

Supplementary Information

Synthesis and preclinical evaluation of a novel fluorine-18 labeled small-molecule PET radiotracer for imaging of CXCR3 receptor in mouse models of atherosclerosis

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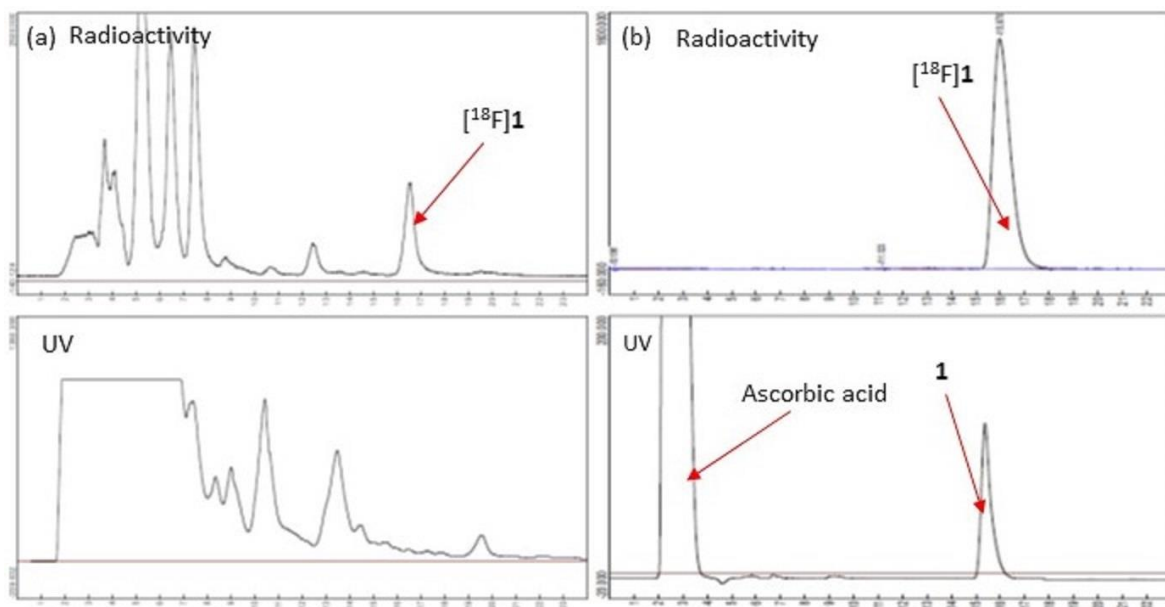


Figure S1. (a) The semi-preparative HPLC of $[^{18}\text{F}]\mathbf{1}$ and (b) The analytical HPLC of $[^{18}\text{F}]\mathbf{1}$. Co-injection of nonradioactive standard $\mathbf{1}$ confirmed that the collected product was authentic.

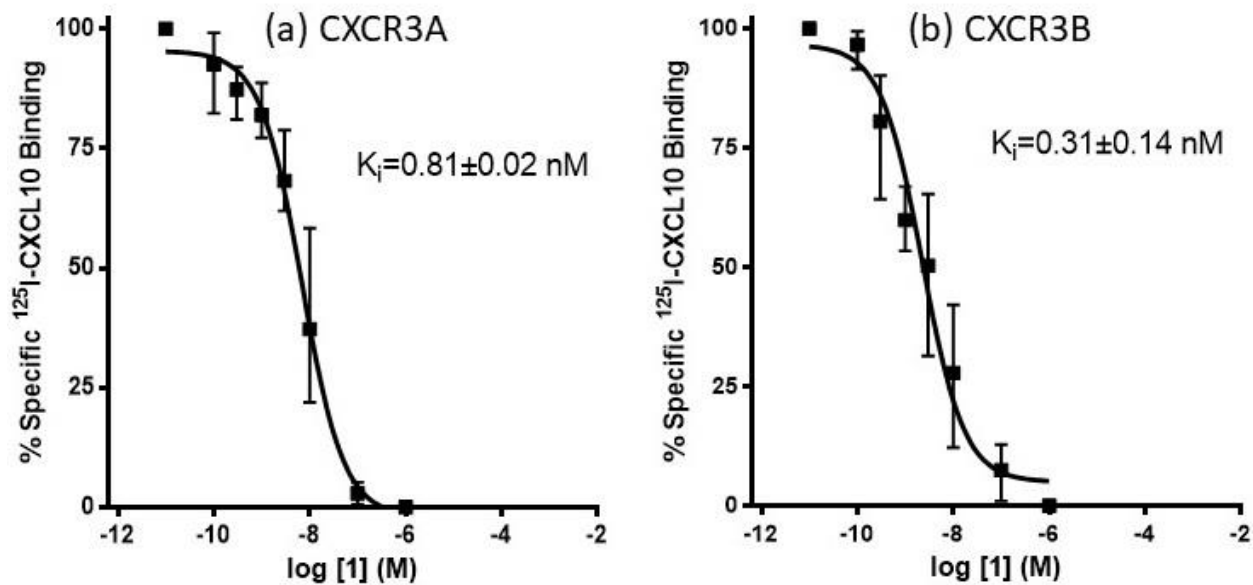


Figure S2. Competitive binding curves of cell-binding assays of compound $\mathbf{1}$ for (a) CXCR3A and (b) CXCR3B

