## Contents

# 1 General Information

All reactions were carried out in flame dried glassware under a nitrogen atmosphere using standard Schlenk techniques. Glassware and stir bars contaminated with transition metals were treated with *aqua regia* (conc. HCl/conc. $HNO_3$ 3:1) prior to cleaning. For cleaning, glassware and stir bars were kept in a $^{i}$PrOH/KOH bath overnight, rinsed with $H_2O$, kept in a citric acid/$H_2O$ bath overnight and finally rinsed with dest. $H_2O$ and dried at 120 °C. Solutions and reagents were added with nitrogen-flushed disposable syringes/needles. Solvents were added using glass syringes and stainless steel needles (stored at 120 °C). Analytical thin layer chromatography (TLC) was performed on silica gel 60 G/$UV_{254}$ aluminium sheets (*Macherey-Nagel*). Flash column chromatography was performed on silica gel Davisil LC60A (40-63 µm, pore size 60 Å, *Grace*) using the indicated solvents. NMR spectra were recorded on AV400 or AV500 instruments (*Bruker*) at the Institut für Chemie of *Technische Universität Berlin*. Chemical shifts are reported in parts per million (ppm) and are referenced to the residual solvent resonance as the internal standard according to the standard literature.[1] Data are reported as follows: chemical shift, multiplicity (br s = broad singlet, s = singlet, d = doublet, t = triplet, q = quartet, sept = septet, m = multiplet, $m_c$ = centrosymmetric multiplet, app = apparent), coupling constants (Hz), integration and – if possible – atom assignment. The assignment refers to the atom number shown in the corresponding molecule figure and was achieved by analysis of DEPT (DEPT 135) and 2D-NMR spectra (COSY, HMQC, HMBC, NOESY). If a distinct assignment was not possible, atoms were marked with "*" and can be interchanged. Designation "*Ar*" refers to atoms of an aromatic system where a distinct assignment was not possible. Melting points (m.p.) were determined using a Leica Galen III melting point apparatus (*Wagner & Munz*). Infrared (IR) spectra were recorded on a Cary 630 FT-IR spectrometer equipped with an ATR unit (*Agilent Technologies).* Mass spectra (HRMS) were obtained from the Analytical Facility at the Institut für Chemie at *Technische Universität Berlin* (ESI/APCI: LTQ Orbitrap XL, *Thermo Scientific*; EI: GC-system 5975C, HP-5MS, *Agilent Technologies*).

All hydrogenation reactions were carried out in glass vials (50 x 14 mm, *Schütt*), equipped with a magnetic stir bar, a rubber septum pinched with a needle (0.90 x 50 mm, *Braun*) in autoclaves BR-100 or BR-300 (including the appropriate heating blocks; *Berghof*).

## 1.1 Solvents

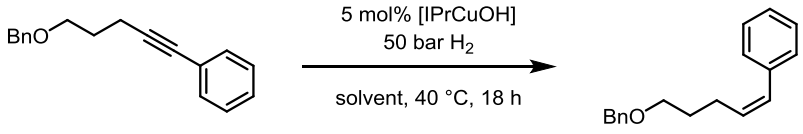
THF and 1,4-dioxane were dried over sodium/benzophenone and distilled under a $N_2$ atmosphere prior to use. $Et_3N$, $CH_2Cl_2$ and $Et_2O$ were dried over $CaH_2$ and distilled under a $N_2$ atmosphere prior to use. Acetonitrile (99.9%, extra dry) was purchased from *Acros*. Benzene (puriss., absolute) was purchased from *Sigma Aldrich*. Solvents (technical grade) for extraction/chromatography (EtOAc, cyclohexane, $CH_2Cl_2$, $Et_2O$, *tert*-butyl methyl ether) were distilled under reduced pressure prior to use.

## 1.2 Chemicals

The following chemicals were purchased commercially: Ethynylbenzene (**S2**), 1,2-Diphenylethyne (**3k**), Dodec-6-yne (**3o**), Methyl-non-2-ynoate (**3q**), ß-(*E*)-bromostyrene The following chemicals were synthesized according to literature procedures: (5-(Benzyloxy)pent-1-yn-1-yl)benzene (**1**),[2] Methyl 4-(5-(benzyloxy)pent-1-yn-1-yl)benzoate (**3a**),[2] 1-(5-(Benzyloxy)pent-1-yn-1-yl)-4-methoxybenzene (**3b**),[2] 1-(4-(5-(Benzyloxy)pent-1-yn-1-yl)phenyl)ethan-1-one (**3f**),[2] 2-(5-(Benzyloxy)pent-1-yn-1-yl)thiophene (**3g**),[2] 2-(5-(Benzyloxy)pent-1-yn-1-yl)pyridine (**3h**),[2] 3-(5-(Benzyloxy)pent-1-yn-1-yl)pyridine (**3i**),[2] 4-(5-(benzyloxy)pent-1-yn-1-yl)pyridine (**3j**),[2] ((Pent-4-yn-1-yloxy)methyl)benzene (**S1**),[2] 6-(Benzyloxy)hex-2-yn-1-ol (**S4**),[2] [IPrCuOH],[3] [IPr*CuOH].[4]

# 2 Additional screening results

## 2.1 Influence of the solvent

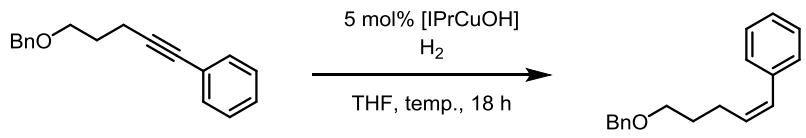



**1** **2**

| Entry | Solvent | Conversion [%][a] | *Z* / *E* / alkane[a] |
|---|---|---|---|
| **1** | THF | 87 | >99 / 0 / 0 |
| **2** | DMF | 25 | >99 / 0 / 0 |
| **3** | benzene | 32 | >99 / 0 / 0 |
| **4** | toluene | 26 | >99 / 0 / 0 |
| **5** | chlorobenzene | 13 | >99 / 0 / 0 |
| **6** | 1,2-dichlorobenzene | 5 | >99 / 0 / 0 |
| **7** | 2-Me-THF | 27 | >99 / 0 / 0 |
| **8** | *n*-hexane | 4 | >99 / 0 / 0 |
| **9** | 1,4-dioxane | 15 | >99 / 0 / 0 |

[a] Determined by GC analysis and $^1$H NMR.

## 2.2 Influence of pressure and temperature



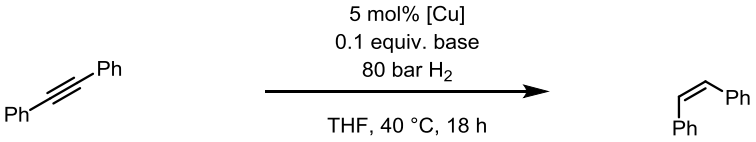

**1** **2**

| Entry | Pressure [bar] | Temperature [°C] | Conversion [%][a] | *Z*/*E*/alkane[a] |
|---|---|---|---|---|
| **1** | 50 | 40 | 87 | >99 / 0 / 0 |
| **2** | 70 | 40 | 98 | >99 / 0 / 0 |
| **3** | 80 | 40 | full (93%) | >99 / 0 / 0 |
| **4** | 100 | 40 | full | >99 / 0 / 0 |
| **5** | 50 | 60 | full | >99 / 0 / 0 |
| **6** | 40 | 60 | 95 | >99 / 0 / 0 |
| **7** | 30 | 60 | 61 | >99 / 0 / 0 |
| **8** | 1 | 60 | 0 | 0 / 0 / 0 |

[a] Determined by GC analysis and $^1$H NMR.

## 2.3 Investigation of *in situ* activation of the catalyst

To probe whether an *in situ* activation of the copper(I) hydroxide catalyst was possible, it was attempted to generate an active catalyst directly from the corresponding copper(I) halide complexes with a variety of hydroxides. None of the reactions displayed any turnover, demonstrating the need for a preactivated catalyst.

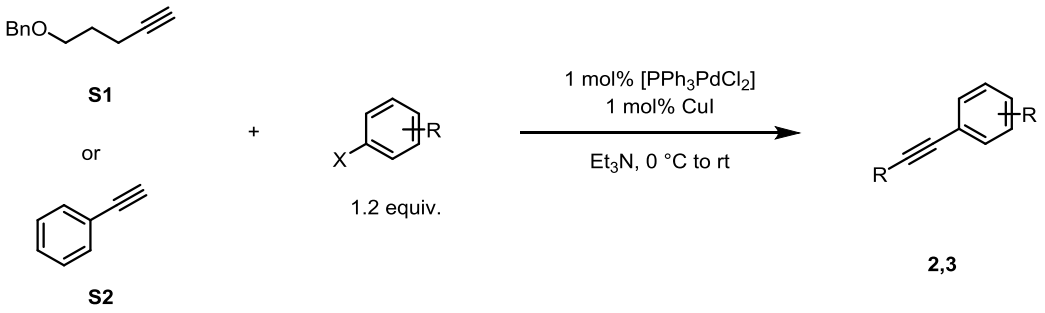



**3k** **4k**

with [IPrCuCl]: LiOH: 0% conv.
NaOH: 0% conv.
CsOH: 0% conv.

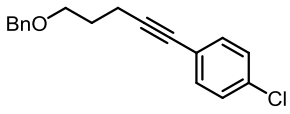
with [IPrCuBr]: LiOH: 0% conv.
NaOH: 0% conv.
CsOH: 0% conv.

## 3.1 General procedure – Sonogashira coupling (GP1)




According to a literature procedure, the terminal alkyne (**S1, S2**, 1.0 equiv.) is added dropwise to a stirred mixture of $[(PPh_3)_2PdCl_2]$ (1 mol%), CuI (1 mol%) and the corresponding aryl halide (1.2 equiv.) in $Et_3N$ (0.2 M) at 0 °C. After complete addition the mixture is allowed to warm to r.t. and stirred until full conversion of the starting material is detected by TLC or NMR analysis (for reaction time see corresponding substrates). The reaction is quenched by adding $H_2O$ (5 mL/mmol) and extracted with *tert*-butyl methyl ether (5 mL/mmol). The layers are separated and the organic phase is washed with aq. HCl-solution (2M, 5 mL/mmol), brine (5 mL/mmol) and dried over $MgSO_4$. After filtration, all volatiles are removed under reduced pressure to afford the crude product. Purification by flash column chromatography (cyclohexane/*tert*-butyl methyl ether) affords the pure products (**2, 3**).

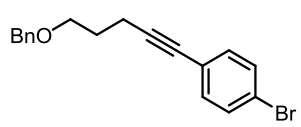
### 3.1.1 1-(5-(Benzyloxy)pent-1-yn-1-yl)-4-chlorobenzene (**3c**)




**3c**
$C_{18}H_{17}ClO$
Mw = 284.78 g/mol

Prepared from **S1** (0.70 g, 4.0 mmol, 1.0 equiv.) and 1-chloro-4-iodobenzene (1.1 g, 4.8 mmol, 1.2 equiv.) using $[(PPh_3)_2PdCl_2]$ (28 mg, 40 µmol, 1 mol%) and CuI (7.6 mg, 40 µmol, 1 mol%) following **GP1**. The reaction mixture was stirred for 22 h at rt. Purification by flash column chromatography (cyclohexane/*tert*-butyl methyl ether 100:1) yielded internal alkyne **3c** (0.66 g, 2.3 mmol, 58%) as a pale yellow oil. $\mathbf{R_f}$ = 0.67(cyclohexane/*tert*-butyl methyl ether 10:1). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 1.83 ($m_c$, 2H), 2.45 (t, $^3J$ = 7.1 Hz, 2H), 3.54 (t, $^3J$ = 6.2 Hz, 2H), 4.46 (s, 2H), 7.15-7.21 (m, 5H), 7.26-7.27 (m, 4H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 16.3, 228.8, 68.7, 73.0, 79.8, 90.7, 122.4, 127.5, 127.6, 128.4, 128.5, 132.8, 133.5, 138.5 ppm. **HRMS** (APCI) calcd for $C_{18}H_{18}ClO^+$ $[(M+H)^+]$: 285.1041, found: 285.1035. **IR** (ATR) ν = 2856 (w), 1489 (s), 1453 (m), 1089 (s), 1027 (m), 1014 (s), 827 (s), 733 (s), 696 (s), 521 (s), 472 (m) $cm^{-1}$.

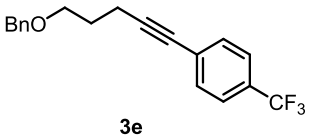
### 3.1.2 1-(5-(Benzyloxy)pent-1-yn-1-yl)-4-bromobenzene (**3d**)



**3d**
$C_{18}H_{17}BrO$
Mw = 329.24 g/mol

Prepared from **S1** (1.0 g, 5.7 mmol, 1.0 equiv.) and 1,4-dibromobenzene (1.6 g, 6.9 mmol, 1.2 equiv.) using $[(PPh_3)_2PdCl_2]$ (40 mg, 57 µmol, 1 mol%) and CuI (11 mg, 57 µmol, 1 mol%) following **GP1**. The reaction mixture was stirred for 48 h at rt. Purification by flash column chromatography (cyclohexane/*tert*-butyl methyl ether 100:1) yielded internal alkyne **3d** (0.72 g, 2.2 mmol, 38%) as a colorless oil. $\mathbf{R_f}$ = 0.35 (cyclohexane/*tert*-butyl methyl ether 10:1). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 1.91 ($m_c$, 2H), 2.53 (t, $^3J$ = 7.1 Hz, 2H), 3.62 (t, $^3J$ = 6.2 Hz, 2H), 4.54 (s, 2H), 7.22 ($m_c$, 2H), 7.27-7.30 (m, 1H), 7.33-7.37 (m, 4H), 7.41 ($m_c$, 2H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 16.5, 28.9, 68.9, 73.1, 80.0, 91.1, 121.8, 123.1, 127.7, 127.8, 128.5, 131.5, 133.2, 138.6 ppm. **HRMS** (EI) calcd for $C_{18}H_{17}BrO^+$ [$(M)^+$]: 328.0457, found: 328.0461. **IR** (ATR) ν = 2858 (w), 1484 (s), 1453 (m), 1099 (s), 1069 (s), 1028 (s), 1010 (s), 822 (s), 735 (s), 697 (s), 522 (s), 457 (s) $cm^{-1}$.

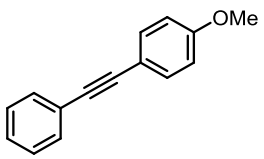
### 3.1.3 1-(5-(Benzyloxy)pent-1-yn-1-yl)-4-(trifluoromethyl)benzene (**3e**)



**3e**
$C_{19}H_{17}F_3O$
Mw = 318.34 g/mol

Prepared from **S1** (1.2 g, 6.9 mmol, 1.0 equiv.) and 4-bromobenzotriflouride (1.6 g, 6.9 mmol, 1.2 equiv.) using $[(PPh_3)_2PdCl_2]$ (97 mg, 140 µmol, 1 mol%) and CuI (26 mg, 140 µmol, 1 mol%) following **GP1**. The reaction mixture was stirred for 48 h at rt. Purification by flash column chromatography (cyclohexane/*tert*-butyl methyl ether 100:1) yielded internal alkyne **3e** (1.0 g, 3.3 mmol, 47%) as a colorless oil. $\mathbf{R_f}$ = 0.38 (cyclohexane/*tert*-butyl methyl ether 10:1). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 1.93 ($m_c$, 2H), 2.57 (t, $^3J$ = 7.1 Hz, 2H), 3.64 (t, $^3J$ = 6.1 Hz, 2H), 4.55 (s, 2H), 7.27-7.31 (m, 1H), 7.33-7.38 (m, 4H), 7.45-7.46 (m, 2H), 7.53-7.54 (m, 2H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 16.5, 28.9, 68.8, 73.1, 79.9, 92.6, 124.2 (q, $^1J$ = 272 Hz), 125.2 (q, $^3J$ = 4.0 Hz), 127.7, 127.8, 127.9, 128.5, 129.5 (q, $^2J$ = 32.5 Hz), 131.9, 138.6 ppm. **$^{19}$F NMR** (470 MHz, $CDCl_3$): δ = -62.7 ppm. **HRMS** (EI) calcd for $C_{19}H_{17}FO^+$ [$(M)^+$]: 318.1226-, found: 318.1229. **IR** (ATR) ν = 2858 (w), 1615 (m), 1321 (s), 1164 (s), 1121 (s), 1104 (s), 1066 (s), 1017 (m), 841 (s), 735 (m), 697 (s), 598 (m) $cm^{-1}$.

### 3.1.4 1-Methoxy-4-(phenylethynyl)benzene (**3l**)

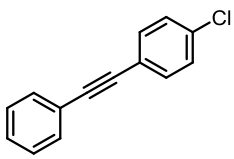


**3l**
$C_{15}H_{12}O$
Mw = 208.26 g/mol

Prepared from **S2** (1.0 g, 9.8 mmol, 1.0 equiv.) and 1-iodo-4-methoxybenzene (2.5 g, 11. mmol, 1.1 equiv.) using $[(PPh_3)_2PdCl_2]$ (69 mg, 98 µmol, 1 mol%) and CuI (19 mg, 98 µmol, 1 mol%) in $Et_3N$ (50 mL) following **GP1**. The reaction mixture was stirred for 24 h at rt. Purification by flash column chromatography on silica gel using cyclohexane/*tert*-butyl methyl ether 100:1 as eluent yielded **3l** (2.0 g, 9.8 mmol, 99%) as a white solid. $\boldsymbol{R_f}$ = 0.54 (cyclohexane/*tert*-butyl methyl ether 10:1). **$^1$H NMR** (500 MHz, $CD_2Cl_2$): δ = 3.83 (s, 3H), 6.89 ($m_c$, 2H), 7.30-7.36 (m, 3H), 7.48 ($m_c$, 2H), 7.52 (m, 2H) ppm. **$^{13}$C NMR** (126 MHz, $CD_2Cl_2$): δ = 55.4, 88.2, 89.5, 114.1,

115.5, 123.8, 128.1, 128.4, 131.6, 133.2, 159.8 ppm. **HRMS** (EI) calcd for $C_{15}H_{12}O^+$ [$(M)^+$]: 208.0883, found: 208.0883.
The data is in accordance with the literature.[5]

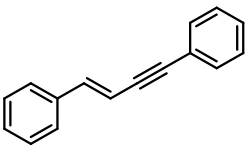
### 3.1.5 1-Chloro-4-(phenylethynyl)benzene (**3m**)




**3m**
$C_{14}H_9Cl$
Mw = 212.68 g/mol

Prepared from **S2** (0.41 g, 4.0 mmol, 1.0 equiv.) and 1-chloro-4-iodobenzene (0.96 g, 4.8 mmol, 1.2 equiv.) using [$(PPh_3)_2PdCl_2$] (28 mg, 40 µmol, 1 mol%) and CuI (7.6 mg, 40 µmol, 1 mol%) in $Et_3N$ (15 mL) following **GP1**. The reaction mixture was stirred for 24 h at rt Purification by flash column chromatography on silica gel using pentane as eluent yielded **3m** (0.64 g, 3.0 mmol, 75%) as a white solid. $\boldsymbol{R_f}$ = 0.55 (cyclohexane). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 7.32-7.38 (m, 5H), 7.45-7.47 ($m_c$, 2H), 7.51-7.55 (m, 2H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 88.4, 90.5, 121.9, 123.1, 128.5, 128.6, 128.8, 131.7, 133.0, 134.4 ppm. **HRMS** (EI) calcd for $C_{14}H_9Cl^+$ [$(M)^+$]: 212.0387, found: 212.0393.
The data is in accordance with the literature.[6]

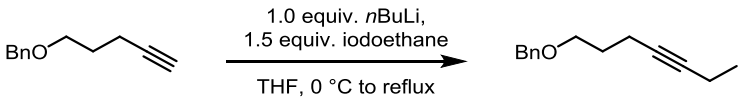
3.1.6 (*E*)-But-1-en-3-yne-1,4-diyldibenzene (**7**)



**7**
$C_{16}H_{12}$
Mw = 204.27 g/mol

Prepared from **S2** (0.41 g, 4.0 mmol, 1.0 equiv.) and ß-(*E*)-bromostyrene (0.88 g, 4.8 mmol, 1.2 equiv.) using [$(PPh_3)_2PdCl_2$] (28 mg, 40 µmol, 1 mol%) and CuI (7.6 mg, 40 µmol, 1 mol%) in $Et_3N$ (15 mL) following **GP1**. The reaction mixture was stirred for 23 h at rt. Purification by flash column chromatography on silica gel using cyclohexane as eluent yielded **7** (0.55 g, 2.7 mmol, 67%) as a pale yellow solid. *E*/*Z*-**7** = 99:1 as judged by $^1$H NMR. $\boldsymbol{R_f}$ = 0.31 (cyclohexane). **$^1$H NMR** (500 MHz, $CD_2Cl_2$): δ = 6.43 (d, $^3J$ = 16.2 Hz, 1H), 7.07 (d, $^3J$ = 16.2 Hz, 1H), 7.30-7.38 (m, 6H), 7.44-7.51 (m, 4H) ppm. **$^{13}$C NMR** (126 MHz, $CD_2Cl_2$): δ = 89.2, 92.0, 108.4, 123.8, 126.7, 128.7, 128.8, 129.1, 129.2, 131.9, 136.7, 141.7 ppm. **HRMS** (EI) calcd for $C_{16}H_{12}^+$ [$(M)^+$]: 204.0939, found: 204.0930.
The data is in accordance with the literature.[7]

3.1.7 ((Hept-4-yn-1-yloxy)methyl)benzene (**3n**)

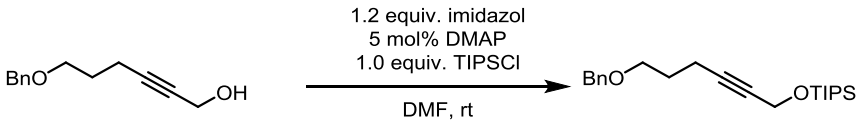



**S1**

**3n**
$C_{14}H_{18}O$
Mw = 202.30 g/mol

On the basis of a literature procedure[8] a solution of **S1** (0.70 g, 4.0 mmol, 1.0 equiv.) in THF (13 mL) was cooled to 0 °C. *n*-Butyllithium (2.5M in hexane, 1.6 mL, 4.0 mmol, 1.0 equiv.) was added dropwise. After 20 min the mixture was allowed to warm to rt. Then, iodoethane was added and the mixture was heated to reflux for 22 h. After cooling down to rt the reaction was quenched by the addition of $H_2O$ (30 mL). The layers were separated and the aqueous layer was extracted with TBME (3 x 10 mL). The combined organic layers were washed with brine (30 mL) and dried over $Na_2SO_4$. After filtration and concentration under reduced pressure the crude product was purified by flash column chromatography on silica gel using cyclohexane/*tert*-butyl methyl ether 150:1 as eluent to yield **3n** (0.69 g, 3.4 mmol, 85%) as a colorless liquid. $\boldsymbol{R_f}$ = 0.62 (cyclohexane/*tert*-butyl methyl ether 10:1). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 1.10 (t, $^3J$ = 7.5 Hz, 3H), 1.79 ($m_c$, 2H), 2.15 (qt, $^3J$ = 7.5 Hz, $^5J$ = 2.4 Hz, 2H), 2.27 (tt, $^3J$ = 7.1 Hz, $^5J$ = 2.4 Hz, 2H), 3.57 (t, $^3J$ = 6.3 Hz, 2H), 4.52 (s, 2H), 7.28 ($m_c$, 1H), 7.32-7.36 (m, 4H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 13.5, 14.5, 15.7, 29.4, 69.1, 73.1, 78.9, 82.1, 127.6, 127.7, 128.5, 138.8 ppm. **HRMS** (EI) calcd for $C_{16}H_{12}^+$ [$(M)^+$]: 204.0939, found: 204.0930.
The data is in accordance with the literature.[2]

### 3.1.8 ((6-(Benzyloxy)hex-2-yn-1-yl)oxy)triisopropylsilane (**3p**)




**S4**

**3p**
$C_{22}H_{36}O_2Si$
Mw = 360.61 g/mol

In a flame-dried 25 mL Schlenk flask, **S4** (0.50 g, 2.5 mmol, 1.0 equiv.), imidazol (0.20 g, 2.9 mmol, 1.2 equiv.) and 4-(dimethylamino)pyridine (DMAP, 15 mg, 0.12 mmol, 5 mol%) were dissolved in DMF (5 mL). Triisopropylsilylchloride (0.47 g, 2.5 mmol, 1.0 equiv.) was added dropwise. The reaction was stirred overnight at rt and was quenched by addition of water (50 mL). The aqueous phase was extracted with TBME (3 x 15 mL), the combined organic layers were washed with brine (20 mL) and dried over $MgSO_4$. After filtration and removal of all volatiles under reduced pressure the crude product was purified by flash column chromatography on silica gel using cyclohexane/*tert*-butyl methyl ether 50:1 as eluent to afford **3p** (0.776 g, 2.15 mmol, 88%) as a colorless oil. $\boldsymbol{R_f}$ = 0.48 (cyclohexane/*tert*-butyl methyl ether 30:1). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 1.06-1.09 (m, 18H), 1.10-1.16 (m, 3H), 1.81 ($m_c$, 2H), 2.34 (tt, $^3J$ = 7.1 Hz, $^5J$ = 2.2 Hz, 2H), 3.56 (t, $^3J$ = 6.2 Hz, 2H), 4.35 (t, $^5J$ = 2.2 Hz, 2H), 4.51 (s, 2H), 7.27-7.36 (m, 5H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 12.2, 15.8, 18.1, 29.0, 52.3, 69.1, 73.1, 79.3, 84.5, 127.7, 127.8, 128.5, 138.7 ppm. **$^{29}$Si NMR** (99 MHz, $CDCl_3$): δ = 16.0 ppm. **HRMS** (APCI) calcd for $C_{22}H_{35}O_2Si^+$ [$(M-H)^+$]: 359.2401, found: 359.2410. **IR** (ATR) ν = 2942 (s), 2864 (s), 1454 (m), 1364 (m), 1141 (s), 1082 (s), 1065 (s), 882 (s), 733 (s), 680 (s), 659 (m) $cm^{-1}$.

### 3.1.9 1,4-Diphenylbuta-1,3-diyne (**5**)


**5**
$C_{16}H_{10}$
Mw = 202.26 g/mol

Following a literature procedure,[9] in a flame-dried 25 mL Schlenk flask $CuCl_2$ (0.79 g, 5.9 mmol, 1.0 equiv.) was suspended in DMF (12 mL). TMEDA (0.68 g, 5.9 mmol, 1.0 equiv.) and **S2** (0.60 g, 5.9 mmol, 1.0 equiv.) were added and the mixture was heated to 70 °C for 48 h. The reaction mixture was poured onto water (100 mL). The aqueous phase was extracted with TBME (3 x 20 mL). The combined organic layers were washed with brine (50 mL) and dried over $MgSO_4$. After filtration and removal of all volatiles under reduced pressure the crude product was purified by flash column chromatography on silica gel using cyclohexane as eluent to afford **5** (0.33 g, 1.6 mmol, 55%) as a white crystalline solid. $\boldsymbol{R_f}$ = 0.52 (cyclohexane). **$^1$H NMR** (500 MHz, $CDCl_3$): δ = 7.32-7.40 (m, 6H), 7.52-7.55 (m, 4H) ppm. **$^{13}$C NMR** (126 MHz, $CDCl_3$): δ = 74.1, 81.7, 122.0, 128.6, 129.4, 132.7 ppm. **HRMS** (EI) calcd for $C_{16}H_{10}^+$ [$(M)^+$]: 202.0777, found: 202.0787.
The data is in accordance with the literature.[9]

# 4 References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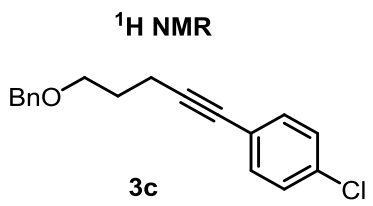
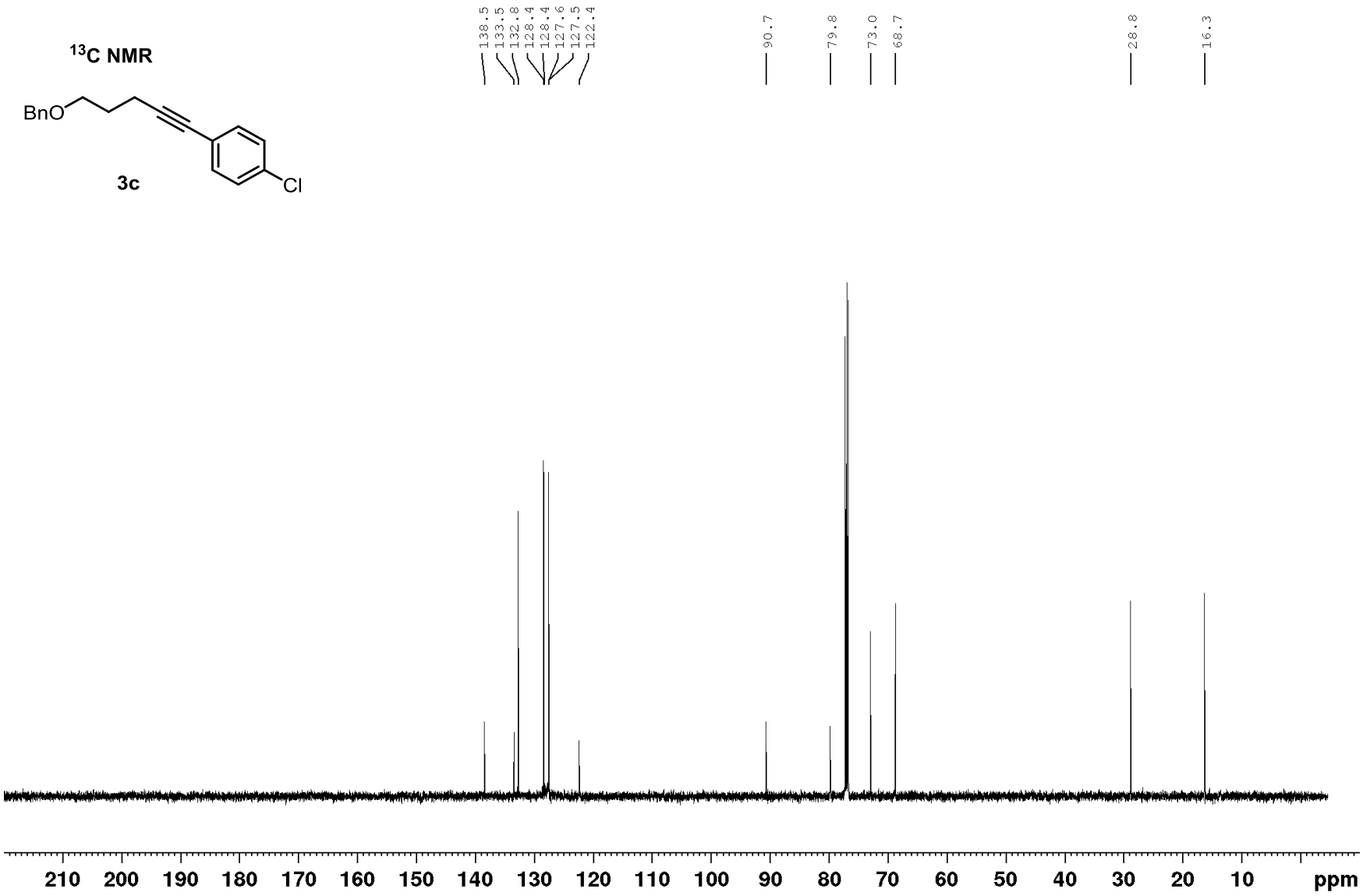
## 5 Spectra

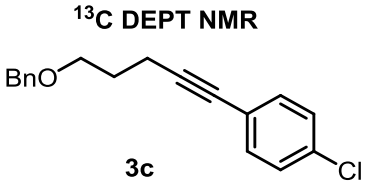
**$^1$H NMR**



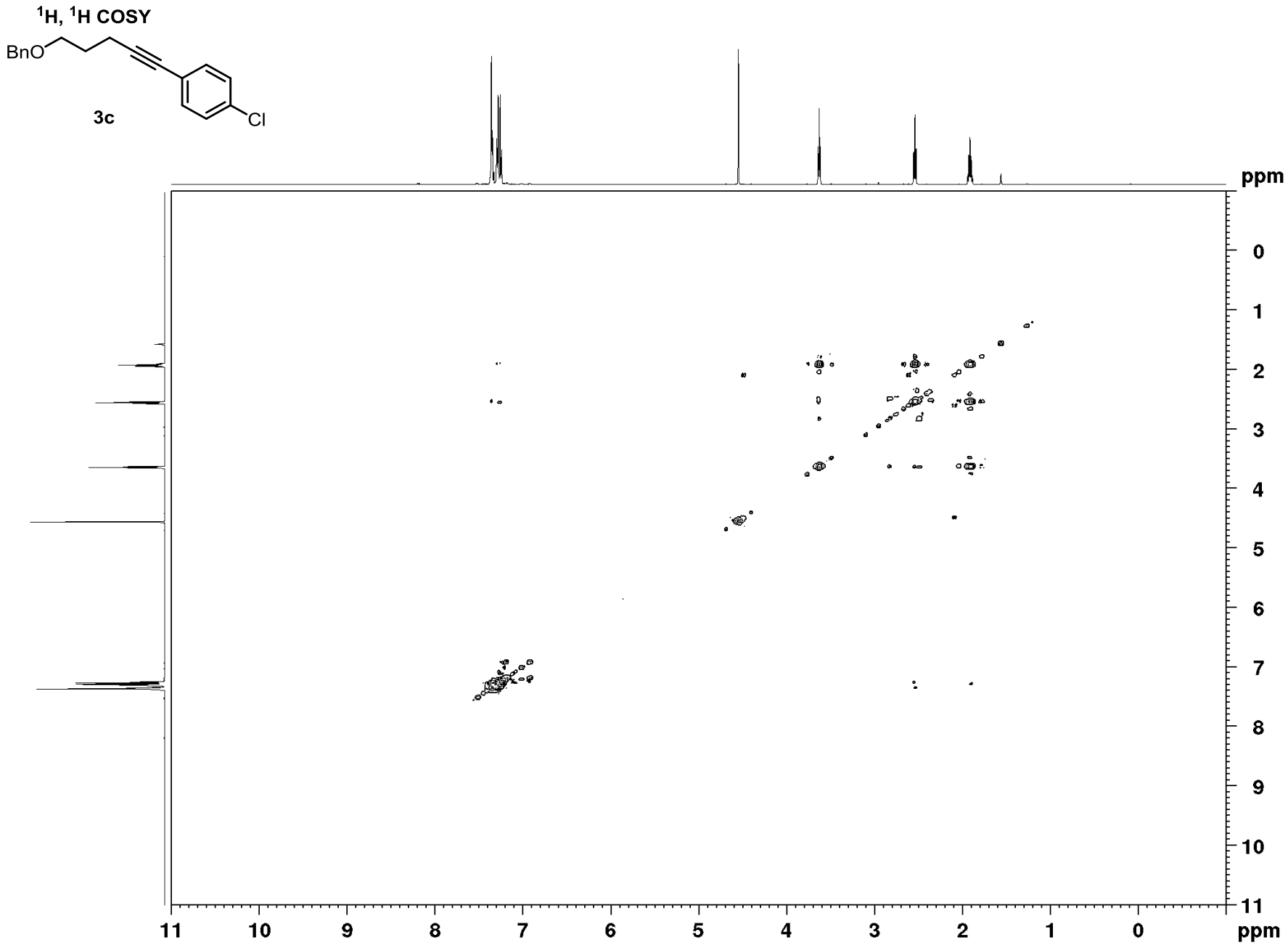

**3c**


$^{13}$C NMR
BnO
Cl
3c
138.5
133.5
132.8
128.4
128.4
127.6
127.5
122.4
90.7
79.8
73.0
68.7
28.8
16.3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

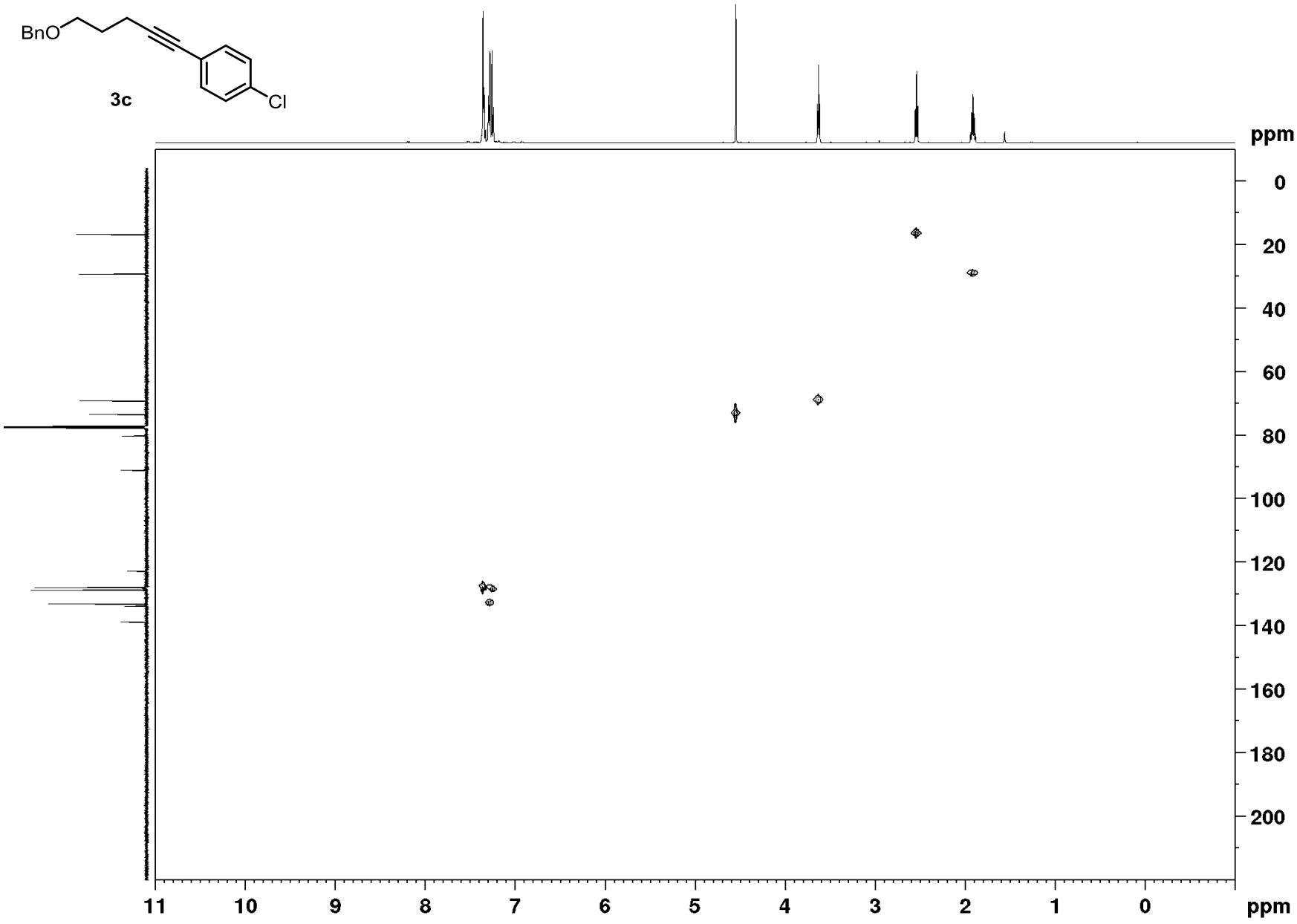
**$^{13}$C DEPT NMR**



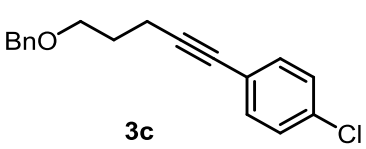

**3c**


$^1$H, $^1$H COSY
BnO
Cl
3c
ppm
0
1
2
3
4
5
6
7
8
9
10
11
ppm
11
10
9
8
7
6
5
4
3
2
1
0

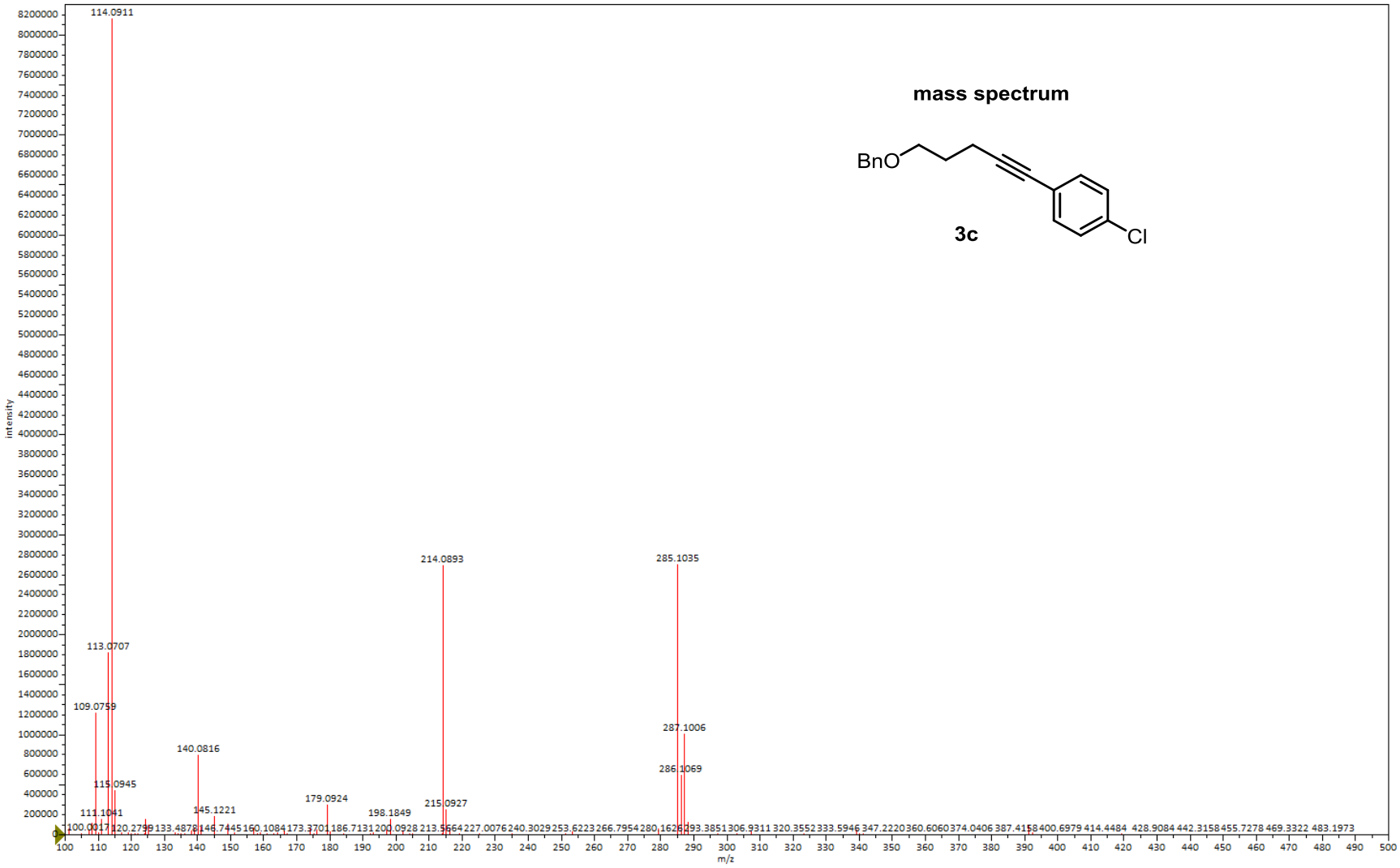
**$^{1}H$, $^{13}C$ HMQC**


BnO
Cl
3c
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^{1}H$, $^{13}C$ HMBC**




**3c**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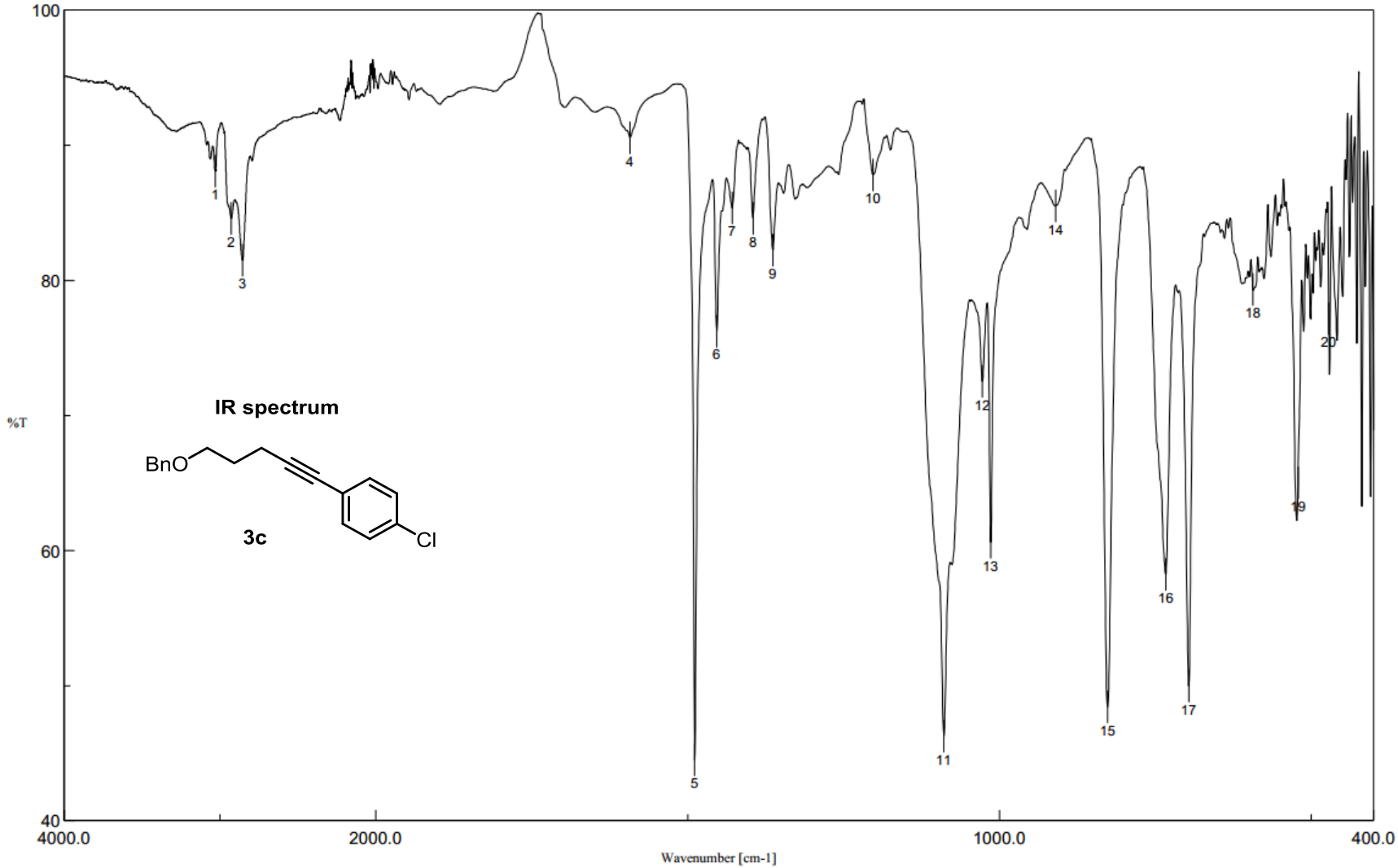
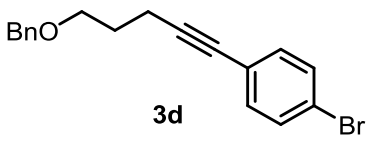
BnO
Cl
3c
intensity
m/z
114.0911
214.0893
285.1035
113.0707
109.0759
287.1006
286.1069
140.0816
115.0945
179.0924
215.0927
145.1221
198.1849
111.1041

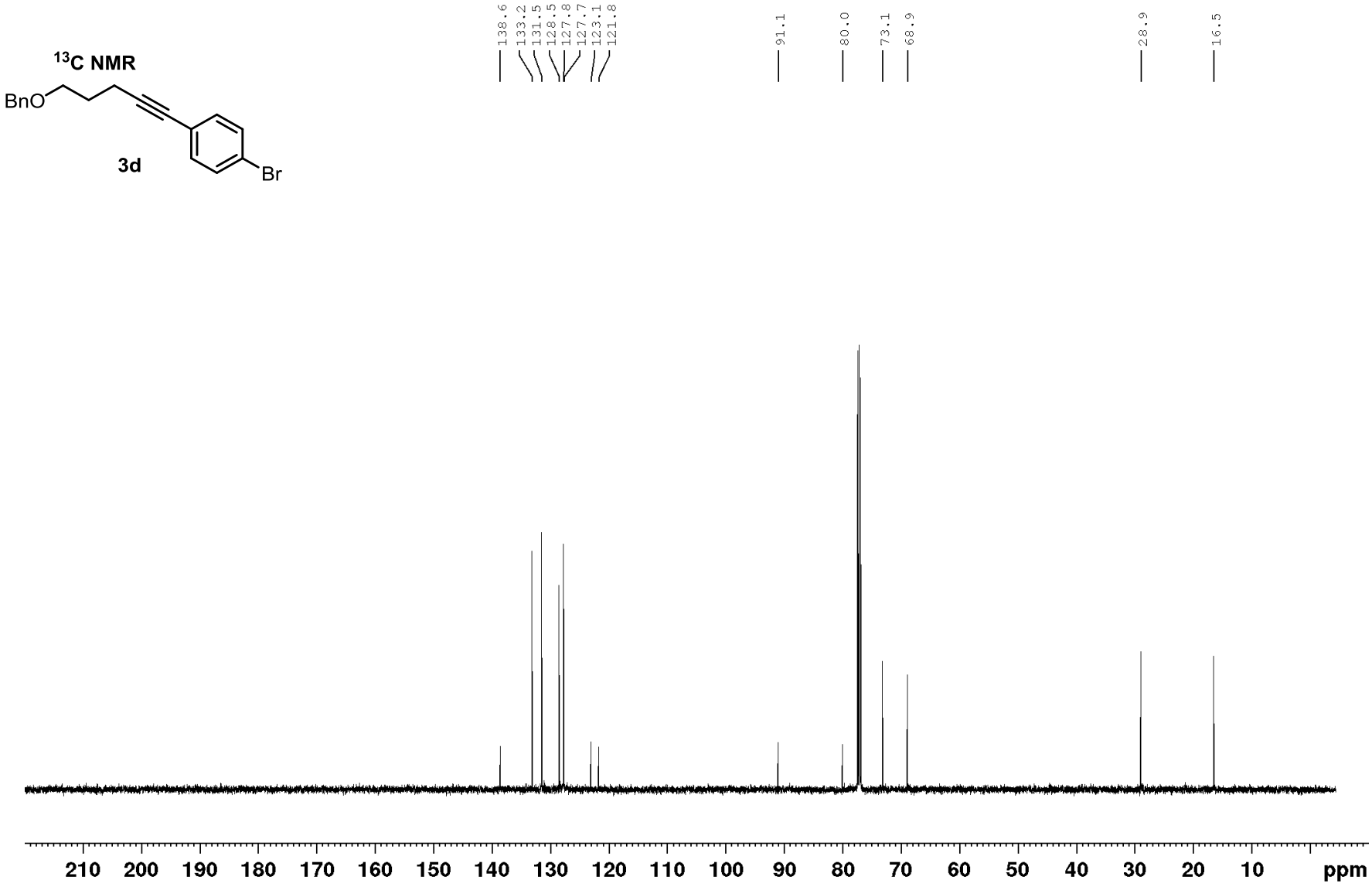

IR spectrum
BnO
Cl
3c
%T
100
80
60
40
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20

