

SUPPORTING INFORMATION

Design, synthesis, experimental and theoretical characterization of a new multitarget 2-thienyl-*N*-acylhydrazone derivative

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Table S1. Details from Rietveld refinements of the crystal structure of LASSBio-1834 (3) and LASSBio-1835 (4).

Chemical formula	C ₁₄ H ₁₄ N ₂ O ₃ S	C ₁₅ H ₁₆ N ₂ O ₃ S
Formula weight (g mol ⁻¹)	290.34	304.36
Crystal system	Monoclinic	Monoclinic
Space group	<i>P</i> 2 ₁ / <i>c</i> (Nr. 14)	<i>P</i> 2 ₁ / <i>c</i> (Nr. 14)
<i>a</i> , <i>b</i> , <i>c</i> (Å)	10.18727(19); 16.2201(3);8.34362(14)	11.27114(17); 9.73916(13); 13.6237(2)
β (°)	90.3514(9)	90.4227(8)
Volume (Å ³)	1378.66(4)	1495.45(4)
<i>Z</i> , <i>Z'</i>	4, 1	4, 1
ρ_{calc} (g cm ⁻³)	1.399	1.352
T (K)	298(2)	298(2)
<i>Data collection</i>		
Diffractometer	STADI P	STADI P
Monochromator	Ge(111)	Ge(111)
Wavelength (Å)	1.54056	1.54056
2 θ range (°)	4-82.735	8-86.735
Step size (°)	1.05	1.05
Time per step (s)	200	200
<i>Refinement</i>		
Number of data points	3360	5250
Number of contributing reflections	922	1117
Number of restraints	47	47
Number of refined parameters	96	96
<i>R_p</i> (%)	2.256	2.615
<i>R_{exp}</i> (%)	2.116	2.243
<i>R_{wp}</i> (%)	3.155	3.433
<i>R_{Bragg}</i> (%)	1.022	1.181
χ^2	1.491	1.530