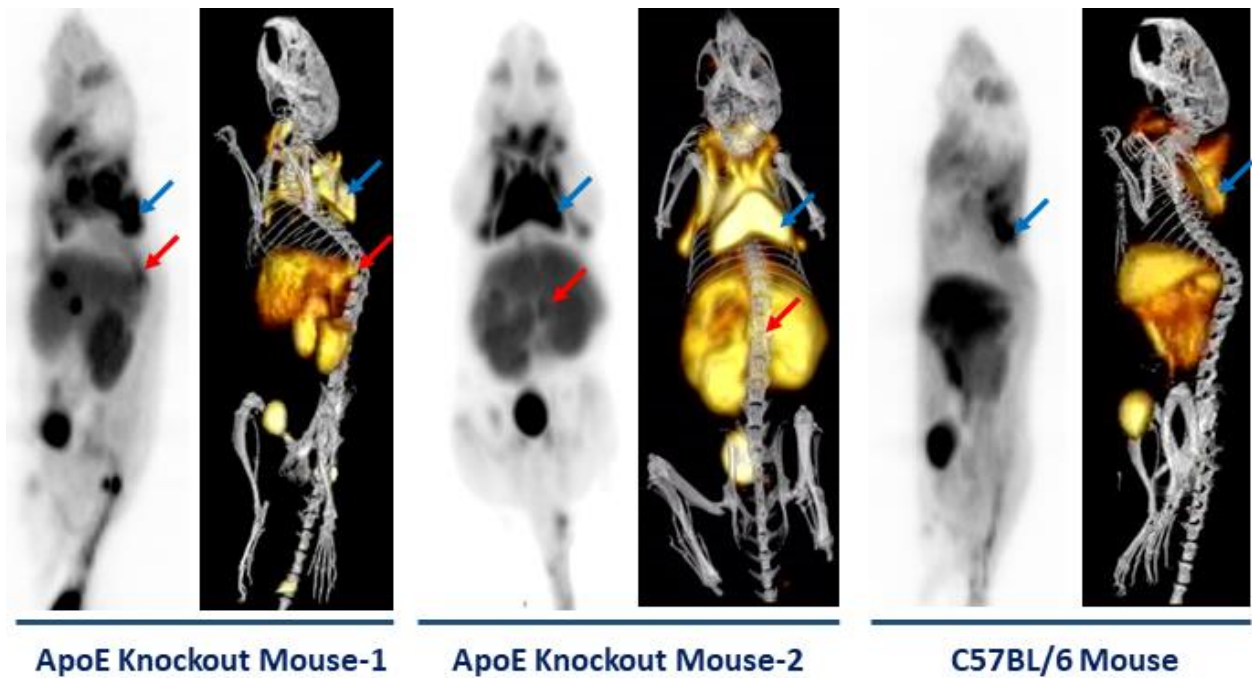
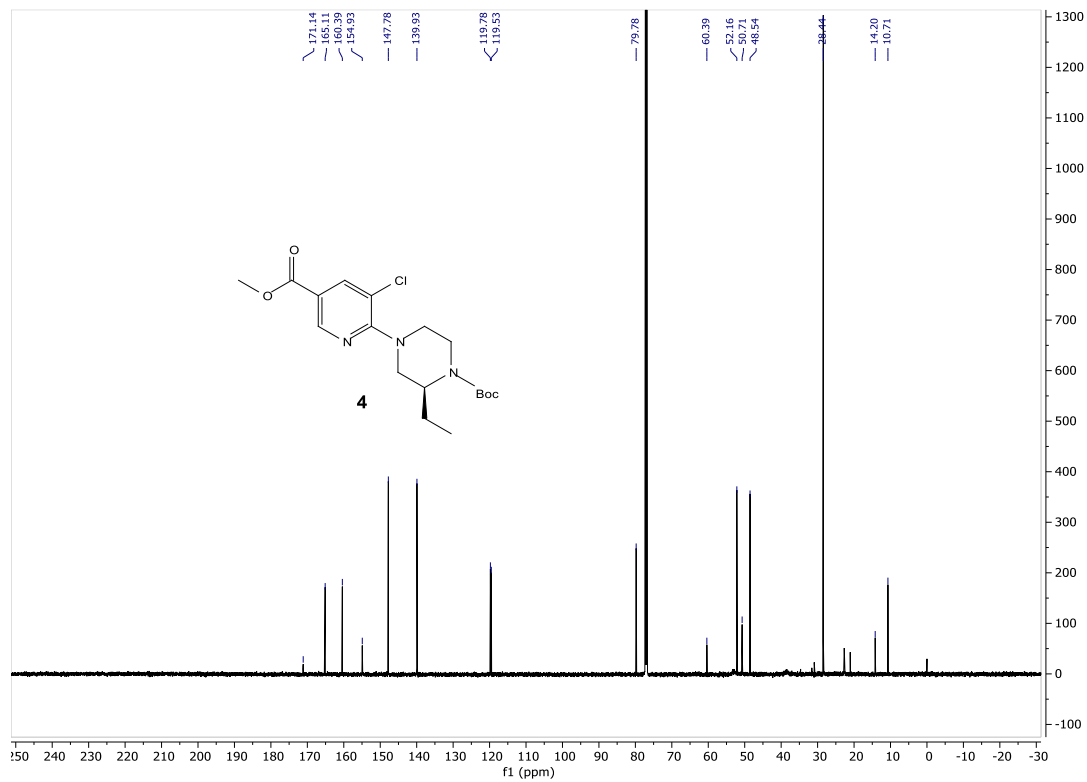
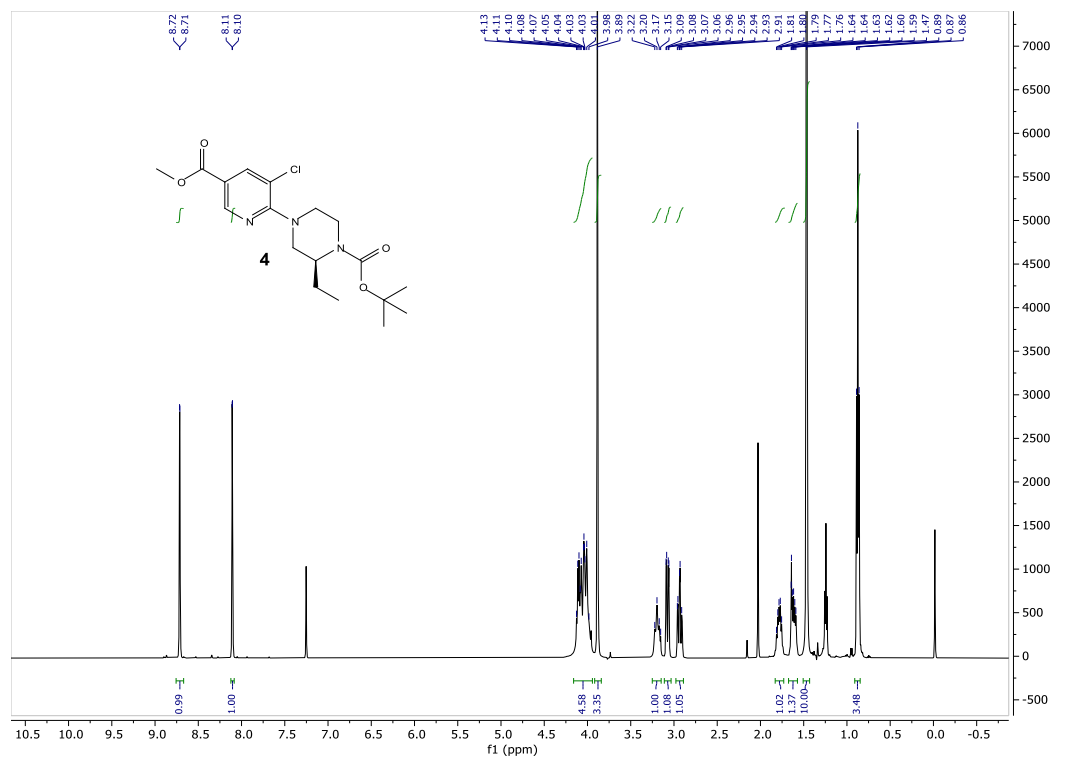


Figure S3. Baseline PET and PET/CT images of two ApoE knockout mice and a C57BL/6 control mouse presented in Figure 3. Atherosclerotic lesions and brown adipose tissues are indicated by red arrows and blue arrows, respectively.

