Supplementary Material

Efficient aqueous Suzuki coupling at room temperature via micellar catalysis with unconventional surfactants

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Email: sunilgg2010@gmail.com

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1. List of Suzuki Cross-Coupling product

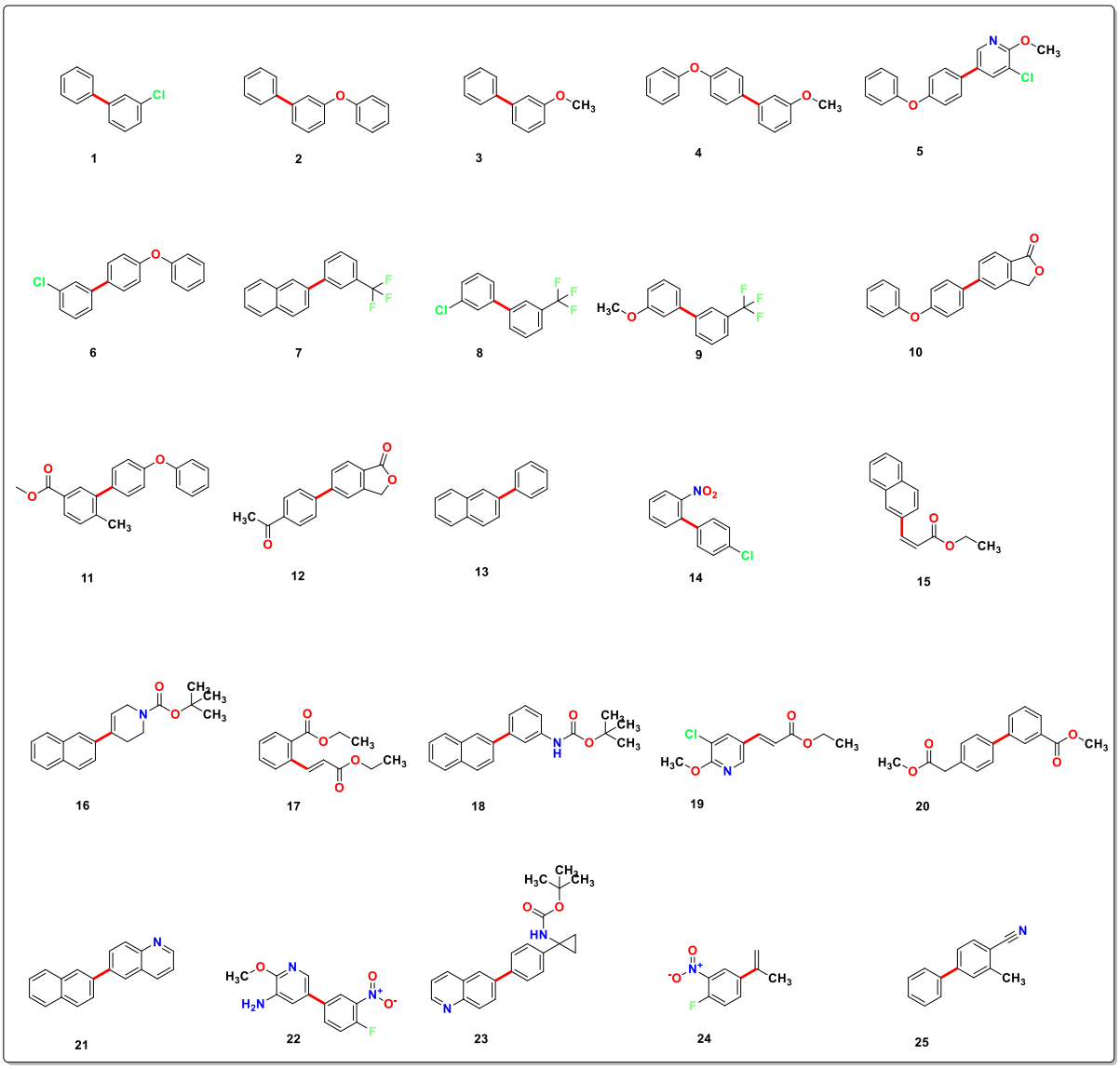


Table S1: List of Suzuki Cross-Coupling product 1-25

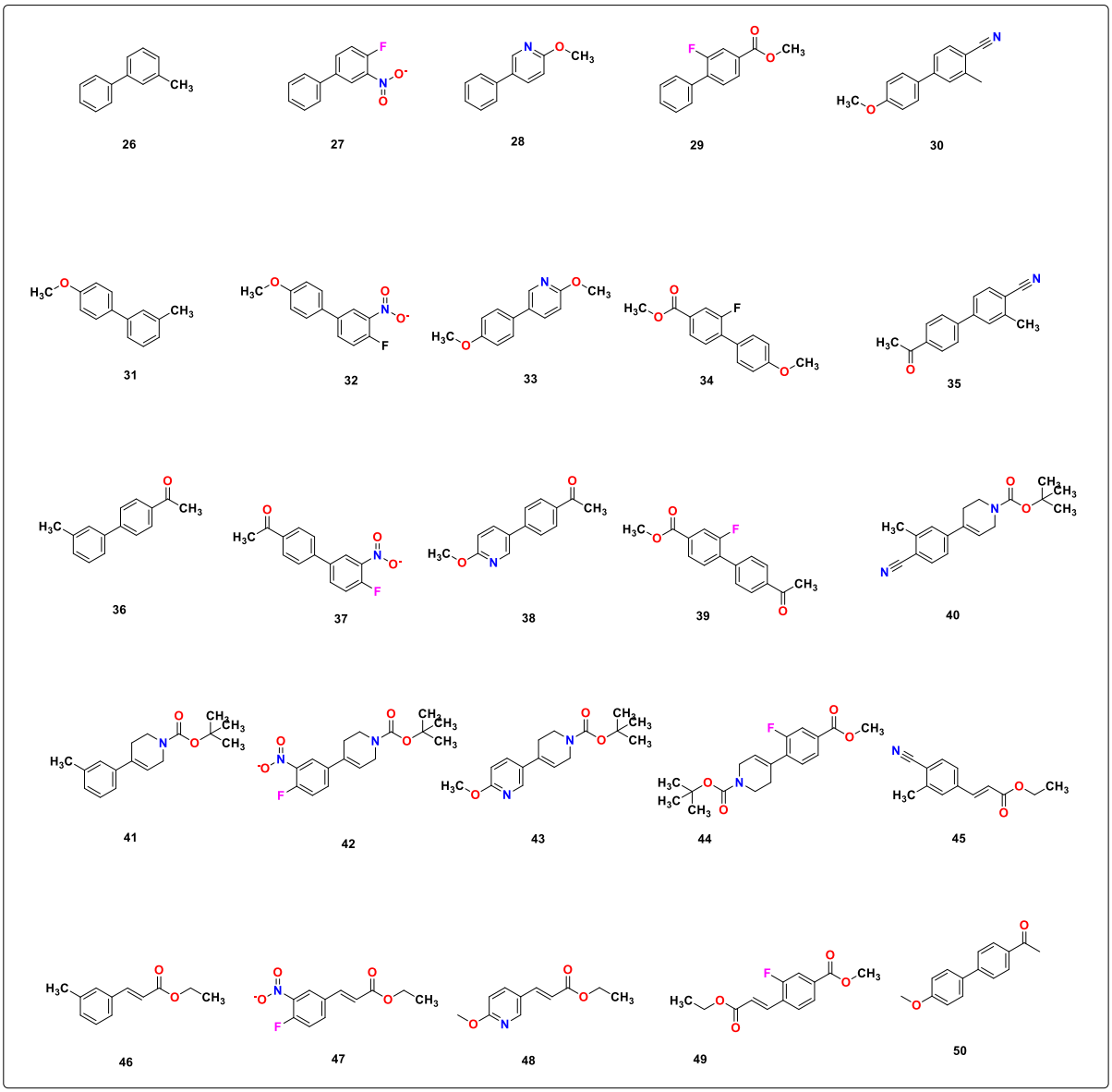


Table S2: List of Suzuki Cross-Coupling product 26-50

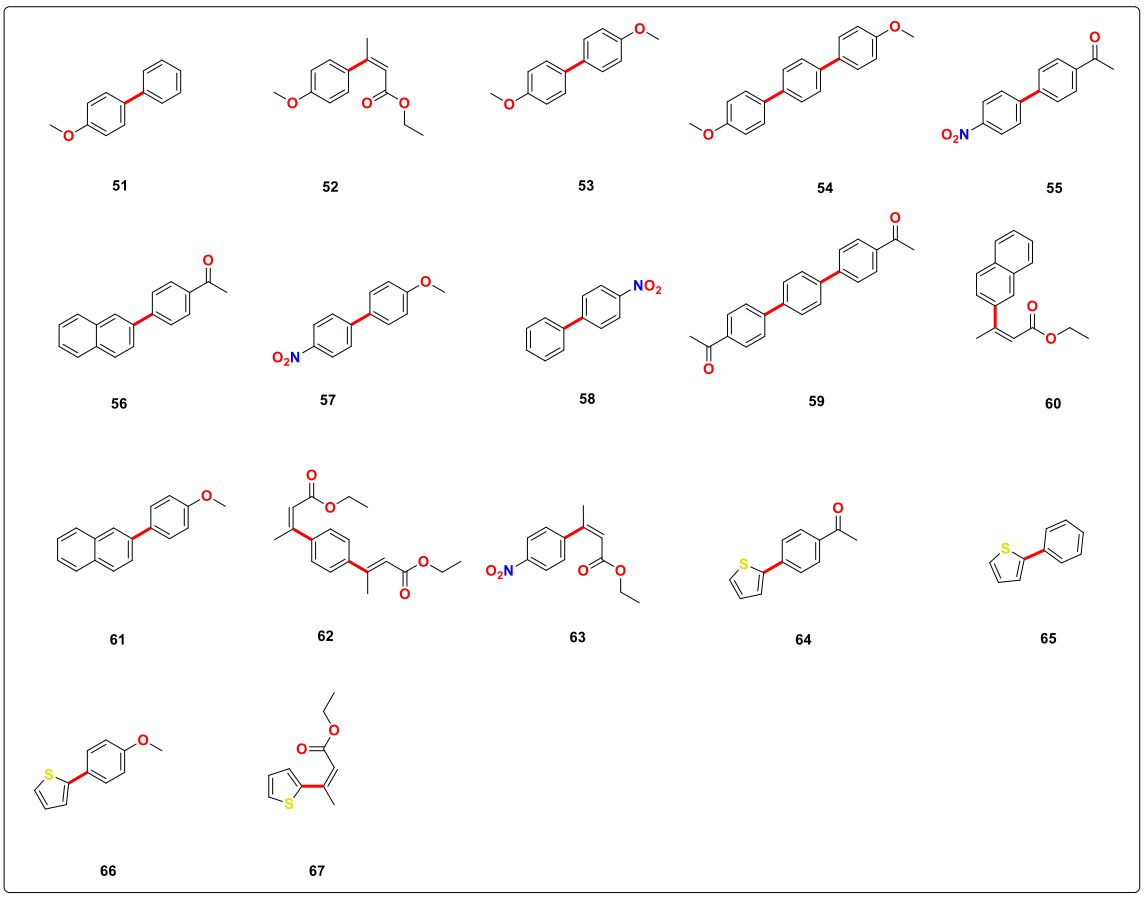


Table S3: List of Suzuki Cross-Coupling product 51-67

2. Scanned copy of spectra's (^{1}H NMR, ^{13}C NMR, and HRMS-ESI) of Suzuki Cross-Coupling product

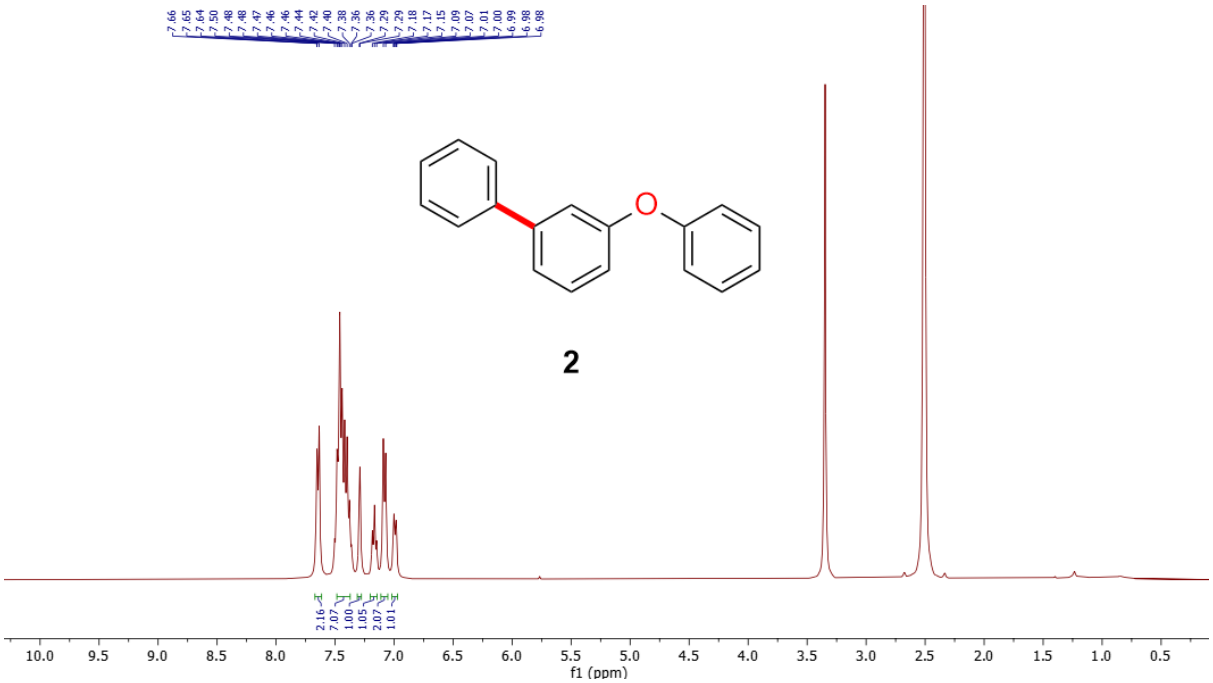


Figure S1: ^{1}H NMR Analysis of 2

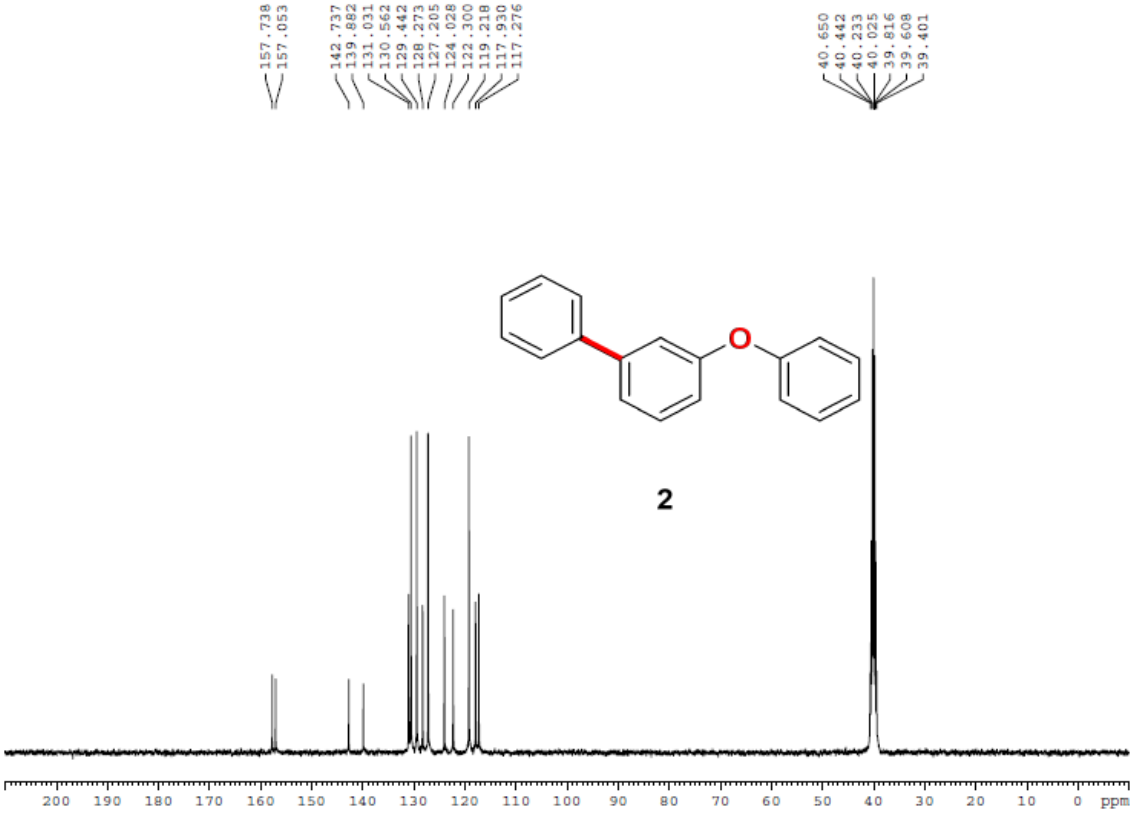
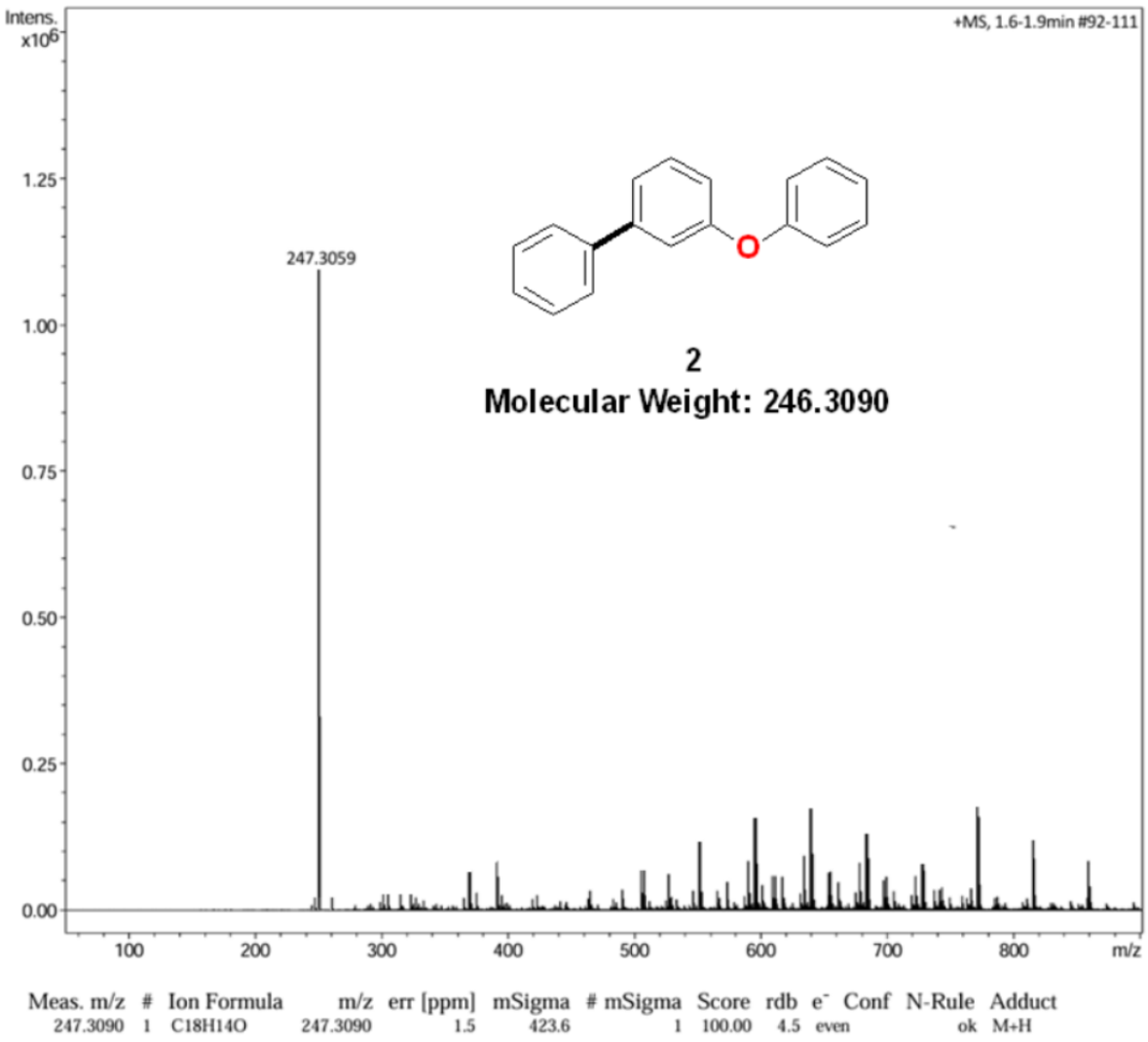


Figure S2: ^{13}C NMR Analysis of 2



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# mSigma	Score	rdb	e⁻	Conf	N-Rule	Adduct
247.3090	1	C18H14O	247.3090	1.5	423.6	1	100.00	4.5	even		ok	M+H

