

Supplementary Material

Antagonism of CGRP signaling by rimegepant at two receptors

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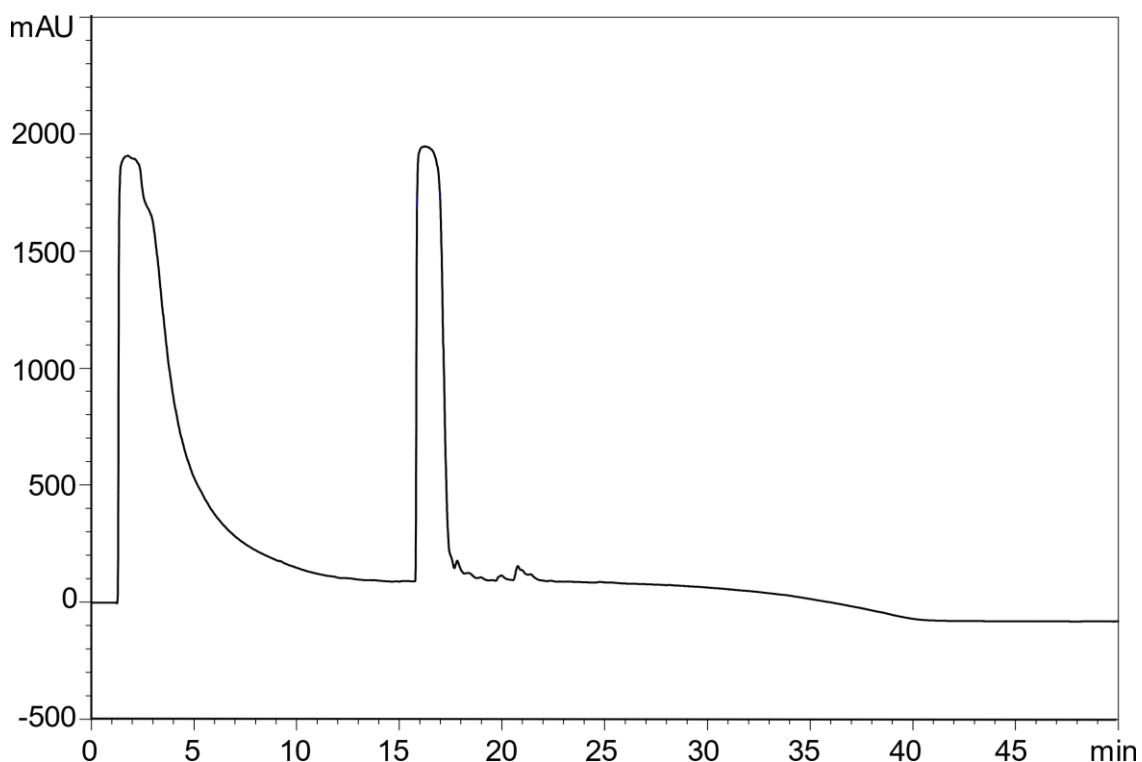
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Christopher Walker

