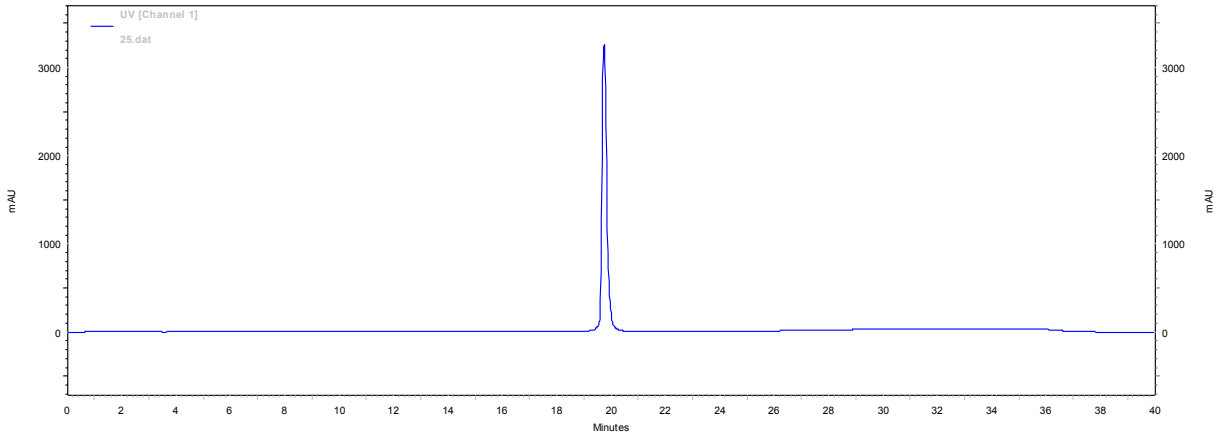

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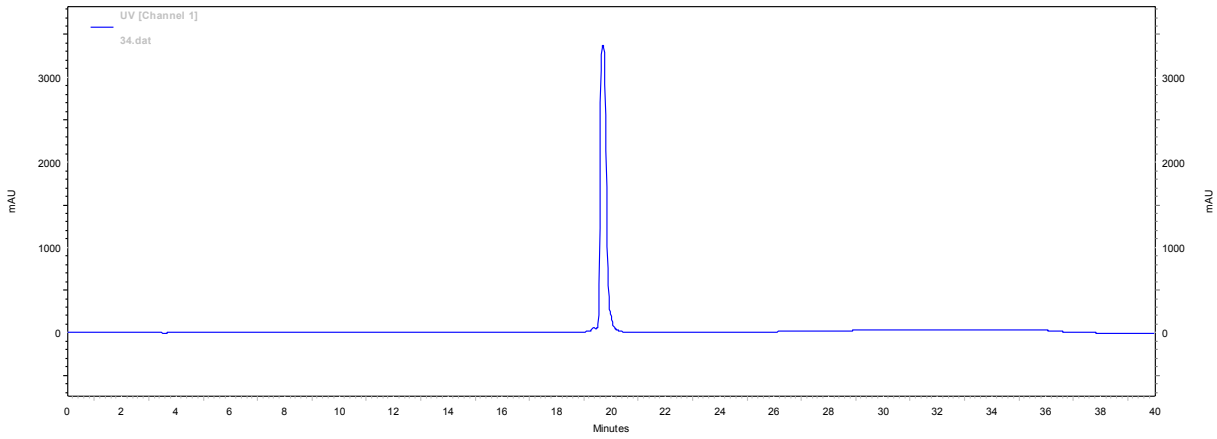