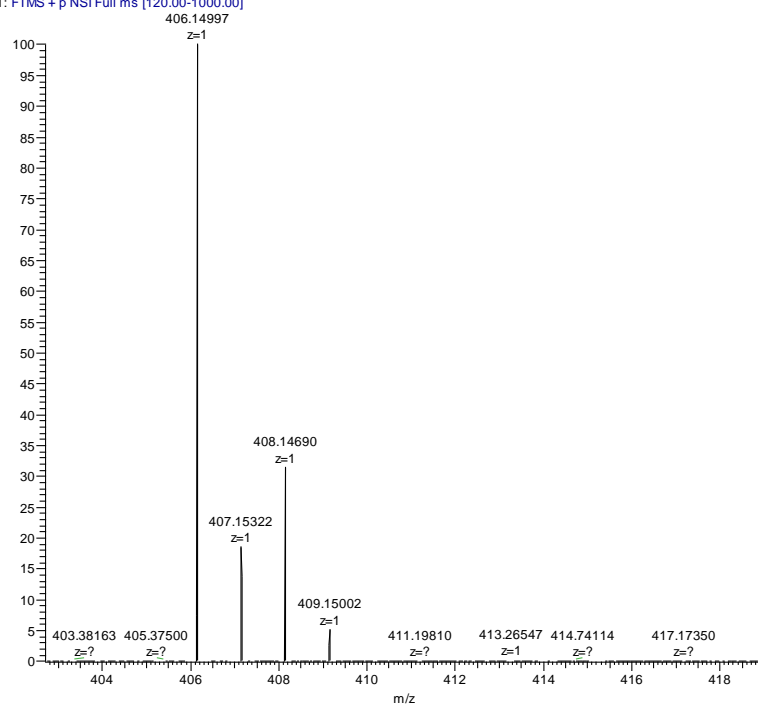
Figure S4. NMR and Mass spectra

(a) Methyl (S)-6-(4-(tert-butoxycarbonyl)-3-ethylpiperazin-1-yl)-5-chloronicotinate (4)

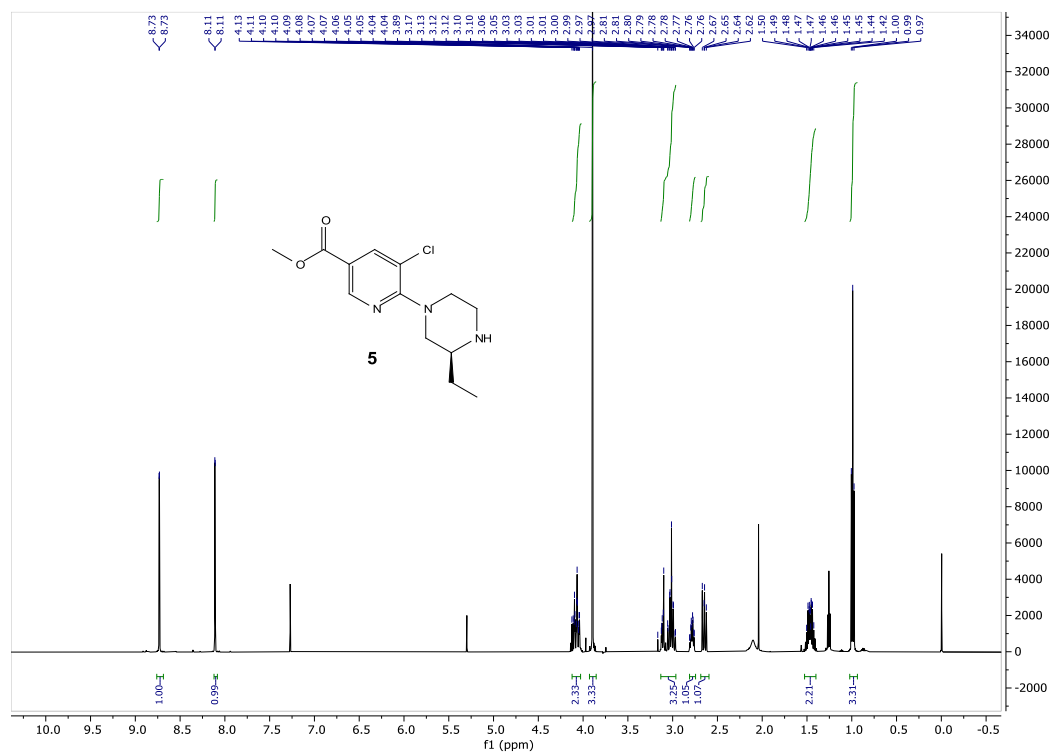


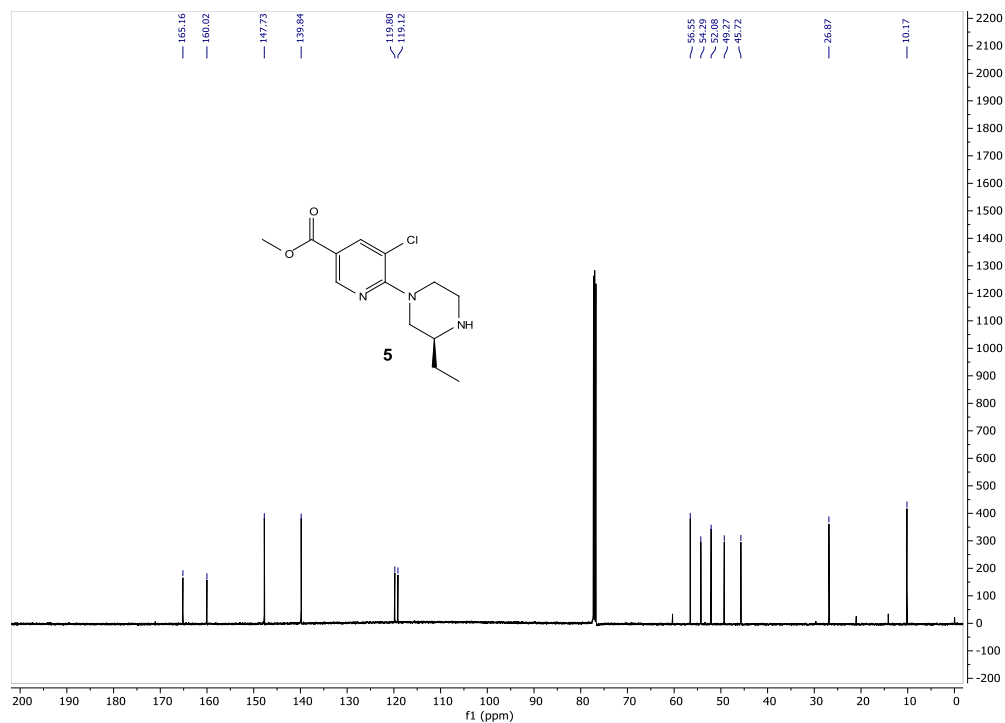
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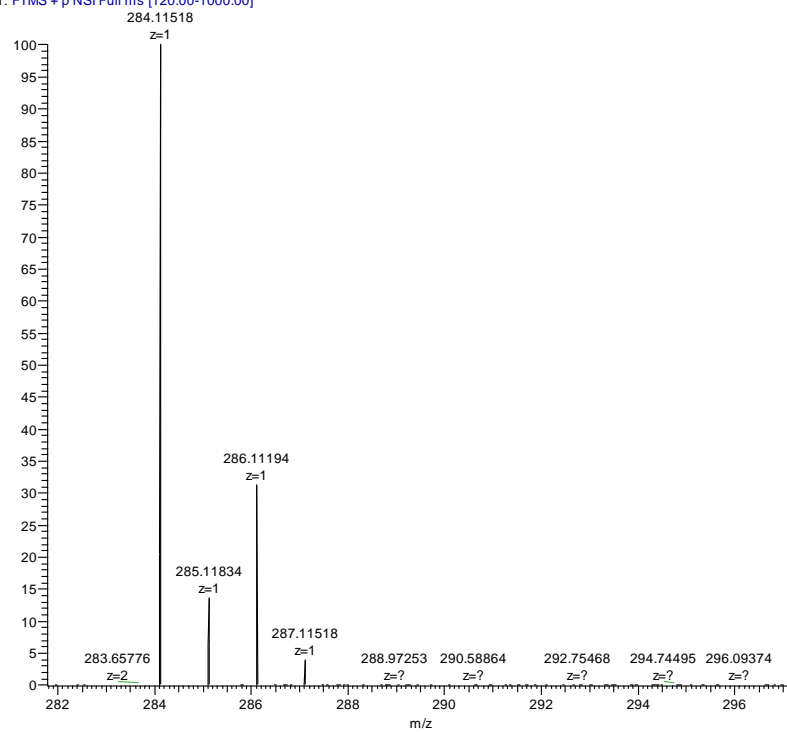


