Supplementary Material

Synthesis of a lysosome-targeting aminoferrocene-based prodrug NCure2

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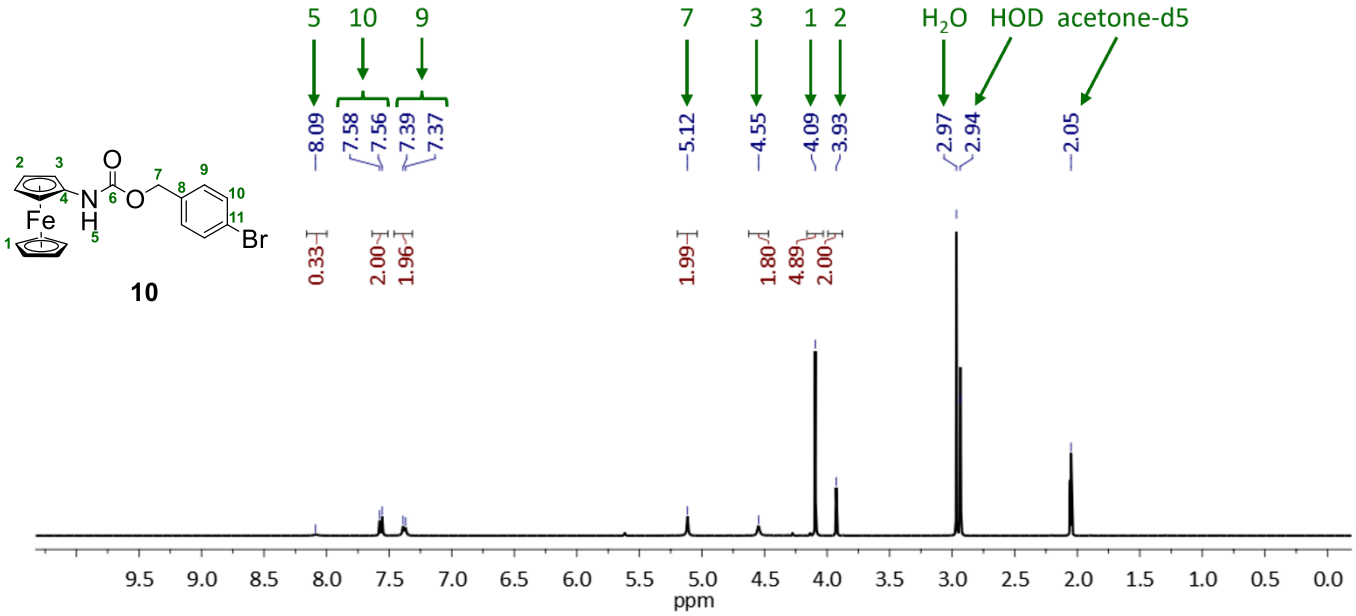
Table of Contents

