

Electronic Supplementary Material (ESI) for RSC Advances. This journal is © The Royal Society of Chemistry 2020

Supporting Information

Boron-Containing Capsaicinoids

:

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Table of Contents

General information.....	S2
NMR, IR, and HRMS Spectra of the Products.....	S3-S98
Antimicrobial and Cytotoxicity Data.....	S99-S106

General Information

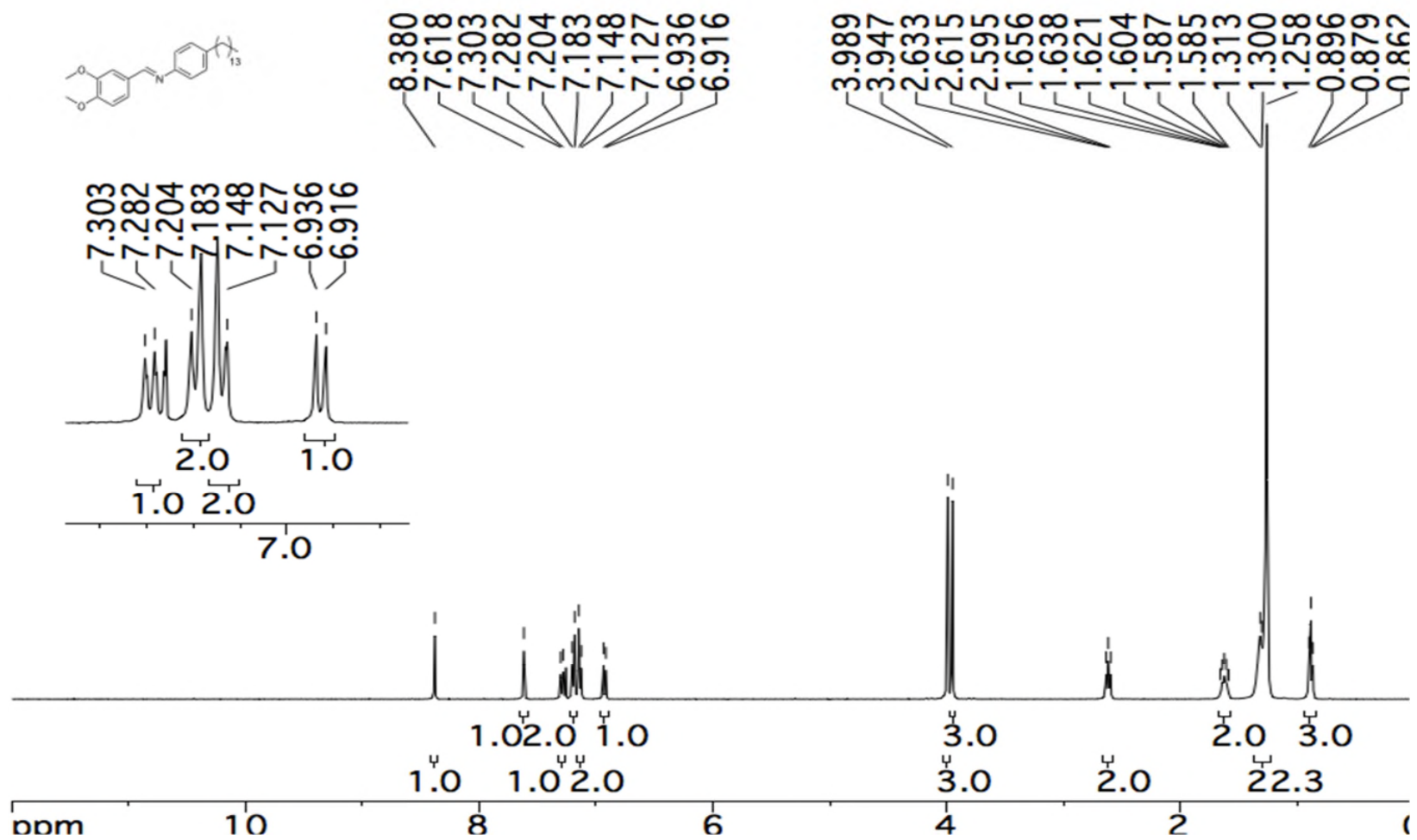
Chemistry Data NMR spectra were recorded on a JEOL JNM-GSX400 FT NMR (^1H : 400 MHz; ^{11}B : 128 MHz; ^{13}C : 100 MHz) spectrometer. ^1H , $^{13}\text{C}\{^1\text{H}\}$, and $^{11}\text{B}\{^1\text{H}\}$ NMR chemical shifts (δ /ppm) are referenced to Me_4Si , Me_4Si , and $\text{BF}_3\cdot\text{OEt}_2$, respectively. Chemical shifts (δ) are reported in ppm [relative to residual solvent peaks (^1H and ^{13}C) or external $\text{BF}_3\cdot\text{OEt}_2$ (^{11}B)]. Multiplicities are reported as singlet (s), doublet (d), triplet (t), quartet (q), quintet (quint), multiplet (m), and broad (br) with coupling constants (J) reported in hertz. High resolution mass spectrometry was performed at DalChem Mass Spec Laboratory (Dalhousie University, Halifax, NS).

Antimicrobial Assay Data Growth of *S. warneri*, *P. vulgaris*, *P. aeruginosa* and *C. albicans* were measured by reading optical density (OD600), or in the case of slow growing microorganisms (MRSA and VRE), PrestoBlue was used to assess metabolic activity by measuring fluorescence (535-560)/(590-615) (excitation/emission) using a Thermo Scientific Varioskan Flash plate reader at time zero and then again after incubation of the plates for 22 h at 37°C. After subtracting the time zero OD600 from the final reading, the percentages of microorganism survival relative to vehicle control wells were calculated.

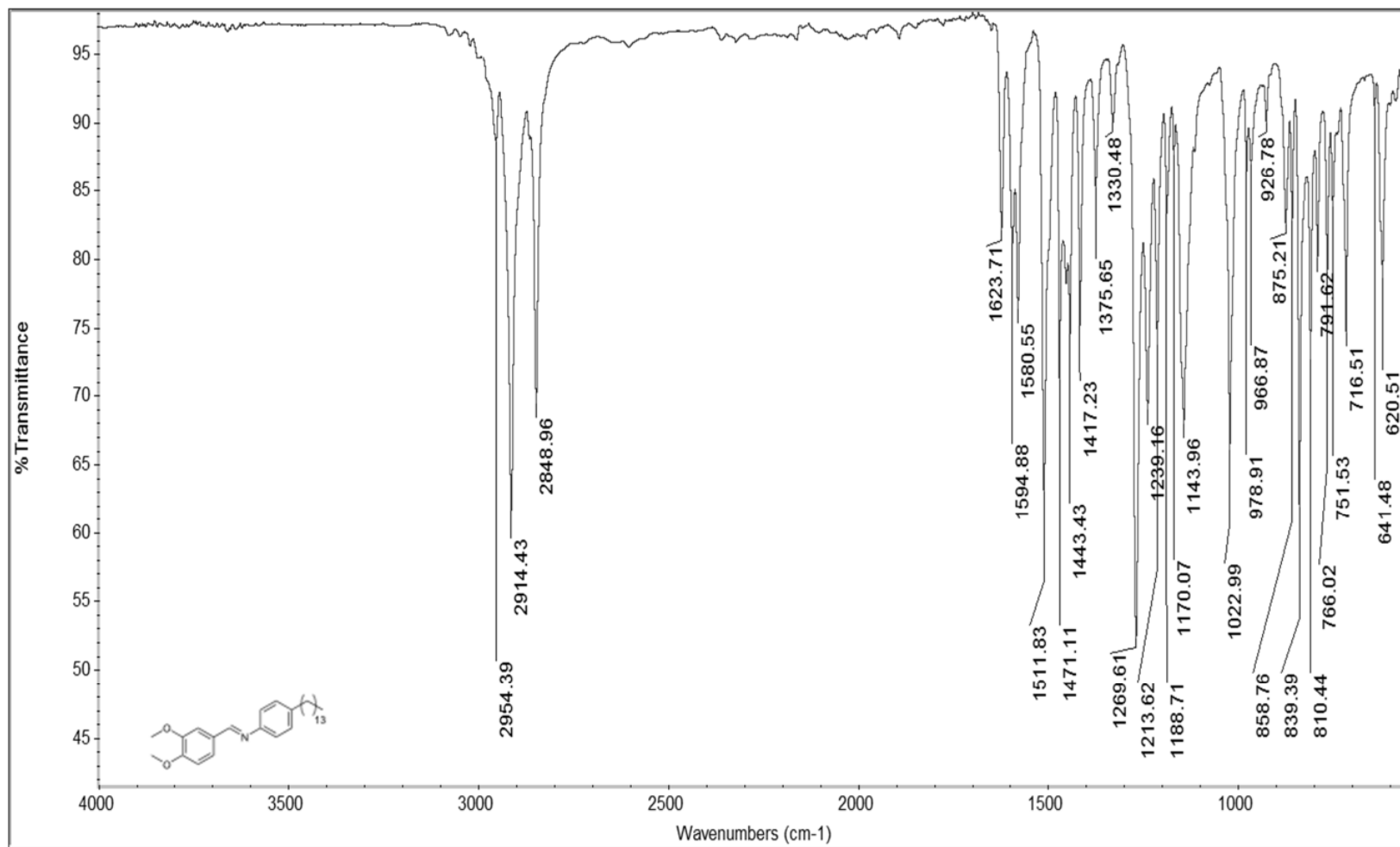
Cytotoxicity Assay Data Alamar blue was added, 24 h after the treatment, and fluorescence was monitored using a Cytation Gen 5 plate reader using 560 nm Ex/590 nm Em both at time zero and 4 h after Alamar blue addition. The inferred percentage of cell viability relative to vehicle control wells were calculated after subtracting the time zero emission 590 nm measurement from the final reading and the IC50 was determined.

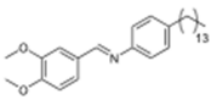
NMR, IR, and HRMS Spectra of the Products

1-(3,4-dimethoxyphenyl)-N-(4-tetradecylphenyl)methanimine(13)— ^1H NMR



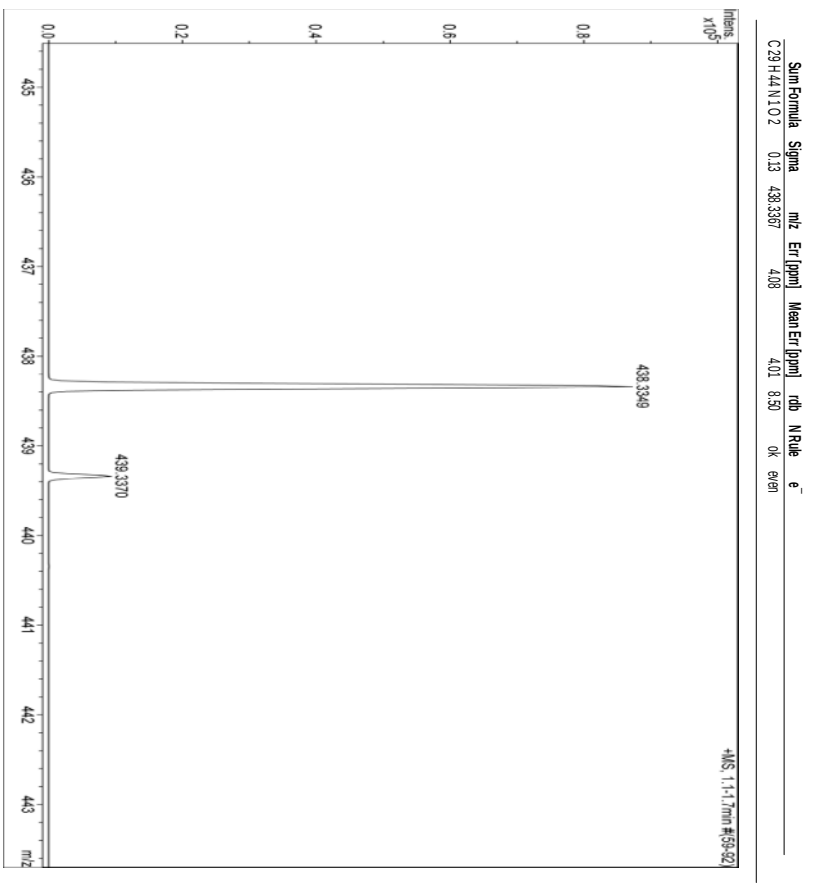
1-(3,4-dimethoxyphenyl)-N-(4-tetradecylphenyl)methanimine (**13**) – IR





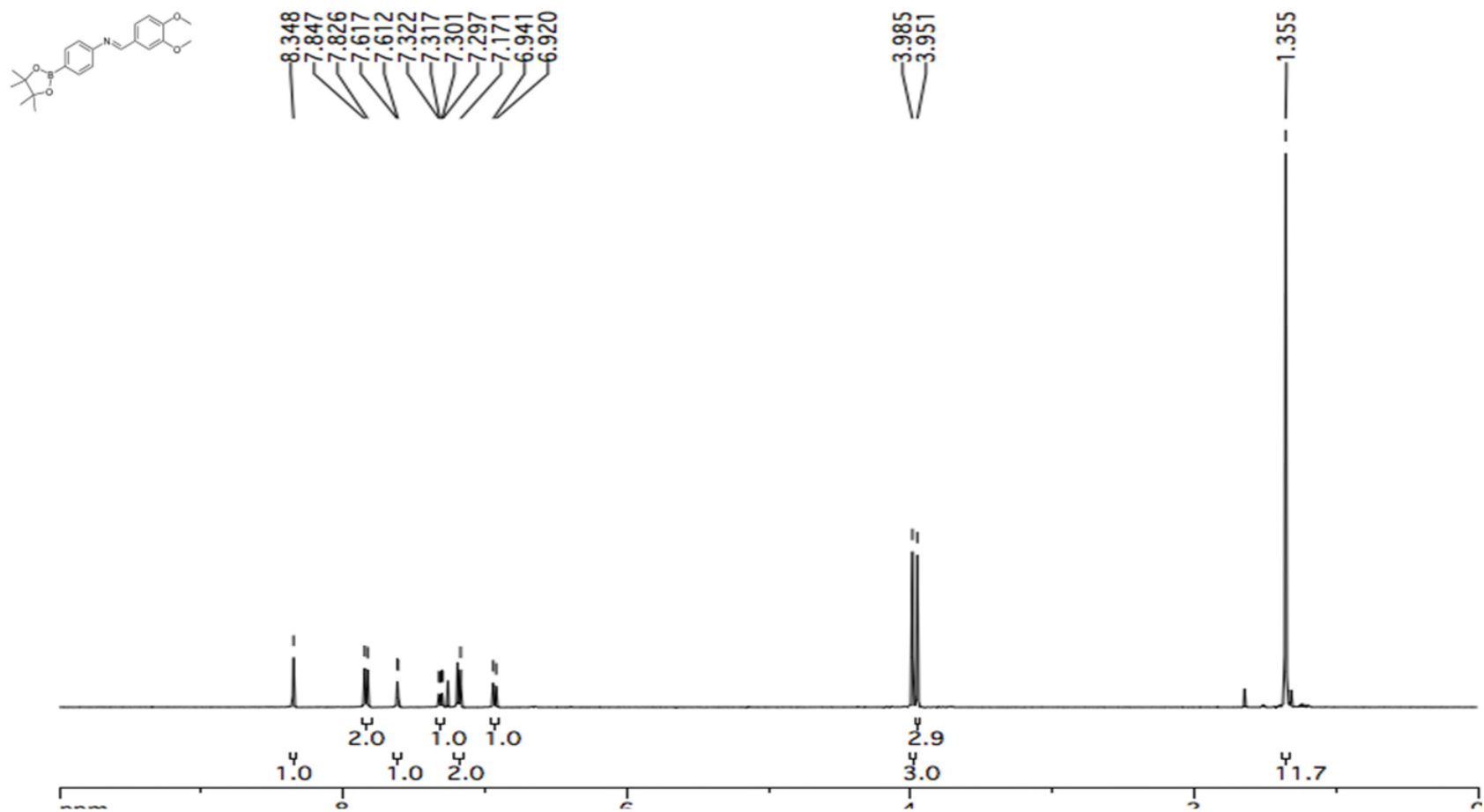
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Comment			

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			Set Detector TOF
			45 V
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		Set P1 Bias Push	399 V
		Set Reflector	1300 V
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		Set Detector TOF	2200 V

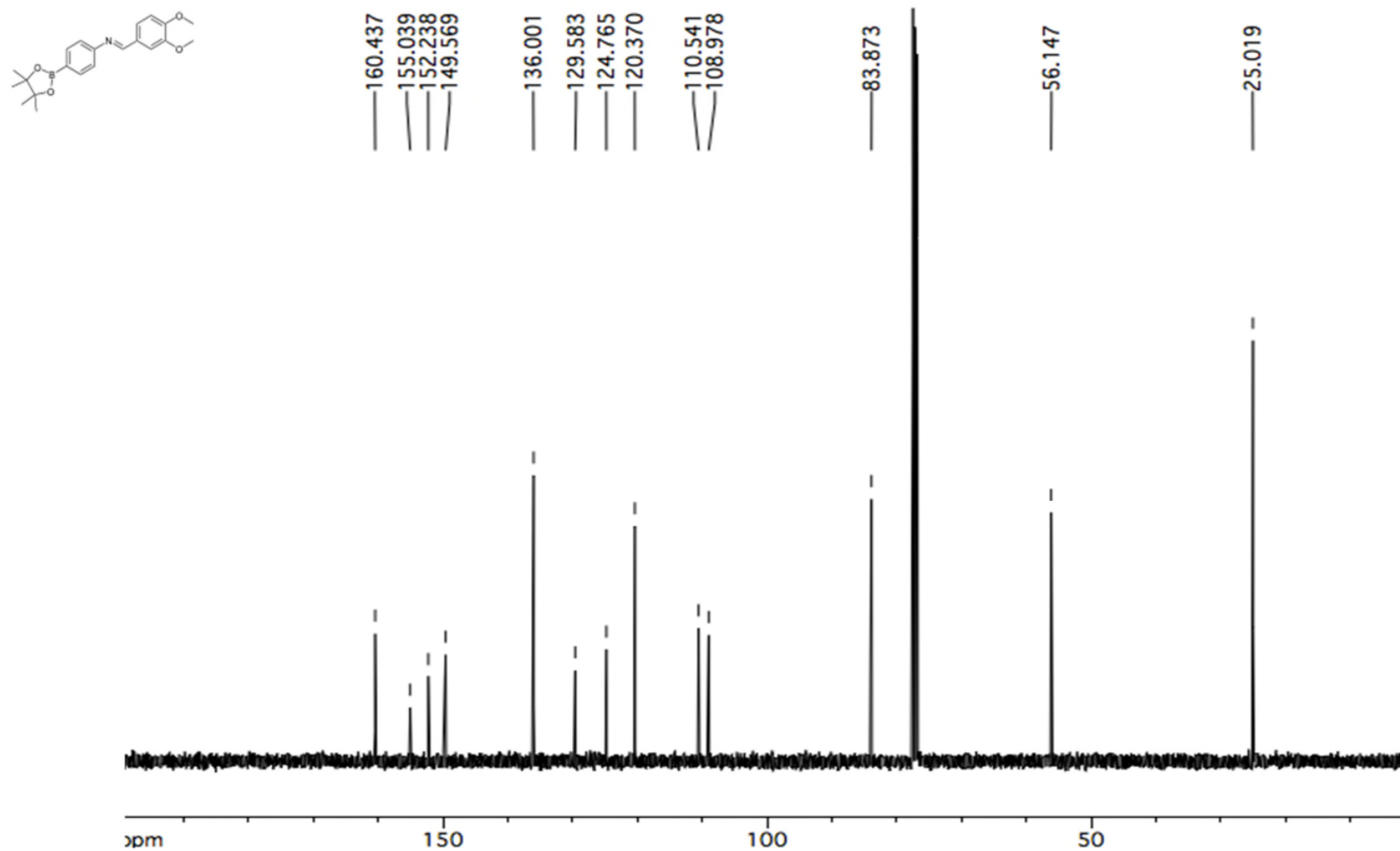


1-(3,4-dimethoxyphenyl)-N-(4-tetradecylphenyl)methanimine(13)- HRMS

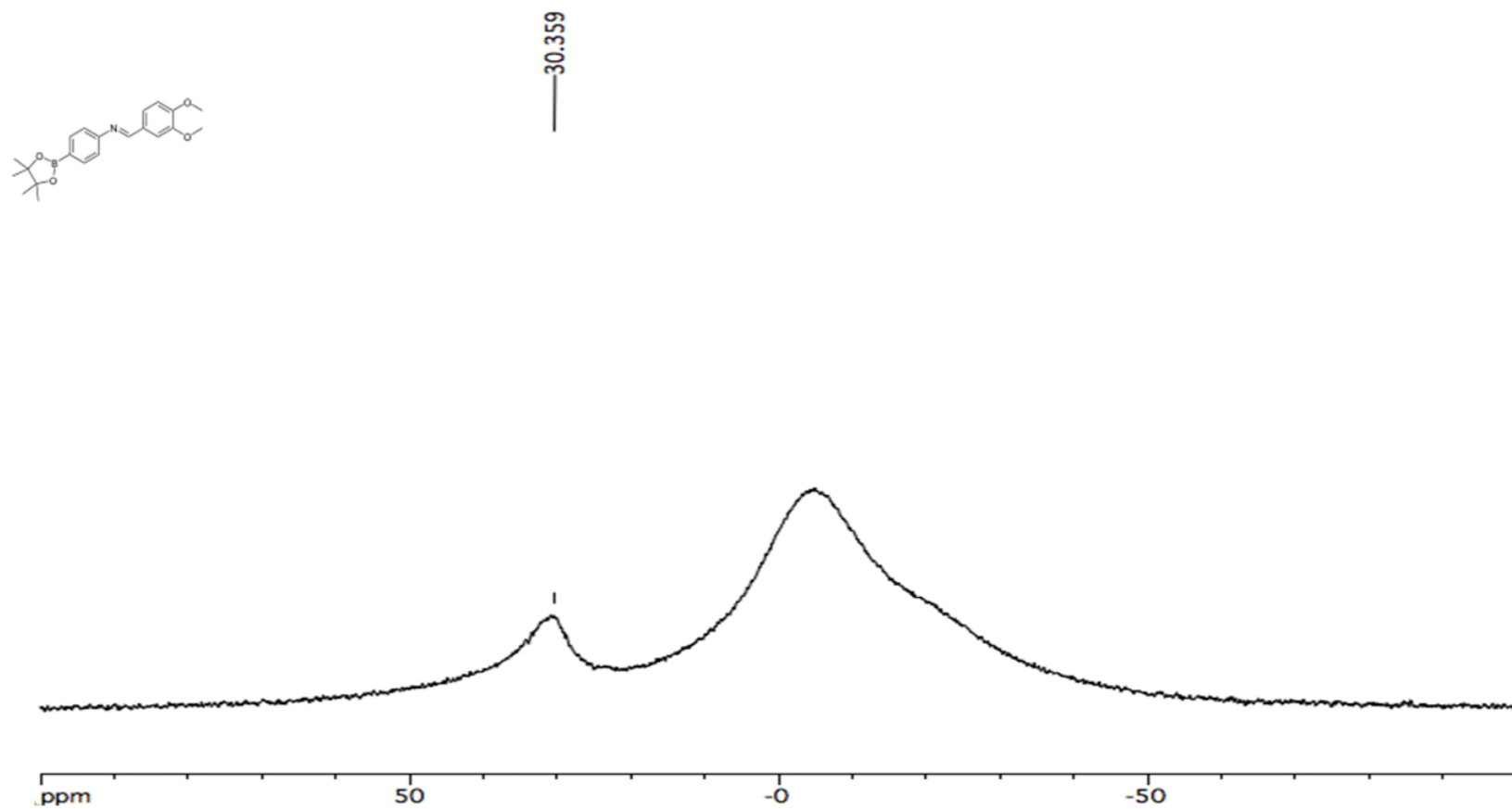
1-(3,4-dimethoxyphenyl)-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**14**) – ^1H NMR



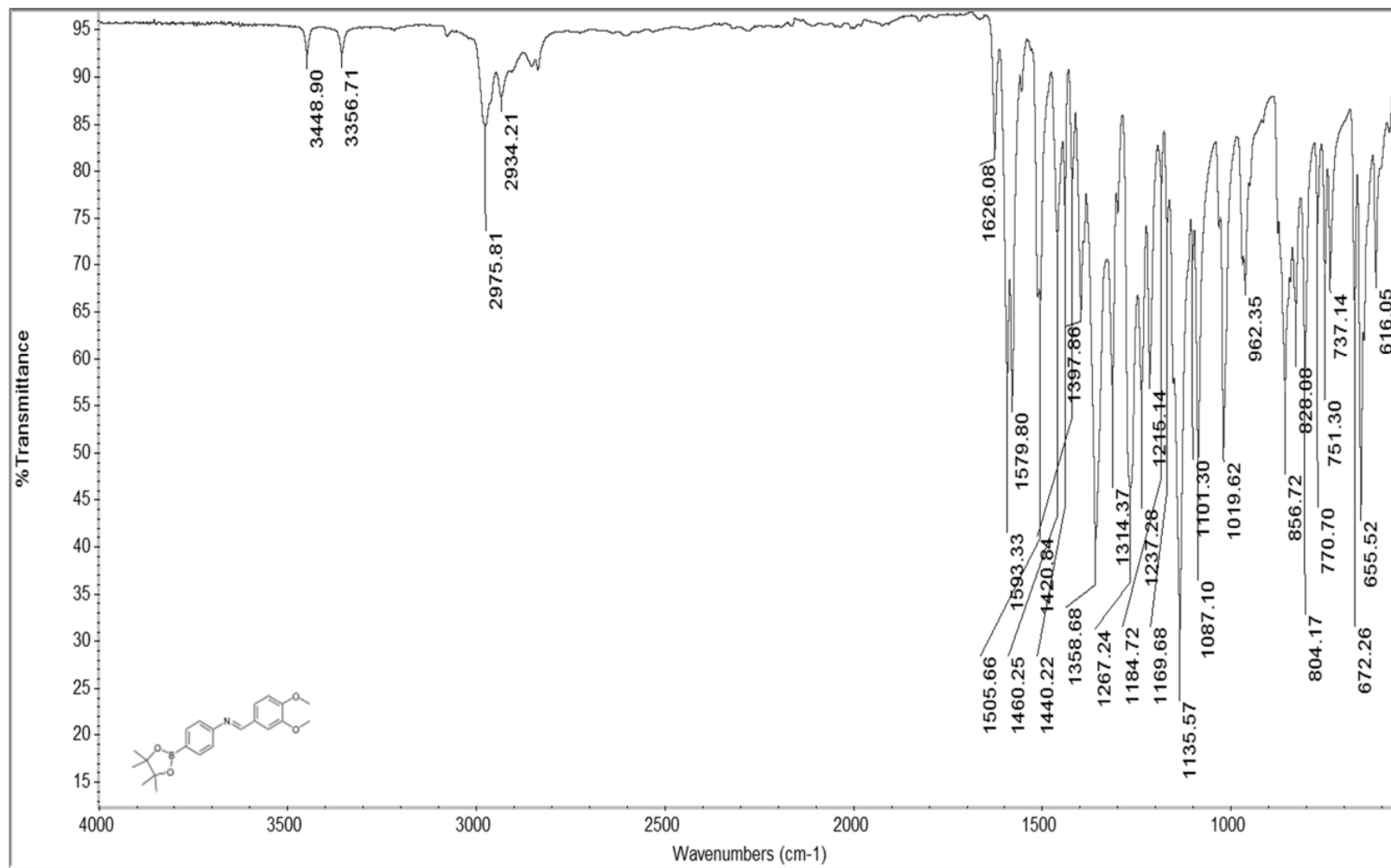
1-(3,4-dimethoxyphenyl)-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**14**) – ^{13}C NMR

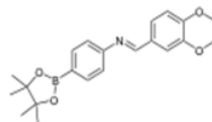


1-(3,4-dimethoxyphenyl)-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**14**) – ^{11}B NMR



1-(3,4-dimethoxyphenyl)-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**14**) – IR





1-(3,4-dimethoxyphenyl)-N-(4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (14) – HRMS

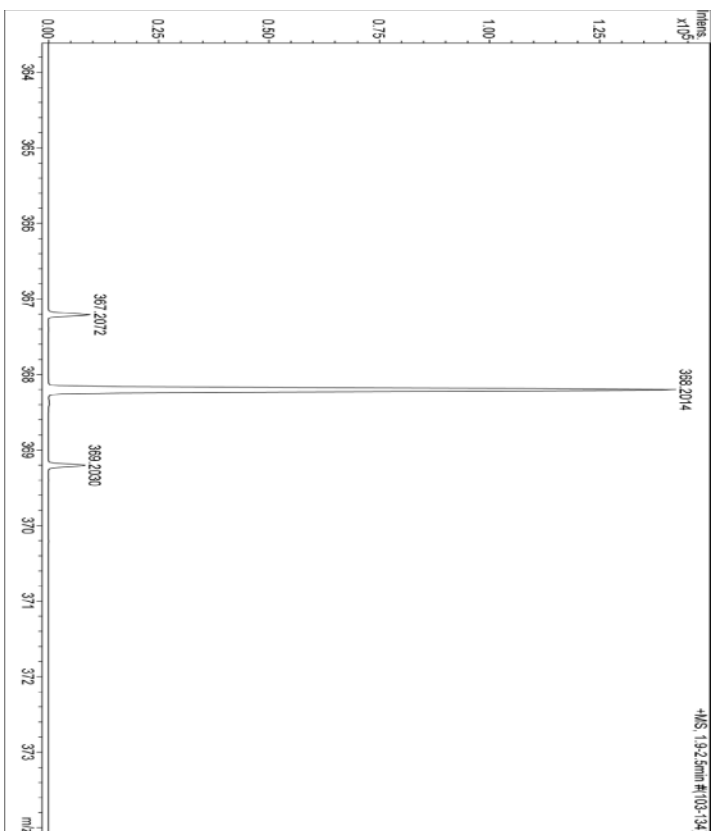
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Comment			

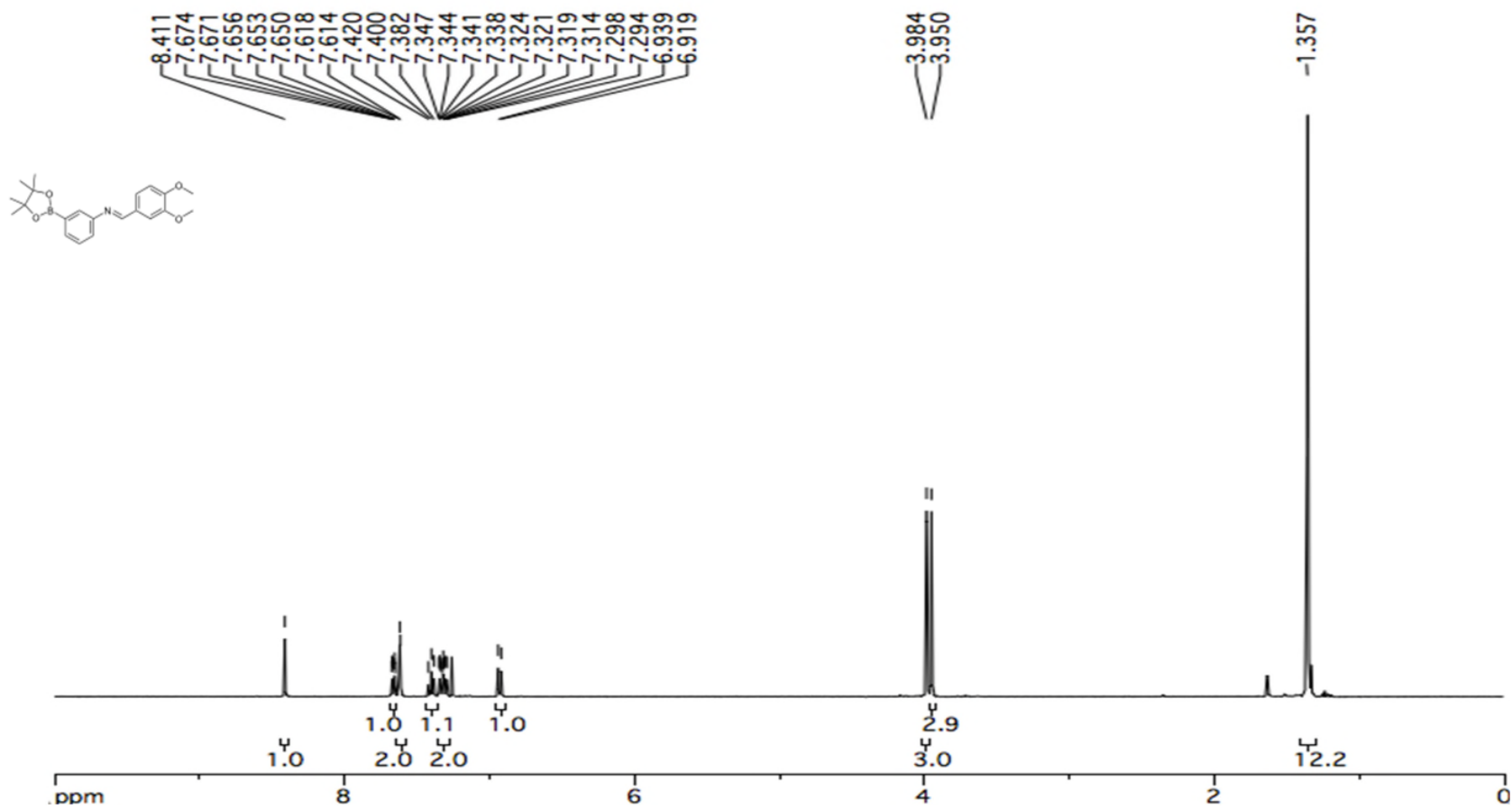
Acquisition Parameter

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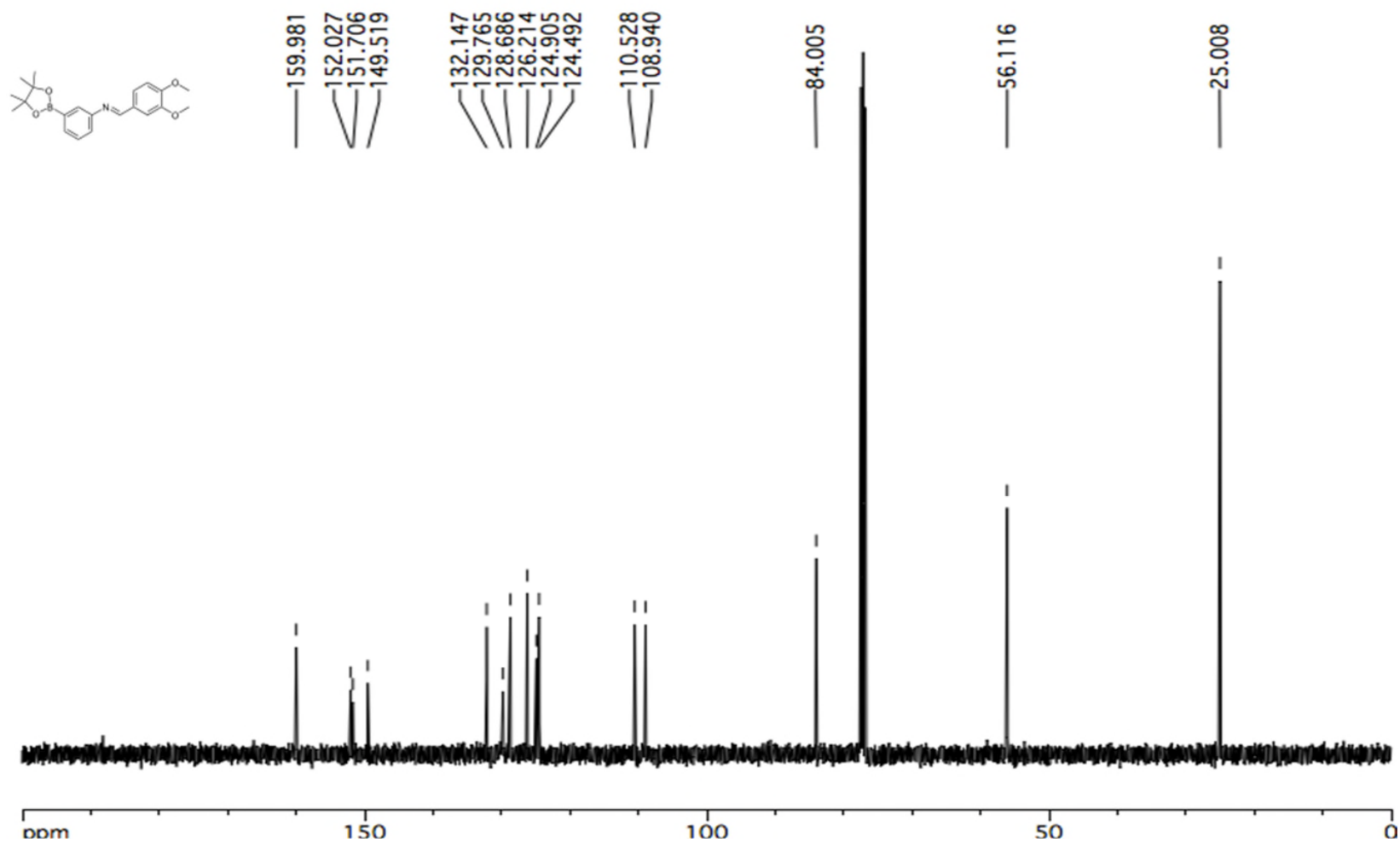
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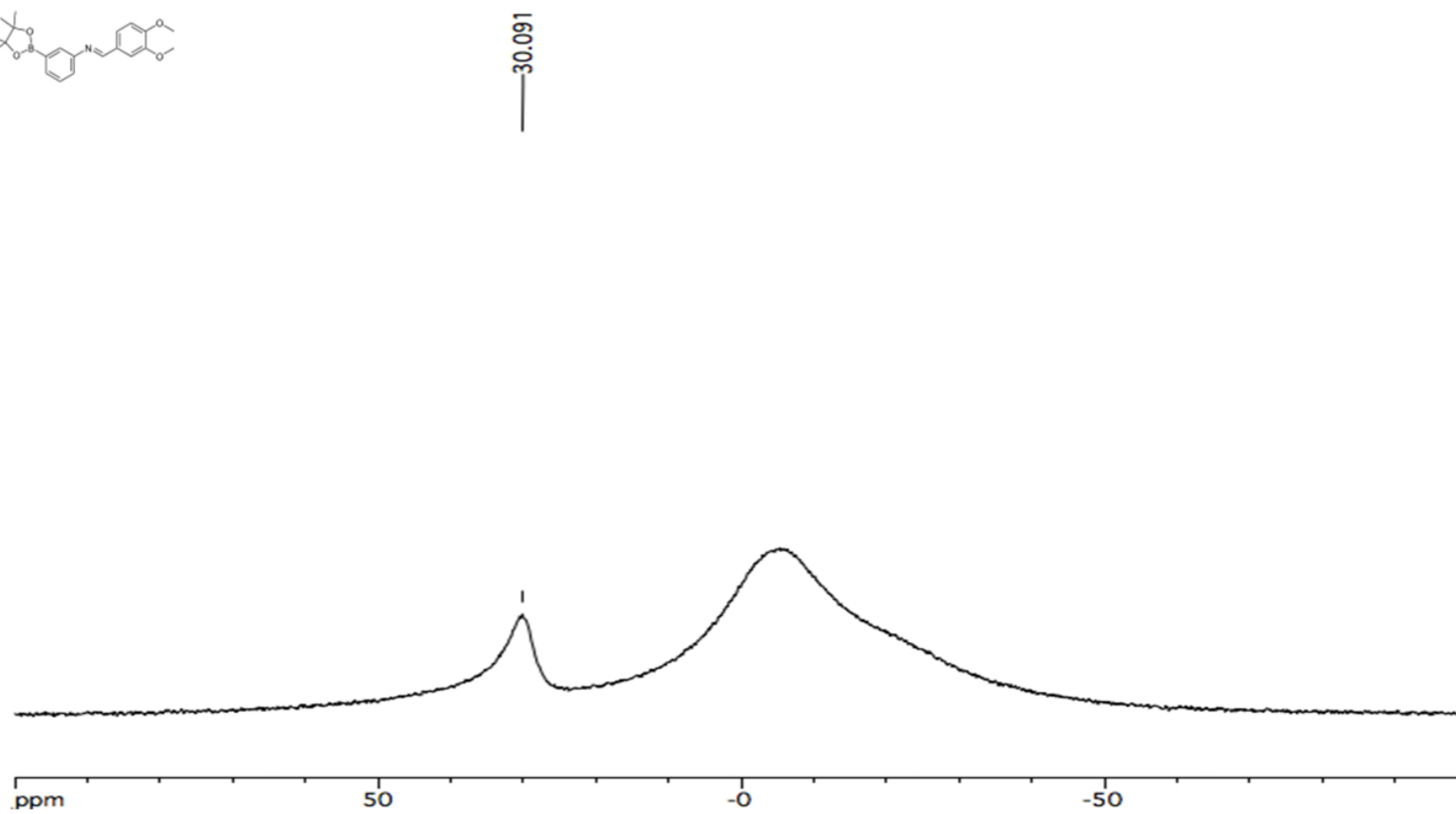
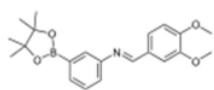
1-(3,4-dimethoxyphenyl)-N-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**15**) – ^1H NMR



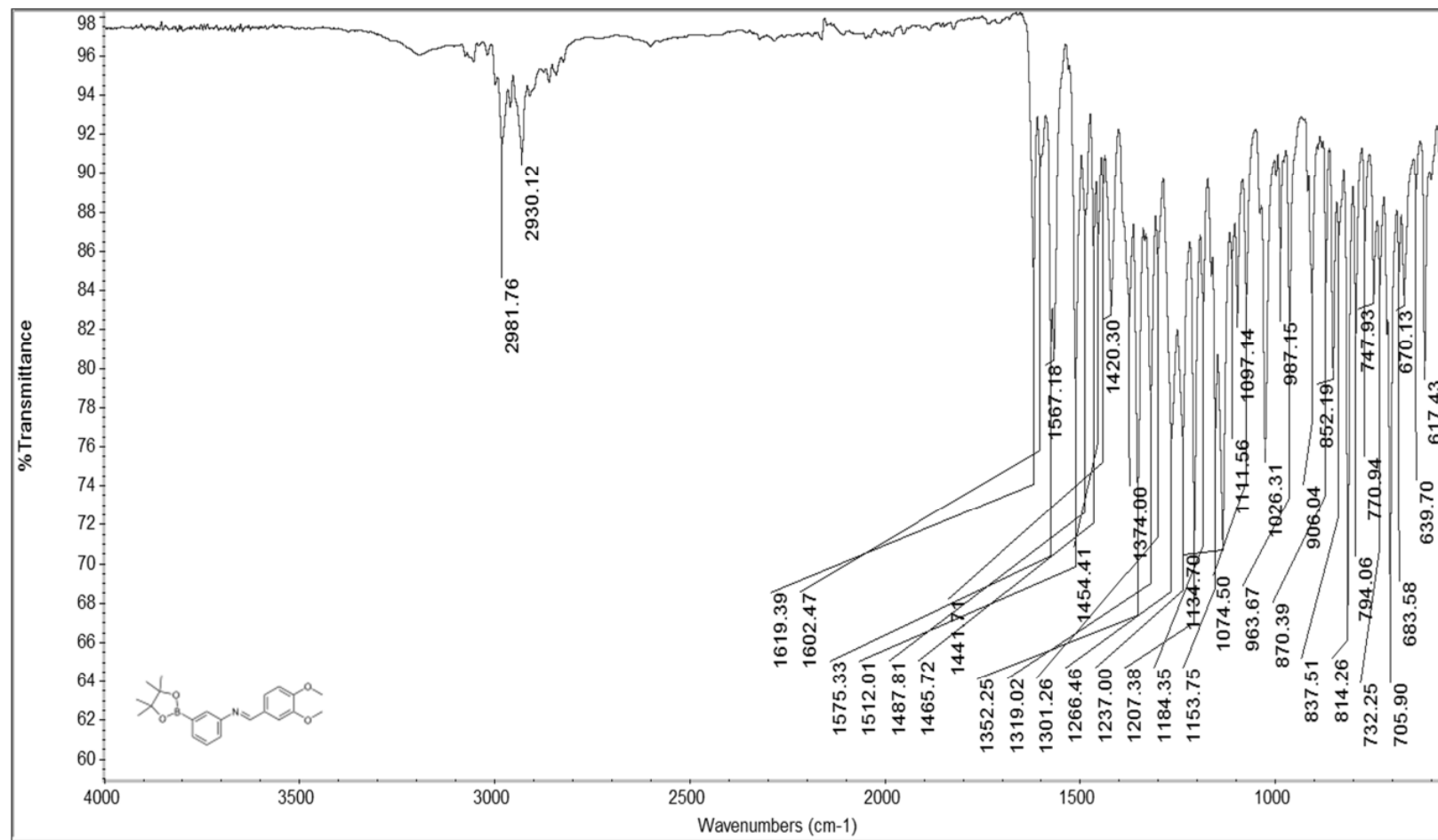
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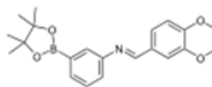


1-(3,4-dimethoxyphenyl)-N-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**15**) – ^{11}B NMR



1-(3,4-dimethoxyphenyl)-N-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (**15**) – IR



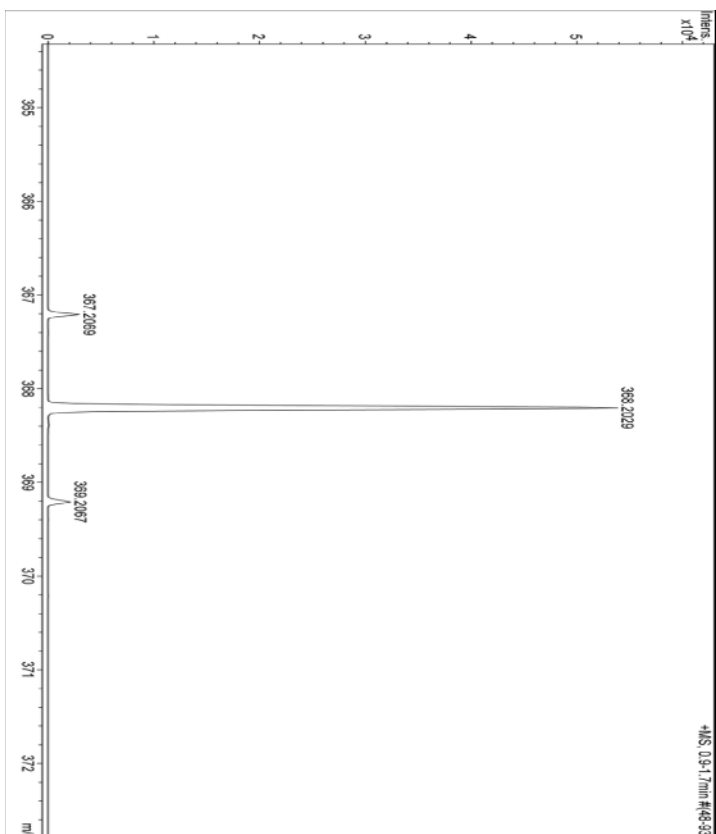


1-(3,4-dimethoxyphenyl)-N-(3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl)methanimine (15) – HRMS