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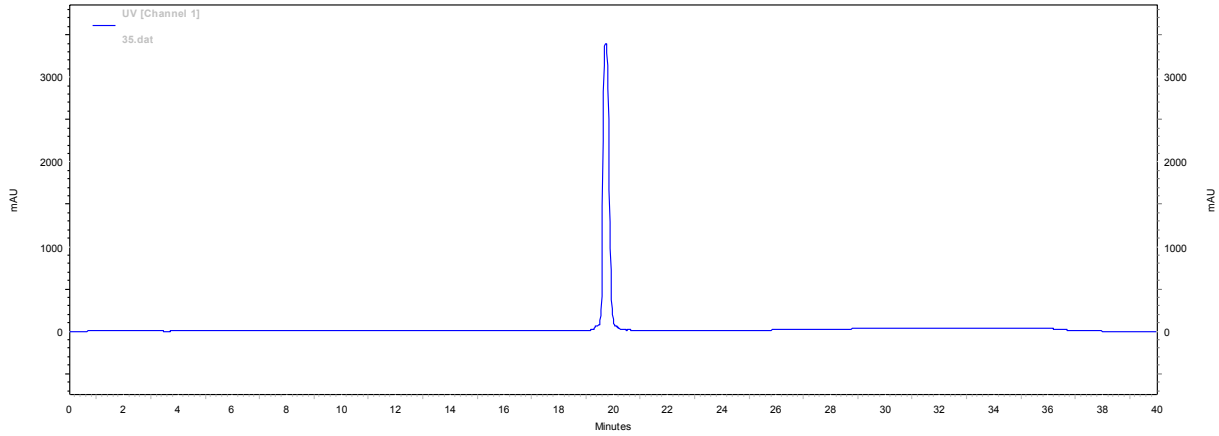

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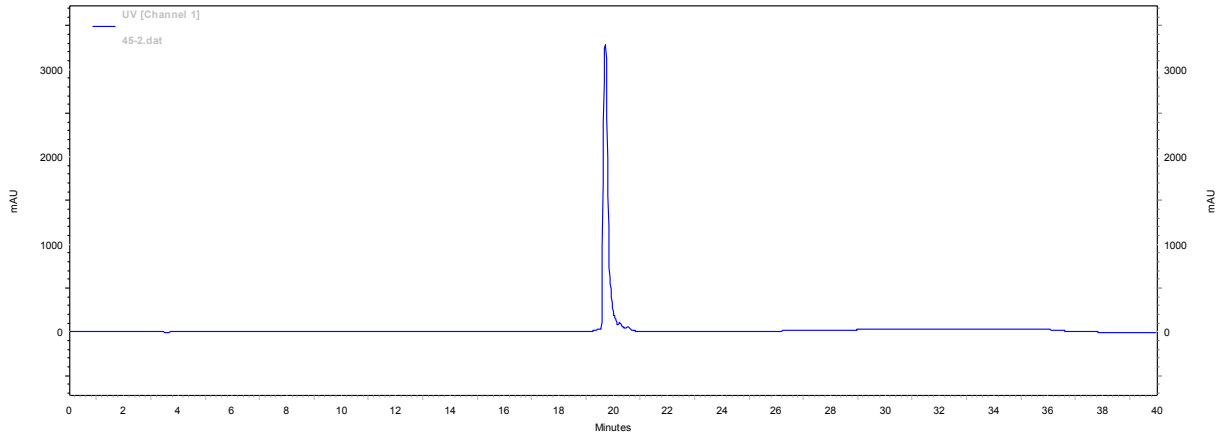

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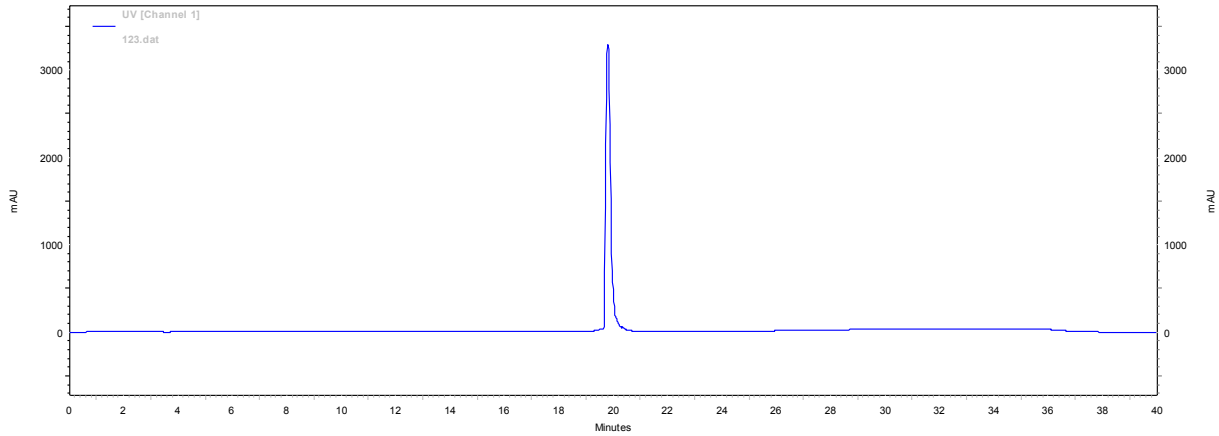