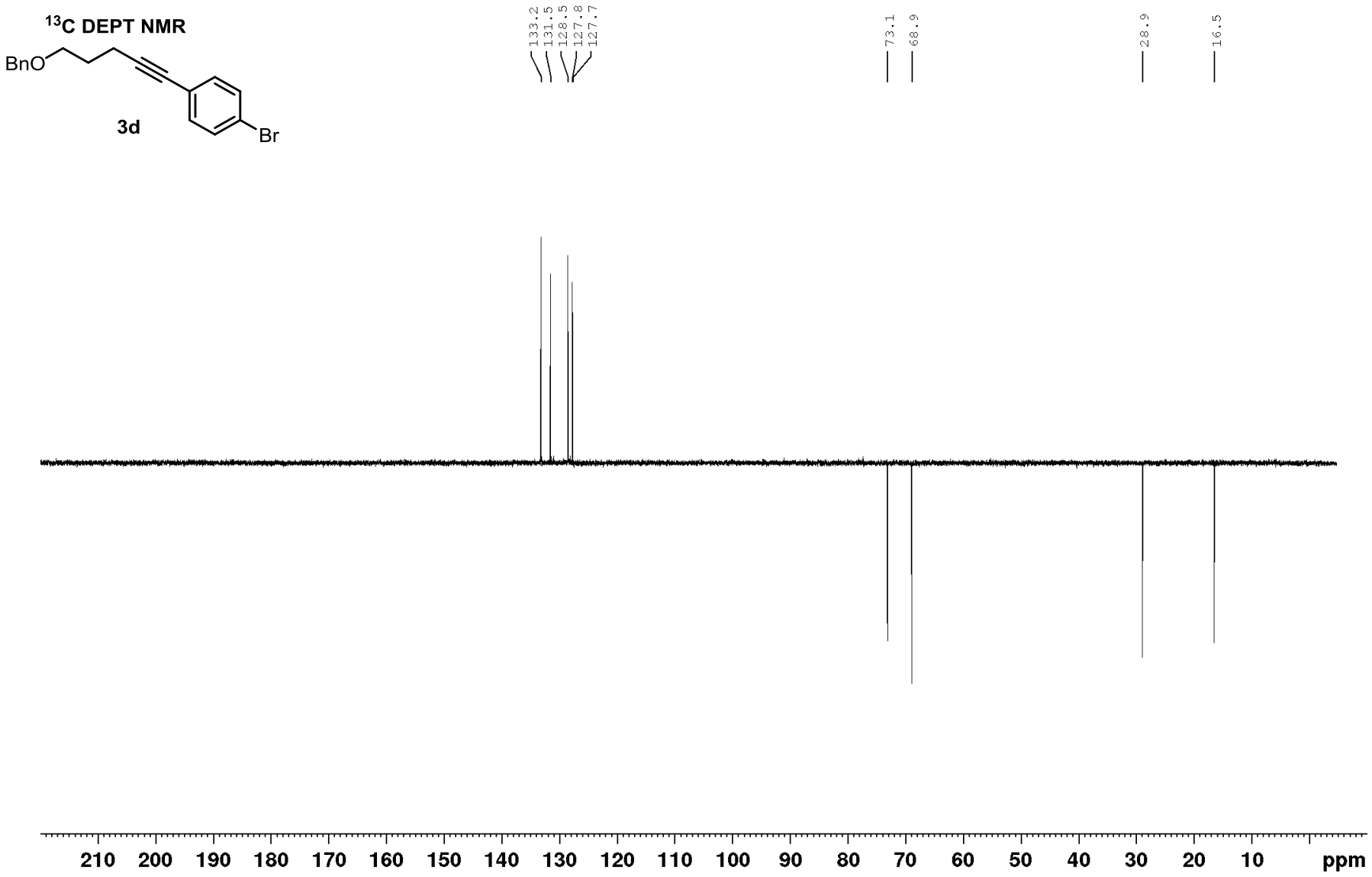
**$^1$H NMR**

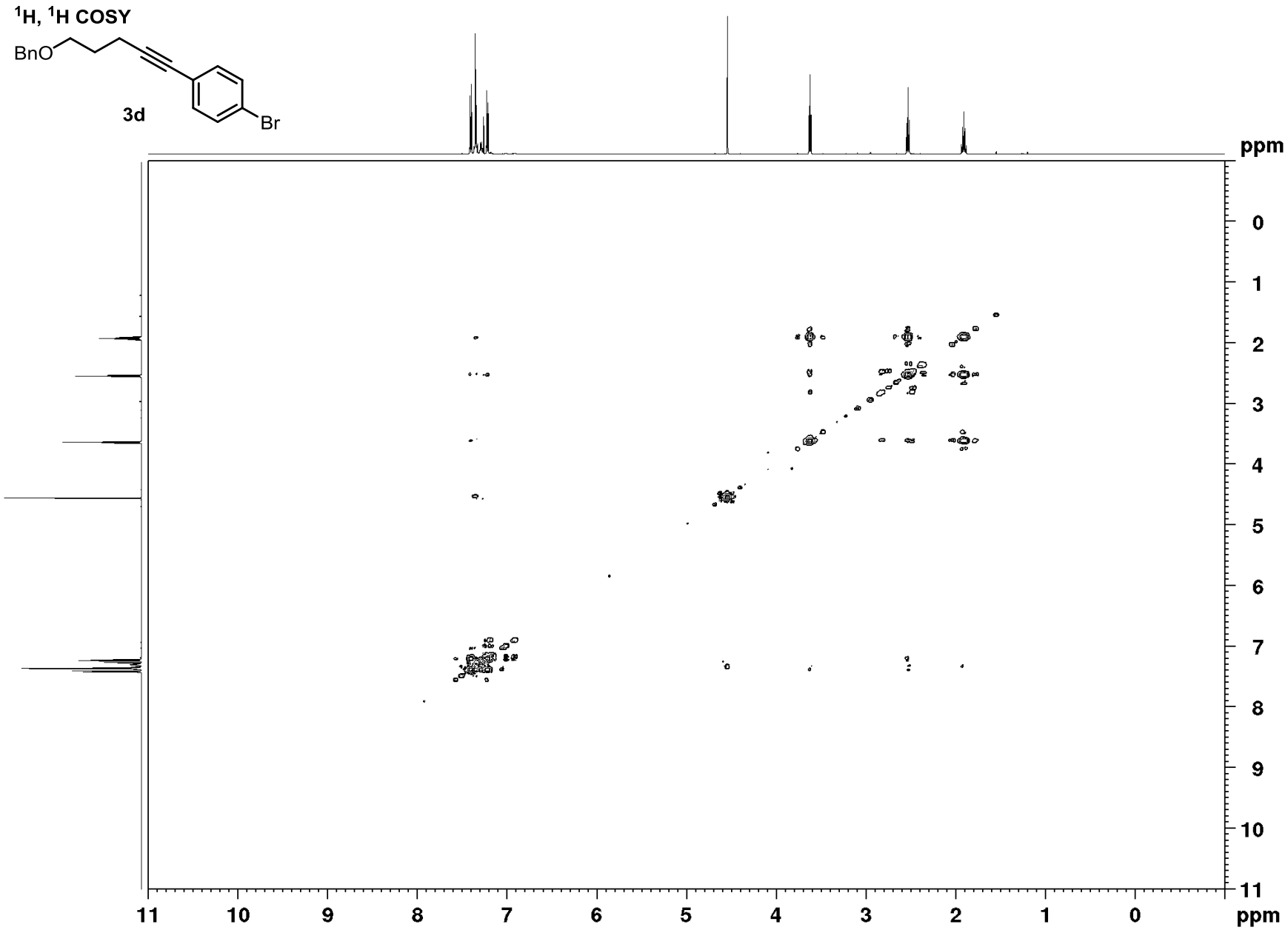

BnO
Br

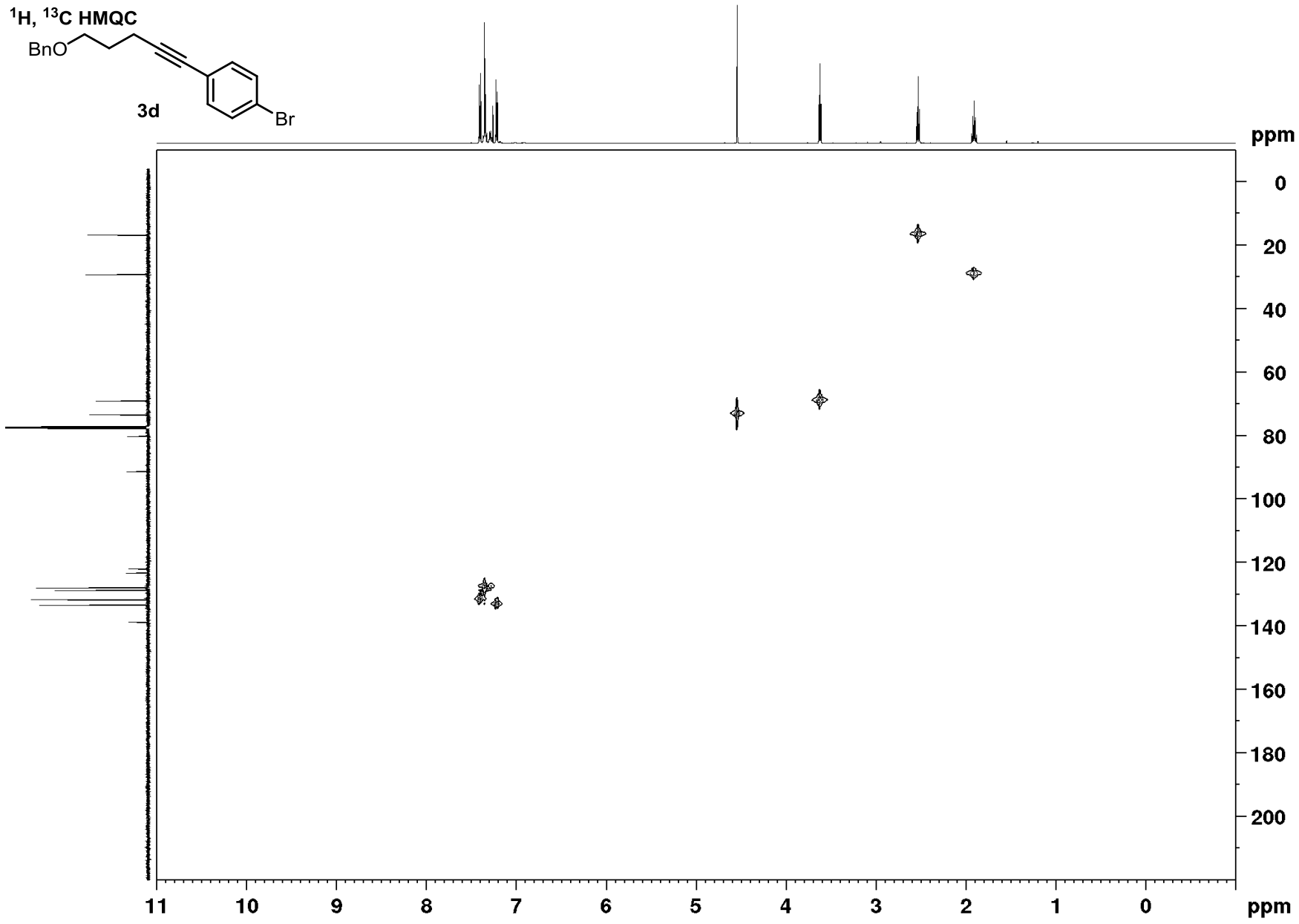
**3d**

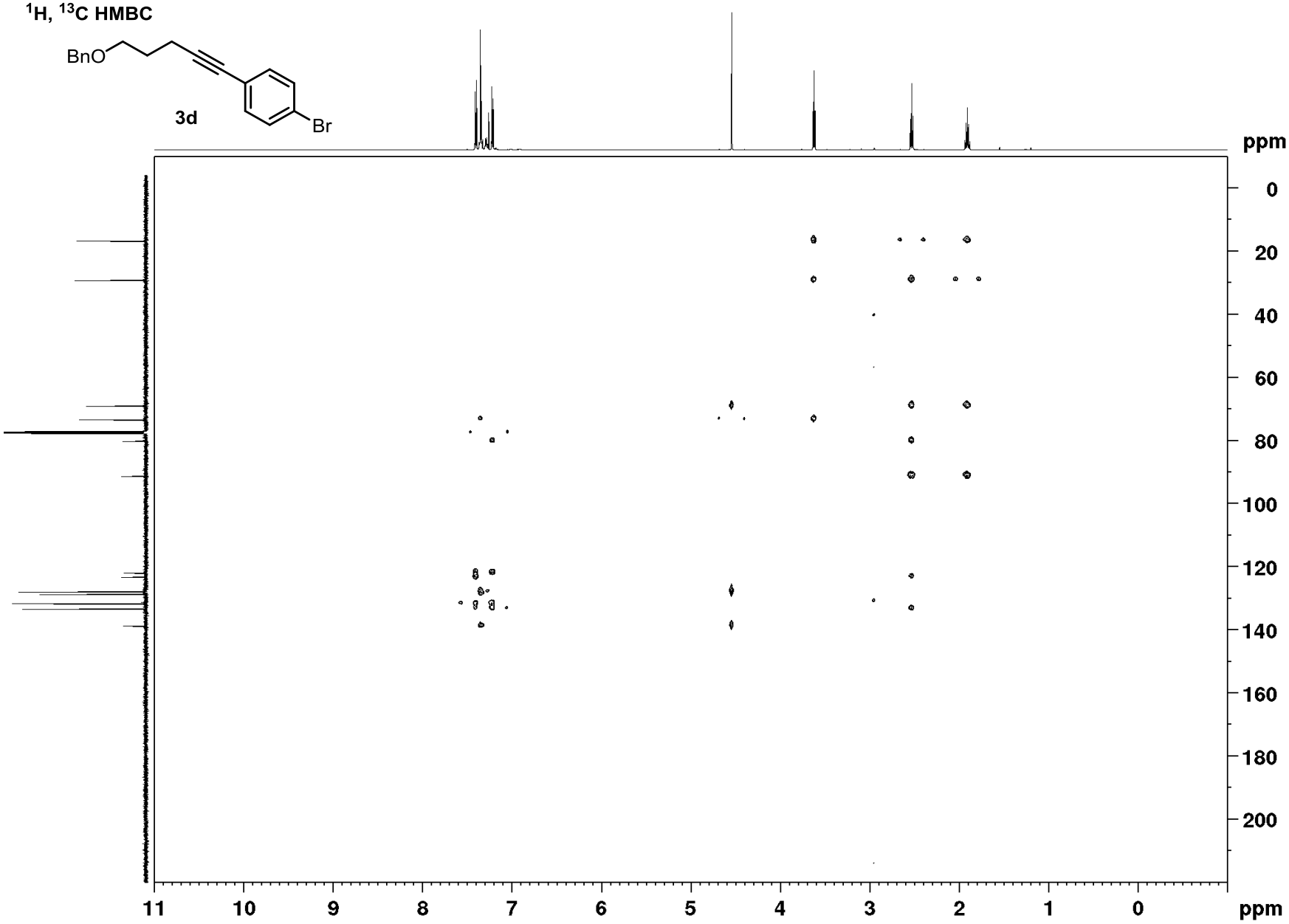

7.42
7.41
7.41
7.40
7.40
7.39
7.37
7.37
7.36
7.36
7.35
7.34
7.34
7.33
7.33
7.30
7.30
7.29
7.29
7.28
7.28
7.27
7.27
7.23
7.23
7.22
7.21
7.21
7.21
4.54
3.64
3.62
3.61
2.54
2.53
2.52
1.94
1.92
1.91
1.90
1.88
1.91
3.76
0.89
1.97
2.00
2.01
2.04
2.01
10
9
8
7
6
5
4
3
2
1
0
ppm

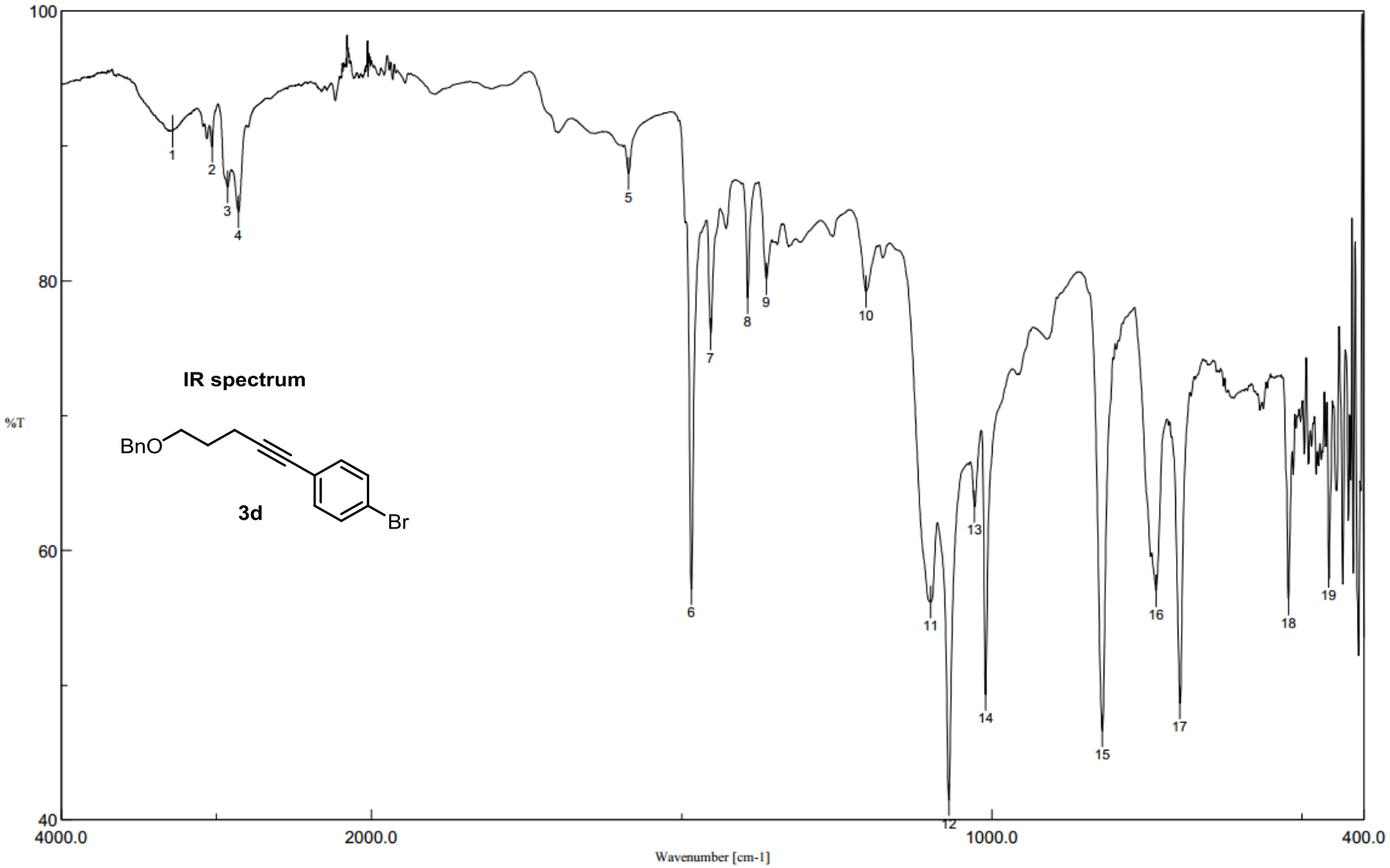

$^{13}$C NMR
BnO
Br
3d
138.6
133.2
131.5
128.5
127.8
127.7
123.1
121.8
91.1
80.0
73.1
68.9
28.9
16.5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


13C DEPT NMR
BnO
3d
Br
133.2
131.5
128.5
127.8
127.7
73.1
68.9
28.9
16.5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

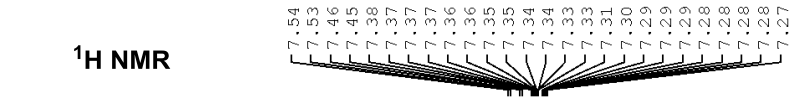

$^1$H, $^1$H COSY
BnO
3d
Br
ppm
0
1
2
3
4
5
6
7
8
9
10
11
11
10
9
8
7
6
5
4
3
2
1
0
ppm


$^{1}$H, $^{13}$C HMQC
BnO
3d
Br
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm


$^{1}$H, $^{13}$C HMBC
BnO
Br
3d
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm


IR spectrum
BnO
Br
3d
%T
100
80
60
40
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

**$^1$H NMR**


7.54
7.53
7.46
7.45
7.38
7.37
7.37
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.31
7.30
7.29
7.29
7.29
7.28
7.28
7.28
7.28
7.27
4.55
3.65
3.64
3.62
2.59
2.57
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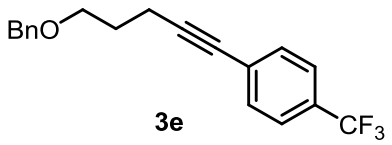
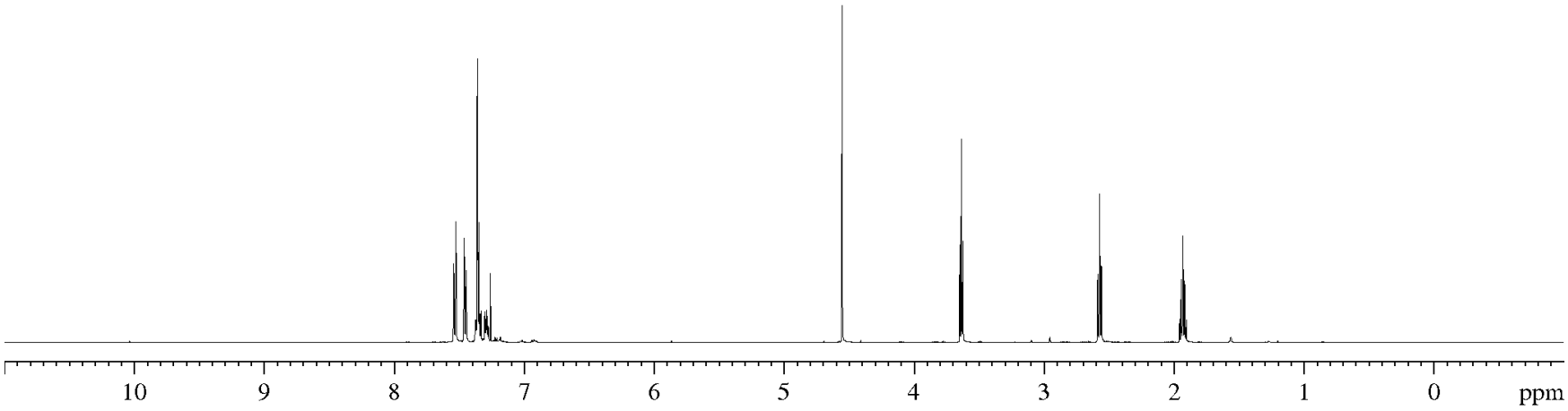
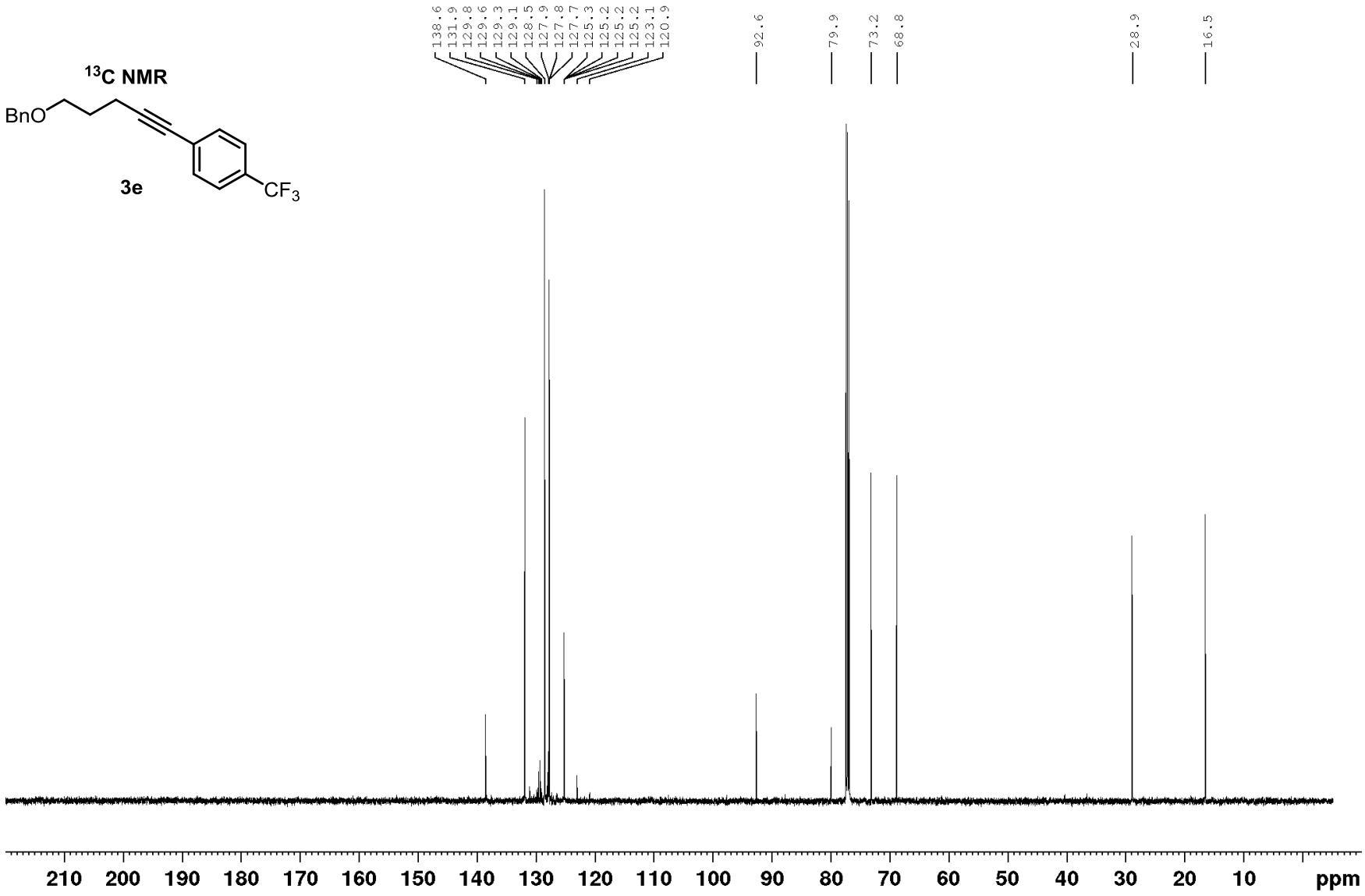
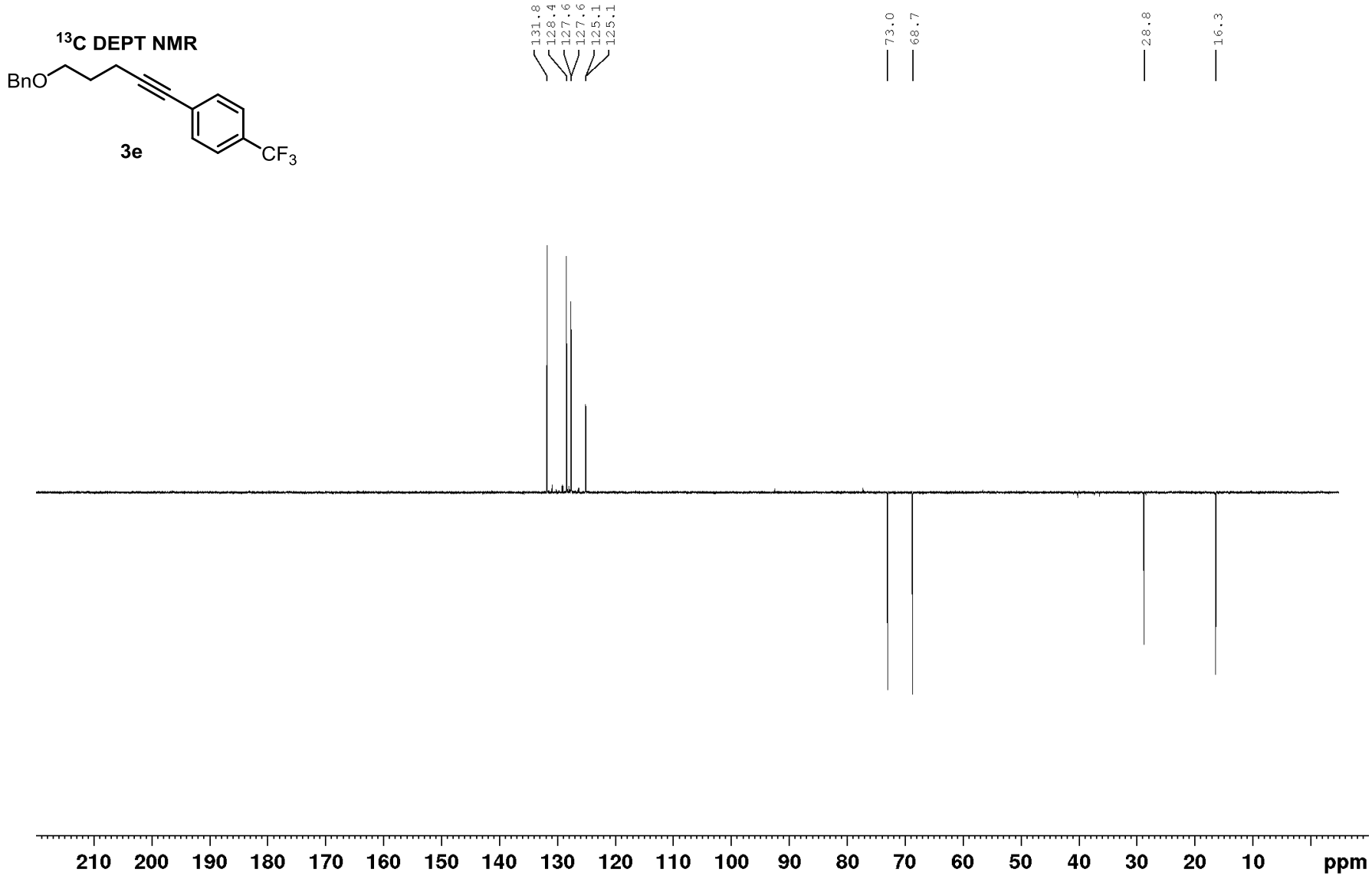
1.96
1.94
1.94
1.93
1.92
1.90


BnO
CF3

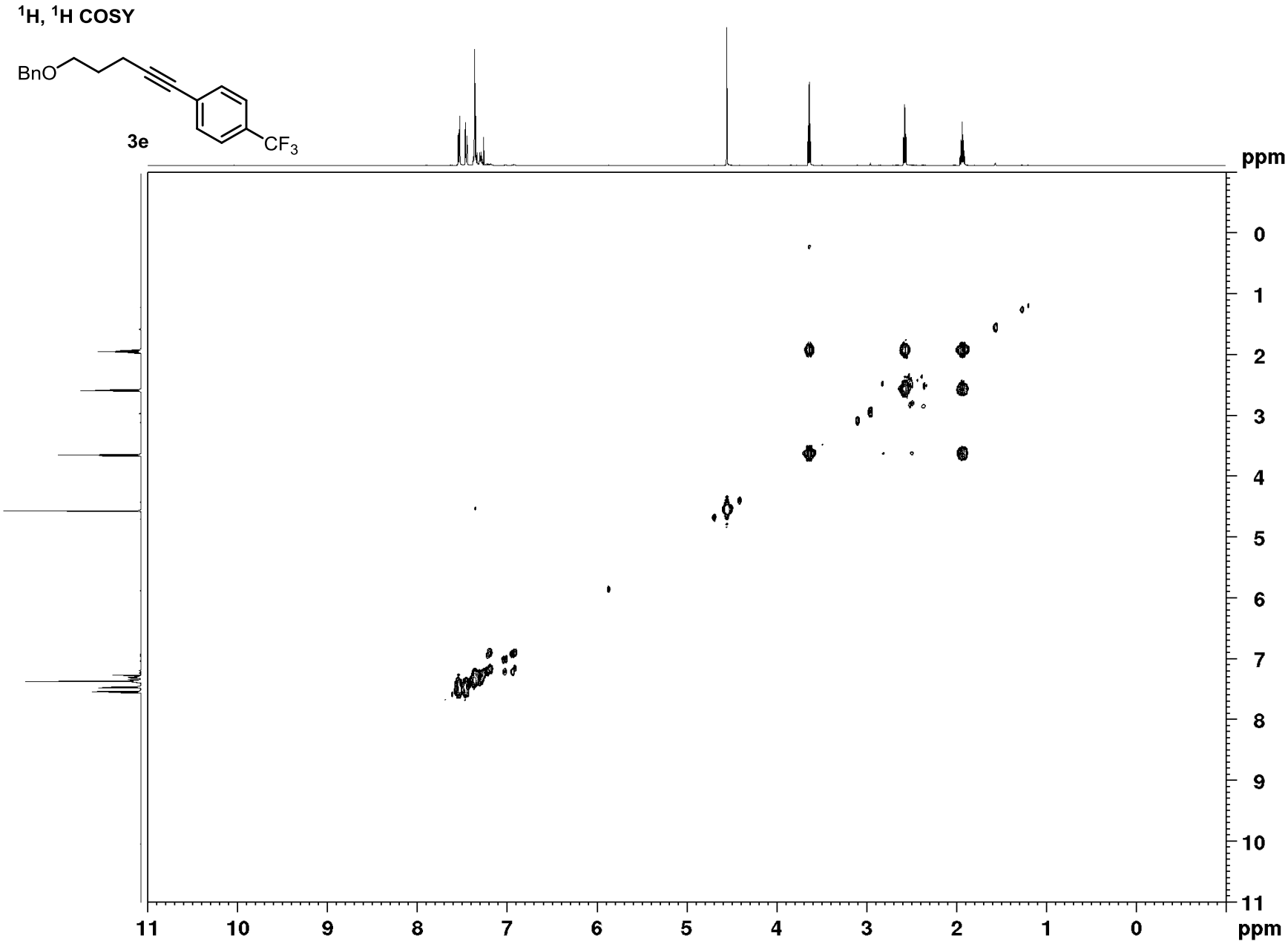
**3e**


10
9
8
7
6
5
4
3
2
1
0
ppm


$^{13}$C NMR
BnO
3e
$CF_3$
138.6
131.9
129.8
129.6
129.3
129.1
128.5
127.9
127.8
127.7
125.3
125.2
125.2
125.2
123.1
120.9
92.6
79.9
73.2
68.8
28.9
16.5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


13C DEPT NMR
BnO
3e
CF3
131.8
128.4
127.6
127.6
125.1
125.1
73.0
68.7
28.8
16.3
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^1$H, $^1$H COSY**



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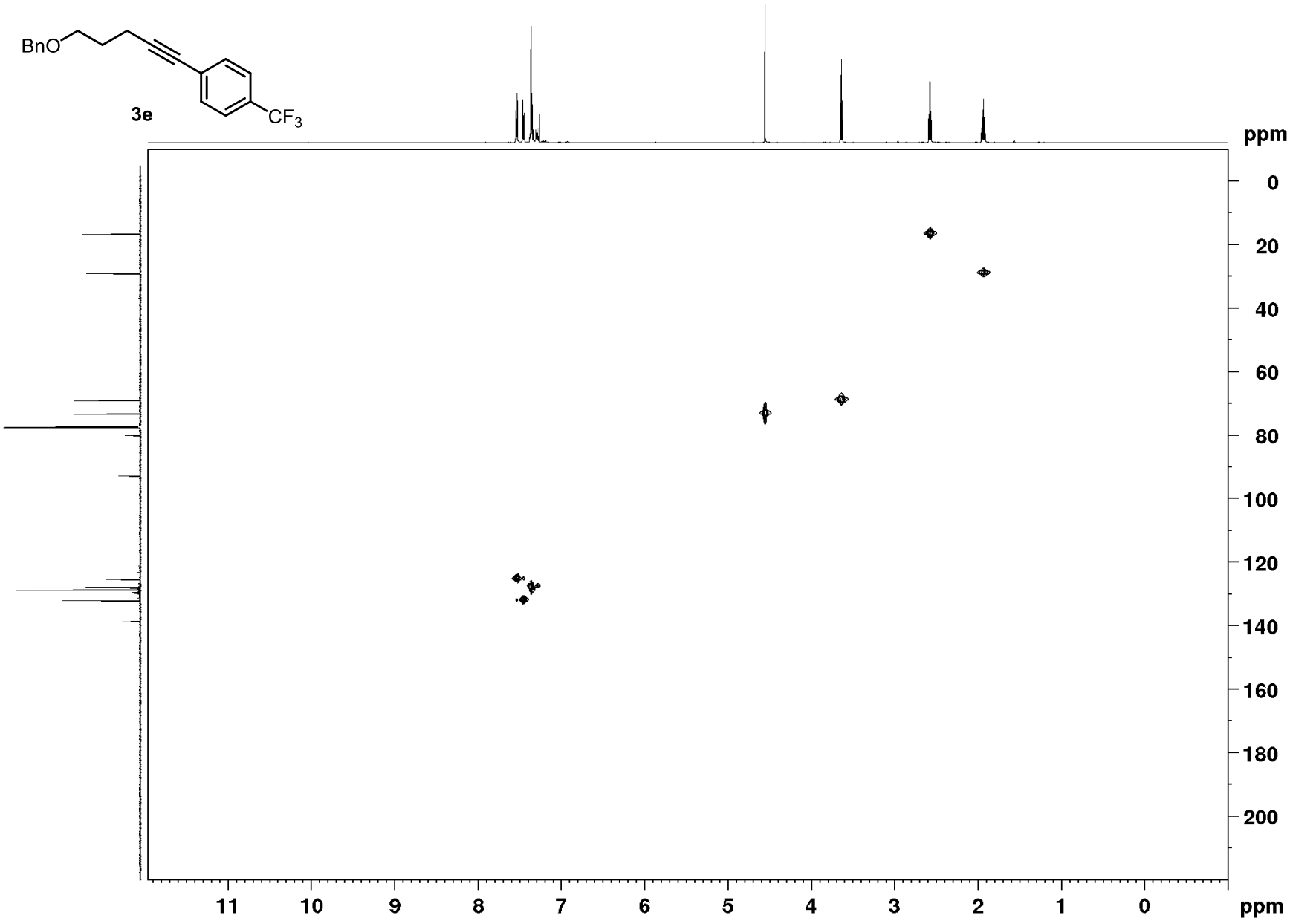
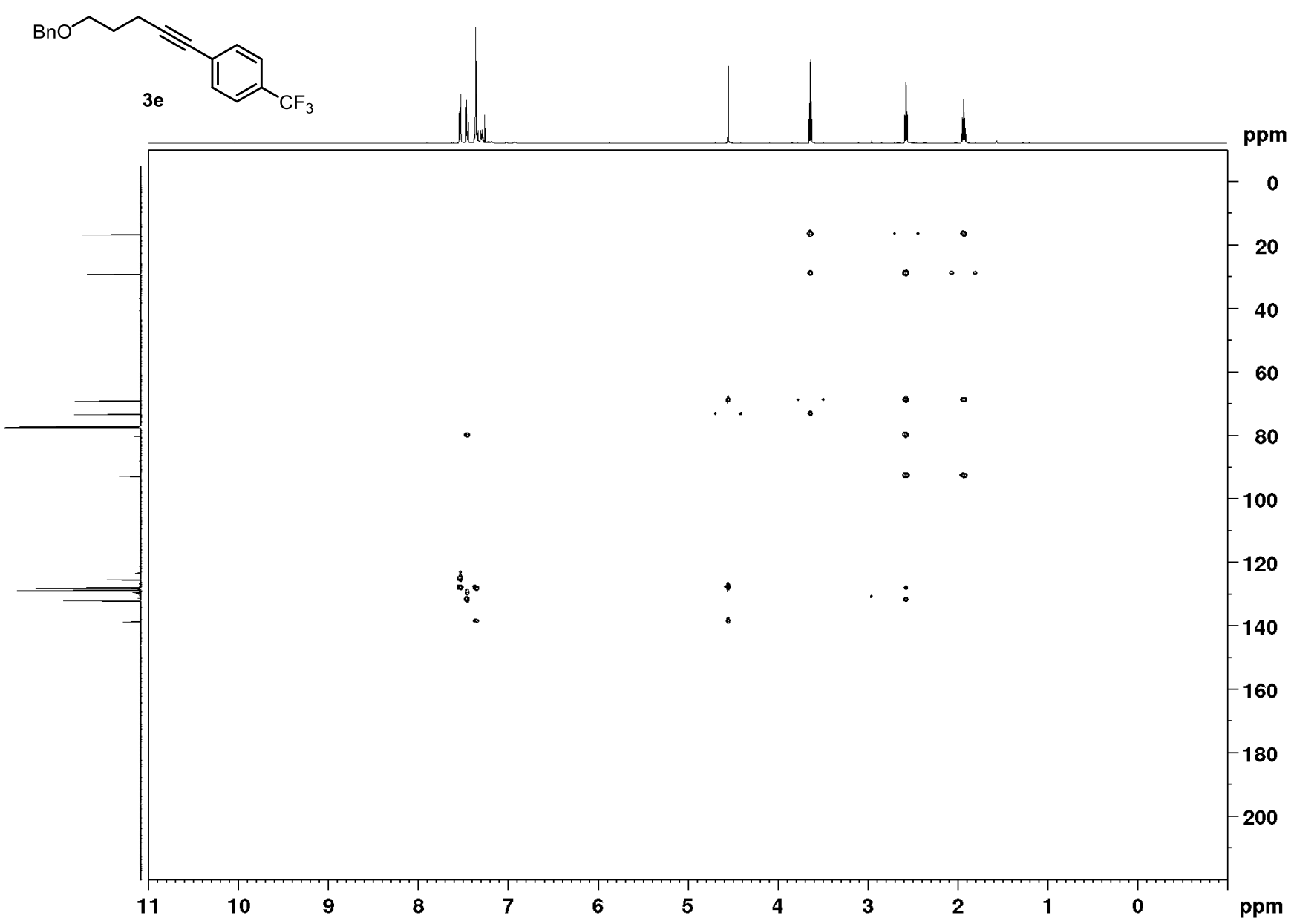
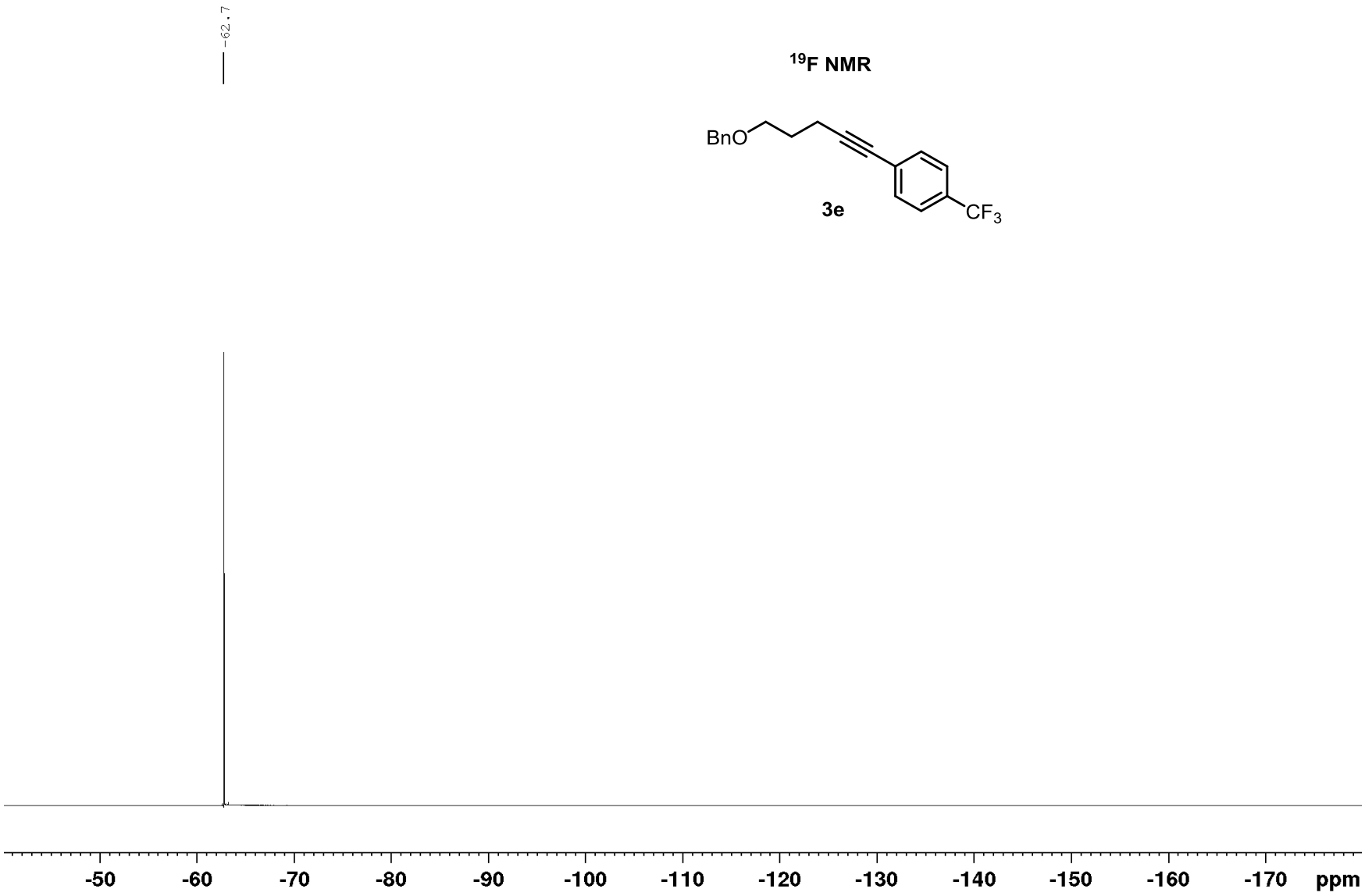
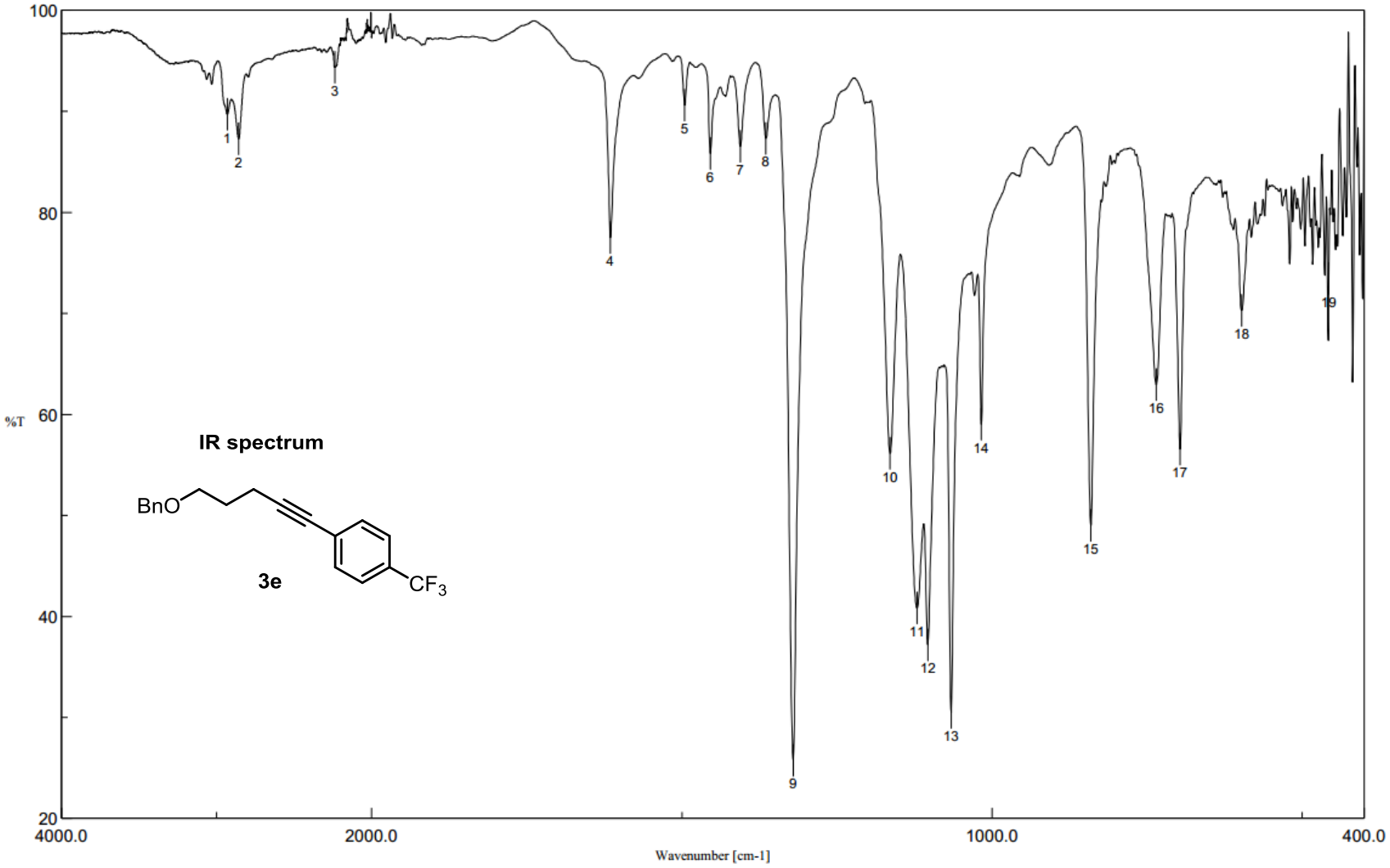

BnO
CF3
3e
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

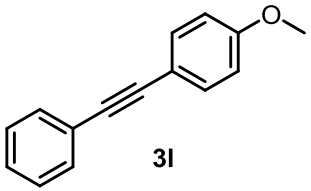
**$^{1}H$, $^{13}C$ HMBC**


BnO
CF3
3e
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm


-62.7
19F NMR
BnO
CF3
3e
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
-170
ppm


IR spectrum
BnO
CF3
3e
%T
100
80
60
40
20
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19

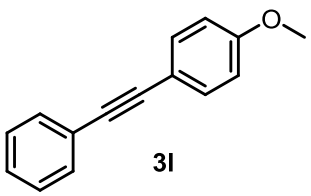
**$^1$H NMR**



**3l**

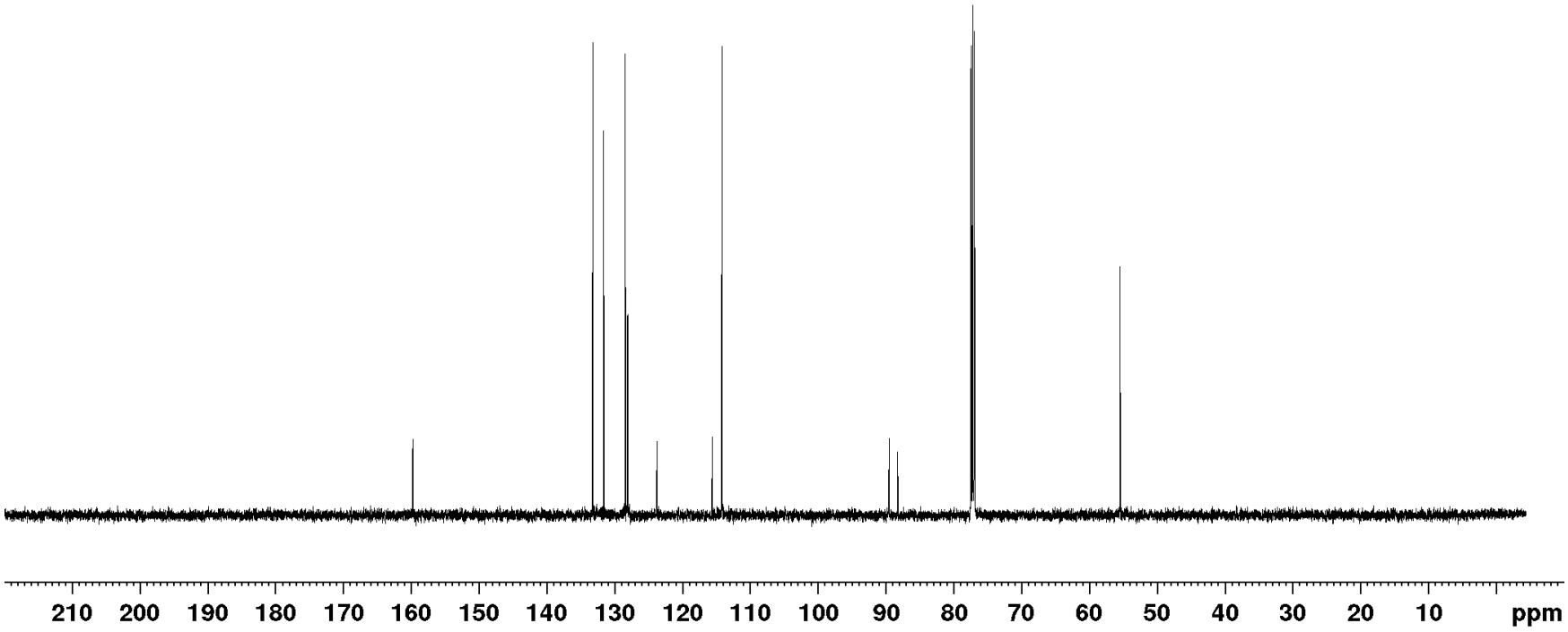

7.53
7.53
7.52
7.51
7.51
7.51
7.49
7.49
7.48
7.47
7.47
7.36
7.36
7.35
7.34
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.30
6.89
6.89
6.88
6.87
3.83
1.91
1.92
2.90
1.97
3.00
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^{13}$C NMR**