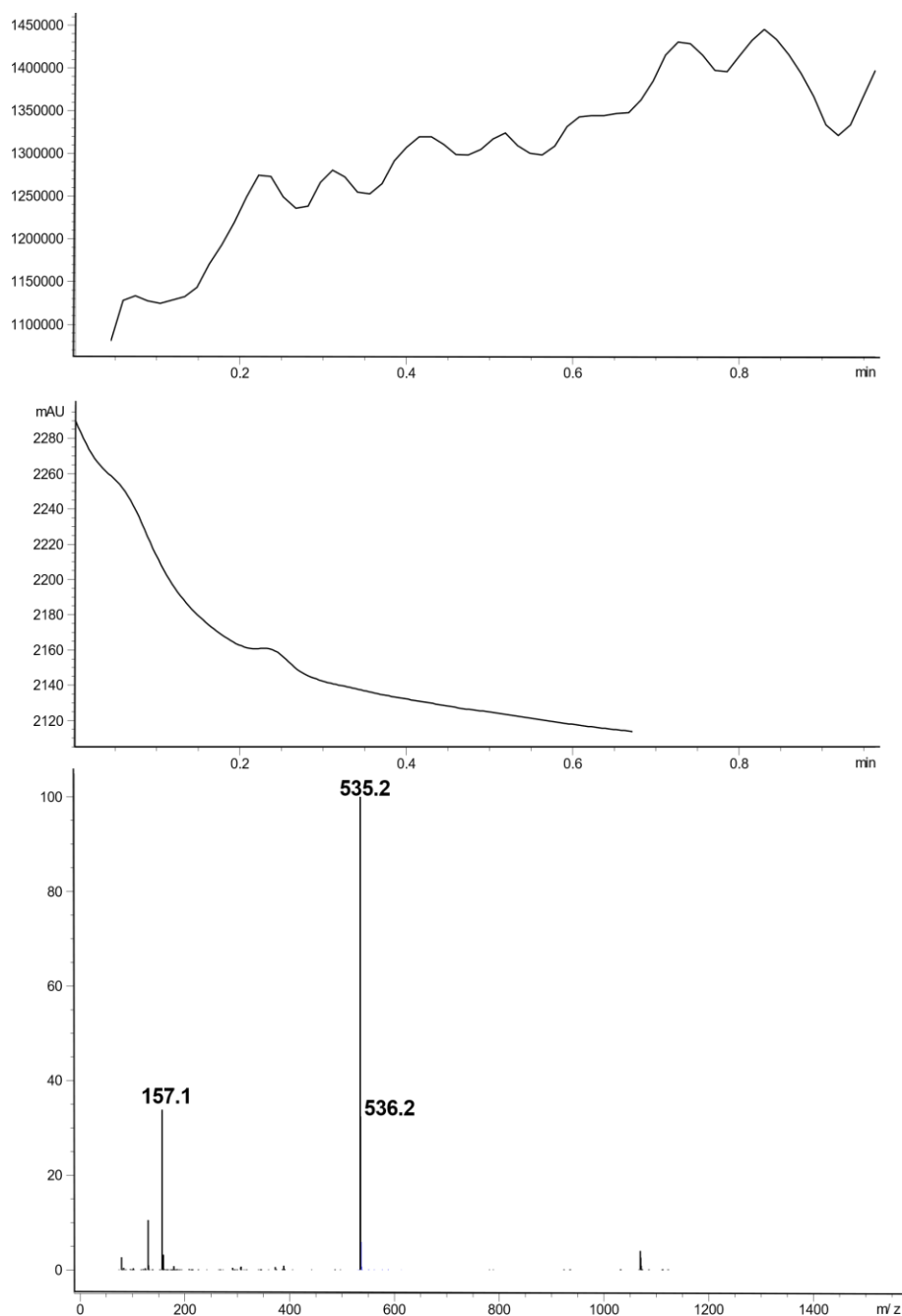
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Supplemental Figure 1. Analytical RP-HPLC chromatogram of rimegepant (BMS-927711), $t_R = 16.2$ min. Chromatographic separations were performed on a Thermo Scientific Dionex Ultimate 3000 HPLC using a Agilent C3, (3.5 μm ; 3.0 \times 150 mm) at a flow rate of 0.3 mL min⁻¹ and a linear gradient of 5-95% B in 50 min at room temperature, *ca.* 2% B per min at a flow rate of 0.3 mL/min. Buffer A: H₂O containing 0.1% TFA (v/v); Buffer B: acetonitrile containing 0.1% TFA (v/v). The peak at 2-5 min corresponds to the absorption of CH₂Cl₂ (solvent).



Supplemental Figure 2. ESI-MS profile of rimegepant (BMS-927711); Ion polarity positive, 25 eV. ESI-MS (m/z $[M+H]^+$ calculated: 535.5; found: 535.2). The ESI-MS data is consistent with previous reports¹.

1. Luo G, Chen L, Conway CM, Denton R, Keavy D, Signor L, et al. Discovery of (5S,6S,9R)-5-amino-6-(2,3-difluorophenyl)-6,7,8,9-tetrahydro-5H-cyclohepta[b]pyridin-9-yl 4-(2-oxo-2,3-dihydro-1H-imidazo[4,5-b]pyridin-1-yl)piperidine-1-carboxylate (BMS-927711): an oral calcitonin gene-related peptide (CGRP) antagonist in clinical trials for treating migraine. *Journal of medicinal chemistry*. 2012;55(23):10644-51.