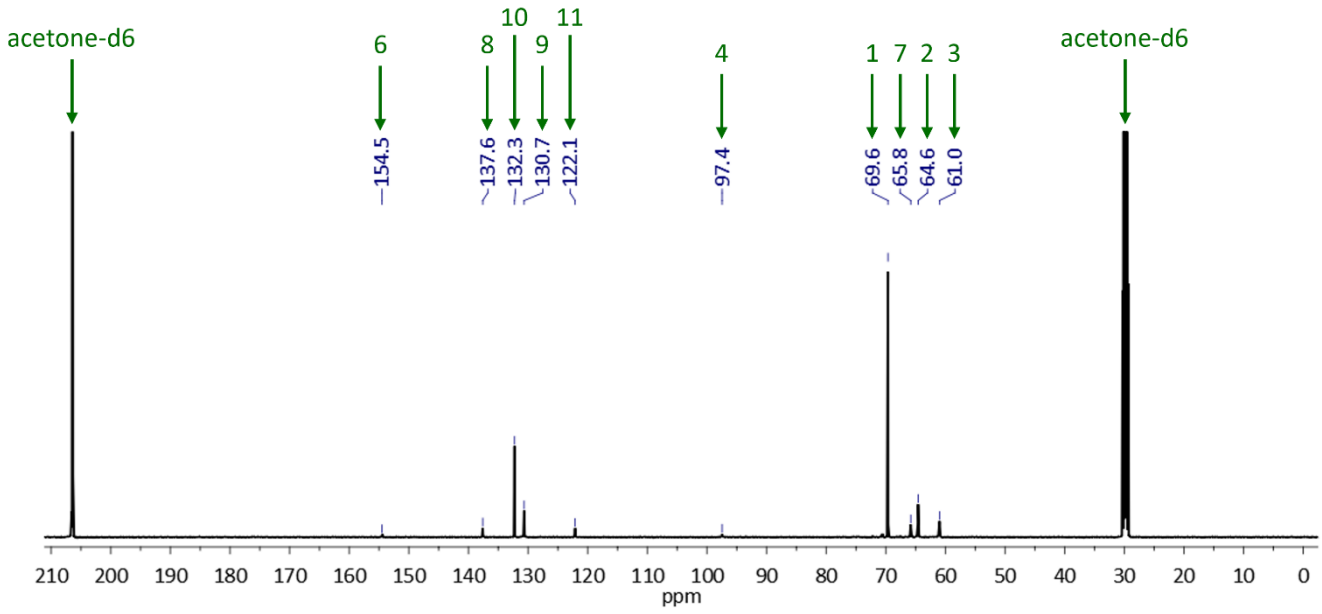
1. NMR Spectra

^{1}H NMR spectrum of 4-bromobenzyl (ferrocenyl)carbamate (**10**, acetone-d6, 400 MHz):