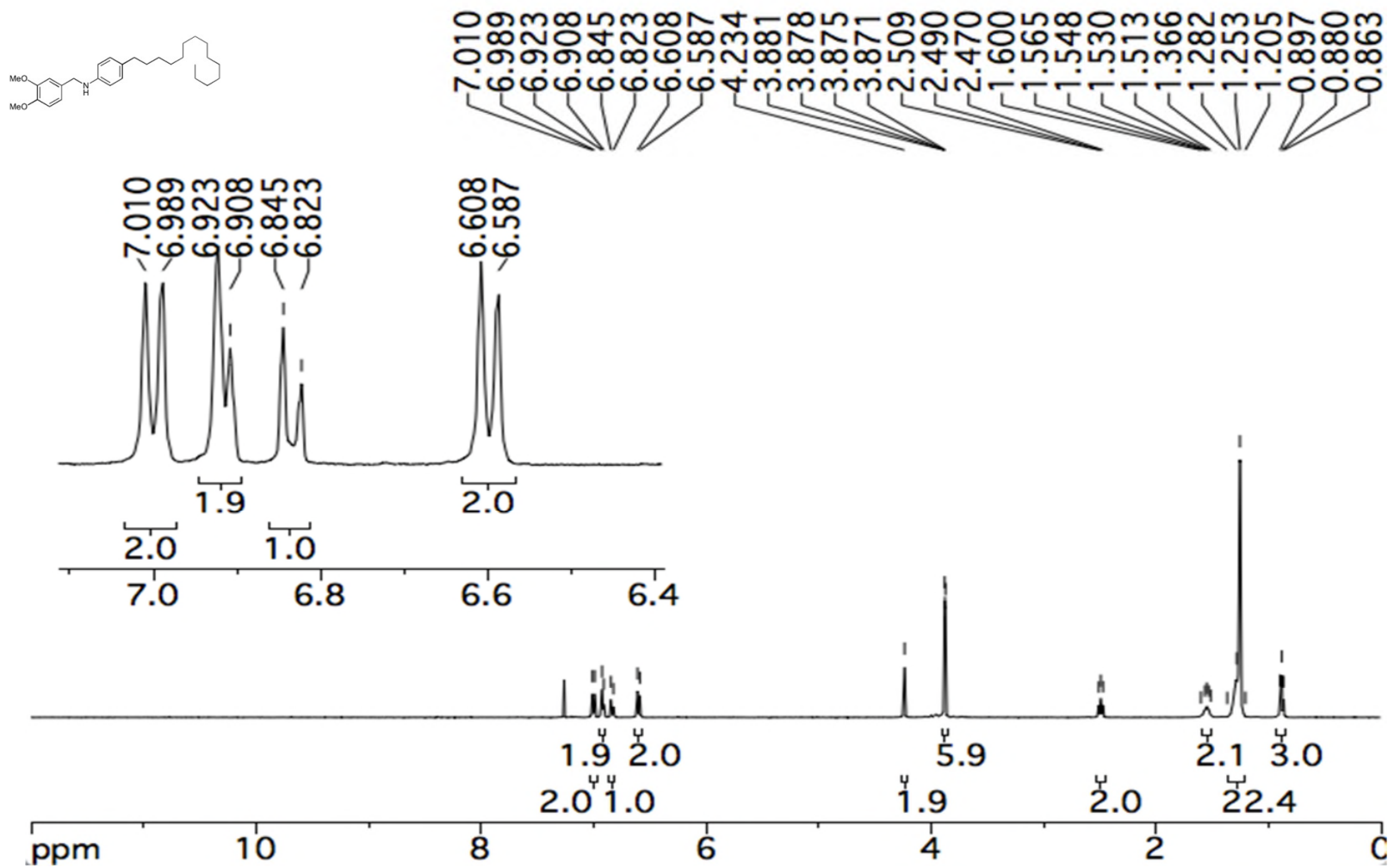
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Sample Name	JM-48		57
Comment			

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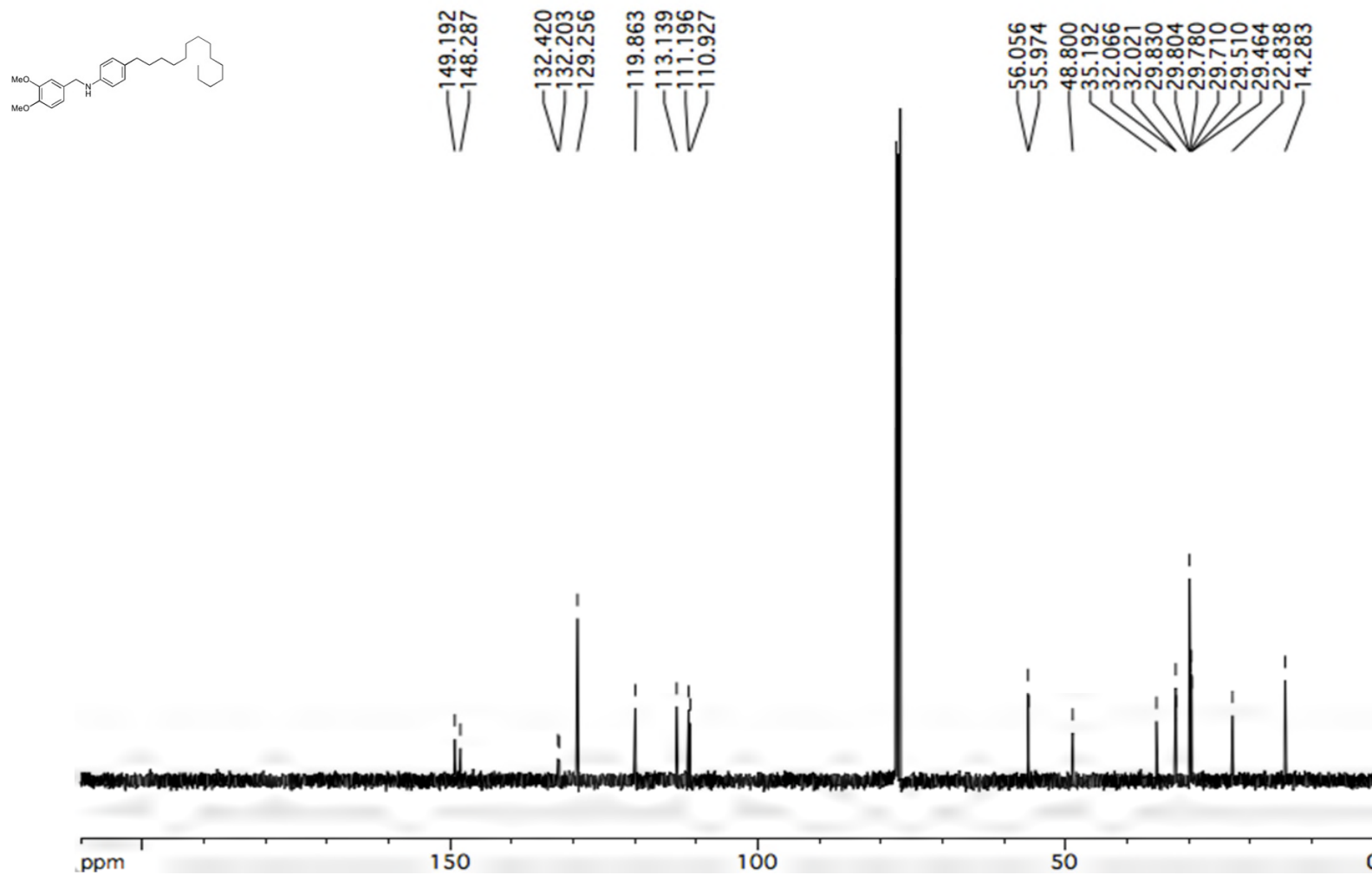
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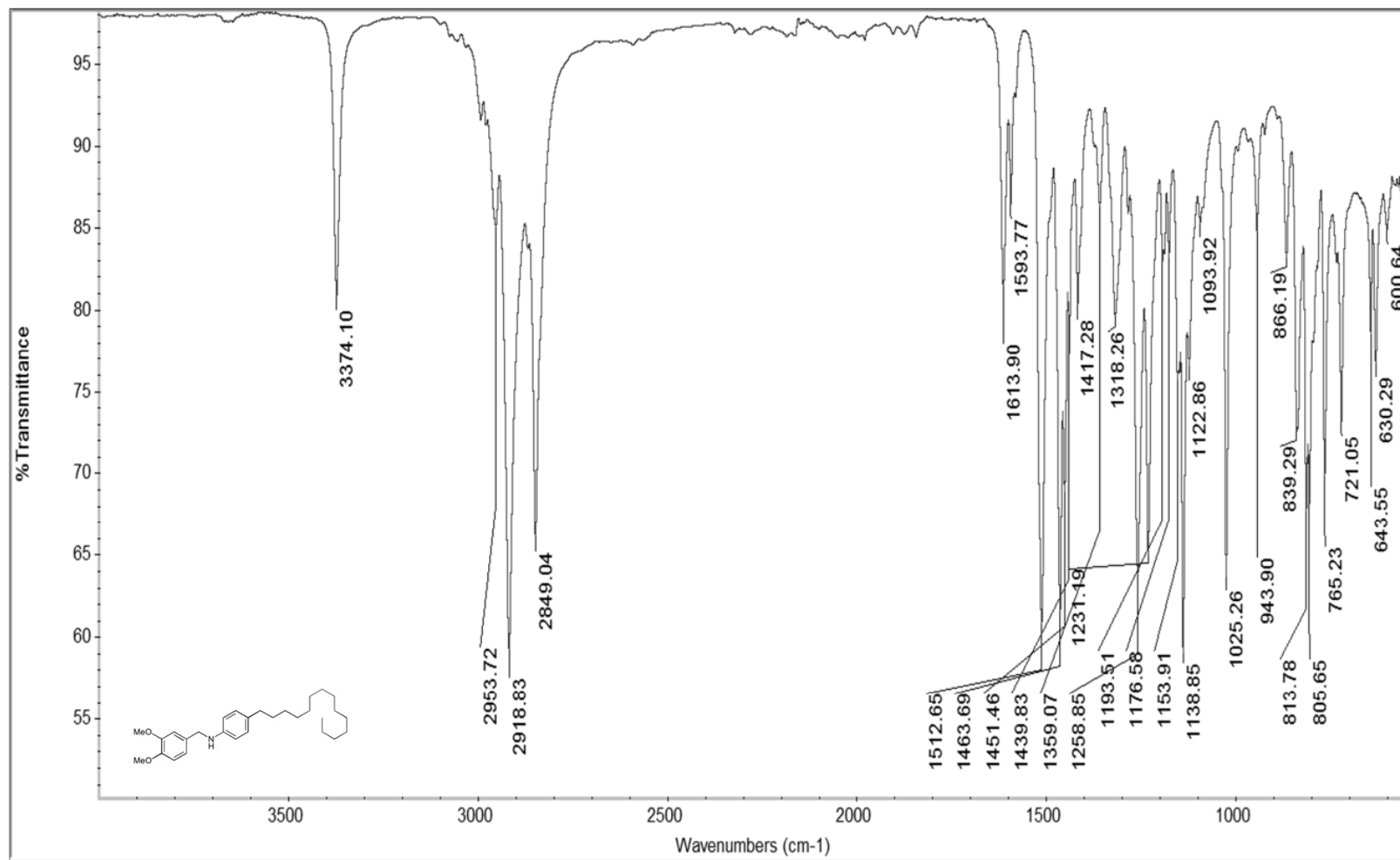
4-tetradecyl-*N*-(3,4-dimethoxybenzyl)aniline (**17**) – ^1H NMR

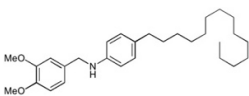


4-tetradecyl-N-(3,4-dimethoxybenzyl)aniline (17) – ^{13}C NMR



4-tetradecyl-N-(3,4-dimethoxybenzyl)aniline (17) – IR

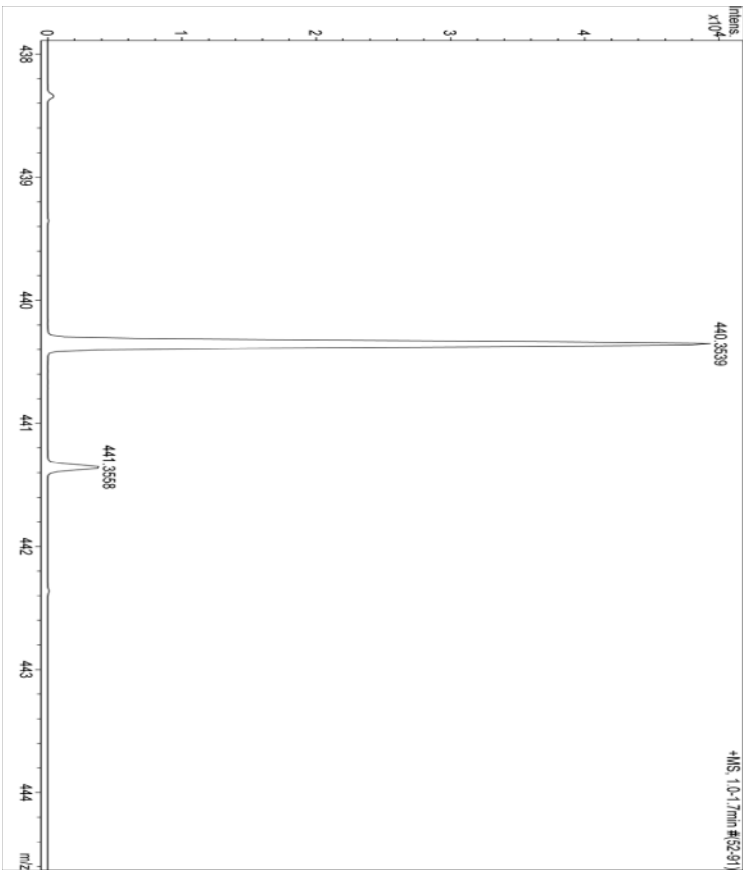




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Sample Name	JM-21		57
Comment			

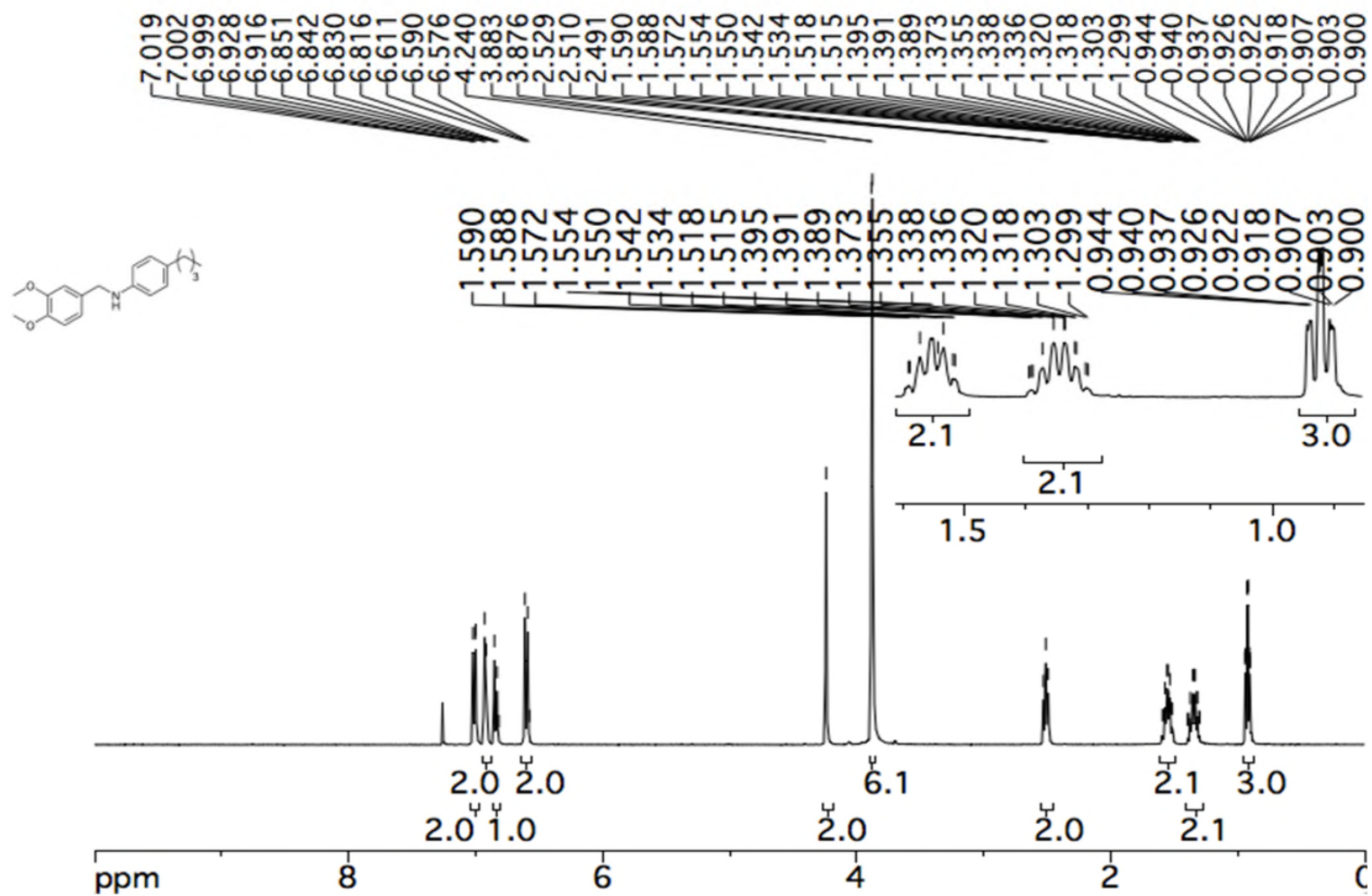
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Scan End	1500 m/z	Set Reflector	1300 V
		Set Flight Tube	9000 V
		Set Detector TOF	2200 V

Sum Formula	Sigma	m/z	Er [ppm]	Mean Er [ppm]	rdv	N Rule	e ⁻
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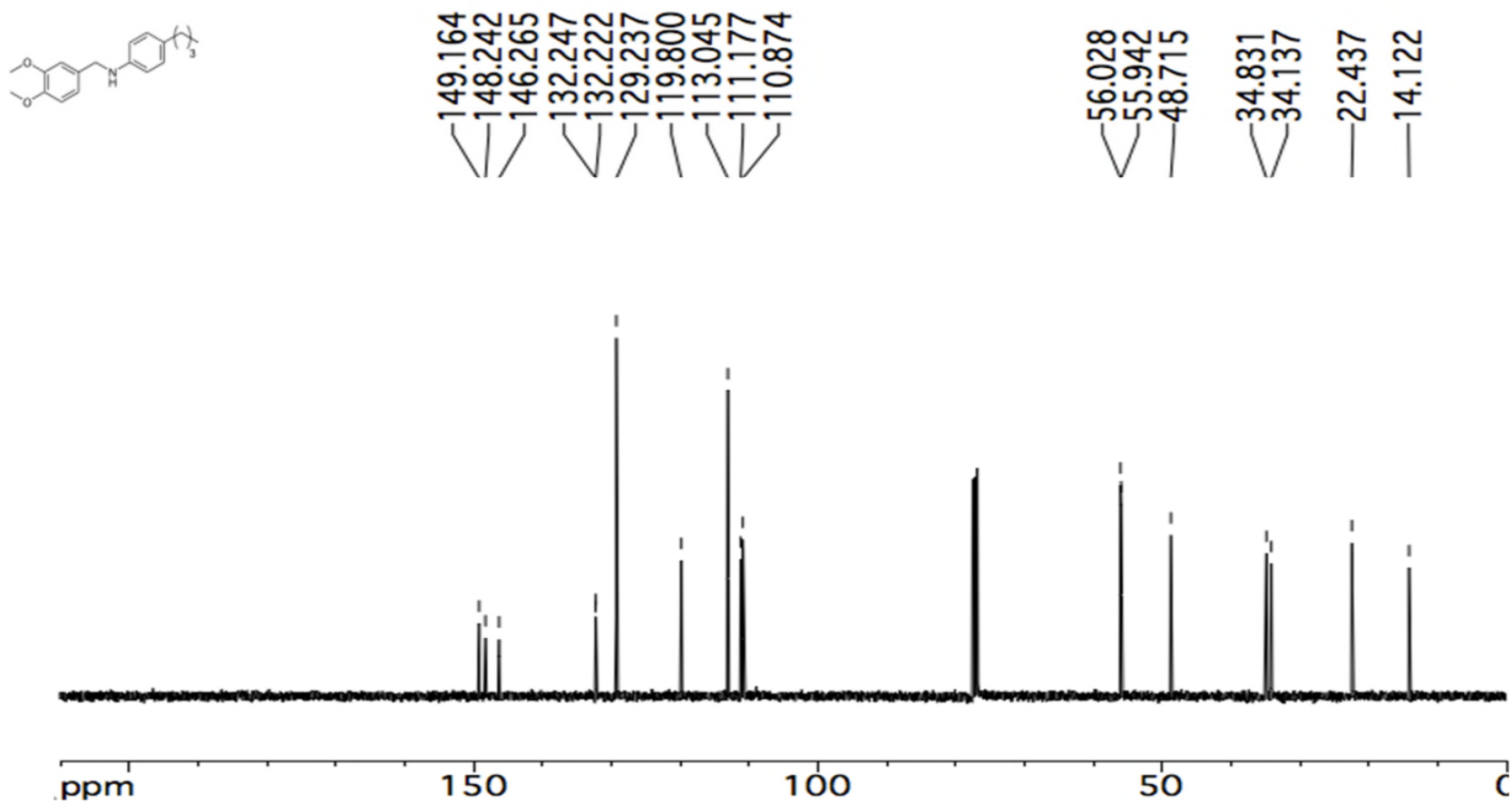


4-tetradecyl-N-(3,4-dimethoxybenzyl)aniline (17) – HRMS

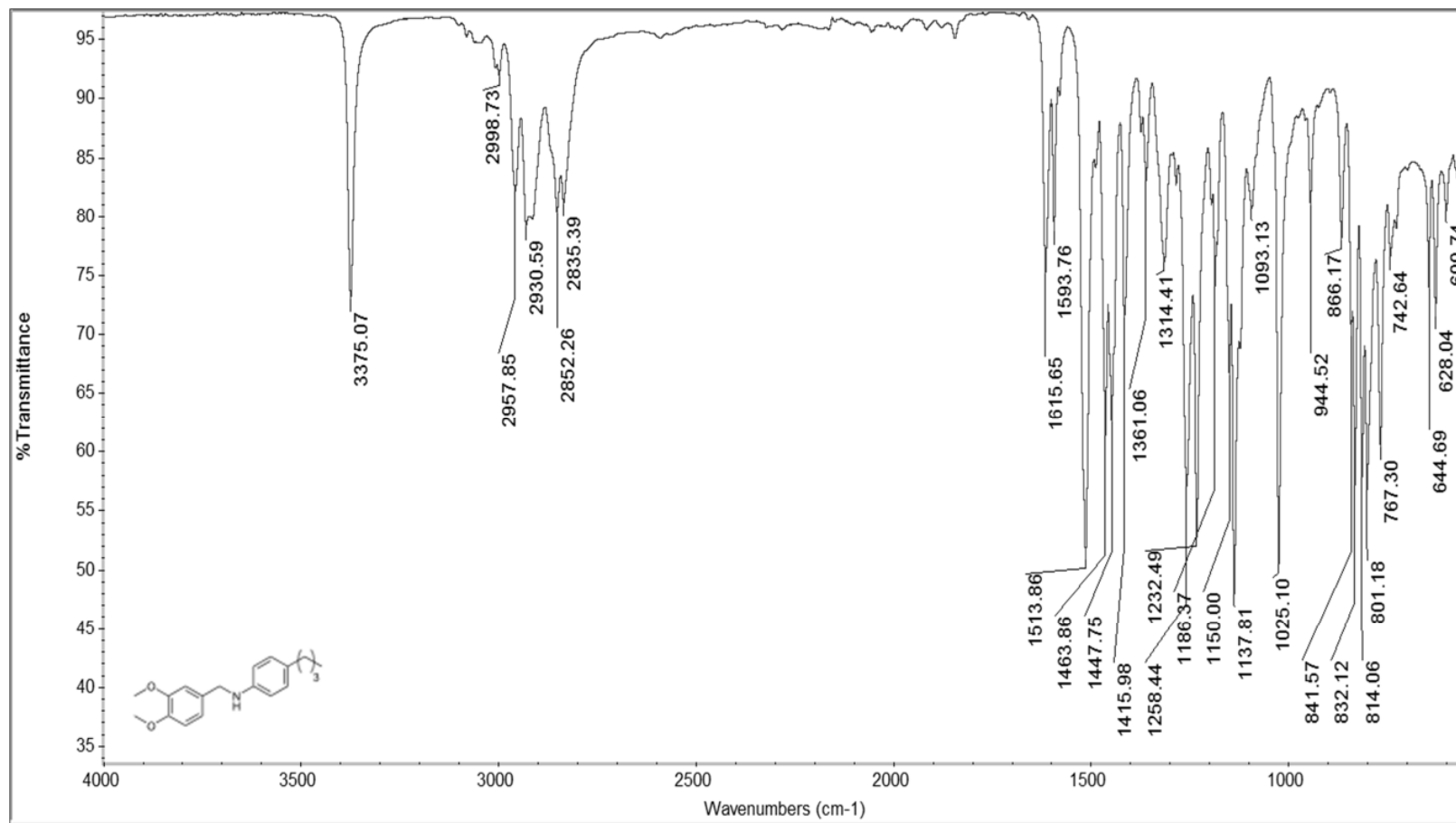
4-butyl-*N*-(3,4-dimethoxybenzyl)aniline (**18**) -¹H NMR

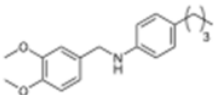


4-butyl-*N*-(3,4-dimethoxybenzyl)aniline (**18**) -¹³C NMR



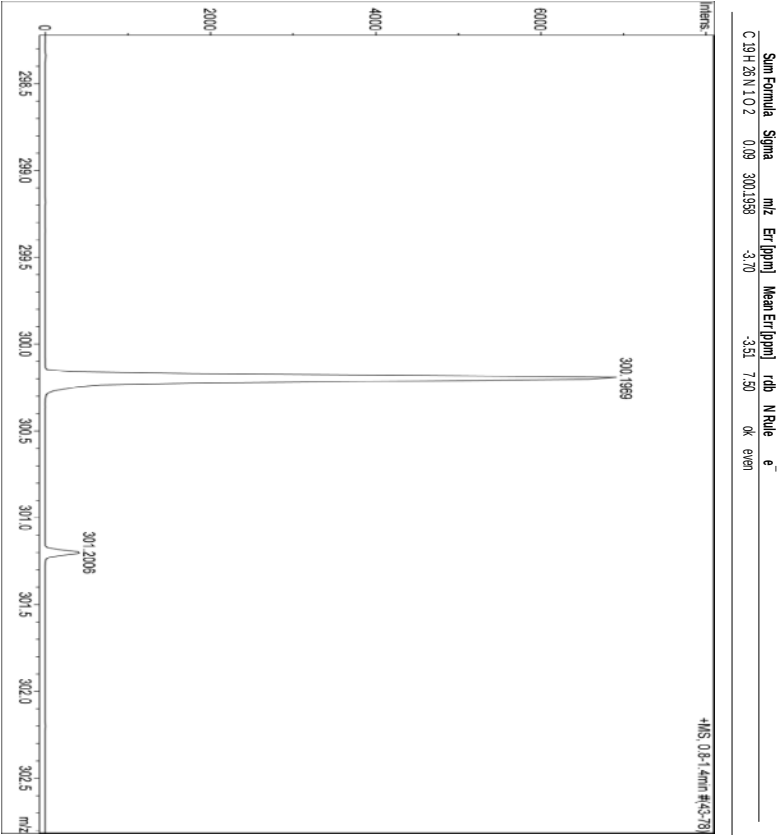
4-butyl-N-(3,4-dimethoxybenzyl)aniline (**18**) - IR





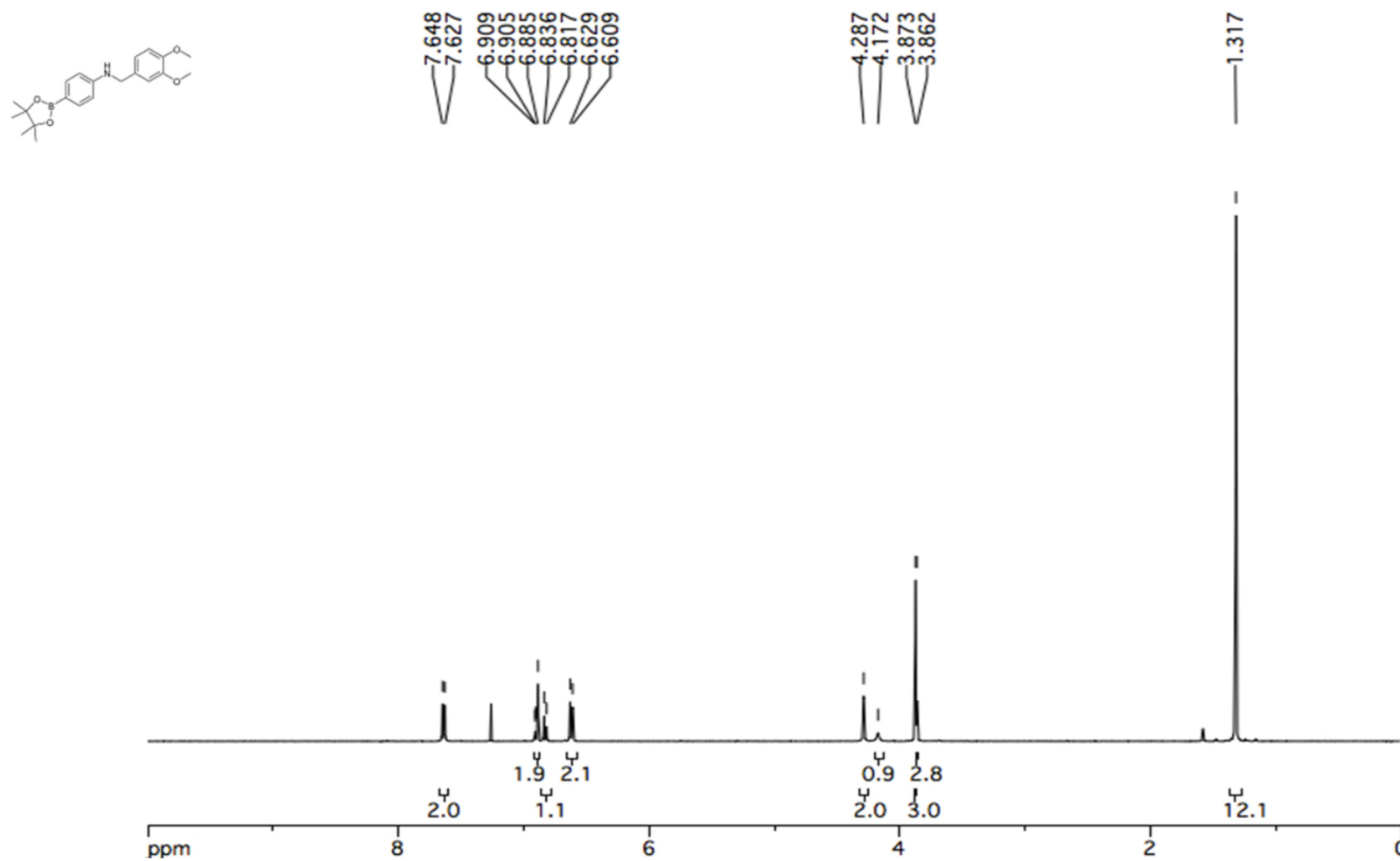
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Comment			

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		Set Detector TOF	2200 V

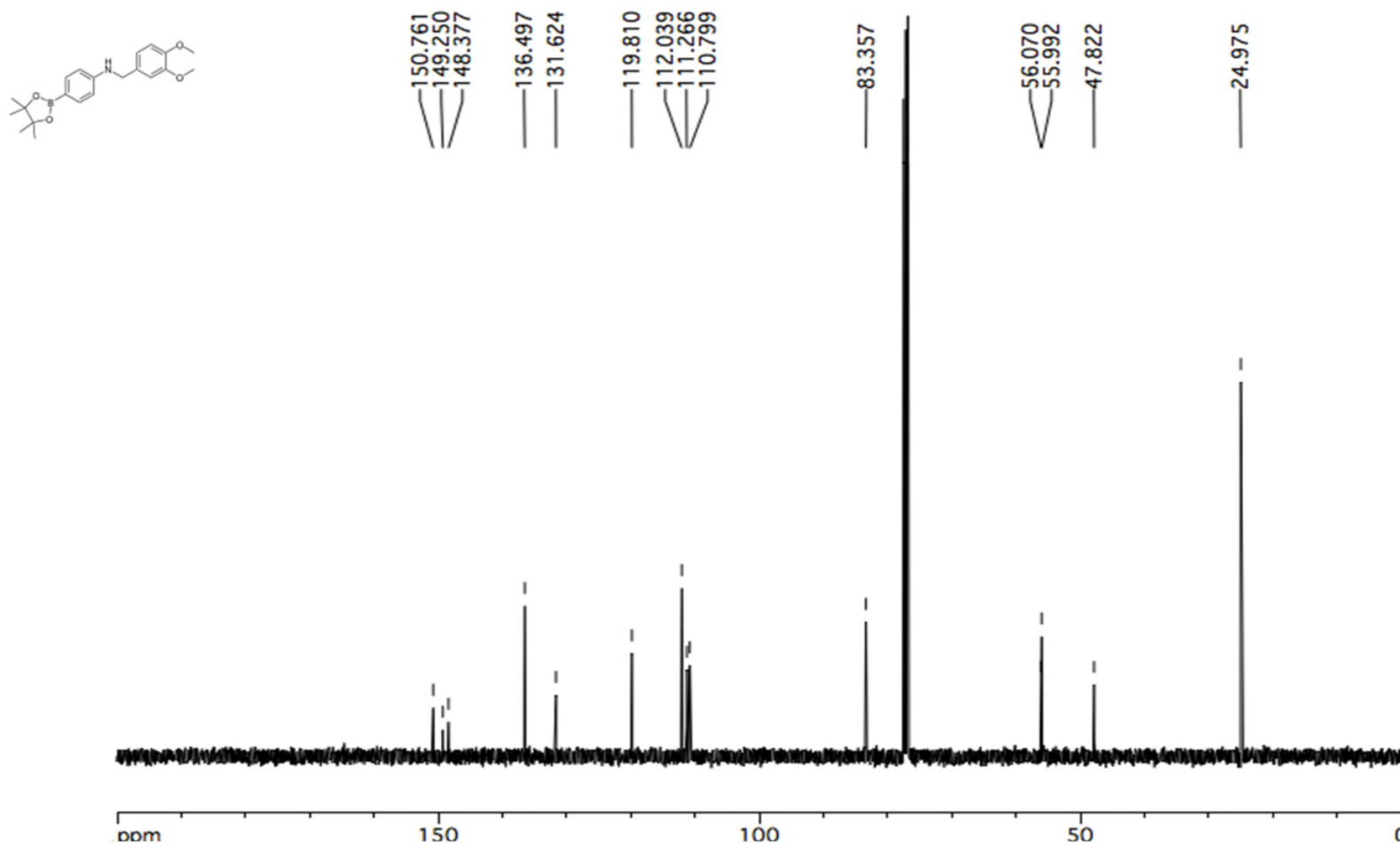


4-butyl-*N*-(3,4-dimethoxybenzyl)aniline (**18**) - HRMS

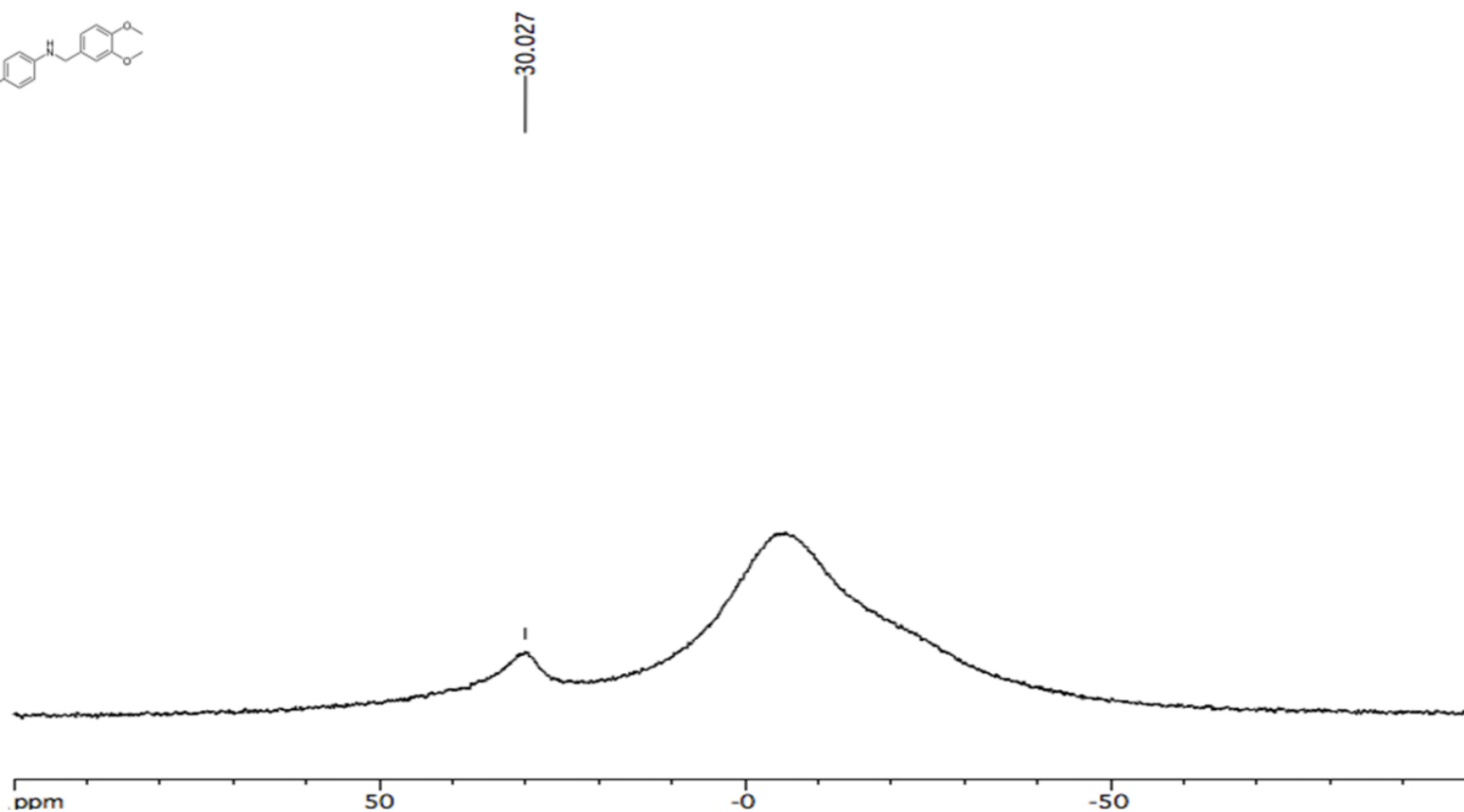
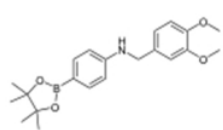
3,4-dimethoxy-N-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-benzenemethanamine (19) – ^1H NMR



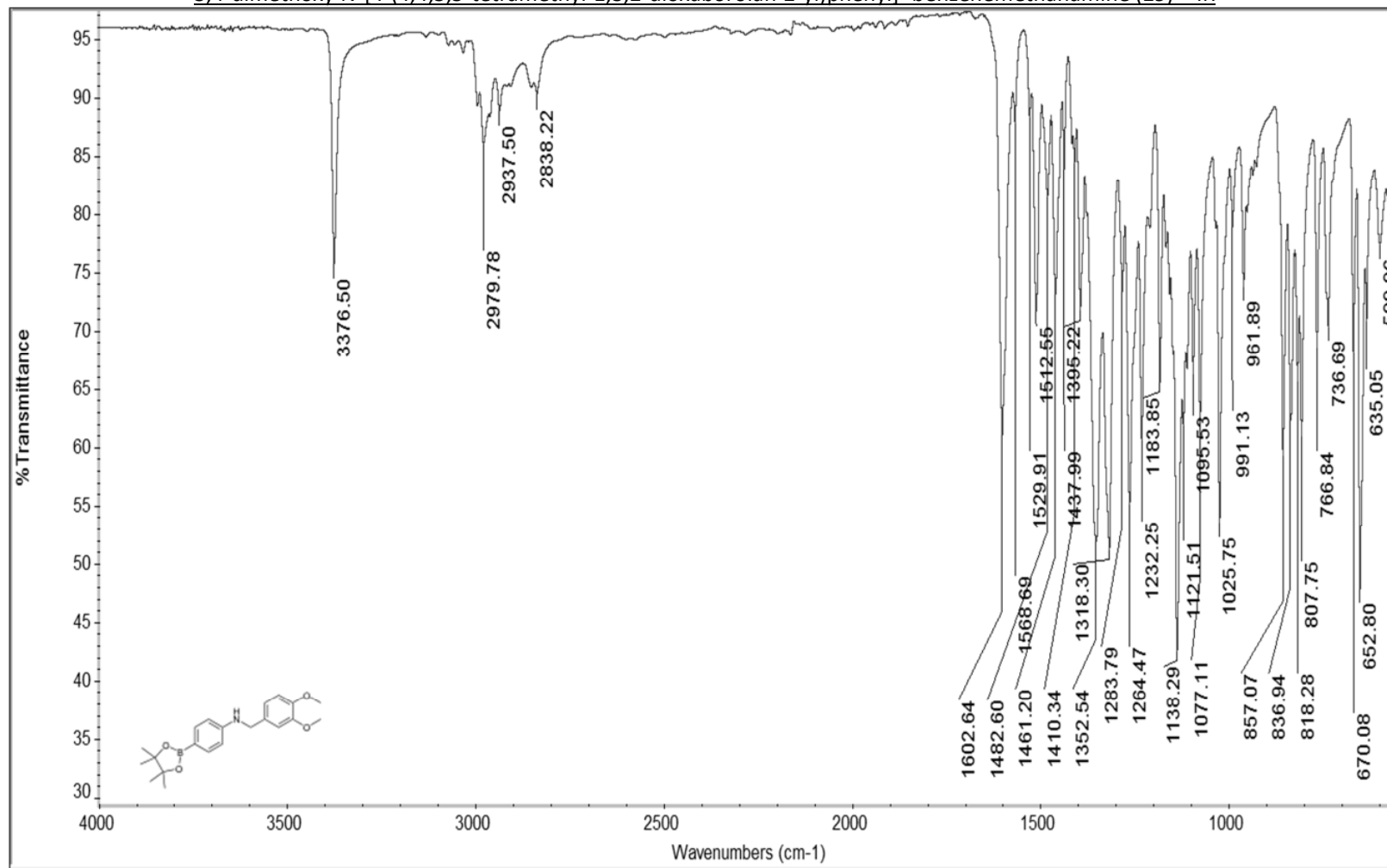
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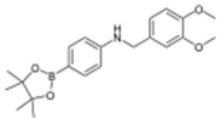


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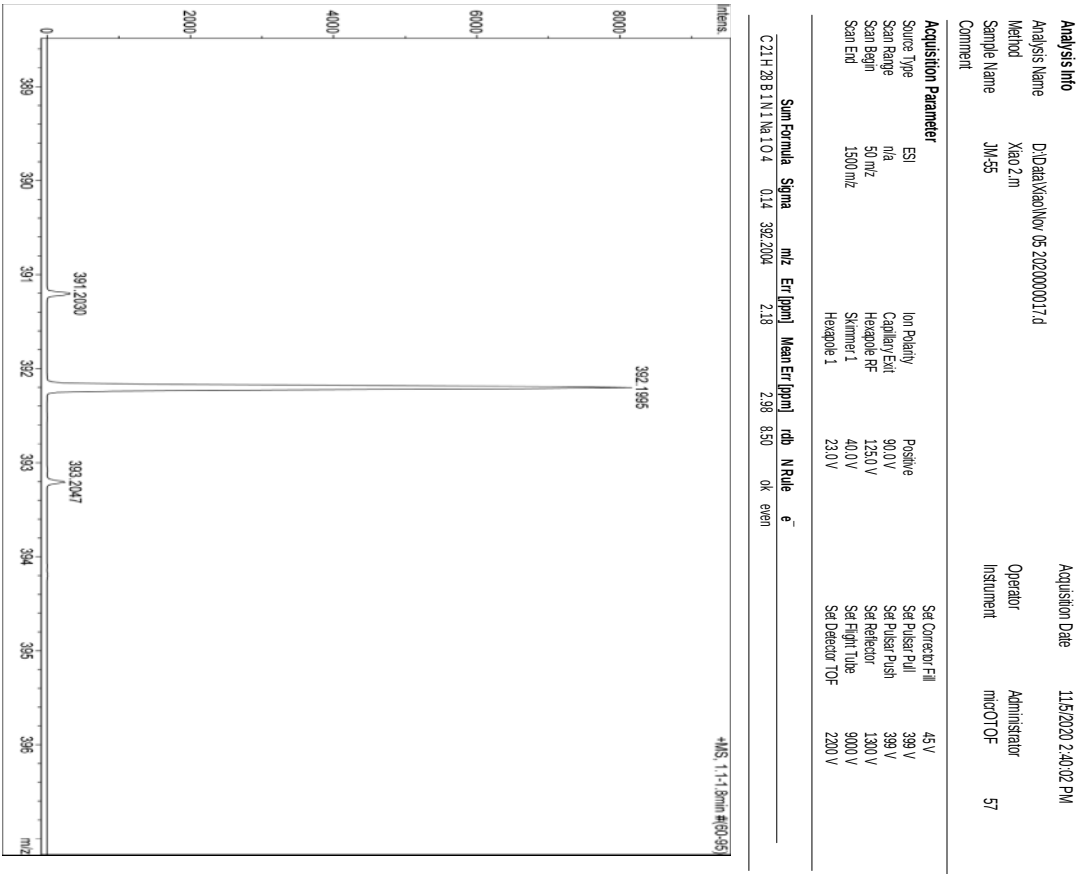