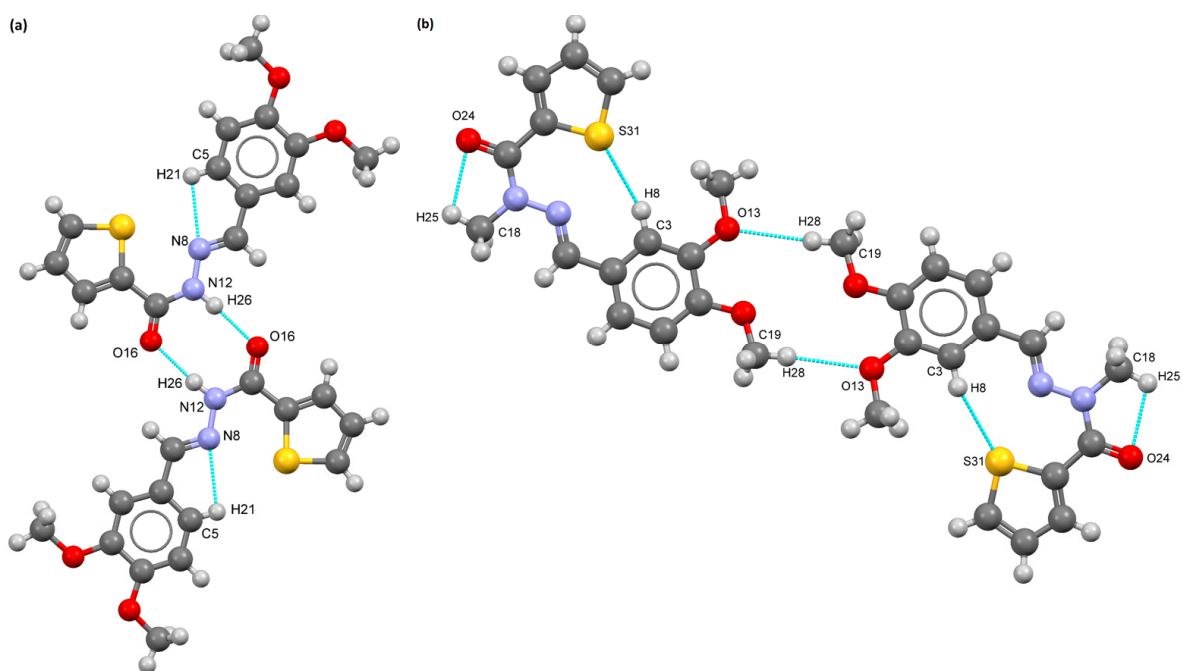


Figure S1. The formation of the crystalline aggregate of LASSBio-1834 (3) molecules (a) and LASSBio-1835 (4) (b) the inter- and intramolecular H-bonds (cyan dashed lines).

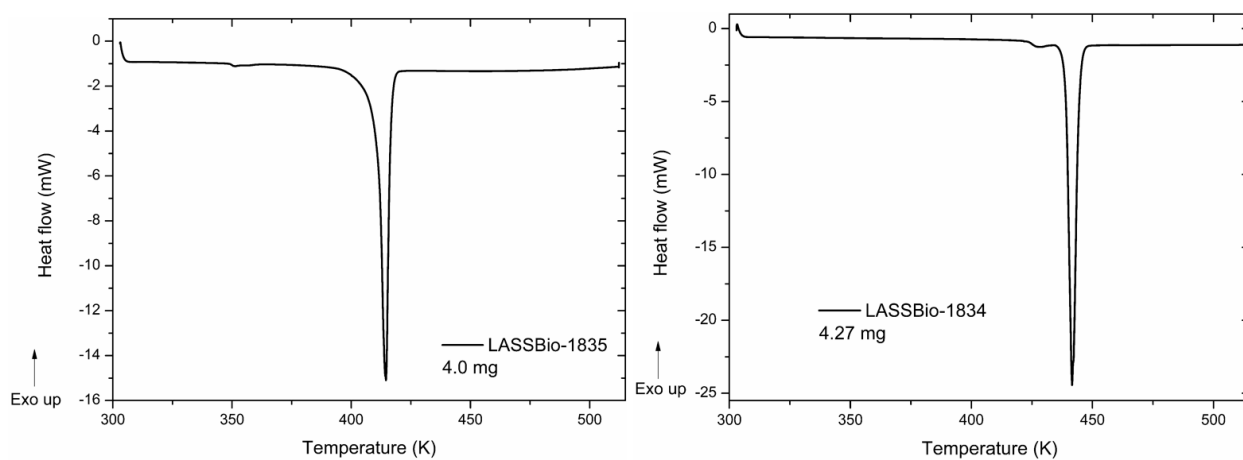


Figure S2. DSC curves of LASSBio-1834 (3) and LASSBio-1835 (4).