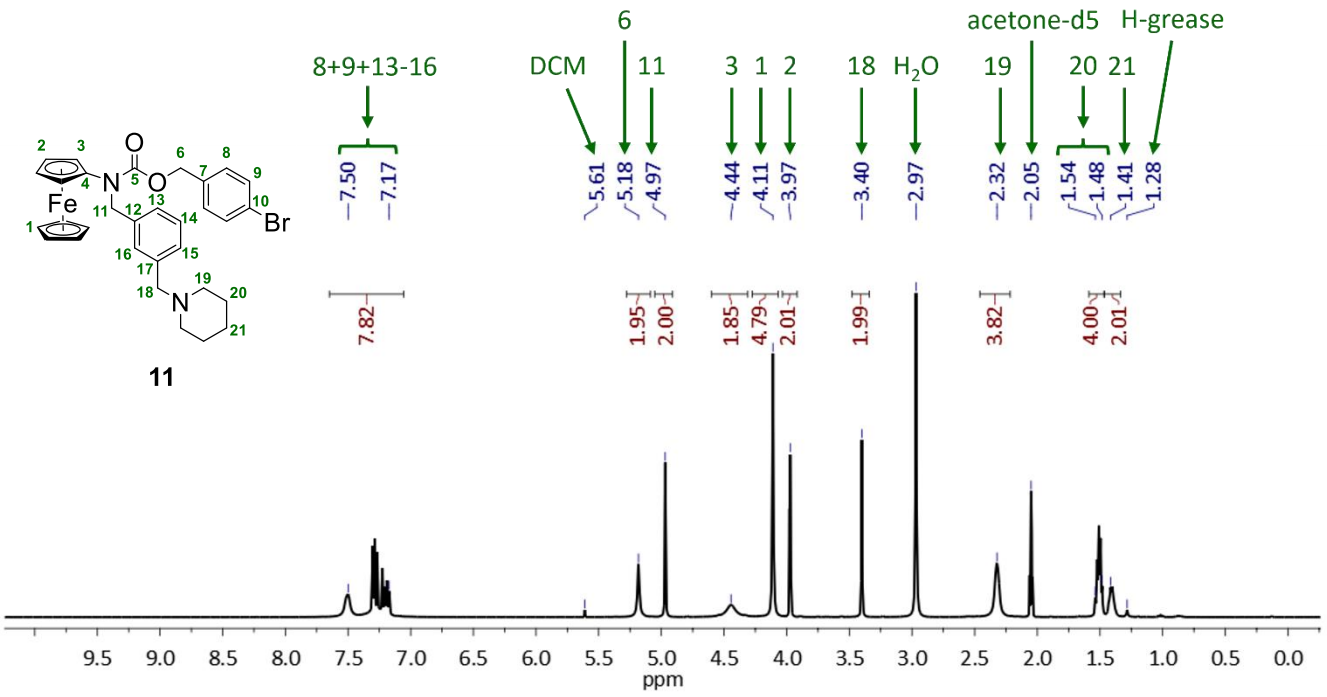


10

^{13}C{^{1}H} NMR spectrum of 4-bromobenzyl (ferrocenyl)carbamate (**10**, acetone-d6, 126 MHz):