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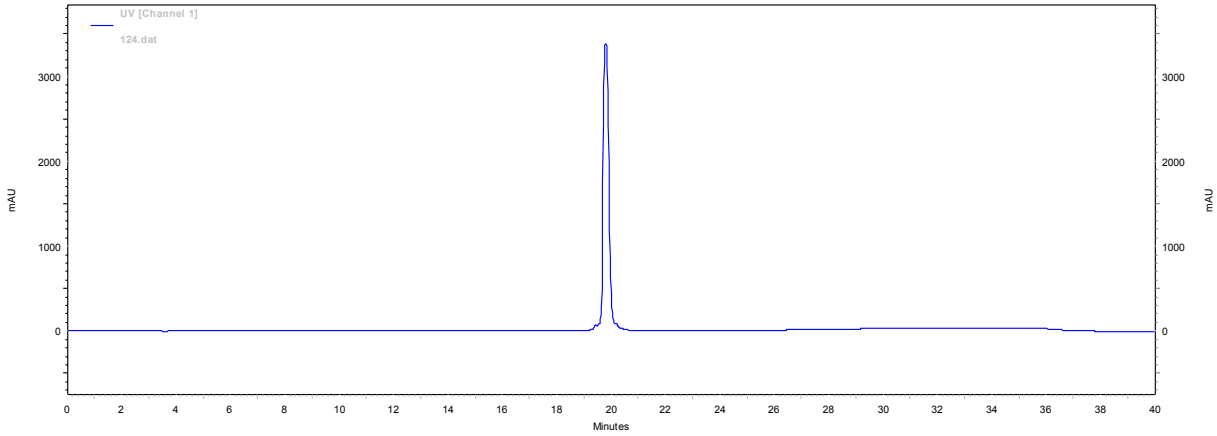

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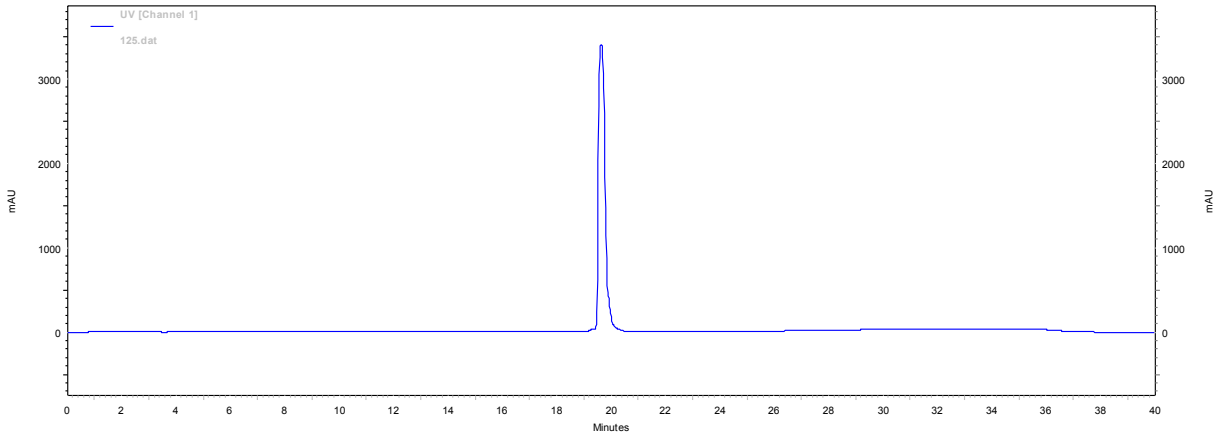