(b) Methyl (S)-5-chloro-6-(3-ethylpiperazin-1-yl)nicotinate (5)

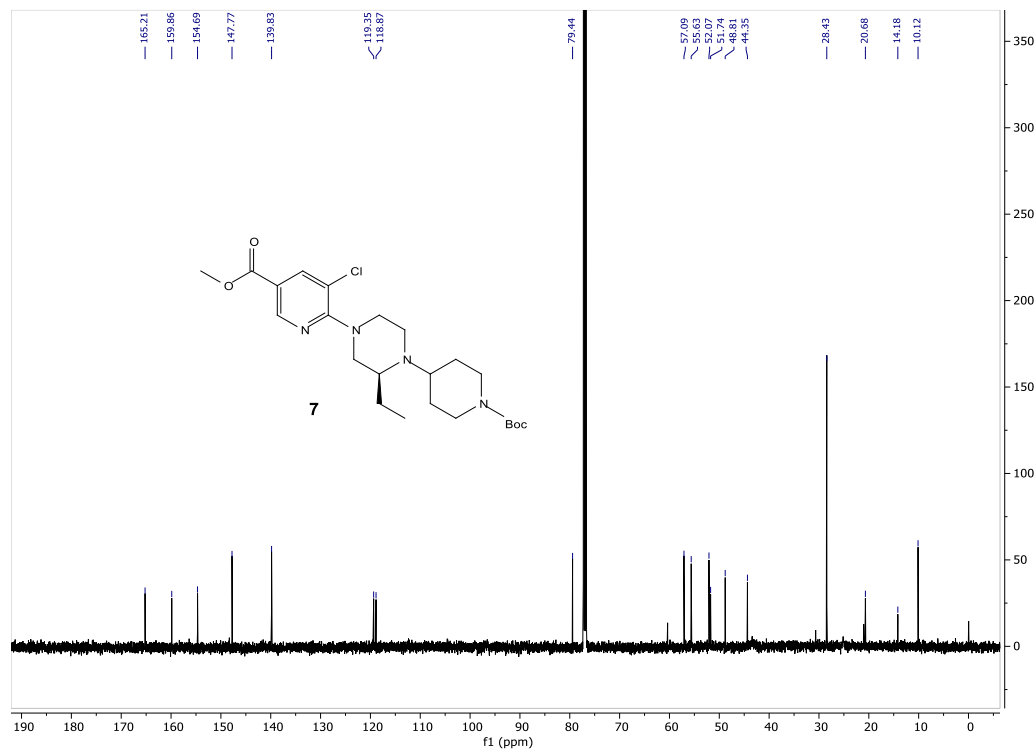
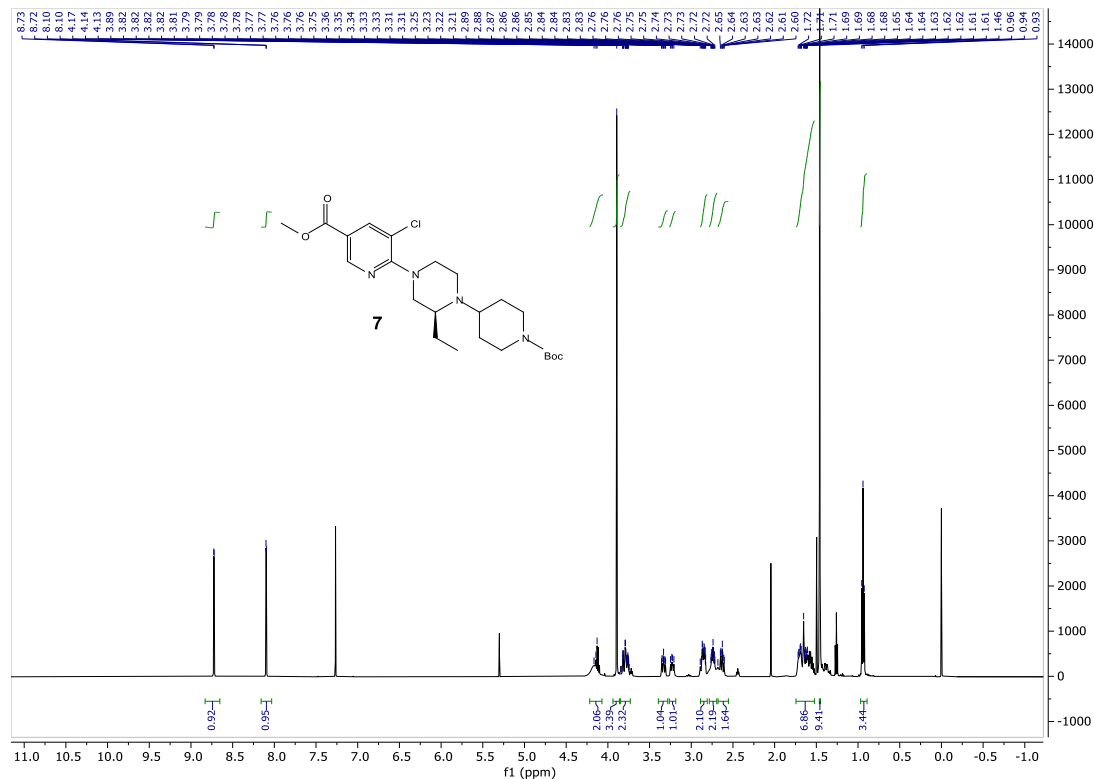