3,4-dimethoxy-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]- benzenemethanamine (**19**) – IR

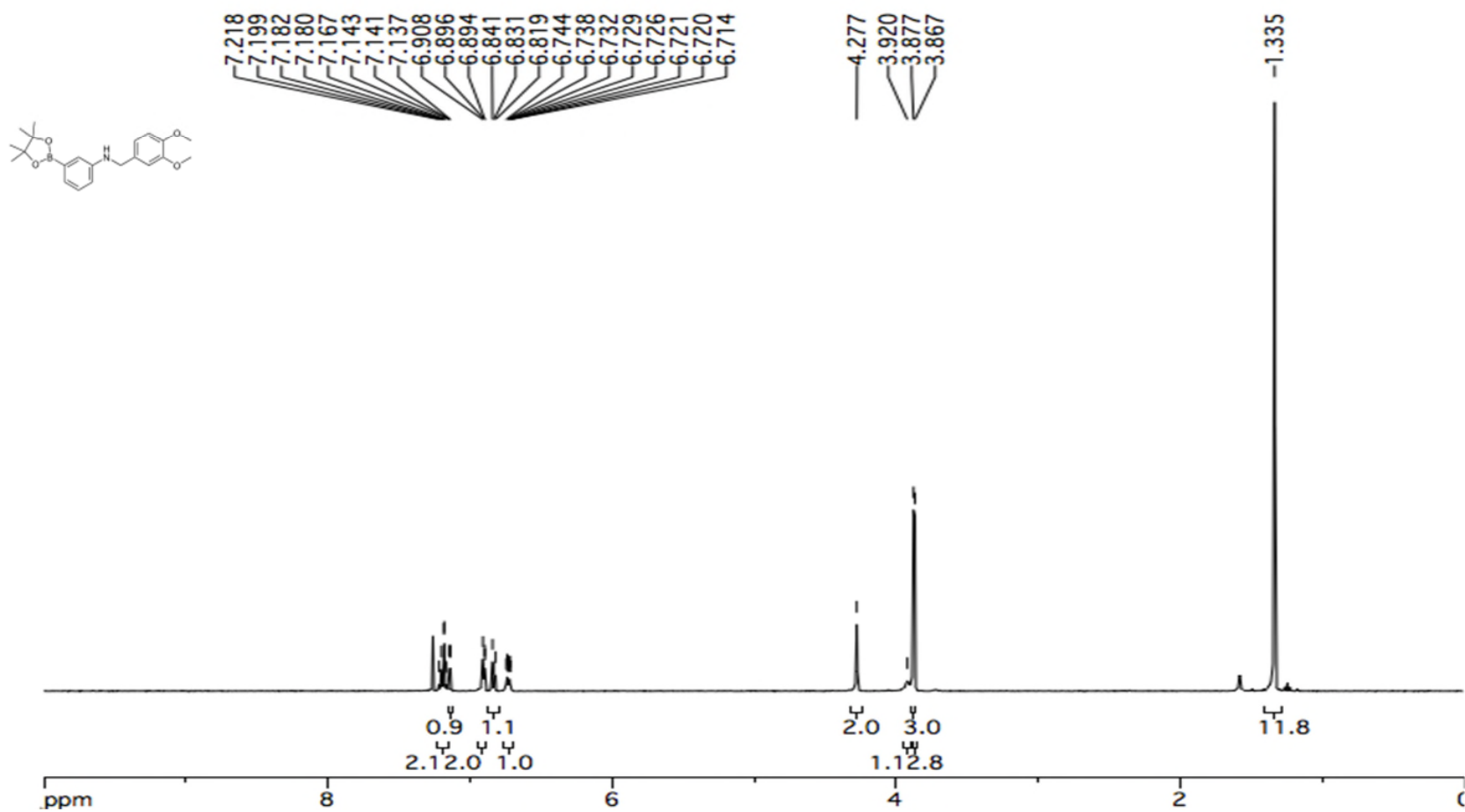




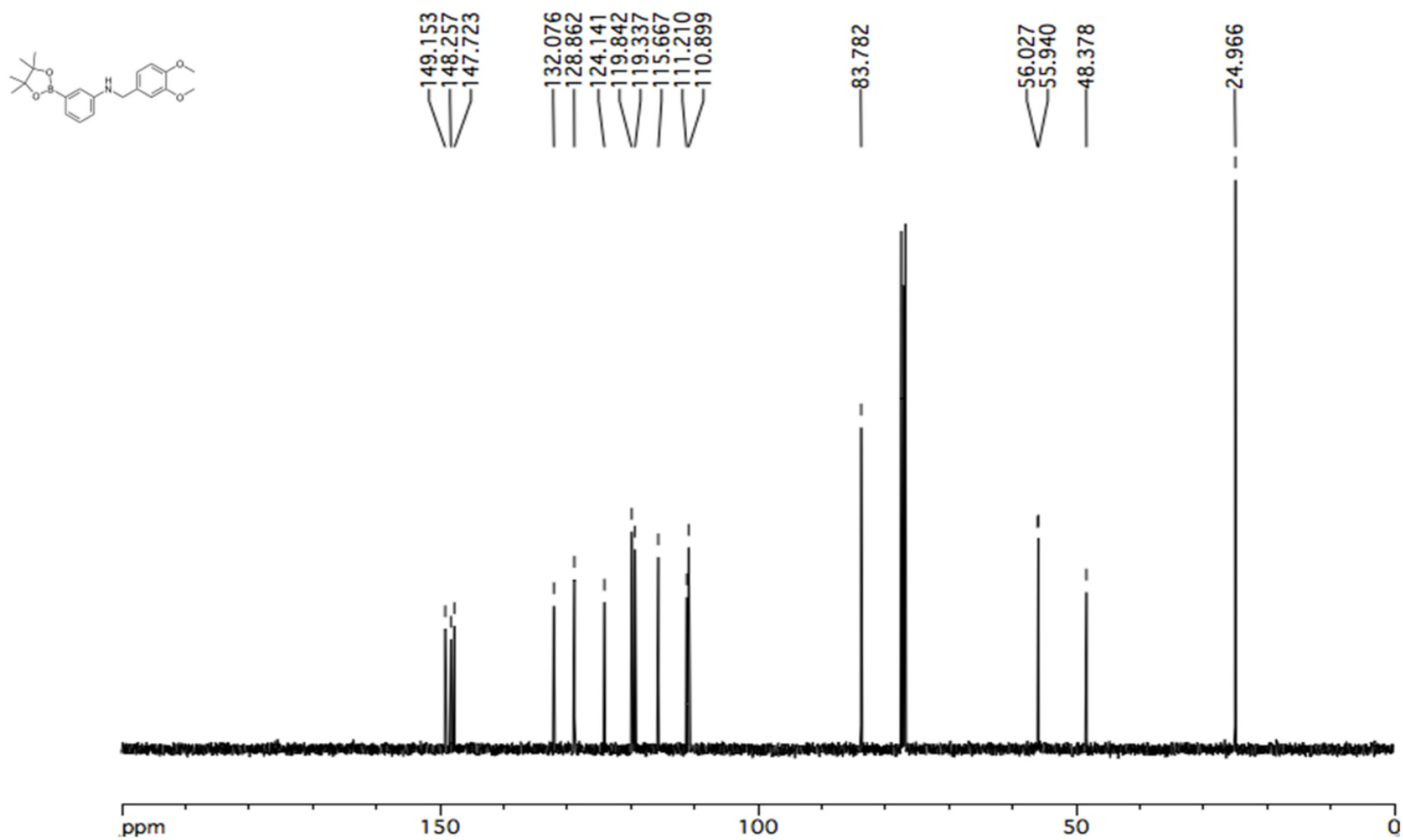
3,4-dimethoxy-N-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]- benzenemethanamine (19) – HRMS



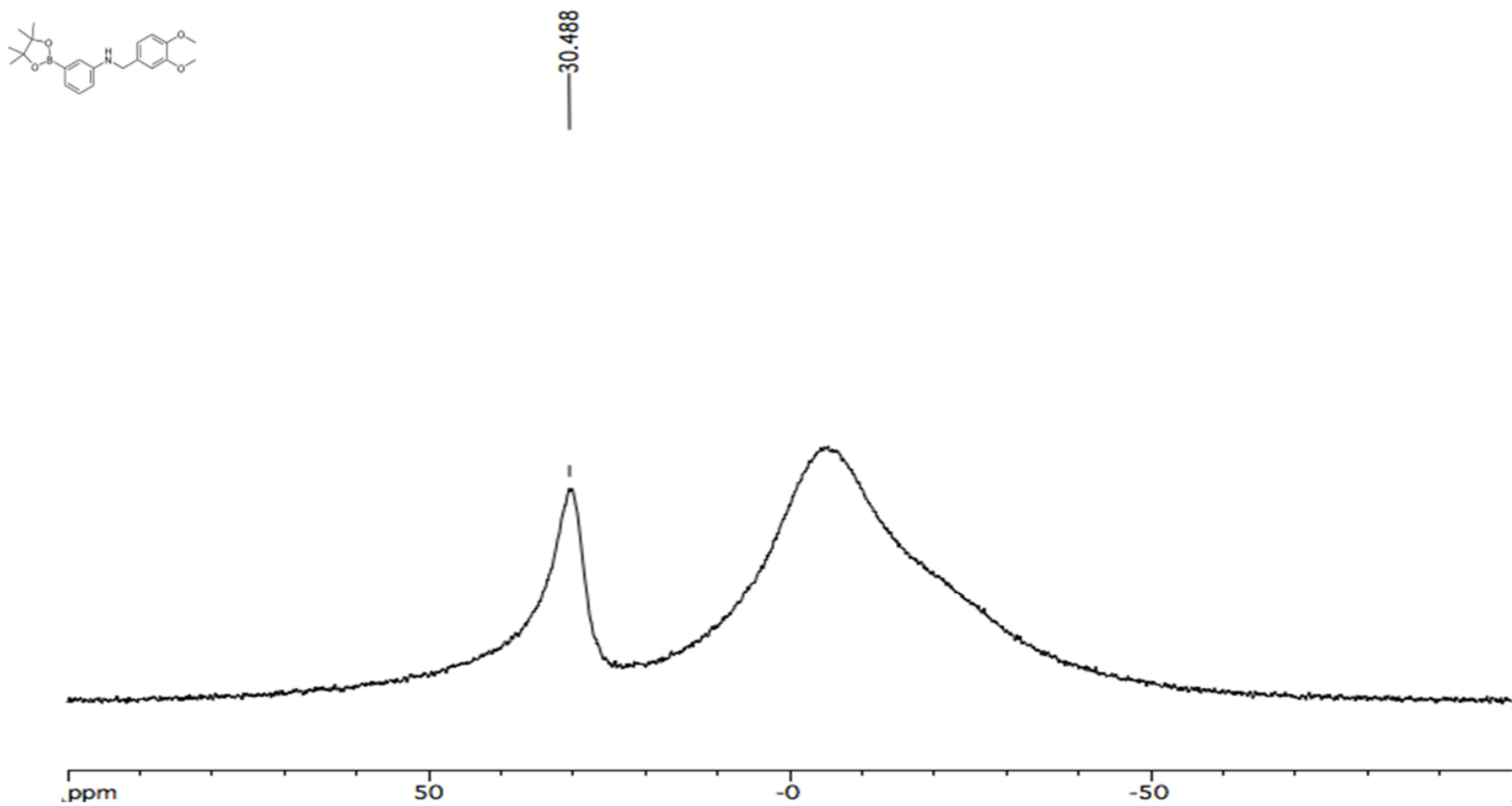
3,4-dimethoxy-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-benzenemethanamine (**20**) – ^1H NMR



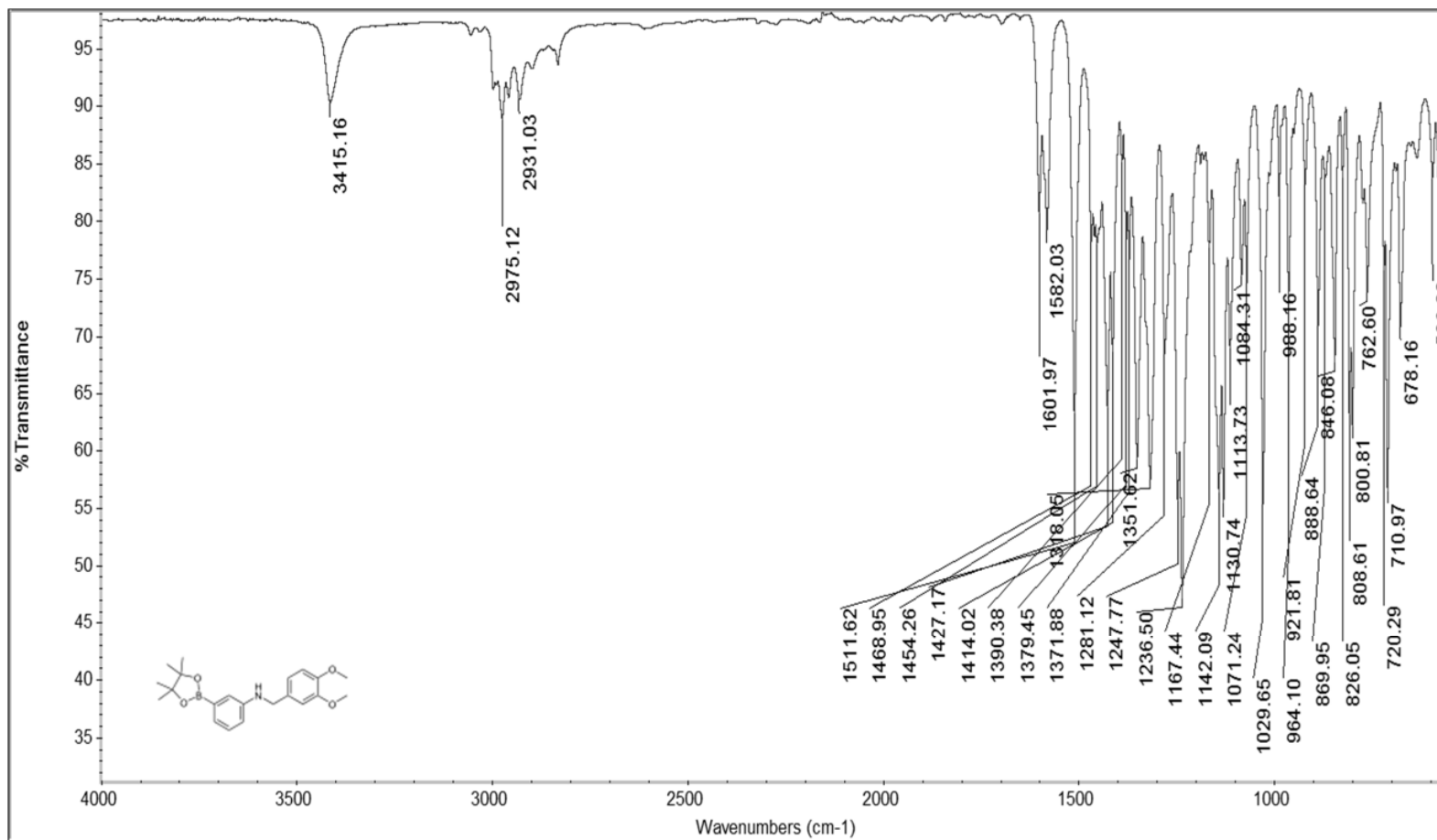
3,4-dimethoxy-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-benzenemethanamine (**20**) – ^{13}C NMR

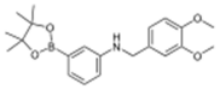


3,4-dimethoxy-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-benzenemethanamine (20) – ^{11}B NMR



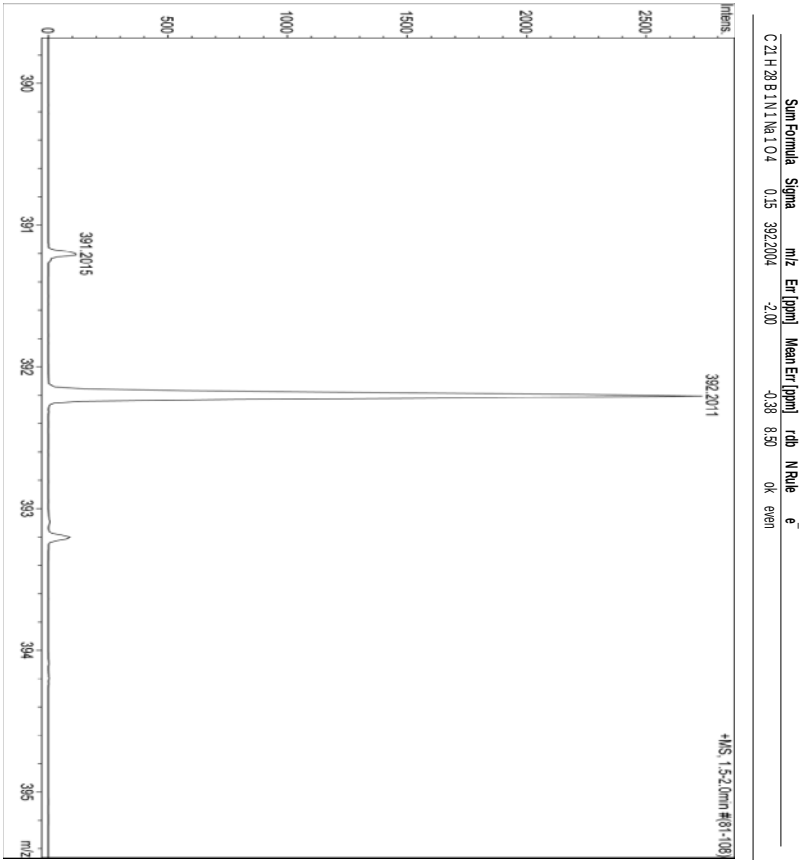
3,4-dimethoxy-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-benzenemethanamine (20) – IR





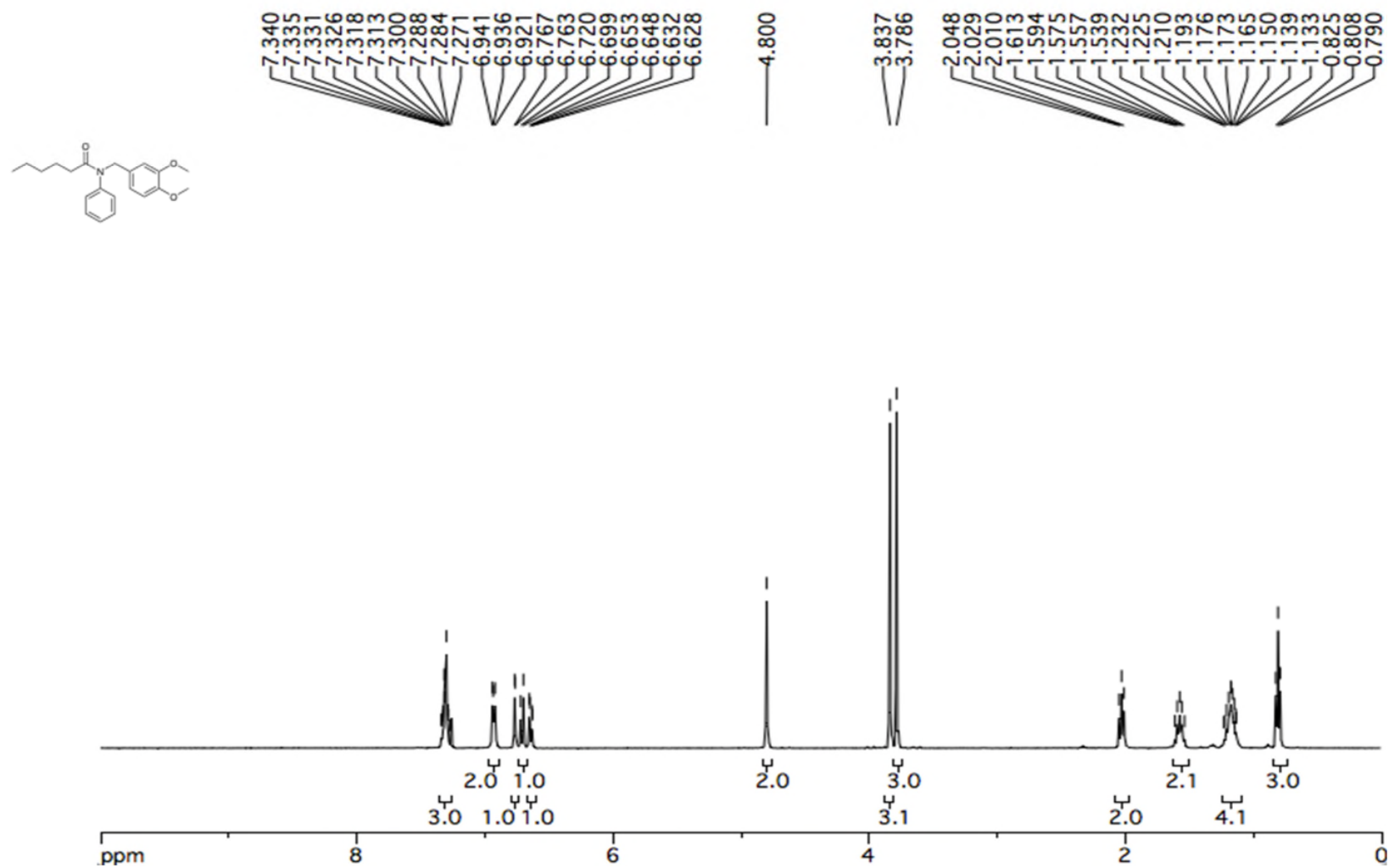
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Method	Xiao 2.m	Operator
Sample Name	JM-54	Administrator
Comment		Instrument
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		57

Acquisition Parameter					
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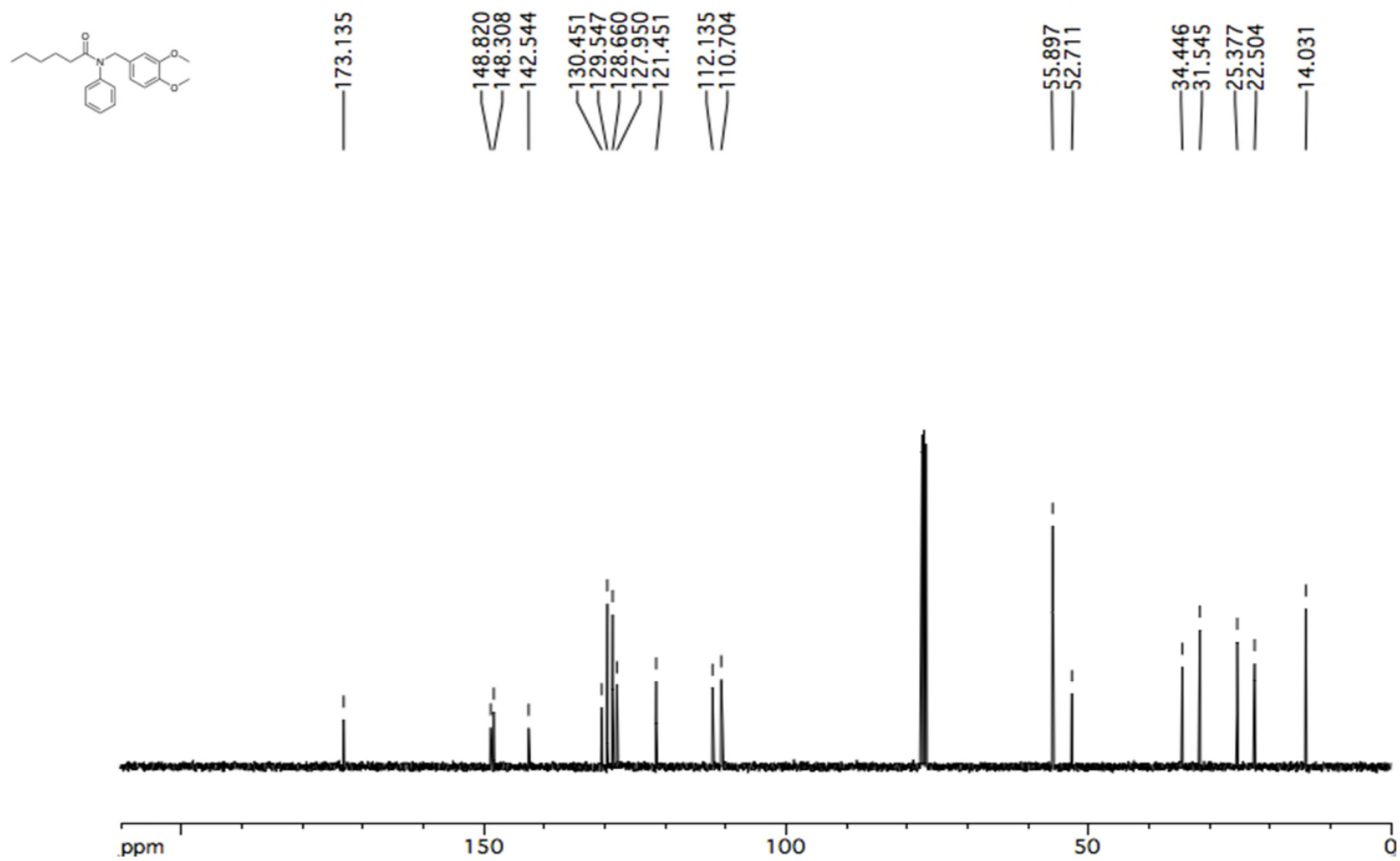


3,4-dimethoxy-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-benzenemethanamine (20) – HRMS

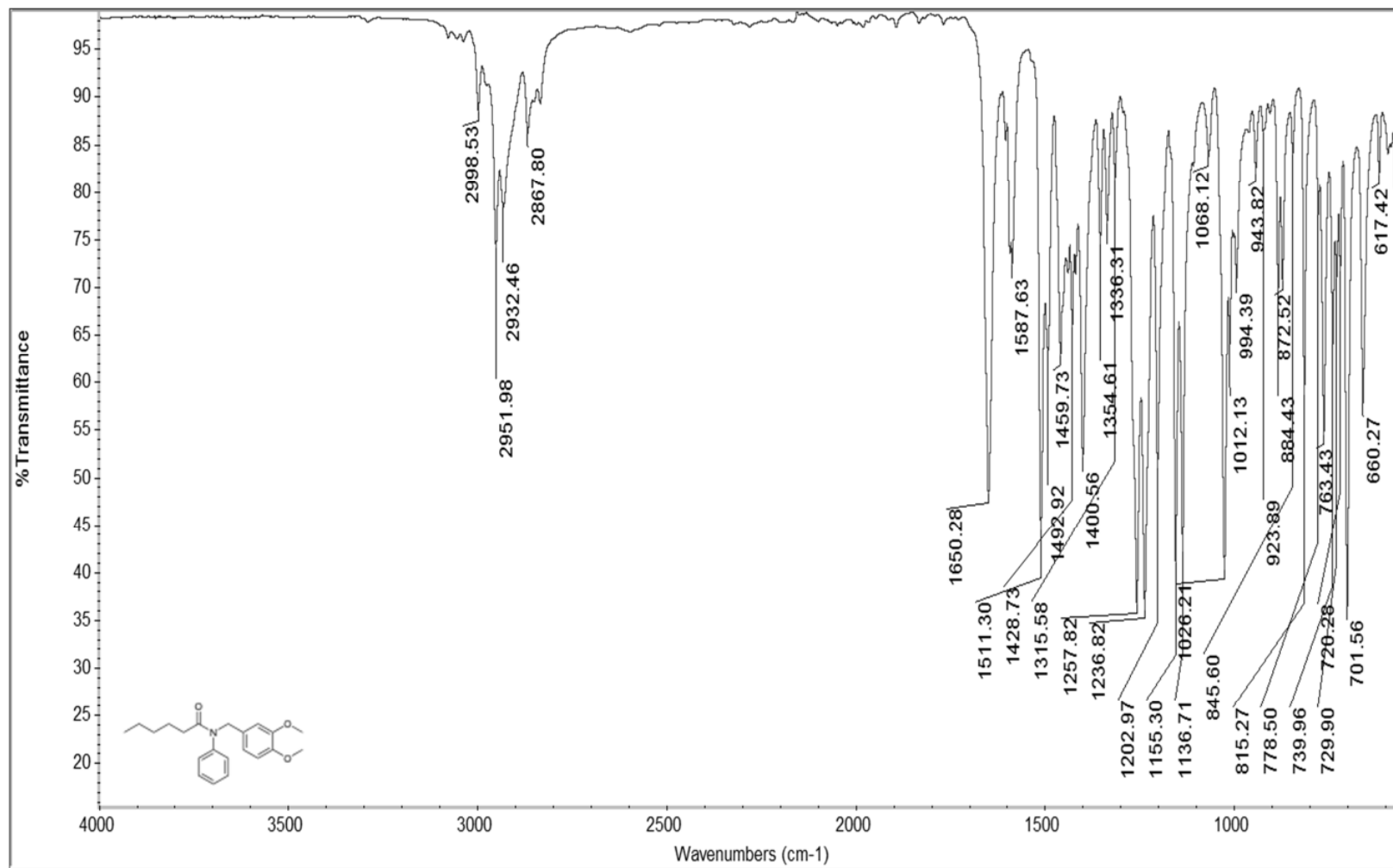
N-[3,4-dimethoxyphenyl)methyl]-*N*-(phenyl)-hexanamide (**21**) – ^1H NMR

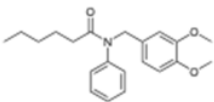


N-[3,4-dimethoxyphenyl)methyl]-*N*-(phenyl)-hexanamide (**21**) – ^{13}C NMR



N-[3,4-dimethoxyphenyl)methyl]-*N*-(phenyl)-hexanamide (**21**) – IR





Analysis Info

Analysis Name D:\Data\Xiao\Nov 06 2020\000011.d
Method Xiao 2.m
Sample Name MFL-93
Comment

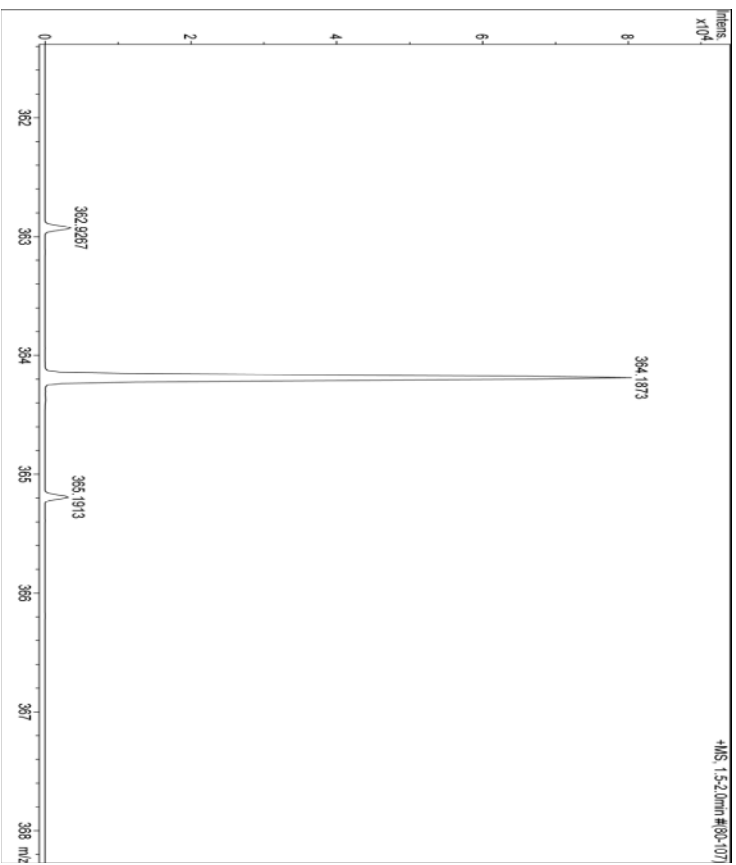
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Operator Administrator
Instrument microTOF 57

Acquisition Parameter

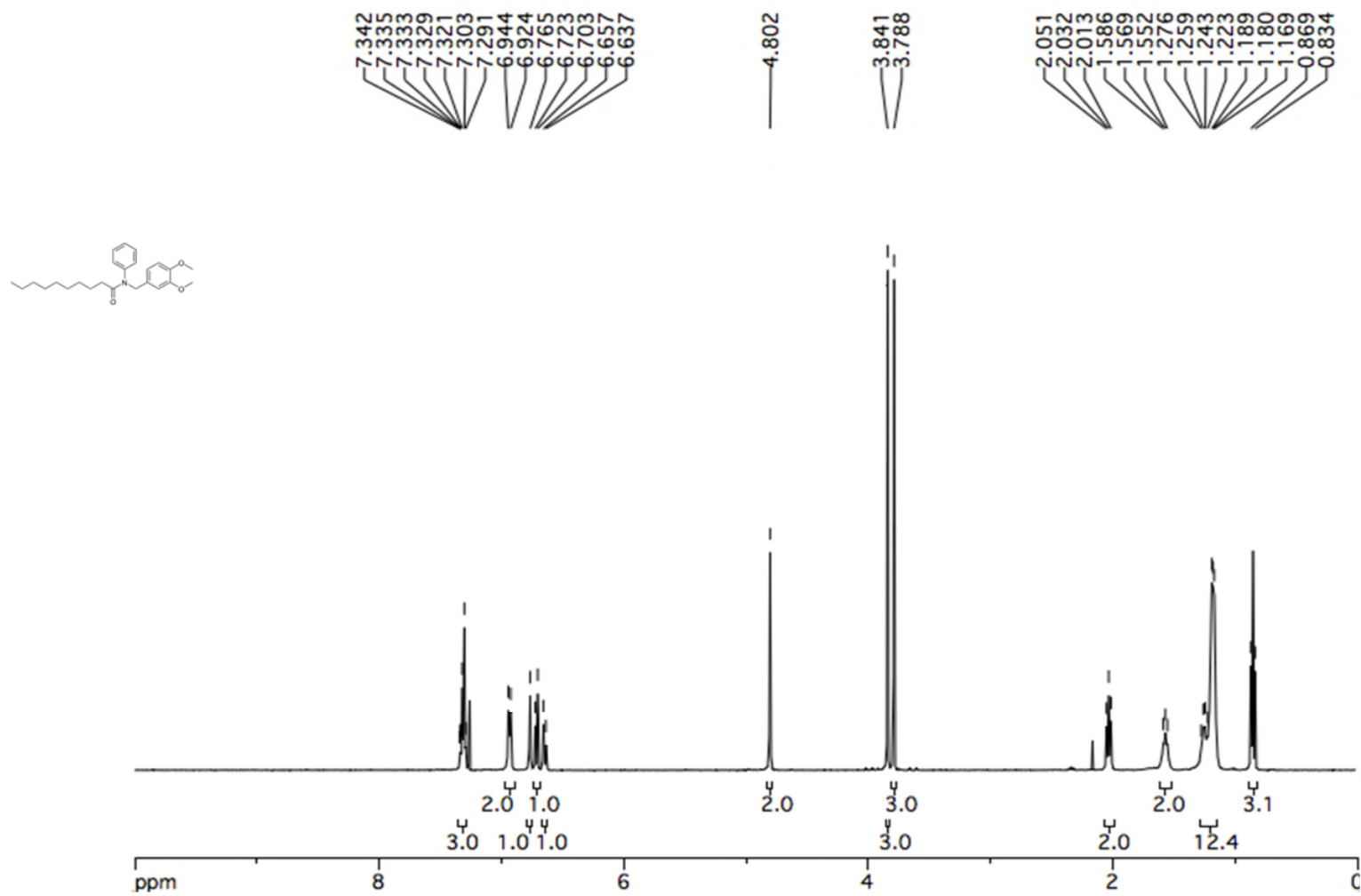
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Scan End	1500 m/z	Skimmer 1	40.0 V	Set Reflector	1300 V
		Hexapole 1	23.0 V	Set Flight Tube	9000 V
				Set Detector TOF	2200 V

Sum Formula	Sigma	m/z	Erf (ppm)	Mean Erf (ppm)	rtb	N Rule	e ⁻
C ₂₁ H ₂₇ N ₁ O ₃	0.11	364.1883	2.67	2.23	8.30	OK	even

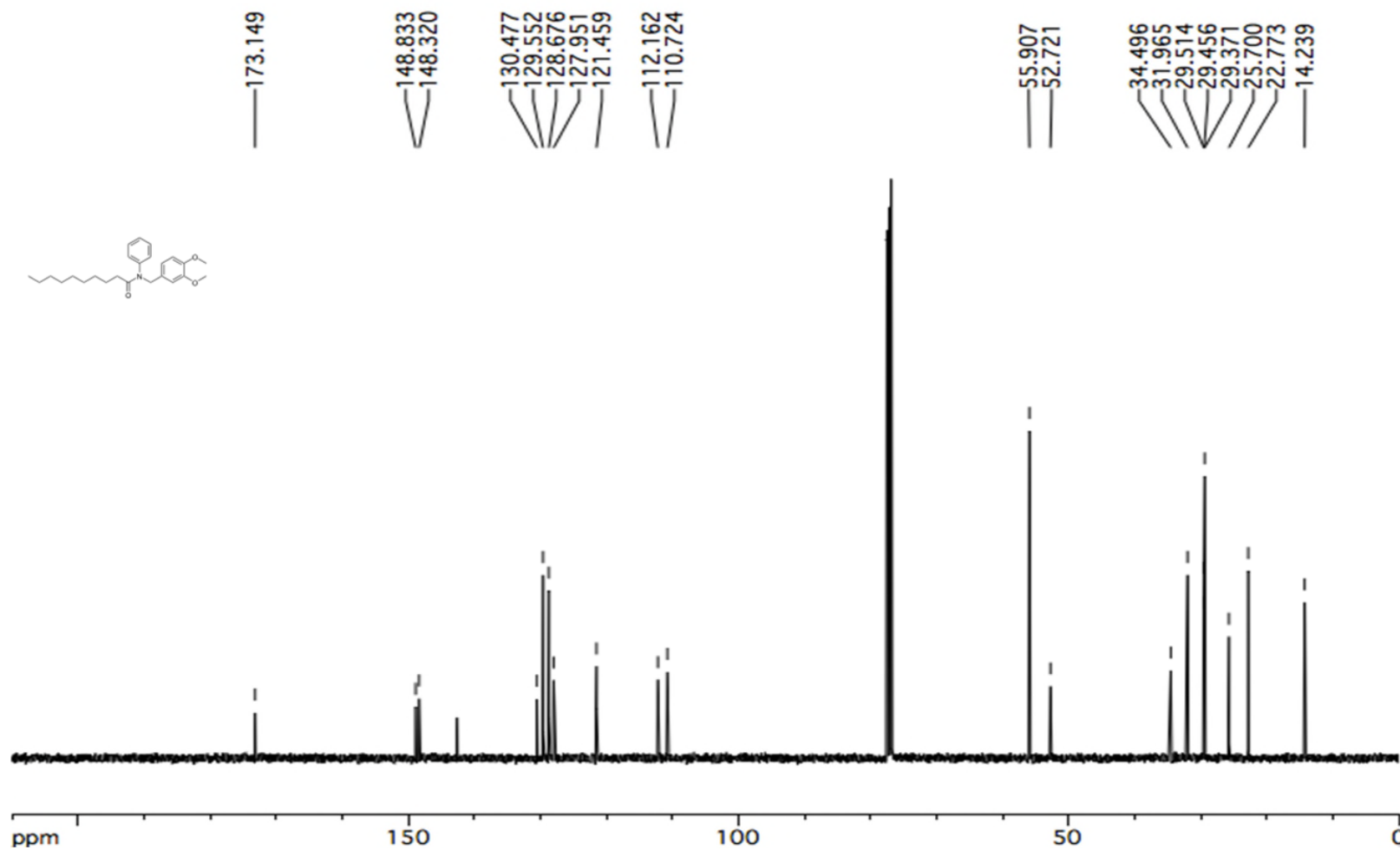


N-[3,4-dimethoxyphenyl)methyl]-N-(phenyl)-hexanamide (21) – HRMS

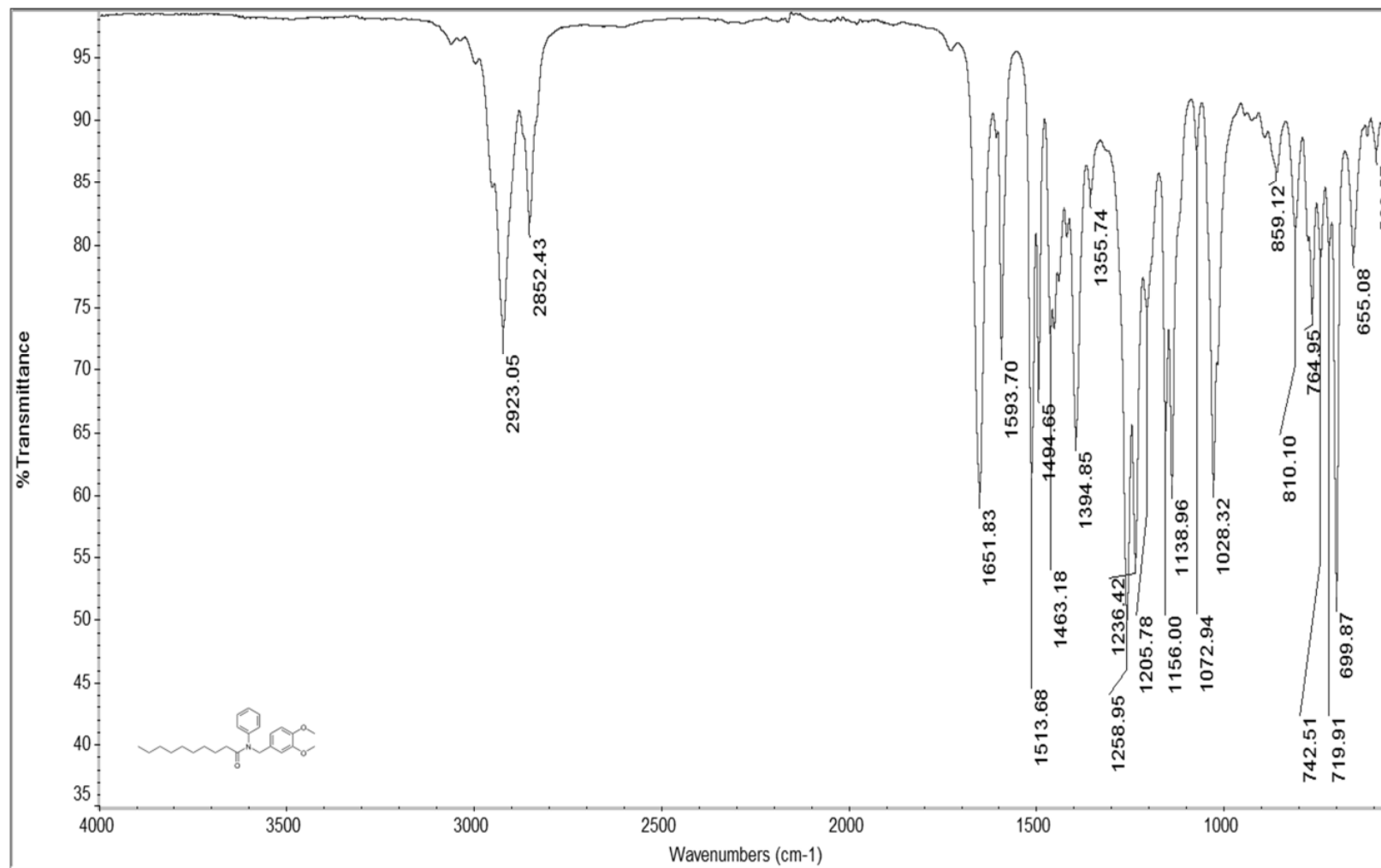
N-[3,4-dimethoxyphenyl)methyl]-*N*-(phenyl)-decanamide (**22**) – ^1H NMR



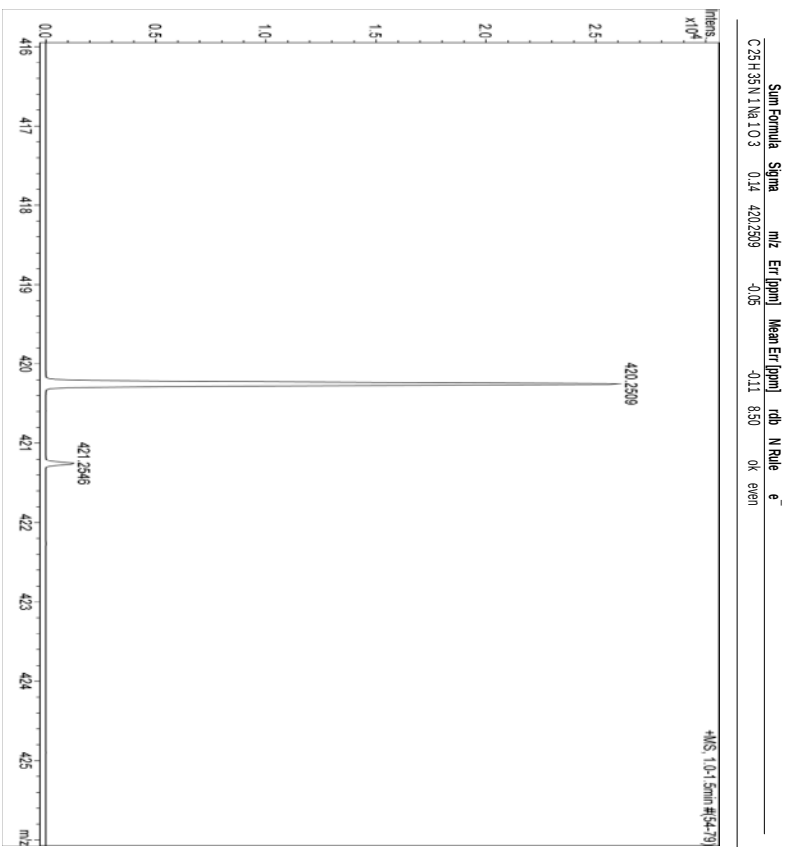
N-[3,4-dimethoxyphenyl)methyl]-*N*-(phenyl)-decanamide (**22**) – ^{13}C NMR