Figure S3: HRMS Analysis of 2

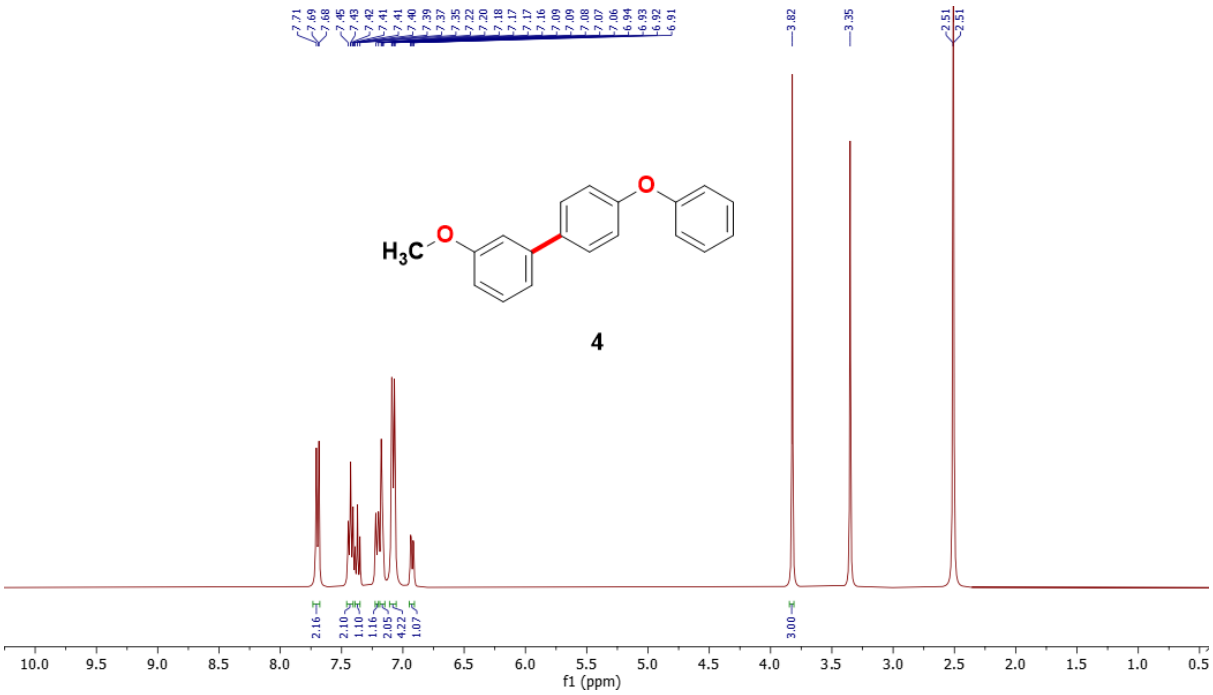


Figure S4: ^{1}H NMR Analysis of 4

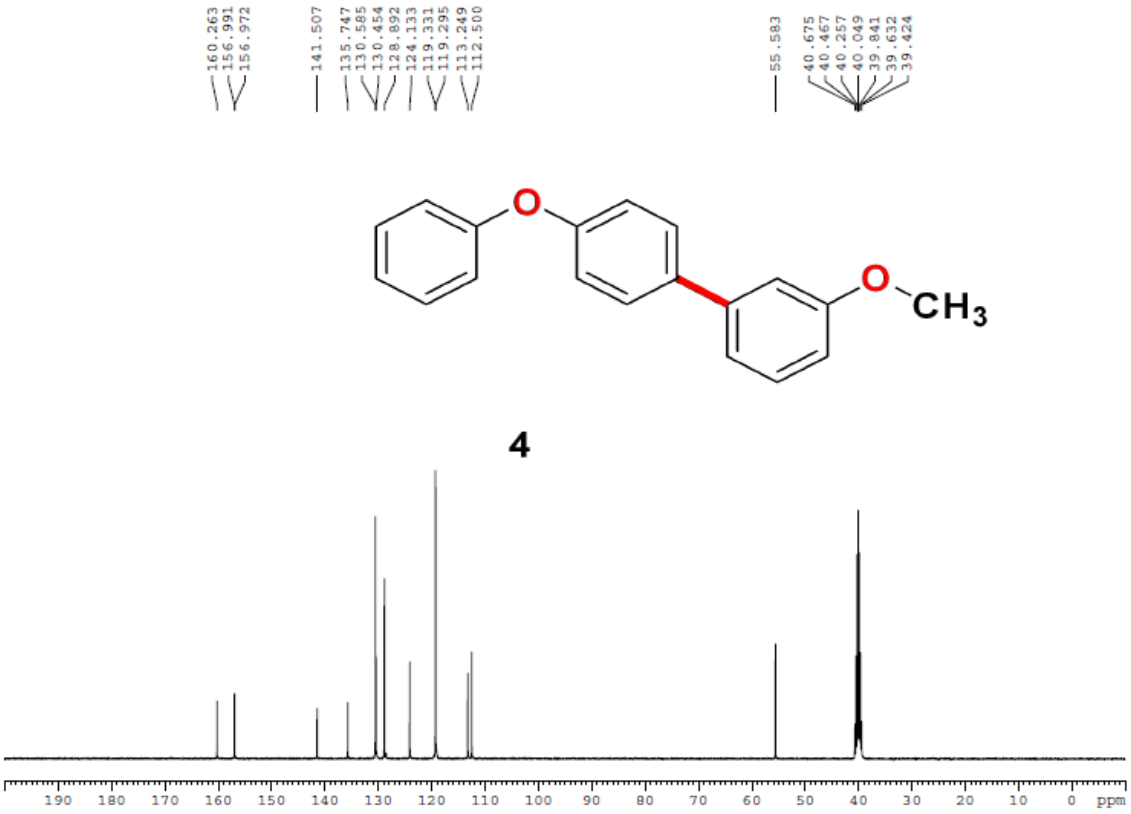


Figure S5: ^{13}C NMR Analysis of 4

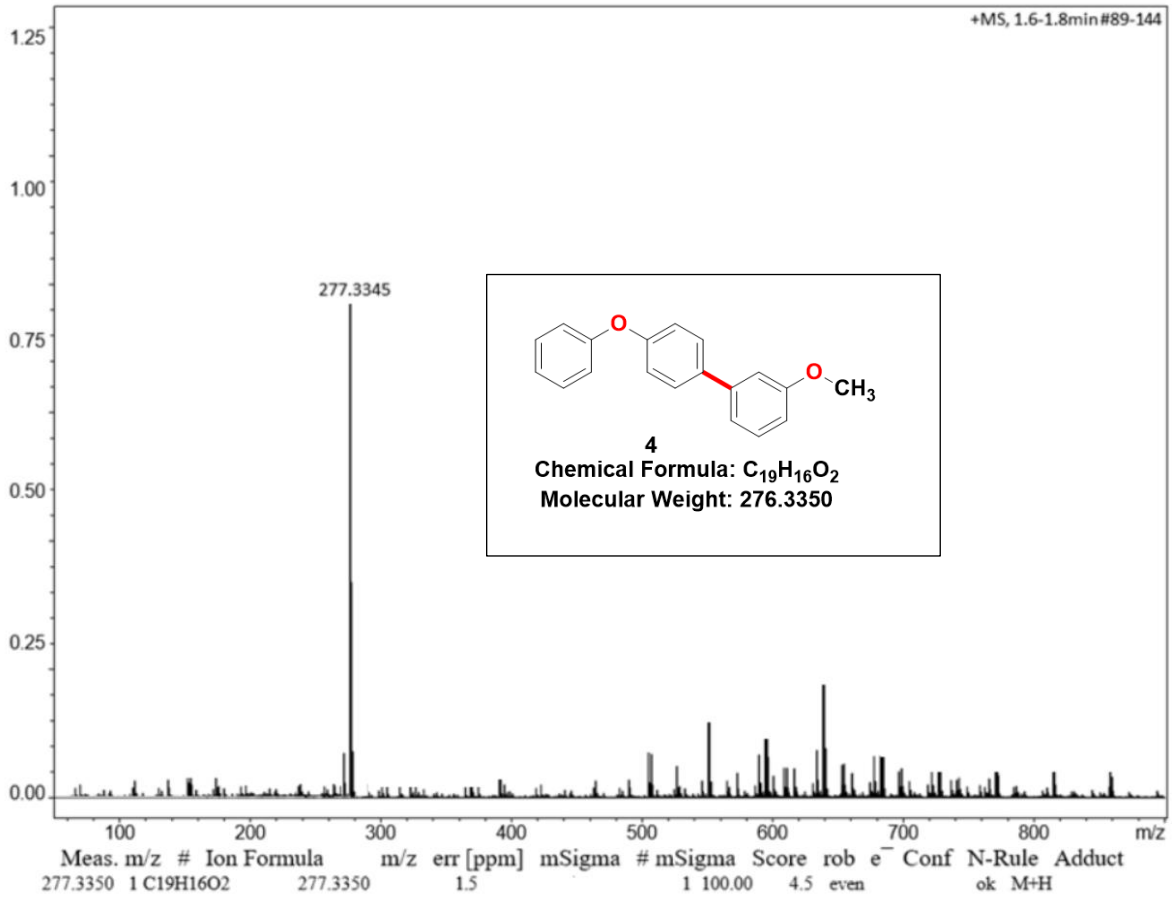


Figure S6: HRMS Analysis of 4

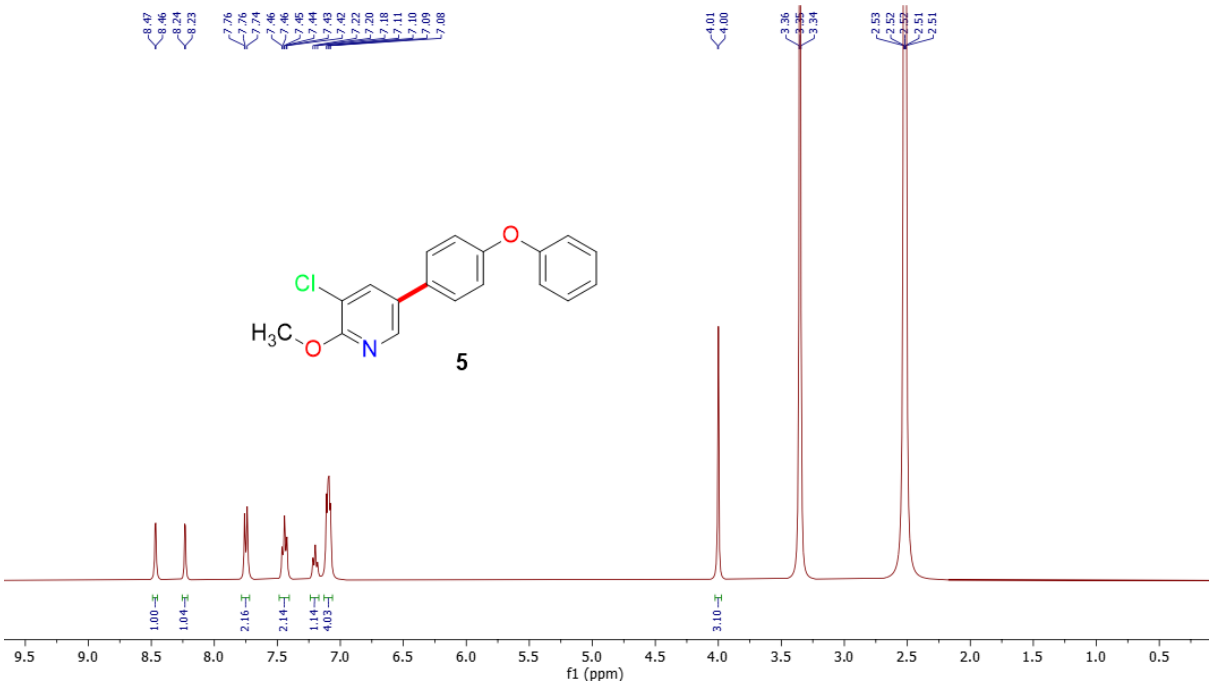


Figure S7: ^{1}H NMR Analysis of 5

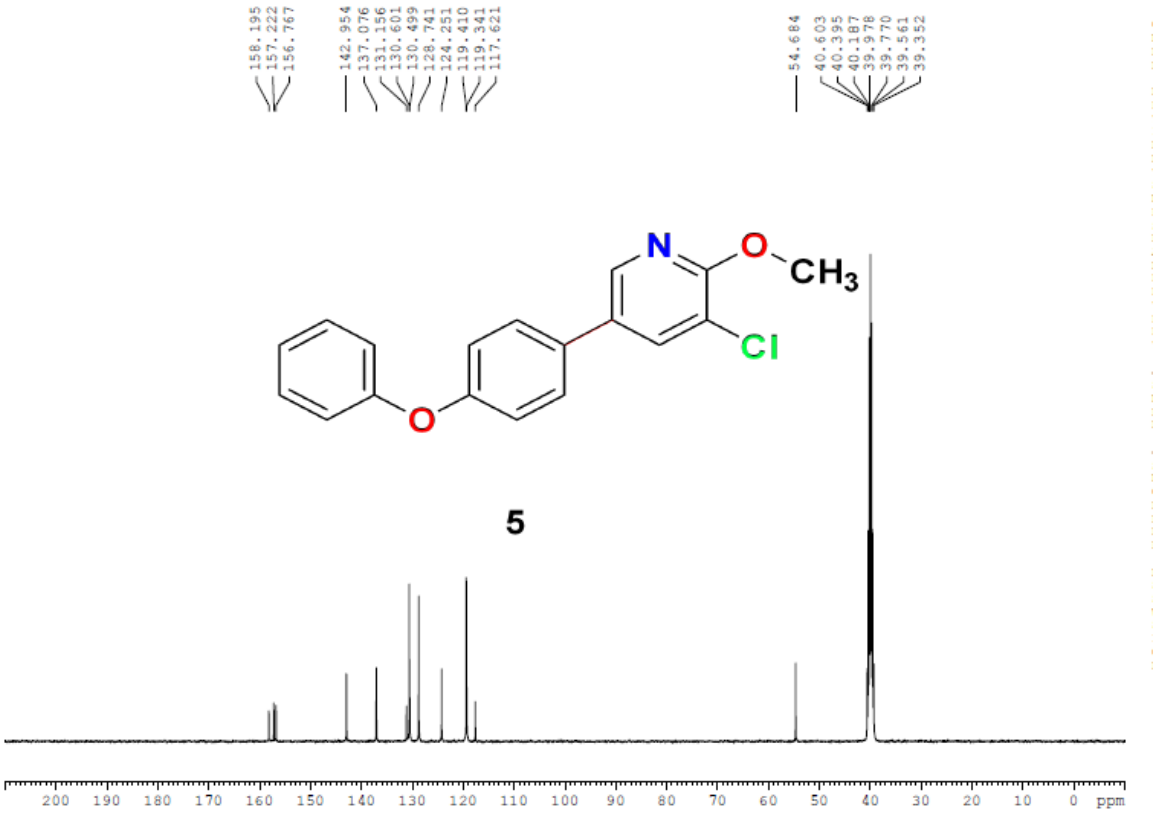


Figure S8: ^{13}C NMR Analysis of 5

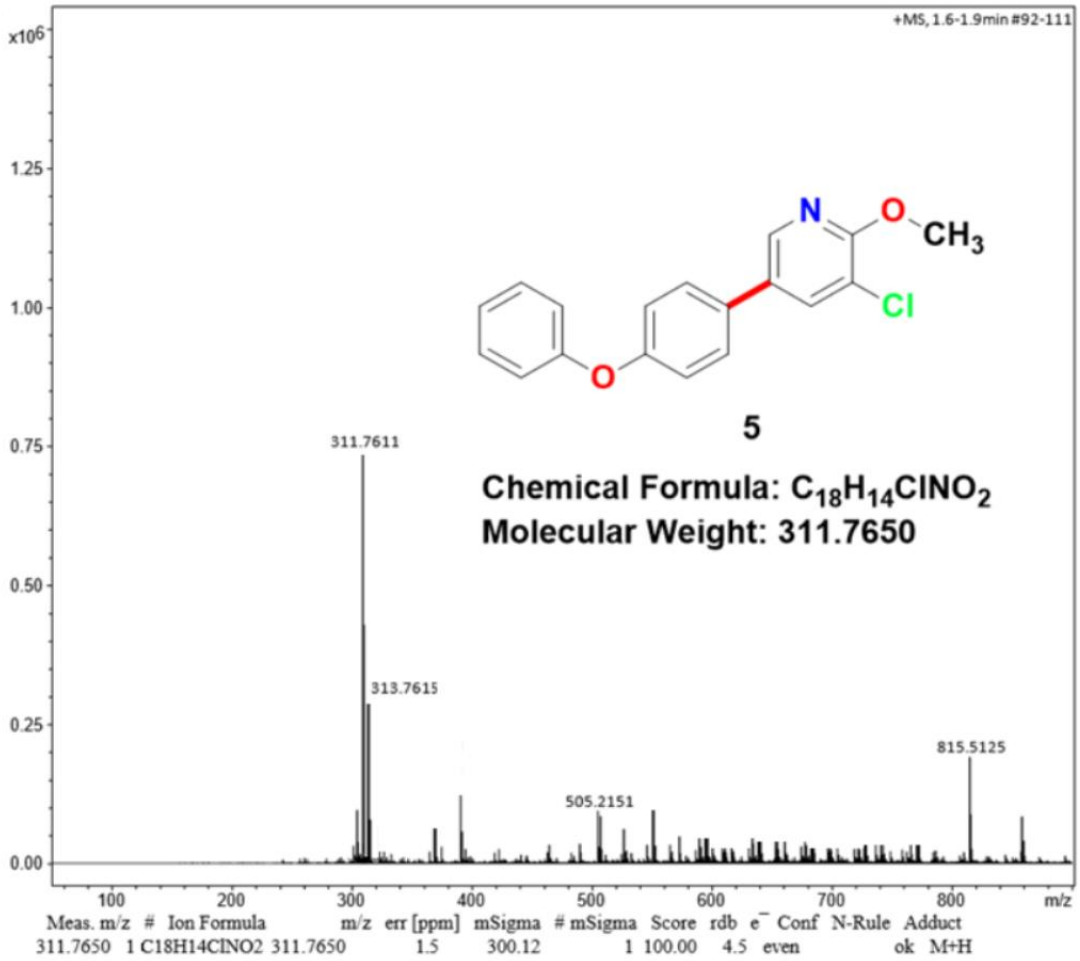


Figure S9: HRMS Analysis of 5

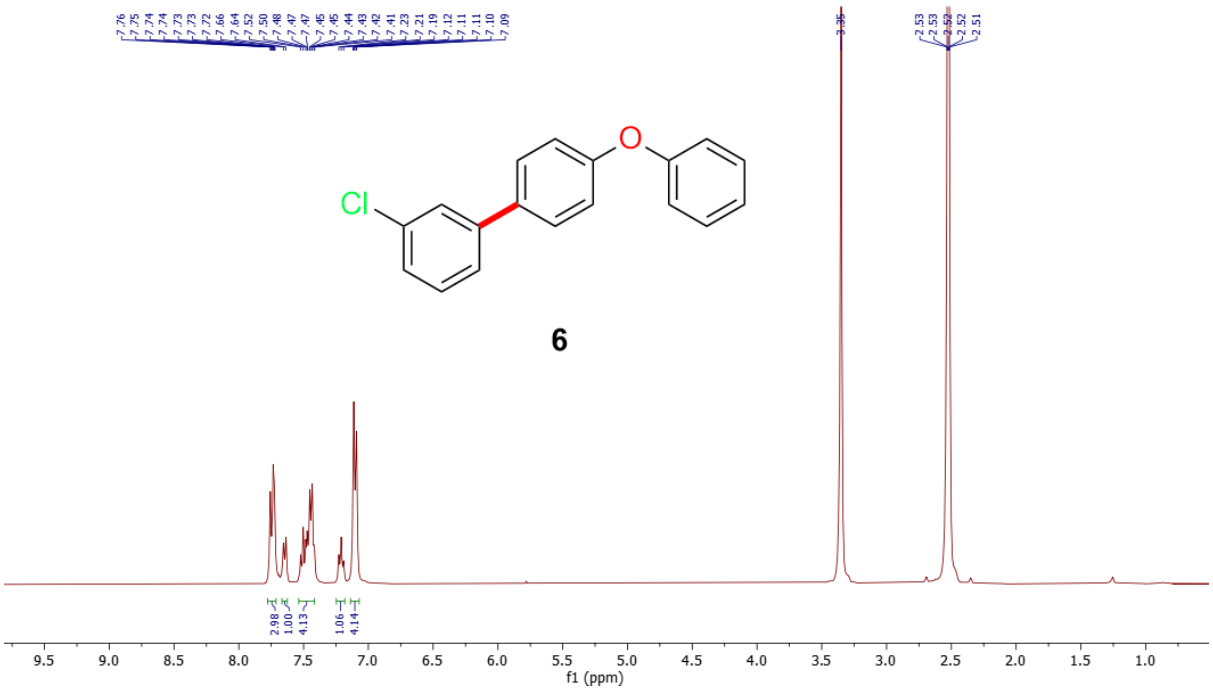


Figure S10: ^{1}H NMR Analysis of 6

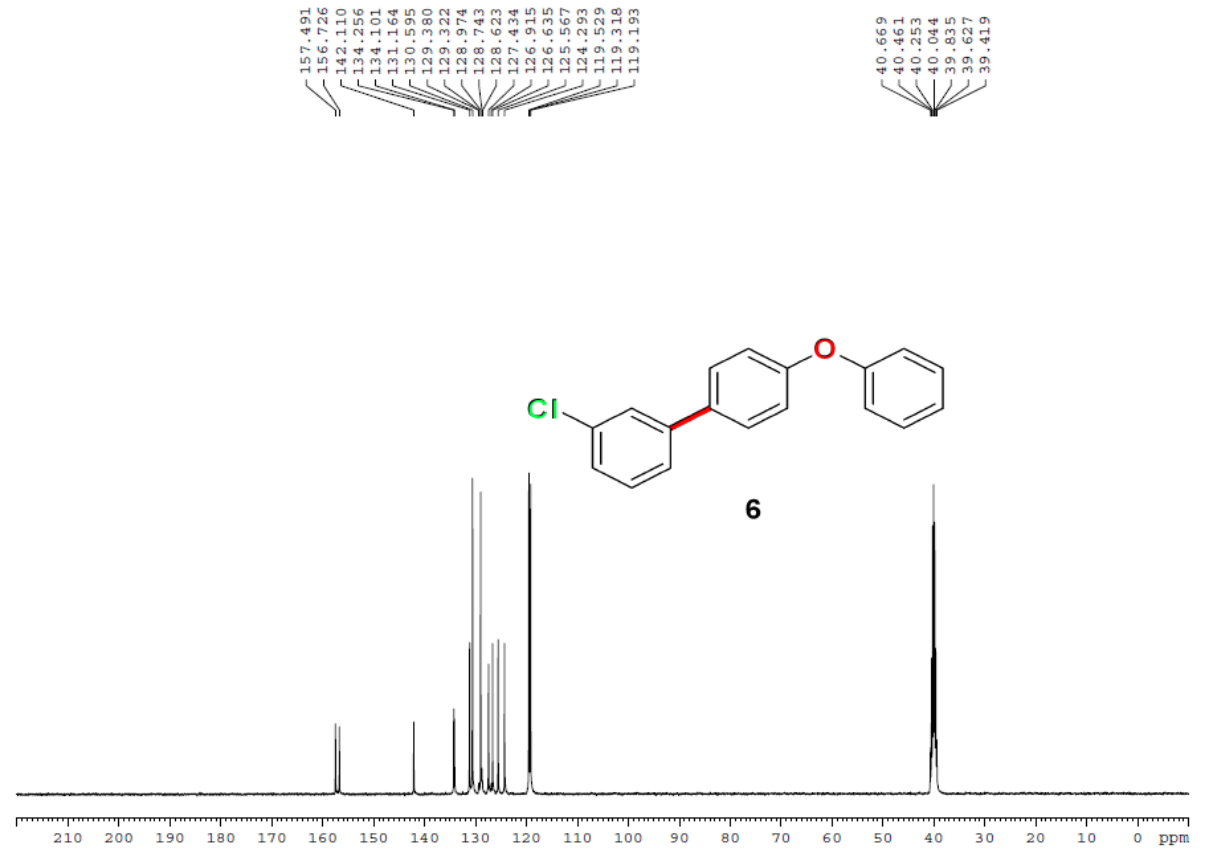


Figure S11: ^{13}C NMR Analysis of 6

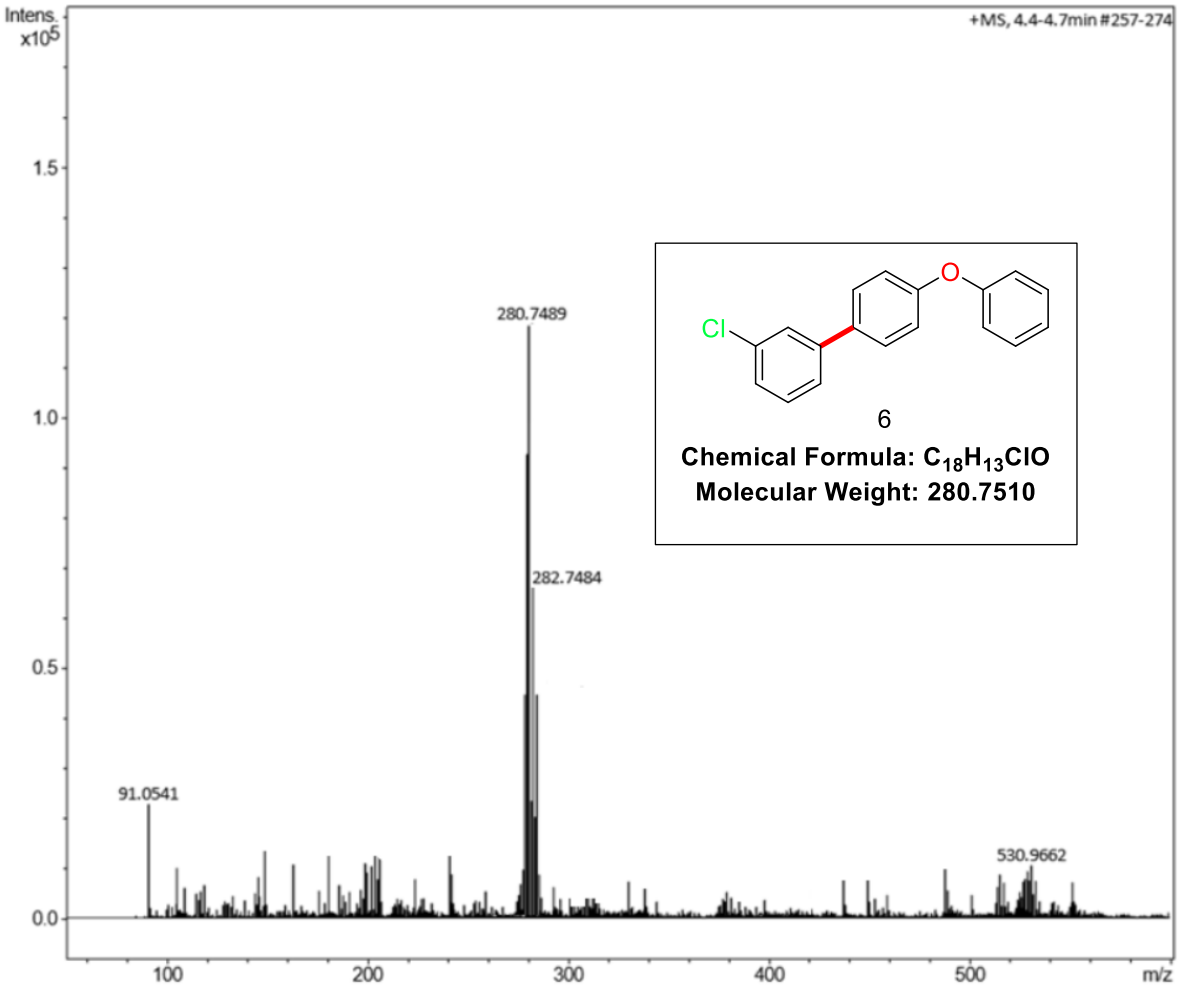


Figure S12: HRMS Analysis of 6

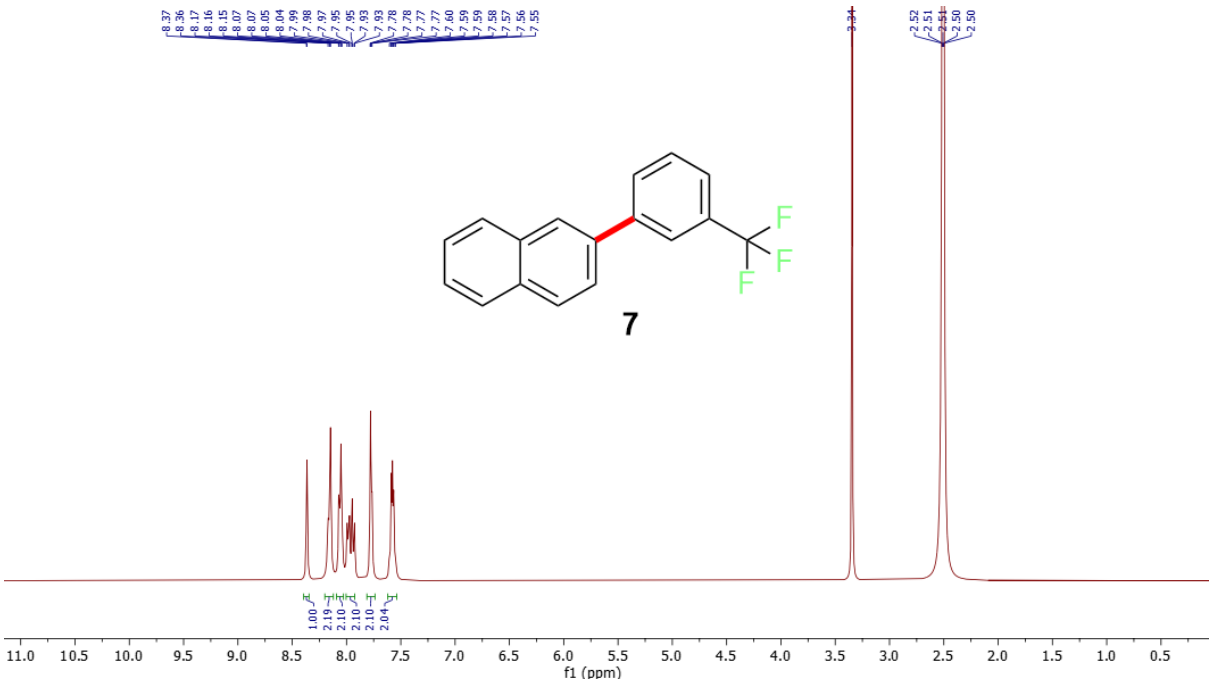


Figure S13: ^{1}H NMR Analysis of 7

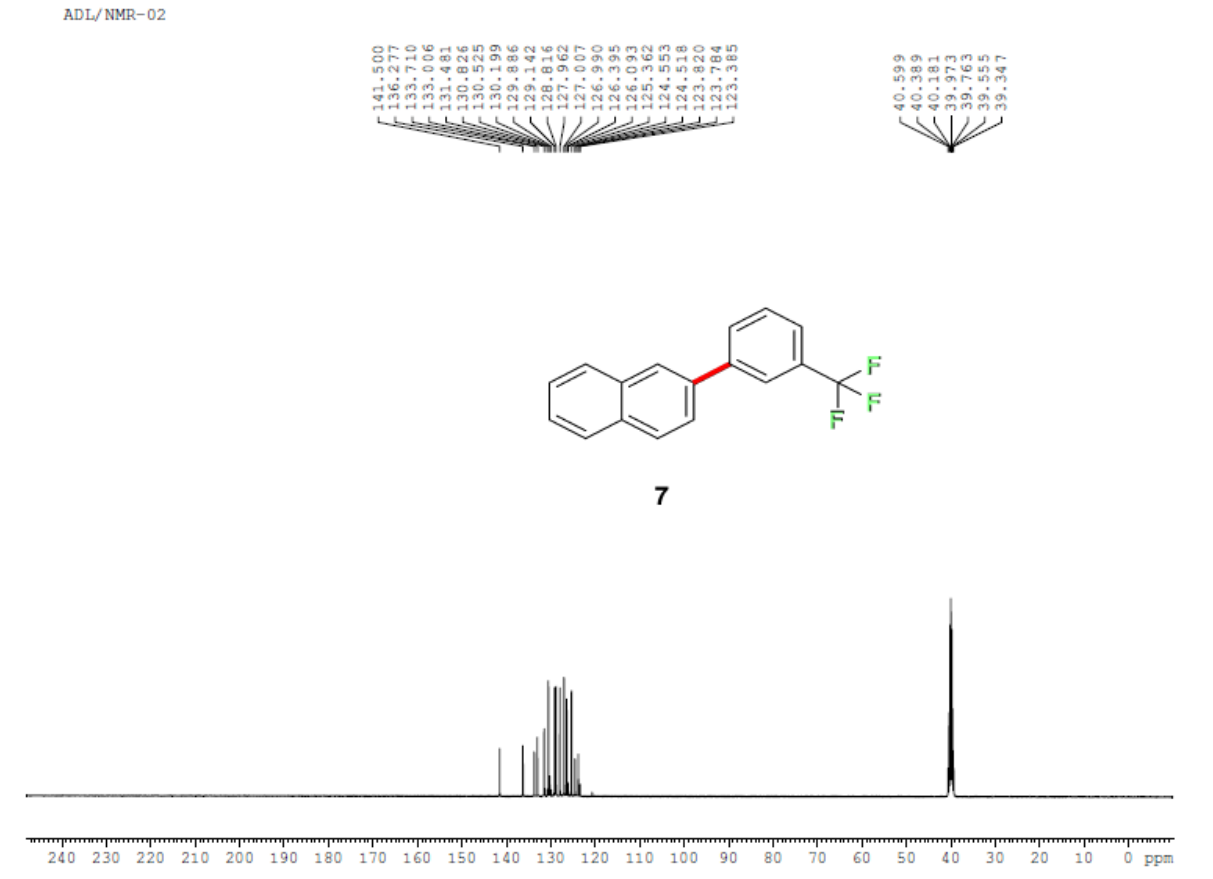


Figure S14: ^{13}C NMR Analysis of 7

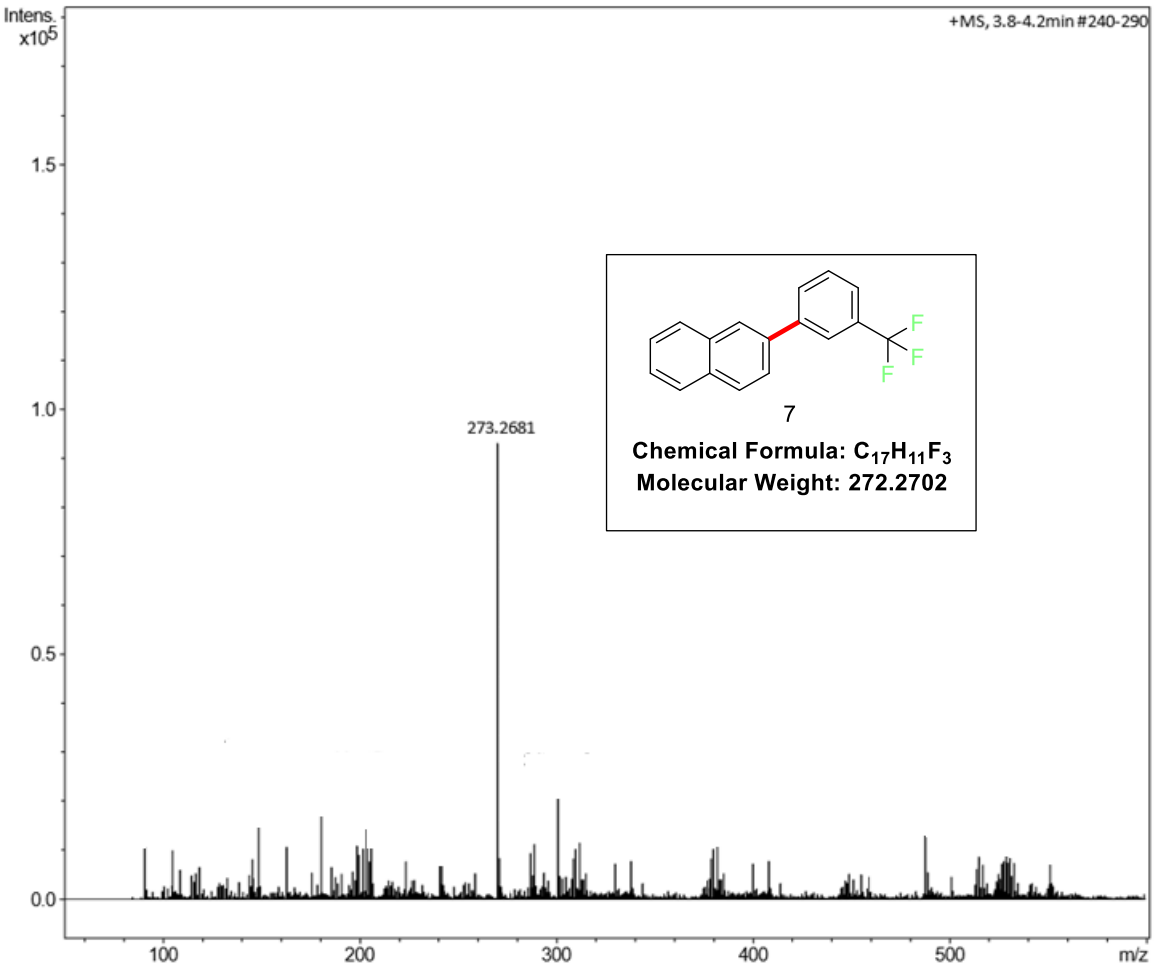


Figure S15: HRMS Analysis of 7

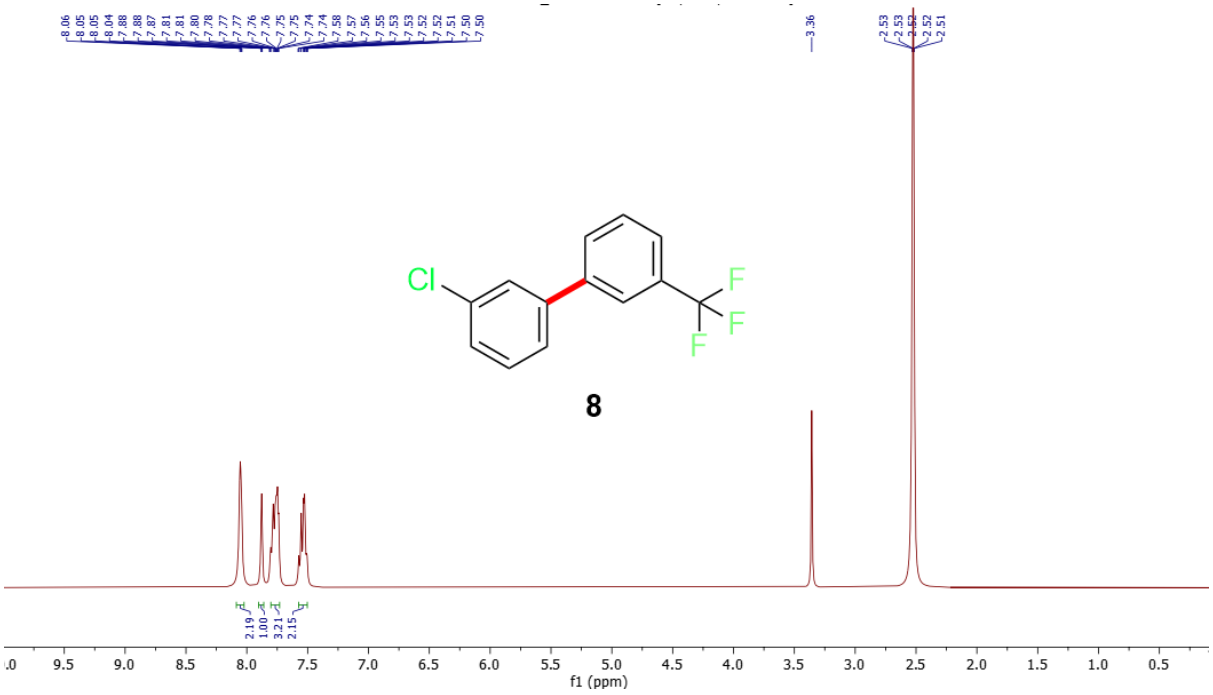


Figure S16: ^{1}H NMR Analysis of 8

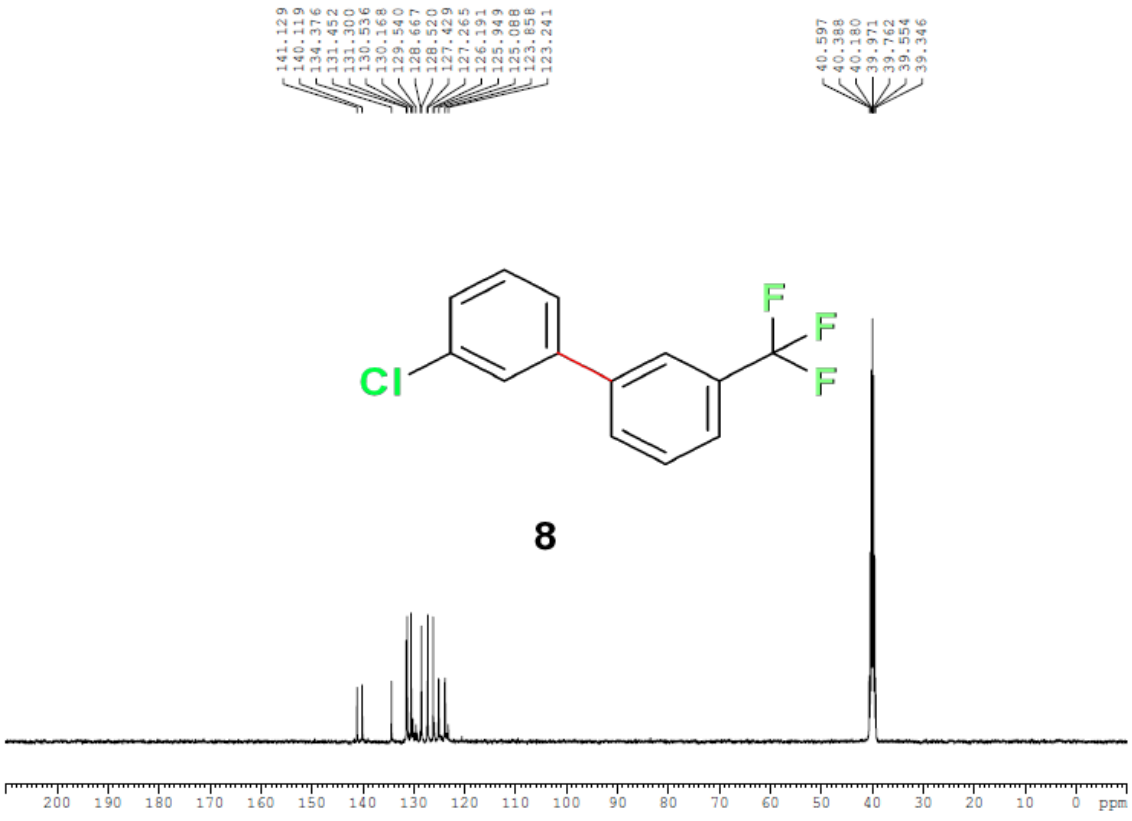


Figure S17: ^{13}C NMR Analysis of 8

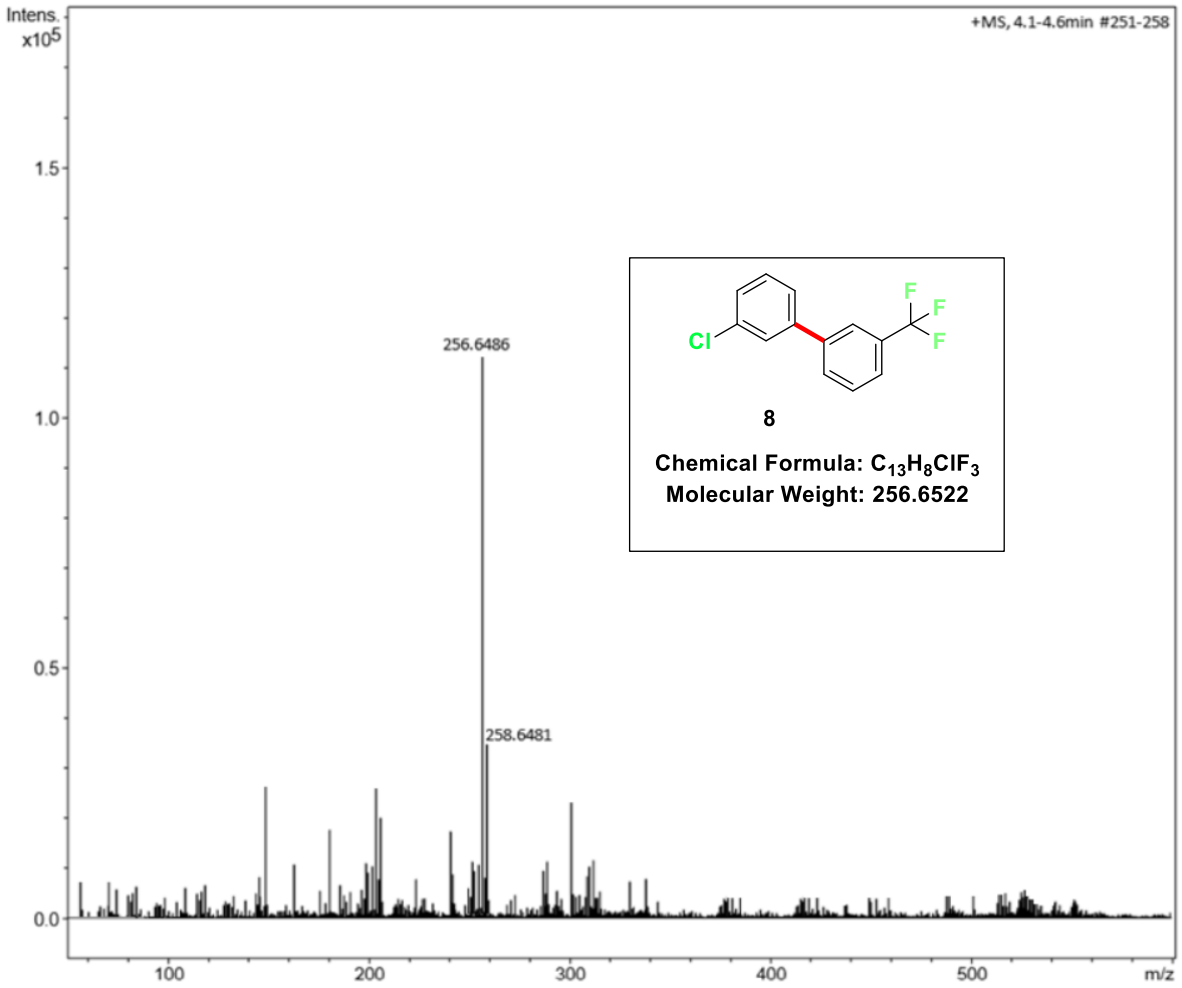


Figure S18: HRMS Analysis of 8

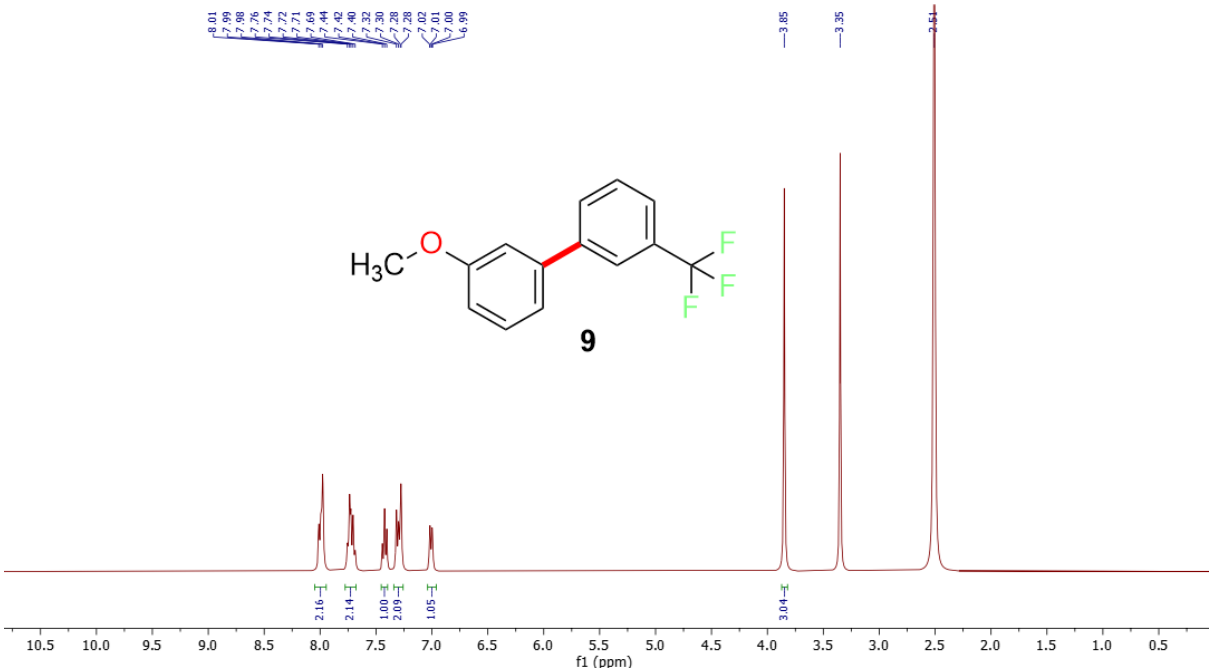


Figure S19: ^{1}H NMR Analysis of 9

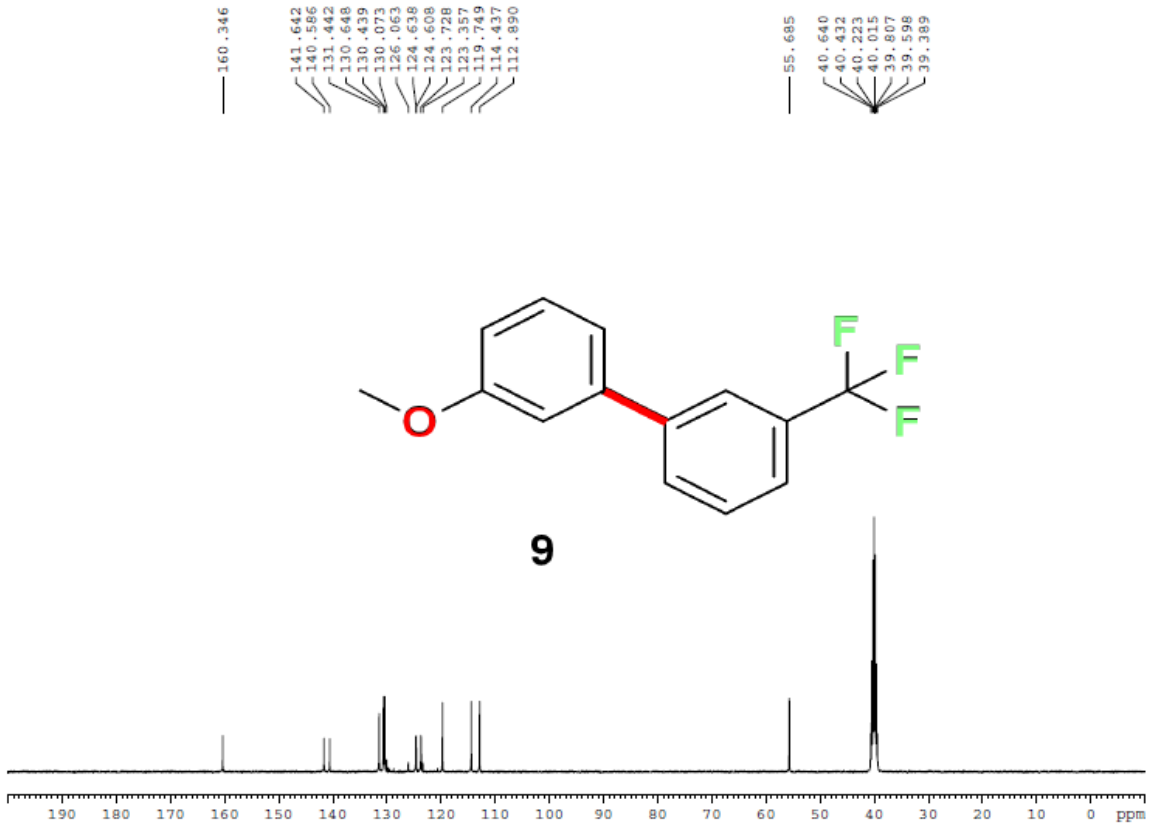


Figure S20: ^{13}C NMR Analysis of 9

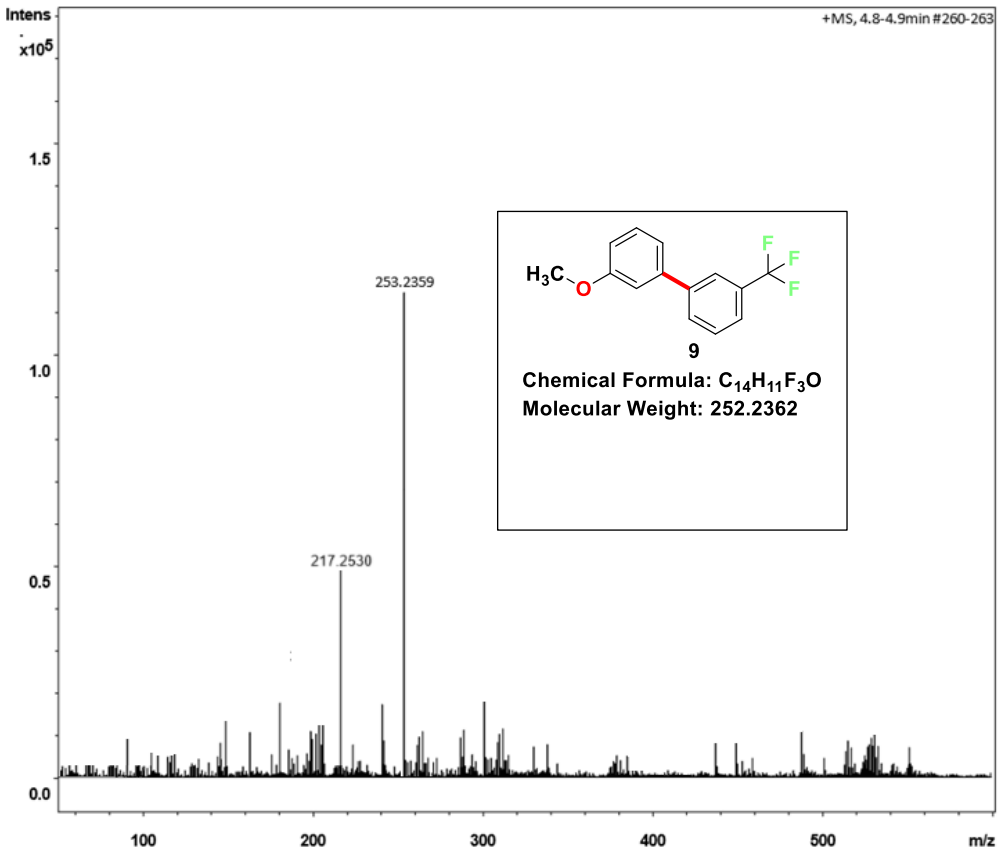


Figure S21: HRMS Analysis of 9

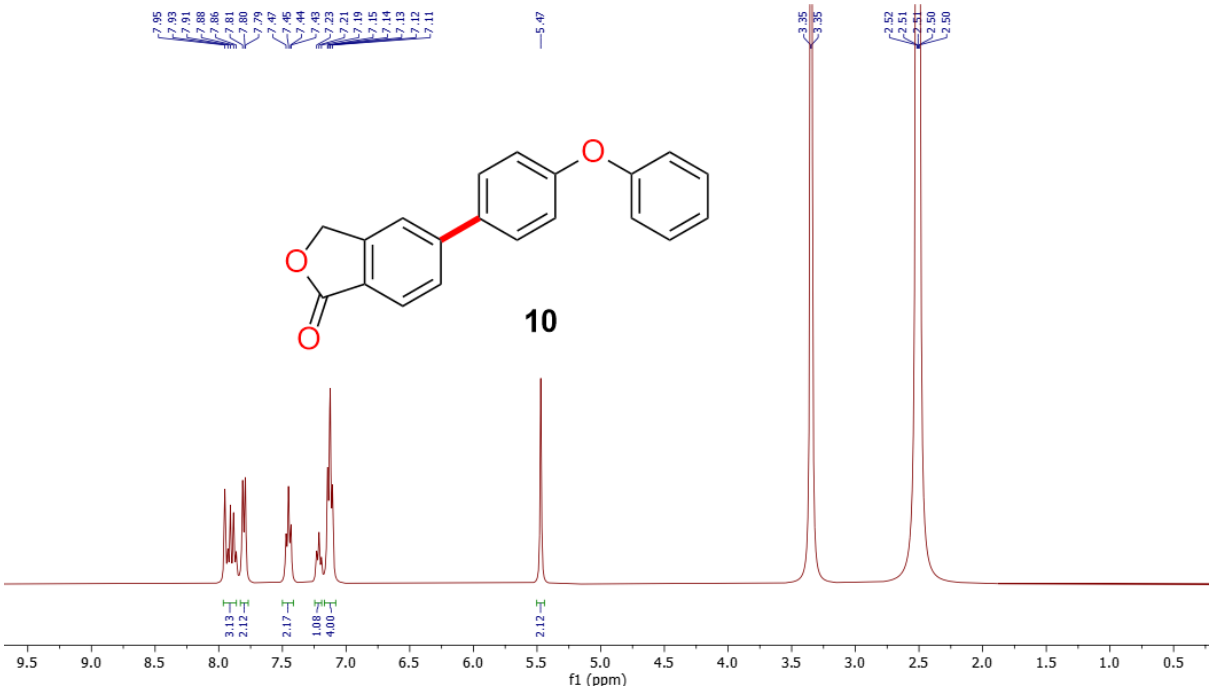


Figure S22: ^{1}H NMR Analysis of 10