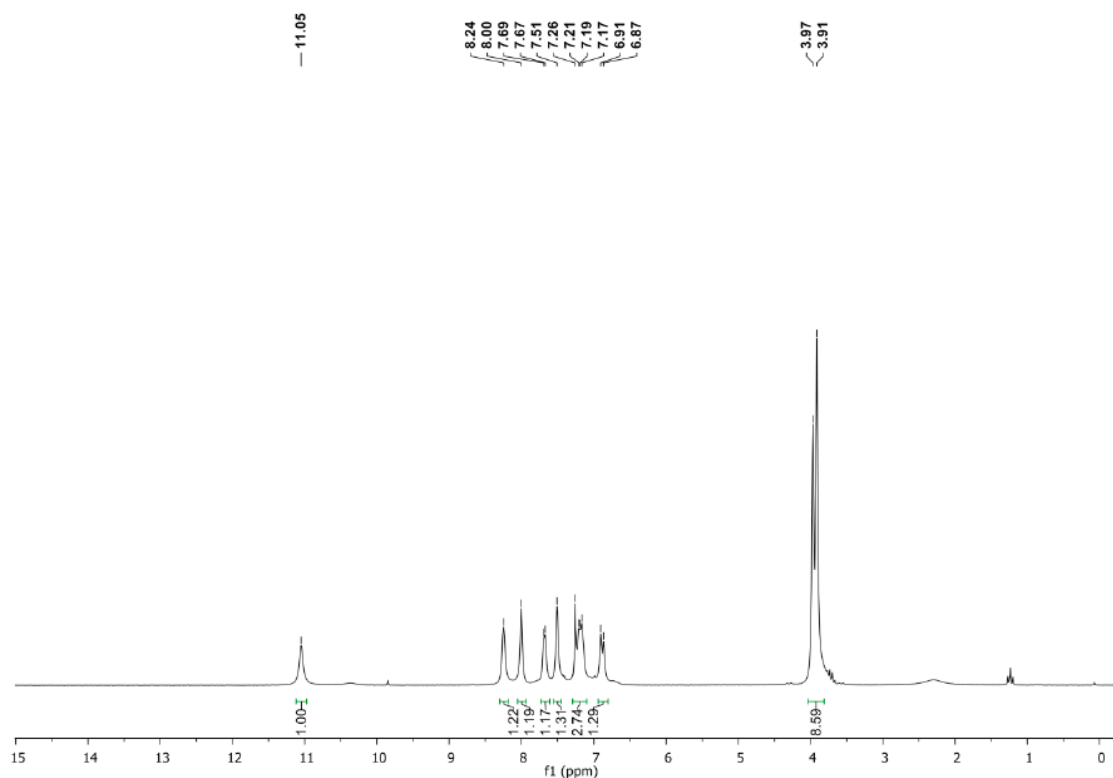


Figure S3. LASSBio-1834 (3) (¹H NMR, 200 MHz, CDCl₃).