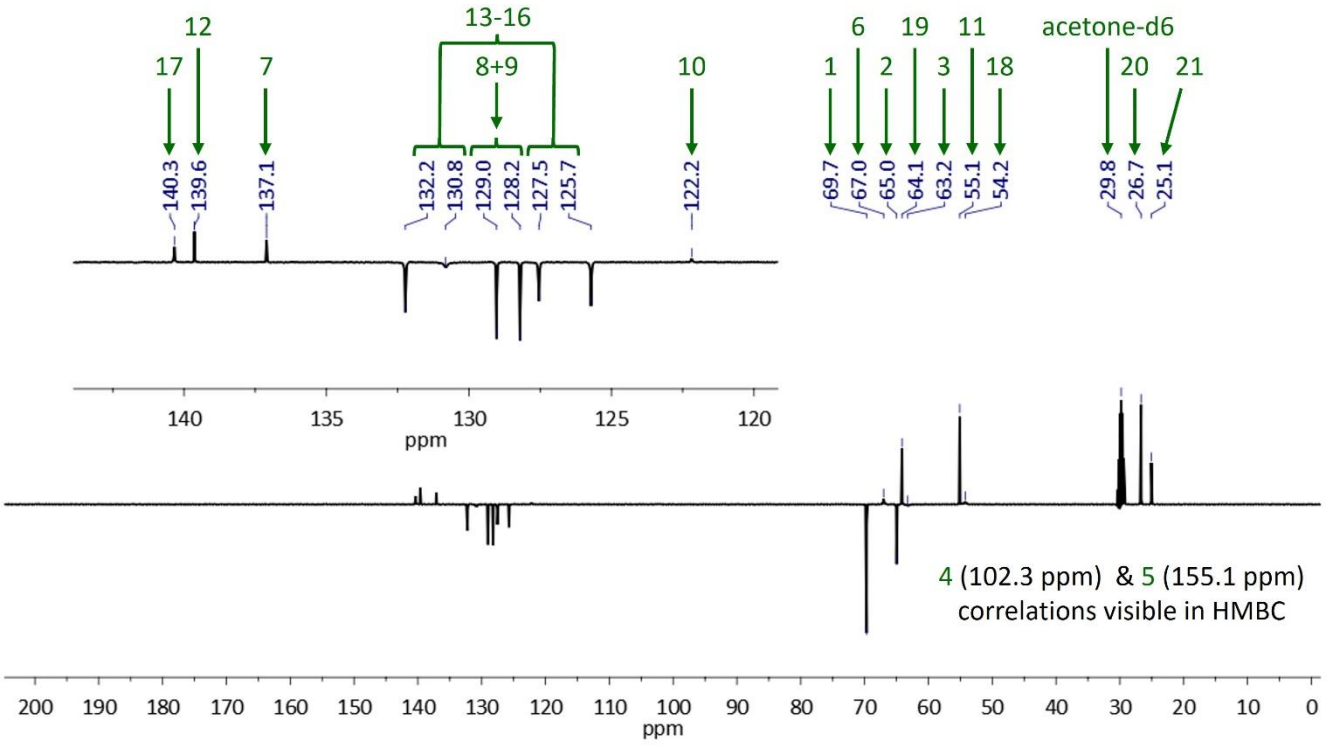


^{1}H NMR spectrum of 4-bromobenzyl (3-(piperidin-1-ylmethyl)benzyl)(ferrocenyl)carbamate (**11**, acetone-d6, 400 MHz):

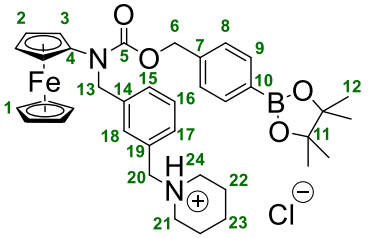


^{13}C{^{1}H} DEPTQ NMR spectrum of 4-bromobenzyl (3-(piperidin-1-ylmethyl)benzyl)(ferrocenyl)carbamate (**11**, acetone-d6, 100 MHz):

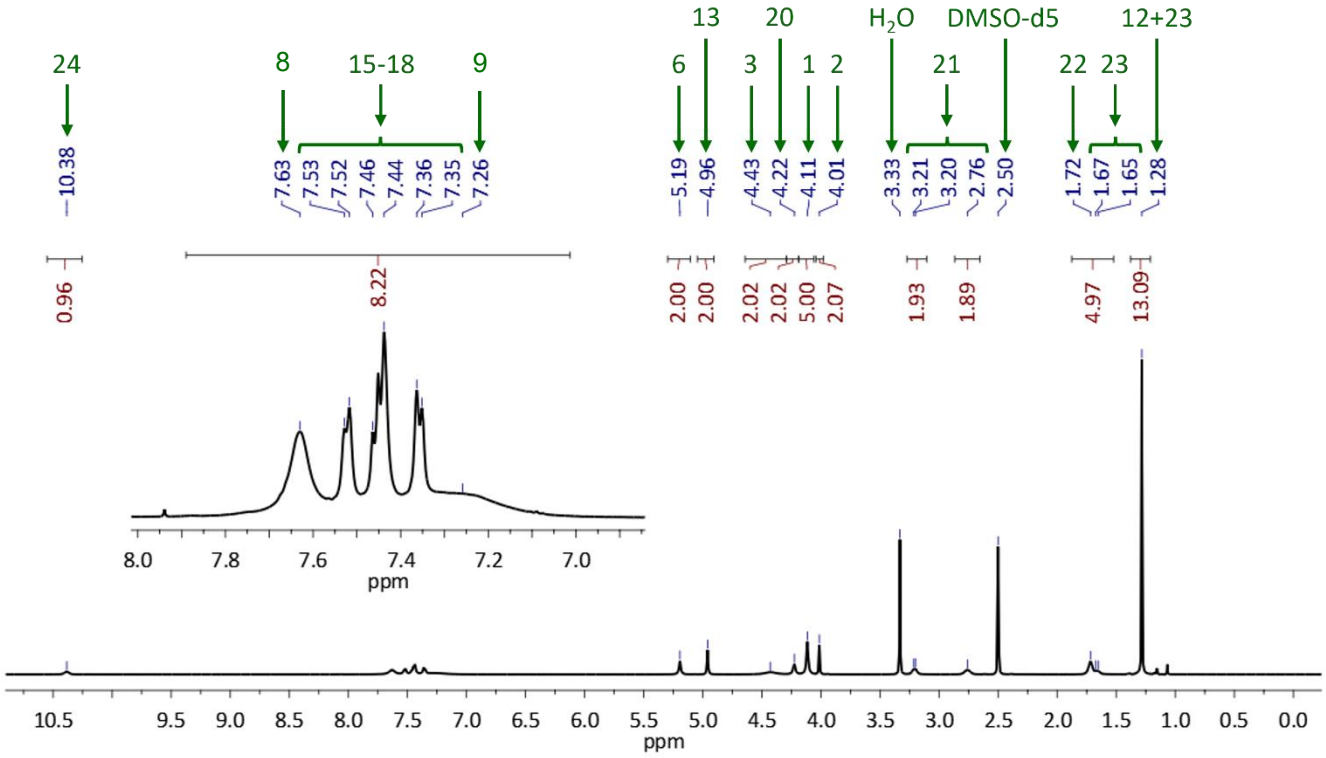
The quaternary carbons 4 and 5 are hard to detect, even with an adequate amount of substance and number of scans.



