Lithium Enolates Derived from Pyroglutaminol:
Mechanism and Stereoselectivity of an Azaaldol Addition

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**Part 1: NMR Characterization**

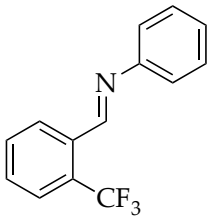
**Part 2: Rapid–inject Fluorine NMR Kinetics**

**Part 3: Selectivity Studies**

**Part 4: Solution Structural Studies**

**Part 1: NMR Spectroscopic Studies**

**Chart 1**

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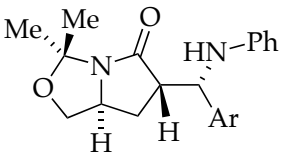


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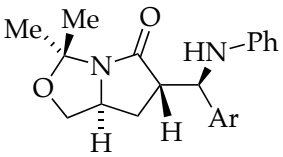


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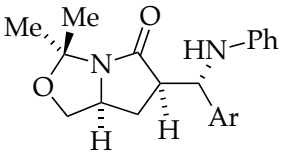


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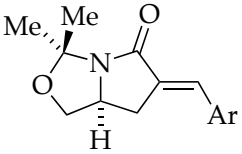


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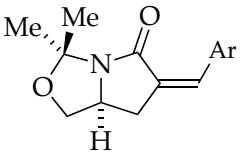


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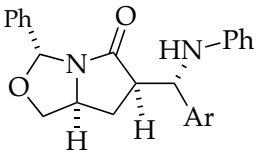


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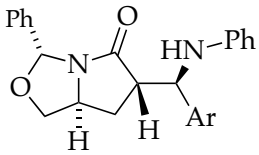


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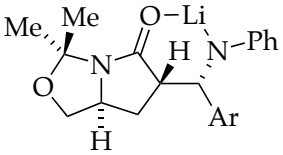
**Chart 2**

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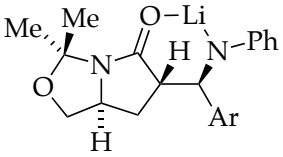


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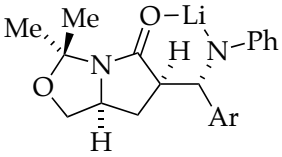


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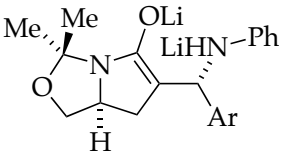


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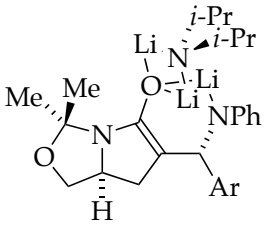


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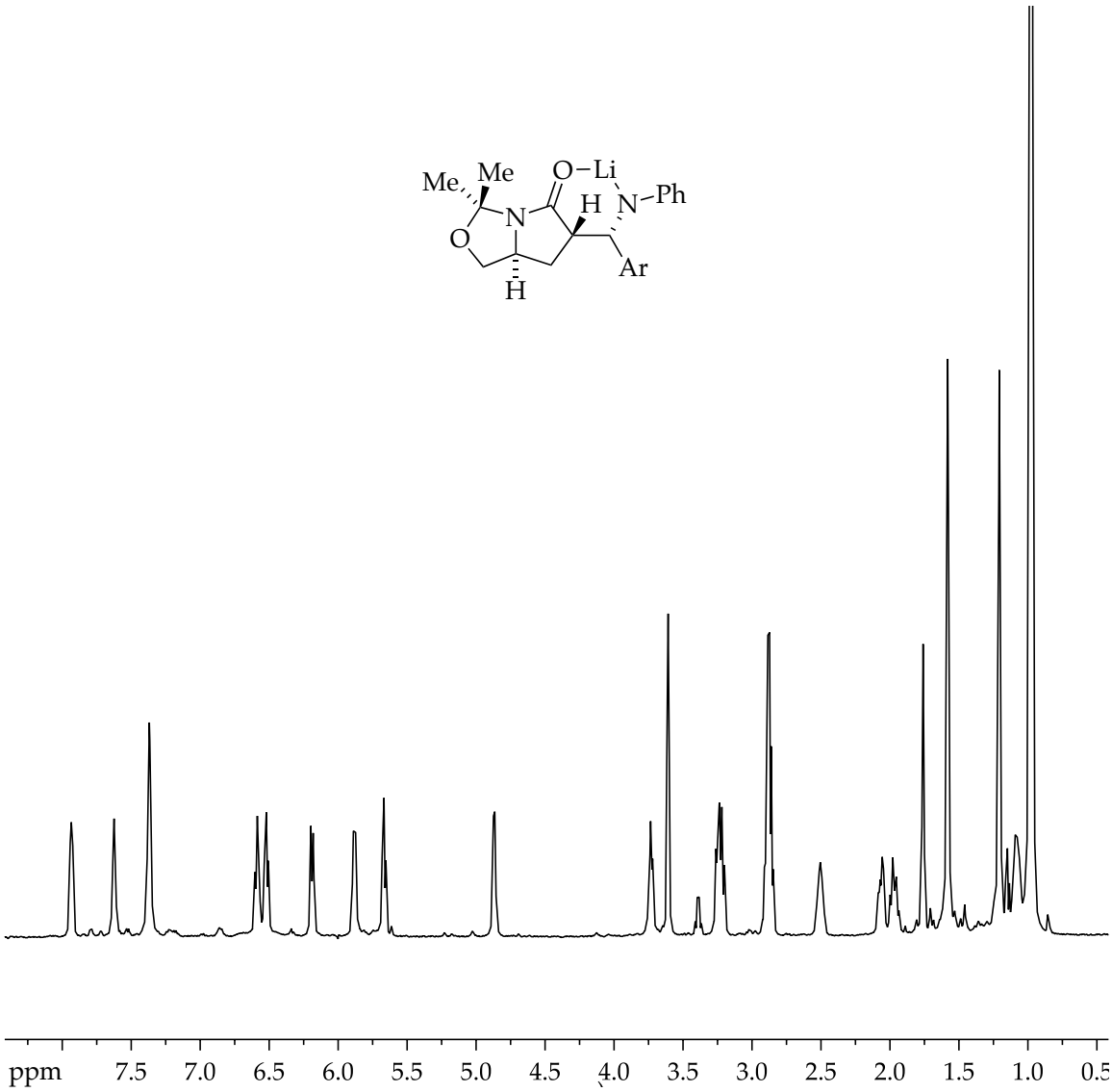



**Figure 1**. $^{1}$H NMR of **8** in THF-$d_8$.

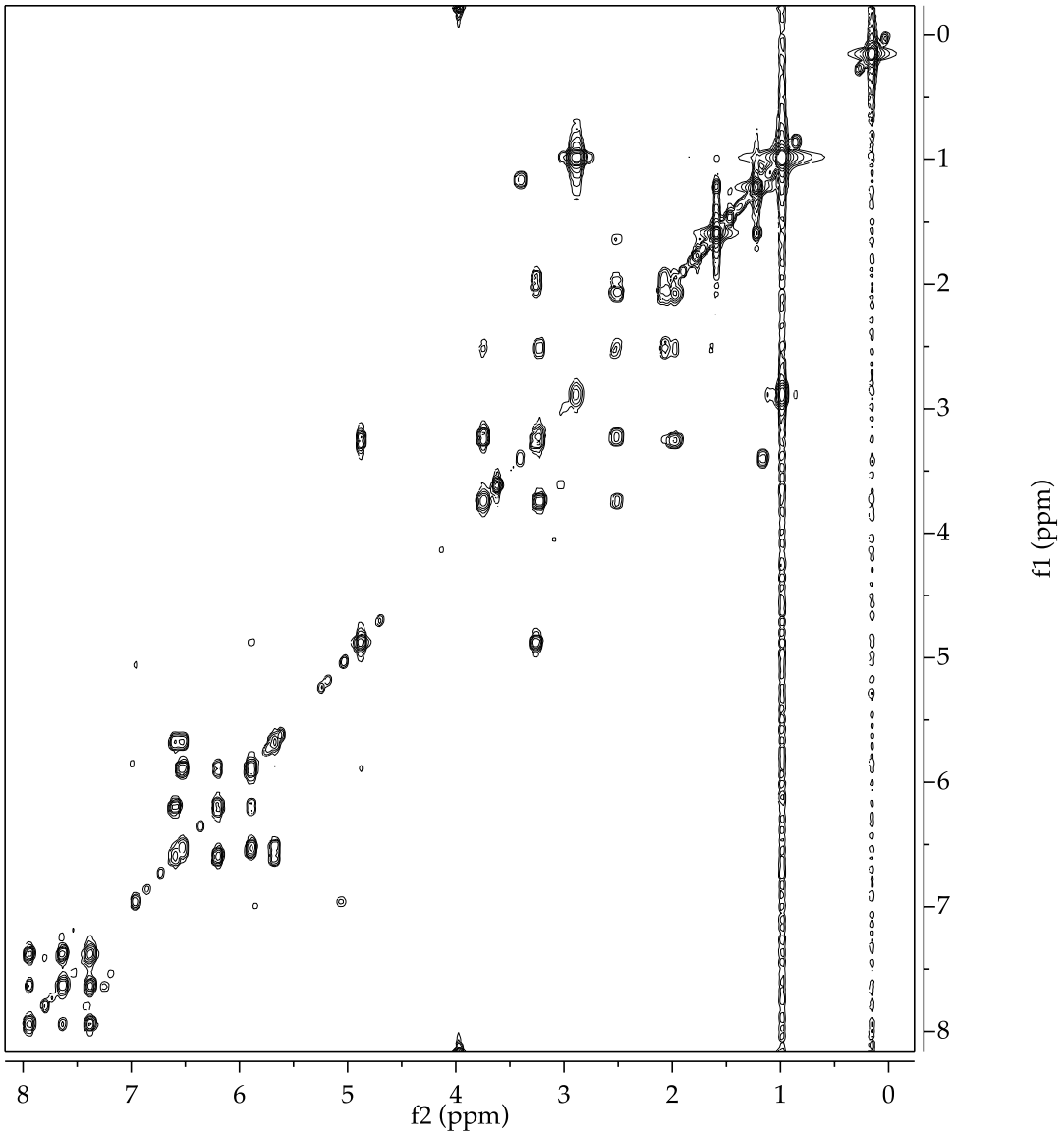
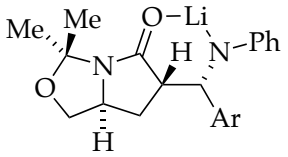



**Figure 2**. $^{1}$H-$^{1}$H COSY of **8** in THF-$d_8$.



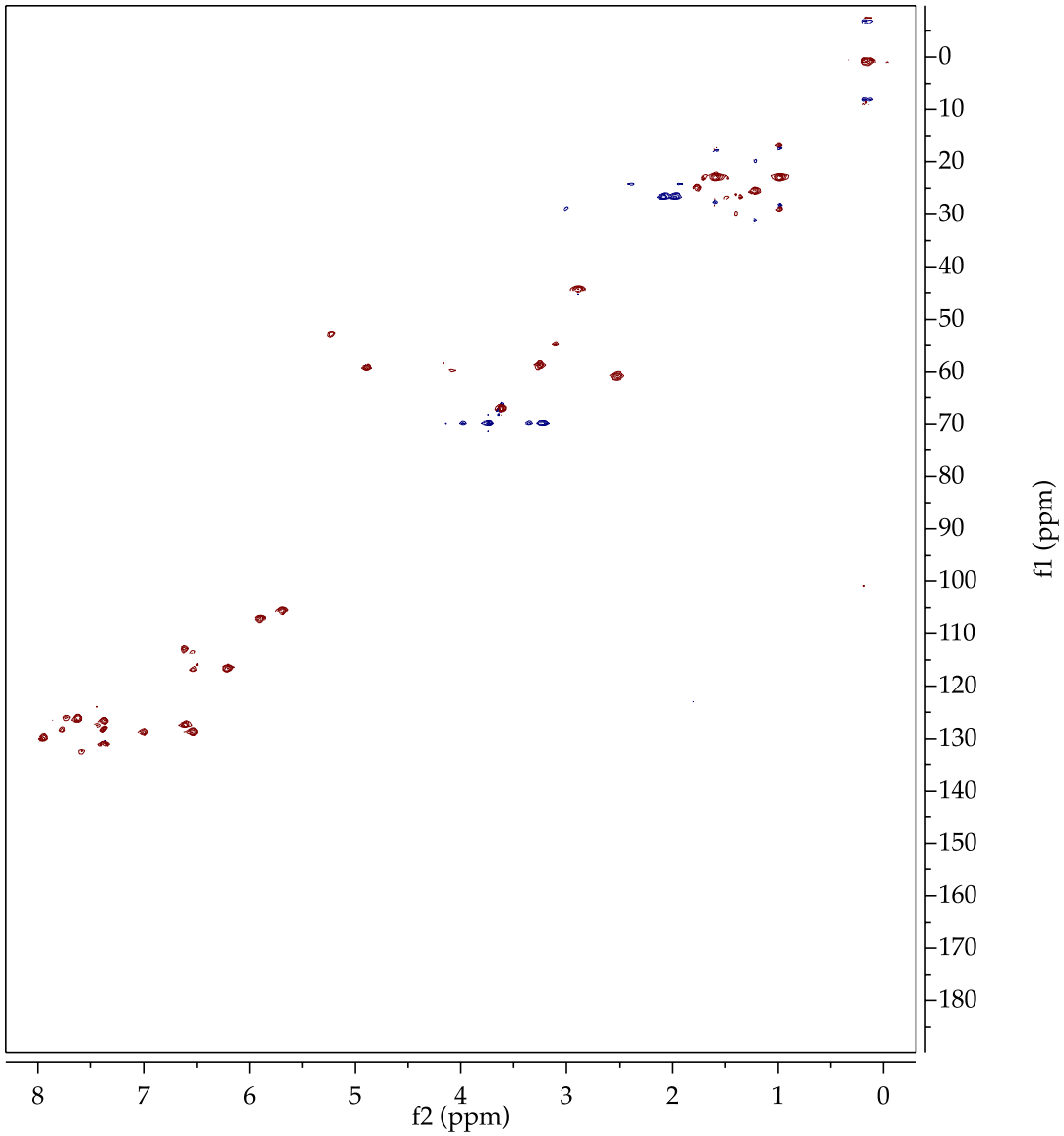
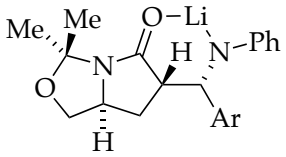



**Figure 3**. $^{1}$H-$^{13}$C HSQC of **8** in THF-$d_8$.



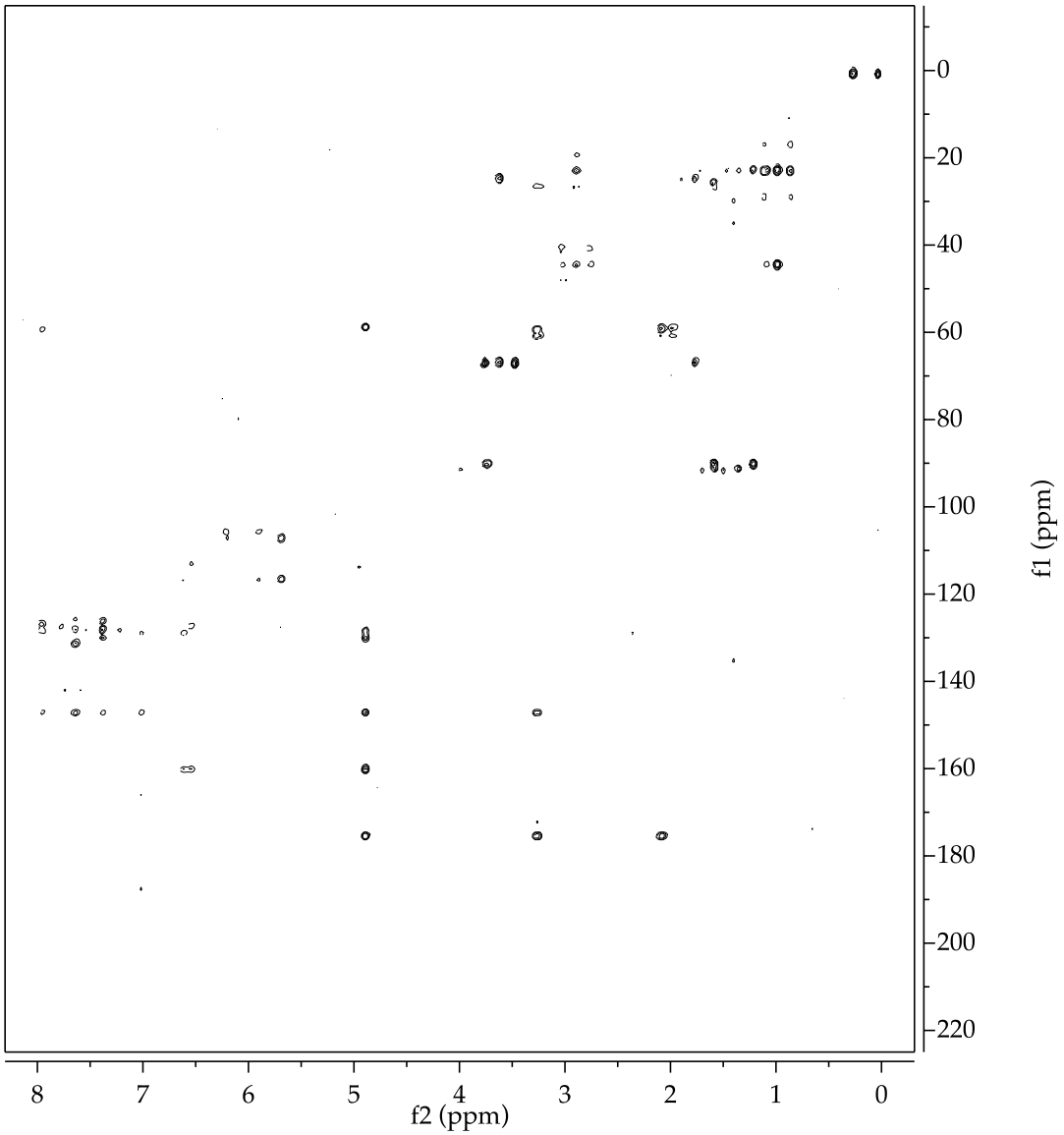
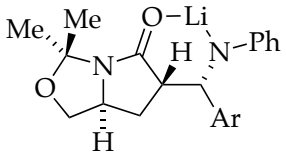



**Figure 4**. $^{1}$H-$^{13}$C HMBC of **8** in THF-$d_8$.



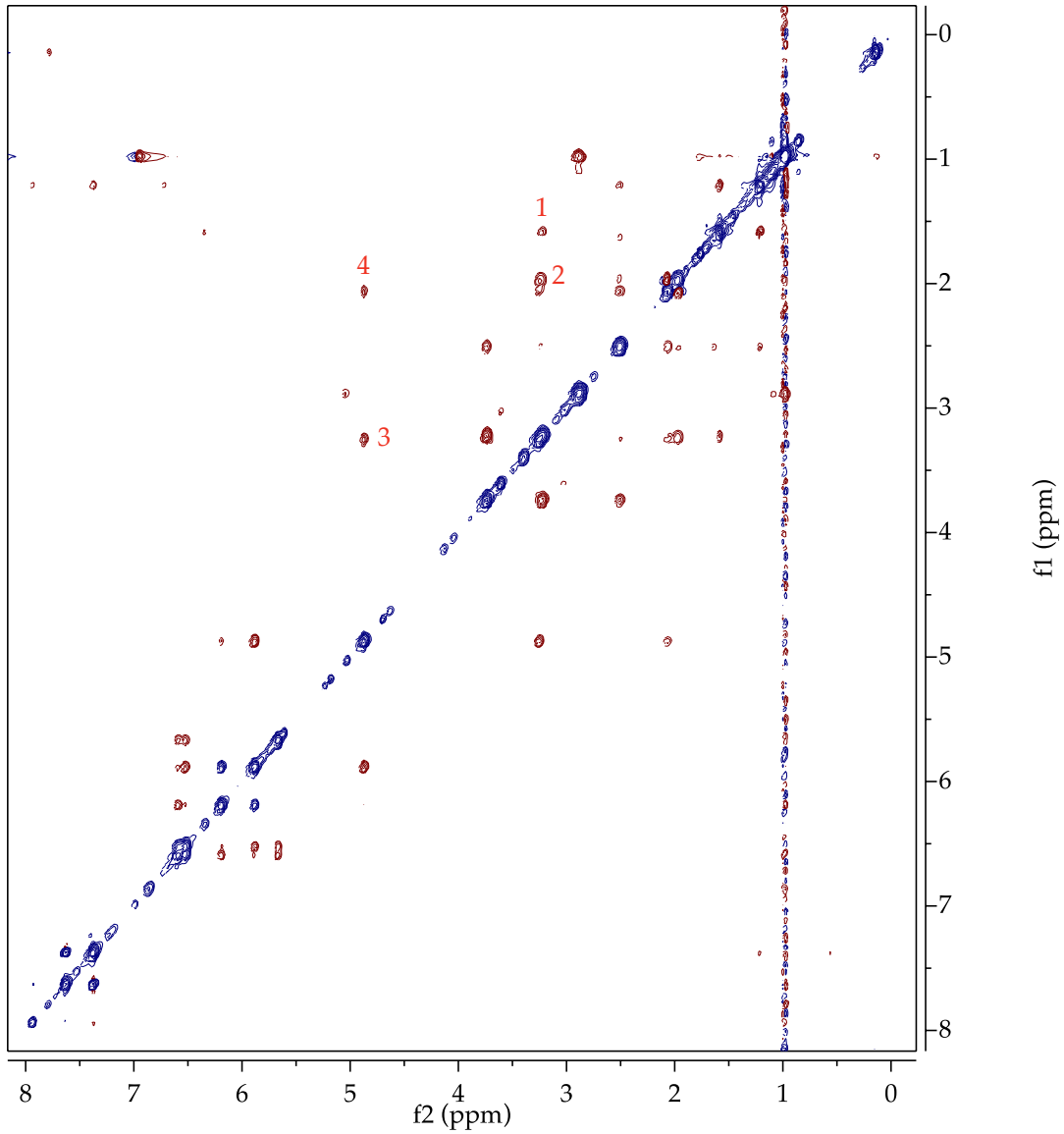
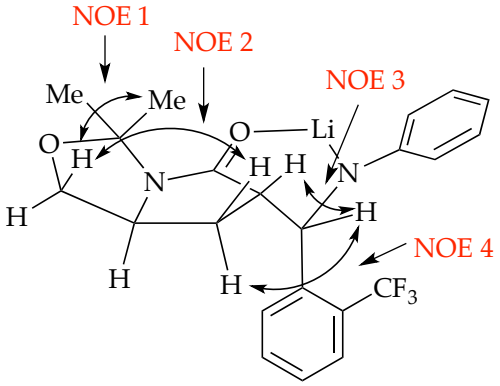



**Figure 5**. $^{1}$H-$^{1}$H ROESY of **8** in THF-$d_8$.



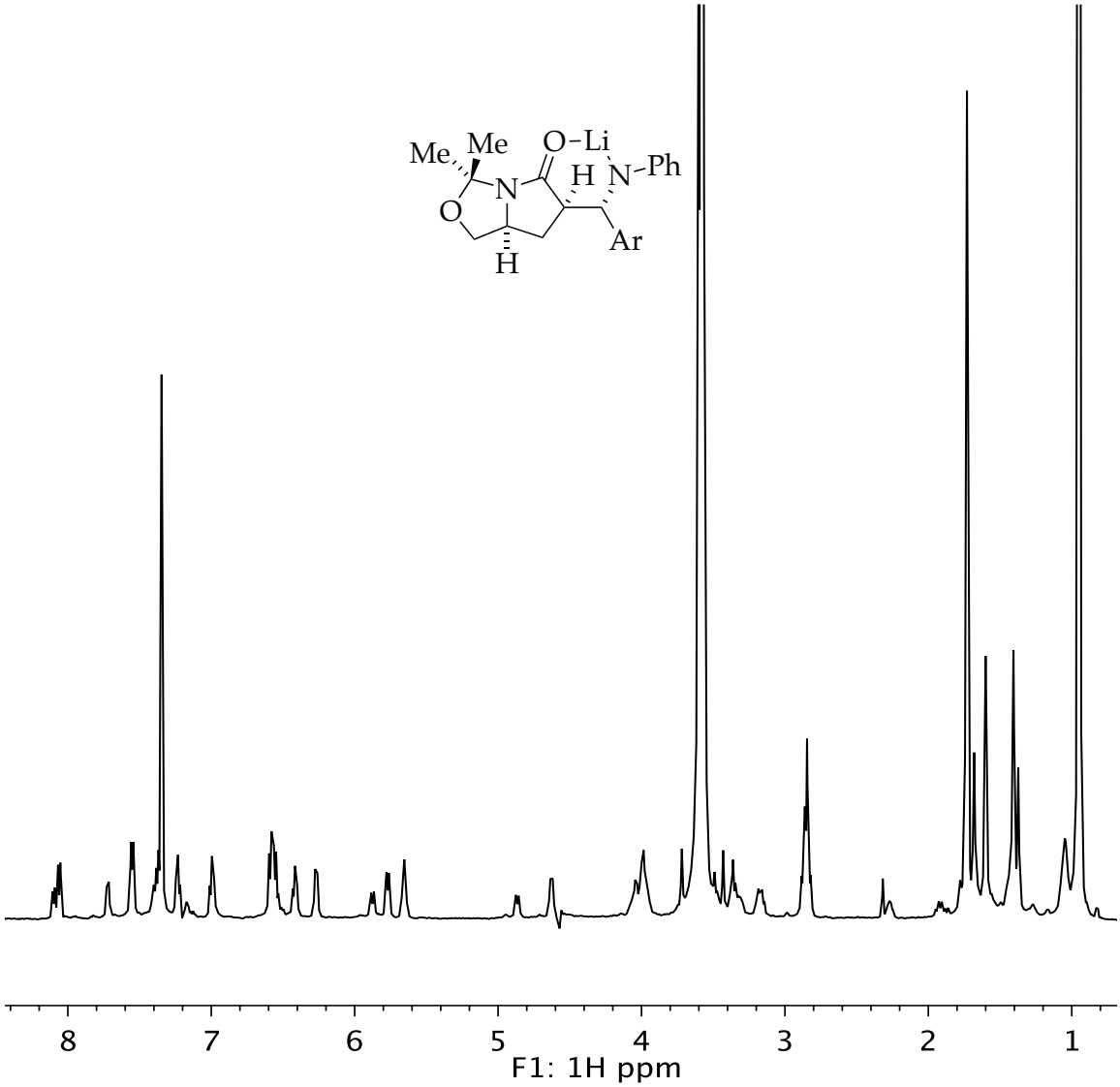



**Figure 6**. $^{1}$H NMR of **10** in THF-$d_8$ in a two : one ratio of **10** : **7**.

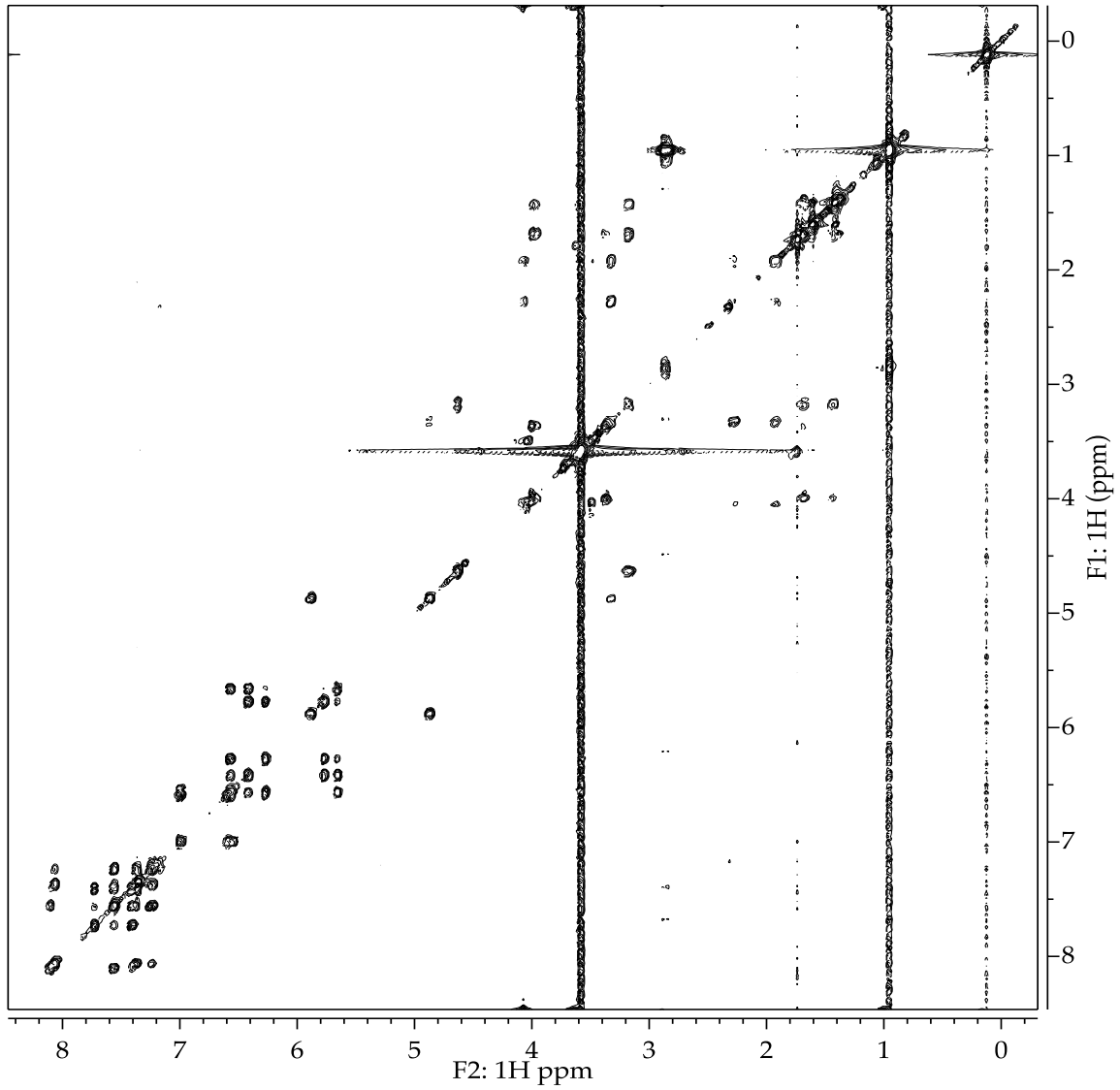
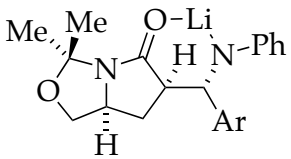



**Figure 7**. $^{1}$H-$^{1}$H COSY of **10** in THF-$d_8$ in a two : one ratio of **10** : **7**.



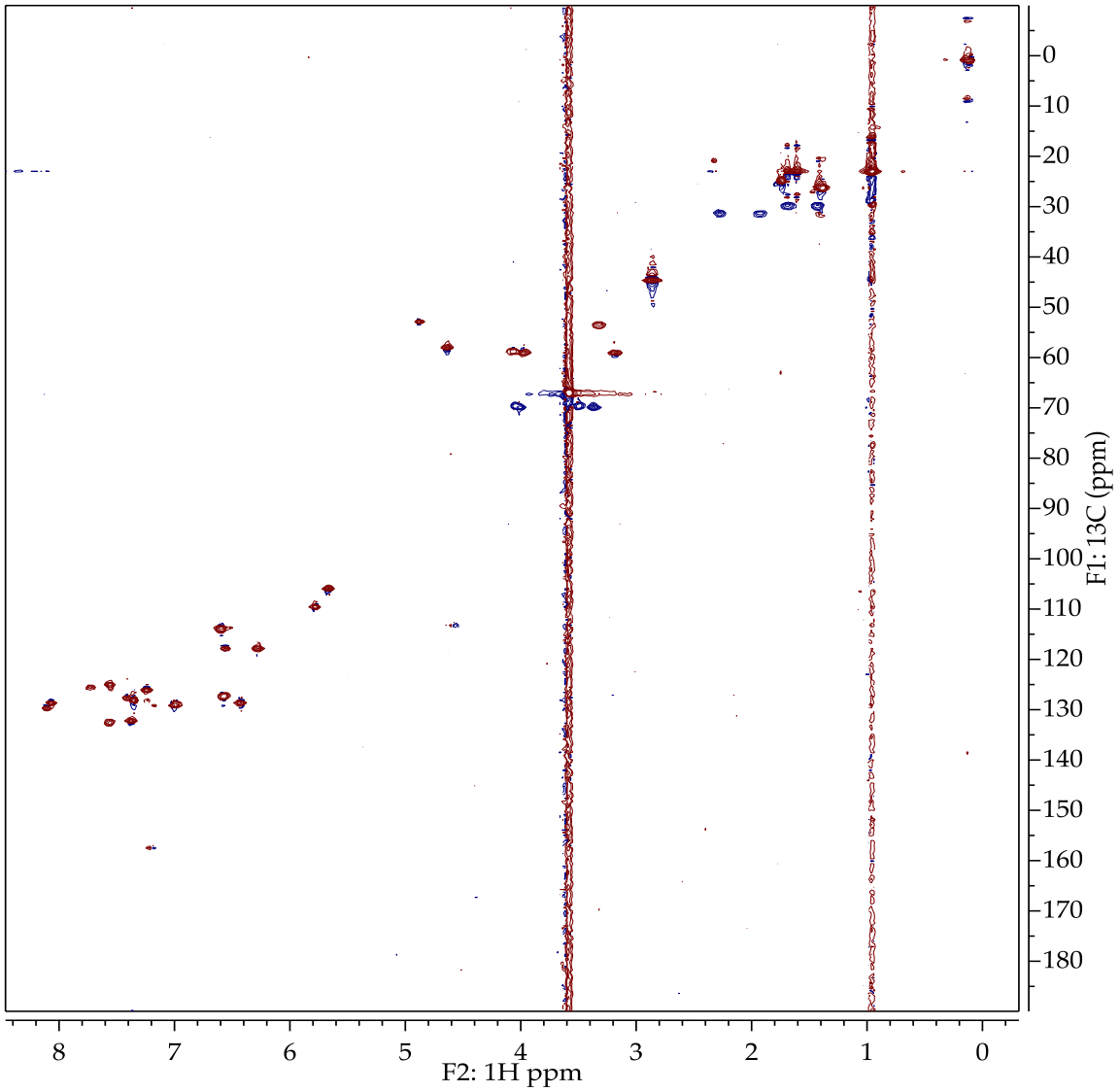
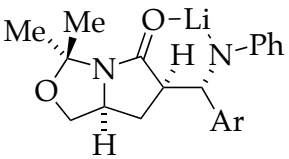



**Figure 8**. $^{1}$H-$^{13}$C HSQC of **10** in THF-$d_8$ in a two : one ratio of **10** : **7**..



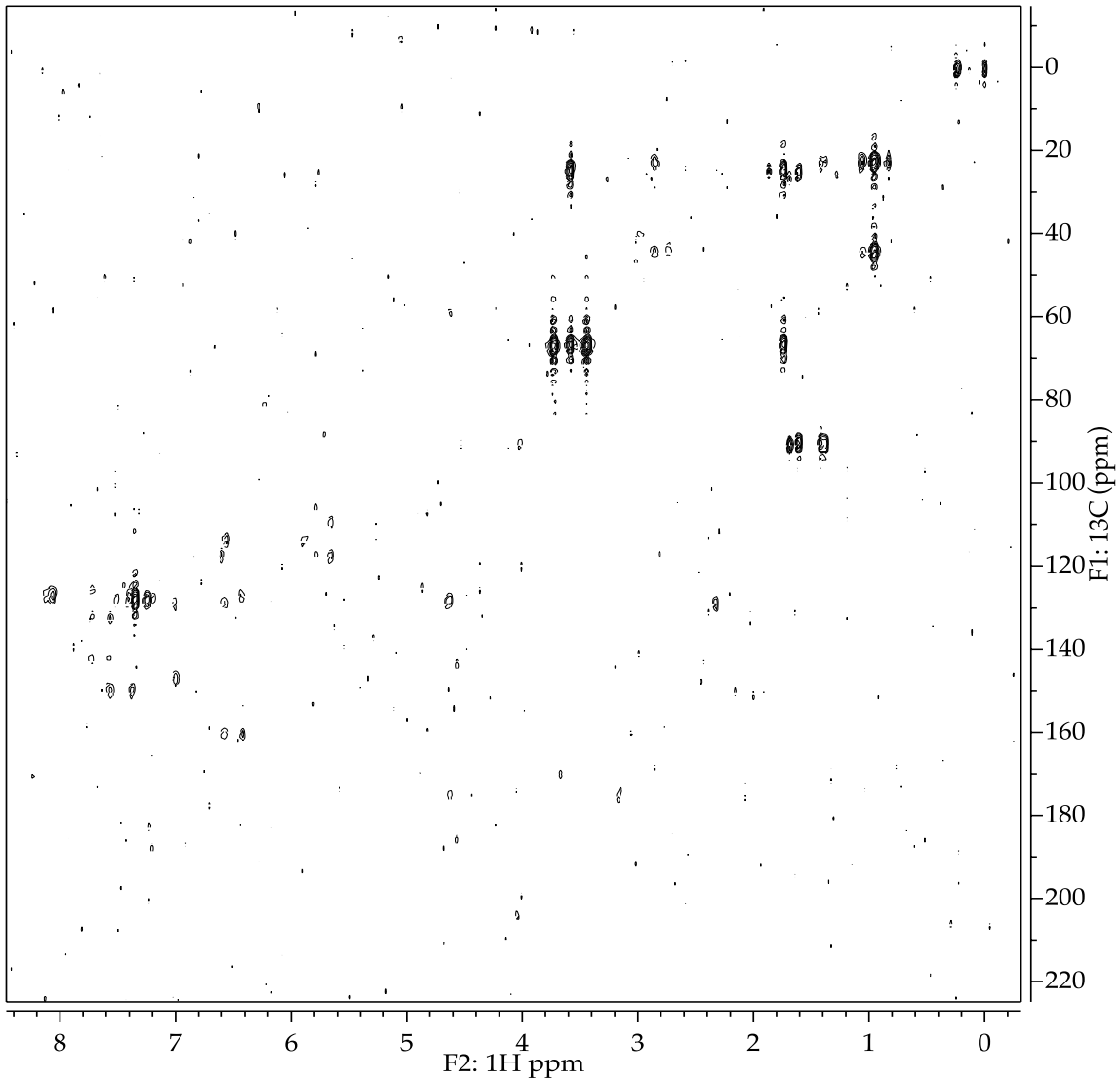
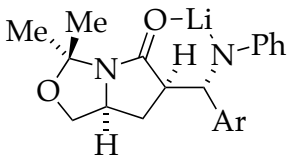