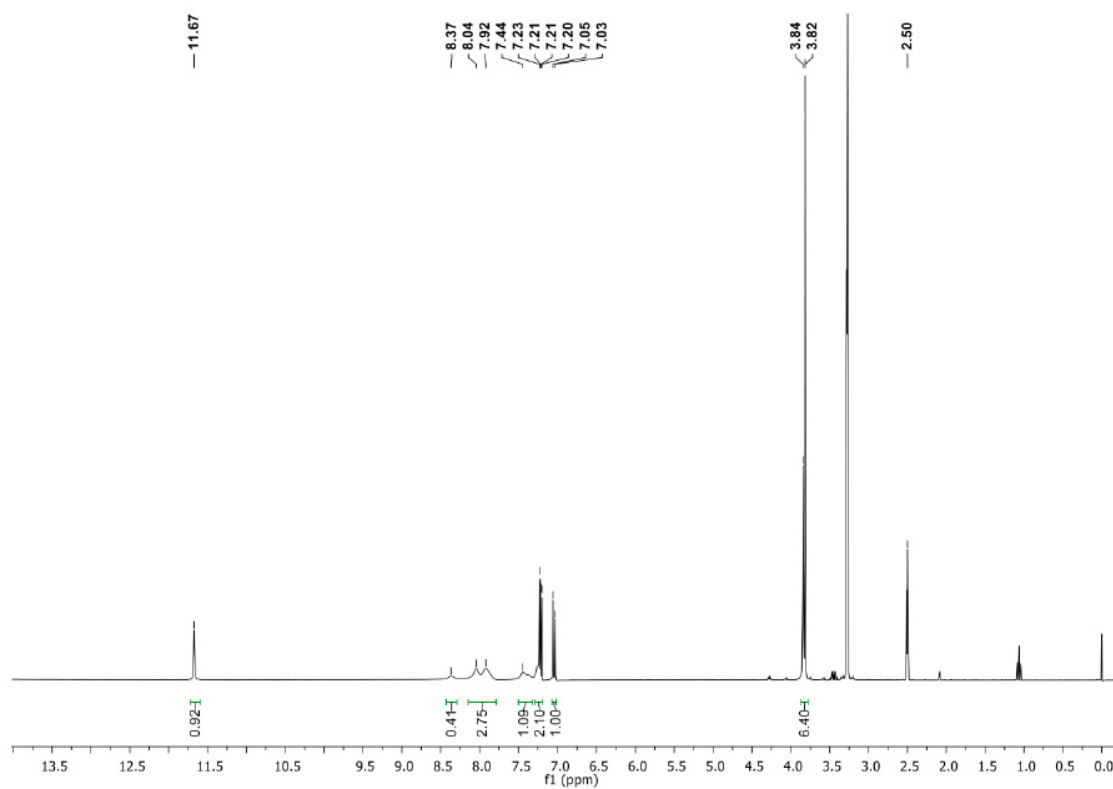


Figure S4. LASSBio-1834 (3) (¹H NMR, 300 MHz, DMSO-*d*₆).

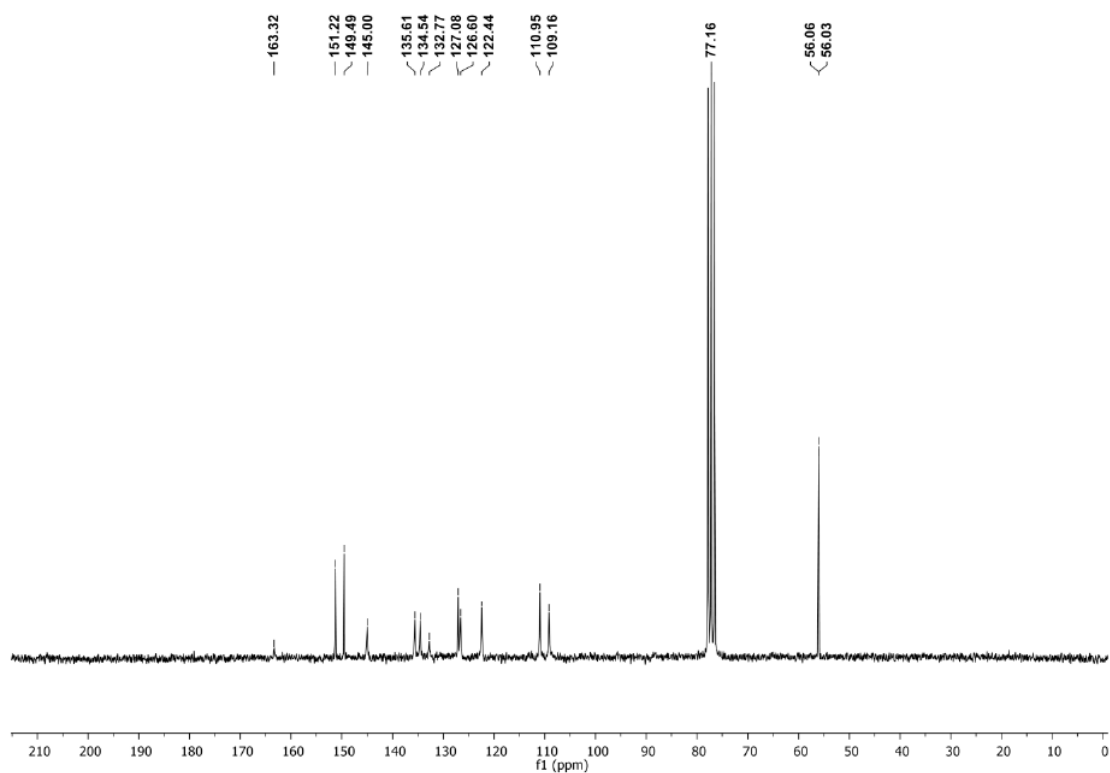


Figure S5. LASSBio-1834 (3) (^{13}C NMR, 50 MHz, CDCl_3).

