

Supporting Information

α -Alkylation of Arylacetonitriles with Primary Alcohols Catalyzed by Backbone Modified N-Heterocyclic Carbene Iridium(I) Complexes

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1. Traces of ^1H and ^{13}C NMR spectra and HRMS analysis of complexes 1d-f

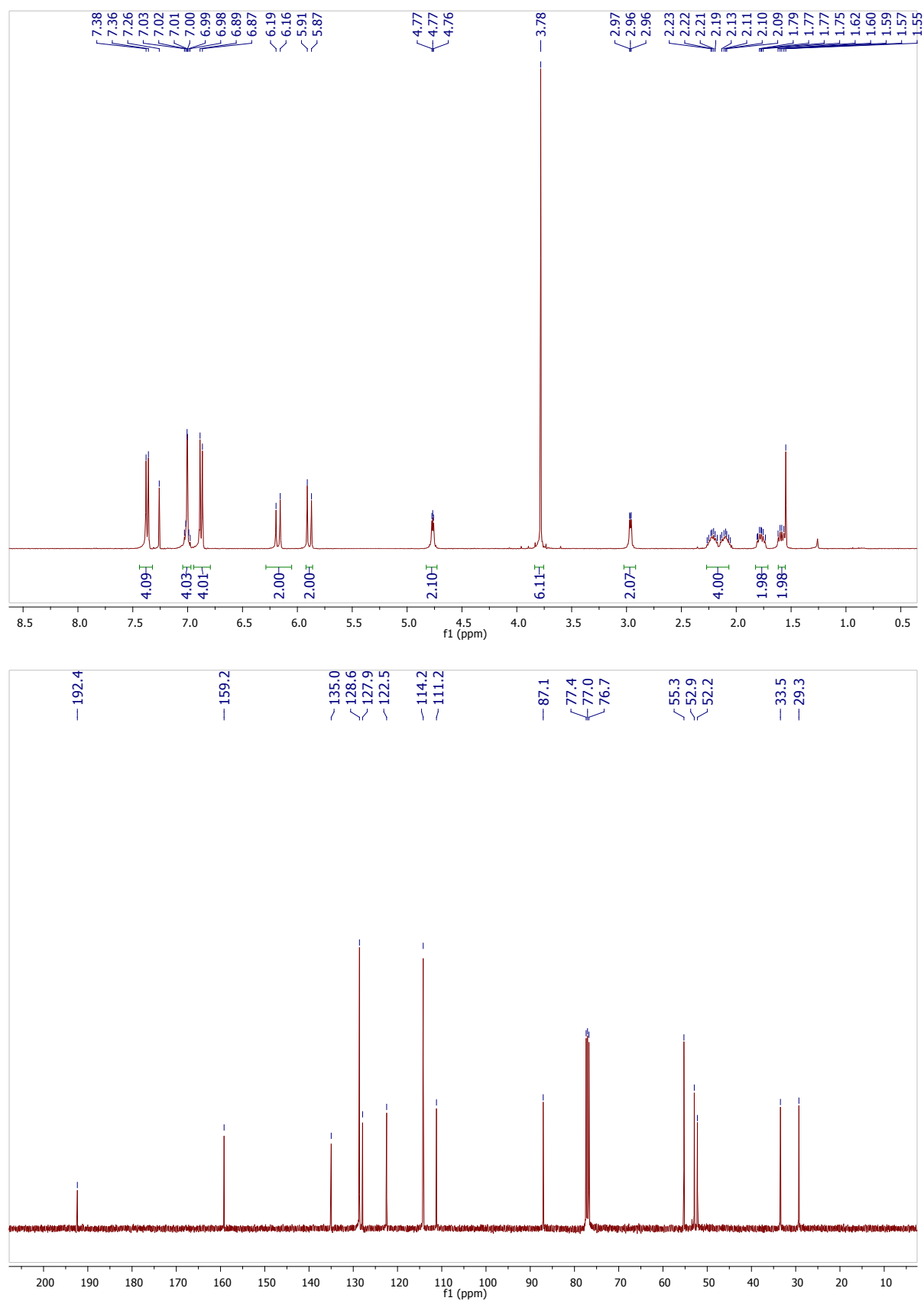


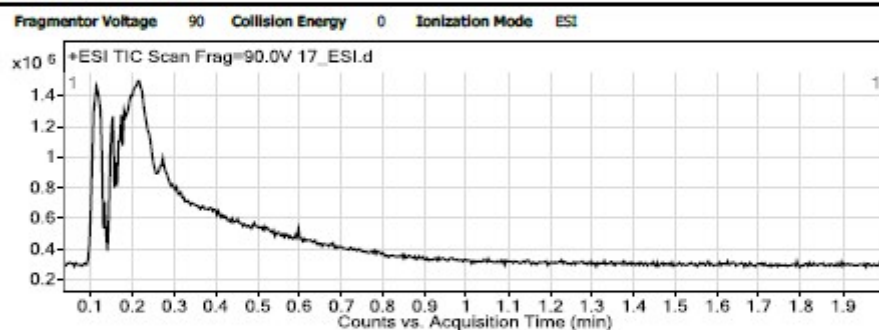
Figure S1. ^1H and ^{13}C spectra of compound 1d.

Qualitative Analysis Report

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| | | | |
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User Chromatograms



User Spectra

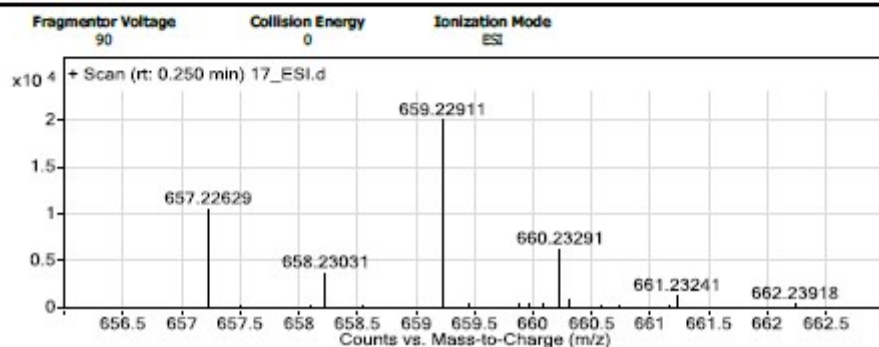


Figure S2. HRMS analysis report of compound **1d**.

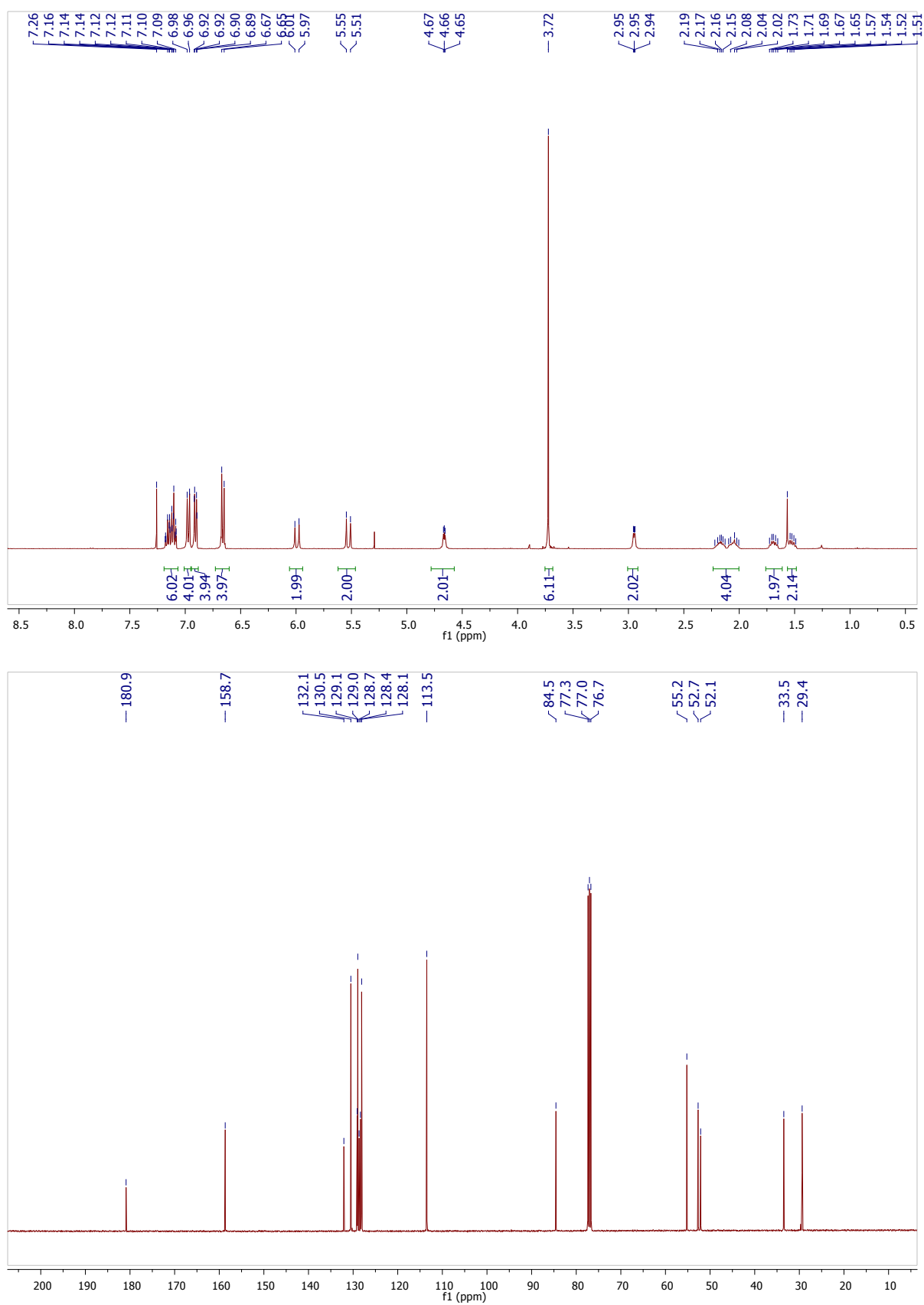


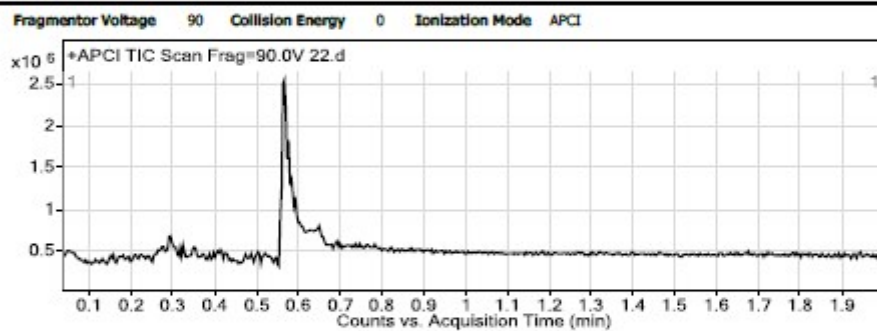
Figure S3. ^1H and ^{13}C NMR spectra of compound 1e.

Qualitative Analysis Report

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User Chromatograms



User Spectra

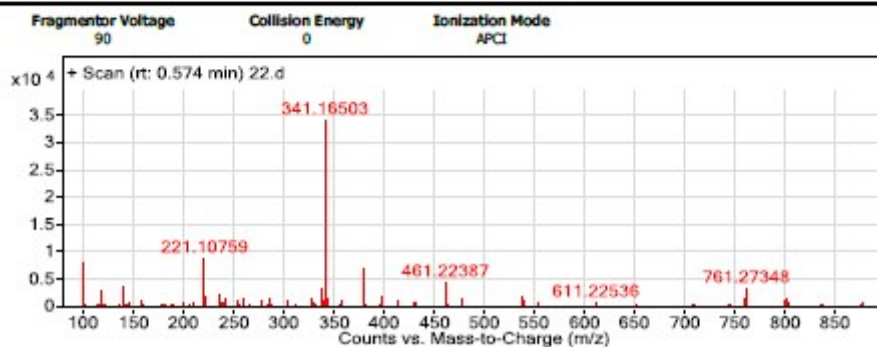


Figure S4. HRMS analysis report of compound **1e**.

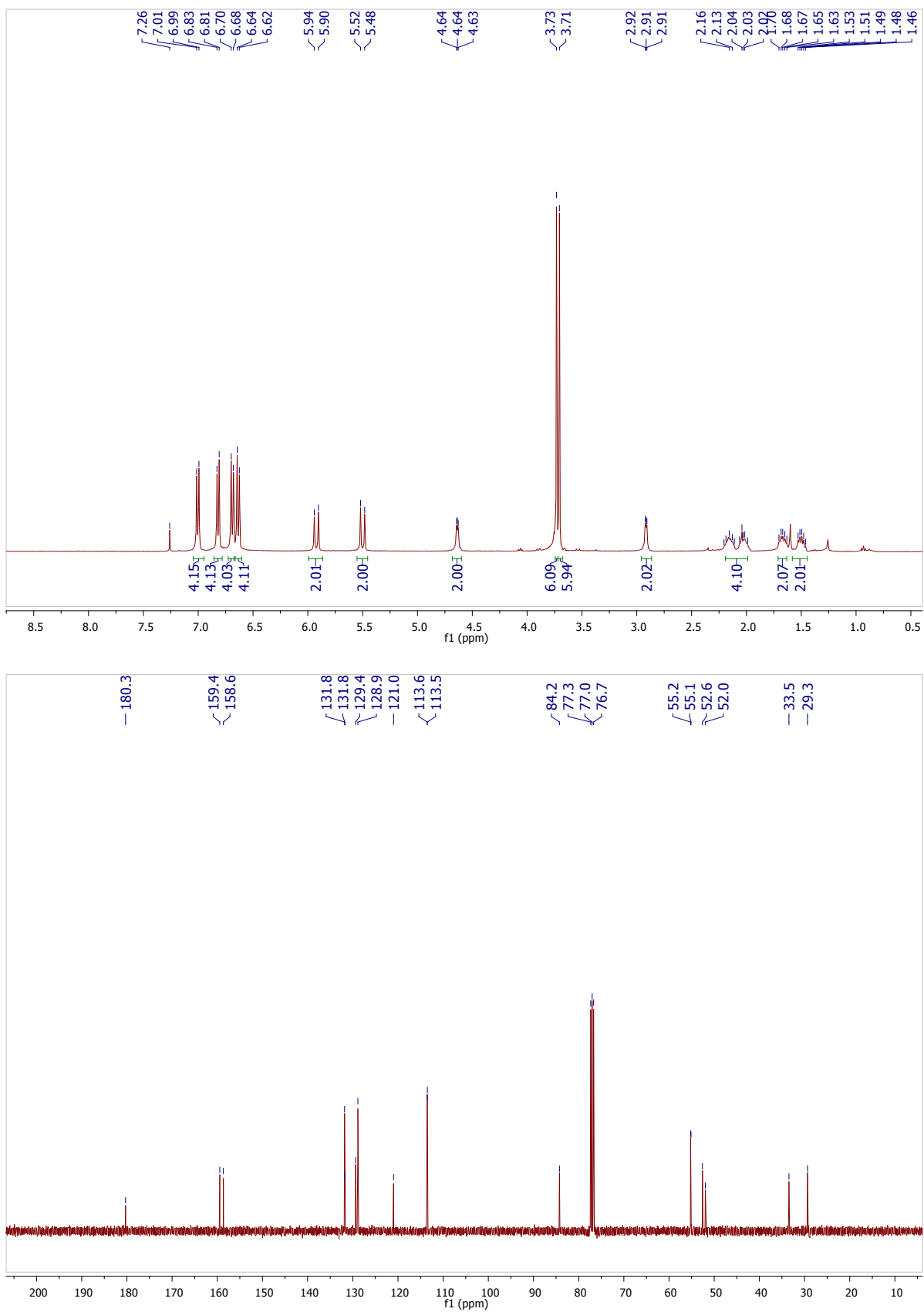


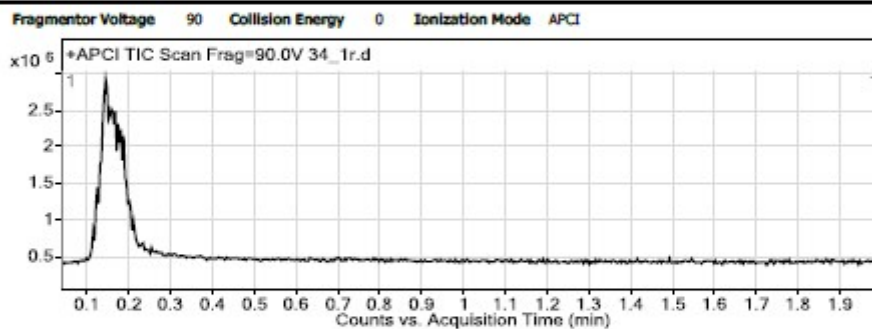
Figure S5. ^1H and ^{13}C NMR spectra of compound 1f.

Qualitative Analysis Report

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User Chromatograms



User Spectra

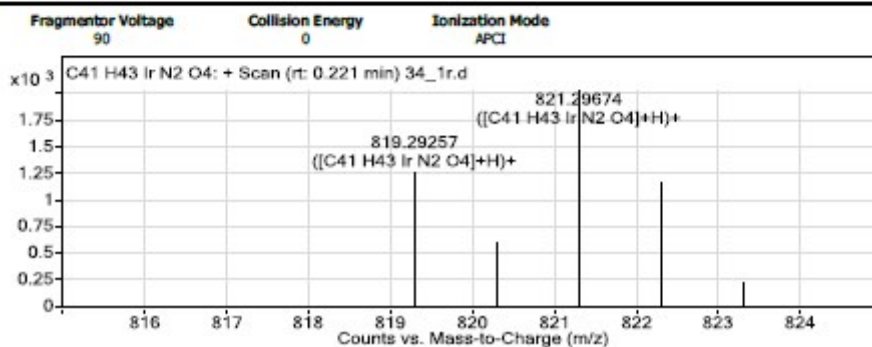


Figure S6. HRMS analysis report of compound **1f**.