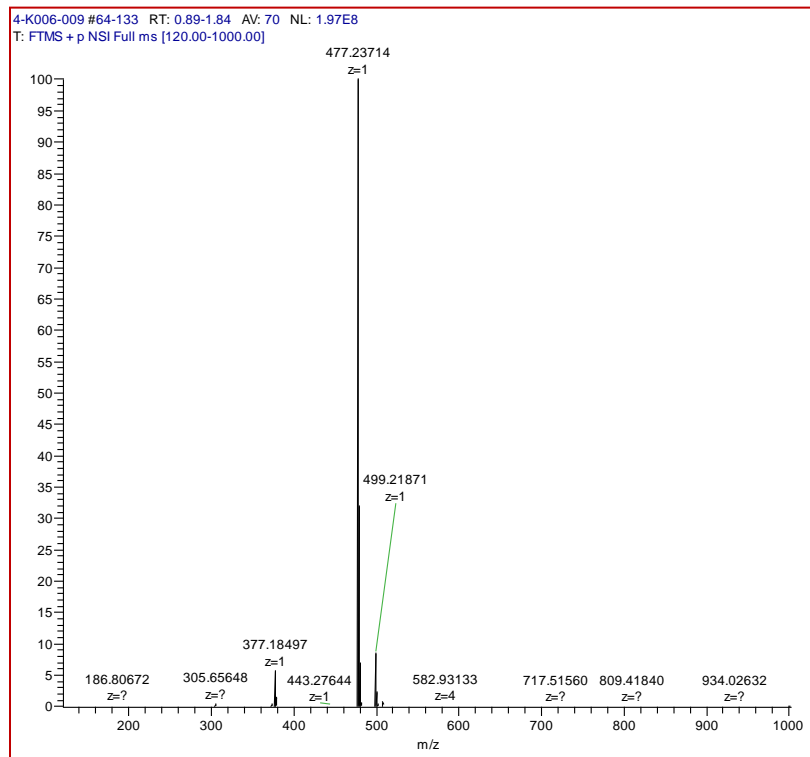
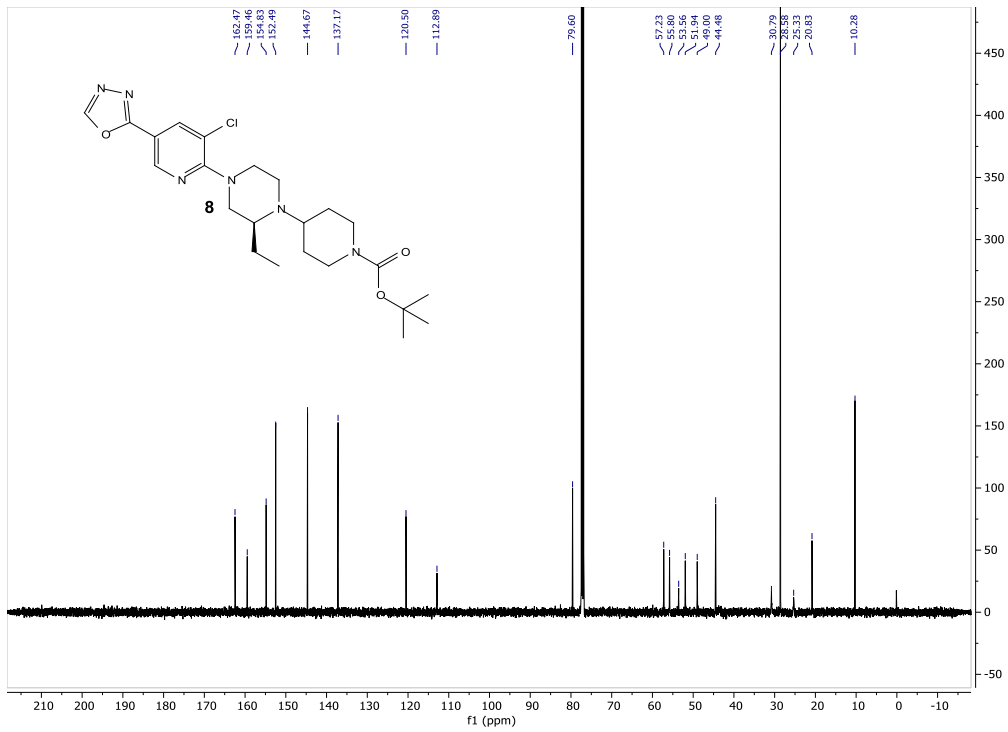


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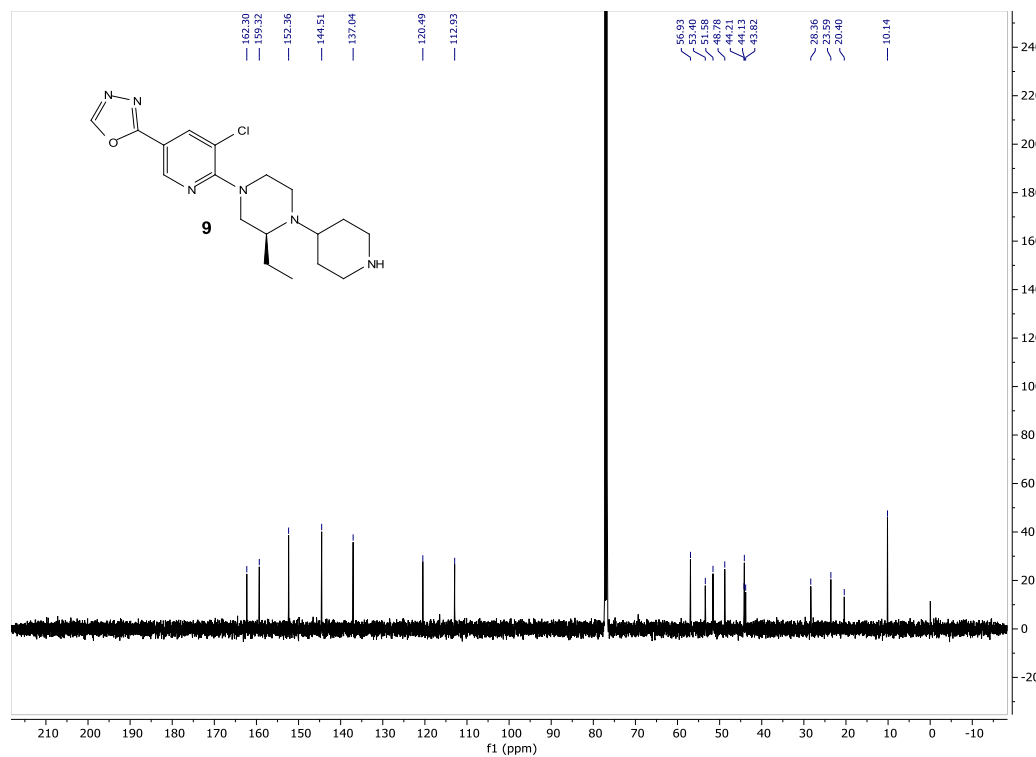
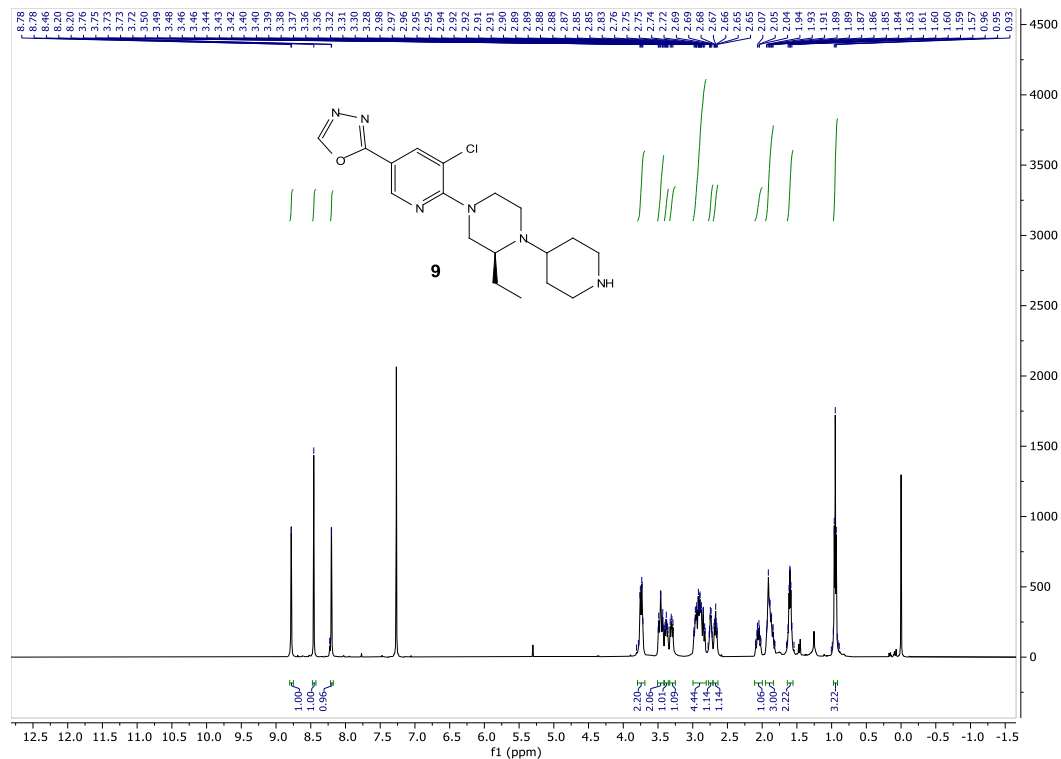