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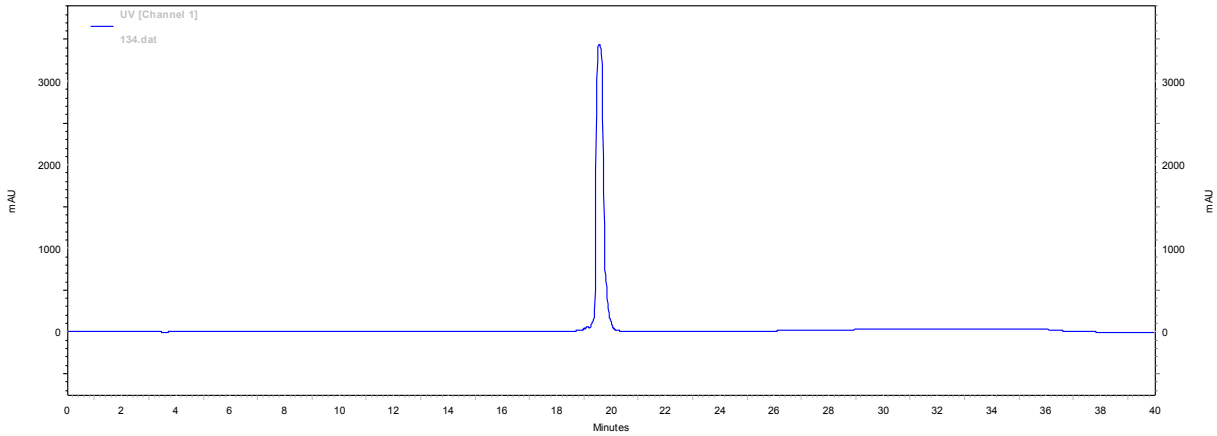

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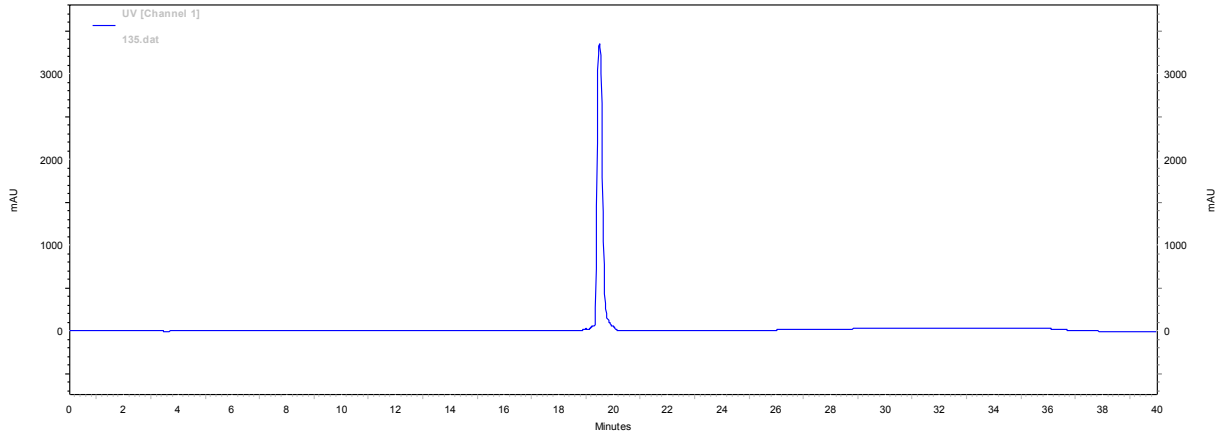

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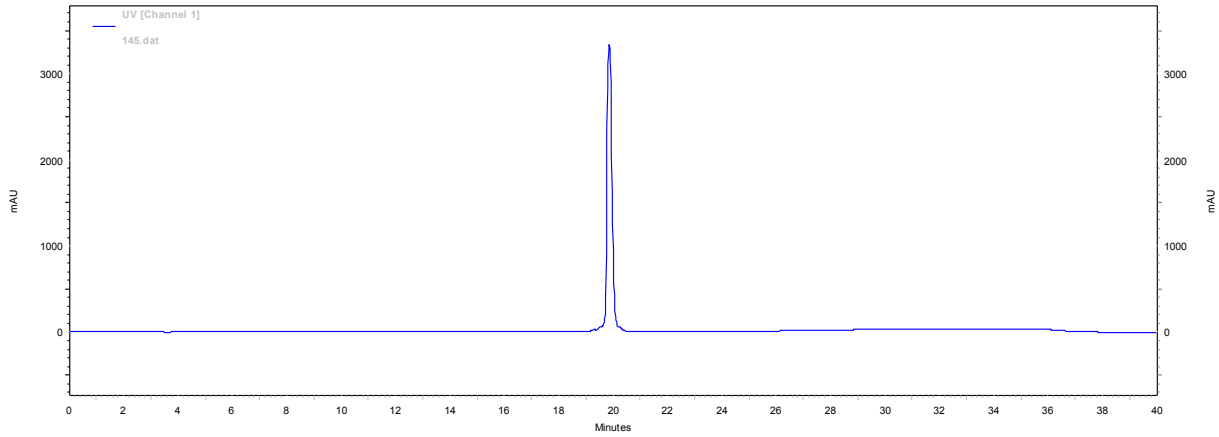