2. Traces of ^1H and ^{13}C NMR spectra of products 4a-p / 6a-e and HRMS analysis of products 4m,n

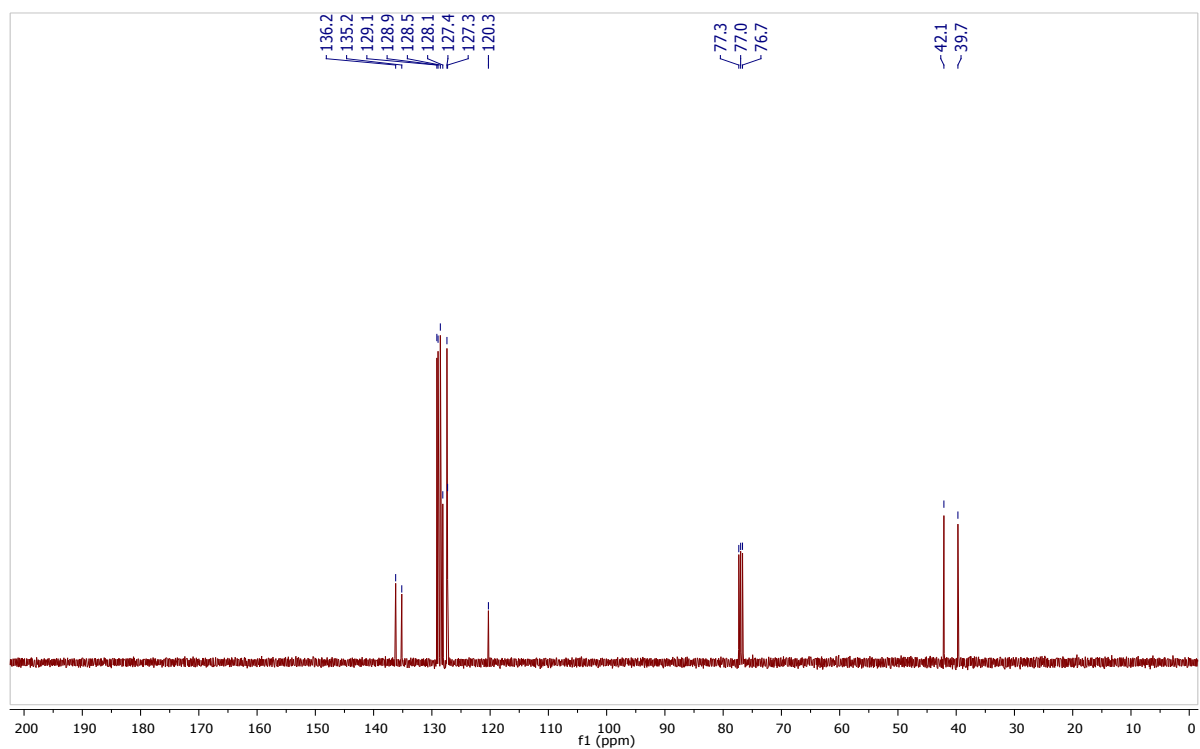
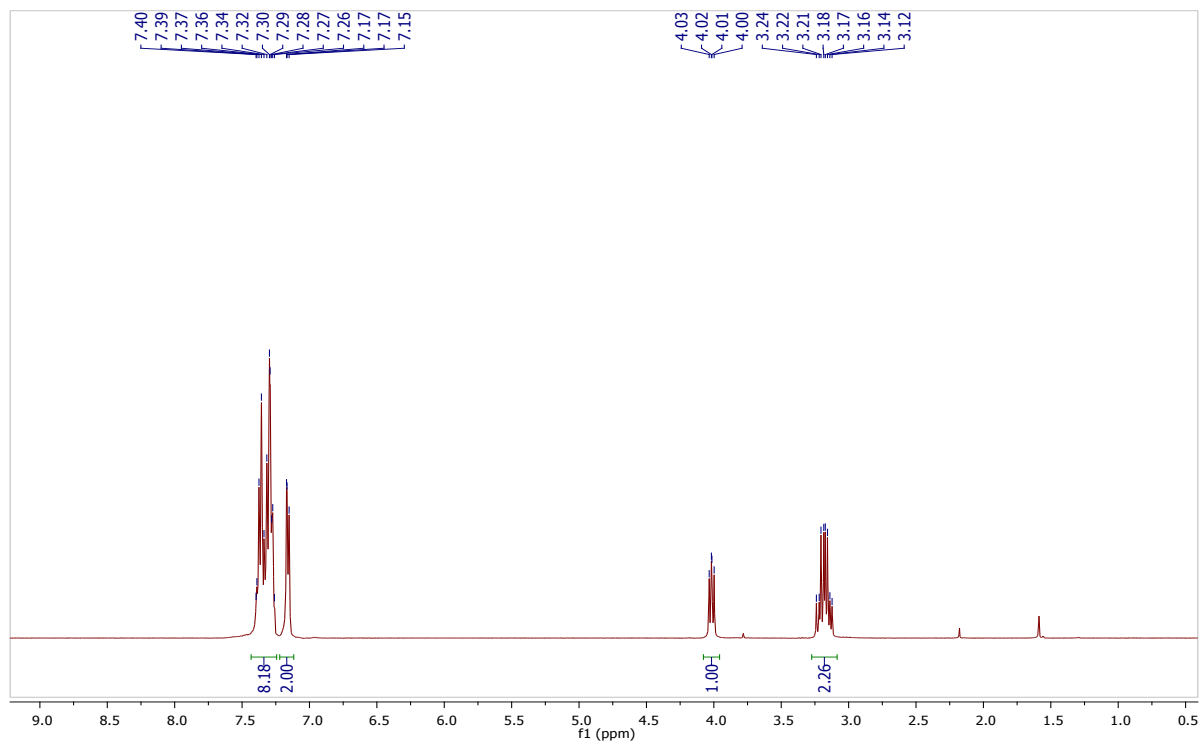
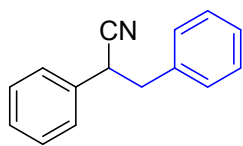


Figure S7. ^1H and ^{13}C NMR spectra of 4a.

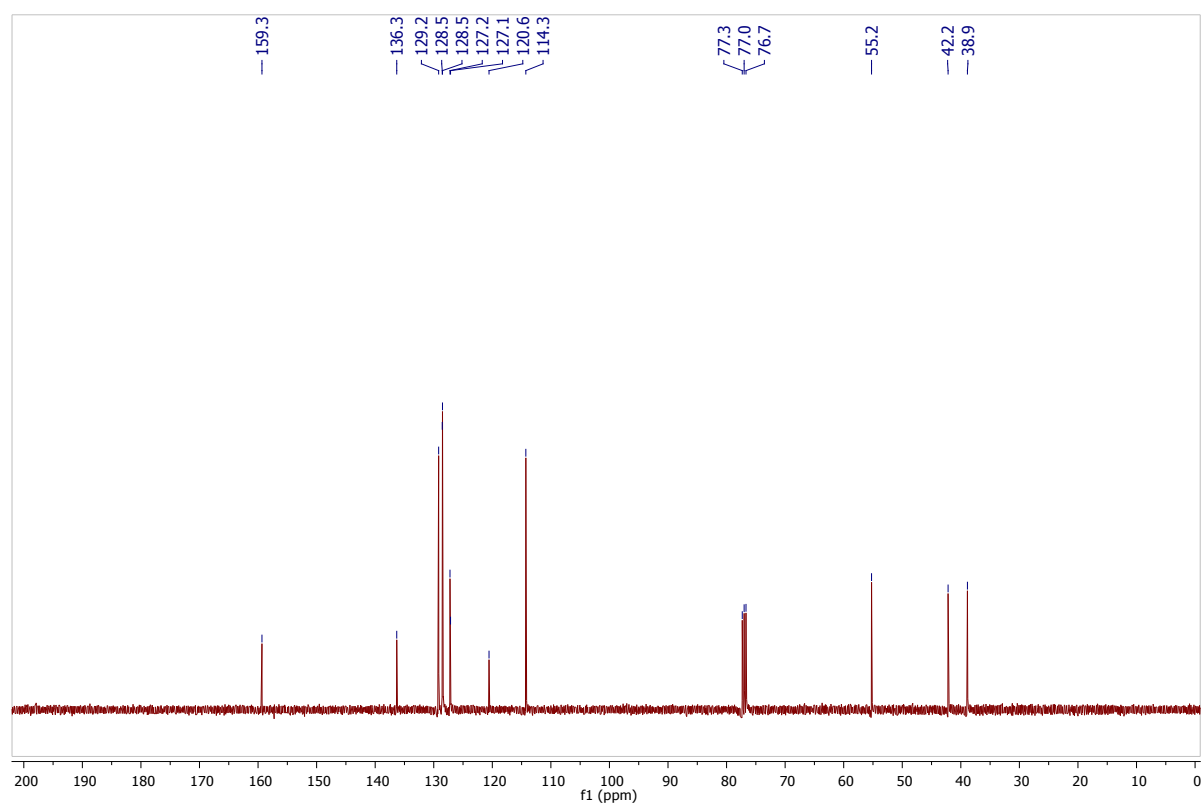
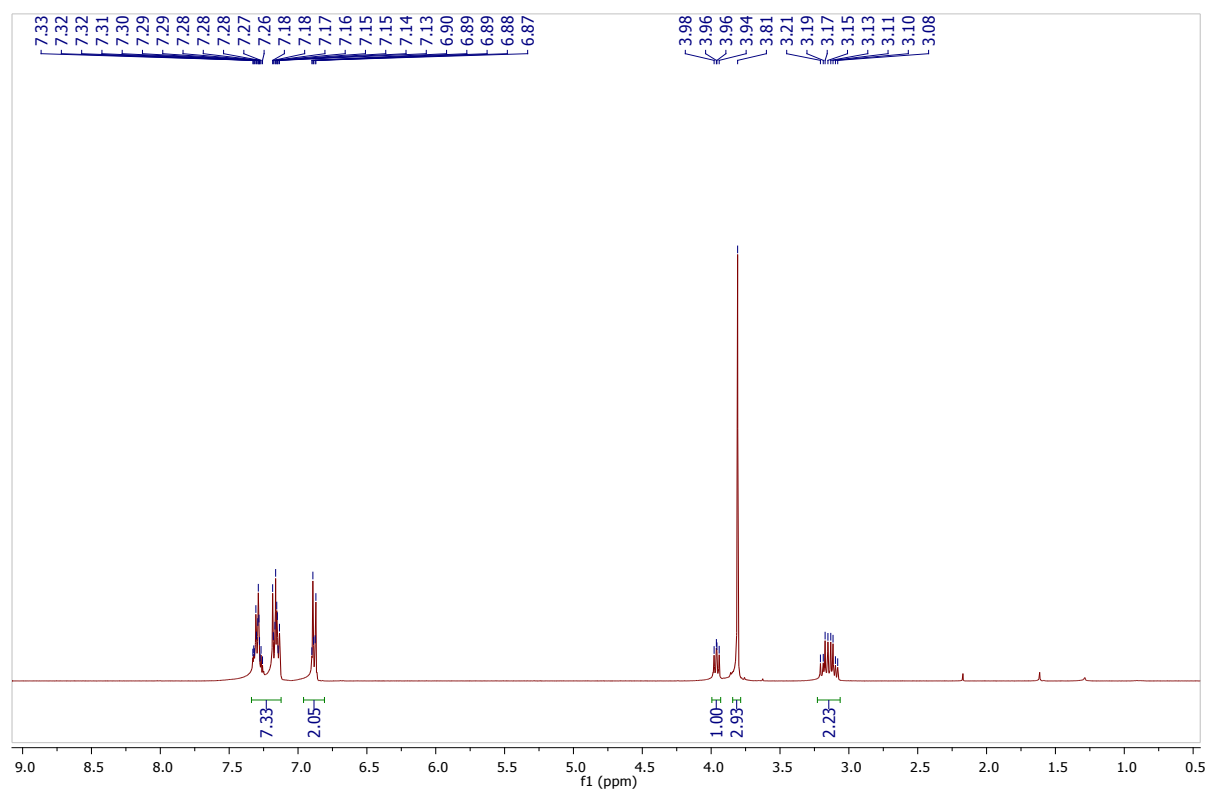
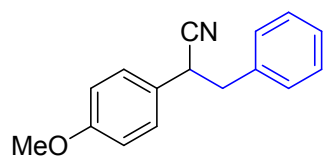


Figure S8. ¹H and ¹³C NMR spectra of 4b.

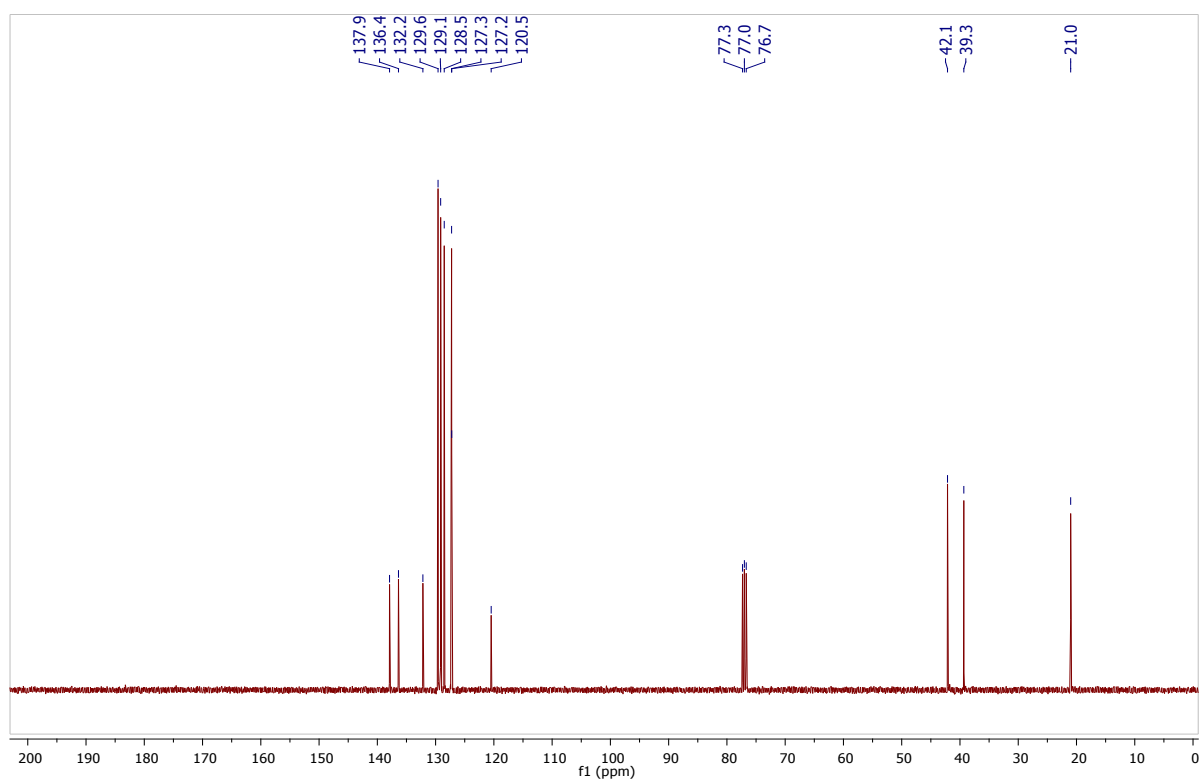
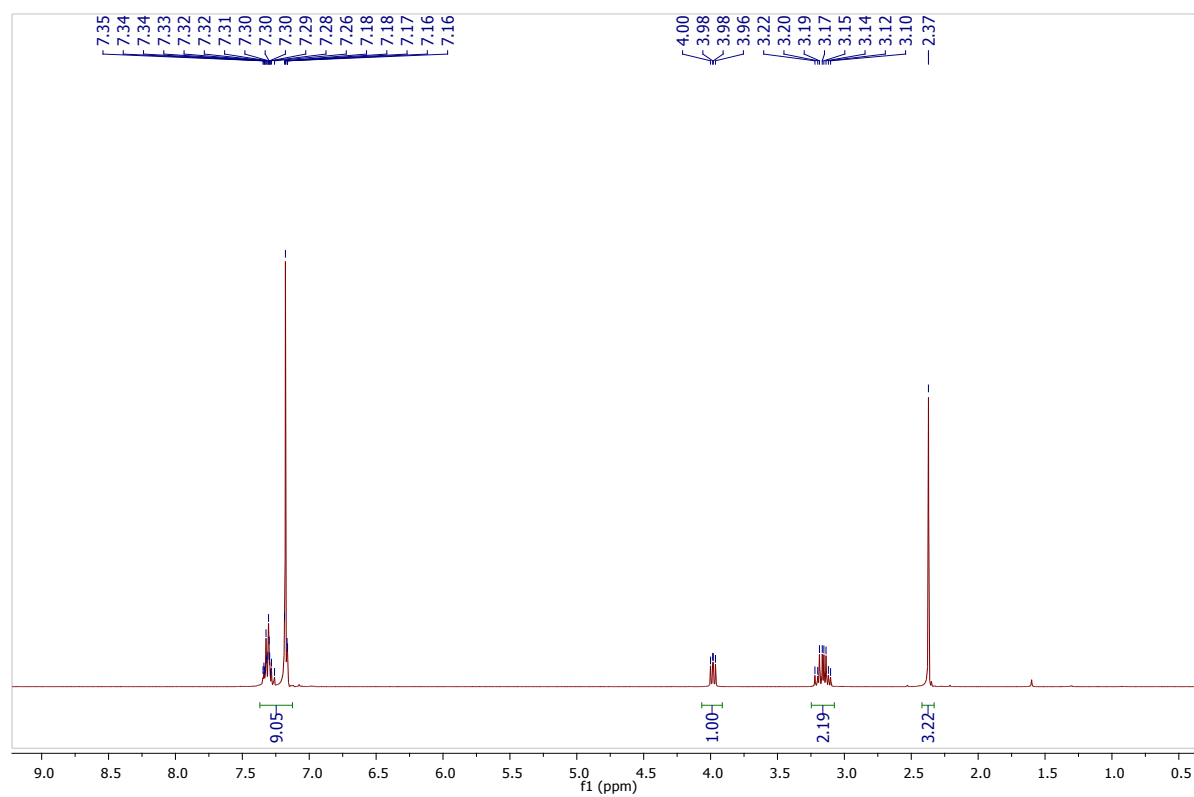
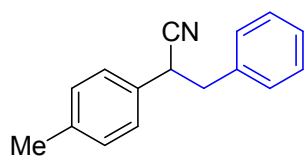


Figure S9. ¹H and ¹³C NMR spectra of 4c.