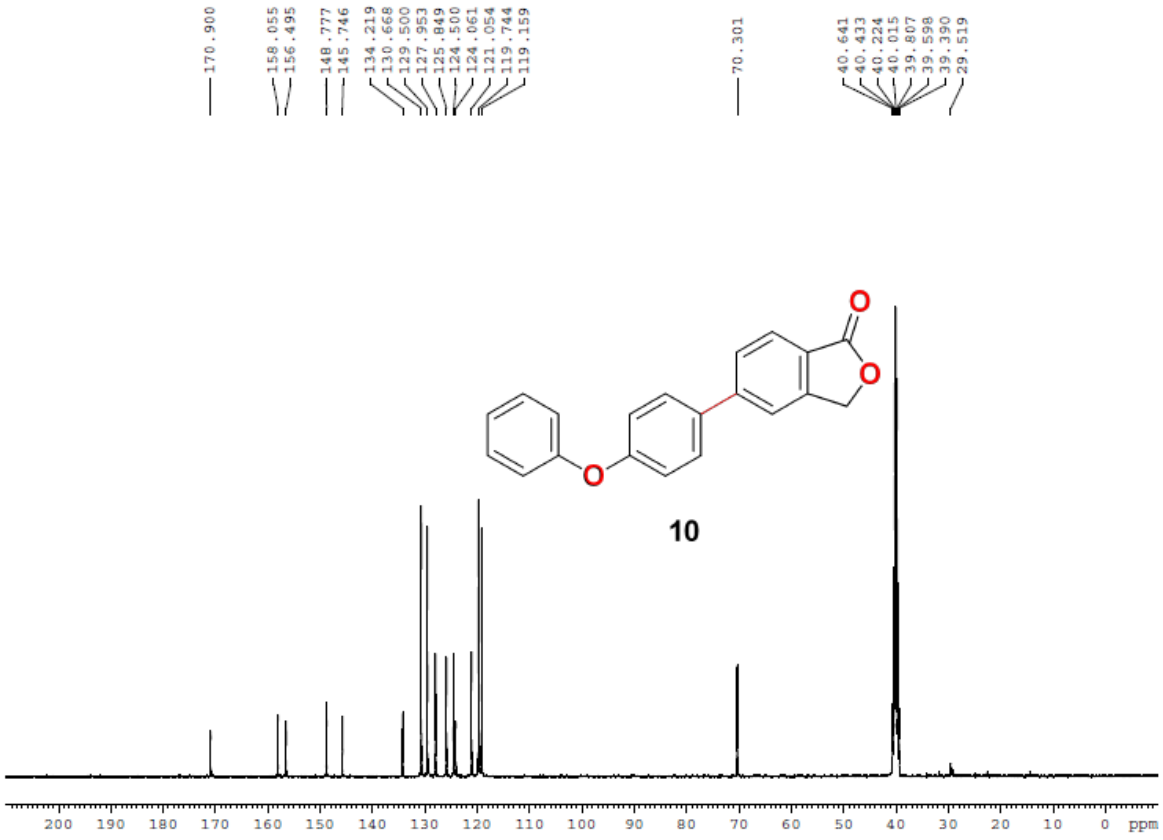


Figure S23: ^{13}C NMR Analysis of 10

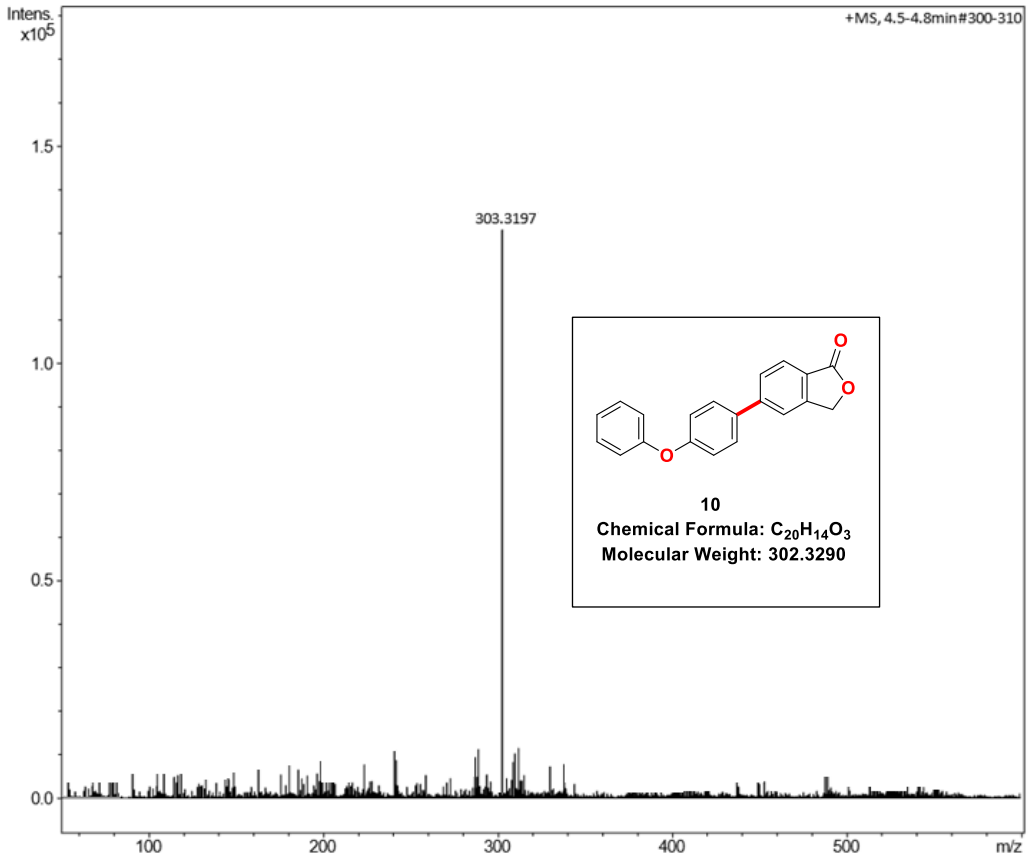


Figure S24: HRMS Analysis of 10

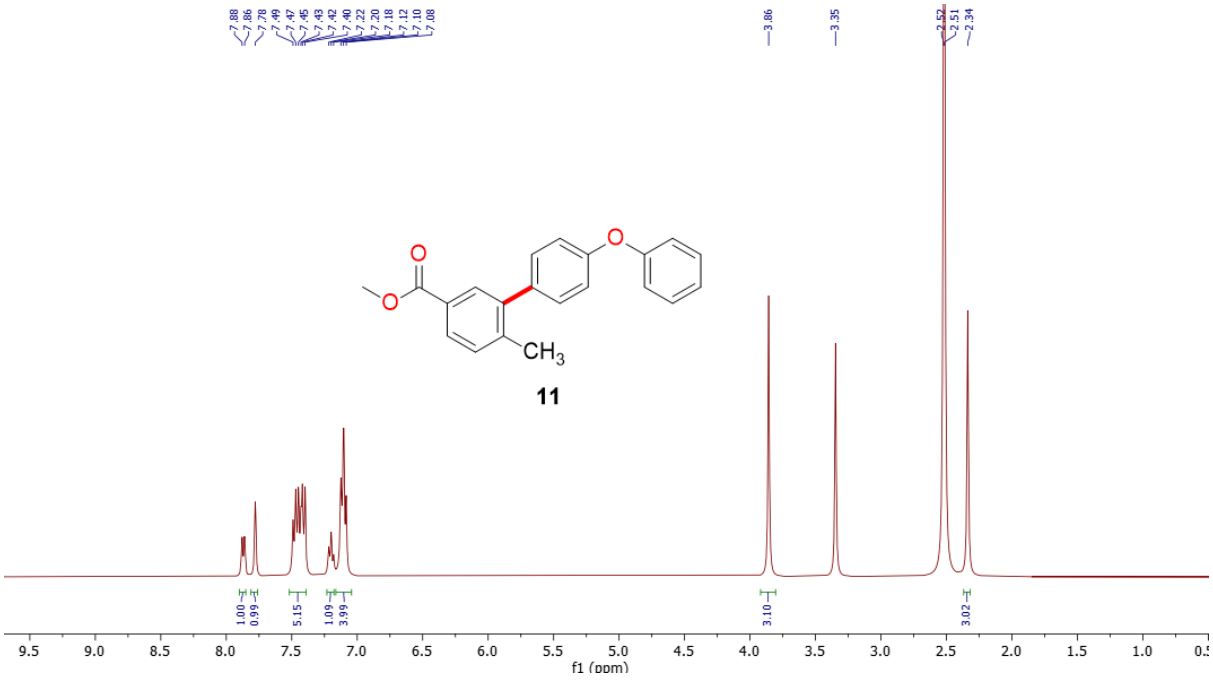


Figure S25: ^{1}H NMR Analysis of 11

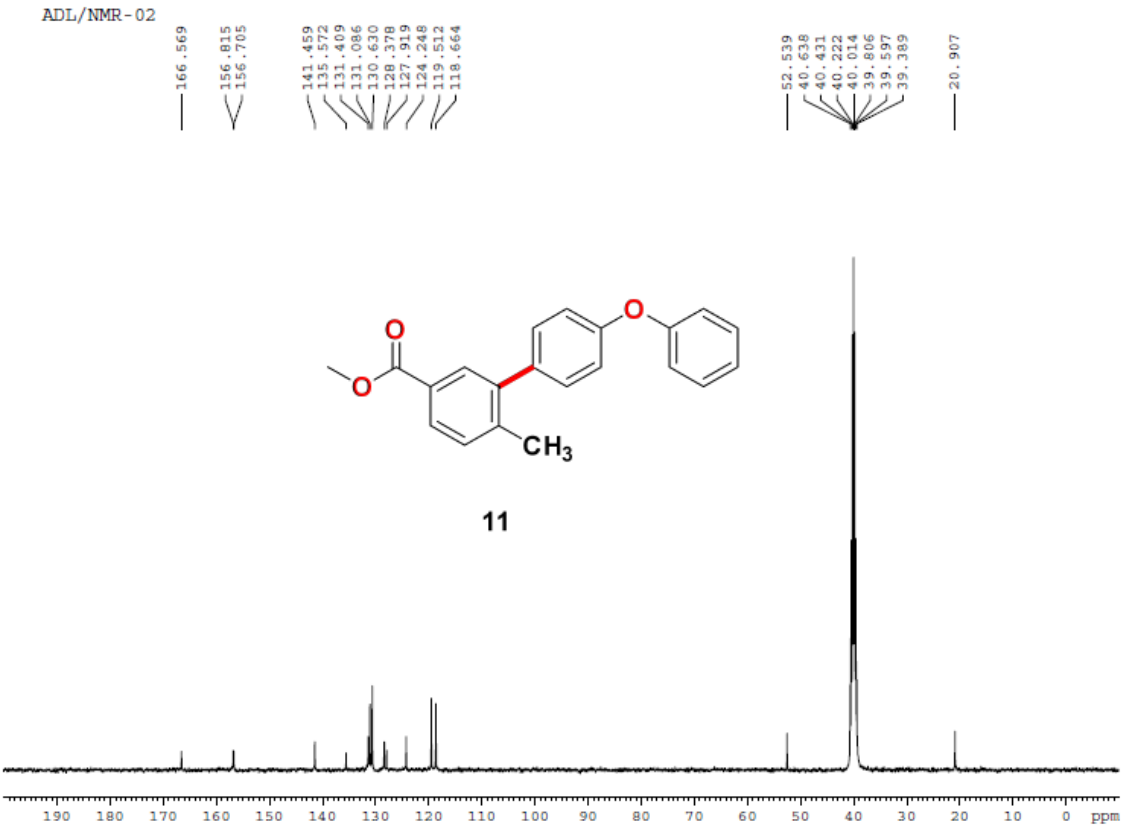


Figure S26: ^{13}C NMR Analysis of 11

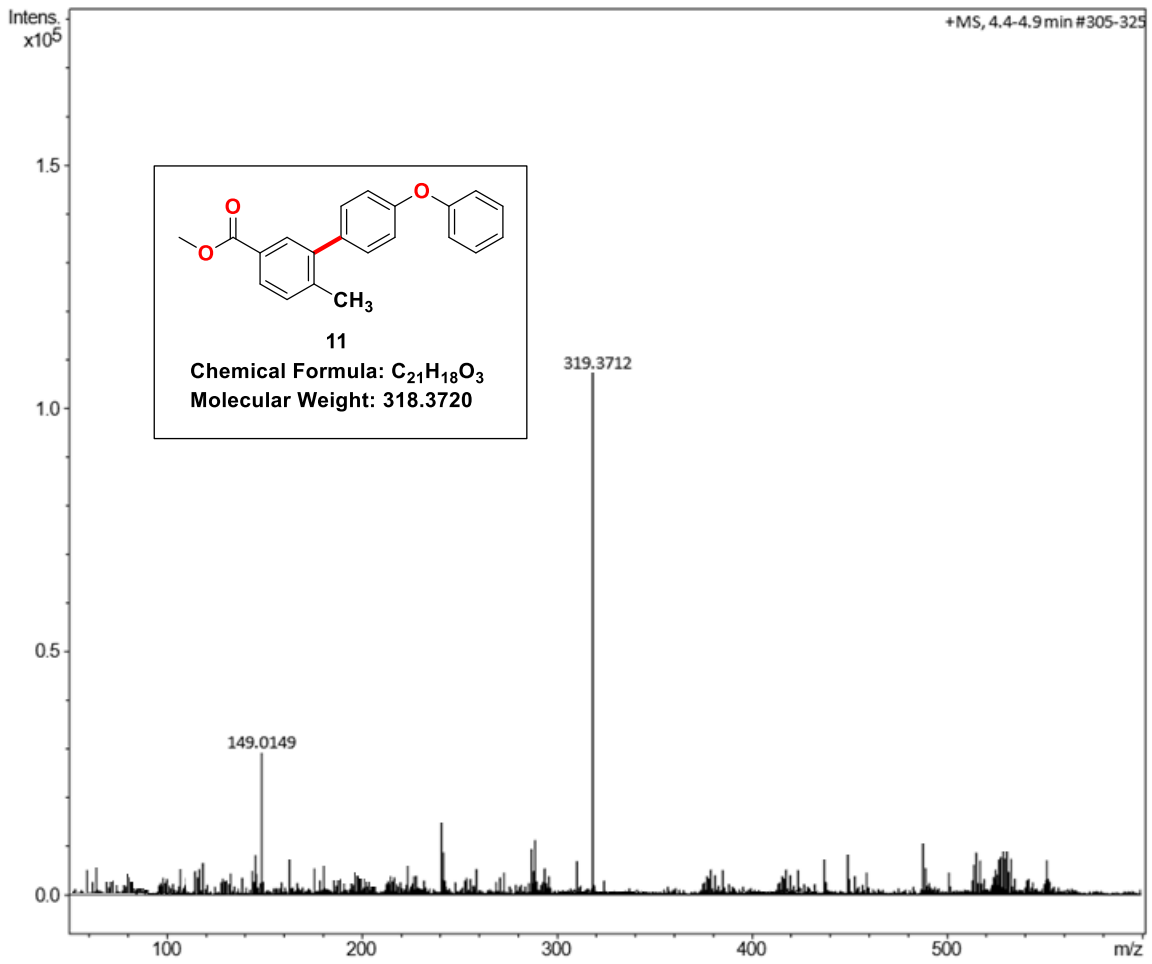


Figure S27: HRMS Analysis of 11

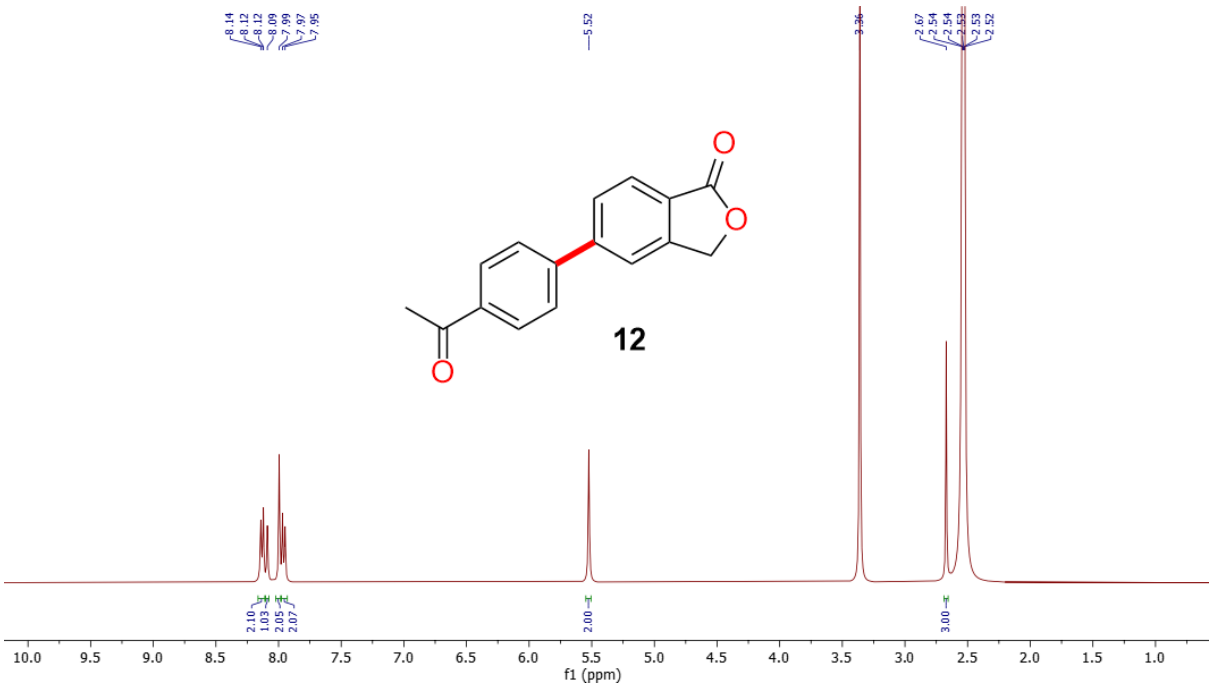


Figure S28: ^{1}H NMR Analysis of 12

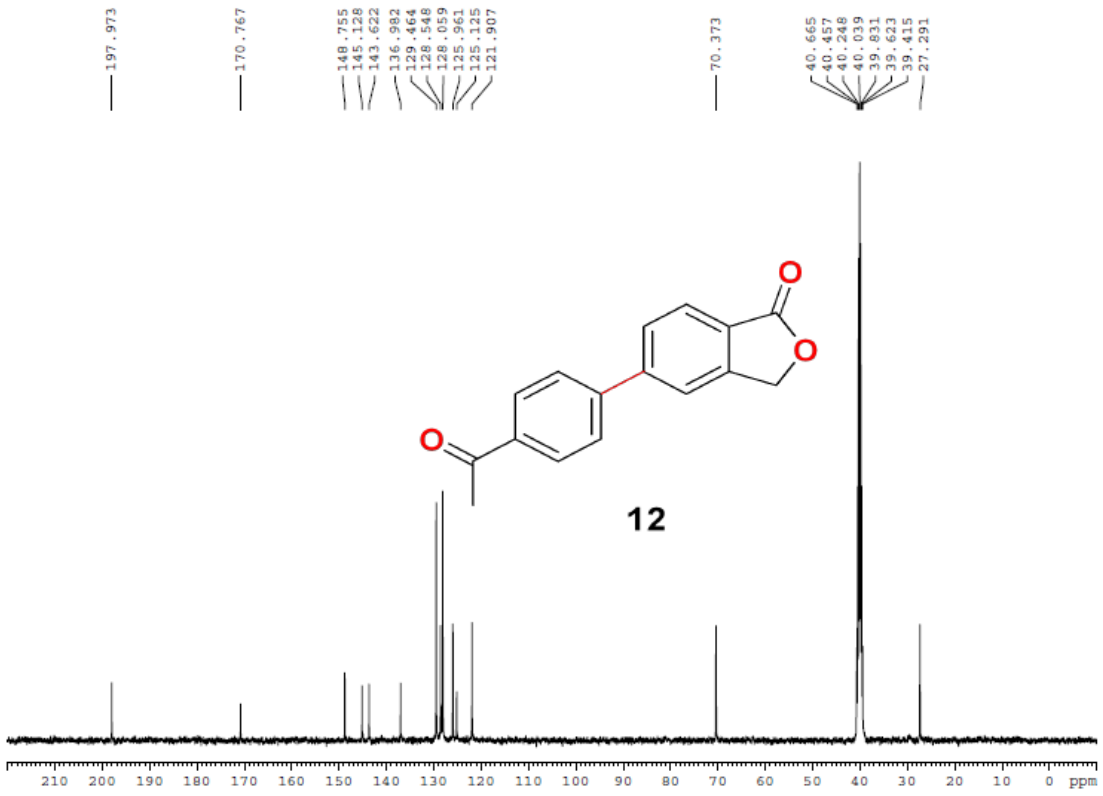


Figure S29: ^{13}C NMR Analysis of 12

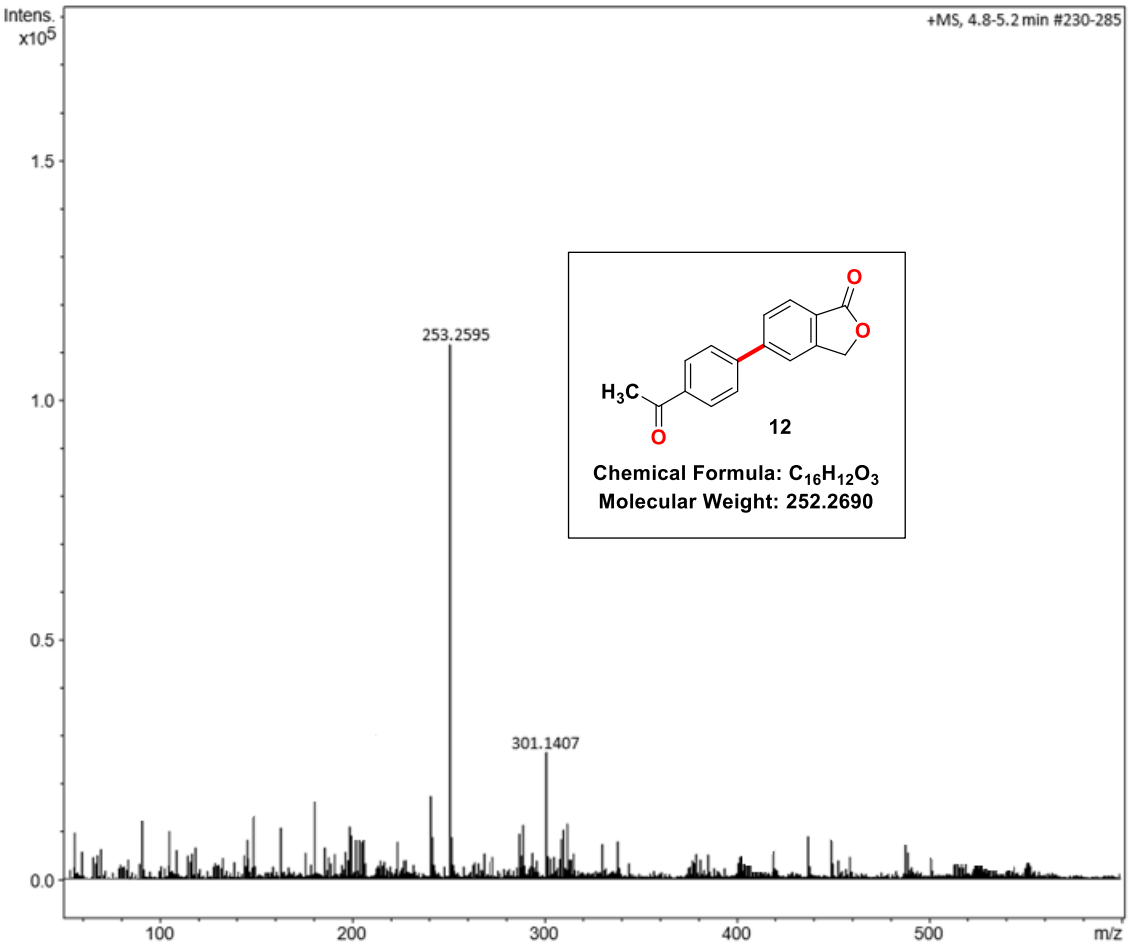


Figure S30: HRMS Analysis of 12

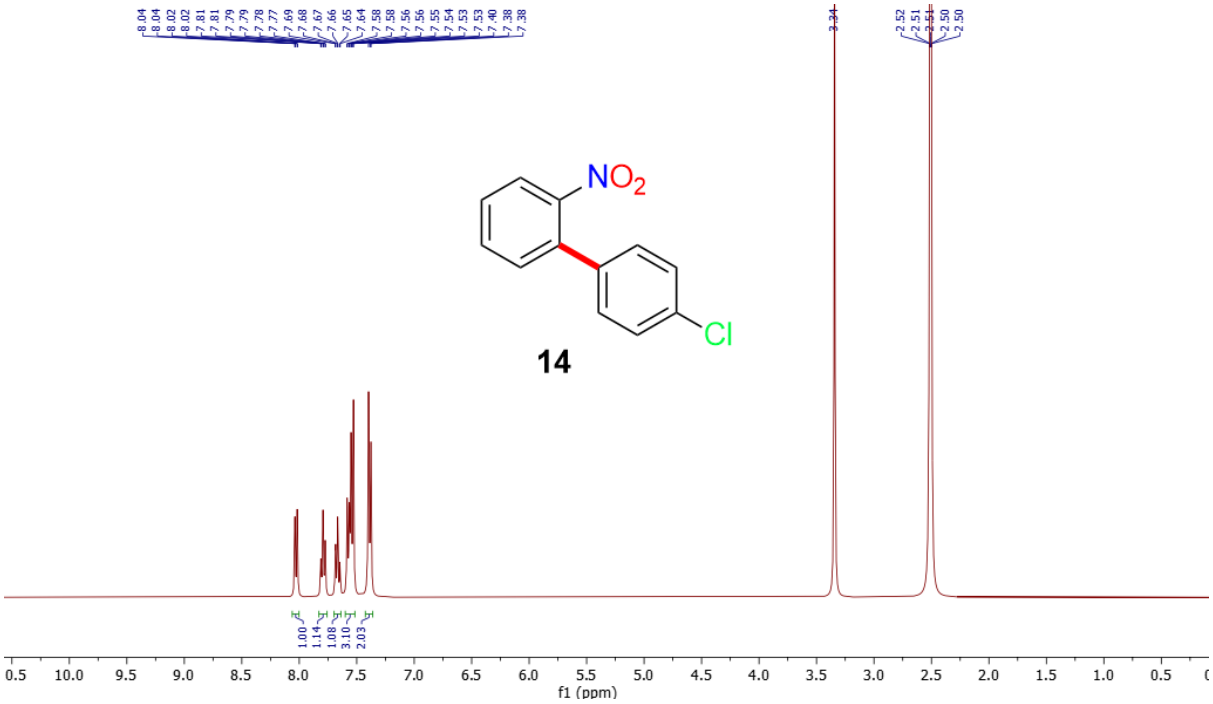


Figure S31: ^{1}H NMR Analysis of 14

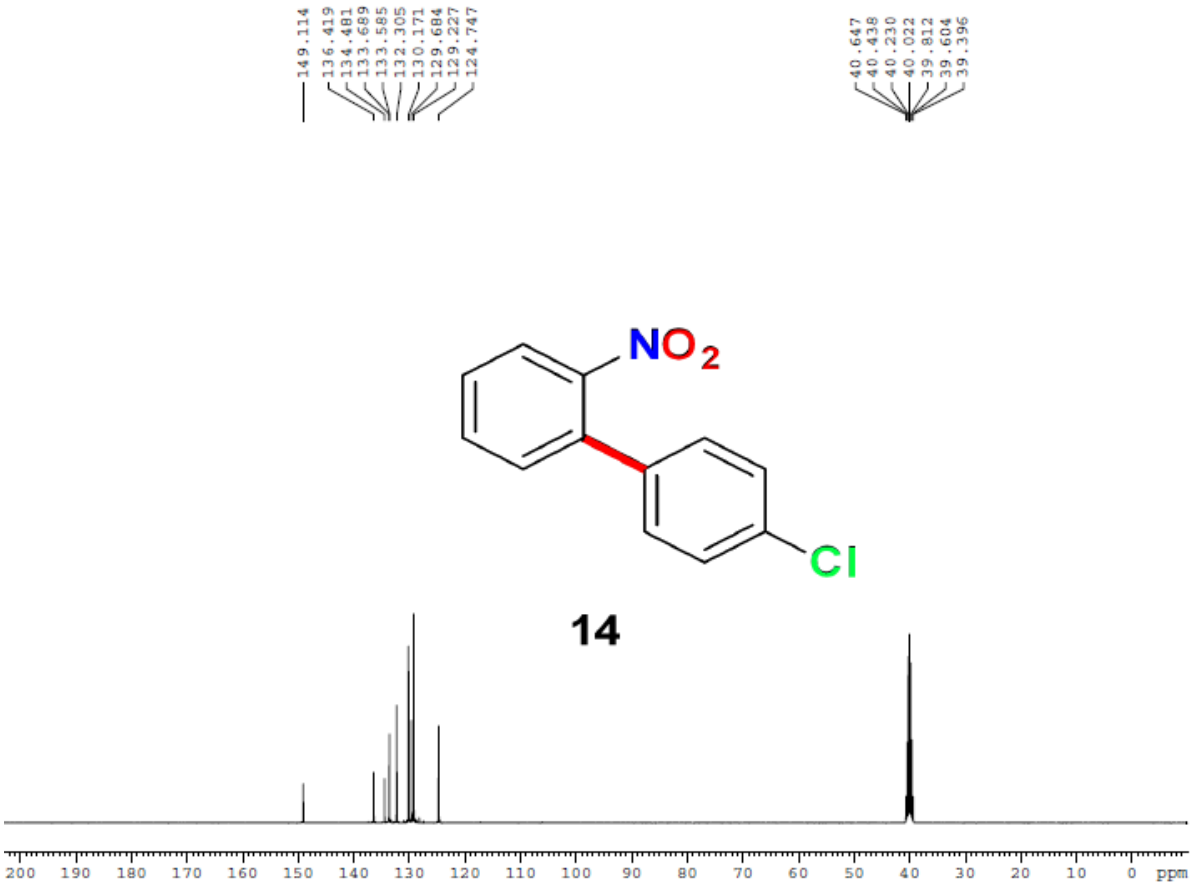


Figure S32: ^{13}C NMR Analysis of 14

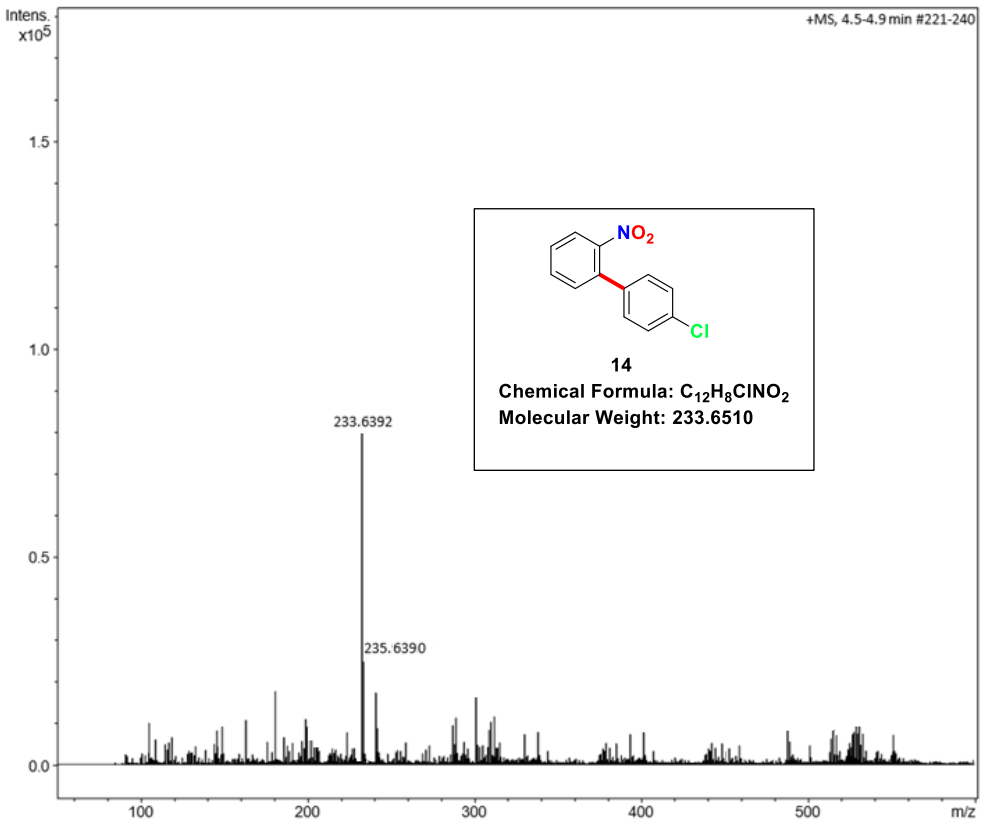


Figure S33: HRMS Analysis of 14

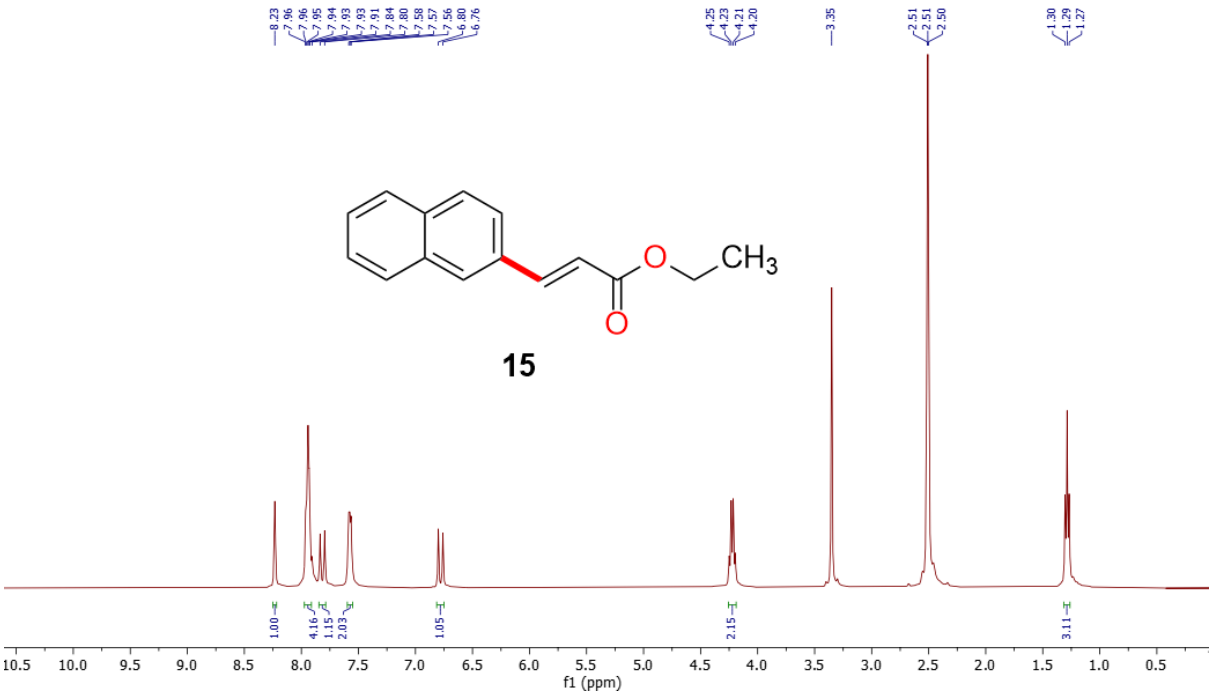


Figure 34: ^{1}H NMR Analysis of 15

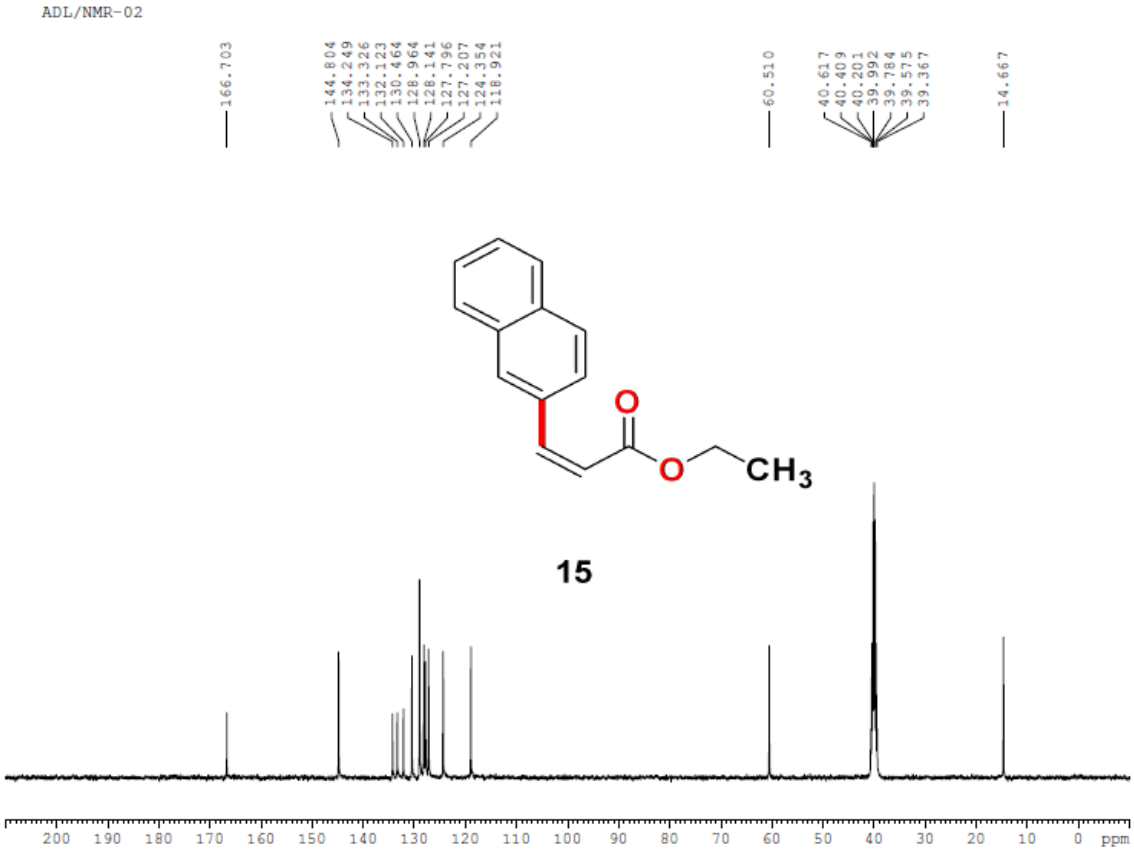


Figure S35: ^{13}C NMR Analysis of 15

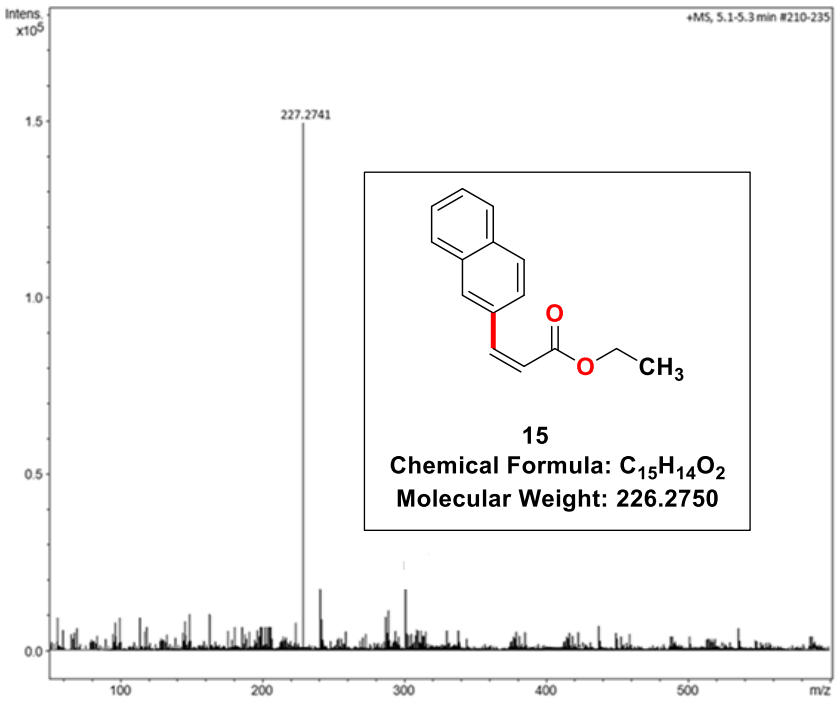


Figure S36: HRMS Analysis of 15

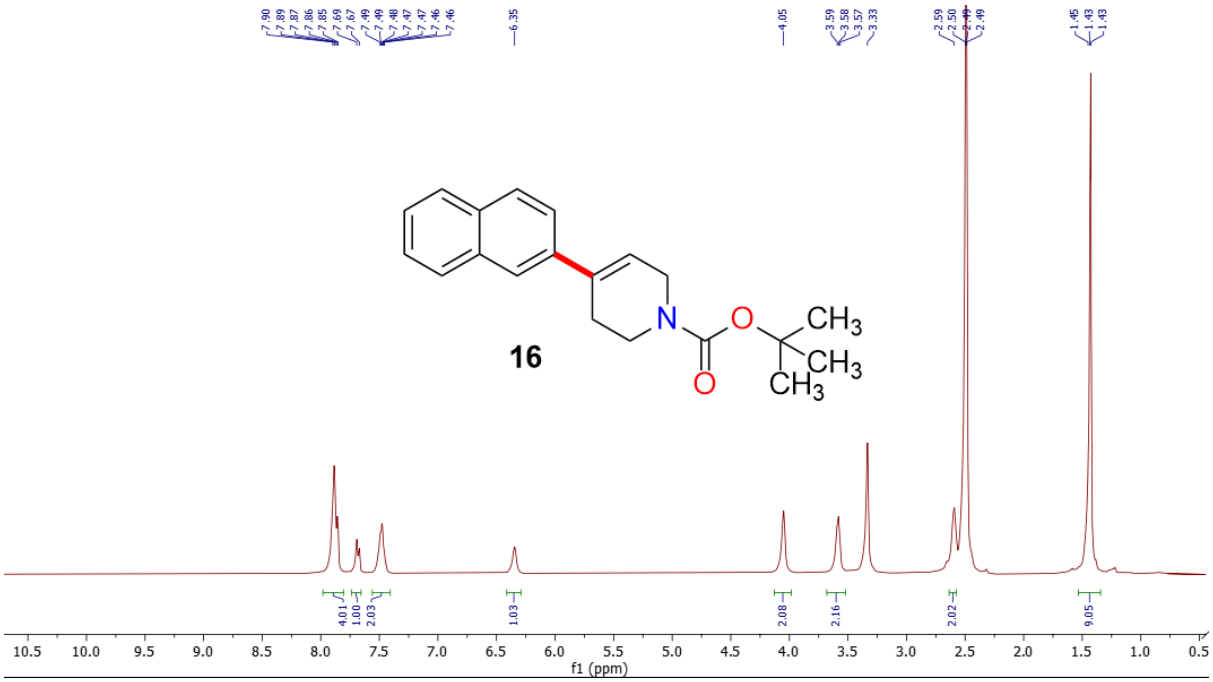


Figure S37: ^{1}H NMR Analysis of 16

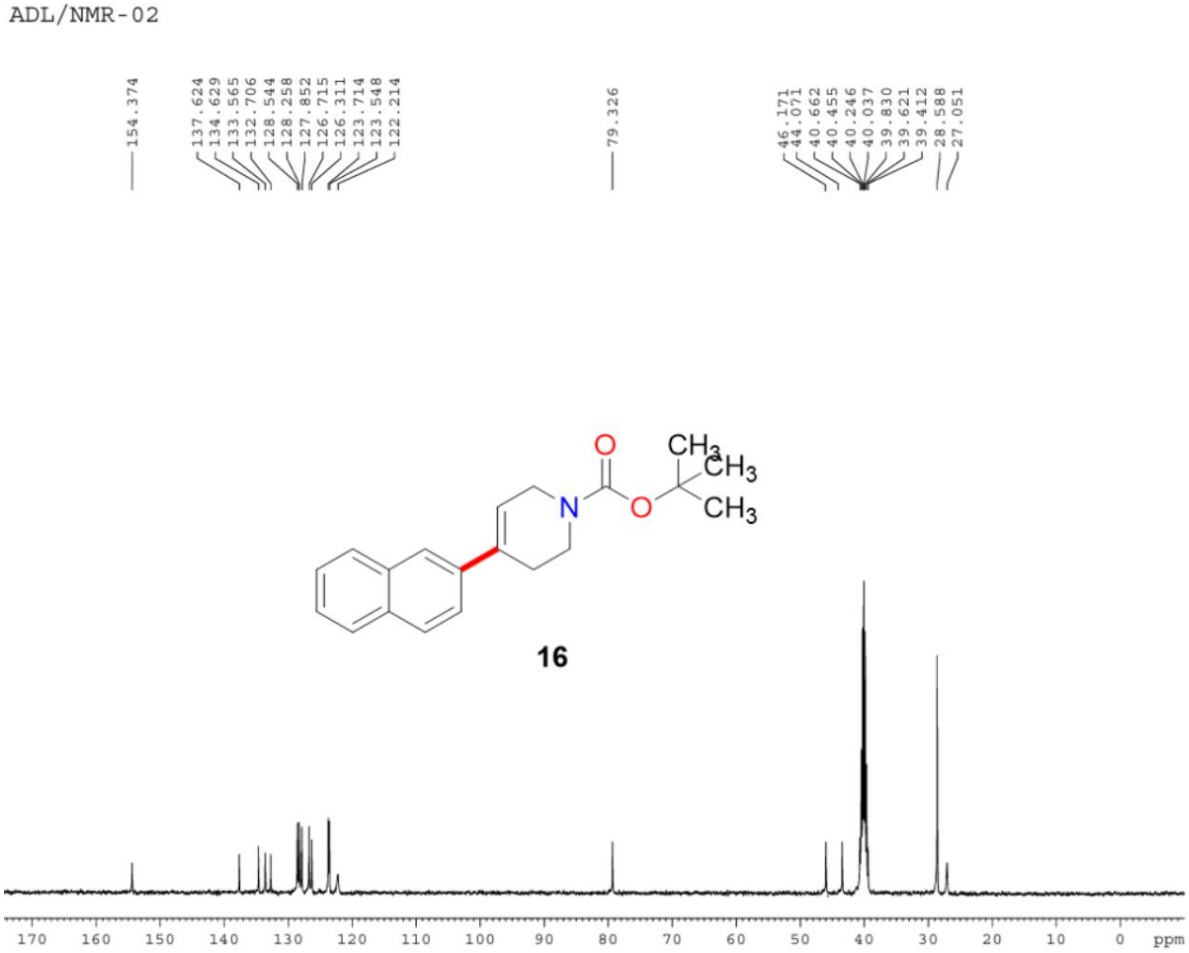


Figure S38: ^{13}C NMR Analysis of 16

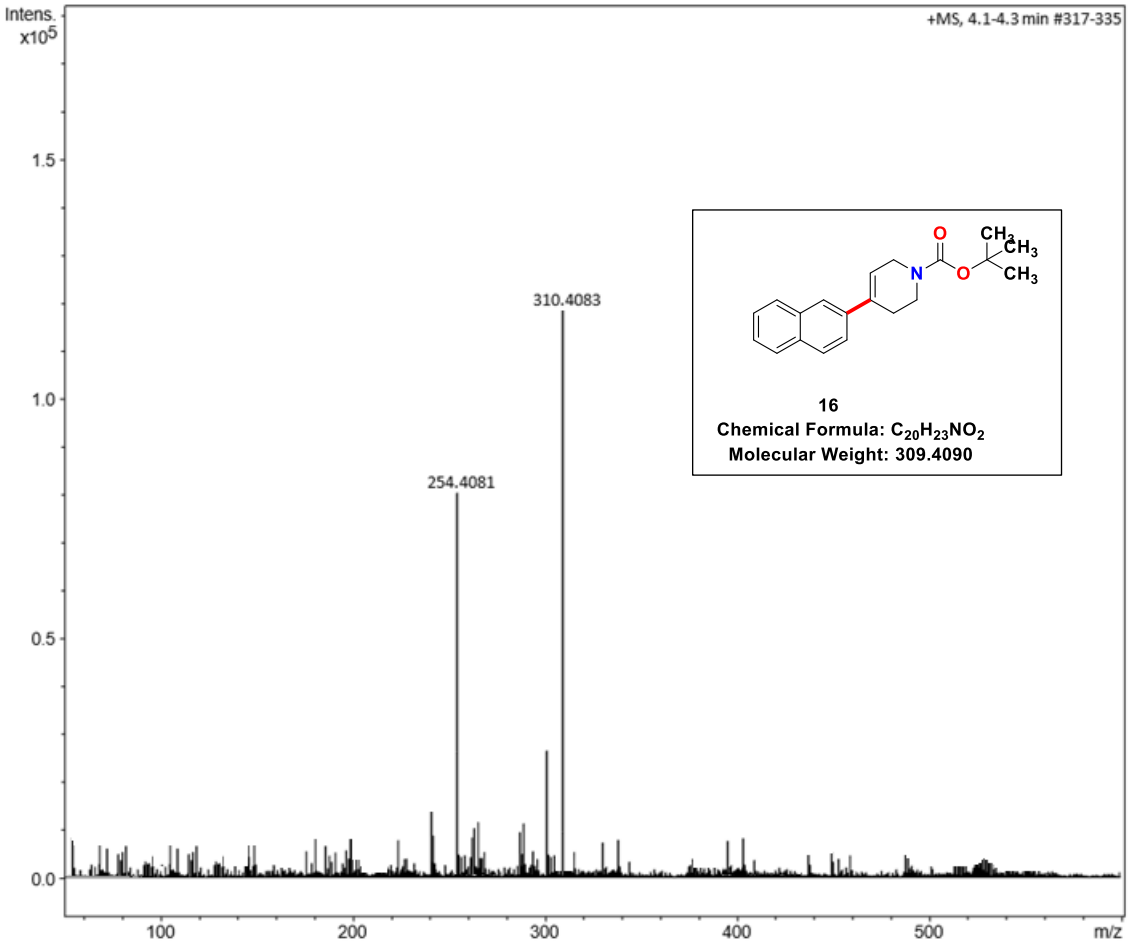


Figure S39: HRMS Analysis of 16

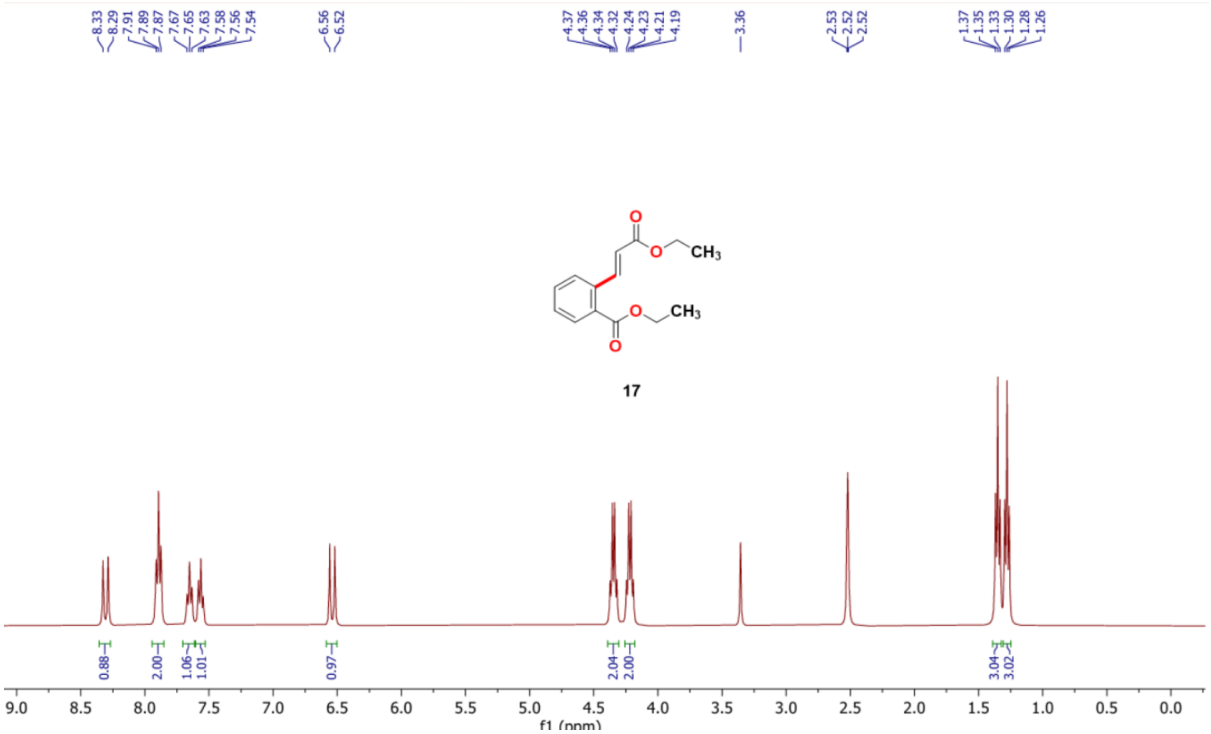


Figure S40: ^{1}HNMR Analysis of 17

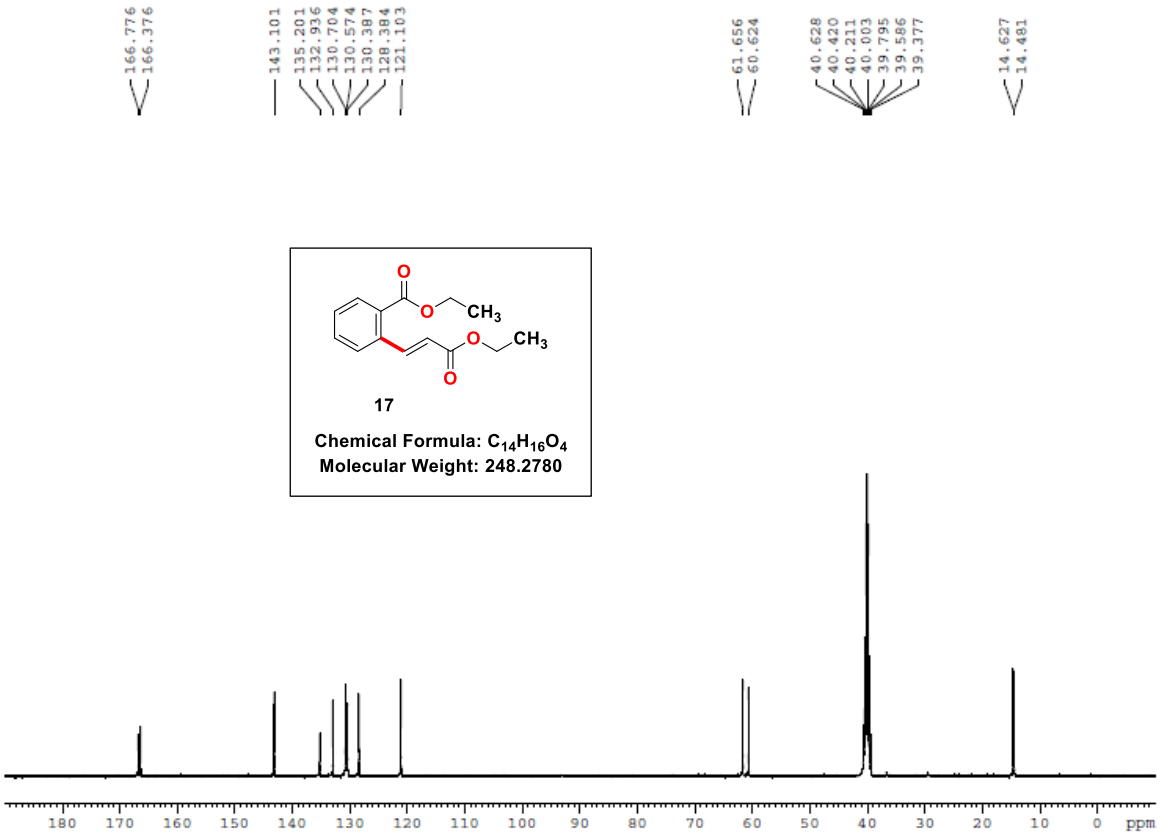