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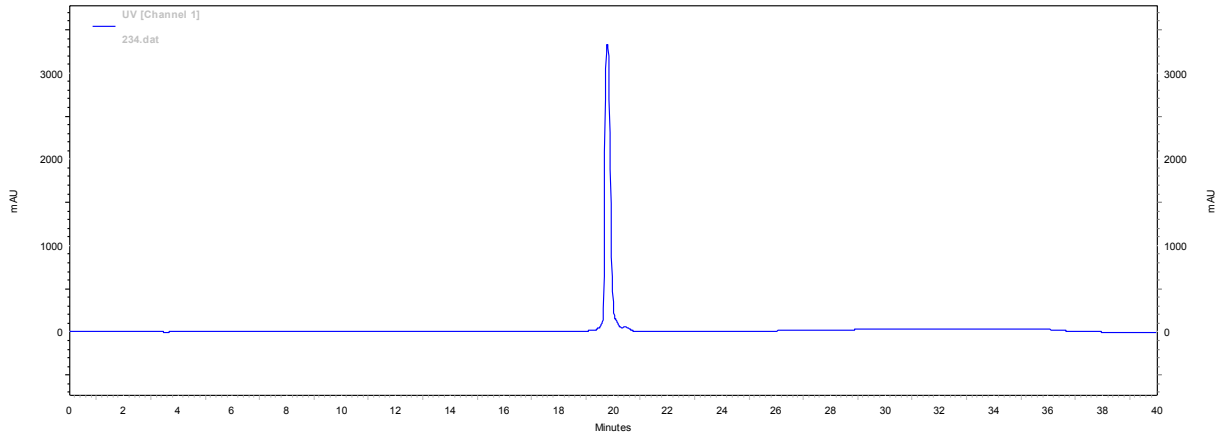

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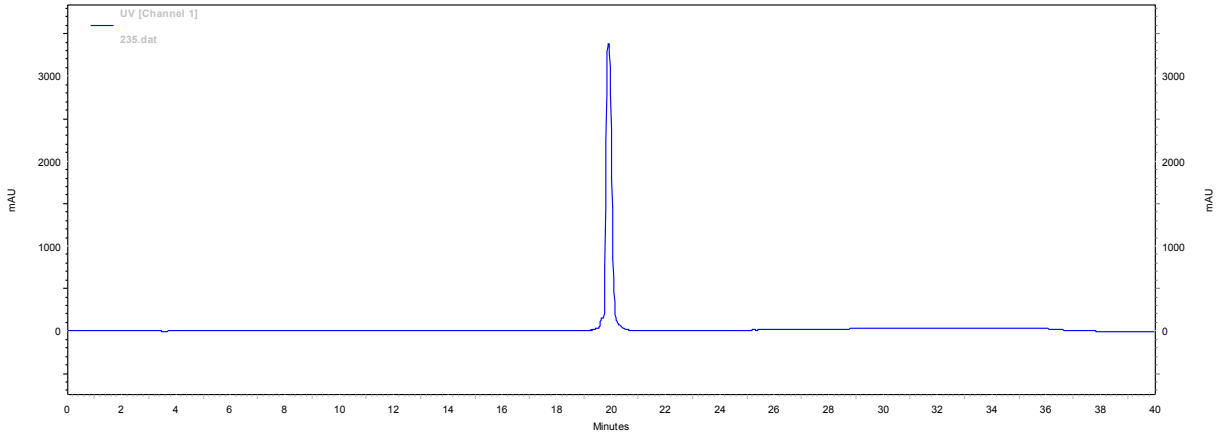