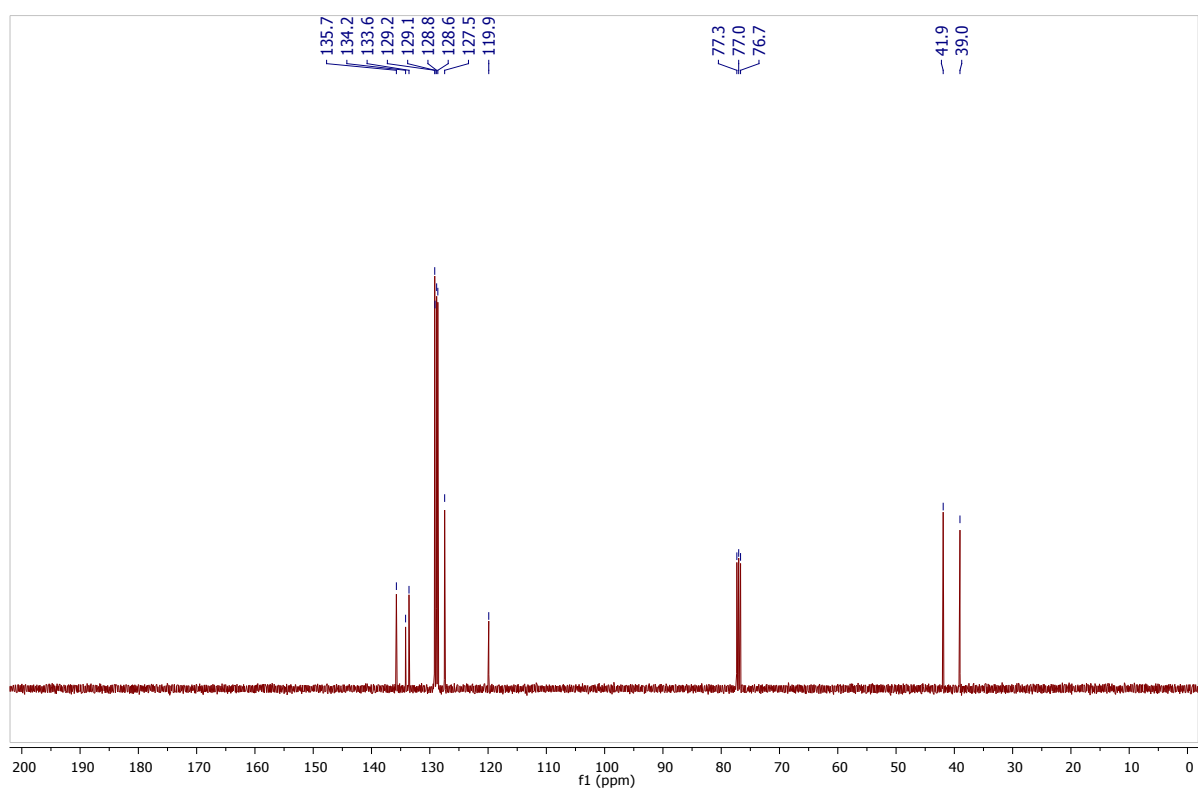
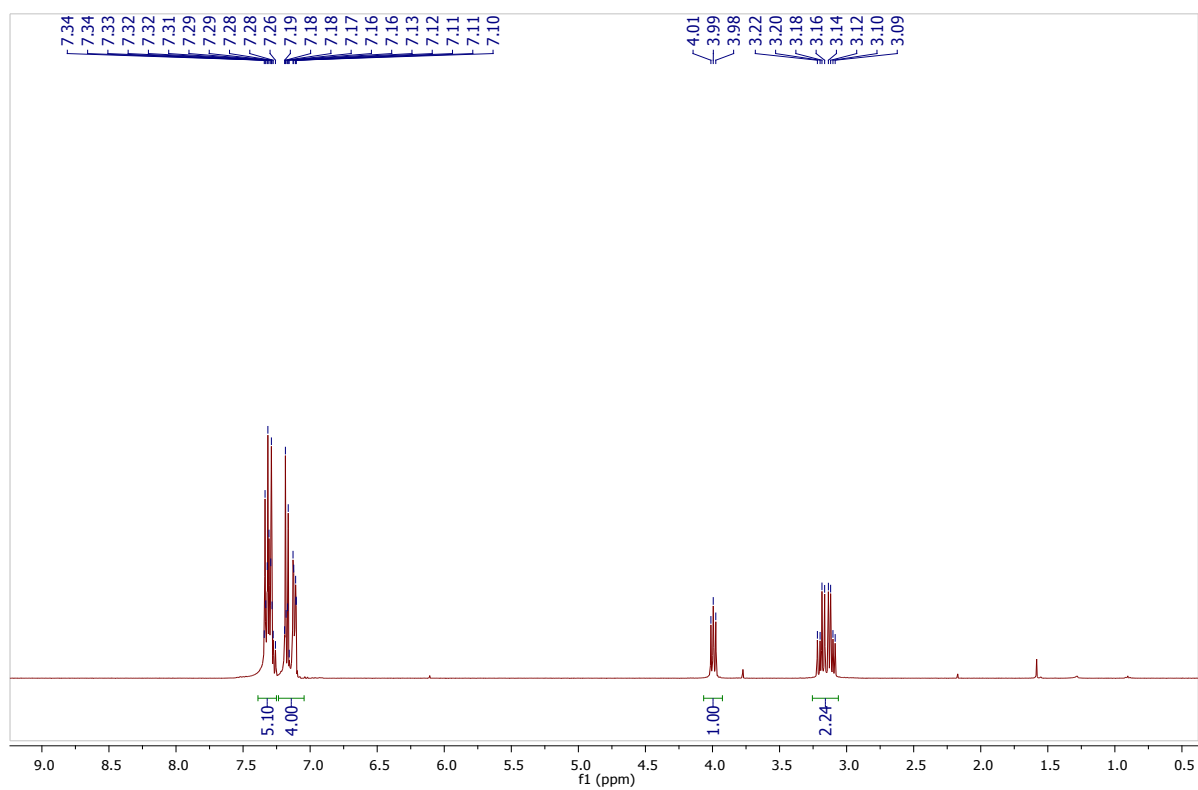
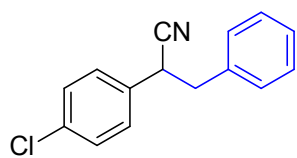


Figure S10. ¹H and ¹³C NMR spectra of 4d.

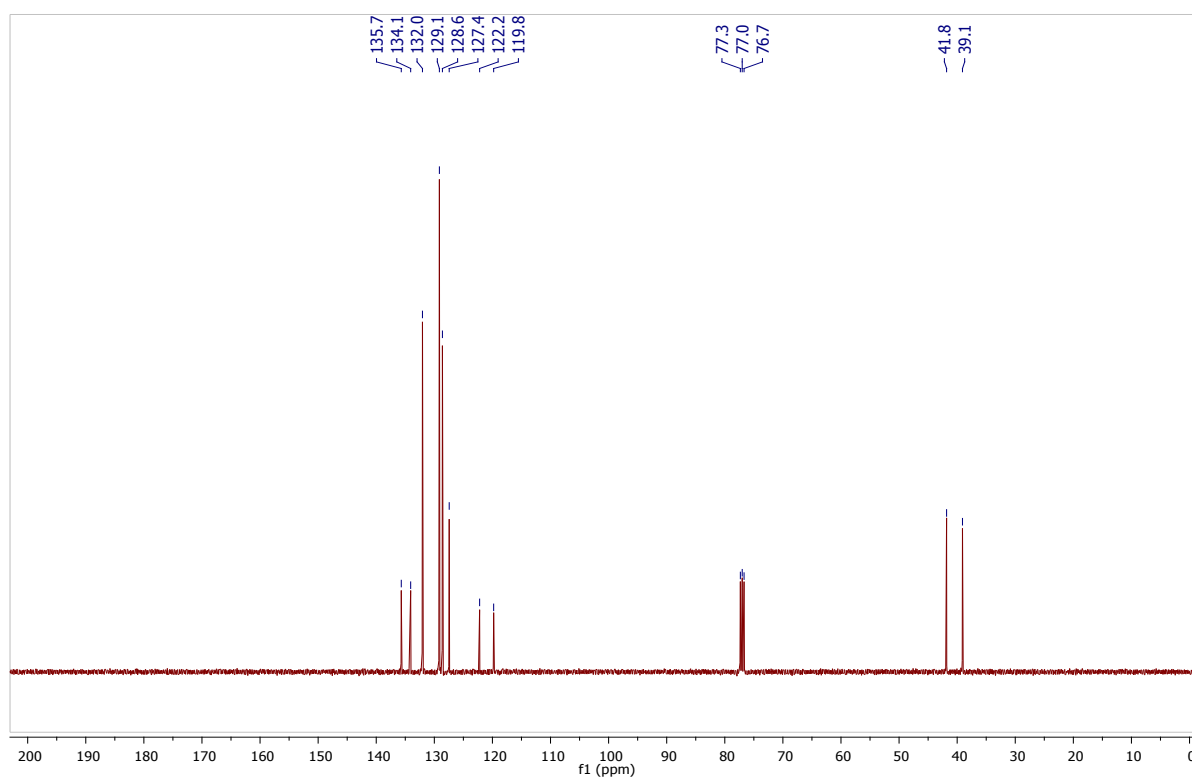
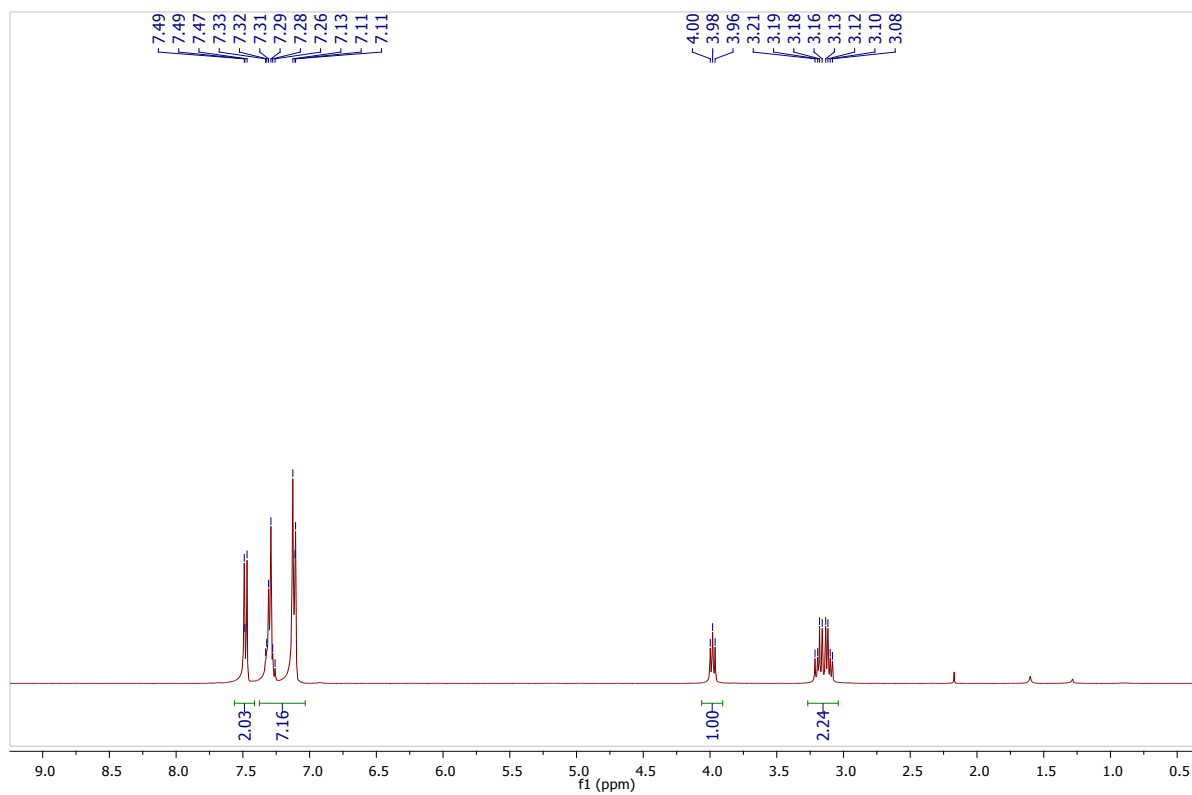
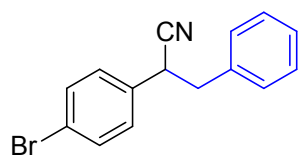


Figure S11. ¹H and ¹³C NMR spectra of 4e.

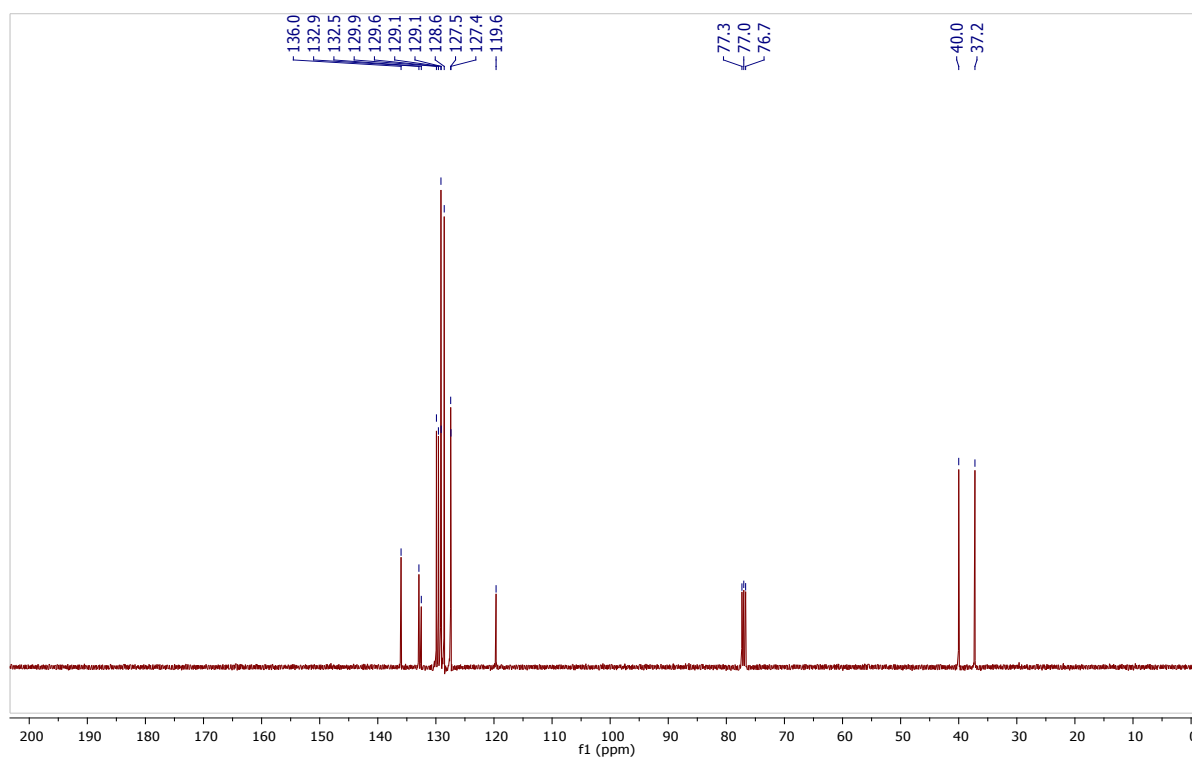
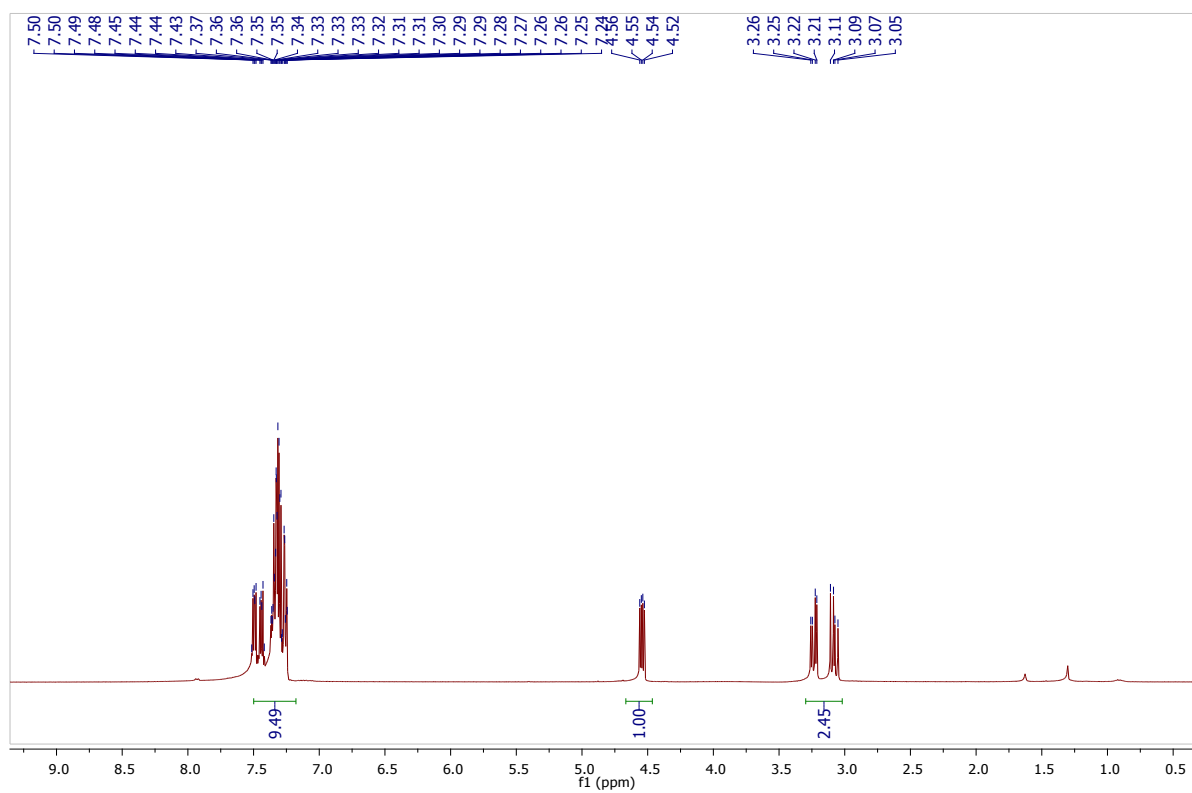
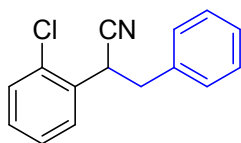


Figure S12. ¹H and ¹³C NMR spectra of 4f.

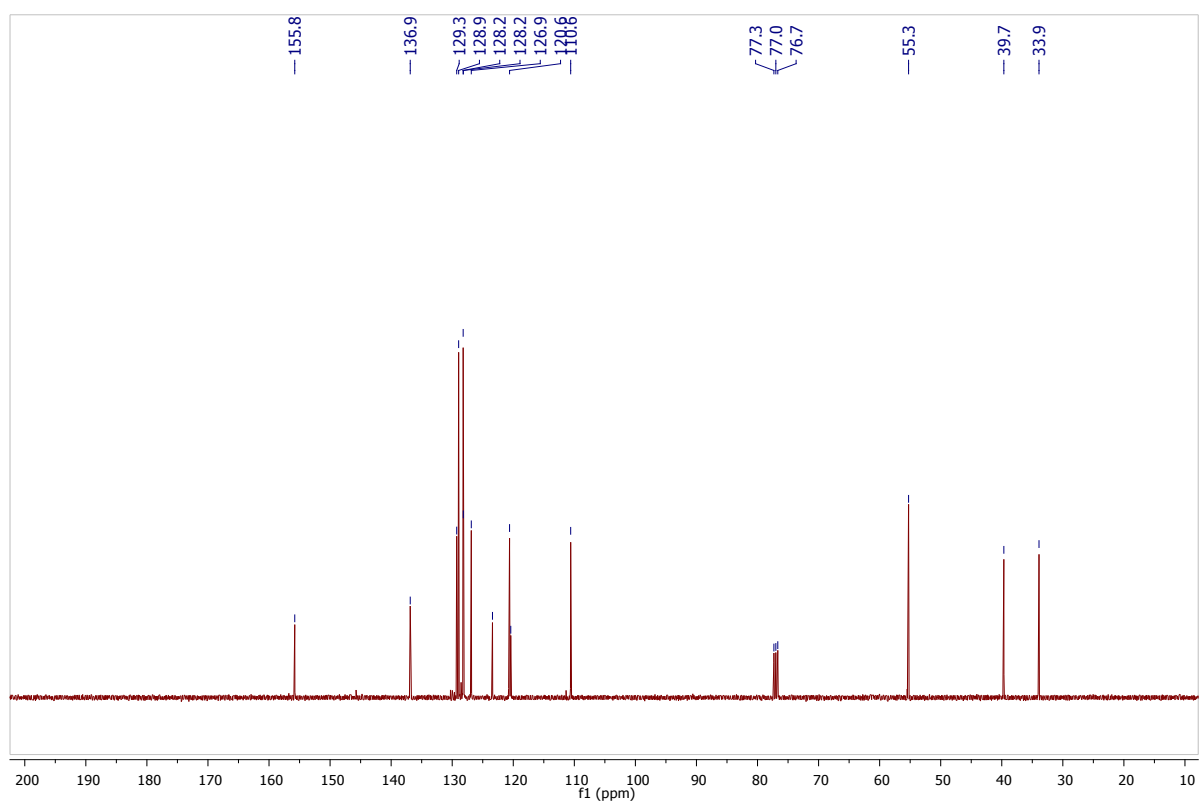
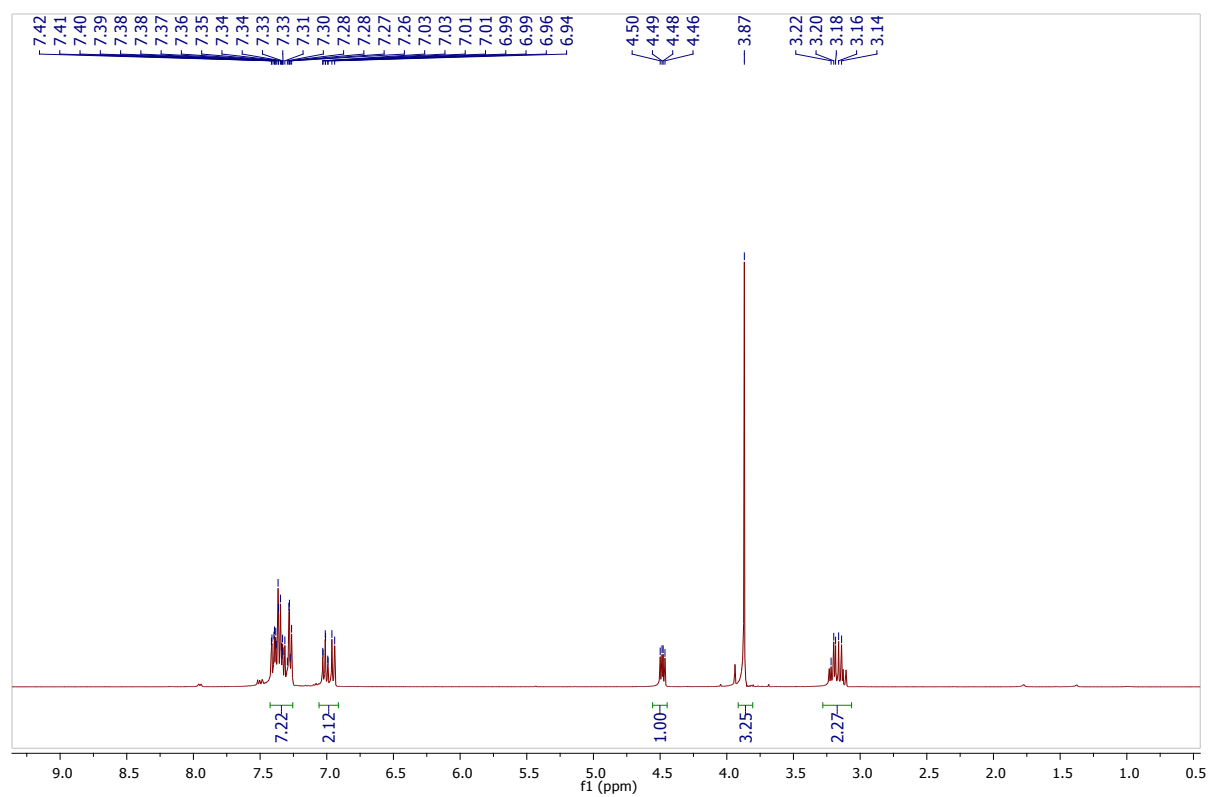
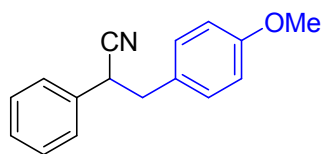


Figure S13. ¹H and ¹³C NMR spectra of 4g.