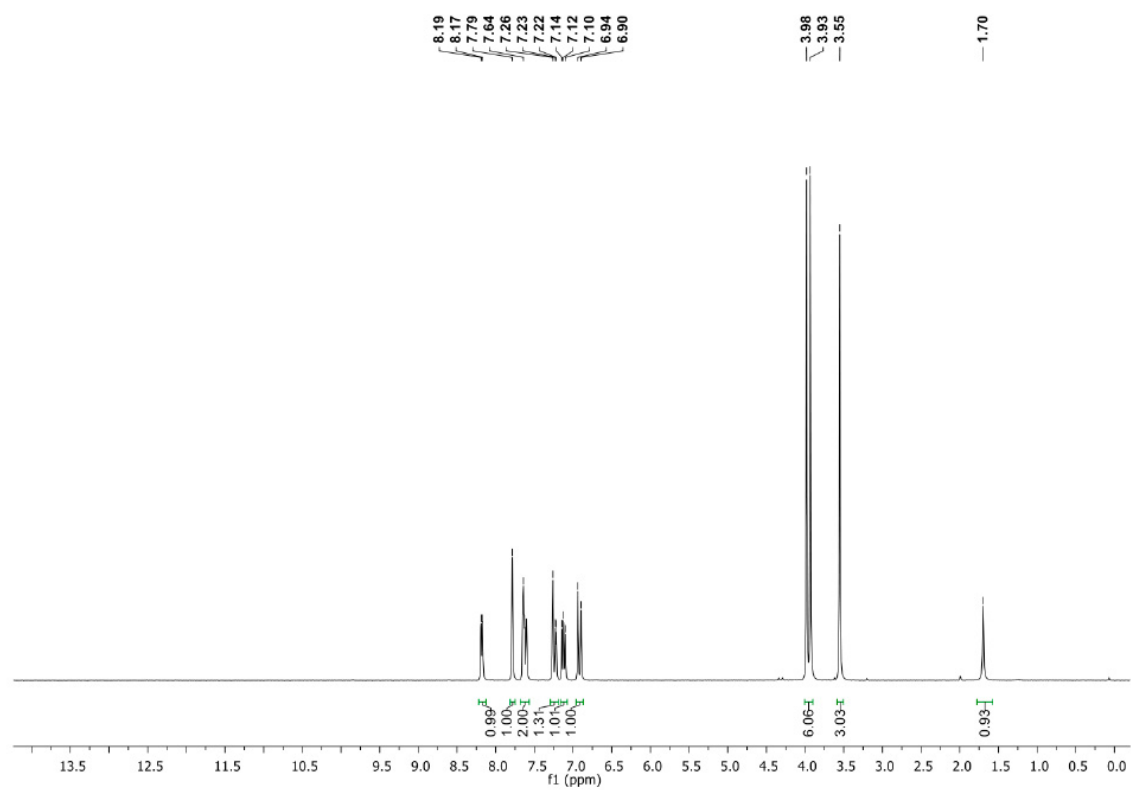


Figure S6. LASSBio-1835 (4) (^1H NMR, 200 MHz, CDCl_3).