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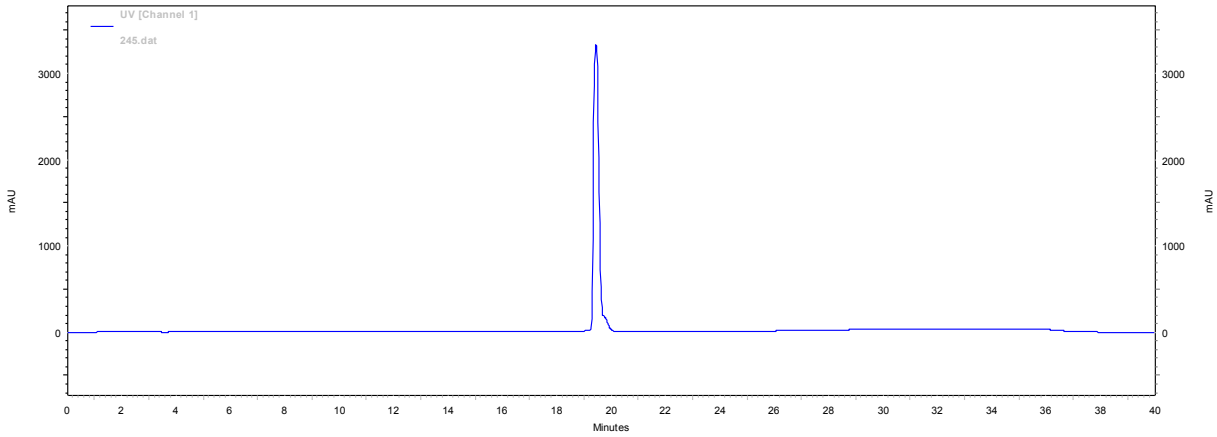

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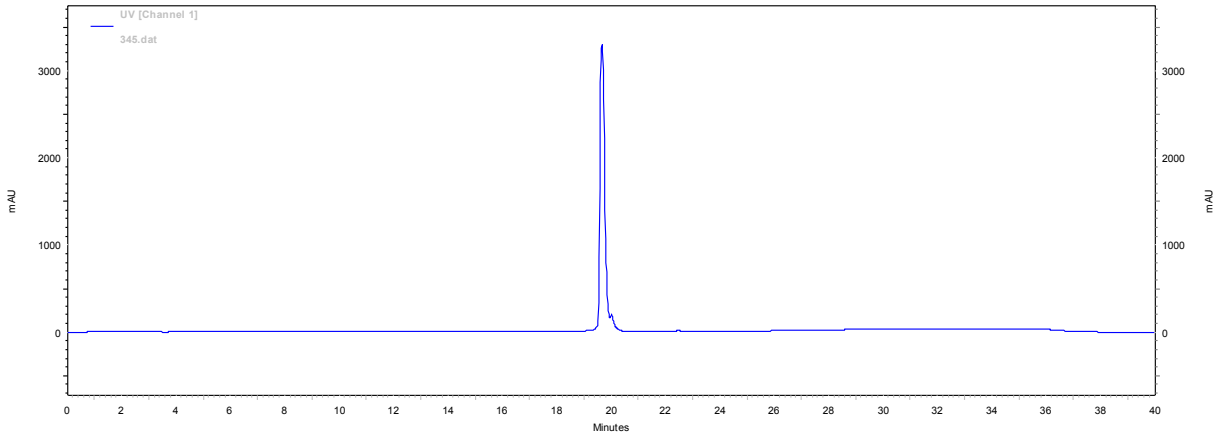