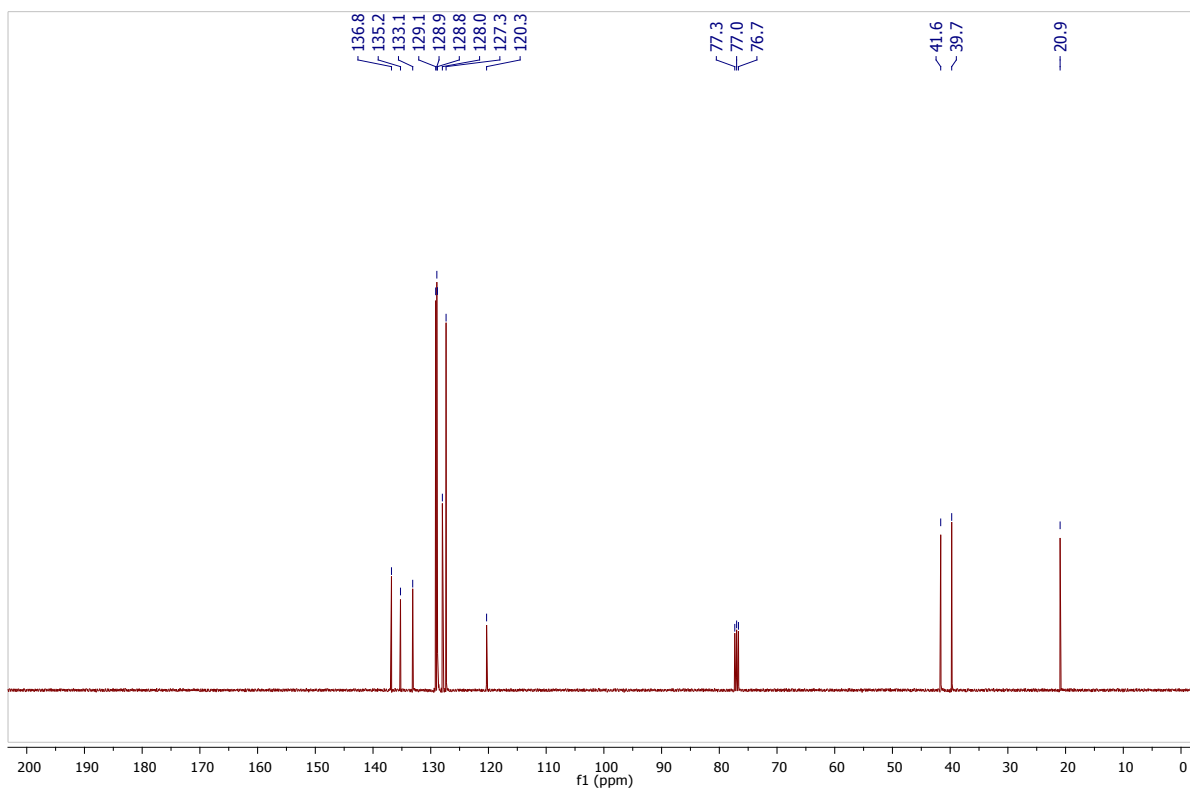
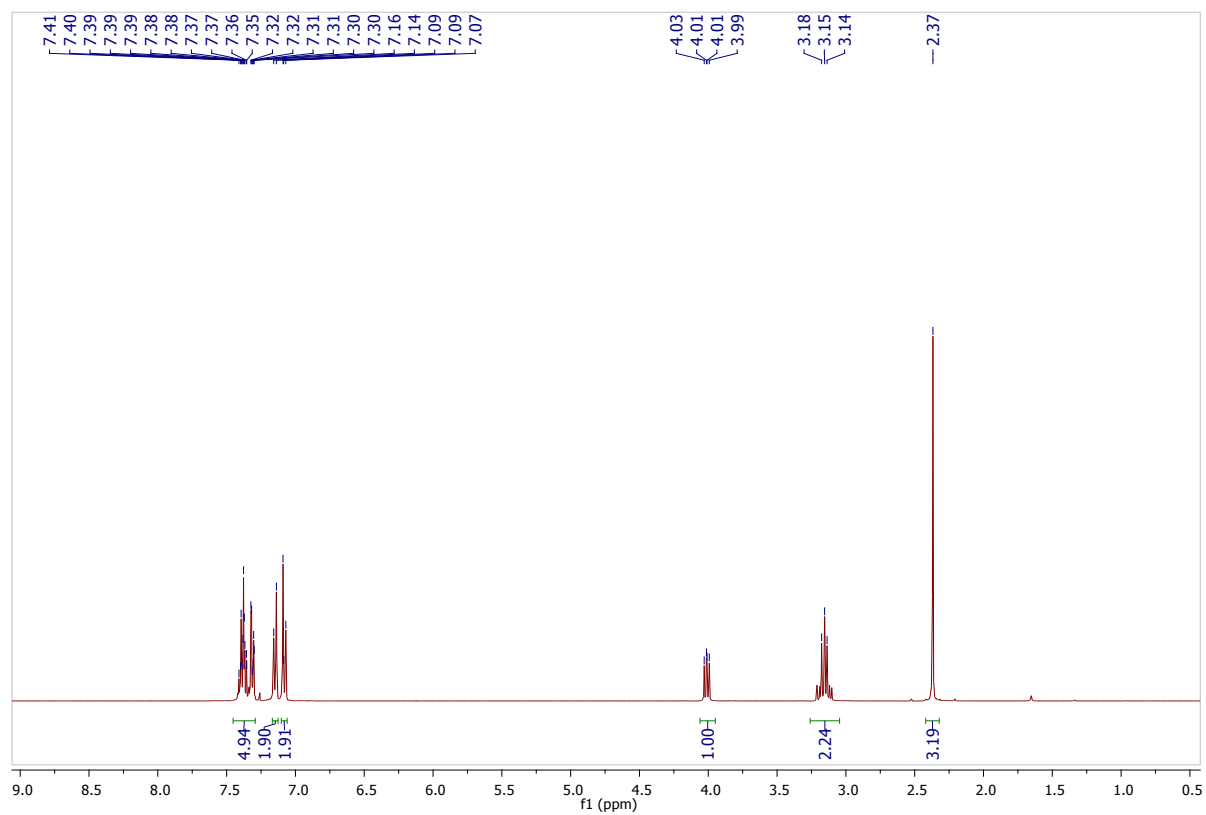
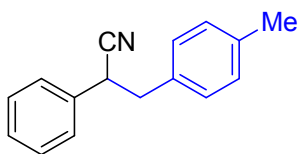


Figure S14. ¹H and ¹³C NMR spectra of 4h.

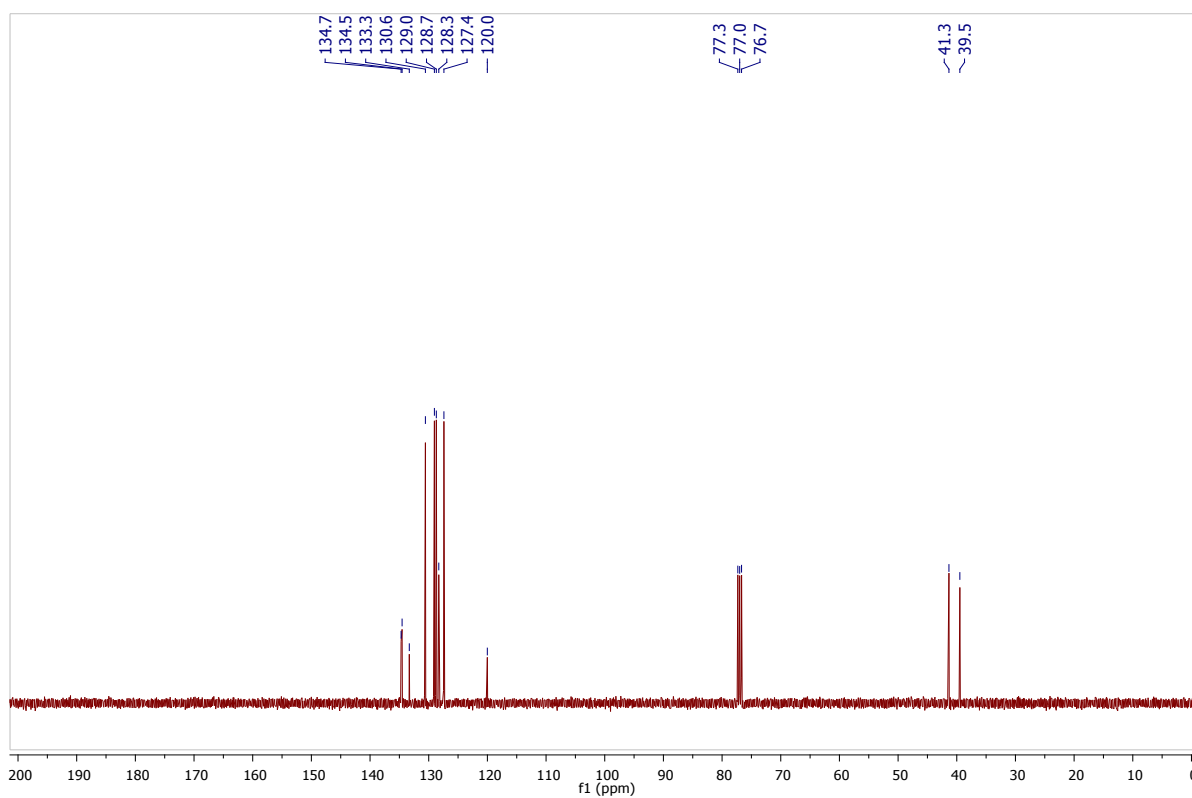
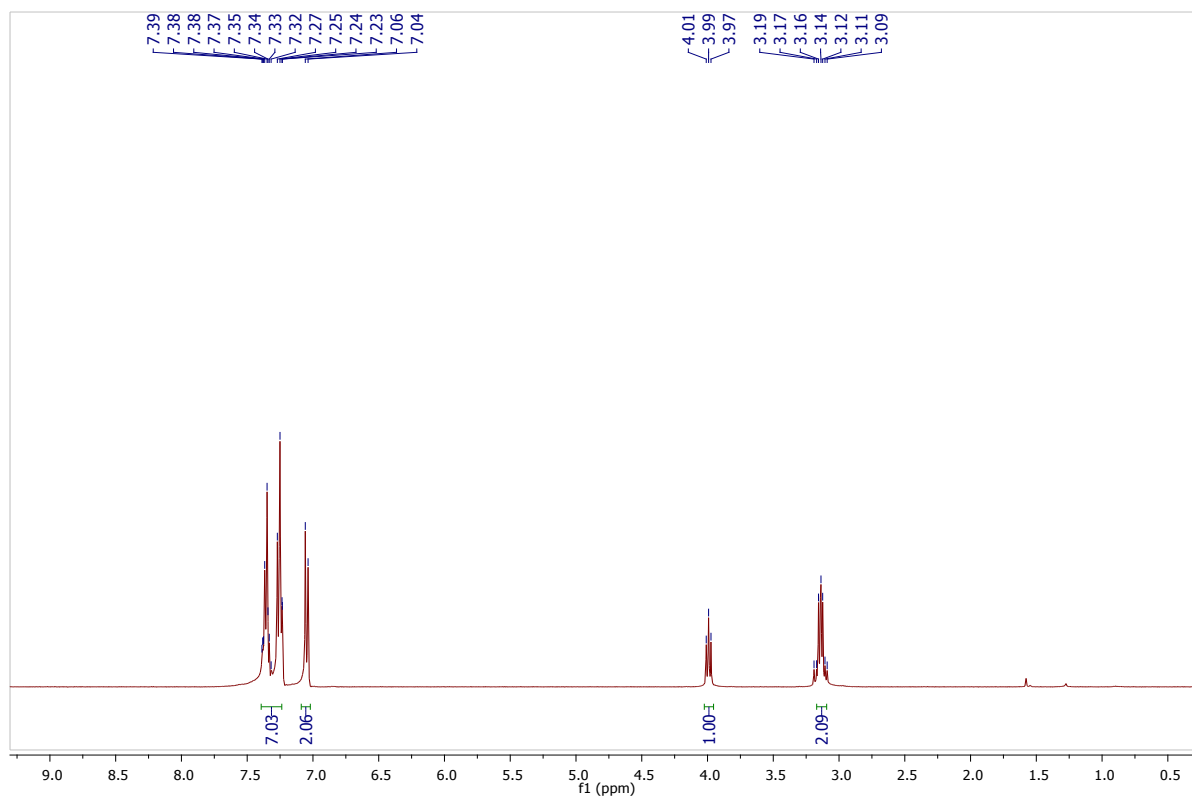
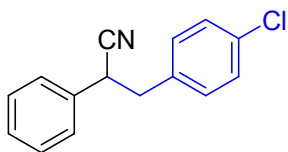


Figure S15. ¹H and ¹³C NMR spectra of 4i.

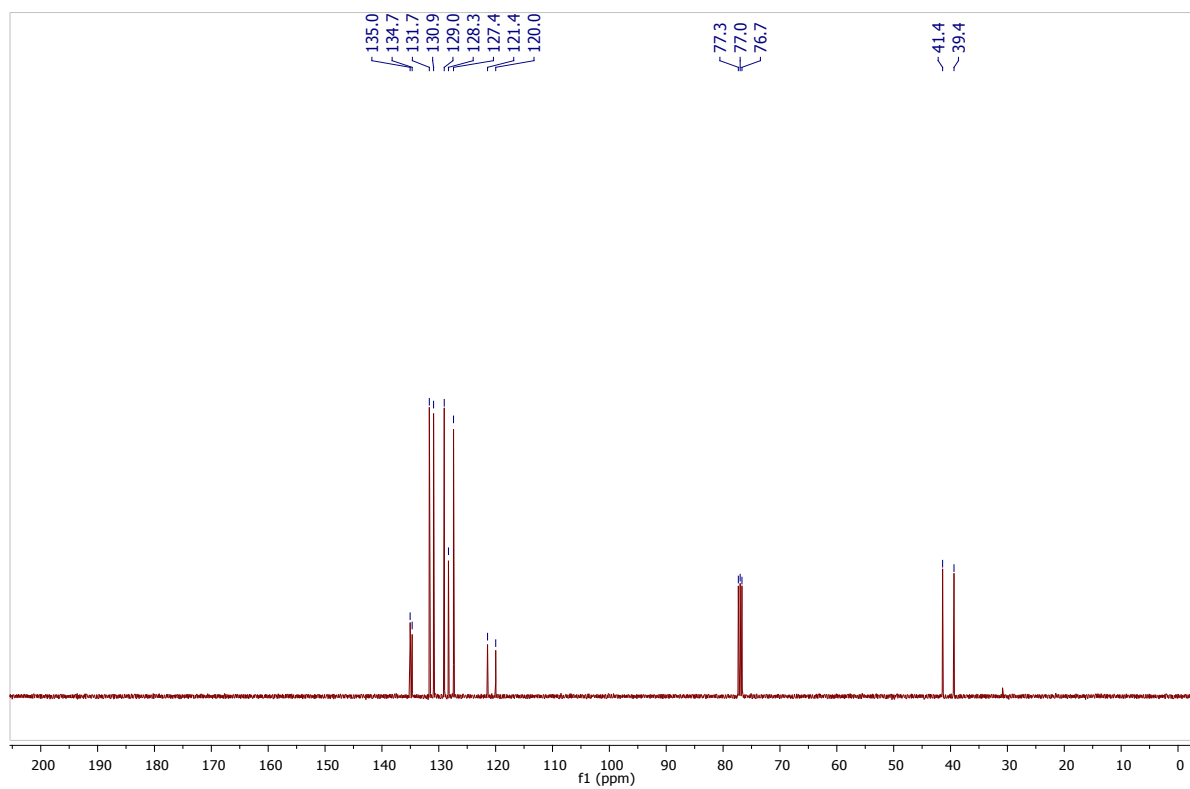
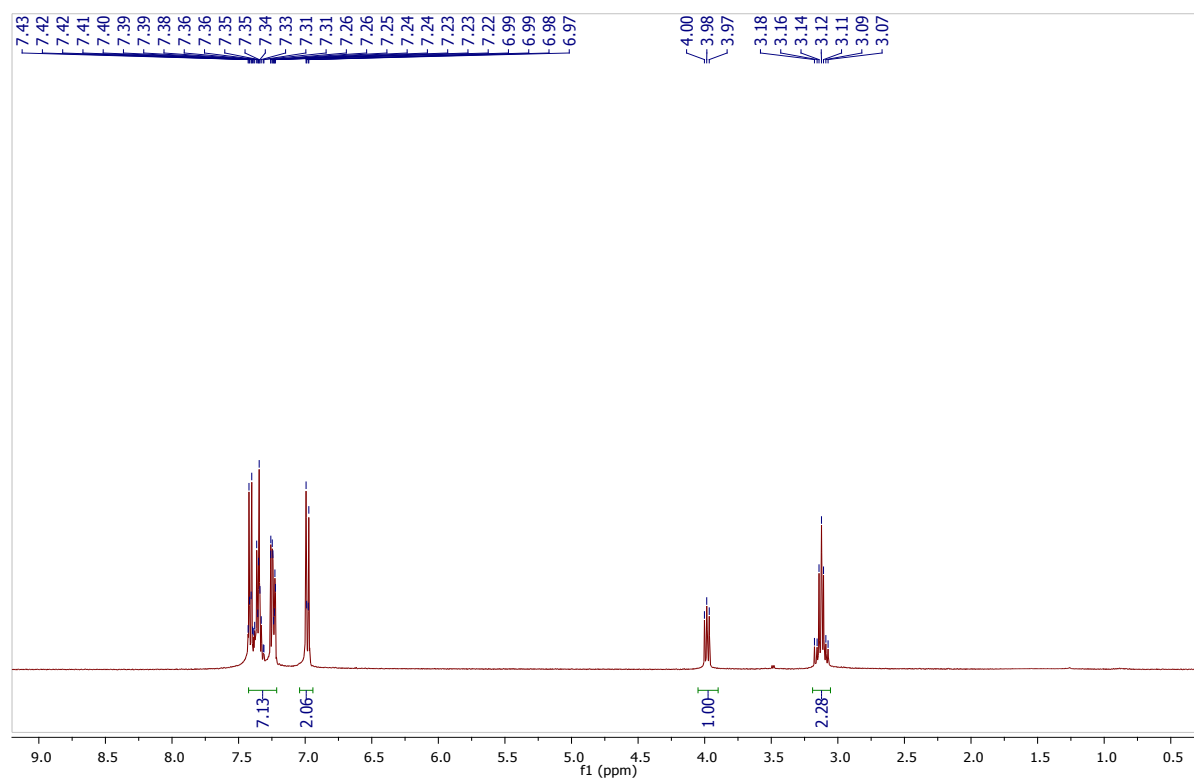
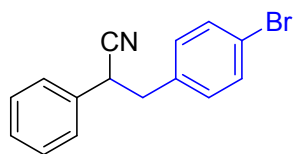


Figure S16. ¹H and ¹³C NMR spectra of 4j.