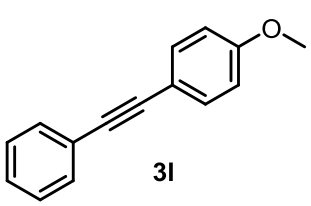


**3l**

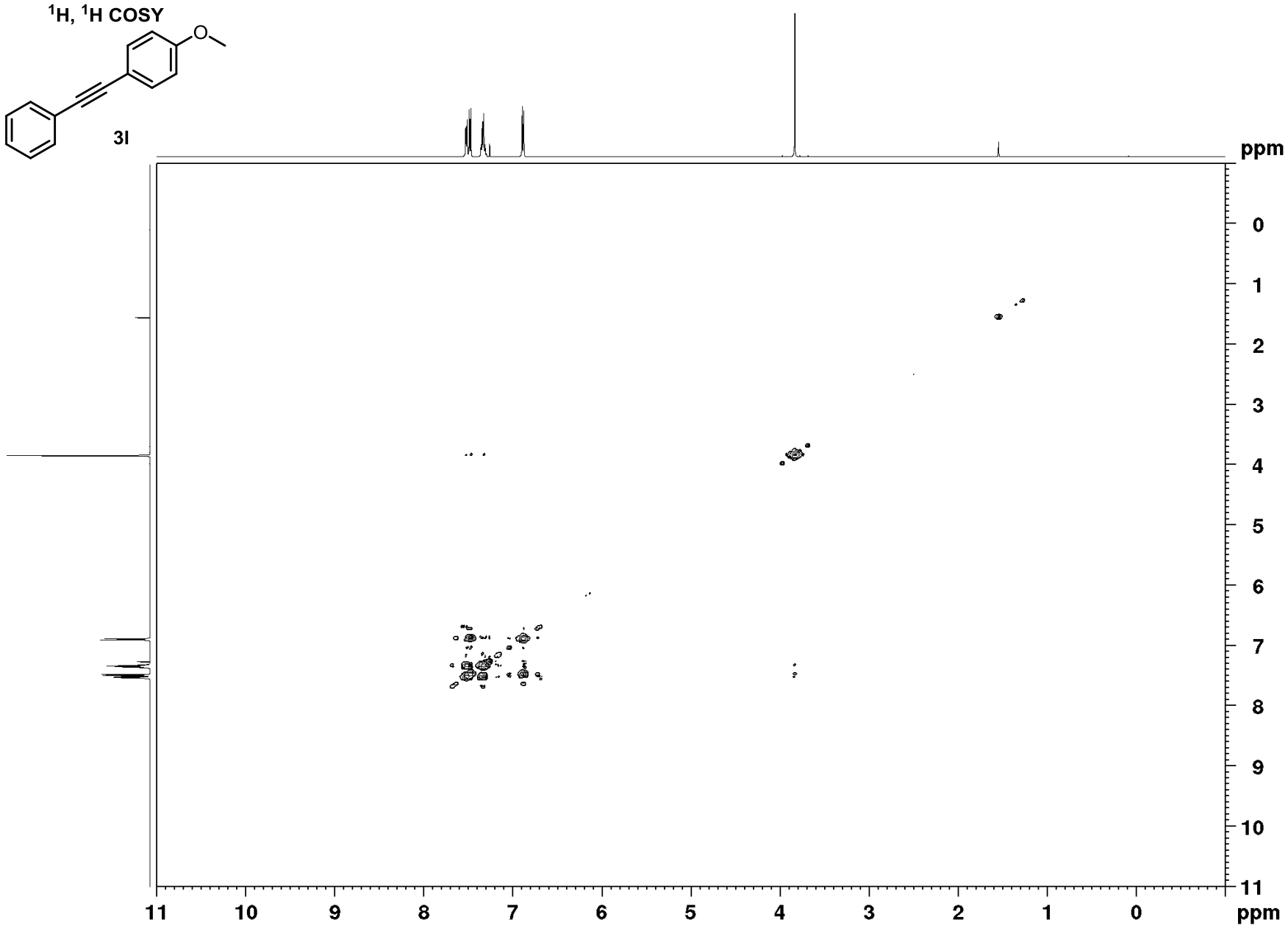
159.8
133.2
131.6
128.4
128.1
123.8
115.5
114.1
89.5
88.2
55.4

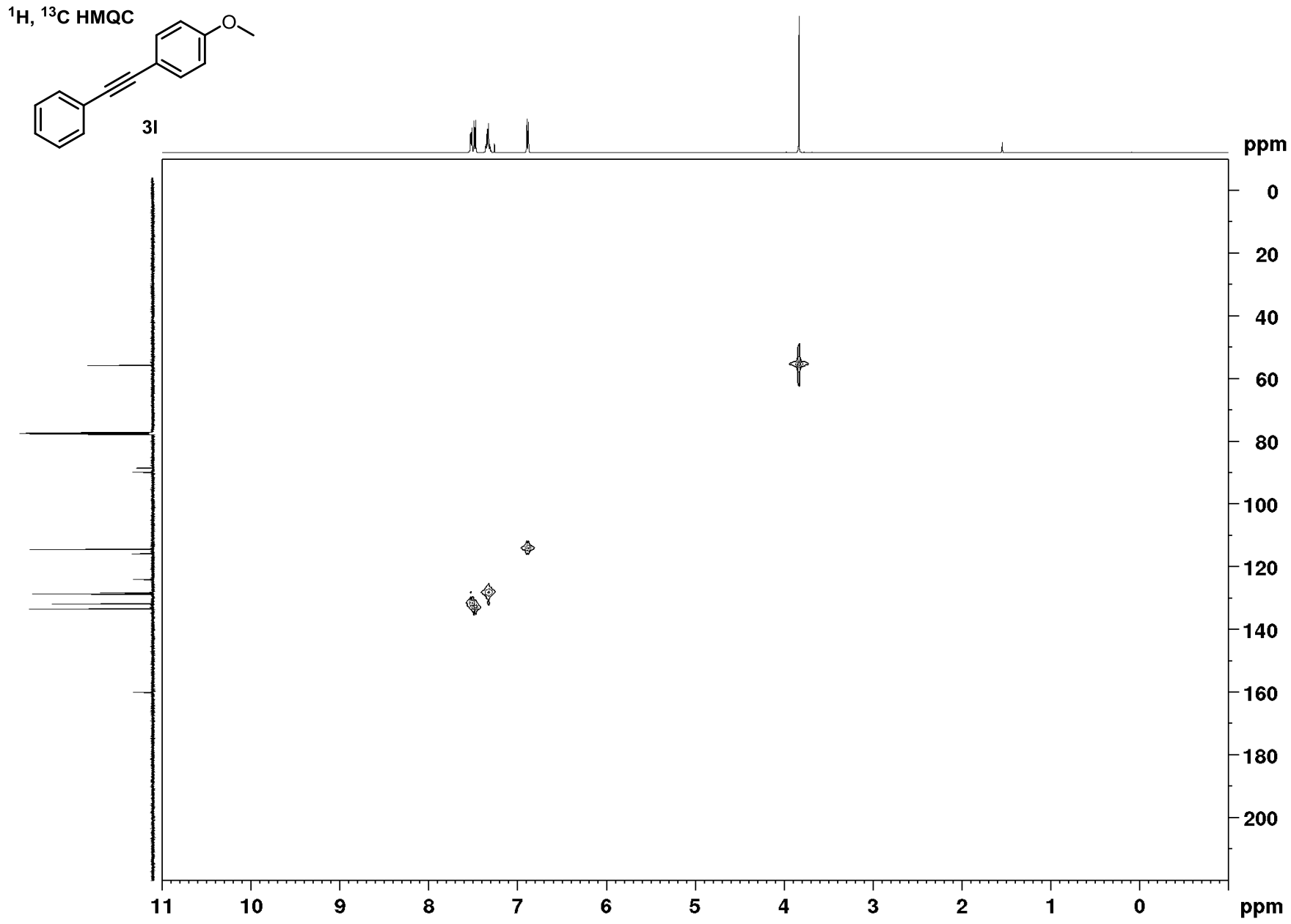


**$^{13}$C DEPT NMR**

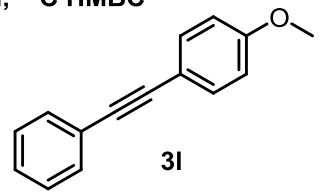


**3l**


$^1$H, $^1$H COSY
O
3l
ppm
0
1
2
3
4
5
6
7
8
9
10
11
11
10
9
8
7
6
5
4
3
2
1
0
ppm

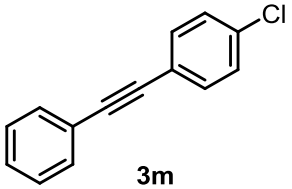

$^{1}$H, $^{13}$C HMQC
O
3l
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

$^{1}H$, $^{13}C$ HMBC

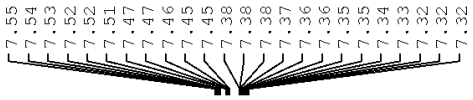


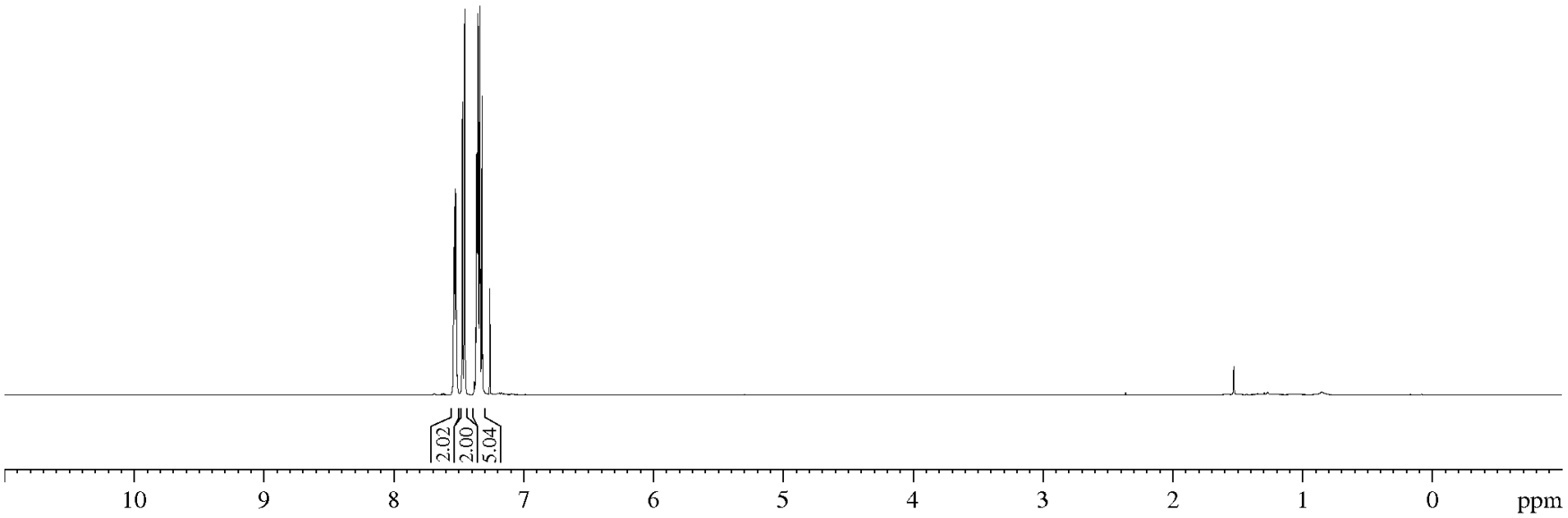
3l

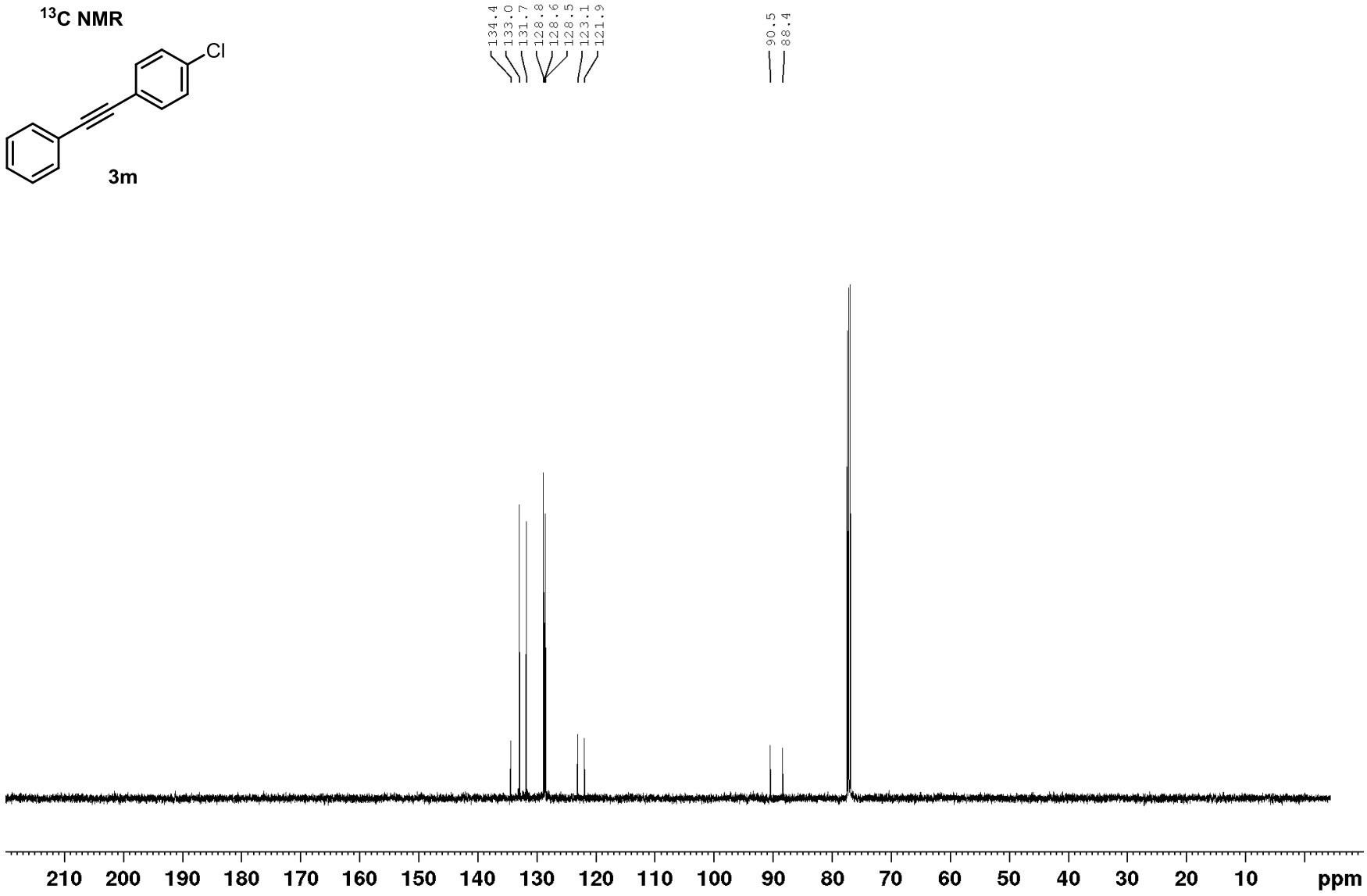
**$^1$H NMR**


Cl

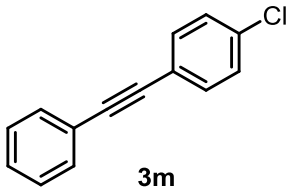
**3m**


7.55
7.54
7.53
7.52
7.52
7.51
7.47
7.47
7.46
7.45
7.45
7.38
7.38
7.37
7.36
7.36
7.35
7.35
7.34
7.33
7.32
7.32
7.32

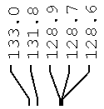

2.02
2.00
5.04
10
9
8
7
6
5
4
3
2
1
0
ppm

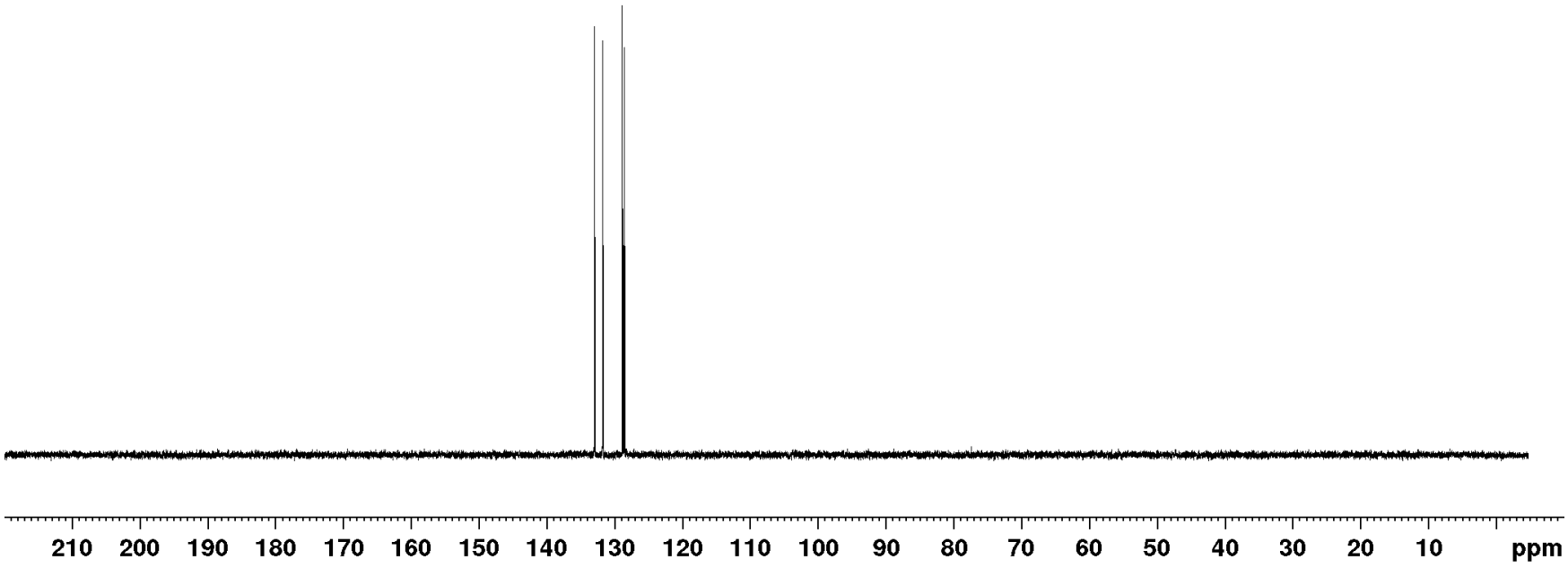

13C NMR
Cl
3m
134.4
133.0
131.7
128.8
128.6
128.5
123.1
121.9
90.5
88.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

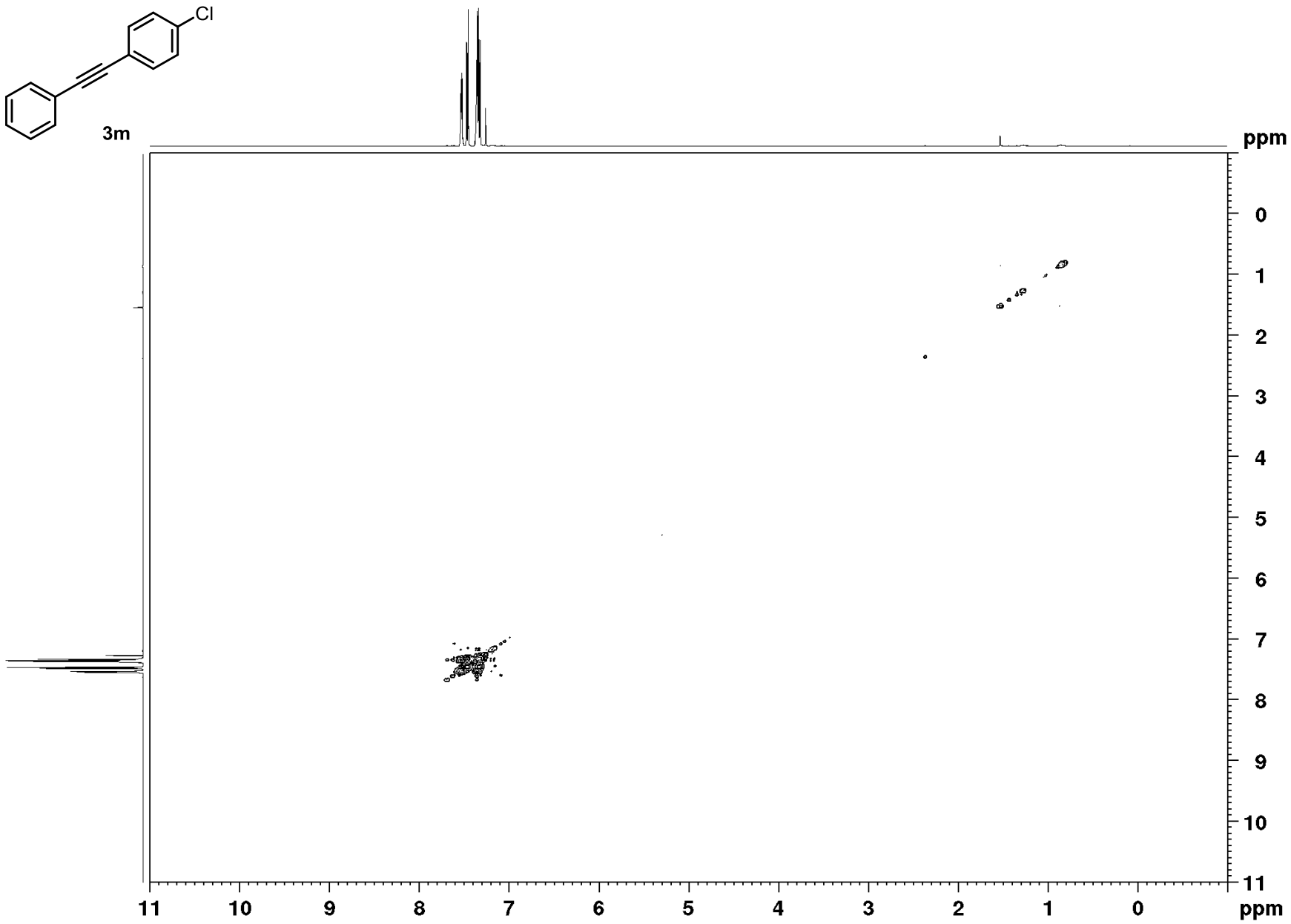
**$^{13}$C DEPT NMR**

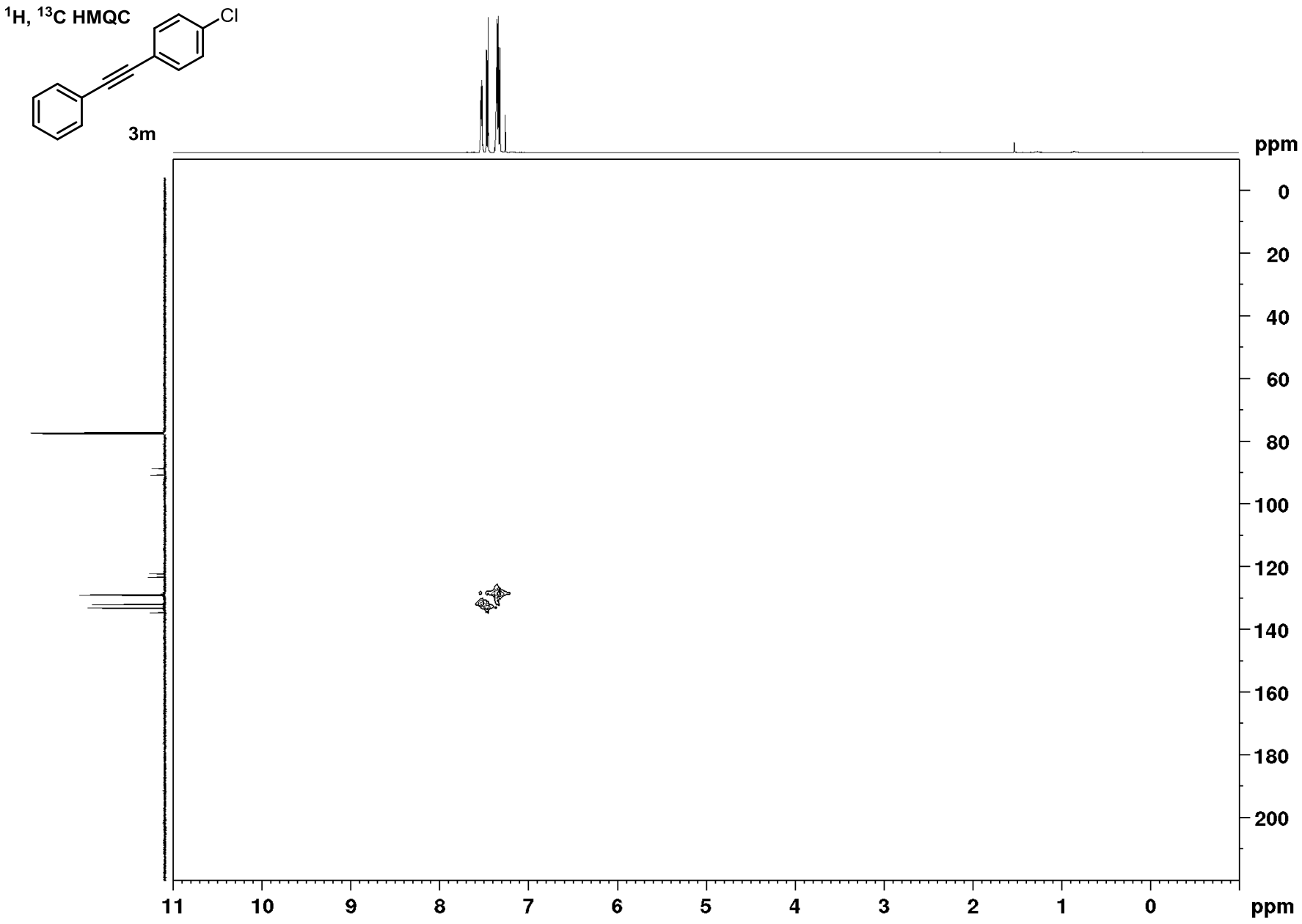


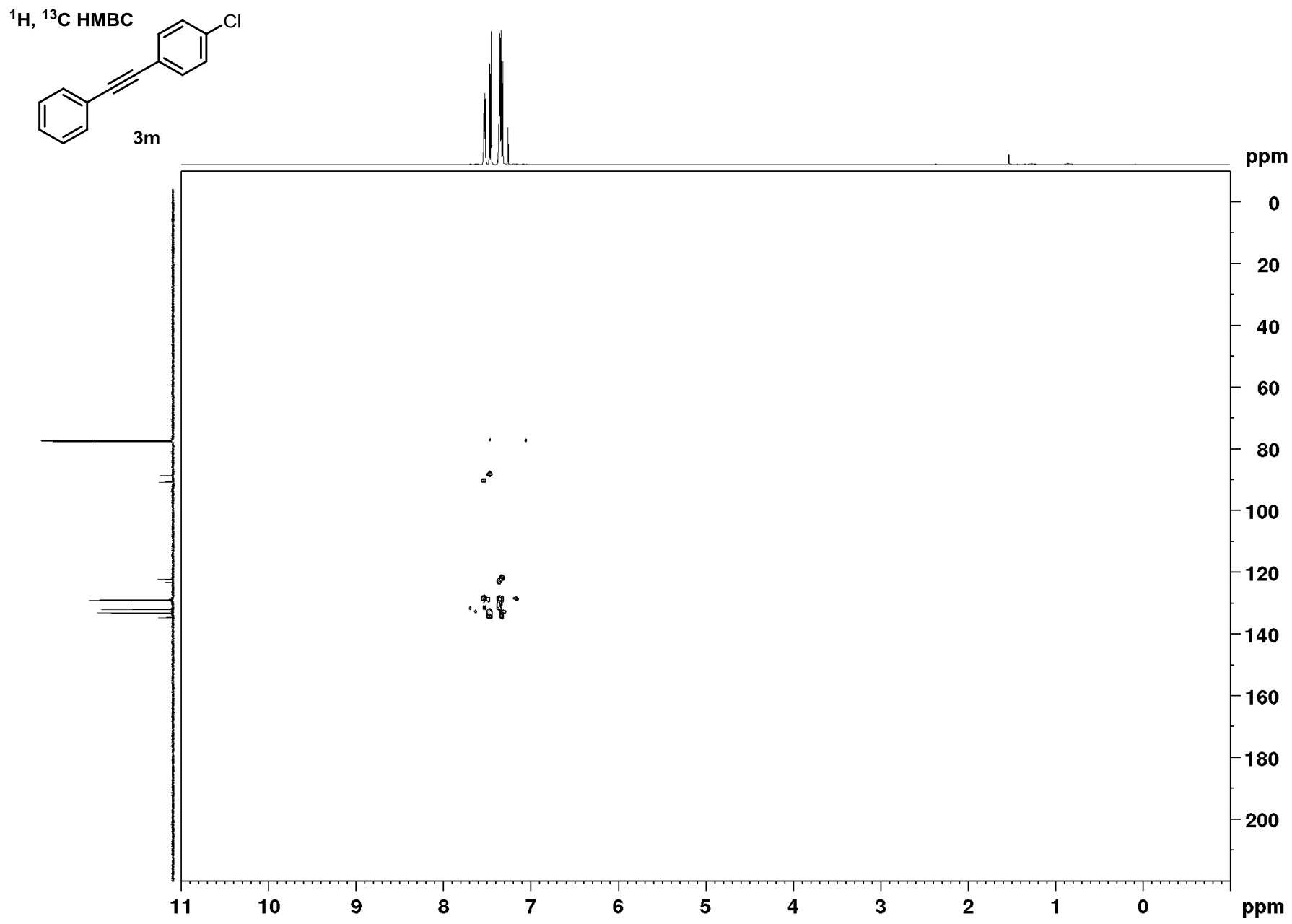

**3m**



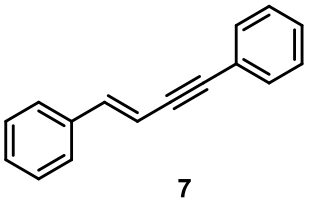




Cl
3m
ppm
0
1
2
3
4
5
6
7
8
9
10
11
11
10
9
8
7
6
5
4
3
2
1
0
ppm

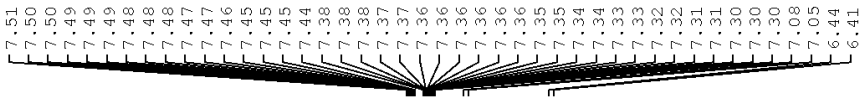

$^{1}$H, $^{13}$C HMQC
Cl
3m
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

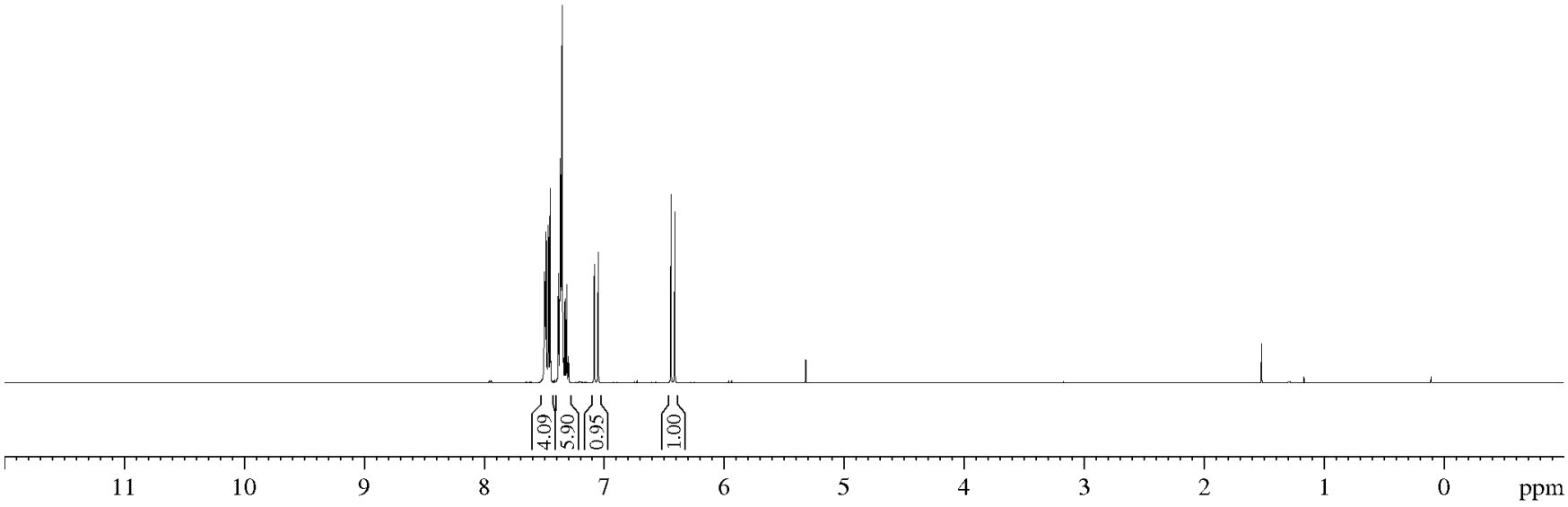

$^{1}$H, $^{13}$C HMBC
Cl
3m
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^1$H NMR**

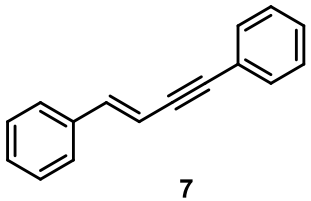


**7**


7.51
7.50
7.50
7.49
7.49
7.49
7.48
7.48
7.48
7.48
7.47
7.47
7.46
7.45
7.45
7.45
7.44
7.38
7.38
7.38
7.37
7.37
7.36
7.36
7.36
7.36
7.36
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.31
7.31
7.30
7.30
7.30
7.08
7.05
6.44
6.41


4.09
5.90
0.95
1.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm

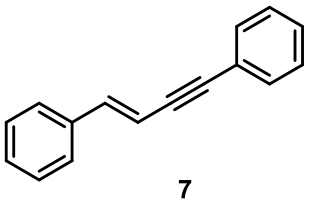
$^{13}$C NMR



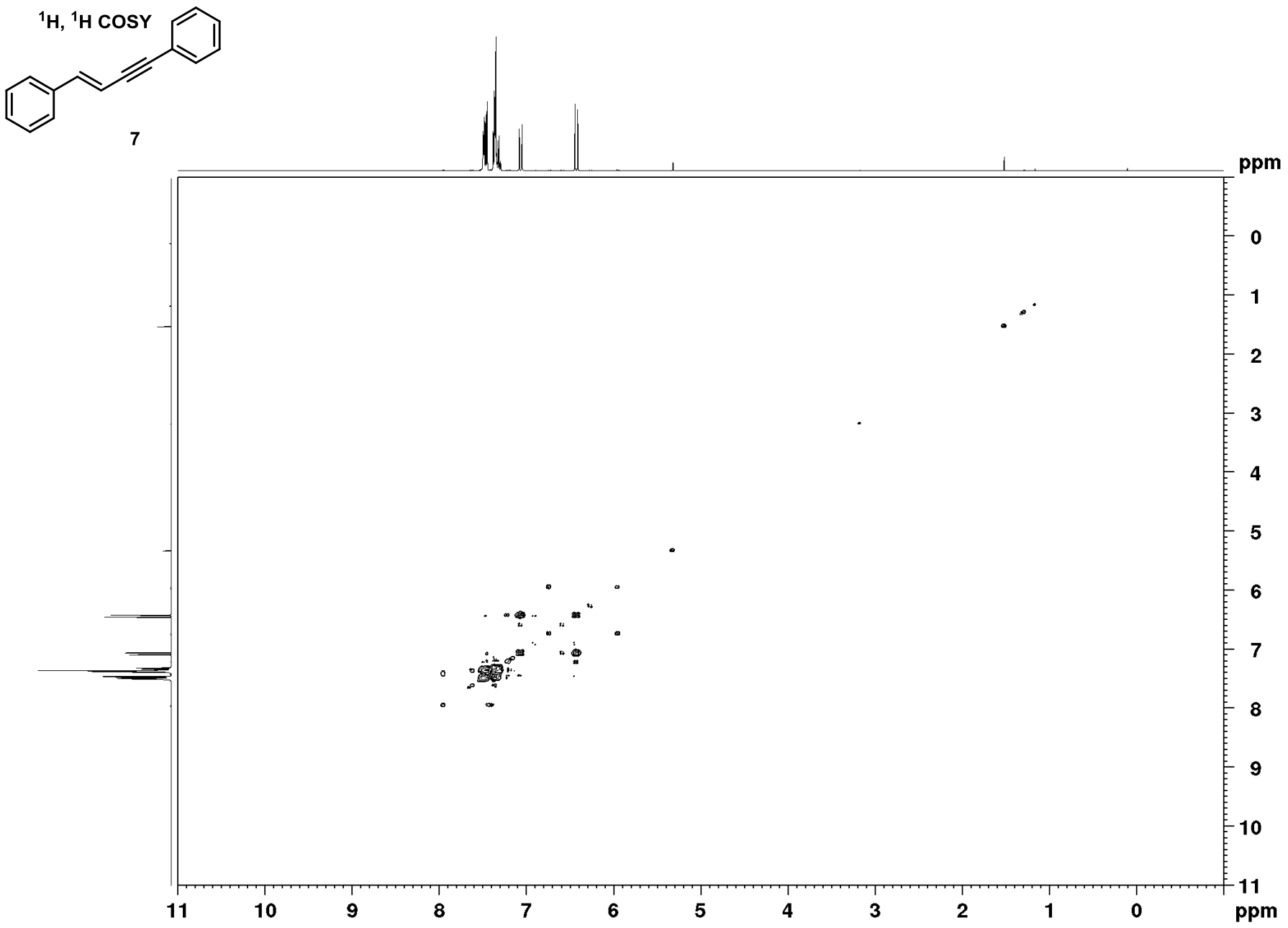
7


141.7
136.7
131.9
129.2
129.1
128.8
128.7
126.7
123.8
108.4
92.0
89.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

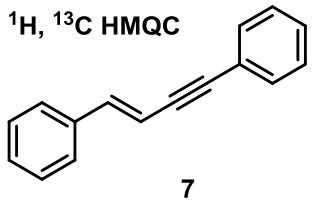
**$^{13}$C DEPT NMR**



**7**

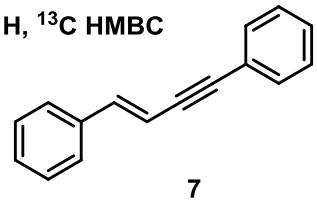

$^1$H, $^1$H COSY
7
ppm
0
1
2
3
4
5
6
7
8
9
10
11
11
10
9
8
7
6
5
4
3
2
1
0
ppm

$^{1}H$, $^{13}C$ HMQC



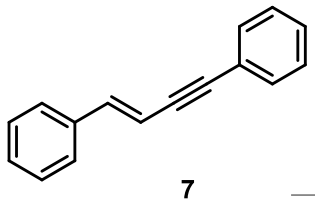
7

$^{1}H$, $^{13}C$ HMBC



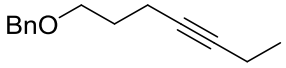
7

$^{1}$H, $^{1}$H NOESY



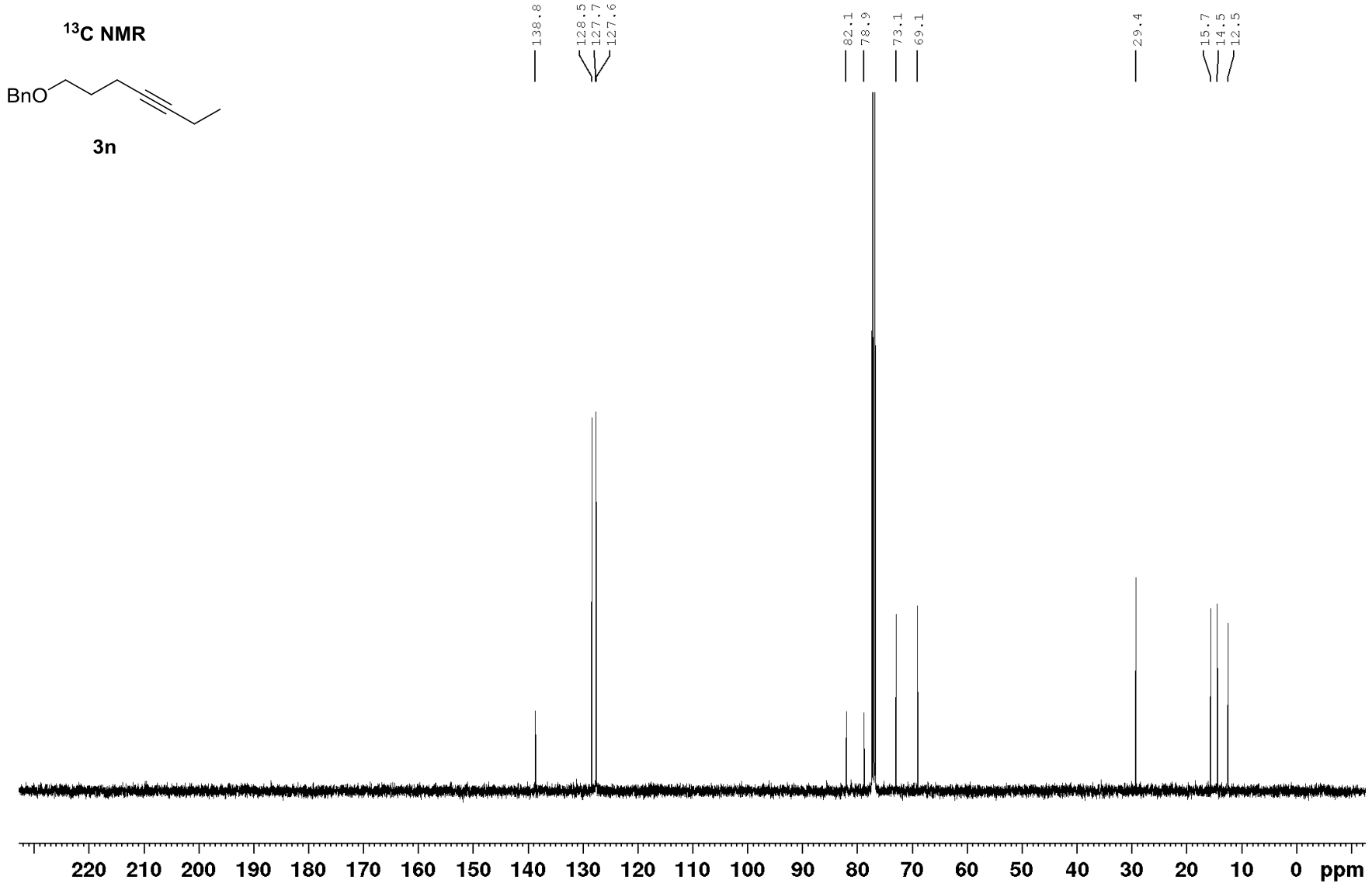
7

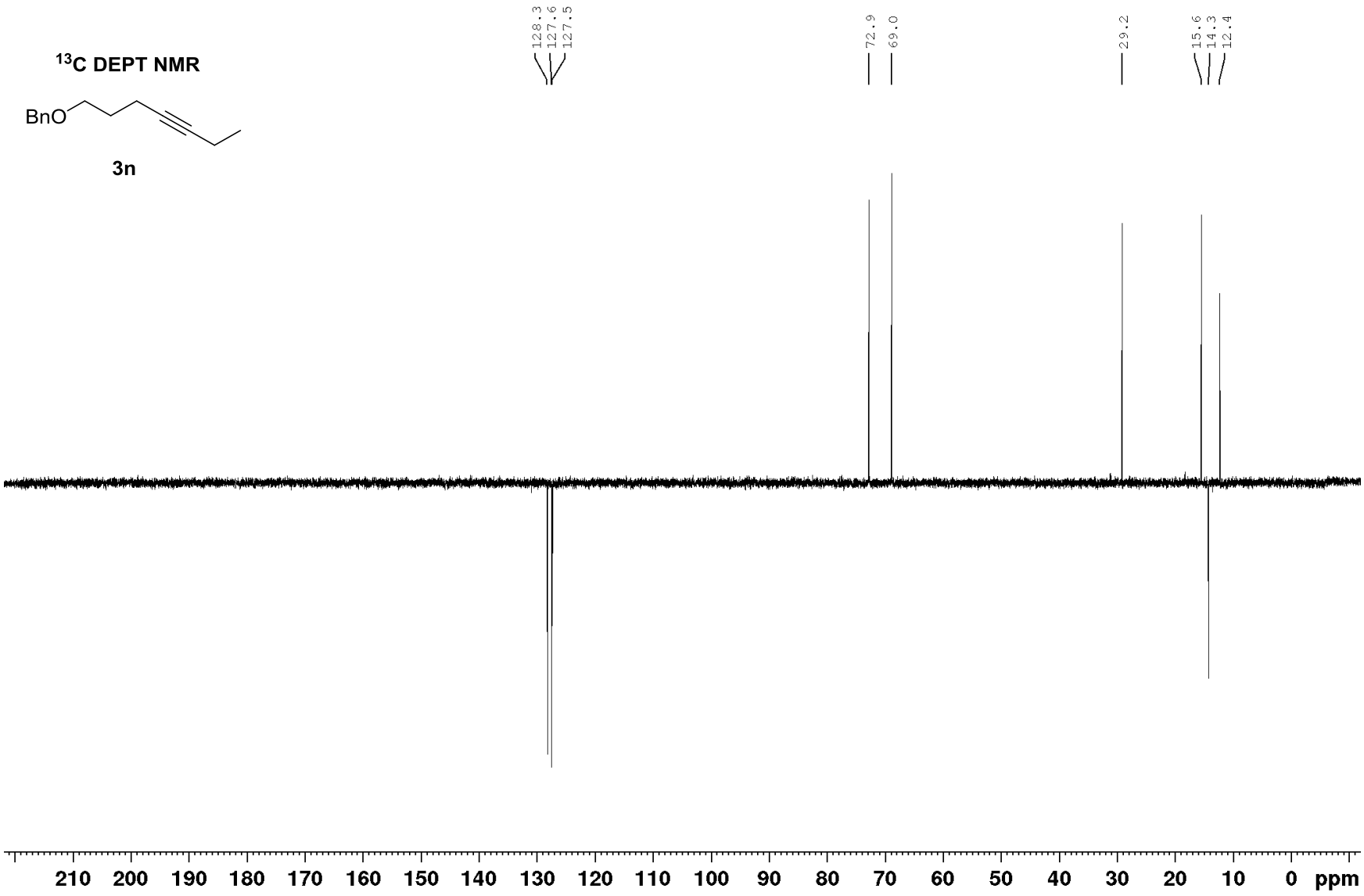
**$^1$H NMR**

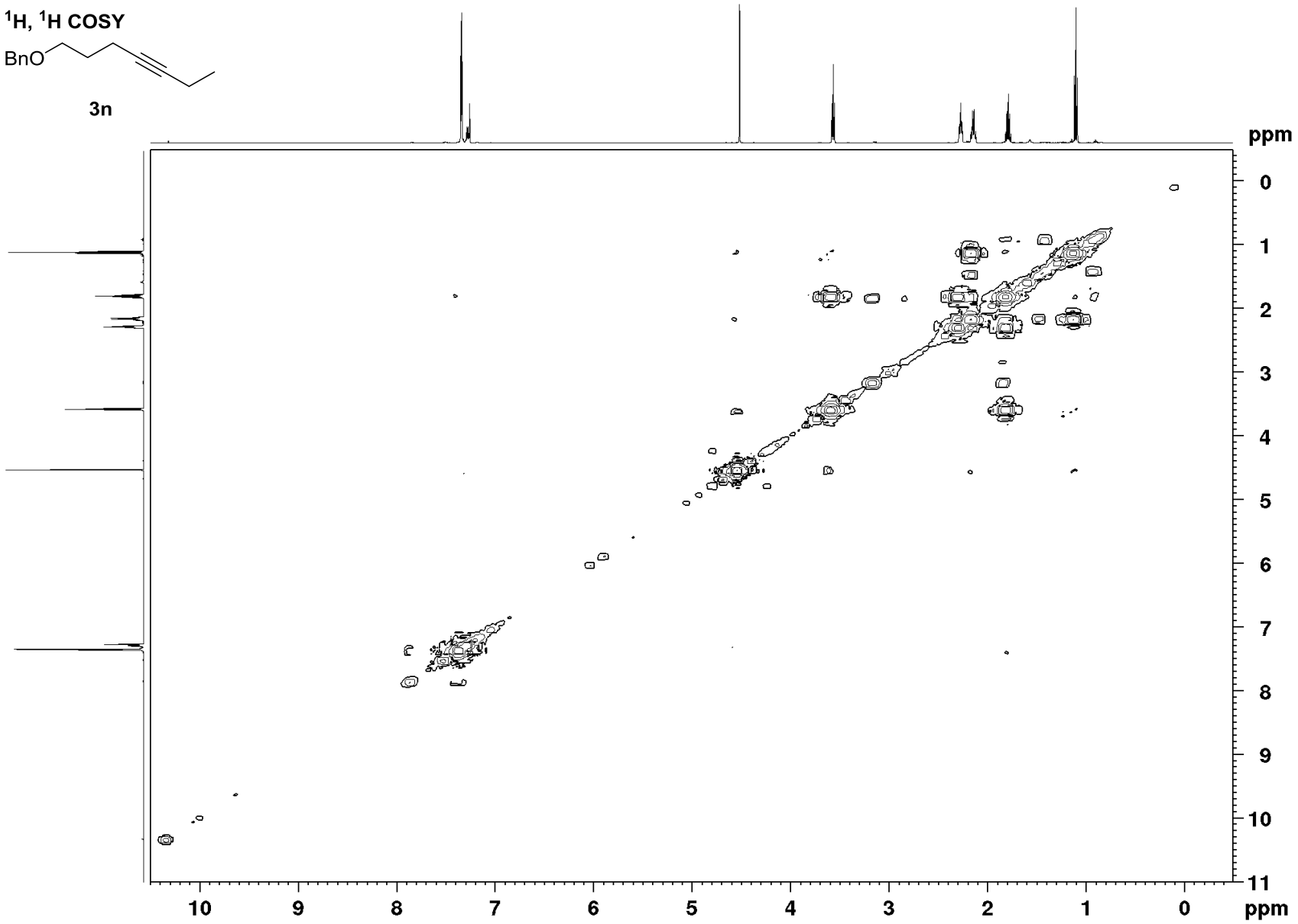

BnO

**3n**

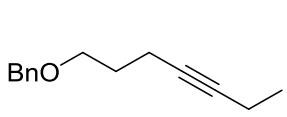

7.36
7.35
7.34
7.33
7.32
7.32
7.30
7.29
7.28
7.28
7.27
4.52
2.29
2.29
2.28
2.28
2.27
2.27
2.26
2.26
2.25
2.17
2.17
2.16
2.16
2.15
2.15
2.14
2.14
2.13
2.12
2.12
1.82
1.80
1.80
1.79
1.78
1.12
1.10
1.09
4.68
2.00
2.02
2.03
1.97
2.07
2.81
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
1.5
1.0
0.5
0.0
ppm


13C NMR
BnO
3n
138.8
128.5
127.7
127.6
82.1
78.9
73.1
69.1
29.4
15.7
14.5
12.5
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


$^{13}$C DEPT NMR
BnO
3n
128.3
127.6
127.5
72.9
69.0
29.2
15.6
14.3
12.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

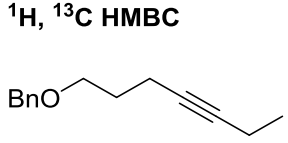

$^1$H, $^1$H COSY
BnO
3n
ppm
0
1
2
3
4
5
6
7
8
9
10
11
10
9
8
7
6
5
4
3
2
1
0
ppm