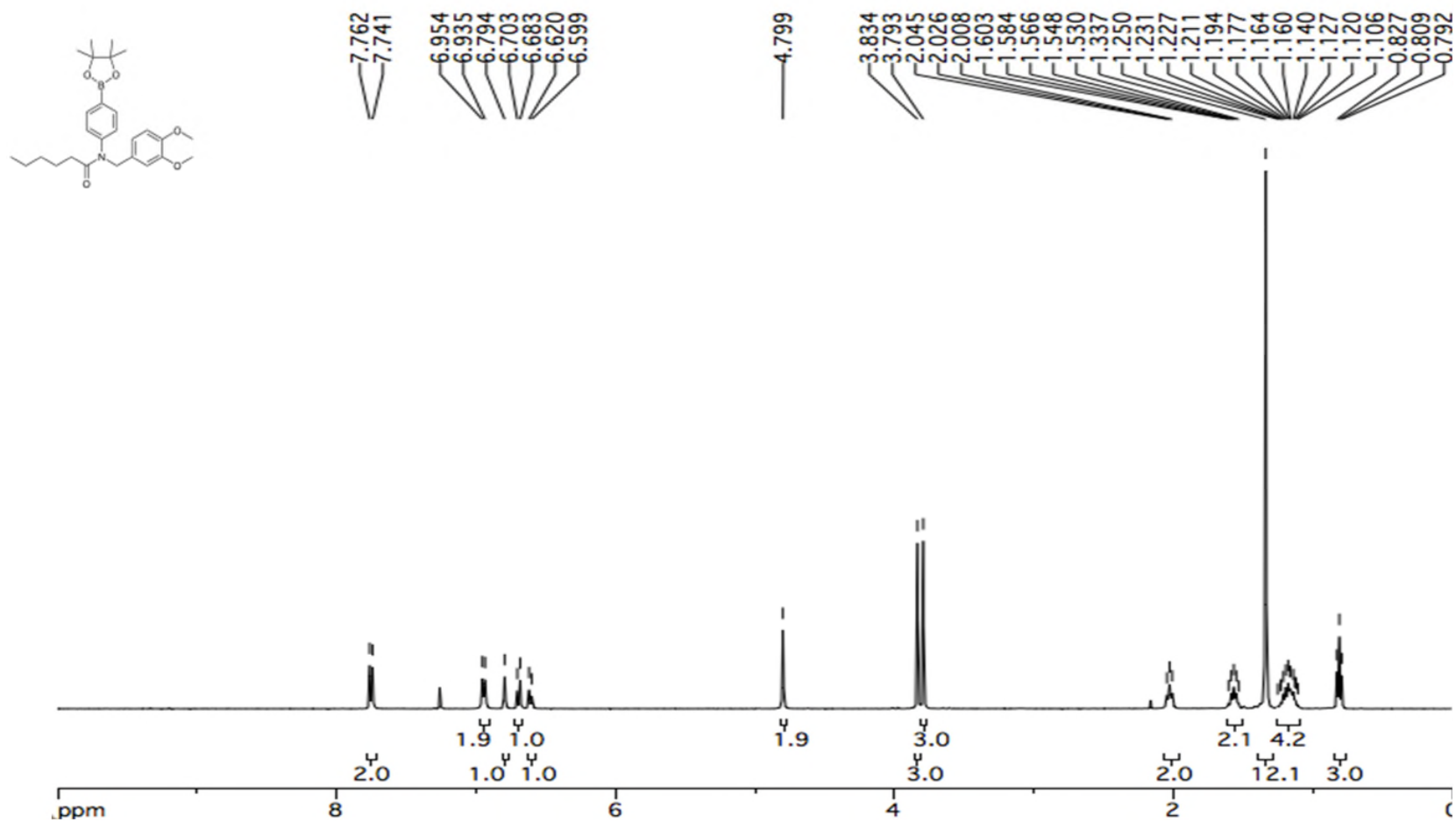
N-[3,4-dimethoxyphenyl)methyl]-*N*-(phenyl)-decanamide (**22**) – IR



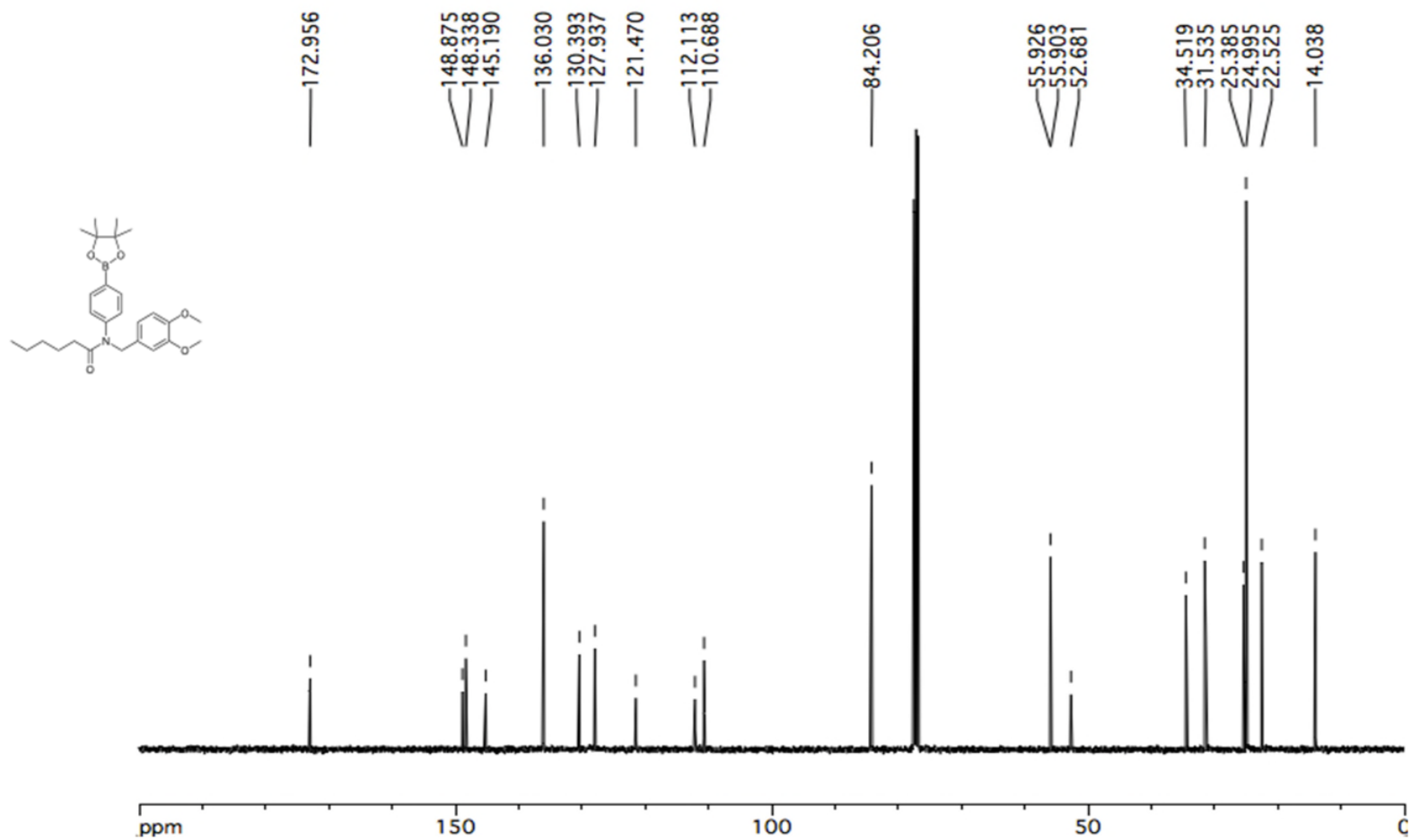
Acquisition Parameter			
Source Type	ESI	Sol Collector Fill	45 V
Scan Range	m/z	Sol Pulsar Pull	399 V
Scan Begin	50 m/z	Sol Pulsar Push	339 V
Scan End	1500 m/z	Sol Retract	1300 V
		Sol Flight Tube	900 V
		Sol Detector (DC)	220 V



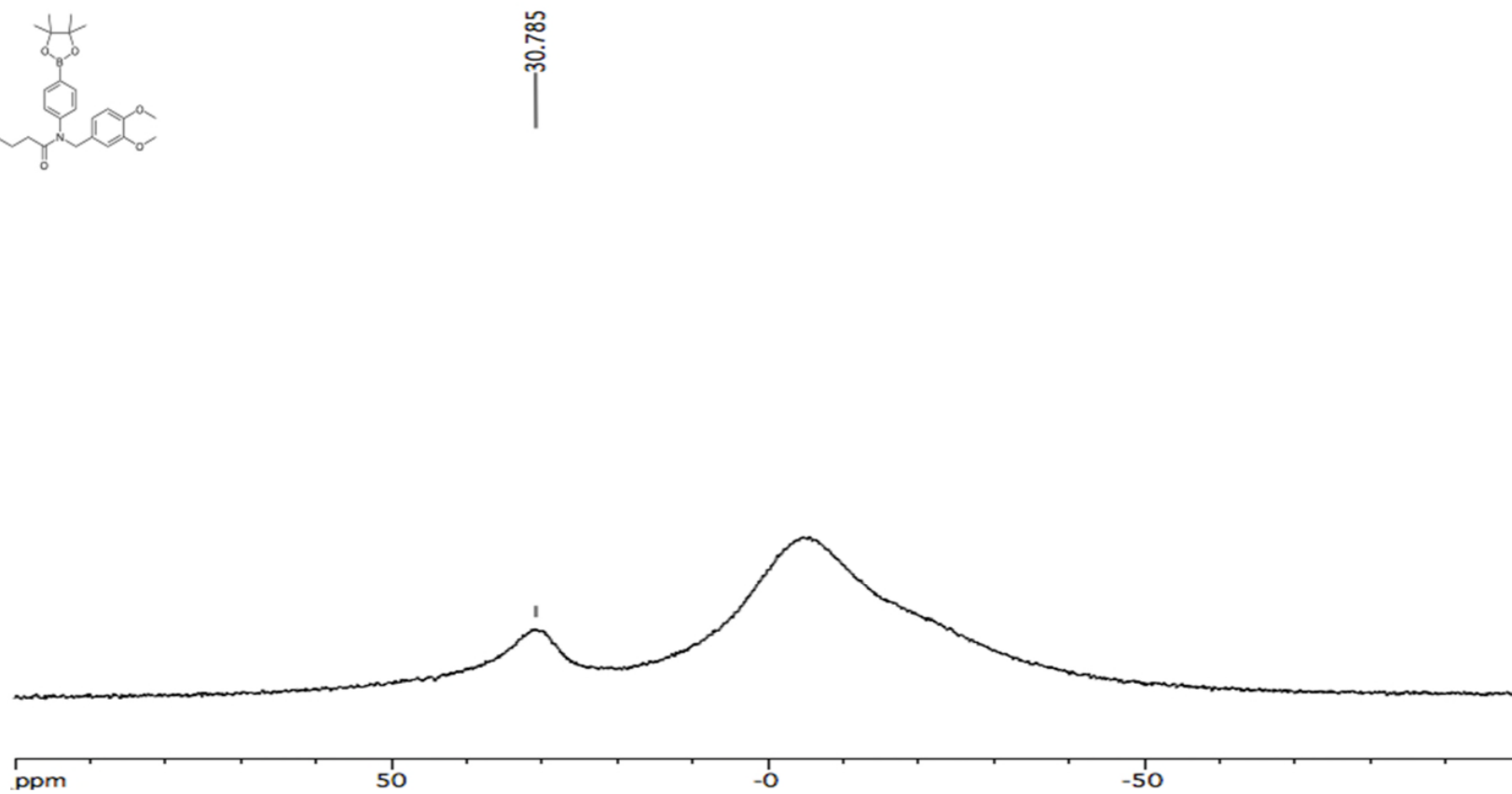
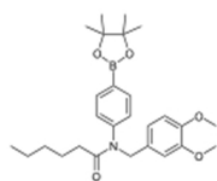
N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**23**) – ^1H NMR



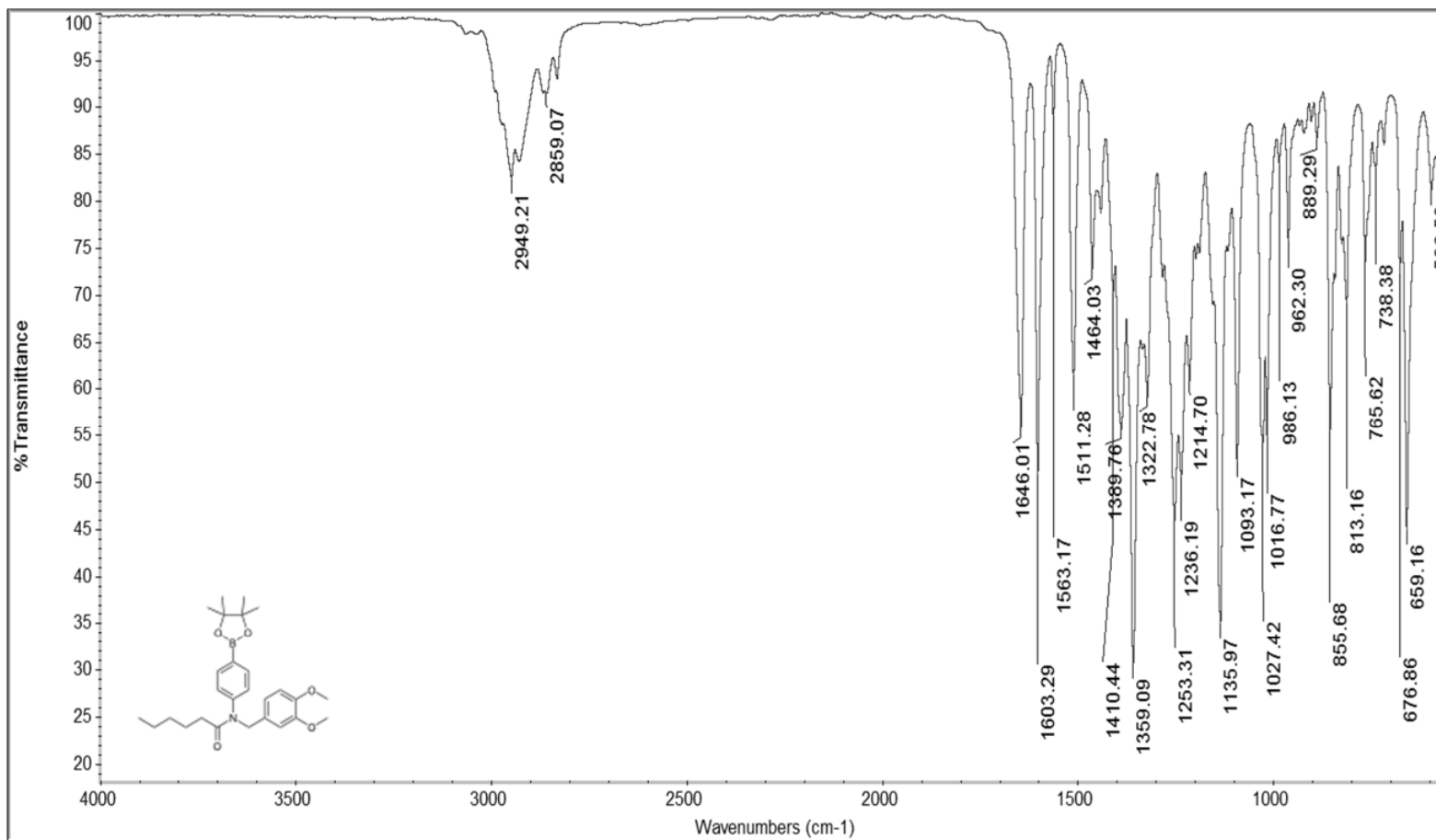
N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**23**) – ^{13}C NMR

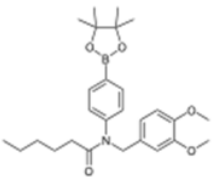


N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**23**) – ^{11}B NMR

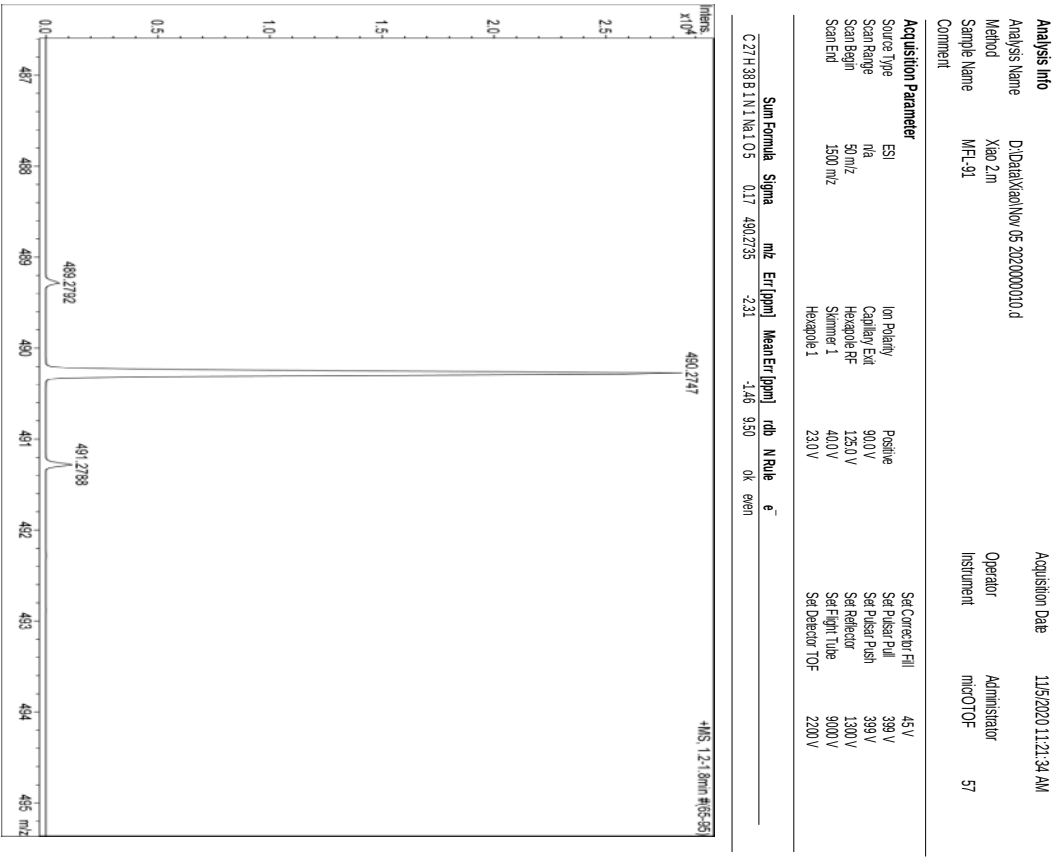


N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**23**) – IR

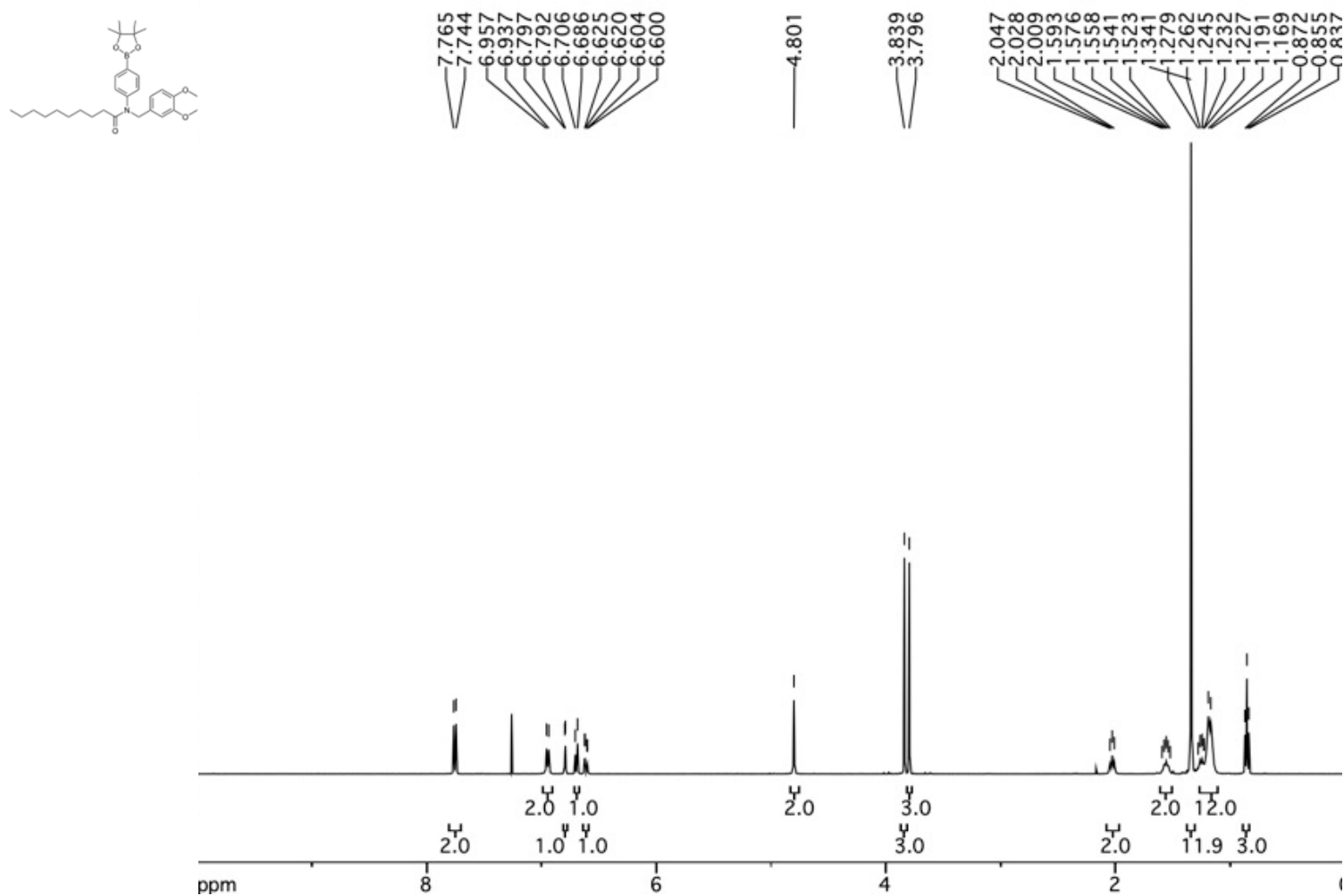




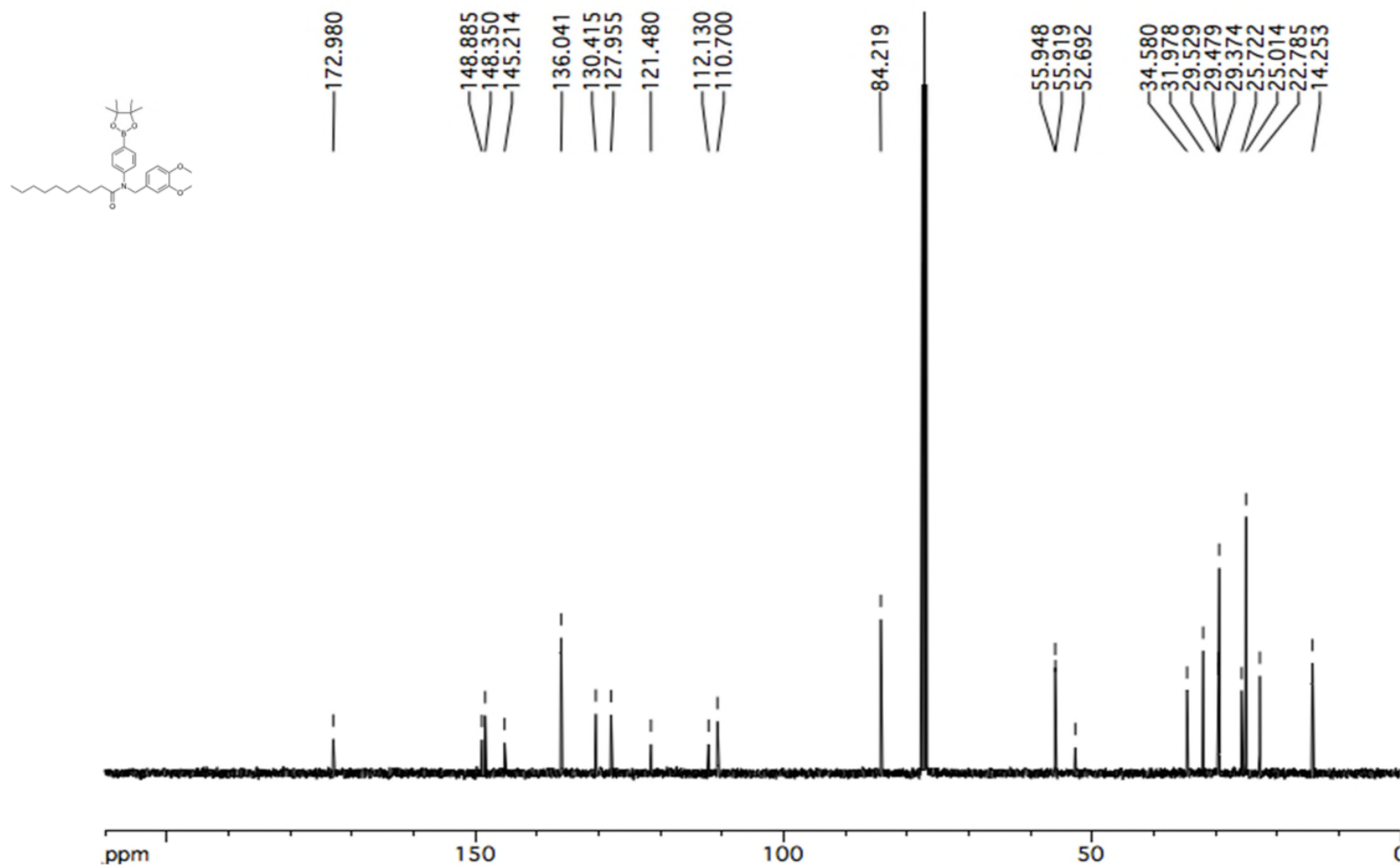
N-(3,4-dimethoxyphenylmethyl)-N-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (23) – HRMS



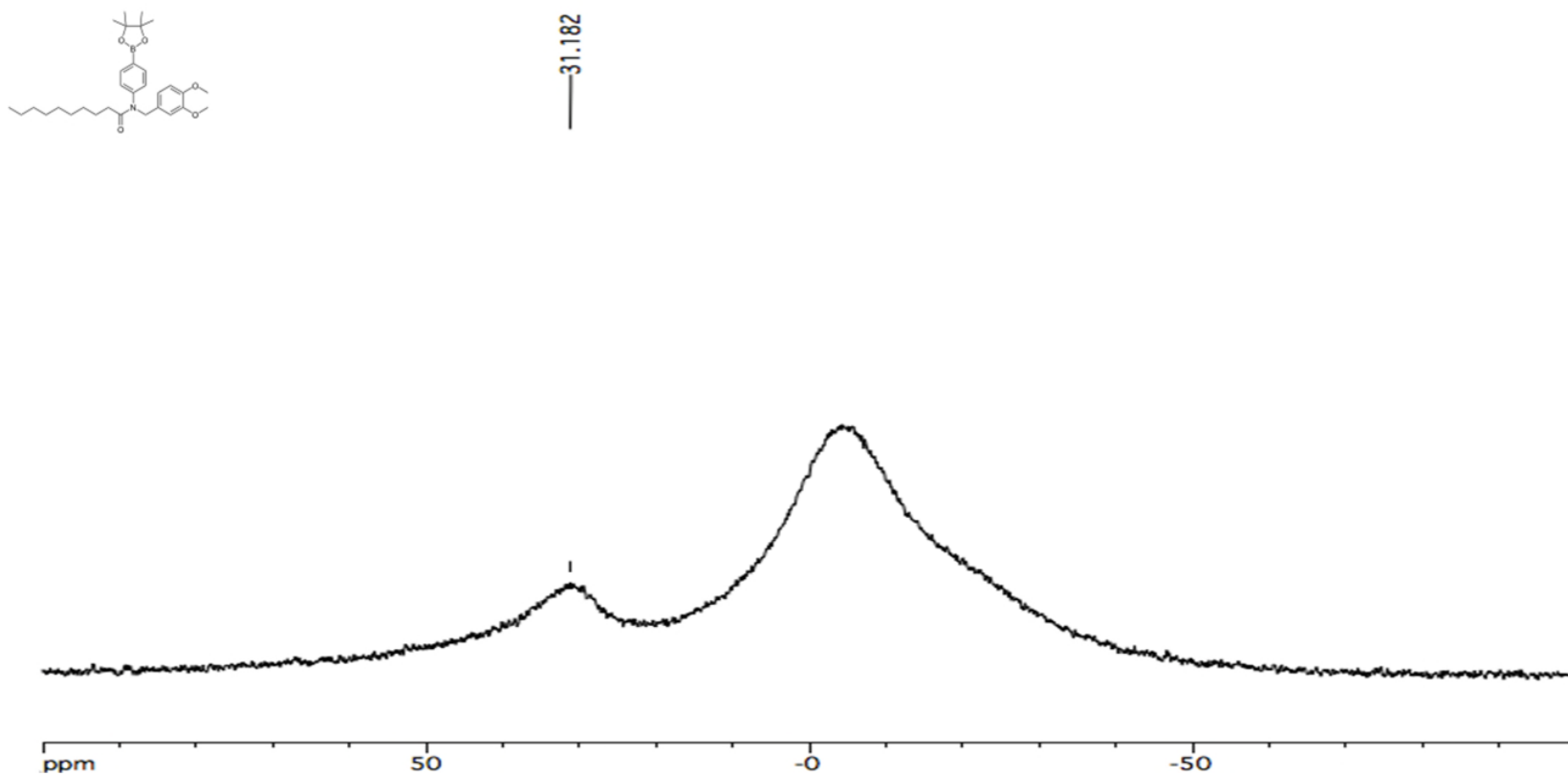
N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**24**) – ^1H NMR



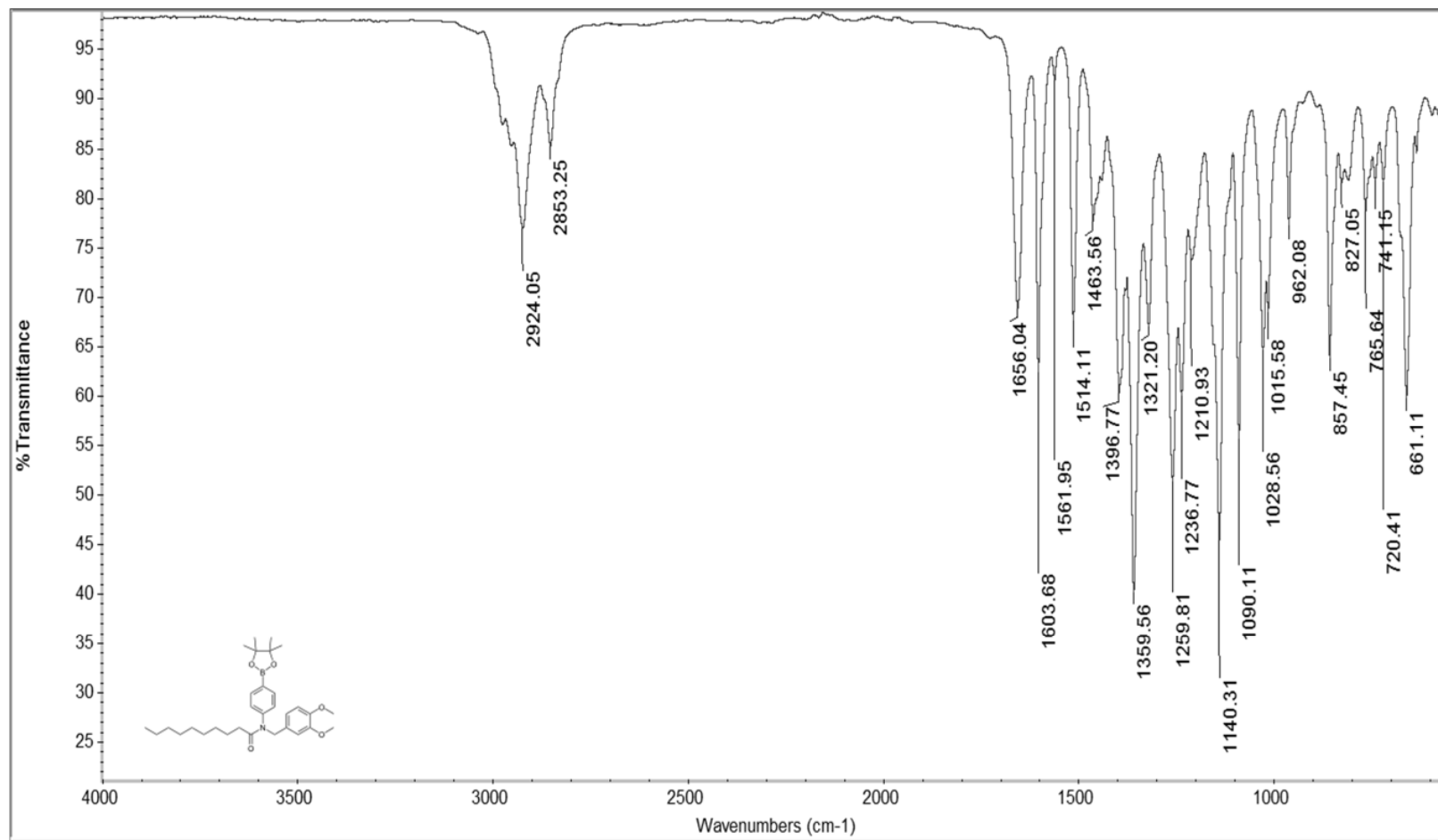
N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**24**)— ^{13}C NMR

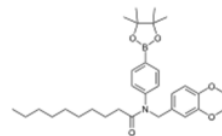


N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**24**) – ^{11}B NMR



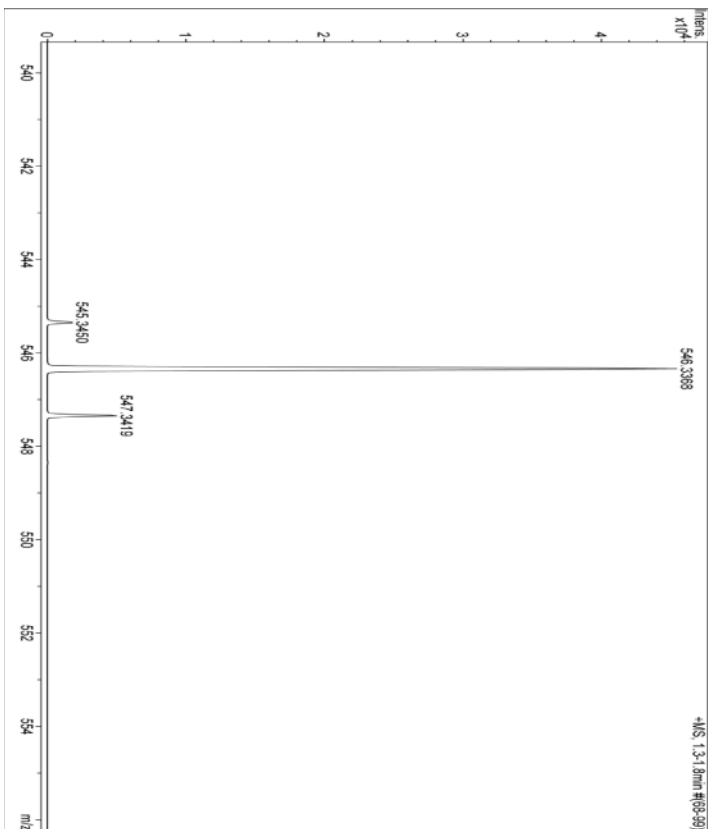
N-(3,4-dimethoxyphenylmethyl)-*N*-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**24**) – IR





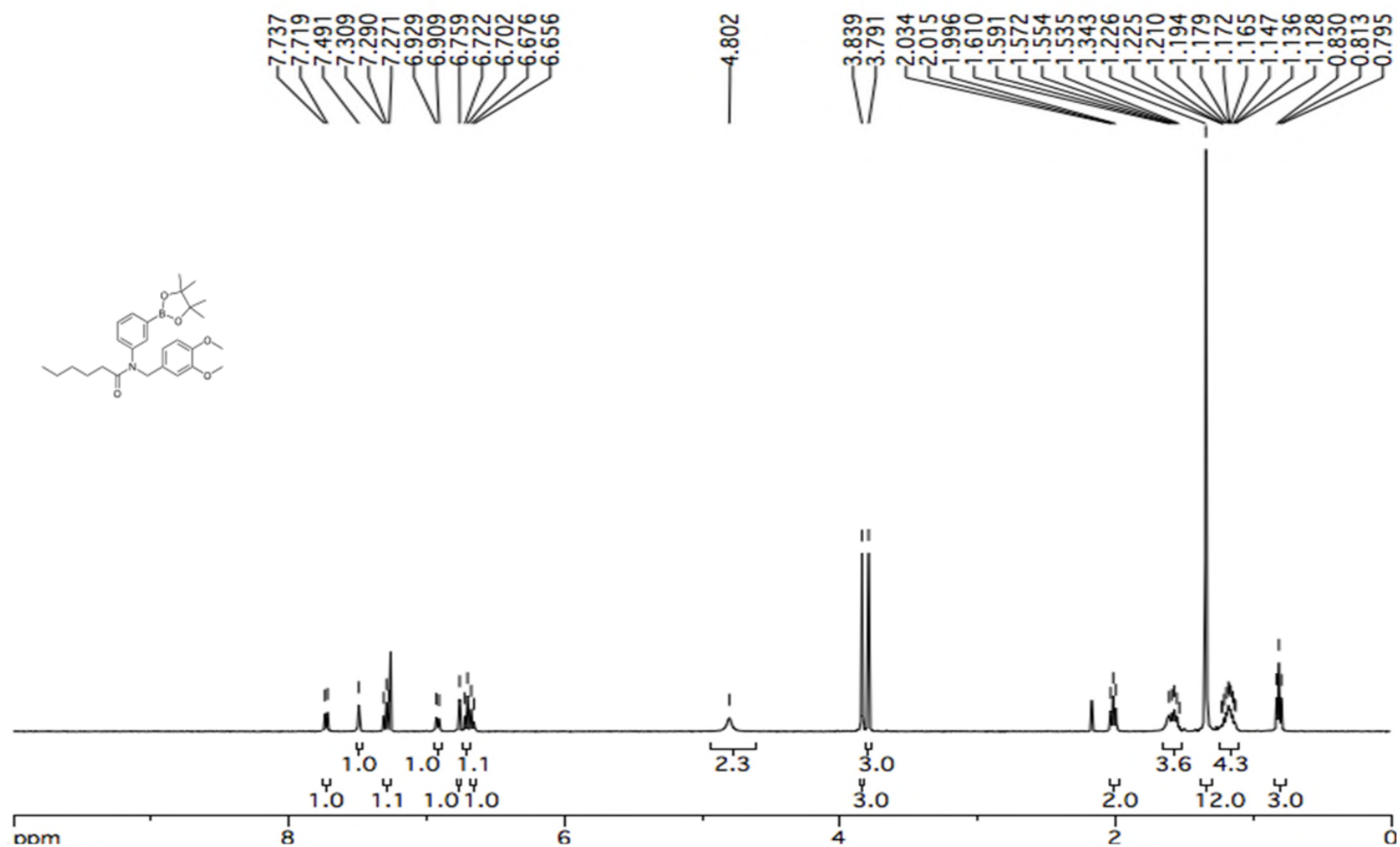
Analysis Info		Acquisition Date
Analysis Name	D:\Data\Xian\Nov_05_2020\000013.d	11/5/2020 1:56:29 PM
Method	Xao 2.m	
Sample Name	MFI-103	
Comment		

Sum Formula	Sigma	m/z	Err (ppm)	Mean Err (ppm)	orb	N Rule	e ⁻
C31H46BINO5	0.13	546.3361	-1.74	-1.33	9.50	OK	even

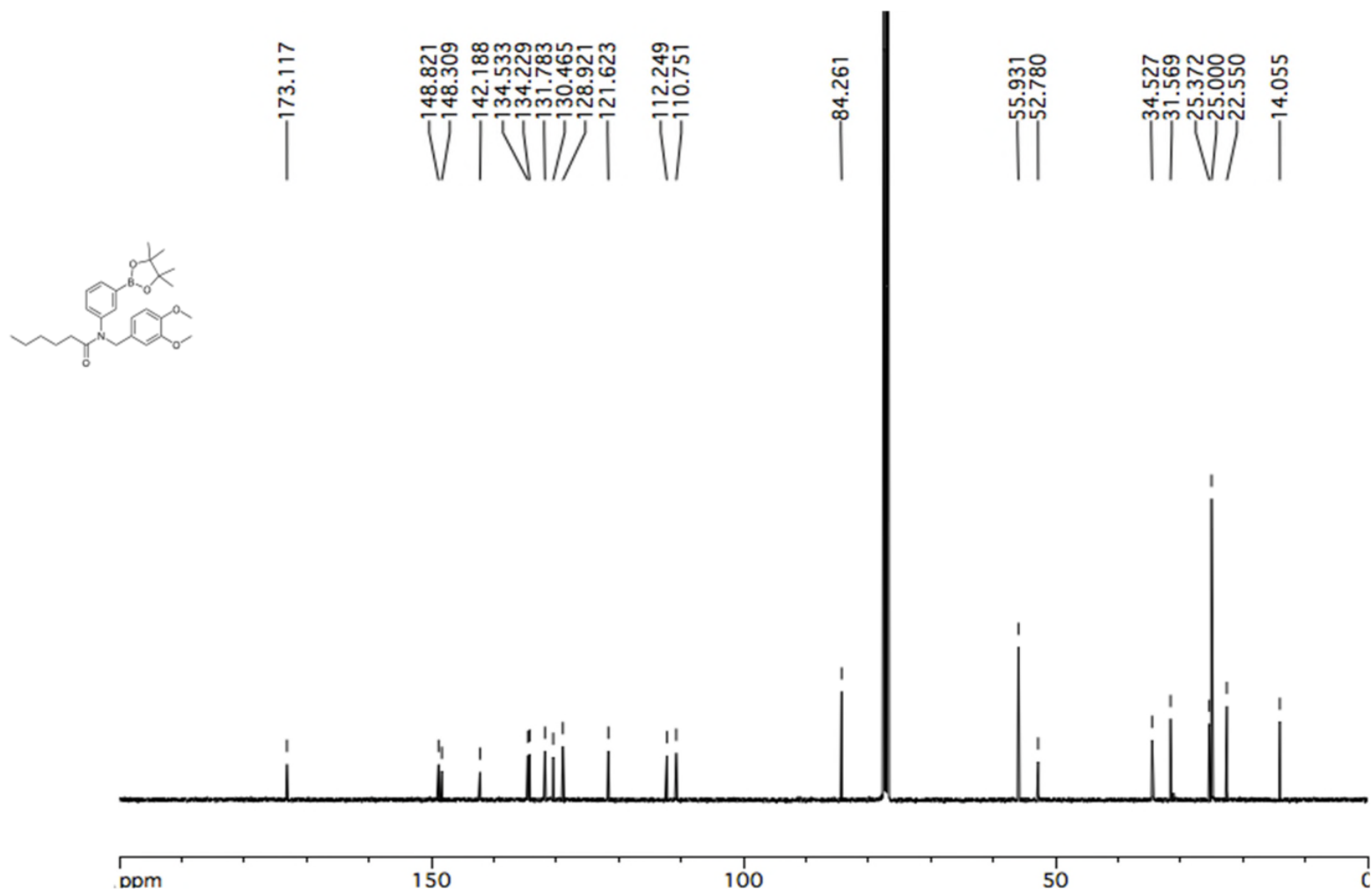


N-(3,4-dimethoxyphenylmethyl)-N-[4-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (24) – HRMS

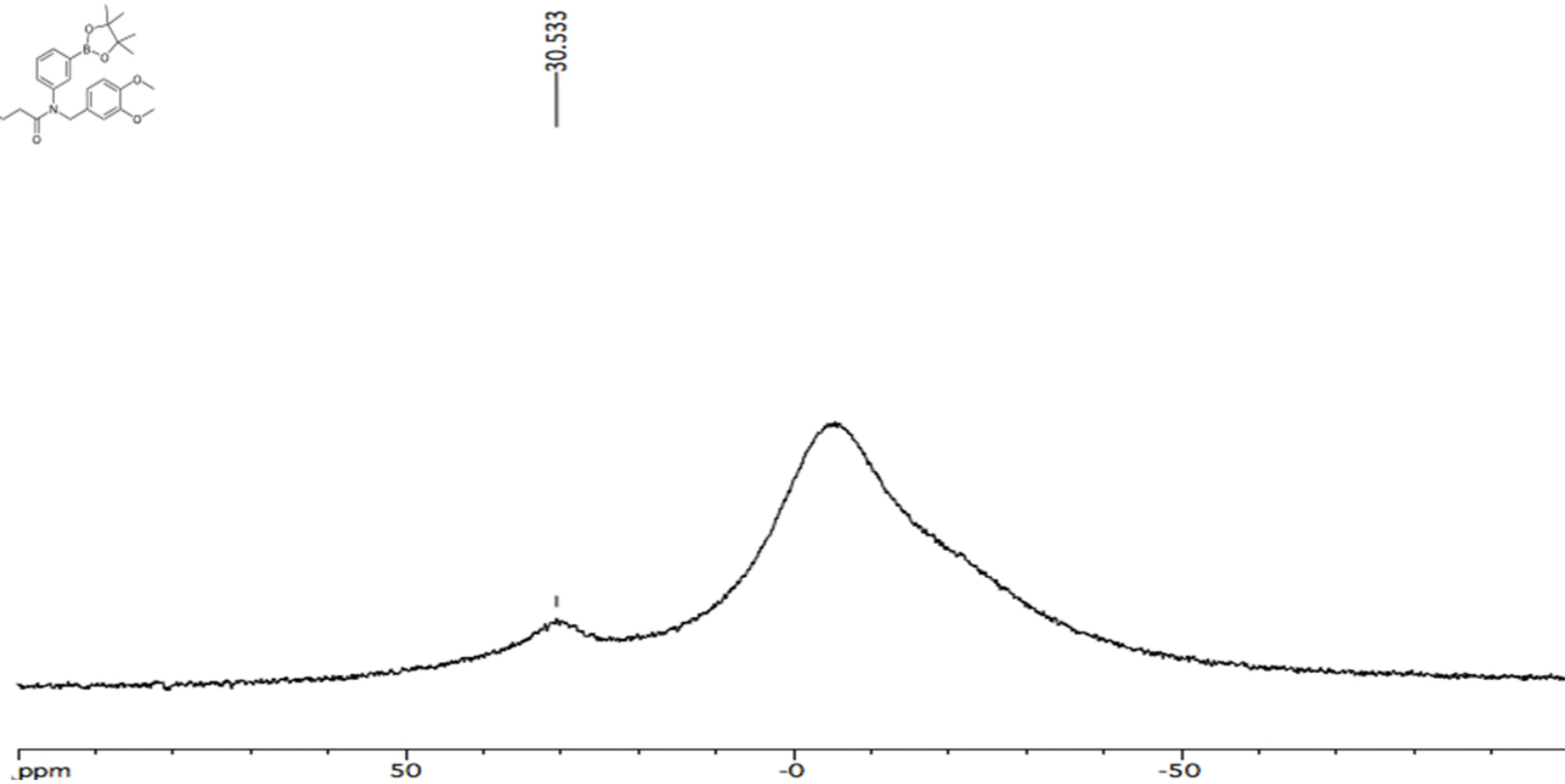
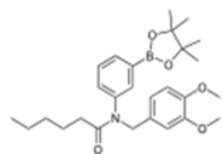
N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**25**) – ^1H NMR