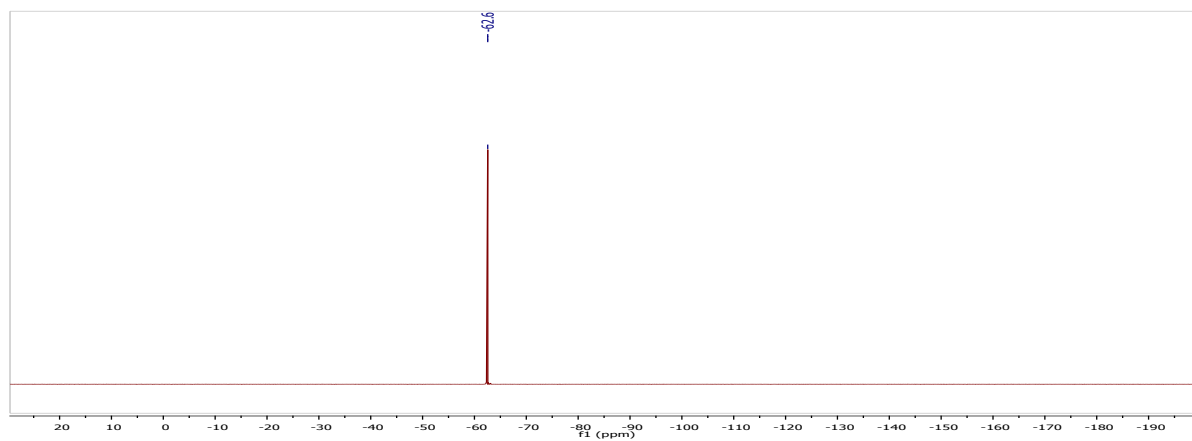
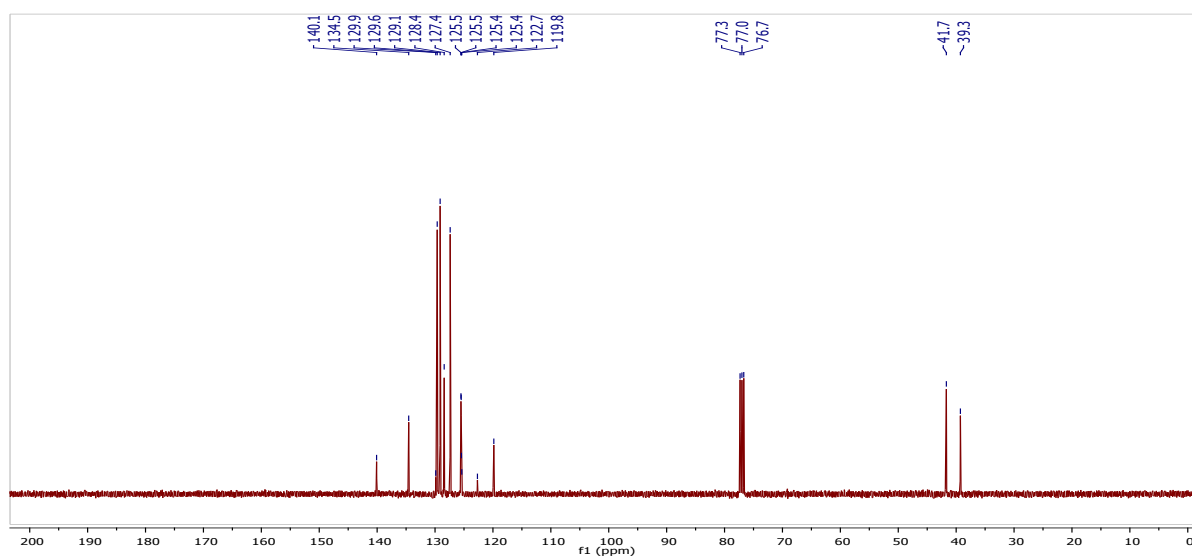
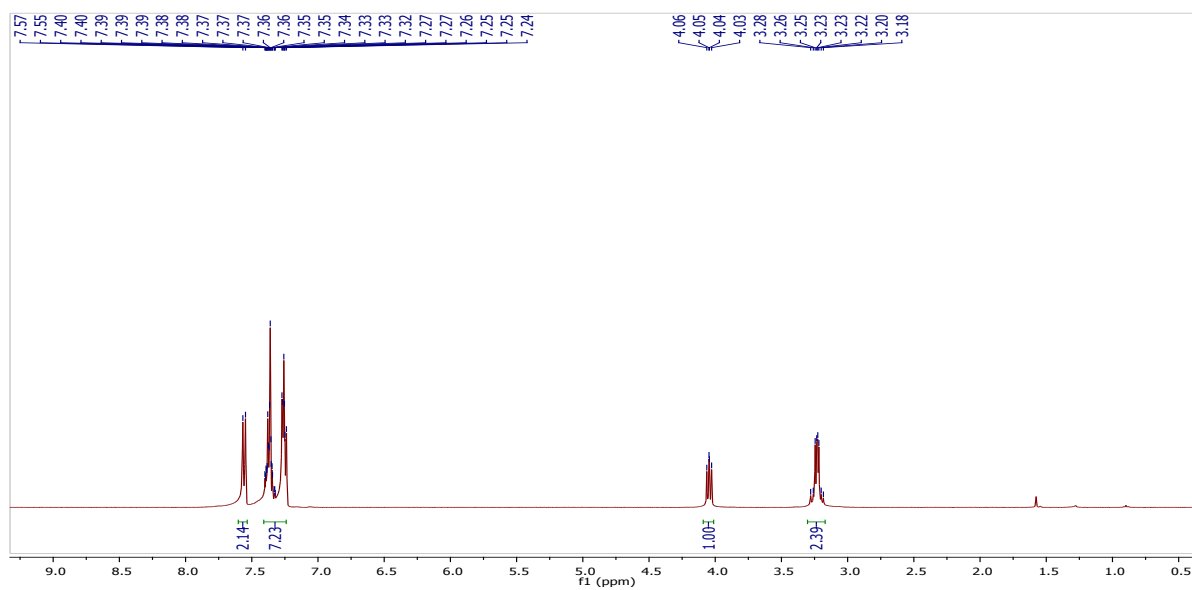
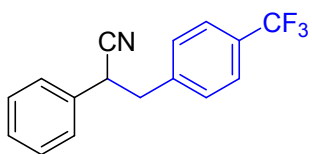


Figure S17. ¹H, ¹³C, and ¹⁹F NMR spectra of 4k.

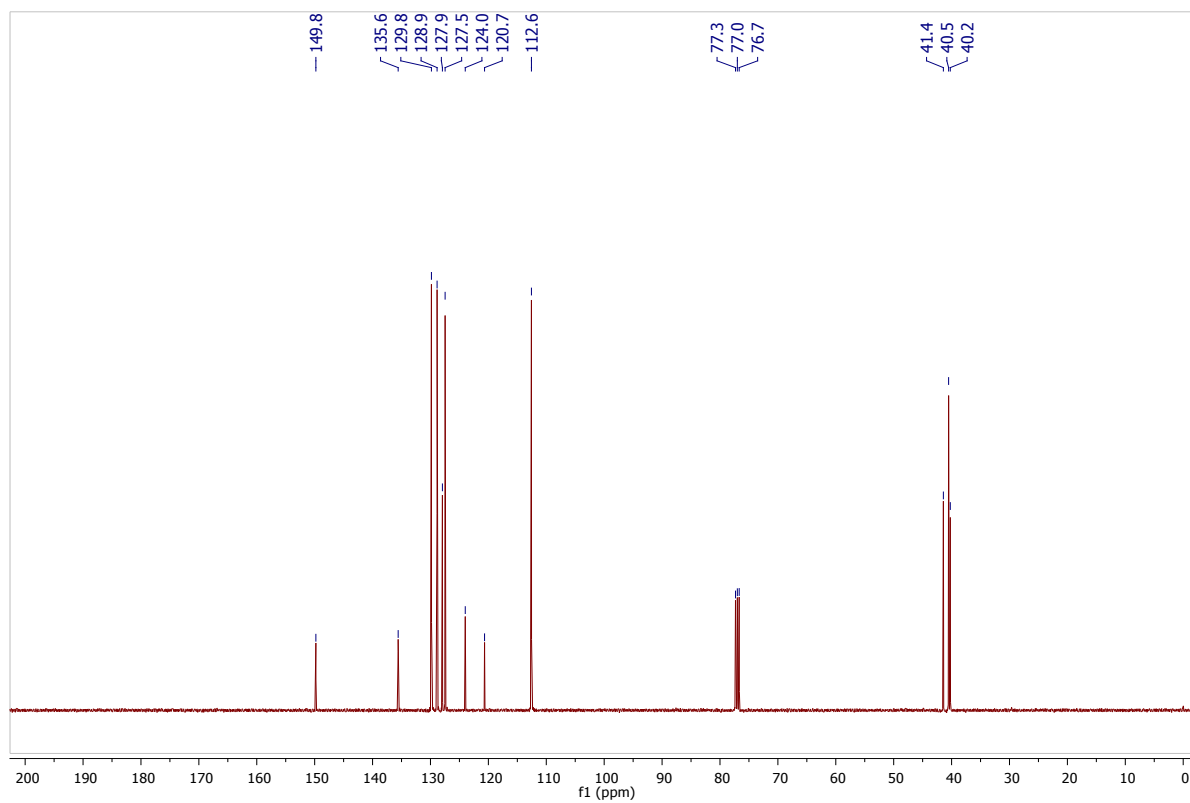
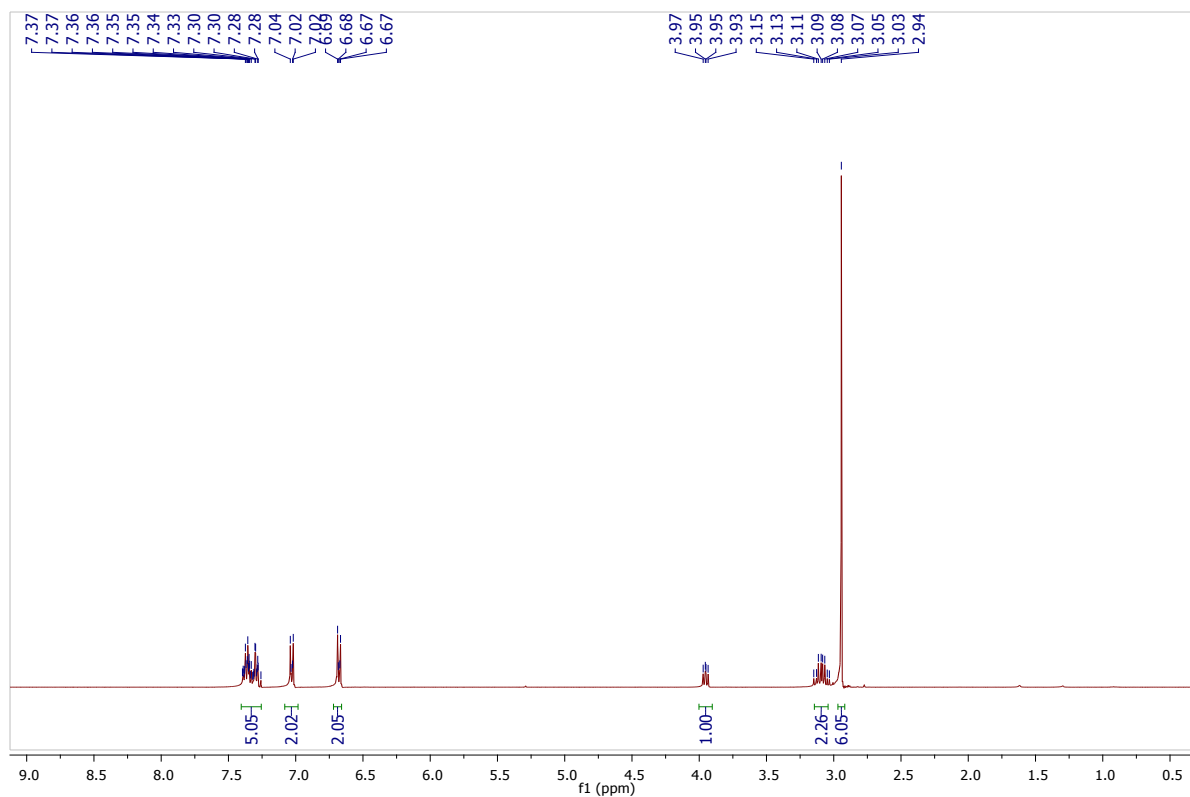
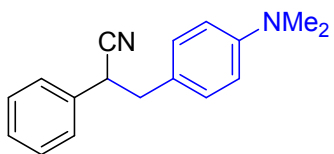


Figure S18. ¹H and ¹³C NMR spectra of 4l.

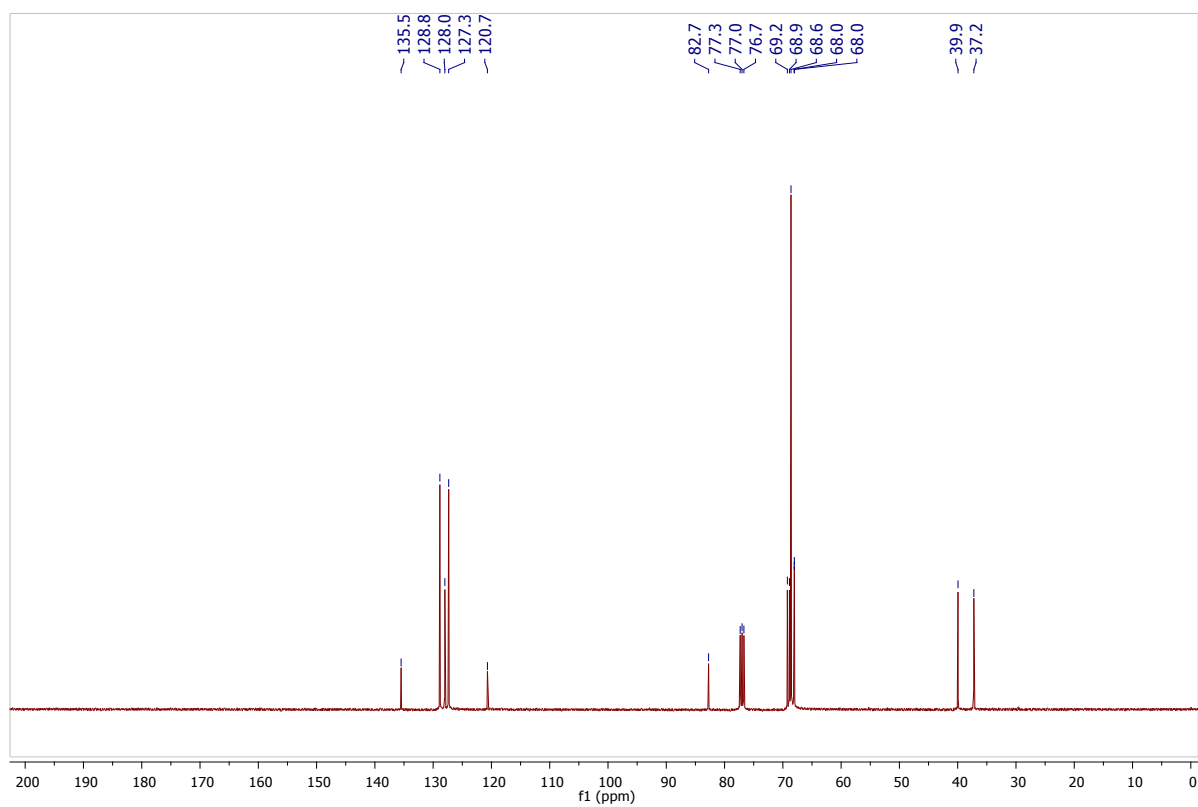
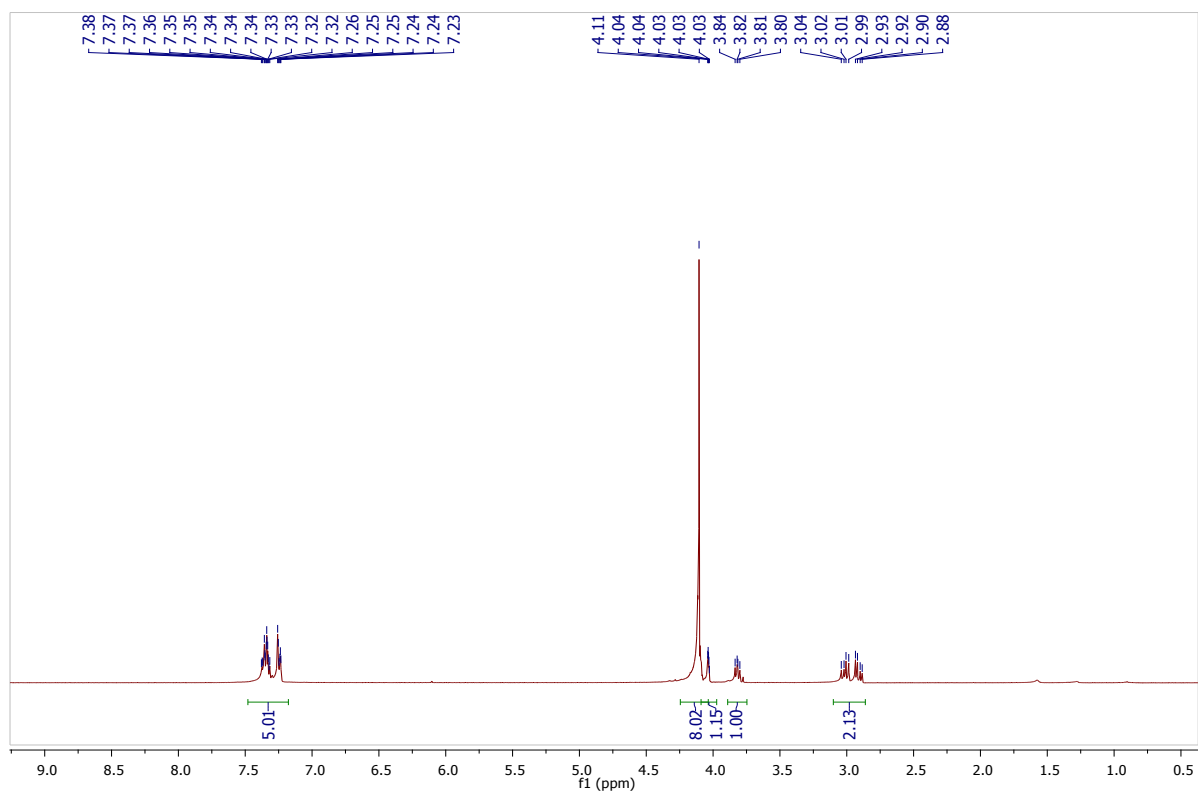
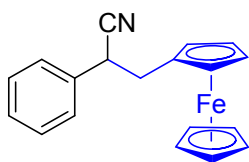
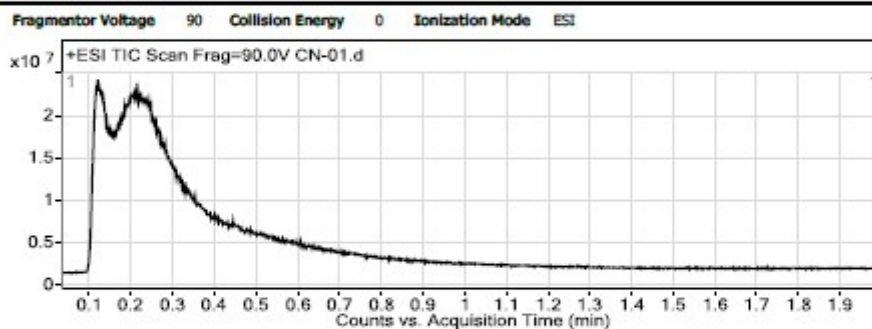


Figure S19. ¹H and ¹³C NMR spectra of **4m**.