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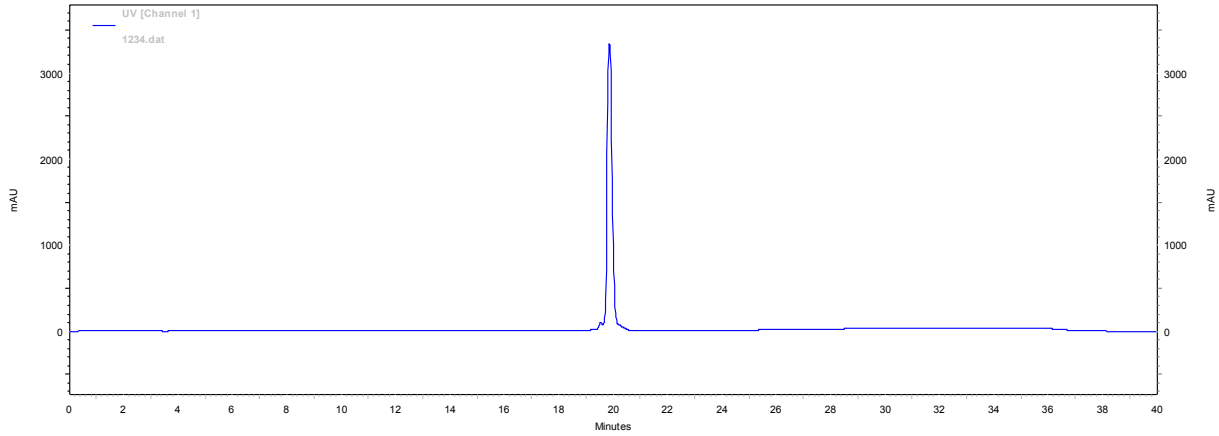

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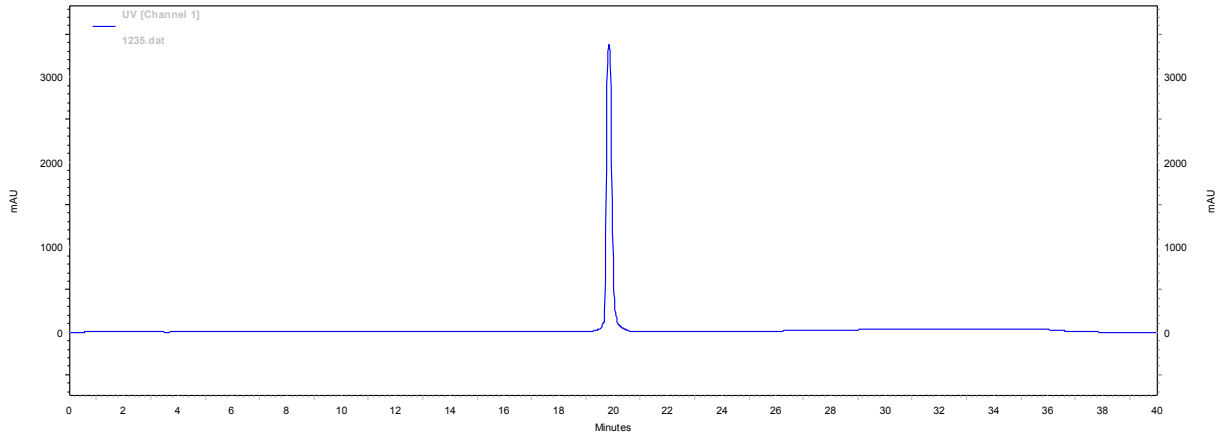

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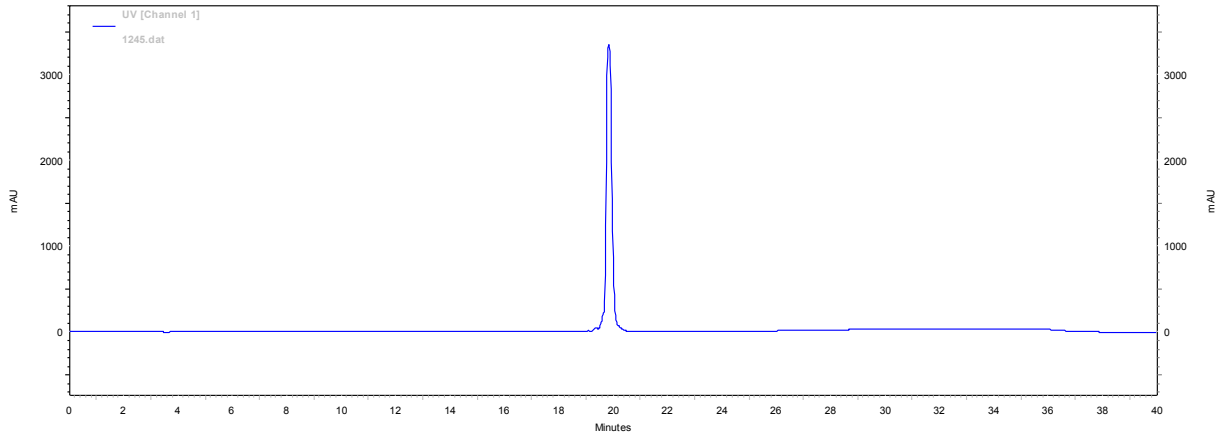