^{1}H NMR spectrum of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl (3-piperidin-1-ylmethyl)benzyl) (ferrocenyl)carbamate hydrochloride salt (**NCure2**·HCl, DMSO-d6, 600 MHz):

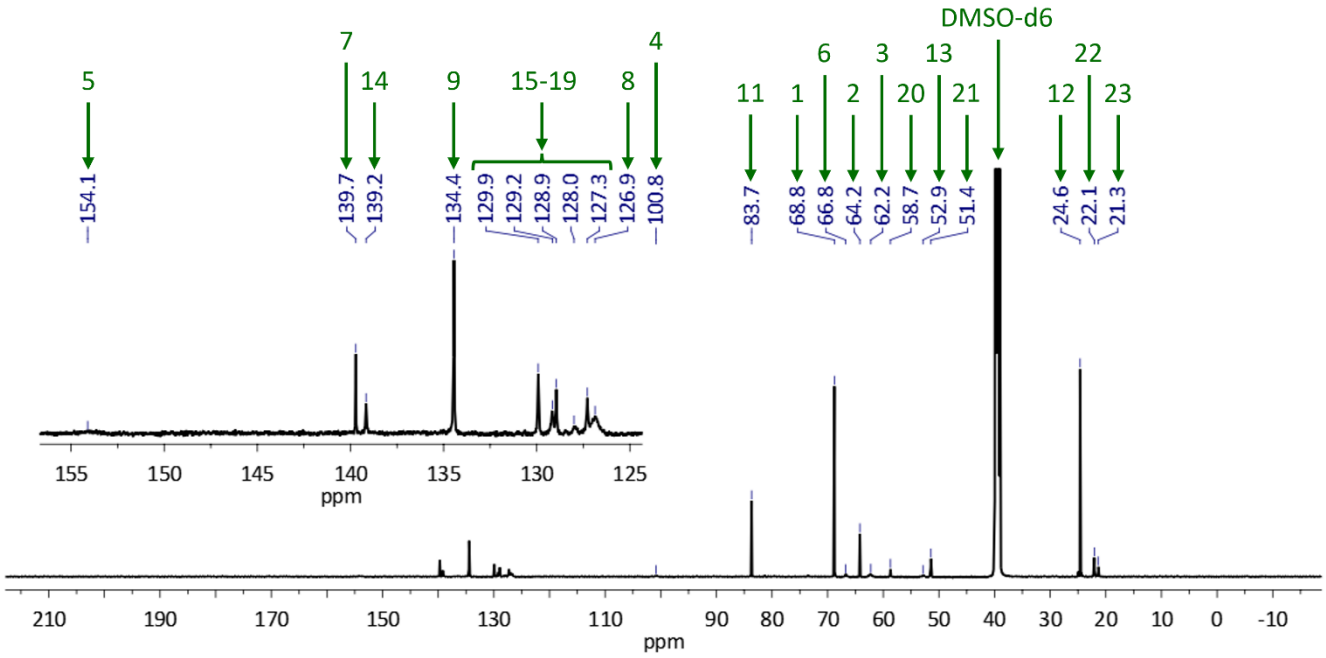


NCure2·HCl



$^{13}C\{^{1}H\}$ NMR spectrum of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl (3-piperidin-1-ylmethyl)benzyl) (ferrocenyl)carbamate hydrochloride salt (**NCure2**·HCl, DMSO-d6, 151 MHz):

The quaternary carbons 10 are hard to detect, even with an adequate amount of substance and number of scans.