**Figure 9**. $^{1}$H-$^{13}$C HMBC of **10** in THF-$d_8$ in a two : one ratio of **10** : **7**.



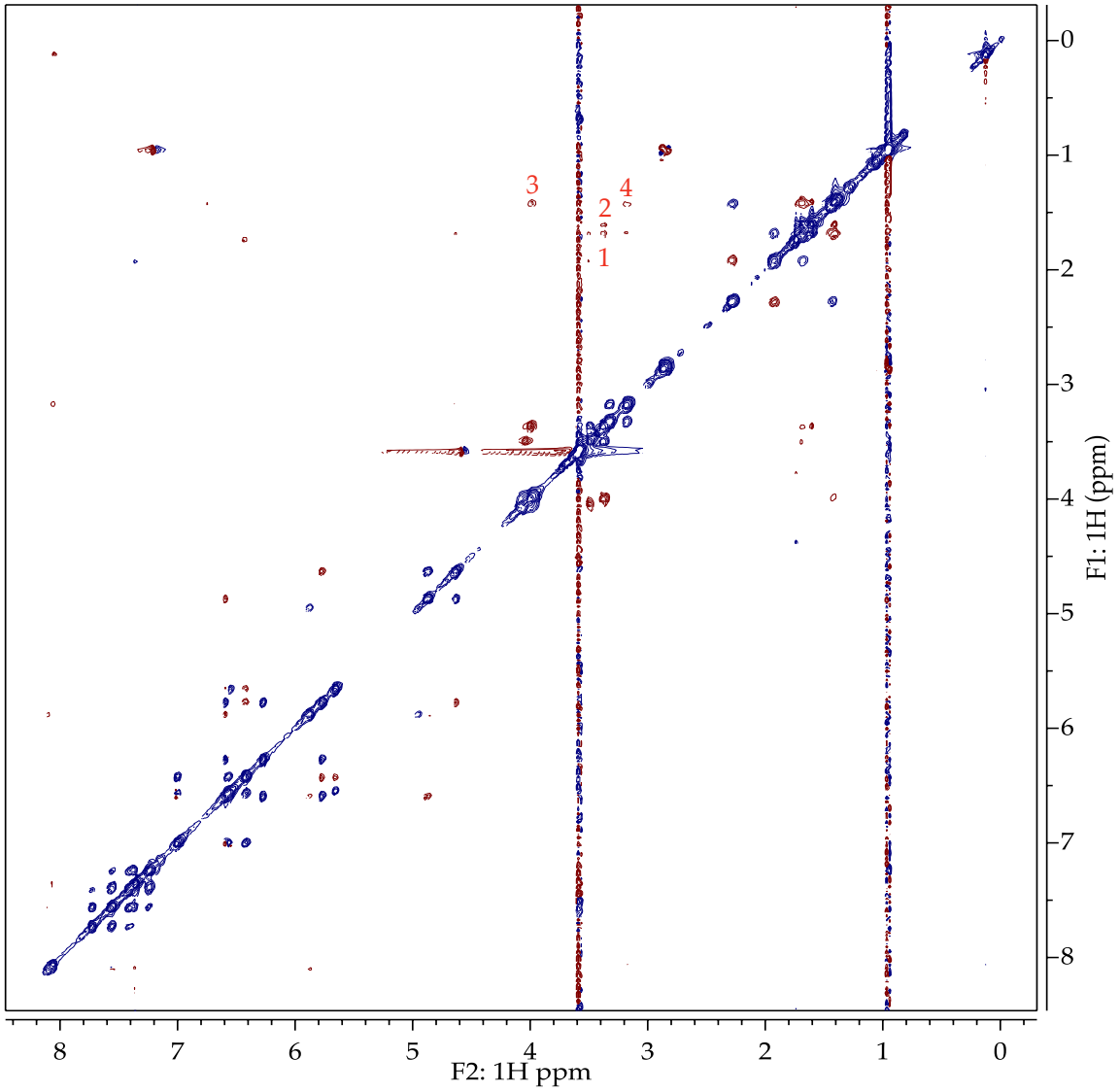
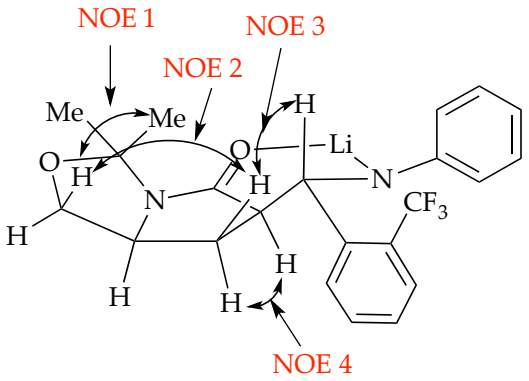



**Figure 10**. $^{1}$H-$^{1}$H ROESY of **10** in THF-$d_8$ in a two : one ratio of **10** : **7**.



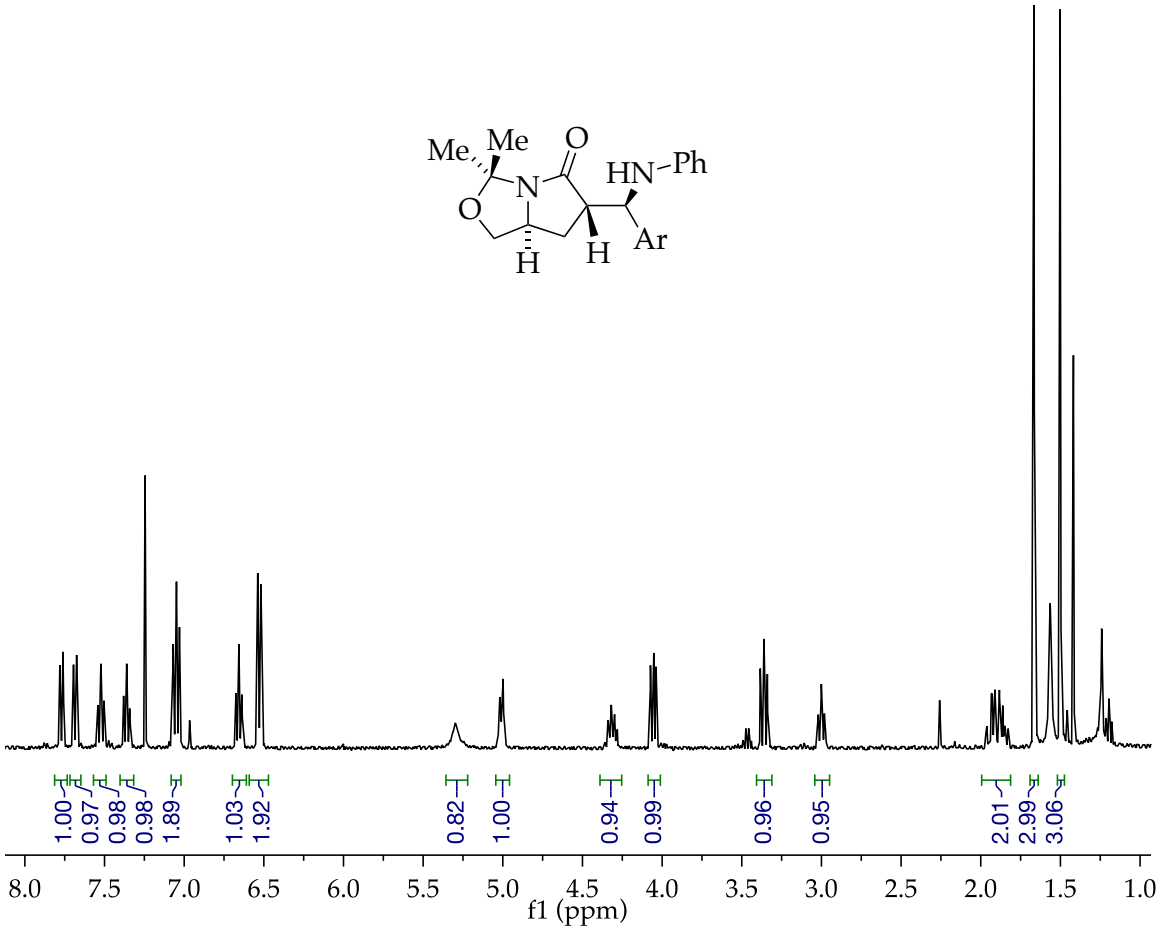



**Figure 11**. $^{1}$H NMR of **6** in $CDCl_3$.

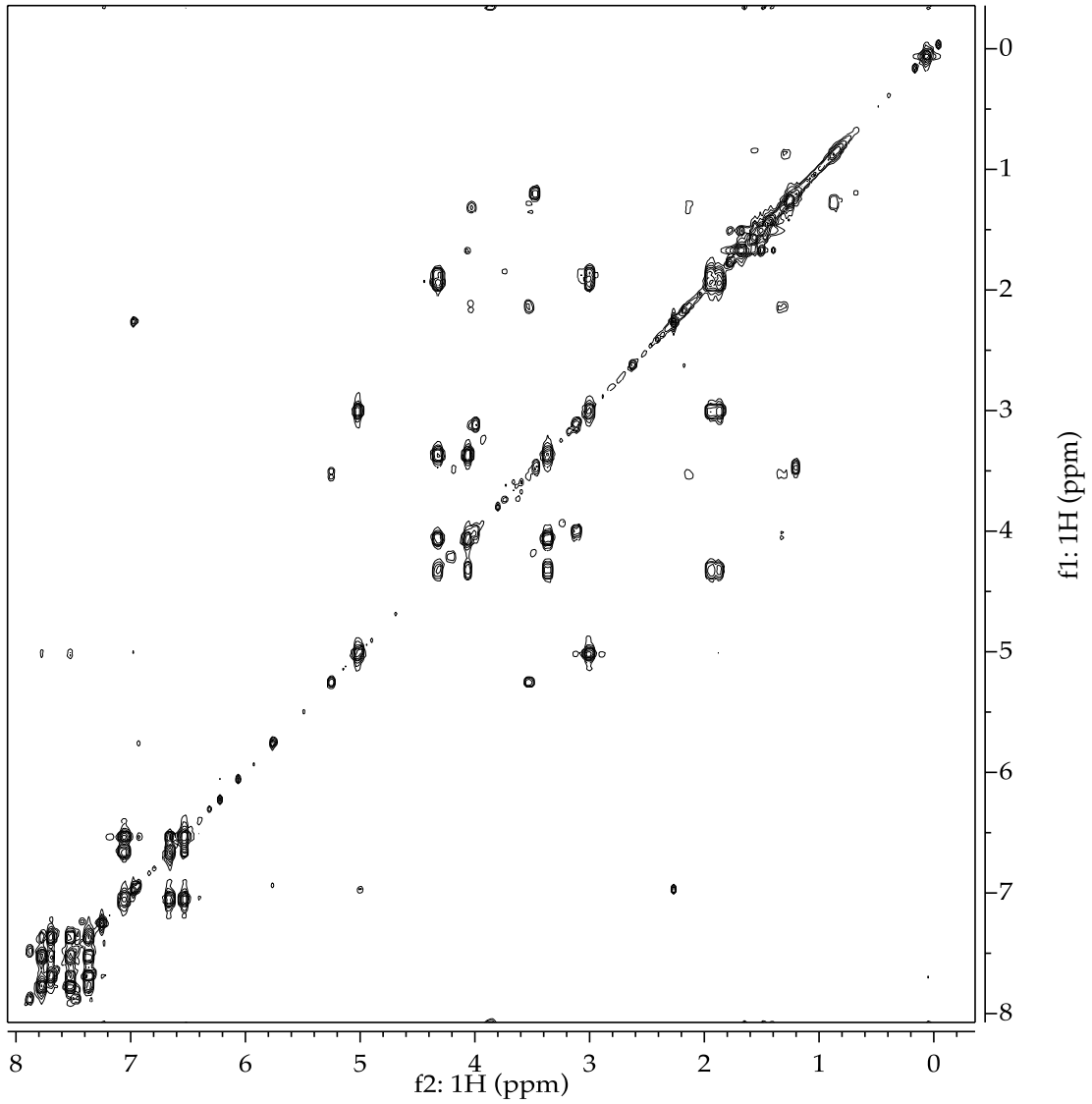
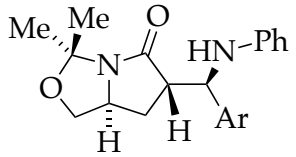



**Figure 12**. $^{1}H$-$^{1}H$ COSY of **6** in $CDCl_3$.



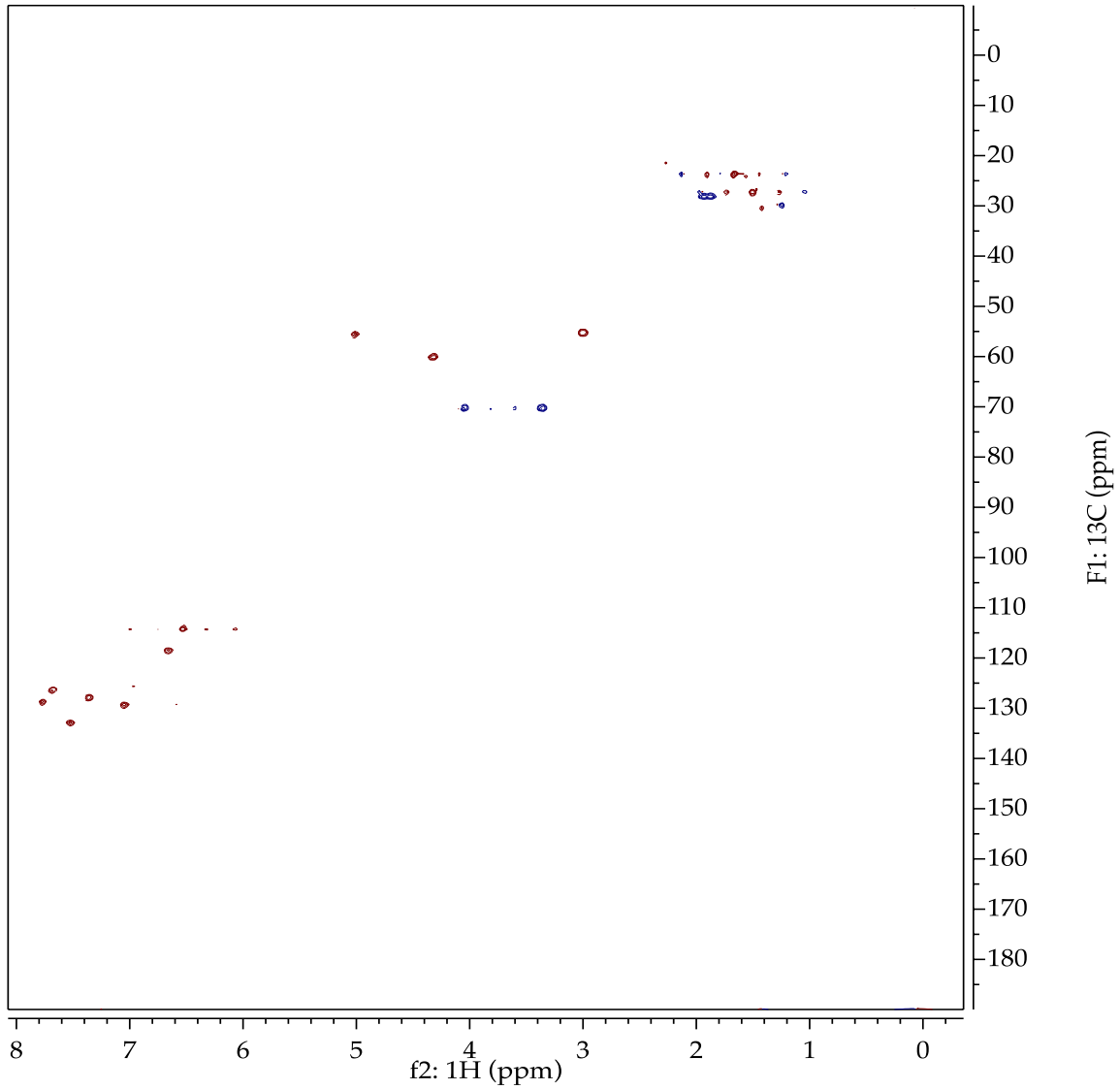
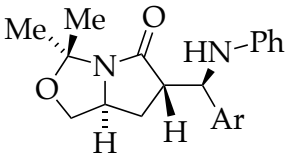



**Figure 13**. $^{1}H$-$^{13}C$ HSQC of **6** in $CDCl_3$.



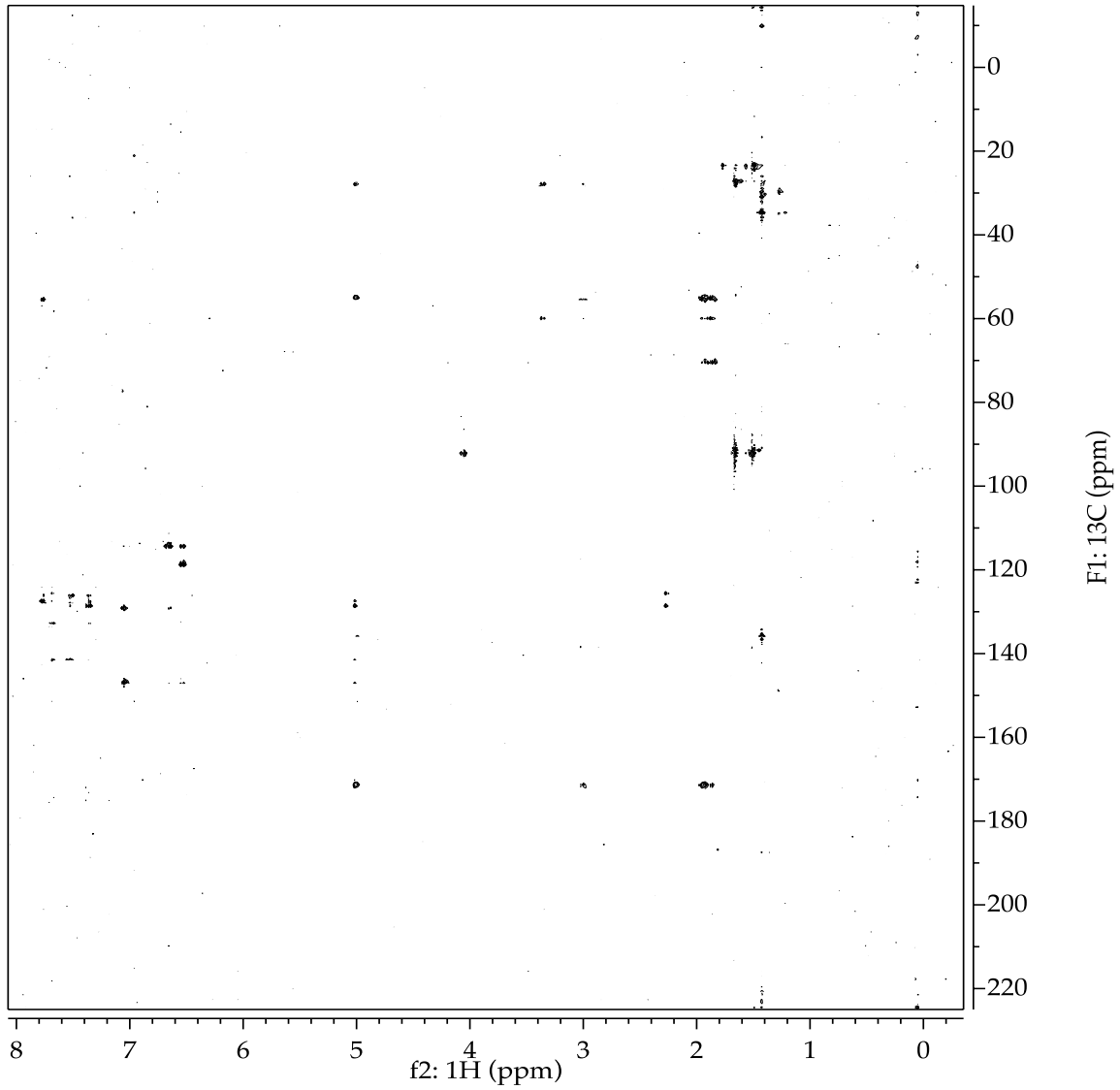
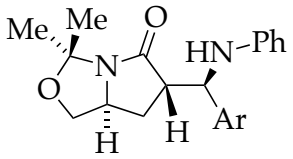



**Figure 14**. $^{1}H$-$^{13}C$ HMBC of **6** in $CDCl_3$.



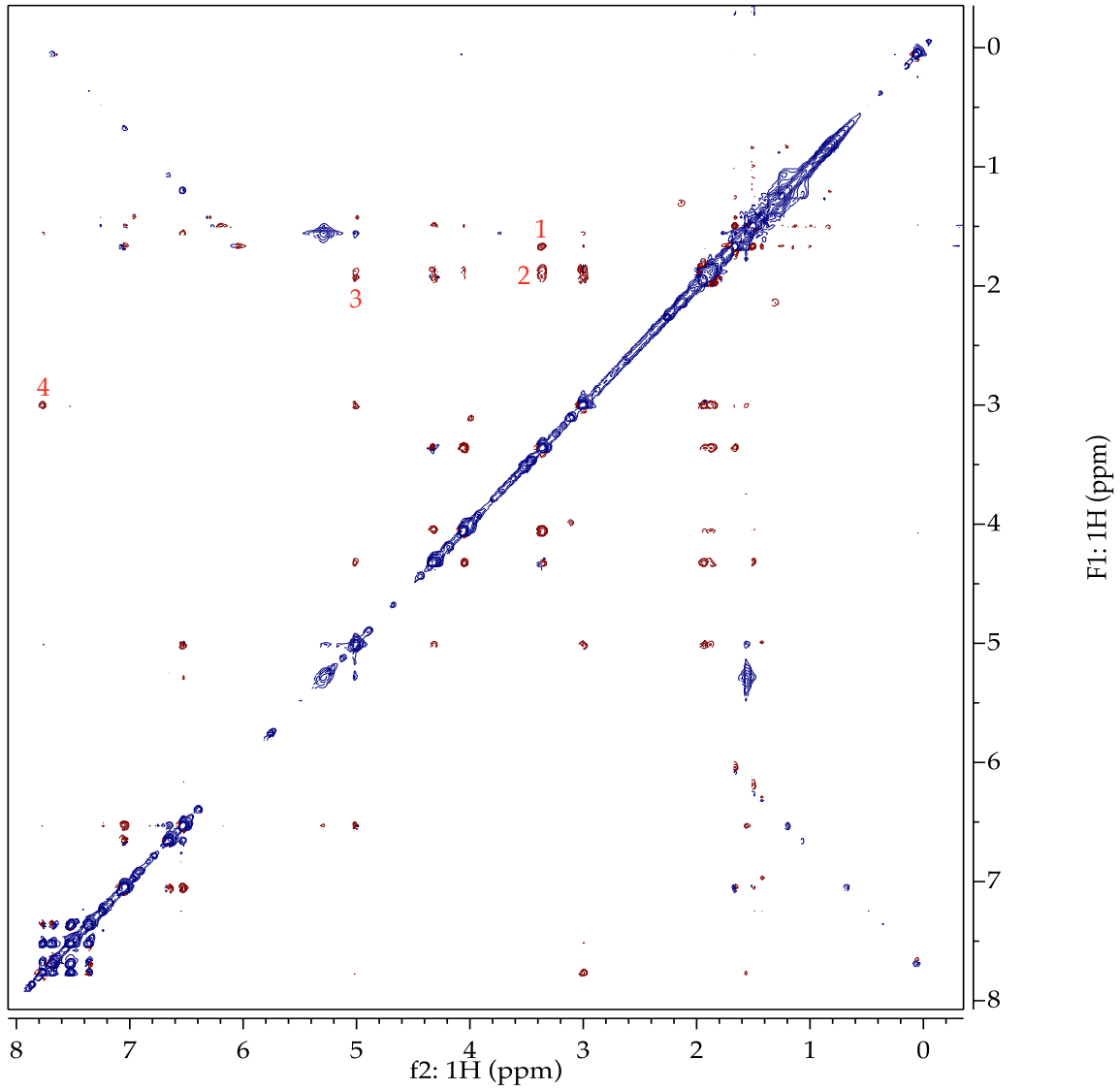
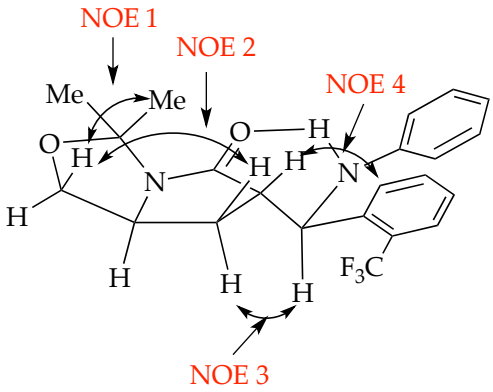