Figure S41: ^{13}C NMR Analysis of 17

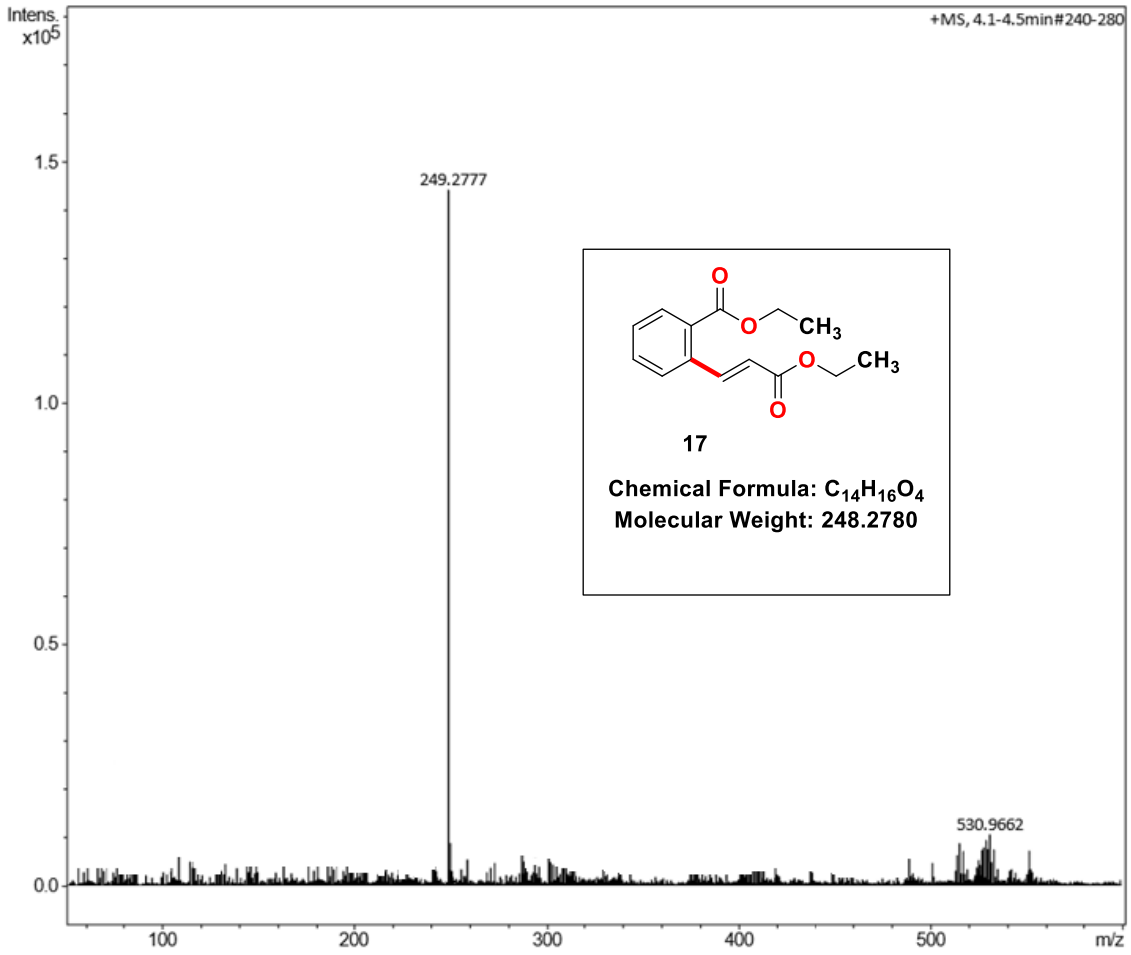


Figure S4: H2RMS Analysis of 17

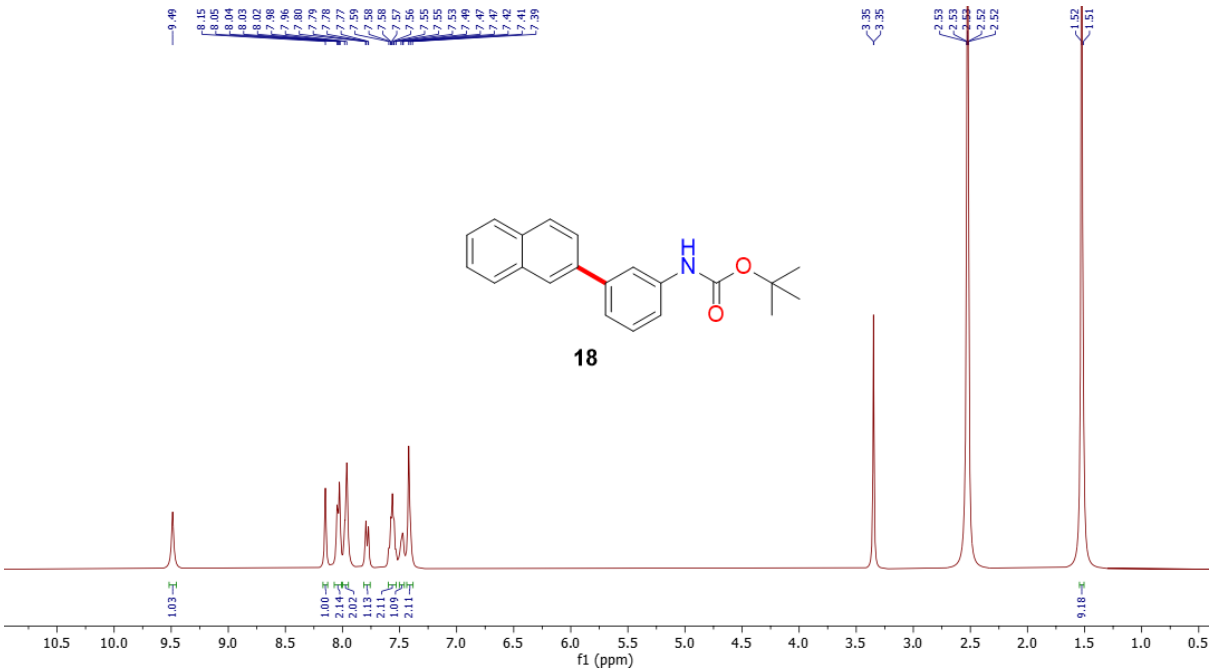


Figure S42: ^{1}H NMR Analysis of 18

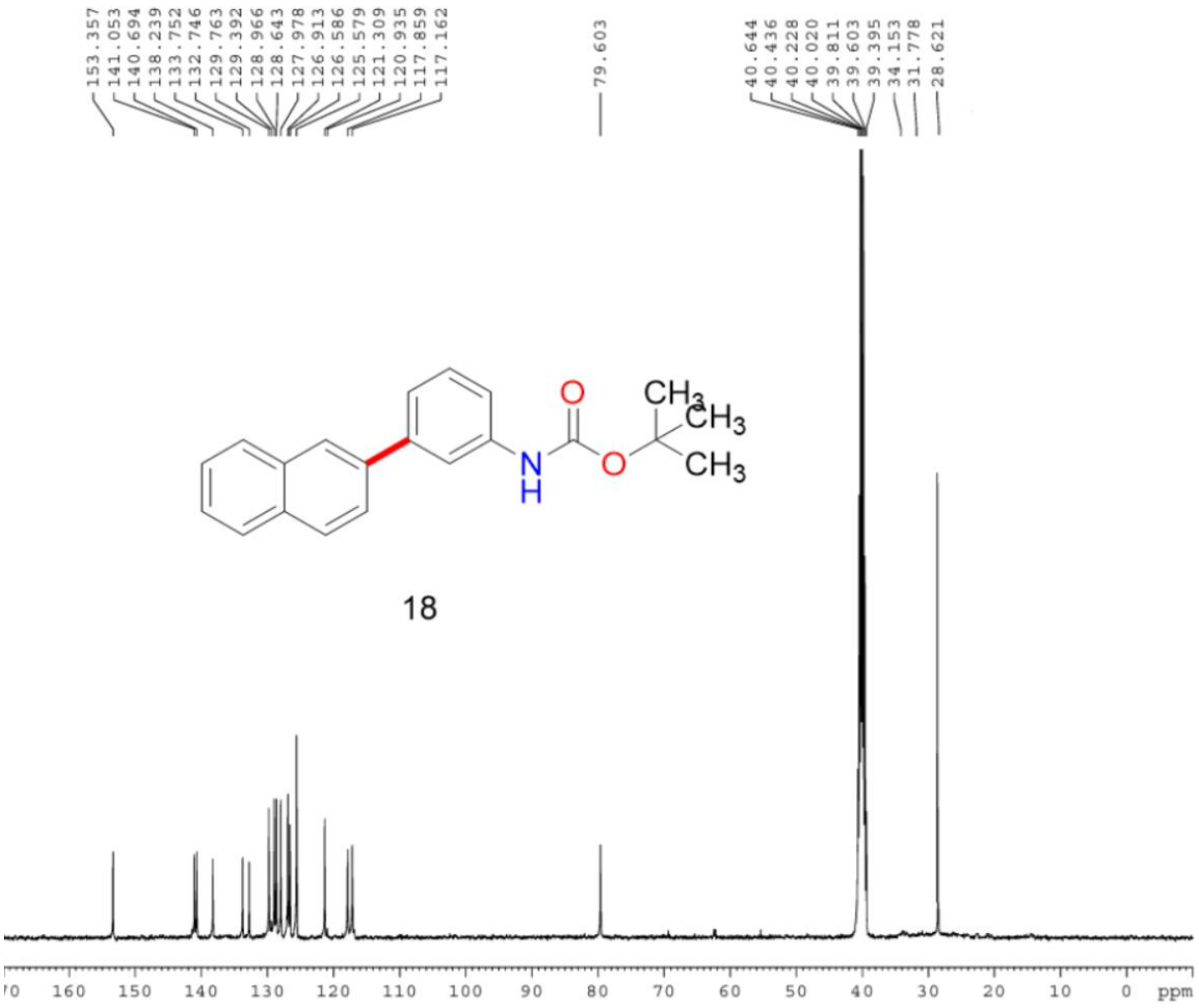


Figure S43: ^{13}C NMR Analysis of 18

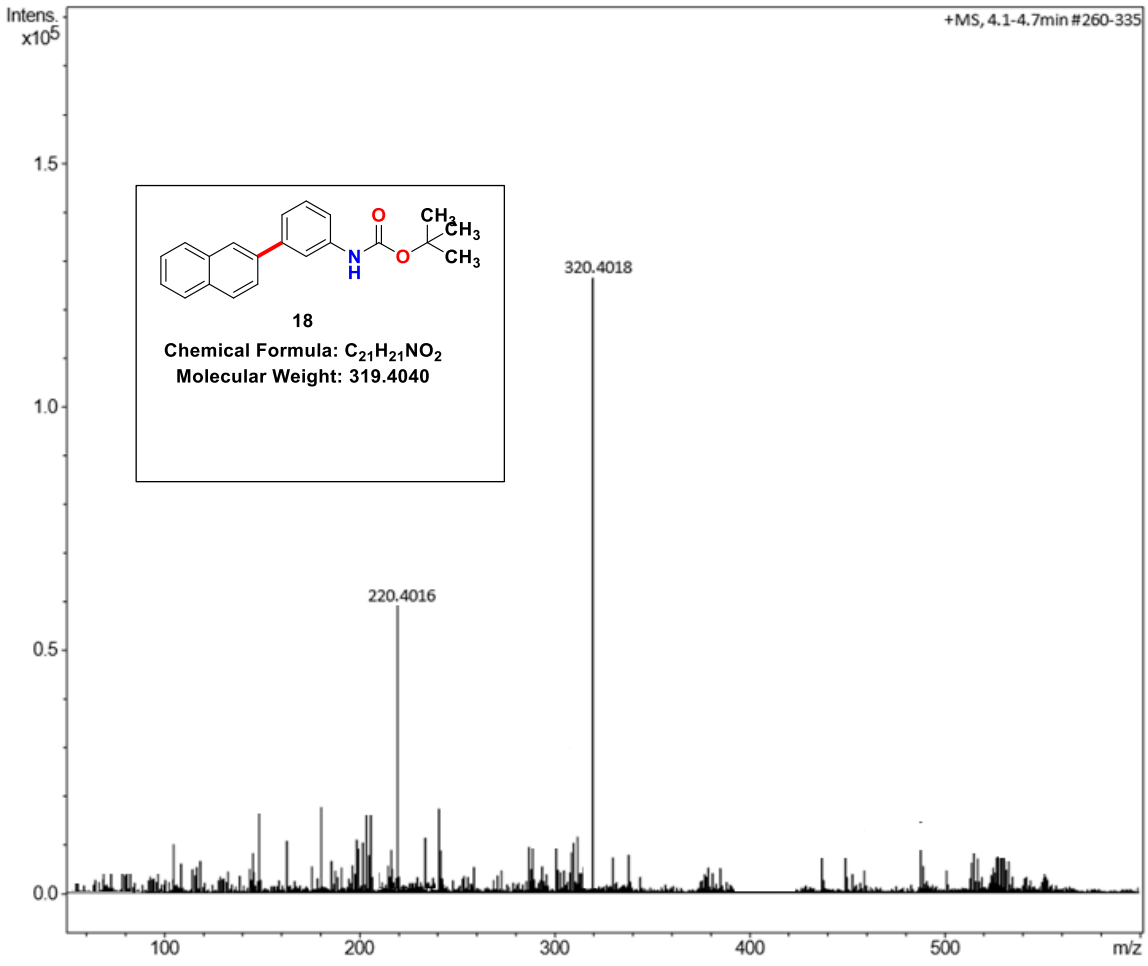


Figure S44: HRMS Analysis of 18

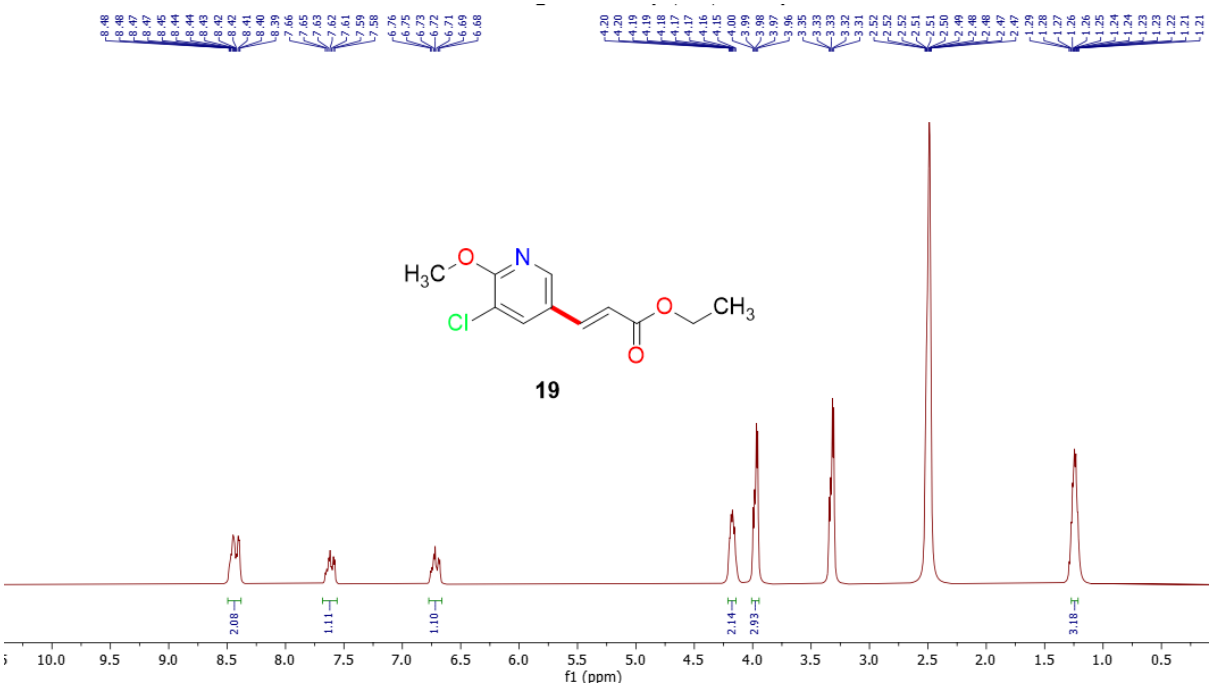


Figure S45: ^{1}H NMR Analysis of 19

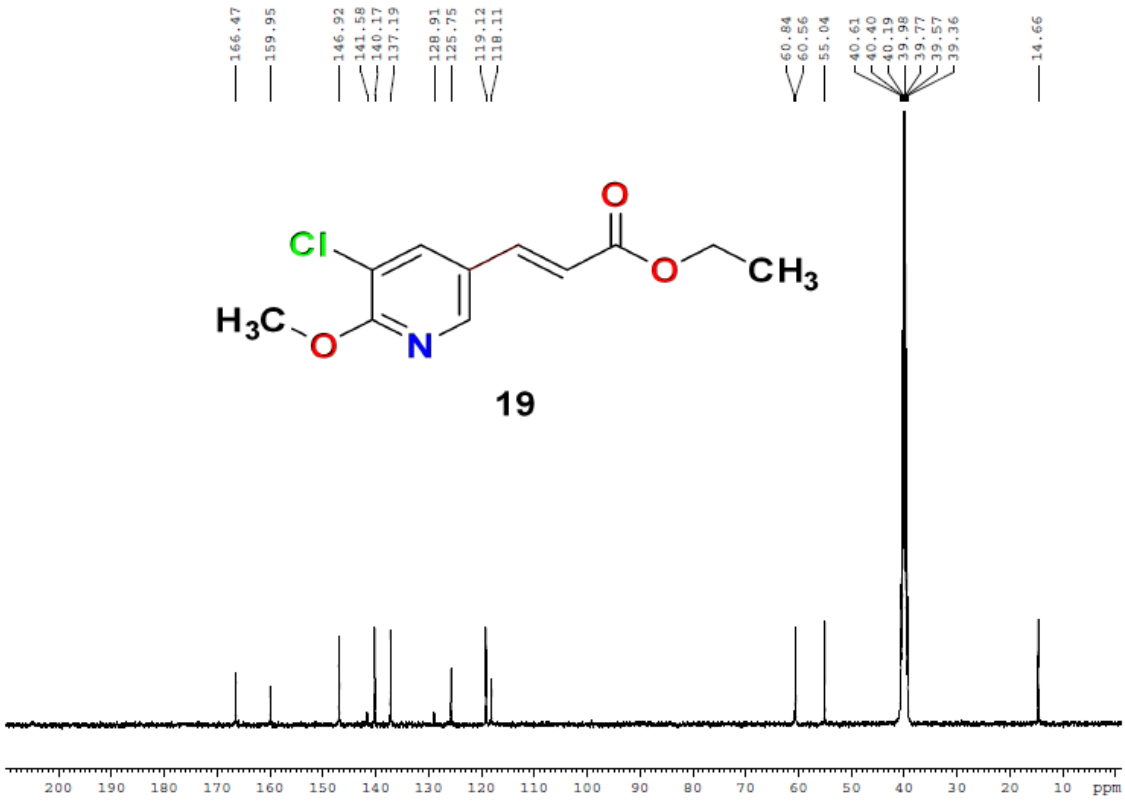


Figure S46: ^{13}C NMR A6nalysis of 19

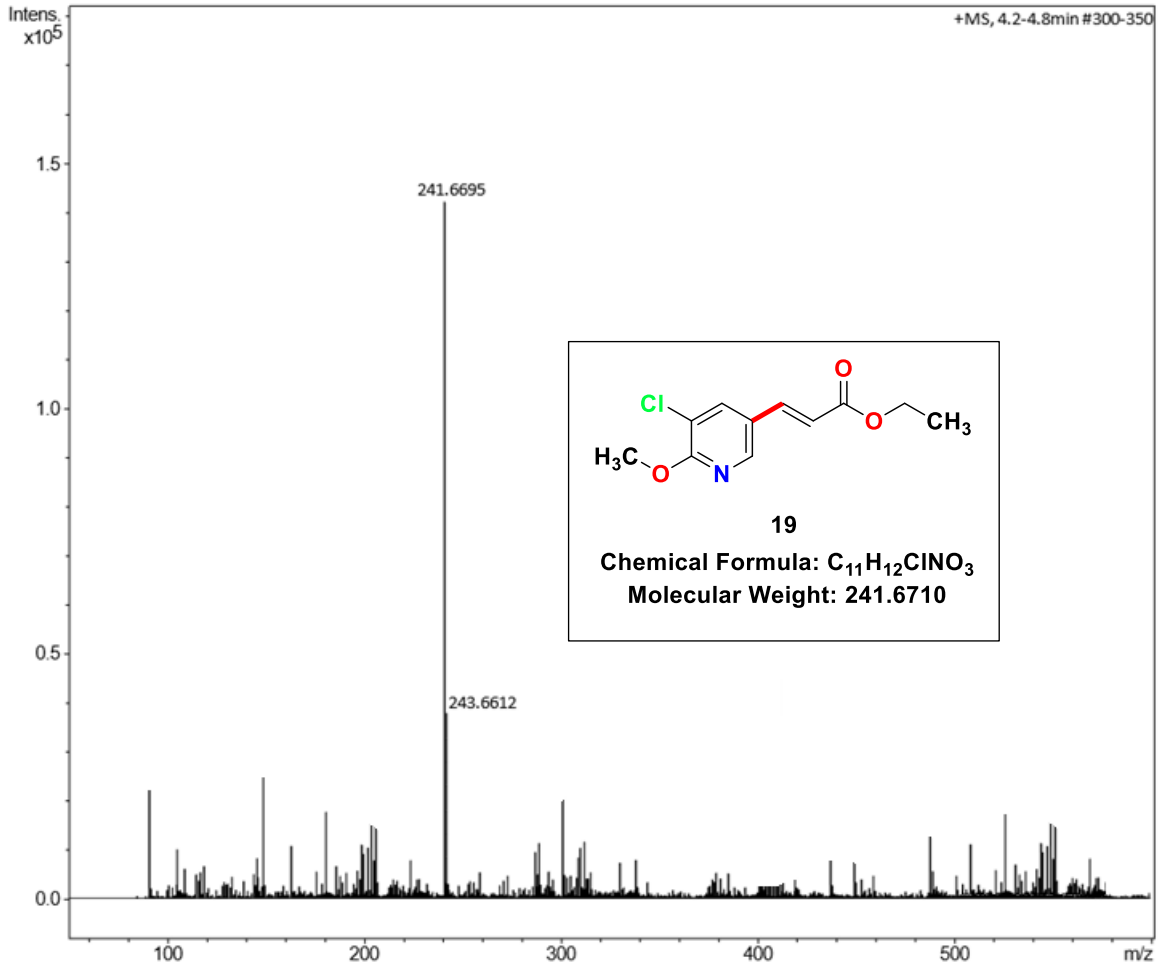


Figure S47: HRMS Analysis of 19

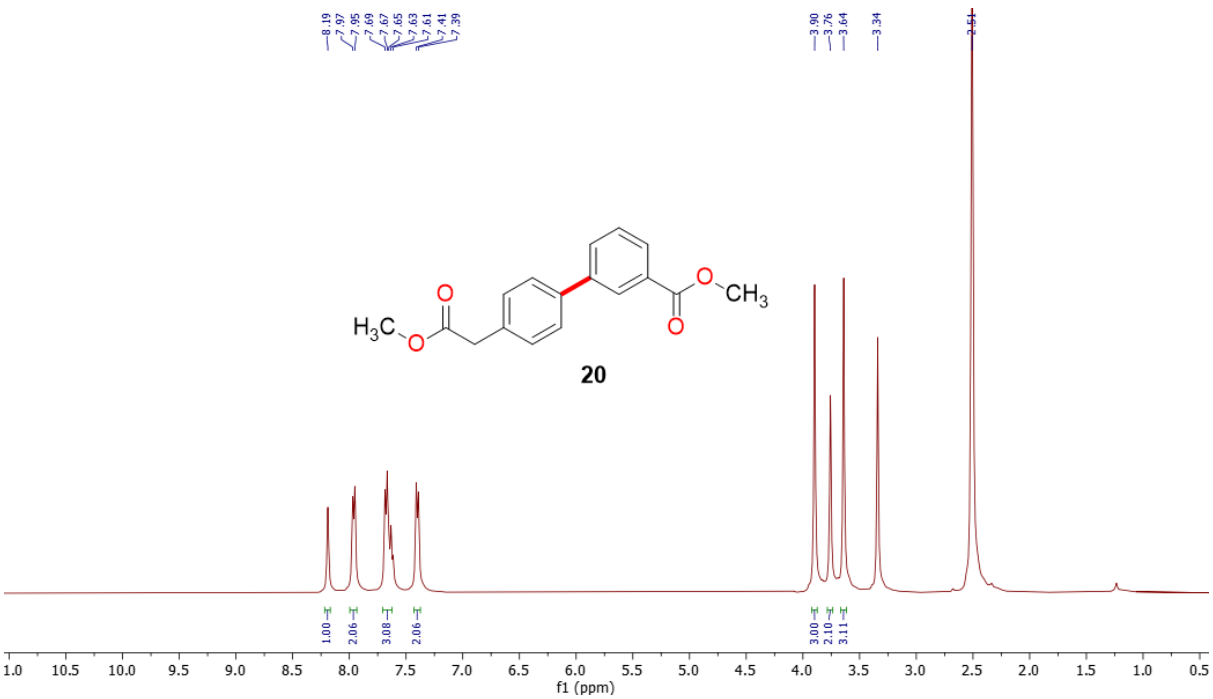


Figure S48: ^{1}H NMR Analysis of 20

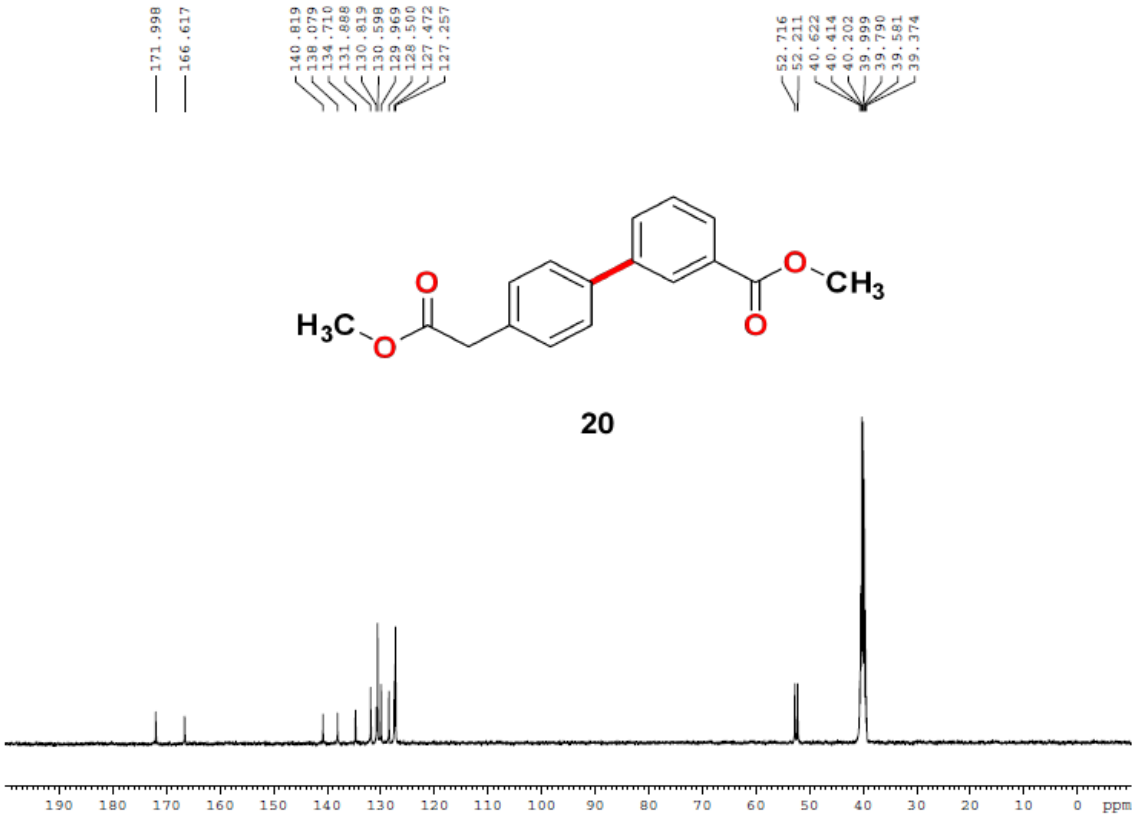


Figure S49: ^{13}C NMR Analysis of 20

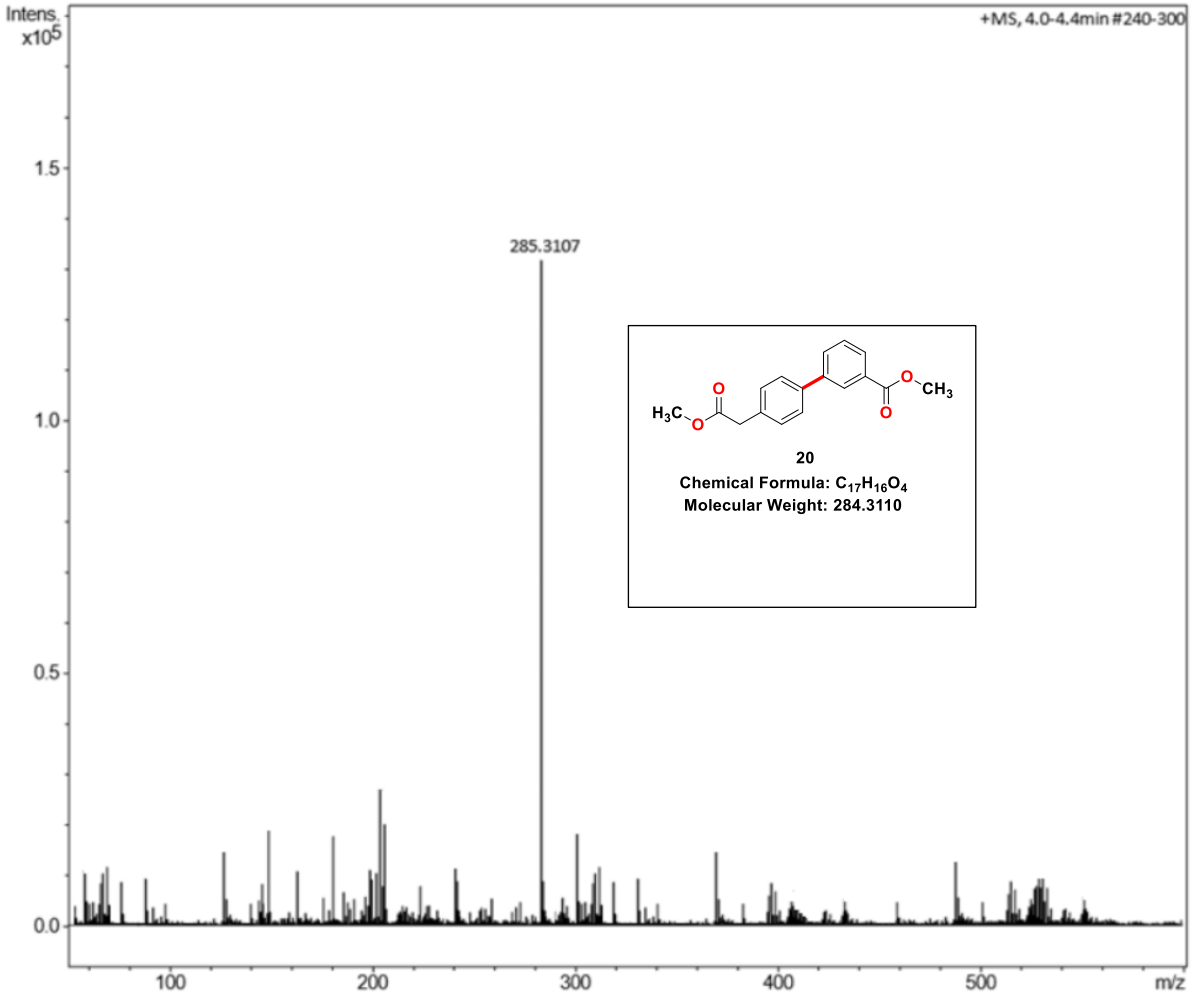


Figure S50: HRMS Analysis of 20

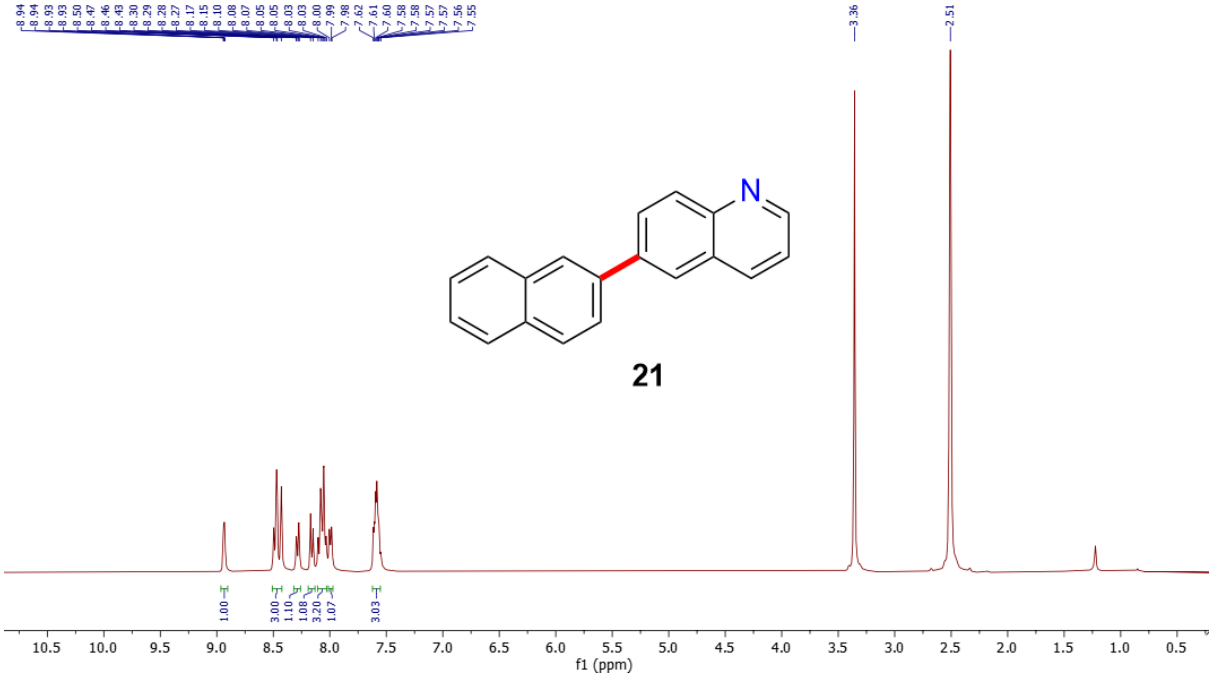


Figure S51: ^{1}H NMR Analysis of 21

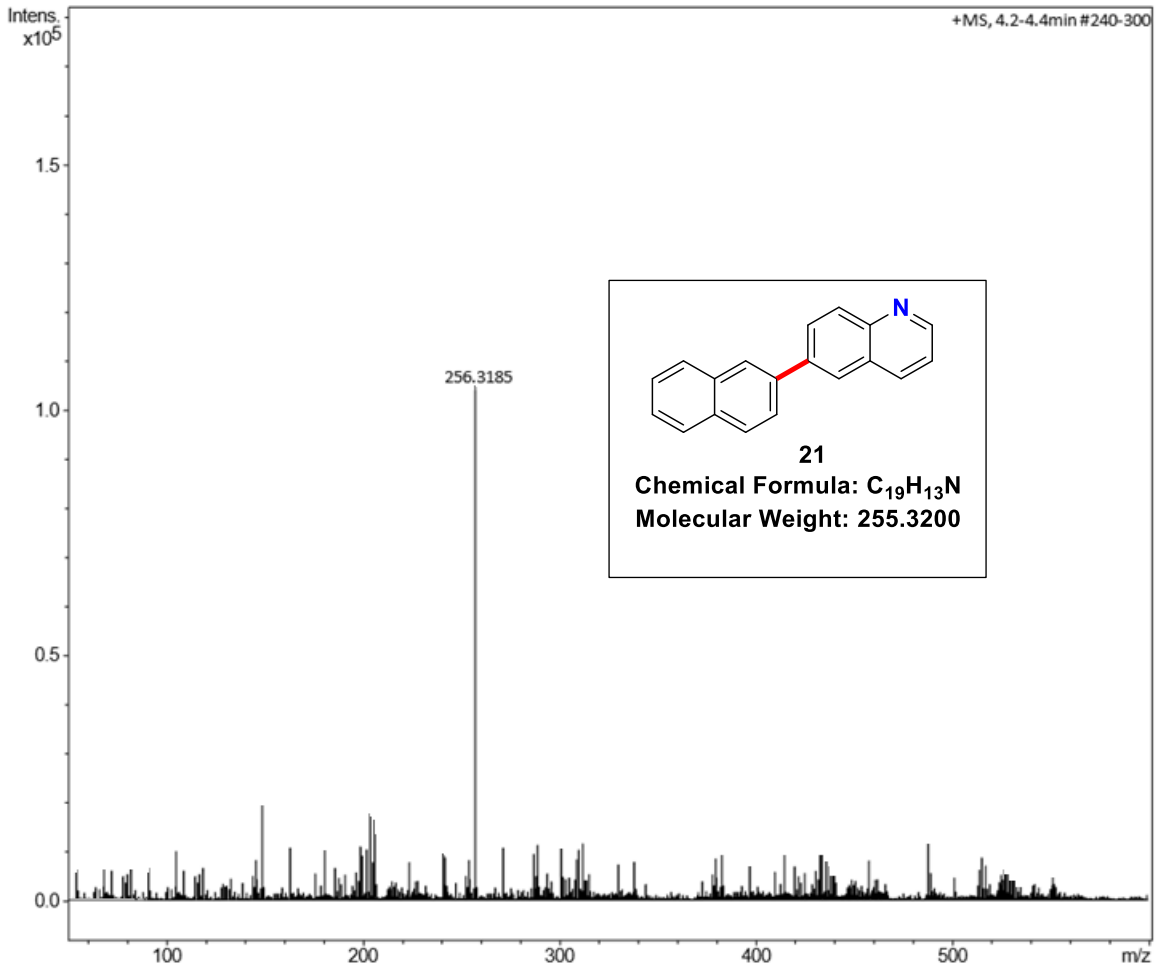


Figure S52: HRMS Analysis of 21

^{13}C NMR*: 21 has solubility issue so ^{13}C not recorded*

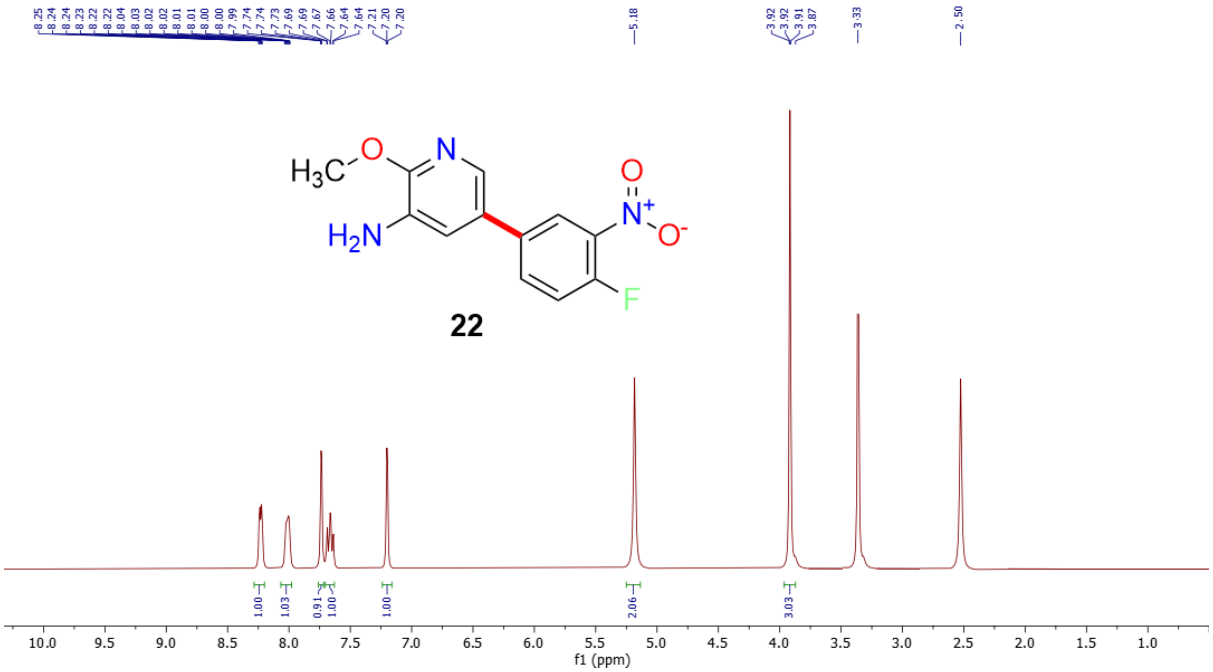


Figure S53: ^{1}H NMR Analysis of 22

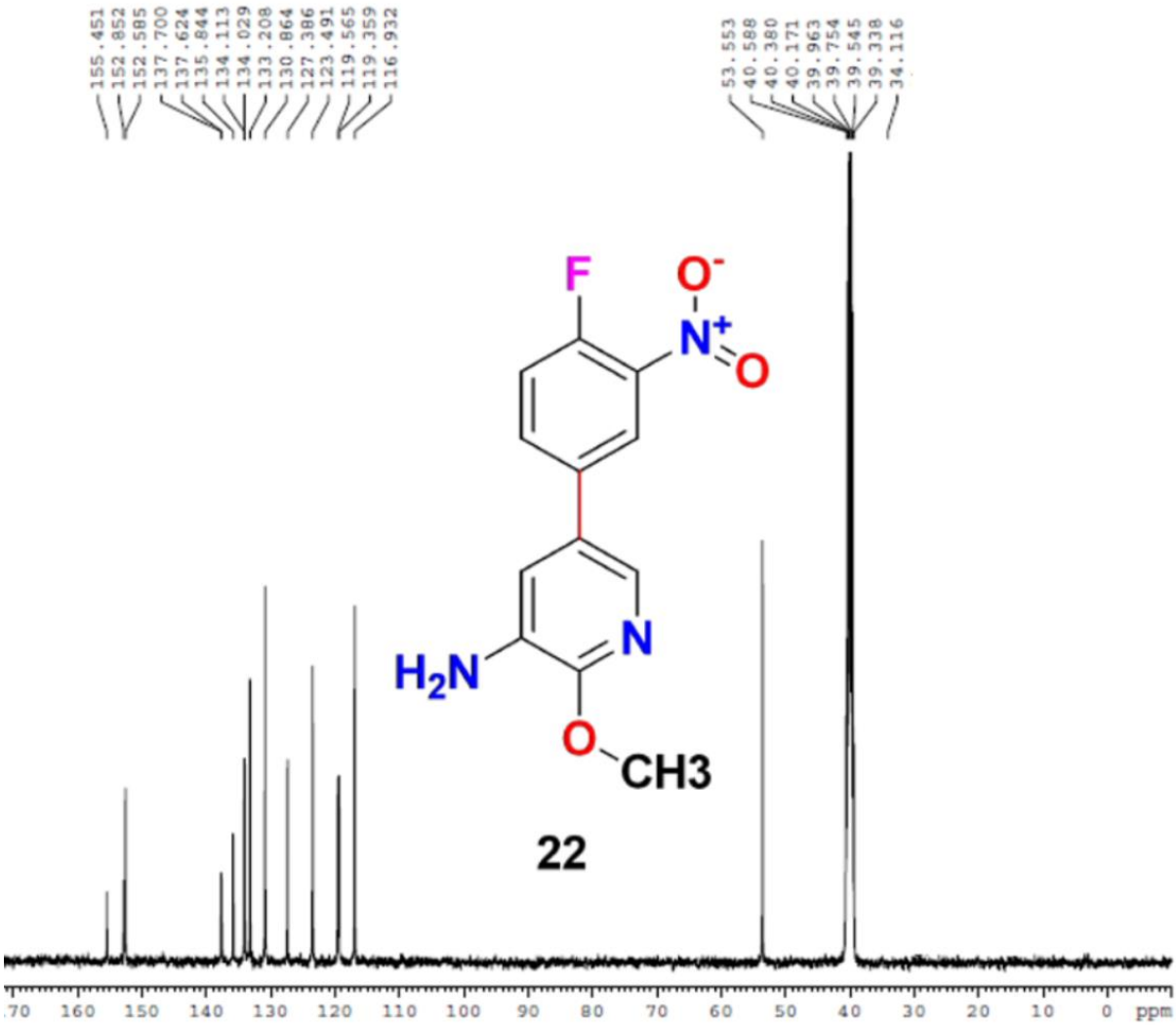


Figure S54: ^{13}C NMR Analysis of 22

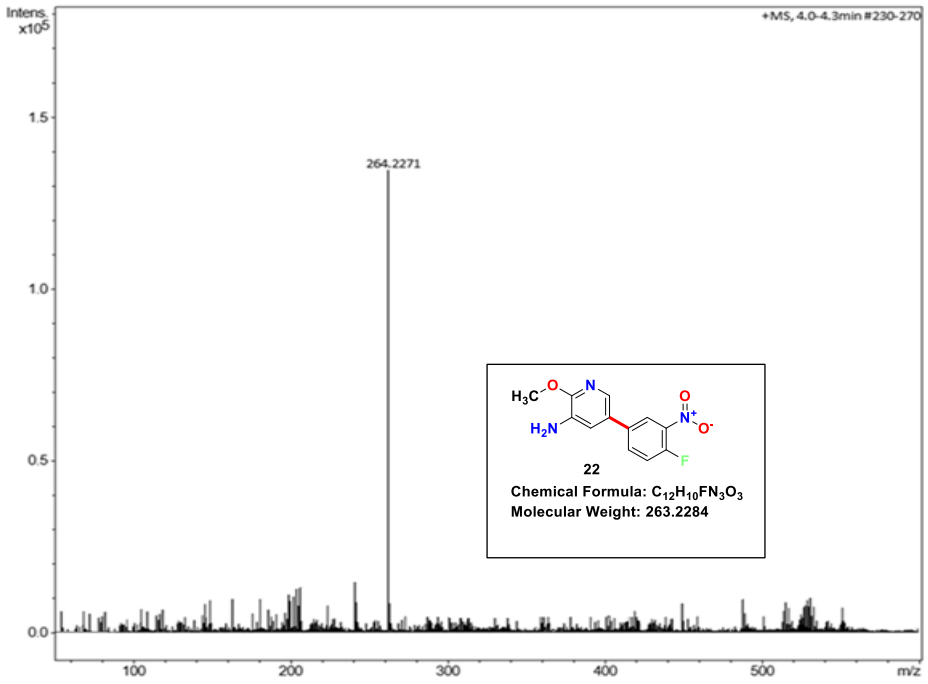


Figure S55: HRMS Analysis of 22

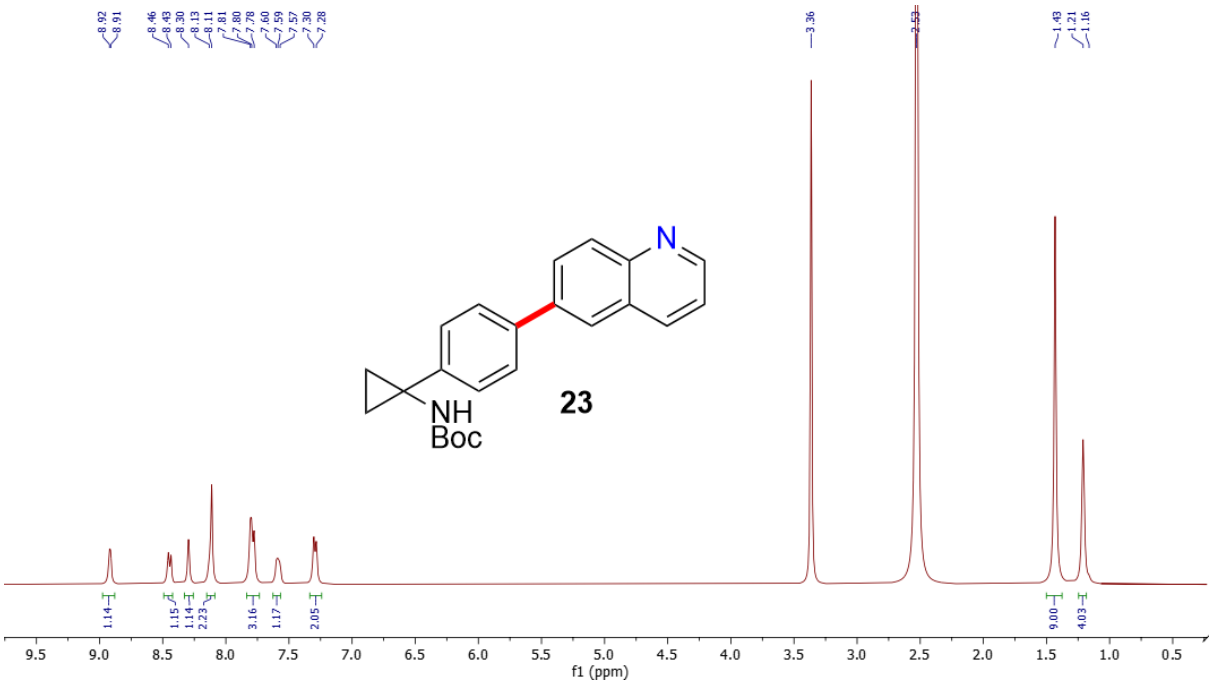


Figure S56: ^{1}H NMR Analysis of 23

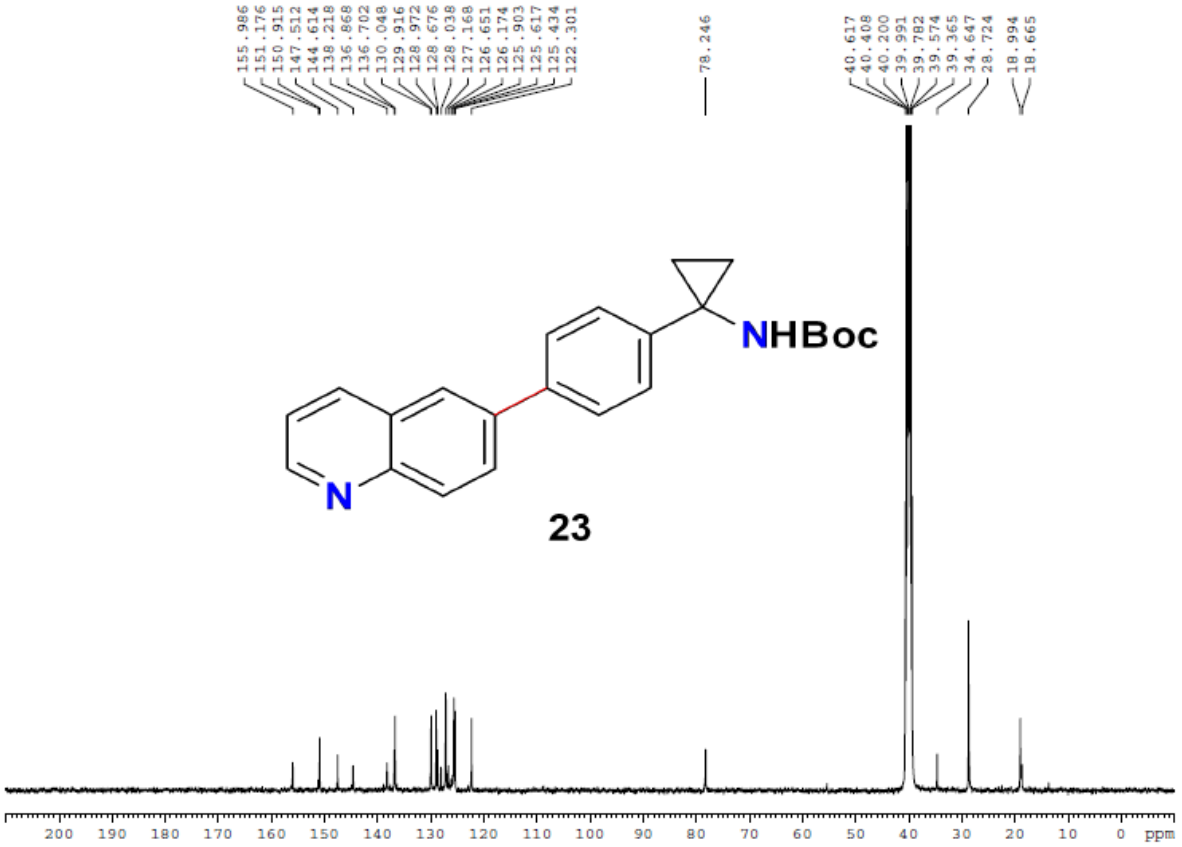


Figure S57: ^{13}C NMR Analysis of 23

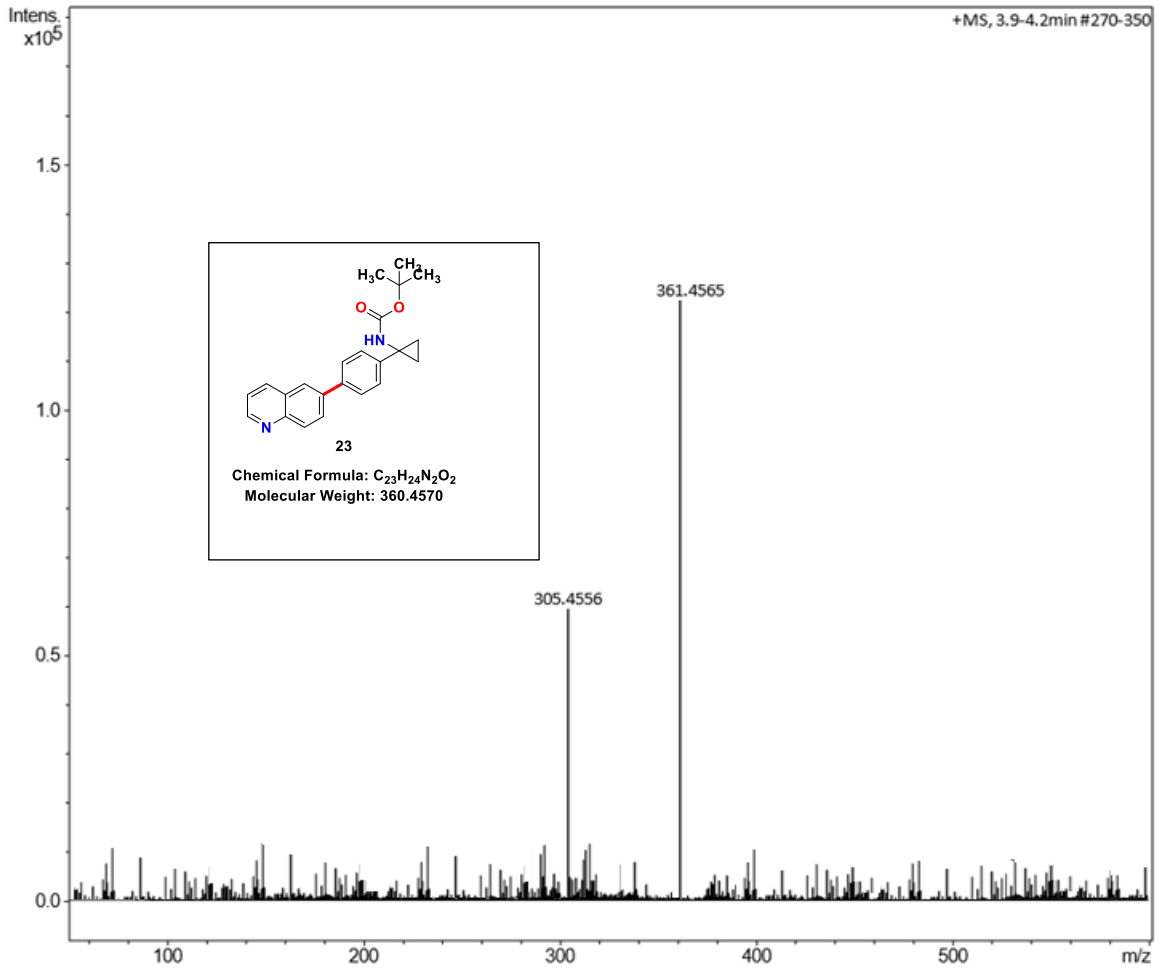


Figure S58: HRMS Analysis of 23