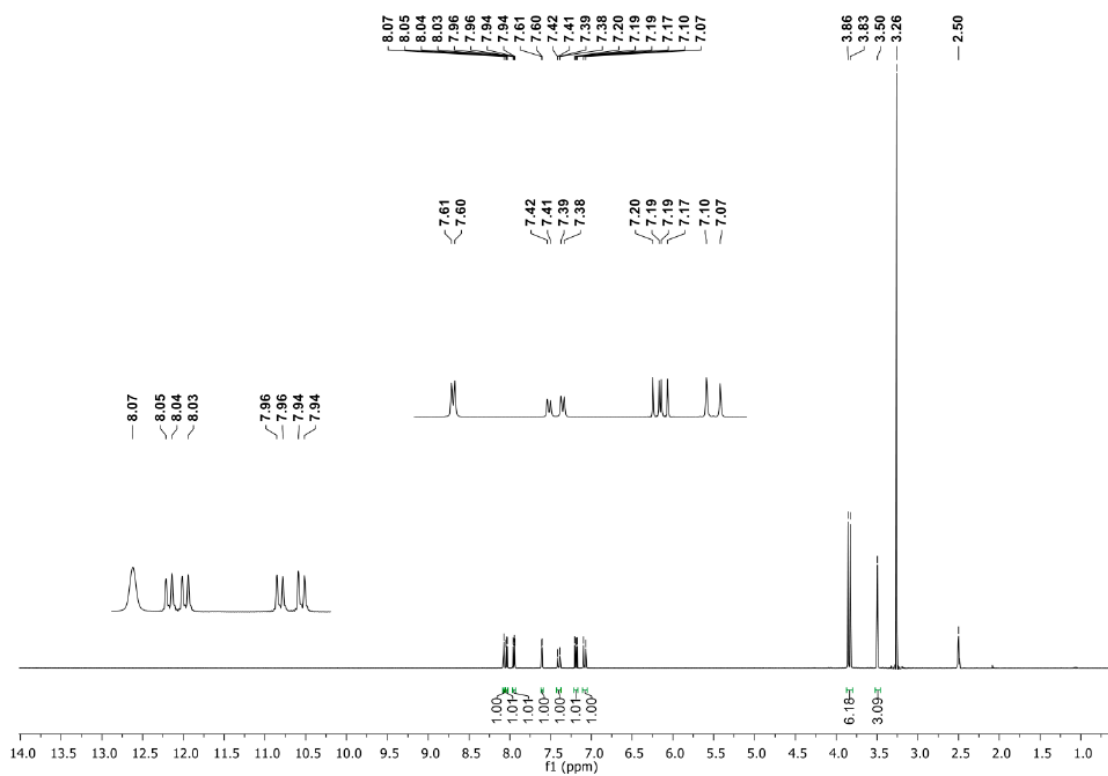


Figure S7. LASSBio-1835 (4) (¹H NMR, 300 MHz, DMSO-*d*₆).