**Figure 15**. $^{1}$H-$^{1}$H NOESY of **6** in $CDCl_3$.



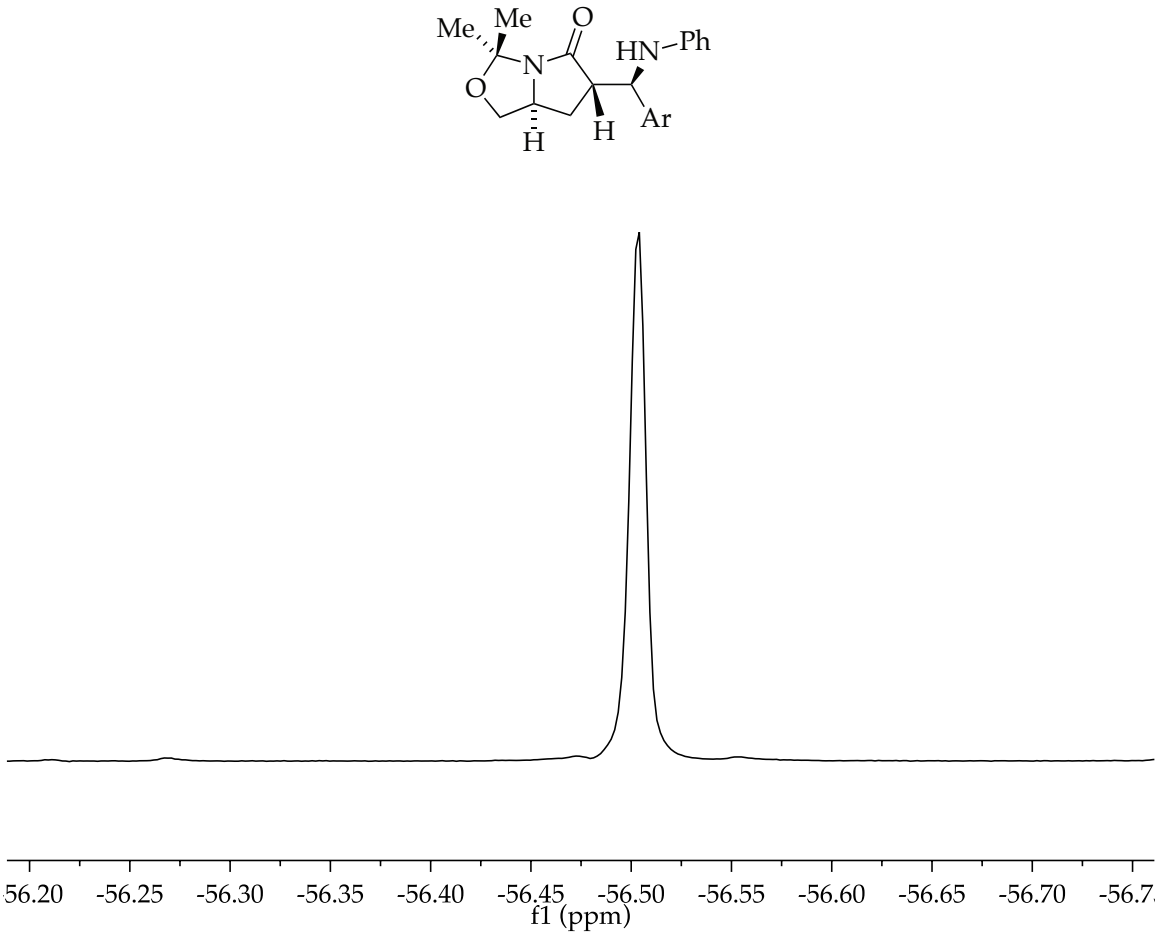



**Figure 16**. $^{19}F$ NMR of **6** in $CDCl_3$.

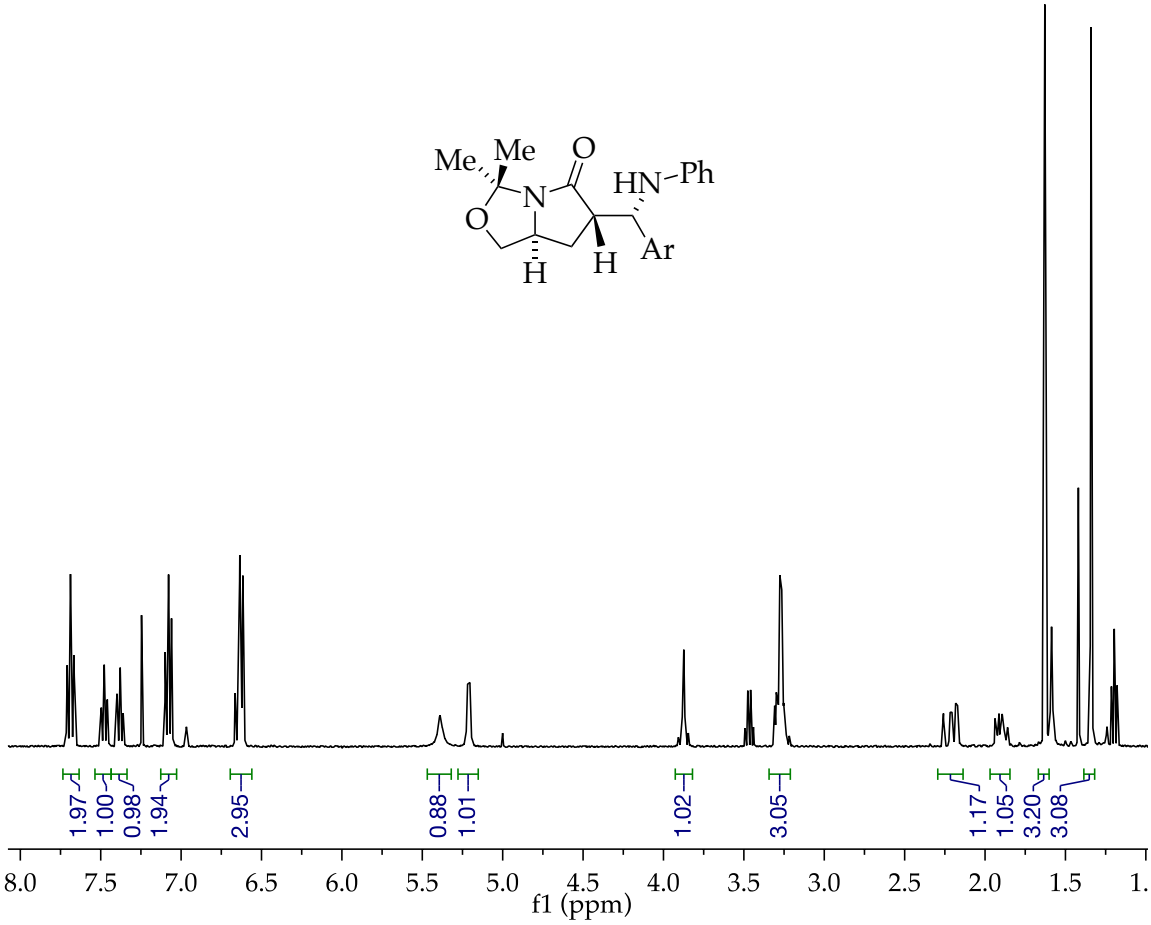



**Figure 17**. $^{1}$H NMR of **4** in $CDCl_3$.

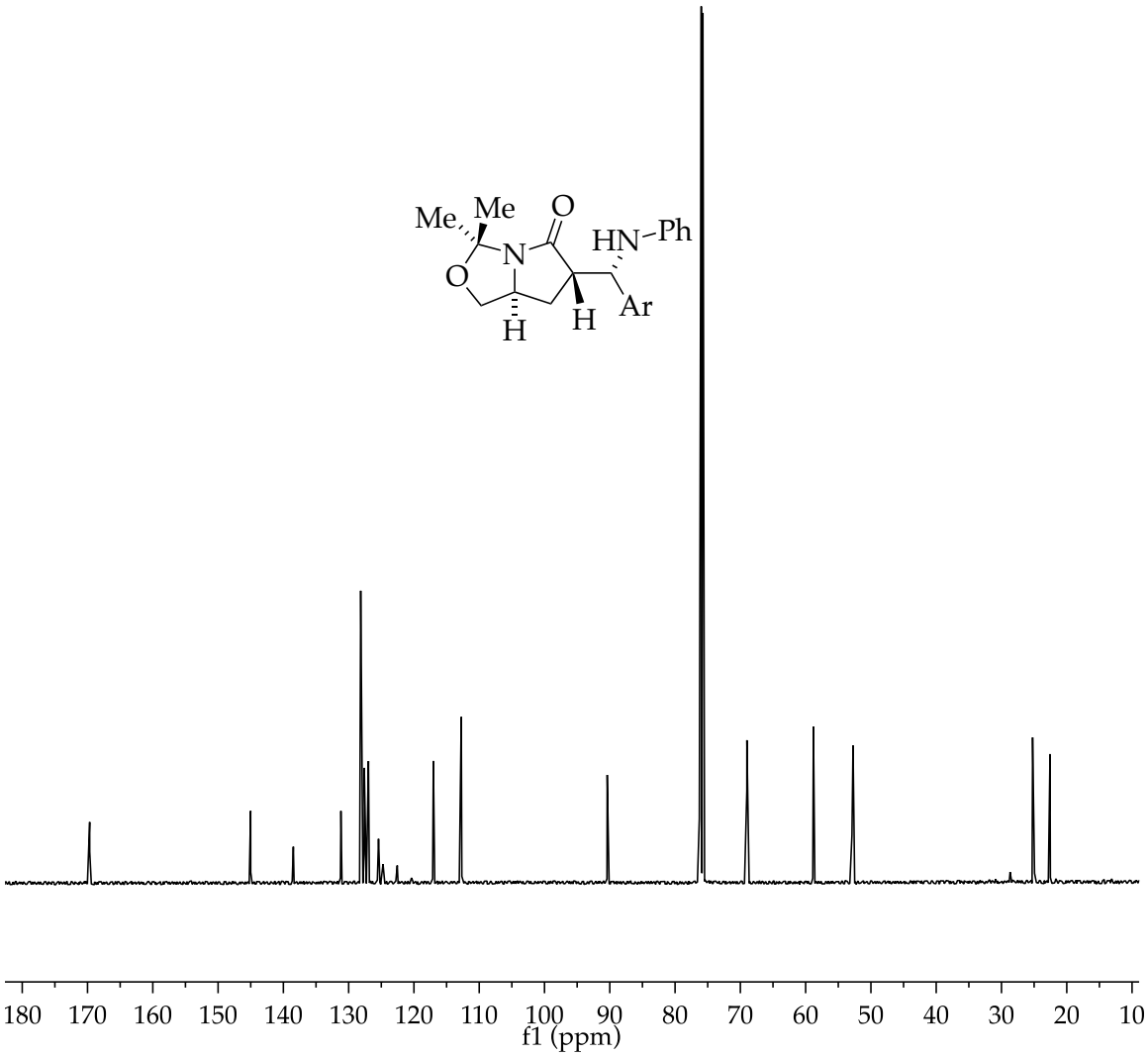



**Figure 18**. $^{13}C$ NMR of **4** in $CDCl_3$.

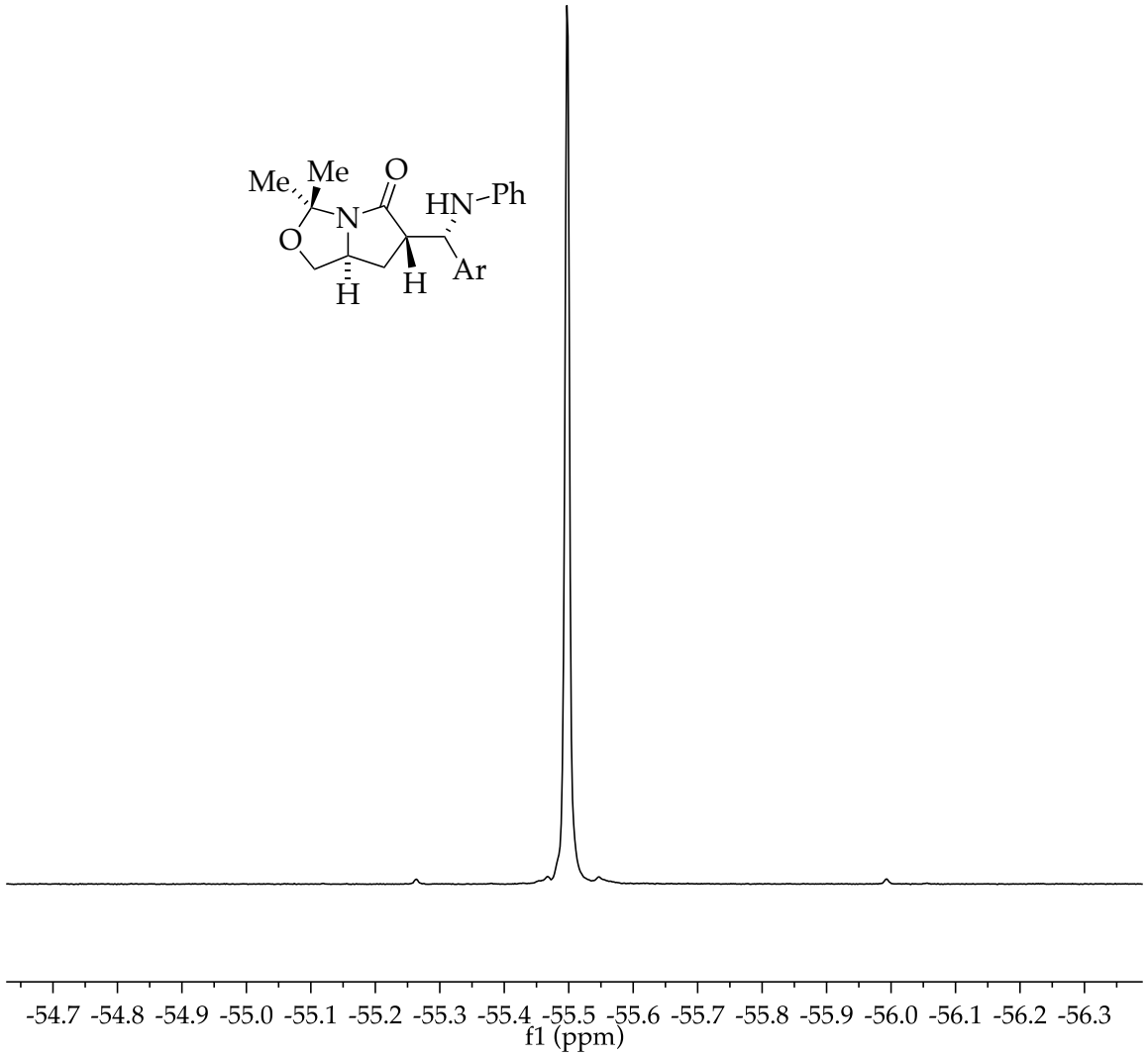



**Figure 19**. $^{19}F$ NMR of **4** in $CDCl_3$.

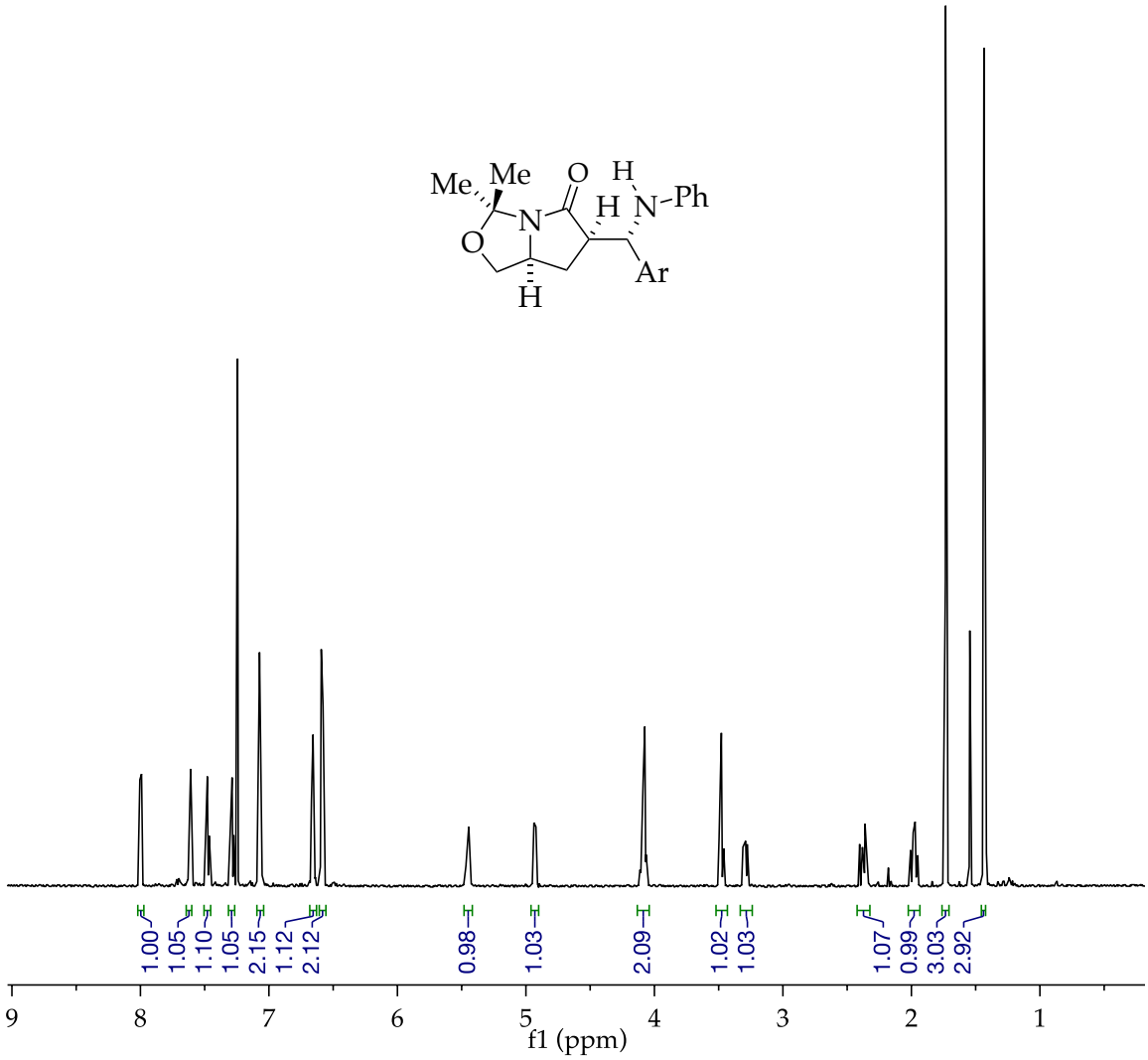



**Figure 20.** $^{1}$H NMR of **7** in $CDCl_3$.

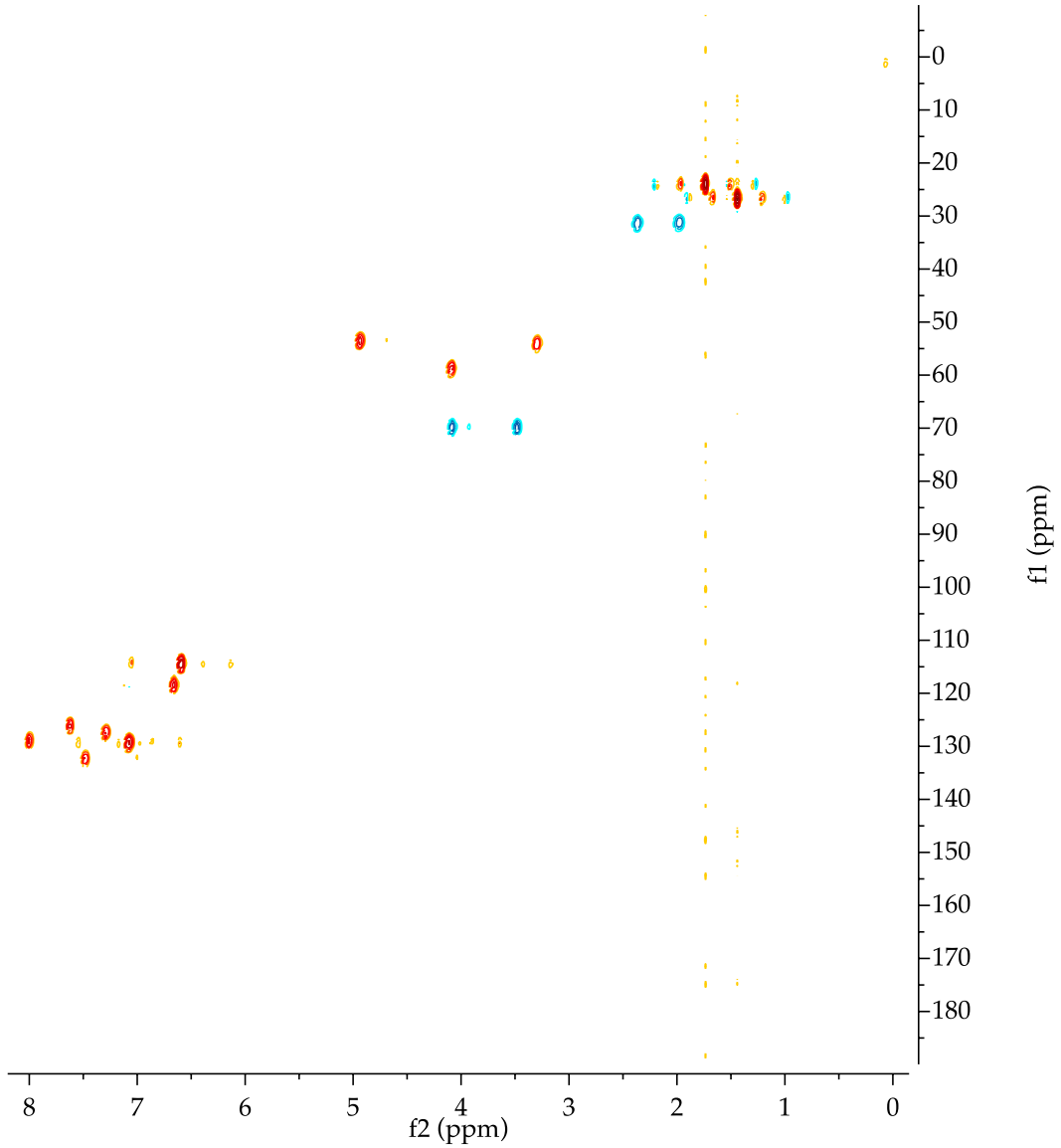



**Figure 21**. $^{1}H$-$^{13}C$ HSQC of **7** in $CDCl_3$.

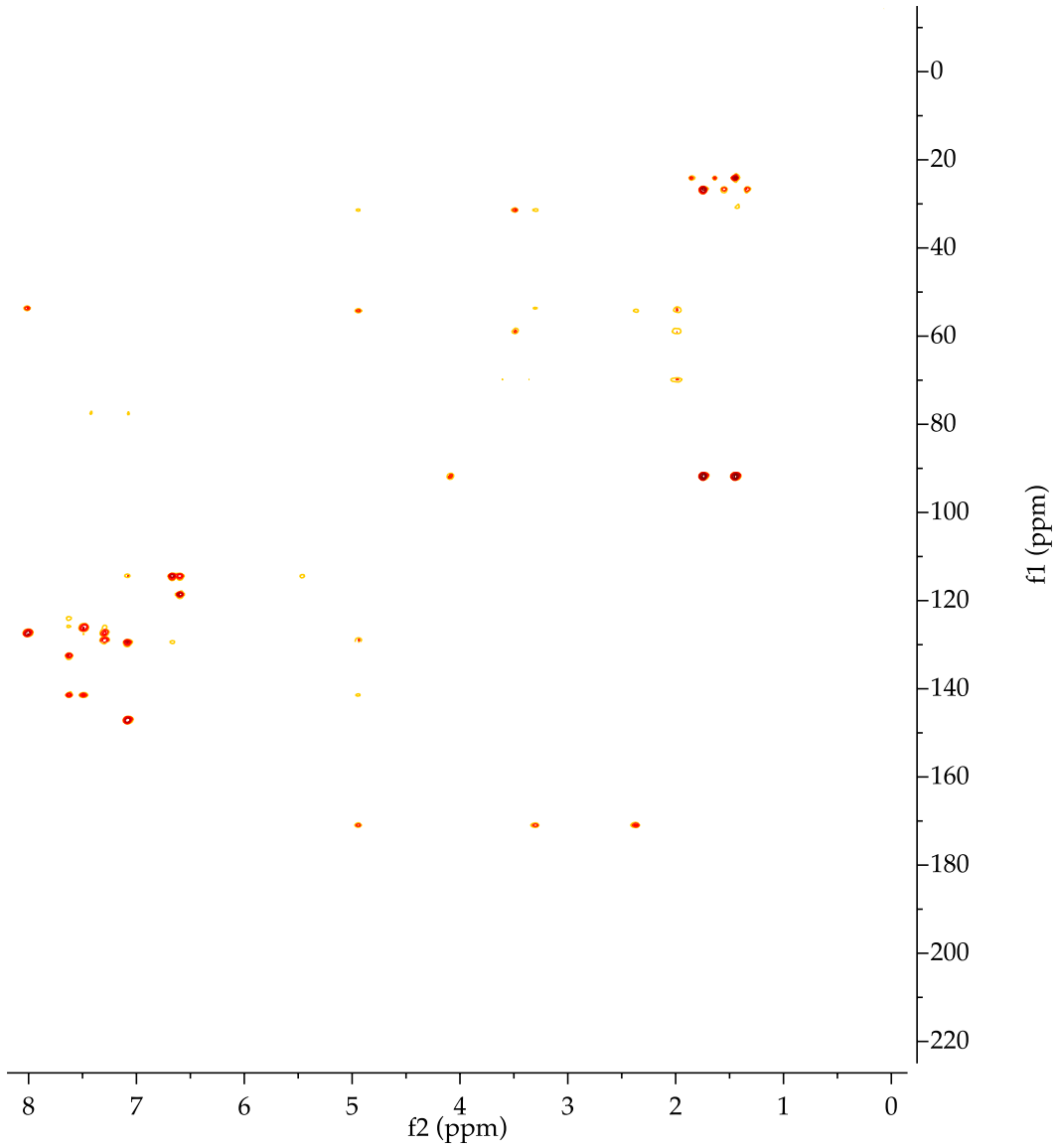



**Figure 22**. $^{1}H$-$^{13}C$ HMBC of **7** in $CDCl_3$.

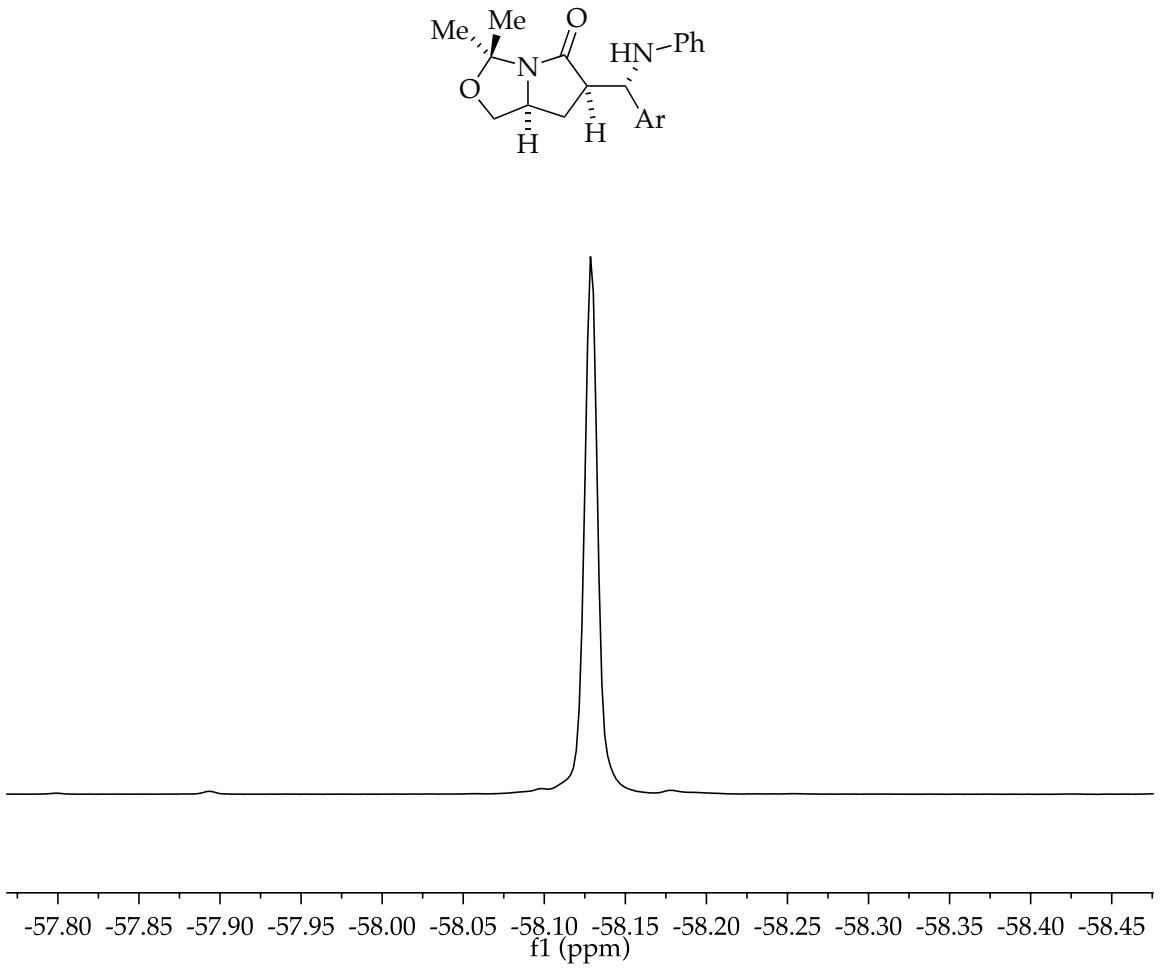



**Figure 23**. $^{19}F$ NMR of **7** in $CDCl_3$.

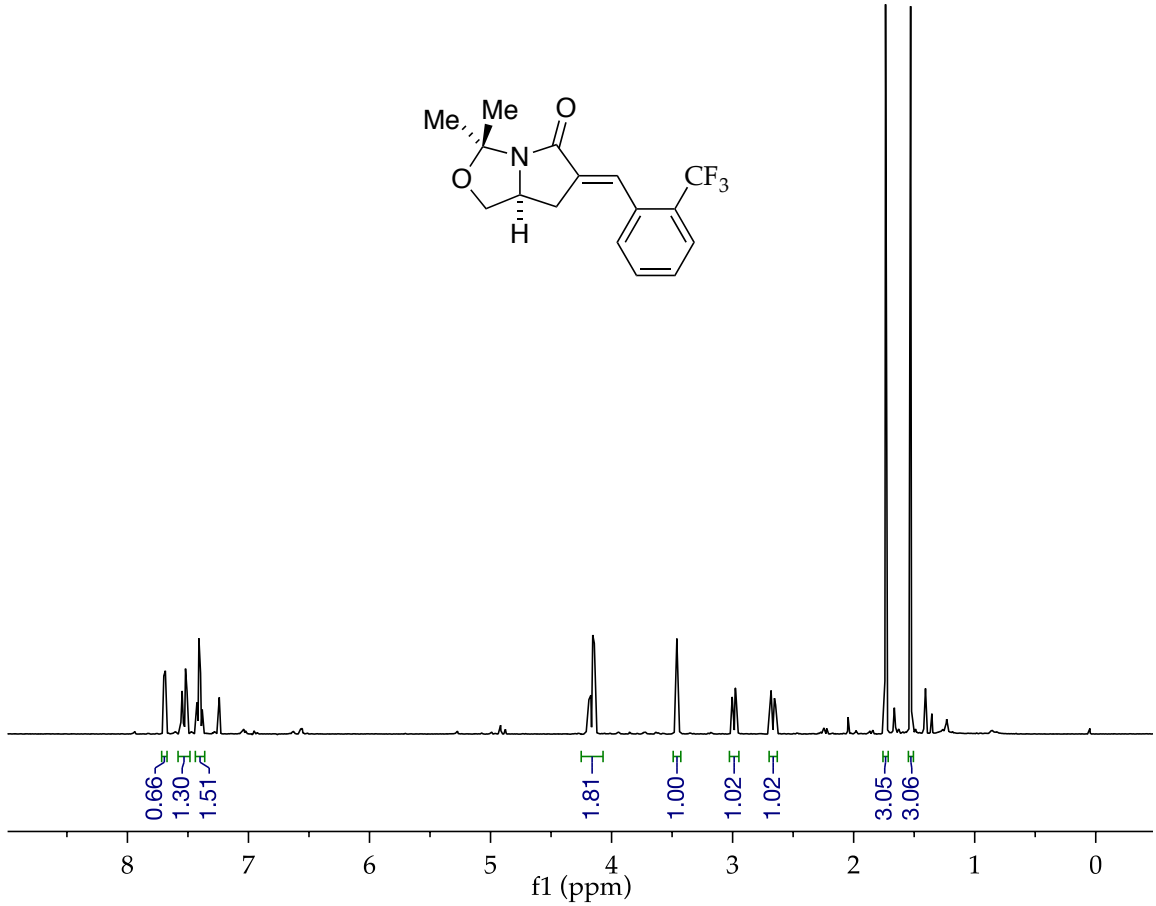



**Figure 24**. $^{1}$H NMR of **15** in $CDCl_3$.

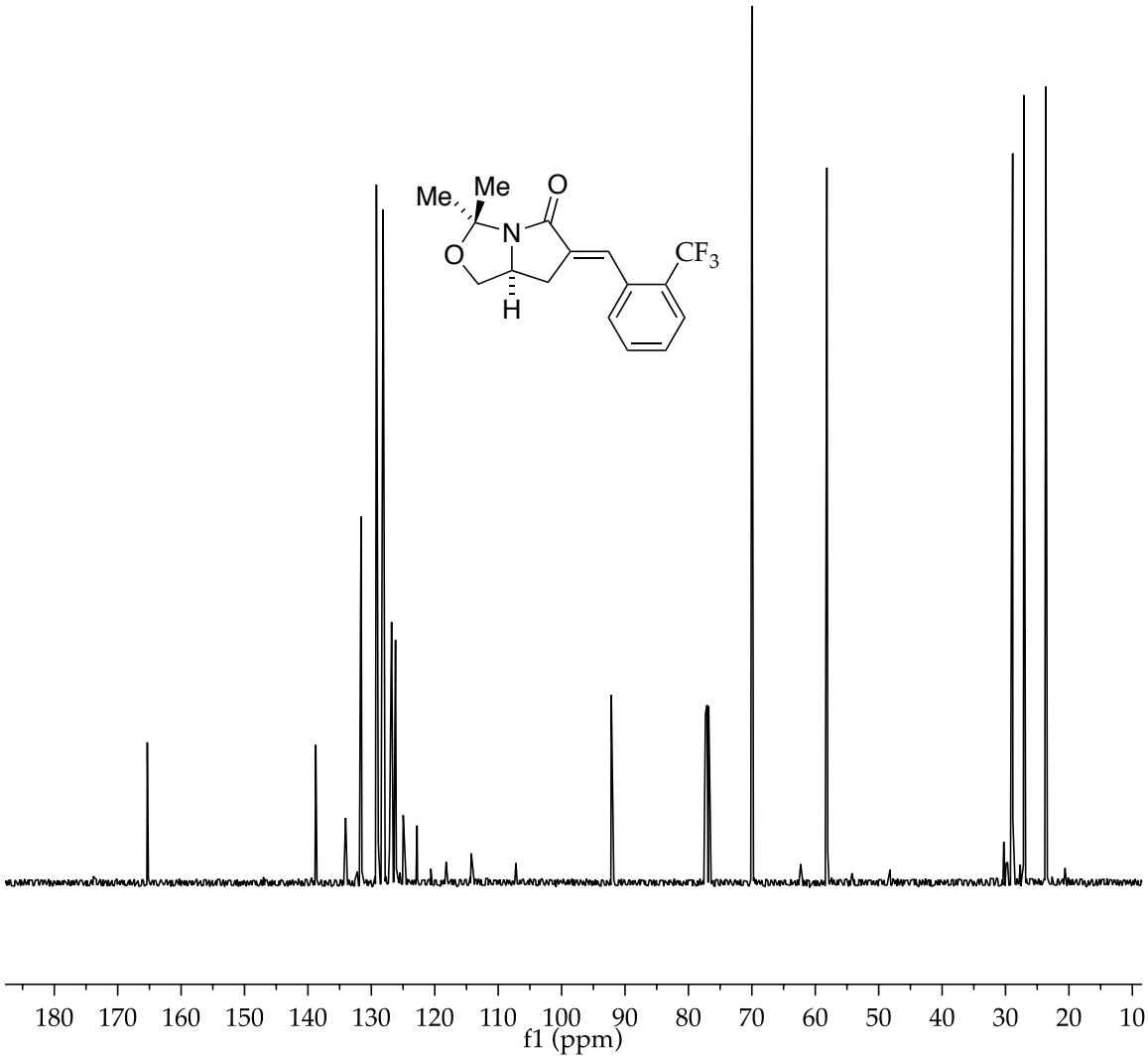



**Figure 25**. $^{13}C$ NMR of **15** in $CDCl_3$.

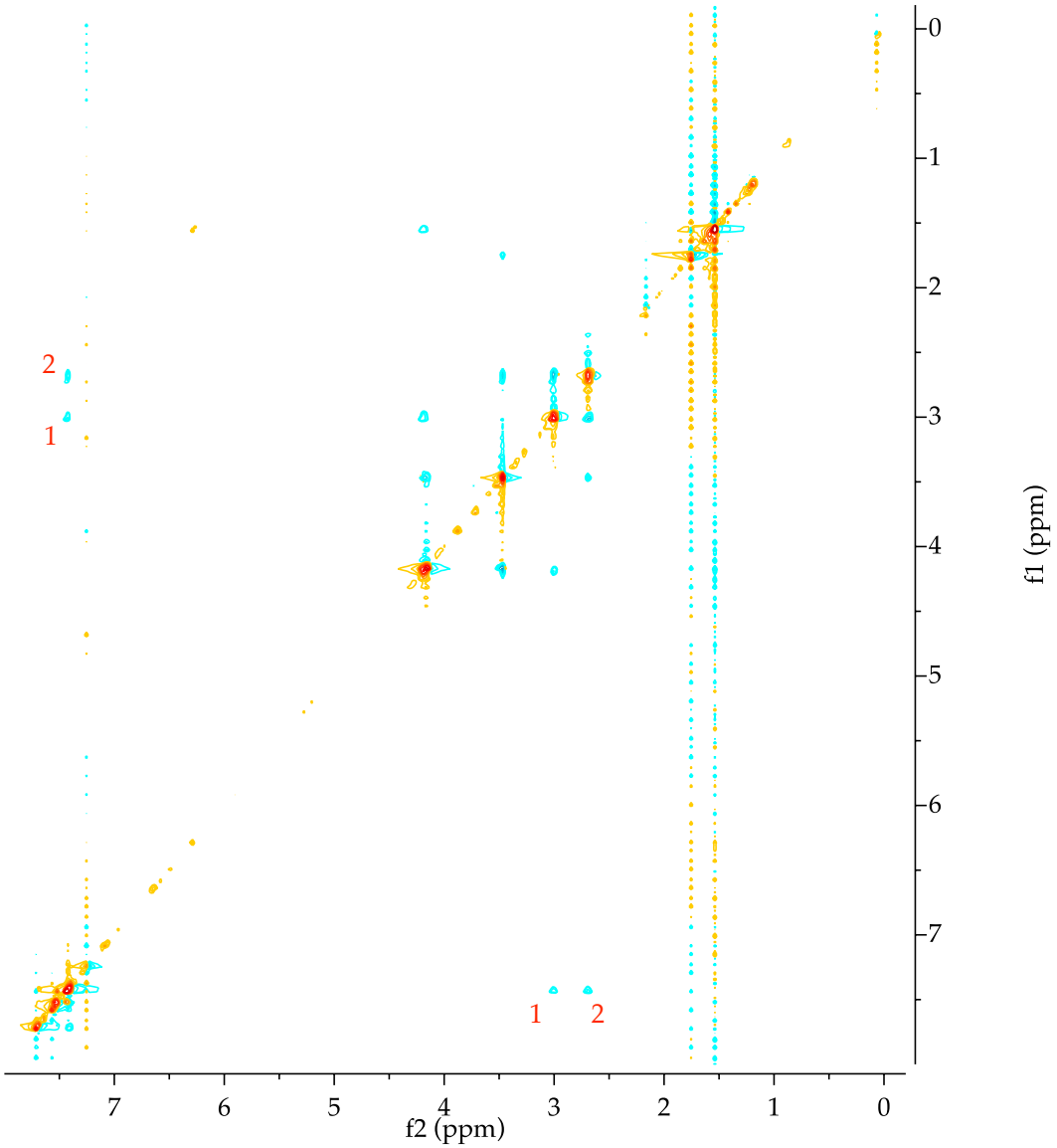
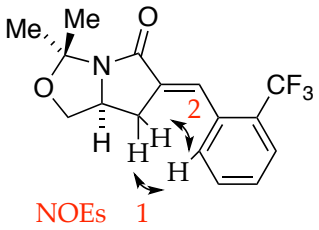