Qualitative Analysis Report

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User Chromatograms



User Spectra

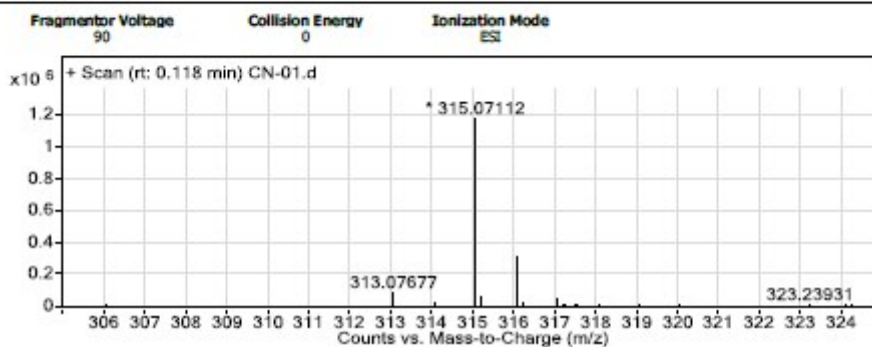


Figure S20. HRMS analysis report of **4m**.

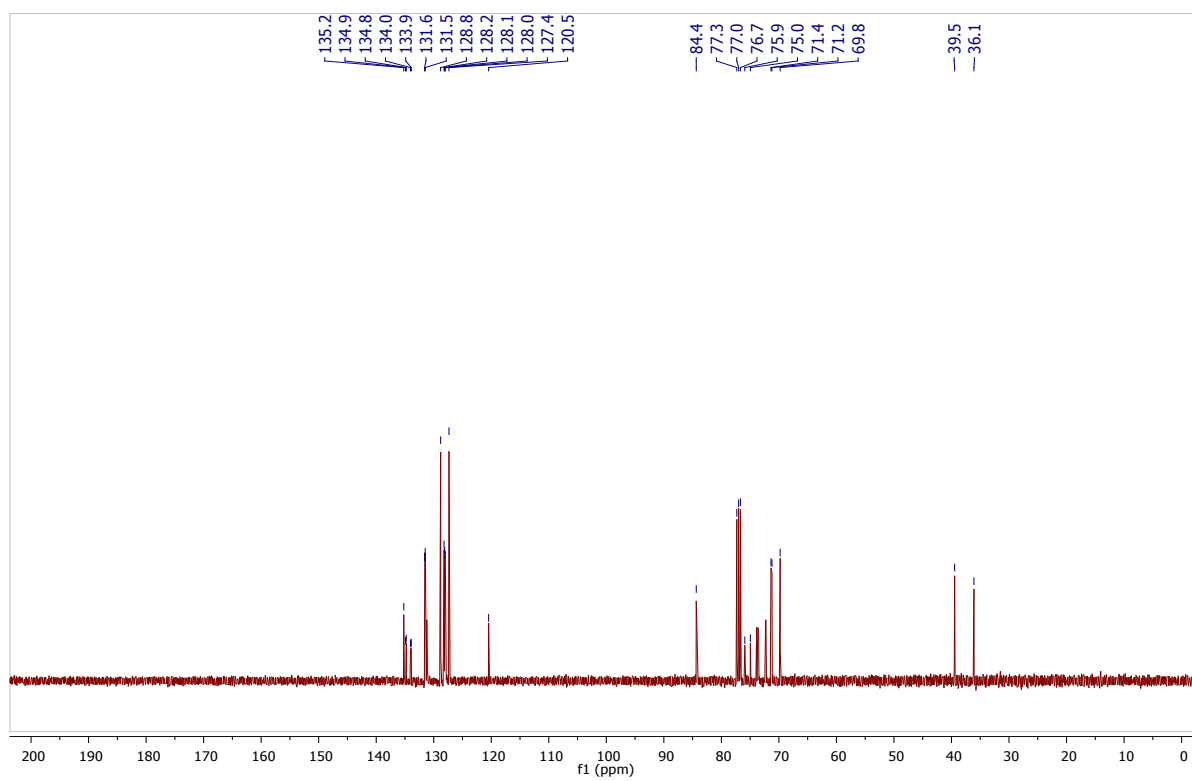
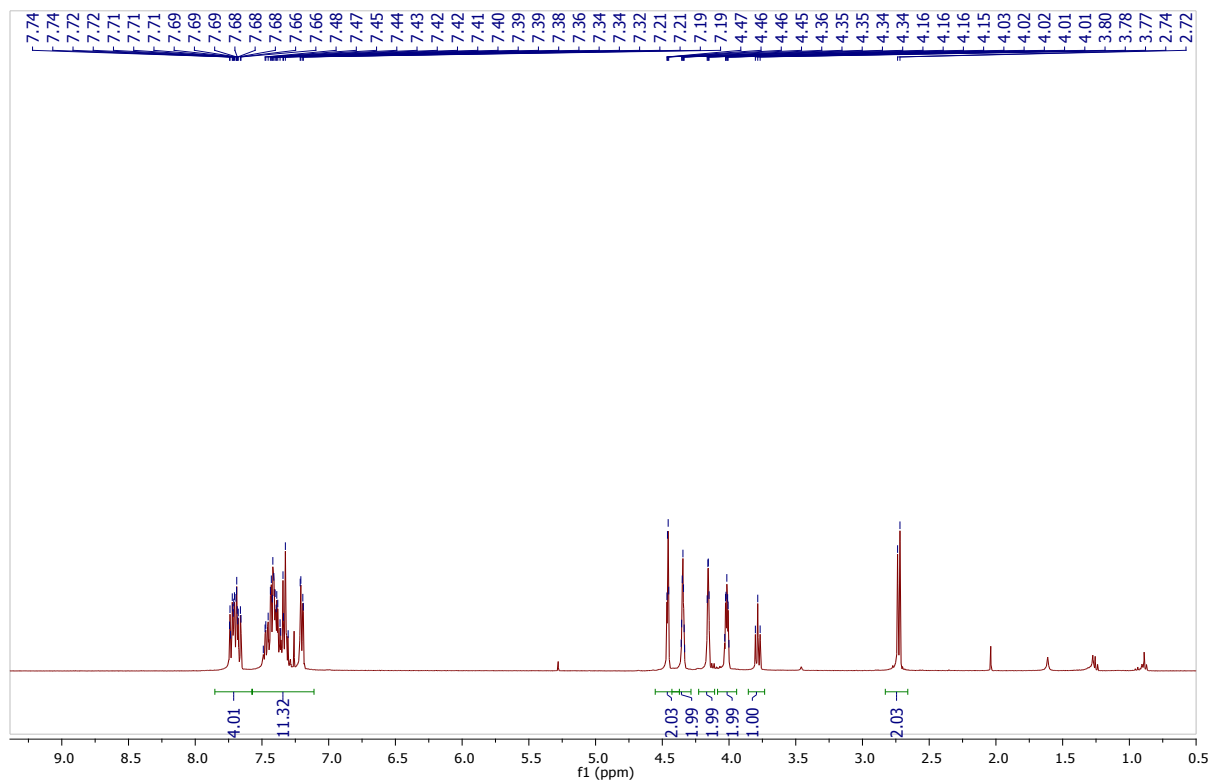
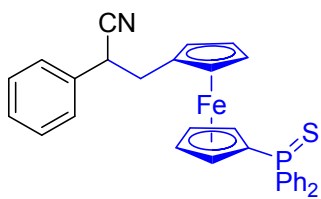


Figure S21. ^1H and ^{13}C NMR spectra of **4n**.

Qualitative Analysis Report

| | | | |
|------------------------|--------------|---------------|---------------------|
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| | | | |
|--------------|------|----------------|-----------------------------|
| Sample Group | | Info. | |
| Stream Name | LC 1 | Acquisition SW | 6200 series TOF/6500 series |
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User Spectra

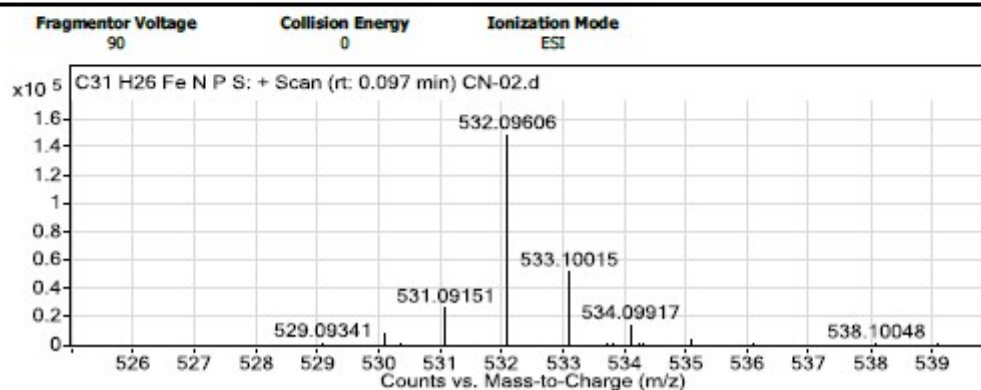


Figure S22. HRMS analysis report of **4n**.

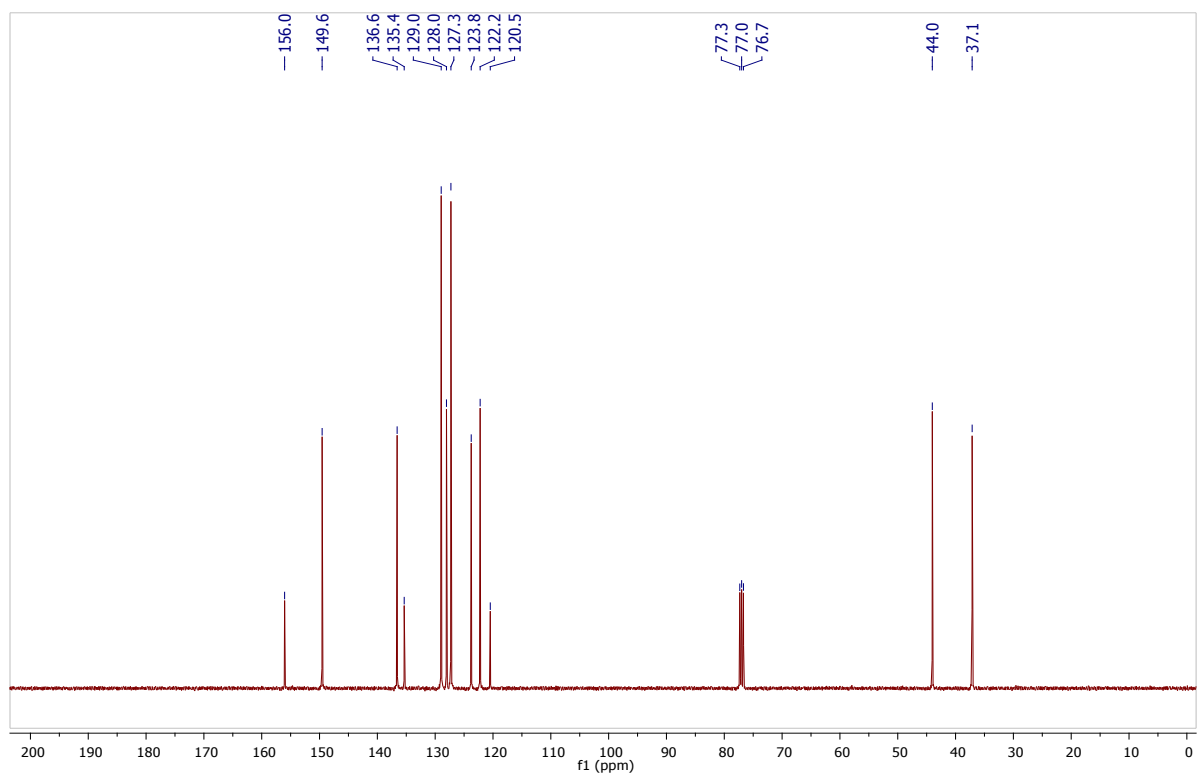
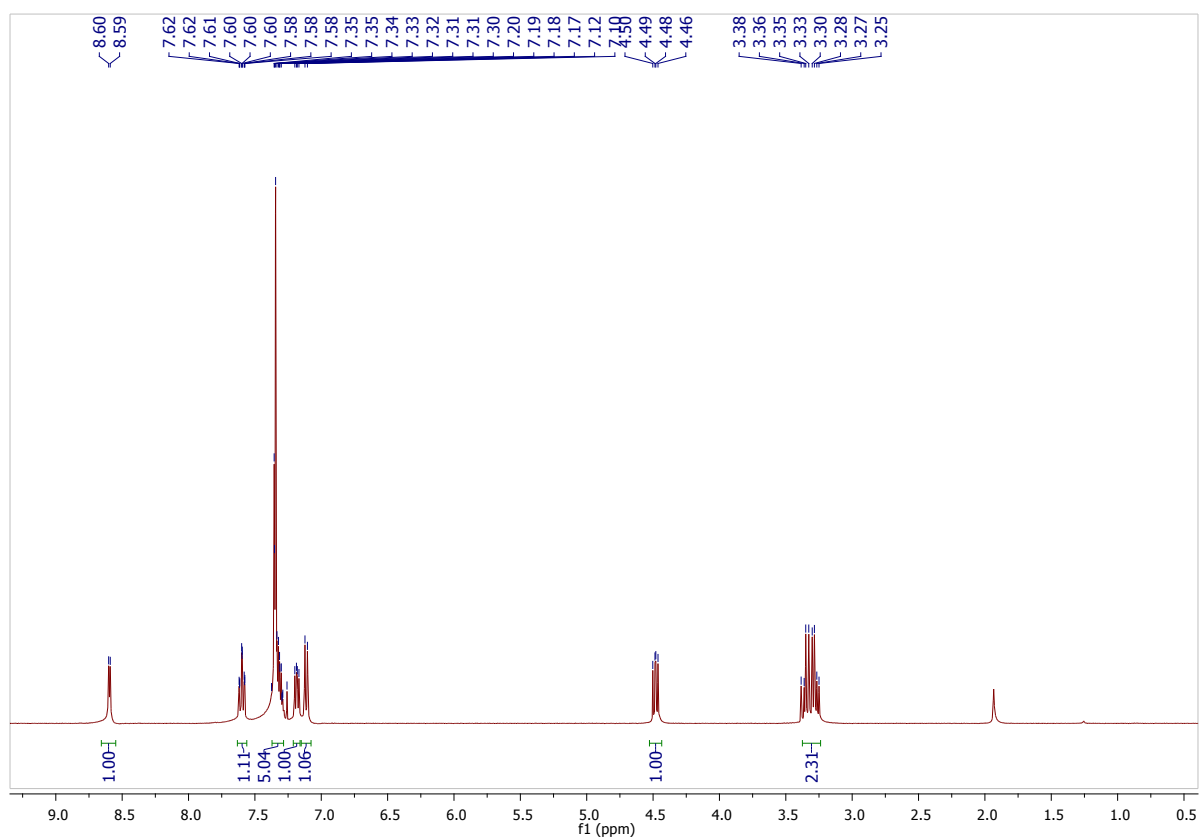
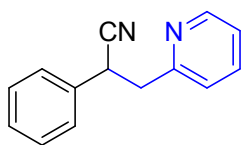


Figure S23. ¹H and ¹³C NMR spectra of **40**.