$^{1}H$, $^{13}C$ HMQC

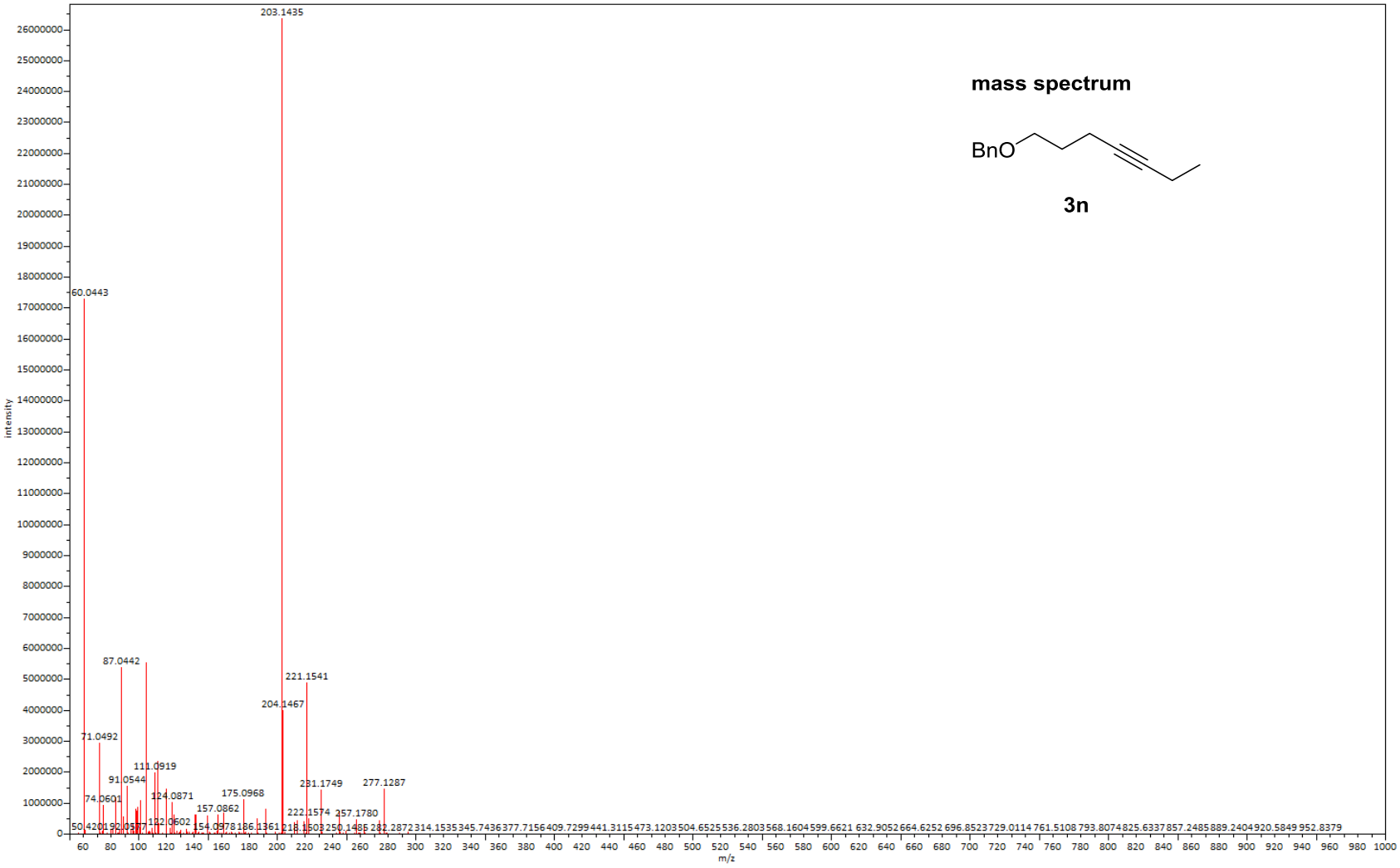



**3n**

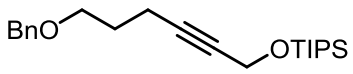
**$^{1}H$, $^{13}C$ HMBC**




**3n**

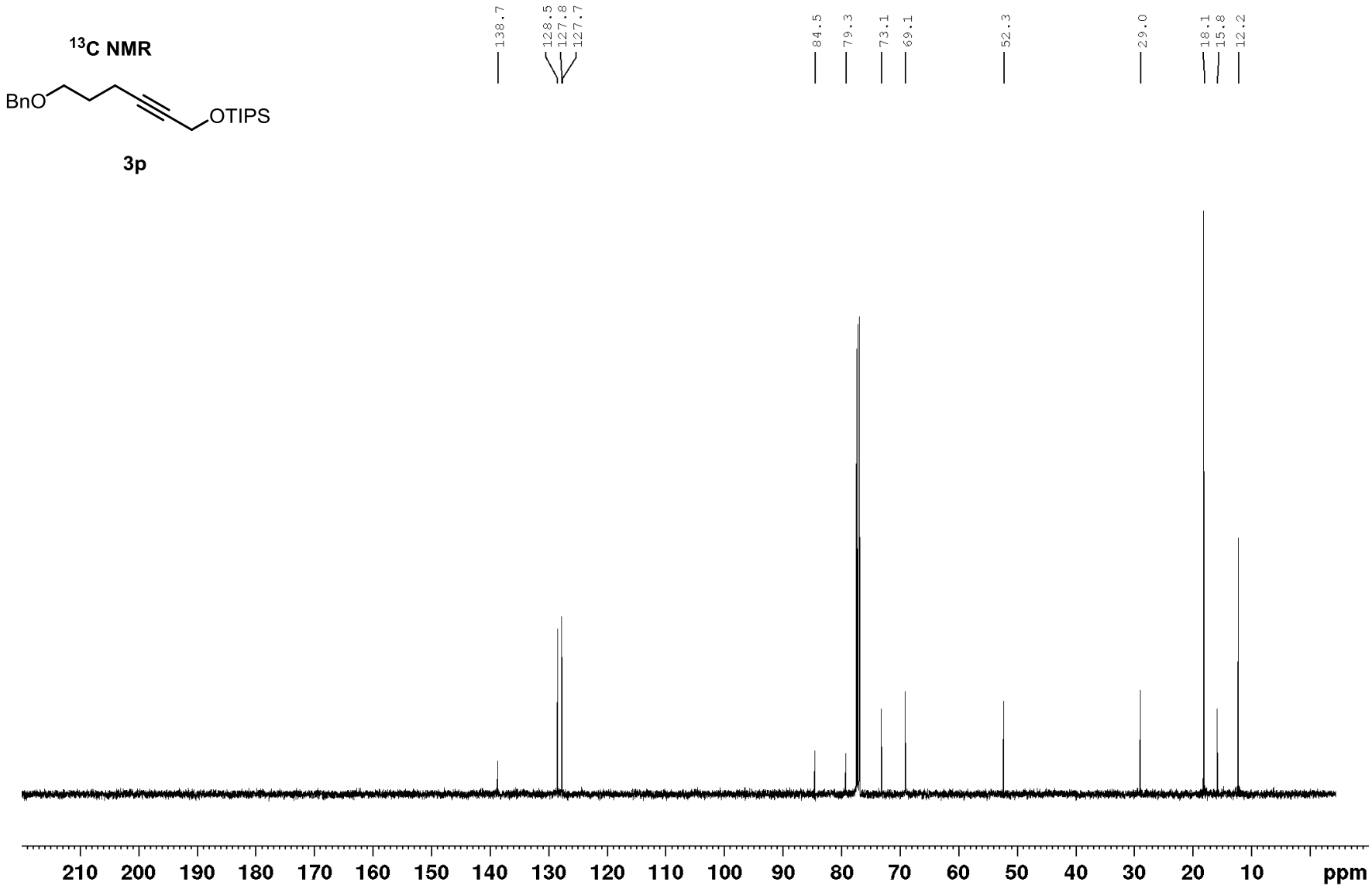

mass spectrum
BnO
3n
intensity
m/z
203.1435
60.0443
87.0442
221.1541
204.1467
71.0492
111.0919
91.0544
231.1749
277.1287
74.0601
124.0871
175.0968
222.1574
257.1780
157.0862

**$^1$H NMR**

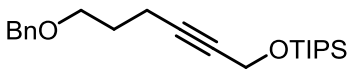

BnO
OTIPS

**3p**


7.36
7.36
7.35
7.34
7.34
7.33
7.33
7.32
7.29
7.29
7.29
7.28
7.28
7.28
7.28
7.27
7.27
7.27
4.51
4.36
4.35
4.35
3.58
3.56
3.55
2.36
2.35
2.35
2.34
2.34
2.33
2.33
2.32
2.32
1.84
1.83
1.81
1.80
1.79
1.16
1.15
1.15
1.14
1.13
1.12
1.11
1.10
1.09
1.08
1.07
1.07
1.06
4.66
2.00
2.00
2.01
2.01
2.02
3.17
17.79
10
9
8
7
6
5
4
3
2
1
0
ppm

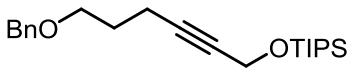

13C NMR
BnO
OTIPS
3p
138.7
128.5
127.8
127.7
84.5
79.3
73.1
69.1
52.3
29.0
18.1
15.8
12.2
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



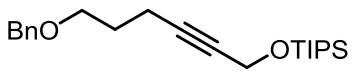

**3p**

**$^1$H, $^1$H COSY**



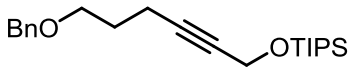

**3p**

**$^{1}H$, $^{13}C$ HMQC**



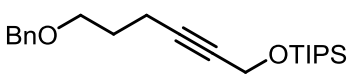

**3p**

**$^{1}H$, $^{13}C$ HMBC**

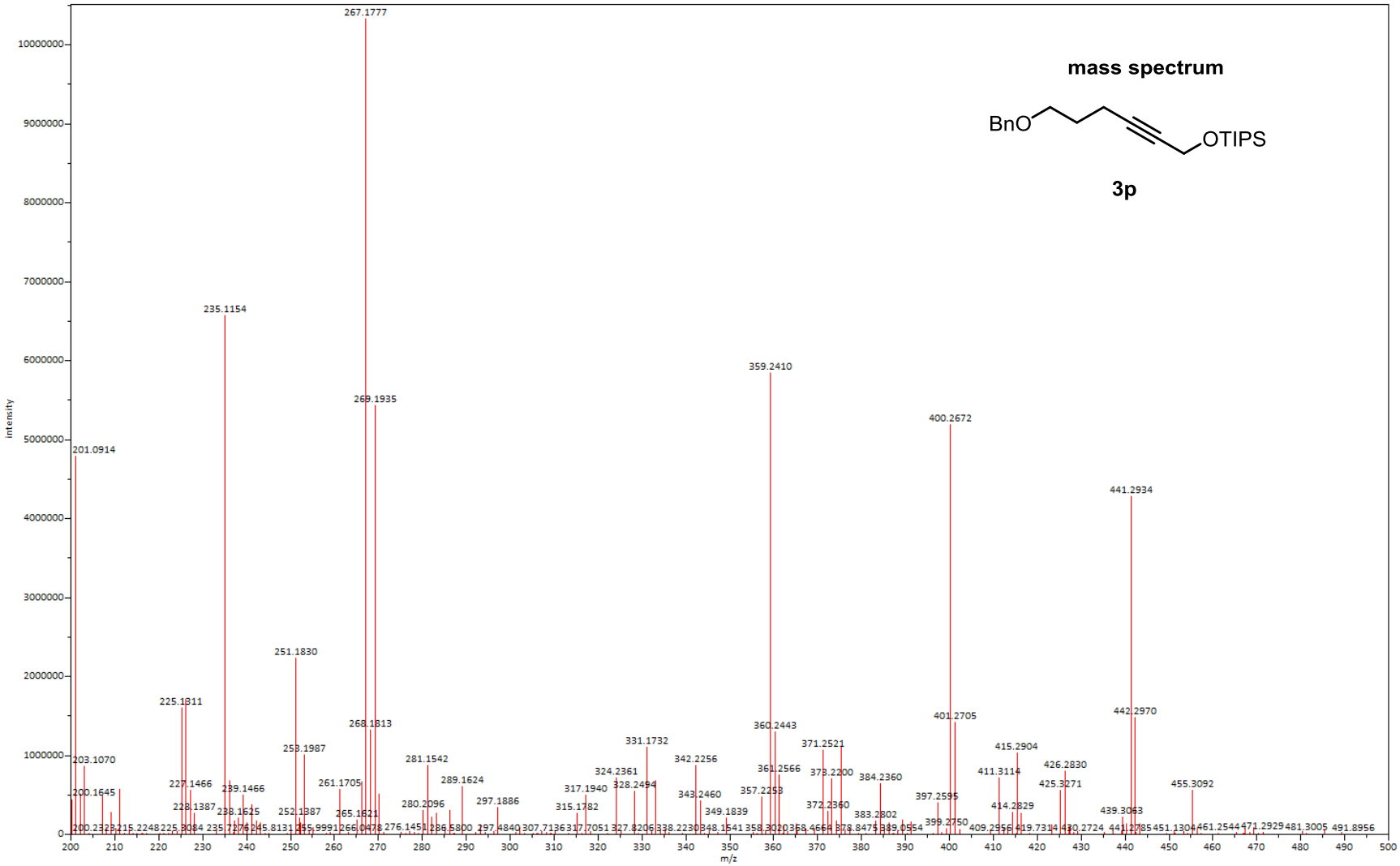


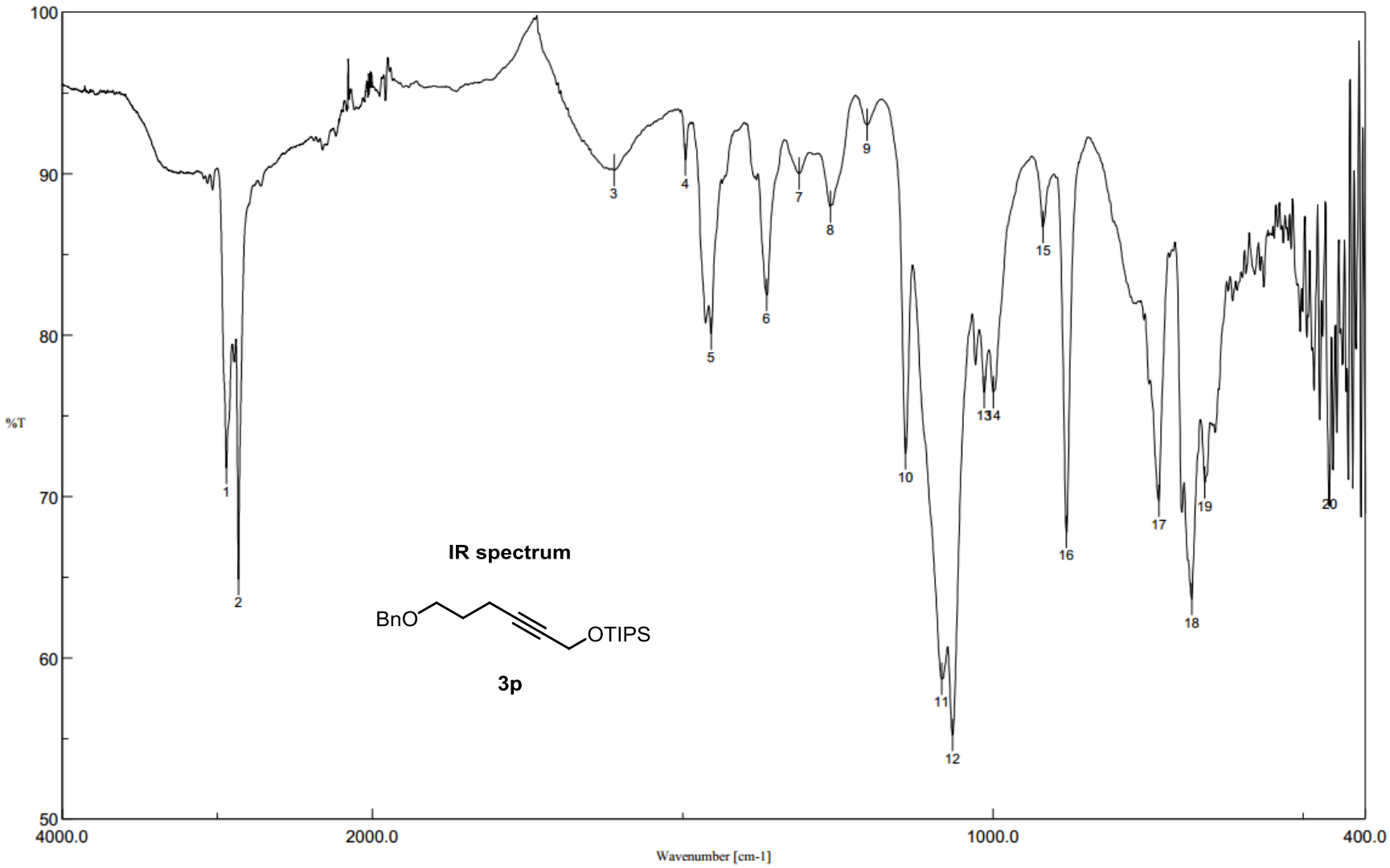

**3p**

**$^{29}$Si DEPT NMR**

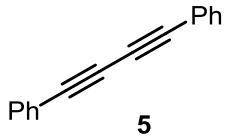



**3p**


mass spectrum
BnO
OTIPS
3p
intensity
m/z
267.1777
235.1154
359.2410
269.1935
400.2672
201.0914
441.2934
251.1830
225.1811
268.1813
401.2705
442.2970
360.2443
331.1732
371.2521
415.2904
203.1070
281.1542
342.2256
426.2830
289.1624
324.2361
361.2566
373.2200
384.2360
411.3114
227.1466
239.1466
317.1940
328.2494
425.3271
455.3092
200.1645
297.1886
357.2253
414.2829
228.1387
238.1625
280.2096
315.1782
372.2360
439.3063
252.1387
253.1987
343.2460
383.2802
261.1705
265.1621
349.1839
397.2595
399.2750

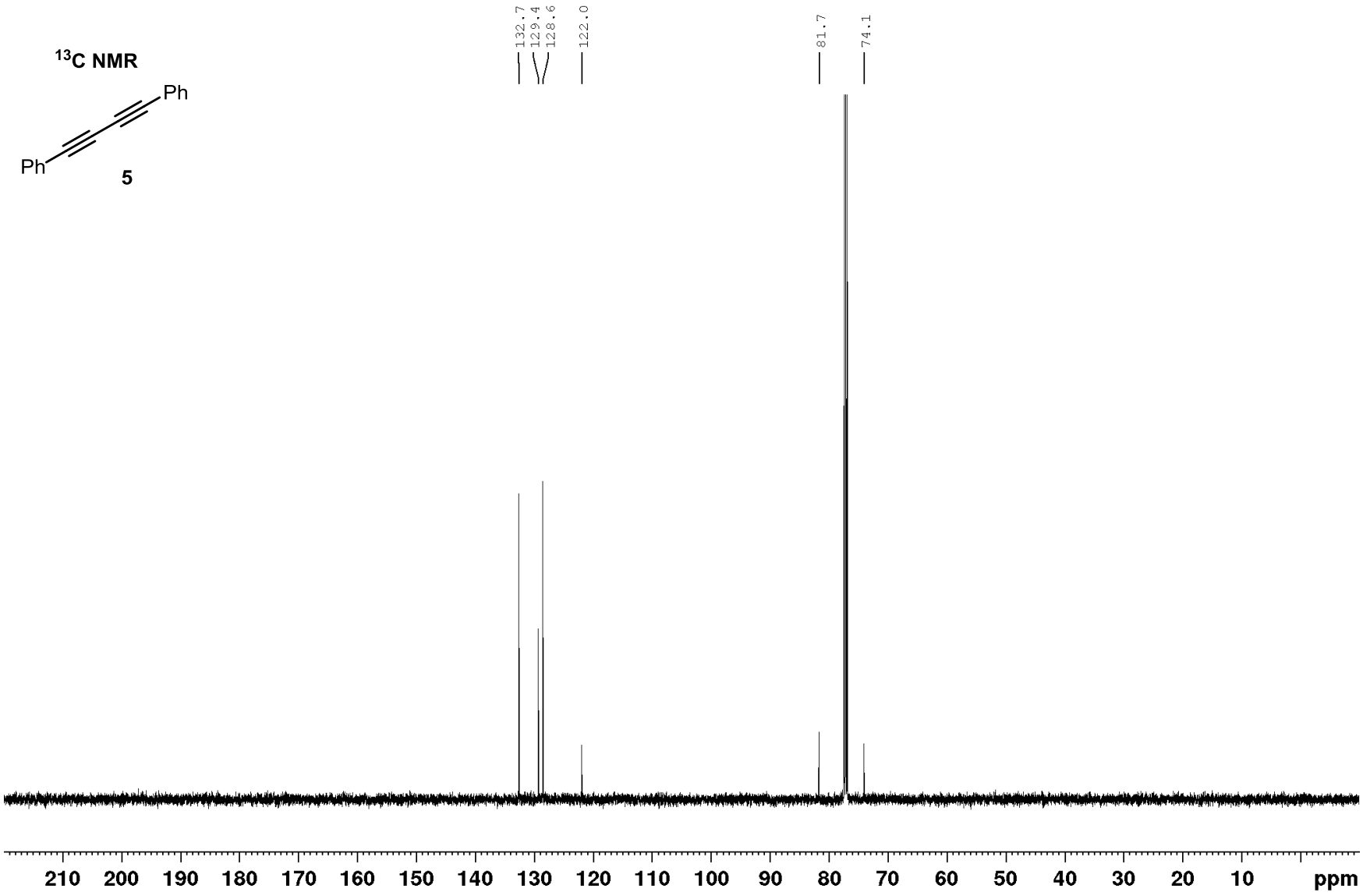

100
90
80
70
60
50
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
IR spectrum
BnO
OTIPS
3p

**$^1$H NMR**

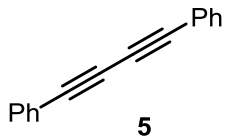

Ph
Ph

**5**


7.55
7.54
7.54
7.54
7.53
7.53
7.52
7.40
7.39
7.39
7.39
7.38
7.37
7.37
7.36
7.36
7.36
7.35
7.34
7.34
7.34
7.33
7.33
7.32
3.99
6.01
11
10
9
8
7
6
5
4
3
2
1
0
ppm

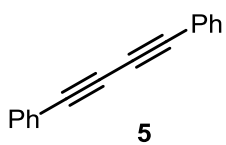

$^{13}$C NMR
Ph
Ph
5
132.7
129.4
128.6
122.0
81.7
74.1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



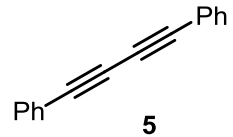

**5**

**$^1$H, $^1$H COSY**




**5**

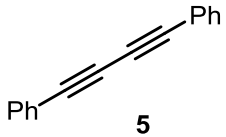
$^{1}H$, $^{13}C$ HMQC


Ph
Ph

5

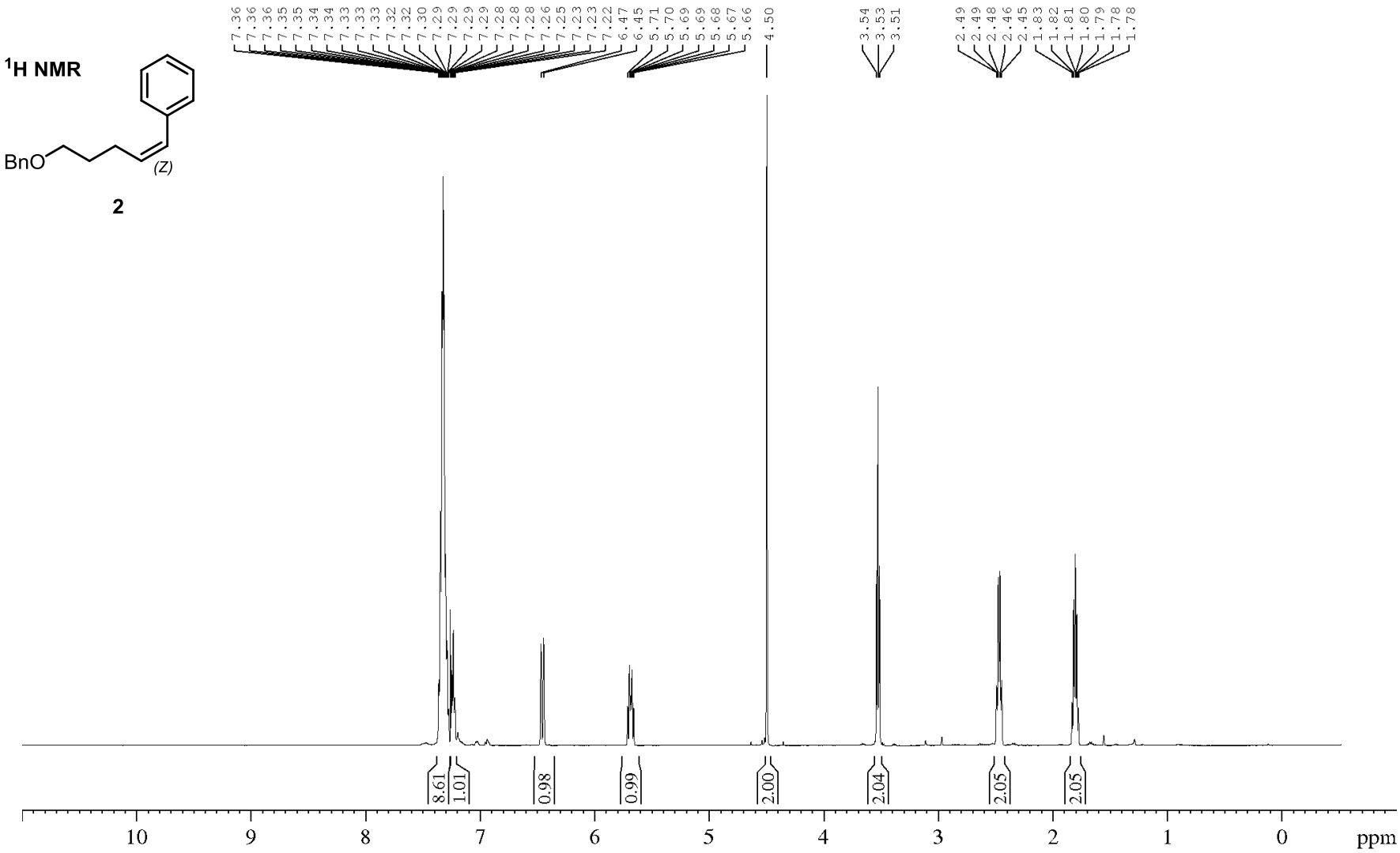

ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

$^{1}H$, $^{13}C$ HMBC

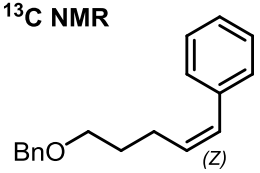

Ph
Ph

**5**


ppm
0
20
40
60
80
100
120
140
160
180
200
12
11
10
9
8
7
6
5
4
3
2
1
0
ppm


1H NMR
BnO
(Z)
2
7.36 7.36 7.36 7.35 7.35 7.34 7.34 7.33 7.33 7.33 7.32 7.32 7.30 7.29 7.29 7.29 7.29 7.28 7.28 7.28 7.26 7.25 7.23 7.23 7.22 6.47 6.45 5.71 5.70 5.69 5.69 5.68 5.67 5.66 4.50
3.54 3.53 3.51
2.49 2.49 2.48 2.46 2.45
1.83 1.82 1.81 1.80 1.79 1.78 1.78
8.61 1.01 0.98 0.99 2.00 2.04 2.05 2.05
10 9 8 7 6 5 4 3 2 1 0 ppm

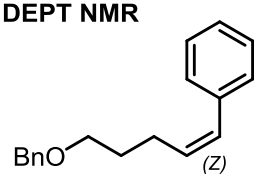
**$^{13}$C NMR**


BnO
(Z)

**2**

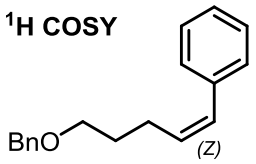

138.7
137.8
132.4
129.5
128.9
128.5
128.3
127.7
127.6
126.6
73.0
69.9
30.1
25.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



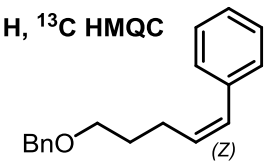

**2**

$^1$H, $^1$H COSY




**2**

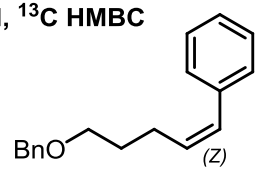
$^{1}H$, $^{13}C$ HMQC


BnO
(Z)

**2**


ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

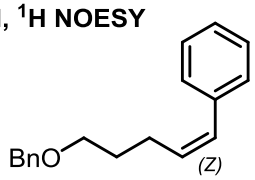
$^{1}H$, $^{13}C$ HMBC


BnO
(Z)

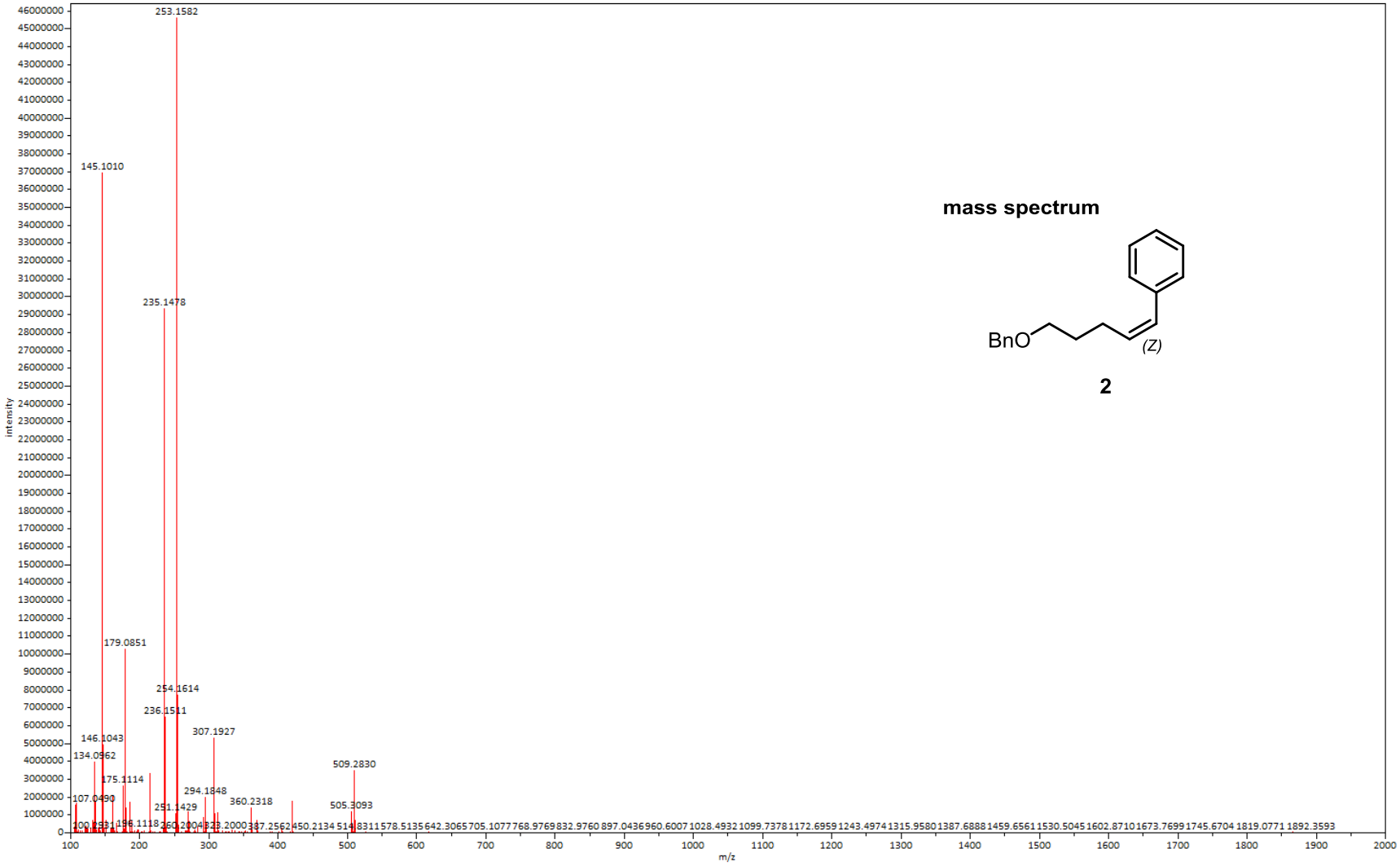
**2**


ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

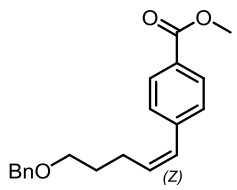
**$^1$H, $^1$H NOESY**




**2**


mass spectrum
BnO
(Z)
2
intensity
m/z
253.1582
145.1010
235.1478
179.0851
254.1614
236.1511
307.1927
146.1043
134.0962
509.2830
175.1114
294.1848
107.0490
251.1429
360.2318
505.3093

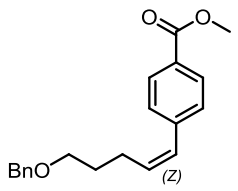
**$^1$H NMR**


O
O
BnO
(Z)

**4a**


8.00
7.99
7.98
7.36
7.35
7.35
7.34
7.34
7.33
7.33
7.32
7.32
7.30
7.29
7.29
7.29
7.28
7.27
7.27
7.26
6.47
6.45
5.81
5.79
5.78
5.78
5.77
5.75
4.48
3.92
3.91
3.52
3.51
3.49
2.48
2.48
2.47
2.46
2.45
2.45
2.44
2.43
1.82
1.81
1.79
1.78
1.77
1.98
6.80
1.00
1.01
2.00
3.00
2.10
2.06
2.11
10
9
8
7
6
5
4
3
2
1
0
ppm

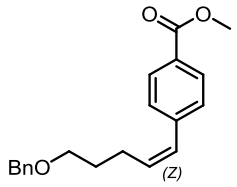
**$^{13}$C NMR**


O
O
BnO
(Z)

**4a**

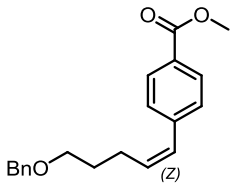

167.1
142.4
138.6
134.6
129.6
128.8
128.7
128.5
128.2
127.7
127.6
73.1
69.7
52.1
30.0
25.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



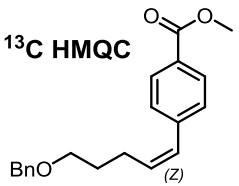

**4a**

**$^1$H, $^1$H COSY**



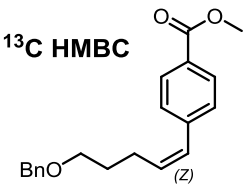

**4a**

$^{1}H$, $^{13}C$ HMQC

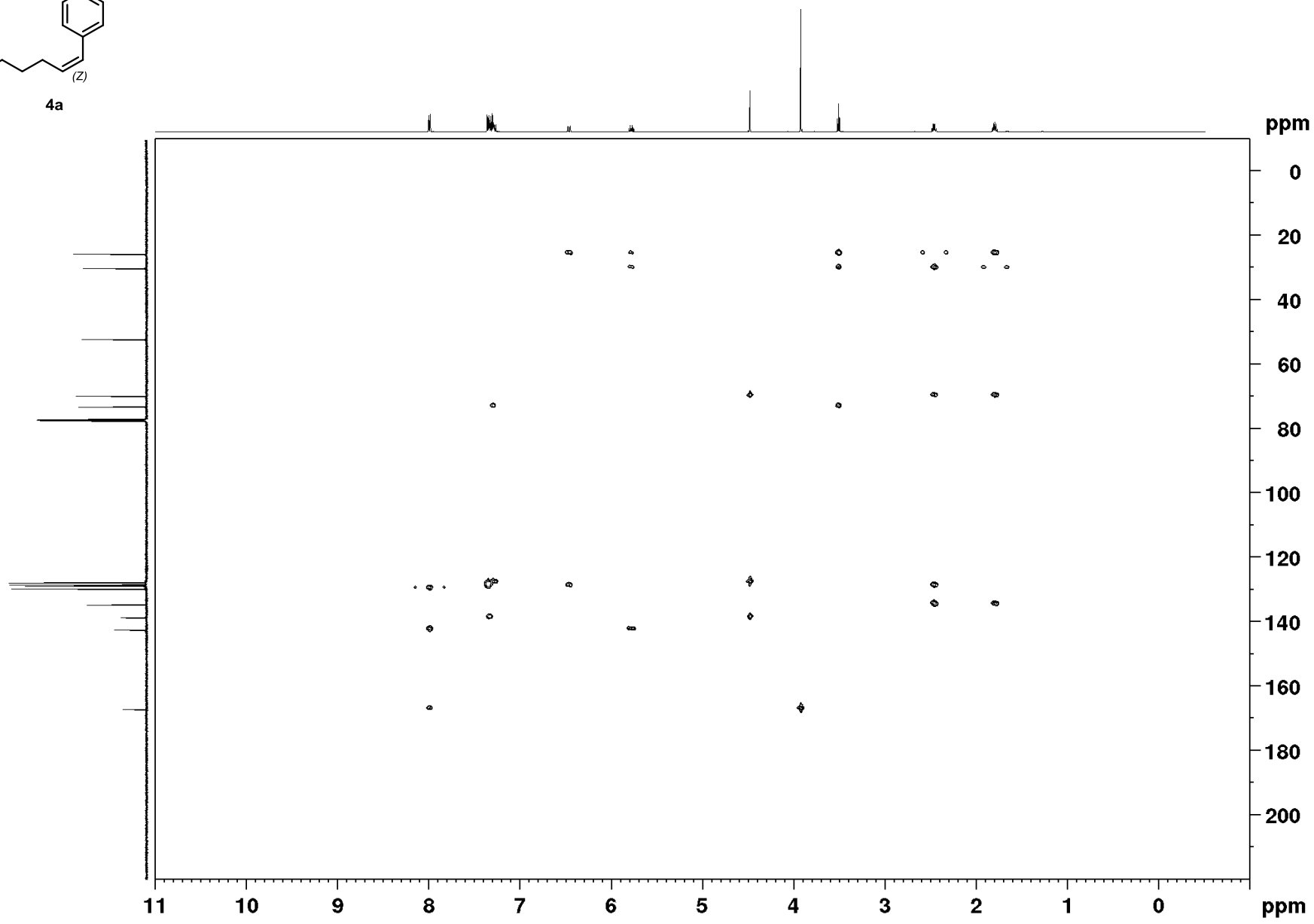



**4a**

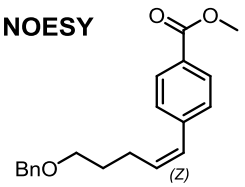
$^{1}H$, $^{13}C$ HMBC



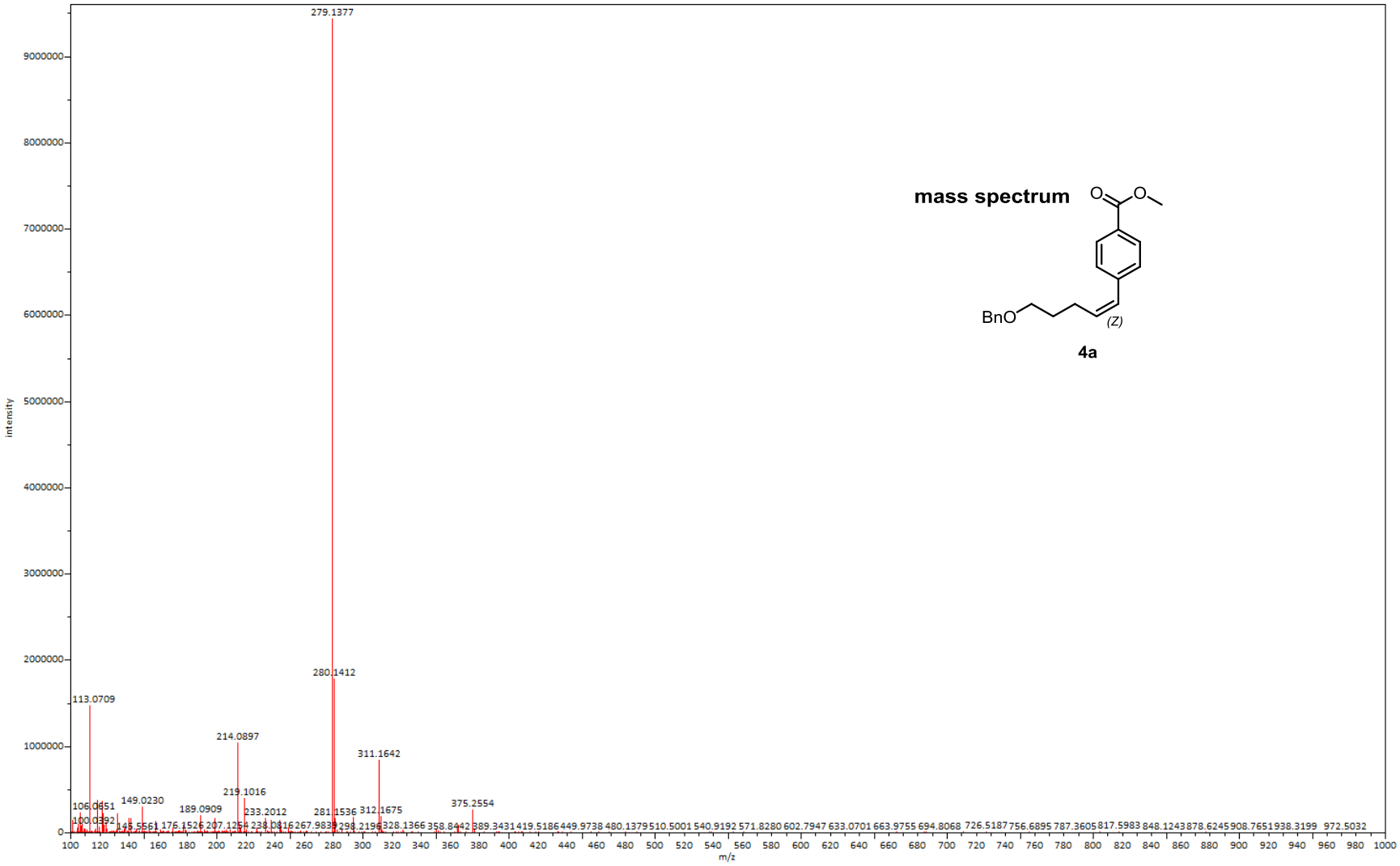

**4a**



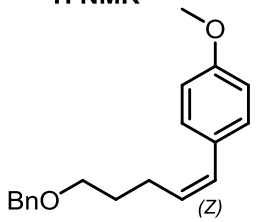
**$^1$H, $^1$H NOESY**




**4a**

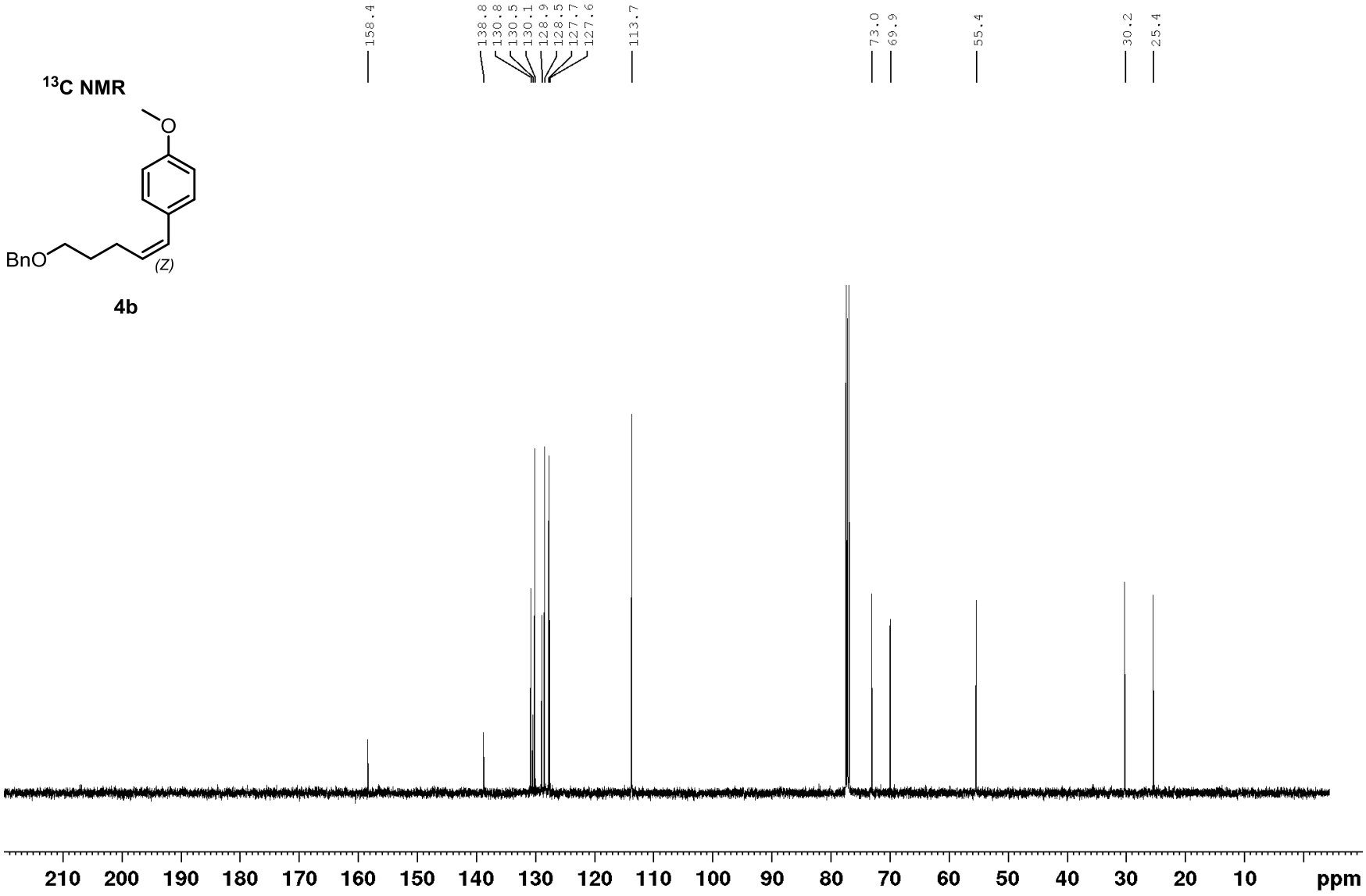

mass spectrum
BnO
(Z)
4a
intensity
m/z
279.1377
280.1412
113.0709
214.0897
311.1642
219.1016
149.0230
106.0651
189.0909
233.2012
281.1536
312.1675
375.2554

**$^1$H NMR**

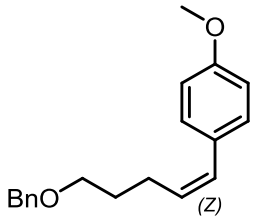

O
BnO
(Z)

**4b**


7.36
7.35
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.27
7.27
7.27
7.27
7.26
7.25
7.24
6.87
6.87
6.85
6.39
6.37
5.60
5.59
5.58
5.58
5.57
5.57
5.55
4.49
3.81
3.53
3.53
3.52
3.52
3.51
2.47
2.45
2.44
2.42
1.82
1.81
1.80
1.79
1.78
1.76
4.81
1.91
1.97
0.99
1.00
2.00
3.05
2.03
2.03
2.04
11
10
9
8
7
6
5
4
3
2
1
0
ppm

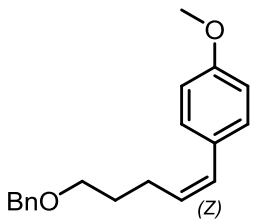

158.4
138.8
130.8
130.5
130.1
128.9
128.5
127.7
127.6
113.7
73.0
69.9
55.4
30.2
25.4
$^{13}$C NMR
O
BnO
(Z)
4b
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



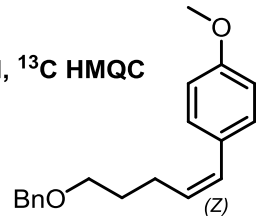

**4b**

**$^1$H, $^1$H COSY**



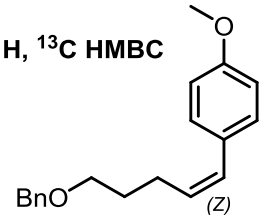

**4b**

$^{1}H$, $^{13}C$ HMQC



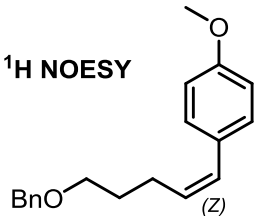

**4b**

$^{1}H$, $^{13}C$ HMBC

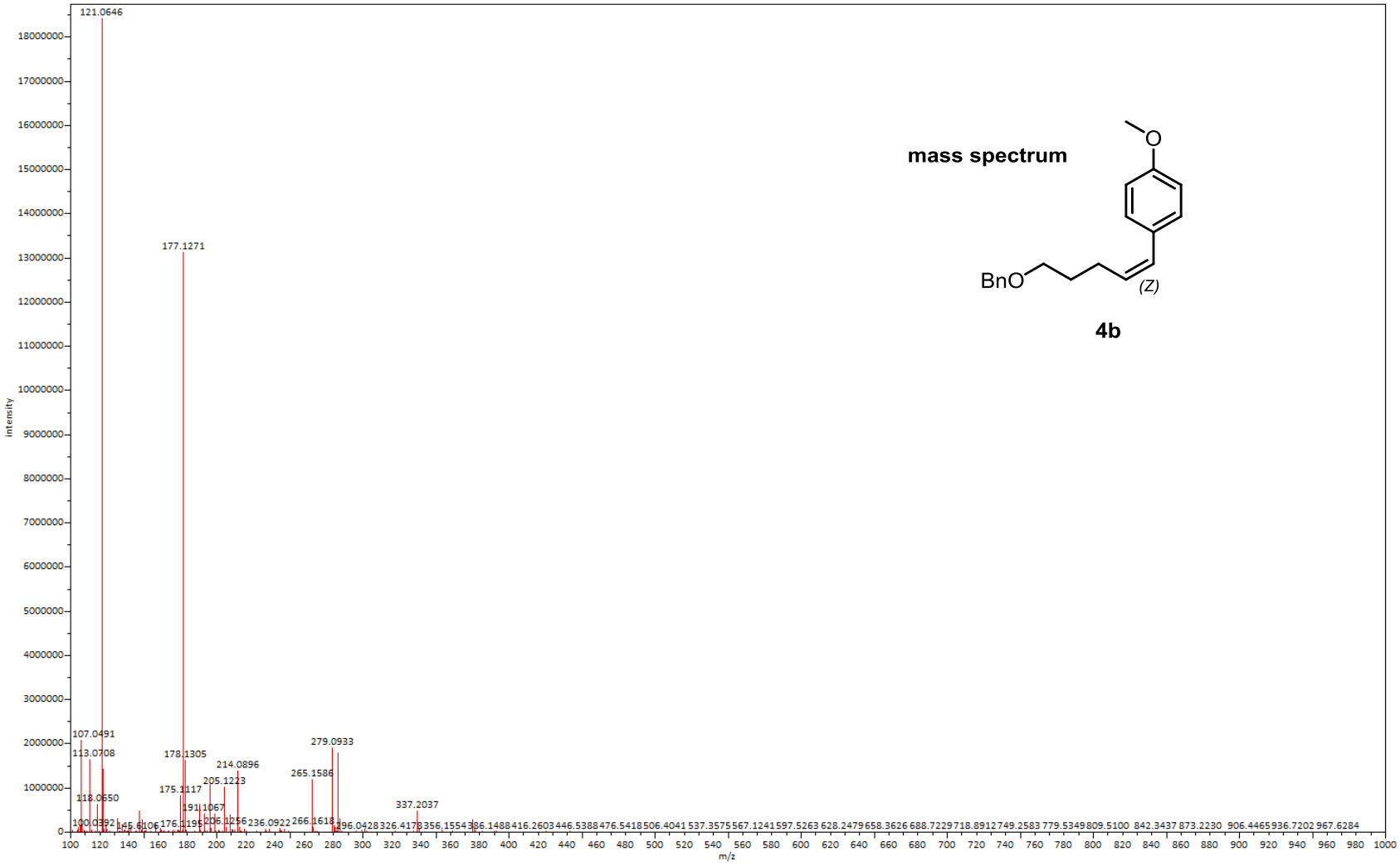



**4b**

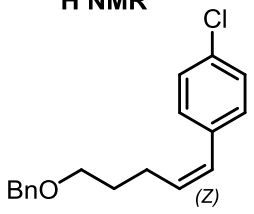
$^1$H, $^1$H NOESY




**4b**


mass spectrum
BnO
(Z)
4b
intensity
m/z
121.0646
177.1271
107.0491
113.0708
118.0650
178.1305
214.0896
205.1223
175.1117
191.1067
279.0933
265.1586
337.2037

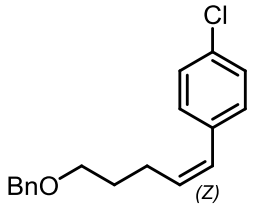
**$^1$H NMR**


Cl
BnO
(Z)

**4c**


7.36
7.34
7.34
7.33
7.33
7.31
7.29
7.27
7.23
7.21
6.40
6.37
5.72
5.70
5.69
5.69
5.68
5.66
4.48
3.52
3.51
3.50
2.44
2.44
2.43
2.43
2.41
2.41
2.40
2.40
1.81
1.80
1.78
1.77
1.76
1.99
4.71
1.98
0.98
0.99
2.00
2.02
2.02
2.02
11
10
9
8
7
6
5
4
3
2
1
0
ppm

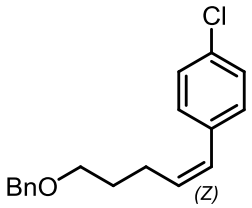
**$^{13}$C NMR**


Cl
BnO
(Z)

**4c**

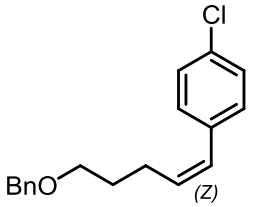

138.6
136.2
133.1
132.4
130.2
128.5
128.4
128.3
127.7
127.7
73.1
69.7
30.0
25.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