**Figure 26**. $^{1}$H-$^{1}$H NOESY of **15** in $CDCl_3$.



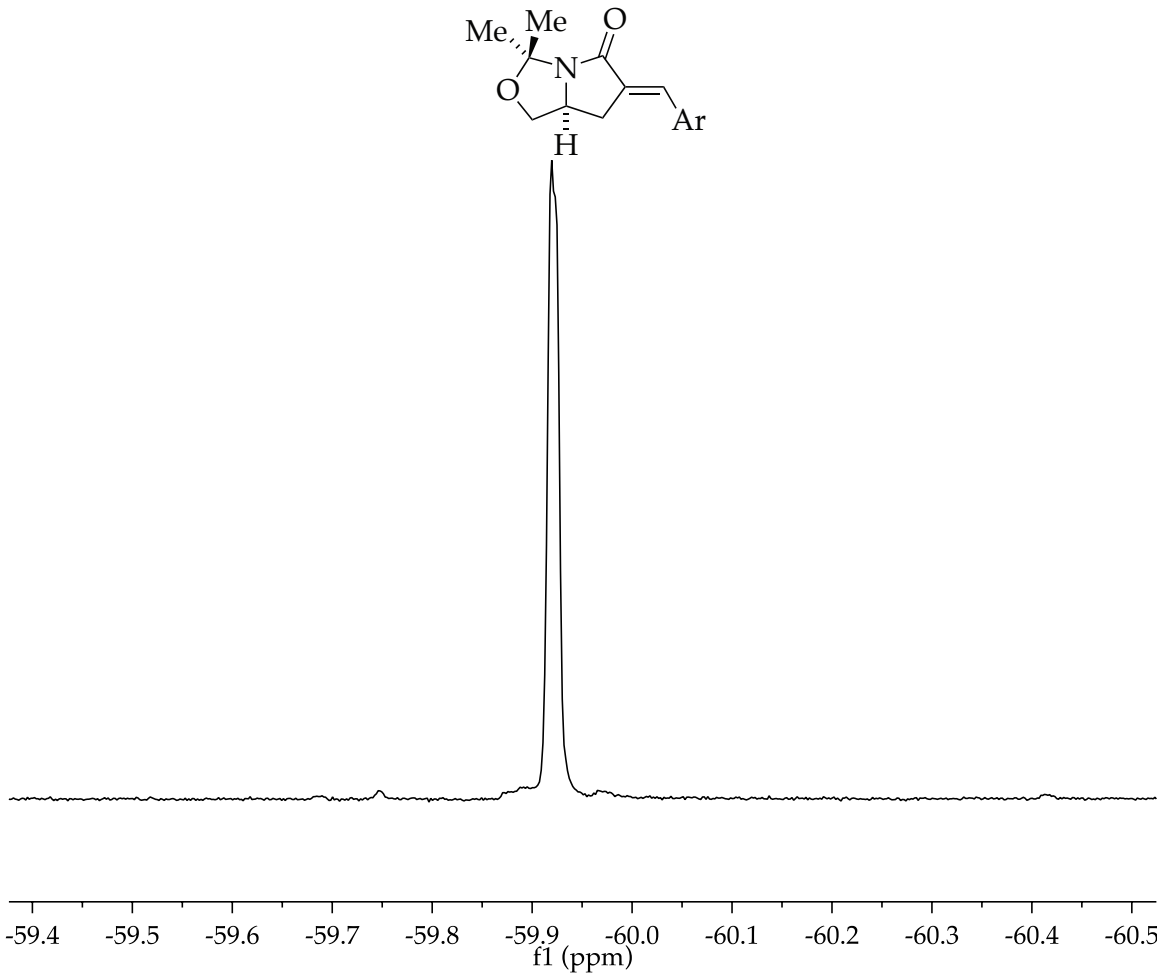



**Figure 27**. $^{19}$F NMR of **15** in $CDCl_3$.

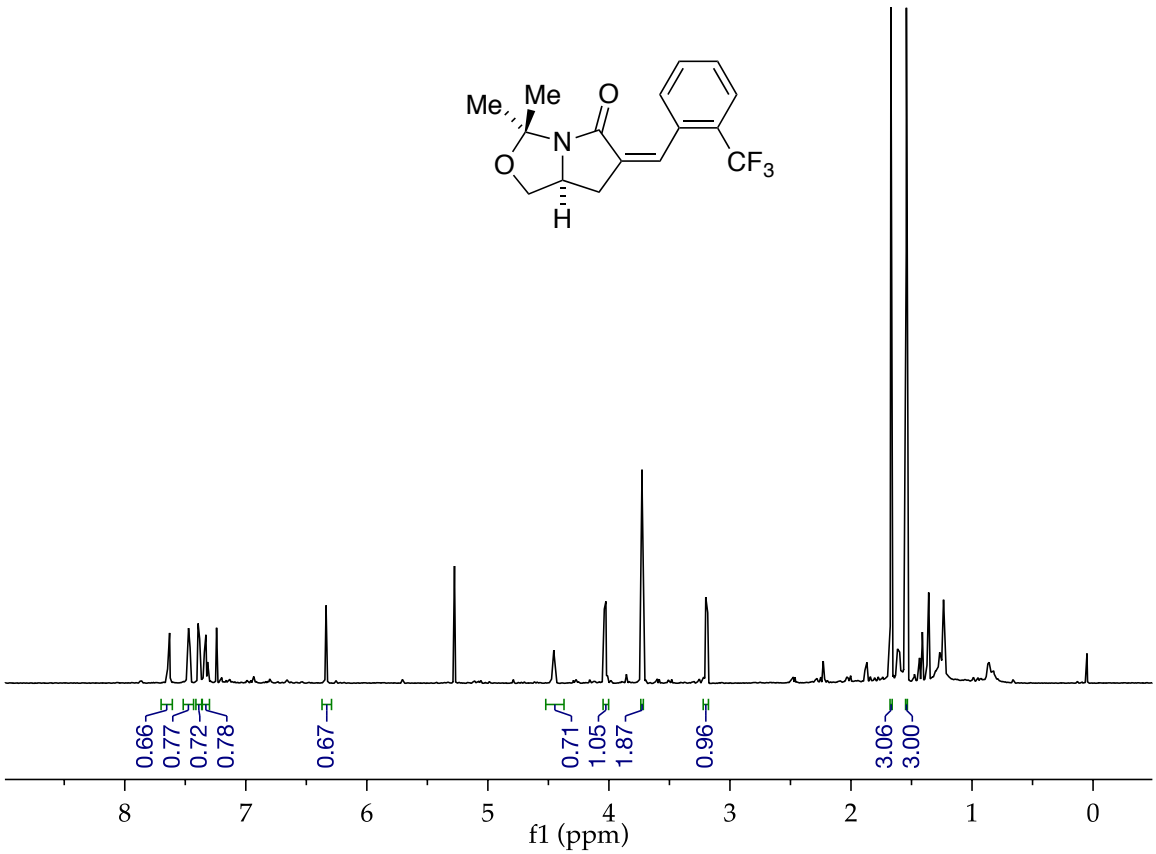



**Figure 28**. $^{1}$H NMR of **16** in $CDCl_3$.

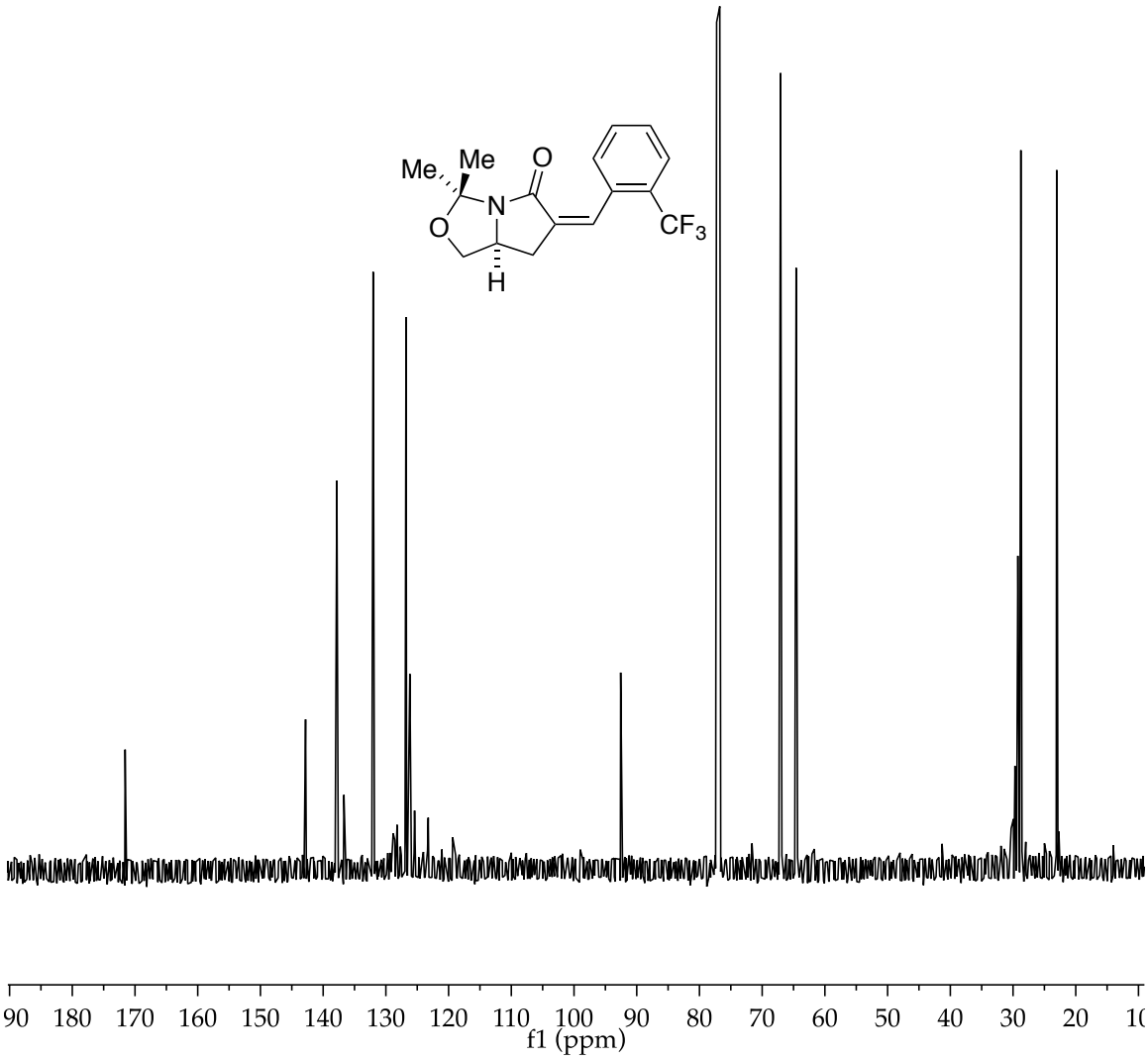



**Figure 29**. $^{13}C$ NMR of **16** in $CDCl_3$.

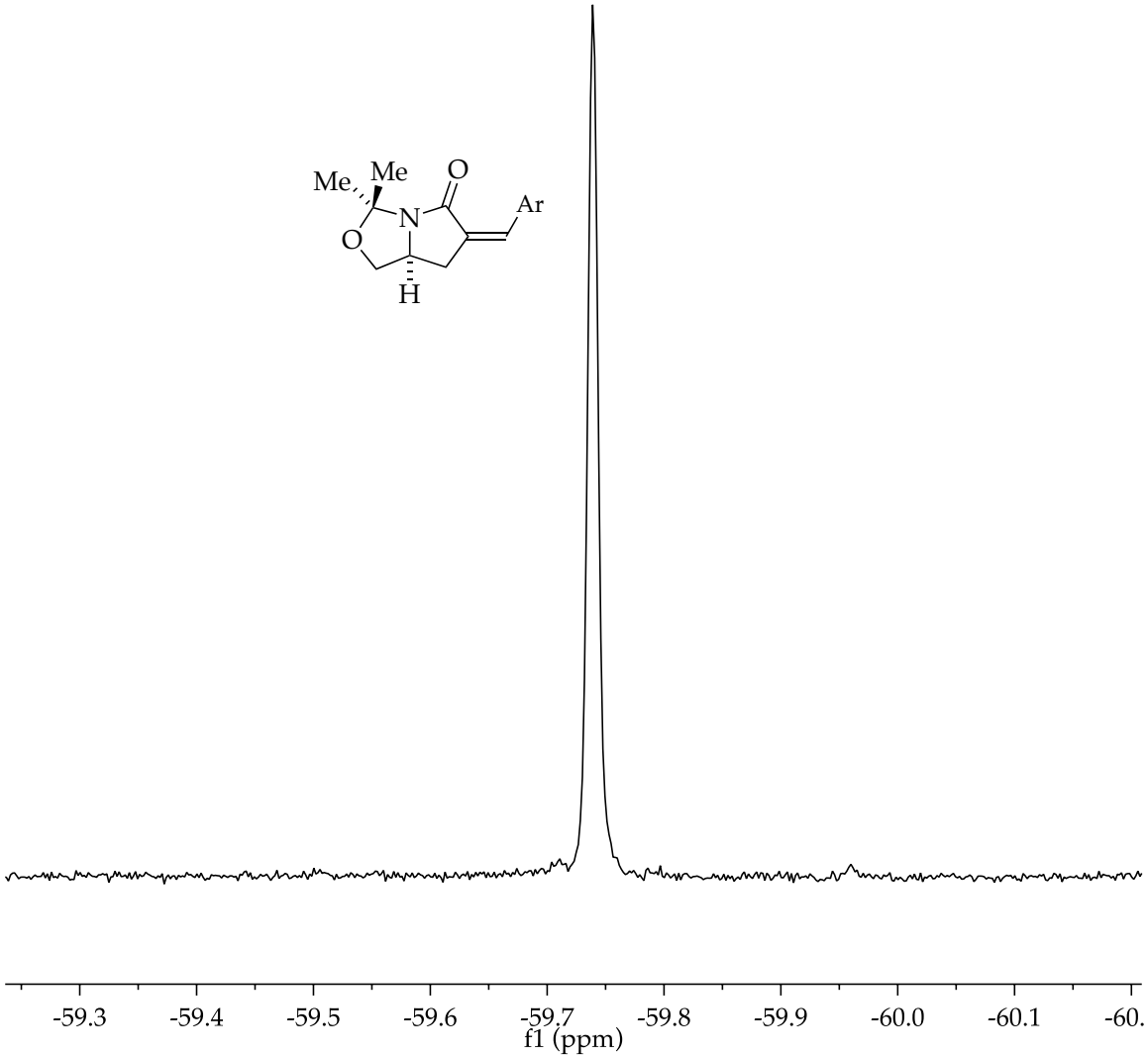



**Figure 30**. $^{19}F$ NMR of **16** in $CDCl_3$.

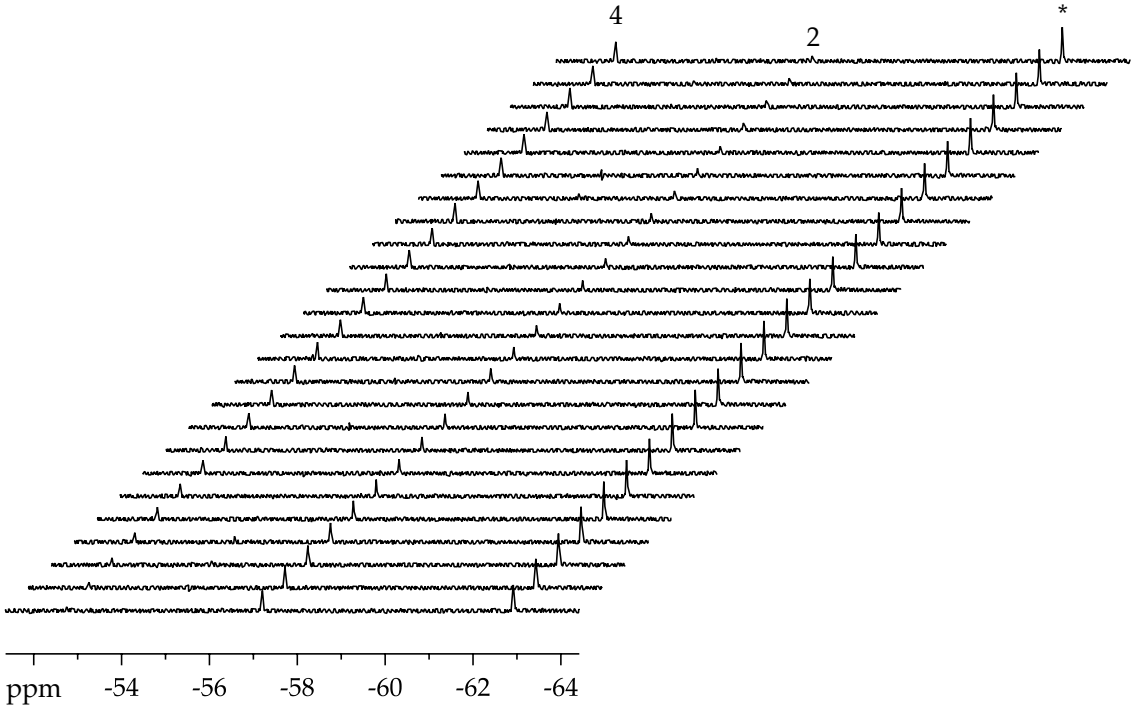



**Figure 31**. Representative $^{19}$F NMR spectra for the condensation of lithium enolate **3** with imine **2** under pseudo-first-order conditions at –70 °C. *α, α, α-trifluorotoluene standard.

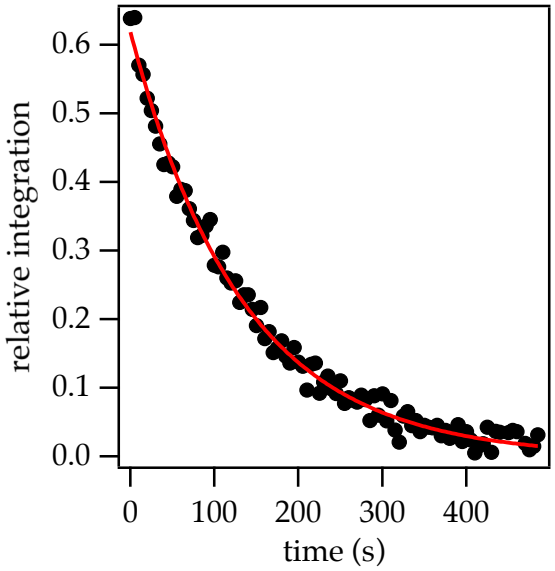



**Figure 32**. Representative curve fitting for the condensation of lithium enolate **3** with imine **2** under pseudo-first-order conditions observed using $^{19}$F NMR spectroscopy.

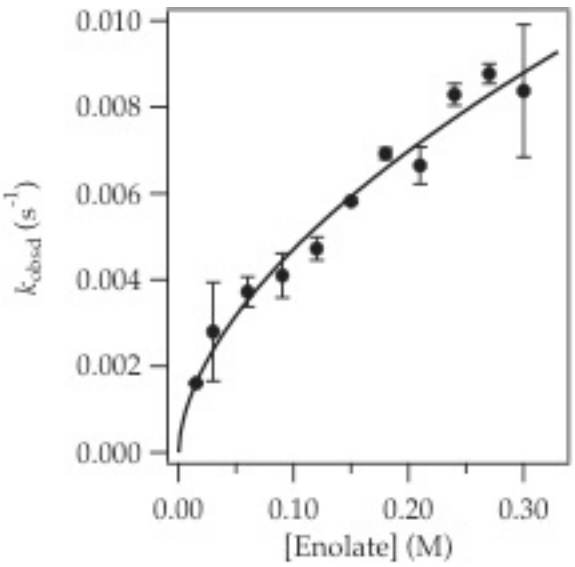



**Figure 33**. Plot of $k_{obsd}$ vs concentration of enolate **3** for the addition of lithium enolate **3** to imine **2** (0.003 M) in 12.3 M THF at –70 °C. The curve depicts an unweighted least-squares fit to $y = k[\mathbf{3}]^n$ [$k = 0.017 \pm 0.001$, $n = 0.57 \pm 0.05$].

| [Enolate] (M) | $k_{obsd}$ 1 x $10^{-3}$ ($s^{-1}$) | $k_{obsd}$ 1 x $10^{-3}$ ($s^{-1}$) |
|---|---|---|
| 0.015 | 1.61 | 0 |
| 0.03 | 3.94 | 1.66 |
| 0.06 | 4.07 | 3.38 |
| 0.09 | 4.62 | 3.59 |
| 0.12 | 5.00 | 4.45 |
| 0.15 | 5.87 | 5.78 |
| 0.18 | 7.04 | 6.80 |
| 0.21 | 7.08 | 6.22 |
| 0.24 | 8.55 | 8.04 |
| 0.27 | 9.01 | 8.55 |
| 0.30 | 9.91 | 6.84 |

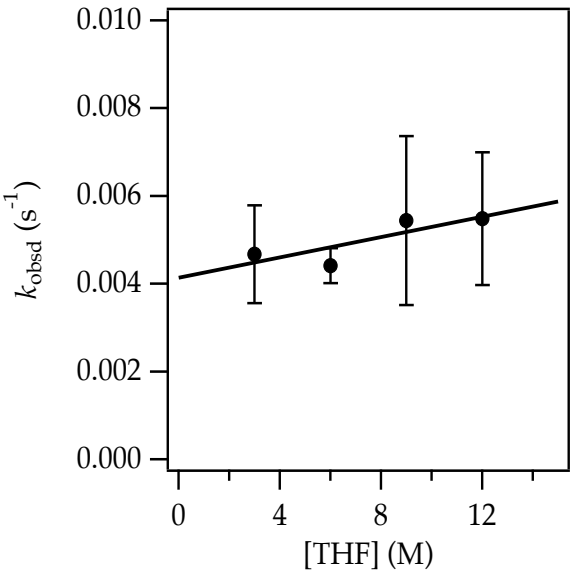



**Figure 34**. Plot of $k_{obsd}$ vs THF concentration (M) in toluene cosolvent for the addition of lithium enolate **3** (0.10 M) to imine **2** (0.005 M) at –70 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k + k'[THF]$ [$k = (4.1 \pm 0.5) \times 10^{-3}$, $k' = (1.2 \pm 0.6) \times 10^{-4}$].

| [THF] (M) | $k_{obsd}$ 1 x $10^{-3}$ ($s^{-1}$) | $k_{obsd}$ 1 x $10^{-3}$ ($s^{-1}$) |
|---|---|---|
| 3.0 | 5.79 | 3.60 |
| 6.0 | 4.81 | 4.02 |
| 9.0 | 7.37 | 3.51 |
| 12.3 | 7.00 | 3.98 |

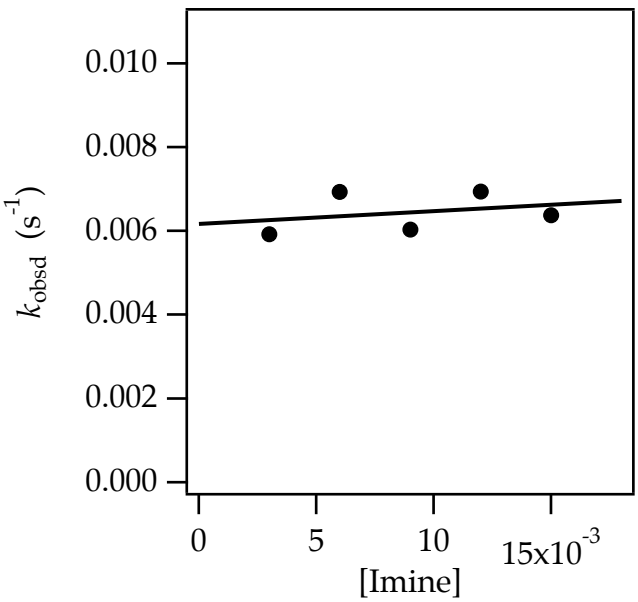



**Figure 35**. Plot of $k_{obsd}$ vs imine concentration (M) in THF for the addition of lithium enolate **3** (0.20 M) to imine **2** at –70 °C. The curve depicts an unweighted least-squares fit to $k_{obsd} = k + k'$[imine] [$k = (6.2 \pm 0.6) \times 10^{-3}$, $k' = (3.1 \pm 0.6) \times 10^{-2}$].

| [Imine] (M) | $k_{obsd}$ 1 x $10^{-3}$ ($s^{-1}$) |
|---|---|
| 0.003 | 5.92 |
| 0.006 | 6.93 |
| 0.009 | 6.03 |
| 0.012 | 6.94 |
| 0.015 | 6.38 |

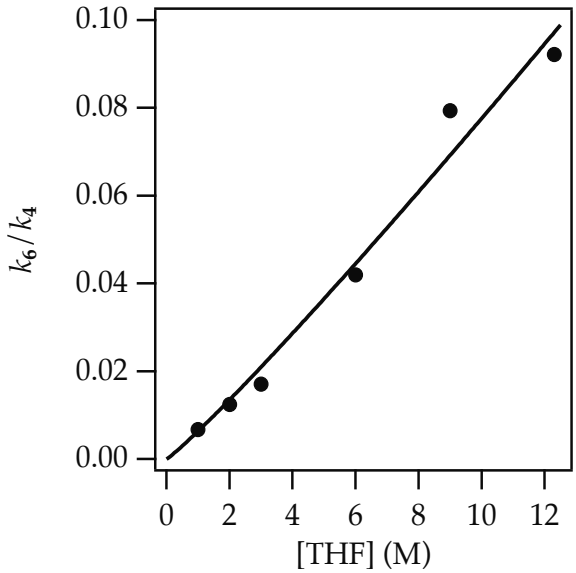



**Figure 36**. Plot of $k_6/k_4$ vs tetrahydrofuran (THF) concentration (M) as determined by carrying out the addition of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –78 °C and monitoring the proportions of **6** and **4** in quenched aliquots with $^{19}$F NMR spectroscopy. The curve depicts an unweighted least-squares fit to $y = k[\text{THF}]^n$ [$k = (6.4 \pm 2.0) \times 10^{-3}$, $n = 1.09 \pm 0.13$]

| [THF] (M) | $k_6/k_4$ |
|---|---|
| 1.0 | 0.007 |
| 2.0 | 0.013 |
| 3.0 | 0.017 |
| 6.0 | 0.042 |
| 9.0 | 0.077 |
| 12.3 | 0.091 |

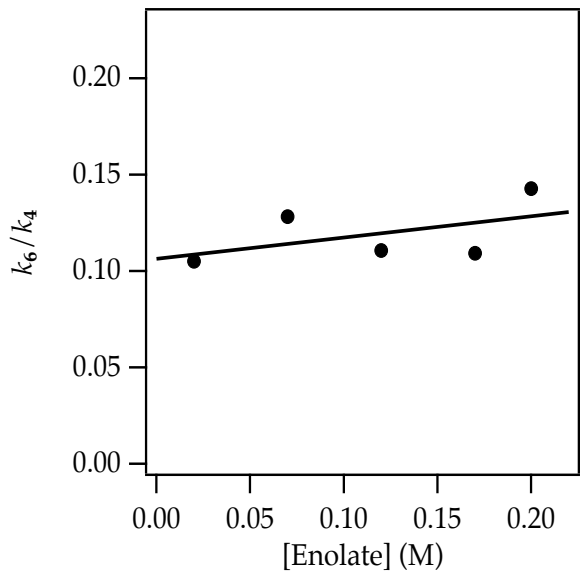



**Figure 37**. Plot of $k_6/k_4$ vs enolate concentration (M) as determined by carrying out the addition of lithium enolate **3** with imine **2** in a fixed ratio at –78 °C in 12.3 M THF and monitoring the proportions of **6** and **4** in quenched aliquots with $^{19}$F NMR spectroscopy. The curve depicts an unweighted least-squares fit to $k_6/k_4 = k + k'$[enolate] [$k = (1.1 \pm 0.1) \times 10^{-1}$, $k' = (1.1 \pm 0.1) \times 10^{-1}$].

| [Enolate] (M) | $k_6/k_4$ |
|---|---|
| 0.02 | 0.103 |
| 0.07 | 0.126 |
| 0.12 | 0.107 |
| 0.17 | 0.106 |
| 0.20 | 0.142 |

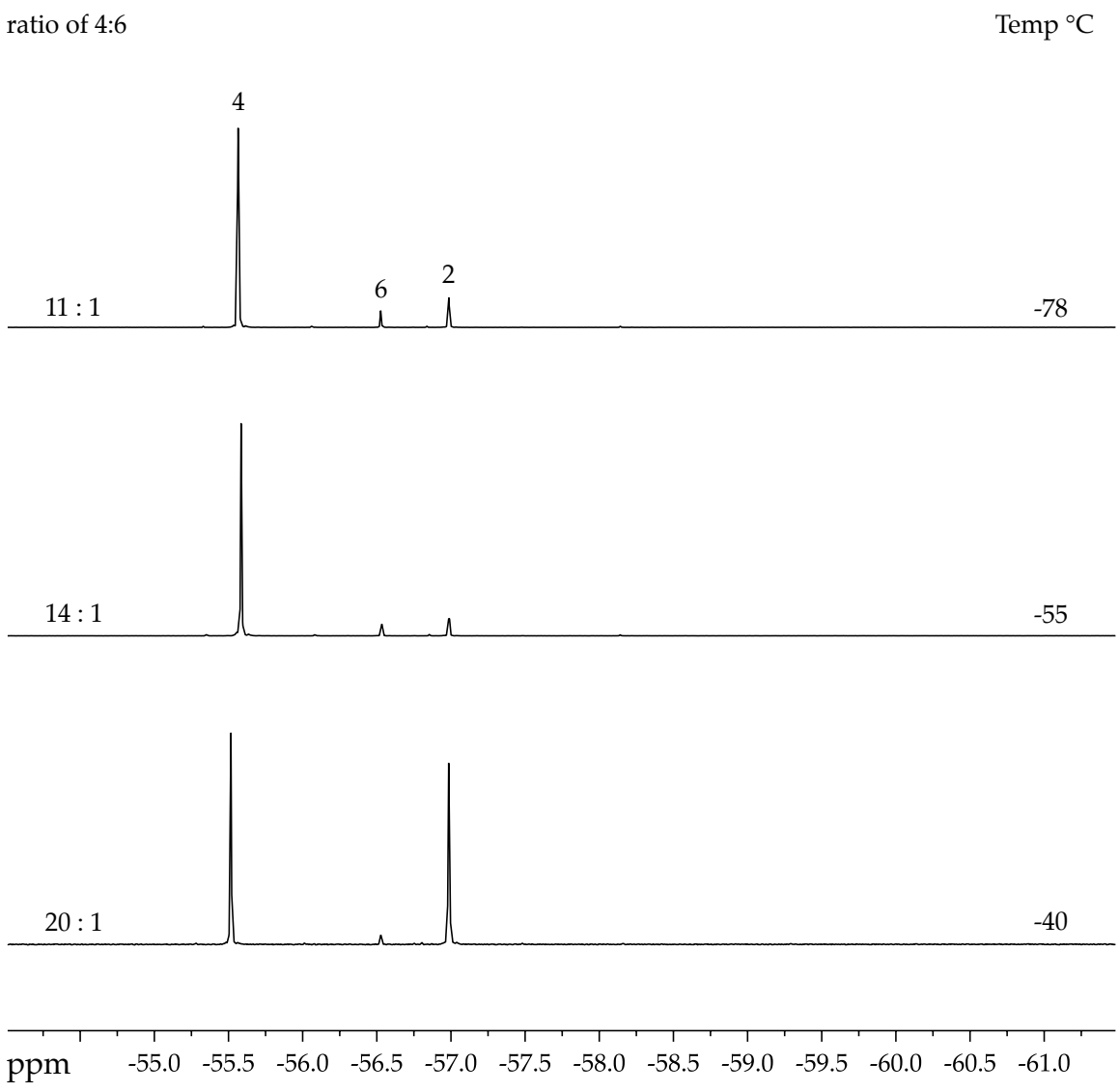



**Figure 38**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) in 12.3 M THF conducted at various temperatures.

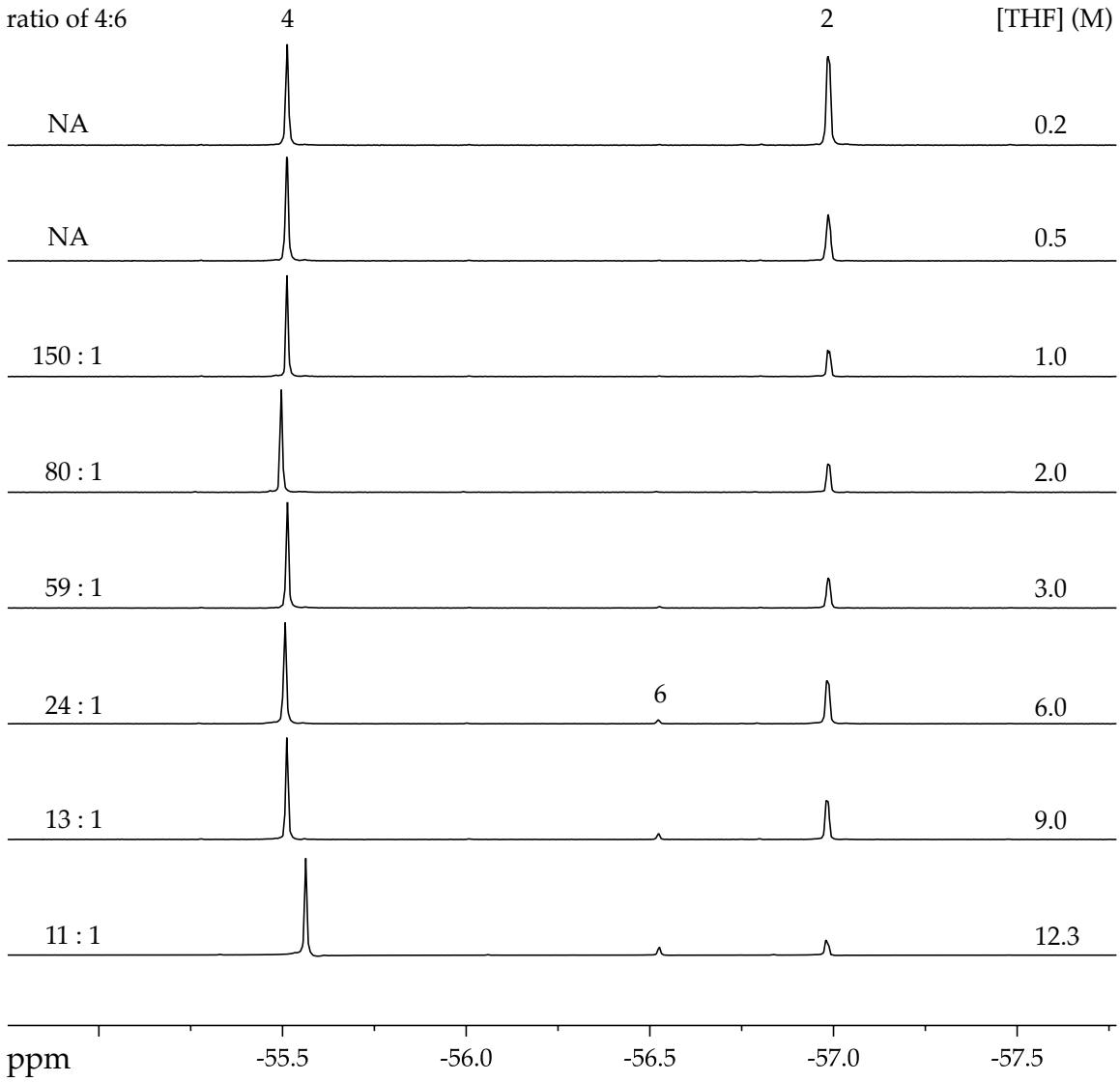



**Figure 39**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –78 °C with varying THF concentration.

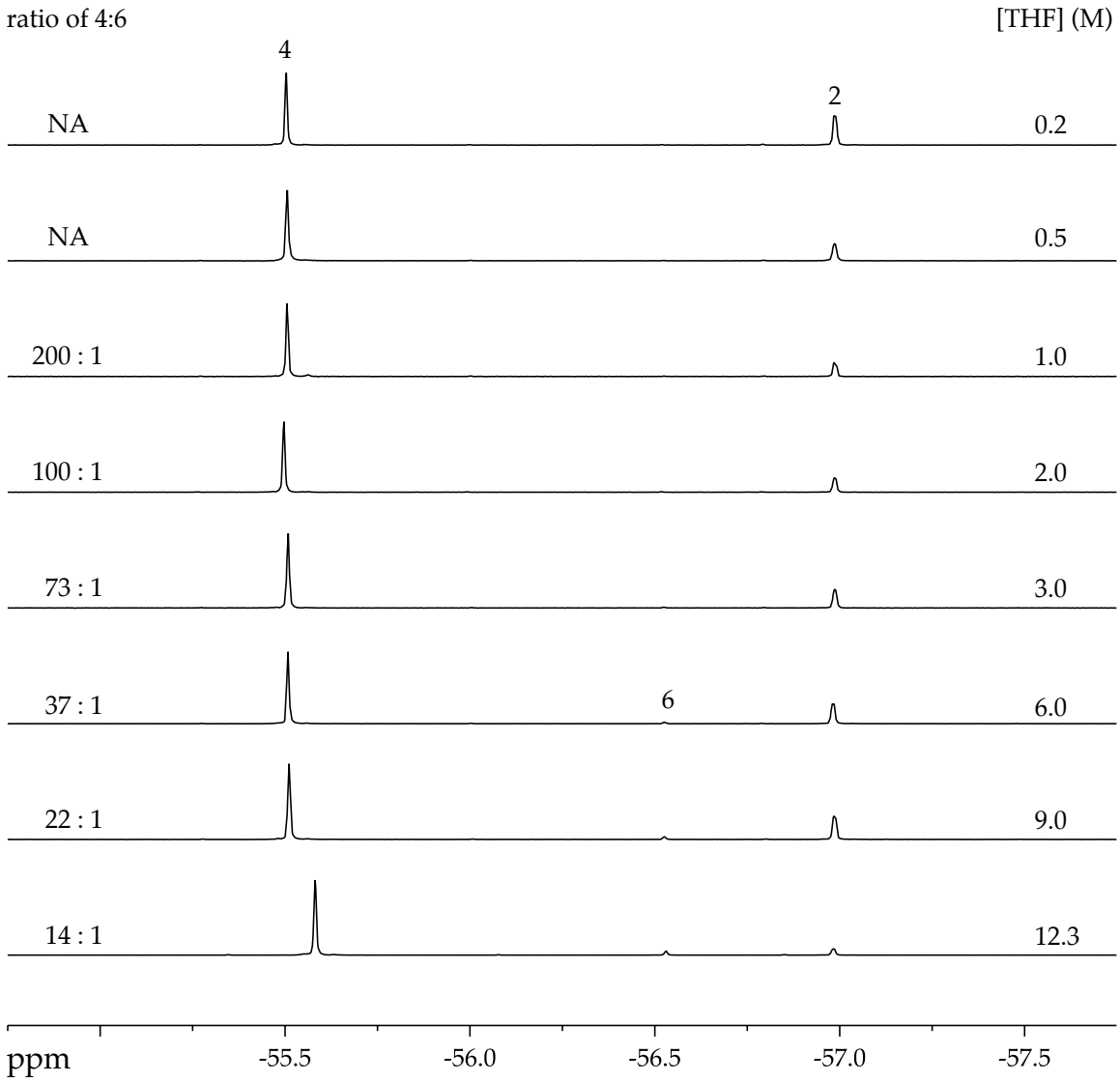



**Figure 40**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –55 °C with varying THF concentration.

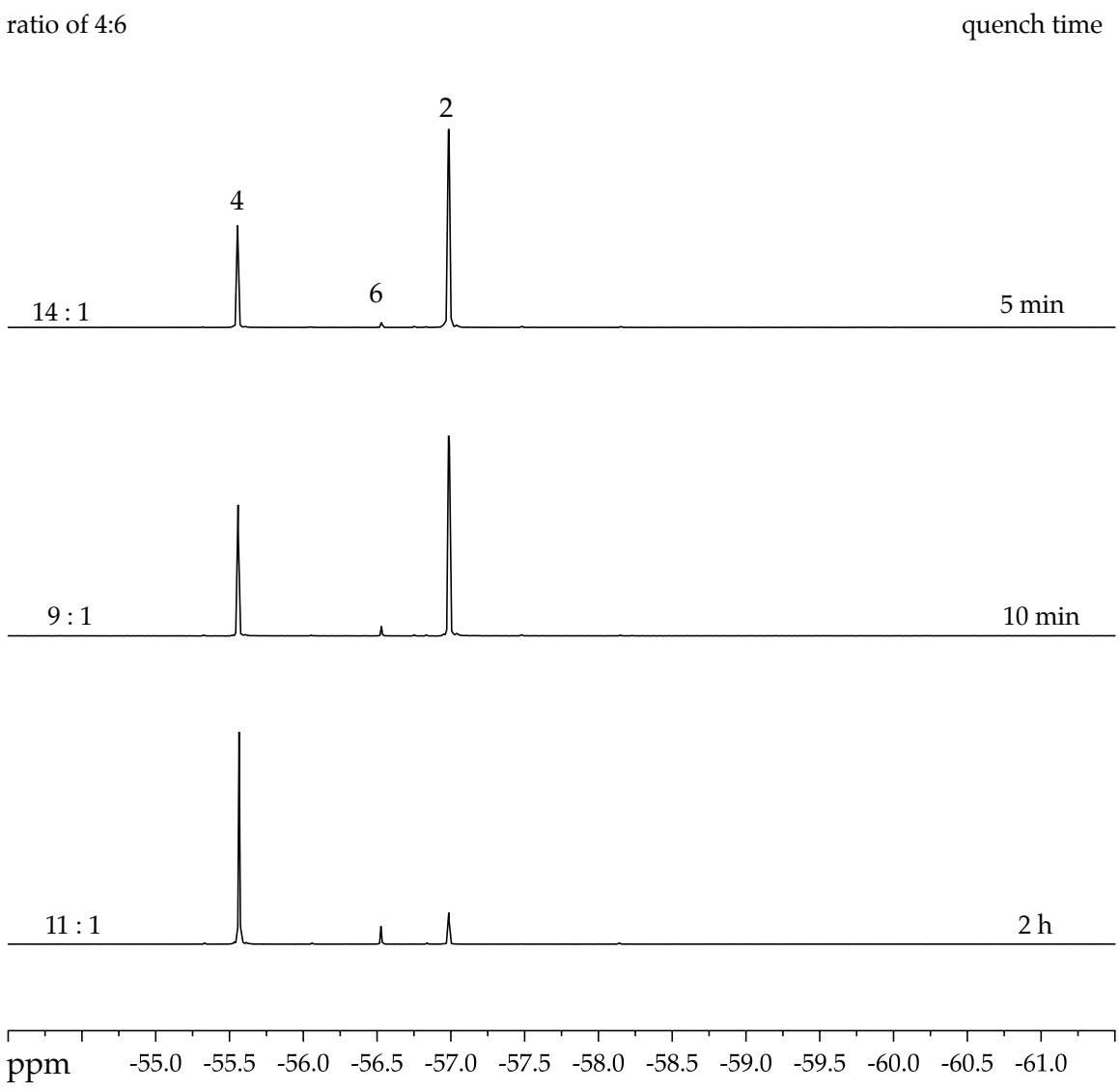



**Figure 41**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –78 °C in 12.3 M THF with quenching at different % conversions throughout the reaction.

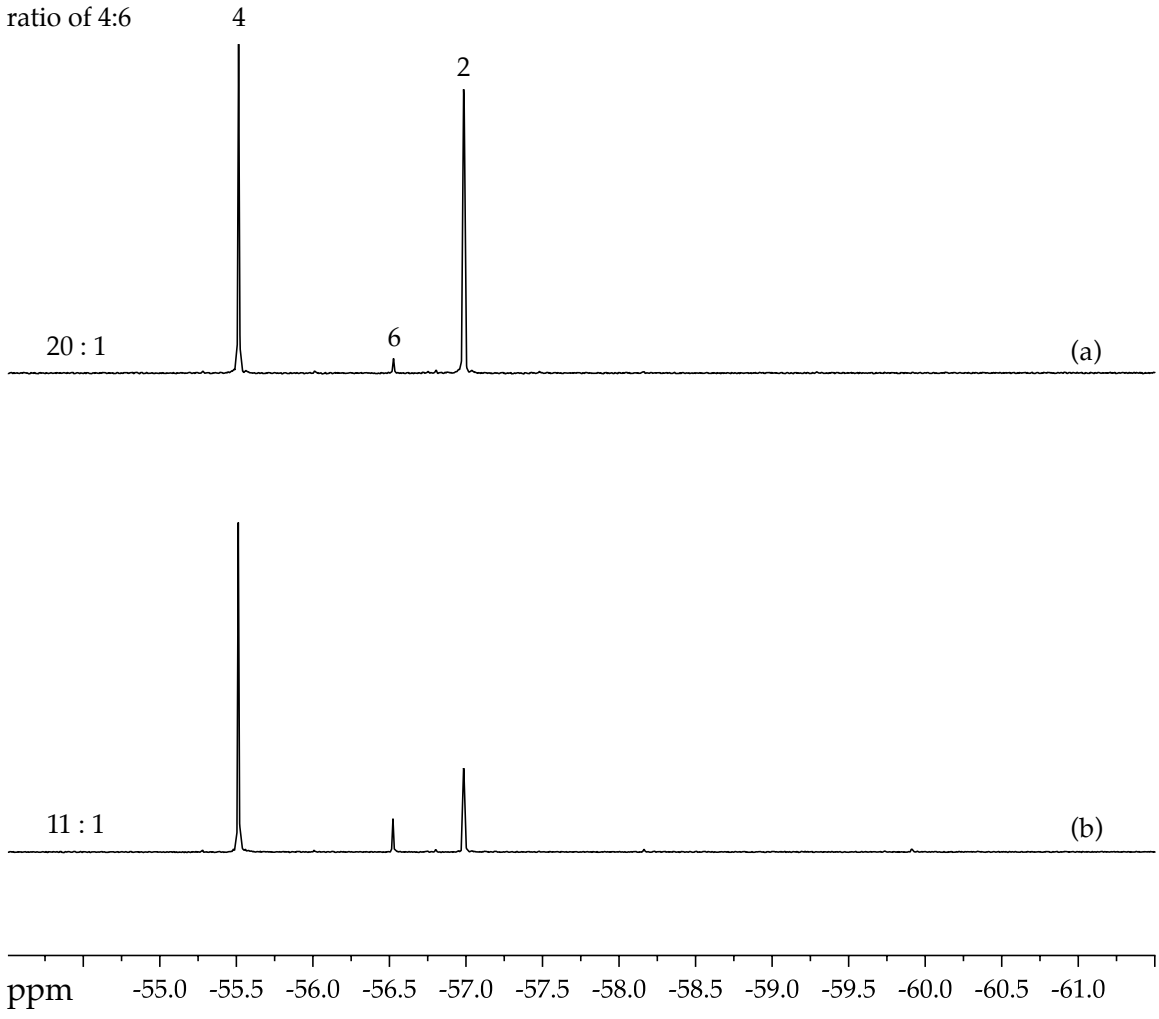



**Figure 42**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) in 12.3 M THF. The top spectrum (a) shows the product ratio for the reaction conducted at –40 °C and the bottom spectrum (b) shows the product ratio for the reaction conducted at –78 °C and then warmed to –40 °C for 1 hour before quenching.