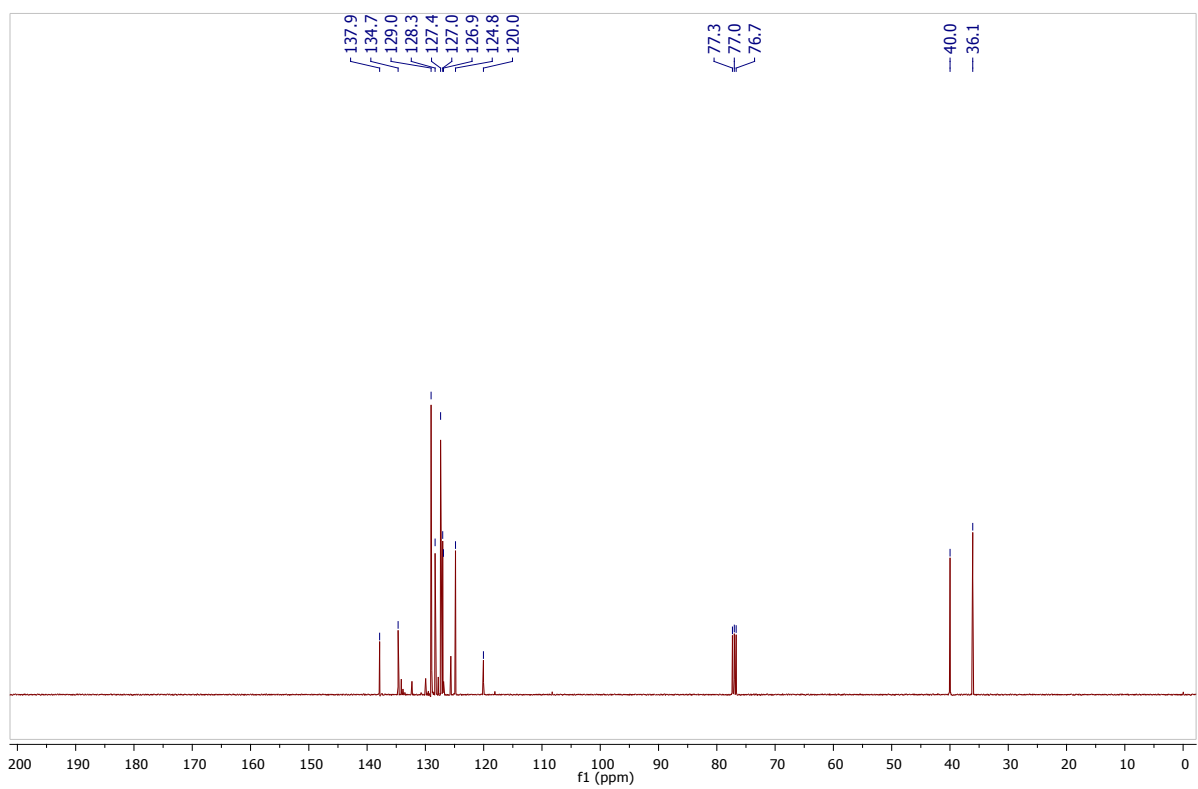
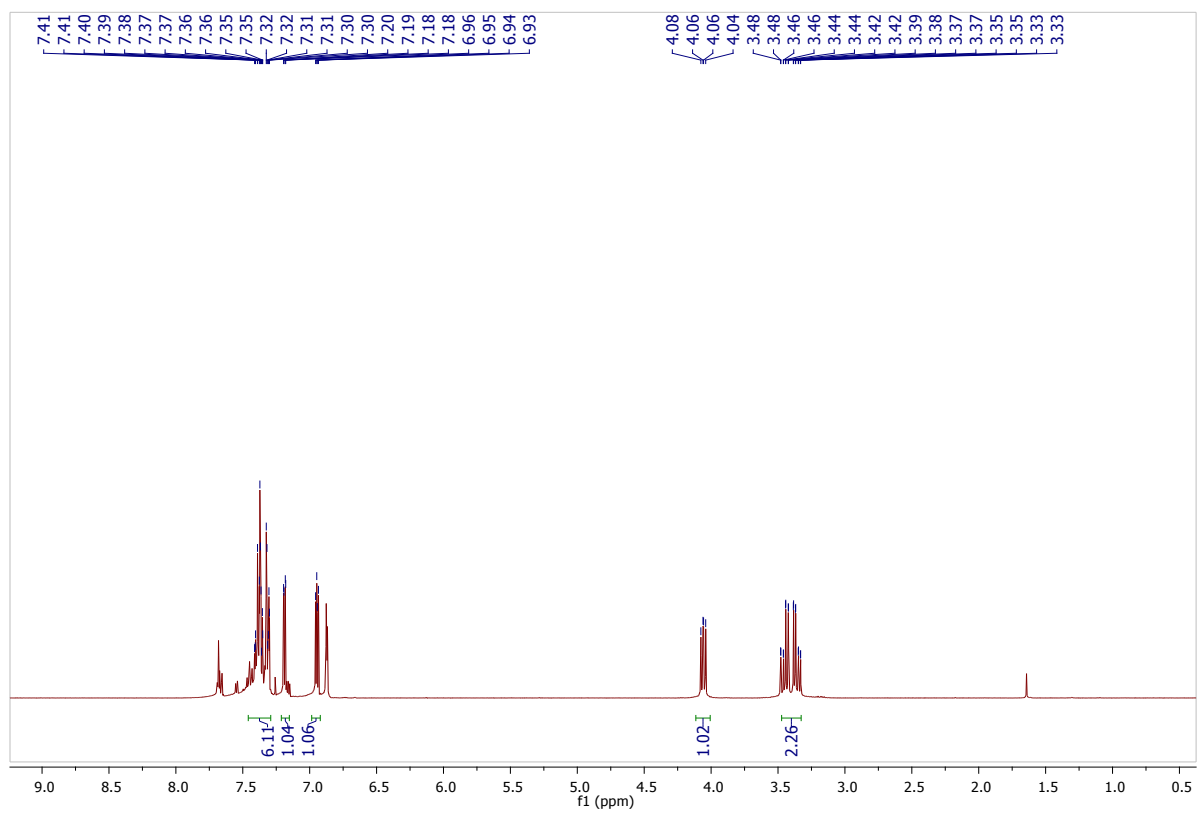
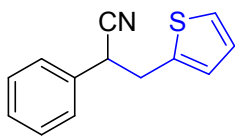


Figure S24. ^1H and ^{13}C NMR spectra of **4p**.

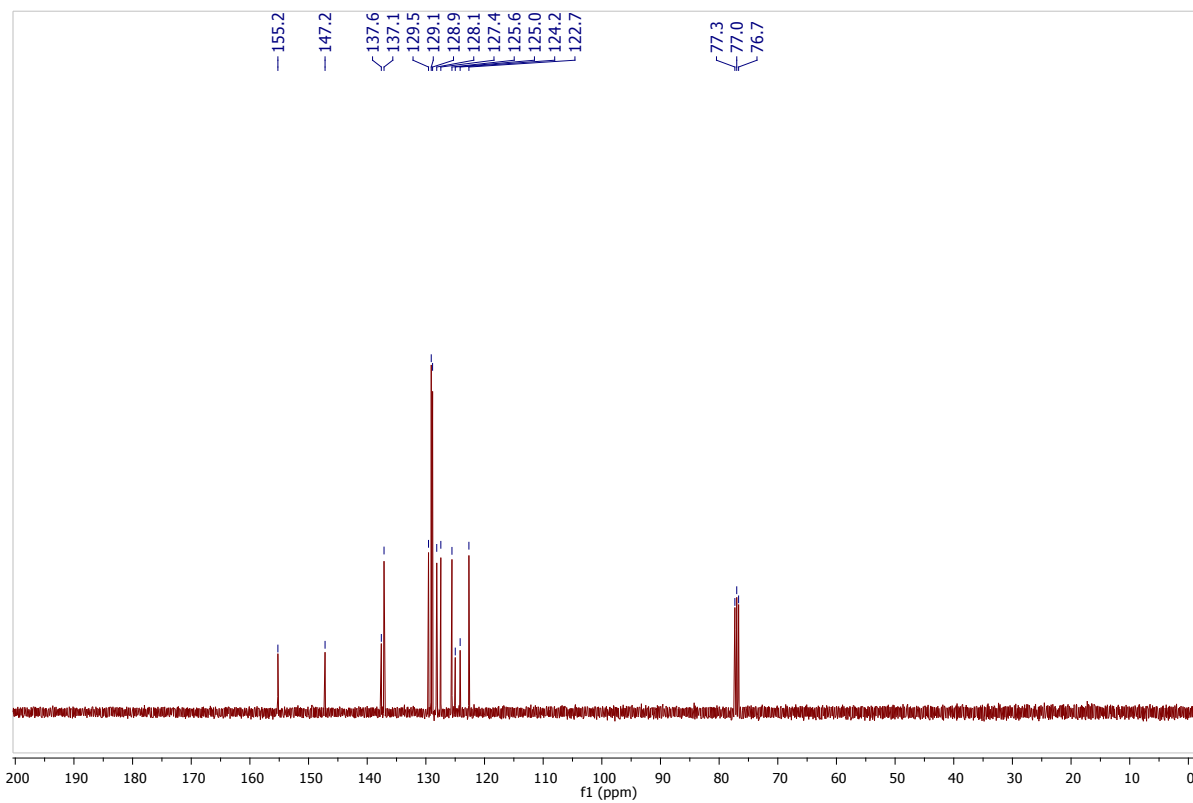
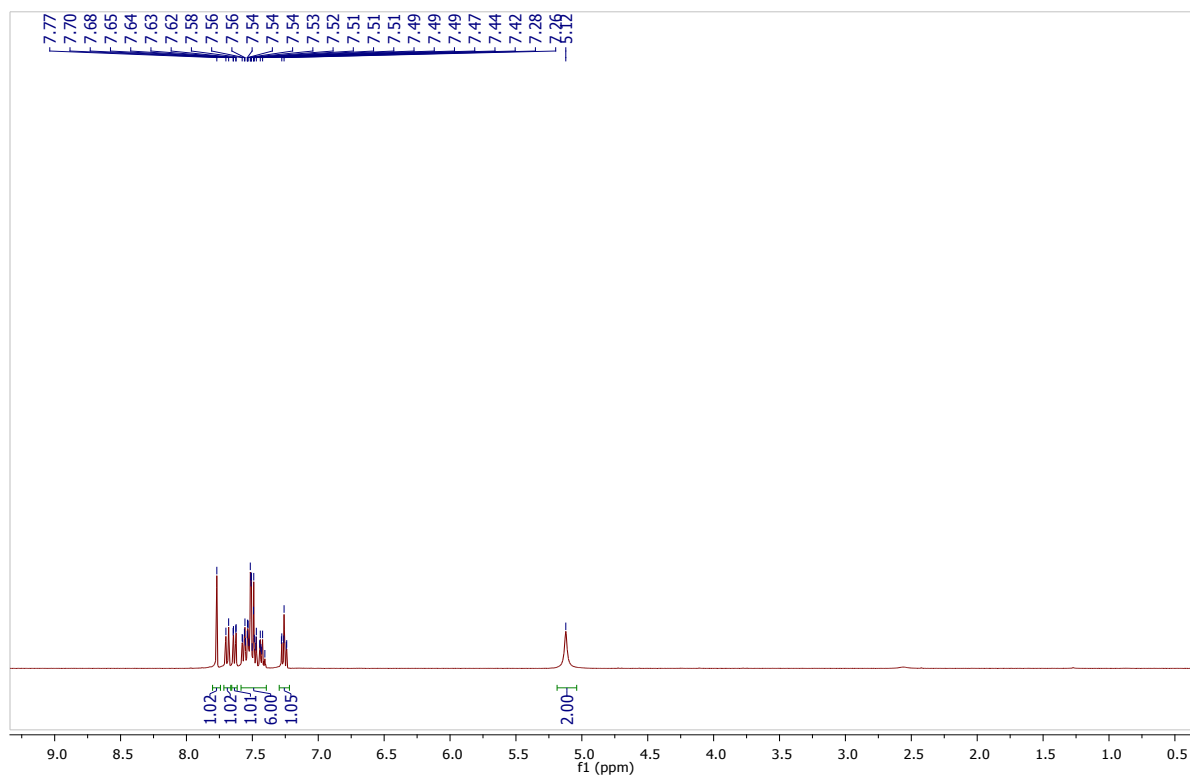
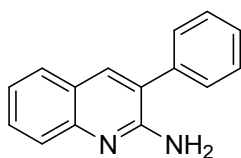


Figure S25. ¹H and ¹³C NMR spectra of 6a.

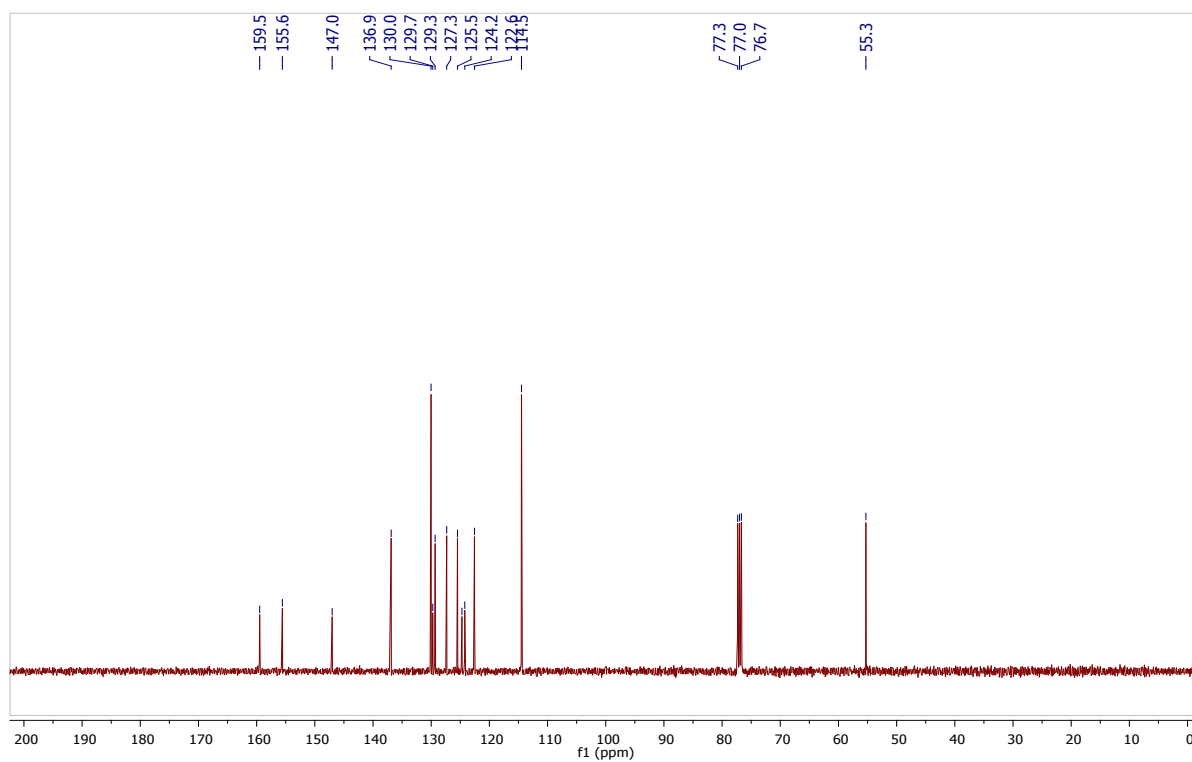
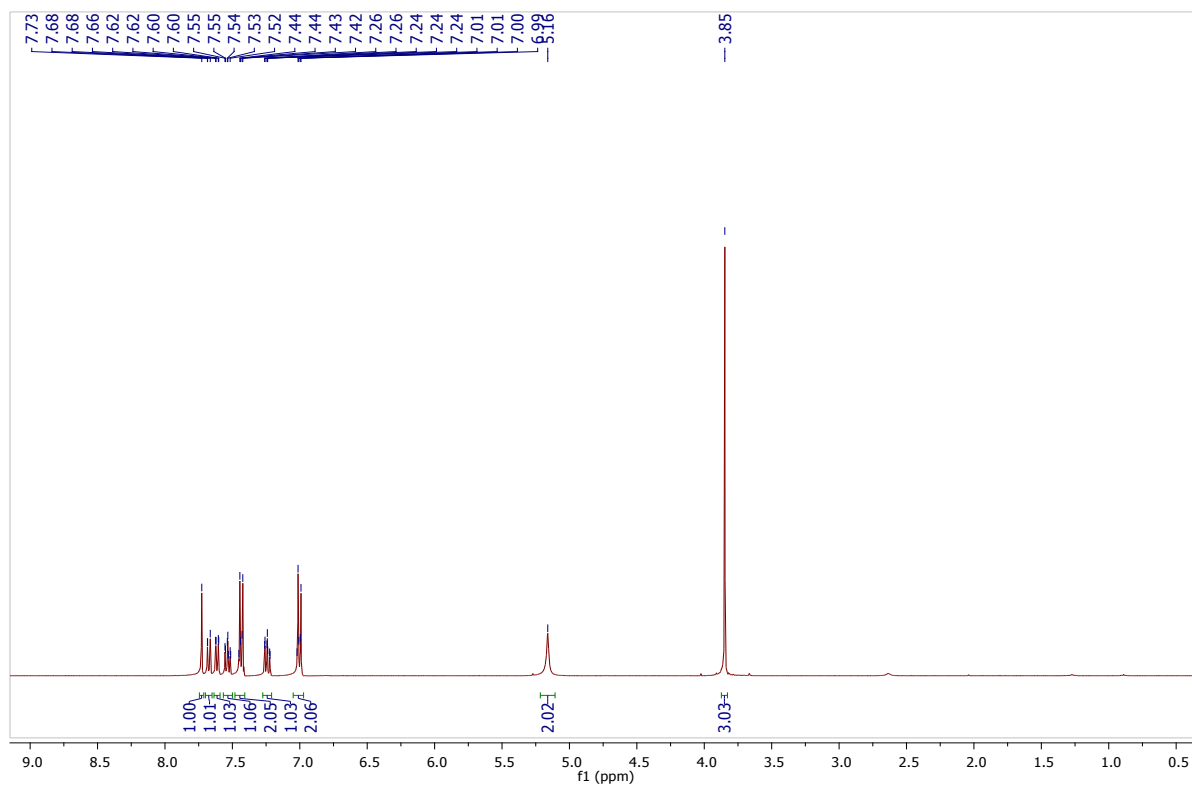
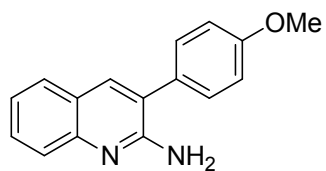


Figure S26. ^1H and ^{13}C NMR spectra of **6b**.