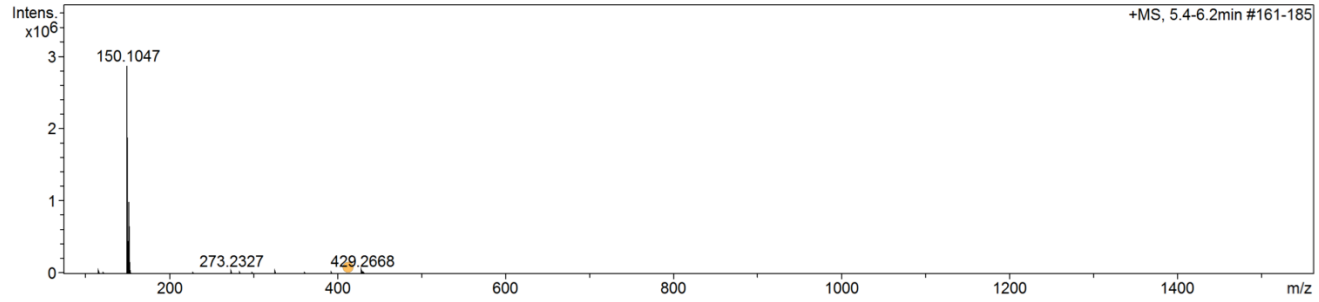


2. HRMS Data

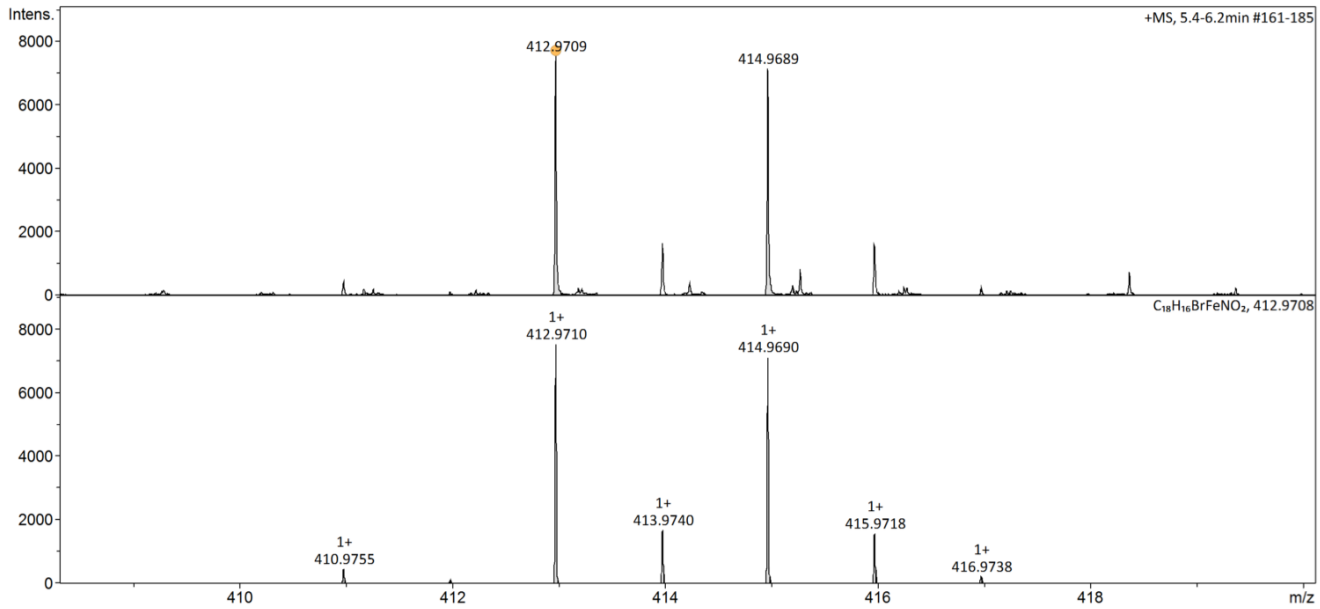
HRMS of 4-bromobenzyl (ferrocenyl)carbamate (**10**):