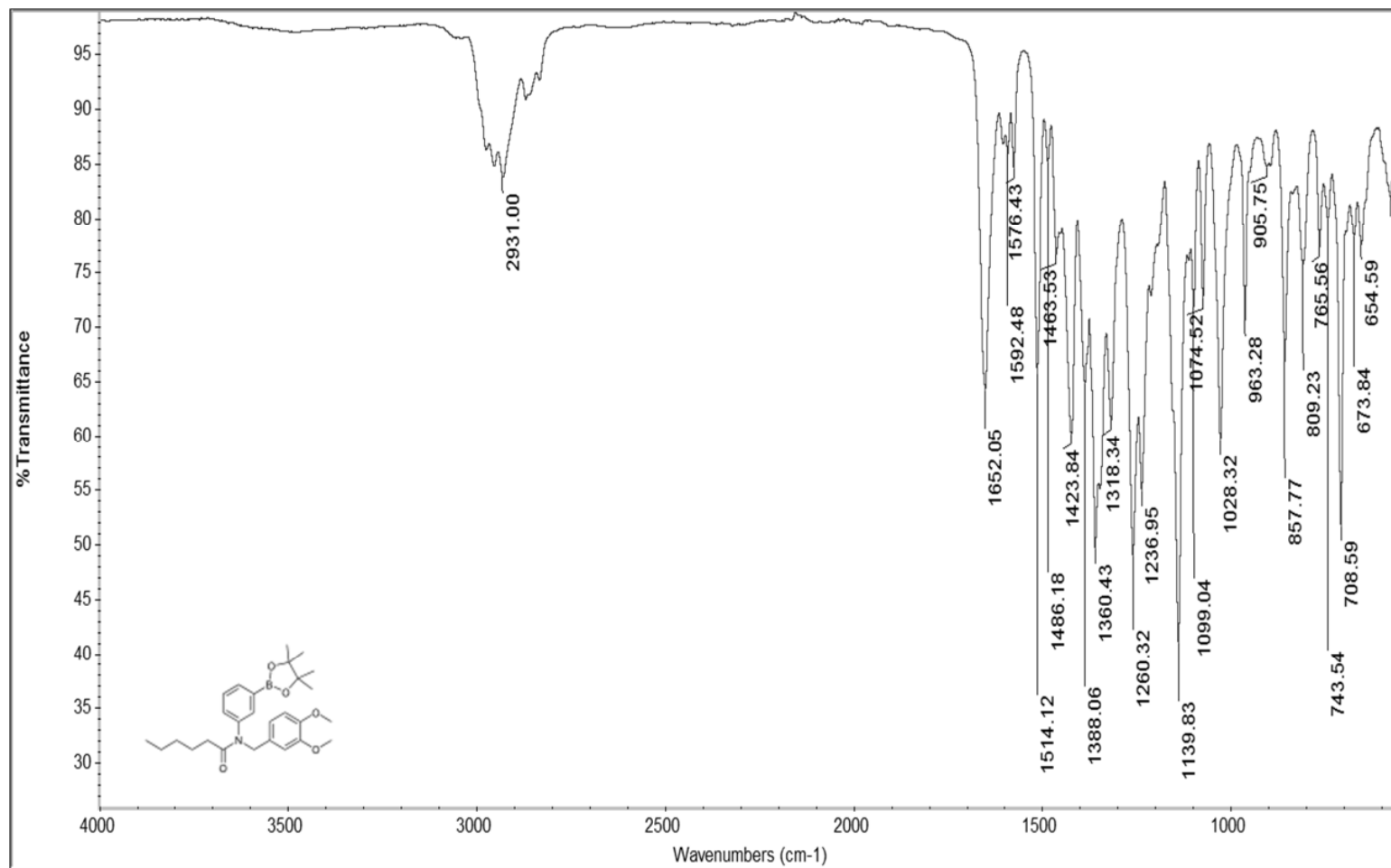
N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**25**) – ^{13}C NMR

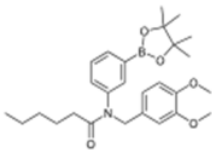


N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**25**) – ^{11}B NMR

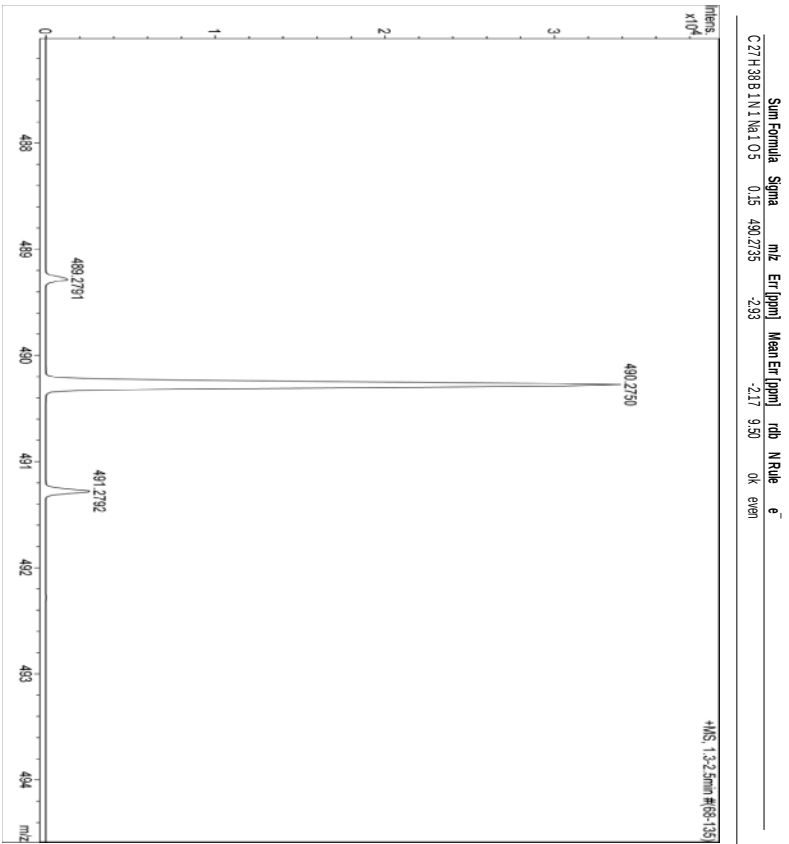


N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (**25**) – IR



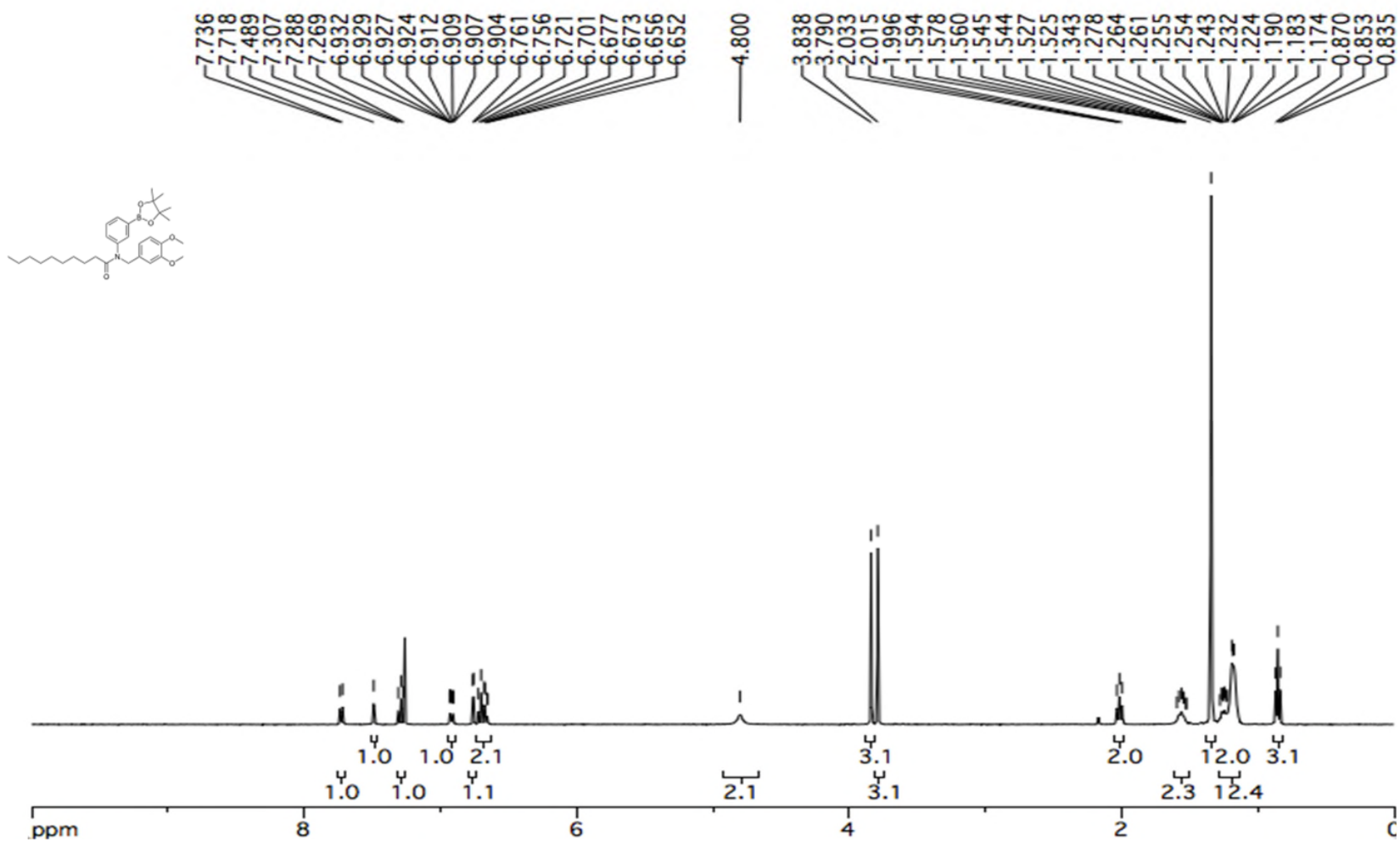


Analysis Info		Acquisition Date	
Analysis Name	D:\Data\Xiao\Nov 05 2020\000011.d	11/5/2020 11:31:10 AM	
Method	Xiao 2.m	Operator	Administrator
Sample Name	MFL-98	Instrument	micrOTOF
Comment	57		
Acquisition Parameter			
Source type	ESI	Ion Polarity	Positive
Scan Range	na	Capillary Exit	90.0 V
Scan Begin	50 m/z	Hexapole RF	125.0 V
Scan End	1500 m/z	Skimmer 1	40.0 V
		Hexapole 1	23.0 V
		Set Corrector Fill	45 V
		Set Pulsar Pull	39 V
		Set Pulsar Push	39 V
		Set Reflector	1300 V
		Set Flight Tube	9000 V
		Set Detector TOF	2200 V

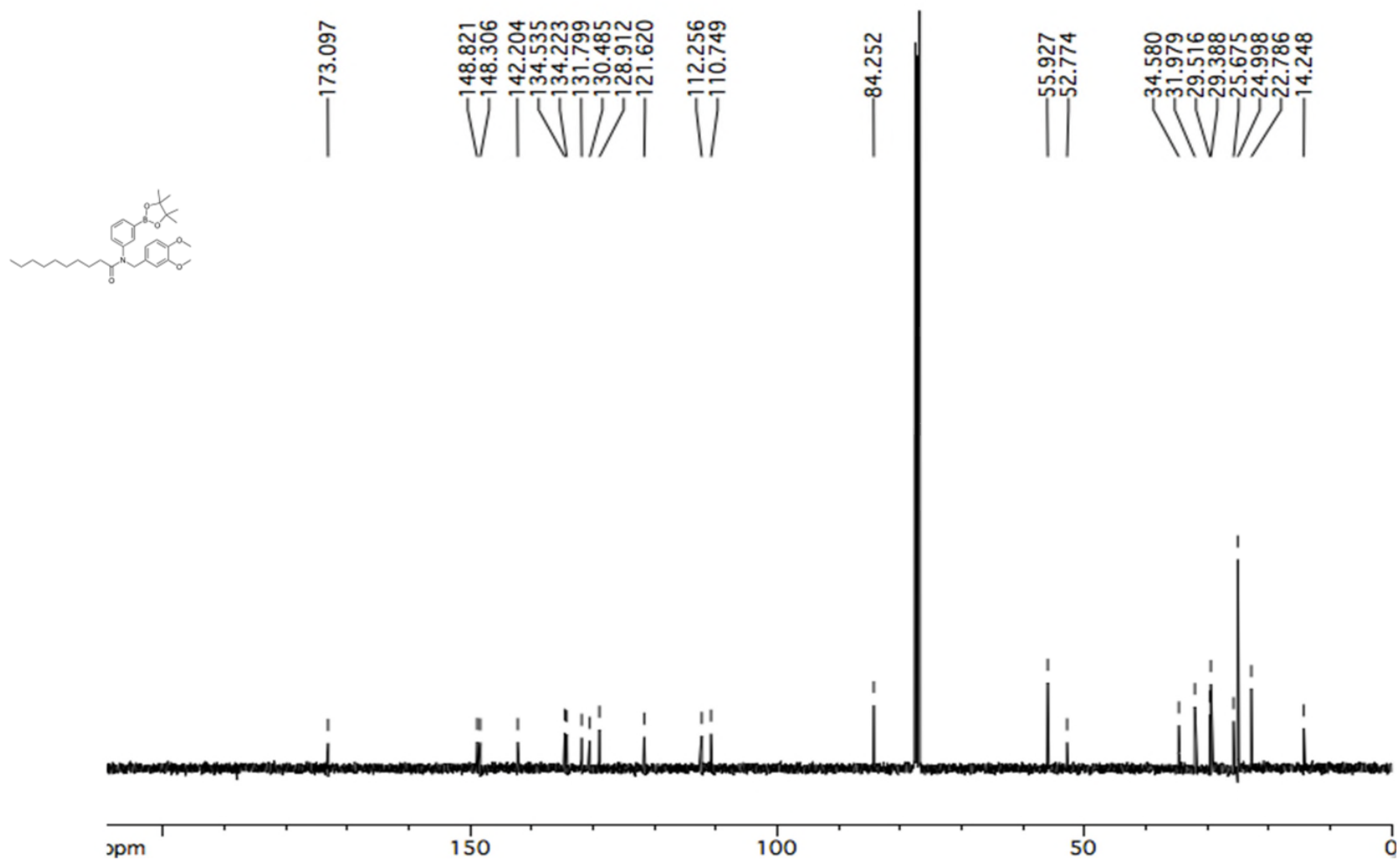


N-(3,4-dimethoxyphenylmethyl)-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-hexanamide (25) – HRMS

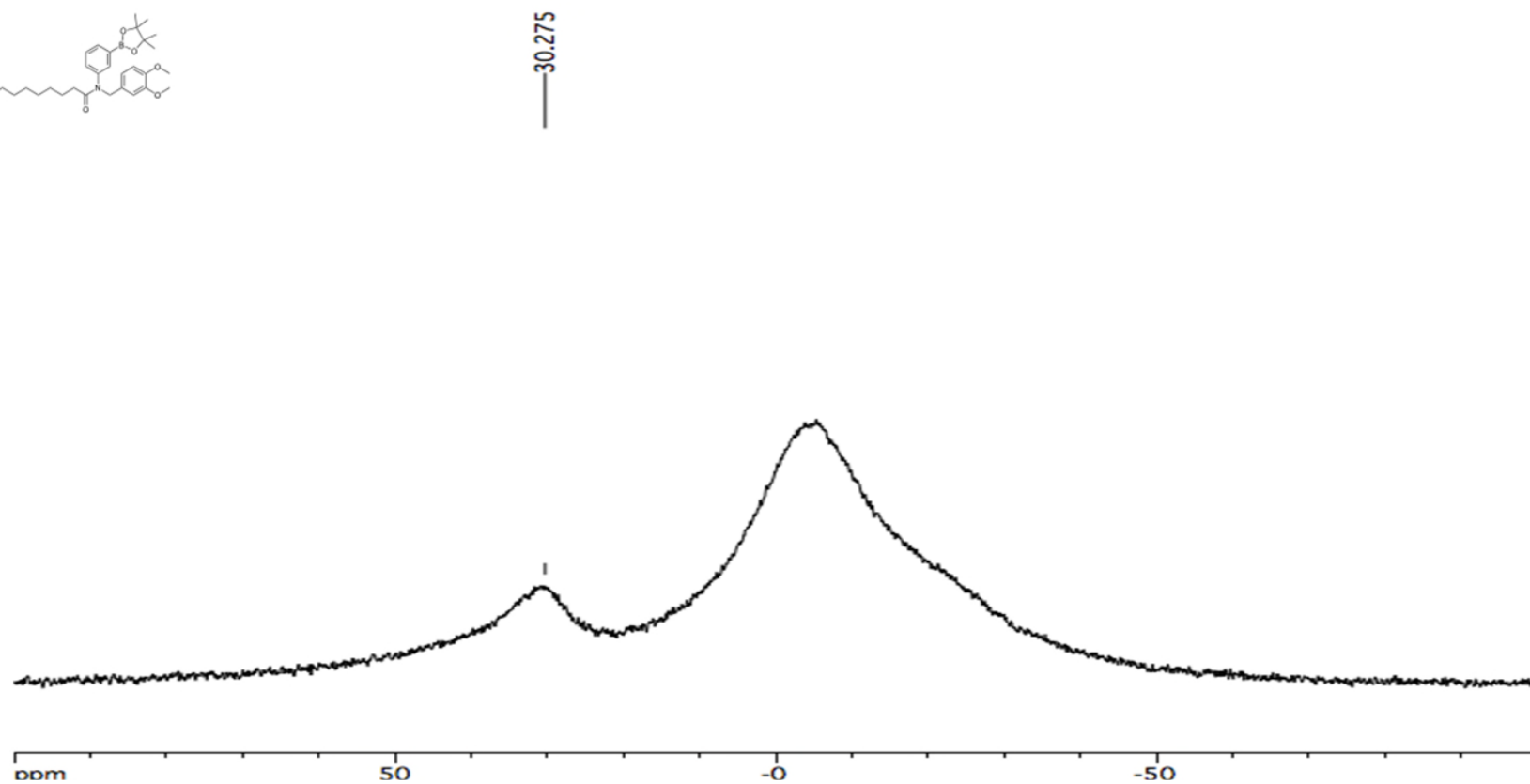
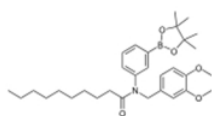
N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**26**) – ^1H NMR



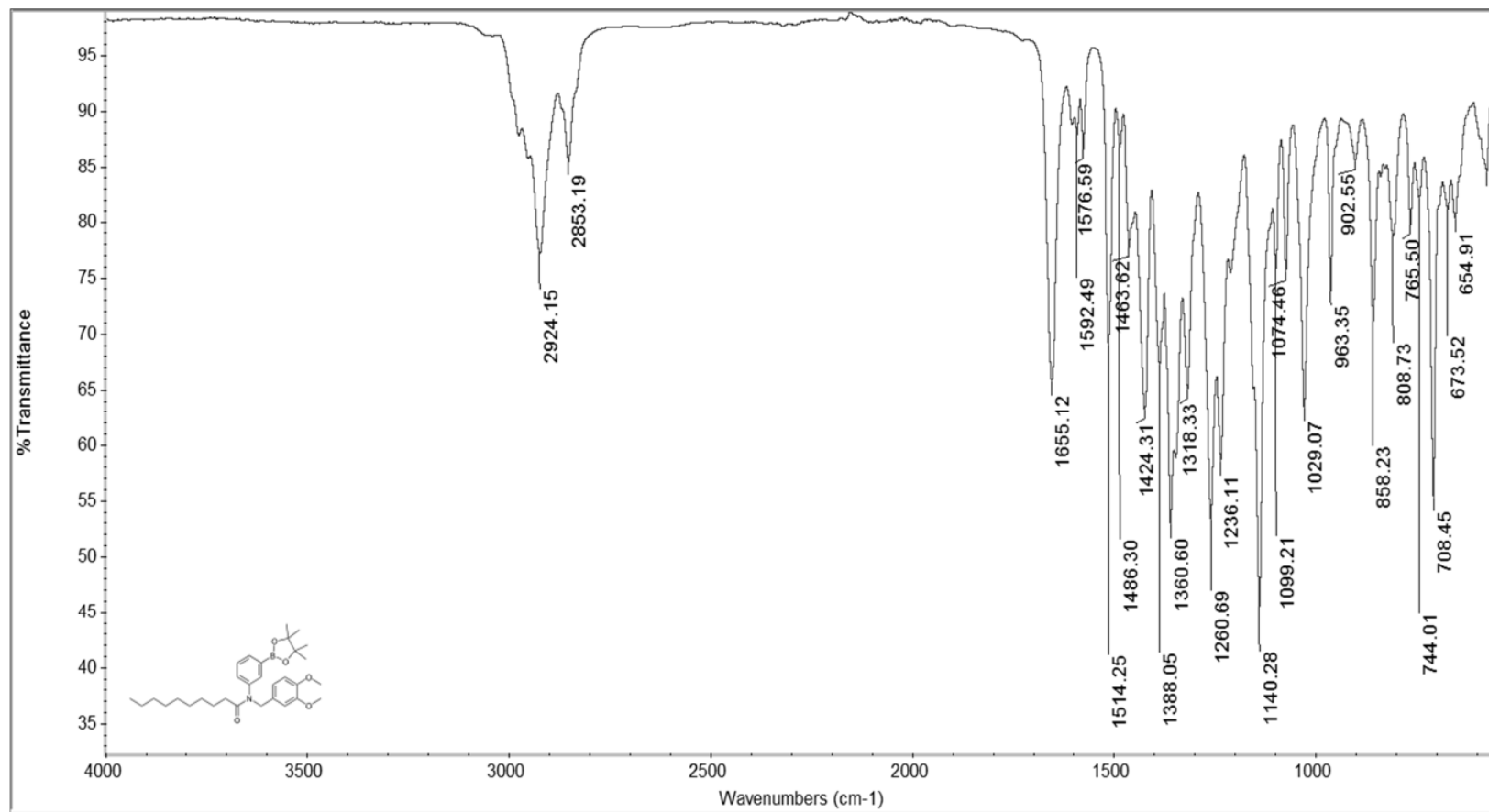
N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**26**) – ^{13}C NMR

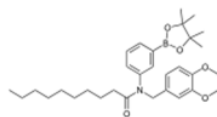


N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (**26**) – ^{11}B NMR



N-(3,4-dimethoxyphenylmethyl)-*N*-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (26) – IR





Analysis Info

Analysis Name D:\Data\Xiao\Nov 05 2020\00014.d
 Method Xiao 2.m
 Sample Name MF-102
 Comment

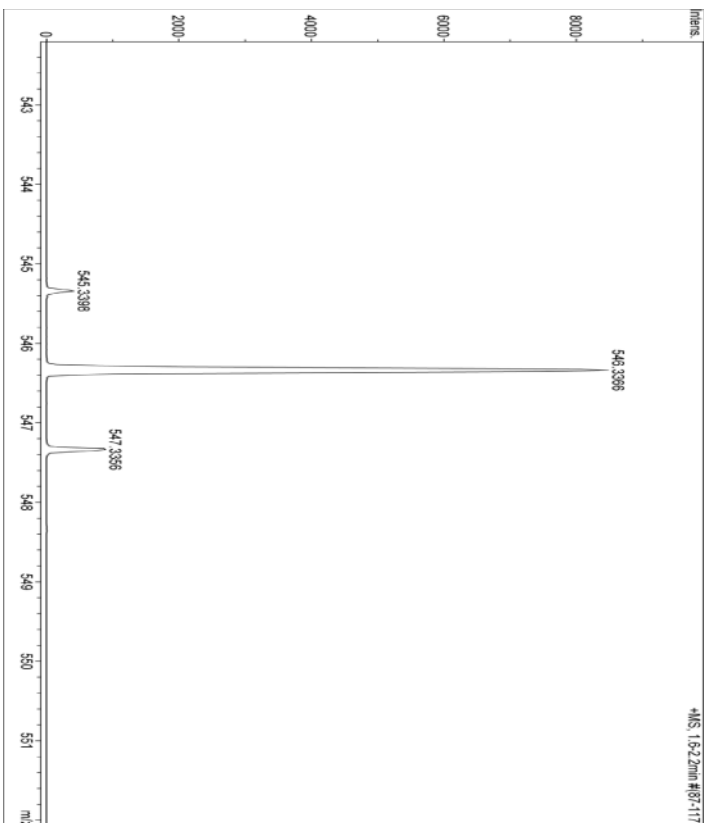
Acquisition Date 11/5/2020 2:06:14 PM

Operator Administrator
 Instrument microTOF 57

Acquisition Parameter

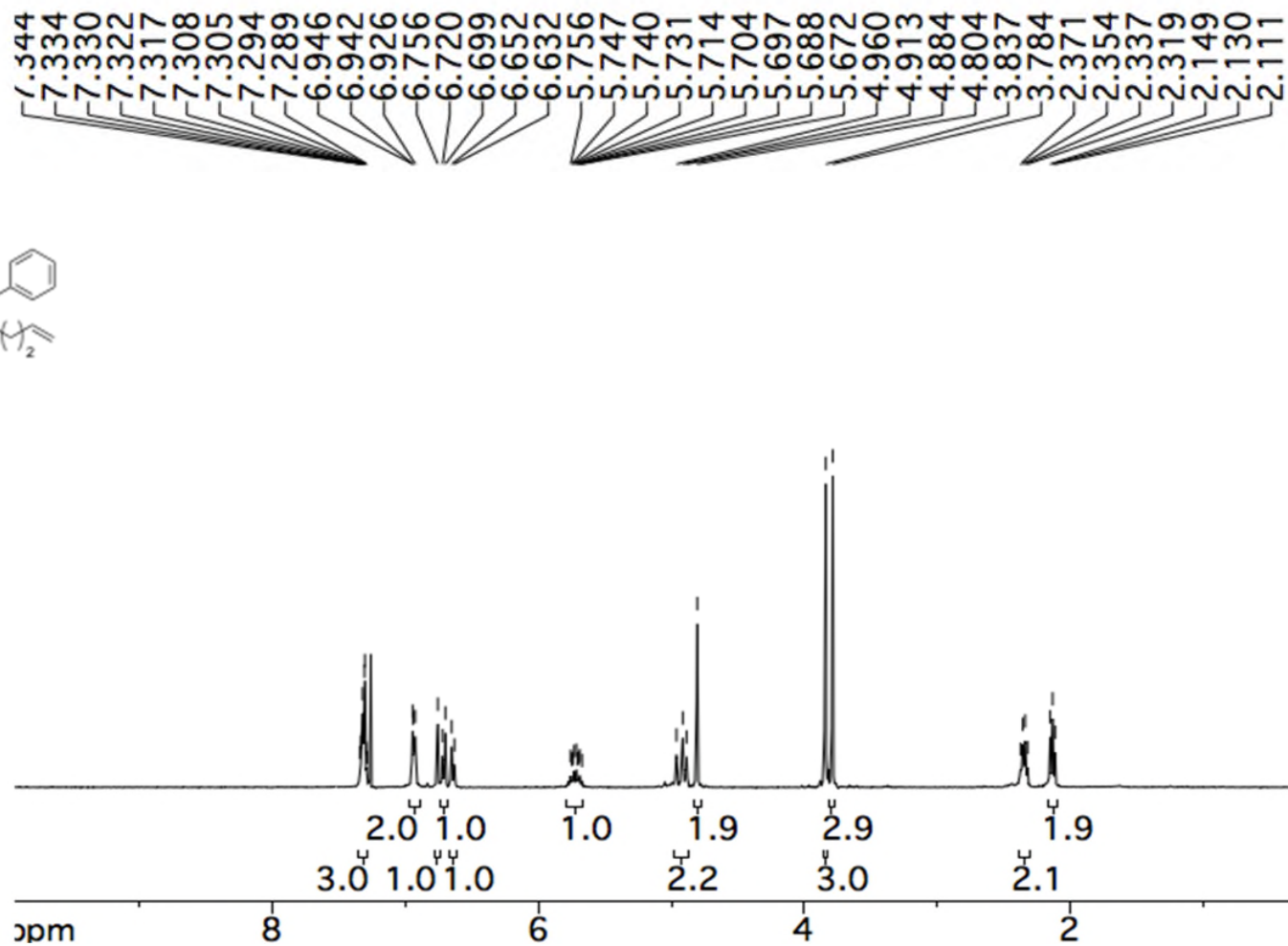
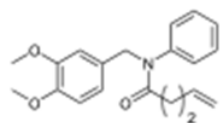
Source Type	ESI	Ion Polarity	Positive	Set Cone Volt	45 V
Scan Range	na	Cylindrical Exit	90.0 V	Set PLSA PUL	390 V
Scan Begin	50 m/z	Hexapole RF	125.0 V	Set PLSA PUL	390 V
Scan End	1500 m/z	Skimmer 1	40.0 V	Set Reflector	1300 V
			23.0 V	Set Flight Tube	9000 V
				Set Detector TOF	2200 V

Sum Formula	Sigma	m/z	Err (ppm)	Mean Err (ppm)	rtb	N Rule	e ⁻
C31H46B1N1O5	0.13	546.3361	-0.35	0.99	9.50	OK	even

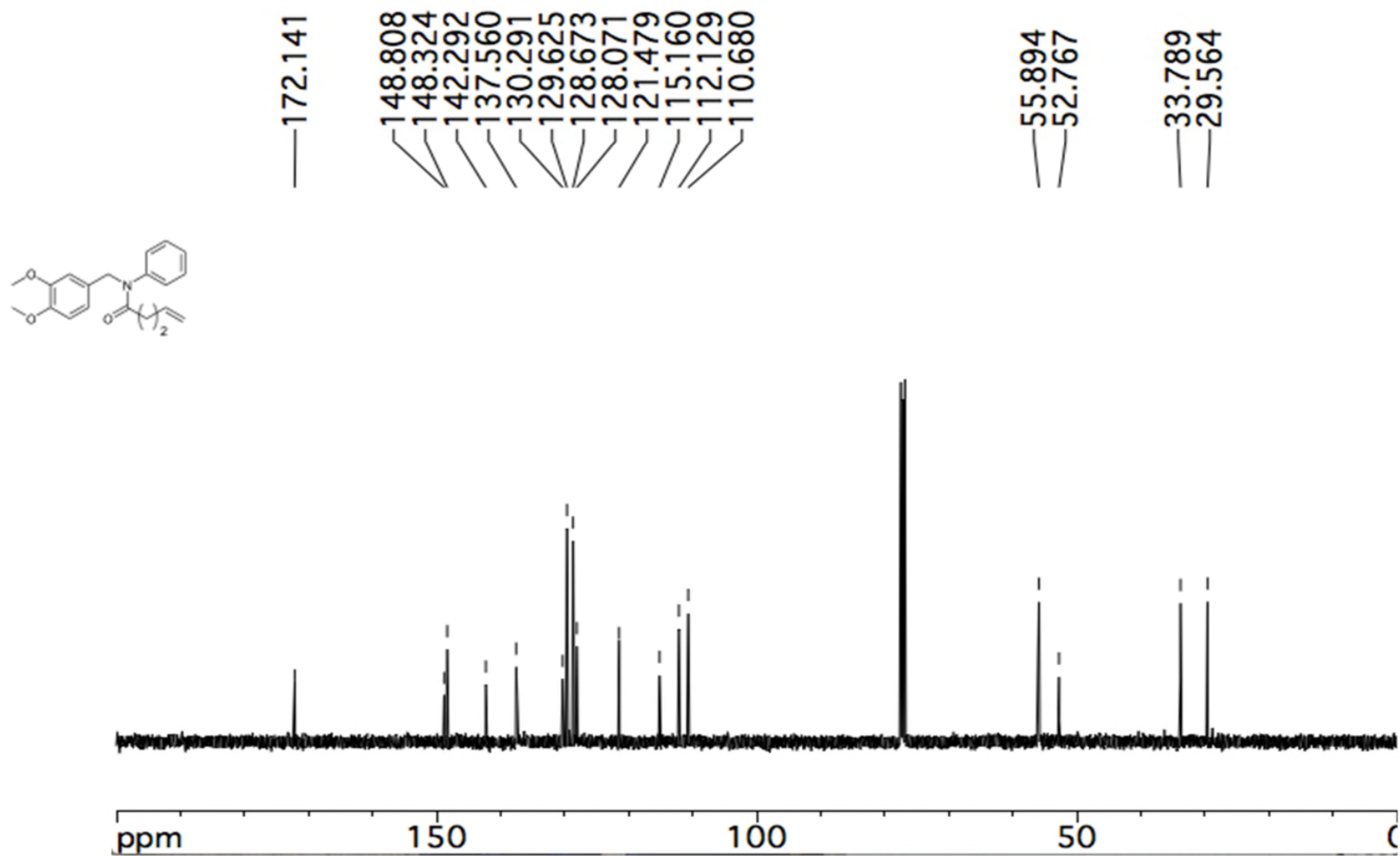


N-(3,4-dimethoxyphenylmethyl)-N-[3-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)phenyl]-decanamide (26) – HRMS

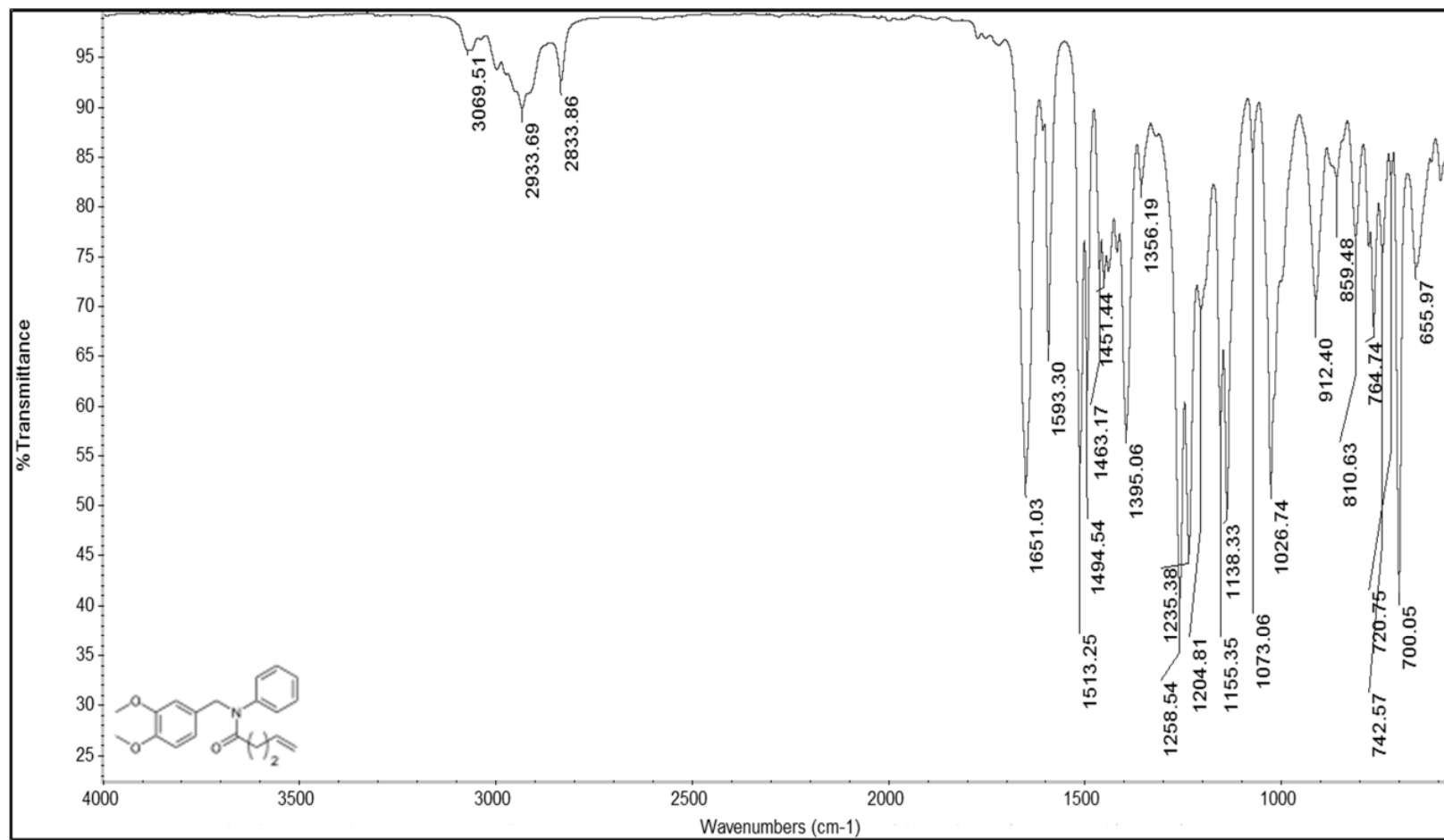
N-(3,4-dimethoxybenzyl)-*N*-phenylpent-4-enamide (**27**) – ^1H NMR

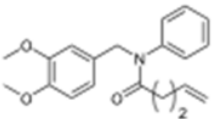


N-(3,4-dimethoxybenzyl)-*N*-phenylpent-4-enamide (**27**) – ^{13}C NMR



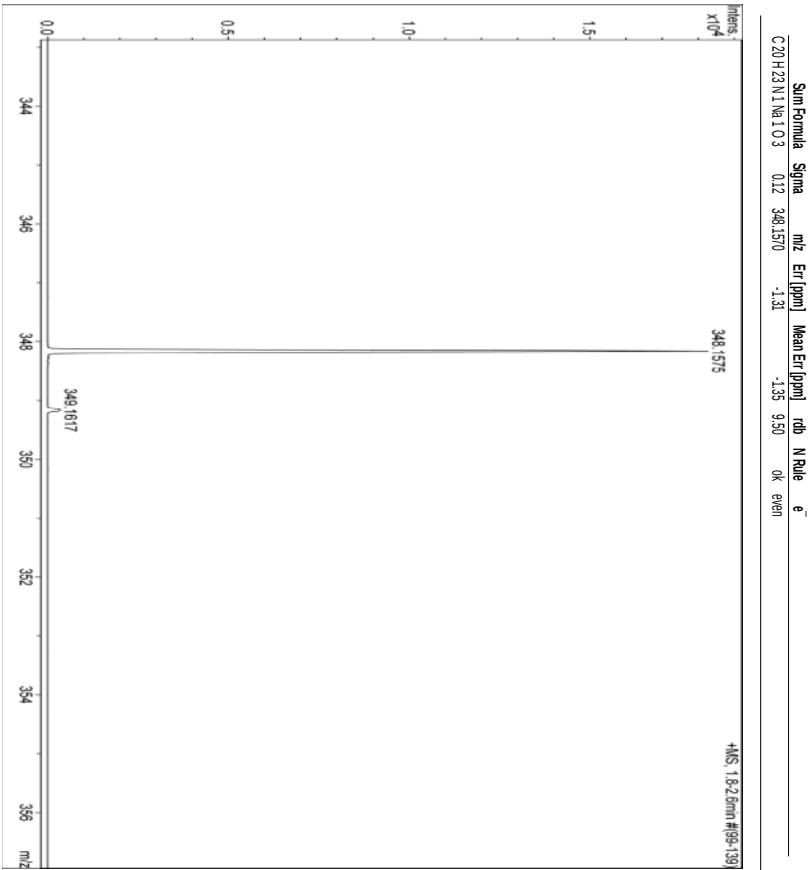
N-(3,4-dimethoxybenzyl)-*N*-phenylpent-4-enamide (**27**) – IR





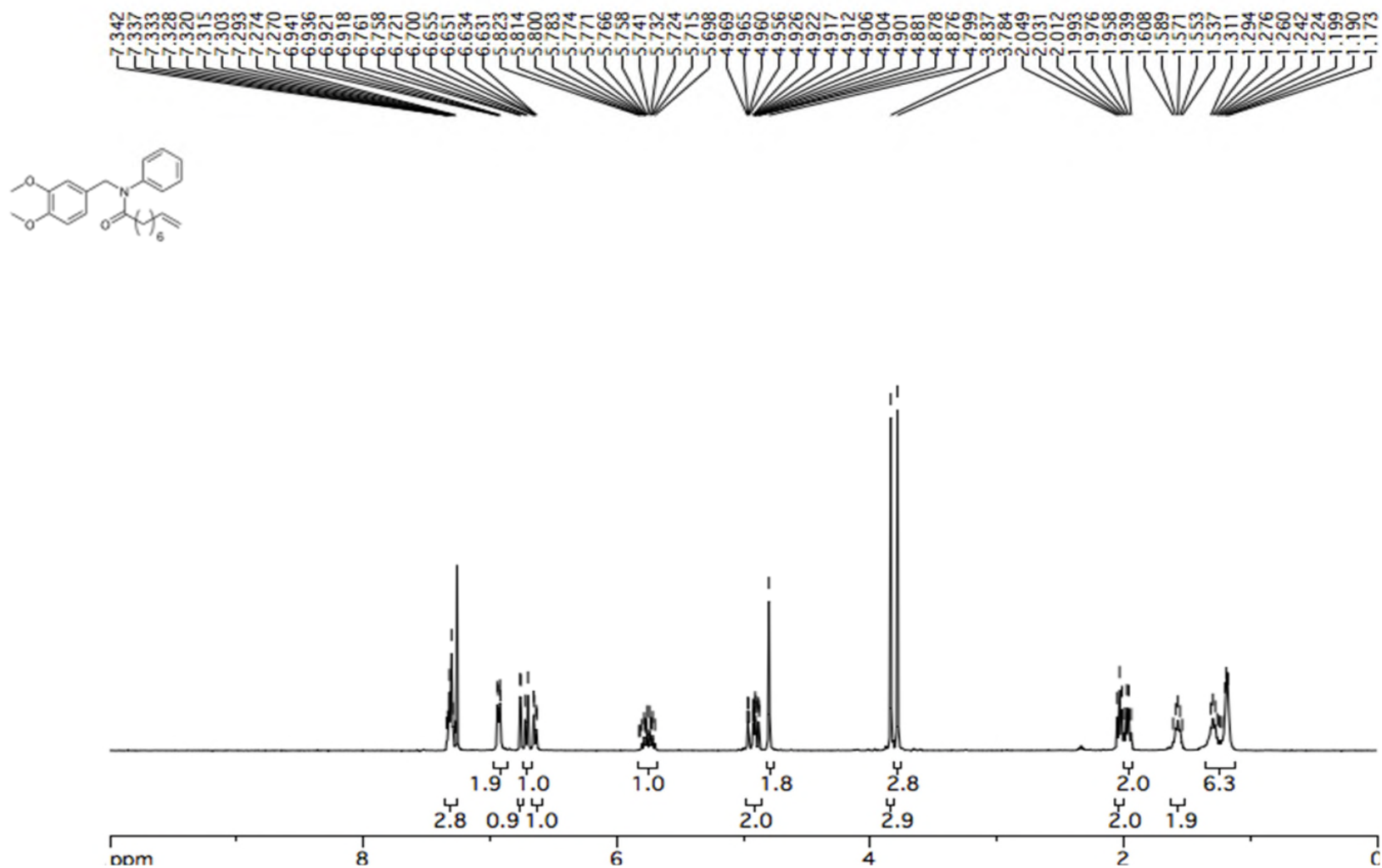
Analysis Info		Acquisition Date	
Analysis Name	D:\Data\XenNov 05 2020\000012.d	Operator	Administrator
Method	Xiao 2.m	Instrument	micrOTOF
Sample Name	JM-34		57
Comment			

Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Scan Range	n/a	Capillary Exit	90.0 V
Scan Begin	50 m/z	Hexapole RF	125.0 V
Scan End	150 m/z	Skimmer 1	40.0 V
		Hexapole 1	23.0 V
			Set Detector TOF
			Set Detector Fill
			Set Pulsar Pull
			Set Pulsar Push
			Set Reflector
			Set Flight Tube
			Set Detector TOF