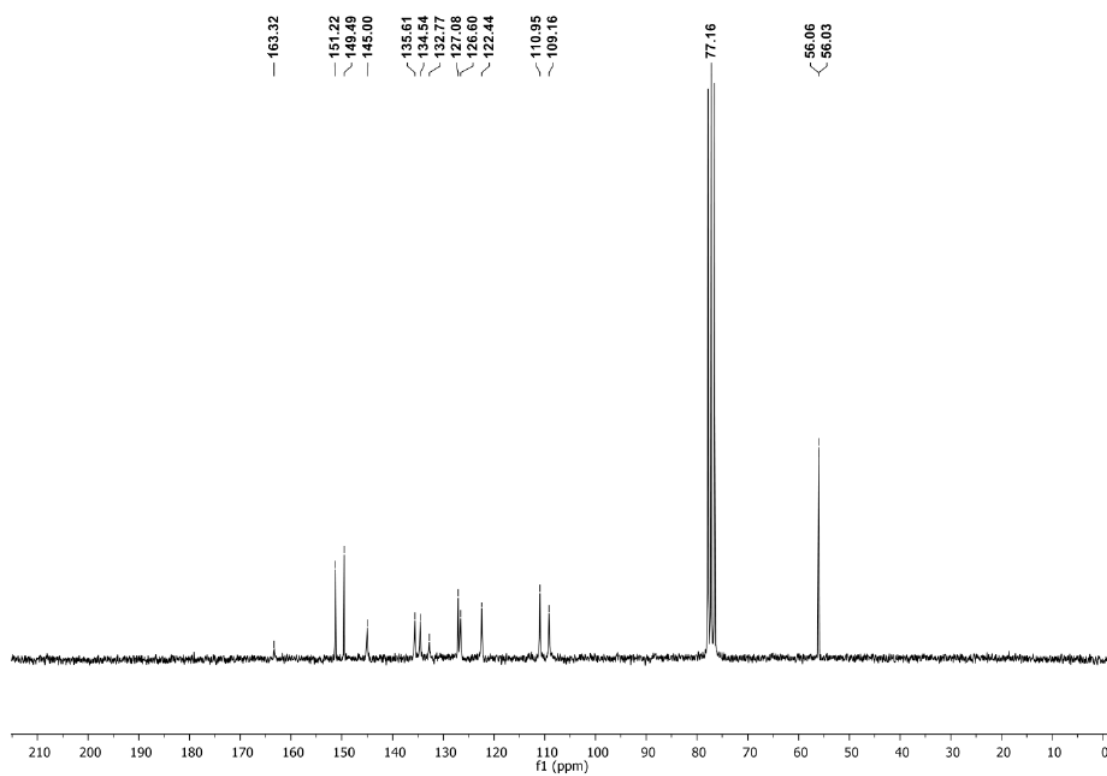


Figure S8. LASSBio-1835 (4) (¹³C NMR, 50 MHz, CDCl₃).