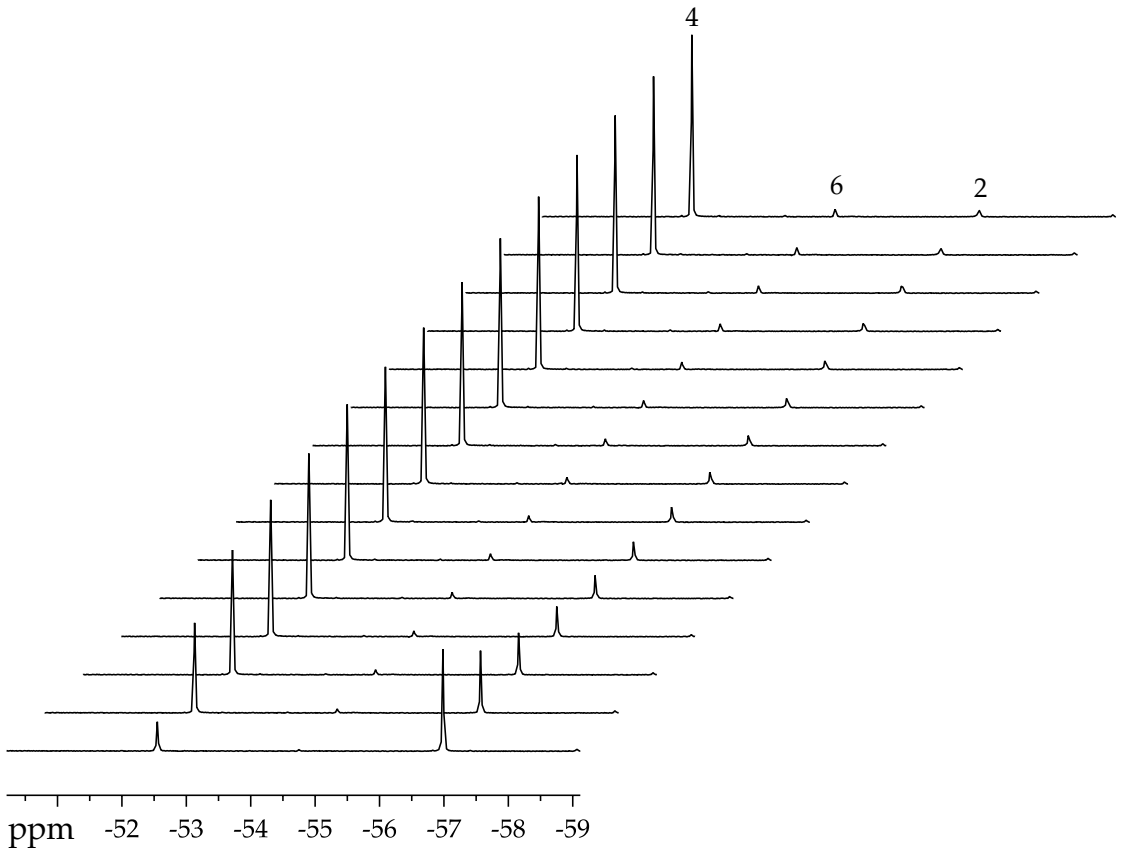



**Figure 43**. $^{19}$F NMR spectroscopy following the **4**:**6** product ratio *in situ* from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –55 °C in 12.3 M THF demonstrating the product ratios do not change during the reaction.

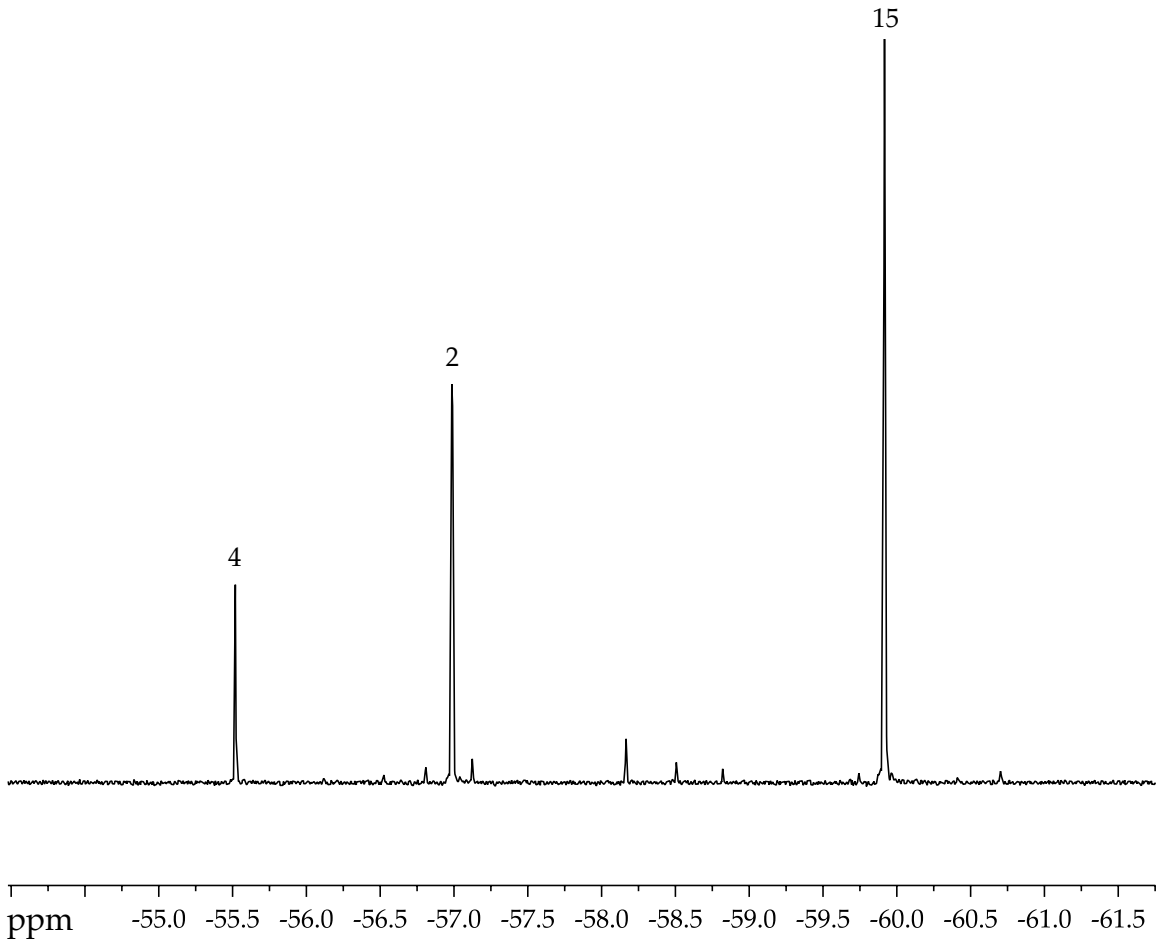



**Figure 44**. Crude $^{19}$F spectrum from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –55 °C in 0.15 M THF and run for 4 hours.

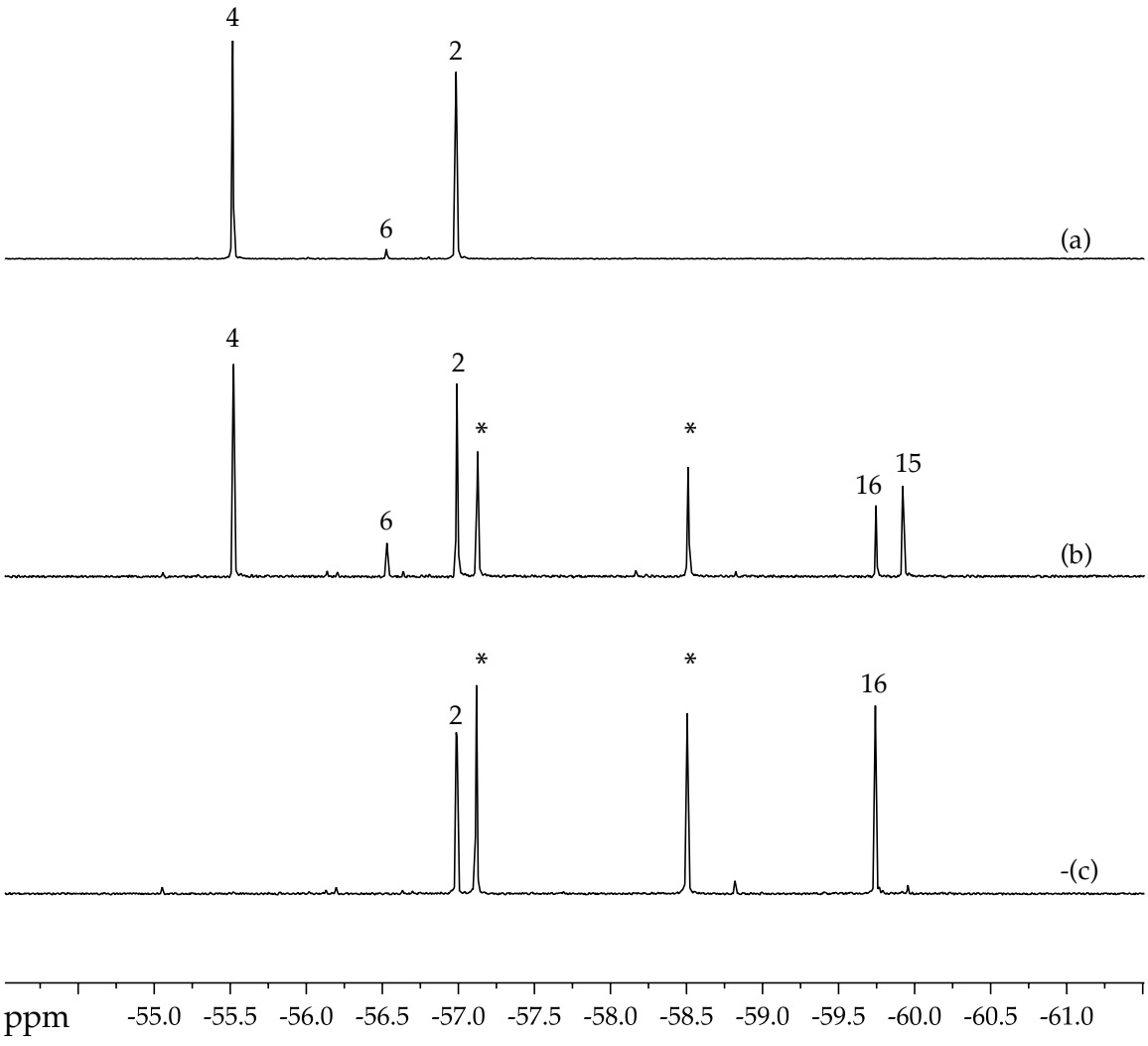



**Figure 45**. Crude $^{19}$F spectrum from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –78 °C in 12.3 M THF. The spectra show the product distribution for: (a) the reaction quenched without warming; (b) the reaction quenched after warming to 0 °C for 10 minutes; (c) the reaction quenched after being warmed to 25 °C for 30 minutes. * uncharacterized dimerized product lacking aniline fragments.

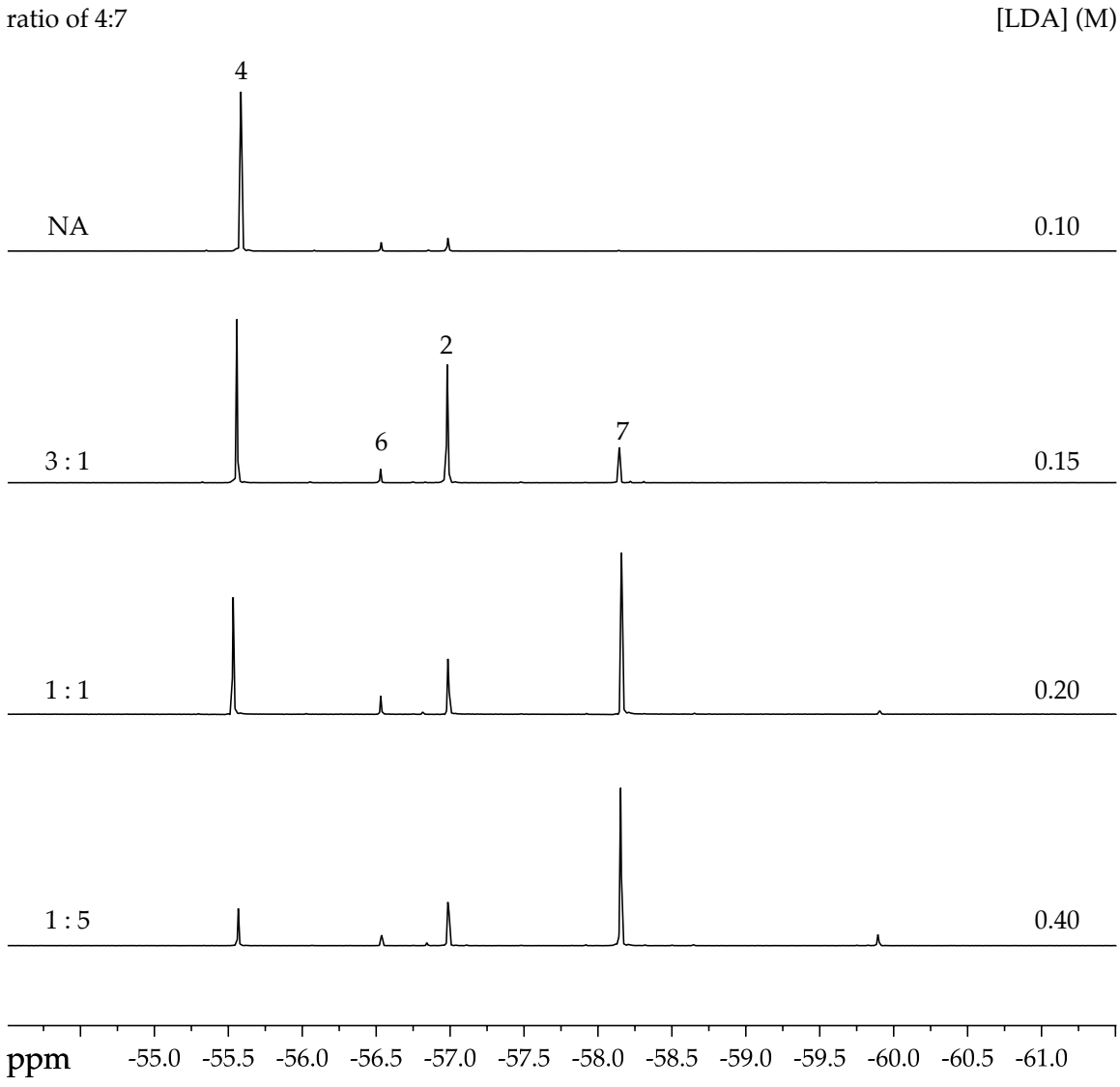



**Figure 46**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –78 °C with varying LDA concentration.

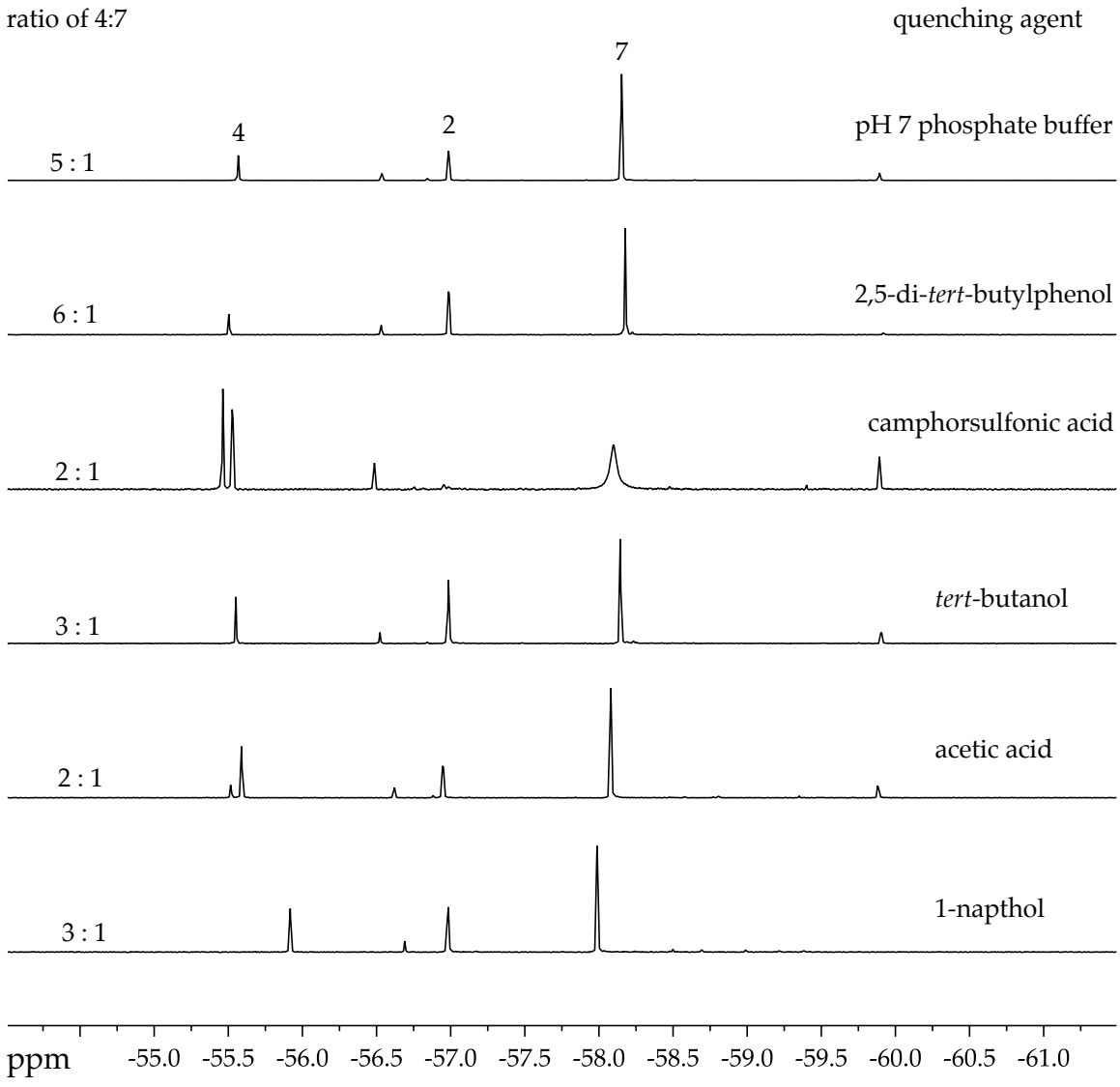



**Figure 47**. Crude $^{19}$F spectra from the condensation of lithium enolate **3** (0.10 M) with imine **2** (0.13 M) at –78 °C with 0.40 M LDA and various quenching conditions.

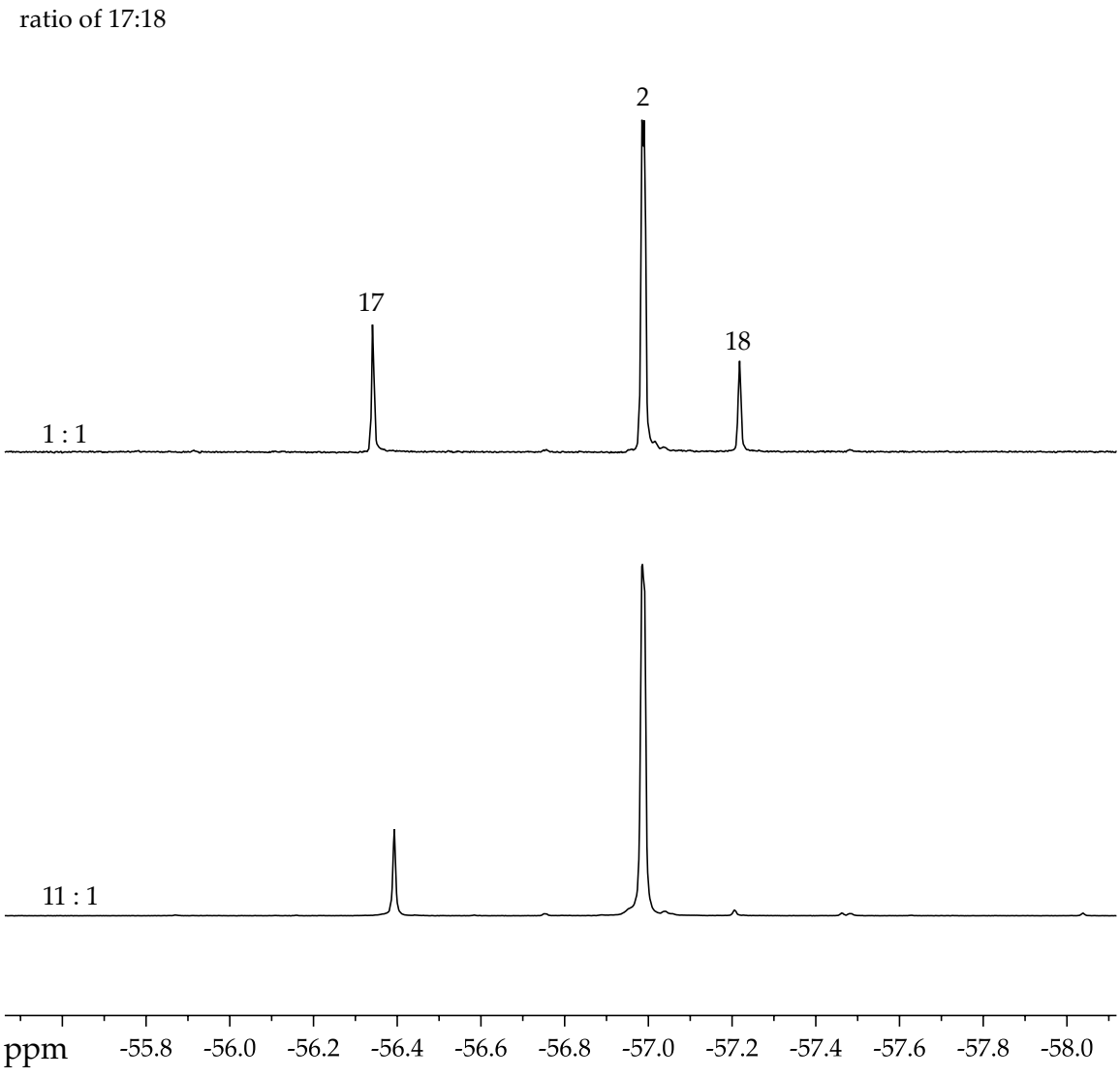



**Figure 48**. Crude $^{19}$F spectra from the condensation of lithium enolate **3b** (0.10 M) with imine **2** (0.13 M) at –55 °C in 12.3 M THF for the top spectrum and 1.0 M THF for the bottom spectrum.

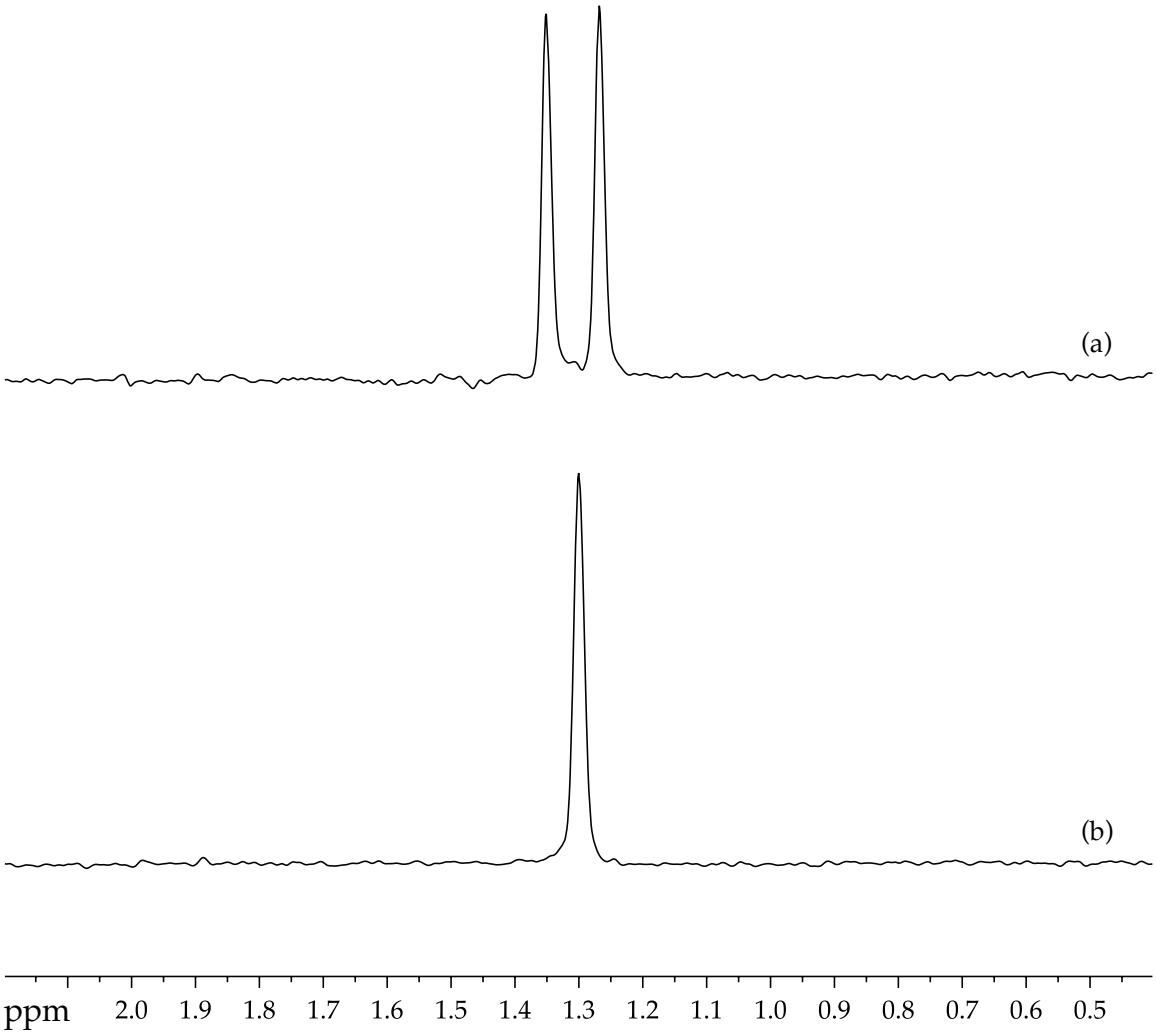



**Figure 49**. $^{6}$Li NMR spectra for a 0.10 M solution of [$^{6}$Li]$^{15}$N **8** in 12.3 M THF with 0.11 M [$^{6}$Li ]LDA at –80 °C: (a) $^{6}$Li spectrum; and (b) $^{6}$Li{$^{15}$N} spectrum.

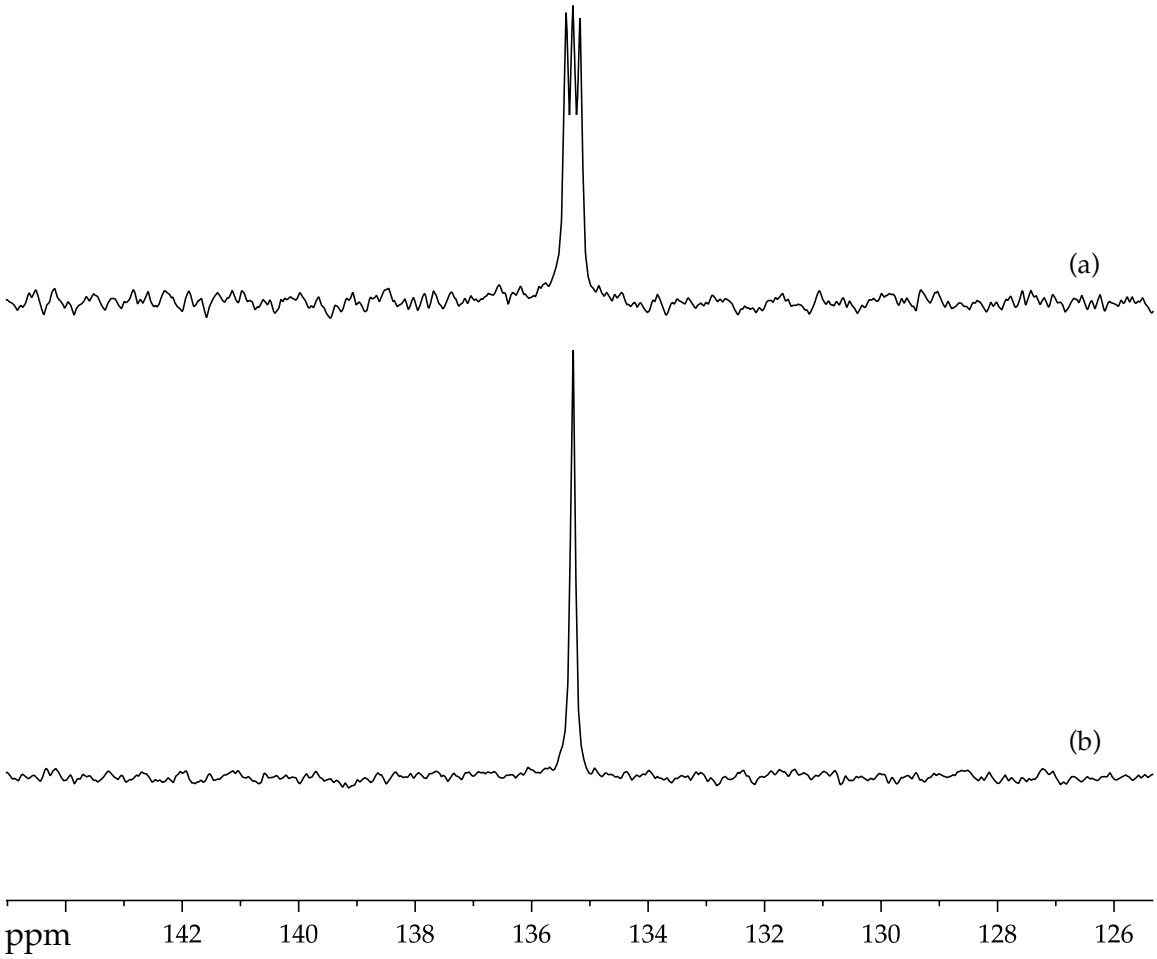



**Figure 50**. $^{15}$N NMR spectra for a 0.10 M solution of [$^{6}$Li]$^{15}$N **8** in 12.3 M THF with 0.11 M [$^{6}$Li ]LDA at –80 °C: (a) $^{15}$N spectrum; and (b) $^{15}$N{$^{6}$Li} spectrum.

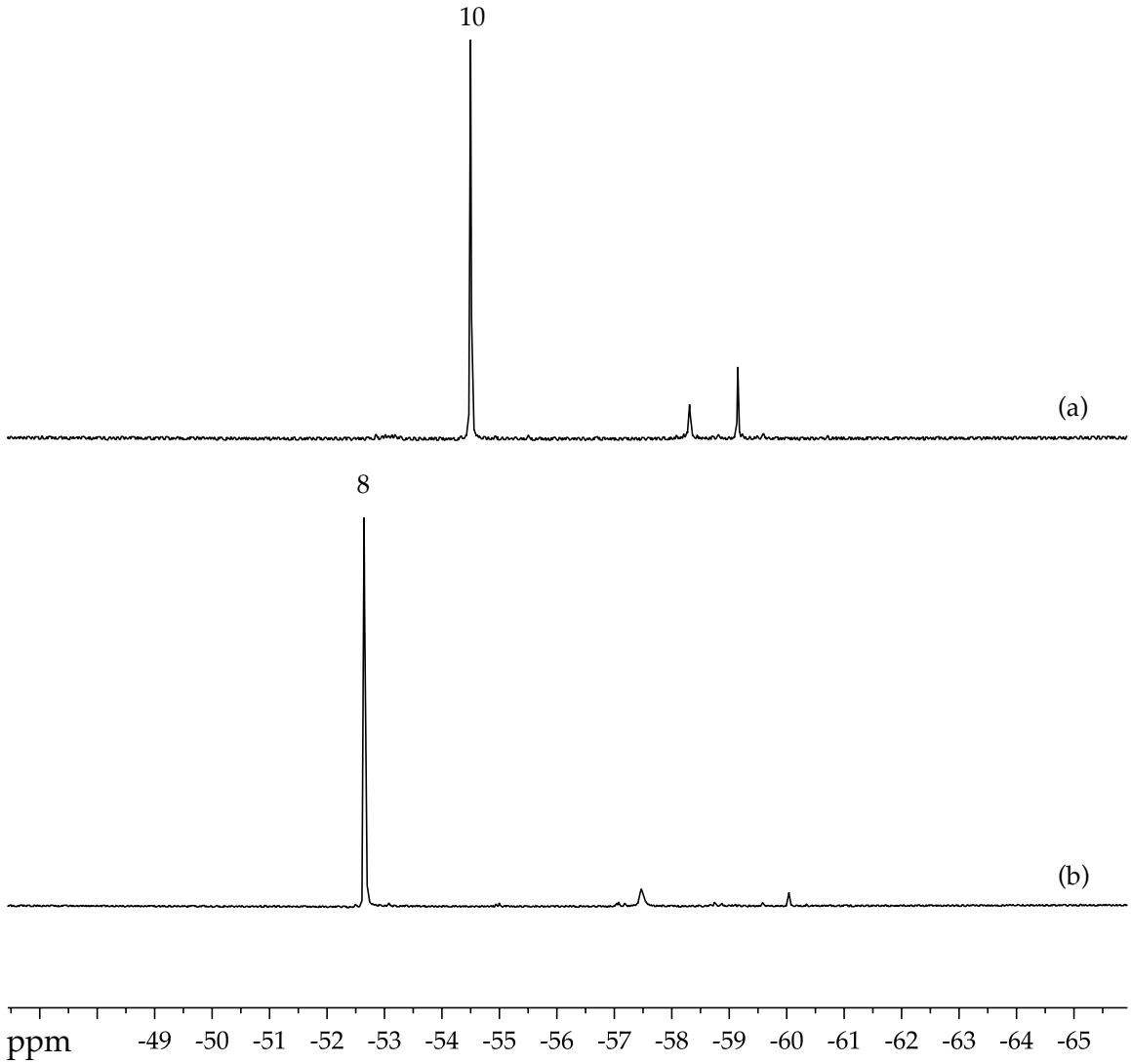



**Figure 51**. $^{19}$F NMR spectra for 0.10 M solutions of: (a) [$^{6}$Li]**10** in 12.3 M THF with 0.11 M [$^{6}$Li ]LDA at –80 °C; (b) [$^{6}$Li]**8** in 12.3 M THF with 0.11 M [$^{6}$Li ]LDA at –80 °C.

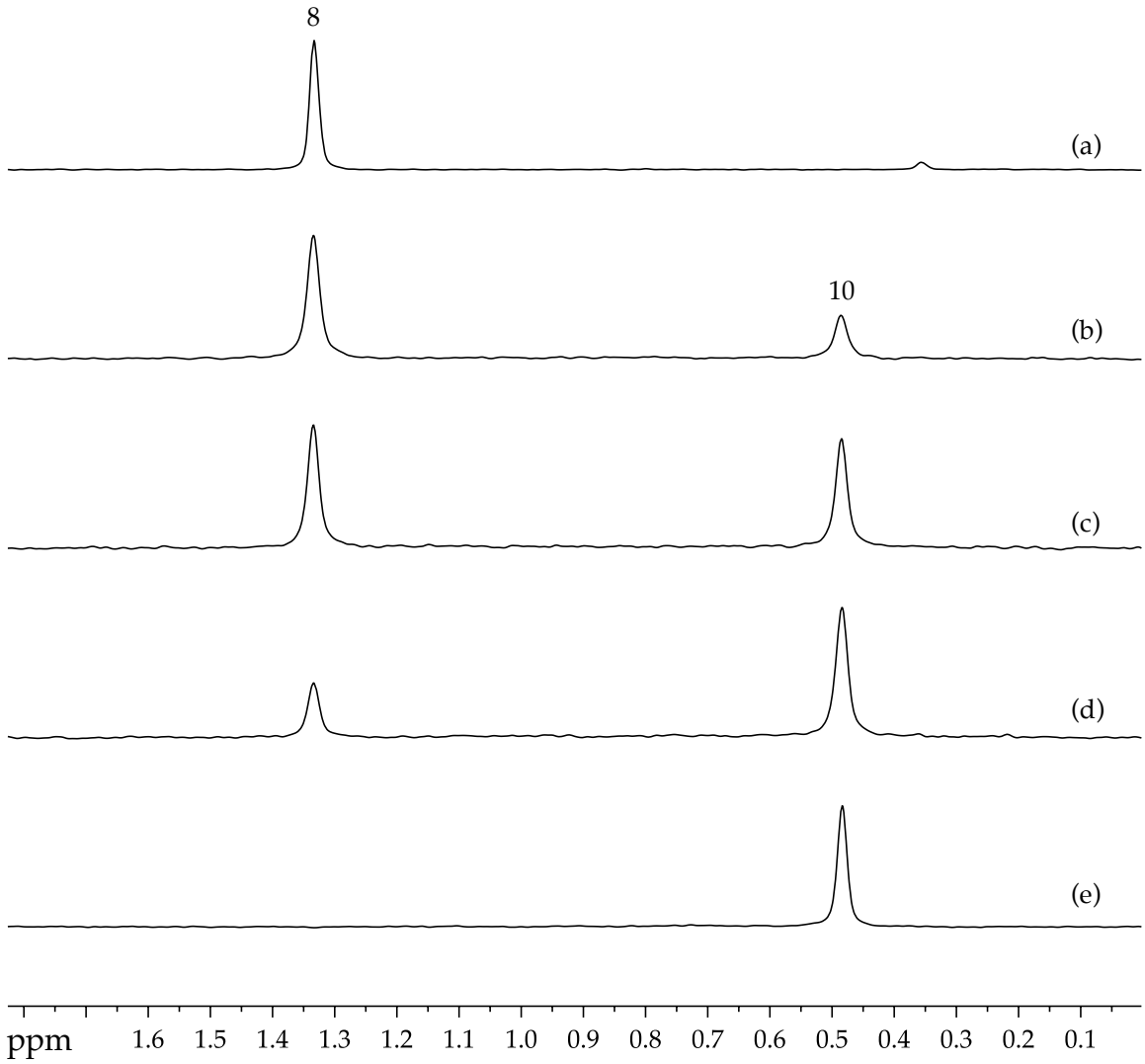



**Figure 52**. $^{6}$Li NMR spectra for 0.10 M total concentration solutions of [$^{6}$Li]**8** and [$^{6}$Li]**10** in 12.3 M THF with 0.11 M [$^{6}$Li ]LDA at –80 °C.