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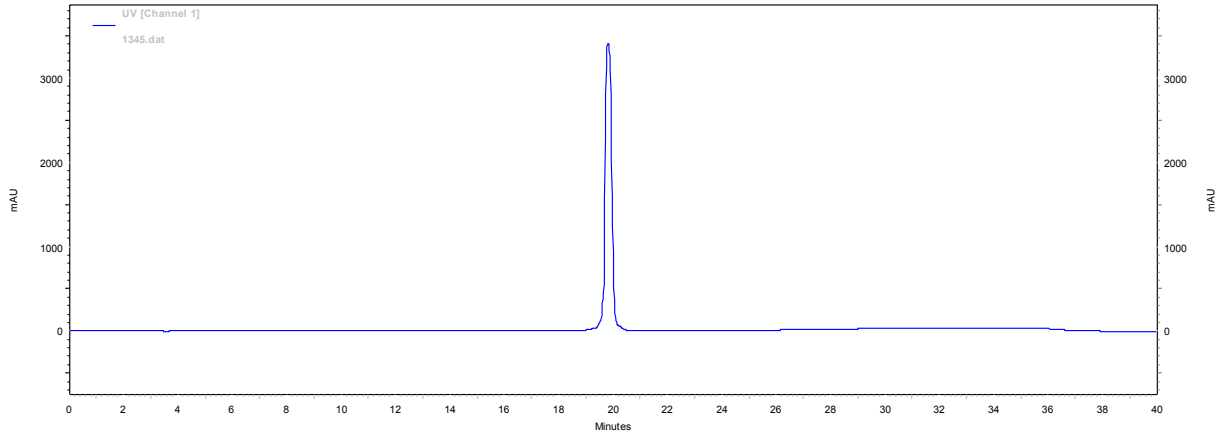

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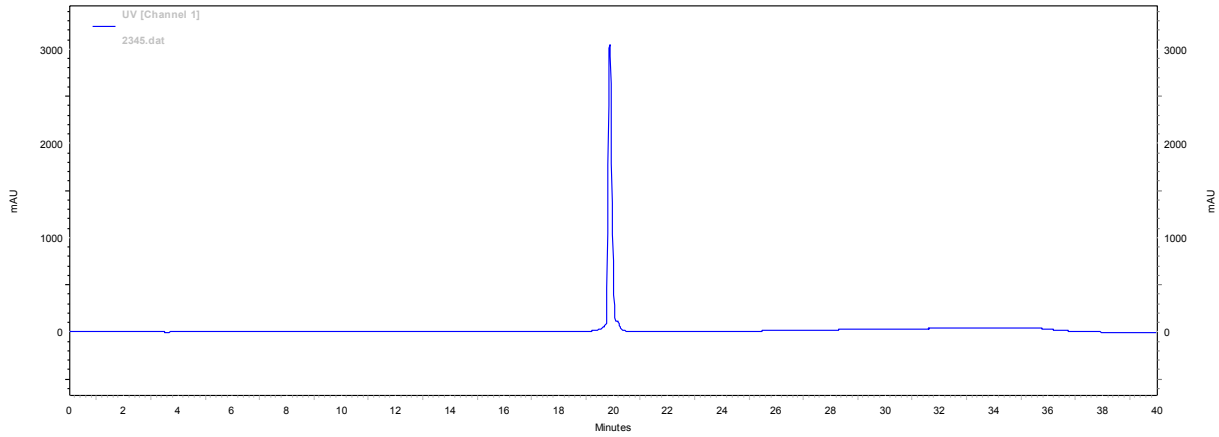

RcC(O)-DDDDD-NH_2 (20.1 min)