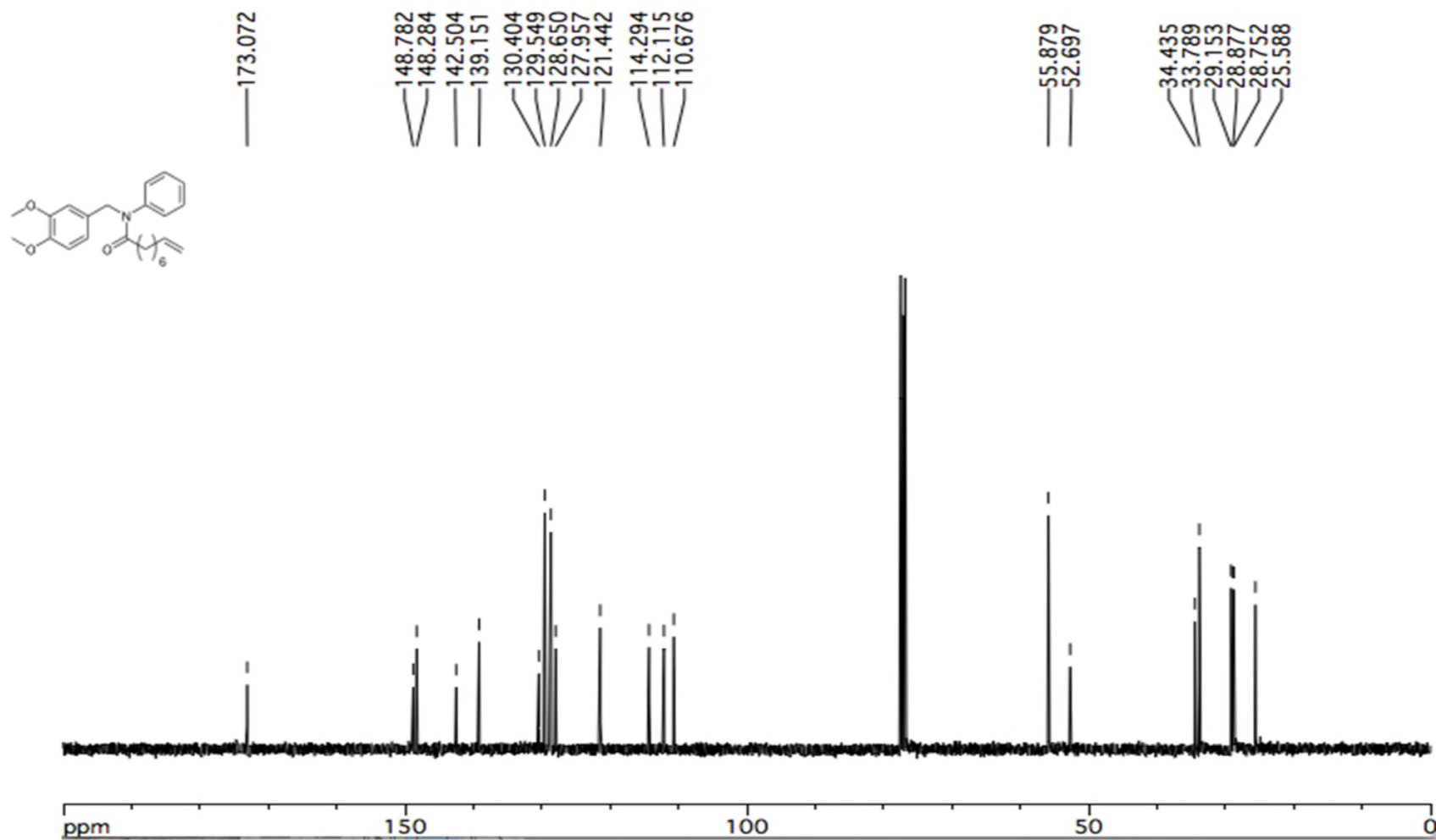


N-(3,4-dimethoxybenzyl)-N-phenylpent-4-enamide (27) – HRMS

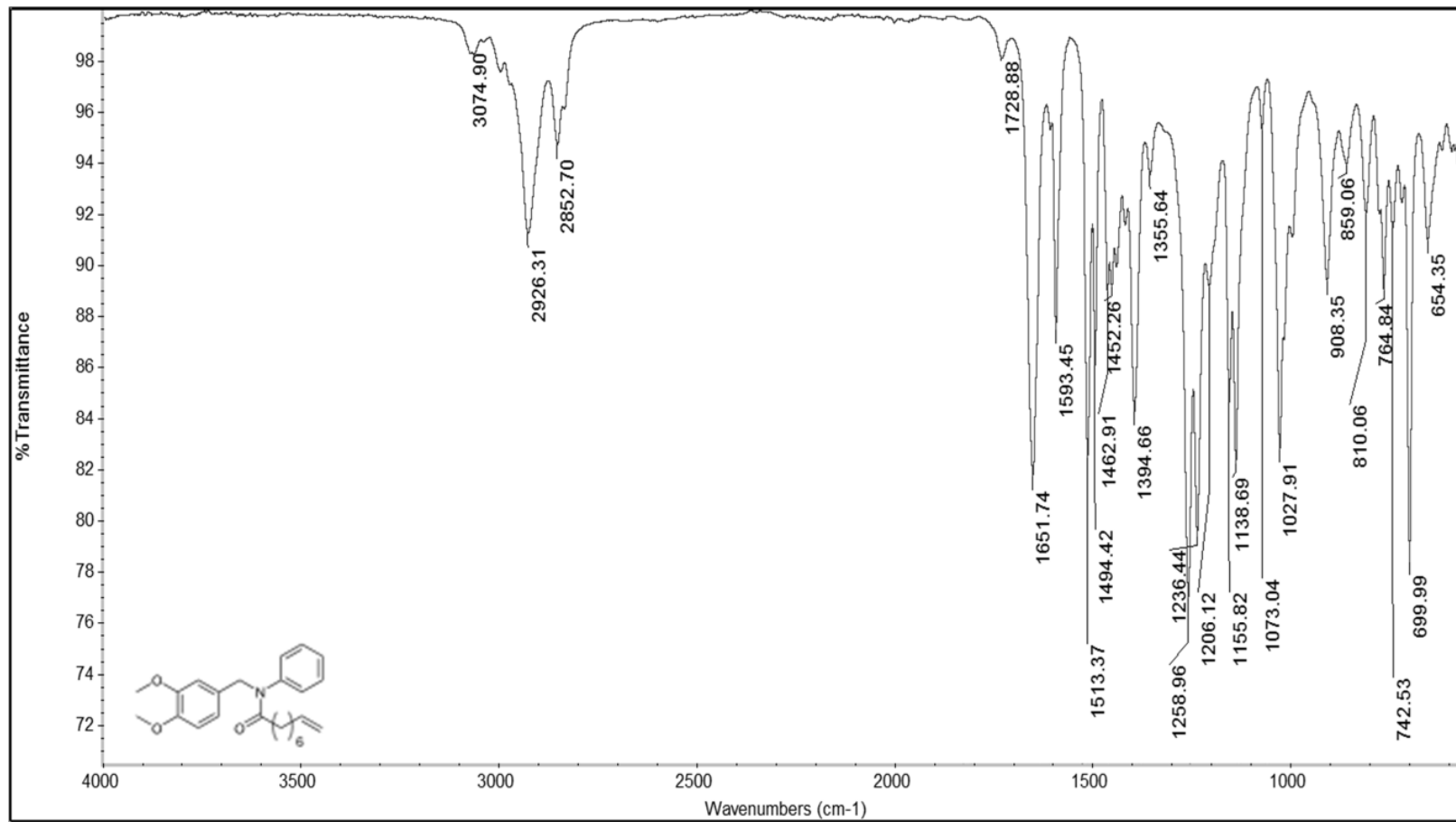
N-(3,4-dimethoxybenzyl)-*N*-phenylnon-8-enamide (**28**) – ^1H NMR

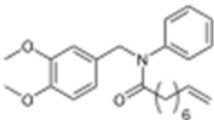


N-(3,4-dimethoxybenzyl)-*N*-phenylnon-8-enamide (**28**) – ^{13}C NMR

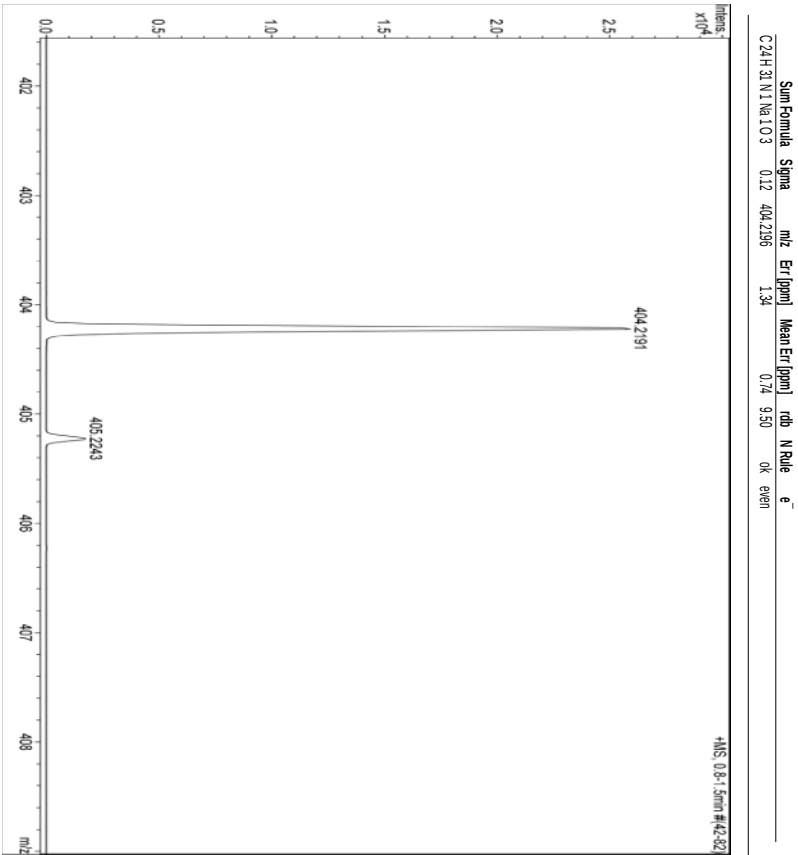


N-(3,4-dimethoxybenzyl)-*N*-phenylnon-8-enamide (**28**) – IR



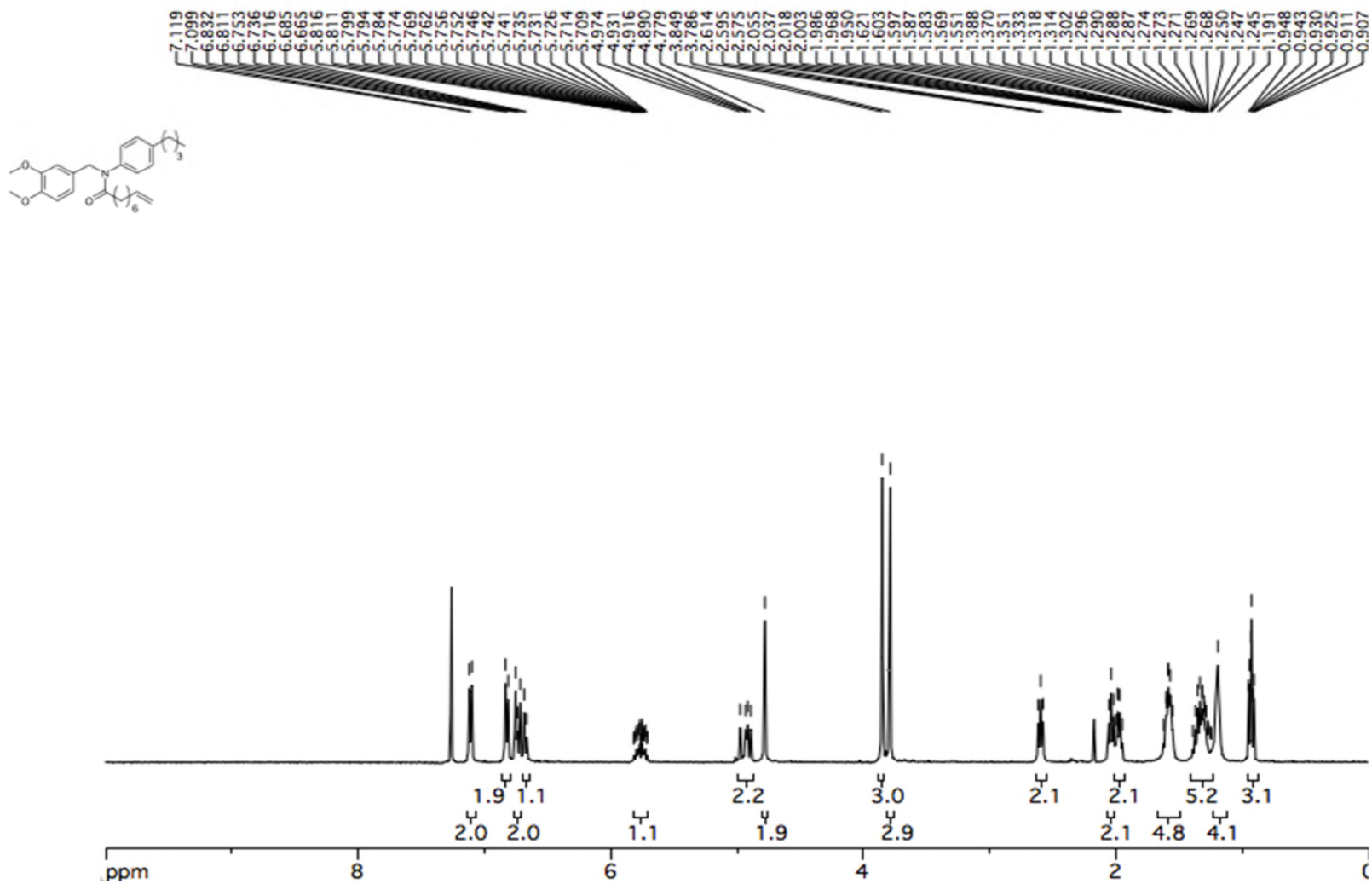


Analysis Info		Acquisition Date	
Analysis Name	D:\Data\Xian\Nov 05 2020\000015.d	11/5/2020 2:15:24 PM	
Method	Xiao 2.m	Operator	Administrator
Sample Name	JW-38	Instrument	micrOTOF
Comment			57
Acquisition Parameter			
Source Type	ESI	Ion Polarity	Positive
Scan Range	n/a	Capillary Exit	900 V
Scan Begin	50 m/z	Hexapole RF	125.0 V
Scan End	1500 m/z	Skimmer 1	400 V
		Hexapole 1	230 V
		Set Corrector Fill	45 V
		Set Pulsar Pull	399 V
		Set Pulsar Push	399 V
		Set Reflector	1300 V
		Set Flight Tube	9000 V
		Set Detector TOF	2200 V

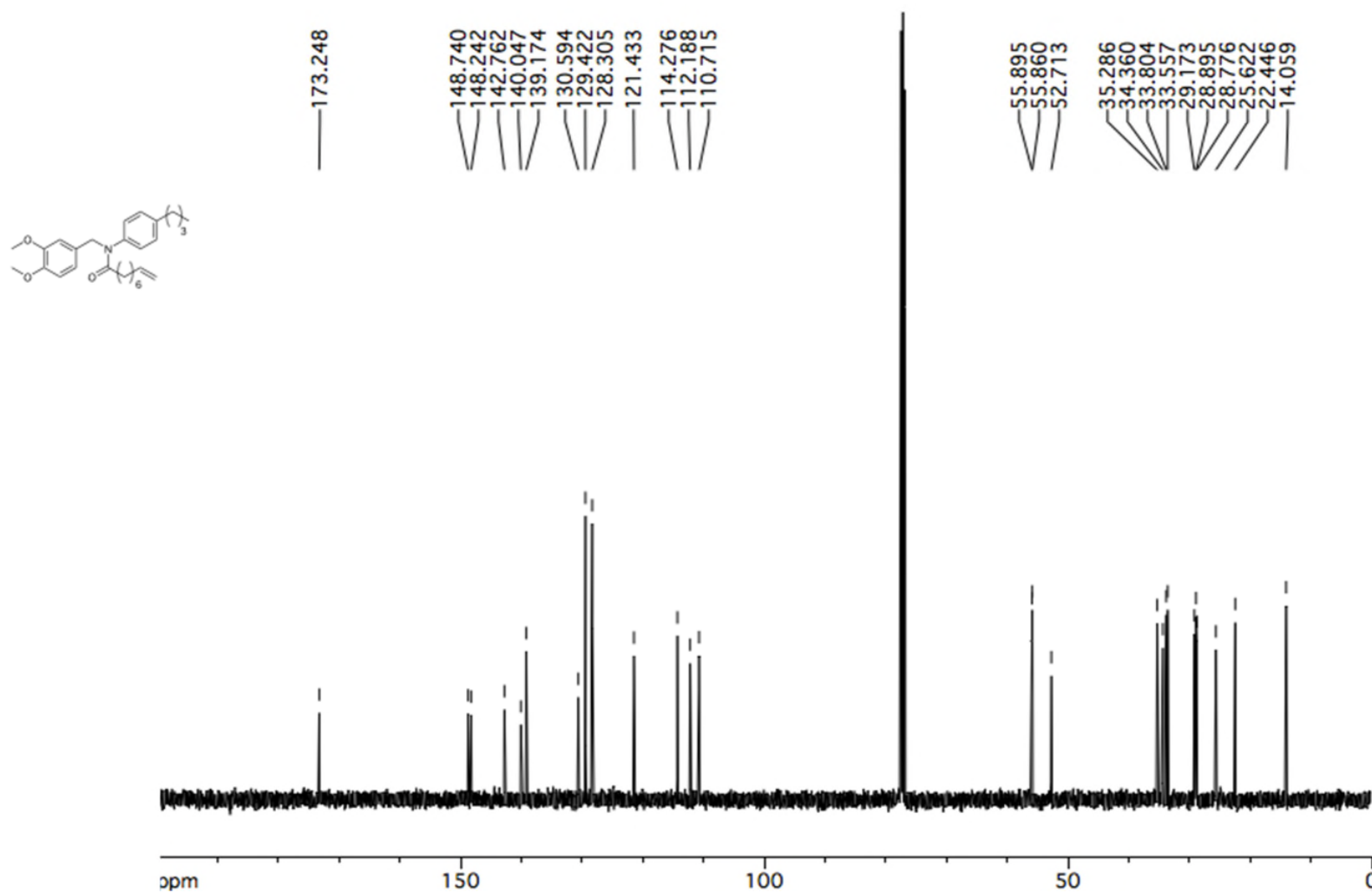


N-(3,4-dimethoxybenzyl)-N-phenylnon-8-enamide (28) – HRMS

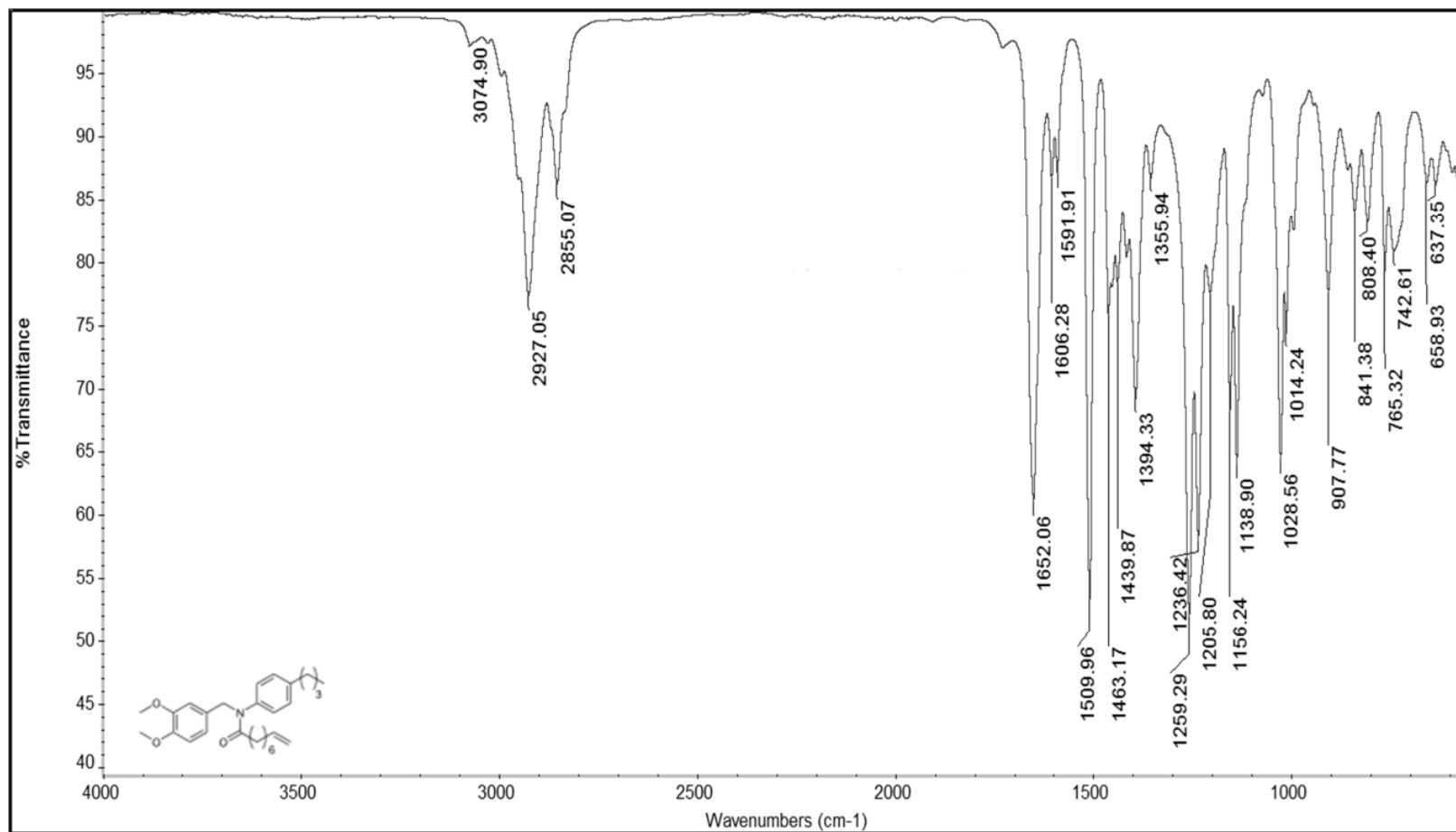
N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)non-8-enamide (**29**) – ^1H NMR

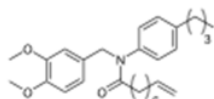


N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)non-8-enamide (**29**) – ^{13}C NMR



N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)non-8-enamide (**29**) – IR





Analysis Info

Analysis Name D:\Data\Kao\Nov 05 2020\000001.d

Method Xeo 2.m

Sample Name JM-52

Comment

Acquisition Date 11/5/2020 9:50:03 AM

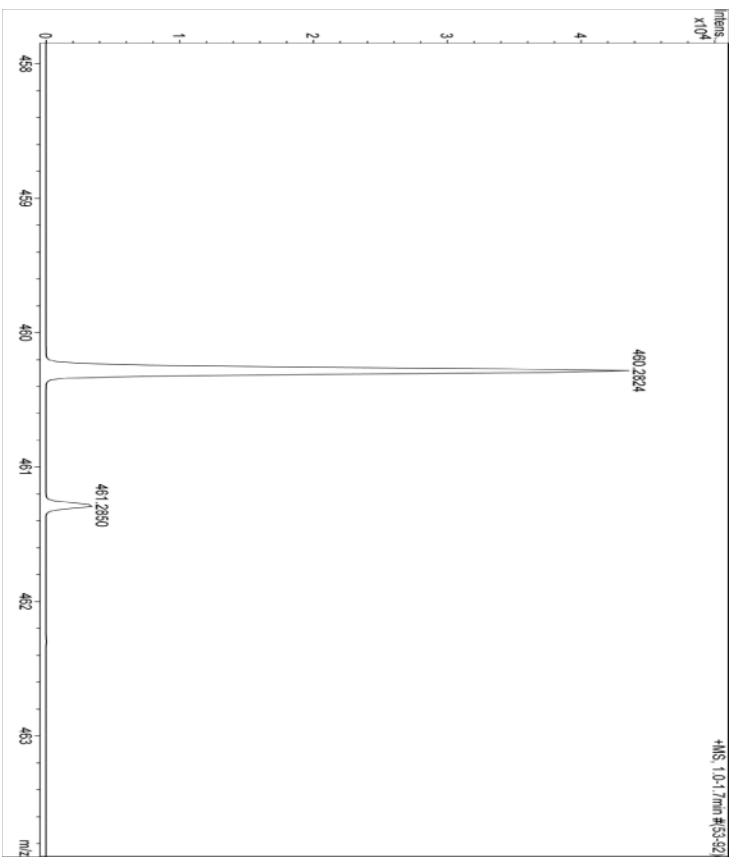
Operator Administrator

Instrument microTOF 57

Acquisition Parameter

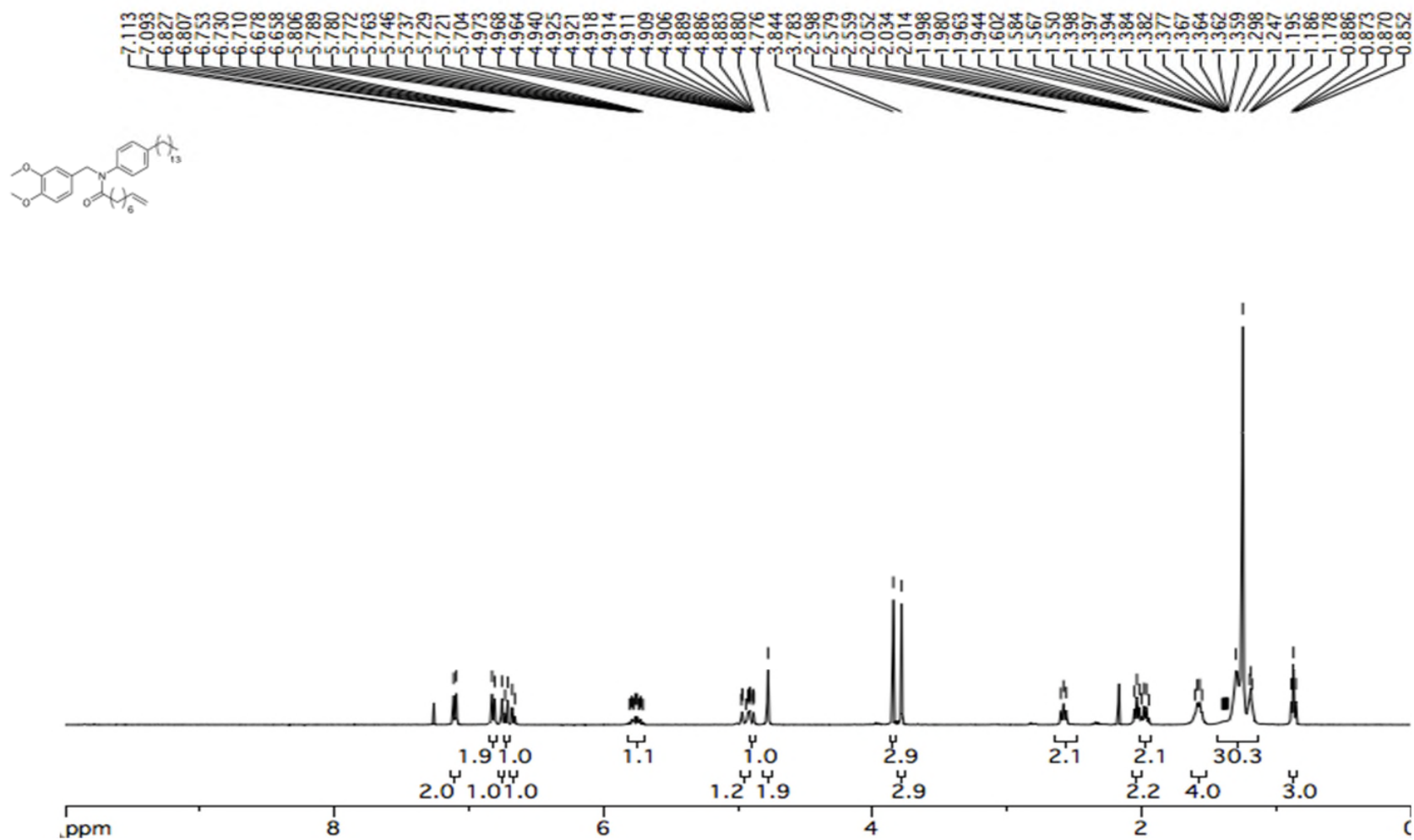
Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	45 V
Scan Range	n/a	Capillary Exit	900 V	Set Pulsar Pull	399 V
Scan Begin	50 m/z	Heapole RF	125.0 V	Set Pulsar Push	399 V
Scan End	1500 m/z	Skimmer 1	400 V	Set Reflector	1300 V
		Heapole 1	230 V	Set Flight Tube	9000 V
				Set Detector TOF	2200 V

Sum Formula	Sigma	m/z	Err [ppm]	Mean Err [ppm]	rdn	N Rule	e ⁻
C28H39N1Na1O3	0.14	460.2822	-0.46	-0.22	9.50	OK	even

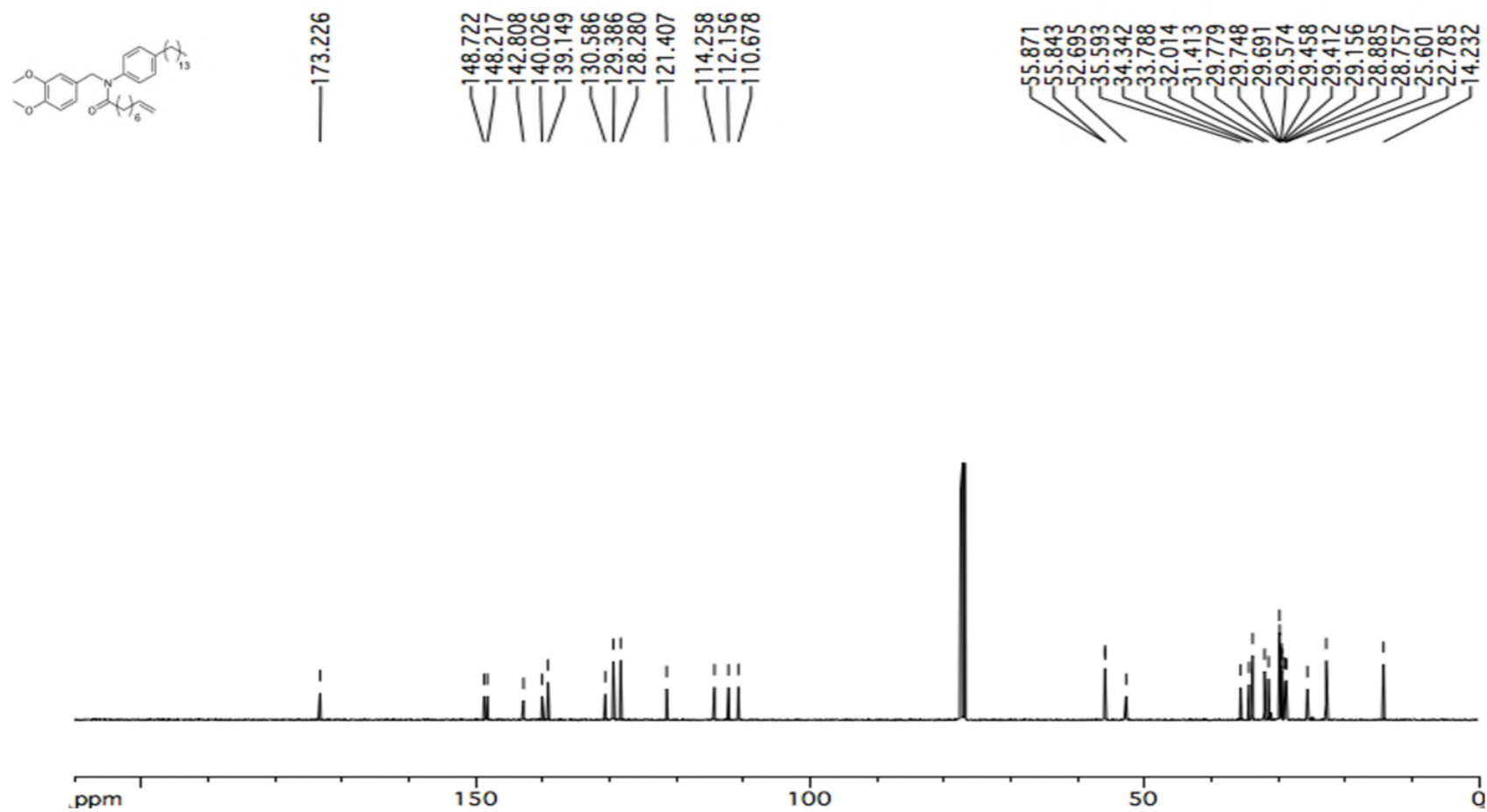


N-(4-butylphenyl)-N-(3,4-dimethoxybenzyl)non-8-enamide (29) – HRMS

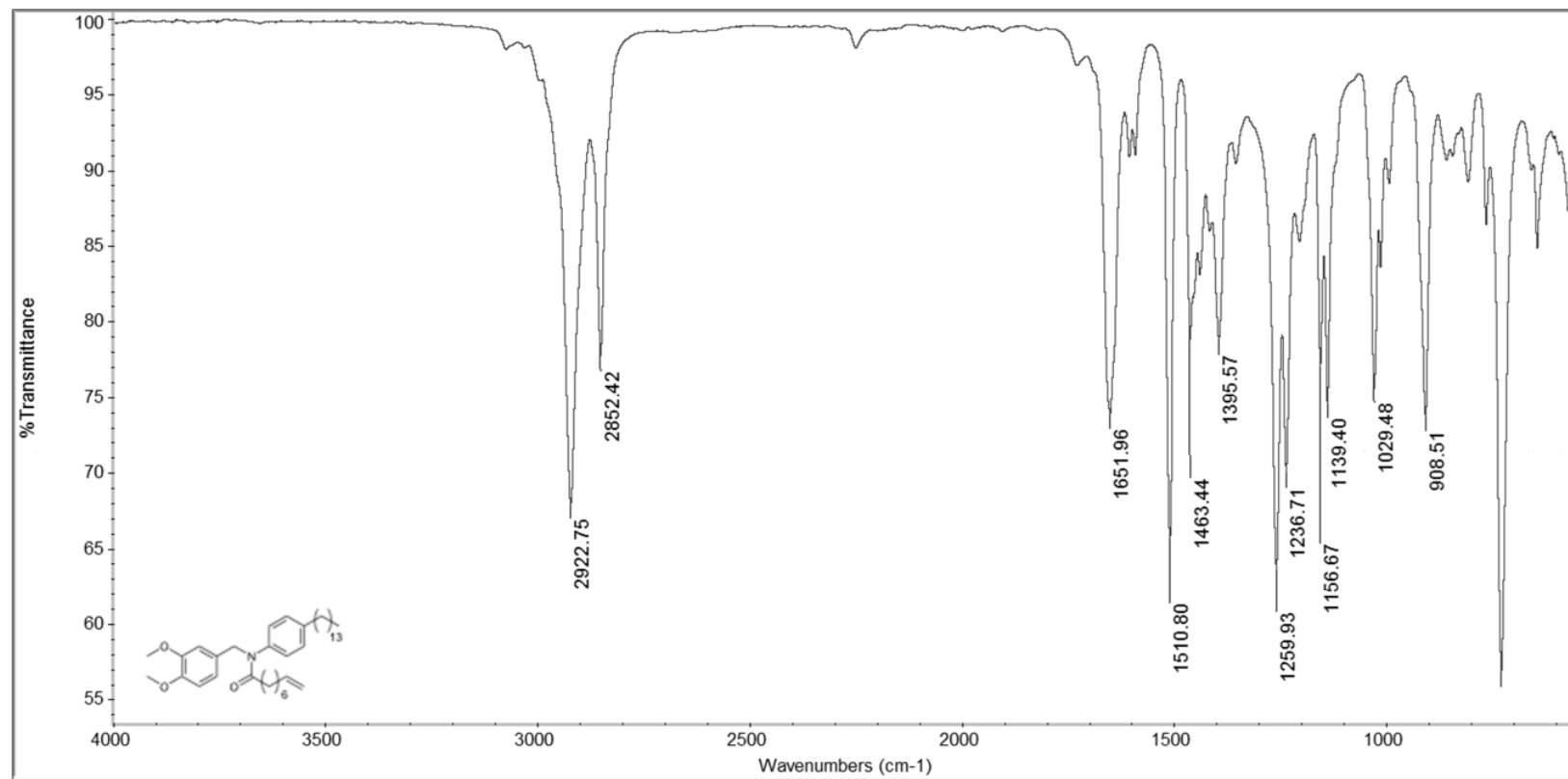
N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)non-8-enamide (**30**) – ^1H NMR

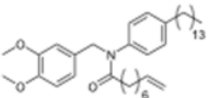


N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)non-8-enamide (**30**) – ^{13}C NMR



N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)non-8-enamide (30) – IR

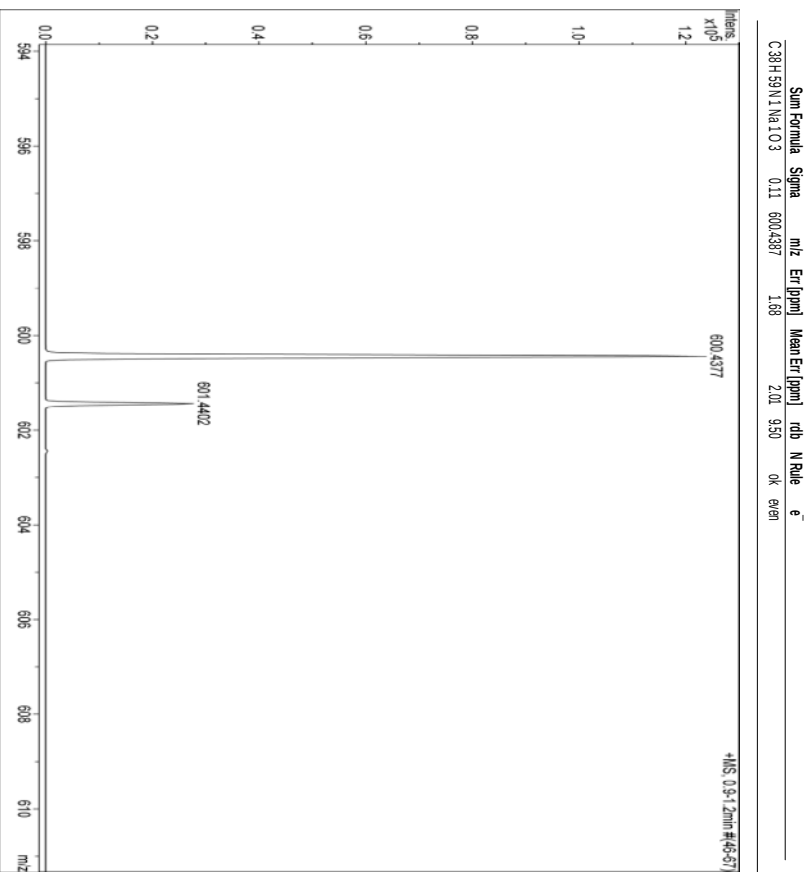




Analysis Info

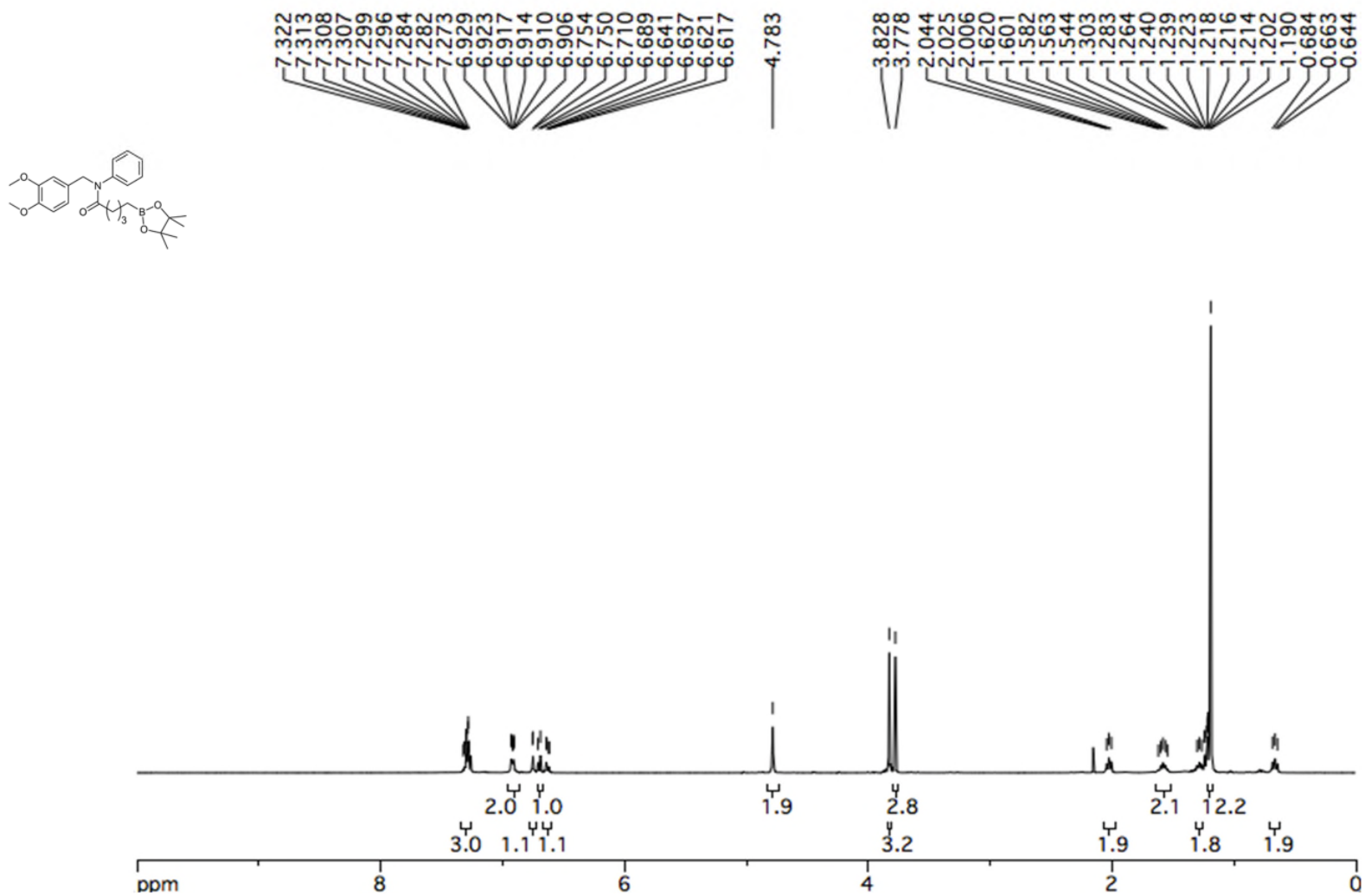
Analysis Name	D:\Data\Kao\Nov 05 2020\000005.d	Acquisition Date	11/5/2020 10:38:59 AM
Method	Xiao 2.m	Operator	Administrator
Sample Name	JW-72	Instrument	micro TOF 57
Comment			

Acquisition Parameter							
Source Type	ESI	Ion Polarity	Positive	Set Detector Fill	45 V		
Scan Range	na	Capillary Exit	90.0 V	Set Pulsar Pull	399 V		
Scan Begin	50 m/z	Headspace RF	125.0 V	Set Pulsar Push	399 V		
Scan End	1500 m/z	Skimmer 1	400 V	Set Detector	1300 V		
		Headspace 1	230 V	Set Flight Tube	9000 V		
				Set Detector TOF	2200 V		