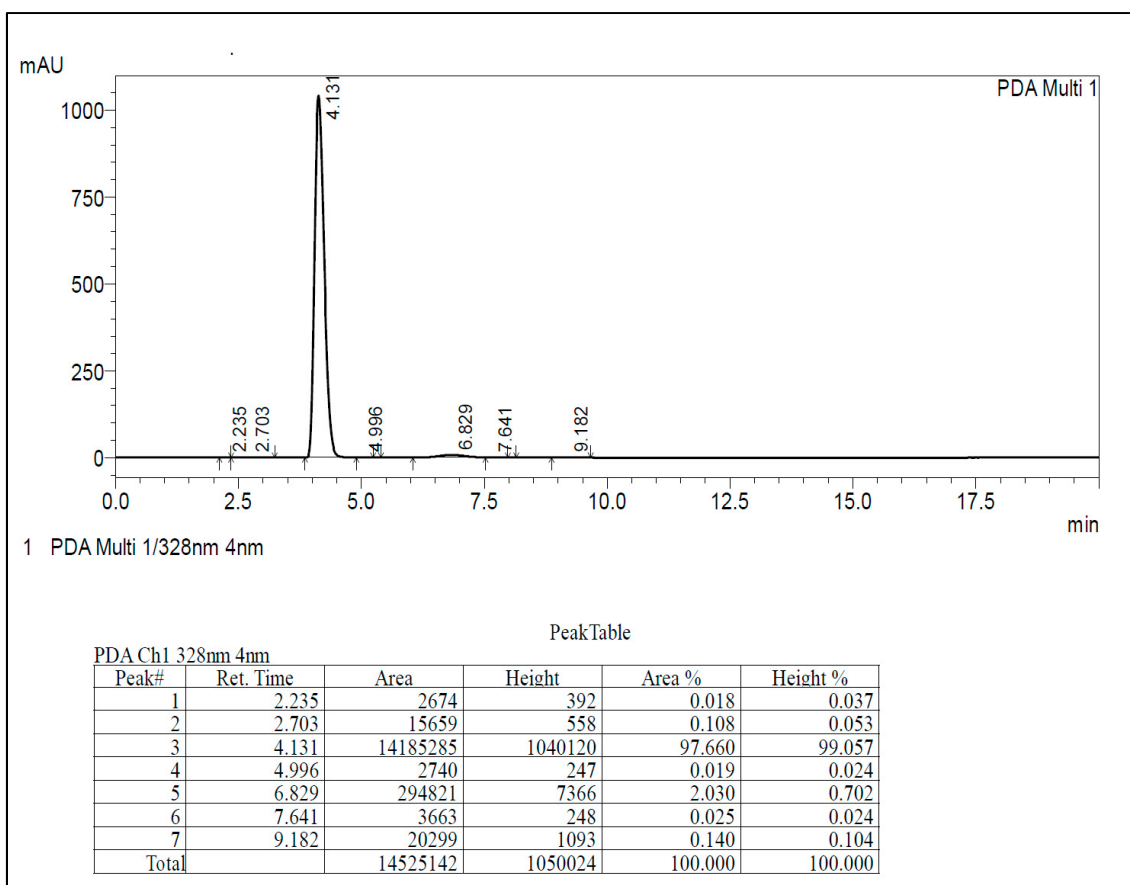


Figure S9. LASSBio-1834 (3) chromatogram.

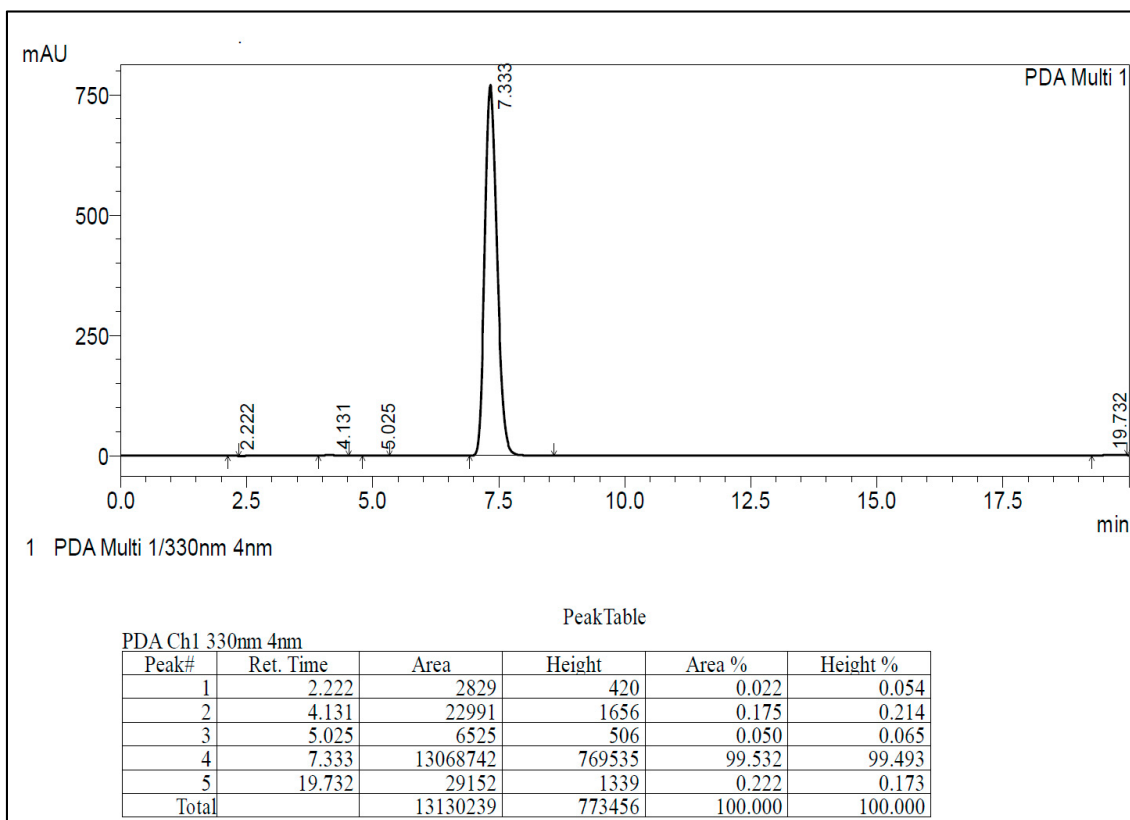


Figure S10. LASSBio-1835 (4) chromatogram.