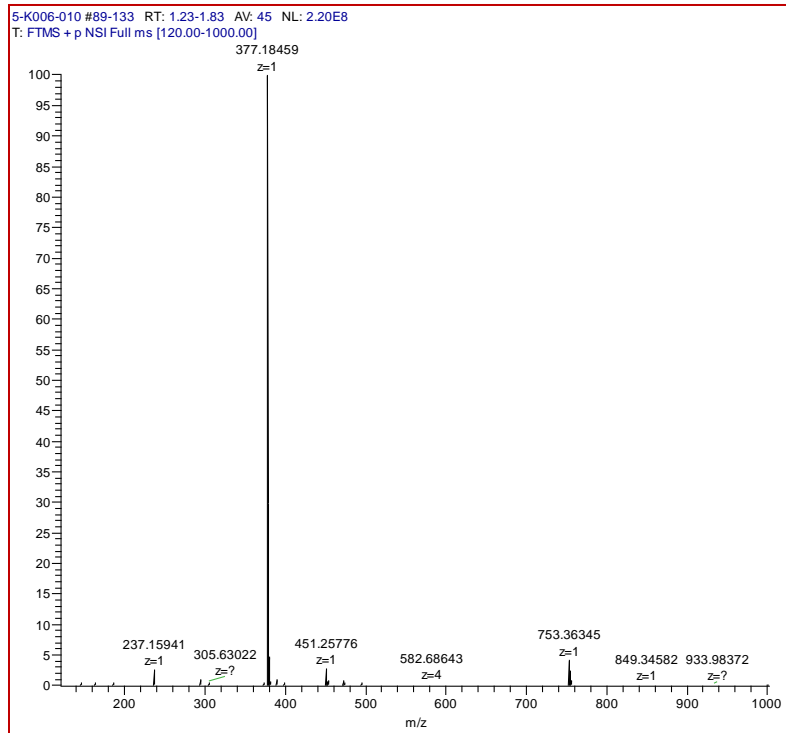
(c) Methyl (S)-6-(4-(1-(tert-butoxycarbonyl)piperidin-4-yl)-3-ethylpiperazin-1-yl)-5-chloronicotinate (7)



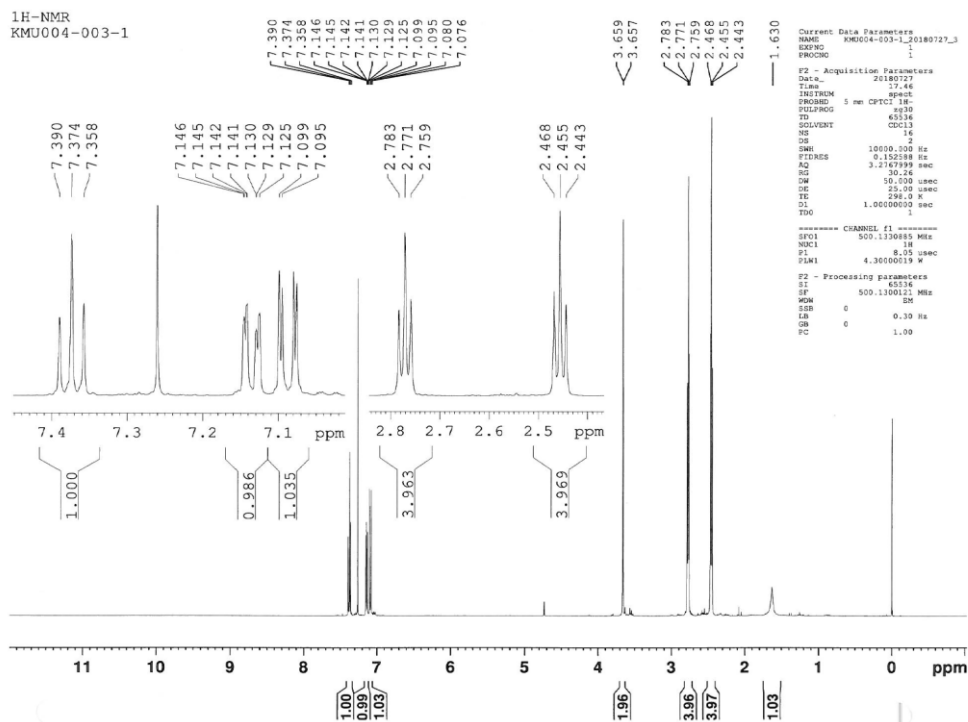


(e) (S)-2-(5-Chloro-6-(3-ethyl-4-(piperidin-4-yl)piperazin-1-yl)pyridin-3-yl)-1,3,4-oxadiazole
 (9)