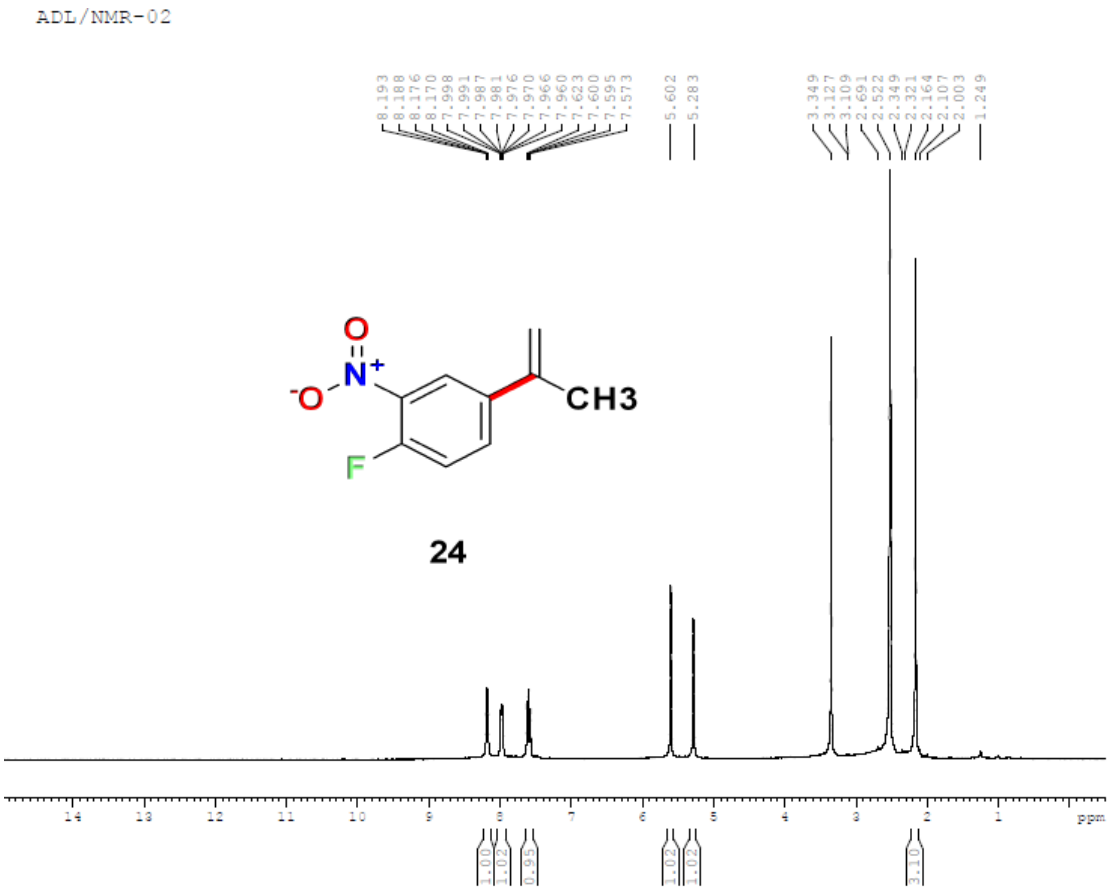


Figure S59: ^{1}H NMR Analysis of 24

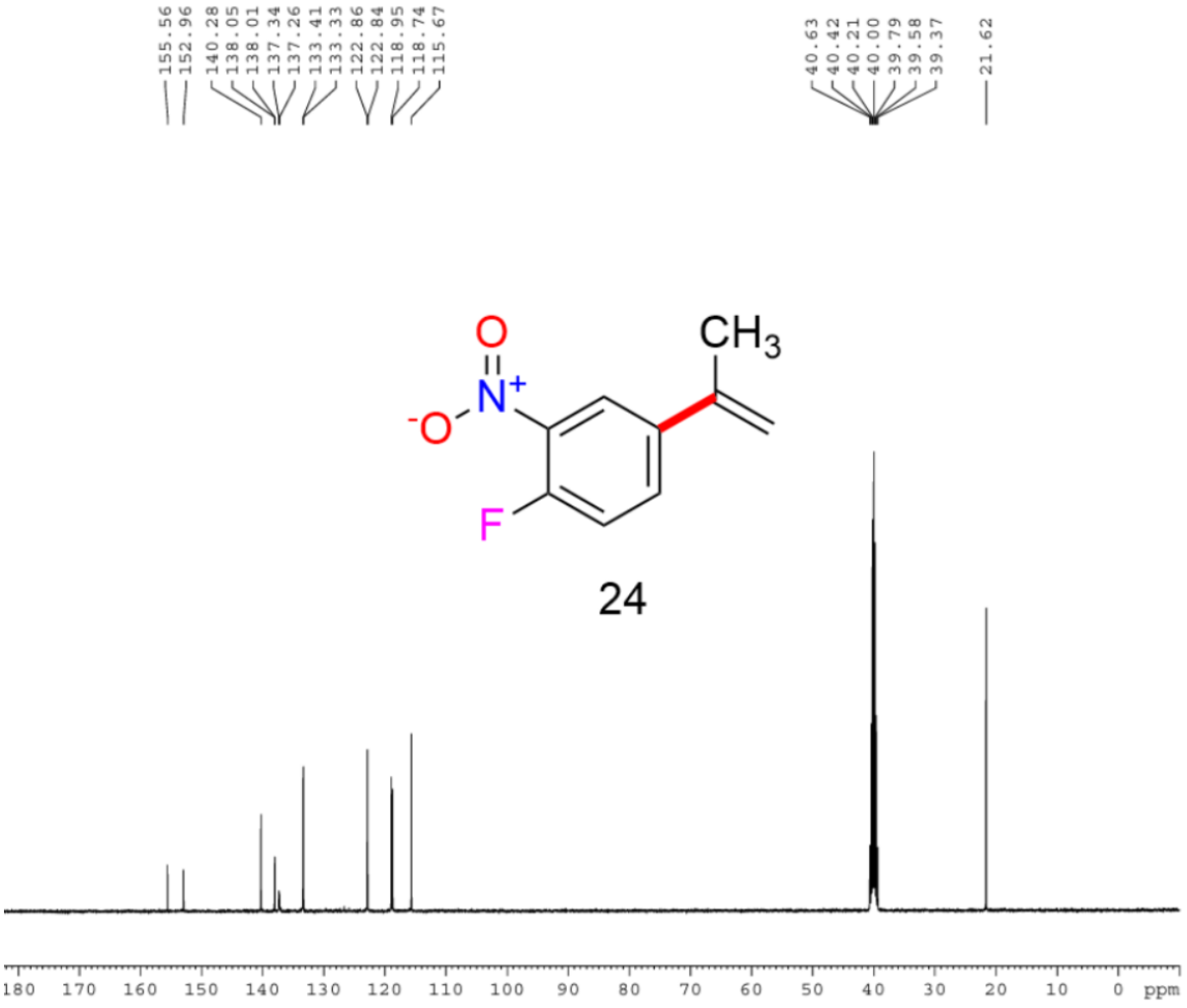


Figure S60: ^{13}C NMR Analysis of 24

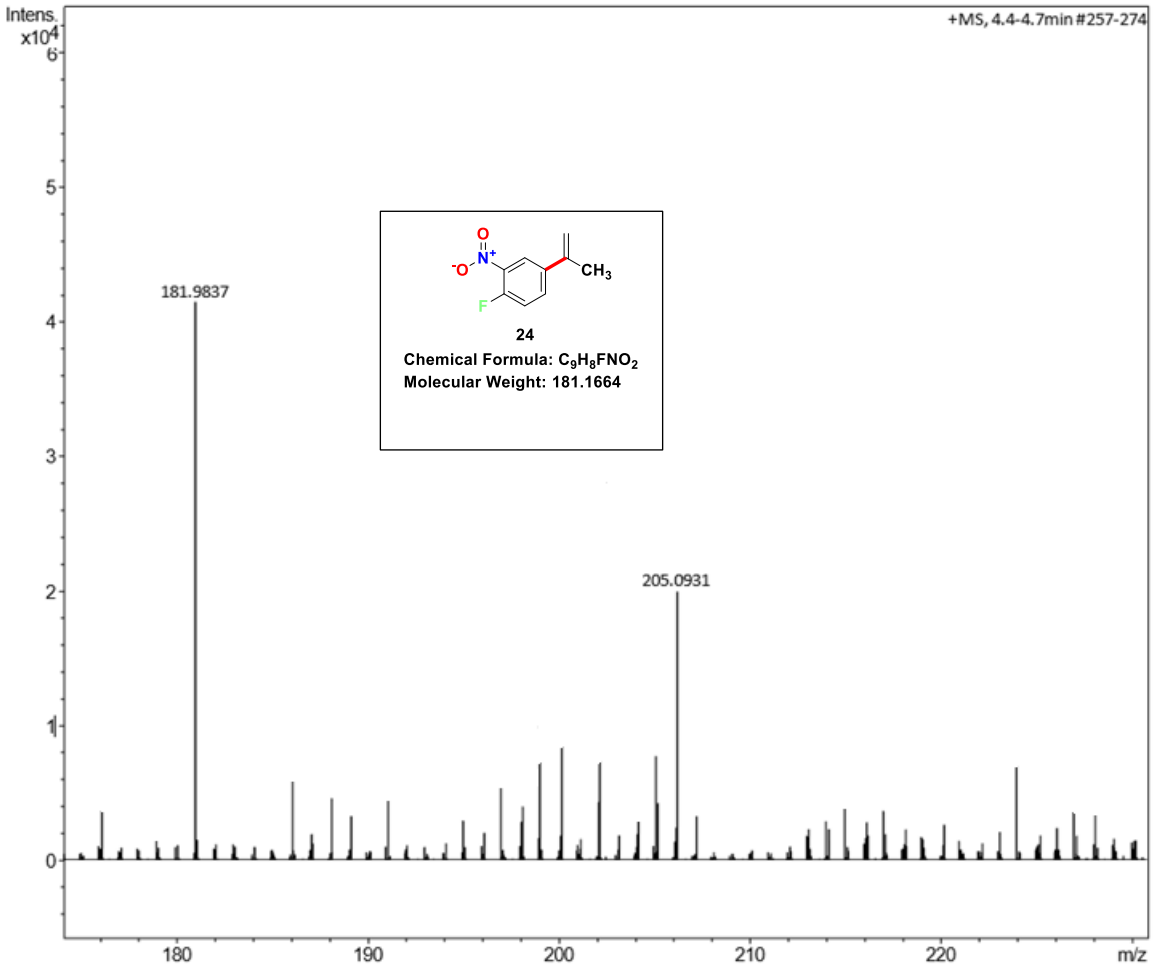


Figure S61: HRMS Analysis of 24

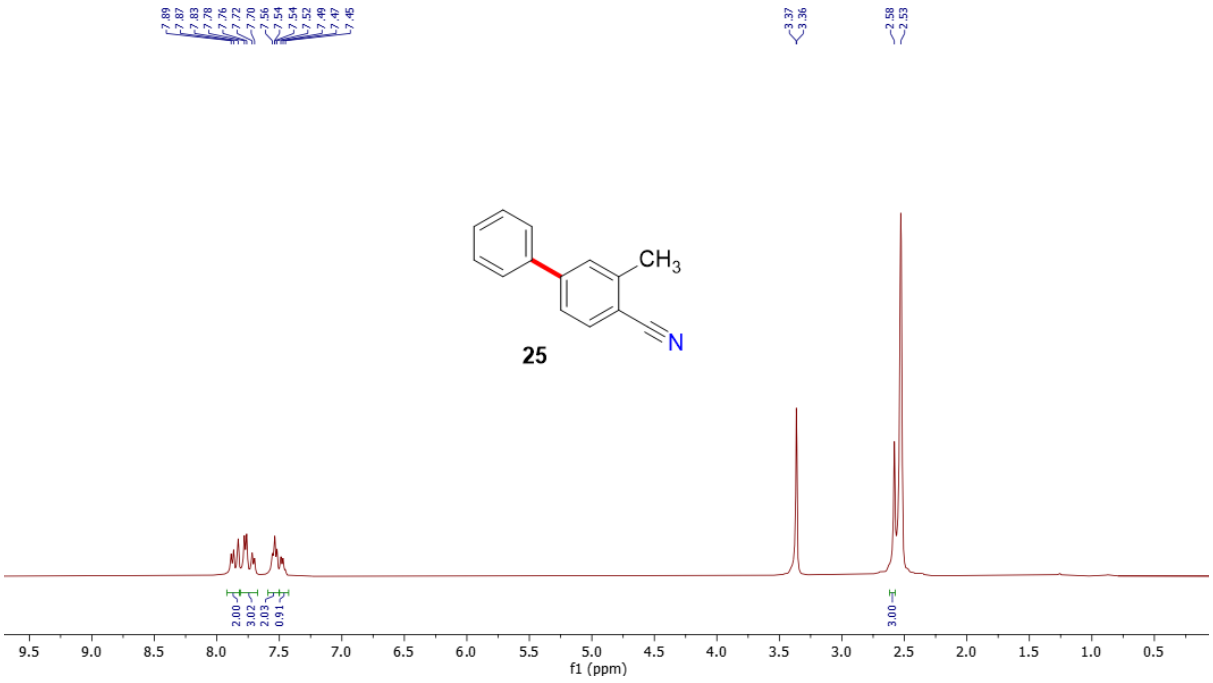


Figure S6: ^{1}H NMR Analysis of 25

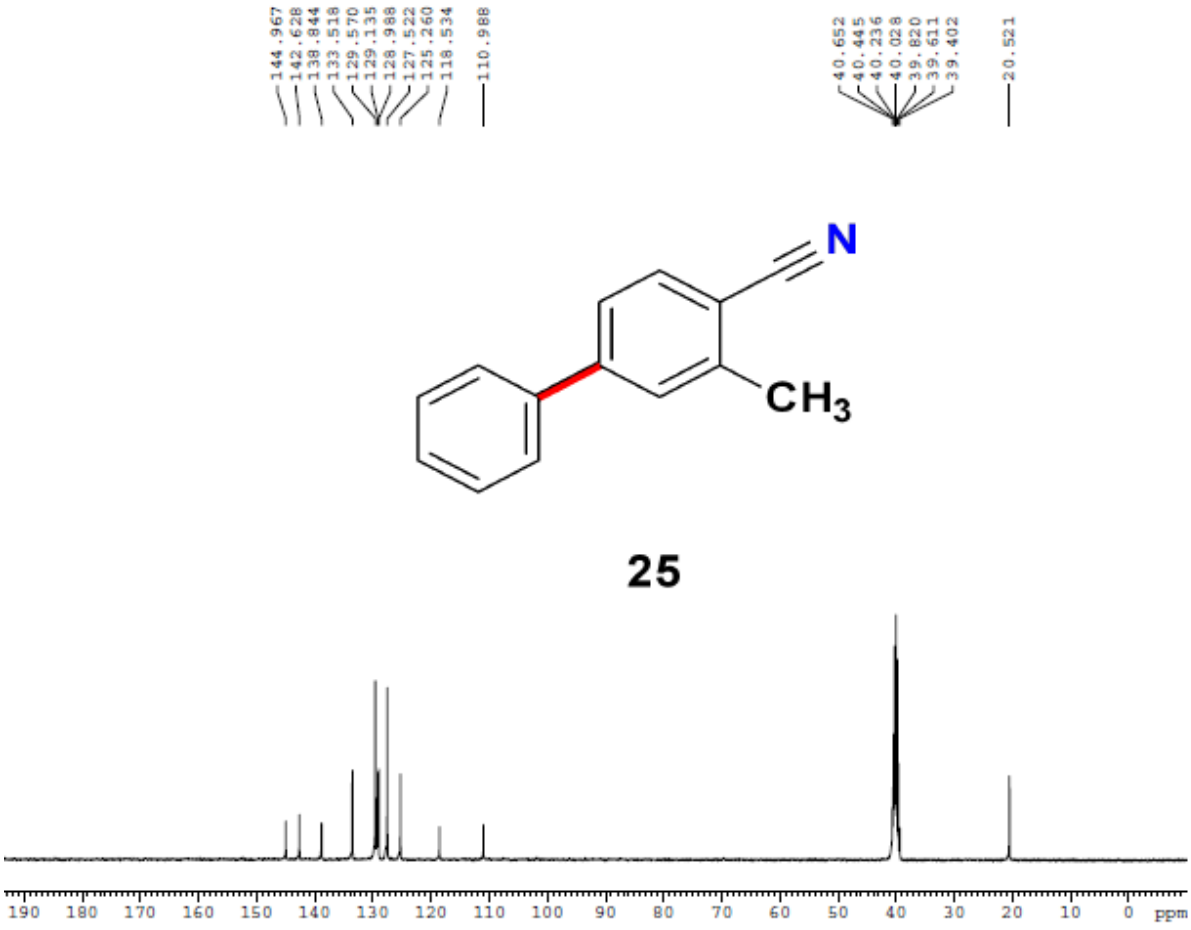


Figure S63: ^{13}C NMR Analysis of 25

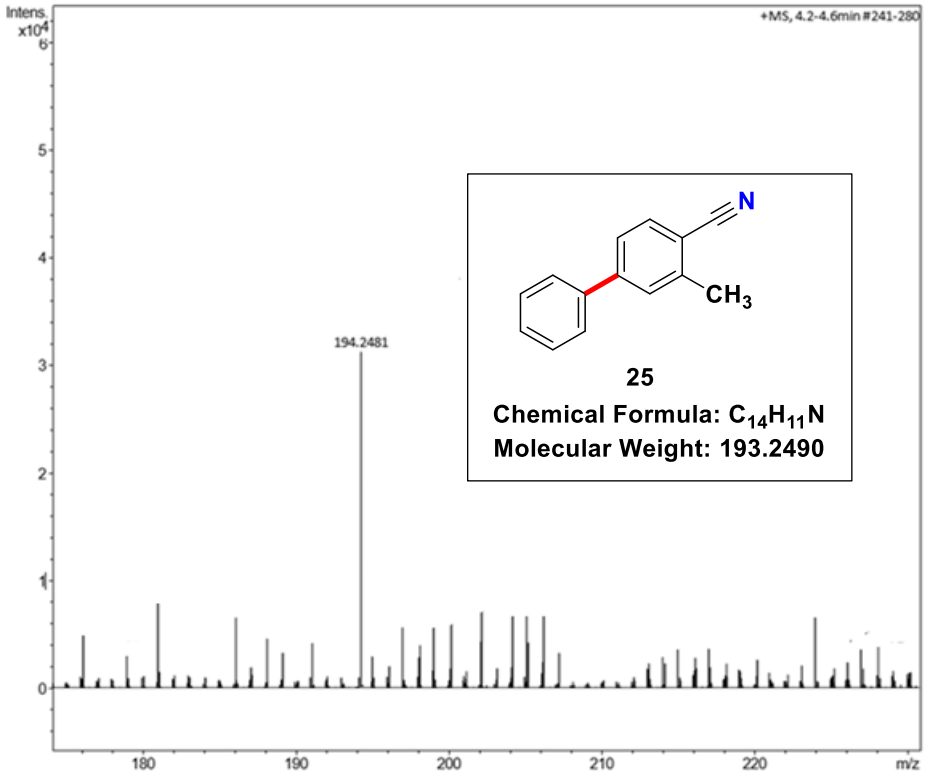


Figure S64: HRMS Analysis of 25

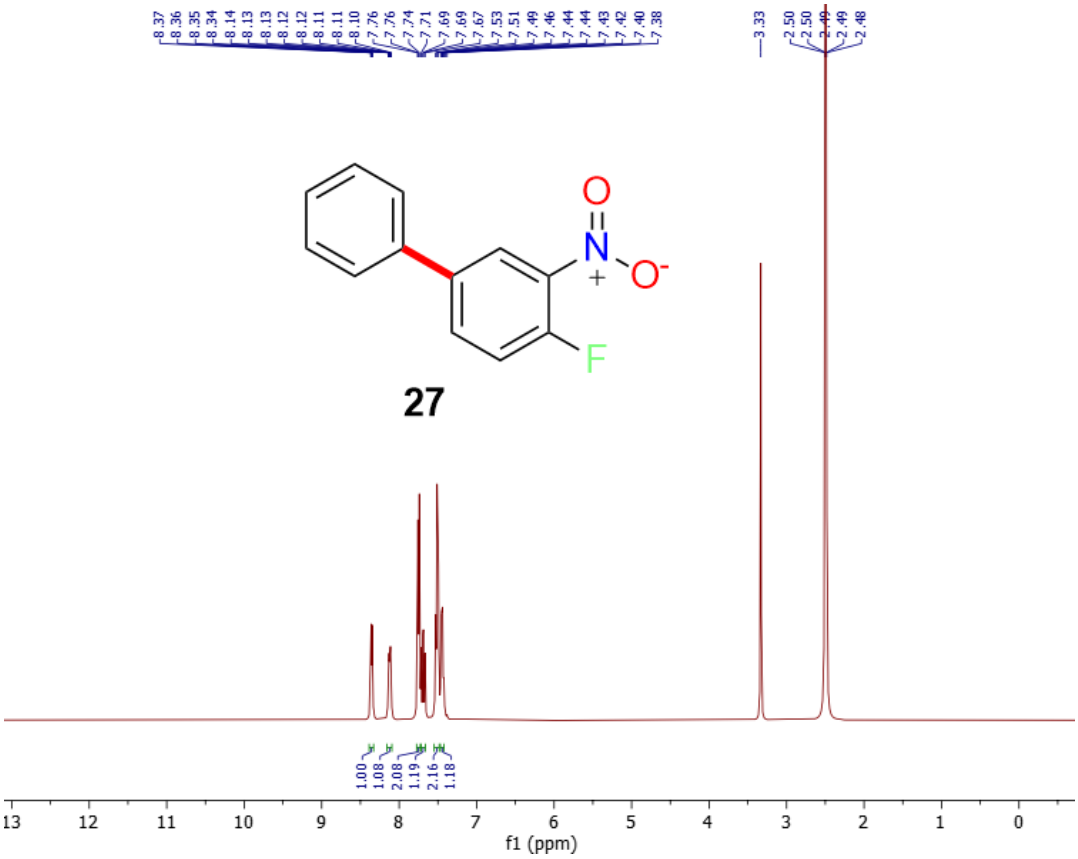


Figure S65: ^{1}H NMR Analysis of 27

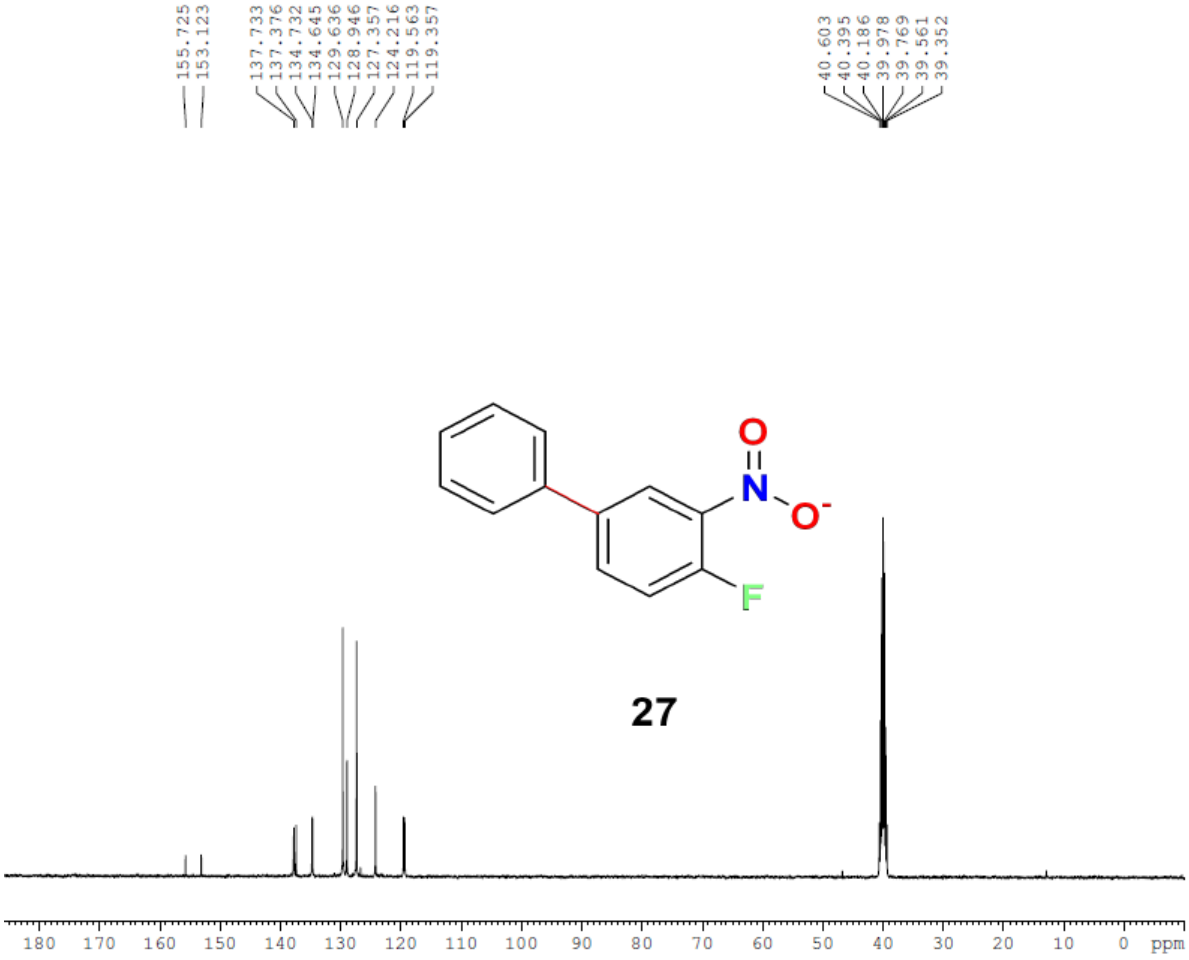


Figure S66: ^{13}C NMR Analysis of 27

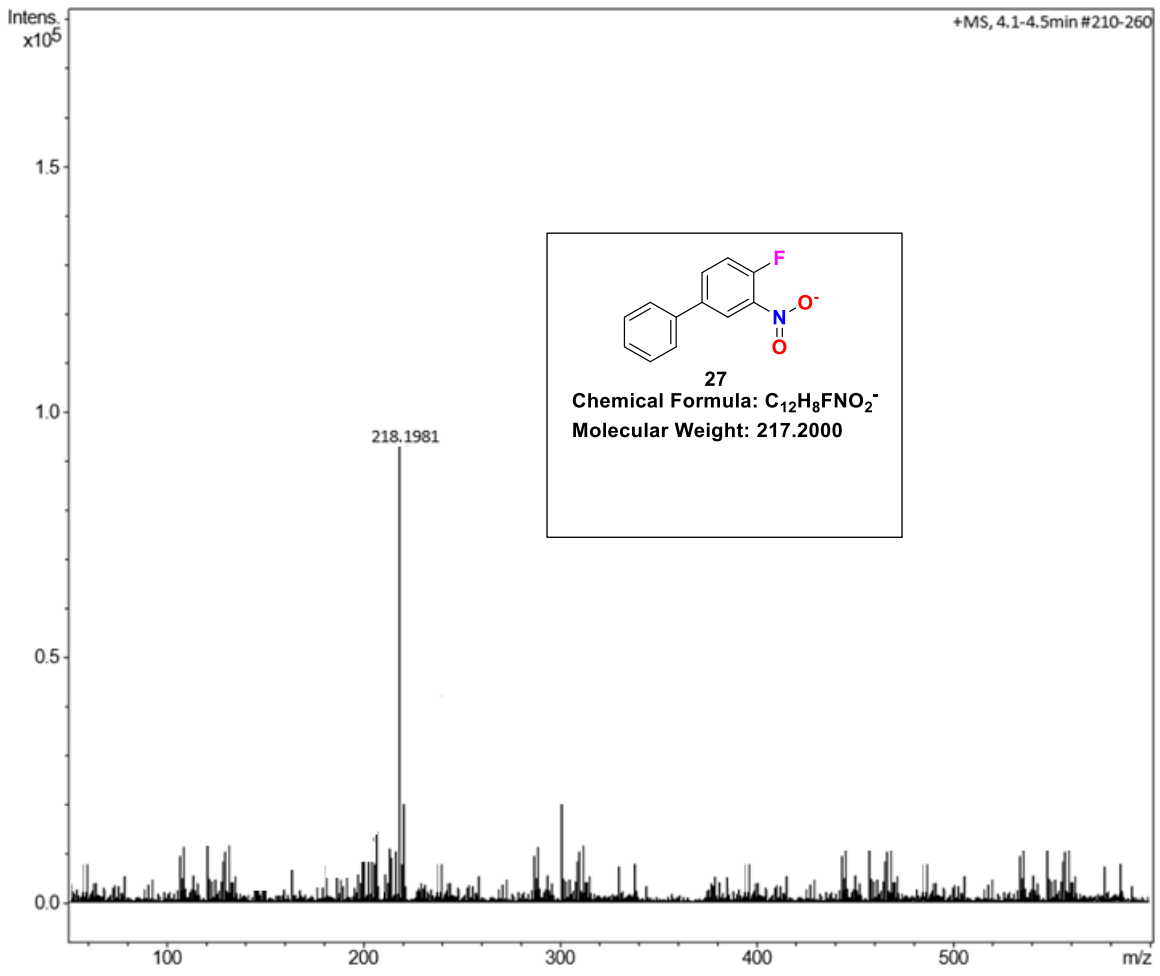


Figure S67: HRMS Analysis of 27

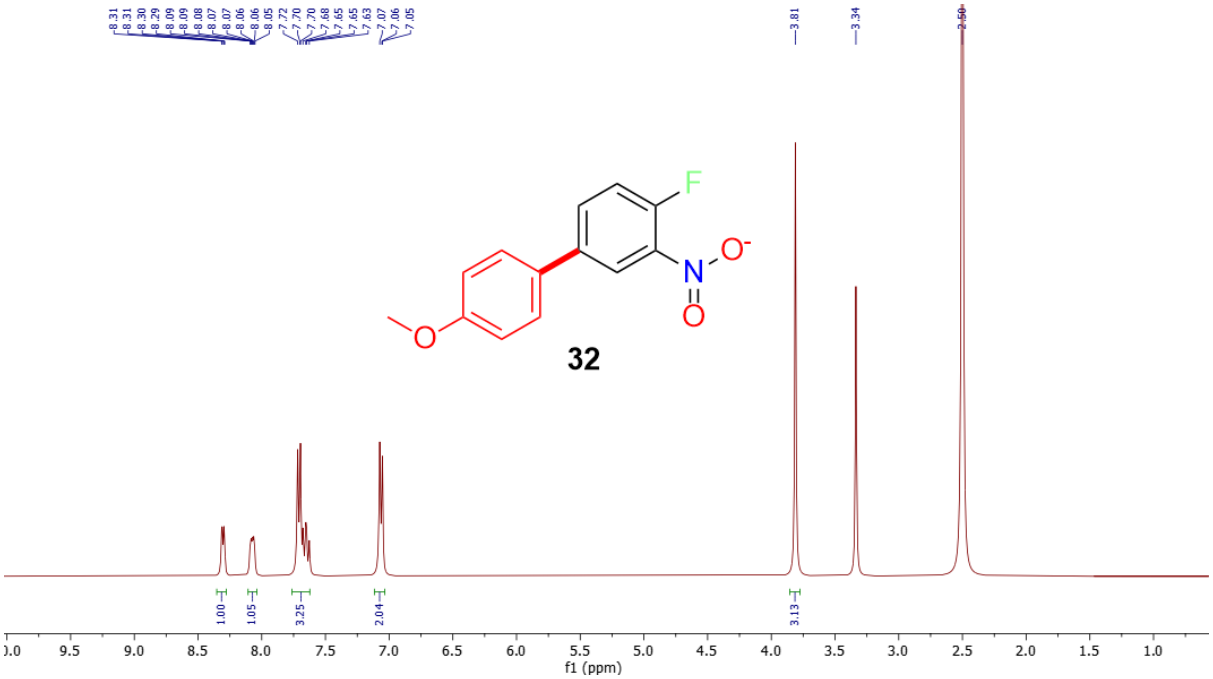


Figure S68: ^{1}H NMR Analysis of 32

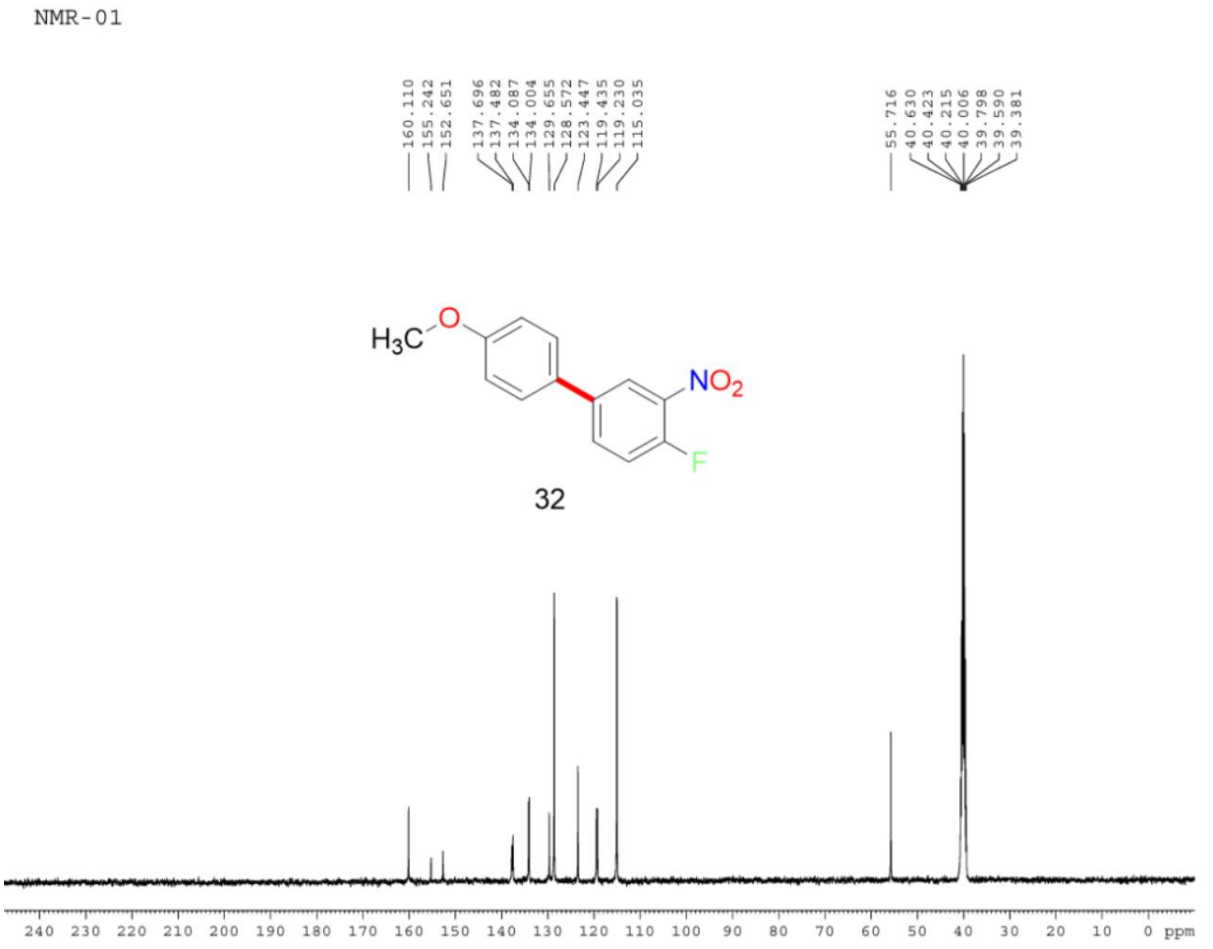


Figure S69: ^{13}C NMR Analysis of 32

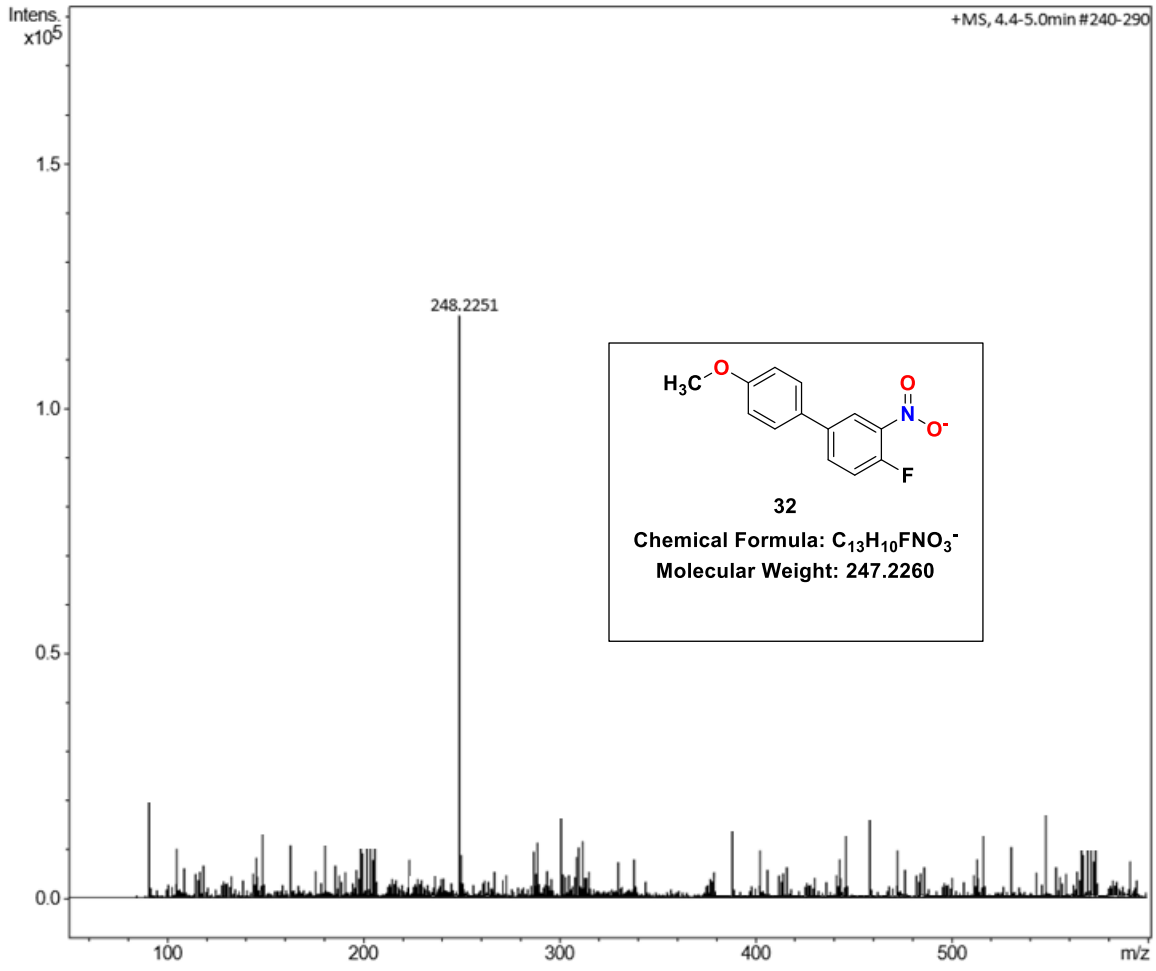


Figure S70: HRMS Analysis of 32

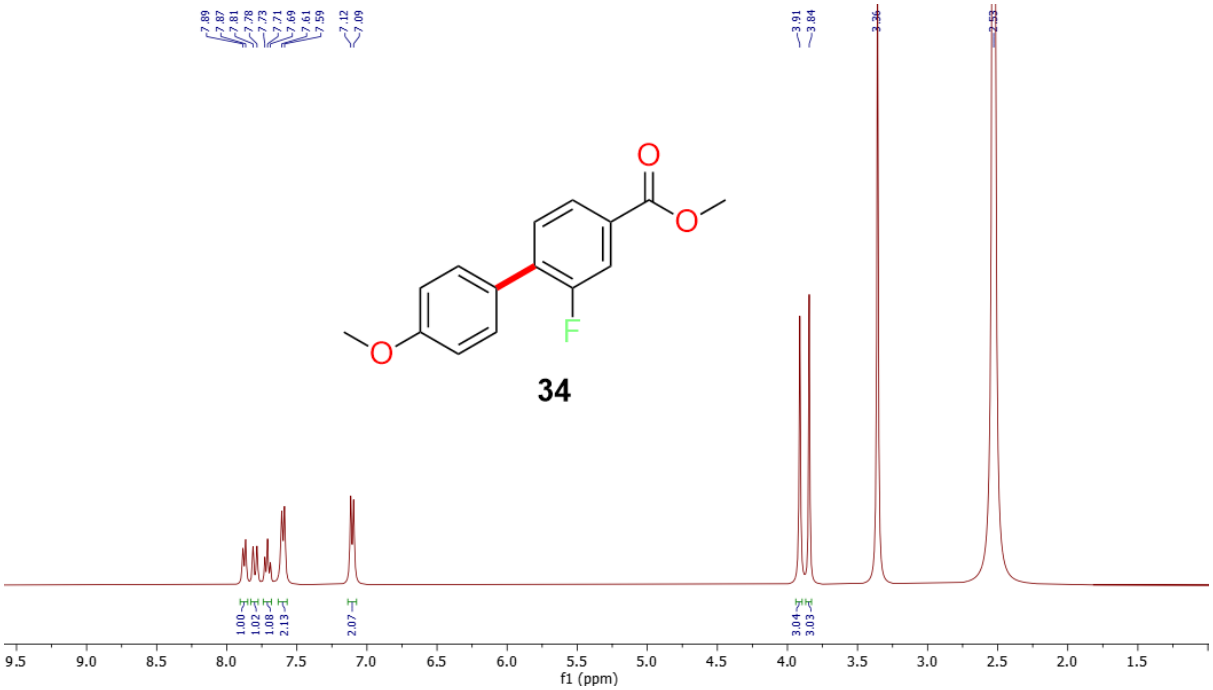


Figure S71: ^{1}H NMR Analysis of 34

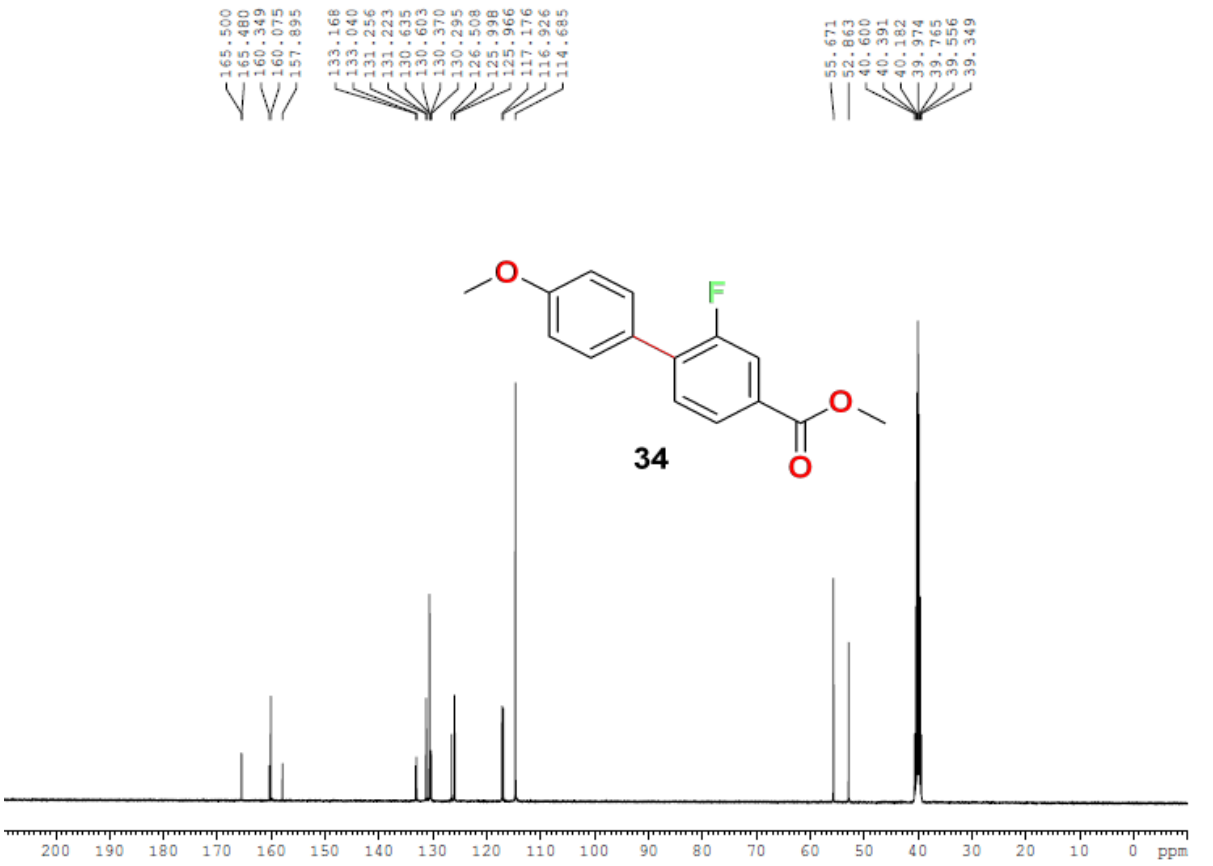


Figure S72: ^{13}C NMR Analysis of 34

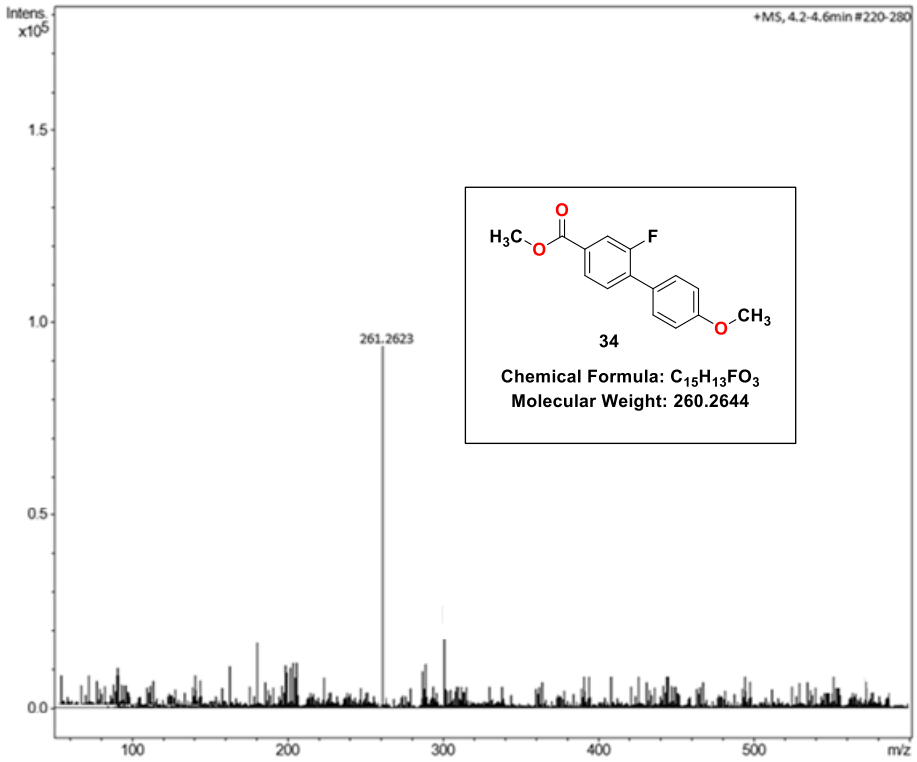


Figure S73: HRMS Analysis of 34

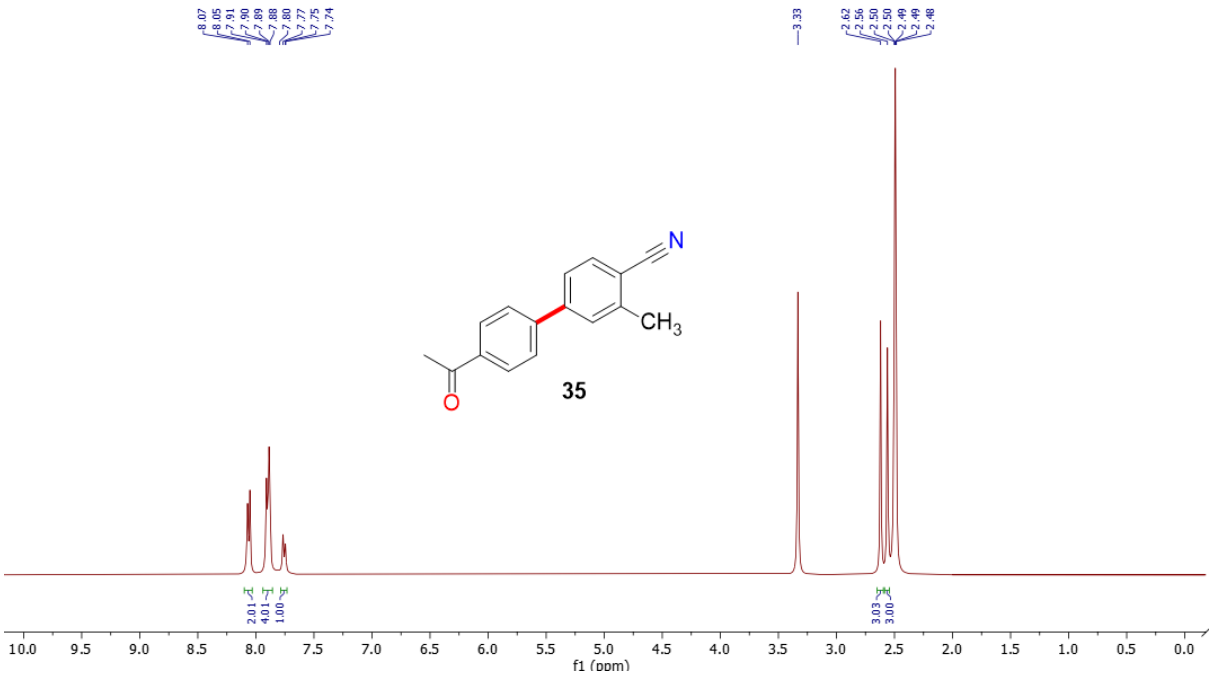


Figure S74: ^{1}H NMR Analysis of 35

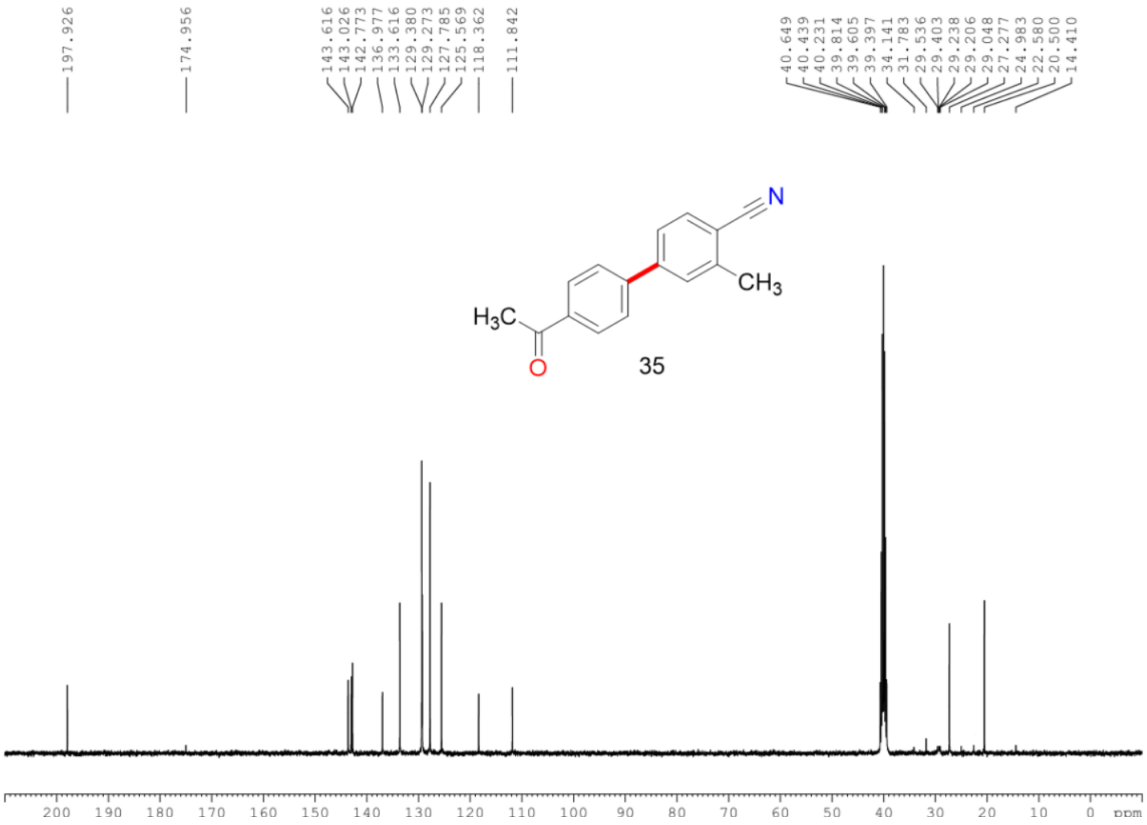


Figure S75: ^{13}C NMR Analysis of 35

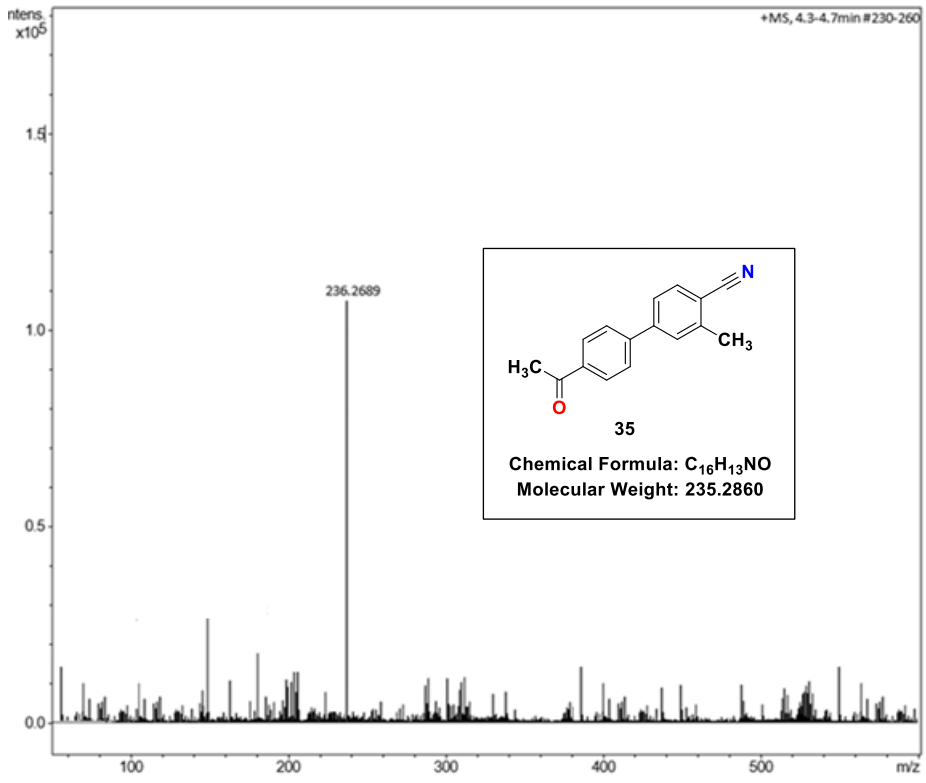


Figure S76: HRMS Analysis of 35

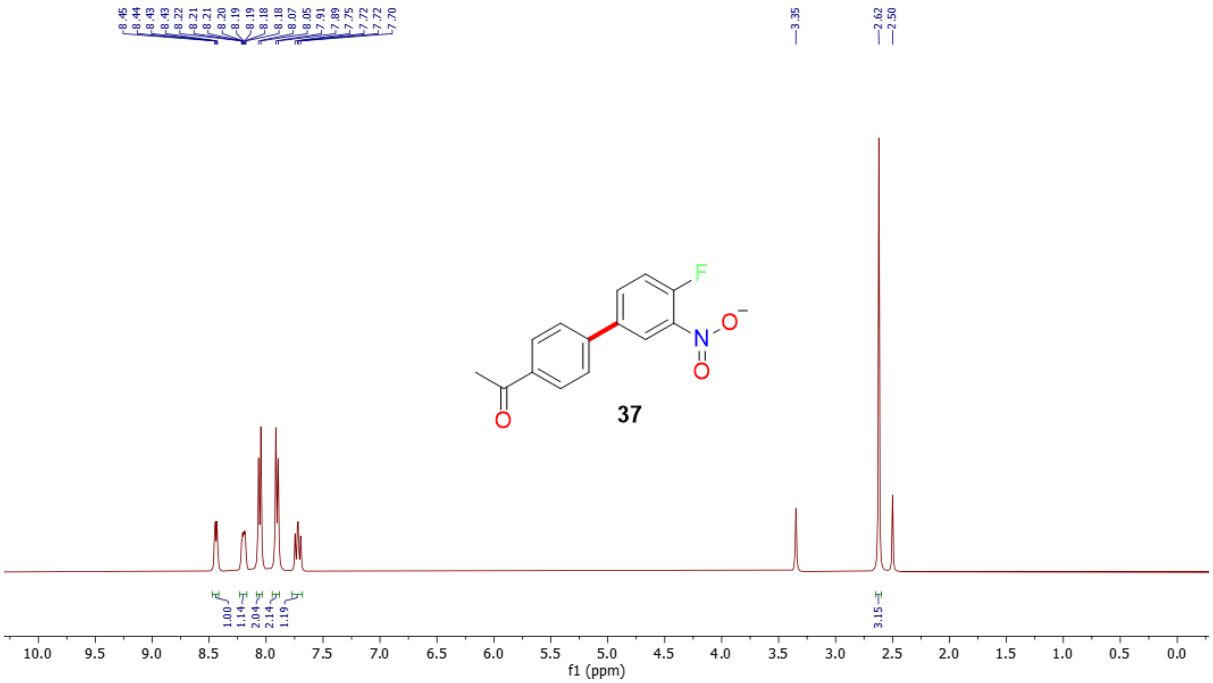


Figure S77: ^{1}H NMR Analysis of 37