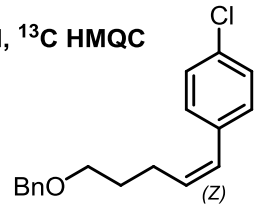

**4c**

**$^1$H, $^1$H COSY**



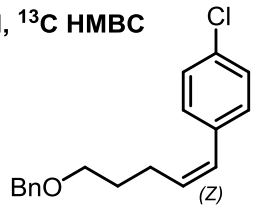

**4c**

$^{1}H$, $^{13}C$ HMQC



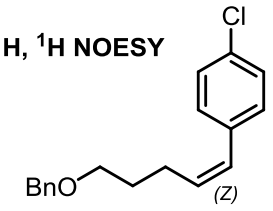

**4c**

$^{1}H$, $^{13}C$ HMBC

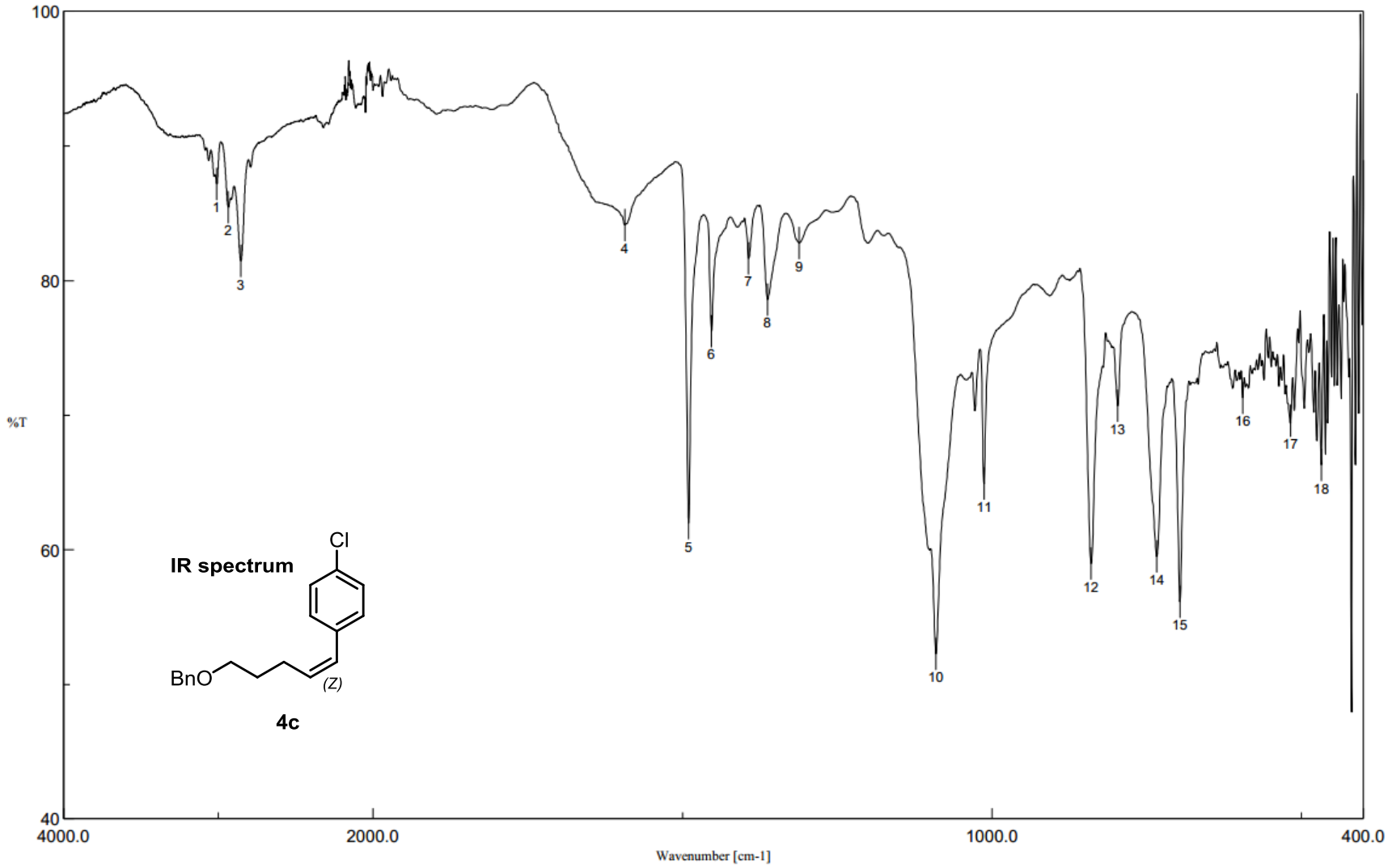


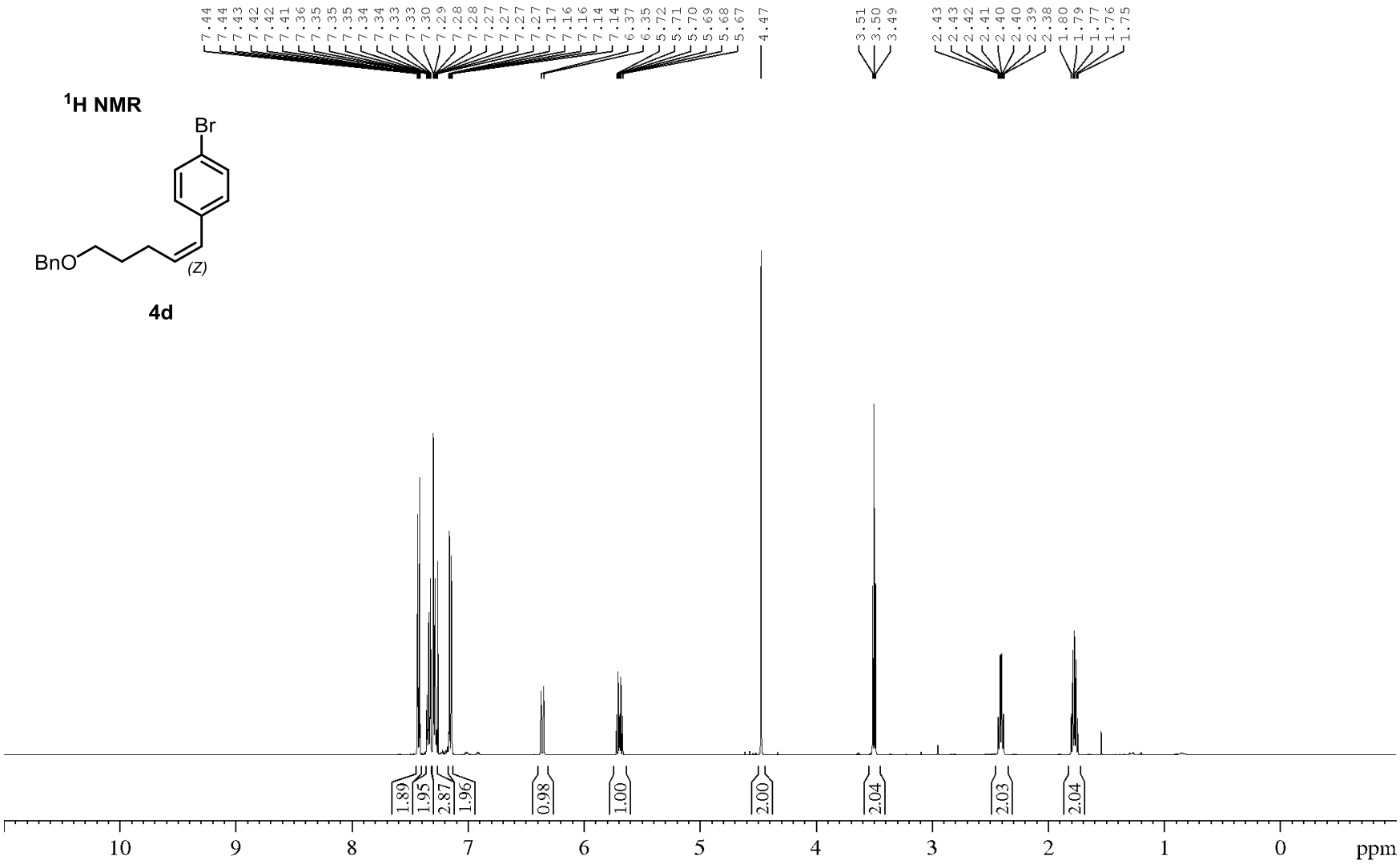

**4c**

$^1$H, $^1$H NOESY

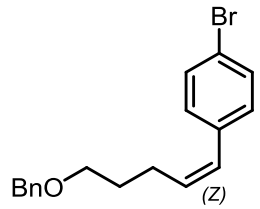



**4c**


100
80
60
40
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
IR spectrum
Cl
BnO
(Z)
4c


7.44
7.44
7.43
7.42
7.42
7.41
7.36
7.35
7.35
7.35
7.34
7.34
7.33
7.33
7.30
7.29
7.28
7.28
7.27
7.27
7.27
7.27
7.17
7.16
7.16
7.14
7.14
6.37
6.35
5.72
5.71
5.70
5.69
5.68
5.67
4.47
3.51
3.50
3.49
2.43
2.43
2.42
2.41
2.40
2.40
2.39
2.38
1.80
1.79
1.77
1.76
1.75
1H NMR
Br
BnO
(Z)
4d
1.89
1.95
2.87
1.96
0.98
1.00
2.00
2.04
2.03
2.04
10
9
8
7
6
5
4
3
2
1
0
ppm

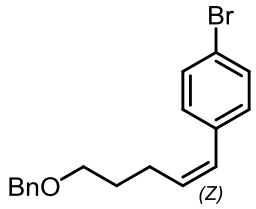
**$^{13}$C NMR**


Br
BnO
(Z)

**4d**

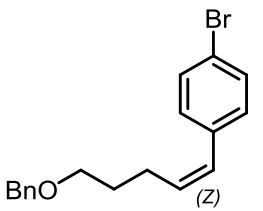

138.6
136.6
133.2
131.4
130.5
128.5
128.4
127.7
127.7
120.5
73.1
69.7
30.0
25.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**

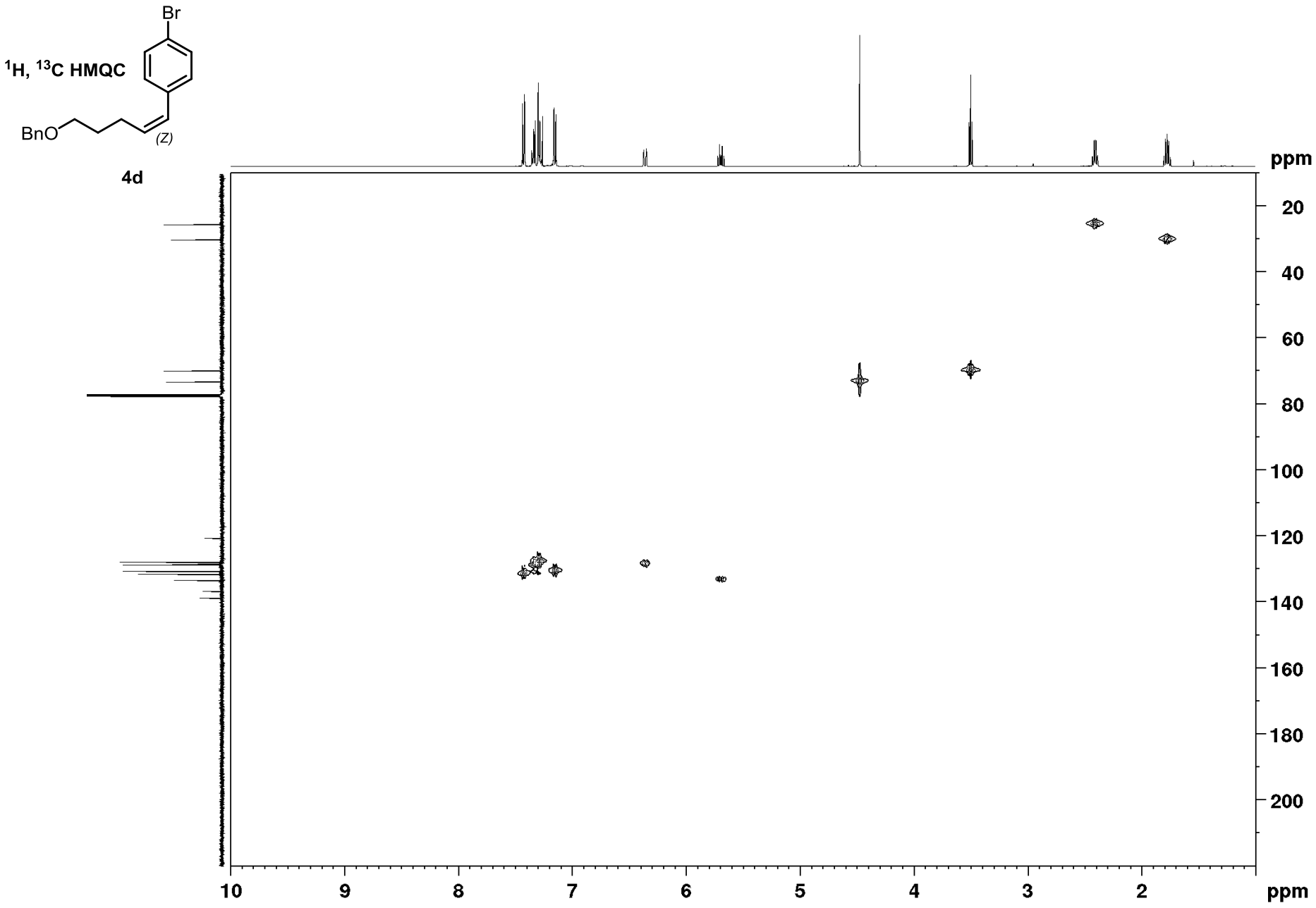



**4d**

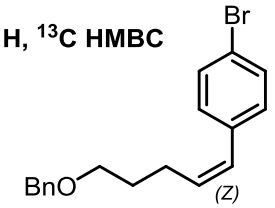
**$^1$H, $^1$H COSY**



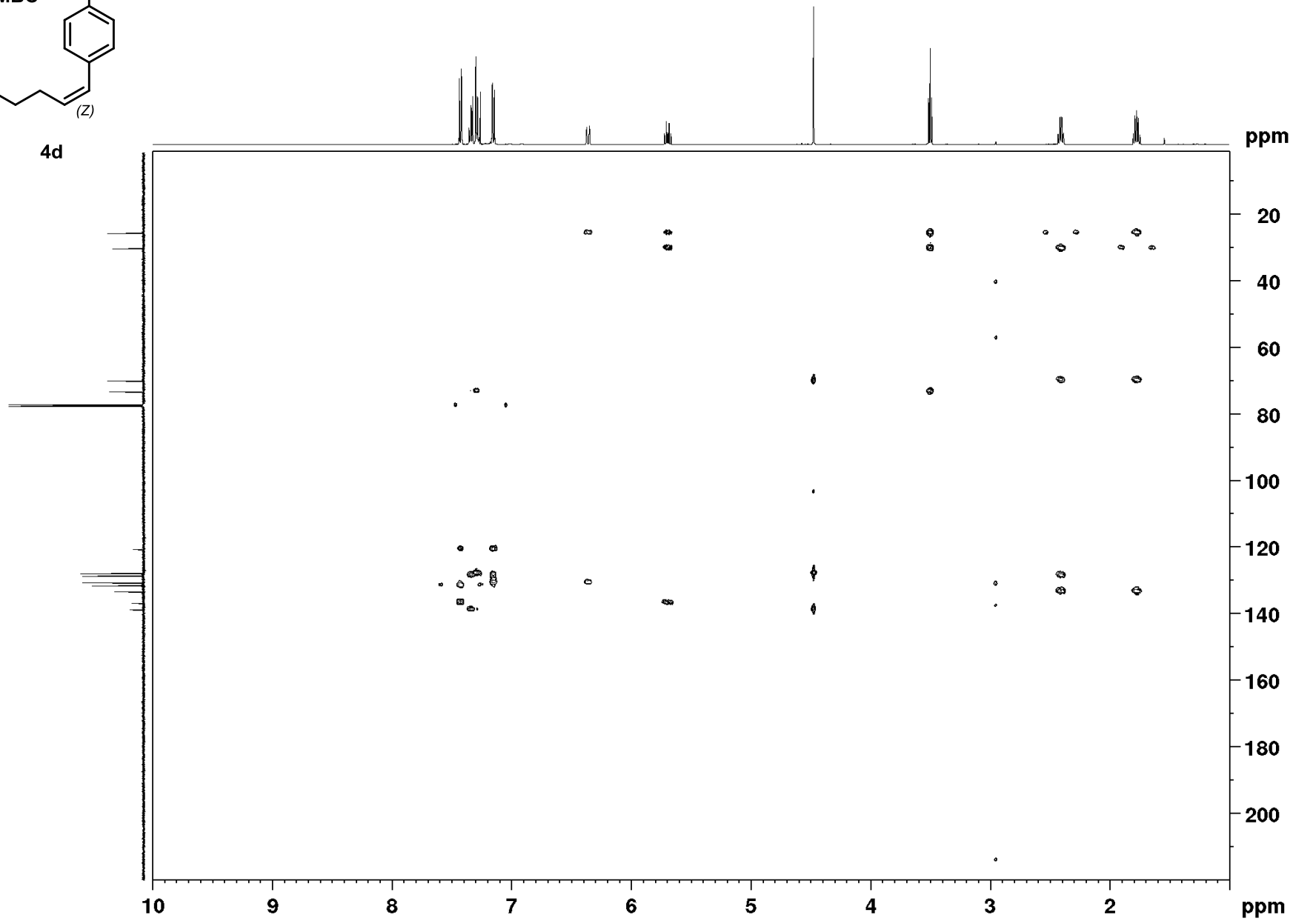

**4d**


Br
BnO
(Z)
$^{1}$H, $^{13}$C HMQC
4d
ppm
20
40
60
80
100
120
140
160
180
200
10
9
8
7
6
5
4
3
2
ppm

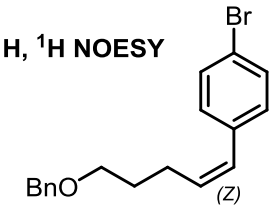
$^{1}$H, $^{13}$C HMBC



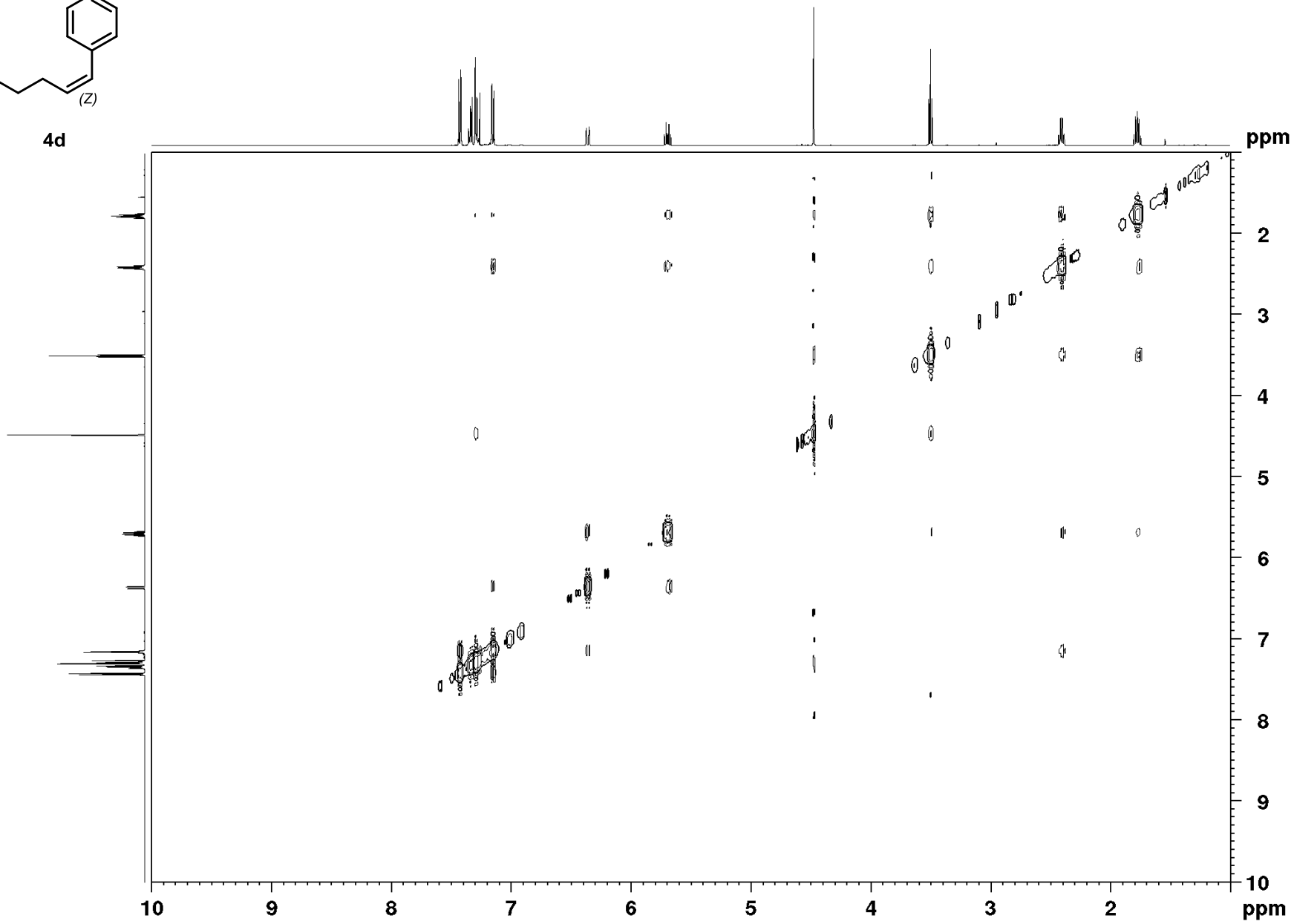

**4d**

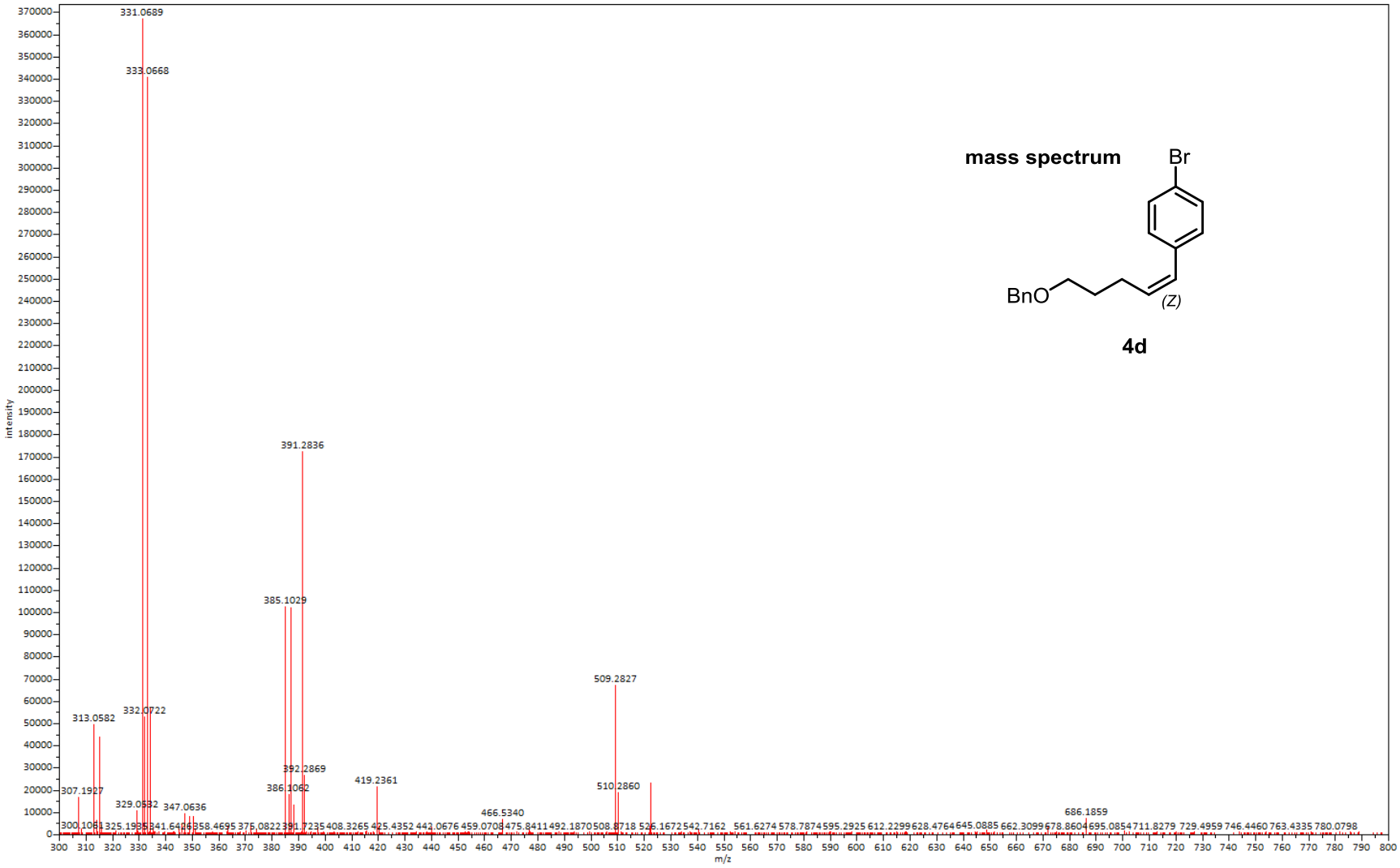


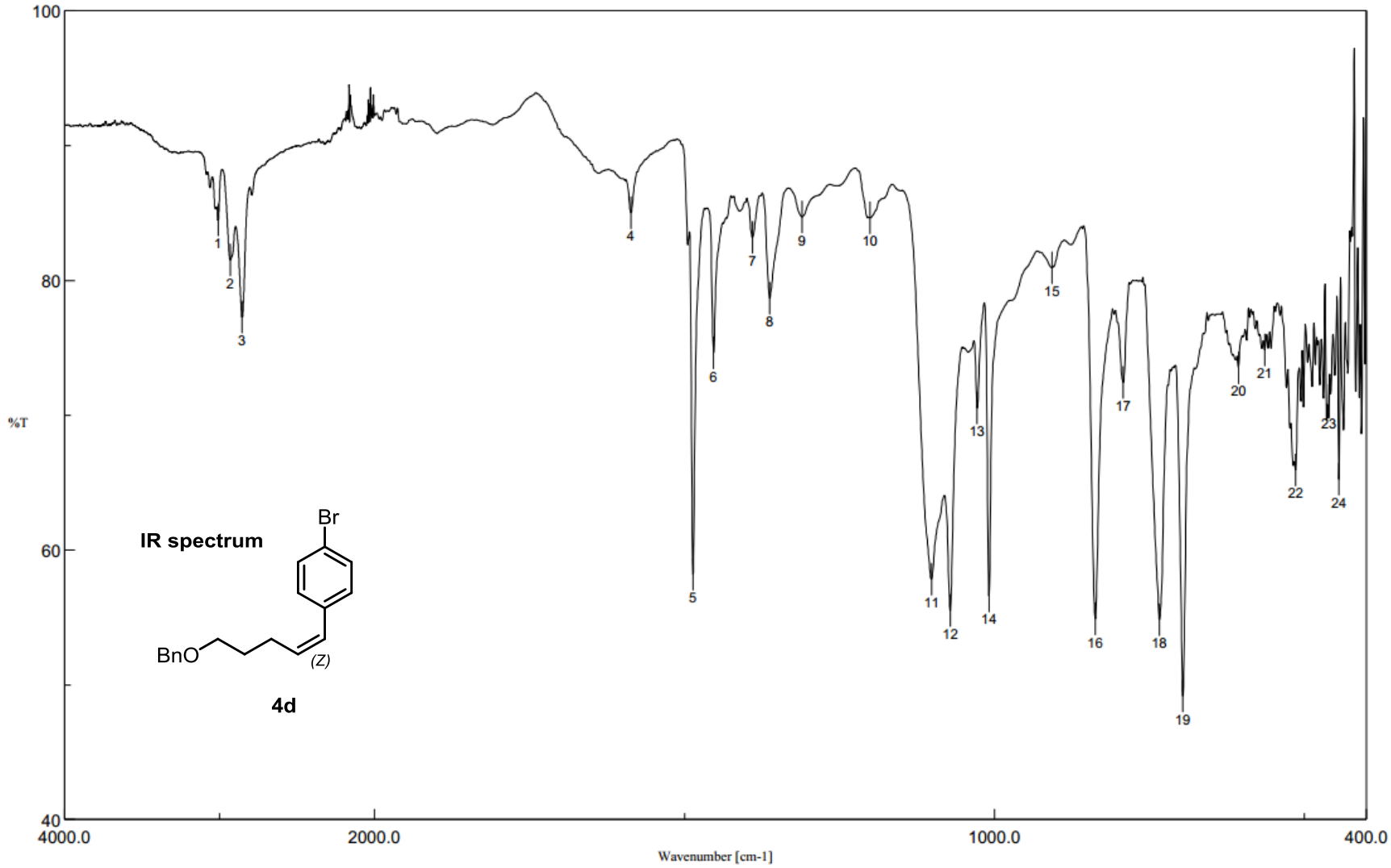
$^1$H, $^1$H NOESY



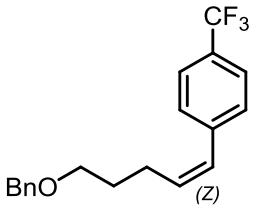

**4d**




mass spectrum
Br
BnO
(Z)
4d
intensity
m/z
331.0689
333.0668
391.2836
385.1029
509.2827
332.0722
313.0582
392.2869
386.1062
419.2361
510.2860
307.1927
329.0532
347.0636
466.5340
686.1859

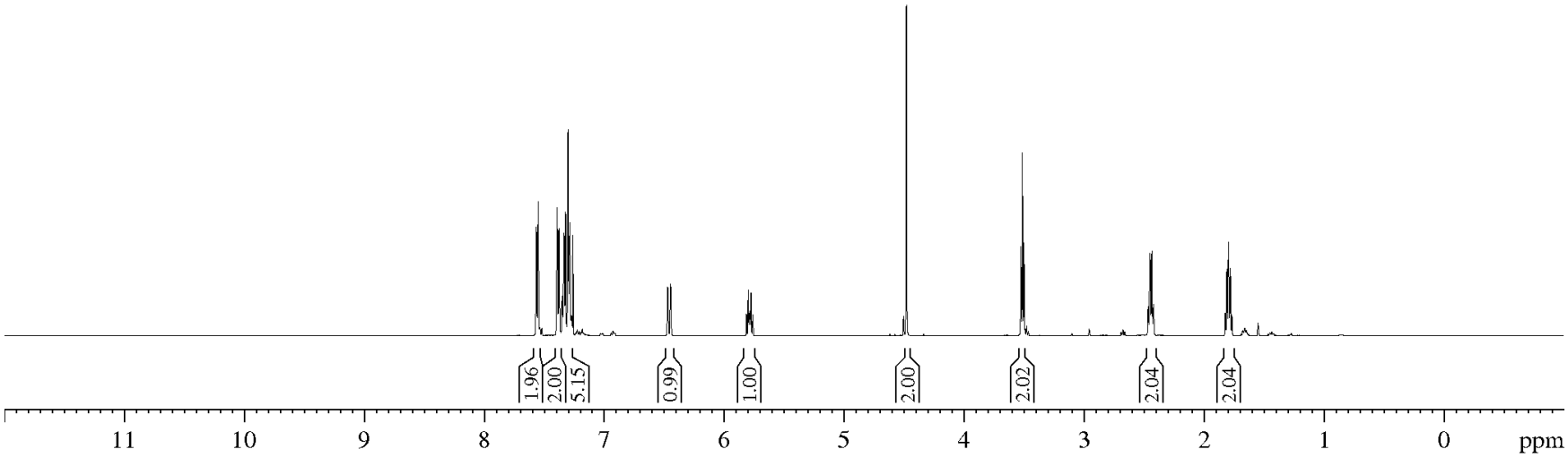

IR spectrum
Br
BnO
(Z)
4d
%T
100
80
60
40
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24

**$^1$H NMR**

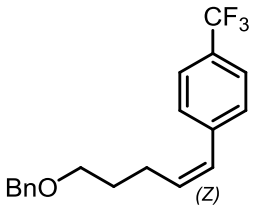

CF3
BnO
(Z)

**4e**


7.57
7.55
7.39
7.38
7.35
7.34
7.33
7.33
7.32
7.30
7.29
7.28
7.27
7.27
7.26
6.47
6.45
5.81
5.80
5.79
5.78
5.78
5.76
4.48
3.53
3.51
3.50
2.46
2.45
2.43
2.42
1.82
1.81
1.79
1.78
1.77


1.96
2.00
5.15
0.99
1.00
2.00
2.02
2.04
2.04
11
10
9
8
7
6
5
4
3
2
1
0
ppm

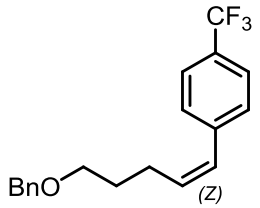
**$^{13}$C NMR**


CF3
BnO
(Z)

**4e**

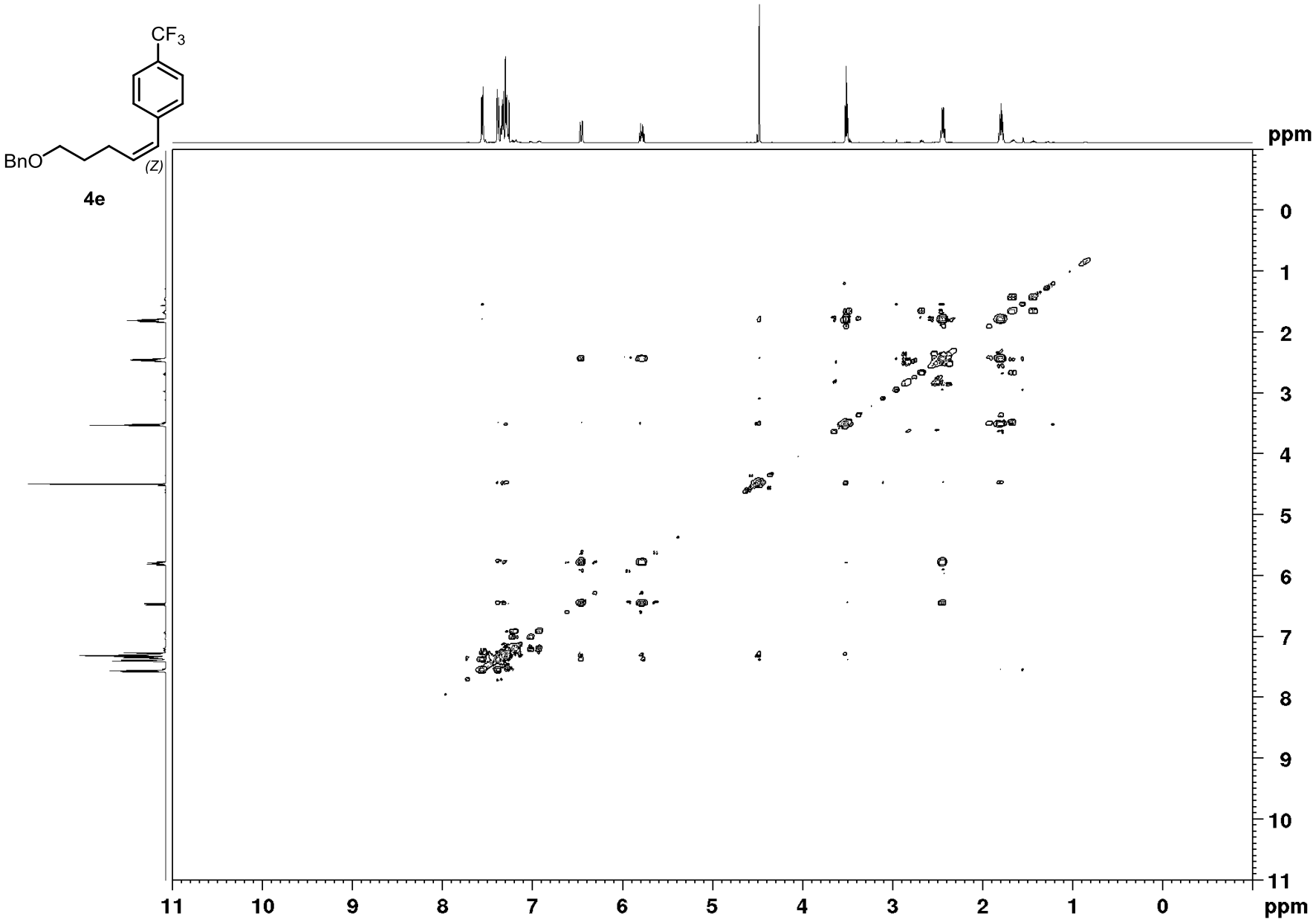

141.3
138.6
134.6
129.1
128.5
128.3
127.7
127.7
125.3
125.2
125.2
125.2
73.1
69.7
30.0
25.5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

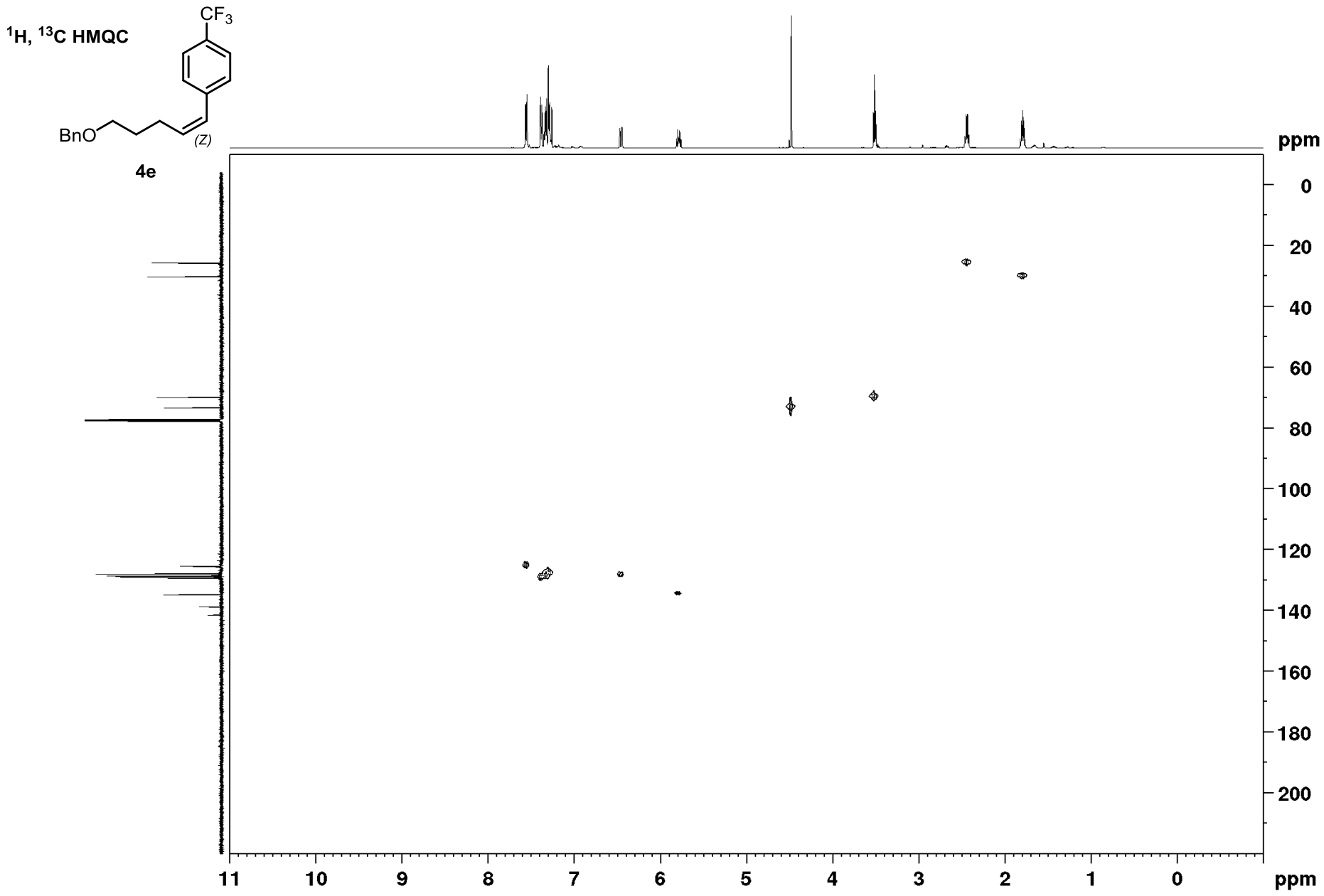
**$^{13}$C DEPT NMR**

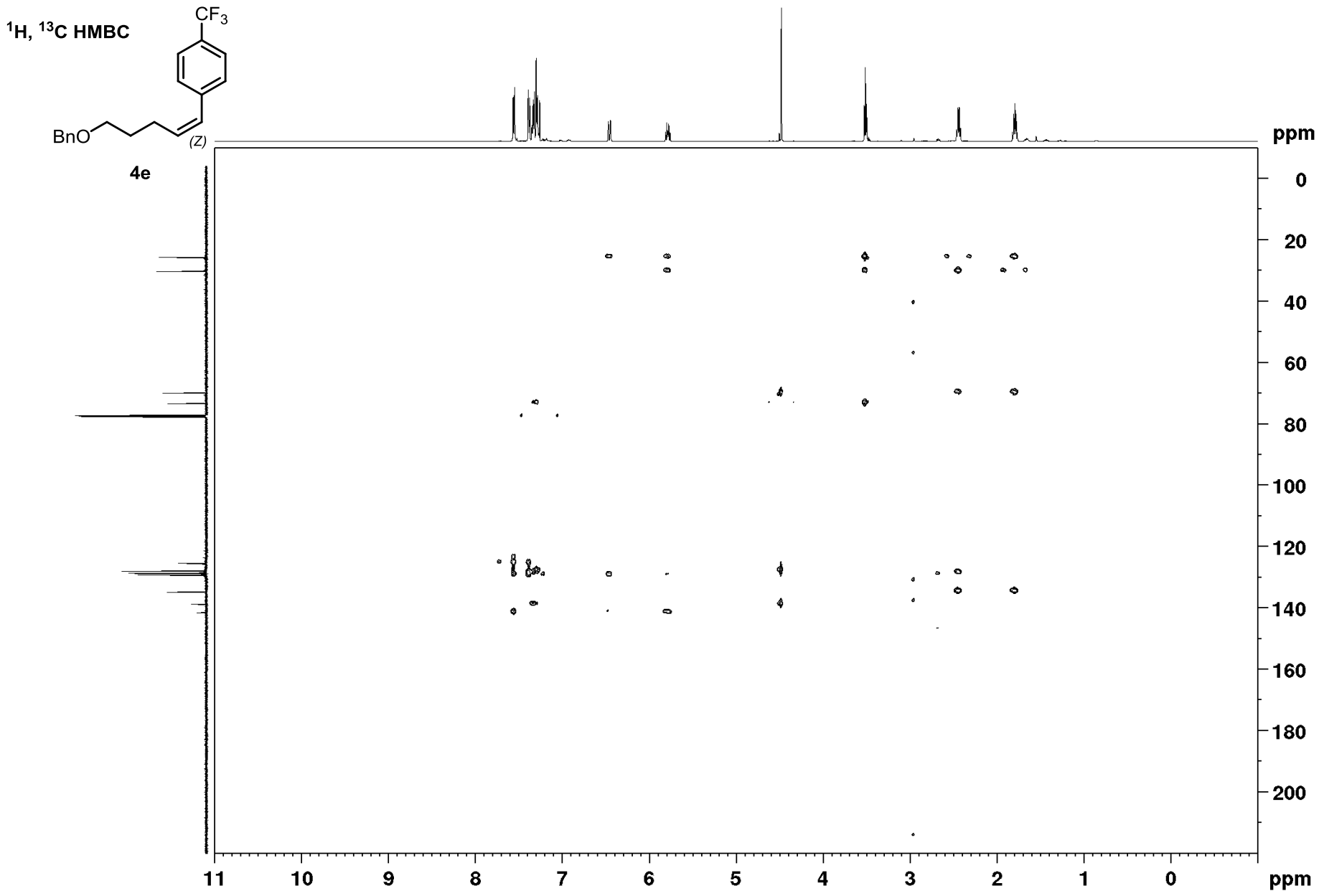



**4e**

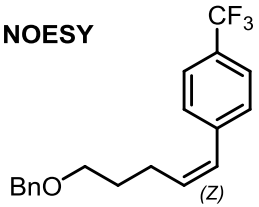
**$^1$H, $^1$H COSY**



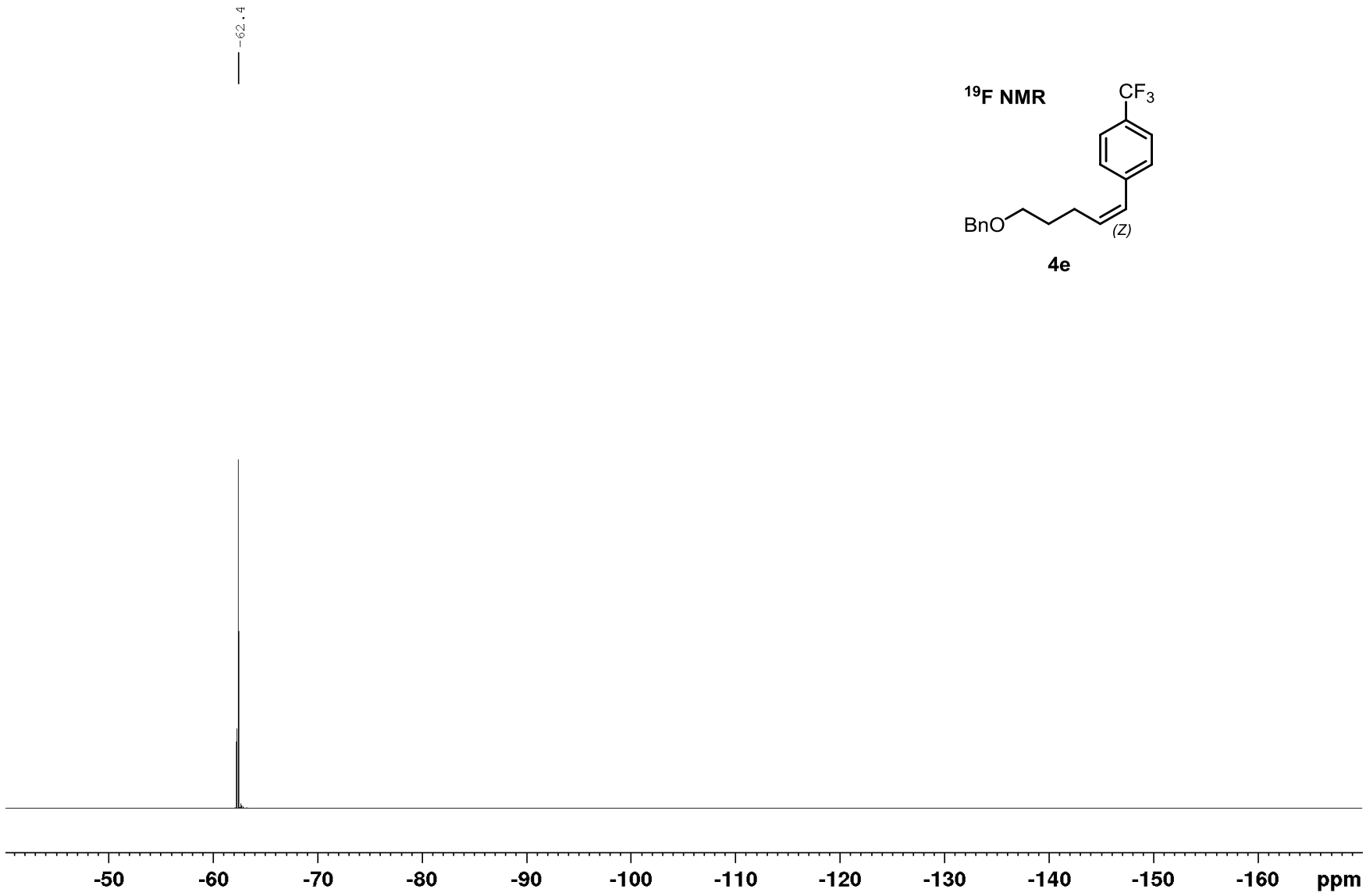

$^1$H, $^{13}$C HMQC
CF3
BnO
(Z)
4e
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

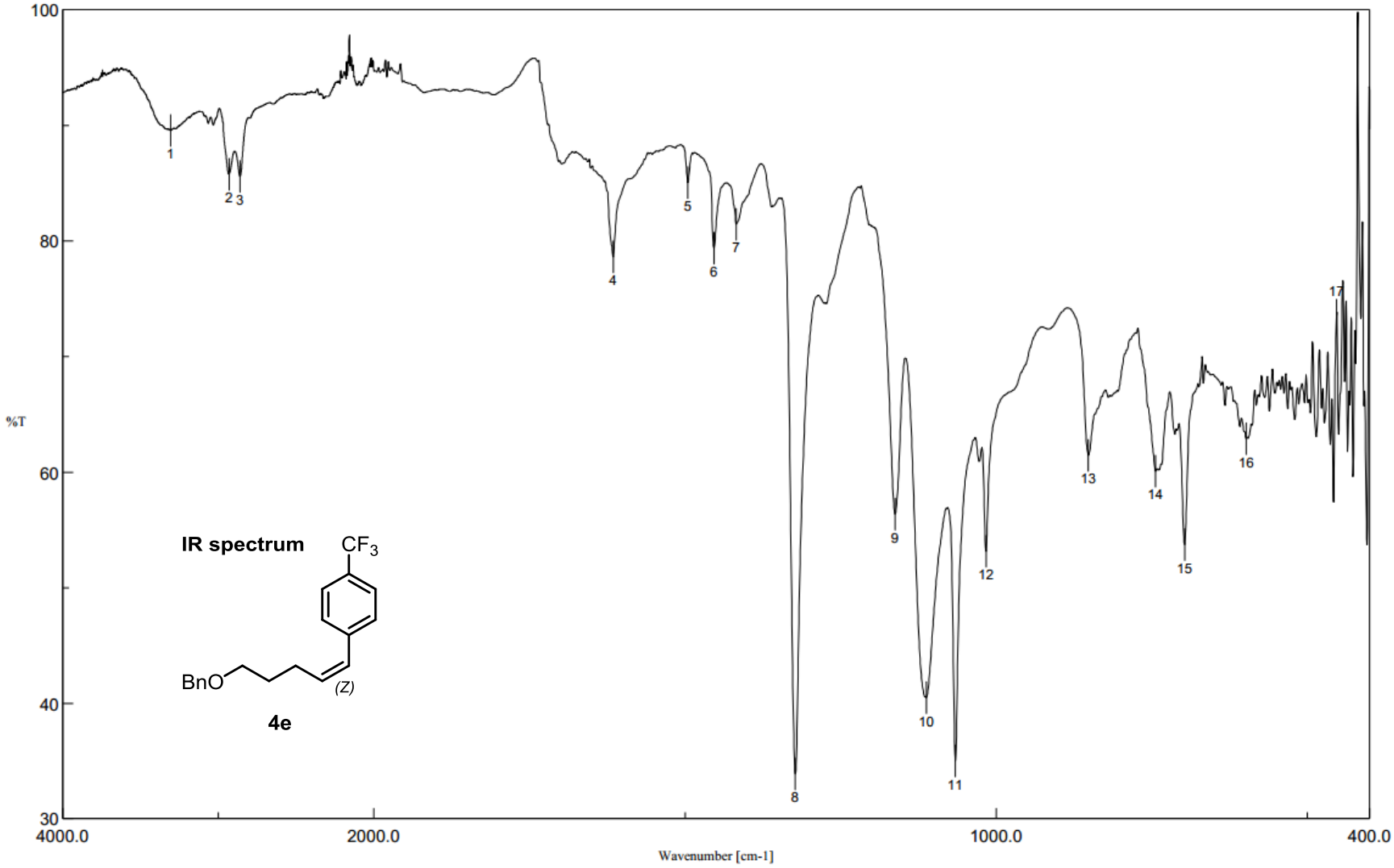

$^1$H, $^{13}$C HMBC
CF3
BnO
(Z)
4e
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