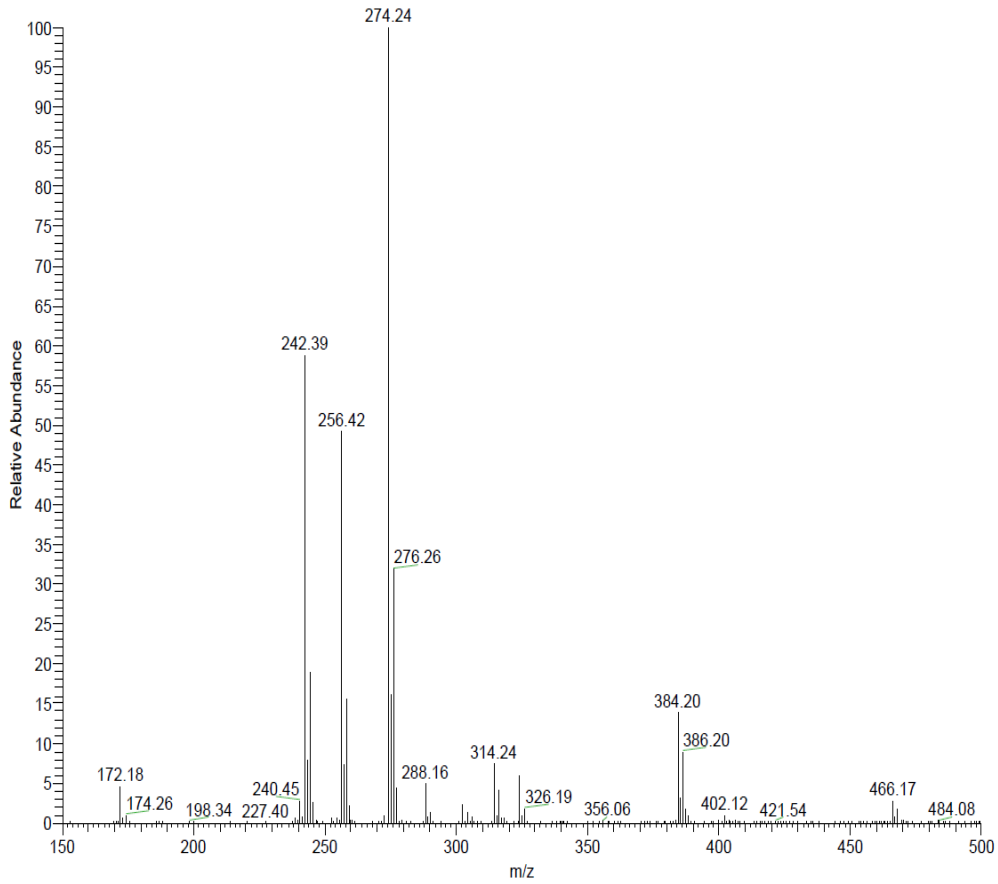
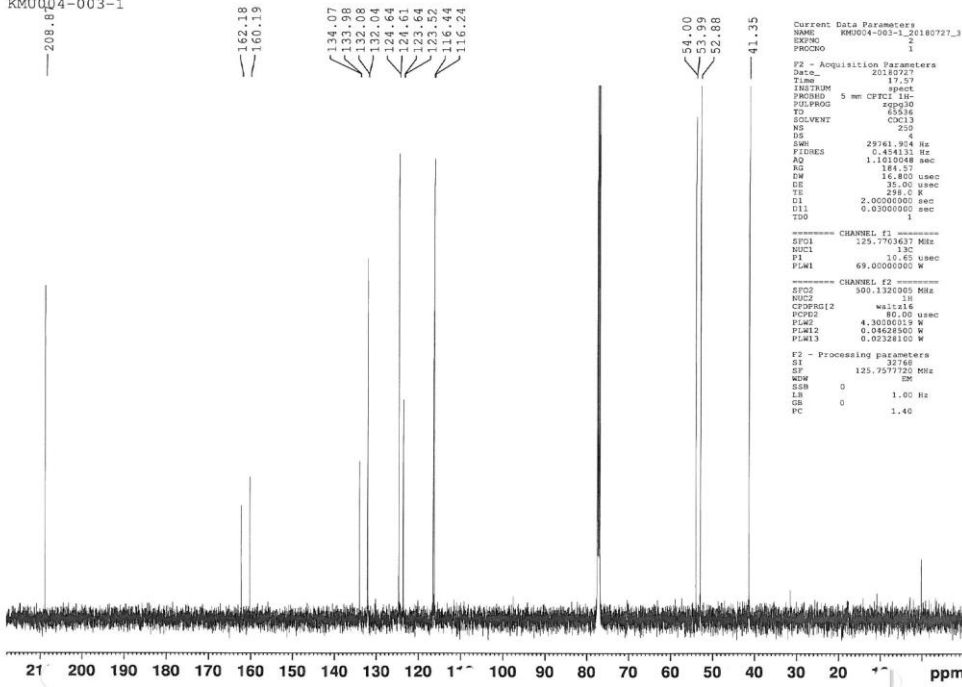




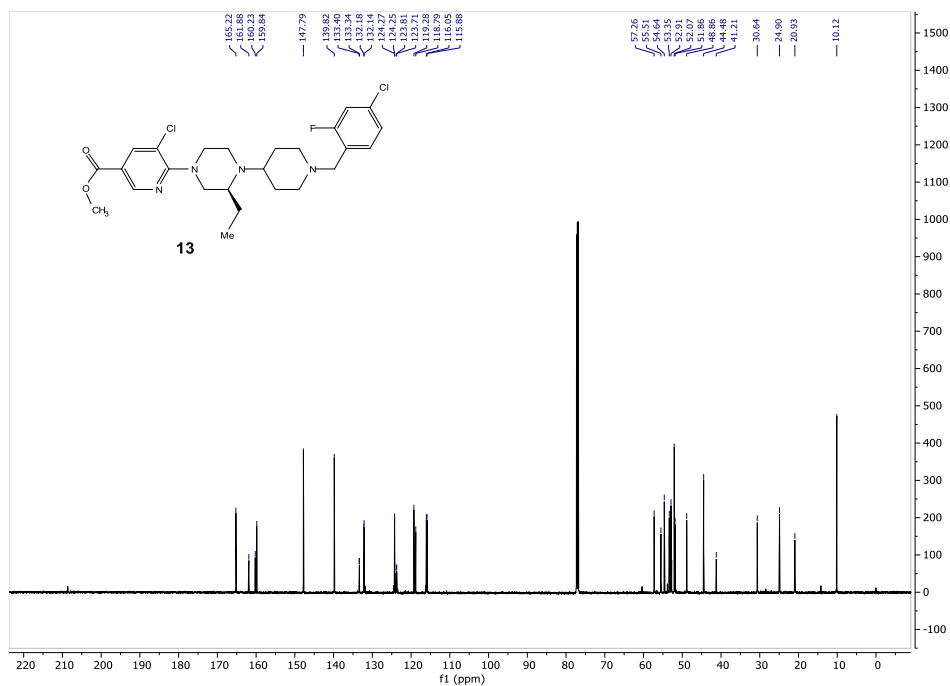
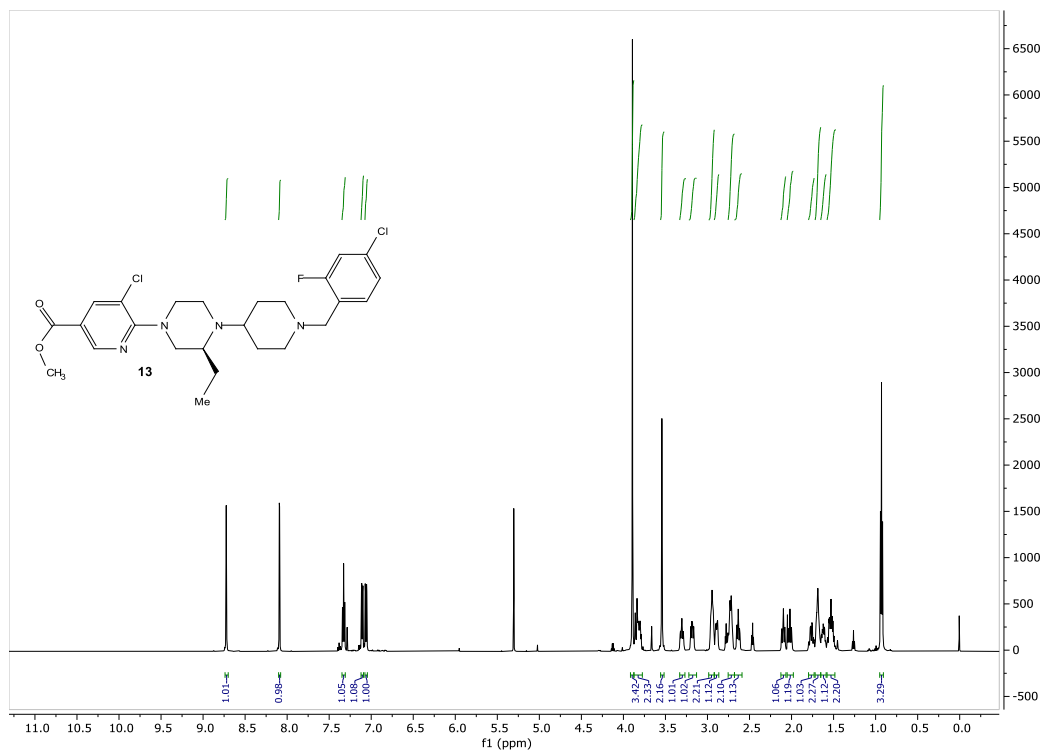
(f) *N*-(4-Chloro-2-fluorobenzyl)-4-piperidinone (12)