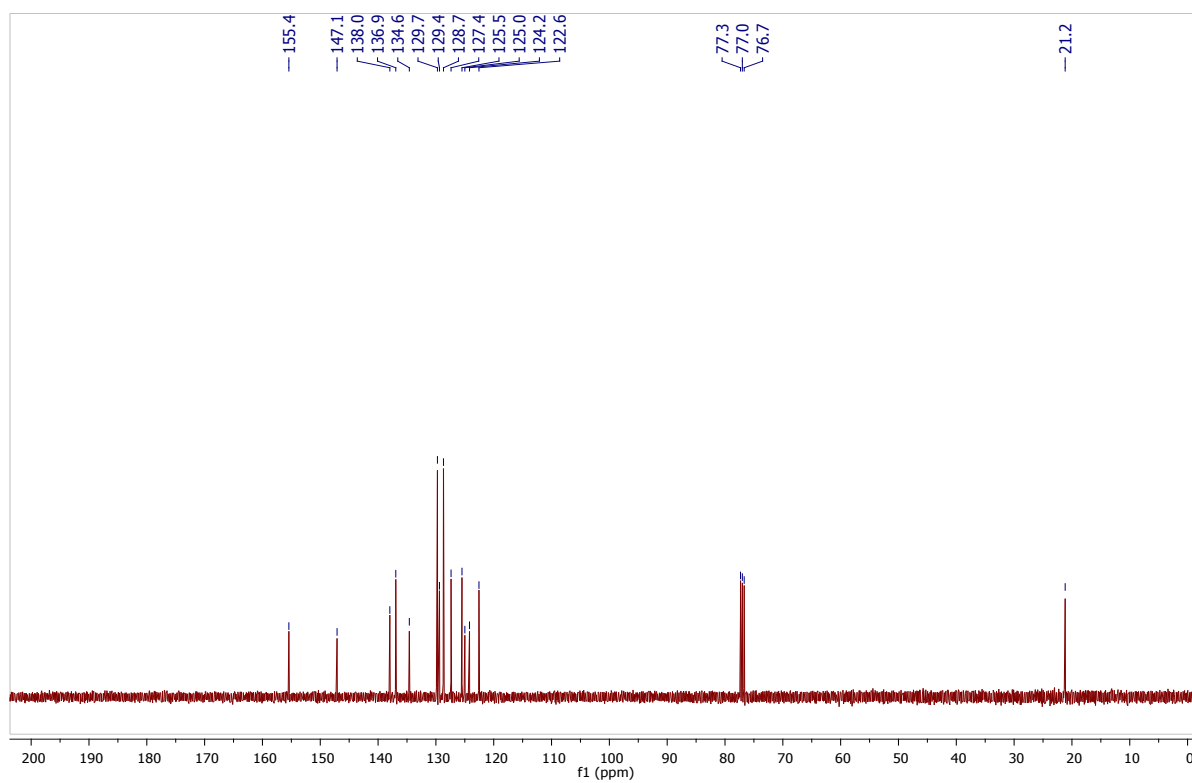
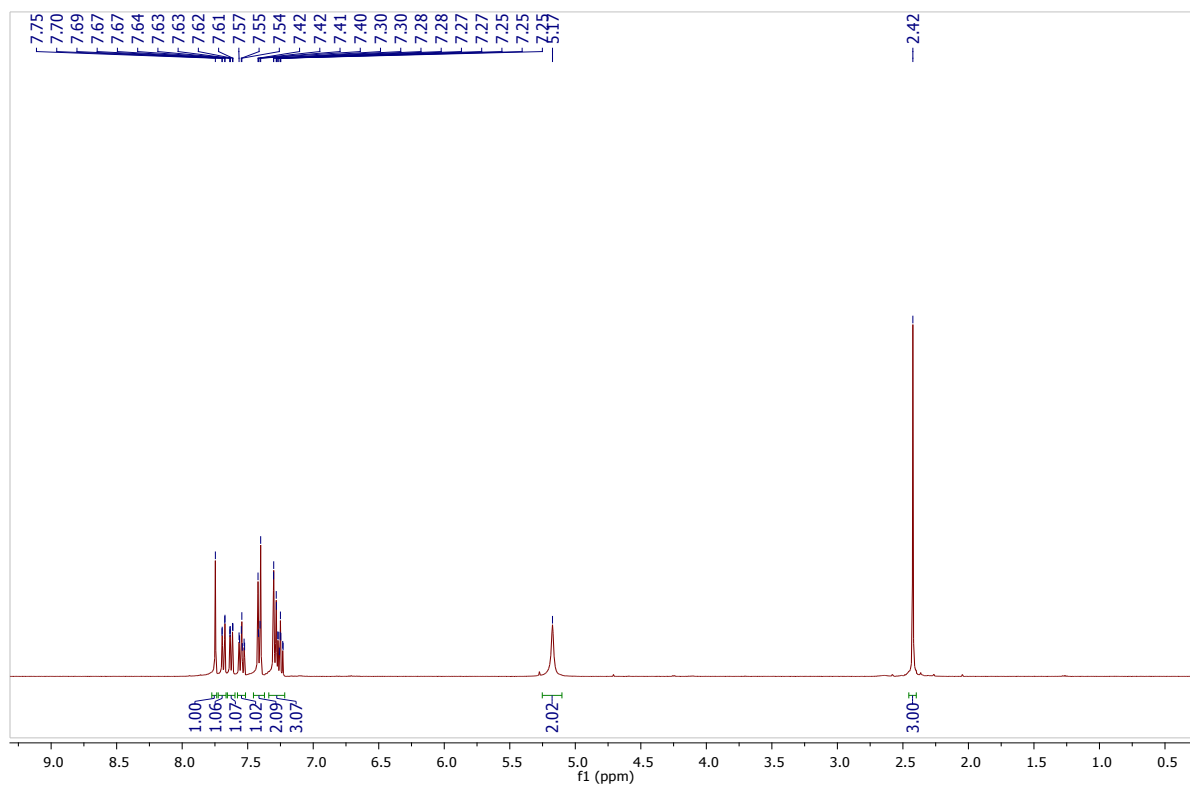
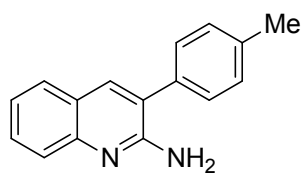


Figure S27. ^1H and ^{13}C NMR spectra of 6c.

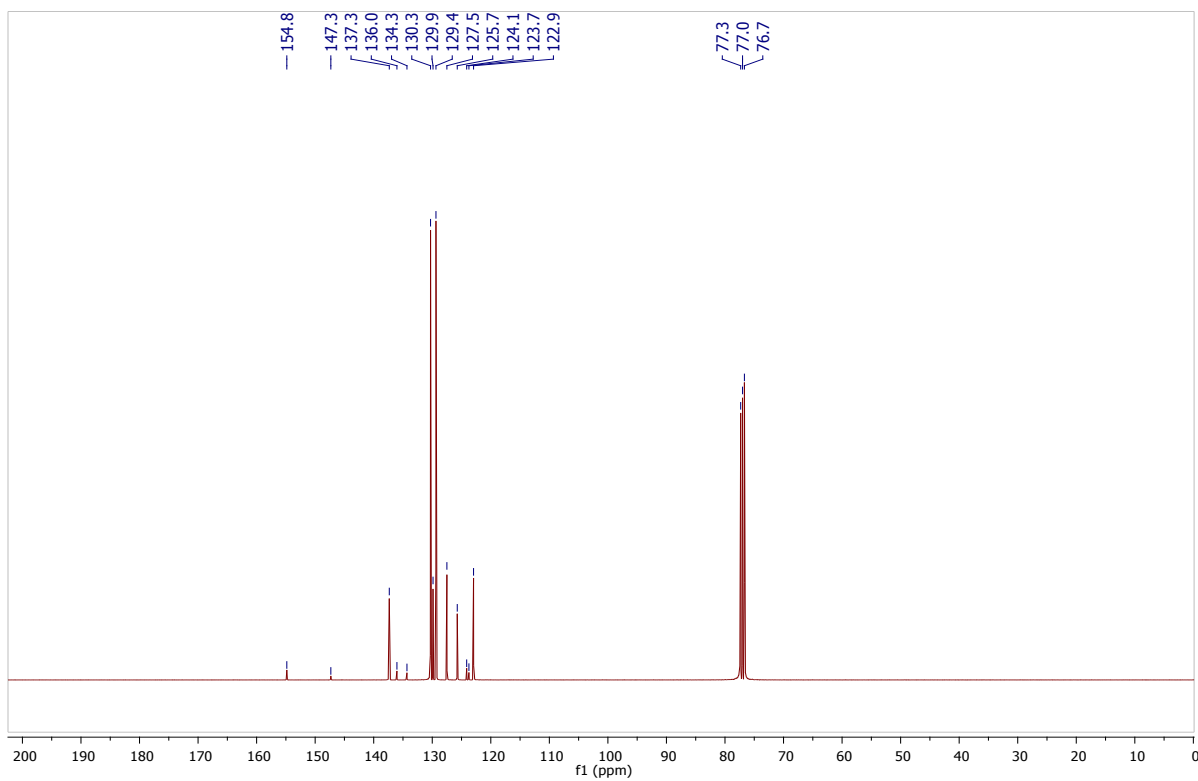
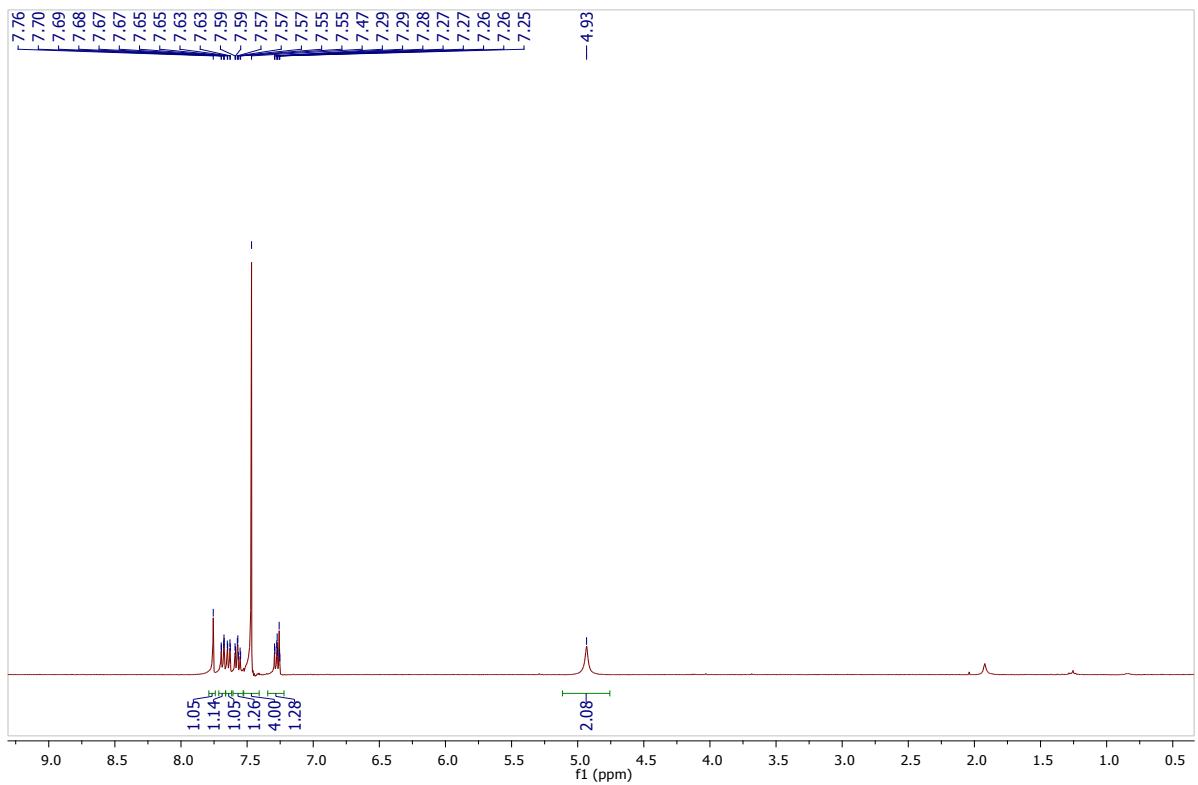
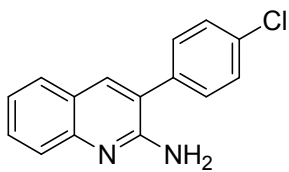


Figure S28. ¹H and ¹³C NMR spectra of 6d.

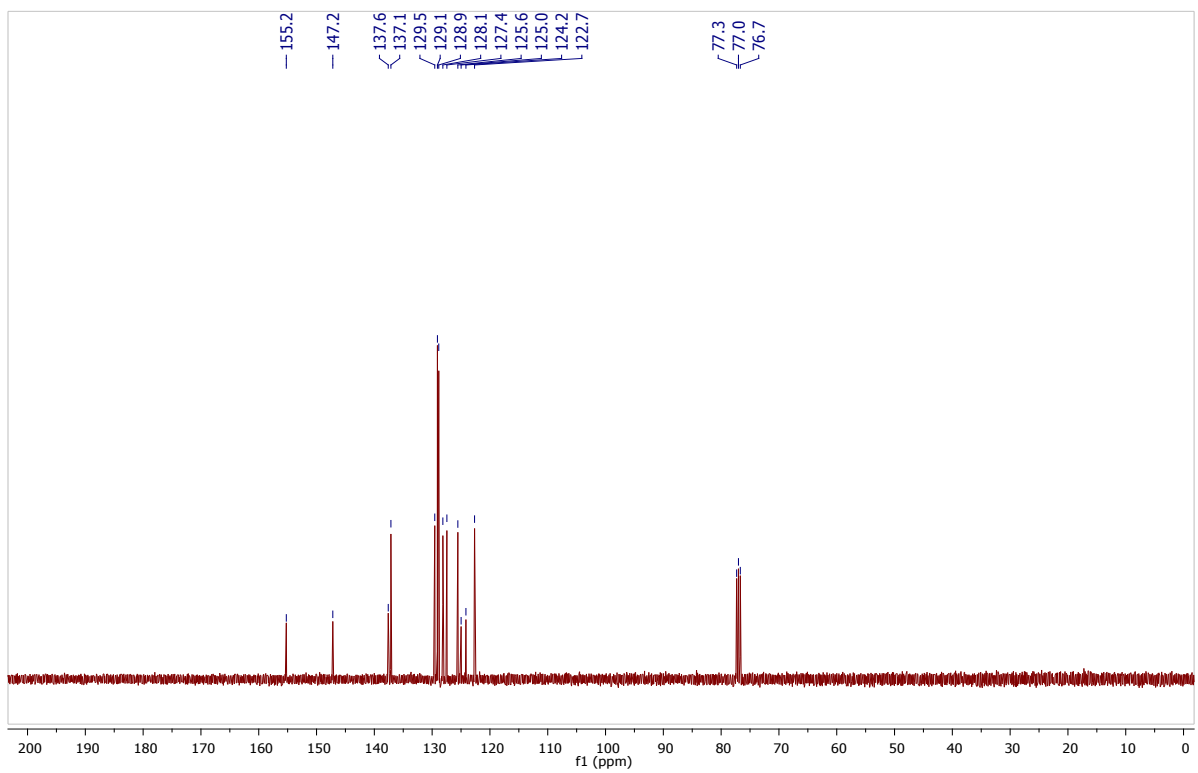
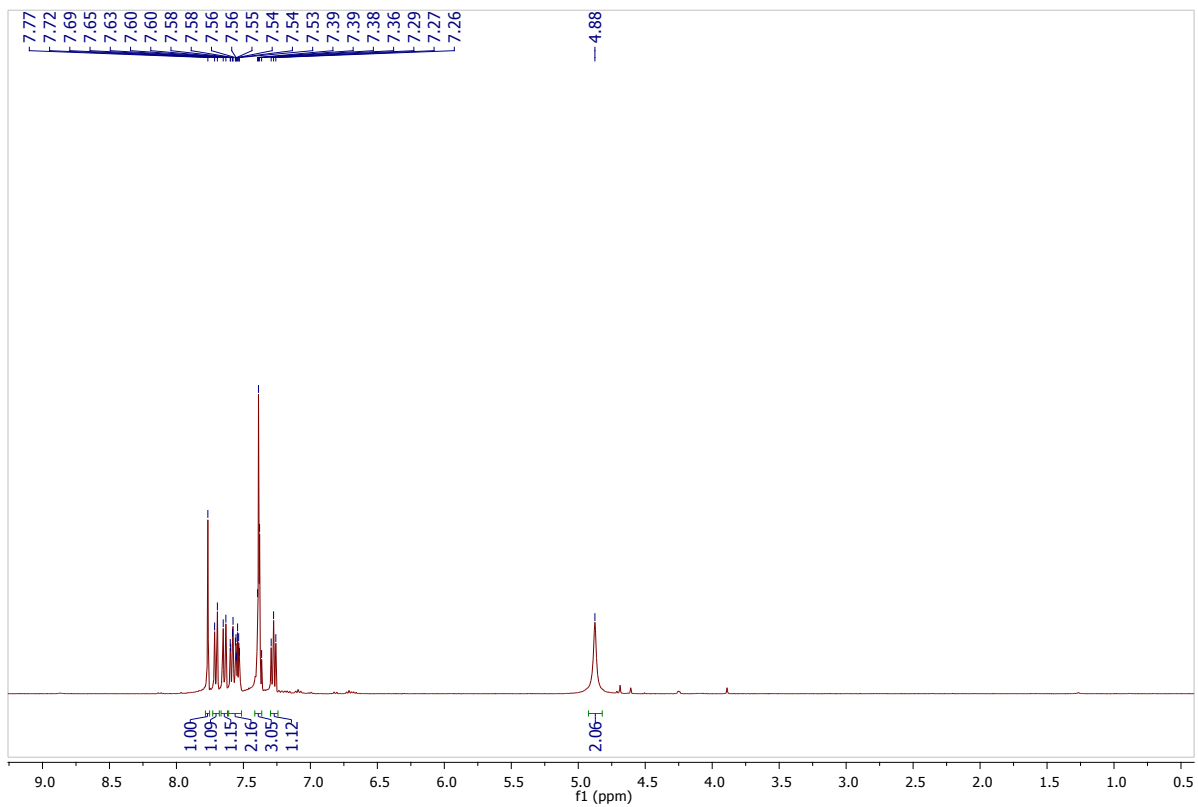
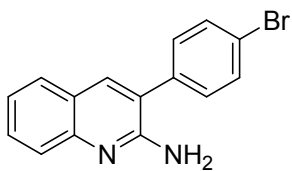
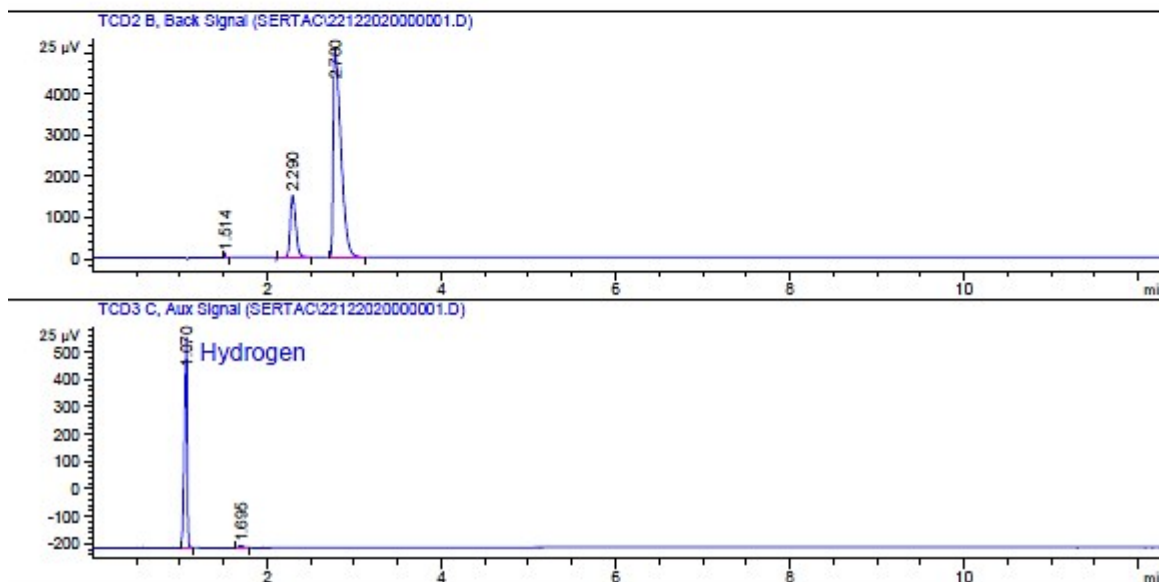


Figure S29. ¹H and ¹³C NMR spectra of 6e.

```

=====
Acq. Operator   : gozde
Acq. Instrument : Instrument 1           Location : Vial 1
Injection Date  : 12/22/2020 2:43:50 PM
                                           Inj Volume : Manually

Acq. Method     : C:\CHEM32\1\METHODS\23112020.M
Last changed    : 12/22/2020 2:38:44 PM by gozde
Analysis Method : C:\CHEM32\1\METHODS\22122020.M
Last changed    : 12/22/2020 3:07:52 PM by gozde
Sample Info     : CN
  
```



Signal 2: TCD2 B, Back Signal

| RetTime [min] | Type | Area [25 µV*s] | Amt/Area | Amount [% mole] | Grp | Name |
|---------------|------|----------------|------------|-----------------|-----|------|
| 1.795 | - | - | - | - | - | CO2 |
| 2.290 | BB | 6839.18994 | 0.00000 | 0.00000 | - | - |
| 2.780 | BB S | 3.11195e4 | 2.27134e-3 | 70.68298 | - | N2 |
| 4.250 | - | - | - | - | - | CO |

Totals : 70.68298

Signal 3: TCD3 C, Aux Signal

| RetTime [min] | Type | Area [25 µV*s] | Amt/Area | Amount [% mole] | Grp | Name |
|---------------|------|----------------|------------|-----------------|-----|------|
| 1.070 | BB | 1806.53967 | 5.30129e-3 | 9.57700 | - | H2 |

Totals : 9.57700

Figure S30. GC traces to confirm H₂ evolution.