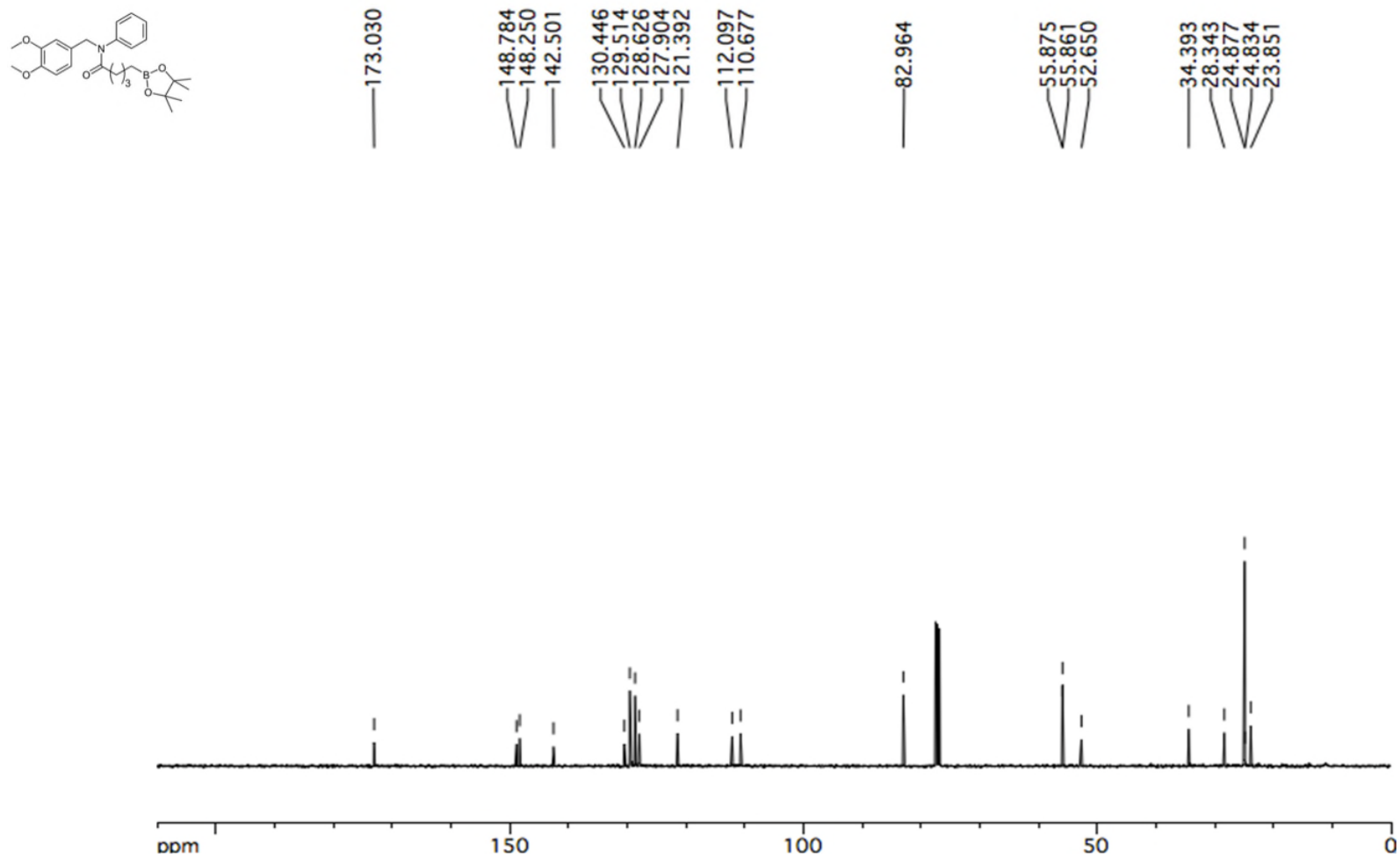


N-(3,4-dimethoxybenzyl)-N-(4-tetradecylphenyl)non-8-enamide (30) – HRMS

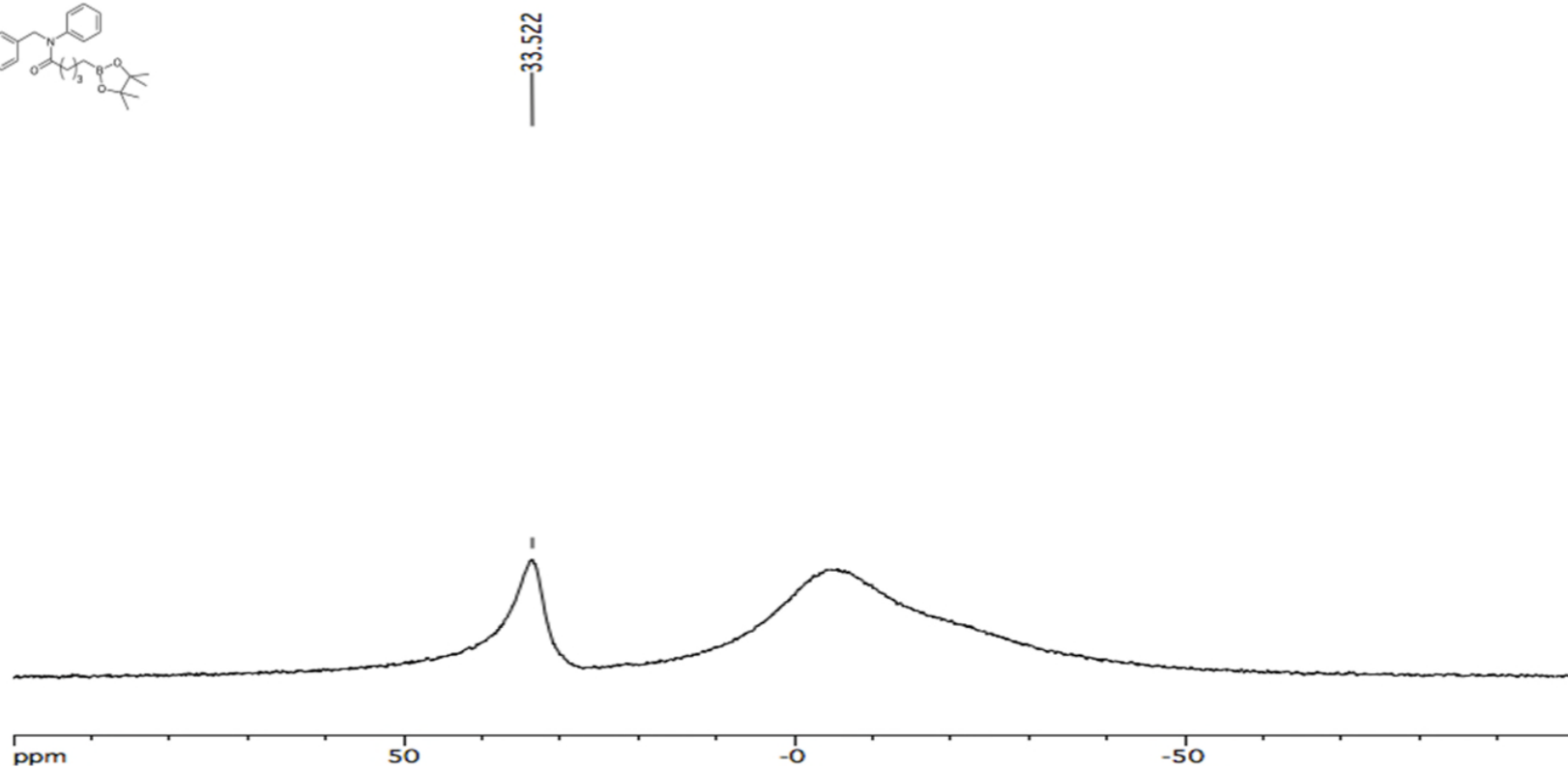
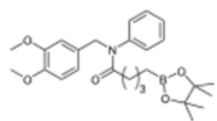
N-(3,4-dimethoxybenzyl)-*N*-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentanamide (**31**) – ^1H NMR



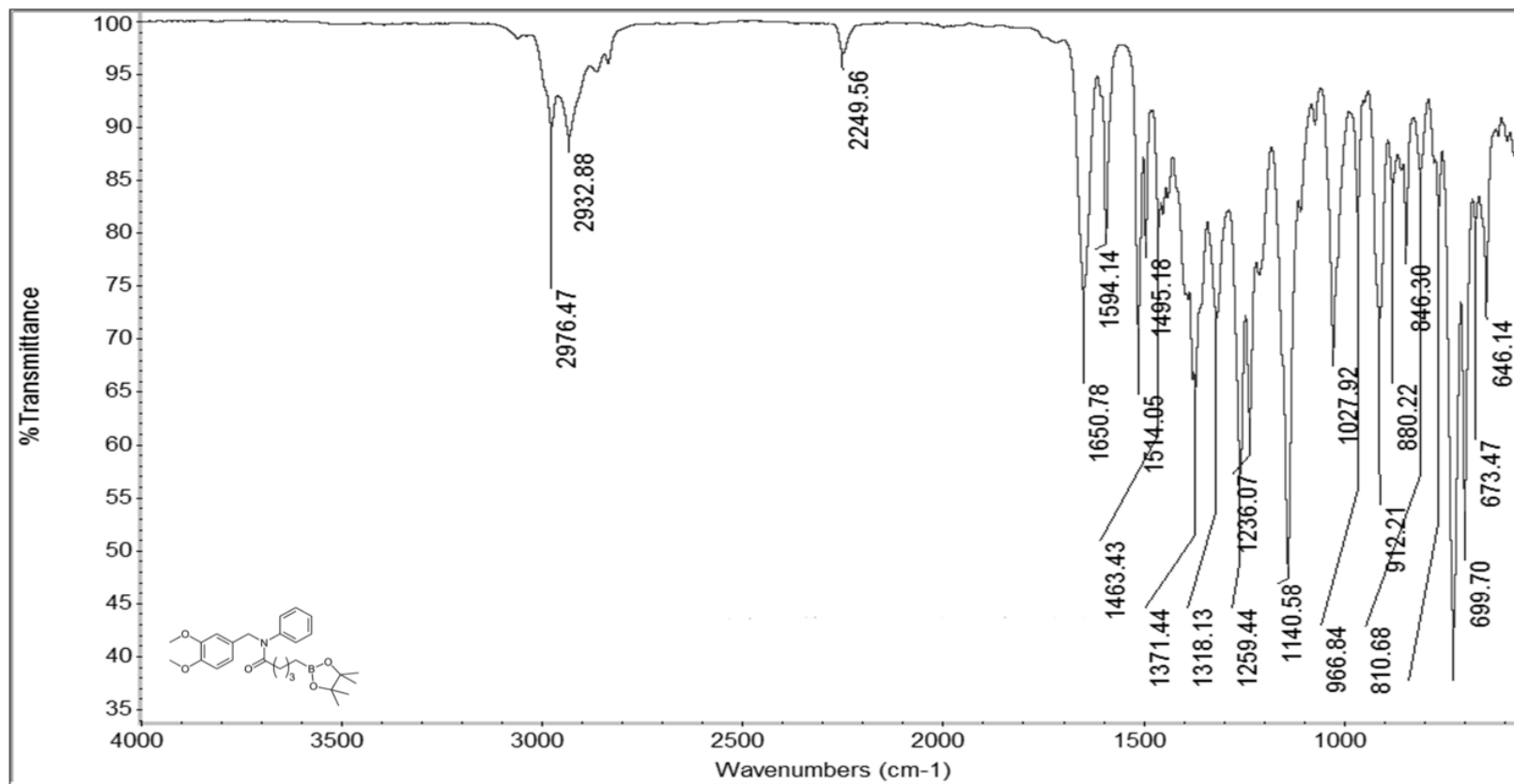
N-(3,4-dimethoxybenzyl)-*N*-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentanamide (**31**) – ^{13}C NMR

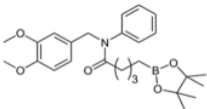


N-(3,4-dimethoxybenzyl)-*N*-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentanamide (**31**) – ^{11}B NMR

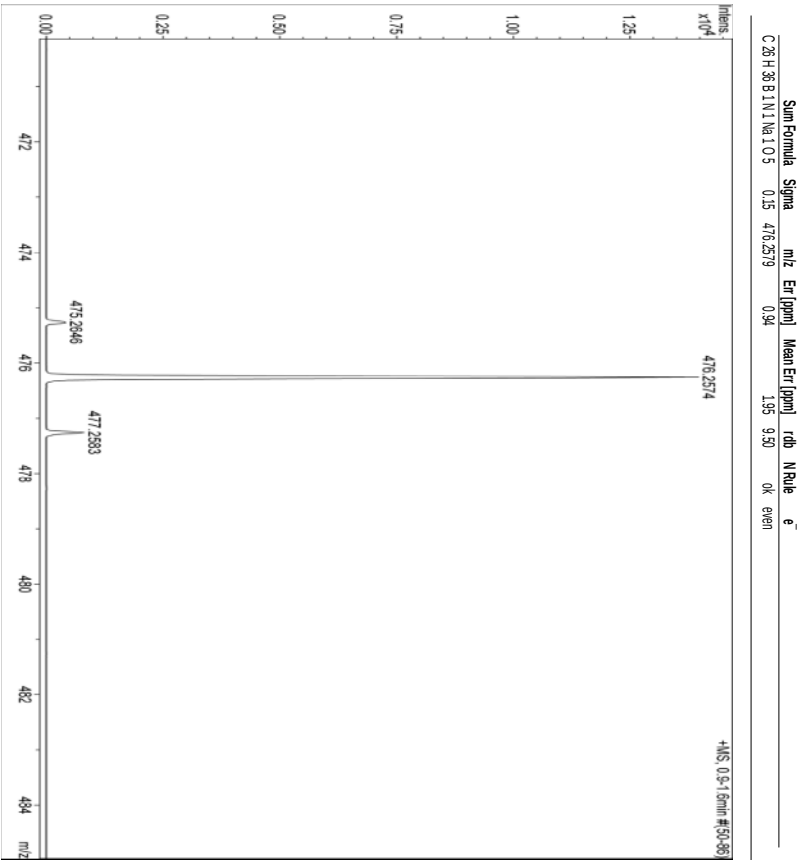


N-(3,4-dimethoxybenzyl)-*N*-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentanamide (**31**) – IR



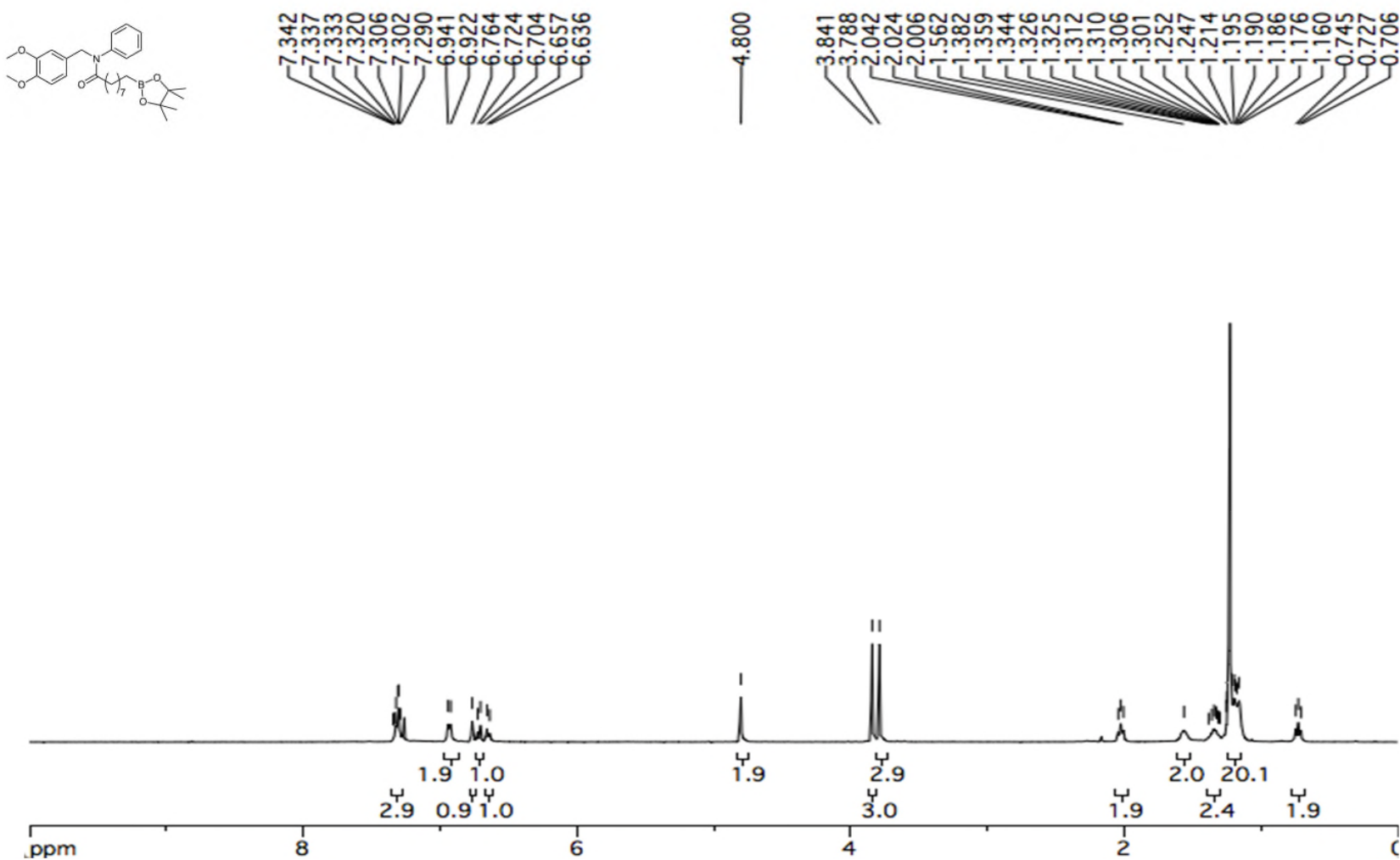


Analysis Info			Acquisition Date		
Analysis Name	D:\Data\Xiao\Nov 05 2020\00002020.d		11/5/2020 3:06:15 PM		
Method	Xiao 2.m		Operator		
Sample Name	JM-47		Administrator		
Comment			Instrument		
			microTOF		
			57		
Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Corrector Fill	45 V
Scan Range	na	Capillary Exit	90.0 V	Set Pulsar Pull	399 V
Scan Begin	50 m/z	Hexapole RF	125.0 V	Set Pulsar Push	399 V
Scan End	1500 m/z	Skimmer 1	40.0 V	Set Reflector	1300 V
		Hexapole 1	23.0 V	Set FWHM Tube	9000 V
				Set Detector TOF	2200 V

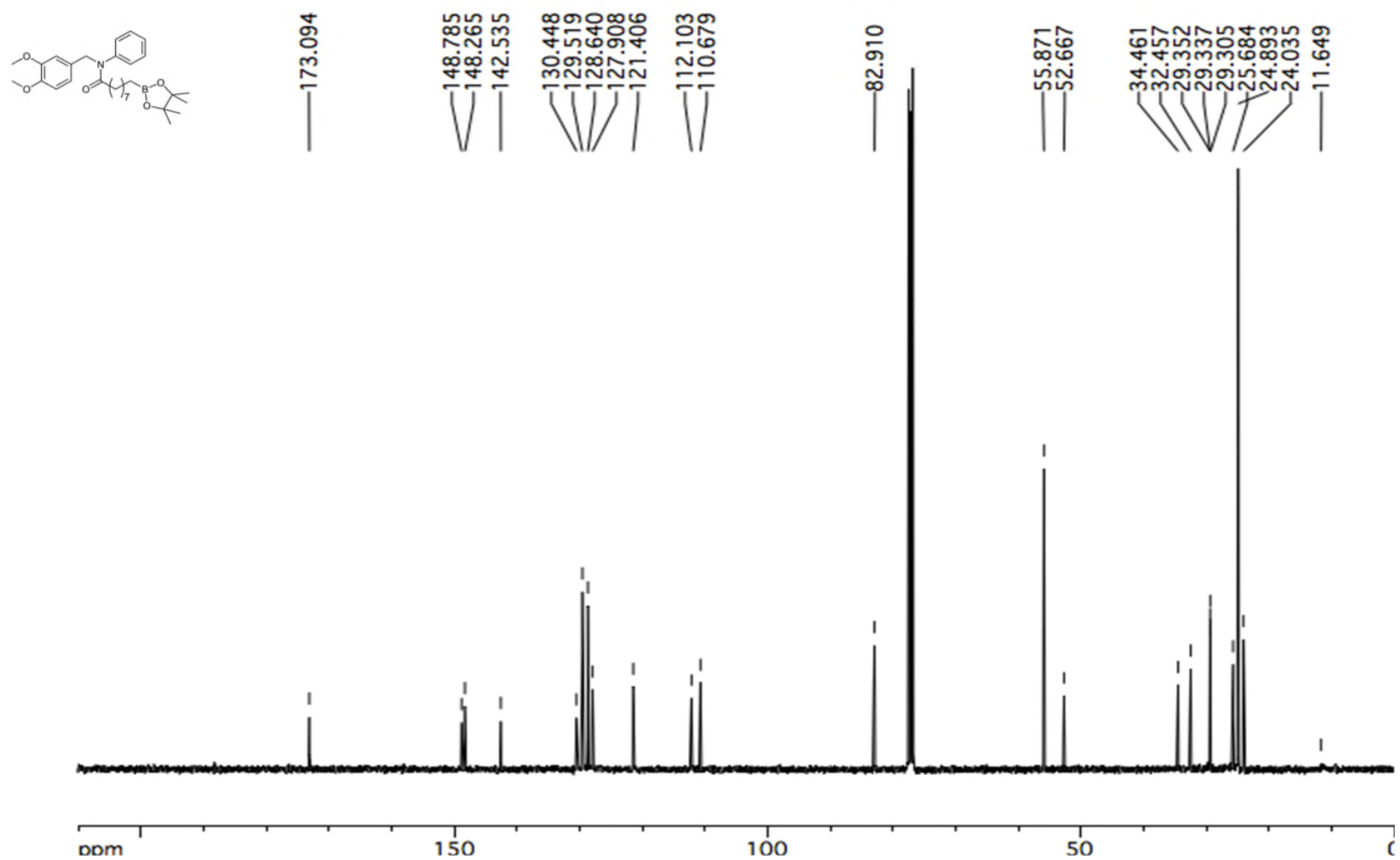


N-(3,4-dimethoxybenzyl)-*N*-phenyl-5-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)pentanamide (**31**) – HRMS

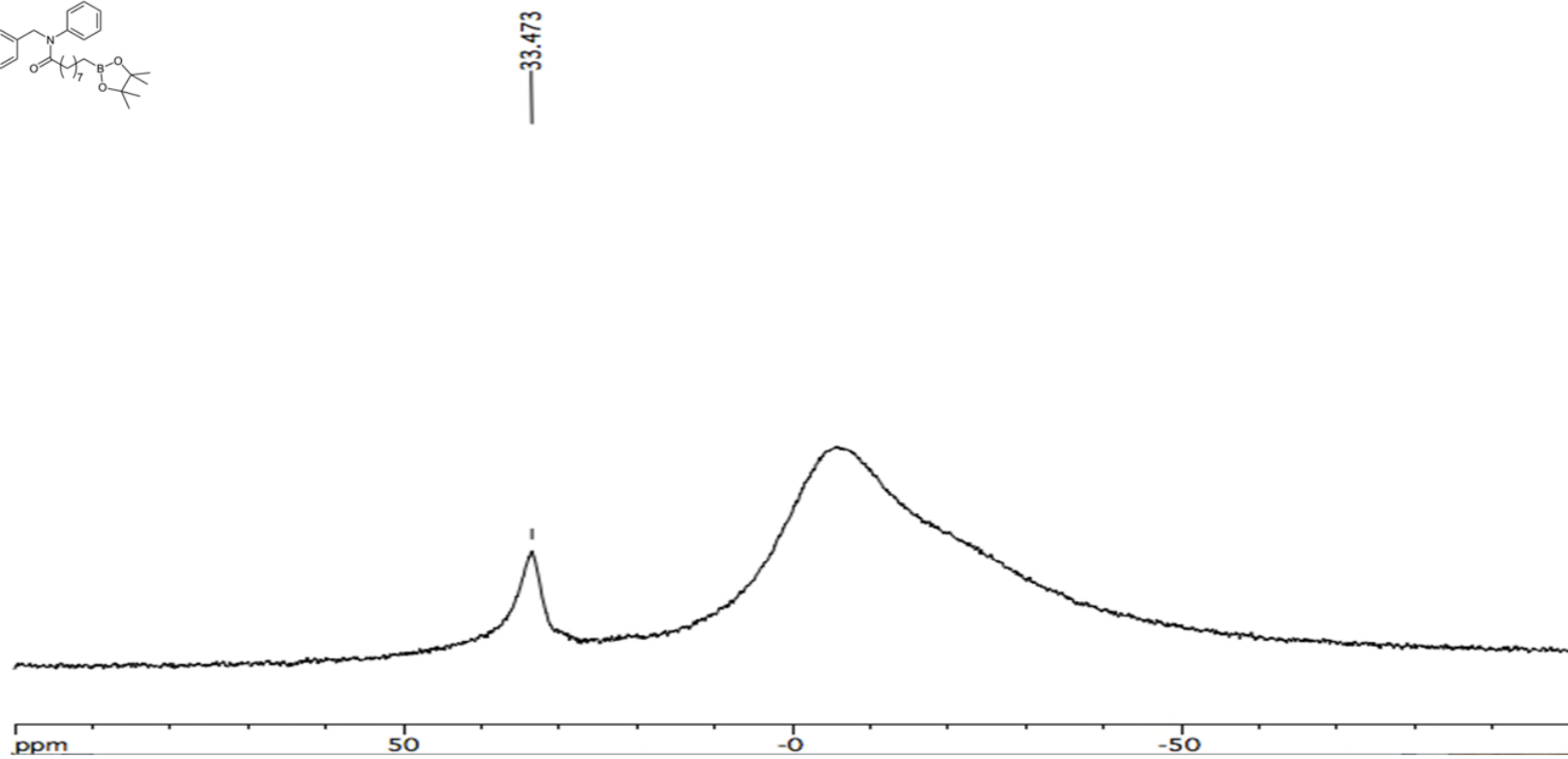
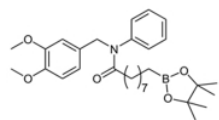
N-(3,4-dimethoxybenzyl)-*N*-phenyl-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**32**) – ^1H NMR



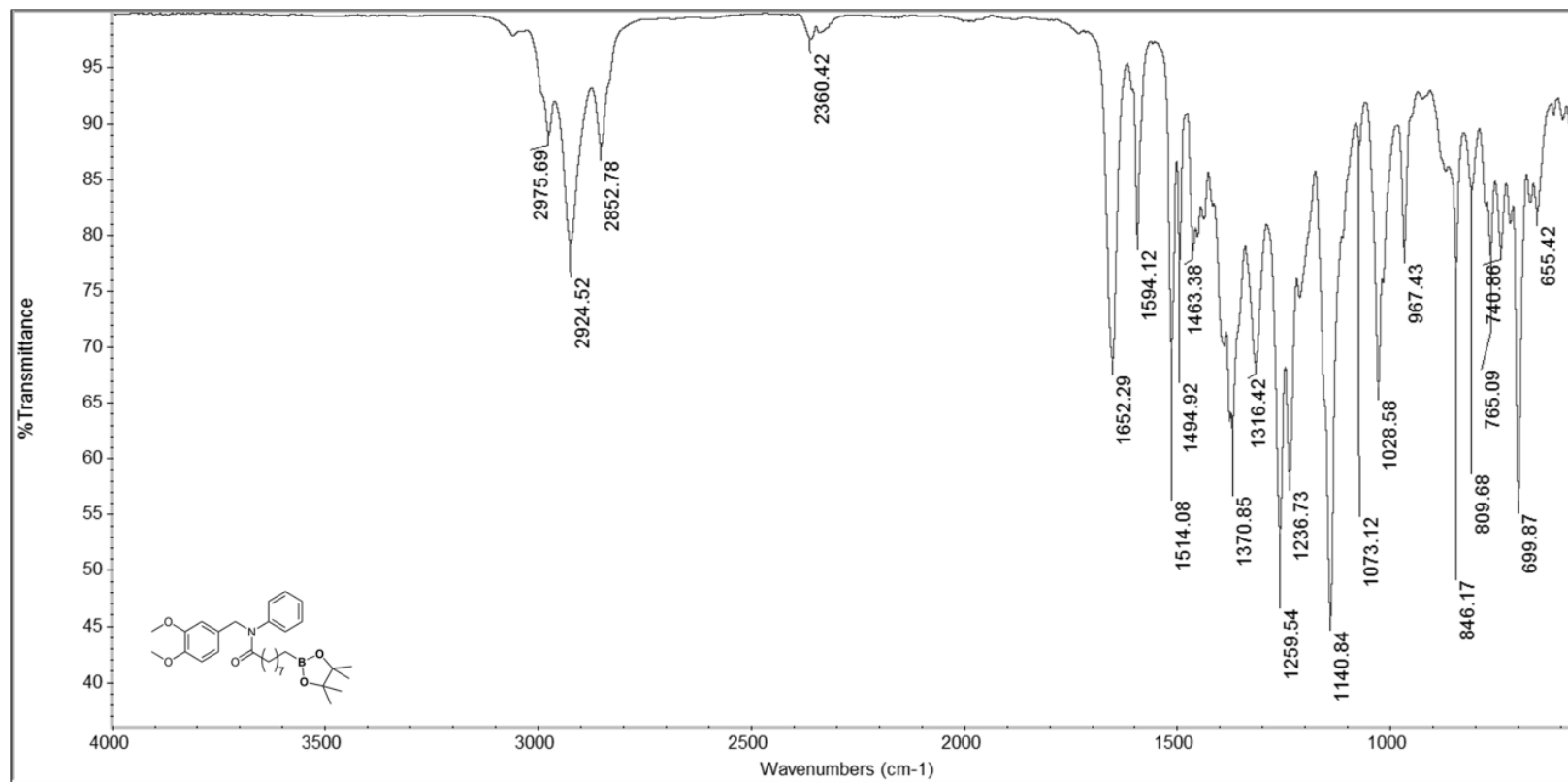
N-(3,4-dimethoxybenzyl)-*N*-phenyl-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**32**) – ^{13}C NMR

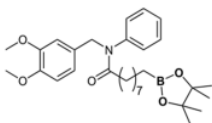


N-(3,4-dimethoxybenzyl)-*N*-phenyl-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**32**) – ^{11}B NMR



N-(3,4-dimethoxybenzyl)-*N*-phenyl-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**32**) – IR





Analysis Info

Analysis Name D:\Data\Kao\Nov 05 2002\000008.d
Method Xeo 2.m
Sample Name JM-61
Comment

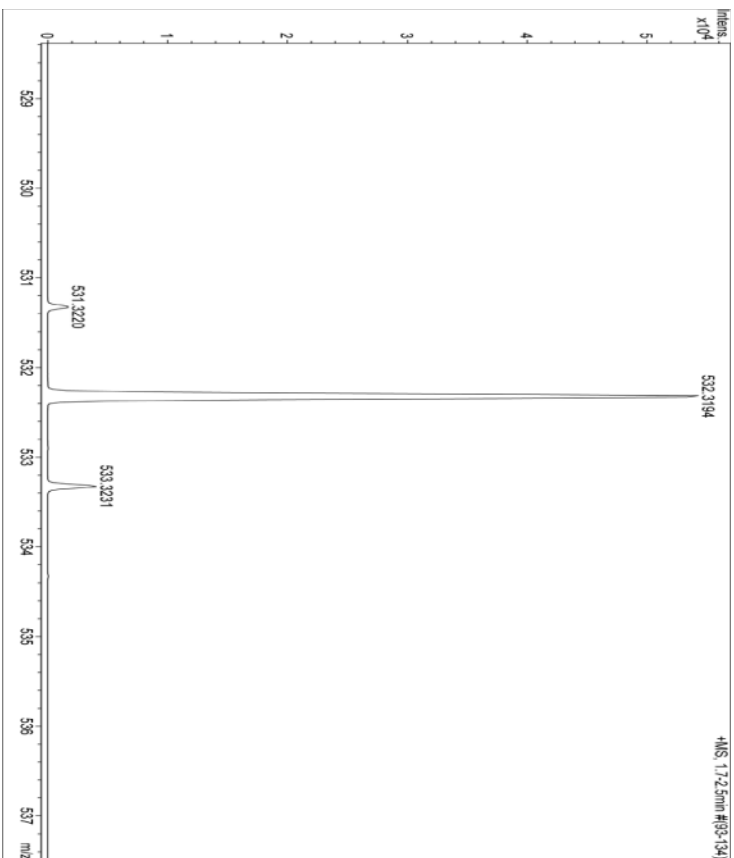
Acquisition Date 11/6/2002 10:57:50 AM

Operator Administrator
Instrument microTOF 57

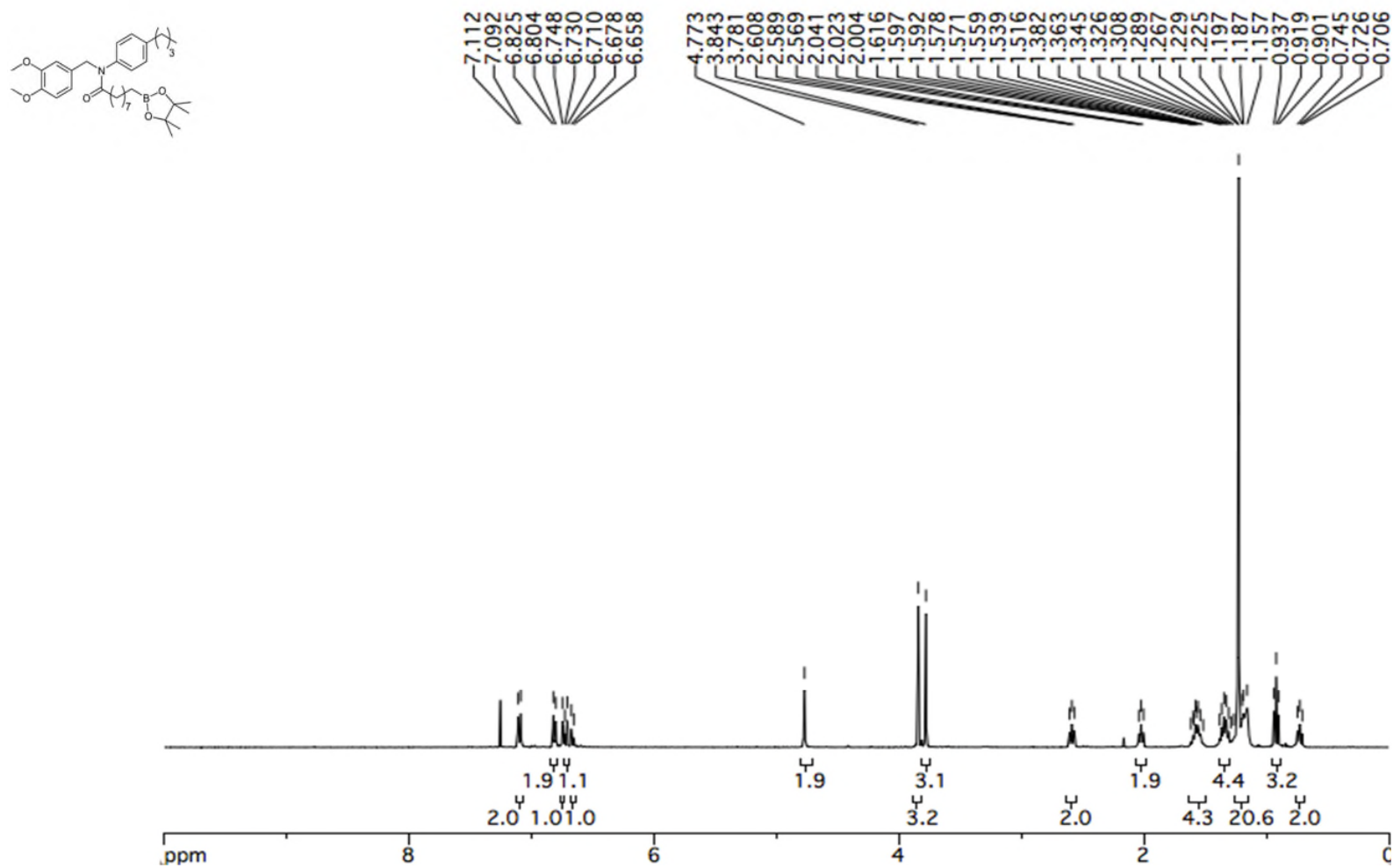
Acquisition Parameter

Source Type	ESI	Ion Planity	Positive	Set Corrector Fill	45 V
Scan Range	n/a	Capillary Exit	90.0 V	Set Pulsar Pull	399 V
Scan Begin	50 m/z	Hexapole RF	125.0 V	Set Pulsar Push	399 V
Scan End	1500 m/z	Skimmer 1	40.0 V	Set Flight Tube	9000 V
		Hexapole 1	23.0 V	Set Detector TOF	2200 V

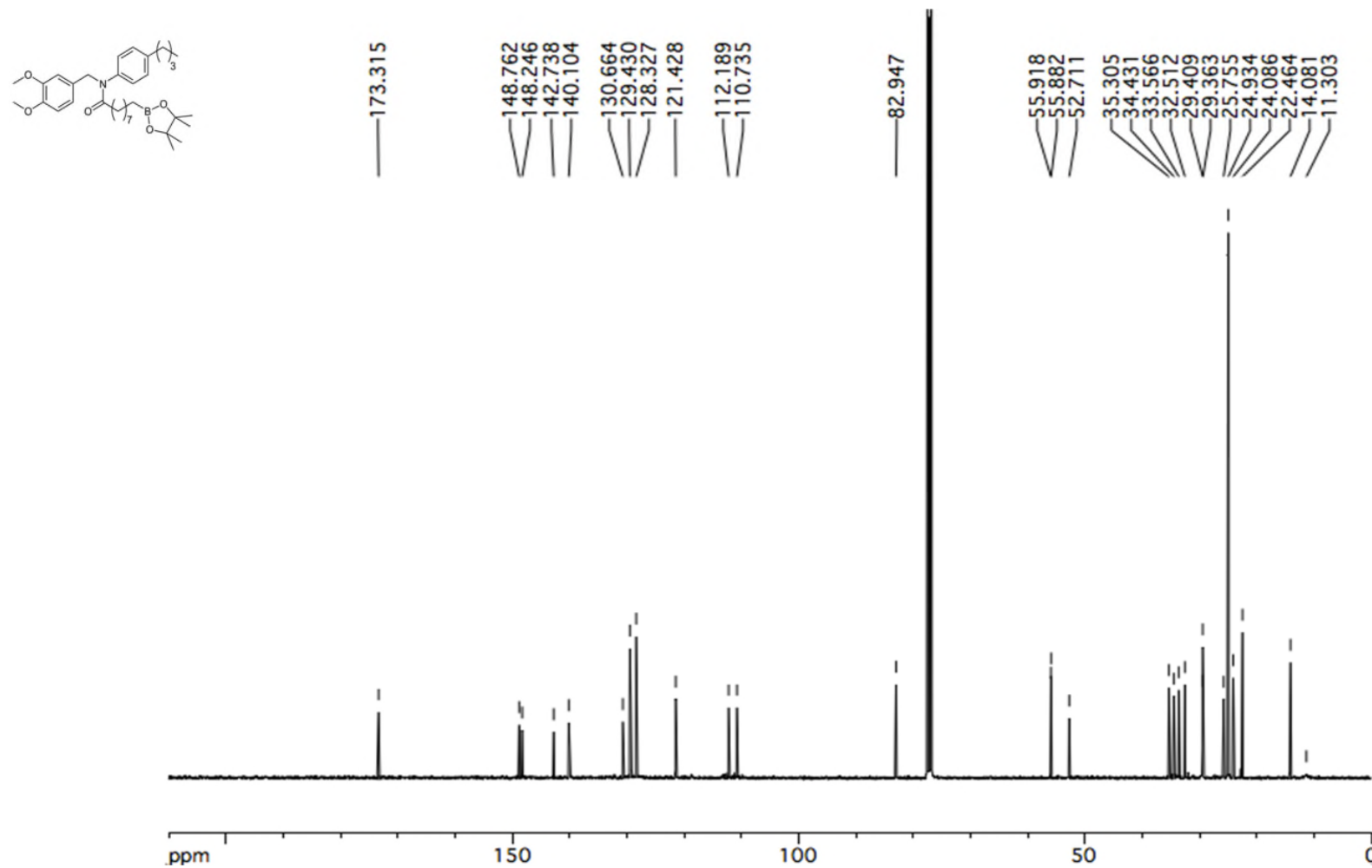
Sum Formula	Sigma	m/z	Err (ppm)	Mean Err (ppm)	rtb	N Rule	e ⁻
C30H44B1N1Na1O5	0.15	532.3205	2.02	2.98	950	OK	even



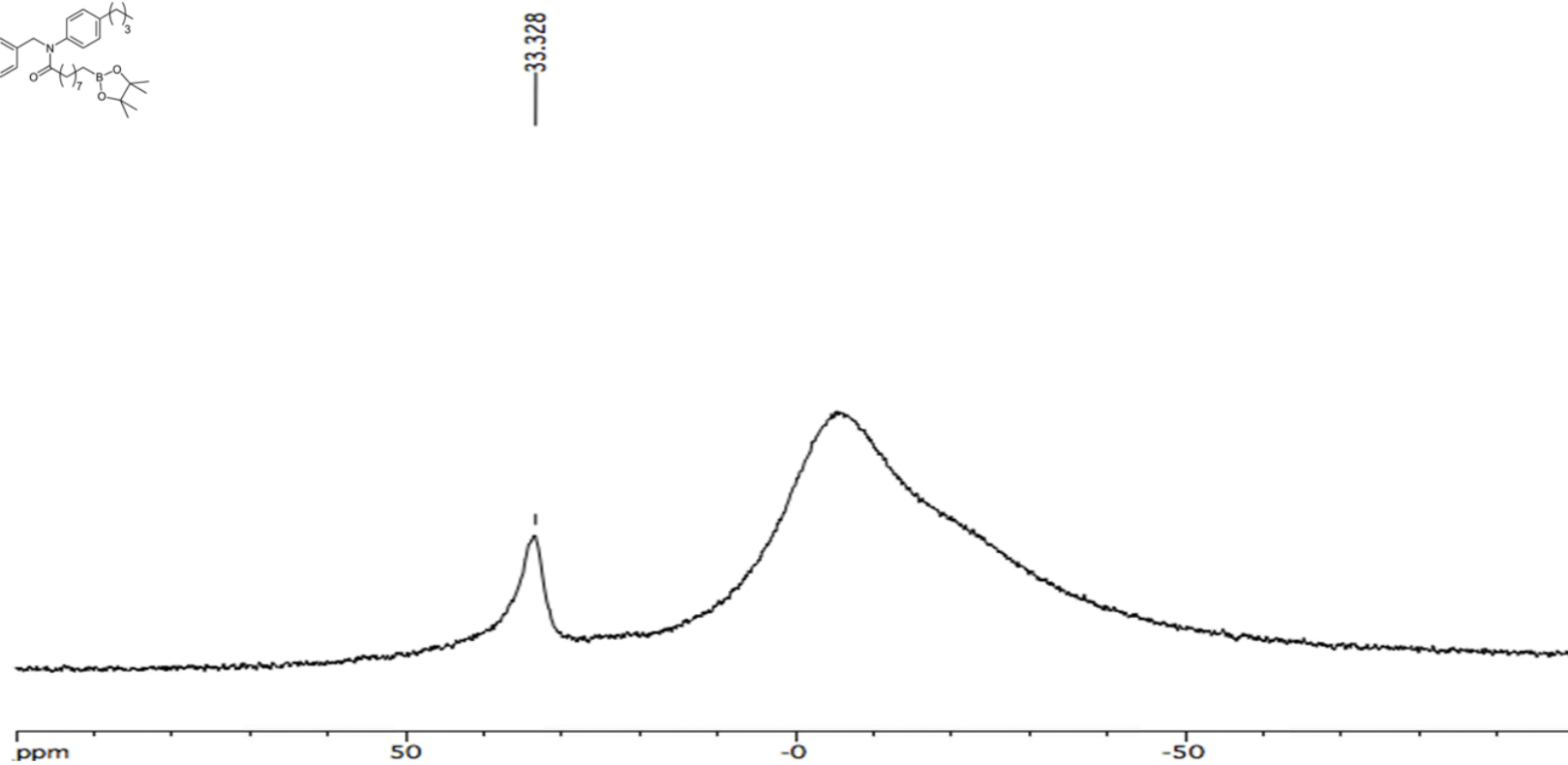
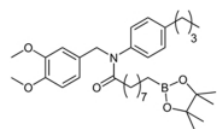
N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**33**) – ^1H NMR



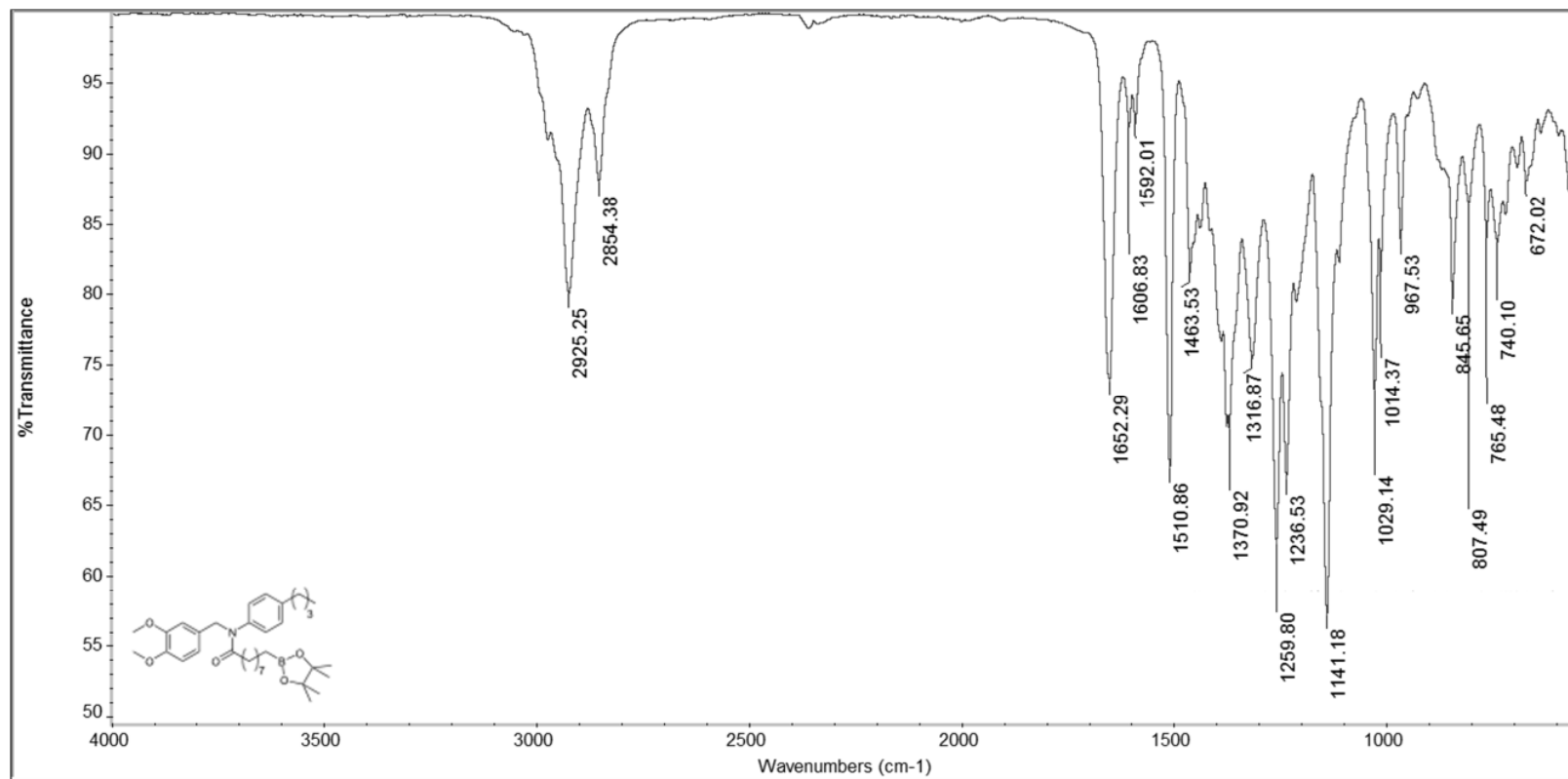
N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**33**) – ^{13}C NMR