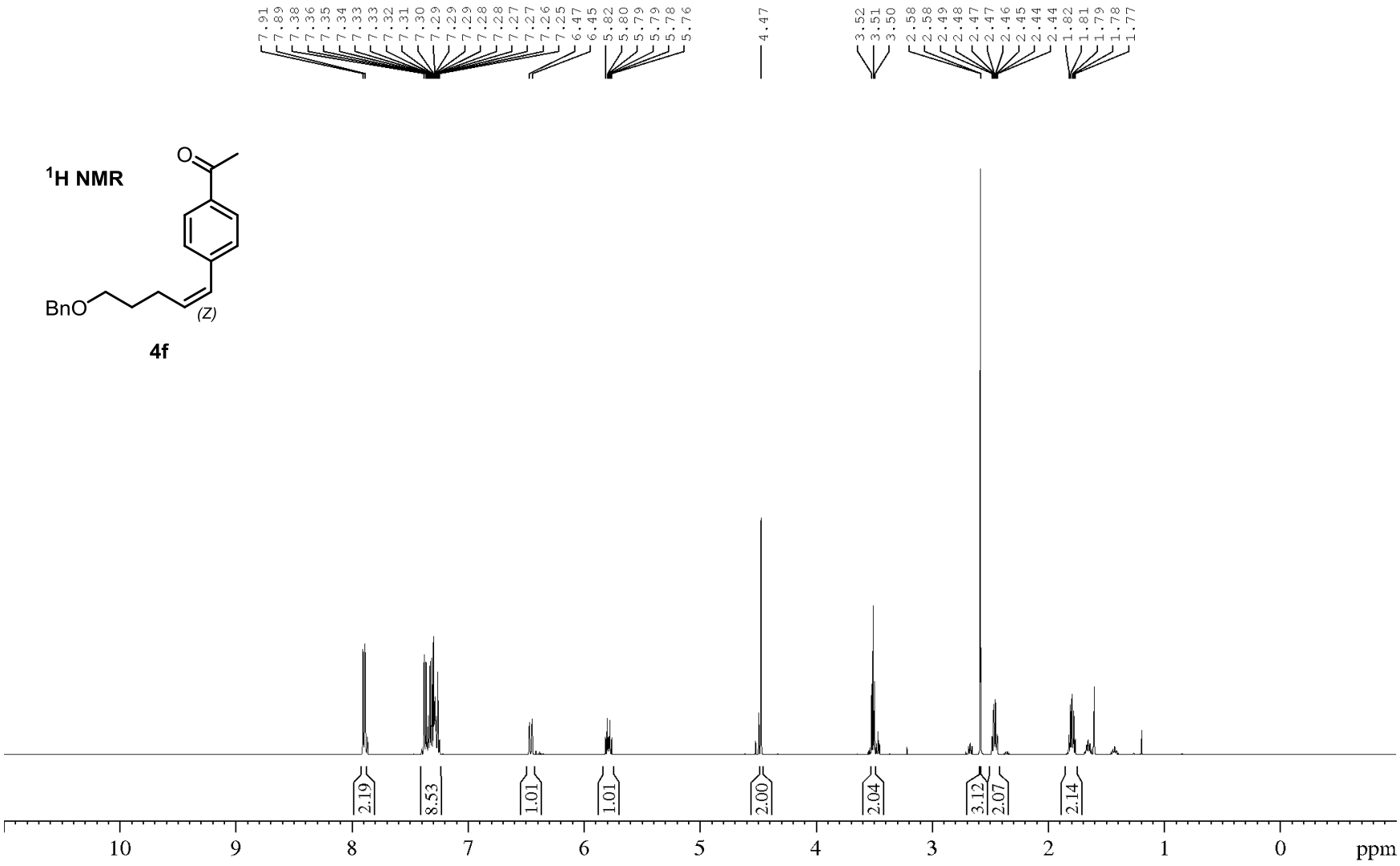
**$^1$H, $^1$H NOESY**

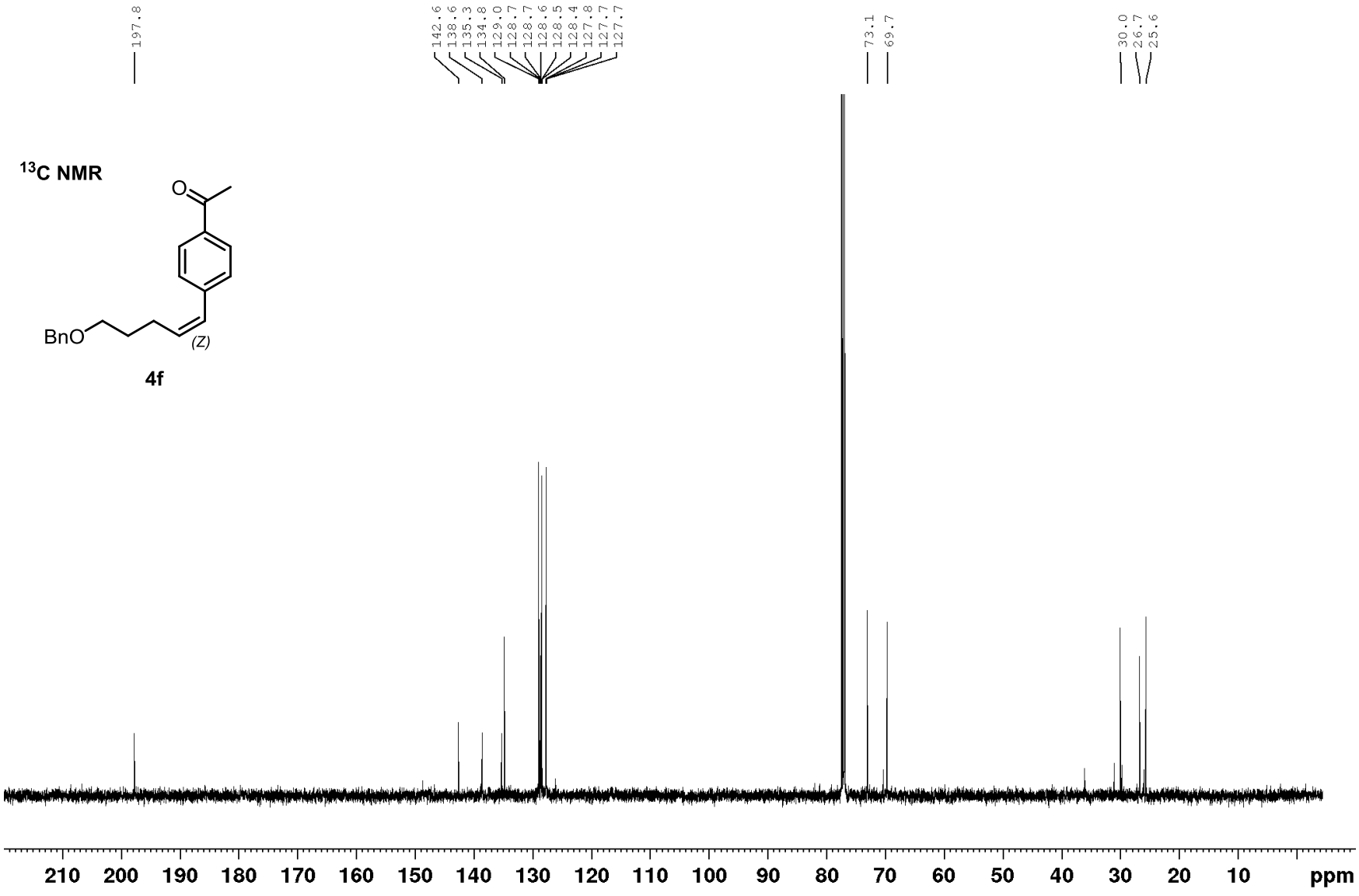


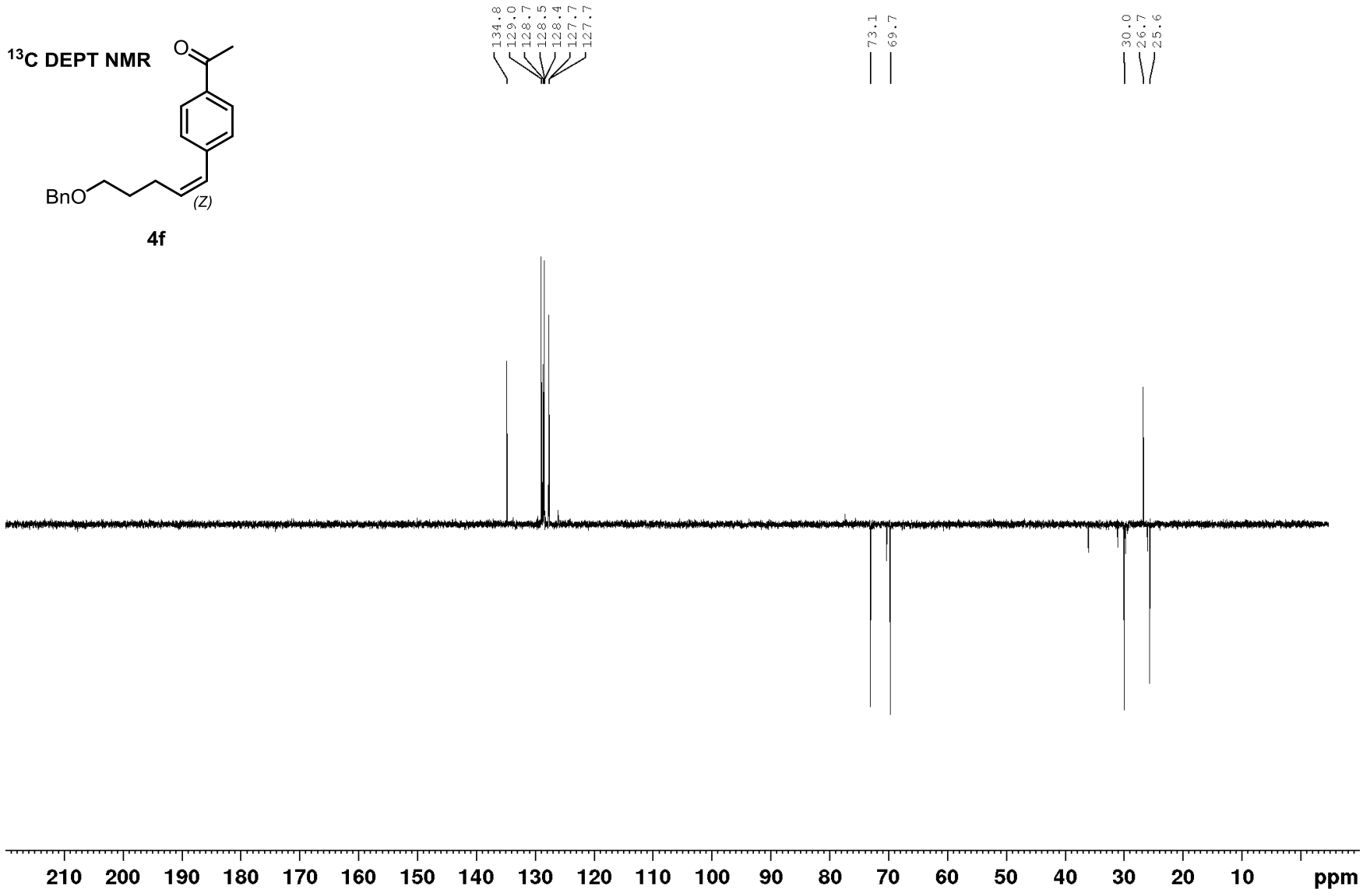

**4e**


-62.4
19F NMR
CF3
BnO
(Z)
4e
-50
-60
-70
-80
-90
-100
-110
-120
-130
-140
-150
-160
ppm

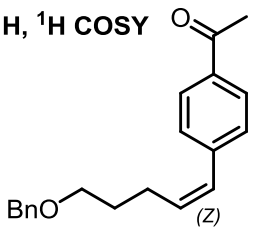

100
80
60
40
30
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
IR spectrum
CF3
BnO
(Z)
4e


7.91
7.89
7.38
7.36
7.35
7.34
7.33
7.32
7.31
7.30
7.29
7.29
7.29
7.28
7.28
7.27
7.27
7.26
7.25
6.47
6.45
5.82
5.80
5.79
5.79
5.78
5.76
4.47
3.52
3.51
3.50
2.58
2.58
2.49
2.48
2.47
2.47
2.46
2.45
2.44
2.44
1.82
1.81
1.79
1.78
1.77
1H NMR
O
BnO
(Z)
4f
2.19
8.53
1.01
1.01
2.00
2.04
3.12
2.07
2.14
10
9
8
7
6
5
4
3
2
1
0
ppm

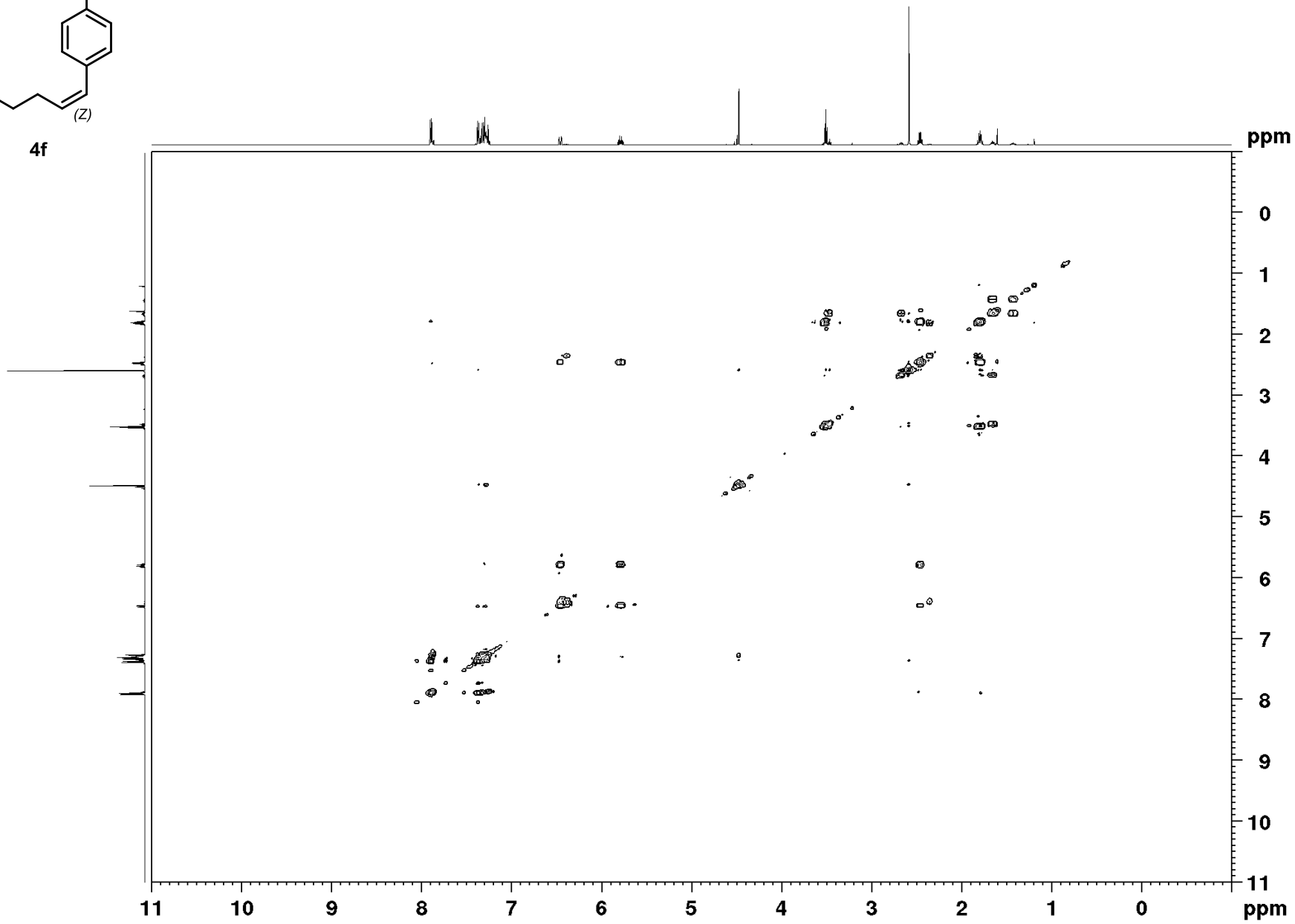

197.8
142.6
138.6
135.3
134.8
129.0
128.7
128.7
128.6
128.5
128.4
127.8
127.7
127.7
73.1
69.7
30.0
26.7
25.6
13C NMR
O
BnO
(Z)
4f
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


13C DEPT NMR
O
BnO
(Z)
4f
134.8
129.0
128.7
128.5
128.4
127.7
127.7
73.1
69.7
30.0
26.7
25.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

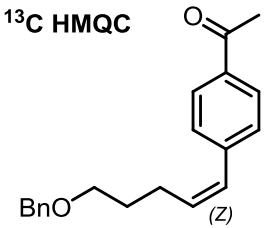
$^1$H, $^1$H COSY




**4f**

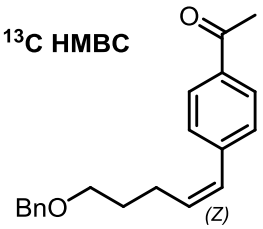


$^{1}H$, $^{13}C$ HMQC

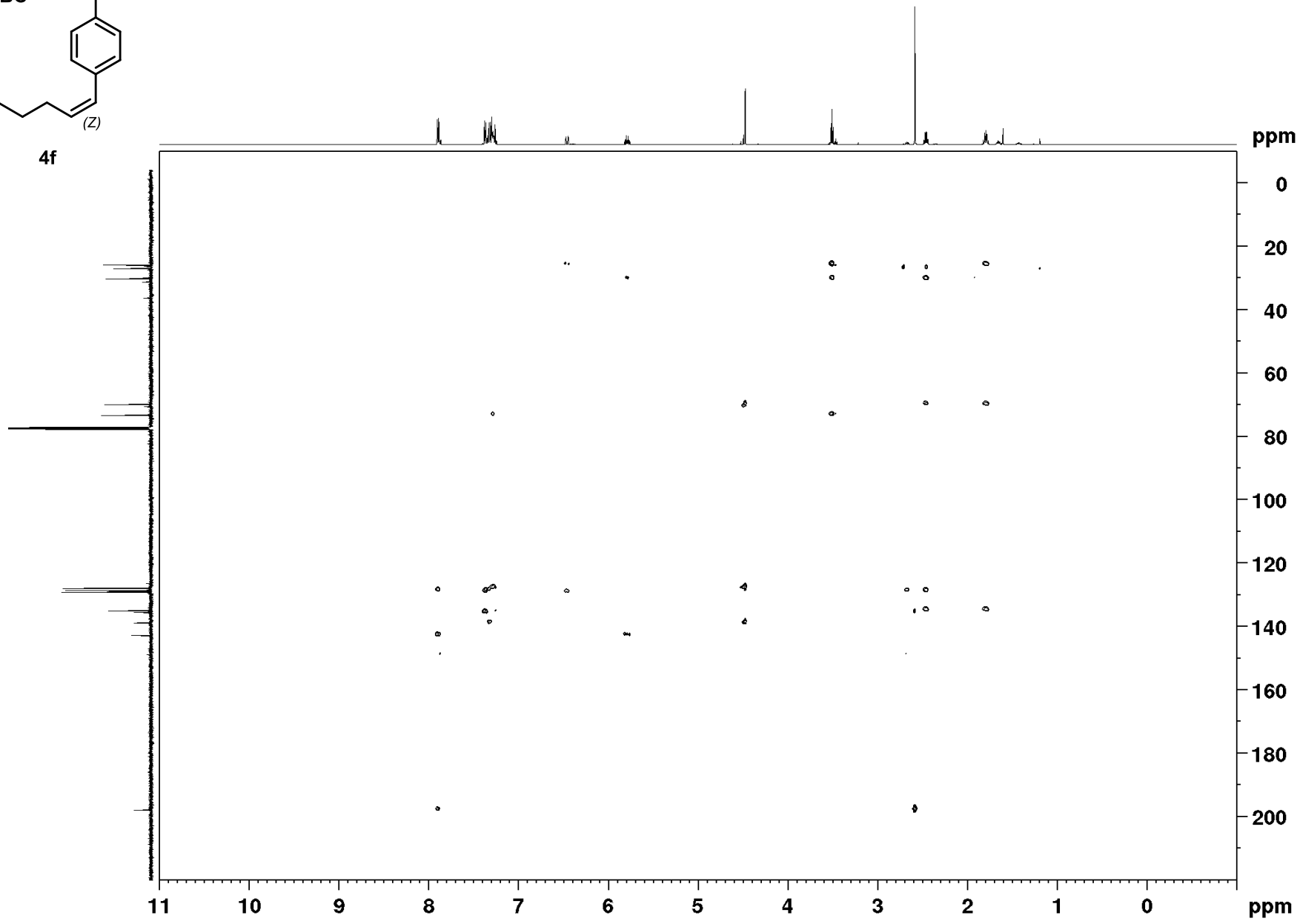



**4f**

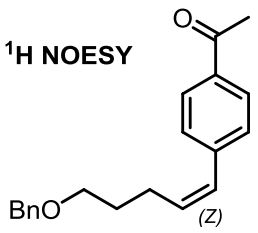
$^{1}H$, $^{13}C$ HMBC



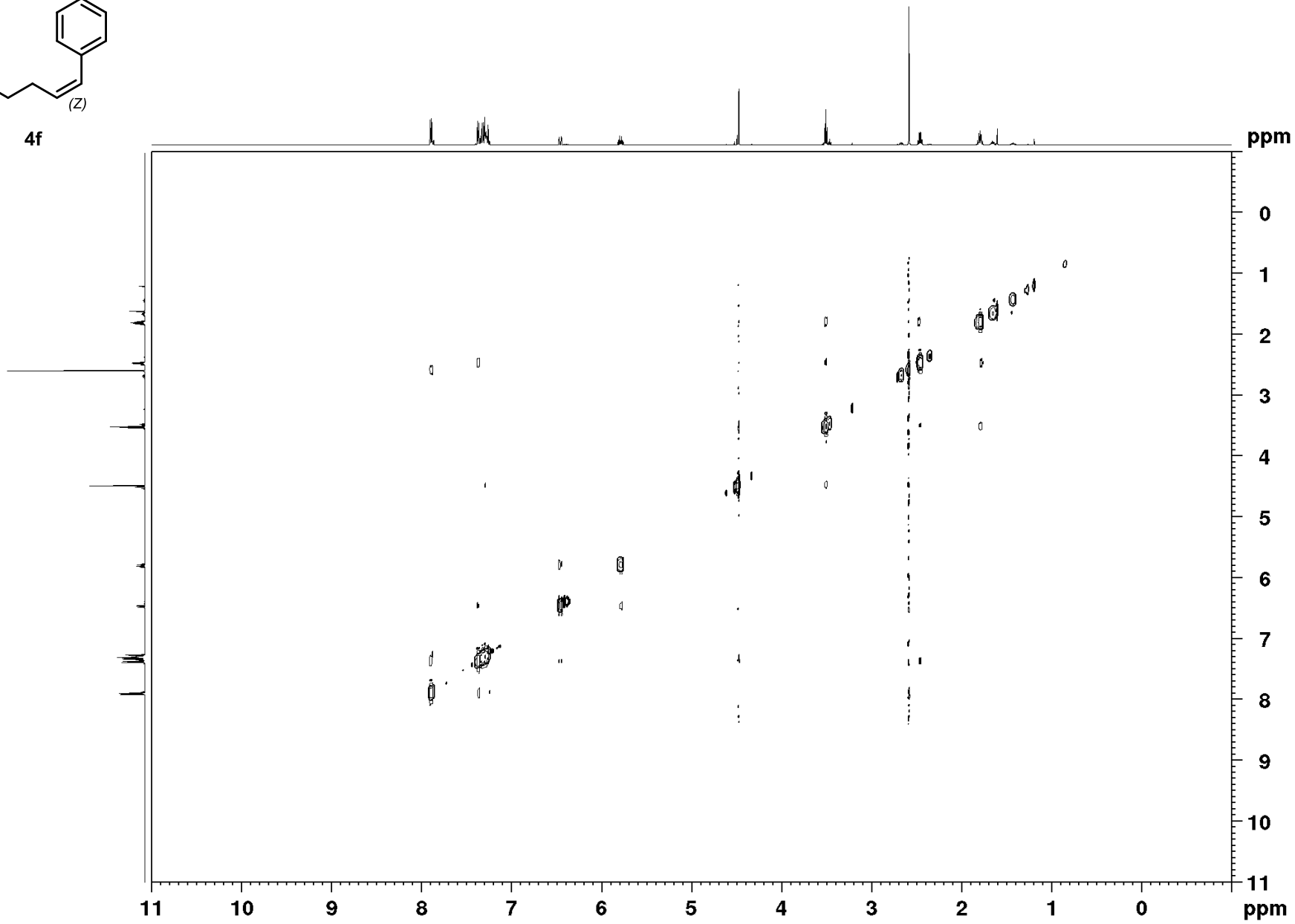

**4f**



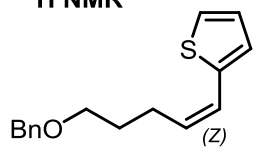
$^1$H, $^1$H NOESY




**4f**



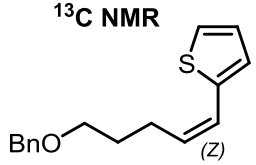
**$^1$H NMR**


S
BnO
(Z)

**4g**


7.36
7.36
7.35
7.34
7.33
7.32
7.32
7.31
7.30
7.29
7.28
7.27
7.27
7.27
7.26
7.26
7.26
7.26
7.25
7.25
7.24
7.02
7.01
7.00
6.99
6.56
6.56
6.54
6.54
5.62
5.60
5.59
5.59
5.58
5.56
4.52
3.57
3.56
3.55
2.56
2.55
2.54
2.54
2.53
2.52
2.51
2.51
1.88
1.86
1.85
1.83
1.82
3.94
0.92
1.28
1.93
0.99
1.00
2.07
2.07
2.06
2.06
11
10
9
8
7
6
5
4
3
2
1
0
ppm

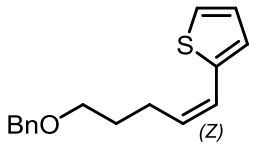
**$^{13}$C NMR**


S
BnO
(Z)

**4g**

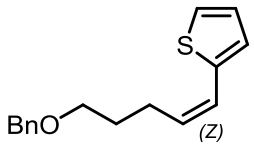

140.8
138.8
130.5
128.5
127.8
127.6
127.3
126.9
125.1
122.3
73.1
70.0
29.7
26.1
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



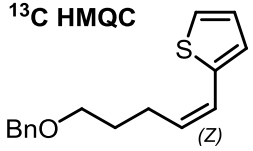

**4g**

**$^1$H, $^1$H COSY**



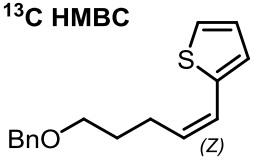

**4g**

$^{1}H$, $^{13}C$ HMQC



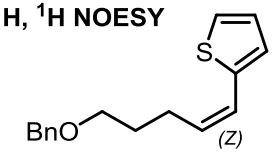

**4g**

$^{1}H$, $^{13}C$ HMBC

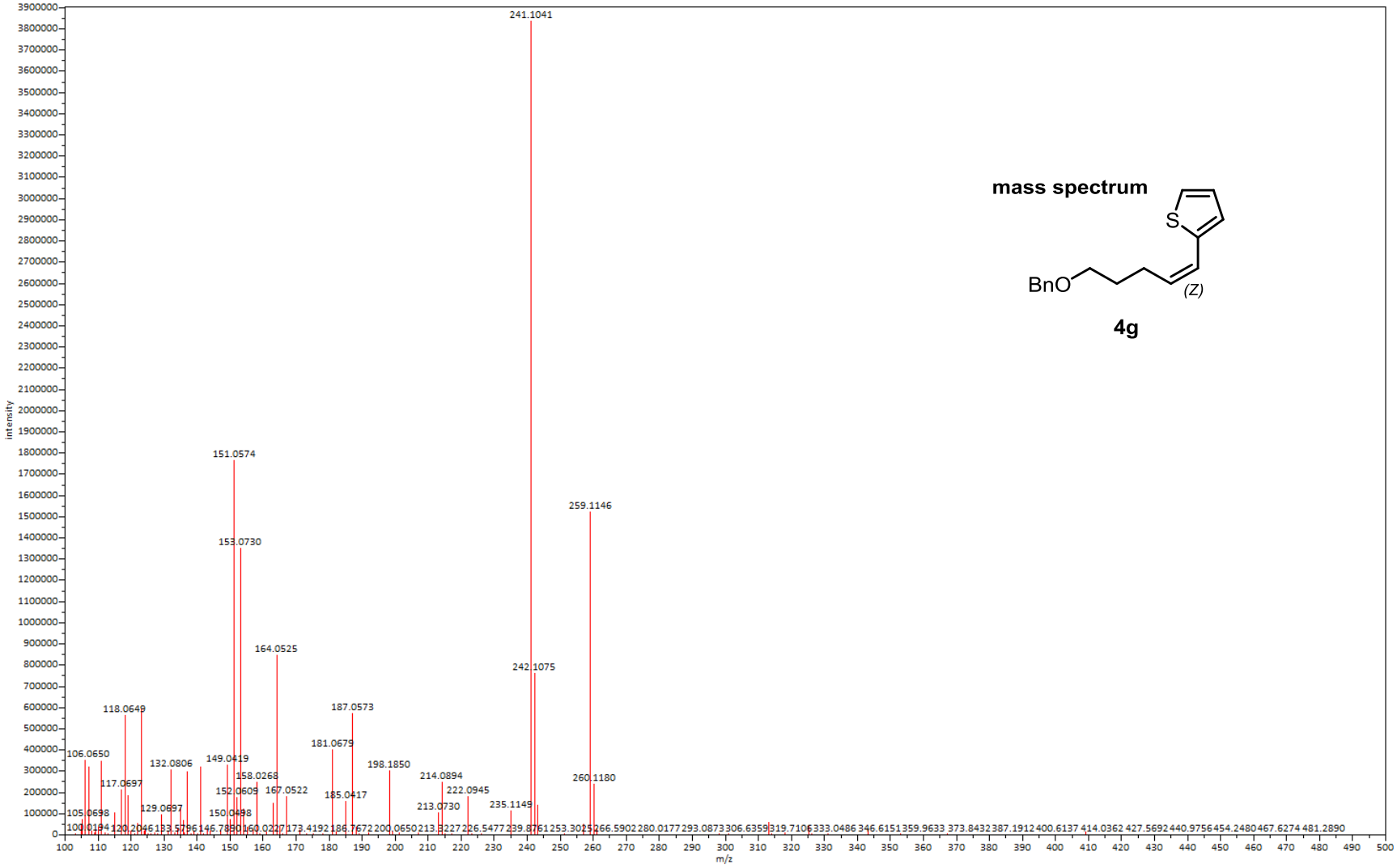


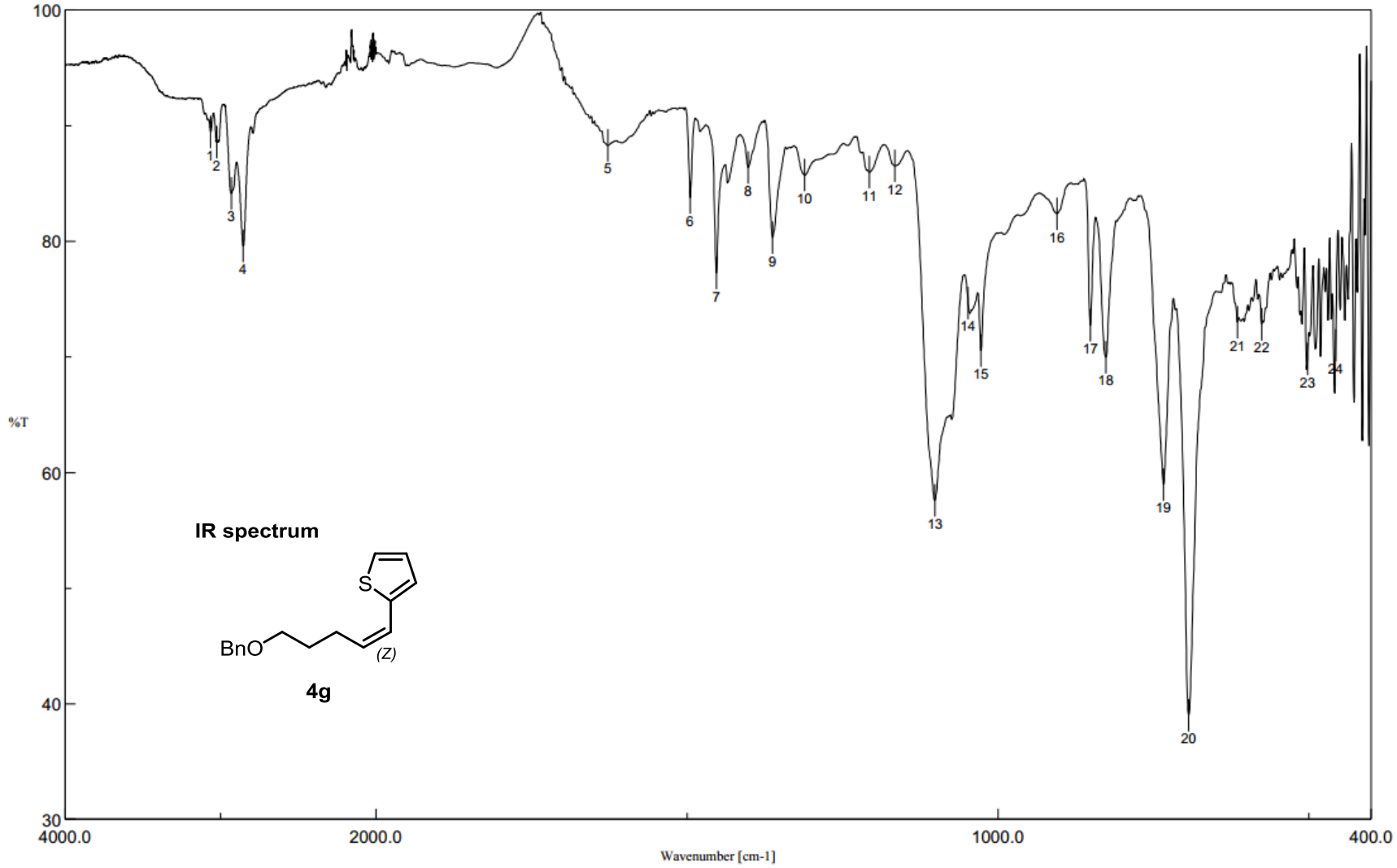

**4g**

$^1$H, $^1$H NOESY

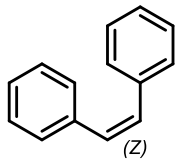



**4g**

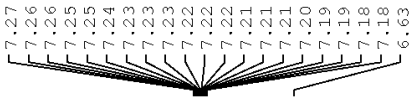

mass spectrum
BnO
S
(Z)
4g
intensity
m/z
241.1041
151.0574
153.0730
259.1146
164.0525
242.1075
118.0649
187.0573
181.0679
106.0650
132.0806
149.0419
198.1850
214.0894
158.0268
222.0945
117.0697
167.0522
260.1180
185.0417
213.0730
129.0697
235.1149
150.0498

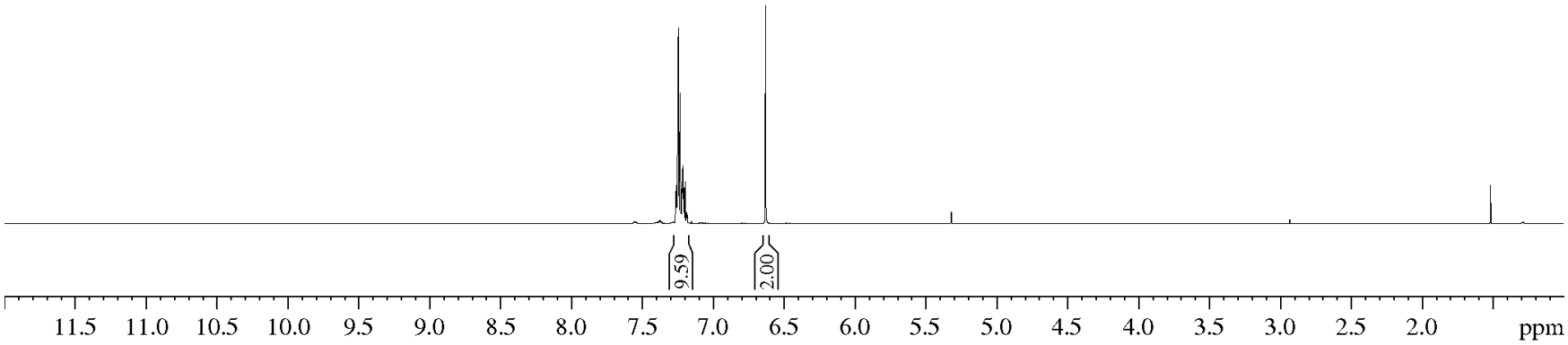

100
80
60
40
30
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
21
22
23
24
IR spectrum
S
BnO
(Z)
4g

**$^1$H NMR**

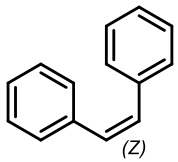

(Z)

**4k**


7.27
7.26
7.26
7.25
7.25
7.24
7.23
7.23
7.23
7.22
7.22
7.22
7.21
7.21
7.21
7.20
7.19
7.19
7.18
7.18
6.63


9.59
2.00
11.5
11.0
10.5
10.0
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
4.0
3.5
3.0
2.5
2.0
ppm

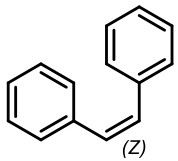
$^{13}$C NMR


(Z)

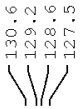
**4k**

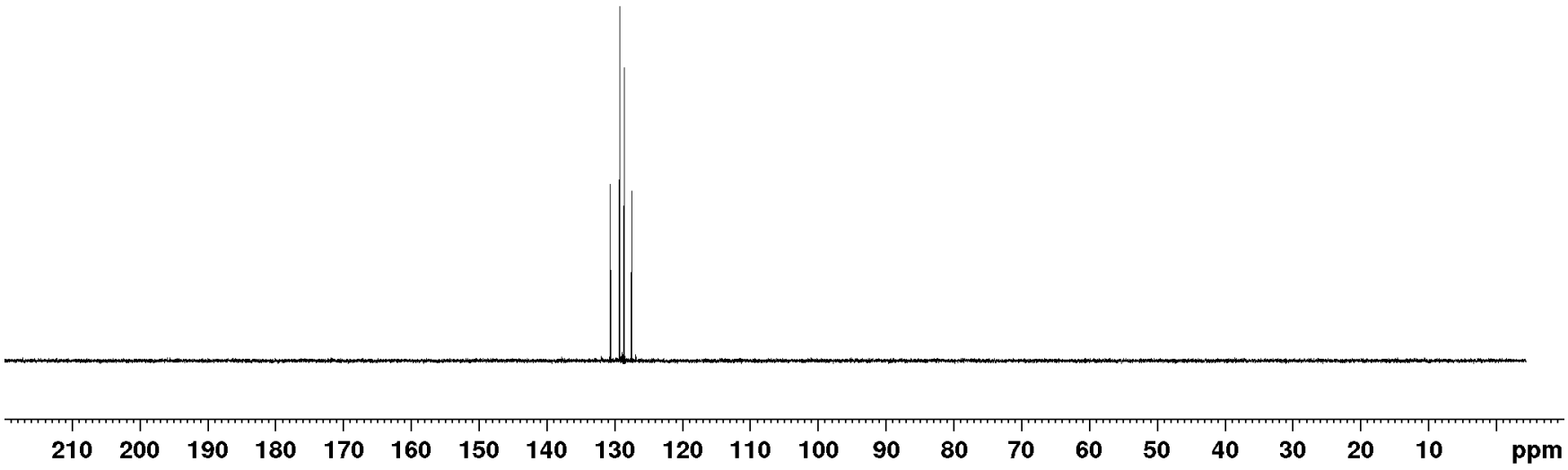

137.8
130.6
129.2
128.6
127.5
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**

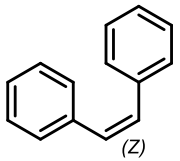



**4k**



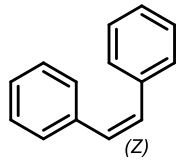



$^{1}$H, $^{1}$H COSY



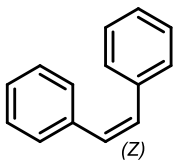

**4k**

$^{1}H$, $^{13}C$ HMQC



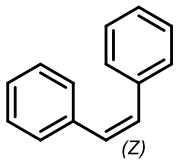

**4k**

$^{1}H$, $^{13}C$ HMBC



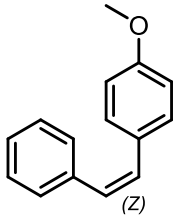

**4k**

**$^1$H, $^1$H NOESY**



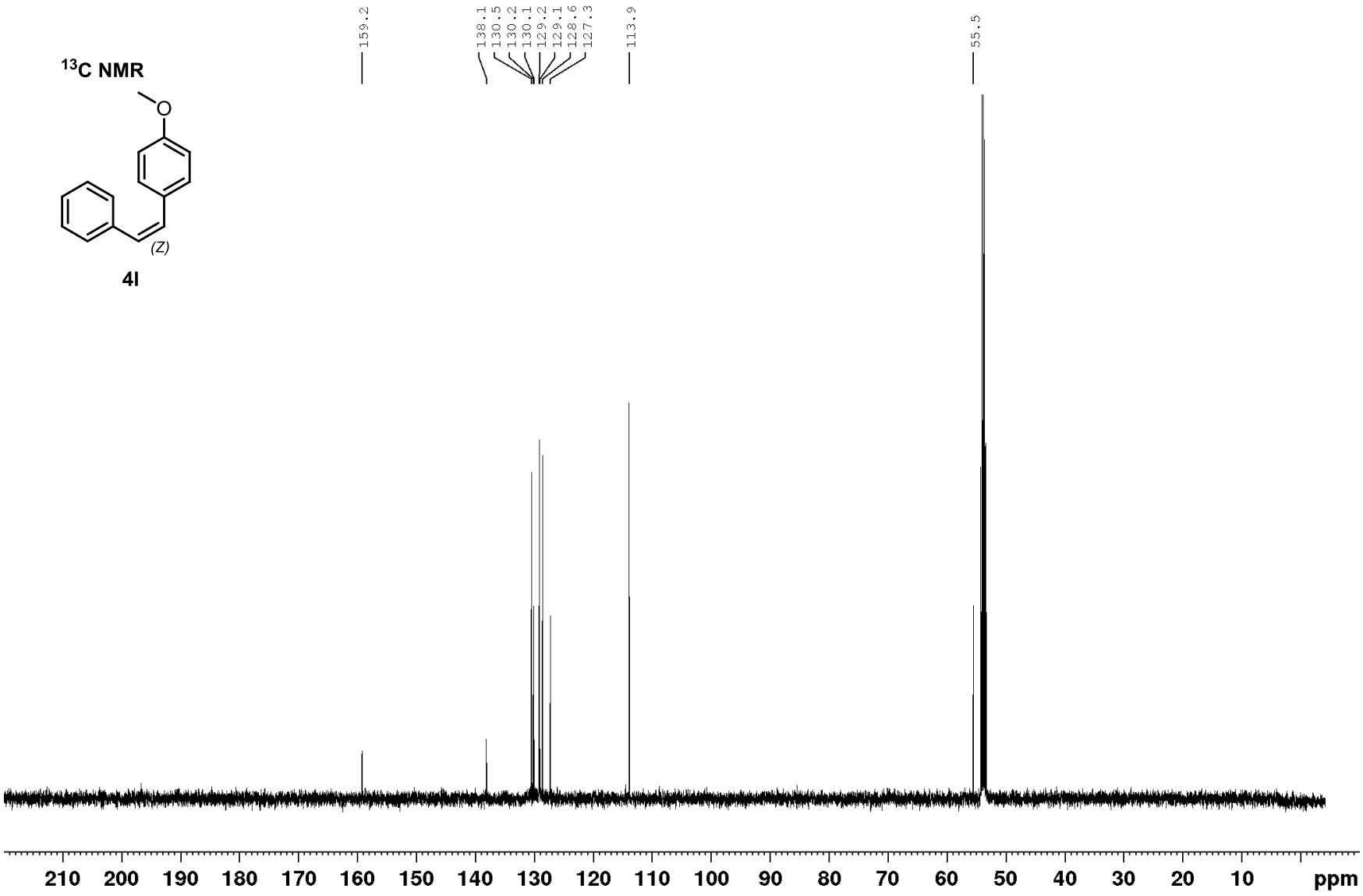

**4k**

**$^1$H NMR**

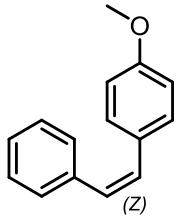

O
(Z)

**4l**


7.27
7.27
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.22
7.20
7.20
7.20
7.18
7.17
7.17
7.17
6.76
6.74
6.56
6.54
6.53
6.51
3.77
6.79
2.00
2.07
3.26
10
9
8
7
6
5
4
3
2
1
0
ppm

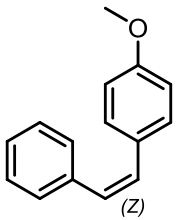

159.2
138.1
130.5
130.2
130.1
129.2
129.1
128.6
127.3
113.9
55.5
$^{13}$C NMR
O
(Z)
4l
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



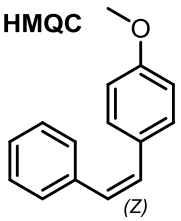

**4l**

$^1$H, $^1$H COSY



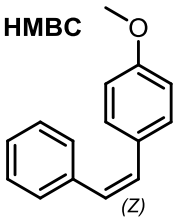

4l

$^{1}H$, $^{13}C$ HMQC



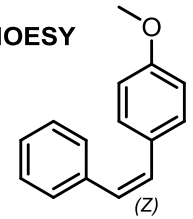

**4l**

$^{1}H$, $^{13}C$ HMBC

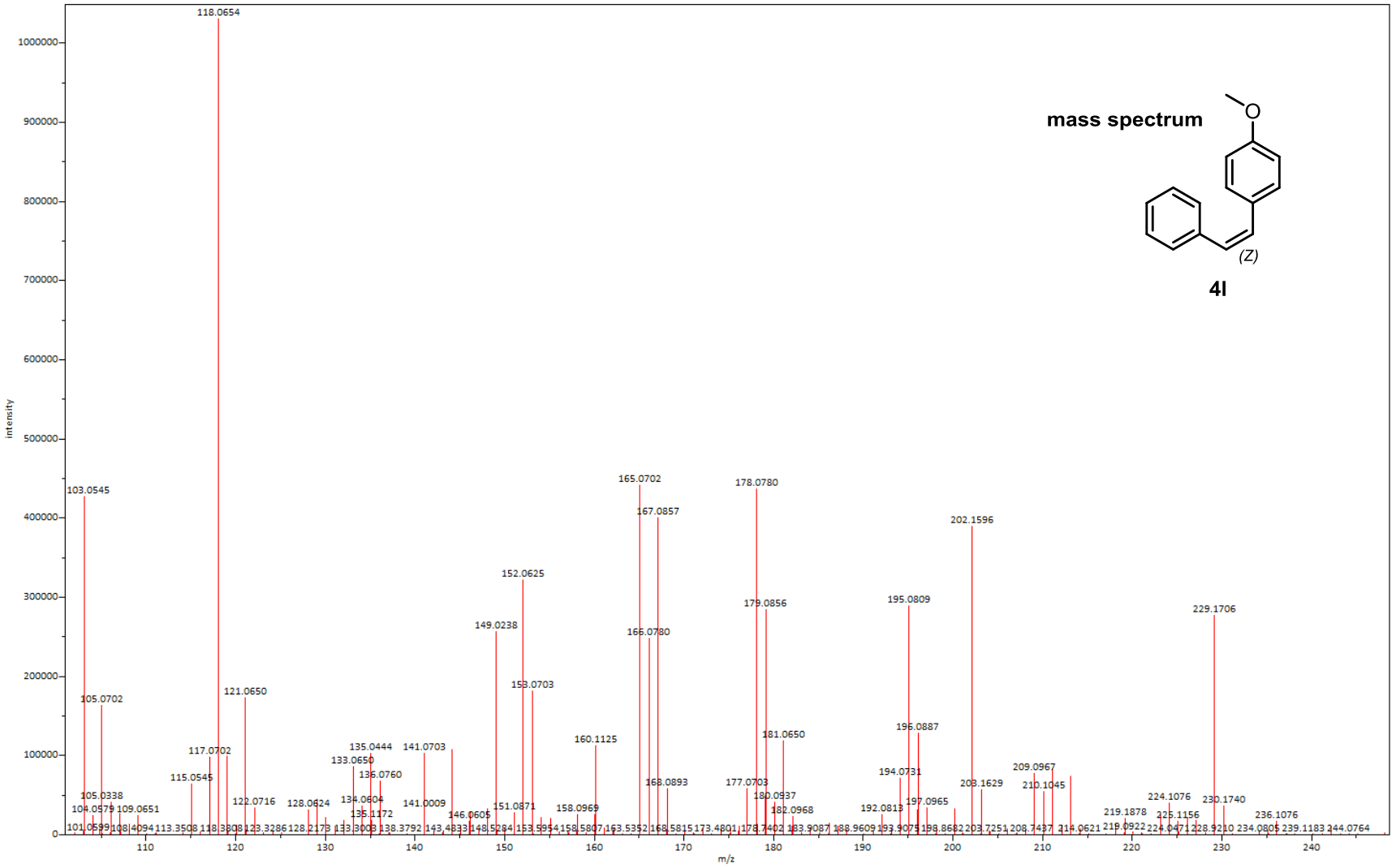



**4l**

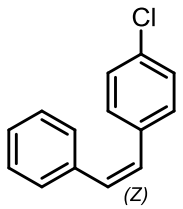
$^1$H, $^1$H NOESY




**4l**


mass spectrum
(Z)
4l
intensity
m/z
118.0654
103.0545
105.0702
121.0650
117.0702
115.0545
122.0716
105.0338
104.0579
109.0651
128.0624
135.0444
133.0650
136.0760
134.0804
135.1172
141.0703
141.0009
146.0605
149.0238
152.0625
153.0703
151.0871
158.0969
160.1125
165.0702
167.0857
166.0780
168.0893
178.0780
179.0856
177.0703
180.0937
181.0650
182.0968
195.0809
196.0887
194.0731
197.0965
192.0813
202.1596
203.1629
209.0967
210.1045
219.1878
224.1076
225.1156
230.1740
229.1706
236.1076

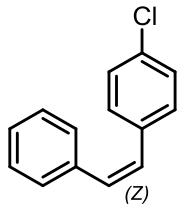
**$^1$H NMR**


Cl
(Z)

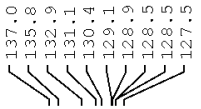
**4m**

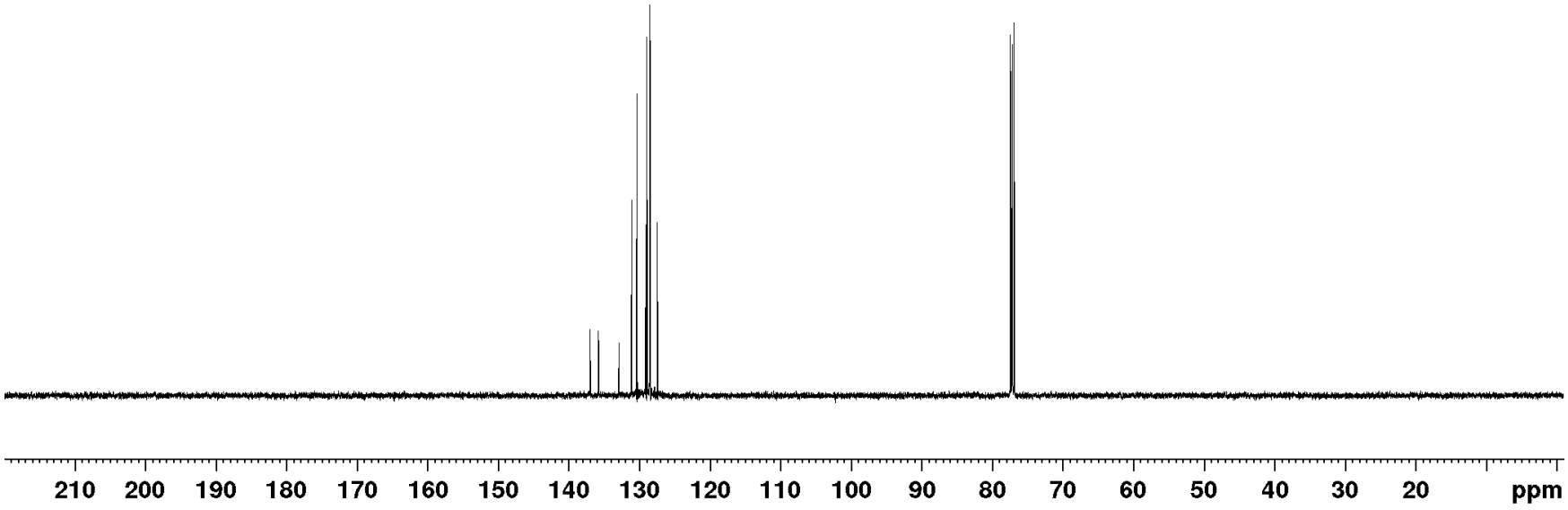

7.27
7.27
7.27
7.26
7.26
7.25
7.25
7.24
7.23
7.23
7.22
7.22
7.21
7.21
7.20
7.20
7.19
7.18
7.18
7.17
7.17
6.65
6.63
6.55
6.53
4.92
4.04
1.00
1.01
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^{13}$C NMR**

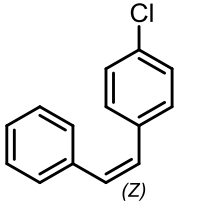

Cl
(Z)