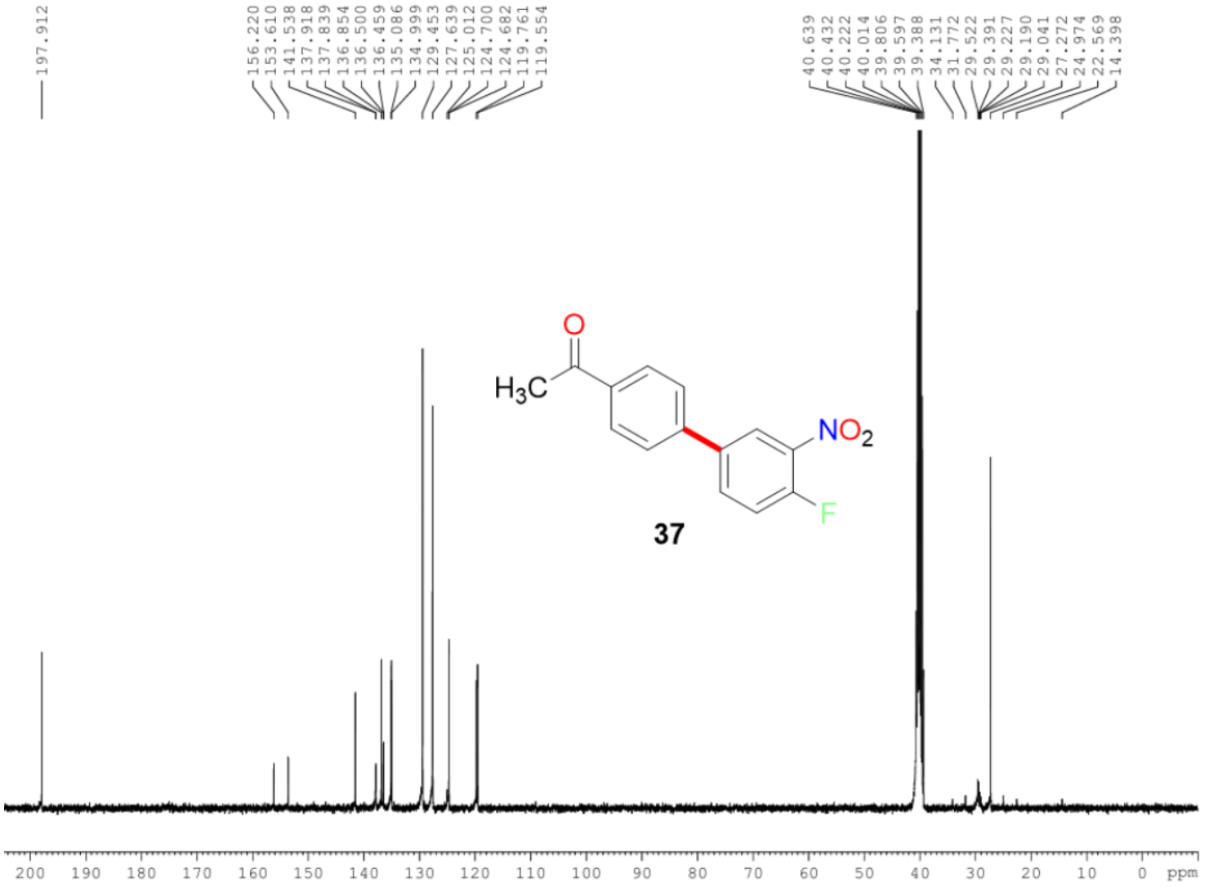


Figure S78: ^{13}C NMR Analysis of 37

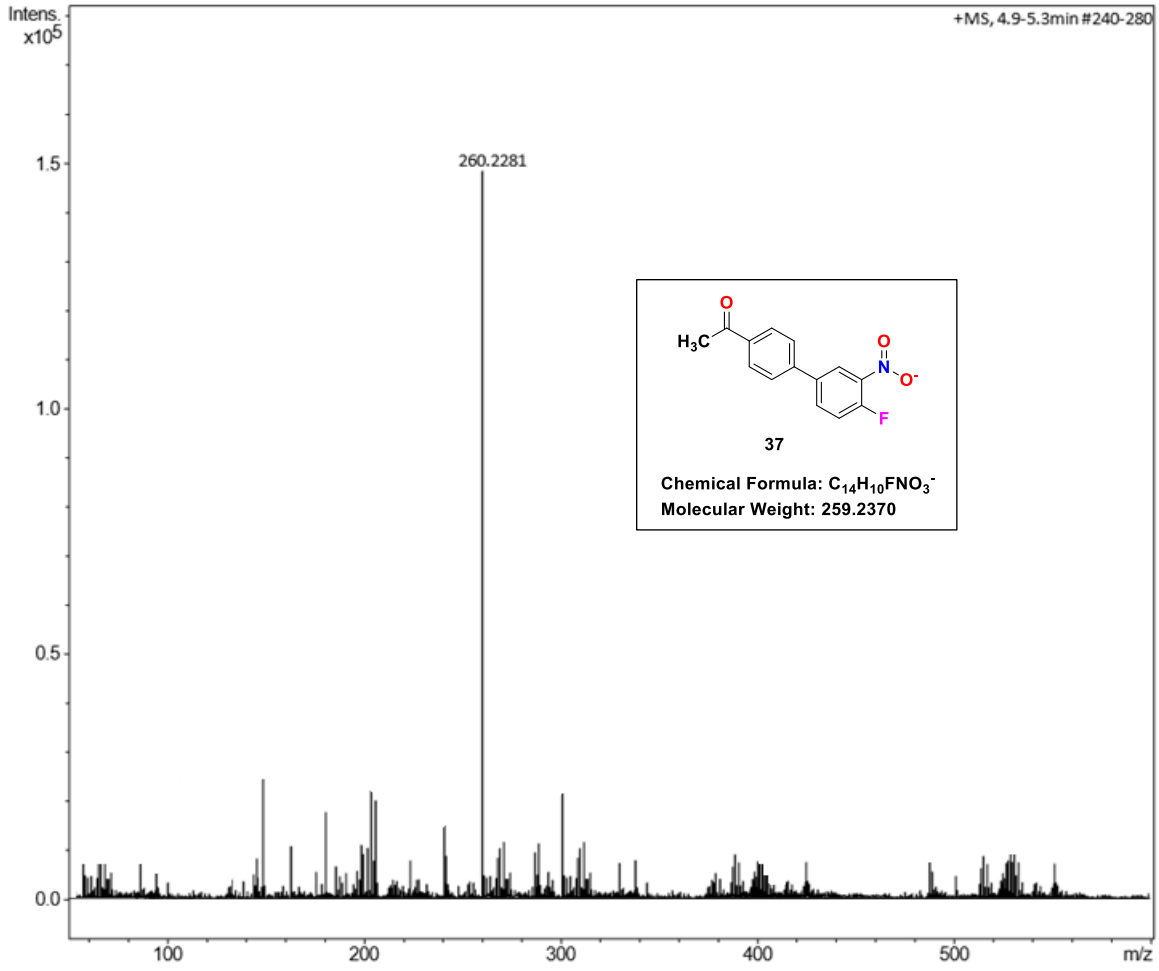


Figure S79: HRMS Analysis of 37

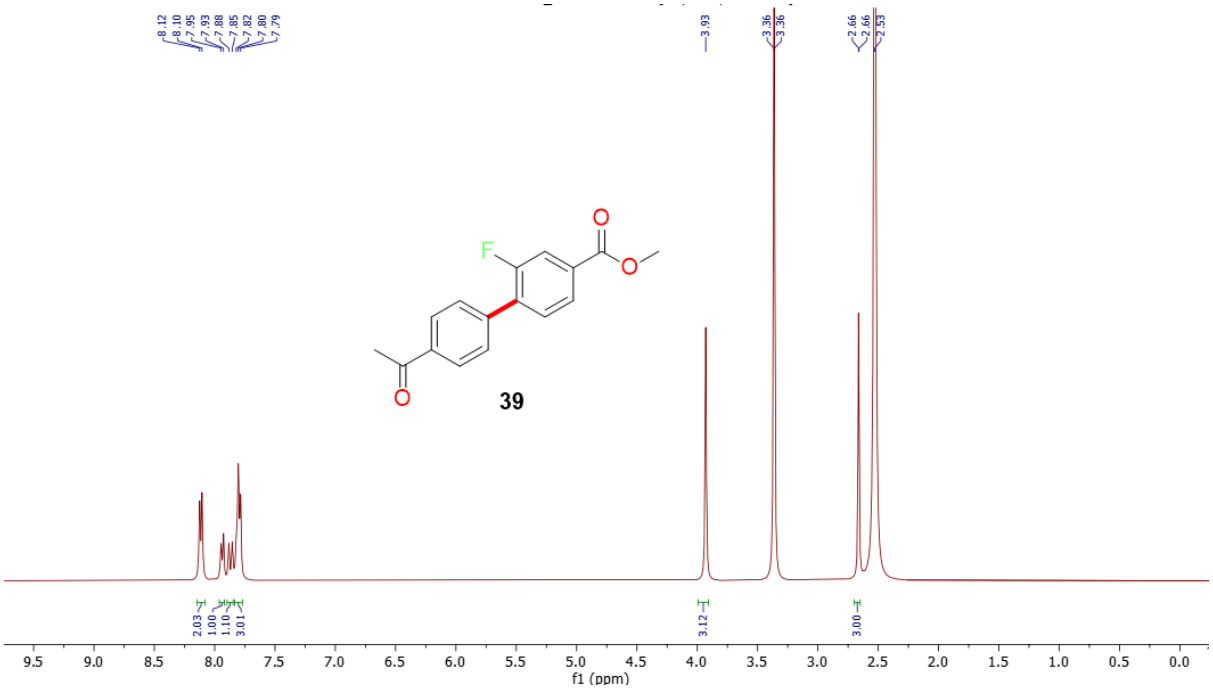


Figure S80: ^{1}H NMR Analysis of 39

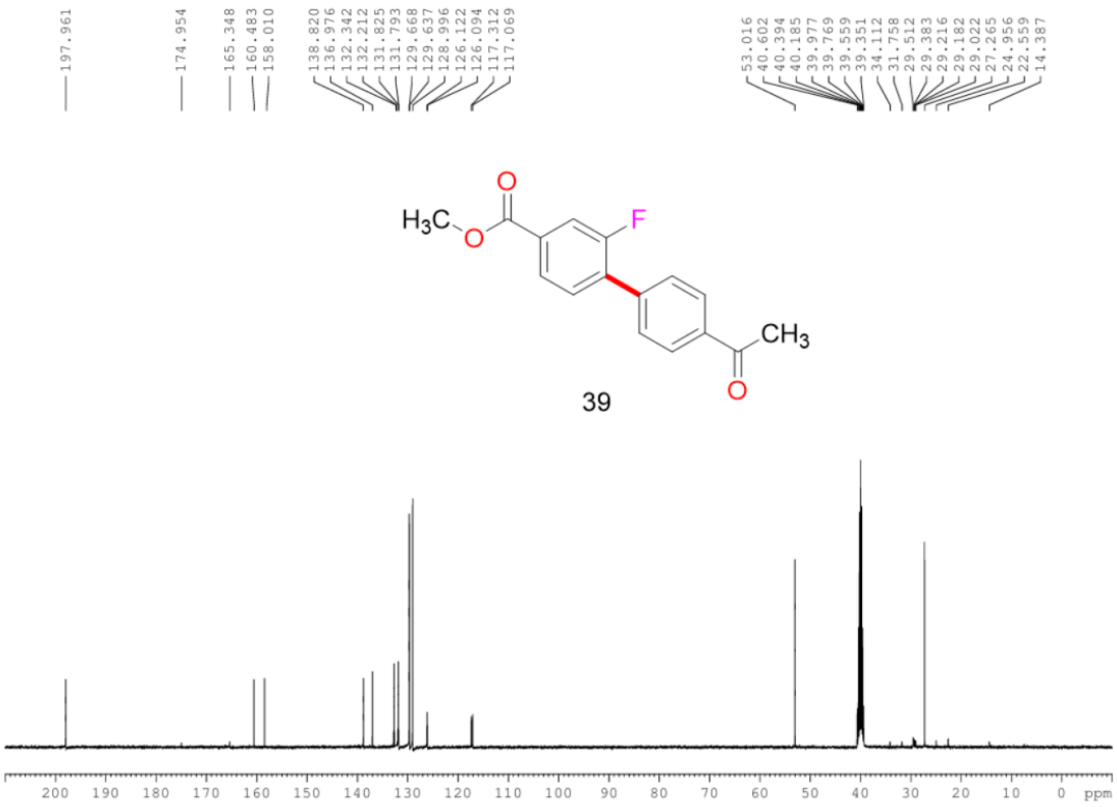


Figure S81: ^{13}C NMR Analysis of 39

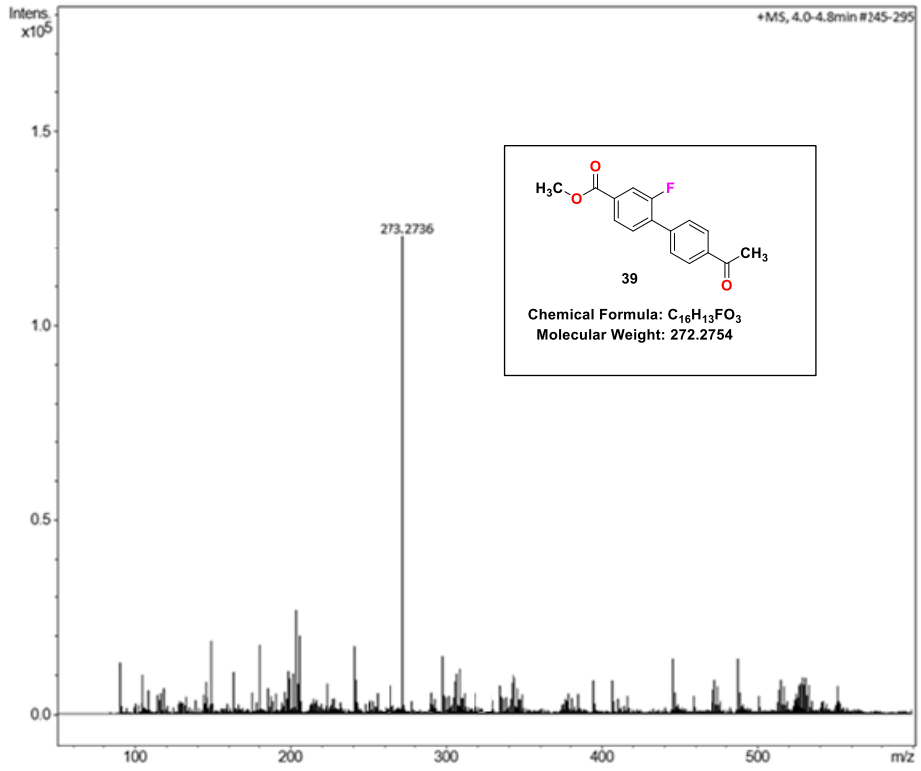


Figure S82: HRMS Analysis of 39

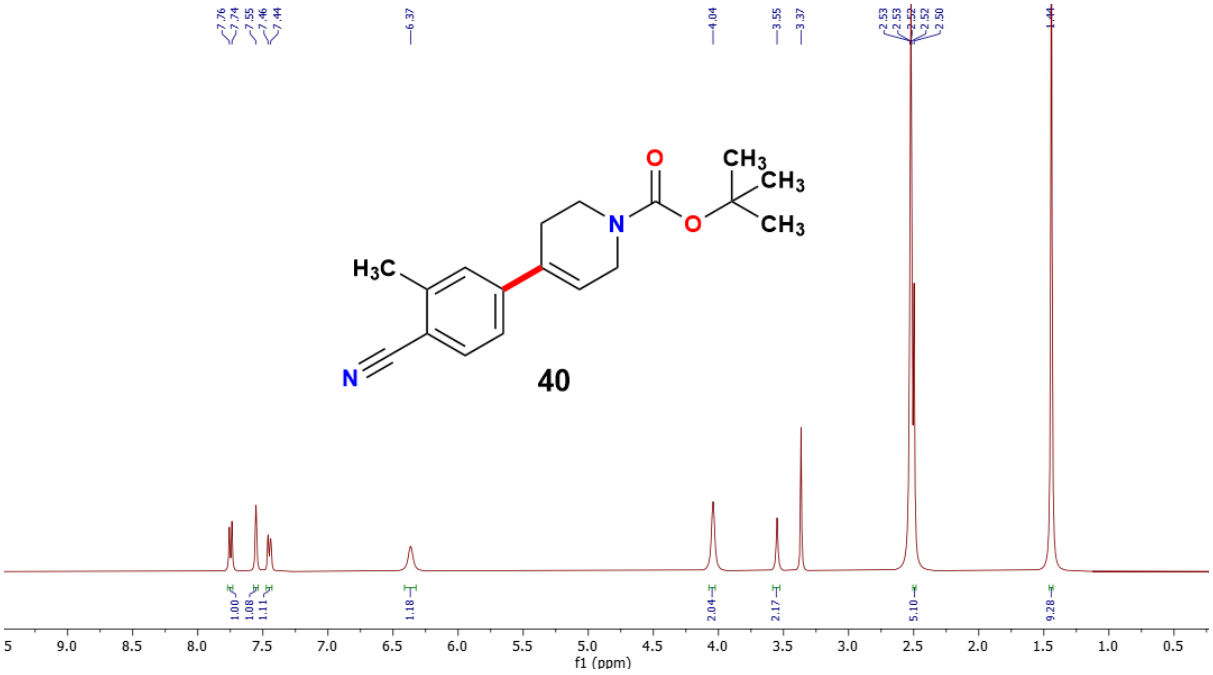


Figure S83: ^{1}H NMR (DMSO-D6) Analysis of 40

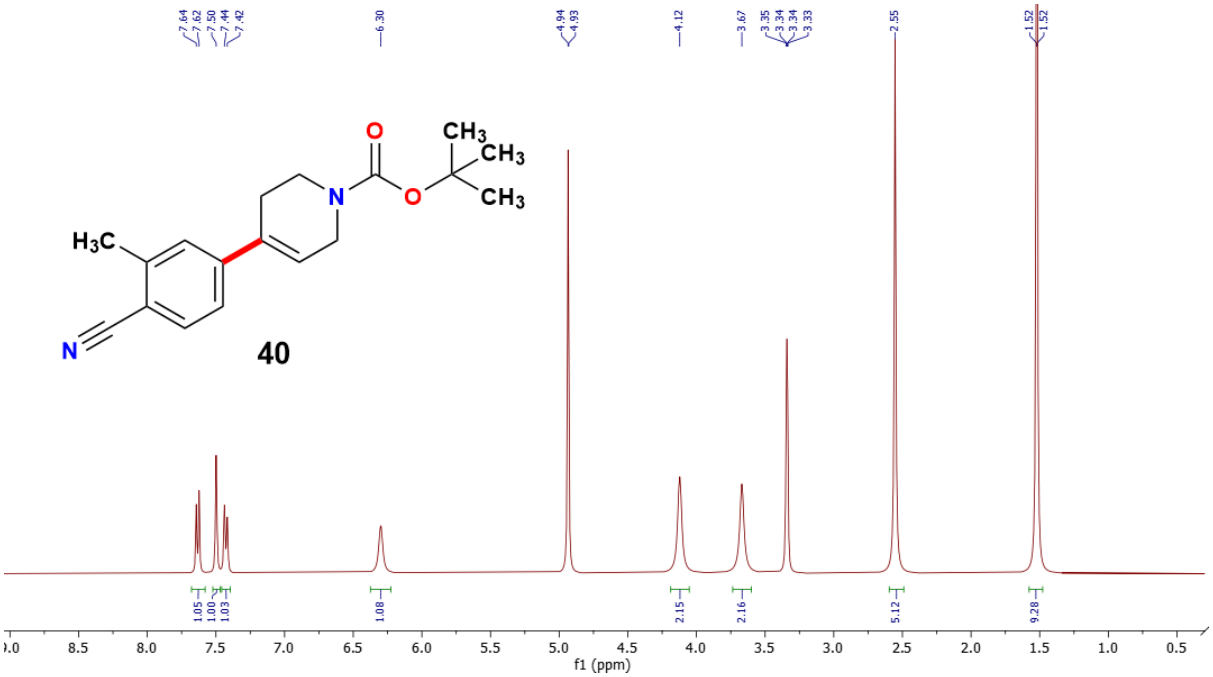


Figure S84: ^{1}H NMR (MeOD) Analysis of 40

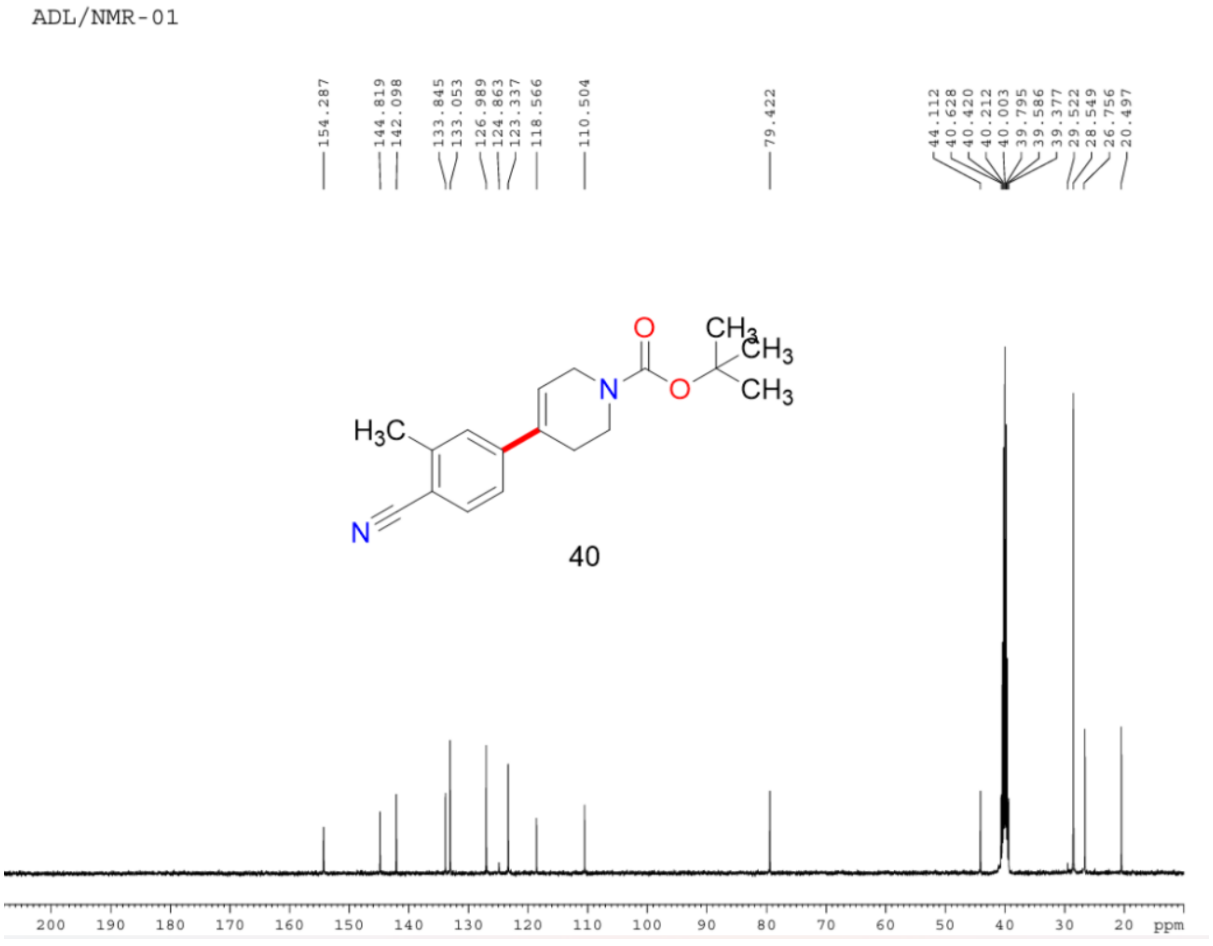


Figure S85: ^{13}C NMR Analysis of 40

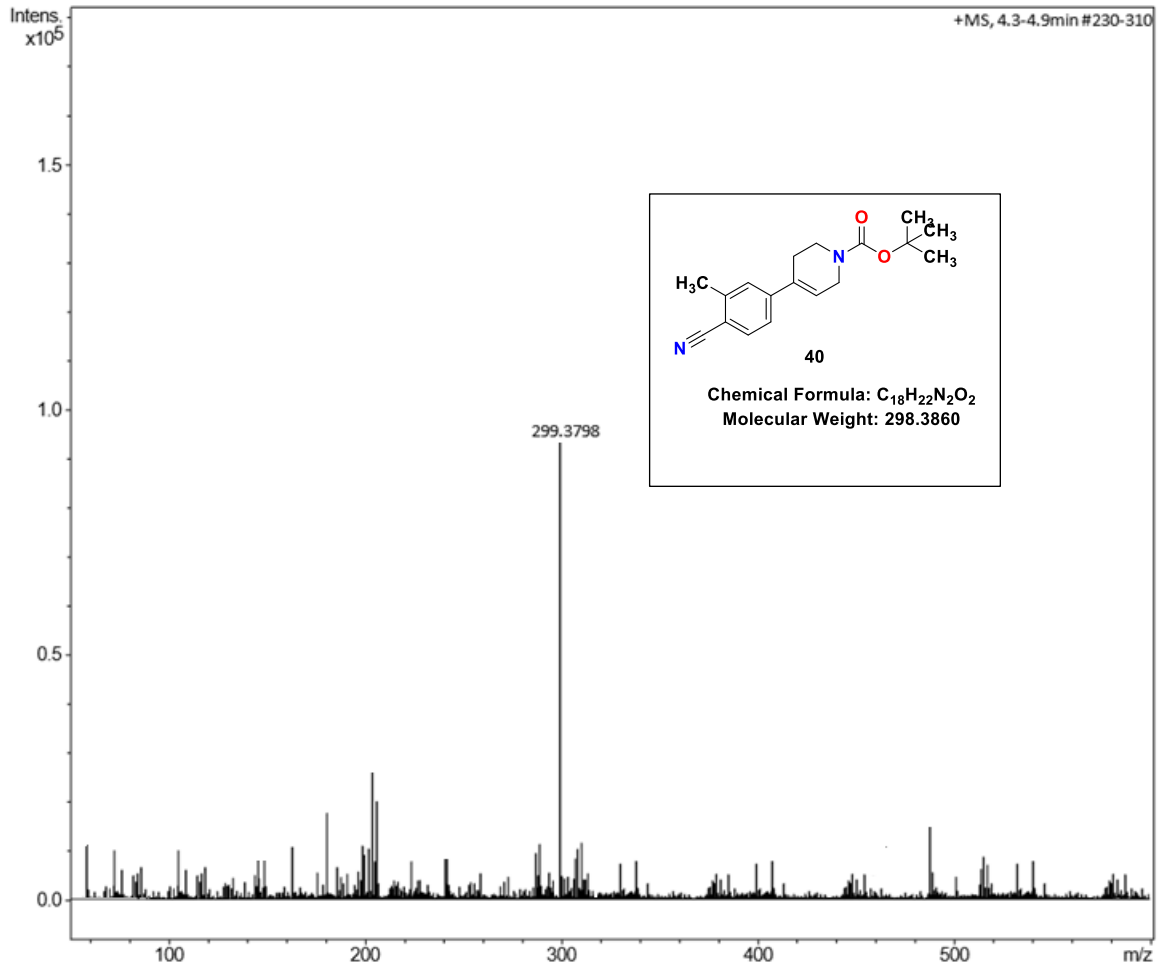


Figure S86: HRMS Analysis of 40

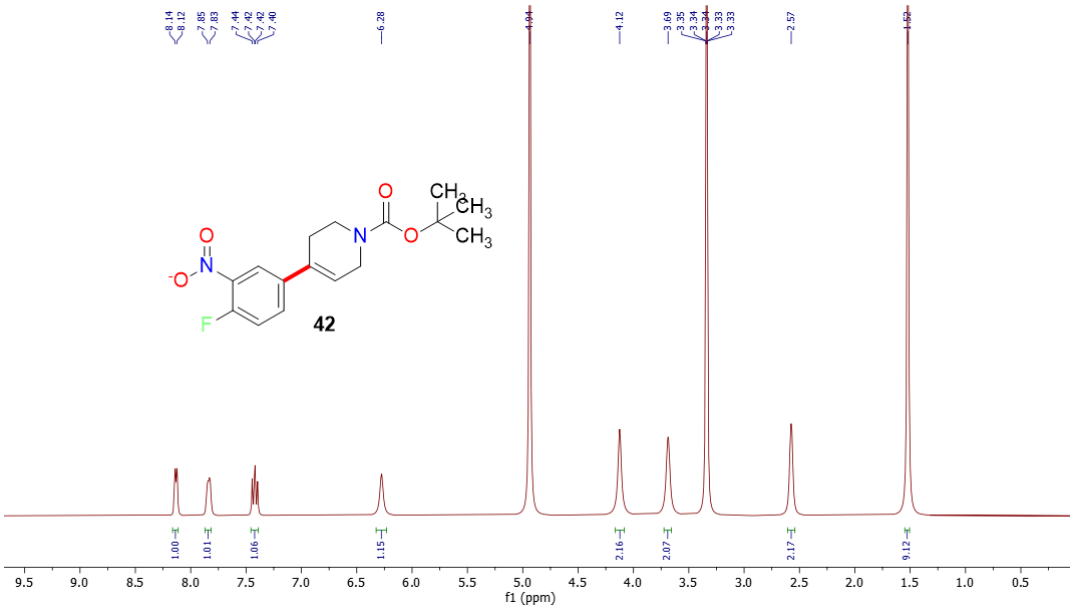


Figure S87: ^{1}H NMR Analysis of 40

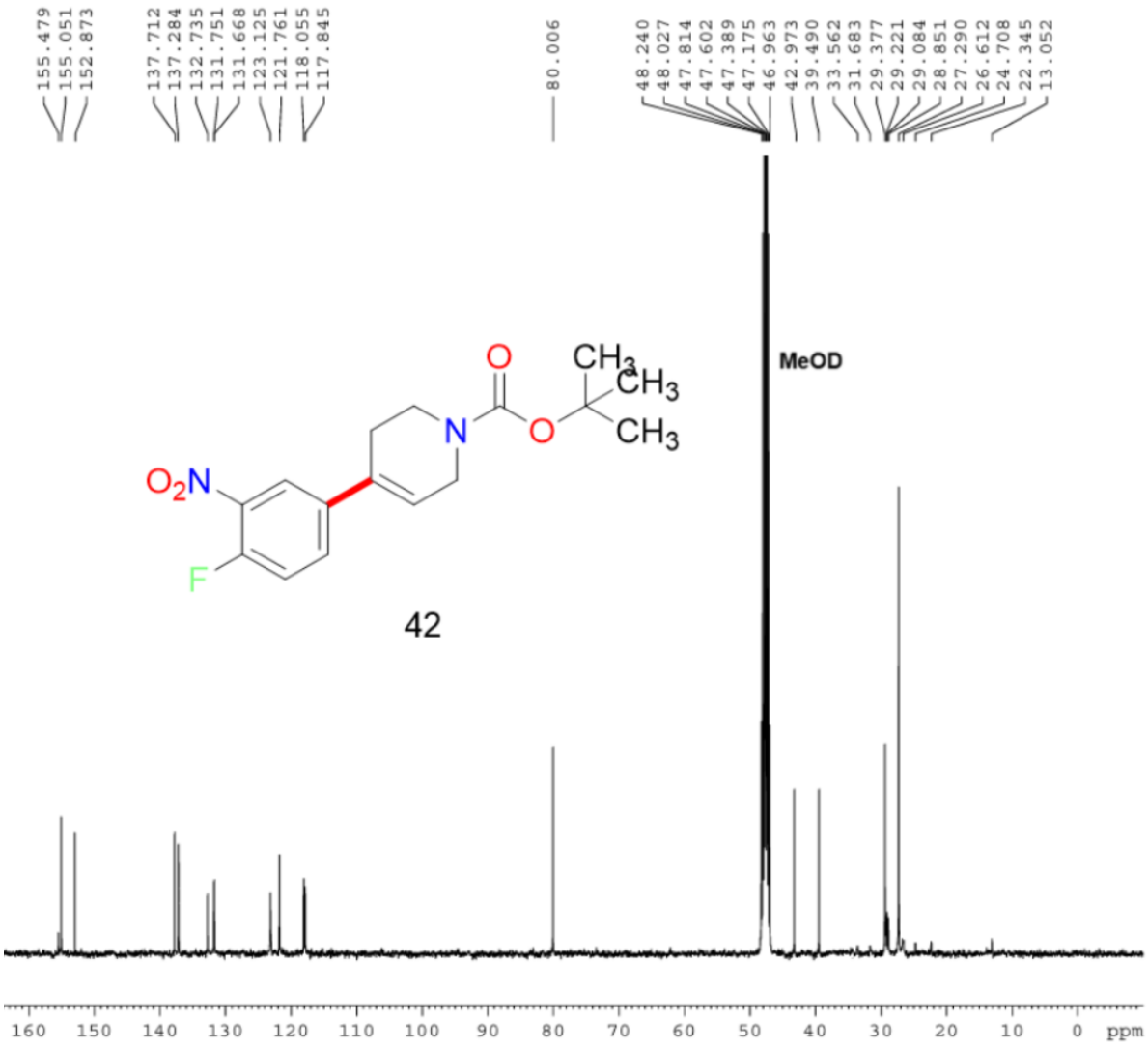


Figure S88: ^{13}C NMR Analysis of 42

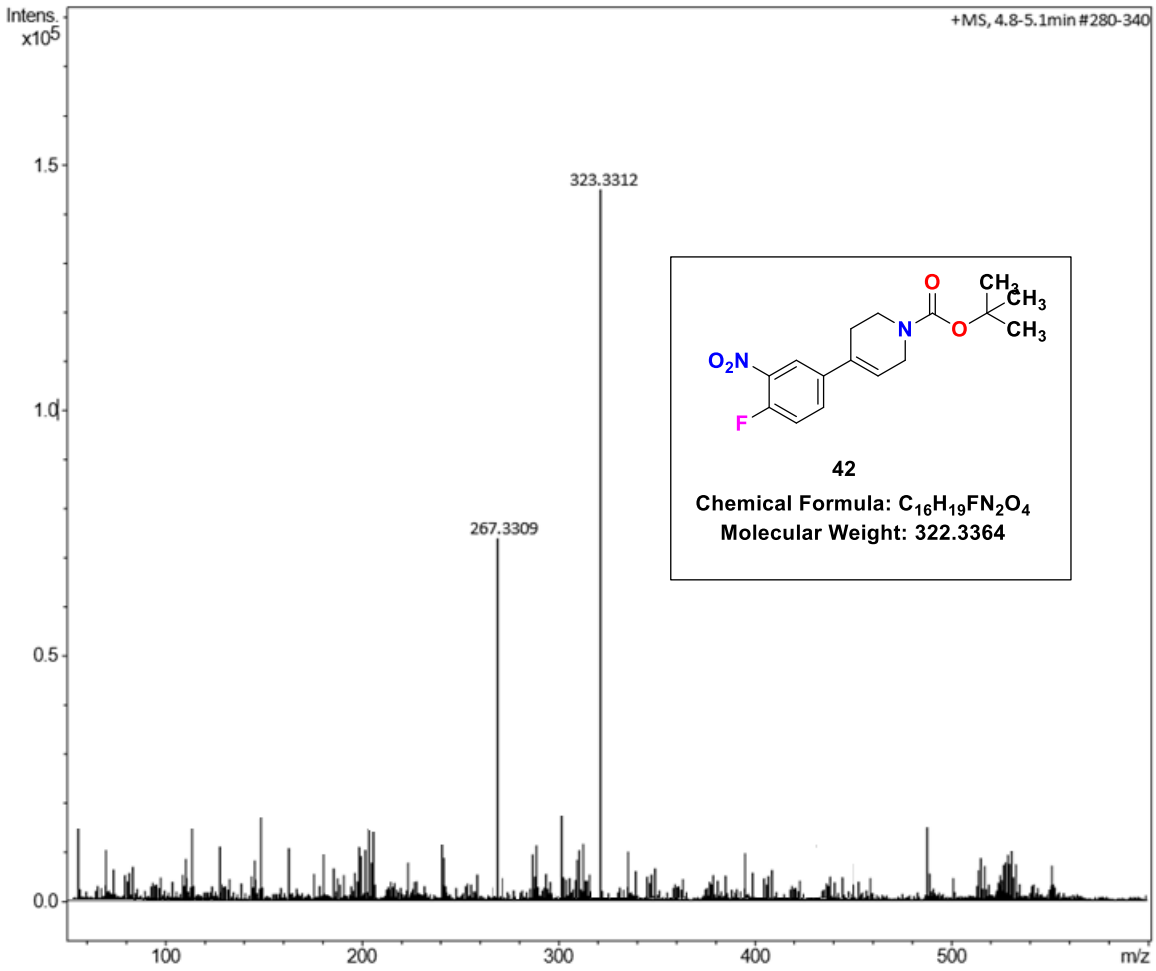


Figure S89: HRMS Analysis of 42

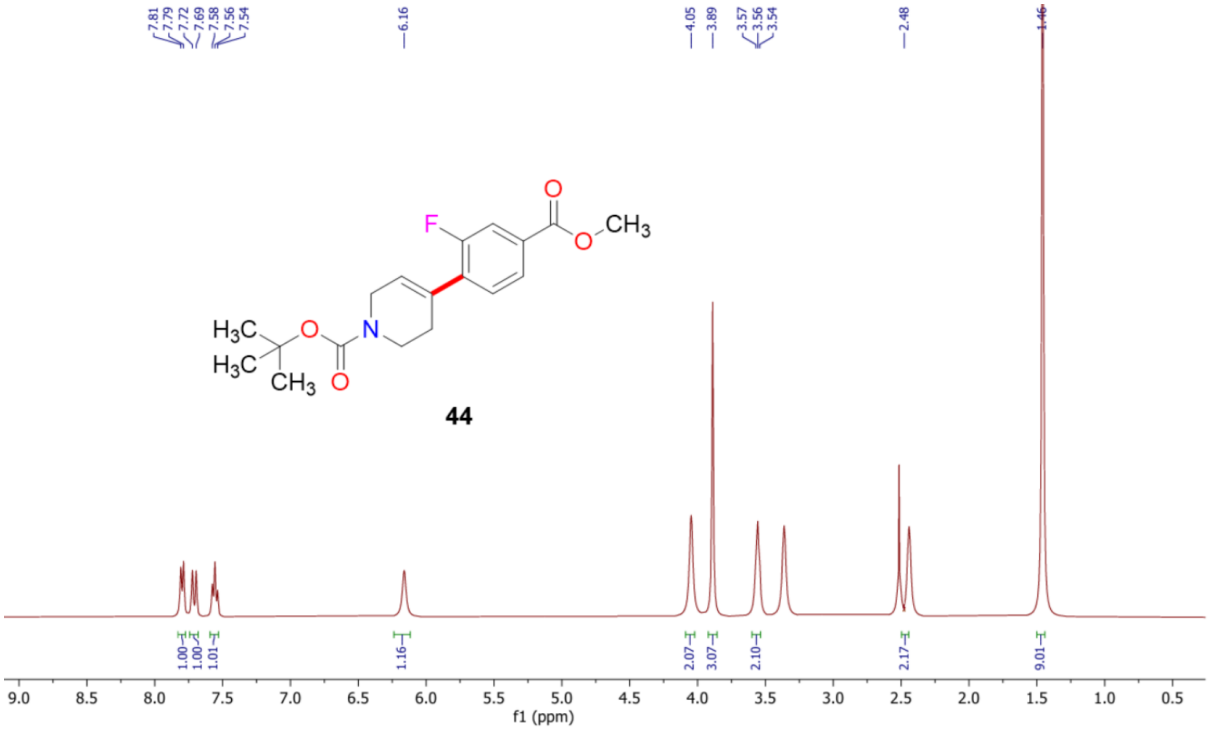


Figure S90: ^{1}H NMR Analysis of 44

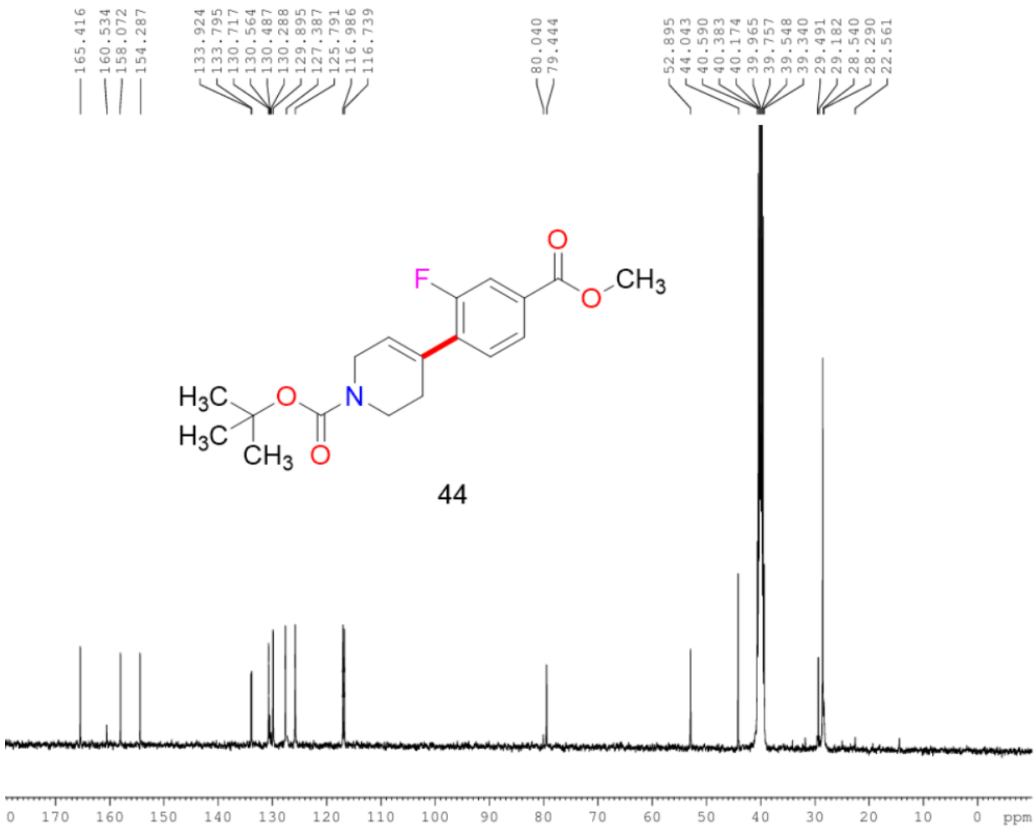


Figure S91: ^{13}C NMR Analysis of 44

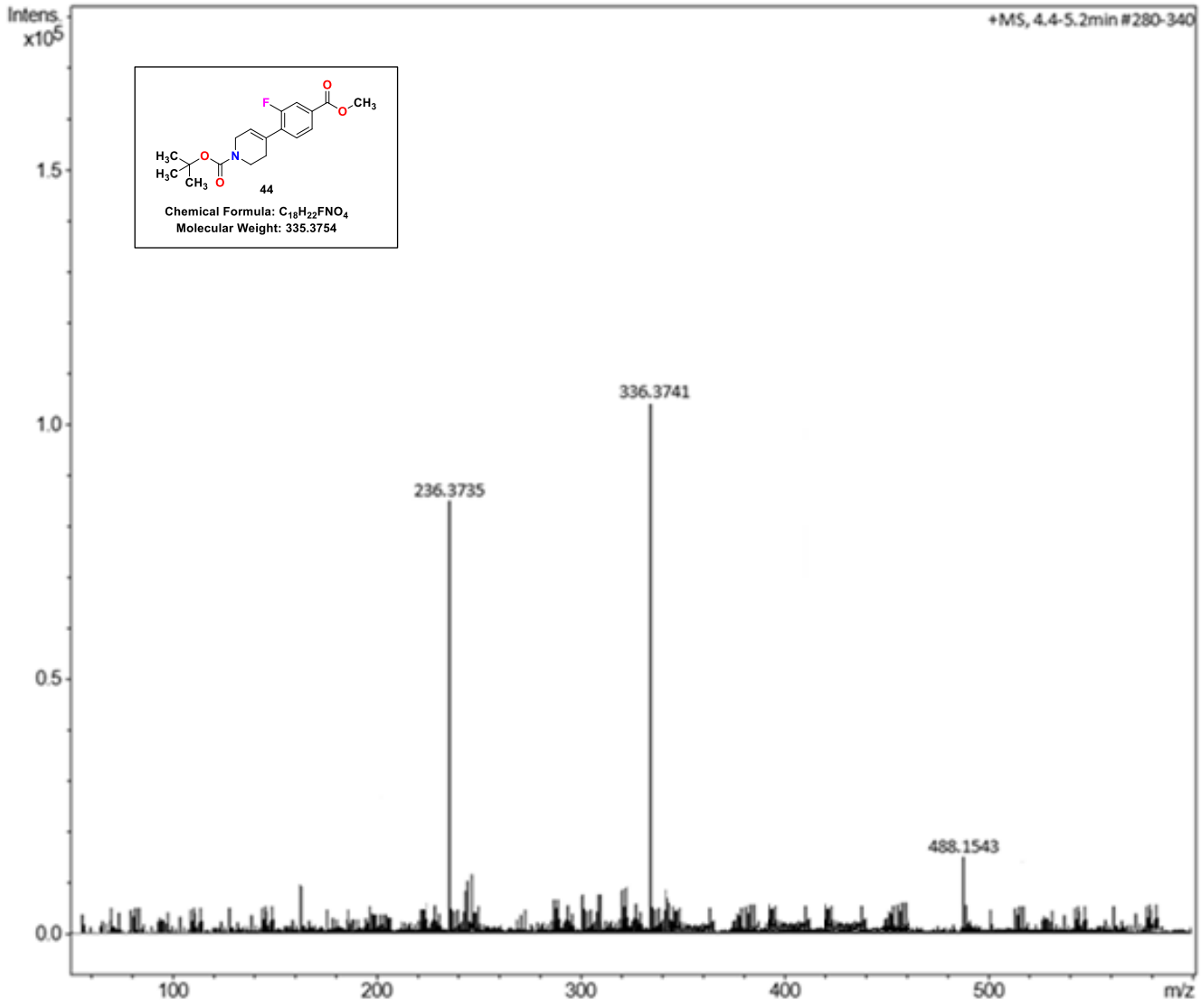


Figure S92: HRMS Analysis of 44

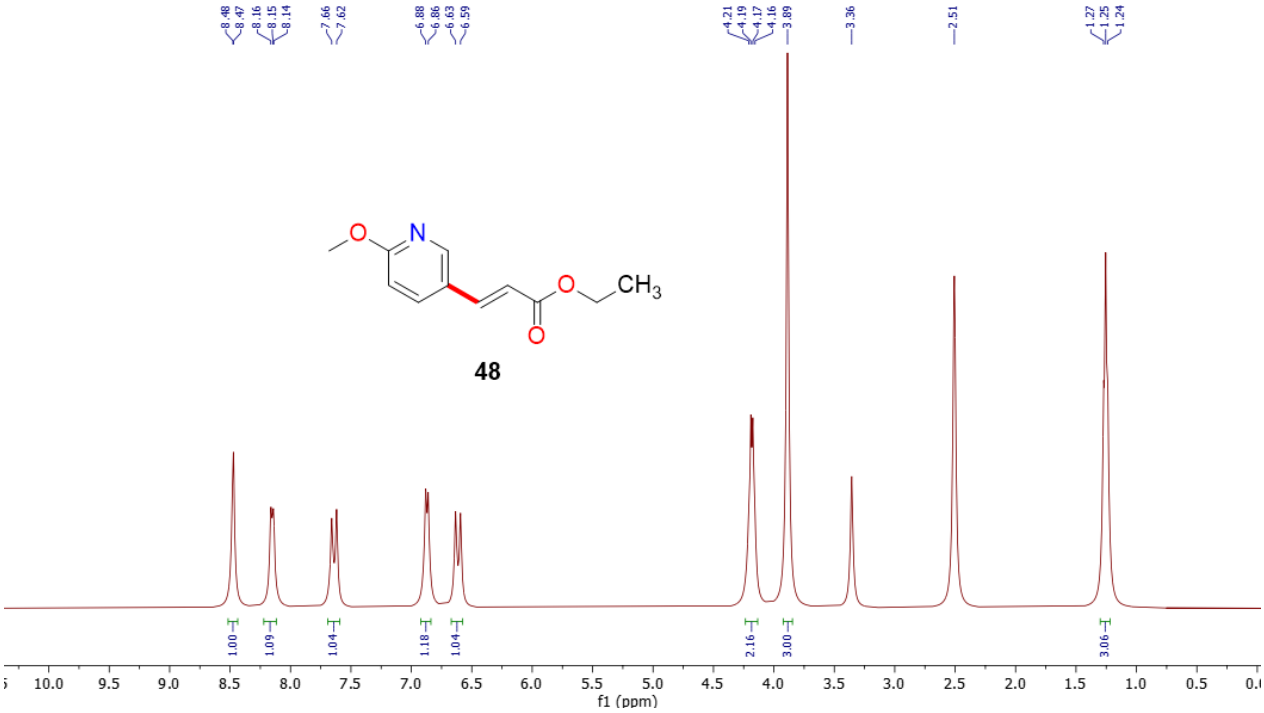


Figure S93: ^{1}H NMR Analysis of 48

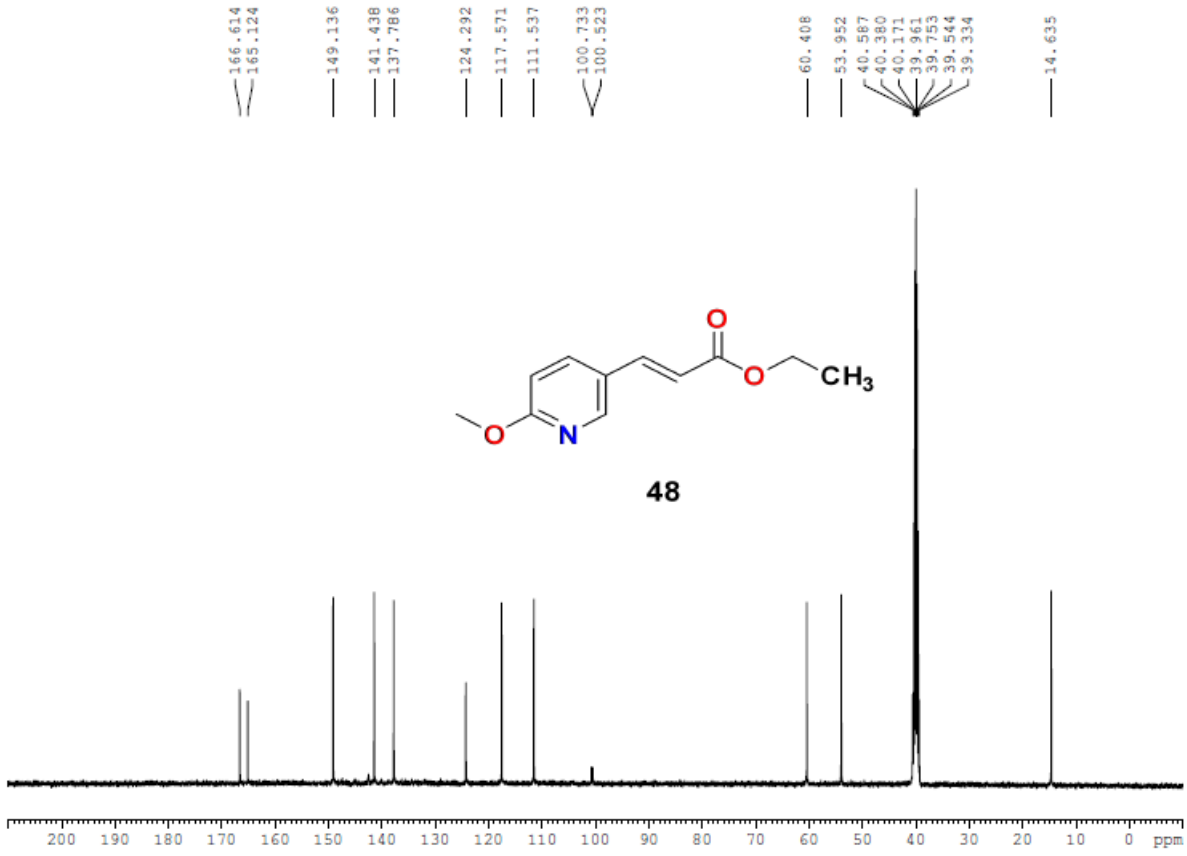


Figure S94: ^{13}C NMR Analysis of 48

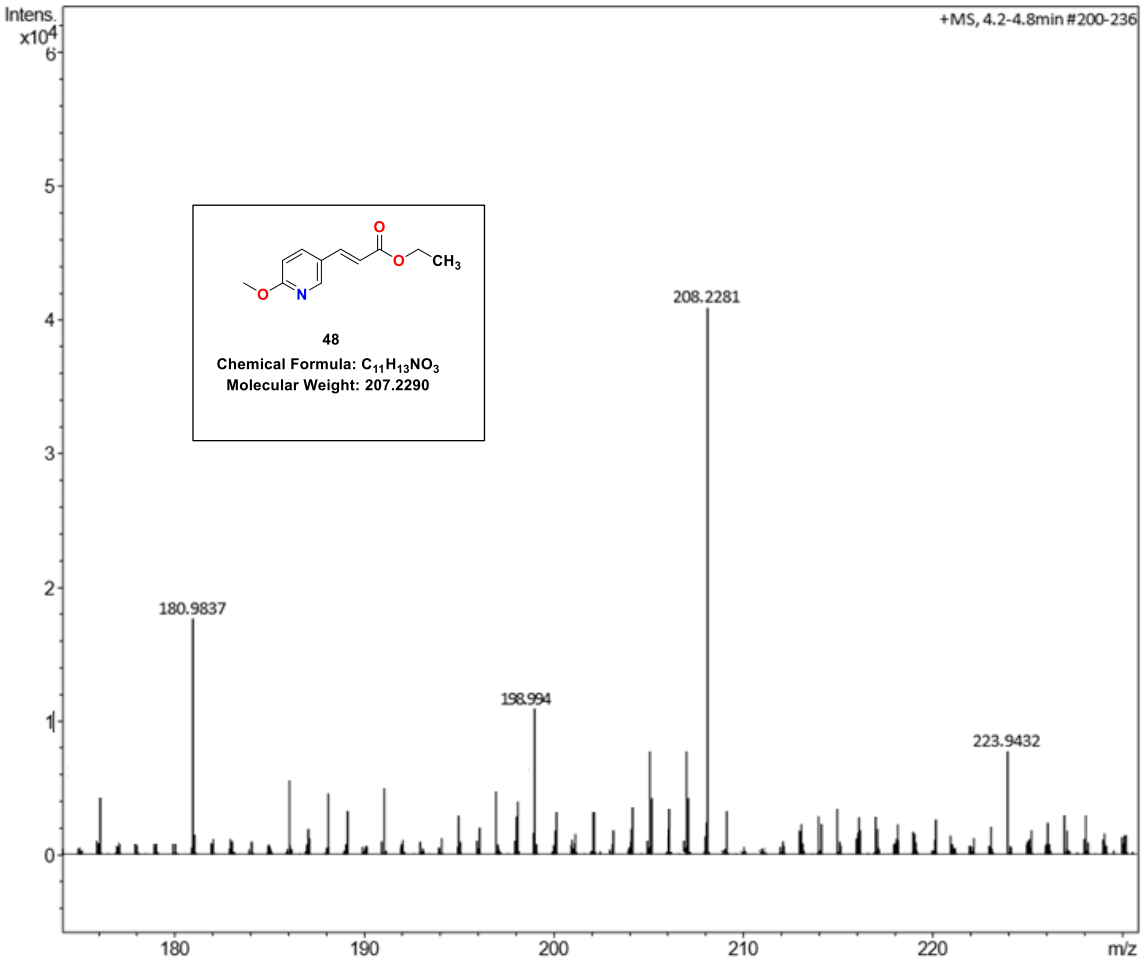
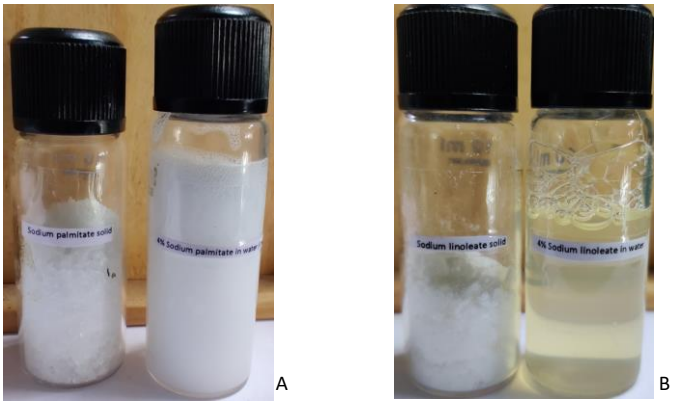


Figure S95: HRMS Analysis of 48