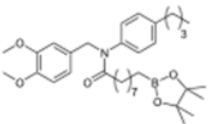


N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**33**) – ^{11}B NMR

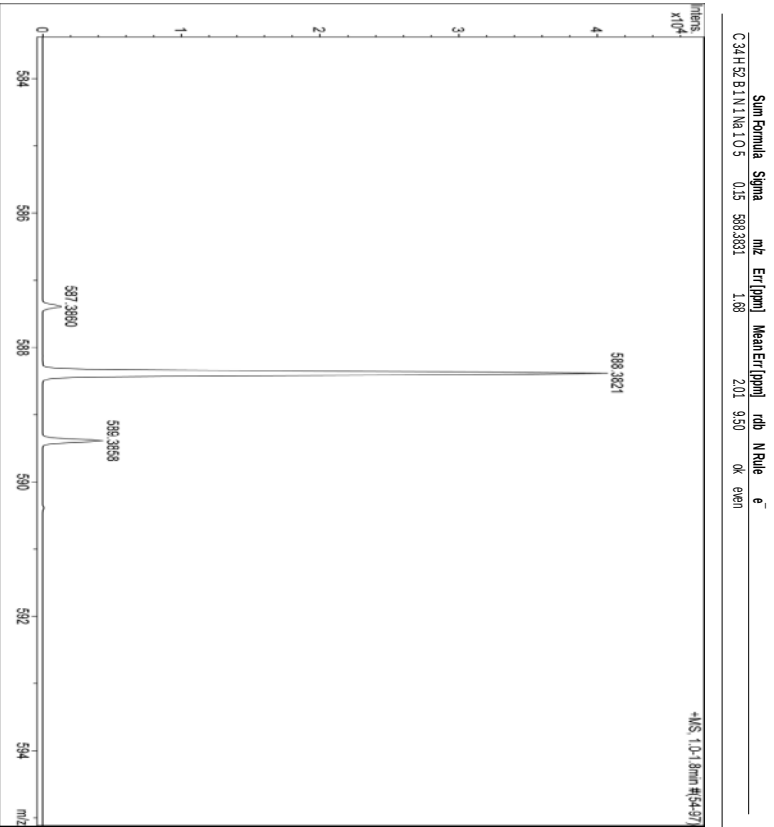


N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**33**) – IR



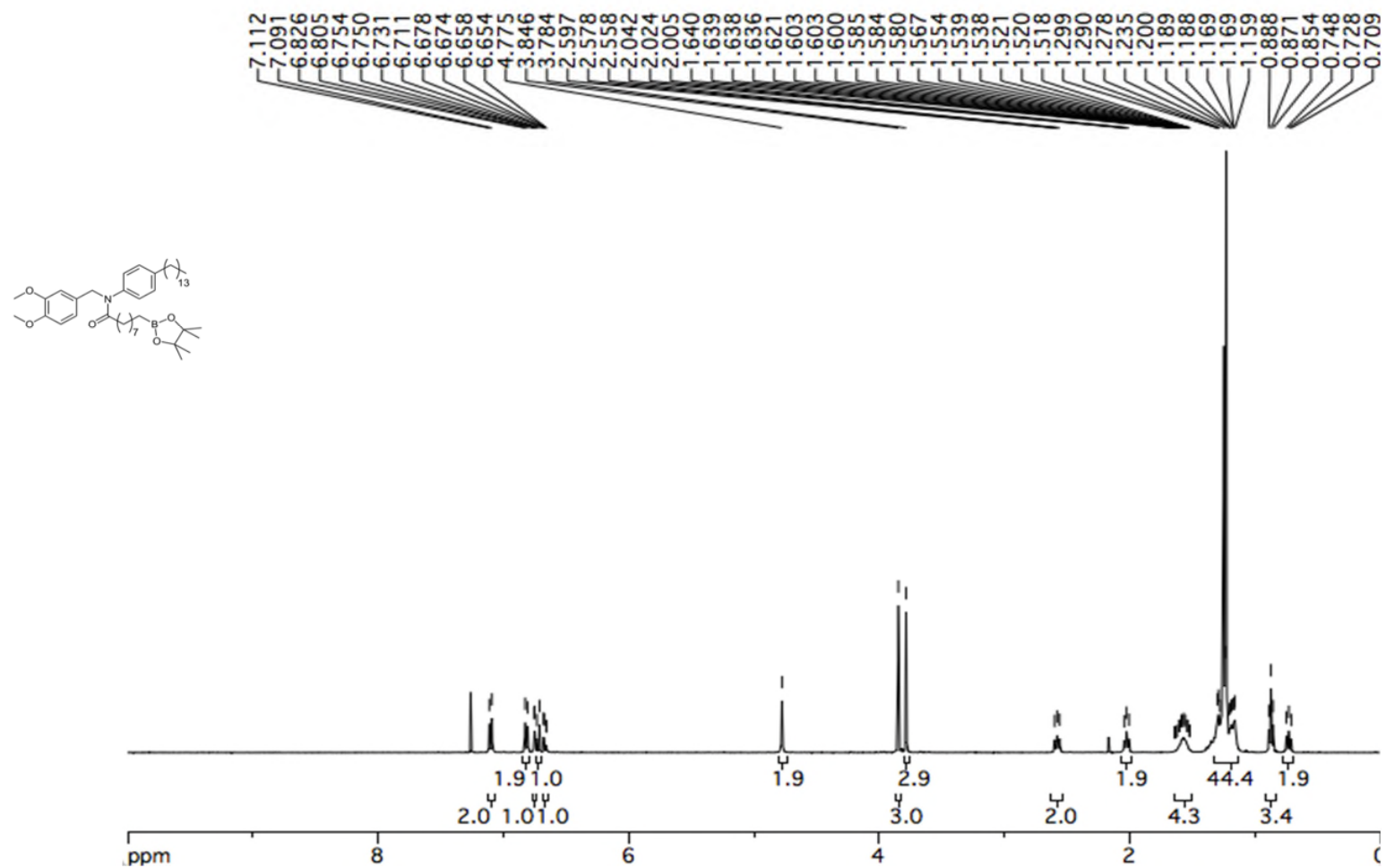


Analysis Info		Acquisition Date	
Analysis Name	D:\Data\Xiao\Nov 05 2020\000007.d	11/5/2020 10:47:50 AM	
Method	Xao 2.m	Operator	Administrator
Sample Name	JM-69	Instrument	micrOTOF
Comment	57		
Acquisition Parameter			
Source type	ESI	Ion Polarity	Positive
Scan Range	m/z	Capillary Exit	900 V
Scan Begin	50 m/z	Headspace RF	1250 V
Scan End	1500 m/z	Skimmer 1	400 V
		Headspace 1	230 V
		Set Corrector Fill	45 V
		Set Pulse Pull	399 V
		Set Pulse Push	399 V
		Set Reflector	1300 V
		Set Flight Tube	9000 V
		Set Detector TOF	2200 V

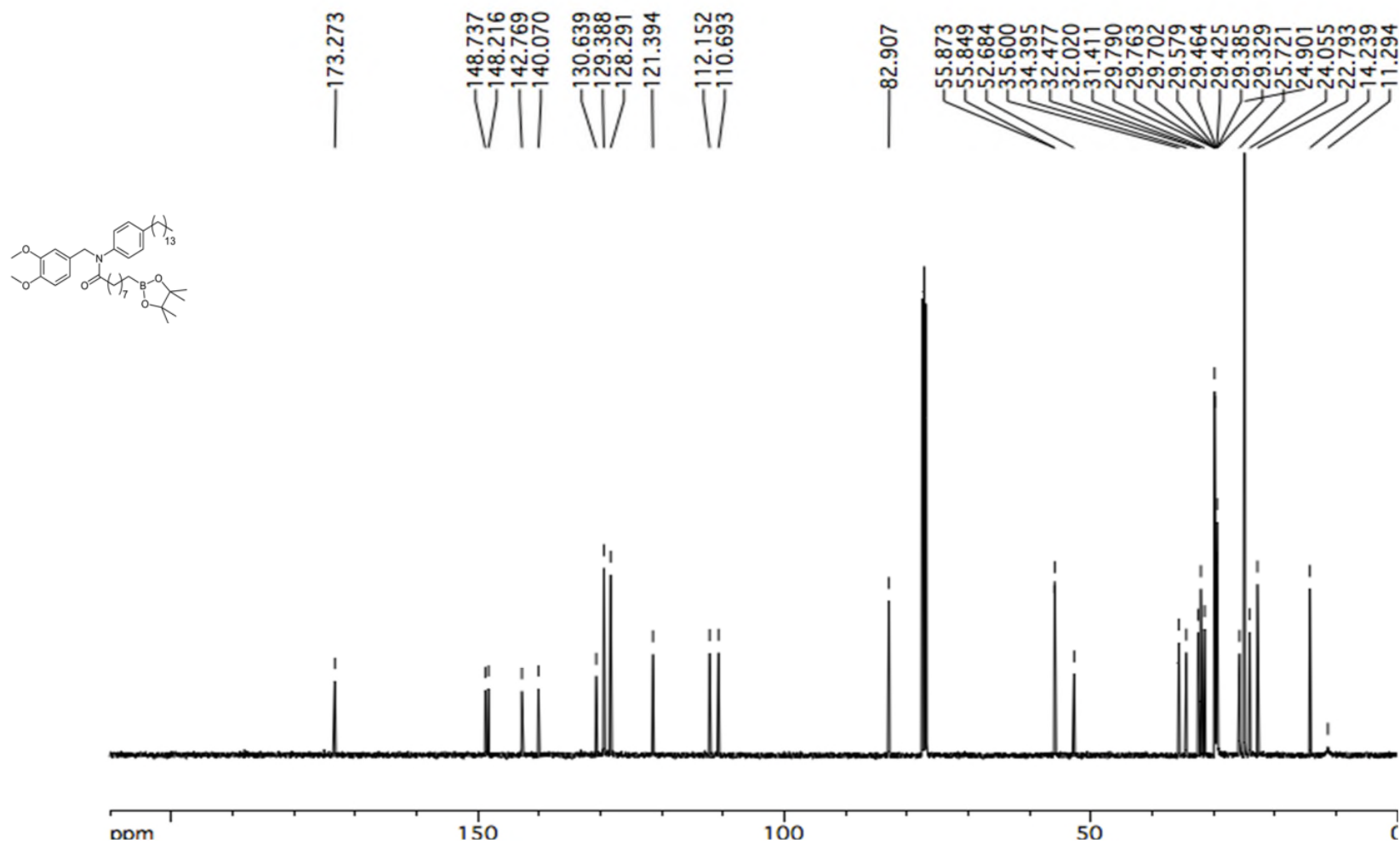


N-(4-butylphenyl)-*N*-(3,4-dimethoxybenzyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**33**) – HRMS

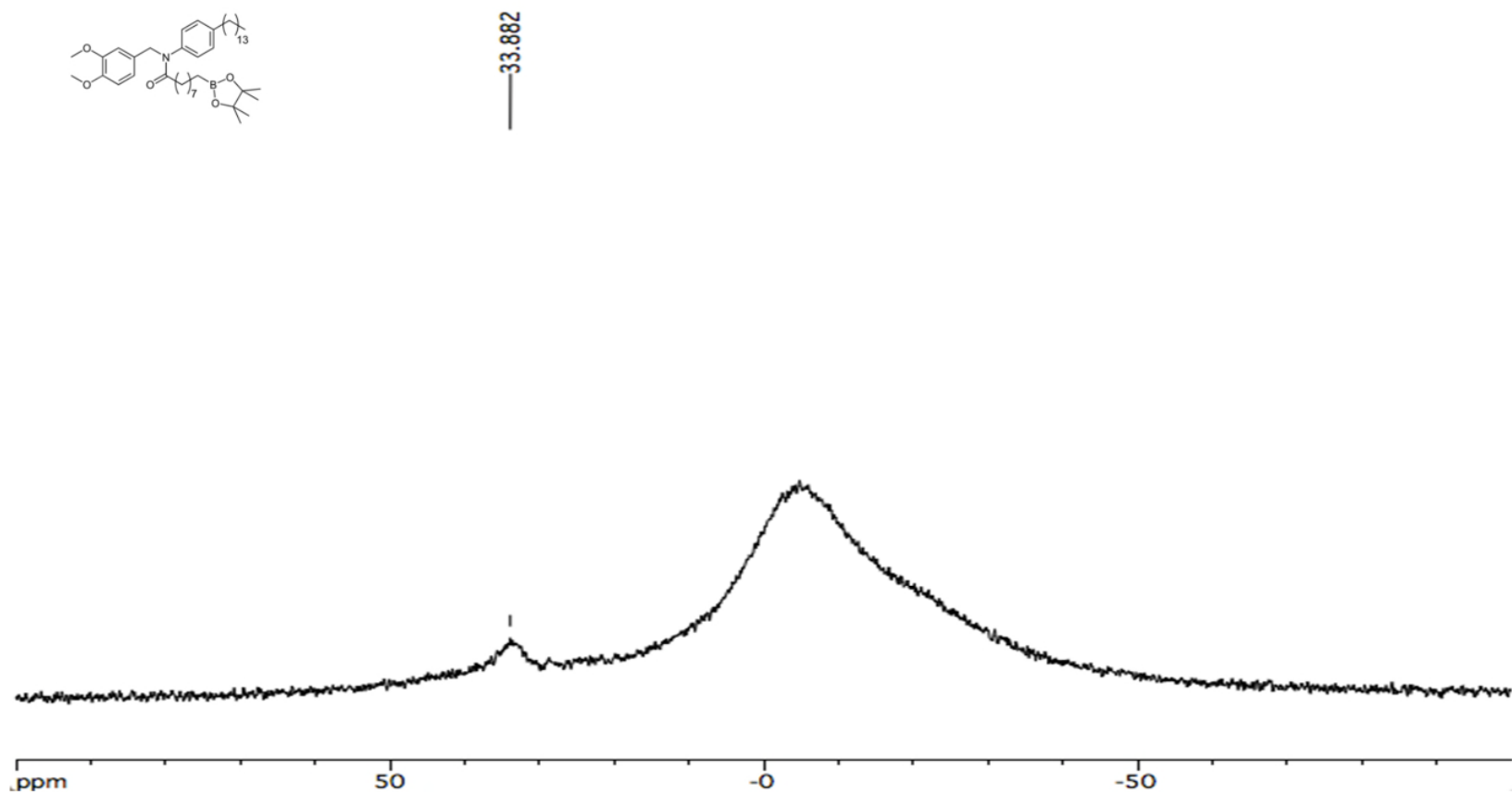
N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**34**) – ^1H NMR



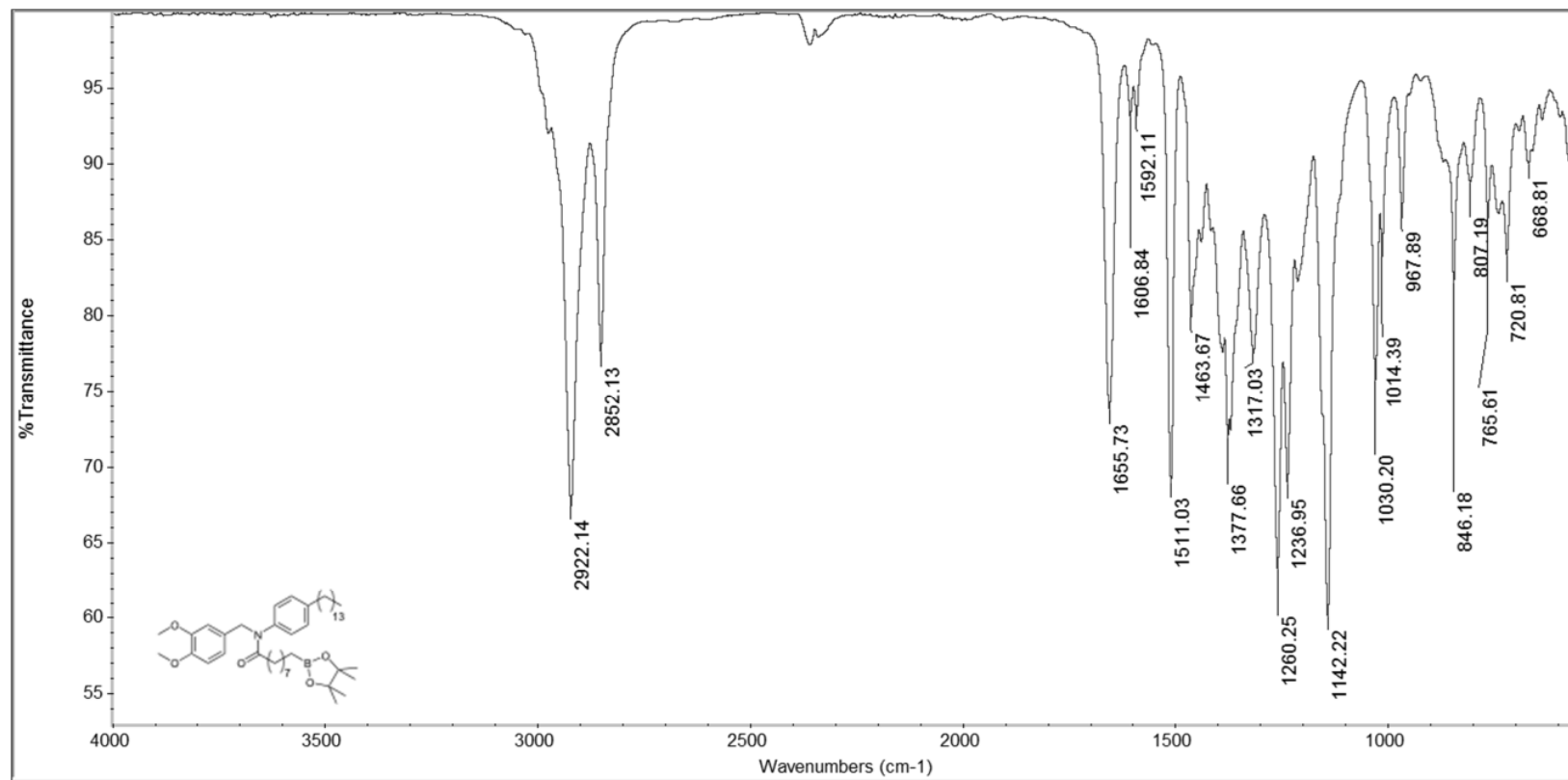
N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**34**) – ^{13}C NMR

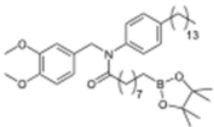


N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (34) – ^{11}B NMR



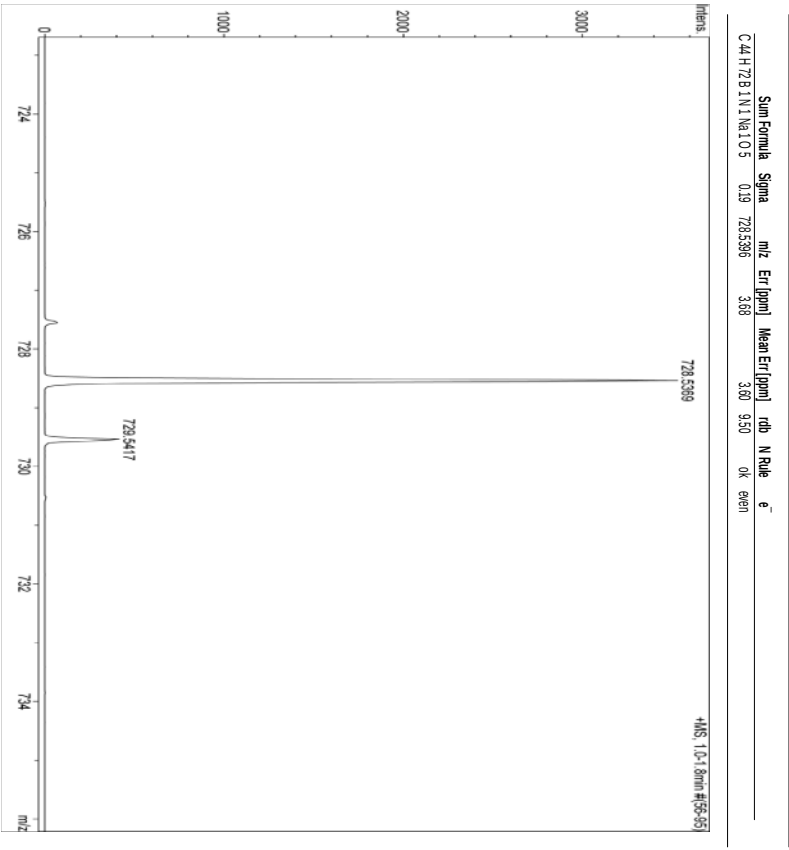
N-(3,4-dimethoxybenzyl)-*N*-(4-tetradecylphenyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (**34**) – IR





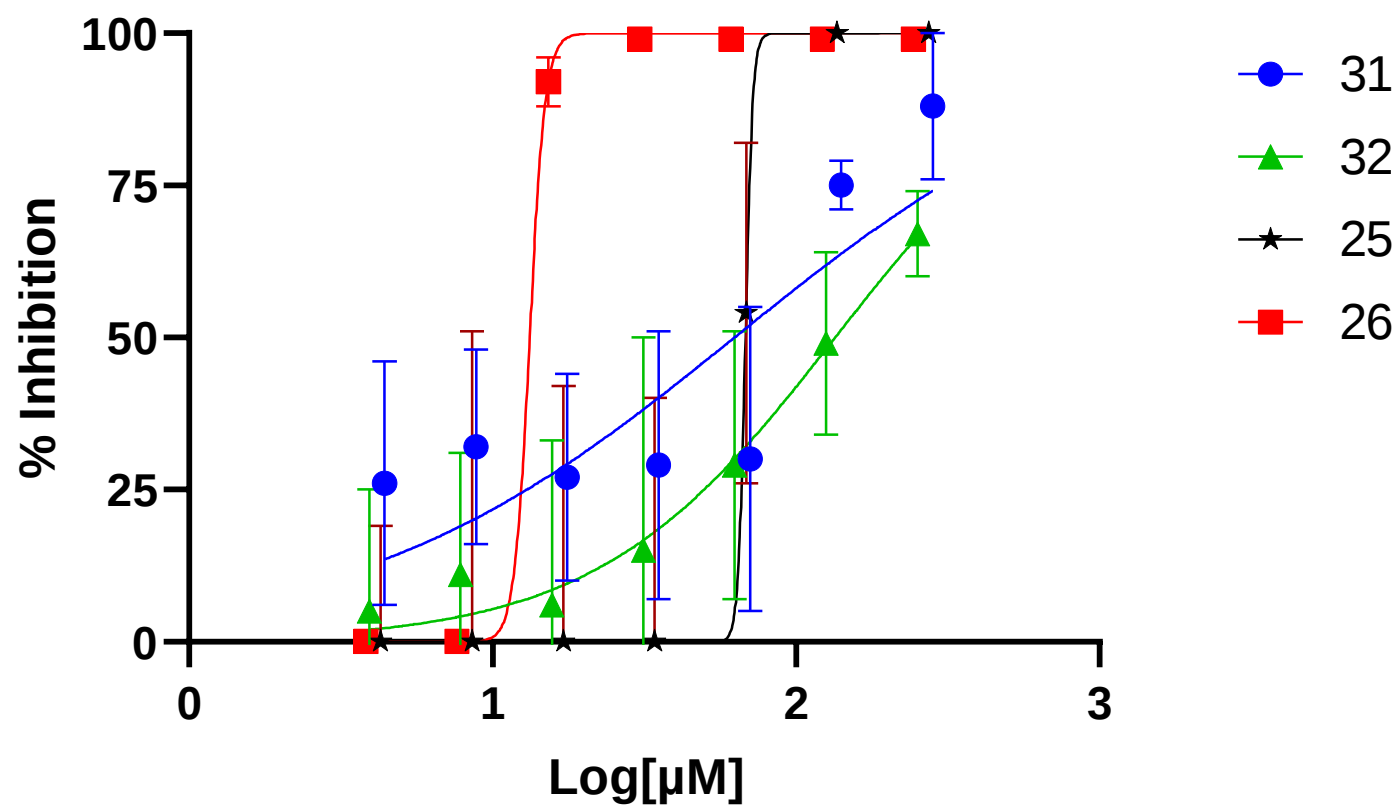
Analysis Info		Acquisition Date	
Analysis Name	D:\Data\Xiao\Nov 05 2020\000009.d	Operator	Administrator
Method	Xiao 2.m	Instrument	micrOTOF
Sample Name	JM-74		57
Comment			

Acquisition Parameter		Set/Corrector Fill	
Source Type	ESI	Set Puffer Fill	399 V
Scan Range	m/z	Set Puffer Push	399 V
Scan Begin	50 m/z	Set Puffer	1300 V
Scan End	1500 m/z	Set Flight Tube	9000 V
		Set Detector TOF	2200 V

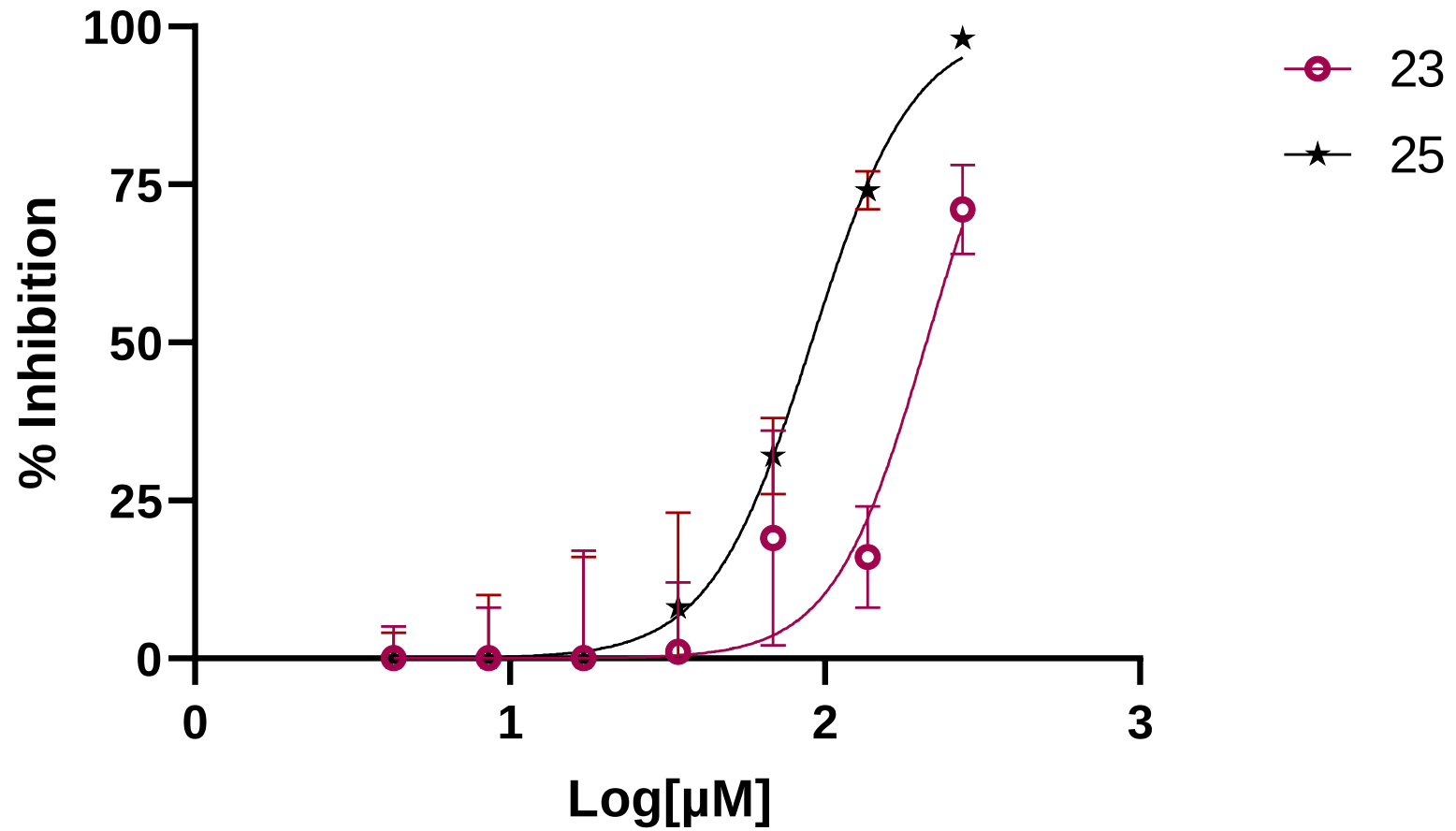


N-(3,4-dimethoxybenzyl)-N-(4-tetradecylphenyl)-9-(4,4,5,5-tetramethyl-1,3,2-dioxaborolan-2-yl)nonamide (34) – HRMS

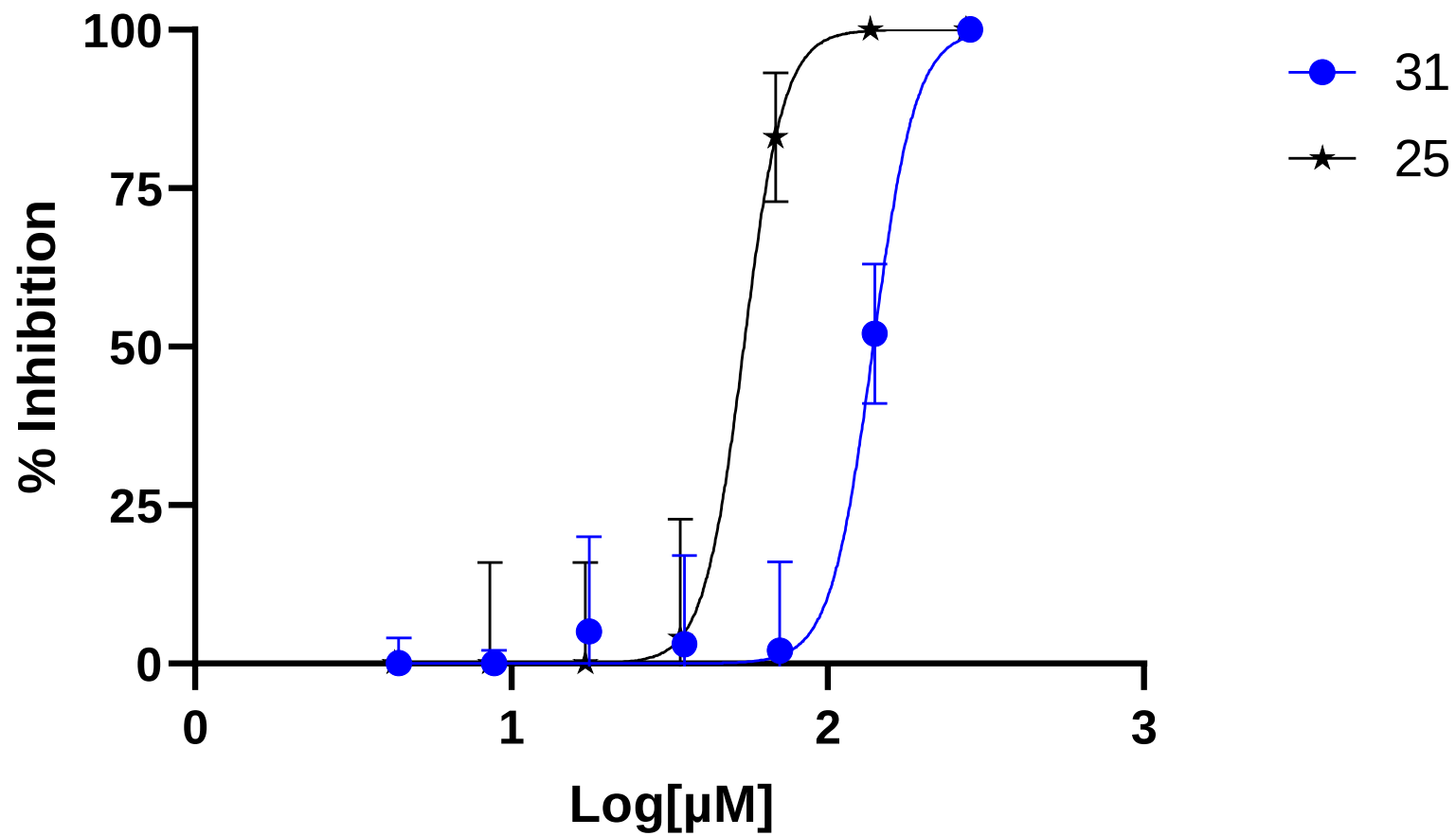
S.aureus methicillin-resistant (MRSA 310)



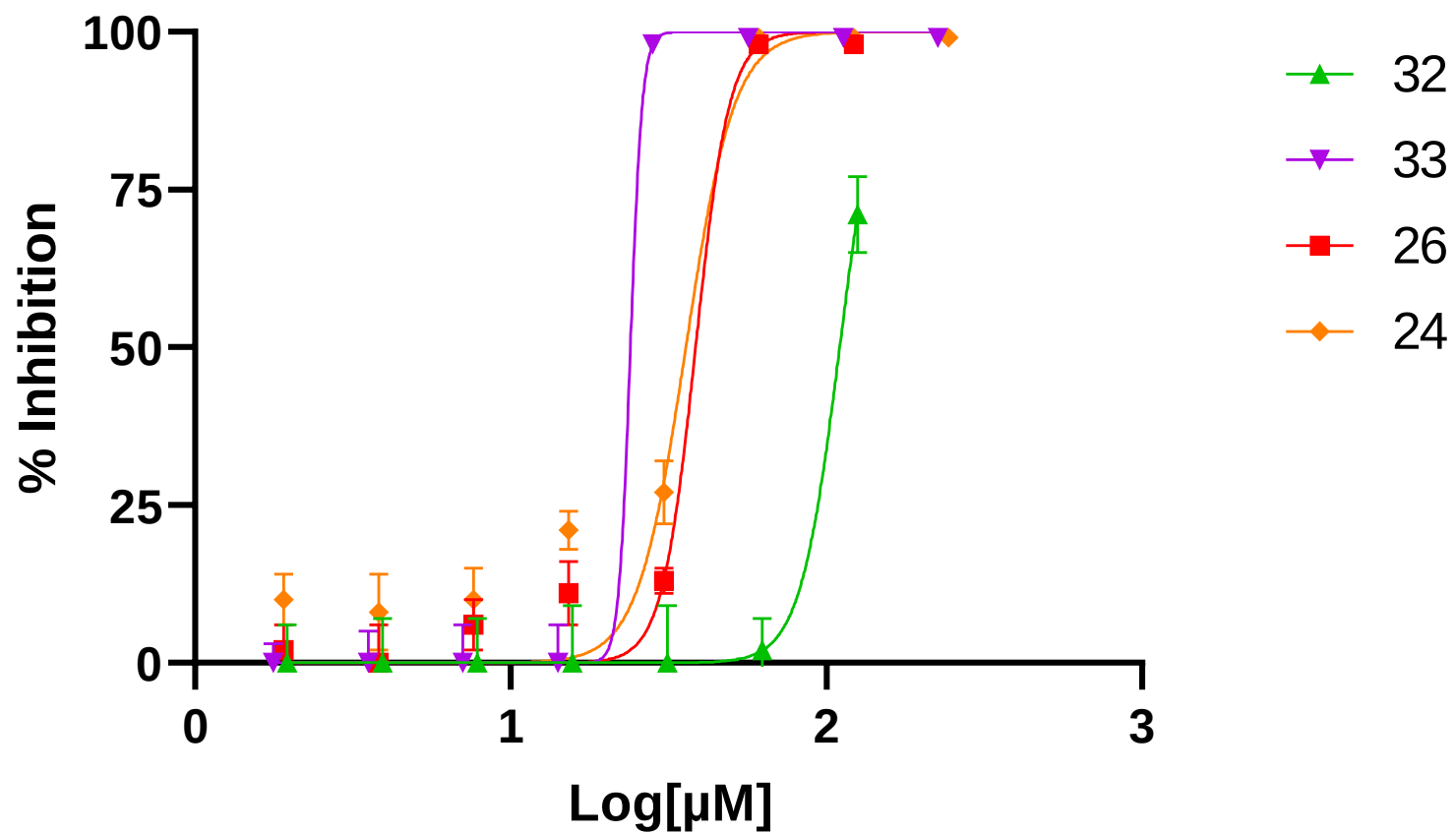
E.faecium vancomycin-resistance (VRE)



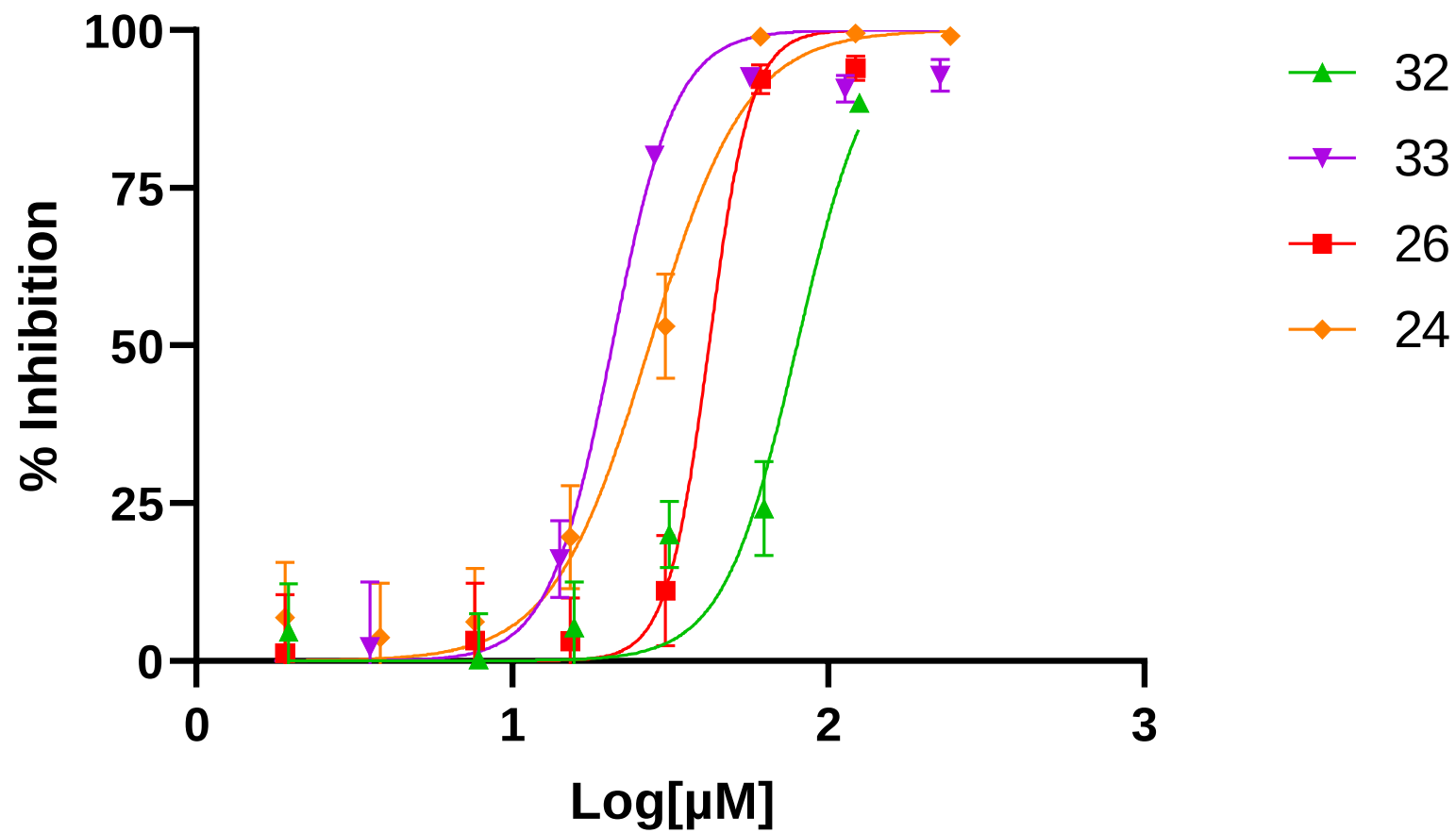
S.warneri (ATCC 17917)



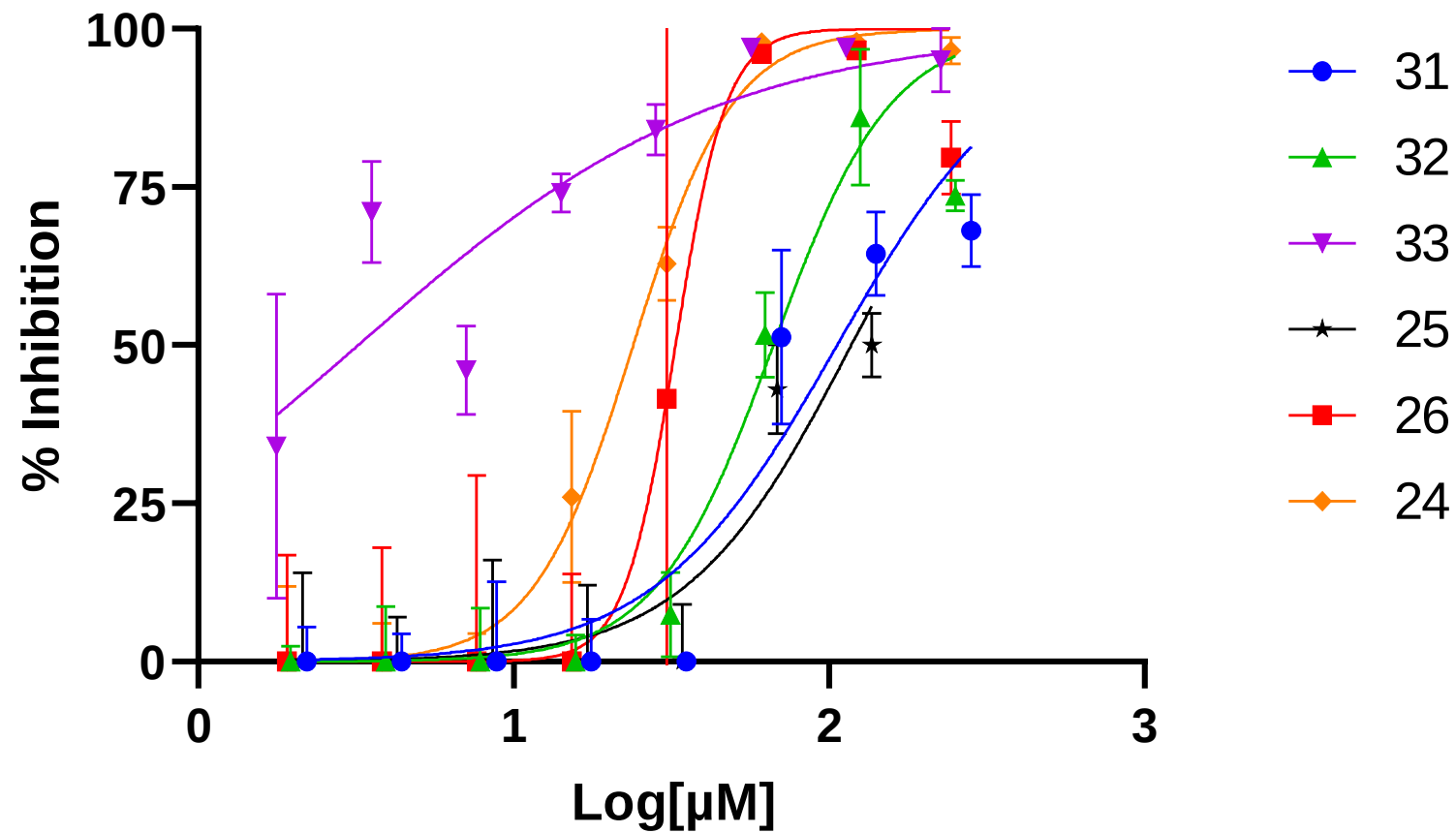
BJ (CRL-2522)



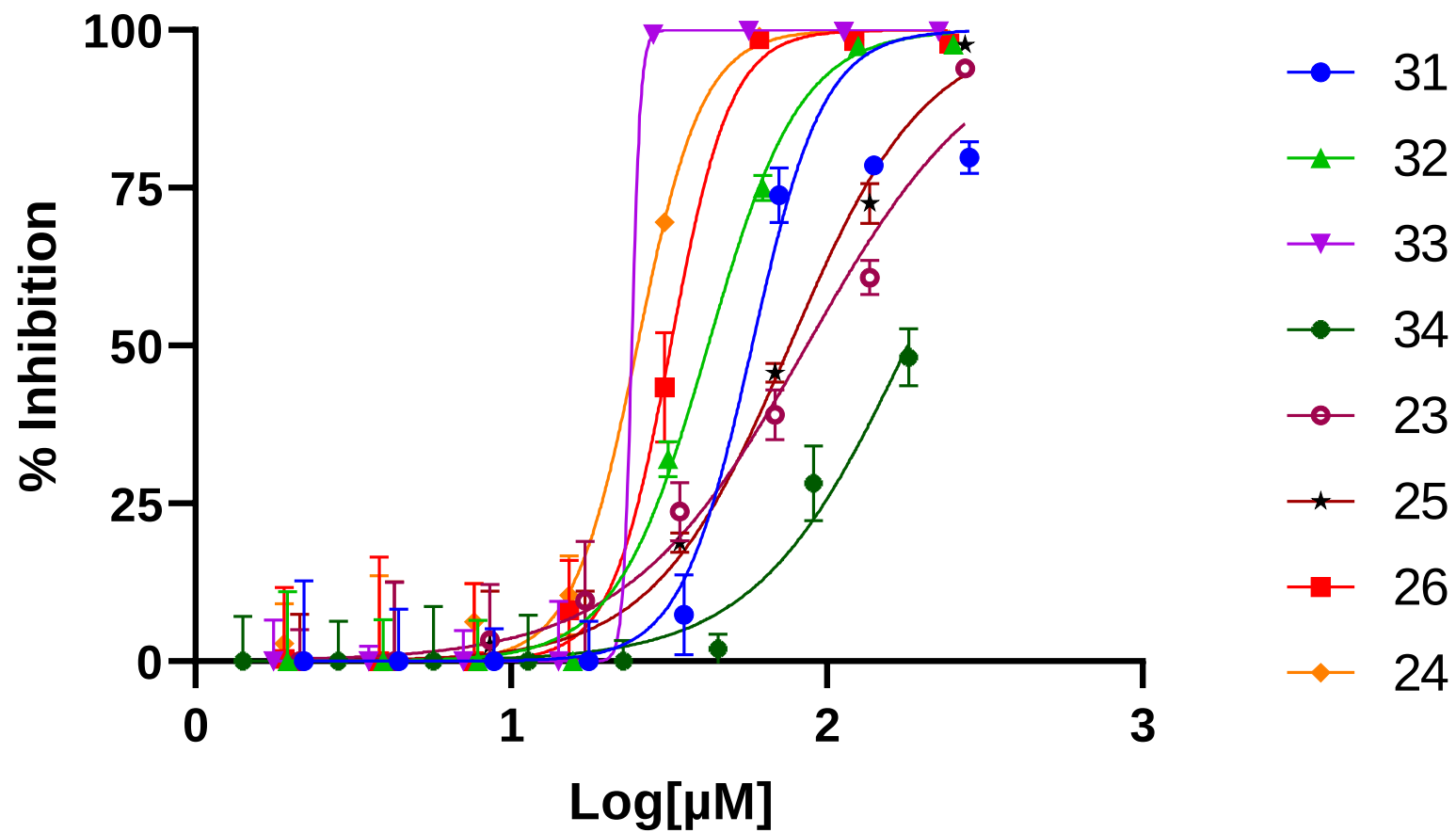
Vero (ATCC CCL-81)



MCF7 (HTB-22)



HTB26 (MDA-MB-231)



HCT116 (ATCC CCL-247)