**4m**

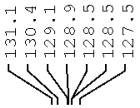

137.0
135.8
132.9
131.1
130.4
129.1
128.9
128.5
128.5
127.5

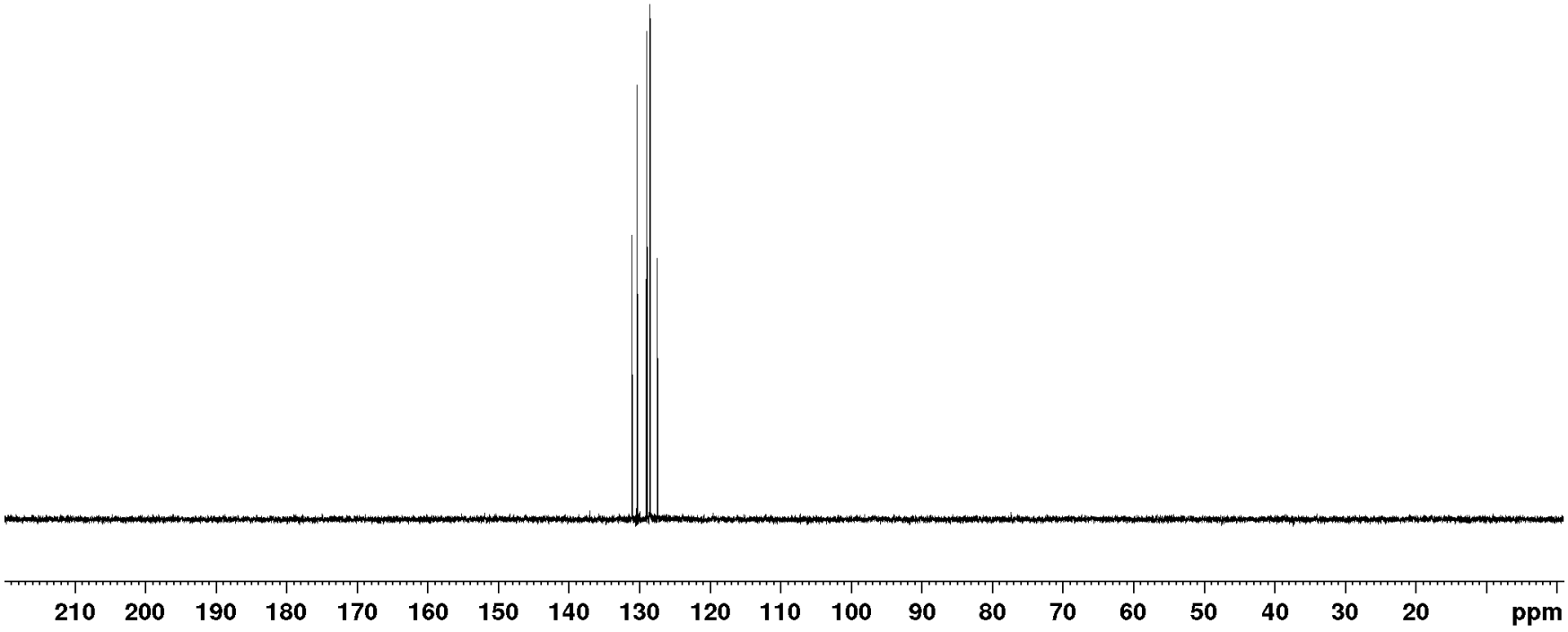

210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

**$^{13}$C DEPT NMR**

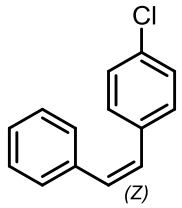



**4m**



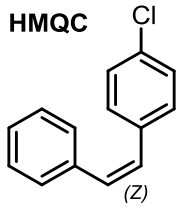



**$^1$H, $^1$H COSY**



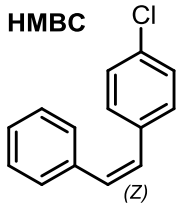

**4m**

$^{1}H$, $^{13}C$ HMQC



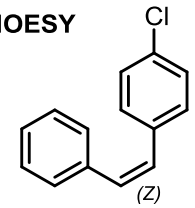

4m

$^{1}$H, $^{13}$C HMBC

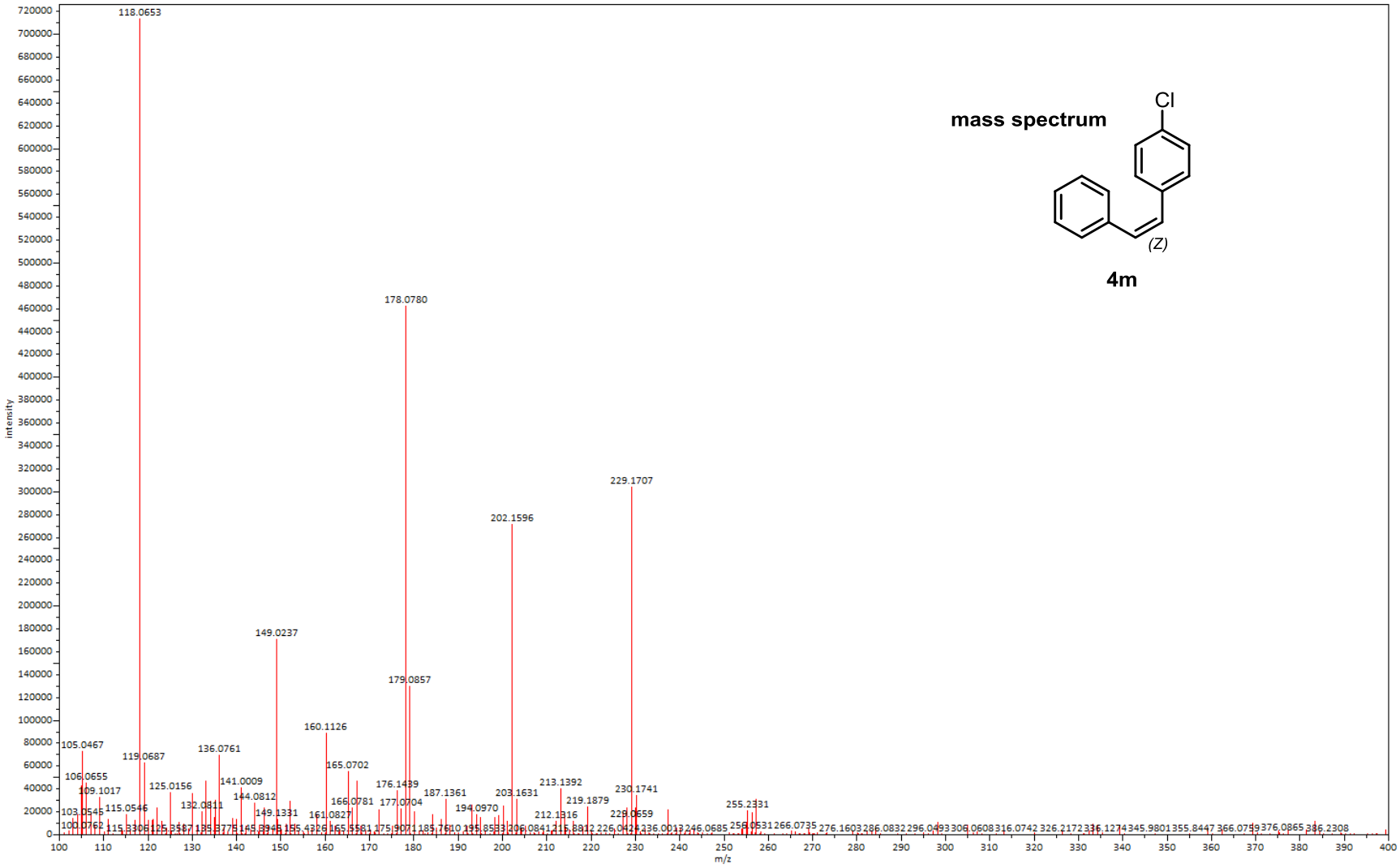


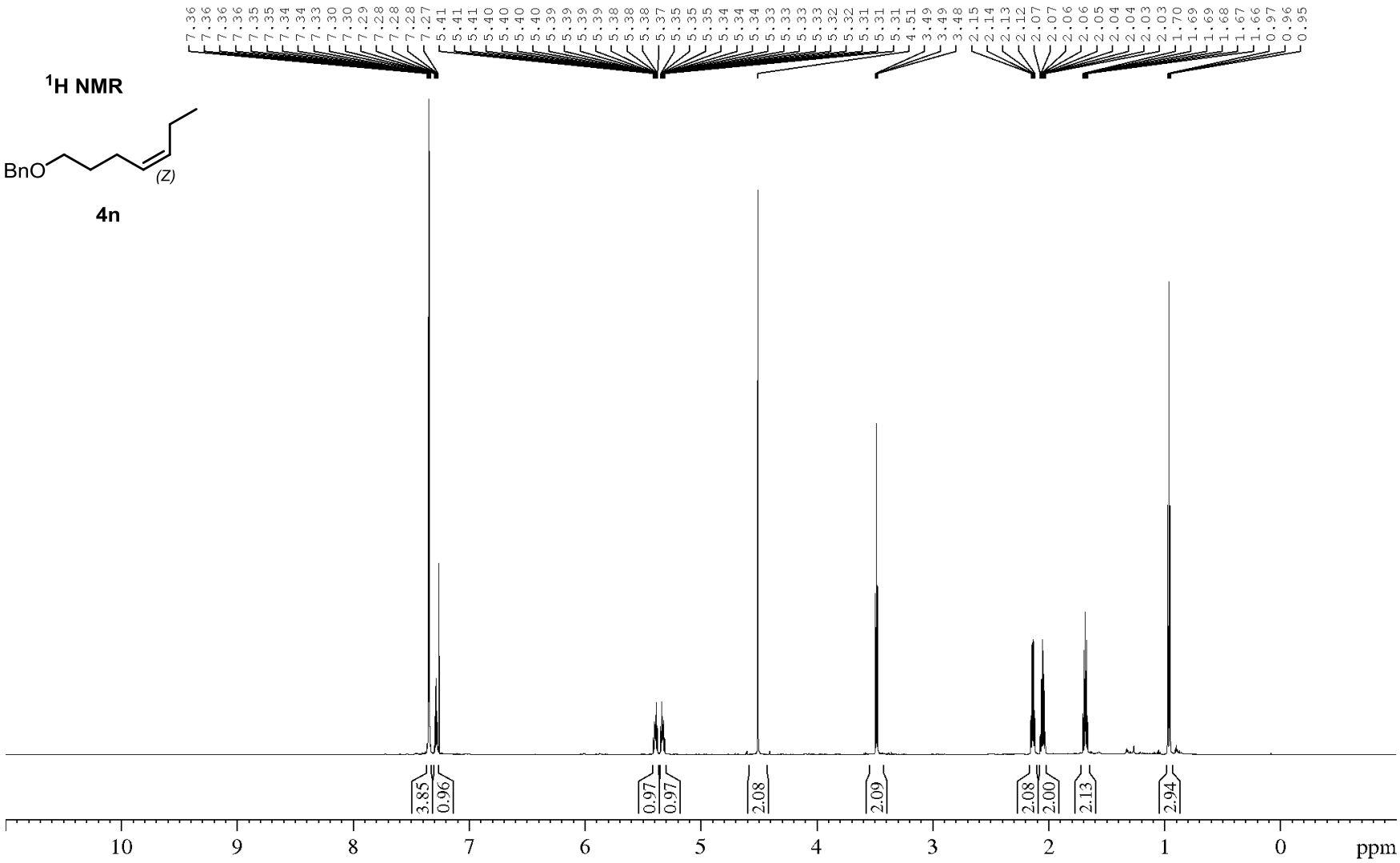

4m

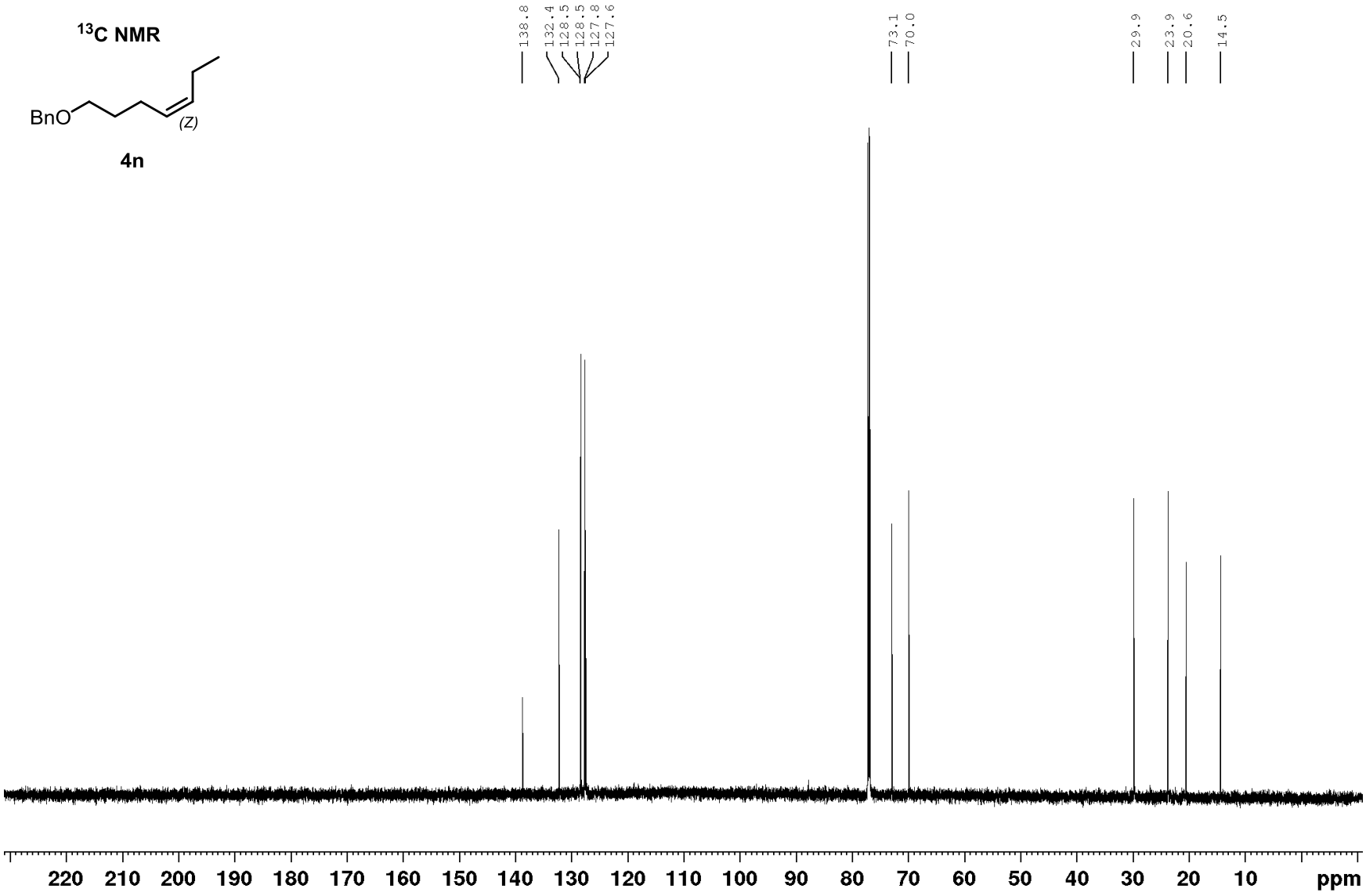
$^1$H, $^1$H NOESY



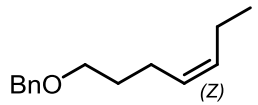

4m


mass spectrum
Cl
(Z)
4m
intensity
m/z
118.0653
178.0780
229.1707
202.1596
149.0237
179.0857
160.1126
105.0467
119.0687
136.0761
165.0702
106.0655
109.1017
141.0009
144.0812
125.0156
176.1439
187.1361
213.1392
230.1741
203.1631
219.1879
115.0546
132.0811
177.0704
194.0970
149.1331
166.0781
161.0827
212.1316
228.0659
255.2331


7.36 7.36 7.36 7.35 7.35 7.34 7.34 7.33 7.30 7.30 7.29 7.28 7.28 7.28 7.27
5.41 5.41 5.40 5.40 5.40 5.39 5.39 5.39 5.39 5.38 5.38 5.38 5.37 5.35 5.35 5.35 5.34 5.34 5.34 5.33 5.33 5.33 5.33 5.32 5.32 5.31 5.31 5.31
4.51 3.49 3.49 3.48
2.15 2.14 2.13 2.12 2.07 2.07 2.06 2.06 2.05 2.04 2.04 2.03 2.03
1.70 1.69 1.69 1.68 1.67 1.66 0.97 0.96 0.95
1H NMR
BnO
(Z)
4n
3.85 0.96 0.97 0.97 2.08 2.09 2.08 2.00 2.13 2.94
10 9 8 7 6 5 4 3 2 1 0 ppm

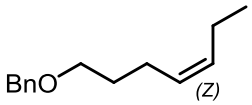

$^{13}$C NMR
BnO
(Z)
4n
138.8
132.4
128.5
128.5
127.8
127.6
73.1
70.0
29.9
23.9
20.6
14.5
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



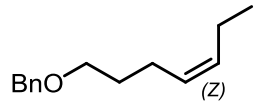

**4n**

**$^1$H, $^1$H COSY**



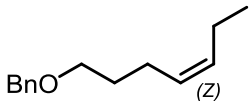

**4n**

**$^{1}H$, $^{13}C$ HMQC**

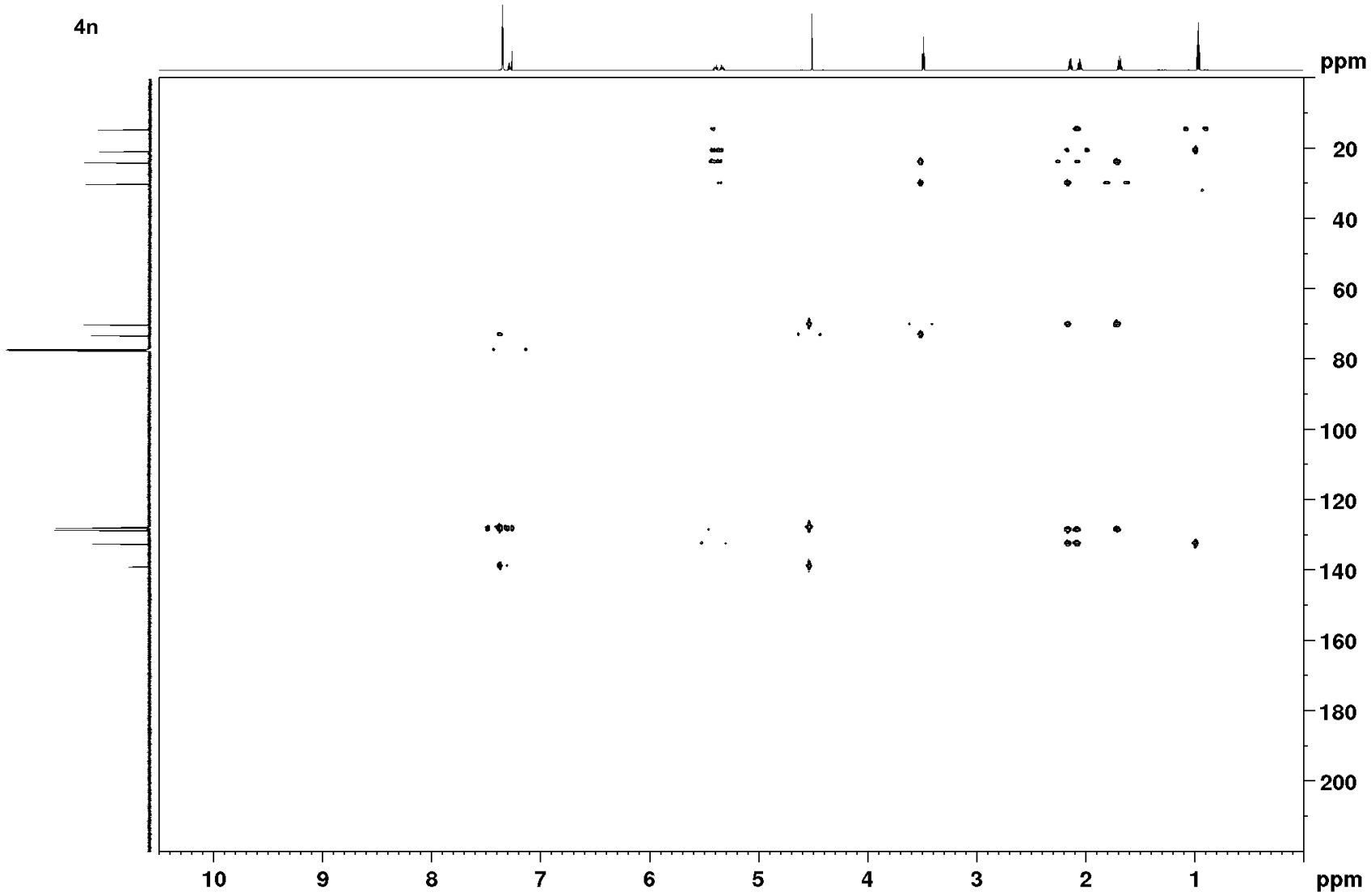



**4n**

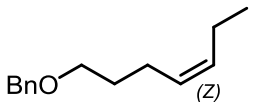
**$^{1}H$, $^{13}C$ HMBC**



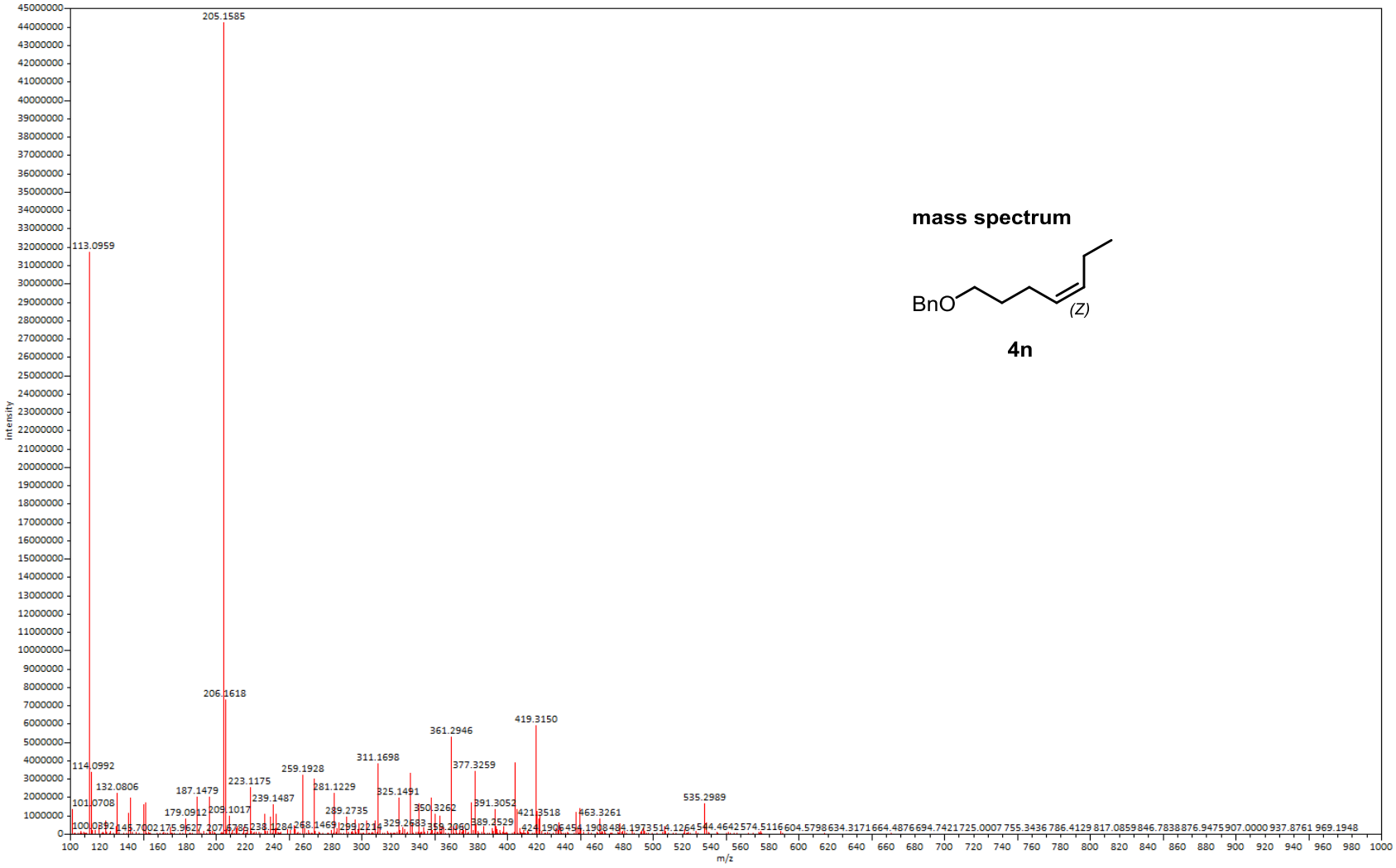

**4n**



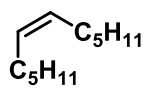
$^1$H, $^1$H NOESY




**4n**


mass spectrum
BnO
(Z)
4n
intensity
m/z
205.1585
113.0959
206.1618
114.0992
132.0806
101.0708
187.1479
179.0912
209.1017
223.1175
239.1487
259.1928
281.1229
289.2735
311.1698
325.1491
329.2683
350.3262
361.2946
377.3259
391.3052
419.3150
421.3518
463.3261
535.2989

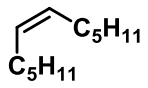
**$^1$H NMR**


C5H11
C5H11

**4o**


5.39
5.36
5.36
5.35
5.32
2.04
2.03
2.01
2.00
1.36
1.35
1.33
1.32
1.32
1.32
1.31
1.31
1.30
1.29
1.29
1.29
1.28
1.28
0.91
0.89
0.88
2.00
4.14
12.53
6.24
12
11
10
9
8
7
6
5
4
3
2
1
0
-1
-2
-3
ppm

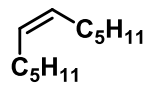
$^{13}$C NMR



4o

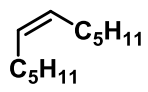

130.1
31.7
29.6
27.3
22.7
14.2
220 210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm

**$^{13}$C DEPT NMR**



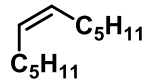

**4o**

$^1$H, $^1$H COSY



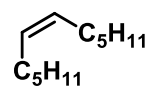

4o

$^{1}H$, $^{13}C$ HMQC



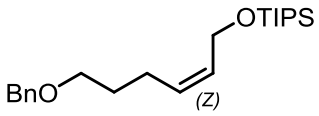

4o

$^{1}H$, $^{13}C$ HMBC




4o

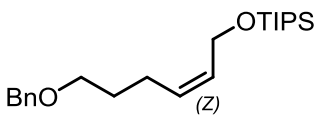
**$^1$H NMR**


OTIPS
BnO
(Z)

**4p**


7.36 7.35 7.35 7.34 7.33 7.31 7.30 7.29 7.29 7.28 7.28 7.27 7.26
5.60 5.59 5.58 5.57 5.56 5.45 5.44 5.43 5.43 5.43 5.42 5.42 5.42 5.41 5.41 5.41 5.39 5.39 4.50 4.31 4.30
3.49 3.48 3.47
2.17 2.15 2.14 2.12 1.72 1.71 1.69 1.68 1.67 1.14 1.13 1.12 1.11 1.10 1.09 1.08 1.07 1.06 1.06 1.05 1.04
3.82 0.93 1.00 1.01 2.04 2.04 2.05 2.02 2.06 21.53
10 9 8 7 6 5 4 3 2 1 0 ppm

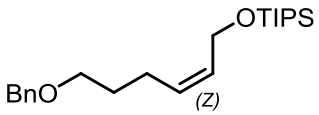
**$^{13}$C NMR**


OTIPS
BnO
(Z)

**4p**

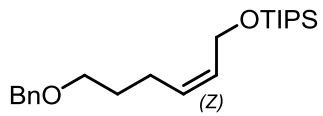

138.8
130.7
129.7
128.5
127.7
127.7
127.7
127.7
127.6
127.6
73.0
69.8
59.8
29.7
24.4
18.2
12.2
200
180
160
140
120
100
80
60
40
20
0
ppm

**$^{13}$C DEPT NMR**



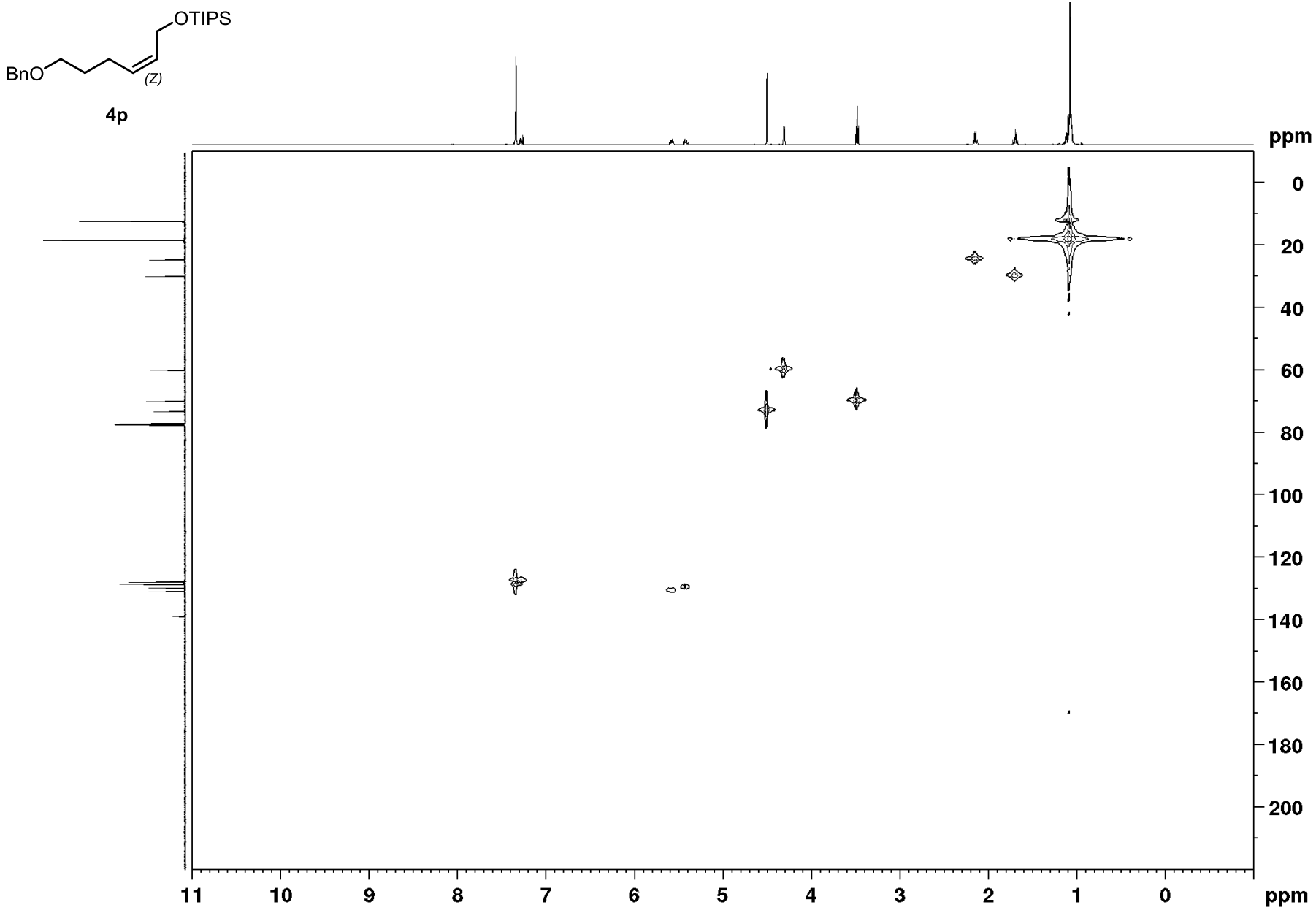

**4p**

**$^1$H, $^1$H COSY**

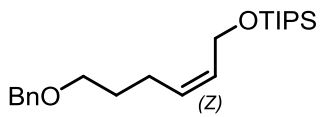



**4p**

**$^{1}H$, $^{13}C$ HMQC**

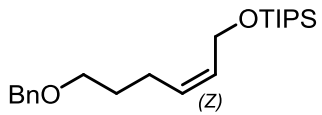

OTIPS
BnO
(Z)
4p
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^{1}H$, $^{13}C$ HMBC**



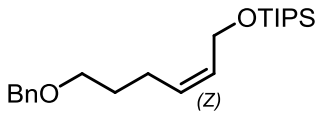

**4p**

**$^1$H, $^1$H NOESY**

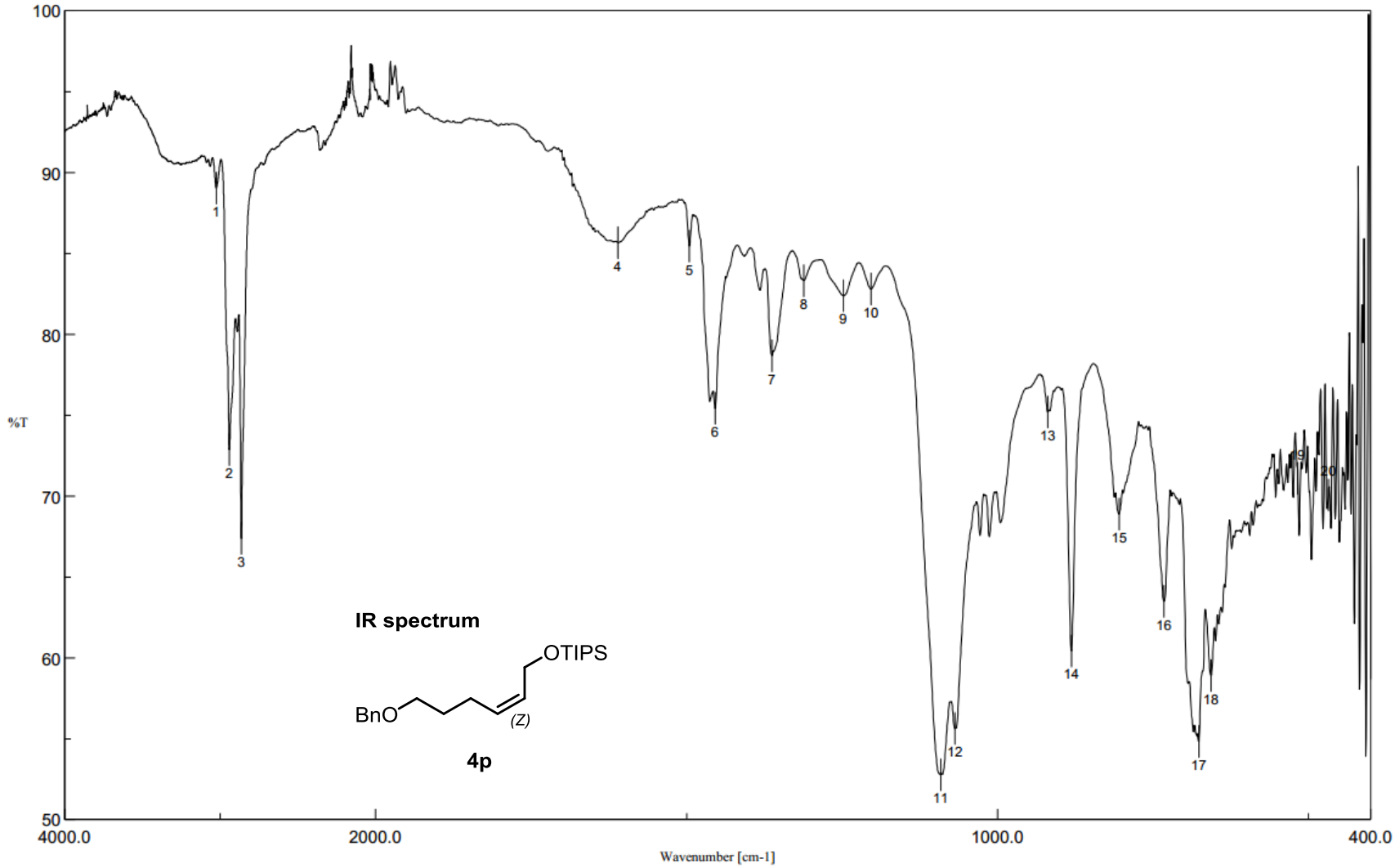


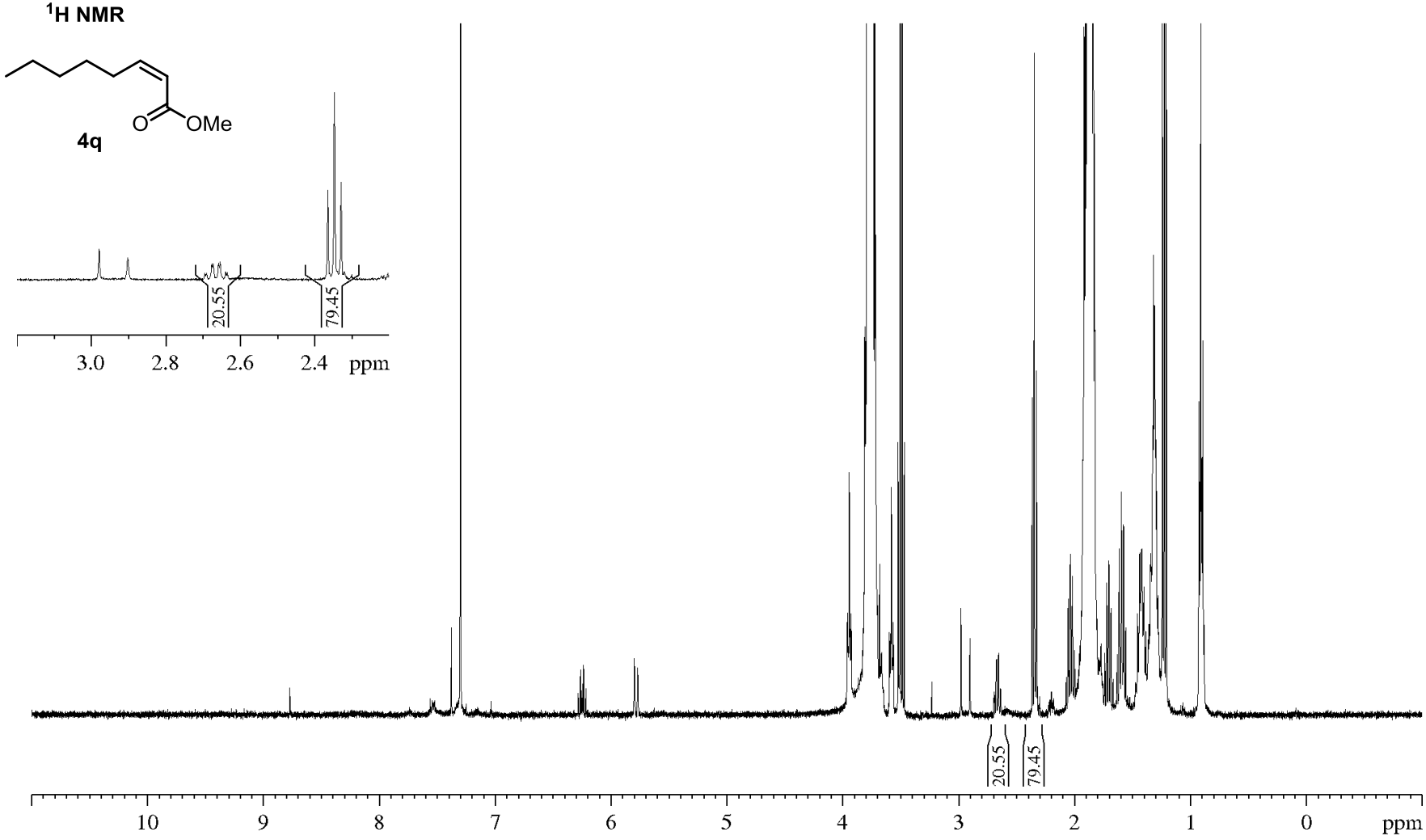

**4p**

**$^{29}$Si DEPT NMR**

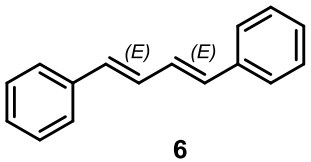



**4p**

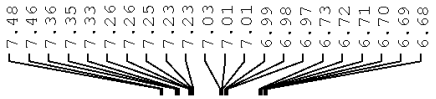

100
90
80
70
60
50
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16
17
18
19
20
IR spectrum
OTIPS
BnO
(Z)
4p

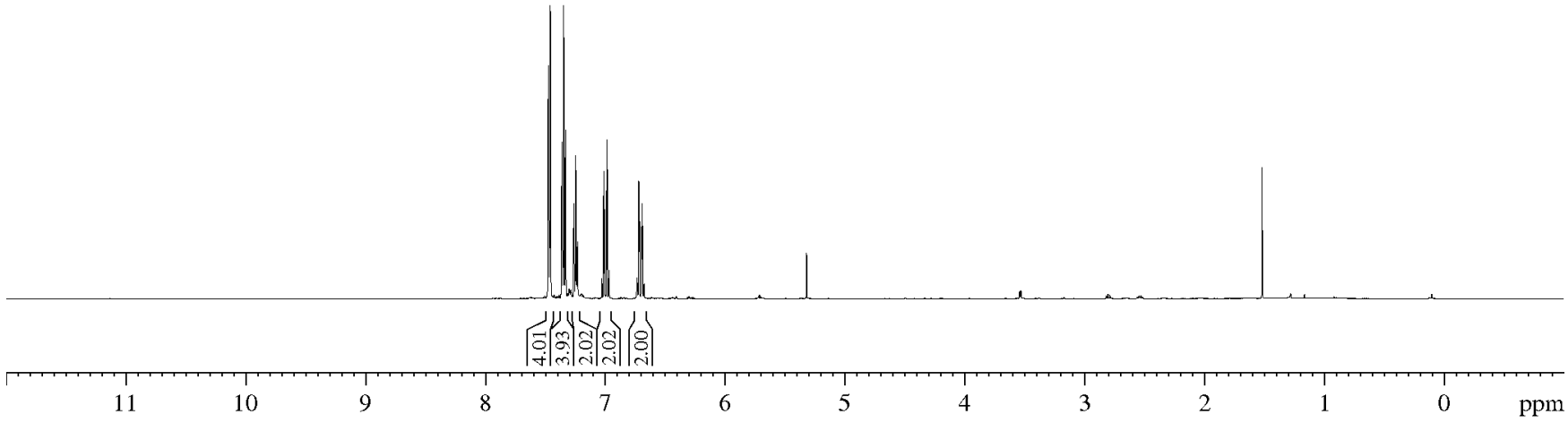

1H NMR
O
OMe
4q
20.55
79.45
3.0
2.8
2.6
2.4
ppm
20.55
79.45
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^1$H NMR**

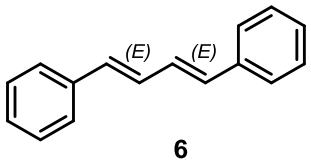

(E)
(E)

**6**


7.48
7.46
7.36
7.35
7.33
7.26
7.26
7.25
7.23
7.23
7.03
7.01
7.01
6.99
6.98
6.97
6.73
6.72
6.71
6.70
6.69
6.68


4.01
3.93
2.02
2.02
2.00
11
10
9
8
7
6
5
4
3
2
1
0
ppm

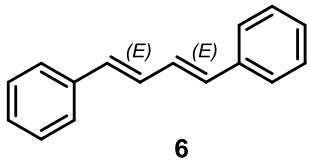
**$^{13}$C NMR**


(E)
(E)

**6**

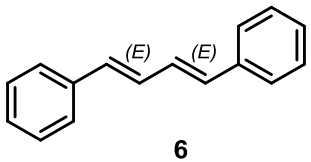

137.8
133.2
129.6
129.1
128.0
126.8
210
200
190
180
170
160
150
140
130
120
110
100
90
80
70
60
50
40
30
20
ppm

**$^{13}$C DEPT NMR**



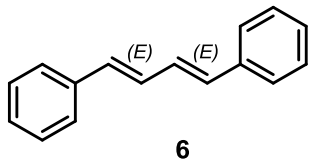

**6**

**$^1$H, $^1$H COSY**



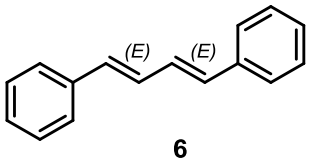

**6**

$^{1}H$, $^{13}C$ HMQC

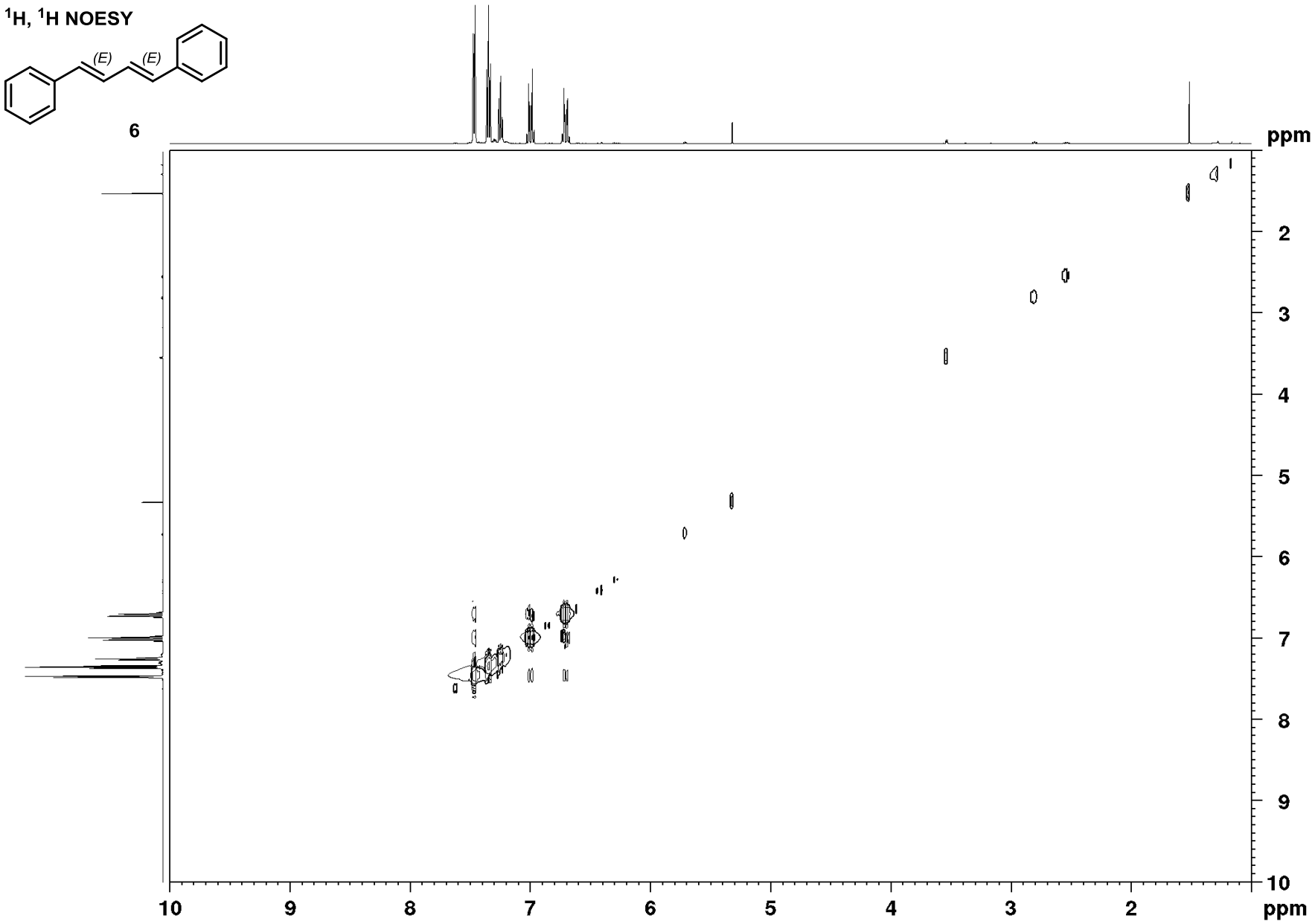



6

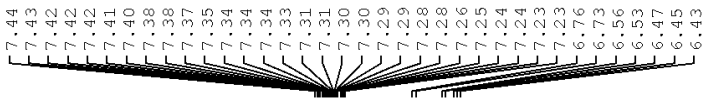
**$^{1}H$, $^{13}C$ HMBC**

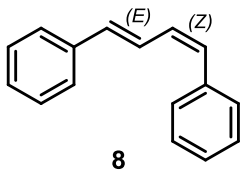



**6**

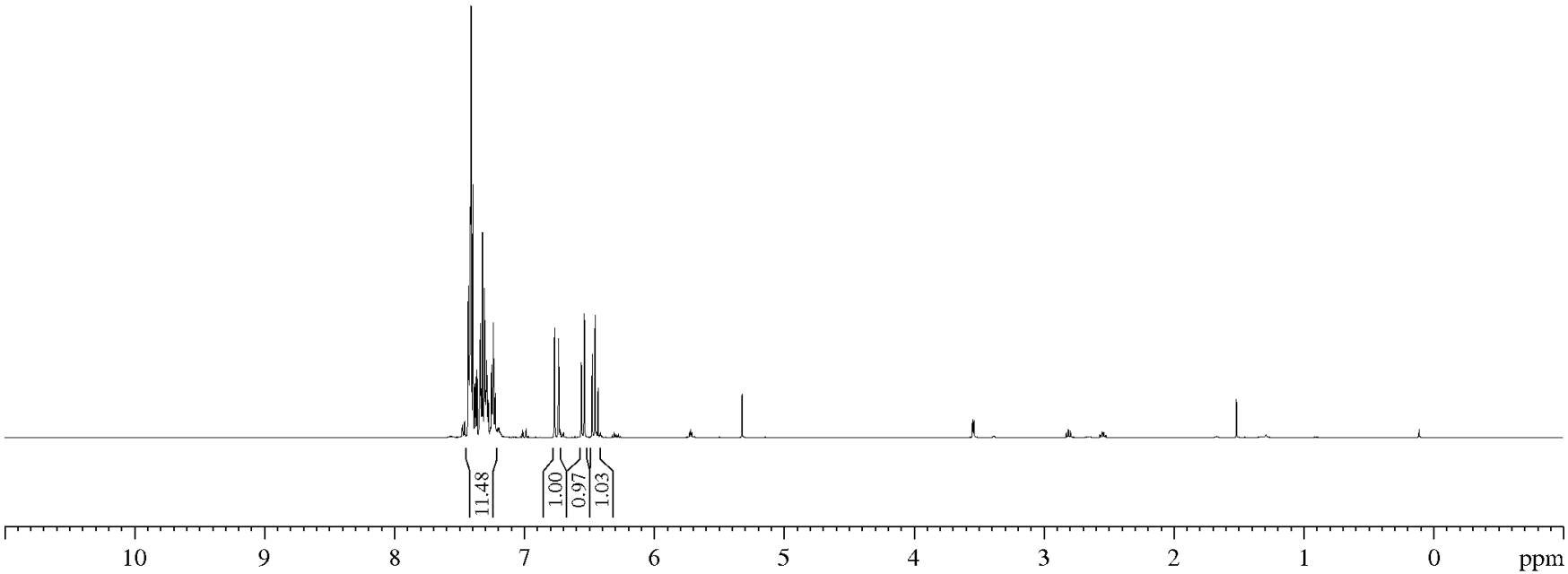

$^1$H, $^1$H NOESY
(E)
(E)
6
ppm
2
3
4
5
6
7
8
9
10
10
9
8
7
6
5
4
3
2
ppm

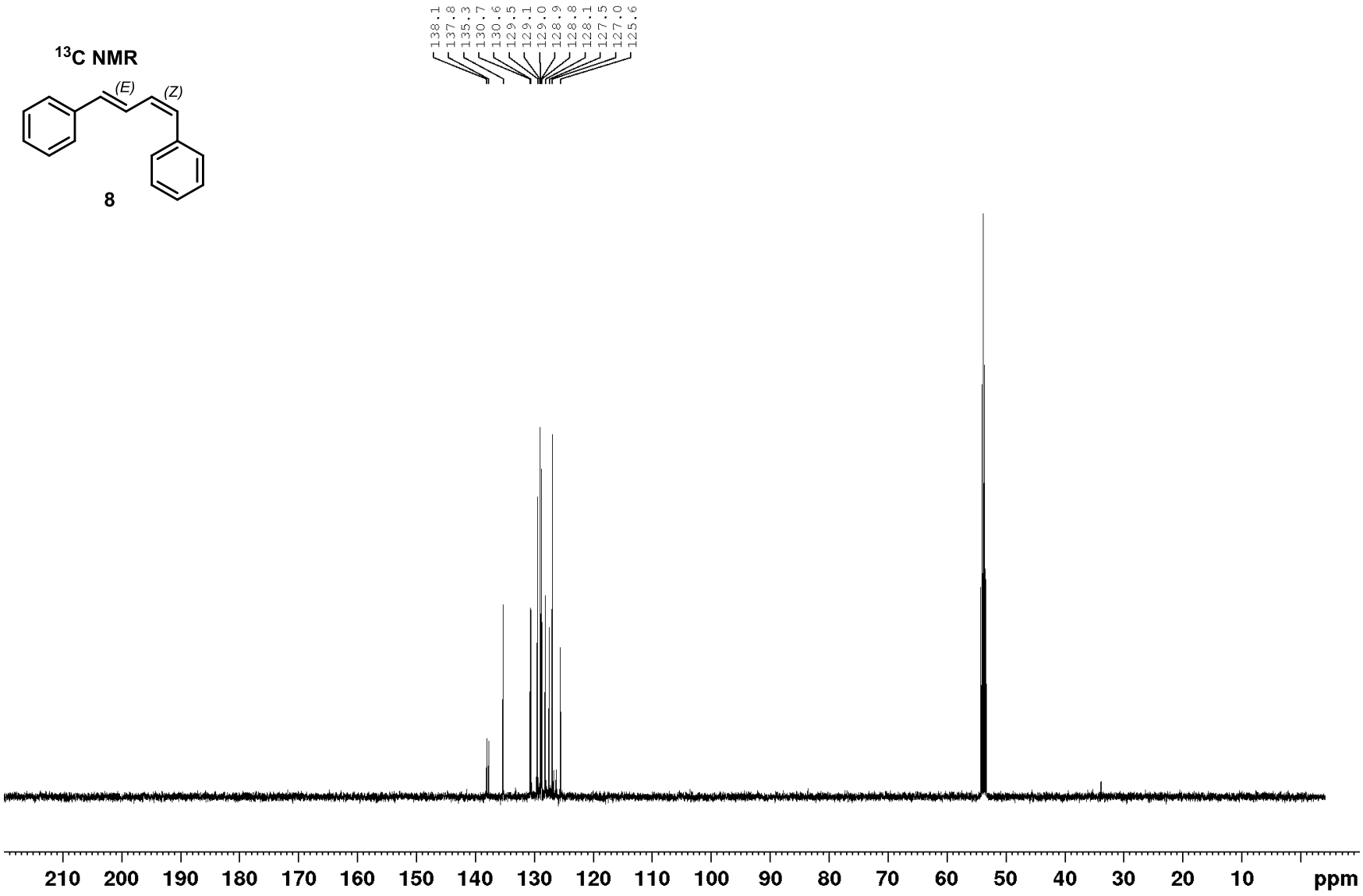
**$^1$H NMR**


7.44
7.43
7.42
7.42
7.42
7.41
7.40
7.38
7.38
7.37
7.35
7.34
7.34
7.34
7.33
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.26
7.25
7.24
7.24
7.23
7.23
6.76
6.73
6.56
6.53
6.47
6.45
6.43