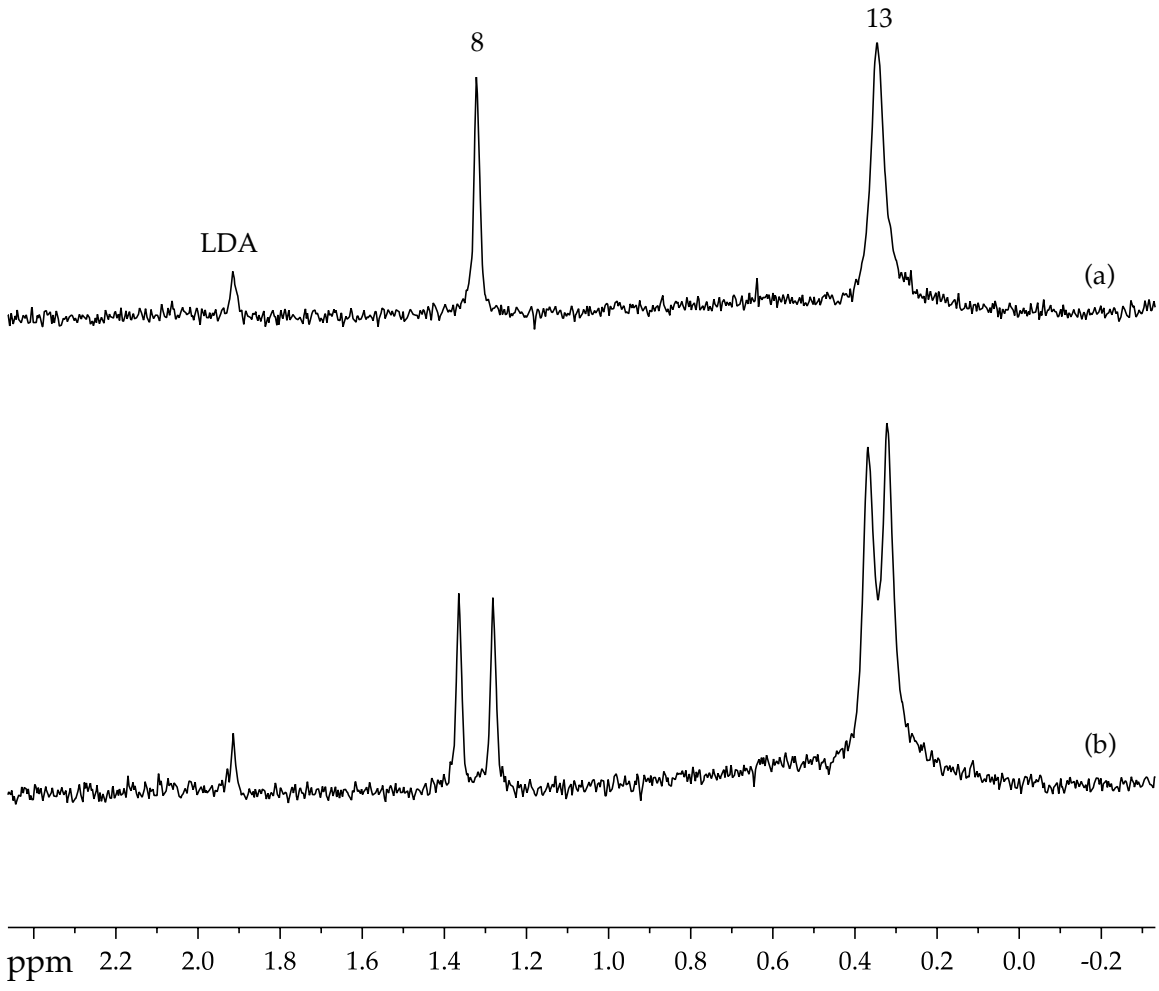



**Figure 53**. $^{6}$Li NMR spectra for a 0.10 M solution of [$^{6}$Li,$^{15}$N]**13** in 12.3 M THF with 0.20 M [$^{6}$Li ]LDA at –80 °C: (a) $^{6}$Li spectrum; and (b) $^{6}$Li{$^{15}$N} spectrum.

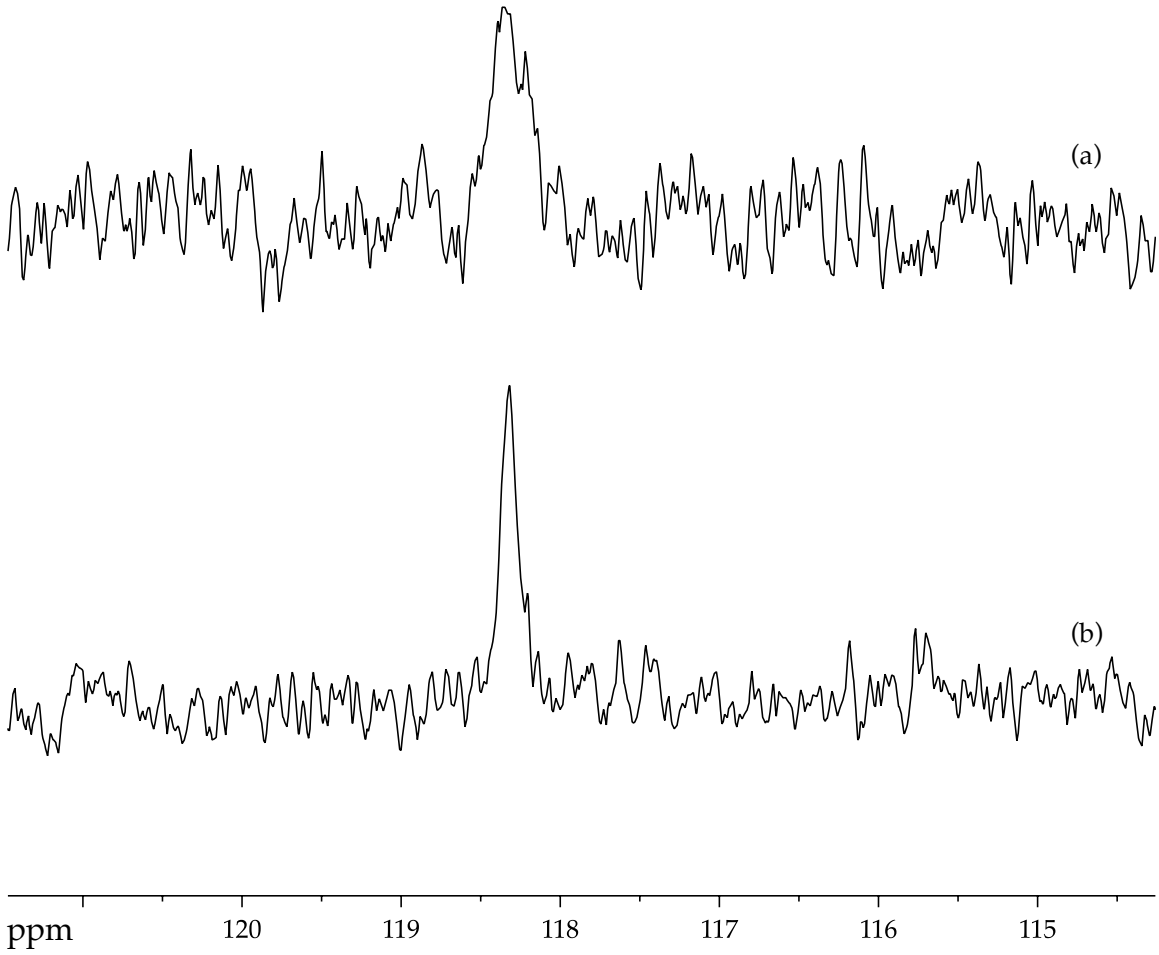



**Figure 54**. $^{15}$N NMR spectra for a 0.10 M solution of [$^{6}$Li,$^{15}$N]**13** in 12.3 M THF with 0.20 M [$^{6}$Li]LDA at –80 °C: (a) $^{15}$N spectrum; and (b) $^{15}$N{$^{6}$Li} spectrum.

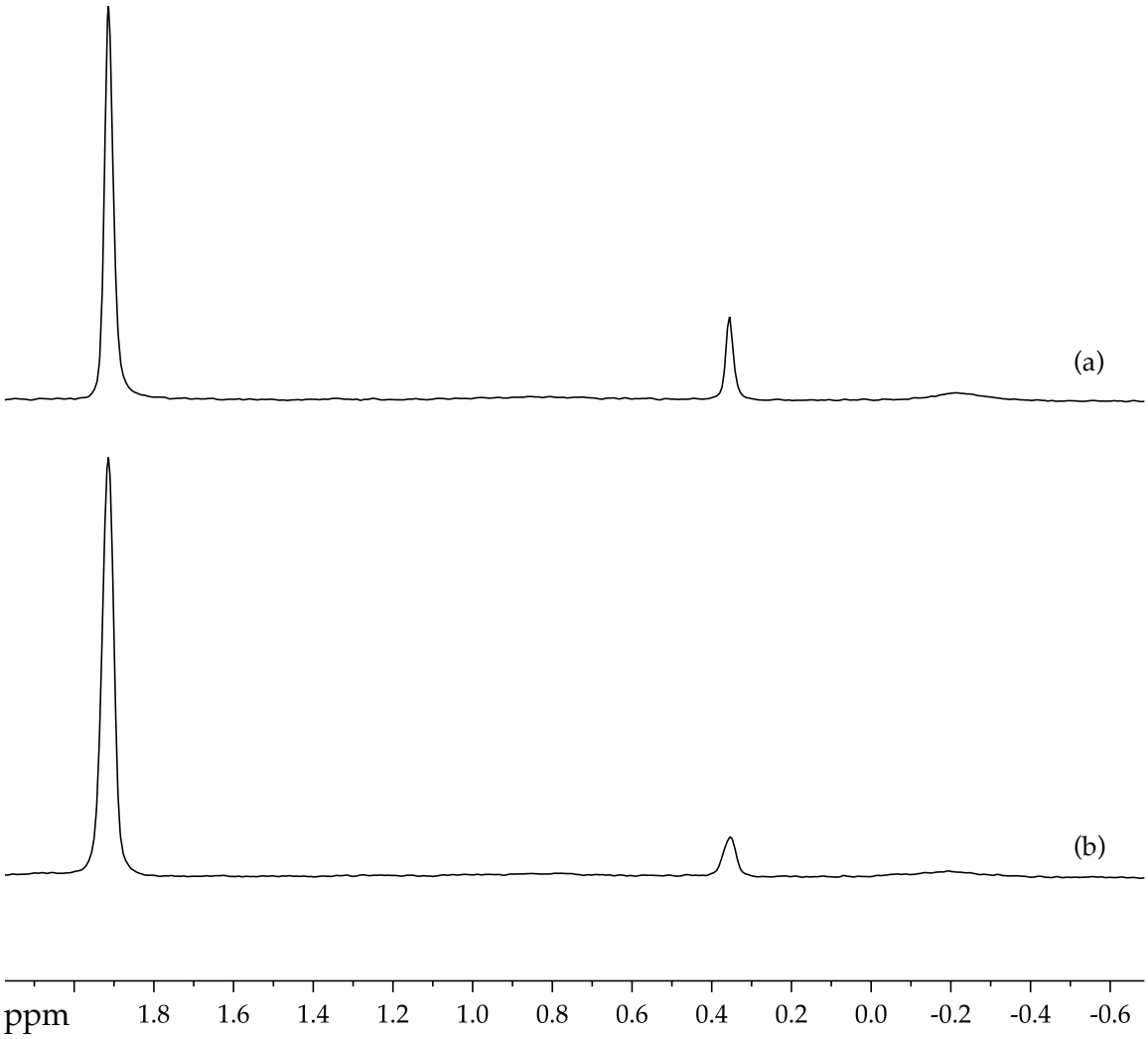



**Figure 55**. $^{6}$Li NMR spectra for 0.10 M solutions of [$^{6}$Li]**13** in 12.3 M THF with 0.40 M [$^{6}$Li ]LDA at –80 °C generated from: (a) 0.10 M **4**; and (b) 0.10 M **6**.

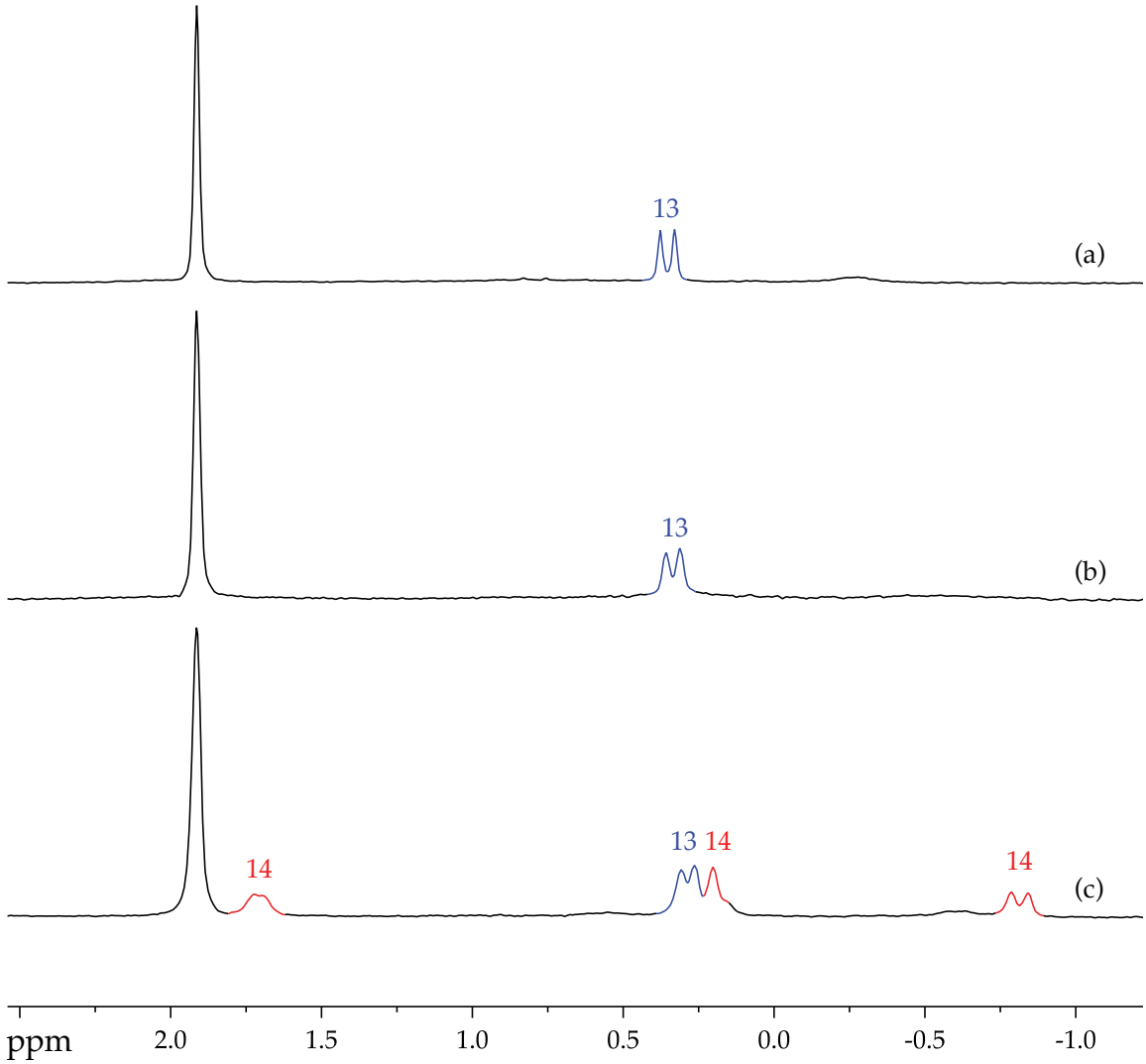



**Figure 56**. $^{6}$Li NMR spectra for a 0.10 M solution of [$^{6}$Li]**13** in 12.3 M THF with 0.60 M [$^{6}$Li ]LDA at: (a) –80 °C; (b) –100 °C; (c) –120 °C.

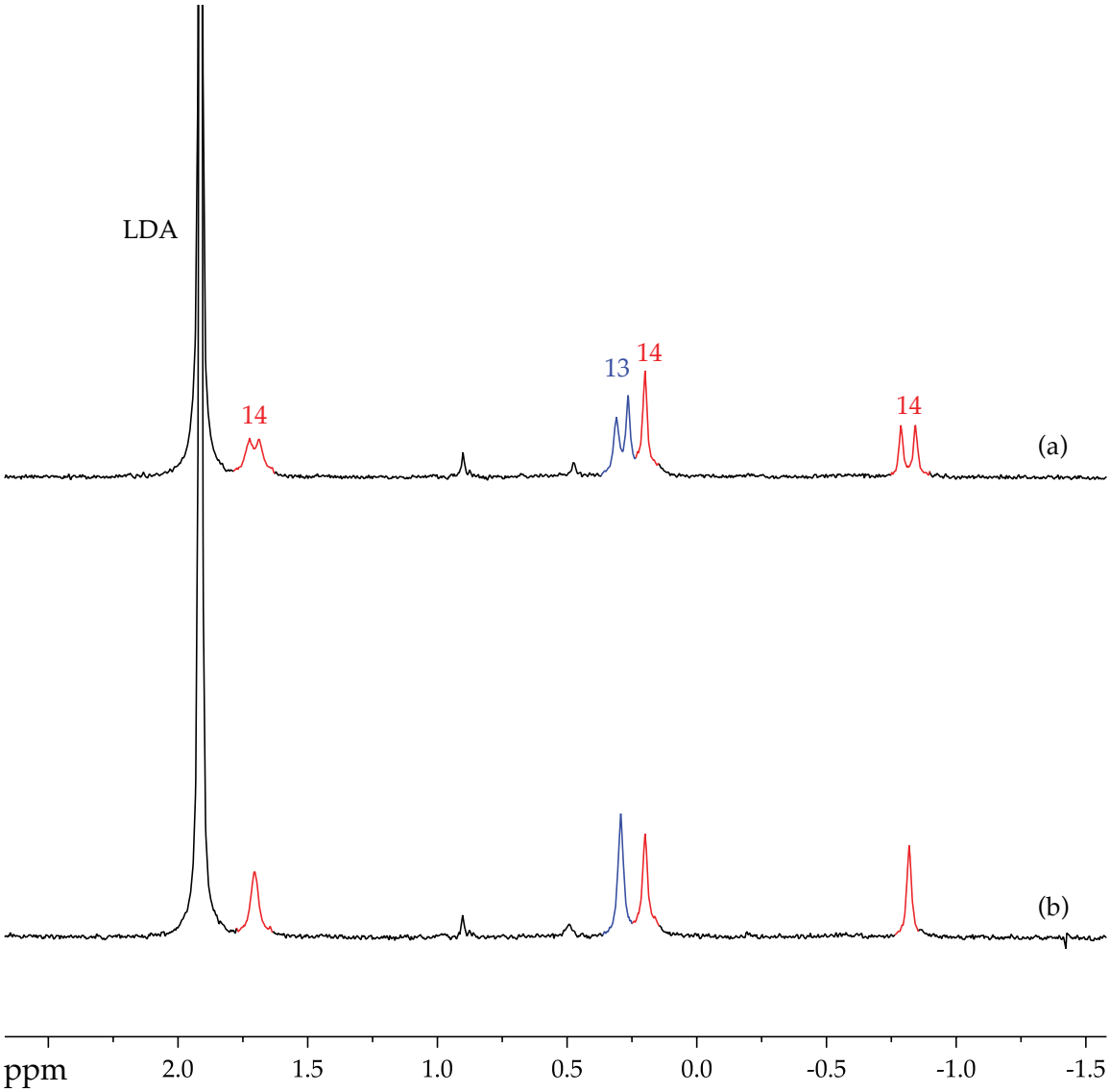



**Figure 57**. $^{6}$Li NMR spectra for a 0.10 M solution of [$^{6}$Li**,** $^{15}$N]**13** in 12.3 M THF with 0.60 M [$^{6}$Li ]LDA at –120 °C: (a) $^{6}$Li spectrum; (b) $^{6}$Li{$^{15}$N} spectrum.

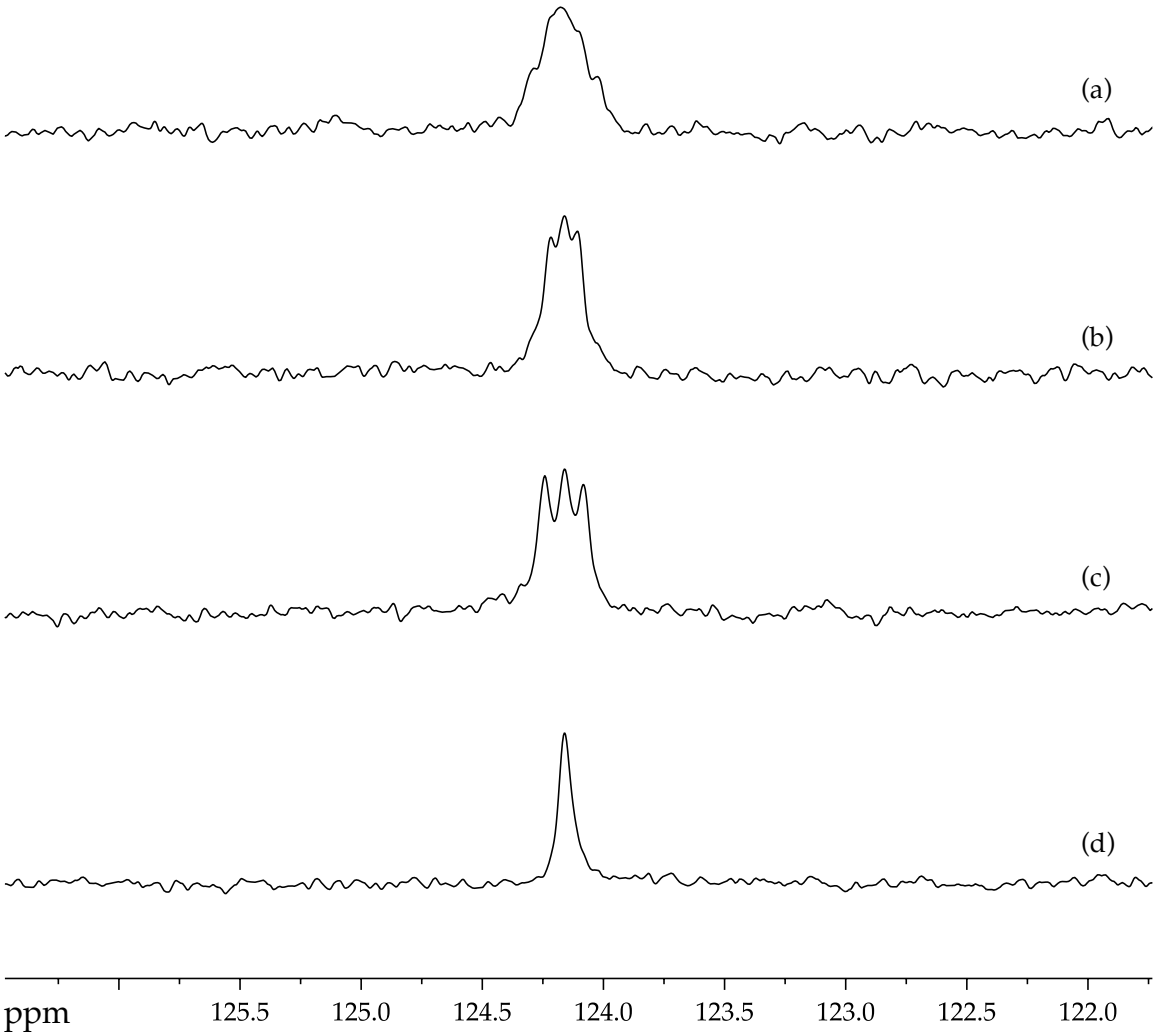



**Figure 58**. $^{15}$N NMR spectra for a 0.10 M solution of [$^{6}$Li**,** $^{15}$N]**13** in 12.3 M THF with 0.60 M [$^{6}$Li ]LDA at –120 °C: (a) $^{15}$N spectrum; (b) single frequency $^{15}$N{$^{6}$Li}; (c) single frequency $^{15}$N{$^{6}$Li''}; (d) $^{15}$N{$^{6}$Li}.

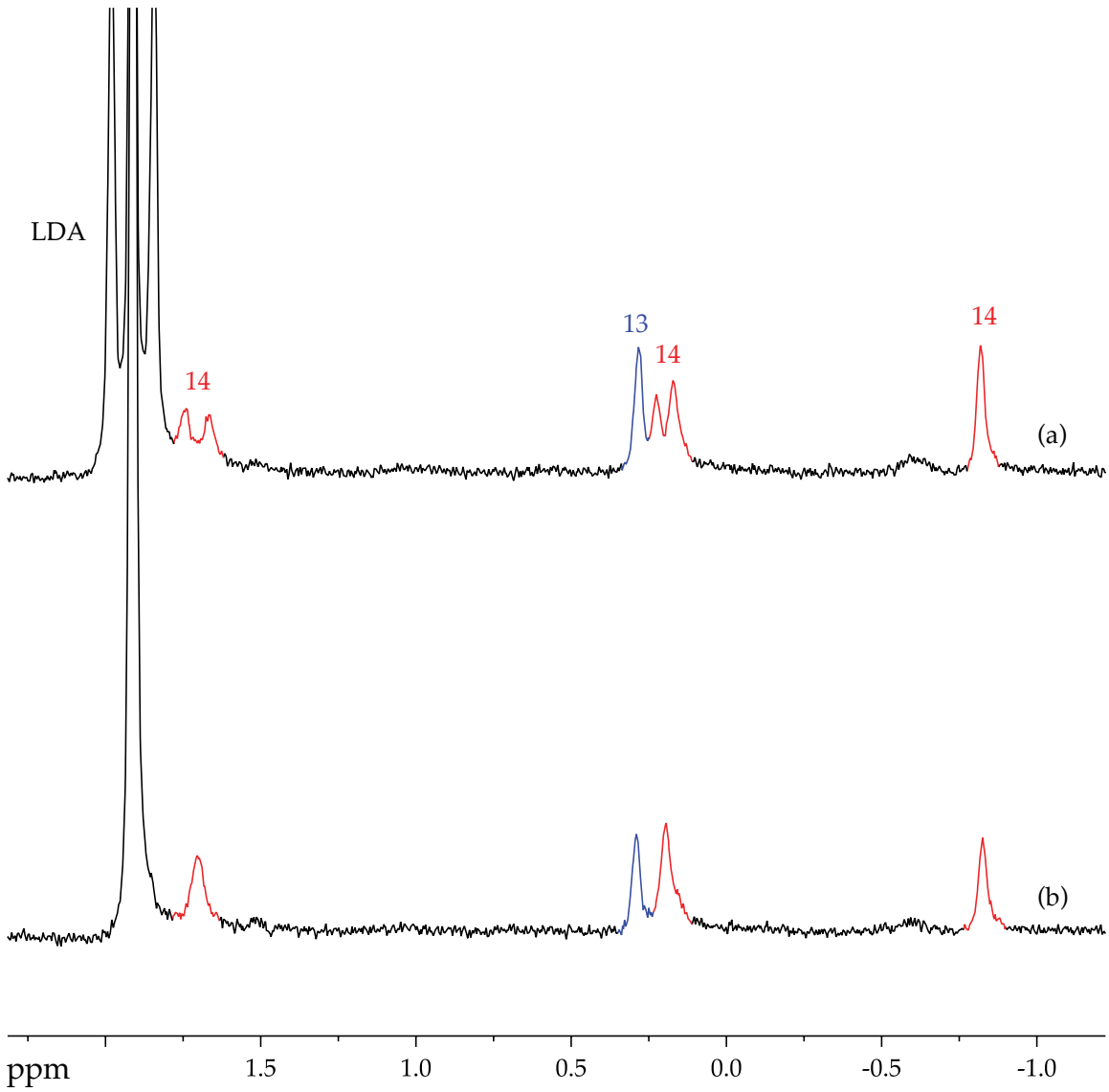



**Figure 59**. $^{6}$Li NMR spectra for a 0.10 M solution of [$^{6}$Li]**13** in 12.3 M THF with 0.60 M [$^{6}$Li, $^{15}$N]LDA at –120 °C: (a) $^{6}$Li spectrum; (b) $^{6}$Li{$^{15}$N} spectrum.

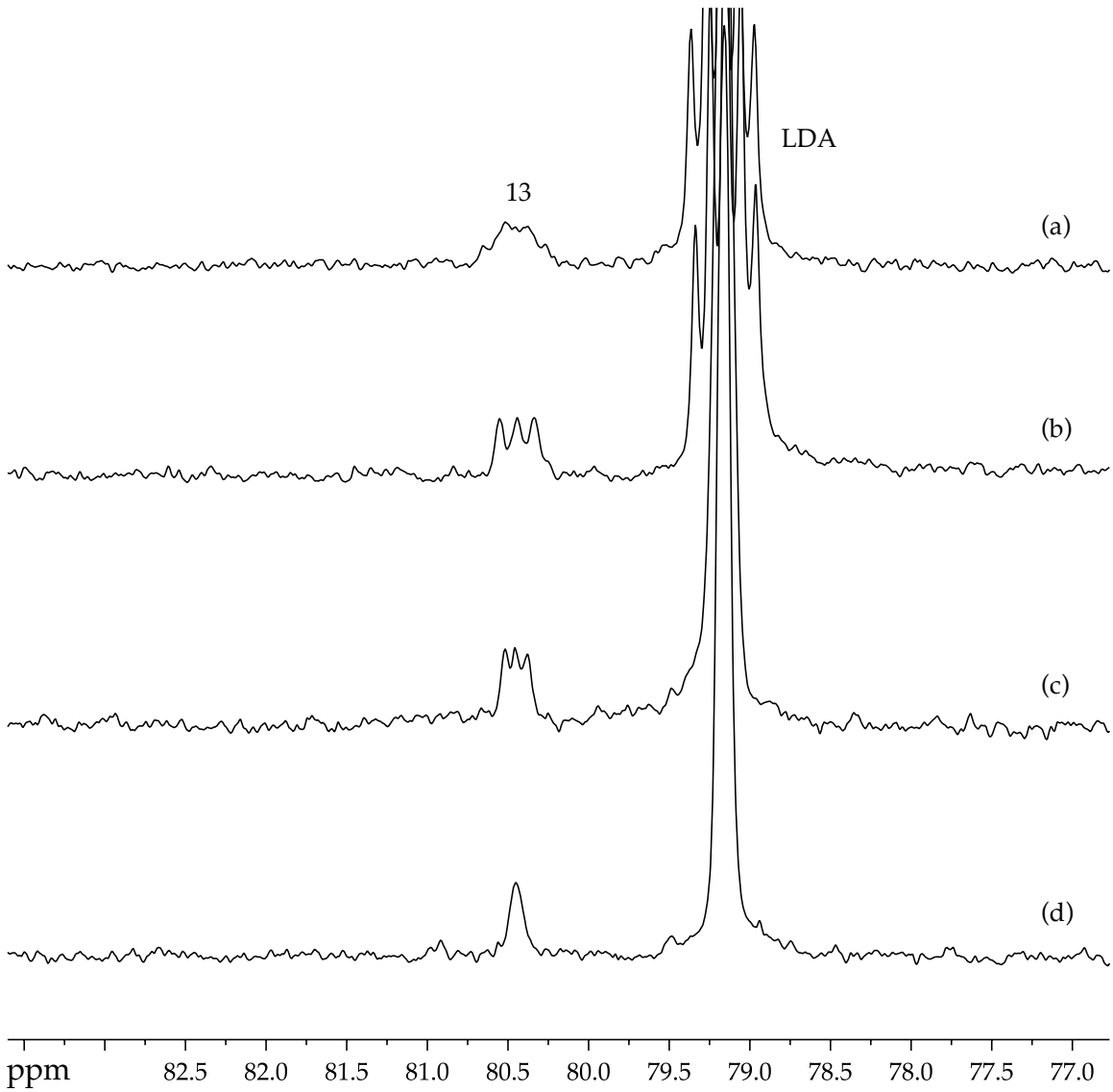
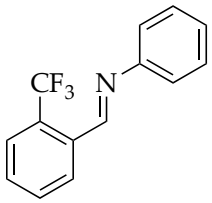


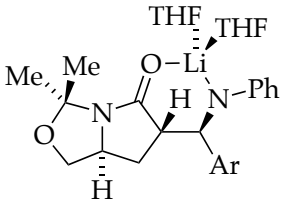

**Figure 60**. $^{15}$N NMR spectra for a 0.10 M solution of [$^{6}$Li]**13** in 12.3 M THF with 0.60 M [$^{6}$Li, $^{15}$N]LDA at –120 °C: (a) $^{15}$N spectrum; (b) single frequency $^{15}$N{$^{6}$Li}; (c) single frequency $^{15}$N{$^{6}$Li'}; (d) $^{15}$N{$^{6}$Li}.

## Part 2: Computational Studies

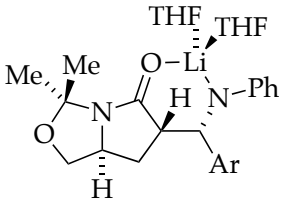
**Chart 3**



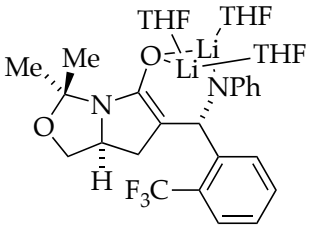
**2**



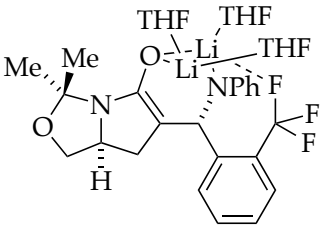
**8b**



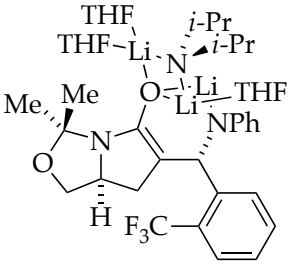
**8a**



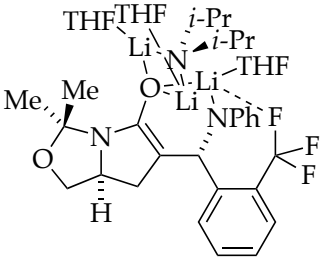
**13b**



**13a**

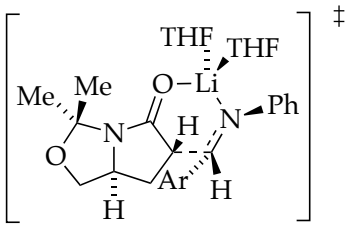


**14a**

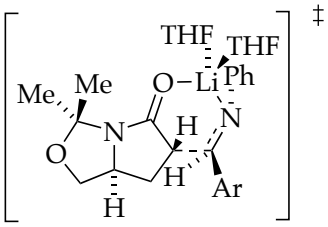


**14b**

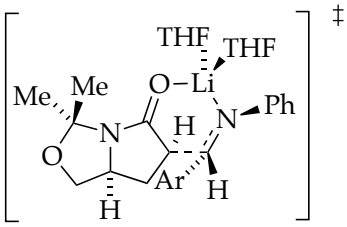
**Chart 4**



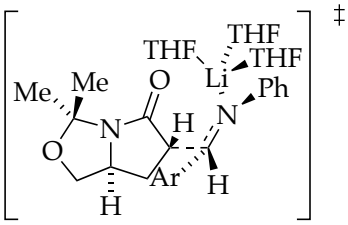

**11a**



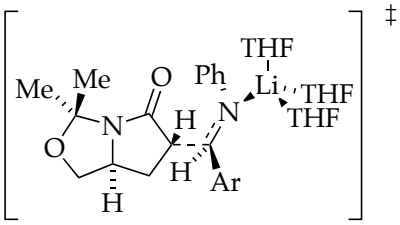

**11b**




**12c**

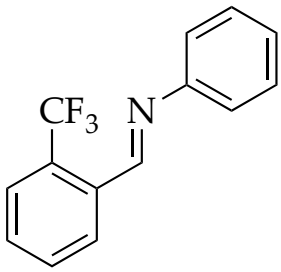


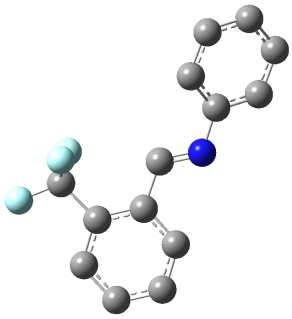

**12a**




**12b**

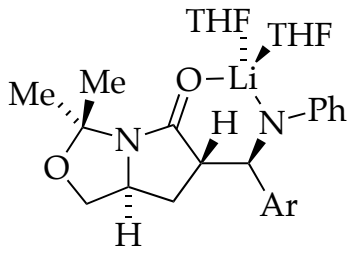
**Table 1.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the azaaldol products and reagents at –70 °C with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

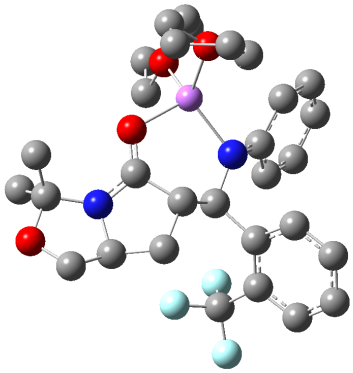


**2**
G = -893.785925
$G_{MP2}$ = -891.190811

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | -0.12117400 | 1.49870900 | -0.13407600 |
| C | -1.39702900 | 2.06291200 | -0.19897200 |
| C | -1.55528600 | 3.44176000 | -0.32617600 |
| C | -0.42952300 | 4.26505100 | -0.39055900 |
| C | 0.84319600 | 3.70878600 | -0.32902100 |
| C | 1.02626200 | 2.32235700 | -0.19878600 |
| C | 2.39806700 | 1.77974900 | -0.13595600 |
| H | 2.50910400 | 0.70115800 | -0.00087400 |
| N | 3.41777300 | 2.55131600 | -0.22106800 |
| C | 4.71397400 | 2.00479100 | -0.21533500 |
| C | 5.72983500 | 2.75534900 | 0.39924600 |
| C | 7.03530200 | 2.27352600 | 0.44158000 |
| C | 7.35510300 | 1.05259200 | -0.15888200 |
| C | 6.35712100 | 0.31744800 | -0.80235900 |
| C | 5.04420100 | 0.78421800 | -0.83162900 |
| H | 4.27890300 | 0.22378400 | -1.36119800 |
| H | 6.60282200 | -0.62145700 | -1.29167600 |
| H | 8.37730200 | 0.68499300 | -0.13967500 |
| H | 7.80843000 | 2.85716500 | 0.93426000 |
| H | 5.46708900 | 3.70774300 | 0.84967100 |
| H | 1.73011800 | 4.33097500 | -0.37820200 |
| H | -0.54449400 | 5.34089800 | -0.48946400 |
| H | -2.55315600 | 3.86784100 | -0.37457800 |
| H | -2.26642100 | 1.41797000 | -0.15019500 |
| F | -1.20150500 | -0.61153000 | 0.03565900 |
| F | 0.65729700 | -0.35505300 | 1.13122700 |
| F | 0.68948800 | -0.54522500 | -1.03338100 |