A B

Figure S96. (A) Sodium palmitate and its 4% aqueous solution; (B) Sodium Linoleate and its 4% aqueous solution.

As shown in figure-S1 the solid form of sodium palmitate and its 4% aqueous solution (A), sodium palmitate forms the emulsion in water used as it is for reaction while in sodium linoleate (B) is clearly soluble in water.

Comparison of Surfactant Pricing

The surfactants listed in the table vary significantly in price, which can be attributed to differences in their composition, purity, and applications. Below is a comparative analysis based on pricing:

1. **High-Cost Surfactants**
    - **TGPS-750M is the most expensive surfactant at $1316 per 100g,** indicating its specialized nature, likely due to its high efficiency in catalytic reactions.
    - TEAB is also expensive at $258 per 50 mL, suggesting it is a high-purity reagent used for specific reactions.
    - P105 ($80 per 5g) and PS-750M (₹380 per 5g) are also relatively costly, likely due to their specialized applications in catalysis.
2. **Moderately Priced Surfactants**
    - PTS ($76 per 10 mL) and Brij L23 ($77 per 100 mL) fall in the mid-range pricing, suggesting they are used for specialized applications but are more accessible than high-cost surfactants.
    - CTAB ($113 per 100g) and TTAB ($164 per 100g), which are cationic surfactants, are moderately priced, possibly due to their widespread use in various industrial and biochemical applications.