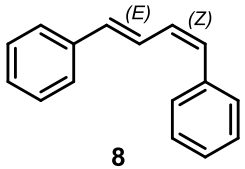

(E)
(Z)

**8**

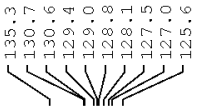

11.48
1.00
0.97
1.03
10
9
8
7
6
5
4
3
2
1
0
ppm

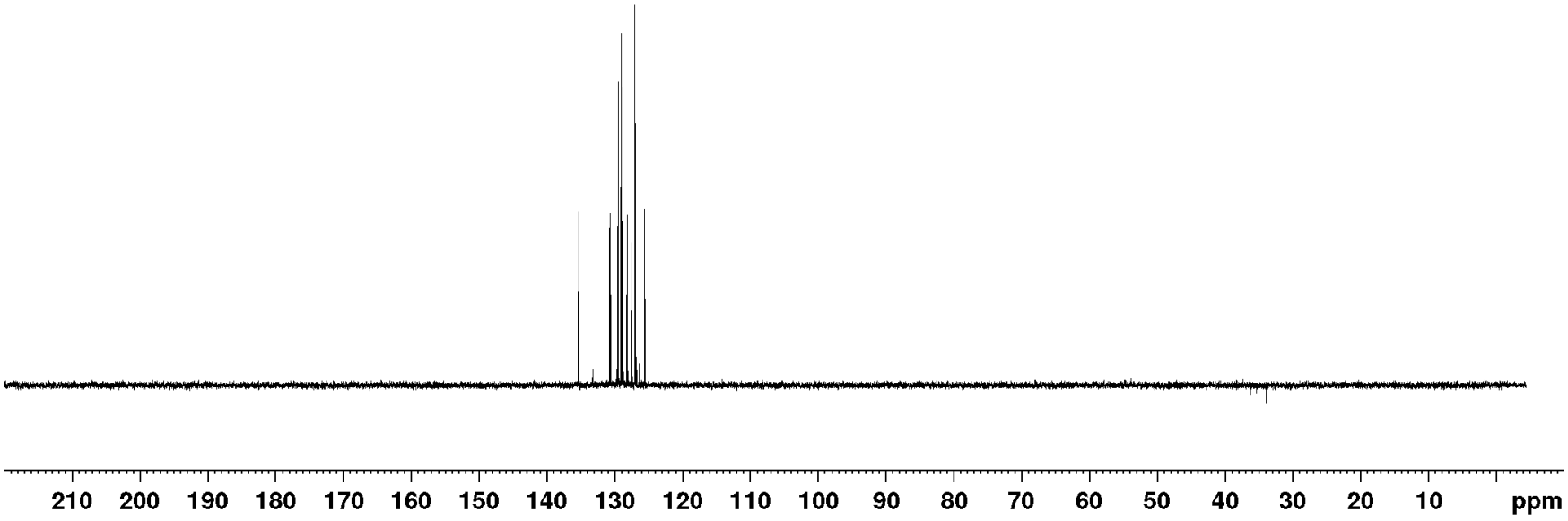

13C NMR
(E)
(Z)
8
138.1
137.8
135.3
130.7
130.6
129.5
129.1
129.0
128.9
128.8
128.1
127.5
127.0
125.6
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**

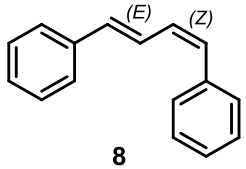



**8**



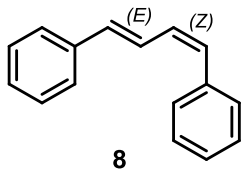



$^1$H, $^1$H COSY



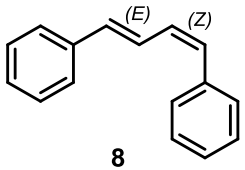

8

$^{1}H$, $^{13}C$ HMQC



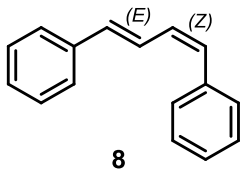

8

**$^{1}H$, $^{13}C$ HMBC**



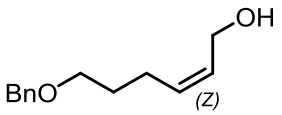

**8**

**$^1$H, $^1$H NOESY**

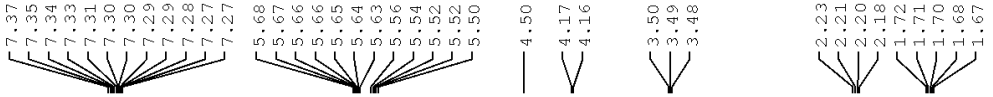


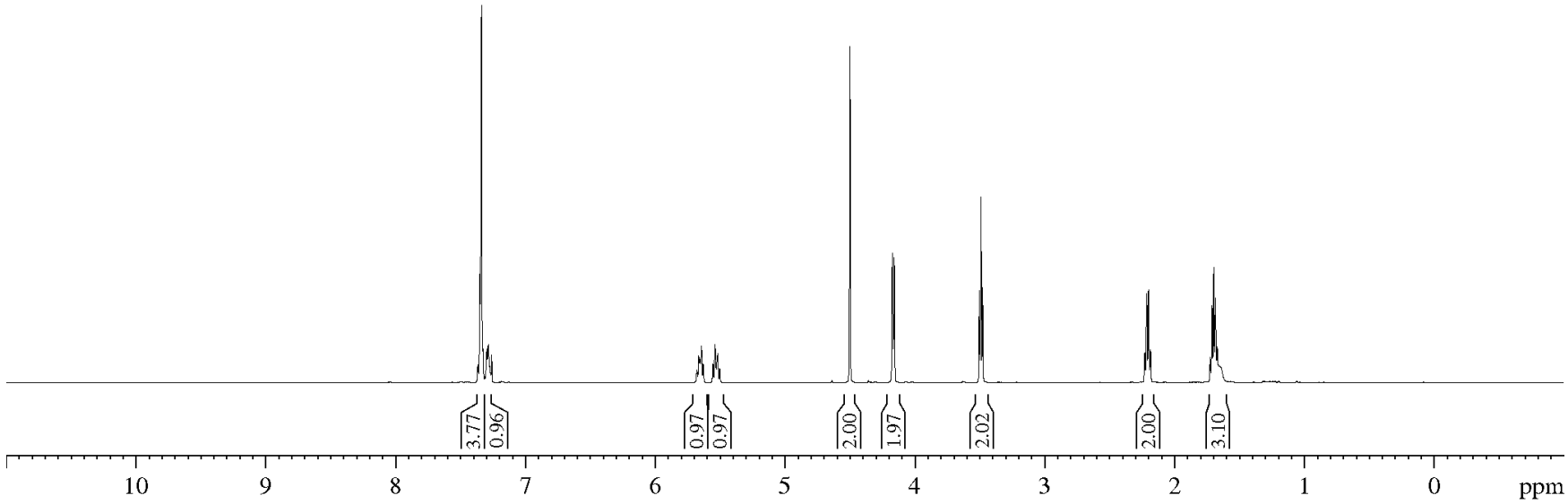

**8**

**$^1$H NMR**

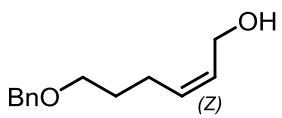

OH
BnO
(Z)

**9**


7.37
7.35
7.34
7.33
7.31
7.30
7.30
7.29
7.29
7.28
7.27
7.27
5.68
5.67
5.66
5.66
5.65
5.64
5.63
5.56
5.54
5.52
5.52
5.50
4.50
4.17
4.16
3.50
3.49
3.48
2.23
2.21
2.20
2.18
1.72
1.71
1.70
1.68
1.67


3.77
0.96
0.97
0.97
2.00
1.97
2.02
2.00
3.10
10
9
8
7
6
5
4
3
2
1
0
ppm

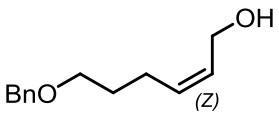
**$^{13}$C NMR**


OH
BnO
(Z)

**9**

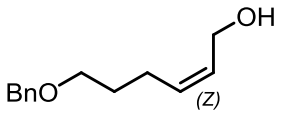

138.5
132.3
129.4
128.5
127.8
127.7
73.0
69.3
58.5
29.4
24.0
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



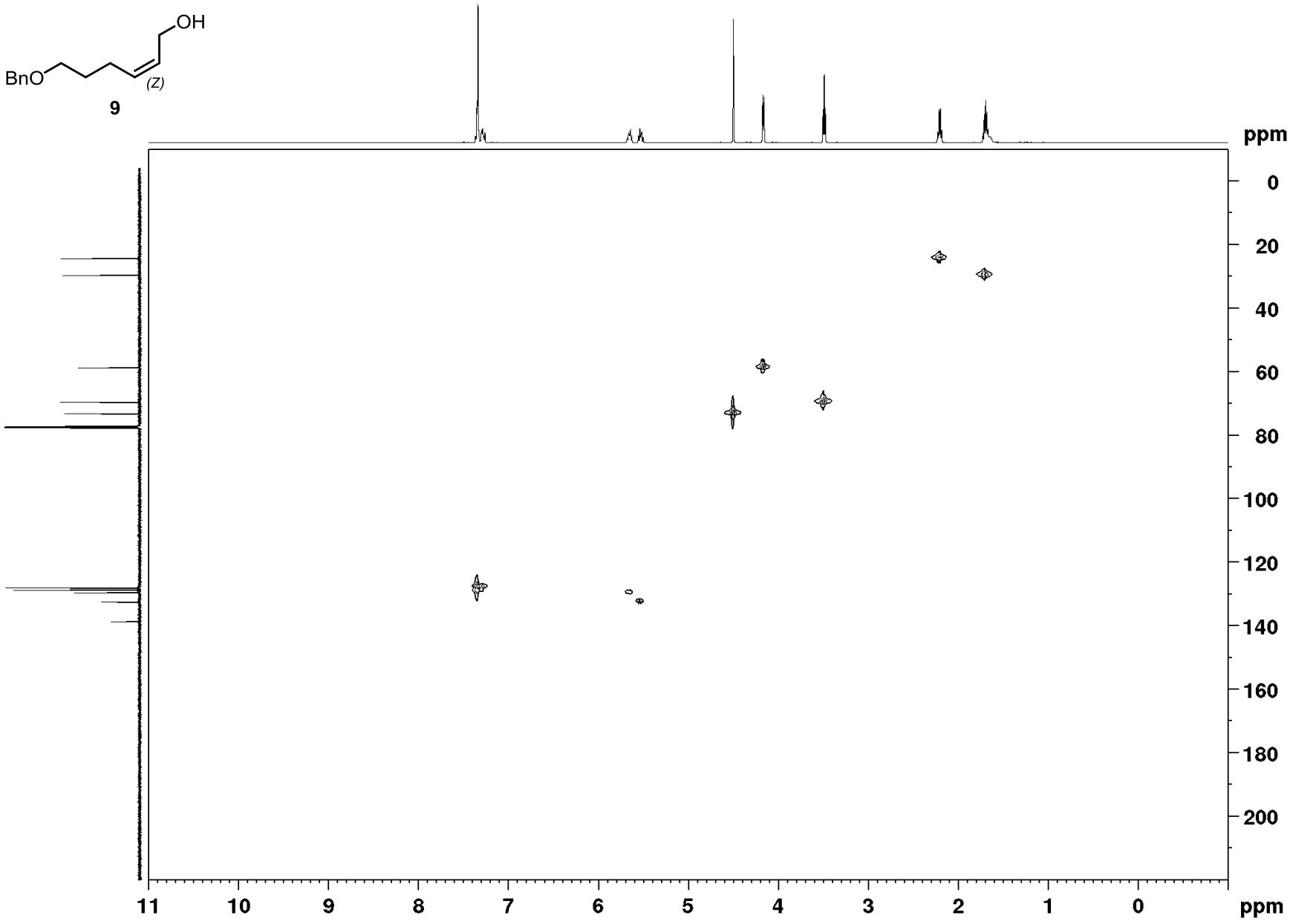

**9**

**$^1$H, $^1$H COSY**

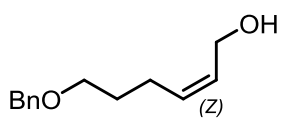



**9**

**$^{1}H$, $^{13}C$ HMQC**


OH
BnO
(Z)
9
ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

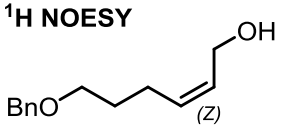
**$^{1}H$, $^{13}C$ HMBC**


OH
BnO
(Z)

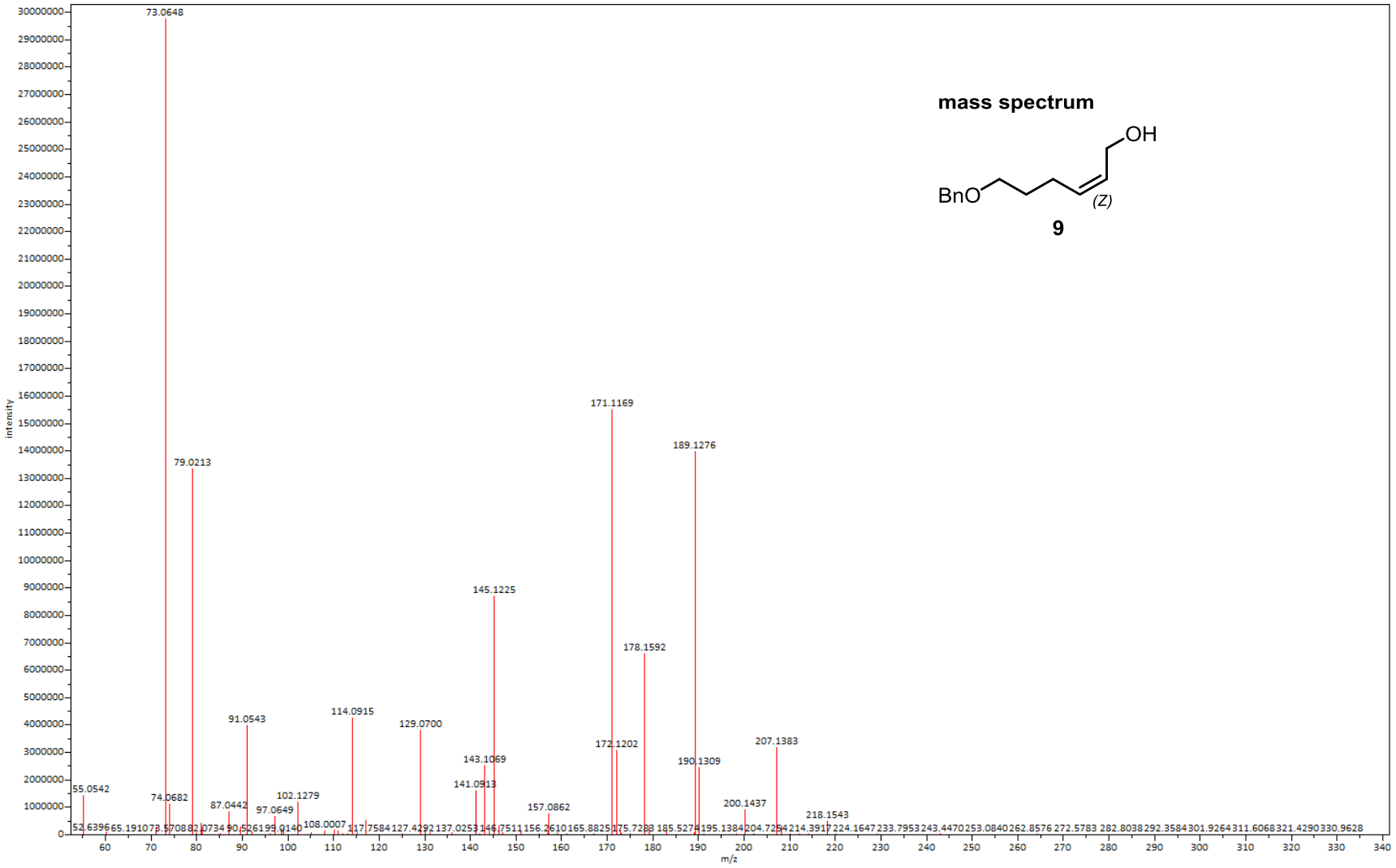
**9**

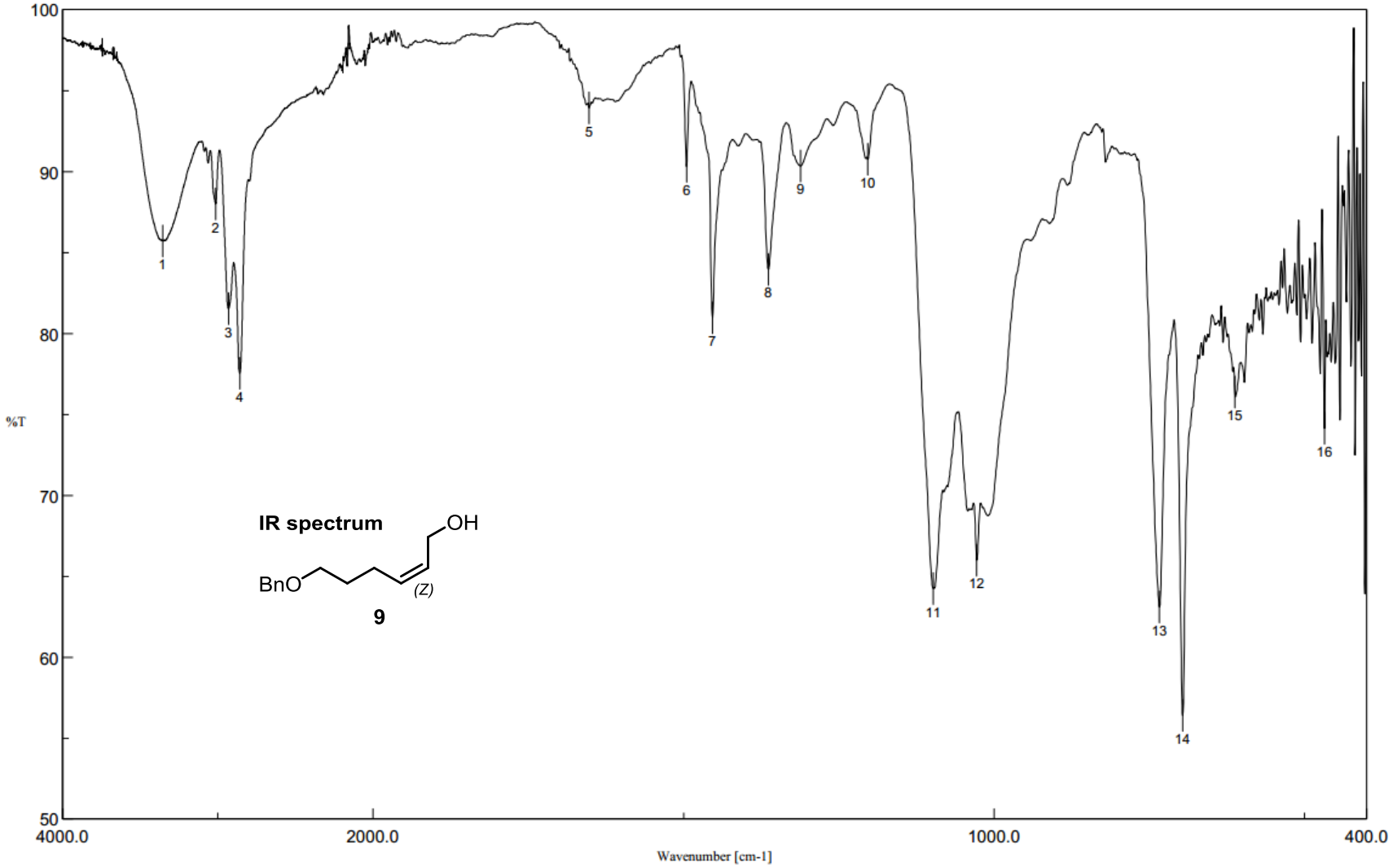

ppm
0
20
40
60
80
100
120
140
160
180
200
11
10
9
8
7
6
5
4
3
2
1
0
ppm

**$^1$H, $^1$H NOESY**

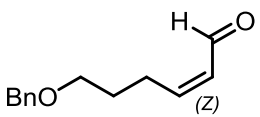



**9**


mass spectrum
OH
BnO
(Z)
9
intensity
m/z
73.0648
79.0213
171.1169
189.1276
145.1225
178.1592
114.0915
91.0543
129.0700
172.1202
143.1069
207.1383
190.1309
55.0542
74.0682
141.0913
102.1279
87.0442
200.1437
157.0862
97.0649
218.1543
108.0007

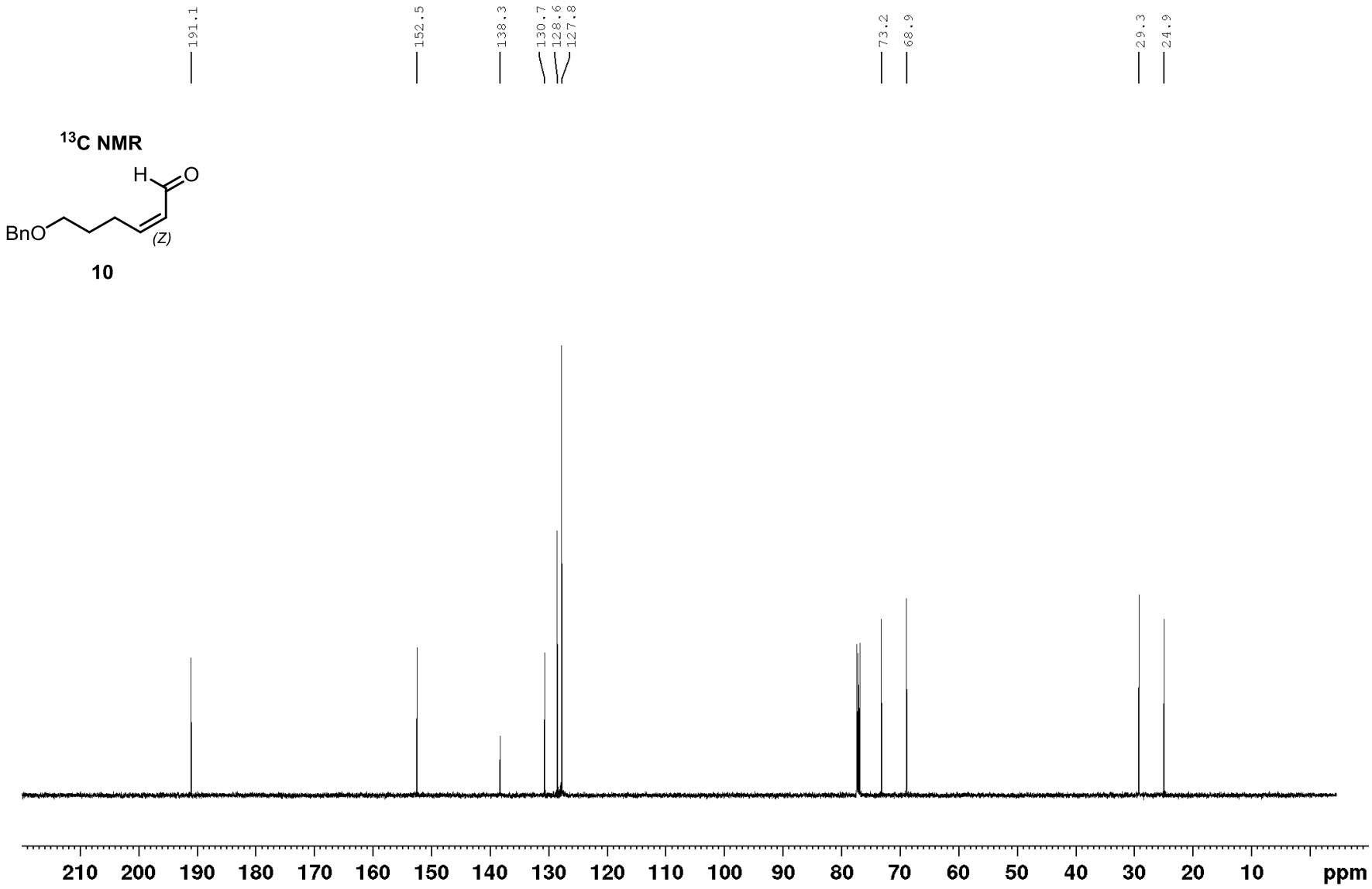

IR spectrum
OH
BnO
(Z)
9
%T
100
90
80
70
60
50
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
16

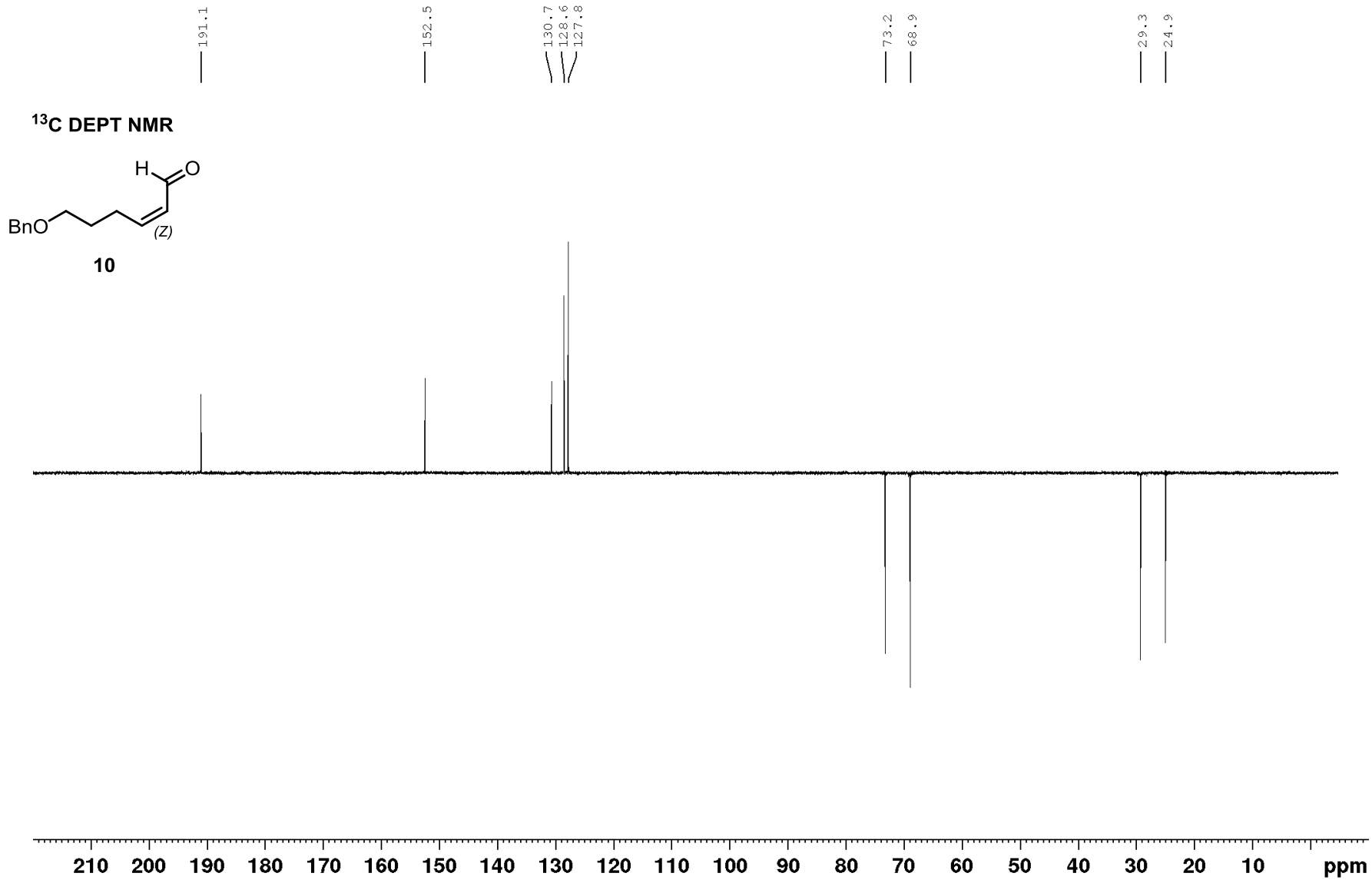
**$^1$H NMR**


H
O
BnO
(Z)

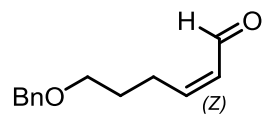
**10**


10.09
10.07
7.37
7.36
7.36
7.35
7.35
7.34
7.34
7.34
7.33
7.33
7.32
7.31
7.31
7.31
7.31
7.30
7.30
7.29
7.29
7.28
7.28
7.28
7.27
7.27
6.65
6.63
6.63
6.62
6.61
6.59
6.00
5.99
5.99
5.98
5.98
5.97
5.97
5.97
5.96
5.95
5.95
4.49
3.53
3.52
3.50
2.76
2.75
2.74
2.73
2.71
2.71
1.85
1.84
1.82
1.81
1.79
0.92
4.60
1.00
0.86
2.24
2.33
2.28
2.32
10
9
8
7
6
5
4
3
2
1
0
ppm


191.1
152.5
138.3
130.7
128.6
127.8
73.2
68.9
29.3
24.9
13C NMR
H
O
BnO
(Z)
10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

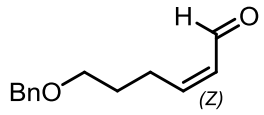

191.1
152.5
130.7
128.6
127.8
73.2
68.9
29.3
24.9
13C DEPT NMR
H
O
BnO
(Z)
10
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^1$H, $^1$H COSY**



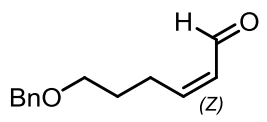

**10**

**$^{1}H$, $^{13}C$ HMQC**



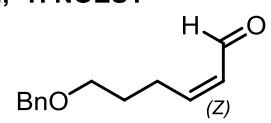

**10**

**$^{1}H$, $^{13}C$ HMBC**

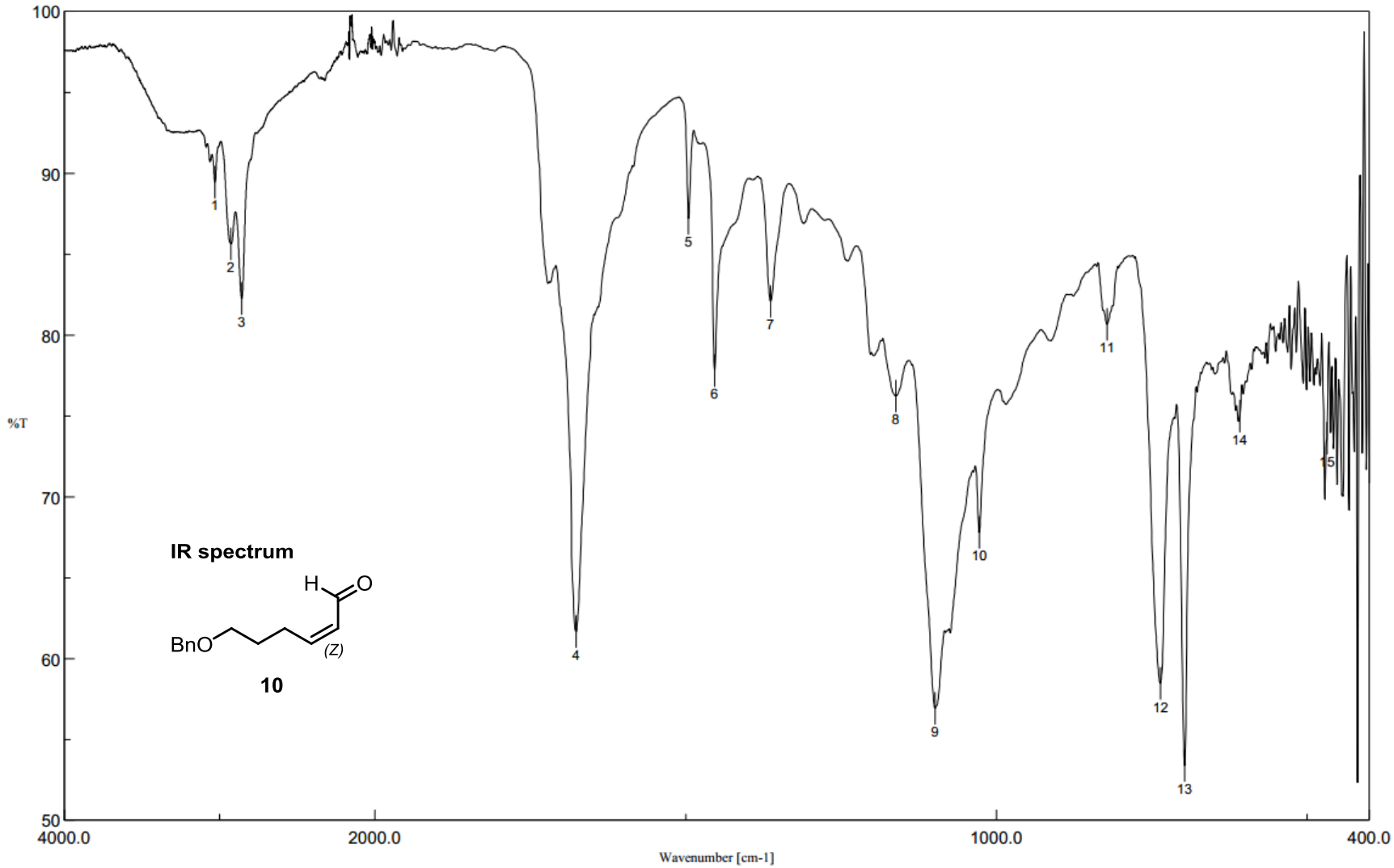



**10**

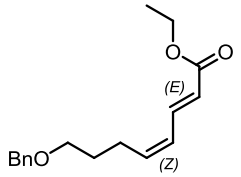
**$^1$H, $^1$H NOESY**




**10**

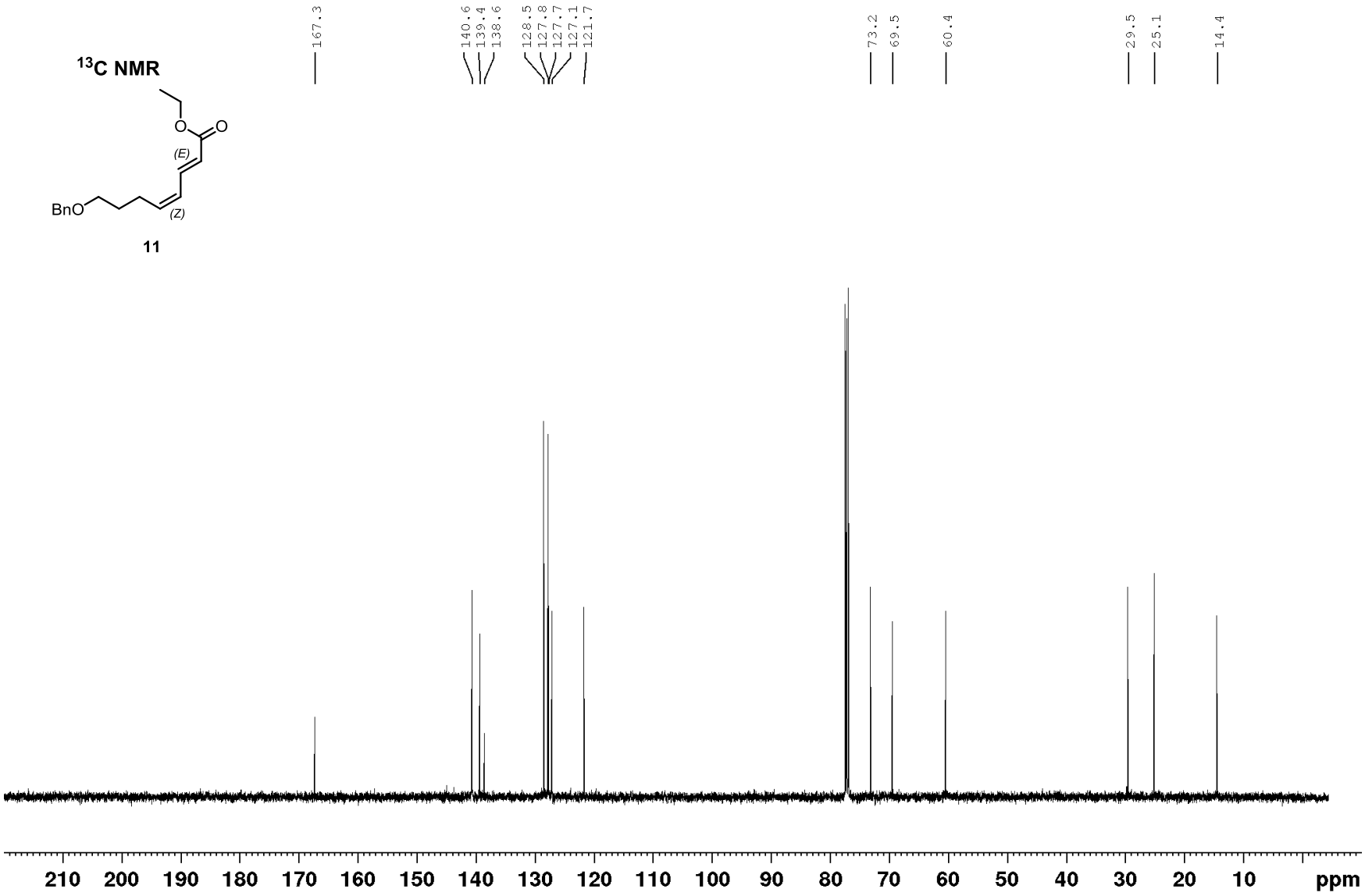

100
90
80
70
60
50
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
1
2
3
4
5
6
7
8
9
10
11
12
13
14
15
IR spectrum
H
O
BnO
(Z)
10

**$^1$H NMR**

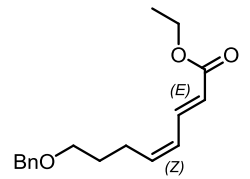

O
O
(E)
BnO
(Z)

**11**


7.65 7.64 7.62 7.62 7.62 7.61 7.59 7.59 7.36 7.35 7.34 7.34 7.33 7.31 7.30 7.29 7.29 7.29 7.28 7.28 7.28 7.27 7.27 7.27 6.16 6.14 6.12 5.89 5.87 5.86 5.85 5.84 5.83 5.82 4.50 4.23 4.22 4.20 4.19 3.50 3.49 3.47 2.44 2.44 2.43 2.41 2.41 2.40 2.40 1.77 1.76 1.74 1.73 1.72 1.31 1.29 1.28
0.95 3.96 0.96 1.04 1.92 2.01 2.05 2.10 2.00 2.10 3.15
10 9 8 7 6 5 4 3 2 1 0 ppm

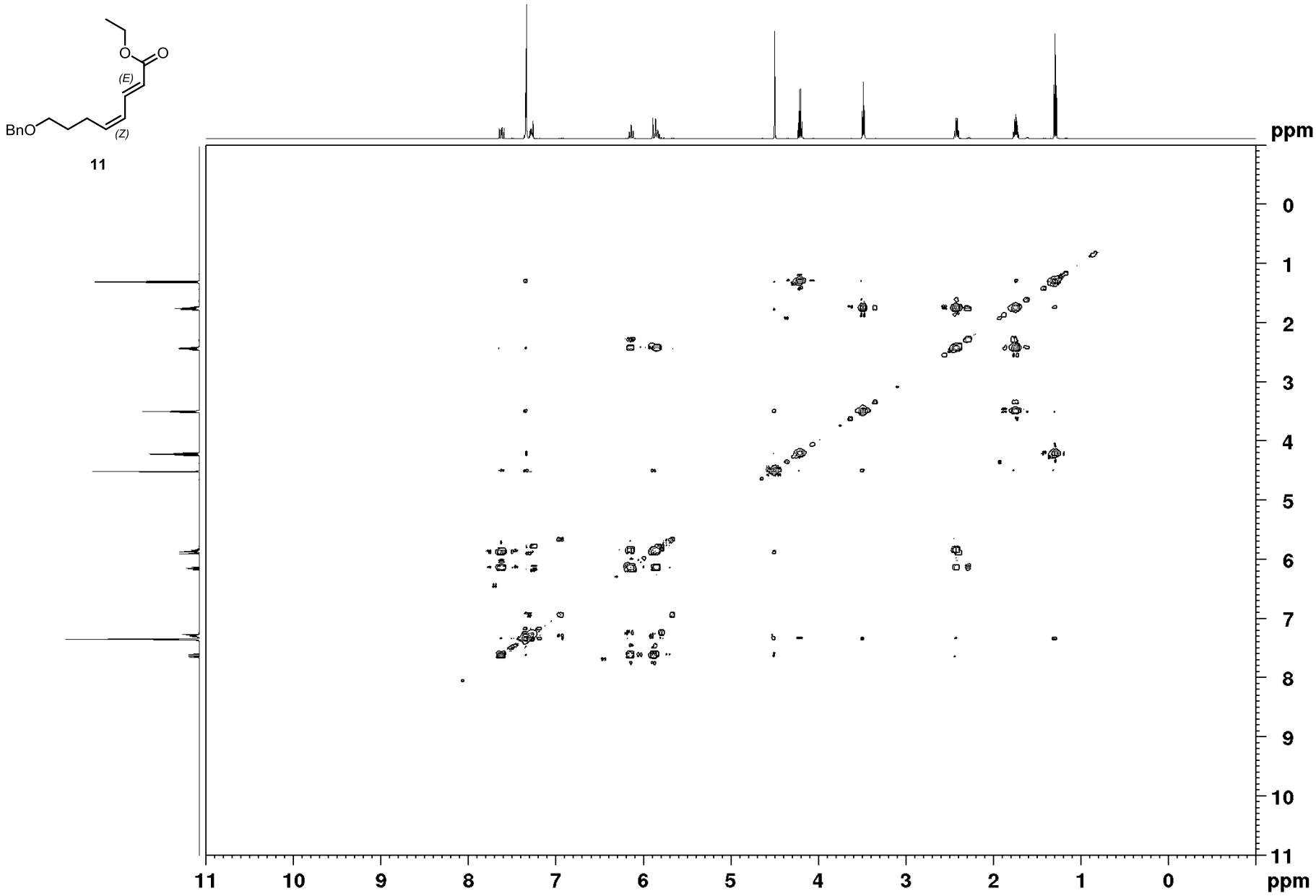

13C NMR
11
167.3
140.6
139.4
138.6
128.5
127.8
127.7
127.1
121.7
73.2
69.5
60.4
29.5
25.1
14.4
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 ppm

**$^{13}$C DEPT NMR**



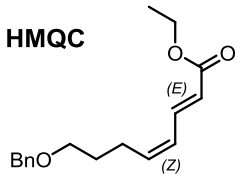

**11**

**$^1$H, $^1$H COSY**



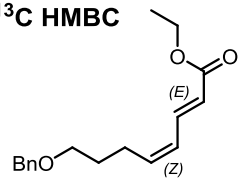

**11**

$^{1}H$, $^{13}C$ HMQC



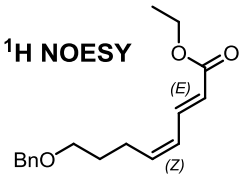

11

$^{1}H$, $^{13}C$ HMBC

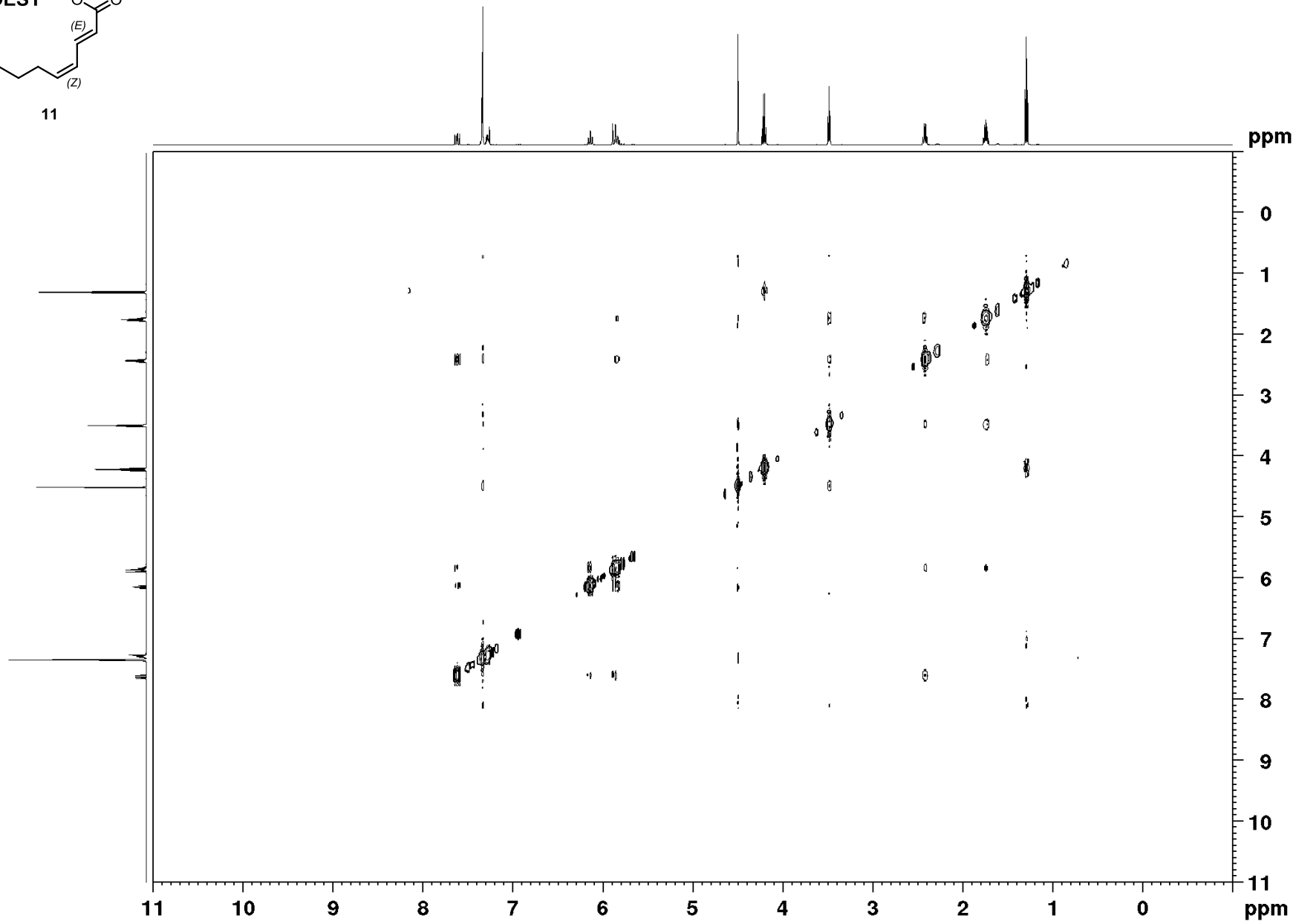


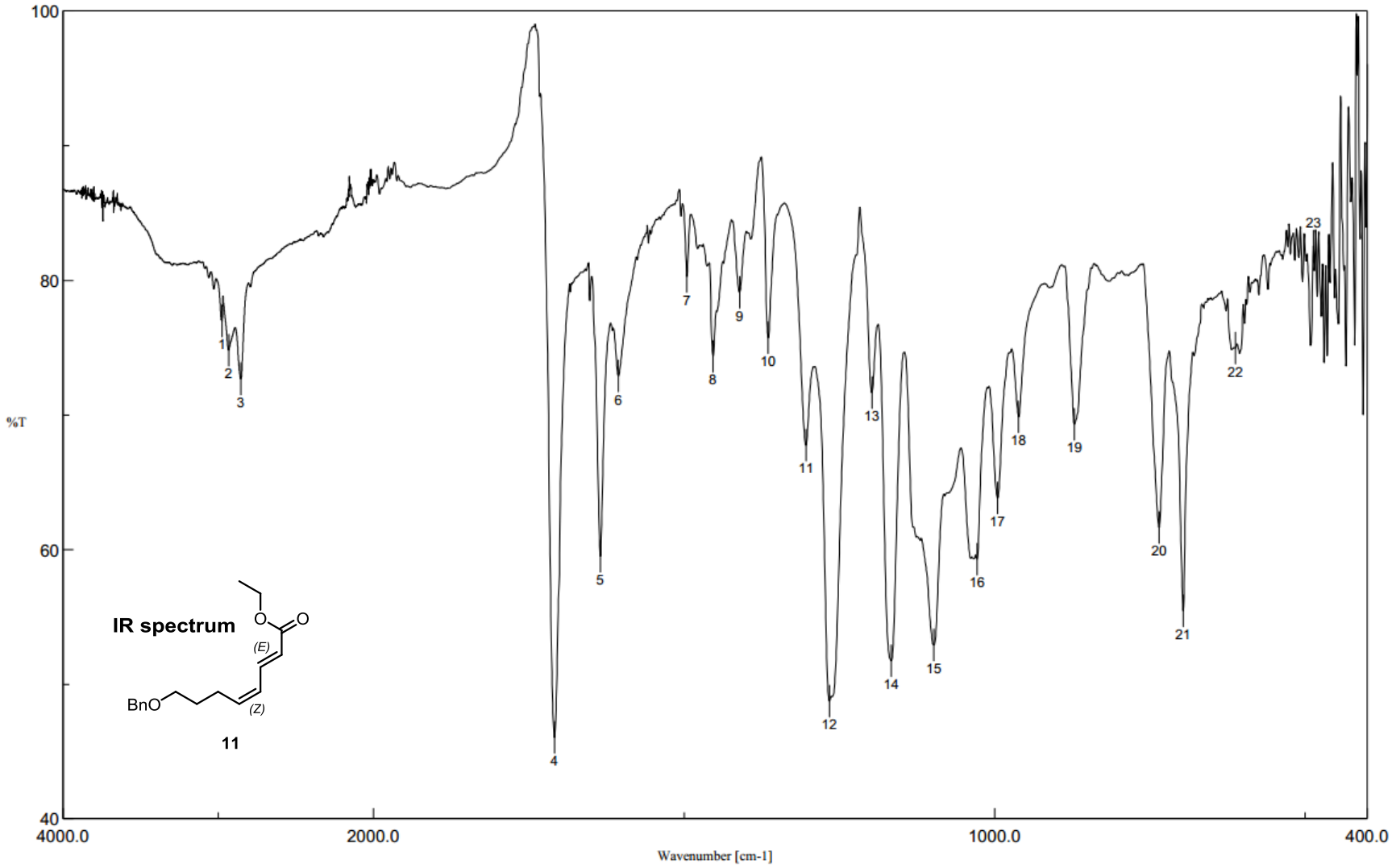

11

$^1$H, $^1$H NOESY




**11**




100
80
60
40
%T
4000.0
2000.0
1000.0
400.0
Wavenumber [cm-1]
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20
21
22
23
IR spectrum
O
O
(E)
BnO
(Z)
11