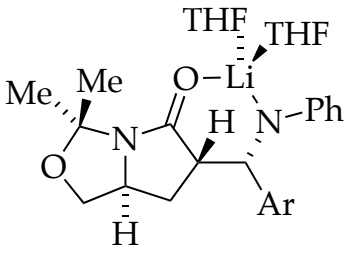


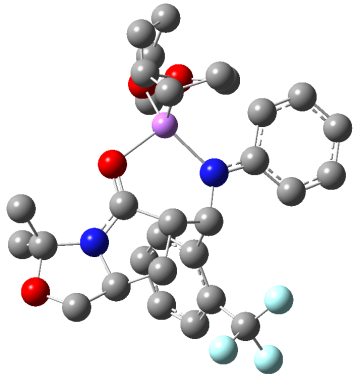



**8b**
G = –1883.008658
$G_{MP2}$ = –-1877.821459

| Atom | X | Y | Z |
|---|---|---|---|
| Li | 0.00000000 | 0.00000000 | 0.00000000 |
| C | -2.00218500 | 1.85353100 | -0.23974500 |
| C | -2.90997400 | 0.94368600 | 0.60036700 |
| C | -4.22001200 | 1.77200600 | 0.71262200 |
| C | -4.19177800 | 2.72631700 | -0.49196200 |
| C | -4.48082800 | 4.21906600 | -0.33166300 |
| H | -5.51502600 | 4.50500300 | -0.53736900 |
| H | -4.20215400 | 4.56863700 | 0.67524100 |
| O | -3.65994600 | 4.82028100 | -1.33757300 |
| C | -2.42214100 | 4.09150100 | -1.44865800 |
| N | -2.76911400 | 2.79238300 | -0.83686800 |
| C | -2.09440300 | 3.95157800 | -2.93293400 |
| H | -2.90280900 | 3.42694900 | -3.44962600 |
| H | -1.97656200 | 4.94252000 | -3.38263800 |
| H | -1.16354200 | 3.39041000 | -3.06074400 |
| C | -1.31864000 | 4.81258900 | -0.67029300 |
| H | -0.38765900 | 4.24240200 | -0.69510100 |
| H | -1.15423400 | 5.79705900 | -1.11831400 |
| H | -1.61672800 | 4.95316600 | 0.37382200 |
| H | -4.76463700 | 2.32906700 | -1.33655100 |
| H | -5.12042700 | 1.15982000 | 0.73364600 |
| H | -4.19438000 | 2.35640100 | 1.64065900 |
| H | -2.43823100 | 0.83000100 | 1.58193900 |
| C | -2.96032500 | -0.52132600 | 0.02359100 |
| H | -3.20624800 | -0.45454200 | -1.05028100 |
| C | -4.09841900 | -1.29897100 | 0.73044600 |
| C | -5.36961600 | -1.58935000 | 0.18491700 |
| C | -6.31997900 | -2.29908300 | 0.93432900 |
| C | -6.03767700 | -2.72055000 | 2.22934100 |
| C | -4.78764900 | -2.44018700 | 2.78026200 |
| C | -3.84014100 | -1.74678600 | 2.03302600 |
| H | -2.84809300 | -1.56252100 | 2.43227900 |
| H | -4.54666000 | -2.77051700 | 3.78759900 |
| H | -6.78472000 | -3.26926300 | 2.79587300 |
| H | -7.28447300 | -2.52210500 | 0.49367100 |
| C | -5.76716700 | -1.18742600 | -1.21560500 |
| F | -7.06083900 | -1.46942300 | -1.48481100 |
| F | -5.03666800 | -1.80040000 | -2.17892600 |
| F | -5.62268500 | 0.15036000 | -1.43856400 |
| N | -1.64758100 | -1.08368500 | 0.27657000 |
| C | -1.36771900 | -2.33833600 | -0.21041800 |
| C | -0.16293000 | -2.96747700 | 0.22914700 |
| C | 0.24311000 | -4.21023600 | -0.23934600 |
| C | -0.52857700 | -4.91758700 | -1.17152800 |
| C | -1.72322100 | -4.33777300 | -1.60231400 |
| C | -2.14242200 | -3.08946500 | -1.14070600 |
| H | -3.08151600 | -2.69425500 | -1.50461000 |
| H | -2.35363600 | -4.86831200 | -2.31457500 |
| H | -0.21782100 | -5.89504200 | -1.52989300 |
| H | 1.16679300 | -4.64443800 | 0.14139500 |
| H | 0.43531500 | -2.45391200 | 0.97955200 |
| O | -0.77024100 | 1.76544200 | -0.36355500 |
| O | 1.14717800 | -0.33539900 | -1.60254200 |
| C | 0.41423700 | -0.48254900 | -2.84591900 |
| C | 1.36557900 | -1.20550400 | -3.79989900 |
| C | 2.16271000 | -2.09541700 | -2.83392600 |
| C | 2.31868700 | -1.18493700 | -1.61463200 |
| H | 3.20820900 | -0.54501000 | -1.69280200 |
| H | 2.35172600 | -1.73155300 | -0.66945600 |
| H | 3.12725400 | -2.41860300 | -3.23801200 |
| H | 1.57986400 | -2.98252700 | -2.56505700 |
| H | 2.02753500 | -0.48955200 | -4.30247200 |
| H | 0.83002200 | -1.77360600 | -4.56616900 |
| H | -0.48580900 | -1.07703900 | -2.65050100 |
| H | 0.12338800 | 0.51702000 | -3.18193800 |
| O | 1.31044500 | 0.24214000 | 1.51166000 |
| C | 1.96946300 | 1.51740800 | 1.60559300 |
| C | 1.32089500 | 2.19576100 | 2.80934300 |

| | | | |
|---|---|---|---|
| C | 1.13708400 | 1.01265300 | 3.77743300 |
| C | 0.90755400 | -0.18835000 | 2.83660100 |
| H | -0.14038400 | -0.49185800 | 2.76131100 |
| H | 1.50527400 | -1.06099600 | 3.12359600 |
| H | 0.30455200 | 1.15754100 | 4.47220200 |
| H | 2.04416200 | 0.86576800 | 4.37415600 |
| H | 0.35175200 | 2.61318500 | 2.51502700 |
| H | 1.93301400 | 3.00126400 | 3.22654000 |
| H | 3.04818200 | 1.36611800 | 1.76038800 |
| H | 1.81120500 | 2.03619600 | 0.65770600 |

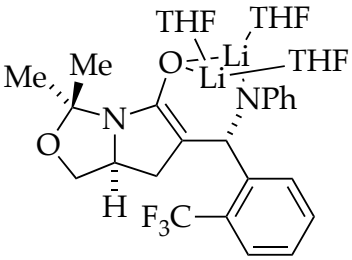


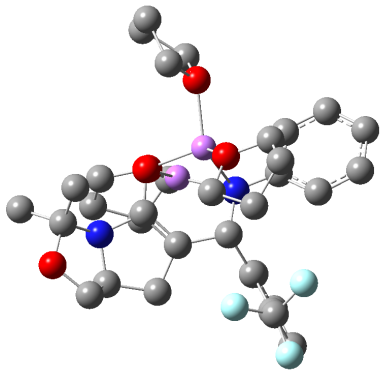



**8a**
G = –1883.004630
$G_{MP2}$ = –-1877.819029

| Atom | X | Y | Z |
|---|---|---|---|
| Li | 0.00000000 | 0.00000000 | 0.00000000 |
| N | -0.98542700 | 1.64968600 | -0.50317800 |
| C | -2.40227300 | 1.64107400 | -0.80880400 |
| C | -2.76417800 | 0.18808500 | -1.28781800 |
| C | -2.55128300 | -0.89321200 | -0.22127400 |
| N | -3.76094200 | -1.35204500 | 0.16149500 |
| C | -4.89129900 | -0.74872900 | -0.55135000 |
| C | -4.21846900 | -0.07657200 | -1.75828300 |
| H | -4.74191200 | 0.82245000 | -2.07837400 |
| H | -4.20293100 | -0.77669100 | -2.60306400 |
| C | -5.77621500 | -1.98512200 | -0.70956300 |
| H | -6.84599900 | -1.77100200 | -0.76569300 |
| H | -5.47827500 | -2.57337100 | -1.59206400 |
| O | -5.54548400 | -2.71121000 | 0.50219100 |
| C | -4.17100400 | -2.55805600 | 0.90627800 |
| C | -4.15030200 | -2.32776500 | 2.41526400 |
| H | -4.71355200 | -1.42498700 | 2.66653000 |
| H | -4.60553000 | -3.18183000 | 2.92658000 |
| H | -3.11911600 | -2.21311400 | 2.76338900 |
| C | -3.35955900 | -3.78699000 | 0.48893100 |
| H | -2.30371800 | -3.65834800 | 0.73777500 |
| H | -3.75066300 | -4.66549400 | 1.01077600 |
| H | -3.44930600 | -3.95616000 | -0.58898600 |
| H | -5.39182400 | -0.01224800 | 0.08915100 |
| O | -1.46015700 | -1.29460200 | 0.21797900 |
| H | -2.04783800 | -0.00476100 | -2.09303300 |
| H | -2.63234500 | 2.26936900 | -1.67681800 |
| C | -3.29656800 | 2.11056000 | 0.37617600 |
| C | -4.42878700 | 2.95971900 | 0.31141600 |
| C | -5.12515400 | 3.30821500 | 1.48220200 |
| C | -4.72987500 | 2.83385900 | 2.72624500 |
| C | -3.61165100 | 2.00502900 | 2.80894800 |
| C | -2.91294500 | 1.66990000 | 1.65387800 |
| H | -2.01668100 | 1.06429300 | 1.72152800 |
| H | -3.27551400 | 1.63082700 | 3.77290600 |
| H | -5.28079900 | 3.11973400 | 3.61774800 |
| H | -5.98050300 | 3.96986600 | 1.40931200 |
| C | -5.03416800 | 3.50576500 | -0.96357100 |
| F | -5.90838300 | 2.61658700 | -1.52578100 |
| F | -5.75111100 | 4.62992300 | -0.74074600 |
| F | -4.14143500 | 3.81615000 | -1.92986400 |
| C | -0.34430900 | 2.86410900 | -0.53273000 |
| C | 1.06810900 | 2.89163900 | -0.31383000 |
| C | 1.80627400 | 4.06765200 | -0.34139900 |
| C | 1.19110000 | 5.30097700 | -0.58686800 |
| C | -0.18762400 | 5.30742900 | -0.80330400 |
| C | -0.94180900 | 4.13494300 | -0.77693400 |
| H | -2.00749600 | 4.20923500 | -0.95251000 |
| H | -0.69828700 | 6.24986800 | -0.99614600 |
| H | 1.76777600 | 6.22142100 | -0.60856200 |
| H | 2.88204100 | 4.02197300 | -0.17411100 |
| H | 1.57851700 | 1.94822900 | -0.13034200 |
| O | 1.12513200 | -0.01984700 | 1.66361400 |
| C | 2.51476300 | -0.39964900 | 1.71332500 |

| | | | |
|---|---|---|---|
| C | 3.21222500 | 0.73546800 | 2.46136000 |
| C | 2.14360500 | 1.13097700 | 3.49285900 |
| C | 0.83615000 | 0.94443900 | 2.71033300 |
| H | 0.50775600 | 1.86837400 | 2.22525900 |
| H | 0.02256400 | 0.55052100 | 3.32868300 |
| H | 2.25888800 | 2.15495900 | 3.85924300 |
| H | 2.18015000 | 0.45588600 | 4.35607000 |
| H | 3.41240800 | 1.57030300 | 1.78076600 |
| H | 4.15789200 | 0.42323900 | 2.91500500 |
| H | 2.61091800 | -1.35319800 | 2.25262100 |
| H | 2.85185800 | -0.53883100 | 0.68344700 |
| O | 1.25296100 | -0.73786100 | -1.41863400 |
| C | 1.10711700 | -2.11465400 | -1.81922600 |
| C | 0.62782800 | -2.05668100 | -3.26793700 |
| C | 1.40459200 | -0.84345500 | -3.80513000 |
| C | 1.45107600 | 0.10053100 | -2.59348900 |
| H | 0.64739400 | 0.84211900 | -2.59339700 |
| H | 2.40837700 | 0.62082700 | -2.49359600 |
| H | 0.92798700 | -0.37642600 | -4.67196800 |
| H | 2.41613900 | -1.14447100 | -4.10161100 |
| H | -0.45193200 | -1.86865200 | -3.29912600 |
| H | 0.83078700 | -2.98006000 | -3.81915000 |
| H | 2.07903900 | -2.62381000 | -1.74197600 |
| H | 0.39963300 | -2.58214900 | -1.13061500 |

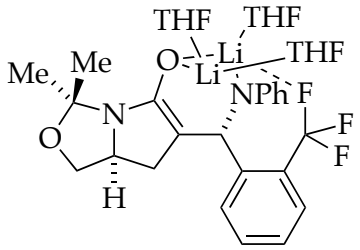


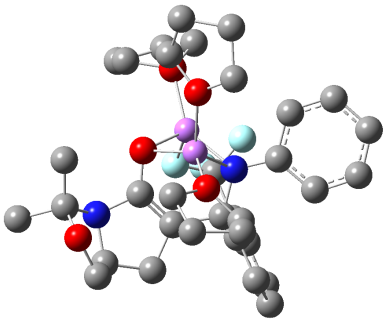



**13b**
G = –-2122.348710
$G_{MP2}$ = –-2116.456993

| Atom | X | Y | Z |
|---|---|---|---|
| Li | 0.00000000 | 0.00000000 | 0.00000000 |
| N | -1.24707400 | -1.11450200 | 1.33238800 |
| C | -1.90291600 | -1.99775200 | 0.35582300 |
| C | -0.85171600 | -2.92409500 | -0.28204500 |
| C | 0.46839800 | -2.61275200 | -0.51558400 |
| N | 1.20920000 | -3.74033100 | -1.02219700 |
| C | 0.21433200 | -4.78661800 | -1.36190800 |
| C | -1.10537500 | -4.36463100 | -0.68391300 |
| H | -1.31318000 | -5.00764300 | 0.18353300 |
| H | -1.95462200 | -4.49769200 | -1.36649300 |
| C | 0.23392900 | -4.74871500 | -2.88919800 |
| H | -0.05232400 | -5.69229100 | -3.36434900 |
| H | -0.42515600 | -3.94773400 | -3.26387900 |
| O | 1.59625200 | -4.49474000 | -3.19766900 |
| C | 2.13920900 | -3.61646500 | -2.17976900 |
| C | 3.51363200 | -4.18008300 | -1.81471700 |
| H | 3.40529100 | -5.18409500 | -1.39319100 |
| H | 4.15024300 | -4.24292000 | -2.70415000 |
| H | 4.00203600 | -3.53712500 | -1.07490700 |
| C | 2.25387300 | -2.21158200 | -2.77934000 |
| H | 2.69157900 | -1.50703700 | -2.07158700 |
| H | 2.88033600 | -2.27562100 | -3.67504200 |
| H | 1.26968700 | -1.83454900 | -3.07439400 |
| H | 0.56235700 | -5.76868100 | -1.02025600 |
| O | 1.12793400 | -1.52559400 | -0.19151200 |
| Li | 0.48745300 | -1.92819800 | 1.57972400 |
| O | 1.59143200 | -2.76974000 | 2.90258700 |
| C | 2.60843100 | -3.69905600 | 2.42248400 |
| C | 2.52370100 | -4.93916700 | 3.33672300 |
| C | 1.19930800 | -4.74331400 | 4.09991200 |
| C | 1.10520400 | -3.22306300 | 4.18131100 |
| H | 1.74305300 | -2.81917000 | 4.98054500 |
| H | 0.09260100 | -2.83061900 | 4.30469300 |
| H | 1.19755100 | -5.22205400 | 5.08364800 |
| H | 0.35545000 | -5.13748100 | 3.52255200 |
| H | 3.36579800 | -4.95958900 | 4.03700600 |
| H | 2.54460900 | -5.87064500 | 2.76448400 |
| H | 2.37798200 | -3.91090600 | 1.37457600 |
| H | 3.58416500 | -3.20488500 | 2.47973700 |
| H | -2.37662600 | -1.39155200 | -0.43456700 |
| C | -3.03106100 | -2.86972700 | 0.96241800 |
| C | -4.21461000 | -3.22417400 | 0.27881900 |

| | | | |
|---|---|---|---|
| C | -5.16552000 | -4.05960300 | 0.88205300 |
| C | -4.96185000 | -4.55935000 | 2.16423500 |
| C | -3.80136900 | -4.21024900 | 2.85465200 |
| C | -2.85968900 | -3.37792100 | 2.25502200 |
| H | -1.96689400 | -3.07902900 | 2.79555600 |
| H | -3.63374700 | -4.58027800 | 3.86328600 |
| H | -5.70672600 | -5.20533400 | 2.62014200 |
| H | -6.06964000 | -4.31399300 | 0.34122900 |
| C | -4.54810700 | -2.68022600 | -1.08955200 |
| F | -3.54877400 | -2.83057600 | -1.99634500 |
| F | -5.63795300 | -3.27035900 | -1.62824000 |
| F | -4.82176400 | -1.34289500 | -1.05899600 |
| C | -1.99904500 | -0.13718100 | 1.95210100 |
| C | -3.35074100 | 0.20084000 | 1.66488600 |
| C | -4.00068100 | 1.23812500 | 2.33825400 |
| C | -3.35833100 | 1.98801500 | 3.32302800 |
| C | -2.02910900 | 1.66969500 | 3.62994800 |
| C | -1.37172200 | 0.64010500 | 2.96957800 |
| H | -0.34175100 | 0.40103900 | 3.23238100 |
| H | -1.50139200 | 2.22695600 | 4.40226700 |
| H | -3.87545600 | 2.78904100 | 3.84369300 |
| H | -5.03718200 | 1.45491300 | 2.08461200 |
| H | -3.90106300 | -0.35309800 | 0.91518200 |
| O | -0.95221700 | 0.81811900 | -1.53412900 |
| C | -1.81992900 | 1.96558700 | -1.32316800 |
| C | -2.61251300 | 2.12661800 | -2.62222500 |
| C | -2.69980400 | 0.67984300 | -3.13430900 |
| C | -1.33242200 | 0.11730300 | -2.74481400 |
| H | -0.57588500 | 0.31861100 | -3.51483600 |
| H | -1.34319800 | -0.95370600 | -2.52604900 |
| H | -2.88221600 | 0.61386200 | -4.21134800 |
| H | -3.49530600 | 0.13420800 | -2.61805000 |
| H | -2.06422900 | 2.75386400 | -3.33571600 |
| H | -3.59215000 | 2.58276400 | -2.45214400 |
| H | -2.46806800 | 1.75301300 | -0.46644400 |
| H | -1.18856300 | 2.82670500 | -1.08427200 |
| O | 1.28754400 | 1.48404200 | 0.44275200 |
| C | 2.12007600 | 1.39744400 | 1.62275700 |
| C | 3.56277000 | 1.54502600 | 1.13361100 |
| C | 3.39172200 | 2.43110600 | -0.10917600 |
| C | 2.08315900 | 1.89828200 | -0.69414000 |
| H | 2.25389700 | 1.02663200 | -1.33762400 |
| H | 1.51168900 | 2.64511100 | -1.25165500 |
| H | 4.22462100 | 2.35459200 | -0.81452500 |
| H | 3.28409000 | 3.48318000 | 0.18034500 |
| H | 3.96849200 | 0.56745100 | 0.84977400 |
| H | 4.21776300 | 1.98206500 | 1.89337100 |
| H | 1.83161400 | 2.20418200 | 2.30729600 |
| H | 1.93008000 | 0.43770400 | 2.11223600 |

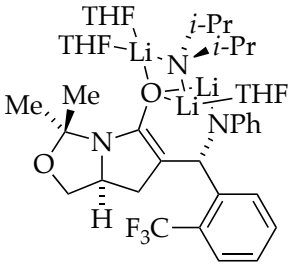


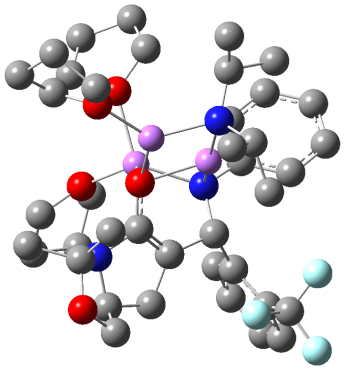



**13a**
G = –-2122.354571
$G_{MP2}$ = –-2116.464263

| Atom | X | Y | Z |
|---|---|---|---|
| Li | 0.00000000 | 0.00000000 | 0.00000000 |
| Li | -2.08265600 | -0.02872300 | 1.37696000 |
| N | -2.00011500 | -0.17306500 | -0.59170400 |
| C | -2.09441900 | -1.57670700 | -0.97818400 |
| C | -1.30120000 | -2.47459700 | -0.03846600 |
| C | -0.62407300 | -2.12830500 | 1.10242200 |
| N | -0.10601700 | -3.29401900 | 1.78806300 |
| C | -0.21199100 | -4.40942100 | 0.81781500 |
| C | -1.27241400 | -3.97252400 | -0.20866900 |
| H | -2.24266700 | -4.44291100 | 0.01754100 |
| H | -1.00418400 | -4.31144200 | -1.22253200 |
| C | 1.23359800 | -4.53840900 | 0.25738000 |
| H | 1.57512300 | -5.58318700 | 0.25510300 |
| H | 1.30597400 | -4.15074700 | -0.76625500 |

| | | | |
|---|---|---|---|
| O | 2.06610700 | -3.74251000 | 1.09912900 |
| C | 1.28054600 | -3.34861500 | 2.26295600 |
| C | 1.39991700 | -4.44769500 | 3.33526900 |
| H | 1.00309100 | -5.40450400 | 2.98410000 |
| H | 2.45242700 | -4.59364100 | 3.59902300 |
| H | 0.84425900 | -4.16101200 | 4.23398400 |
| C | 1.89222900 | -2.05565400 | 2.79269300 |
| H | 1.33010200 | -1.68814200 | 3.65421300 |
| H | 2.92006300 | -2.27090700 | 3.10498400 |
| H | 1.90320100 | -1.27545100 | 2.03380900 |
| H | -0.50160600 | -5.33439300 | 1.32462600 |
| O | -0.45707200 | -0.94639000 | 1.64711500 |
| H | -1.65150600 | -1.71723700 | -1.98578500 |
| C | -3.53749600 | -2.14894200 | -1.18018300 |
| C | -4.65897200 | -2.00060000 | -0.32829400 |
| C | -5.88229400 | -2.61520700 | -0.63483700 |
| C | -6.03127400 | -3.39898100 | -1.77421600 |
| C | -4.93883900 | -3.56992300 | -2.61978000 |
| C | -3.72871400 | -2.95090600 | -2.31608400 |
| H | -2.88516800 | -3.08547000 | -2.98936700 |
| H | -5.02606200 | -4.17734600 | -3.51713900 |
| H | -6.98723100 | -3.86584600 | -1.99246800 |
| H | -6.72533000 | -2.47814100 | 0.03217400 |
| C | -4.65310200 | -1.16129800 | 0.91945800 |
| F | -3.54983100 | -1.38664900 | 1.71441200 |
| F | -4.67005600 | 0.17424800 | 0.68386400 |
| F | -5.71195000 | -1.40736400 | 1.72456100 |
| C | -2.37727900 | 0.77420600 | -1.51795600 |
| C | -2.79685400 | 0.53613100 | -2.85692400 |
| C | -3.12014600 | 1.58639100 | -3.71936400 |
| C | -3.05356000 | 2.91770500 | -3.31045100 |
| C | -2.65510200 | 3.18055300 | -1.99308900 |
| C | -2.32770300 | 2.14637700 | -1.12573900 |
| H | -2.02408500 | 2.37310300 | -0.10430500 |
| H | -2.60647500 | 4.20817500 | -1.63556200 |
| H | -3.31430300 | 3.72596100 | -3.98783000 |
| H | -3.43927800 | 1.34916100 | -4.73312500 |
| H | -2.89400900 | -0.47968600 | -3.22203600 |
| O | -2.39285200 | 1.22638300 | 2.87535800 |
| C | -3.58456600 | 1.98597100 | 3.14820100 |
| C | -4.35643000 | 1.16733700 | 4.19956900 |
| C | -3.26299800 | 0.28129100 | 4.86276000 |
| C | -1.96514800 | 0.69122000 | 4.14611400 |
| H | -1.27716200 | -0.12713600 | 3.92700100 |
| H | -1.43311800 | 1.47995100 | 4.69795500 |
| H | -3.47320300 | -0.77865100 | 4.69537400 |
| H | -3.19099200 | 0.44041700 | 5.94278600 |
| H | -5.11734700 | 0.54632100 | 3.71961400 |
| H | -4.86201000 | 1.81921200 | 4.91823500 |
| H | -3.29285400 | 2.97074100 | 3.54048000 |
| H | -4.11220700 | 2.11957200 | 2.20328800 |
| O | 0.81531700 | 1.73013200 | 0.57322900 |
| C | 0.91394900 | 2.21207300 | 1.93235400 |
| C | 1.74684900 | 3.49153000 | 1.84804200 |
| C | 1.33423600 | 4.04498700 | 0.47505700 |
| C | 1.19595900 | 2.76911600 | -0.36029200 |
| H | 2.14767800 | 2.48342300 | -0.82562300 |
| H | 0.42395400 | 2.83349400 | -1.13155900 |
| H | 2.06071200 | 4.74458700 | 0.05080600 |
| H | 0.36908000 | 4.55997600 | 0.54674300 |
| H | 2.81776700 | 3.25523500 | 1.86033900 |
| H | 1.54124700 | 4.17994200 | 2.67353700 |
| H | -0.09680300 | 2.40789600 | 2.30992000 |
| H | 1.36575100 | 1.42149100 | 2.53683100 |
| O | 1.35597600 | -0.43352500 | -1.40671500 |
| C | 1.03645200 | -0.73468900 | -2.77731100 |
| C | 2.38428200 | -0.70053100 | -3.49112800 |
| C | 3.30244600 | -1.36277000 | -2.44767300 |
| C | 2.68466500 | -0.93259100 | -1.10156400 |
| H | 3.23457500 | -0.10997000 | -0.63152100 |
| H | 2.60447800 | -1.76111900 | -0.39062100 |
| H | 4.34808100 | -1.05481400 | -2.54062200 |
| H | 3.26772400 | -2.45292500 | -2.55070400 |
| H | 2.68590500 | 0.33728500 | -3.67562600 |
| H | 2.37125400 | -1.22923200 | -4.44916500 |
| H | 0.57803100 | -1.73194500 | -2.83995800 |
| H | 0.31098200 | 0.00771300 | -3.11766600 |

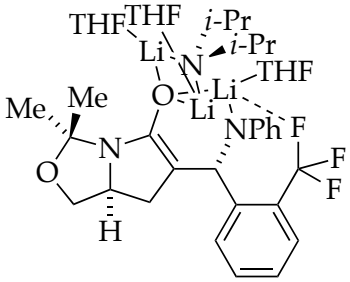


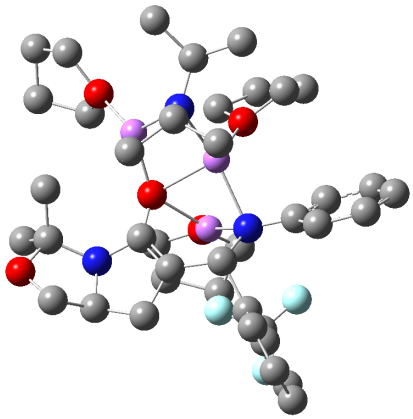



**14a**
G = –-2421.556736
$G_{MP2}$ = –-2414.743725

| Atom | X | Y | Z |
|---|---|---|---|
| Li | 0.00000000 | 0.00000000 | 0.00000000 |
| N | -1.44324100 | 0.19277100 | 1.46923300 |
| C | -2.18089700 | -0.88125500 | 0.77438800 |
| C | -1.53388500 | -2.23435600 | 1.08620300 |
| C | -0.19208300 | -2.46458200 | 1.14758200 |
| N | 0.11935700 | -3.80781500 | 1.57371000 |
| C | -1.17630100 | -4.54229700 | 1.60670300 |
| C | -2.28761700 | -3.48123600 | 1.48735000 |
| H | -2.80813100 | -3.35699400 | 2.44835900 |
| H | -3.05545500 | -3.79258500 | 0.76698900 |
| C | -1.03611700 | -5.49292000 | 0.42127800 |
| H | -1.61838400 | -6.41436900 | 0.51746900 |
| H | -1.31768800 | -4.98911300 | -0.51727000 |
| O | 0.34118200 | -5.83920800 | 0.43938700 |
| C | 1.09436800 | -4.67526400 | 0.84459300 |
| C | 2.17252400 | -5.18251600 | 1.80398600 |
| H | 1.70402900 | -5.65826300 | 2.67051800 |
| H | 2.81292500 | -5.91929100 | 1.30622000 |
| H | 2.79295200 | -4.35070900 | 2.15396600 |
| C | 1.71261000 | -4.05767600 | -0.41520700 |
| H | 2.47857500 | -3.31973900 | -0.16833100 |
| H | 2.18596100 | -4.86451400 | -0.98374700 |
| H | 0.95041900 | -3.59404800 | -1.04867000 |
| H | -1.25314300 | -5.12618400 | 2.53176600 |
| O | 0.79058900 | -1.58187900 | 1.00909800 |
| Li | 2.19692600 | -1.03441600 | -0.12858400 |
| O | 4.06155600 | -1.45195600 | 0.32841000 |
| C | 5.13515900 | -1.67210200 | -0.62040200 |
| C | 6.42215500 | -1.57910000 | 0.19778200 |
| C | 5.97395900 | -2.13078100 | 1.56066800 |
| C | 4.55571100 | -1.56910400 | 1.68469700 |
| H | 4.55182600 | -0.57072100 | 2.13965000 |
| H | 3.86895800 | -2.21108600 | 2.24273100 |
| H | 6.61814400 | -1.81902300 | 2.38805900 |
| H | 5.95253300 | -3.22661400 | 1.54077700 |
| H | 6.74091800 | -0.53442200 | 0.29196300 |
| H | 7.24233000 | -2.14708100 | -0.25060000 |
| H | 5.00907000 | -2.66737500 | -1.06552400 |
| H | 5.04747500 | -0.91931800 | -1.40664900 |
| N | 1.46323600 | 0.37241100 | -1.29614500 |
| C | 1.09199000 | 0.02281000 | -2.67754200 |
| H | 1.06090200 | 0.92271200 | -3.31433800 |
| C | -0.32104100 | -0.58617000 | -2.73495000 |
| H | -0.59381000 | -0.90828300 | -3.74849400 |
| H | -0.39372600 | -1.47454800 | -2.08936300 |
| H | -1.07506400 | 0.13959100 | -2.40618500 |
| C | 2.08676000 | -0.95283400 | -3.35060000 |
| H | 1.80355000 | -1.18317900 | -4.38764700 |
| H | 3.09977700 | -0.53732500 | -3.36156700 |
| H | 2.11863900 | -1.90516500 | -2.80033300 |
| C | 2.09508700 | 1.69560700 | -1.16659900 |
| H | 2.42337800 | 1.76823000 | -0.11617600 |
| C | 1.12569100 | 2.88121900 | -1.39014800 |
| H | 1.61928100 | 3.84700700 | -1.21286500 |
| H | 0.74300900 | 2.89665000 | -2.41819800 |
| H | 0.26240500 | 2.81253000 | -0.71843200 |
| C | 3.37307600 | 1.91712700 | -2.01036400 |
| H | 4.11497100 | 1.13397900 | -1.81073800 |
| H | 3.15690700 | 1.90691600 | -3.08536800 |
| H | 3.83431700 | 2.88727300 | -1.78125900 |
| Li | 0.10887700 | -0.46640200 | 2.57133900 |
| O | -0.14319100 | -1.25354500 | 4.42953200 |
| C | 0.15960800 | -2.60865600 | 4.85061900 |
| C | -1.03543000 | -3.07781100 | 5.71212300 |
| C | -2.07934800 | -1.95467700 | 5.54361300 |
| C | -1.20298500 | -0.73949900 | 5.25432200 |
| H | -0.78196600 | -0.31627100 | 6.17973900 |
| H | -1.69528100 | 0.05524200 | 4.68928200 |
| H | -2.70866400 | -1.82170200 | 6.42890500 |
| H | -2.72872000 | -2.15189700 | 4.68491100 |

| | | | |
|---|---|---|---|
| H | -0.73963200 | -3.17418000 | 6.76236300 |
| H | -1.41703100 | -4.04950100 | 5.38657300 |
| H | 0.30761400 | -3.19617200 | 3.94121700 |
| H | 1.09364200 | -2.59777200 | 5.42809900 |
| H | -2.13780600 | -0.73285700 | -0.32122200 |
| C | -3.68886000 | -0.92888500 | 1.11291200 |
| C | -4.68868300 | -1.32724800 | 0.19924200 |
| C | -6.03189200 | -1.38662000 | 0.59299800 |
| C | -6.40775600 | -1.05562400 | 1.89168300 |
| C | -5.43185900 | -0.64960700 | 2.80070400 |
| C | -4.09691000 | -0.58815400 | 2.40667500 |
| H | -3.33351700 | -0.24481200 | 3.09558300 |
| H | -5.71039700 | -0.37164000 | 3.81428300 |
| H | -7.45308300 | -1.10396300 | 2.18327700 |
| H | -6.78365000 | -1.68926800 | -0.12667600 |
| C | -4.36897700 | -1.65634000 | -1.23989600 |
| F | -3.40625400 | -2.60489500 | -1.36629200 |
| F | -5.44639000 | -2.11646900 | -1.91407300 |
| F | -3.92372000 | -0.57107200 | -1.92971300 |
| C | -1.88168800 | 1.49506800 | 1.26434200 |
| C | -2.74247300 | 1.93854300 | 0.22310100 |
| C | -3.06965200 | 3.28747400 | 0.07604000 |
| C | -2.57878200 | 4.25915700 | 0.94896200 |
| C | -1.75242700 | 3.84414700 | 1.99890500 |
| C | -1.42043600 | 2.50326600 | 2.15673400 |
| H | -0.80760600 | 2.19064300 | 3.00008900 |
| H | -1.37632900 | 4.57369600 | 2.71479200 |
| H | -2.84344100 | 5.30553000 | 0.82638200 |
| H | -3.72729800 | 3.57845200 | -0.74103900 |
| H | -3.16101100 | 1.22710800 | -0.47872800 |
| O | 1.67271100 | 0.83216200 | 3.16704400 |
| C | 2.40384600 | 0.67390100 | 4.39146500 |
| C | 2.32023700 | 2.04174300 | 5.08966400 |
| C | 2.11012200 | 3.03869500 | 3.91619600 |
| C | 2.03798900 | 2.13488500 | 2.67138600 |
| H | 3.01519300 | 2.06443400 | 2.17274400 |
| H | 1.28416800 | 2.43719700 | 1.94449500 |
| H | 2.92265000 | 3.76634500 | 3.83238500 |
| H | 1.17797800 | 3.59664900 | 4.04070800 |
| H | 3.22290000 | 2.25430800 | 5.67054200 |
| H | 1.46962600 | 2.06951500 | 5.77753500 |
| H | 1.94228200 | -0.14596600 | 4.94090700 |
| H | 3.44844200 | 0.41497100 | 4.15796900 |



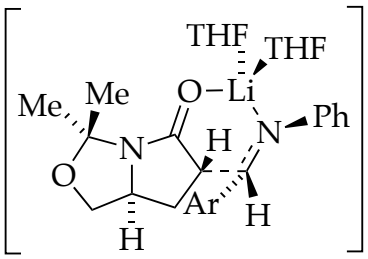



**14b**
G = –-2421.547332
$G_{MP2}$ = –-2414.740985

| Atom | X | Y | Z |
|---|---|---|---|
| N | 0.00000000 | 0.00000000 | 0.00000000 |
| C | -0.38675900 | -0.90044000 | -1.08905800 |
| C | 0.45091300 | -2.18238700 | -1.08450500 |
| C | 1.71302100 | -2.37432600 | -0.59450800 |
| N | 2.06944000 | -3.77908200 | -0.58146100 |
| C | 1.00857200 | -4.50526200 | -1.32647200 |
| C | -0.13106500 | -3.49876300 | -1.55105400 |
| H | -1.01690200 | -3.78641700 | -0.97139600 |
| H | -0.45547600 | -3.48804800 | -2.60403900 |
| C | 1.75326900 | -4.97049200 | -2.57335400 |
| H | 1.33839500 | -5.87451300 | -3.03003300 |
| H | 1.78359000 | -4.17076300 | -3.33155900 |
| O | 3.04982000 | -5.27829100 | -2.08515700 |
| C | 3.37250700 | -4.34252500 | -1.02816800 |
| C | 3.99782300 | -5.18293200 | 0.08917900 |
| H | 3.26839500 | -5.91106100 | 0.45554800 |
| H | 4.87328600 | -5.72597400 | -0.28444000 |
| H | 4.30524100 | -4.54755700 | 0.92628700 |

| | | | |
|---|---|---|---|
| C | 4.37155300 | -3.33841800 | -1.60657600 |
| H | 4.80672600 | -2.70064100 | -0.83581000 |
| H | 5.18252500 | -3.90447000 | -2.07656300 |
| H | 3.90335800 | -2.71866000 | -2.37493700 |
| H | 0.68126700 | -5.38209600 | -0.75483500 |
| O | 2.51265100 | -1.50191800 | 0.01109400 |
| Li | 4.04717400 | -0.58372700 | -0.67300300 |
| O | 5.71269700 | -0.93238900 | 0.47251000 |
| C | 7.09268100 | -0.76288600 | 0.04951000 |
| C | 7.94552900 | -1.61951500 | 0.99924100 |
| C | 6.93212200 | -2.63339700 | 1.55522100 |
| C | 5.66750400 | -1.78429900 | 1.63811000 |
| H | 5.66911800 | -1.16094300 | 2.54287700 |
| H | 4.72871500 | -2.33989900 | 1.59181300 |
| H | 7.22591300 | -3.04733100 | 2.52452800 |
| H | 6.78832000 | -3.46462800 | 0.85605200 |
| H | 8.35048100 | -1.00478500 | 1.81107900 |
| H | 8.78789500 | -2.08995700 | 0.48431000 |
| H | 7.16237300 | -1.09998900 | -0.99033400 |
| H | 7.34384200 | 0.30004200 | 0.08889500 |
| N | 3.52651500 | 1.08758200 | -1.57931400 |
| C | 3.16381700 | 1.12024800 | -3.00758400 |
| H | 3.88553900 | 1.73112800 | -3.57594400 |
| C | 1.77125100 | 1.72877300 | -3.29060300 |
| H | 1.56531100 | 1.78709400 | -4.36956300 |
| H | 0.98459200 | 1.11405800 | -2.83641300 |
| H | 1.67836000 | 2.73502700 | -2.87369600 |
| C | 3.21969400 | -0.28519600 | -3.63066500 |
| H | 2.92367700 | -0.27642400 | -4.68834400 |
| H | 4.23595300 | -0.69641900 | -3.57099400 |
| H | 2.53662100 | -0.96673900 | -3.10489800 |
| C | 4.38007200 | 2.21835200 | -1.18303500 |
| H | 4.55150600 | 2.09597900 | -0.10054300 |
| C | 3.76397300 | 3.62756400 | -1.36504100 |
| H | 4.39804300 | 4.40123000 | -0.90901100 |
| H | 3.65962400 | 3.88112000 | -2.42668600 |
| H | 2.76886700 | 3.68718100 | -0.91124300 |
| C | 5.78856800 | 2.22606300 | -1.83400400 |
| H | 6.27272600 | 1.24960800 | -1.72400800 |
| H | 5.74079400 | 2.44682500 | -2.90693000 |
| H | 6.43695400 | 2.98747500 | -1.37790500 |
| Li | 1.97898300 | 0.63510500 | -0.28198100 |
| O | 2.59512500 | 1.42731000 | 1.64722100 |
| C | 3.51220000 | 0.88618000 | 2.61268400 |
| C | 3.33775900 | 1.73031500 | 3.89954600 |
| C | 2.44639500 | 2.91524100 | 3.44994400 |
| C | 2.51250500 | 2.83841800 | 1.92397700 |
| H | 3.40915200 | 3.33981700 | 1.53478000 |
| H | 1.62685600 | 3.22041000 | 1.41625000 |
| H | 2.79355200 | 3.87949200 | 3.83317500 |
| H | 1.41369000 | 2.77120700 | 3.78275100 |
| H | 4.30815300 | 2.07207000 | 4.27355900 |
| H | 2.86308600 | 1.15420600 | 4.69966300 |
| H | 3.25809400 | -0.16662700 | 2.74184000 |
| H | 4.53474100 | 0.96730500 | 2.21961400 |
| Li | 0.94172200 | -1.18310800 | 1.23872000 |
| O | 1.35501000 | -1.80296500 | 3.07606100 |
| C | 1.95772700 | -3.12183400 | 3.19006900 |
| C | 1.25889600 | -3.82298600 | 4.37150300 |
| C | 0.00524800 | -2.96359300 | 4.61660900 |
| C | 0.48400900 | -1.57436900 | 4.20532400 |
| H | 1.05438000 | -1.08781900 | 5.00976600 |
| H | -0.31287000 | -0.90650200 | 3.87403000 |
| H | -0.33830400 | -2.99752500 | 5.65485000 |
| H | -0.81849200 | -3.28009300 | 3.97033600 |
| H | 1.90415900 | -3.81817100 | 5.25711300 |
| H | 1.01721700 | -4.86463000 | 4.14234300 |
| H | 1.81511900 | -3.63110500 | 2.23266300 |
| H | 3.03344300 | -2.99841000 | 3.35925600 |
| H | -0.23540300 | -0.42124700 | -2.07670800 |
| C | -1.90349800 | -1.25451900 | -1.10925200 |
| C | -2.68798900 | -1.69893600 | -0.01741500 |
| C | -4.05502100 | -1.96574300 | -0.18430900 |
| C | -4.67512200 | -1.81948300 | -1.42110300 |
| C | -3.91548900 | -1.40608400 | -2.51150300 |
| C | -2.56012500 | -1.13221100 | -2.34208300 |
| H | -1.97809000 | -0.79898600 | -3.19802700 |
| H | -4.37339300 | -1.28762700 | -3.49015900 |
| H | -5.73537600 | -2.03040400 | -1.52581200 |
| H | -4.63592900 | -2.30127100 | 0.66680100 |
| C | -2.16113800 | -1.90198300 | 1.38140900 |
| F | -0.92603700 | -2.50019000 | 1.41775100 |
| F | -2.05091700 | -0.76417000 | 2.10146100 |
| F | -2.95793100 | -2.72470300 | 2.11057600 |
| C | -0.68282200 | 1.20550300 | 0.09500900 |
| C | -0.66178400 | 1.89818100 | 1.33686300 |
| C | -1.28611400 | 3.12830100 | 1.51393300 |
| C | -1.97508100 | 3.74206000 | 0.46215300 |
| C | -2.02278800 | 3.07964400 | -0.76505300 |
| C | -1.40145600 | 1.84444200 | -0.95119300 |
| H | -1.46883600 | 1.37536600 | -1.92570900 |
| H | -2.55642900 | 3.52810700 | -1.60114500 |
| H | -2.47000100 | 4.69917700 | 0.60079200 |
| H | -1.24975700 | 3.60658000 | 2.49178900 |
| H | -0.15076600 | 1.42361500 | 2.17110400 |

**Table 2.** Optimized geometries at B3LYP level of theory with 6-31G(d) basis set for the azaaldol transition states at –70 °C with free energies (Hartrees) and Cartesian coordinates (X, Y, Z) (Note: $G_{MP2}$ includes single point MP2 corrections to B3LYP/6-31G(d) optimized structures).