    - SDS ($132 per 100g) is also in this range, reflecting its extensive utility in biochemical research and catalysis.

- Tween 80 (₹70 per 500 mL) and Span-80 ($44 per 250 mL) are also relatively inexpensive, making them widely used in emulsification and industrial applications.
- TX-100 ($56 per 100 mL) and NP-9 ($34 per 100 mL) are also on the lower end, indicating their accessibility for large-scale applications.
-

3. Low-Cost Surfactants

- **Linoleic Acid Sodium Salt (~$1 per kg) and Sodium Palmitate ($9 per kg)** are the most affordable surfactants, likely due to their natural origin and ease of synthesis.

Table S4. Pricing of Surfactant for Comparison

Sr No.	Surfactant	Price
1	• Product Name: TGPS-750M (2% water) • 1309573-60-1	• $1316 /100g
2	• Product Name: Sodium Palmitate • CAS: 408-35-5	• $9/Kg
3	• Product Name: LINOLEIC ACID SODIUM SALT • CAS: 822-17-3	• ~$1/Kg
4	• Product Name: PTS (15% in water) • CAS: 263015-34-5	• $76/10 mL
5	• Product Name: CTAB • CAS: 57-09-0	• $113/100g
6	• Product Name: SDS • CAS: 151-21-3	• $132/100g
7	• Product name: NP-9 • CAS: 127087-87-0	• $34/100 mL
8	• Product name: P105 • CAS: 9003-11-6	• $80/5g
9	• Product name: TX-100 • CAS: 9036-19-5	• $56/100 mL
10	• Product Name: Span-80 • CAS: 1338-43-8	• $44/250 mL
11	• Product Name: TEAB •	• $258/50 ML
12	• Product Name: TTAB • CAS: 1119-97-7	• $164/100g
13	• Product Name: Brij L23 (30% in water) • CAS: 9002-92-0	• $77/100 mL
14	• Product Name: Tween 80 • CAS: 9005-65-6	• ₹70/500 mL
15	• Product Name: PS-750M • CAS: 2135447-74-2	• ₹380/5g