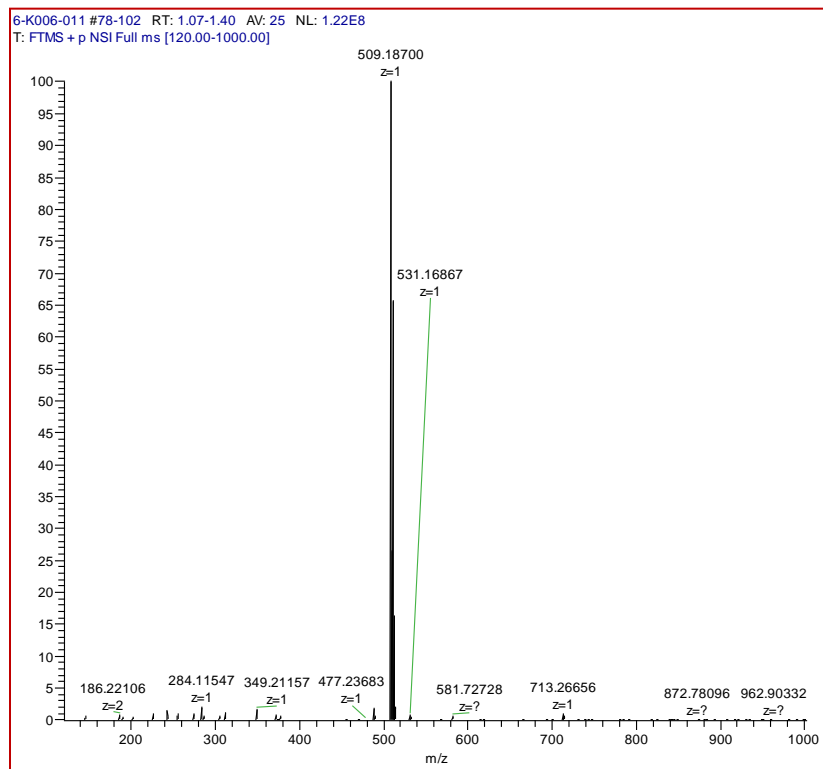
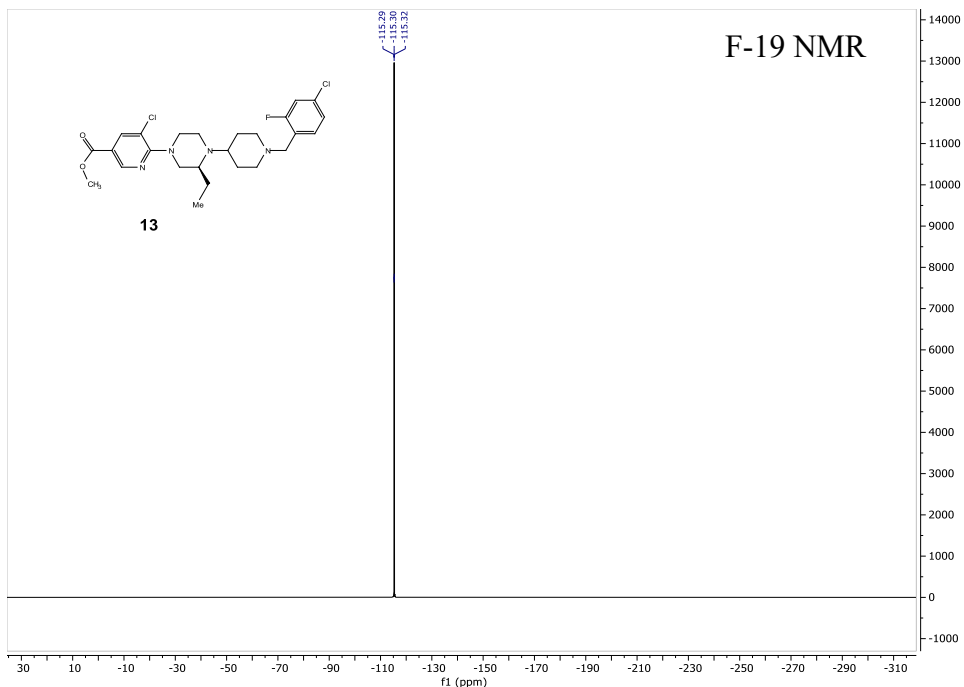


13C-NMR
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(g) Methyl (S)-5-chloro-6-(4-(1-(4-chloro-2-fluorobenzyl)piperidin-4-yl)-3-ethylpiperazin-1-yl)nicotinate (13)





(h) (S)-2-(5-chloro-6-(4-(1-(4-chloro-2-fluorobenzyl)piperidin-4-yl)-3-ethylpiperazin-1-yl)pyridin-3-yl)-1,3,4-oxadiazole (1)