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	5.2 Bar
Focus	Not active	Set Capillary	700 V	Set Dry Heater	220 °C
Scan Begin	80 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.2 l/min
Scan End	1550 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	250 °C



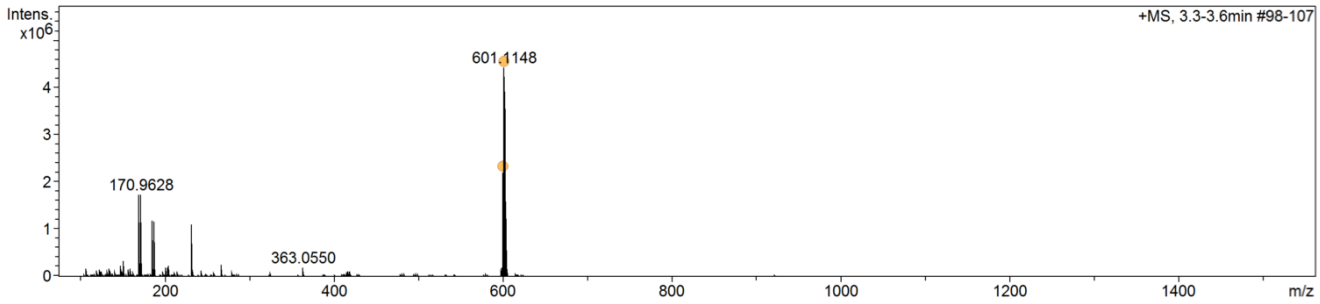
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
412.9709	1	C18H16BrFeNO2	412.9708	0.4	117.9	1	100.00	11.0	odd	ok



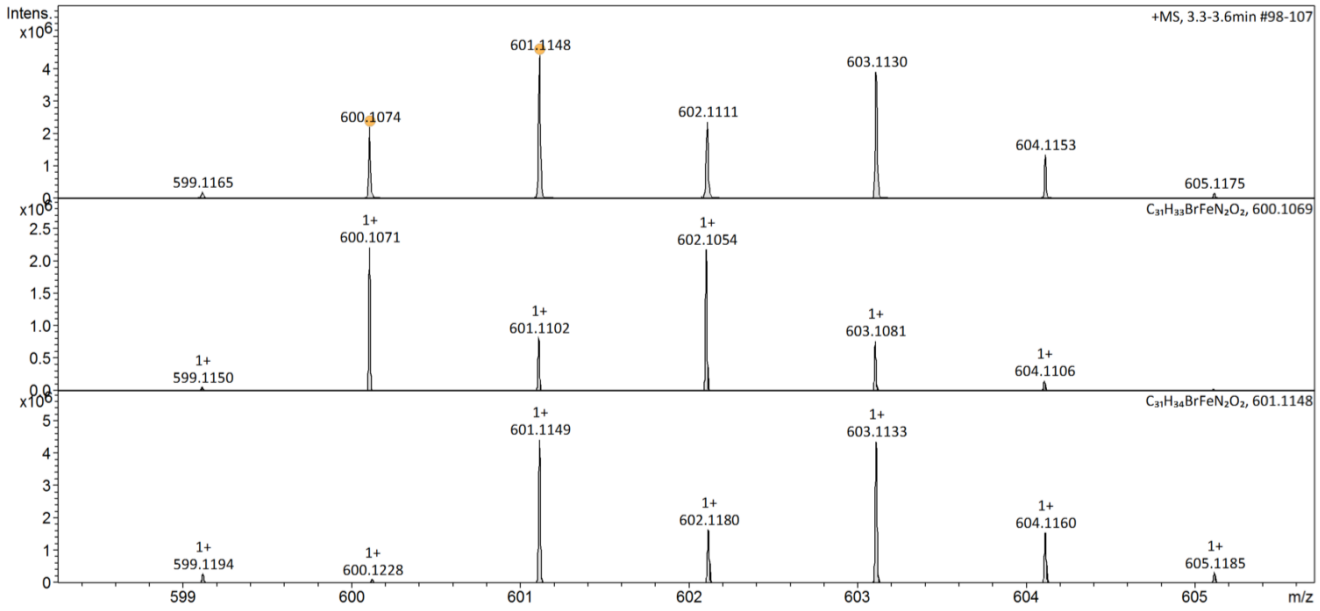
HRMS of 4-bromobenzyl (3-(piperidin-1-ylmethyl)benzyl)(ferrocenyl)carbamate (**11**):