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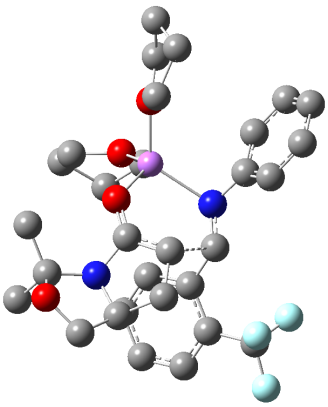
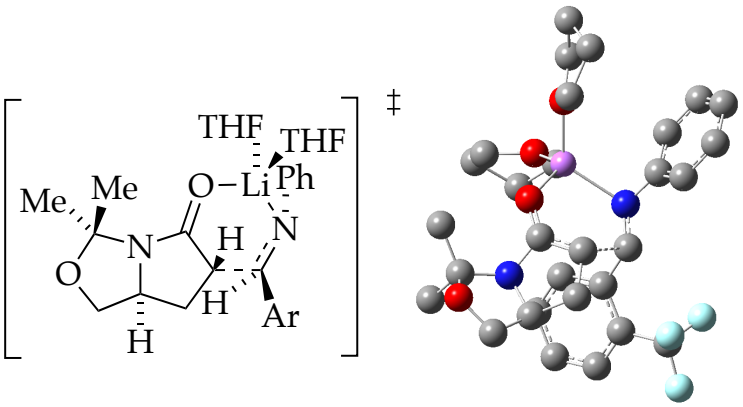


**11a**
G = –1882.979910
$G_{MP2}$ = –-1877.780702

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 1.36879900 | -0.00353800 | 0.63637600 |
| C | 1.59698700 | -1.25990200 | 1.23490400 |
| O | 2.66302300 | -1.71347500 | 1.74723000 |
| Li | 3.87577400 | -0.85455900 | 2.85737400 |
| O | 5.63548600 | -1.16343700 | 1.99713300 |
| C | 5.71609200 | -1.07553700 | 0.55277000 |
| C | 7.16965800 | -0.71020100 | 0.24915700 |
| C | 7.91911400 | -1.39379000 | 1.40344000 |
| C | 6.95653600 | -1.17868300 | 2.57420300 |
| H | 7.13446200 | -0.21487500 | 3.06657900 |
| H | 6.99338000 | -1.97301300 | 3.32613300 |
| H | 8.90830900 | -0.96658600 | 1.59403200 |
| H | 8.04372700 | -2.46392000 | 1.19896100 |
| H | 7.30396400 | 0.37622000 | 0.29643300 |
| H | 7.48892800 | -1.05494400 | -0.73906500 |
| H | 5.43647800 | -2.04826400 | 0.13112500 |
| H | 4.99561500 | -0.32674100 | 0.21729800 |
| O | 4.14602900 | -1.65057800 | 4.67388300 |
| C | 3.89680100 | -3.06205300 | 4.88514100 |
| C | 3.71902400 | -3.23606300 | 6.39836800 |
| C | 3.21126700 | -1.85231100 | 6.83604600 |
| C | 3.99770200 | -0.92181500 | 5.91411600 |
| H | 4.99537900 | -0.70470300 | 6.32084200 |
| H | 3.49272600 | 0.01846900 | 5.68107700 |
| H | 3.38905500 | -1.64191700 | 7.89483300 |
| H | 2.13692300 | -1.75436000 | 6.64418600 |
| H | 4.68141900 | -3.45532100 | 6.87544800 |
| H | 3.02904300 | -4.04874500 | 6.64400900 |
| H | 2.99591100 | -3.33208000 | 4.32271600 |
| H | 4.74150600 | -3.62809800 | 4.47983100 |
| N | 0.38096400 | -1.97314200 | 1.33065100 |
| C | -0.70338000 | -1.19778400 | 0.69528600 |
| C | -1.41098900 | -2.24189100 | -0.20121800 |
| O | -0.55702000 | -3.37997100 | -0.22080300 |
| C | 0.20026100 | -3.39753800 | 1.00673500 |
| C | 1.47989100 | -4.17072900 | 0.70864100 |
| H | 2.03860600 | -3.69059500 | -0.09743200 |
| H | 2.12238400 | -4.23154600 | 1.58782000 |
| H | 1.20087900 | -5.18002100 | 0.38921500 |
| C | -0.62354600 | -4.08204600 | 2.10942400 |
| H | -0.87874800 | -5.10504400 | 1.81282100 |
| H | -0.05196600 | -4.11390400 | 3.04295200 |
| H | -1.55162000 | -3.53479300 | 2.30423200 |
| H | -2.40361100 | -2.50143800 | 0.19723400 |
| H | -1.53608300 | -1.90052100 | -1.23389300 |
| H | -1.39373200 | -0.82799000 | 1.46202900 |
| H | 2.20275200 | 0.53766300 | 0.20823000 |
| H | 0.05213800 | -0.15792800 | -1.09126500 |
| H | -0.56560700 | 0.92494100 | 0.15554500 |
| N | 3.01291900 | 1.10869200 | 3.01496000 |
| C | 4.03529200 | 1.88640900 | 2.44057200 |
| C | 3.95740800 | 2.56230100 | 1.20202700 |
| C | 5.03838500 | 3.30217100 | 0.72203600 |
| C | 6.22324900 | 3.40044500 | 1.45410500 |
| C | 6.31384200 | 2.74168800 | 2.68470100 |

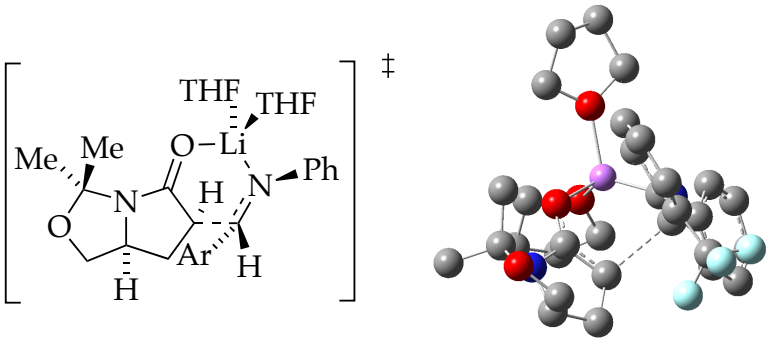
| | | | |
|---|---|---|---|
| C | 5.24273000 | 1.99366500 | 3.16430300 |
| H | 5.30670600 | 1.49603300 | 4.12858200 |
| H | 7.22147800 | 2.82057800 | 3.27896800 |
| H | 7.05704300 | 3.98695600 | 1.07826900 |
| H | 4.94964100 | 3.80872500 | -0.23627900 |
| H | 3.05325100 | 2.50453600 | 0.60615100 |
| C | 1.76678000 | 1.35445600 | 2.64347800 |
| C | 0.61910100 | 0.84079700 | 3.42151900 |
| C | 0.71754400 | -0.35898900 | 4.14753700 |
| C | -0.35216100 | -0.85347900 | 4.88707300 |
| C | -1.55679800 | -0.15210700 | 4.94059400 |
| C | -1.67050300 | 1.05685000 | 4.25749800 |
| C | -0.60232900 | 1.55830600 | 3.50837400 |
| C | -0.76381400 | 2.91810800 | 2.87575200 |
| F | -0.60686100 | 2.90006900 | 1.52407500 |
| F | -1.98421200 | 3.45120300 | 3.10564600 |
| F | 0.14520500 | 3.80534000 | 3.34810000 |
| H | -2.58993900 | 1.62746600 | 4.31566700 |
| H | -2.39563700 | -0.53199600 | 5.51655100 |
| H | -0.24834800 | -1.79701000 | 5.41730600 |
| H | 1.64477600 | -0.91457800 | 4.09909300 |
| H | 1.55910400 | 2.23293800 | 2.03959100 |




**11b**
G = –1882.972173
$G_{MP2}$ = –-1877.775583

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.83318500 | 1.12558700 | 0.57563300 |
| C | 2.14043800 | 0.62502700 | 0.81184400 |
| O | 3.17928100 | 1.28944800 | 1.08278000 |
| Li | 3.14993700 | 2.84134200 | 2.15034600 |
| O | 3.09298200 | 4.62431000 | 1.21189500 |
| C | 2.98831600 | 4.85312800 | -0.21129000 |
| C | 2.83251500 | 6.36657500 | -0.36917600 |
| C | 3.64698100 | 6.89881300 | 0.82084700 |
| C | 3.33662000 | 5.86859800 | 1.91010000 |
| H | 2.43351100 | 6.12978900 | 2.47558100 |
| H | 4.15747300 | 5.70613900 | 2.61427300 |
| H | 3.36987000 | 7.91464100 | 1.11724200 |
| H | 4.71715100 | 6.89543000 | 0.58188600 |
| H | 1.77905100 | 6.65410300 | -0.27065200 |
| H | 3.19301000 | 6.72526700 | -1.33770600 |
| H | 3.90183000 | 4.48540900 | -0.69596000 |
| H | 2.13744000 | 4.27762300 | -0.58527700 |
| O | 5.10818900 | 2.96057800 | 2.69183000 |
| C | 5.94718500 | 3.14465400 | 1.52822900 |
| C | 7.28781100 | 2.50058800 | 1.87932600 |
| C | 6.84340200 | 1.32618100 | 2.76351000 |
| C | 5.67320300 | 1.92654000 | 3.54576400 |
| H | 6.00393500 | 2.40287600 | 4.47579800 |
| H | 4.88806200 | 1.20631900 | 3.77937600 |
| H | 7.63453400 | 0.95429400 | 3.42157900 |
| H | 6.49840400 | 0.49335000 | 2.14076500 |
| H | 7.91260400 | 3.19845000 | 2.44973800 |
| H | 7.84623300 | 2.18941700 | 0.99121400 |
| H | 5.47509400 | 2.64543400 | 0.67275400 |
| H | 6.01425700 | 4.21775100 | 1.32503300 |
| N | 2.10909700 | -0.78295000 | 0.84376400 |
| C | 0.75430500 | -1.25943700 | 0.49641600 |
| C | 1.03024500 | -2.39637600 | -0.51604500 |
| O | 2.41150600 | -2.29619400 | -0.84678700 |
| C | 3.10408200 | -1.70028900 | 0.26896200 |
| C | 4.34854500 | -1.03188800 | -0.30342200 |
| H | 4.07325300 | -0.28452000 | -1.05084900 |
| H | 4.92985800 | -0.54517500 | 0.48086500 |
| H | 4.95896400 | -1.80187800 | -0.78558900 |

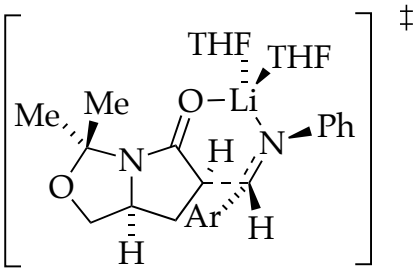
| | | | |
|---|---|---|---|
| C | 3.46893500 | -2.78439200 | 1.29478700 |
| H | 4.11727300 | -3.53889000 | 0.83658400 |
| H | 3.98795500 | -2.33671800 | 2.14854000 |
| H | 2.57077400 | -3.28446500 | 1.67218300 |
| H | 0.79964000 | -3.38103300 | -0.08286700 |
| H | 0.45718100 | -2.28702200 | -1.44237000 |
| H | 0.25466100 | -1.65746000 | 1.38858200 |
| H | 0.75037200 | 2.12769200 | 0.17340100 |
| H | -0.01197800 | 0.03147500 | -1.10320100 |
| H | -1.04299000 | -0.00980600 | 0.32791000 |
| N | 1.44584500 | 2.38883800 | 3.31532700 |
| C | 2.07337700 | 1.60117100 | 4.30098800 |
| C | 2.68834000 | 2.28980700 | 5.36820500 |
| C | 3.32155800 | 1.60448900 | 6.40259300 |
| C | 3.37238500 | 0.20795400 | 6.39976900 |
| C | 2.77723300 | -0.48762500 | 5.34367600 |
| C | 2.13501100 | 0.19110100 | 4.30829400 |
| H | 1.71664800 | -0.37063500 | 3.47984500 |
| H | 2.81673000 | -1.57453100 | 5.32048200 |
| H | 3.86646500 | -0.32909100 | 7.20489000 |
| H | 3.77147900 | 2.16468200 | 7.21925000 |
| H | 2.62948700 | 3.37518100 | 5.37707700 |
| C | 0.35531500 | 1.89707100 | 2.72851700 |
| C | -0.66505900 | 2.84291900 | 2.19864700 |
| C | -0.27198600 | 4.08877100 | 1.67960200 |
| C | -1.19881800 | 4.99625100 | 1.17972300 |
| C | -2.56185800 | 4.69256400 | 1.19586700 |
| C | -2.97931900 | 3.48280700 | 1.74081300 |
| C | -2.05118800 | 2.56380100 | 2.24619700 |
| C | -2.58649700 | 1.32774100 | 2.92664500 |
| F | -2.22975000 | 1.27631700 | 4.23170700 |
| F | -3.93650500 | 1.26446500 | 2.88806000 |
| F | -2.13965200 | 0.16930000 | 2.36725400 |
| H | -4.03600100 | 3.24822600 | 1.79216900 |
| H | -3.29266800 | 5.39468300 | 0.80525400 |
| H | -0.85914900 | 5.94818100 | 0.77756900 |
| H | 0.78656700 | 4.32326700 | 1.66944300 |
| H | -0.03831300 | 0.94575400 | 3.08005800 |




**12c**
G = –1882.976722
$G_{MP2}$ = –-1877.778538

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | -1.04068100 | -0.16756600 | 1.09109000 |
| C | -1.05616400 | -1.53716100 | 1.50013100 |
| O | -1.84245000 | -2.09492700 | 2.32034500 |
| Li | -3.20062200 | -1.05105500 | 3.14644400 |
| O | -3.68544400 | -2.04069200 | 4.82004600 |
| C | -4.29208100 | -1.47607600 | 6.00566100 |
| C | -4.34363900 | -2.61180600 | 7.03603500 |
| C | -3.19063200 | -3.52409000 | 6.58543200 |
| C | -3.27344500 | -3.40303400 | 5.06485600 |
| H | -4.02747400 | -4.08685800 | 4.65035800 |
| H | -2.32937100 | -3.55583700 | 4.53832600 |
| H | -3.29549500 | -4.55660100 | 6.93165500 |
| H | -2.23049500 | -3.13792700 | 6.94781800 |
| H | -5.29768200 | -3.14757900 | 6.96988500 |
| H | -4.23266900 | -2.24673000 | 8.06114600 |
| H | -3.66616500 | -0.64019200 | 6.33811400 |
| H | -5.28204400 | -1.08999500 | 5.74195300 |
| O | -4.80781900 | -1.33194400 | 1.94639700 |
| C | -4.88161800 | -2.67953500 | 1.41825400 |
| C | -5.28459400 | -2.52414800 | -0.04801800 |
| C | -6.16884500 | -1.26908000 | -0.00166000 |
| C | -5.44343500 | -0.40336900 | 1.03074800 |
| H | -6.10295300 | 0.24848900 | 1.60719400 |

| | | | |
|---|---|---|---|
| H | -4.66707600 | 0.21594100 | 0.56750700 |
| H | -7.17636600 | -1.52482900 | 0.34812900 |
| H | -6.26353800 | -0.76748300 | -0.96944300 |
| H | -5.80096500 | -3.40751300 | -0.43607500 |
| H | -4.39822000 | -2.34586000 | -0.66777600 |
| H | -3.90303500 | -3.14331300 | 1.55986300 |
| H | -5.64021800 | -3.23631700 | 1.98553400 |
| N | -0.05068900 | -2.24576400 | 0.82747600 |
| C | 0.78073900 | -1.33061200 | 0.03048700 |
| C | 2.09780000 | -1.40102900 | 0.80858200 |
| O | 2.15949000 | -2.75290500 | 1.26454700 |
| C | 0.81941500 | -3.32017800 | 1.32334000 |
| C | 0.55232800 | -3.76922300 | 2.75670300 |
| H | 0.59575700 | -2.92445000 | 3.44500300 |
| H | -0.42561100 | -4.24688100 | 2.84584400 |
| H | 1.33066300 | -4.48806300 | 3.03306200 |
| C | 0.79137500 | -4.51117800 | 0.35644200 |
| H | 1.57268300 | -5.22932500 | 0.62624000 |
| H | -0.18137300 | -5.01310200 | 0.39661300 |
| H | 0.97052900 | -4.17915600 | -0.67054200 |
| H | 2.98294400 | -1.20597800 | 0.19357400 |
| H | 2.09058600 | -0.69836100 | 1.65342000 |
| H | 0.93674800 | -1.73872800 | -0.97630900 |
| H | -1.99324400 | 0.33390100 | 0.96752500 |
| H | 0.66714700 | 0.85697500 | 0.14216000 |
| H | -0.46897800 | 0.13314600 | -0.98613800 |
| N | -2.41386600 | 0.88877800 | 3.48734000 |
| C | -3.34621300 | 1.79620300 | 2.96639500 |
| C | -4.59870900 | 1.86874800 | 3.61847500 |
| C | -5.59351500 | 2.74202200 | 3.19165200 |
| C | -5.38201000 | 3.57222400 | 2.08559200 |
| C | -4.15365100 | 3.51310500 | 1.42508700 |
| C | -3.14773600 | 2.64604100 | 1.85234400 |
| H | -2.20815600 | 2.62832400 | 1.31055600 |
| H | -3.97046700 | 4.15172800 | 0.56382000 |
| H | -6.15718100 | 4.25559300 | 1.75027800 |
| H | -6.53828100 | 2.78172600 | 3.72933000 |
| H | -4.75627600 | 1.23672500 | 4.48847900 |
| C | -1.13595900 | 1.01619600 | 3.13496900 |
| C | -0.09192600 | 0.38770700 | 3.98029000 |
| C | -0.42986900 | -0.66816400 | 4.84520300 |
| C | 0.50977800 | -1.25011700 | 5.69146400 |
| C | 1.82451600 | -0.78645300 | 5.71097500 |
| C | 2.17690900 | 0.28464100 | 4.89409900 |
| C | 1.23801700 | 0.87804100 | 4.04445700 |
| C | 1.67088700 | 2.10416200 | 3.28014000 |
| F | 0.94675900 | 3.19777400 | 3.62382200 |
| F | 2.96789500 | 2.41562900 | 3.49533300 |
| F | 1.53343500 | 1.96556700 | 1.93471500 |
| H | 3.18522400 | 0.67962800 | 4.92611100 |
| H | 2.56419200 | -1.23702900 | 6.36615300 |
| H | 0.21245000 | -2.06882000 | 6.34264700 |
| H | -1.45317300 | -1.01808100 | 4.85483400 |
| H | -0.81596500 | 1.90739800 | 2.60267200 |

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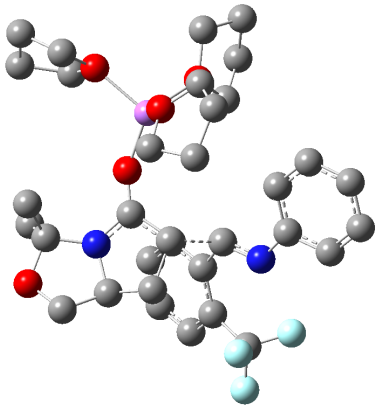
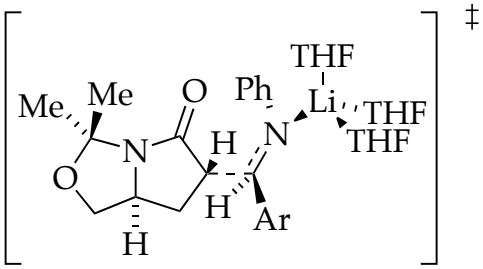
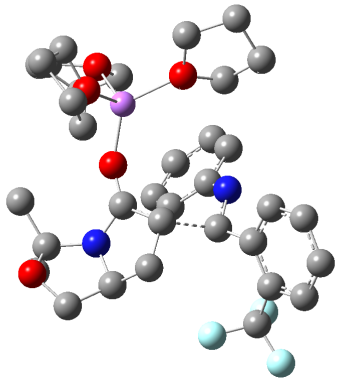


**12a**
G = –-2115.306637
$G_{MP2}$ = –-2109.450425

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.97238700 | 0.75435100 | 0.89986000 |
| C | 1.95628500 | -0.19572100 | 1.34558600 |
| O | 3.07224300 | 0.02744400 | 1.91231000 |
| Li | 4.46867800 | 1.21770800 | 2.12329500 |
| O | 6.10359600 | 0.12997900 | 2.56897300 |

| | | | |
|---|---|---|---|
| C | 5.88192200 | -0.95280000 | 3.50949800 |
| C | 6.73483400 | -2.12497200 | 3.01250800 |
| C | 7.86671400 | -1.41273300 | 2.25465600 |
| C | 7.12381900 | -0.23991400 | 1.61605600 |
| H | 6.64581100 | -0.53390300 | 0.67233000 |
| H | 7.74937000 | 0.63812700 | 1.43379200 |
| H | 8.35932700 | -2.04977000 | 1.51424200 |
| H | 8.62906700 | -1.04799100 | 2.95320500 |
| H | 6.15669200 | -2.75494900 | 2.32754300 |
| H | 7.09178900 | -2.75556800 | 3.83193900 |
| H | 6.19988700 | -0.60998500 | 4.50217500 |
| H | 4.80989500 | -1.16621200 | 3.52721500 |
| O | 4.47673400 | 2.46238900 | 3.70208800 |
| C | 3.38213100 | 2.61931200 | 4.64678200 |
| C | 4.04334600 | 2.96459200 | 5.98016900 |
| C | 5.27781700 | 3.75837300 | 5.52673300 |
| C | 5.69531600 | 3.00574900 | 4.26104100 |
| H | 6.37721600 | 2.17570700 | 4.48220900 |
| H | 6.16418800 | 3.64807800 | 3.50907600 |
| H | 6.07587100 | 3.78803600 | 6.27450000 |
| H | 4.99860300 | 4.79035800 | 5.28550400 |
| H | 4.34652000 | 2.05278200 | 6.50862800 |
| H | 3.37913000 | 3.53406400 | 6.63624200 |
| H | 2.72754400 | 3.42278300 | 4.29176200 |
| H | 2.81514800 | 1.68564700 | 4.65885500 |
| O | 4.94723300 | 2.27625600 | 0.49831900 |
| C | 5.29304500 | 3.68448900 | 0.55717800 |
| C | 4.86555800 | 4.29378200 | -0.78478800 |
| C | 3.76991400 | 3.32612400 | -1.26016500 |
| C | 4.30411400 | 1.98459800 | -0.76805000 |
| H | 5.05149500 | 1.56746200 | -1.45771900 |
| H | 3.53209000 | 1.23706700 | -0.57673200 |
| H | 3.62004800 | 3.34546000 | -2.34365300 |
| H | 2.81853700 | 3.56060600 | -0.77130900 |
| H | 5.70559000 | 4.30274100 | -1.48909600 |
| H | 4.50473100 | 5.31976800 | -0.67230000 |
| H | 4.75047800 | 4.12362200 | 1.40040100 |
| H | 6.36955000 | 3.77177400 | 0.74308700 |
| N | 1.46537000 | -1.47471800 | 1.16690400 |
| C | 0.17929100 | -1.46761600 | 0.45192000 |
| C | 0.43144700 | -2.57065300 | -0.57521300 |
| O | 1.28302900 | -3.48759300 | 0.11868100 |
| C | 2.17665700 | -2.74556300 | 0.96956300 |
| C | 3.52334100 | -2.56478600 | 0.25580900 |
| H | 3.37445700 | -2.08582400 | -0.71765900 |
| H | 4.19675800 | -1.94080200 | 0.84708600 |
| H | 3.97913600 | -3.54643800 | 0.09078100 |
| C | 2.31425100 | -3.53486400 | 2.27137200 |
| H | 2.70511800 | -4.53759600 | 2.06813200 |
| H | 2.99607000 | -3.01867100 | 2.95540900 |
| H | 1.33678400 | -3.62547400 | 2.75215300 |
| H | -0.46317900 | -3.12023800 | -0.87926500 |
| H | 0.92659500 | -2.16819000 | -1.47363500 |
| H | -0.62352800 | -1.77163500 | 1.13450200 |
| H | 1.35776100 | 1.71073000 | 0.55880600 |
| H | 0.26260800 | 0.10967300 | -1.06473300 |
| H | -1.03094500 | 0.34090900 | 0.11372200 |
| N | -0.72945700 | 2.65145500 | 2.02883200 |
| C | -0.12087500 | 3.84768700 | 1.75546100 |
| C | -0.97245300 | 4.93315500 | 1.40861700 |
| C | -0.47619000 | 6.19757200 | 1.13410900 |
| C | 0.90289000 | 6.45519700 | 1.18253700 |
| C | 1.76308600 | 5.40758800 | 1.50878100 |
| C | 1.27579000 | 4.12592700 | 1.78333200 |
| H | 1.98190500 | 3.33770800 | 2.02676100 |
| H | 2.83695200 | 5.58987000 | 1.55598000 |
| H | 1.29086600 | 7.44786700 | 0.96958200 |
| H | -1.16675400 | 6.99935300 | 0.87969900 |
| H | -2.03868500 | 4.72744900 | 1.38076300 |
| C | -0.01731500 | 1.61336000 | 2.46986500 |
| C | -0.76262900 | 0.47945900 | 3.11700000 |
| C | 0.01954100 | -0.38551400 | 3.90513700 |
| C | -0.50967300 | -1.47384700 | 4.58947900 |
| C | -1.87455900 | -1.73540200 | 4.50340300 |
| C | -2.67845500 | -0.89235600 | 3.74137200 |
| C | -2.15674600 | 0.21153600 | 3.04830800 |
| C | -3.18486900 | 1.06244000 | 2.31118500 |
| F | -2.91408700 | 1.24244200 | 1.00179300 |
| F | -4.40908000 | 0.45141000 | 2.33207500 |
| F | -3.37896400 | 2.26510400 | 2.87796200 |
| H | -3.74133400 | -1.08806000 | 3.68497600 |
| H | -2.31671700 | -2.57761100 | 5.02835000 |
| H | 0.13992800 | -2.10796200 | 5.18783900 |
| H | 1.08581700 | -0.18775800 | 3.96784900 |
| H | 0.92601600 | 1.79440300 | 3.00953700 |



**12b**
G = –2115.312487
$G_{MP2}$ = –-2109.455260

| Atom | X | Y | Z |
|---|---|---|---|
| C | 0.00000000 | 0.00000000 | 0.00000000 |
| C | 0.84751700 | 0.89541600 | 0.88897100 |
| C | 1.88677100 | 0.06712600 | 1.42543400 |
| O | 2.99552800 | 0.41846700 | 1.90966900 |
| Li | 4.25655300 | 1.76617200 | 1.91062200 |
| O | 5.24968100 | 1.64656300 | 0.14744300 |
| C | 4.48690700 | 1.25280400 | -1.01727100 |
| C | 5.26491500 | 1.81436500 | -2.20426400 |
| C | 6.71736300 | 1.64168700 | -1.73123200 |
| C | 6.61343700 | 1.93715400 | -0.22809800 |
| H | 6.81290400 | 2.99218500 | -0.00461200 |
| H | 7.28680700 | 1.32208400 | 0.37764300 |
| H | 7.42228400 | 2.30777200 | -2.23718800 |
| H | 7.04892000 | 0.61047400 | -1.89795500 |
| H | 5.02871000 | 2.87531200 | -2.34944100 |
| H | 5.04839000 | 1.28522500 | -3.13684500 |
| H | 4.42731800 | 0.15771400 | -1.05695000 |
| H | 3.47597700 | 1.65085400 | -0.90410400 |
| O | 5.54431800 | 1.37849300 | 3.38695400 |
| C | 6.47653100 | 0.27966800 | 3.25967500 |
| C | 6.56650100 | -0.36594200 | 4.64608500 |
| C | 5.17756000 | -0.06941200 | 5.23026900 |
| C | 4.89534200 | 1.32936400 | 4.69074200 |
| H | 5.33893400 | 2.10894700 | 5.32367100 |
| H | 3.83226500 | 1.53475400 | 4.55559700 |
| H | 5.14351600 | -0.10559800 | 6.32234900 |
| H | 4.43138300 | -0.77134000 | 4.84471600 |
| H | 7.34695700 | 0.11876100 | 5.24480800 |
| H | 6.79746900 | -1.43408500 | 4.59035900 |
| H | 6.08517900 | -0.42134700 | 2.51239000 |
| H | 7.43326000 | 0.67831100 | 2.90484600 |
| O | 3.88280500 | 3.72309400 | 2.02412100 |
| C | 3.03903400 | 4.35324500 | 3.02058600 |
| C | 2.88202300 | 5.78185500 | 2.51293300 |
| C | 4.29001600 | 6.08381900 | 1.96938200 |
| C | 4.77675100 | 4.70907400 | 1.46583000 |
| H | 5.80385700 | 4.49268800 | 1.78551500 |
| H | 4.72561700 | 4.61711200 | 0.37582200 |
| H | 4.93723700 | 6.44566900 | 2.77595400 |
| H | 4.29383000 | 6.83866600 | 1.17732800 |
| H | 2.56747600 | 6.47701100 | 3.29689500 |
| H | 2.13756900 | 5.81513500 | 1.70881700 |
| H | 2.11213100 | 3.77501700 | 3.08734600 |
| H | 3.55217600 | 4.33413100 | 3.99338600 |
| N | 1.45825500 | -1.26669700 | 1.41338100 |
| C | 0.21393900 | -1.39789300 | 0.62960600 |
| C | 0.52084700 | -2.59047400 | -0.31213500 |
| O | 1.88279800 | -2.94500100 | -0.07449800 |
| C | 2.24868400 | -2.48816700 | 1.24497000 |
| C | 3.76187000 | -2.30861500 | 1.23923800 |
| H | 4.06452100 | -1.57724100 | 0.48819500 |
| H | 4.12098700 | -1.97646100 | 2.21447100 |
| H | 4.21473100 | -3.27509000 | 0.99545100 |
| C | 1.82247300 | -3.53077100 | 2.29191700 |
| H | 2.31133300 | -4.48981100 | 2.09054700 |
| H | 2.09817000 | -3.19272100 | 3.29611500 |
| H | 0.73894300 | -3.68636000 | 2.27556500 |
| H | -0.14471200 | -3.44199400 | -0.11058800 |
| H | 0.42629500 | -2.32475100 | -1.37045100 |
| H | -0.62689200 | -1.64173200 | 1.28765100 |
| H | 1.15601000 | 1.87251200 | 0.53117100 |
| H | 0.35391900 | 0.00519000 | -1.04489400 |
| H | -1.06173900 | 0.26028000 | -0.02602600 |
| N | 0.39837800 | 2.30097800 | 3.46930200 |

| | | | |
|---|---|---|---|
| C | 0.87688100 | 1.62685200 | 4.58215200 |
| C | 1.30354900 | 2.42175100 | 5.67659400 |
| C | 1.77062000 | 1.85568800 | 6.85861200 |
| C | 1.83952000 | 0.46554700 | 7.00408200 |
| C | 1.42857900 | -0.33839400 | 5.93590000 |
| C | 0.96053900 | 0.22016500 | 4.74829500 |
| H | 0.67997200 | -0.43944500 | 3.93402800 |
| H | 1.47284200 | -1.42243600 | 6.02838600 |
| H | 2.19477800 | 0.02003100 | 7.92967500 |
| H | 2.07190400 | 2.50397300 | 7.67944500 |
| H | 1.21866700 | 3.50077600 | 5.57658900 |
| C | -0.32109700 | 1.64465100 | 2.55723800 |
| C | -1.22789400 | 2.50502500 | 1.72759000 |
| C | -0.73765700 | 3.70881800 | 1.19655400 |
| C | -1.53471100 | 4.55373500 | 0.43333200 |
| C | -2.86826600 | 4.22160600 | 0.18326200 |
| C | -3.38899400 | 3.05077200 | 0.72279900 |
| C | -2.58618800 | 2.19749400 | 1.49310200 |
| C | -3.24099400 | 0.99063500 | 2.11935700 |
| F | -3.10621200 | 0.97406100 | 3.46358200 |
| F | -4.56779200 | 0.93386700 | 1.85996400 |
| F | -2.72323100 | -0.18864800 | 1.66903600 |
| H | -4.42991000 | 2.79587600 | 0.56148700 |
| H | -3.49980000 | 4.87309500 | -0.41408100 |
| H | -1.11789800 | 5.47476800 | 0.03274500 |
| H | 0.29438000 | 3.96849000 | 1.40559600 |
| H | -0.73315600 | 0.66500400 | 2.80306300 |

**Part 4: Full References**

Gaussian 03, Revision B.04, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.;Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A. Gaussian, Inc., Wallingford CT, 2004.