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	5.2 Bar
Focus	Not active	Set Capillary	700 V	Set Dry Heater	220 °C
Scan Begin	80 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.2 l/min
Scan End	1550 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	250 °C



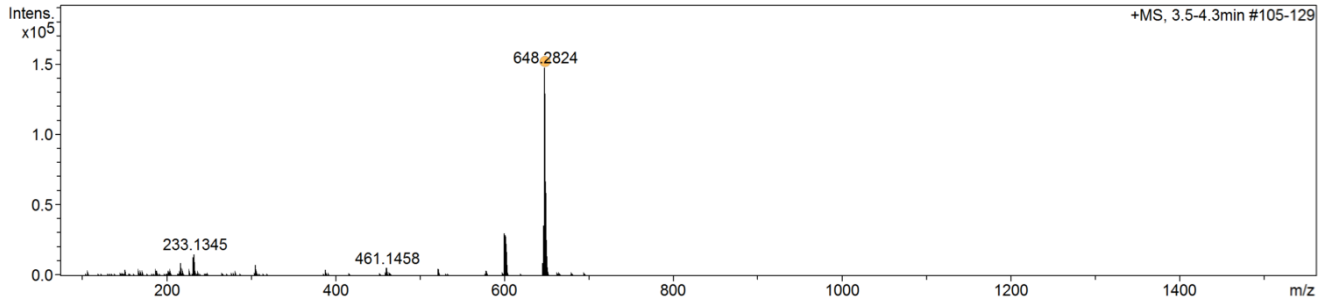
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
600.1074	1	C31H33BrFeN2O2	600.1069	-0.5	413.9	1	100.00	16.0	odd	ok
601.1148	1	C31H34BrFeN2O2	601.1148	0.3	76.9	1	100.00	15.5	even	ok



HRMS of 4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)benzyl (3-piperidin-1-ylmethyl)benzyl) (ferrocenyl)carbamate hydrochloride salt (**NCure2**·HCl):

Acquisition Parameter

Source Type	APPI	Ion Polarity	Positive	Set Nebulizer	5.2 Bar
Focus	Not active	Set Capillary	700 V	Set Dry Heater	220 °C
Scan Begin	80 m/z	Set End Plate Offset	-500 V	Set Dry Gas	1.2 l/min
Scan End	1550 m/z	Set Charging Voltage	0 V	Set Divert Valve	Waste
		Set Corona	0 nA	Set APCI Heater	250 °C



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻ Conf	N-Rule
648.2824	1	C37H45BFeN2O4	648.2816	-0.1	15.1	1	100.00	17.0	odd	ok